Supporting Information

Photooxidative Tandem Cyclization of Enamines to Polysubstituted Pyrroles: A Combined Experimental and Theoretical Study

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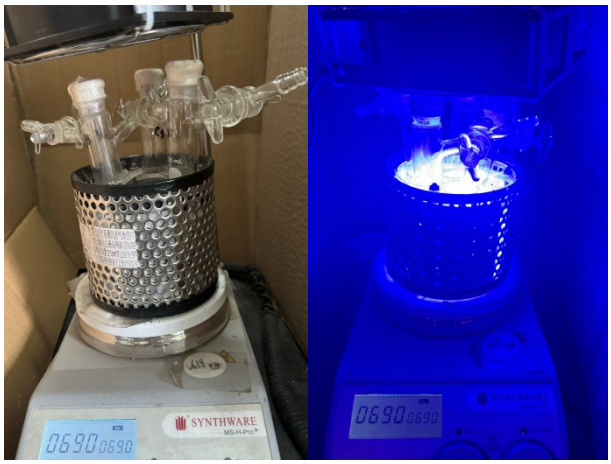
I. General Remarks

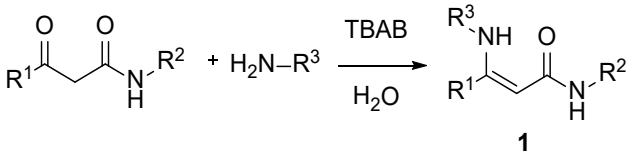
All reagents were purchased from commercial sources and used without further treatment, unless otherwise indicated. All solvents under the optimization conditions were anhydrous solvents (Water ≤50 ppm) purchased by the reagent company without further purification. Petroleum ether (PE) used here refers to the 60–90 °C boiling point fraction of petroleum. Ethyl acetate is abbreviated as EA. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker Avance/600 (^{1}H: 600 MHz, ^{13}C: 150 MHz) or Bruker Avance/400 (^{1}H: 400 MHz, ^{19}F: 376 MHz, ^{13}C: 100 MHz at 25 °C); fluorine nuclear magnetic resonance (^{19}F NMR) spectra were recorded on a Bruker Avance/600 spectrometer. Data are represented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, dd = double doublet, t = triplet, q = quartet, and m = multiplet), and coupling constants in Hertz (Hz). Solvents were ultra-solvents from Energy Chemical, such as MeCN, NMP, THF, DMSO, EtOH, Dioxane and DMF. All other reagents were purchased as reagent grade and used without further purification. All high-resolution mass spectra (HRMS) were measured on a mass spectrometer by using electrospray ionization orthogonal acceleration time-of-flight (ESI-OA-TOF), and the purity of all samples used for HRMS (>95%) was confirmed by ^{1}H NMR and ^{13}C NMR spectroscopic analysis. Melting points were measured on a melting point apparatus equipped with a thermometer and were uncorrected. All reactions were monitored by thin-layer chromatography (TLC) with GF254 silica gel-coated plates. Flash chromatography was carried out on SiO_2 (silica gel 200–300 mesh).

II. General setup for the reaction



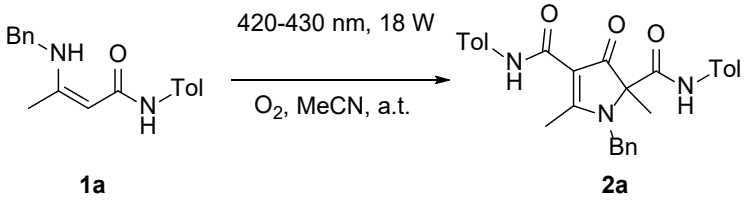
III. General Procedures

1. General Procedure for the Preparation of Reagents[1].



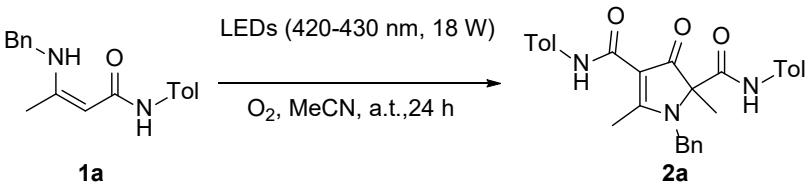
Amine (10 mmol) was added to a suspension of 1,3-dicarbonyl compounds (10 mmol) and TBAB (0.5 mmol) in water (20 mL) at room temperature. The resulting mixture was stirred at room temperature for 12 h, then filtered, washed with water (3 × 30 mL), and dried in vacuo to afford corresponding enamino amides **1**.

2. General Procedure for the synthesis of product 2 (2a as an example).



To a 15 mL Schlenk tube were added **1a** (140 mg, 0.5 mmol), and MeCN (2 mL) under an O_2 atmosphere. The reaction mixture was stirred for 24 h under irradiation from 420-430 nm blue LED at room temperature (the whole process was closely monitored by TLC). The reaction mixture was treated with H_2O (5 mL) and extracted with DCM (3 × 10 mL). The combined organic layer was dried over anhydrous Na_2SO_4 and concentrated on a rotary evaporator. The crude reaction mixture was purified by flash silica gel column chromatography (PE : EA =9 : 1) to get white solid **2a** (87.6 mg, 75%).

3. Average yield and value of stdev for 2a.



Entry	**2a**/%	Average (%)	stdev[a]
1	76	75	0.9
2	75		

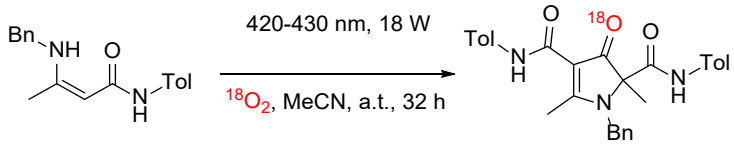
3	74
4	75
5	75
6	74
7	76
8	75
9	74
10	76

[a]stdev: $S = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i-\bar{x})}$

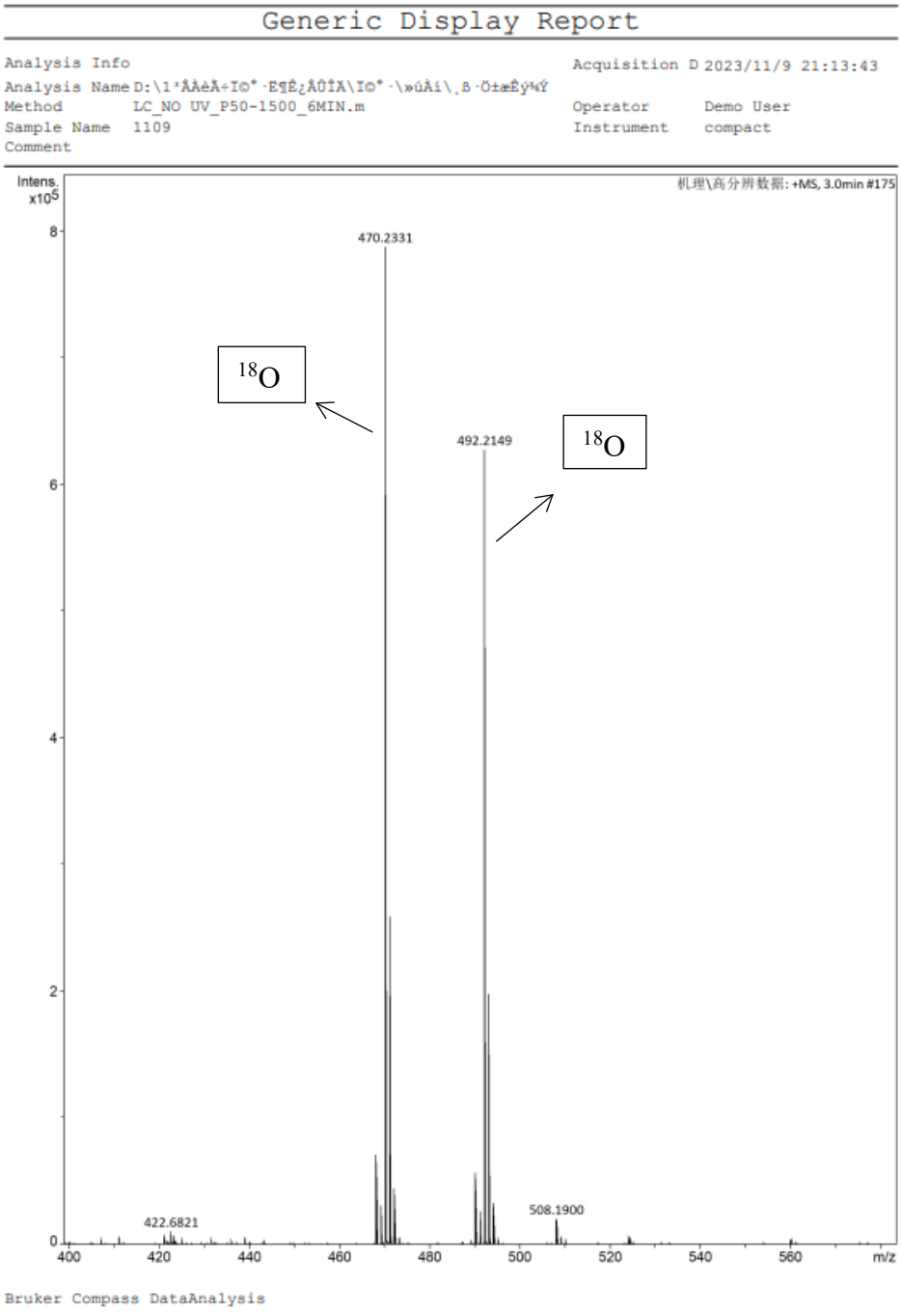
IV. Mechanistic Studies

1. Oxygen Labelling Reactions

The reactions are conducted under standard conditions with $^{18}O_2$ instead of O_2.



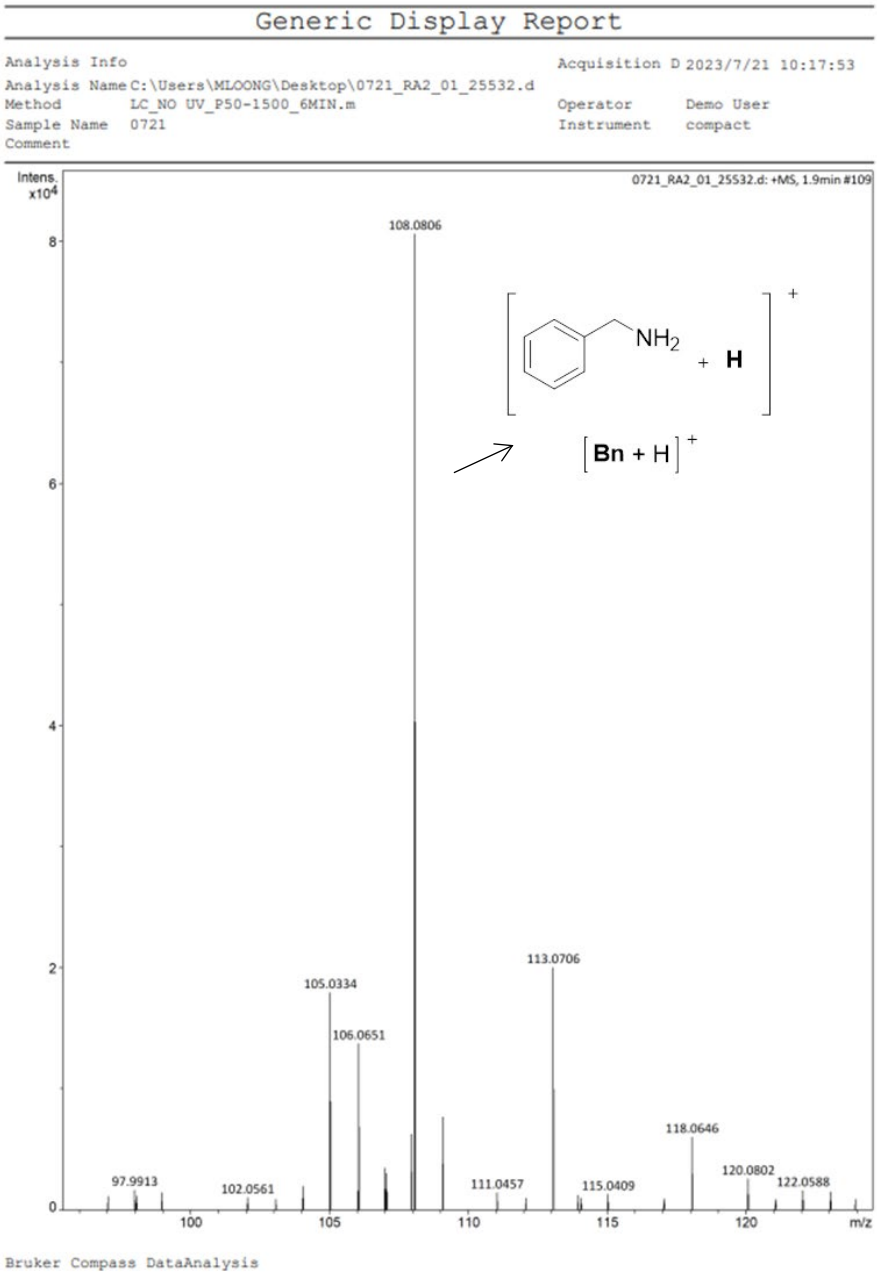
Yield = 75%



2. Analytical data of ESI(+)-MS

To a 15 mL Schlenk tube were added **1a** (140 mg, 0.5 mmol), and MeCN (2 mL) under an O_2 atmosphere. The reaction mixture was stirred for 24 h under irradiation from 420-430 nm blue LED at room temperature (the whole process was closely monitored by TLC). The excess MeCN was removed under reduced pressure. The reaction was diluted with MeOH (1/100) prior to the injection into the mass spectrometer.

The positive-ion mode of ESI-MS spectrum showed the signals corresponding to the [**Bn** + H]$^+$ (m/z 108.0806), [**Int-8'** + Na]$^+$ (m/z 317.1259), [**Int-16'** + H]$^+$ (m/z 575.3015).



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Comment

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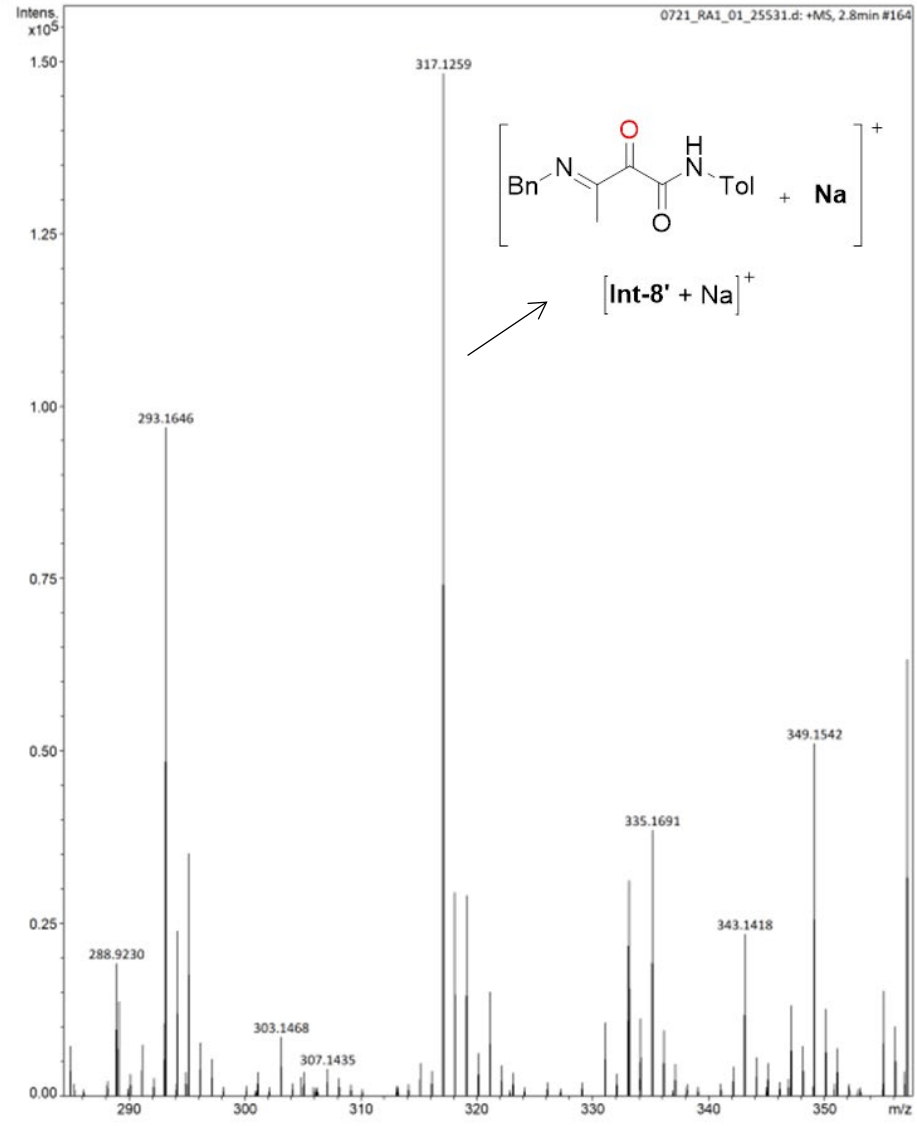
Instrument compact



Bruker Compass DataAnalysis

Generic Display Report

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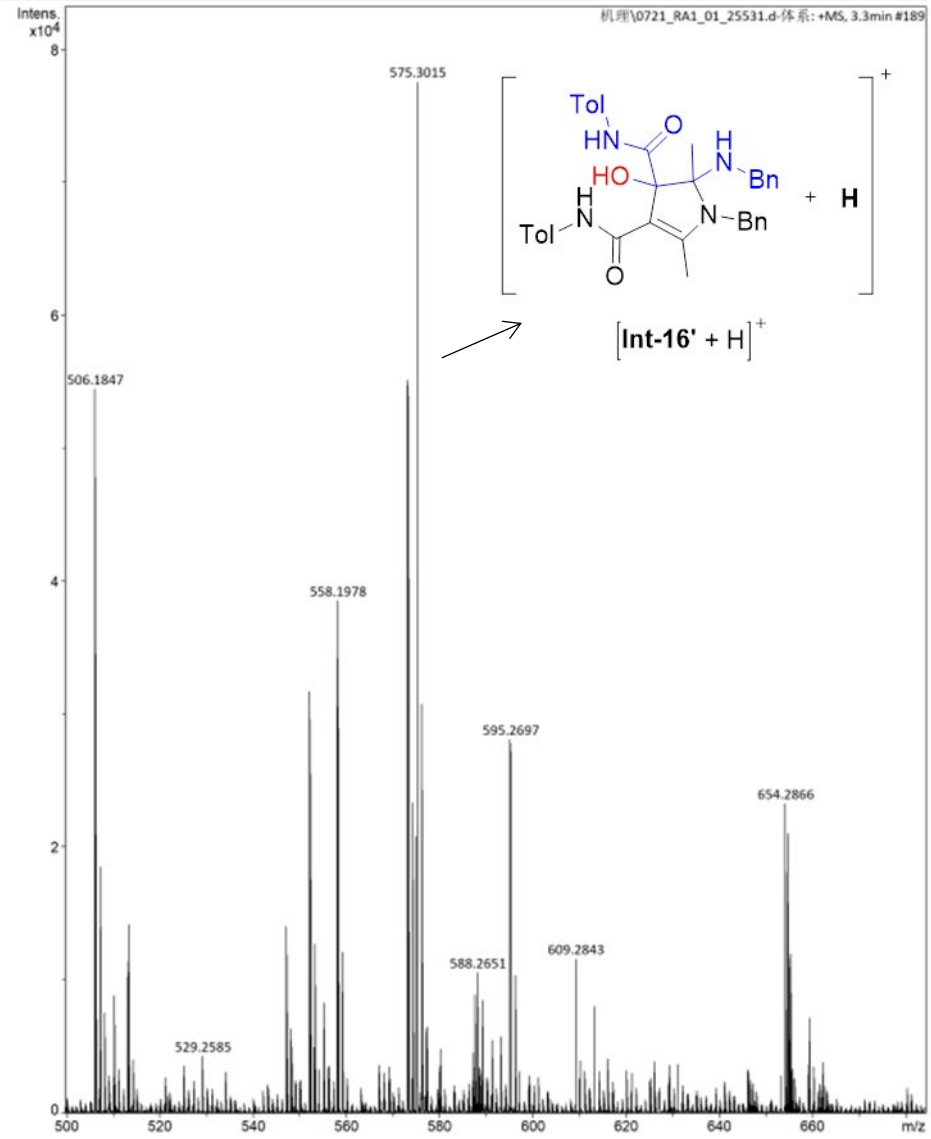
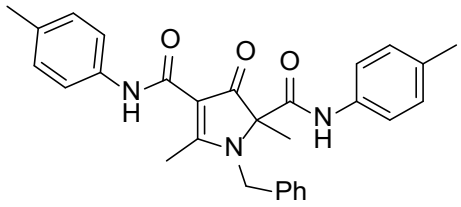
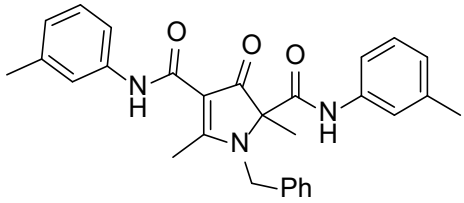


Bruker Compass DataAnalysis

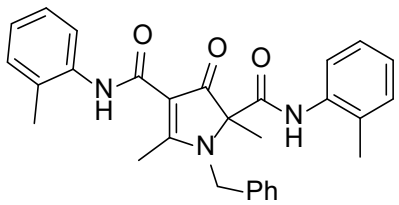
V. Analytical Data of Compounds



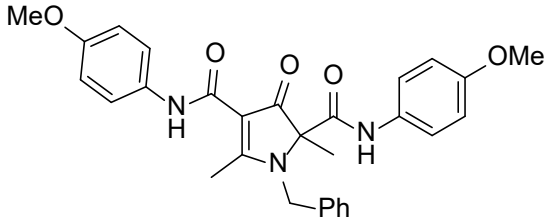
1-Benzyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-*p*-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2a) The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (87.6 mg, 75%); Mp: 165-166 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.06 (s, 1H), 9.13 (s, 1H), 7.54 - 7.52 (m, 2H), 7.43 - 7.40 (m, 2H), 7.39 - 7.35 (m, 2H), 7.33 - 7.29 (m, 1H), 7.19 - 7.12 (m, 6H), 5.31 (q, J = 17.6 Hz, 2H), 2.74 (s, 3H), 2.32 (d, J = 2.0 Hz, 6H), 1.71 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.8, 182.2, 163.9, 161.6, 136.2, 136.1, 134.7, 134.4, 133.0, 129.6, 129.4, 129.1, 127.9, 126.0, 120.13, 120.10, 103.1, 74.6, 48.9, 22.7, 20.93, 20.89, 15.6. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{29}N_3O_3Na$ 490.2101; Found 490.2101.



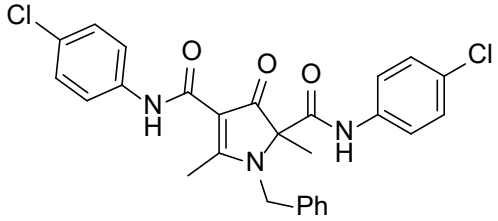
1-Benzyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-*m*-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2b). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (81.8 mg, 70%); Mp: 167-168 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.07 (s, 1H), 9.14 (s, 1H), 7.52 (s, 1H), 7.43 - 7.41 (m, 1H), 7.39 - 7.36 (m, 3H), 7.35 - 7.31 (m, 2H), 7.24 - 7.22 (m, 2H), 7.20 - 7.17 (m, 2H), 6.97 (d, J = 7.2 Hz, 1H), 6.89 (d, 1H), 5.34 (dd, J = 48.6, 17.4 Hz, 2H), 2.75 (s, 3H), 2.35 (s, 6H), 1.71 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.8, 182.3, 164.0, 161.6, 139.1, 138.7, 138.6, 136.9, 136.1, 129.2, 128.9, 128.7, 127.9, 126.0, 125.8, 124.3, 120.7, 117.18, 117.15, 103.1, 74.7, 48.9, 22.7, 21.6, 21.5, 15.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{29}N_3O_3Na$ 490.2101; Found 490.2095.



1-Benzyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-*o*-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2c). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (78.3 mg, 67%); Mp: 151-152 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.08 (s, 1H), 9.25 (s, 1H), 8.22 (dd, J = 8.4, 1.8 Hz, 1H), 7.86 (dd, J = 7.8, 1.2 Hz, 1H), 7.40 - 7.37 (m, 2H), 7.33 - 7.30 (m, 1H), 7.22 - 7.19 (m, 6H), 7.09 (td, J = 7.2, 1.2 Hz, 1H), 7.01 (td, J = 7.8, 1.8 Hz, 1H), 5.34 (dd, J = 55.8, 18.0 Hz, 2H), 2.76 (s, 3H), 2.40 (s, 3H), 2.34 (s, 3H), 1.77 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.2, 182.4, 164.3, 161.6, 137.0, 136.1, 135.0, 130.7, 130.3, 129.2, 128.9, 127.9, 127.5, 126.8, 126.6, 126.0, 125.4, 123.6, 122.0, 121.5, 103.3, 74.7, 48.9, 22.9, 18.2, 17.7, 15.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{29}N_3O_3Na$ 490.2101; Found 490.2095.

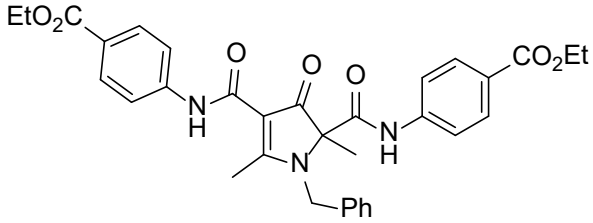


1-Benzyl-*N*^{2},*N*^{4}-bis(4-methoxyphenyl)-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2d). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (93.6 mg, 75%); Mp: 106-107 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.99 (s, 1H), 9.06 (s, 1H), 7.56 - 7.34 (m, 2H), 7.45 - 7.43 (m, 2H), 7.39 - 7.35 (m, 2H), 7.32 - 7.29 (m, 1H), 7.17 (d, J = 6.8 Hz, 2H), 6.88 - 6.86 (m, 4H), 5.44 - 5.19 (dd, J = 37.2, 17.6 Hz, 2H), 3.80 (s, 6H), 2.74 (s, 3H), 1.70 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.9, 182.2, 163.9, 161.5, 156.85, 155.89, 136.2, 131.8, 130.0, 129.1, 127.9, 126.0, 121.8, 121.7, 114.2, 114.1, 103.0, 74.5, 55.5, 48.9, 22.7, 15.6. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{29}N_3O_5Na$ 522.1999; Found 522.1995.

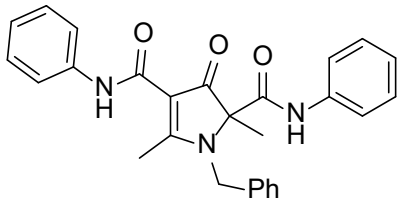


1-Benzyl-*N*^{2},*N*^{4}-bis(4-chlorophenyl)-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2e). The product was isolated by flash chromatography (eluent: EA/PE = 1/4) as a white solid (72.2 mg, 57%); Mp: 98-99 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.11 (s, 1H), 9.22 (s, 1H), 7.62 - 7.58 (m, 2H), 7.51 - 7.48 (m, 2H), 7.40 - 7.36 (m, 2H), 7.33 - 7.32 (m, 2H), 7.30 - 7.28 (m, 2H), 7.27 (d, J = 2.0 Hz, 1H), 7.17

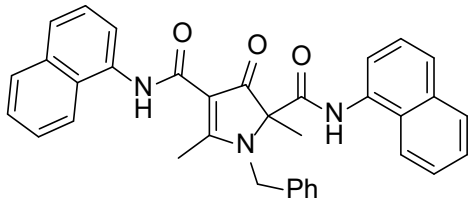
(d, *J* = 6.8 Hz, 2H), 5.31 (dd, *J* = 26.4, 17.6 Hz, 2H), 2.74 (s, 3H), 1.71 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.6, 182.5, 164.0, 161.5, 137.2, 135.8, 135.5, 130.1, 129.2, 129.1, 128.9, 128.3, 128.0, 126.0, 121.3, 121.2, 102.9, 74.6, 49.0, 22.8, 15.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{23}Cl_2N_3O_3Na$ 530.1009; Found 530.1003.



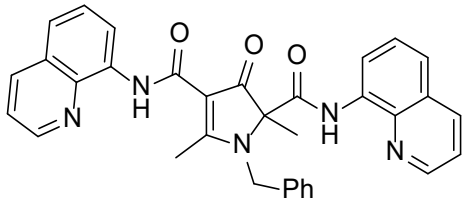
Diethyl 4,4'-((1-benzyl-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarbonyl)bis(azanediyl))dibenzoate (2f). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (83.1 mg, 57%); Mp: 145-146 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.31 (s, 1H), 9.39 (s, 1H), 8.04 - 8.00 (m, 4H), 7.73 - 7.72 (m, 2H), 7.64 - 7.62 (m, 2H), 7.41 - 7.37(m, 2H), 7.34 - 7.31 (m, 1H), 7.18 (d, *J* = 6.6 Hz, 2H), 5.33 (dd, *J* = 30.0, 17.4 Hz, 2H), 4.38 - 4.34 (m, 4H), 2.75 (s, 3H), 1.74 (s, 3H), 1.40 - 1.37 (m, 6H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.5, 182.7, 166.4, 166.0, 164.1, 161.6, 142.8, 140.9, 135.7, 130.8, 130.7, 129.3, 128.1, 126.8, 125.9, 125.2, 119.3, 119.0, 102.9, 74.8, 61.0, 60.8, 49.1, 22.8, 15.8, 14.40, 14.35. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{33}H_{33}N_3O_7Na$ 606.2211; Found 606.2212.



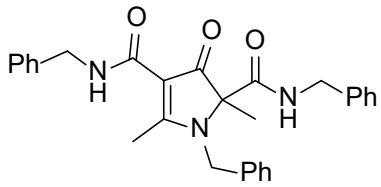
1-Benzyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-diphenyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2g). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (76.8 mg, 70%); Mp: 174-175 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.12 (s, 1H), 9.21 (s, 1H), 7.66 - 7.63 (m, 2H), 7.56 - 7.54 (m, 2H), 7.40 - 7.27 (m, 7H), 7.19 - 7.13 (m, 3H), 7.10 - 7.06 (m, 1H), 5.39 - 5.24 (dd, *J* = 29.2, 17.6 Hz, 2H), 2.74 (s, 3H), 1.72 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.8, 182.4, 164.0, 161.7, 138.6, 137.0, 136.1, 129.2, 129.1, 128.9, 127.9, 126.0, 125.0, 123.5, 120.1, 103.0, 74.7, 48.9, 22.7, 15.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{27}H_{25}N_3O_3Na$ 462.1788; Found 462.1790.



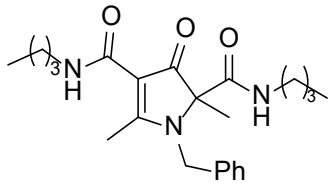
1-Benzyl-2,5-dimethyl-*N*^{2},*N*^{4}-di(naphthalen-1-yl)-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2h). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (80.9 mg, 60%); Mp: 167-168 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.90 (s, 1H), 10.00 (s, 1H), 8.36 (m, 2H), 8.13 (d, J = 8.4 Hz, 1H), 8.03 (d, J = 7.8 Hz, 1H), 7.89 (d, J = 7.8 Hz, 2H), 7.72 (d, J = 7.8 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.63 - 7.59 (m, 2H), 7.55 - 7.52 (m, 2H), 7.49 (q, J = 7.8 Hz, 2H), 7.42 - 7.39 (m, 2H), 7.35 - 7.34 (m, 1H), 7.25 - 7.24 (m, 2H), 5.46 (d, J = 17.4 Hz, 1H), 5.36 (d, J = 17.4 Hz, 1H), 2.83 (s, 3H), 1.92 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 195.7, 182.8, 164.7, 162.1, 136.2, 134.28, 134.26, 133.7, 131.7, 129.3, 128.9, 128.8, 128.1, 126.92, 126.87, 126.4, 126.3, 126.2, 126.1, 126.05, 125.9, 125.7, 124.2, 121.1, 120.7, 119.7, 118.6, 103.7, 75.1, 49.2, 23.3, 15.9. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{35}H_{29}N_3O_3Na$ 562.2101; Found 562.2097.



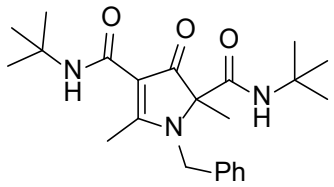
1-Benzyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di(quinolin-8-yl)-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2i).The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (82.5 mg, 61%); Mp: 222-223 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 12.11 (s, 1H), 11.04 (s, 1H), 8.99 (dd, J = 4.2, 1.8 Hz, 1H), 8.93 (dd, J = 4.2, 1.8 Hz, 1H), 8.91 (dd, J = 7.8, 1.8 Hz, 1H), 8.63 (dd, J = 7.2, 1.8 Hz, 1H), 8.15 (dd, J = 8.4, 1.8 Hz, 1H), 8.11 (dd, J = 8.4, 1.8 Hz, 1H), 7.54 - 7.50 (m, 3H), 7.48 - 7.44 (m, 2H), 7.41 (q, J = 4.2 Hz, 1H), 7.36 - 7.34 (m, 2H), 7.31 - 7.28 (m, 1H), 7.23 (d, J = 7.2 Hz, 2H), 5.27 (d, J = 17.4 Hz, 1H), 5.08 (d, J = 17.4 Hz, 1H), 2.90 (s, 3H), 1.89 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.1, 182.2, 164.1, 162.6, 148.9, 148.7, 139.5, 139.2, 136.3, 136.22, 136.18, 136.1, 134.1, 129.3, 128.3, 128.1, 128.0, 127.4, 127.2, 126.3, 122.6, 121.9, 121.4, 121.1, 117.1, 117.0, 103.8, 76.7, 48.8, 21.1, 15.7. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{33}H_{27}N_5O_3H$ 542.2187; Found 542.2186.



***N*^{2},*N*^{4},1-Tribenzyl-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide(2j).** The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (75.9 mg, 65%); Mp: 121-122 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.46 (t, J = 6.0 Hz, 1H), 7.53 (t, J = 6.0 Hz, 1H), 7.37 - 7.32 (m, 7H),7.31 - 7.27 (m, 3H), 7.25 - 7.24 (m, 1H), 7.23 - 7.21 (m, 2H), 7.13 (d, J = 6.8 Hz, 2H), 5.21 (dd, J = 27.2, 17.6 Hz, 2H), 4.60 - 4.52 (m, 2H), 4.50 - 4.47 (m, 1H), 4.32 (dd, J = 15.2, 5.2 Hz, 1H), 2.69 (s, 3H), 1.57 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.1, 181.8, 166.5, 163.8, 139.3, 137.6, 136.5, 129.2, 128.9, 128.7, 127.9, 127.8, 127.7, 127.5, 127.2, 126.1, 102.7, 74.5, 48.7,43.7, 42.6, 22.6, 15.5. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{29}N_3O_3Na$ 490.2101; Found 490.2099.

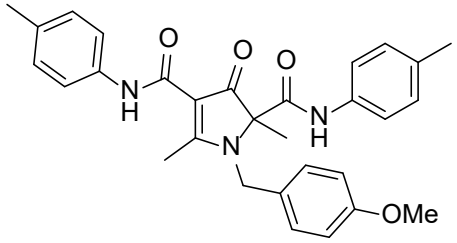


1-Benzyl-*N*^{2},*N*^{4}-diethyl-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2k). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (58.3 mg, 68%); Mp: 136-137 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.10 (t, J = 6.0 Hz, 1H), 7.35 - 7.32 (m, 2H), 7.29 - 7.27 (m, 1H), 7.17 (t, J = 6.0 Hz, 1H), 7.12 (d, J = 7.2 Hz, 2H), 5.19 (dd, J = 42.6, 18.0 Hz, 2H), 3.40 - 3.30 (m, 2H), 3.29 - 3.23 (m, 1H), 3.21 - 3.15 (m, 1H), 2.66 (s, 3H), 1.58 - 1.55 (m, 2H), 1.54 (s, 3H), 1.52 - 1.47 (m, 2H), 1.44 - 1.37 (m, 2H), 1.36 - 1.30 (m, 2H), 0.96 - 0.91 (m, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.3, 181.4, 166.4, 163.9, 136.6, 129.1, 127.8, 126.1, 102.7, 74.4, 48.6, 39.5, 38.3, 32.0, 31.4, 22.5, 20.4, 20.1, 15.3, 13.9, 13.8. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{33}N_3O_3H$ 400.2595; Found 400.2602.

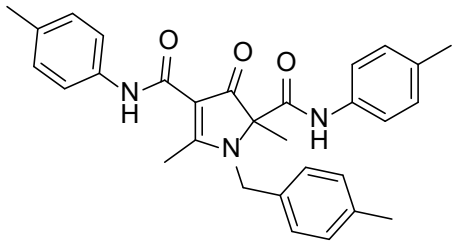


1-Benzyl-*N*^{2},*N*^{4}-di-tert-butyl-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2l). The product was isolated by flash chromatography (eluent: EA/PE

= 1/3) as a white solid (59.9 mg, 60%); Mp: 137-138 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.34 - 7.32 (m, 1H), 7.31 - 7.29 (m, 1H), 7.28 - 7.26 (m, 1H), 7.10 (d, J = 7.2 Hz, 2H), 7.05 (s, 1H), 5.18 (dd, J = 36.0, 17.6 Hz, 2H), 2.63 (s, 3H), 1.51 (s, 3H), 1.43 (s, 9H), 1.34 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 195.4, 181.3, 165.6, 163.6, 136.8, 129.1, 127.7, 126.0, 103.5, 74.5, 51.7, 50.6, 48.6, 29.3, 28.6, 22.8, 15.4. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{23}H_{33}N_3O_3Na$ 422.2414; Found 422.2416.

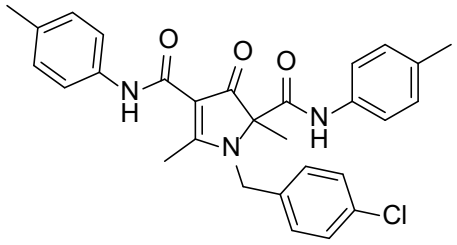


1-(4-Methoxybenzyl)-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-p-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2m). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (91.9 mg, 74%); Mp: 98-99 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.05 (s, 1H), 9.11 (s, 1H), 7.53 - 7.51 (m, 2H), 7.42 - 7.41 (m, 2H), 7.15 - 7.10 (m, 6H), 6.89 - 6.88 (m, 2H), 5.24 (q, J = 17.4 Hz, 2H), 3.80 (s, 3H), 2.75 (s, 3H), 2.32 (d, J = 4.2 Hz, 6H), 1.69 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.8, 182.1, 163.9, 161.6, 159.2, 136.1, 134.6, 134.4, 133.0, 129.6, 129.4, 128.0, 127.4, 120.10, 120.07, 114.5, 103.0, 74.6, 55.4, 48.5, 22.9, 20.92, 20.88, 15.6. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{30}H_{31}N_3O_4Na$ 520.2207; Found 520.2211.

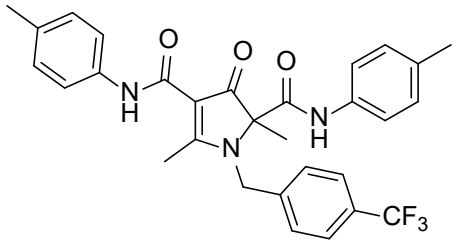


2,5-Dimethyl-1-(4-methylbenzyl)-3-oxo-*N*^{2},*N*^{4}-di-p-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2n). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (87.8 mg, 73%); Mp: 93-94 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.05 (s, 1H), 9.10 (s, 1H), 7.53 - 7.52 (m, 2H), 7.42 - 7.40 (m, 2H), 7.17 - 7.15 (m, 3H), 7.13 - 7.12 (m, 3H), 7.05 (d, J = 7.8 Hz, 2H), 5.27 (dd, J = 54.6, 17.4 Hz, 2H), 2.74 (s, 3H), 2.34 (s, 3H), 2.32 (d, J = 3.6 Hz, 6H), 1.69 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.9, 182.3, 164.1, 161.7, 137.8, 136.2, 134.8, 134.5, 133.2, 133.1, 129.9, 129.7, 129.5, 126.1, 120.22, 120.20, 103.1, 74.8, 48.8, 22.8, 21.2, 21.04, 21.00,

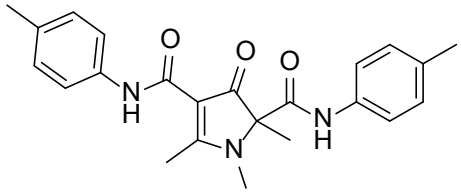
15.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{31}N_3O_3Na$ 504.2258; Found 504.2258.



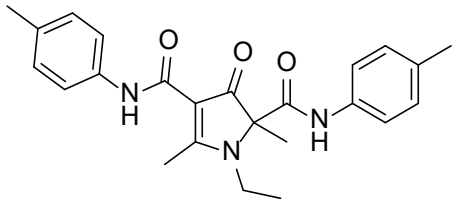
1-(4-Chlorobenzyl)-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-p-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2o). The product was isolated by flash chromatography (eluent: EA/PE = 1/1) as a white solid (77.7 mg, 62%); Mp: 187-188 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.01 (s, 1H), 9.15 (s, 1H), 7.53 - 7.51 (m, 2H), 7.41 - 7.40 (m, 2H), 7.35 - 7.34 (m, 2H), 7.15 - 7.12 (m, 6H), 5.27 (dd, J = 20.4, 17.4 Hz, 2H), 2.72 (s, 3H), 2.32 (d, J = 3.0 Hz, 6H), 1.70 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.0, 182.2, 163.9, 161.6, 136.1, 134.90, 134.88, 134.4, 133.9, 133.2, 129.7, 129.53, 129.45, 127.6, 120.3, 120.2, 103.4, 74.5, 48.4, 23.1, 21.1, 21.0, 15.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{29}H_{28}ClN_3O_3Na$ 524.1711; Found 524.1712.



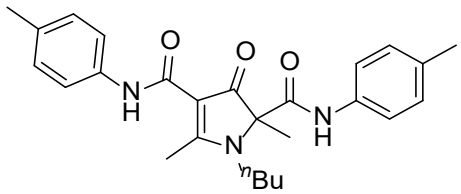
2,5-Dimethyl-3-oxo-*N*^{2},*N*^{4}-di-p-tolyl-1-(4-(trifluoromethyl)benzyl)-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2p). The product was isolated by flash chromatography (eluent: EA/PE = 1/1) as a white solid (81.6 mg, 61%); Mp: 96-97 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.01 (s, 1H), 9.18 (s, 1H), 7.64 (d, J = 8.4 Hz, 2H), 7.53 - 7.52 (m, 2H), 7.41 - 7.40 (m, 2H), 7.32 (d, J = 8.4 Hz, 2H), 7.14 (t, J = 8.4 Hz, 4H), 5.35 (s, 2H), 2.71 (s, 3H), 2.32 (d, J = 1.8 Hz, 6H), 1.73 (s, 3H). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -62.63. **^{13}C NMR** (151 MHz, $CDCl_3$) δ 195.1, 182.3, 163.9, 161.5, 140.5, 136.1, 135.0, 134.4, 133.3, 129.7, 129.5, 126.5, 126.3 (q, J = 3.0 Hz), 120.27, 120.25, 103.5, 74.5, 48.5, 23.2, 21.1, 21.0, 15.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{30}H_{28}N_3O_3Na$ 558.1975; Found 558.1973.



1,2,5-Trimethyl-3-oxo-*N*^{2},*N*^{4}-di-p-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2q). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (65.5mg, 67%); Mp: 200-201 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.01 (s, 1H), 9.21 (s, 1H), 7.52 - 7.50 (m, 2H), 7.42 - 7.41 (m, 2H), 7.13 (dd, J = 15.0, 7.8 Hz, 4H), 3.50 (s, 3H), 2.83 (s, 3H), 2.31 (d, J = 6.6 Hz, 6H), 1.76 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.9, 181.0, 163.9, 161.8, 136.2, 134.7, 134.6, 133.0, 129.7, 129.5, 120.20, 120.17, 102.5, 74.1, 31.7, 22.7, 21.04, 21.00, 14.7. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{23}H_{25}N_3O_3Na$ 414.1788; Found 414.1793.

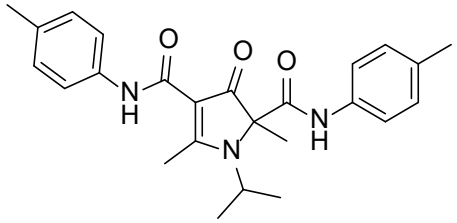


1-Ethyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-*p*-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2r). The product was isolated by flash chromatography (eluent: EA/PE = 1/5) as a colourless liquid (59.8 mg, 59%); **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 9.17 (s, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.41 (d, J = 8.4 Hz, 2H), 7.12 (t, J = 8.8 Hz, 4H), 4.13 - 3.94 (m, 2H), 2.85 (s, 3H), 2.31 (d, J = 3.2 Hz, 6H), 1.79 (s, 3H), 1.39 (t, J = 7.2 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.5, 180.9, 163.69, 161.72, 136.1, 134.6, 134.5, 132.9, 129.6, 129.4, 120.1, 120.0, 102.6, 74.5, 40.2, 23.1, 20.9, 20.9, 15.6, 15.0. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{24}H_{27}N_3O_3Na$ 428.1945; Found 428.1945.

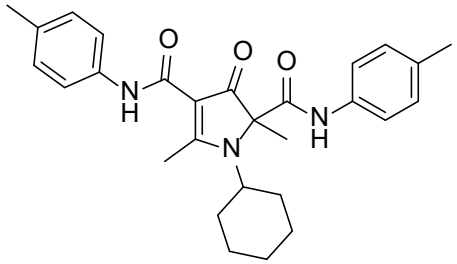


1-Butyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-p-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2s). The product was isolated by flash chromatography (eluent: EA/PE = 1/3) as a white solid (68.2 mg, 63%); Mp: 169-170 ºC. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 10.04 (s, 1H), 9.13 (s, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.42 (d, J = 8.4 Hz, 2H),

7.12 (dd, J = 16.2, 8.4 Hz, 4H), 4.01 - 3.93 (m, 1H), 3.85 - 3.76 (m, 1H), 2.83 - 2.82 (m, 3H), 2.31 (d, J = 6.0 Hz, 6H), 1.83 - 1.76 (m, 4H), 1.65 - 1.58 (m, 1H), 1.44 - 1.39 (m, 2H), 1.01 - 0.98 (m, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.4, 180.9, 163.7, 161.7, 136.1, 134.6, 134.5, 132.9, 129.5, 129.4, 120.2, 120.0, 102.6, 74.6, 45.4, 32.4, 22.9, 20.91, 20.87, 20.4, 15.1, 13.6. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{26}H_{31}N_3O_3Na$ 456.2258; Found 456.2254.

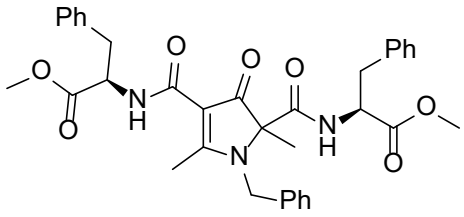


1-Isopropyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-*p*-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2t). The product was isolated by flash chromatography (eluent: EA/PE = 1/5) as a white solid (48.2 mg, 46%); Mp: 191-192 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.09 (s, 1H), 9.16 (s, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 8.0 Hz, 2H), 7.12 (t, J = 8.8 Hz, 4H), 4.62 - 4.54 (m, 1H), 2.97 (s, 3H), 2.31 (d, J = 3.2 Hz, 6H), 1.80 (s, 3H), 1.71 (d, J = 7.2 Hz, 3H), 1.50 (d, J = 7.2 Hz, 3H). **^{13}C NMR** (151 MHz, MeOD-d_4) δ 194.7, 182.5, 164.3, 162.7, 135.8, 134.7, 133.0, 128.9, 128.9, 121.6, 119.9, 101.9, 77.3, 49.8, 21.5, 19.9, 19.52, 19.47, 19.4, 15.1. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{25}H_{29}N_3O_3Na$ 442.2101; Found 442.2101.

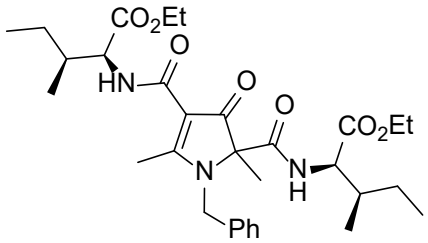


1-Cyclohexyl-2,5-dimethyl-3-oxo-*N*^{2},*N*^{4}-di-*p*-tolyl-2,3-dihydro-1*H*-pyrrole-2,4-dicarboxamide (2u). The product was isolated by flash chromatography (eluent: EA/PE = 1/5) as a white solid (36.7 mg, 32%); Mp: 227-228 ºC. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 10.13 (s, 1H), 9.12 (s, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.40 (d, J = 7.2 Hz, 2H), 7.12 (dd, J = 11.2, 8.0 Hz, 4H), 4.11 - 4.05 (m, 1H), 2.99 (s, 3H), 2.46 (d, J = 10.8 Hz, 1H), 2.31 (d, J = 4.0 Hz, 6H), 2.00 - 1.86 (m, 5H), 1.80 (s, 3H), 1.75 (d, J = 13.6 Hz, 1H), 1.47 - 1.37 (m, 2H), 1.25 - 1.18 (m, 1H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.1, 181.1, 163.7, 161.9, 136.2, 134.5, 132.8, 129.5, 129.3, 120.3, 120.1, 103.1, 75.8, 59.3,

32.7, 32.0, 26.7, 26.5, 25.4, 22.9, 20.9, 20.9, 17.4. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{28}H_{33}N_3O_3Na$ 482.2414; Found 482.2413.

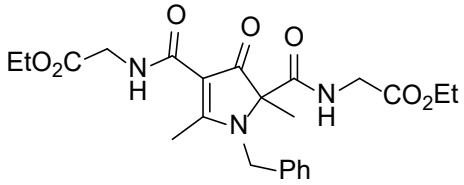


Methyl (1-benzyl-4-(((*R*)-1-methoxy-1-oxo-3-phenylpropan-2-yl)carbamoyl)-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2-carbonyl)-*L*-phenylalaninate (2y). The product was isolated by flash chromatography (eluent: EA/PE = 1/1) as a yellow liquid (64.1 mg, 42%); dr: 3:1. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.60 (d, J = 7.2 Hz, 0.3H), 8.57 (d, J = 7.2 Hz, 1H), 7.60 (d, J = 8.4 Hz, 0.3H), 7.53 (d, J = 7.9 Hz, 1H), 7.34 - 7.30 (m, 4H), 7.29 - 7.27 (m, 4H), 7.25 - 7.21 (m, 5H), 7.21 - 7.19 (m, 1H), 7.15 - 7.13 (m, 2H), 7.10 - 7.08 (m, 1H), 7.07 - 7.06 (m, 2H), 7.04 - 7.03 (m, 1H), 5.05 - 5.01 (m, 2.4H), 4.93 - 4.90 (m, 0.3H), 4.89 - 4.85 (m, 1H), 4.77 - 4.74 (m, 1.4H), 4.44 (d, J = 5.4 Hz, 0.4H), 3.74 (s, 1H), 3.73 (s, 3H), 3.70 (s, 1H), 3.69 (s, 3H), 3.22 (dd, J = 13.8, 5.4 Hz, 1H), 3.18 (d, J = 6.0 Hz, 0.3H), 3.16 (d, J = 6.6 Hz, 1H), 3.14 (d, J = 6.0 Hz, 1H), 3.11 (d, J = 7.2 Hz, 1H), 3.09 (d, J = 7.2 Hz, 0.3H), 3.04 (dd, J = 13.8, 7.8 Hz, 1H), 2.99 (dd, J = 13.8, 7.8 Hz, 0.3H), 2.56 (s, 3H), 2.55 (s, 1H), 1.52 (s, 1H), 1.34 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.4, 181.4, 172.54, 172.46, 171.3, 171.1, 166.1, 165.8, 163.5, 163.3, 136.7, 136.5, 136.3, 136.2, 135.8, 135.4, 129.4, 129.3, 129.0, 128.8, 128.7, 128.6, 128.5, 127.9, 127.8, 127.7, 127.6, 127.24, 127.21, 126.90, 126.87, 126.0, 125.9, 102.1, 74.3, 74.1, 53.3, 53.2, 52.5, 52.4, 52.1, 48.6, 48.4, 38.5, 38.4, 38.0, 37.9, 22.01, 21.96, 15.21, 15.15. **HRMS** (ESI-TOF) m/z: $[M+H]^+$ Calcd for $C_{35}H_{37}N_3O_7H$ 612.2704; Found 612.2709.

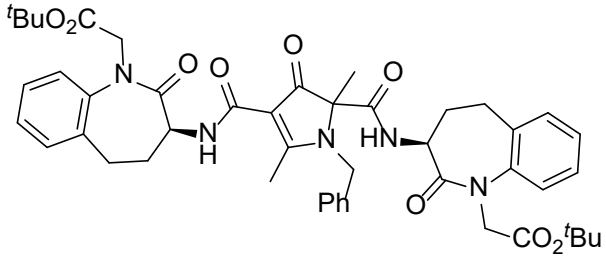


Ethyl (1-benzyl-4-(((2*S*,3*S*)-1-ethoxy-3-methyl-1-oxopentan-2-yl)carbamoyl)-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2-carbonyl)-*D*-isoleucinate (2z). The product was isolated by flash chromatography (eluent: EA/PE = 1/1) as a yellow liquid (67.1 mg, 47%); dr: 3:2. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.62 (d, J = 8.4 Hz, 1H), 8.59

(d, J = 8.4 Hz, 0.7H), 7.69 (t, J = 8.4 Hz, 1.8H), 7.33 (t, J = 7.2 Hz, 3.7H), 7.29 - 7.27 (m, 1.5H), 7.12 (d, J = 7.2 Hz, 3.5H), 5.17 - 5.13 (m, 3.4H), 4.63 - 4.58 (m, 1.7H), 4.42 (dd, J = 8.4, 4.8 Hz, 1.7H), 4.24 - 4.21 (m, 2H), 4.20 - 4.15 (m, 4.6H), 2.64 (s, 2H), 2.63 (s, 3H), 1.98 - 1.94 (m, 3.5H), 1.62 (s, 2H), 1.58 (s, 3H), 1.56 - 1.52 (m, 1.7H), 1.48 - 1.42 (m, 1.6H), 1.30 - 1.27 (m, 6H), 1.27 - 1.24 (m, 6.6H), 1.00 (d, J = 6.6 Hz, 2H), 0.98 - 0.97 (m, 3H), 0.96 - 0.94 (m, 6H), 0.94 - 0.91 (m, 7H), 0.90 (d, J = 7.2 Hz, 2H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.9, 194.8, 181.5, 181.4, 172.3, 171.9, 171.0, 170.6, 166.5, 166.2, 163.63, 163.62, 136.4, 136.3, 129.0, 127.73, 127.70, 126.0, 125.9, 102.4, 102.3, 74.4, 74.3, 61.22, 61.19, 60.9, 60.8, 56.8, 56.0, 48.6, 48.5, 37.7, 37.64, 37.62, 37.4, 25.3, 25.12, 25.09, 22.4, 22.1, 15.83, 15.79, 15.6, 15.3, 15.2, 14.3, 14.23, 14.15, 11.7, 11.6, 11.5. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{31}H_{45}N_3O_7Na$ 594.3150; Found 594.3155.



Diethyl 2,2'-((1-benzyl-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarbonyl)bis(azanediyl))diacetate (2aa). The product was isolated by flash chromatography (eluent: EA/PE = 1/1) as a yellow liquid (57.4 mg, 50%); **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.53 (t, J = 5.4 Hz, 1H), 7.64 (t, J = 5.4 Hz, 1H), 7.34 - 7.32 (m, 2H), 7.28 (d, J = 7.2 Hz, 1H), 7.12 (d, J = 7.2 Hz, 2H), 5.14 (s, 2H), 4.23 - 4.18 (m, 4H), 4.12 (dd, J = 18.0, 5.4 Hz, 1H), 4.08 - 4.03 (m, 2H), 3.87 (dd, J = 18.0, 5.4 Hz, 1H), 2.63 (s, 3H), 1.60 (s, 3H), 1.27 (q, J = 7.2 Hz, 6H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 194.7, 181.6, 170.3, 169.0, 166.7, 163.9, 136.2, 129.0, 127.8, 126.0, 102.2, 74.4, 61.6, 61.2, 48.6, 41.4, 40.7, 22.2, 15.3, 14.2, 14.1. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{23}H_{29}N_3O_7Na$ 482.1898; Found 482.1899.



Di-*tert*-butyl 2,2'-((3*S*,3'*S*)-((1-benzyl-2,5-dimethyl-3-oxo-2,3-dihydro-1*H*-pyrrole-2,4-dicarbonyl)bis(azanediyl))bis(2-oxo-2,3,4,5-tetrahydro-1*H*-

benzo[*b*]azepine-3,1-diyl))diacetate (2ab). The product was isolated by flash chromatography (eluent: EA/PE = 1/1) as a white solid (118.7 mg, 57%), dr: 1:1. Mp: 133-134 °C. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.76 (d, J = 7.2 Hz, 1H), 8.71 (d, J = 7.2 Hz, 1H), 7.81 (d, J = 7.2 Hz, 1H), 7.78 (d, J = 6.6 Hz, 1H), 7.31 - 7.27 (m, 6H), 7.25 - 7.22 (m, 7H), 7.20 - 7.16 (m, 5H), 7.13 - 7.09 (m, 4H), 7.06 (d, J = 7.8 Hz, 4H), 5.06 - 4.93 (m, 4H), 4.84 - 4.78 (m, 3H), 4.76 - 4.70 (m, 2H), 4.67 - 4.60 (m, 2H), 4.44 - 4.39 (m, 1H), 4.37 - 4.34 (m, 1H), 4.24 (d, J = 16.8 Hz, 1H), 4.20 (d, J = 3.0 Hz, 1H), 4.18 (d, J = 3.6 Hz, 1H), 3.47 - 3.37 (m, 4H), 2.64 - 2.56 (m, 7H), 2.53 (s, 3H), 2.52 (s, 3H), 2.21 - 2.15 (m, 2H), 2.11 - 2.03 (m, 3H), 1.51 (s, 3H), 1.46 - 1.38 (m, 39H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 194.3, 194.2, 181.1, 181.0, 171.52, 171.50, 170.4, 170.2, 167.9, 167.62, 167.55, 165.8, 165.5, 163.1, 163.0, 141.0, 140.9, 140.6, 140.4, 136.4, 136.3, 136.01, 135.99, 135.69, 135.65, 129.7, 129.56, 129.55, 128.9, 127.92, 127.88, 127.72, 127.68, 127.64, 127.59, 127.2, 127.1, 126.81, 126.77, 126.0, 125.9, 122.59, 122.56, 122.5, 102.3, 102.1, 82.21, 82.19, 81.93, 81.90, 74.44, 74.38, 51.1, 51.0, 50.1, 50.0, 49.1, 49.0, 48.5, 48.2, 36.2, 36.1, 35.6, 28.4, 28.3, 28.02, 27.96, 22.3, 22.0, 15.1, 15.0. **HRMS** (ESI-TOF) m/z: $[M+Na]^+$ Calcd for $C_{47}H_{55}N_5O_9Na$ 856.3892; Found 856.3887.

VI. Theoretical Studies

1. Complete Reference for Gaussian 16

Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

2. Computational Method for Global and Local Reactivity Index

The global reactivity index (GRI) values were also calculated using M06-2X functional and the 6-31G(d) basis set for all atoms. The ω (electrophilicity index)[2,3] values were calculated according to eq 1. In eq 1, the μ (electronic chemical potential) value could be obtained by $\mu = (\mathcal{E}_{HOMO} + \mathcal{E}_{LUMO})/2$ and the η(chemical hardness) value could be obtained by $\eta = \mathcal{E}_{HOMO} - \mathcal{E}_{LUMO}$[4].

$$\omega = (\mu)^2/2\eta \qquad \text{(eq 1)}$$

$$N = \mathcal{E}_{HOMO}(\text{Nu}) - \mathcal{E}_{HOMO}(\text{TCE}) \qquad \text{(eq 2)}$$

The $\mathcal{E}_{HOMO}$ values refer to the orbital energies of the highest occupied molecular orbital (HOMO), and the corresponding orbital and the $\mathcal{E}_{LUMO}$ values refer to the orbital energies of the lowest unoccupied molecular orbital (LUMO). The N (nucleophilicity index) values were calculated with eq 2[5-7]. In eq 2, tetracyanoethylene (TCE) with the lowest HOMO energy among the organic molecules serves as a reference.

The condensed local electrophilicity ($\omega°$)[8,9] and local nucleophilicity ($N°$)[10,11] at the atomic site k may be defined in terms of the related condensed Fukui functions f_k^+ and f_k^-, as

$$\omega° = \omega \cdot f_k^+ \qquad \text{(eq 3)}$$

$$N° = N \cdot f_k^- \qquad \text{(eq 4)}$$

Where the condensed Fukui functions at the atomic site k, for the nucleophilic attack (f_k^+) and for the electrophilic attack (f_k^-), may be written in terms of the respective population q_k (N) of the N−electronic system of k atomic site, as[12,13]

$$f_k^+ = q_k(N) - q_k(N+1) \qquad \text{(eq 5)}$$

$$f_k^- = q_k(N-1) - q_k(N) \qquad \text{(eq 6)}$$

3. Detailed information of reactivity index calculation.

Complex	E_{HOMO}	E_{LUMO}	E_{TCE}	η	μ	ω	N	f_k^-	$N°$
Int-5	-0.2509	-0.0208	-0.3350	6.2605	-3.6971	1.0916	2.2890	0.1104	0.253
Int-13	-0.2447	0.01306	-0.3350	7.0140	-3.1516	0.7081	2.4577	0.1424	0.350

Table S1. The calculated condensed local nucleophilicity index ($N°$) values of the complexes **Int-5** and **Int-13**.

4. Substitute Effect of Nucleophilic Cyclization Step.

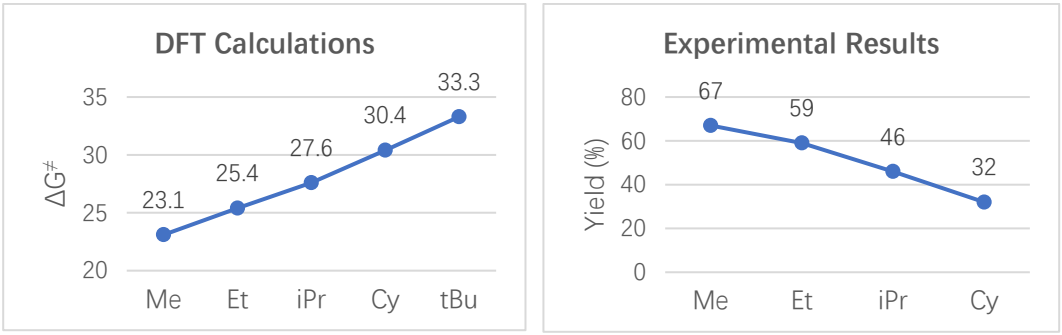


Figure S1. Calculated relative activation free energy for the nucleophilic cyclization step using different substitute groups (Left). The values given in kcal/mol are the relative free energies calculated by the SMD(acetonitrile)/M06-2x/6-311+g(d,p)//SMD(acetonitrile)/M06-2x/6-31g(d) level of theory. Isolated yields of different substitute groups (Right).

A combination of DFT calculations and experimental investigations were further employed to explore the steric effect for the nucleophilic cyclization step. As shown in Figure S1, DFT calculated results show that the relative activation free energy for the nucleophilic cyclization step increases gradually accompanied by the increase of steric hindrance in R^1 of acetoacetamides **1**, suggesting a lower yield would be observed experimentally when a large steric hindrance reactant was used. The calculated results are well consistent with experimental observations.

5. The intrinsic reaction coordinate (IRC) analysis of the transition state TS-22.

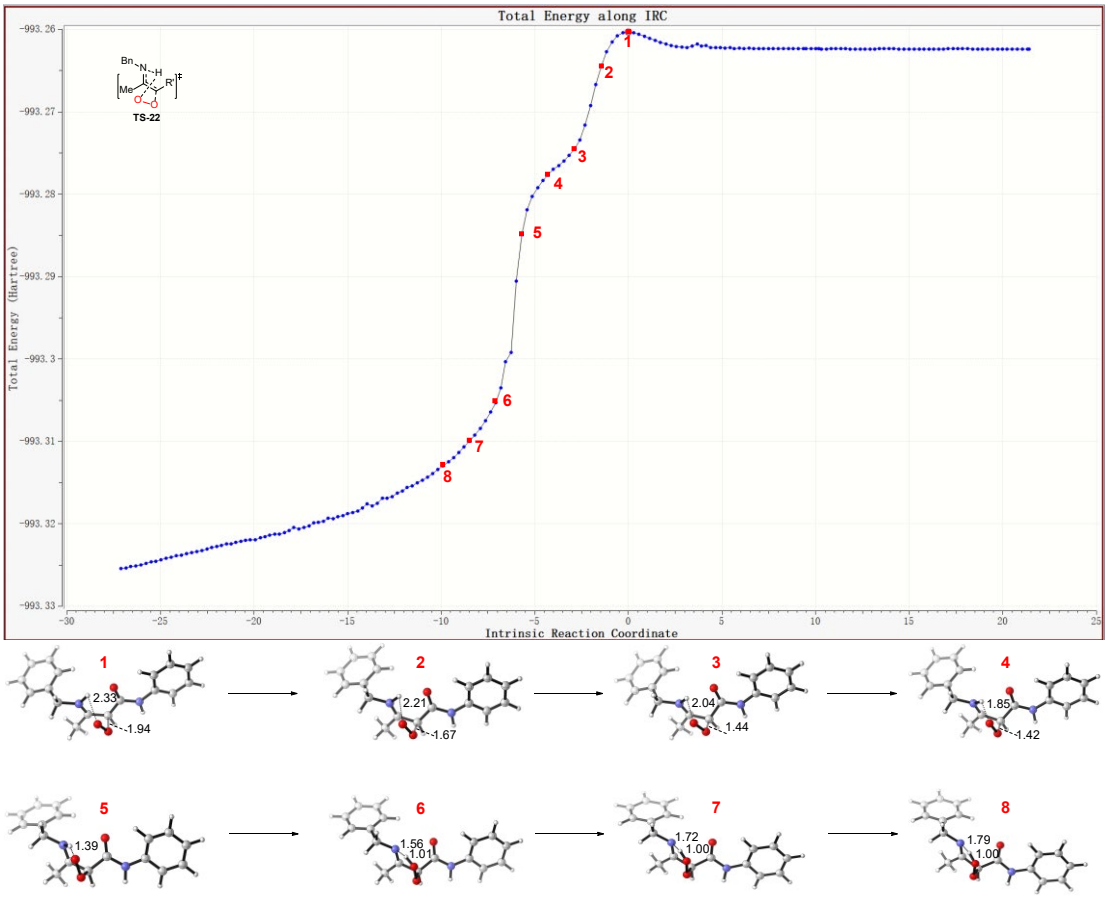


Figure S2. The calculated intrinsic reaction coordinate (IRC) and the snapshots along the IRC path of the transition state **TS-22**. The black values of geometric information are the bond lengths given in angstroms.

As shown in Figure S2, the calculated intrinsic reaction coordinate (IRC) and the snapshots along the IRC path of the transition state TS-22 shows that a concerted but asynchronous process could be observed.

6. Kinetic experiments.

To quantitatively explore the effect of steric hindrance on the reaction, we make the greatest efforts to conduct kinetic experimental studies. In the kinetic experiments, we selected methyl (**2q**), ethyl (**2r**), isopropyl (**2t**), and cyclohexyl (**2u**) substituted enamines as reactants and monitored the time-dependent curves for each product. As shown in Figure S3, we plotted the kinetic curves for product formation over the first six hours (left) and for the entire reaction process (right). The measurement results indicate that the rate of product formation follows the trend: Et > ^{i}Pr ≈ Me > Cy, suggesting that steric hindrance did not well correlation with the reaction rate. We

speculate that this lack of apparent regularity may stem from the complex nature of photochemical reactions. Taking this reaction as an example, in addition to the nucleophilic cyclization step, the rate at which amino moiety of acetoacetamides **Int-9** is oxidized by $^1O_2$ will also determine the rate of product formation (Figure 3). However, this step is not affected by steric hindrance. Although we cannot quantitatively discuss the effect of steric hindrance on the reaction, the observed decrease in yield with increasing steric hindrance suggests that steric effects do impact the nucleophilic cyclization step, thereby further influencing product formation.

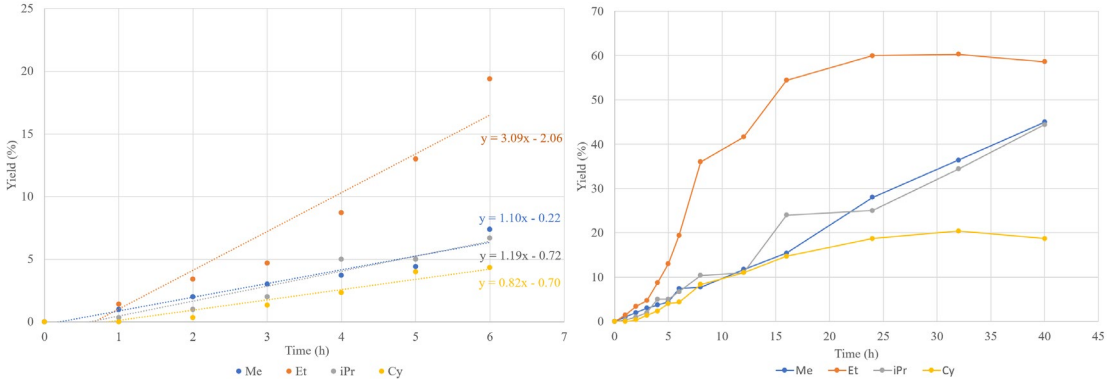


Figure S3. Kinetic experiments. The formation rate of products over the first six hours (left) and for the entire reaction process (right).

7. Absolute Calculation Energies, Enthalpies, and Free Energies.

Geometry	$E_{(M06\text{-}2X)}$[1]	$G_{(M06\text{-}2X)}$[2]	$H_{(M06\text{-}2X)}$[3]	$E_{(M06\text{-}2X)}$[4]	IF[5]
Int-1	-936.867251	0.237628	0.307039	-937.138700	-
Int-2	-862.904836	0.25962	0.325982	-863.153295	-
TS-3	-1799.764479	0.524622	0.633915	-1800.279929	224.15*i*
Int-4	-1799.797303	0.525615	0.6357	-1800.313238	-
Int-5	-1799.787675	0.524676	0.63541	-1800.306649	-
TS-6	-1799.747629	0.527903	0.635114	-1800.267647	214.75*i*
Int-7	-1799.749460	0.528977	0.636621	-1800.270277	-
Int-8	-917.016489	0.248309	0.319608	-917.281676	-
Int-9	-843.045334	0.269692	0.338872	-843.289418	-
TS-10	-1760.068663	0.553852	0.659722	-1760.574548	234.49*i*
Int-11	-1760.070317	0.552378	0.660976	-1760.576988	-

Int-12	-1760.096495	0.551651	0.661253	-1760.604186	-
Int-12^{Me}	-1298.168562	0.396049	0.487723	-1298.555046	-
Int-12^{Et}	-1376.761138	0.449723	0.547922	-1377.16943	-
Int-12^{iPr}	-1455.355451	0.504514	0.607285	-1455.785784	-
Int-12^{Cy}	-1688.735304	0.63206	0.744569	-1689.22514	-
Int-12^{tBu}	-1533.93608	0.559296	0.665888	-1534.388916	-
Int-13	-1760.086445	0.550113	0.661607	-1760.596136	-
Int-13^{Me}	-1298.161658	0.397318	0.48864	-1298.551023	-
Int-13^{Et}	-1376.752991	0.45095	0.548749	-1377.164551	-
Int-13^{iPr}	-1455.346348	0.505272	0.607949	-1455.780232	-
Int-13^{Cy}	-1688.727324	0.635787	0.745146	-1689.220743	-
Int-12^{tBu}	-1533.927679	0.560526	0.666958	-1534.383603	-
TS-14	-1760.055732	0.553665	0.660652	-1760.566024	142.90*i*
TS-14^{Me}	-1298.131186	0.399643	0.48745	-1298.521779	145.43*i*
TS-14^{Et}	-1376.720339	0.453614	0.547641	-1377.132908	142.02*i*
TS-14^{iPr}	-1455.309107	0.506808	0.606782	-1455.744151	141.41*i*
TS-14^{Cy}	-1688.687614	0.637258	0.744445	-1689.181851	174.05*i*
TS-14^{tBu}	-1533.88535	0.564832	0.666523	-1534.341322	182.95*i*
Int-15	-1760.056343	0.554839	0.662227	-1760.567073	-
Int-16	-1760.104869	0.556566	0.662979	-1760.613685	-
TS-17	-1760.064397	0.549526	0.659766	-1760.571927	63.53*i*
Int-18	-1433.272429	0.407056	0.502143	-1433.689188	-
$BnNH_2$	-326.763022	0.116050	0.155972	-326.863332	-
TS-19	-1433.271212	0.410091	0.501156	-1433.68605	93.19*i*
Int-20	-1433.339375	0.411914	0.504634	-1433.749517	-
$^1O_2$	-150.200053	-0.014863	0.007357	-150.253163	-
$O_2^{-\cdot}$	-150.343064	-0.01676	0.006321	-150.429631	-
Int-21	-842.853315	0.270471	0.33918	-843.089269	-
TS-22	-993.260342	0.273549	0.34687	-993.559874	236.91*i*

Int-23	-993.333303	0.276642	0.348673	-993.62931	-
TS-24	-993.228477	0.266294	0.340643	-993.527379	2418.59*i*
Int-25	-993.331648	0.274841	0.348785	-993.630556	-
TS-26	-993.319002	0.274587	0.346724	-993.623417	327.88*i*
H_2O	-76.380526	0.003554	0.025002	-76.429678	-

[1]The electronic energy calculated by M06-2X functional with 6-31G(d) basis set. [2]The thermal correction to Gibbs free energy was calculated by M06-2X functional with 6-31G(d) basis set. [3]The thermal correction to enthalpy calculated by M06-2X functional with 6-31G(d) basis set. [4]The electronic energy calculated by M06-2X functional with 6-311+G(d,p) basis set. [5]The M06-2X functional with 6-31G(d) basis set calculated imaginary frequencies for the transition state.

8. Geometries for All the Optimized Compounds and Transition State.

Int-1

C	0.09907500	-0.64228400	0.25783800
C	-1.28599700	-1.22968400	0.49043100
N	1.03245300	-1.50769700	0.20472400
C	-2.40731100	-0.66730900	-0.39723300
O	-2.17354600	-0.18845300	-1.48113900
O	-1.49538000	-2.12406600	1.26777800
C	2.39310800	-1.13923700	0.10802400
C	2.99372500	-0.30235200	1.05594000
C	3.16495200	-1.70954800	-0.90853200
C	4.35450900	-0.02535400	0.96781300
H	2.39311100	0.11426500	1.85922500
C	4.51965200	-1.40395300	-1.00393200
H	2.68996000	-2.37648700	-1.62169200
C	5.11983800	-0.56401200	-0.06637700
H	4.81722100	0.61828000	1.70985500
H	5.11007800	-1.83479100	-1.80680700
H	6.17929600	-0.33843600	-0.13507300
C	0.17813900	0.83865400	0.13386200
C	-0.59737000	1.62921400	0.98830700
C	0.96969400	1.44761800	-0.84714400
C	-0.56228700	3.01791900	0.88190800
H	-1.21963300	1.16052000	1.74807700
C	0.99168300	2.83308400	-0.95837100
H	1.55500700	0.83572100	-1.52694500
C	0.23174400	3.62003900	-0.09104700
H	-1.15753400	3.62569600	1.55586900
H	1.60119800	3.30140600	-1.72476400
H	0.25539100	4.70177600	-0.17961400
O	-3.59830900	-0.82780800	0.14660800
C	-4.71799800	-0.38101900	-0.65407400
H	-4.57415300	0.67814700	-0.88421300
H	-4.71370300	-0.94372100	-1.59147400
C	-5.97104000	-0.62468100	0.15175900
H	-6.84072700	-0.30049500	-0.42616100
H	-6.08345000	-1.68763700	0.38176500
H	-5.94604300	-0.06030600	1.08787400

Int-2

C	-0.30469700	0.34743600	-0.15644600
C	-1.64078900	0.63409400	-0.08104300
H	-1.95626900	1.66811600	-0.04141300
N	0.15765000	-0.92431700	-0.33289200
H	-0.57408400	-1.61188700	-0.50682200
C	-2.67203000	-0.38599700	-0.09157000
O	-2.49640900	-1.59248700	-0.23318400
C	1.43047200	-1.44711000	-0.02453900
C	1.84880800	-2.58470400	-0.72463700
C	2.25174500	-0.91262300	0.97501800
C	3.07738800	-3.17098900	-0.43879000
H	1.20332600	-2.99861000	-1.49455900
C	3.48782800	-1.49622100	1.23950500
H	1.92071300	-0.05547300	1.55142500

C	3.90904200	-2.62469100	0.53785700	C	6.60988000	-1.21441300	0.39282000
H	3.38722600	-4.05426200	-0.98908700	H	6.53769400	-0.10313100	2.23710700
H	4.11767500	-1.07099300	2.01513000	H	6.35529400	-2.28961500	-1.45806500
H	4.87082700	-3.07791800	0.75550000	H	7.67962500	-1.39062500	0.44491000
C	0.67270900	1.47013200	-0.15934100	C	-3.44966700	-0.92878600	1.52448600
C	1.70897700	1.49901700	-1.10063600	C	-3.67893800	-0.04061200	2.57377000
C	0.53826200	2.52439900	0.74857800	C	-4.46854000	-1.73966600	1.02730500
C	2.59344500	2.57202300	-1.13298600	C	-4.95479200	0.04557900	3.12405100
H	1.81217100	0.68516400	-1.81286000	H	-2.86286100	0.58053400	2.93148900
C	1.43086200	3.59350200	0.71892800	C	-5.74123700	-1.63828700	1.58106100
H	-0.25681200	2.49573300	1.48792900	H	-4.26166300	-2.43956000	0.22368400
C	2.45917700	3.61936300	-0.22084700	C	-5.98737700	-0.74833500	2.62665400
H	3.38870700	2.59154900	-1.87174400	H	-5.14108900	0.73801900	3.93871300
H	1.32419000	4.40352100	1.43375700	H	-6.54068000	-2.26523900	1.19922100
H	3.15482900	4.45261100	-0.24377900	H	-6.98185100	-0.67755000	3.05543600
O	-3.89914200	0.13703800	0.07128100	C	-2.62068200	-0.59271400	-1.36358700
C	-4.98749000	-0.79888400	0.06791300	C	-3.59696000	0.40314400	-1.21992100
H	-4.83937400	-1.52093400	0.87662700	C	-2.45608300	-1.23061300	-2.59884900
H	-4.98339900	-1.34721800	-0.87896900	C	-4.39592000	0.75275800	-2.30237900
C	-6.26211200	-0.00691100	0.25159200	H	-3.71054100	0.91942300	-0.27212200
H	-6.24639500	0.53781800	1.19988600	C	-3.27262200	-0.89058400	-3.67308600
H	-6.39262300	0.71137000	-0.56281400	H	-1.70148900	-2.00375100	-2.70912200
H	-7.11944800	-0.68578400	0.25592500	C	-4.23978200	0.10229400	-3.52709700
TS-3				H	-5.13802900	1.53713000	-2.18986300
C	-1.71771500	-0.94559000	-0.24725900	H	-3.14942200	-1.39786900	-4.62439200
C	-0.30256300	-1.07868600	-0.47144100	H	-4.86972100	0.37345500	-4.36862900
H	-0.00660400	-1.00465200	-1.51276400	C	2.46071800	1.85023300	0.20415800
N	-2.12769300	-1.00785900	1.00287600	C	1.96959000	2.85383700	1.04790500
H	-1.36441800	-1.01525500	1.68940800	C	3.48947900	2.15037300	-0.69691500
C	0.34104900	-2.20846600	0.25627300	C	2.52278700	4.13234100	1.00953100
O	0.18217900	-2.44399500	1.43795300	H	1.15854000	2.62390900	1.73295000
C	1.84181700	0.48724700	0.22147300	C	4.03001700	3.43126400	-0.73985100
C	0.31098700	0.51133600	0.41423100	H	3.85671500	1.38220500	-1.37102700
N	2.45271400	-0.62511900	0.19550400	C	3.55255500	4.42335000	0.11753300
C	-0.31416100	1.52450200	-0.57414900	H	2.14454100	4.90172900	1.67566800
O	0.05984500	1.66126700	-1.71875900	H	4.82333100	3.65690500	-1.44579100
O	-0.06221600	0.53279600	1.62379700	H	3.97853400	5.42147300	0.08442200
C	3.85332400	-0.75666400	0.25946300	O	1.03884300	-2.99793000	-0.56870700
C	4.59700300	-0.25652200	1.33486300	C	1.81794600	-4.01645800	0.07551200
C	4.49180100	-1.50714800	-0.73488200	H	1.15844600	-4.64290400	0.68283800
C	5.96809700	-0.49083100	1.39759500	H	2.53580600	-3.52785000	0.74389800
H	4.09231500	0.30430900	2.11638400	C	2.50779600	-4.81853200	-1.00398100
C	5.86594100	-1.71930800	-0.67405500	H	1.77390800	-5.28116200	-1.67029600
H	3.89684300	-1.90424400	-1.55256700	H	3.17135700	-4.18525200	-1.59952000

H	3.10603000	-5.61080300	-0.54509200
O	-1.30069000	2.22372200	-0.01925300
C	-1.88932900	3.23582300	-0.85928000
H	-1.10322100	3.93893000	-1.15125700
H	-2.27676300	2.76170000	-1.76567100
C	-2.97966700	3.91174200	-0.06121400
H	-3.44119800	4.69710800	-0.66644400
H	-3.75644700	3.19736000	0.22833600
H	-2.57033000	4.36756500	0.84481300

Int-4

C	1.74294900	-0.71453900	-0.06608600
C	0.22218700	-0.84081700	0.03382500
H	-0.06288200	-1.05071300	1.06458500
N	2.20746100	-0.39994700	-1.21390100
H	0.71600800	0.51990700	-1.91346600
C	-0.26286900	-1.98805200	-0.84054100
O	-0.28887800	-1.98569100	-2.04650700
C	-1.94199900	0.50060200	-0.18096900
C	-0.41192800	0.52979100	-0.35134100
N	-2.48064000	-0.65051700	-0.17904000
C	0.16929900	1.52812900	0.67240900
O	-0.17640500	1.53165300	1.83235600
O	-0.16092500	0.89767500	-1.67392400
C	-3.87139600	-0.87603600	-0.20859400
C	-4.68421000	-0.33556100	-1.21211200
C	-4.41973900	-1.75214400	0.73404700
C	-6.03893200	-0.65222400	-1.24967500
H	-4.24593000	0.32068200	-1.95843300
C	-5.78025900	-2.04438800	0.70179600
H	-3.77099400	-2.18504700	1.49009100
C	-6.59477300	-1.49778500	-0.28974000
H	-6.66323100	-0.23362100	-2.03341600
H	-6.20229600	-2.71173500	1.44717300
H	-7.65300300	-1.73711400	-0.32055200
C	3.58686600	-0.25131500	-1.47826600
C	4.01797200	0.94526200	-2.05879900
C	4.49862800	-1.28644600	-1.24913400
C	5.36475400	1.12152500	-2.36349000
H	3.29152200	1.73035000	-2.24984200
C	5.83967100	-1.10864100	-1.57793700
H	4.14995100	-2.22195800	-0.82142000
C	6.27972000	0.09577500	-2.12611000
H	5.69716800	2.05926000	-2.79832300
H	6.54371200	-1.91643600	-1.40248700
H	7.32743300	0.23072800	-2.37537100
C	2.51191400	-0.85459300	1.20220500
C	3.45095400	0.11619200	1.57071100
C	2.25343000	-1.93161900	2.05655400
C	4.12766300	0.00343400	2.78161700
H	3.64125700	0.96195500	0.91485100
C	2.95202500	-2.05404600	3.25431800
H	1.51377900	-2.67767500	1.77564000
C	3.88591600	-1.08523400	3.61944000
H	4.84464800	0.76561300	3.07011700
H	2.76005200	-2.90042200	3.90609200
H	4.42075400	-1.17475600	4.55990700
C	-2.62427400	1.82269200	-0.04201400
C	-2.18624500	2.93348800	-0.77419500
C	-3.66127600	1.97765800	0.88719800
C	-2.80213800	4.17157400	-0.60056800
H	-1.37089200	2.82467300	-1.48229800
C	-4.26335900	3.21816300	1.06540700
H	-3.98459700	1.12869600	1.48174600
C	-3.84076100	4.31654900	0.31595800
H	-2.46475400	5.02410800	-1.18186800
H	-5.06048300	3.32911800	1.79391600
H	-4.31514700	5.28337900	0.45359800
O	-0.56980600	-3.04828800	-0.08542200
C	-1.07141800	-4.19263600	-0.79828300
H	-0.31596400	-4.52272400	-1.51708500
H	-1.96363400	-3.88750400	-1.35402000
C	-1.38317600	-5.25973600	0.22503600
H	-0.48329000	-5.53841700	0.78097200
H	-2.13899900	-4.90761900	0.93281800
H	-1.76841900	-6.15009300	-0.27952700
O	1.10755100	2.31232100	0.15797800
C	1.71747700	3.24400200	1.07797300
H	0.94921100	3.95097500	1.40507500
H	2.07184200	2.69063700	1.95218500
C	2.84488000	3.92925800	0.34313300
H	3.31381300	4.66503600	1.00239000
H	3.60632600	3.20614800	0.03425900
H	2.47166500	4.44678100	-0.54520600

Int-5

C	1.63564600	-1.05630100	0.13177100
C	1.50680700	0.22918100	-0.28984100
N	0.58000300	-1.97029200	0.04417300
H	-0.91326700	0.38280800	-2.16000000

C	2.71564600	1.07548900	-0.52113000
O	3.77710900	1.03485200	0.05993400
C	-1.04922900	0.31052300	0.07757400
C	0.18086300	0.88192300	-0.68310200
N	-1.96796500	-0.14757400	-0.67236400
C	0.20969100	2.35528200	-0.18986800
O	0.94804100	2.77778300	0.66929100
O	-0.05800600	0.85371800	-2.05789600
C	-3.17954000	-0.67613300	-0.17617400
C	-4.36249400	-0.31417400	-0.82711900
C	-3.22063600	-1.59318000	0.88107900
C	-5.58074600	-0.83347100	-0.39821300
H	-4.31244200	0.37994100	-1.66092000
C	-4.44031600	-2.12424200	1.28989900
H	-2.29571100	-1.89187000	1.36594300
C	-5.62416800	-1.74134100	0.65920300
H	-6.49664400	-0.53648800	-0.90003600
H	-4.46482800	-2.83983800	2.10624900
H	-6.57350900	-2.15464700	0.98499100
C	-0.00377600	-2.42152200	-1.16307300
C	0.43457700	-2.00532800	-2.42310900
C	-1.04382700	-3.35463700	-1.06927200
C	-0.18973900	-2.49570200	-3.56793700
H	1.24271600	-1.28877300	-2.50840900
C	-1.65366300	-3.84305400	-2.21942900
H	-1.36914800	-3.69005000	-0.08828200
C	-1.23739000	-3.41003600	-3.47816000
H	0.15759100	-2.16064800	-4.54099800
H	-2.46160300	-4.56295000	-2.12773300
H	-1.71797300	-3.78556900	-4.37579200
H	0.63461400	-2.70900700	0.73979800
O	-0.75441400	3.06555900	-0.76371000
O	2.48991900	1.91699700	-1.54455300
C	-0.91921200	4.40800700	-0.26359700
C	-2.08875900	5.01956400	-0.99810700
H	0.00821500	4.96160800	-0.43466400
H	-1.09331200	4.35533700	0.81567500
H	-2.24727500	6.04214900	-0.64468300
H	-1.89766600	5.04975600	-2.07442700
H	-3.00206700	4.44483800	-0.81889600
C	3.48552600	2.92722100	-1.75860300
C	2.96116700	3.84432900	-2.83975900
H	4.42514300	2.44812300	-2.04865900
H	3.65047800	3.45992800	-0.81669600
H	3.68404600	4.64226800	-3.03100400
H	2.79731900	3.29304100	-3.76999800
H	2.01431200	4.29843100	-2.53181900
C	2.84218700	-1.63189700	0.78882700
C	3.39638300	-1.04152000	1.92926600
C	3.34921500	-2.85229000	0.32729000
C	4.45793300	-1.65569100	2.58633500
H	2.98604700	-0.10539700	2.29421900
C	4.42731900	-3.45291500	0.97150100
H	2.90283700	-3.32151900	-0.54609900
C	4.98006200	-2.85619500	2.10395300
H	4.87830400	-1.19832800	3.47665900
H	4.82836100	-4.38922500	0.59617900
H	5.81225400	-3.33022800	2.61560400
C	-1.17417100	0.60552800	1.53969300
C	-2.15169200	1.54431300	1.89783400
C	-0.34750800	0.06574600	2.52855500
C	-2.29842900	1.93818400	3.22467700
H	-2.79230500	1.96872000	1.12845700
C	-0.50652800	0.45447200	3.85729500
H	0.40464200	-0.67283200	2.27735800
C	-1.47498800	1.39280800	4.20818100
H	-3.05657100	2.66907400	3.48821400
H	0.13340700	0.02098100	4.61972100
H	-1.58870700	1.69654200	5.24422000

TS-6

C	1.54891100	-0.39164000	-0.59311400
C	1.44402900	0.94225100	-0.71338100
N	0.23536200	-0.98177500	-0.82304700
C	2.55530300	1.91501300	-0.83975600
O	2.50083400	2.88089400	-1.56853200
C	-0.90492700	0.37564200	-0.24313300
C	0.02079400	1.40493000	-1.07325200
N	-2.05858500	0.22532600	-0.91823700
C	-0.25990500	2.77218500	-0.41214200
O	0.38866700	3.23853300	0.49873900
O	-0.27166800	1.28530900	-2.35918000
H	-1.94333800	0.62406200	-1.86770700
H	-0.00754500	-0.73978100	-1.80120100
C	-3.25093600	-0.43800100	-0.57791800
C	-4.39726700	-0.10675400	-1.30908000
C	-3.33019000	-1.40830800	0.42892900
C	-5.60779500	-0.73599600	-1.03648400
H	-4.32763600	0.64746800	-2.08847000

C	-4.54937000	-2.02276100	0.69893000
H	-2.44253900	-1.69795500	0.98271100
C	-5.69340500	-1.69354100	-0.02730800
H	-6.48780400	-0.47022500	-1.61431000
H	-4.59758500	-2.77633300	1.47936800
H	-6.63824100	-2.18230900	0.18734600
C	-0.14459600	-2.33558600	-0.54901500
C	-1.02874400	-2.92499400	-1.45653100
C	0.24861400	-3.02492400	0.60053200
C	-1.55212900	-4.18691500	-1.19652000
H	-1.31387800	-2.38515000	-2.35628800
C	-0.27563300	-4.29197100	0.84465300
H	0.96476400	-2.60011500	1.29347200
C	-1.18323400	-4.87168400	-0.04043500
H	-2.24679400	-4.63298900	-1.90102500
H	0.03167400	-4.82678200	1.73768000
H	-1.59036900	-5.85653500	0.16462000
O	-1.35365600	3.34464100	-0.91272600
O	3.61397700	1.61803300	-0.08397900
C	4.74569400	2.49860400	-0.20494700
C	5.84335500	1.93149300	0.66572300
H	4.44468000	3.50071600	0.11427700
H	5.04257900	2.54955000	-1.25619200
H	6.72487200	2.57639100	0.61164800
H	5.51967300	1.87377500	1.70909700
H	6.12447300	0.92939600	0.32906000
C	-1.77140600	4.56044200	-0.26727900
C	-3.09062100	4.96510500	-0.88346100
H	-0.99957600	5.32174200	-0.41514100
H	-1.86275700	4.37401700	0.80734300
H	-3.44879700	5.88637300	-0.41562200
H	-2.98009200	5.14114000	-1.95718000
H	-3.84157100	4.18377700	-0.73208000
C	2.70870100	-1.28413500	-0.38365400
C	2.95524100	-2.32130200	-1.29265300
C	3.52723400	-1.14537200	0.74279600
C	4.02233600	-3.19079900	-1.08942700
H	2.31379500	-2.44042100	-2.16215600
C	4.58858700	-2.02350200	0.94708100
H	3.32557700	-0.35156100	1.45400600
C	4.83970700	-3.04384800	0.03109800
H	4.21316700	-3.98508100	-1.80417600
H	5.21716800	-1.91136300	1.82513700
H	5.66778400	-3.72727500	0.19215200
C	-0.95602300	0.46496500	1.25044100
C	-2.01106300	1.23015200	1.77530200
C	0.01057300	-0.03101900	2.12782600
C	-2.10270000	1.47317000	3.14098800
H	-2.75705300	1.64625200	1.10373500
C	-0.09297900	0.20097400	3.49836200
H	0.86140200	-0.58999000	1.76317200
C	-1.14737700	0.95068900	4.01123200
H	-2.92478900	2.07018800	3.52339200
H	0.66442700	-0.20340300	4.16253800
H	-1.22103100	1.13290000	5.07877700

Int-7

C	1.50451200	-0.45139100	-0.57001700
C	1.50994700	0.87141400	-0.75972700
N	0.09136700	-0.90870200	-0.72219600
C	2.69727600	1.74529600	-0.92364200
O	2.74483500	2.65109900	-1.72409300
C	-0.81151500	0.35555500	-0.26993600
C	0.10801100	1.40650900	-1.12054800
N	-2.03216400	0.28974600	-0.93322700
C	-0.10209700	2.78763600	-0.47659900
O	0.62543800	3.27014600	0.36436300
O	-0.17853800	1.28515900	-2.40135800
H	-1.92634000	0.69011700	-1.87471100
H	-0.08454000	-0.79664100	-1.74203800
C	-3.20736500	-0.38855500	-0.61685900
C	-4.29666400	-0.22602900	-1.48897400
C	-3.36424000	-1.21368100	0.50826900
C	-5.50175600	-0.87458600	-1.24786900
H	-4.18100800	0.41478000	-2.35953700
C	-4.57938500	-1.85307900	0.73997100
H	-2.53529200	-1.37916800	1.18788900
C	-5.65677700	-1.69346800	-0.12940000
H	-6.32586400	-0.73539300	-1.94164500
H	-4.67420300	-2.49323300	1.61255600
H	-6.59793600	-2.19968000	0.05880800
C	-0.35291500	-2.24120500	-0.33892400
C	-1.16796100	-2.90960400	-1.24915900
C	-0.03636300	-2.80392200	0.89498000
C	-1.70870200	-4.14434400	-0.90488300
H	-1.39098300	-2.45785900	-2.21239900
C	-0.58167200	-4.04163900	1.22650400
H	0.62874200	-2.30257000	1.58706500
C	-1.42403800	-4.70731300	0.33716200

H	-2.35234800	-4.66163400	-1.60870700
H	-0.34124200	-4.48593800	2.18677600
H	-1.84753900	-5.66900500	0.60839200
O	-1.21330100	3.37274400	-0.92003900
O	3.69499100	1.42413900	-0.09916500
C	-1.55587800	4.61864500	-0.28870900
C	-2.87829500	5.06696500	-0.86662200
H	-0.75884700	5.34314100	-0.48036600
H	-1.61596900	4.45774900	0.79255800
H	-3.17914800	6.01283800	-0.40756500
H	-2.79892900	5.21536300	-1.94728000
H	-3.65667300	4.32322900	-0.67167800
C	4.89873300	2.20414400	-0.22739100
C	5.90684100	1.62414700	0.73760200
H	4.66406500	3.24788500	0.00072900
H	5.24445800	2.14892400	-1.26331300
H	6.84082100	2.18954800	0.67610200
H	5.53558300	1.67872400	1.76509800
H	6.11647100	0.57847500	0.49397000
C	2.55696000	-1.47156000	-0.40672600
C	2.62415200	-2.54219000	-1.30855000
C	3.46164800	-1.40667700	0.65860300
C	3.59726500	-3.52405500	-1.15565500
H	1.91830500	-2.59990200	-2.13343200
C	4.43118800	-2.39542700	0.80954600
H	3.39999000	-0.58382900	1.36256700
C	4.50162000	-3.45228000	-0.09609600
H	3.64875700	-4.34562200	-1.86306600
H	5.12853300	-2.34055600	1.63979300
H	5.25784800	-4.22182100	0.02481700
C	-0.86953300	0.61517900	1.21642100
C	-1.93699600	1.41303700	1.66044200
C	0.11854600	0.26338100	2.14210100
C	-2.02556800	1.82057300	2.98707400
H	-2.69878400	1.72514000	0.95318400
C	0.02002100	0.66109000	3.47494300
H	0.99332300	-0.30310500	1.84881700
C	-1.05027100	1.43821500	3.90606500
H	-2.86297300	2.43655100	3.30042900
H	0.79758300	0.36565000	4.17247400
H	-1.12007100	1.74954300	4.94362000

Int-8

C	0.80896000	0.78492900	-0.88830100
C	-0.39750000	-0.12323200	-0.97419000
C	0.64238900	2.24054600	-1.22508100
H	0.79924500	2.85576100	-0.33210300
H	1.38983100	2.53231300	-1.97079600
H	-0.35275900	2.45220200	-1.61853900
N	1.88415300	0.19876400	-0.54770400
C	3.09093600	1.00586200	-0.44142300
C	4.26458500	0.20782400	0.08111700
C	4.36663100	-1.16674000	-0.14376700
C	5.29398700	0.85940800	0.76530200
C	5.47924200	-1.87592900	0.30581900
H	3.56458200	-1.67942900	-0.66572500
C	6.40860900	0.15337400	1.21295500
C	6.50445700	-1.21859800	0.98419100
H	5.54475700	-2.94505900	0.12572200
H	7.19891000	0.67383400	1.74592400
H	7.37024500	-1.77193000	1.33530400
H	5.21863500	1.92835000	0.95123100
H	2.92037700	1.87977000	0.20198600
H	3.34017400	1.40639300	-1.43605400
C	-1.66404000	0.36160600	-0.24393000
O	-1.62384200	1.35917100	0.46049800
N	-2.72005500	-0.44852100	-0.46650300
H	-2.52728900	-1.24812700	-1.06510600
C	-4.02649500	-0.35022800	0.04686400
C	-4.43936100	0.68466400	0.89361000
C	-4.93247600	-1.34974100	-0.32988900
C	-5.75592400	0.70267900	1.35089900
H	-3.74286100	1.45743200	1.18730500
C	-6.24052800	-1.31626000	0.13592100
H	-4.60107600	-2.14886400	-0.98779800
C	-6.66101300	-0.28842700	0.98021900
H	-6.07157800	1.50770100	2.00767400
H	-6.93247800	-2.09746100	-0.16315700
H	-7.68293900	-0.26191900	1.34437100
O	-0.38106000	-1.19205700	-1.53833400

Int-9

C	-0.78917900	2.23355500	0.07123200
C	0.57688100	2.12676500	0.19119600
H	1.13683900	3.02276100	0.43114100
C	-1.45161700	3.56905800	0.26401200
H	-0.70418000	4.33524200	0.47266000
H	-2.01219900	3.85892200	-0.63110300
H	-2.15896000	3.53344400	1.09967400
N	-1.58529100	1.17853400	-0.20277800

H	-1.09321200	0.30740000	-0.39180500	C	4.29747800	1.91144600	2.51113600
C	-3.00356600	1.23777400	-0.50475700	H	2.27694200	1.91897400	1.76282200
C	-3.68303200	-0.07619600	-0.18346200	C	6.02462700	2.40110000	0.90141500
C	-3.33014800	-0.80845200	0.95379000	C	5.64813200	2.08023300	2.20476700
C	-4.70017800	-0.55727200	-1.01035300	H	3.99788100	1.64940400	3.52160000
C	-3.98643000	-1.99866700	1.25931700	H	7.07438100	2.52117600	0.65047100
H	-2.53406700	-0.44531600	1.59838800	H	6.40248100	1.95368800	2.97541400
C	-5.36187900	-1.74503700	-0.70336600	H	5.34843900	2.81971600	-1.10130100
C	-5.00571800	-2.46976800	0.43251000	H	2.35529100	3.75983400	-0.77116500
H	-3.70134300	-2.55903800	2.14483400	H	3.08397400	2.56880100	-1.84153200
H	-6.14965000	-2.10783400	-1.35691400	C	-1.27361100	1.07516100	-0.77342500
H	-5.51598900	-3.39833300	0.66994100	O	-1.13748300	2.07685100	-0.06608600
H	-4.97192200	0.00171100	-1.90243700	N	-2.47826700	0.68974800	-1.29266400
H	-3.17632900	1.48660500	-1.56068200	H	-2.48633200	-0.24135500	-1.69669300
H	-3.46148600	2.03427500	0.09016500	C	-3.73866900	1.28056200	-1.12297600
C	1.29153600	0.88112100	0.00526800	C	-3.95970000	2.48647100	-0.44496100
O	0.74897600	-0.20452100	-0.25831800	C	-4.83059700	0.59468700	-1.67881000
N	2.66239700	0.98727600	0.14263700	C	-5.26106600	2.97446000	-0.32199900
H	3.01560900	1.91484900	0.34798200	H	-3.12820700	3.02430300	-0.01341700
C	3.64295200	-0.00432400	0.02536700	C	-6.11886300	1.09292500	-1.54436800
C	3.37343000	-1.35249700	-0.25591200	H	-4.65603300	-0.34057700	-2.20538200
C	4.97698300	0.39853300	0.20580000	C	-6.34585400	2.28877400	-0.86007600
C	4.42793100	-2.25950300	-0.35056500	H	-5.42006200	3.90822300	0.20985500
H	2.35311000	-1.67674100	-0.39723400	H	-6.95020300	0.53999900	-1.97201300
C	6.01486100	-0.51857500	0.10787700	H	-7.35325600	2.67772500	-0.75156600
H	5.19019800	1.44203800	0.42420500	C	-0.92815700	-1.57267900	0.79640000
C	5.74941200	-1.85931300	-0.17206300	C	0.32684200	-0.73251400	0.49522900
H	4.20223500	-3.29948500	-0.56899600	C	-0.94679500	-1.98782800	2.24820200
H	7.03696800	-0.18074200	0.25157800	H	-0.83134700	-1.08954400	2.86016000
H	6.55939500	-2.57747400	-0.24921200	H	-1.85769100	-2.51168600	2.53853600
TS-10				H	-0.08156100	-2.62895000	2.45792200
C	1.11656600	0.86993400	-1.42934900	N	-1.76802100	-1.86648000	-0.11076200
C	-0.13036400	0.20991900	-1.17046600	C	-2.91136600	-2.71445700	0.20219400
H	-0.36469800	-0.57587700	-1.88069200	C	-4.12449700	-1.93255800	0.67977200
C	2.07003200	0.31432700	-2.44125000	C	-5.40291500	-2.42303100	0.39081700
H	1.81822100	-0.72629800	-2.65611200	C	-4.01187300	-0.75420600	1.42157600
H	1.98321200	0.88679700	-3.37258200	C	-6.54188500	-1.76104800	0.84171400
H	3.10591800	0.37126400	-2.09604500	H	-5.50277400	-3.33244600	-0.19726200
N	1.44918000	1.91573600	-0.71418600	C	-5.15114900	-0.08947400	1.87638100
H	0.73576800	2.22437900	-0.04825800	C	-6.41914000	-0.58996700	1.58998100
C	2.66272600	2.71166000	-0.84538000	H	-7.52531500	-2.15549300	0.60301400
C	3.69968400	2.41536900	0.22026000	H	-5.04414300	0.83012000	2.44466600
C	3.32584800	2.07493200	1.52437900	H	-7.30519000	-0.06642200	1.93664700
C	5.05386300	2.56565500	-0.08595600	H	-3.03279600	-0.32934500	1.62763900

H	-2.66476300	-3.48472100	0.94522700	N	-2.51128200	0.72385200	-1.23313500
H	-3.18637900	-3.24321500	-0.71600000	H	-2.53300800	-0.23851500	-1.56105200
C	1.43379200	-1.63194300	-0.13099200	C	-3.76911200	1.31782500	-1.03330300
O	1.20245200	-2.57213500	-0.87968300	C	-3.97450000	2.51247500	-0.33258400
N	2.66322800	-1.19791200	0.24678100	C	-4.87108600	0.63421700	-1.56978900
H	2.62477700	-0.41717500	0.90426900	C	-5.27364800	2.99452000	-0.16938100
C	3.92160800	-1.64211500	-0.18570900	H	-3.13352500	3.04689900	0.08496400
C	4.09710000	-2.66525600	-1.12729800	C	-6.15741900	1.12542100	-1.39414200
C	5.04387900	-0.99543200	0.34916700	H	-4.70608900	-0.29321300	-2.11298100
C	5.38805500	-3.02227600	-1.51475500	C	-6.36922900	2.31153600	-0.68890100
H	3.23571000	-3.16950200	-1.54221000	H	-5.42234500	3.91997300	0.37948100
C	6.32306100	-1.36287700	-0.04863700	H	-6.99813500	0.57538000	-1.80676100
H	4.89991300	-0.20416000	1.07961700	H	-7.37464200	2.69576100	-0.54937400
C	6.50520000	-2.38113100	-0.98484600	C	-0.88168300	-1.60728600	0.62934400
H	5.51476400	-3.81686200	-2.24436400	C	0.28144400	-0.66079700	0.25194100
H	7.17946100	-0.84778900	0.37736300	C	-0.74054300	-2.11624000	2.04132300
H	7.50406200	-2.66974900	-1.29619500	H	-0.58326100	-1.25251300	2.69096500
O	0.70187600	0.10480500	1.36458900	H	-1.59918300	-2.69098500	2.38880000
Int-11				H	0.16053500	-2.73817300	2.11754300
C	1.07884400	0.89376800	-1.51561400	N	-1.79939100	-1.87387700	-0.21062900
C	-0.15893700	0.18720400	-1.12483400	C	-2.89666900	-2.76351600	0.14544600
H	-0.44580800	-0.52698900	-1.89416800	C	-4.09982100	-2.00217300	0.67723100
C	1.88737600	0.41903100	-2.67719600	C	-5.38860700	-2.45887100	0.38218900
H	1.62716800	-0.61733100	-2.90016600	C	-3.95870500	-0.86149800	1.47222400
H	1.65138900	1.02913100	-3.55756200	C	-6.51126200	-1.79814400	0.87562800
H	2.95993700	0.48895300	-2.48113900	H	-5.51048400	-3.33880800	-0.24515700
N	1.47400600	1.85834000	-0.74953400	C	-5.08053400	-0.19604900	1.96619200
H	0.85698800	2.04237300	0.04814800	C	-6.36019800	-0.66177300	1.67017500
C	2.67123900	2.68129200	-0.88625900	H	-7.50404300	-2.16475900	0.63129200
C	3.69502200	2.40650300	0.19699100	H	-4.95211800	0.69564100	2.57320400
C	3.31036900	2.12387700	1.51216600	H	-7.23353600	-0.13776700	2.04714000
C	5.05221600	2.52156500	-0.10965100	H	-2.96860600	-0.46817300	1.68925100
C	4.27581800	1.98572400	2.50823600	H	-2.60031900	-3.53018600	0.87302800
H	2.26034800	1.98781000	1.75782600	H	-3.19989200	-3.29367100	-0.76311800
C	6.01658700	2.38021100	0.88760100	C	1.42370700	-1.58611800	-0.31392600
C	5.63013900	2.11993300	2.20101000	O	1.23620000	-2.47940600	-1.13318800
H	3.96802200	1.76929100	3.52688300	N	2.61899800	-1.19460200	0.18838100
H	7.06890500	2.47230500	0.63589200	H	2.49404900	-0.44630100	0.88037500
H	6.37931900	2.01276400	2.97960400	C	3.90616800	-1.63967300	-0.13825400
H	5.35458900	2.72975800	-1.13283800	C	4.15433000	-2.63765700	-1.09075100
H	2.33593000	3.72179600	-0.82256500	C	4.98285300	-1.02746300	0.51732400
H	3.10038900	2.53367400	-1.87691800	C	5.47028300	-3.00411700	-1.36935600
C	-1.29741900	1.12850500	-0.76655600	H	3.32609500	-3.11373300	-1.59727000
O	-1.11764100	2.16748500	-0.13876300	C	6.28831700	-1.40284800	0.22652200

H	4.78140500	-0.25442500	1.25383200	H	-7.75784800	2.26084300	0.51564000
C	6.54232800	-2.39562700	-0.72046200	C	-0.72564800	-1.50234000	0.08718000
H	5.65345800	-3.77918100	-2.10796800	C	0.22741000	-0.29493800	0.08265600
H	7.10915600	-0.91367800	0.74349200	C	-0.49057400	-2.47755100	1.21193200
H	7.56180900	-2.69013400	-0.94830700	H	-0.58346800	-1.95350300	2.16661300
O	0.67808800	0.14048200	1.21276800	H	-1.19066300	-3.31229600	1.19877000
Int-12				H	0.53089400	-2.87162000	1.15890000
C	0.74373200	1.98723700	-0.89111100	N	-1.58892700	-1.56751500	-0.84362400
C	-0.30696800	0.89629400	-0.74689700	C	-2.53560800	-2.67138400	-0.92276900
H	-0.54697500	0.51864300	-1.74291800	C	-3.84629000	-2.33525000	-0.22986000
C	0.59281200	2.88188700	-2.09323800	C	-5.05558400	-2.73230300	-0.80865300
H	-0.44802400	2.88757500	-2.42850600	C	-3.87742000	-1.65996200	0.99378200
H	0.90306000	3.90812000	-1.88736300	C	-6.26923600	-2.47361000	-0.17431000
H	1.20349600	2.49178600	-2.91702200	H	-5.04377500	-3.24777300	-1.76592500
N	1.65046000	2.04666500	-0.00144500	C	-5.08993300	-1.39920000	1.63071800
H	0.98755200	0.89705200	1.34851100	C	-6.28982600	-1.80701800	1.05019400
C	2.75670900	2.99058200	-0.09740500	H	-7.19868900	-2.78640000	-0.64102100
C	4.03340300	2.28363700	0.30379400	H	-5.09581000	-0.86606000	2.57702400
C	4.18950300	1.80765100	1.61091200	H	-7.23444500	-1.59630600	1.54271100
C	5.05037700	2.06231500	-0.62332100	H	-2.95337200	-1.31416600	1.45002900
C	5.34880800	1.13574500	1.98467200	H	-2.13265500	-3.60574600	-0.51295300
H	3.39395500	1.96891200	2.33531500	H	-2.73949100	-2.85090300	-1.98251600
C	6.21645700	1.38886500	-0.25134500	C	1.53448500	-0.77579100	-0.61700600
C	6.36860500	0.92661100	1.05241400	O	1.60277000	-0.84941400	-1.83471600
H	5.46029000	0.77241800	3.00230900	N	2.51762900	-1.11596200	0.25370400
H	7.00050400	1.22166900	-0.98425900	H	2.28321000	-0.99680600	1.23517800
H	7.27211900	0.39846000	1.34264600	C	3.80425200	-1.60855000	-0.03187100
H	4.93102000	2.41885300	-1.64358400	C	4.38329900	-1.54695200	-1.30452000
H	2.55505700	3.81536200	0.59775500	C	4.52556400	-2.16195500	1.03433300
H	2.86979900	3.41429700	-1.10102000	C	5.67494800	-2.03812500	-1.49057400
C	-1.55288000	1.53379200	-0.11287400	H	3.83073800	-1.11694900	-2.12851500
O	-1.45587500	2.37901800	0.76446200	C	5.81214300	-2.64646200	0.83274200
N	-2.72846500	1.10785700	-0.65277900	H	4.06868400	-2.20284600	2.02007200
H	-2.64487100	0.32398600	-1.29540600	C	6.39614900	-2.58702500	-0.43296300
C	-4.03951200	1.47400000	-0.30285500	H	6.11954600	-1.98363200	-2.47998200
C	-4.35889000	2.26987700	0.80379700	H	6.35926100	-3.07071600	1.66923800
C	-5.06720200	0.97252200	-1.11494000	H	7.40097900	-2.96540400	-0.59153300
C	-5.69750300	2.54476900	1.08328000	O	0.46600500	0.06241400	1.42289100
H	-3.57160200	2.65897000	1.43382000	**Int-12^{Me}**			
C	-6.39504200	1.25232100	-0.82021700	C	-0.10467300	2.18858800	0.60248200
H	-4.81229600	0.35434000	-1.97228300	C	0.52530800	0.80545300	0.59611400
C	-6.72045900	2.04169200	0.28387100	H	0.59249800	0.44125500	1.62423100
H	-5.93656400	3.16019100	1.94573900	C	0.38475000	3.14408600	1.65618400
H	-7.17818500	0.84791900	-1.45484600	H	1.24580500	2.73775600	2.19153500

H	0.66187800	4.10414300	1.20949100	H	-6.54995000	-0.58518800	2.05906100
H	-0.41335900	3.33487400	2.38395600	H	-6.91953400	-0.69489600	-2.21844000
N	-0.96791700	2.46505000	-0.29139800	H	-7.98304800	-0.73316800	0.03509200
H	-0.61420400	1.08958100	-1.57281700	O	-0.35481100	0.13819900	-1.57935600
C	-1.56190400	3.79313000	-0.30780200	H	1.89783300	-3.70667000	0.22278400
H	-0.83666400	4.53123300	-0.67217000	H	-2.41898500	3.79395700	-0.98404900
H	-1.89744500	4.11021800	0.68639200	**Int-12^{Et}**			
C	1.93869800	0.98007300	0.01389200	C	0.26378600	-1.99650800	0.92231900
O	2.19202800	1.88649100	-0.76663300	C	-0.53159400	-0.72234300	0.67401400
N	2.84604800	0.07662400	0.47420200	H	-0.66582400	-0.19955200	1.62449100
H	2.44671700	-0.67220900	1.04011700	C	-0.07683000	-2.74767200	2.18457600
C	4.18813000	-0.08476900	0.09110100	H	-1.02581200	-2.39342200	2.59420700
C	4.89178100	0.83591700	-0.69561700	H	-0.15027800	-3.82301800	2.00623800
C	4.83825900	-1.23903800	0.55144300	H	0.69947600	-2.57834800	2.94020300
C	6.22662500	0.58531300	-1.01080700	N	1.13308000	-2.32336700	0.05370200
H	4.39837600	1.72816600	-1.05349500	H	0.62830500	-1.22631200	-1.43903200
C	6.16888400	-1.47269700	0.22952900	C	2.01212200	-3.46743700	0.23683000
H	4.28669000	-1.94905200	1.16327900	H	1.75612400	-4.21276100	-0.52524000
C	6.87383800	-0.56069000	-0.55650300	H	1.89699100	-3.93996700	1.21872100
H	6.76387100	1.30490200	-1.62172700	C	-1.90155300	-1.14874300	0.11985100
H	6.65538600	-2.37215200	0.59465700	O	-2.04566900	-2.21592200	-0.45896200
H	7.91354800	-0.74207400	-0.80930800	N	-2.90169000	-0.25754700	0.36072300
C	0.14847100	-1.65902400	-0.09503200	H	-2.59585600	0.62007500	0.78257100
C	-0.32015700	-0.20252200	-0.21397400	C	-4.23561700	-0.30616400	-0.07824900
C	-0.38176100	-2.62740500	-1.11970200	C	-4.83054600	-1.44318300	-0.63975600
H	0.44023800	-3.22236400	-1.53178200	C	-4.99485100	0.86209000	0.08207000
H	-1.07972900	-3.32528400	-0.64119000	C	-6.16714900	-1.39166700	-1.03317700
H	-0.89127300	-2.11962300	-1.93754800	H	-4.25291000	-2.34771700	-0.76579700
N	0.87753200	-1.98189400	0.89562700	C	-6.32604100	0.89581300	-0.31282800
C	1.25098400	-3.38156200	1.04749800	H	-4.52850100	1.74300700	0.51746300
H	0.37269000	-4.03829400	1.06208600	C	-6.92268100	-0.23274700	-0.87577600
H	1.79660000	-3.50726800	1.98472200	H	-6.61921300	-2.27831300	-1.46811900
C	-1.74683900	-0.22134600	0.41237500	H	-6.89761700	1.80960300	-0.18117800
O	-1.89794400	-0.18894800	1.62368100	H	-7.96228300	-0.20732900	-1.18613700
N	-2.73444600	-0.34725500	-0.51032800	C	-0.37188900	1.63789100	-0.38421600
H	-2.42350600	-0.31503400	-1.47706700	C	0.21953600	0.22520400	-0.29047800
C	-4.12178200	-0.44458500	-0.30249000	C	0.10459500	2.49148400	-1.53101600
C	-4.71328100	-0.46564400	0.96643300	H	-0.74672600	2.98491500	-2.01082600
C	-4.92934600	-0.52826700	-1.44503200	H	0.76939400	3.27849400	-1.15434800
C	-6.09956000	-0.56978800	1.07091200	H	0.63860800	1.90545100	-2.27815700
H	-4.09653600	-0.40068400	1.85137600	N	-1.15069600	2.03186500	0.54000900
C	-6.30912400	-0.63146100	-1.32275600	C	-1.65242700	3.40383500	0.50919600
H	-4.46367300	-0.51206000	-2.42706900	H	-0.83647200	4.11049200	0.30905600
C	-6.90512100	-0.65270800	-0.06164300	C	1.64226500	0.45264900	0.30594800

O	1.79545000	0.62656600	1.50503900	H	3.92217700	2.19630300	-1.28512700
N	2.62066500	0.49123900	-0.63439800	C	6.49282400	-0.16056500	0.40673600
H	2.31476300	0.27356800	-1.57855900	H	4.79151600	-1.07316900	1.36173000
C	4.00579600	0.64757200	-0.44807300	C	6.93626300	0.83431700	-0.46470400
C	4.58939600	0.95060500	0.78836300	H	6.33370200	2.45459400	-1.74471400
C	4.82008700	0.48276300	-1.57723400	H	7.20411000	-0.82572700	0.88693500
C	5.97484000	1.08249600	0.87416900	H	7.99512300	0.95114800	-0.67200500
H	3.96729600	1.07837200	1.66278800	C	0.38610300	-1.71725200	-0.56017600
C	6.19856100	0.61944500	-1.47394800	C	-0.30891100	-0.36300000	-0.35240000
H	4.36090300	0.24666800	-2.53380300	C	-0.02051500	-2.43734200	-1.82017400
C	6.78666700	0.92003700	-0.24519500	H	0.44051200	-1.94038700	-2.67982900
H	6.41952200	1.31734500	1.83676400	H	0.28321900	-3.48410500	-1.81657000
H	6.81415700	0.48849200	-2.35867400	H	-1.10412500	-2.38137300	-1.96094900
H	7.86359900	1.02597600	-0.16318200	N	1.20010200	-2.10962400	0.33251400
O	0.28114800	-0.31522600	-1.58933900	C	1.87627300	-3.40536900	0.22374200
H	-2.36711300	3.50258000	-0.31987500	H	1.18855700	-4.16800800	-0.16331800
C	3.45447100	-3.00895400	0.04368500	C	-1.68477300	-0.69830700	0.29831800
H	3.58739100	-2.56427500	-0.94799600	O	-1.76067600	-0.98064200	1.48429000
H	3.71876500	-2.25546200	0.79405200	N	-2.72105000	-0.67531500	-0.57888300
H	4.14356700	-3.85275000	0.14292700	H	-2.47753700	-0.37321500	-1.51793900
C	-2.32701500	3.73854100	1.83016900	C	-4.08939700	-0.86857400	-0.32067500
H	-1.61262800	3.66030400	2.65565500	C	-4.59046900	-1.28962500	0.91729800
H	-2.72506900	4.75731600	1.81398800	C	-4.97524600	-0.61331300	-1.37677500
H	-3.15307700	3.04785300	2.03015800	C	-5.96660600	-1.44684400	1.07796500
Int-12^{iPr}				H	-3.91263600	-1.48766000	1.73529300
C	-0.39273800	1.80159400	0.96717800	C	-6.34326400	-0.77688000	-1.19973900
C	0.43399100	0.56841400	0.63237000	H	-4.57971800	-0.28538200	-2.33480900
H	0.61398300	0.00468000	1.55073100	C	-6.84946600	-1.19502000	0.03121700
C	-0.01112500	2.51473200	2.23988600	H	-6.34687500	-1.77376300	2.04130100
H	1.00313300	2.23706500	2.53897500	H	-7.01518500	-0.57472900	-2.02832400
H	-0.06152700	3.60036300	2.13057600	H	-7.91817400	-1.32204600	0.17091200
H	-0.68937000	2.21759100	3.04873600	O	-0.46710800	0.23599500	-1.61670500
N	-1.30991700	2.13425100	0.15206800	C	-3.60867400	2.85277600	0.07326300
H	-0.82724700	1.12925200	-1.40438800	H	-3.67780000	2.52156600	-0.96952000
C	-2.17931500	3.28095200	0.39468900	H	-3.92025400	2.02373000	0.71814000
H	-2.13419800	3.60052800	1.44338000	H	-4.30214600	3.68655300	0.22180700
C	1.76510600	1.07640100	0.05659300	C	2.32941600	-3.82102400	1.61833800
O	1.81422700	2.10758100	-0.59848600	H	1.47745800	-3.88159600	2.30264400
N	2.84678200	0.31556700	0.38191200	H	2.82046900	-4.79868500	1.58871200
H	2.63393500	-0.55275400	0.86947900	H	3.03938700	-3.08816200	2.01957900
C	4.19772200	0.53912400	0.06357300	C	3.06509700	-3.27818100	-0.72828400
C	4.63809200	1.53970500	-0.81221400	H	3.75607300	-2.50676100	-0.36896900
C	5.13719200	-0.30583800	0.67315200	H	3.60943800	-4.22610900	-0.78540100
C	6.00270100	1.67579100	-1.06389900	H	2.74036900	-3.00326300	-1.73689600

C	-1.71939100	4.42984600	-0.49949700	H	2.85103100	3.01285200	1.50320500
H	-2.37031700	5.30005600	-0.37002100	C	5.58618800	2.88369300	-1.24117900
H	-0.69191400	4.72276400	-0.25972600	H	4.19790200	1.66068500	-2.34575800
H	-1.75243800	4.12396000	-1.55118600	C	5.81999300	3.59663100	-0.06500100

Int-12^{Cy}

C	0.93761400	-1.47935800	1.05436300	H	4.99764500	4.19038300	1.83207900
C	-0.28703900	-0.70711000	0.58419500	H	6.34560900	2.84076700	-2.01602800
H	-0.72458600	-0.18530200	1.43803000	H	6.76209000	4.11397200	0.08522100
C	0.80177300	-2.15492300	2.39519900	O	0.51604300	-0.24154100	-1.67789600
H	-0.25390700	-2.32273100	2.62649600	C	3.18536100	-2.17548200	0.64631600
H	1.32671800	-3.11160400	2.43027800	C	3.28829500	-3.48988900	-0.13418900
H	1.21237100	-1.50533000	3.17777600	C	4.35632100	-1.24910000	0.30319200
N	1.94874800	-1.50048400	0.28360900	H	3.22724200	-2.40091000	1.72184400
H	1.16995400	-0.91628800	-1.38025400	C	4.63137500	-4.17820200	0.11834200
C	-1.27658600	-1.74511900	0.03197100	H	3.18163800	-3.26239000	-1.20420300
O	-0.87935200	-2.73311300	-0.56849000	H	2.45244600	-4.14383600	0.14237000
N	-2.58453800	-1.48742000	0.31211100	C	5.69962100	-1.93532300	0.55621100
H	-2.76573000	-0.59253100	0.76149400	H	4.27259900	-0.97060100	-0.75754900
C	-3.71009900	-2.26951700	-0.00630100	H	4.27204300	-0.32321400	0.88625800
C	-3.67782500	-3.35109300	-0.89580600	C	5.79987900	-3.24960400	-0.22157100
C	-4.92063300	-1.91974300	0.60998500	H	4.69238400	-5.10152400	-0.46806900
C	-4.85009600	-4.06014500	-1.15397700	H	4.69615400	-4.46655200	1.17659600
H	-2.75001200	-3.62830200	-1.37509000	H	6.51903500	-1.26230500	0.28064800
C	-6.08112600	-2.63330100	0.33722000	H	5.80404600	-2.14276600	1.63018500
H	-4.93991000	-1.08674700	1.30803600	H	6.75321700	-3.74592300	-0.00859900
C	-6.05382300	-3.71165600	-0.54710700	H	5.78416500	-3.03182100	-1.29859400
H	-4.81409700	-4.89662400	-1.84584100	C	-3.11897100	2.33632200	-0.23478700
H	-7.00863800	-2.34684000	0.82372700	C	-4.44012500	1.68830900	0.18349000
H	-6.95895500	-4.27180100	-0.75883500	C	-2.86225500	3.60877900	0.58247100
C	-1.06800400	1.30706200	-0.81484200	H	-3.19289500	2.61384300	-1.29633400
C	0.08476000	0.35379600	-0.47692600	C	-5.60698200	2.66842600	0.04971200
C	-0.90510400	2.10565700	-2.08833400	H	-4.34617700	1.36265400	1.22997600
H	-1.60912100	1.74812600	-2.84801300	H	-4.61403400	0.78961000	-0.42122800
H	-1.11142900	3.16434200	-1.91006300	C	-4.02671100	4.59255000	0.45086200
H	0.10174100	2.00470700	-2.49362100	H	-2.73362300	3.31957800	1.63465100
N	-2.03246100	1.39334400	0.00695300	H	-1.92223000	4.06954100	0.25571000
C	1.19051300	1.25396400	0.15166300	C	-5.34995600	3.94133000	0.85986500
O	1.08730700	1.65499500	1.30107200	H	-6.53675200	2.18806200	0.37364200
N	2.20080400	1.55284100	-0.70487600	H	-5.73656800	2.93397600	-1.00860200
H	2.14843800	1.08071000	-1.60280000	H	-3.83271900	5.48175000	1.06068500
C	3.38739900	2.25992300	-0.44263700	H	-4.09790200	4.92934600	-0.59256600
C	3.61357800	2.97740300	0.73816800	H	-6.17687000	4.64839400	0.73029800
C	4.38095700	2.21970800	-1.43118400	H	-5.30955900	3.68553800	1.92781900
C	4.82960500	3.63707800	0.91277800				

Int-12^{tBu}

C	-0.47954000	1.82831800	0.97352400

C	0.45292500	0.66692400	0.63700600	H	-6.20477200	-2.15179600	1.80733400
H	0.66859500	0.10642700	1.54906800	H	-6.80599700	-1.01790700	-2.29126500
C	-0.23752300	2.41892000	2.33826300	H	-7.73250500	-1.82865700	-0.12479700
H	0.83561100	2.39976500	2.55570300	O	-0.35917600	0.28897200	-1.63192300
H	-0.59962300	3.43901800	2.44772200	C	-3.26247300	2.99210400	-1.03258400
H	-0.72978300	1.78534100	3.08661700	H	-2.67279400	3.07028800	-1.95261400
N	-1.33173200	2.14448000	0.08489500	H	-3.73082700	2.00103800	-1.00761900
H	-0.76622800	1.16371300	-1.41215500	H	-4.05376800	3.74815400	-1.05998400
C	-2.36467800	3.18941000	0.19460100	C	2.70448800	-3.23331400	1.91424500
C	1.74878300	1.25847900	0.06479100	H	1.94595900	-3.17503200	2.70199900
O	1.74910200	2.31390200	-0.55099400	H	3.31001900	-4.13081200	2.07645600
N	2.86495700	0.51865200	0.32406800	H	3.35435900	-2.35521100	2.00270900
H	2.70578800	-0.35230400	0.82646200	C	3.13813500	-3.32035100	-0.53247400
C	4.19217300	0.78341400	-0.05950500	H	3.74396400	-2.40724500	-0.49199000
C	4.56088000	1.82037000	-0.92652500	H	3.79676900	-4.17332700	-0.33708500
C	5.18343200	-0.05935600	0.46478900	H	2.74466400	-3.42406200	-1.54604700
C	5.90495900	1.99374400	-1.25393500	C	-1.72172400	4.57799100	0.11905400
H	3.80621500	2.47653700	-1.33489000	H	-2.50187900	5.34433100	0.06122900
C	6.51783000	0.12434100	0.12462200	H	-1.09895700	4.79324600	0.99118900
H	4.89749400	-0.85687800	1.14569400	H	-1.09616800	4.65427300	-0.77671100
C	6.88943700	1.15495100	-0.73849400	C	1.11462800	-4.49037500	0.48254000
H	6.17858500	2.80069500	-1.92741400	H	0.31963500	-4.38835600	1.22917500
H	7.26903600	-0.54014500	0.54069900	H	0.64916300	-4.63652000	-0.49450200
H	7.93163600	1.30142200	-1.00334100	H	1.69059900	-5.39145500	0.71837200
C	0.57924700	-1.62830400	-0.54413500	C	-3.22423400	3.02266600	1.45338500
C	-0.20259100	-0.30924600	-0.36759600	H	-3.56996300	1.98566300	1.53781900
C	0.35320800	-2.27974300	-1.88596200	H	-2.69211400	3.28610300	2.36979900
H	0.82182800	-1.66413100	-2.66024500	H	-4.10486500	3.66965400	1.38132100
H	0.75058200	-3.28833700	-1.94674400	**Int-13**			
H	-0.71862800	-2.30729000	-2.10834700	C	-0.26323500	-1.95254800	1.22561500
N	1.26757900	-2.00963400	0.45106100	C	-1.00081600	-0.89477500	0.75974900
C	2.03744900	-3.26643200	0.53390900	C	-0.84789200	-3.30554300	1.55445800
C	-1.57609200	-0.72033900	0.24070400	H	-0.41103600	-3.68464600	2.48177700
O	-1.68396600	-0.97783100	1.43000100	H	-0.63301500	-4.03033700	0.76053700
N	-2.57553400	-0.78260100	-0.67685100	H	-1.92729800	-3.25648100	1.68566500
H	-2.31537300	-0.47487800	-1.60982300	N	1.06762900	-1.81312400	1.48697800
C	-3.93495400	-1.07539400	-0.46957700	C	2.05815000	-2.86943400	1.64381600
C	-4.44960600	-1.53225100	0.75006900	C	3.13492800	-2.75146700	0.58478800
C	-4.79617600	-0.89411400	-1.56104000	C	2.92105900	-3.25959800	-0.70161400
C	-5.81410900	-1.79746300	0.85795400	C	4.33460900	-2.09545900	0.86391800
H	-3.79066700	-1.67467200	1.59461200	C	3.89260700	-3.11621800	-1.68916500
C	-6.15311900	-1.16417300	-1.43616200	H	1.98865800	-3.77481500	-0.92431200
H	-4.38976300	-0.54016400	-2.50524800	C	5.30986300	-1.94779400	-0.12369600
C	-6.67249100	-1.61796400	-0.22347500	C	5.09046700	-2.45715400	-1.40131800

H	3.71898700	-3.52048300	-2.68216600	N	-1.45084800	2.60074600	0.45919900
H	6.23557100	-1.42662100	0.10554800	H	-0.95822200	2.64068300	1.34649200
H	5.84785800	-2.34315900	-2.17127200	C	-2.24606600	3.70923500	0.12464600
H	4.50641500	-1.69725800	1.86145400	C	-3.01379700	3.78786200	-1.04410700
H	2.51265200	-2.80493200	2.63916400	C	-2.24727400	4.78324500	1.02573600
H	1.56518900	-3.83881000	1.56355300	C	-3.76678700	4.93489000	-1.29088700
C	-2.48451300	-0.91371700	0.67653400	H	-3.01927000	2.96277600	-1.74185800
O	-3.16993200	-0.02831600	1.17975600	C	-3.00260600	5.91912300	0.76410200
N	-3.02205600	-1.95398700	-0.04146800	H	-1.65026600	4.71694000	1.93170600
H	-2.35654300	-2.57424700	-0.48816900	C	-3.76906000	6.00360500	-0.39848600
C	-4.37101600	-2.31136900	-0.19811000	H	-4.35968100	4.98606400	-2.19942000
C	-5.44389900	-1.52824300	0.24906500	H	-2.99097100	6.74116100	1.47348400
C	-4.63204500	-3.52662000	-0.84926100	H	-4.35969500	6.89061800	-0.60388800
C	-6.74885200	-1.97398200	0.04353300	O	0.22225000	1.00700900	1.64649400
H	-5.25169100	-0.58788000	0.74473900	H	1.09215100	1.37213600	1.36274600
C	-5.93833800	-3.95306300	-1.05046700	H	1.45382300	-0.87855000	1.44762300
H	-3.79792400	-4.13309500	-1.19384800	**Int-13^{Me}**			
C	-7.00950000	-3.17911400	-0.60316600	C	-1.54218100	2.29615400	-0.84886100
H	-7.57218100	-1.35892000	0.39528800	C	-0.75956200	1.22951000	-0.49861300
H	-6.11796600	-4.89648800	-1.55733700	C	-2.98948500	2.18660000	-1.25502500
H	-8.03088300	-3.51164000	-0.75809700	H	-3.15741200	2.73797900	-2.18480100
C	0.80212700	0.26764400	-0.57243200	H	-3.63755900	2.62934500	-0.48988400
C	-0.33076500	0.43919900	0.47435100	H	-3.29642800	1.15498300	-1.41302000
C	0.53793700	-0.51258600	-1.82481800	N	-1.03654000	3.56943700	-0.85574300
H	-0.50388500	-0.81976000	-1.89394900	C	-1.74775300	4.72146400	-1.38244600
H	1.18332800	-1.40079200	-1.83161300	H	-1.90138900	4.67224200	-2.46825600
H	0.79856800	0.08761000	-2.70354200	H	-2.71991000	4.83303000	-0.89696200
N	1.90753200	0.80950700	-0.25977600	C	-1.23145600	-0.17832500	-0.56686200
C	3.03866500	0.69081600	-1.16158400	O	-0.60720500	-1.03801500	-1.18133100
C	4.32070400	1.22699200	-0.56554100	N	-2.37679600	-0.45191300	0.14077300
C	4.47387400	1.43556400	0.80574500	H	-2.74762600	0.31061300	0.69642900
C	5.41341200	1.44935300	-1.40930100	C	-3.12405600	-1.63968800	0.18222500
C	5.69963100	1.85393900	1.32487800	C	-2.76507600	-2.81439900	-0.49300800
H	3.63226300	1.26171000	1.46960900	C	-4.29889500	-1.62020100	0.94926300
C	6.63807000	1.86541000	-0.89387400	C	-3.58495800	-3.93774000	-0.39484000
C	6.78576600	2.06810700	0.47889300	H	-1.85837700	-2.84097900	-1.07965600
H	5.80476200	2.01116900	2.39452200	C	-5.10159400	-2.74982700	1.03979900
H	7.47676500	2.03376000	-1.56306100	H	-4.57528200	-0.70814500	1.47265600
H	7.73927800	2.39331100	0.88389800	C	-4.75127600	-3.91980700	0.36535800
H	5.30187800	1.28716100	-2.47933600	H	-3.29742800	-4.84172100	-0.92405600
H	3.19429100	-0.36691600	-1.42825800	H	-6.00612900	-2.71300400	1.63950900
H	2.82181200	1.21431800	-2.10307200	H	-5.37812200	-4.80307400	0.43370600
C	-1.32551800	1.42473800	-0.20056500	C	0.89530600	2.40394500	1.02097800
O	-1.86592700	1.13858100	-1.25972200	C	0.71088900	1.43556600	-0.17810800

C	0.03410800	2.24196500	2.23725600	C	4.50286600	-1.52325800	1.11385400
H	-0.55727700	1.32905700	2.18910300	C	5.58713500	0.61984600	-0.27176300
H	-0.63873700	3.10603200	2.31182600	H	3.58601200	0.98619300	-0.98955300
H	0.65130600	2.22629300	3.14160100	C	5.86039400	-1.24808400	1.21376700
N	1.78709000	3.29256600	0.85505600	H	4.07198700	-2.36376500	1.65219500
C	2.03452200	4.25487700	1.91693400	C	6.41492300	-0.17308500	0.51863200
H	1.12133200	4.80786200	2.16922300	H	6.00355200	1.46205000	-0.81686800
H	2.38886600	3.75722400	2.82758300	H	6.48694200	-1.87959100	1.83655900
C	1.36587400	0.11301100	0.30791900	H	7.47582600	0.04264100	0.59442900
O	0.95708000	-0.45491900	1.31100000	C	-1.99127600	-0.83543100	1.14239700
N	2.43206000	-0.26416200	-0.43704500	C	-1.21252200	-0.33526900	-0.10428100
H	2.59689800	0.31195400	-1.25706700	C	-1.23244100	-1.22937200	2.37407100
C	3.25744400	-1.38910200	-0.27882500	H	-0.17946500	-0.96344300	2.29639100
C	3.14949500	-2.28757000	0.78995200	H	-1.32231000	-2.31452200	2.51279900
C	4.23964300	-1.59361100	-1.25812200	H	-1.66405100	-0.74730800	3.25740200
C	4.02205300	-3.37279700	0.85974100	N	-3.25148900	-0.88656300	0.99802300
H	2.39381900	-2.13593100	1.54749700	C	-4.08902300	-1.35364100	2.09800300
C	5.10112200	-2.67959700	-1.17302400	H	-3.72573500	-2.32786600	2.45246000
H	4.31897400	-0.89290400	-2.08529600	H	-4.00040100	-0.65692200	2.94221500
C	4.99828900	-3.57891300	-0.11147200	C	-0.76629600	1.10143100	0.28438900
H	3.93063400	-4.06504200	1.69164800	O	-0.06484300	1.29253300	1.26799700
H	5.85552000	-2.82226100	-1.94085700	N	-1.28390900	2.06213800	-0.51753700
H	5.67064000	-4.42815600	-0.04396100	H	-1.81748800	1.70862800	-1.30625000
O	1.41132300	1.96557400	-1.28715600	C	-1.09651500	3.45233100	-0.44824400
H	2.02626300	2.62921300	-0.89327400	C	-0.36761200	4.08670900	0.56554200
H	-0.02871700	3.63812700	-0.91892300	C	-1.68757800	4.22191600	-1.45998300
H	-1.15402900	5.60933300	-1.15825700	C	-0.24240300	5.47512000	0.54977700
H	2.79516500	4.96622000	1.59079400	H	0.09175700	3.49927400	1.34757300
Int-13^{Et}				C	-1.55333800	5.60436400	-1.46046500
C	-0.17747800	-2.55041700	-0.66239700	H	-2.25161600	3.72373700	-2.24410900
C	-0.00985700	-1.22019400	-0.38854900	C	-0.82830900	6.24222900	-0.45365800
C	0.95896700	-3.47730500	-1.01713600	H	0.32496900	5.95838200	1.33980800
H	0.71534900	-4.05337600	-1.91378200	H	-2.01792300	6.18400200	-2.25241100
H	1.13792800	-4.19152800	-0.20520400	H	-0.72235900	7.32232500	-0.45304900
H	1.88215000	-2.93475900	-1.20914100	O	-2.10309300	-0.30455900	-1.20267200
N	-1.41829300	-3.13167800	-0.60920300	H	-2.99965400	-0.34481600	-0.79272000
C	-1.74385400	-4.45423600	-1.13001900	H	-2.19814300	-2.48614900	-0.65451700
H	-0.93959800	-5.14729100	-0.87547600	H	-2.63416600	-4.79489000	-0.59266400
C	1.30595100	-0.53367200	-0.49187900	C	-2.01748400	-4.45875600	-2.63138800
O	1.45819900	0.46893300	-1.18274900	H	-2.28981400	-5.46379700	-2.96905200
N	2.31062100	-1.07174600	0.27454700	H	-2.84468600	-3.78149200	-2.86826900
H	2.04418800	-1.84698100	0.87097400	H	-1.13848600	-4.13061200	-3.19540100
C	3.66998500	-0.72308100	0.31695200	C	-5.53689400	-1.45917100	1.64814600
C	4.22148900	0.36077600	-0.37969900	H	-6.17212700	-1.80381000	2.46920900

H	-5.90587200	-0.48593100	1.30998000
H	-5.63036600	-2.16717100	0.81864400

Int-13^{iPr}

C	-1.11995400	-2.13694200	-0.70144400
C	-0.30562900	-1.06306500	-0.46162900
C	-0.60854100	-3.53860900	-0.92672200
H	-1.10075800	-3.99357600	-1.78957900
H	-0.82255300	-4.16763600	-0.05485900
H	0.46463000	-3.55466900	-1.10580500
N	-2.47973200	-1.98806000	-0.72802400
C	-3.45593600	-3.00931800	-1.10466400
H	-3.09109900	-3.97269700	-0.73883000
C	1.17819400	-1.13735400	-0.52089000
O	1.83213600	-0.37762000	-1.22890500
N	1.75687900	-2.06989100	0.30508900
H	1.12323000	-2.57483300	0.91453400
C	3.10987200	-2.42702100	0.41923300
C	4.14766400	-1.79743200	-0.28178300
C	3.41400100	-3.47814400	1.29766900
C	5.45998800	-2.23022200	-0.09636200
H	3.92399600	-0.98241500	-0.95443700
C	4.72731200	-3.89409700	1.47328800
H	2.60780700	-3.96470500	1.84076800
C	5.76315100	-3.27278700	0.77517700
H	6.25548200	-1.73455400	-0.64533900
H	4.93998600	-4.70912000	2.15863100
H	6.78996600	-3.59703800	0.91051800
C	-1.88468300	0.35282700	0.93759100
C	-0.90019400	0.32049000	-0.26769500
C	-1.49771200	-0.36684600	2.19936300
H	-0.43395000	-0.60099400	2.19819700
H	-2.06662100	-1.30315200	2.26159900
H	-1.73336600	0.23216000	3.08286500
N	-2.95418700	1.00169700	0.72393600
C	-3.96837100	1.15563000	1.76727300
H	-3.92487500	0.31583600	2.47301900
C	0.19851200	1.34373600	0.13382900
O	0.86527700	1.17936100	1.14626600
N	0.26688700	2.41549200	-0.69159600
H	-0.34011000	2.36133900	-1.50423000
C	1.12717300	3.52305900	-0.61435300
C	2.05852800	3.71169600	0.41450700
C	1.02314600	4.47713900	-1.63602800
C	2.86810000	4.84667900	0.40287900
H	2.14496800	2.97946100	1.20447200
C	1.83707200	5.60267100	-1.63222600
H	0.29812300	4.32487300	-2.43126200
C	2.76721700	5.79604100	-0.61064700
H	3.58834300	4.98374000	1.20417800
H	1.74236000	6.33075200	-2.43222500
H	3.40392400	6.67494300	-0.60668700
O	-1.59582600	0.75752200	-1.41936100
H	-2.39404600	1.21444800	-1.06050900
H	-2.81586000	-1.04158800	-0.87240500
C	-3.65435900	-3.07386000	-2.61982300
H	-4.38097200	-3.85020300	-2.88103200
H	-4.03224300	-2.11210200	-2.98576500
H	-2.71575200	-3.29008200	-3.13931500
C	-5.34175900	1.17831800	1.10724500
H	-6.12583500	1.29674300	1.86157000
H	-5.40721400	2.01367700	0.40152700
H	-5.52773200	0.24916200	0.55961700
C	-3.69397900	2.45711100	2.51967100
H	-2.71324500	2.43276900	3.00548000
H	-3.71245400	3.30248500	1.82325900
H	-4.45821900	2.62104700	3.28566900
C	-4.76934100	-2.68523600	-0.39888700
H	-4.62809600	-2.63286800	0.68529600
H	-5.15442700	-1.71889200	-0.74607200
H	-5.52183500	-3.44785000	-0.62011100

Int-13^{Cy}

C	-0.38287200	-1.92423600	-1.13023700
C	0.54999200	-1.00048900	-0.75777700
C	-0.09029400	-3.40036600	-1.25755200
H	-0.53602300	-3.78458000	-2.17917000
H	-0.52364400	-3.95818000	-0.41914700
H	0.97896800	-3.60441600	-1.28380500
N	-1.65200200	-1.56158600	-1.51720300
C	1.99284600	-1.34630800	-0.59271000
O	2.86865200	-0.78514500	-1.24143200
N	2.25431700	-2.29650700	0.36113800
H	1.45259000	-2.61799200	0.89225400
C	3.48360500	-2.87309200	0.71883000
C	4.70018000	-2.56875500	0.09342500
C	3.46243800	-3.80990800	1.76308000
C	5.86580700	-3.20427000	0.51919100
H	4.72656400	-1.84462800	-0.70779300
C	4.63352800	-4.43130500	2.17660400

H	2.51681800	-4.04294600	2.24642200	H	-5.12025300	-3.71376300	-2.19491100
C	5.84696500	-4.13339000	1.55589800	H	-6.58421800	-3.18289300	-0.26244600
H	6.80281600	-2.96127800	0.02641800	H	-5.89377100	-1.56189700	-0.15924400
H	4.59546100	-5.15224800	2.98778200	C	-2.99495800	1.65139400	1.00357100
H	6.76288600	-4.61864700	1.87746700	C	-2.74968100	2.99662000	1.69852800
C	-0.90231900	0.66729800	0.45071800	C	-4.30668100	1.68697300	0.21829200
C	0.18944800	0.47382200	-0.63827200	H	-3.07113700	0.87009500	1.77517400
C	-0.70884100	0.01136400	1.79096300	C	-3.92359400	3.36329300	2.60937800
H	0.28455900	-0.42698300	1.87108600	H	-2.62288400	3.76505900	0.92362900
H	-1.46037600	-0.77557700	1.92416500	H	-1.81393500	2.95037800	2.26795900
H	-0.84333000	0.74040500	2.59594500	C	-5.48277300	2.04430100	1.12845700
N	-1.89431700	1.37254300	0.08793400	H	-4.20989400	2.43495200	-0.58078000
C	1.40335000	1.30234600	-0.13026500	H	-4.47048000	0.71553500	-0.26387500
O	1.93731800	1.04462300	0.93961600	C	-5.24314100	3.38122500	1.83403200
N	1.73472700	2.32690800	-0.95122600	H	-3.74068200	4.33709900	3.07659900
H	1.19408700	2.36886800	-1.81024400	H	-3.99246600	2.62649700	3.42148900
C	2.75403200	3.28056500	-0.79386200	H	-6.40953300	2.07887300	0.54541300
C	3.60781200	3.32691700	0.31530800	H	-5.60886300	1.25432700	1.88224500
C	2.89897400	4.22622900	-1.81869700	H	-6.07576200	3.61077300	2.50821500
C	4.58776000	4.31630900	0.38154800	H	-5.20745100	4.18192600	1.08235200
H	3.50299800	2.59966000	1.10764600	**Int-13^{tBu}**			
C	3.88071600	5.20543400	-1.73662800	C	1.20453400	1.81184300	-0.81366800
H	2.23404900	4.18472000	-2.67774800	C	0.23456200	0.90599900	-0.48969400
C	4.73369800	5.25770000	-0.63389200	C	0.88506500	3.24068500	-1.17195300
H	5.24550800	4.34427600	1.24538400	H	1.32118500	3.50755800	-2.13620200
H	3.97837700	5.92989100	-2.53955500	H	1.29953700	3.92192100	-0.42113900
H	5.50096800	6.02251500	-0.56875200	H	-0.18787200	3.41029600	-1.23987100
O	-0.29122200	1.00001500	-1.85787900	N	2.53965200	1.45922600	-0.76819200
H	-1.07938900	1.53542700	-1.59967600	C	3.64646300	1.99249300	-1.60098600
H	-1.84984700	-0.56778500	-1.48254800	C	-1.21686000	1.25440300	-0.49397400
C	-2.83723600	-2.37987800	-1.26619400	O	-2.01943200	0.65949800	-1.20432100
C	-3.24851100	-2.33921900	0.21127300	N	-1.57918400	2.24767100	0.38088100
C	-3.97427800	-1.88751700	-2.16242200	H	-0.83427900	2.61523600	0.96290000
H	-2.60829800	-3.41651600	-1.53902500	C	-2.83195800	2.86110300	0.54602900
C	-4.53934100	-3.12145500	0.46101500	C	-3.99384100	2.45575500	-0.12481700
H	-3.39361300	-1.28432300	0.49337100	C	-2.89618600	3.93876200	1.44207000
H	-2.42766400	-2.72870500	0.82715900	C	-5.18976100	3.13364200	0.10773500
C	-5.26763300	-2.66394100	-1.90591500	H	-3.95493600	1.62260800	-0.81134100
H	-4.14154500	-0.81981300	-1.95526900	C	-4.09679700	4.60015800	1.66505300
H	-3.67006300	-1.96900000	-3.21182100	H	-1.99355000	4.25173200	1.96081500
C	-5.66952500	-2.60371300	-0.43071800	C	-5.25521200	4.20329500	0.99649500
H	-4.82045900	-3.05509600	1.51775700	H	-6.08361200	2.81127400	-0.41853400
H	-4.36553300	-4.18429600	0.24215100	H	-4.12445500	5.43157500	2.36304400
H	-6.06944100	-2.26883800	-2.53902600	H	-6.19394400	4.72006400	1.16839200

C	1.48199000	-0.67765700	1.05465100
C	0.57747700	-0.55258800	-0.21484700
C	1.09053200	0.15460000	2.24529400
H	0.03545200	0.42117800	2.18407300
H	1.68538000	1.07576700	2.24310200
H	1.27439500	-0.36988400	3.18427200
N	2.47233300	-1.45128900	0.88982000
C	3.51873600	-1.76621800	1.87937000
C	-0.69599500	-1.37813300	0.12646800
O	-1.37632800	-1.11764300	1.10923500
N	-0.90826500	-2.40732800	-0.72756200
H	-0.25470300	-2.44918300	-1.50396100
C	-1.95092700	-3.34862500	-0.72377600
C	-2.92047000	-3.43053800	0.28345800
C	-1.99252000	-4.24810700	-1.79856700
C	-3.91372300	-4.40527900	0.19674400
H	-2.89443300	-2.74075500	1.11496800
C	-2.98898700	-5.21282300	-1.86959000
H	-1.23652900	-4.18013000	-2.57701800
C	-3.95877000	-5.29855700	-0.87032100
H	-4.66179200	-4.46120600	0.98220000
H	-3.00601700	-5.89990000	-2.71024400
H	-4.73825500	-6.05177700	-0.92458800
O	1.25839100	-1.13272300	-1.30658400
H	1.97396000	-1.66592400	-0.87715600
H	2.65623800	0.45565800	-0.69117300
C	3.35201200	1.82857300	-3.09702100
H	4.21823600	2.14417300	-3.68861300
H	3.14243100	0.77754700	-3.32450300
H	2.49243300	2.42501400	-3.41576700
C	4.64075400	-2.44206400	1.08494600
H	5.43901000	-2.77590300	1.75535700
H	4.25333400	-3.30932500	0.54053800
H	5.06918800	-1.74224600	0.35836900
C	2.95670900	-2.75833900	2.90206600
H	2.14211800	-2.31835100	3.48488500
H	2.57755900	-3.65280300	2.39707500
H	3.74864500	-3.06193000	3.59475400
C	4.85041400	1.11341700	-1.24117600
H	5.11038700	1.22620300	-0.18310500
H	4.63179900	0.05617000	-1.43766500
H	5.71758200	1.39835600	-1.84377400
C	3.99801100	3.44281000	-1.25390800
H	3.28109700	4.16427500	-1.64970900
H	4.06021900	3.56819600	-0.16785500
H	4.97604700	3.68329700	-1.68375200
C	4.08827900	-0.51797200	2.56589000
H	5.04236300	-0.77178600	3.03945400
H	4.27328900	0.27121600	1.82786400
H	3.42851500	-0.12305100	3.34081700

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C	1.39688200	-2.36903200	-0.61087700
C	1.65621800	-1.05740200	-0.68180800
C	2.31832100	-3.54717800	-0.61230100
H	2.03439500	-4.24852700	-1.40467100
H	2.27721900	-4.08849300	0.33968800
H	3.34787000	-3.23132300	-0.78718700
N	-0.03494400	-2.59734600	-0.57065600
C	-0.51304900	-3.85855100	0.02243800
C	-2.02160600	-3.94324300	0.00298900
C	-2.73787100	-4.08456700	1.19202600
C	-2.71640300	-3.91767100	-1.21137700
C	-4.12855700	-4.20053700	1.17278900
H	-2.20288600	-4.11120600	2.13827400
C	-4.10410100	-4.02379700	-1.23272700
C	-4.81407300	-4.16793900	-0.03865800
H	-4.67276400	-4.31500900	2.10538900
H	-4.63234200	-4.00376400	-2.18116700
H	-5.89601000	-4.25734100	-0.05635900
H	-2.16729000	-3.82410200	-2.14609700
H	-0.08511800	-4.70107100	-0.53342900
H	-0.14075200	-3.90829400	1.04937100
C	2.99073000	-0.40494400	-0.76931100
O	3.20440500	0.50166000	-1.56283600
N	3.91391600	-0.87335600	0.12772600
H	3.57538100	-1.54635400	0.80693600
C	5.24735400	-0.46518000	0.30591800
C	5.89106300	0.47599900	-0.50800900
C	5.95260400	-1.06043000	1.36188100
C	7.22137700	0.80478000	-0.25077900
H	5.35591700	0.94112900	-1.32292100
C	7.27703200	-0.72068000	1.60443900
H	5.45041200	-1.79242100	1.98904100
C	7.92287600	0.21686000	0.79821200
H	7.71080400	1.53601700	-0.88749000
H	7.80506600	-1.19251700	2.42755200
H	8.95782600	0.48369600	0.98643300
C	-0.63916900	-0.96114100	0.13724300

C	0.38595500	-0.21663800	-0.81344000
C	-0.38753100	-1.14079700	1.60834800
H	0.66097500	-1.37496000	1.79614100
H	-1.01330600	-1.93712700	2.02213400
H	-0.62741700	-0.20812800	2.12675000
N	-1.88302500	-0.69480700	-0.27405700
C	-3.12418900	-0.74003900	0.46750500
C	-3.73830800	0.64256500	0.59479000
C	-2.94170100	1.74574600	0.91972500
C	-5.10575200	0.83222300	0.39208400
C	-3.50184500	3.01568700	1.03260000
H	-1.87368800	1.61041500	1.07818200
C	-5.67164500	2.10166400	0.51256100
C	-4.87062200	3.19688100	0.82885500
H	-2.86739900	3.86485000	1.27564500
H	-6.73671300	2.23528100	0.34737300
H	-5.30790400	4.18727100	0.91217400
H	-5.72968900	-0.01911100	0.13031200
H	-3.83184300	-1.41698600	-0.02629800
H	-2.92823200	-1.15455700	1.46030900
C	0.58590800	1.17787600	-0.16260000
O	1.16831800	1.34317300	0.90524500
N	-0.02398000	2.12817400	-0.91054200
H	-0.39917600	1.70395800	-1.76789800
C	-0.31468800	3.45698200	-0.59261700
C	0.13320200	4.07624700	0.58256500
C	-1.12500800	4.17411400	-1.48516700
C	-0.23963700	5.39345700	0.84791500
H	0.76106900	3.52609100	1.27038000
C	-1.48592400	5.48633500	-1.20683200
H	-1.47370200	3.68574400	-2.39139000
C	-1.04762700	6.10622400	-0.03555400
H	0.11197700	5.86500300	1.76116400
H	-2.11586500	6.02573200	-1.90796700
H	-1.33021800	7.13119400	0.18241300
O	-0.12633800	-0.16258000	-2.05237500
H	-1.87530500	-0.36004300	-1.24468700
H	-0.41742700	-2.44496500	-1.51262400

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C	-1.01393700	2.56325600	-0.60217600
C	-0.60617200	1.28694700	-0.55487300
C	-2.38156600	3.14515500	-0.77932000
H	-2.37348200	3.88274900	-1.58926600
H	-2.71445100	3.65842000	0.13033200
H	-3.10926800	2.37071700	-1.02561800
N	0.10672000	3.45955300	-0.48841100
C	-0.11570700	4.81886800	-0.00330000
C	-1.44635200	0.06902300	-0.70530300
O	-1.08333600	-0.86911600	-1.40283200
N	-2.60986900	0.07417100	0.01964400
H	-2.73351300	0.84858200	0.66279200
C	-3.60254200	-0.91923300	0.08188000
C	-3.61874600	-2.05654000	-0.73649100
C	-4.63365000	-0.72643200	1.01275700
C	-4.65798100	-2.97680800	-0.60755000
H	-2.82873000	-2.21502700	-1.45584200
C	-5.66120800	-1.65363300	1.12847700
H	-4.61966200	0.15852200	1.64385500
C	-5.68101500	-2.78876000	0.31779800
H	-4.66016400	-3.85484800	-1.24689700
H	-6.44945600	-1.48611000	1.85623000
H	-6.48288800	-3.51451800	0.40760500
C	1.37252300	2.30669200	0.46602200
C	0.92210400	1.14338600	-0.49477000
C	0.88733800	2.45887000	1.87598000
H	-0.17298100	2.21654200	1.95405000
H	1.05790000	3.47621800	2.24101800
H	1.44531400	1.76459300	2.51182100
N	2.61429300	2.67915700	0.18366200
C	3.42725800	3.61342700	0.93727300
C	1.27135500	-0.18163600	0.24257500
O	0.72641500	-0.52868600	1.28623700
N	2.24110000	-0.84160000	-0.43005600
H	2.45858700	-0.33534100	-1.29837700
C	2.84654900	-2.06826500	-0.14877600
C	2.55604800	-2.81772200	0.99981500
C	3.78882400	-2.55277200	-1.06773200
C	3.20670600	-4.03220600	1.20884100
H	1.82872800	-2.44615600	1.70891700
C	4.42861500	-3.76560400	-0.84442100
H	4.01045900	-1.96691400	-1.95593200
C	4.14205000	-4.51570000	0.29675900
H	2.97377400	-4.60590000	2.10140000
H	5.15476600	-4.12589600	-1.56713800
H	4.64154900	-5.46338500	0.47103600
O	1.54836900	1.28148600	-1.67428700
H	2.87417100	2.38348300	-0.76346700
H	0.64265900	3.43849800	-1.36218900

H	3.52328200	3.29163500	1.97816700
H	0.85574400	5.30939300	0.08693200
H	-0.59106400	4.78158200	0.97952100
H	3.01191300	4.62696500	0.91883000
H	4.42176800	3.63693600	0.49030100
H	-0.74520900	5.39895400	-0.68569000

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C	-0.65326600	2.51836200	-0.56906900
C	-0.55452000	1.18173600	-0.58967500
C	-1.85720800	3.39739600	-0.69817800
H	-1.78945300	3.99706700	-1.61225200
H	-1.93947100	4.08852800	0.14773100
H	-2.77087200	2.80339700	-0.74901100
N	0.65618400	3.11128500	-0.44970900
C	0.85078100	4.44697200	0.12478700
C	-1.65982200	0.19875700	-0.75929600
O	-1.57708800	-0.71852800	-1.56516200
N	-2.72446200	0.38432200	0.08282300
H	-2.61318700	1.10526600	0.78739600
C	-3.89766300	-0.38217900	0.19168000
C	-4.23839300	-1.41283500	-0.69409800
C	-4.76533100	-0.06606500	1.24745100
C	-5.43250800	-2.10771700	-0.50745100
H	-3.57609000	-1.66419300	-1.50966400
C	-5.95114100	-0.76860000	1.41861700
H	-4.49923000	0.73551700	1.93189500
C	-6.29412700	-1.79749000	0.54119100
H	-5.68631700	-2.90539800	-1.19945100
H	-6.60856700	-0.50931100	2.24299800
H	-7.21999400	-2.34772000	0.67451900
C	1.61072000	1.68460600	0.42049800
C	0.89782500	0.68323100	-0.56844000
C	1.18020000	1.85347500	1.84914800
H	0.09279800	1.84252100	1.93069000
H	1.56443400	2.78443800	2.27544800
H	1.57431300	1.01706300	2.43351600
N	2.90362600	1.78138100	0.12058500
C	3.98946700	2.31976500	0.92416500
C	0.93946600	-0.71177000	0.11760200
O	0.31258300	-0.97270300	1.14031900
N	1.75564200	-1.54156100	-0.57139700
H	2.08620300	-1.06815100	-1.42193800
C	2.08994800	-2.87536900	-0.32451800
C	1.64058800	-3.57953200	0.80116000
C	2.92038500	-3.51849100	-1.25396200
C	2.02675600	-4.90678300	0.97852200
H	0.99806300	-3.08602000	1.51778600
C	3.29596400	-4.84222600	-1.06239800
H	3.26521400	-2.96752300	-2.12514000
C	2.85177900	-5.54727800	0.05673100
H	1.67331200	-5.44402200	1.85398400
H	3.93922500	-5.32446000	-1.79251200
H	3.14502700	-6.58145500	0.20646800
O	1.52610200	0.71601700	-1.75387200
H	3.07885900	1.42094200	-0.82486500
H	1.15968500	2.99788500	-1.33734000
C	0.68408600	5.58443900	-0.87404800
H	-0.34428800	5.66894400	-1.23293600
H	0.95877700	6.53137400	-0.39992300
H	1.34160500	5.43213200	-1.73625100
C	4.78103000	1.21434900	1.61478400
H	4.13878300	0.65003300	2.29831100
H	5.19079400	0.51817900	0.87607300
H	5.61171800	1.63802100	2.18756500
H	3.58002600	3.01506800	1.66084900
H	1.87445000	4.45462600	0.51961700
H	0.17123200	4.55250500	0.97476900
H	4.64315500	2.89794300	0.26404500

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C	0.25996000	-2.32161100	-0.54257900
C	0.50044800	-1.00182400	-0.52977400
C	1.23205700	-3.45300400	-0.71217500
H	0.79146500	-4.26041200	-1.30220900
H	1.54611100	-3.87276500	0.24943000
H	2.12509900	-3.09844000	-1.23213800
N	-1.17056900	-2.54536300	-0.46985100
C	-1.81926900	-3.79912400	-0.01084100
C	1.81949100	-0.33224300	-0.68050100
O	1.94850500	0.66694800	-1.37568500
N	2.83727300	-0.90032700	0.03963700
H	2.57868300	-1.66269100	0.65606000
C	4.18591400	-0.51057600	0.10947100
C	4.73377400	0.54220700	-0.63519900
C	5.00955300	-1.24245100	0.97733400
C	6.08839100	0.84268500	-0.49869000
H	4.10685800	1.11306700	-1.30441300
C	6.35675100	-0.92917600	1.10142400
H	4.58084500	-2.05939300	1.55227000

C	6.90766700	0.11824100	0.36274400	H	-6.17267900	-2.00335500	0.28669000
H	6.50272800	1.66107400	-1.08026600	H	-5.45699500	-1.14306300	-1.08924700
H	6.97726300	-1.50779800	1.77906000	H	-2.76301000	-3.44847800	0.42992700
H	7.96021500	0.36459100	0.45879300	H	-4.02859300	-1.72380600	1.55301000
C	-1.75979500	-0.99371700	0.37100400	**TS-14^{Cy}**			
C	-0.78010700	-0.15768200	-0.54093000	C	0.63408500	-2.09489500	-0.80175600
C	-1.46454400	-1.24013000	1.82478700	C	1.19118600	-0.88238700	-0.71248300
H	-0.40533600	-1.45011000	1.97716200	C	1.25987300	-3.42746500	-1.06897800
H	-2.05919100	-2.06865000	2.22014000	H	0.86051200	-3.84608900	-1.99994800
H	-1.71752600	-0.33659900	2.38672900	H	1.07280400	-4.15345200	-0.27243000
N	-3.02920900	-0.75708600	0.01281600	H	2.33886400	-3.31583900	-1.18739000
C	-4.26976600	-1.05880100	0.71858800	N	-0.82426800	-1.96053300	-0.80181100
C	-0.51580700	1.18775100	0.18660700	C	2.64079200	-0.55092700	-0.74356500
O	0.10655900	1.26820400	1.24139400	O	3.06820300	0.37054500	-1.42505000
N	-1.07927000	2.20586000	-0.50448200	N	3.41692600	-1.33074900	0.07206800
H	-1.47202700	1.84765000	-1.38393000	H	2.92053400	-1.99007400	0.66163200
C	-1.09029300	3.57479900	-0.22765200	C	4.80682400	-1.27685100	0.27525700
C	-0.52994300	4.12413300	0.93408000	C	5.66259300	-0.41215500	-0.41931300
C	-1.70135500	4.42117300	-1.16445900	C	5.34023000	-2.15808300	1.22737300
C	-0.58854500	5.50141700	1.13849200	C	7.03007500	-0.44244300	-0.14916400
H	-0.05705400	3.47337000	1.65705600	H	5.26017900	0.27071400	-1.15333900
C	-1.75102800	5.79219900	-0.94572300	C	6.70486000	-2.17417500	1.48432300
H	-2.13506100	3.98963800	-2.06268300	H	4.67303500	-2.82982600	1.76226600
C	-1.19430000	6.34366500	0.20878600	C	7.56187500	-1.31440500	0.79685600
H	-0.15106700	5.91739800	2.04157700	H	7.68484600	0.23239800	-0.69276300
H	-2.22752800	6.43227600	-1.68240400	H	7.09857300	-2.86299500	2.22562200
H	-1.23289500	7.41472100	0.37989100	H	8.62843800	-1.32569600	0.99697800
O	-1.33080800	-0.01342900	-1.75777300	C	-1.07694000	-0.40454400	0.01212500
H	-3.06757900	-0.35524800	-0.93132000	C	0.14005300	0.22703600	-0.78938600
H	-1.56413700	-2.26237200	-1.37785500	C	-0.93188900	-0.65179200	1.49275400
C	-1.03443300	-4.53825800	1.06901500	H	-0.11371800	-1.34492700	1.69805800
H	-0.26461500	-5.18189800	0.63666300	H	-1.85197300	-1.04137800	1.93110300
H	-0.56093100	-3.85334100	1.77819500	H	-0.69288400	0.29702900	1.97769300
H	-1.72656300	-5.17623200	1.62586200	N	-2.23304600	0.16258200	-0.42587500
C	-2.16550300	-4.70179100	-1.19022900	C	0.62791800	1.47633100	-0.01183300
H	-1.26202900	-5.07045000	-1.68627900	O	1.23348700	1.41550200	1.05427100
H	-2.73826400	-5.56454800	-0.83610600	N	0.27207200	2.60043200	-0.67757200
H	-2.77285800	-4.16554600	-1.92709100	H	-0.14043100	2.34826600	-1.58399700
C	-4.88445600	0.22803100	1.26748000	C	0.48147800	3.94141700	-0.34596600
H	-4.19030000	0.72908800	1.94940600	C	1.10845100	4.34784900	0.83998300
H	-5.11380000	0.91510200	0.44472500	C	0.02666400	4.91004100	-1.25273600
H	-5.81270300	0.01523800	1.80738800	C	1.27013400	5.70789200	1.09795700
C	-5.23157100	-1.77737300	-0.22381200	H	1.46145100	3.60240500	1.53958200
H	-4.79787800	-2.71463200	-0.58789600	C	0.19618200	6.26174100	-0.98064300

H	-0.45990300	4.58820300	-2.16979800	C	0.72031100	-1.02420800	-0.65552400
C	0.81992700	6.67152200	0.19835900	C	1.37965900	-3.45184700	-0.96398000
H	1.75807200	6.01307800	2.01924000	H	1.18956900	-3.86686100	-1.95872300
H	-0.16186100	6.99784200	-1.69431500	H	1.32692700	-4.26888500	-0.24228600
H	0.95249900	7.72746000	0.41129800	H	2.39865100	-3.06093400	-0.96148200
O	-0.26048000	0.50233800	-2.04172500	N	-1.03090100	-2.50333700	-0.57291800
H	-2.07899700	0.63515800	-1.32195700	C	-1.63622000	-3.85518200	-0.26314500
H	-1.07134400	-1.60287600	-1.73847900	C	2.05861400	-0.38272200	-0.78382200
C	-3.44990400	0.44187400	0.31748900	O	2.24918200	0.52336900	-1.58335900
C	-3.34592500	1.74623100	1.12143500	N	3.00302200	-0.84851200	0.09037800
C	-4.62580400	0.51602200	-0.66027900	H	2.68398400	-1.53167700	0.76923700
H	-3.63776100	-0.38657600	1.01387000	C	4.33725800	-0.43119200	0.24089700
C	-4.65468900	2.06413300	1.84807300	C	4.95725600	0.51294200	-0.58789600
H	-3.10252000	2.55655400	0.41857500	C	5.06791400	-1.01879000	1.28360800
H	-2.51511300	1.67819000	1.83292400	C	6.28980300	0.85259600	-0.35810700
C	-5.93666900	0.83576000	0.06125700	H	4.40253300	0.97201600	-1.39305400
H	-4.41062300	1.30407400	-1.39708000	C	6.39436800	-0.66845300	1.49866900
H	-4.70446700	-0.42855000	-1.21053600	H	4.58338700	-1.75240300	1.92265300
C	-5.82592700	2.13224900	0.86625600	C	7.01665400	0.27225800	0.67772200
H	-4.55912100	3.00648300	2.39859300	H	6.76078400	1.58601500	-1.00610600
H	-4.85317500	1.27920000	2.59144500	H	6.94243600	-1.13435400	2.31200300
H	-6.75423600	0.90347100	-0.66478800	H	8.05310300	0.54739400	0.84453600
H	-6.18197000	0.00876700	0.74215800	C	-1.51192800	-0.98526600	0.27779500
H	-6.76188700	2.32821900	1.40126600	C	-0.53493500	-0.16194500	-0.66329800
H	-5.66782400	2.97223000	0.17562000	C	-1.14183500	-1.18703000	1.72220000
C	-1.63682300	-3.18328300	-0.54748200	H	-0.11391500	-1.54344400	1.80844900
C	-1.51200100	-3.75145400	0.86631800	H	-1.81111500	-1.89409900	2.20945500
C	-3.10591200	-2.93891900	-0.88902800	H	-1.20603100	-0.22670100	2.23959300
H	-1.25679200	-3.93753400	-1.25036800	N	-2.81083600	-0.69085000	-0.04700800
C	-2.24138300	-5.09812200	0.92117300	C	-3.88924200	-0.09169800	0.77354400
H	-1.98501400	-3.06979300	1.57940200	C	-0.24877600	1.19839600	0.02007900
H	-0.46429500	-3.86283200	1.16381700	O	0.38160800	1.30365100	1.06890600
C	-3.86964900	-4.26552700	-0.82645200	N	-0.79014800	2.20501200	-0.70329100
H	-3.53520400	-2.23310200	-0.16750400	H	-1.21278000	1.82784500	-1.56027200
H	-3.19213600	-2.48764200	-1.88495400	C	-0.86184600	3.57020400	-0.41811400
C	-3.71594900	-4.93144000	0.54368800	C	-0.29143200	4.14377000	0.72688100
H	-2.15123600	-5.52494400	1.92535500	C	-1.55406500	4.38499400	-1.32629400
H	-1.76025400	-5.80072300	0.22707800	C	-0.42033600	5.51468200	0.94277900
H	-4.92750100	-4.09292000	-1.05048000	H	0.24323400	3.51728800	1.42787300
H	-3.48150400	-4.93813600	-1.60318600	C	-1.67183400	5.75003800	-1.09679100
H	-4.22197500	-5.90293100	0.54998100	H	-1.99652300	3.93329300	-2.21034400
H	-4.20799000	-4.30749600	1.30243300	C	-1.10512100	6.32593600	0.04092600

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C	0.42733800	-2.32905700	-0.67917000	H	0.02553800	5.95034600	1.83235200
				H	-2.21041700	6.36583200	-1.81100100

H	-1.19717100	7.39230600	0.22066000
O	-1.10115100	-0.04235500	-1.87776600
H	-2.77297400	-0.26785400	-0.98621600
H	-1.41068100	-2.19316700	-1.48292000
C	-3.15685800	-3.69090400	-0.22448300
H	-3.47135700	-3.02954700	0.58069000
H	-3.53855900	-3.29526700	-1.17222000
H	-3.59859200	-4.67817500	-0.05825500
C	-1.31378500	-4.83810600	-1.40134000
H	-1.43281500	-4.35775500	-2.37896600
H	-0.31233800	-5.26122700	-1.33213900
H	-2.02383500	-5.66882100	-1.34539800
C	-1.14940200	-4.39808700	1.08216400
H	-1.66638900	-3.92413300	1.91886600
H	-1.36960400	-5.46952300	1.12133500
H	-0.07402000	-4.27197800	1.22797600
C	-3.58735100	1.39312700	1.02185600
H	-2.64926800	1.51299500	1.57742300
H	-3.49413600	1.93083700	0.07150900
H	-4.39260900	1.85639300	1.60326800
C	-5.15097600	-0.21683700	-0.08725500
H	-5.41743200	-1.27008000	-0.22794100
H	-5.99121800	0.29512700	0.39202300
H	-4.99286100	0.23461600	-1.07336900
C	-4.15038400	-0.77908600	2.11721900
H	-4.23241800	-1.86532300	2.02016900
H	-3.38752600	-0.54672600	2.86252600
H	-5.10571100	-0.40809400	2.50299000

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C	-1.37870900	-2.32955600	0.61402700
C	-1.66493100	-1.02789200	0.67769500
C	-2.24308000	-3.54426200	0.68076900
H	-1.92208800	-4.19698900	1.50045600
H	-2.19911100	-4.12476300	-0.24710300
H	-3.27976600	-3.25524300	0.86124400
N	0.08597900	-2.49579300	0.54929200
C	0.56809800	-3.75916600	-0.06944600
C	2.07221100	-3.88650600	-0.04686700
C	2.78199600	-4.03226700	-1.23841200
C	2.76377500	-3.91848500	1.16897000
C	4.16686900	-4.20583500	-1.22074500
H	2.24732100	-4.01615300	-2.18507400
C	4.14541600	-4.08026800	1.18846200
C	4.85068200	-4.22698500	-0.00859400
H	4.70716500	-4.32294600	-2.15519900
H	4.67283000	-4.10267100	2.13724200
H	5.92801500	-4.36082400	0.00807900
H	2.21651500	-3.82083600	2.10436400
H	0.12018200	-4.58445600	0.49146900
H	0.18525300	-3.79468500	-1.09170600
C	-3.00990900	-0.39838000	0.77152500
O	-3.22862400	0.51680000	1.55254600
N	-3.93060700	-0.90083400	-0.10774100
H	-3.58723900	-1.58528400	-0.77320400
C	-5.27114000	-0.51519400	-0.28679700
C	-5.92123400	0.43831700	0.50703200
C	-5.97442800	-1.14718000	-1.32223000
C	-7.25718800	0.74347400	0.24984800
H	-5.38733200	0.93102600	1.30646600
C	-7.30466200	-0.83088200	-1.56471200
H	-5.46624500	-1.88861300	-1.93333800
C	-7.95727900	0.11918600	-0.77887900
H	-7.75215700	1.48478100	0.87036300
H	-7.83187400	-1.33059100	-2.37170100
H	-8.99674200	0.36777200	-0.96718700
C	0.62332100	-1.03951900	-0.07872400
C	-0.39201600	-0.18596800	0.80368400
C	0.41455000	-1.12808200	-1.57388800
H	-0.62779000	-1.34697300	-1.81171000
H	1.04883600	-1.89915300	-2.02091800
H	0.67078400	-0.16786100	-2.02650000
N	1.89952600	-0.75959100	0.34940000
C	3.12628800	-0.74892200	-0.41011400
C	3.72898300	0.64091200	-0.52548300
C	2.93118600	1.74025700	-0.86045900
C	5.09259400	0.84170800	-0.30603900
C	3.48486200	3.01349000	-0.96979900
H	1.86653100	1.59710000	-1.03099000
C	5.65297100	2.11441100	-0.41975400
C	4.84988600	3.20414400	-0.74881500
H	2.84881400	3.85835100	-1.22388600
H	6.71506500	2.25455500	-0.24078200
H	5.28197400	4.19713600	-0.82891000
H	5.71904800	-0.00557400	-0.03654700
H	3.86523600	-1.42433500	0.04310600
H	2.92712400	-1.14247800	-1.41106200
C	-0.57312800	1.18785100	0.11704100
O	-1.14275400	1.33622700	-0.96071100

N	0.01741600	2.15409400	0.86073100
H	0.37220300	1.74540800	1.73462500
C	0.29639300	3.48238500	0.53361600
C	-0.11983800	4.07700000	-0.66578600
C	1.06465400	4.22551900	1.44208900
C	0.24294100	5.39535600	-0.93906500
H	-0.71523400	3.50673400	-1.36598100
C	1.41600400	5.53849600	1.15554100
H	1.38923800	3.75635300	2.36718700
C	1.00983900	6.13358900	-0.03999200
H	-0.08335200	5.84747400	-1.87136800
H	2.01345700	6.09805400	1.86922200
H	1.28531900	7.15907400	-0.26458300
O	0.07663400	-0.10298100	2.05675100
H	1.88044200	-0.35137200	1.28596000
H	0.44347500	-2.41197300	1.51331300

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C	-0.36230800	-2.51865600	-0.02341000
C	-1.02009600	-1.35250400	0.19524600
C	-0.90896700	-3.91313000	-0.02184000
H	-0.24287000	-4.57483300	0.53951900
H	-0.99848700	-4.30940100	-1.03949500
H	-1.88901000	-3.94451900	0.45464100
N	1.00185200	-2.32962000	-0.17722500
C	1.80758100	-3.28916200	-0.93962200
C	3.24702500	-3.34096200	-0.47359100
C	4.29104600	-2.95376200	-1.31342300
C	3.54174400	-3.77203600	0.82546900
C	5.61160100	-2.97977100	-0.86044400
H	4.07015600	-2.62861300	-2.32747200
C	4.85643900	-3.79416300	1.28117600
C	5.89549900	-3.39359300	0.43818200
H	6.41531600	-2.67210200	-1.52259300
H	5.07328900	-4.12660400	2.29192500
H	6.92113600	-3.40920300	0.79386700
H	2.72942200	-4.07674800	1.48213800
H	1.35952900	-4.27404900	-0.79706100
H	1.77083700	-3.07231800	-2.01466000
C	-2.43344100	-1.07036800	0.46757800
O	-2.77043400	-0.06743400	1.09191000
N	-3.34653400	-1.95378200	-0.06883500
H	-2.98642800	-2.61290800	-0.74795600
C	-4.74490800	-1.93482100	0.04757600
C	-5.44547100	-1.10515000	0.93443000
C	-5.46132600	-2.82873600	-0.76325900
C	-6.83628100	-1.18037600	0.99062300
H	-4.90595900	-0.41099200	1.56198500
C	-6.84710600	-2.89044300	-0.69480900
H	-4.91937600	-3.47584800	-1.44837300
C	-7.54796900	-2.06428100	0.18378700
H	-7.36615800	-0.53126000	1.68185600
H	-7.37977800	-3.58922900	-1.33296100
H	-8.63091300	-2.11018200	0.23740000
C	1.30170100	-0.88169500	-0.29266200
C	-0.02520300	-0.22679900	0.32971900
C	1.53285800	-0.48506100	-1.74669200
H	0.66890800	-0.78077000	-2.34548600
H	2.43065400	-0.96644200	-2.14171100
H	1.65382900	0.59629500	-1.84281300
N	2.42586800	-0.57750300	0.60222300
C	3.49329600	0.32787000	0.17095900
C	3.11169600	1.78519000	0.31749800
C	3.11314600	2.64748100	-0.77950900
C	2.76202400	2.29136400	1.57463900
C	2.76880300	3.99240400	-0.62952800
H	3.38684100	2.26331400	-1.75963600
C	2.41990700	3.63144200	1.72971600
C	2.42280100	4.48651600	0.62505300
H	2.76826900	4.64999100	-1.49390800
H	2.15405500	4.01288300	2.71152300
H	2.14823000	5.53064400	0.74369400
H	2.76870100	1.62824900	2.43732000
H	4.34417000	0.11280200	0.82602700
H	3.82559500	0.13257000	-0.85653800
C	-0.52527100	1.01670300	-0.43338000
O	-1.01048700	0.92834800	-1.55343600
N	-0.38229300	2.17650800	0.25955200
H	-0.07954700	2.04936800	1.22095100
C	-0.80105800	3.45889000	-0.12650500
C	-0.96298900	3.83334600	-1.46579700
C	-1.01101100	4.40510200	0.88564300
C	-1.33355100	5.14167500	-1.77203300
H	-0.79682600	3.10753200	-2.25006900
C	-1.37588100	5.70721000	0.56521500
H	-0.87823300	4.10886700	1.92322300
C	-1.54064000	6.08476500	-0.76787700
H	-1.45486100	5.42370800	-2.81390600
H	-1.53259300	6.42852700	1.36170300

H	-1.82665300	7.10113800	-1.01927900
O	0.22060500	0.09577800	1.67696500
H	2.81888900	-1.44202300	0.95619200
H	1.20799600	-0.00754700	1.74765700

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C	0.40124200	-1.80356300	-1.73618200
C	-0.57560700	-1.50329100	-0.86537400
C	0.57455100	-2.94639700	-2.67217600
H	1.55193000	-3.42477600	-2.55496700
H	0.49485900	-2.59941100	-3.70917700
H	-0.21454400	-3.67352300	-2.48558000
N	1.37848000	-0.74552100	-1.70354200
C	2.62270800	-0.73409700	-2.48298600
C	3.83249800	-1.10635300	-1.65053200
C	4.92791700	-0.24318800	-1.60227700
C	3.88488400	-2.31415400	-0.94673900
C	6.07016200	-0.58598400	-0.87659700
H	4.88909300	0.70011400	-2.14191700
C	5.02195600	-2.65636100	-0.22044100
C	6.11989300	-1.79420700	-0.18640700
H	6.91711000	0.09317400	-0.85271700
H	5.05201000	-3.59746000	0.32036700
H	7.00686300	-2.06411000	0.37860500
H	3.03417900	-2.99080000	-0.95697500
H	2.49158600	-1.42690700	-3.31622000
H	2.74249400	0.26806800	-2.90174900
C	-1.77467600	-2.31355300	-0.54154100
O	-2.10747300	-3.31857300	-1.16520700
N	-2.43427800	-1.80113300	0.53705600
H	-1.95102600	-0.99118000	0.97620200
C	-3.61146900	-2.26366600	1.13701200
C	-4.33016000	-3.38609700	0.70101500
C	-4.08206400	-1.53408700	2.24071100
C	-5.49595400	-3.75628300	1.37033400
H	-3.97605900	-3.95480600	-0.14704300
C	-5.24405200	-1.91751000	2.89689800
H	-3.52514500	-0.66168500	2.57398300
C	-5.96175300	-3.03396500	2.46583900
H	-6.04427800	-4.62745000	1.02343400
H	-5.59033300	-1.33953400	3.74854200
H	-6.87048900	-3.33444900	2.97755400
C	1.06334900	0.16522700	-0.81762800
C	-0.34295600	-0.09999400	-0.31114000
C	1.77280800	1.44830500	-0.63537600
H	1.54854000	2.09746400	-1.49277100
H	2.85364300	1.30648300	-0.57801000
H	1.41052100	1.92151800	0.28021600
N	1.96457900	-0.85743300	1.26697700
C	3.09753000	-0.52055600	2.13470400
C	3.15242600	0.96761500	2.38737800
C	4.19939500	1.74593400	1.89067000
C	2.12183100	1.59609700	3.09493100
C	4.21442500	3.12752600	2.08336000
H	5.00242700	1.26411300	1.33681800
C	2.13017400	2.97558200	3.28683800
C	3.17720500	3.74591900	2.77832000
H	5.03410400	3.71999900	1.68743700
H	1.32173600	3.45098700	3.83454600
H	3.18448100	4.82152200	2.92711800
H	1.30196300	0.99953900	3.48958300
H	3.05030300	-1.04808600	3.10059500
H	4.02092600	-0.83686000	1.63690600
C	-1.17205000	0.86116700	-1.33011100
O	-1.09549400	0.79844700	-2.54670100
N	-1.91647500	1.70662400	-0.59239000
H	-1.77232900	1.53520800	0.41102400
C	-2.79754100	2.71107800	-1.01627000
C	-3.02858200	3.00652400	-2.36534300
C	-3.46430100	3.43877700	-0.02135300
C	-3.92143000	4.02384200	-2.69785100
H	-2.51520700	2.44529600	-3.13433000
C	-4.35096800	4.44990200	-0.36993000
H	-3.27891600	3.20147000	1.02292100
C	-4.58595600	4.74968700	-1.71216000
H	-4.09599100	4.24753800	-3.74622000
H	-4.86044200	5.00495900	0.41200100
H	-5.27864500	5.53946200	-1.98465400
O	-0.63991600	0.17772600	0.96571100
H	1.91599100	-1.86880500	1.14854200
H	1.07297500	-0.55488200	1.67120800

Int-18

C	0.09645600	-1.82066500	0.51327500
C	-0.62263300	-0.70843000	0.70033600
C	-0.15274400	-3.08559300	-0.23293900
H	-1.05180700	-2.98417200	-0.84312200
H	0.68881100	-3.31583800	-0.89461500
H	-0.28900900	-3.92976500	0.45180200
N	1.36829900	-1.65127300	1.19903500

C	2.39449800	-2.69440800	1.24410800
C	3.30160000	-2.69527300	0.02886100
C	3.27131600	-1.68681200	-0.93405800
C	4.20966500	-3.75069000	-0.10354700
C	4.14858900	-1.73627400	-2.01967700
H	2.56510300	-0.86293100	-0.85320300
C	5.08392400	-3.79361600	-1.18436100
C	5.05561800	-2.78366600	-2.14751500
H	4.11735600	-0.94842900	-2.76641900
H	5.78575900	-4.61687900	-1.27716500
H	5.73603500	-2.81751500	-2.99285900
H	4.22927800	-4.53854300	0.64566700
H	2.97718200	-2.53626800	2.15510300
H	1.88416200	-3.65528600	1.34578900
C	-1.95721400	-0.35334900	0.16463700
O	-2.16387900	0.76058800	-0.29784400
N	-2.89542900	-1.34373400	0.25575600
H	-2.61502000	-2.18359000	0.75152500
C	-4.23663700	-1.31968500	-0.16974800
C	-4.82344900	-0.23265600	-0.83000400
C	-5.00207500	-2.46547700	0.09014200
C	-6.16092300	-0.30984300	-1.21611100
H	-4.24213100	0.65476300	-1.03346600
C	-6.33332400	-2.52476200	-0.30102000
H	-4.54346500	-3.30866900	0.60040400
C	-6.92402200	-1.44513900	-0.95787200
H	-6.60680300	0.53858700	-1.72683100
H	-6.90999200	-3.42026400	-0.09020600
H	-7.96431100	-1.49037200	-1.26356000
C	1.45465800	-0.47505300	1.74149100
C	0.20000900	0.33931100	1.45765900
C	2.58705700	0.04734200	2.52844900
H	3.45523100	0.19791400	1.87537200
H	2.27739000	0.99891900	2.96537000
H	2.87823400	-0.64486300	3.32458000
C	0.71797200	1.34452100	0.30524500
O	1.27599300	0.99158600	-0.72733600
N	0.45122200	2.59158400	0.72358500
H	-0.02360700	2.53549700	1.64396800
C	0.68315500	3.81502700	0.08869200
C	1.29334300	3.91498000	-1.16859800
C	0.28358200	4.97928900	0.75937200
C	1.49484900	5.17285200	-1.73342700
H	1.60110400	3.01638800	-1.68670600
C	0.49227600	6.22605300	0.18258200
H	-0.19024100	4.89248400	1.73351100
C	1.10037400	6.33196000	-1.06875300
H	1.96845300	5.24182800	-2.70846100
H	0.17775100	7.11889800	0.71476000
H	1.26340000	7.30596000	-1.51898900
O	-0.30874600	0.97738200	2.49715600

$BnNH_2$

N	2.88102100	0.40524000	0.00004800
C	1.89966500	-0.67188100	-0.00010800
C	0.42755200	-0.28470200	0.00000800
C	-0.54124700	-1.29622600	0.00004100
C	0.00424000	1.04400000	-0.00001100
C	-1.89737500	-0.98732500	0.00002600
H	-0.22272100	-2.33679700	0.00005900
C	-1.35660700	1.35898700	-0.00001300
C	-2.31114300	0.34655100	-0.00000900
H	-2.63398600	-1.78568000	0.00005000
H	-1.66706900	2.39988900	-0.00003000
H	-3.36918300	0.59064700	-0.00000700
H	0.73875600	1.84451100	-0.00000500
H	2.09036700	-1.30464300	-0.87514300
H	2.09043100	-1.30502100	0.87463900
H	2.72797500	1.00175400	0.81227800
H	2.72776700	1.00223800	-0.81178700

TS-19

C	-0.52004900	-1.86969400	0.20907400
C	-1.04739000	-0.72857200	0.70758100
C	-1.01250400	-2.81314600	-0.83607500
H	-1.91459600	-2.41107900	-1.30029500
H	-0.26038000	-2.95799900	-1.61828500
H	-1.25015200	-3.79343900	-0.40903100
N	0.75391800	-2.07029600	0.81068600
C	1.63560500	-3.21698900	0.54892300
C	2.88265800	-2.85065800	-0.22340700
C	2.79435600	-2.19124500	-1.45244500
C	4.13623200	-3.20221700	0.27880600
C	3.94924200	-1.89152200	-2.16949000
H	1.82233800	-1.89239500	-1.83294400
C	5.29305900	-2.90640000	-0.44161900
C	5.20059700	-2.25077400	-1.66709400
H	3.87321300	-1.37675500	-3.12256800
H	6.26365600	-3.18405400	-0.04206700
H	6.09990000	-2.01582300	-2.22838400

H	4.20571200	-3.70867800	1.23842300
H	1.90232300	-3.64944800	1.51725400
H	1.04526400	-3.95866500	0.00821400
C	-2.27207700	-0.01512400	0.28056000
O	-2.24152100	1.17839100	0.01219000
N	-3.39846200	-0.79145200	0.22798600
H	-3.30365900	-1.74280700	0.56748200
C	-4.69757300	-0.42342400	-0.16504100
C	-5.03310100	0.84427900	-0.65752200
C	-5.69142200	-1.40655000	-0.05485500
C	-6.35133000	1.10493000	-1.02937800
H	-4.27475900	1.60878200	-0.74379200
C	-6.99975400	-1.12944300	-0.42909700
H	-5.42482200	-2.38880500	0.32705800
C	-7.34036600	0.13125400	-0.91981800
H	-6.60116900	2.09097600	-1.41002500
H	-7.75523000	-1.90375600	-0.33559300
H	-8.36247600	0.34960300	-1.21193900
C	1.04206300	-1.08886700	1.64438000
C	-0.02842400	-0.07328200	1.59343500
C	2.26765000	-0.98164800	2.46385800
H	3.13721500	-0.74478900	1.83976400
H	2.11283800	-0.18065300	3.19057600
H	2.47536000	-1.92149600	2.98586900
C	0.88517700	0.76954400	0.26973700
O	1.17020700	0.32386400	-0.81744500
N	1.08582500	1.97275200	0.80715300
H	0.63049500	2.02103300	1.74187300
C	1.66401200	3.10609400	0.21458400
C	2.22857800	3.08521900	-1.06559900
C	1.67179300	4.29008900	0.96219400
C	2.79164500	4.25069600	-1.58169400
H	2.22335100	2.16980700	-1.64335300
C	2.23792100	5.44382500	0.43322800
H	1.23215000	4.29322000	1.95585800
C	2.80136900	5.43176600	-0.84302600
H	3.22762800	4.22914400	-2.57610300
H	2.23783200	6.35581300	1.02253200
H	3.24277400	6.33318000	-1.25585800
O	-0.25388300	0.75939700	2.55442700

Int-20

C	0.74661200	0.57313500	-0.48048900
C	0.77086200	-0.66570700	0.16533600
C	1.79068200	1.14374300	-1.38360200
H	2.32224300	0.34084600	-1.89740500
H	1.34826800	1.81058100	-2.12655500
H	2.51704200	1.72403700	-0.80243200
N	-0.38103400	1.25677300	-0.22598000
C	-0.70747700	2.58375500	-0.73076600
C	0.22623900	3.68134400	-0.25510500
C	0.99273100	3.56641000	0.90579700
C	0.29172100	4.86509100	-0.99599100
C	1.80518900	4.62078400	1.32291300
H	0.96913300	2.64656600	1.48363600
C	1.09776000	5.92046600	-0.57773500
C	1.85826200	5.80115100	0.58537000
H	2.39821600	4.51595800	2.22654600
H	1.13795600	6.83331100	-1.16446300
H	2.49185900	6.62065600	0.91044200
H	-0.29348500	4.95693600	-1.90796300
H	-0.73818000	2.56486000	-1.82522300
H	-1.72718100	2.79907800	-0.40455900
C	1.80364900	-1.71813600	0.12706800
O	1.51776800	-2.90789300	0.17164000
N	3.10027800	-1.25997900	0.05862200
H	3.24018600	-0.26546600	0.19453800
C	4.28326500	-2.00298900	-0.08696400
C	4.32189300	-3.39527000	-0.24371000
C	5.48517400	-1.27879600	-0.08896400
C	5.55216000	-4.03256100	-0.39977200
H	3.40382200	-3.96403300	-0.23922900
C	6.70201800	-1.93008900	-0.24246700
H	5.45315600	-0.19850500	0.02893400
C	6.74541100	-3.31559500	-0.39982200
H	5.56858800	-5.11180000	-0.52144300
H	7.61960200	-1.34946100	-0.24028500
H	7.69535800	-3.82635800	-0.52011400
C	-1.27780200	0.48146000	0.61627700
C	-0.46754800	-0.80957200	0.87771800
C	-1.59389400	1.17118500	1.94670900
H	-2.15118600	2.09882100	1.78702900
H	-2.19326700	0.50290500	2.56989500
H	-0.66351500	1.39411400	2.47588900
C	-2.57654700	0.15037500	-0.15628700
O	-2.87858600	0.73228100	-1.18559800
N	-3.32163800	-0.80523600	0.45733000
H	-2.85948900	-1.29449000	1.22481300
C	-4.56991500	-1.32298800	0.06136800

C	-5.33800600	-0.78848800	-0.98009600
C	-5.05152800	-2.42478100	0.78172800
C	-6.57011000	-1.36560300	-1.28483000
H	-4.97535900	0.06057800	-1.54146500
C	-6.28114500	-2.98754100	0.46487600
H	-4.45300700	-2.83519700	1.59098000
C	-7.05033500	-2.46148200	-0.57308300
H	-7.15862200	-0.94454800	-2.09466000
H	-6.63763300	-3.84138700	1.03294500
H	-8.01080100	-2.90103900	-0.82218900
O	-0.89204200	-1.70359800	1.60141600

$^1O_2$

O	0.00000000	0.00000000	0.59837100
O	0.00000000	0.00000000	-0.59837100

$O_2^{-\cdot}$

O	0.00000000	0.00000000	0.66388900
O	0.00000000	0.00000000	-0.66388900

Int-21

C	-0.96178900	2.07551000	-0.12929600
C	0.42474300	1.97365900	0.19509100
H	0.87651300	2.82432000	0.69049600
C	-1.71092600	3.32343600	0.21310600
H	-2.07672400	3.80359900	-0.69999300
H	-2.57323400	3.08793200	0.84448500
H	-1.05930800	4.01801000	0.74202800
N	-1.55266500	1.07096300	-0.72773600
H	-0.95847600	0.25075800	-0.91907700
C	-2.95624400	0.97979400	-1.12202800
C	-3.62980400	-0.15501100	-0.38087800
C	-3.65608000	-0.15636000	1.01670600
C	-4.23322000	-1.19645400	-1.08469600
C	-4.28635800	-1.19003200	1.70262600
H	-3.18140700	0.65390000	1.56607600
C	-4.86941000	-2.22932100	-0.39701400
C	-4.89547900	-2.22775200	0.99565600
H	-4.30434700	-1.18619000	2.78812800
H	-5.34012000	-3.03585400	-0.95057800
H	-5.38792900	-3.03357900	1.53115100
H	-4.20649000	-1.19633600	-2.17104700
H	-2.97361900	0.79609200	-2.20012500
H	-3.44287200	1.93492700	-0.92312200
C	1.25608400	0.79037400	-0.10763700
O	0.80167700	-0.21826500	-0.65656900
N	2.54731200	0.93781100	0.27781500
H	2.79217300	1.81747600	0.72360000
C	3.60994000	0.02403500	0.14310100
C	3.47780300	-1.24198600	-0.44157000
C	4.85578400	0.44157400	0.63307500
C	4.59617900	-2.06915500	-0.52472200
H	2.52251200	-1.57226800	-0.82175400
C	5.95812900	-0.39637700	0.54132700
H	4.95106900	1.42525300	1.08537200
C	5.83488600	-1.65905400	-0.03938400
H	4.48841400	-3.04959700	-0.97829800
H	6.91613300	-0.05996100	0.92490800
H	6.69633700	-2.31505400	-0.11103400

TS-22

C	1.07250300	1.30277900	0.61020600
C	-0.31278800	1.36195500	0.85059900
H	-0.62139900	1.81043000	1.78857600
C	2.04768500	1.97118000	1.52736900
H	1.56577000	2.22886300	2.47086700
H	2.90319600	1.31890200	1.72954200
H	2.42858700	2.88887700	1.06380800
N	1.48466500	0.84187100	-0.55399300
H	0.76673700	0.41237800	-1.13858000
C	2.86373400	0.83498100	-1.01689300
C	3.67669800	-0.31125700	-0.44483400
C	3.09151100	-1.55449700	-0.19218000
C	5.03888000	-0.13459100	-0.19431600
C	3.86100700	-2.60727200	0.29809200
H	2.02935300	-1.69766900	-0.37474500
C	5.81023400	-1.18869500	0.29222000
C	5.22259100	-2.42796400	0.53973400
H	3.39562800	-3.56906000	0.49209100
H	6.86810000	-1.03824300	0.48572100
H	5.82094500	-3.24863900	0.92354700
H	5.49554600	0.83473200	-0.37903700
H	3.33624600	1.79045600	-0.77412800
H	2.82259700	0.75910600	-2.10684600
C	-1.26771000	0.46140700	0.18272000
O	-0.97897100	-0.19567500	-0.82126200
N	-2.51095700	0.44394600	0.75488900
H	-2.62702800	0.99813200	1.59614900
C	-3.65145300	-0.26943400	0.35102500
C	-3.73213300	-1.00908300	-0.83679700
C	-4.76619700	-0.21310300	1.20134900
C	-4.91532600	-1.67761300	-1.14806200

H	-2.88227500	-1.05832600	-1.50151100
C	-5.93772000	-0.88338000	0.87455700
H	-4.70452600	0.36160200	2.12208800
C	-6.02152500	-1.62387400	-0.30463700
H	-4.96493900	-2.24760200	-2.07128000
H	-6.78804300	-0.82602200	1.54744300
H	-6.93587700	-2.14940900	-0.56065500
O	-0.59709800	2.80255000	-0.41143000
O	-0.07449700	2.54831700	-1.54983800

Int-23

C	0.78761900	1.48729800	-0.68073900
C	-0.45273400	0.88738500	-1.32764700
H	-0.74624800	1.52626500	-2.17237700
C	0.77778400	2.96366100	-0.40881400
H	0.88587000	3.14663700	0.66560300
H	1.62570000	3.43987100	-0.91525100
H	-0.14839300	3.42754400	-0.74958100
N	1.75344500	0.69675700	-0.43662100
C	2.97120500	1.22658700	0.15744300
C	4.01988400	0.15170100	0.34128800
C	4.07218600	-0.96557800	-0.49552600
C	4.98548900	0.29138400	1.34189800
C	5.06992200	-1.92575500	-0.33283400
H	3.32459100	-1.08539700	-1.27422600
C	5.98587900	-0.66459100	1.50387300
C	6.03042100	-1.77844800	0.66621100
H	5.09592200	-2.79084000	-0.98907200
H	6.72609900	-0.54294600	2.28923800
H	6.80623500	-2.52735800	0.79374100
H	4.94897000	1.15478500	2.00221000
H	2.74933700	1.69549600	1.12557600
H	3.37724800	2.02389000	-0.48248900
C	-1.63267100	0.86287400	-0.33771300
O	-1.67419800	1.62456900	0.61616000
N	-2.59090200	-0.03454200	-0.67997800
H	-2.36288200	-0.63709500	-1.46483600
C	-3.80323900	-0.31287000	-0.02244000
C	-4.27878100	0.42724900	1.06683000
C	-4.55879200	-1.38604300	-0.51395300
C	-5.49781100	0.07993100	1.64717000
H	-3.70271900	1.25685000	1.45100000
C	-5.77199800	-1.71777300	0.07558400
H	-4.18489000	-1.95552500	-1.36118500
C	-6.25048600	-0.98650700	1.16286500
H	-5.85873100	0.65897500	2.49209000
H	-6.34399100	-2.55261100	-0.31783600
H	-7.19769500	-1.24563300	1.62483000
O	-0.22918000	-0.37497900	-1.91587200
O	0.05321300	-1.31156200	-0.86994000
H	0.94583900	-0.97567200	-0.60501400

TS-24

C	-0.85355200	1.06569900	0.49297000
C	0.39162000	0.31232400	0.85955500
H	0.60255800	0.46390900	2.25736700
C	-0.76339500	2.57006700	0.43741400
H	-0.85071800	2.91810900	-0.59819900
H	-1.58951000	3.01100000	1.00585200
H	0.18320500	2.92972000	0.83752600
N	-1.91970000	0.39077600	0.31562800
C	-3.14641300	1.11264300	0.03133700
C	-4.30016800	0.18623600	-0.29739800
C	-4.15321500	-1.19951500	-0.35773900
C	-5.55866500	0.74225700	-0.55466200
C	-5.24327300	-2.01456500	-0.66875500
H	-3.17998500	-1.63428600	-0.15767000
C	-6.64656900	-0.06777900	-0.86483200
C	-6.49195300	-1.45397600	-0.92320800
H	-5.11240000	-3.09214100	-0.71176400
H	-7.61598000	0.38123100	-1.06086200
H	-7.33914800	-2.08880700	-1.16486400
H	-5.68306600	1.82232000	-0.50979700
H	-3.00766400	1.81481100	-0.80434700
H	-3.42975700	1.73373500	0.89497700
C	1.68847500	0.62400500	0.16129800
O	1.84391600	1.66017100	-0.46997400
N	2.64889800	-0.33508400	0.32280400
H	2.35429700	-1.19132400	0.77929800
C	3.95905400	-0.34575600	-0.18714200
C	4.56837800	0.76259800	-0.78910900
C	4.68012300	-1.54104600	-0.05371600
C	5.87992500	0.65538100	-1.24935300
H	4.02247900	1.68886300	-0.89531800
C	5.98700200	-1.62984500	-0.51578600
H	4.20487900	-2.39904800	0.41504300
C	6.59756700	-0.53068900	-1.11978200
H	6.34246200	1.52068900	-1.71511500
H	6.52828700	-2.56439200	-0.40334000
H	7.61797500	-0.59928300	-1.48279700

O	0.24087000	-0.95951500	1.25117900
O	0.41507900	-0.64302000	2.88265600
H	1.27913500	-1.05428600	3.12754200

Int-25

C	-0.74311800	1.12886400	-0.16995500
C	0.38167700	0.33966100	-0.30326300
C	-0.71409800	2.57879800	0.20829200
H	-1.25208900	3.16718400	-0.54199500
H	-1.22181700	2.72227800	1.16876000
H	0.30870100	2.93319000	0.29262000
N	-1.94656300	0.57174400	-0.39742300
C	-3.22062300	1.26930200	-0.43401500
C	-4.36409300	0.32627300	-0.13051000
C	-4.23479000	-0.67932600	0.83193100
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C	-5.31018100	-1.51450500	1.12751900
H	-3.28766800	-0.81054000	1.34881500
C	-6.66234300	-0.34997800	-0.49261800
C	-6.52755100	-1.35097400	0.46785900
H	-5.19666600	-2.29362600	1.87545300
H	-7.60490200	-0.21955200	-1.01583100
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H	-5.68729800	1.25373800	-1.54932700
H	-3.38409500	1.74268300	-1.41097200
H	-3.20324700	2.06825200	0.31351700
C	1.76593400	0.70398700	0.01671700
O	2.11959800	1.77736300	0.50427500
N	2.66390000	-0.30317900	-0.28114700
H	2.29135700	-1.08499300	-0.80804200
C	4.05544400	-0.30455100	-0.11322800
C	4.76599400	0.67838100	0.59072400
C	4.75709100	-1.38258400	-0.67605900
C	6.15057200	0.56922500	0.71241200
H	4.23930400	1.51291700	1.02955300
C	6.13627200	-1.47613500	-0.54475300
H	4.20572600	-2.14706600	-1.21788000
C	6.84686700	-0.49780300	0.15115400
H	6.68803700	1.33850100	1.25959900
H	6.65642200	-2.31890900	-0.99025800
H	7.92492400	-0.56834800	0.25402600
O	0.17728900	-0.95481900	-0.73934200
O	-0.16075800	-1.81021200	0.39906400
H	0.72688700	-1.99571300	0.76505800
H	-1.94452100	-0.38705700	-0.73025700

TS-26

C	1.04750400	-1.53708200	0.29450300
C	-0.28000400	-1.43807400	-0.26854200
C	1.37943700	-1.66375500	1.74214700
H	1.89848500	-2.61478900	1.90840300
H	2.05778500	-0.85826600	2.04435700
H	0.47622700	-1.63267500	2.34482200
N	1.99704600	-1.47473500	-0.60635000
C	3.42647300	-1.43934500	-0.33491400
C	3.92508700	-0.02683600	-0.08983000
C	3.29346000	1.07384000	-0.67619400
C	5.05206500	0.17308000	0.70998000
C	3.79187400	2.35831800	-0.46556100
H	2.41107400	0.92938900	-1.29726500
C	5.55026500	1.45771500	0.91637200
C	4.92069000	2.55383300	0.32855100
H	3.29553800	3.20855900	-0.92369300
H	6.42531800	1.60236400	1.54280200
H	5.30524200	3.55591200	0.49202300
H	5.53771900	-0.68152200	1.17450200
H	3.92481300	-1.87122000	-1.20756500
H	3.64787200	-2.07840100	0.52238800
C	-1.44357400	-0.87459400	0.48432800
O	-1.50831700	-0.82241400	1.70874000
N	-2.41945900	-0.43533500	-0.36504900
H	-2.21549600	-0.55709500	-1.35295100
C	-3.65422000	0.15307800	-0.05310000
C	-4.11437200	0.35149700	1.25547300
C	-4.45323200	0.55611600	-1.13334000
C	-5.35785800	0.94786000	1.45957500
H	-3.50706900	0.04297400	2.09408200
C	-5.68977400	1.14805500	-0.91155000
H	-4.09304200	0.40147600	-2.14722100
C	-6.15239600	1.34939900	0.38914000
H	-5.70491100	1.09679300	2.47793700
H	-6.29314900	1.45325400	-1.76116500
H	-7.11822100	1.81258200	0.56361700
O	-0.37707800	-1.60215800	-1.52607500
O	0.35751700	-0.15139500	-2.45332900
H	0.01571400	0.52495300	-1.84125500
H	1.66746600	-1.21468700	-1.55094700

H_2O

O	0.00000000	0.00000000	0.11986300
H	0.00000000	0.76139600	-0.47945100

H	0.00000000	-0.76139600	-0.47945100

VII. References

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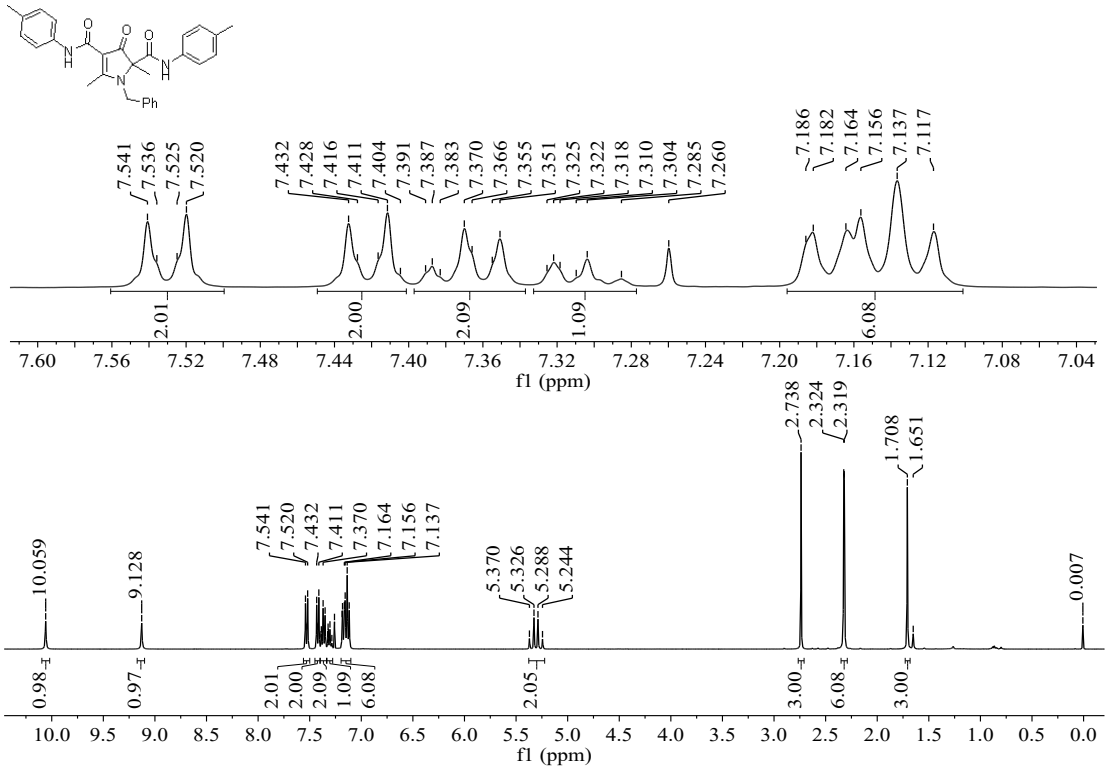
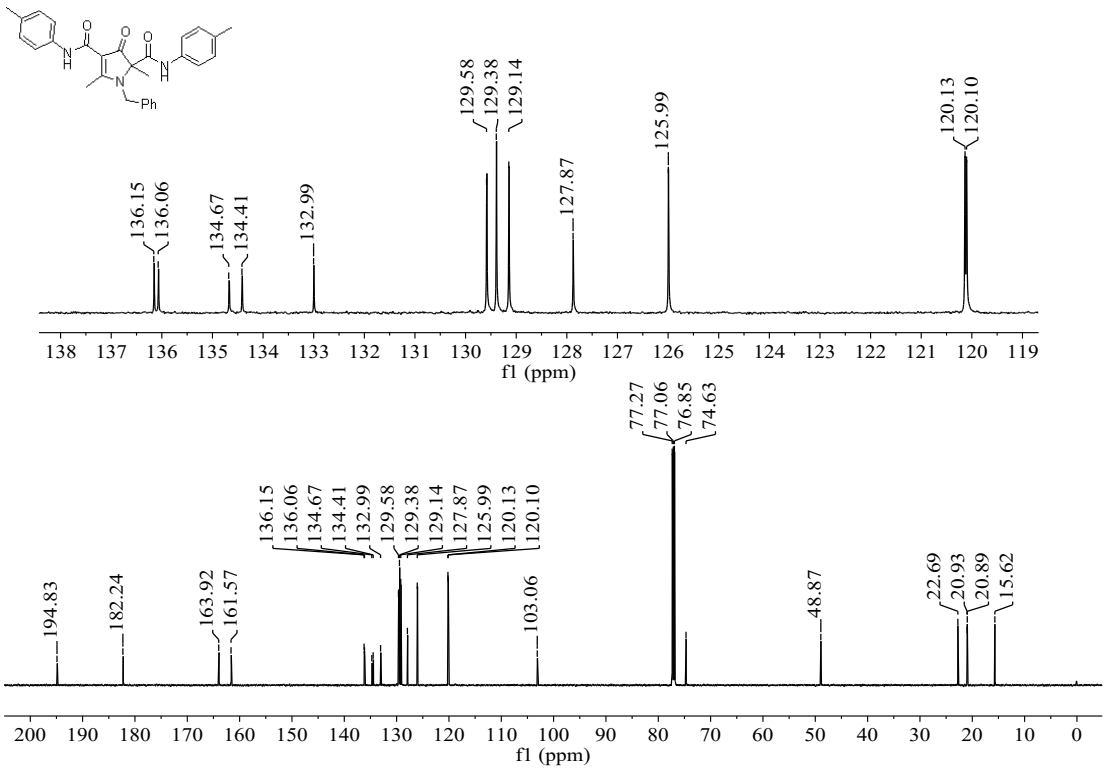
VIII. ^{1}H and ^{13}C NMR Spectra

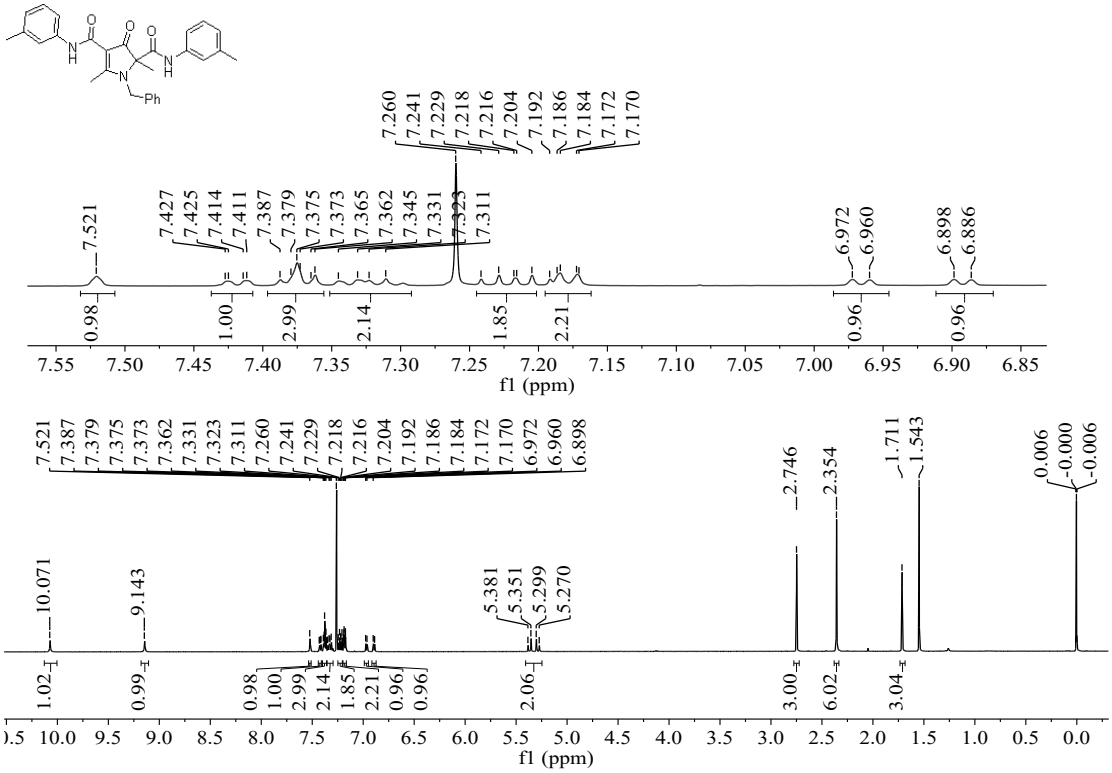
^{1}H NMR spectra of compound 2a (400 MHz, $CDCl_3$)



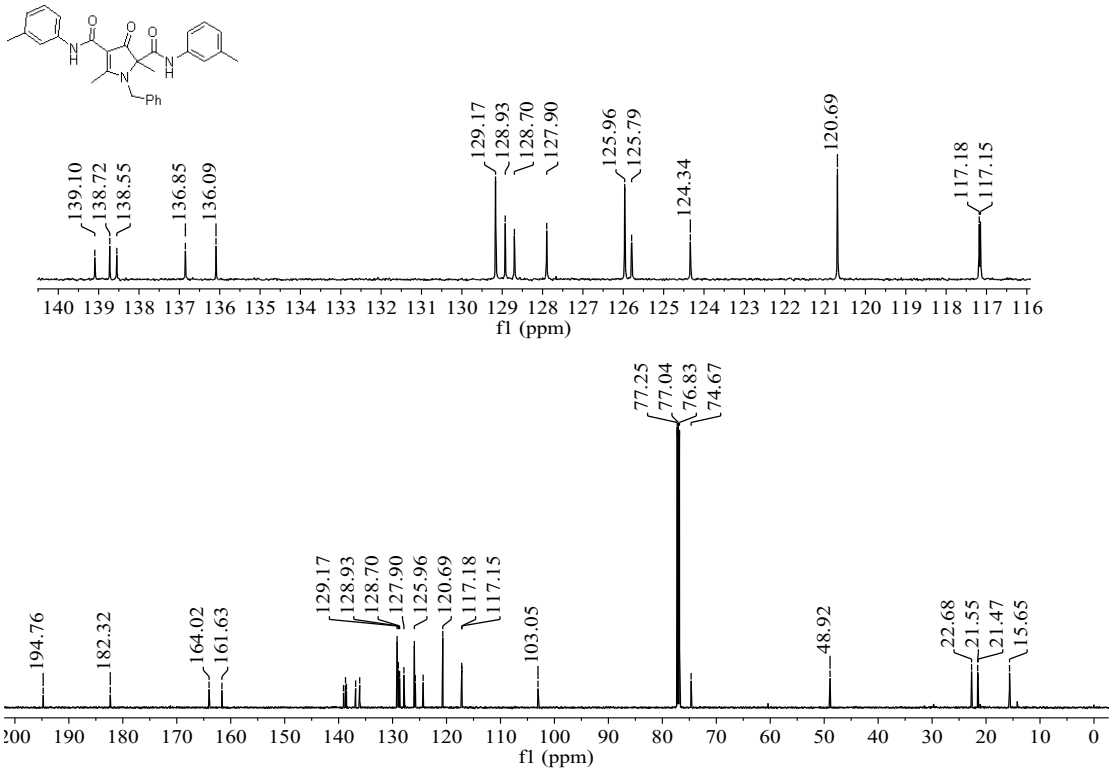
^{13}C NMR spectra of compound 2a (151 MHz, $CDCl_3$)



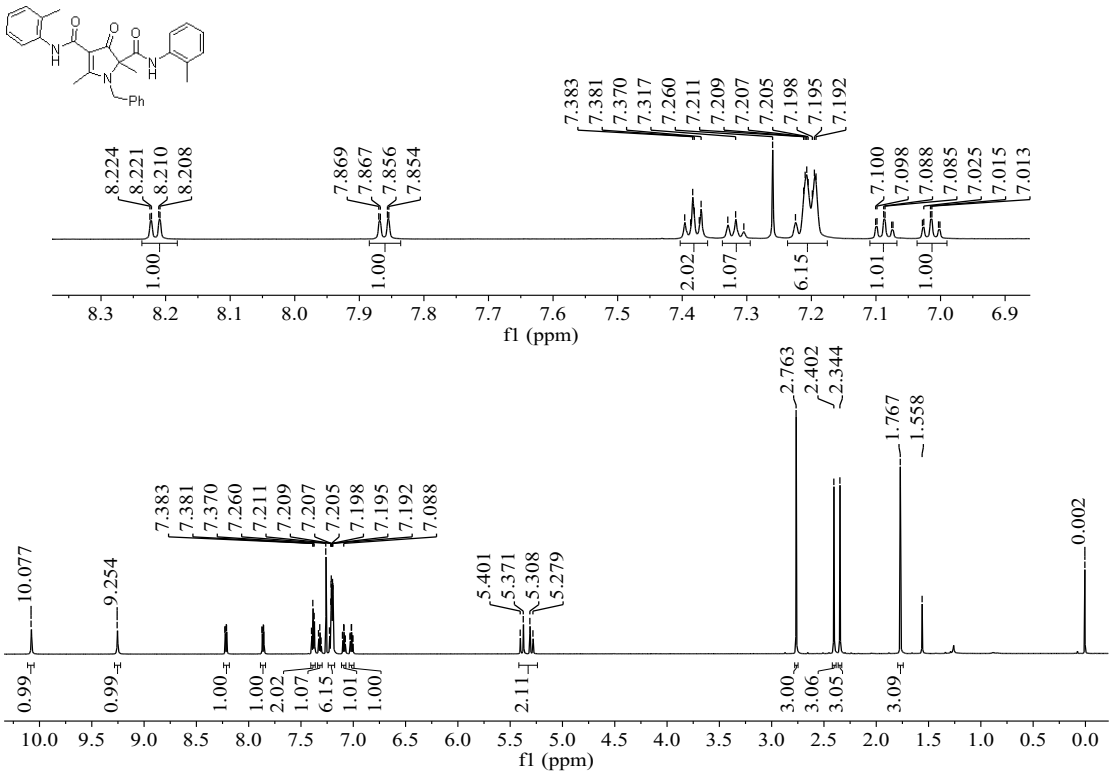
^{1}H NMR spectra of compound 2b (600 MHz, $CDCl_3$)



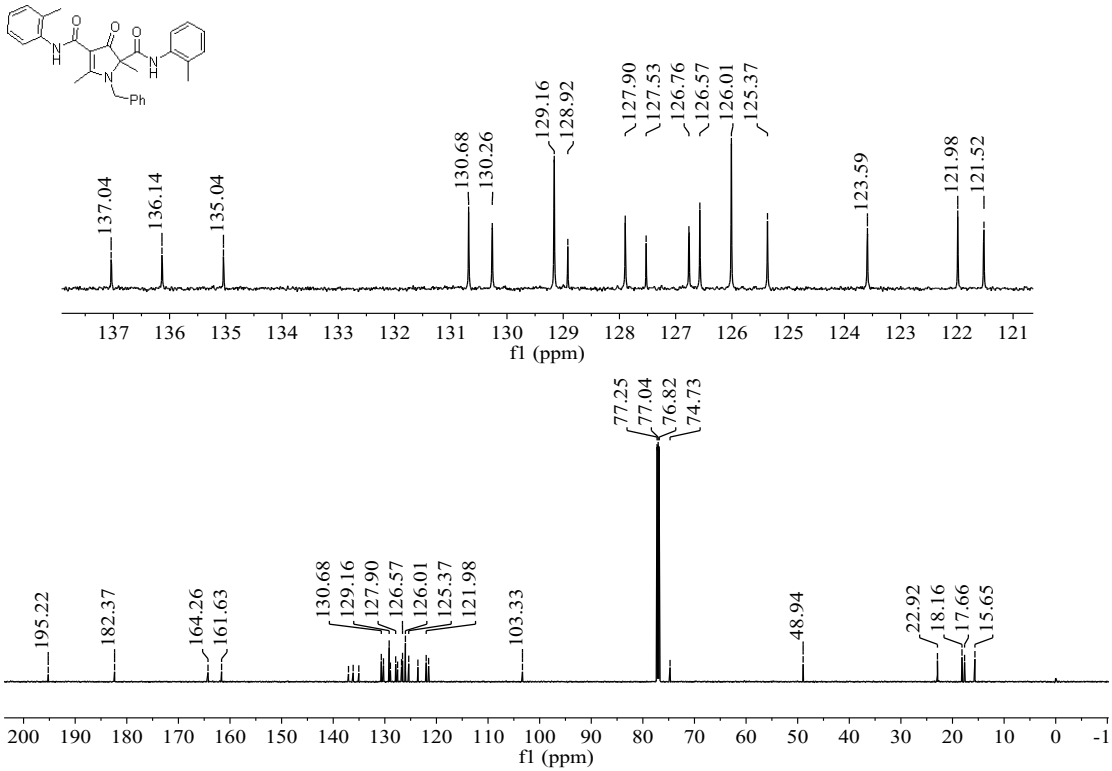
^{13}C NMR spectra of compound 2b (151 MHz, $CDCl_3$)



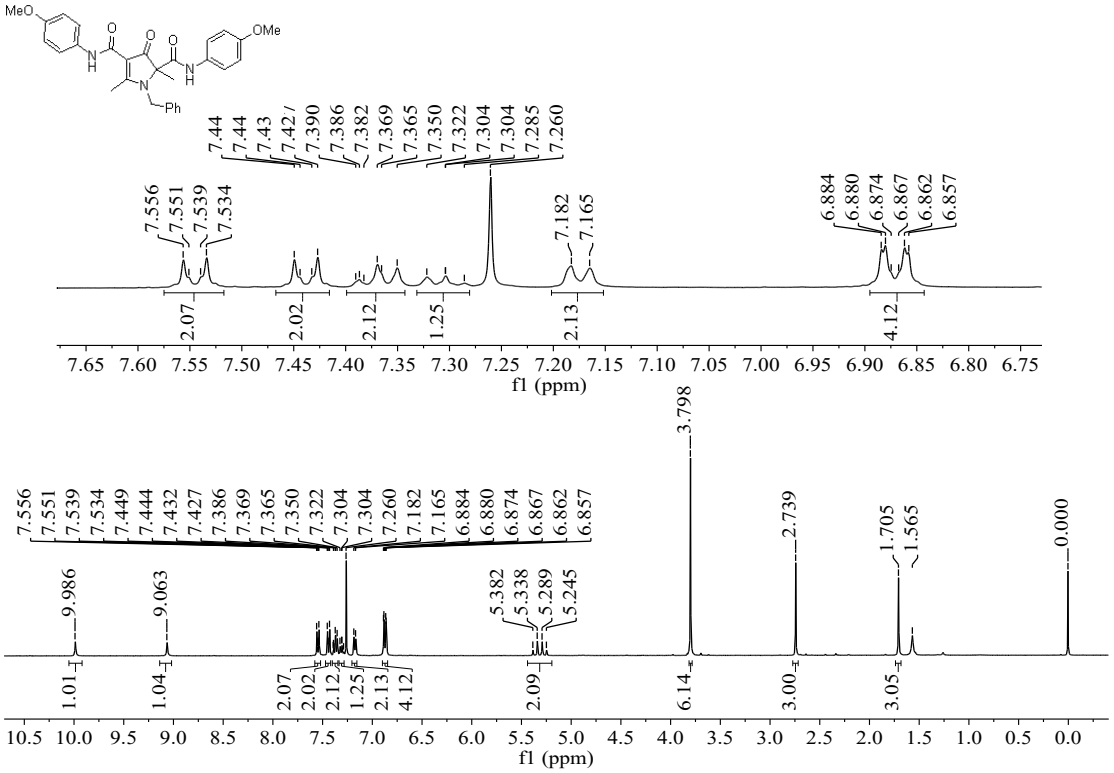
^{1}H NMR spectra of compound 2c (600 MHz, $CDCl_3$)



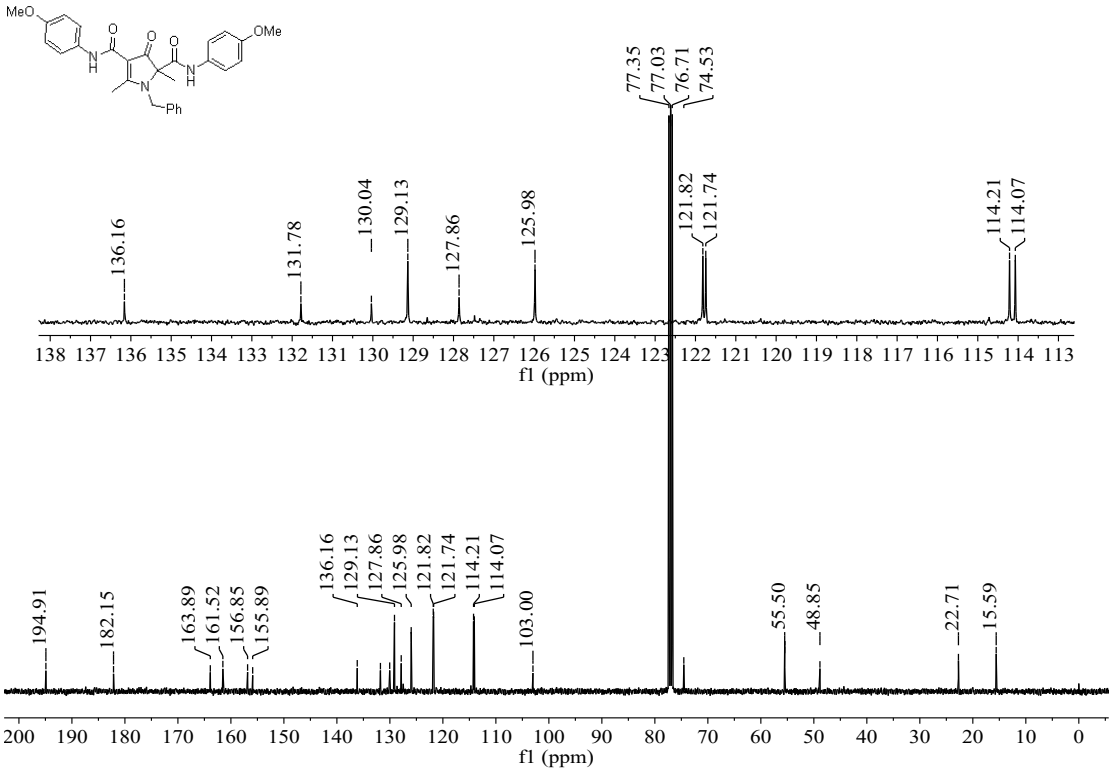
^{13}C NMR spectra of compound 2c (151 MHz, $CDCl_3$)



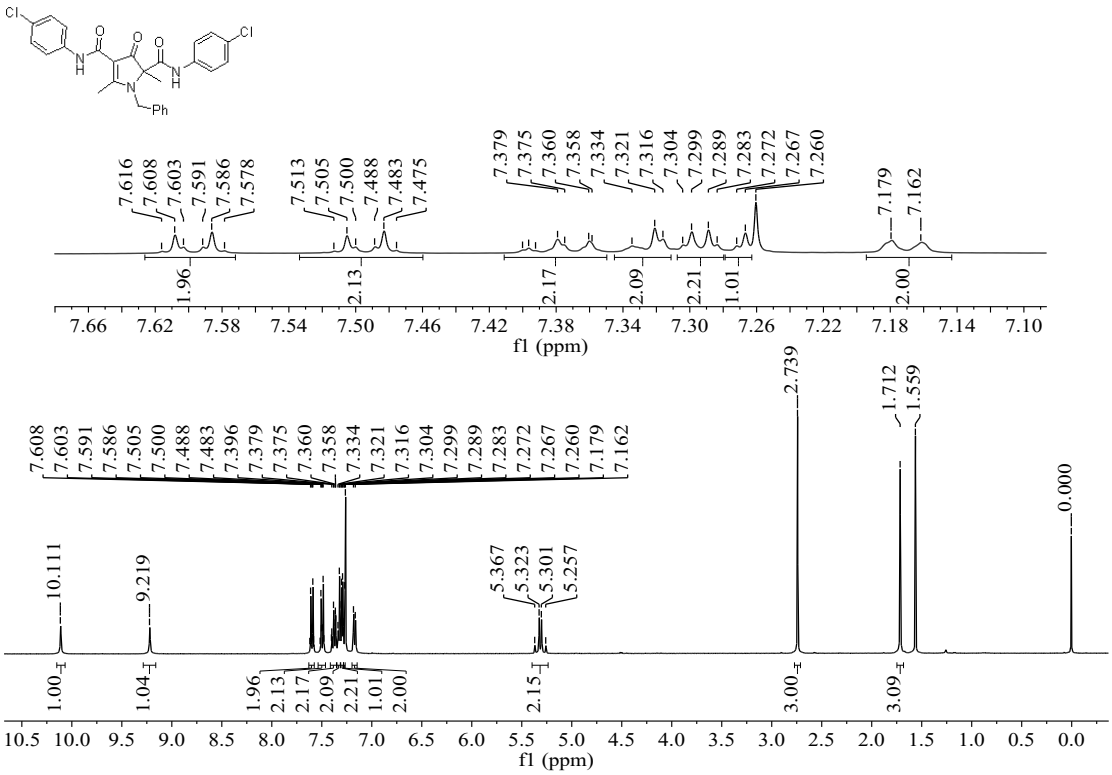
^{1}H NMR spectra of compound 2d (400 MHz, $CDCl_3$)



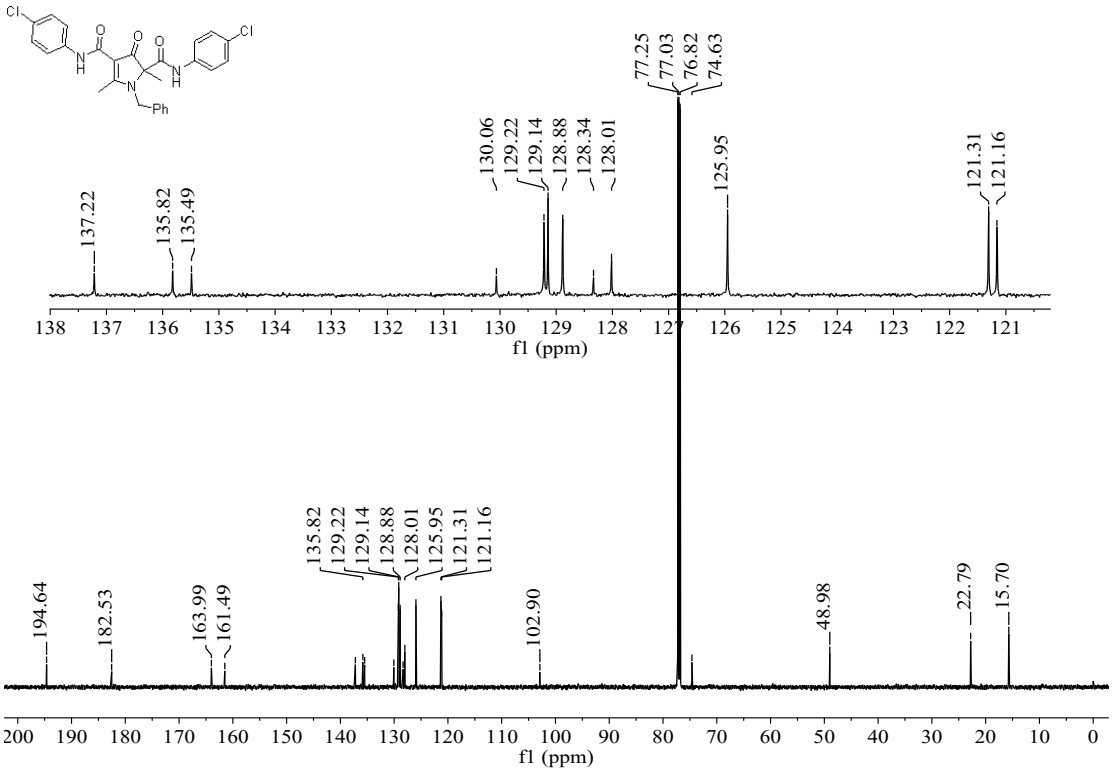
^{13}C NMR spectra of compound 2d (101 MHz, $CDCl_3$)



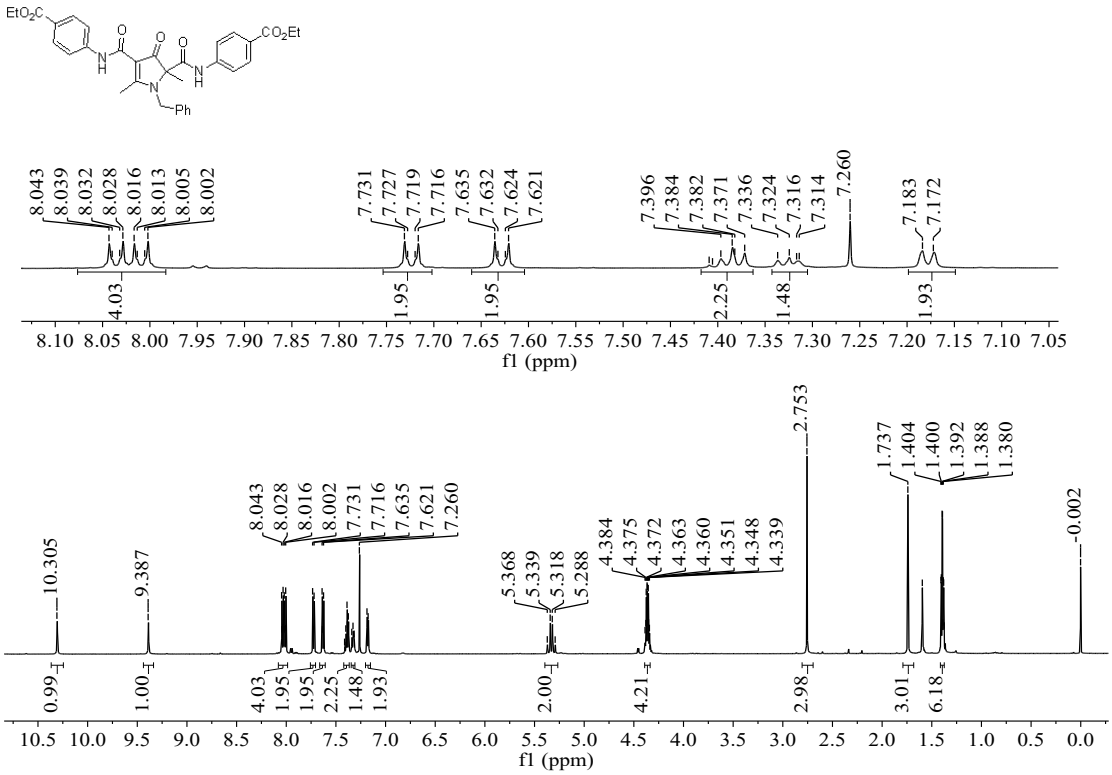
^{1}H NMR spectra of compound 2e (400 MHz, $CDCl_3$)



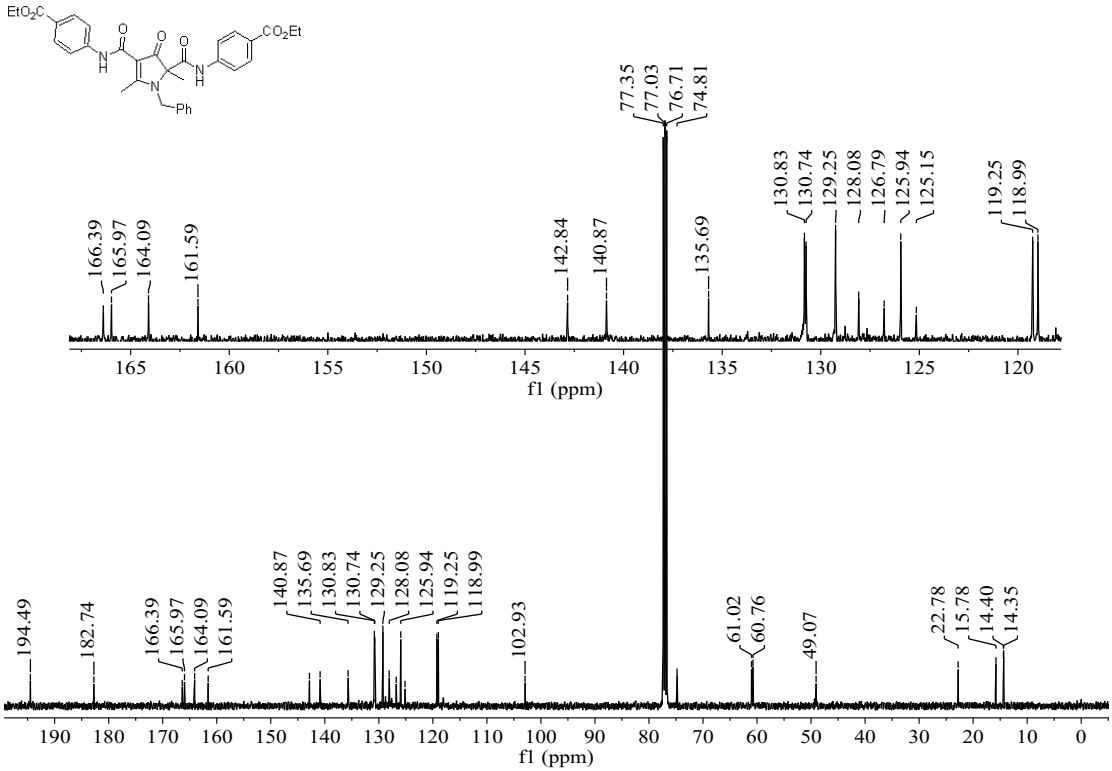
^{13}C NMR spectra of compound 2e (151 MHz, $CDCl_3$)



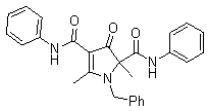
^{1}H NMR spectra of compound 2f (600 MHz, $CDCl_3$)

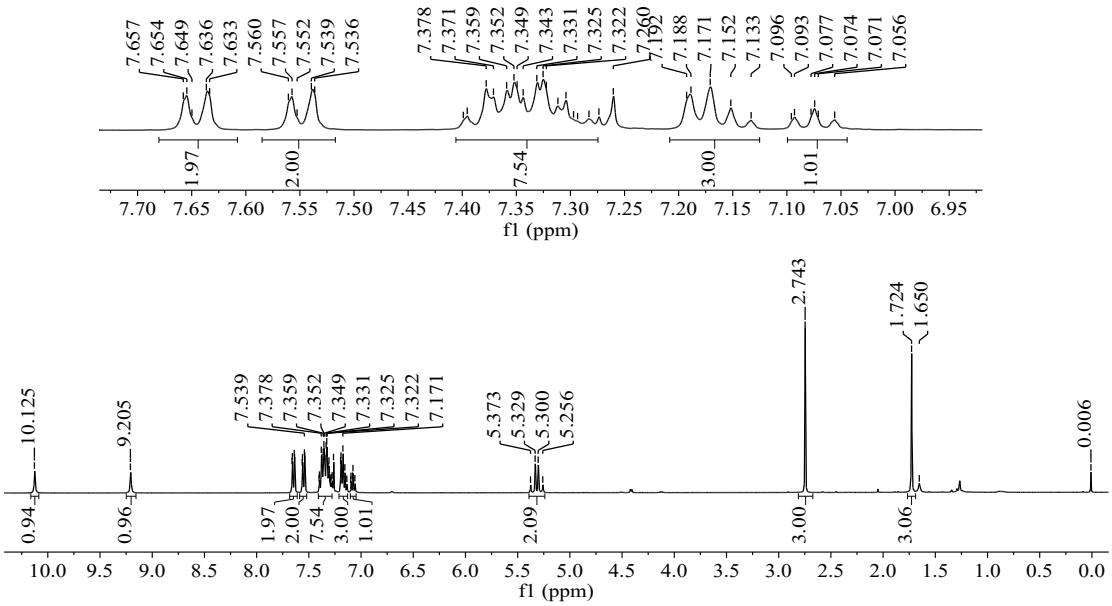


^{13}C NMR spectra of compound 2f (101 MHz, $CDCl_3$)

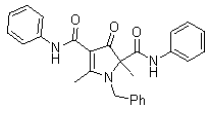


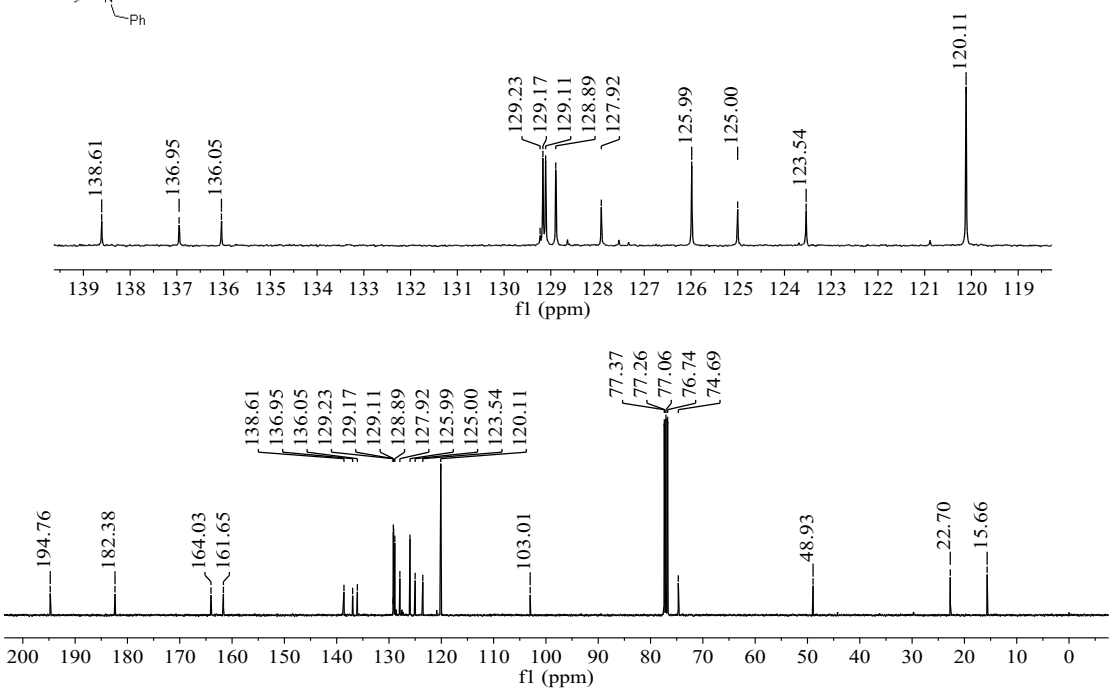
^{1}H NMR spectra of compound 2g (400 MHz, $CDCl_3$)



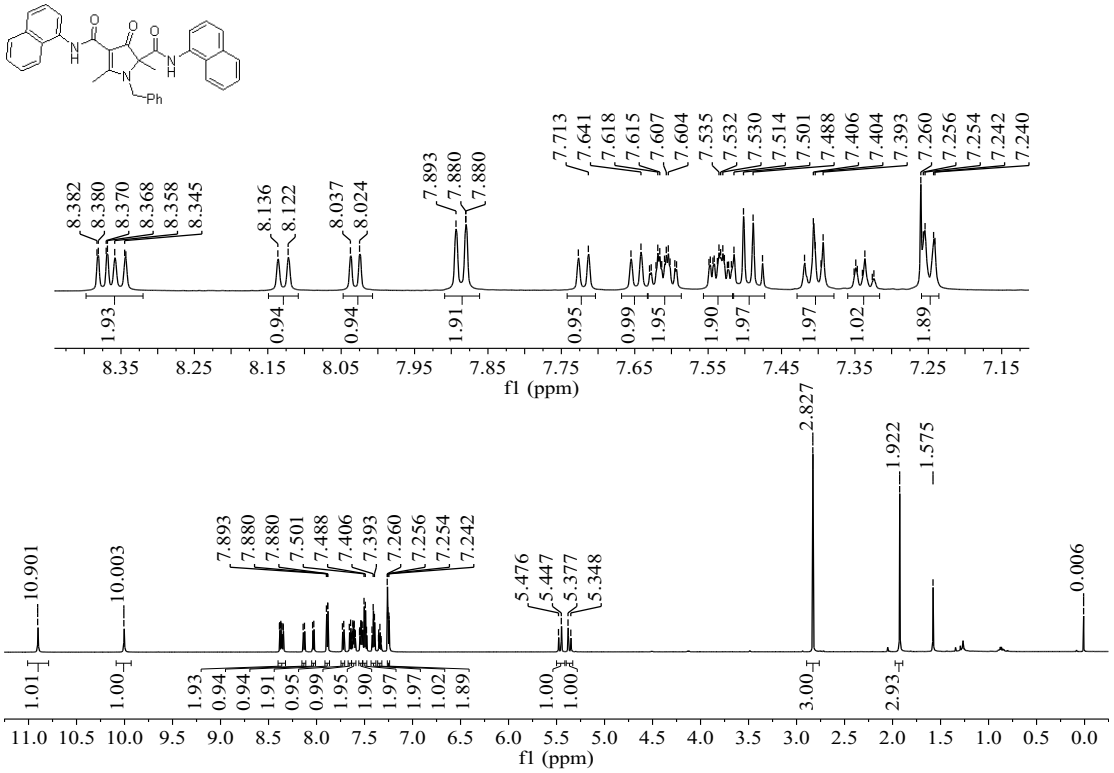


^{13}C NMR spectra of compound 2g (101 MHz, $CDCl_3$)

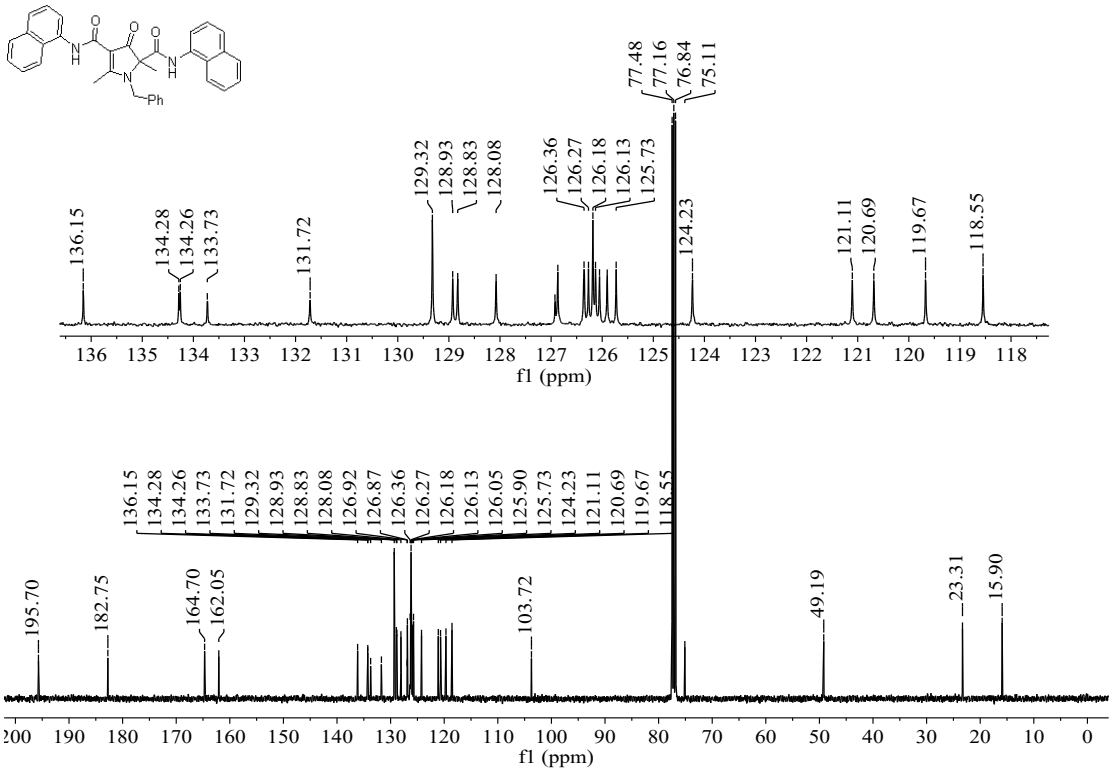




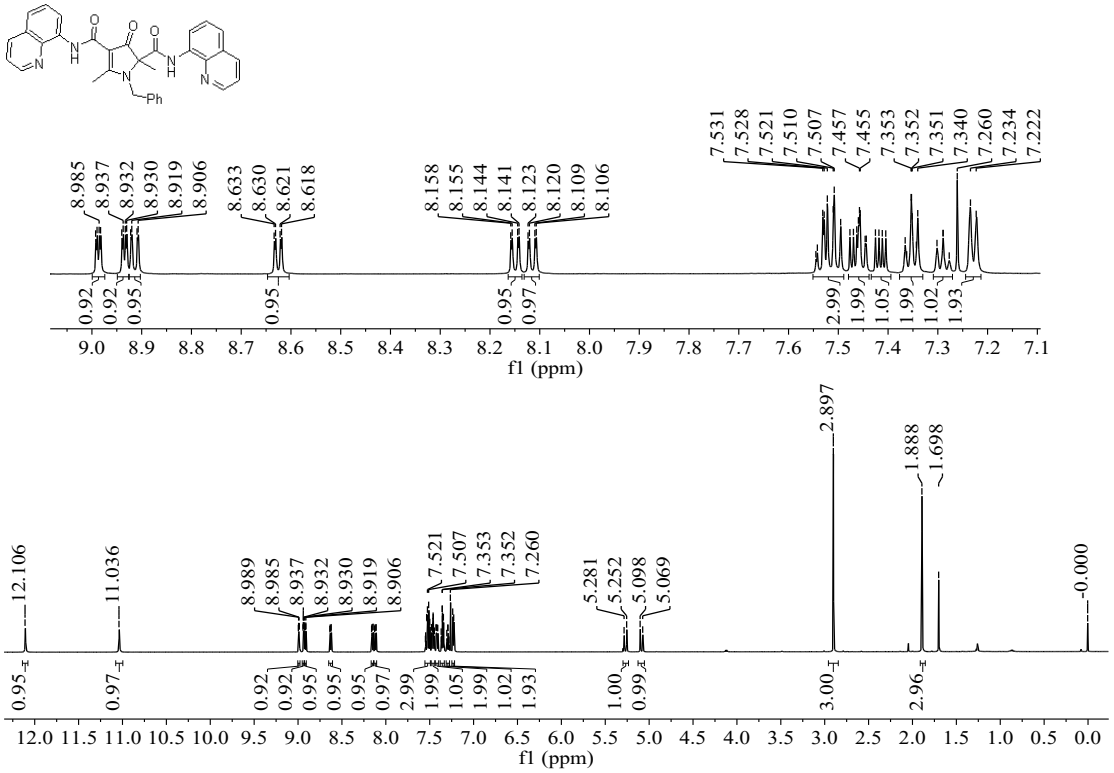
^{1}H NMR spectra of compound 2h (600 MHz, $CDCl_3$)



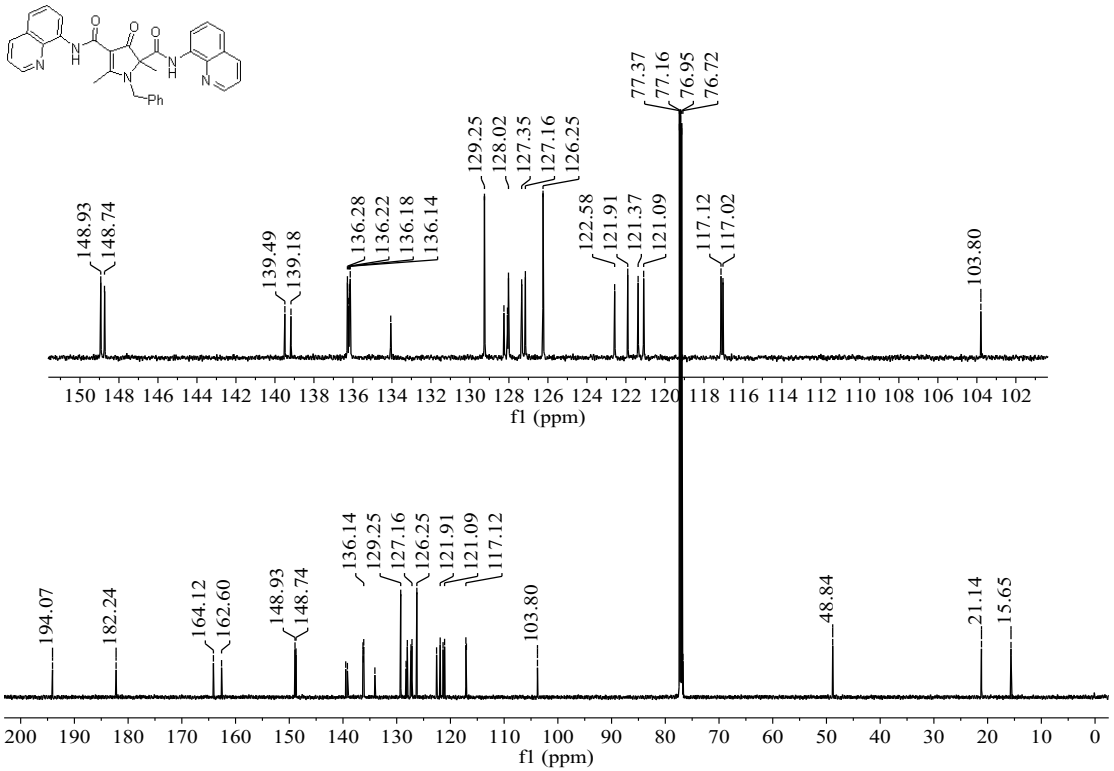
^{13}C NMR spectra of compound 2h (101 MHz, $CDCl_3$)



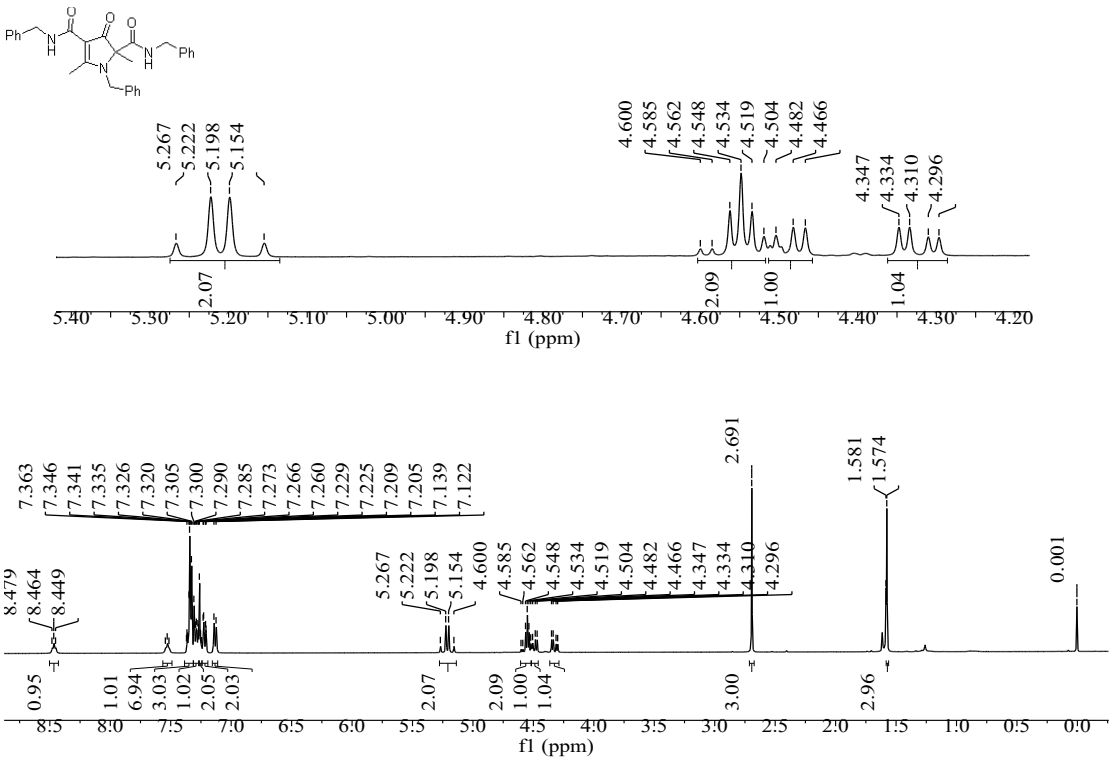
^{1}H NMR spectra of compound 2i (600 MHz, $CDCl_3$)



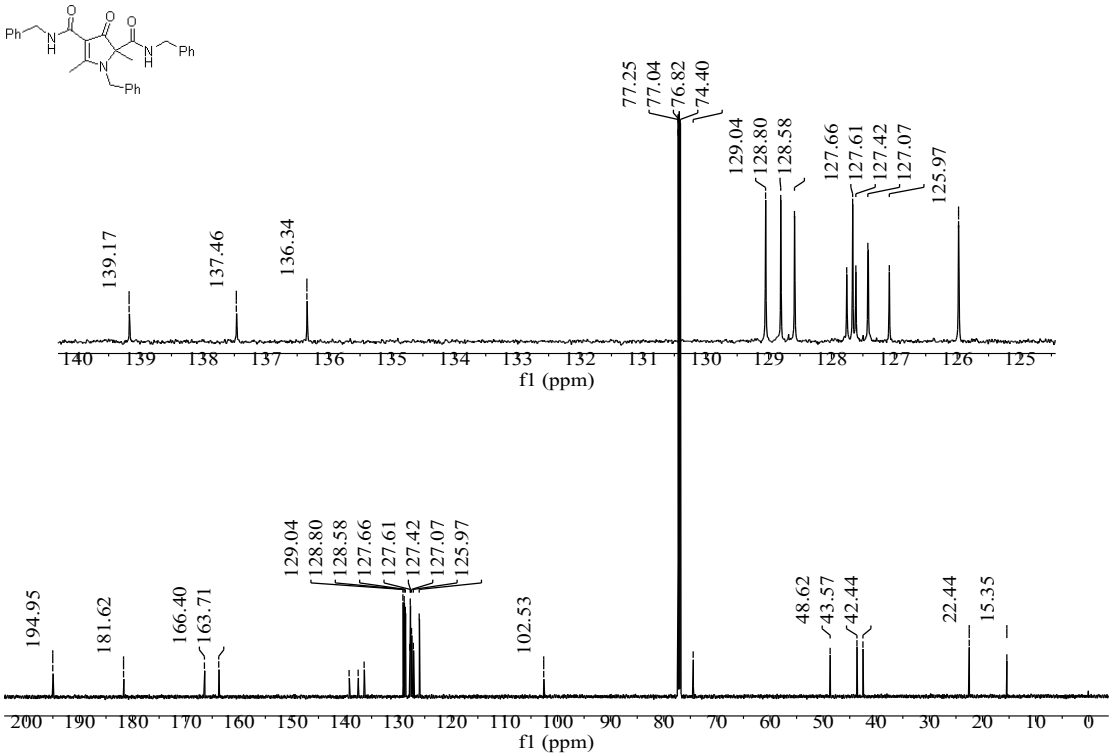
^{13}C NMR spectra of compound 2i (151 MHz, $CDCl_3$)



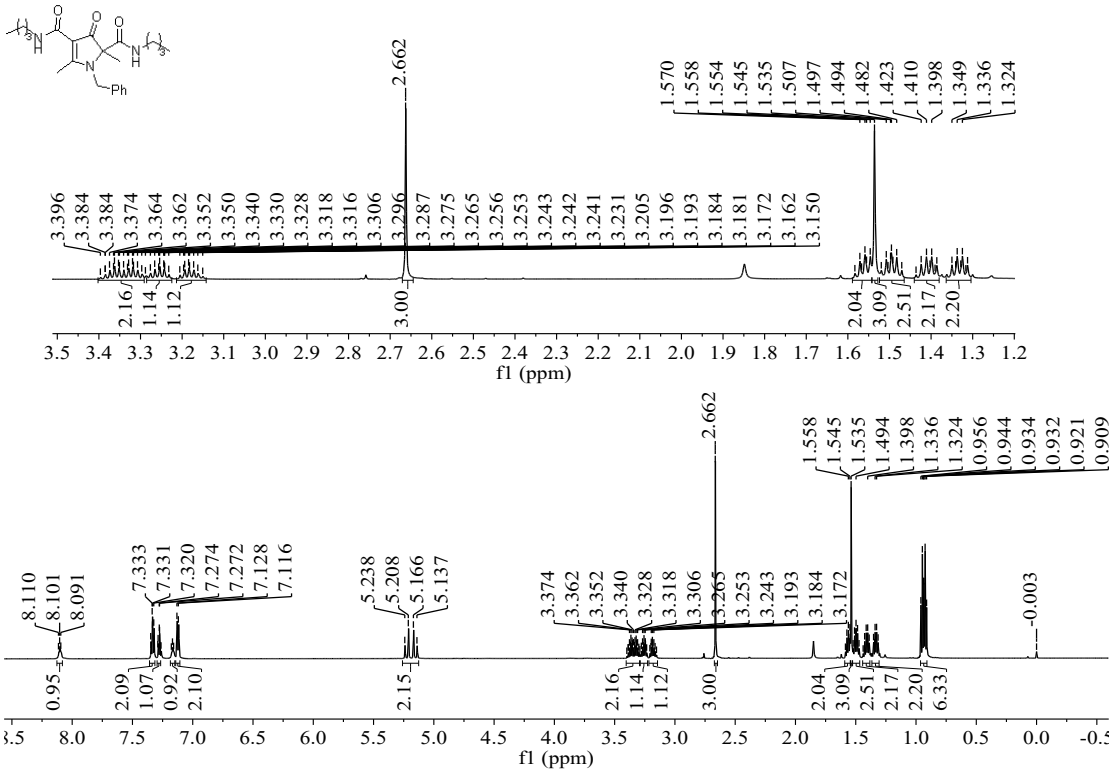
^{1}H NMR spectra of compound 2j (400 MHz, $CDCl_3$)



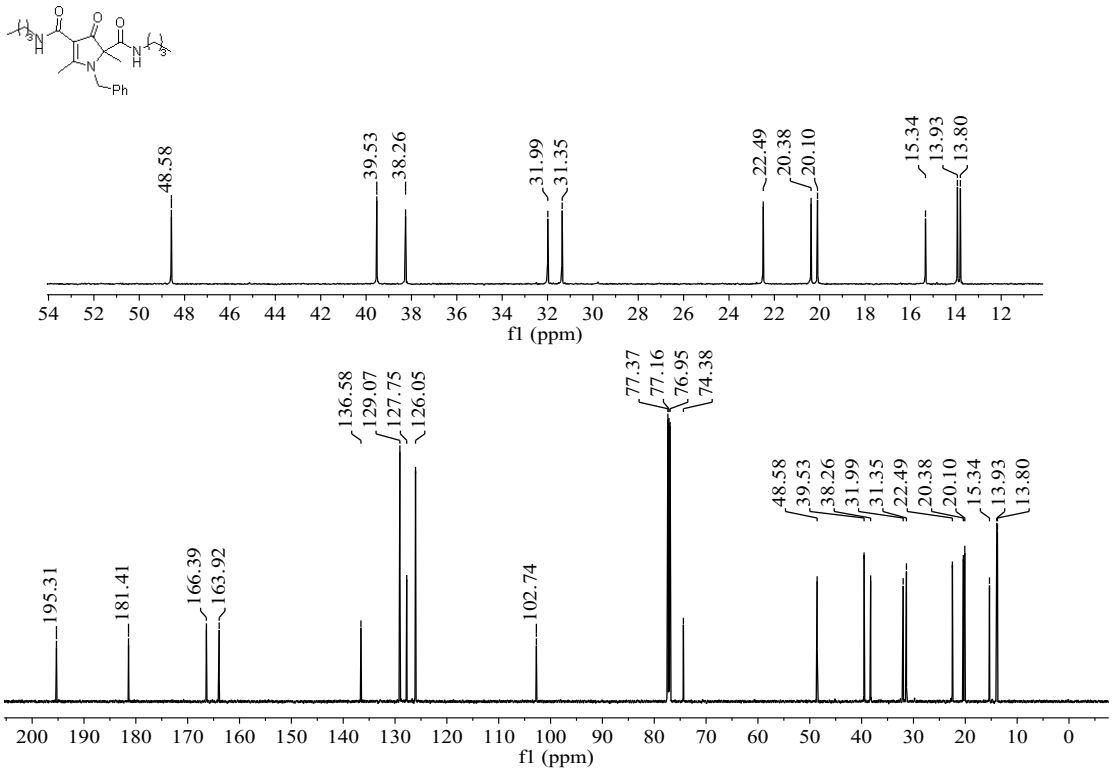
^{13}C NMR spectra of compound 2j (151 MHz, $CDCl_3$)



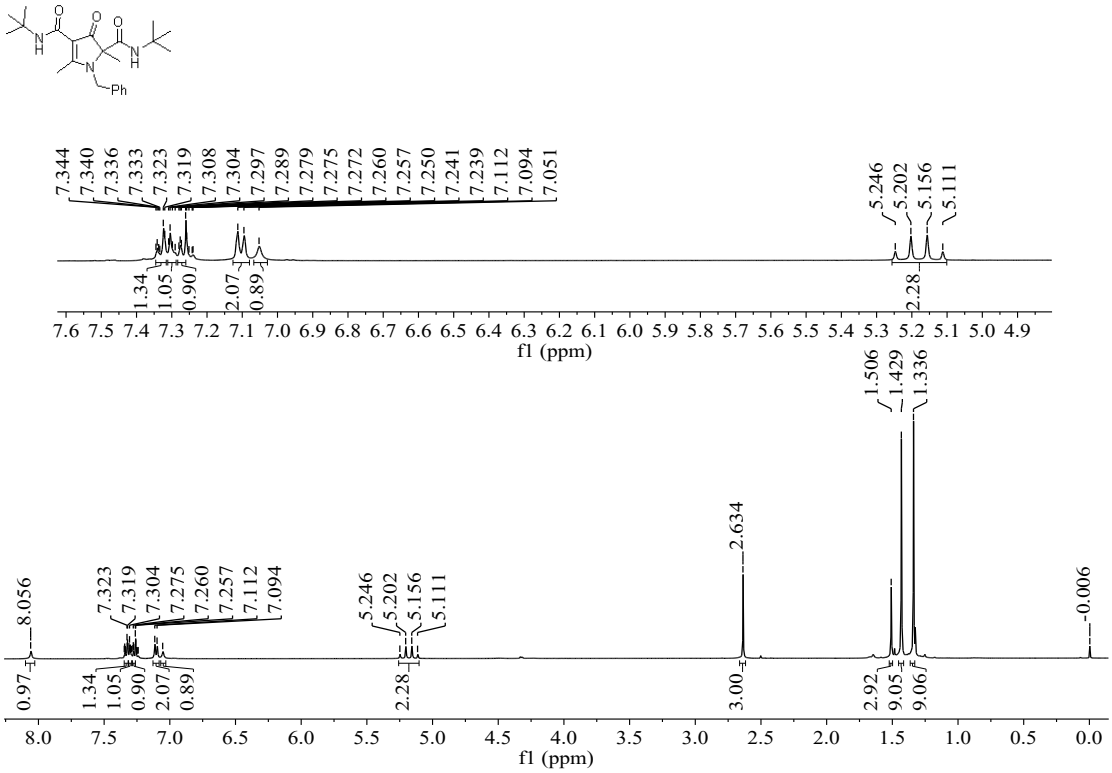
^{1}H NMR spectra of compound 2k (600 MHz, $CDCl_3$)



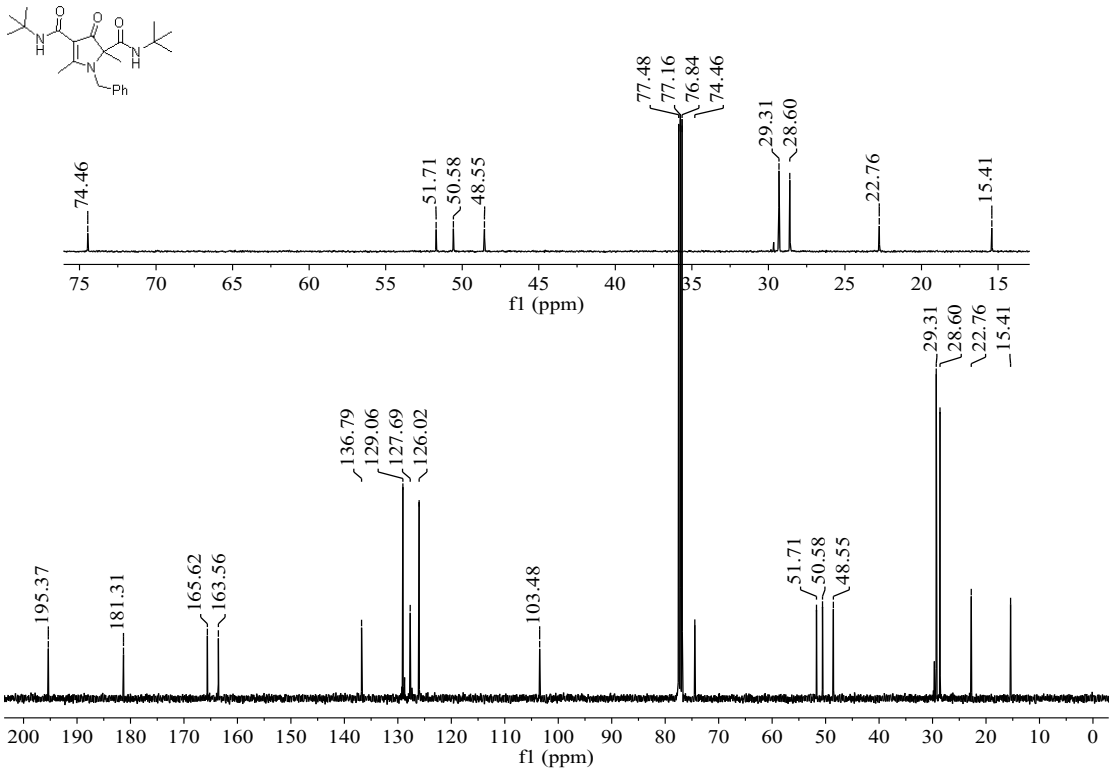
^{13}C NMR spectra of compound 2k (151 MHz, $CDCl_3$)



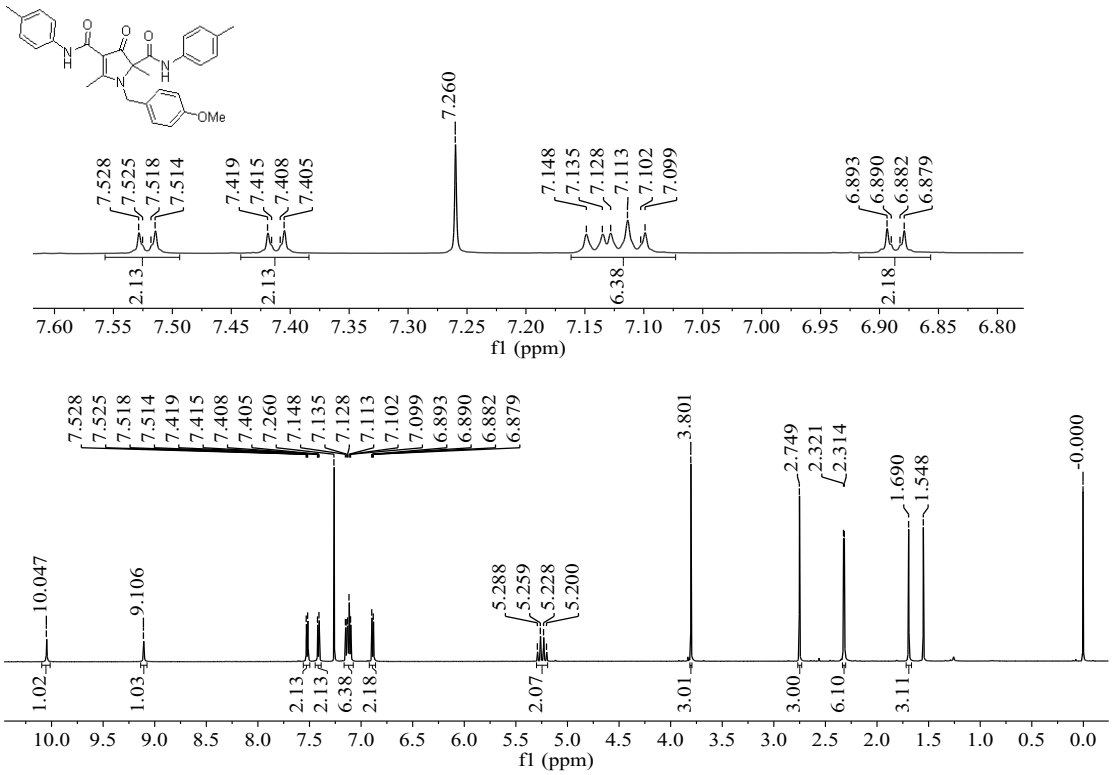
^{1}H NMR spectra of compound 2l (400 MHz, $CDCl_3$)



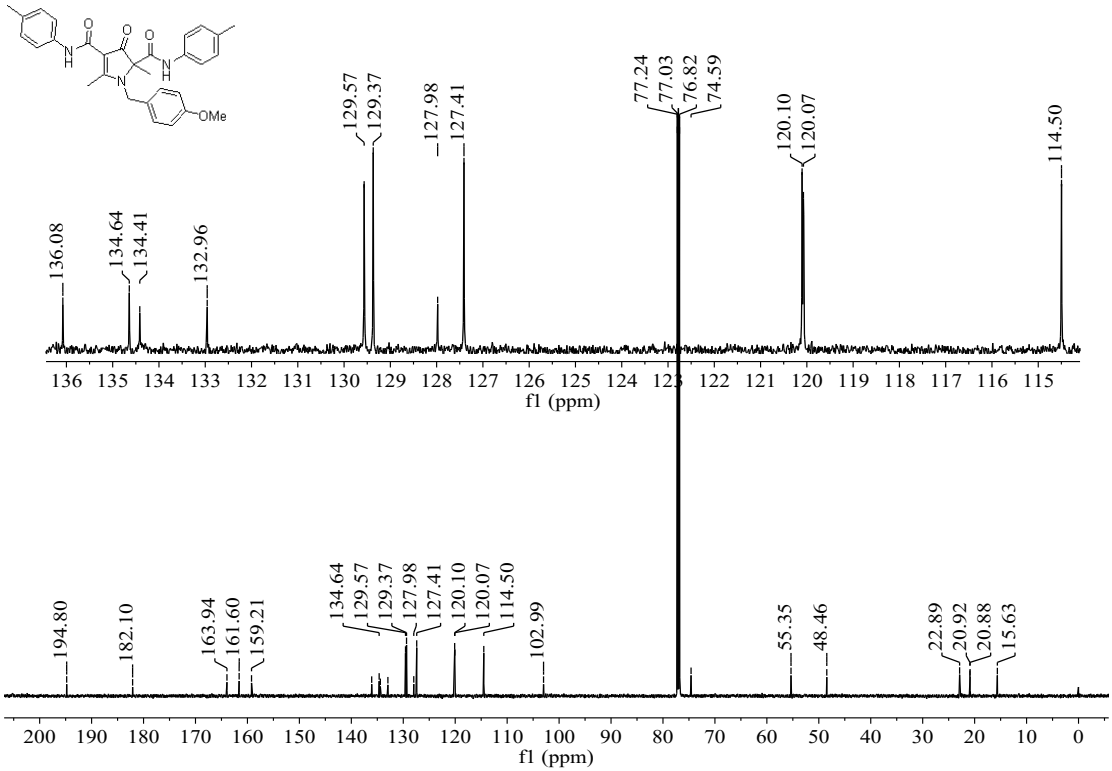
^{13}C NMR spectra of compound 2l (101 MHz, $CDCl_3$)



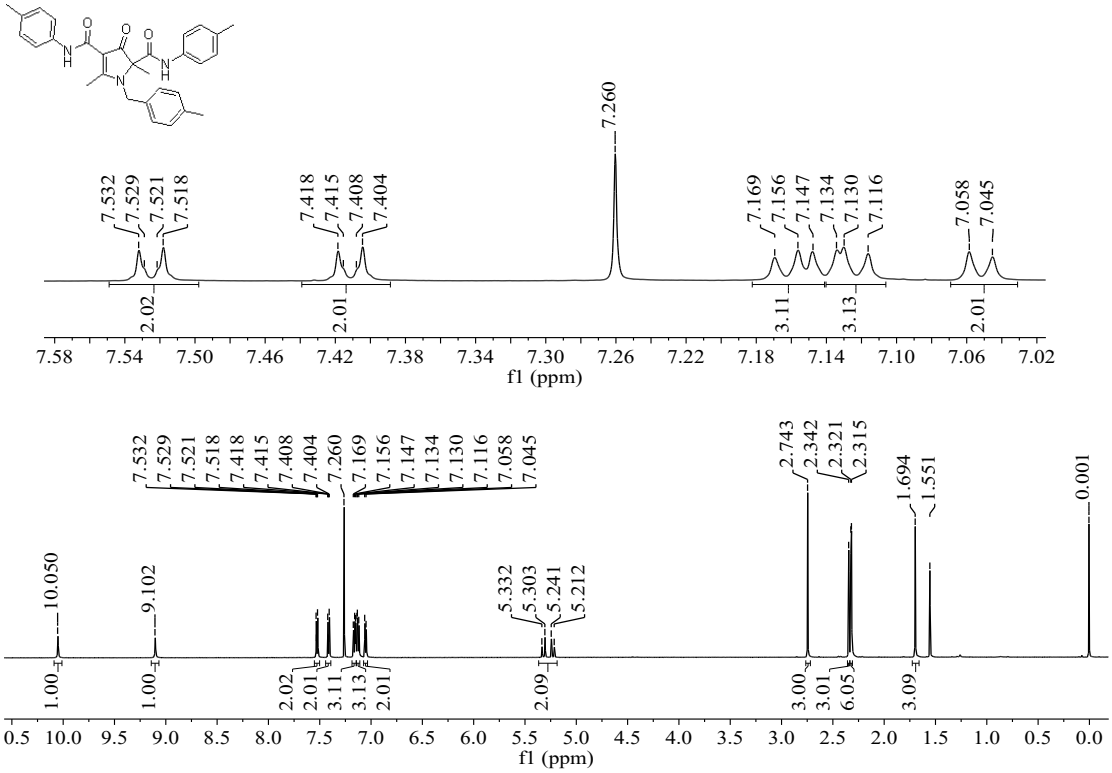
^{1}H NMR spectra of compound 2m (600 MHz, $CDCl_3$)



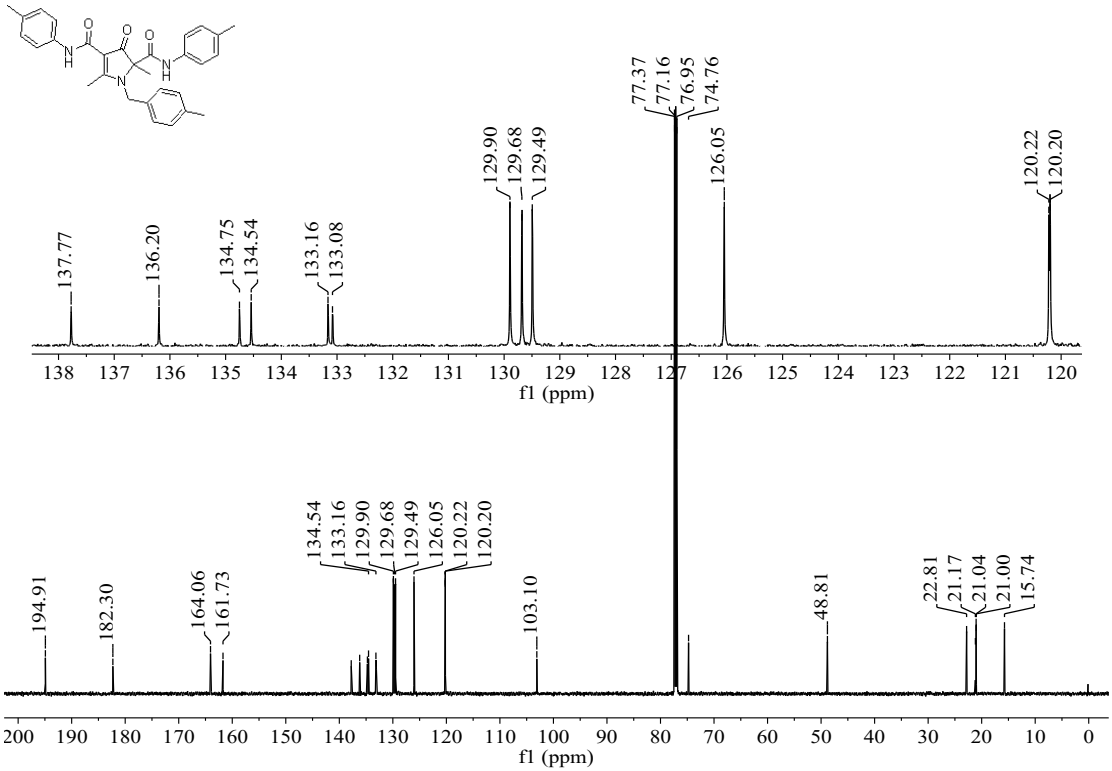
^{13}C NMR spectra of compound 2m (151 MHz, $CDCl_3$)



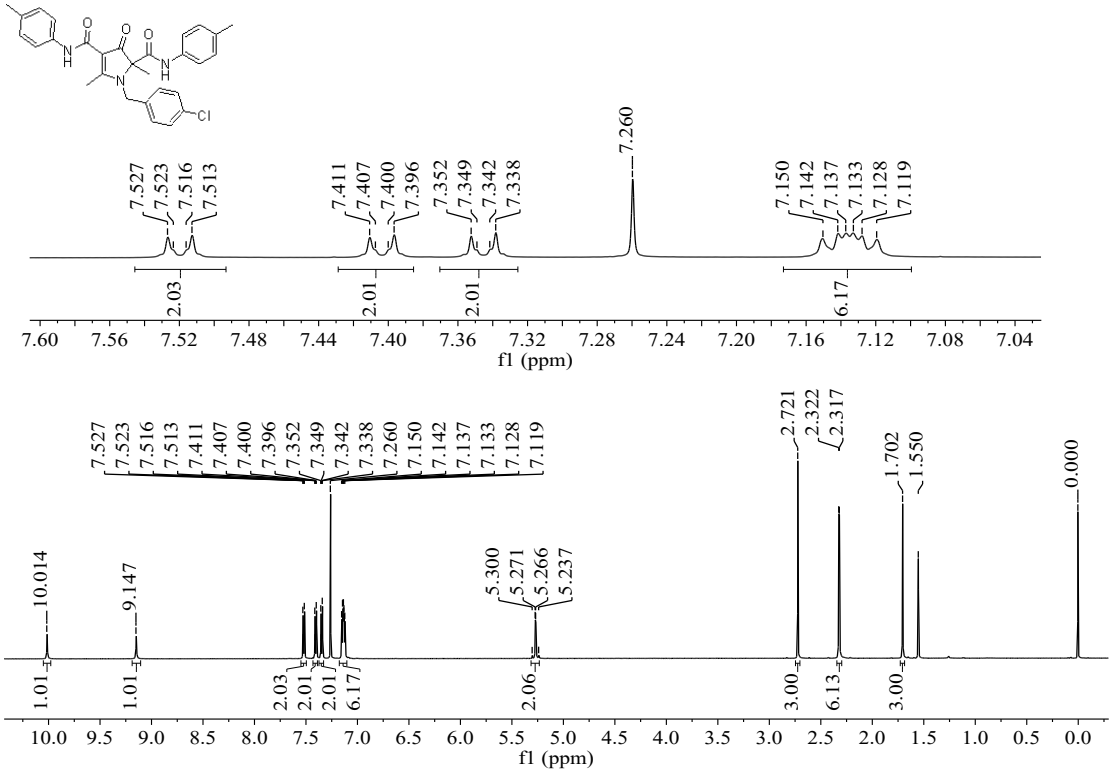
^{1}H NMR spectra of compound 2n (600 MHz, $CDCl_3$)



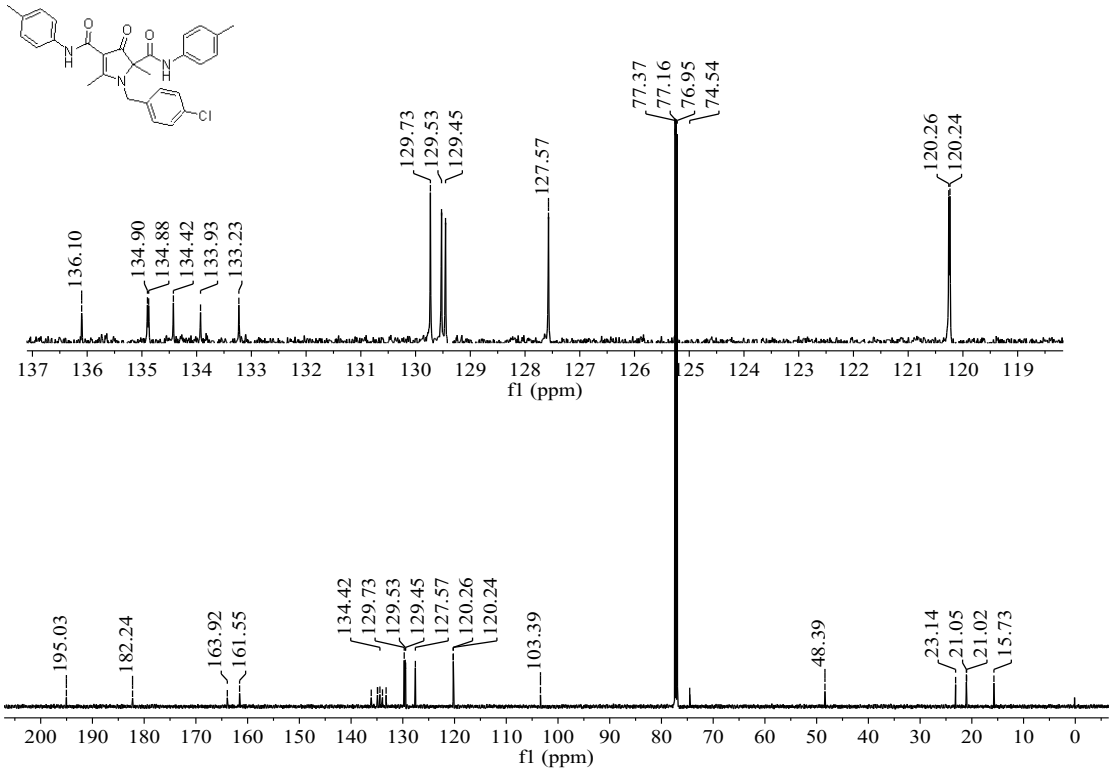
^{13}C NMR spectra of compound 2n (151 MHz, $CDCl_3$)



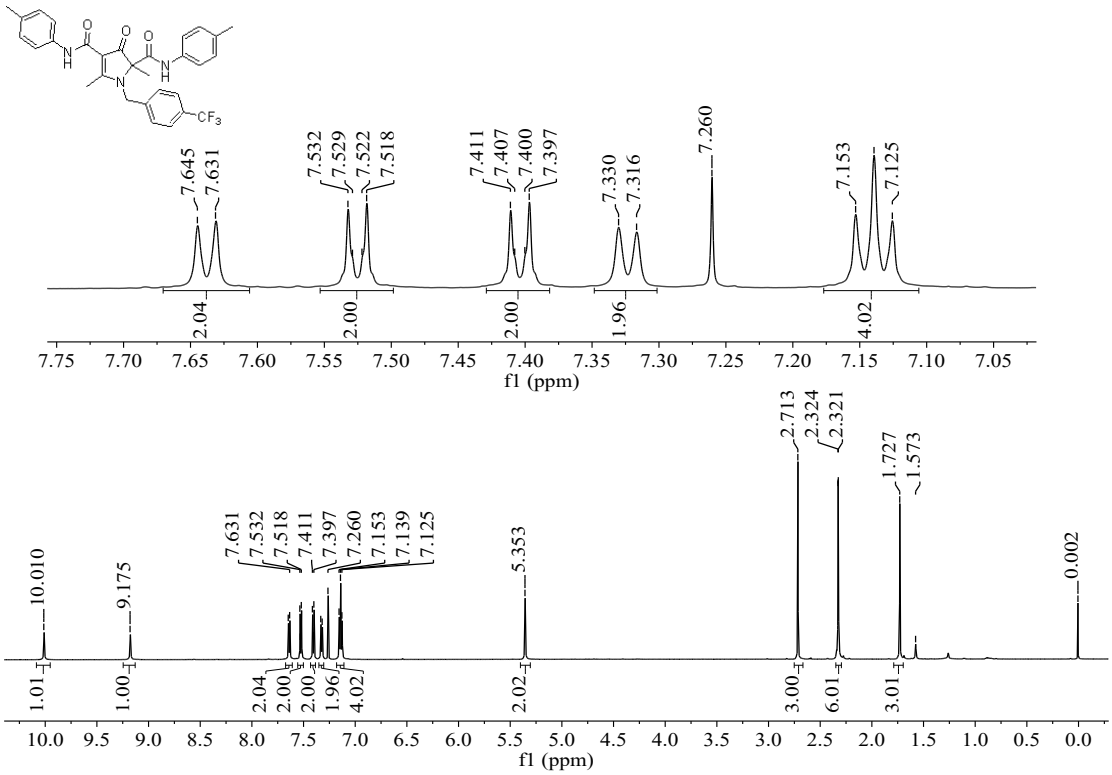
^{1}H NMR spectra of compound 2o (600 MHz, $CDCl_3$)



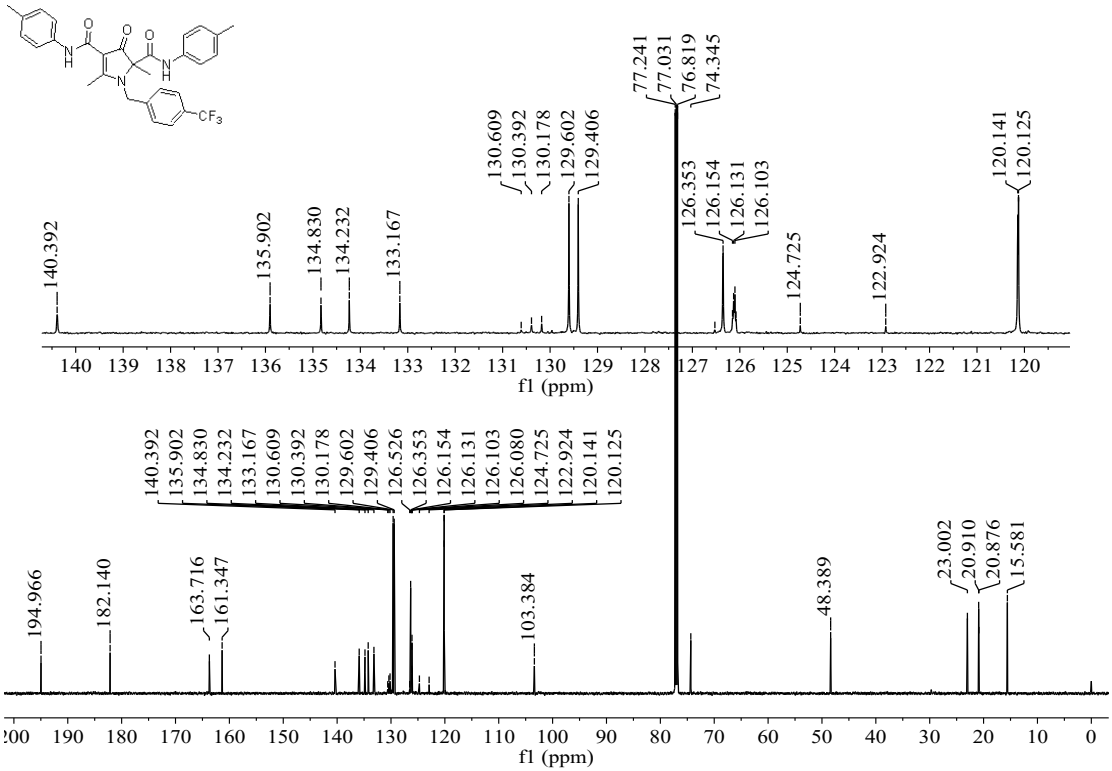
^{13}C NMR spectra of compound 2o (151 MHz, $CDCl_3$)



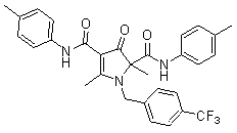
^{1}H NMR spectra of compound 2p (400 MHz, $CDCl_3$)

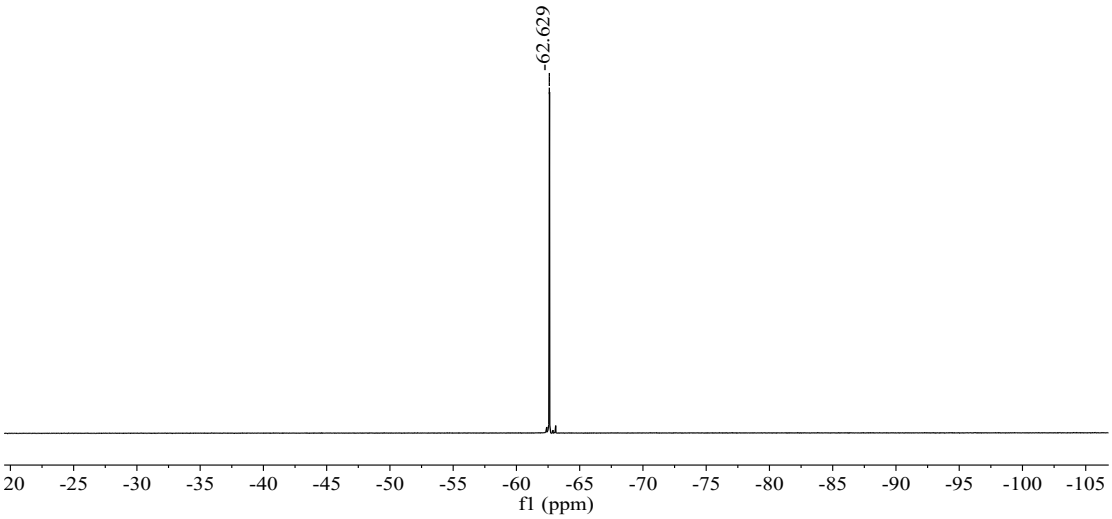


^{13}C NMR spectra of compound 2p (151 MHz, $CDCl_3$)

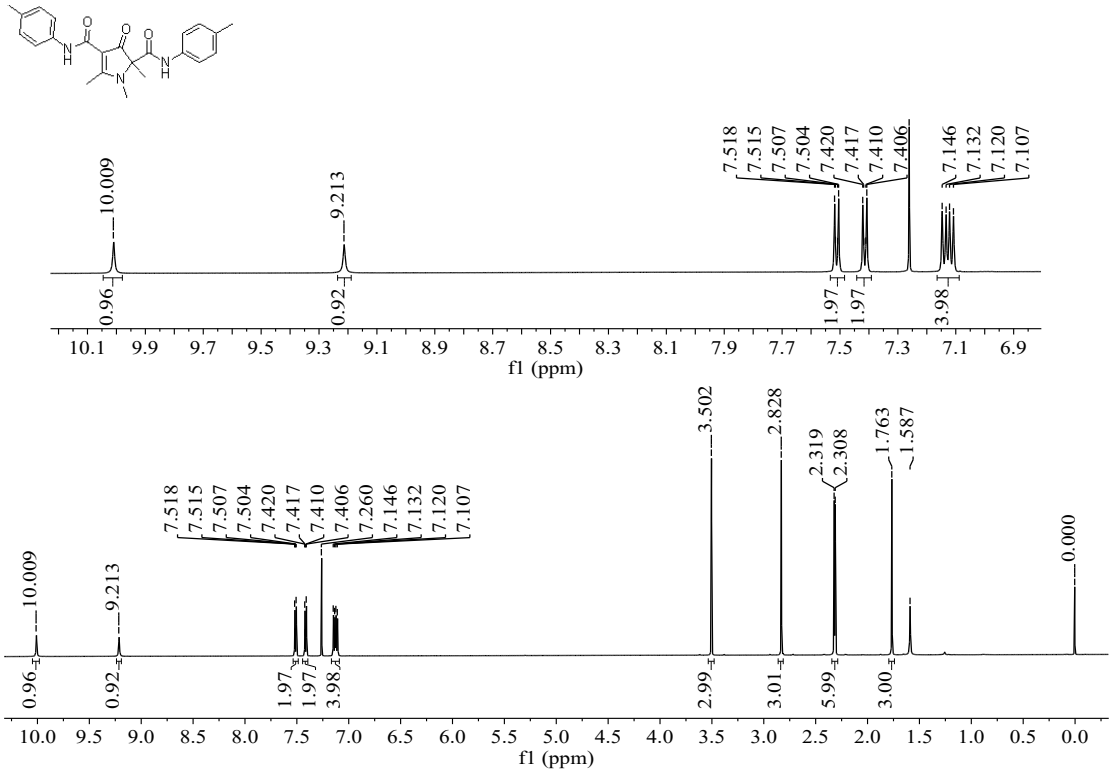


^{19}F NMR spectra of compound 2p (376 MHz, $CDCl_3$)

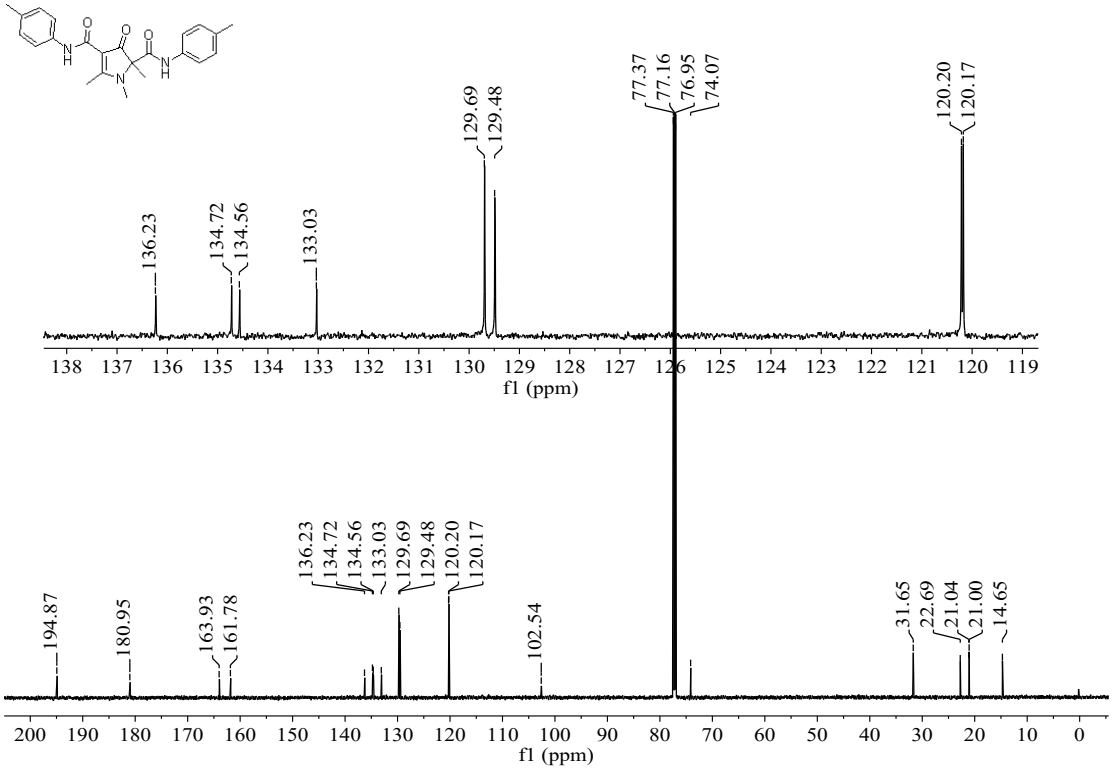




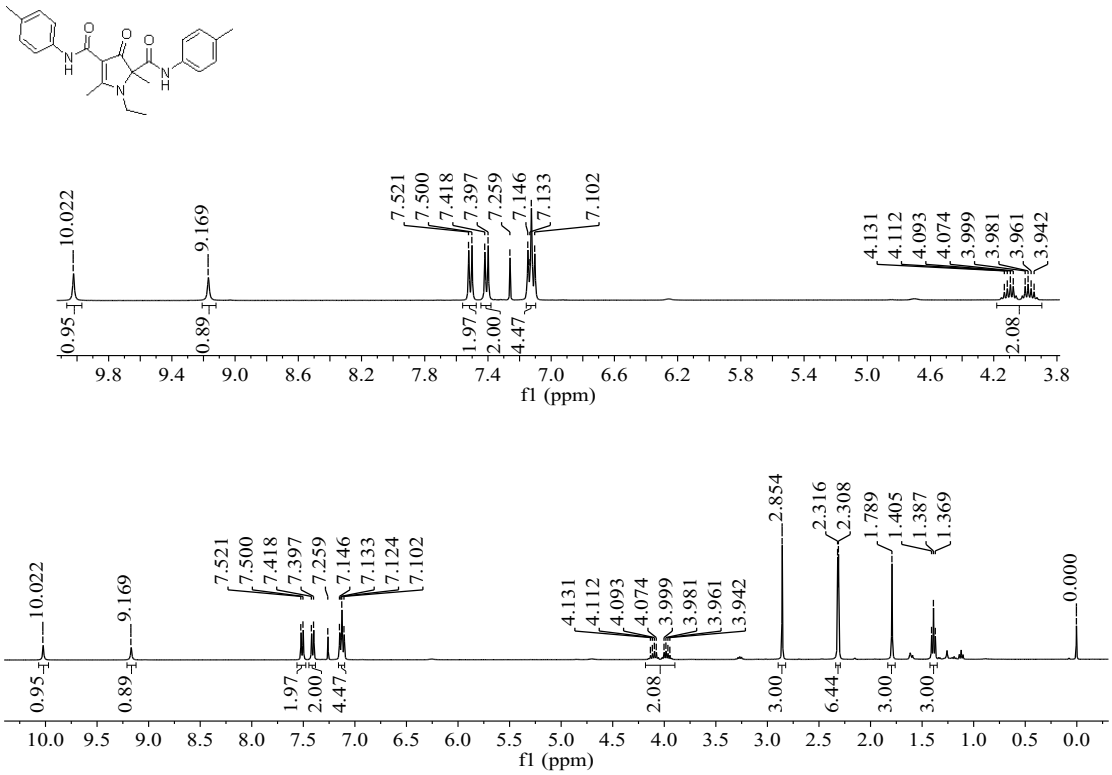
^{1}H NMR spectra of compound 2q (600 MHz, $CDCl_3$)



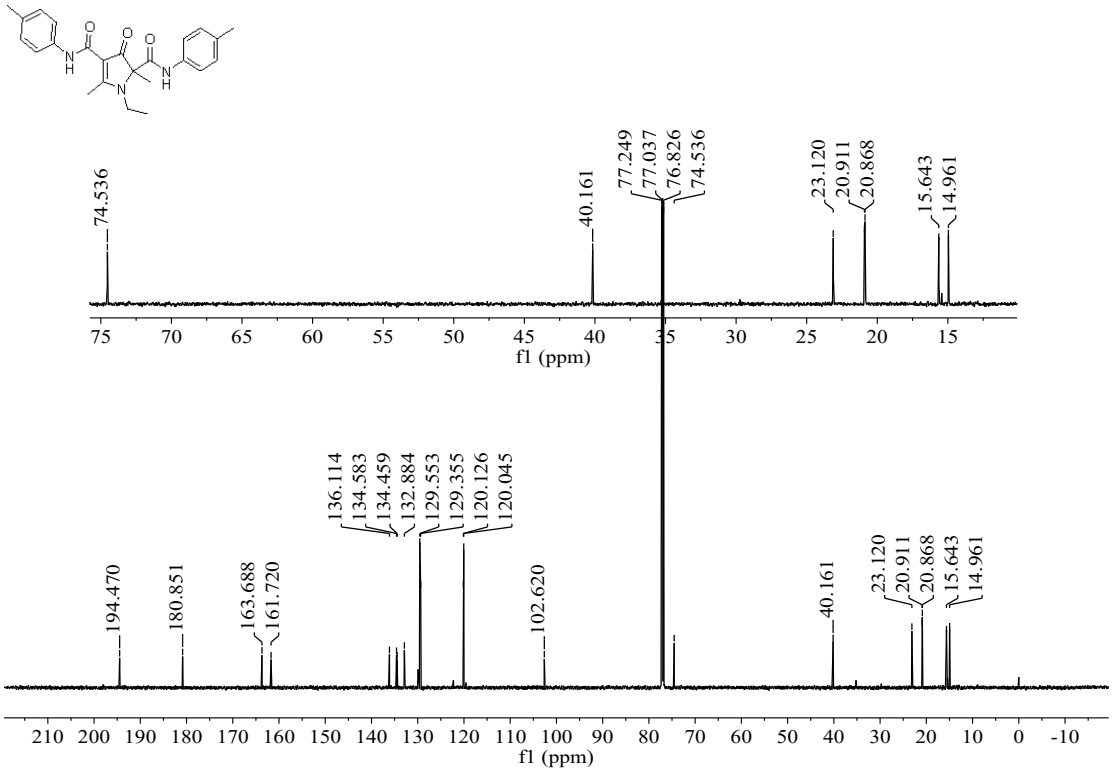
^{13}C NMR spectra of compound 2q (151 MHz, $CDCl_3$)



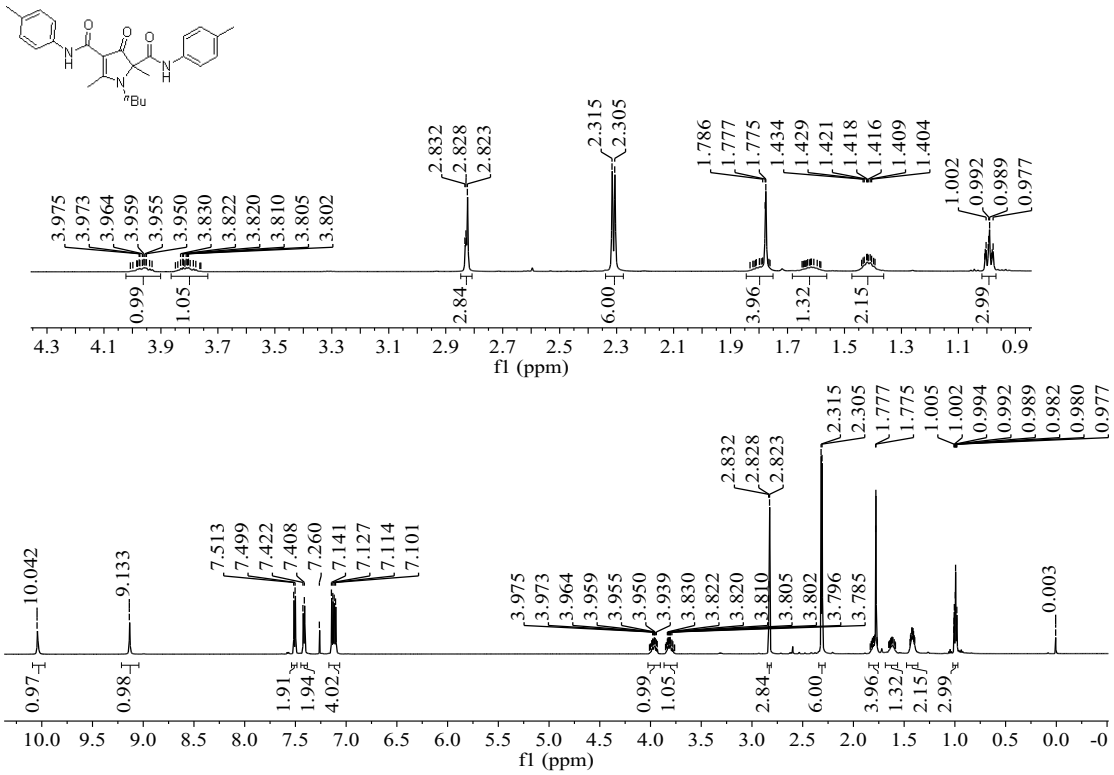
^{1}H NMR spectra of compound 2r (400 MHz, $CDCl_3$)



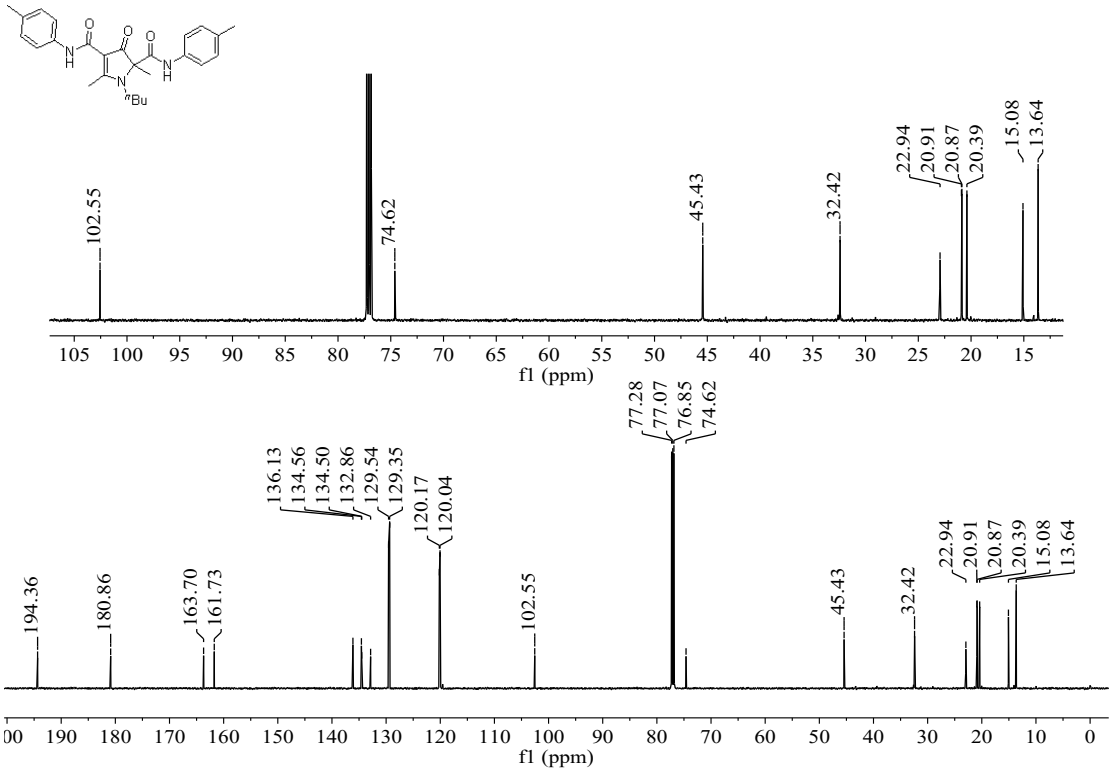
^{13}C NMR spectra of compound 2r (151 MHz, $CDCl_3$)



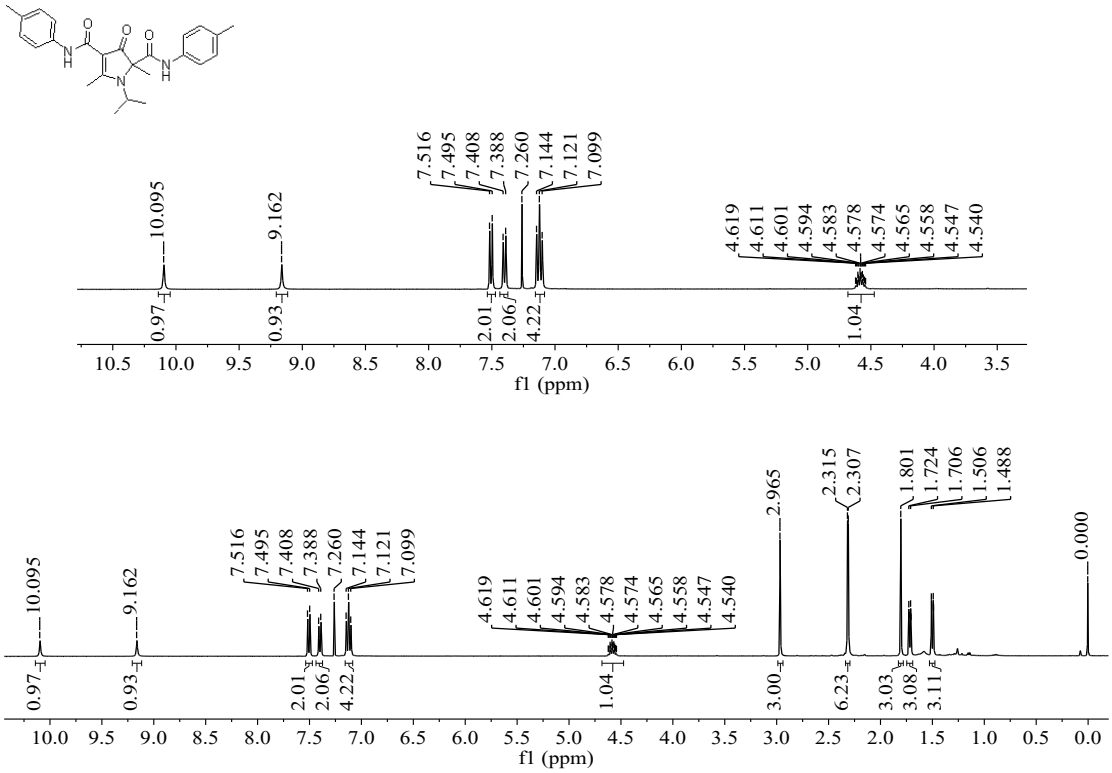
^{1}H NMR spectra of compound 2s (600 MHz, $CDCl_3$)



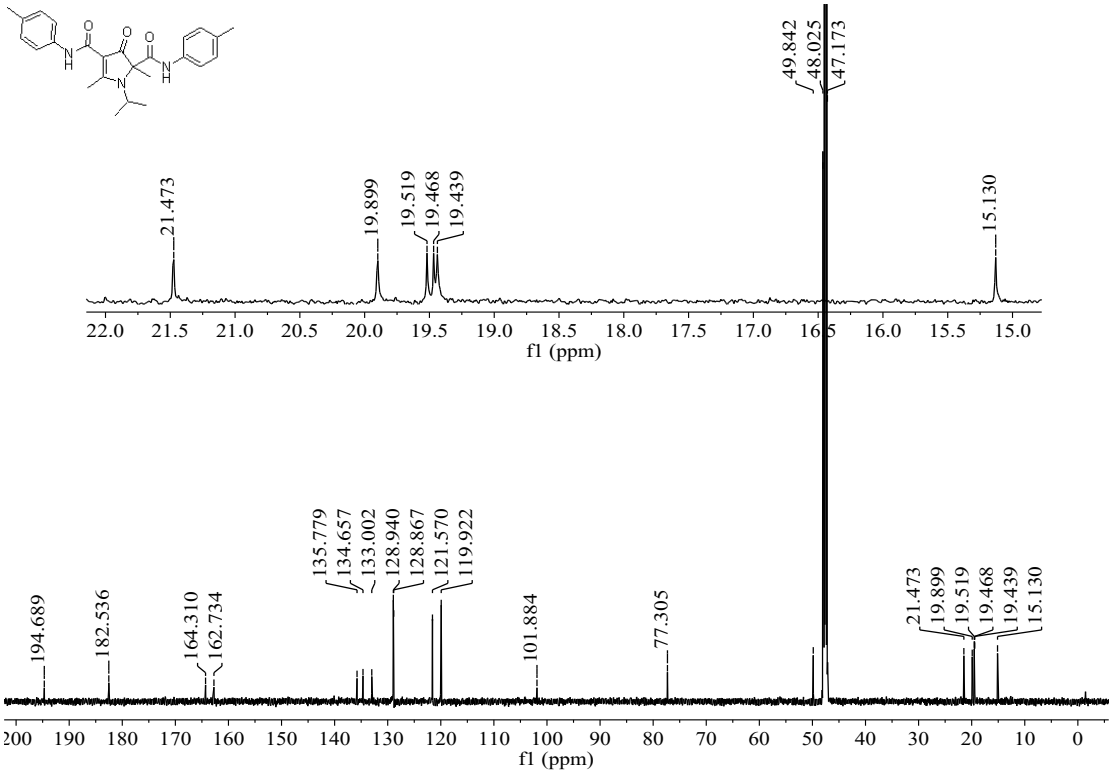
^{13}C NMR spectra of compound 2s (151 MHz, $CDCl_3$)



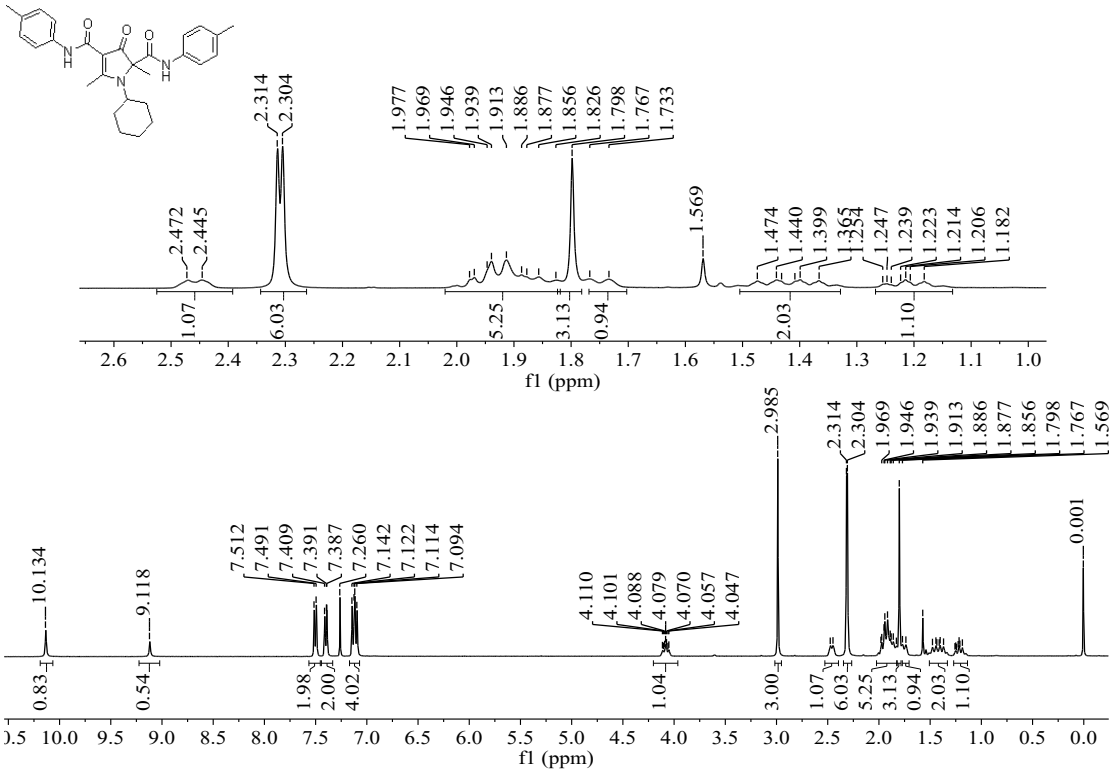
^{1}H NMR spectra of compound 2t (400 MHz, $CDCl_3$)



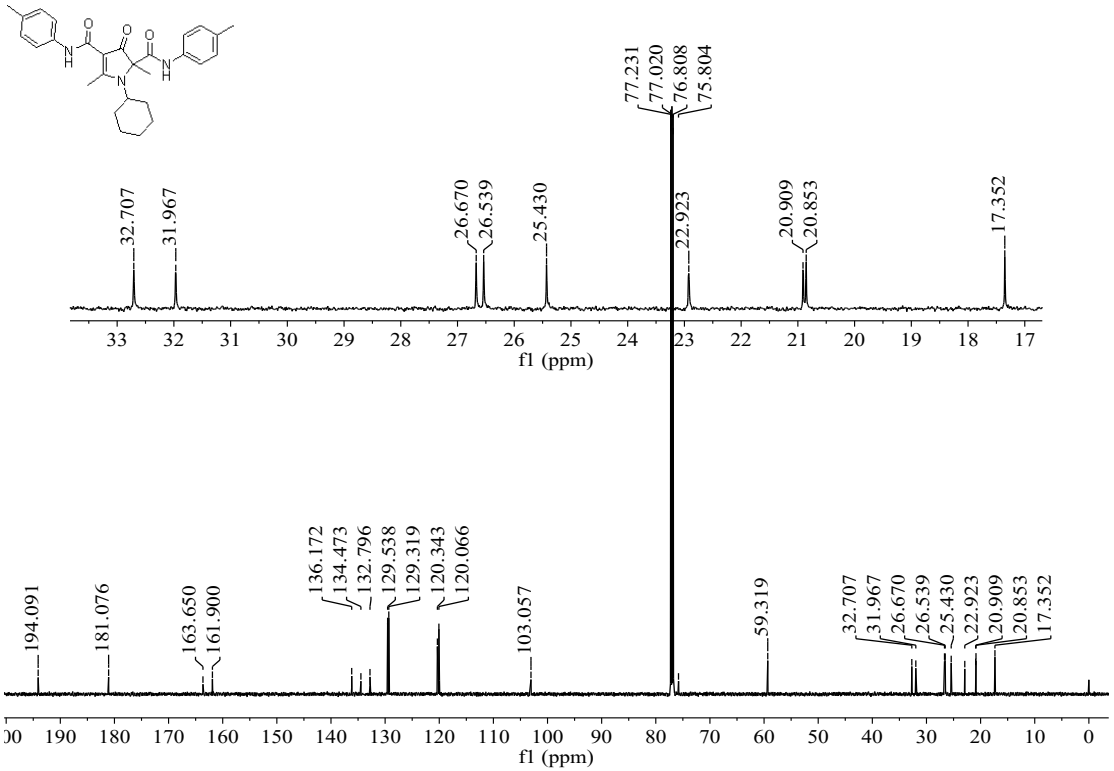
^{13}C NMR spectra of compound 2t (151 MHz, MeOD-*d_4*)



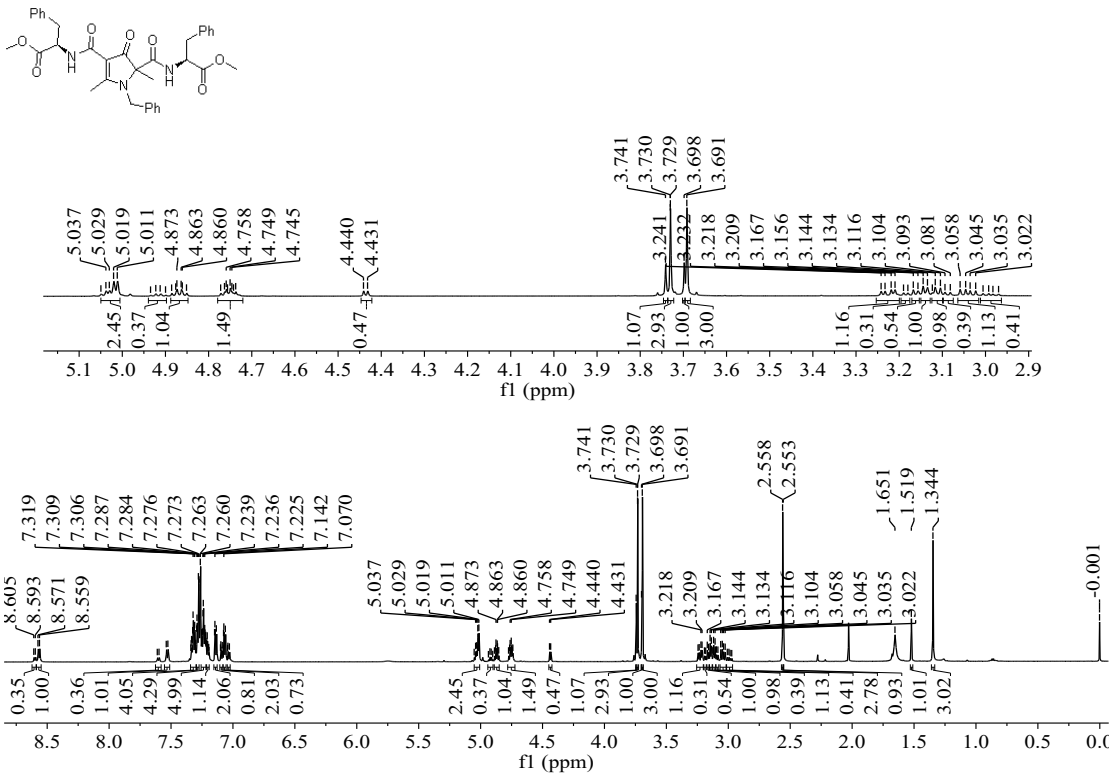
^{1}H NMR spectra of compound 2u (400 MHz, $CDCl_3$)



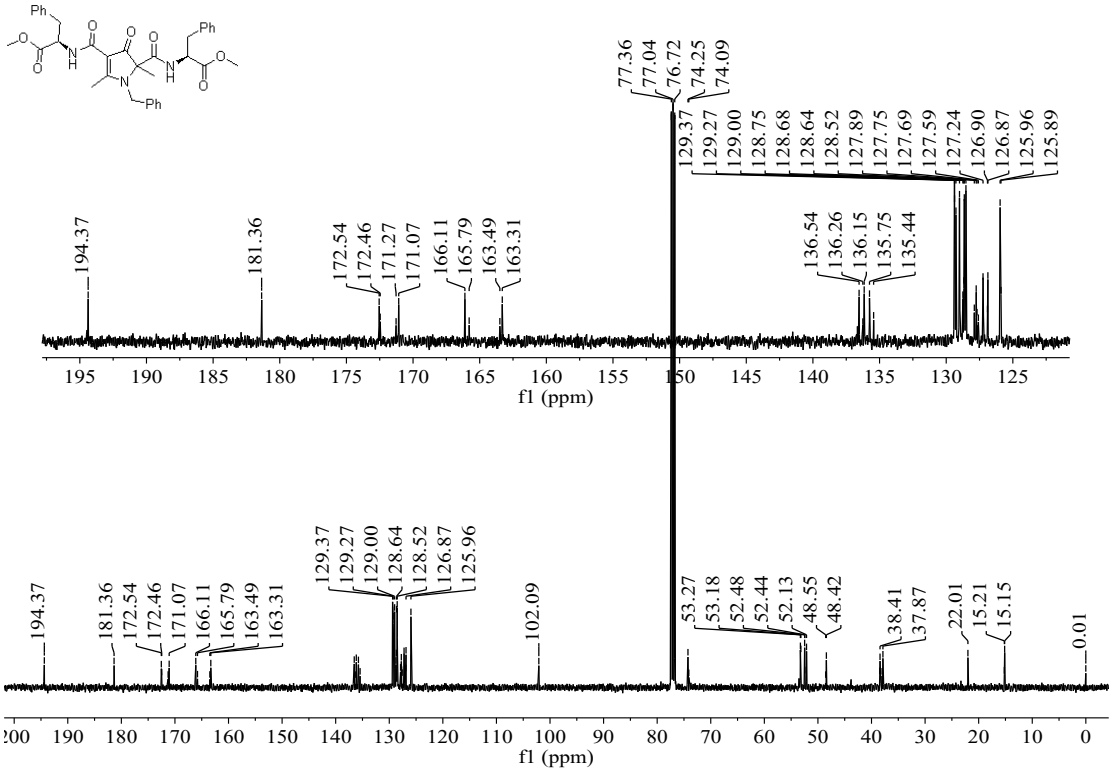
^{13}C NMR spectra of compound 2u (151 MHz, $CDCl_3$)



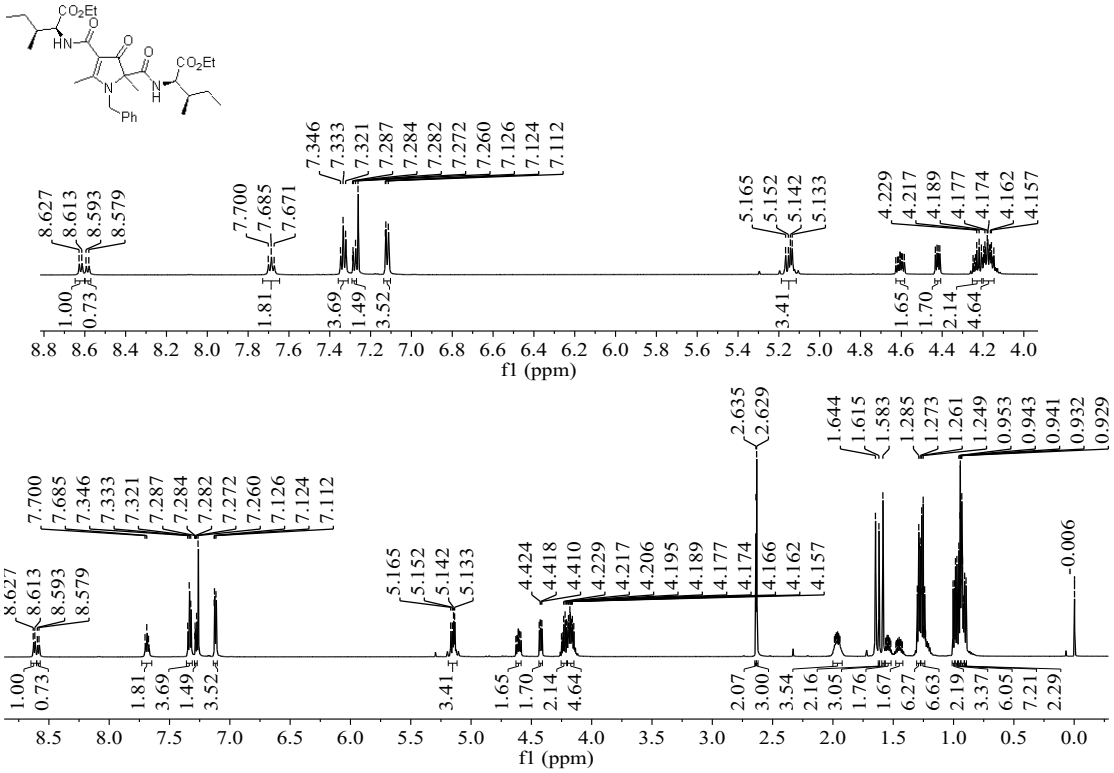
^{1}H NMR spectra of compound 2y (600 MHz, $CDCl_3$)



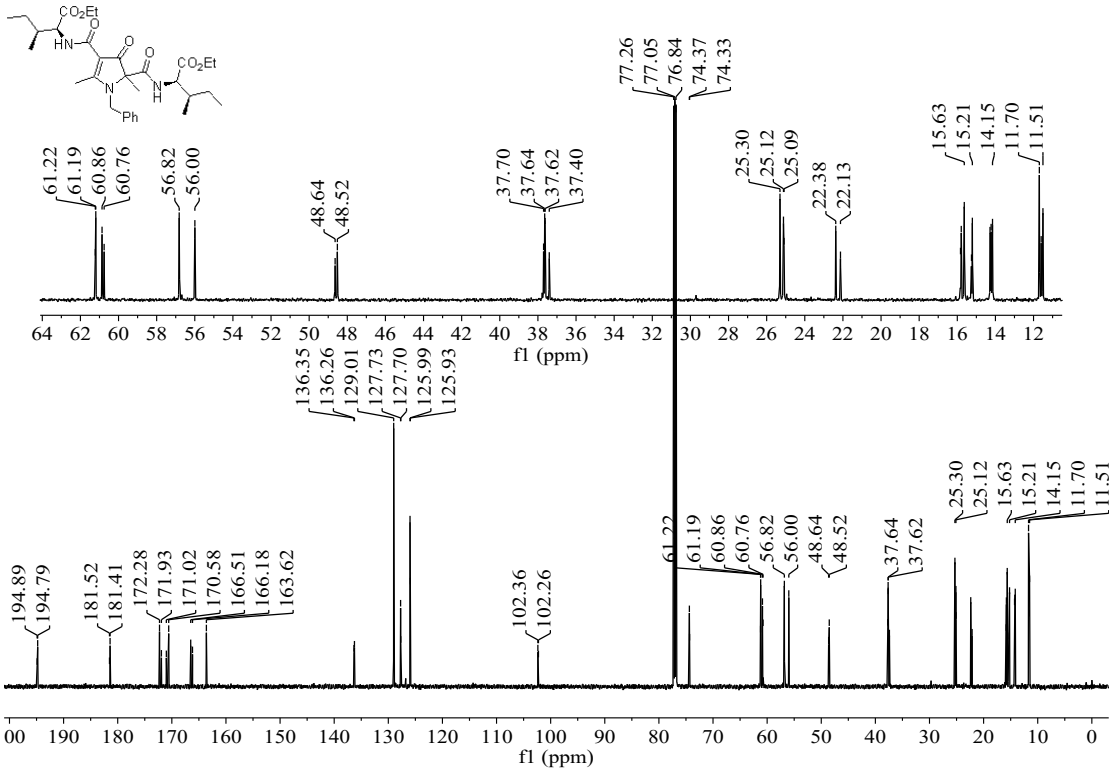
^{13}C NMR spectra of compound 2y (101 MHz, $CDCl_3$)



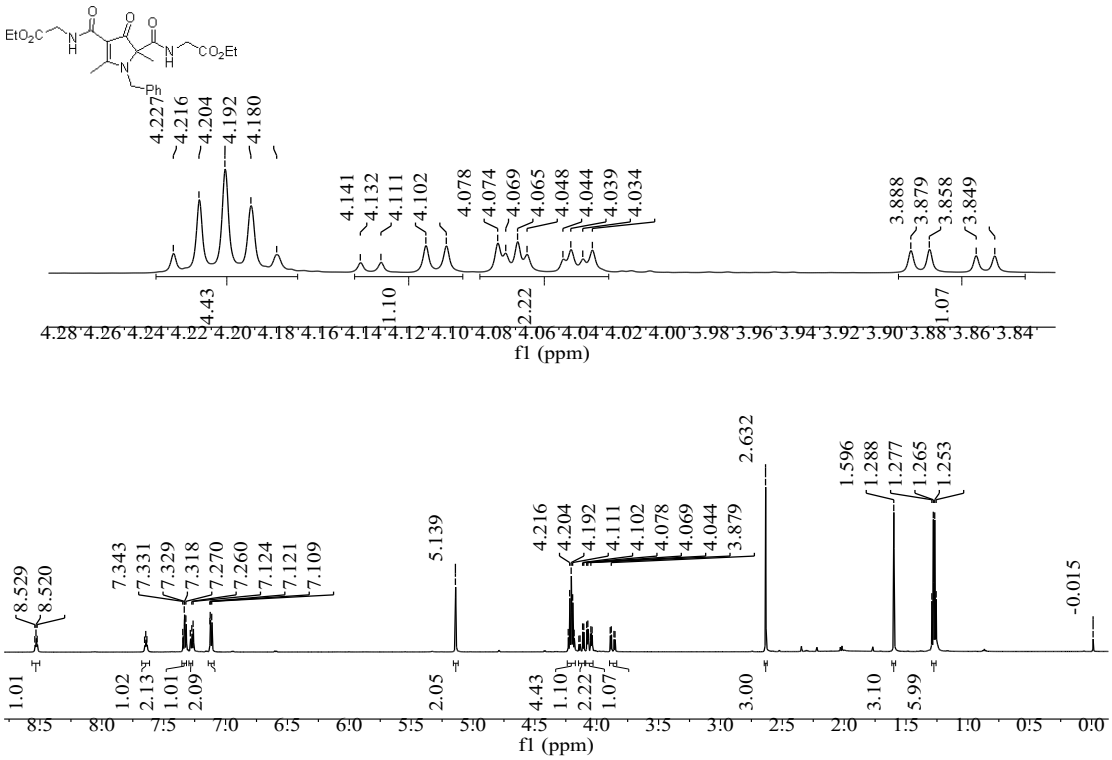
^{1}H NMR spectra of compound 2z (600 MHz, $CDCl_3$)



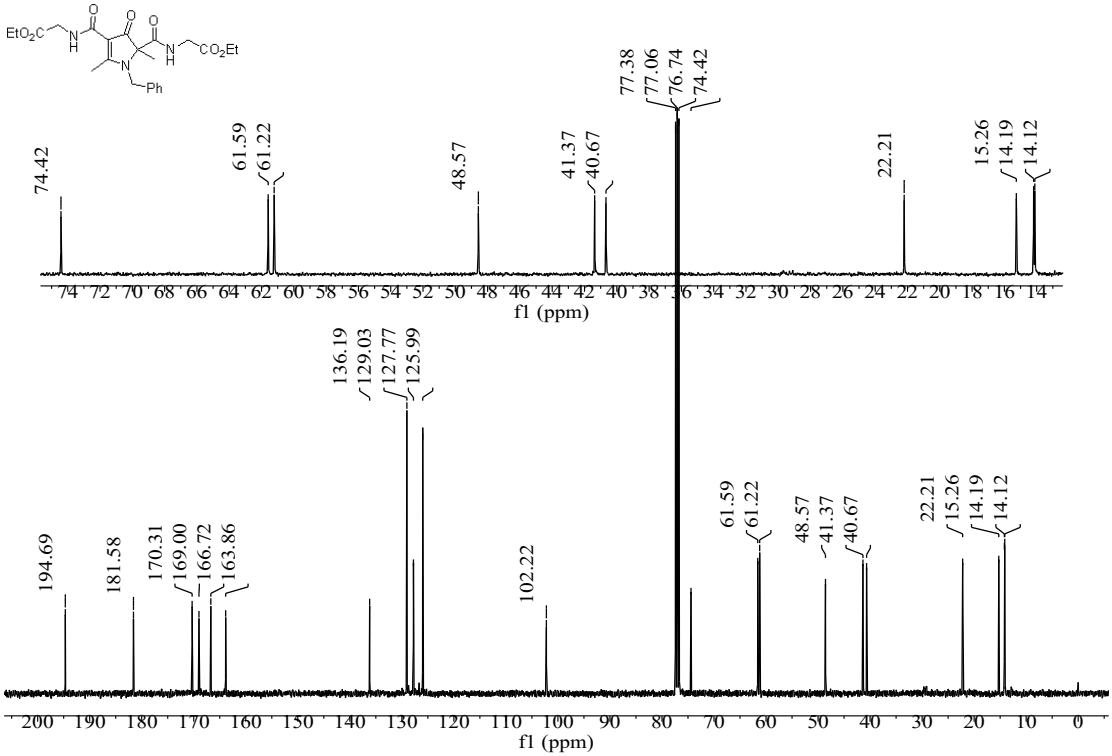
^{13}C NMR spectra of compound 2z (151 MHz, $CDCl_3$)



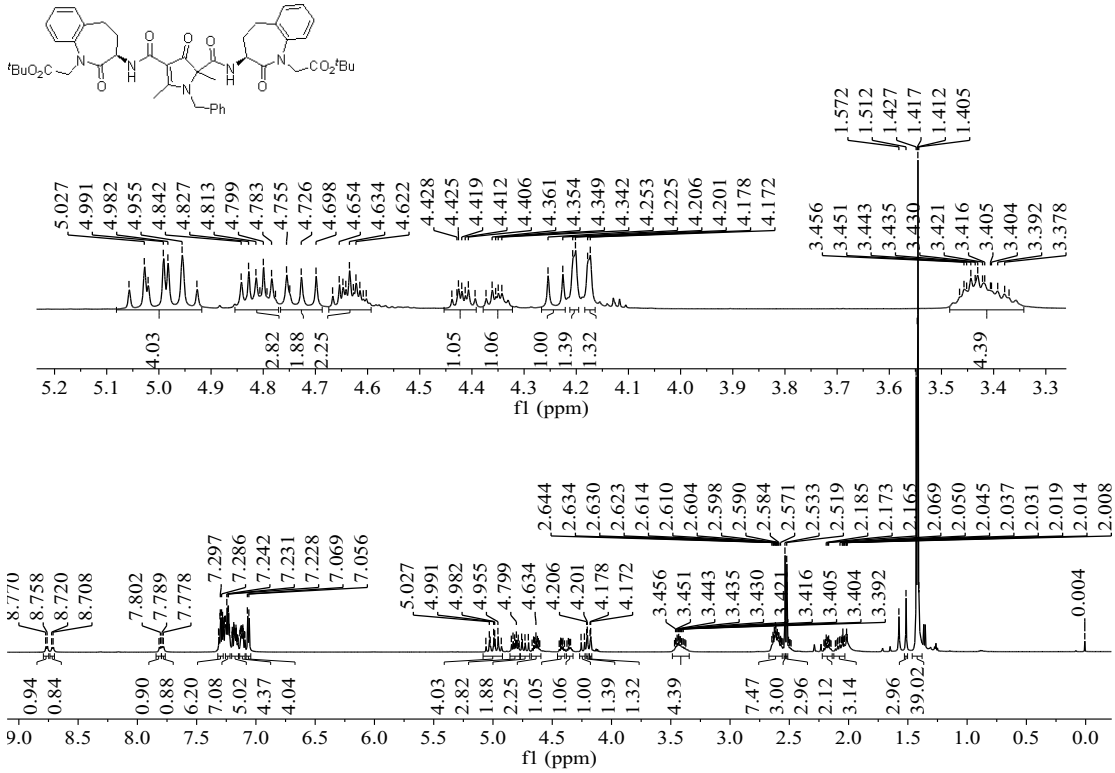
^{1}H NMR spectra of compound 2aa (600 MHz, $CDCl_3$)



^{13}C NMR spectra of compound 2aa (101 MHz, $CDCl_3$)



^{1}H NMR spectra of compound 2ab (600 MHz, $CDCl_3$)



^{13}C NMR spectra of compound 2ab (101 MHz, $CDCl_3$)