Supporting Information

Enantioconvergent and Diastereoselective Synthesis of Atropisomeric Hydrazides Bearing a Cyclic Quaternary Stereocenter through Ternary Catalysis

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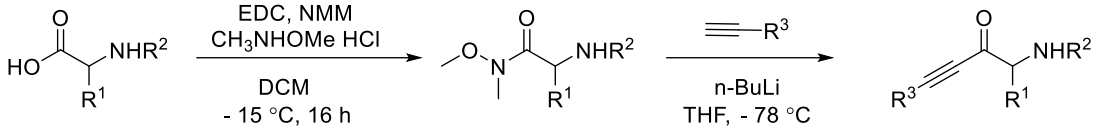
1.General information

All reactions were carried out under nitrogen atmosphere in a glovebox. Reagents were purchased from commercial sources and used without further purification. ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded at 25 ℃ (all substrates) on a Bruker AMX500 (500 MHz) spectrometer. ^{1}H NMR, ^{19}F NMR and ^{13}C NMR spectra were recorded at 60 ℃ (all products) on a Bruker AMX500 (500 MHz) spectrometer. Chemical shifts were reported in parts per million (ppm), and the residual solvent peak was used as an internal reference: ^{1}H (chloroform δ 7.26), ^{13}C (chloroform δ 77.0). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constants (Hz) and integration. Melting point (MP) was obtained on Buchi B-540. For thin layer chromatography (TLC), Merck pre-coated TLC plates (Merck 60 F254) were used, and compounds were visualized with a UV light at 254 nm. High resolution mass spectra (HRMS) were obtained on a Finnigan/MAT 95XL-T spectrometer. Specific rotations were measured using an Anton Paar MCP-150 digital polarimeter using a 1 cm glass cell. Enantiomeric excesses (ee) were determined by HPLC analysis on ThermoFisher HPLC units, including the following instruments: pump, LPG3400SDN; detector, VWD-3400RS; column, Chiralcel OD-H, Chiralpak AD-H, Chiralpak IA, Chiralpak IB-3. All chiral phosphoric acids were purchased from commercial sources. *Tert*-butyl (2-methyl-4-oxo-6-phenylhex-5-yn-3-yl)carbamate **(1a)** and *tert*-butyl (6-(4-methoxyphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate **(1e)** were synthesized by the reported procedure.[1] *Tert*-butyl (3-oxo-1,5-diphenylpent-4-yn-2-yl)carbamate **(1k)**, *tert*-butyl (3-oxo-5-phenylpent-4-yn-2-yl)carbamate **(1j)** were synthesized by the reported procedure.[2] Diethyl (*E*)-diazene-1,2-dicarboxylate **(2a)**, dibenzyl (*E*)-diazene-1,2-dicarboxylate **(2b)** and diisopropyl (*E*)-diazene-1,2-dicarboxylate **(2c)** were purchased from commercial sources . Ethyl 2-(((tert-butoxycarbonyl)oxy)methyl)acrylate **(4a)**, methyl 2-(((tert-butoxycarbonyl)oxy)methyl)acrylate **(4h)** and isopropyl 2-(((tert-butoxycarbonyl)oxy)methyl)acrylate **(4i)** were synthesized by the reported procedure.[3]

2. General procedure for the synthesis of substrates 1 and 3

A: Typical procedure for the preparation of **1**[4]:

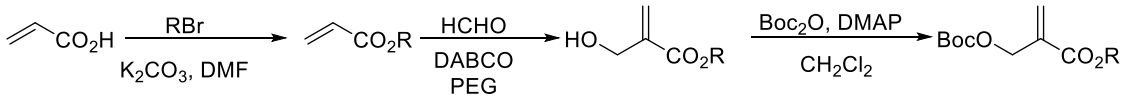


SI-1 **1**

To a solution of amino acid (10 mmol, 1.0 equiv.), N,O-dimethyl hydroxylamine hydrochloride (11.0 mmol, 1.1 equiv.), NMM (11 mmol, 1.1 equiv.) in DCM (20 mL) at -15 °C was slowly added EDC (11 mmol, 1.1 equiv.) in four equal portion over 15 min. The mixture was stirred at -15 °C for 16 h and then washed with 1N aqueous HCl (2 × 20 mL), saturated aqueous $NaHCO_3$ (2 × 25 mL) and saturated aqueous brine (1 × 25 mL). The organic layer was then dried with Na_2SO_4 and concentrated to afford tert-butyl (1-(methoxy(methyl)amino)-3-methyl-1-oxobutan-2-yl) carbamate as a white solid in quantitative yield.

To a stirred solution of arylacetylene (15.4 mmol, 4.0 equiv.) in THF (15 mL) at -78 °C, a solution of 2.5 M n-BuLi in hexanes (14.8 mmol, 3.85 equiv.) was added dropwise. The solution was stirred for 45 min. Then, a solution of **SI-1** (3.85 mmol) in THF (10 mL) was dropwise added at -78 °C and stirred for 1 h at the same temperature. The mixture was then allowed to warm to -20 °C and after 2 h, the reaction was quenched by addition of a 1 M NaH_2PO_4 solution (60 mL). The aqueous phase was diluted by addition of 50 mL of water, then extracted with EtOAc (3 × 40 mL). The combined organic layers were washed with brine, then dried over Na_2SO_4 and evaporated in vacuo. Purification of the residue by flash chromatography silica.

B: Typical procedure for the preparation of **4**[3]:



SI-2 **SI-3** **4**

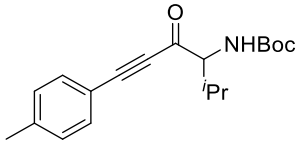
Under nitrogen atmosphere, a mixture of acrylic acid (5.40 g, 75 mmol) and K_2CO_3 (10.35 g) in DMF (125 mL) was stirred at 0 °C for 45 min. After slowly adding alkyl bromide (63 mmol), the reaction mixture was stirred at 100 °C through an oil bath for 24 h. The reaction mixture was added into water (1 L) and the resulting mixture was then extracted with Et_2O (250 mL × 2). The organic layer was dried over Na_2SO_4, concentrated, and purified by flash column to

provide the intermediate **SI-2**.

A mixture of **SI-2** (10 mmol), methyl aldehyde (0.36 g, 12 mmol) and triethylene diamine (1.12 g, 10 mmol) in polyethylene glycol was stirred at 25 ℃ for 24 h. The resulting reaction mixture was diluted with Et_2O (50 mL) and washed with water. The organic layer was dried over Na_2SO_4, concentrated, and purified by flash column to provide the intermediate **SI-3**. The mixture of dibutyldicarbonate (1.31 g, 6 mmol) and 4-dimethylaminopyridine (0.12 g, 1 mmol) in DCM (10 mL) was slowly added (30 min) to the solution of **SI-3** (5 mmol, 1 equiv.) in DCM (10 mL). The mixture was stirred at 0 °C for 5 h. The resulting reaction mixture was washed with 1 N of aqueous HCl, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried over Na_2SO_4, concentrated and purified by flash column to provide product **4**.

3. Characterization of substrates

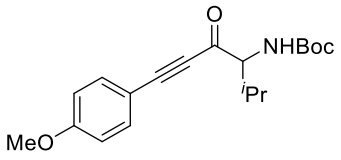
***tert*-butyl (2-methyl-4-oxo-6-(p-tolyl)hex-5-yn-3-yl)carbamate (1d)**



White solid, m.p. 100-102 ℃, 62% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.9 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 5.18 (d, *J* = 9.2 Hz, 1H), 4.50 (dd, *J* = 9.1, 3.9 Hz, 1H), 2.49 (s, 1H), 2.39 (s, 3H), 1.46 (s, 9H), 1.08 (d, *J* = 6.9 Hz, 3H), 0.89 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.10, 155.83, 141.87, 133.22, 129.49, 116.52, 94.89, 86.63, 79.83, 65.90, 30.58, 28.32, 21.77, 19.72, 16.73. **HRMS** (ESI, m/z): calcd. for $C_{19}H_{25}NO_3$ $[M+Na]^+$ 338.1726, found 338.1758.

***tert*-butyl (6-(4-methoxyphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1e)**

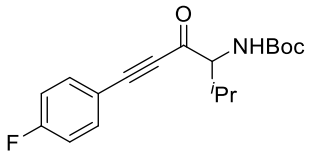


White solid, m.p. 90-92 ℃, 48% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 (d, *J* = 8.2 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 5.18 (d, *J* = 9.2 Hz, 1H), 4.49 (dd, *J* = 9.5, 3.8 Hz, 1H), 3.85 (s, 3H), 2.48 (dd, *J* = 12.2, 6.6 Hz, 1H), 1.46 (s, 9H), 1.07 (d, *J* = 6.9 Hz, 3H), 0.88 (d, *J* = 6.9 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.00,

161.94, 155.84, 135.28, 114.44, 111.35, 95.46, 86.77, 79.78, 65.81, 55.43, 30.62, 28.31, 19.71, 16.74. **HRMS** (ESI, m/z): calcd. for $C_{19}H_{25}NO_4$ $[M+Na]^+$ 354.1676, found 354.1679.

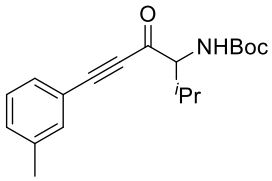
***tert*-butyl (6-(4-fluorophenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1f)**



White solid, m.p. 88-90 ℃, 55% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.50 (m, 2H), 7.10 (t, *J* = 8.4 Hz, 2H), 5.21 (d, *J* = 9.1 Hz, 1H), 4.51 (dd, *J* = 9.1, 4.0 Hz, 1H), 2.48 (s, 1H), 1.46 (s, 9H), 1.09 (d, *J* = 6.8 Hz, 3H), 0.90 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.97, 163.12, 160.48 (d, *J* = 1176.84 Hz), 135.48 (d, *J* = 8.82 Hz), 116.24 (d, *J* = 22.68 Hz), 115.77 (d, *J* = 3.78 Hz), 92.90, 86.67, 79.87, 65.90, 30.44, 28.28, 19.68, 16.72. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -105.57. **HRMS** (ESI, m/z): calcd. for $C_{18}H_{22}FNO_3$ $[M+H]^+$ 320.1657, found 320.1655.

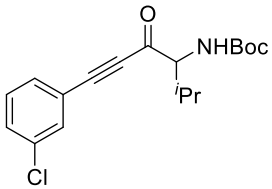
***tert*-butyl (2-methyl-4-oxo-6-(m-tolyl)hex-5-yn-3-yl)carbamate (1g)**



White solid, m.p. 74-76 ℃, 55% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 5.6 Hz, 2H), 7.29 – 7.27 (m, 2H), 5.17 (d, *J* = 9.2 Hz, 1H), 4.50 (dd, *J* = 9.4, 3.9 Hz, 1H), 2.50 (qq, *J* = 6.7, 3.3 Hz, 1H), 2.36 (s, 3H), 1.46 (s, 9H), 1.08 (d, *J* = 6.8 Hz, 3H), 0.89 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.13, 155.84, 138.54, 133.65, 132.00, 130.33, 128.59, 119.44, 94.56, 86.49, 79.88, 65.94, 30.56, 28.32, 21.15, 19.73, 16.72. **HRMS** (ESI, m/z): calcd. for $C_{19}H_{25}NO_3$ $[M+Na]^+$ 338.1726, found 338.1722.

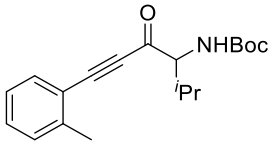
***tert*-butyl (6-(3-chlorophenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1h)**



White solid, m.p. 74-76 ℃, 65% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (s, 1H), 7.46 (t, *J* = 9.1 Hz, 2H), 7.34 (t, *J* = 7.0 Hz, 1H), 5.18 (d, *J* = 9.0 Hz, 1H), 4.49 (dd, *J* = 9.6, 4.0 Hz, 1H), 2.49 (s, 1H), 1.46 (s, 9H), 1.08 (d, *J* = 6.9 Hz, 3H), 0.89 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.98, 155.81, 134.62, 132.74, 131.27, 131.17, 129.97, 121.36, 91.81, 87.14, 80.00, 65.97, 30.39, 28.30, 19.71, 16.74. **HRMS** (ESI, m/z): calcd. for $C_{18}H_{22}ClNO_3$ $[M+Na]^+$ 358.1180, found 358.1175.

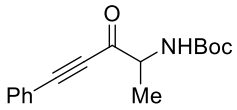
***tert*-butyl (2-methyl-4-oxo-6-(o-tolyl)hex-5-yn-3-yl)carbamate (1i)**



White solid, m.p. 59-61 ℃, 68% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.6 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.25 (s, 1H), 7.21 (t, *J* = 7.5 Hz, 1H), 5.18 (d, *J* = 9.1 Hz, 1H), 4.51 (d, *J* = 12.3 Hz, 1H), 2.50 (s, 3H), 1.46 (s, 9H), 1.08 (d, *J* = 6.8 Hz, 3H), 0.90 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.06, 155.82, 142.33, 133.75, 131.12, 129.88, 125.95, 119.47, 93.29, 90.51, 79.91, 66.01, 30.71, 28.32, 20.67, 19.76, 16.74. **HRMS** (ESI, m/z): calcd. for $C_{19}H_{25}NO_3$ $[M+Na]^+$ 338.1726, found 338.1729.

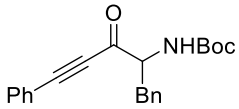
***tert*-butyl (3-oxo-5-phenylpent-4-yn-2-yl)carbamate (1j)**



White solid, m.p. 95-97 ℃, 70% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (t, *J* = 5.9 Hz, 2H), 7.52 – 7.44 (m, 1H), 7.44 – 7.36 (m, 2H), 5.33 (s, 1H), 4.53 (q, *J* = 8.1, 7.4 Hz, 1H), 1.52 – 1.44 (m, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.18, 155.14, 133.18, 131.07, 128.69, 119.59, 94.29, 85.88, 79.91, 56.97, 28.33, 17.74. **HRMS** (ESI, m/z): calcd. for $C_{16}H_{19}NO_3$ $[M+Na]^+$ 372.1570, found 372.1563.

***tert*-butyl (3-oxo-1,5-diphenylpent-4-yn-2-yl)carbamate (1k)**

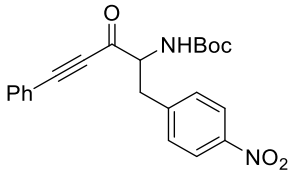


White solid, m.p. 93-95 ℃, 70% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.5 Hz, 2H), 7.47 (q, *J* = 7.1 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.34 – 7.14 (m, 5H), 5.14 (dd, *J* = 8.1, 3.9 Hz, 1H), 4.79 (t, *J* = 6.7 Hz, 1H), 3.28

(qd, *J* = 14.1, 6.5 Hz, 2H), 1.43 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.97, 155.12, 133.25, 131.15, 129.54, 129.26, 128.69, 127.06, 119.53, 94.81, 86.41, 80.00, 62.08, 37.44, 28.32. **HRMS** (ESI, m/z): calcd. for $C_{22}H_{23}NO_3$ $[M+Na]^+$ 296.1257, found 296.1251.

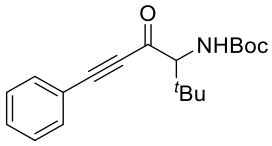
***tert*-butyl (1-(4-nitrophenyl)-3-oxo-5-phenylpent-4-yn-2-yl)carbamate (1l)**



White solid, m.p. 165-167 ℃, 70% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.8 Hz, 2H), 7.57 (d, *J* = 7.3 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 1H), 7.41 (dd, *J* = 12.2, 8.0 Hz, 4H), 5.26 (d, *J* = 7.8 Hz, 1H), 4.85 (q, *J* = 6.7 Hz, 1H), 3.47 (dd, *J* = 14.1, 6.0 Hz, 1H), 3.31 (dd, *J* = 14.1, 6.2 Hz, 1H), 1.43 (s, 9H). **^{13}C NMR** (126 MHz, CDCl3) δ 184.66, 154.95, 147.15, 143.81, 133.29, 131.53, 130.48, 128.82, 123.67, 119.08, 95.72, 86.13, 80.43, 61.69, 37.48, 28.27. **HRMS** (ESI, m/z): calcd. for $C_{22}H_{22}N_2O_5$ $[M+Na]^+$ 417.1421, found 417.1428.

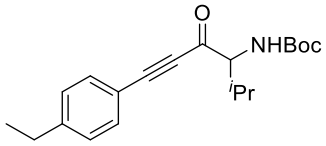
***tert*-butyl (2,2-dimethyl-4-oxo-6-phenylhex-5-yn-3-yl)carbamate (1m)**



White solid, m.p. 113-115 ℃, 2% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57 (d, *J* = 6.0 Hz, 2H), 7.47 (q, *J* = 5.9 Hz, 1H), 7.39 (q, *J* = 5.9 Hz, 2H), 5.22 (d, *J* = 16.1 Hz, 1H), 4.50 (s, 1H), 2.13 – 1.96 (m, 1H), 1.78 – 1.63 (m, 1H), 1.48 – 1.29 (m, 13H), 0.91 (q, *J* = 5.7 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.15, 155.36, 133.07, 130.94, 128.59, 119.57, 93.97, 86.14, 79.80, 61.11, 31.29, 28.23, 27.14, 22.30, 13.73. **HRMS** (ESI, m/z): calcd. for $C_{19}H_{25}NO_3$ $[M+H]^+$ 316.1907, found 316.1913.

***tert*-butyl (6-(4-ethylphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1n)**

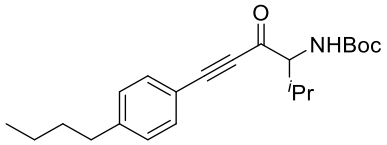


White solid, m.p. 53-55 ℃, 61% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 5.19 (d, *J* =

9.0 Hz, 1H), 4.51 (dd, *J* = 9.1, 3.9 Hz, 1H), 2.68 (q, *J* = 7.6 Hz, 2H), 2.50 (s, 1H), 1.46 (s, 9H), 1.24 (t, *J* = 7.6 Hz, 3H), 1.08 (d, *J* = 6.9 Hz, 3H), 0.89 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.10, 155.83, 148.07, 133.34, 128.31, 116.72, 94.94, 86.61, 79.83, 65.91, 30.60, 29.03, 28.32, 19.71, 16.74, 15.14. **HRMS** (ESI, m/z): calcd. for $C_{20}H_{27}NO_3$ $[M+K]^+$ 368.1623, found 368.1627.

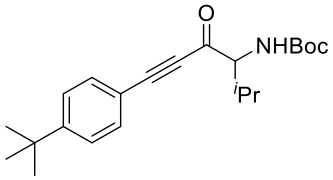
***tert*-butyl (6-(4-butylphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1o)**



White solid, m.p. 92-94 ℃, 53% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.1 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 5.19 (d, *J* = 9.1 Hz, 1H), 4.50 (dd, *J* = 9.3, 3.9 Hz, 1H), 2.64 (t, *J* = 7.8 Hz, 2H), 2.49 (qt, *J* = 7.1, 4.4 Hz, 1H), 1.62 – 1.57 (m, 2H), 1.46 (s, 9H), 1.37 – 1.30 (m, 2H), 1.08 (d, *J* = 6.9 Hz, 3H), 0.91 (dt, *J* = 16.0, 6.9 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.08, 155.83, 146.82, 133.26, 128.84, 116.69, 94.97, 86.63, 79.82, 65.91, 35.78, 33.19, 30.61, 28.31, 22.27, 19.71, 16.73, 13.88. **HRMS** (ESI, m/z): calcd. for $C_{22}H_{31}NO_3$ $[M+K]^+$ 396.1936, found 396.1934.

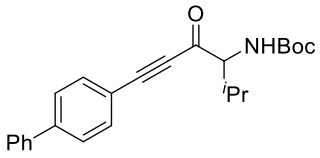
***tert*-butyl (6-(4-(tert-butyl)phenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1p)**



White solid, m.p. 54-56 ℃, 40% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 5.28 (d, *J* = 5.8 Hz, 1H), 4.52 (d, *J* = 5.0 Hz, 1H), 2.50 (s, 1H), 1.46 (t, *J* = 2.8 Hz, 9H), 1.32 (s, 9H), 1.08 (d, *J* = 6.8 Hz, 3H), 0.90 (d, *J* = 7.2 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.00, 155.80, 154.81, 133.07, 125.72, 116.53, 94.75, 86.58, 79.69, 65.91, 35.05, 30.98, 30.57, 28.29, 19.67, 16.75. **HRMS** (ESI, m/z): calcd. for $C_{22}H_{31}NO_3$ $[M+Na]^+$ 380.2196, found 380.2197.

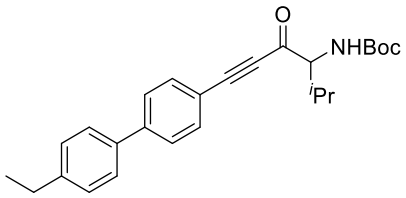
***tert*-butyl (6-([1,1'-biphenyl]-4-yl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1q)**



White solid, m.p. 114-116 ℃, 50% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.4 Hz, 2H), 7.63 – 7.55 (m, 4H), 7.47 – 7.41 (m, 2H), 7.41 – 7.35 (m, 1H), 5.23 (d, *J* = 10.3 Hz, 1H), 4.54 (dd, *J* = 9.3, 3.9 Hz, 1H), 2.52 (s, 1H), 1.47 (s, 9H), 1.10 (d, *J* = 6.9 Hz, 3H), 0.91 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.08, 155.87, 143.87, 139.68, 133.72, 129.02, 128.29, 127.33, 127.15, 118.34, 94.23, 87.46, 79.89, 66.00, 30.58, 28.36, 19.77, 16.81. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{27}NO_3$ $[M+Na]^+$ 400.1883, found 400.1885.

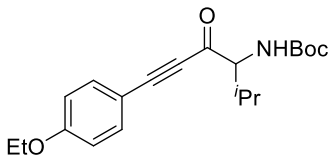
***tert*-butyl (6-(4'-ethyl-[1,1'-biphenyl]-4-yl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1r)**



White solid, m.p. 142-144 ℃, 58% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (q, *J* = 8.3 Hz, 4H), 7.52 (d, *J* = 6.5 Hz, 2H), 7.29 (d, *J* = 6.4 Hz, 2H), 5.20 (s, 1H), 4.53 (d, *J* = 7.9 Hz, 1H), 2.70 (q, *J* = 7.6 Hz, 2H), 2.61 – 2.29 (m, 1H), 1.47 (s, 9H), 1.27 (t, *J* = 7.6 Hz, 3H), 1.09 (d, *J* = 6.9 Hz, 3H), 0.91 (d, *J* = 6.9 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.01, 155.80, 144.57, 143.81, 136.97, 133.65, 128.50, 127.06, 127.02, 117.91, 94.41, 87.34, 79.83, 65.91, 30.55, 28.51, 28.29, 19.69, 16.72, 15.48. **HRMS** (ESI, m/z): calcd. for $C_{26}H_{31}NO_3$ $[M+K]^+$ 444.1936, found 444.1935.

***tert*-butyl (6-(4-ethoxyphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1s)**

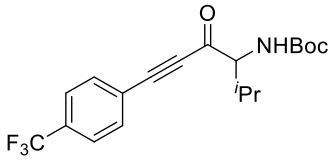


White solid, m.p. 109-111 ℃, 57% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.4 Hz, 2H), 6.89 (d, *J* = 8.4 Hz, 2H), 5.22 (d, *J* = 9.0 Hz, 1H), 4.49 (dd, *J* = 9.1, 3.9 Hz, 1H), 4.06 (q, *J* = 7.0 Hz, 2H), 2.49 (s, 1H), 1.49 – 1.39 (m, 12H), 1.08 (d, *J* = 6.9 Hz, 3H), 0.89 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.96, 161.35, 155.83, 135.27, 114.86, 111.09, 95.62, 86.75, 79.74, 65.81, 63.75, 30.63, 28.30,

19.70, 16.74, 14.61. **HRMS** (ESI, m/z): calcd. for $C_{20}H_{27}NO_4$ $[M+Na]^+$ 368.1832, found 368.1829.

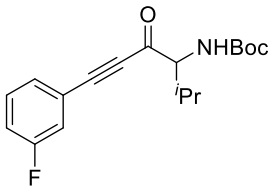
***tert*-butyl (2-methyl-4-oxo-6-(4-(trifluoromethyl)phenyl)hex-5-yn-3-yl)carbamate (1t)**



White solid, m.p. 88-90 ℃, 65% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 – 7.58 (m, 4H), 5.14 (d, *J* = 8.6 Hz, 1H), 4.52 (d, *J* = 8.8 Hz, 1H), 2.49 (s, 1H), 1.46 (s, 9H), 1.09 (d, *J* = 6.8 Hz, 3H), 0.90 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.94, 155.81, 133.25, 132.48 (q, *J* = 32.76 Hz), 125.63 (q, *J* = 3.78 Hz), 123.46, 123.49 (q, *J* = 289.80 Hz), 91.27, 87.86, 80.07, 66.00, 30.35, 28.30, 19.71, 16.74. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.22. **HRMS** (ESI, m/z): calcd. for $C_{19}H_{22}F_3NO_3$ $[M+H]^+$ 370.1625, found 370.1622.

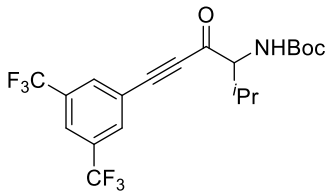
***tert*-butyl (6-(3-fluorophenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1u)**



White solid, m.p. 93-95 ℃, 48% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.38 (t, *J* = 4.9 Hz, 2H), 7.28 (d, *J* = 6.9 Hz, 1H), 7.25 – 7.12 (m, 1H), 5.14 (d, *J* = 9.0 Hz, 1H), 4.50 (d, *J* = 12.2 Hz, 1H), 2.49 (s, 1H), 1.46 (s, 9H), 1.08 (d, *J* = 6.9 Hz, 3H), 0.89 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.99, 162.22 (d, *J* = 248.22 Hz), 155.80, 130.44 (d, *J* = 7.56 Hz), 128.99 (d, *J* = 2.52 Hz), 121.43 (d, *J* = 8.82 Hz), 119.72 (d, *J* = 23.94 Hz), 118.45 (d, *J* = 85 Hz), 92.00, 86.91, 80.02, 65.98, 30.42, 28.31, 19.71, 16.74.**^{19}F NMR** (471 MHz, $CDCl_3$) δ -111.53. **HRMS** (ESI, m/z): calcd. for $C_{18}H_{22}FNO_3$ $[M+Na]^+$ 342.1476, found 342.1476.

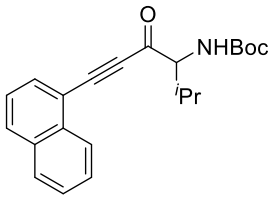
***tert*-butyl (6-(3,5-bis(trifluoromethyl)phenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1v)**



White solid, m.p. 95-97 ℃, 55% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02 (d, *J* = 1.6 Hz, 2H), 7.96 (s, 1H), 5.13 (d, *J* = 9.0 Hz, 1H), 4.50 (d, *J* = 4.8 Hz, 1H), 2.48 (s, 1H), 1.46 (s, 9H), 1.10 (d, *J* = 6.9 Hz, 3H), 0.91 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 186.72, 155.78, 132.93, 132.53 (q, J = 34.02 Hz), 124.17 (q, J = 3.78 Hz), 122.56 (q, J = 273.42 Hz), 122.20, 88.59, 88.29, 80.21, 65.97, 30.16, 28.26, 19.69, 16.75.**^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.26. **HRMS** (ESI, m/z): calcd. for $C_{20}H_{21}F_6NO_3$ $[M+Na]^+$ 460.1318, found 460.1314.

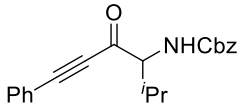
***tert*-butyl (2-methyl-6-(naphthalen-1-yl)-4-oxohex-5-yn-3-yl)carbamate (1w)**



White solid, m.p. 80-82 ℃, 48% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.3 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.87 (dd, *J* = 11.4, 7.6 Hz, 2H), 7.64 (t, *J* = 7.0 Hz, 1H), 7.61 – 7.55 (m, 1H), 7.51 – 7.45 (m, 1H), 5.26 (d, *J* = 9.0 Hz, 1H), 4.62 (dd, *J* = 9.0, 3.9 Hz, 1H), 2.59 (qd, *J* = 10.6 Hz, 1H), 1.47 (s, 9H), 1.13 (d, *J* = 6.8 Hz, 3H), 0.95 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.05, 155.89, 133.59, 133.05, 131.88, 128.61, 127.87, 127.03, 125.65, 125.18, 117.19, 92.46, 91.42, 79.99, 66.10, 30.75, 28.35, 19.80, 16.86. **HRMS** (ESI, m/z): calcd. for $C_{22}H_{25}NO_3$ $[M+Na]^+$ 374.1726, found 374.1724.

benzyl (2-methyl-4-oxo-6-phenylhex-5-yn-3-yl)carbamate (1x)

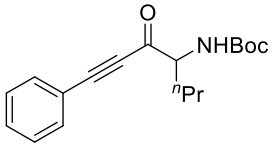


Yellow liquid, 70% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.2 Hz, 2H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.35 (td, *J* = 18.5, 17.1, 9.4 Hz, 7H), 5.46 (s, 1H), 5.13 (d, *J* = 4.4 Hz, 2H), 4.59 (dd, *J* = 9.0, 3.9 Hz, 1H), 2.53 (pd, *J* = 6.6, 3.8 Hz, 1H), 1.09 (d, *J* = 6.9 Hz, 3H), 0.89 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (126

MHz, $CDCl_3$) δ 186.54, 156.48, 136.28, 133.24, 131.18, 128.73, 128.58, 128.23, 128.15, 119.51, 94.53, 86.60, 67.16, 66.41, 30.58, 19.74, 16.68. **HRMS** (ESI, m/z): calcd. for $C_{21}H_{21}NO_3$ $[M+Na]^+$ 358.1413, found 358.1417.

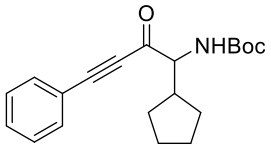
***tert*-butyl (3-oxo-1-phenylhept-1-yn-4-yl)carbamate (1y)**



White solid, m.p. 105-107 ℃, 48% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 6.8 Hz, 2H), 7.47 (q, *J* = 5.9 Hz, 1H), 7.39 (q, *J* = 6.6, 6.1 Hz, 2H), 5.21 (d, *J* = 18.2 Hz, 1H), 4.51 (d, *J* = 11.6 Hz, 1H), 2.00 (tt, *J* = 10.8, 5.7 Hz, 1H), 1.74 – 1.61 (m, 1H), 1.56 – 1.31 (m, 11H), 1.07 – 0.89 (m, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.18, 155.37, 133.09, 130.95, 128.60, 119.58, 94.00, 86.15, 79.80, 60.99, 33.77, 28.24, 18.48, 13.75. **HRMS** (ESI, m/z): calcd. for $C_{18}H_{23}NO_3$ $[M+H]^+$ 302.1760, found 302.1756.

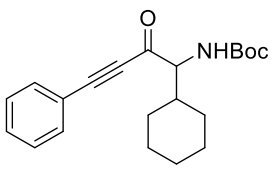
***tert*-butyl (1-cyclopentyl-2-oxo-4-phenylbut-3-yn-1-yl)carbamate (1z)**



White solid, m.p. 101-103 ℃, 38% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.1 Hz, 2H), 7.51 – 7.44 (m, 1H), 7.40 (dt, *J* = 8.0, 4.1 Hz, 2H), 5.21 (d, *J* = 8.7 Hz, 1H), 4.53 (d, *J* = 12.2 Hz, 1H), 2.46 (h, *J* = 8.0 Hz, 1H), 1.91 – 1.81 (m, 1H), 1.67 (tt, *J* = 9.9, 5.5 Hz, 3H), 1.60 – 1.50 (m, 3H), 1.45 (s, 9H), 1.35 – 1.21 (m, 1H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.17, 155.66, 133.07, 130.90, 128.58, 119.64, 93.81, 86.66, 79.84, 63.83, 41.55, 29.20, 28.23, 27.44, 25.26, 25.01. **HRMS** (ESI, m/z): calcd. for $C_{20}H_{25}NO_3$ $[M+H]^+$ 328.1907, found 3288.1913.

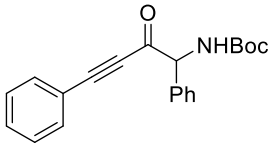
***tert*-butyl (1-cyclohexyl-2-oxo-4-phenylbut-3-yn-1-yl)carbamate (1aa)**



White solid, m.p. 108-110 ℃, 25% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (d, *J* = 6.7 Hz, 2H), 7.47 (dd, *J* = 7.4, 2.8 Hz, 1H), 7.40 (t, *J* = 7.8 Hz, 2H), 5.20 (d, *J* = 9.0 Hz, 1H), 4.48 (d, *J* = 6.0 Hz, 1H), 2.09 (s, 1H), 1.84 – 1.74 (m, 3H), 1.67 (d, *J* = 12.9 Hz, 1H), 1.57 (d, *J* = 11.1 Hz, 1H), 1.46 (s, 9H), 1.27 (dd, *J* = 22.3, 12.8 Hz, 3H), 1.19 – 1.02 (m, 2H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 187.17, 155.66, 133.08, 130.93, 128.59, 119.61, 93.96, 86.73, 79.76, 65.65, 40.38, 29.94, 28.24, 27.21, 26.12, 26.01, 25.83. **HRMS** (ESI, m/z): calcd. for $C_{21}H_{27}NO_3$ $[M+Na]^+$ 364.1883, found 364.1889.

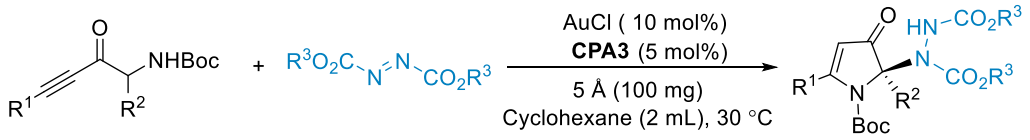
***tert*-butyl (2-oxo-1,4-diphenylbut-3-yn-1-yl)carbamate (1ab)**



White solid, m.p. 110-112 ℃, 40% yield.

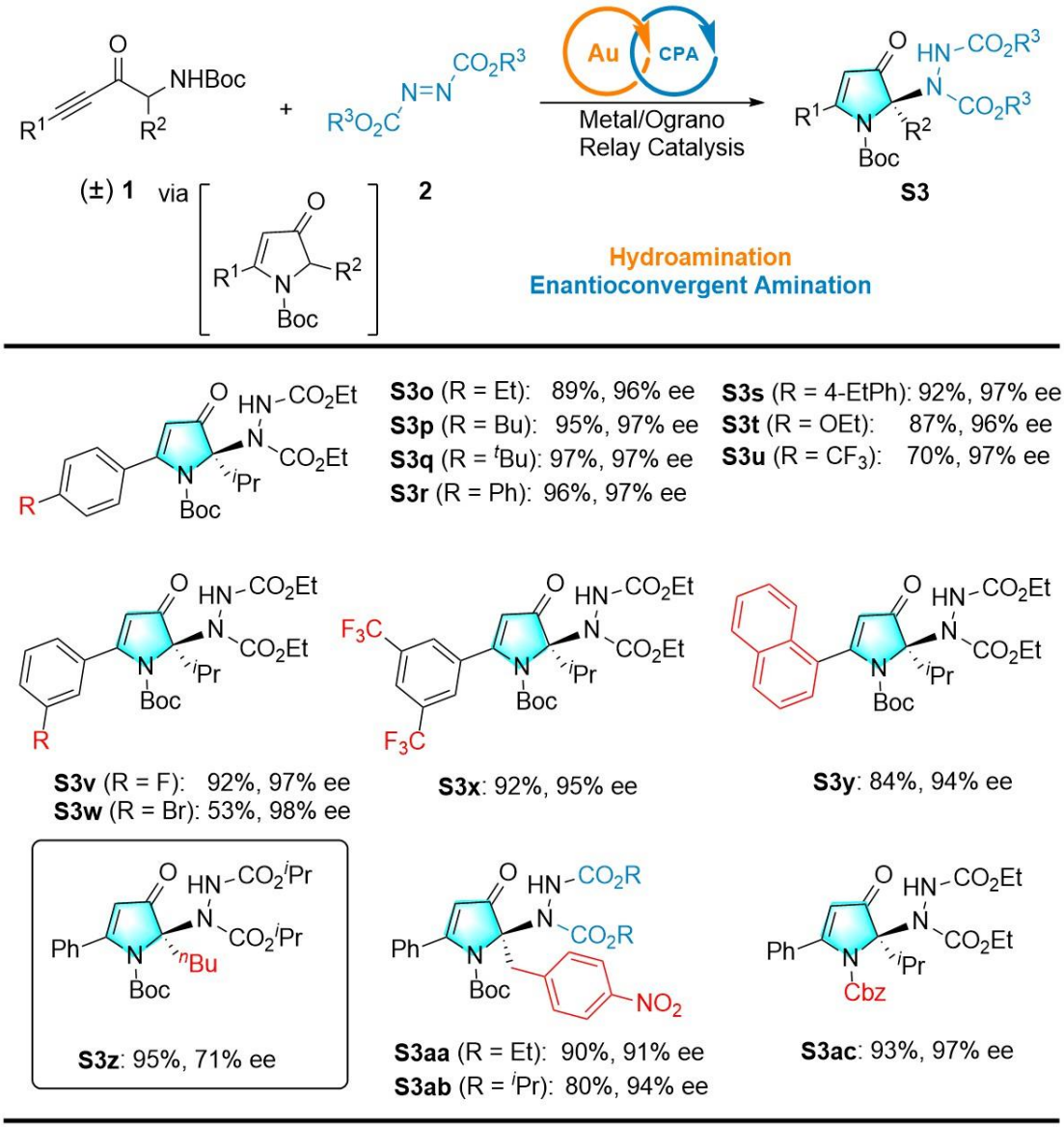
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (qd, *J* = 10.0, 3.4 Hz, 7H), 7.34 (dd, *J* = 7.4, 4.5 Hz, 3H), 5.87 (s, 1H), 5.54 (d, *J* = 6.9 Hz, 1H), 1.43 (s, 9H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 183.18, 154.74, 135.88, 133.04, 131.05, 128.98, 128.63, 128.56, 127.96, 119.37, 95.60, 86.16, 80.12, 65.78, 28.24. **HRMS** (ESI, m/z): calcd. for $C_{21}H_{21}NO_3$ $[M+Na]^+$ 358.1413, found 358.1419.

4. General procedure for the synthesis of product

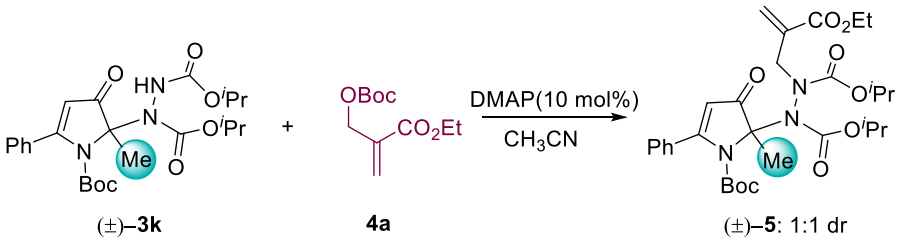


1 **2** **3**

To a 4 mL vial was added **1** (0.12 mmol, 1.2 equiv.), which was taken into the glovebox, where **CPA3** (0.005 mmol, 5 mol%), AuCl (0.01 mmol, 10 mol%), 5Å (100 mg), diethyl (E)-diazene-1,2-dicarboxylate (0.10 mmol, 1.0 equiv.) and cyclohexane (2 mL) were added. The reaction mixture was taken outside the glovebox. The vial was then sealed and the reaction mixture was allowed to stir at 30 ℃ for 18 h. The crude reaction mixture was directly purified by silica gel column chromatography with hexanes/ethyl acetate (8:1 v/v) as eluent to afford the product **3**.

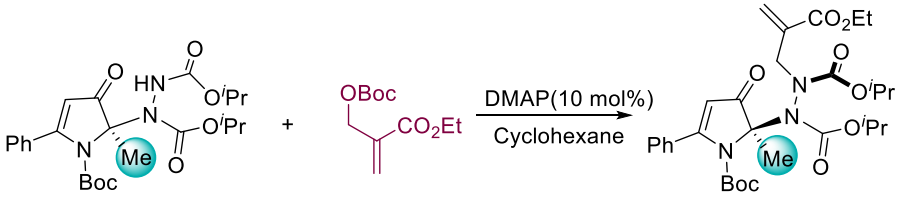


Scheme S1. Substrate scope for gold and CPA relay reaction



To a 4 mL vial was added **3k** (0.1 mmol), DMAP (10 mol%), CH_3CN (2 mL) and ethyl 2-(((tert-butoxycarbonyl)oxy)methyl)acrylate (0.3 mmol). The reaction mixture was allowed to stir at 30 ℃ for 6 h. The crude reaction mixture was directly purified by silica gel column chromatography with hexanes/ethyl acetate (8:1 v/v) as eluent to afford the product **5** (90%

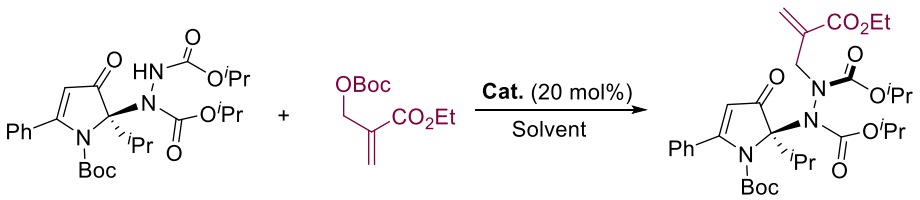
yield, 1:1 dr).



3k 80% ee + **4a** → **5**: 2:1 dr

To a 4 mL vial was added **3k** (0.1 mmol), DMAP (10 mol%), cyclohexane (2 mL) and ethyl 2-(((tert-butoxycarbonyl)oxy)methyl)acrylate (0.3 mmol). The reaction mixture was allowed to stir at 30 ℃ for 6 h. The crude reaction mixture was directly purified by silica gel column chromatography with hexanes/ethyl acetate (8:1 v/v) as eluent to afford the product **5** (92% yield, 2:1 dr, 80% ee, 80% ee).

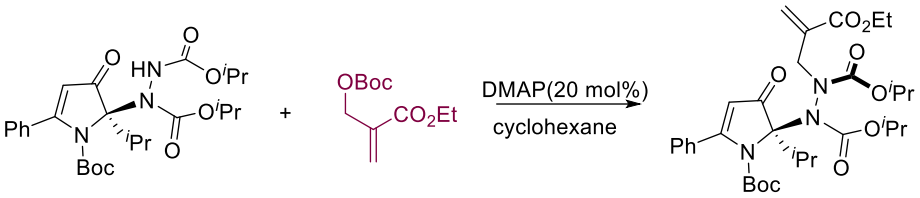
Table S1. Reaction conditions screening[a]



3c: 97% ee + **4a** → **6a**

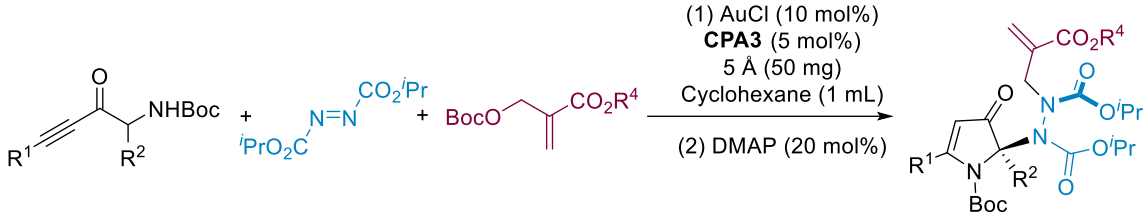
Entry	**Cat.**	Solvent	yield (%)[b]	dr[c]	ee (%)[d]
1	DMAP	cyclohexane	92	> 98:2	97
2	DMAP	toluene	88	8:1	97
3	DMAP	THF	< 5	/	/
4	DMAP	$CHCl_3$	76	6:1	97
5	Quinine	cyclohexane	< 5	/	/
6	Quinidine	cyclohexane	< 5	/	/
7	$(DHQ)_2PHAL$	cyclohexane	< 5	/	/
8[e]	DMAP	cyclohexane	75	> 98:2	97
9[f]	DMAP	cyclohexane	79	> 98:2	97

[a] Reaction conditions: **3c** (1.0 equiv., 0.05 mmol), **4a** (3.0 equiv., 0.15 mmol), **Cat.** (20 mol%), and solvent (0.5 M), 30 ℃, N_2, 6 hours. [b]Isolated yield. [c]Determined by ^1H NMR. [d] Determined by HPLC. [e] 2.0 equiv. instead of 3.0 equiv. **4a**. [f]10 mol% instead of 20 mol% DMAP.



3c **4a** **6a**

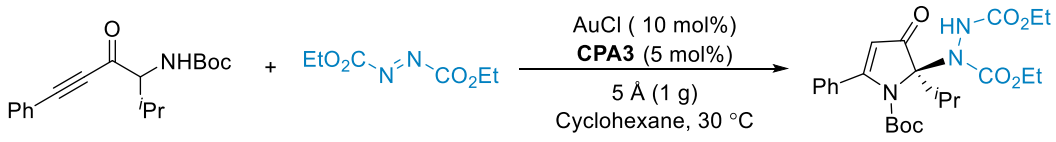
To a 4 mL vial was added **3c** (0.1 mmol), DMAP (20 mol%), cyclohexane (2 mL) and ethyl 2-(((tert-butoxycarbonyl)oxy)methyl)acrylate (0.3 mmol). The reaction mixture was allowed to stir at 30 ℃ for 6 h. The crude reaction mixture was directly purified by silica gel column chromatography with hexanes/ethyl acetate (8:1 v/v) as eluent to afford the product **6a** (92% yield, > 98:2 dr).



(±)-1 **2c** **4** **6**

To a 4 mL vial was added α-amino-ynone (0.12 mmol, 1.2 equiv.), which was taken into the glovebox , where **CPA3** (0.005 mmol, 5 mol%), AuCl (0.01 mmol, 10 mol%), 5Å (100 mg), diisopropyl (E)-diazene-1,2-dicarboxylate (0.10 mmol, 1.0 equiv.) and cyclohexane (2 mL)were added. The reaction mixture was taken outside the glovebox. The vial was then sealed and the reaction mixture was allowed to stir at 30 ℃ for 18 h. Then compound **4** (0.3 mmol, 3.0 equiv.) and DMAP (20 mol%) were added. The reaction mixture was allowed to stir at 30 ℃ until TLC indicated the reaction was completed. The solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography with hexane\ethyl acetate (10:1 v\v) as eluent to afford product **6**.

5. One-mmol-scale reaction

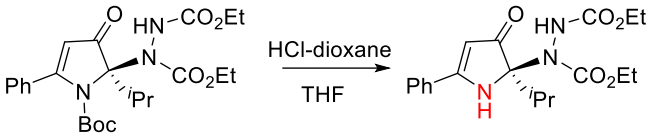


1a **2b** **3b**

To a 50 mL vial was added **1a** (1.2 mmol, 1.2 equiv.), which was taken into the glovebox, where

CPA3 (0.05 mmol, 5 mol%), AuCl (0.1 mmol, 10 mol%), 5Å (1 g), diethyl (E)-diazene-1,2-dicarboxylate (1.0 mmol, 1.0 equiv.) and cyclohexane (20 mL) were added. The reaction mixture was taken outside the glovebox. The vial was then sealed and the reaction mixture was allowed to stir at 30 ℃ for 24 h. The solvent was removed under reduced pressure. Then the residue was directly purified by silica gel column chromatography with hexanes/ethyl acetate (8:1 v/v) as eluent to afford the diethyl 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (451 mg, 95% yield, 97% ee).

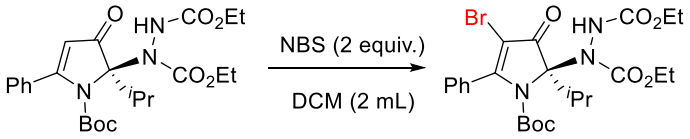
6. Synthetic Transformations of Product



3b
97% ee

9
60%, 97% ee

To the tube was added **3b** (1.0 equiv., 0.2 mmol) and THF (2 mL). Then HCl-dioxane (5.0 equiv., 1.0 mmol) was added to the mixture solution and stirred at 30 ℃ for 20 h. After complete consumption of the starting material. The mixture solution was quenched by aq. NaOH and extracted with EtOAc. The combined organic phase washed with brine, dried over Na_2SO_4, and concentrated in vacuum. The crude reaction mixture was purified by silica gel column chromatography with hexanes/ethyl acetate (5:1 v/v) as eluent to afford the diethyl 1-(2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (44 mg, 60% yield).

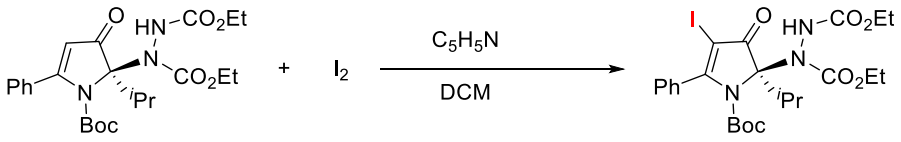


3b
97% ee

10
91%, 96% ee

The NBS (2.0 equiv., 0.4 mmol) was dissolved in DCM (2 mL) containing compound **3b** (1.0 equiv., 0.2 mmol). The resulting mixture was stirred for 1 h at 30 ℃. Subsequently, the solvent was removed under reduced to obtain a yellow oil residue. The residue was purified by column chromatography on silica gel (PE: EA=10: 1) to afford product as a white solid (91% yield, 96%

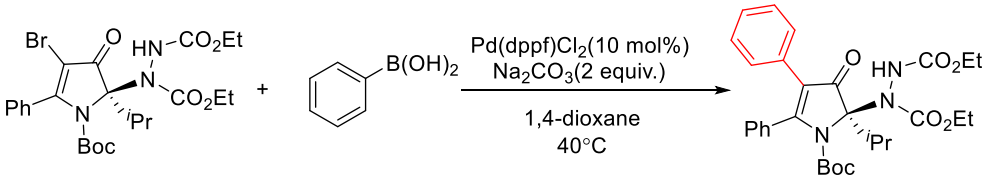
ee).



3b
97% ee

11
96% ee

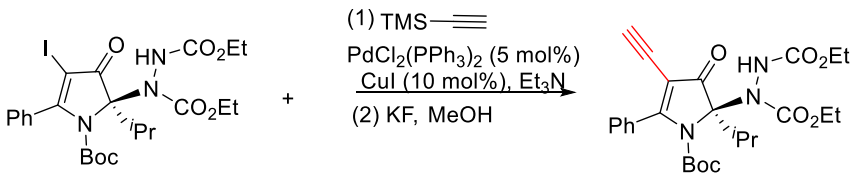
The **3b** (1.0 equiv., 0.2 mmol) and pyridine (1.2 equiv., 0.24 mmol) were dissolved in DCM (2 mL). Then iodine (2.0 equiv., 0.4 mmol) was added to the solution. The resulting mixture was stirred at rt. After complete consumption of the starting material. The mixture solution was quenched by aq. Na_2SO_3 and extracted with DCM. The combined organic phase washed with brine, dried over Na_2SO_4, and concentrated in vacuum. The crude reaction mixture was purified by silica gel column chromatography with hexanes/ethyl acetate (5:1 v/v) as eluent to afford product as white solid (88% yield, 96% ee).



10
97% ee

12
88%, 96% ee

To a solution of **10** (1.0 equiv., 2 mmol) in 1,4-dioxane (2 mL) was added 2 M aqueous Na_2CO_3 (2.0 equiv., 0.4 mmol), boric acid (2.0 equiv., 0.4 mmol) and $PdCl_2$(dppf) (10% mol). The flask was flushed with nitrogen gas. The reaction mixture was allowed to stir at 40 ℃ until the starting material was complete consumption. The 1,4-dioxane was evaporated, and the residue was extracted with EtOAc (3 × 5 mL) and washed with brine, dried over sodium sulfate and concentrated in vacuum. The residue was purified by column chromatography to afford product **12** (88% yield, 96% ee).

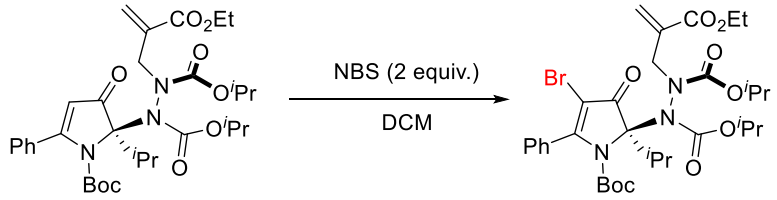


11
96% ee

13
75%, 96% ee

Palladium(II)bis(triphenylphosphine) dichloride (10 mol%), **11** (1.0 equiv., 0.2 mmol), and cuprous iodide (1.2 equiv., 0.24 mmol) were added to an oven-dried Schlenk tube equipped

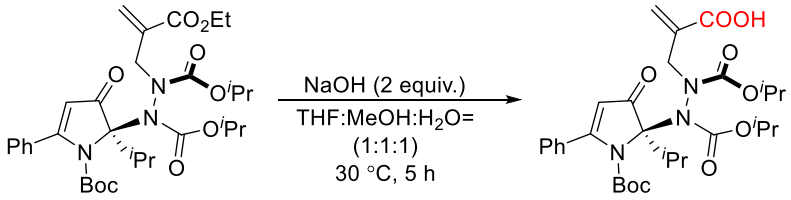
with a stir bar. The tube was then sealed, evacuated, and backfilled with nitrogen three times using standard Schlenk techniques. Et_3N (2 mL) and trimethylsilylacetylene (3.0 equiv., 0.6 mmol) were sequentially added by syringe at ambient temperature. The resulting mixture was vigorously stirred and heated at 40 °C (oil bath) for 24 h. After the mixture was cooled to room temperature, water (10 mL) was added. The resulting mixture was extracted with ethyl acetate (5 mL × 3). The combined organic layers were then washed with brine, dried over Na_2SO_4, and concentrated in vacuum. The residue was used without further purification. Then the mixture was added KF (2 equiv., 0.4 mmol) and MeOH (2 mL), and the resulting mixture was stirred at room temperature until TLC indicated the reaction was complete. The reaction mixture was diluted with water (5 mL) and extracted with ethyl acetate (5 mL × 3). The combined organic phase washed with brine, dried over Na_2SO_4, and concentrated in vacuum. The residue was purified by column chromatography to give product **13** (70% yield, 96% ee).



6a
96% ee

14
88%, 96% ee

The NBS (0.4 mmol, 47.1 mg) was dissolved in DCM (2 mL) containing compound **6a** (0.2 mmol, 123 mg). The resulting mixture was stirred for 1 h at 30 ℃. Subsequently, the solvent was removed under reduced to obtain a yellow oil residue. The residue was purified by column chromatography on silica gel (PE: EA=10: 1) to afford product as a white solid (88% yield, 96% ee).



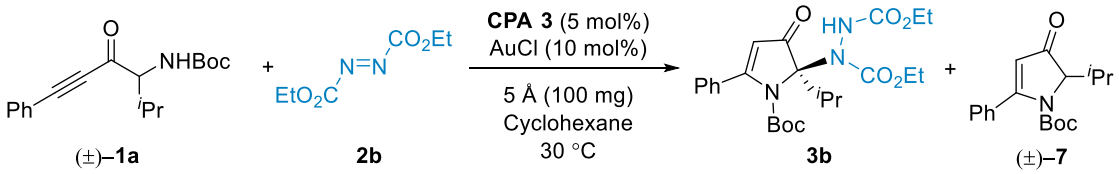
6a
96% ee

15
84%, 99% ee

The NaOH (0.4 mmol, 16 mg) was dissolved in THF:MeOH:H_2O (1:1:1=0.5 mL:0.5 mL:0.5 mL) containing compound **6a** (0.2 mmol, 123 mg). The resulting mixture was stirred for 5 h at 30 ℃. Subsequently, the volatiles were evaporated under reduced pressure. The residual

aqueous solution was acidified with 3N HCl solution (pH < 1) and extracted with ethyl acetate. The combined organic layers were dried with Na_2SO_4, filtered and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (PE:EA=5:1) to afford product as a white solid (84% yield, 99% ee).

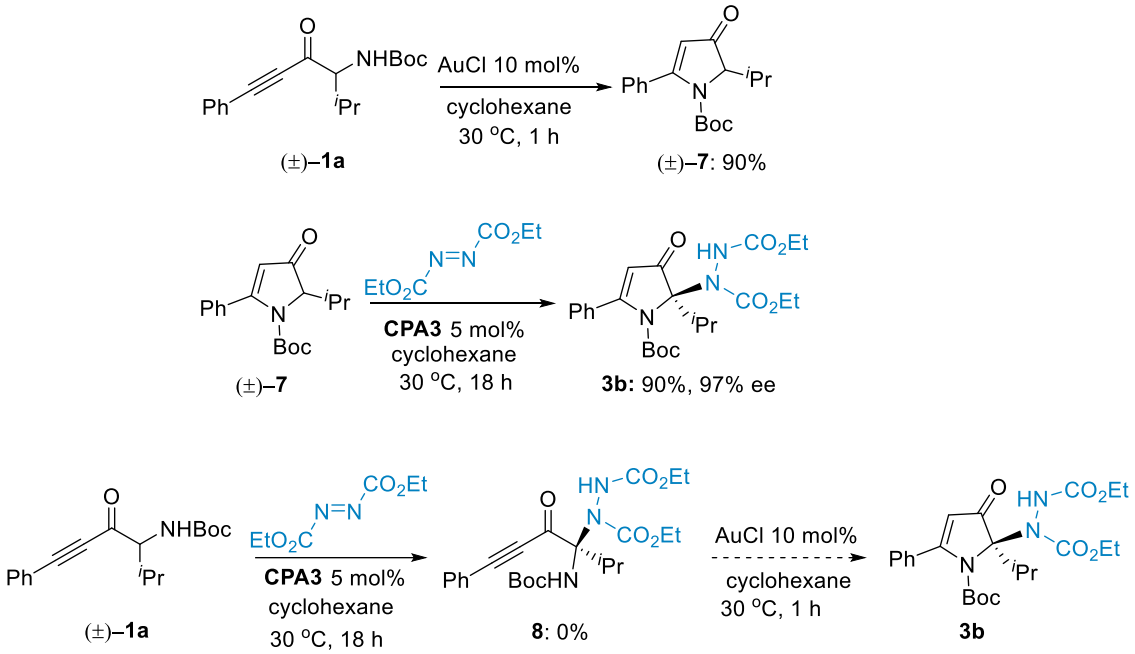
7. NMR revealed the catalytic reaction profile



To a 4 mL vial was added **1a** (0.12 mmol, 1.2 equiv.), which was taken into the glovebox, where **CPA3** (0.005 mmol, 5mol%), AuCl (0.01 mmol, 10 mol%), 5Å (100 mg), diethyl (E)-diazene-1,2-dicarboxylate (0.1 mmol, 1.0 equiv.) and cyclohexane (2 mL) were added. The reaction mixture was taken outside the glovebox. The vial was then sealed and the reaction mixture was allowed to stir at 30 ℃ for the given time. The reaction mixture was filtered through silica gel and the solvent was removed under reduced pressure. Real time content was determined by **^{1}H NMR** using 1,1,2,2-tetrachloroethane as the internal standard.

Entry	Time (h)	**1a** (%)	**7** (%)	**3b** (%)
1	0	120	0	0
2	0.15	70	50	0
3	0.30	45	75	0
4	0.45	10	95	10
5	1	0	78	30
6	2	0	60	55
7	4	0	48	69
8	6	0	35	77
9	8	0	30	83
10	12	0	28	88
11	16	0	23	92
12	18	0	17	97

8. Control reactions and the stepwise reactions



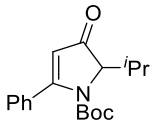
To a 4 mL vial was added tert-butyl (2-methyl-4-oxo-6-phenylhex-5-yn-3-yl)carbamate (**1a**) (0.12 mmol), which was taken into the glovebox, where AuCl (0.01 mmol, 10 mol %) and cyclohexane (2 mL) were added. The reaction mixture was stirred at 30 ℃ for 1 h. The crude reaction mixture was directly purified by silica gel column chromatography with hexane and ethyl acetate (5:1 v/v) as eluent to afford the product **7** in 90% yield.

To a 4 mL vial was added **7** (0.1 mmol, 1.2 equiv.), which was taken into the glovebox, where **CPA3** (5 mol%), 5Å (100 mg) and cyclohexane (2 mL) were added. Then diethyl (E)-diazene-1,2-dicarboxylate (1.0 equiv.) was added. The reaction mixture was stirred at 30 ℃ for 18 h. The crude reaction mixture was directly purified by silica gel column chromatography with hexane and ethyl acetate (5:1 v/v) as eluent to afford the product **3b** (90% yield, 97% ee).

To a 4 mL vial was added the tert-butyl (2-methyl-4-oxo-6-phenylhex-5-yn-3-yl)carbamate (**1a**) (0.12 mmol, 1.2 equiv.), **CPA3** (0.005 mmol, 5mol%), 5Å (100 mg), diethyl (E)-diazene-1,2-dicarboxylate (0.10 mmol, 1.0 equiv.) and cyclohexane (2 mL). The vial was then sealed and the reaction mixture was allowed to stir at 30 ℃ for 18 h. The reaction mixture was filtered through silica gel and the solvent was removed under reduced pressure. The residue was checked by crude **^{1}H NMR**. No target material was obtained by crude **^{1}H NMR**.

9. Characterization of products

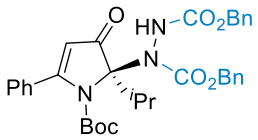
***tert*-butyl 2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrole-1-carboxylate (7)**



White solid, m.p. 108-110 ℃, 90% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (q, *J* = 6.5, 5.8 Hz, 5H), 5.60 (s, 1H), 4.19 (d, *J* = 3.6 Hz, 1H), 2.62 (s, 1H), 1.24 (s, 9H), 1.18 (d, *J* = 7.2 Hz, 3H), 1.03 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 200.74, 172.86, 150.34, 133.29, 130.08, 127.99, 127.07, 113.55, 82.57, 71.53, 32.07, 27.64, 17.18, 17.10. **HRMS** (ESI, m/z): calcd. for $C_{18}H_{23}NO_3$ $[M+Na]^+$ 324.1567, found 324.1569.

dibenzyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3a)

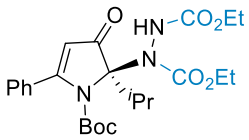


White solid, m.p. 73-75 ℃, 93% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.28 (m, 10H), 7.26 – 7.14 (m, 5H), 5.50 (s, 1H), 5.18 (s, 2H), 5.10 (s, 2H), 2.97 (p, J = 6.8 Hz, 1H), 1.13 – 0.97 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.24, 168.46, 155.17, 150.23, 136.21, 135.39, 133.84, 129.58, 128.40, 128.25, 128.16, 127.96, 126.60, 111.42, 86.46, 83.18, 68.84, 67.41, 32.32, 27.30, 17.08, 14.80. **HRMS** (ESI, m/z): calcd. for $C_{34}H_{37}N_3O_7$ $[M+Na]^+$ 599.2632, found 599.2635.

Specific Rotation: $[\alpha]^{25}_D$ = −89.6 (*c* = 1.0, $CHCl_3$). 93% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 7.718 min for minor isomer, t_R = 9.913 min for major isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3b)

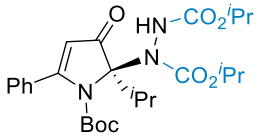


White solid, m.p. 111-113 ℃, 96% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 – 7.31 (m, 5H), 5.60 (s, 1H), 4.18 (dddt, *J* = 37.2, 30.3, 10.8, 7.5 Hz, 4H), 2.97 (p, *J* = 6.9 Hz, 1H), 1.67 (s, 1H), 1.31 (dt, *J* = 11.8, 5.1 Hz, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.18 – 0.89 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.33, 168.27, 155.17, 150.27, 133.98, 129.60, 128.02, 126.55, 111.42, 86.56, 83.02, 63.09, 61.54, 32.42, 27.29, 17.08, 14.74, 14.44, 14.11. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{33}N_3O_7$ $[M+Na]^+$ 498.2211, found 498.2214.

Specific Rotation: $[\alpha]^{25}_D$ = –93.8 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.488 min for major isomer, t_R = 5.492 min for minor isomer).

diisopropyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3c)

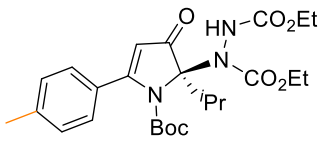


White solid, m.p. 100-102 ℃, 92% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.33 (m, 5H), 7.22 (s, 1H), 5.59 (s, 1H), 5.03 (h, *J* = 6.0 Hz, 1H), 4.89 (h, *J* = 6.2 Hz, 1H), 3.05 – 2.90 (m, 1H), 1.31 (td, *J* = 11.8, 10.8, 6.4 Hz, 6H), 1.21 (q, *J* = 5.2, 4.7 Hz, 6H), 1.15 – 1.02 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.49, 168.08, 154.89, 154.59, 150.18, 134.02, 129.56, 128.02, 126.54, 111.50, 86.62, 82.88, 71.30, 69.08, 32.59, 27.30, 21.71, 17.12, 14.73. **HRMS** (ESI, m/z): calcd. for $C_{26}H_{37}N_3O_7$ $[M+Na]^+$ 526.2524, found 526.2524.

Specific Rotation: $[\alpha]^{25}_D$ = –47.1 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 3.858 min for minor isomer, t_R = 4.288 min for major isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(p-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3d)

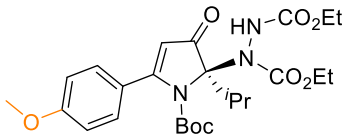


White solid, m.p. 117-119 ℃, 87% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.26 – 7.17 (m, 4H), 5.57 (s, 1H), 4.30 – 4.02 (m, 4H), 2.96 (p, J = 6.8 Hz, 1H), 2.38 (s, 3H), 1.91 (s, 1H), 1.29 (d, J = 17.5 Hz, 3H), 1.20 (t, J = 7.1 Hz, 3H), 1.07 (d, J = 22.9 Hz, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.35, 168.55, 155.19, 150.41, 139.97, 131.04, 128.62, 126.55, 111.12, 86.68, 82.97, 63.09, 61.55, 32.53, 27.10, 21.18, 17.11, 14.79, 14.44, 14.11. **HRMS** (ESI, m/z): calcd. for $C_{25}H_{35}N_3O_7$ $[M+H]^+$ 490.2548 , found 490.2546.

Specific Rotation: $[\alpha]^{25}_D$ = –66.0 (c = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.298 min for major isomer, t_R = 5.285 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-5-(4-methoxyphenyl)-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3e)

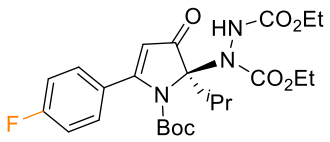


Yellow liquid, 83% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (d, J = 8.7 Hz, 2H), 6.92 (d, J = 8.7 Hz, 2H), 5.57 (s, 1H), 4.33 – 4.02 (m, 4H), 3.84 (s, 3H), 2.95 (p, J = 6.8 Hz, 1H), 1.85 (s, 1H), 1.30 (t, J = 7.2 Hz, 3H), 1.22 – 1.17 (m, 3H), 1.16 – 0.96 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.32, 168.26, 161.21, 155.21, 150.52, 128.15, 126.14, 113.60, 110.80, 86.87, 82.93, 63.09, 61.56, 55.41, 32.61, 27.42, 17.13, 14.85, 14.44, 14.10. **HRMS** (ESI, m/z): calcd. for $C_{25}H_{35}N_3O_8$ $[M+Na]^+$ 528.2316, found 528.232.

Specific Rotation: $[\alpha]^{25}_D$ = –33.0 (c = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.142 min for major isomer, t_R = 6.545 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-5-(4-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3f)

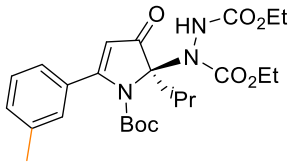


White solid, m.p. 59-61 ℃, 95% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (t, *J* = 4.5 Hz, 2H), 7.21 (s, 1H), 7.10 (t, *J* = 7.4 Hz, 2H), 5.73 – 5.48 (m, 1H), 4.34 – 4.06 (m, 4H), 3.11 – 2.82 (m, 1H), 2.08 (s, 1H), 1.32 (d, *J* = 6.2 Hz, 3H), 1.21 (t, *J* = 5.8 Hz, 3H), 1.08 (dd, *J* = 42.2, 4.7 Hz, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.14, 167.10, 163.55 (d, *J* = 250.74 Hz), 155.15, 150.15, 130.00, 128.54 (d, *J* = 7.56 Hz), 115.17 (d, *J* = 21.42 Hz), 111.51 (d, *J* = 13.86 Hz), 86.66, 83.27, 63.12, 61.59, 32.37, 27.37, 17.03, 14.73, 14.41, 14.09.**^{19}F NMR** (471 MHz, $CDCl_3$) δ -110.02. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{32}FN_3O_7$ $[M+Na]^+$ 516.2116, found 516.2118.

Specific Rotation: $[\alpha]^{25}_D$ = –53.3 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.587 min for major isomer, t_R = 8.672 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(m-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3g)

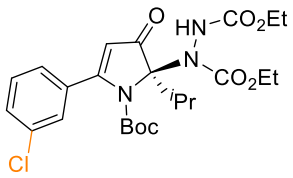


Yellow liquid, 94% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.27 (d, *J* = 7.8 Hz, 1H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.18 – 7.12 (m, 2H), 5.58 (s, 1H), 4.31 – 4.05 (m, 4H), 2.97 (p, *J* = 6.6 Hz, 1H), 2.38 (s, 3H), 2.05 (s, 1H), 1.34 – 1.28 (m, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.15 – 1.00 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.42, 168.58, 155.19, 150.33, 137.69, 133.83, 130.31, 127.97, 127.11, 123.73, 111.19, 86.53, 82.91, 63.11, 61.55, 32.42, 27.29, 21.09, 17.10, 14.73, 14.44, 14.10. **HRMS** (ESI, m/z): calcd. for $C_{25}H_{35}N_3O_7$ $[M+H]^+$ 490.2548 , found 490.2552.

Specific Rotation: $[\alpha]^{25}_D$ = –44.3 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.318 min for major isomer, t_R = 8.210 min for minor isomer).

diethyl (*R*)1-(1-(tert-butoxycarbonyl)-5-(3-chlorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3h)

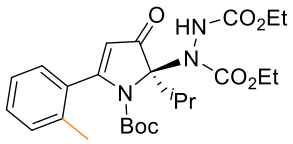


White solid, m.p. 69-72 ℃, 81% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 8.2 Hz, 1H), 7.33 (d, *J* = 5.8 Hz, 2H), 7.26 (t, *J* = 9.0 Hz, 1H), 5.61 (s, 1H), 4.37 – 4.03 (m, 4H), 2.97 (p, *J* = 6.8 Hz, 1H), 1.88 (s, 1H), 1.31 (d, *J* = 6.9 Hz, 3H), 1.22 (d, *J* = 7.1 Hz, 3H), 1.08 (d, *J* = 35.4 Hz, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.13, 166.37, 155.24, 155.17, 149.97, 135.62, 134.16, 129.51, 129.45, 126.77, 124.79, 111.84, 86.54, 83.40, 63.18, 61.63, 32.32, 27.36, 17.06, 14.69, 14.44, 14.12. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{32}ClN_3O_7$ $[M+Na]^+$ 532.1821 , found 532.1828.

Specific Rotation: $[\alpha]^{25}_D$ = –111.9 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.842 min for major isomer, t_R = 8.125 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(o-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3i)

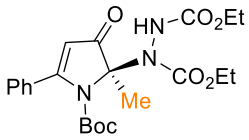


White solid, m.p. 101-103 ℃. 65% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.18 (t, *J* = 7.8 Hz, 2H), 7.10 (d, *J* = 7.5 Hz, 1H), 5.46 (s, 1H), 4.22 (ddt, *J* = 38.6, 14.0, 7.5 Hz, 4H), 3.03 (s, 1H), 2.29 (s, 3H), 1.79 (s, 1H), 1.35 – 1.28 (m, 3H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.16 – 1.01 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.09, 168.26, 155.02, 149.95, 134.34, 129.95, 128.87, 126.91, 125.20, 111.17, 85.08, 82.86, 63.09, 61.49, 31.32, 27.26, 16.83, 14.47, 14.40, 14.19, 14.11. **HRMS** (ESI, m/z): calcd. for $C_{25}H_{35}N_3O_7$ $[M+Na]^+$ 512.2367, found 512.2371.

Specific Rotation: $[\alpha]^{25}_D$ = –70.3 (*c* = 1.0, $CHCl_3$). 88% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.878 min for major isomer, t_R = 6.818 min for minor isomer).

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3j)

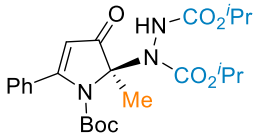


White solid, m.p. 93-95 ℃, 95% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (q, *J* = 5.9 Hz, 3H), 7.35 (d, *J* = 5.8 Hz, 2H), 5.58 (s, 1H), 4.27 (tt, *J* = 15.2, 7.8 Hz, 2H), 4.21 – 4.06 (m, 2H), 1.66 (s, 3H), 1.32 (td, *J* = 7.2, 2.9 Hz, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.10 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.76, 167.39, 154.19, 149.72, 133.64, 129.66, 127.96, 126.68, 108.58, 83.09, 81.99, 62.92, 61.75, 27.32, 20.49, 14.37, 14.14. **HRMS** (ESI, m/z): calcd. for $C_{22}H_{29}N_3O_7$ $[M+Na]^+$ 470.1898, found 470.1902.

Specific Rotation: $[\alpha]^{25}_D$ = -60.2 (*c* = 1.0, $CHCl_3$). 91% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.880 min for major isomer, t_R = 5.837 min for minor isomer).

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3k)

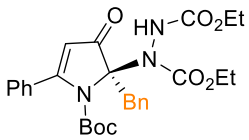


White sold, m.p. 82-84 ℃, 95% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (q, *J* = 5.9 Hz, 3H), 7.38 – 7.33 (m, 2H), 5.57 (s, 1H), 5.03 (h, *J* = 6.2 Hz, 1H), 4.90 (h, *J* = 6.2 Hz, 1H), 1.66 (s, 3H), 1.36 – 1.28 (m, 6H), 1.21 (dd, *J* = 6.4, 2.7 Hz, 6H), 1.10 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.86, 167.12, 153.65, 149.62, 133.70, 129.63, 127.95, 126.66, 108.63, 82.90, 82.04, 71.02, 69.36, 27.32, 21.84, 21.81, 21.72, 21.67, 20.67. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{33}N_3O_7$ $[M+Na]^+$ 498.2211, found 498.2213.

Specific Rotation: $[\alpha]^{25}_D$ = -52.8 (*c* = 1.0, $CHCl_3$). 80% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 7.995 min for minor isomer, t_R =10.362 min for major isomer).

diethyl (*R*)-1-(2-benzyl-1-(tert-butoxycarbonyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3l)

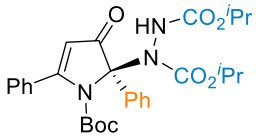


White solid, m.p. 83-85 ℃, 95% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 – 7.26 (m, 1H), 7.24 – 7.17 (m, 7H), 6.85 (d, *J* = 7.1 Hz, 2H), 5.19 (s, 1H), 4.38 – 4.23 (m, 2H), 4.17 (dqd, *J* = 10.7, 7.2, 3.6 Hz, 2H), 3.85 (d, *J* = 12.7 Hz, 1H), 3.17 (s, 1H), 1.40 – 1.29 (m, 3H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.11 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.73, 168.56, 154.25, 149.99, 133.49, 132.75, 130.85, 129.07, 127.91, 127.53, 127.40, 126.77, 111.38, 83.67, 83.00, 63.01, 61.91, 39.59, 27.40, 14.45, 14.21. **HRMS** (ESI, m/z): calcd. for $C_{28}H_{33}N_3O_7$ $[M+H]^+$ 524.2392, found 524.2388.

Specific Rotation: $[\alpha]^{25}_D$ = -63.0 (*c* = 1.0, $CHCl_3$). 85% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.875 min for major isomer, t_R = 7.067 min for minor isomer).

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-2,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3m)

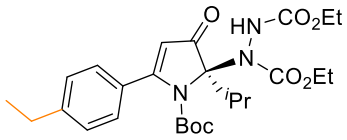


White solid, m.p. 101-103 ℃, 92% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.6 Hz, 2H), 7.45 (dt, *J* = 22.3, 3.7 Hz, 5H), 7.33 (p, *J* = 7.1, 6.7 Hz, 3H), 7.03 (s, 1H), 5.57 (s, 1H), 4.90 (dp, *J* = 51.0, 6.2 Hz, 2H), 1.41 (d, *J* = 6.3 Hz, 1H), 1.34 (d, *J* = 6.3 Hz, 1H), 1.25 (dd, *J* = 11.6, 5.8 Hz, 6H), 1.17 (d, *J* = 6.4 Hz, 2H), 1.12 (s, 9H), 1.02 (d, *J* = 6.3 Hz, 2H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 192.61, 167.60, 154.37, 150.62, 133.90, 133.00, 129.89, 129.01, 128.14, 128.09, 127.30, 127.13, 126.56, 109.69, 87.41, 83.20, 69.37, 68.72, 27.30, 21.76, 21.70. **HRMS** (ESI, m/z): calcd. for $C_{29}H_{35}N_3O_7$ $[M]^+$ 537.2475, found 537.2479.

Specific Rotation: $[\alpha]^{25}_D$ = -71.5 (*c* = 1.0, $CHCl_3$). 40% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 17.608 min for major isomer, t_R = 23.788 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-5-(4-ethylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3o)

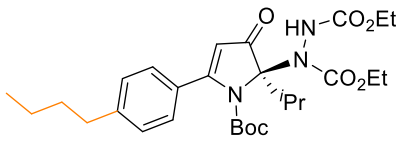


Yellow liquid, 89% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 5.59 (s, 1H), 4.32 – 4.06 (m, 4H), 2.97 (p, *J* = 6.7 Hz, 1H), 2.69 (q, *J* = 7.6 Hz, 2H), 1.95 (s, 1H), 1.31 (t, *J* = 7.1 Hz, 3H), 1.23 (dt, *J* = 16.4, 7.4 Hz, 6H), 1.14 – 1.02 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.43, 168.58, 155.21, 150.40, 146.45, 131.24, 127.47, 126.64, 111.08, 86.67, 82.92, 63.09, 61.55, 32.51, 28.69, 27.29, 17.11, 15.39, 14.78, 14.44, 14.11. **HRMS** (ESI, m/z): calcd. for $C_{26}H_{37}N_3O_7$ $[M+Na]^+$ 526.2524 , found 526.2522.

Specific Rotation: $[\alpha]^{25}_D$ = –39.1(*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R =6.093 min for major isomer, t_R = 8.385 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-5-(4-butylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3p)



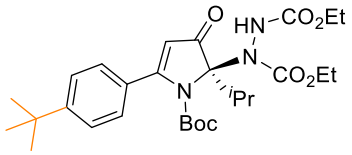
Yellow liquid, 95% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 5.58 (s, 1H), 4.16 (ddtt, *J* = 24.8, 14.1, 10.6, 7.3 Hz, 4H), 2.97 (p, *J* = 6.8 Hz, 1H), 2.65 (t, *J* = 7.7 Hz, 2H), 2.02 (s, 1H), 1.61 (p, *J* = 7.5 Hz, 2H), 1.38 (dt, *J* = 14.8, 7.4 Hz, 2H), 1.31 (q, *J* = 7.0 Hz, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.19 – 0.98 (m, 15H), 0.93 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.43, 168.60, 155.21, 150.41, 145.08, 131.19, 128.03, 126.55, 111.08, 86.68, 82.93, 63.09, 61.55, 35.38, 33.40, 32.52, 27.30, 22.08, 17.11, 14.77, 14.44, 14.10, 13.63. **HRMS** (ESI, m/z): calcd. for $C_{28}H_{41}N_3O_7$ $[M+Na]^+$ 554.2837, found 554.2832.

Specific Rotation: $[\alpha]^{25}_D$ = –35.1 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.615

min for major isomer, t_R = 7.620 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-5-(4-(tert-butyl)phenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3q)

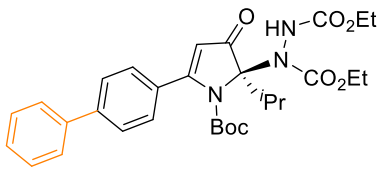


Yellow liquid, 97% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.2 Hz, 2H), 7.36 (s, 1H), 7.29 (d, *J* = 8.2 Hz, 2H), 5.59 (s, 1H), 4.32 – 4.05 (m, 4H), 2.97 (p, *J* = 6.8 Hz, 1H), 2.08 (s, 1H), 1.33 (s, 12H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.13 – 1.01 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.44, 168.54, 155.21, 153.38, 150.36, 130.98, 126.39, 124.87, 111.02, 86.63, 82.87, 63.08, 61.53, 34.74, 32.49, 31.12, 27.24, 17.11, 14.75, 14.44, 14.11. **HRMS** (ESI, m/z): calcd. for $C_{28}H_{41}N_3O_7$ $[M+Na]^+$ 554.2837, found 554.2830.

Specific Rotation: $[\alpha]^{25}_D$ = –47.1 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.837 min for major isomer, t_R = 7.988 min for minor isomer).

diethyl (*R*) 1-(5-([1,1'-biphenyl]-4-yl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3r)



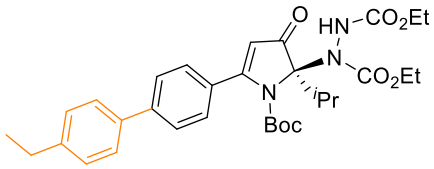
Yellow liquid, 96% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 19.5, 7.6 Hz, 4H), 7.50 – 7.40 (m, 4H), 7.36 (d, *J* = 7.4 Hz, 1H), 5.66 (s, 1H), 4.31 – 4.09 (m, 4H), 3.00 (h, *J* = 6.8 Hz, 1H), 1.86 (s, 1H), 1.31 (t, *J* = 6.8 Hz, 3H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.09 (d, *J* = 19.5 Hz, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.39, 168.04, 155.23, 150.35, 142.91, 140.19, 132.78, 128.90, 127.87, 127.10, 127.01, 126.69, 111.44, 86.72, 83.20, 63.16, 61.61, 32.54, 27.37, 17.16, 14.81, 14.47, 14.16. **HRMS** (ESI, m/z): calcd. for $C_{30}H_{37}N_3O_7$ $[M+Na]^+$ 574.2524 , found 574.2524.

Specific Rotation: $[\alpha]^{25}_D$ = –23.2 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel OD

column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R =8.958 min for major isomer, t_R = 12.823 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-5-(4'-ethyl-[1,1'-biphenyl]-4-yl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3s)

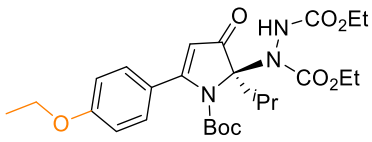


White solid, m.p. 124-126 ℃, 92% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 6.0 Hz, 2H), 7.52 (d, *J* = 6.0 Hz, 2H), 7.42 (d, *J* = 6.0 Hz, 2H), 7.37 (s, 1H), 7.31 – 7.25 (m, 2H), 5.66 (s, 1H), 4.33 – 4.07 (m, 4H), 2.99 (hept, *J* = 6.4 Hz, 1H), 2.70 (qd, *J* = 7.5, 2.2 Hz, 2H), 1.91 (s, 1H), 1.29 (dd, *J* = 13.5, 6.1 Hz, 6H), 1.22 (dt, *J* = 9.2, 4.6 Hz, 3H), 1.18 – 1.04 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.71, 168.19, 155.23, 150.38, 144.22, 142.88, 137.52, 132.45, 128.43, 127.07, 126.93, 126.49, 111.34, 86.74, 83.19, 63.16, 61.61, 32.56, 28.46, 27.37, 17.16, 15.29, 14.82, 14.47, 14.15. **HRMS** (ESI, m/z): calcd. for $C_{32}H_{41}N_3O_7$ $[M+Na]^+$ 602.2837 , found 602.2833.

Specific Rotation: $[\alpha]^{25}_D$ = –33.3 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 7.387 min for major isomer, t_R = 9.898 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-5-(4-ethoxyphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3t)



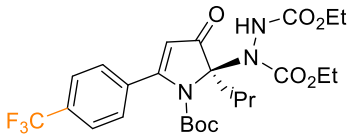
Yellow liquid, 87% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (s, 1H), 7.29 (d, *J* = 8.6 Hz, 2H), 6.90 (d, *J* = 8.6 Hz, 2H), 5.57 (s, 1H), 4.37 – 4.03 (m, 6H), 2.96 (h, *J* = 6.7 Hz, 1H), 1.87 (s, 1H), 1.42 (t, *J* = 7.0 Hz, 3H), 1.30 (t, *J* = 7.4 Hz, 3H), 1.20 (t, *J* = 7.1 Hz, 3H), 1.13 (s, 9H), 1.10 (d, *J* = 6.6 Hz, 3H), 1.03 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.31, 168.33, 160.52, 155.22, 150.55, 128.14, 125.95, 114.19, 110.72, 86.88, 82.93, 63.76, 63.08, 61.56, 32.62, 27.42, 17.13, 14.85,

14.54, 14.44, 14.10. **HRMS** (ESI, m/z): calcd. for $C_{26}H_{37}N_3O_8$ $[M+Na]^+$ 542.2473, found 542.247.

Specific Rotation: $[\alpha]^{25}_D$ = –30.5 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 8.558 min for major isomer, t_R = 10.087 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3u)

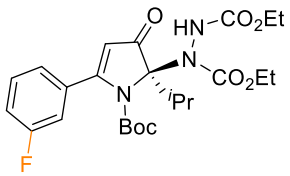


White solid, m.p. 47-49 °C, 70% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.2 Hz, 2H), 7.31 (s, 1H), 5.64 (s, 1H), 4.28 – 4.06 (m, 4H), 2.99 (hept, *J* = 6.7 Hz, 1H), 1.85 (s, 1H), 1.31 (q, *J* = 7.1, 6.0 Hz, 3H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.12 – 1.04 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.05, 166.25, 155.16, 149.86, 131.76 (q, *J* = 34.02 Hz), 127.03, 125.02 (q, *J* = 16.83 Hz), 123.71 (q, *J* = 273.42 Hz), 122.62, 112.22, 86.52, 83.58, 63.21, 61.66, 32.30, 27.27, 17.03, 14.67, 14.42, 14.12.**^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.06. **HRMS** (ESI, m/z): calcd. for $C_{25}H_{32}F_3N_3O_7$ $[M+H]^+$ 544.2192 , found 544.2199.

Specific Rotation: $[\alpha]^{25}_D$ = –38.0 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.103 min for major isomer, t_R = 7.122 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-5-(3-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3v)



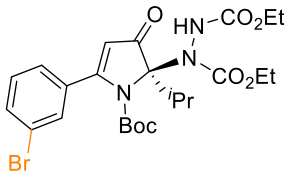
Yellow liquid, 93% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.35 (m, 1H), 7.21 (s, 1H), 7.19 – 7.09 (m, 2H), 7.06 (d, *J* = 9.0 Hz, 1H), 5.61 (s, 1H), 4.32 – 3.96 (m, 4H), 2.97 (p, *J* = 6.9 Hz, 1H), 2.02 (s, 1H), 1.31

(t, J = 7.2 Hz, 3H), 1.24 – 1.19 (m, 3H), 1.08 (d, J = 32.4 Hz, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.18, 166.79, 162.38 (d, J = 248.22 Hz), 155.16, 150.00, 135.90, 129.81 (d, J = 8.82 Hz), 122.39 (d, J = 3.78 Hz), 116.38 (d, J = 21.42 Hz), 113.83 (d, J = 23.94 Hz), 111.80, 86.56, 83.37, 63.16, 61.60, 32.35, 27.33, 17.01, 14.69, 14.42, 14.09.**^{19}F NMR** (471 MHz, $CDCl_3$) δ -112.91. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{32}FN_3O_7$ $[M+Na]^+$ 516.2116 , found 516.2116.

Specific Rotation: $[\alpha]^{25}_D$ = –40.1 (c = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.587 min for major isomer, t_R = 8.523 min for minor isomer).

diethyl (*R*) 1-(5-(3-bromophenyl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3w)

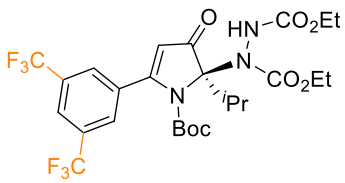


White solid, m.p. 62-64 ℃, 53% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.34 (m, 4H), 5.60 (s, 1H), 4.29 – 4.07 (m, 4H), 2.98 (p, J = 7.1 Hz, 1H), 1.70 (s, 1H), 1.32 (dd, J = 7.0, 3.5 Hz, 3H), 1.21 (t, J = 7.1 Hz, 3H), 1.13 – 1.03 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.37, 168.29, 155.18, 150.29, 134.00, 129.59, 128.02, 126.56, 111.44, 86.56, 83.03, 63.11, 61.56, 32.43, 27.29, 17.09, 14.75, 14.44, 14.12. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{32}BrN_3O_7$ $[M+Na]^+$ 576.1316 , found 576.132.

Specific Rotation: $[\alpha]^{25}_D$ = –26.5 (c = 1.0, $CHCl_3$). 98% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.903 min for major isomer, t_R = 9.100 min for minor isomer).

diethyl (*R*) 1-(5-(3,5-bis(trifluoromethyl)phenyl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3x)

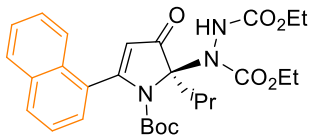


Yellow liquid, 92% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (s, 1H), 7.79 (s, 2H), 5.71 (s, 1H), 4.40 – 4.09 (m, 4H), 3.00 (p, *J* = 6.8 Hz, 1H), 1.81 (s, 1H), 1.35 – 1.30 (m, 3H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.18 – 1.05 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 192.60, 164.31, 155.10, 149.49, 132.04 (q, J = 34.02 Hz), 126.76, 122.88 (q, J = 3.78 Hz), 122.87 (q, J = 273.42 Hz), 112.96, 86.64, 83.98, 63.31, 61.73, 32.21, 27.20, 17.04, 14.62, 14.40, 14.08.**^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.15. **HRMS** (ESI, m/z): calcd. for $C_{26}H_{31}F_6N_3O_7$ $[M+Na]^+$ 634.1958 , found 634.1957.

Specific Rotation: $[\alpha]^{25}_D$ = −103.1 (*c* = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel IB-3 column, *n*-Hexane/*i*-PrOH = 97:3, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 7.627 min for major isomer, t_R = 9.477 min for minor isomer).

diethyl (*R*) 1-(1-(tert-butoxycarbonyl)-2-isopropyl-5-(naphthalen-1-yl)-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3y)

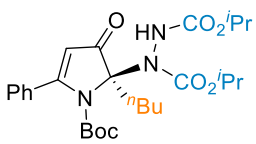


Yellow liquid, 84% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.2 Hz, 1H), 7.85 (dd, *J* = 14.2, 8.0 Hz, 2H), 7.47 (dt, *J* = 15.7, 7.3 Hz, 3H), 7.33 (d, *J* = 7.1 Hz, 1H), 5.64 (s, 1H), 4.40 – 4.19 (m, 4H), 3.06 (dt, *J* = 14.5, 7.5 Hz, 1H), 1.82 (s, 1H), 1.33 – 1.08 (m, 12H), 0.64 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.03, 167.28, 155.48, 155.08, 149.83, 133.21, 132.42, 131.12, 129.29, 127.94, 126.71, 126.28, 125.71, 124.69, 124.51, 112.04, 85.24, 82.72, 63.37, 61.57, 31.37, 26.84, 16.82, 14.51, 14.44, 14.20. **HRMS** (ESI, m/z): calcd. for $C_{28}H_{35}N_3O_7$ $[M+H]^+$ 526.2548, found 526.2552.

Specific Rotation: $[\alpha]^{25}_D$ = -60.7 (*c* = 1.0, $CHCl_3$). 94% ee (HPLC condition: Chiralcel IA column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 7.070 min for major isomer, t_R = 7.887 min for minor isomer).

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-butyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3z)

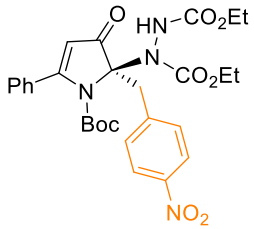


Yellow liquid, 92% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.34 (m, 5H), 5.61 (s, 1H), 5.02 (p, *J* = 6.2 Hz, 1H), 4.89 (h, *J* = 6.2 Hz, 1H), 2.46 – 2.36 (m, 1H), 1.95 (s, 1H), 1.36 – 1.26 (m, 10H), 1.21 (dd, *J* = 6.2, 2.5 Hz, 7H), 1.10 (s, 9H), 0.86 (q, *J* = 6.5 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.95, 168.21, 153.73, 149.75, 133.69, 129.56, 127.90, 126.49, 110.77, 84.07, 82.73, 77.00, 70.91, 69.22, 34.03, 27.23, 24.25, 22.54, 21.75, 21.72, 21.62, 21.59, 13.49. **HRMS** (ESI, m/z): calcd. for $C_{27}H_{39}N_3O_7$ $[M]^+$ 517.2788, found 517.2780.

Specific Rotation: $[\alpha]^{25}_D$ = -79.5 (*c* = 1.0, $CHCl_3$). 71% ee (HPLC condition: Chiralcel IB column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 9.267 min for major isomer, t_R = 13.410 min for minor isomer).

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3aa)

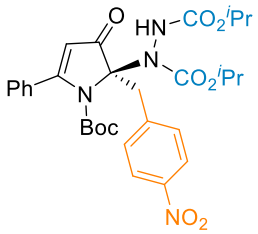


White solid, m.p. 94-96 ℃, 90% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.5 Hz, 2H), 7.31 (d, *J* = 8.3 Hz, 2H), 7.22 – 7.16 (m, 3H), 7.07 (s, 1H), 6.82 (d, *J* = 7.0 Hz, 2H), 5.15 (s, 1H), 4.23 (dt, *J* = 10.4, 6.1 Hz, 2H), 4.13 – 4.06 (m, 2H), 3.89 (d, *J* = 12.6 Hz, 1H), 3.18 (s, 1H), 1.39 – 1.06 (m, 6H), 1.04 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.10, 168.01, 153.16, 149.23, 146.78, 139.69, 132.01, 130.83, 128.77, 126.96, 125.63, 122.03, 110.21, 82.77, 82.49, 62.37, 61.22, 38.51, 26.49, 13.55, 13.30. **HRMS** (ESI, m/z): calcd. for $C_{28}H_{32}N_4O_9$ $[M+H]^+$ 569.2242, found 569.2268.

Specific Rotation: $[\alpha]^{25}_D$ = -48.5 (*c* = 1.0, $CHCl_3$). 91% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 24.872 min for minor isomer, t_R = 26.570 min for major isomer).

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3ab)

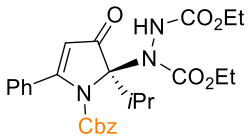


White solid, m.p. 97-99 ℃, 80% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 8.8, 2.3 Hz, 2H), 7.40 (d, *J* = 6.8 Hz, 2H), 7.31 (d, *J* = 4.8 Hz, 1H), 7.27 (t, *J* = 7.5 Hz, 2H), 6.92 (d, *J* = 8.4 Hz, 2H), 5.23 (s, 1H), 5.07 (pd, *J* = 6.3, 2.4 Hz, 1H), 4.93 (dqd, *J* = 8.8, 6.7, 3.5 Hz, 1H), 3.99 (d, *J* = 12.6 Hz, 1H), 3.26 (s, 1H), 1.36 (d, *J* = 13.8 Hz, 6H), 1.23 (dt, *J* = 6.3, 3.3 Hz, 6H), 1.13 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.15, 168.66, 153.52, 150.04, 147.62, 140.75, 132.91, 131.70, 129.65, 127.84, 126.49, 122.89, 111.11, 83.48, 83.37, 71.46, 69.82, 39.57, 27.35, 21.93, 21.84, 21.74, 21.69. **HRMS** (ESI, m/z): calcd. for $C_{30}H_{36}N_4O_9$ $[M+Na]^+$ 619.2374, found 619.2394.

Specific Rotation: $[\alpha]^{25}_D$ = -30.9 (*c* = 1.0, $CHCl_3$). 94% ee (HPLC condition: Chiralcel IA column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 15.263 min for minor isomer, t_R = 16.523 min for major isomer).

diethyl (*R*)-1-(1-((benzyloxy)carbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3ac)

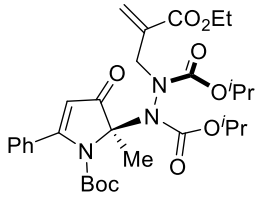


White solid, m.p. 92-94 ℃, 93% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 – 7.27 (m, 5H), 7.24 – 7.17 (m, 3H), 6.86 (d, *J* = 7.3 Hz, 2H), 5.63 (s, 1H), 4.92 (s, 2H), 4.24 (tt, *J* = 16.0, 8.6 Hz, 2H), 4.16 – 3.98 (m, 2H), 2.99 (hept, *J* = 6.8 Hz, 1H), 1.30 (d, *J* = 10.6 Hz, 3H), 1.17 – 1.08 (m, 6H), 1.03 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 192.95, 167.72, 154.96, 151.11, 134.32, 133.06, 129.81, 128.37, 128.12, 128.05, 126.64, 112.25, 86.89, 68.28, 63.19, 61.63, 32.39, 17.18, 14.82, 14.44, 14.04. **HRMS** (ESI, m/z): calcd. for $C_{27}H_{31}N_3O_7$ $[M+Na]^+$ 532.2054, found 532.2062.

Specific Rotation: $[\alpha]^{25}_D$ = -127.2 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel IB-3 column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 7.165 min for major isomer, t_R = 7.907 min for minor isomer).

Diisopropyl (*R*, *R*) -1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (5)

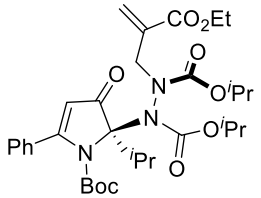


Yellow liquid, 80% yield, 1:1 dr.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.32 (m, 10H), 6.40 (s, 1H), 6.34 (s, 1H), 6.01 (s, 1H), 5.80 (s, 1H), 5.57 (s, 1H), 5.51 (s, 1H), 5.01 (p, *J* = 6.2 Hz, 1H), 4.92 (dp, *J* = 12.9, 6.4 Hz, 2H), 4.84 (q, *J* = 6.2 Hz, 1H), 4.76 (s, 1H), 4.56 (d, *J* = 17.6 Hz, 1H), 4.43 (d, *J* = 16.8 Hz, 1H), 4.32 (d, *J* = 16.9 Hz, 1H), 4.23 (dqd, *J* = 14.2, 7.1, 1.8 Hz, 4H), 1.77 (s, 3H), 1.71 (s, 3H), 1.43 – 1.27 (m, 18H), 1.20 (p, *J* = 9.0, 6.6 Hz, 12H), 1.11 (s, 9H), 1.05 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.69, 170.06, 167.51, 166.35, 166.03, 156.35, 153.89, 153.13, 149.21, 149.01, 137.38, 135.87, 134.65, 134.31, 129.50, 127.87, 127.58, 126.65, 124.72, 108.60, 108.27, 82.32, 81.56, 70.28, 60.52, 60.20, 54.42, 53.55, 27.42, 27.25, 21.90, 21.86, 21.83, 21.76, 21.70, 21.54, 14.09, 14.05. **HRMS** (ESI, m/z): calcd. for $C_{30}H_{41}N_3O_9$ $[M+Na]^+$ 610.2735, found 610.2730.

Specific Rotation: $[\alpha]^{25}_D$ = -123.5 (*c* = 1.0, $CHCl_3$). 80% , 80% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R =5.425 min for major isomer, t_R =8.065 min for minor isomer, t_R =6.025 min for minor isomer, t_R =6.810 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6a)



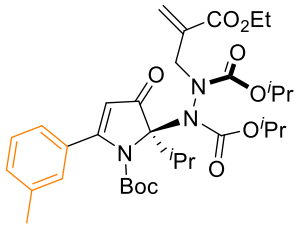
Yellow liquid, 73% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.24 (m, 5H), 6.22 (s, 1H), 5.60 (s, 1H), 5.38 (s, 1H), 4.87 (dp, *J* = 23.2, 6.5 Hz, 2H), 4.67 – 4.44 (m, 1H), 4.23 – 4.07 (m, 3H), 3.35 – 2.80 (m, 1H), 1.18 (ddd, *J* = 20.3, 14.1, 6.7 Hz, 15H), 1.08 – 0.93 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.21, 166.21, 153.40, 148.89, 137.49, 134.41, 129.33, 127.90, 126.58, 110.16, 82.27, 70.74,

60.24, 55.57, 31.41, 27.33, 21.90, 21.69, 17.68, 16.05, 14.08. **HRMS** (ESI, m/z): calcd. for $C_{32}H_{45}N_3O_9$ $[M+Na]^+$ 638.3048, found 638.3052.

Specific Rotation: $[\alpha]^{25}_D$ = -85.9 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel IA column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.058 min for major isomer, t_R = 7.042 min for minor isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(m-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6b)

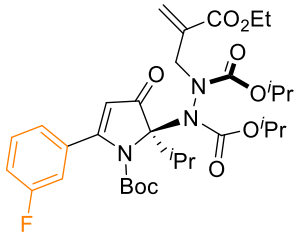


Yellow liquid, 66% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (dd, *J* = 25.0, 7.7 Hz, 2H), 7.09 – 7.01 (m, 2H), 6.22 (s, 1H), 5.60 (s, 1H), 5.37 (s, 1H), 4.87 (ddt, *J* = 16.6, 10.4, 6.2 Hz, 2H), 4.53 (d, *J* = 20.2 Hz, 1H), 4.23 – 4.05 (m, 3H), 3.15-3.06 (m, 1H), 2.28 (s, 3H), 1.19 (dt, *J* = 24.4, 7.3 Hz, 15H), 1.09 – 0.91 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.25, 166.22, 148.96, 137.50, 134.26, 130.06, 127.88, 127.15, 123.76, 109.93, 82.12, 70.87, 60.24, 55.60, 31.78, 27.34, 21.89, 21.69, 21.09, 17.68, 16.04, 14.09. **HRMS** (ESI, m/z): calcd. for $C_{33}H_{47}N_3O_9$ $[M+H]^+$ 630.3385, found 630.3392.

Specific Rotation: $[\alpha]^{25}_D$ = -79.6 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 3.632 min for minor isomer, t_R = 4.355 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(3-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6c)

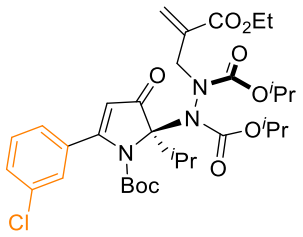


Yellow liquid, 61% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (td, *J* = 8.0, 5.6 Hz, 1H), 7.17 – 7.00 (m, 3H), 6.29 (s, 1H), 5.67 (s, 1H), 5.47 (s, 1H), 4.95 (ddq, *J* = 25.7, 12.9, 6.4 Hz, 2H), 4.62 (s, 1H), 4.40 – 4.12 (m, 3H), 3.20 (s, 1H), 1.40 – 1.20 (m, 16H), 1.12 (d, *J* = 13.5 Hz, 11H), 1.00 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.01, 166.22, 162.34 (d, *J* = 246.96), 148.67, 136.97 (d, *J* = 131.04), 129.62 (d, *J* = 7.56), 123.86, 122.41, 116.08 (d, *J* = 23.94), 113.96 (d, *J* = 24.94), 110.59, 82.60, 70.87, 60.30, 55.57, 31.16, 27.41, 21.91, 21.70, 17.57, 16.00, 14.09. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -110.02. **HRMS** (ESI, m/z): calcd. for $C_{32}H_{44}FN_3O_9$ $[M+H]^+$ 634.3135, found 634.3143.

Specific Rotation: $[\alpha]^{25}_D$ = -98.3 (*c* = 1.0, $CHCl_3$). 91% ee (HPLC condition: Chiralcel IB column, *n*-Hexane/*i*-PrOH = 95:5, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.815 min for minor isomer, t_R = 9.412 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(3-chlorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6d)

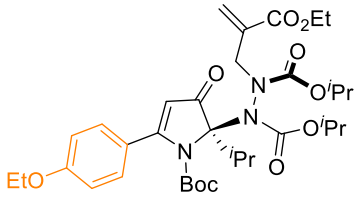


Yellow liquid, 70% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 – 7.21 (m, 3H), 7.16 (d, *J* = 7.5 Hz, 1H), 6.21 (s, 1H), 5.59 (s, 1H), 5.39 (s, 1H), 4.87 (dtd, *J* = 26.3, 12.8, 12.0, 5.7 Hz, 2H), 4.72 – 4.44 (m, 1H), 4.24 – 4.08 (m, 3H), 3.31 – 2.76 (m, 1H), 1.19 (ddd, *J* = 29.7, 13.9, 6.7 Hz, 15H), 1.05 (d, *J* = 11.6 Hz, 12H), 0.92 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.92, 166.17, 153.50, 148.60, 137.45, 136.08, 134.02, 129.31, 126.82, 124.76, 110.56, 82.63, 70.83, 60.27, 55.54, 31.19, 27.39, 21.88, 21.67, 17.61, 15.96, 14.08. **HRMS** (ESI, m/z): calcd. for $C_{32}H_{44}ClN_3O_9$ $[M+Na]^+$ 672.2658, found 672.2662.

Specific Rotation: $[\alpha]^{25}_D$ = -70.9 (*c* = 1.0, $CHCl_3$). 98% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 3.682 min for minor isomer, t_R = 4.778 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethoxyphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6e)

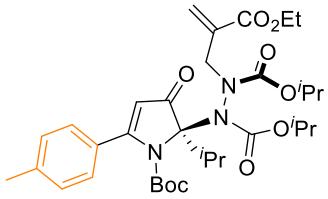


Yellow liquid, 69% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.9 Hz, 2H), 6.89 (d, *J* = 8.9 Hz, 2H), 6.29 (s, 1H), 5.67 (s, 1H), 5.42 (s, 1H), 4.94 (ddt, *J* = 24.2, 12.7, 6.3 Hz, 2H), 4.61 (dd, *J* = 25.1, 12.1 Hz, 1H), 4.29 – 4.18 (m, 3H), 4.07 (q, *J* = 7.0 Hz, 2H), 3.17-3.11 (m, 1H), 1.41 (d, *J* = 7.0 Hz, 3H), 1.31 – 1.18 (m, 18H), 1.13 (s, 9H), 1.00 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.85, 166.22, 160.32, 149.15, 137.43, 128.17, 128.11, 126.33, 125.93, 123.66, 114.08, 109.47, 82.19, 70.68, 63.69, 60.24, 55.55, 31.48, 27.46, 27.36, 21.89, 21.69, 17.63, 16.11, 14.53, 14.08. **HRMS** (ESI, m/z): calcd. for $C_{34}H_{49}N_3O_{10}$ $[M+Na]^+$ 682.331, found 682.3315.

Specific Rotation: $[\alpha]^{25}_D$ = -122.8 (*c* = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel IB-3 column, *n*-Hexane/*i*-PrOH = 80:20, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.238 min for minor isomer, t_R = 5.705 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(p-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6f)

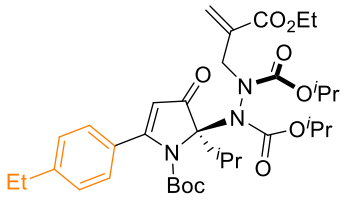


Yellow liquid, 55% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (d, *J* = 7.8 Hz, 2H), 7.17 (d, *J* = 7.9 Hz, 2H), 6.29 (s, 1H), 5.67 (s, 1H), 5.43 (s, 1H), 4.95 (dp, *J* = 17.2, 6.3 Hz, 2H), 4.62 (s, 1H), 4.34 – 3.97 (m, 3H), 3.18 (s, 1H), 2.38 (s, 3H), 1.40 – 1.18 (m, 16H), 1.11 (d, *J* = 14.6 Hz, 11H), 1.01 (d, *J* = 7.0 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.15, 166.25, 153.44, 149.04, 139.65, 137.49, 131.46, 128.51, 126.61, 123.79, 109.88, 82.25, 70.78, 60.25, 55.61, 31.46, 27.39, 21.91, 21.71, 21.17, 17.71, 16.09, 14.09. **HRMS** (ESI, m/z): calcd. for $C_{33}H_{47}N_3O_9$ $[M+Na]^+$ 652.3204, found 652.3219.

Specific Rotation: $[\alpha]^{25}_{D}$ = -103.4 (*c* = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel IB column, *n*-Hexane/*i*-PrOH = 99:1, flow rate = 0.75 mL/min, wavelength = 254 nm, t_R = 8.290 min for minor isomer, t_R = 10.952 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6g)

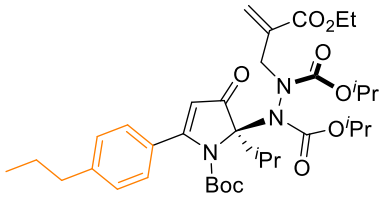


Yellow liquid, 63% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 2H), 7.20 (d, *J* = 8.1 Hz, 2H), 6.29 (s, 1H), 5.68 (s, 1H), 5.44 (s, 1H), 4.94 (ddq, *J* = 24.5, 12.4, 6.3 Hz, 2H), 4.60 (d, *J* = 18.3 Hz, 1H), 4.32 – 4.14 (m, 3H), 3.39 – 2.95 (m, 1H), 2.68 (q, *J* = 7.6 Hz, 2H), 1.34 – 1.21 (m, 18H), 1.15 – 1.00 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.29, 166.22, 165.86, 149.00, 146.13, 137.49, 131.65, 127.36, 126.67, 126.58, 125.97, 123.71, 109.82, 82.16, 70.68, 60.23, 55.57, 31.42, 27.34, 27.26, 21.90, 21.69, 17.74, 16.07, 15.38, 14.08. **HRMS** (ESI, m/z): calcd. for $C_{34}H_{49}N_3O_7$ $[M+Na]^+$ 666.3361, found 666.3366.

Specific Rotation: $[\alpha]^{25}_{D}$ = -148.6 (*c* = 1.0, $CHCl_3$). 98% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.545 min for minor isomer, t_R = 6.045 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-propylphenyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6h)



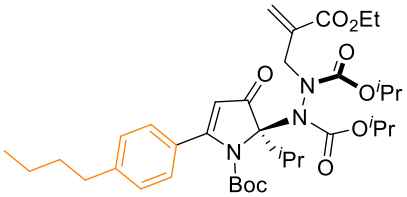
Yellow liquid, 61% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.29 – 7.23 (m, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 6.29 (s, 1H), 5.68 (s, 1H), 5.44 (s, 1H), 4.94 (dp, *J* = 23.7, 6.2 Hz, 2H), 4.63 (s, 1H), 4.43 – 4.10 (m, 3H), 3.18 (s, 1H), 2.62 (t, *J* = 7.6 Hz, 2H), 1.66 (dt, *J* = 14.9, 8.0 Hz, 3H), 1.40 – 1.19 (m, 15H), 1.17 – 0.99 (m, 14H), 0.95 (t, *J* = 7.3 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.27, 166.25, 153.39,

149.02, 144.50, 137.50, 131.67, 127.97, 126.59, 123.95, 109.88, 82.19, 70.77, 60.25, 55.58, 37.82, 31.35, 27.36, 24.30, 21.91, 21.70, 17.72, 16.08, 14.09, 13.49. **HRMS** (ESI, m/z): calcd. for $C_{35}H_{51}N_3O_9$ $[M+H]^+$ 658.3698, found 658.3705.

Specific Rotation: $[\alpha]^{25}_D$ = -159.6 (*c* = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 99:1, flow rate = 0.5 mL/min, wavelength = 254 nm, t_R = 6.245 min for minor isomer, t_R = 7.915 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-butylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6i)

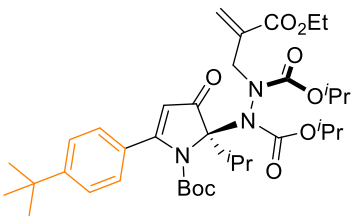


Yellow liquid, 63% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.15 (m, 4H), 6.29 (s, 1H), 5.68 (s, 1H), 5.44 (s, 1H), 4.94 (dp, *J* = 23.8, 6.3 Hz, 2H), 4.63 (s, 1H), 4.40 – 4.07 (m, 3H), 3.17 (s, 1H), 2.64 (t, *J* = 7.7 Hz, 2H), 1.74 – 1.56 (m, 3H), 1.46 – 1.19 (m, 18H), 1.15 – 1.00 (m, 13H), 0.93 (t, *J* = 7.4 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.27, 166.25, 153.34, 149.02, 144.75, 137.50, 131.63, 127.92, 126.60, 123.77, 109.84, 82.19, 70.77, 60.25, 55.59, 35.39, 33.42, 31.44, 27.35, 22.10, 21.91, 21.70, 17.72, 16.08, 14.09, 13.64. **HRMS** (ESI, m/z): calcd. for $C_{36}H_{53}N_3O_9$ $[M+H]^+$ 672.3855, found 678.3859.

Specific Rotation: $[\alpha]^{25}_D$ = -208.6 (*c* = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 99:1, flow rate = 0.5 mL/min, wavelength = 254 nm, t_R = 8.730 min for major isomer, t_R = 11.938 min for minor isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-(tert-butyl)phenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6j)

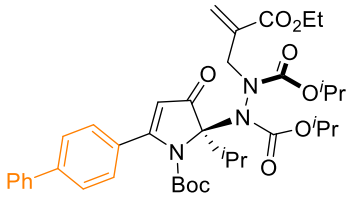


Yellow liquid, 68% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 8.3 Hz, 2H), 6.30 (s, 1H), 5.68 (s, 1H), 5.45 (s, 1H), 4.94 (ddd, *J* = 23.4, 12.6, 6.4 Hz, 2H), 4.62 (s, 1H), 4.44 – 4.03 (m, 3H), 3.18 (s, 1H), 1.41 – 1.18 (m, 25H), 1.17 – 0.97 (m, 14H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.19, 166.24, 153.05, 148.96, 137.50, 131.39, 126.42, 126.35, 124.76, 123.71, 109.76, 82.11, 70.74, 60.23, 55.55, 34.71, 31.14, 27.29, 21.91, 21.69, 17.71, 16.07, 14.08. **HRMS** (ESI, m/z): calcd. for $C_{36}H_{53}N_3O_9$ $[M+Na]^+$ 694.3674, found 694.3672.

Specific Rotation: $[\alpha]^{25}_D$ = -94.3 (*c* = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 99:1, flow rate = 0.5 mL/min, wavelength = 254 nm, t_R = 11.073 min for major isomer, t_R = 13.707 min for minor isomer).

diisopropyl (*R*, *R*)-1-(5-([1,1'-biphenyl]-4-yl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6k)

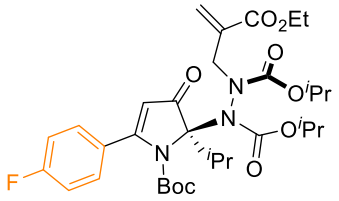


Yellow liquid, 65% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 (dd, *J* = 13.4, 7.5 Hz, 4H), 7.47 – 7.33 (m, 5H), 6.30 (s, 1H), 5.69 (s, 1H), 5.51 (s, 1H), 4.96 (ddt, *J* = 21.5, 13.2, 6.2 Hz, 2H), 4.64 (s, 1H), 4.43 – 4.10 (m, 3H), 3.21 (s, 1H), 1.29 (ddp, *J* = 28.3, 22.0, 8.7, 7.7 Hz, 15H), 1.19 – 1.00 (m, 15H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.14, 166.26, 153.40, 148.97, 142.65, 140.32, 137.53, 133.24, 128.86, 127.79, 127.14, 127.01, 126.60, 110.14, 82.47, 70.84, 60.29, 55.60, 31.38, 27.43, 21.95, 21.74, 17.72, 16.10, 14.12. **HRMS** (ESI, m/z): calcd. for $C_{38}H_{49}N_3O_9$ $[M+H]^+$ 692.3542, found 692.3549.

Specific Rotation: $[\alpha]^{25}_D$ = -126.8 (*c* = 1.0, $CHCl_3$). 93% ee (HPLC condition: Chiralcel IA column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.247 min for minor isomer, t_R = 7.067 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6l)

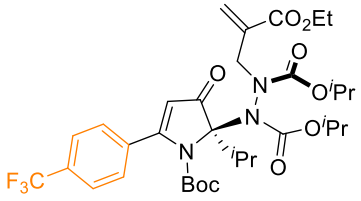


White solid, m.p. 70-72 ℃, 65% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (dd, *J* = 8.3, 5.2 Hz, 2H), 7.08 (t, *J* = 8.3 Hz, 2H), 6.29 (s, 1H), 5.67 (s, 1H), 5.44 (s, 1H), 4.94 (ddt, *J* = 24.7, 13.4, 6.5 Hz, 2H), 4.60 (d, *J* = 20.6 Hz, 1H), 4.22 (ddt, *J* = 11.7, 7.0, 4.3 Hz, 3H), 3.37 – 2.89 (m, 1H), 1.26 (ddd, *J* = 27.0, 14.3, 6.7 Hz, 15H), 1.12 (s, 12H), 1.00 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.90, 166.18, 164.41, 162.42, 153.28, 148.82, 137.47 (d, *J* = 5.04 Hz), 137.44 (d, *J* = 1.26 Hz), 128.58 (d, *J* = 8.82 Hz), 123.76, 115.02 (d, *J* = 22.68 Hz), 110.37, 82.52, 70.76, 60.26, 55.56, 31.43, 27.44, 21.89, 21.68, 17.57, 16.02, 14.07. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -112.50. **HRMS** (ESI, m/z): calcd. for $C_{32}H_{44}FN_3O_9$ $[M+Na]^+$ 656.2954, found 656.2956.

Specific Rotation: $[\alpha]^{25}_D$ = -255.1 (*c* = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.507 min for minor isomer, t_R = 6.155 min for major isomer).

diisopropyl (*R, R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6m)



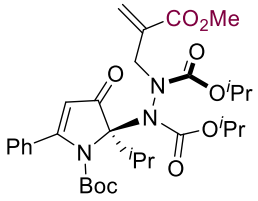
White solid, m.p. 74-76 ℃, 60% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.9 Hz, 2H), 7.48 (d, *J* = 7.9 Hz, 2H), 6.30 (s, 1H), 5.67 (s, 1H), 5.49 (s, 1H), 4.97 (dtq, *J* = 18.9, 12.9, 7.1 Hz, 2H), 4.62 (d, *J* = 20.5 Hz, 1H), 4.33 – 4.16 (m, 3H), 3.18 (dd, *J* = 27.6, 11.3 Hz, 1H), 1.34 – 1.20 (m, 15H), 1.17 – 0.98 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.80, 166.13, 157.49, 153.37, 153.33, 148.51, 137.80 (q, *J* = 83.16 Hz), 127.03, 125.96, 124.79 (q, *J* = 535.50 Hz), 124.87 (q, *J* = 2.52 Hz), 123.68, 110.90, 82.81, 70.82, 60.25, 55.53, 30.98, 27.29, 21.86, 21.64, 17.51, 15.91, 14.03. **^{19}F NMR** (471 MHz, $CDCl_3$) δ -63.05. **HRMS** (ESI, m/z): calcd. for $C_{33}H_{44}F_3N_3O_9$ $[M+Na]^+$ 706.2922, found

706.2925.

Specific Rotation: $[\alpha]^{25}_{D}$ = -258.4 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.222 min for minor isomer, t_R = 5.358 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(methoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6n)

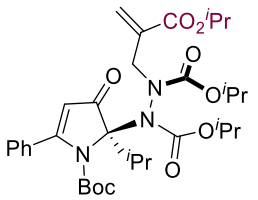


Yellow liquid, 63% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (q, *J* = 7.9 Hz, 5H), 6.28 (s, 1H), 5.69 (s, 1H), 5.43 (s, 1H), 4.94 (dh, *J* = 26.8, 7.7, 7.1 Hz, 2H), 4.71 – 4.46 (m, 1H), 4.28 (dt, *J* = 16.7, 7.3 Hz, 1H), 3.73 (s, 3H), 3.45 – 2.80 (m, 1H), 1.23 (dt, *J* = 14.7, 7.1 Hz, 15H), 1.14 – 1.00 (m, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.19, 166.69, 153.42, 148.89, 137.33, 134.40, 129.34, 127.91, 126.58, 124.25, 110.14, 82.31, 70.74, 55.39, 51.33, 31.37, 27.32, 21.88, 21.67, 17.67, 15.99. **HRMS** (ESI, m/z): calcd. for $C_{31}H_{43}N_3O_9$ $[M+Na]^+$ 624.2891, found 624.2891.

Specific Rotation: $[\alpha]^{25}_{D}$ = -78.2 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 5.047 min for minor isomer, t_R = 8.123 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(isopropoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6o)



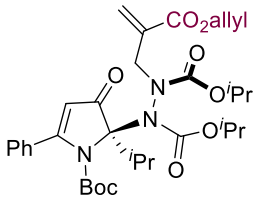
Yellow liquid, 75% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.41 – 7.33 (m, 5H), 6.28 (s, 1H), 5.65 (s, 1H), 5.46 (s, 1H), 5.08 (pd, *J* = 6.2, 2.9 Hz, 1H), 4.96 (ddt, *J* = 20.6, 14.2, 7.1 Hz, 2H), 4.73 – 4.56 (m, 1H), 4.29 (d, *J* = 18.0 Hz, 1H), 3.20-3.08 (m, 1H), 1.33 – 1.19 (m, 18H), 1.15 – 1.00 (m, 15H). **^{13}C NMR** (126 MHz, CDCl3) δ 194.14, 165.69, 158.10, 153.42, 148.88, 137.71, 134.43, 129.32, 127.90,

126.57, 123.17, 110.19, 82.23, 70.76, 67.66, 55.73, 31.31, 27.33, 21.90, 21.74, 21.69, 17.70, 16.11. **HRMS** (ESI, m/z): calcd. for $C_{33}H_{47}N_3O_9$ $[M+Na]^+$ 652.3204, found 652.3211.

Specific Rotation: $[\alpha]^{25}_D$ = -101.6 (*c* = 1.0, $CHCl_3$). 90% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 97:3, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 7.025 min for minor isomer, t_R = 10.262 min for major isomer).

diisopropyl (*R*, *R*)-1-(2-((allyloxy)carbonyl)allyl)-2-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (6p)

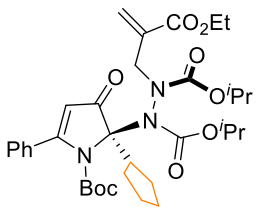


Yellow liquid, 72% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.54 – 7.31 (m, 5H), 6.33 (s, 1H), 5.95 (ddt, *J* = 16.5, 11.0, 5.6 Hz, 1H), 5.72 (s, 1H), 5.45 (s, 1H), 5.32 (d, *J* = 17.2 Hz, 1H), 5.20 (d, *J* = 10.6 Hz, 1H), 4.95 (dp, *J* = 18.1, 6.5 Hz, 2H), 4.66 (s, 3H), 4.30 (d, *J* = 17.8 Hz, 1H), 3.42 – 2.93 (m, 1H), 1.38 – 1.20 (m, 12H), 1.19 – 0.75 (m, 15H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.21, 165.82, 158.31, 153.30, 148.89, 137.28, 134.39, 132.42, 129.34, 127.90, 126.58, 124.11, 117.55, 110.17, 82.30, 70.78, 64.95, 55.54, 31.35, 27.34, 21.90, 21.69, 17.64, 16.04. **HRMS** (ESI, m/z): calcd. for $C_{33}H_{45}N_3O_9$ $[M+Na]^+$ 650.3048, found 650.3951.

Specific Rotation: $[\alpha]^{25}_D$ = -147.7 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 4.567 min for minor isomer, t_R = 6.203 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-cyclopentyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6q)



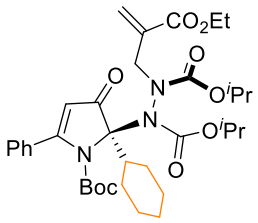
Yellow liquid, 55% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (dt, *J* = 20.0, 6.5 Hz, 5H), 6.30 (d, *J* = 5.6 Hz, 1H), 5.76

(d, J = 5.5 Hz, 1H), 5.53 (d, J = 5.7 Hz, 1H), 5.08 – 4.84 (m, 2H), 4.86 – 4.59 (m, 1H), 4.32 (dd, J = 17.4, 5.6 Hz, 1H), 4.22 (dt, J = 13.2, 6.5 Hz, 2H), 3.36 (s, 1H), 2.49 – 2.21 (m, 1H), 1.86 – 1.69 (m, 2H), 1.52 (dq, J = 22.1, 9.3, 7.4 Hz, 5H), 1.26 (dq, J = 27.6, 6.6 Hz, 13H), 1.04 (s, 9H), 0.87 (dd, J = 15.3, 7.5 Hz, 2H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.83, 168.95, 166.41, 153.33, 149.08, 137.84, 134.65, 129.32, 127.98, 126.51, 123.88, 110.75, 82.25, 70.77, 60.28, 55.34, 42.87, 29.61, 27.32, 26.19, 24.95, 23.80, 21.95, 21.71, 14.14. **HRMS** (ESI, m/z): calcd. for $C_{34}H_{47}N_3O_9$ $[M+H]^+$ 642.3385 , found 642.3391.

Specific Rotation: $[\alpha]^{25}_D$ = 97.0 (c = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.393 min for minor isomer, t_R = 6.952 min for major isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-cyclohexyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6r)

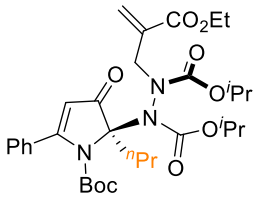


Yellow liquid, 53% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 – 7.28 (m, 5H), 6.30 (s, 1H), 5.69 (s, 1H), 5.40 (s, 1H), 4.95 (dp, J = 18.3, 6.3 Hz, 2H), 4.59 (d, J = 19.6 Hz, 1H), 4.21 (dtq, J = 11.1, 7.7, 3.9 Hz, 3H), 2.97 (s, 1H), 1.97 (d, J = 13.9 Hz, 1H), 1.83 – 1.70 (m, 3H), 1.63 (d, J = 13.1 Hz, 2H), 1.37 – 1.18 (m, 19H), 1.13 – 1.04 (m, 9H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.60, 170.80, 166.43, 157.71, 149.01, 137.47, 134.59, 129.50, 128.05, 128.01, 126.84, 126.69, 126.33, 109.95, 82.34, 70.78, 60.41, 55.69, 27.62, 27.53, 27.39, 27.10, 26.39, 26.35, 22.09, 21.96, 21.84, 14.23. **HRMS** (ESI, m/z): calcd. for $C_{35}H_{49}N_3O_9$ $[M+Na]^+$ 678.3361 , found 678.3364.

Specific Rotation: $[\alpha]^{25}_D$ = 55.5 (c = 1.0, $CHCl_3$). 95% ee (HPLC condition: Chiralcel IC column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 21.308 min for major isomer, t_R = 29.04 min for minor isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-5-phenyl-2-propyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6s)



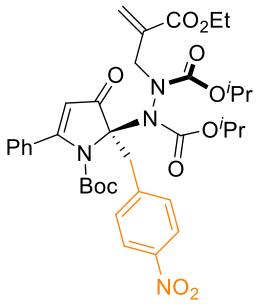
Yellow liquid, 1:2 dr, 48% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.30 (m, 5H), 6.41 (s, 1H), 6.01 (s, 1H), 5.59 (s, 1H), 4.87 (ddt, *J* = 37.9, 12.0, 6.0 Hz, 2H), 4.59 (dd, *J* = 17.8, 7.5 Hz, 1H), 4.49 – 4.32 (m, 1H), 4.24 (q, *J* = 7.0 Hz, 2H), 2.84 (q, *J* = 13.1, 12.6 Hz, 1H), 1.80 (td, *J* = 11.6, 5.7 Hz, 1H), 1.35 – 1.25 (m, 11H), 1.17 (dd, *J* = 10.7, 6.2 Hz, 6H), 1.10 (s, 9H), 0.86 (dt, *J* = 18.9, 7.3 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 195.89, 171.40, 171.40, 154.13, 149.04, 136.07, 134.97, 129.44, 127.91, 127.51, 126.79, 110.87, 84.24, 82.11, 70.38, 60.67, 55.08, 27.49, 22.55, 22.02, 21.83, 21.73, 15.58, 14.15, 13.82, 13.67.**^{1}H NMR** (500 MHz, $CDCl_3$) δ 7.37 (q, *J* = 5.8, 4.3 Hz, 5H), 6.34 (s, 1H), 5.80 (s, 1H), 5.54 (s, 1H), 5.01 (p, *J* = 6.3 Hz, 1H), 4.90 (dt, *J* = 13.8, 6.9 Hz, 1H), 4.74 (d, *J* = 16.9 Hz, 1H), 4.31 (dd, *J* = 16.9, 3.7 Hz, 1H), 4.21 (q, *J* = 7.2 Hz, 2H), 2.61 (td, *J* = 12.6, 4.4 Hz, 1H), 1.90 – 1.77 (m, 1H), 1.42 – 1.27 (m, 11H), 1.23 – 1.17 (m, 6H), 1.05 (s, 9H), 0.88 (dt, *J* = 20.9, 7.3 Hz, 3H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 195.88, 169.00, 166.42, 153.33, 149.26, 137.24, 134.51, 129.44, 127.98, 126.59, 125.09, 110.43, 84.45, 82.37, 70.56, 60.26, 53.52, 27.30, 22.60, 21.92, 21.82, 21.60, 15.72, 14.12, 14.01, 13.57.**HRMS** (ESI, m/z): calcd. for $C_{32}H_{45}N_3O_9$ $[M+H]^+$ 616.3229 , found 616.3234.

Specific Rotation: $[\alpha]^{25}_D$ = 107.6 (*c* = 1.0, $CHCl_3$). 80% ee (HPLC condition: Chiralcel IC column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 21.055 min for minor isomer, t_R = 42.46 min for major isomer). 80% ee (HPLC condition: Chiralcel IC column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 21.672 min for major isomer, t_R = 29.73 min for minor isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6t)

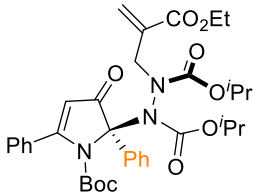


White solid, m.p. 83-85 °C, 79% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.6 Hz, 2H), 7.32 (d, *J* = 8.6 Hz, 2H), 7.27 – 7.12 (m, 3H), 6.76 (d, *J* = 7.1 Hz, 2H), 6.30 (s, 1H), 5.73 (s, 1H), 5.10 (s, 1H), 5.05 – 4.79 (m, 2H), 4.77 – 4.60 (m, 1H), 4.19 – 4.08 (m, 3H), 4.05 (d, *J* = 12.2 Hz, 1H), 3.19 (d, *J* = 11.8 Hz, 1H), 1.41 – 1.21 (m, 9H), 1.16 (dd, *J* = 9.5, 6.2 Hz, 6H), 1.00 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.74, 168.84, 166.22, 157.34, 153.07, 149.35, 147.58, 141.00, 137.46, 133.37, 131.80, 129.33, 127.82, 126.35, 124.53, 122.82, 110.47, 83.02, 70.98, 62.17, 60.37, 54.29, 27.45, 27.30, 21.99, 21.91, 21.78, 21.58, 14.09. **HRMS** (ESI, m/z): calcd. for $C_{36}H_{44}N_4O_{11}$ $[M+Na]^+$ 731.2899, found 731.2894.

Specific Rotation: $[\alpha]^{25}_D$ = 41.5 (*c* = 1.0, $CHCl_3$). 94% ee (HPLC condition: Chiralcel IA column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 8.142 min for major isomer, t_R = 13.795 min for minor isomer).

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-2,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6u)



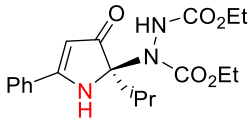
White solid, m.p. 78-80 °C, 65% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.98 (dd, *J* = 6.9, 3.0 Hz, 2H), 7.56 – 7.29 (m, 8H), 5.74 (s, 1H), 5.60 (s, 1H), 5.13 – 4.85 (m, 2H), 4.41 (d, *J* = 18.7 Hz, 2H), 4.15 (qd, *J* = 7.0, 1.6 Hz, 3H), 1.63 – 1.51 (m, 2H), 1.46 – 1.38 (m, 2H), 1.33 – 1.17 (m, 11H), 1.08 (s, 9H).**^{13}C NMR** (126 MHz, $CDCl_3$) δ 194.91, 167.94, 166.21, 157.08, 153.46, 149.76, 135.49, 134.31, 132.53, 129.82, 129.36, 128.98, 128.13, 127.87, 126.25, 123.87, 109.20, 88.14, 82.32, 70.94, 59.89, 53.04, 27.16, 21.89, 21.79, 21.61, 13.99. **HRMS** (ESI, m/z): calcd. for $C_{35}H_{43}N_3O_9$ $[M+H]^+$ 650.3072 ,

found 650.3077.

Specific Rotation: $[\alpha]^{25}_{D}$ = 103.3 (*c* = 1.0, $CHCl_3$). 40% ee (HPLC condition: Chiralcel IC column, *n*-Hexane/*i*-PrOH = 99:1, flow rate = 0.25 mL/min, wavelength = 254 nm, t_R = 17.608 min for major isomer, t_R = 23.788 min for minor isomer).

diethyl (*R*)-1-(2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (9)

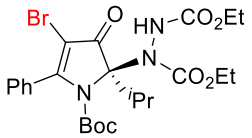


Yellow solid, m.p. 83-85 ℃, 60% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.6 Hz, 2H), 7.51 – 7.45 (m, 3H), 7.34 (s, 1H), 6.71 (s, 1H), 5.53 (s, 1H), 4.27 – 4.08 (m, 4H), 2.41 (dt, *J* = 13.3, 7.2 Hz, 1H), 1.31 (t, *J* = 7.1 Hz, 3H), 1.17 – 1.01 (m, 9H). **^{13}C NMR** (126 MHz, CDCl3) δ 198.18, 172.82, 155.39, 131.69, 130.41, 128.87, 126.37, 97.24, 83.13, 62.88, 62.43, 33.70, 16.76, 14.34, 14.20, 13.97. **HRMS** (ESI, m/z): calcd. for $C_{19}H_{25}N_3O_5$ $[M+Na]^+$ 398.1686, found 398.1690.

Specific Rotation: $[\alpha]^{25}_{D}$ = -191.2 (*c* = 1.0, $CHCl_3$). 98% ee (HPLC condition: Chiralcel OD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 6.915 min for major isomer, t_R = 8.052 min for minor isomer).

diethyl (*R*)-1-(4-bromo-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (10)



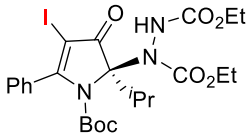
White solid, m.p. 70-72 ℃, 91% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 – 7.39 (m, 3H), 7.36 (dt, *J* = 7.0, 3.7 Hz, 2H), 4.47 – 4.00 (m, 4H), 3.00 (h, *J* = 6.8 Hz, 1H), 1.31 (d, *J* = 7.1 Hz, 3H), 1.20 (d, *J* = 7.1 Hz, 3H), 1.12 (d, *J* = 6.4 Hz, 3H), 1.11 – 0.86 (m, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 188.10, 163.80, 155.02, 149.74, 132.68, 129.73, 128.09, 127.42, 85.24, 83.60, 63.37, 61.65, 32.27, 27.23, 16.91, 14.53, 14.14. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{32}BrN_3O_7$ $[M+Na]^+$ 576.1316, found 576.1318.

Specific Rotation: $[\alpha]^{25}_{D}$ = -182.4 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel AD

column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 8.790 min for minor isomer, t_R = 13.622 min for major isomer).

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-4-iodo-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (11)

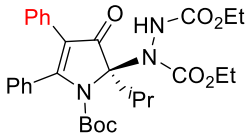


White solid, m.p. 123-125 ℃, 88% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49 – 7.40 (m, 3H), 7.32 (dt, *J* = 6.2, 3.2 Hz, 2H), 4.35 – 4.10 (m, 4H), 3.06 – 2.76 (m, *J* = 6.6 Hz, 1H), 1.30 (t, *J* = 7.3 Hz, 3H), 1.22 (t, *J* = 7.1 Hz, 3H), 1.11 (d, *J* = 6.5 Hz, 3H), 1.03 (s, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 189.94, 167.67, 154.97, 149.54, 134.45, 129.62, 128.12, 127.44, 84.86, 83.60, 63.33, 61.62, 32.16, 27.24, 16.97, 14.53, 14.47, 14.27. **HRMS** (ESI, m/z): calcd. for $C_{24}H_{32}IN_3O_7$ $[M+Na]^+$ 624.1177, found 624.1182.

Specific Rotation: $[\alpha]^{25}_D$ = -173.3 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 12.172 min for minor isomer, t_R = 16.498 min for major isomer).

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-4,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (12)



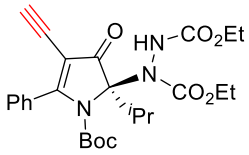
White solid, m.p. 68-70 ℃, 80% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.33 – 7.25 (m, 3H), 7.21 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.19 – 7.08 (m, 3H), 7.06 (dd, *J* = 7.9, 1.9 Hz, 2H), 4.31 – 4.12 (m, 4H), 3.07 (p, *J* = 6.7 Hz, 1H), 1.33 – 1.28 (m, 3H), 1.23 (t, *J* = 7.1 Hz, 3H), 1.13 (d, *J* = 6.9 Hz, 6H), 1.03 (s, 9H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 192.47, 162.04, 156.34, 155.18, 150.56, 129.91, 129.43, 128.95, 128.00, 127.87, 127.72, 126.88, 85.28, 82.89, 63.11, 61.53, 31.46, 27.30, 22.50, 17.37, 14.64, 14.28. **HRMS** (ESI, m/z): calcd. for $C_{30}H_{37}N_3O_7$ $[M+Na]^+$ 574.2524, found 574.2527.

Specific Rotation: $[\alpha]^{25}_D$ = -267.3 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 10.018

min for minor isomer, t_R = 11.532 min for major isomer).

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-4-ethynyl-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (13)

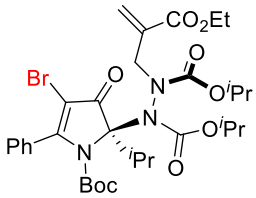


Yellow solid, m.p. 88-90 ℃, 75% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 – 7.38 (m, 5H), 4.28 – 4.13 (m, 4H), 3.09 (s, 1H), 2.99 (p, *J* = 6.8 Hz, 1H), 1.52 (s, 1H), 1.33 – 1.29 (m, 3H), 1.21 (t, *J* = 7.1 Hz, 3H), 1.12 (d, *J* = 6.7 Hz, 3H), 1.09 – 1.00 (m, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 190.85, 168.51, 154.95, 149.85, 129.96, 128.97, 127.91, 127.28, 106.41, 86.01, 84.35, 83.75, 83.47, 63.38, 61.66, 32.56, 27.21, 16.99, 14.61, 14.44, 14.07. **HRMS** (ESI, m/z): calcd. for $C_{26}H_{33}N_3O_7$ $[M+Na]^+$ 522.2211, found 522.2217.

Specific Rotation: $[\alpha]^{25}_D$ = -44.2 (*c* = 1.0, $CHCl_3$). 96% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 12.568 min for minor isomer, t_R = 16.138 min for major isomer).

diisopropyl (*R*)-1-(4-bromo-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (14)



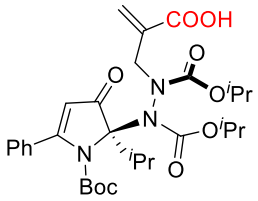
White solid, m.p. 64-66 ℃, 88% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (d, *J* = 5.2 Hz, 3H), 7.39 – 7.31 (m, 2H), 6.30 (s, 1H), 5.67 (s, 1H), 4.97 (dq, *J* = 19.8, 6.1 Hz, 2H), 4.78 – 4.50 (m, 1H), 4.29 – 4.15 (m, 3H), 3.43 – 2.98 (m, 1H), 1.39 – 1.21 (m, 15H), 1.14 (d, *J* = 6.6 Hz, 3H), 1.00 (d, *J* = 16.9 Hz, 12H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 189.16, 166.15, 153.16, 148.45, 137.67, 133.15, 129.50, 127.99, 127.41, 123.61, 82.77, 71.00, 60.24, 55.67, 31.09, 27.23, 21.88, 21.76, 17.63, 15.88, 14.09. **HRMS** (ESI, m/z): calcd. for $C_{32}H_{44}BrN_3O_9$ $[M+H]^+$ 694.2334, found 694.2338.

Specific Rotation: $[\alpha]^{25}_D$ = -394.4 (*c* = 1.0, $CHCl_3$). 97% ee (HPLC condition: Chiralcel IB-3

column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 3.858 min for major isomer, t_R = 4.705 min for minor isomer).

(*R*, *R*)-2-((2-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-1,2-bis(isopropoxycarbonyl)hydrazineyl)methyl)acrylic acid (15)



White solid, m.p. 73-75 ℃, 84% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.72 (s, 1H), 7.36 – 7.23 (m, 5H), 6.34 (s, 1H), 5.76 (s, 1H), 5.39 (s, 1H), 4.87 (ddq, *J* = 30.4, 13.1, 6.7 Hz, 2H), 4.61 (s, 1H), 4.22 (d, *J* = 17.2 Hz, 1H), 3.17-3.08 (m, 1H), 1.17 (td, *J* = 15.0, 13.6, 6.8 Hz, 12H), 1.10 – 0.90 (m, 15H). **^{13}C NMR** (126 MHz, CDCl3) δ 194.39, 170.88, 153.45, 148.91, 137.00, 134.39, 129.37, 127.91, 126.61, 110.24, 82.53, 70.94, 54.86, 31.32, 27.34, 21.88, 21.65, 17.67, 16.01. **HRMS** (ESI, m/z): calcd. for $C_{30}H_{41}N_3O_9$ $[M+Na]^+$ 610.2735, found 610.273.

Specific Rotation: $[\alpha]^{25}_D$ = -123.5 (*c* = 1.0, $CHCl_3$). 99% ee (HPLC condition: Chiralcel AD column, *n*-Hexane/*i*-PrOH = 90:10, flow rate = 1.0 mL/min, wavelength = 254 nm, t_R = 11.763 min for minor isomer, t_R = 21.272 min for major isomer).

10. X-ray Crystallographic

Data X-ray Crystallographic Data of Compound 3b

Bond precision:	C-C = 0.0074 A	Wavelength=1.34139	
Cell:	a=10.4813(16) alpha=97.915(6)	b=10.5048(16) beta=92.615(6)	c=13.991(2) gamma=118.101(6)
Temperature:	298 K		

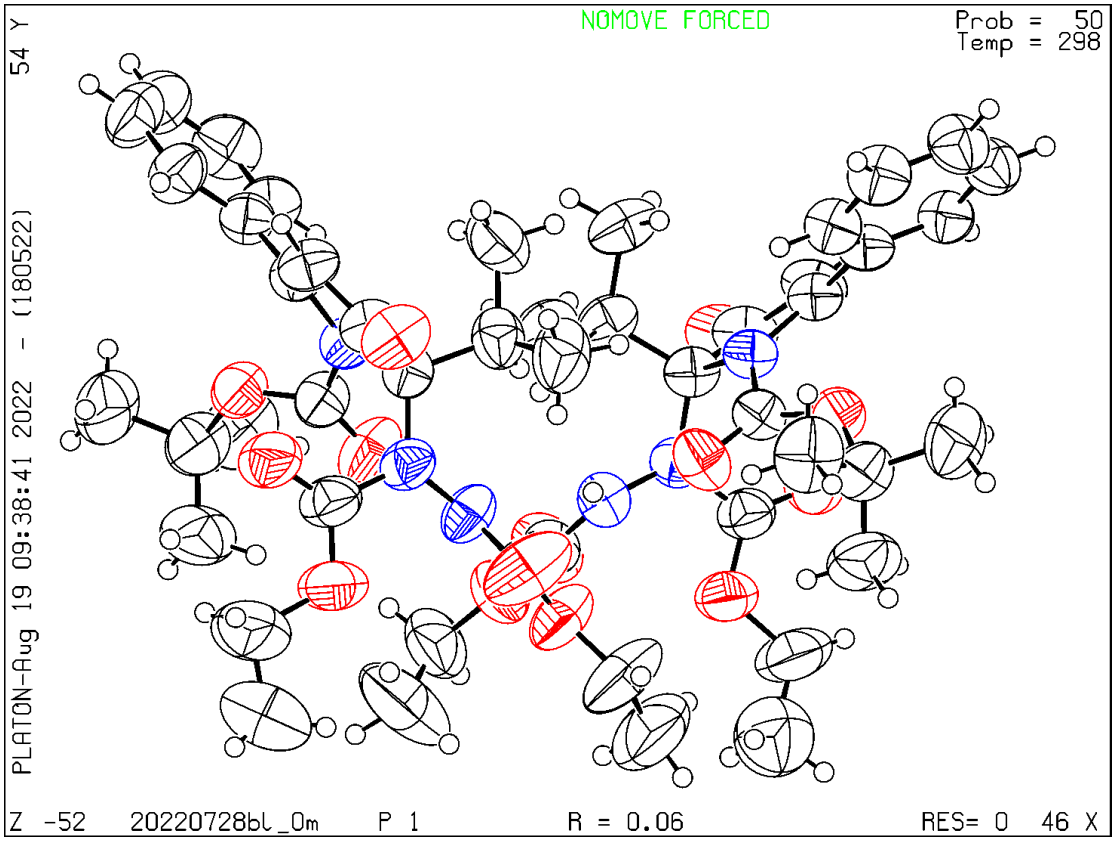
	Calculated		Reported
Volume Space group Hall group	1335.1(4) P 1		1335.2(4) P 1
Moiety formula	P 1 C24 H32 N3	O7	P 1 0.074(C24 H32 N3 O7)
Sum formula	C24 H32 N3	O7	C1.78 H2.37 N0.22 O0.52
Mr	474.53		35.15
Dx,g cm-3	1.180		1.180
Z	2		27
Mu (mm-1)	0.460		0.460
F000	506.0		506.0
F000’	507.26		
h,k,lmax	14,14,18		14,14,18
Nref	13830[6915]		12815
Tmin,Tmax			0.659,0.753
Tmin’			

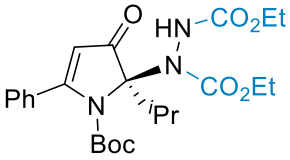
Correction method= # Reported T Limits: Tmin=0.659 Tmax=0.753 AbsCorr = NONE

Data completeness= 1.85/0.93 Theta(max)= 65.108

R(reflections)=0.0555(8481) wR2(reflections)= 0.1707(12815)

S = 1.009 Npar= 623





CCDC: 2202374

Data X-ray Crystallographic Data of Compound 6t

Bond precision:	C-C = 0.0029 A	Wavelength=1.54184	
Cell:	a=15.78147(11)	b=14.09396(13)	c=16.78114(12)
	alpha=90	beta=98.9652(7)	gamma=90
Temperature:	301 K		

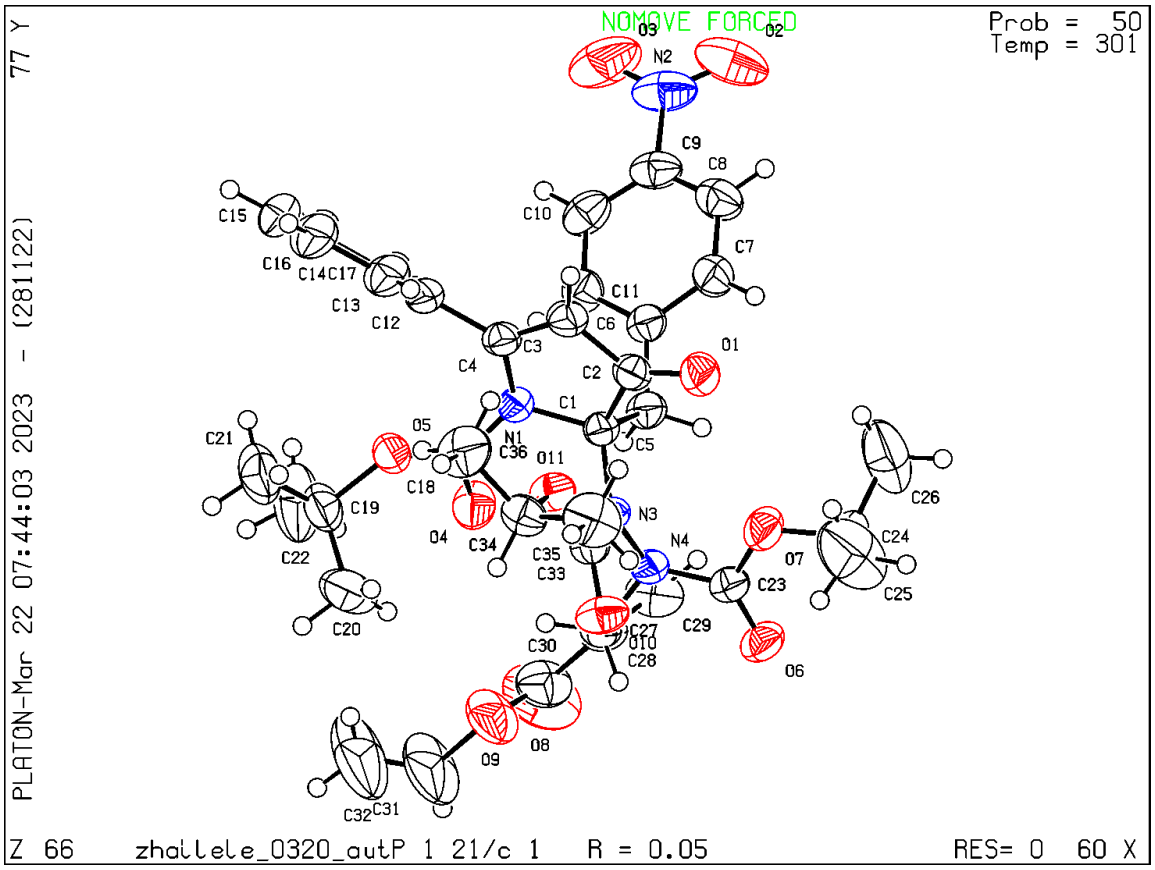
	Calculated		Reported
Volume Space group Hall group	3686.92(5) P 21/c -P 2ybc		3686.92(5) P 1 21/c 1 -P 2ybc
Moiety formula	C36 H42 N4	O11	C36 H42 N4 O11
Sum formula	C36 H42 N4	O11	C36 H42 N4 O11
Mr	706.74		706.73
Dx,g cm-3	1.273		1.273
Z	4		4
Mu (mm-1)	0.792		0.792
F000	1496.0		1496.0
F000’	1501.04		
h,k,lmax	19,17,21		19,17,20
Nref	7736		7355
Tmin,Tmax	0.945,0.969		0.697,1.000
Tmin’	0.939		

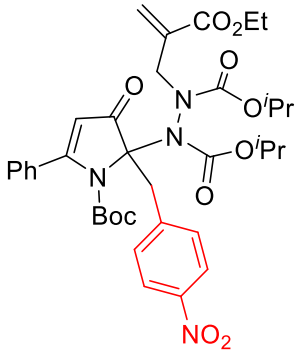
Correction method= # Reported T Limits: Tmin=0.697 Tmax=1.000 AbsCorr = MULTI-SCAN

Data completeness= 0.951 Theta(max)= 76.415

R(reflections)= 0.0489(6676) wR2(reflections)= 0.1379(7355)

S = 1.059 Npar= 476

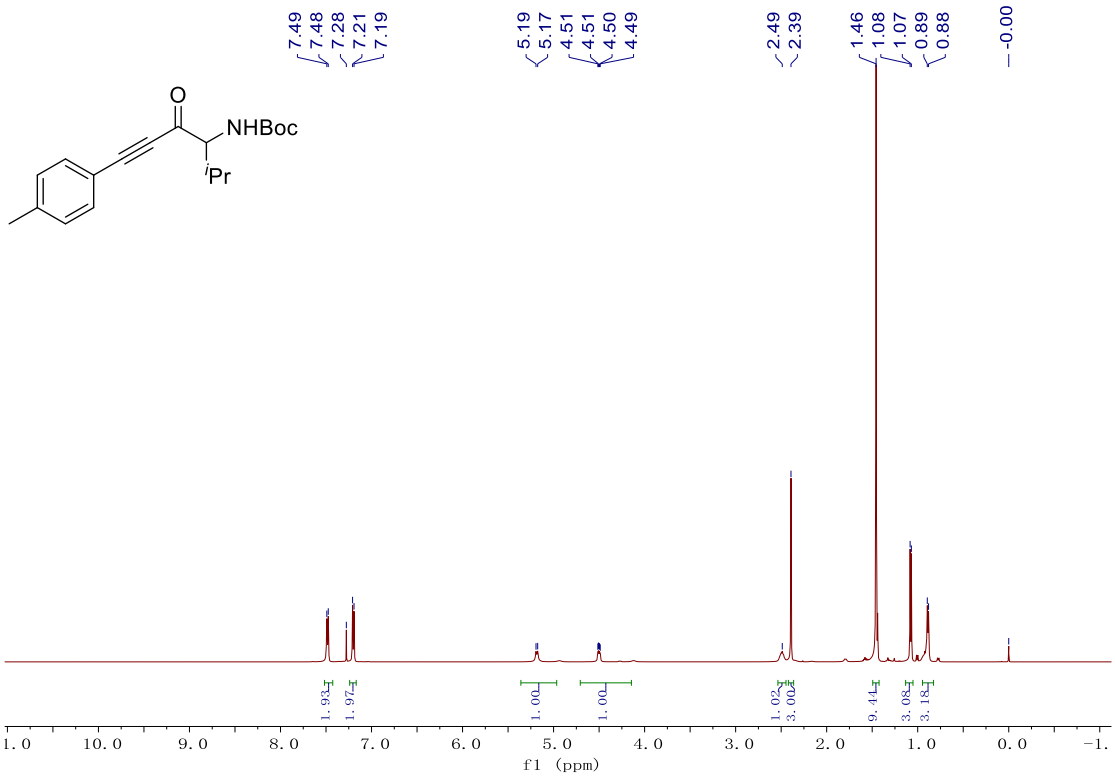


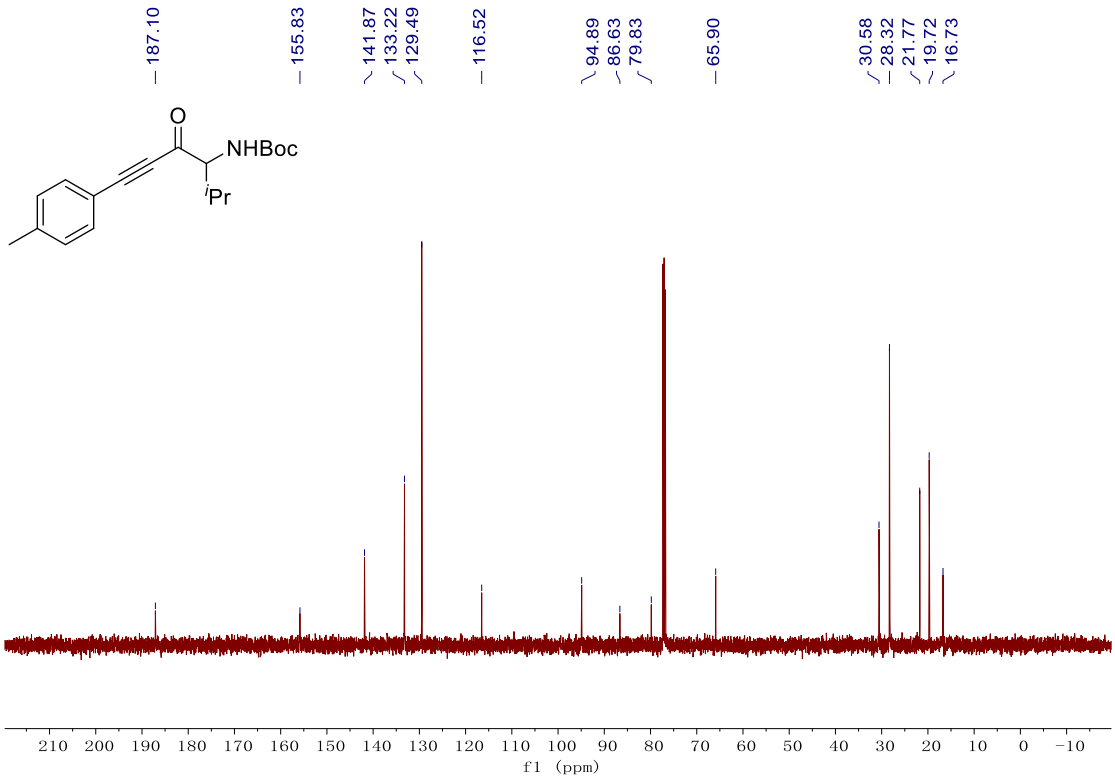


CCDC: 2250756

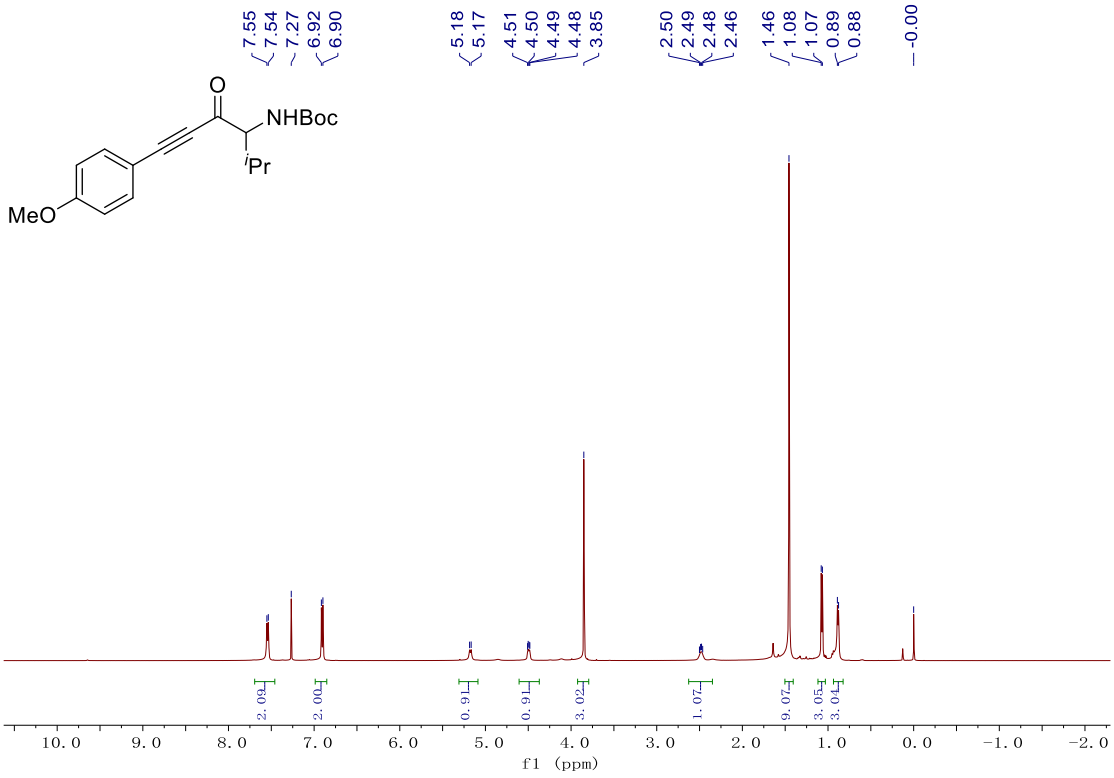
11. ^{1}H NMR, ^{13}C NMR, ^{19}F NMR and HPLC spectra.

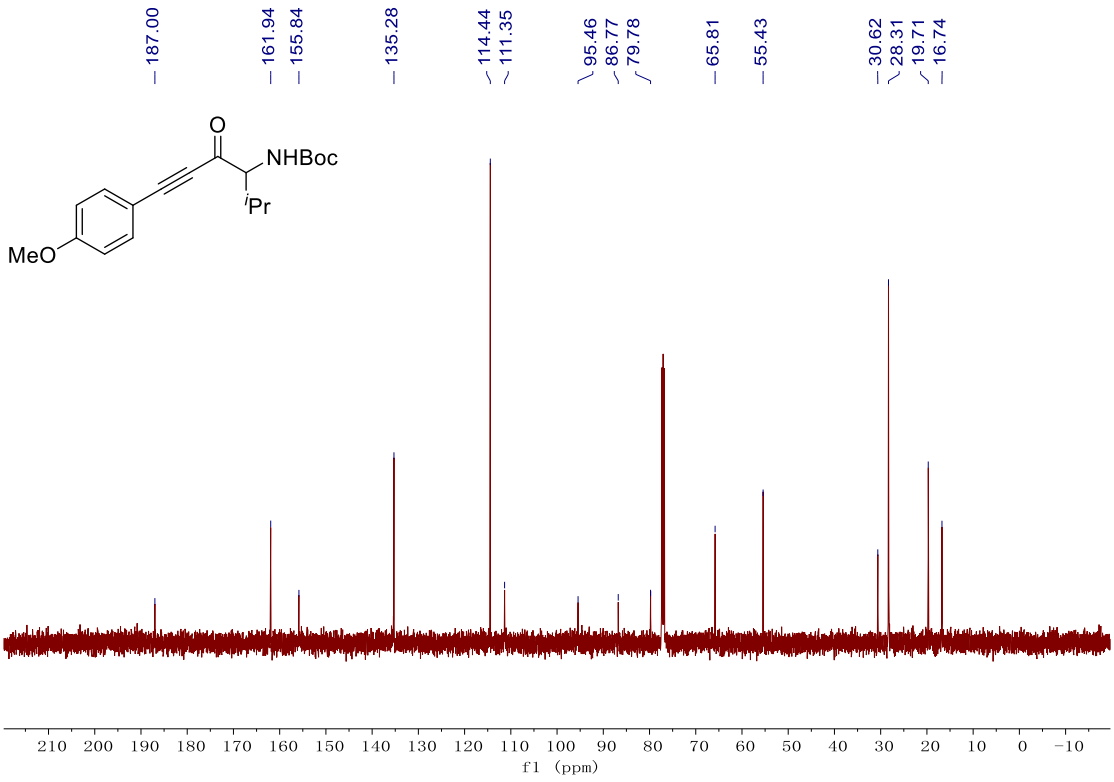
***tert*-butyl (2-methyl-4-oxo-6-(p-tolyl)hex-5-yn-3-yl)carbamate (1d)**



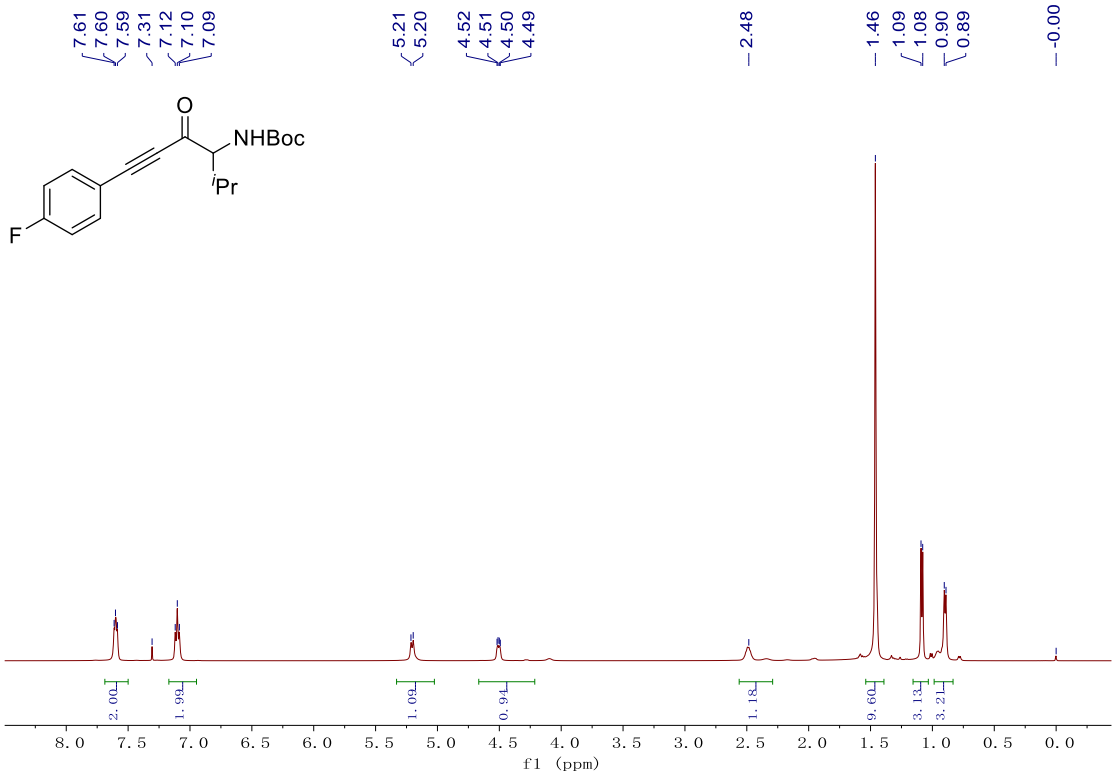


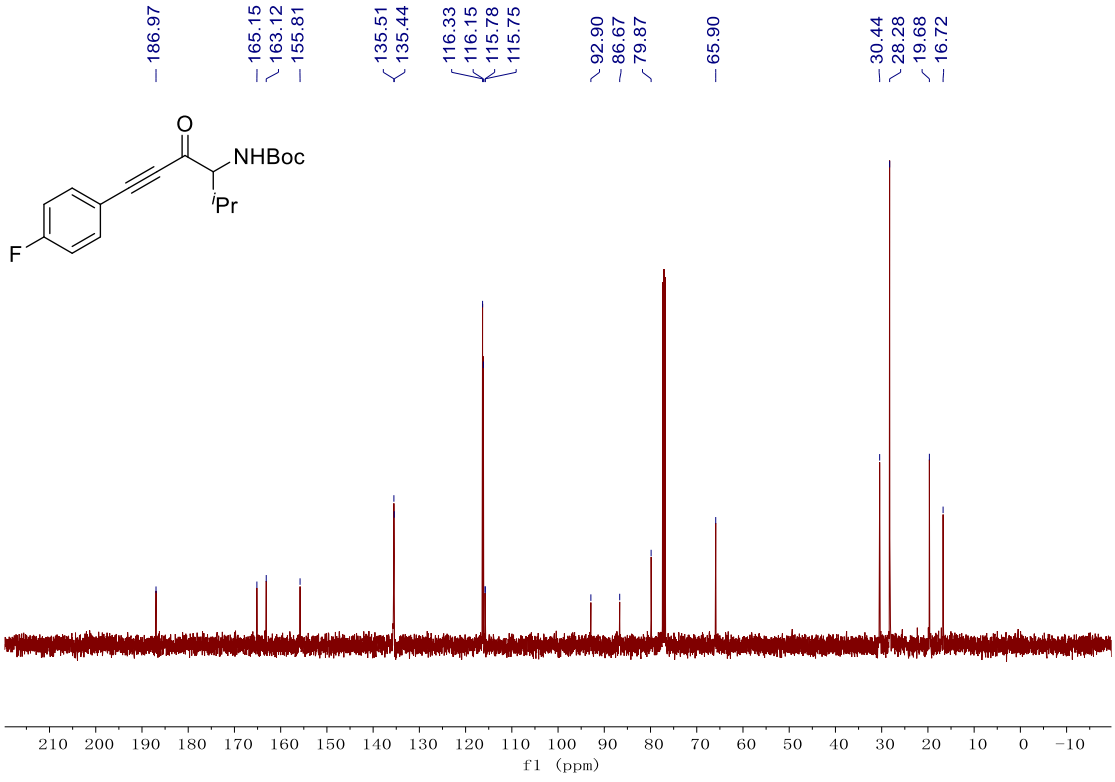
tert-butyl (6-(4-methoxyphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1e)

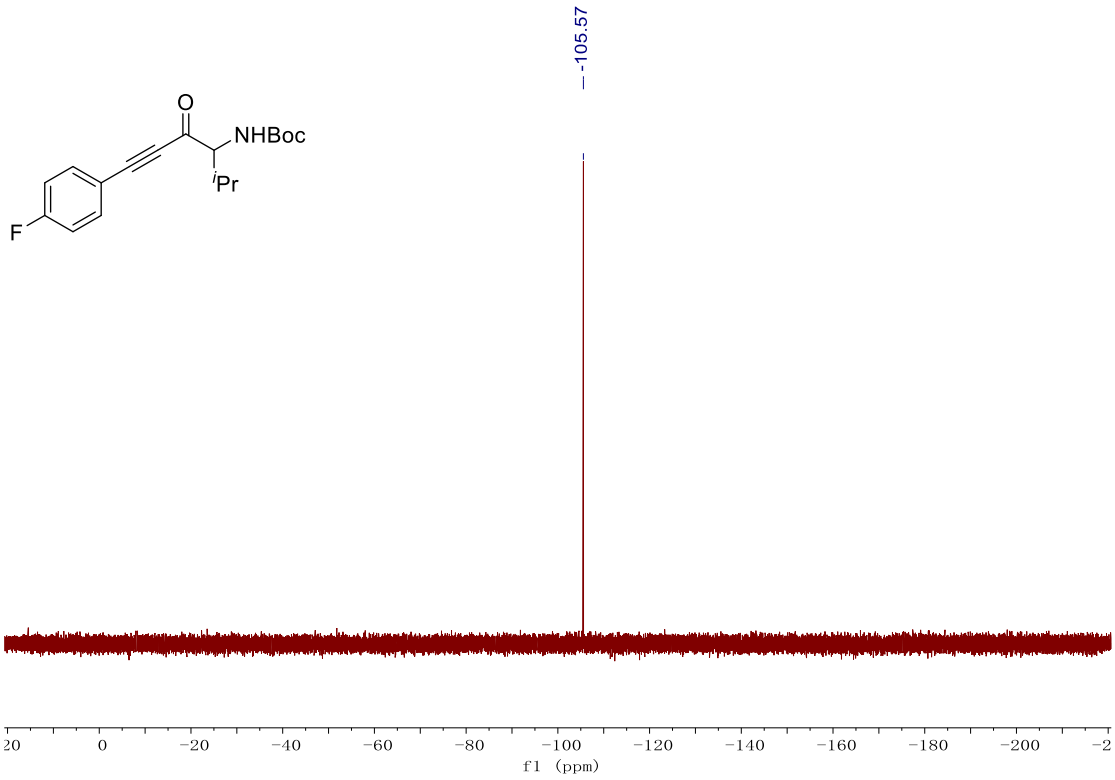




tert-butyl (6-(4-fluorophenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1f)



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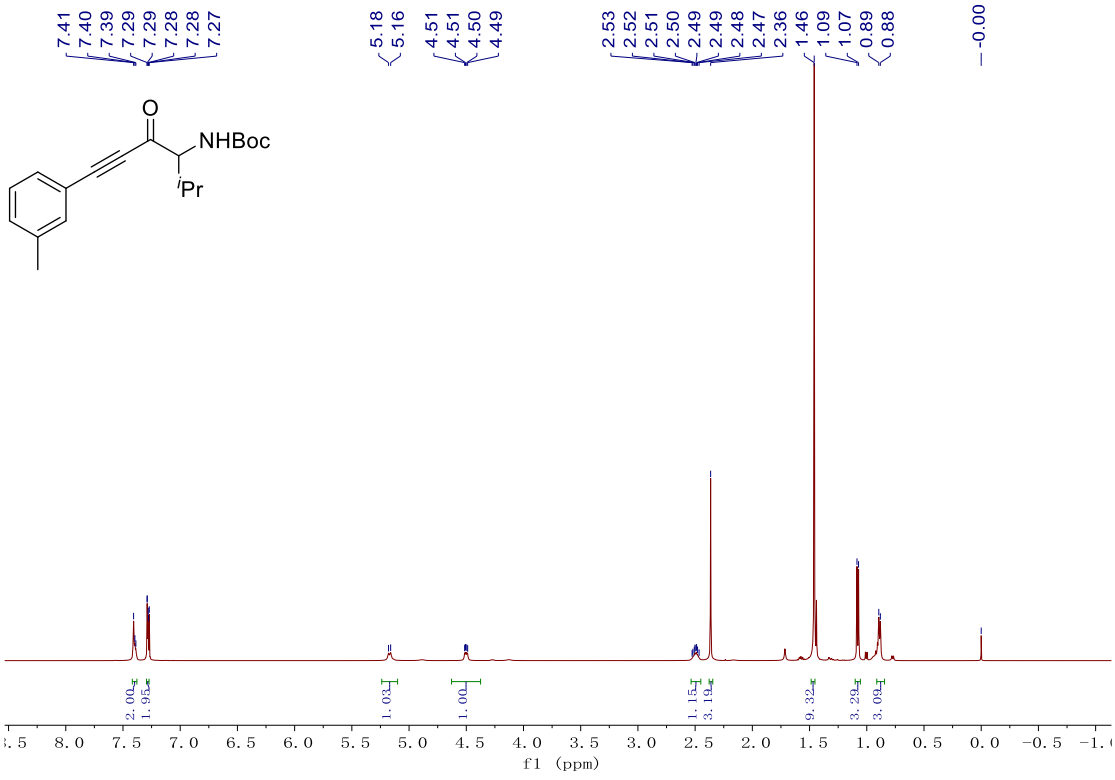
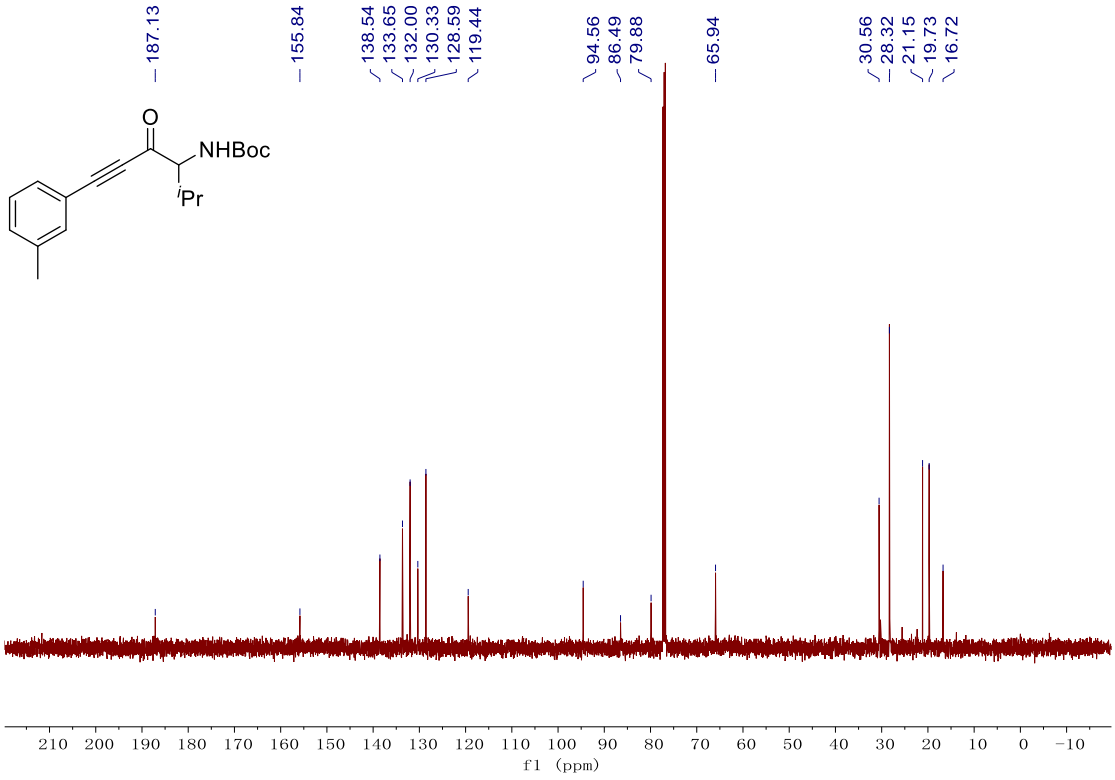
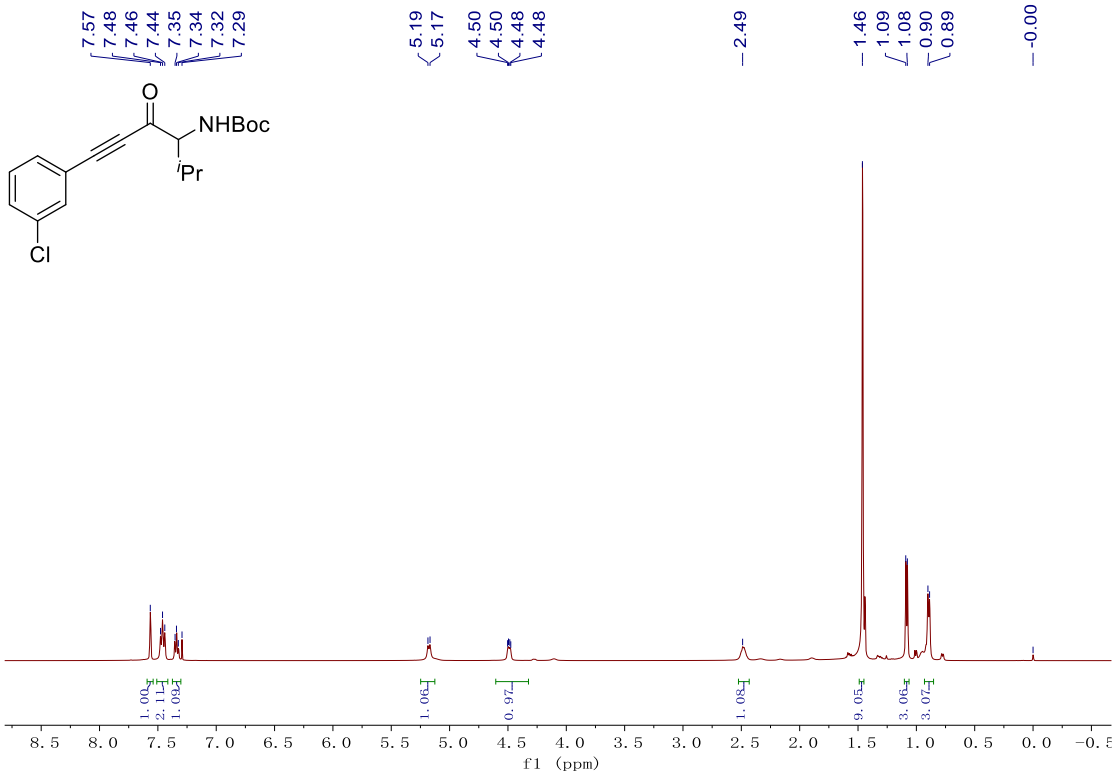
NHBoc
iPr
F
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

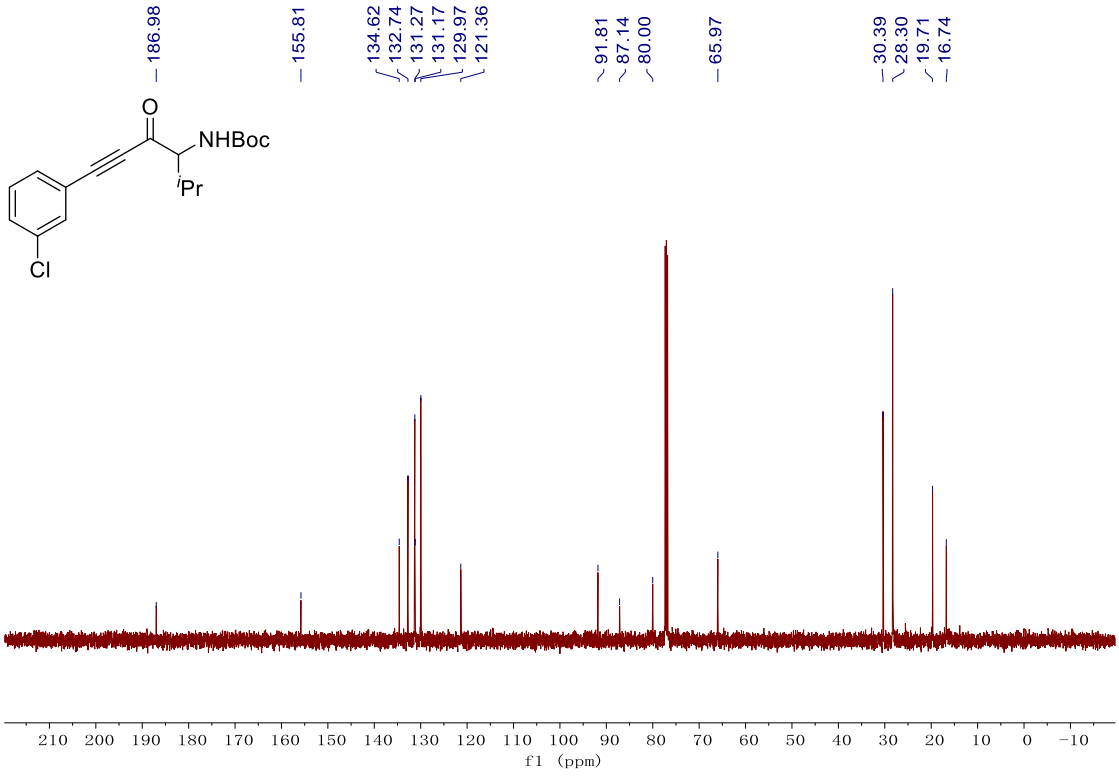
tert-butyl (2-methyl-4-oxo-6-(m-tolyl)hex-5-yn-3-yl)carbamate (1g)



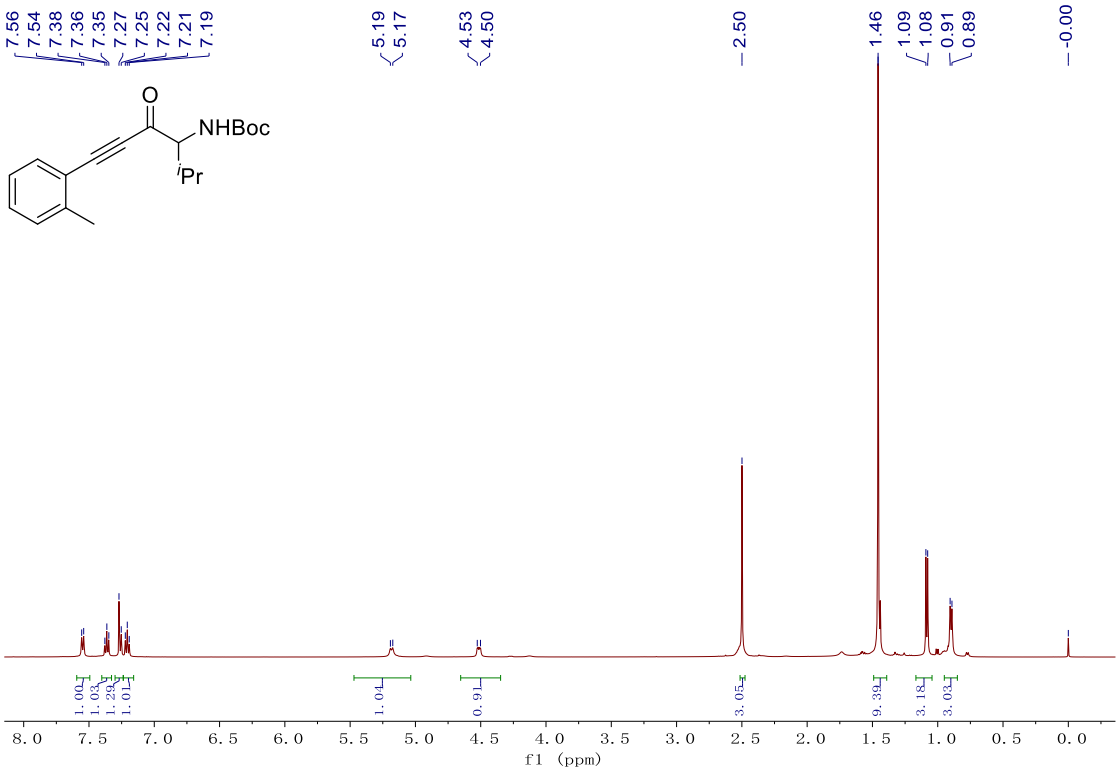


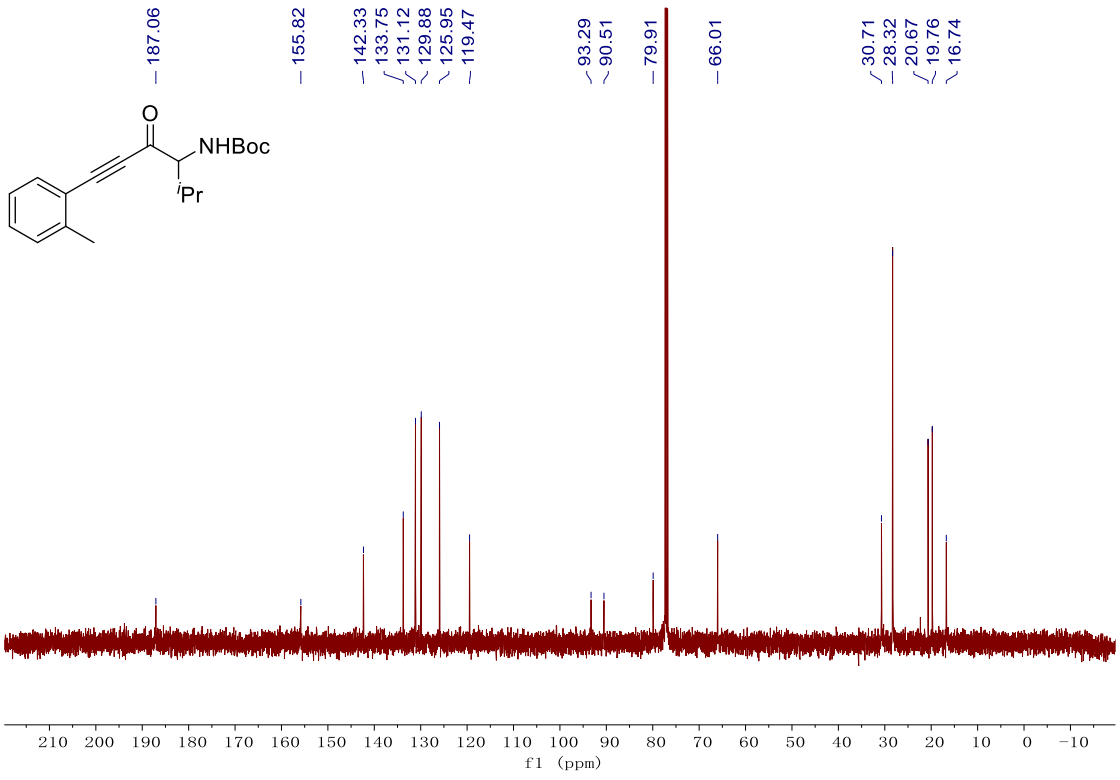
tert-butyl (6-(3-chlorophenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1h)



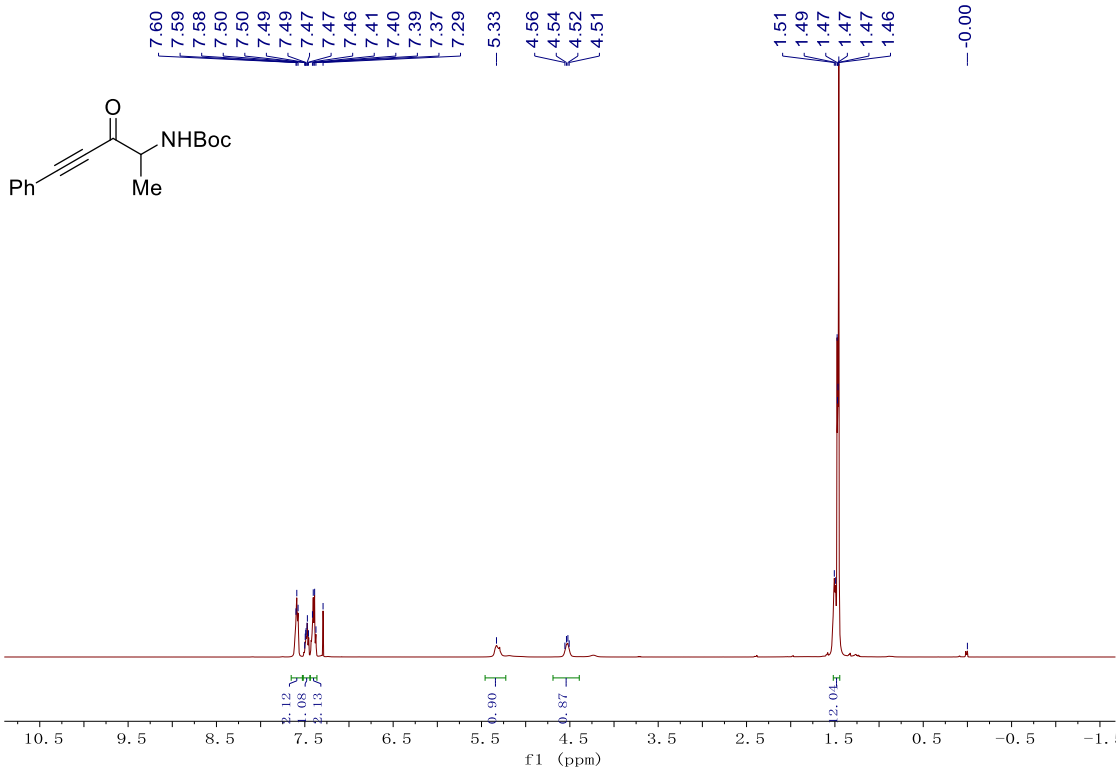


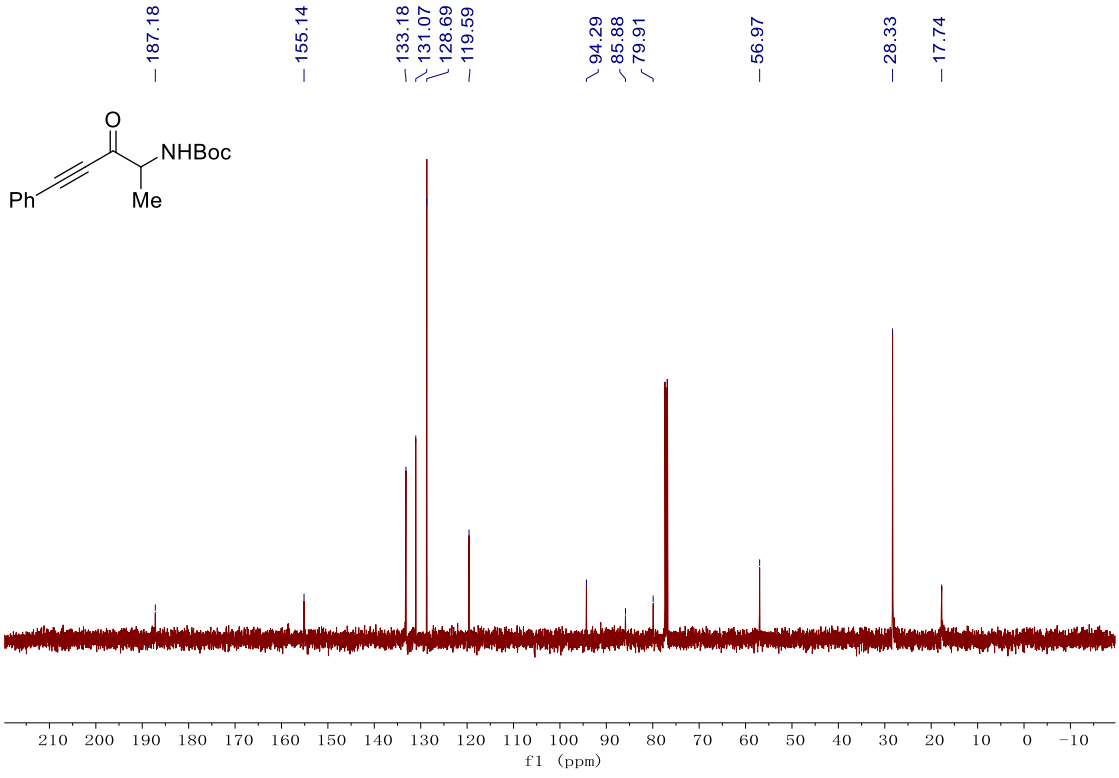
tert-butyl (2-methyl-4-oxo-6-(o-tolyl)hex-5-yn-3-yl)carbamate (1i)



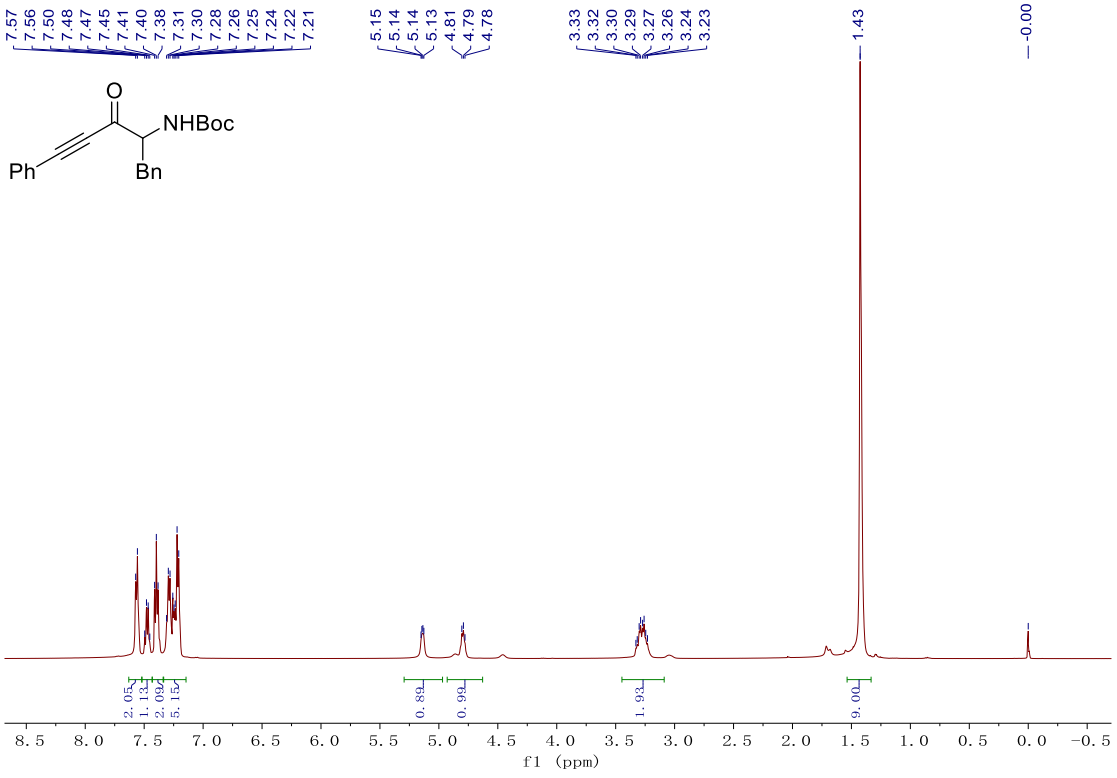


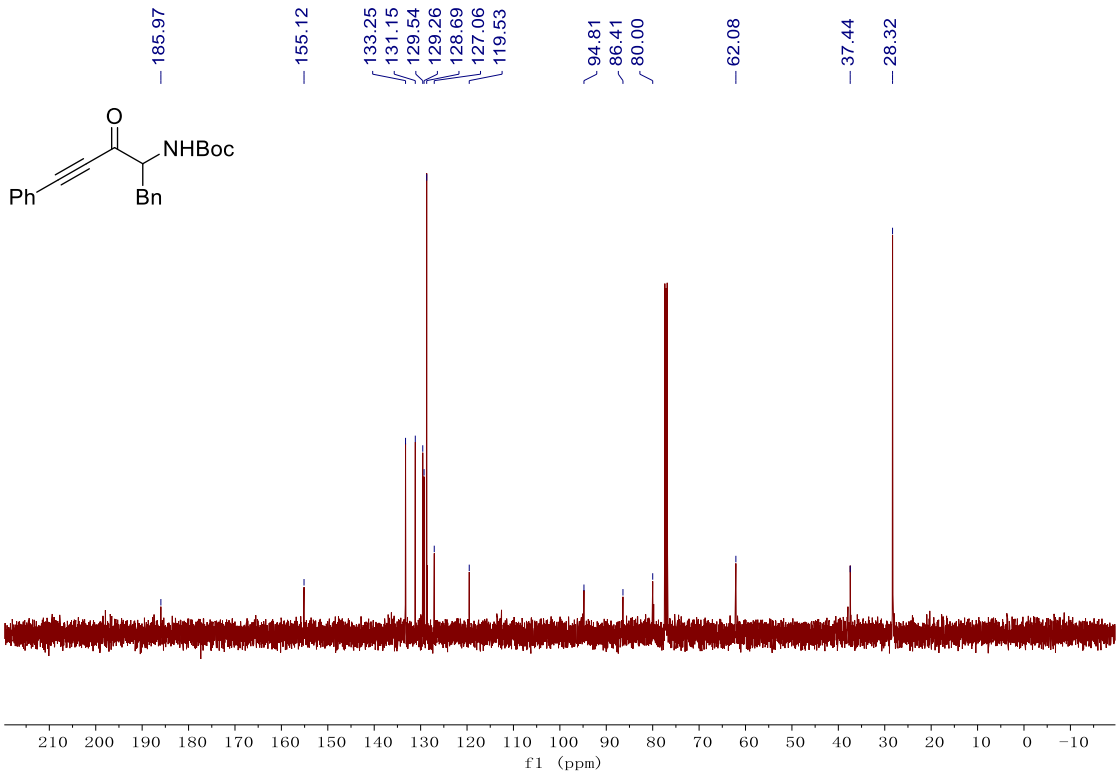
tert-butyl (3-oxo-5-phenylpent-4-yn-2-yl)carbamate (1j)



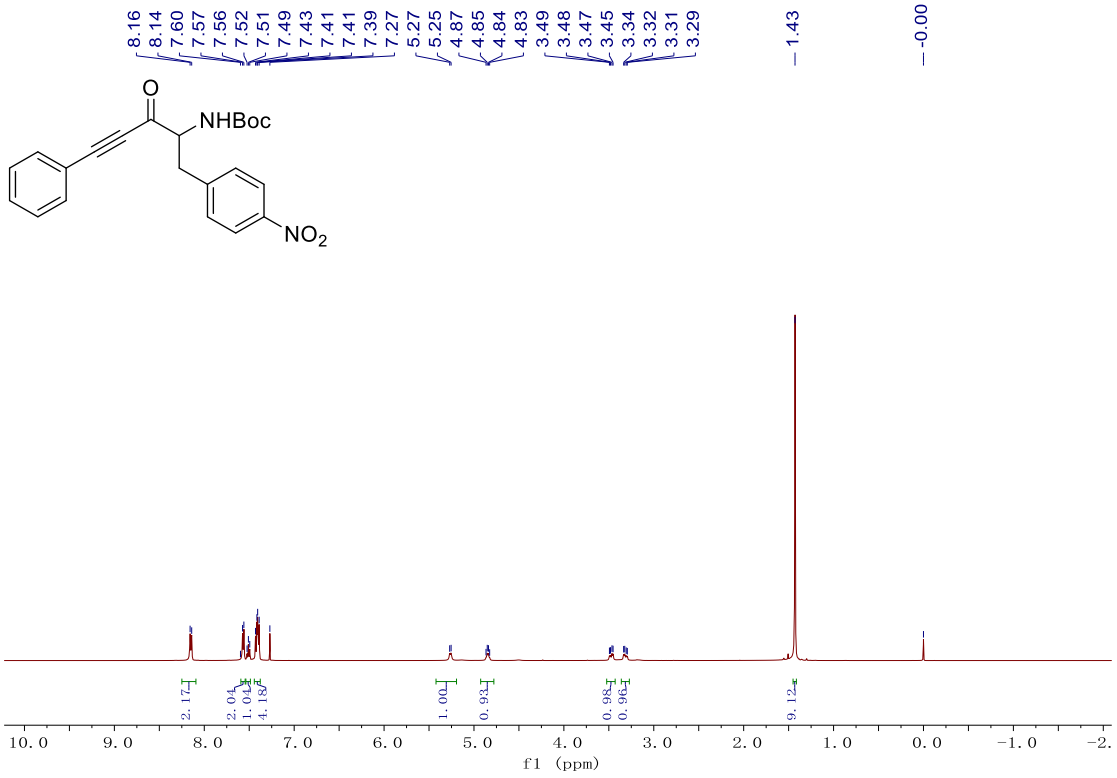


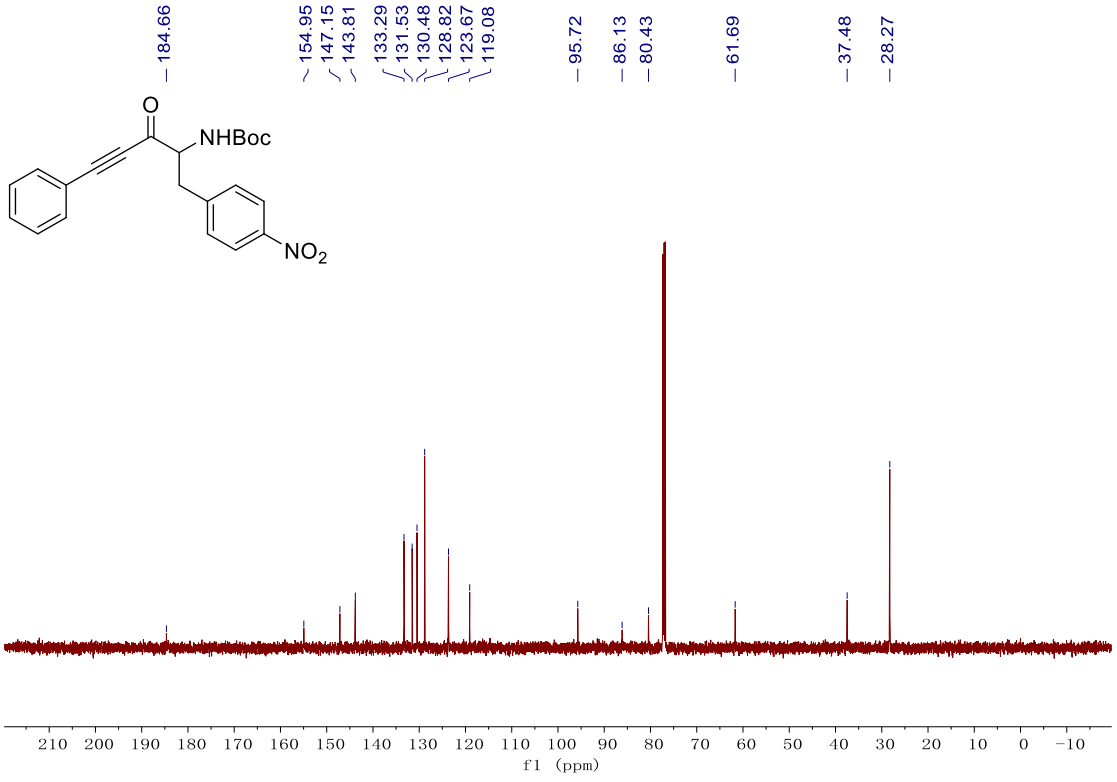
tert-butyl (3-oxo-1,5-diphenylpent-4-yn-2-yl)carbamate (1k)



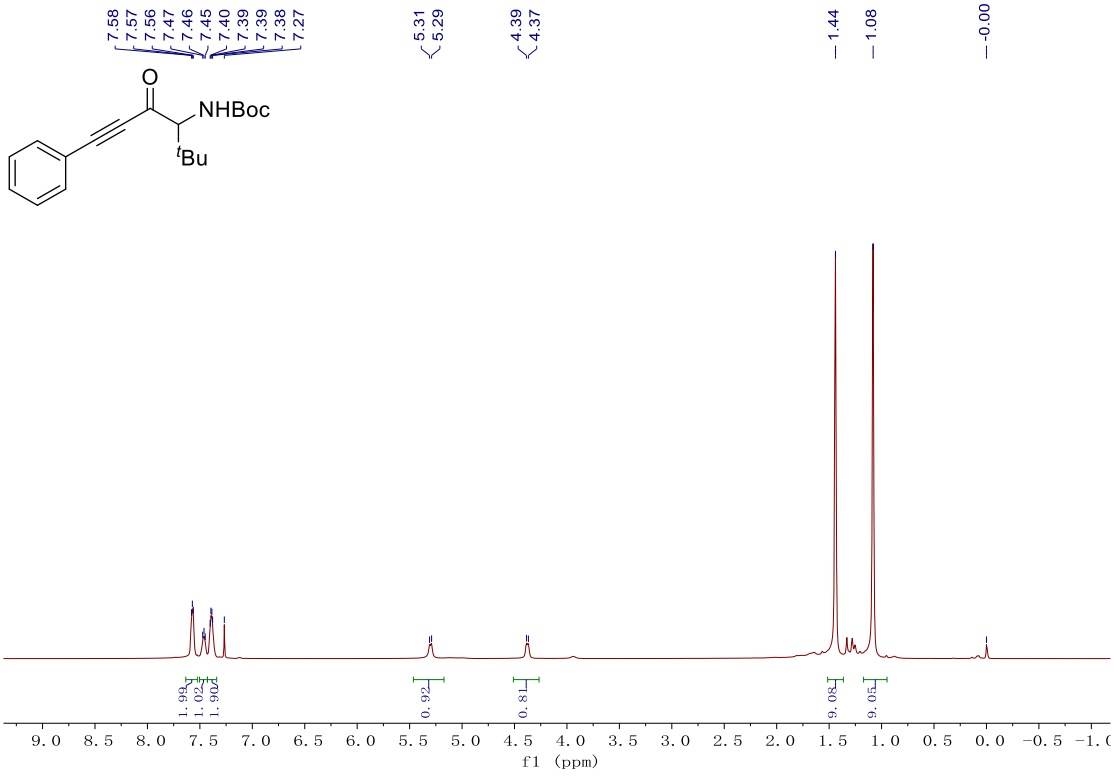


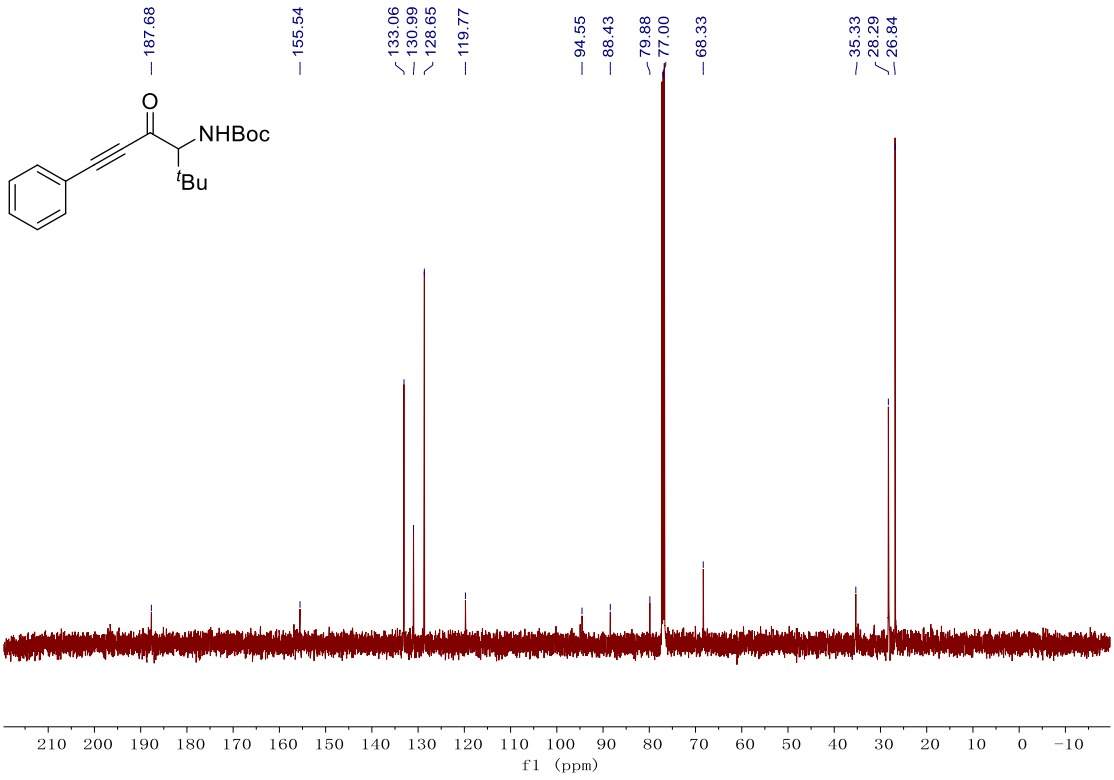
tert-butyl (1-(4-nitrophenyl)-3-oxo-5-phenylpent-4-yn-2-yl)carbamate (1l)



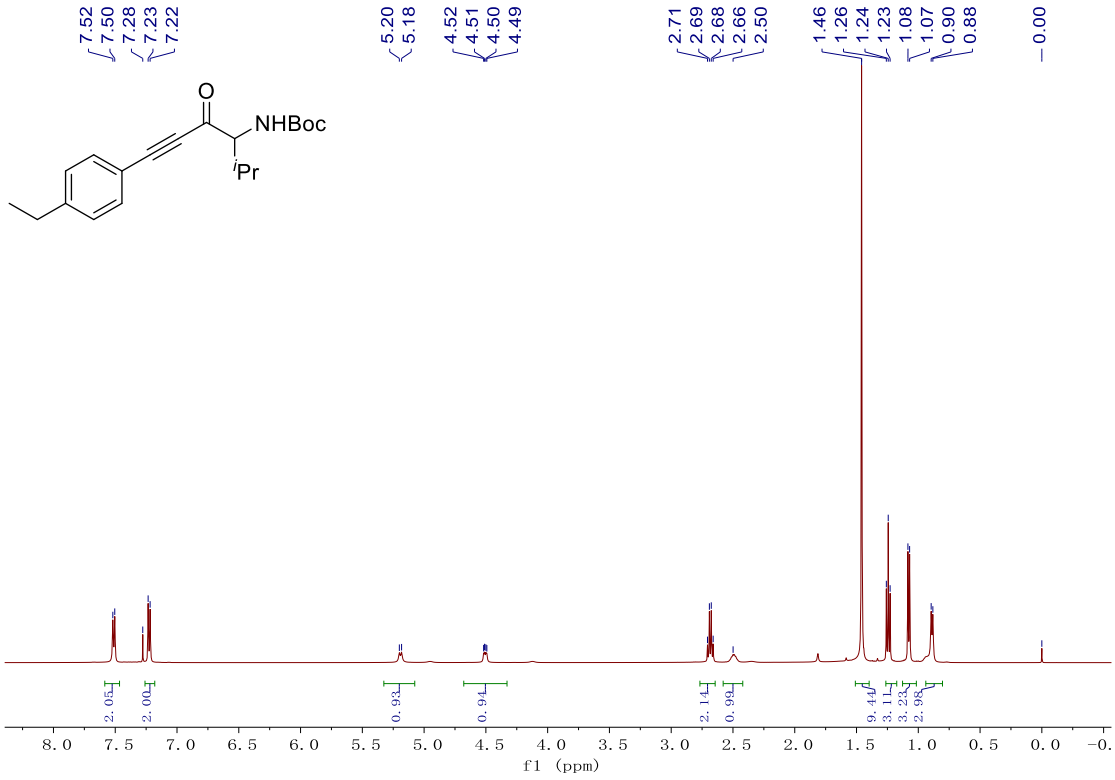


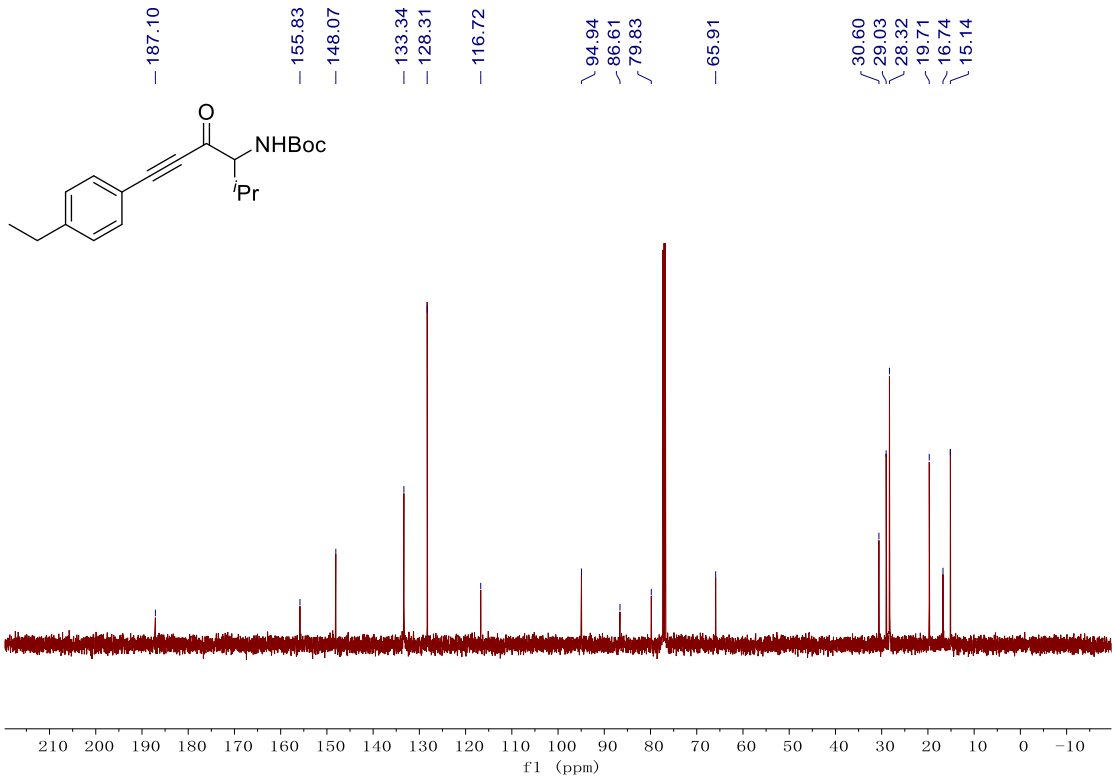
tert-butyl (2,2-dimethyl-4-oxo-6-phenylhex-5-yn-3-yl)carbamate (1m)



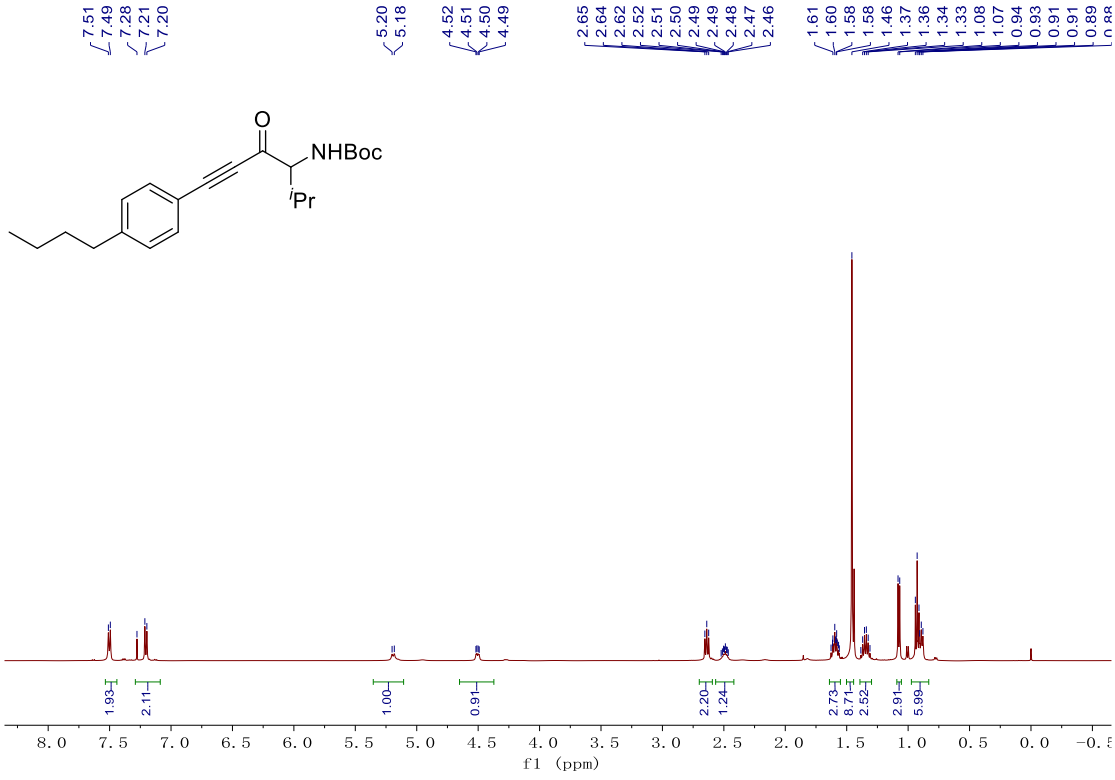


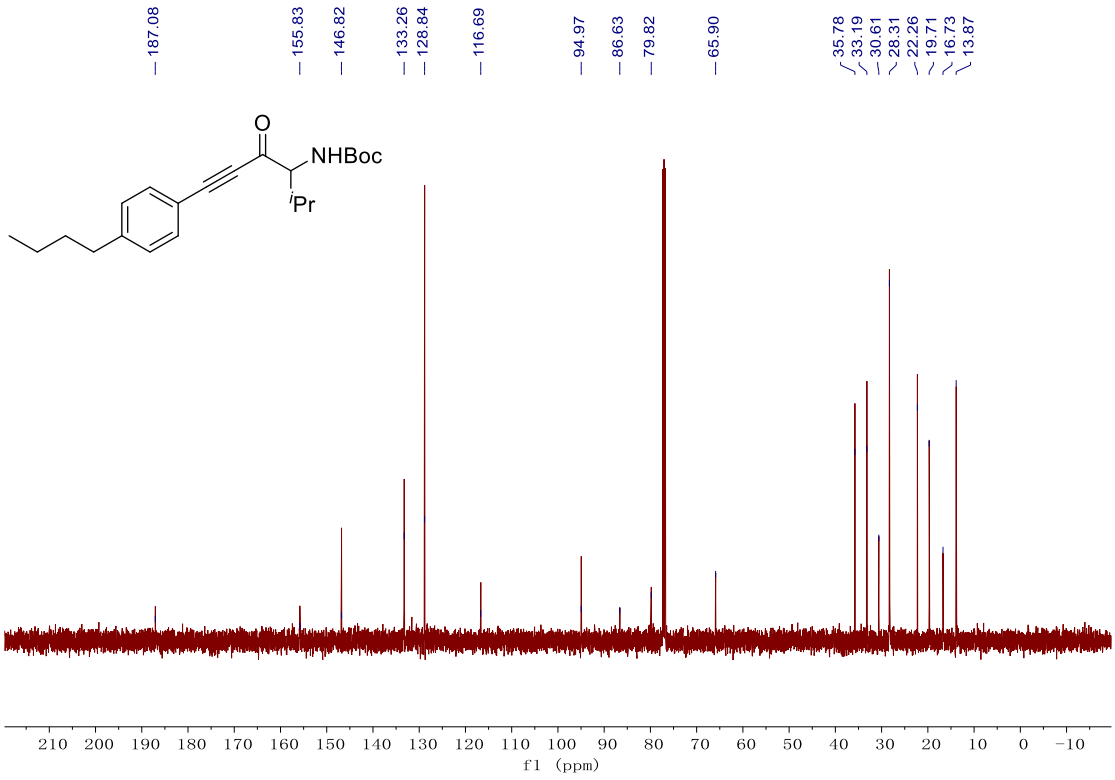
tert-butyl (6-(4-ethylphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1n)



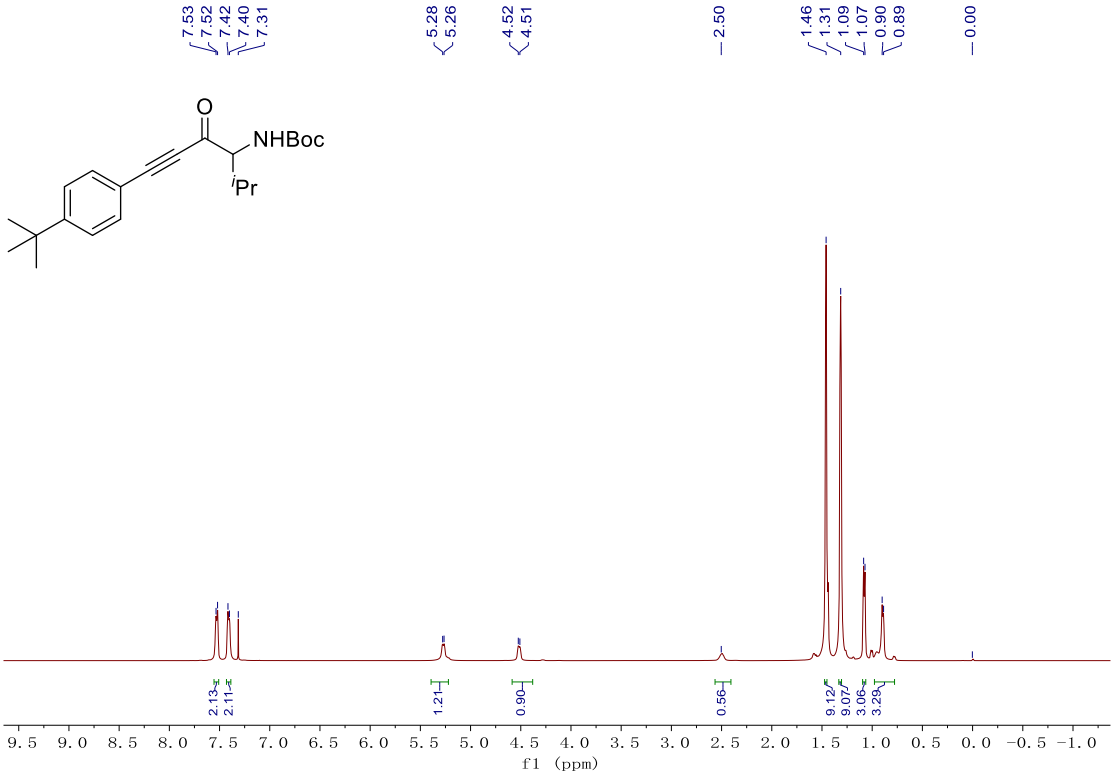


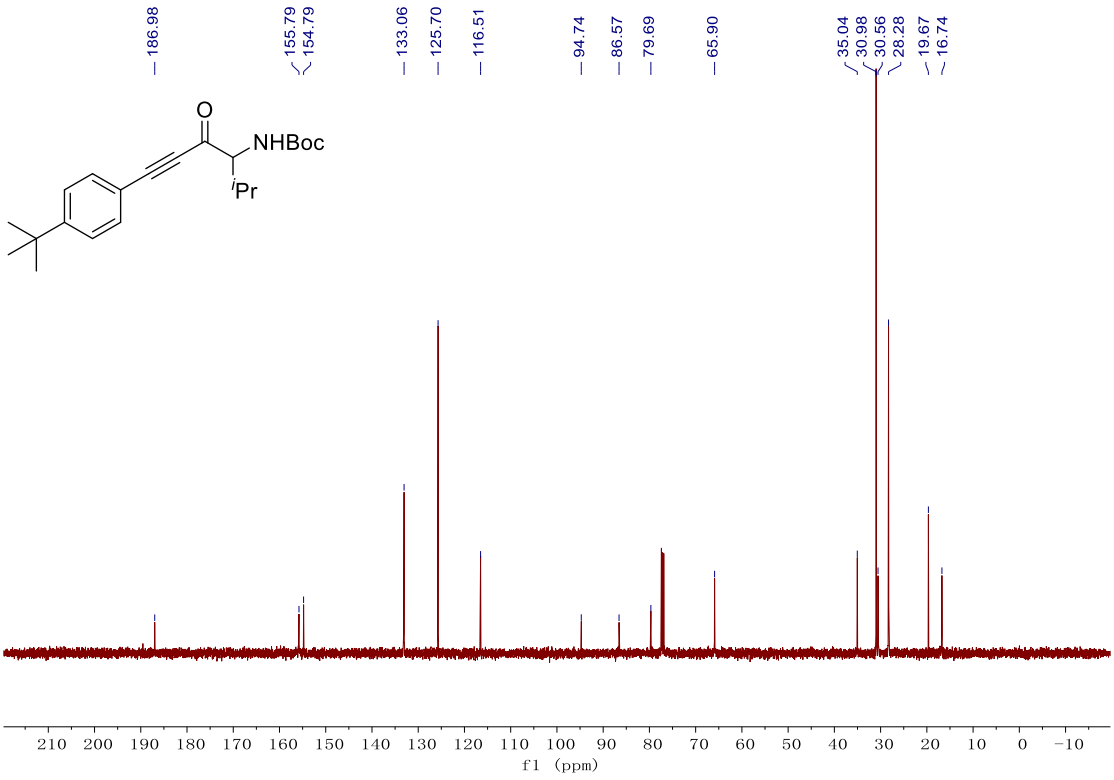
tert-butyl (6-(4-butylphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1o)



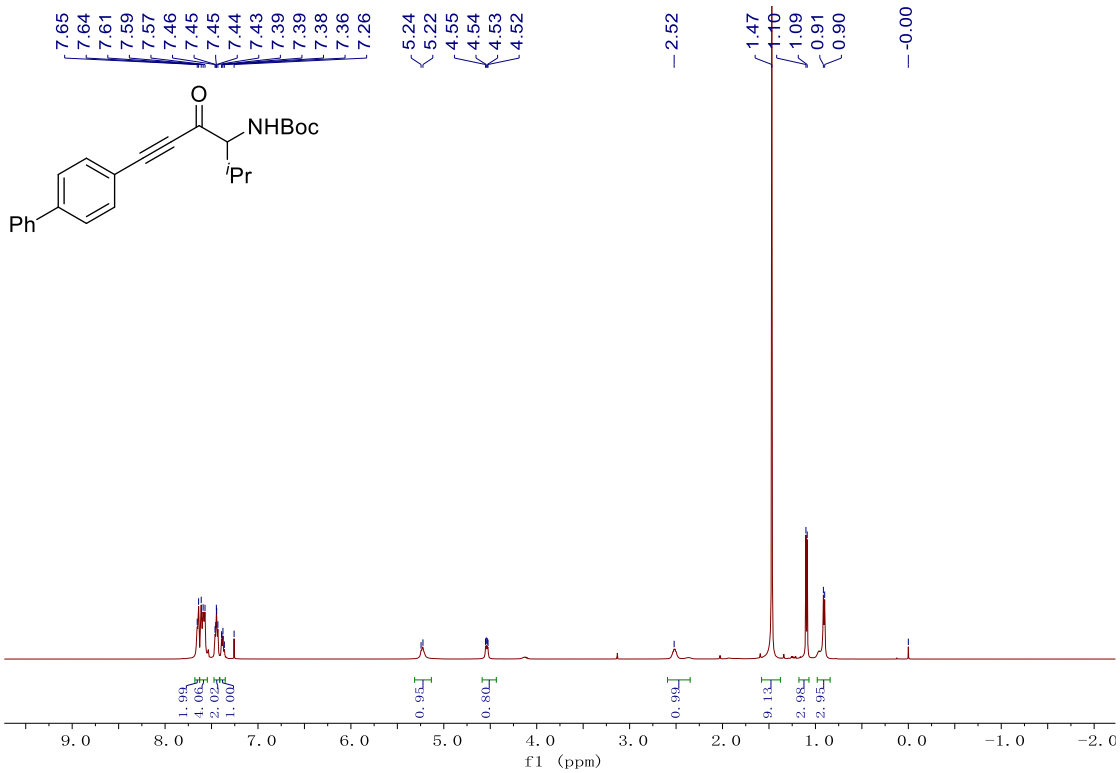


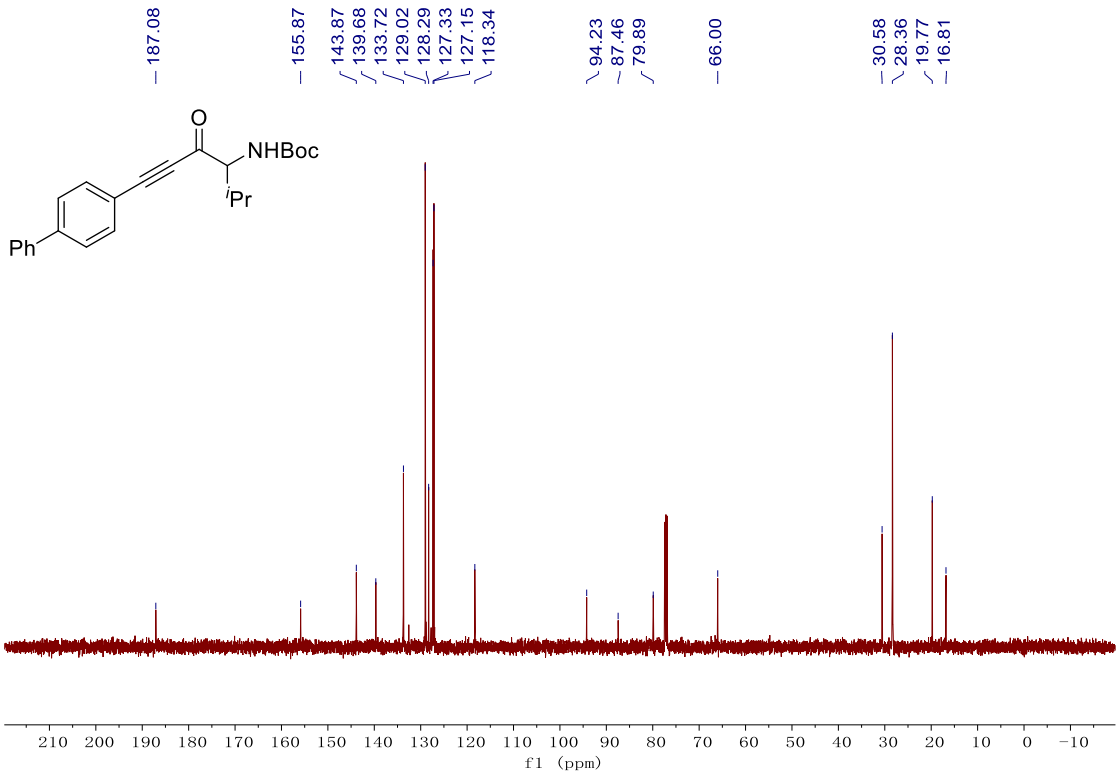
tert-butyl (6-(4-(tert-butyl)phenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1p)



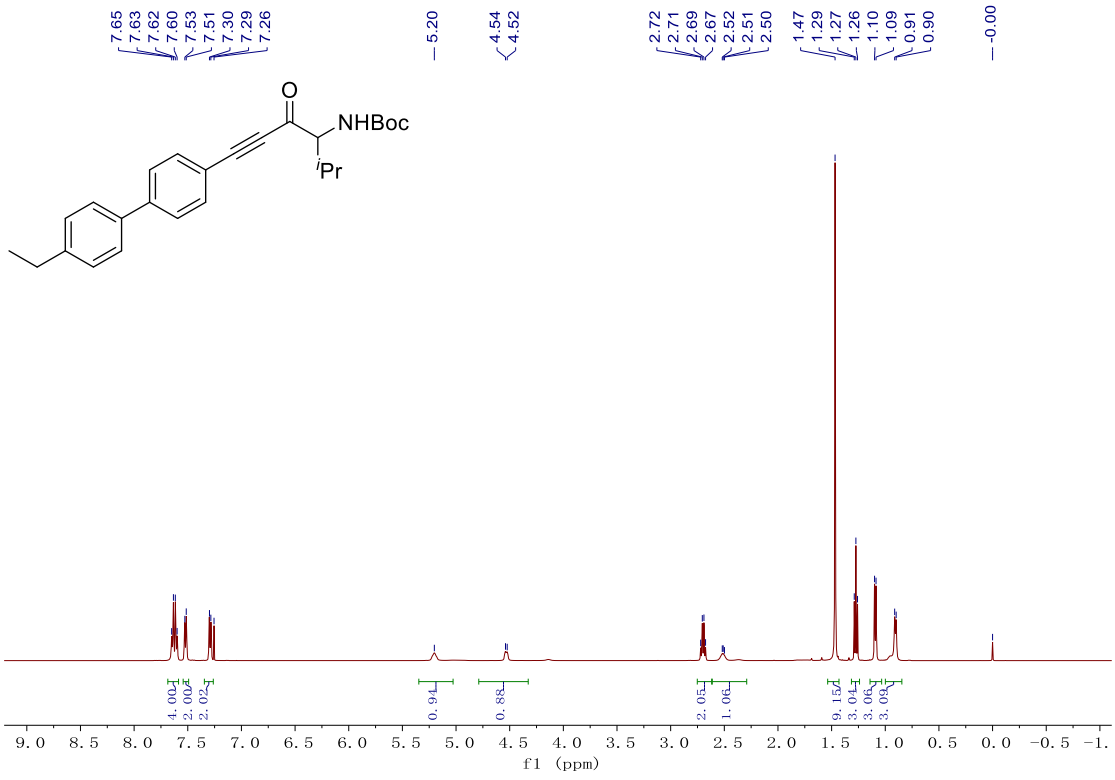


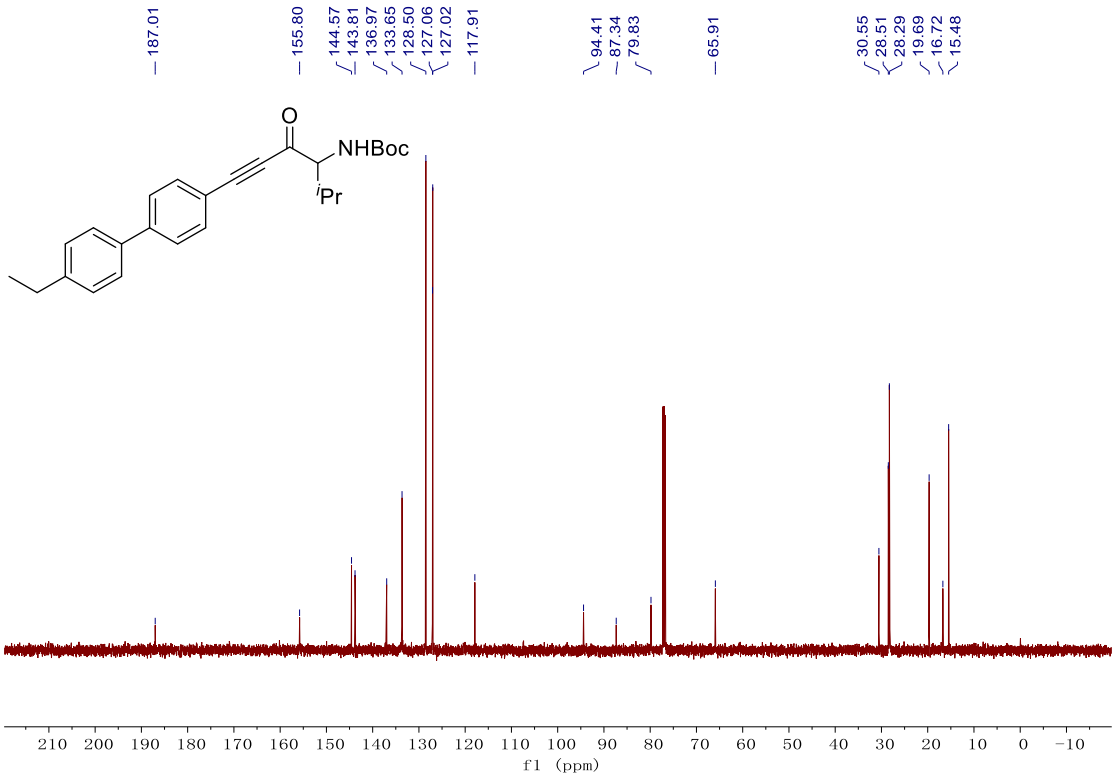
tert-butyl (6-([1,1'-biphenyl]-4-yl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1q)



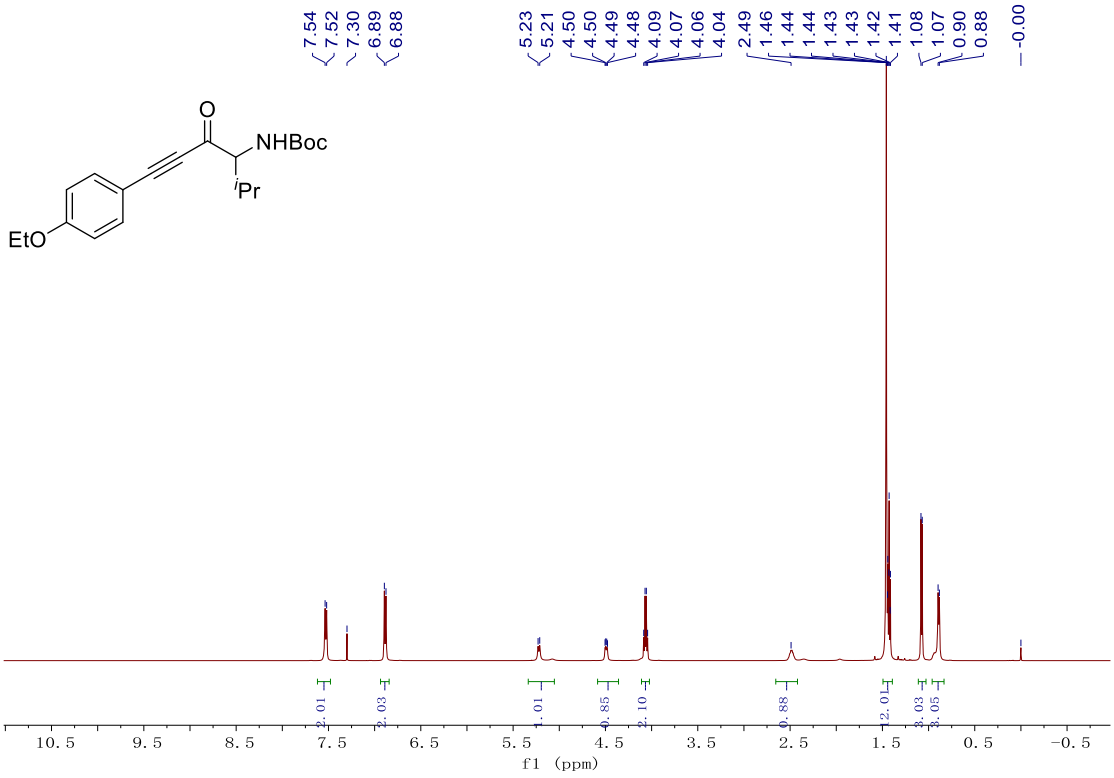


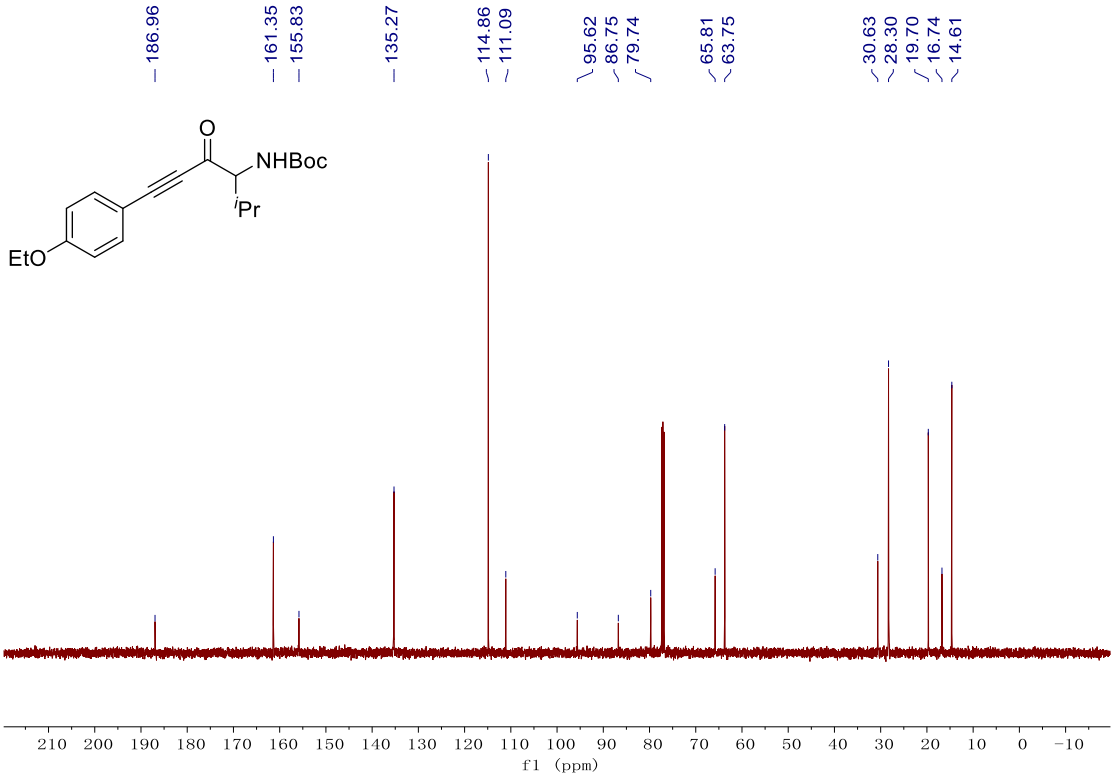
tert-butyl (6-(4'-ethyl-[1,1'-biphenyl]-4-yl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1r)



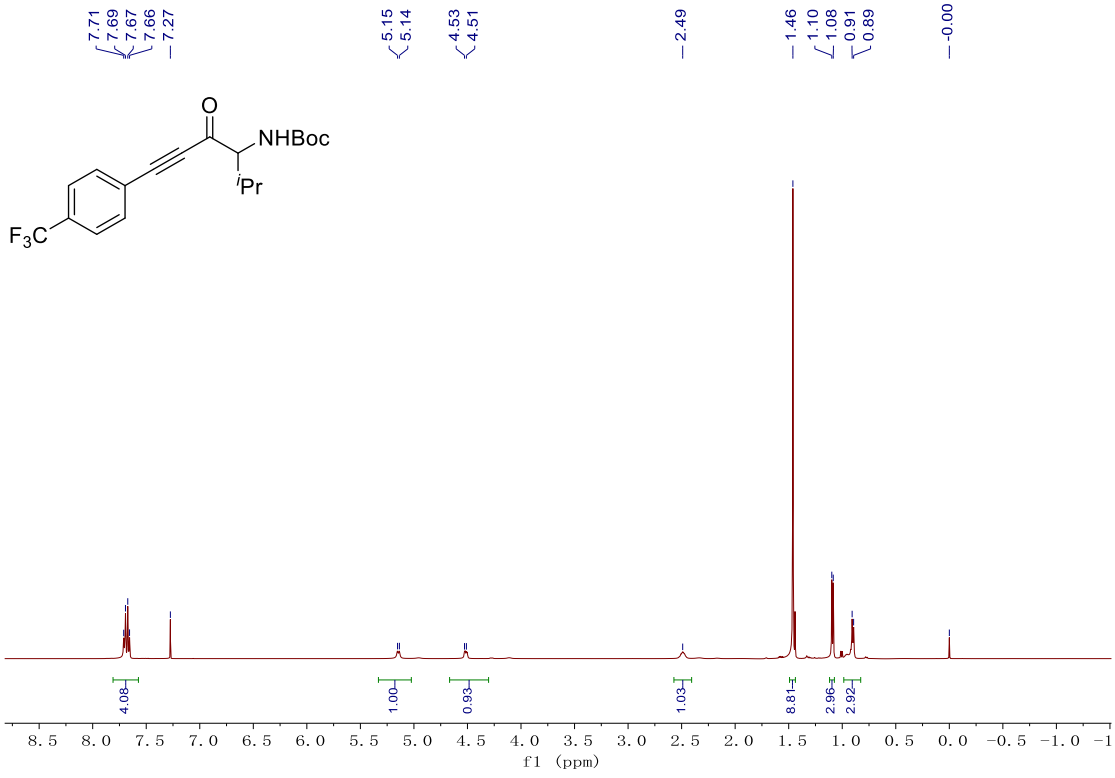


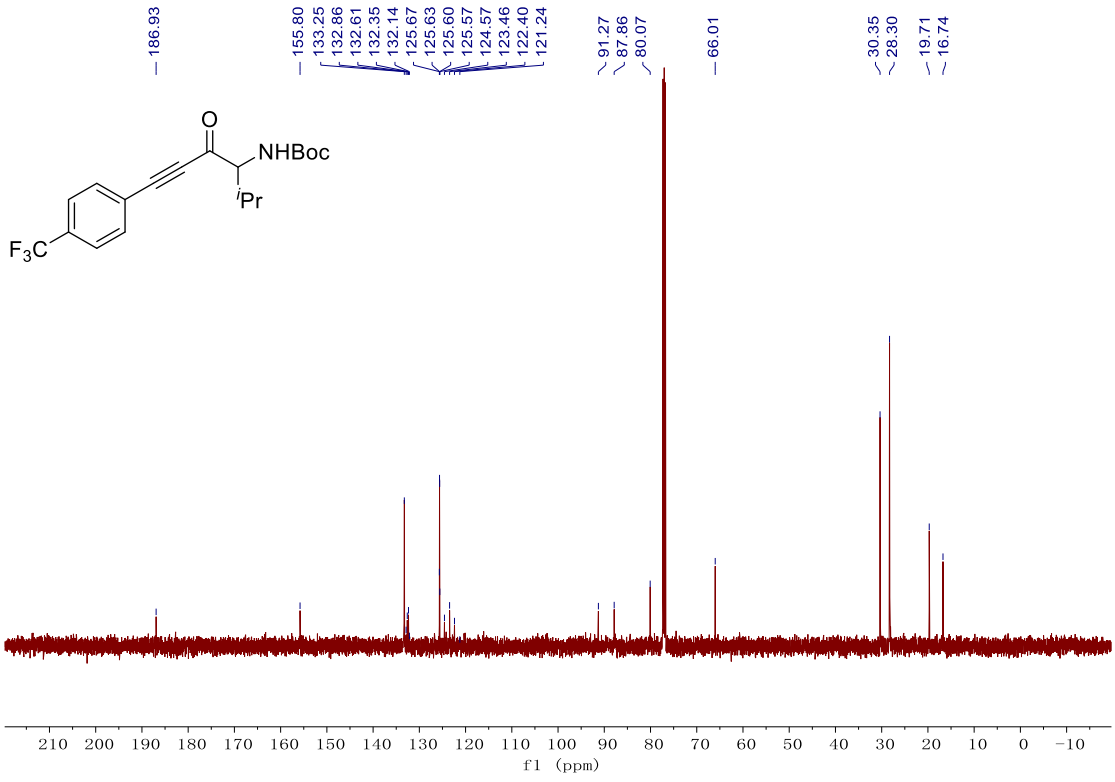
tert-butyl (6-(4-ethoxyphenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1s)

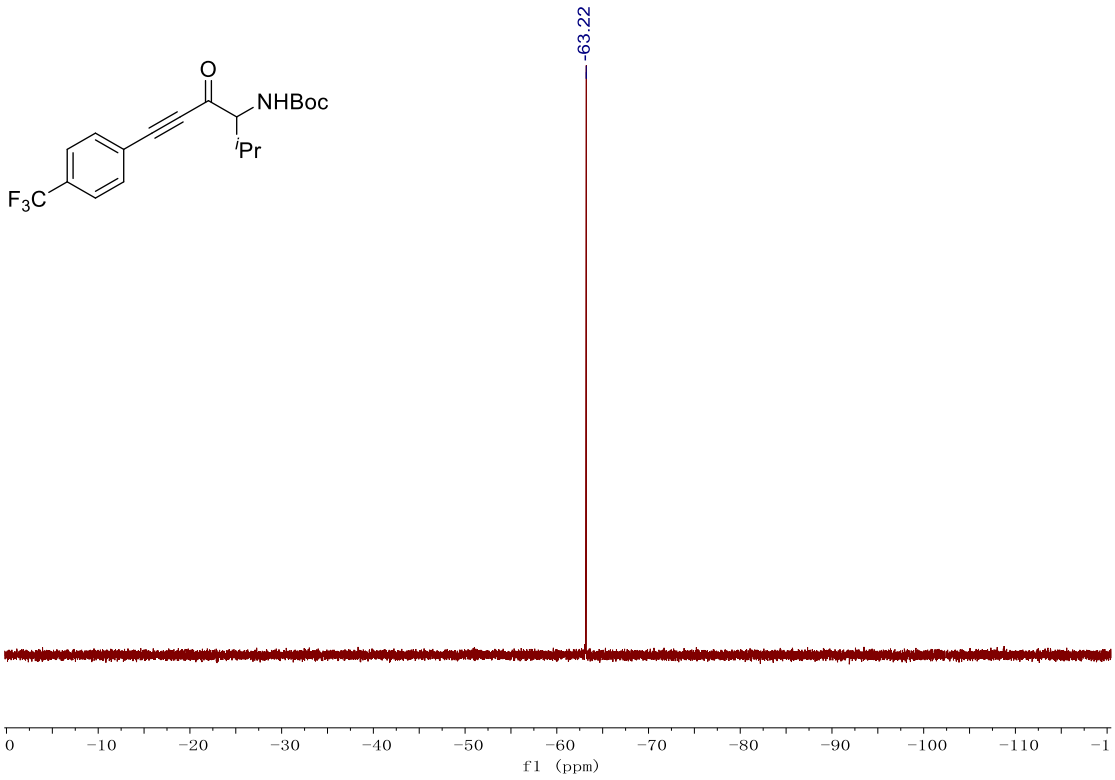




tert-butyl (2-methyl-4-oxo-6-(4-(trifluoromethyl)phenyl)hex-5-yn-3-yl)carbamate (1t)



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O
NHBoc
iPr
F3C
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−10
−20
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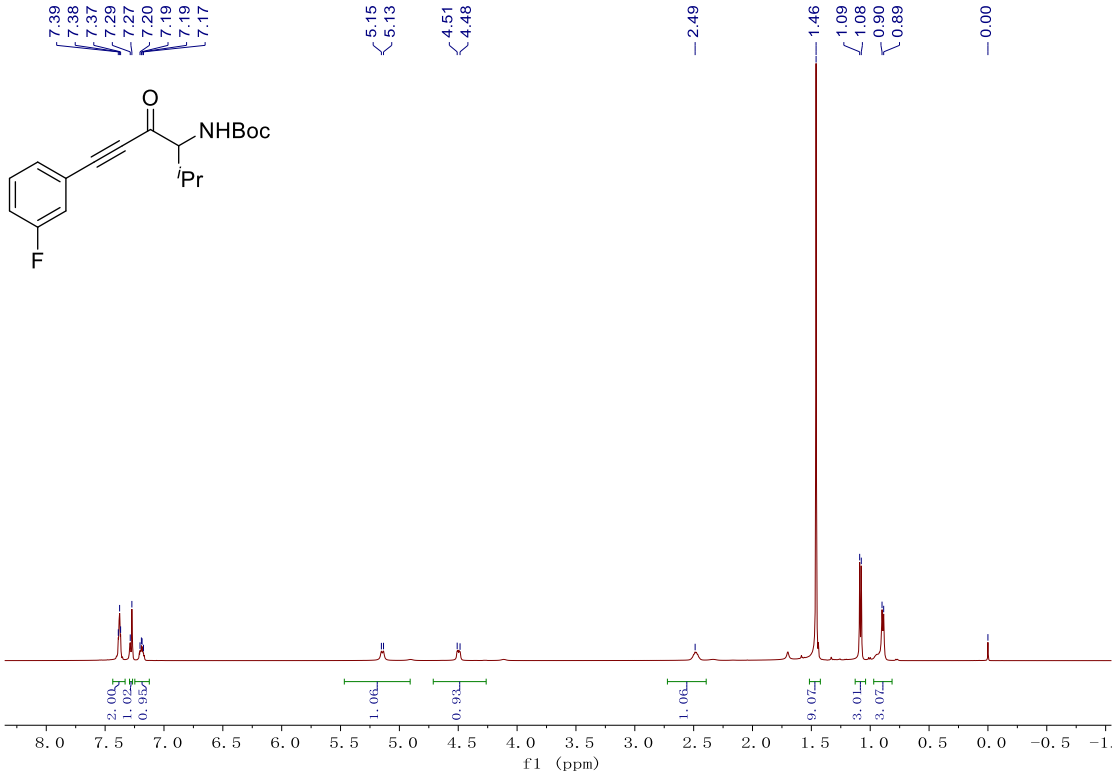
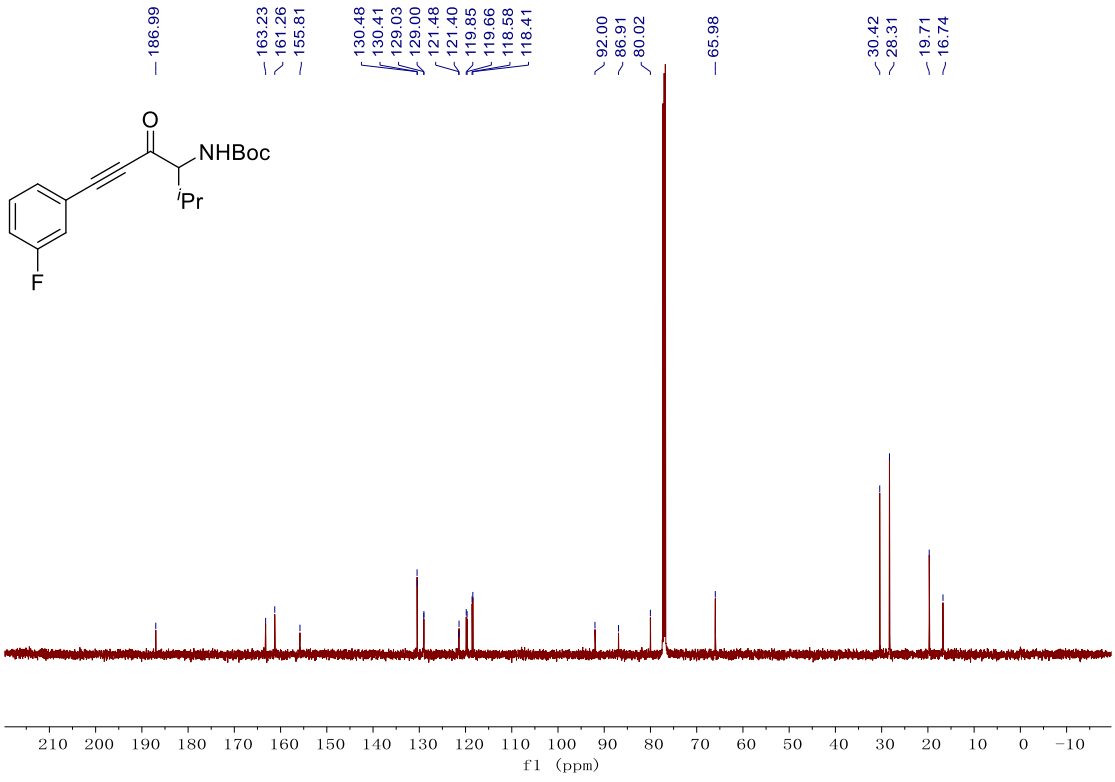
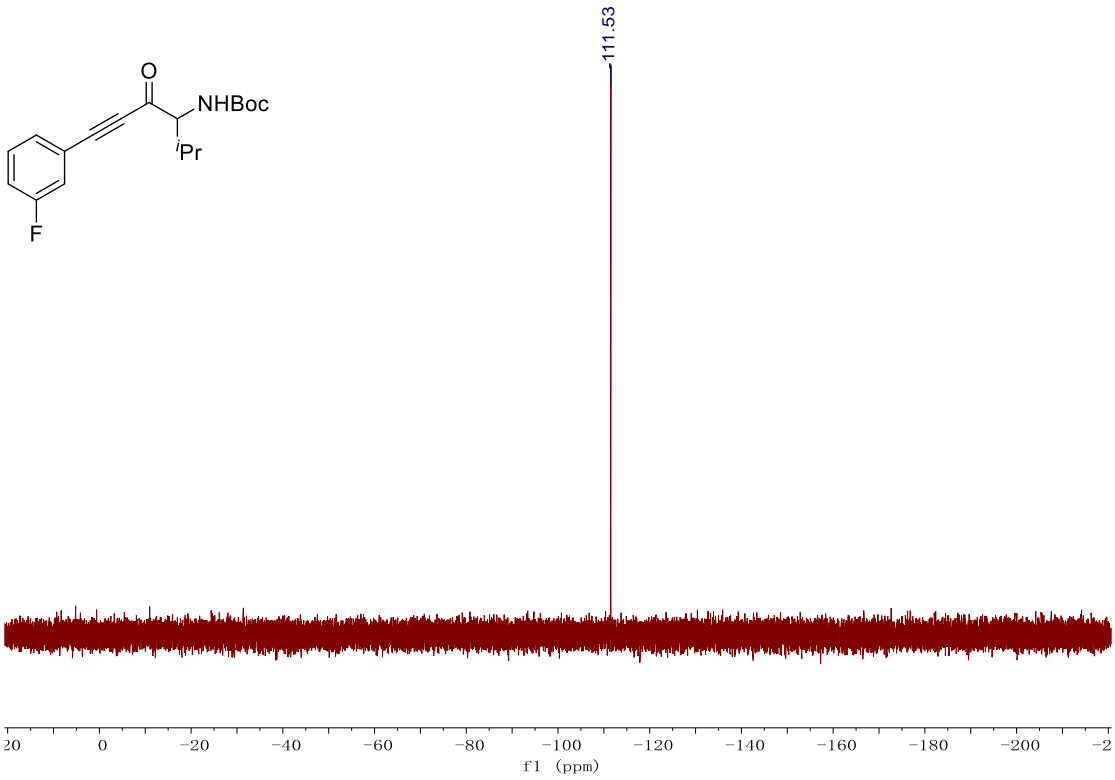
−40
−50
−60
−70
−80
−90
−100
−110
−1
f1 (ppm)

tert-butyl (6-(3-fluorophenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate (1u)

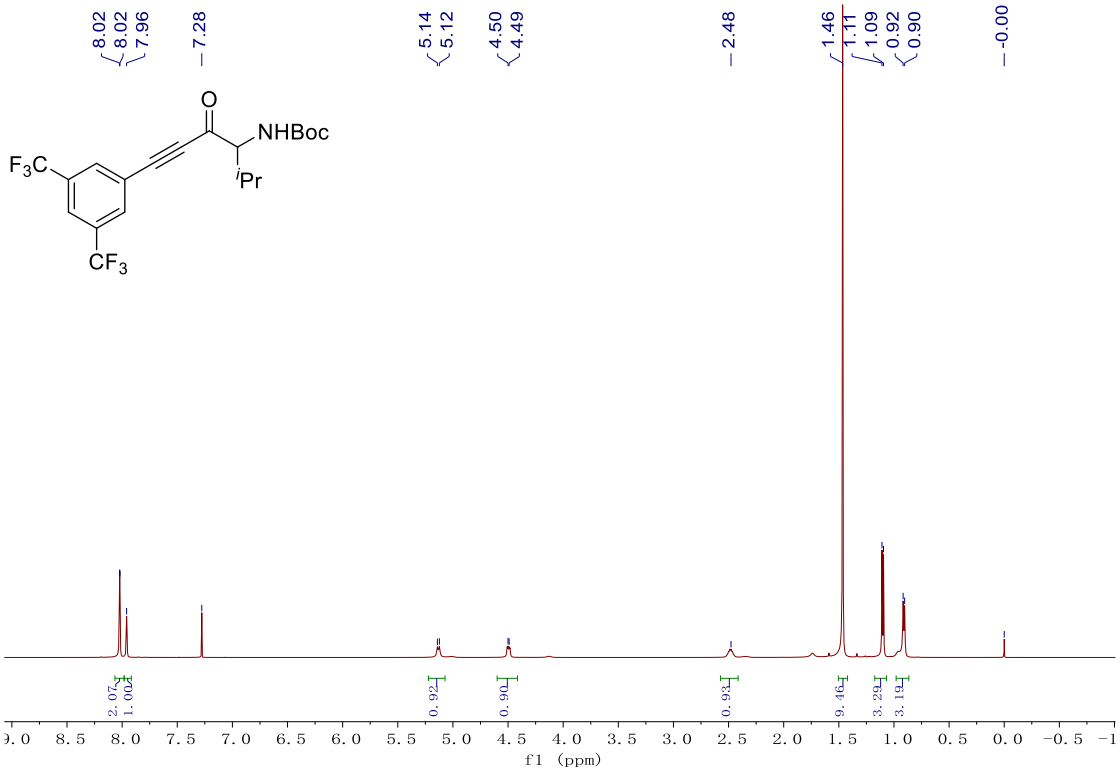


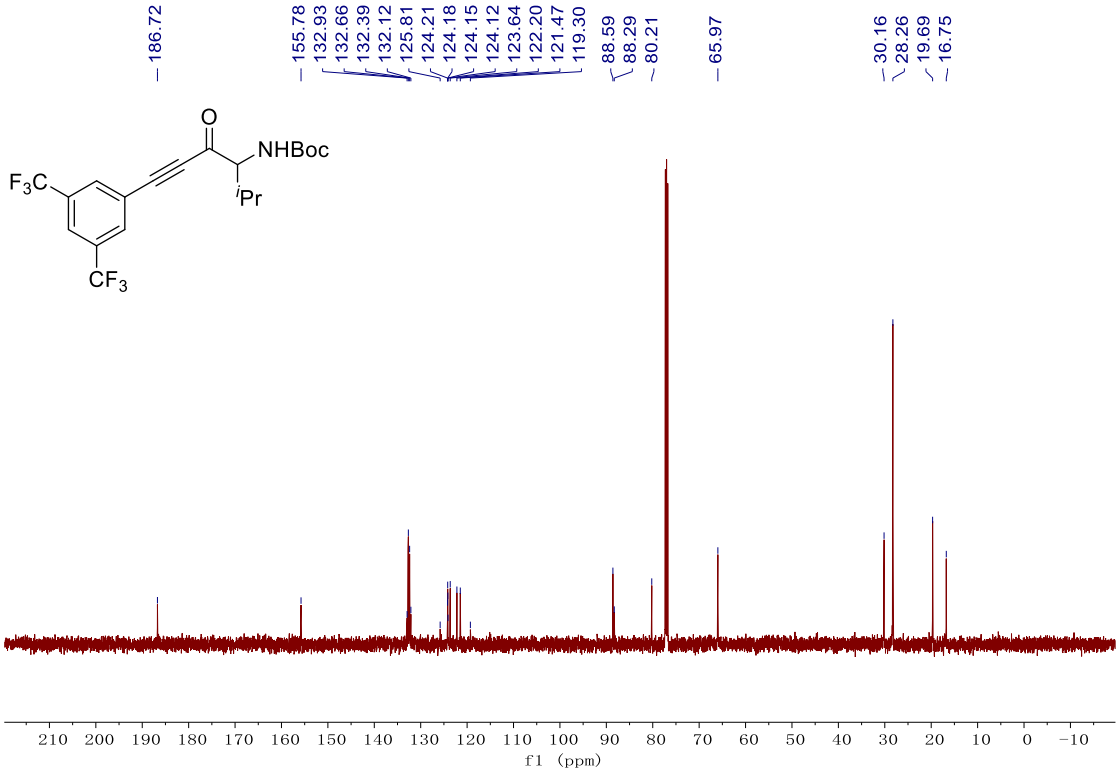


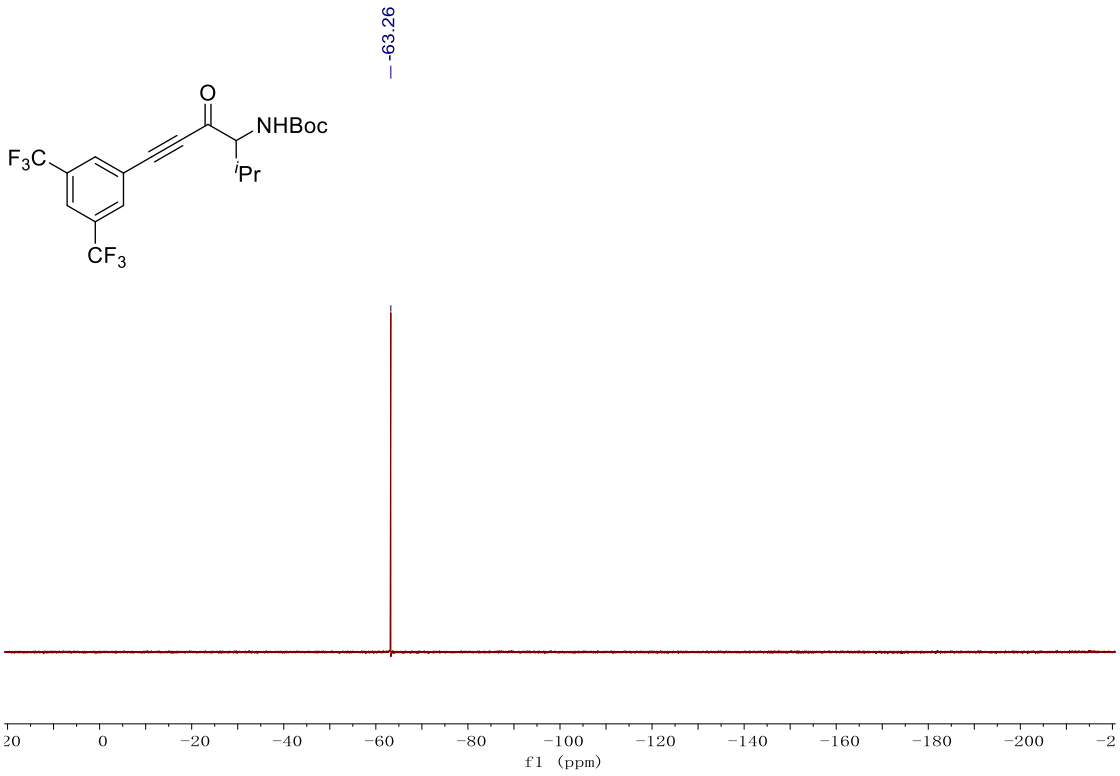

O
NHBoc
iPr
F
111.53
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

***tert*-butyl (6-(3,5-bis(trifluoromethyl)phenyl)-2-methyl-4-oxohex-5-yn-3-yl)carbamate**

(1v)



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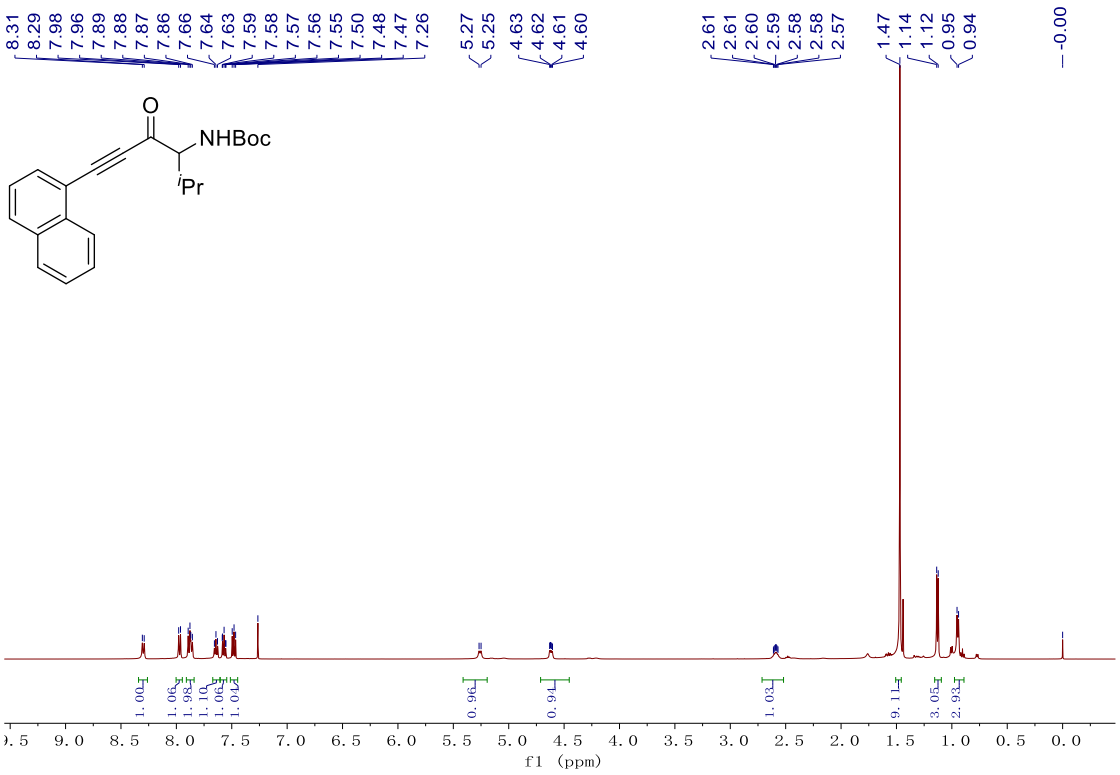
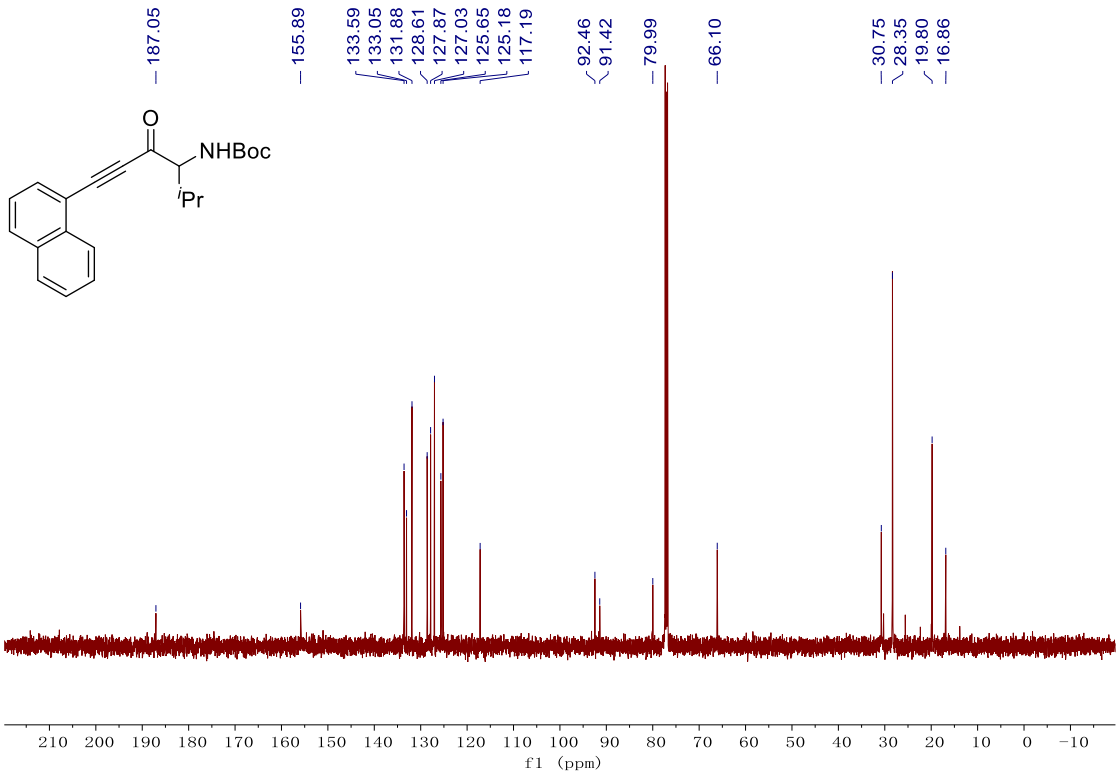
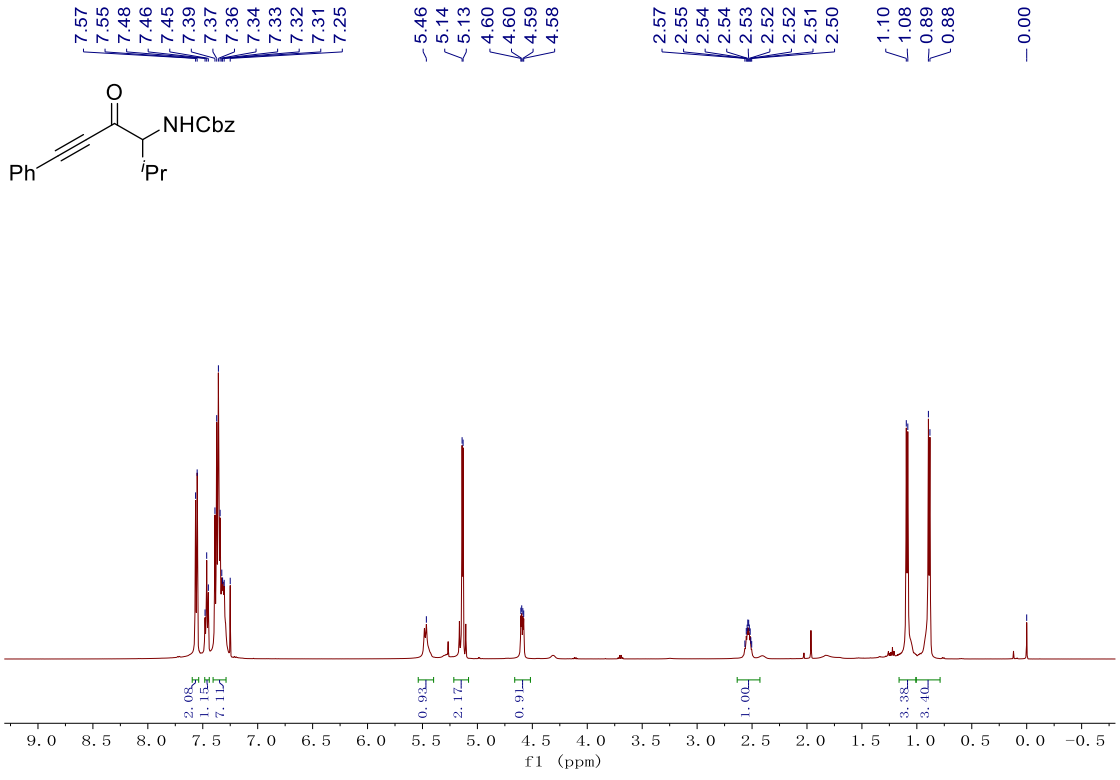
NHBoc
F3C
iPr
CF3
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

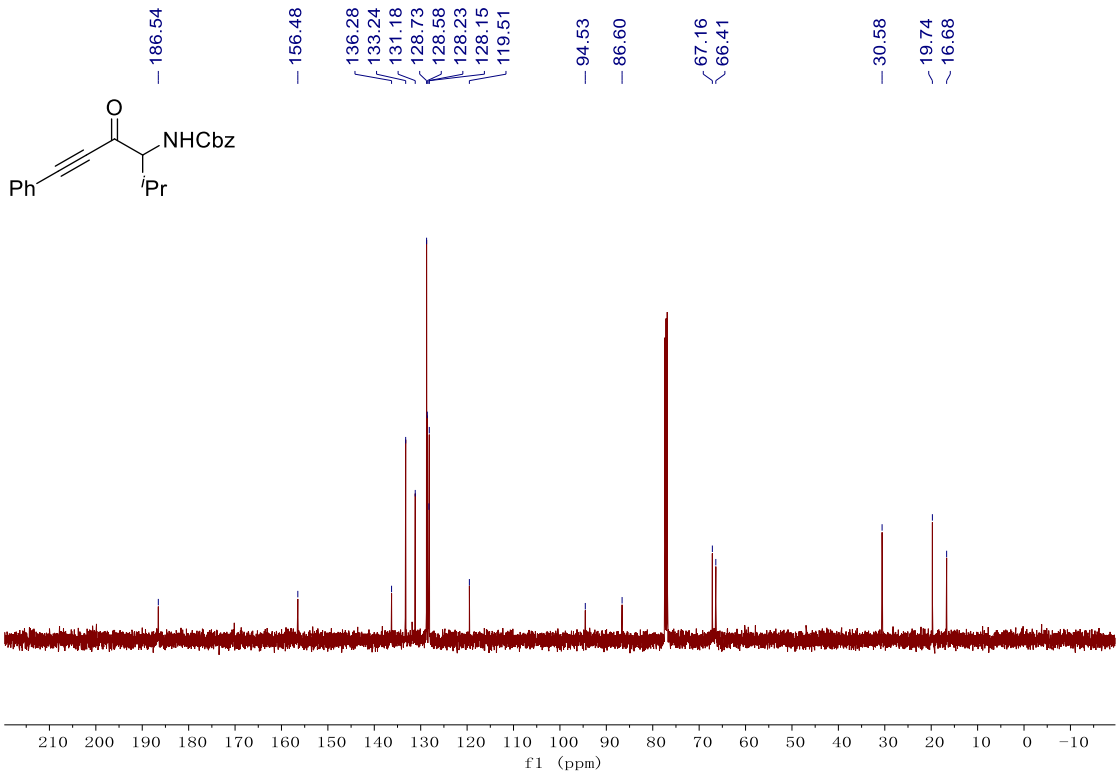
tert-butyl (2-methyl-6-(naphthalen-1-yl)-4-oxohex-5-yn-3-yl)carbamate (1w)



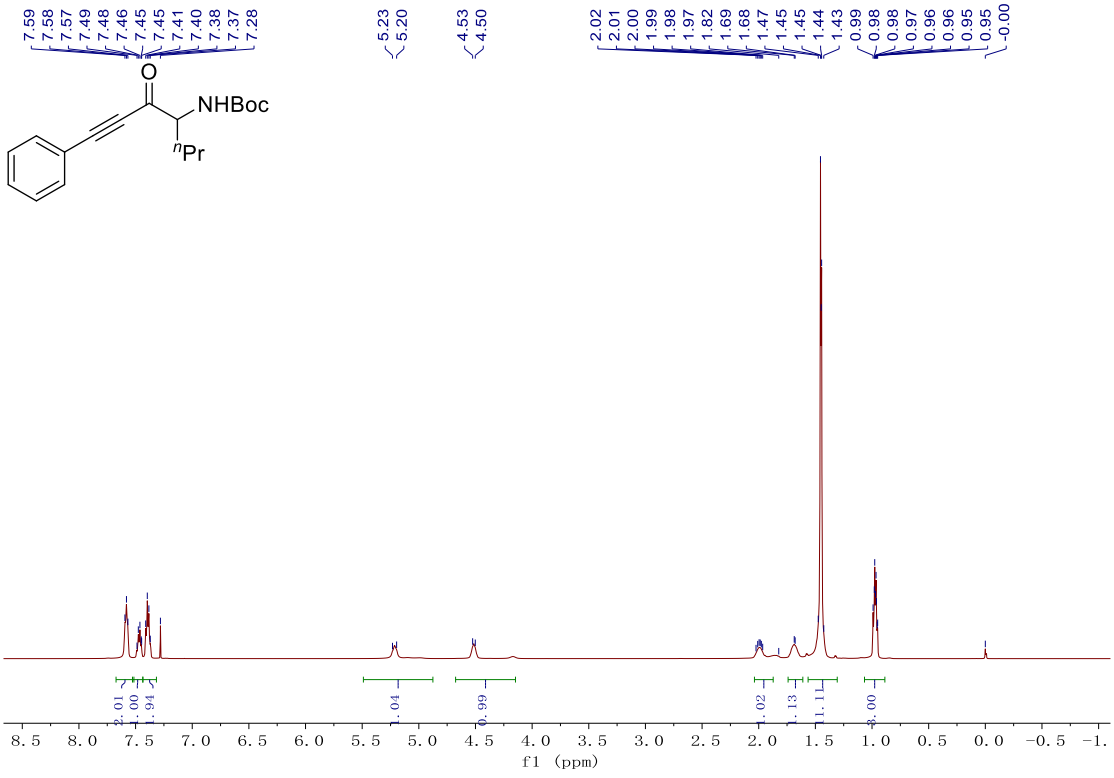


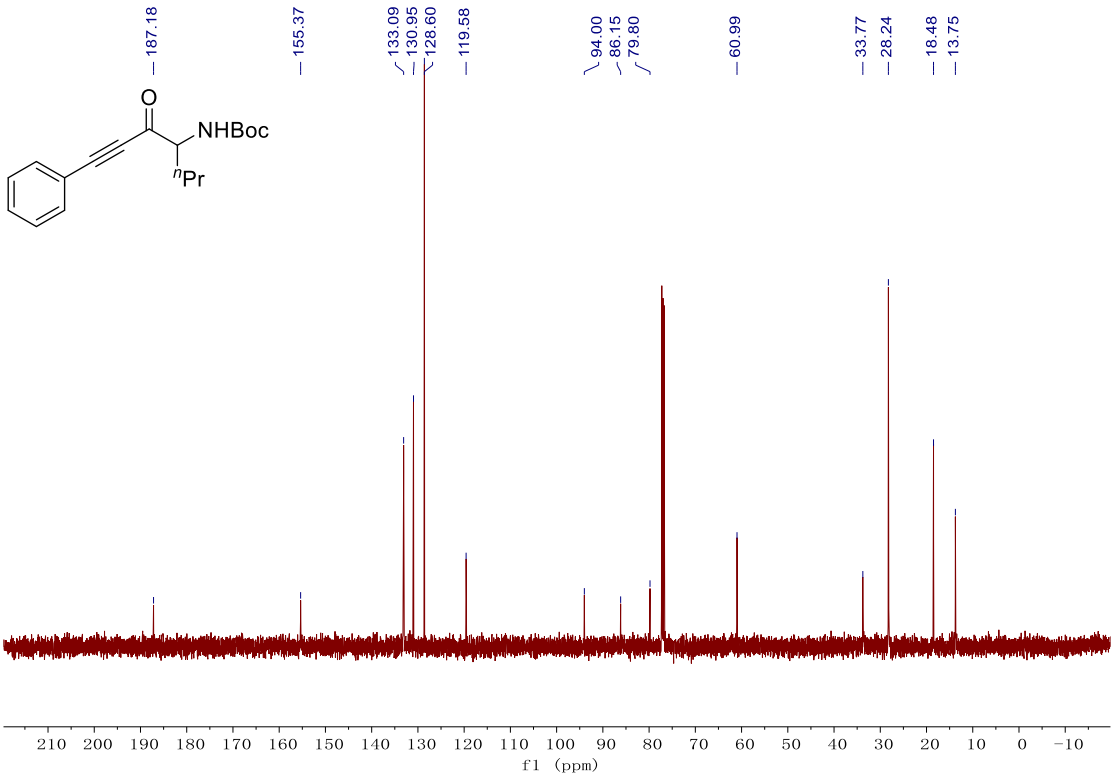
benzyl (2-methyl-4-oxo-6-phenylhex-5-yn-3-yl)carbamate (1x)



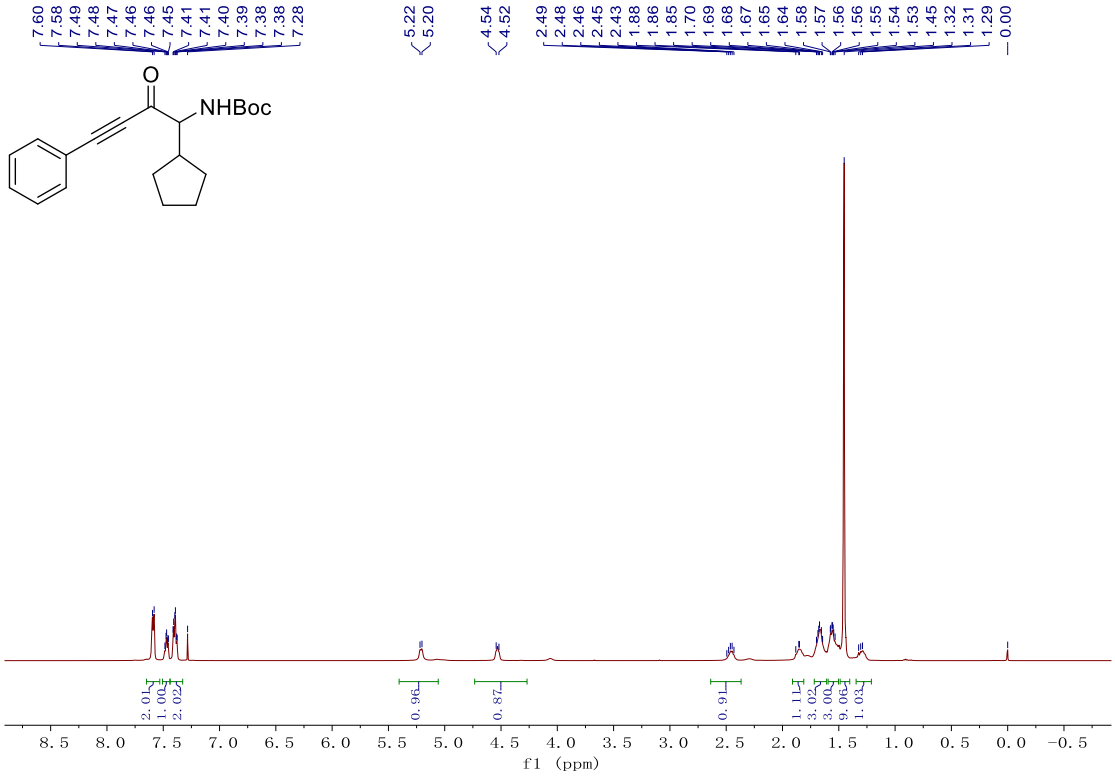


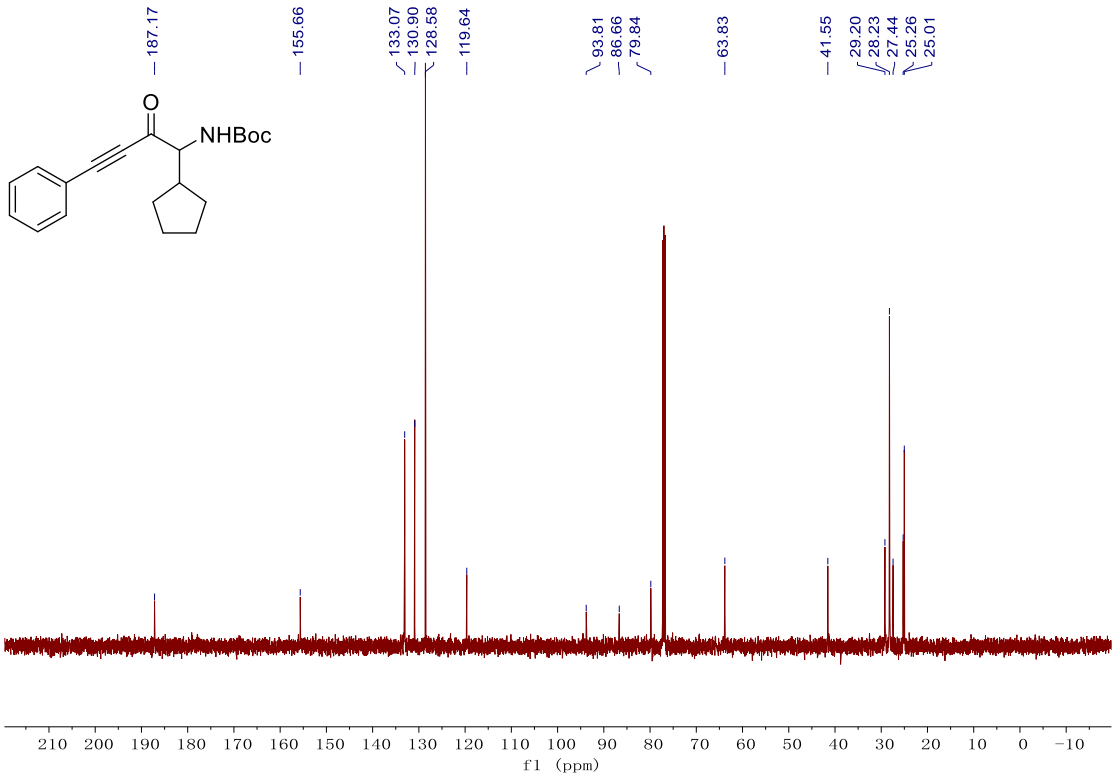
tert-butyl (3-oxo-1-phenylhept-1-yn-4-yl)carbamate (1y)



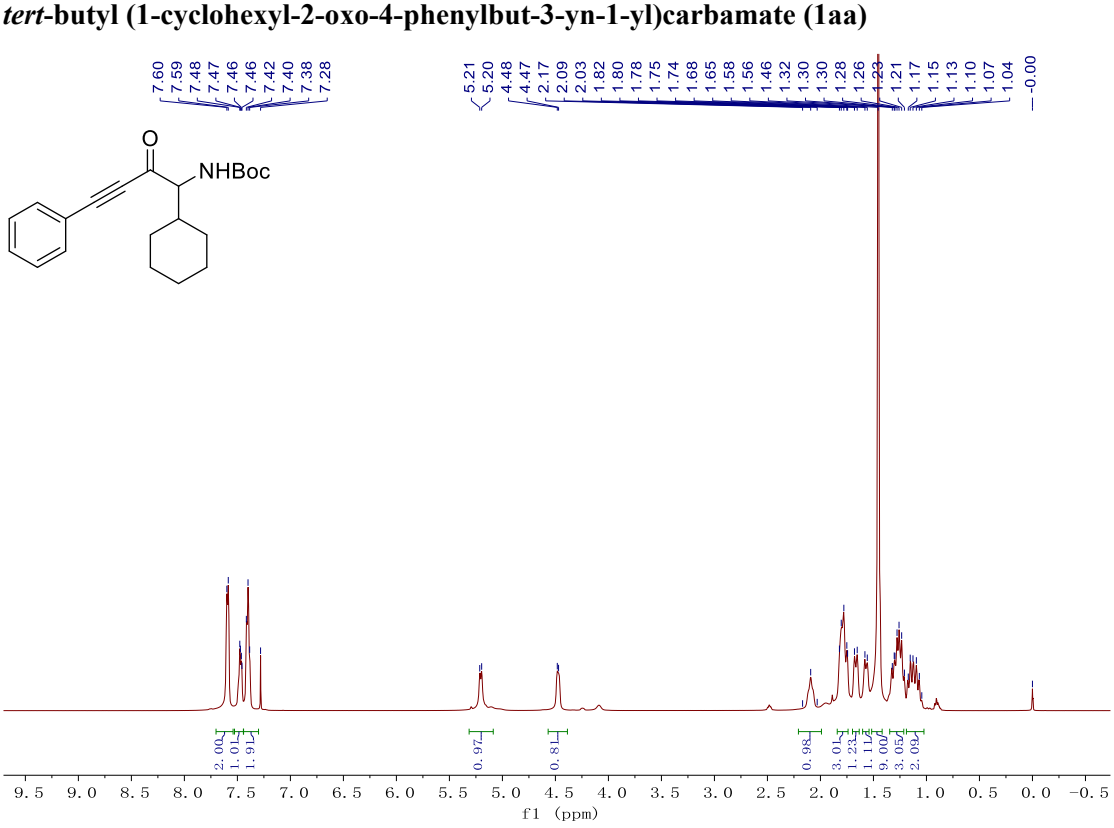


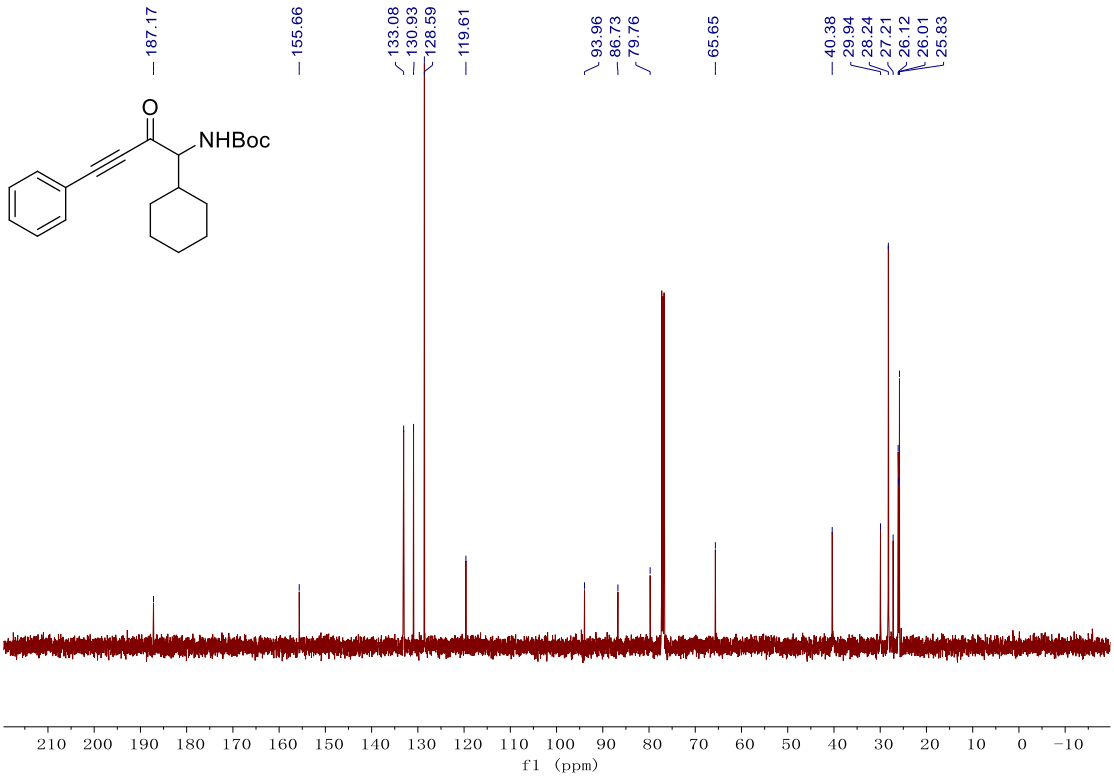
tert-butyl (1-cyclopentyl-2-oxo-4-phenylbut-3-yn-1-yl)carbamate (1z)



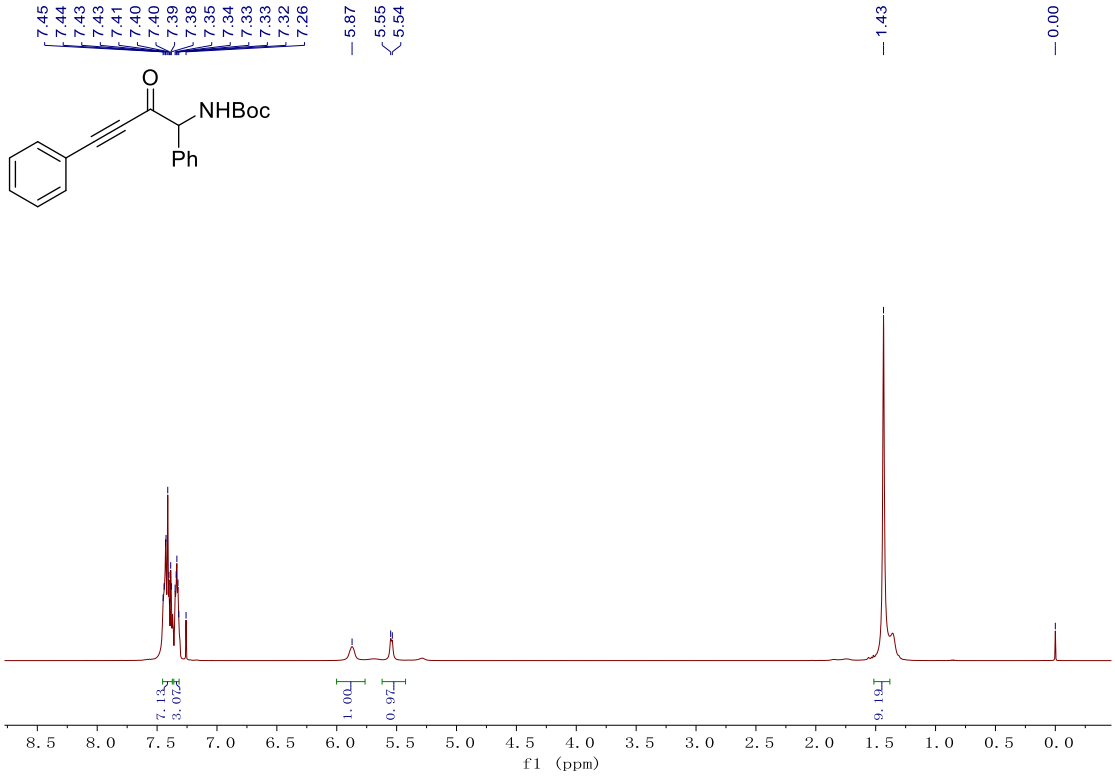


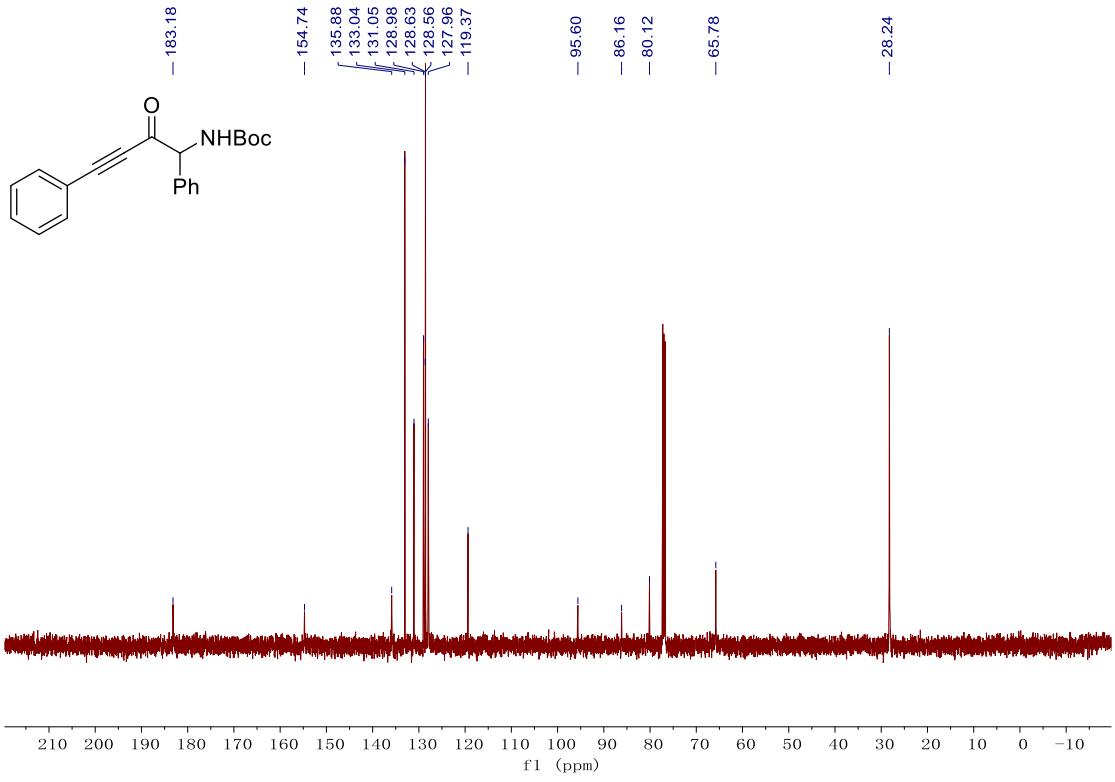
***tert*-butyl (1-cyclohexyl-2-oxo-4-phenylbut-3-yn-1-yl)carbamate (1aa)**



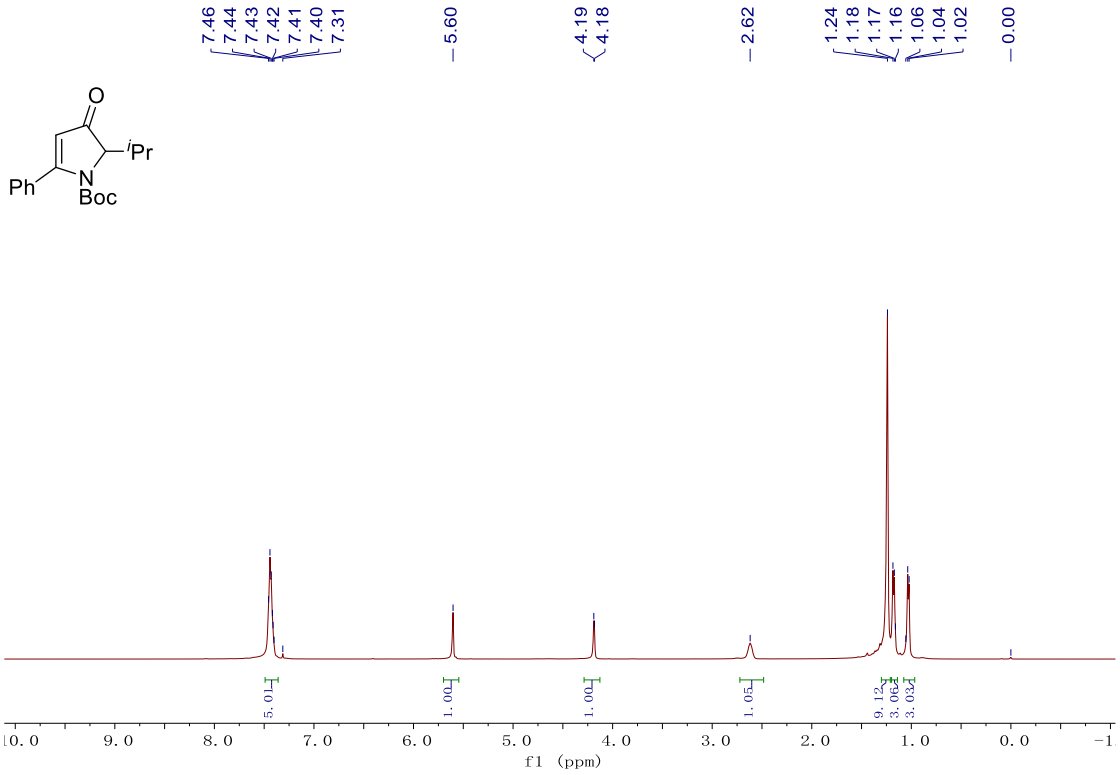


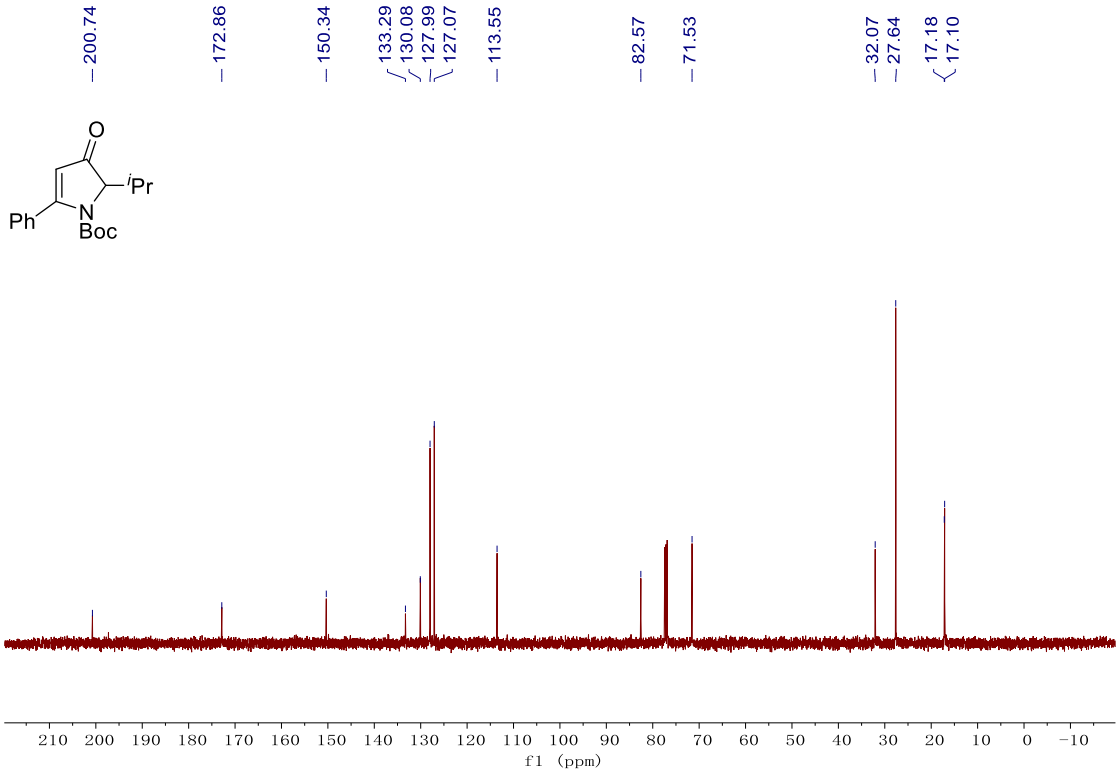
tert-butyl (2-oxo-1,4-diphenylbut-3-yn-1-yl)carbamate (1ab)



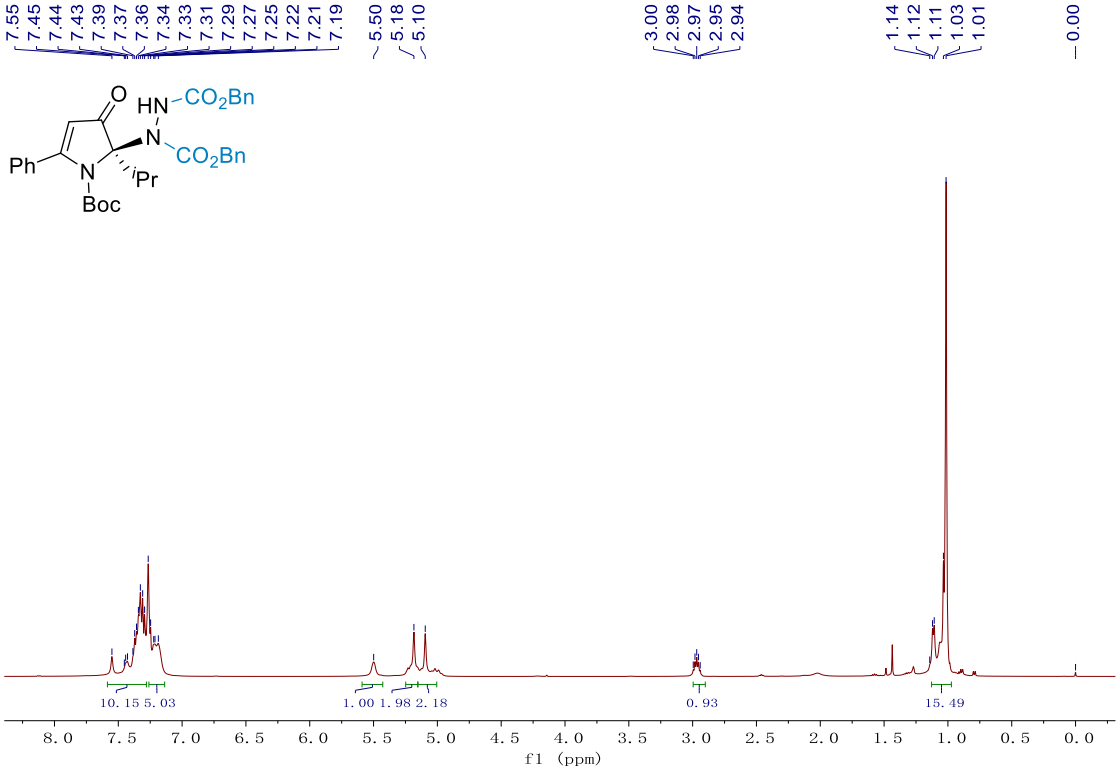


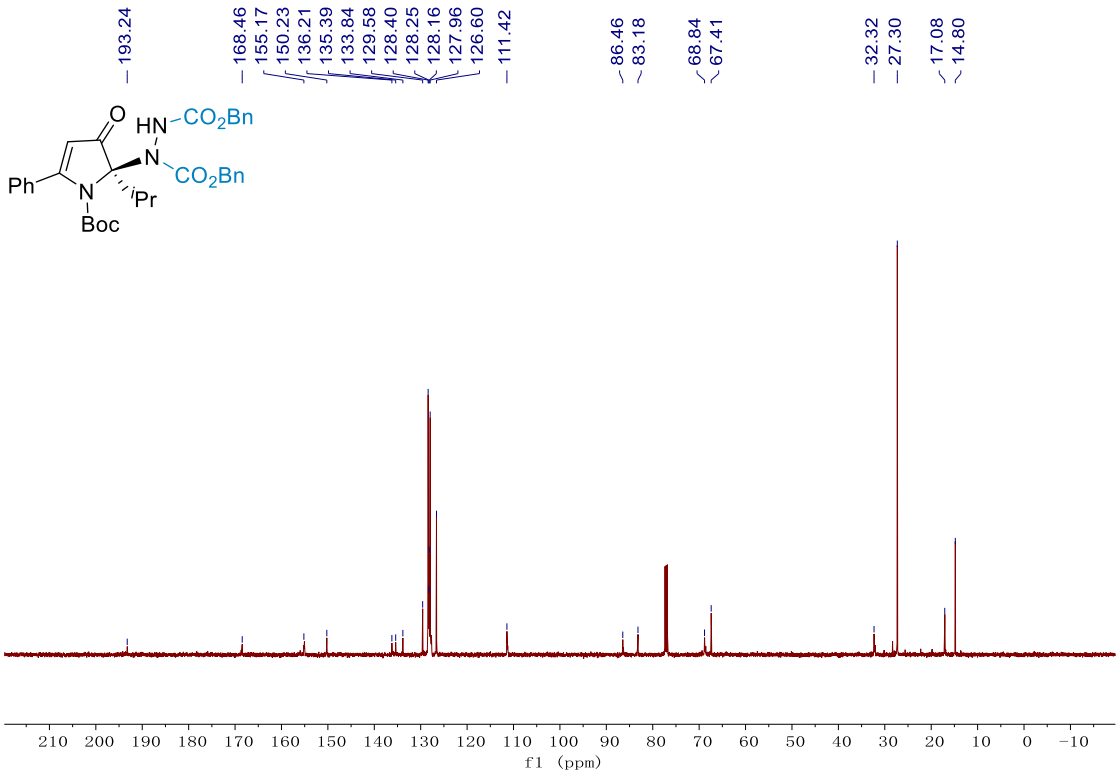
tert-butyl 2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrole-1-carboxylate (7)



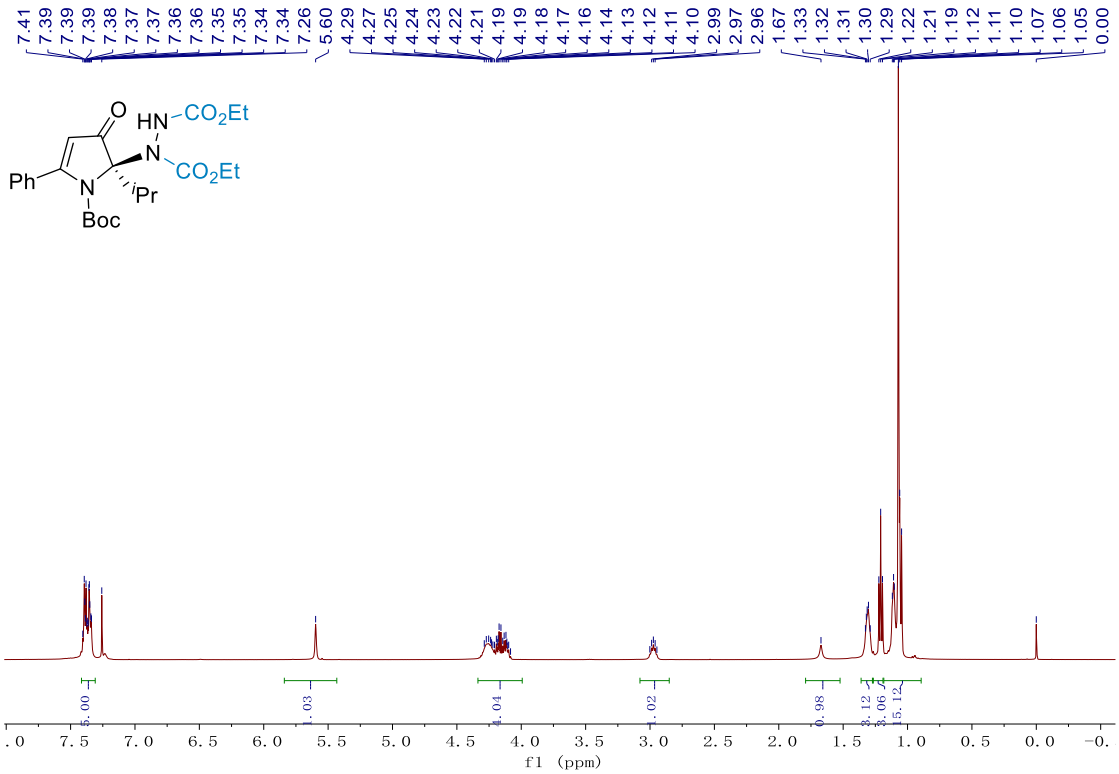


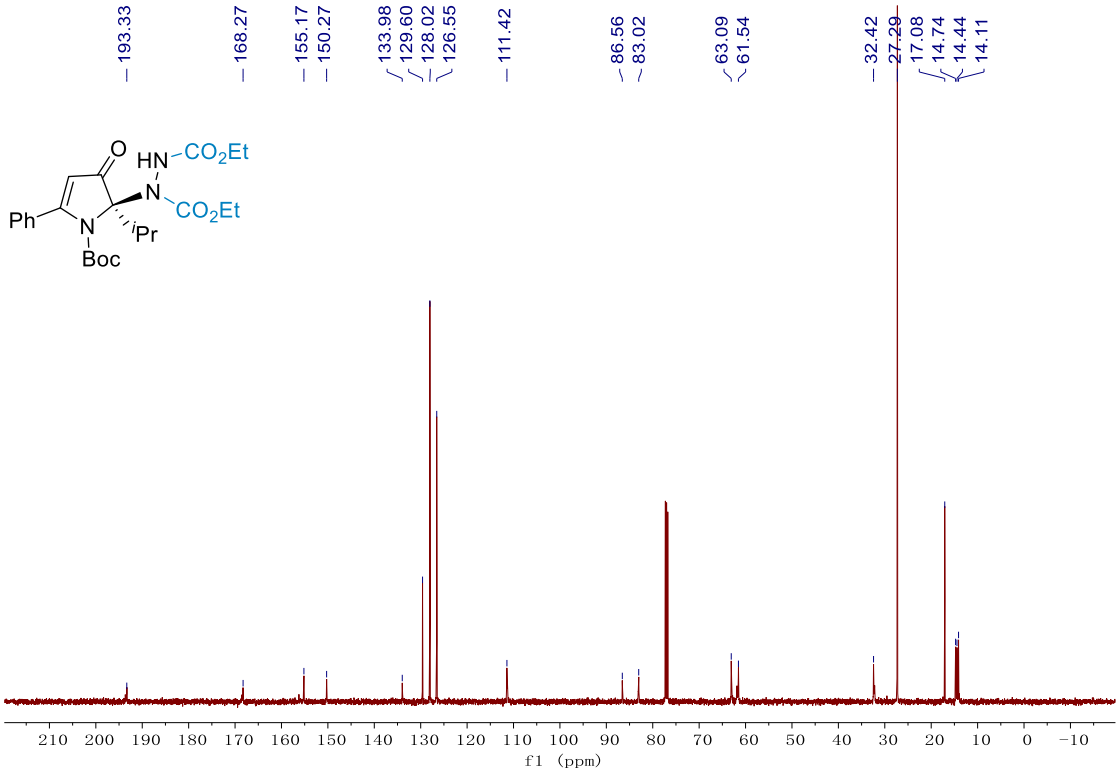
Dibenzyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3a)



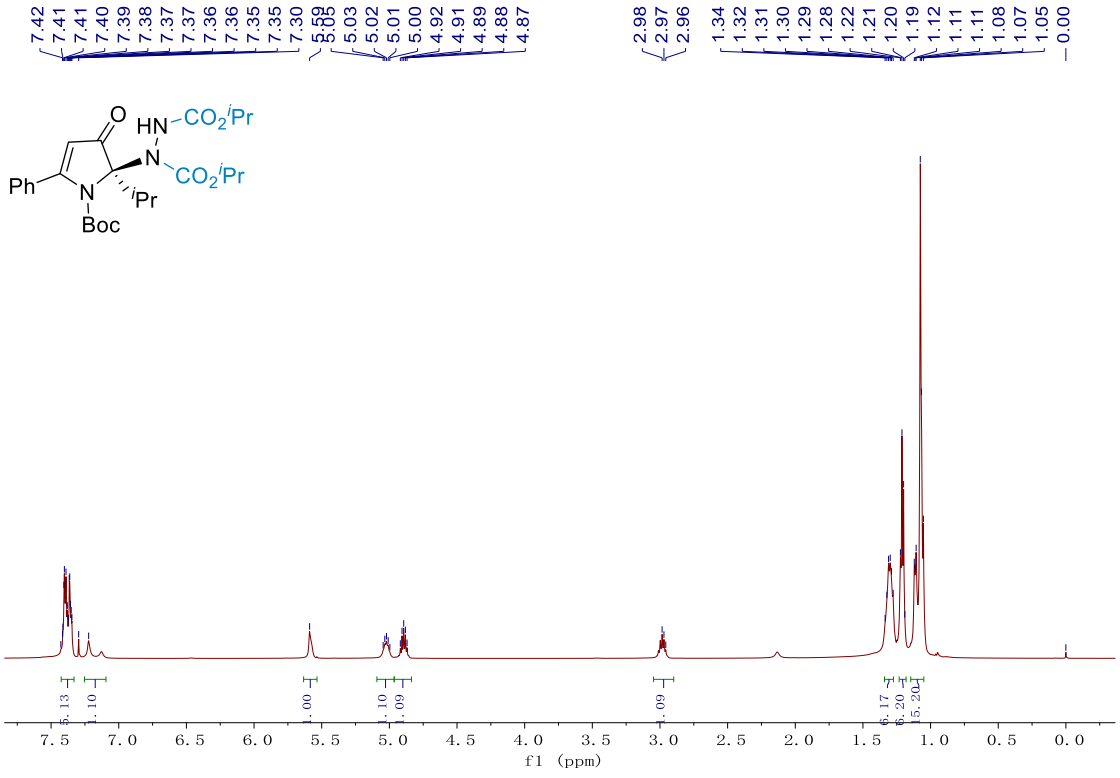


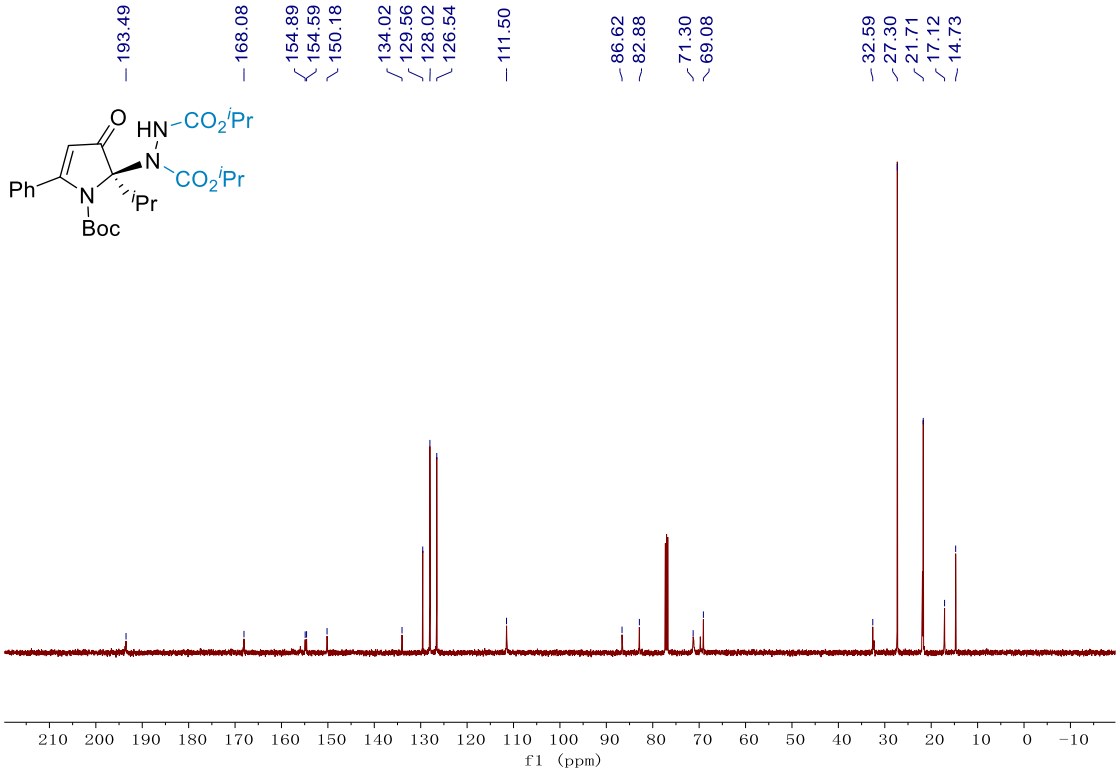
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3b)



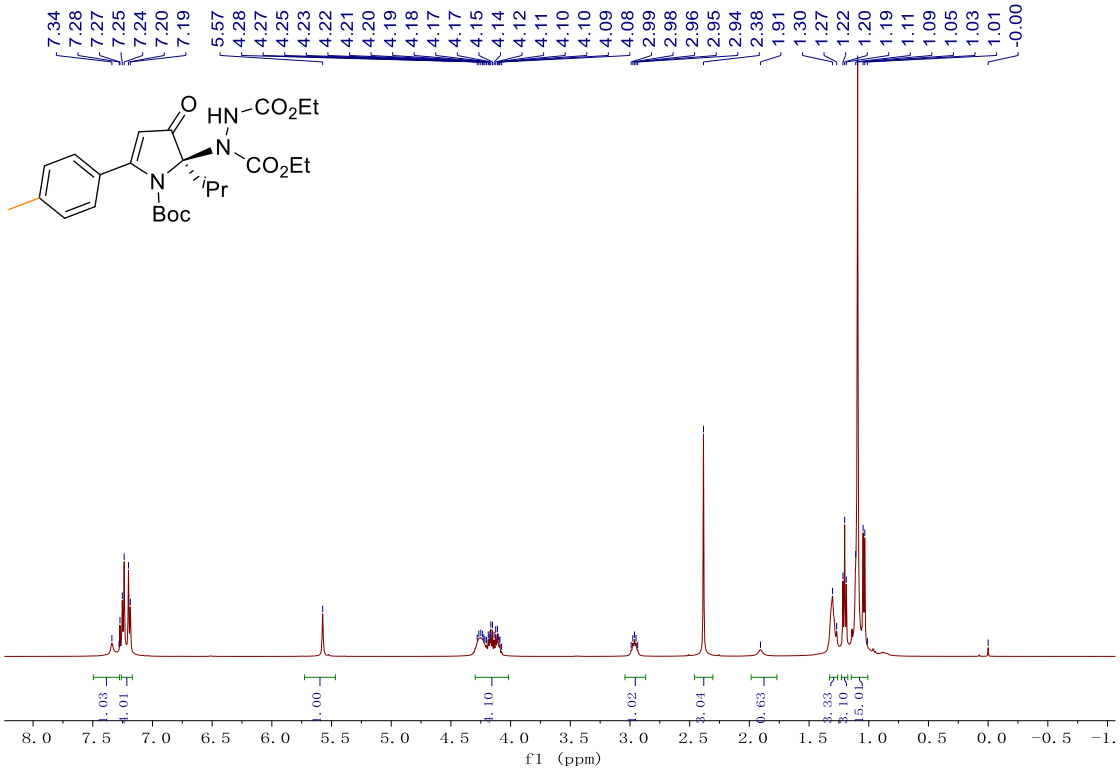


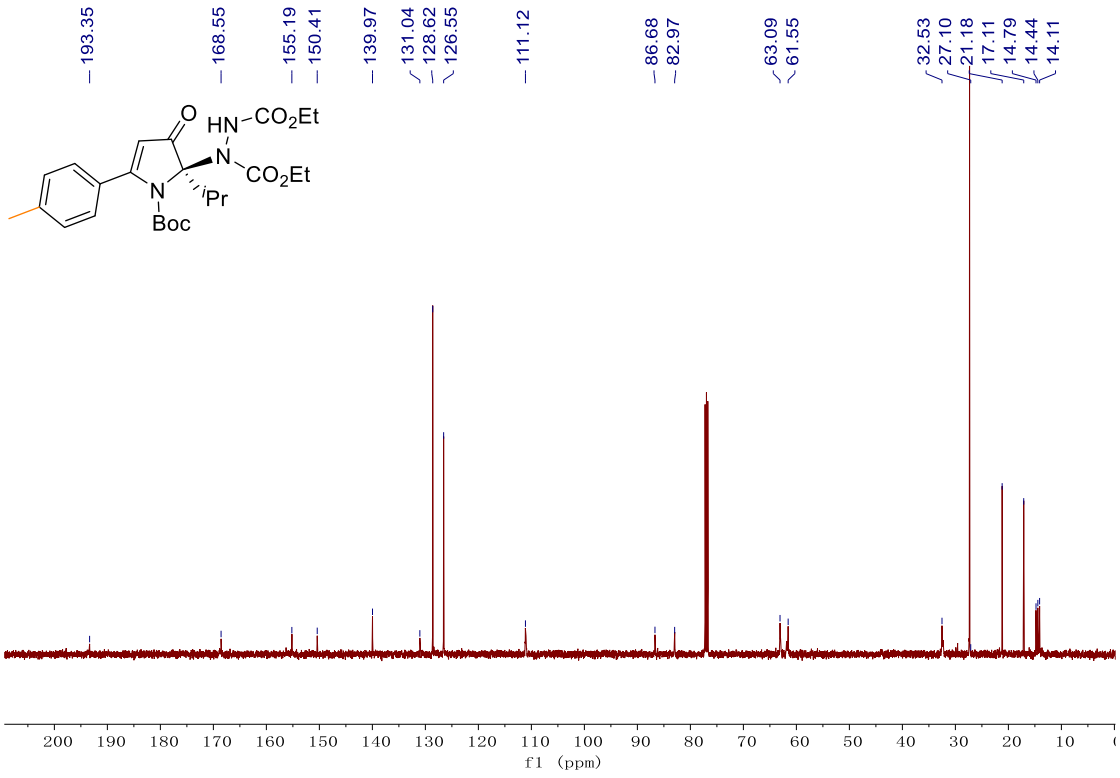
diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3c)



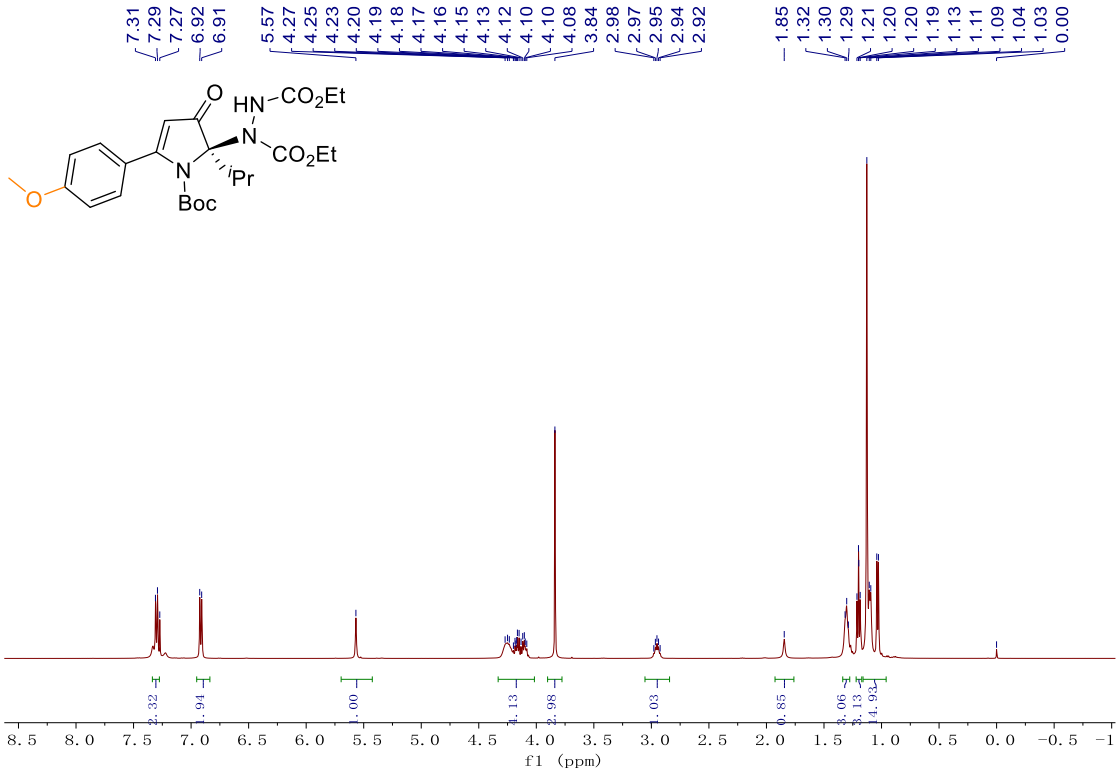


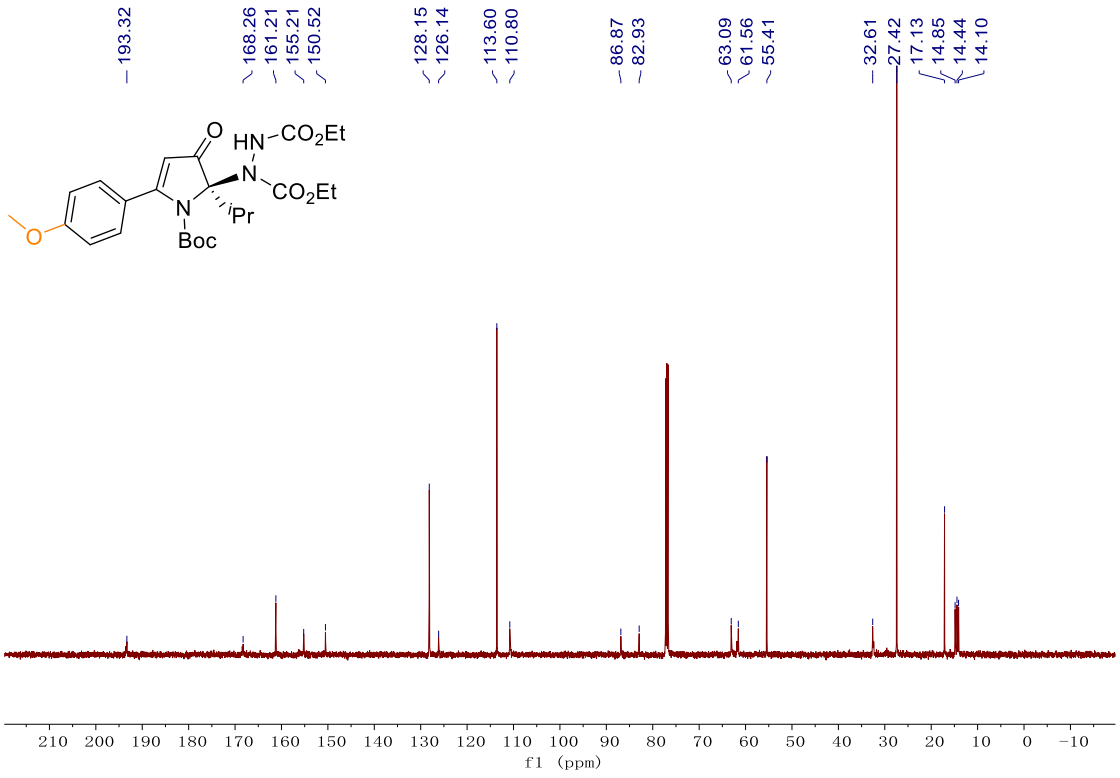
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(p-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3d)



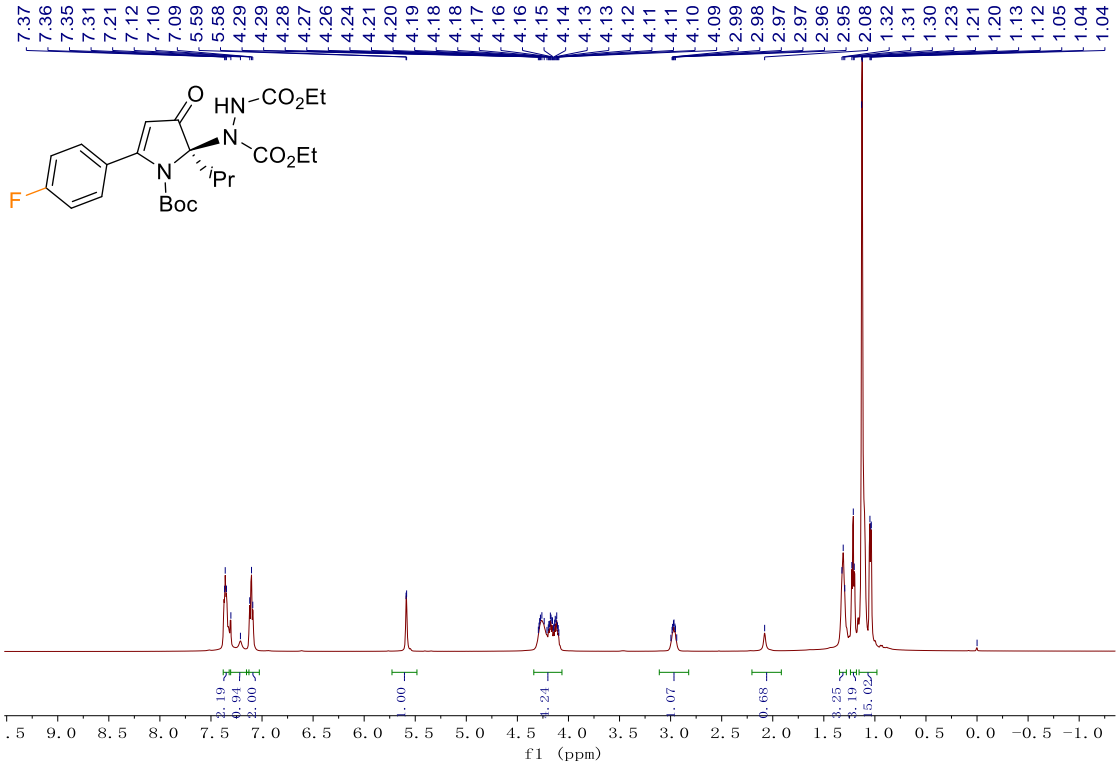


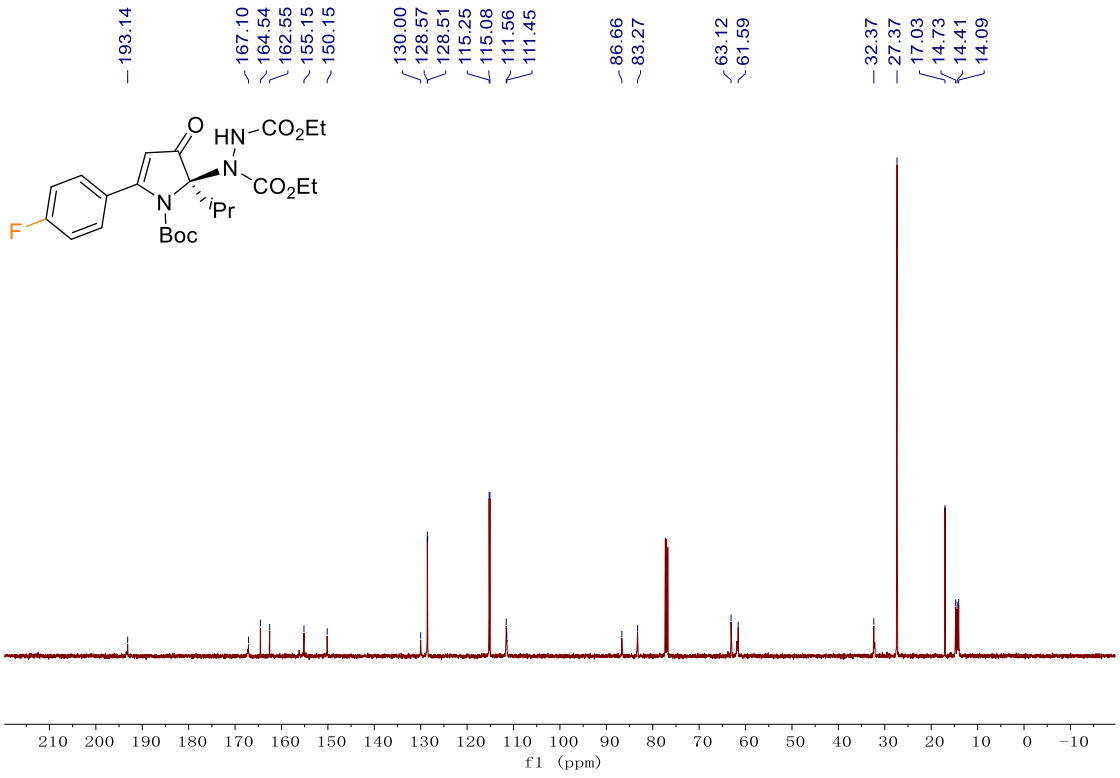
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-5-(4-methoxyphenyl)-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3e)

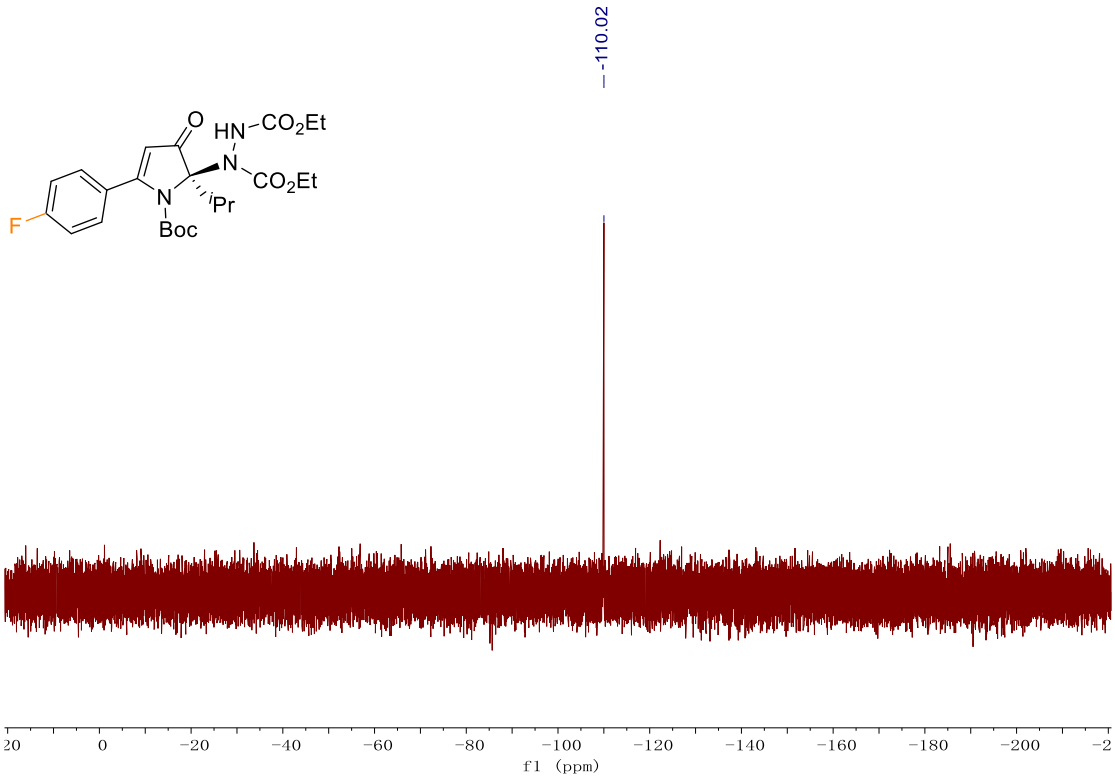




diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3f)






-110.02
O
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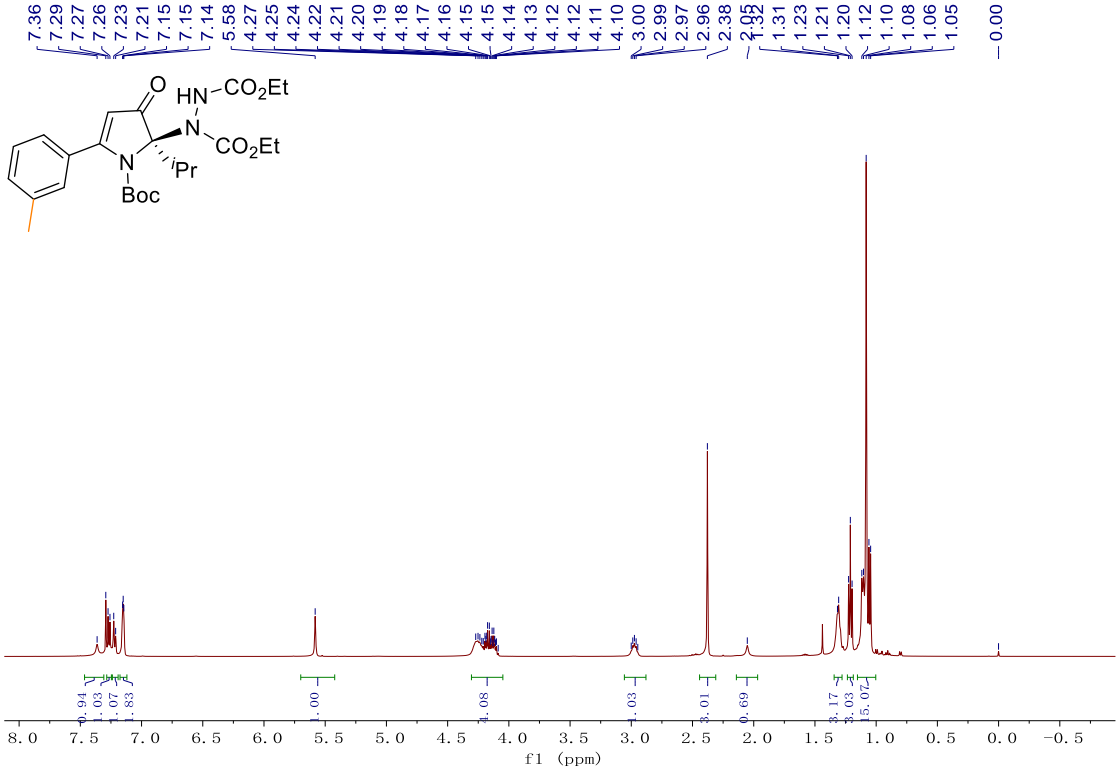
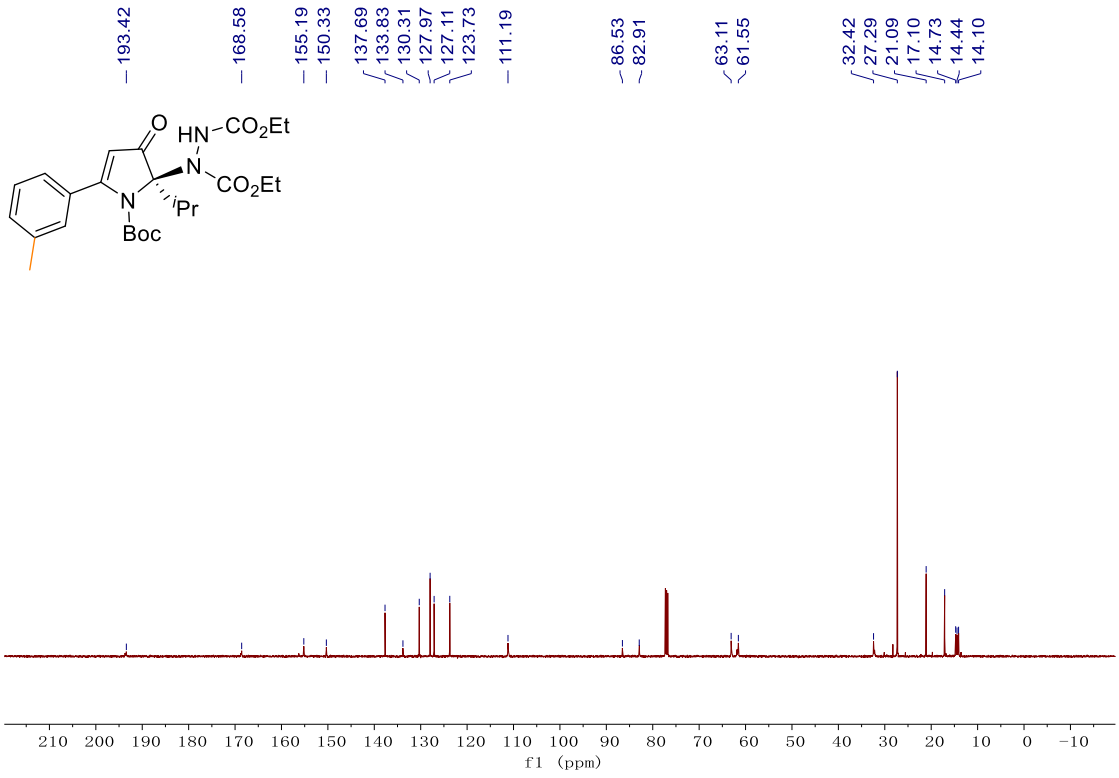
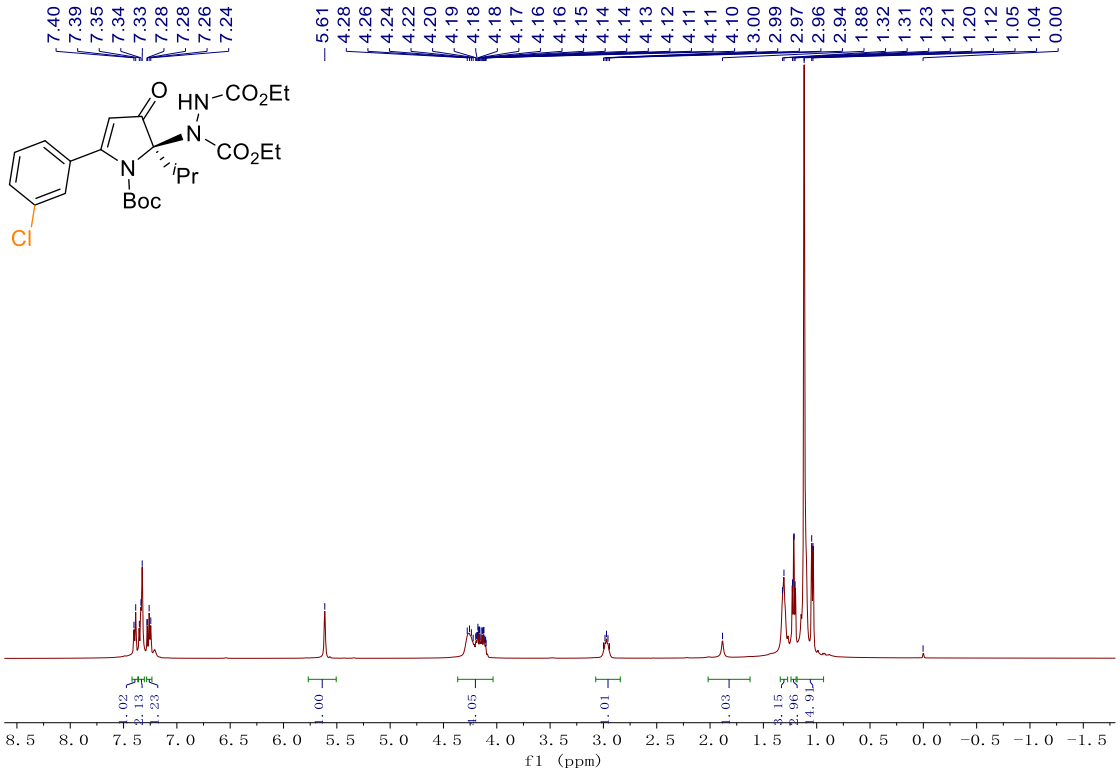
CO2Et
N
CO2Et
iPr
N
Boc
F
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

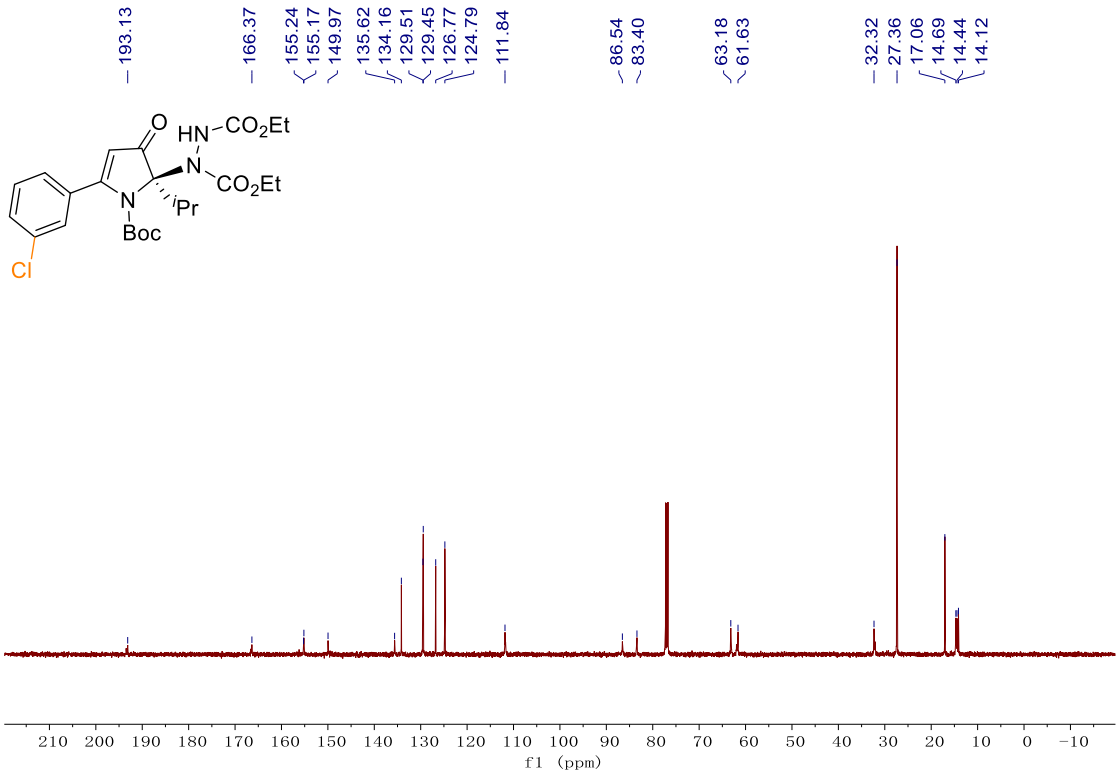
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(m-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3g)



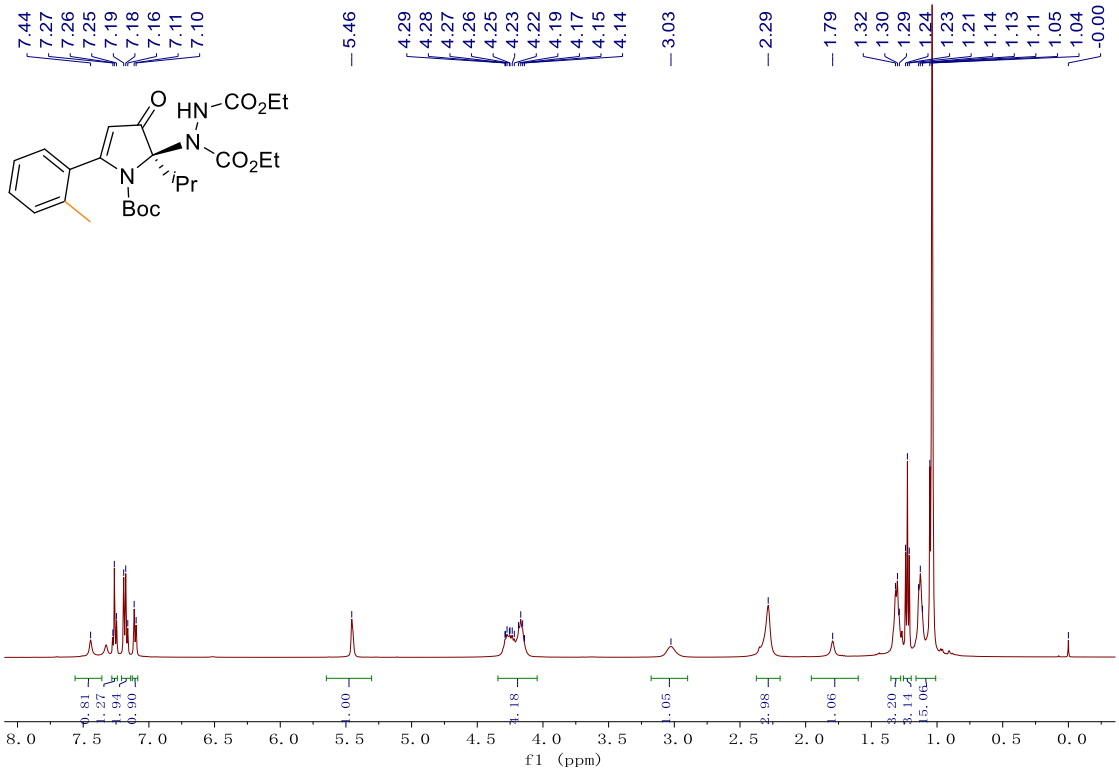


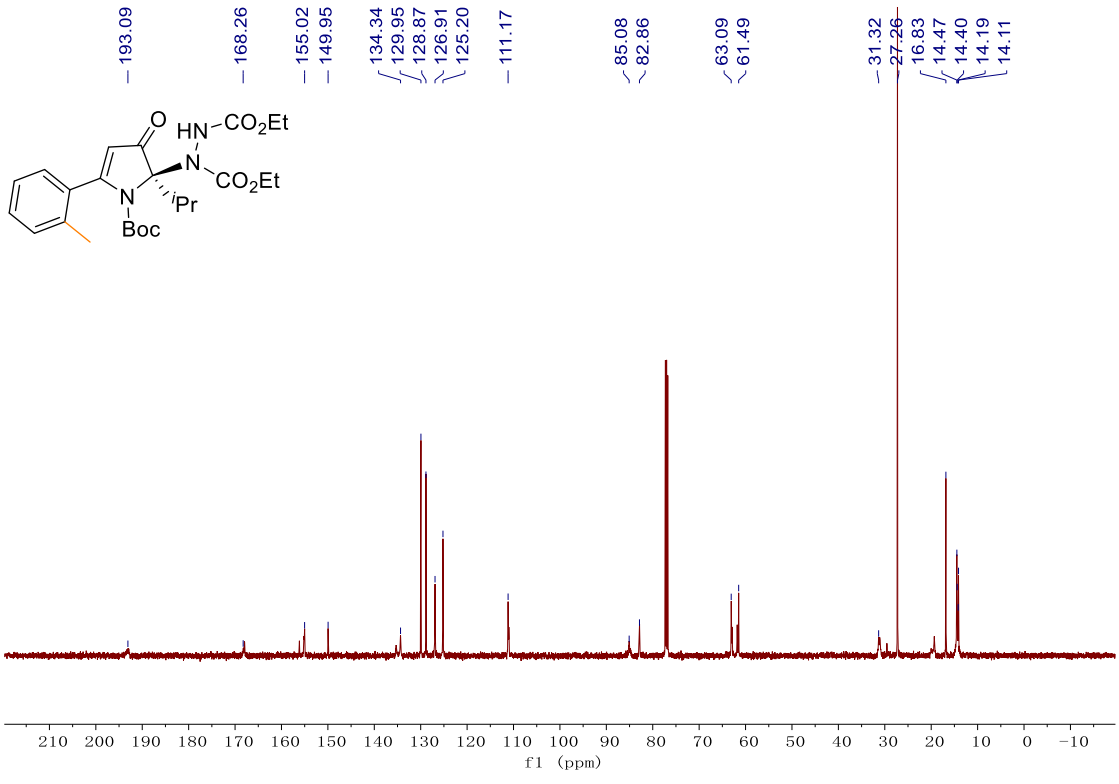
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(3-chlorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3h)



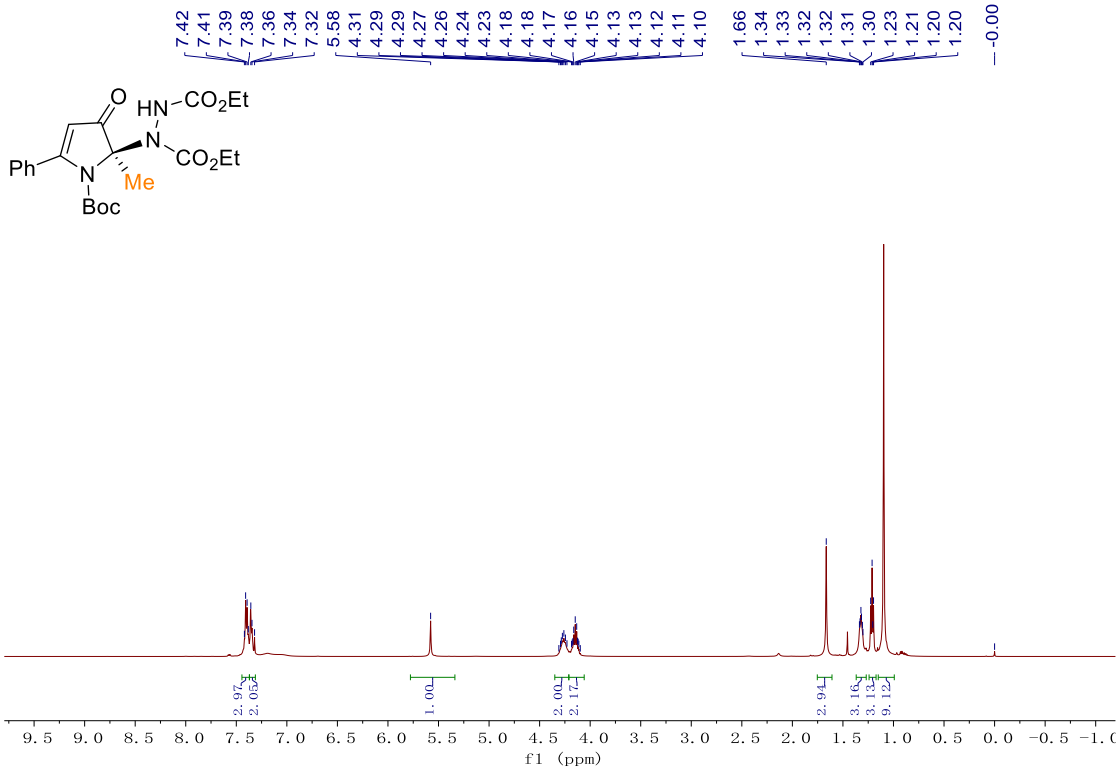


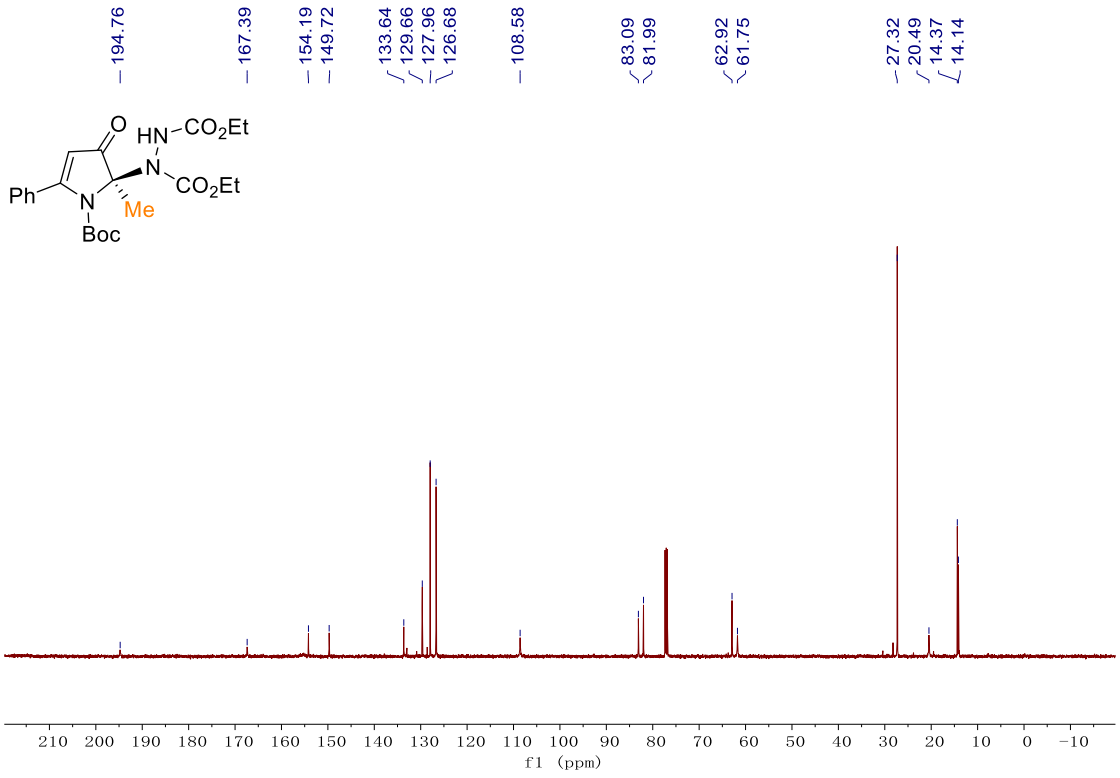
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(o-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3i)



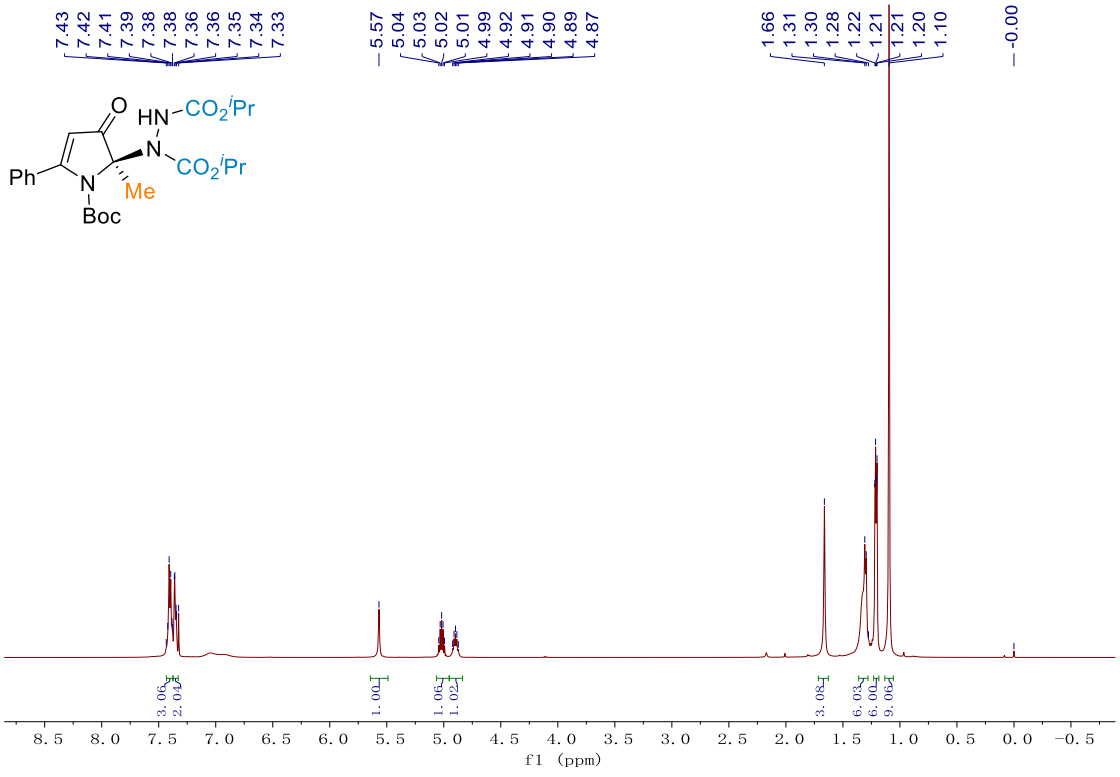


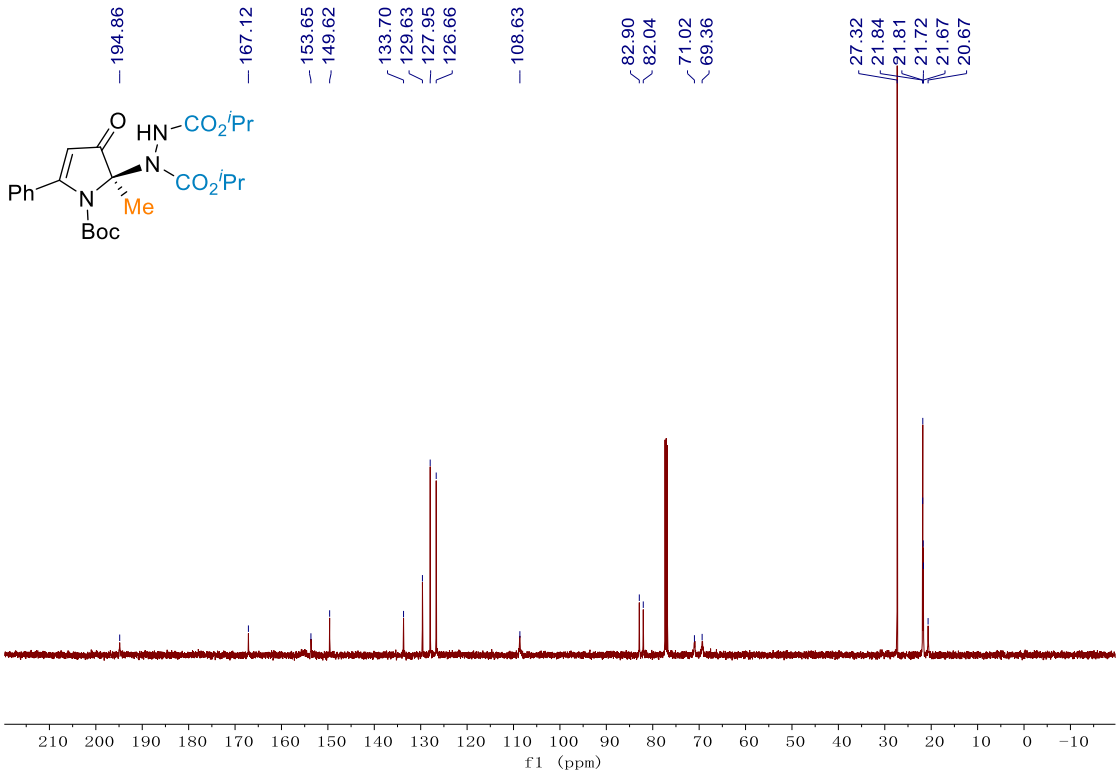
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3j)



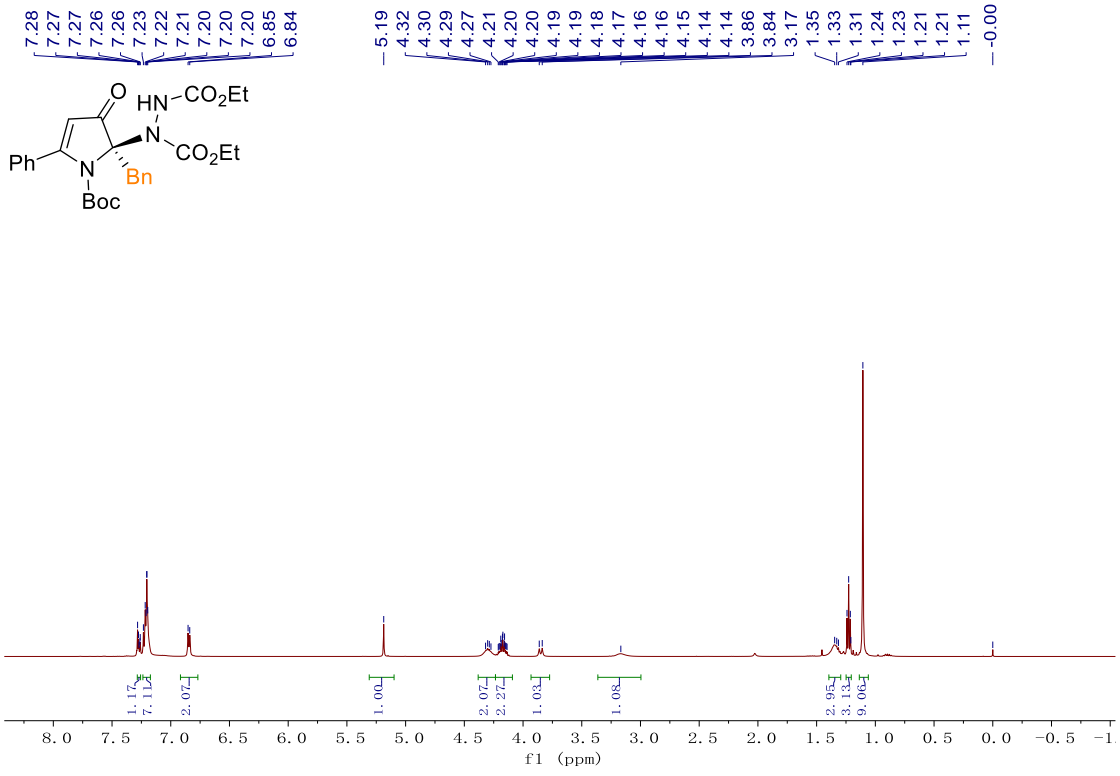


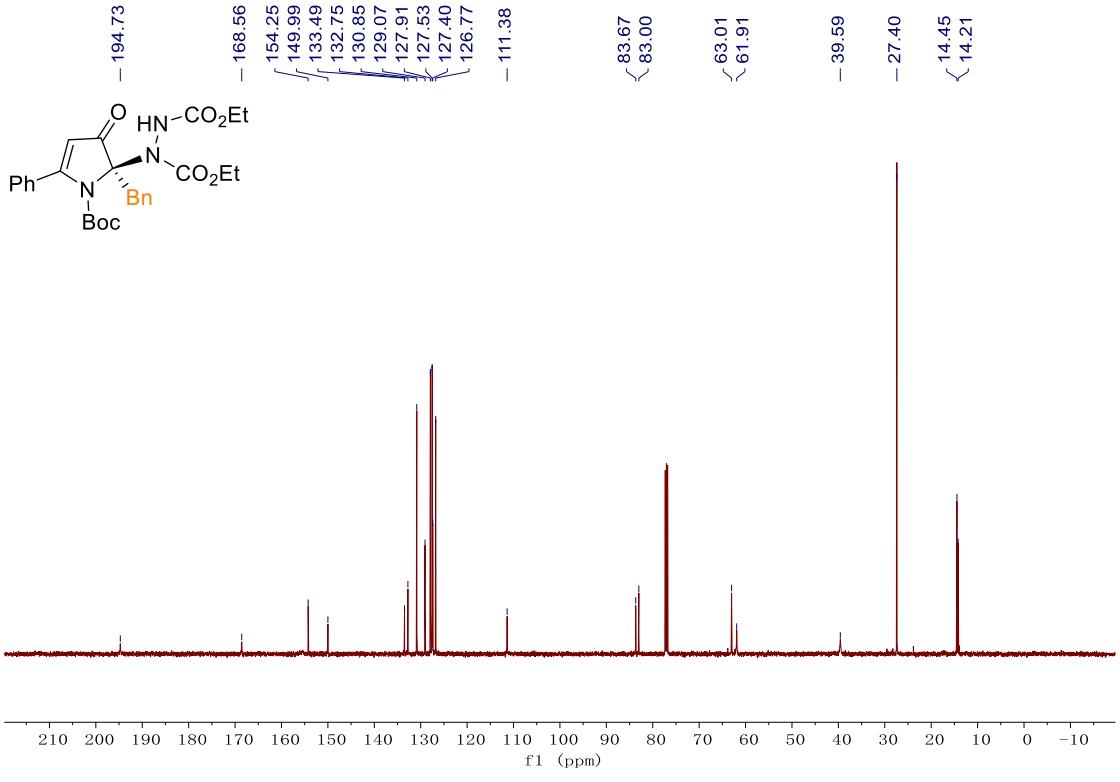
diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3k)



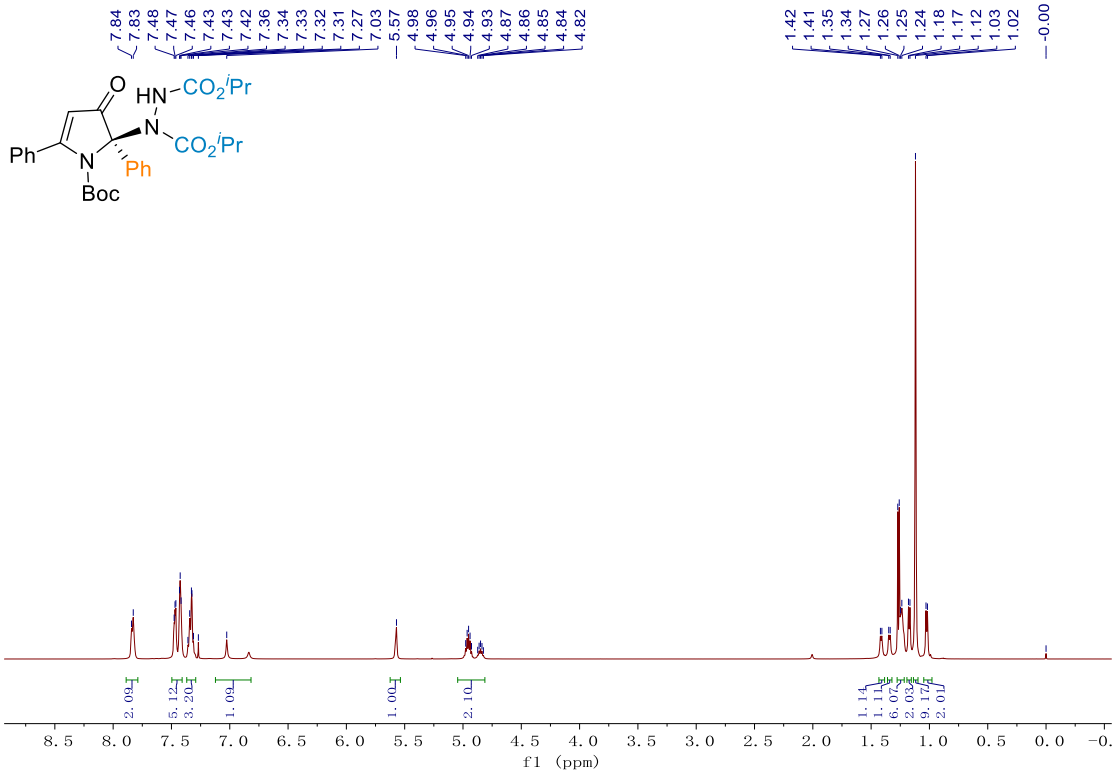


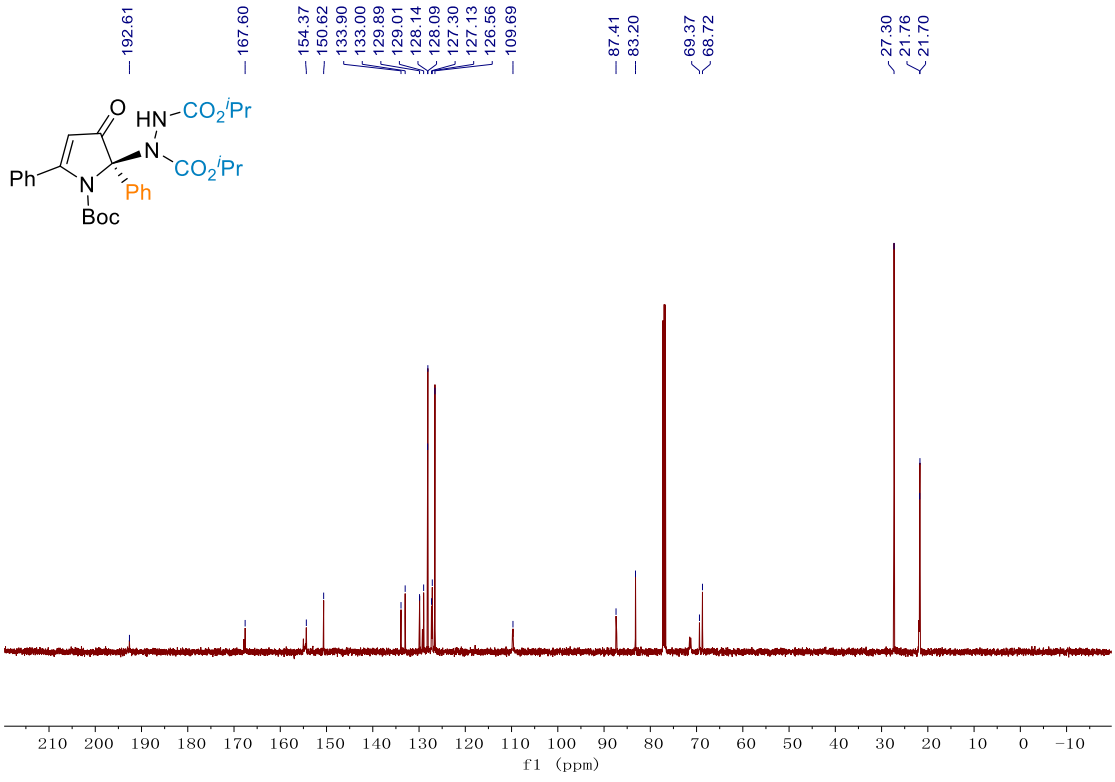
diethyl (*R*)-1-(2-benzyl-1-(tert-butoxycarbonyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3l)



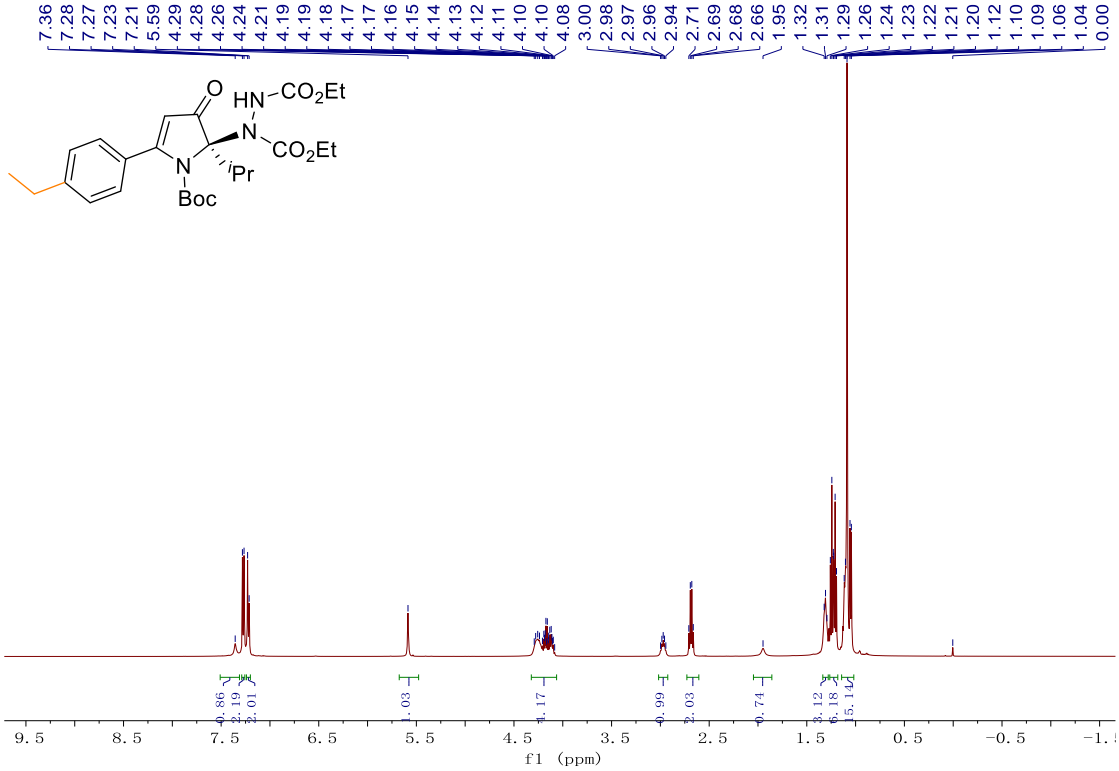


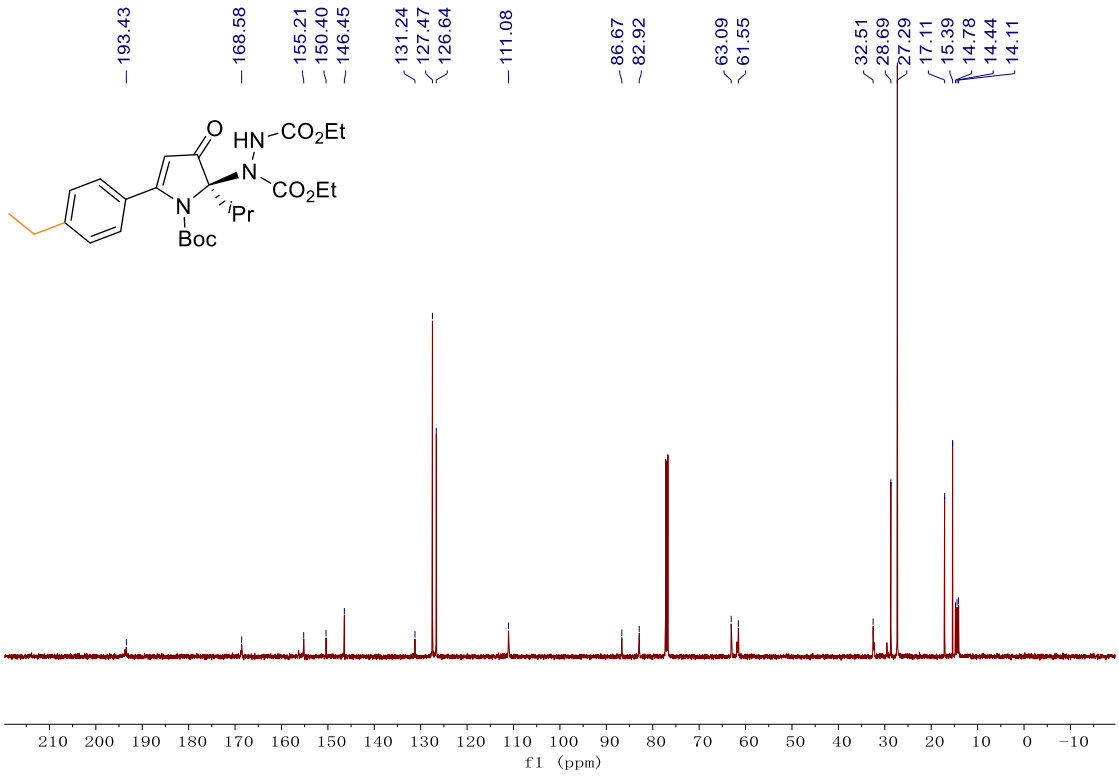
diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-2,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3m)



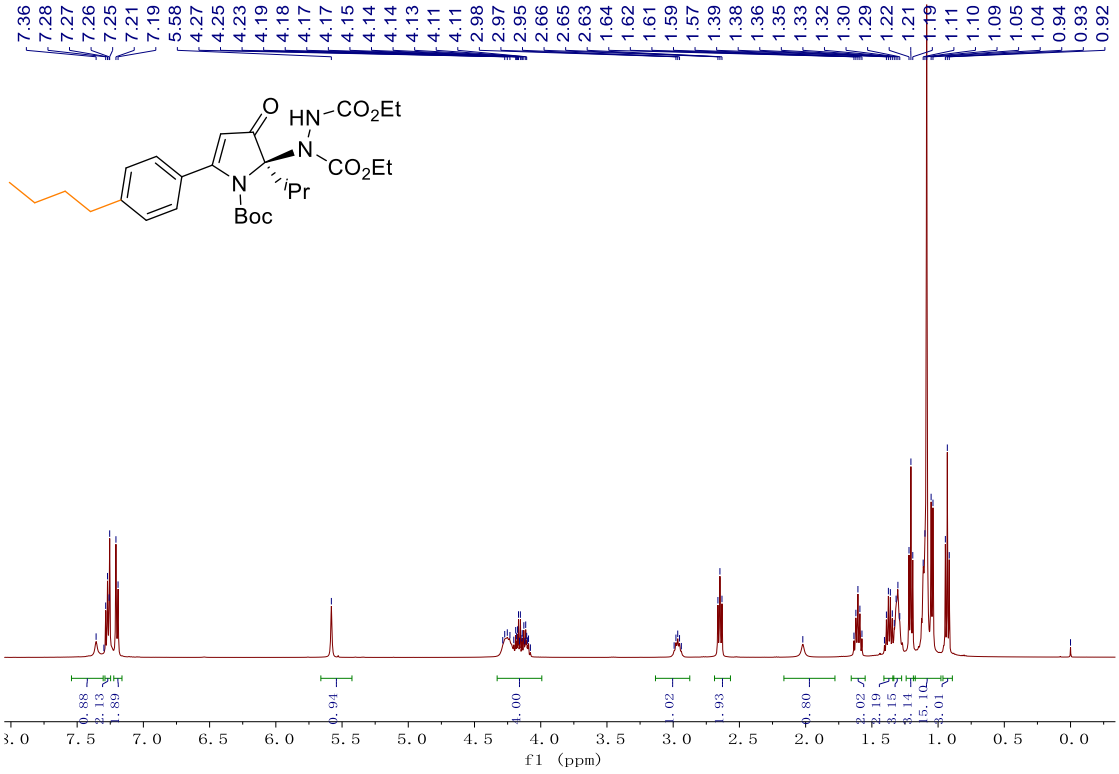


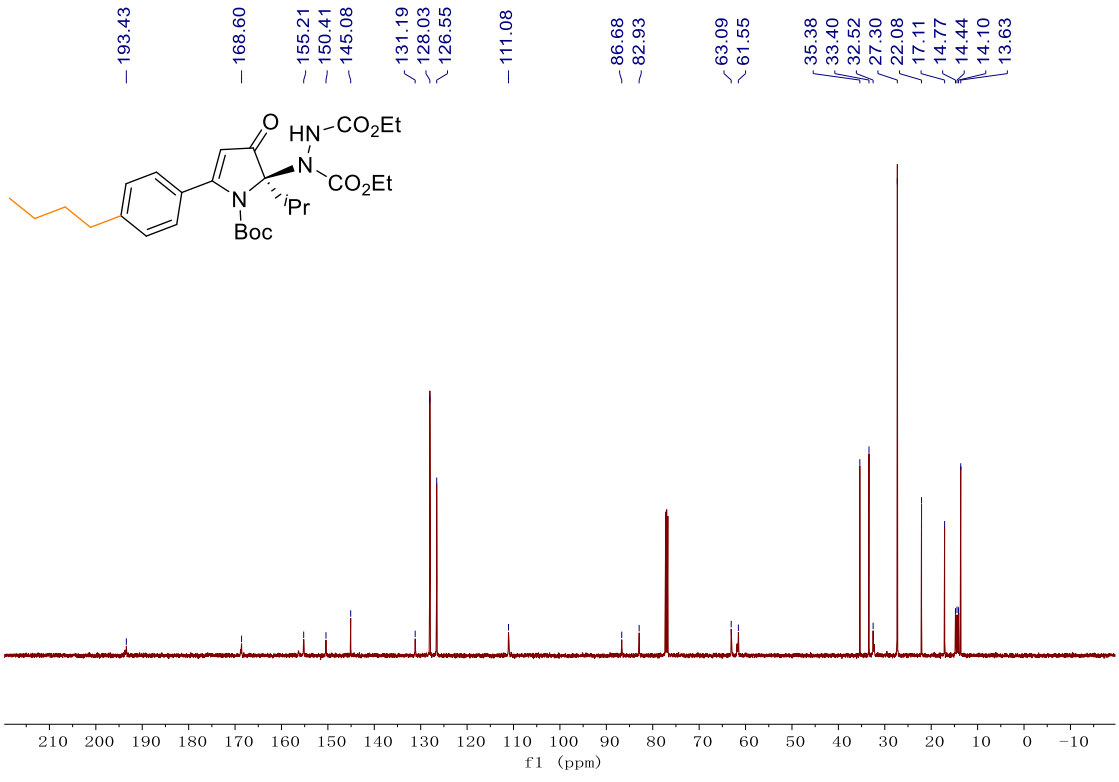
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3o)



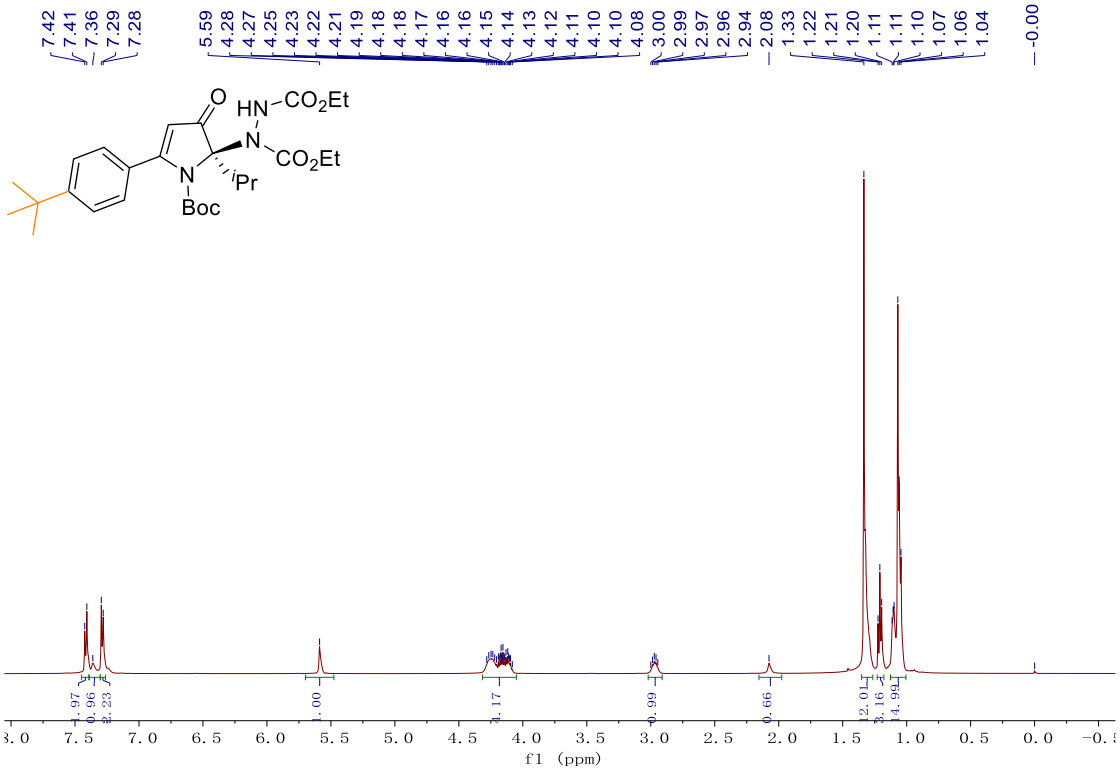


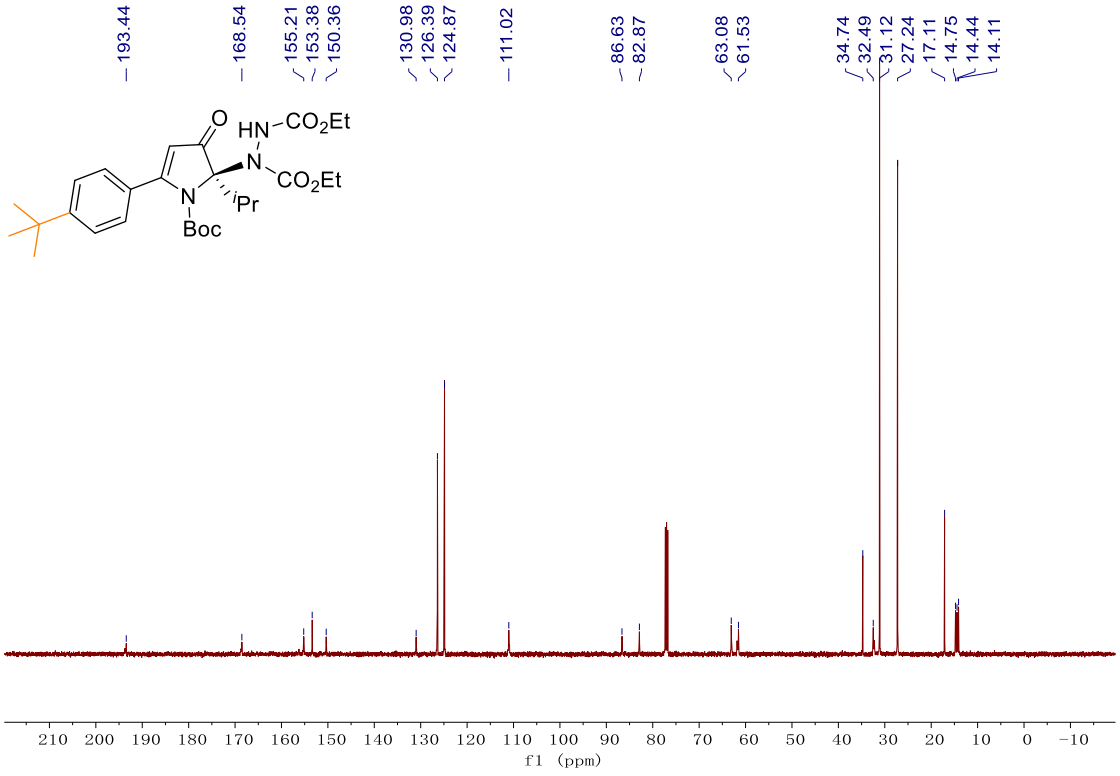
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-butylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3p)



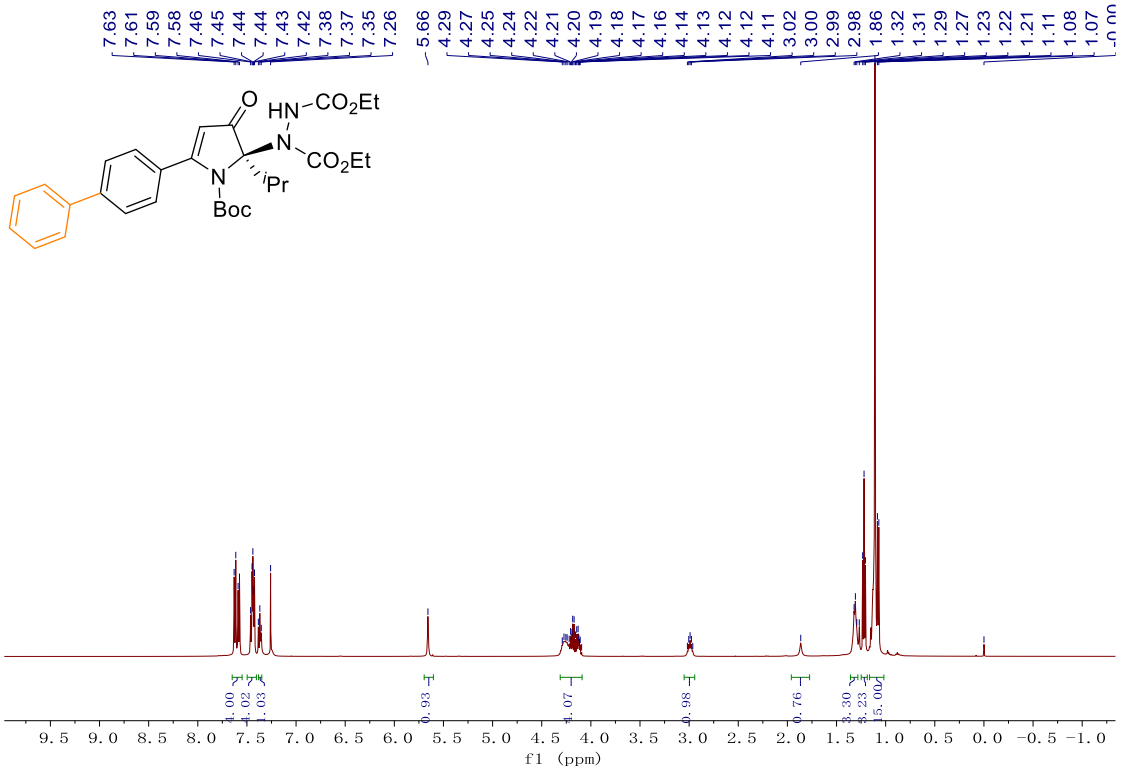


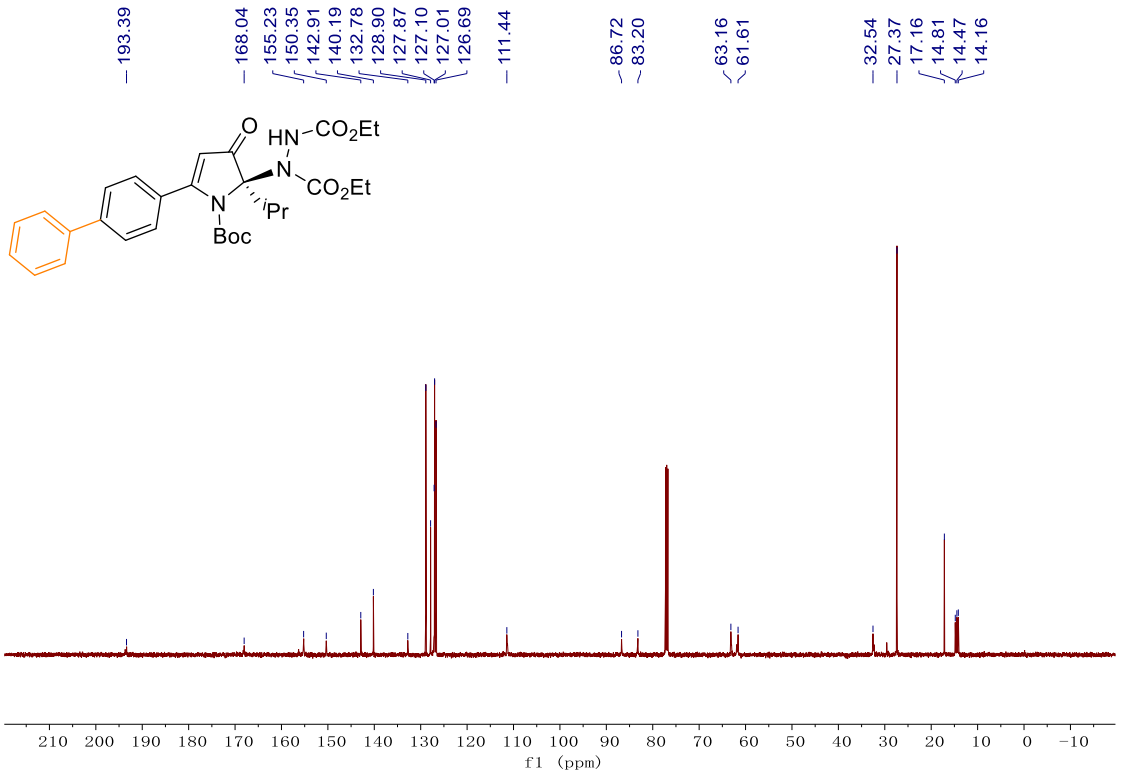
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-(tert-butyl)phenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3q)



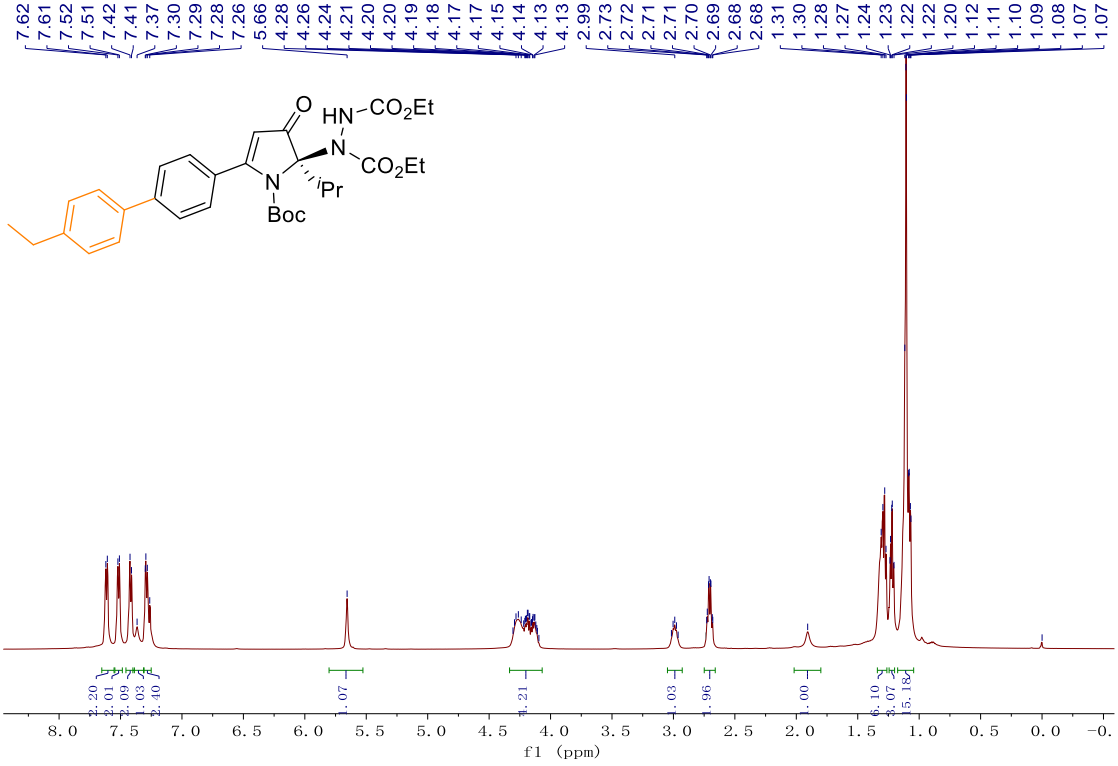


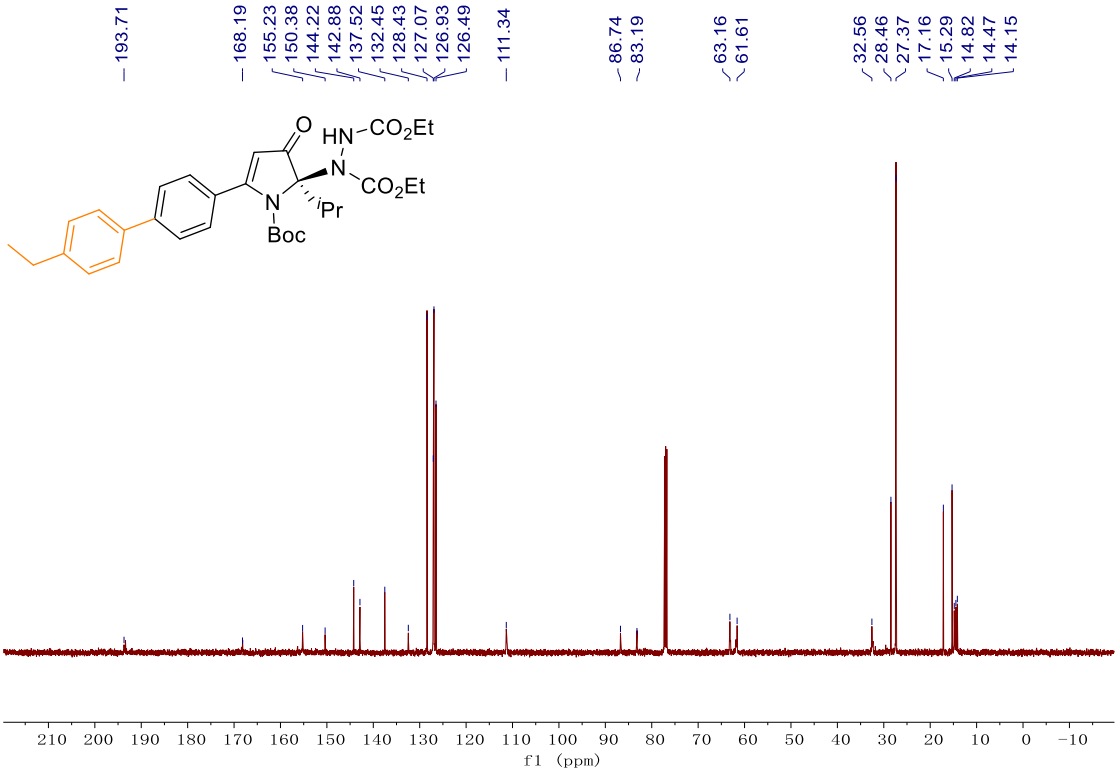
diethyl (*R*)-1-(5-([1,1'-biphenyl]-4-yl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3r)



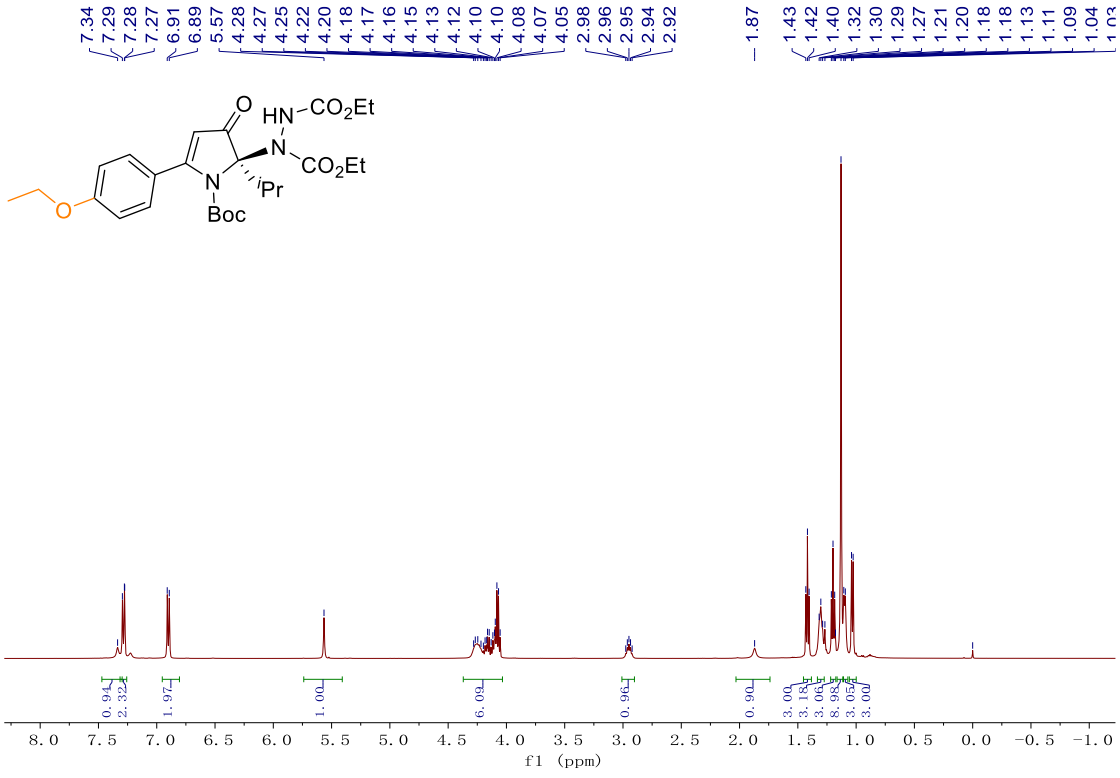


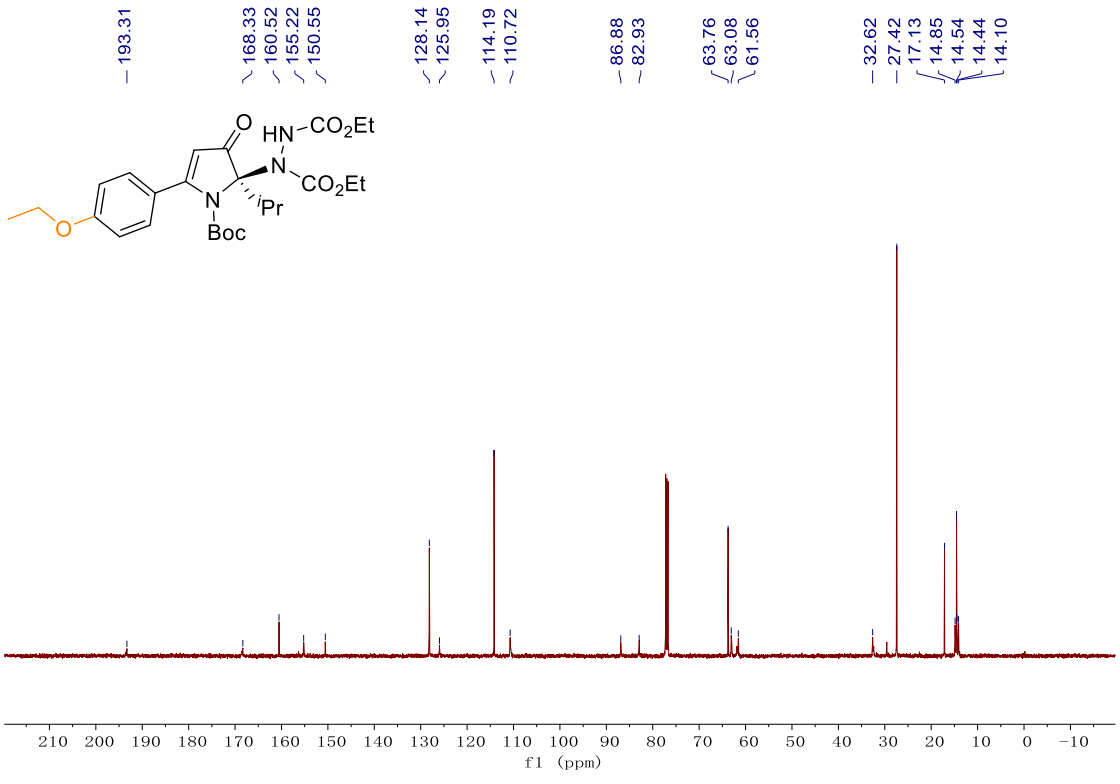
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4'-ethyl-[1,1'-biphenyl]-4-yl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3s)



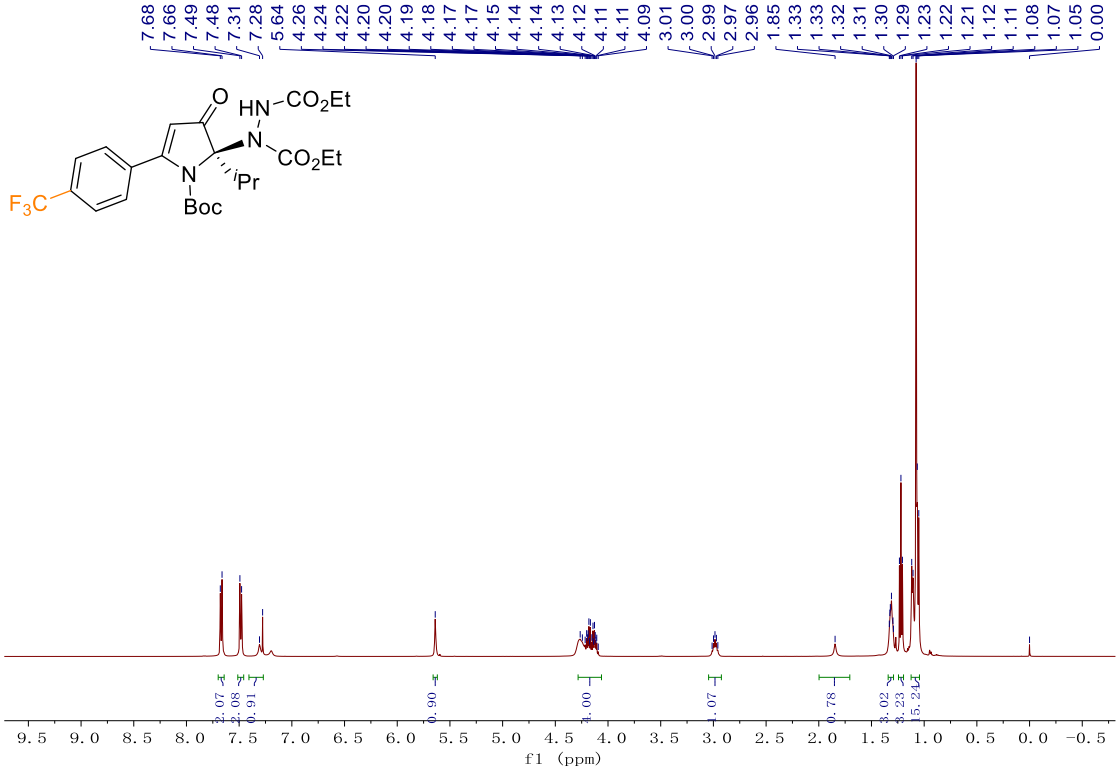


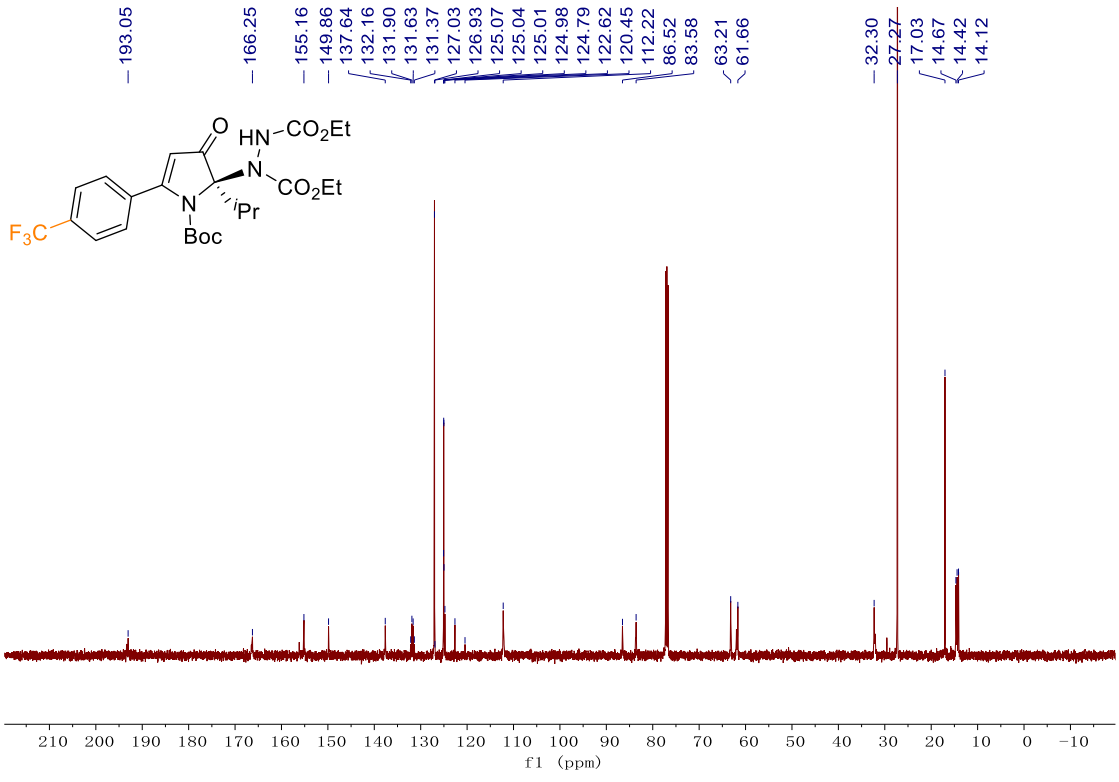
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethoxyphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3t)

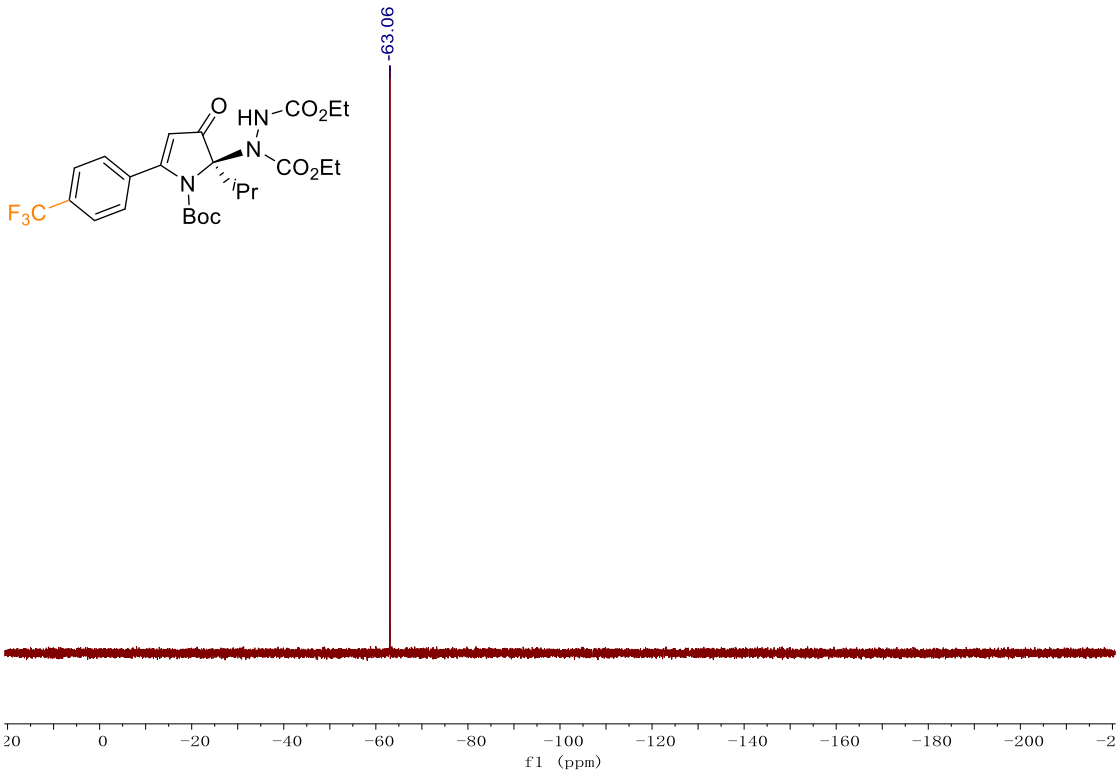




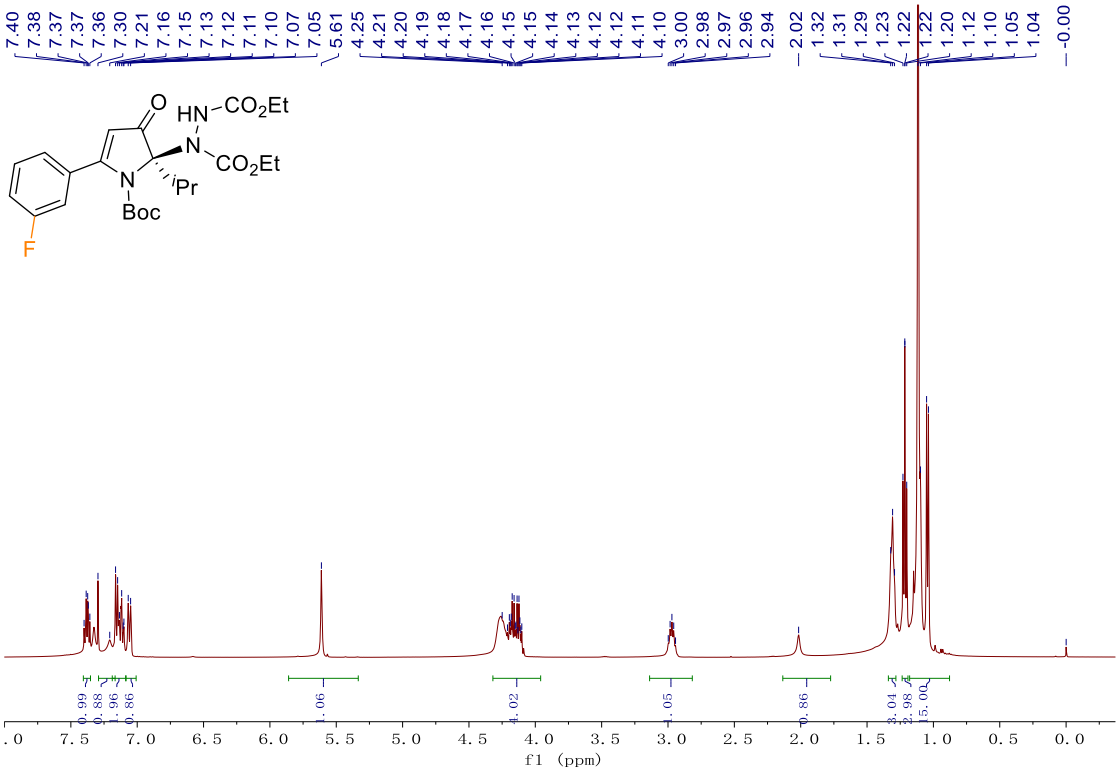
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3u)

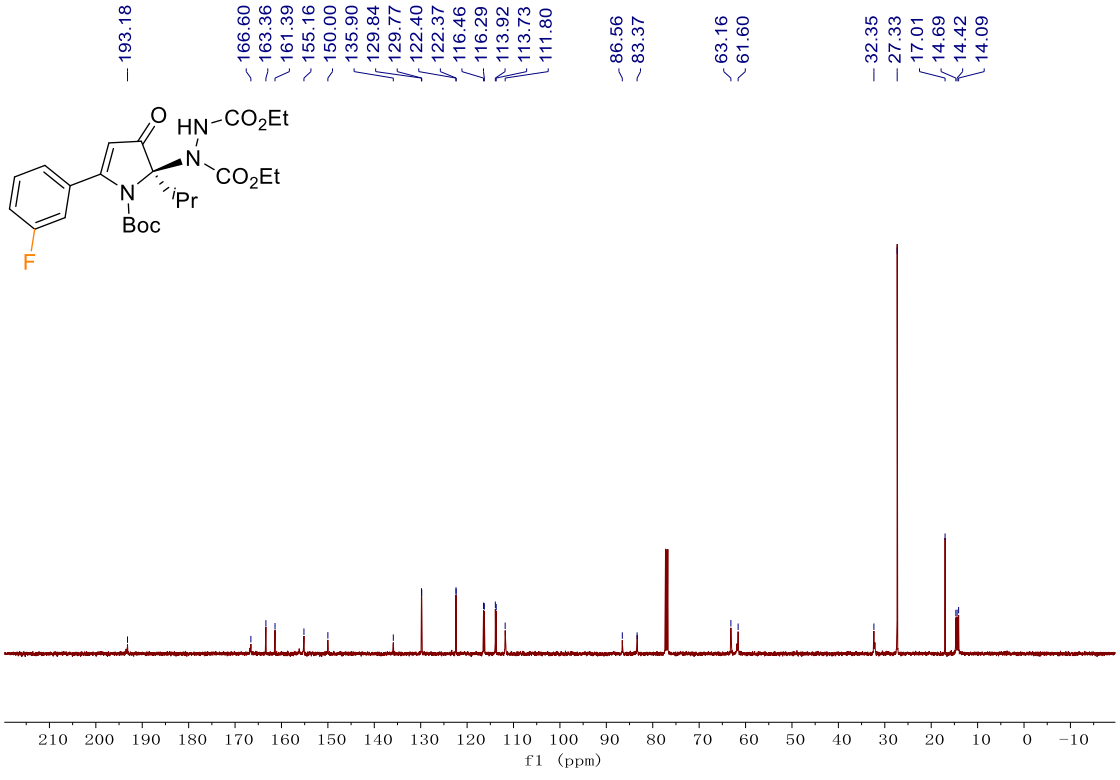


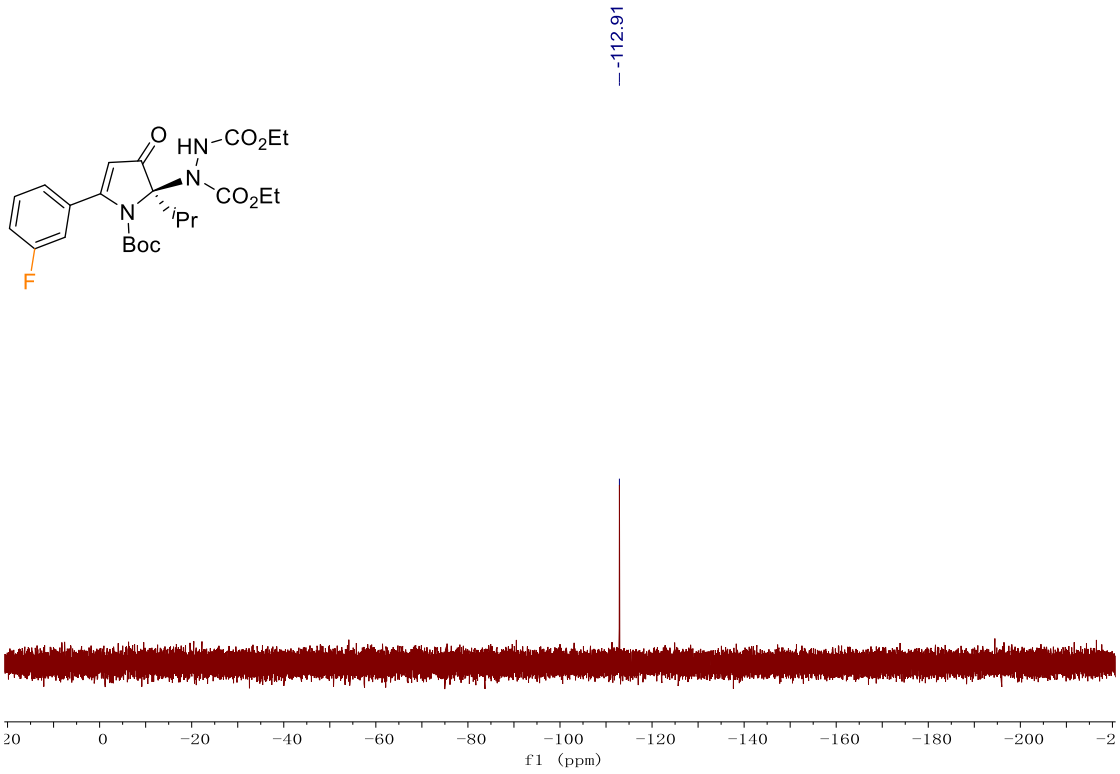



-63.06
O
HN
CO2Et
N
CO2Et
N
iPr
Boc
F3C
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(3-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3v)






-112.91
O
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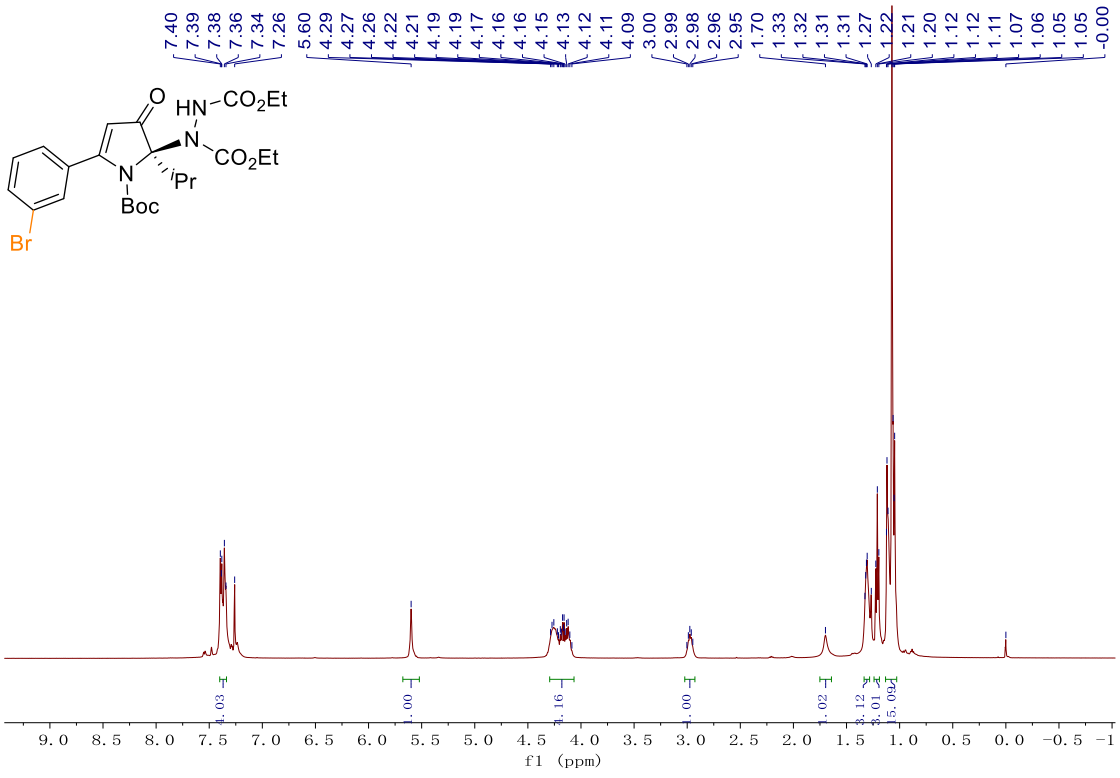
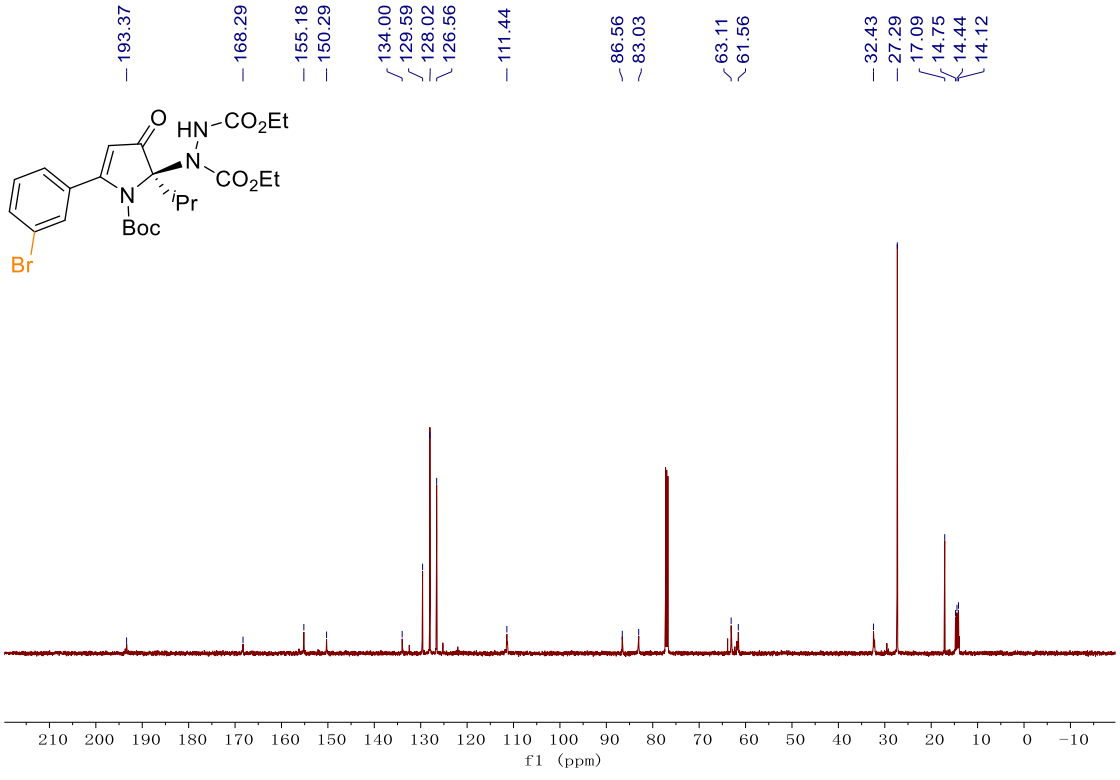
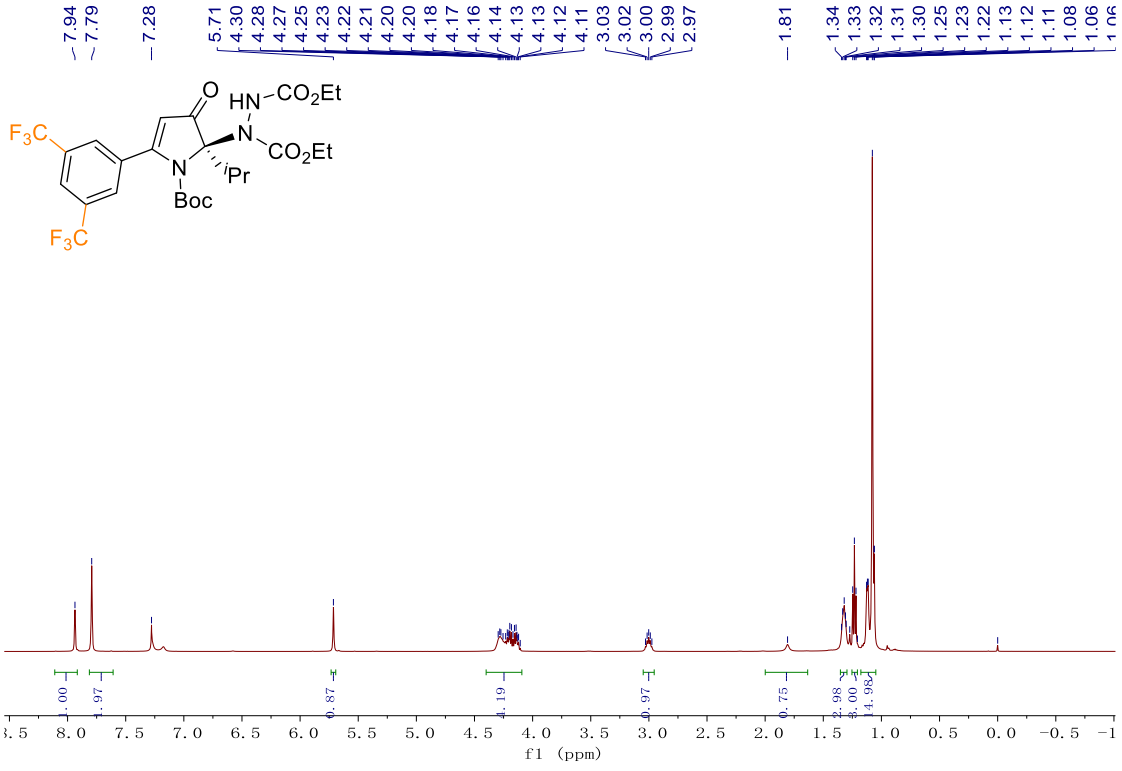
CO2Et
N
CO2Et
N
iPr
Boc
F
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

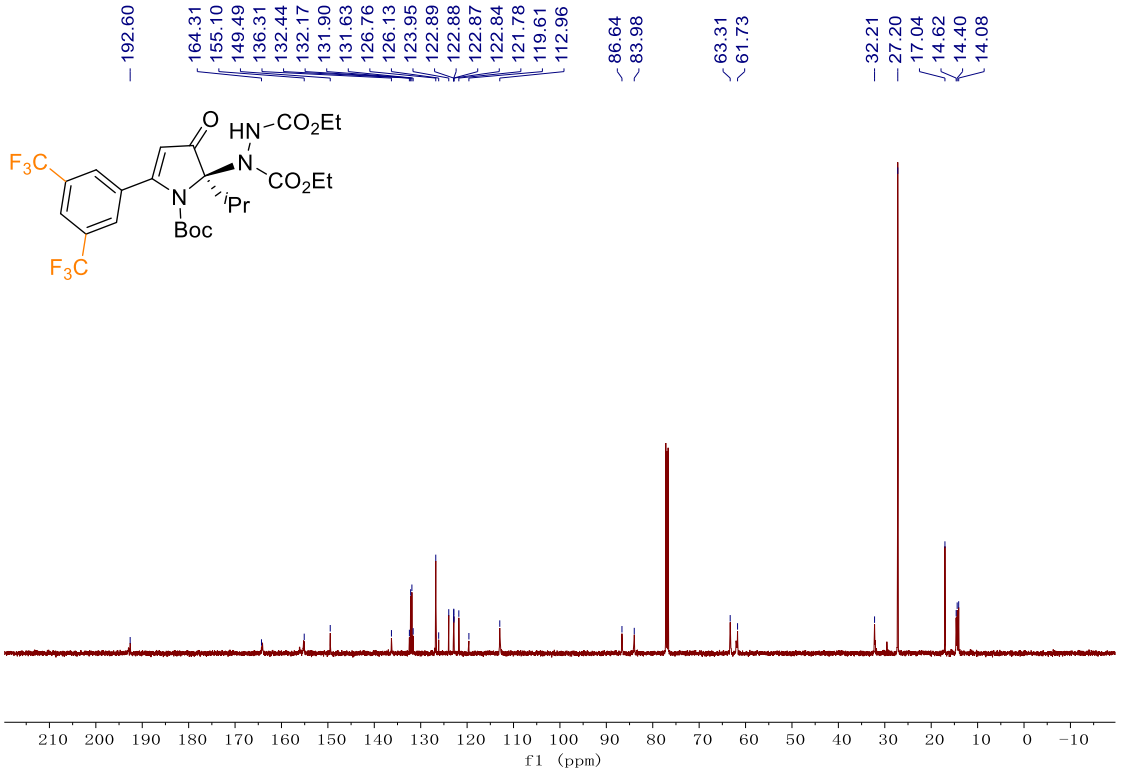
diethyl (*R*)-1-(5-(3-bromophenyl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3w)

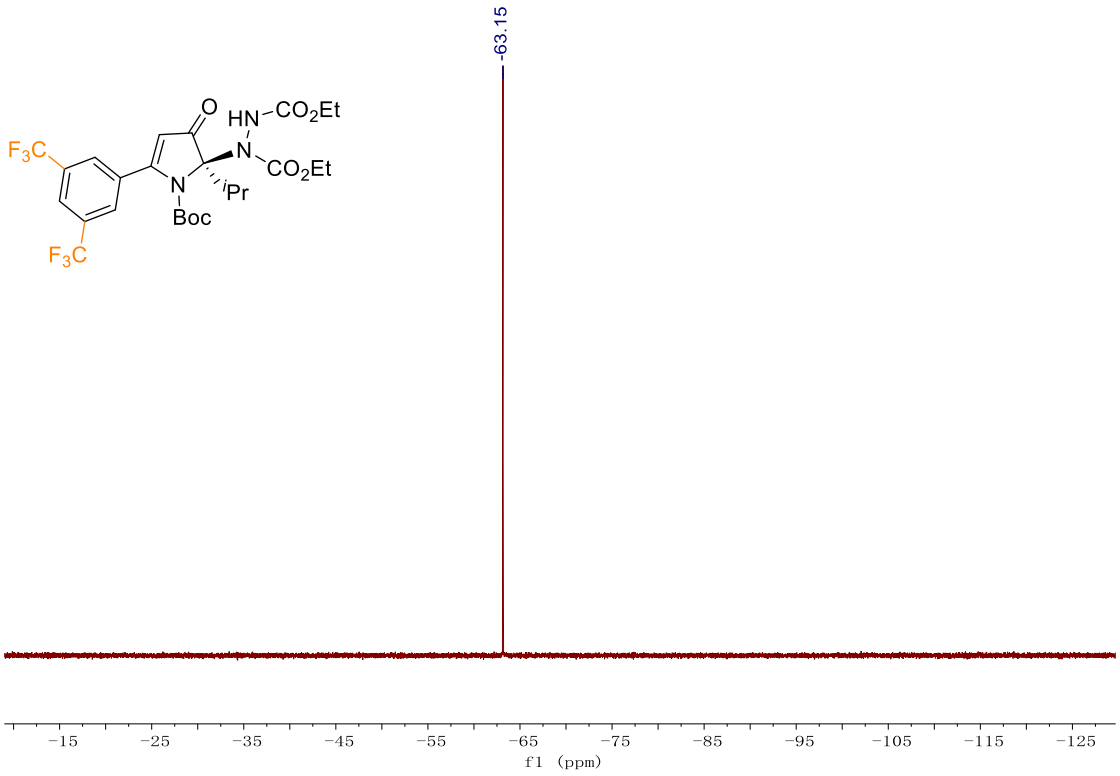




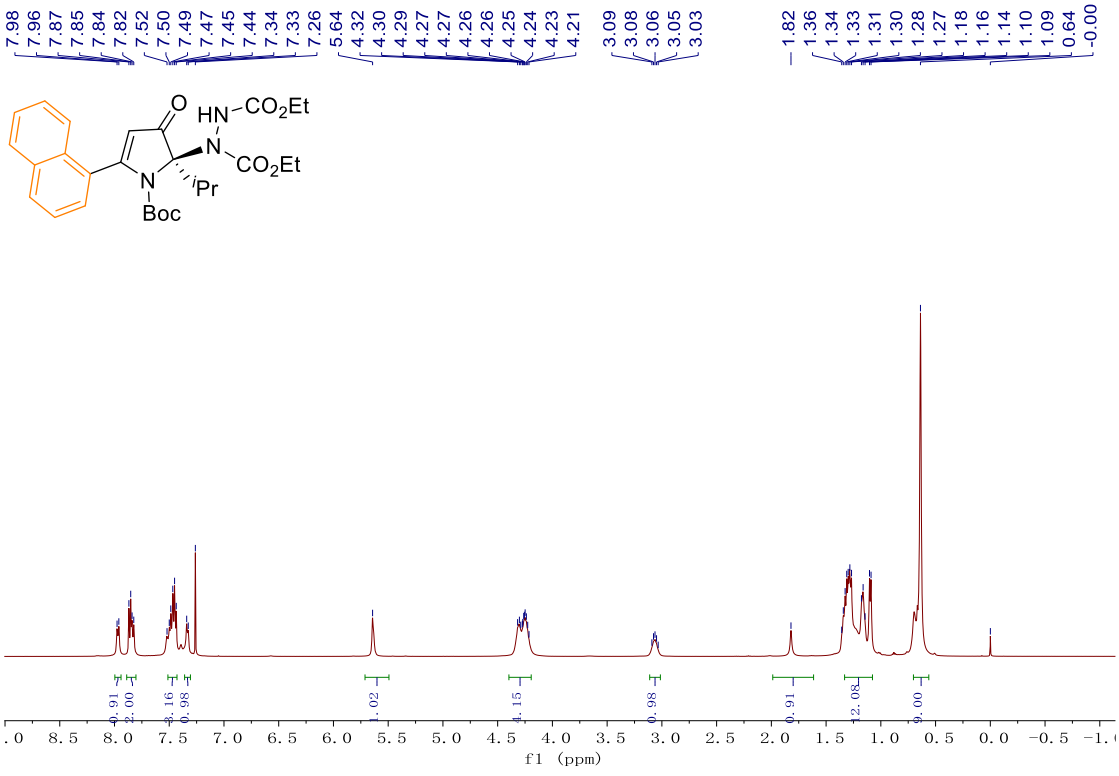
diethyl (*R*)-1-(5-(3,5-bis(trifluoromethyl)phenyl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3x)

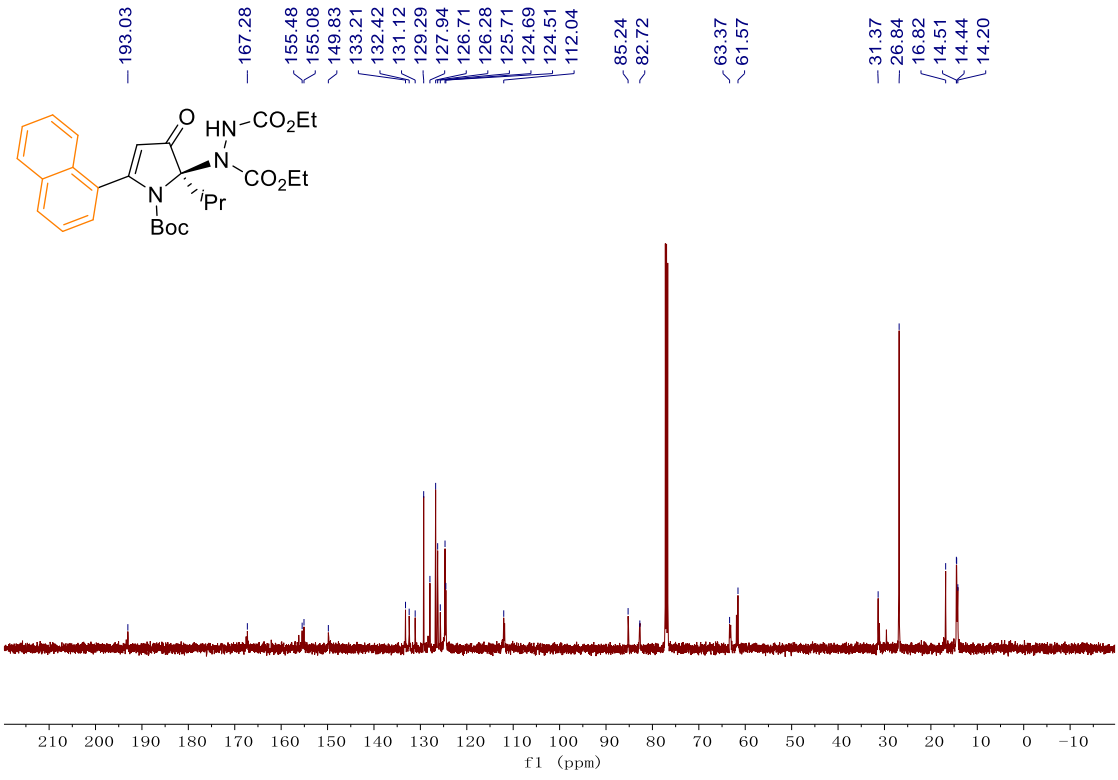




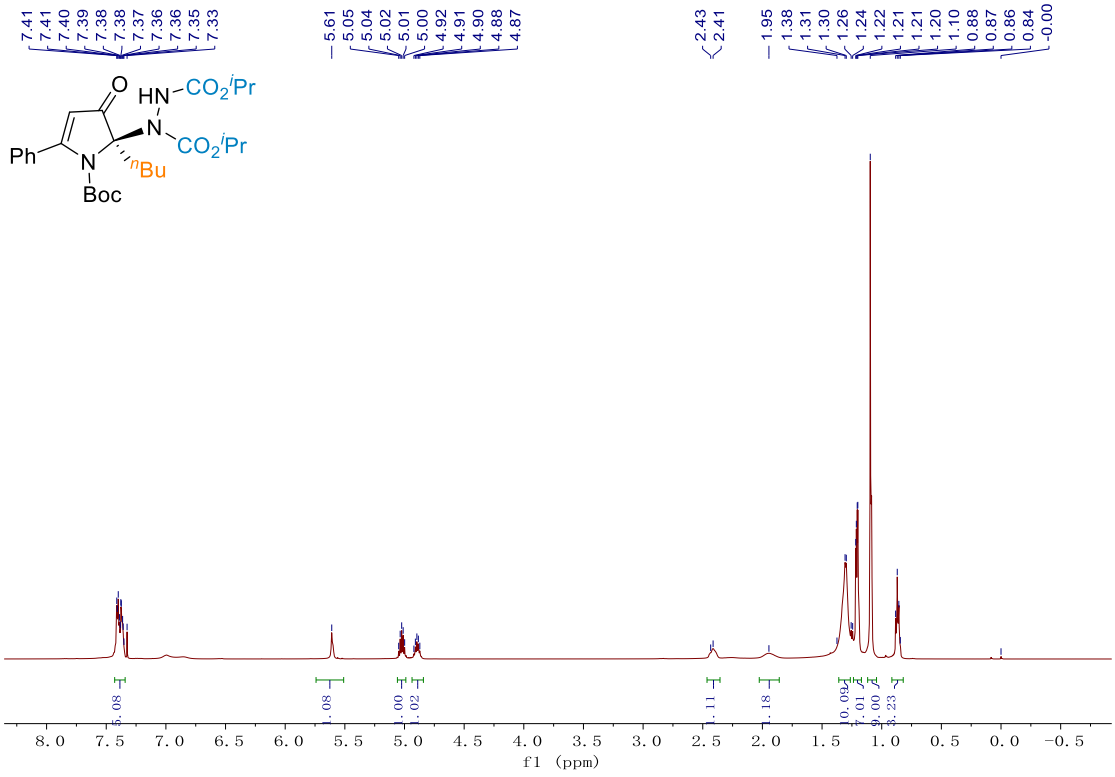

-63.15
O
HN
CO2Et
N
CO2Et
F3C
N
iPr
Boc
F3C
−15
−25
−35
−45
−55
−65
−75
−85
−95
−105
−115
−125
f1 (ppm)

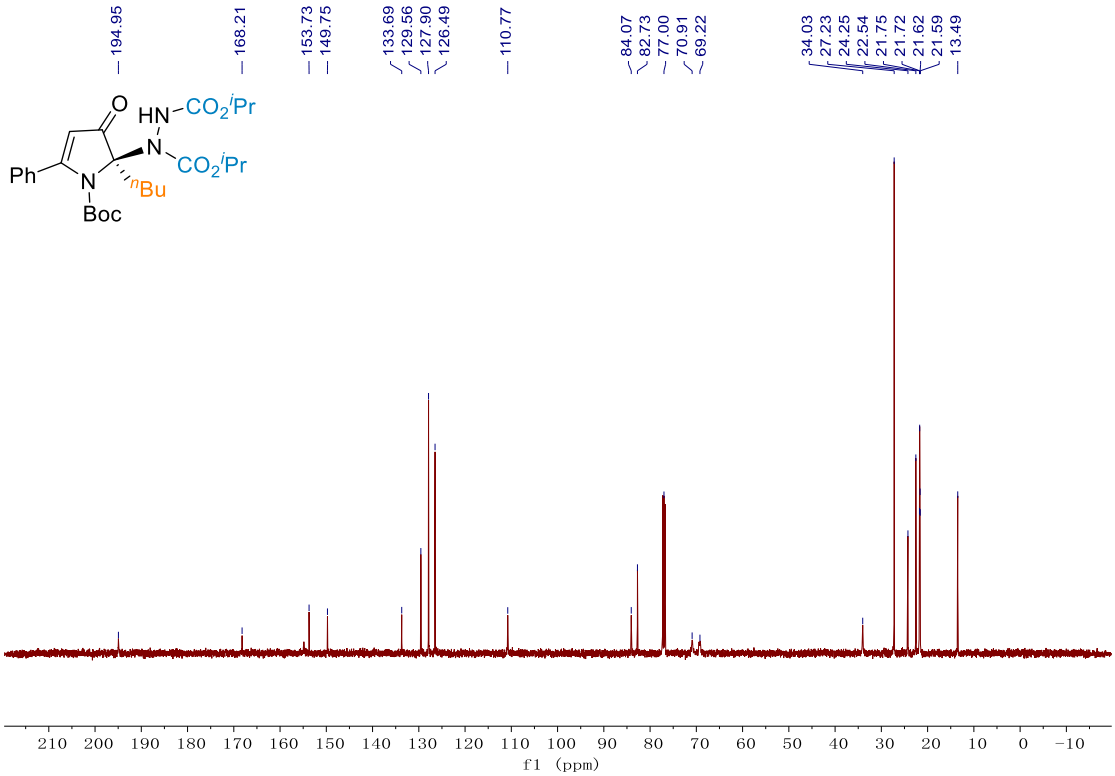
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-5-(naphthalen-1-yl)-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3y)



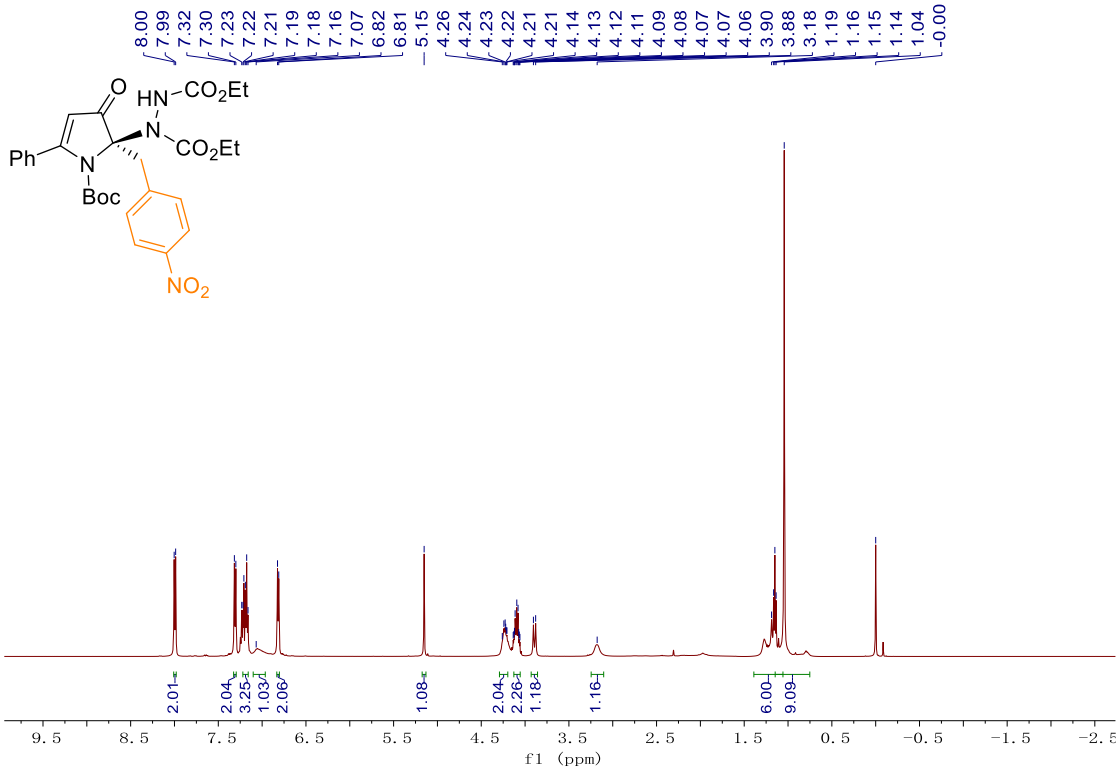


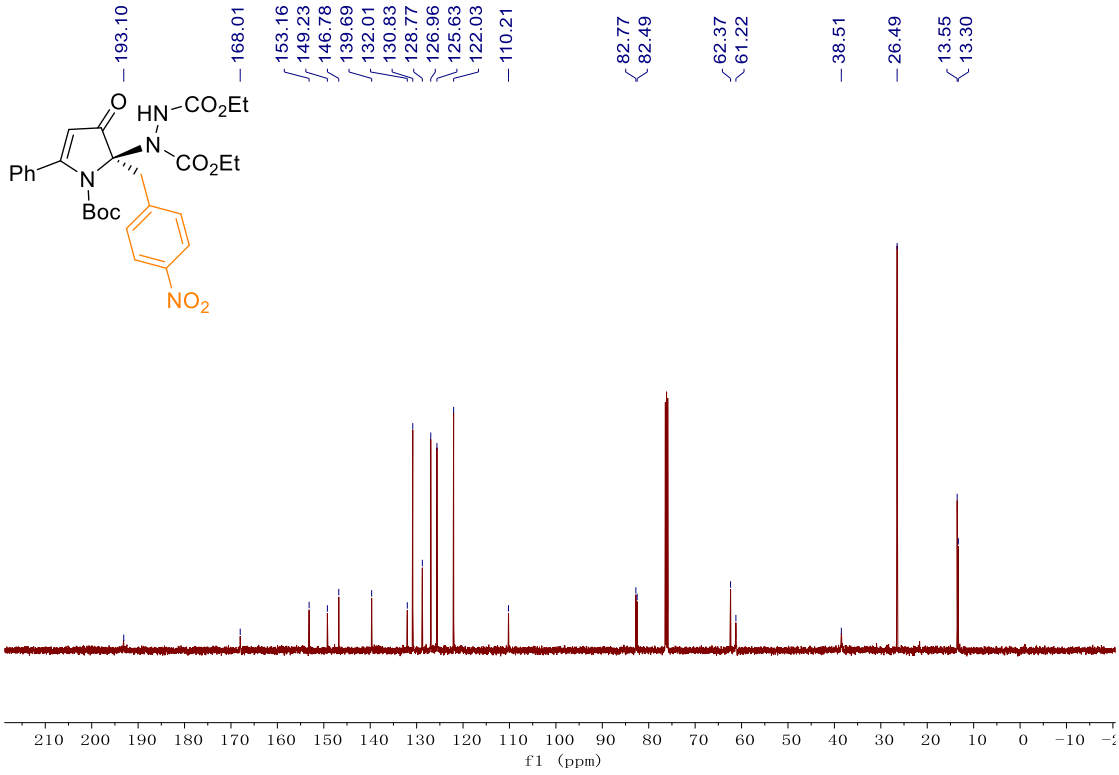
diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-butyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3z)



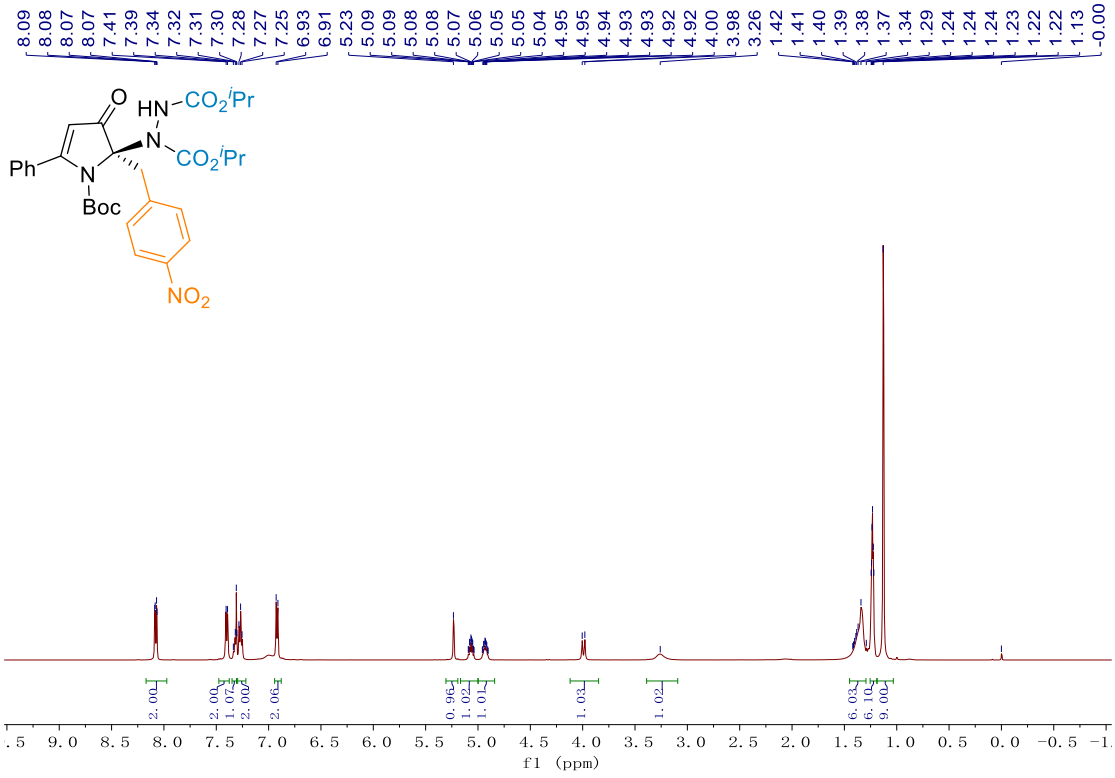


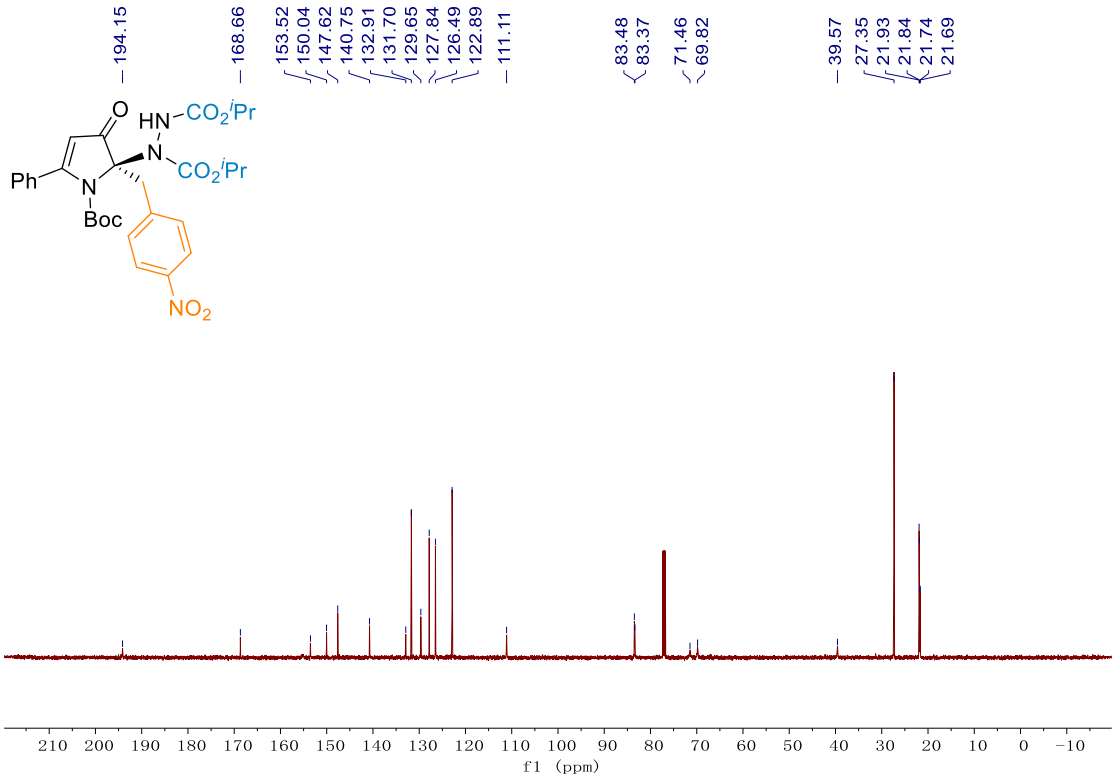
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3aa)



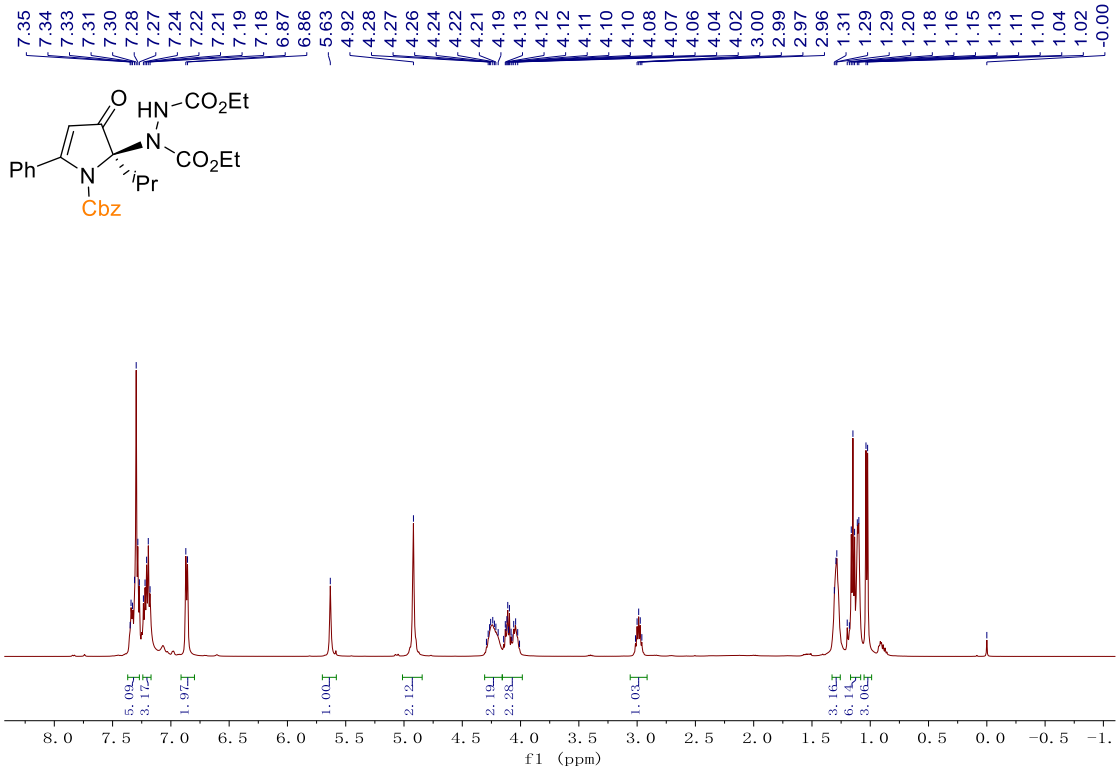


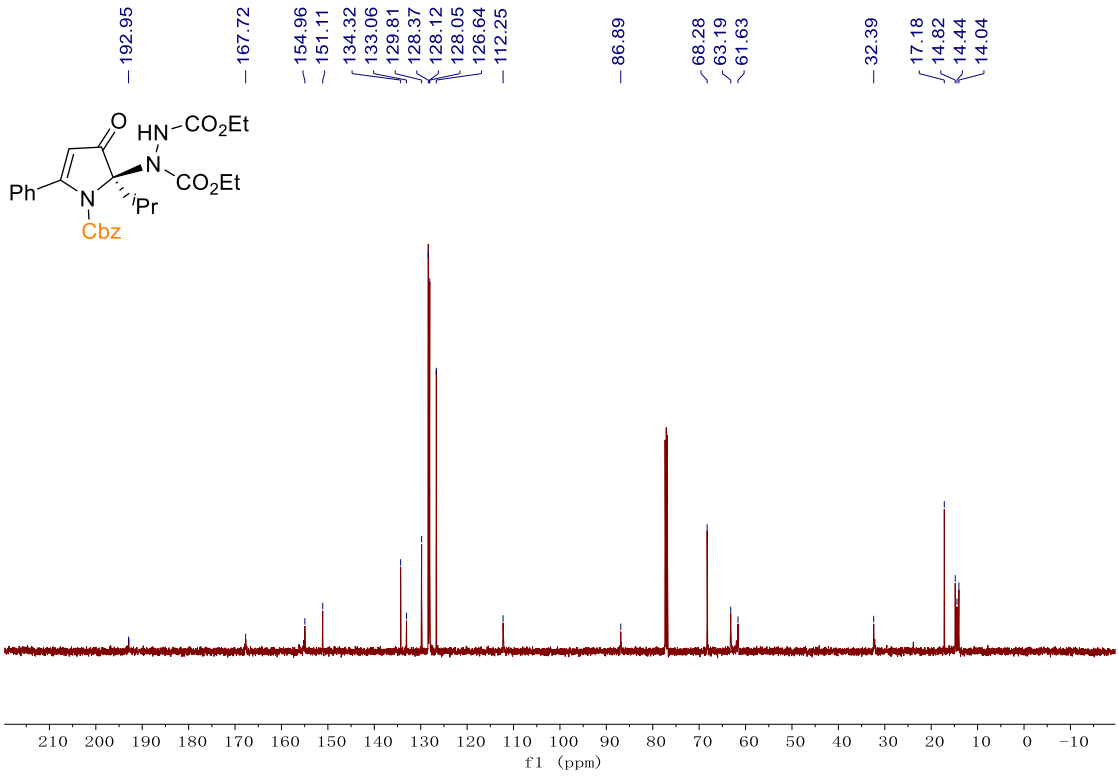
diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3ab)



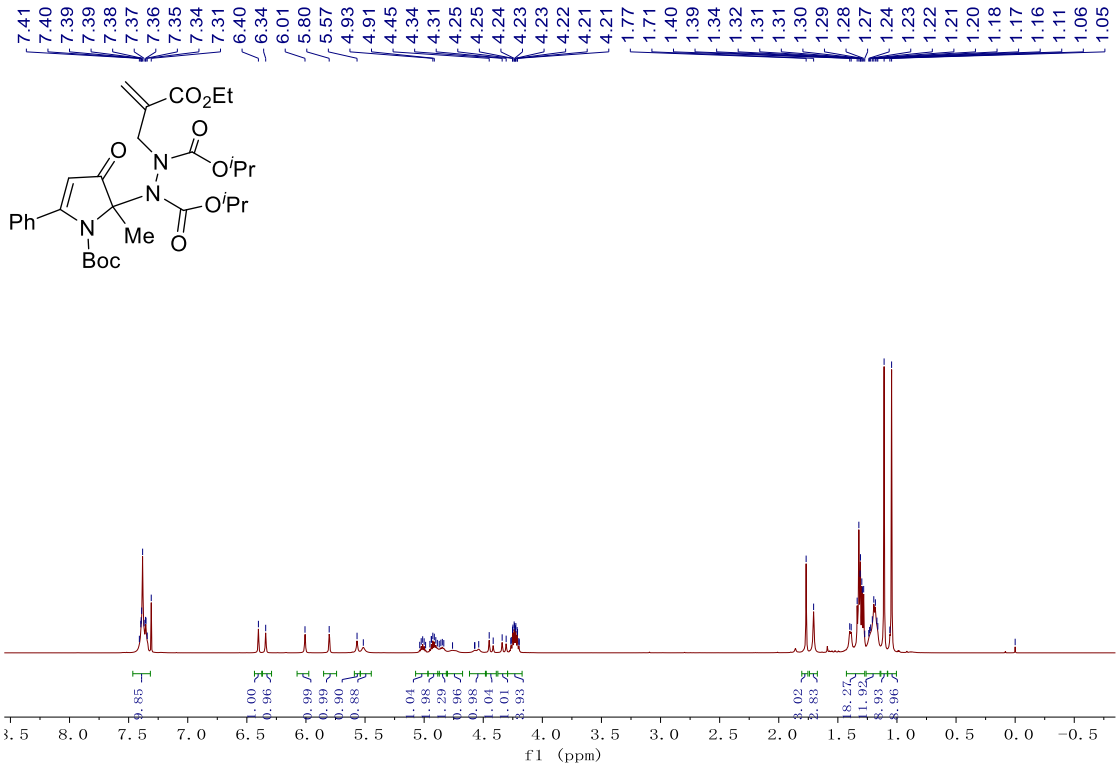


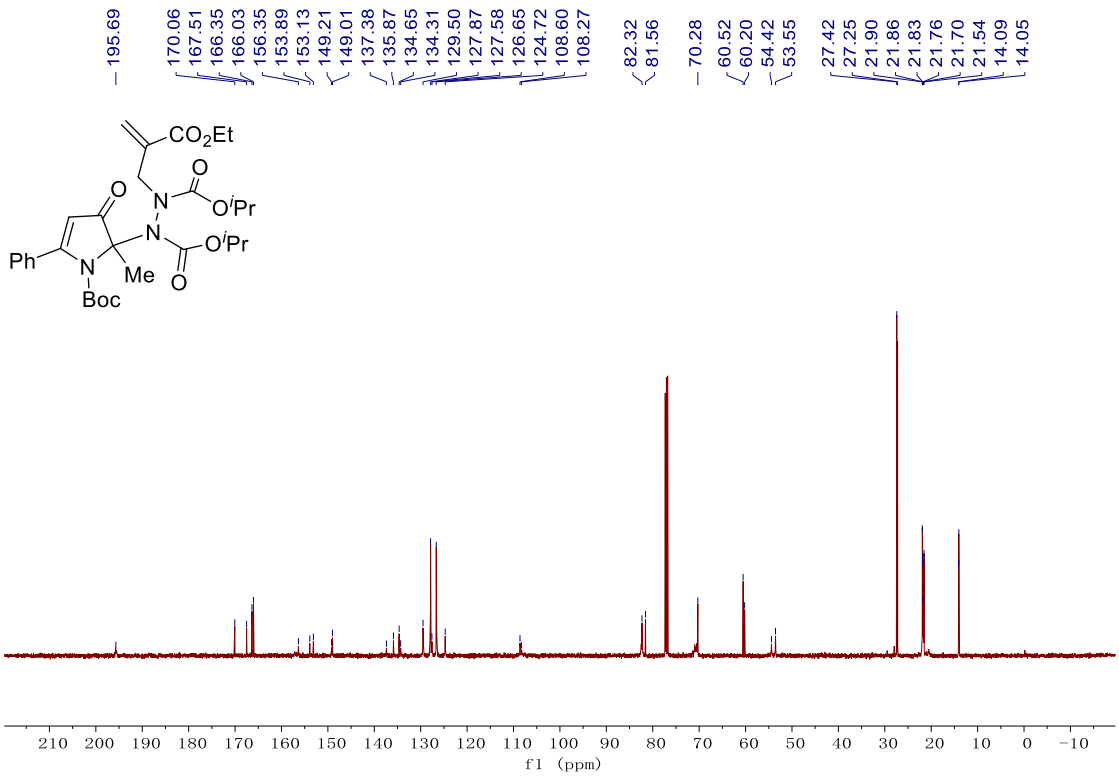
diethyl (*R*)-1-(1-((benzyloxy)carbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3ac)



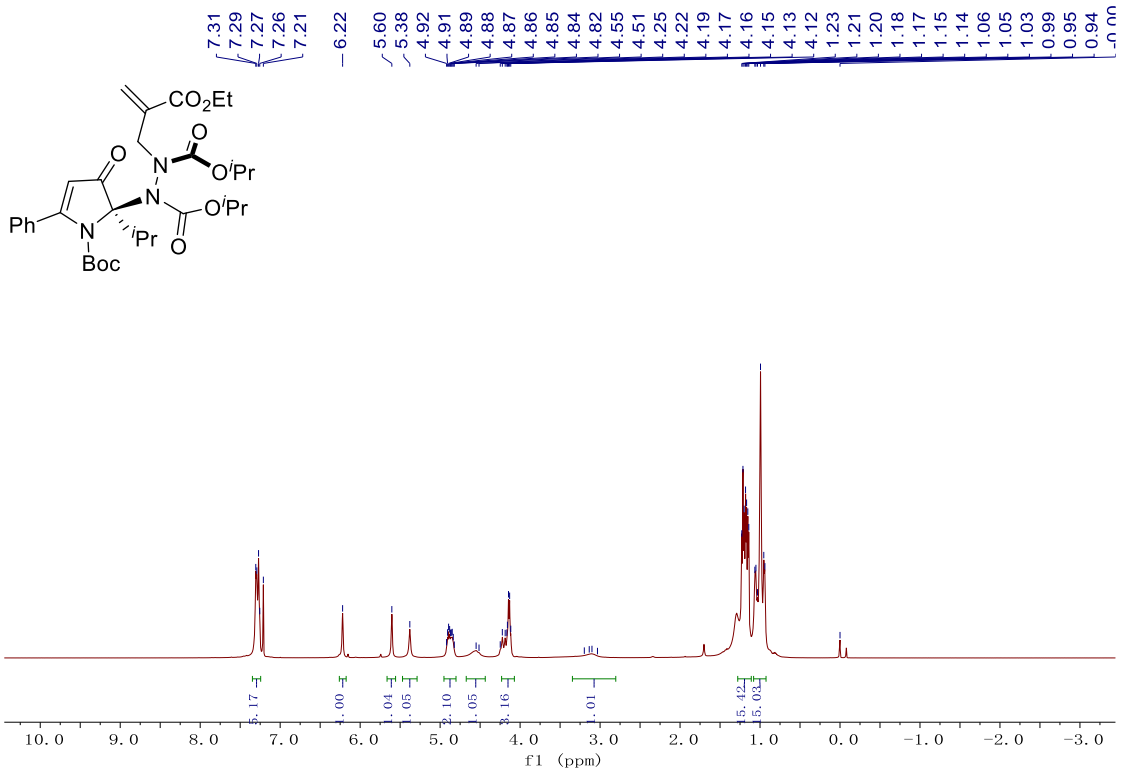


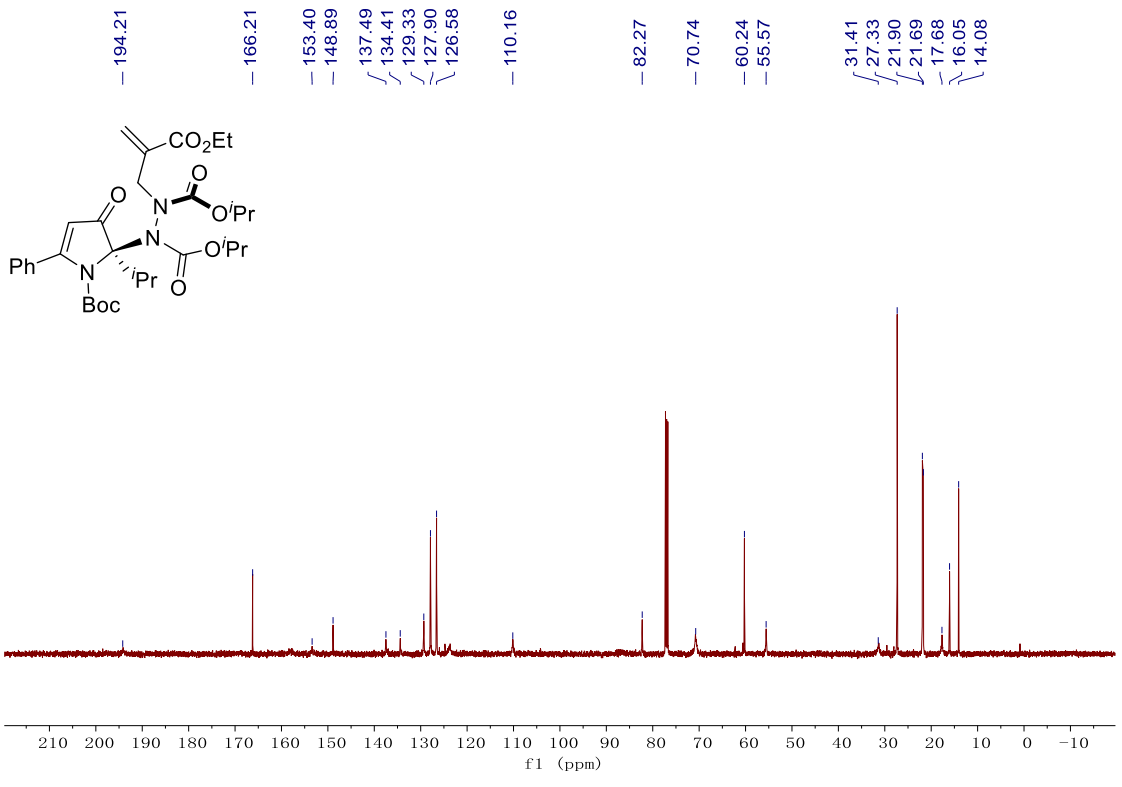
diisopropyl-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (5)



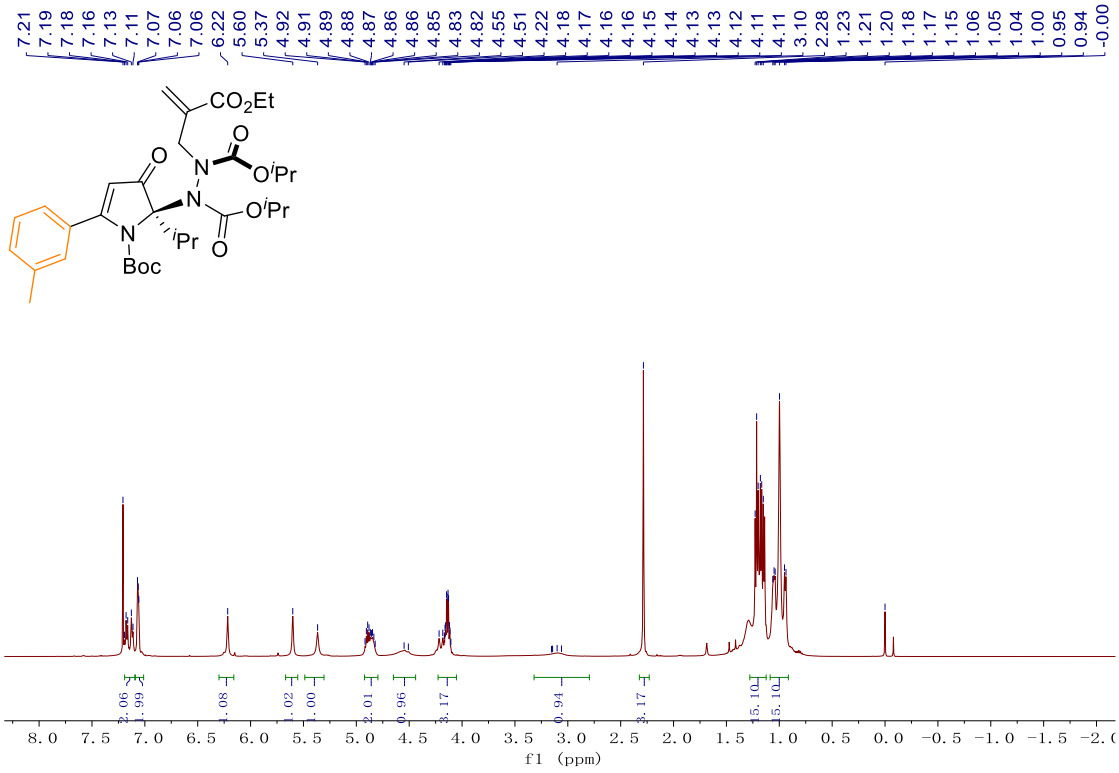


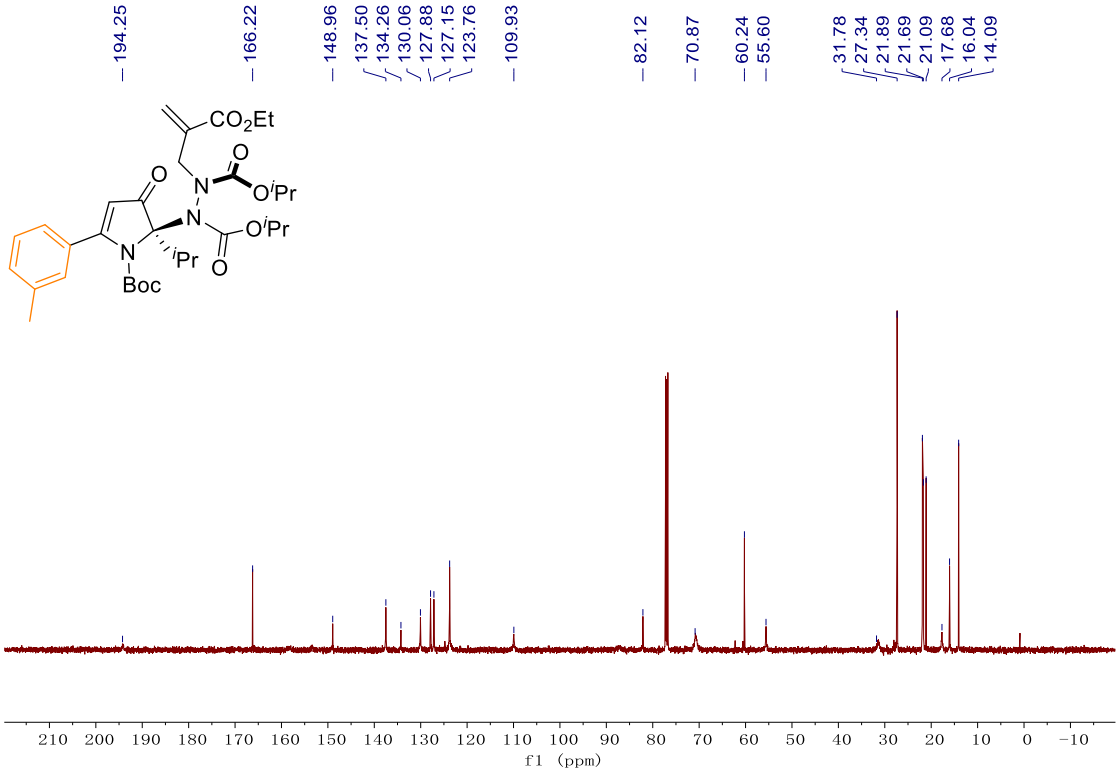
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6a)



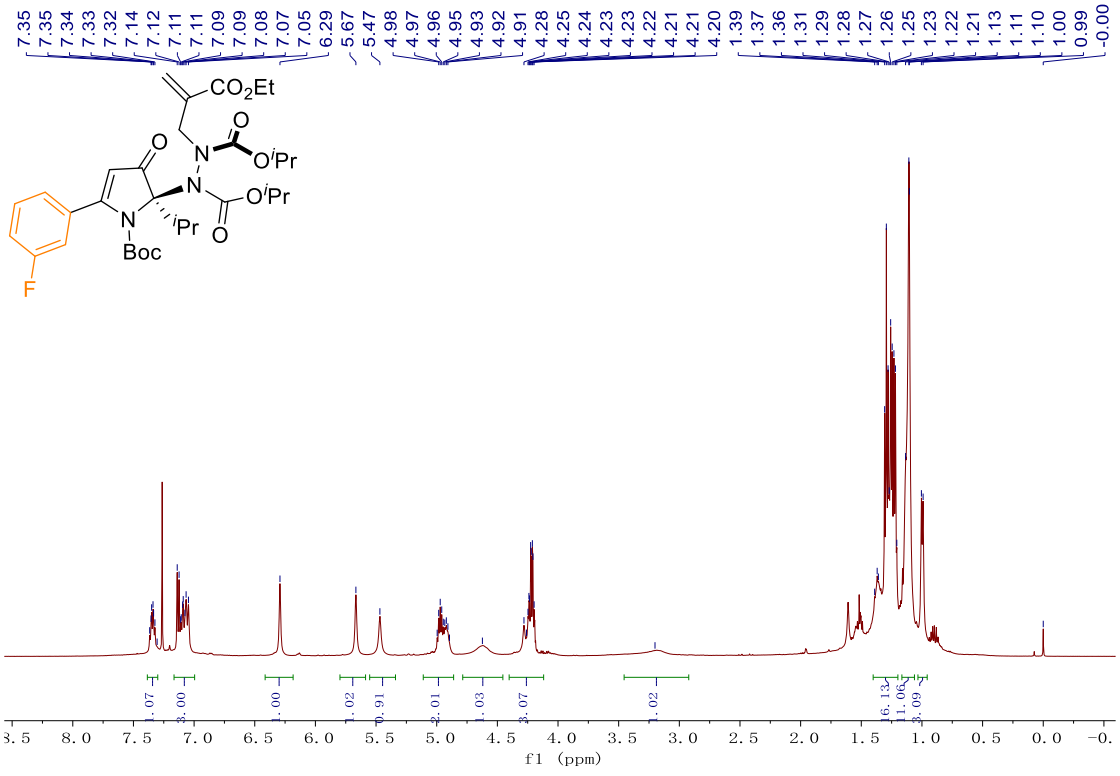


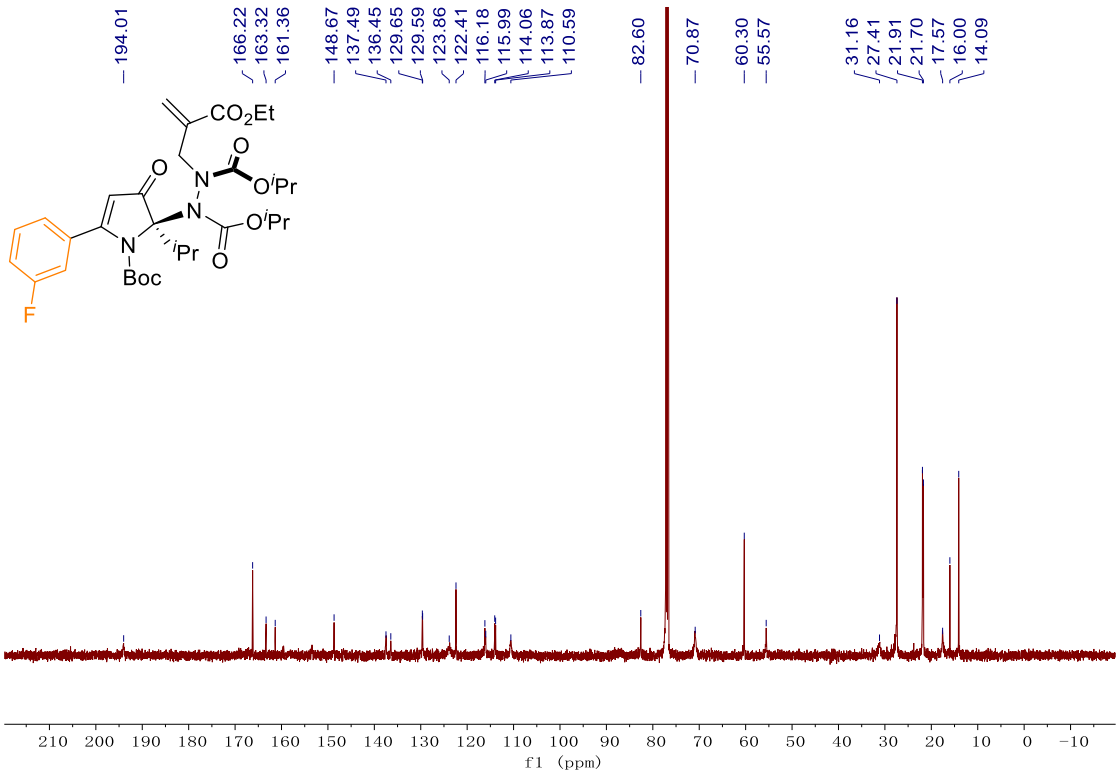
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(m-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6b)

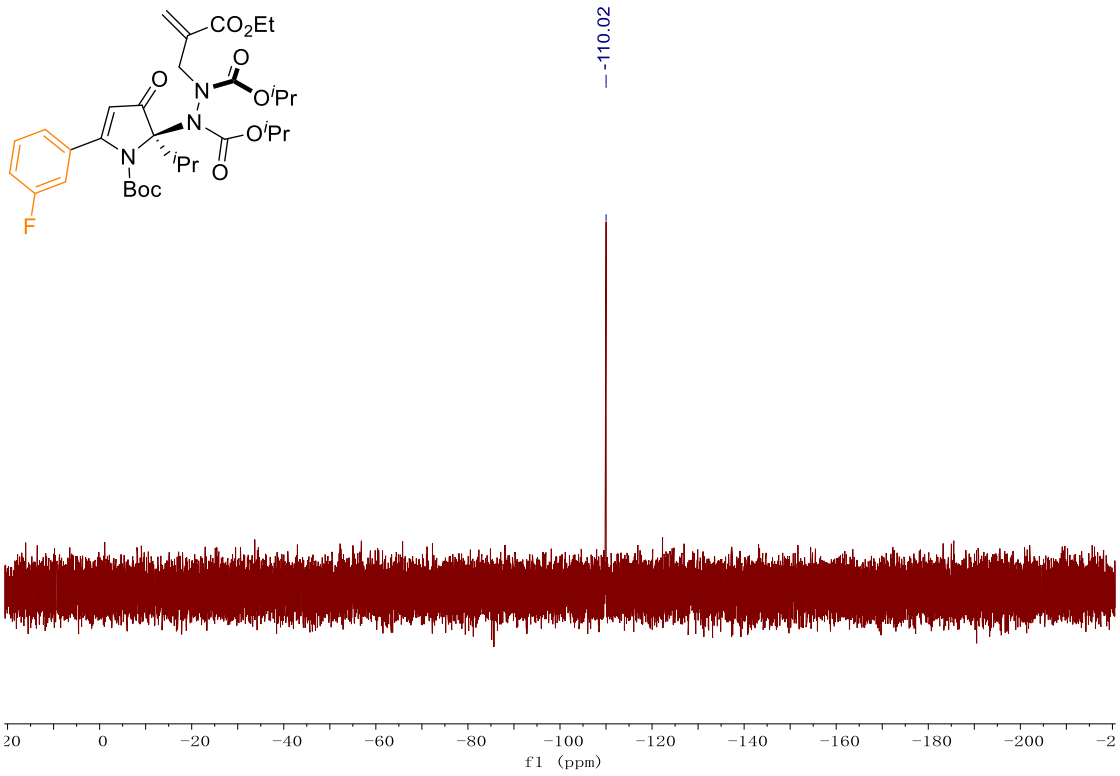




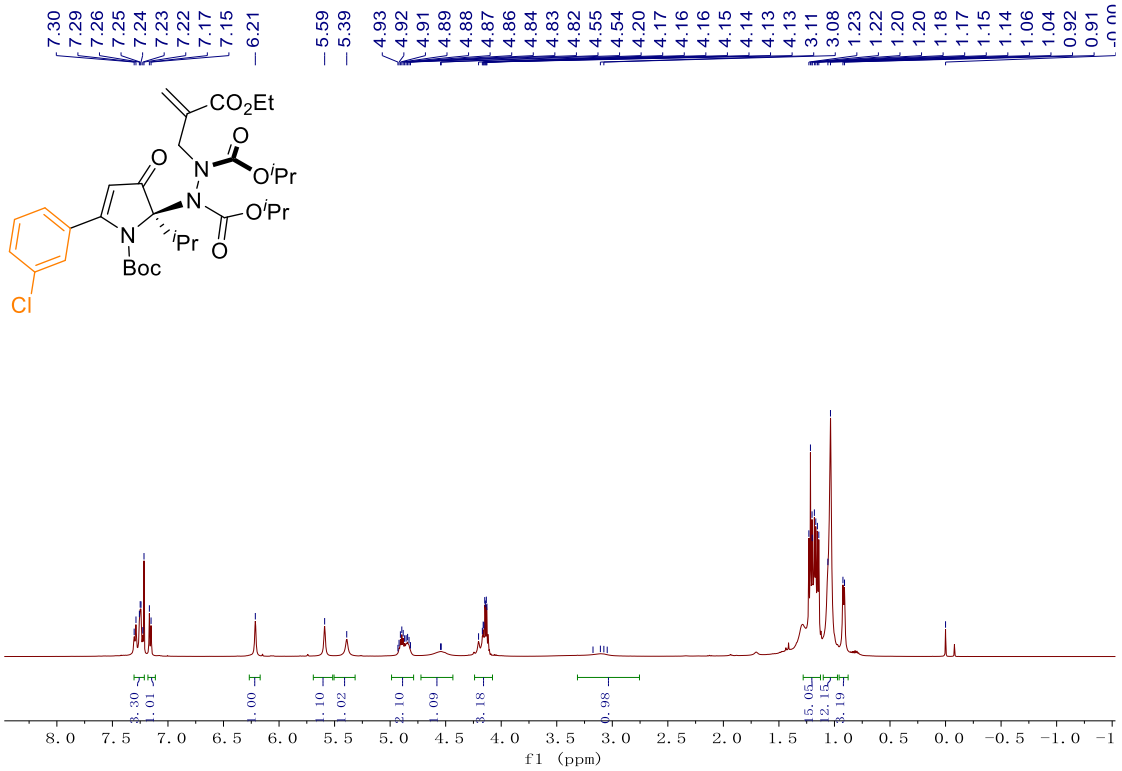
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(3-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6c)

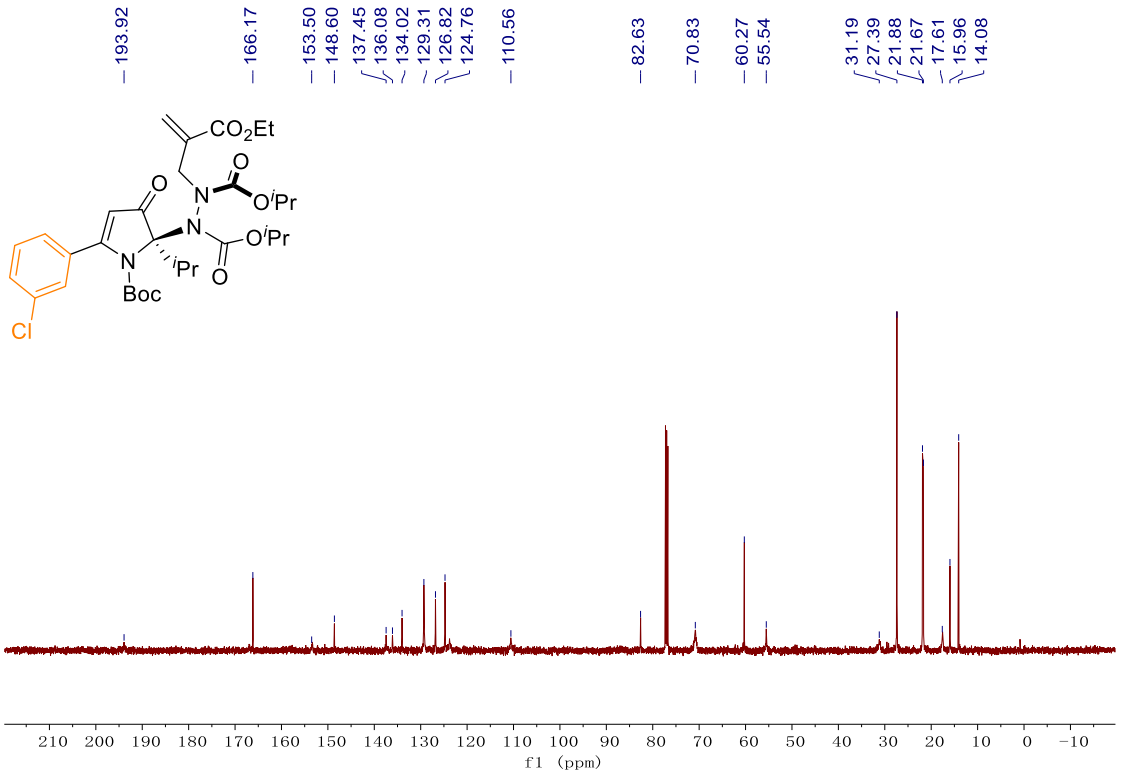




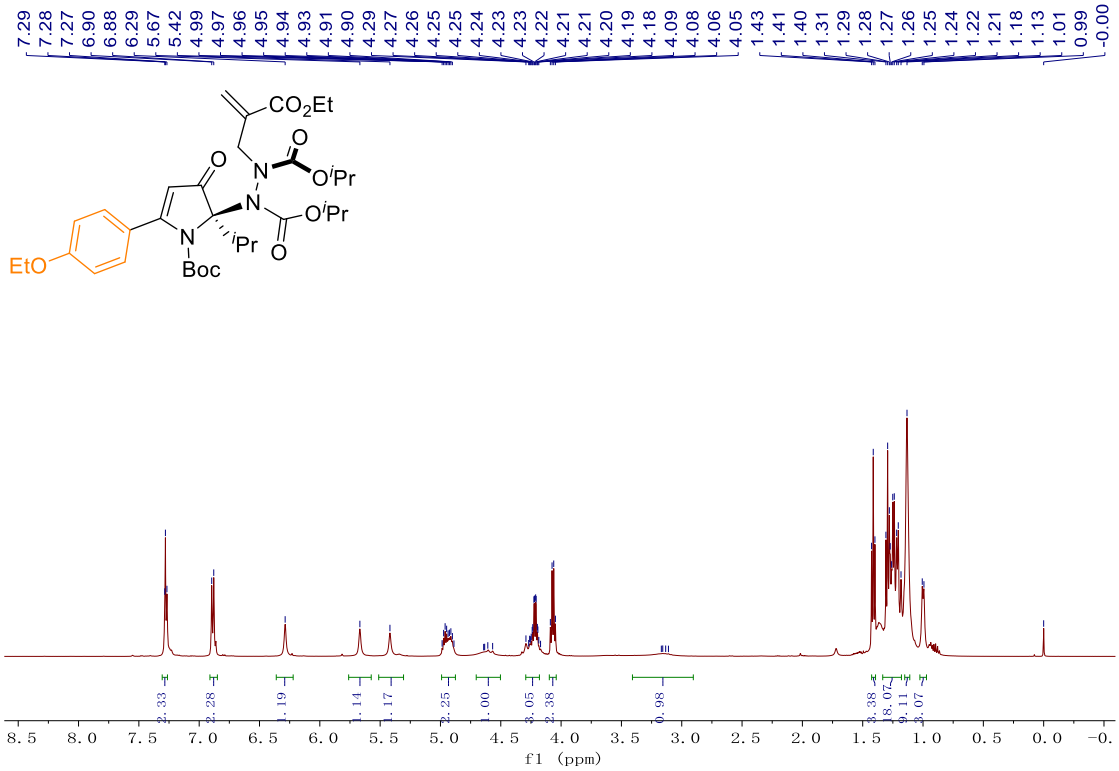

CO2Et
O
N
O
iPr
O
N
O
iPr
N
iPr
O
Boc
F
-110.02
20
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
-2
f1 (ppm)

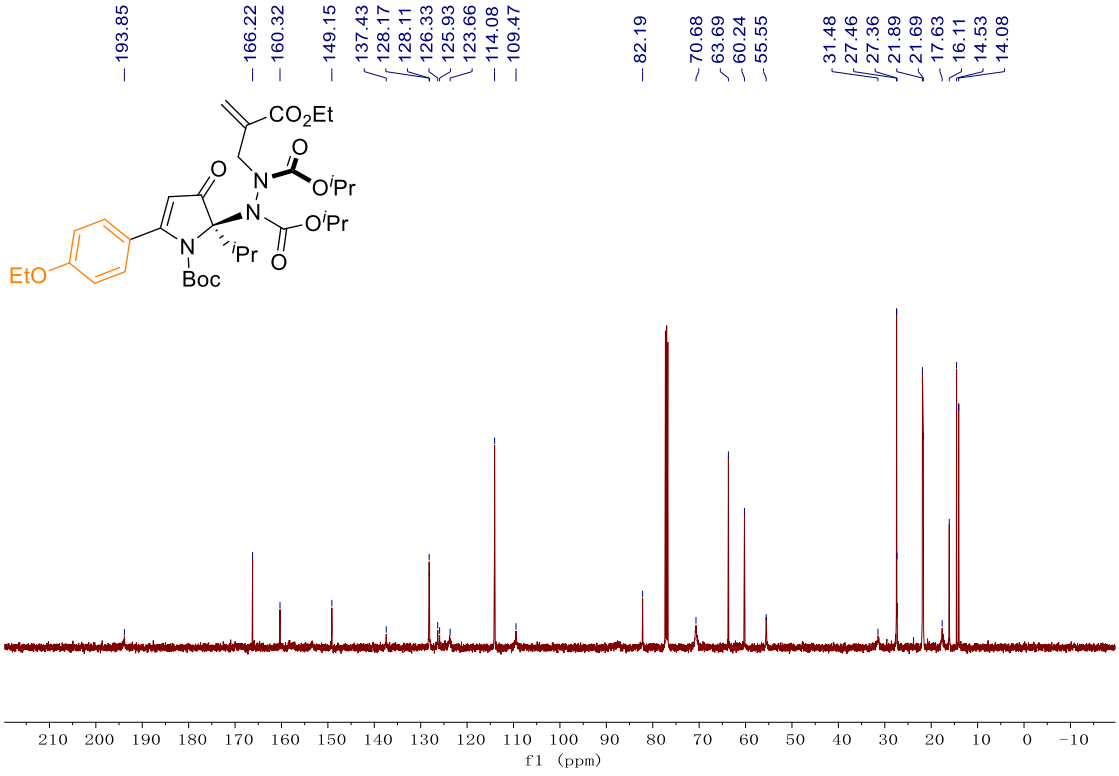
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(3-chlorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6d)



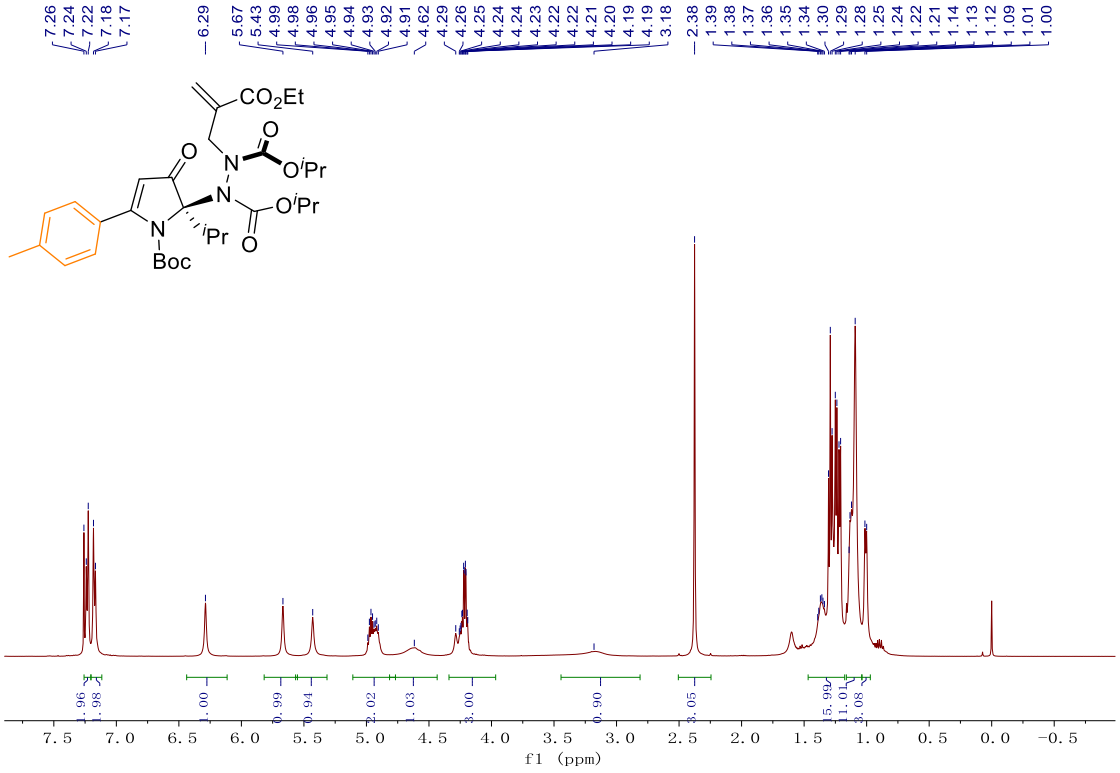


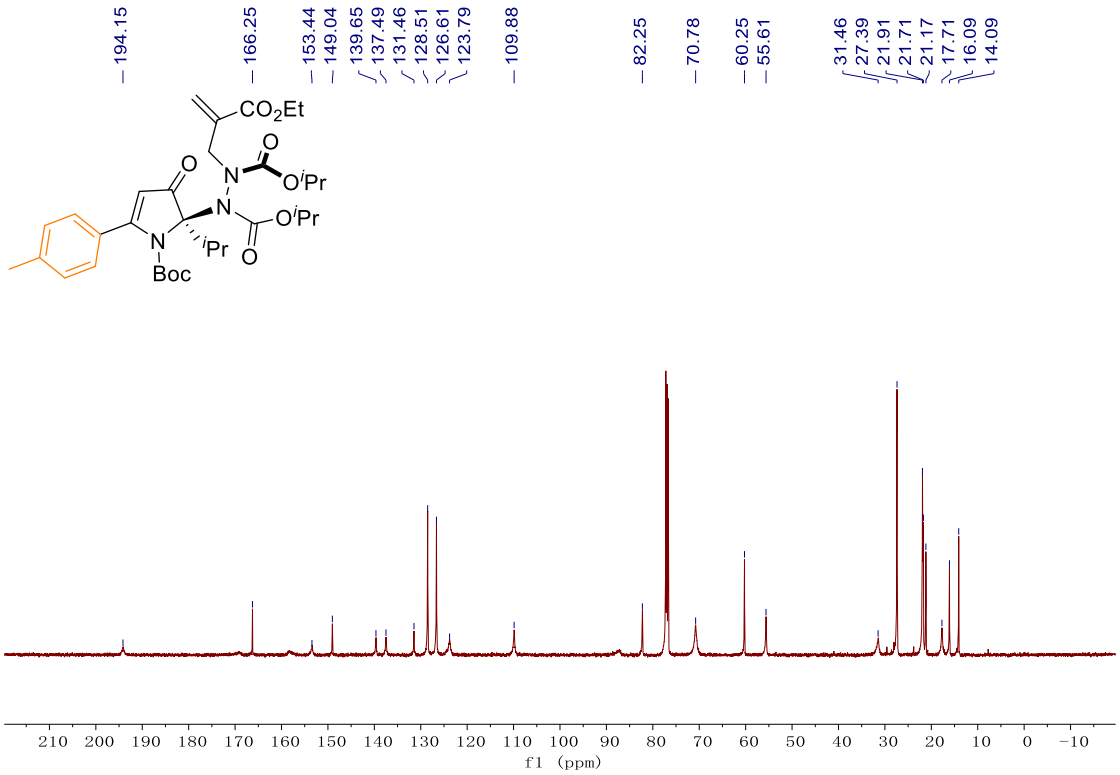
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethoxyphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6e)



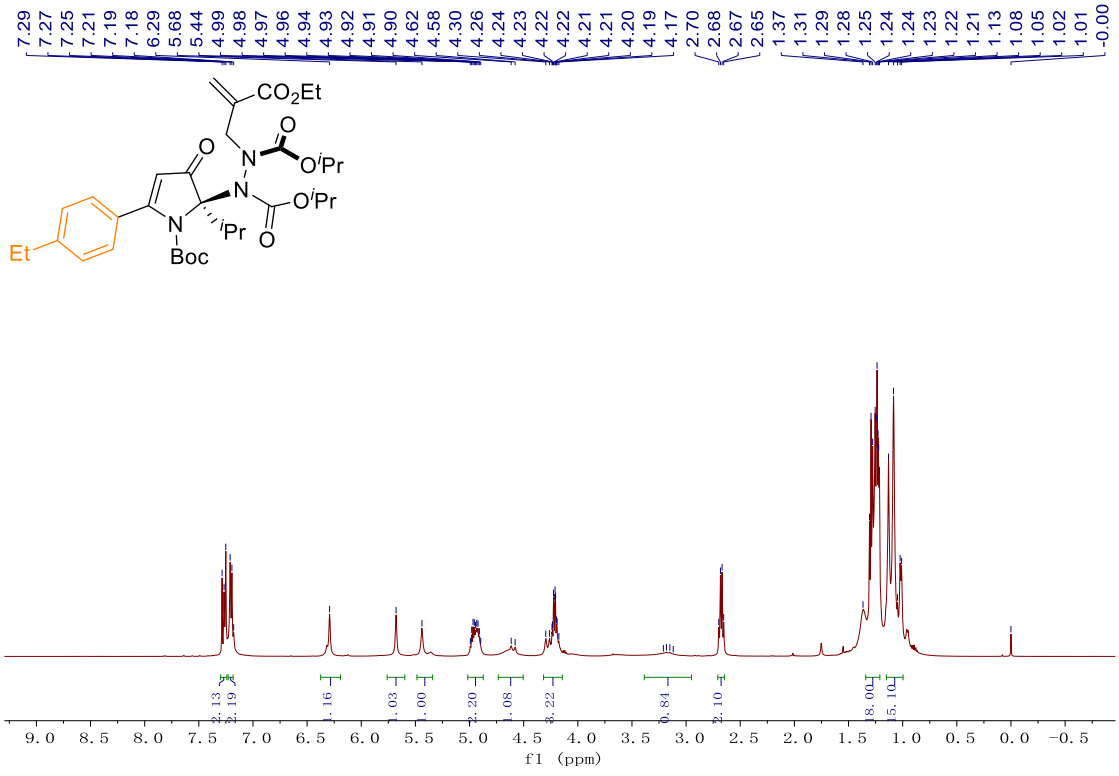


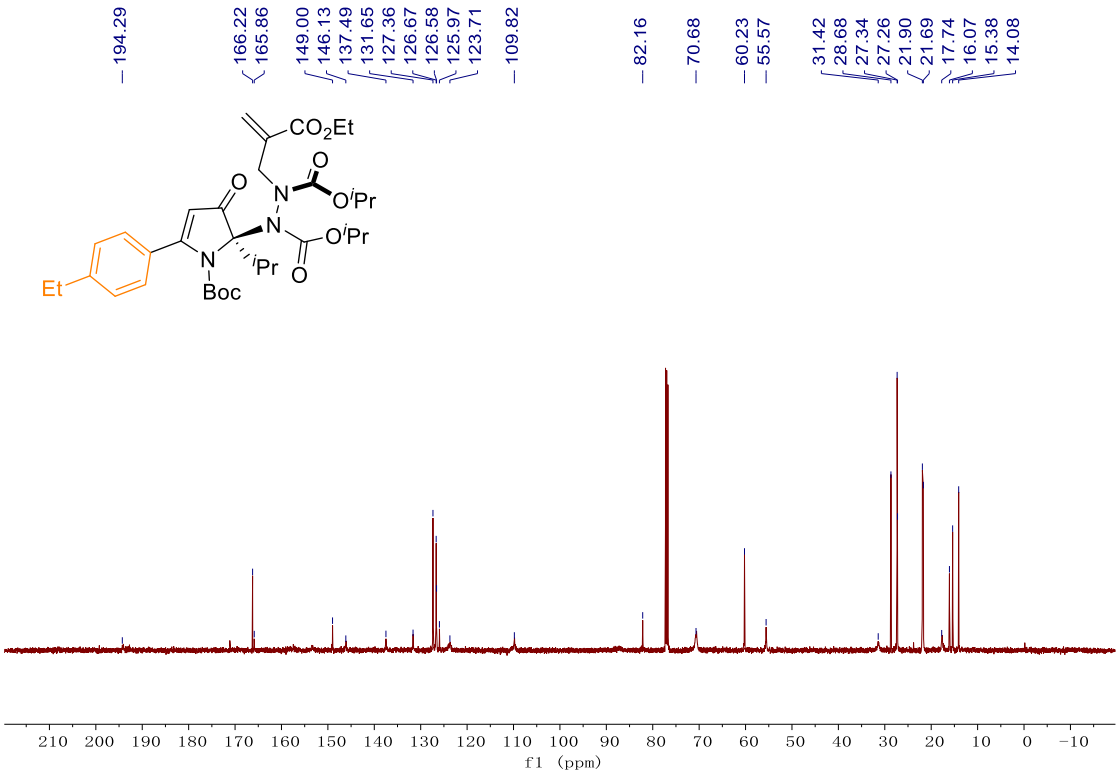
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(p-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6f)



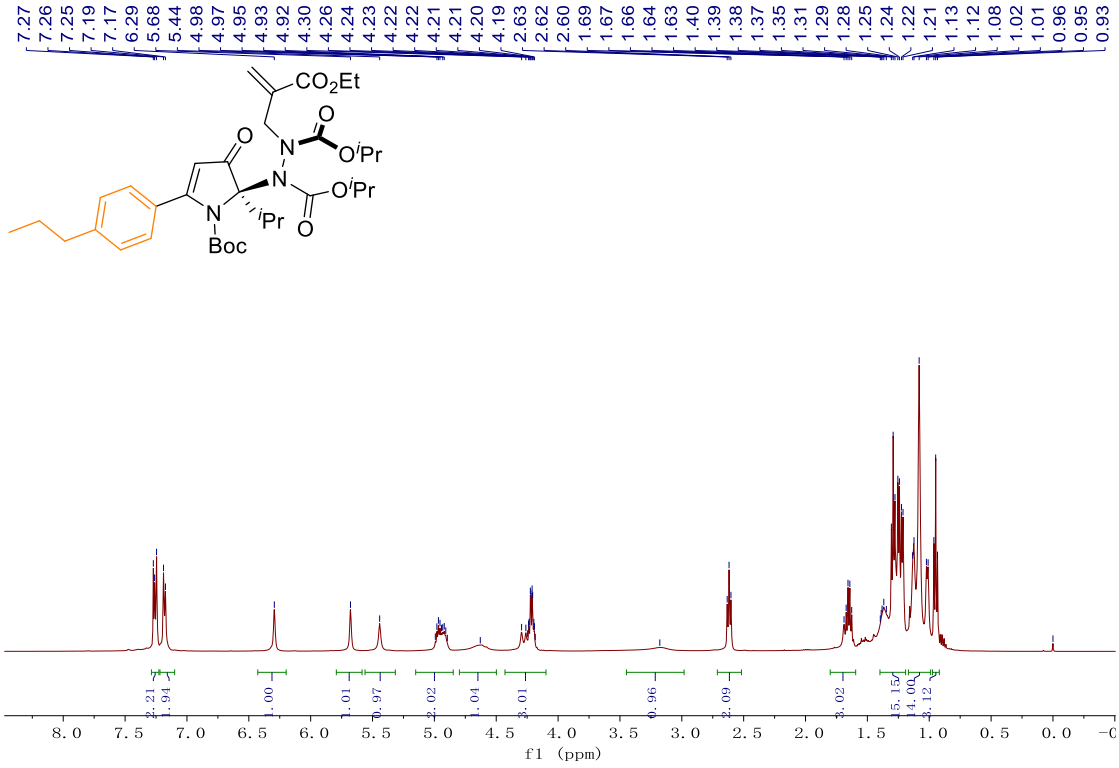


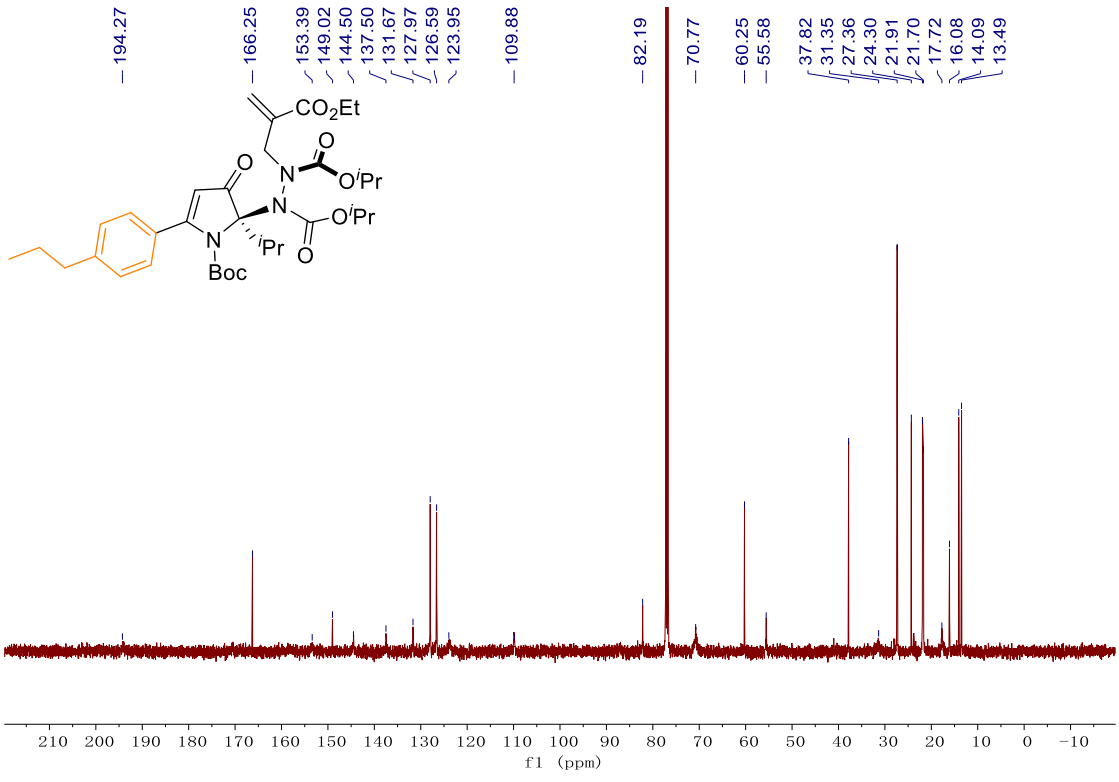
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6g)



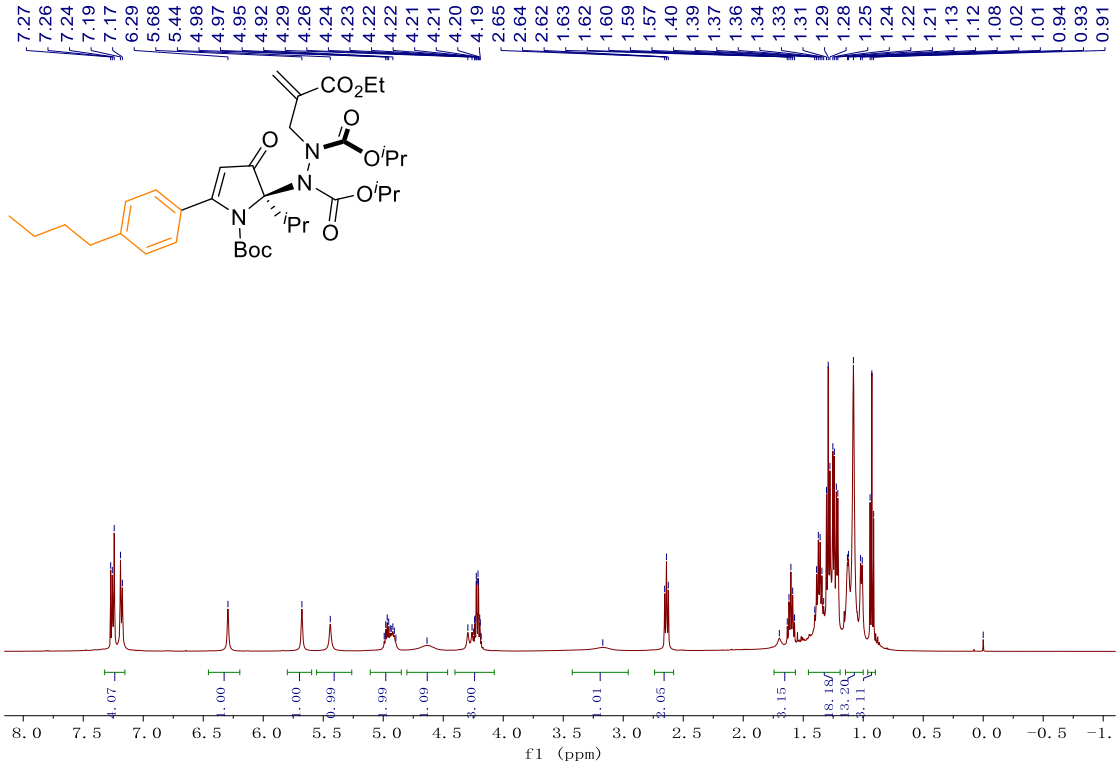


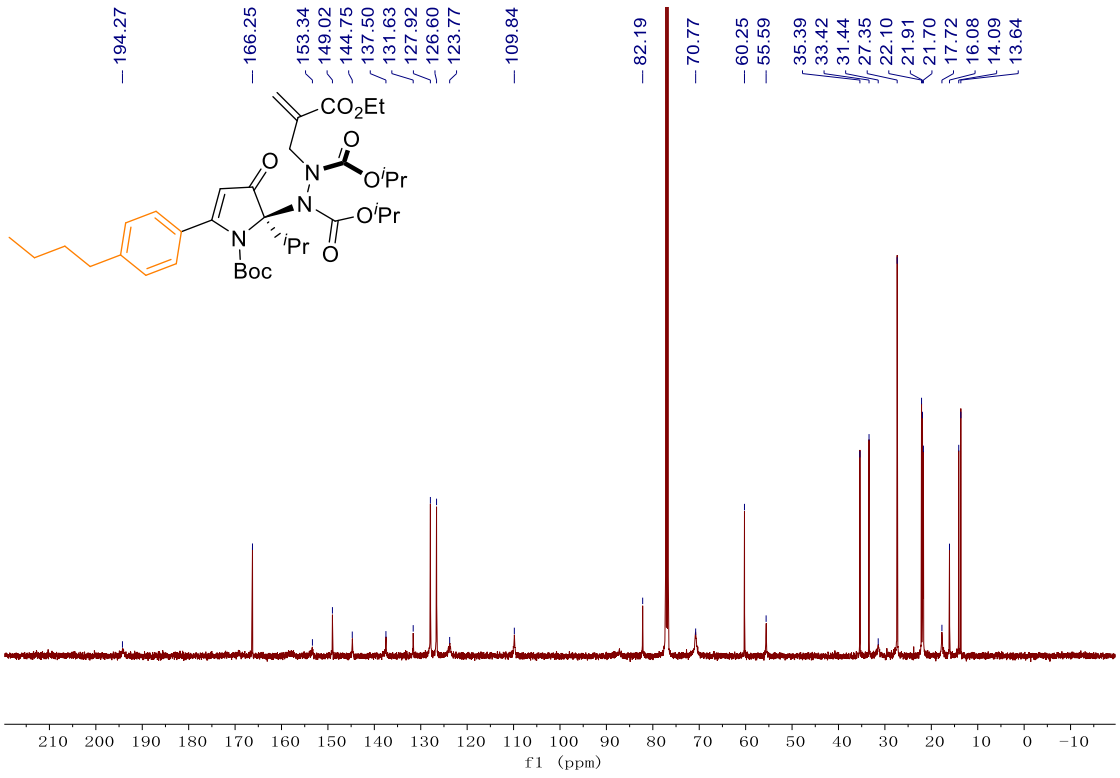
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-propylphenyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6h)



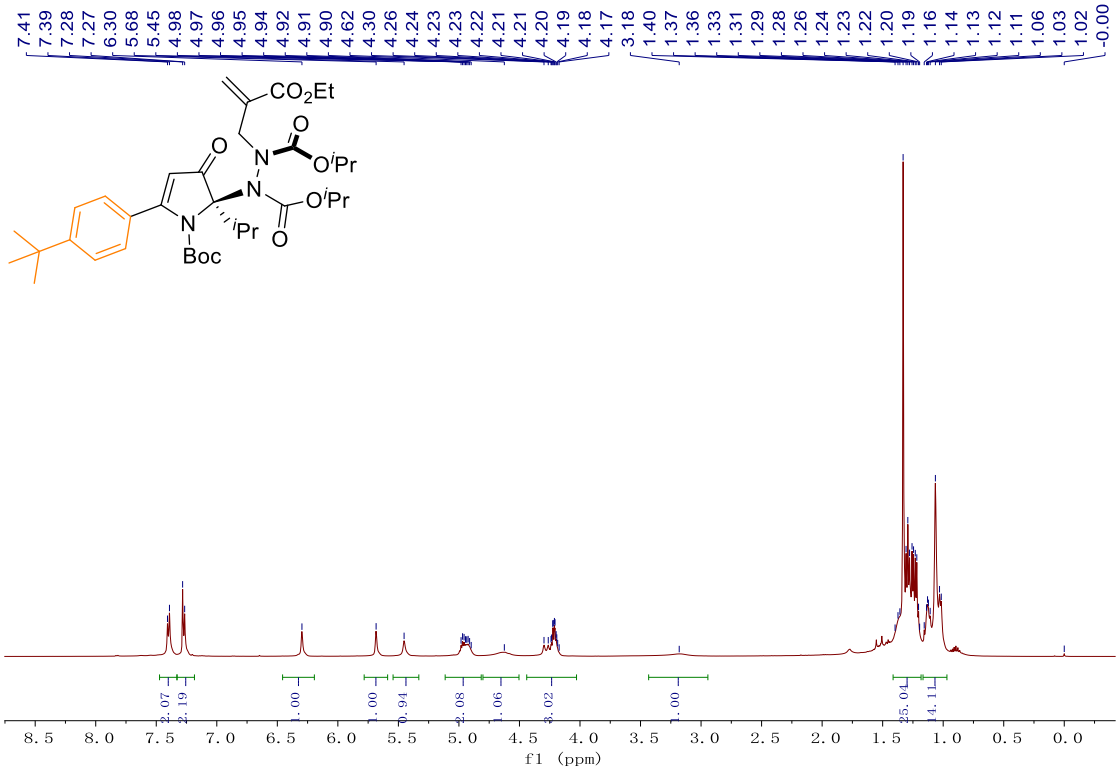


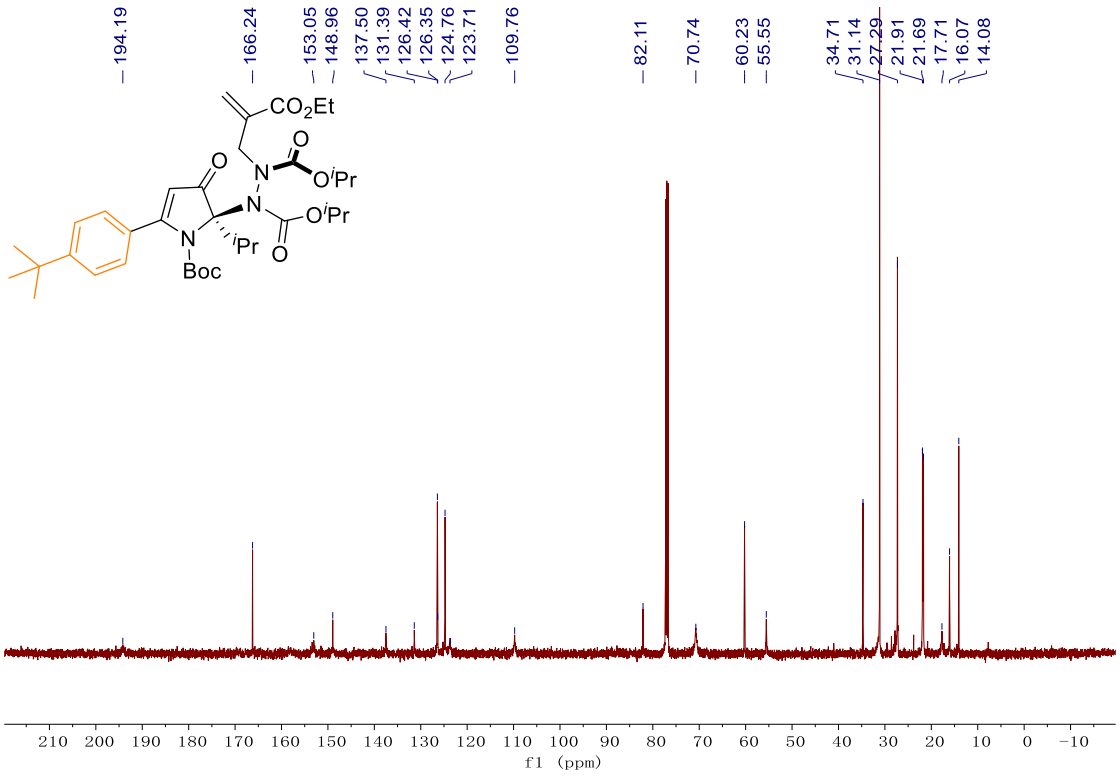
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-butylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6i)



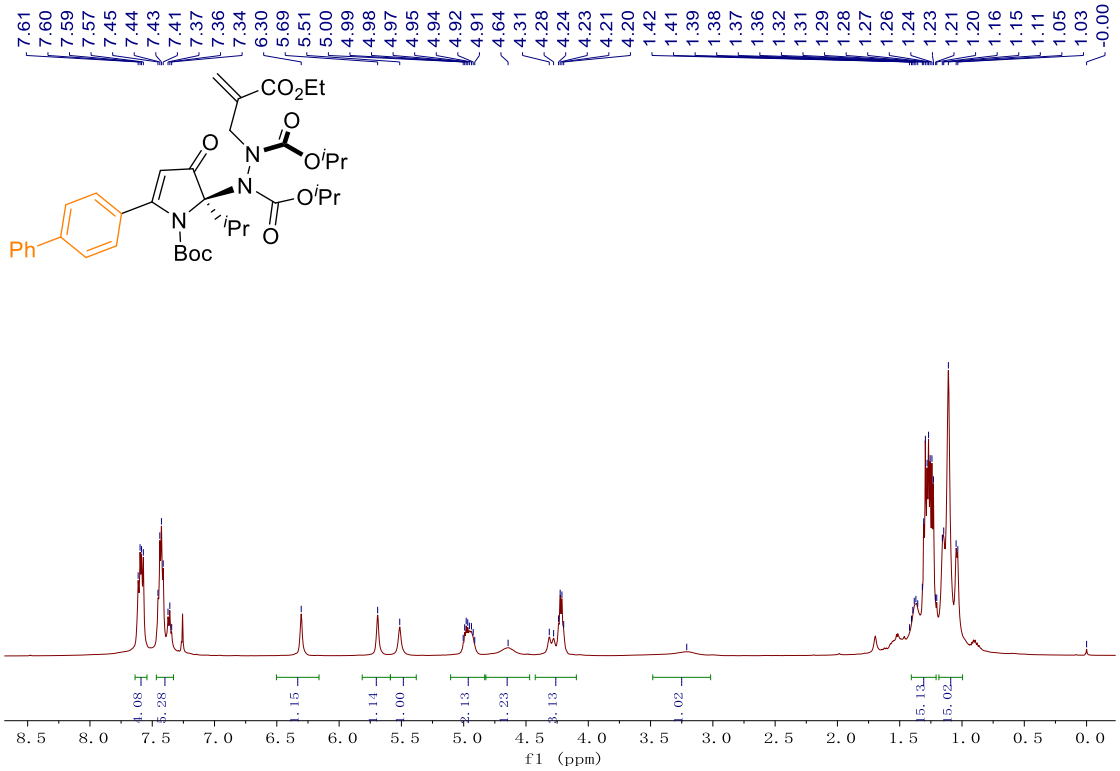


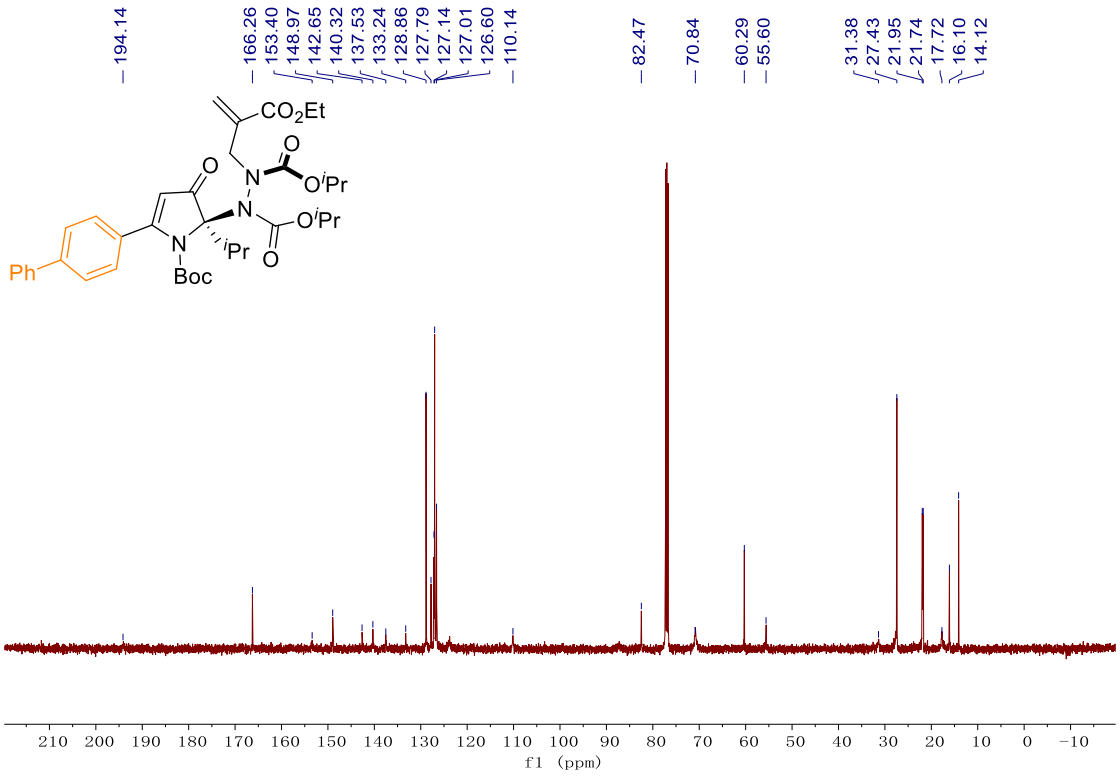
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-(tert-butyl)phenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6j)



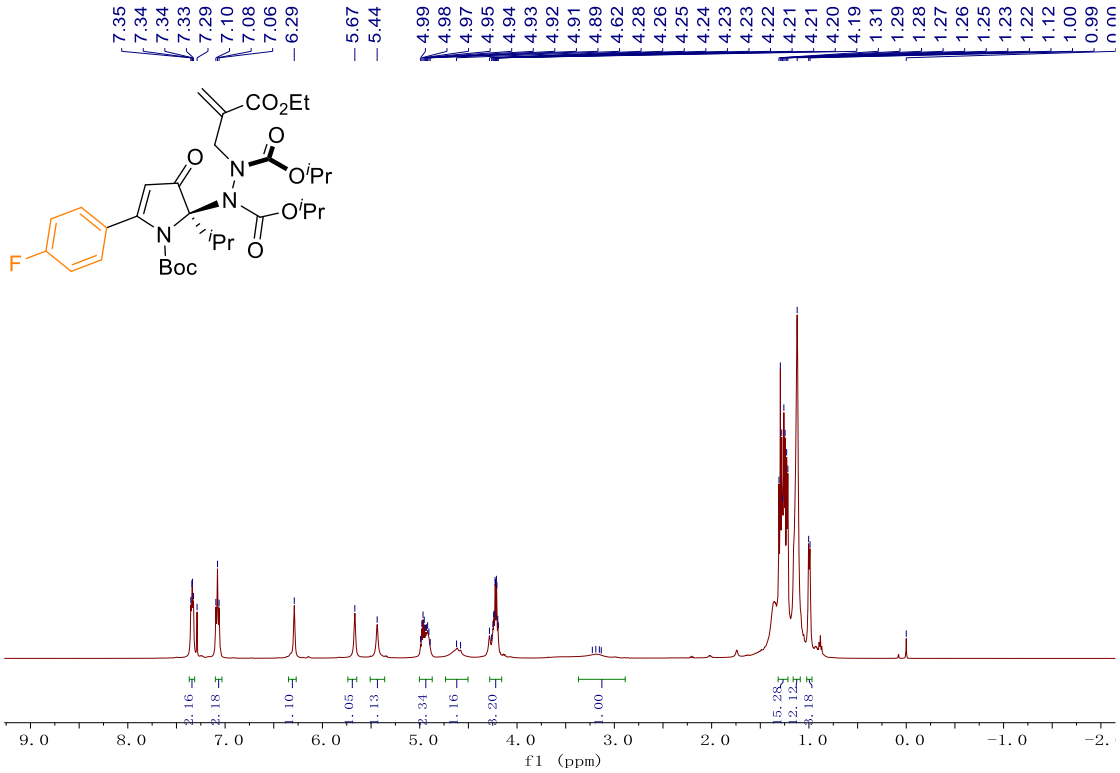


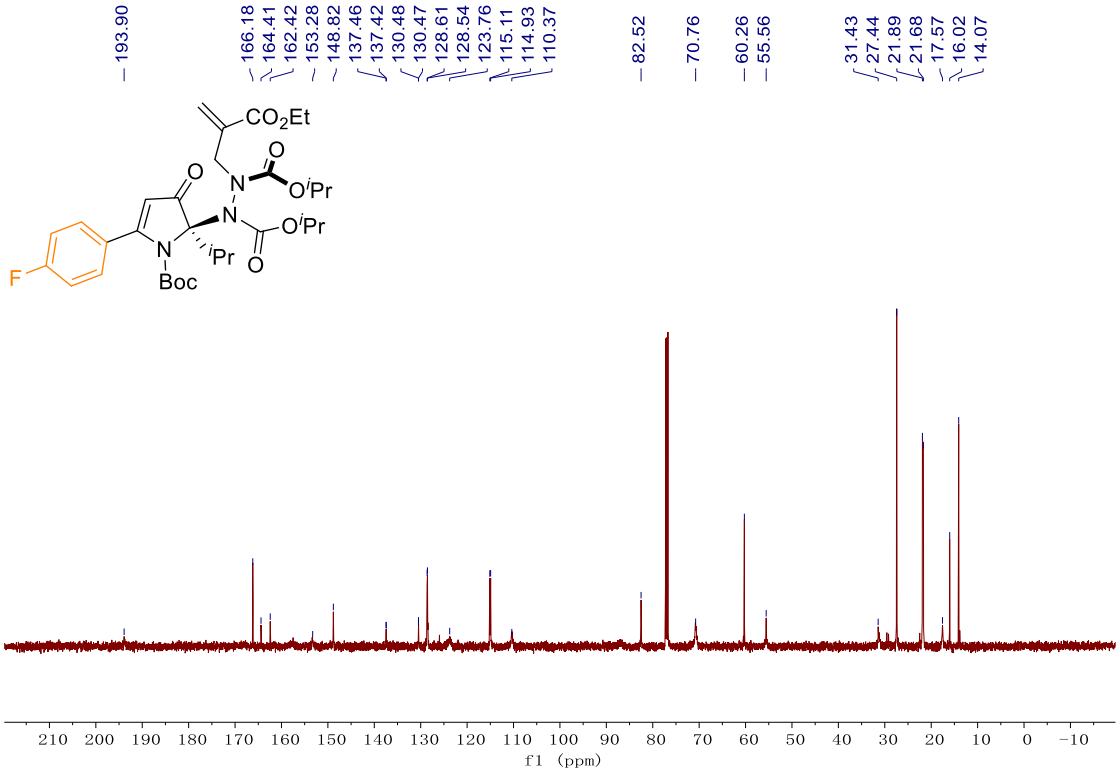
diisopropyl (*R*, *R*)-1-(5-([1,1'-biphenyl]-4-yl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6k)

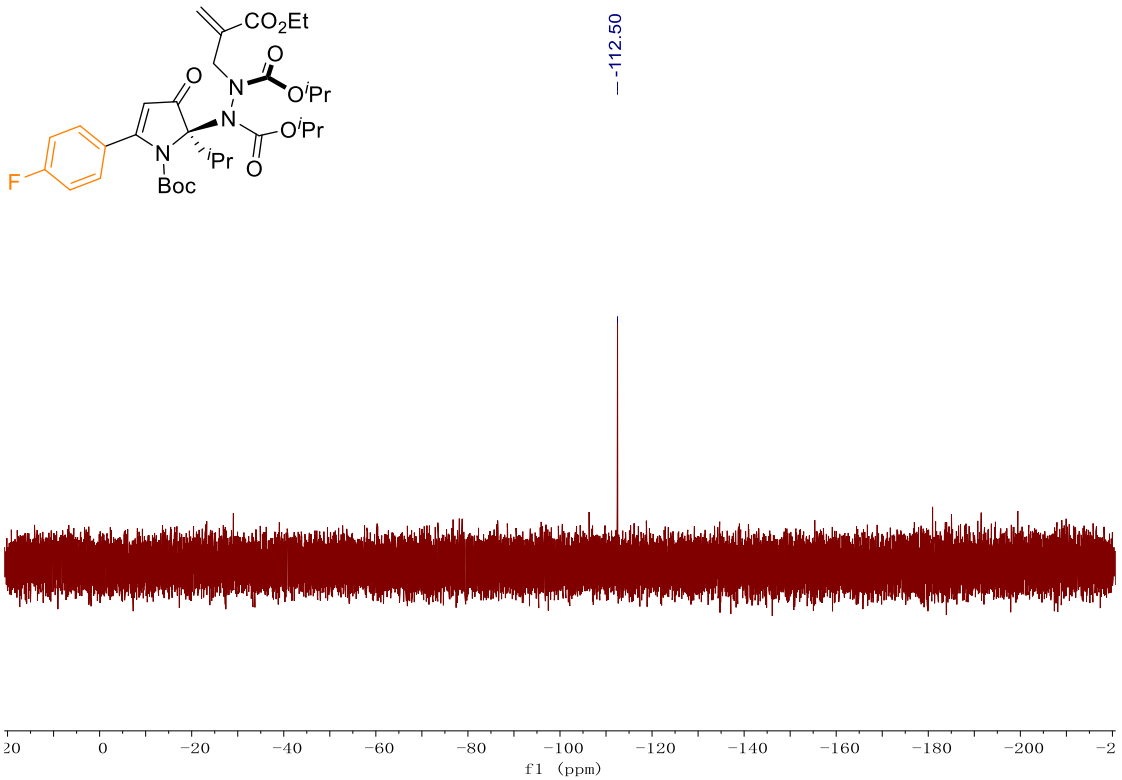




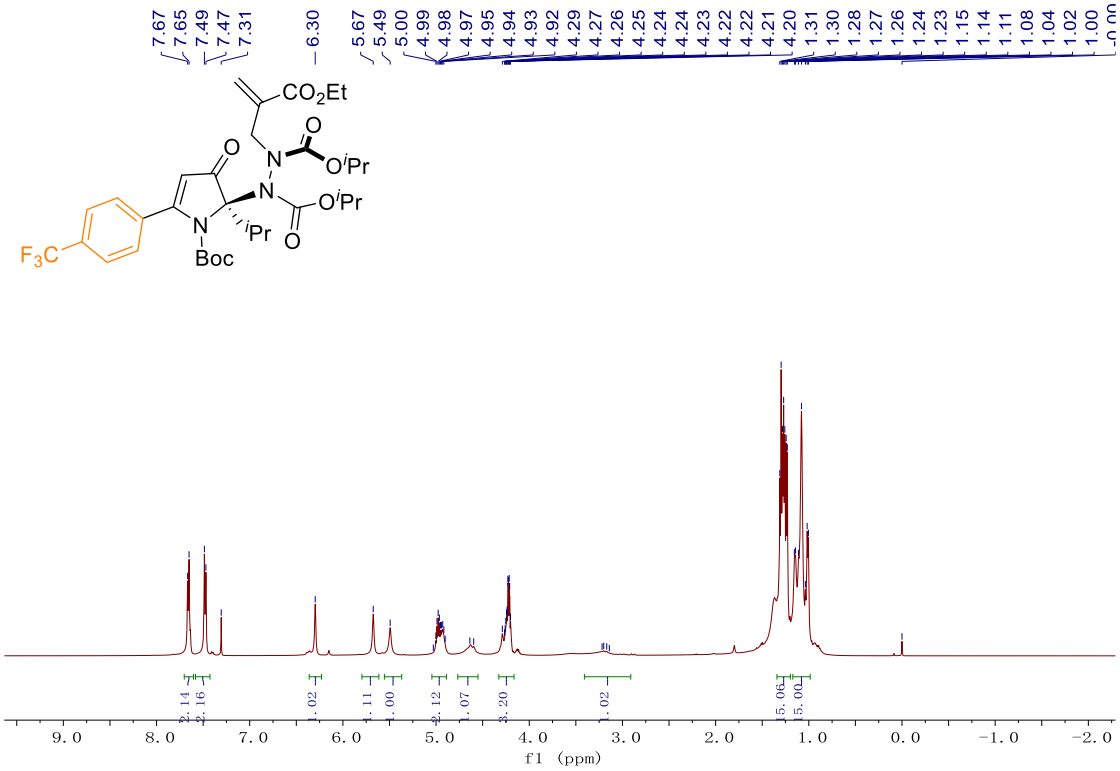
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6l)

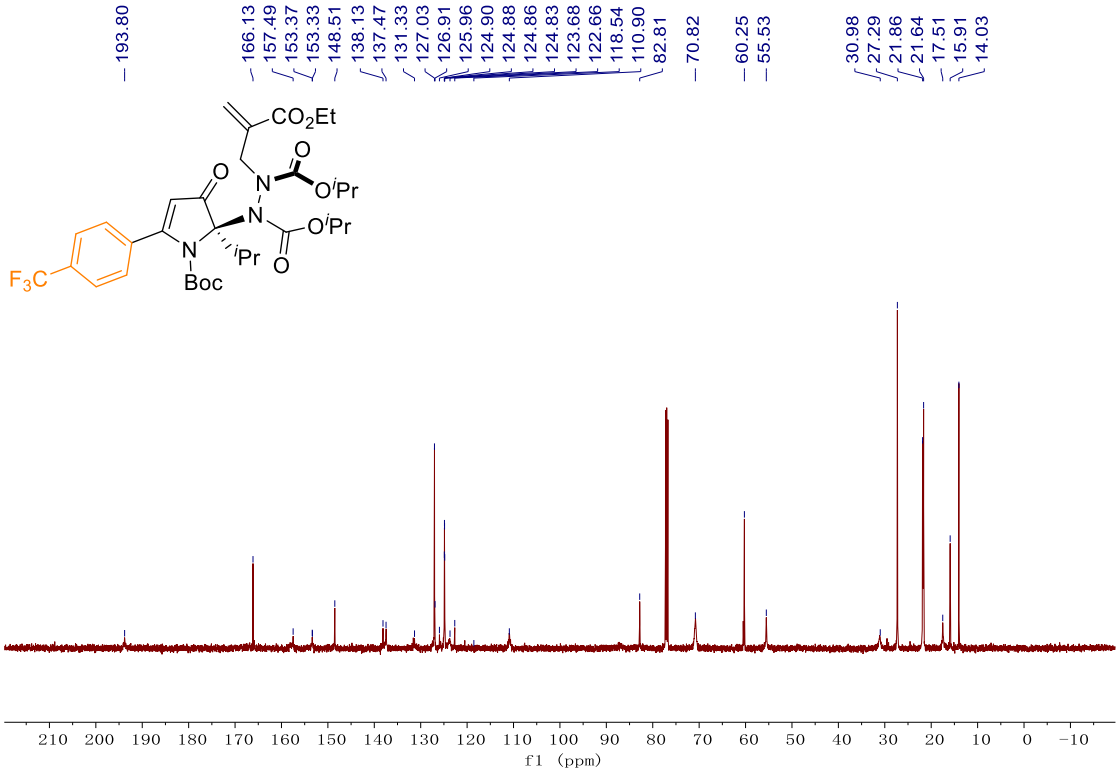


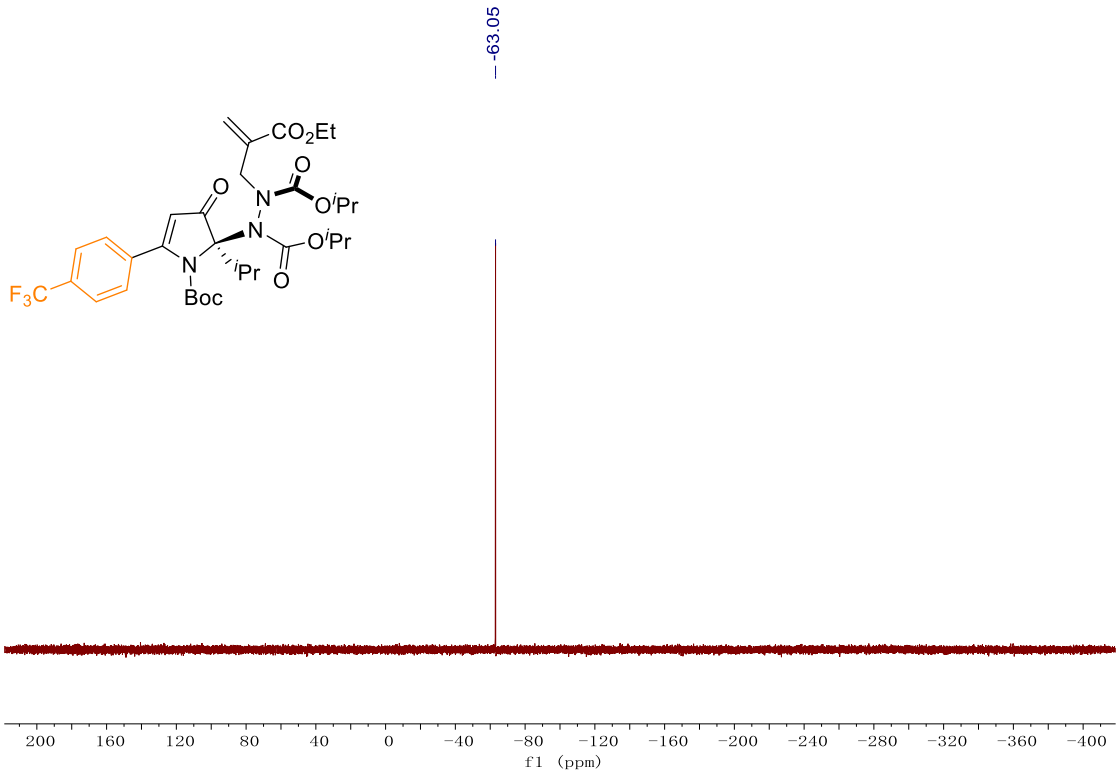



CO2Et
O
N
O
OiPr
N
O
OiPr
O
iPr
N
Boc
F
-112.50
20
0
−20
−40
−60
−80
−100
−120
−140
−160
−180
−200
−2
f1 (ppm)

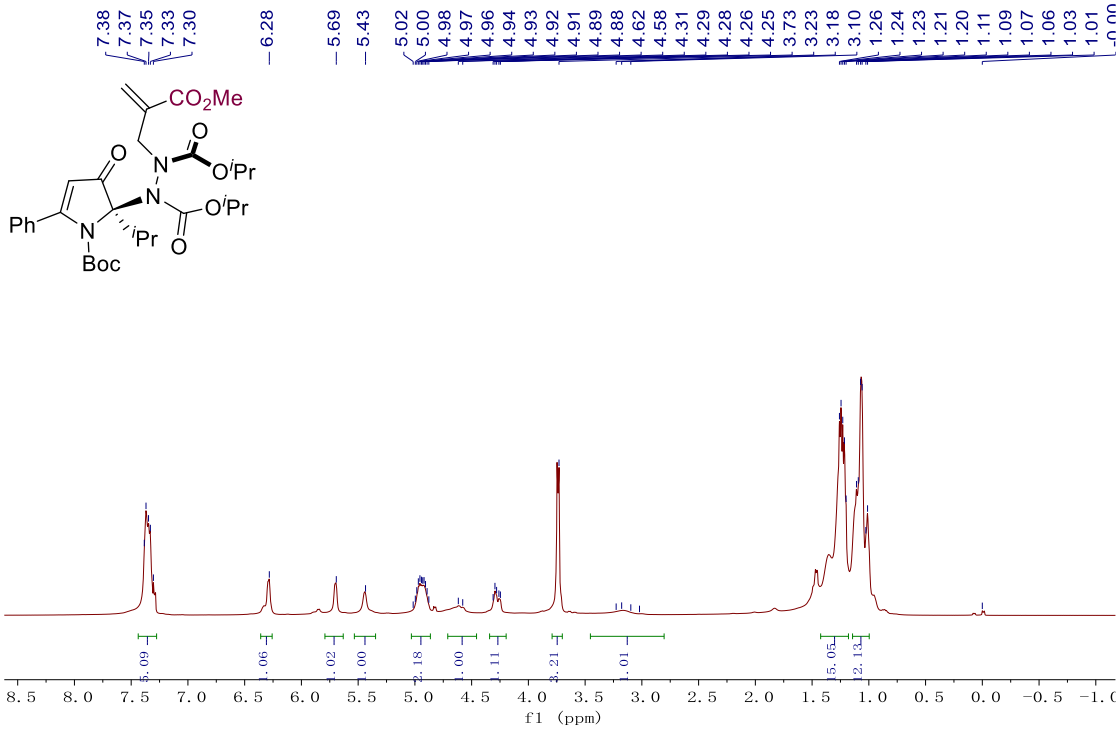
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6m)

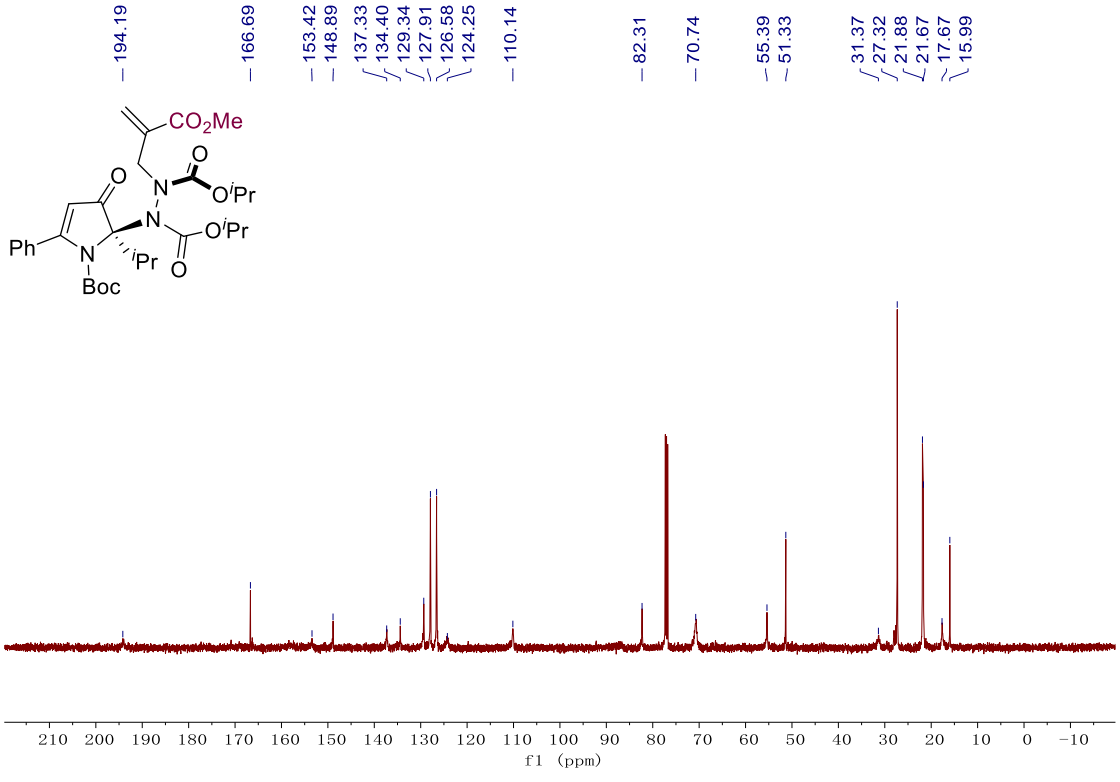




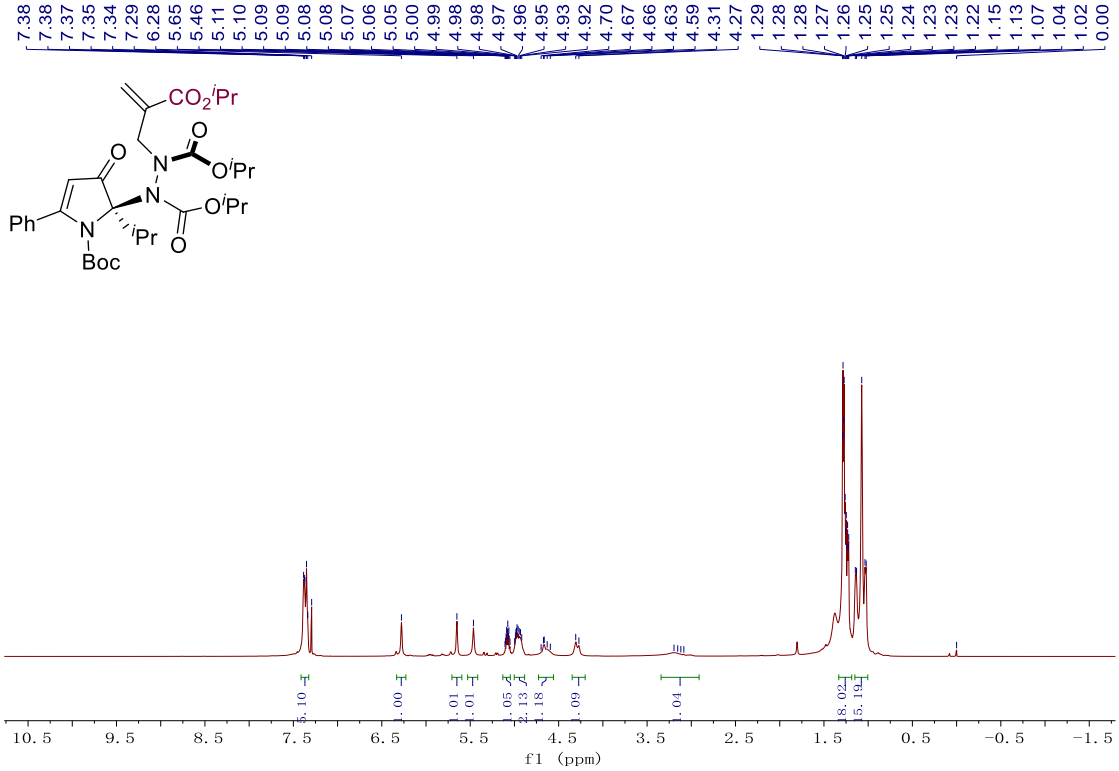

-63.05
CO2Et
O
N
OiPr
O
N
OiPr
O
N
iPr
Boc
F3C
200
160
120
80
40
0
−40
−80
−120
−160
−200
−240
−280
−320
−360
−400
f1 (ppm)

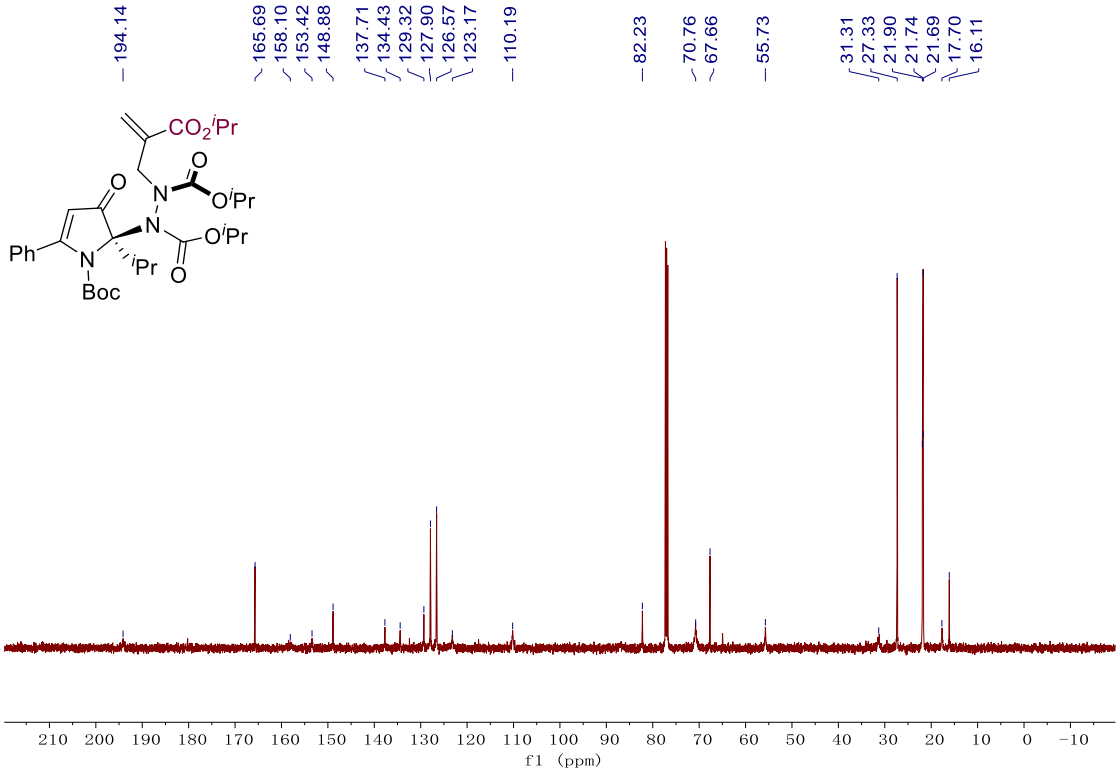
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(methoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6n)



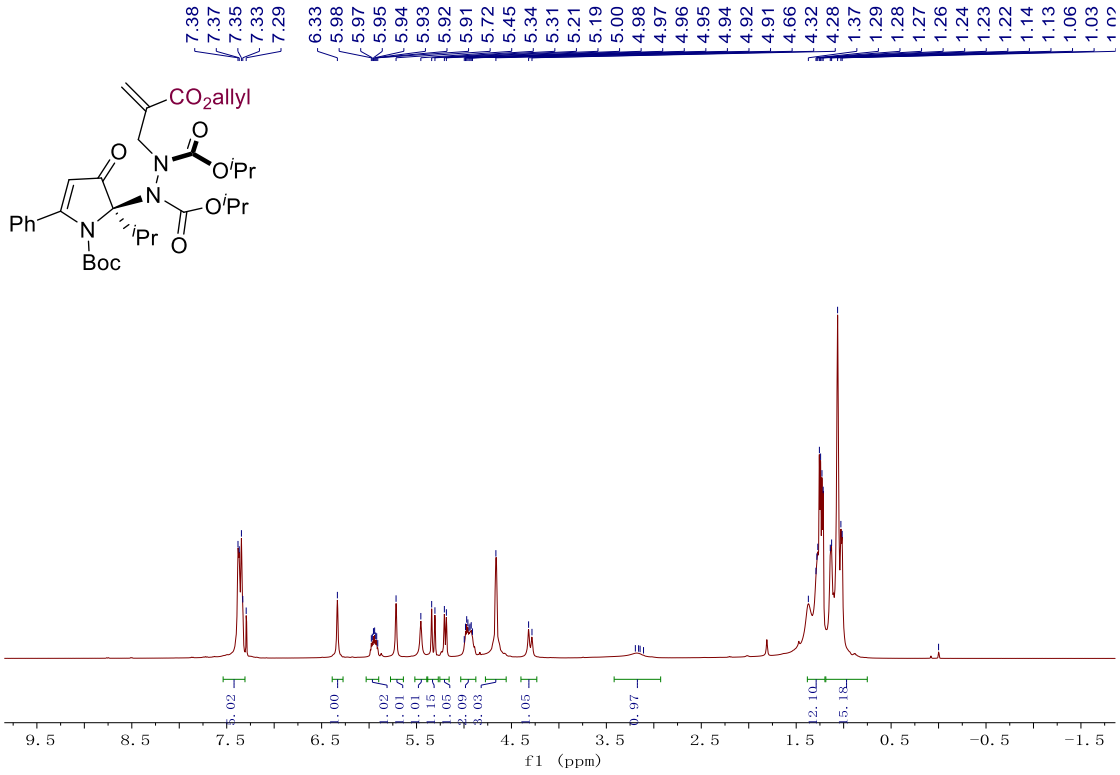


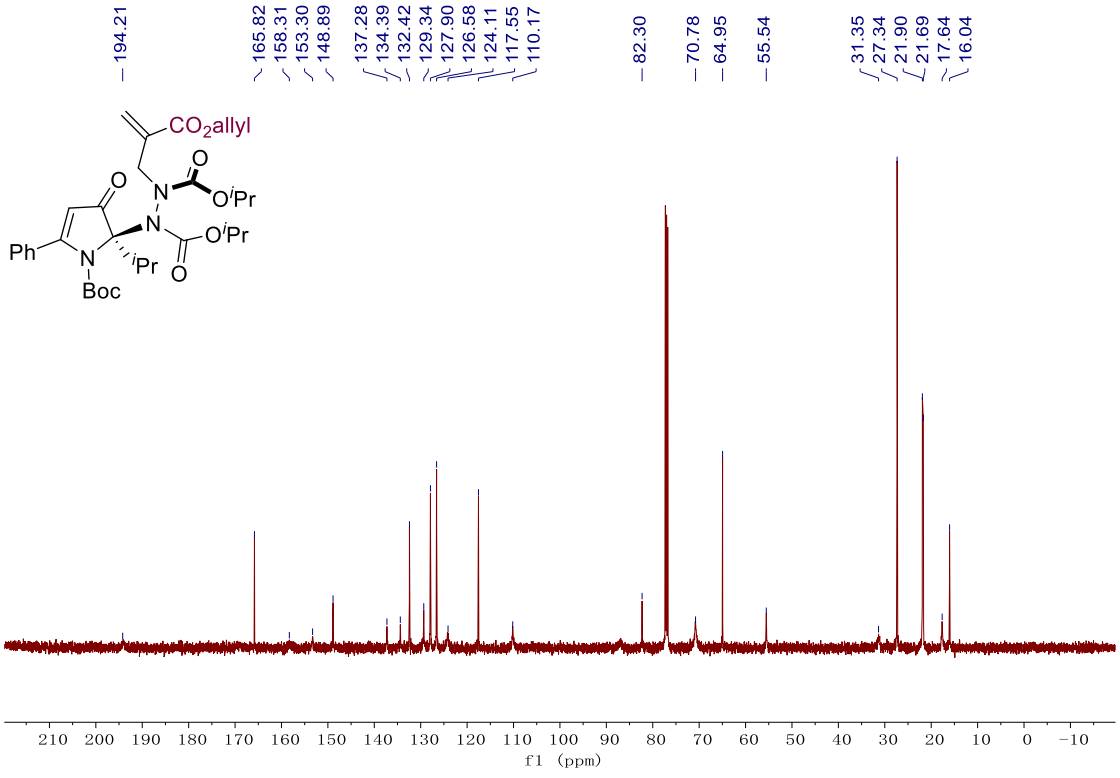
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(isopropoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6o)



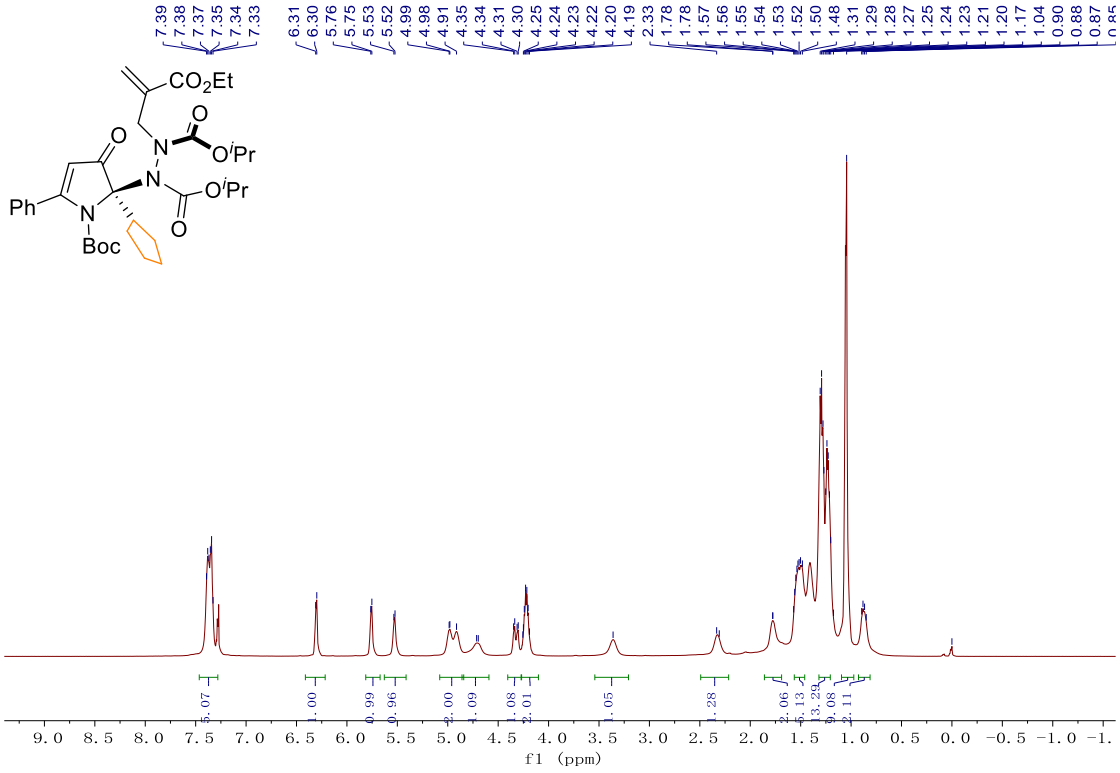


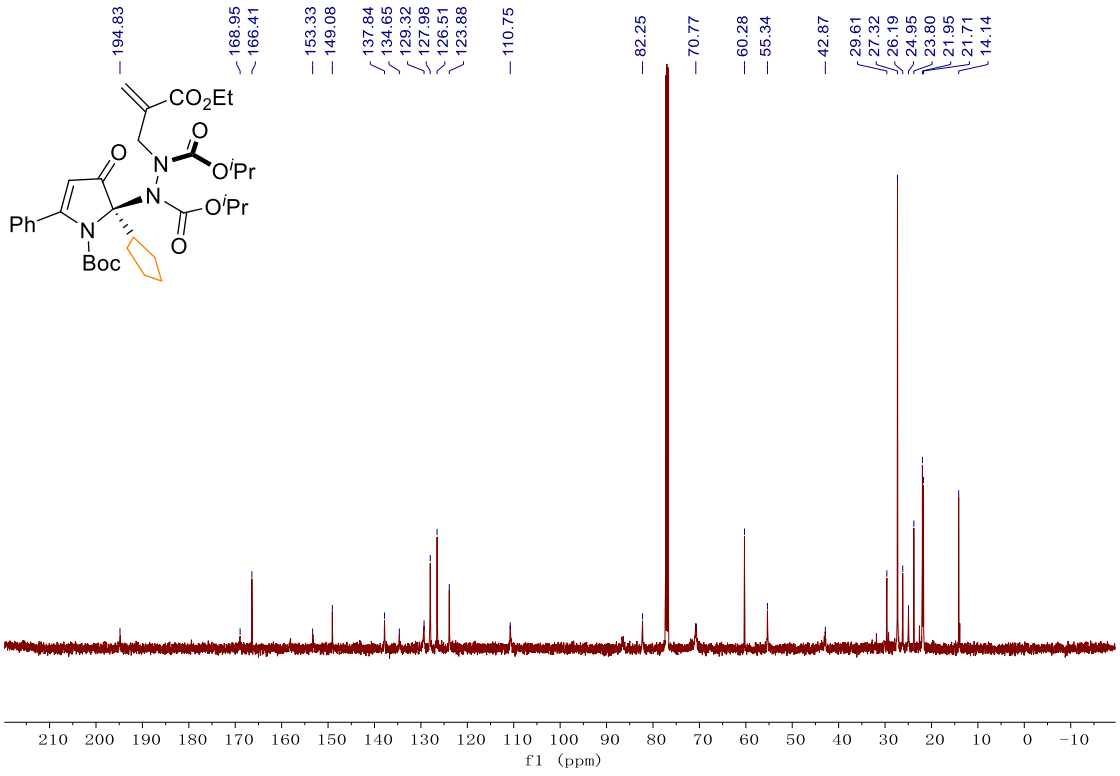
diisopropyl (*R*, *R*)-1-(2-((allyloxy)carbonyl)allyl)-2-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (6p)



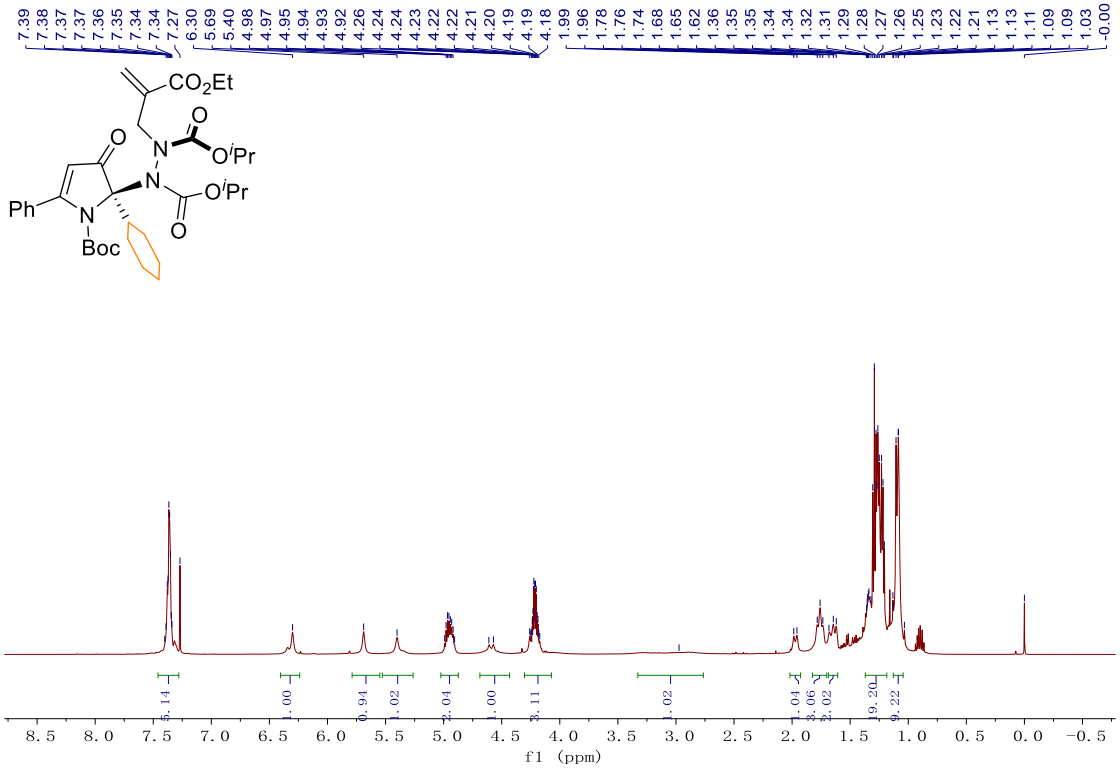


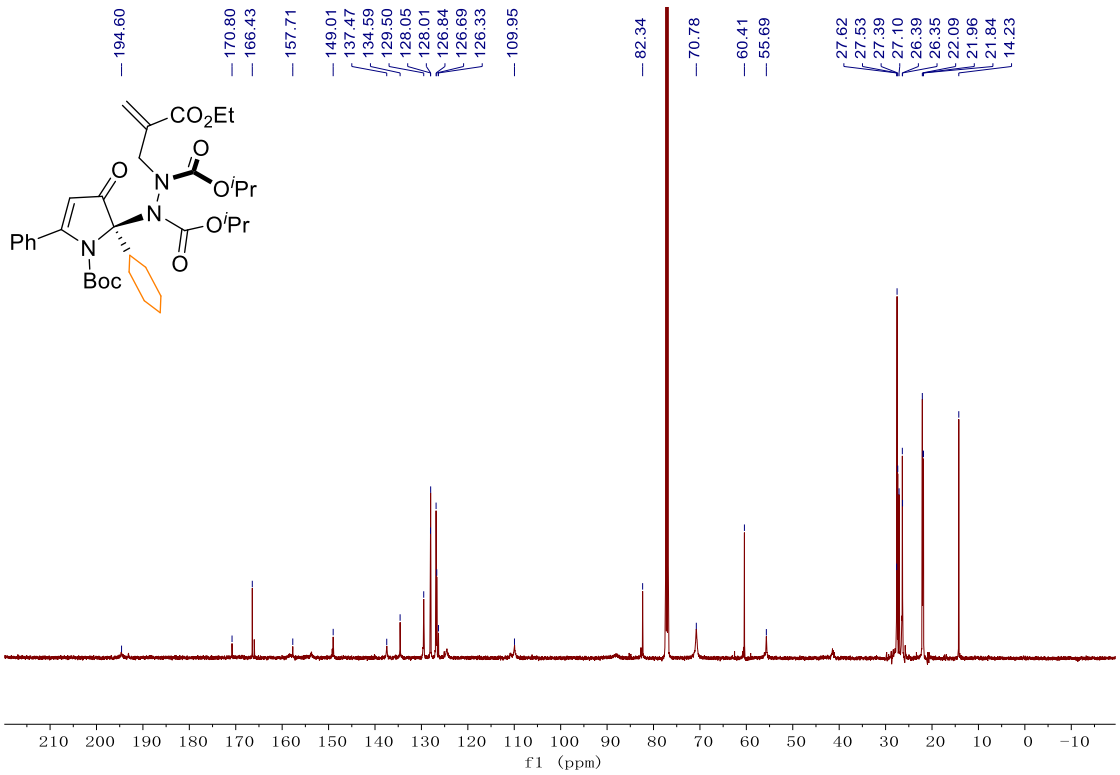
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-cyclopentyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6q)



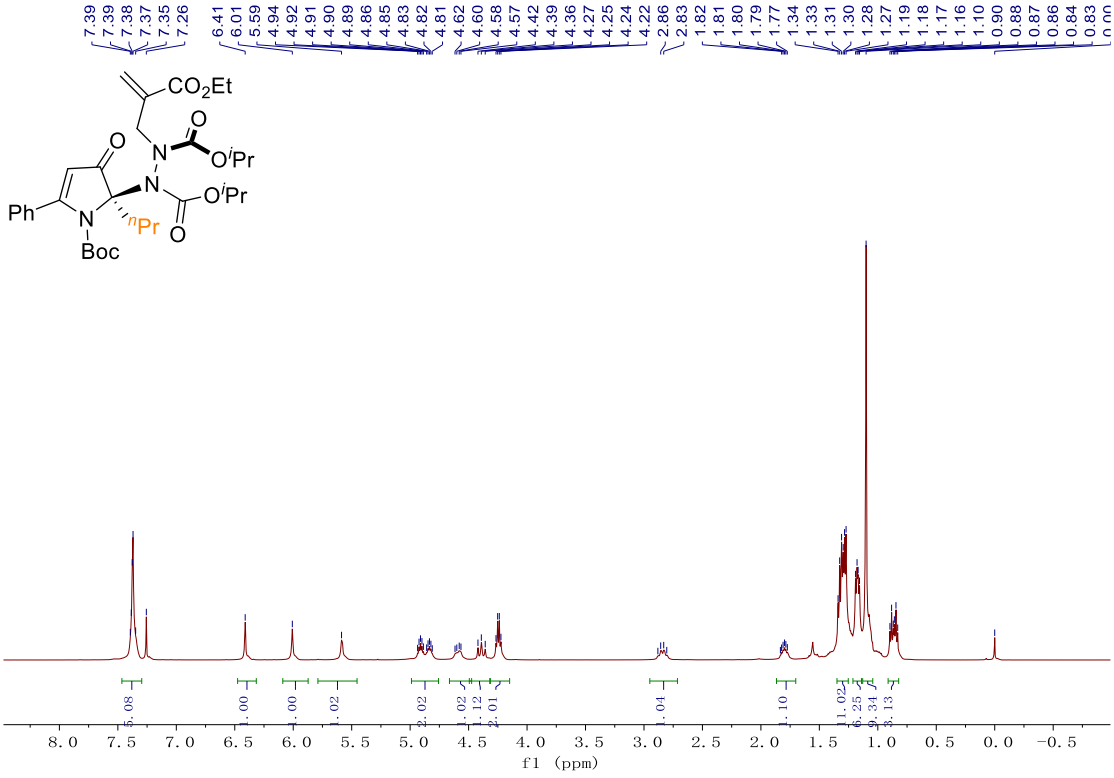


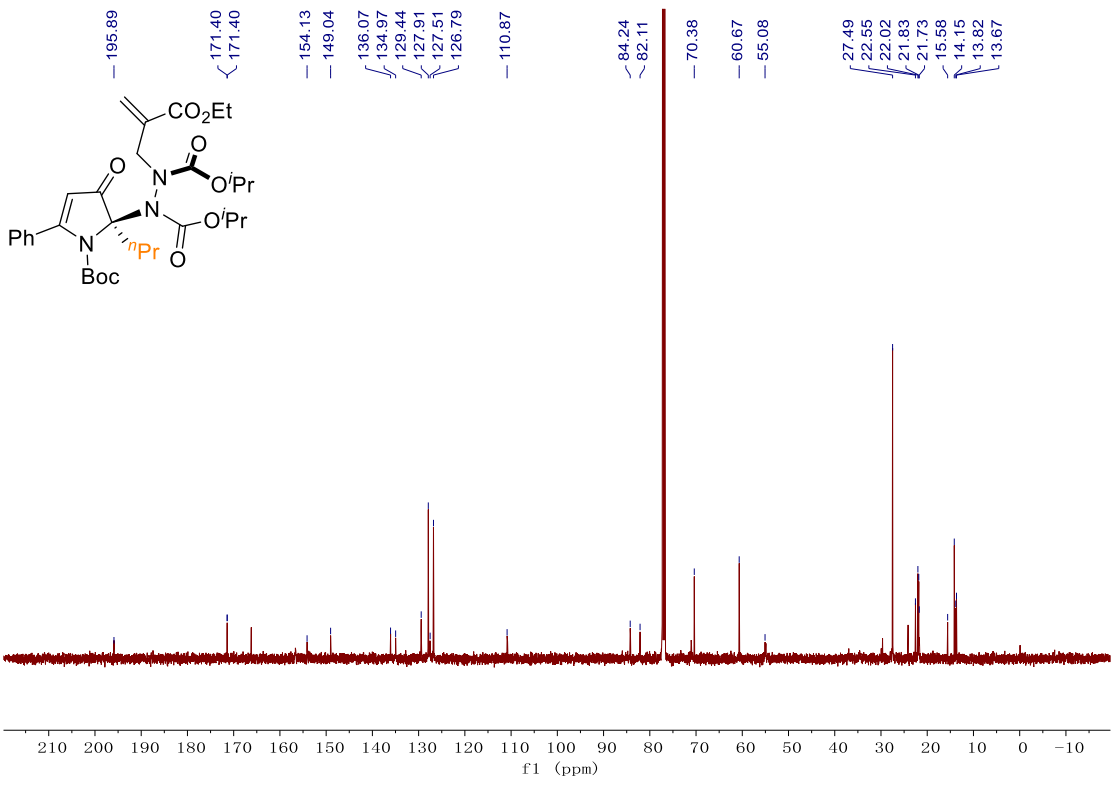
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-cyclohexyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6r)



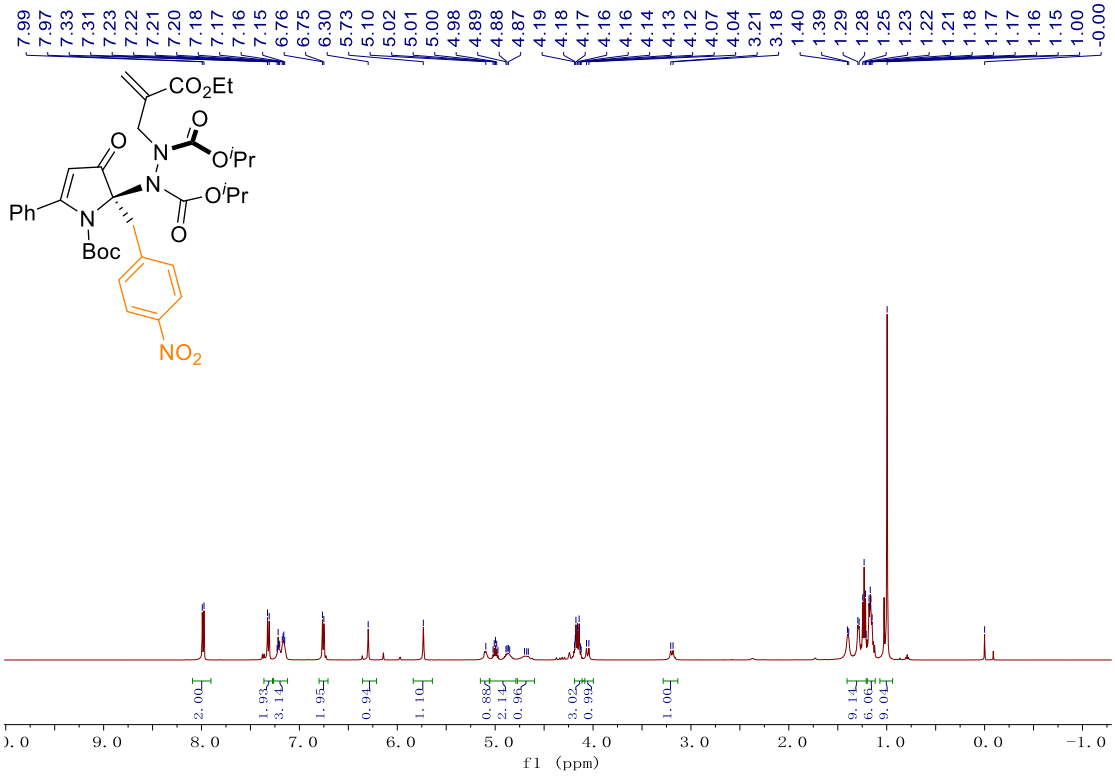


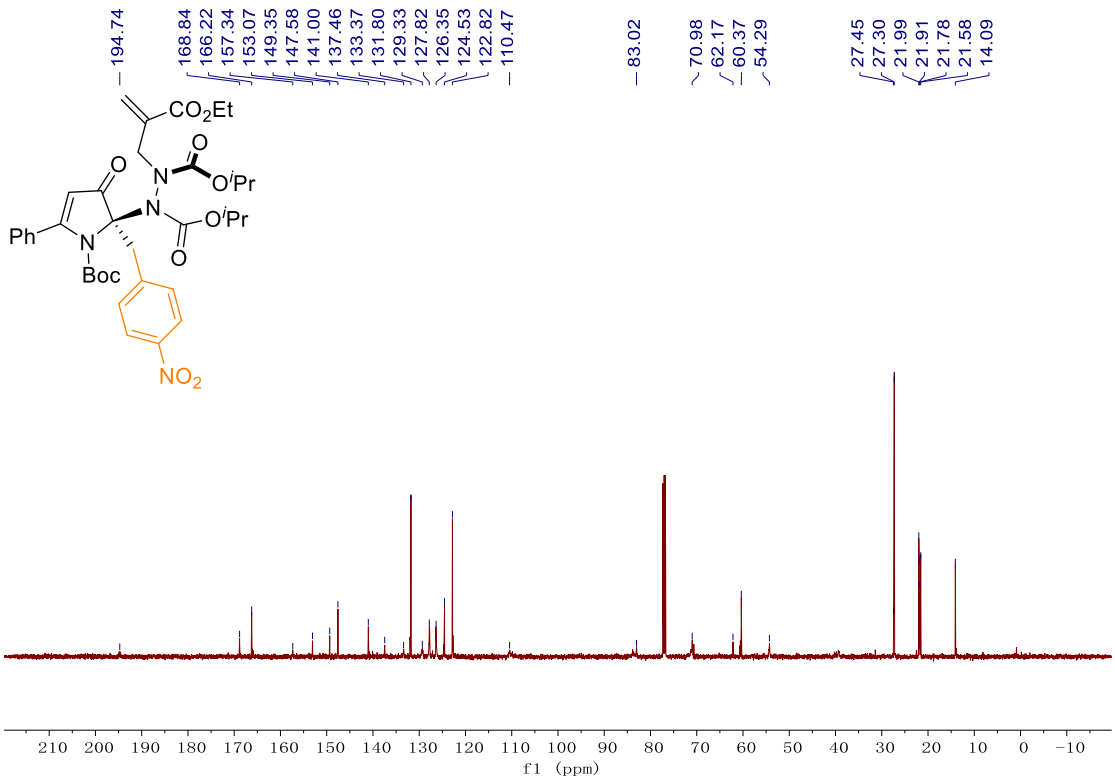
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-5-phenyl-2-propyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6s)



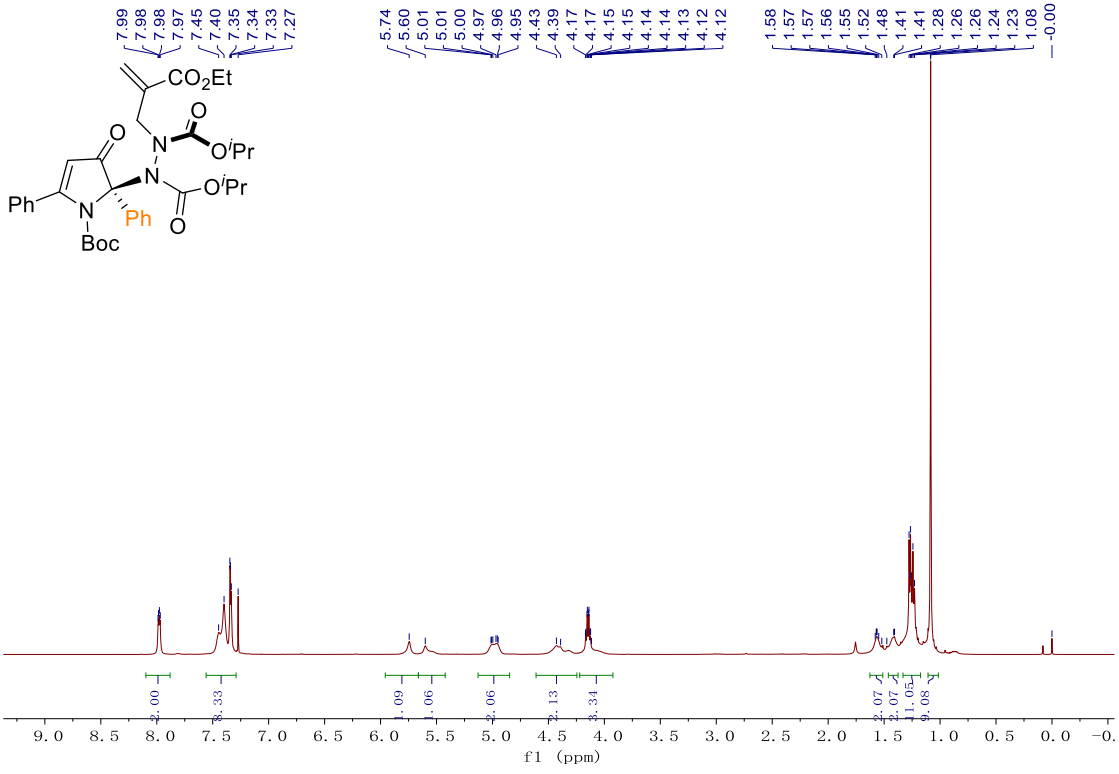


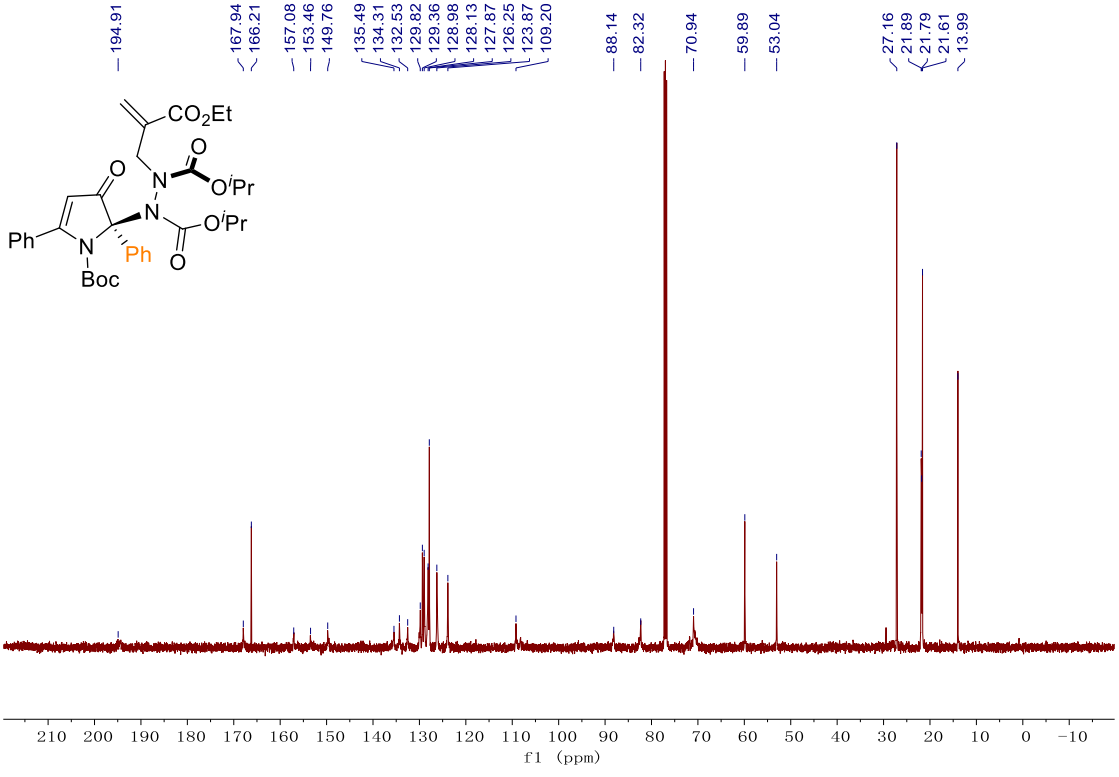
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6t)



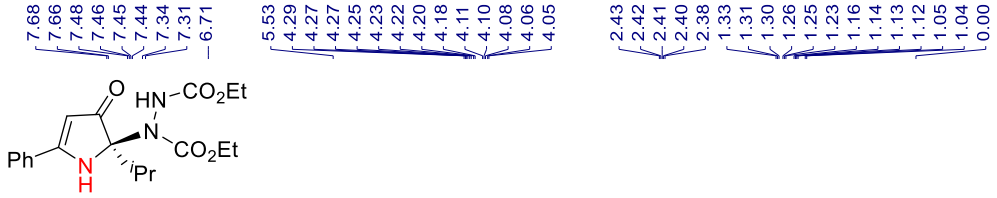


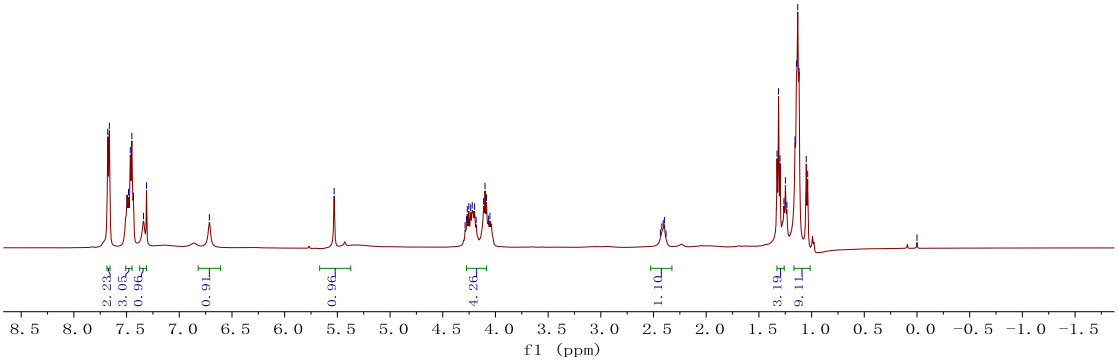
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-2,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6u)

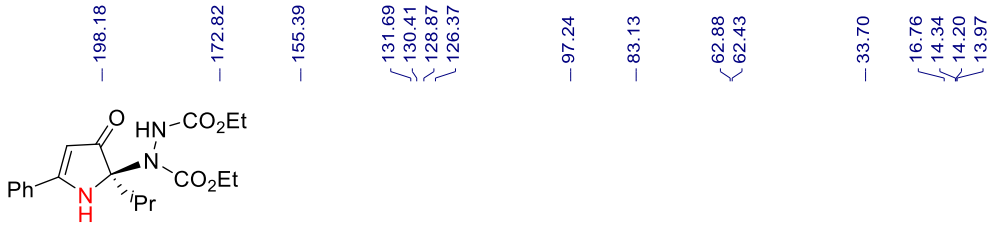


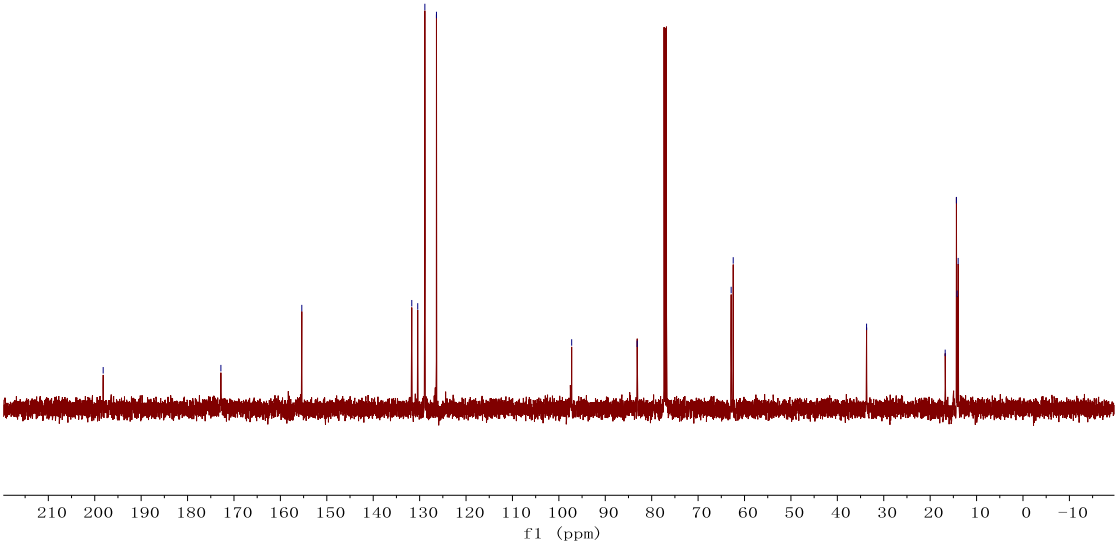


diethyl (*R*)-1-(2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (9)

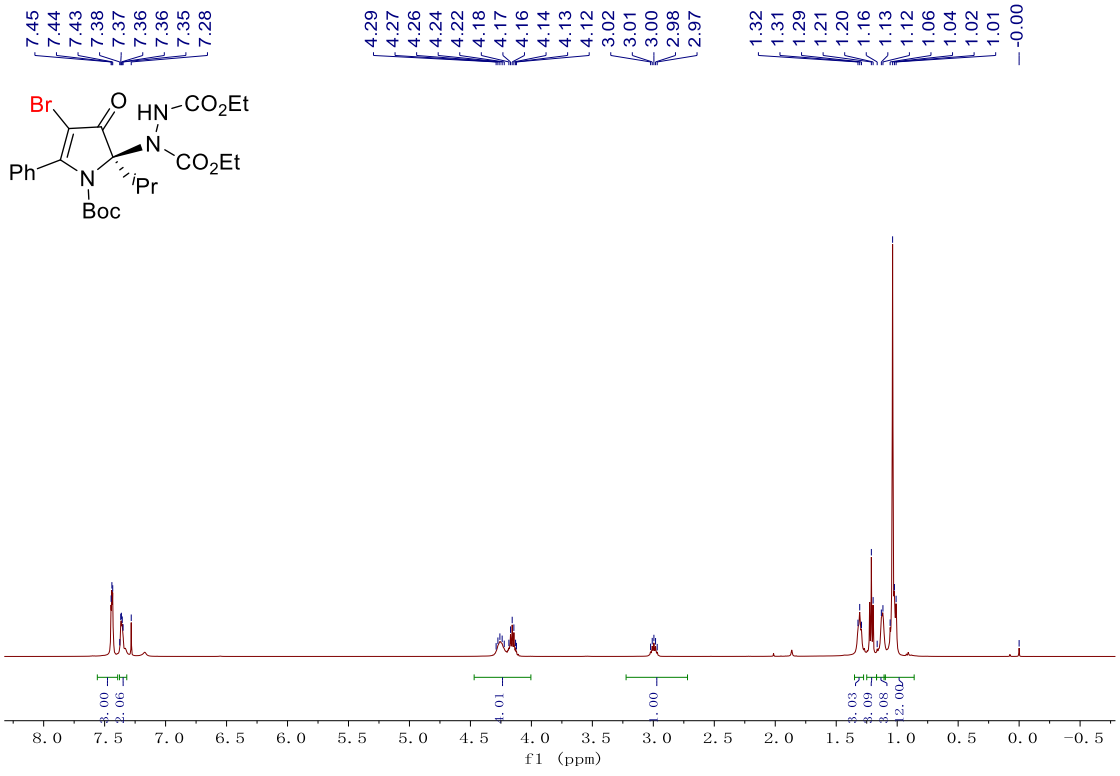


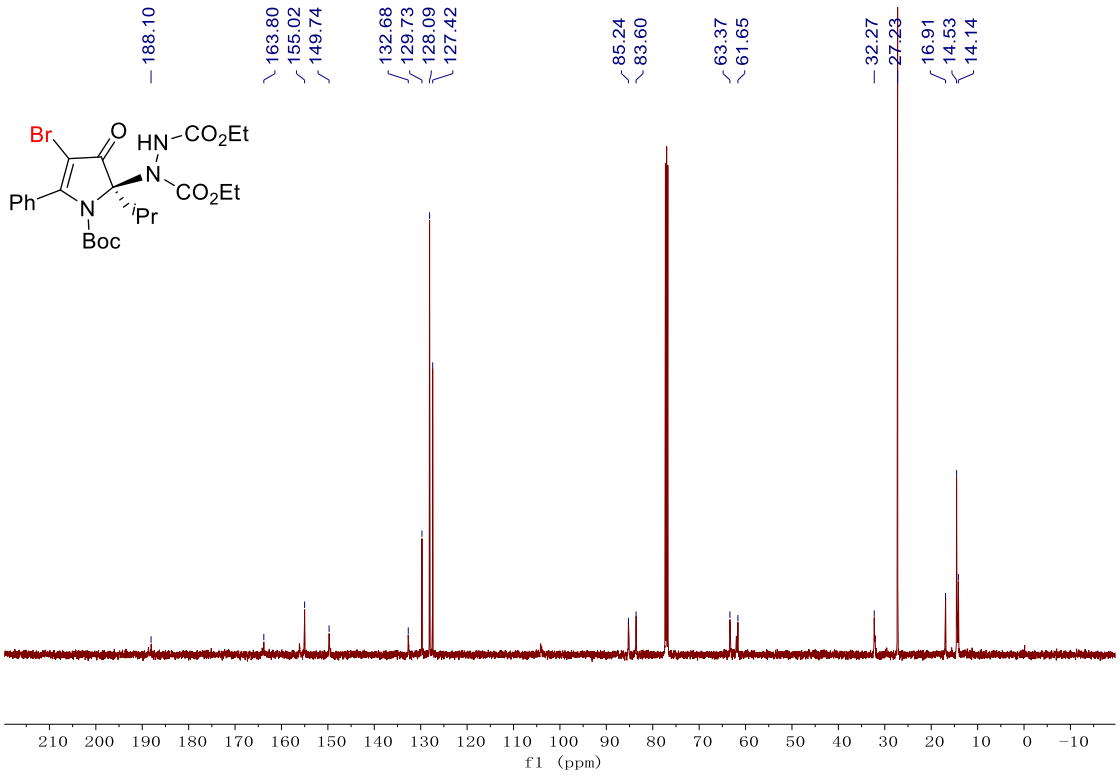




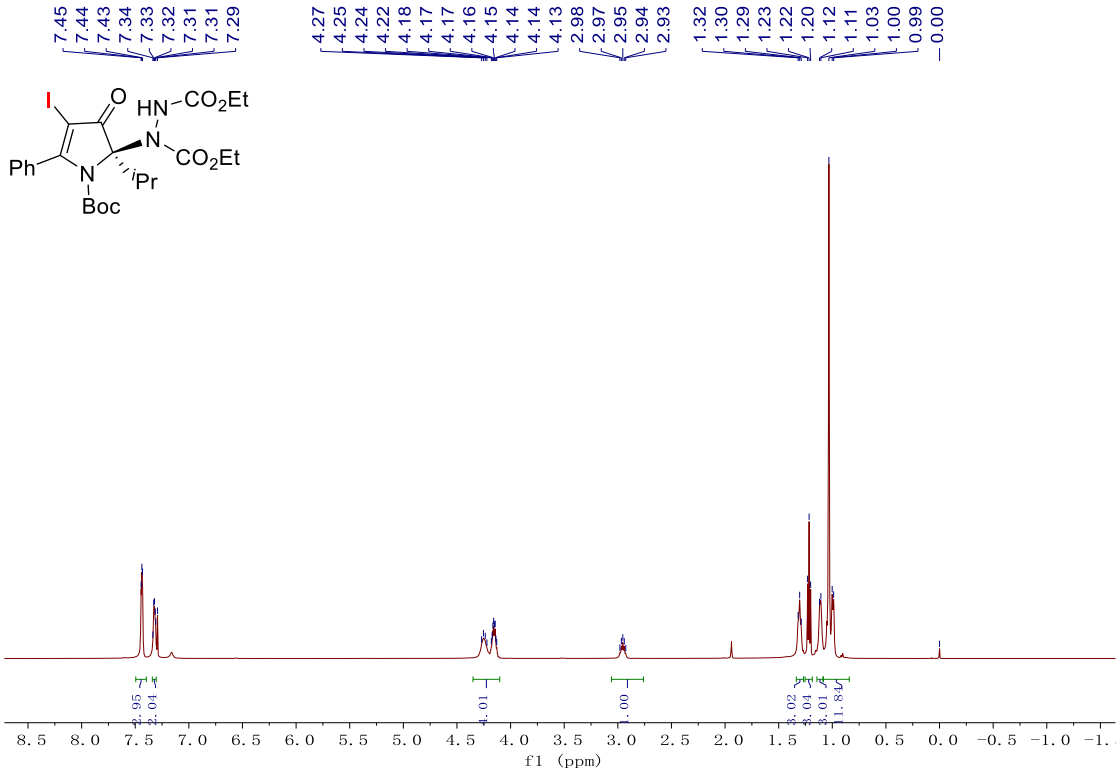


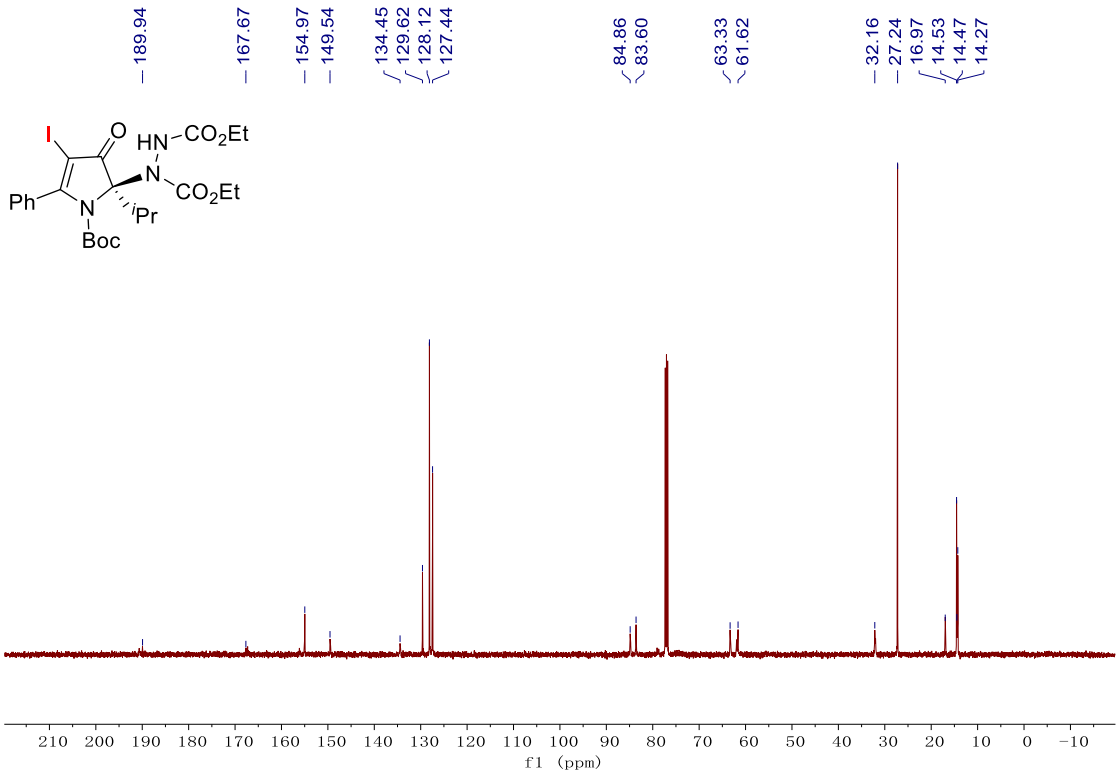
diethyl (*R*)-1-(4-bromo-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (10)



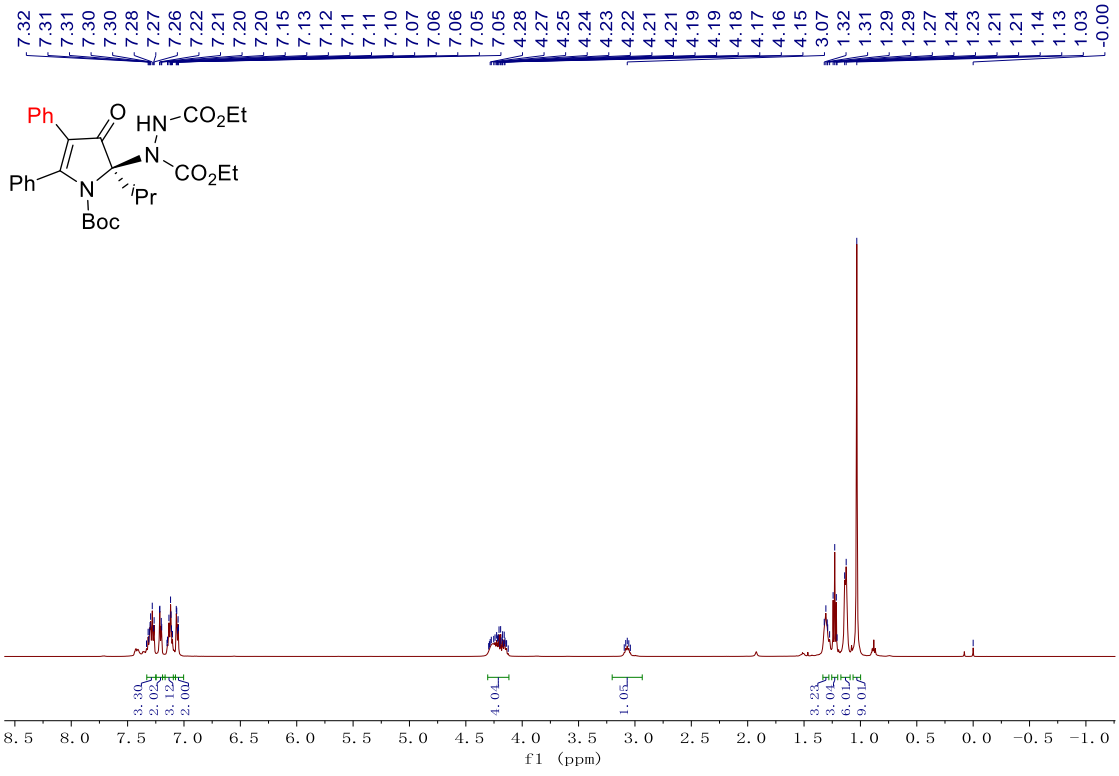


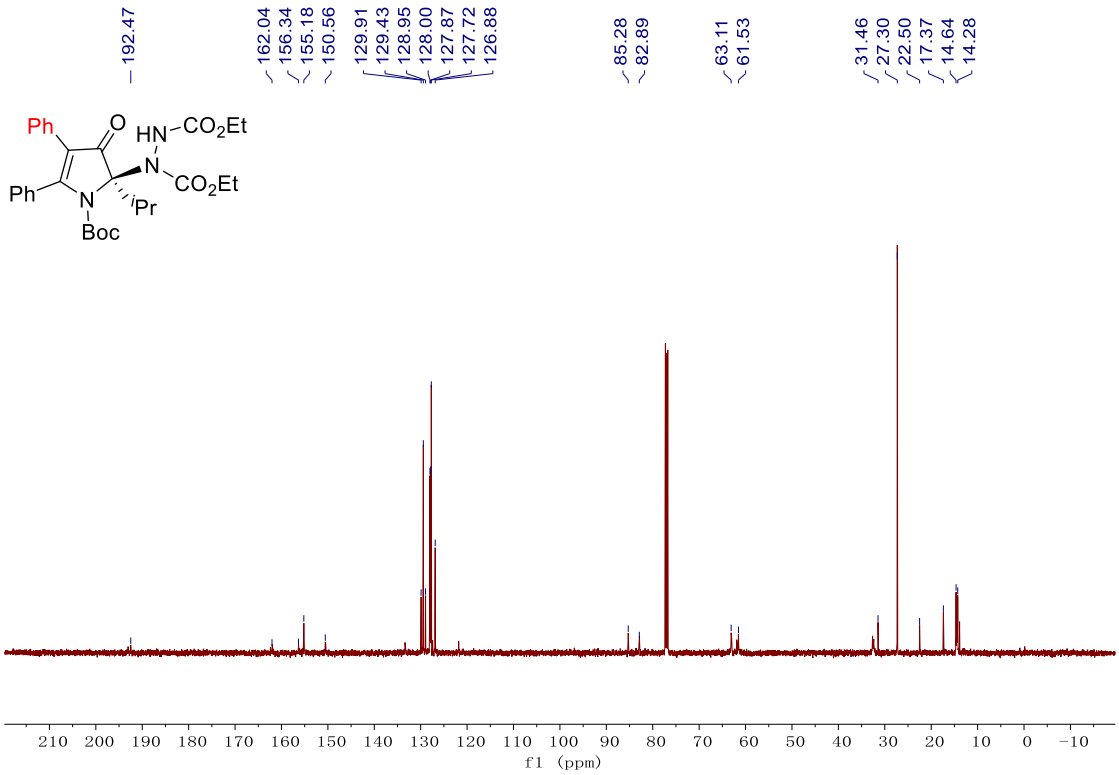
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-4-iodo-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (11)



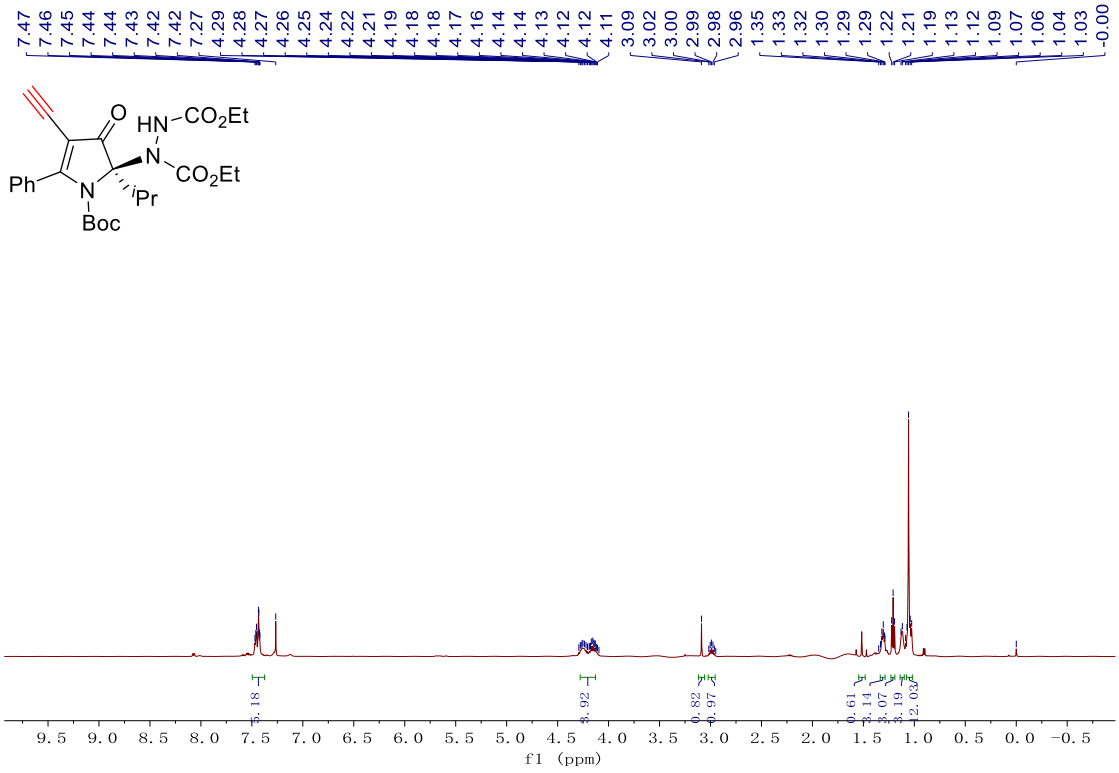


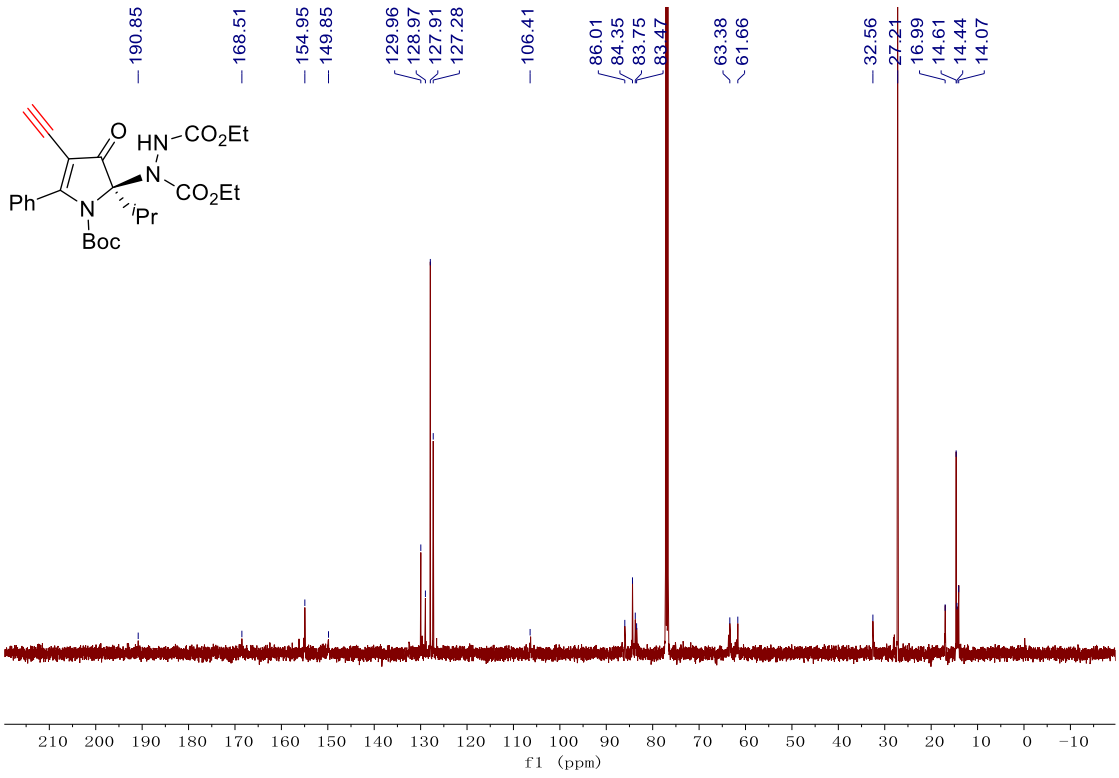
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-4,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (12)



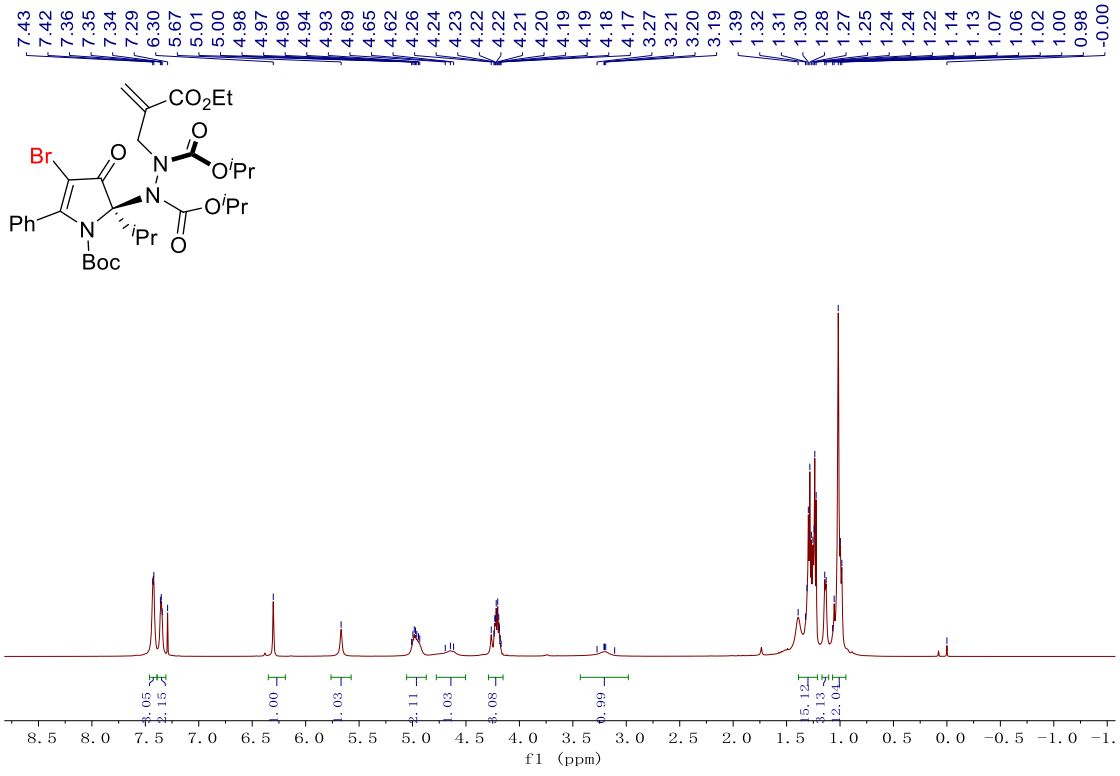


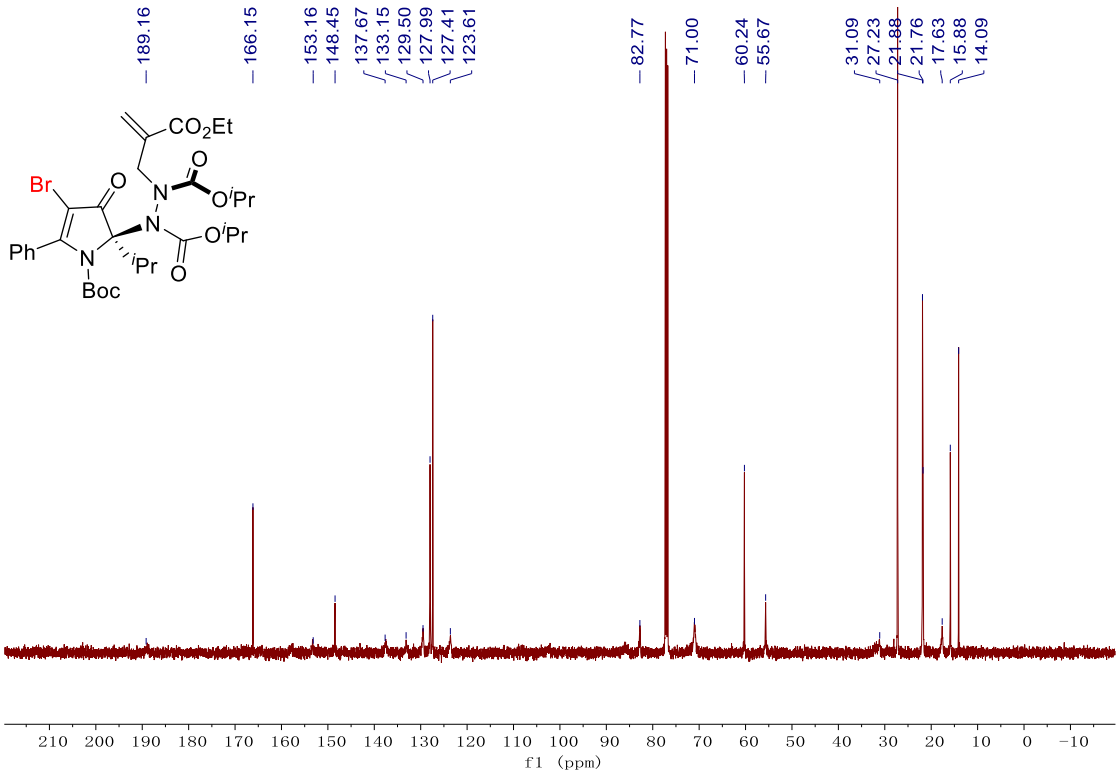
diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-4-ethynyl-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (13)



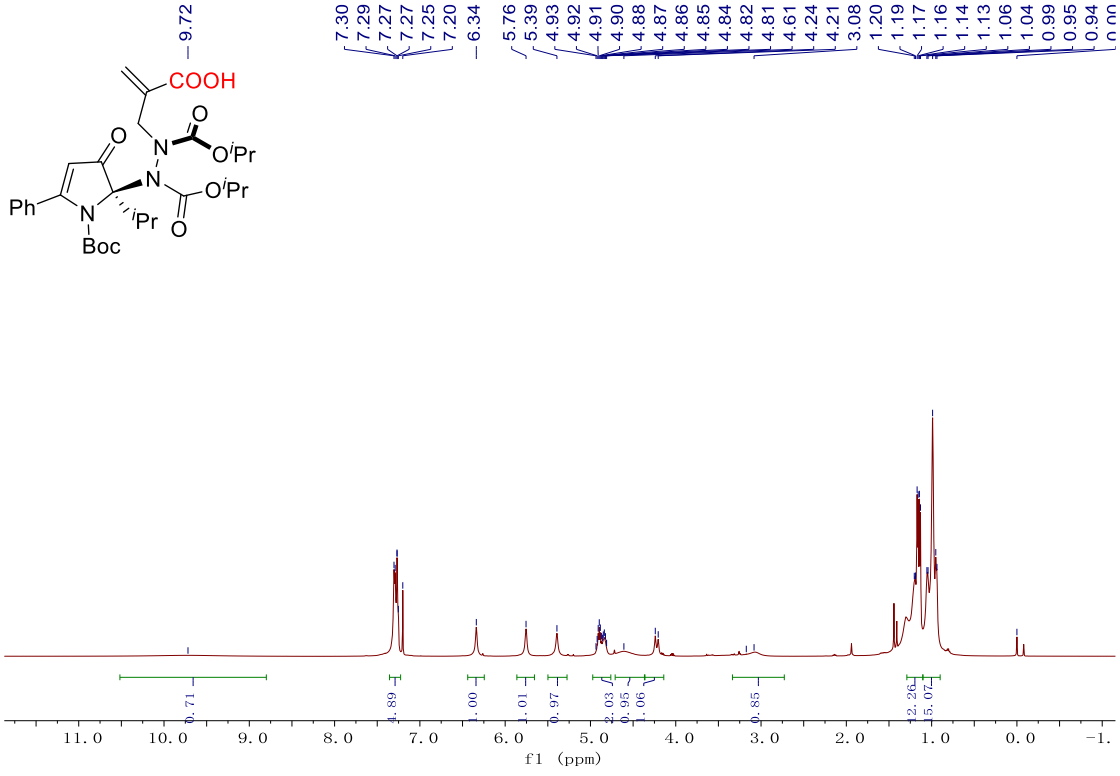


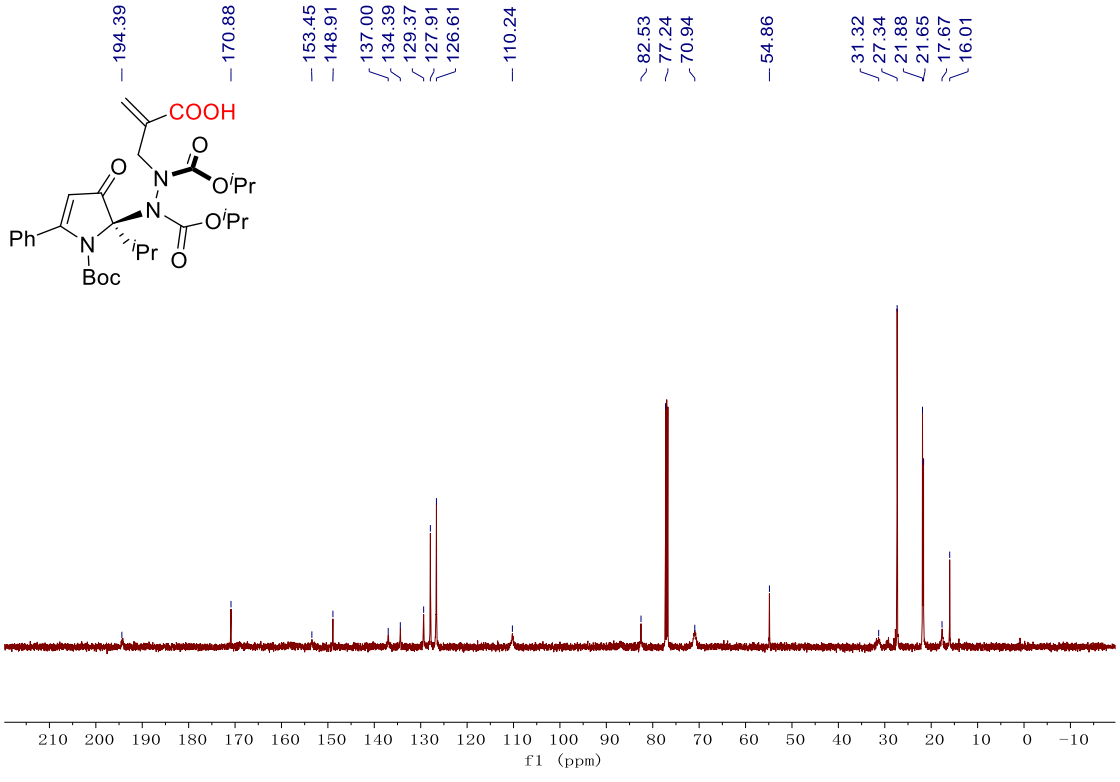
diisopropyl (*R*, *R*)-1-(4-bromo-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (14)



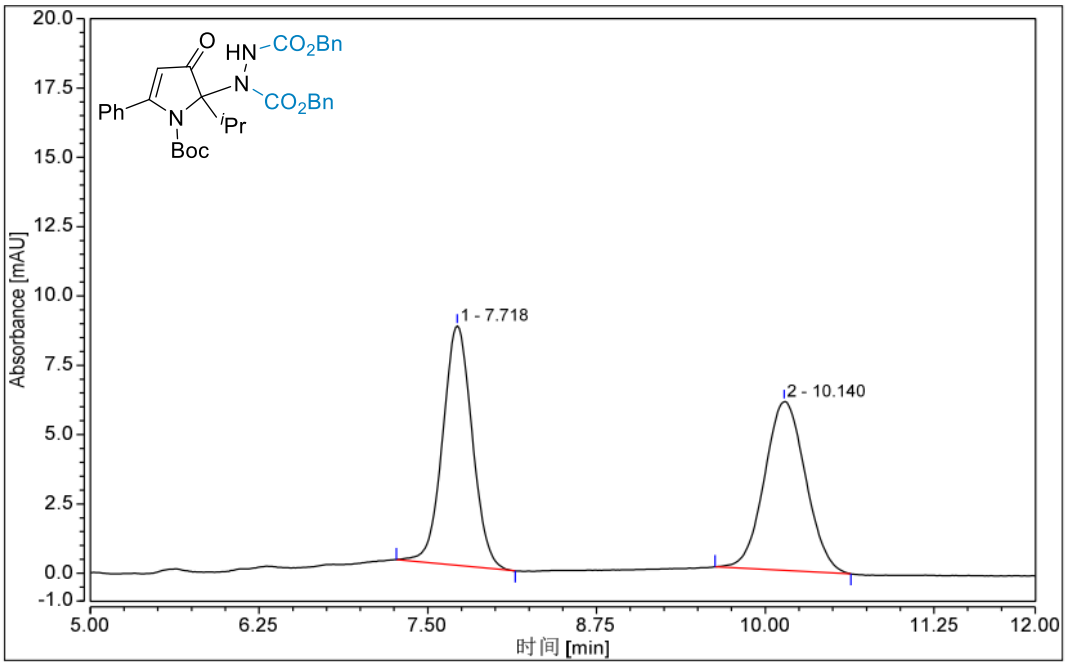


(*R*, *R*)-2-((2-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-1,2-bis(isopropoxycarbonyl)hydrazineyl)methyl)acrylic acid (15)

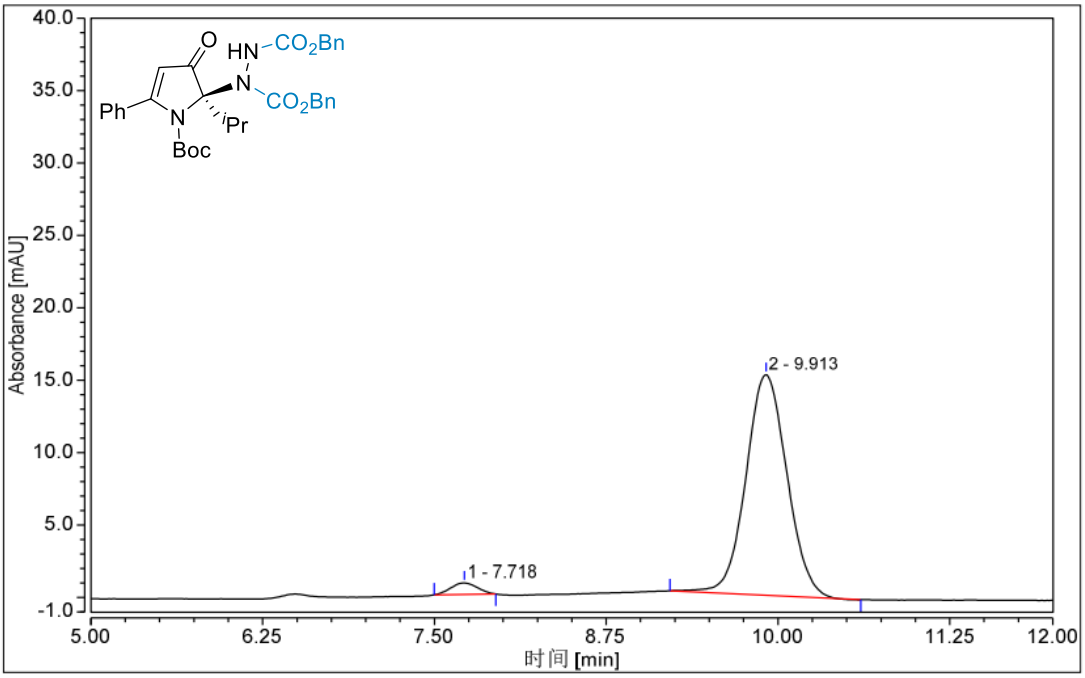




Dibenzyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3a)

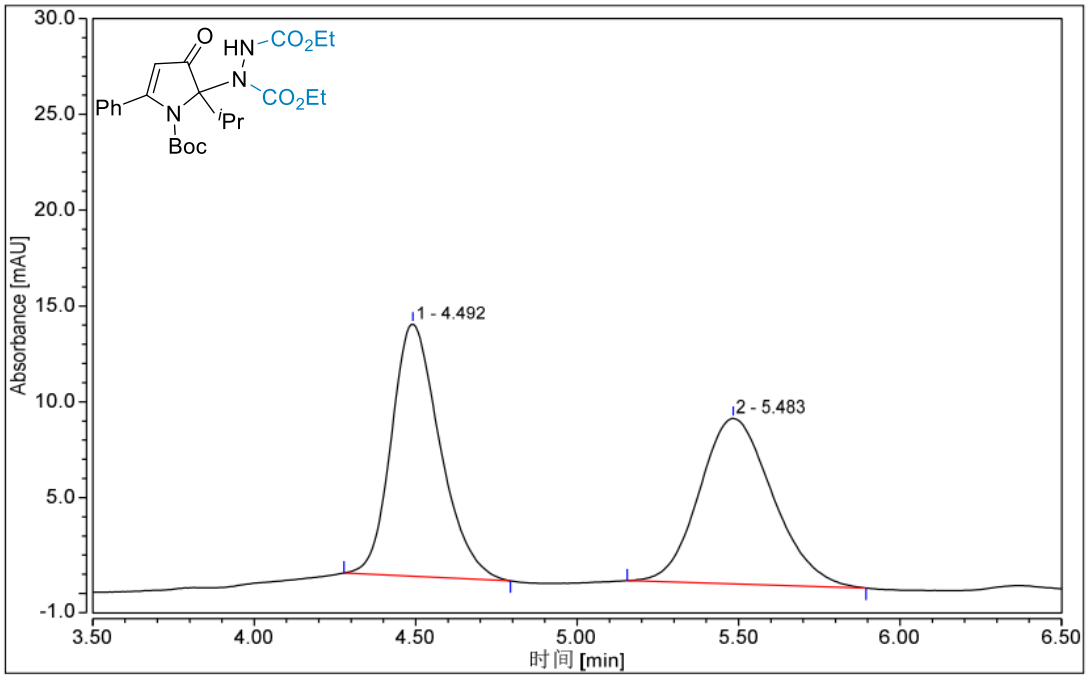


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.718	2.184	8.633	50.38	58.64
2	10.140	2.151	6.090	49.62	41.36

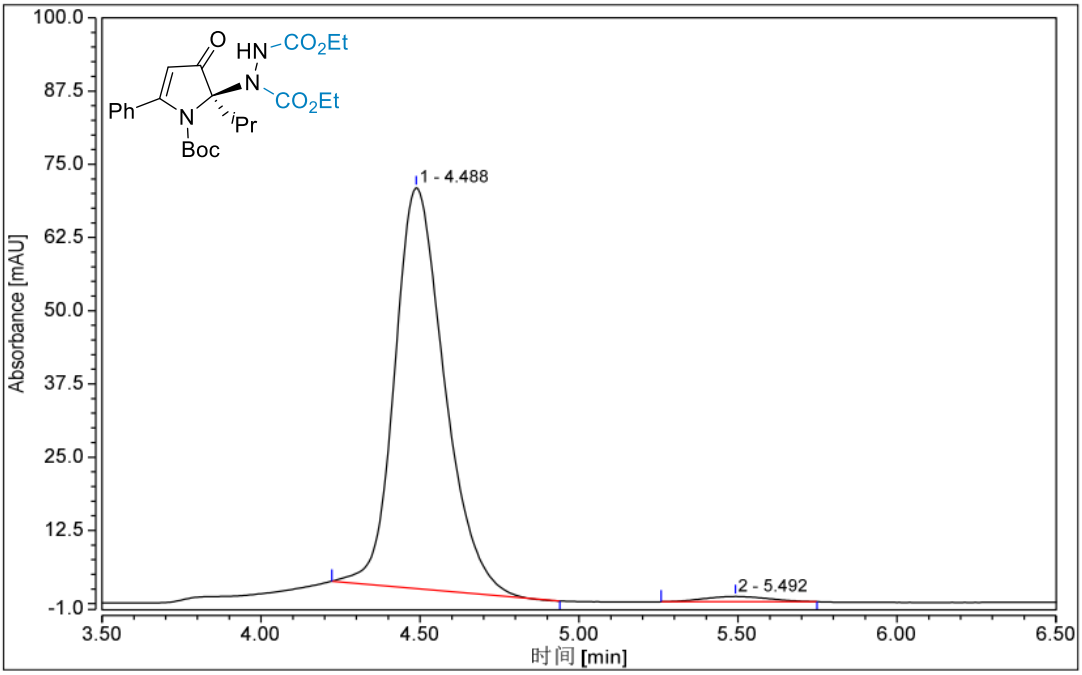


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.718	0.179	0.801	3.29	4.99
2	9.913	5.280	15.247	96.71	95.01

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3b)

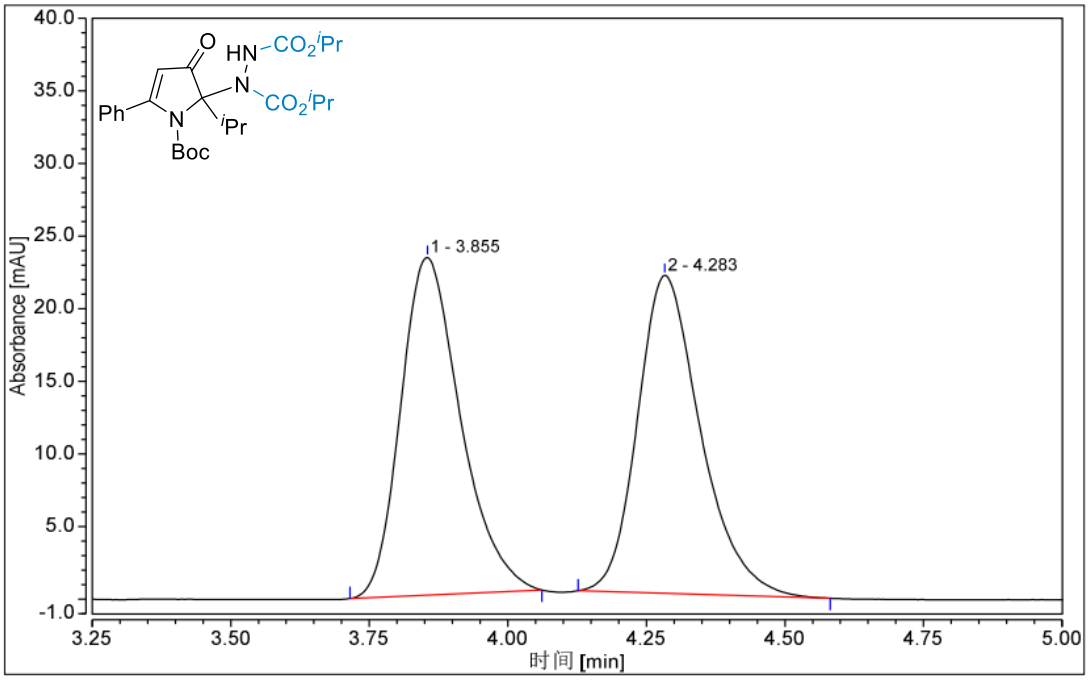


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.492	2.293	13.163	50.20	60.37
2	5.483	2.274	8.641	49.80	39.63

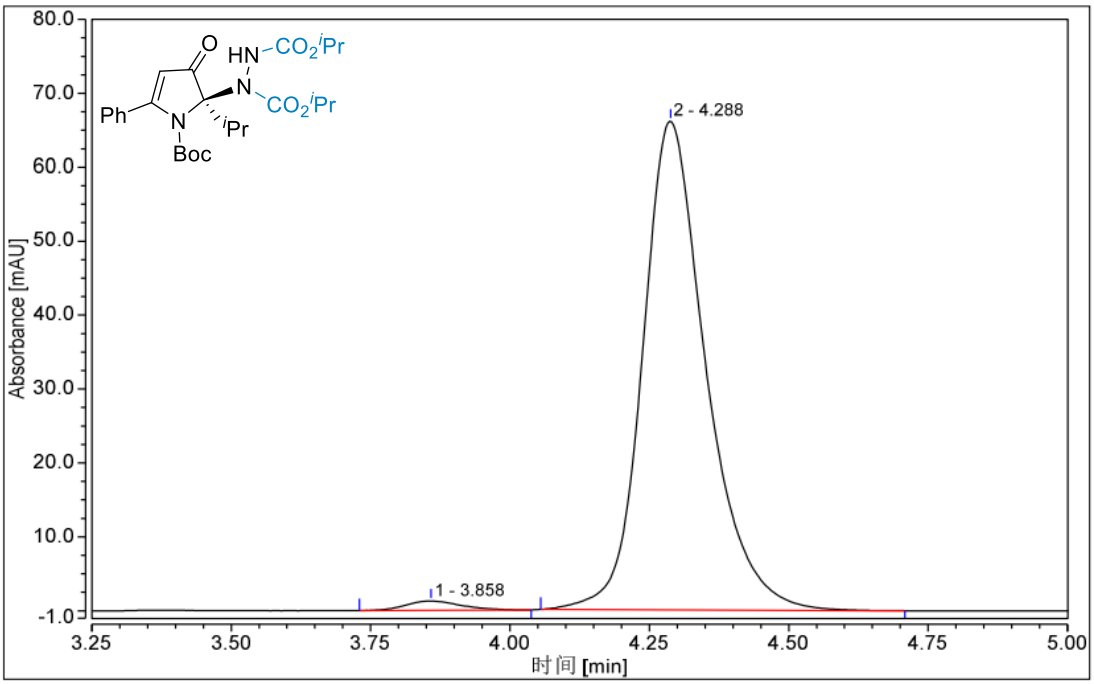


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.488	12.437	68.436	98.30	98.69
2	5.492	0.215	0.909	1.70	1.31

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3c)

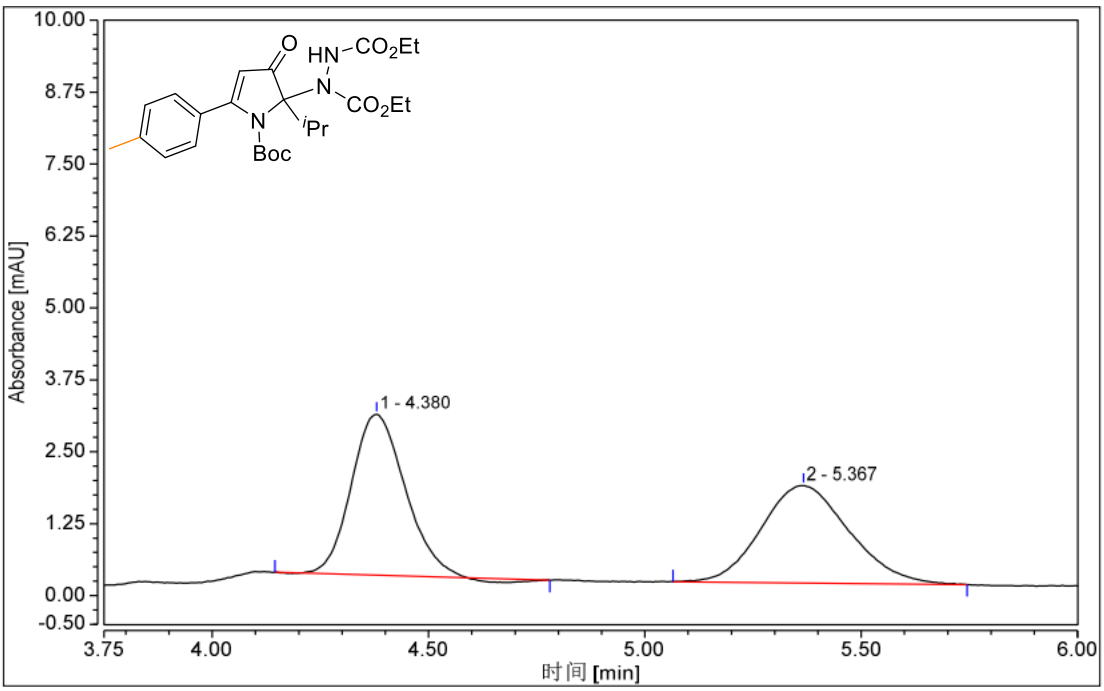


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.855	2.912	23.251	50.19	51.49
2	4.283	2.890	21.901	49.81	48.51

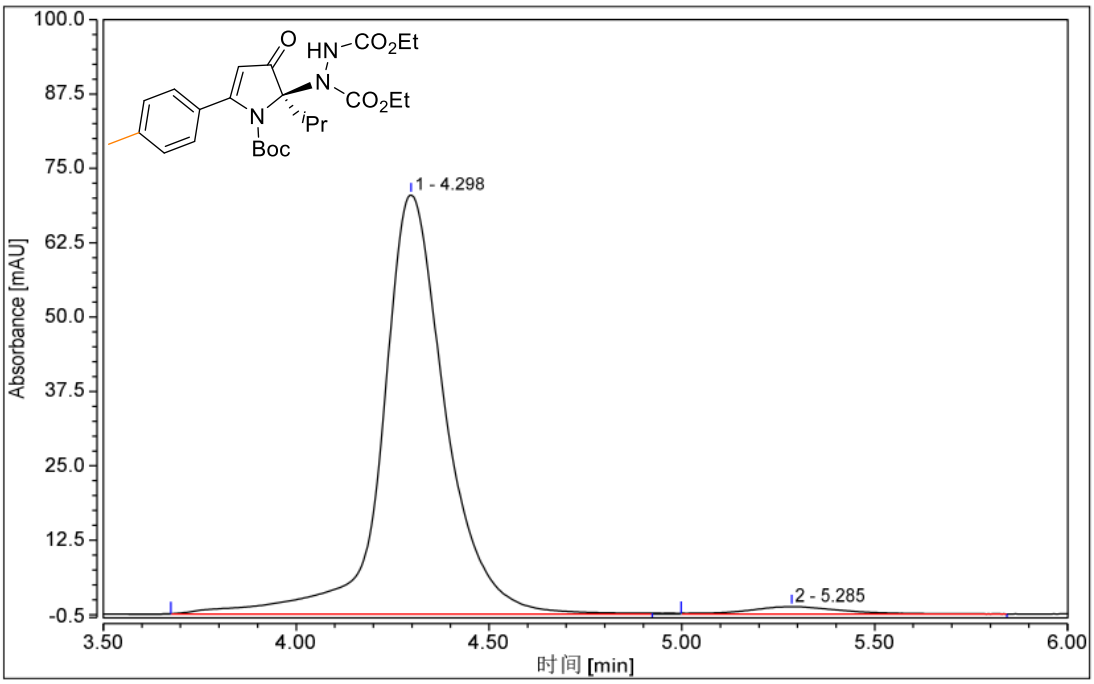


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.858	0.141	1.249	1.60	1.85
2	4.288	8.684	66.096	98.40	98.15

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(p-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3d)

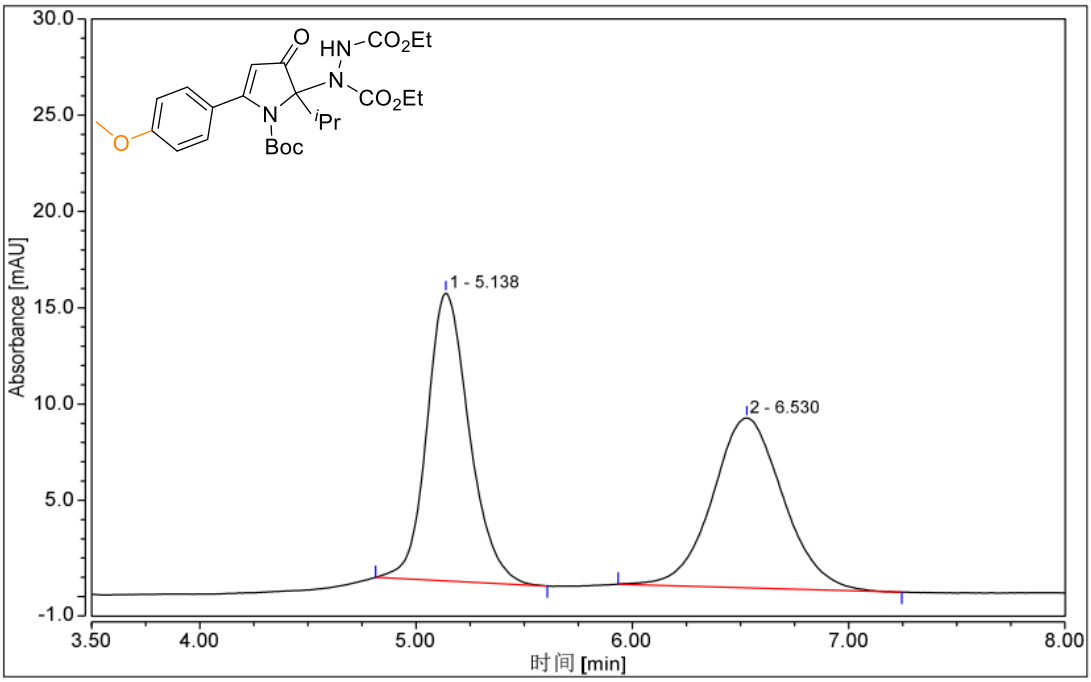


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.380	0.398	2.796	49.99	62.24
2	5.367	0.399	1.697	50.01	37.76

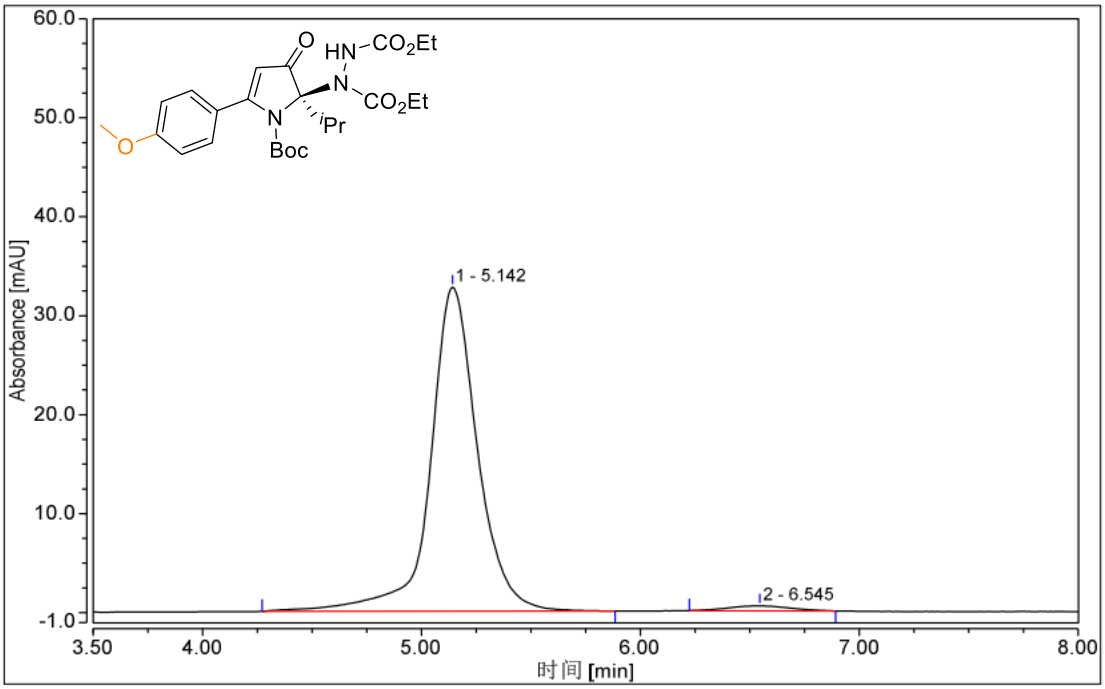


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.298	13.451	70.466	97.54	98.28
2	5.285	0.340	1.235	2.46	1.72

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-5-(4-methoxyphenyl)-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3e)

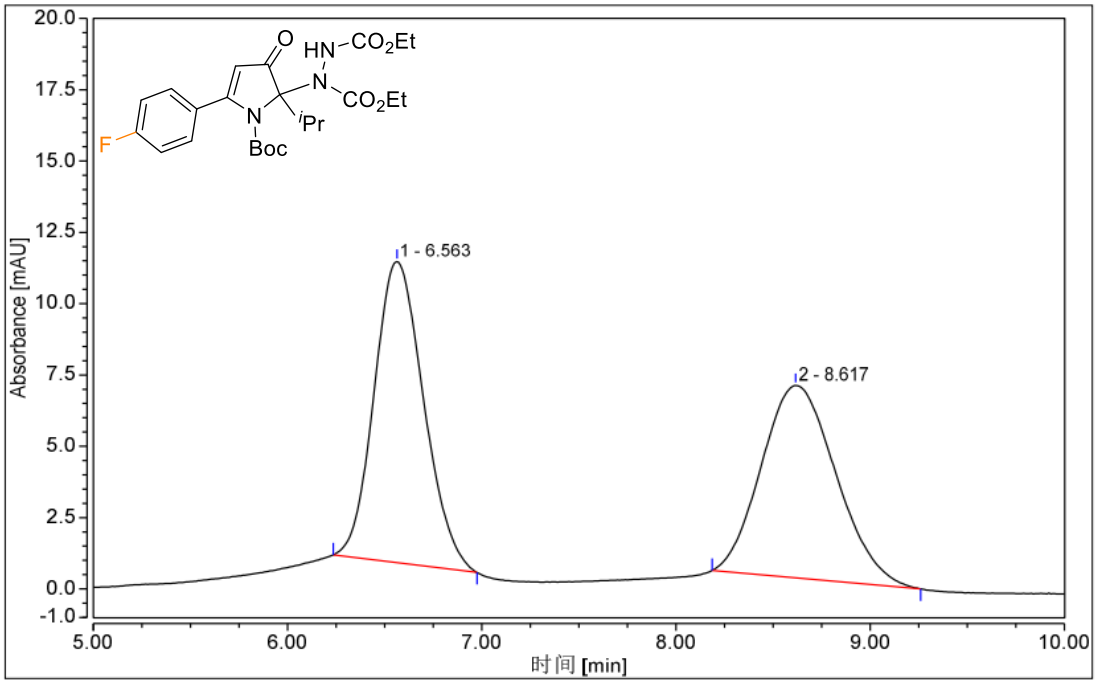


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.138	3.395	14.950	50.35	62.87
2	6.530	3.348	8.830	49.65	37.13

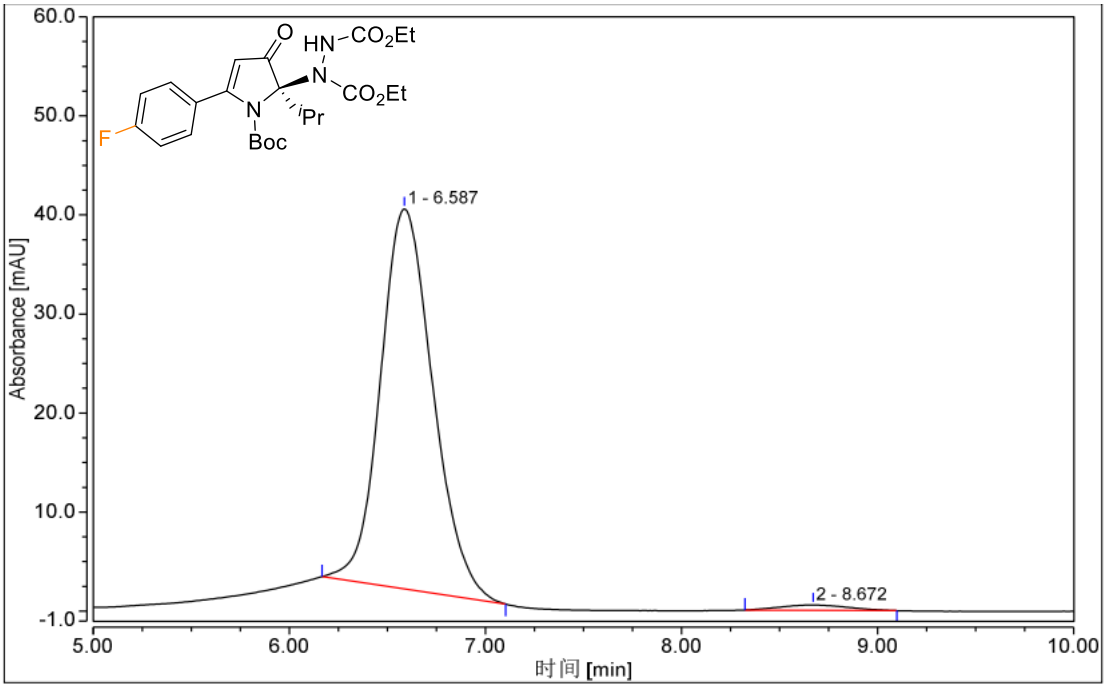


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.142	8.194	32.752	98.06	98.52
2	6.545	0.162	0.492	1.94	1.48

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3f)

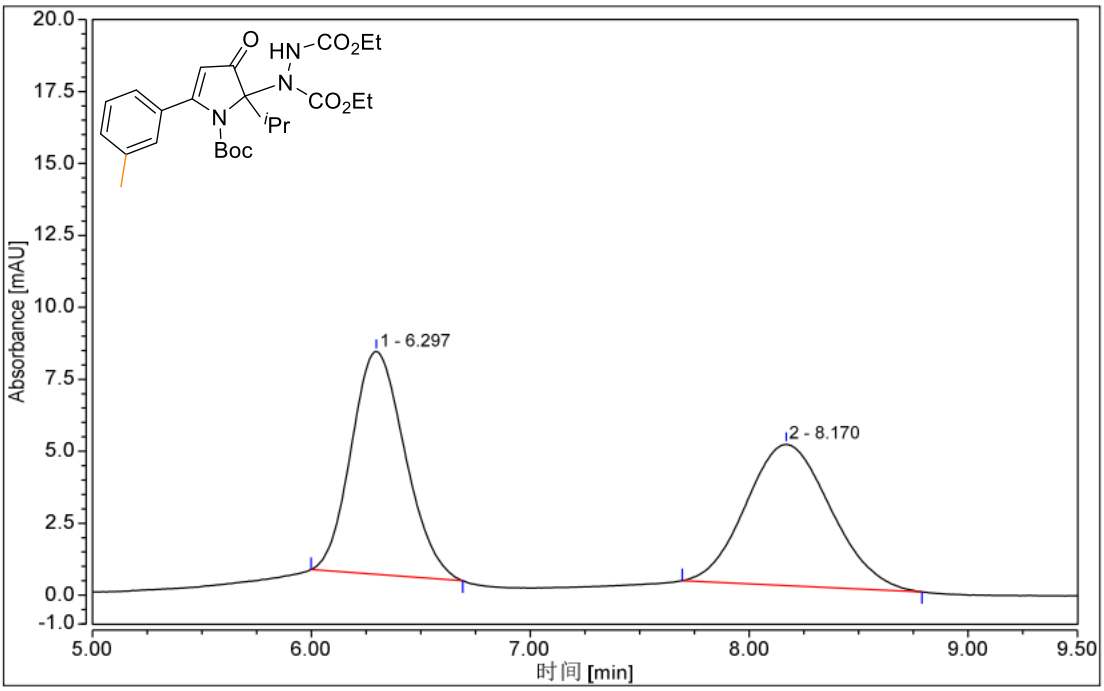


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.563	3.114	10.558	50.90	61.02
2	8.617	3.004	6.745	49.10	38.98

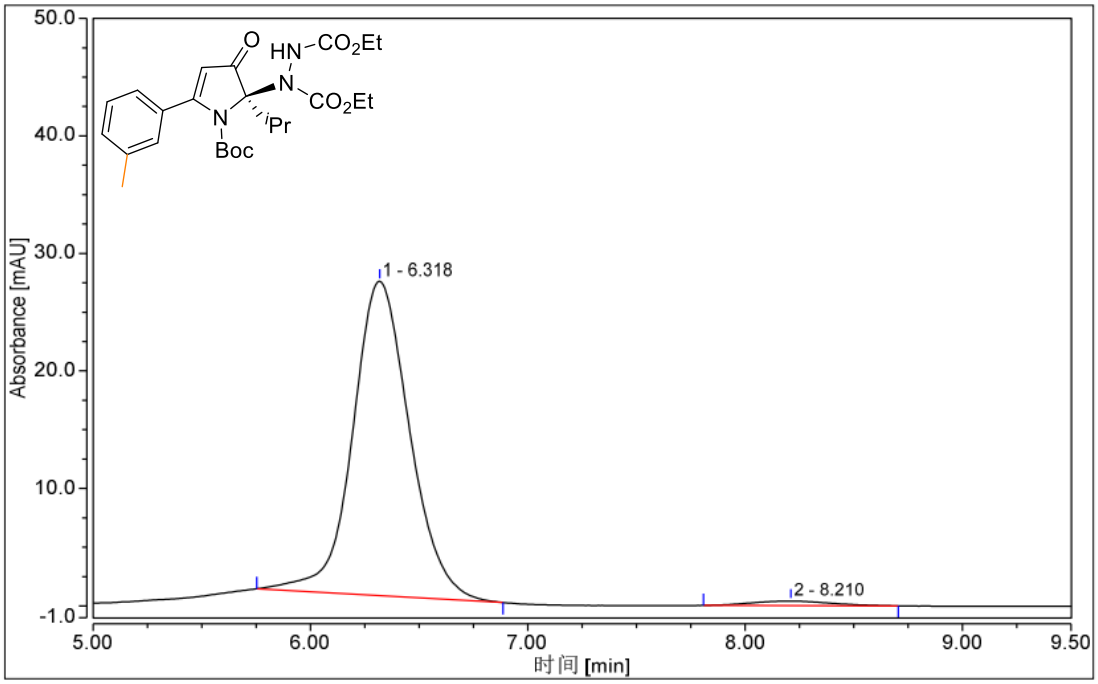


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.587	11.907	38.374	98.26	98.64
2	8.672	0.211	0.531	1.74	1.36

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(m-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3g)

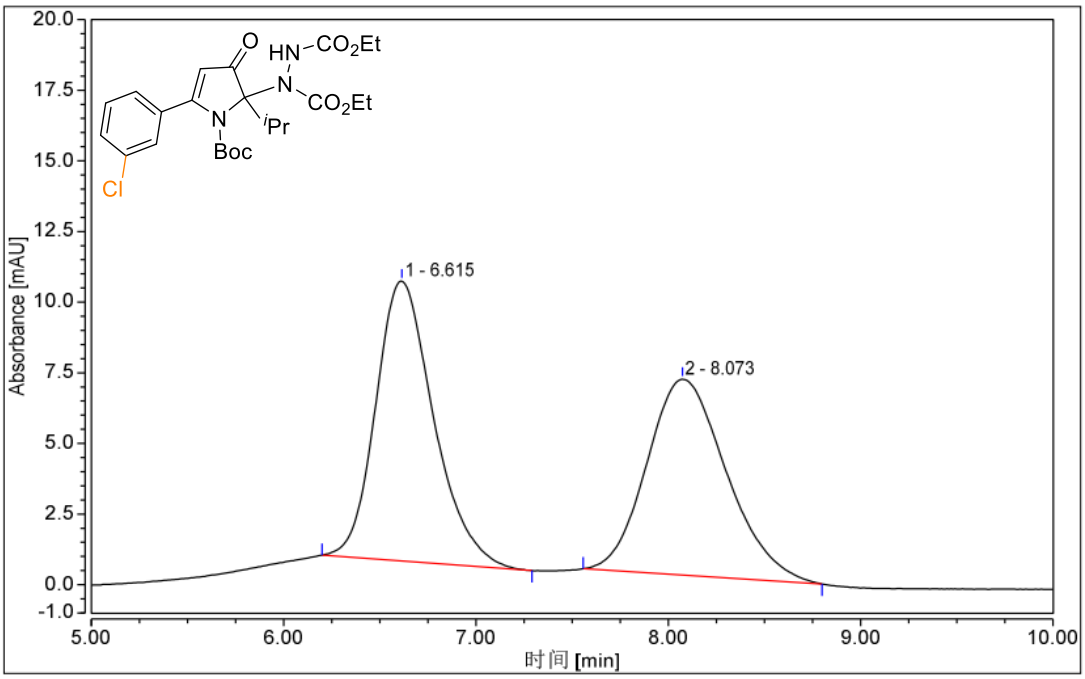


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.297	2.204	7.745	50.04	61.23
2	8.170	2.201	4.904	49.96	38.77

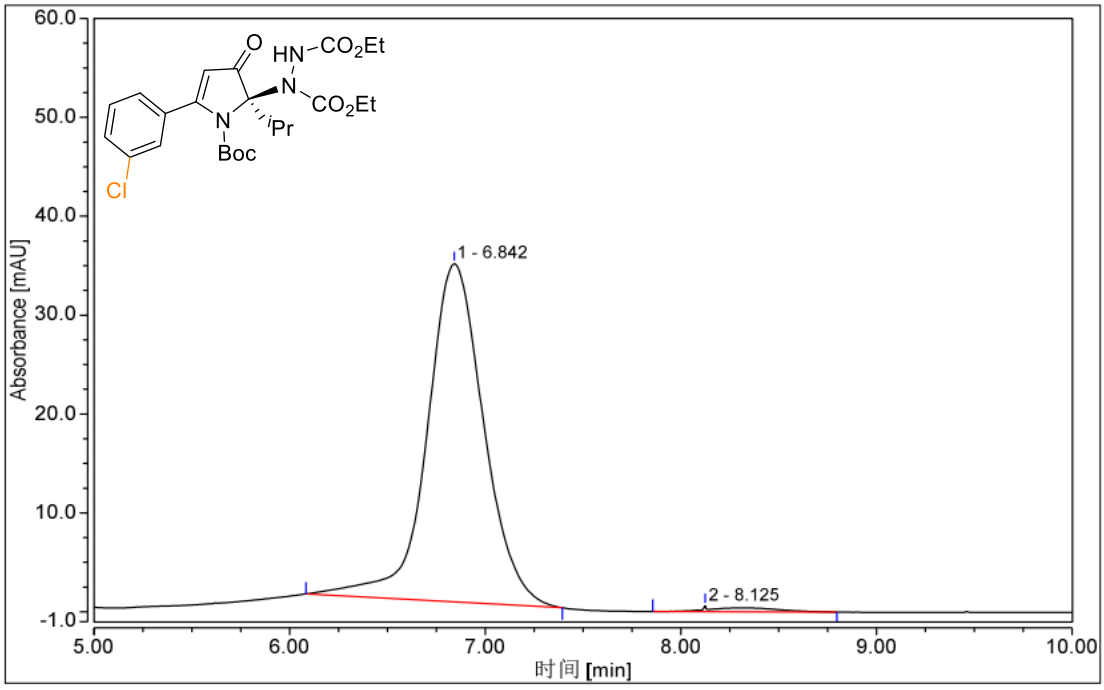


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.318	8.145	26.761	98.05	98.55
2	8.210	0.162	0.392	1.95	1.45

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(3-chlorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3h)

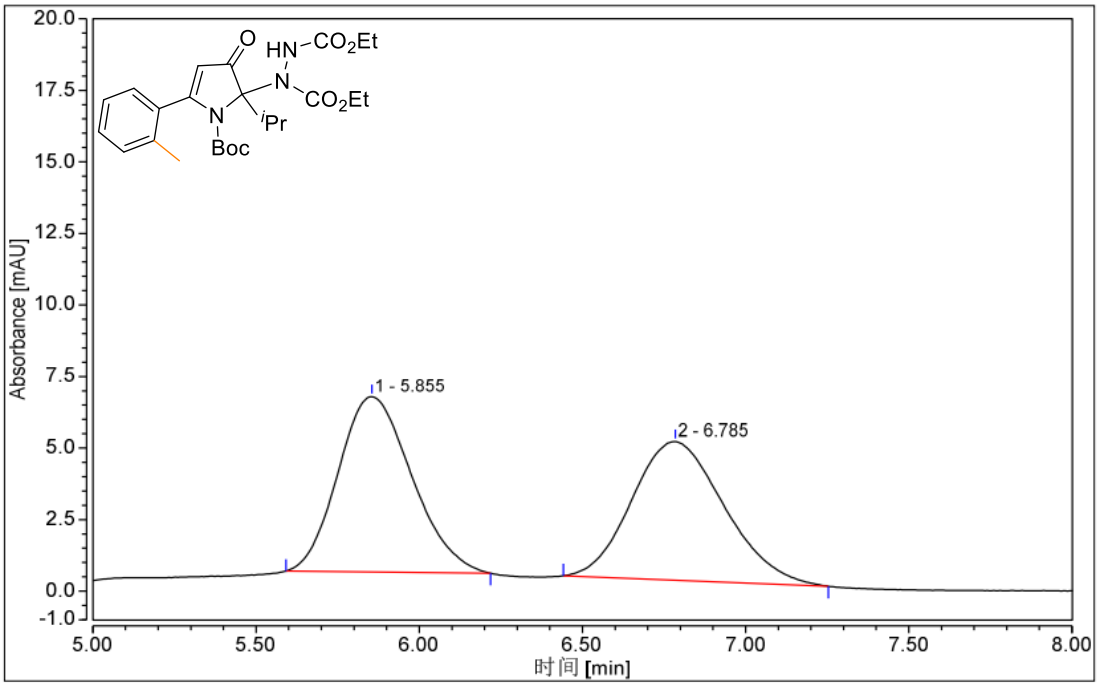


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.615	3.457	9.912	50.99	58.83
2	8.073	3.323	6.937	49.01	41.17

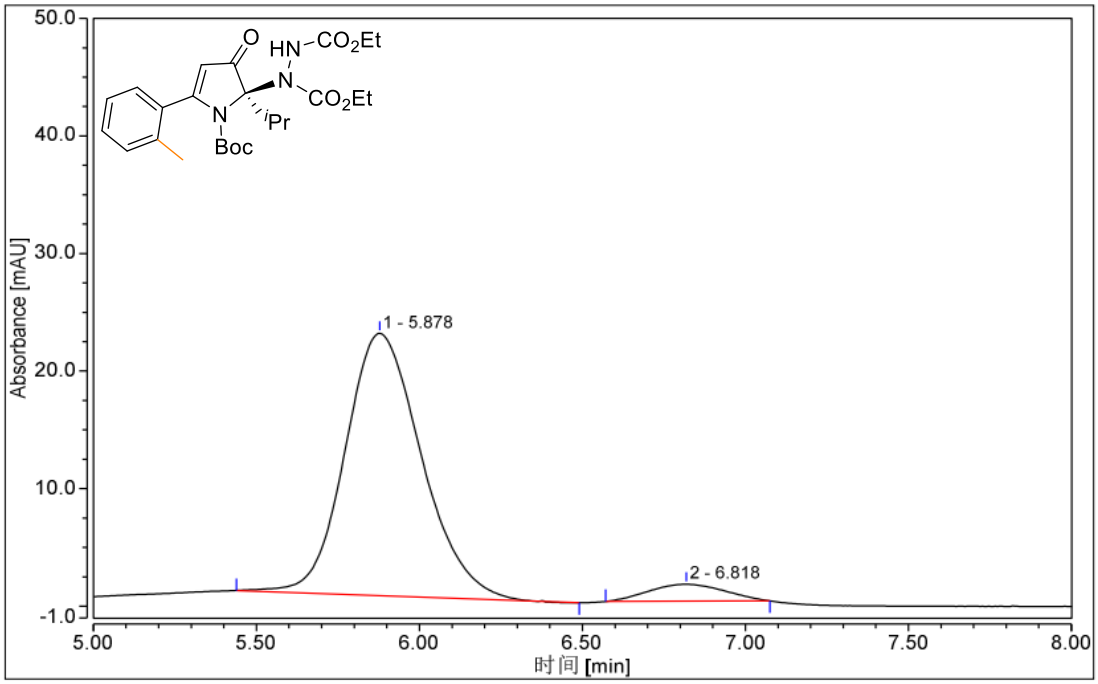


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.842	11.553	34.202	98.60	98.29
2	8.125	0.164	0.593	1.40	1.71

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(o-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3i)

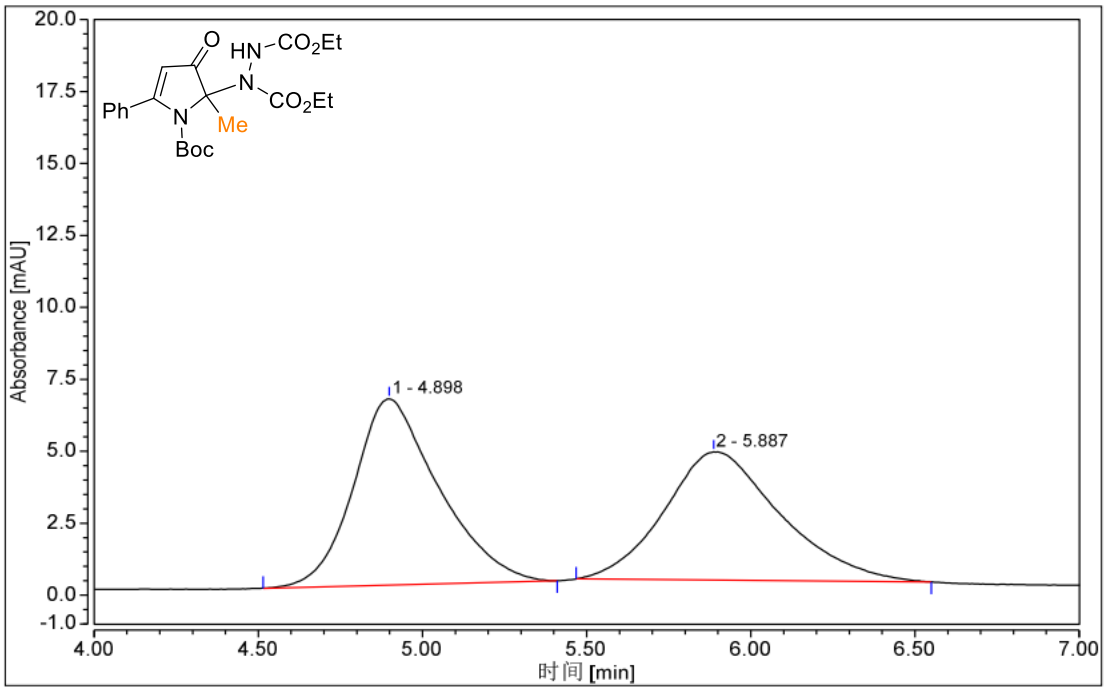


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.855	1.602	6.130	50.25	55.86
2	6.785	1.587	4.844	49.75	44.14

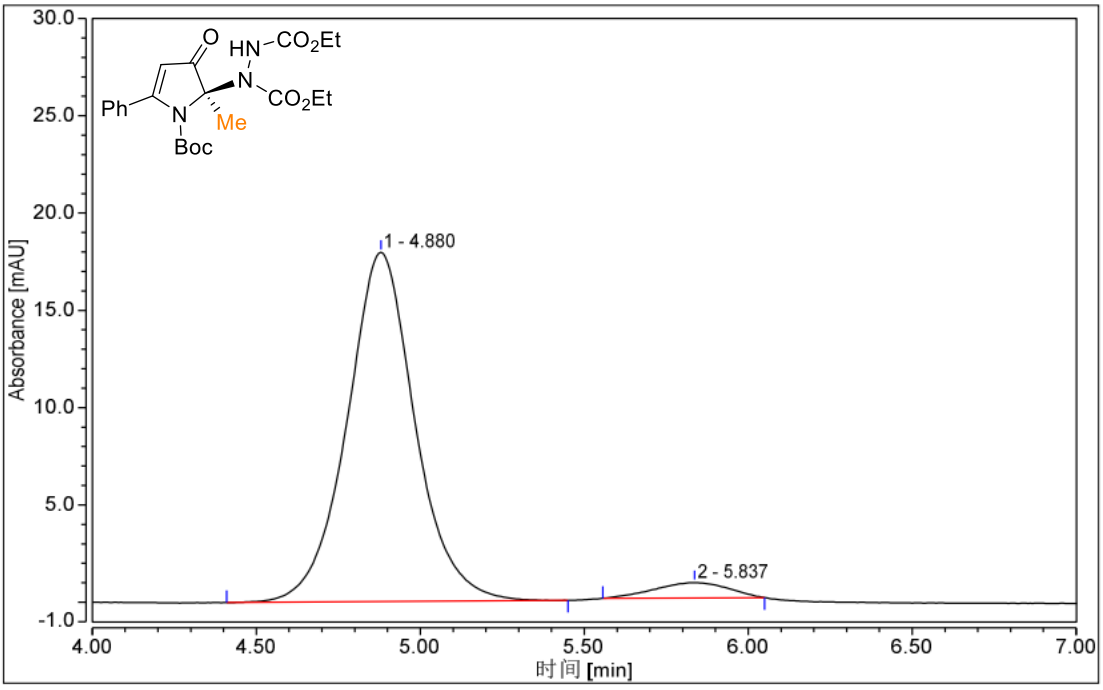


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.878	6.069	22.307	94.00	93.94
2	6.818	0.387	1.440	6.00	6.06

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3j)

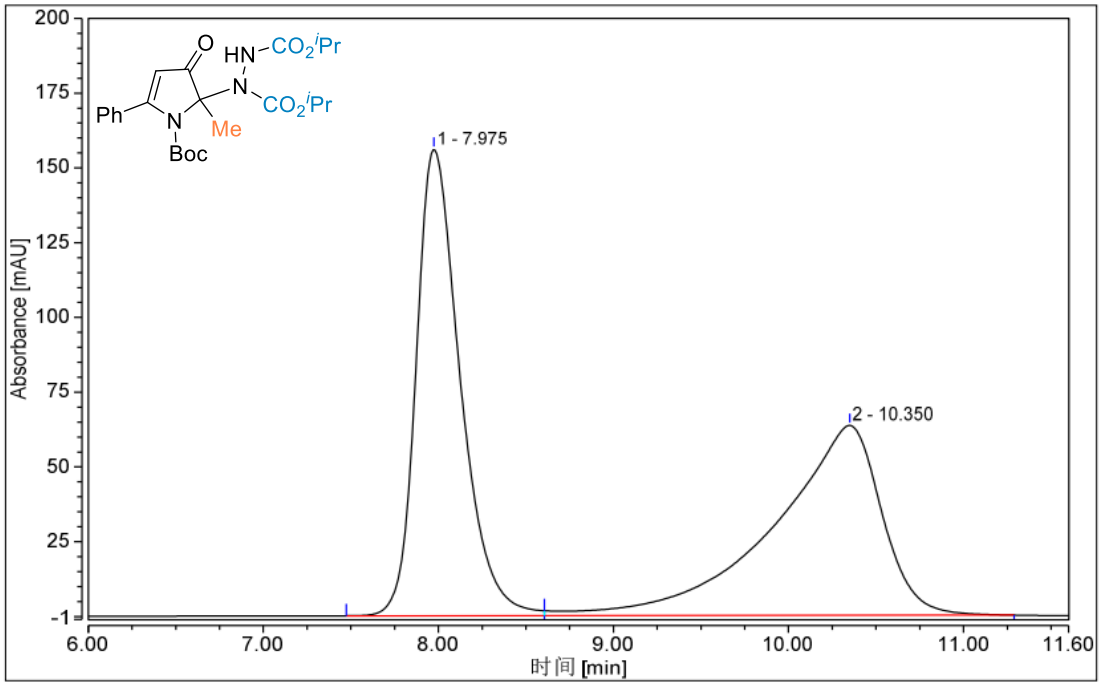


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.898	1.948	6.470	51.61	59.24
2	5.887	1.826	4.451	48.39	40.76

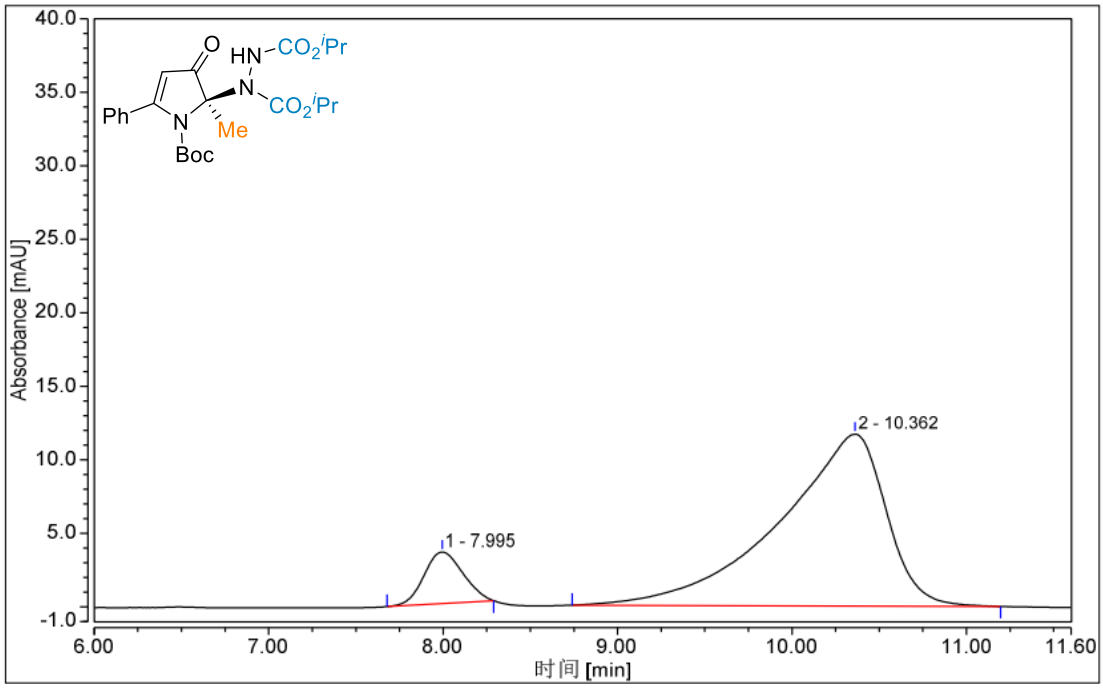


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.880	4.308	17.946	95.48	95.78
2	5.837	0.204	0.791	4.52	4.22

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3k)

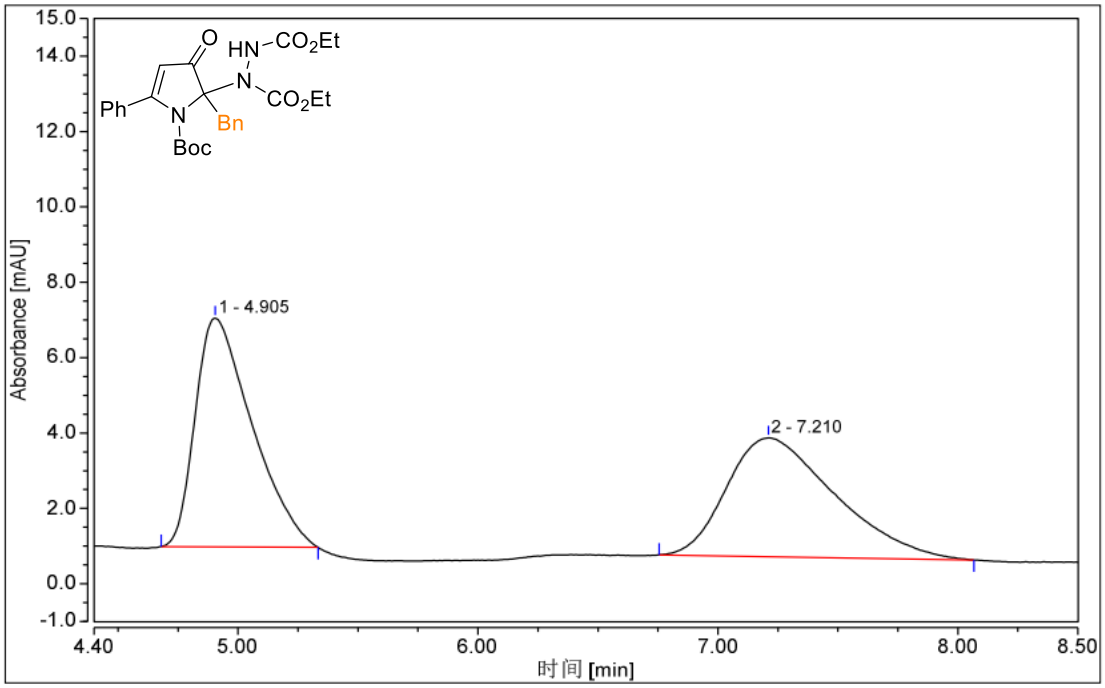


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.975	45.426	155.950	50.07	71.06
2	10.350	45.304	63.498	49.93	28.94

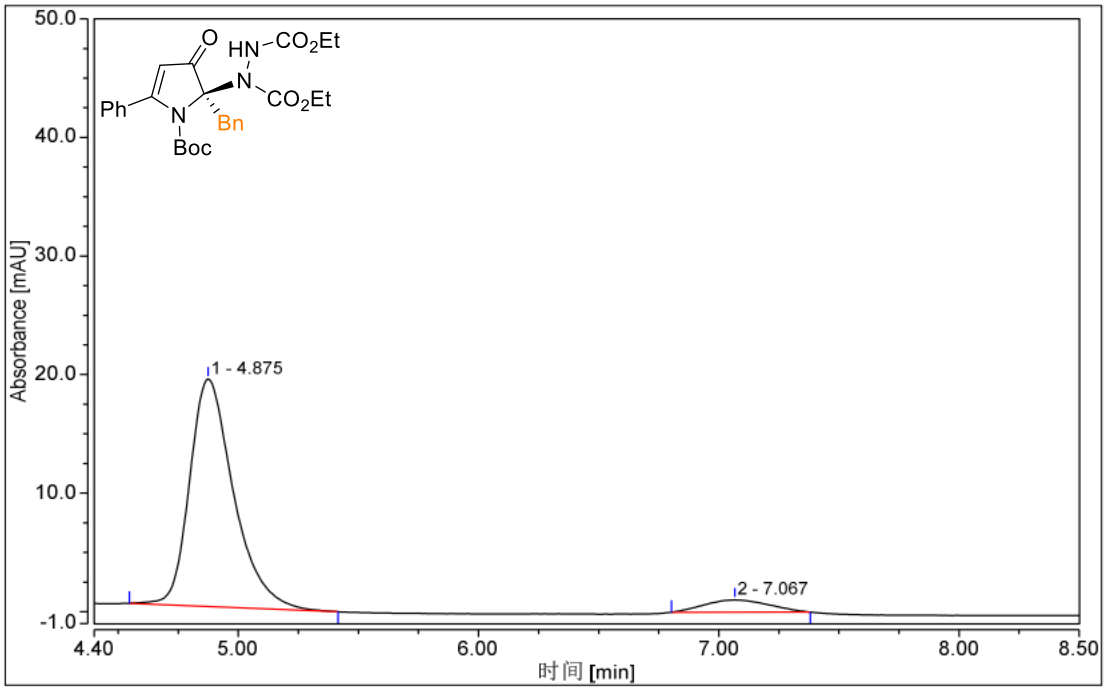


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.995	0.906	3.508	9.87	23.08
2	10.362	8.268	11.688	90.13	76.92

diethyl (*R*)-1-(2-benzyl-1-(tert-butoxycarbonyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3l)

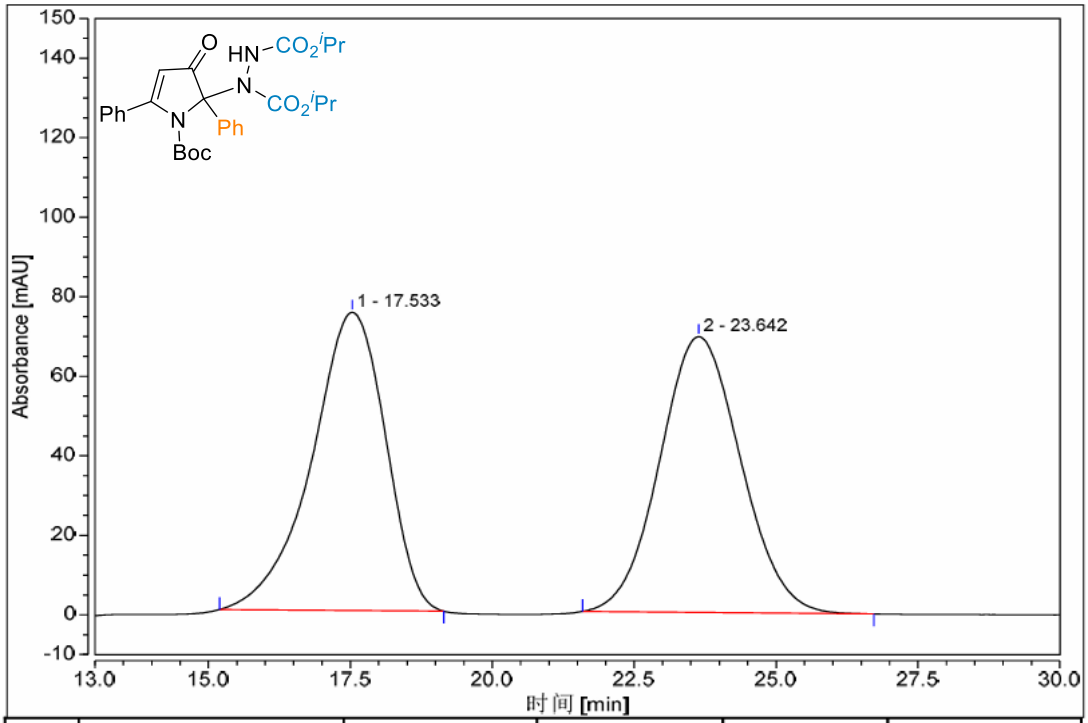


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.905	1.666	6.073	50.25	65.81
2	7.210	1.650	3.155	49.75	34.19

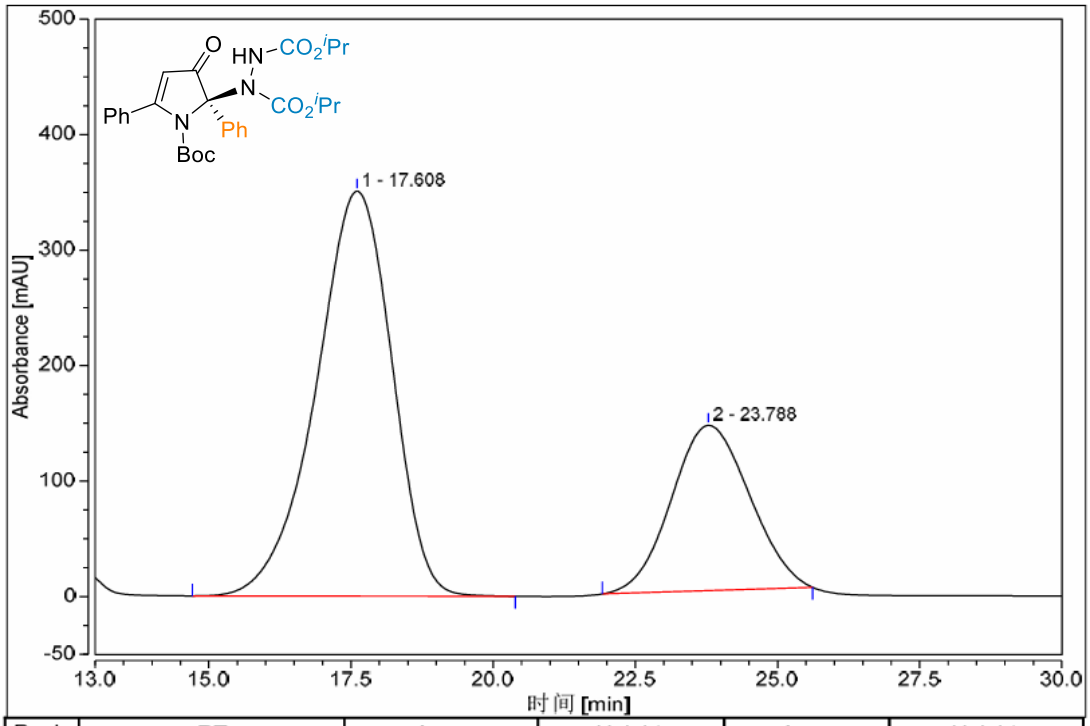


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.875	4.077	19.186	92.73	94.92
2	7.067	0.319	1.027	7.27	5.08

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-2,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (3m)

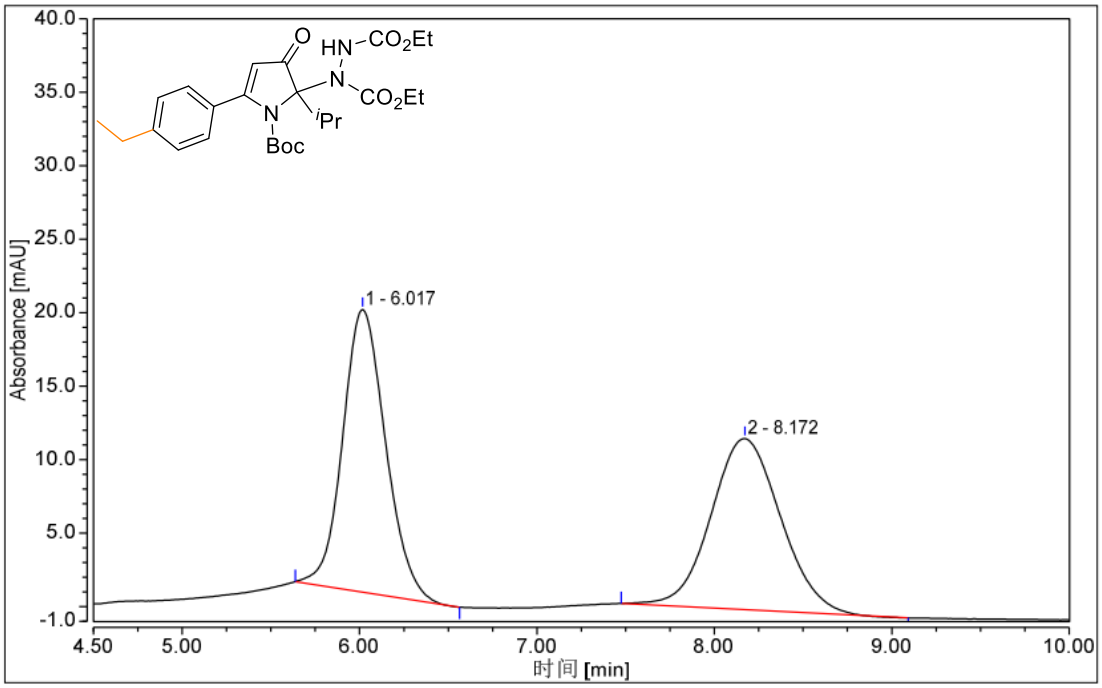


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	17.533	112.815	74.985	49.57	51.94
2	23.642	114.766	69.373	50.43	48.06

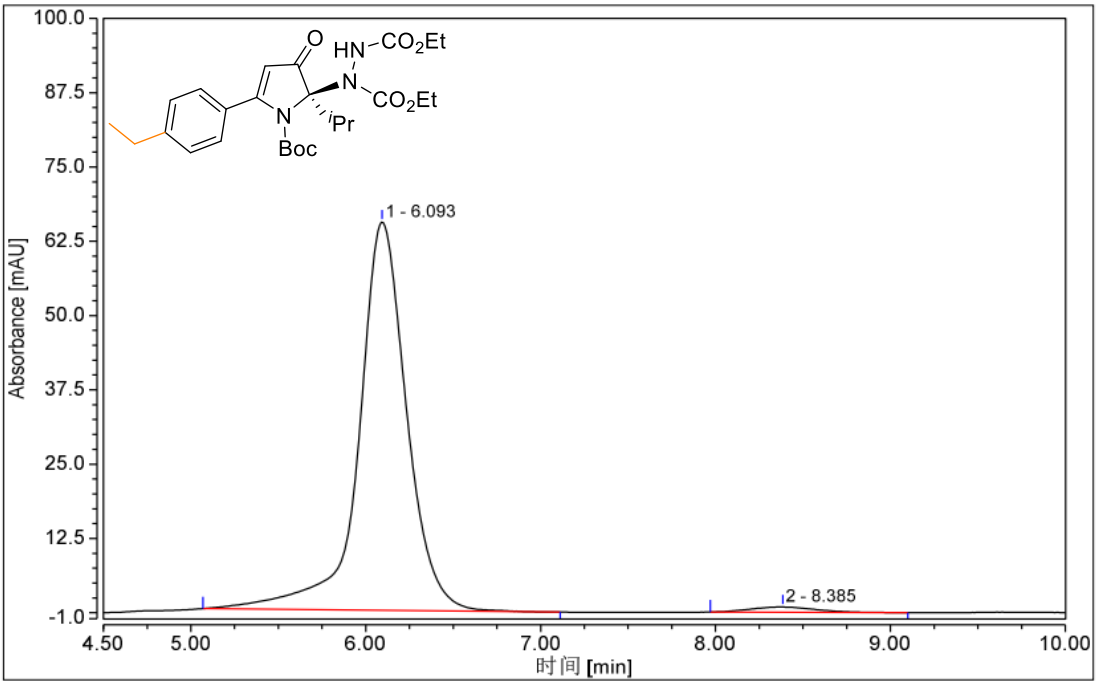


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	17.608	541.174	350.431	70.36	71.02
2	23.788	228.001	142.990	29.64	28.98

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3o)

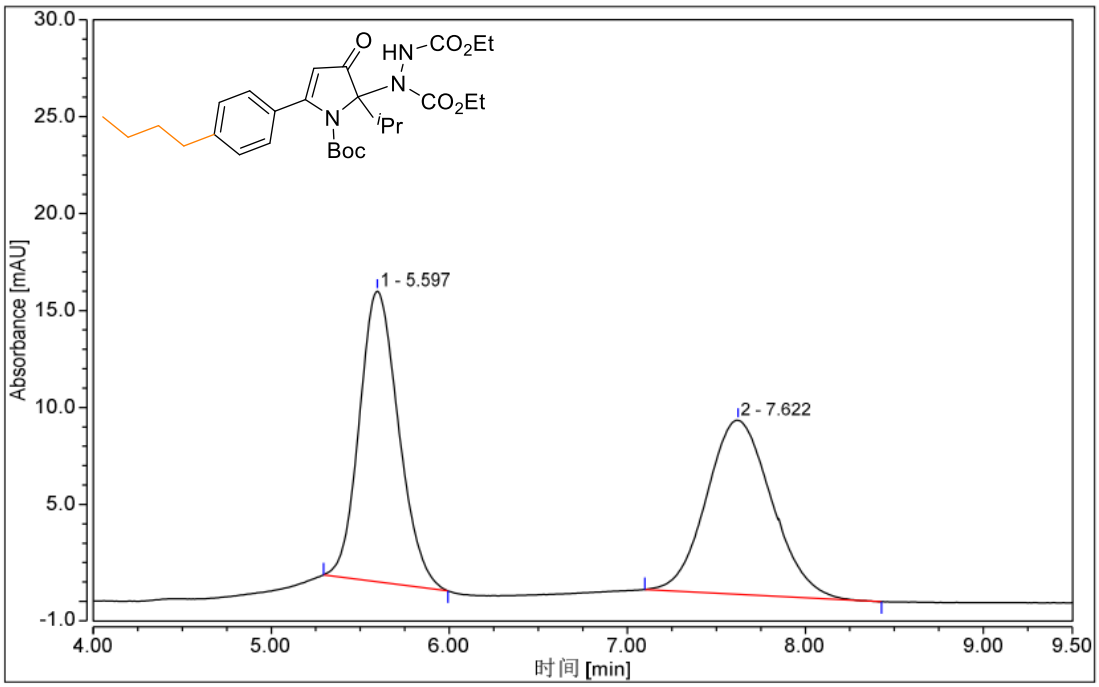


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.017	5.392	19.227	50.38	62.27
2	8.172	5.311	11.652	49.62	37.73

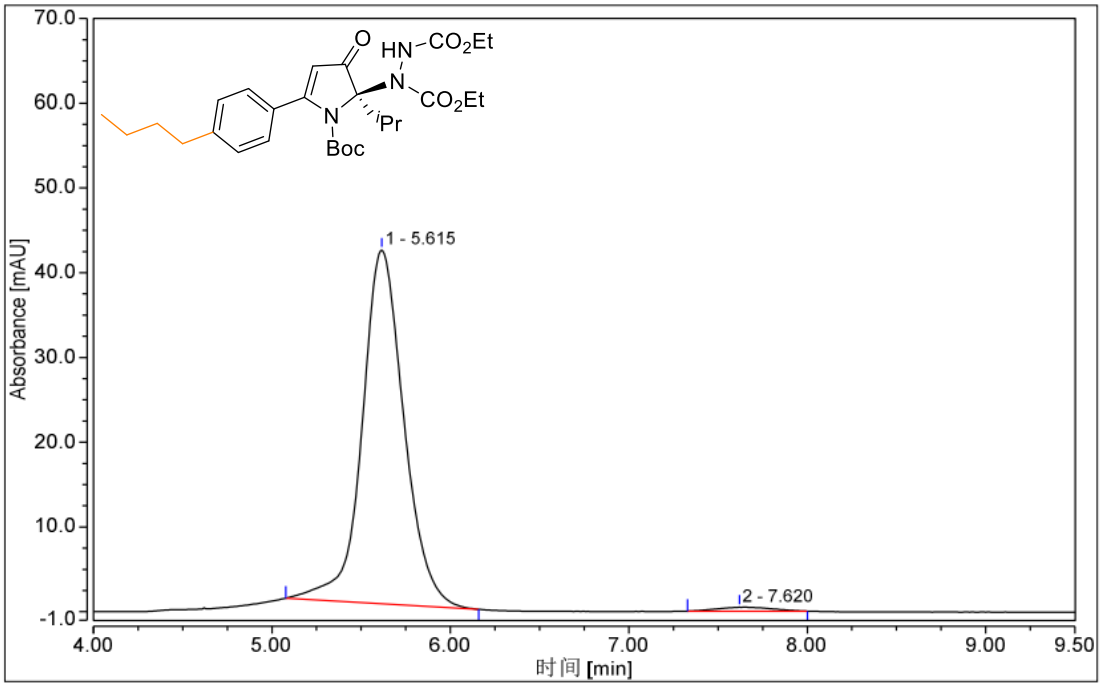


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.093	20.871	65.336	98.24	98.66
2	8.385	0.375	0.887	1.76	1.34

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-butylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3p)

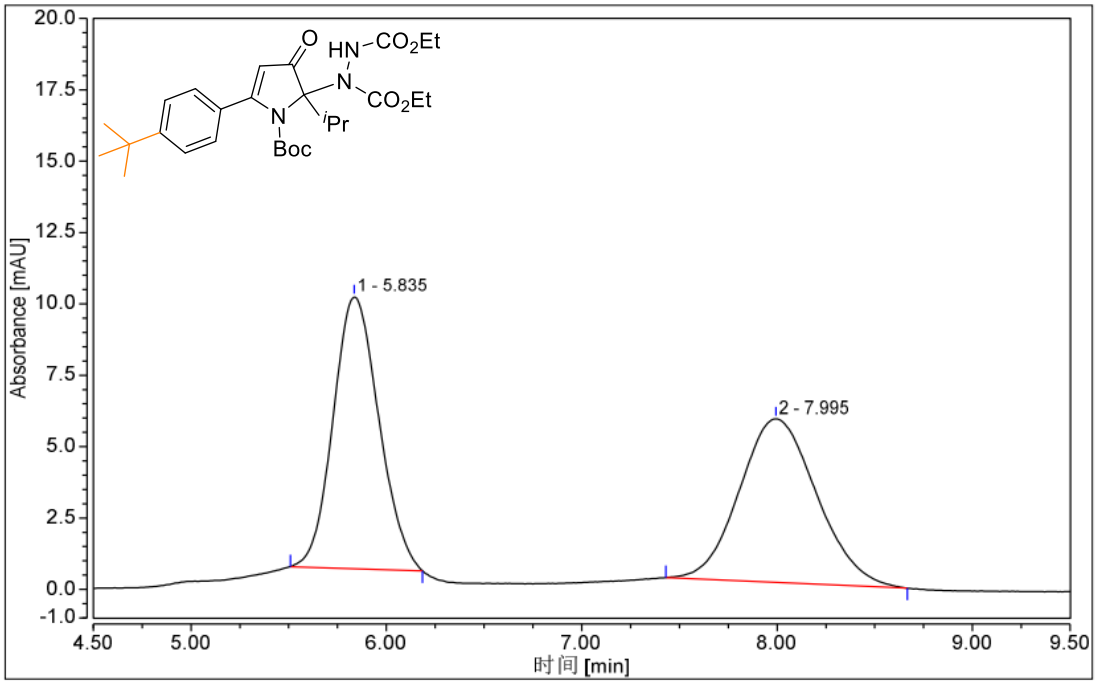


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.597	3.837	14.999	50.19	62.57
2	7.622	3.809	8.975	49.81	37.43

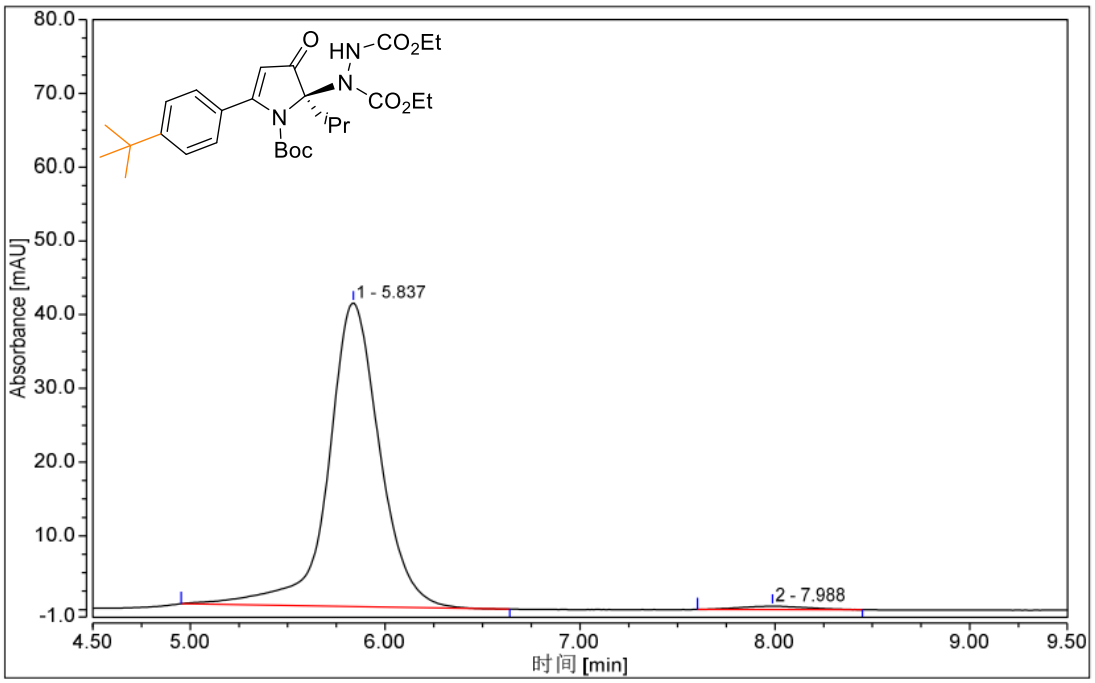


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.615	11.352	41.726	98.58	98.88
2	7.620	0.163	0.471	1.42	1.12

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-(tert-butyl)phenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3q)

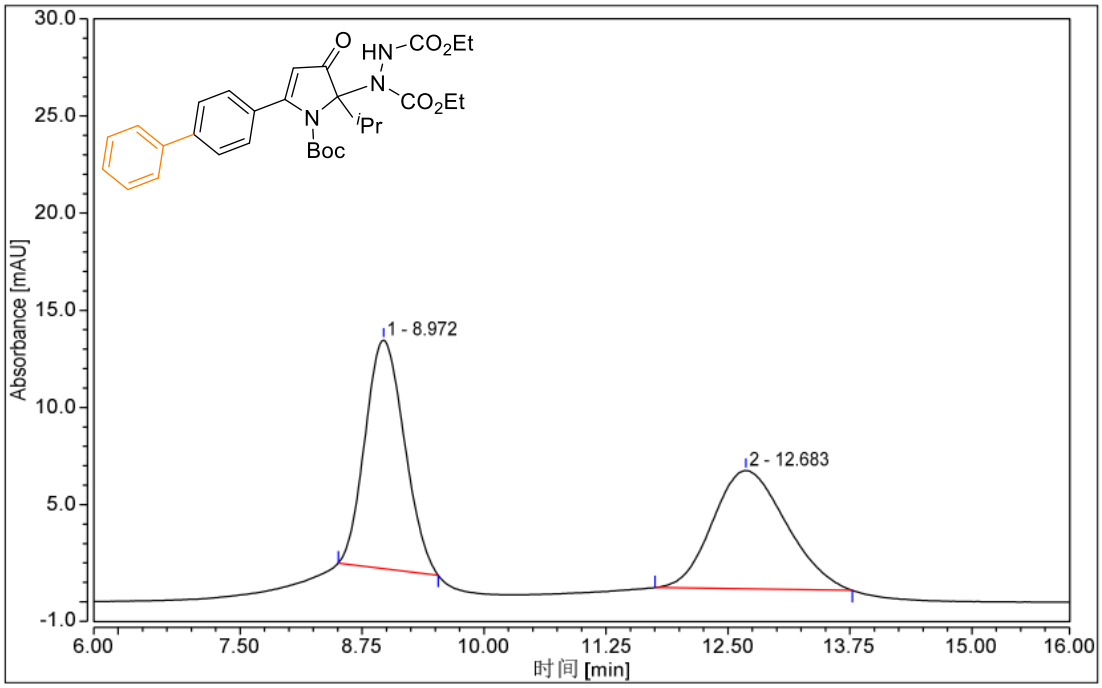


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.835	2.585	9.523	49.61	62.42
2	7.995	2.626	5.734	50.39	37.58

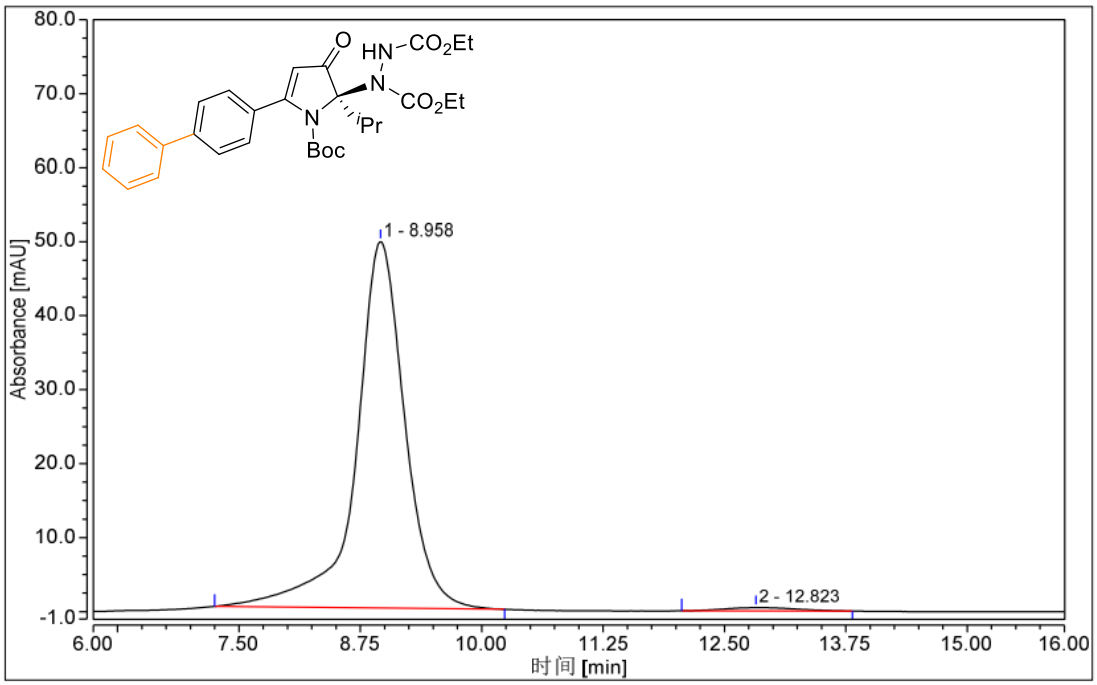


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.837	12.608	41.175	98.55	98.91
2	7.988	0.186	0.455	1.45	1.09

diethyl (*R*)-1-(5-([1,1'-biphenyl]-4-yl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3r)

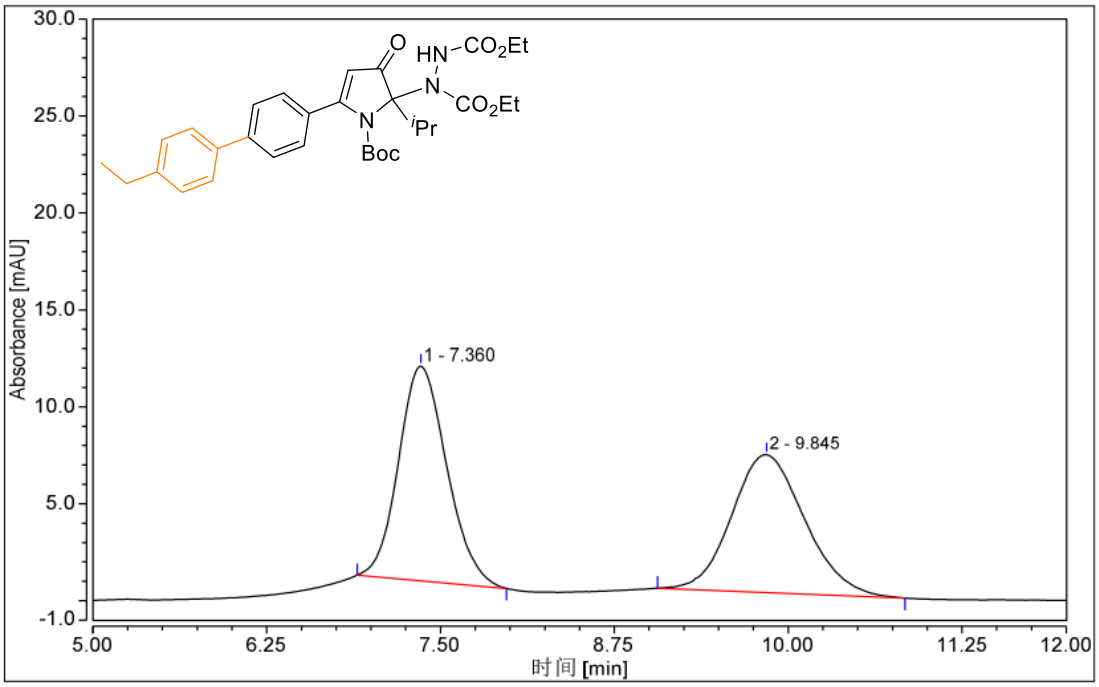


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.972	5.488	11.756	50.81	65.88
2	12.683	5.314	6.088	49.19	34.12

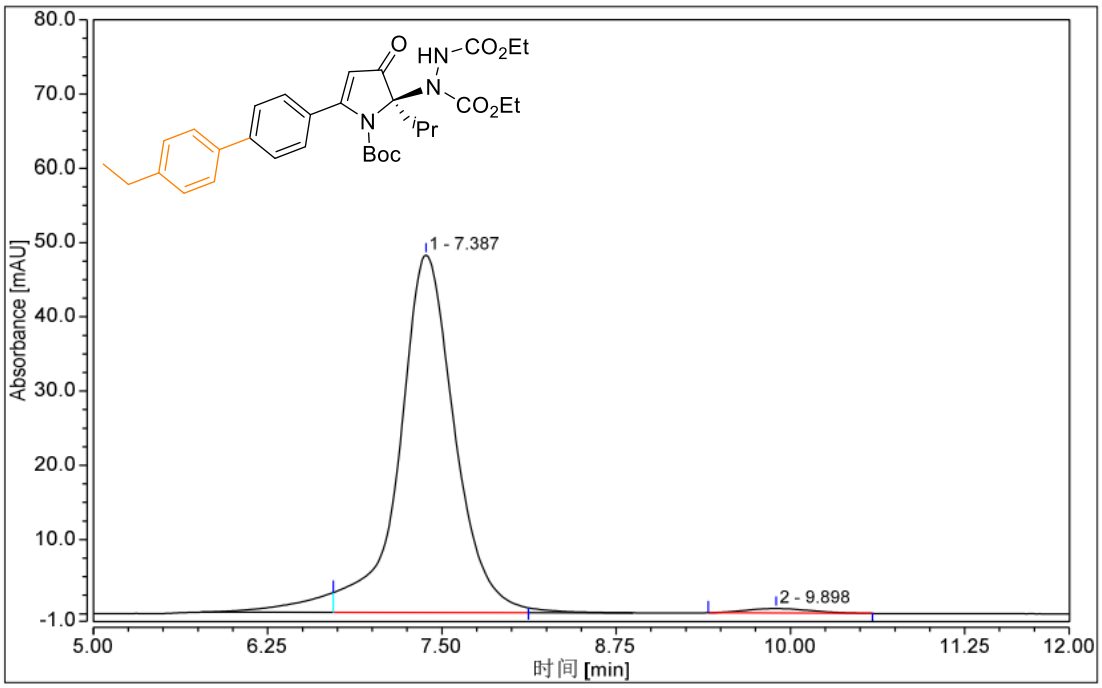


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.958	28.908	49.543	98.68	99.07
2	12.823	0.388	0.463	1.32	0.93

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4'-ethyl-[1,1'-biphenyl]-4-yl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3s)

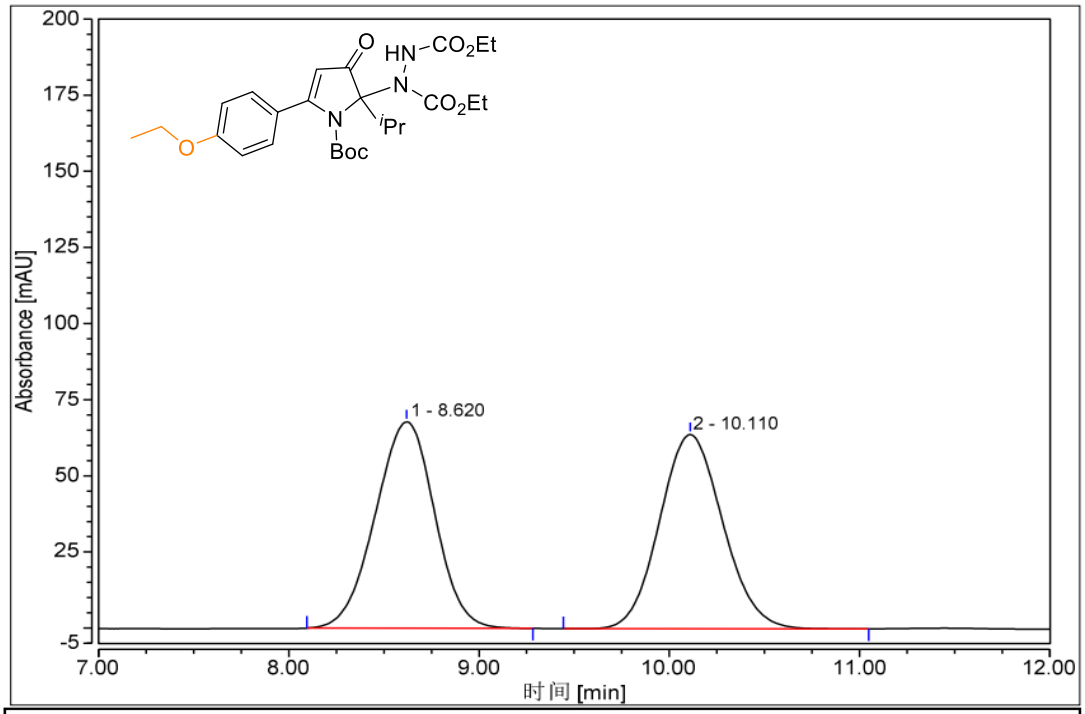


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.360	4.458	11.083	50.74	60.92
2	9.845	4.328	7.110	49.26	39.08

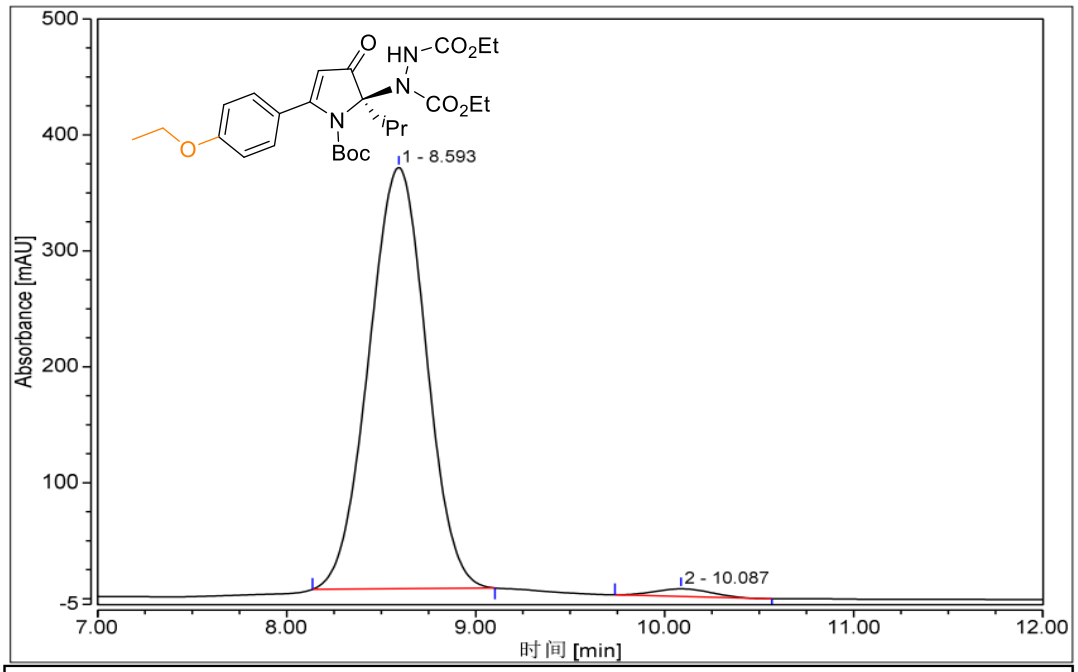


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.387	21.991	48.124	98.54	98.76
2	9.898	0.327	0.604	1.46	1.24

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethoxyphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3t)

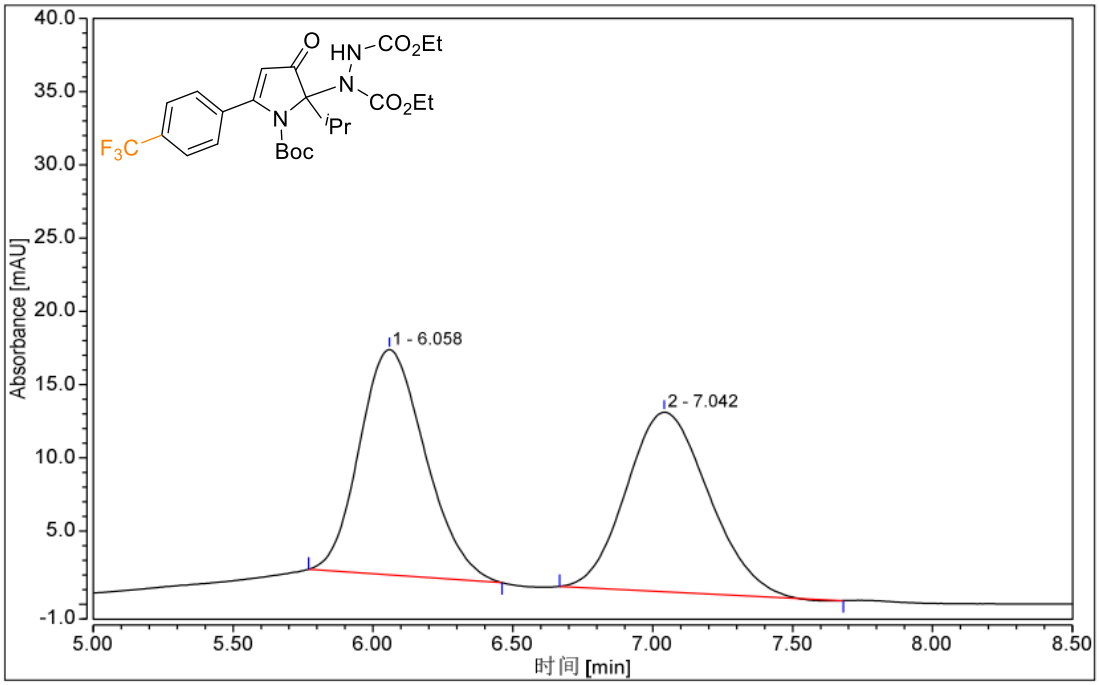


Peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.620	24.519	67.788	50.02	51.53
2	10.110	24.499	63.771	49.98	48.47

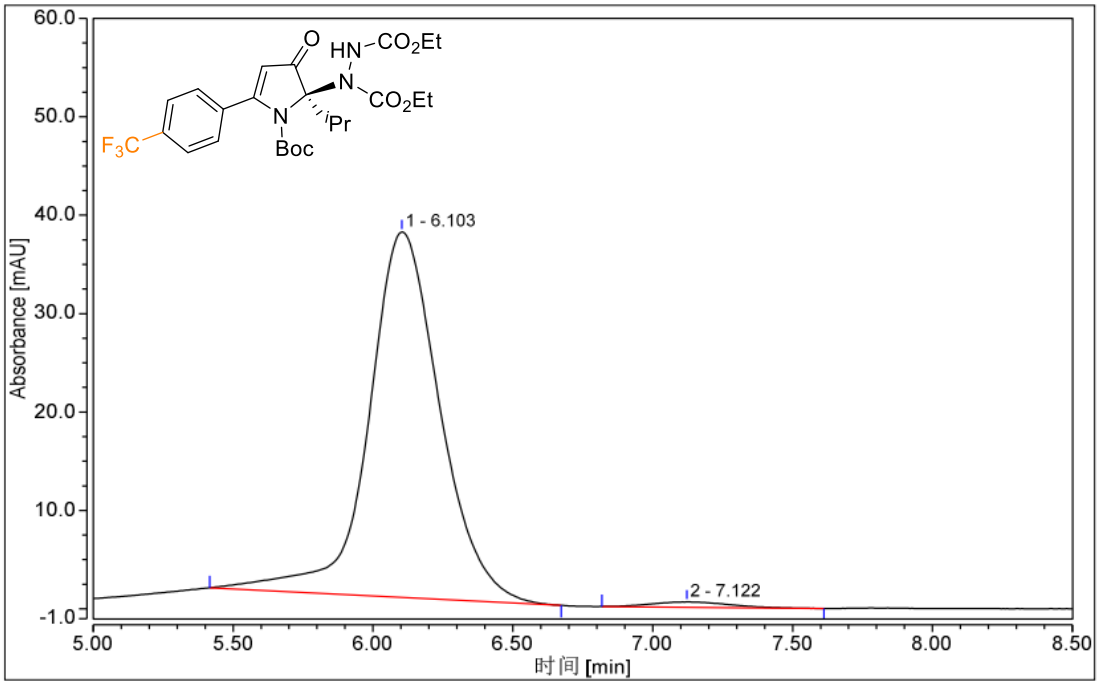


Peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.593	127.856	363.457	98.25	98.22
2	10.087	2.275	6.572	1.75	1.78

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3u)

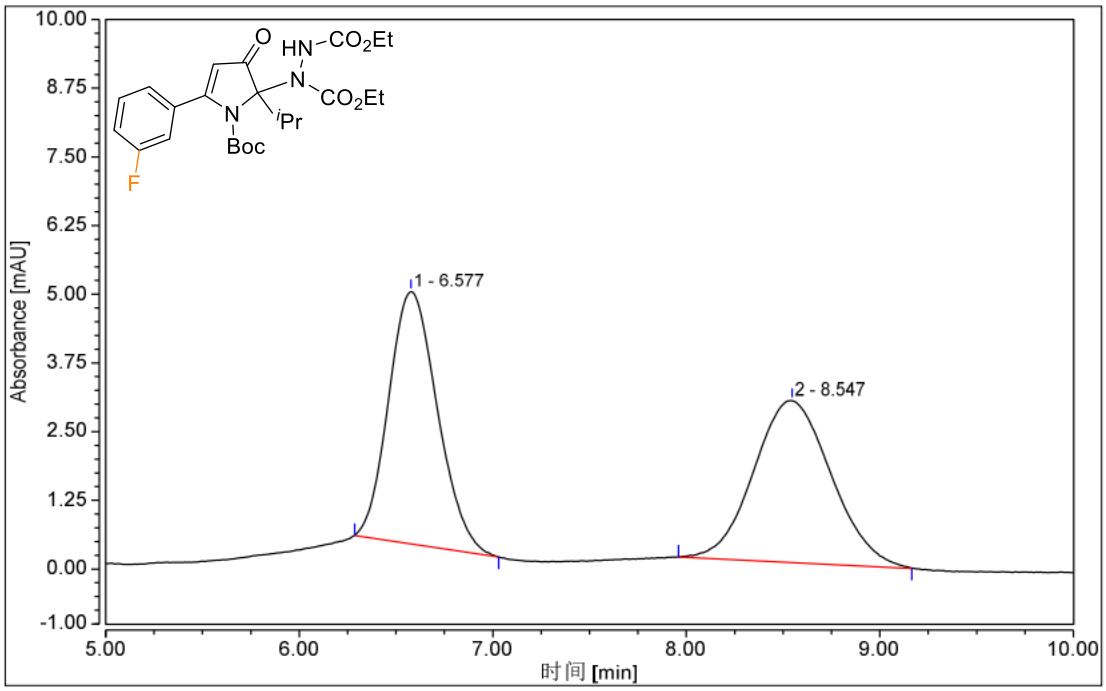


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.058	4.205	15.379	50.12	55.66
2	7.042	4.185	12.249	49.88	44.34

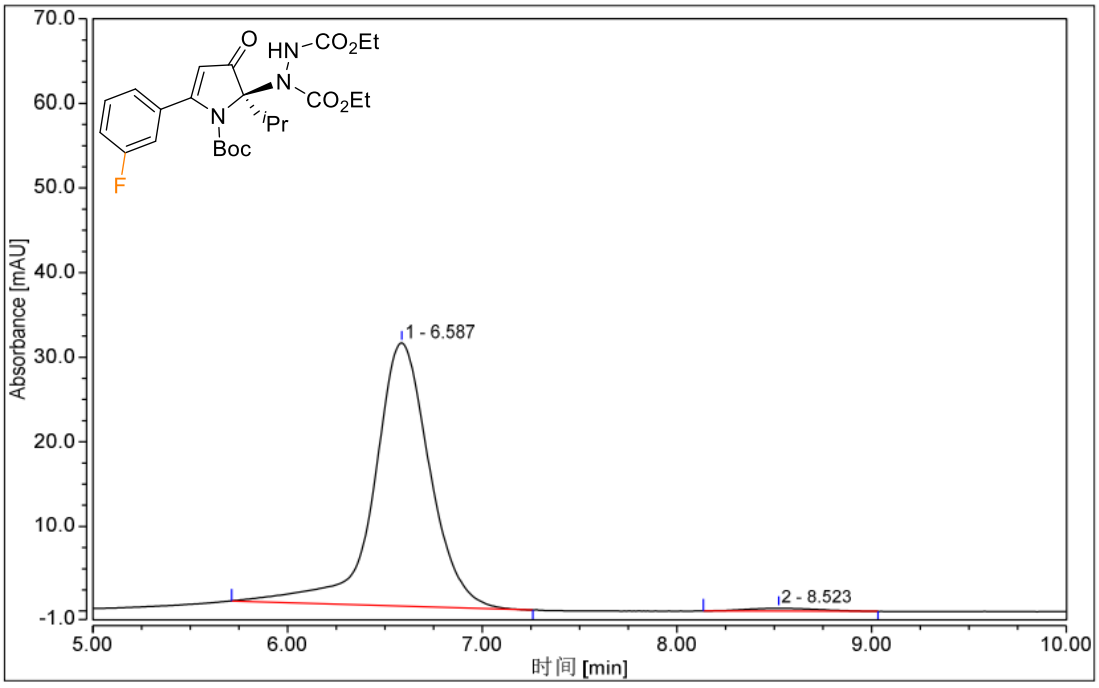


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.103	11.036	37.135	98.45	98.55
2	7.122	0.174	0.544	1.55	1.45

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-5-(3-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3v)

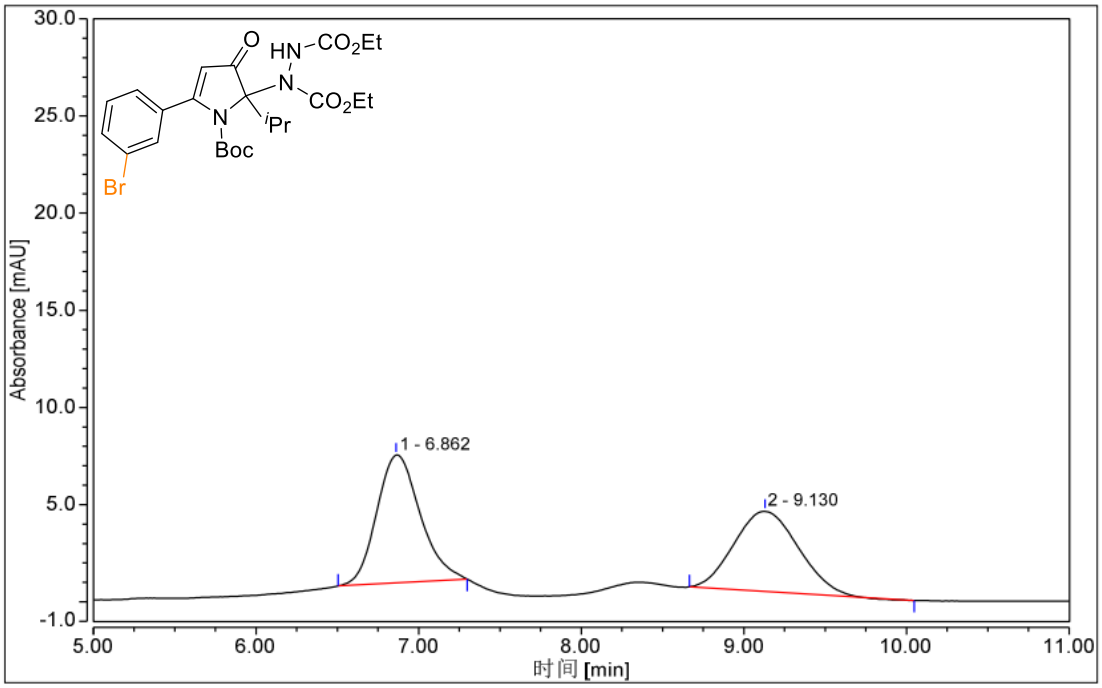


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.577	1.340	4.592	49.51	60.87
2	8.547	1.366	2.952	50.49	39.13

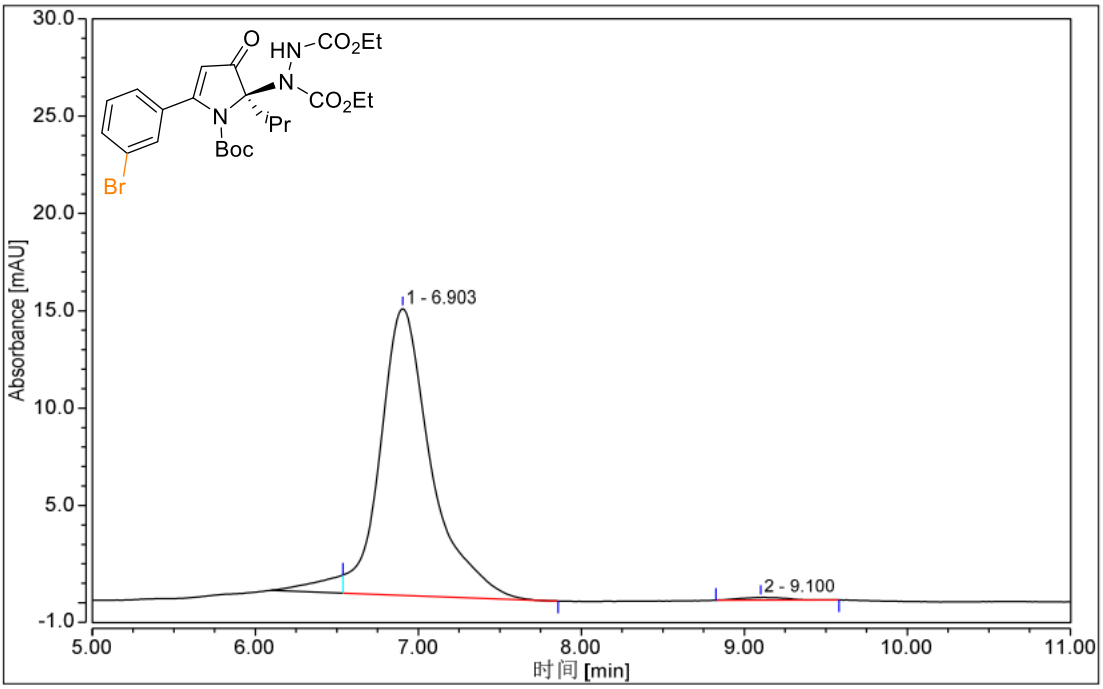


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.587	10.346	31.117	98.60	98.94
2	8.523	0.147	0.334	1.40	1.06

diethyl (*R*)-1-(5-(3-bromophenyl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3w)

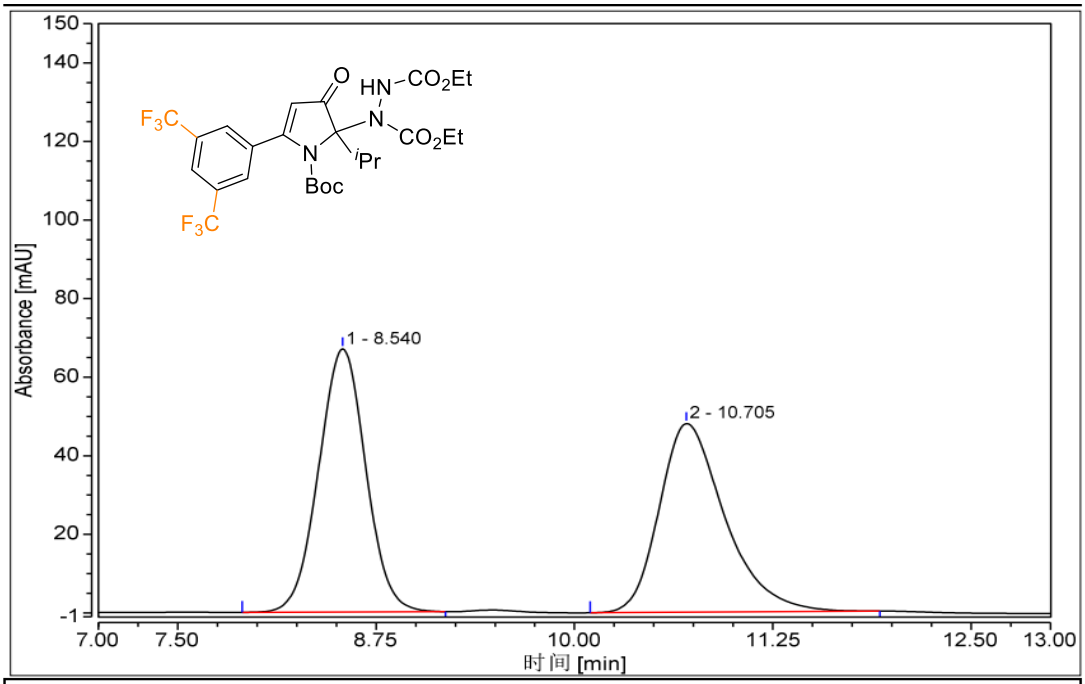


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.862	2.039	6.584	51.89	61.49
2	9.130	1.890	4.123	48.11	38.51

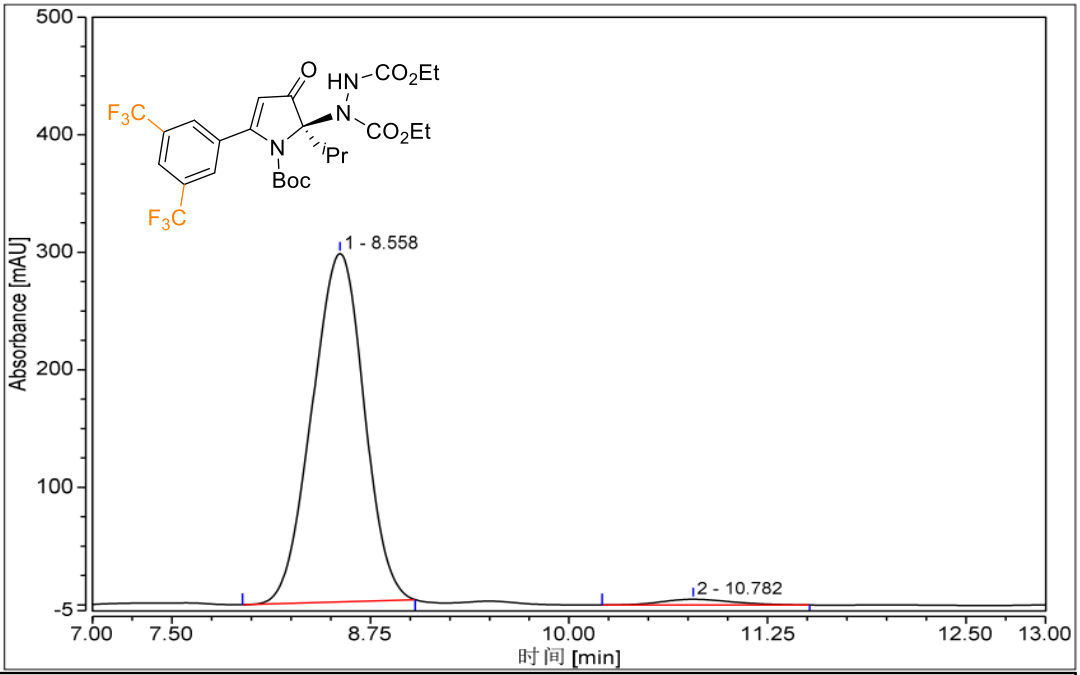


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.903	5.279	14.730	99.19	99.07
2	9.100	0.043	0.138	0.81	0.93

diethyl (*R*)-1-(5-(3,5-bis(trifluoromethyl)phenyl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3x)

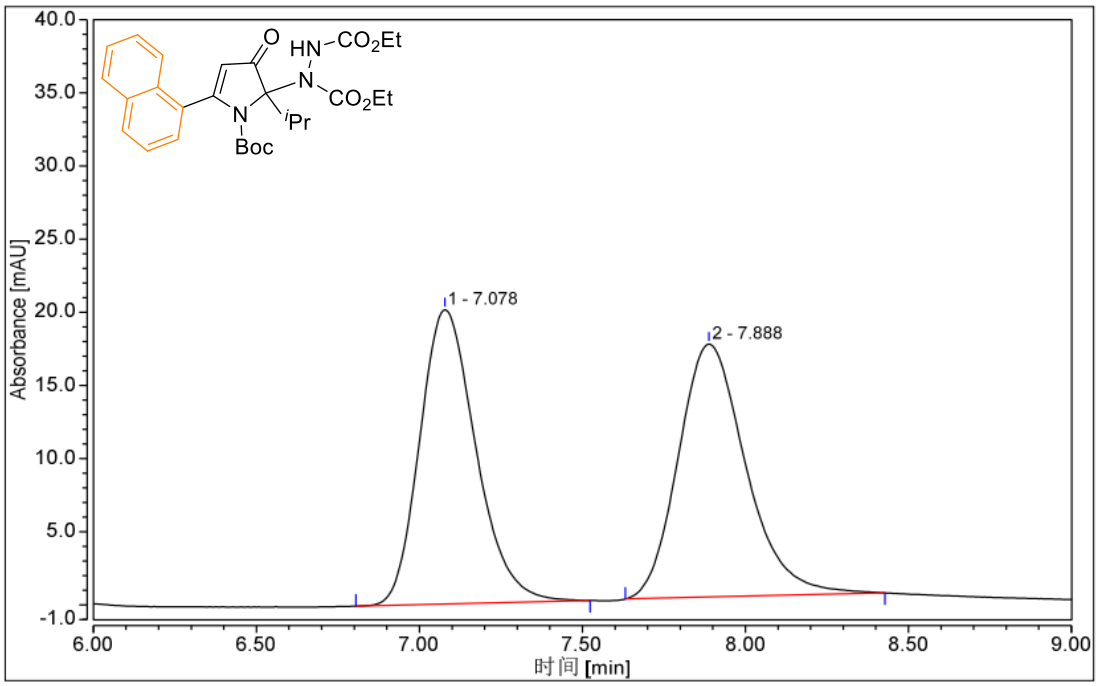


Peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.540	23.063	67.011	50.12	58.27
2	10.705	22.956	47.999	49.88	41.73

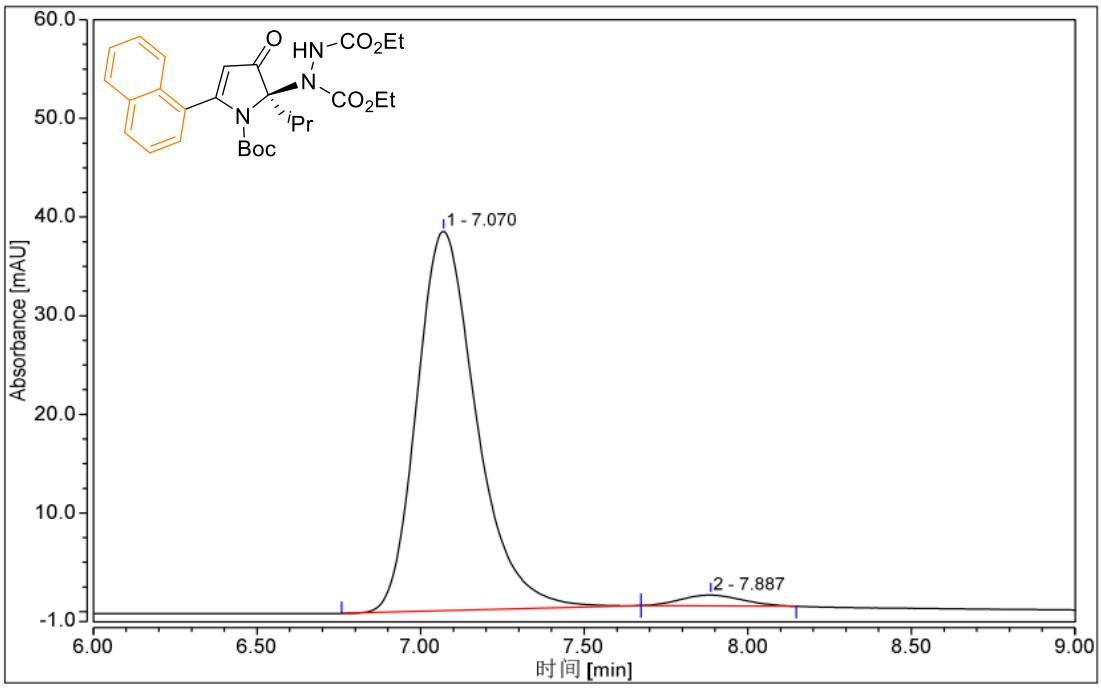


Peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	8.558	112.426	296.360	97.78	98.38
2	10.782	2.556	4.895	2.22	1.62

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-5-(naphthalen-1-yl)-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3y)

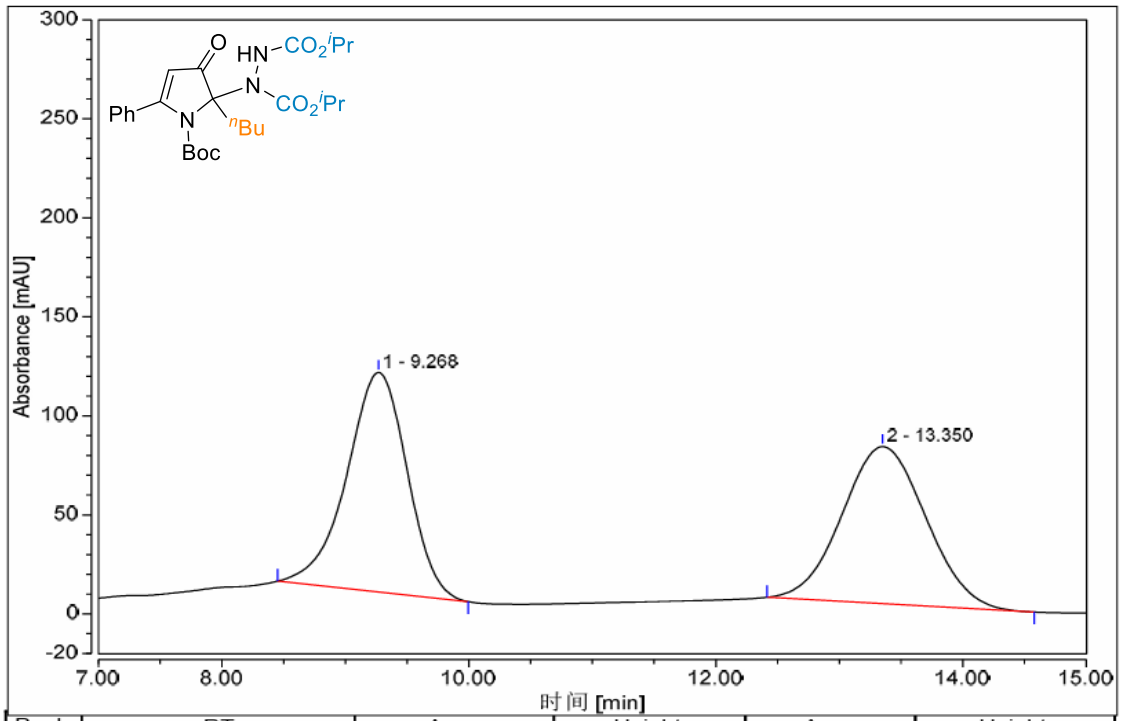


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.078	4.021	20.128	49.22	53.78
2	7.888	4.148	17.299	50.78	46.22

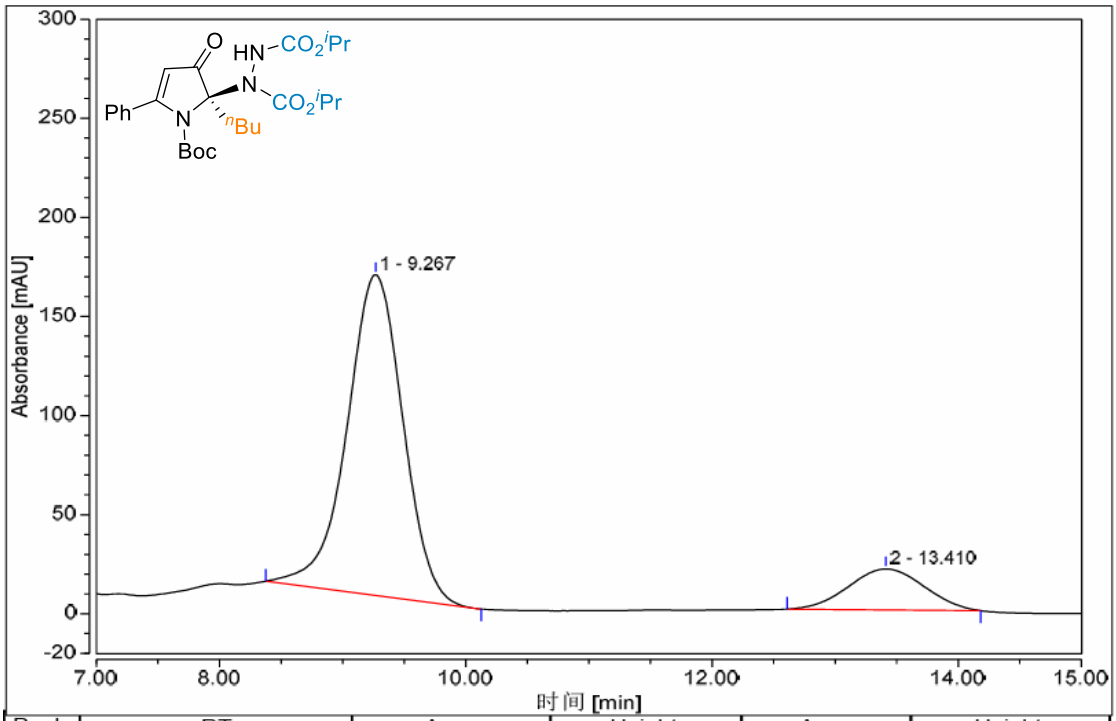


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.070	8.121	38.463	97.11	97.20
2	7.887	0.242	1.110	2.89	2.80

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-butyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3z)

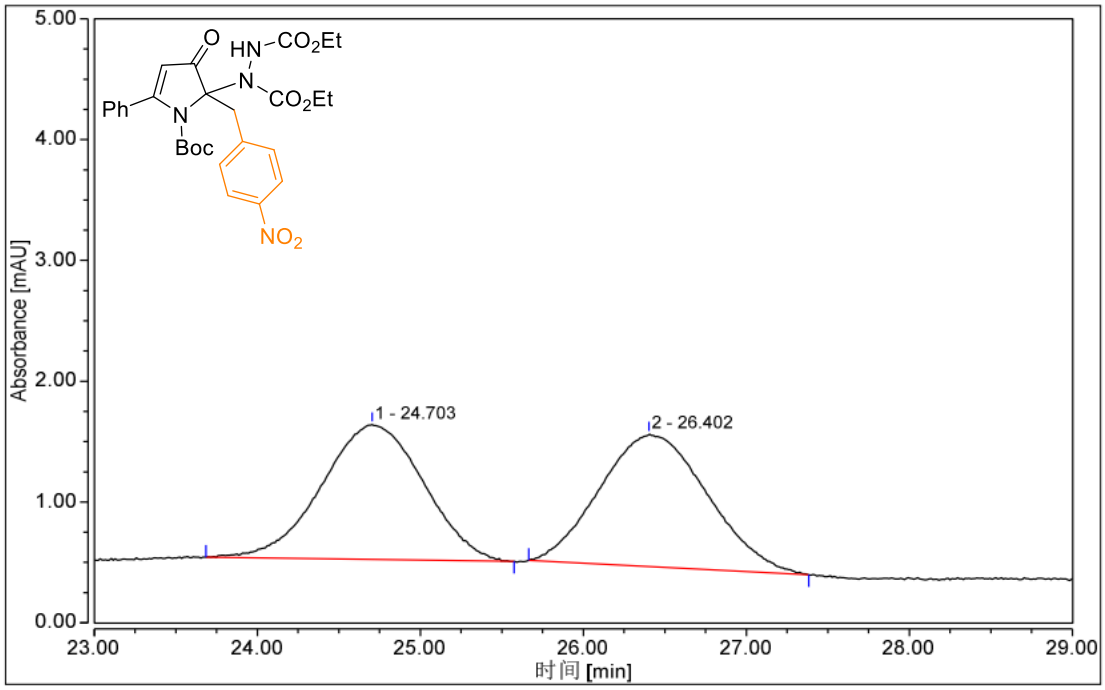


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	9.268	62.818	110.827	50.14	58.28
2	13.350	62.476	79.327	49.86	41.72

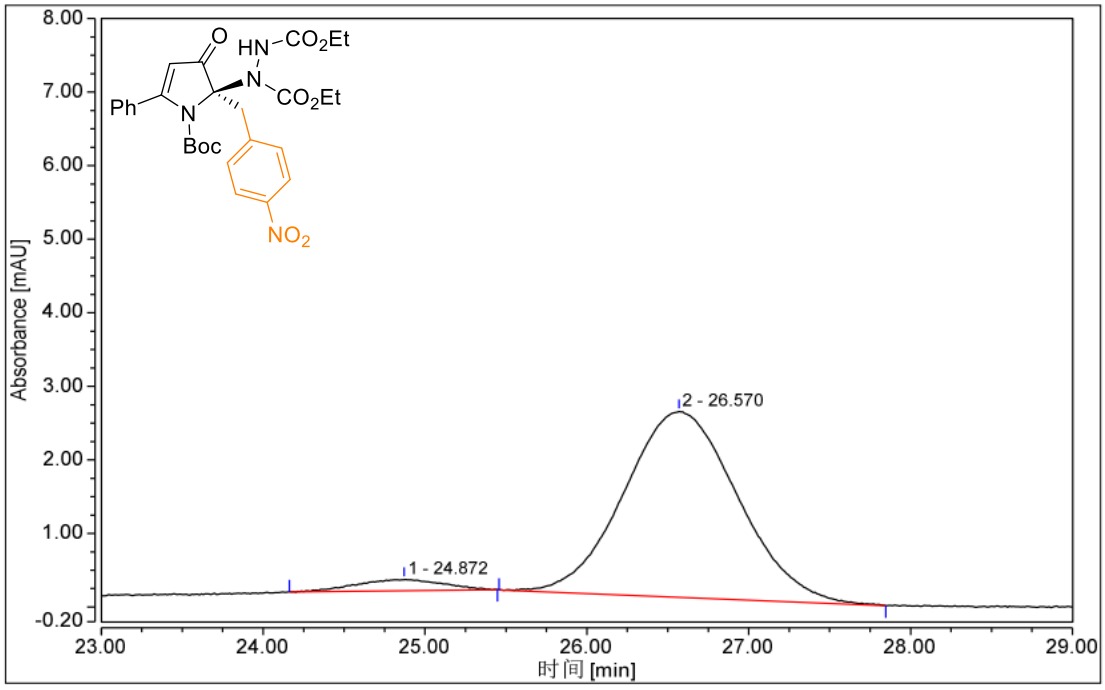


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	9.267	85.248	161.804	85.29	88.69
2	13.410	14.708	20.629	14.71	11.31

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3aa)

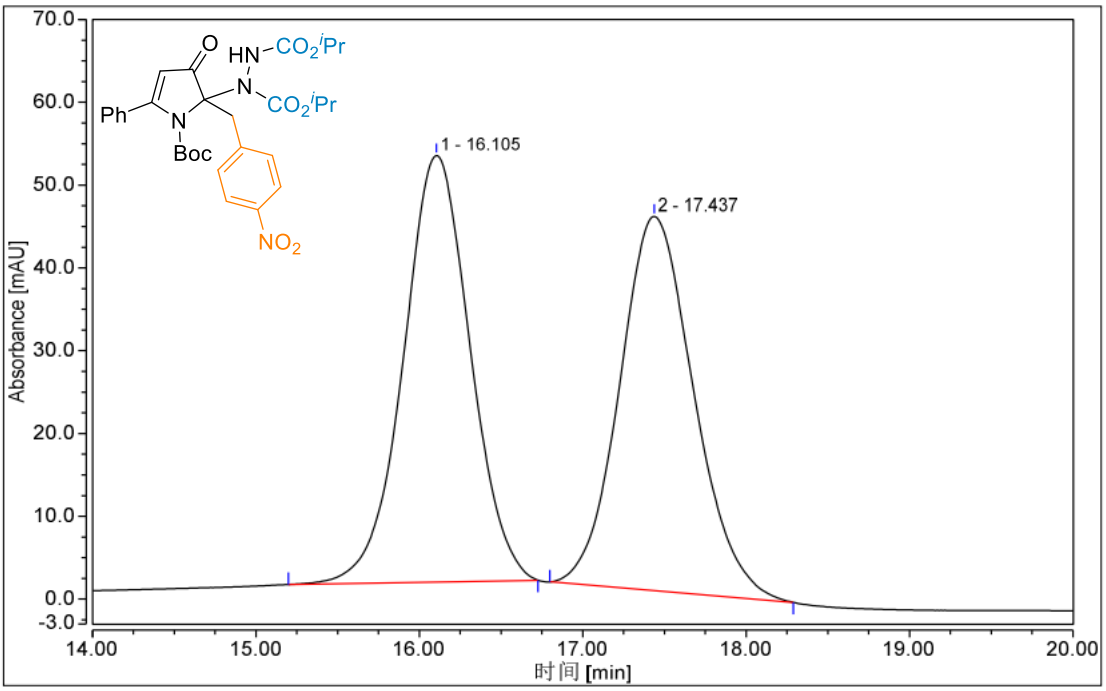


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	24.703	0.805	1.117	49.02	50.41
2	26.402	0.838	1.099	50.98	49.59

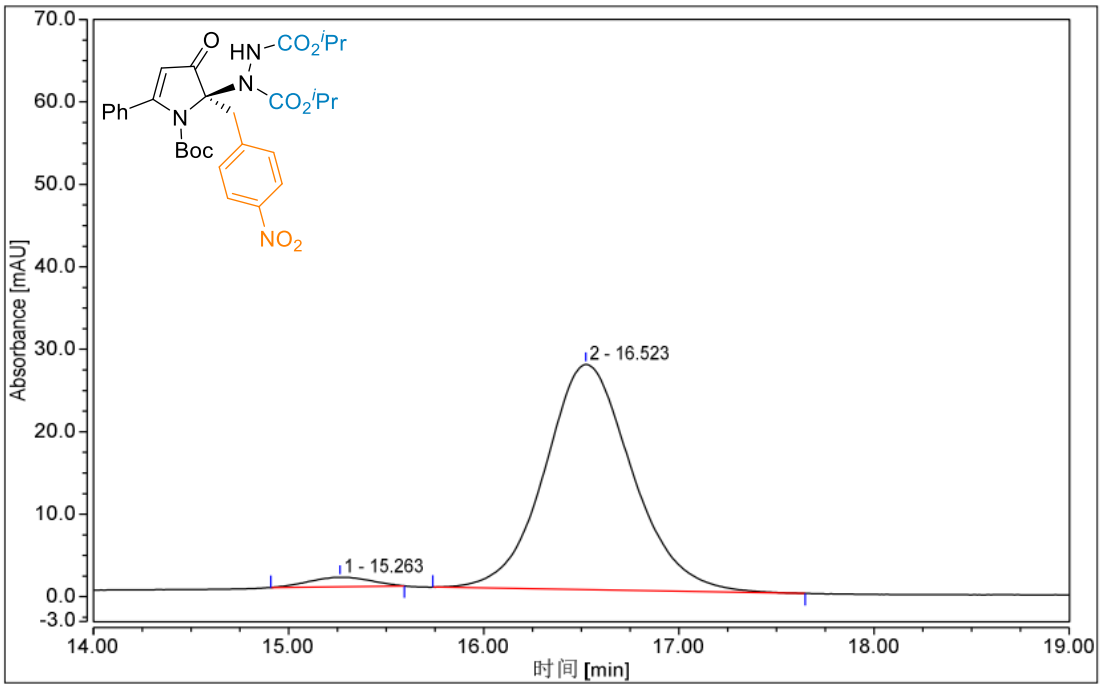


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	24.872	0.094	0.154	4.37	5.73
2	26.570	2.065	2.528	95.63	94.27

diisopropyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3ab)

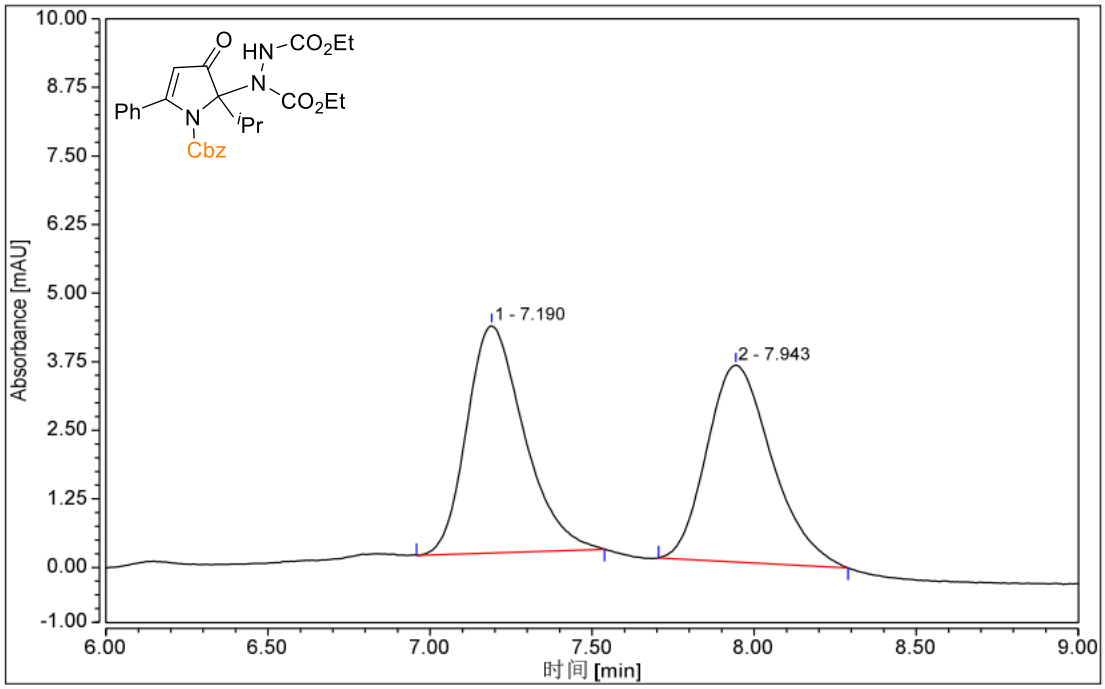


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	16.105	24.335	51.492	50.63	53.25
2	17.437	23.732	45.203	49.37	46.75

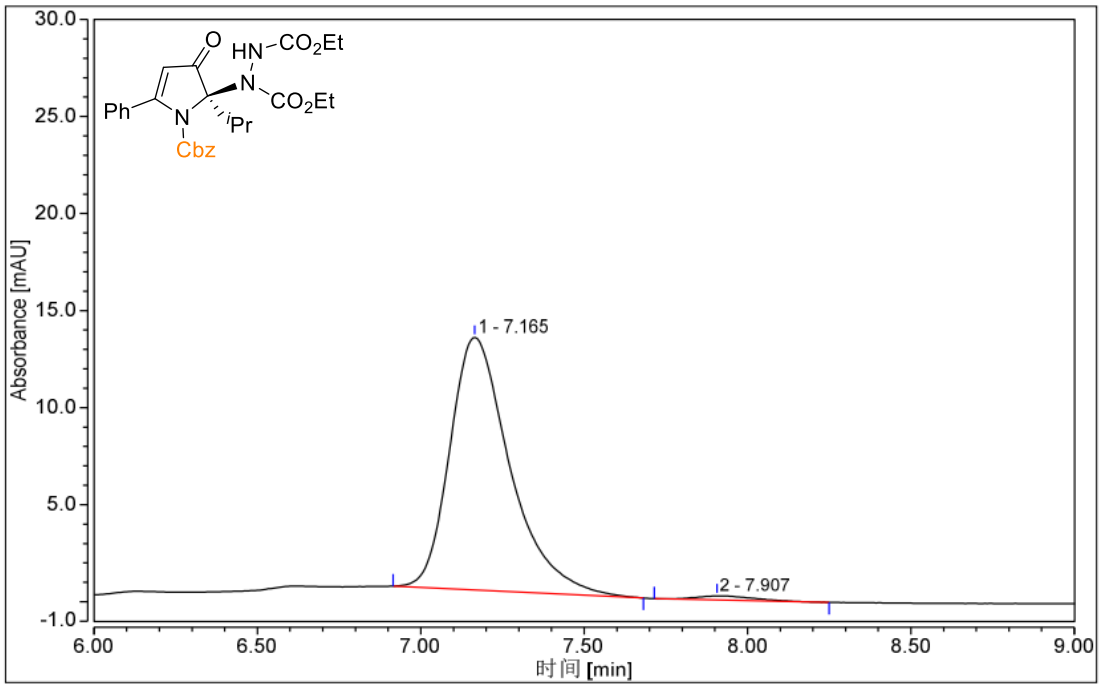


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	15.263	0.414	1.142	2.83	4.01
2	16.523	14.195	27.319	97.17	95.99

diethyl (*R*)-1-(1-((benzyloxy)carbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (S3ac)

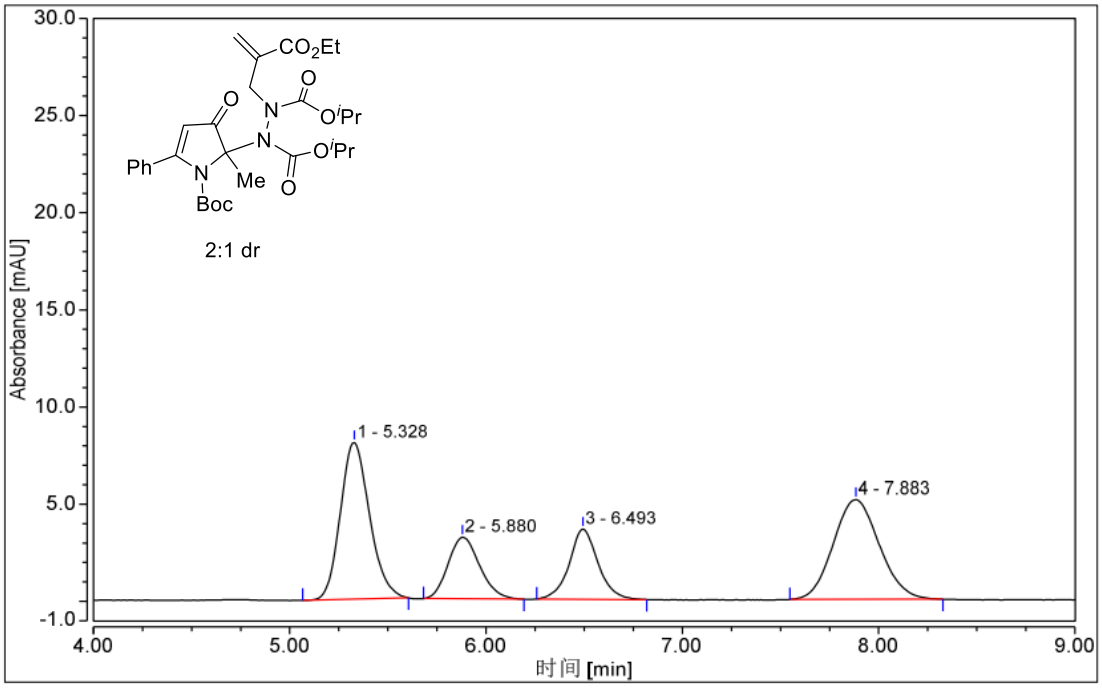


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.190	0.851	4.147	50.37	53.60
2	7.943	0.838	3.591	49.63	46.40

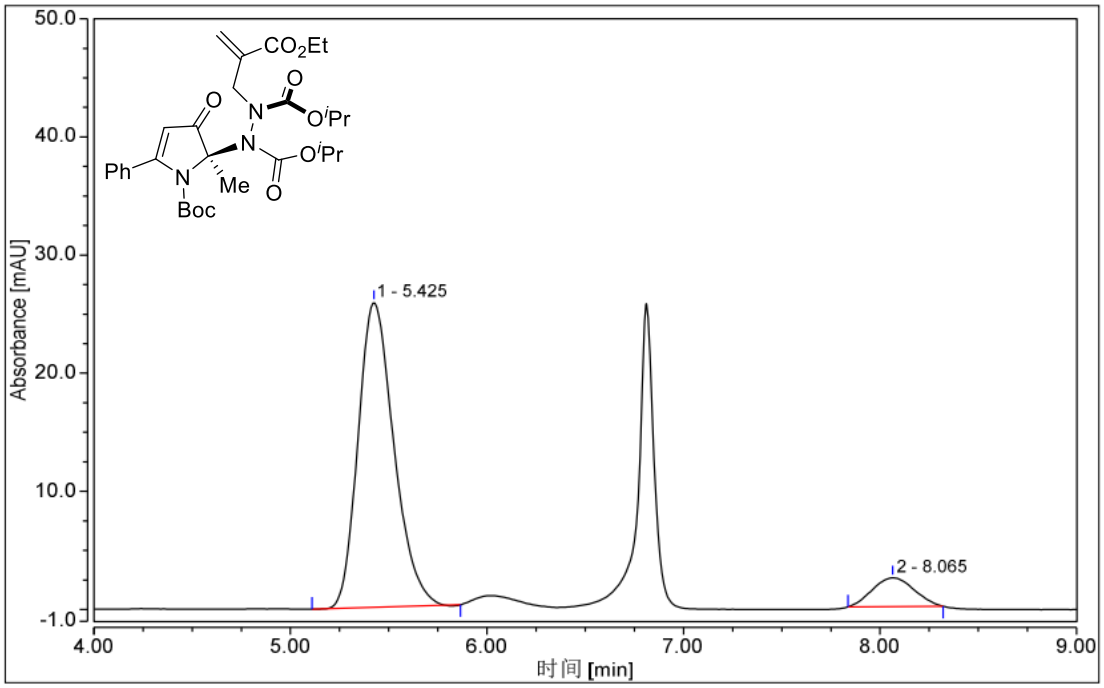


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.165	2.778	13.012	98.47	98.42
2	7.907	0.043	0.208	1.53	1.58

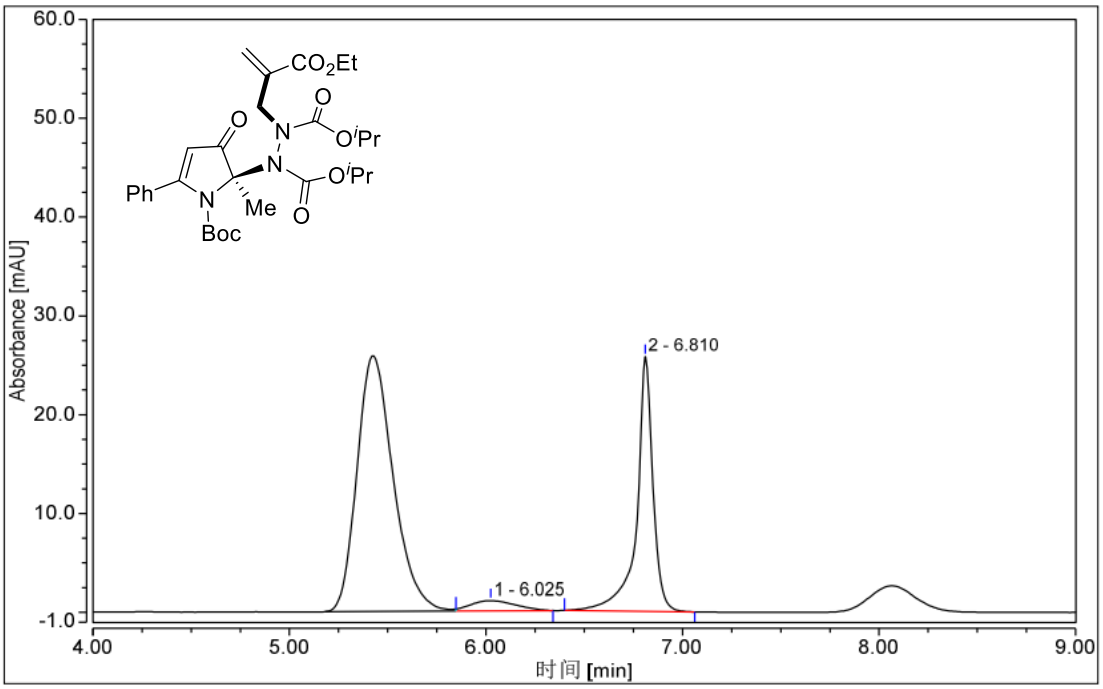
Diisopropyl-1-(1-(tert-butoxycarbonyl)-2-methyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (5)



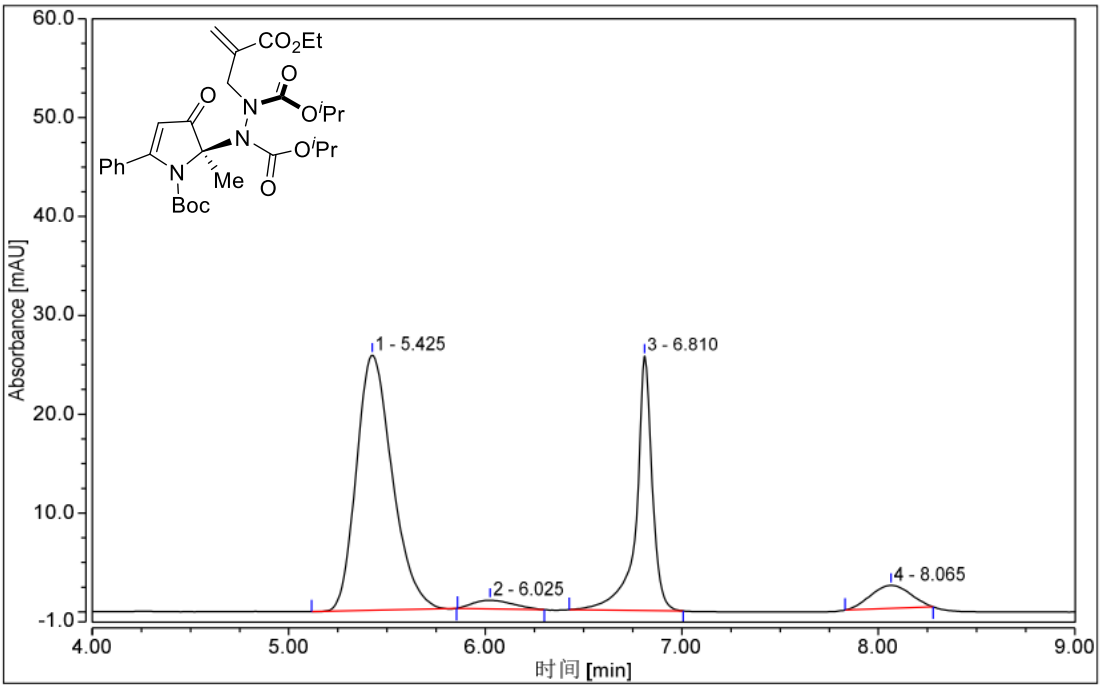
Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.328	1.390	8.065	34.81	40.32
2	5.880	0.592	3.176	14.83	15.88
3	6.493	0.615	3.620	15.40	18.10
4	7.883	1.396	5.141	34.97	25.70



Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.425	5.444	25.812	90.06	91.34
2	8.065	0.601	2.447	9.94	8.66

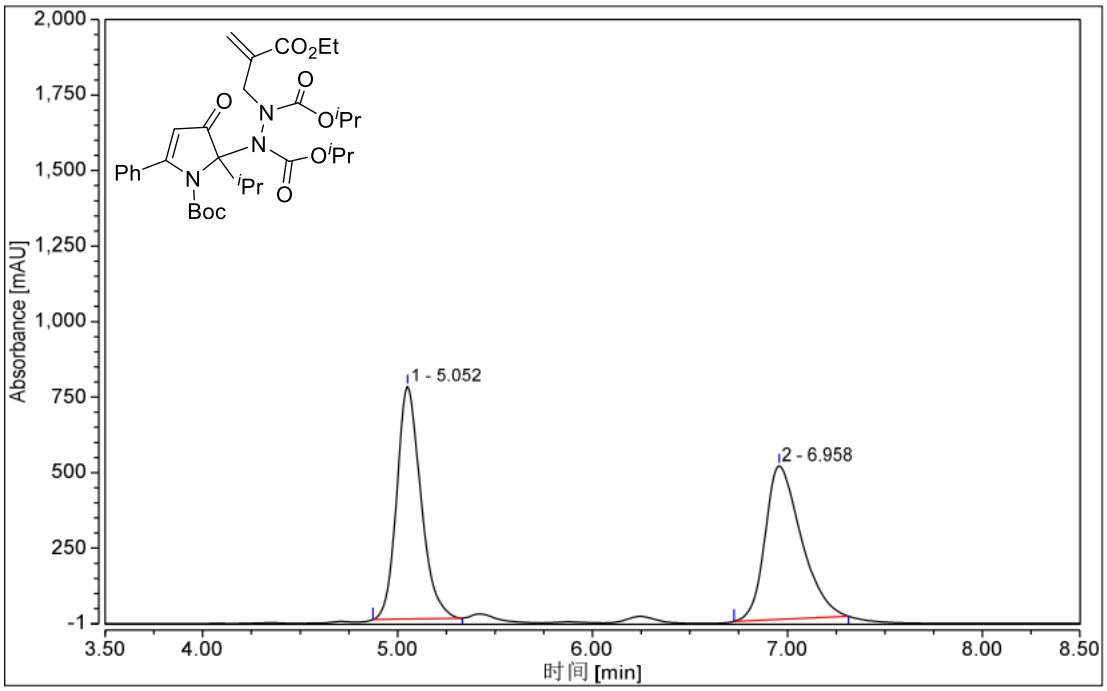


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.025	0.271	1.025	9.89	3.83
2	6.810	2.471	25.779	90.11	96.17

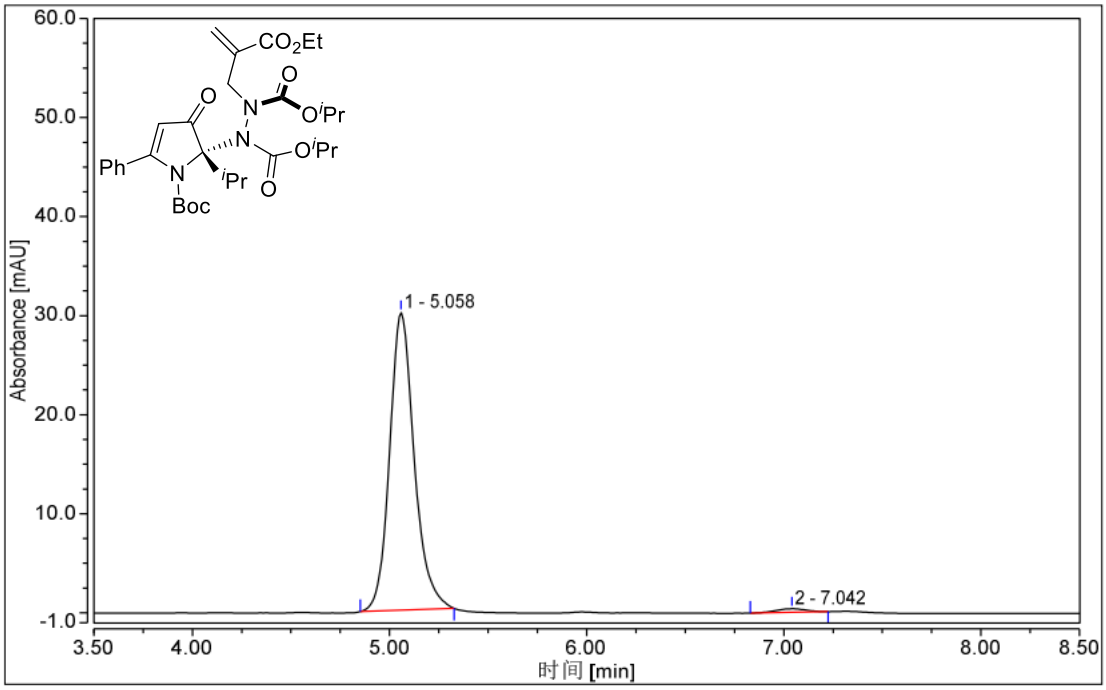


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.425	5.460	25.830	63.09	47.18
2	6.025	0.203	0.858	2.34	1.57
3	6.810	2.444	25.734	28.24	47.00
4	8.065	0.547	2.331	6.32	4.26

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6a)

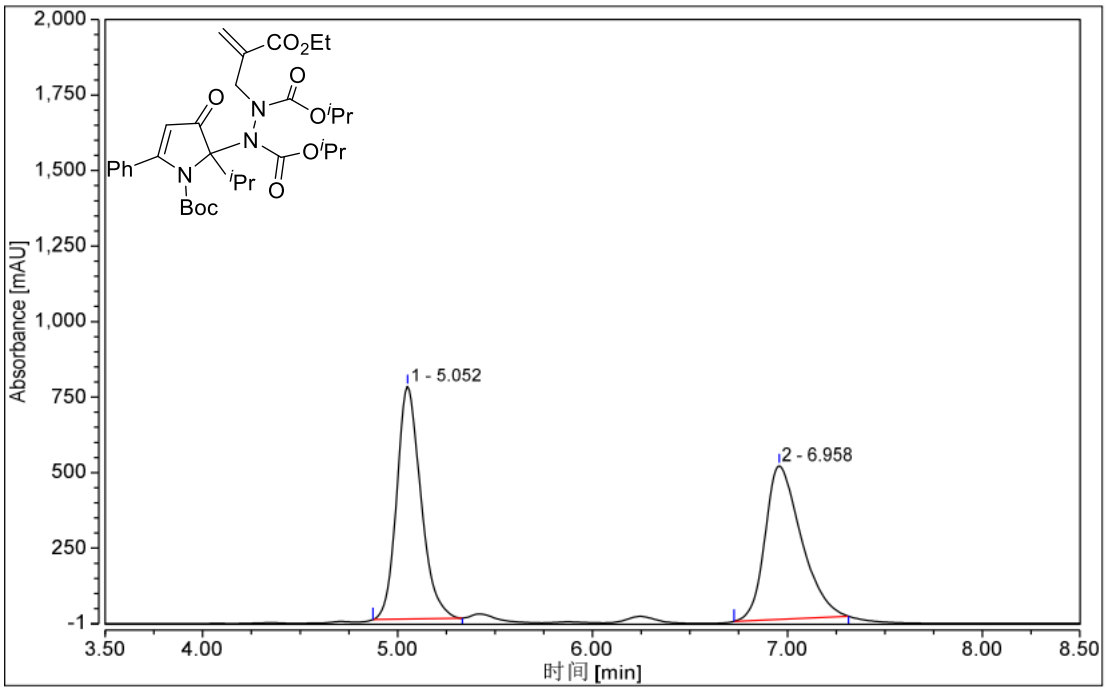


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.052	110.657	769.644	50.36	60.23
2	6.958	109.067	508.193	49.64	39.77

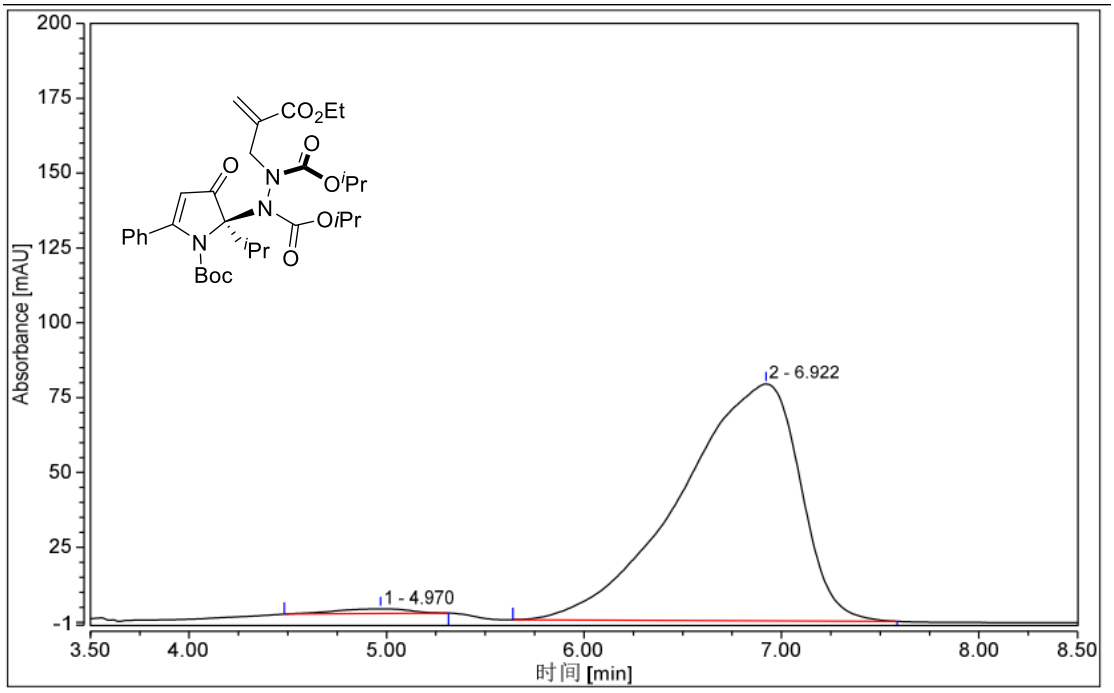


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.058	4.350	30.052	98.54	98.79
2	7.042	0.064	0.367	1.46	1.21

diisopropyl (*S*, *S*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (*ent*-6a)

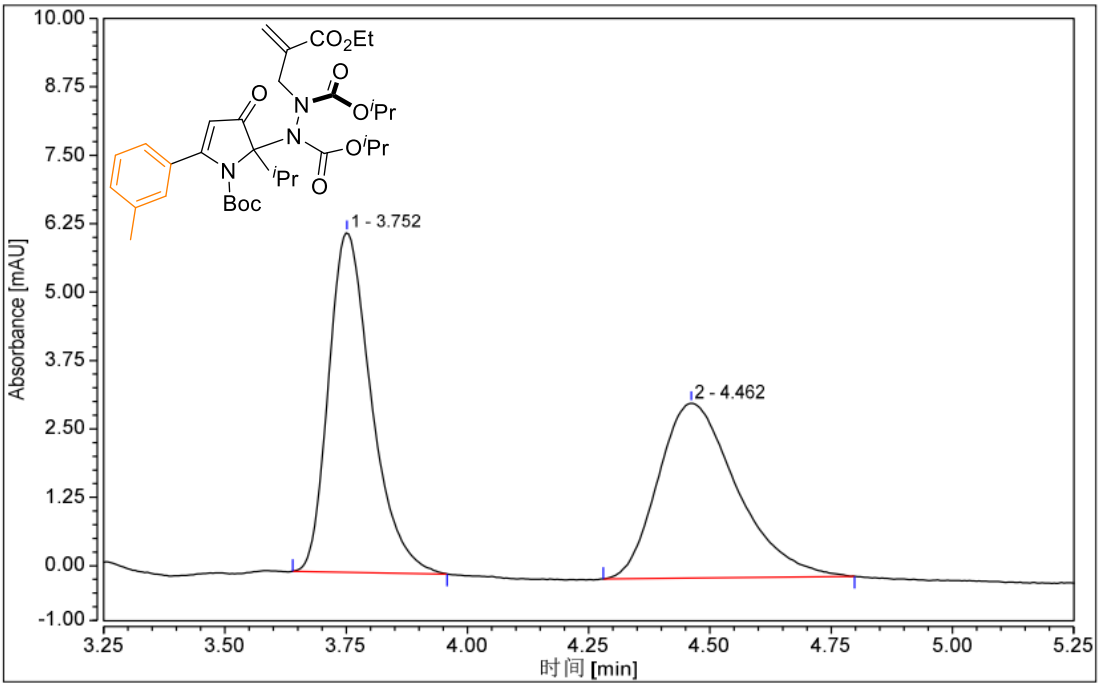


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.052	110.657	769.644	50.36	60.23
2	6.958	109.067	508.193	49.64	39.77

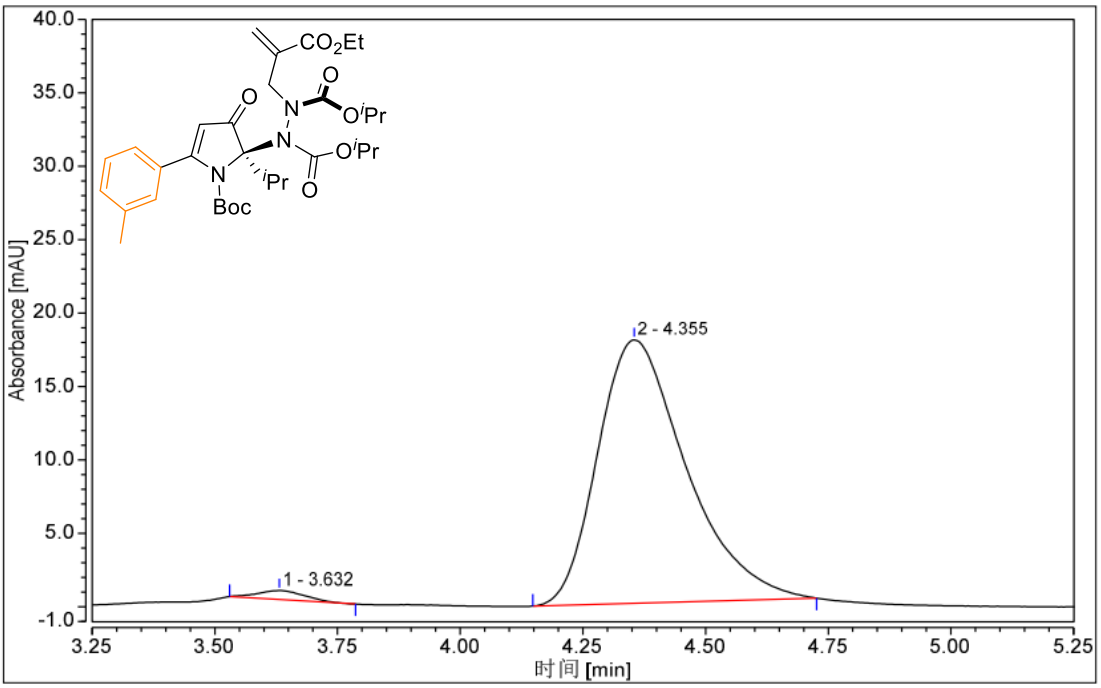


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.970	0.682	1.581	1.22	1.96
2	6.922	55.364	79.074	98.78	98.04

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(m-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6b)

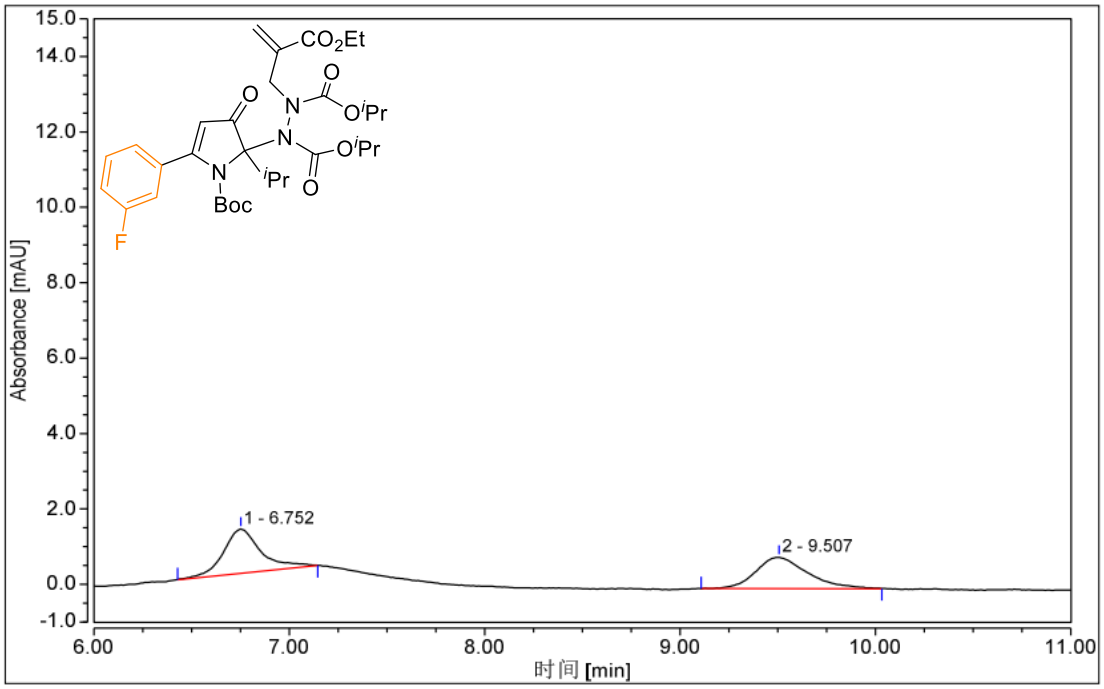


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.752	0.634	6.208	51.34	66.01
2	4.462	0.601	3.197	48.66	33.99

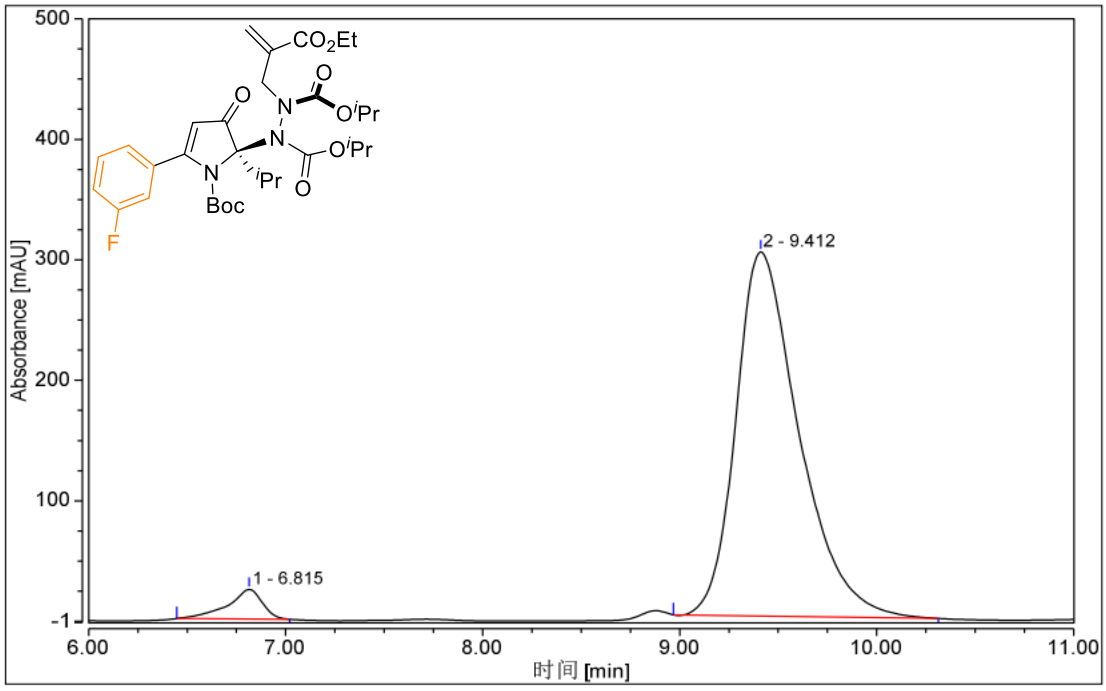


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.632	0.068	0.608	1.77	3.28
2	4.355	3.749	17.937	98.23	96.72

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(3-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6c)

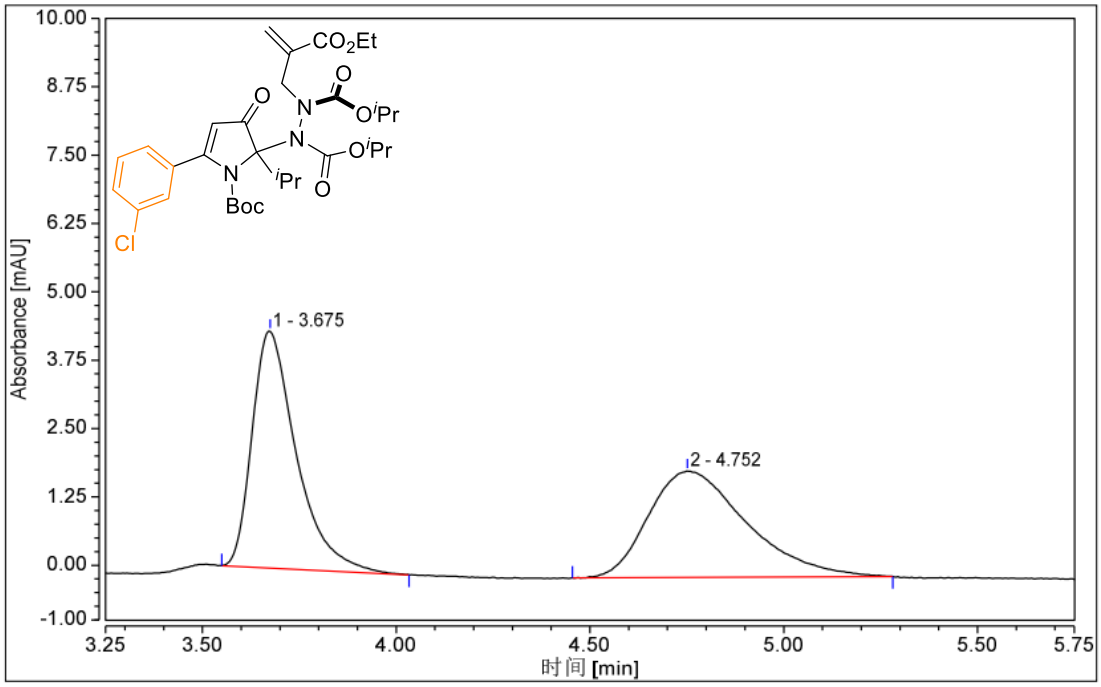


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.752	0.262	1.174	50.67	58.60
2	9.507	0.255	0.829	49.33	41.40

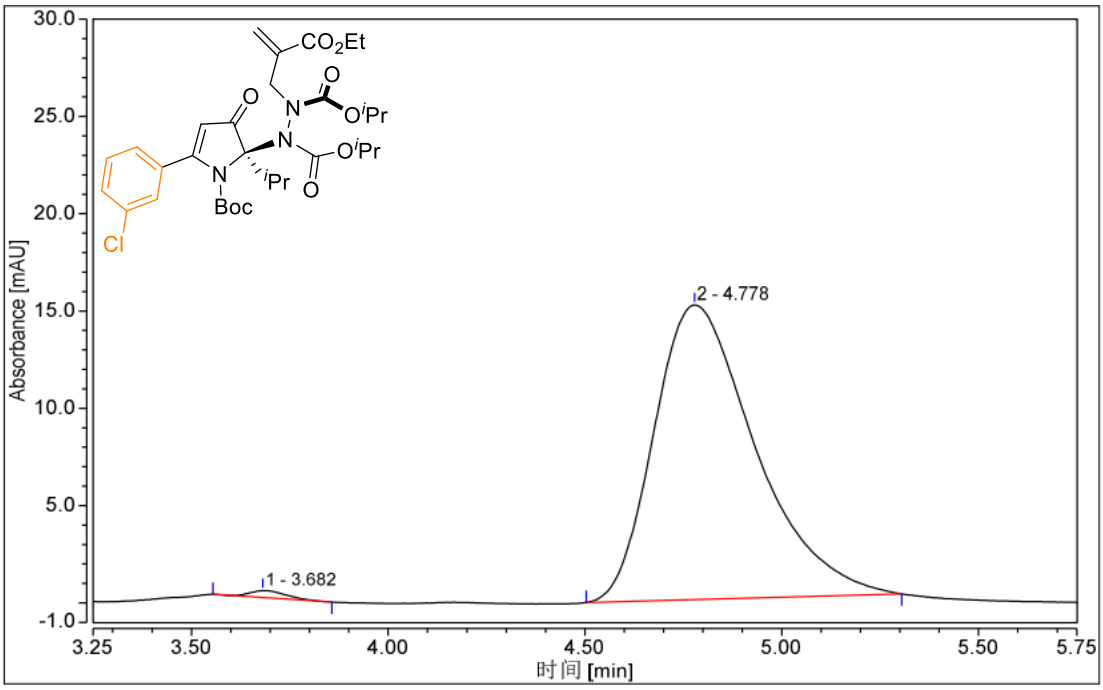


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.815	5.017	24.524	4.28	7.51
2	9.412	112.084	302.153	95.72	92.49

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(3-chlorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6d)

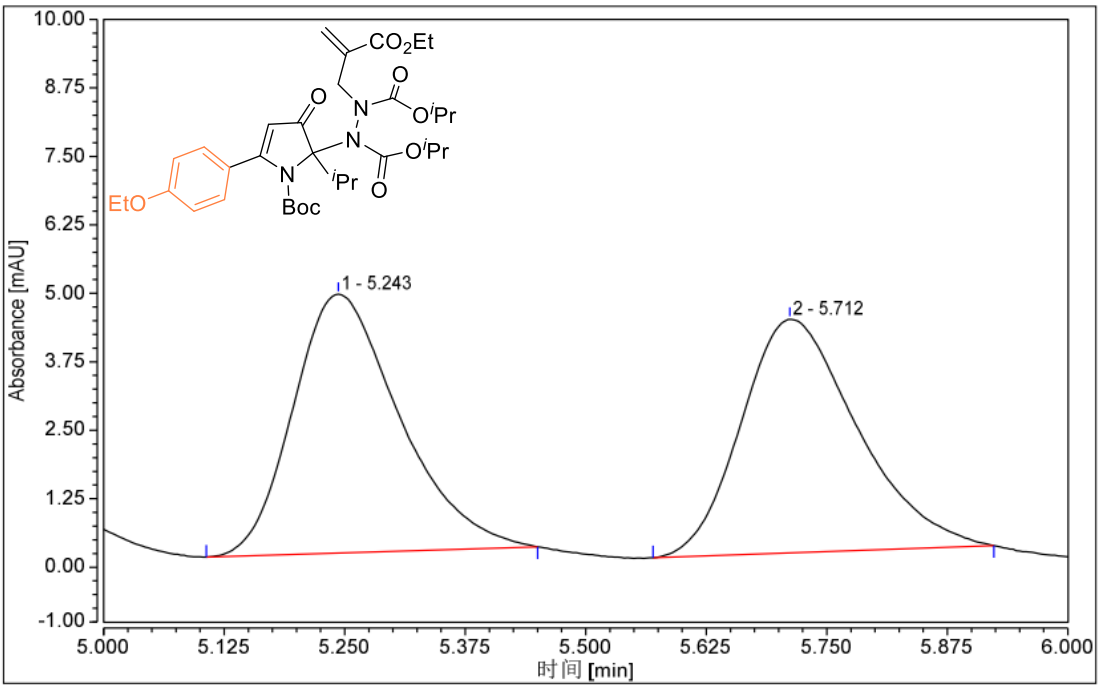


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.675	0.573	4.330	50.06	68.99
2	4.752	0.571	1.947	49.94	31.01

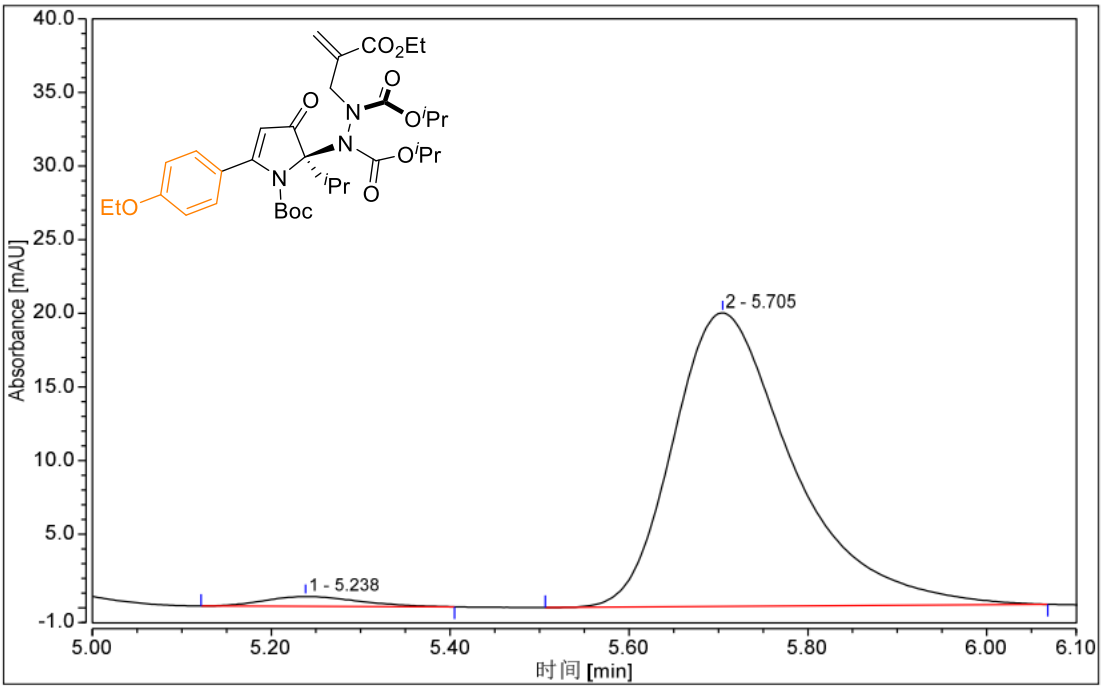


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.682	0.039	0.360	0.85	2.32
2	4.778	4.503	15.140	99.15	97.68

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethoxyphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6e)

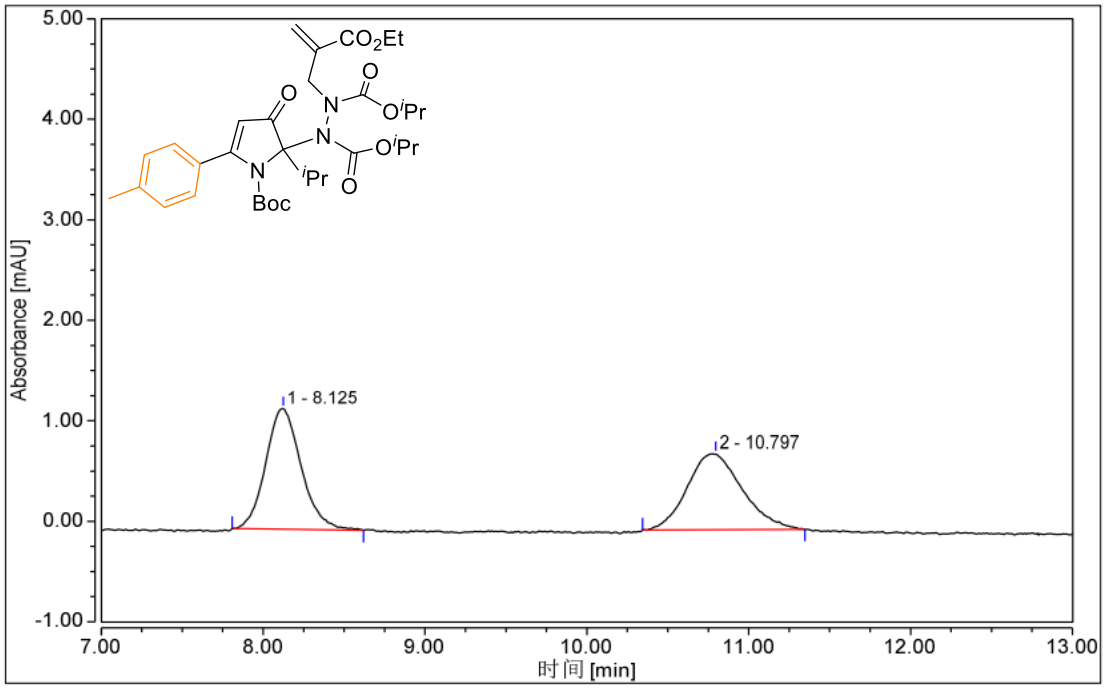


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.243	0.605	4.724	50.42	52.56
2	5.712	0.595	4.265	49.58	47.44

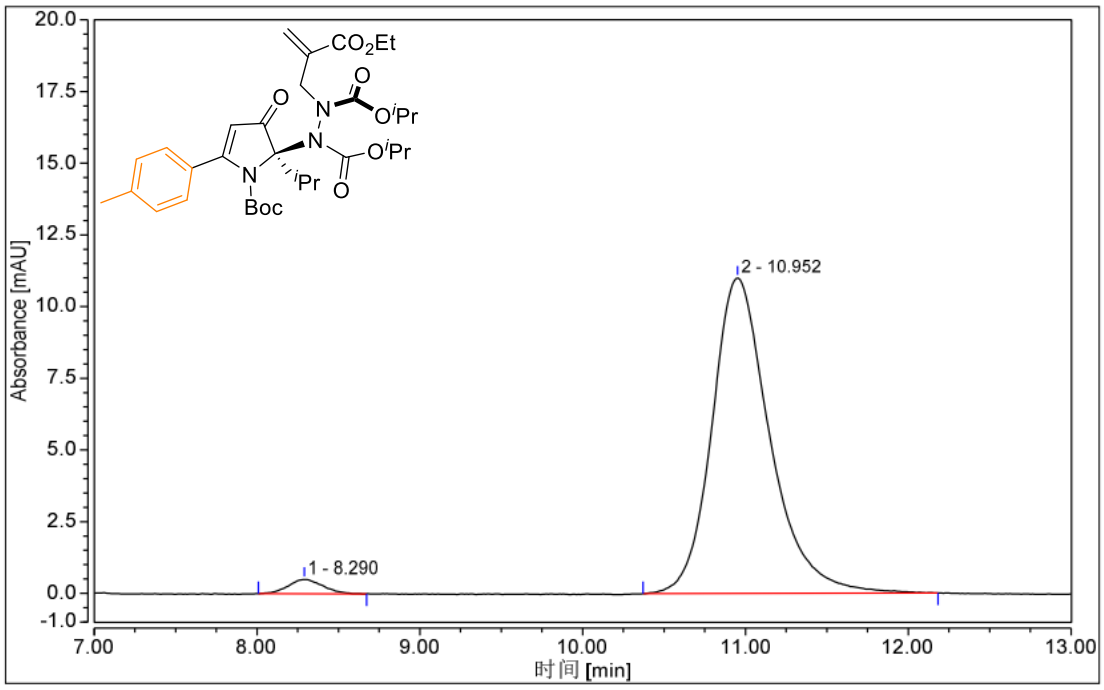


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.238	0.081	0.666	2.56	3.23
2	5.705	3.090	19.936	97.44	96.77

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(p-tolyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6f)

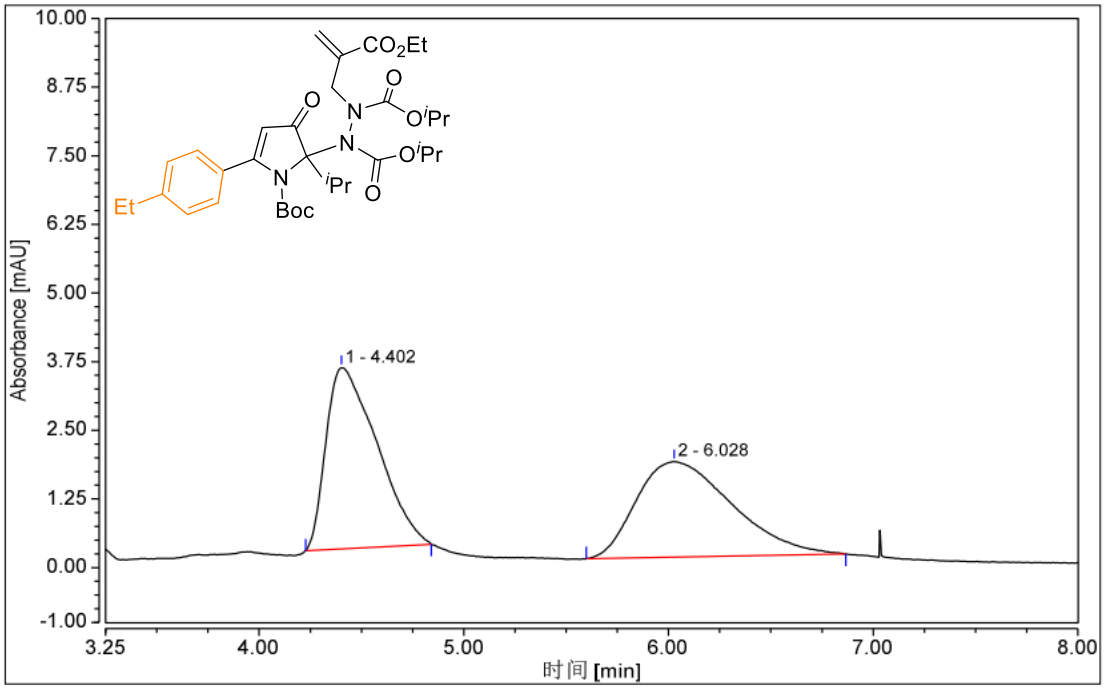


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.125	0.305	1.199	50.69	61.33
2	10.797	0.297	0.756	49.31	38.67

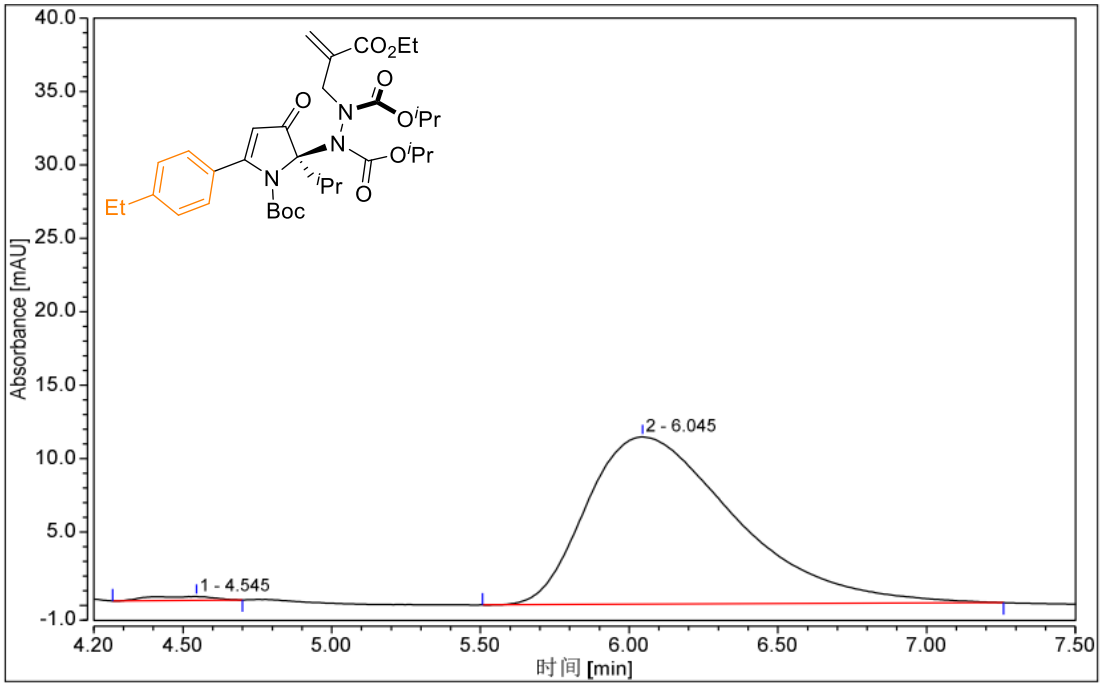


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.290	0.122	0.503	2.62	4.37
2	10.952	4.533	10.994	97.38	95.63

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-ethylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6g)

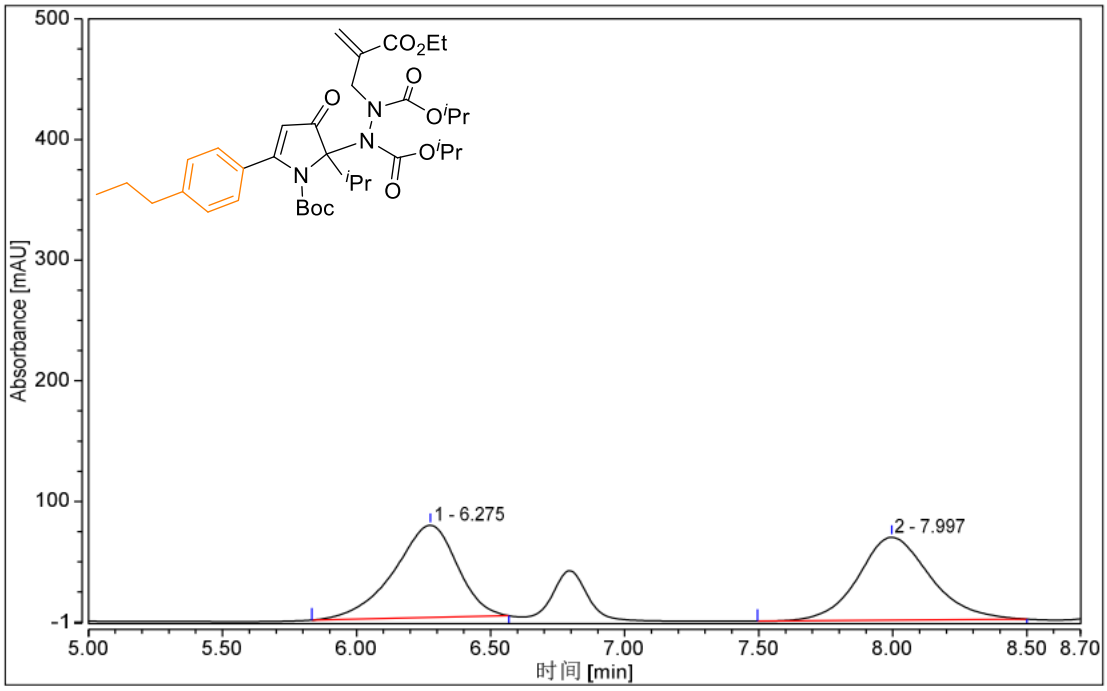


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.402	0.951	3.304	50.22	65.52
2	6.028	0.943	1.739	49.78	34.48

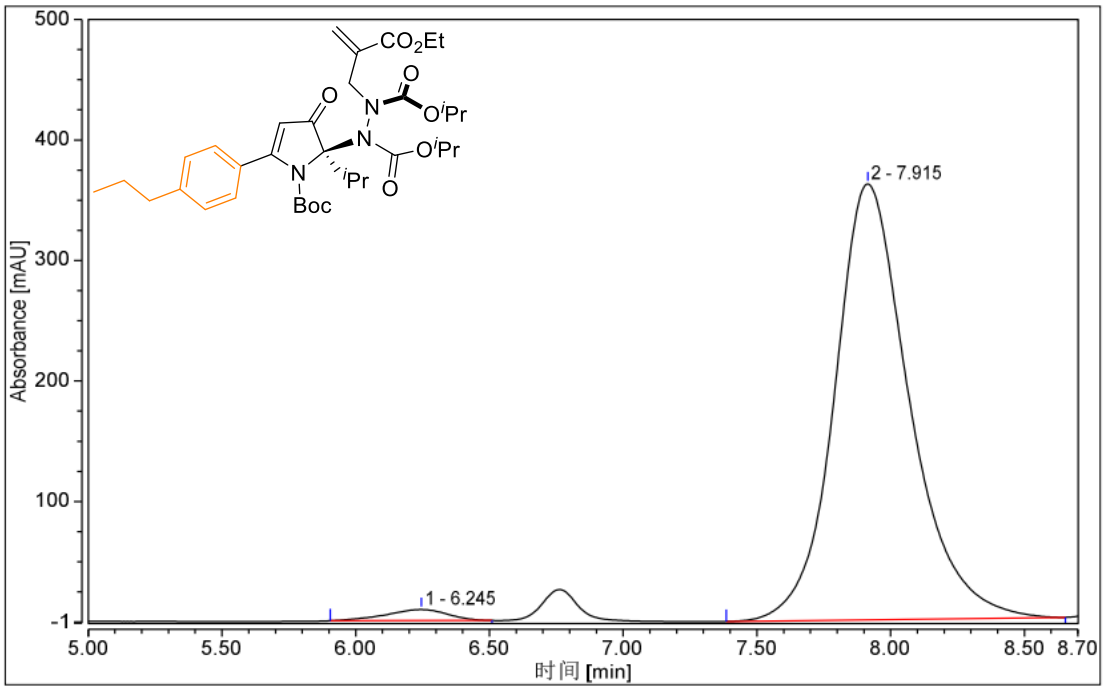


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.545	0.068	0.256	1.02	2.19
2	6.045	6.614	11.397	98.98	97.81

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-propylphenyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6h)

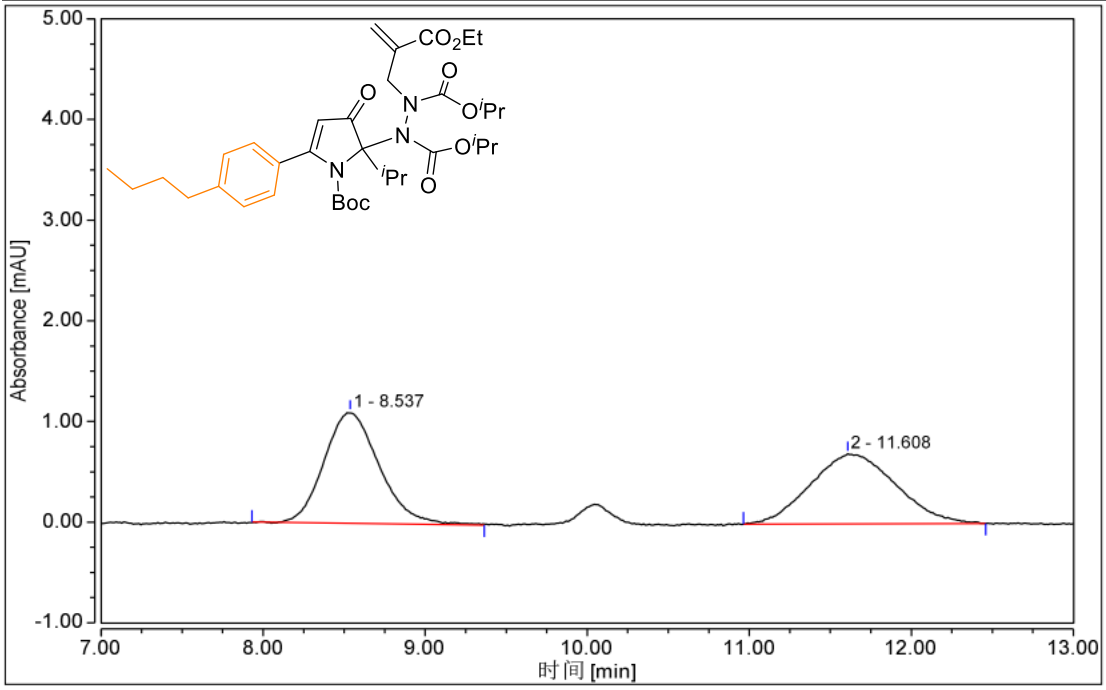


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.275	21.007	76.397	49.49	52.66
2	7.997	21.437	68.670	50.51	47.34

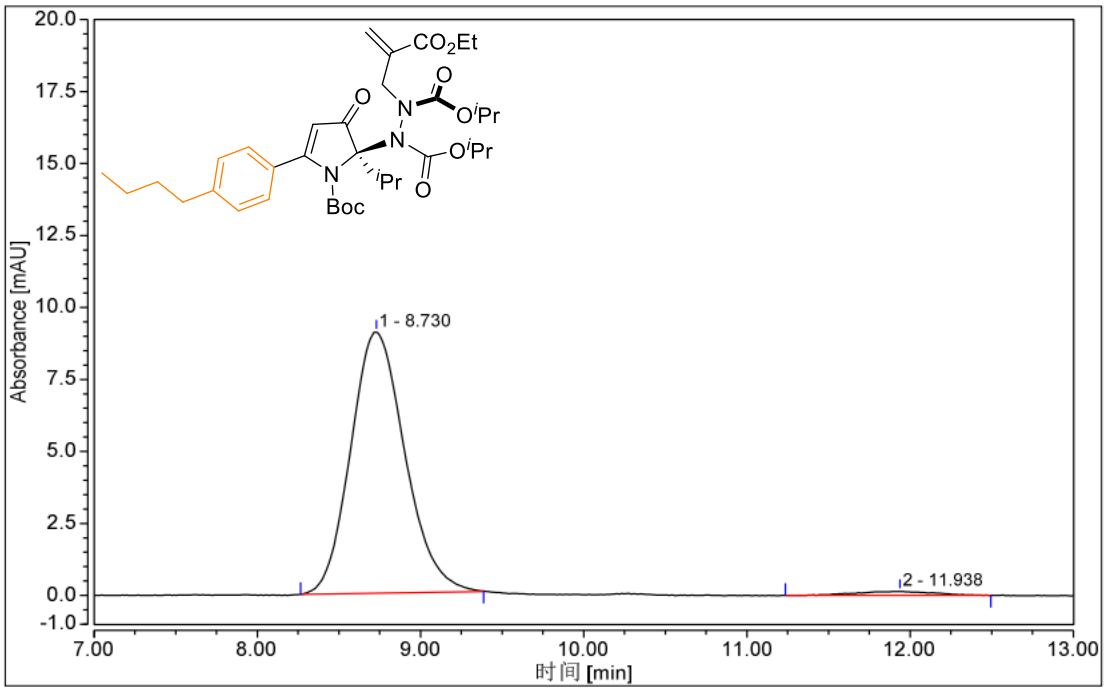


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.245	2.441	9.119	2.04	2.46
2	7.915	117.012	361.694	97.96	97.54

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-butylphenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6i)

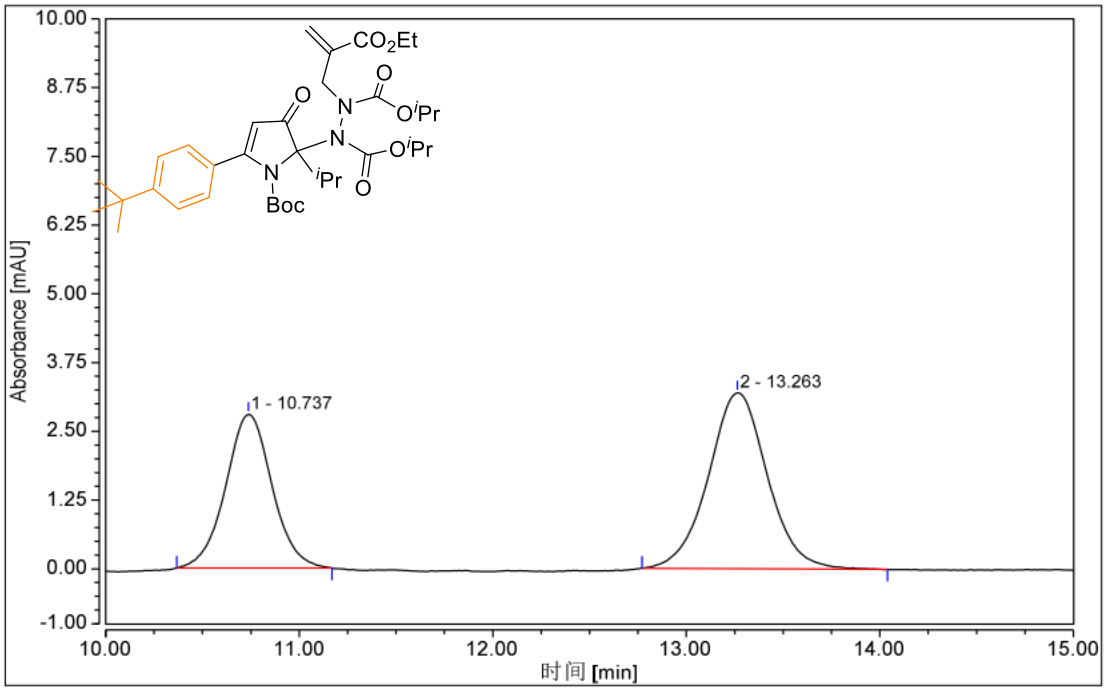


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.537	0.433	1.102	50.56	61.26
2	11.608	0.423	0.697	49.44	38.74

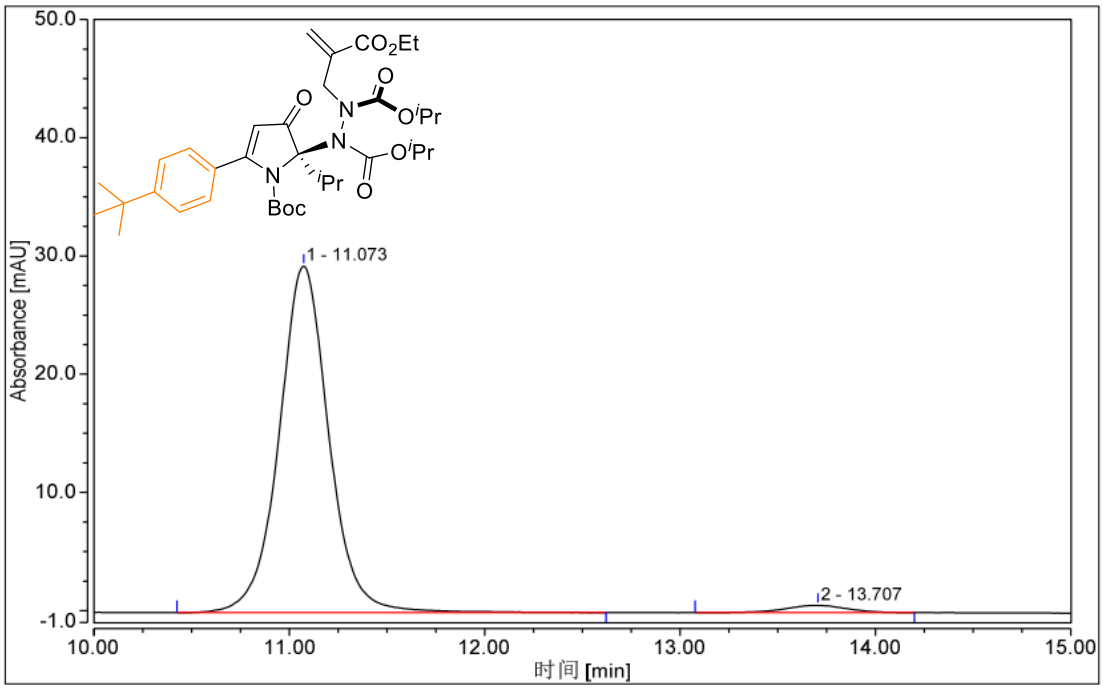


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.730	3.494	9.071	97.86	98.47
2	11.938	0.077	0.141	2.14	1.53

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-(tert-butyl)phenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6j)

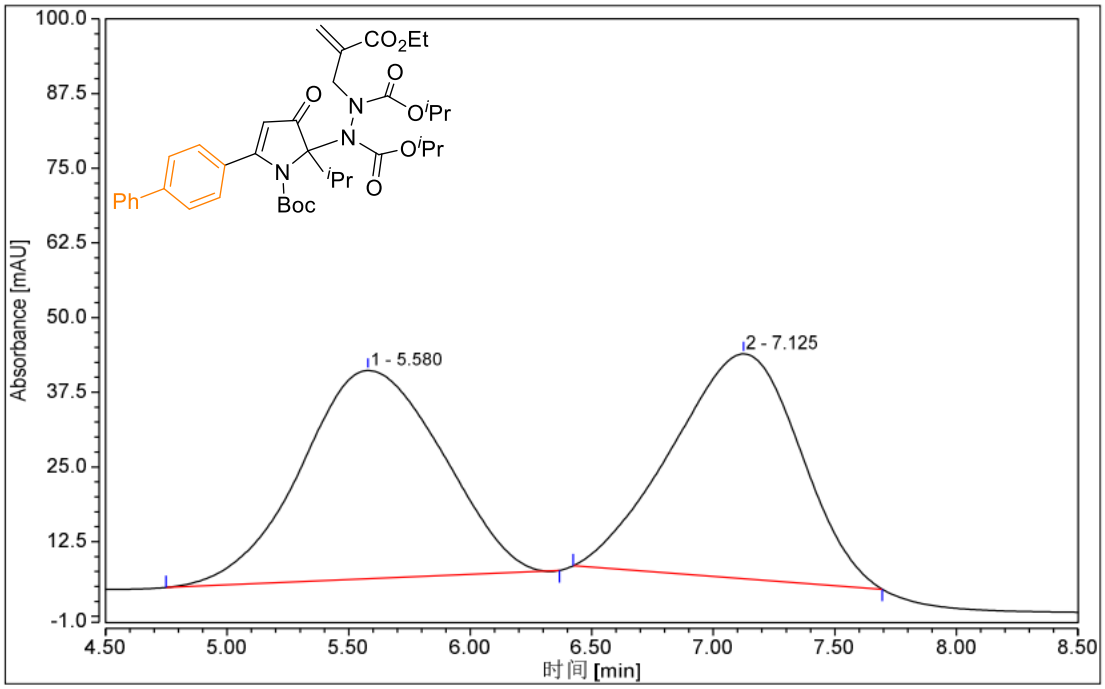


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	10.737	0.776	2.797	40.77	46.63
2	13.263	1.128	3.200	59.23	53.37

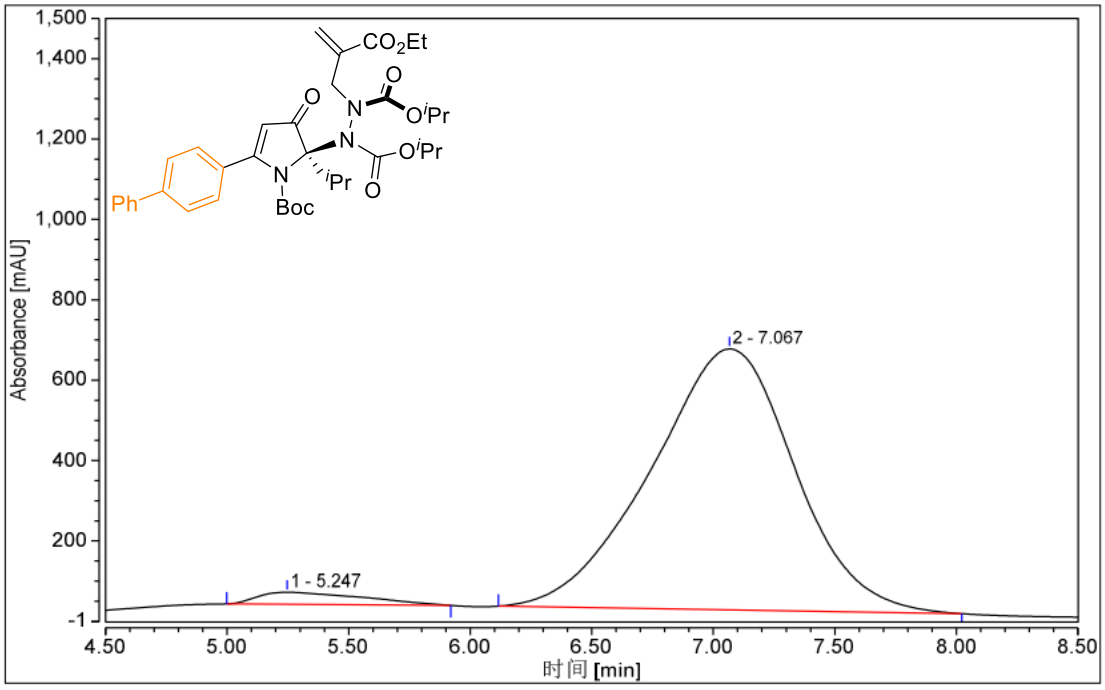


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	11.073	8.672	29.312	97.45	97.93
2	13.707	0.227	0.619	2.55	2.07

diisopropyl (*R*, *R*)-1-(5-([1,1'-biphenyl]-4-yl)-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6k)

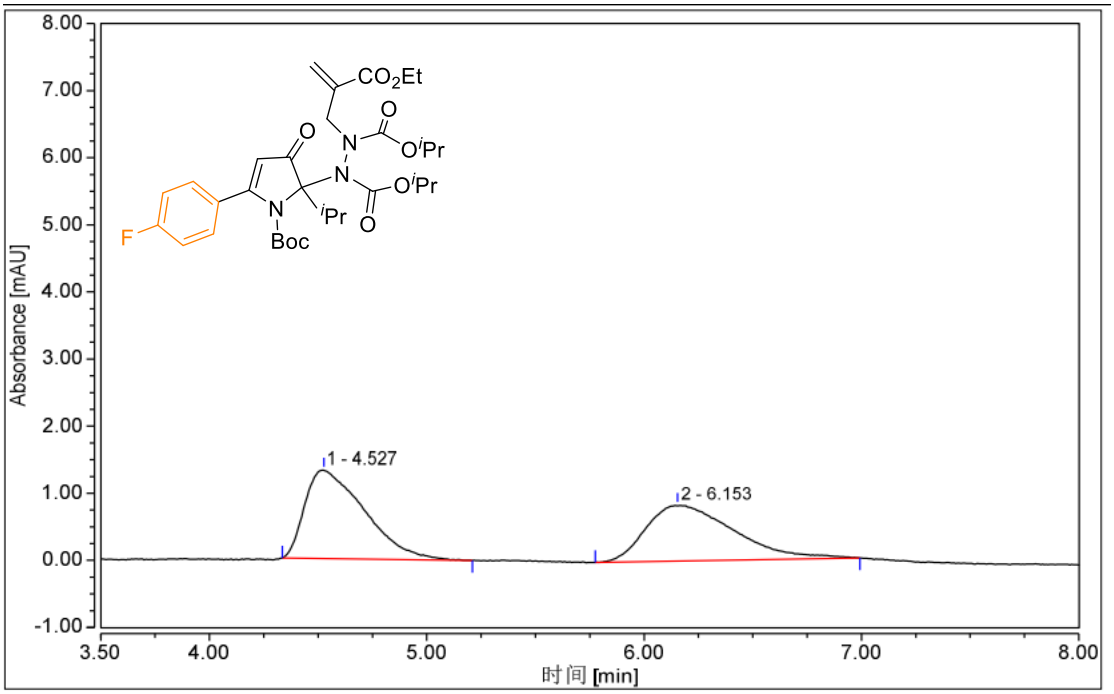


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.580	23.357	34.851	50.35	48.07
2	7.125	23.032	37.645	49.65	51.93

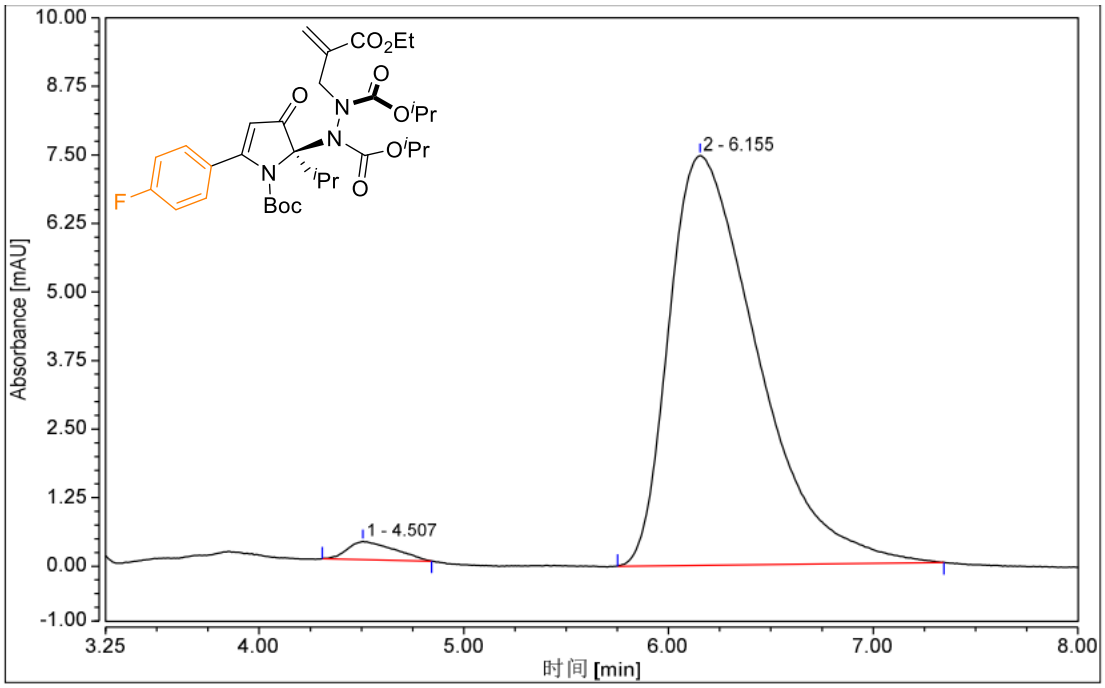


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.247	15.005	29.887	3.26	4.40
2	7.067	444.681	649.462	96.74	95.60

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-5-(4-fluorophenyl)-2-isopropyl-3-oxo-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6l)

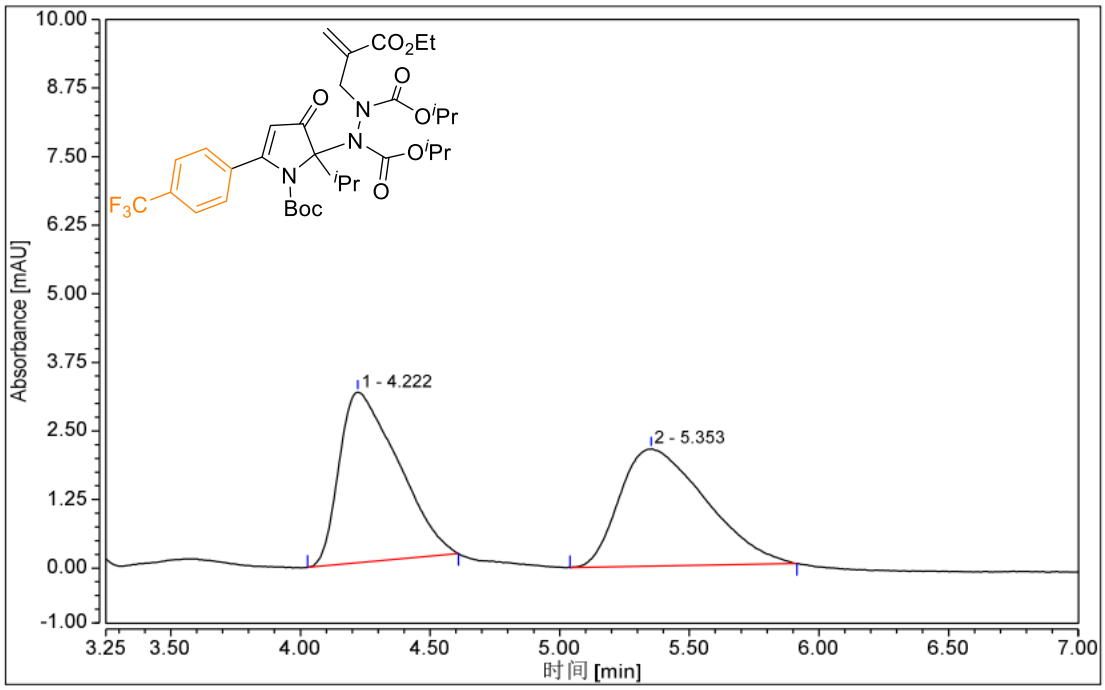


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.527	0.417	1.321	51.75	61.31
2	6.153	0.389	0.833	48.25	38.69

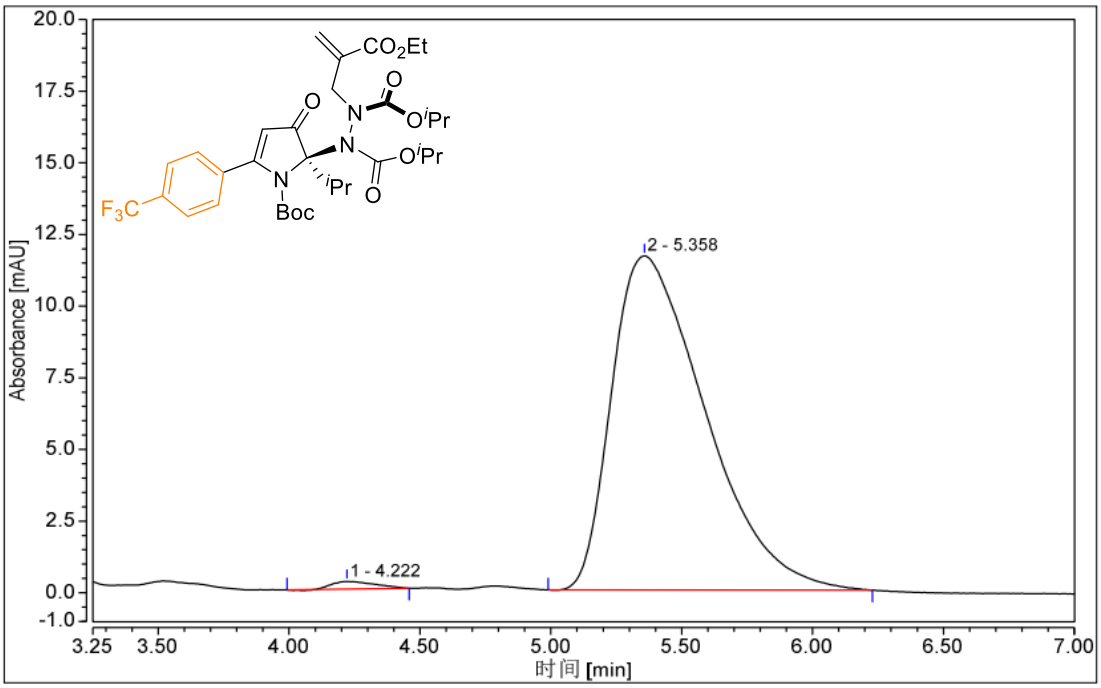


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.507	0.087	0.330	2.28	4.23
2	6.155	3.744	7.470	97.72	95.77

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-(4-(trifluoromethyl)phenyl)-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6m)

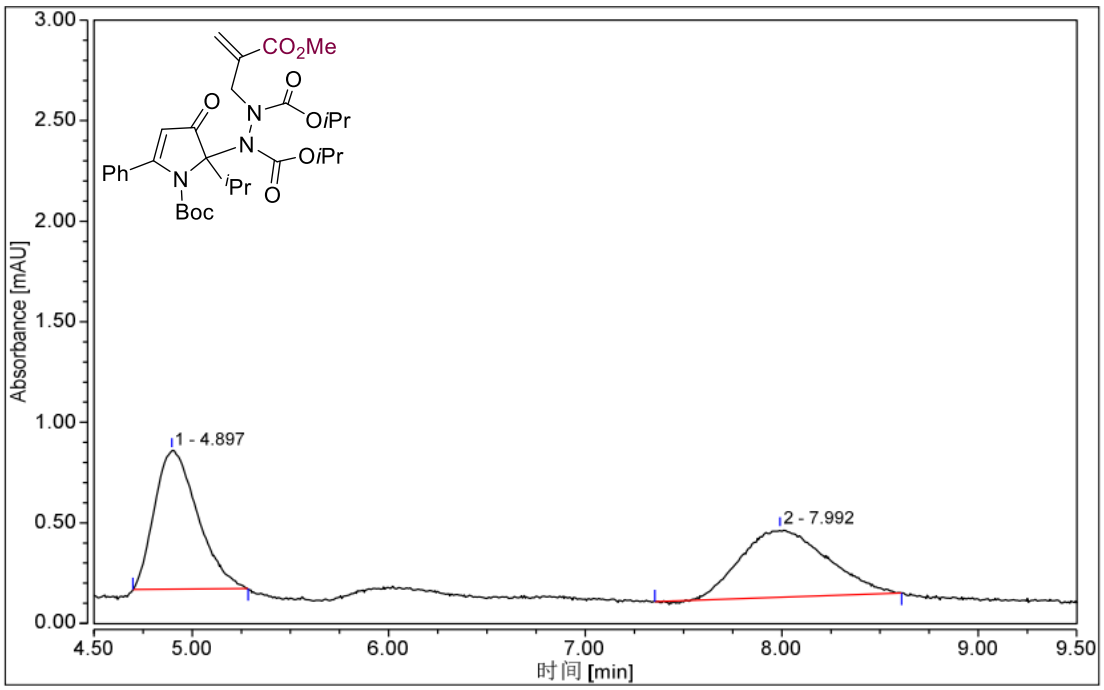


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.222	0.815	3.112	49.84	59.29
2	5.353	0.821	2.136	50.16	40.71

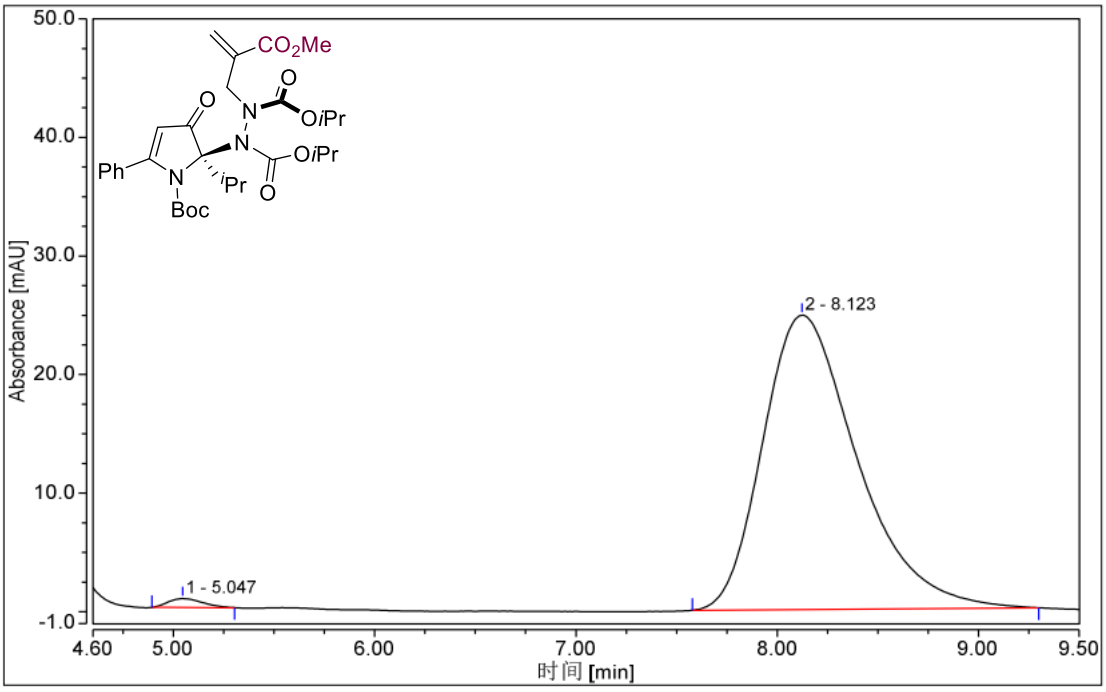


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.222	0.050	0.270	1.02	2.26
2	5.358	4.833	11.657	98.98	97.74

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(methoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6n)

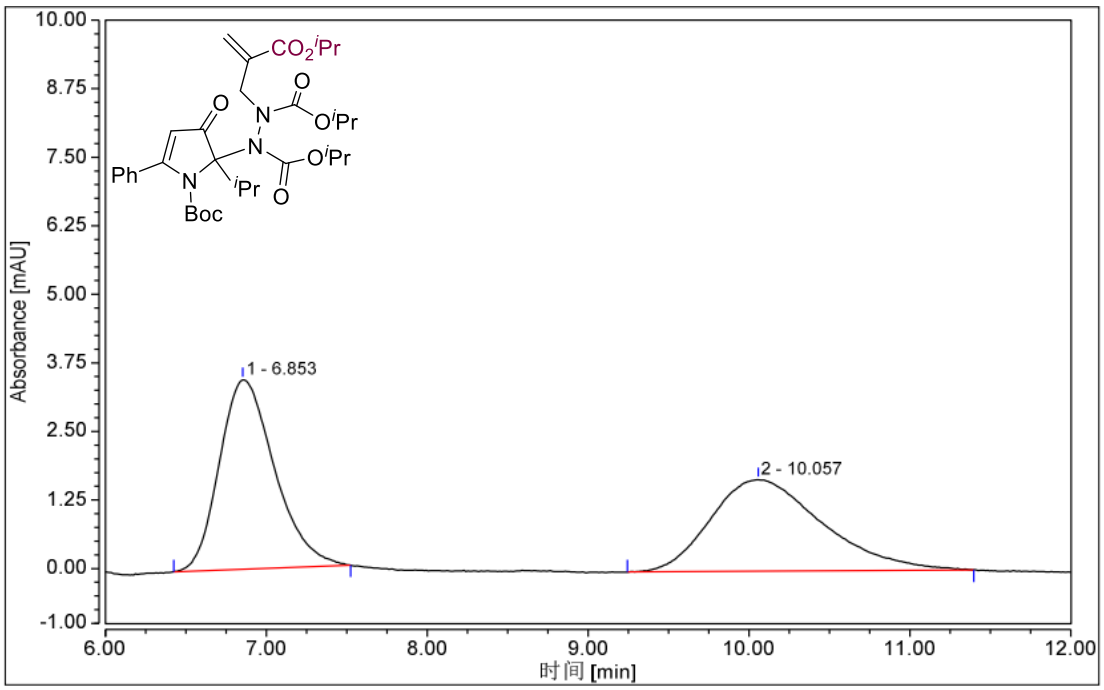


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.897	0.176	0.691	50.64	67.12
2	7.992	0.171	0.339	49.36	32.88

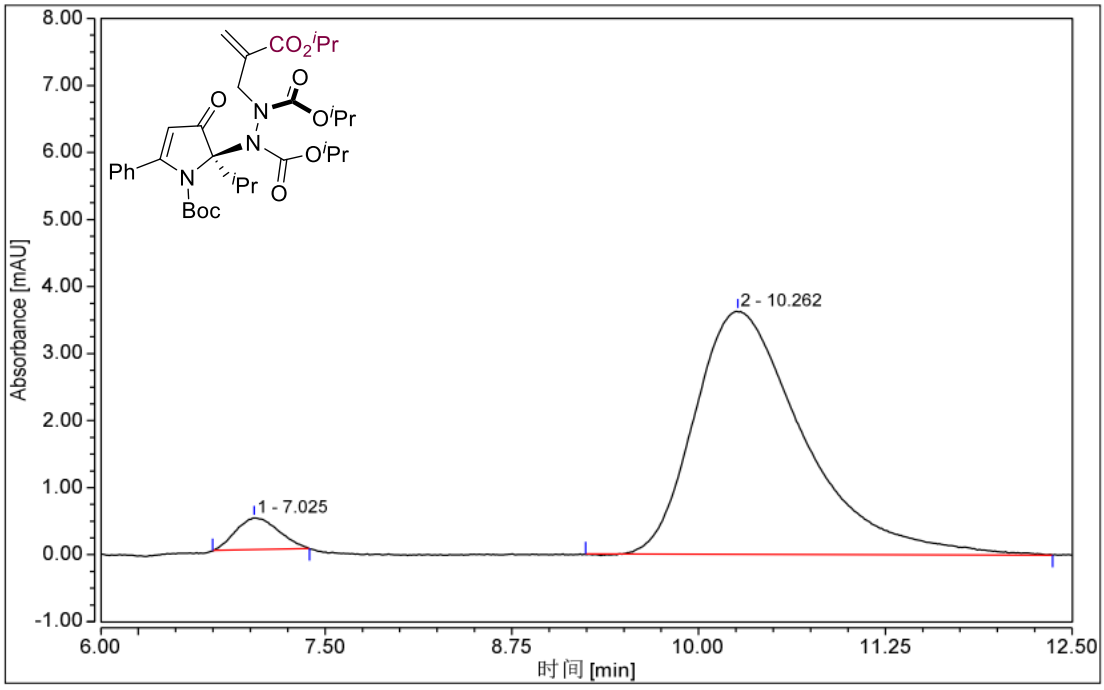


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	5.047	0.148	0.744	1.08	2.91
2	8.123	13.522	24.827	98.92	97.09

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(isopropoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6o)

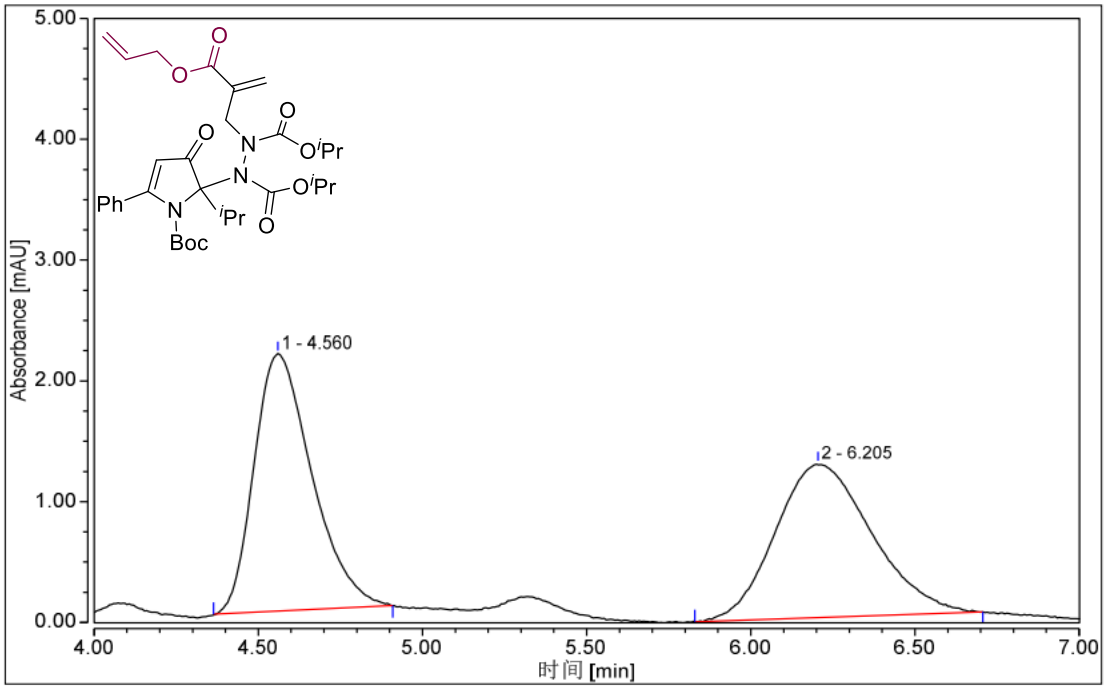


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.853	1.373	3.457	50.53	67.41
2	10.057	1.344	1.671	49.47	32.59

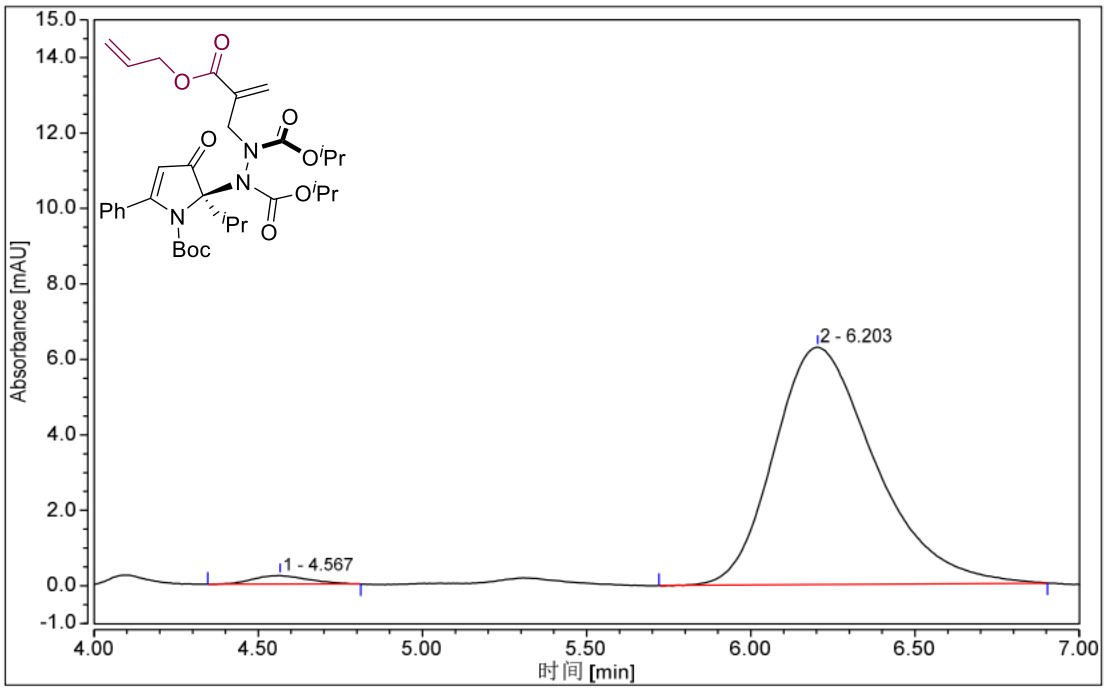


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	7.025	0.157	0.474	4.85	11.54
2	10.262	3.072	3.632	95.15	88.46

diisopropyl (*R*, *R*)-1-(2-((allyloxy)carbonyl)allyl)-2-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (6p)

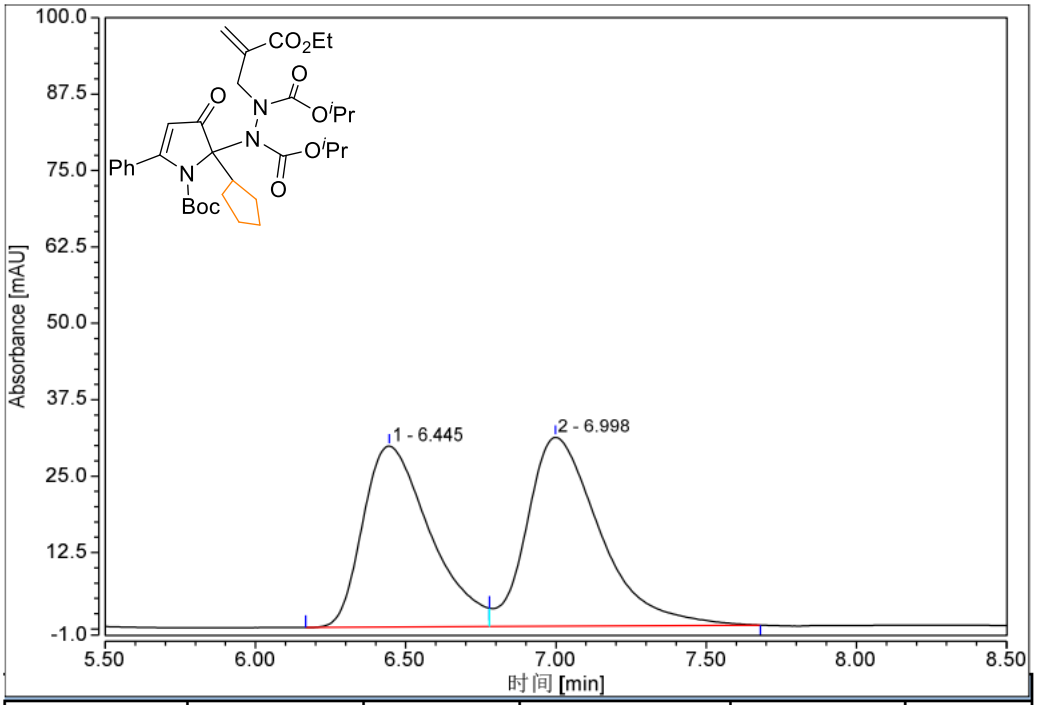


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.560	0.435	2.132	50.23	62.64
2	6.205	0.431	1.271	49.77	37.36

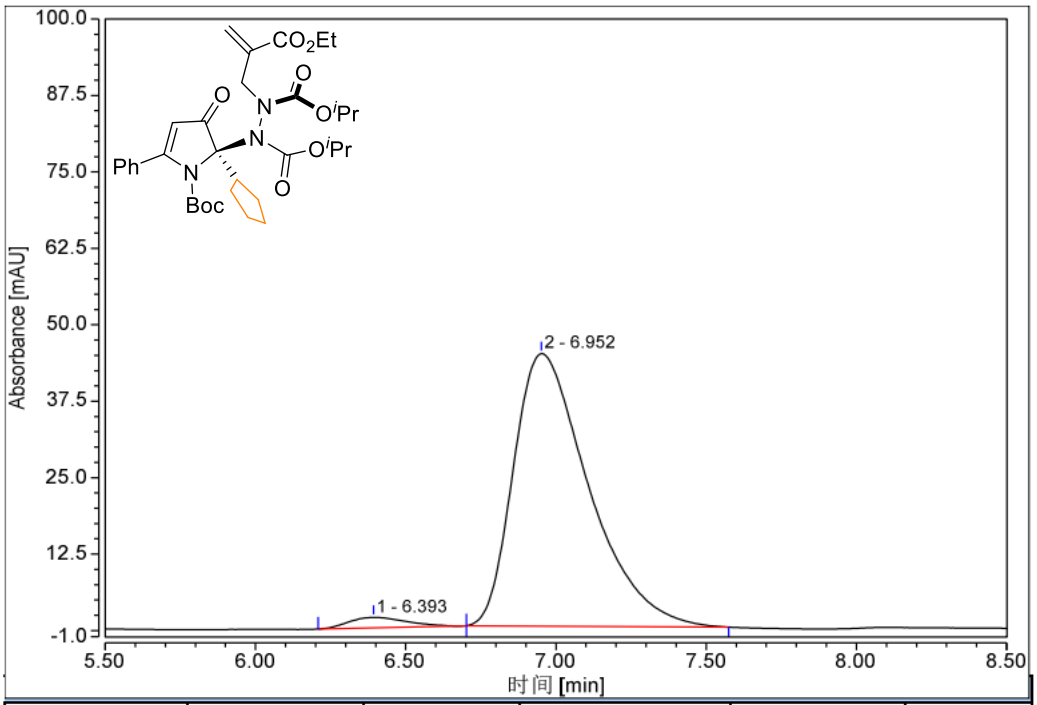


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	4.567	0.043	0.226	1.89	3.48
2	6.203	2.245	6.290	98.11	96.52

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-cyclopentyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6q)

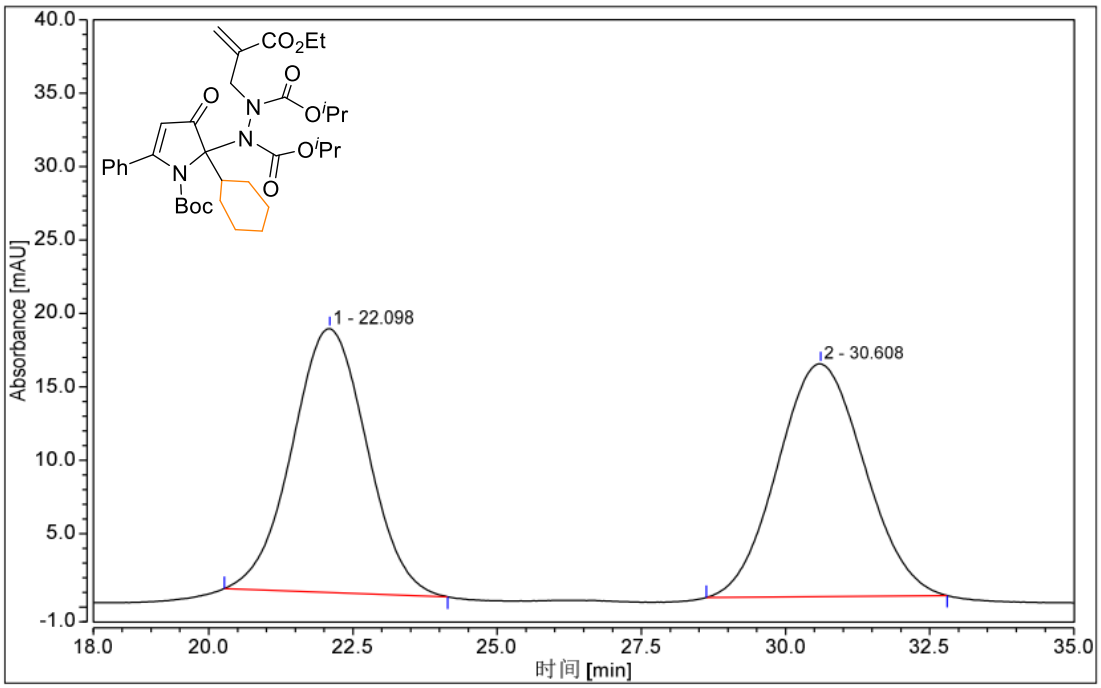


Peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	6.445	7.655	29.58	46.86	48.929
2	6.998	8.679	30.88	53.14	51.071

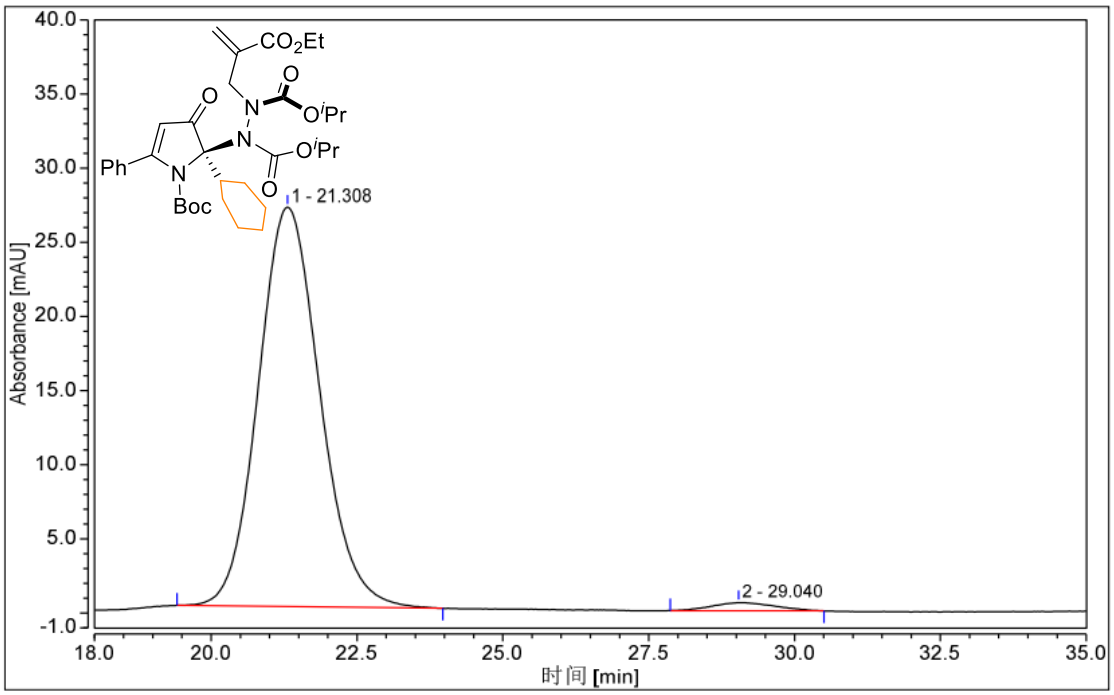


Peak	RT min	Area mAU*min	Height mAU	Area %	Height %
1	6.393	0.370	1.70	2.78	3.680
2	6.952	12.942	44.57	97.22	96.320

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-cyclohexyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6r)

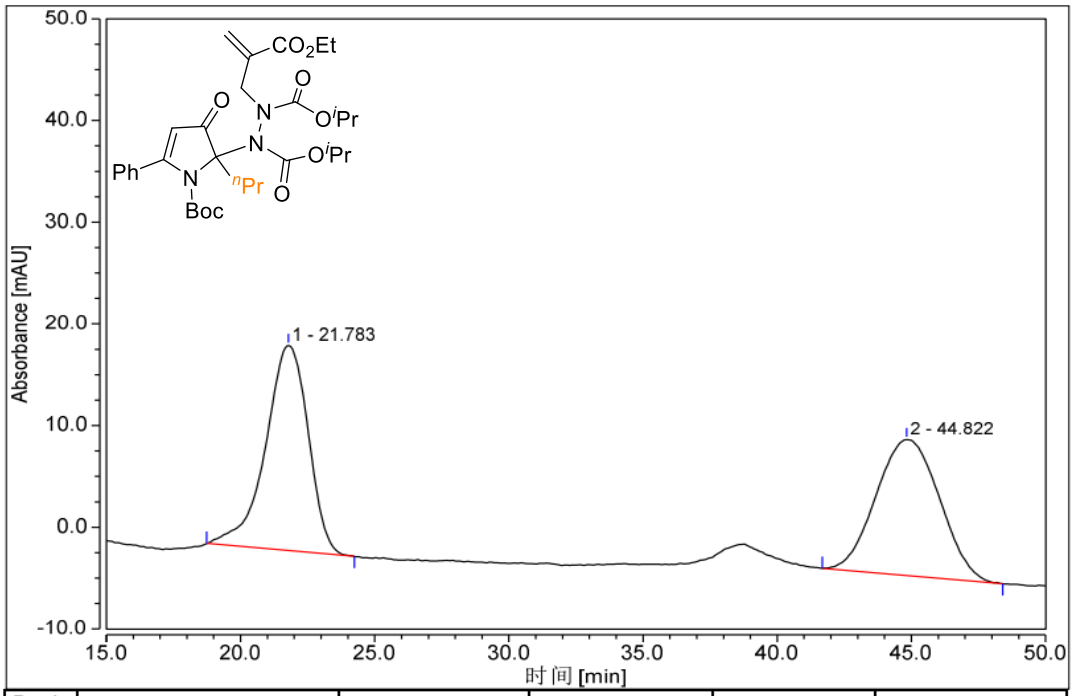


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	22.098	27.052	17.974	49.45	53.15
2	30.608	27.655	15.846	50.55	46.85

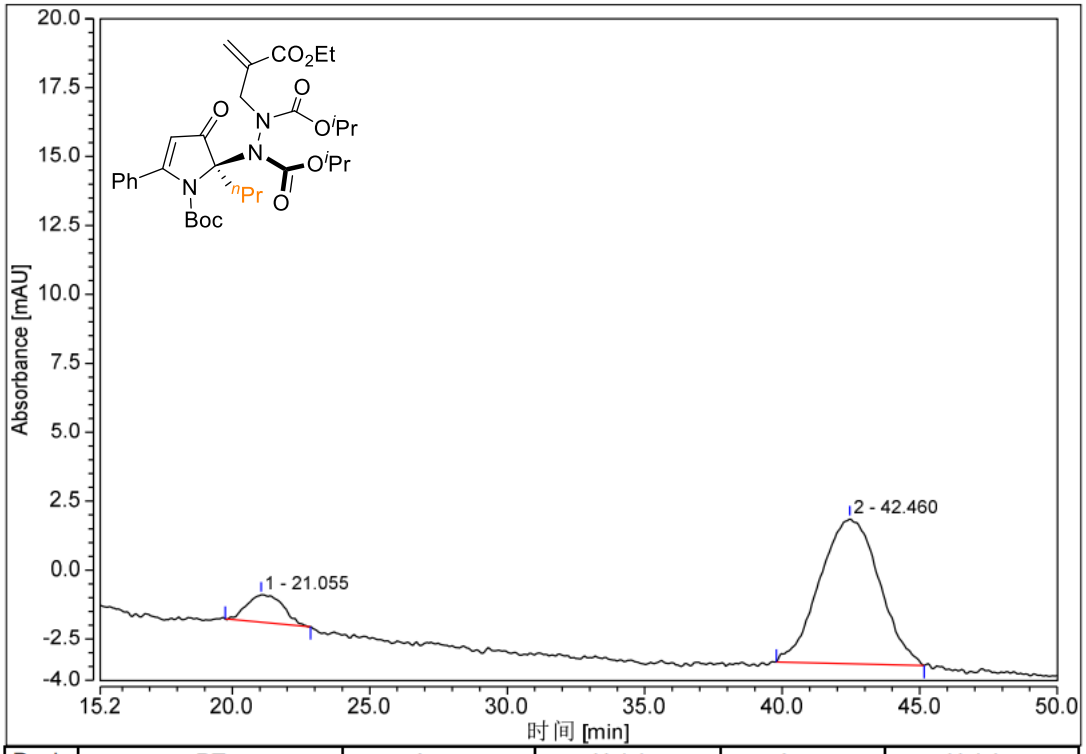


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	21.308	32.997	26.938	97.98	98.01
2	29.040	0.679	0.547	2.02	1.99

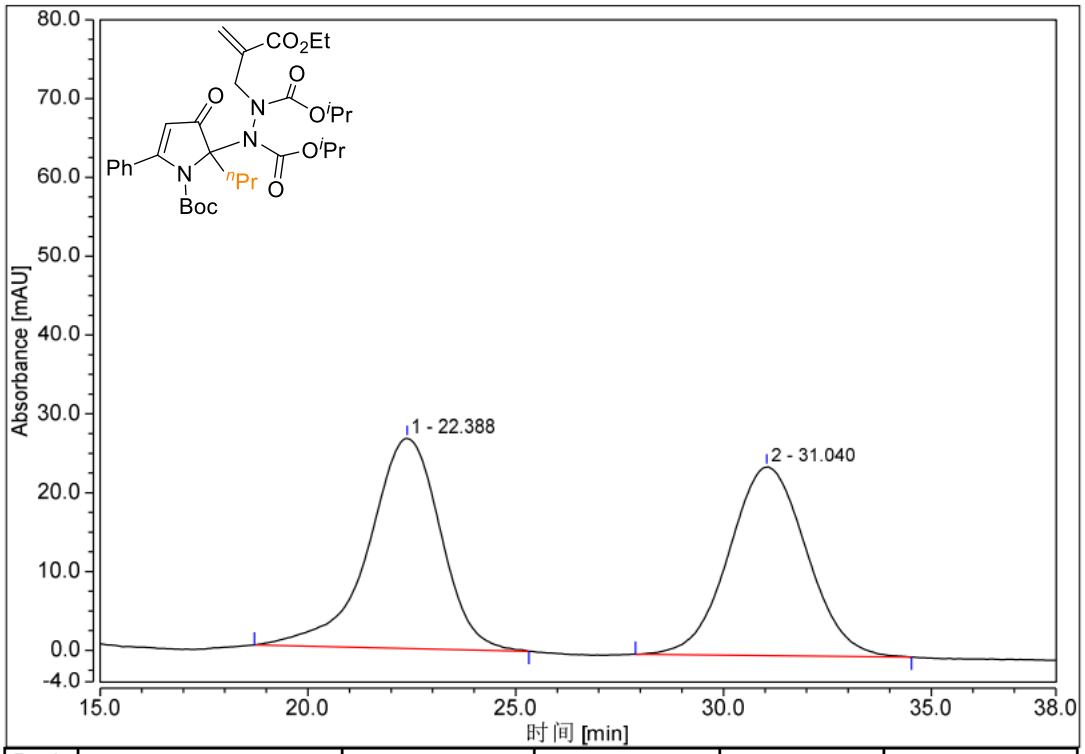
diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-5-phenyl-2-propyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6s)



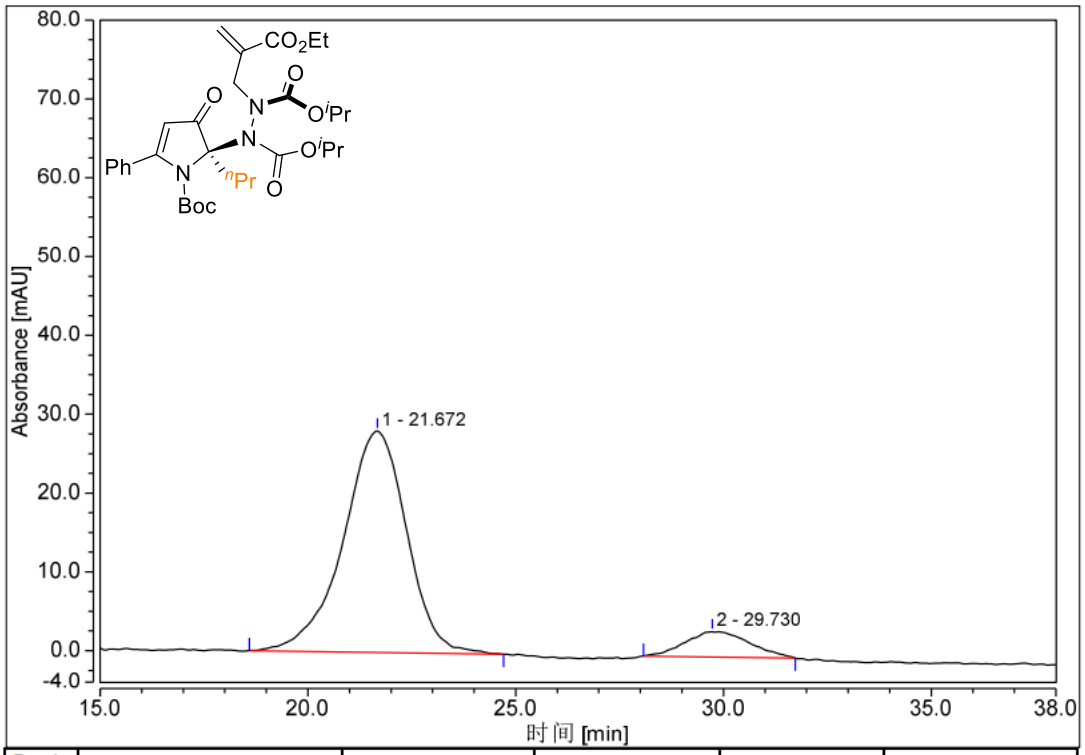
Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	21.783	37.245	20.164	50.37	60.13
2	44.822	36.704	13.372	49.63	39.87



Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	21.055	1.535	0.998	10.44	15.95
2	42.460	13.163	5.262	89.56	84.05

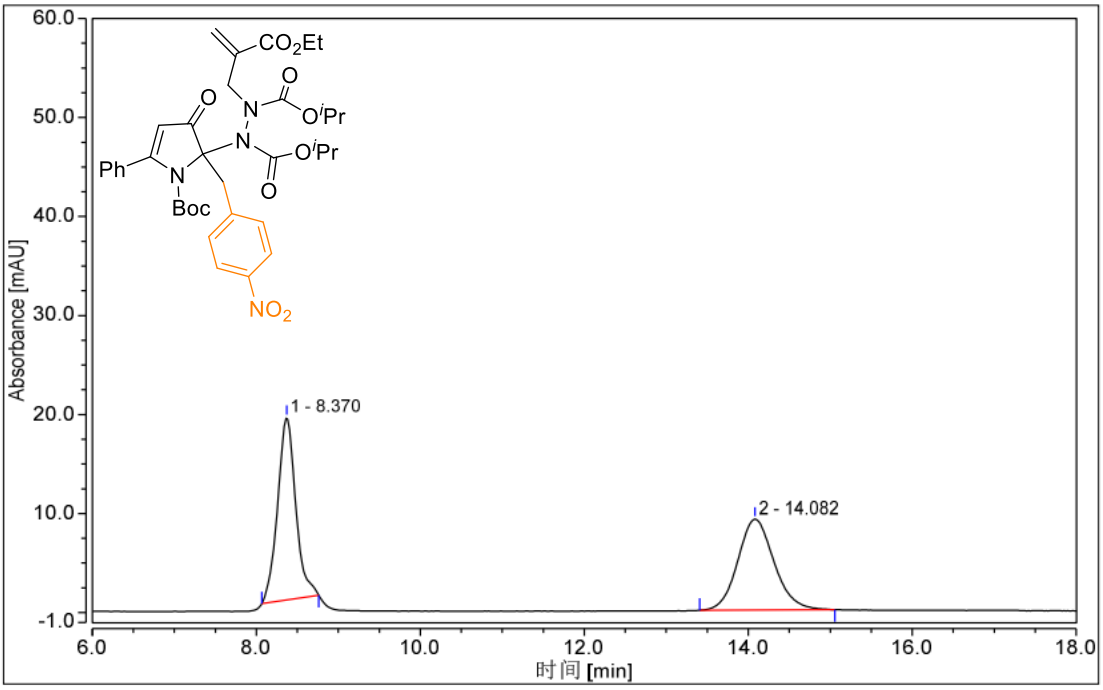


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	22.388	53.400	26.634	50.76	52.67
2	31.040	51.798	23.932	49.24	47.33

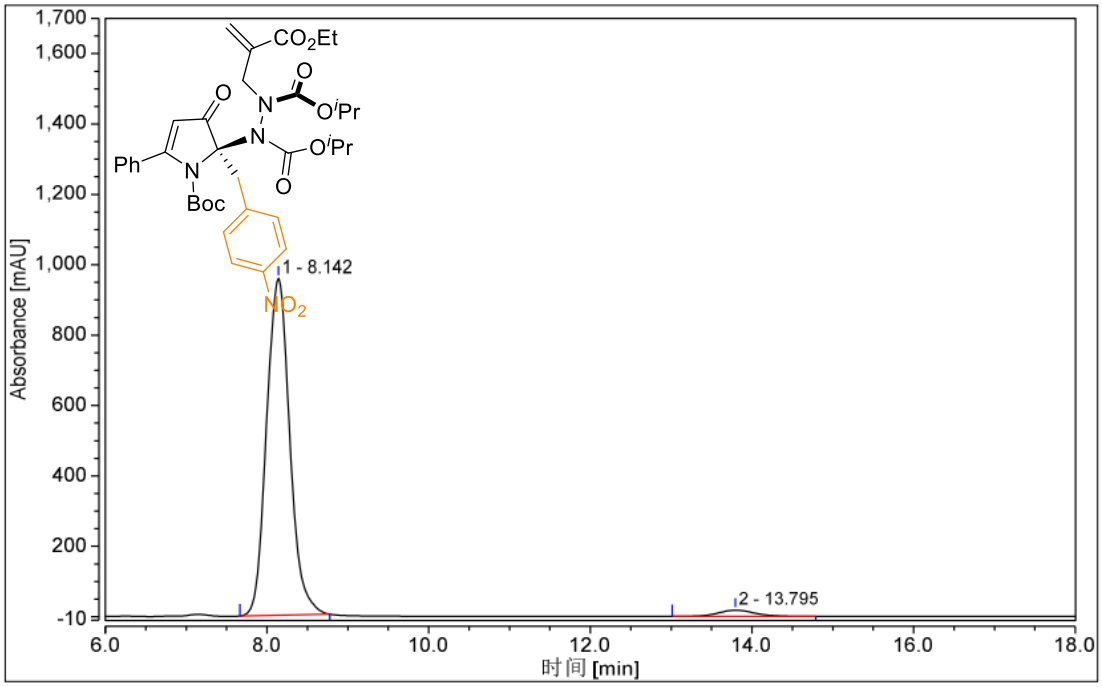


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	21.672	49.748	28.078	89.62	89.82
2	29.730	5.764	3.182	10.38	10.18

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-2-(4-nitrobenzyl)-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6t)

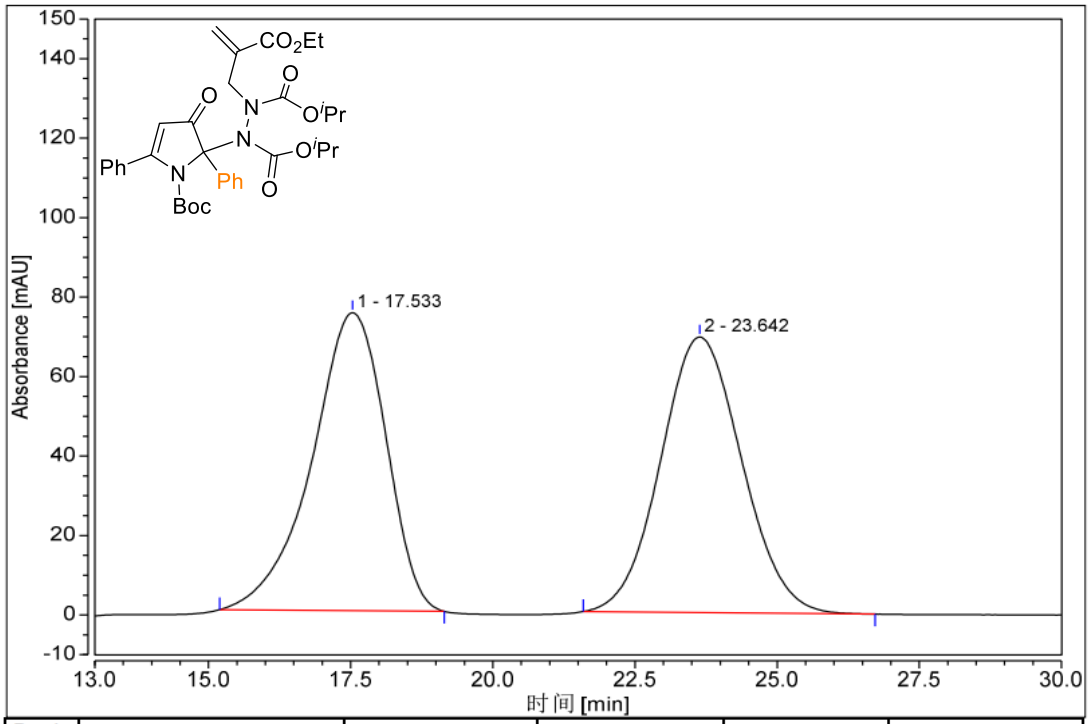


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.370	4.730	18.435	50.23	66.78
2	14.082	4.688	9.170	49.77	33.22

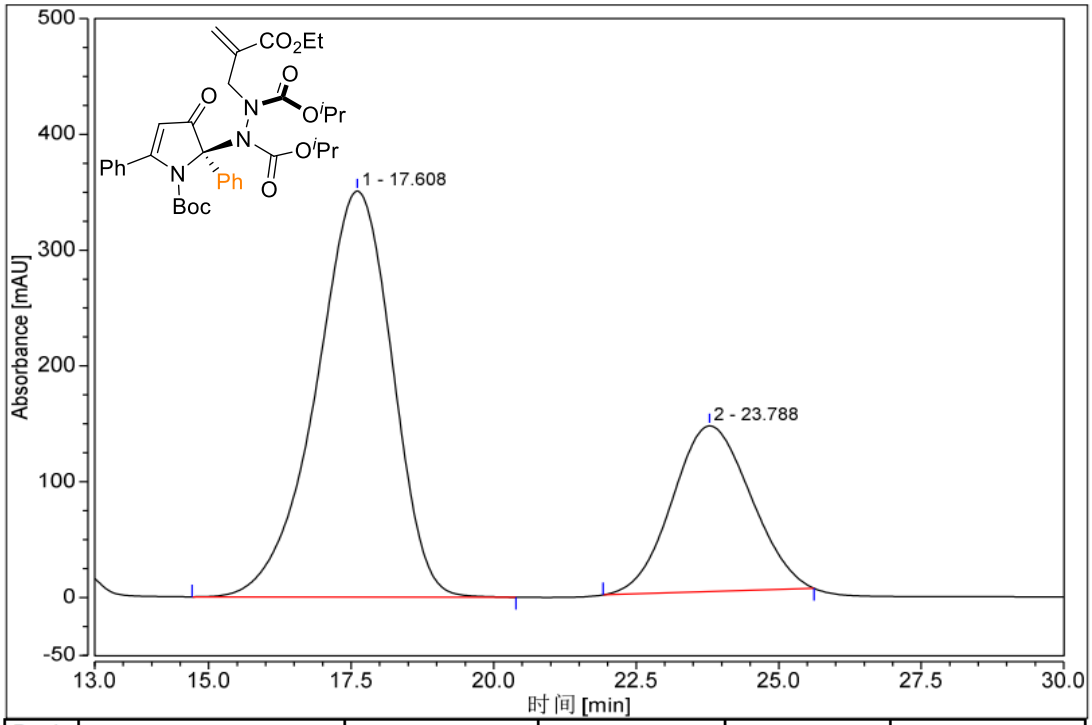


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.142	317.782	957.775	97.13	98.18
2	13.795	9.395	17.794	2.87	1.82

diisopropyl (*R*, *R*)-1-(1-(tert-butoxycarbonyl)-3-oxo-2,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (6u)

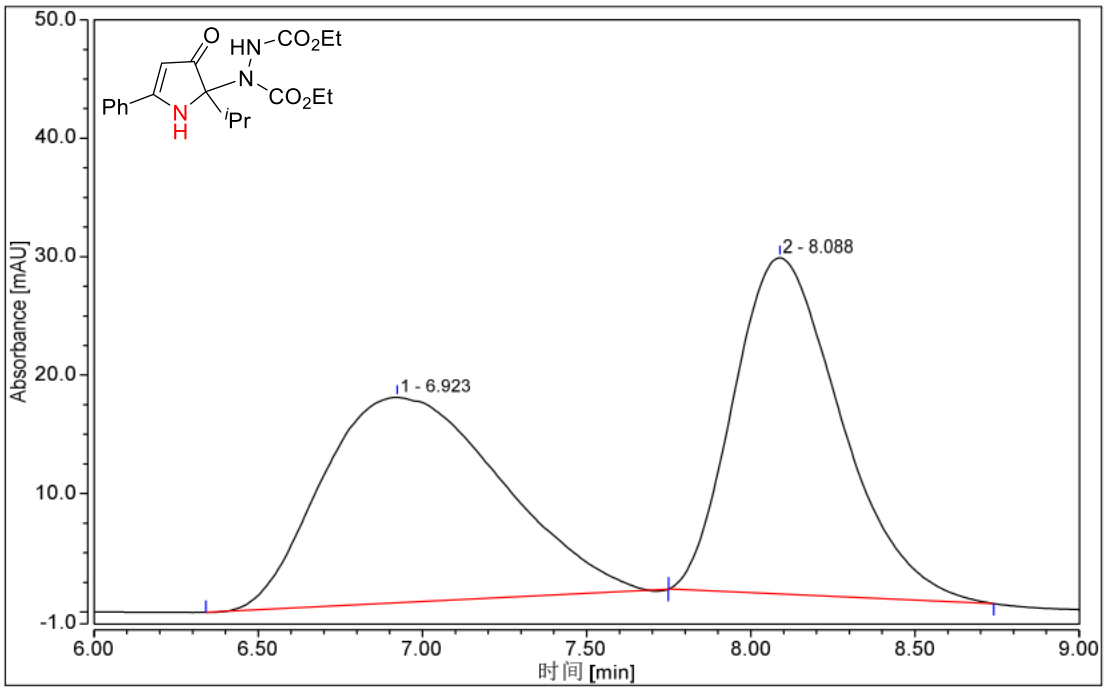


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	17.533	112.815	74.985	49.57	51.94
2	23.642	114.766	69.373	50.43	48.06

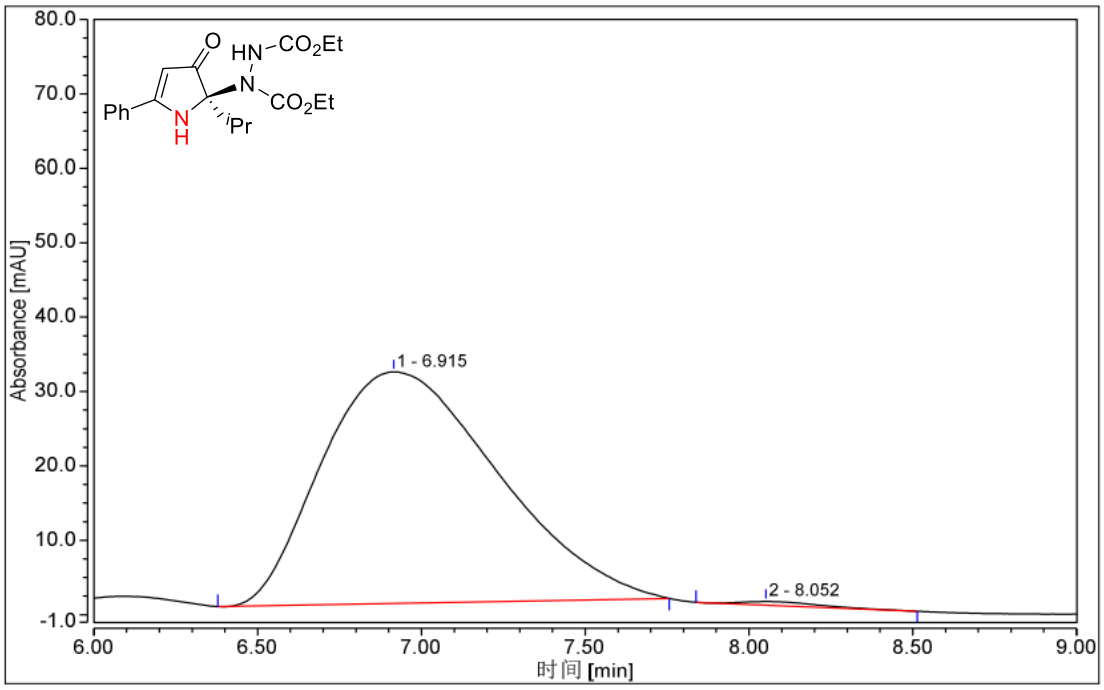


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	17.608	541.174	350.431	70.36	71.02
2	23.788	228.001	142.990	29.64	28.98

diethyl (*R*)-1-(2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (9)

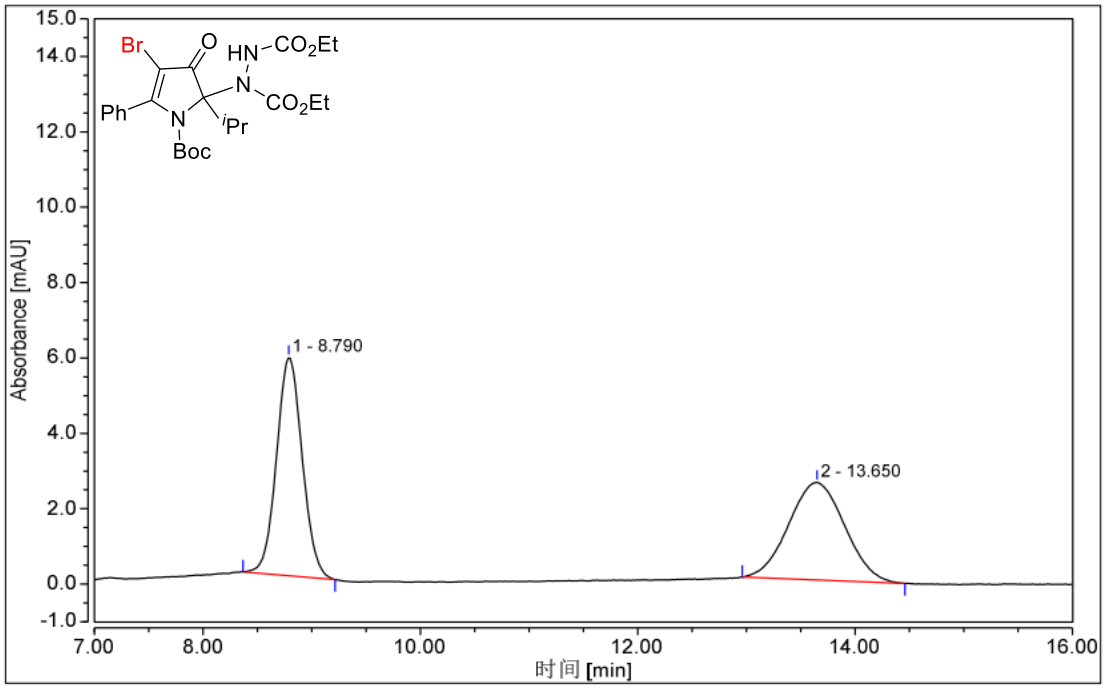


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.923	10.958	17.352	50.48	37.93
2	8.088	10.747	28.392	49.52	62.07

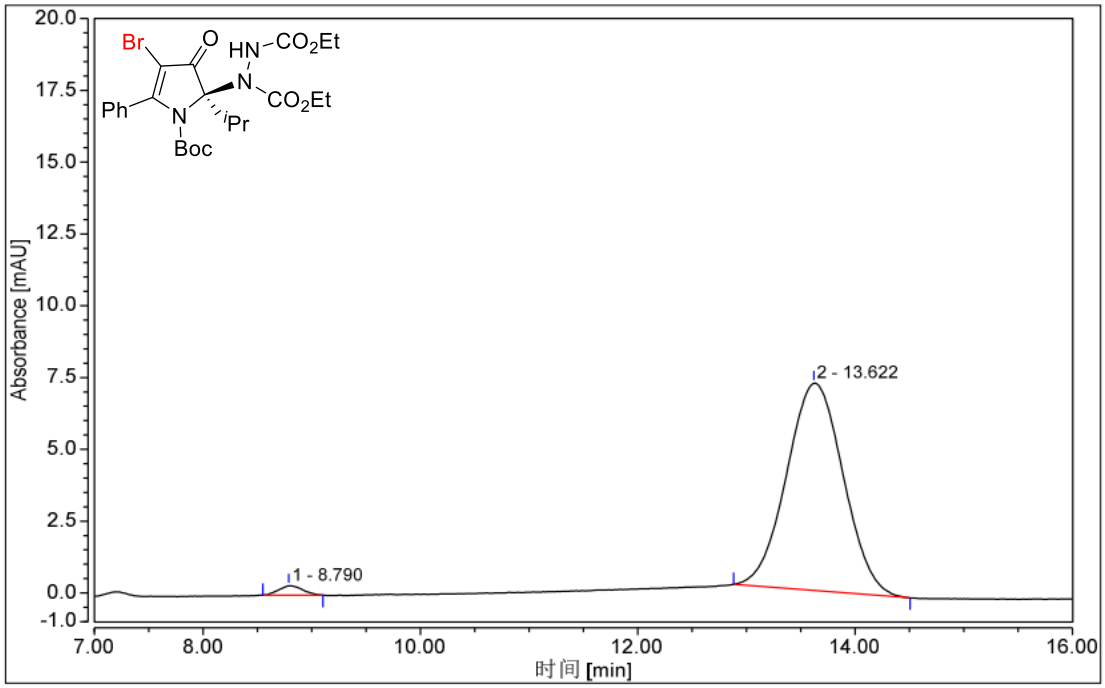


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	6.915	19.398	31.113	99.29	98.44
2	8.052	0.139	0.492	0.71	1.56

diethyl (*R*)-1-(4-bromo-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (10)

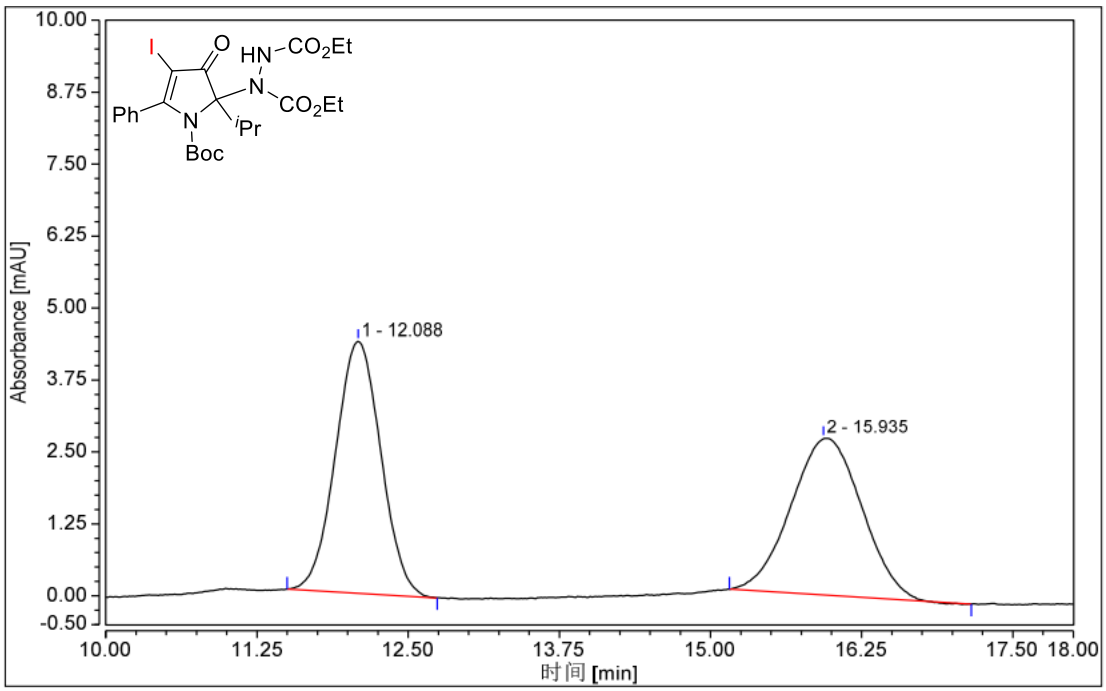


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.790	1.587	5.791	50.66	69.10
2	13.650	1.545	2.589	49.34	30.90

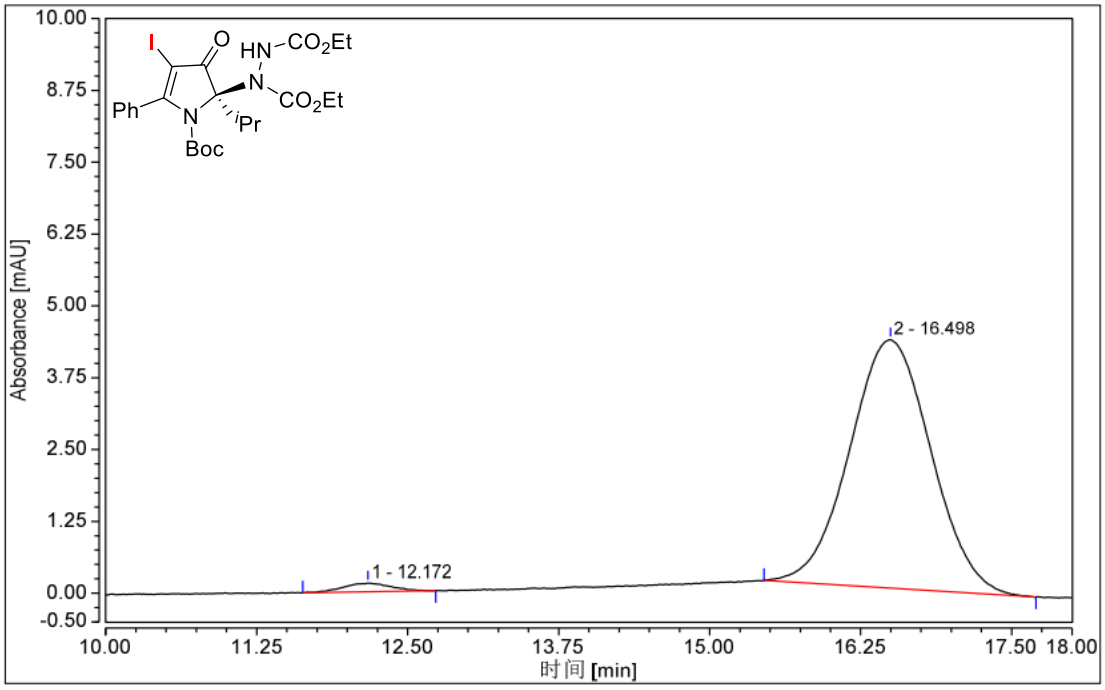


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	8.790	0.086	0.330	1.93	4.37
2	13.622	4.363	7.222	98.07	95.63

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-4-iodo-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (11)

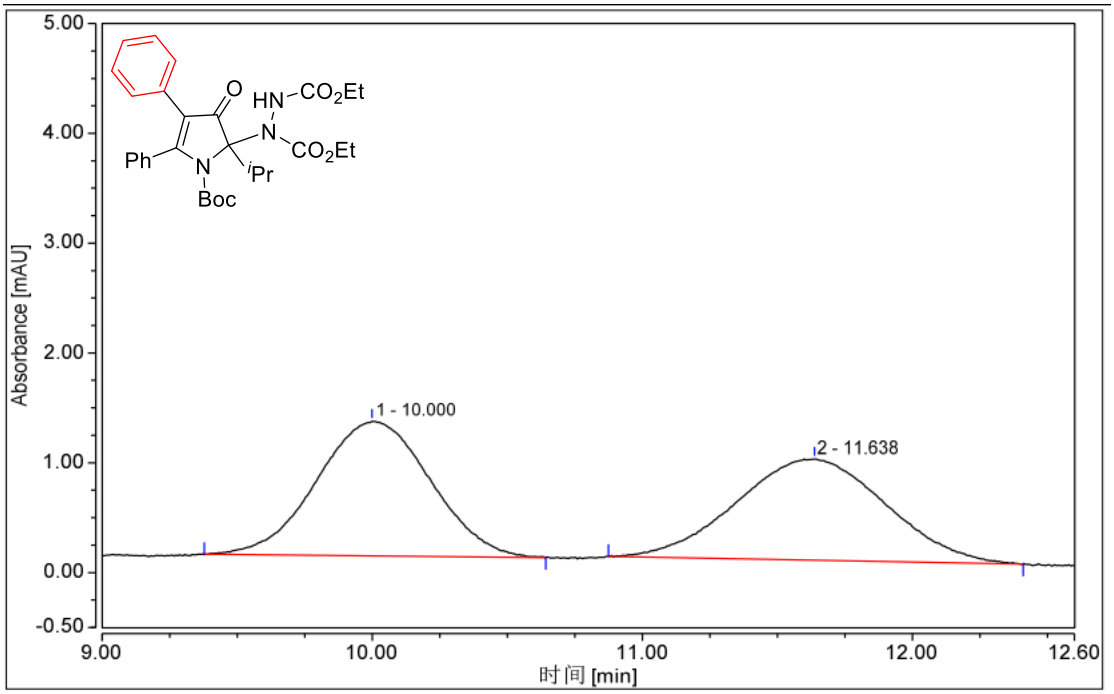


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	12.088	1.902	4.377	50.67	61.66
2	15.935	1.851	2.721	49.33	38.34

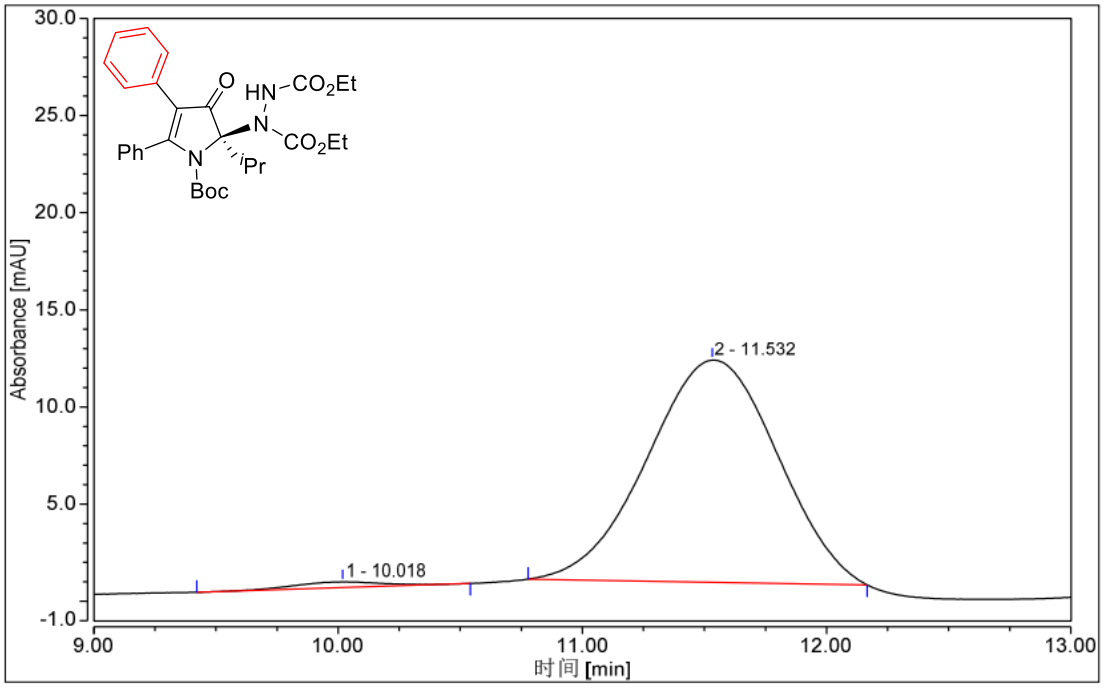


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	12.172	0.068	0.155	1.96	3.46
2	16.498	3.381	4.323	98.04	96.54

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-4,5-diphenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (12)

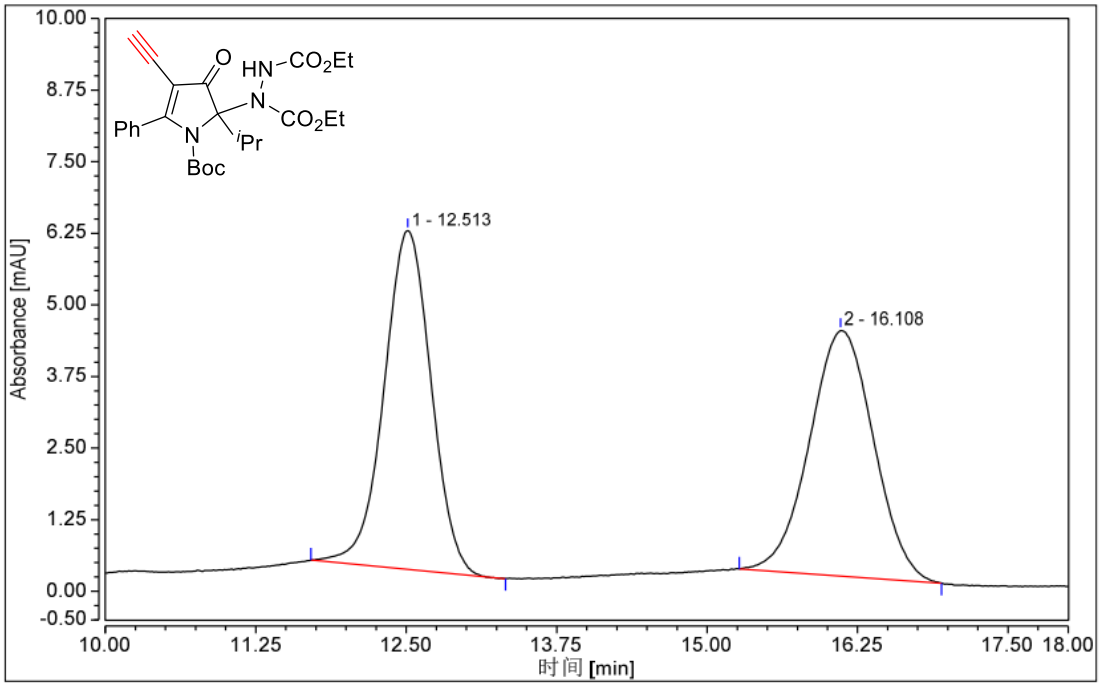


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	10.000	0.598	1.228	50.51	57.09
2	11.638	0.586	0.923	49.49	42.91

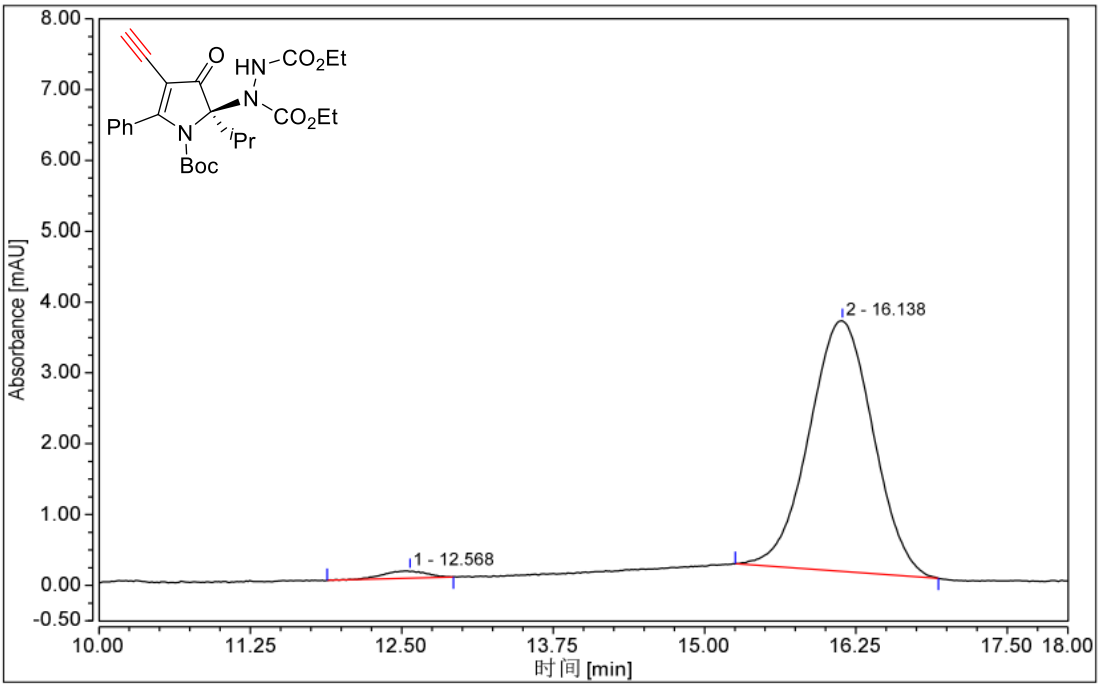


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	10.018	0.121	0.297	1.68	2.53
2	11.532	7.052	11.448	98.32	97.47

diethyl (*R*)-1-(1-(tert-butoxycarbonyl)-4-ethynyl-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)hydrazine-1,2-dicarboxylate (13)

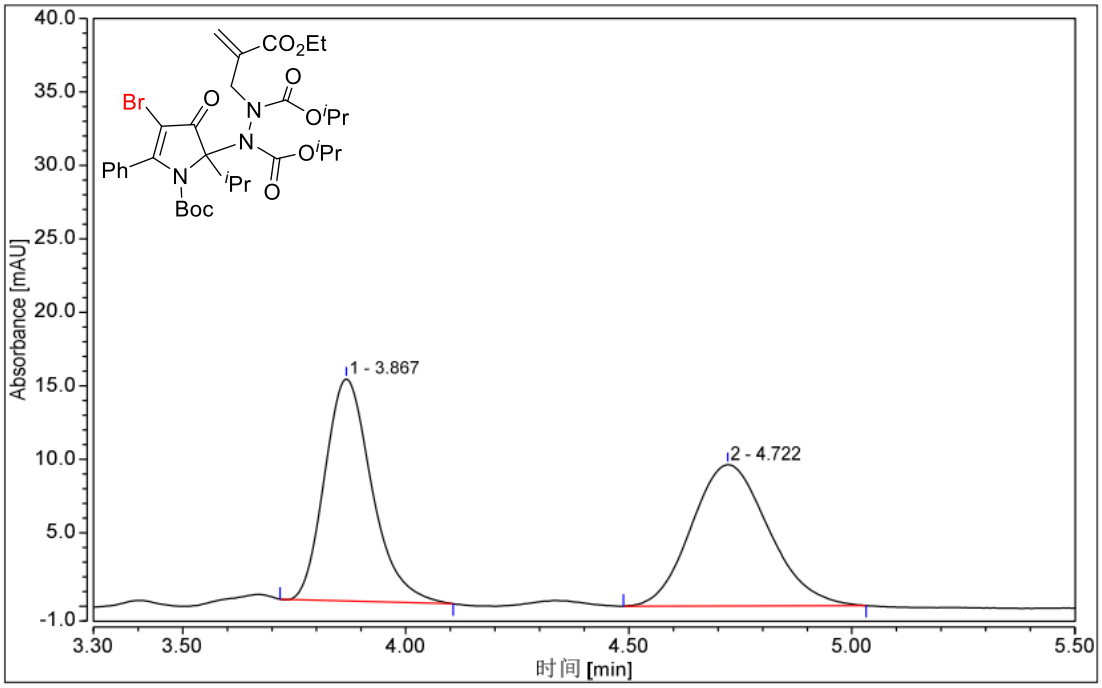


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	12.513	2.681	5.918	50.29	57.95
2	16.108	2.649	4.294	49.71	42.05

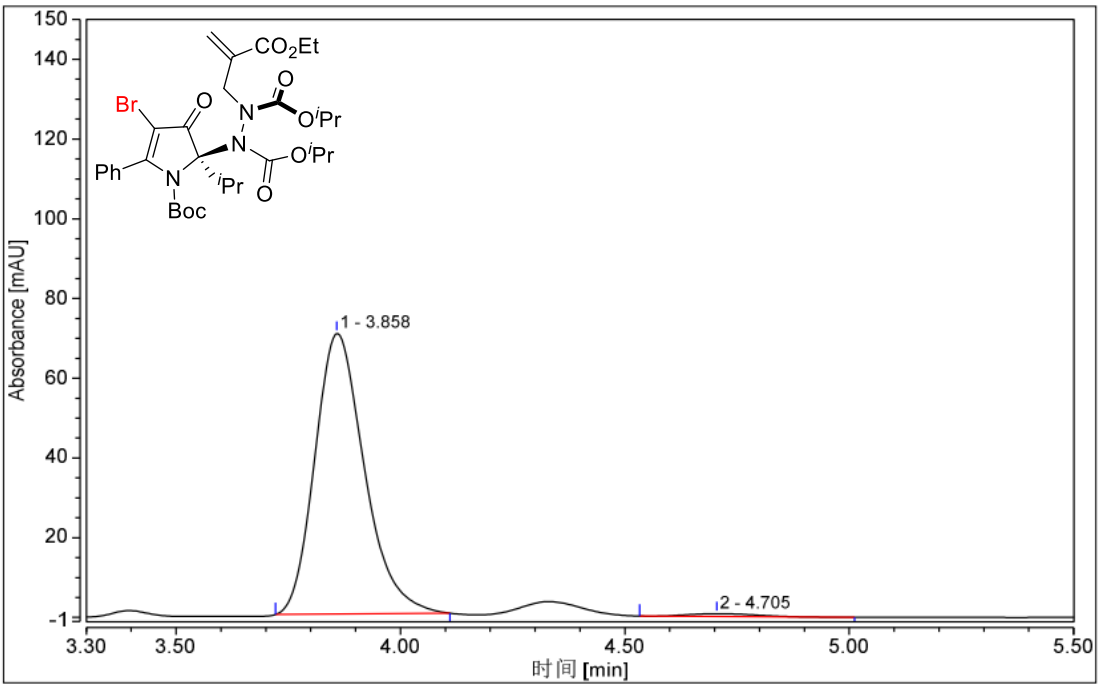


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	12.568	0.042	0.104	1.88	2.86
2	16.138	2.169	3.539	98.12	97.14

diisopropyl (*R*)-1-(4-bromo-1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-2-(2-(ethoxycarbonyl)allyl)hydrazine-1,2-dicarboxylate (14)

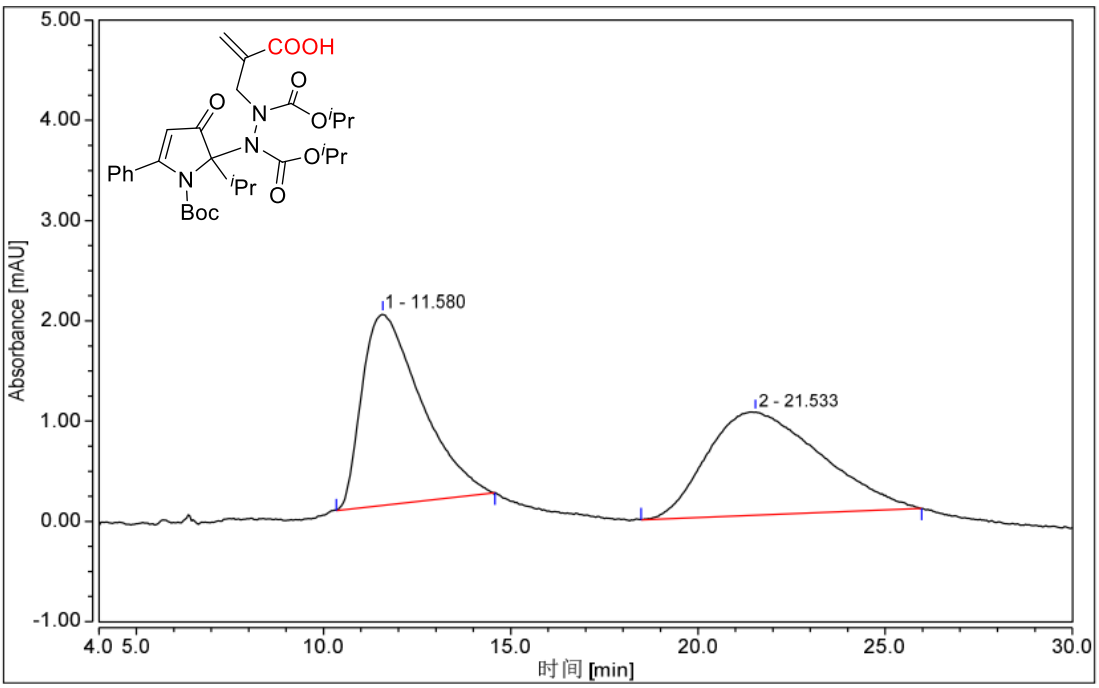


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.867	1.851	15.110	49.00	61.13
2	4.722	1.926	9.608	51.00	38.87

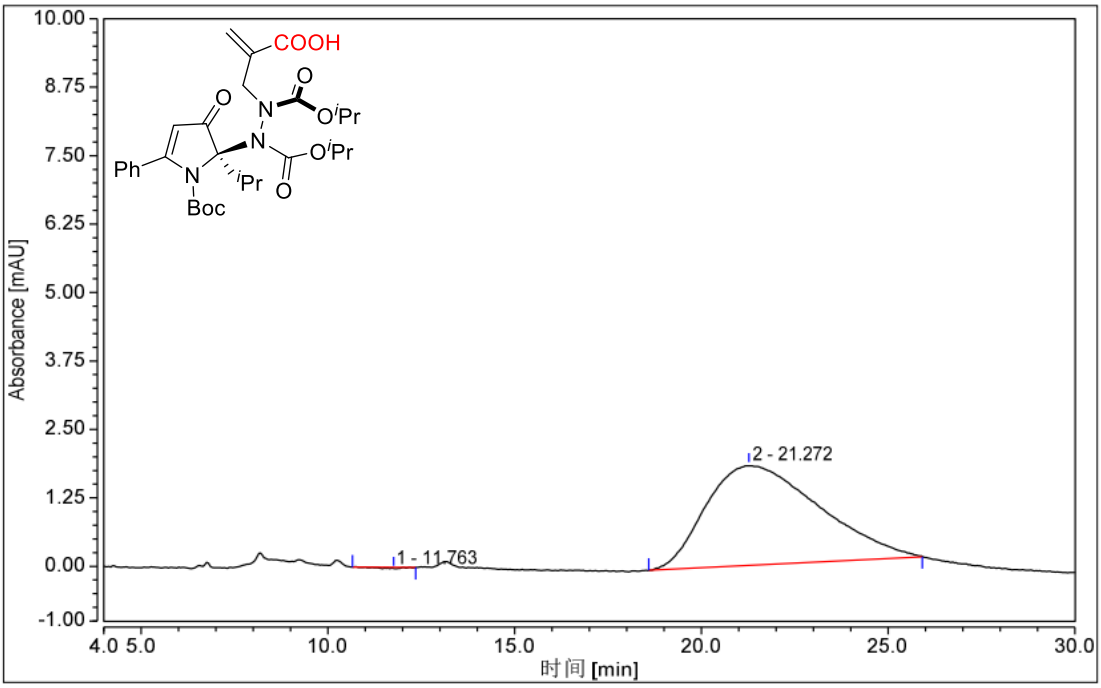


Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	3.858	9.001	70.413	98.60	98.98
2	4.705	0.128	0.727	1.40	1.02

(*R*, *R*)-2-((2-(1-(tert-butoxycarbonyl)-2-isopropyl-3-oxo-5-phenyl-2,3-dihydro-1H-pyrrol-2-yl)-1,2-bis(isopropoxycarbonyl)hydrazineyl)methyl)acrylic acid (15)



Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	11.580	3.502	1.918	49.14	64.99
2	21.533	3.624	1.033	50.86	35.01



Peak	RT min	Aera mAU*min	Height mAU	Area %	Height %
1	11.763	0.017	0.028	0.26	1.52
2	21.272	6.391	1.831	99.74	98.48

12. Computational Methods

Geometry optimizations and frequency calculations were performed at M06-2X/6-31G(d) level. IRC calculations were performed to verify the nature of transition states located, except for the N-N rotational transition state of 3c, whose imaginary frequency was too low for the calculation to succeed. Instead, manual inspections were employed to verify its nature. Higher level single-point energy calculations were performed at M06-2X/6-311+G(2d,p) level. A slightly larger basis set, 6-311++G(2d,p) was used for TDDFT simulations of CD spectra to ensure the accuracy of the result. Solvent effect was incorporated using the SMD[5] implicit reaction field model. Dichloromethane was used as the solvent for the reaction profile of N-alkylation of **3c**, and cyclohexane for the barrier of rotation around the N-N axis of **3c**. Relative free energies and enthalpies were computed at the temperature of 298 K and reported in kcal/mol unless otherwise stated. An entropy correction term, of the magnitude of 7.06 kJ/mol at 298 K, was included to account for the change of state from gaseous to standard state of 1 M.[6] For the Quasi-harmonic approximation treatment of low frequencies, the python program GoodVibes[7] was employed, with a frequency cutoff of 100 cm^{-1} and the option of a linked job. Graphics of optimized structures were rendered using the CYLview program.[8] All DFT calculations were carried out with the Gaussian 16 suite of programs.[9]

Barrier of Rotation around the N–N axis of 3c

The substrate **3c** also has an N–N axis, whose rotational barrier was calculated to be 22.4 kcal/mol. An estimation of rotational rate constant using the Eyring equation gave a value of 2.36×10^{-4} $M\cdot S^{-1}$, suggesting a slow but measurable interconversion between the two configurations **3c-1** and **3c-2**. Given this equilibrium, it seems that the reaction diastereoselectivity is governed by steps of N-arylation reaction.

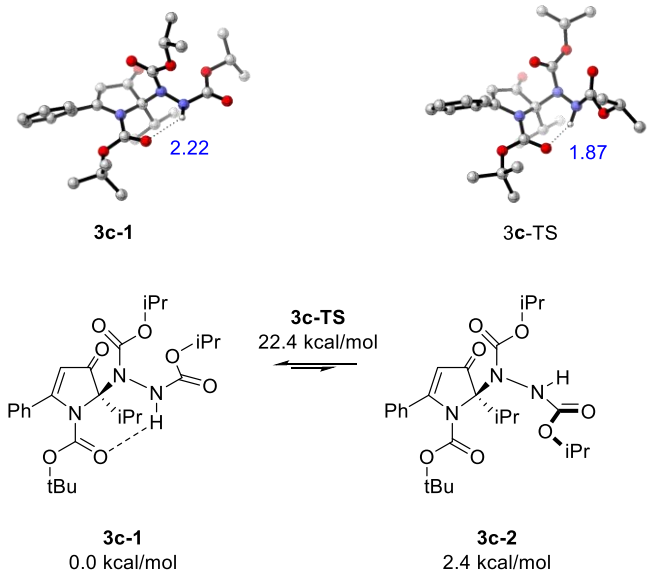


Figure S1. Rotation barrier of **3c**

Diastereoselectivity of *N*-alkylation of 3c through Morita-Baylis-Hillman Reaction

The diastereoselectivity-determining transition states, **TS4**, contain many low-lying frequencies (<100 cm^{-1}), which may introduce errors to the calculated free energy values. One way to treat such frequencies is to use quasi-harmonic approximation to correct the values. As shown in **Table S2**, after correction, the energy difference for **3c** reduced to 3.0 kcal/mol while that of **3k** to 1.4 kcal/mol. Another less commonly used method is to ignore the entropic contribution entirely and compare the difference in enthalpy instead. Again, this treatment led to reduced energy differences, 2.0 kcal/mol for **3c** and 0.8 kcal/mol for **3k**, which seems to agree with the experimental result better.

Table S2. Diastereoselectivity-determining transition states **TS4**

Entry	H_{corr} [a]	G_{corr} [a]	E_L [a]	E_H [b]	H_H [b]	G_H [b]	QH-G_H [b,c]
RR-**TS4**	1.142197	0.967944	-2891.180524	-2892.085129	-2890.942932	-2891.117185	-2891.099924
RS-**TS4**	1.142539	0.971931	-2891.178554	-2892.082296	-2890.939757	-2891.110365	-2891.095097
3k-*RR*-**TS4**	1.082237	0.912270	-2812.596138	-2813.478135	-2812.395898	-2812.565865	-2812.548528
3k-*RS*-**TS4**	1.082089	0.914441	-2812.593862	-2813.476777	-2812.394688	-2812.562336	-2812.546319
$\Delta_{RS\text{-}RR}$/kcal·mol^{-1}					2.0	4.3	3.0
$\Delta_{3k,\ RS\text{-}RR}$/kcal·mol^{-1}					0.8	2.2	1.4

a) at 6-31G(d) level. b) at 6-311+G(2d,p) level. c) Quasi-harmonic approximation corrected

CD Spectra

To further validate the assignment of configuration of the N-N axis, we turned to simulate CD spectra of conformers of **6a** and compare them to experimentally obtained one (**Figure S2**). Only two of the lowest-energy conformers, namely *RR*-**6a** and *RS*-**6a**, were chosen for comparison. Result shown in **Figure S3** is consistent with the assignment of **6a** as *RR*-**6a**.

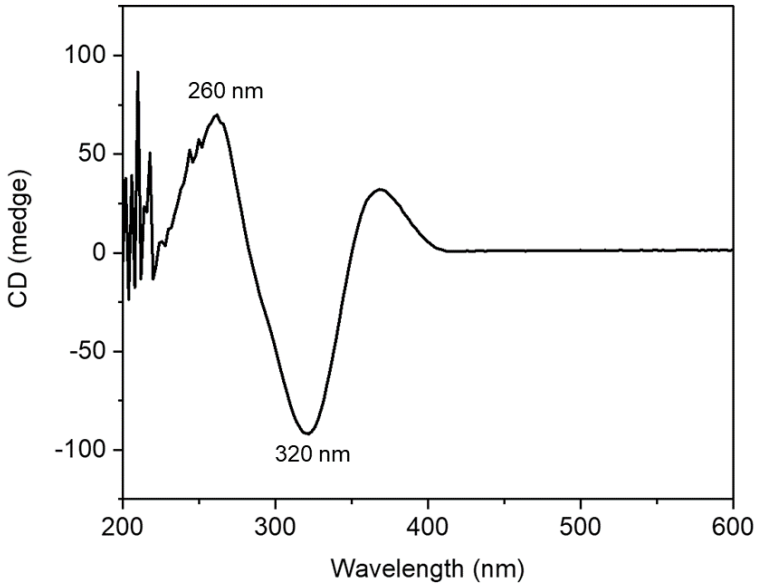


Figure S2. Experimental CD spectrum

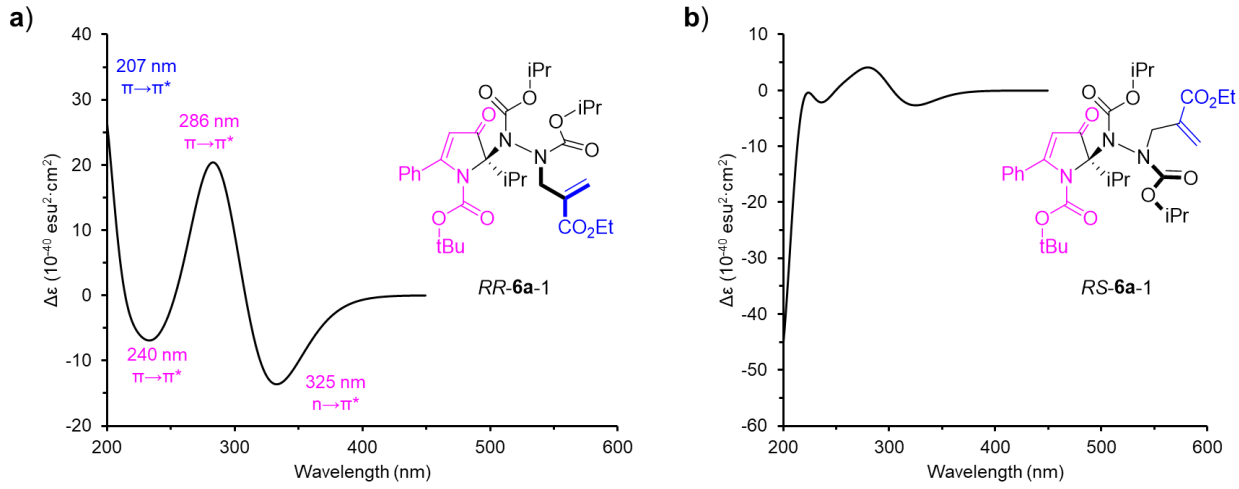


Figure S3. Computationally simulated CD spectra of a) *RR*-**6a** and b) *RS*-**6a**. The colors of assignment of peaks are based on the location of the corresponding molecular orbitals of the electronic transitions. Peak positions of *RR*-**6a** were marked to be compared with the experimental spectrum.

Atomic Coordinates and Associated Thermodynamics Data

N-alkylation of 3c to Synthesize *RR*-6a

3c

C	2.14504400	0.77928000	1.09357300
C	1.68621800	1.44421500	2.18047100
H	2.22809800	2.20999700	2.71822500
C	0.27112800	1.15841600	2.34339200
O	-0.53481700	1.63936300	3.11086000
C	-0.08789800	0.04117300	1.32197000
N	1.16084200	-0.03759600	0.52746700
C	1.32994600	-1.08538000	-0.36886700
O	0.38308000	-1.59269300	-0.94169700
O	2.59762200	-1.45015000	-0.46872600
C	3.04422700	-2.41211300	-1.48303600
C	2.70132900	-1.89441200	-2.87385800
H	3.12533300	-0.89540600	-3.01992800
H	1.62210900	-1.85588200	-3.03390500
H	3.13936500	-2.56486500	-3.61969300
C	4.55153500	-2.43162500	-1.26867700
H	4.97172900	-1.43246300	-1.42338500
H	5.01607900	-3.12351800	-1.97699500
H	4.78932000	-2.75811000	-0.25165900
C	2.43355000	-3.77812600	-1.19686900
H	1.35627100	-3.77800000	-1.36992100
H	2.63025800	-4.06877000	-0.15967800
H	2.89616800	-4.52052300	-1.85469400
C	3.45712800	0.99801700	0.45434800
C	5.91938800	1.54952500	-0.73333000
C	3.52514000	1.29790000	-0.91180700

C	4.62144800	0.98549700	1.22328400
C	5.85193600	1.25301200	0.62565000
C	4.75219000	1.57858000	-1.50011600
H	2.61243800	1.32521000	-1.50220700
H	4.56222200	0.75049900	2.28212800
H	6.75689800	1.23055400	1.22483700
H	4.80024500	1.82086800	-2.55755300
H	6.87809000	1.76228700	-1.19652800
C	-0.35247900	-1.28467800	2.08448000
H	-0.59413800	-2.02487800	1.31634400
C	-1.54121600	-1.16827100	3.04270600
H	-1.25961900	-0.62430900	3.94832500
H	-1.85876800	-2.17400800	3.33565500
H	-2.39352500	-0.65037800	2.59658100
C	0.88620900	-1.77157600	2.84205400
H	1.17527100	-1.07542300	3.63653800
H	1.75028300	-1.92753700	2.18784800
H	0.65215900	-2.73091900	3.31355700
N	-1.22822300	0.40478800	0.49568900
C	-1.16759300	1.60554900	-0.19638200
O	-0.35016700	2.46618700	0.05449300
O	-2.10776300	1.67617700	-1.13686700
C	-2.26982300	2.95943500	-1.79515400
H	-1.27097500	3.35090100	-2.00592200
C	-3.02481700	3.89582600	-0.86917300
H	-4.00157800	3.46825400	-0.62072000
H	-3.17836300	4.86107500	-1.36087600
H	-2.46599000	4.06275400	0.05534300
C	-3.01479100	2.66225300	-3.08044000
H	-2.45089000	1.96369300	-3.70473200

H	-3.16545600	3.58878900	-3.64154300
H	-3.99429800	2.22548800	-2.85943900
N	-2.06812200	-0.58485800	0.03738000
C	-3.42366700	-0.40189900	0.20545900
O	-3.93293000	0.39027200	0.96630800
O	-4.07697600	-1.26304700	-0.58387800
C	-5.52084800	-1.27919300	-0.45842600
H	-5.85338100	-0.24239300	-0.35760000
C	-6.03871400	-1.88321900	-1.74809000
H	-7.13211000	-1.90537500	-1.73189400
H	-5.67207400	-2.90816700	-1.86457900
H	-5.71463800	-1.29357600	-2.61019100
C	-5.90980800	-2.07776300	0.77301400
H	-6.99918700	-2.10154800	0.87279700
H	-5.49019700	-1.62619000	1.67585100
H	-5.54563800	-3.10669100	0.68562300
H	-1.74592900	-1.07916900	-0.79078300

Zero-point correction= 0.619904 (Hartree/Particle)

Thermal correction to Energy= 0.657596

Thermal correction to Enthalpy= 0.658540

Thermal correction to Gibbs Free Energy= 0.549382

Sum of electronic and zero-point Energies= -1702.643752

Sum of electronic and thermal Energies= -1702.606059

Sum of electronic and thermal Enthalpies= -1702.605115

Sum of electronic and thermal Free Energies= -1702.714274

E(RM062X/6-311+G(2d,p)) = -1703.79554975

4a-CONF1

C	-2.30554400	-0.47509700	-1.39997200
C	-2.38329400	1.00065700	-1.67740800

H	-3.41303200	1.35759500	-1.65394500
H	-1.93326800	1.23049600	-2.64440400
C	-3.04857200	-1.02619900	-0.22418800
O	-2.98748900	-2.17575300	0.15322800
O	-3.80318900	-0.09440000	0.36572700
C	-4.55376000	-0.52565100	1.51540500
H	-3.85618700	-0.92205400	2.25884600
H	-5.22426500	-1.33508800	1.21214800
C	-5.31112600	0.67518200	2.03262900
H	-4.62057000	1.47391100	2.31694000
H	-5.89436800	0.38982500	2.91252000
H	-5.99653500	1.05827200	1.27141200
O	-1.71962900	1.74906000	-0.64444900
C	-0.38514100	1.80717600	-0.75012400
O	0.25768000	1.34367400	-1.66373300
O	0.06825100	2.46239100	0.30992400
C	1.50482400	2.69764700	0.47198400
C	2.02168400	3.56492700	-0.66964800
H	3.05555800	3.85506700	-0.45826200
H	1.41999400	4.47576700	-0.75300800
H	1.99707600	3.03107100	-1.62096100
C	1.57038900	3.45307700	1.79260800
H	1.16017400	2.84348200	2.60338300
H	0.99950500	4.38442900	1.73034000
H	2.61052100	3.69513500	2.02832600
C	2.24283000	1.36827100	0.57715600
H	1.78944200	0.74633500	1.35580100
H	3.28417500	1.55938500	0.85427900
H	2.22728500	0.82471400	-0.36870700
C	-1.58663900	-1.31320800	-2.14583800

H -1.01850800 -0.95733300 -2.99988100

H -1.55497000 -2.37384300 -1.91424500

Zero-point correction= 0.288917 (Hartree/Particle)

Thermal correction to Energy= 0.306943

Thermal correction to Enthalpy= 0.307887

Thermal correction to Gibbs Free Energy= 0.241084

Sum of electronic and zero-point Energies= -805.531183

Sum of electronic and thermal Energies= -805.513158

Sum of electronic and thermal Enthalpies= -805.512214

Sum of electronic and thermal Free Energies= -805.579016

E(RM062X/6-311+G(2d,p)) = -806.085072131

4a-CONF2

C -1.52237600 -1.73258000 0.01308400

C -0.61377500 -1.61913700 -1.17634000

H -1.16624700 -1.34170000 -2.07555900

H -0.09406900 -2.56516000 -1.34784100

C -2.37301600 -0.55388100 0.36711500

O -3.12482600 -0.50021400 1.31476800

O -2.20763300 0.44411100 -0.50626800

C -2.98567800 1.63180700 -0.27444100

H -2.82036000 1.96484000 0.75387200

H -4.04507500 1.38200900 -0.38716800

C -2.52917000 2.65909800 -1.28343300

H -1.46873500 2.88437900 -1.14036200

H -3.10175700 3.58214800 -1.15678500

H -2.67550500 2.29361700 -2.30380700

O 0.37895400 -0.61727700 -0.90630600

C 0.58741600 0.30233800 -1.85739200

O 0.04511000 0.33121700 -2.93723700

O 1.50383500 1.14340500 -1.39264100

C 2.10758700 2.14019900 -2.28030000

C 1.06942500 3.17280900 -2.70008500

H 1.55794400 3.94393300 -3.30429900

H 0.63630100 3.65505400 -1.81819000

H 0.27252100 2.71807200 -3.29140100

C 3.16870600 2.77646700 -1.39229000

H 3.90463300 2.03028700 -1.07784300

H 2.70924000 3.21338100 -0.50056200

H 3.68507300 3.56790500 -1.94290700

C 2.75471000 1.44895300 -3.47545800

H 3.41841100 0.64821400 -3.13295200

H 3.35530000 2.17895600 -4.02669400

H 2.00819400 1.03034300 -4.15233900

C -1.63006400 -2.83872000 0.74710800

H -1.03501400 -3.72088700 0.52936400

H -2.32436800 -2.88404400 1.58071000

Zero-point correction= 0.288943 (Hartree/Particle)

Thermal correction to Energy= 0.306901

Thermal correction to Enthalpy= 0.307845

Thermal correction to Gibbs Free Energy= 0.241889

Sum of electronic and zero-point Energies= -805.531641

Sum of electronic and thermal Energies= -805.513683

Sum of electronic and thermal Enthalpies= -805.512739

Sum of electronic and thermal Free Energies= -805.578695

E(RM062X/6-311+G(2d,p)) = -806.085269474

DMAP

N -0.08665800 -1.60267000 -1.19259700

C -0.00641700 -1.78221400 0.13238300

H	-0.95432200	-1.83312100	0.66547700
C	1.08759700	-1.53989000	-1.83406300
H	1.03561900	-1.39450400	-2.91177600
C	1.17195600	-1.90281000	0.85002400
H	1.12700500	-2.04252700	1.92303700
C	2.40778400	-1.83636500	0.16637500
C	2.33057500	-1.64536000	-1.23244000
H	3.22233800	-1.58269700	-1.84379400
N	3.59880500	-1.94928500	0.81479400
C	4.84009200	-1.83117400	0.07214300
H	5.67640700	-1.91296500	0.76588900
H	4.91033400	-0.86283700	-0.43828500
H	4.93568200	-2.62434700	-0.67958000
C	3.62365900	-2.15307600	2.25145900
H	4.65870000	-2.25721600	2.57591600
H	3.08318100	-3.06453700	2.53340300
H	3.17550700	-1.30701100	2.78758700

Zero-point correction= 0.164337 (Hartree/Particle)

Thermal correction to Energy= 0.172890

Thermal correction to Enthalpy= 0.173834

Thermal correction to Gibbs Free Energy= 0.129495

Sum of electronic and zero-point Energies= -381.933881

Sum of electronic and thermal Energies= -381.925328

Sum of electronic and thermal Enthalpies= -381.924384

Sum of electronic and thermal Free Energies= -381.968722

E(RM062X/6-311+G(2d,p)) = -382.213973036

INT1-CONF2

C	-2.21179900	-1.46591000	-0.87621800
C	-2.12141900	-0.46940400	-1.95386800

H	-2.89071600	0.29869700	-1.87665800
H	-2.12691700	-0.90362300	-2.95994000
C	-2.90733600	-1.23274300	0.32267600
O	-2.79549100	-1.86489600	1.39115100
O	-3.83318000	-0.21571600	0.24079100
C	-4.31162700	0.27860200	1.48164100
H	-3.46541200	0.54994700	2.12461300
H	-4.88363400	-0.49650600	2.00421600
C	-5.17413400	1.48729600	1.18193600
H	-4.58735900	2.25573100	0.66978400
H	-5.57211100	1.91136100	2.10892500
H	-6.01555900	1.21055600	0.53917300
O	-0.79782900	0.21915500	-1.97442400
C	-0.60356500	1.11912400	-1.02184100
O	-1.46006600	1.61658500	-0.32467500
O	0.70883300	1.39156500	-0.97532600
C	1.19134500	2.52601600	-0.19859200
C	0.87762500	2.35625800	1.28459100
H	1.42695800	3.11277900	1.85498300
H	1.20280800	1.36677900	1.62249300
H	-0.18828600	2.46392600	1.48645000
C	2.69774500	2.47089000	-0.42361200
H	2.92839800	2.51355200	-1.49271200
H	3.10806400	1.54191100	-0.01210200
H	3.18190200	3.31649700	0.07385500
C	0.60813200	3.81599800	-0.76520000
H	0.83764700	3.89750900	-1.83272000
H	1.05068300	4.67473000	-0.25065800
H	-0.47490000	3.84995000	-0.62950200
C	-1.24261000	-2.57856800	-0.89103400

H	-1.08546400	-3.00317900	-1.88862000
H	-1.53211600	-3.37494000	-0.20156800
N	0.15528400	-2.16699100	-0.44423800
C	0.32218200	-1.75190600	0.83055800
H	-0.57187300	-1.79703600	1.44851400
C	1.18953900	-2.11879200	-1.30201100
H	0.98533800	-2.44777400	-2.31480600
C	1.53302700	-1.30381600	1.28821300
H	1.61034100	-0.99619500	2.32287700
C	2.64684200	-1.23130400	0.40646400
C	2.42932000	-1.66942500	-0.92572100
H	3.21773700	-1.64959500	-1.66605300
N	3.84126700	-0.76090300	0.81169700
C	4.94660400	-0.67237700	-0.13233100
H	5.80316500	-0.22671000	0.37068200
H	4.68112100	-0.04312500	-0.98953800
H	5.23229700	-1.66460900	-0.49894300
C	4.02080100	-0.30663200	2.18375700
H	5.05031400	0.02480900	2.31113800
H	3.82640400	-1.11629600	2.89512600
H	3.35312800	0.53271200	2.41220300

Zero-point correction= 0.456991 (Hartree/Particle)

Thermal correction to Energy= 0.483888

Thermal correction to Enthalpy= 0.484833

Thermal correction to Gibbs Free Energy= 0.399283

Sum of electronic and zero-point Energies= -1187.463605

Sum of electronic and thermal Energies= -1187.436708

Sum of electronic and thermal Enthalpies= -1187.435764

Sum of electronic and thermal Free Energies= -1187.521313

E(RM062X/6-311+G(2d,p)) = -1188.29755972

INT1

C	-2.30759800	-0.41940500	-1.13227800
C	-2.30903700	1.03147700	-1.36692500
H	-3.29464600	1.47418400	-1.22238300
H	-1.93019600	1.29396400	-2.35883300
C	-3.17110300	-1.02237000	-0.20024500
O	-3.18491200	-2.22038100	0.13673200
O	-4.07525500	-0.15081100	0.37348100
C	-4.96502600	-0.72347500	1.32213200
H	-4.39526400	-1.19714700	2.12956500
H	-5.56677600	-1.50707500	0.84771500
C	-5.84054300	0.39360800	1.85122900
H	-5.23137400	1.16717600	2.32844200
H	-6.54717000	0.00339700	2.58994700
H	-6.40915500	0.85589600	1.03862700
O	-1.49974800	1.83049900	-0.40091700
C	-0.19806700	1.85110800	-0.61097000
O	0.38313000	1.34572700	-1.55159900
O	0.36875700	2.54112100	0.38658400
C	1.80239400	2.79922300	0.39320900
C	2.19750200	3.61717300	-0.83185400
H	3.24407000	3.92455300	-0.73944400
H	1.57985300	4.51905700	-0.89595200
H	2.08097300	3.03965600	-1.75021500
C	1.99033000	3.61955500	1.66364800
H	1.67189000	3.04646100	2.53986400
H	1.40045700	4.53994900	1.61570900
H	3.04467700	3.88532300	1.78324600
C	2.57423600	1.48695300	0.48718200

H	2.19861000	0.89188000	1.32738600
H	3.63430500	1.70054400	0.66128400
H	2.47350700	0.90640100	-0.43135600
C	-1.37269500	-1.30844400	-1.84741200
H	-1.08938800	-0.91616800	-2.82787100
H	-1.79274200	-2.31160300	-1.96531300
N	-0.03269100	-1.54295200	-1.15416100
C	-0.00660500	-1.76841600	0.17470600
H	-0.97659300	-1.81514600	0.65807300
C	1.11997400	-1.51545400	-1.84582000
H	1.03082500	-1.32950600	-2.91009300
C	1.17041300	-1.94685200	0.85404400
H	1.12685400	-2.12175100	1.92070200
C	2.41031300	-1.87998600	0.16192700
C	2.33906900	-1.69083500	-1.24391400
H	3.22898600	-1.64280800	-1.85697300
N	3.58787600	-1.96735800	0.80602900
C	4.83434800	-1.83258200	0.06514000
H	5.66757100	-1.89158700	0.76366700
H	4.88054700	-0.86725200	-0.45178200
H	4.94228300	-2.63301400	-0.67498700
C	3.61674200	-2.13620300	2.25229400
H	4.65381900	-2.19061700	2.57947000
H	3.11040600	-3.06047500	2.55010900
H	3.13370700	-1.29181000	2.75751900

Zero-point correction= 0.456961 (Hartree/Particle)

Thermal correction to Energy= 0.484080

Thermal correction to Enthalpy= 0.485024

Thermal correction to Gibbs Free Energy= 0.398042

Sum of electronic and zero-point Energies= -1187.465498

Sum of electronic and thermal Energies= -1187.438379

Sum of electronic and thermal Enthalpies= -1187.437435

Sum of electronic and thermal Free Energies= -1187.524417

E(RM062X/6-311+G(2d,p)) = -1188.30092019

INT2

C	-0.36104200	3.83126100	-0.80166700
H	-0.93744000	4.42567500	-0.09977100
H	0.14856800	4.35614300	-1.60570000
C	-0.29052000	2.50582700	-0.69404400
C	-0.95707800	1.76026000	0.41703000
O	-0.54268600	0.69814000	0.83459300
O	-2.00796600	2.39862700	0.92281300
C	-2.81124500	1.61931100	1.82808000
H	-3.02056700	0.66168800	1.34177200
H	-2.23979400	1.43512700	2.74366800
C	-4.06977900	2.41086900	2.09931200
H	-4.62031700	2.57920900	1.16956800
H	-3.83504900	3.38001200	2.54958600
H	-4.71330800	1.85587000	2.78798100
C	0.45401800	1.64618300	-1.68037500
H	0.82931300	2.25720300	-2.50454100
H	-0.21314900	0.86870000	-2.06566500
N	1.61210300	0.95812000	-1.06837100
C	2.70739700	1.66616700	-0.71269100
H	2.67402100	2.72950800	-0.92478800
C	3.78833400	1.07636900	-0.12121700
H	4.63766200	1.69535300	0.13419100
C	1.55712700	-0.37192500	-0.82644000
H	0.62687600	-0.85876600	-1.11847300

C	2.60480000	-1.03158200	-0.24300800
H	2.50621000	-2.09549700	-0.07388000
C	3.77797600	-0.32511500	0.13990100
N	4.81958500	-0.94205100	0.71614600
C	5.99513000	-0.17869700	1.11713900
H	6.71194000	-0.85569000	1.57892500
H	5.72918100	0.59543800	1.84447600
H	6.46967900	0.29490000	0.25118400
C	4.77421900	-2.37965200	0.95544500
H	5.71576300	-2.69028600	1.40443000
H	4.63779700	-2.92667100	0.01679200
H	3.95774500	-2.63816300	1.63804300
C	-2.18297400	-0.50738400	-1.27208000
O	-2.54762700	0.67073400	-1.42587600
O	-1.26047500	-1.12490500	-1.85414300
O	-2.93753800	-1.18590000	-0.31267000
C	-2.64419800	-2.53942000	0.05943000
C	-2.93850700	-3.49218700	-1.09849100
H	-3.98161500	-3.38630700	-1.41711600
H	-2.77871700	-4.53077700	-0.78706000
H	-2.28535100	-3.26754500	-1.94334200
C	-1.20756500	-2.69634200	0.56547200
H	-0.49972600	-2.73017100	-0.26350500
H	-1.11757000	-3.62039700	1.14840300
H	-0.95242500	-1.84648100	1.20740900
C	-3.61619100	-2.80311900	1.20901600
H	-4.64514000	-2.61591700	0.88554000
H	-3.39498100	-2.14242100	2.05462400
H	-3.54048800	-3.84073200	1.55023300

Zero-point correction= 0.455286 (Hartree/Particle)

Thermal correction to Energy= 0.483099

Thermal correction to Enthalpy= 0.484043

Thermal correction to Gibbs Free Energy= 0.395380

Sum of electronic and zero-point Energies= -1187.473336

Sum of electronic and thermal Energies= -1187.445522

Sum of electronic and thermal Enthalpies= -1187.444578

Sum of electronic and thermal Free Energies= -1187.533241

E(RM062X/6-311+G(2d,p)) = -1188.31031817

RR-**6a**-CONF1

C	1.79723600	-2.26379600	-0.21946200
C	0.92748700	-3.30087900	-0.28827400
H	1.18712400	-4.34592900	-0.19181800
C	-0.40323900	-2.78400400	-0.54868200
O	-1.46417100	-3.36722100	-0.62423000
C	-0.25287400	-1.25286400	-0.81336000
N	1.16258300	-1.04056200	-0.43193700
C	1.65633700	0.24062000	-0.25200000
O	1.13888300	1.20464300	-0.78295400
O	2.69326300	0.25595300	0.57368500
C	3.44962200	1.48950600	0.80807800
C	2.56075200	2.49383700	1.53193600
H	2.16505100	2.05401400	2.45374200
H	1.72706900	2.80718600	0.89960200
H	3.15582100	3.37397200	1.79822400
C	4.58359300	1.01416400	1.70597700
H	4.18507700	0.57395400	2.62497900
H	5.22427700	1.86015200	1.97116100
H	5.18874400	0.26107800	1.19083600
C	3.99501000	2.03666100	-0.50595000

H	3.19578900	2.38935800	-1.16078100
H	4.57396100	1.26562100	-1.02542100
H	4.66382000	2.87538500	-0.28820800
C	3.26264900	-2.39498400	-0.09259600
C	6.02353600	-2.77135900	0.06191400
C	3.80079300	-3.23577600	0.88309800
C	4.11177600	-1.74790100	-0.99865400
C	5.48578300	-1.94157000	-0.92431900
C	5.18042100	-3.41559300	0.96375400
H	3.13828400	-3.73211300	1.58622200
H	3.69082800	-1.10449300	-1.76769400
H	6.13921600	-1.44554000	-1.63581000
H	5.59422400	-4.06084600	1.73246900
H	7.09784100	-2.91640100	0.12280800
C	-0.47387600	-0.91504000	-2.31356000
H	-0.53756800	0.17469400	-2.35271500
C	-1.76355900	-1.51017700	-2.88183000
H	-1.64438000	-2.57738000	-3.09361500
H	-2.00147400	-1.00312800	-3.82279500
H	-2.60998900	-1.40872000	-2.20288400
C	0.71676900	-1.34097000	-3.17559700
H	0.92949800	-2.41195400	-3.08215800
H	1.62234600	-0.78037000	-2.92844500
H	0.47791300	-1.14156000	-4.22491100
N	-1.14366400	-0.48738100	0.05853300
C	-1.15331600	-0.77359800	1.41225200
O	-0.47834400	-1.65072500	1.90834100
O	-1.96398000	0.05451300	2.07543000
C	-2.11244500	-0.18487600	3.49831500
H	-1.13243500	-0.47186800	3.88818200

C	-3.11488500	-1.30526200	3.70458400
H	-4.08833800	-1.01617000	3.29418500
H	-3.23363700	-1.50762900	4.77336400
H	-2.77675200	-2.22180400	3.21317200
C	-2.56115500	1.13667200	4.08793800
H	-1.82227000	1.91929500	3.89370900
H	-2.68590200	1.03451400	5.16969600
H	-3.51906000	1.44147500	3.65412400
N	-2.01266600	0.47556200	-0.41817700
C	-3.37385500	0.18987900	-0.38240200
O	-4.21211900	1.04097300	-0.60046100
O	-3.61808000	-1.08873800	-0.10799600
C	-5.00055000	-1.51925100	-0.19472800
H	-5.61307700	-0.75916000	0.29889500
C	-5.40427800	-1.65721900	-1.65263900
H	-6.45945700	-1.94052900	-1.71535800
H	-4.80763700	-2.43662300	-2.13815700
H	-5.26958400	-0.71401800	-2.18884900
C	-5.05896200	-2.83612700	0.55232400
H	-6.07487200	-3.23941000	0.50932500
H	-4.77909500	-2.70621900	1.60099100
H	-4.37305200	-3.55499700	0.09409300
C	-1.63770500	1.88240100	-0.21302500
H	-2.45393800	2.38304000	0.31702100
H	-0.76356200	1.88908200	0.43513000
C	-1.90156400	2.33092300	-2.67173600
H	-1.63918300	2.89406800	-3.56220300
C	-1.33130600	2.60955800	-1.50099100
C	-0.33716600	3.72373800	-1.44854300
O	0.19952300	4.22531300	-2.41093900

O	-0.12809700	4.13831800	-0.19043000
C	0.79469800	5.22943500	-0.02838900
H	0.51039800	6.03489100	-0.71092800
H	1.79599100	4.88433800	-0.30811700
C	0.72594500	5.66682800	1.41679800
H	-0.27972100	6.01860400	1.66375600
H	1.43116900	6.48533700	1.58656900
H	0.98120900	4.84288400	2.08967600
H	-2.63951000	1.53850400	-2.76494000

Zero-point correction= 0.754442 (Hartree/Particle)

Thermal correction to Energy= 0.800986

Thermal correction to Enthalpy= 0.801930

Thermal correction to Gibbs Free Energy= 0.673528

Sum of electronic and zero-point Energies= -2086.253976

Sum of electronic and thermal Energies= -2086.207432

Sum of electronic and thermal Enthalpies= -2086.206488

Sum of electronic and thermal Free Energies= -2086.334890

E(RM062X/6-311+G(2d,p)) = -2087.65806389

RR-**6a**-CONF2

C	1.58825200	-1.98241100	-0.74762900
C	0.72246200	-3.02038600	-0.86579800
H	0.99785300	-4.05971200	-0.98019200
C	-0.63378200	-2.50437300	-0.85439500
O	-1.69193900	-3.09757300	-0.85484100
C	-0.52863100	-0.94685600	-0.89925800
N	0.92513600	-0.75952200	-0.67659600
C	1.42480800	0.47676900	-0.30171600
O	0.85376300	1.50978900	-0.59175000
O	2.53305400	0.35927200	0.41670900

C	3.30005000	1.54396400	0.81484000
C	2.47343500	2.36665400	1.79547800
H	2.16335600	1.74571000	2.64296500
H	1.58497900	2.77744800	1.31076600
H	3.08404900	3.19158000	2.17782800
C	4.51670700	0.93444600	1.49729400
H	4.21096000	0.32169100	2.35092100
H	5.17604500	1.73009100	1.85602700
H	5.07333700	0.30516000	0.79514100
C	3.71612500	2.34535700	-0.41318100
H	2.85571600	2.78804800	-0.91900000
H	4.25856800	1.70495400	-1.11685900
H	4.38812900	3.14984100	-0.09803000
C	3.05747000	-2.08649500	-0.83999800
C	5.81843600	-2.38625800	-1.11896800
C	3.72560800	-3.09979000	-0.14945100
C	3.77669700	-1.22712600	-1.67974000
C	5.15008500	-1.38212900	-1.82275900
C	5.10519800	-3.24229500	-0.28364600
H	3.16564700	-3.76401100	0.50267700
H	3.25450000	-0.44759800	-2.22938400
H	5.70100000	-0.71943200	-2.48341100
H	5.62082700	-4.02421300	0.26513000
H	6.89268500	-2.50141000	-1.22653600
C	-0.93549900	-0.39887600	-2.29700900
H	-1.02013000	0.68165000	-2.16114100
C	-2.27478900	-0.94743800	-2.79282400
H	-2.16155600	-1.96535000	-3.17967400
H	-2.63522700	-0.31421900	-3.61019200
H	-3.03405900	-0.98203600	-2.01190200

C	0.14642200	-0.64960500	-3.34976700
H	0.38482700	-1.71448800	-3.44925400
H	1.06650200	-0.10220300	-3.12896900
H	-0.22360200	-0.30159300	-4.31925700
N	-1.31805100	-0.33739900	0.17393500
C	-1.21647400	-0.72172000	1.50316800
O	-1.87813700	-0.22586100	2.38991000
O	-0.28645400	-1.66089000	1.65566600
C	-0.08888800	-2.19414200	2.98971500
H	-0.11882700	-1.35092600	3.68552100
C	1.28890100	-2.82489100	2.96435800
H	1.30612900	-3.66632600	2.26373800
H	1.54452600	-3.19608000	3.96089700
H	2.04279400	-2.09328000	2.65747000
C	-1.19632800	-3.18361500	3.30089500
H	-2.16969800	-2.68708900	3.30518000
H	-1.02976900	-3.63092200	4.28551500
H	-1.20606000	-3.98111700	2.55043600
N	-2.24108500	0.66341200	-0.06511000
C	-3.58833900	0.34484000	0.07794800
O	-4.45132700	1.19948400	0.07034200
O	-3.79380100	-0.96382700	0.18695300
C	-5.17347500	-1.40412800	0.23614700
H	-5.72692500	-0.68912700	0.85072600
C	-5.74153600	-1.43903900	-1.17166900
H	-6.79320000	-1.73987400	-1.13889600
H	-5.19212700	-2.16236400	-1.78348600
H	-5.68045000	-0.45274600	-1.64052700
C	-5.13637000	-2.76786900	0.89504400
H	-6.14808000	-3.17994500	0.95142100

H	-4.73109800	-2.69678100	1.90808000
H	-4.50881100	-3.44894700	0.31216200
C	-1.85667300	2.02876200	0.32567900
H	-2.63014200	2.42781200	0.98820400
H	-0.93286200	1.95361000	0.89634600
C	-2.35140600	2.86359400	-1.99084800
H	-2.16767100	3.55778200	-2.80525500
C	-1.66065200	2.94990300	-0.85562600
C	-0.64147400	4.03512100	-0.72978700
O	-0.17315700	4.66260300	-1.65325100
O	-0.32448800	4.26566300	0.55267500
C	0.63132300	5.31306300	0.79126600
H	0.31497900	6.20865200	0.24959300
H	1.60140300	4.99845700	0.39099100
C	0.68036300	5.54699200	2.28378300
H	-0.29606800	5.87258700	2.65342800
H	1.41398900	6.32612400	2.50944900
H	0.96664400	4.63497000	2.81571800
H	-3.11333500	2.10074800	-2.12854300

Zero-point correction= 0.754380 (Hartree/Particle)

Thermal correction to Energy= 0.800929

Thermal correction to Enthalpy= 0.801873

Thermal correction to Gibbs Free Energy= 0.673902

Sum of electronic and zero-point Energies= -2086.254571

Sum of electronic and thermal Energies= -2086.208023

Sum of electronic and thermal Enthalpies= -2086.207078

Sum of electronic and thermal Free Energies= -2086.335049

E(RM062X/6-311+G(2d,p)) = -2087.65783943

E(RM062X/6-311+G(2d,p)) = -2087.65824516

RR-**INT3**

C	-1.64791800	-0.69155500	-1.07358500
H	-1.13695600	-1.28538100	-1.82413900
H	-1.17725500	0.23113800	-0.75315400
C	-2.79275700	-1.10307400	-0.52538700
C	-3.42177300	-2.39537700	-0.89627900
O	-4.39179600	-2.85801700	-0.32271800
O	-2.82819600	-2.99544000	-1.92656500
C	-3.19686800	-4.36224800	-2.15930900
H	-3.19124500	-4.89079700	-1.20228400
H	-4.21317700	-4.39487800	-2.56570600
C	-2.17606400	-4.93409900	-3.11611000
H	-1.17977100	-4.86153700	-2.67047800
H	-2.18198600	-4.38945500	-4.06506600
H	-2.40182100	-5.98536900	-3.31763400
C	-3.46169100	-0.33827600	0.58450700
H	-2.72107400	0.24511400	1.13322100
H	-3.98293100	-1.01393600	1.26231500
N	-4.45925300	0.62473400	0.05551000
C	-4.10832400	1.91630000	-0.13675900
H	-3.10133000	2.18037200	0.17417300
C	-4.97532200	2.82239700	-0.68367100
H	-4.63915200	3.84314200	-0.80605400
C	-5.69174800	0.20021300	-0.30449600
H	-5.89299300	-0.85222000	-0.13333400
C	-6.61258500	1.04737700	-0.85564100
H	-7.58372300	0.64927400	-1.11667200
C	-6.28290400	2.41597700	-1.07383200
N	-7.15736800	3.27382500	-1.61741400

C	-6.78223900	4.66708300	-1.82689400
H	-7.62635300	5.19458800	-2.26750300
H	-5.92718000	4.74385000	-2.50674800
H	-6.52553700	5.14937400	-0.87795300
C	-8.48275600	2.81398500	-2.01470300
H	-9.03165400	3.65225500	-2.43970000
H	-9.03905400	2.43263700	-1.15209800
H	-8.41199800	2.02343200	-2.76914200
N	-0.01023600	-0.79296000	1.35900800
N	0.72756100	0.39316500	1.55910800
C	0.11150800	1.58051400	1.30713500
O	-1.08692100	1.73192100	1.10653600
O	0.99053400	2.60120400	1.30476200
C	0.48002000	3.92136100	1.03395000
H	-0.48605800	4.01737200	1.53713400
C	1.48995400	4.88251300	1.63034100
H	2.45589800	4.78344600	1.12417500
H	1.63065100	4.68018600	2.69605400
H	1.13954100	5.91201300	1.51121200
C	0.31625100	4.08769100	-0.46704000
H	1.27792300	3.91751500	-0.96395600
H	-0.03002900	5.09888000	-0.70312100
H	-0.41202600	3.36862200	-0.85271900
C	-0.89287700	-1.05333200	2.29639500
O	-1.63791200	-2.07814000	2.25583200
O	-1.04492200	-0.17655000	3.32782400
C	-1.98082300	-0.51893300	4.35875200
H	-2.86816300	-0.95472700	3.88991100
C	-2.33468700	0.78974300	5.04185300
H	-1.44024900	1.23974100	5.48549700

H	-3.06845000	0.61883800	5.83559500
H	-2.75546400	1.49673300	4.32020700
C	-1.35833300	-1.52800000	5.31091800
H	-0.47069100	-1.09783600	5.78800900
H	-1.06756900	-2.42998300	4.76612500
H	-2.07168100	-1.80649200	6.09381600
C	2.17956500	0.30077000	1.58524400
C	2.61889400	-1.14148200	1.94920000
H	2.07609100	-1.77956100	1.24860700
C	2.19400200	-1.52574000	3.37088700
H	2.08198600	-2.61299300	3.42228800
H	1.24746400	-1.06419300	3.65971800
H	2.94680500	-1.21676100	4.10406000
C	4.11985000	-1.37551700	1.77464600
H	4.71711700	-0.74804800	2.44633500
H	4.45418300	-1.19985800	0.74700900
H	4.34067100	-2.41934300	2.02282600
C	2.82302000	1.30360800	2.58732200
O	2.49669500	1.39594700	3.75278200
C	3.90403400	1.97488000	1.88282900
H	4.65251600	2.60578400	2.34281400
C	3.85902300	1.62631600	0.57462900
N	2.82455700	0.72936800	0.30446300
C	2.19936900	0.53442200	-0.92004400
O	1.45408000	-0.39547700	-1.13906300
O	2.51179600	1.51067600	-1.77593000
C	2.20997600	1.39196900	-3.20113800
C	2.89596300	2.62081800	-3.78464400
H	2.47977000	3.53519600	-3.34977100
H	2.74715100	2.65036800	-4.86803400

H	3.97095600	2.59194000	-3.57678000
C	2.81924600	0.11701100	-3.77422300
H	2.34728800	-0.77569700	-3.35915900
H	3.89486300	0.08553000	-3.57290100
H	2.67486900	0.11298800	-4.85923500
C	0.70311300	1.45473300	-3.41912000
H	0.20895000	0.56965400	-3.01448700
H	0.49698400	1.51359300	-4.49278800
H	0.28895100	2.34799900	-2.94062900
C	4.87121900	1.99237400	-0.43585000
C	6.88306900	2.66050600	-2.25493400
C	5.37519500	3.29403200	-0.47837600
C	5.38404500	1.02274200	-1.30606000
C	6.38985800	1.35510600	-2.20599100
C	6.37347100	3.62748800	-1.39145400
H	4.97368800	4.04643700	0.19466100
H	4.99775500	0.00671800	-1.26816300
H	6.78974700	0.59565200	-2.87133900
H	6.75236200	4.64427700	-1.42648200
H	7.66442000	2.92006400	-2.96271500
C	0.25992500	-3.88751300	0.30582500
O	1.01324300	-3.89546900	1.26106800
O	-1.00672900	-3.55509900	0.31688900
H	-1.22074400	-2.97638600	1.15893800
O	0.60436300	-4.26204000	-0.94216200
C	1.95441200	-4.71644300	-1.22269400
C	2.98615000	-3.65610300	-0.83771800
H	2.64978500	-2.66706100	-1.16994200
H	3.93884500	-3.88587900	-1.32721000
H	3.14076600	-3.62719100	0.24109700

C	2.20967800	-6.04489800	-0.51801000
H	2.18284300	-5.92026700	0.56620800
H	3.19412900	-6.43018600	-0.80340100
H	1.45325000	-6.78014400	-0.81228000
C	1.93970100	-4.90836100	-2.73544400
H	1.72019200	-3.96022800	-3.23756600
H	1.17792800	-5.64015100	-3.02276500
H	2.91423800	-5.26907300	-3.07781000

Zero-point correction= 1.075169 (Hartree/Particle)

Thermal correction to Energy= 1.141591

Thermal correction to Enthalpy= 1.142536

Thermal correction to Gibbs Free Energy= 0.970673

Sum of electronic and zero-point Energies= -2890.116302

Sum of electronic and thermal Energies= -2890.049880

Sum of electronic and thermal Enthalpies= -2890.048935

Sum of electronic and thermal Free Energies= -2890.220798

E(RM062X/6-311+G(2d,p)) = -2892.09845441

RR-**INT4**-CONF1

C	-1.36850200	0.49659900	0.04235400
H	-0.85641300	-0.44714300	0.23293600
H	-1.63315500	0.53983200	-1.02424500
C	-2.57543700	0.63631300	0.89991100
C	-2.73922700	-0.00431500	2.12864300
O	-3.77598700	-0.00839200	2.82514600
O	-1.63002800	-0.70835100	2.57685600
C	-1.85987500	-1.54854900	3.69745200
H	-2.19603400	-0.95395600	4.55401100
H	-2.65910300	-2.26426600	3.46850200
C	-0.56201100	-2.26517900	4.00627700

H	0.21188000	-1.55047600	4.30004800
H	-0.20821100	-2.81472200	3.12832500
H	-0.70565200	-2.97370600	4.82815800
C	-3.78069800	1.35035900	0.42196400
H	-3.57962400	1.93728400	-0.47361500
H	-4.23801000	2.00503500	1.17171900
N	-4.90983800	0.40614100	0.04215500
C	-4.84755600	-0.26485500	-1.12622000
H	-3.99662100	-0.03180100	-1.75761800
C	-5.79464200	-1.18097200	-1.49490900
H	-5.69059800	-1.67587800	-2.45118000
C	-5.92334600	0.16097500	0.89332100
H	-5.89234000	0.71052800	1.82476500
C	-6.91288500	-0.74595500	0.60152900
H	-7.69959000	-0.89834000	1.32816200
C	-6.88493200	-1.46112400	-0.62335900
N	-7.83576100	-2.35638200	-0.94700700
C	-7.76098500	-3.07956300	-2.20869500
H	-8.61457200	-3.75187300	-2.27819600
H	-6.84306300	-3.67462400	-2.26819100
H	-7.79001700	-2.39079100	-3.06010800
C	-8.93032500	-2.62026000	-0.02388500
H	-9.59234000	-3.36246200	-0.46716900
H	-9.50793700	-1.70994400	0.17064500
H	-8.55631700	-3.00965100	0.92951900
N	-0.27002500	1.51463300	0.24116200
N	1.01459100	1.12398000	-0.12361000
C	1.40871800	1.28571700	-1.43702200
O	2.55472700	1.15003200	-1.81518500
O	0.36780000	1.57694000	-2.22574200

C	0.66064600	1.84374400	-3.61751500
H	1.41692200	1.12380000	-3.94217100
C	-0.64564200	1.62075500	-4.35300800
H	-1.41148900	2.30950400	-3.98106100
H	-0.99787700	0.59443000	-4.21390100
H	-0.50499600	1.80002100	-5.42274400
C	1.18763100	3.26084000	-3.75110400
H	0.44001000	3.97374700	-3.38623600
H	1.39956700	3.48440100	-4.80117600
H	2.10972700	3.38316000	-3.17691300
C	-0.56980100	2.84618800	-0.00180600
O	-1.69959800	3.27684900	-0.12260300
O	0.53227800	3.60456500	-0.06558900
C	0.33590000	5.03373000	-0.10814000
H	-0.48034600	5.24084400	-0.80697500
C	1.64243900	5.61360500	-0.61301000
H	2.45890400	5.32744700	0.05618500
H	1.57448600	6.70512700	-0.64813000
H	1.87143300	5.24663600	-1.61721900
C	-0.02475500	5.53252000	1.28141600
H	0.79498100	5.32282600	1.97682700
H	-0.93479000	5.04724300	1.64457100
H	-0.19427400	6.61363200	1.25911000
C	2.03964900	0.77709200	0.86670000
C	1.43218900	0.65096700	2.28879600
H	0.49931900	0.09101700	2.16238600
C	1.11521500	2.00032700	2.94267700
H	0.40633700	1.82951400	3.76002500
H	0.67871000	2.71885300	2.24935000
H	2.01828600	2.45371600	3.36413500

C	2.35452600	-0.15047500	3.21262800
H	3.36883300	0.26556800	3.23413100
H	2.41570600	-1.20264600	2.92093400
H	1.96429900	-0.10408400	4.23411800
C	3.24553100	1.77485800	0.84996800
O	3.13578300	2.96665800	1.05205400
C	4.45015900	0.99288300	0.64864400
H	5.45993300	1.37328800	0.71662100
C	4.10265300	-0.29572300	0.42009300
N	2.72301800	-0.48380500	0.47324100
C	2.00899400	-1.54427400	-0.07032900
O	0.87547800	-1.80605800	0.27193700
O	2.71852300	-2.17309300	-1.00079500
C	2.22725500	-3.39841300	-1.62928400
C	3.39799100	-3.80125300	-2.51655200
H	3.61878100	-3.01120500	-3.24073400
H	3.15388700	-4.71857200	-3.06011000
H	4.29158100	-3.97860700	-1.90861100
C	1.95893700	-4.46992600	-0.57883300
H	1.13073700	-4.19458300	0.07627800
H	2.85671800	-4.63961100	0.02478200
H	1.70653300	-5.40670700	-1.08567600
C	0.99373800	-3.07516300	-2.46478500
H	0.14474300	-2.80931400	-1.83237100
H	0.72548800	-3.94909200	-3.06682700
H	1.20916700	-2.24169900	-3.14214400
C	5.04850700	-1.42068800	0.28829400
C	6.91140700	-3.49413600	0.11558900
C	6.20380200	-1.26395800	-0.48065900
C	4.83272100	-2.61988600	0.97812400

C	5.76327000	-3.64895100	0.89500700
C	7.12888200	-2.30178600	-0.57076800
H	6.36360800	-0.33641500	-1.02269500
H	3.93979900	-2.74054000	1.58696200
H	5.59362000	-4.57344400	1.43888500
H	8.01876600	-2.17726800	-1.18000700
H	7.63405600	-4.30160400	0.04668300

Zero-point correction= 0.922339 (Hartree/Particle)

Thermal correction to Energy= 0.978264

Thermal correction to Enthalpy= 0.979208

Thermal correction to Gibbs Free Energy= 0.828539

Sum of electronic and zero-point Energies= -2468.170458

Sum of electronic and thermal Energies= -2468.114533

Sum of electronic and thermal Enthalpies= -2468.113589

Sum of electronic and thermal Free Energies= -2468.264257

E(RM062X/6-311+G(2d,p)) = -2469.85495422

RR-**INT4**-CONF2

C	1.17469300	-0.54101100	0.07018200
H	0.56263000	0.31944300	0.34143000
H	1.37553400	-0.49444400	-1.00964800
C	2.44167800	-0.55797700	0.84202000
C	2.57353100	-0.07178900	2.14194000
O	3.63904900	0.02928400	2.78580000
O	1.38735400	0.33619900	2.73283200
C	1.53523000	1.05488300	3.94806000
H	2.11316000	0.46528300	4.66697300
H	2.09369000	1.98249000	3.76681700
C	0.14724000	1.35096800	4.47452200
H	-0.37221000	0.42067300	4.72260400

H	-0.44197100	1.88727600	3.72352800
H	0.20498600	1.96489600	5.37888400
C	3.70630800	-1.02377200	0.23447400
H	3.54452200	-1.52893800	-0.72023900
H	4.29594000	-1.68288500	0.88164100
N	4.66560800	0.11501100	-0.07023300
C	4.43369300	0.91745900	-1.12936600
H	3.58325400	0.64785800	-1.74670800
C	5.21612700	2.00469500	-1.40757300
H	4.98015400	2.60160800	-2.27834400
C	5.68547100	0.39520300	0.76256000
H	5.79171900	-0.26934800	1.60987100
C	6.51463300	1.47065000	0.55870100
H	7.31535200	1.64211800	1.26537400
C	6.30650000	2.32979200	-0.55112400
N	7.09292800	3.39601200	-0.78298100
C	6.84297600	4.25348100	-1.93322500
H	7.59275100	5.04279800	-1.95215600
H	5.85109800	4.71492800	-1.87363100
H	6.91301200	3.68672600	-2.86778000
C	8.17856000	3.71207700	0.13469100
H	8.67915900	4.61541500	-0.21013100
H	8.91167300	2.89879600	0.17159500
H	7.79785700	3.88892100	1.14645300
N	0.20073200	-1.68798700	0.26519800
N	-1.10079300	-1.41450400	-0.14646000
C	-1.43450000	-1.60893500	-1.47243900
O	-2.57447200	-1.54909600	-1.88695500
O	-0.35683900	-1.83741400	-2.23392700
C	-0.58947300	-1.90216000	-3.66246200

H	-1.49537500	-2.49178100	-3.82514100
C	-0.77283700	-0.49431900	-4.20297300
H	0.12237300	0.10479500	-4.00305200
H	-1.63748900	-0.01208300	-3.73941800
H	-0.93438700	-0.52832800	-5.28465100
C	0.62000200	-2.60564800	-4.24386300
H	1.53410400	-2.04985600	-4.00803100
H	0.52226400	-2.66802500	-5.33153800
H	0.71124300	-3.61877500	-3.84422500
C	0.54266200	-3.01923100	0.05763600
O	-0.26571000	-3.91431300	-0.07981500
O	1.86846700	-3.20420800	0.05219500
C	2.31443200	-4.57470300	-0.08401100
H	1.64944200	-5.20011700	0.51733900
C	3.72470900	-4.61561900	0.47093400
H	4.39864500	-4.00355000	-0.13750800
H	4.09272500	-5.64593800	0.46076800
H	3.74662800	-4.24764500	1.50069700
C	2.24127300	-4.98837800	-1.54331200
H	2.86231000	-4.32308600	-2.15373500
H	1.21002700	-4.94451700	-1.90104300
H	2.60952100	-6.01224400	-1.66218000
C	-2.19557500	-1.16318600	0.79816000
C	-1.67658600	-1.06905000	2.25681000
H	-0.76441200	-0.46481600	2.20982700
C	-1.33482200	-2.43510500	2.86222500
H	-0.64834100	-2.28226400	3.70208300
H	-0.87175800	-3.11572700	2.14708700
H	-2.23457000	-2.92852400	3.24446300
C	-2.68927700	-0.34909400	3.15264400

H	-3.68671300	-0.79865400	3.07930000
H	-2.76748800	0.71446400	2.90944800
H	-2.37219900	-0.43404200	4.19624800
C	-3.33507500	-2.22915600	0.66660500
O	-3.15821400	-3.41954100	0.80967500
C	-4.57426600	-1.51108900	0.43238700
H	-5.56055100	-1.95361100	0.41479700
C	-4.29517600	-0.19615800	0.27876300
N	-2.93436400	0.06891700	0.41580600
C	-2.27208500	1.24449700	0.09610100
O	-1.20639700	1.54638300	0.59186900
O	-2.94057500	1.94023200	-0.81849600
C	-2.54364400	3.30367500	-1.17298300
C	-3.65646900	3.72952400	-2.12159100
H	-3.69425300	3.06456400	-2.98996100
H	-3.47836100	4.75139600	-2.46897500
H	-4.62473600	3.69373700	-1.61096300
C	-2.52215800	4.19594600	0.06296400
H	-1.74986300	3.88717800	0.76978400
H	-3.49691900	4.17863100	0.56065000
H	-2.31697700	5.22491200	-0.24887200
C	-1.19762200	3.27466200	-1.88765600
H	-0.39577500	2.97582000	-1.21014800
H	-0.97659800	4.27348800	-2.27735000
H	-1.23304600	2.57747100	-2.73080900
C	-5.30845300	0.86963500	0.13995200
C	-7.31333700	2.80403000	-0.04121500
C	-6.34337700	0.72149900	-0.78522700
C	-5.28433400	1.98754500	0.98187300
C	-6.28663200	2.94684200	0.89434500

C	-7.33870100	1.69223000	-0.87985500
H	-6.35485500	-0.14512500	-1.43978300
H	-4.48473300	2.09678000	1.71109000
H	-6.26807300	3.80733300	1.55667900
H	-8.13412600	1.57724600	-1.60977000
H	-8.09201200	3.55743200	-0.11242000

Zero-point correction= 0.922383 (Hartree/Particle)

Thermal correction to Energy= 0.978308

Thermal correction to Enthalpy= 0.979253

Thermal correction to Gibbs Free Energy= 0.828922

Sum of electronic and zero-point Energies= -2468.166437

Sum of electronic and thermal Energies= -2468.110512

Sum of electronic and thermal Enthalpies= -2468.109567

Sum of electronic and thermal Free Energies= -2468.259897

E(RM062X/6-311+G(2d,p)) = -2469.85153773

RR-**TS3**

C	1.77682000	-0.15424400	-1.33915900
H	1.55096100	0.47584400	-2.19322500
H	1.02772800	-0.87031200	-1.01707500
C	2.92463300	-0.02947400	-0.67025800
C	3.93527800	1.00134200	-1.02337600
O	4.92977200	1.22216800	-0.35744100
O	3.64498900	1.65975300	-2.14510200
C	4.36848200	2.88014100	-2.36366900
H	4.30679900	3.48524500	-1.45415600
H	5.41993100	2.64432300	-2.55661300
C	3.71497800	3.57864700	-3.53318300
H	2.67509600	3.81233100	-3.29067300
H	3.74390900	2.95009900	-4.42840900

H	4.24314600	4.51215900	-3.74942000
C	3.22027300	-0.85611800	0.55263100
H	2.29004000	-1.11318300	1.06047200
H	3.88288400	-0.32054300	1.23143900
N	3.87730100	-2.13678200	0.19251900
C	3.14812600	-3.27292100	0.12303400
H	2.09860400	-3.17506500	0.38630300
C	3.70843800	-4.46334000	-0.25318100
H	3.07543100	-5.33983200	-0.28447600
C	5.19148400	-2.15803400	-0.12635400
H	5.70557000	-1.20472600	-0.05728600
C	5.82079400	-3.30873800	-0.51192800
H	6.87580900	-3.26363500	-0.74599200
C	5.08961900	-4.52902500	-0.59107500
N	5.67182400	-5.67757000	-0.96252900
C	4.89322200	-6.90940400	-1.00894300
H	5.54968900	-7.72877600	-1.29631200
H	4.08395600	-6.83417800	-1.74309600
H	4.46293200	-7.13535200	-0.02784700
C	7.08602300	-5.70059300	-1.31698400
H	7.35439000	-6.71061400	-1.62162700
H	7.70878000	-5.41412600	-0.46283000
H	7.29021900	-5.01978000	-2.14963400
N	0.08620100	0.74601400	0.96639600
N	-1.00743600	-0.09725100	1.24056900
C	-0.80942000	-1.43983600	1.17433300
O	0.26858300	-1.99463300	0.99634100
O	-1.96380300	-2.11751200	1.33356000
C	-1.91296900	-3.55376100	1.23862200
H	-1.00644000	-3.89261400	1.74784500

C	-3.14930400	-4.05643200	1.95870600
H	-4.05421200	-3.71406600	1.44556300
H	-3.17070900	-3.68984100	2.98907700
H	-3.15217200	-5.15037500	1.97451500
C	-1.87950700	-3.95106500	-0.22730300
H	-2.75672100	-3.53904000	-0.73875700
H	-1.88935400	-5.04099200	-0.32822200
H	-0.97643500	-3.56235000	-0.70621800
C	0.98927400	0.81459100	1.93988500
O	2.01919900	1.50562900	1.82652200
O	0.76863200	0.06673600	3.06666700
C	1.71408800	0.20671100	4.13069000
H	2.71944400	0.24819900	3.69914300
C	1.55686400	-1.03691700	4.98760600
H	0.53796000	-1.09372500	5.38562800
H	2.25860500	-1.01568100	5.82726300
H	1.74555200	-1.93725800	4.39447900
C	1.44199800	1.48831500	4.90385600
H	0.43959900	1.45562000	5.34555000
H	1.50805300	2.35006800	4.23423400
H	2.17233000	1.61359300	5.71043900
C	-2.35249700	0.45982900	1.30185200
C	-2.28982700	2.00858200	1.39763800
H	-1.59766700	2.29621200	0.60371400
C	-1.71899400	2.47650800	2.74167100
H	-1.25507600	3.45883000	2.61174500
H	-0.97241900	1.78607000	3.13688400
H	-2.51303700	2.56349800	3.49142400
C	-3.63855600	2.68175500	1.14157500
H	-4.39215400	2.38857500	1.88123200

H	-4.02825100	2.46452300	0.14281900
H	-3.50652300	3.76607100	1.21945600
C	-3.17506500	-0.11401900	2.49410100
O	-2.77911600	-0.12748200	3.64118900
C	-4.46608600	-0.52228300	1.96520400
H	-5.32206900	-0.81530900	2.55782300
C	-4.43504900	-0.42961900	0.61362100
N	-3.21107100	0.04926100	0.14846600
C	-2.67179300	-0.12065900	-1.11870000
O	-1.71406400	0.50838100	-1.51008000
O	-3.32593800	-1.06596100	-1.79831400
C	-3.11863200	-1.23920300	-3.23531200
C	-4.14996700	-2.30246800	-3.59072900
H	-3.94885000	-3.23055200	-3.04595900
H	-4.11198500	-2.51265800	-4.66367800
H	-5.15708800	-1.95685200	-3.33457800
C	-3.41420400	0.06128400	-3.97432700
H	-2.71173700	0.84890900	-3.69506100
H	-4.43514600	0.39504200	-3.76330600
H	-3.32821200	-0.11476700	-5.05121100
C	-1.70550400	-1.74338400	-3.50401200
H	-0.96197800	-0.97751000	-3.27777200
H	-1.61866500	-2.01926600	-4.55998800
H	-1.50027600	-2.63255700	-2.89930400
C	-5.59570300	-0.64713400	-0.27275600
C	-7.87525200	-0.99937200	-1.84886100
C	-6.44668300	-1.73095700	-0.04515500
C	-5.89554100	0.26578400	-1.29093300
C	-7.03363800	0.09279000	-2.06995500
C	-7.57907000	-1.90958500	-0.83705000

H	-6.21208600	-2.43928900	0.74443200
H	-5.23895700	1.11518900	-1.46350600
H	-7.26477100	0.80999900	-2.85195500
H	-8.22957300	-2.76079900	-0.66115500
H	-8.76024000	-1.13642200	-2.46278300
C	1.34656000	4.10178900	-0.14859500
O	0.69106900	4.39417000	0.82813100
O	1.57681700	2.87868700	-0.59236800
H	1.26508500	2.22615300	0.08569100
O	1.95451900	4.96195200	-0.97717900
C	1.87161700	6.39594500	-0.74048600
C	0.42351700	6.86470600	-0.83707200
H	-0.01444300	6.53711700	-1.78572200
H	0.39443200	7.95854700	-0.80483800
H	-0.17581700	6.47282600	-0.01399100
C	2.50751900	6.74665700	0.60090300
H	1.91783400	6.36089800	1.43357700
H	2.57970500	7.83504500	0.69347600
H	3.51843700	6.32919100	0.65662400
C	2.69588200	6.97349400	-1.88505300
H	2.26601200	6.68737800	-2.85017000
H	3.72627500	6.60655700	-1.83669400
H	2.71151800	8.06541000	-1.81977400

Zero-point correction= 1.075062 (Hartree/Particle)

Thermal correction to Energy= 1.141446

Thermal correction to Enthalpy= 1.142390

Thermal correction to Gibbs Free Energy= 0.969303

Sum of electronic and zero-point Energies= -2890.108989

Sum of electronic and thermal Energies= -2890.042605

Sum of electronic and thermal Enthalpies= -2890.041661

Sum of electronic and thermal Free Energies= -2890.214748

E(RM062X/6-311+G(2d,p)) = -2892.09019114

RR-**TS4**-CONF1

C	0.02035100	1.58509300	-0.60276700
H	-0.45324600	1.19341000	-1.49348900
H	0.93404900	1.07006500	-0.31321700
C	-0.12247000	2.92456200	-0.29828700
C	-1.09813900	3.77279900	-0.94160300
O	-1.27370500	4.96442100	-0.69456900
O	-1.80896400	3.14576700	-1.90724600
C	-2.86420100	3.90027500	-2.50218500
H	-3.60869700	4.14041000	-1.73506100
H	-2.46451000	4.84376400	-2.88800600
C	-3.46303900	3.05553100	-3.60549200
H	-3.86954900	2.12862600	-3.19357500
H	-2.70423300	2.80801600	-4.35439200
H	-4.26806500	3.60755700	-4.10058400
C	0.58373000	3.51341800	0.87678800
H	0.65861500	2.79898600	1.69818300
H	0.08149500	4.41986900	1.21887700
N	1.99099000	3.90817100	0.55519800
C	3.03570500	3.17786200	0.99342300
H	2.78410900	2.33005000	1.62412900
C	4.32633500	3.48511000	0.64626400
H	5.12274500	2.85951400	1.02694400
C	2.20223400	4.96374300	-0.26132900
H	1.30633700	5.48229800	-0.59009000
C	3.45975300	5.33928600	-0.64467400
H	3.56561200	6.19848600	-1.29314200

C	4.59186800	4.60078500	-0.19424300
N	5.84115800	4.94047800	-0.54920800
C	6.97448400	4.16137500	-0.06800600
H	7.89354500	4.61505600	-0.43501400
H	6.92417700	3.12864700	-0.43008500
H	7.00455800	4.15122200	1.02664200
C	6.06766800	6.07911600	-1.43039900
H	7.13703200	6.17671500	-1.60871800
H	5.70296200	7.00600900	-0.97527300
H	5.56579300	5.93583900	-2.39323200
N	-0.96591000	0.35403000	0.65111800
N	-0.18703100	-0.70986300	1.11112300
C	0.96254200	-0.42260600	1.79905500
O	1.32657400	0.69854000	2.11614800
O	1.65726700	-1.53547000	2.07638700
C	2.95617200	-1.37201800	2.68472900
H	2.88147200	-0.56986500	3.42356800
C	3.26516200	-2.69381300	3.35922400
H	3.34217600	-3.49340700	2.61487400
H	2.48045900	-2.95347200	4.07559600
H	4.21764700	-2.62311400	3.89260400
C	3.95688900	-1.01141200	1.60003400
H	3.96076600	-1.79216000	0.83134700
H	4.96250800	-0.92458700	2.02314400
H	3.69132600	-0.05806000	1.13277300
C	-1.63324500	1.03138100	1.60105000
O	-2.37755000	1.98736500	1.31454200
O	-1.45043700	0.64445600	2.87832200
C	-2.25386200	1.29042400	3.88417700
H	-2.28500300	2.36025000	3.65836900

C	-1.53000800	1.04340500	5.19440200
H	-1.46433100	-0.03211400	5.39055100
H	-2.07060000	1.51701000	6.01940500
H	-0.51585300	1.45223300	5.15766000
C	-3.66014800	0.71406900	3.86738200
H	-3.62754100	-0.35530500	4.10567100
H	-4.12113000	0.84800800	2.88401700
H	-4.27989300	1.21601600	4.61808900
C	-0.53080700	-2.08085000	0.72918000
C	-1.93890300	-2.13771000	0.07100200
H	-1.94486600	-1.31336800	-0.64501300
C	-3.06292100	-1.91947300	1.08778900
H	-3.97673500	-1.62900100	0.56014900
H	-2.82435600	-1.14552100	1.81903900
H	-3.27099600	-2.83947700	1.64399600
C	-2.17292600	-3.44093400	-0.69404600
H	-2.08475100	-4.32083900	-0.04678300
H	-1.48082800	-3.55322000	-1.53334500
H	-3.19005100	-3.43043000	-1.09965200
C	-0.46288400	-3.04862500	1.95237100
O	-1.04477100	-2.84521700	2.99761200
C	0.35013500	-4.18325800	1.55262600
H	0.48195100	-5.09296100	2.12215300
C	0.90255500	-3.92057900	0.34161500
N	0.49106500	-2.69086800	-0.16101300
C	1.03415000	-1.95727300	-1.20564700
O	0.39591500	-1.11177200	-1.79457800
O	2.30788500	-2.28043500	-1.41835000
C	3.03341200	-1.74921000	-2.57406900
C	4.38196700	-2.44859400	-2.46605200

H	4.88535700	-2.17507100	-1.53327000
H	5.01935000	-2.15553700	-3.30535100
H	4.24897800	-3.53533500	-2.48780900
C	2.33032100	-2.14139400	-3.86841700
H	1.34167000	-1.68493400	-3.94268900
H	2.23322900	-3.22992500	-3.93259300
H	2.93394900	-1.80187400	-4.71598200
C	3.18982200	-0.23895200	-2.43412300
H	2.23523200	0.27502700	-2.55984500
H	3.88712300	0.12116200	-3.19740700
H	3.60254100	0.00762700	-1.44964100
C	1.72655900	-4.86417700	-0.43849800
C	3.21783300	-6.74738200	-1.86359600
C	2.70933100	-5.61755000	0.20811000
C	1.48532300	-5.06663100	-1.80278600
C	2.22488100	-6.00795900	-2.50917200
C	3.45759900	-6.55100500	-0.50576000
H	2.89389600	-5.46061300	1.26713100
H	0.70876500	-4.49528000	-2.30590300
H	2.02595800	-6.16678500	-3.56483900
H	4.22776000	-7.12406600	0.00117800
H	3.79851800	-7.47771900	-2.41882600
C	-4.86207500	0.83434000	-0.45797300
O	-5.27178500	0.77689300	0.68460000
O	-3.68974600	1.29702600	-0.84017300
H	-3.15973700	1.60473900	-0.03702800
O	-5.53303900	0.44105200	-1.54901300
C	-6.88438300	-0.08822000	-1.43529200
C	-6.88306600	-1.37584800	-0.61758600
H	-6.15585800	-2.08288300	-1.03155600

H	-7.87475000	-1.83701800	-0.66796700
H	-6.63876000	-1.18219000	0.42809500
C	-7.81856600	0.96715100	-0.85194300
H	-7.58326500	1.17237800	0.19332100
H	-8.85176900	0.61149200	-0.91768600
H	-7.73856000	1.89665500	-1.42543400
C	-7.25314800	-0.38025400	-2.88503800
H	-6.55790600	-1.10628300	-3.31768900
H	-7.21496200	0.53696300	-3.48093000
H	-8.26586200	-0.79031200	-2.93777200

Zero-point correction= 1.075044 (Hartree/Particle)

Thermal correction to Energy= 1.141253

Thermal correction to Enthalpy= 1.142197

Thermal correction to Gibbs Free Energy= 0.967944

Sum of electronic and zero-point Energies= -2890.105479

Sum of electronic and thermal Energies= -2890.039271

Sum of electronic and thermal Enthalpies= -2890.038327

Sum of electronic and thermal Free Energies= -2890.212579

E(RM062X/6-311+G(2d,p)) = -2892.08512891

RR-**TS4**-CONF2

C	1.12366500	1.13406500	1.03208400
H	0.82149100	1.77259700	1.85099900
H	0.54383500	1.25000300	0.11930200
C	2.42845000	0.70508600	0.94991900
C	3.34069300	0.73994400	2.07086500
O	4.47997000	0.27714400	2.04642900
O	2.86049300	1.37654000	3.16140000
C	3.78583300	1.59345000	4.22871700
H	4.20211700	0.63852800	4.56114600

H	4.61632900	2.20953900	3.86580800
C	3.02763900	2.28043300	5.34322500
H	2.20474000	1.64914800	5.69136100
H	2.61304200	3.23296300	5.00057500
H	3.69707900	2.47548500	6.18605200
C	2.93676500	0.00681600	-0.26469100
H	2.14290200	-0.07607600	-1.00895800
H	3.32801800	-0.99543800	-0.06674100
N	4.06324500	0.74788700	-0.91118700
C	3.80946500	1.91313600	-1.54701200
H	2.77117700	2.22819000	-1.55684100
C	4.79844200	2.65091100	-2.13458900
H	4.52740100	3.57025500	-2.63592000
C	5.33289700	0.30112400	-0.82324300
H	5.47226400	-0.62168700	-0.27423000
C	6.38068400	0.98282700	-1.38276600
H	7.37509600	0.57114200	-1.27598300
C	6.14987300	2.20299400	-2.07523800
N	7.14841600	2.89698400	-2.64044800
C	6.87075100	4.14993500	-3.33201400
H	7.80607500	4.55167400	-3.71789600
H	6.42932700	4.88411800	-2.64977000
H	6.18659900	3.99022800	-4.17205300
C	8.51774800	2.40472800	-2.55620600
H	9.17402100	3.10386400	-3.07118100
H	8.61006800	1.42261200	-3.03186200
H	8.84191100	2.32475600	-1.51328600
N	-0.24012100	-0.28838900	1.60447500
N	-1.37142500	-0.38522300	0.79550700
C	-1.28756600	-0.77199900	-0.51824400

O	-2.23423200	-0.73581800	-1.28513200
O	-0.05366900	-1.18475300	-0.86053000
C	0.05759600	-1.72335100	-2.19996900
H	-0.84963600	-2.30201200	-2.39229300
C	0.17920900	-0.58721800	-3.20241800
H	1.07810000	0.00801600	-3.00129800
H	-0.69788600	0.06297300	-3.15587800
H	0.25892200	-0.99101900	-4.21679400
C	1.26671100	-2.63948600	-2.20074800
H	2.19439800	-2.07424800	-2.06405000
H	1.32713800	-3.15872700	-3.16215800
H	1.19400400	-3.38499500	-1.40360000
C	0.23002100	-1.47616700	2.01252300
O	-0.20634500	-2.61842200	1.78930200
O	1.31521400	-1.30093100	2.79736400
C	2.01711900	-2.48672500	3.20976900
H	1.27929300	-3.21800200	3.55214200
C	2.91809900	-2.05327700	4.35067400
H	3.68483100	-1.36835200	3.97395800
H	3.41478200	-2.92507700	4.78771700
H	2.34283800	-1.54894500	5.13315500
C	2.81297800	-3.05243100	2.04457000
H	3.54920800	-2.30956500	1.71630100
H	2.14938700	-3.31095400	1.21476500
H	3.34759100	-3.95624200	2.35550800
C	-2.66885500	0.09955100	1.26237500
C	-2.64512300	0.37308900	2.78985900
H	-1.72249700	0.93266900	2.95702700
C	-2.59879700	-0.91788500	3.61394000
H	-2.22149400	-0.68817900	4.61585100

H	-1.96495200	-1.68376100	3.16329300
H	-3.60027800	-1.34711000	3.72079000
C	-3.82018100	1.24221500	3.23990100
H	-4.78580900	0.79294700	2.98062200
H	-3.77410700	2.24556900	2.80702200
H	-3.78682300	1.34623700	4.32934000
C	-3.79758600	-0.91449700	0.89418100
O	-3.76765600	-2.08458100	1.21180900
C	-4.83831700	-0.17015000	0.20735000
H	-5.80900800	-0.55766600	-0.06927900
C	-4.40013900	1.09271400	-0.01097900
N	-3.12906600	1.30070900	0.51703300
C	-2.27237500	2.36446900	0.29226300
O	-1.38836600	2.65825400	1.07021700
O	-2.53151900	2.95996400	-0.86913100
C	-1.85313000	4.19747800	-1.24976500
C	-2.52059500	4.54130400	-2.57503800
H	-2.35894500	3.74192000	-3.30474600
H	-2.10203600	5.47054000	-2.97242000
H	-3.59848700	4.67256200	-2.43301700
C	-2.11475900	5.28940700	-0.21898900
H	-1.67901700	5.03941600	0.75001100
H	-3.19148200	5.44868700	-0.10192400
H	-1.66758100	6.22444800	-0.57098300
C	-0.36395700	3.92845100	-1.44386300
H	0.13285300	3.73535600	-0.49094400
H	0.10064200	4.80115600	-1.91414600
H	-0.22390400	3.06620400	-2.10535000
C	-5.20897900	2.18022900	-0.59755600
C	-6.85130700	4.17970200	-1.64952000

C	-5.95901700	1.93813500	-1.75042100
C	-5.29065100	3.42788500	0.03224600
C	-6.11229700	4.42021100	-0.48953000
C	-6.77270900	2.93900700	-2.27749700
H	-5.88826500	0.97149200	-2.24048500
H	-4.71856600	3.61453900	0.93815200
H	-6.17837800	5.38235100	0.00976100
H	-7.34432900	2.74687700	-3.18026600
H	-7.48851500	4.95783500	-2.05872800
C	-0.81189400	-4.75046800	-0.56448200
O	0.16093900	-5.20186100	0.00825000
O	-1.47274200	-3.66269500	-0.22471900
H	-1.02846500	-3.22913800	0.57018500
O	-1.39172300	-5.27450000	-1.65185500
C	-0.91685700	-6.53335200	-2.20803300
C	0.50401600	-6.37436000	-2.73809600
H	0.54363300	-5.55847400	-3.46727200
H	0.80790400	-7.29763200	-3.24207400
H	1.20703200	-6.16814900	-1.92921600
C	-1.02708700	-7.64888800	-1.17311200
H	-0.30580300	-7.51808600	-0.36547100
H	-0.84096800	-8.61142500	-1.66014500
H	-2.03697700	-7.66846400	-0.75017200
C	-1.88762200	-6.78051600	-3.35683300
H	-1.85247100	-5.95225500	-4.07126600
H	-2.91094500	-6.87233400	-2.98013600
H	-1.62178800	-7.70451900	-3.87855100

Zero-point correction= 1.076026 (Hartree/Particle)

Thermal correction to Energy= 1.141698

Thermal correction to Enthalpy= 1.142642

Thermal correction to Gibbs Free Energy= 0.971660

Sum of electronic and zero-point Energies= -2890.103704

Sum of electronic and thermal Energies= -2890.038032

Sum of electronic and thermal Enthalpies= -2890.037088

Sum of electronic and thermal Free Energies= -2890.208069

E(RM062X/6-311+G(2d,p)) = -2892.08649840

RR-**TS4**-CONF3

C	-0.30134900	-0.25511900	0.18982200
H	0.09476900	-0.02164600	-0.79177400
H	0.18867800	-1.04965400	0.73822100
C	-1.56057200	0.14852300	0.53256000
C	-2.27856100	1.15317500	-0.21658000
O	-3.37346600	1.61891000	0.13520200
O	-1.70158100	1.53052400	-1.36051500
C	-2.37646800	2.54852700	-2.11022300
H	-3.37820800	2.19637700	-2.37959900
H	-2.49112300	3.43596500	-1.48033600
C	-1.52999100	2.83255700	-3.33045300
H	-1.43082700	1.93569400	-3.94889700
H	-0.53038000	3.15855900	-3.03126500
H	-1.99550400	3.61972200	-3.93049600
C	-2.11278200	-0.12793700	1.89280500
H	-2.23981200	0.80015800	2.45496100
H	-1.44153100	-0.78543800	2.45156400
N	-3.45010600	-0.78535400	1.85904500
C	-4.52708800	-0.19994700	2.42290700
H	-4.35328400	0.76393800	2.88643600
C	-5.76525100	-0.78182300	2.39735900
H	-6.58825900	-0.25393200	2.85951500

C	-3.58502500	-1.98770700	1.25636800
H	-2.67951600	-2.39870800	0.82373100
C	-4.78682900	-2.63232100	1.18524900
H	-4.82817500	-3.59011500	0.68467800
C	-5.95110100	-2.02715200	1.73682600
N	-7.15830700	-2.60235100	1.63714300
C	-8.32665100	-1.93215300	2.18850000
H	-9.20295400	-2.55890700	2.02863500
H	-8.48646200	-0.96419800	1.69948100
H	-8.21019600	-1.76954200	3.26493200
C	-7.32058900	-3.82379700	0.86020900
H	-6.99177700	-3.67285500	-0.17397000
H	-8.37351300	-4.10148700	0.85533400
H	-6.74726500	-4.64696300	1.29981100
N	1.17957100	1.09808500	1.06665100
N	2.43552200	1.08443000	0.43720900
C	2.48539300	1.28019200	-0.91819200
O	1.53338800	1.53470000	-1.63146000
O	3.74298400	1.12135100	-1.37990300
C	3.94724400	1.24425900	-2.79976100
H	3.10372100	0.75924300	-3.30029200
C	4.00930600	2.71267800	-3.18210200
H	4.81495600	3.20766500	-2.62919800
H	3.06400200	3.20885100	-2.94969600
H	4.20580000	2.81593600	-4.25398900
C	5.23844500	0.50022300	-3.08494100
H	6.08113300	1.00495600	-2.59989300
H	5.42517100	0.46964400	-4.16264100
H	5.17865600	-0.52481700	-2.70417000
C	0.61060700	2.31886500	1.14946500

O	-0.50100000	2.50588300	1.65120500
O	1.34455400	3.36021700	0.65121700
C	0.77555500	4.66652900	0.77552600
H	-0.29769300	4.59765900	0.57234300
C	1.46113400	5.51891000	-0.27741200
H	1.27596300	5.11623300	-1.27760300
H	2.54278400	5.53194600	-0.10476300
H	1.08846400	6.54737700	-0.23923900
C	0.99506800	5.19643500	2.18491700
H	2.06814600	5.26646500	2.39644800
H	0.53100600	4.52772900	2.91475200
H	0.55451500	6.19312800	2.29440600
C	3.62359900	0.69725800	1.19076000
C	3.31568900	0.61556600	2.71097600
H	2.39350200	0.03375900	2.76932500
C	3.07472400	1.99938600	3.32486900
H	2.47093100	1.89440100	4.23229300
H	2.56677200	2.67600900	2.63662500
H	4.02354600	2.46997800	3.60310900
C	4.40368100	-0.11744900	3.49746500
H	5.37488500	0.38386000	3.41886600
H	4.52074200	-1.15501800	3.17220400
H	4.12465300	-0.12755100	4.55634900
C	4.82167300	1.66686500	0.94309900
O	4.74966100	2.87071800	1.07847100
C	5.97617600	0.84844500	0.61053700
H	6.99271700	1.20633200	0.52042300
C	5.57041600	-0.43509600	0.45209500
N	4.21188400	-0.59079000	0.71510000
C	3.38495100	-1.60592100	0.25816700

O	2.31246500	-1.84649300	0.77040400
O	3.91276500	-2.22190700	-0.79776900
C	3.29348800	-3.42039000	-1.36138900
C	4.27976900	-3.81683500	-2.45229400
H	4.35566400	-3.02891900	-3.20816600
H	3.94444500	-4.73672400	-2.94014600
H	5.27201000	-3.98771900	-2.02108000
C	3.19644700	-4.51689600	-0.30677300
H	2.52104200	-4.23616800	0.50320900
H	4.18708200	-4.73315400	0.10647600
H	2.81605100	-5.42890900	-0.77756400
C	1.93666600	-3.06022800	-1.95580000
H	1.20899400	-2.82833400	-1.17599400
H	1.56554000	-3.90391500	-2.54645700
H	2.03537600	-2.19316800	-2.61783900
C	6.45404000	-1.58554600	0.18093700
C	8.20353000	-3.71594100	-0.27657200
C	6.28050700	-2.79823500	0.85954000
C	7.51193700	-1.44602500	-0.72130400
C	8.37987600	-2.51083900	-0.95251400
C	7.15510100	-3.85508700	0.63473600
H	5.46601100	-2.90856900	1.57183400
H	7.64159800	-0.50763100	-1.25294400
H	9.19239000	-2.39768500	-1.66358400
H	7.01923300	-4.78955200	1.17102300
H	8.88144000	-4.54492300	-0.45571200
C	-6.44777200	0.39949700	-0.99614000
O	-6.65611800	1.55643600	-1.29170100
O	-5.28237600	-0.07941300	-0.58600000
H	-4.65849300	0.67475200	-0.41428600

O -7.33038000 -0.60241900 -1.02364300

C -8.63621100 -0.40557500 -1.64961100

C -9.45043400 0.64093700 -0.89655600

H -9.52096600 0.38086100 0.16466800

H -10.46499200 0.66445300 -1.30709700

H -9.00949600 1.63363900 -0.99140200

C -8.45022900 -0.03951400 -3.11818400

H -7.99533700 0.94680600 -3.22717300

H -9.42526700 -0.03078400 -3.61495800

H -7.81771000 -0.78272600 -3.61455100

C -9.28287300 -1.77834300 -1.51838900

H -9.37716600 -2.05640200 -0.46343600

H -8.68333100 -2.53727500 -2.03060600

H -10.28173500 -1.76261600 -1.96399500

Zero-point correction= 1.074489 (Hartree/Particle)

Thermal correction to Energy= 1.140781

Thermal correction to Enthalpy= 1.141726

Thermal correction to Gibbs Free Energy= 0.967071

Sum of electronic and zero-point Energies= -2890.095134

Sum of electronic and thermal Energies= -2890.028842

Sum of electronic and thermal Enthalpies= -2890.027898

Sum of electronic and thermal Free Energies= -2890.202552

E(RM062X/6-311+G(2d,p)) = -2892.07731702

RR-**TS4**-CONF4

C 0.99809600 -0.51184100 0.01073500

H 0.31044500 -0.25683200 -0.78601100

H 0.77279500 -1.43764100 0.53185000

C 2.31978600 -0.11569900 -0.10004500

C 2.75523600 0.90579400 -1.01734500

O	3.89878300	1.35405100	-1.06863400
O	1.79337600	1.31437900	-1.88479800
C	2.17644600	2.31243900	-2.83052600
H	2.26756700	3.27716300	-2.31468200
H	3.15987100	2.06620900	-3.24123600
C	1.11455100	2.34575100	-3.90816200
H	0.13507700	2.54932100	-3.46819700
H	1.07376300	1.38424800	-4.42943100
H	1.34560000	3.12627100	-4.63991800
C	3.35391500	-0.56152600	0.87491800
H	2.91246100	-1.18136600	1.65976200
H	3.87611300	0.27242300	1.34992000
N	4.42947500	-1.38340700	0.23129300
C	4.15048800	-2.64120300	-0.17420400
H	3.13746300	-2.98194200	0.01167500
C	5.08322900	-3.43267000	-0.78379600
H	4.79814500	-4.43421500	-1.07630300
C	5.65494000	-0.86830800	0.00419200
H	5.80113900	0.15665800	0.32114900
C	6.64452700	-1.59407200	-0.60521400
H	7.60589700	-1.12220200	-0.75691900
C	6.39529700	-2.93034400	-1.02130900
N	7.34099700	-3.67986600	-1.60735200
C	7.04474800	-5.04930400	-2.00897700
H	7.94100600	-5.48906900	-2.44275400
H	6.24536600	-5.07488000	-2.75714800
H	6.74281400	-5.65303500	-1.14664600
C	8.66883200	-3.12718100	-1.84260700
H	9.28241200	-3.88272600	-2.33025500
H	9.14728000	-2.84311200	-0.89925700

H	8.61697000	-2.24731200	-2.49247700
N	-0.13717300	0.48101200	1.33379600
N	-1.35729600	-0.18637100	1.50106800
C	-1.41858300	-1.38728900	2.16329800
O	-2.46321900	-1.97510400	2.38803200
O	-0.20926300	-1.85722000	2.51155400
C	-0.19615900	-3.13866800	3.17775800
H	-1.03631600	-3.16013600	3.87652900
C	-0.34413400	-4.24783800	2.14996000
H	0.48384200	-4.21153700	1.43246700
H	-1.28937900	-4.14817600	1.61022400
H	-0.32842300	-5.22357500	2.64546200
C	1.11935800	-3.19922800	3.92829800
H	1.96306800	-3.16120200	3.23024700
H	1.18195900	-4.13402700	4.49316600
H	1.20186200	-2.36228800	4.62688200
C	0.40572500	0.83184600	2.54568600
O	-0.11406600	0.78135900	3.64962500
O	1.65852200	1.30885400	2.34788200
C	2.28282300	1.97131100	3.45917000
H	1.50469200	2.50363900	4.01489500
C	3.26667600	2.95751500	2.85554400
H	4.03133900	2.43098500	2.27304300
H	3.76552700	3.52410600	3.64811500
H	2.74860900	3.65209500	2.18955300
C	2.94707200	0.95030900	4.36854500
H	3.72119400	0.39926300	3.82257100
H	2.20505900	0.24316400	4.74726100
H	3.41880700	1.45108700	5.22032500
C	-2.63585300	0.40120800	1.09934300

C	-2.45081000	1.83810400	0.55206000
H	-1.60265200	1.77809200	-0.13119700
C	-2.14747700	2.85657700	1.65469100
H	-1.71945700	3.75542600	1.19735700
H	-1.45880000	2.47420800	2.41049800
H	-3.06646400	3.15107000	2.17167800
C	-3.65090400	2.30969300	-0.26939400
H	-4.57965000	2.30232100	0.31307400
H	-3.79466900	1.70142900	-1.16673600
H	-3.46698500	3.33946500	-0.59192100
C	-3.67803500	0.37985700	2.26416000
O	-3.47606300	0.87779200	3.35136600
C	-4.88210900	-0.25209300	1.75275400
H	-5.82949400	-0.30795700	2.27075800
C	-4.62708300	-0.74282200	0.51686600
N	-3.32908600	-0.45841200	0.10332400
C	-2.64664800	-0.97765700	-0.98380600
O	-1.72336600	-0.39045600	-1.50919200
O	-3.11404700	-2.17533200	-1.32386400
C	-2.64136800	-2.85419400	-2.53041400
C	-3.50768100	-4.10656800	-2.55993100
H	-3.34870400	-4.70372500	-1.65671200
H	-3.25283000	-4.71452100	-3.43282300
H	-4.56681500	-3.83387100	-2.61731600
C	-2.89763600	-1.99628400	-3.76408300
H	-2.30748400	-1.07834200	-3.74540600
H	-3.96025400	-1.74285800	-3.83526900
H	-2.62302100	-2.56857100	-4.65590300
C	-1.16806100	-3.21391700	-2.37075200
H	-0.53635200	-2.32395800	-2.39082000

H	-0.86944200	-3.87642700	-3.18948000
H	-1.01088900	-3.74312200	-1.42497700
C	-5.62669600	-1.37265900	-0.36926200
C	-7.61085600	-2.48556500	-1.98973700
C	-6.49078900	-2.34191900	0.14457500
C	-5.76558300	-0.95595600	-1.69862000
C	-6.75675600	-1.50719200	-2.50233200
C	-7.47575700	-2.90086400	-0.66719200
H	-6.37626400	-2.66794400	1.17425000
H	-5.10358300	-0.19073400	-2.09758100
H	-6.86465900	-1.17256700	-3.52984700
H	-8.13649900	-3.66211200	-0.26399000
H	-8.38071600	-2.91921600	-2.62077500
C	0.36570200	3.81793800	-0.57899000
O	-0.54633000	3.52549300	-1.32372400
O	0.88929600	3.03445200	0.35234100
H	0.44199400	2.15334400	0.37649200
O	1.01535600	4.98296300	-0.54410900
C	0.56232000	6.10783600	-1.35699500
C	0.70861400	5.78918600	-2.84053000
H	1.74123400	5.50354600	-3.06804700
H	0.46673400	6.68356200	-3.42393800
H	0.03688200	4.98328200	-3.14052800
C	-0.86977600	6.47657400	-0.98372900
H	-1.57627100	5.70704500	-1.29967100
H	-1.13768400	7.41886800	-1.47187100
H	-0.95172700	6.61617100	0.09939600
C	1.52209400	7.21978700	-0.95255900
H	2.55473400	6.93083000	-1.17079900
H	1.43629600	7.42983900	0.11788600

H 1.28888400 8.13234100 -1.50865000

Zero-point correction= 1.075406 (Hartree/Particle)

Thermal correction to Energy= 1.141635

Thermal correction to Enthalpy= 1.142579

Thermal correction to Gibbs Free Energy= 0.969918

Sum of electronic and zero-point Energies= -2890.098449

Sum of electronic and thermal Energies= -2890.032219

Sum of electronic and thermal Enthalpies= -2890.031275

Sum of electronic and thermal Free Energies= -2890.203937

E(RM062X/6-311+G(2d,p)) = -2892.07993225

RR-**TS4**-CONF5

C 1.19589000 -0.75936400 0.17586600

H 0.47912700 -0.73546400 -0.63883600

H 1.09422300 -1.59146400 0.86442700

C 2.45820800 -0.22756800 -0.02175900

C 2.76987300 0.67544500 -1.10014200

O 3.86947500 1.19476700 -1.27909900

O 1.73977400 0.89431200 -1.95513300

C 2.02828300 1.74418600 -3.06488300

H 2.30903000 2.73696200 -2.69676200

H 2.88693100 1.34354900 -3.61477200

C 0.78915000 1.79985900 -3.92962300

H -0.05376000 2.18682900 -3.35197600

H 0.53595400 0.80183900 -4.30105500

H 0.96332000 2.45497100 -4.78923800

C 3.54647600 -0.39113000 0.98497400

H 3.19967500 -0.95976200 1.84903100

H 3.93947500 0.56277900 1.34413200

N 4.72778300 -1.12797600 0.42687300

C	4.62629200	-2.45300500	0.18814800
H	3.67134000	-2.90387600	0.43676100
C	5.65854700	-3.17988800	-0.33646200
H	5.51414400	-4.23983700	-0.49601700
C	5.87121700	-0.48405700	0.11934900
H	5.87721000	0.58183900	0.30781100
C	6.95130500	-1.13847100	-0.41292300
H	7.83887000	-0.56279300	-0.63760000
C	6.88727500	-2.53635300	-0.66045600
N	7.92575400	-3.21576900	-1.17221600
C	7.81586200	-4.64951900	-1.40962200
H	8.76427200	-5.01418500	-1.79989700
H	7.02950200	-4.86849700	-2.13999200
H	7.59427900	-5.18410500	-0.47990500
C	9.16170300	-2.51862600	-1.50466700
H	9.87237200	-3.23670600	-1.91034100
H	9.60199200	-2.05532200	-0.61519300
H	8.98368500	-1.74219100	-2.25613200
N	-0.06981800	0.32989300	1.29879500
N	-1.36158300	-0.22084400	1.32201400
C	-1.60021700	-1.42166400	1.94269500
O	-2.71129500	-1.90876000	2.06399000
O	-0.47647800	-2.00651800	2.38866800
C	-0.62762200	-3.29212600	3.02725400
H	-1.50110900	-3.23918500	3.68333600
C	-0.82771800	-4.36943500	1.97446900
H	0.03500200	-4.40139900	1.29948000
H	-1.73112900	-4.17567400	1.39098900
H	-0.92711700	-5.34776200	2.45490300
C	0.63961000	-3.48988800	3.83645700

H	1.51312400	-3.52019200	3.17546400
H	0.58859100	-4.43435700	4.38589000
H	0.77408100	-2.67450100	4.55299100
C	0.43862000	0.59303700	2.54574400
O	1.61589300	0.86458400	2.74106400
O	-0.47158700	0.55287300	3.54812600
C	-0.01824100	0.92889400	4.85664400
H	0.97641100	0.49919000	5.01209600
C	-1.02152100	0.32915300	5.82417500
H	-2.02066400	0.72517600	5.61693600
H	-0.74972100	0.57677000	6.85489600
H	-1.05459800	-0.76002000	5.72320400
C	0.05165400	2.44474600	4.95415000
H	-0.94466000	2.87380700	4.80046700
H	0.73243600	2.84459900	4.19764300
H	0.41185500	2.74733100	5.94283000
C	-2.53521400	0.49989500	0.82782000
C	-2.15847800	1.90960100	0.30705000
H	-1.26003500	1.76166600	-0.29281300
C	-1.86014000	2.90319900	1.43212300
H	-1.35193600	3.77336000	1.00330500
H	-1.23521600	2.47643400	2.21817200
H	-2.78591700	3.25097900	1.90137500
C	-3.22006400	2.49357300	-0.62550700
H	-4.19865100	2.57884800	-0.13841400
H	-3.33241000	1.89913400	-1.53661900
H	-2.90390600	3.49884900	-0.92140700
C	-3.66473000	0.58327000	1.90438100
O	-3.50387200	1.05752200	3.01009300
C	-4.88003000	0.07733500	1.29071900

H	-5.86775600	0.11650000	1.72886700
C	-4.57604300	-0.43354000	0.07350300
N	-3.22685100	-0.28248600	-0.23033100
C	-2.50486500	-0.87550900	-1.25267800
O	-1.46712300	-0.40309600	-1.66853900
O	-3.07699500	-2.00504700	-1.66058200
C	-2.58294700	-2.71541600	-2.84007700
C	-3.55227800	-3.88551600	-2.94503900
H	-3.49424200	-4.51305700	-2.05023100
H	-3.30513900	-4.49550200	-3.81874500
H	-4.57889400	-3.51893600	-3.04977500
C	-2.68121500	-1.82373000	-4.07226000
H	-2.04801600	-0.93940600	-3.97619100
H	-3.71763700	-1.51115100	-4.23405400
H	-2.35407700	-2.39115500	-4.94934300
C	-1.16025700	-3.20837500	-2.59560400
H	-0.44335400	-2.38587700	-2.61103500
H	-0.89176700	-3.92560500	-3.37790800
H	-1.09953700	-3.71721700	-1.62782700
C	-5.56031500	-0.95611300	-0.89546700
C	-7.51134700	-1.85485100	-2.68040800
C	-6.55781300	-1.83223200	-0.46219300
C	-5.54809000	-0.52460700	-2.22710800
C	-6.52280800	-0.96865000	-3.11293900
C	-7.52642100	-2.28488300	-1.35576000
H	-6.56011400	-2.17078700	0.56975400
H	-4.77964500	0.16756800	-2.56356700
H	-6.51257200	-0.62286400	-4.14233300
H	-8.29182000	-2.97511700	-1.01463700
H	-8.26821600	-2.20567600	-3.37540300

C	0.93239200	3.58754900	-0.49029600
O	0.00794200	3.46729200	-1.26772500
O	1.27816800	2.72221000	0.44999500
H	0.70219300	1.91612500	0.44041300
O	1.77054700	4.62375100	-0.42615400
C	1.52110500	5.82129100	-1.22239100
C	1.66351100	5.51616200	-2.70954100
H	2.65463900	5.09971700	-2.91764200
H	1.55873400	6.44655200	-3.27723800
H	0.89875800	4.81287900	-3.04531800
C	0.15286300	6.40352800	-0.88063800
H	-0.65676500	5.77416800	-1.25374600
H	0.06167800	7.39593600	-1.33321900
H	0.05177500	6.51163100	0.20458000
C	2.62779400	6.76322500	-0.76413800
H	3.60951800	6.31725600	-0.95032800
H	2.53542900	6.97105500	0.30624200
H	2.56265000	7.70789500	-1.31168200

Zero-point correction= 1.075624 (Hartree/Particle)

Thermal correction to Energy= 1.141612

Thermal correction to Enthalpy= 1.142557

Thermal correction to Gibbs Free Energy= 0.970641

Sum of electronic and zero-point Energies= -2890.099043

Sum of electronic and thermal Energies= -2890.033054

Sum of electronic and thermal Enthalpies= -2890.032110

Sum of electronic and thermal Free Energies= -2890.204026

E(RM062X/6-311+G(2d,p)) = -2892.08032741

RR-**TS4**-CONF6

C	1.07769600	-0.51414000	-0.58588000

H	0.25571600	-0.07536700	-1.14144700
H	1.06273400	-1.59849200	-0.55248200
C	2.34251000	0.08817600	-0.72986100
C	2.52665400	1.37397600	-1.32313900
O	3.58348300	2.00230000	-1.38216200
O	1.38450100	1.90500500	-1.87953200
C	1.52789900	3.22039400	-2.40391100
H	1.81844800	3.90575300	-1.59706400
H	2.33122000	3.23802300	-3.14749400
C	0.20303900	3.62203900	-3.01643100
H	-0.60337500	3.53281500	-2.28216300
H	-0.04032300	2.98264800	-3.87081000
H	0.24894800	4.65921300	-3.36366500
C	3.56411000	-0.58422300	-0.22518600
H	3.32764800	-1.38447400	0.48098800
H	4.26304900	0.10669900	0.25275900
N	0.86799300	2.59663200	0.87238600
C	2.06880300	3.02762800	1.30923700
H	2.77375300	2.24801000	1.56860500
C	2.33965700	4.36581800	1.41416900
H	3.31602000	4.66697100	1.76825700
C	-0.09045800	3.46608200	0.49174700
H	-1.00327000	3.02465900	0.10654600
C	0.10748200	4.81746300	0.57527400
H	-0.68853500	5.47738100	0.25780600
C	1.34994100	5.32543100	1.05651500
N	1.57707100	6.64361500	1.15815000
C	2.87034100	7.13032400	1.62364400
H	2.85219800	8.21870700	1.63173300
H	3.67630600	6.79804400	0.96080300

H	3.07814200	6.77704200	2.63896200
C	0.54688200	7.59662900	0.76457000
H	0.30537000	7.49816200	-0.29951300
H	0.91461600	8.60502200	0.94576400
H	-0.36598600	7.44847900	1.35065100
N	0.24153700	-0.33156600	1.07005400
N	-0.92420700	-1.10748000	1.10062500
C	-0.80110300	-2.46224600	0.84986800
O	0.24695000	-3.07392400	0.83033400
O	-1.99758400	-3.00820800	0.58763900
C	-2.06312500	-4.45257600	0.55134000
H	-1.19870700	-4.80597600	-0.01714400
C	-2.02497600	-4.99313900	1.97022700
H	-2.87364300	-4.60503100	2.54246200
H	-1.09923000	-4.69886100	2.47237500
H	-2.07918000	-6.08611600	1.95412800
C	-3.35260300	-4.78367400	-0.17374400
H	-4.21444500	-4.44302800	0.40981400
H	-3.43256800	-5.86602500	-0.31061200
H	-3.37895100	-4.30319400	-1.15642800
C	1.09754200	-0.49453000	2.13577400
O	2.10946700	0.18928900	2.24419800
O	0.74727000	-1.42815100	3.03465600
C	1.63618400	-1.62571000	4.15321300
H	2.66216000	-1.55625300	3.78109000
C	1.34275100	-3.02633100	4.65519800
H	1.52783600	-3.76198000	3.86755500
H	0.29530300	-3.10297100	4.96612800
H	1.98068700	-3.26036100	5.51275100
C	1.39460700	-0.55822200	5.20802000

H	0.37612300	-0.63553700	5.60361800
H	1.54024400	0.43996100	4.78648300
H	2.09706100	-0.68965600	6.03729900
C	-2.23099600	-0.49067600	1.33851800
C	-2.09450100	0.89163300	2.03607200
H	-1.30899000	1.39713200	1.48074300
C	-1.65683700	0.77734200	3.49811900
H	-1.20128000	1.72339700	3.81056600
H	-0.94078300	-0.03024600	3.65019700
H	-2.51342500	0.58067700	4.15075000
C	-3.36022900	1.74117500	1.92192200
H	-4.22806000	1.24994900	2.37601200
H	-3.59976900	1.98193100	0.88189500
H	-3.19811400	2.68389900	2.45520000
C	-3.15220500	-1.41834900	2.19583700
O	-2.81717600	-1.88277900	3.26615700
C	-4.41396200	-1.53201600	1.48939700
H	-5.30665100	-2.00772700	1.87155400
C	-4.29357700	-0.93836400	0.27488600
N	-3.03500800	-0.37583200	0.09743400
C	-2.49961400	0.22530900	-1.03214200
O	-1.64140700	1.08482200	-0.95504400
O	-3.00816200	-0.28702300	-2.14184300
C	-2.67829200	0.27088300	-3.45855000
C	-3.51266000	-0.59258100	-4.39465100
H	-3.20968800	-1.64149000	-4.32109900
H	-3.37330800	-0.25899500	-5.42698300
H	-4.57469500	-0.51429500	-4.13912900
C	-3.12105100	1.72683200	-3.53283500
H	-2.58895800	2.34289900	-2.80548500

H	-4.19880900	1.80587600	-3.35698900
H	-2.90827800	2.11254100	-4.53506400
C	-1.18930900	0.09487000	-3.73254400
H	-0.57786700	0.74168400	-3.09914500
H	-0.99093300	0.33866600	-4.78167300
H	-0.89827700	-0.94774000	-3.56500700
C	-5.39006600	-0.77693300	-0.70154100
C	-7.54604400	-0.46870000	-2.44767600
C	-5.69169000	0.48369400	-1.23025900
C	-6.17964900	-1.87723100	-1.04133800
C	-7.25037000	-1.72288700	-1.91963200
C	-6.76864700	0.63636400	-2.09535000
H	-5.09018100	1.34576100	-0.95071800
H	-5.94267300	-2.85417100	-0.62992000
H	-7.85222700	-2.58489000	-2.19007900
H	-7.00347000	1.61822000	-2.49542700
H	-8.38234900	-0.34874800	-3.12956200
C	5.42541800	-1.79743600	-1.02958700
O	5.89453300	-1.87326400	0.08681600
O	4.28774800	-1.20121500	-1.34821100
O	5.95683200	-2.29866800	-2.14945300
C	7.22164900	-3.02180400	-2.10149800
C	8.33776000	-2.10185600	-1.61760500
H	8.35757900	-1.18726000	-2.21933500
H	9.30024500	-2.61026600	-1.73393900
H	8.20655000	-1.83490500	-0.56800200
C	7.08391200	-4.27126500	-1.23771400
H	6.94759900	-4.01560500	-0.18595200
H	7.98822200	-4.88004200	-1.33749300
H	6.22971000	-4.86806000	-1.57416200

C	7.44351400	-3.40568000	-3.55949300
H	7.50031800	-2.51053400	-4.18636800
H	6.62170900	-4.03235100	-3.91933700
H	8.37904800	-3.96354700	-3.65995300
H	0.69077000	1.58193900	0.79930500

Zero-point correction= 1.076225 (Hartree/Particle)

Thermal correction to Energy= 1.142130

Thermal correction to Enthalpy= 1.143074

Thermal correction to Gibbs Free Energy= 0.971136

Sum of electronic and zero-point Energies= -2890.090926

Sum of electronic and thermal Energies= -2890.025021

Sum of electronic and thermal Enthalpies= -2890.024077

Sum of electronic and thermal Free Energies= -2890.196015

E(RM062X/6-311+G(2d,p)) = -2892.07067193

***RR*-TS5**

C	1.33173000	-0.74610200	0.60620900
H	1.21116000	-0.88423800	1.68290700
H	0.71576800	0.11072500	0.31999700
C	2.76261400	-0.49032500	0.24789800
C	3.84659300	-0.87907200	1.11463100
O	5.04608900	-0.72430900	0.89154600
O	3.43257100	-1.45217000	2.27968400
C	4.45141100	-1.73839100	3.23542000
H	5.20293000	-2.40216500	2.79722000
H	4.95971700	-0.80846200	3.51495800
C	3.77852100	-2.38242100	4.42843800
H	3.27812700	-3.30936200	4.13253700
H	3.03210300	-1.71017000	4.86196600
H	4.52083100	-2.61841300	5.19656600

C	3.08792300	0.22518900	-0.90011300
H	2.35791400	0.26766200	-1.70324600
H	4.12561600	0.21393300	-1.22454200
N	3.01907700	2.09864800	-0.61106100
C	3.12557300	2.98447100	-1.60695700
H	3.30962900	2.57317800	-2.59781000
C	3.01221400	4.34373700	-1.40989900
H	3.10599200	5.00866000	-2.25872700
C	2.80001500	2.53695800	0.62570900
H	2.71956700	1.75605000	1.38393600
C	2.67493500	3.87548600	0.93481100
H	2.49759700	4.16476000	1.96273900
C	2.77668600	4.84079400	-0.10030100
N	2.65380600	6.16507800	0.14607300
C	2.76776900	7.12268100	-0.94239400
H	2.65084400	8.12854400	-0.54111700
H	1.99143500	6.95916200	-1.69884100
H	3.74784100	7.05591600	-1.42858800
C	2.41012400	6.63017200	1.50186100
H	2.33703100	7.71668900	1.49431400
H	3.22680700	6.34189900	2.17374900
H	1.47286600	6.22263000	1.89861400
N	0.65765900	-1.89759100	-0.08813000
N	-0.59507800	-1.67417100	-0.61628600
C	-0.72215600	-1.16935100	-1.89590500
O	-1.80100200	-0.98683700	-2.42369200
O	0.45853800	-0.89291600	-2.45304200
C	0.40675400	-0.33435300	-3.79058200
H	-0.41511900	-0.82387500	-4.31855800
C	0.14848000	1.15880300	-3.69334500

H	0.94246500	1.64652600	-3.11597100
H	-0.81180600	1.35230800	-3.20713700
H	0.12560500	1.60109600	-4.69405900
C	1.72885100	-0.68035000	-4.44583300
H	2.56655700	-0.20698200	-3.92285300
H	1.72588200	-0.32617700	-5.48095500
H	1.88243600	-1.76290500	-4.44897900
C	1.32826400	-2.99409500	-0.59314700
O	0.95037800	-3.66655800	-1.53072600
O	2.42440500	-3.24021300	0.13217100
C	3.42307700	-4.08447800	-0.47964700
H	2.91775700	-4.97341700	-0.86835100
C	4.38565300	-4.44620300	0.63346200
H	4.90003100	-3.54375700	0.97999900
H	5.13418100	-5.15297300	0.26309000
H	3.85774400	-4.90350600	1.47539000
C	4.11180700	-3.32429300	-1.60277300
H	4.63566400	-2.45483000	-1.19070100
H	3.38690900	-2.98686900	-2.34946200
H	4.84142400	-3.97296000	-2.09804800
C	-1.82168700	-2.04741800	0.09838400
C	-1.49744100	-2.79247600	1.42261200
H	-0.66046300	-2.24695500	1.86582100
C	-1.08007100	-4.25020500	1.19850900
H	-0.53890600	-4.60369700	2.08173800
H	-0.45144000	-4.38766000	0.31750800
H	-1.96035700	-4.88694700	1.06365400
C	-2.66513100	-2.72939800	2.40859100
H	-3.59030900	-3.12038600	1.96969800
H	-2.84350600	-1.70919500	2.75843900

H	-2.42561600	-3.34674000	3.28025700
C	-2.76414500	-2.89672800	-0.81860700
O	-2.41110500	-3.91895000	-1.36645500
C	-4.06178200	-2.24889400	-0.81400300
H	-4.96328600	-2.64680100	-1.25838600
C	-3.95529100	-1.06268400	-0.16730500
N	-2.67496000	-0.85919800	0.33684400
C	-2.13942500	0.29629600	0.89050300
O	-1.24687500	0.25790800	1.71202000
O	-2.69503500	1.38659300	0.37591900
C	-2.36644600	2.71580500	0.89762000
C	-3.23216100	3.62612900	0.03743200
H	-2.95264700	3.53751700	-1.01697200
H	-3.10090300	4.66613800	0.34968400
H	-4.28813000	3.35709200	0.14421400
C	-2.76740700	2.81703200	2.36438400
H	-2.20230100	2.11584800	2.98203800
H	-3.83799100	2.62168000	2.48074500
H	-2.56403300	3.83254400	2.71880500
C	-0.88415100	3.01046600	0.68361900
H	-0.25940400	2.42819200	1.36275800
H	-0.70392900	4.07538800	0.86544400
H	-0.59531700	2.78666200	-0.34971000
C	-5.07515800	-0.14205700	0.10962900
C	-7.27981100	1.48805700	0.63791700
C	-5.98526100	0.15856200	-0.90654700
C	-5.27729300	0.37231100	1.39576400
C	-6.37859000	1.17915900	1.65819900
C	-7.08086700	0.97748800	-0.64270100
H	-5.82142500	-0.23631500	-1.90493300

H -4.57986800 0.12793100 2.19384500

H -6.53517600 1.56654800 2.66053500

H -7.77789000 1.21605800 -1.43999700

H -8.13618700 2.12287900 0.84404700

Zero-point correction= 0.920249 (Hartree/Particle)

Thermal correction to Energy= 0.975997

Thermal correction to Enthalpy= 0.976941

Thermal correction to Gibbs Free Energy= 0.827568

Sum of electronic and zero-point Energies= -2468.164316

Sum of electronic and thermal Energies= -2468.108568

Sum of electronic and thermal Enthalpies= -2468.107624

Sum of electronic and thermal Free Energies= -2468.256997

E(RM062X/6-311+G(2d,p)) = -2469.84517810

RS-**TS4**-CONF1

C -2.27025800 0.60104300 -0.83724100

H -2.01715000 1.24281100 -1.67260700

H -2.07952100 -0.45469600 -1.00743800

C -3.32916400 0.97944800 -0.03135700

C -3.89515100 2.30548200 -0.06823200

O -4.80390900 2.71039500 0.65534400

O -3.35894300 3.09624400 -1.02723200

C -3.78435300 4.45806400 -1.03565700

H -3.56223300 4.91044700 -0.06383400

H -4.86856600 4.50047000 -1.18676800

C -3.03647200 5.15597300 -2.15053900

H -1.96036500 5.11252900 -1.96344800

H -3.24956800 4.68212800 -3.11381300

H -3.34422200 6.20472400 -2.20680200

C -3.75525200 0.11445100 1.10646500

H	-2.91769700	-0.46698100	1.49746500
H	-4.19462500	0.71173600	1.90749600
N	-4.79577900	-0.88935500	0.71864800
C	-4.48371100	-2.19269100	0.57314500
H	-3.45132000	-2.45544100	0.78459300
C	-5.41345600	-3.11558700	0.16906900
H	-5.10201100	-4.14659300	0.06763800
C	-6.04687500	-0.46055900	0.44201100
H	-6.20563600	0.60798400	0.55642900
C	-7.03146700	-1.32093200	0.04117900
H	-8.01540800	-0.91941900	-0.16045100
C	-6.74814600	-2.70932200	-0.10544900
N	-7.69180600	-3.58521000	-0.48580200
C	-7.36165000	-4.99715700	-0.62930400
H	-8.25941500	-5.53892000	-0.92249800
H	-6.59637700	-5.14598500	-1.39873500
H	-6.99779700	-5.41160700	0.31682200
C	-9.04614700	-3.12627900	-0.76741700
H	-9.65448000	-3.98373200	-1.04973900
H	-9.49275800	-2.65740800	0.11580500
H	-9.05362500	-2.40624800	-1.59283700
N	-0.50257900	0.70788200	0.08756500
C	-0.63178600	1.04363000	1.38256000
O	-1.27679000	2.05657700	1.71514300
O	-0.09874200	0.22278700	2.30271700
C	-0.11649700	0.68861000	3.66560300
H	-1.06910000	1.19666800	3.83711500
C	-0.02738900	-0.55125000	4.53432800
H	0.90930900	-1.08564400	4.34917500
H	-0.06377400	-0.27020500	5.59132400

H	-0.86080400	-1.22837300	4.32375300
C	1.03488000	1.65790500	3.87214600
H	1.98689000	1.15297800	3.67982700
H	0.94492900	2.50106200	3.18064100
H	1.03245000	2.03858500	4.89897400
C	0.37472300	4.37308100	0.21066900
O	1.18439400	3.86106400	0.96079900
O	-0.87381300	3.99477000	0.04735100
H	-1.06247700	3.19491100	0.64257200
O	0.60766400	5.42559200	-0.58678200
C	1.88706600	6.11908400	-0.54100000
C	3.00543200	5.19684700	-1.01320100
H	2.78714500	4.82800600	-2.02123100
H	3.94604700	5.75617000	-1.05130100
H	3.12756200	4.34836400	-0.33725900
C	2.14281800	6.66862600	0.85913400
H	2.33279200	5.86706100	1.57417500
H	3.01348900	7.33154100	0.83271600
H	1.27881600	7.25089500	1.19636800
C	1.68671200	7.26145000	-1.52969500
H	1.44537600	6.86868700	-2.52225600
H	0.86917400	7.91160400	-1.20319200
H	2.60104400	7.85766500	-1.60197300
N	0.27976400	-0.41283000	-0.18544900
C	-0.23897700	-1.64971700	0.10388300
O	-1.25834700	-1.84801700	0.74502500
O	0.53172700	-2.63210200	-0.38733400
C	0.02608200	-3.98042400	-0.28080800
H	-0.38422800	-4.10308800	0.72534800
C	-1.05313300	-4.19736300	-1.32794300

H	-0.64059200	-4.02964900	-2.32859500
H	-1.89142000	-3.51212200	-1.17426000
H	-1.42807800	-5.22421300	-1.27303800
C	1.22991500	-4.87900600	-0.48431900
H	1.61651600	-4.76533800	-1.50245100
H	0.94495000	-5.92459500	-0.33550900
H	2.02474600	-4.62554100	0.22344400
C	1.42009300	-0.24983900	-1.09770700
C	1.77304700	1.25891900	-1.31438500
H	1.63611100	1.72501900	-0.33493400
C	0.86537900	1.96768400	-2.32052200
H	-0.18927100	1.78390000	-2.12650300
H	1.09117100	1.65871800	-3.34710700
H	1.04071700	3.04755300	-2.24785300
C	3.23552400	1.44555800	-1.73122700
H	3.49710300	0.83801600	-2.60561000
H	3.92511600	1.20666700	-0.91706600
H	3.39279900	2.49356300	-2.00326200
C	1.14433400	-0.97980500	-2.44303700
O	0.11641600	-0.82589500	-3.07482200
C	2.30510700	-1.79741400	-2.73001000
H	2.49949500	-2.32582600	-3.65325100
C	3.12425900	-1.77623600	-1.64505100
N	2.62341400	-0.97371900	-0.62852200
C	3.05005500	-0.87263200	0.68968100
O	2.78589300	0.08586900	1.38098500
O	3.72970600	-1.95941800	1.05045900
C	4.47591200	-2.00533500	2.30758700
C	5.16929300	-3.35921700	2.23121900
H	4.43222700	-4.16688400	2.18343400

H	5.79177500	-3.50687300	3.11855600
H	5.80558300	-3.41123800	1.34144700
C	5.50071300	-0.87817100	2.35856000
H	5.01834700	0.10139100	2.34877800
H	6.19108300	-0.95103700	1.51237300
H	6.08145200	-0.96886500	3.28192200
C	3.50585900	-1.95398700	3.48069900
H	3.05433700	-0.96475900	3.57095800
H	4.04321000	-2.18461400	4.40614300
H	2.71319600	-2.69757300	3.34557500
C	4.46444000	-2.39646300	-1.59673900
C	7.01828100	-3.52386800	-1.65906100
C	4.64070400	-3.70929200	-2.03785400
C	5.57548600	-1.64365000	-1.19843100
C	6.84662300	-2.20417200	-1.23598300
C	5.91489500	-4.27365200	-2.05852900
H	3.77806300	-4.29030100	-2.35055300
H	5.44001800	-0.61571200	-0.87120800
H	7.70552500	-1.61183900	-0.93466100
H	6.04297300	-5.29949600	-2.38995600
H	8.01133100	-3.96236100	-1.68056900

Zero-point correction= 1.075846 (Hartree/Particle)

Thermal correction to Energy= 1.141594

Thermal correction to Enthalpy= 1.142539

Thermal correction to Gibbs Free Energy= 0.971931

Sum of electronic and zero-point Energies= -2890.102708

Sum of electronic and thermal Energies= -2890.036960

Sum of electronic and thermal Enthalpies= -2890.036015

Sum of electronic and thermal Free Energies= -2890.206623

E(RM062X/6-311+G(2d,p)) = -2892.08229609

RS-**TS4**-CONF2

C	-2.30094500	0.50324800	-0.90766500
H	-2.05691100	1.15425600	-1.73836800
H	-2.06463800	-0.54356900	-1.07260400
C	-3.38451800	0.83558100	-0.11570400
C	-3.99143000	2.14365000	-0.14226300
O	-4.91957800	2.51106400	0.57666500
O	-3.46720200	2.96315400	-1.08372400
C	-3.93115100	4.31242200	-1.07711500
H	-3.75250800	4.74909000	-0.08962000
H	-5.01080500	4.32761600	-1.26319400
C	-3.16751800	5.05494900	-2.15156600
H	-2.09761200	5.03871500	-1.92755900
H	-3.33344100	4.59567600	-3.13107200
H	-3.50366000	6.09546400	-2.19717300
C	-3.78911500	-0.05675400	1.00875200
H	-2.93724000	-0.62814900	1.38419500
H	-4.23520500	0.51635000	1.82362600
N	-4.81177900	-1.07406400	0.60912200
C	-4.46748700	-2.36264800	0.41288500
H	-3.42353000	-2.60299800	0.59192100
C	-5.38058600	-3.29760700	-0.00054900
H	-5.04423400	-4.31573600	-0.14294500
C	-6.07957700	-0.67129100	0.37248500
H	-6.26458100	0.38817500	0.52527000
C	-7.04857700	-1.54496700	-0.03781800
H	-8.04763100	-1.16479300	-0.20363800
C	-6.73098000	-2.91939200	-0.23538500
N	-7.65818100	-3.80812400	-0.62639200

C	-7.29751600	-5.20822700	-0.80717000
H	-8.19032300	-5.76701600	-1.08329700
H	-6.55175600	-5.32410300	-1.60122900
H	-6.89616300	-5.63058200	0.11997000
C	-9.02604100	-3.37457900	-0.88093500
H	-9.61139800	-4.23440400	-1.20195600
H	-9.48184500	-2.95948600	0.02439900
H	-9.05688900	-2.61781000	-1.67209700
N	-0.55269200	0.68361500	0.04706900
C	-0.70922500	0.96655100	1.35147300
O	-1.41605100	1.92643700	1.71624400
O	-0.12890400	0.14952800	2.24597600
C	-0.18088800	0.56027500	3.62523100
H	-1.15824100	1.01466400	3.80717300
C	-0.03751300	-0.70758200	4.44506400
H	0.92123000	-1.19276500	4.23745100
H	-0.08327700	-0.47068000	5.51251200
H	-0.84182800	-1.41108000	4.20866500
C	0.92102400	1.57445000	3.88118900
H	1.89777400	1.12151700	3.68272400
H	0.79921000	2.43718800	3.21917600
H	0.88986100	1.91653200	4.92099500
C	0.13984800	4.37013000	0.33999100
O	0.97415100	3.83970200	1.04975200
O	-1.09844000	3.96345400	0.16822200
H	-1.25219500	3.12159700	0.71559600
O	0.33196000	5.47441400	-0.39577700
C	1.58756000	6.20718900	-0.31575600
C	2.73380000	5.35467300	-0.84848100
H	2.52345000	5.04184700	-1.87694400

H	3.65473200	5.94709300	-0.85419900
H	2.88806800	4.47045600	-0.22706800
C	1.83516200	6.68047900	1.11346700
H	2.06302400	5.84542200	1.77718300
H	2.67933300	7.37729100	1.12114400
H	0.95261000	7.20710500	1.49167100
C	1.34090200	7.39948800	-1.23245900
H	1.10263200	7.05927700	-2.24496600
H	0.50619900	8.00216700	-0.86126400
H	2.23494300	8.02839300	-1.27582700
N	0.28705700	-0.38868800	-0.24840400
C	-0.16276400	-1.65651700	0.02475900
O	-1.17902500	-1.91905500	0.64806600
O	0.66761000	-2.58780600	-0.46800500
C	0.41094600	-3.96185300	-0.10587200
H	-0.65973800	-4.14790800	-0.23051700
C	1.22218300	-4.79129200	-1.08149600
H	2.28999000	-4.58553200	-0.94717000
H	0.94508000	-4.56133500	-2.11456500
H	1.04773400	-5.85575300	-0.89916100
C	0.83039500	-4.18669300	1.33675700
H	1.89655600	-3.95988400	1.44370300
H	0.66212800	-5.23058800	1.61926300
H	0.26002300	-3.54402300	2.01262700
C	1.42043700	-0.14226500	-1.15153700
C	1.71639100	1.38712700	-1.30209400
H	1.55585500	1.80474600	-0.30468800
C	0.79137300	2.10678400	-2.28497200
H	-0.25889200	1.88469000	-2.10556700
H	1.03200500	1.84755100	-3.32182300

H	0.93345600	3.18759900	-2.16694800
C	3.17356400	1.64416400	-1.70091000
H	3.46014600	1.08404000	-2.59895000
H	3.86831400	1.39501900	-0.89427000
H	3.29407300	2.70780900	-1.92773000
C	1.16902600	-0.82070600	-2.52704300
O	0.13951600	-0.66635600	-3.15643500
C	2.35228900	-1.59149500	-2.84497800
H	2.56222700	-2.07569500	-3.78879300
C	3.17171900	-1.58842700	-1.75976800
N	2.65158500	-0.83867300	-0.71339800
C	3.05538600	-0.79790300	0.61545600
O	2.76582900	0.12248400	1.34710400
O	3.74570900	-1.89118200	0.93763200
C	4.49996500	-1.96763200	2.19039500
C	5.19189800	-3.31924700	2.07512700
H	4.45371200	-4.12539000	2.01243700
H	5.82083000	-3.48990000	2.95375200
H	5.82165600	-3.34969800	1.17972500
C	5.52419200	-0.84076500	2.26045900
H	5.04004700	0.13833300	2.25746100
H	6.22301100	-0.90321300	1.42085000
H	6.09594800	-0.93964000	3.18858200
C	3.54638900	-1.94224000	3.37821900
H	3.09298600	-0.95683200	3.49612100
H	4.10143400	-2.18876200	4.28913100
H	2.75398000	-2.68600200	3.24564300
C	4.52839100	-2.17050000	-1.73892600
C	7.11477700	-3.21633200	-1.85655300
C	4.74745400	-3.44154900	-2.27516500

C 5.61331400 -1.41704500 -1.27613300

C 6.90078900 -1.93661200 -1.34061900

C 6.03759500 -3.96604000 -2.32299100

H 3.90457400 -4.02051900 -2.64186700

H 5.44482600 -0.41850500 -0.88037300

H 7.73924200 -1.34302500 -0.98843000

H 6.19906800 -4.96009500 -2.72834800

H 8.12043000 -3.62336000 -1.89917700

Zero-point correction= 1.075815 (Hartree/Particle)

Thermal correction to Energy= 1.141496

Thermal correction to Enthalpy= 1.142440

Thermal correction to Gibbs Free Energy= 0.972404

Sum of electronic and zero-point Energies= -2890.102826

Sum of electronic and thermal Energies= -2890.037145

Sum of electronic and thermal Enthalpies= -2890.036201

Sum of electronic and thermal Free Energies= -2890.206237

E(RM062X/6-311+G(2d,p)) = -2892.08209233

TBHC

O 0.14910400 -0.00002600 1.47613300

C 0.06499400 -0.00000200 0.01311200

C 0.70207100 1.26760600 -0.54335300

H 0.26825400 2.15009900 -0.06202800

H 0.49833000 1.32760500 -1.61693300

H 1.78276400 1.27203900 -0.39255200

C 0.70209700 -1.26757400 -0.54341400

H 1.78281000 -1.27192900 -0.39276300

H 0.49820900 -1.32762600 -1.61696200

H 0.26841200 -2.15008100 -0.06199600

C -1.43760900 -0.00001300 -0.23328800

H	-1.89853100	0.88915300	0.20734800
H	-1.89849700	-0.88927000	0.20719900
H	-1.63479700	0.00007300	-1.30893700
C	1.32938700	-0.00013200	2.07439400
O	2.42521600	-0.00024700	1.56228900
O	1.12323800	-0.00012700	3.39827400
H	2.00163400	-0.00021700	3.82072400

Zero-point correction= 0.153467 (Hartree/Particle)

Thermal correction to Energy= 0.162481

Thermal correction to Enthalpy= 0.163425

Thermal correction to Gibbs Free Energy= 0.120154

Sum of electronic and zero-point Energies= -421.928149

Sum of electronic and thermal Energies= -421.919135

Sum of electronic and thermal Enthalpies= -421.918191

Sum of electronic and thermal Free Energies= -421.961462

E(RM062X/6-311+G(2d,p)) = -422.230428921

TS1-CONF2

C	-2.45433000	0.07146400	-1.18653700
C	-2.54241900	1.47935300	-0.71215700
H	-3.47497900	1.67439700	-0.18529600
H	-2.42793800	2.19392800	-1.52906200
C	-3.18462700	-0.99325600	-0.53018800
O	-3.08636800	-2.18959100	-0.77393000
O	-4.04646700	-0.54338700	0.42268900
C	-4.80487800	-1.54878300	1.09755600
H	-4.12188500	-2.25823200	1.57618500
H	-5.40171400	-2.10553000	0.36772500
C	-5.68014100	-0.84773100	2.11337800
H	-5.06944900	-0.29537000	2.83354800

H	-6.28067900	-1.58158700	2.65873400
H	-6.35699100	-0.14382400	1.62029300
O	-1.51134000	1.79339600	0.28163000
C	-0.34655400	2.20946400	-0.20844700
O	-0.13023200	2.50685800	-1.36374400
O	0.52458800	2.25055800	0.79871700
C	1.87956300	2.74917200	0.57670200
C	1.82838500	4.21954100	0.17819200
H	2.84664300	4.61903700	0.13862400
H	1.26291700	4.79238300	0.92038400
H	1.36499200	4.34877200	-0.80165900
C	2.52236000	2.58333500	1.94789900
H	2.52136800	1.52878100	2.24265400
H	1.97437900	3.15749600	2.70117700
H	3.55639400	2.93862200	1.91996000
C	2.60430400	1.89087600	-0.45421100
H	2.54171400	0.83573000	-0.16929900
H	3.66070400	2.17776400	-0.47774100
H	2.18263000	2.01726500	-1.45213000
C	-1.50497400	-0.30327200	-2.12515400
H	-1.05359400	0.46423000	-2.74820700
H	-1.59818400	-1.28540500	-2.57938000
N	0.18671200	-0.80003200	-1.28210200
C	0.19649200	-0.98049400	0.03794500
H	-0.70257900	-0.65455700	0.56121900
C	1.25377300	-1.18301700	-1.99171000
H	1.19655700	-1.02512500	-3.06679200
C	1.26589200	-1.53210100	0.71463400
H	1.20711000	-1.64449900	1.78960300
C	2.41031700	-1.94731100	-0.01250600

C	2.37264500	-1.74997300	-1.41810600
H	3.20398600	-2.03246600	-2.05131000
N	3.48424100	-2.49746500	0.60166200
C	4.65112600	-2.87853400	-0.17711300
H	5.39249900	-3.31757600	0.48965100
H	5.10110900	-2.01144200	-0.67591400
H	4.39107300	-3.62199700	-0.93854900
C	3.50508800	-2.61746900	2.05020200
H	4.45011100	-3.06536200	2.35423700
H	2.68945600	-3.25670300	2.40646200
H	3.41410000	-1.63649800	2.53279100

Zero-point correction= 0.454705 (Hartree/Particle)

Thermal correction to Energy= 0.481879

Thermal correction to Enthalpy= 0.482823

Thermal correction to Gibbs Free Energy= 0.395112

Sum of electronic and zero-point Energies= -1187.457266

Sum of electronic and thermal Energies= -1187.430092

Sum of electronic and thermal Enthalpies= -1187.429147

Sum of electronic and thermal Free Energies= -1187.516858

E(RM062X/6-311+G(2d,p)) = -1188.28856031

TS1-CONF3

C	-1.74482800	-1.76977800	-1.06618200
C	-2.23555800	-0.65228700	-1.91857500
H	-3.21500100	-0.29751900	-1.59547400
H	-2.27817400	-0.93227400	-2.97390500
C	-2.29428200	-2.01980200	0.25210600
O	-1.77513900	-2.70662600	1.12449400
O	-3.50570900	-1.44284700	0.44359000
C	-4.02226600	-1.50471300	1.77181500

H	-3.27325600	-1.11200900	2.46757900
H	-4.21436800	-2.54814000	2.04361500
C	-5.29010600	-0.67915600	1.79893100
H	-5.07552600	0.35778500	1.52414000
H	-5.72526000	-0.69142900	2.80252800
H	-6.02759200	-1.07933200	1.09680100
O	-1.33028600	0.49884100	-1.95697200
C	-1.31026600	1.26558400	-0.87333300
O	-1.95797200	1.08132700	0.13442500
O	-0.45774100	2.26641000	-1.10194400
C	-0.31850200	3.34962500	-0.13265500
C	0.28258900	2.81941500	1.16340400
H	0.46654000	3.65575000	1.84544800
H	1.23849900	2.32870900	0.95539500
H	-0.38831200	2.11003100	1.65208800
C	0.65601500	4.29436500	-0.82475700
H	0.23404500	4.65832200	-1.76650500
H	1.59838400	3.78107200	-1.03909400
H	0.86352000	5.15262200	-0.17915300
C	-1.66141500	4.03841700	0.08718700
H	-2.10165500	4.31836400	-0.87558600
H	-1.50392300	4.95143900	0.66984300
H	-2.35958300	3.39567000	0.62523300
C	-0.65585400	-2.52593000	-1.45921600
H	-0.36380300	-2.51985800	-2.50771300
H	-0.45275600	-3.44990100	-0.92590300
N	1.05439700	-1.75980800	-0.87655500
C	1.02031600	-0.92405200	0.16025600
H	0.02368100	-0.64660600	0.50549800
C	2.24074900	-2.15628000	-1.34604600

H	2.21843900	-2.84856200	-2.18542500
C	2.15940200	-0.44299800	0.77368400
H	2.06038500	0.21958800	1.62374700
C	3.43210600	-0.83557500	0.28702000
C	3.44012200	-1.72732900	-0.81634200
H	4.36601400	-2.08264200	-1.25030700
N	4.57940500	-0.38493200	0.84789300
C	5.86318500	-0.83197800	0.33396600
H	6.65789200	-0.35289900	0.90420200
H	5.98386800	-0.56080500	-0.72108000
H	5.97516300	-1.91864500	0.42900900
C	4.52450900	0.51617400	1.98681300
H	5.54065700	0.77847300	2.27898200
H	4.02646100	0.04799900	2.84417100
H	3.98831900	1.43893700	1.73529400

Zero-point correction= 0.454611 (Hartree/Particle)

Thermal correction to Energy= 0.481867

Thermal correction to Enthalpy= 0.482811

Thermal correction to Gibbs Free Energy= 0.394165

Sum of electronic and zero-point Energies= -1187.453265

Sum of electronic and thermal Energies= -1187.426009

Sum of electronic and thermal Enthalpies= -1187.425065

Sum of electronic and thermal Free Energies= -1187.513711

E(RM062X/6-311+G(2d,p)) = -1188.28396192

TS1

C	0.48943500	2.14347700	-1.18350600
C	1.54583800	1.15793200	-1.52501700
H	2.55324100	1.56989400	-1.43400200
H	1.41519600	0.77512600	-2.54155600

C	0.63240300	2.99593100	-0.01975200
O	-0.20515800	3.77505900	0.41511300
O	1.84501200	2.85875600	0.57919200
C	2.06683700	3.67796300	1.72882300
H	1.29756800	3.46566400	2.47846900
H	1.97338900	4.73218100	1.44785100
C	3.45245700	3.36068300	2.24717100
H	3.52922200	2.30432900	2.52090200
H	3.66795900	3.96548800	3.13277500
H	4.20835300	3.57770100	1.48677000
O	1.46831500	0.01657200	-0.61348800
C	2.40453400	-0.91149500	-0.78585900
O	3.27451300	-0.87592800	-1.62860700
O	2.20533200	-1.86683200	0.12173500
C	3.08806800	-3.02987800	0.17035700
C	4.51377000	-2.59336900	0.48866900
H	5.12783500	-3.47997700	0.67552300
H	4.52431600	-1.97249800	1.39049300
H	4.95290700	-2.03120200	-0.33677200
C	2.50799600	-3.84069300	1.32228600
H	1.47005900	-4.11619900	1.11177900
H	2.53528000	-3.26112100	2.25008500
H	3.09105800	-4.75517300	1.46356500
C	2.99634800	-3.81365800	-1.13425400
H	1.95034300	-4.04413100	-1.36166400
H	3.53927300	-4.75778600	-1.02516700
H	3.42830400	-3.25591200	-1.96651700
C	-0.70943700	2.19459100	-1.87065100
H	-0.77682200	1.72431800	-2.84856600
H	-1.34131300	3.06646600	-1.73021500

N	-2.07038700	1.00620900	-1.09443100
C	-1.76585200	0.38121900	0.04113100
H	-0.74870200	0.53637500	0.40077100
C	-3.29535100	0.85412600	-1.60639800
H	-3.49986400	1.38892600	-2.53191200
C	-2.65905700	-0.42454100	0.71762500
H	-2.34501700	-0.90645200	1.63454600
C	-3.96521700	-0.60576800	0.19719100
C	-4.26376500	0.07083900	-1.01403300
H	-5.23643100	-0.01011500	-1.48203700
N	-4.88142200	-1.38305100	0.82246600
C	-6.20739700	-1.54573800	0.24987500
H	-6.78405700	-2.22216500	0.87953000
H	-6.15357900	-1.97478800	-0.75727800
H	-6.73840300	-0.58803300	0.19182600
C	-4.54578900	-2.02937600	2.08045700
H	-5.41538000	-2.57908300	2.43875800
H	-4.26477600	-1.29292700	2.84223400
H	-3.71633000	-2.73548700	1.95730400

Zero-point correction= 0.454079 (Hartree/Particle)

Thermal correction to Energy= 0.481696

Thermal correction to Enthalpy= 0.482640

Thermal correction to Gibbs Free Energy= 0.391330

Sum of electronic and zero-point Energies= -1187.453739

Sum of electronic and thermal Energies= -1187.426122

Sum of electronic and thermal Enthalpies= -1187.425178

Sum of electronic and thermal Free Energies= -1187.516488

E(RM062X/6-311+G(2d,p)) = -1188.28582197

TS2-CONF2

C	1.98578200	-1.07211900	-1.18397000
C	1.24728300	-2.23939600	-1.08016500
H	1.69250300	-3.07870200	-0.55858000
H	0.56650500	-2.49279300	-1.88671500
C	3.10385500	-0.77986600	-0.32277800
O	3.75615900	0.26186400	-0.35392200
O	3.41481200	-1.77339600	0.54649800
C	4.53424400	-1.52654800	1.39990400
H	4.35050000	-0.62020100	1.98588400
H	5.42660200	-1.35207900	0.78967800
C	4.69733000	-2.73975100	2.28912600
H	3.79750100	-2.90123700	2.88962500
H	5.54501600	-2.59571100	2.96535300
H	4.88025400	-3.63635600	1.68973100
O	-0.13925400	-2.18880200	0.20490800
C	-1.31135600	-2.03956700	-0.27379400
O	-1.62477600	-1.80814900	-1.44814200
O	-2.25272800	-2.16071600	0.70935900
C	-3.65897000	-1.98070700	0.42452300
C	-4.15599000	-3.02908300	-0.56815400
H	-5.24728900	-2.97572800	-0.64419600
H	-3.88674800	-4.03096400	-0.21642800
H	-3.72161800	-2.87243600	-1.55590800
C	-4.31443400	-2.20099500	1.78503400
H	-3.93692500	-1.47560900	2.51271700
H	-4.09519000	-3.20764400	2.15468600
H	-5.39990600	-2.08601500	1.70711400
C	-3.93157100	-0.55767300	-0.05913400
H	-3.51595300	0.16116000	0.65645800
H	-5.01170500	-0.38857100	-0.12440600

H	-3.48815600	-0.38597700	-1.04171600
C	1.59621300	0.02587900	-2.11413200
H	0.88370700	-0.32797800	-2.86263300
H	2.45680000	0.46574300	-2.62430800
N	0.92799200	1.17361200	-1.41845600
C	1.63387900	2.26271800	-1.04721300
H	2.68143600	2.25979700	-1.32011200
C	-0.38144400	1.08079000	-1.09599900
H	-0.88516200	0.17216300	-1.41975700
C	1.06007100	3.29122000	-0.34748200
H	1.67889600	4.13706200	-0.08049200
C	-0.31312700	3.22897200	0.01497600
C	-1.02514900	2.07008500	-0.40436900
H	-2.07768800	1.94254300	-0.18957100
N	-0.90774000	4.20948900	0.71289900
C	-2.31767900	4.10271500	1.06550800
H	-2.60141300	4.97898800	1.64566400
H	-2.50335100	3.20836500	1.66996200
H	-2.94537000	4.06064100	0.16891100
C	-0.14308900	5.37929300	1.12587300
H	-0.79481100	6.04322500	1.69144500
H	0.24176400	5.92362800	0.25676500
H	0.69923700	5.09078200	1.76358800

Zero-point correction= 0.455209 (Hartree/Particle)

Thermal correction to Energy= 0.482377

Thermal correction to Enthalpy= 0.483321

Thermal correction to Gibbs Free Energy= 0.394511

Sum of electronic and zero-point Energies= -1187.455964

Sum of electronic and thermal Energies= -1187.428797

Sum of electronic and thermal Enthalpies= -1187.427853

Sum of electronic and thermal Free Energies= -1187.516663

E(RM062X/6-311+G(2d,p)) = -1188.29100831

TS2-CONF3

C	-1.99639200	-1.49083000	-1.20591000
C	-2.47613400	-0.46495200	-2.00783000
H	-3.35084700	0.07594600	-1.66516100
H	-2.38237200	-0.55979200	-3.08655000
C	-2.35023100	-1.61466400	0.18648900
O	-1.74766500	-2.31926000	0.99440100
O	-3.45689800	-0.92399400	0.54524300
C	-3.68239100	-0.80073600	1.94702700
H	-2.77084700	-0.42932100	2.42720600
H	-3.90779800	-1.78444600	2.37345000
C	-4.83397600	0.16304800	2.13173300
H	-4.58392700	1.13543800	1.69830600
H	-5.04701400	0.29731400	3.19636600
H	-5.73710000	-0.21430700	1.64264900
O	-1.35168300	1.02472000	-2.08855000
C	-1.11640500	1.54567800	-0.93708700
O	-1.80269700	1.46882600	0.07465400
O	0.07608700	2.22520600	-0.96563000
C	0.50675500	3.00286200	0.17483900
C	0.77503800	2.10838900	1.38346200
H	1.20094100	2.70713200	2.19606600
H	1.49468100	1.32456900	1.12143900
H	-0.14472600	1.63691500	1.73152600
C	1.81096600	3.62995000	-0.30941000
H	1.63050000	4.26394500	-1.18339000
H	2.52664000	2.84977900	-0.59168100

H	2.25670000	4.24182900	0.48105300
C	-0.50828300	4.09824900	0.49599200
H	-0.72669200	4.68006000	-0.40616400
H	-0.09360400	4.77678900	1.24896800
H	-1.43773500	3.67226100	0.87595000
C	-0.88527500	-2.37554000	-1.65225600
H	-0.75834600	-2.33569000	-2.73730700
H	-1.02676800	-3.41714700	-1.35344900
N	0.44226100	-1.98990000	-1.06192700
C	1.02217900	-2.75149100	-0.11261800
H	0.48798100	-3.65141400	0.16503800
C	1.02403500	-0.82833000	-1.43370000
H	0.47589300	-0.23177000	-2.15667000
C	2.20794800	-2.39917400	0.47612400
H	2.61823600	-3.05226200	1.23429200
C	2.85853100	-1.19282800	0.09997600
C	2.20835800	-0.40850000	-0.89333400
H	2.61190300	0.53879500	-1.22595100
N	4.01625400	-0.80555000	0.66064700
C	4.62959900	0.45715700	0.27000700
H	5.57426300	0.56876900	0.79961000
H	3.98377200	1.30564200	0.52541400
H	4.83124900	0.47752500	-0.80598700
C	4.62928700	-1.61816700	1.70329200
H	5.56022900	-1.14737500	2.01497300
H	4.85502700	-2.62342300	1.33212100
H	3.97135700	-1.70232400	2.57511300

Zero-point correction= 0.455433 (Hartree/Particle)

Thermal correction to Energy= 0.482116

Thermal correction to Enthalpy= 0.483061

Thermal correction to Gibbs Free Energy= 0.398578

Sum of electronic and zero-point Energies= -1187.455311

Sum of electronic and thermal Energies= -1187.428627

Sum of electronic and thermal Enthalpies= -1187.427683

Sum of electronic and thermal Free Energies= -1187.512166

E(RM062X/6-311+G(2d,p)) = -1188.28921322

TS2

C	-0.21780000	1.93532400	-1.24236200
C	1.14497300	1.70868200	-1.27898200
H	1.80383400	2.38399400	-0.74561100
H	1.58240500	1.26304500	-2.16725300
C	-0.85640500	2.77487200	-0.25648900
O	-2.06953800	2.93945900	-0.17125900
O	0.00251000	3.40258800	0.58427500
C	-0.59718900	4.26355200	1.55498000
H	-1.29764700	3.68694400	2.16783700
H	-1.16913200	5.04505600	1.04384700
C	0.52117700	4.84879700	2.38907300
H	1.08241100	4.05631900	2.89246500
H	0.10869200	5.51880300	3.14903500
H	1.21259400	5.41931200	1.76213500
O	1.62932700	0.19980200	-0.21430700
C	2.85225100	-0.15092300	-0.37430100
O	3.71060200	0.42994500	-1.03451500
O	3.11014000	-1.31065900	0.30625900
C	4.43087000	-1.89894200	0.29231800
C	5.45537800	-0.95193000	0.91334100
H	6.41168400	-1.47162400	1.03567800
H	5.11264600	-0.62874800	1.90237600

H	5.60629300	-0.07245400	0.28649400
C	4.26552900	-3.13504100	1.17203200
H	3.50609900	-3.80300300	0.75294800
H	3.95406000	-2.84623000	2.18096100
H	5.21097800	-3.68177800	1.24160500
C	4.82328900	-2.31531200	-1.12356000
H	4.04488600	-2.95539900	-1.55339000
H	5.75782200	-2.88577200	-1.09579700
H	4.95814100	-1.44273300	-1.76370700
C	-1.16058200	1.19093500	-2.12219800
H	-0.62376700	0.64870600	-2.90520200
H	-1.90505200	1.83998800	-2.58903900
N	-1.96464600	0.17406300	-1.36554100
C	-3.31201200	0.20583800	-1.38298400
H	-3.76237000	0.99589100	-1.97234500
C	-1.32626300	-0.76205600	-0.62761700
H	-0.24005800	-0.69342200	-0.60768000
C	-4.07020300	-0.70266600	-0.69365700
H	-5.14713900	-0.61815300	-0.74749400
C	-3.43736900	-1.71783800	0.07518200
C	-2.01423800	-1.70802300	0.08245000
H	-1.44690700	-2.42909200	0.65557500
N	-4.14214400	-2.62917100	0.76398200
C	-3.45279200	-3.65643100	1.53502700
H	-4.19501400	-4.31019000	1.98981300
H	-2.84424200	-3.21091300	2.32923300
H	-2.80646600	-4.26088700	0.89022300
C	-5.59862700	-2.58237100	0.75870000
H	-5.97839800	-3.37888300	1.39645100
H	-5.99257700	-2.72694000	-0.25312600

H -5.96049600 -1.62396600 1.14555700

Zero-point correction= 0.454905 (Hartree/Particle)

Thermal correction to Energy= 0.482211

Thermal correction to Enthalpy= 0.483155

Thermal correction to Gibbs Free Energy= 0.392729

Sum of electronic and zero-point Energies= -1187.453901

Sum of electronic and thermal Energies= -1187.426595

Sum of electronic and thermal Enthalpies= -1187.425651

Sum of electronic and thermal Free Energies= -1187.516077

E(RM062X/6-311+G(2d,p)) = -1188.28980386

Barrier of Rotation around N–N bond of **3c** in Cyclohexane

cyclohexane-**3c1**-CONF2

C 2.14032400 0.78500200 1.09446200

C 1.68006000 1.46406200 2.16785600

H 2.21646700 2.24152400 2.69313900

C 0.26087800 1.17884500 2.33688500

O -0.53737200 1.66115500 3.10529100

C -0.09922500 0.05199600 1.32254400

N 1.15558500 -0.04188800 0.53724500

C 1.32899200 -1.09335600 -0.34776000

O 0.39119200 -1.61156200 -0.92575100

O 2.60204200 -1.45449000 -0.43827200

C 3.06115300 -2.40023300 -1.45578500

C 2.71961800 -1.87526400 -2.84498700

H 3.13925200 -0.87324800 -2.98198900

H 1.64067500 -1.84083100 -3.00640700

H 3.16223400 -2.53599300 -3.59681800

C 4.56820800 -2.40484600 -1.23485600

H 4.97546600 -1.39759000 -1.36975900

H	5.04783200	-3.08010400	-1.94940000
H	4.80500500	-2.74167100	-0.22122000
C	2.46173800	-3.77518100	-1.18683900
H	1.38486000	-3.78016000	-1.36094500
H	2.65769700	-4.07529100	-0.15240200
H	2.93041600	-4.50908000	-1.85005600
C	3.45102100	0.99389700	0.44765300
C	5.90852200	1.51517600	-0.76337100
C	3.50852800	1.31469400	-0.91345700
C	4.62424100	0.94510700	1.19935200
C	5.85182500	1.19856600	0.59070700
C	4.73272400	1.57968400	-1.51358600
H	2.58678800	1.37320700	-1.48710700
H	4.57255100	0.69334300	2.25455600
H	6.76361800	1.14946100	1.17764900
H	4.77204300	1.84048600	-2.56693100
H	6.86521500	1.71740700	-1.23501900
C	-0.37764300	-1.26320300	2.09595600
H	-0.61638100	-2.01063700	1.33359100
C	-1.57548100	-1.12642600	3.04088200
H	-1.29739900	-0.58114600	3.94639000
H	-1.91156400	-2.12599000	3.33485100
H	-2.41393600	-0.59496100	2.58521700
C	0.85276200	-1.74608700	2.86929300
H	1.14113500	-1.03923100	3.65440400
H	1.72081100	-1.91649600	2.22379600
H	0.61155700	-2.69611700	3.35581100
N	-1.22971900	0.41006600	0.48336200
C	-1.16557300	1.61156400	-0.20555900
O	-0.33858100	2.46374400	0.03529500

O	-2.11511900	1.69072800	-1.13941900
C	-2.27643500	2.98064500	-1.77700800
H	-1.27774100	3.36701600	-1.99960100
C	-3.00532700	3.91517900	-0.82780600
H	-3.97609600	3.48897200	-0.55637800
H	-3.16740400	4.88496800	-1.30805600
H	-2.42280300	4.07285500	0.08298200
C	-3.04661500	2.70644700	-3.05329000
H	-2.50453400	2.00470700	-3.69289300
H	-3.19543500	3.63863300	-3.60552300
H	-4.02763000	2.28034400	-2.82004700
N	-2.06403800	-0.58200200	0.02356700
C	-3.42238800	-0.41337300	0.18375100
O	-3.94929300	0.37567800	0.93132300
O	-4.05768000	-1.29452600	-0.60483700
C	-5.49797900	-1.32490600	-0.48637200
H	-5.84388200	-0.29068100	-0.40217000
C	-6.00295500	-1.95687200	-1.76851300
H	-7.09611400	-1.99251600	-1.76123900
H	-5.62332000	-2.97884300	-1.86600100
H	-5.67881000	-1.38039300	-2.63913100
C	-5.88742700	-2.10567700	0.75696800
H	-6.97700500	-2.14559000	0.84987500
H	-5.48274700	-1.62831200	1.65274200
H	-5.50637400	-3.13015400	0.69372800
H	-1.73003400	-1.08959400	-0.79062000

Zero-point correction= 0.620867 (Hartree/Particle)

Thermal correction to Energy= 0.658670

Thermal correction to Enthalpy= 0.659614

Thermal correction to Gibbs Free Energy= 0.549707

Sum of electronic and zero-point Energies= -1702.631169

Sum of electronic and thermal Energies= -1702.593366

Sum of electronic and thermal Enthalpies= -1702.592422

Sum of electronic and thermal Free Energies= -1702.702329

E(RM062X/6-311+G(2d,p)) = -1703.78235030

cyclohexane-**3c1**

C	1.80751000	0.09884200	1.47539500
C	1.08354000	0.06565900	2.61652900
H	1.39699300	0.47395500	3.56685000
C	-0.27660600	-0.34917600	2.30031900
O	-1.25727800	-0.39339400	3.00639300
C	-0.28220300	-0.78174700	0.80436100
N	1.07262400	-0.36194400	0.37635700
C	1.54502400	-0.75062800	-0.86691100
O	0.79762100	-0.94225300	-1.80809900
O	2.86178800	-0.90787900	-0.86402700
C	3.61190300	-1.11690300	-2.10290700
C	3.37240100	0.04685300	-3.05689500
H	3.62198700	0.99302900	-2.56546800
H	2.33609400	0.07874900	-3.39803500
H	4.02213300	-0.06557900	-3.93030000
C	5.05288700	-1.12426700	-1.60949500
H	5.29066700	-0.17658300	-1.11556500
H	5.73504400	-1.26574000	-2.45285800
H	5.20809400	-1.93677200	-0.89346400
C	3.23216900	-2.46080100	-2.71256100
H	2.20677300	-2.45343600	-3.08462300
H	3.33562200	-3.25527300	-1.96642200
H	3.90806900	-2.68337300	-3.54429700

C	3.14424000	0.70819600	1.32824500
C	5.62586200	1.96229600	1.11977100
C	3.33853900	1.72666600	0.38811500
C	4.19065000	0.32829000	2.16726500
C	5.43232600	0.95100300	2.05607900
C	4.57360400	2.35430300	0.28987800
H	2.50962200	2.03243400	-0.24555100
H	4.03327200	-0.46400200	2.89319800
H	6.24755200	0.64489500	2.70414000
H	4.71709300	3.15283200	-0.43182800
H	6.59219200	2.45025600	1.03806600
C	-0.44420500	-2.32229400	0.71413300
H	-0.45438600	-2.55741600	-0.35393500
C	-1.76184000	-2.79829700	1.33201400
H	-1.70393800	-2.80009800	2.42357100
H	-1.96199800	-3.82130700	0.99800700
H	-2.60602900	-2.16679100	1.04938300
C	0.73303600	-3.06206000	1.35642700
H	0.79614000	-2.86683900	2.43211400
H	1.69609500	-2.80519800	0.90330100
H	0.58396900	-4.13827200	1.22625200
N	-1.31601100	-0.09850000	0.04338700
C	-1.31472700	1.28719100	0.06527200
O	-0.67374200	1.93274700	0.86592200
O	-2.09857000	1.79123600	-0.89099200
C	-2.26213600	3.22968800	-0.89140200
H	-1.29551800	3.67189500	-0.63548200
C	-3.30368700	3.60955700	0.14557500
H	-4.26736800	3.15777700	-0.11077900
H	-3.42646400	4.69648500	0.17359500

H	-3.00156600	3.26985700	1.13965300
C	-2.66772200	3.59442500	-2.30553200
H	-1.90049500	3.28950700	-3.02205200
H	-2.80915500	4.67614300	-2.38442100
H	-3.60730100	3.09993100	-2.57113600
N	-1.92187100	-0.75103700	-1.00864400
C	-3.29719000	-0.74878500	-1.13425000
O	-3.84665200	-1.03549300	-2.17443700
O	-3.90476500	-0.44065600	0.01466500
C	-5.34665800	-0.54458400	0.02213900
H	-5.71539400	-0.09099700	-0.90284900
C	-5.75367300	-2.00715700	0.08577500
H	-6.84485000	-2.09064900	0.09332300
H	-5.36616200	-2.46630700	1.00129500
H	-5.37255600	-2.55352800	-0.77991600
C	-5.80219600	0.24273000	1.23493700
H	-6.89376800	0.22465900	1.30317000
H	-5.47251800	1.28295800	1.17335300
H	-5.38680100	-0.19601000	2.14740700
H	-1.40665000	-0.72928600	-1.88445700

Zero-point correction= 0.620793 (Hartree/Particle)

Thermal correction to Energy= 0.658597

Thermal correction to Enthalpy= 0.659541

Thermal correction to Gibbs Free Energy= 0.549462

Sum of electronic and zero-point Energies= -1702.631270

Sum of electronic and thermal Energies= -1702.593465

Sum of electronic and thermal Enthalpies= -1702.592521

Sum of electronic and thermal Free Energies= -1702.702601

E(RM062X/6-311+G(2d,p)) = -1703.78236592

cyclohexane-**3c2**

C	-1.76551600	-1.47809700	0.21877200
C	-1.46886000	-2.66558300	0.78976600
H	-1.93210100	-3.61196600	0.54893100
C	-0.22068900	-2.53203300	1.52355100
O	0.44372900	-3.37884700	2.07767600
C	0.18750900	-1.02605700	1.47288100
N	-0.88271400	-0.45808300	0.61676300
C	-1.22222900	0.89174400	0.70518600
O	-0.44291400	1.75458700	1.04315500
O	-2.50969800	1.07578700	0.41502200
C	-3.04399100	2.40935400	0.15875300
C	-2.26628100	3.07023900	-0.97367400
H	-2.29103200	2.43593700	-1.86576100
H	-1.22678200	3.25005400	-0.69333300
H	-2.73400800	4.02848400	-1.22080300
C	-4.47374700	2.10852600	-0.27386800
H	-4.47512300	1.46809300	-1.16203000
H	-4.99760100	3.04015100	-0.50773700
H	-5.01491600	1.59333700	0.52557500
C	-3.02181000	3.23267200	1.44145800
H	-2.00055000	3.46836500	1.74318500
H	-3.51408000	2.68206400	2.24971100
H	-3.56953700	4.16705300	1.28187300
C	-2.74879100	-1.27274700	-0.86086500
C	-4.53538000	-0.98758600	-2.98220500
C	-2.35944100	-0.58590900	-2.01711800
C	-4.02834800	-1.81972400	-0.77387500
C	-4.92206800	-1.66984100	-1.83195700
C	-3.24957200	-0.45127200	-3.07490500

H	-1.35375200	-0.17657700	-2.07871300
H	-4.32555100	-2.34524300	0.12908400
H	-5.92128200	-2.08725000	-1.75583200
H	-2.94109000	0.07196300	-3.97502000
H	-5.23164200	-0.87555500	-3.80769700
C	0.16967600	-0.44279000	2.90969300
H	0.40459500	0.61826200	2.80660100
C	1.22760500	-1.08415800	3.81049800
H	0.98789300	-2.12560500	4.03451700
H	1.27196600	-0.52851000	4.75268800
H	2.22405300	-1.06639300	3.36027500
C	-1.21531400	-0.57751100	3.54947700
H	-1.47874300	-1.62760500	3.71806300
H	-2.00914000	-0.11950300	2.94989900
H	-1.21145500	-0.07883200	4.52328300
N	1.51622100	-0.89003900	0.88928600
C	1.83290200	-1.62126500	-0.25487200
O	1.07762500	-2.40603300	-0.77943100
O	3.08348200	-1.36673400	-0.64744100
C	3.51856300	-2.04407600	-1.85035200
H	2.67845900	-2.04021700	-2.55057800
C	3.91418100	-3.47083000	-1.51240300
H	4.72765400	-3.47258300	-0.77963300
H	4.25909300	-3.98597000	-2.41417600
H	3.06389400	-4.02052700	-1.10293500
C	4.67077200	-1.21937600	-2.38837900
H	4.35052000	-0.19429400	-2.59233700
H	5.04294500	-1.66053300	-3.31746400
H	5.49167300	-1.19218200	-1.66468400
N	2.17217600	0.30600000	1.08264000

C	2.14852600	1.22040300	0.04262700
O	1.48038400	1.10848500	-0.95836300
O	2.96995200	2.23345500	0.33668300
C	2.99469500	3.33079400	-0.60525000
H	1.96133600	3.52219400	-0.90957300
C	3.55529400	4.51259200	0.16114400
H	3.57355200	5.39812800	-0.48053900
H	4.57760100	4.30288500	0.49149300
H	2.94215600	4.73012200	1.03946900
C	3.83305700	2.95512900	-1.81486900
H	3.90584500	3.80653000	-2.49859800
H	3.37830300	2.11946400	-2.35085500
H	4.84420700	2.67585400	-1.50043800
H	3.01789800	0.26407300	1.63960100

Zero-point correction= 0.620575 (Hartree/Particle)

Thermal correction to Energy= 0.658315

Thermal correction to Enthalpy= 0.659260

Thermal correction to Gibbs Free Energy= 0.550308

Sum of electronic and zero-point Energies= -1702.628527

Sum of electronic and thermal Energies= -1702.590787

Sum of electronic and thermal Enthalpies= -1702.589842

Sum of electronic and thermal Free Energies= -1702.698794

E(RM062X/6-311+G(2d,p)) = -1703.77937750

cyclohexane-**3c**-**TS**

C	-1.40680500	-1.60763000	0.02723900
C	-0.83624200	-2.75744900	0.44734700
H	-1.06796500	-3.74706500	0.07946500
C	0.33491500	-2.43905900	1.24280800
O	1.19561800	-3.17922500	1.66572100

C	0.39370400	-0.88696000	1.40364700
N	-0.79141900	-0.47065100	0.58161600
C	-1.46043300	0.72262500	0.82350100
O	-0.89405800	1.73300000	1.20656400
O	-2.76199800	0.60900900	0.61344000
C	-3.63608100	1.78317800	0.54186700
C	-3.11782000	2.76124000	-0.50581700
H	-2.99416500	2.25160100	-1.46704300
H	-2.16758700	3.20777700	-0.20813200
H	-3.85225300	3.56197000	-0.63674400
C	-4.95769000	1.17024700	0.09766900
H	-4.84160300	0.68043300	-0.87489200
H	-5.71964000	1.95042700	0.01234900
H	-5.29820900	0.42589100	0.82364000
C	-3.75225900	2.41197600	1.92434900
H	-2.80559000	2.85363600	2.23955400
H	-4.05712200	1.65808700	2.65718100
H	-4.51602700	3.19565900	1.90192400
C	-2.42911200	-1.49562900	-1.02829300
C	-4.29161800	-1.33975700	-3.09552300
C	-2.23574600	-0.58969200	-2.07719700
C	-3.54934400	-2.32677100	-1.02189400
C	-4.48190000	-2.24284900	-2.05275500
C	-3.16339600	-0.51779700	-3.10905800
H	-1.34421800	0.03231900	-2.08502000
H	-3.69595000	-3.02189200	-0.20026400
H	-5.35795800	-2.88367400	-2.03985800
H	-3.00490000	0.17659400	-3.92851900
H	-5.01751600	-1.27832300	-3.90045100
C	0.21780200	-0.50007900	2.89908700

H	0.09132900	0.58533100	2.94805400
C	1.45522000	-0.86628700	3.71749000
H	1.65906100	-1.93872500	3.67125400
H	1.28502300	-0.58818900	4.76265600
H	2.33864100	-0.33591900	3.35571300
C	-1.04268200	-1.14193200	3.48733200
H	-0.93572400	-2.22973700	3.56306300
H	-1.94284600	-0.92589800	2.90079600
H	-1.20758700	-0.75617500	4.49740300
N	1.68115000	-0.44573100	0.90520900
C	2.09848200	-1.08307100	-0.32594500
O	1.35971700	-1.30102200	-1.25442400
O	3.35118800	-1.47309300	-0.21188700
C	3.96308800	-1.99788500	-1.41329800
H	3.56013100	-1.42918400	-2.25664500
C	3.61108800	-3.46966300	-1.54435900
H	3.96601500	-4.02008800	-0.66738400
H	4.08441500	-3.89070700	-2.43680400
H	2.52959600	-3.60134500	-1.62918400
C	5.44834200	-1.74148300	-1.25865400
H	5.63342600	-0.67263600	-1.12614400
H	5.98187100	-2.08574100	-2.14951200
H	5.84050500	-2.27797200	-0.38895100
N	1.80891300	0.97830500	0.92396800
C	2.47149600	1.64485200	-0.06943500
O	3.18951100	1.15657400	-0.91916300
O	2.23334800	2.96165800	0.07409200
C	2.82204100	3.82517400	-0.92253800
H	3.83432300	3.46240800	-1.12177900
C	1.99025100	3.77130700	-2.19301000

H	2.41215600	4.44104800	-2.94863400
H	0.96321100	4.08788200	-1.98231900
H	1.97546000	2.75742100	-2.60032200
C	2.86076100	5.20605800	-0.29784000
H	3.31617100	5.91737600	-0.99287300
H	3.44539600	5.19756500	0.62573300
H	1.84722500	5.54773600	-0.06535400
H	0.94940700	1.44747700	1.21743000

Zero-point correction= 0.619568 (Hartree/Particle)

Thermal correction to Energy= 0.656763

Thermal correction to Enthalpy= 0.657707

Thermal correction to Gibbs Free Energy= 0.550082

Sum of electronic and zero-point Energies= -1702.596435

Sum of electronic and thermal Energies= -1702.559240

Sum of electronic and thermal Enthalpies= -1702.558296

Sum of electronic and thermal Free Energies= -1702.665922

E(RM062X/6-311+G(2d,p)) = -1703.74733631

Diastereoselectivity of the N-alkylation Reaction

3k-*RR*-**TS4**

C	1.27748300	0.97924300	-0.74725000
H	0.63153100	1.11383300	-1.60538100
H	1.40940400	-0.05399200	-0.43685000
C	2.28042000	1.89415300	-0.50421700
C	2.35222400	3.16987000	-1.17897600
O	3.19826000	4.03642600	-0.96712300
O	1.40542600	3.33265900	-2.13042800
C	1.33412800	4.62328100	-2.73560200
H	1.14848700	5.37313700	-1.95956900
H	2.29422200	4.85846800	-3.20743200

C	0.20794800	4.58573300	-3.74512800
H	-0.73641800	4.35707000	-3.24429500
H	0.39881500	3.82377100	-4.50723900
H	0.12052800	5.55652400	-4.24267300
C	3.18450100	1.71928800	0.67059700
H	2.67665300	1.19273100	1.48095100
H	3.54954800	2.68330700	1.02949800
N	4.39801400	0.90290100	0.35685100
C	4.51609300	-0.36468200	0.80047500
H	3.69705800	-0.72630600	1.41508000
C	5.59834100	-1.14226700	0.47902300
H	5.63765300	-2.15280200	0.86301400
C	5.35248400	1.42969900	-0.44143000
H	5.16745100	2.44680100	-0.77486100
C	6.46481200	0.71991500	-0.80058400
H	7.19674400	1.19799700	-1.43776200
C	6.63520200	-0.61732800	-0.34007400
N	7.71600800	-1.34406200	-0.66544100
C	7.84411200	-2.71329900	-0.18398400
H	8.78130900	-3.12897400	-0.54988800
H	7.01993300	-3.33590800	-0.54873300
H	7.85248800	-2.74424400	0.91083500
C	8.75618900	-0.77155300	-1.51062700
H	9.54793100	-1.50740600	-1.64079000
H	9.18607800	0.12387800	-1.04968500
H	8.36029200	-0.50695800	-2.49705100
N	-0.21898200	1.08058700	0.62247900
N	-0.61409600	-0.17646500	1.08206900
C	0.30599400	-0.98902600	1.68223700
O	1.46663900	-0.68988200	1.91410900

O	-0.23150400	-2.18484000	1.97458200
C	0.64417500	-3.18447400	2.53927300
H	1.31142700	-2.68365700	3.24570600
C	-0.26110000	-4.16410000	3.25906600
H	-0.93207800	-4.65593600	2.54692100
H	-0.86350800	-3.64975400	4.01338600
H	0.34180900	-4.93070100	3.75452400
C	1.44011400	-3.82691400	1.41634700
H	0.75334600	-4.26745500	0.68522100
H	2.08685600	-4.61587700	1.81257600
H	2.06501300	-3.08359200	0.91248100
C	0.01434200	1.98652500	1.58555100
O	0.35789000	3.15399800	1.31379000
O	-0.10766600	1.57282900	2.86015800
C	-0.02087800	2.57260400	3.89140300
H	0.79218500	3.25794600	3.63519000
C	0.30553000	1.81477200	5.16446700
H	-0.49293900	1.10145700	5.39389100
H	0.40377000	2.51092700	6.00290500
H	1.24376400	1.26251400	5.05514100
C	-1.33731600	3.32691000	3.97080500
H	-2.14762500	2.62868600	4.20822800
H	-1.56021300	3.80691000	3.01415400
H	-1.29188300	4.09076400	4.75408000
C	-1.99153900	-0.59415200	0.87819400
C	-2.85385000	0.56132800	0.38314200
H	-2.48481700	0.92146200	-0.57903200
C	-2.65102000	-1.14290700	2.17961500
O	-2.68391200	-0.51568800	3.21729800
C	-3.26601100	-2.41331700	1.83709000

H	-3.92937500	-2.98140300	2.47475800
C	-2.92790100	-2.73692900	0.56361100
N	-2.13033400	-1.76221900	-0.03120800
C	-1.28991300	-1.89702200	-1.12873200
O	-0.84359800	-0.93730000	-1.71851400
O	-1.03697100	-3.17720900	-1.39220500
C	-0.35674500	-3.56997300	-2.62770200
C	-0.39341600	-5.09073400	-2.55386700
H	0.14729600	-5.44695800	-1.67130500
H	0.07544300	-5.51644800	-3.44580500
H	-1.42840600	-5.44408100	-2.49718700
C	-1.13636900	-3.07393000	-3.83999600
H	-1.15449300	-1.98347500	-3.88672200
H	-2.16315000	-3.45274000	-3.81163700
H	-0.65756300	-3.45224200	-4.74860000
C	1.07898800	-3.05819500	-2.61404300
H	1.11508500	-1.97109700	-2.70270200
H	1.62409000	-3.49946400	-3.45464800
H	1.57767600	-3.35857600	-1.68648800
C	-3.45761000	-3.89042400	-0.18952600
C	-4.57210700	-6.05365800	-1.55933300
C	-3.56422100	-5.13594400	0.43335300
C	-3.92201200	-3.72920200	-1.50065100
C	-4.48157600	-4.80554700	-2.17882100
C	-4.11352100	-6.21606300	-0.25421100
H	-3.20384800	-5.25914800	1.45079300
H	-3.85681300	-2.75576800	-1.98051800
H	-4.84863400	-4.67159300	-3.19202100
H	-4.18288300	-7.18410700	0.23215500
H	-5.00375700	-6.89489300	-2.09304100

C	-2.26597500	4.01128900	-0.34250200
O	-2.65660200	3.87362900	0.80150800
O	-1.02081200	3.90265000	-0.75269800
H	-0.43699500	3.60447400	0.02103800
O	-3.03627100	4.30774800	-1.39739200
C	-4.46906000	4.50602800	-1.23289000
C	-5.12688900	3.22539800	-0.72791400
H	-4.85413100	2.38437400	-1.37452200
H	-6.21513400	3.34174400	-0.75851100
H	-4.82631400	3.00162600	0.29703200
C	-4.73716100	5.69577200	-0.31674000
H	-4.43048700	5.48512200	0.70872600
H	-5.80776000	5.92416800	-0.32456200
H	-4.19597900	6.57658200	-0.67790000
C	-4.93007700	4.81505100	-2.65246500
H	-4.70144000	3.97788200	-3.31926800
H	-4.42688600	5.71010600	-3.03116300
H	-6.01001600	4.98854600	-2.66537600
H	-3.88125200	0.19926100	0.27509000
H	-2.83127700	1.37679900	1.11002700

Zero-point correction= 1.017705 (Hartree/Particle)

Thermal correction to Energy= 1.081293

Thermal correction to Enthalpy= 1.082237

Thermal correction to Gibbs Free Energy= 0.912270

Sum of electronic and zero-point Energies= -2811.578432

Sum of electronic and thermal Energies= -2811.514845

Sum of electronic and thermal Enthalpies= -2811.513901

Sum of electronic and thermal Free Energies= -2811.683867

E(RM062X/6-311+G(2d,p)) = -2813.47813451

3k-*RS*-**TS4**-CONF2

C	-2.18338300	0.66206700	-0.80567600
H	-1.87094400	1.31983400	-1.60969200
H	-1.96632000	-0.39032700	-0.96697200
C	-3.26276200	1.02808400	-0.03128900
C	-3.86077400	2.34292600	-0.08913500
O	-4.76649900	2.74056400	0.64064400
O	-3.36461400	3.11951500	-1.07734000
C	-3.77503700	4.48644300	-1.06977400
H	-4.85242200	4.54423700	-1.26145900
H	-3.58515600	4.91297400	-0.08025200
C	-2.97587900	5.19960700	-2.13801200
H	-3.15495300	4.75033700	-3.11988800
H	-1.90851500	5.13927300	-1.90798500
H	-3.26898700	6.25311700	-2.18277900
C	-3.70670400	0.14420500	1.08674800
H	-4.16152300	0.72705600	1.88958200
H	-2.87175200	-0.43804200	1.48287000
N	-4.73220200	-0.85907500	0.66459200
C	-5.98857800	-0.44109300	0.39499600
H	-6.16553100	0.62045100	0.54181000
C	-6.95787300	-1.30347300	-0.03741700
H	-7.94752900	-0.91099400	-0.22880000
C	-4.39984200	-2.15315600	0.48143700
H	-3.36512600	-2.40769500	0.69251600
C	-5.31362600	-3.07686500	0.04514400
H	-4.98645600	-4.09972100	-0.08514800
C	-6.65298100	-2.68239600	-0.22433500
N	-7.58177000	-3.56023700	-0.63478000
C	-8.93953000	-3.11125100	-0.91588200

H	-9.53048400	-3.96588700	-1.24045800
H	-8.94716300	-2.35960500	-1.71249400
H	-9.40495000	-2.68410400	-0.02112600
C	-7.23404500	-4.96495400	-0.80584700
H	-8.12589600	-5.51244700	-1.10638400
H	-6.86273500	-5.39191800	0.13163700
H	-6.46894200	-5.09000200	-1.57978100
N	-0.42691300	0.72005300	0.21804700
N	0.34222600	-0.39454300	-0.10363700
C	-0.13465400	-1.64414500	0.19488200
O	-1.16236700	-1.88123800	0.80696500
O	0.71127000	-2.58854600	-0.25066400
C	0.25201700	-3.95715800	-0.20690500
H	-0.22021600	-4.11716200	0.76636000
C	-0.74610500	-4.18844100	-1.32877300
H	-0.27143600	-3.99975300	-2.29743200
H	-1.60963600	-3.52468500	-1.22694500
H	-1.09907800	-5.22422700	-1.30813900
C	1.50090700	-4.80505200	-0.34464400
H	1.96053200	-4.64291200	-1.32532300
H	1.24566200	-5.86449800	-0.25057500
H	2.22942000	-4.54703700	0.42944100
C	-0.56308600	0.99207900	1.52083400
O	-1.23043200	1.97605000	1.90619000
O	-0.00817200	0.14593000	2.40679900
C	-0.02887100	0.55772300	3.78627300
H	-1.00446300	1.00638100	3.99129400
C	1.07158400	1.57925400	4.02092500
H	2.04919600	1.13042900	3.81759700
H	1.04976100	1.93094500	5.05765900

H	0.93981600	2.43577600	3.35331600
C	0.14167800	-0.70851800	4.60356600
H	1.10404400	-1.18199000	4.38524300
H	-0.65578900	-1.42232100	4.37621600
H	0.10578600	-0.47201600	5.67142400
C	1.37322700	-0.20996900	-1.11485600
C	1.51128100	1.25776600	-1.50998700
H	1.73337500	1.85631400	-0.62489500
C	1.07935700	-1.03655400	-2.39662400
O	0.00222900	-0.99852600	-2.96014100
C	2.30623600	-1.72108600	-2.74743200
H	2.49439900	-2.25514900	-3.66868400
C	3.20664600	-1.53493100	-1.74497700
N	2.70287800	-0.73733400	-0.72452700
C	3.15206400	-0.64039200	0.59071700
O	2.81242200	0.25836400	1.32506600
O	3.94846800	-1.66477800	0.89086000
C	4.72308400	-1.68418300	2.13043500
C	5.56580400	-2.94325000	1.97449800
H	4.92532200	-3.82583500	1.88196100
H	6.20982800	-3.06887300	2.84976500
H	6.19513200	-2.87185500	1.08104800
C	5.61400000	-0.45058300	2.21982800
H	5.02453900	0.46489700	2.29854600
H	6.26410600	-0.38806000	1.34098900
H	6.24749400	-0.53375500	3.10849700
C	3.77641200	-1.80156400	3.31806800
H	3.19413800	-0.88686800	3.44245200
H	4.35554100	-1.98144900	4.22943000
H	3.09085300	-2.64292600	3.17058000

C	4.61512100	-1.97516300	-1.78275500
C	7.28347100	-2.77100400	-1.98177700
C	4.93222400	-3.25650600	-2.23765400
C	5.64116100	-1.08757000	-1.43636300
C	6.96911600	-1.48330700	-1.54233900
C	6.26439000	-3.65493200	-2.32816600
H	4.13434500	-3.94365500	-2.50424800
H	5.39405700	-0.08449500	-1.09736800
H	7.76091800	-0.78752800	-1.28137100
H	6.50403600	-4.65706900	-2.66996800
H	8.32136200	-3.08095800	-2.05664900
C	1.75903300	5.81172500	-0.95131000
C	1.46677400	6.83000000	-2.04744400
H	0.72886000	7.56086200	-1.70227200
H	1.07214700	6.33032400	-2.93777300
H	2.38364200	7.36029700	-2.32088700
C	2.73679100	4.75477300	-1.45541900
H	2.98906400	4.04077600	-0.66979400
H	3.65513800	5.24438700	-1.79562800
H	2.30040200	4.21665300	-2.30402500
C	2.26300700	6.51313500	0.30591500
H	2.48784900	5.79569400	1.09640100
H	1.50979800	7.22041000	0.66869100
H	3.17317300	7.07308300	0.06823100
O	0.45292000	5.21915100	-0.70984500
C	0.29637100	4.25783800	0.21272400
O	1.18360300	3.79066000	0.90201400
O	-0.97191200	3.91695900	0.24755300
H	-1.09383400	3.13147700	0.88717100
H	0.58570100	1.61563600	-1.96654700

H 2.32739700 1.33853200 -2.23485200

Zero-point correction= 1.017961 (Hartree/Particle)

Thermal correction to Energy= 1.081267

Thermal correction to Enthalpy= 1.082211

Thermal correction to Gibbs Free Energy= 0.915517

Sum of electronic and zero-point Energies= -2811.577452

Sum of electronic and thermal Energies= -2811.514147

Sum of electronic and thermal Enthalpies= -2811.513202

Sum of electronic and thermal Free Energies= -2811.679897

E(RM062X/6-311+G(2d,p)) = -2813.47764516

3k-*RS*-**TS4**-CONF3

C	-2.18348000	0.66220600	-0.80557500
H	-1.87098500	1.31991900	-1.60961200
H	-1.96648700	-0.39021000	-0.96681900
C	-3.26281900	1.02833600	-0.03119600
C	-3.86076600	2.34320700	-0.08912500
O	-4.76661600	2.74085900	0.64049100
O	-3.36438300	3.11980200	-1.07720800
C	-3.77479600	4.48673500	-1.06972500
H	-3.58509400	4.91326800	-0.08016700
H	-4.85214700	4.54453600	-1.26160200
C	-2.97544800	5.19989700	-2.13782300
H	-1.90812300	5.13954600	-1.90762100
H	-3.15436700	4.75063700	-3.11973200
H	-3.26854000	6.25340900	-2.18262900
C	-3.70689600	0.14449900	1.08682100
H	-2.87199500	-0.43774600	1.48305900
H	-4.16179600	0.72738700	1.88958300
N	-4.73236100	-0.85877700	0.66457600

C	-4.40005600	-2.15290500	0.48165600
H	-3.36539700	-2.40748600	0.69295900
C	-5.31382400	-3.07660800	0.04531400
H	-4.98670200	-4.09950500	-0.08478700
C	-5.98865300	-0.44074100	0.39466700
H	-6.16556500	0.62083600	0.54130600
C	-6.95792400	-1.30310800	-0.03781900
H	-7.94751500	-0.91058100	-0.22944900
C	-6.65310100	-2.68208200	-0.22446400
N	-7.58188600	-3.55992000	-0.63492400
C	-7.23425300	-4.96470100	-0.80564100
H	-8.12611600	-5.51219300	-1.10614400
H	-6.46907700	-5.08998800	-1.57946700
H	-6.86307800	-5.39147900	0.13198000
C	-8.93954300	-3.11086100	-0.91641000
H	-9.53050800	-3.96550600	-1.24094200
H	-9.40511900	-2.68349100	-0.02184200
H	-8.94693100	-2.35937900	-1.71317700
N	-0.42693500	0.72009000	0.21813600
C	-0.56306300	0.99220100	1.52090800
O	-1.23026200	1.97628700	1.90622300
O	-0.00826100	0.14600600	2.40690400
C	-0.02886000	0.55784600	3.78635900
H	-1.00440300	1.00659700	3.99141500
C	0.14162800	-0.70838900	4.60367400
H	1.10394900	-1.18193600	4.38530800
H	0.10581100	-0.47186600	5.67153000
H	-0.65590200	-1.42213800	4.37637800
C	1.07170000	1.57928100	4.02094200
H	2.04926300	1.13034200	3.81763200

H	0.94001400	2.43577400	3.35328000
H	1.04992300	1.93103600	5.05765400
C	0.29684700	4.25786300	0.21265100
O	1.18400200	3.79057100	0.90196200
O	-0.97148000	3.91713700	0.24744200
H	-1.09351100	3.13169900	0.88708000
O	0.45353100	5.21916400	-0.70990500
C	1.75972900	5.81155600	-0.95135900
C	2.73733900	4.75446100	-1.45545700
H	2.30088800	4.21641400	-2.30407700
H	3.65576800	5.24394000	-1.79564200
H	2.98948800	4.04041900	-0.66983200
C	2.26379200	6.51289800	0.30586800
H	2.48853900	5.79542800	1.09635400
H	3.17403200	7.07272600	0.06818600
H	1.51067600	7.22027200	0.66864300
C	1.46762200	6.82987200	-2.04749500
H	1.07291800	6.33025300	-2.93782200
H	0.72981900	7.56084600	-1.70232300
H	2.38457000	7.36003100	-2.32094000
N	0.34210300	-0.39458500	-0.10351100
C	-0.13487200	-1.64413600	0.19506300
O	-1.16262500	-1.88112900	0.80711600
O	0.71101600	-2.58861600	-0.25039300
C	0.25164300	-3.95718700	-0.20666700
H	-0.22076400	-4.11712500	0.76652400
C	-0.74631700	-4.18840800	-1.32869000
H	-0.27147200	-3.99981500	-2.29728100
H	-1.60979200	-3.52455100	-1.22703300
H	-1.09941200	-5.22415300	-1.30807000

C	1.50048300	-4.80519200	-0.34417300
H	1.96032600	-4.64307000	-1.32475300
H	1.24512300	-5.86461700	-0.25018300
H	2.22885900	-4.54726600	0.43007100
C	1.37307500	-0.21014800	-1.11478500
C	1.51123900	1.25755400	-1.51001400
H	1.73344300	1.85614800	-0.62497800
C	1.07907700	-1.03679500	-2.39648600
O	0.00191100	-0.99875800	-2.95992800
C	2.30590600	-1.72139200	-2.74735000
H	2.49399300	-2.25547800	-3.66860400
C	3.20639800	-1.53520800	-1.74497200
N	2.70271500	-0.73757700	-0.72450700
C	3.15197200	-0.64065500	0.59071000
O	2.81238900	0.25809800	1.32508800
O	3.94837200	-1.66506100	0.89079700
C	4.72307700	-1.68448200	2.13031400
C	5.56575300	-2.94357200	1.97430900
H	4.92524100	-3.82614100	1.88182600
H	6.20985000	-3.06921200	2.84952000
H	6.19500400	-2.87219400	1.08080400
C	5.61403400	-0.45090600	2.21963500
H	5.02460600	0.46459100	2.29839800
H	6.26406900	-0.38840100	1.34074100
H	6.24759900	-0.53409400	3.10825100
C	3.77649700	-1.80183900	3.31802400
H	3.19427700	-0.88711700	3.44247800
H	4.35569400	-1.98177100	4.22933400
H	3.09088600	-2.64316600	3.17057800
C	4.61488100	-1.97540200	-1.78284200

C	7.28324900	-2.77114000	-1.98202900
C	4.93200200	-3.25675300	-2.23770400
C	5.64091000	-1.08774700	-1.43657300
C	6.96887400	-1.48343500	-1.54262900
C	6.26417800	-3.65512700	-2.32829900
H	4.13413200	-3.94394700	-2.50420600
H	5.39379000	-0.08466200	-1.09761600
H	7.76066600	-0.78761000	-1.28175500
H	6.50384200	-4.65727000	-2.67007200
H	8.32114800	-3.08105200	-2.05696600
H	0.58566900	1.61547800	-1.96655200
H	2.32732100	1.33820100	-2.23492900

Zero-point correction= 1.017963 (Hartree/Particle)

Thermal correction to Energy= 1.081268

Thermal correction to Enthalpy= 1.082212

Thermal correction to Gibbs Free Energy= 0.915520

Sum of electronic and zero-point Energies= -2811.577451

Sum of electronic and thermal Energies= -2811.514146

Sum of electronic and thermal Enthalpies= -2811.513201

Sum of electronic and thermal Free Energies= -2811.679893

E(RM062X/6-311+G(2d,p)) = -2813.47764531

3k-*RS*-**TS4**-CONF4

C	-2.23676700	0.62144000	-0.89786400
H	-1.94758100	1.31176400	-1.68278500
H	-1.98420400	-0.41800300	-1.08788200
C	-3.32236400	0.92755000	-0.10698100
C	-3.94150100	2.23392800	-0.09881000
O	-4.84569100	2.58309700	0.65690900
O	-3.46345100	3.06352400	-1.05238500

C	-3.90532000	4.41921300	-0.98861500
H	-3.70814600	4.81442900	0.01246300
H	-4.98686300	4.45783800	-1.16034100
C	-3.14223800	5.19008500	-2.04312200
H	-2.07016800	5.15066800	-1.83178100
H	-3.32535700	4.77065100	-3.03733700
H	-3.46390600	6.23615000	-2.04610400
C	-3.72665400	-0.00293600	0.98819800
H	-2.87318600	-0.58585000	1.34199500
H	-4.16853200	0.54435200	1.82269700
N	-4.74908300	-1.00522300	0.55723500
C	-4.40486400	-2.28757300	0.32153000
H	-3.36079300	-2.53367600	0.49276000
C	-5.31866800	-3.20968300	-0.11795900
H	-4.98248100	-4.22310700	-0.29108800
C	-6.01809200	-0.59648200	0.33735300
H	-6.20497500	0.45666400	0.52633100
C	-6.98733900	-1.45751600	-0.09766100
H	-7.98759200	-1.07363300	-0.24605500
C	-6.66959600	-2.82487800	-0.33914200
N	-7.59748800	-3.70092300	-0.75565200
C	-7.24079600	-5.09773900	-0.96790000
H	-8.13639900	-5.64871700	-1.25053000
H	-6.49945900	-5.19859200	-1.76815800
H	-6.83551600	-5.53990800	-0.05183900
C	-8.96468800	-3.25861700	-0.99931000
H	-9.54599000	-4.10414800	-1.36284000
H	-9.42764900	-2.88466000	-0.07965500
H	-8.99093400	-2.46763200	-1.75626600
N	-0.48295300	0.71883600	0.13060200

C	-0.64405700	0.96170300	1.43654700
O	-1.34802300	1.91685700	1.82911400
O	-0.07546800	0.11574300	2.31388300
C	-0.11948700	0.50167300	3.70000300
H	-1.10711800	0.92413300	3.90337100
C	0.07276100	-0.77580000	4.49468400
H	1.04295600	-1.22810100	4.26563300
H	0.03450100	-0.55983600	5.56684000
H	-0.71286400	-1.49910200	4.25555400
C	0.95536400	1.54316400	3.96389100
H	1.94466200	1.11767100	3.76651100
H	0.81323900	2.40616600	3.30658500
H	0.91300800	1.87843000	5.00546200
C	0.18978500	4.28653000	0.28336600
O	1.04779700	3.82167400	1.01054500
O	-1.06785200	3.90909400	0.23100200
H	-1.20387800	3.10468700	0.84258200
O	0.37145600	5.28030300	-0.59849200
C	1.67060500	5.91890000	-0.74098100
C	2.70912100	4.90867500	-1.21838400
H	2.34468800	4.39268100	-2.11336400
H	3.63293700	5.43538800	-1.47912700
H	2.93086800	4.17150400	-0.44510200
C	2.07580300	6.59248100	0.56617000
H	2.27829100	5.85654300	1.34549400
H	2.97866800	7.18925300	0.40145300
H	1.27893900	7.26242500	0.90578600
C	1.41299100	6.96473500	-1.81972300
H	1.08397700	6.48434500	-2.74651800
H	0.63668300	7.66459700	-1.49524600

H	2.32896100	7.52717400	-2.02280200
N	0.33761100	-0.35487200	-0.20292300
C	-0.09188200	-1.63103800	0.05440100
O	-1.11174100	-1.92625700	0.65487000
O	0.78361600	-2.52797200	-0.42873100
C	0.53404700	-3.92184000	-0.14752100
H	-0.53430300	-4.10755200	-0.29092000
C	1.35856100	-4.69052000	-1.16131300
H	2.42227800	-4.46575500	-1.02436900
H	1.06995100	-4.42376400	-2.18224600
H	1.20940900	-5.76548700	-1.02352000
C	0.94118900	-4.21995300	1.28486400
H	2.00764100	-4.00593200	1.41321600
H	0.76461000	-5.27517200	1.51509600
H	0.36840100	-3.60737100	1.98630300
C	1.39245700	-0.09367200	-1.17501300
C	1.52903500	1.39899700	-1.46358100
H	1.71927600	1.93809900	-0.53352700
C	1.13573200	-0.83031600	-2.51769800
O	0.07705700	-0.74741600	-3.11025900
C	2.36949300	-1.49646100	-2.87644000
H	2.58077400	-1.97733500	-3.82162000
C	3.24142800	-1.37927000	-1.83932600
N	2.71559500	-0.63932400	-0.78689500
C	3.12597300	-0.62476300	0.54458100
O	2.78149900	0.24126300	1.31503400
O	3.89143000	-1.68061900	0.81691200
C	4.66258800	-1.75332700	2.05868100
C	5.45539300	-3.04071300	1.87692900
H	4.78012700	-3.89616500	1.77307300

H	6.09879300	-3.20694200	2.74585300
H	6.08196900	-2.97826400	0.98083100
C	5.59812700	-0.55497400	2.17011100
H	5.04045800	0.38141000	2.23972700
H	6.27072500	-0.51328800	1.30774400
H	6.20650000	-0.66293800	3.07356500
C	3.72104800	-1.85333500	3.25247000
H	3.18174100	-0.91682500	3.40405700
H	4.30347000	-2.07780600	4.15191800
H	2.99705300	-2.66040600	3.10022200
C	4.64389300	-1.83752100	-1.86634000
C	7.30304500	-2.66824300	-2.04808000
C	4.95250400	-3.08978200	-2.40276200
C	5.67431300	-0.99569900	-1.43158000
C	6.99795800	-1.40861400	-1.52846700
C	6.27954900	-3.50641200	-2.48408100
H	4.15045200	-3.73954700	-2.74176200
H	5.43538400	-0.01328000	-1.03167500
H	7.79368100	-0.74759500	-1.19810500
H	6.51190100	-4.48598700	-2.89024400
H	8.33728500	-2.99164800	-2.11599100
H	0.61527300	1.78102400	-1.92412600
H	2.36684500	1.53382600	-2.15471800

Zero-point correction= 1.018169 (Hartree/Particle)

Thermal correction to Energy= 1.081358

Thermal correction to Enthalpy= 1.082302

Thermal correction to Gibbs Free Energy= 0.915067

Sum of electronic and zero-point Energies= -2811.576773

Sum of electronic and thermal Energies= -2811.513585

Sum of electronic and thermal Enthalpies= -2811.512640

Sum of electronic and thermal Free Energies= -2811.679876

E(RM062X/6-311+G(2d,p)) = -2813.47697217

3k-*RS*-**TS4**

C	-2.21586000	0.71201100	-0.77597900
H	-1.89998700	1.34551000	-1.59732300
H	-1.99682200	-0.34487500	-0.90460100
C	-3.28968300	1.09957400	-0.00810900
C	-3.85398100	2.43034800	-0.06398300
O	-4.76460700	2.84326500	0.64939300
O	-3.30952100	3.20473300	-1.02812700
C	-3.71196800	4.57418200	-1.04241200
H	-3.48012500	5.02630100	-0.07267700
H	-4.79554500	4.63375500	-1.19135900
C	-2.95441100	5.25394100	-2.16181000
H	-1.87861800	5.19008900	-1.97870900
H	-3.18058200	4.78173900	-3.12291600
H	-3.24238000	6.30816400	-2.21995300
C	-3.76275200	0.22566400	1.10545700
H	-2.93273100	-0.32114000	1.55850100
H	-4.28047400	0.81063800	1.86790500
N	-4.72982000	-0.81655700	0.64265600
C	-4.35787200	-2.10743900	0.52805700
H	-3.34156200	-2.33356200	0.83811100
C	-5.20993600	-3.06179100	0.03541800
H	-4.85264600	-4.08053400	-0.03412900
C	-5.96616700	-0.43454600	0.25349600
H	-6.17816700	0.62560400	0.35548400
C	-6.87545100	-1.32792800	-0.24056100
H	-7.85092800	-0.96188400	-0.53131300

C	-6.52428300	-2.70260100	-0.37159700
N	-7.38838100	-3.60719100	-0.85789600
C	-6.98514600	-5.00056600	-0.99719500
H	-7.81650900	-5.56691000	-1.41361300
H	-6.12620700	-5.09435700	-1.67029900
H	-6.72142700	-5.43049700	-0.02507900
C	-8.72317200	-3.19458300	-1.27309700
H	-9.26981200	-4.07085200	-1.61696000
H	-9.27201400	-2.74794600	-0.43760300
H	-8.67339200	-2.46919200	-2.09244500
N	-0.43815500	0.82472600	0.23368500
C	-0.56822600	1.21614000	1.50535800
O	-1.25619500	2.21729200	1.80091800
O	0.03771200	0.48442700	2.45700800
C	-0.09349000	0.94947900	3.81171500
H	-0.06724500	2.04246400	3.80053700
C	-1.41734100	0.46899100	4.38303300
H	-1.47262000	-0.62403700	4.32941300
H	-1.51465500	0.77252000	5.43048300
H	-2.25048000	0.89627900	3.81882200
C	1.10732600	0.40300500	4.55837500
H	1.10601300	-0.69227400	4.53580300
H	2.03131900	0.76235900	4.09763500
H	1.08198300	0.72969900	5.60258500
C	0.49315800	4.30488200	0.07051700
O	1.30072400	3.81439500	0.83599700
O	-0.79561700	4.04338300	0.03129900
H	-1.01239500	3.30772700	0.69884300
O	0.76731800	5.21339800	-0.87770600
C	2.11854500	5.72557300	-1.04372500

C	3.07305900	4.59867200	-1.42653600
H	2.67167600	4.04355400	-2.28142700
H	4.03789300	5.02619800	-1.71849700
H	3.23073400	3.91035300	-0.59473400
C	2.56483500	6.45765200	0.21773600
H	2.68892800	5.76708200	1.05309300
H	3.52055500	6.95683900	0.02840000
H	1.82748500	7.21998900	0.49036300
C	1.96602200	6.70578500	-2.20112000
H	1.61301900	6.18661400	-3.09765500
H	1.24575500	7.48911400	-1.94551600
H	2.92884000	7.17460600	-2.42414700
N	0.33028100	-0.31489100	0.00549400
C	-0.16886800	-1.53197900	0.38816700
O	-1.18002200	-1.70480500	1.04826800
O	0.63226700	-2.52626300	-0.03331600
C	0.12635100	-3.87315200	0.08933200
H	-0.33366800	-3.96718600	1.07680700
C	-0.89953600	-4.12195400	-1.00356100
H	-0.43368800	-4.00572600	-1.98785200
H	-1.73256200	-3.41677000	-0.92615800
H	-1.29584500	-5.13896000	-0.92186300
C	1.34021300	-4.77331300	-0.02585700
H	1.79835300	-4.66368900	-1.01445700
H	1.04460800	-5.81796400	0.10750800
H	2.08373600	-4.51748100	0.73421300
C	1.33405800	-0.22034300	-1.04756400
C	1.53410300	1.22474300	-1.49652900
H	1.80388400	1.83656500	-0.63358700
C	0.95483700	-1.07737700	-2.28673200

O	-0.14097700	-1.01478500	-2.81093100
C	2.13667000	-1.82565700	-2.66039300
H	2.26684000	-2.39562300	-3.57007300
C	3.08257900	-1.64384600	-1.70050300
N	2.65181000	-0.79611500	-0.68680600
C	3.16042600	-0.69168400	0.60662600
O	2.89233500	0.23416100	1.33656100
O	3.92482600	-1.74581100	0.88759500
C	4.77615000	-1.78424300	2.07443400
C	5.58719400	-3.05544900	1.85767400
H	4.92699500	-3.92559700	1.78858400
H	6.27459900	-3.20414200	2.69562100
H	6.16904200	-2.98326100	0.93255000
C	5.69227700	-0.56669400	2.11823300
H	5.12759700	0.35689200	2.25718300
H	6.27603500	-0.49818700	1.19434100
H	6.38930500	-0.67824400	2.95469900
C	3.90191800	-1.89453200	3.31597200
H	3.32633500	-0.98062200	3.46669800
H	4.53390200	-2.06453700	4.19353000
H	3.21056800	-2.73817300	3.21783200
C	4.47230000	-2.13622900	-1.78150200
C	7.10177800	-3.02972100	-2.06466500
C	4.72651400	-3.44840300	-2.18432700
C	5.54100000	-1.26747900	-1.52903700
C	6.84934400	-1.71198600	-1.67740000
C	6.03990500	-3.89525600	-2.31624200
H	3.89571200	-4.12071400	-2.37883200
H	5.34125700	-0.24151500	-1.22946800
H	7.67404000	-1.03094300	-1.48951700

H 6.23136000 -4.92067400 -2.61695400

H 8.12460300 -3.37774800 -2.17242500

H 0.61980200 1.61695900 -1.94675900

H 2.33971500 1.23995000 -2.23722600

Zero-point correction= 1.017697 (Hartree/Particle)

Thermal correction to Energy= 1.081145

Thermal correction to Enthalpy= 1.082089

Thermal correction to Gibbs Free Energy= 0.914441

Sum of electronic and zero-point Energies= -2811.576165

Sum of electronic and thermal Energies= -2811.512718

Sum of electronic and thermal Enthalpies= -2811.511774

Sum of electronic and thermal Free Energies= -2811.679422

E(RM062X/6-311+G(2d,p)) = -2813.47677735

RR-**TS4**

C 0.02035100 1.58509300 -0.60276700

H -0.45324600 1.19341000 -1.49348900

H 0.93404900 1.07006500 -0.31321700

C -0.12247000 2.92456200 -0.29828700

C -1.09813900 3.77279900 -0.94160300

O -1.27370500 4.96442100 -0.69456900

O -1.80896400 3.14576700 -1.90724600

C -2.86420100 3.90027500 -2.50218500

H -3.60869700 4.14041000 -1.73506100

H -2.46451000 4.84376400 -2.88800600

C -3.46303900 3.05553100 -3.60549200

H -3.86954900 2.12862600 -3.19357500

H -2.70423300 2.80801600 -4.35439200

H -4.26806500 3.60755700 -4.10058400

C 0.58373000 3.51341800 0.87678800

H	0.65861500	2.79898600	1.69818300
H	0.08149500	4.41986900	1.21887700
N	1.99099000	3.90817100	0.55519800
C	3.03570500	3.17786200	0.99342300
H	2.78410900	2.33005000	1.62412900
C	4.32633500	3.48511000	0.64626400
H	5.12274500	2.85951400	1.02694400
C	2.20223400	4.96374300	-0.26132900
H	1.30633700	5.48229800	-0.59009000
C	3.45975300	5.33928600	-0.64467400
H	3.56561200	6.19848600	-1.29314200
C	4.59186800	4.60078500	-0.19424300
N	5.84115800	4.94047800	-0.54920800
C	6.97448400	4.16137500	-0.06800600
H	7.89354500	4.61505600	-0.43501400
H	6.92417700	3.12864700	-0.43008500
H	7.00455800	4.15122200	1.02664200
C	6.06766800	6.07911600	-1.43039900
H	7.13703200	6.17671500	-1.60871800
H	5.70296200	7.00600900	-0.97527300
H	5.56579300	5.93583900	-2.39323200
N	-0.96591000	0.35403000	0.65111800
N	-0.18703100	-0.70986300	1.11112300
C	0.96254200	-0.42260600	1.79905500
O	1.32657400	0.69854000	2.11614800
O	1.65726700	-1.53547000	2.07638700
C	2.95617200	-1.37201800	2.68472900
H	2.88147200	-0.56986500	3.42356800
C	3.26516200	-2.69381300	3.35922400
H	3.34217600	-3.49340700	2.61487400

H	2.48045900	-2.95347200	4.07559600
H	4.21764700	-2.62311400	3.89260400
C	3.95688900	-1.01141200	1.60003400
H	3.96076600	-1.79216000	0.83134700
H	4.96250800	-0.92458700	2.02314400
H	3.69132600	-0.05806000	1.13277300
C	-1.63324500	1.03138100	1.60105000
O	-2.37755000	1.98736500	1.31454200
O	-1.45043700	0.64445600	2.87832200
C	-2.25386200	1.29042400	3.88417700
H	-2.28500300	2.36025000	3.65836900
C	-1.53000800	1.04340500	5.19440200
H	-1.46433100	-0.03211400	5.39055100
H	-2.07060000	1.51701000	6.01940500
H	-0.51585300	1.45223300	5.15766000
C	-3.66014800	0.71406900	3.86738200
H	-3.62754100	-0.35530500	4.10567100
H	-4.12113000	0.84800800	2.88401700
H	-4.27989300	1.21601600	4.61808900
C	-0.53080700	-2.08085000	0.72918000
C	-1.93890300	-2.13771000	0.07100200
H	-1.94486600	-1.31336800	-0.64501300
C	-3.06292100	-1.91947300	1.08778900
H	-3.97673500	-1.62900100	0.56014900
H	-2.82435600	-1.14552100	1.81903900
H	-3.27099600	-2.83947700	1.64399600
C	-2.17292600	-3.44093400	-0.69404600
H	-2.08475100	-4.32083900	-0.04678300
H	-1.48082800	-3.55322000	-1.53334500
H	-3.19005100	-3.43043000	-1.09965200

C	-0.46288400	-3.04862500	1.95237100
O	-1.04477100	-2.84521700	2.99761200
C	0.35013500	-4.18325800	1.55262600
H	0.48195100	-5.09296100	2.12215300
C	0.90255500	-3.92057900	0.34161500
N	0.49106500	-2.69086800	-0.16101300
C	1.03415000	-1.95727300	-1.20564700
O	0.39591500	-1.11177200	-1.79457800
O	2.30788500	-2.28043500	-1.41835000
C	3.03341200	-1.74921000	-2.57406900
C	4.38196700	-2.44859400	-2.46605200
H	4.88535700	-2.17507100	-1.53327000
H	5.01935000	-2.15553700	-3.30535100
H	4.24897800	-3.53533500	-2.48780900
C	2.33032100	-2.14139400	-3.86841700
H	1.34167000	-1.68493400	-3.94268900
H	2.23322900	-3.22992500	-3.93259300
H	2.93394900	-1.80187400	-4.71598200
C	3.18982200	-0.23895200	-2.43412300
H	2.23523200	0.27502700	-2.55984500
H	3.88712300	0.12116200	-3.19740700
H	3.60254100	0.00762700	-1.44964100
C	1.72655900	-4.86417700	-0.43849800
C	3.21783300	-6.74738200	-1.86359600
C	2.70933100	-5.61755000	0.20811000
C	1.48532300	-5.06663100	-1.80278600
C	2.22488100	-6.00795900	-2.50917200
C	3.45759900	-6.55100500	-0.50576000
H	2.89389600	-5.46061300	1.26713100
H	0.70876500	-4.49528000	-2.30590300

H	2.02595800	-6.16678500	-3.56483900
H	4.22776000	-7.12406600	0.00117800
H	3.79851800	-7.47771900	-2.41882600
C	-4.86207500	0.83434000	-0.45797300
O	-5.27178500	0.77689300	0.68460000
O	-3.68974600	1.29702600	-0.84017300
H	-3.15973700	1.60473900	-0.03702800
O	-5.53303900	0.44105200	-1.54901300
C	-6.88438300	-0.08822000	-1.43529200
C	-6.88306600	-1.37584800	-0.61758600
H	-6.15585800	-2.08288300	-1.03155600
H	-7.87475000	-1.83701800	-0.66796700
H	-6.63876000	-1.18219000	0.42809500
C	-7.81856600	0.96715100	-0.85194300
H	-7.58326500	1.17237800	0.19332100
H	-8.85176900	0.61149200	-0.91768600
H	-7.73856000	1.89665500	-1.42543400
C	-7.25314800	-0.38025400	-2.88503800
H	-6.55790600	-1.10628300	-3.31768900
H	-7.21496200	0.53696300	-3.48093000
H	-8.26586200	-0.79031200	-2.93777200

Zero-point correction= 1.075044 (Hartree/Particle)

Thermal correction to Energy= 1.141253

Thermal correction to Enthalpy= 1.142197

Thermal correction to Gibbs Free Energy= 0.967944

Sum of electronic and zero-point Energies= -2890.105479

Sum of electronic and thermal Energies= -2890.039271

Sum of electronic and thermal Enthalpies= -2890.038327

Sum of electronic and thermal Free Energies= -2890.212579

E(RM062X/6-311+G(2d,p)) = -2892.08512891

RS-**TS4**

C	-2.27025800	0.60104300	-0.83724100
H	-2.01715000	1.24281100	-1.67260700
H	-2.07952100	-0.45469600	-1.00743800
C	-3.32916400	0.97944800	-0.03135700
C	-3.89515100	2.30548200	-0.06823200
O	-4.80390900	2.71039500	0.65534400
O	-3.35894300	3.09624400	-1.02723200
C	-3.78435300	4.45806400	-1.03565700
H	-3.56223300	4.91044700	-0.06383400
H	-4.86856600	4.50047000	-1.18676800
C	-3.03647200	5.15597300	-2.15053900
H	-1.96036500	5.11252900	-1.96344800
H	-3.24956800	4.68212800	-3.11381300
H	-3.34422200	6.20472400	-2.20680200
C	-3.75525200	0.11445100	1.10646500
H	-2.91769700	-0.46698100	1.49746500
H	-4.19462500	0.71173600	1.90749600
N	-4.79577900	-0.88935500	0.71864800
C	-4.48371100	-2.19269100	0.57314500
H	-3.45132000	-2.45544100	0.78459300
C	-5.41345600	-3.11558700	0.16906900
H	-5.10201100	-4.14659300	0.06763800
C	-6.04687500	-0.46055900	0.44201100
H	-6.20563600	0.60798400	0.55642900
C	-7.03146700	-1.32093200	0.04117900
H	-8.01540800	-0.91941900	-0.16045100
C	-6.74814600	-2.70932200	-0.10544900
N	-7.69180600	-3.58521000	-0.48580200

C	-7.36165000	-4.99715700	-0.62930400
H	-8.25941500	-5.53892000	-0.92249800
H	-6.59637700	-5.14598500	-1.39873500
H	-6.99779700	-5.41160700	0.31682200
C	-9.04614700	-3.12627900	-0.76741700
H	-9.65448000	-3.98373200	-1.04973900
H	-9.49275800	-2.65740800	0.11580500
H	-9.05362500	-2.40624800	-1.59283700
N	-0.50257900	0.70788200	0.08756500
C	-0.63178600	1.04363000	1.38256000
O	-1.27679000	2.05657700	1.71514300
O	-0.09874200	0.22278700	2.30271700
C	-0.11649700	0.68861000	3.66560300
H	-1.06910000	1.19666800	3.83711500
C	-0.02738900	-0.55125000	4.53432800
H	0.90930900	-1.08564400	4.34917500
H	-0.06377400	-0.27020500	5.59132400
H	-0.86080400	-1.22837300	4.32375300
C	1.03488000	1.65790500	3.87214600
H	1.98689000	1.15297800	3.67982700
H	0.94492900	2.50106200	3.18064100
H	1.03245000	2.03858500	4.89897400
C	0.37472300	4.37308100	0.21066900
O	1.18439400	3.86106400	0.96079900
O	-0.87381300	3.99477000	0.04735100
H	-1.06247700	3.19491100	0.64257200
O	0.60766400	5.42559200	-0.58678200
C	1.88706600	6.11908400	-0.54100000
C	3.00543200	5.19684700	-1.01320100
H	2.78714500	4.82800600	-2.02123100

H	3.94604700	5.75617000	-1.05130100
H	3.12756200	4.34836400	-0.33725900
C	2.14281800	6.66862600	0.85913400
H	2.33279200	5.86706100	1.57417500
H	3.01348900	7.33154100	0.83271600
H	1.27881600	7.25089500	1.19636800
C	1.68671200	7.26145000	-1.52969500
H	1.44537600	6.86868700	-2.52225600
H	0.86917400	7.91160400	-1.20319200
H	2.60104400	7.85766500	-1.60197300
N	0.27976400	-0.41283000	-0.18544900
C	-0.23897700	-1.64971700	0.10388300
O	-1.25834700	-1.84801700	0.74502500
O	0.53172700	-2.63210200	-0.38733400
C	0.02608200	-3.98042400	-0.28080800
H	-0.38422800	-4.10308800	0.72534800
C	-1.05313300	-4.19736300	-1.32794300
H	-0.64059200	-4.02964900	-2.32859500
H	-1.89142000	-3.51212200	-1.17426000
H	-1.42807800	-5.22421300	-1.27303800
C	1.22991500	-4.87900600	-0.48431900
H	1.61651600	-4.76533800	-1.50245100
H	0.94495000	-5.92459500	-0.33550900
H	2.02474600	-4.62554100	0.22344400
C	1.42009300	-0.24983900	-1.09770700
C	1.77304700	1.25891900	-1.31438500
H	1.63611100	1.72501900	-0.33493400
C	0.86537900	1.96768400	-2.32052200
H	-0.18927100	1.78390000	-2.12650300
H	1.09117100	1.65871800	-3.34710700

H	1.04071700	3.04755300	-2.24785300
C	3.23552400	1.44555800	-1.73122700
H	3.49710300	0.83801600	-2.60561000
H	3.92511600	1.20666700	-0.91706600
H	3.39279900	2.49356300	-2.00326200
C	1.14433400	-0.97980500	-2.44303700
O	0.11641600	-0.82589500	-3.07482200
C	2.30510700	-1.79741400	-2.73001000
H	2.49949500	-2.32582600	-3.65325100
C	3.12425900	-1.77623600	-1.64505100
N	2.62341400	-0.97371900	-0.62852200
C	3.05005500	-0.87263200	0.68968100
O	2.78589300	0.08586900	1.38098500
O	3.72970600	-1.95941800	1.05045900
C	4.47591200	-2.00533500	2.30758700
C	5.16929300	-3.35921700	2.23121900
H	4.43222700	-4.16688400	2.18343400
H	5.79177500	-3.50687300	3.11855600
H	5.80558300	-3.41123800	1.34144700
C	5.50071300	-0.87817100	2.35856000
H	5.01834700	0.10139100	2.34877800
H	6.19108300	-0.95103700	1.51237300
H	6.08145200	-0.96886500	3.28192200
C	3.50585900	-1.95398700	3.48069900
H	3.05433700	-0.96475900	3.57095800
H	4.04321000	-2.18461400	4.40614300
H	2.71319600	-2.69757300	3.34557500
C	4.46444000	-2.39646300	-1.59673900
C	7.01828100	-3.52386800	-1.65906100
C	4.64070400	-3.70929200	-2.03785400

C	5.57548600	-1.64365000	-1.19843100
C	6.84662300	-2.20417200	-1.23598300
C	5.91489500	-4.27365200	-2.05852900
H	3.77806300	-4.29030100	-2.35055300
H	5.44001800	-0.61571200	-0.87120800
H	7.70552500	-1.61183900	-0.93466100
H	6.04297300	-5.29949600	-2.38995600
H	8.01133100	-3.96236100	-1.68056900

Zero-point correction= 1.075846 (Hartree/Particle)

Thermal correction to Energy= 1.141594

Thermal correction to Enthalpy= 1.142539

Thermal correction to Gibbs Free Energy= 0.971931

Sum of electronic and zero-point Energies= -2890.102708

Sum of electronic and thermal Energies= -2890.036960

Sum of electronic and thermal Enthalpies= -2890.036015

Sum of electronic and thermal Free Energies= -2890.206623

E(RM062X/6-311+G(2d,p)) = -2892.08229609

13. Reference

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