Supporting Information

Atroposelective Synthesis of *N*-Aryl Peptoid Atropisomers via Palladium(II)-Catalyzed Asymmetric C–H Alkynylation Strategy

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Content

1. General Information

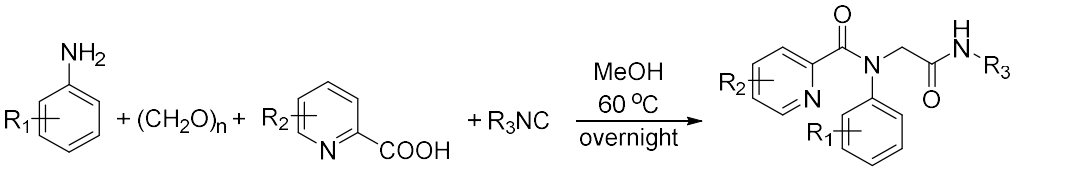
All the materials and solvents were purchased from commercial suppliers and used without additional purification. $Pd(MeCN)_2Cl_2$ were purchased from Adamas and used without additional purification. NMR spectra were recorded on a Bruker Avance operating for ^1H NMR at 400 MHz, ^{13}C NMR at 100 MHz, and ^{19}F NMR at 376 MHz, using TMS as internal standard. The peaks were internally referenced to $CDCl_3$ (7.26 ppm) or residual undeuterated solvent signal of $CDCl_3$ (77.16 ppm for ^{13}C NMR). The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad. High-resolution mass spectra (HRMS) were recorded on an Agilent Mass spectrometer using ESI-TOF (electrospray ionization-time of flight). High pressure liquid chromatography (HPLC) analyses were performed on a Shimadzu instrument using a chiral stationary phase column (Daicel Co. CHIRALPAK). The chiral HPLC methods were calibrated with the corresponding racemic mixtures.

2. Experimental Section

2.1 Preparation of Substrates

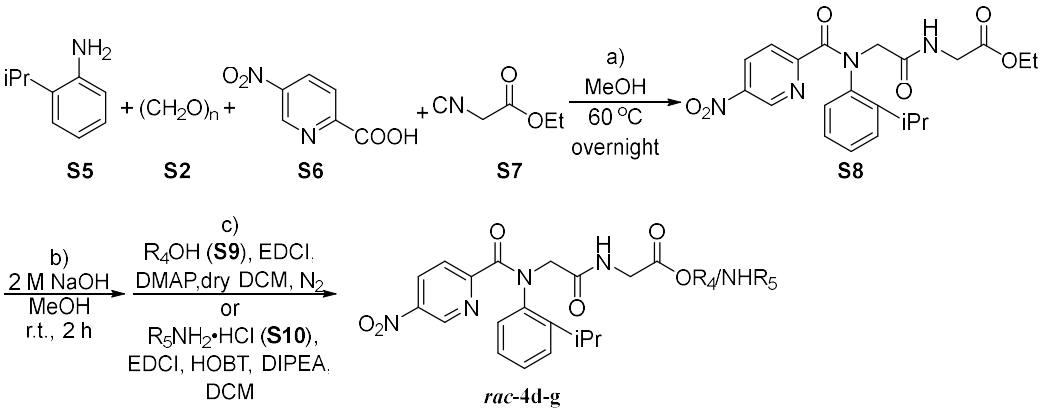
Synthesis and Characterization of Starting Materials

General Procedure A (Ugi reaction) for the Preparation of Compound *rac*-1a-1m, *rac*-4a-4c, *rac*-4h-4p and *rac*-4u-4v:



To a solution of the amine (**S1**) (5.0 mmol, 1.0 equiv) in methanol (10 mL, 0.5 M) was added paraformaldehyde (**S2**) (1.2 equiv). After being stirred for 1h at room temperature, picolinic acid (**S3**) (1.2 equiv) and isocyanide (**S4**) (1.2 equiv) was added. The mixture was then stirred overnight at 60 °C under air followed by cooling. The resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by silica gel column chromatography to afford the product.[1]

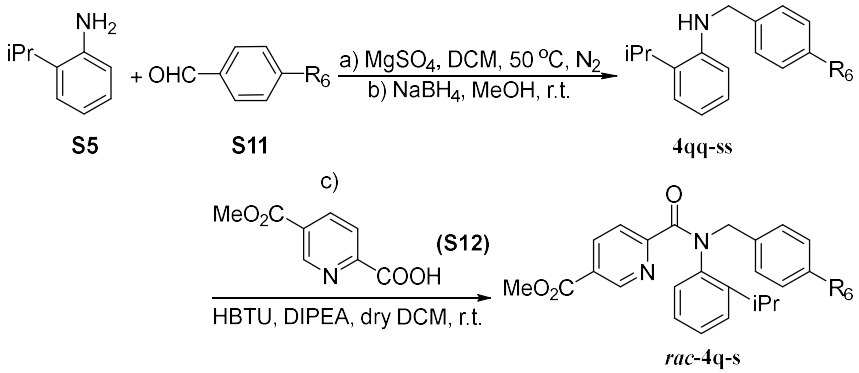
General Procedure B for the Preparation of Compound *rac*-4d-4g:



To a solution of the amine (**S5**) (5.0 mmol, 1.0 equiv) in methanol (10 mL, 0.5 M) was added paraformaldehyde (**S2**) (1.2 equiv). After being stirred for 1h at room temperature, picolinic acid (**S6**) (1.2 equiv) and isocyanide (**S7**) (1.2 equiv) was added. The mixture was then stirred overnight at 60 °C under air followed by cooling. The resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by silica gel column chromatography to afford the product **S8**. Then **S8** was solved in MeOH (5 mL), 2 M NaOH (5 mL) was added into the solution at room temperature. After being stirred for extra 2 h, the reaction was quenched with 1 M HCl and diluted with ethyl acetate. The organic layer was washed by brine, and the combined organic phase was dried over anhydrous Na_2SO_4. Evaporation of organic solvent gave the corresponding product without any purification. Then the product was solved in anhydrous DCM (20 mL), R_4OH (**S9**) (2.0 equiv), EDCI (2.0 equiv) and DMAP (0.2 equiv) were added into the mixture in turn [or R_5NH_2 (1.5 equiv), EDCI (2.0 equiv), HOBT (1.2

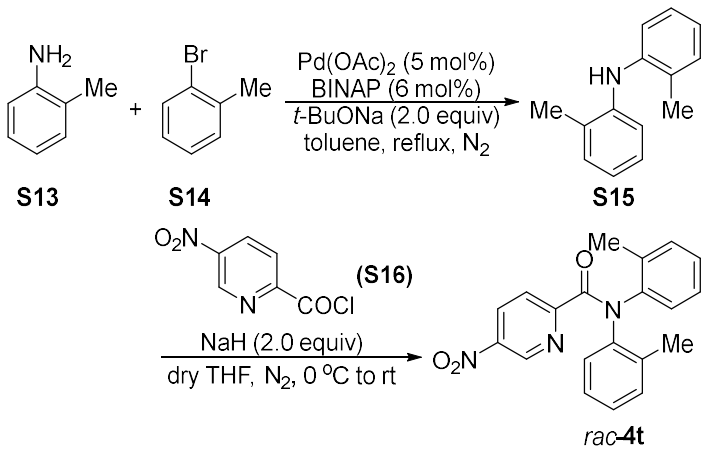
equiv) and DIPEA (3.0 equiv) were added into the mixture in turn]. After being stirred at room temperature overnight. The reaction was diluted with dichloromethane and water was added to the mixture. The aqueous phase was separated and the organic phase was washed with brine. The combined organic layers were dried over Na_2SO_4, filtered, concentrated, and the residue was purified by silica gel column chromatography to afford the product.

General Procedure C for the Preparation of Compound *rac*-4q-4s:



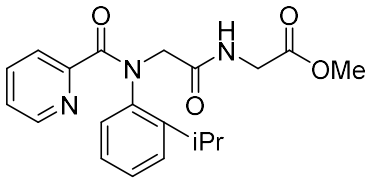
To a solution of the amine (**S5**) (10.0 mmol, 1.0 equiv) and aldehyde (**S11**) (1.5 equiv) in DCM (20 mL, 0.5 M) was added anhydrous $MgSO_4$. The mixture was then stirred for 8 h at 50 °C under N_2 followed by cooling. The reaction mixture was filtered through a celite pad and then evaporation of organic solvent gave the corresponding product without any purification. Then the product was solved in MeOH (30 mL), and $NaBH_4$ (2.0 equiv) was added in portions. After being stirred for 4 h at room temperature, the reaction mixture was quenched with water and extracted with EtOAc. The combined organic layers were dried over Na_2SO_4, filtered, concentrated, and the residue was purified by silica gel column chromatography to afford the product **4qq-ss**. Then the product was solved in anhydrous DCM (30 mL), picolinic acid (**S12**) (1.5 equiv), HBTU (1.5 equiv) and DIPEA (3.0 equiv) were added into the mixture in turn. After being stirred at room temperature overnight. The reaction was diluted with dichloromethane and water was added to the mixture. The aqueous phase was separated and the organic phase was washed with brine. The combined organic layers were dried over Na_2SO_4, filtered, concentrated, and the residue was purified by silica gel column chromatography to afford the product.

General Procedure D for the Preparation of Compound *rac*-4t:



The o-toluidine (**S13**) (1.0 equiv) and 2-bromotoluene (**S14**) (1.0 equiv) was solved in toluene (0.5 M), $Pd(OAc)_2$ (5 mol%), BINAP (6 mol%) and *t*-BuONa (2.0 equiv) were added into the mixture in turn. Then the mixture was refluxed for 12 h under N_2 in oil bath. Afterwards the resulting solution was filtered through a plug of Celite and concentrated in vacuo. The residue was purified by silica gel column chromatography to afford the product **S15**. Then the product **S15** (1.5 equiv) was solved in anhydrous THF (0.5 M), NaH (2.0 equiv, 60% dispersion in mineral oil) was added into the solution under the N_2 atmosphere at 0 ºC, and the mixture was stirred for extra 1h. Then the picolinoyl chloride (**S16**) (1.0 equiv) was solved in anhydrous THF and added into the system dropwise, then warm to room temperature overnight. After being stirred overnight, the reaction was quenched with water at 0 ºC and diluted with ethyl acetate. The organic layer was washed by brine, and the combined organic phase was dried over anhydrous Na_2SO_4. Evaporation of organic solvent and purification by column chromatography gave the corresponding product *rac*-**4t**.

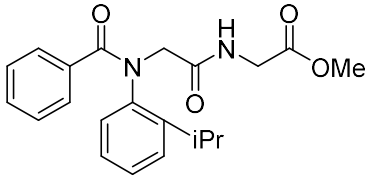
Methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-1a)



The title compound ***rac*-1a** was prepared according to the general procedure A and was purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1a** was obtained as a light yellow solid, *E*: *Z* = 4: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 4.6 Hz, 1H), 7.59-7.52 (m, 2H), 7.38-7.35 (m, 1H), 7.25 (d, *J* = 8.7 Hz, 1H), 7.17 (d, *J* = 3.9 Hz, 2H), 7.12-7.09 (m, 1H), 7.04-7.00 (m, 1H), 4.94 (d, *J* = 14.9 Hz, 1H), 4.21 (dd, *J* = 18.2, 5.9 Hz, 1H), 4.01 (dd, *J* = 18.2, 5.0 Hz, 1H), 3.98 (d, *J* = 14.8 Hz, 1H), 3.76 (s, 3H), 3.15-3.09 (m, 1H), 1.16 (d, *J* = 6.8 Hz, 3H), 0.99 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.26, 169.92, 168.76, 152.79, 148.28, 145.59, 140.35, 136.09, 129.02, 128.70, 126.86, 126.44, 124.43, 123.94, 55.27, 52.42, 41.20, 27.99, 24.88, 22.85; **HRMS** (ESI-TOF) calcd for $[C_{20}H_{23}N_3O_4+Na^+]$: 392.1581, found: 392.1581.

Methyl *N*-benzoyl-*N*-(2-isopropylphenyl)glycylglycinate (*rac*-1b)

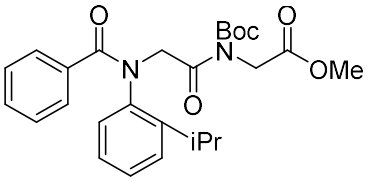


The title compound ***rac*-1b** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1b** was obtained as a brown solid, *E*: *Z* > 99: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (dd, *J* = 22.7, 7.5 Hz, 4H), 7.25-7.11 (m, 6H), 4.84 (d, *J* = 14.8 Hz, 1H), 4.19-3.99 (m, 3H), 3.75 (s, 3H), 2.96-2.89 (m, 1H), 1.08 (d, *J* = 6.8 Hz, 3H), 0.73 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 171.55, 170.26, 169.02, 145.16, 140.69, 134.46, 130.23, 128.94, 128.91, 127.63, 127.22, 126.96, 55.57, 52.37, 41.16, 27.71, 25.21, 22.30; **HRMS** (ESI-TOF) calcd for

[$C_{21}H_{24}N_2O_4$+Na^+]: 391.1628, found: 391.1629.

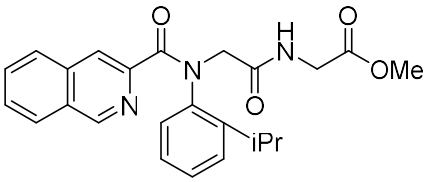
Methyl *N*-(*N*-benzoyl-*N*-(2-isopropylphenyl)glycyl)-*N*-(tert-butoxycarbonyl)glycinate (*rac*-1c)



The title compound ***rac*-1c** was prepared according to the general procedure A then reacted with Boc_2O and purified by flash chromatography (petroleum ether: ethyl acetate = 8: 1). ***rac*-1c** was obtained as light yellow solid, *E*: *Z* > 99: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 7.6 Hz, 2H), 7.21-7.15 (m, 3H), 7.13-7.05 (m, 3H), 5.51 (d, *J* = 17.8 Hz, 1H), 4.66-4.54 (m, 2H), 4.41 (d, *J* = 17.3 Hz, 1H), 3.72 (s, 3H), 3.20-3.13 (m, 1H), 1.49 (s, 9H), 1.16 (d, *J* = 6.8 Hz, 3H), 0.85 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.71, 170.66, 169.30, 151.90, 145.36, 141.23, 135.10, 129.79, 129.33, 128.81, 128.46, 127.48, 126.94, 126.60, 84.38, 57.16, 52.26, 45.39, 27.88, 27.63, 25.12, 22.43; **HRMS** (ESI-TOF) calcd for [$C_{26}H_{32}N_2O_6$+Na^+]: 491.2152, found: 491.2154.

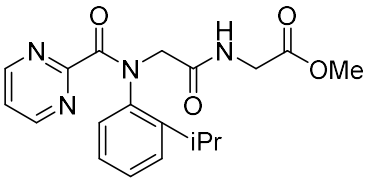
Methyl *N*-(2-isopropylphenyl)-*N*-(isoquinoline-3-carbonyl)glycylglycinate (*rac*-1d)



The title compound ***rac*-1d** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1d** was obtained as a light yellow solid, *E*: *Z* = 5: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.5 Hz, 1H), 7.73-7.67 (m, 3H), 7.57 (t, *J* = 7.2 Hz, 1H), 7.46 (t, *J* = 7.4 Hz, 1H), 7.41 (d, *J* = 5.9 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.16-7.10 (m, 2H), 7.01-6.97 (m, 1H), 5.05 (d, *J* = 14.9 Hz, 1H), 4.22 (dd, *J* = 18.1, 6.0 Hz, 1H), 4.04 (dd, *J* = 18.1, 5.0 Hz 1H), 4.00 (d, *J* = 14.9 Hz, 1H), 3.75 (s, 3H), 3.27-3.17 (m, 1H), 1.18 (d, *J* = 6.8 Hz, 3H), 1.03 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.27, 169.76, 168.70, 152.45, 146.52, 145.45, 140.54, 136.24, 129.77, 129.63, 129.09, 128.63, 127.71, 127.61, 127.43, 126.80, 126.37, 120.66, 55.33, 52.39, 41.22, 27.98, 24.78, 23.10; **HRMS** (ESI-TOF) calcd for [$C_{24}H_{25}N_3O_4$+Na^+]: 442.1737, found: 442.1739.

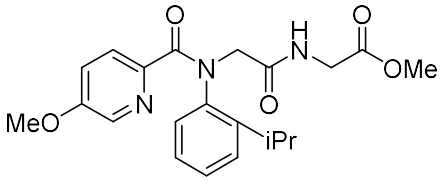
Methyl *N*-(2-isopropylphenyl)-*N*-(pyrimidine-2-carbonyl)glycylglycinate (*rac*-1e)



The title compound ***rac*-1e** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1e** was obtained as a light yellow solid, *E*: *Z* = 8: 1.

^{1}H NMR (400 MHz, $(CD_3)_2SO$) δ 8.65 (d, *J* = 4.9 Hz, 2H), 8.53 (t, *J* = 5.8 Hz, 1H), 7.34-7.31 (m, 2H), 7.27 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.18 (td, *J* = 7.4, 1.4 Hz, 1H), 6.99 (td, *J* = 7.6, 1.6 Hz, 1H), 5.00 (d, *J* = 16.0 Hz, 1H), 3.96 (d, *J* = 5.8 Hz, 2H), 3.85 (d, *J* = 16.0 Hz, 1H), 3.66 (s, 3H), 3.27-3.20 (m, 1H), 1.22 (dd, *J* = 9.8, 6.9 Hz, 6H); **^{13}C NMR (101 MHz, $(CD_3)_2SO$)** δ 170.65, 167.91, 166.69, 162.15, 157.26, 146.52, 139.17, 131.15, 129.10, 126.90, 126.03, 121.56, 52.18, 51.84, 41.06, 27.88, 24.81, 23.42; **HRMS** (ESI-TOF) calcd for $[C_{19}H_{22}N_4O_4+Na^+]$: 393.1533, found: 393.1534.

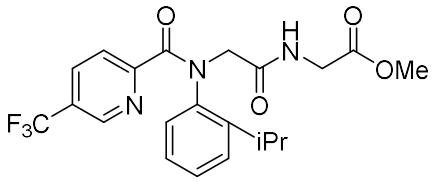
Methyl *N*-(2-isopropylphenyl)-*N*-(5-methoxypicolinoyl)glycylglycinate (*rac*-1f)



The title compound ***rac*-1f** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1f** was obtained as a reddish brown solid, *E*: *Z* = 4: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 2.7 Hz, 1H), 7.56 (d, *J* = 8.8 Hz, 1H), 7.44 (t, *J* = 5.8 Hz, 1H), 7.22-7.16 (m, 3H), 7.04-7.00 (m, 2H), 4.88 (d, *J* = 14.9 Hz, 1H), 4.15 (dd, *J* = 18.1, 5.9 Hz, 1H), 4.01-3.94 (m, 2H), 3.73 (s, 3H), 3.72 (s, 3H), 3.11-3.04 (m, 1H), 1.14 (d, *J* = 6.9 Hz, 3H), 0.96 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.22, 169.40, 168.92, 156.04, 145.40, 144.59, 141.03, 135.96, 128.70, 128.37, 126.78, 126.34, 125.41, 119.49, 55.53, 55.49, 52.29, 41.14, 27.96, 24.72, 22.92; **HRMS** (ESI-TOF) calcd for $[C_{21}H_{25}N_3O_5+Na^+]$: 422.1686, found: 422.1687.

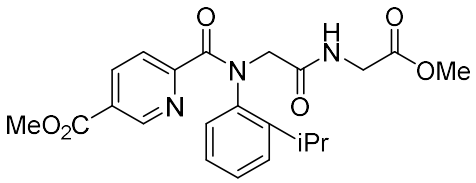
Methyl *N*-(2-isopropylphenyl)-*N*-(5-(trifluoromethyl)picolinoyl)glycylglycinate (*rac*-1g)



The title compound ***rac*-1g** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1g** was obtained as a brown solid, *E*: *Z* = 7: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46 (s, 1H), 7.80 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.30 -7.25 (m, 1H), 7.22-7.14 (m, 3H), 6.98-6.94 (m, 1H), 4.97 (d, *J* = 15.1 Hz, 1H), 4.12 (dd, *J* = 18.3, 6.0 Hz, 1H), 3.99 (dd, *J* = 18.1, 5.2 Hz, 1H), 3.91 (d, *J* = 15.1 Hz, 1H), 3.70 (s, 3H), 3.17-3.10 (m, 1H), 1.15 (d, *J* = 6.9 Hz, 3H), 1.05 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.26, 168.49, 168.20, 156.13, 145.71, 144.96 (q, J_{CF} = 4.0 Hz), 139.83, 133.51 (q, J_{CF} = 3.0 Hz), 129.03, 129.01, 127.19 (q, J_{CF} = 19.2 Hz), 126.96, 126.48, 125.47 (q, J_{CF} = 235.3 Hz), 123.73, 54.94, 52.39, 41.16, 28.02, 24.69, 22.94; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -62.70; **HRMS** (ESI-TOF) calcd for $[C_{21}H_{22}F_3N_3O_4+Na^+]$: 460.1454, found: 460.1455.

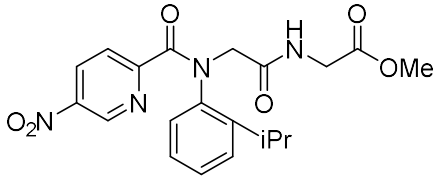
Methyl 6-((2-isopropylphenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (*rac*-1h)



The title compound ***rac*-1h** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 4: 1: 1%). ***rac*-1h** was obtained as a light yellow solid, *E*: *Z* = 5: 1.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.83 (s, 1H), 8.17 (d, *J* = 8.1 Hz, 1H), 7.63 (d, *J* = 8.1 Hz, 1H), 7.37 (t, *J* = 5.7 Hz, 1H), 7.25 (d, *J* = 7.6 Hz, 1H), 7.19 -7.14 (m, 2H), 7.01-6.94 (m, 1H), 4.99 (d, *J* = 15.0 Hz, 1H), 4.15 (dd, *J* = 18.2, 4.9 Hz, 1H), 4.02 (dd, *J* = 17.7, 4.9 Hz, 1H), 3.94 (d, *J* = 15.8 Hz, 1H), 3.86 (s, 3H), 3.73 (s, 3H), 3.19-3.13 (m, 1H),1.16 (d, *J* = 6.2 Hz, 3H), 1.07 (d, *J* = 6.1 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 170.28, 168.94, 168.36, 164.99, 156.40, 149.23, 145.73, 139.87, 137.26, 129.19, 128.88, 126.85, 126.37, 125.97, 123.39, 54.63, 52.47, 52.30, 41.14, 27.93, 24.73, 22.88; **HRMS** (ESI-TOF) calcd for [$C_{22}H_{25}N_3O_6$+Na^+]: 450.1635, found: 450.1637.

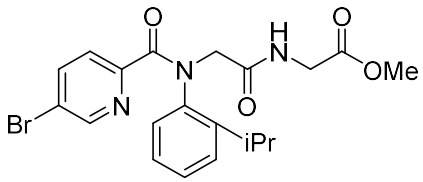
Methyl *N*-(2-isopropylphenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (*rac*-1i)



The title compound ***rac*-1i** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 4: 1: 1%). ***rac*-1i** was obtained as a reddish brown solid, *E*: *Z* = 10: 1.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.98 (d, *J* = 2.3 Hz, 1H), 8.36 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.79 (d, *J* = 8.6 Hz, 1H), 7.20-7.12 (m, 4H), 6.95 (td, *J* = 6.9, 2.0 Hz, 1H), 4.98 (d, *J* = 15.1 Hz, 1H), 4.14 (dd, *J* = 18.2, 5.8 Hz, 1H), 4.01 (dd, *J* = 18.2, 5.2 Hz, 1H), 3.90 (d, *J* = 15.1 Hz, 1H), 3.72 (s, 3H), 3.21-3.12 (m, 1H), 1.17 (d, *J* = 6.9 Hz, 3H), 1.12 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR (101 MHz, CDCl$_3$)** δ 170.31, 167.91, 167.89, 158.00, 145.90, 143.62, 143.44, 139.43, 131.51, 129.28, 129.17, 127.11, 126.56, 124.33, 54.74, 52.48, 41.18, 28.07, 24.70, 23.05; **HRMS** (ESI-TOF) calcd for [$C_{20}H_{22}N_4O_6$+Na^+]: 437.1431, found: 437.1430.

Methyl *N*-(5-bromopicolinoyl)-*N*-(2-isopropylphenyl)glycylglycinate (*rac*-1j)

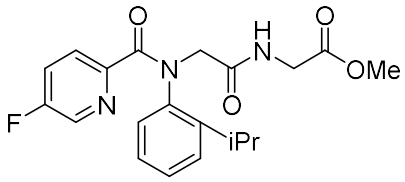


The title compound ***rac*-1j** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1j** was obtained as a white solid, *E*: *Z* = 5: 1.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.29 (d, *J* = 1.9 Hz, 1H), 7.74 (dd, *J* = 8.3, 2.3 Hz, 1H), 7.53 (d, *J* = 8.3 Hz, 1H), 7.21-7.17 (m, 4H), 7.04-7.00 (m, 1H), 4.93 (d, *J* = 14.8 Hz, 1H), 4.21 (dd, *J* = 18.2, 6.0 Hz, 1H), 4.02 (dd, *J* = 18.2, 5.0 Hz, 1H), 3.93 (d, *J* = 14.8 Hz, 1H), 3.77 (s, 3H), 3.16-3.09 (m, 1H), 1.19 (d,

J = 6.9 Hz, 3H), 1.06 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 170.29, 168.92, 168.47, 151.09, 149.20, 145.63, 140.28, 138.91, 128.91, 128.87, 126.99, 126.52, 125.47, 122.01, 55.27, 52.46, 41.21, 28.05, 24.75, 23.04; **HRMS** (ESI-TOF) calcd for [$C_{20}H_{22}BrN_3O_4$+Na^+]: 470.0686, found: 470.0687.

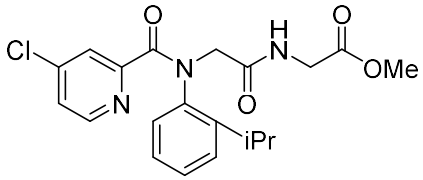
Methyl *N*-(5-fluoropicolinoyl)-*N*-(2-isopropylphenyl)glycylglycinate (*rac*-1k)



The title compound ***rac*-1k** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1k** was obtained as a light yellow solid, *E*: *Z* = 6: 1.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.03 (d, *J* = 2.8 Hz, 1H), 7.62 (dd, *J* = 8.7, 4.4 Hz, 1H), 7.33 (t, *J* = 5.4 Hz, 1H), 7.25 (td, *J* = 8.4, 2.8 Hz, 1H), 7.20-7.14 (m, 3H), 7.00-6.95 (m, 1H), 4.91 (d, *J* = 15.0 Hz, 1H), 4.12 (dd, *J* = 18.1, 5.9 Hz, 1H), 3.98 (dd, *J* = 18.2, 5.2 Hz, 1H), 3.91 (d, *J* = 15.0 Hz, 1H), 3.70 (s, 3H), 3.12-3.05 (m, 1H), 1.13 (d, *J* = 6.9 Hz, 3H), 1.00 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 170.27, 168.63, 168.52, 159.18 (d, J_{CF} = 262.6 Hz), 148.86 (d, J_{CF} = 4.0 Hz), 145.53, 140.47, 136.41 (d, J_{CF} = 24.2 Hz), 128.92, 128.64, 126.80, 126.35, 125.73 (d, J_{CF} = 5.1 Hz), 122.82 (d, J_{CF} = 19.2 Hz), 55.03, 52.30, 41.12, 27.94, 24.68, 22.90; **^{19}F NMR (376 MHz, CDCl$_3$)** δ -123.33; **HRMS** (ESI-TOF) calcd for [$C_{20}H_{22}FN_3O_4$+Na^+]: 410.1486, found: 410.1488.

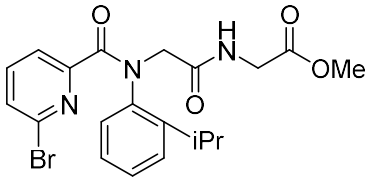
Methyl *N*-(4-chloropicolinoyl)-*N*-(2-isopropylphenyl)glycylglycinate (*rac*-1l)



The title compound ***rac*-1l** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1l** was obtained as a light yellow solid, *E*: *Z* = 5: 1.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.12 (d, *J* = 5.2 Hz, 1H), 7.62 (d, *J* = 1.7 Hz, 1H), 7.21-7.18 (m, 4H), 7.11 (dd, *J* = 5.3, 2.0 Hz, 1H), 7.04-6.99 (m, 1H), 4.93 (d, *J* = 14.9 Hz, 1H), 4.19 (dd, *J* = 18.2, 5.8 Hz, 1H), 4.02 (dd, *J* = 18.2, 5.1 Hz, 1H), 3.94 (d, *J* = 14.9 Hz, 1H), 3.77 (s, 3H),3.17-3.10 (m, 1H), 1.18 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 170.20, 168.66, 168.35, 154.15, 149.01, 145.64, 144.32, 140.04, 129.01, 128.85, 126.90, 126.45, 124.66, 124.45, 55.14, 52.40, 41.19, 28.03, 24.77, 22.91; **HRMS** (ESI-TOF) calcd for [$C_{20}H_{22}ClN_3O_4$+Na^+]: 426.1191, found: 426.1194.

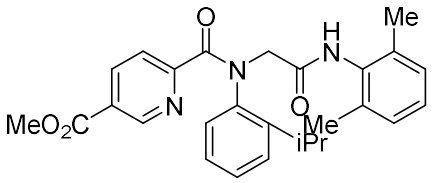
Methyl *N*-(6-bromopicolinoyl)-*N*-(2-isopropylphenyl)glycylglycinate (*rac*-1m)



The title compound ***rac*-1m** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-1m** was obtained as a light yellow solid, *E*: *Z* = 8: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 7.6 Hz, 1H), 7.44 (t, *J* = 7.8 Hz, 1H), 7.27 (d, *J* = 7.6 Hz, 1H), 7.24-7.16 (m, 4H), 7.00 (td, *J* = 6.8, 2.0 Hz,1H), 4.94 (d, *J* = 14.9 Hz, 1H), 4.15 (dd, *J* = 18.2, 5.8 Hz, 1H), 4.00 (dd, *J* = 18.2, 5.1 Hz, 1H), 3.91 (d, *J* = 15.0 Hz, 1H), 3.73 (s, 3H), 3.14-3.07 (m, 1H), 1.17 (d, *J* = 6.9 Hz, 3H), 1.13 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.25, 168.34, 167.86, 153.26, 145.56, 140.24, 140.02, 138.46, 129.11, 128.93, 128.82, 126.95, 126.35, 123.04, 54.96, 52.37, 41.17, 27.99, 24.80, 23.05; **HRMS** (ESI-TOF) calcd for $[C_{20}H_{22}BrN_3O_4+Na^+]$: 470.0686, found: 470.0687.

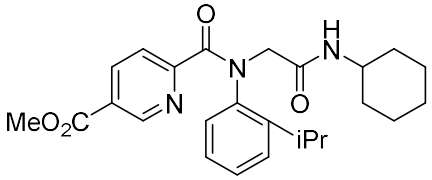
Methyl 6-((2-((2,6-dimethylphenyl)amino)-2-oxoethyl)(2-isopropylphenyl)carbamoyl)nicotinate (*rac*-4a)



The title compound ***rac*-4a** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4a** was obtained as a white solid, *E*: *Z* = 11: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.21-8.18 (m, 2H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.24-7.19 (m, 3H), 7.10-7.06 (m, 3H), 6.99 (td, *J* = 7.7, 2.3 Hz, 1H), 5.12 (d, *J* = 14.9 Hz, 1H), 4.03 (d, *J* = 14.9 Hz, 1H), 3.88 (s, 3H), 3.24-3.16 (m, 1H), 2.29 (s, 6H), 1.23 (d, *J* = 6.8 Hz, 3H), 1.11 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.23, 166.66, 165.00, 156.31, 149.34, 145.74, 140.19, 137.38, 135.28, 133.68, 129.11, 129.03, 128.22, 127.32, 127.05, 126.38, 126.13, 123.24, 55.56, 52.53, 28.12, 24.80, 22.96, 18.60; **HRMS** (ESI-TOF) calcd for $[C_{27}H_{29}N_3O_4+Na^+]$: 482.2050, found: 482.2052.

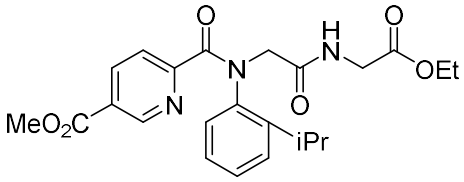
Methyl 6-((2-(cyclohexylamino)-2-oxoethyl)(2-isopropylphenyl)carbamoyl)nicotinate (*rac*-4b)



The title compound ***rac*-4b** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4b** was obtained as a white solid, *E*: *Z* = 7: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 7.58 (d, *J* = 8.1 Hz, 1H), 7.17-7.13 (m, 3H), 7.02-6.96 (m, 1H), 6.57 (d, *J* = 8.2 Hz, 1H), 4.80 (d, *J* = 14.8 Hz, 1H), 3.92 (d, *J* = 15.0 Hz, 1H), 3.87 (s, 3H), 3.16-3.10 (m, 1H), 1.99-1.89 (m, 2H), 1.74-1.68 (m, 2H), 1.62-1.57 (m, 1H), 1.43-1.32 (m, 2H), 1.29-1.21 (m, 4H), 1.18 (d, *J* = 6.7 Hz, 3H), 1.04 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 168.99, 167.05, 165.02, 156.52, 149.31, 145.76, 140.06, 137.27, 129.04, 128.86, 126.89, 126.35, 126.01, 123.24, 55.49, 52.49, 48.33, 33.03, 32.86, 27.99, 25.52, 24.87, 24.70, 24.00, 22.86; **HRMS** (ESI-TOF) calcd for $[C_{25}H_{31}N_3O_4+Na^+]$: 460.2207, found: 460.2209.

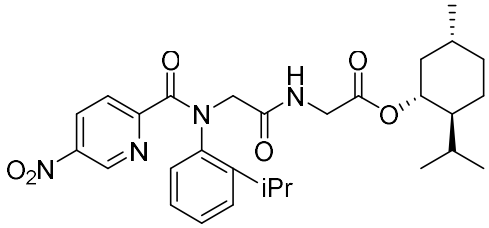
Methyl 6-((2-((2-ethoxy-2-oxoethyl)amino)-2-oxoethyl)(2-isopropylphenyl)carbamoyl)nicotinate (*rac*-4c)



The title compound ***rac*-4c** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4c** was obtained as a light yellow solid, *E*: *Z* = 7: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.19 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.22-7.15 (m, 4H), 7.01-6.97 (m, 1H), 4.97 (d, *J* = 14.9 Hz, 1H), 4.26-417 (m, 3H), 4.01 (dd, *J* = 14.9, 4.9 Hz, 1H), 3.93 (d, *J* = 14.8 Hz, 1H), 3.88 (s, 3H), 3.19-3.13 (m, 1H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.19 (d, *J* = 6.9 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.76, 169.09, 168.28, 165.05, 156.35, 149.26, 145.77, 139.88, 137.30, 129.11, 128.94, 126.94, 126.43, 126.05, 123.47, 61.56, 55.02, 52.49, 41.37, 28.02, 24.78, 22.94, 14.18; **HRMS** (ESI-TOF) calcd for $[C_{23}H_{27}N_3O_6+Na^+]$: 464.1792, found: 464.1792.

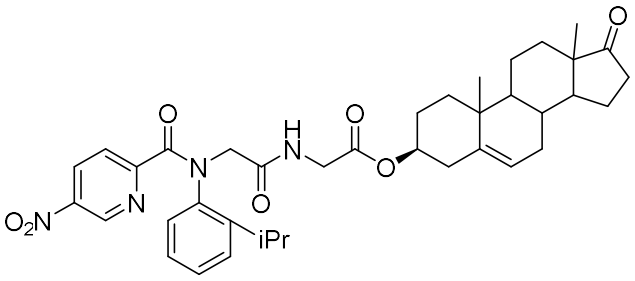
(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl *N*-(2-isopropylphenyl)-*N*-(5-nitropicolinoyl) glycylglycinate (*rac*-4d)



The title compound ***rac*-4d** was prepared according to the general procedure B and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4d** was obtained as a light yellow solid, *E*: *Z* = 11: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, *J* = 2.4 Hz, 1H), 8.39 (dd, *J* = 8.6, 2.4 Hz, 1H), 7.84 (d, *J* = 8.6 Hz, 1H), 7.24-7.17 (m, 3H), 7.00-6.95 (m, 2H), 5.00 (dd, *J* = 15.0, 8.9 Hz, 1H), 4.78 (tdd, *J* = 10.9, 4.5, 2.1 Hz, 1H), 4.21-4.12 (m, 1H), 4.05-3.99 (m, 1H), 3.95-3.88 (m, 1H), 3.22-3.15 (m, 1H), 2.02-1.97 (m, 1H), 1.86-1.79 (m, 1H), 1.71-1.65 (m, 2H), 1.53-1.45 (m, 1H), 1.43-1.36 (m, 1H), 1.21 (dd, *J* = 6.9, 1.8 Hz, 3H), 1.14 (dd, *J* = 6.7, 3.3 Hz, 3H), 1.07-1.00 (m, 2H), 0.92-0.87 (m, 7H), 0.76 (dd, *J* = 6.9, 1.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.47, 167.85, 167.71, 158.05, 145.91, 143.59, 143.41, 139.47, 131.52, 129.24, 129.21, 127.10, 126.55, 124.40, 75.85, 54.75, 46.90, 41.48, 40.78, 34.09, 31.41, 28.07, 26.26, 24.71, 23.37, 23.07, 22.01, 20.74, 16.33; **HRMS** (ESI-TOF) calcd for $[C_{29}H_{38}N_4O_6+Na^+]$: 561.2683, found: 561.2685.

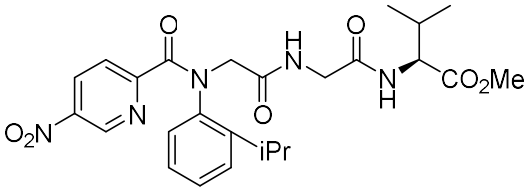
(3*S*)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a]phenanthren-3-yl *N*-(2-isopropylphenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (*rac*-4e)



The title compound ***rac*-4e** was prepared according to the general procedure B and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4e** was obtained as a light yellow powder, *E*: *Z* = 11: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, *J* = 2.5 Hz, 1H), 8.39 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.83 (d, *J* = 8.6 Hz, 1H), 7.23-7.16 (m, 3H), 7.01-6.95 (m, 2H), 5.41 (d, *J* = 4.1 Hz, 1H), 4.99 (d, *J* = 15.0 Hz, 1H), 4.74-4.66 (m, 1H), 4.16 (dd, *J* = 18.3, 6.6 Hz, 1H), 3.99 (ddd, *J* = 18.2, 4.9, 1.8 Hz, 1H), 3.91 (d, *J* = 15.0 Hz, 1H), 3.21-3.14 (m, 1H), 2.48-2.35 (m, 3H), 2.12-2.02 (m, 2H), 1.97-1.85 (m, 4H), 1.71-1.43 (m, 7H), 1.32-1.24 (m, 3H), 1.20 (d, *J* = 6.9 Hz, 3H), 1.14 (d, *J* = 6.8 Hz, 3H), 1.04 (s, 3H), 0.88 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.20, 167.83, 167.79, 158.04, 145.90, 143.61, 143.41, 139.59, 139.48, 131.48, 129.25, 129.20, 127.08, 126.53, 124.35, 122.25, 75.23, 54.75, 51.70, 50.14, 47.52, 41.56, 37.98, 36.86, 36.72, 35.83, 31.45, 31.41, 30.78, 28.06, 27.64, 24.71, 23.04, 21.88, 20.34, 19.33, 13.56. **HRMS** (ESI-TOF) calcd for $[C_{38}H_{46}N_4O_7+Na^+]$: 693.3258, found: 693.3259.

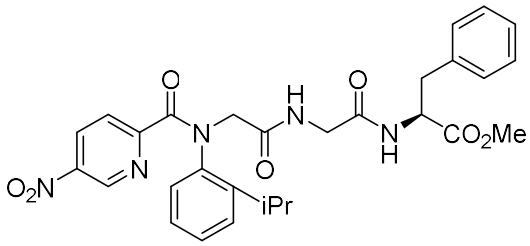
Methyl *N*-(2-isopropylphenyl)-*N*-(5-nitropicolinoyl)glycylglycyl-*L*-valinate (*rac*-4f)



The title compound ***rac*-4f** was prepared according to the general procedure B and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4f** was obtained as a yellow solid, *E*: *Z* = 13: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.00 (t, *J* = 2.4 Hz, 1H), 8.39 (dt, *J* = 8.6, 2.9 Hz, 1H), 7.85 (dd, *J* = 23.0, 8.6 Hz, 1H), 7.26-7.16 (m, 4H), 7.00-6.94 (m, 1H), 6.88-6.81 (m, 1H), 4.93 (dd, *J* = 15.2, 7.0 Hz, 1H), 4.55-4.51 (m, 1H), 4.22-3.88 (m, 3H), 3.72 (d, *J* = 3.3 Hz, 3H), 3.25-3.15 (m, 1H), 2.21-2.11 (m, 1H), 1.20 (dd, *J* = 6.9, 3.1 Hz, 3H), 1.15 (dd, *J* = 6.7, 2.7 Hz, 3H), 0.94-0.89 (m, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 172.35, 168.81, 168.20, 167.78, 157.95, 145.96, 143.64, 143.38, 139.80, 131.52, 129.22, 129.19, 127.11, 126.53, 124.50, 57.47, 54.89, 52.20, 43.15, 31.04, 28.11, 24.66, 23.05, 18.98, 17.96; **HRMS** (ESI-TOF) calcd for $[C_{25}H_{31}N_5O_7+Na^+]$: 536.2115, found: 536.2116.

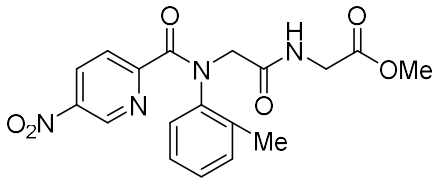
Methyl *N*-(2-isopropylphenyl)-*N*-(5-nitropicolinoyl)glycylglycyl-*L*-phenylalaninate (*rac*-4g)



The title compound ***rac*-4g** was prepared according to the general procedure B and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4g** was obtained as a white solid, *E*: *Z* = 12: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, *J* = 2.4 Hz, 1H), 8.38-8.33 (m, 1H), 7.78 (dd, *J* = 30.2, 8.6 Hz, 1H), 7.25-7.16 (m, 7H), 7.12-7.08 (m, 2H), 7.00 – 6.89 (m, 2H), 4.93-4.81 (m, 2H), 4.12-3.85 (m, 3H), 3.68 (s, 3H), 3.26-3.14 (m, 1H), 3.12-3.03 (m, 2H), 1.20 (dd, *J* = 6.9, 4.1 Hz, 3H), 1.15 (t, *J* = 6.6 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 171.97, 168.56, 168.11, 167.77, 157.91, 145.96, 143.60, 143.41, 139.79, 135.93, 131.56, 129.28, 129.22, 129.18, 128.60, 127.14, 127.10, 126.56, 124.49, 54.85, 53.56, 52.43, 42.95, 37.75, 28.10, 24.71, 23.08; **HRMS** (ESI-TOF) calcd for $[C_{29}H_{31}N_5O_7+Na^+]$: 584.2115, found: 584.2117.

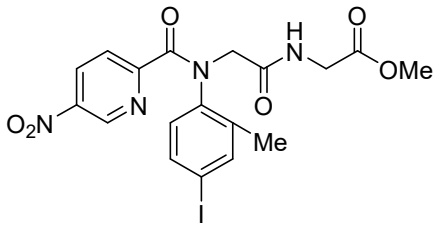
Methyl *N*-(5-nitropicolinoyl)-*N*-(o-tolyl)glycylglycinate (*rac*-4h)



The title compound ***rac*-4h** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4h** was obtained as a brown solid, *E*: *Z* = 11: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.04 (dd, *J* = 2.6, 0.7 Hz, 1H), 8.38 (dd, *J* = 8.6, 2.7 Hz, 1H), 7.78 (dd, *J* = 8.6, 0.8 Hz, 1H), 7.18 (d, *J* = 7.7 Hz, 1H), 7.13-7.07 (m, 3H), 7.01-6.97 (m, 1H), 4.96 (d, *J* = 15.0 Hz, 1H), 4.19 (dd, *J* = 18.2, 5.9 Hz, 1H), 4.02 (dd, *J* = 18.3, 5.0 Hz, 1H), 3.94 (d, *J* = 15.0 Hz, 1H), 3.76 (s, 3H), 2.31 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.28, 167.99, 167.80, 158.10, 143.67, 143.65, 140.76, 135.61, 131.50, 131.19, 129.17, 128.81, 126.92, 123.93, 53.50, 52.46, 41.17, 18.03; **HRMS** (ESI-TOF) calcd for $[C_{18}H_{18}N_4O_6+Na^+]$: 409.1118, found: 409.1119.

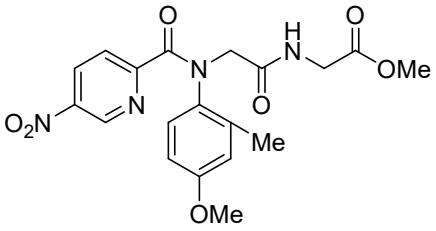
Methyl *N*-(4-iodo-2-methylphenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (*rac*-4i)



The title compound ***rac*-4i** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4i** was obtained as a light yellow solid, *E*: *Z* = 11: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.5 Hz, 1H), 8.45 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.87 (d, *J* = 8.5 Hz, 1H), 7.52 (d, *J* = 2.0 Hz, 1H), 7.33 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.92 (d, *J* = 8.2 Hz, 2H), 4.94 (d, *J* = 14.9 Hz, 1H), 4.20 (dd, *J* = 18.3, 5.9 Hz, 1H), 4.01 (dd, *J* = 18.2, 4.9 Hz, 1H), 3.86 (d, *J* = 14.8 Hz, 1H), 3.78 (s, 3H), 2.29 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.26, 167.72, 167.45, 157.57, 143.87, 143.69, 140.86, 140.02, 138.12, 136.10, 131.77, 130.90, 124.28, 94.46, 53.35, 52.51, 41.16, 17.75; **HRMS** (ESI-TOF) calcd for [$C_{18}H_{17}IN_4O_6$+Na^+]: 535.0085, found: 535.0084.

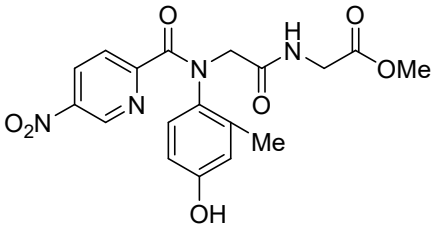
Methyl *N*-(4-methoxy-2-methylphenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (*rac*-4j)



The title compound ***rac*-4j** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4j** was obtained as a yellow solid, *E*: *Z* = 14: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (d, *J* = 2.9 Hz, 1H), 8.37 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.10 (d, *J* = 8.6 Hz, 2H), 6.60 (d, *J* = 2.8 Hz, 1H), 6.48 (dd, *J* = 8.6, 2.9 Hz, 1H), 4.95 (d, *J* = 14.9 Hz, 1H), 4.19 (dd, *J* = 18.2, 6.0 Hz, 1H), 4.00 (dd, *J* = 18.2, 5.0 Hz, 1H), 3.87 (d, *J* = 14.9 Hz, 1H), 3.76 (s, 3H), 3.68 (s, 3H), 2.27 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.30, 168.15, 168.11, 159.29, 158.55, 143.80, 143.54, 137.10, 133.52, 131.46, 130.35, 123.63, 116.18, 111.71, 55.23, 53.51, 52.38, 41.13, 18.27; **HRMS** (ESI-TOF) calcd for [$C_{19}H_{20}N_4O_7$+Na^+]: 439.1224, found: 439.1225.

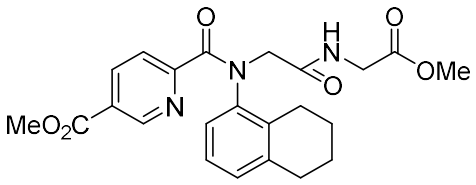
Methyl *N*-(4-hydroxy-2-methylphenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (*rac*-4k)



The title compound ***rac*-4k** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4k** was obtained as a yellow powder, *E*: *Z* = 13: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (d, *J* = 2.5 Hz, 1H), 8.35 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.65 (d, *J* = 8.6 Hz, 1H), 7.53 (s, 1H), 7.46 (t, *J* = 5.8 Hz, 1H), 6.83 (d, *J* = 8.5 Hz, 1H), 6.38 (d, *J* = 2.7 Hz, 1H), 6.18 (dd, *J* = 8.5, 2.8 Hz, 1H), 4.96 (d, *J* = 14.4 Hz, 1H), 4.22 (dd, *J* = 18.2, 6.4 Hz, 1H), 3.98 (dd, *J* = 18.1, 5.0 Hz, 1H), 3.92 (d, *J* = 14.4 Hz, 1H), 3.77 (s, 3H), 2.17 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.11, 169.41, 168.52, 158.21, 156.62, 143.92, 143.60, 136.70, 132.10, 131.49, 130.06, 123.61, 117.61, 113.55, 53.50, 52.57, 41.22, 17.95; **HRMS** (ESI-TOF) calcd for [$C_{18}H_{18}N_4O_7$+H^+]: 403.1248, found: 403.1249.

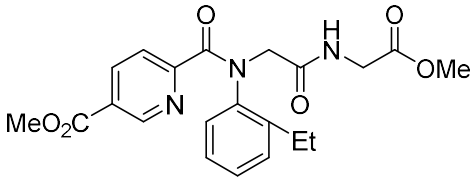
Methyl 6-((2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl) (5,6,7,8-tetrahydronaphthalen-1-yl)carbamoyl)nicotinate (*rac*-4l)



The title compound ***rac*-4l** was prepared according to the general procedure A and purified by flash chromatography (ethyl acetate: dichloromethane: triethylamine = 1: 1: 1%). ***rac*-4l** was obtained as a light yellow powder, *E*: *Z* = 7: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.16 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.25 (t, *J* = 5.0 Hz, 1H), 6.97 (dd, *J* = 6.9, 1.7 Hz, 1H), 6.90-6.84 (m, 2H), 4.93 (d, *J* = 14.9 Hz, 1H), 4.20 (dd, *J* = 18.2, 6.0 Hz, 1H), 4.00 (dd, *J* = 18.1, 5.0 Hz, 1H), 3.88 (d, *J* = 14.8 Hz,1H), 3.88 (s, 3H), 3.76 (s, 3H), 2.88-2.52 (m, 4H), 1.84-1.68 (m, 4H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.25, 169.09, 168.53, 165.10, 156.66, 149.50, 140.75, 139.00, 137.24, 134.83, 129.51, 126.41, 126.00, 125.80, 122.89, 53.56, 52.49, 52.35, 41.15, 29.38, 25.32, 22.64; **HRMS** (ESI-TOF) calcd for $[C_{23}H_{25}N_3O_6+Na^+]$: 462.1635, found: 462.1637.

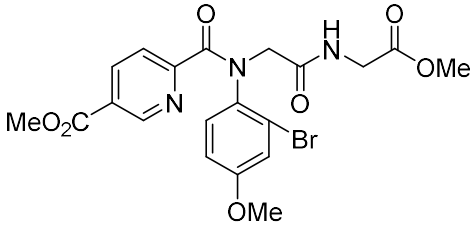
Methyl 6-((2-ethylphenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (*rac*-4m)



The title compound ***rac*-4m** was prepared according to the general procedure A and purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). ***rac*-4m** was obtained as a light yellow solid, *E*: *Z* = 7: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (d, *J* = 1.3 Hz, 1H), 8.16 (dd, *J* = 8.1, 2.0 Hz, 1H), 7.60 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.22-7.19 (m, 2H), 7.16-7.11 (m, 2H), 7.01-6.97 (m, 1H), 4.96 (d, *J* = 14.9 Hz, 1H), 4.19 (dd, *J* = 18.2, 6.0 Hz, 1H), 4.02 (dd, *J* = 18.1, 5.0 Hz, 1H), 3.92 (d, *J* = 14.7 Hz, 1H), 3.87 (s, 3H), 3.76 (s, 3H), 2.63 (q, *J* = 7.5 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.22, 169.07, 168.39, 165.05, 156.47, 149.42, 140.84, 140.64, 137.27, 129.13, 128.82, 128.69, 126.58, 126.03, 123.12, 54.36, 52.49, 52.39, 41.17, 23.45, 13.83. **HRMS** (ESI-TOF) calcd for $[C_{21}H_{23}N_3O_6+Na^+]$: 436.1479, found: 436.1479.

Methyl 6-((2-bromo-4-methoxyphenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (*rac*-4n)

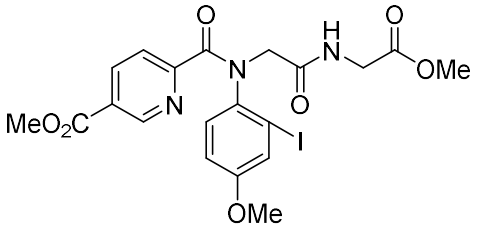


The title compound ***rac*-4n** was prepared according to the general procedure A and purified by flash chromatography (ethyl acetate: dichloromethane: triethylamine = 1: 1: 1%). ***rac*-4n** was obtained as a

brown solid, *E*: *Z* = 8: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (dd, *J* = 2.2, 0.9 Hz, 1H), 8.19 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.68 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.36 (d, *J* = 8.8 Hz, 1H), 7.15 (t, *J* = 5.6 Hz, 1H), 6.95 (d, *J* = 2.8 Hz, 1H), 6.65 (dd, *J* = 8.8, 2.8 Hz, 1H), 5.02 (d, *J* = 15.4 Hz, 1H), 4.16 (dd, *J* = 18.2, 6.0 Hz, 1H), 3.98 (dd, *J* = 18.1, 5.1 Hz, 1H), 3.89 (d, *J* = 15.9 Hz,1H), 3.87 (s, 3H), 3.73 (s, 3H), 3.69 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.19, 168.77, 168.24, 165.06, 159.54, 156.31, 149.39, 137.41, 133.97, 132.05, 126.15, 123.08, 123.02, 118.13, 113.80, 55.63, 53.41, 52.52, 52.36, 41.17; **HRMS** (ESI-TOF) calcd for [$C_{20}H_{20}BrN_3O_7$+Na^+]: 516.0377, found: 516.0379.

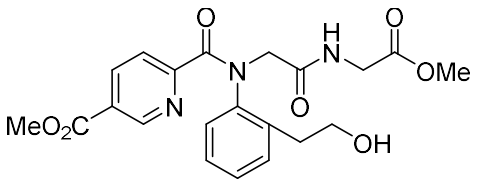
Methyl 6-((2-iodo-4-methoxyphenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (*rac*-4o)



The title compound ***rac*-4o** was prepared according to the general procedure A and purified by flash chromatography (ethyl acetate: dichloromethane: triethylamine =1: 1: 1%). ***rac*-4o** was obtained as a reddish brown solid, *E*: *Z* = 7: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.89 (d, *J* = 1.4 Hz, 1H), 8.22 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.75 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 1H), 7.21 (d, *J* = 2.8 Hz, 1H), 7.05 (t, *J* = 5.6 Hz, 1H), 6.71 (dd, *J* = 8.8, 2.8 Hz, 1H), 5.08 (d, *J* = 15.2 Hz, 1H), 4.21 (dd, *J* = 18.2, 6.0 Hz, 1H), 4.00 (dd, *J* = 18.2, 5.0 Hz, 1H), 3.89 (s, 3H), 3.81 (d, *J* = 15.2 Hz, 1H), 3.76 (s, 3H), 3.71 (s, 3H). **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.18, 168.64, 168.16, 165.11, 159.19, 156.30, 149.34, 137.37, 131.54, 126.13, 124.38, 123.25, 114.56, 99.61, 55.61, 53.84, 52.53, 52.41, 41.20. **HRMS** (ESI-TOF) calcd for [$C_{20}H_{20}IN_3O_7$+Na^+]: 564.0238, found: 564.0240.

Methyl 6-((2-(2-hydroxyethyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (*rac*-4p)

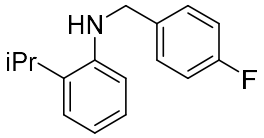


The title compound ***rac*-4p** was prepared according to the general procedure A and purified by flash chromatography (ethyl acetate: dichloromethane: triethylamine =1: 1: 1%). ***rac*-4p** was obtained as a yellow oil, *E*: *Z* = 17: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 1.4 Hz, 1H), 8.32 (dd, *J* = 8.1, 2.0 Hz, 1H), 8.07 (t, *J* = 5.7 Hz, 1H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.24 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.13 (td, *J* = 7.5, 1.4 Hz, 1H), 6.88 (td, *J* = 7.8, 1.6 Hz, 1H), 6.78 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.37 (dd, *J* = 9.1, 3.9 Hz, 1H), 4.55 (d, *J* = 15.8 Hz, 1H), 4.34 (d, *J* = 15.8 Hz, 1H), 4.19 (dd, *J* = 18.0, 6.1 Hz, 1H), 4.07-3.93 (m, 3H), 3.87 (s, 3H), 3.72 (s, 3H), 3.26-3.19 (m, 1H), 2.85-2.79 (m, 1H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.40, 168.87, 168.26, 164.52, 156.11, 148.34, 142.16, 138.62, 137.23, 131.59, 129.54, 128.63, 127.26, 126.59, 124.69, 63.94,

54.67, 52.65, 52.25, 41.06, 35.45. **HRMS** (ESI-TOF) calcd for [$C_{21}H_{23}N_3O_7$+Na^+]: 452.1428, found: 452.1428.

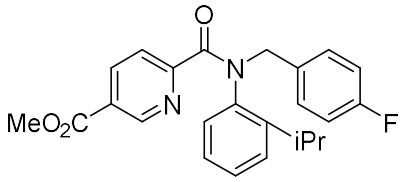
***N*-(4-fluorobenzyl)-2-isopropylaniline (4qq)**



The title compound **4qq** was prepared according to the general procedure C and purified by flash chromatography (petroleum ether: ethyl acetate = 9: 1). **4qq** was obtained as a light yellow oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.37 (m, 2H), 7.23 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.14 (td, *J* = 7.6, 1.6 Hz, 1H), 7.12-7.06 (m, 2H), 6.82 (t, *J* = 7.5 Hz, 1H), 6.66 (d, *J* = 8.0 Hz, 1H), 4.39 (s, 2H), 4.08 (s, 1H), 2.99-2.89 (m, 1H), 1.33 (d, *J* = 6.8 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 162.13 (d, J_{CF} = 246.4 Hz), 144.62, 135.40 (d, J_{CF} = 3.0 Hz), 132.29, 129.08 (d, J_{CF}= 8.1 Hz), 126.81, 125.04, 117.79, 115.55 (d, J_{CF} = 21.2 Hz), 110.79, 47.88, 27.33, 22.37; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -115.54; **HRMS** (ESI-TOF) calcd for [$C_{16}H_{18}FN$+H^+]: 244.1496, found: 244.1495.

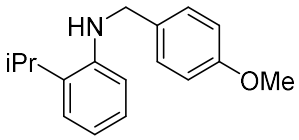
Methyl 6-((4-fluorobenzyl)(2-isopropylphenyl)carbamoyl)nicotinate (*rac*-4q)



The title compound ***rac*-4q** was prepared according to the general procedure C and purified by flash chromatography (petroleum ether: ethyl acetate = 1: 1). ***rac*-4q** was obtained as a light yellow solid, *E*: *Z* = 14: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 1.3 Hz, 1H), 8.13 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.29-7.26 (m, 2H), 7.14-7.12 (m, 2H), 6.94 (t, *J* = 8.7 Hz, 2H), 6.90-6.86 (m, 1H), 6.65 (d, *J* = 7.8 Hz, 1H), 5.48 (d, *J* = 13.9 Hz, 1H), 4.49 (d, *J* = 14.0 Hz, 1H), 3.85 (s, 3H), 3.10-3.03 (m, 1H), 0.99 (d, *J* = 6.8 Hz, 3H), 0.94 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.97, 165.07, 162.39 (d, J_{CF} = 246.4 Hz), 157.22, 149.29, 146.13, 138.73, 137.11, 132.52 (d, J_{CF} = 3.0 Hz), 131.34 (d, J_{CF} = 8.1 Hz), 129.85, 128.50, 126.96, 125.80, 125.73, 123.22, 115.29 (d, J_{CF} = 21.2 Hz), 53.23, 52.42, 27.78, 24.63, 23.12; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -114.53; **HRMS** (ESI-TOF) calcd for [$C_{24}H_{23}FN_2O_3$+Na^+]: 429.1585, found: 429.1587.

2-isopropyl-*N*-(4-methoxybenzyl)aniline (4rr)

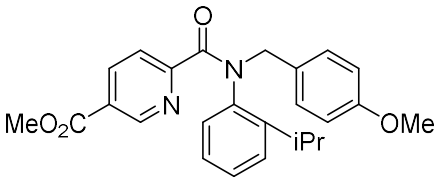


The title compound **4rr** was prepared according to the general procedure C and purified by flash chromatography (petroleum ether: ethyl acetate = 9: 1). **4rr** was obtained as a brown oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, *J* = 8.5 Hz, 2H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.11 (t, *J* = 7.4 Hz, 1H), 6.91 (d, *J* = 8.5 Hz, 2H), 6.77 (t, *J* = 7.4 Hz, 1H), 6.68 (d, *J* = 8.6 Hz, 1H), 4.31 (s, 2H), 3.82 (s,

3H), 3.22 (s, 1H), 2.94-2.83 (m, 1H), 1.27 (d, J = 6.8 Hz, 6H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 158.91, 144.77, 132.21, 131.54, 128.89, 126.76, 124.91, 117.55, 114.09, 110.75, 55.32, 48.10, 27.23, 22.33; **HRMS** (EI-TOF) calcd for $[C_{17}H_{21}NO]^+$: 255.1623, found: 255.1624.

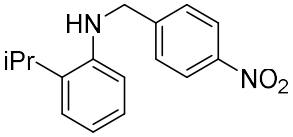
Methyl 6-((2-isopropylphenyl)(4-methoxybenzyl)carbamoyl)nicotinate (*rac*-4r)



The title compound ***rac*-4r** was prepared according to the general procedure C and purified by flash chromatography (petroleum ether: ethyl acetate = 1: 1). ***rac*-4r** was obtained as a light brown solid, *E*: *Z* = 13: 1.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.84 (dd, J = 2.2, 0.9 Hz, 1H), 8.12 (dd, J = 8.2, 2.1 Hz, 1H), 7.51 (dd, J = 8.1, 0.9 Hz, 1H), 7.23-7.20 (m, 2H), 7.14-7.09 (m, 2H), 6.89-6.85 (m, 1H), 6.81-6.77 (m, 2H), 6.66 (d, J = 7.6 Hz, 1H), 5.49 (d, J = 13.8 Hz, 1H), 4.44 (d, J = 13.9 Hz, 1H), 3.86 (s, 3H), 3.76 (s, 3H), 3.12-3.04 (m, 1H), 1.00 (d, J = 6.8 Hz, 3H), 0.94 (d, J = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 167.88, 165.16, 159.17, 157.51, 149.31, 146.19, 138.81, 137.04, 130.91, 130.04, 128.86, 128.37, 126.84, 125.69, 125.59, 123.17, 113.78, 55.23, 53.32, 52.42, 27.76, 24.68, 23.13; **HRMS** (EI-TOF) calcd for $[C_{25}H_{26}N_2O_4]^+$: 418.1893, found: 418.1895.

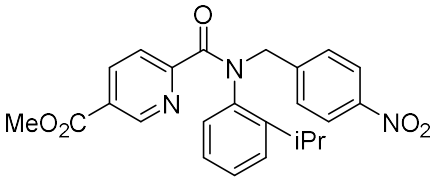
2-isopropyl-*N*-(4-nitrobenzyl)aniline (4ss)



The title compound **4ss** was prepared according to the general procedure C and purified by flash chromatography (petroleum ether: ethyl acetate = 9: 1). **4ss** was obtained as a yellow solid.

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.20 (d, J = 8.6 Hz, 2H), 7.54 (d, J = 8.6 Hz, 2H), 7.20 (dd, J = 7.6, 1.6 Hz, 1H), 7.04 (td, J = 7.6, 1.6 Hz, 1H), 6.79 (t, J = 7.3 Hz, 1H), 6.45 (d, J = 8.0 Hz, 1H), 4.53 (s, 2H), 4.29 (s, 1H), 3.00-2.90 (m, 1H), 1.32 (d, J = 6.8 Hz, 6H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 147.66, 147.23, 143.88, 132.43, 127.73, 126.77, 125.22, 123.95, 118.25, 110.76, 47.81, 27.39, 22.36; **HRMS** (EI-TOF) calcd for $[C_{16}H_{18}N_2O_2]^+$: 270.1368, found: 270.1370.

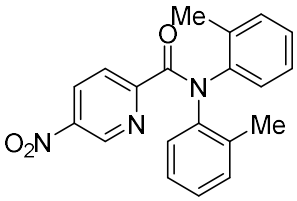
Methyl 6-((2-isopropylphenyl)(4-nitrobenzyl)carbamoyl)nicotinate (*rac*-4s)



The title compound ***rac*-4s** was prepared according to the general procedure C and purified by flash chromatography (petroleum ether: ethyl acetate = 1: 1). ***rac*-4s** was obtained as a light yellow solid, *E*: *Z* = 20: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (s, 1H), 8.19-8.15 (m, 3H), 7.59-7.51 (m, 3H), 7.20-7.14 (m, 2H), 6.95-6.87 (m, 1H), 6.65 (d, *J* = 7.8 Hz, 1H), 5.63 (d, *J* = 14.3 Hz, 1H), 4.56 (d, *J* = 14.3 Hz, 1H), 3.88 (s, 3H), 3.13-3.06 (m, 1H), 1.05 (d, *J* = 6.8 Hz, 3H), 0.99 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 168.30, 165.05, 156.65, 149.31, 147.51, 145.97, 143.96, 138.79, 137.31, 130.25, 129.50, 128.82, 127.23, 126.07, 125.99, 123.76, 123.34, 53.56, 52.55, 27.90, 24.74, 23.15; **HRMS** (EI-TOF) calcd for $[C_{24}H_{23}N_3O_5]^+$: 433.1638, found: 433.1637.

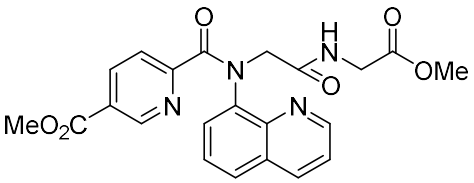
5-nitro-*N*,*N*-di-o-tolylpicolinamide (*rac*-4t)



The title compound ***rac*-4t** was prepared according to the general procedure D and was purified by flash chromatography (petroleum ether: ethyl acetate: triethylamine = 4: 1: 1%). ***rac*-4t** was obtained as a light yellow solid, *E*: *Z* > 99: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.08 (d, *J* = 2.3 Hz, 1H), 8.44 (dd, *J* = 8.5, 2.4 Hz, 1H), 7.93 (d, *J* = 8.5 Hz, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.21 (t, *J* = 7.2 Hz, 1H), 7.16-7.08 (m, 3H), 7.01 (s, 2H), 6.90 (d, *J* = 7.8 Hz, 1H), 2.49 (s, 3H), 2.17 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.37, 159.38, 143.81, 143.69, 142.01, 135.12, 131.77, 131.70, 131.27, 129.68, 128.01, 127.23, 126.74, 126.57, 125.99, 124.45, 18.83, 18.38; **HRMS** (ESI-TOF) calcd for $[C_{20}H_{17}N_3O_3+Na^+]$: 370.1162, found: 370.1164.

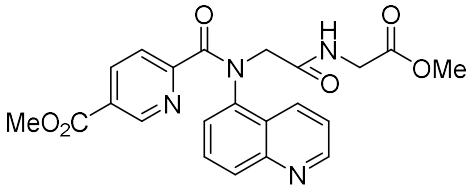
Methyl 6-((2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)(quinolin-8-yl)carbamoyl)nicotinate (*rac*-4u)



The title compound ***rac*-4u** was prepared according to the general procedure A and was purified by flash chromatography (ethyl acetate: triethylamine = 1: 1%). ***rac*-4u** was obtained as a brown solid, *E*: *Z* > 99: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.50 (s, 1H), 8.81 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.51 (s, 1H), 8.09 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.04 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.70 (t, *J* = 6.7 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.34 (dd, *J* = 8.3, 4.2 Hz, 1H), 5.00 (d, *J* = 16.5 Hz, 1H), 4.38 (d, *J* = 13.9 Hz, 1H), 4.15-3.93 (m, 2H), 3.78 (s, 3H), 3.60 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.07, 169.09, 168.75, 164.94, 156.76, 150.31, 148.48, 143.31, 140.22, 137.12, 136.79, 128.96, 128.26, 128.04, 126.80, 125.88, 123.68, 121.85, 55.69, 52.42, 52.03, 41.37; **HRMS** (ESI-TOF) calcd for $[C_{22}H_{20}N_4O_6+Na^+]$: 459.1275, found: 459.1277.

Methyl 6-((2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)(quinolin-5-yl)carbamoyl)nicotinate (*rac*-4v)

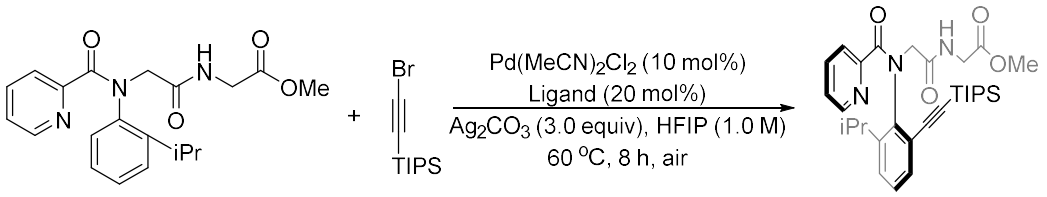


The title compound ***rac*-4v** was prepared according to the general procedure A and was purified by flash chromatography (ethyl acetate: dichloromethane: triethylamine = 1: 1: 1%). ***rac*-4v** was obtained as a yellow solid, *E*: *Z* = 8: 1.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (dd, *J* = 4.3, 1.6 Hz, 1H), 8.55 (s, 1H), 8.48 (d, *J* = 8.4 Hz, 1H), 8.12 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.98 (dd, *J* = 7.3, 2.2 Hz, 1H), 7.68 (d, *J* = 8.1 Hz, 1H), 7.52-7.45 (m, 3H), 7.13 (t, *J* = 5.5 Hz, 1H), 5.00 (d, *J* = 15.0 Hz, 1H), 4.23-4.16 (m, 2H), 4.05 (dd, *J* = 18.2, 5.0 Hz, 1H), 3.81 (s, 3H), 3.76 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.26, 169.31, 168.05, 164.79, 155.77, 150.86, 149.23, 148.78, 138.88, 137.48, 131.63, 130.28, 128.80, 127.26, 126.29, 125.46, 123.21, 122.01, 54.36, 52.48, 52.45, 41.19; **HRMS** (ESI-TOF) calcd for $[C_{22}H_{20}N_4O_6+Na^+]$: 459.1275, found: 459.1277.

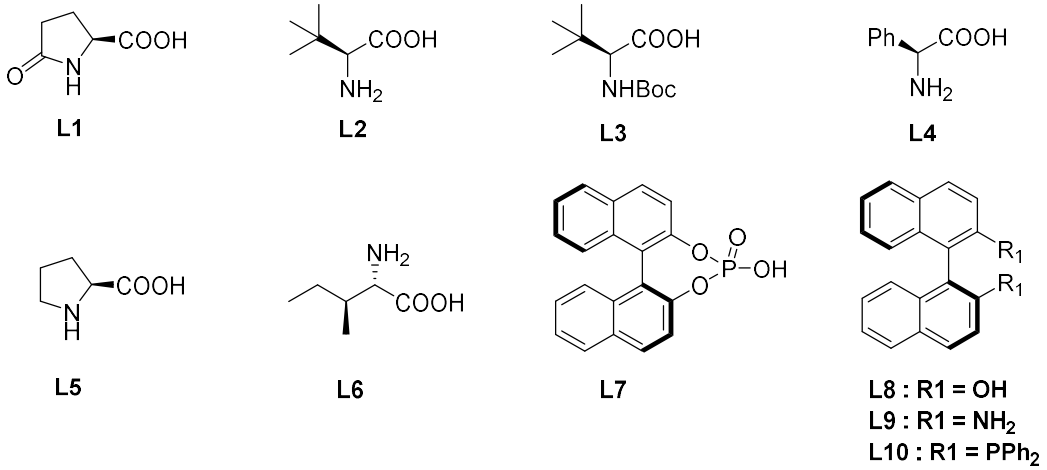
2.2 Optimization of Reaction Conditions

Table S1. Screening of ligands[a]



rac-**1a** **2** **3a**

Entry	Ligand	Yield (%)[b]	ee (%)[c]
1	**L1**	81(78)[d]	93
2	**L2**	N.R.	--
3	**L3**	23	-29
4	**L4**	N.R.	--
5	**L5**	N.R.	--
6	**L6**	N.R.	--
7	**L7**	3	0
8	**L8**	8	0
9	**L9**	N.R.	--
10	**L10**	1	2



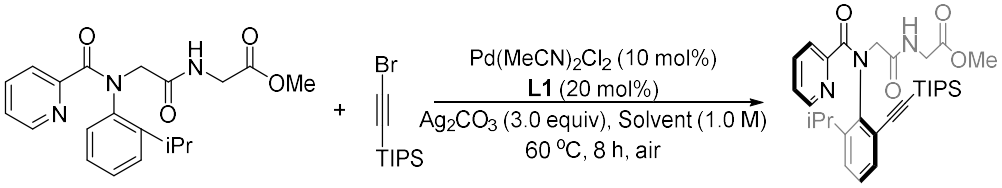
L1 **L2** **L3** **L4**

L5 **L6** **L7**

L8 : R1 = OH
L9 : R1 = NH_2
L10 : R1 = PPh_2

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), Ligand (0.2 equiv), Ag_2CO_3 (3.0 equiv), HFIP (0.1 mL), 60 °C, 8 h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Yield of isolated product is within parentheses.

Table S2. Screening of the solvents[a]

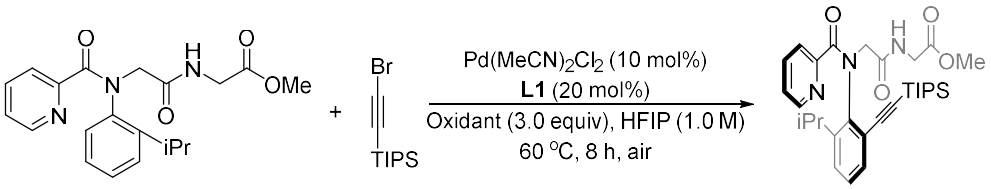


rac-**1a** **2** **3a**

Entry	Solvent	Yield (%)[b]	ee (%)[c]
1	TFE	71	76
2	*t*-AmyOH	21	86
3	MeOH	37	85
4	DCE	31	83
5	MeCN	76	80
6	toluene	10	77
7	HFIP	78[d]	93

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Ag_2CO_3 (3.0 equiv), solvent (0.1 mL), 60 °C, 8 h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Isolated yield.

Table S3. Screening of the oxidants[a]

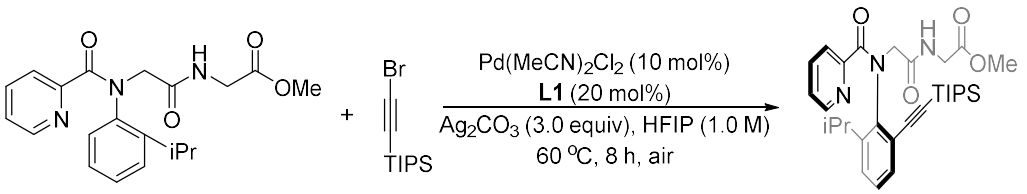


rac-**1a** **2** **3a**

Entry	Oxidant	Yield (%)[b]	ee (%)[c]
1	AgOAc	70	57
2	Ag_3PO_4	68	95
3	AgTFA	N.R.	--
4	AgF	N.R.	--
5	$Cu(OAc)_2$	11	44
6	$Mn(OAc)_2•4H_2O$	16	16
7	Ag_2CO_3	78[d]	93

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Oxidant (3.0 equiv), HFIP (0.1 mL), 60 °C, 8 h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Isolated yield.

Table S4. Screening of the equivalents of 2[a]

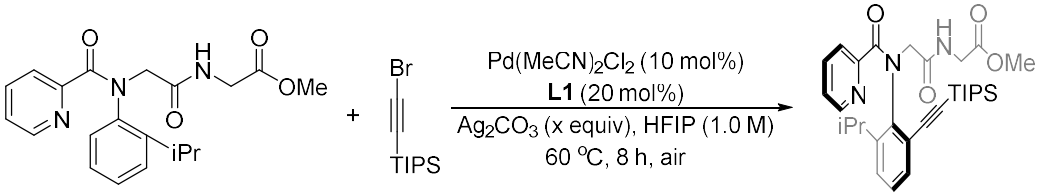


rac-**1a** **2** **3a**

Entry	**2**	Yield (%)[b]	ee (%)[c]
1	1.0 equiv	67	94
2	2.0 equiv	74	93
3	3.0 equiv	76	93
4	4.0 equiv	78 [d]	93
5	5.0 equiv	75	93

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2**, $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Ag_2CO_3 (3.0 equiv), HFIP (0.1 mL), 60 °C, 8 h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Isolated yield.

Table S5. Screening of the equivalents of Ag_2CO_3[a]

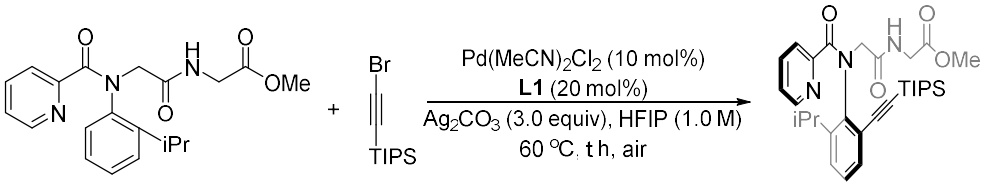


rac-**1a** **2** **3a**

Entry	Ag_2CO_3	Yield (%)[b]	ee (%)[c]
1	1.0 equiv	79	91
2	2.0 equiv	77	93
3	3.0 equiv	78[d]	93
4	4.0 equiv	73	94

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Ag_2CO_3 (x equiv), HFIP (0.1 mL), 60 °C, 8 h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Isolated yield.

Table S6. Investigation of reaction time[a]

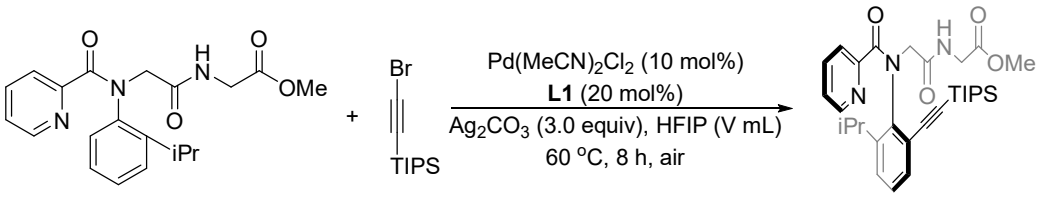


rac-**1a** **2** **3a**

Entry	Reaction time t / h	Yield (%)[b]	ee (%)[c]
1	4	39	96
2	8	78[d]	93
3	12	81	91
4	16	88	87
5	20	94	84
6	24	99	71

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Ag_2CO_3 (3.0 equiv), HFIP (0.1 mL), 60 °C, t h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Isolated yield.

Table S7. Investigation of reaction concentration[a]

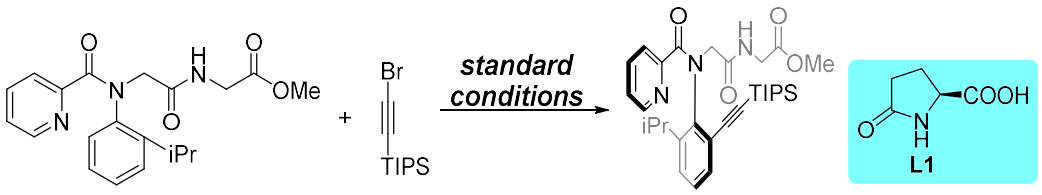


rac-**1a** **2** **3a**

Entry	Reaction concentration V / mL	Yield (%)[b]	ee (%)[c]
1	0.1	78[d]	93
2	0.2	65	95
3	0.3	63	94
4	0.4	59	94
5	0.5	43	93
6	0.6	49	96

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Ag_2CO_3 (3.0 equiv), HFIP (V mL), 60 °C, 8 h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Isolated yield.

Table S8. Optimization of conditions[a]



rac-**1a** **2** **3a**

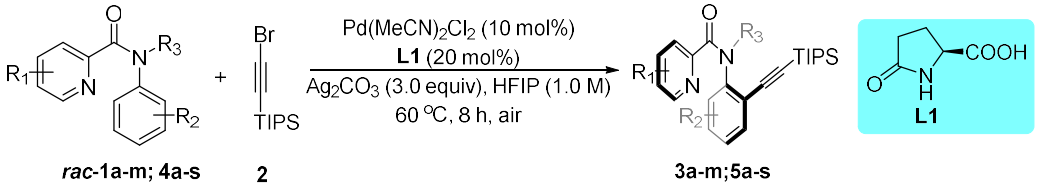
Entry	Deviation from standard conditions	Yield (%)[b]	ee (%)[c]
1	none	81(78)[d]	93
2	add AcOH (40 uL)	76	36
3	add $NaHCO_3$ (1.0 equiv)	60	89
4	add H_2O (40 uL)	37	93
5	24 h instead of 8 h	99	71
6	HFIP (0.2 M) instead of HFIP (1.0 M)	43	93
7	80 °C instead of 60 °C	76	46
8	no **L1**	2	0
9	*D*-**L1**	66	-93

[a]Reaction conditions: *rac*-**1a** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), Ligand (0.2 equiv), Ag_2CO_3 (3.0 equiv), HFIP (0.1 mL), 60 °C, 8 h, air. [b]Determined by ^1H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard. [c]The ee values were determined by chiral HPLC. [d]Yield of isolated product is within parentheses.

2.3 Palladium-Catalyzed Atroposelective Synthesis of N-Aryl Peptoid Atropisomers

2.3.1 General Procedure for Pd-Catalyzed Atroposelective Synthesis of Peptoid Atropisomers

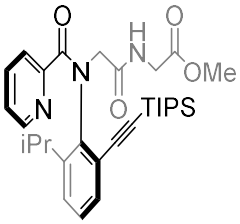
General Procedures for Atroposelective Synthesis of N-aryl peptoid atropisomers via Pd(II)-Catalyzed asymmetric C(sp^2)-H Alkynylation:



rac-1a-m; 4a-s 2 3a-m;5a-s

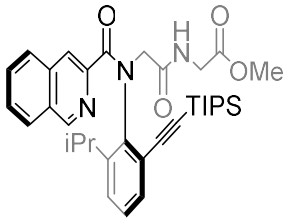
To an oven-dried 10 mL screw-capped vial was added substrate (0.10 mmol), protected alkynyl bromide (0.40 mmol), $Pd(MeCN)_2Cl_2$ (2.60 mg, 0.01 mmol), **L1** (0.02 mmol), Ag_2CO_3 (82.70 mg, 0.30 mmol), HFIP (0.1 mL). The mixture was then stirred for 8 h at 60 °C under air followed by cooling. The resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by preparative TLC to afford the chiral product.[2] Characterization data for products are reported as follows:

Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-picolinoylglycylglycinate (3a)



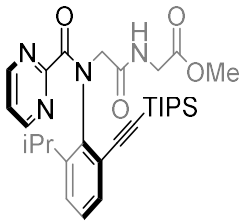
The title compound **3a** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3a** was obtained as a light yellow oil (42.8 mg, 78%, *E*: *Z* = 2: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.35 (d, *J* = 4.5 Hz, 1H), 7.82 (t, *J* = 5.4 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.52 (td, *J* = 7.7, 1.5 Hz, 1H), 7.30-7.27 (m, 1H), 7.16-7.10 (m, 3H), 5.22 (d, *J* = 14.6 Hz, 1H), 4.15 (dd, *J* = 18.0, 5.8 Hz, 1H), 4.03 (dd, *J* = 18.0, 5.4 Hz, 1H), 3.87 (d, *J* = 14.7 Hz, 1H), 3.76 (s, 3H), 3.20-3.14 (m, 1H), 1.10 (s, 21H), 1.05 (d, *J* = 6.8 Hz, 3H), 0.80 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.91, 169.79, 169.18, 152.11, 148.43, 147.55, 141.93, 135.86, 131.37, 128.35, 127.41, 124.71, 123.49, 122.28, 103.79, 96.91, 56.04, 52.30, 41.24, 28.28, 25.09, 22.81, 18.67, 11.34; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{43}N_3O_4Si$+Na^+]: 572.2915, found: 572.2916; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 90/10, rate = 0.8 mL/min, λ = 254 nm, t (major) = 7.9 min, t (minor) = 11.6 min, 93% ee; $[\alpha]_D^{20}$ = -139.2 (c = 1.0, $CHCl_3$).

Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(isoquinoline-3-carbonyl)glycylglycinate (3d)



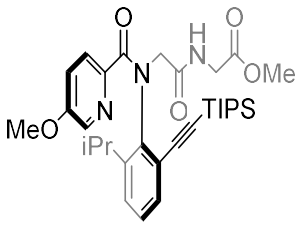
The title compound **3d** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3d** was obtained as a light yellow oil (6.6 mg, 11%, *E*: *Z* = 4: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.04 (d, *J* = 8.6 Hz, 1H), 7.86 (d, *J* = 8.6 Hz, 2H), 7.72 (t, *J* = 8.8 Hz, 2H), 7.60 (td, *J* = 6.8, 1.5 Hz, 1H), 7.49 (td, *J* = 8.0, 1.3 Hz, 1H), 7.28-7.26 (m, 1H), 7.15-7.13 (m, 2H), 5.25 (d, *J* = 14.7 Hz, 1H), 4.14 (dd, *J* = 9.8, 5.8 Hz, 2H), 3.95 (d, *J* = 14.7 Hz, 1H), 3.78 (s, 3H), 3.35-3.28 (m, 1H), 1.13-1.08 (m, 24H), 0.85 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.98, 169.70, 169.22, 151.75, 147.30, 146.54, 142.42, 135.99, 131.33, 129.79, 129.68, 128.19, 127.93, 127.70, 127.34, 127.33, 122.30, 120.44, 104.09, 96.56, 56.34, 52.31, 41.27, 28.30, 25.08, 23.00, 18.68, 11.35; **HRMS** (ESI-TOF) calcd for [$C_{35}H_{45}N_3O_4Si$+Na^+]: 622.3071, found: 622.3072; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 5.5 min, t (major) = 7.3 min, 61% ee; $[\alpha]_D^{20}$ = +59.4 (c = 0.5, $CHCl_3$).

Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(pyrimidine-2-carbonyl)glycylglycinate (3e)



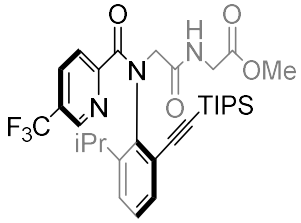
The title compound **3e** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3e** was obtained as a light yellow oil (34.7 mg, 63%, *E*: *Z* = 9: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.50 (d, *J* = 4.8 Hz, 2H), 7.78 (t, *J* = 5.8 Hz, 1H), 7.24 (dd, *J* = 7.3, 1.8 Hz, 1H), 7.12-7.05 (m, 3H), 5.20 (d, *J* = 14.7 Hz, 1H), 4.12 (dd, *J* = 18.0, 5.9 Hz, 1H), 4.00 (dd, *J* = 17.9, 5.5 Hz, 1H), 3.90 (d, *J* = 14.7 Hz, 1H), 3.73 (s, 3H), 3.21-3.14 (m, 1H), 1.09 (s, 21H), 1.04 (d, *J* = 6.8 Hz, 3H), 0.81 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.79, 169.05, 167.49, 160.33, 156.40, 147.20, 141.10, 131.21, 128.40, 126.85, 123.20, 121.25, 103.56, 96.72, 55.85, 52.27, 41.23, 28.17, 25.22, 22.92, 18.64, 11.34; **HRMS** (ESI-TOF) calcd for [$C_{30}H_{42}N_4O_4Si$+Na^+]: 573.2867, found: 573.2867; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 6.9 min, t (minor) = 11.9 min, 83% ee; $[\alpha]_D^{20}$ = -109.2 (c = 1.0, $CHCl_3$).

Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-methoxypicolinoyl)glycylglycinate (3f)



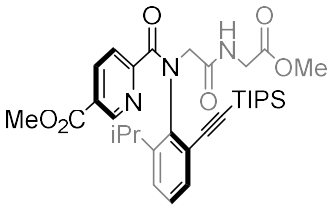
The title compound **3f** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3f** was obtained as a light yellow oil (12.7 mg, 22%, *E*: *Z* = 3: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.10 (d, *J* = 2.8 Hz, 1H), 7.99 (t, *J* = 5.6 Hz, 1H), 7.74 (d, *J* = 8.7 Hz, 1H), 7.44-7.38 (m, 2H), 7.27 (d, *J* = 3.1 Hz, 1H), 7.10 (dd, *J* = 8.7, 2.9 Hz, 1H), 5.29 (d, *J* = 14.6 Hz, 1H), 4.25 (dd, *J* = 18.0, 5.8 Hz, 1H), 4.13 (dd, *J* = 18.0, 5.5 Hz, 1H), 3.98 (d, *J* = 14.6 Hz, 1H), 3.88 (s, 3H), 3.87 (s, 3H), 3.29-3.22 (m, 1H), 1.21 (s, 21H), 1.18 (d, *J* = 6.9 Hz, 3H), 0.90 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.93, 169.33, 167.73, 156.31, 147.30, 144.07, 142.51, 136.22, 131.33, 128.08, 127.38, 125.10, 122.14, 119.28, 103.89, 96.57, 56.21, 55.55, 52.26, 41.20, 28.28, 24.93, 22.94, 18.66, 11.33; **HRMS** (ESI-TOF) calcd for [$C_{32}H_{45}N_3O_5Si$+Na^+]: 602.3020, found: 602.3022; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 85/15, rate = 0.8 mL/min, λ = 254 nm, t (major) = 7.2 min, t (minor) = 9.2 min, 96% ee; $[\alpha]_D^{20}$ = -107.8 (c = 0.5, $CHCl_3$).

Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-(trifluoromethyl)picolinoyl)glycylglycinate (3g)



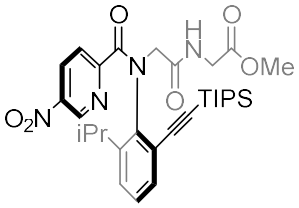
The title compound **3g** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3g** was obtained as a light yellow oil (57.4 mg, 93%, *E*: *Z* = 7: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.51 (s, 1H), 7.86-7.80 (m, 2H), 7.57 (t, *J* = 5.4 Hz, 1H), 7.24 (dd, *J* = 6.1, 3.1 Hz, 1H), 7.18-7.13 (m, 2H), 5.16 (d, *J* = 14.8 Hz, 1H), 4.09 (d, *J* = 5.6 Hz, 2H), 3.84 (d, *J* = 14.8 Hz, 1H), 3.74 (s, 3H), 3.31-3.24 (m, 1H), 1.12-1.07 (m, 24H), 0.92 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.88, 168.60, 168.48, 155.47, 147.60, 144.86 (q, J_{CF} = 2.0 Hz), 141.66, 133.31 (q, J_{CF} = 4.0 Hz), 131.38, 128.63, 127.53, 125.06 (q, J_{CF} = 152.5 Hz), 123.49, 122.20, 103.62, 96.86, 56.02, 52.29, 41.21, 28.30, 24.96, 22.87, 18.63, 11.33; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -62.71; **HRMS** (ESI-TOF) calcd for [$C_{32}H_{42}F_3N_3O_4Si$+Na^+]: 640.2789, found: 640.2791; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 85/15, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 6.6 min, t (major) = 10.2 min, 97% ee; $[\alpha]_D^{20}$ = -109.5 (c = 1.0, $CHCl_3$).

Methyl 6-((2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (3h)



The title compound **3h** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3h** was obtained as a light yellow oil (58.8 mg, 97%, *E*: *Z* = 6: 1). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.86 (dd, *J* = 2.1, 0.9 Hz, 1H), 8.15 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.75 (dd, *J* = 8.1, 0.8 Hz, 1H), 7.64 (t, *J* = 5.6 Hz, 1H), 7.23 (dd, *J* = 5.5, 3.6 Hz, 1H), 7.15-7.13 (m, 2H), 5.18 (d, *J* = 14.8 Hz, 1H), 4.09 (t, *J* = 5.6 Hz, 2H), 3.86 (s, 3H), 3.83 (d, *J* = 14.8 Hz, 1H), 3.74 (s, 3H), 3.28-3.22 (m, 1H), 1.09 (s, 21H), 1.07 (d, *J* = 6.8 Hz, 3H), 0.91 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 169.88, 169.08, 168.78, 165.00, 155.61, 149.20, 147.71, 141.64, 137.14, 131.34, 128.57, 127.49, 126.39, 123.13, 122.25, 103.64, 96.91, 55.96, 52.50, 52.30, 41.24, 28.32, 25.05, 22.90, 18.66, 11.33; **HRMS** (ESI-TOF) calcd for [$C_{33}H_{45}N_3O_6Si$+Na^+]: 630.2970, found: 630.2973; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, λ = 254 nm, t (major) = 15.3 min, t (minor) = 22.3 min, 97% ee; $[\alpha]_D^{20}$ = -159.9 (c = 1.0, $CHCl_3$).

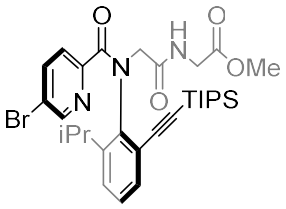
Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (3i)



The title compound **3a**iwas prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3i** was obtained as a light yellow oil (42.2 mg, 71%, *E*: *Z* = 17: 1).

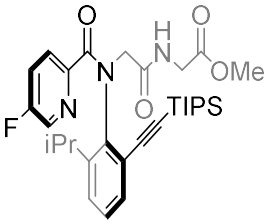
^{1}H NMR (400 MHz, CDCl$_3$) δ 9.02 (d, *J* = 2.5 Hz, 1H), 8.37 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.95 (d, *J* = 8.6 Hz, 1H), 7.44 (t, *J* = 5.6 Hz, 1H), 7.23-7.17 (m, 3H), 5.14 (d, *J* = 14.9 Hz, 1H), 4.10 (t, *J* = 5.9 Hz, 2H), 3.83 (d, *J* = 14.9 Hz, 1H), 3.76 (s, 3H), 3.38-3.31 (m, 1H), 1.10 (s, 21H), 1.02 (d, *J* = 6.8 Hz, 6H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 169.92, 168.30, 167.92, 157.26, 147.80, 143.92, 143.18, 141.40, 131.40, 131.28, 128.86, 127.64, 124.20, 122.25, 103.47, 97.04, 55.92, 52.36, 41.25, 28.34, 25.00, 22.98, 18.67, 11.35; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{42}N_4O_6Si$+Na^+]: 617.2766, found: 617.2768; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 85/15, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 8.9 min, t (major) = 10.4 min, 97% ee; $[\alpha]_D^{20}$ = -92.1 (c = 1.0, $CHCl_3$).

Methyl *N*-(5-bromopicolinoyl)-*N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)glycylglycinate (3j)



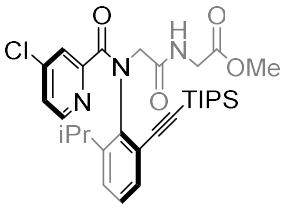
The title compound **3j** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3j** was obtained as a light yellow oil (60.8 mg, 97%, *E*: *Z* = 6: 1). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.30 (dd, *J* = 2.2, 0.6 Hz,1H), 7.68 (dd, *J* = 8.4, 2.3 Hz, 1H), 7.63 (t, *J* = 5.5 Hz, 1H), 7.60 (dd, *J* = 8.4, 0.6 Hz,1H), 7.26-7.22 (m, 1H), 7.16-7.14 (m, 2H), 5.13 (d, *J* = 14.7 Hz, 1H), 4.06 (dd, *J* = 5.6, 2.5 Hz, 2H), 3.81 (d, *J* = 14.8 Hz, 1H), 3.72 (s, 3H), 3.24-3.17 (m, 1H), 1.08-1.05 (m, 24H), 0.89 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 169.87, 168.80, 150.48, 149.10, 147.47, 142.00, 138.66, 131.33, 128.42, 127.47, 125.17, 122.37, 122.12, 103.70, 96.69, 56.06, 52.28, 41.20, 28.28, 24.94, 22.95, 18.65, 11.32; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{42}BrN_3O_4Si$+Na^+]: 650.2020, found: 650.2022; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, λ = 254 nm, t (major) = 10.0 min, t (minor) = 14.3 min, 94% ee; $[\alpha]_D^{20}$ = -149.1 (c = 1.0, $CHCl_3$).

Methyl *N*-(5-fluoropicolinoyl)-*N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)glycylglycinate (3k)



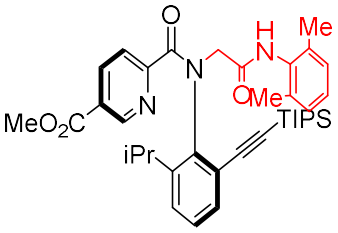
The title compound **3k** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **3k** was obtained as a light yellow oil (43.7 mg, 77%, *E*: *Z* = 5: 1). **^{1}H NMR (400 MHz, CDCl$_3$)** δ 8.07 (d, *J* = 2.7 Hz, 1H), 7.73 (dd, *J* = 8.8, 4.4 Hz, 1H), 7.66 (t, *J* = 5.6 Hz, 1H), 7.25-7.21 (m, 2H), 7.14-7.12 (m, 2H), 5.13 (d, *J* = 14.8 Hz, 1H), 4.05 (dd, *J* = 5.6, 2.8 Hz, 2H), 3.81 (d, *J* = 14.8 Hz, 1H), 3.71 (s, 3H), 3.21-3.14 (m, 1H), 1.07-1.03 (m, 24H), 0.83 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, CDCl$_3$)** δ 169.90, 168.92, 168.61, 159.51 (d, J_{CF} = 161.6 Hz), 148.23 (d, J_{CF} = 5.1 Hz), 147.39, 142.15, 136.45 (d, J_{CF} = 23.2 Hz), 131.31, 128.33, 127.41, 125.60 (d, J_{CF} = 5.1 Hz), 122.66 (d, J_{CF} = 19.2 Hz), 122.15, 103.74, 96.62, 56.10, 52.26, 41.18, 28.26, 24.92, 22.89, 18.63, 11.31; **^{19}F NMR (376 MHz, CDCl$_3$)** δ -122.78; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{42}FN_3O_4Si$+Na^+]: 590.2821, found: 590.2820; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 90/10, rate = 0.8 mL/min, λ = 254 nm, t (major) = 6.7 min, t (minor) = 8.6 min, 96% ee; $[\alpha]_D^{20}$ = -120.8 (c = 1.0, $CHCl_3$).

Methyl *N*-(4-chloropicolinoyl)-*N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)glycylglycinate (3l)



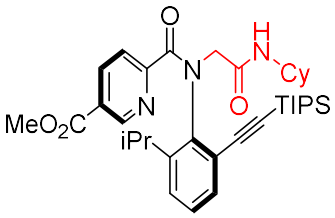
The title compound **3l** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate =2: 1). **3l** was obtained as a light yellow oil (54.8 mg, 94%, *E*: *Z* = 3: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.14 (d, *J* = 5.2 Hz, 1H), 7.74 (d, *J* = 2.0 Hz, 1H), 7.63 (t, *J* = 5.4 Hz, 1H), 7.24 (dd, *J* = 6.3, 2.7 Hz, 1H), 7.17-7.12 (m, 3H), 5.12 (d, *J* = 14.8 Hz, 1H), 4.07 (dd, *J* = 5.4, 4.2 Hz, 2H), 3.83 (d, *J* = 14.8 Hz, 1H), 3.73 (s, 3H), 3.27-3.20 (m, 1H), 1.11-1.07 (m, 24H), 0.94 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.85, 168.85, 168.70, 153.44, 148.90, 147.58, 144.27, 141.69, 131.35, 128.55, 127.49, 125.05, 124.18, 122.15, 103.62, 96.93, 55.96, 52.29, 41.22, 28.33, 24.92, 22.90, 18.63, 11.31; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{42}ClN_3O_4Si$+Na^+]: 606.2525, found: 606.2526; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 97/3, rate = 0.8 mL/min, λ = 254 nm, t (major) = 13.5 min, t (minor) = 21.1 min, 95% ee; $[\alpha]_D^{20}$ = -93.4 (c = 1.0, $CHCl_3$).

Methyl 6-((2-((2,6-dimethylphenyl)amino)-2-oxoethyl)(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)carbamoyl)nicotinate (5a)



The title compound **5a** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5a** was obtained as a white powder (57.5 mg, 90%, *E*: *Z* = 17: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.77 (s, 1H), 8.63 (s, 1H), 8.23 (dd, *J* = 8.1, 1.8 Hz, 1H), 7.94 (d, *J* = 8.2 Hz, 1H), 7.29 (t, *J* = 4.8 Hz, 1H), 7.17 (d, *J* = 4.8 Hz, 2H), 7.08-7.04 (m, 3H), 5.04 (d, *J* = 15.3 Hz, 1H), 4.18 (d, *J* = 15.3 Hz, 1H), 3.88 (s, 3H), 3.51-3.45 (m, 1H), 2.30 (s, 6H), 1.26 (d, *J* = 6.8 Hz, 3H), 1.21 (d, *J* = 6.8 Hz, 3H), 1.06 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.50, 166.66, 165.10, 155.91, 148.61, 147.53, 142.43, 137.24, 135.39, 133.80, 131.44, 128.42, 128.17, 127.88, 127.19, 126.40, 123.68, 122.02, 104.17, 97.14, 56.86, 52.51, 28.78, 24.73, 23.22, 18.67, 18.59, 18.54, 11.39; **HRMS** (ESI-TOF) calcd for [$C_{38}H_{49}N_3O_4Si$+Na^+]: 662.3384, found: 662.3387; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak IC, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 15.3 min, t (major) = 25.1 min, 93% ee; $[\alpha]_D^{20}$ = -55.3 (c = 1.0, $CHCl_3$).

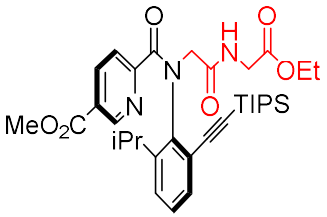
Methyl 6-((2-(cyclohexylamino)-2-oxoethyl)(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)carbamoyl)nicotinatee (5b)



The title compound **5b** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5b** was obtained as a light yellow oil (61.1 mg, 99%, *E*: *Z* = 14: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 8.14 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.73 (d, *J* = 8.1 Hz, 1H), 7.20 (dd, *J* = 6.8, 2.3 Hz, 1H), 7.17-7.10 (m, 3H), 5.18 (d, *J* = 14.7 Hz, 1H), 3.87 (s, 3H), 3.83-3.75 (m, 1H), 3.67 (d, *J* = 14.7 Hz, 1H), 3.27-3.21 (m, 1H), 1.95-1.90 (m, 2H), 1.74-1.67 (m, 2H), 1.41-1.20 (m, 6H), 1.13 (d, *J* = 6.9 Hz, 3H), 1.10 (s, 21H), 0.98 (d, *J* = 6.3 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.28, 167.75, 165.05, 156.03, 149.14, 147.81, 141.90, 137.09, 131.26, 128.51, 127.36, 126.26, 122.87, 122.29, 103.63, 96.73, 56.59, 52.48, 48.21, 32.82, 32.72, 28.46, 25.56, 25.32, 24.63, 22.82, 18.67, 11.35; **HRMS** (ESI-TOF) calcd for $[C_{36}H_{51}N_3O_4Si+Na^+]$: 640.3541, found: 640.3542; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak IC, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 7.9 min, t (major) = 15.7 min, 96% ee; $[\alpha]_D^{20}$ = -182.7 (c = 1.0, $CHCl_3$).

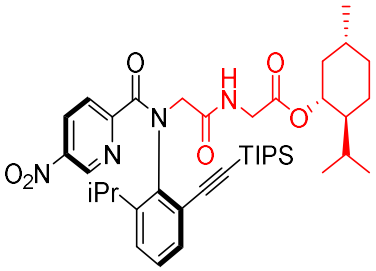
Methyl 6-((2-((2-ethoxy-2-oxoethyl)amino)-2-oxoethyl)(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)carbamoyl)nicotinate (5c)



The title compound **5c** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5c** was obtained as a light yellow oil (50.9 mg, 82%, *E*: *Z* = 6: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 1.3 Hz, 1H), 8.15 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.77 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.61 (t, *J* = 5.5 Hz, 1H), 7.24-7.20 (m, 1H), 7.16-7.11 (m, 2H), 5.18 (d, *J* = 14.7 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 2H), 4.08 (dd, *J* = 8.6, 5.5 Hz, 2H), 3.87 (s, 3H), 3.84 (d, *J* = 14.8 Hz, 1H), 3.30-3.24 (m, 1H), 1.27 (t, *J* = 7.1 Hz, 3H), 1.11-107 (m, 24H), 0.92 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.40, 169.06, 168.74, 165.04, 155.66, 149.18, 147.74, 141.72, 137.13, 131.34, 128.55, 127.48, 126.38, 123.18, 122.27, 103.67, 96.87, 61.39, 56.00, 52.49, 41.41, 28.33, 25.06, 22.89, 18.66, 14.15, 11.35; **HRMS** (ESI-TOF) calcd for $[C_{34}H_{47}N_3O_6Si+Na^+]$: 644.3126, found: 644.3128; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH= 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 6.2 min, t (major) = 8.4 min, 96% ee; $[\alpha]_D^{20}$ = -168.4 (c = 1.0, $CHCl_3$).

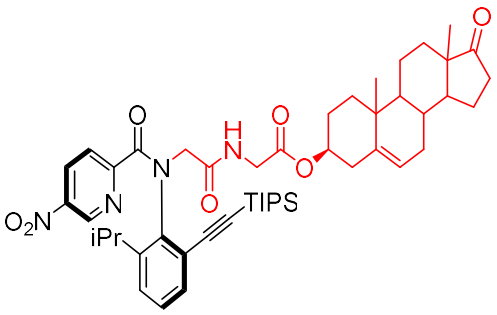
(1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (5d)



The title compound **5d** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5d** was obtained as a light yellow oil (36.6 mg, 51%, *E*: *Z* = 10: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.02 (d, *J* = 2.6 Hz, 1H), 8.37 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.98 (d, *J* = 8.6 Hz, 1H), 7.36 (t, *J* = 4.9 Hz, 1H), 7.24-7.15 (m, 3H), 5.15 (d, *J* = 14.9 Hz, 1H), 4.76 (td, *J* = 10.9, 4.4 Hz, 1H), 4.14-4.02 (m, 2H), 3.83 (d, *J* = 14.9 Hz, 1H), 3.41-3.34 (m, 1H), 2.04-1.98 (m, 1H), 1.89-1.81 (m, 1H), 1.71-1.65 (m, 2H), 1.55-1.45 (m, 1H), 1.43-1.36 (m, 1H), 1.14-0.99 (m, 29H), 0.92-0.86 (m, 7H), 0.75 (d, *J* = 6.9 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.10, 168.16, 167.81, 157.33, 147.83, 143.95, 143.15, 141.52, 131.40, 131.27, 128.82, 127.62, 124.35, 122.31, 103.52, 96.97, 75.73, 55.92, 46.91, 41.59, 40.79, 34.14, 31.39, 28.33, 26.30, 25.01, 23.46, 22.99, 22.00, 20.72, 18.68, 16.38, 11.36; **HRMS** (ESI-TOF) calcd for [$C_{40}H_{58}N_4O_6Si$+Na^+]: 741.4018, found: 741.4018; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 97/3, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 12.8 min, t (major) = 17.3 min, 97% ee; $[\alpha]_D^{20}$ = -147.8 (c = 1.0, $CHCl_3$).

(3S)-10,13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[a] phenanthren-3-yl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (5e)

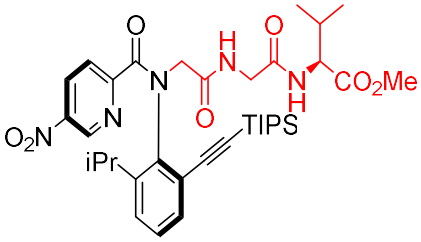


The title compound **5e** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5e** was obtained as a yellow oil (62.1 mg, 73%, *E*: *Z* = 11: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.01 (d, *J* = 2.4 Hz, 1H), 8.36 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.41 (t, *J* = 5.4 Hz, 1H), 7.23-7.14 (m, 3H), 5.39 (d, *J* = 5.0 Hz, 1H), 5.14 (d, *J* = 14.9 Hz, 1H), 4.72-4.64 (m, 1H), 4.13-4.01 (m, 2H), 3.82 (d, *J* = 14.9 Hz, 1H), 3.39-3.32 (m, 1H), 2.48-2.34 (m, 3H), 2.12-2.02 (m, 2H), 1.97-1.79 (m, 5H), 1.70-1.42 (m, 7H), 1.31-1.23 (m, 3H), 1.10 (s, 21H), 1.03 (s, 3H), 1.02-0.98 (m, 5H), 0.87 (s, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 168.82, 168.80, 168.20, 167.88, 157.31, 147.82, 143.93, 143.17, 141.45, 139.64, 131.41, 131.27, 128.85, 127.64, 124.22, 122.27, 122.17, 103.49, 97.03, 75.06, 55.94, 51.70, 50.12, 47.51, 41.63, 37.99, 37.96, 36.86, 36.71, 35.82, 31.45, 31.40, 30.78, 28.34, 27.62, 25.03, 22.99, 21.87, 20.33, 19.31, 18.68, 13.55, 11.35; **HRMS** (ESI-TOF) calcd for [$C_{49}H_{66}N_4O_7Si$+Na^+]: 873.4593, found: 873.4595; Enantiomeric excess was determined by HPLC with

a Daicel Chiralpak AD-H, *n*-Hexane/ *i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 11.1 min, t (major) = 15.6 min, 97% ee; $[\alpha]_D^{20}$ = -103.8 (c = 1.0, $CHCl_3$).

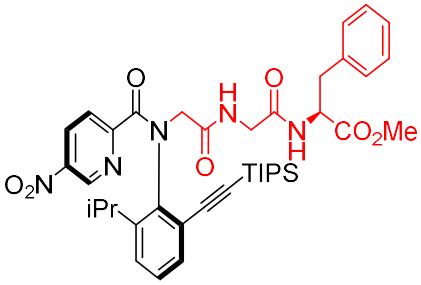
Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycyl-*L*-valinate (5f)



The title compound **5f** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5f** was obtained as a light yellow oil (34.7 mg, 50%, *E*: *Z* = 14: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 2.5 Hz, 1H), 8.39 (dd, *J* = 8.7, 2.5 Hz, 1H), 8.05 (d, *J* = 8.6 Hz, 1H), 7.34 (t, *J* = 5.2 Hz, 1H), 7.27-7.24 (m, 1H), 7.19 (d, *J* = 4.8 Hz, 2H), 6.89 (d, *J* = 8.5 Hz, 1H), 4.87 (d, *J* = 15.1 Hz, 1H), 4.51 (dd, *J* = 8.2, 5.5 Hz, 1H), 4.16 (dd, *J* = 16.8, 6.1 Hz, 1H), 3.99-3.91 (m, 2H), 3.72 (s, 3H), 3.53-3.44 (m, 1H), 2.21-2.13 (m, 1H), 1.17-1.07 (m, 27H), 0.92 (dd, *J* = 10.2, 6.8 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 172.18, 168.64, 168.16, 167.57, 156.97, 147.72, 144.00, 142.89, 141.55, 131.46, 131.31, 128.78, 127.82, 124.73, 122.07, 103.79, 96.92, 57.52, 56.02, 52.07, 43.29, 30.95, 28.27, 24.73, 23.05, 18.93, 18.66, 17.98, 11.36; **HRMS** (ESI-TOF) calcd for $[C_{36}H_{51}N_5O_7Si+Na^+]$: 716.3450, found: 716.3449; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, λ = 254 nm, t (major) = 24.3 min, t (minor) = 41.5 min, 98% ee; $[\alpha]_D^{20}$ = -73.6 (c = 1.0, $CHCl_3$).

Methyl *N*-(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycyl-*L*-phenylalaninate (5g)

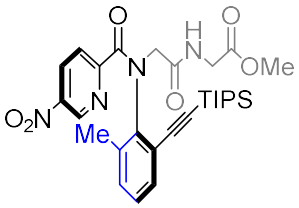


The title compound **5g** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5g** was obtained as a light yellow oil (34.8 mg, 47%, *E*: *Z* = 13: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (d, *J* = 2.5 Hz, 1H), 8.37 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.99 (d, *J* = 8.6 Hz, 1H), 7.27-7.17 (m, 7H), 7.10 (d, *J* = 6.9 Hz, 2H), 6.84 (d, *J* = 7.8 Hz, 1H), 4.93 (d, *J* = 15.0 Hz, 1H), 4.84 (q, *J* = 6.7 Hz, 1H), 4.08 (dd, *J* = 16.8, 6.0 Hz, 1H), 3.94 (dd, *J* = 16.8, 5.3 Hz, 1H), 3.87 (d, *J* = 15.0 Hz, 1H), 3.69 (s, 3H), 3.53-3.46 (m, 1H), 3.17-3.07 (m, 2H), 1.16-1.08 (m, 27H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 171.81, 168.31, 168.16, 167.66, 157.00, 147.76, 143.98, 142.99, 141.48, 135.93, 131.44,

131.31, 129.23, 128.84, 128.55, 127.79, 127.07, 124.55, 122.16, 103.64, 96.90, 55.92, 53.56, 52.30, 43.19, 37.74, 28.24, 24.82, 23.03, 18.69, 11.38; **HRMS** (ESI-TOF) calcd for $[C_{40}H_{51}N_5O_7Si+Na^+]$: 764.3450, found: 764.3453; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 8.8 min, t (minor) = 14.0 min, 97% ee; $[\alpha]_D^{20}$ = -61.1 (c = 1.0, $CHCl_3$).

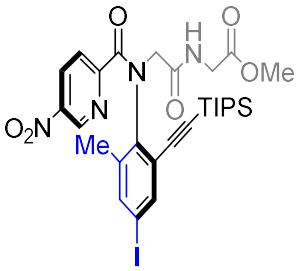
Methyl *N*-(2-methyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (5h)



The title compound **5h** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5h** was obtained as a light yellow oil (40.1 mg, 71%, *E*: *Z* = 20: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.05 (s, 1H), 8.36 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 8.6 Hz, 1H), 7.43 (t, *J* = 5.7 Hz, 1H), 7.21 (dd, *J* = 6.5, 2.7 Hz, 1H), 7.10-7.05 (m, 2H), 5.11 (d, *J* = 14.7 Hz, 1H), 4.10 (dd, *J* = 8.3, 5.6 Hz, 2H), 3.83 (d, *J* = 14.7 Hz, 1H), 3.75 (s, 3H), 2.35 (s, 3H), 1.12 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.90, 168.41, 167.87, 157.58, 143.98, 143.51, 142.80, 137.83, 131.65, 131.62, 131.27, 128.50, 123.65, 122.39, 103.13, 97.42, 54.91, 52.37, 41.31, 18.67, 18.56, 11.34; **HRMS** (ESI-TOF) calcd for $[C_{29}H_{38}N_4O_6Si+Na^+]$: 589.2453, found: 589.2455; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 13.2 min, t (minor) = 16.5 min, 87% ee; $[\alpha]_D^{20}$ = -107.0 (c = 1.0, $CHCl_3$).

Methyl *N*-(4-iodo-2-methyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (5i)

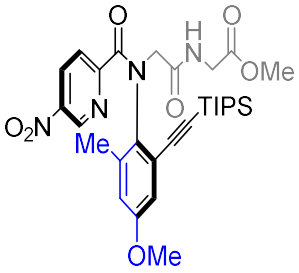


The title compound **5i** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 1: 1). **5i** was obtained as a light yellow oil (26.3 mg, 38%, *E*: *Z* = 17: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.4 Hz, 1H), 8.41 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.96 (d, *J* = 8.6 Hz, 1H), 7.52 (d, *J* = 1.8 Hz, 1H), 7.47 (d, *J* = 1.3 Hz, 1H), 7.29 (t, *J* = 5.2 Hz, 1H), 5.07 (d, *J* = 14.8 Hz, 1H), 4.13 (dd, *J* = 18.2, 5.5 Hz, 1H), 4.05 (dd, *J* = 18.2, 5.3 Hz, 1H), 3.76 (d, *J* = 14.6 Hz, 1H),3.75 (s, 3H), 2.32 (s, 3H), 1.10 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.87, 168.07, 167.44, 157.07, 144.16, 143.47, 143.03, 140.35, 139.86, 139.85, 131.49, 124.13, 124.06, 101.35, 98.98, 93.49, 54.82, 52.40, 41.29, 18.66, 18.27, 11.31; **HRMS** (ESI-TOF) calcd for $[C_{29}H_{37}IN_4O_6Si+Na^+]$: 715.1419, found: 715.1419; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-

PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 16.9 min, t (minor) = 32.5 min, 83% ee; $[\alpha]_D^{20}$ = -69.1 (c = 1.0, $CHCl_3$).

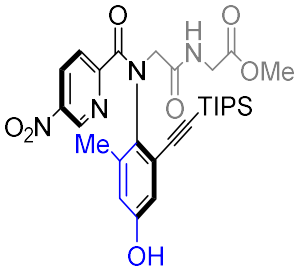
Methyl *N*-(4-methoxy-2-methyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (5j)



The title compound **5j** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 1: 1). **5j** was obtained as a light yellow oil (47.1 mg, 79%, *E*: *Z* = 25: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.12 (d, *J* = 2.5 Hz, 1H), 8.36 (dd, *J* = 8.6, 2.5 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.45 (t, *J* = 5.5 Hz, 1H), 6.70 (d, *J* = 2.9 Hz, 1H), 6.60 (d, *J* = 2.9 Hz, 1H), 5.11 (d, *J* = 14.6 Hz, 1H), 4.10 (t, *J* = 6.3 Hz, 2H), 3.79 (d, *J* = 14.8 Hz, 1H), 3.76 (s, 3H), 3.72 (s, 3H), 2.30 (s, 3H), 1.13 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.87, 168.51, 168.26, 158.70, 157.99, 143.88, 143.71, 139.23, 135.87, 131.23, 123.25, 117.26, 116.02, 103.06, 97.25, 55.43, 55.18, 52.36, 41.30, 18.87, 18.68, 11.36; **HRMS** (ESI-TOF) calcd for $[C_{30}H_{40}N_4O_7Si+Na^+]$: 619.2558, found: 619.2559; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, n-Hexane/i-PrOH = 80/20, rate = 1.0 mL/min, λ = 254 nm, t (major) = 12.7 min, t (minor) = 16.3 min, 94% ee; $[\alpha]_D^{20}$ = -178.6 (c = 1.0, $CHCl_3$).

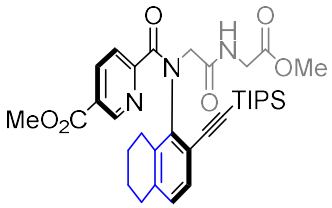
Methyl *N*-(4-hydroxy-2-methyl-6-((triisopropylsilyl)ethynyl)phenyl)-*N*-(5-nitropicolinoyl)glycylglycinate (5k)



The title compound **5k** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 1: 1). **5k** was obtained as a yellow oil (34.3 mg, 59%, *E*: *Z* = 10: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (d, *J* = 2.4 Hz, 1H), 8.30 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.96 (s, 1H), 7.85 (t, *J* = 5.6 Hz, 1H), 7.73 (d, *J* = 8.6 Hz, 1H), 6.59 (d, *J* = 2.8 Hz, 1H), 6.20 (d, *J* = 2.8 Hz, 1H), 5.11 (d, *J* = 14.2 Hz, 1H), 4.09 (d, *J* = 5.6 Hz, 2H), 3.94 (d, *J* = 14.2 Hz, 1H), 3.77 (s, 3H), 2.06 (s, 3H), 1.12 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.08, 169.38, 168.43, 157.63, 156.12, 144.14, 143.93, 138.08, 133.85, 131.24, 122.99, 122.95, 118.51, 118.02, 103.05, 97.39, 54.38, 52.54, 41.43, 18.69, 18.36, 11.32; **HRMS** (ESI-TOF) calcd for $[C_{29}H_{38}N_4O_7Si+Na^+]$: 605.2402, found: 605.2401; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 9.6 min, t (major) = 16.5 min, 94% ee; $[\alpha]_D^{20}$ = -174.5 (c = 1.0, $CHCl_3$).

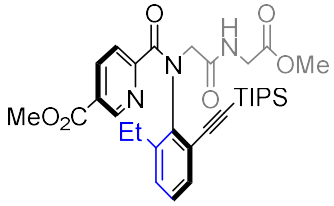
Methyl 6-((2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)(2-((triisopropylsilyl)ethynyl)-5,6,7,8-tetrahydronaphthalen-1-yl)carbamoyl)nicotinate (5l)



The title compound **5l** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5l** was obtained as a light yellow oil (61.3 mg, 99%, *E*: *Z* = 11: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (d, *J* = 2.0 Hz, 1H), 8.13 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.63 (t, *J* = 5.6 Hz, 1H), 7.07 (d, *J* = 7.9 Hz, 1H), 6.84 (d, *J* = 7.9 Hz, 1H), 5.09 (d, *J* = 14.7 Hz, 1H), 4.08 (dd, *J* = 5.5, 2.0 Hz, 2H), 3.87 (s, 3H), 3.78 (d, *J* = 14.7 Hz, 1H), 3.73 (s, 3H), 2.95-2.88 (m, 1H), 2.69-2.57 (m, 3H), 1.79-1.56 (m, 4H), 1.10 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.82, 169.21, 168.96, 165.11, 156.18, 149.31, 142.89, 140.07, 137.04, 130.29, 129.28, 126.32, 122.50, 119.38, 103.63, 96.11, 54.97, 52.49, 52.27, 41.32, 29.63, 25.48, 22.50, 22.21, 18.67, 11.36; **HRMS** (ESI-TOF) calcd for [$C_{34}H_{45}N_3O_6Si$+Na^+]: 642.2970, found: 642.2971; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 6.9 min, t (minor) = 9.0 min, 87% ee; $[\alpha]_D^{20}$ = -100.7 (c = 1.0, $CHCl_3$).

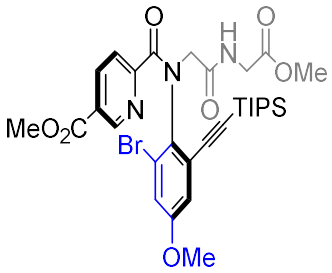
Methyl 6-((2-ethyl-6-((triisopropylsilyl)ethynyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (5m)



The title compound **5m** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5m** was obtained as a light yellow oil (54.0 mg, 91%, *E*: *Z* = 8: 1).

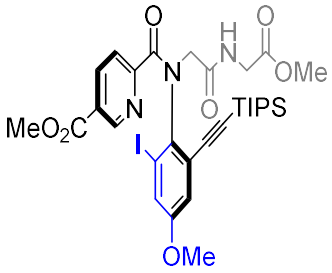
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.84 (dd, *J* = 2.1, 0.8 Hz, 1H), 8.14 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.73 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.59 (t, *J* = 5.5 Hz, 1H), 7.24-7.19 (m, 1H), 7.14-7.08 (m, 2H), 5.14 (d, *J* = 14.7 Hz, 1H), 4.09 (d, *J* = 5.6 Hz, 2H), 3.87 (s, 3H), 3.82 (d, *J* = 15.0 Hz, 1H), 3.75 (s, 3H), 2.72-2.64 (m, 2H), 1.13-1.09 (m, 24H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.85, 169.10, 168.74, 165.06, 155.93, 149.29, 142.97, 142.51, 137.07, 131.30, 129.07, 128.31, 126.32, 122.74, 122.27, 103.48, 97.00, 55.34, 52.49, 52.30, 41.27, 23.57, 18.67, 13.77, 11.35; **HRMS** (ESI-TOF) calcd for [$C_{32}H_{43}N_3O_6Si$+Na^+]: 616.2813, found: 616.2815; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 6.9 min, t (major) = 12.5 min, 94% ee; $[\alpha]_D^{20}$ = -172.5 (c = 1.0, $CHCl_3$).

Methyl 6-((2-bromo-4-methoxy-6-((triisopropylsilyl)ethynyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (5n)



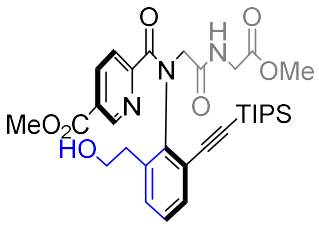
The title compound **5n** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5n** was obtained as a light yellow oil (21.5 mg, 32%, *E*: *Z* = 6: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.87 (d, *J* = 2.0 Hz, 1H), 8.22 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.64 (t, *J* = 5.5 Hz, 1H), 6.94 (d, *J* = 2.8 Hz, 1H), 6.88 (d, *J* = 2.8 Hz, 1H), 5.03 (d, *J* = 14.8 Hz, 1H), 4.14 (dd, *J* = 18.2, 5.6 Hz, 1H), 4.03 (dd, *J* = 18.2, 5.2 Hz, 1H), 3.94-3.90 (m, 4H), 3.75 (s, 6H), 1.09 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.95, 168.61, 168.16, 165.16, 158.73, 155.34, 149.17, 137.17, 136.53, 126.57, 124.88, 124.43, 123.71, 119.05, 118.22, 102.20, 98.79, 55.80, 55.11, 52.54, 52.29, 41.44, 18.62, 11.29; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{40}BrN_3O_7Si+Na^+$]: 696.1711, found: 696.1710; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (minor) = 11.9 min, t (major) = 15.0 min, 90% ee; $[\alpha]_D^{20}$ = -96.8 (c = 0.5, $CHCl_3$).

Methyl 6-((2-iodo-4-methoxy-6-((triisopropylsilyl)ethynyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (5o)



The title compound **5o** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 2: 1). **5o** was obtained as a light brown oil (29.6 mg, 41%, *E*: *Z* = 5: 1). **^{1}H NMR (400 MHz, $CDCl_3$)** δ 8.87 (dd, *J* = 2.1, 0.8 Hz, 1H), 8.23 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.93 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.74 (t, *J* = 5.3 Hz, 1H), 7.19 (d, *J* = 2.9 Hz, 1H), 6.92 (d, *J* = 2.8 Hz, 1H), 5.02 (d, *J* = 14.6 Hz, 1H), 4.19 (dd, *J* = 18.1, 5.6 Hz, 1H), 4.02 (dd, *J* = 18.2, 4.9 Hz, 1H), 3.91 (d, *J* = 14.6 Hz, 1H), 3.91 (s, 3H), 3.75 (s, 3H), 3.74 (s, 3H), 1.08 (s, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.95, 168.45, 168.10, 165.18, 158.45, 155.33, 149.03, 140.05, 137.13, 126.54, 125.46, 124.06, 124.01, 119.07, 102.50, 100.57, 98.49, 55.76, 55.58, 52.54, 52.30, 41.54, 18.62, 11.30; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{40}IN_3O_7Si+Na^+$]: 744.1572, found: 744.1573; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, λ = 254 nm, t (major) = 56.3 min, t (minor) = 77.2 min, 96% ee; $[\alpha]_D^{20}$ = -95.8 (c = 1.0, $CHCl_3$).

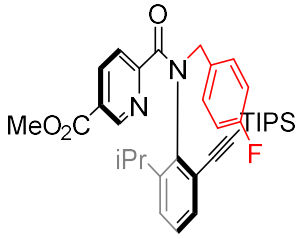
Methyl 6-((2-(2-hydroxyethyl)-6-((triisopropylsilyl)ethynyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (5p)



The title compound **5p** was prepared under the optimized conditions and purified by preparative TLC (ethyl acetate: dichloromethane = 1: 1). **5p** was obtained as a light yellow oil (23.1 mg, 38%, *E*: *Z* = 33: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (d, *J* = 2.0 Hz, 1H), 8.49 (t, *J* = 6.3 Hz, 1H), 8.27 (dd, *J* = 8.2, 2.0 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.23 (dd, *J* = 6.6, 2.7 Hz, 1H), 7.13-7.08 (m, 2H), 5.50 (s, 1H), 5.01 (d, *J* = 16.0 Hz, 1H), 4.38 (dd, *J* = 17.8, 6.8 Hz, 1H), 4.05-3.98 (m, 2H), 3.89 (s, 3H), 3.88-3.80 (m, 2H), 3.74 (s, 3H), 3.39-3.32 (m, 1H), 2.86 (dt, *J* = 14.8, 4.1 Hz, 1H), 1.15-1.10 (m, 21H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.41, 169.01, 168.63, 164.65, 156.10, 147.70, 143.85, 139.04, 137.92, 132.32, 131.73, 128.47, 126.65, 125.20, 123.07, 103.17, 97.27, 63.77, 55.10, 52.65, 52.23, 41.11, 35.75, 18.68, 18.65, 11.42; **HRMS** (ESI-TOF) calcd for [$C_{32}H_{43}N_3O_7Si+Na^+$]: 632.2762, found: 632.2759; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AS-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 9.2 min, t (minor) = 16.0 min, 99% ee; $[\alpha]_D^{20}$ = -23.7 (c = 1.0, $CHCl_3$).

Methyl 6-((4-fluorobenzyl)(2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)carbamoyl)nicotinate (5q)

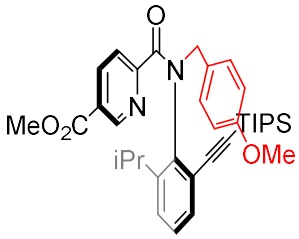


The title compound **5q** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 4: 1). **5q** was obtained as a light yellow oil (51.6 mg, 88%, *E*: *Z* = 11: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, *J* = 2.0 Hz, 1H), 8.10 (dd, *J* = 8.2, 2.2 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.35-7.30 (m, 3H), 7.13 (t, *J* = 7.8 Hz, 1H), 7.01 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.92 (t, *J* = 8.6 Hz, 2H), 5.72 (d, *J* = 14.2 Hz, 1H), 4.58 (d, *J* = 14.2 Hz, 1H), 3.88 (s, 3H), 2.78-2.72 (m, 1H), 1.12 (s, 21H), 0.61 (d, *J* = 6.7 Hz, 3H), 0.37 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 166.42 (d, J_{CF} = 254.8 Hz), 165.19, 163.75, 161.30, 156.73, 149.50, 147.84, 140.40, 136.98, 132.64 (d, J_{CF} = 4.0 Hz), 131.93 (d, J_{CF} = 8.1 Hz), 131.52, 128.15, 127.50, 126.02, 122.90, 122.87, 115.25 (d, J_{CF} = 21.2 Hz), 104.14, 96.96, 53.07, 52.46, 28.04, 23.60, 23.30, 18.69, 18.68, 11.35; **^{19}F NMR (376 MHz, $CDCl_3$)** δ -114.70; **HRMS** (ESI-TOF) calcd for [$C_{35}H_{43}FN_2O_3Si+H^+$]: 587.3100, found: 587.3102; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, n-Hexane/i-PrOH = 90/10, rate = 0.8 mL/min, λ = 254 nm, t (major) = 7.2 min, t (minor) = 9.7 min, 92% ee; $[\alpha]_D^{20}$ = -91.0 (c = 0.28, $CHCl_3$).

Methyl 6-((2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)(4-

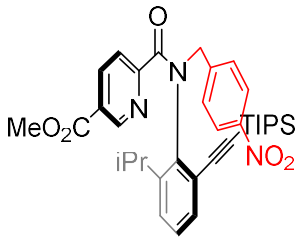
methoxybenzyl)carbamoyl)nicotinate (5r)



The title compound **5r** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 10: 1). **5r** was obtained as a light yellow oil (44.3 mg, 74%, *E*: *Z* = 9: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.95 (dd, *J* = 2.1, 0.9 Hz, 1H), 8.09 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.67 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.31 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.26 (t, *J* = 4.6 Hz, 2H), 7.12 (t, *J* = 7.8 Hz, 1H), 6.99 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.76 (d, *J* = 8.6 Hz, 2H), 5.74 (d, *J* = 14.2 Hz, 1H), 4.54 (d, *J* = 14.1 Hz, 1H), 3.88 (s, 3H), 3.75 (s, 3H), 2.78-2.71 (m, 1H), 1.12 (s, 21H), 0.57 (d, *J* = 6.8 Hz, 3H), 0.33 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 167.48, 165.24, 159.27, 156.96, 149.55, 147.99, 140.50, 136.92, 131.50, 131.42, 128.97, 128.02, 127.45, 125.91, 122.90, 122.82, 113.78, 104.27, 96.82, 55.26, 53.11, 52.43, 28.02, 23.57, 23.36, 18.71, 18.69, 11.37; **HRMS** (ESI-TOF) calcd for [$C_{36}H_{46}N_2O_4Si$+Na^+]: 621.3119, found: 621.3122; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 6.8 min, t (minor) = 12.8 min, 91% ee; $[\alpha]_D^{20}$ = -128.2 (c = 1.0, $CHCl_3$).

Methyl 6-((2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)(4-nitrobenzyl)carbamoyl)nicotinate (5s)

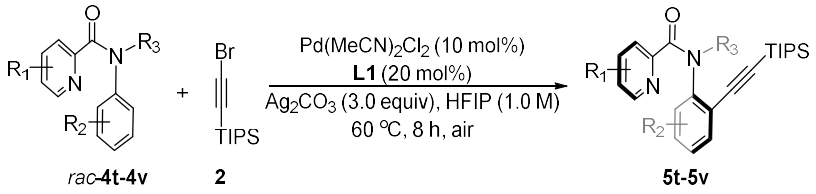


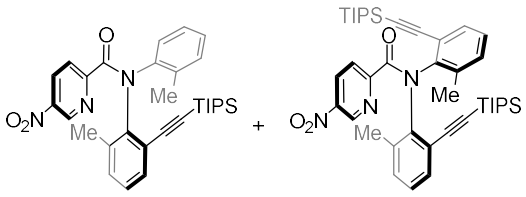
The title compound **5s** was prepared under the optimized conditions and purified by preparative TLC (petroleum ether: ethyl acetate = 10: 1). **5s** was obtained as a light yellow oil (53.3 mg, 87%, *E*: *Z* = 14: 1).

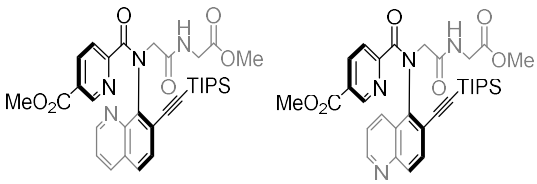
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 1.4 Hz, 1H), 8.16-8.11 (m, 3H), 7.77 (d, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 8.6 Hz, 2H), 7.26 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.15 (t, *J* = 7.8 Hz, 1H), 7.09 (dd, *J* = 7.9, 1.6 Hz, 1H), 5.61 (d, *J* = 14.4 Hz, 1H), 4.78 (d, *J* = 14.5 Hz, 1H), 3.89 (s, 3H), 2.91-2.85 (m, 1H), 1.09 (s, 21H), 0.78 (d, *J* = 6.7 Hz, 3H), 0.51 (d, *J* = 6.8 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 168.05, 165.13, 156.31, 149.20, 147.51, 144.09, 140.56, 137.13, 131.70, 130.88, 128.38, 127.61, 126.26, 123.59, 123.27, 122.82, 103.93, 97.04, 53.55, 52.50, 28.19, 23.90, 23.23, 18.66, 18.63, 11.33; **HRMS** (ESI-TOF) calcd for [$C_{35}H_{43}N_3O_5Si$+Na^+]: 636.2864, found: 636.2864; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 90/10, rate = 0.8 mL/min, λ = 254 nm, t (major) = 9.8 min, t (minor) = 21.3 min, 91% ee; $[\alpha]_D^{20}$ = -82.0 (c = 1.0, $CHCl_3$).

2.3.2 Limitation of the Scope of Substrate and Alkyne

Table S9. Limitation of substrate scope[a]

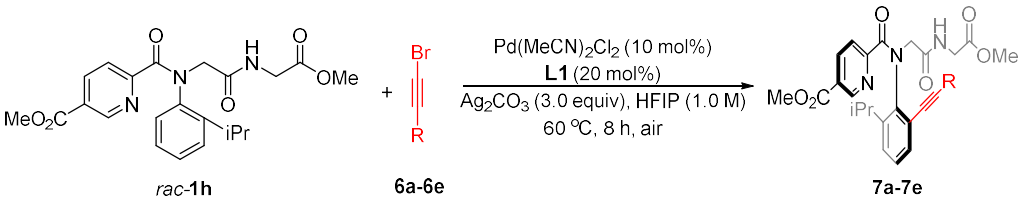




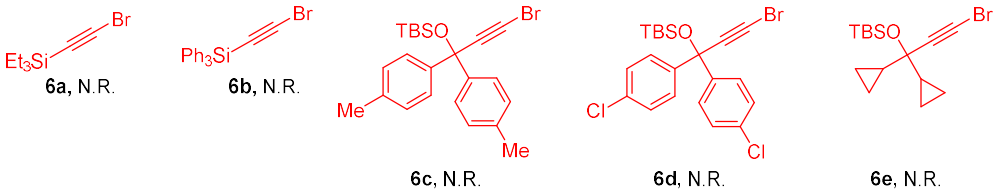


[a]Standard conditions: *rac*-**4** (0.1 mmol, 1.0 equiv), **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Ag_2CO_3 (3.0 equiv), HFIP (0.1 mL, 1.0 M), 60 °C, 8 h, air.

Table S10. Limitation of alkynes scope[a]



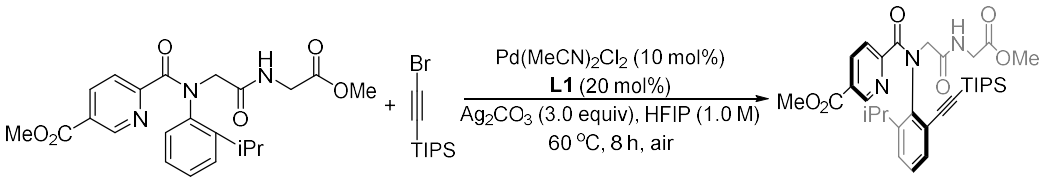
Failed alkyne reagents:



[a]Standard conditions: *rac*-**1h** (0.1 mmol, 1.0 equiv), **6** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (0.1 equiv), **L1** (0.2 equiv), Ag_2CO_3 (3.0 equiv), HFIP (0.1 mL, 1.0 M), 60 °C, 8 h, air.

2.4 Gram-Scale Synthesis and Transformations

2.4.1 Gram-scale synthesis of 3h

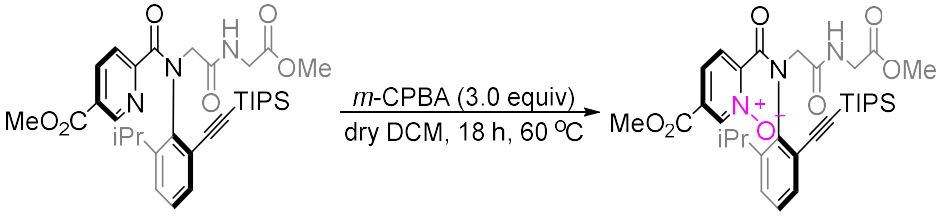


***rac*-1h**, 2.5 mmol, 1.0675 g **2** **3h**, 1.2156 g, 80%, 95% ee, *E* : *Z* = 6: 1

To an oven-dried 50 mL screw-capped vial was added ***rac*-1h** (2.5 mmol, 1.07 g, 1.0 equiv), protected alkynyl bromide **2** (4.0 equiv), $Pd(MeCN)_2Cl_2$ (65 mg, 0.1 equiv), **L1** (65 mg, 0.2 equiv), Ag_2CO_3 (2.07 g, 3.0 equiv), HFIP (2.5 mL). The mixture was then stirred for 8 h at 60 °C under air followed by cooling. The resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by silica gel column chromatography to afford the desired product **3h** (1.22 g, 80% yield, 95% ee, *E*: *Z* = 6: 1).

2.4.2 Transformations

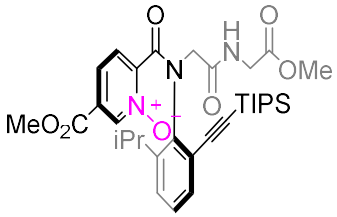
a) Oxidation of 3h



3h, 95% ee, *E* : *Z* = 6: 1 **3ha**, 59%, 95% ee, *E* : *Z* = 11: 1

To an oven-dried 10 mL screw-capped vial containing a stirring bar was added **3h** (0.20 mmol), *m*-CPBA (3.0 equiv), anhydrous DCM (3.0 mL). The mixture was then stirred for 18 h at 60 °C followed by cooling. The resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by preparative TLC (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%) to give **3ha** as a brown oil (73.6 mg, 59%, *E*: *Z* = 11: 1).

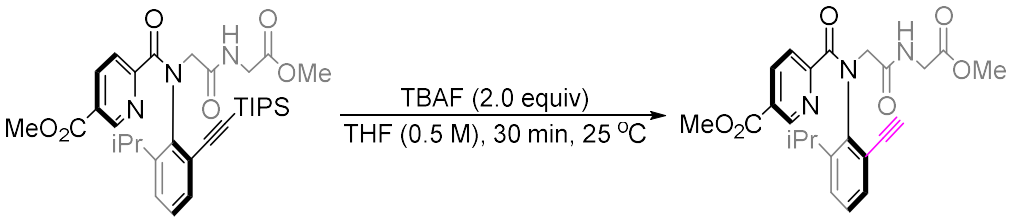
2-((2-isopropyl-6-((triisopropylsilyl)ethynyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)-5-(methoxycarbonyl)pyridine 1-oxide (3ha)



The title compound **3ha** was purified by preparative TLC (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). **3ha** was obtained as a brown oil (73.6 mg, 59%, *E*: *Z* = 11: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (s, 1H), 8.31 (t, *J* = 5.7 Hz, 1H), 7.66-7.60 (m, 2H), 7.28 (dd, *J* = 7.1, 1.9 Hz, 1H), 7.22-7.14 (m, 2H), 5.22 (d, *J* = 16.5 Hz, 1H), 4.34 (dd, *J* = 17.8, 6.4 Hz, 1H), 4.00 (dd, *J* = 17.8, 5.1 Hz, 1H), 3.88 (s, 3H), 3.75 (s, 3H), 3.74-3.67 (m, 2H), 1.16-1.10 (m, 21H), 1.06 (t, *J* = 6.4 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.73, 167.68, 163.14, 162.71, 149.44, 146.99, 139.98, 139.51, 131.64, 129.71, 129.39, 128.36, 125.75, 123.78, 123.46, 103.10, 98.52, 53.88, 53.16, 52.19, 41.38, 28.06, 25.34, 23.57, 18.68, 18.65, 11.36; **HRMS** (ESI-TOF) calcd for [$C_{33}H_{45}N_3O_7Si$ +Na^+]: 646.2919, found: 646.2919; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 8.5 min, t (minor) = 14.2 min, 95% ee; $[\alpha]_D^{20}$ = -391.3 (c = 0.5, $CHCl_3$).

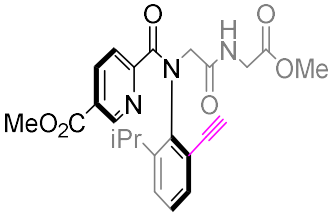
b) Removal of TIPS of 3h



3h, 95% ee, *E* : *Z* = 6: 1 **3hb**, 92%, 95% ee, *E* : *Z* = 10: 1

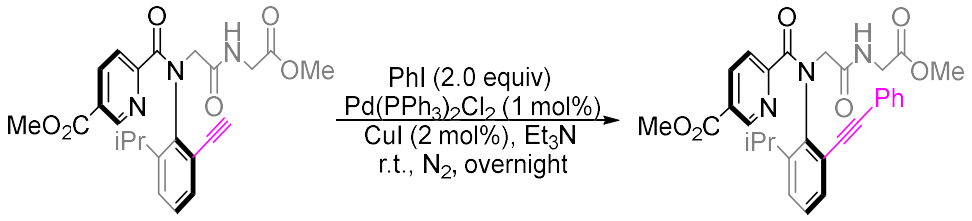
TBAF (1 M in THF) (2.0 equiv) was added dropwise into a solution of **3h** (4.1 mmol, 1.0 equiv) in THF (0.5 M). After being stirred for 30 min at 25 °C, the resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by silica gel column chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%) to afford the product **3hb** as a white foam (1.7011 g, 92%, *E*: *Z* = 10: 1).

Methyl6-((2-ethynyl-6-isopropylphenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (3hb)



The title compound **3hb** was purified by silica gel column chromatography (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). **3hb** was obtained as a white foam (1.7011 g, 92%, *E*: *Z* = 10: 1).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.75 (dd, *J* = 2.1, 0.8 Hz, 1H), 8.20 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.84 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.62 (t, *J* = 5.3 Hz, 1H), 7.26-7.22 (m, 1H), 7.14 (d, *J* = 4.5 Hz, 2H), 4.57 (d, *J* = 14.9 Hz, 1H), 4.28 (d, *J* = 14.9 Hz, 1H), 4.14 (dd, *J* = 18.2, 5.6 Hz, 1H), 4.04 (dd, *J* = 18.2, 5.2 Hz, 1H), 3.85 (s, 3H), 3.73 (s, 3H), 3.33-3.26 (m, 1H), 3.24 (s, 1H), 1.16 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.00, 169.25, 168.26, 165.03, 155.79, 148.64, 147.37, 142.41, 137.33, 130.82, 128.54, 128.22, 126.40, 123.76, 120.92, 82.31, 80.95, 55.85, 52.50, 52.30, 41.35, 28.43, 24.63, 23.07; **HRMS** (ESI-TOF) calcd for [$C_{24}H_{25}N_3O_6$+Na^+]: 474.1635, found: 474.1637; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, λ = 254 nm, t (major) = 29.7 min, t (minor) = 43.4 min, 95% ee; $[\alpha]_D^{20}$ = -44.8 (c = 0.5, $CHCl_3$).

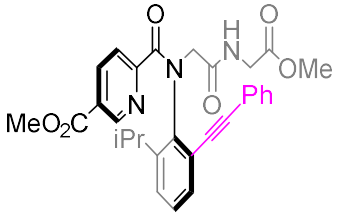
c) Sonogashira coupling of 3hb



3hb, 95% ee, *E* : *Z* = 10: 1 **3hc**, 91%, 91% ee, *E* : *Z* = 17: 1

To an oven-dried 10 mL screw-capped vial containing a stirring bar was added **3hb** (0.10 mmol), PhI (2.0 equiv), $Pd(PPh_3)_2Cl_2$ (0.01 equiv), CuI (0.02 equiv) and Et_3N (0.6 mL). Then the test tube was evacuated and back-filled with dry nitrogen (this sequence was repeated three times). The mixture was stirred overnight at room temperature. Then the resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by preparative TLC (petroleum ether: ethyl acetate: triethylamine = 2: 1: 1%) to give **3hc** as a light yellow oil (48.0 mg, 91%, *E*: *Z* = 17: 1).

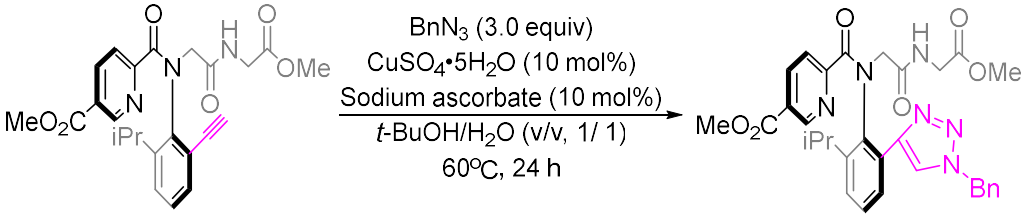
Methyl6-((2-isopropyl-6-(phenylethynyl)phenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (3hc)



The title compound **3hc** was purified by preparative TLC (petroleum ether: ethyl acetate: triethylamine = 2: 1: 1%). **3hc** was obtained as a light yellow oil (48.0 mg, 91%, *E*: *Z* = 17: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 1.4 Hz, 1H), 8.18 (dd, *J* = 8.1, 2.1 Hz, 1H), 7.86 (d, *J* = 8.2 Hz, 1H), 7.63 (t, *J* = 5.2 Hz, 1H), 7.55-7.50 (m, 2H), 7.40-7.35(m, 3H), 7.28 (dd, *J* = 7.5, 2.0 Hz, 1H), 7.21-7.14 (m, 2H), 4.59 (d, *J* = 14.8 Hz, 1H), 4.37 (d, *J* = 14.8 Hz, 1H), 4.02 (dd, *J* = 18.2, 5.8 Hz, 1H), 3.87-3.81 (m, 4H), 3.68 (s, 3H), 3.45-3.36 (m, 1H), 1.24 (dd, *J* = 6.9, 3.7 Hz, 6H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 169.88, 168.19, 165.10, 155.93, 148.60, 147.28, 142.11, 137.43, 131.43, 129.83, 128.94, 128.69, 128.55, 127.78, 126.44, 123.68, 122.36, 121.91, 93.97, 86.86, 55.96, 52.52, 52.27, 41.36, 28.71, 24.51, 23.28; **HRMS** (ESI-TOF) calcd for $[C_{30}H_{29}N_3O_6+Na^+]$: 550.1948, found: 550.1949; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak IF-3, *n*-Hexane/*i*-PrOH = 60/40, rate = 0.6 mL/min, λ = 254 nm, t (minor) = 10.6 min, t (major) = 14.1 min, 91% ee; $[\alpha]_D^{20}$ = -218.9 (c = 0.5, $CHCl_3$).

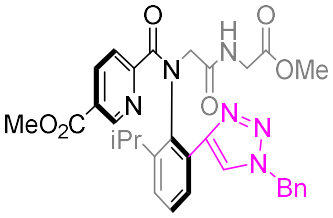
d) Azide-Alkyne cycloaddition of 3hb



3hb, 95% ee, *E* : *Z* = 10: 1 **3hd**, 81%, 97% ee, *E* : *Z* = 4: 1

To an oven-dried 10 mL screw-capped vial containing a stirring bar was added **3hb** (0.10 mmol), BnN_3 (3.0 equiv), $CuSO_4•5H_2O$ (0.1 equiv), Sodium ascorbate (0.1 equiv) and *t*-BuOH/H_2O (v/v, 1/1, 0.4 mL). The mixture was stirred for 24 h at 25 °C. Then the resulting mixture was filtered through a celite pad and concentrated in vacuo. The residue was purified by preparative TLC (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%) to give **3hd** as a white foam (47.3 mg, 81%, *E*: *Z* = 4: 1).

Methyl6-((2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-6-isopropylphenyl)(2-((2-methoxy-2-oxoethyl)amino)-2-oxoethyl)carbamoyl)nicotinate (3hd)



The title compound **3hd** was purified by preparative TLC (petroleum ether: ethyl acetate: triethylamine = 1: 1: 1%). **3hd** was obtained as a white foam (47.3 mg, 81%, *E*: *Z* = 4: 1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.00 (dd, *J* = 8.2, 2.1 Hz, 1H), 7.96-7.93 (m, 1H), 7.63-7.60 (m, 2H), 7.42-7.37 (m, 3H)), 7.34-7.29 (m, 3H), 7.24-7.19 (m, 2H), 5.59-5.46 (m, 2H), 4.39 (d, *J* = 14.8 Hz, 1H), 4.04-3.98 (m, 3H), 3.86 (s, 3H), 3.74 (s, 3H), 3.25-3.18 (m, 1H), 1.15 (d, *J* = 6.7 Hz, 3H), 0.91 (d, *J* = 6.7 Hz, 3H); **^{13}C NMR (101 MHz, $CDCl_3$)** δ 170.08, 169.26, 168.38, 165.08, 156.05, 148.60, 147.46, 145.95, 138.94, 137.17, 134.62, 129.21, 129.15, 128.90, 128.82, 128.13, 128.04, 127.47, 127.19, 123.91, 122.57, 56.46, 54.23, 52.47, 52.25, 41.12, 28.30, 25.08, 23.27; **HRMS** (ESI-TOF) calcd for [$C_{31}H_{32}N_6O_6$+Na^+]: 607.2275, found: 607.2276; Enantiomeric excess was determined by HPLC with a Daicel Chiralpak IF-3, *n*-Hexane/*i*-PrOH = 50/50, rate = 0.8 mL/min, λ = 254 nm, t (major) = 22.5 min, t (minor) = 25.8 min, 97% ee; $[\alpha]_D^{20}$ = -107.6 (c = 1.0, $CHCl_3$).

3. Computational Details

All density functional theory (DFT) calculations were carried out using Gaussian09 software package[3]. All geometry optimizations were performed with ω-B97XD[4] functional using LANL2DZ[5] basis set for palladium and 6-31G(d) basis set for the other atoms. The vibrational frequencies were computed at the same level of theory as for the geometry optimizations, and to evaluate the zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. The single-point energies were computed based on the gas-phase optimized structures, using MN15L functional[6], and def2-TZVPP[7,8] basis set for all atoms, with the inclusion of solvation energy corrections using a self-consistent reaction field (SCRF) based on SMD implicit solvent model[9] with HFIP (ε = 16.7) as solvent. In addition, to correct the Gibbs free energies under pressure of 1 atm to the standard state in solution (1 mol/L), a correction of RT $\ln(c_s/c_g)$ (1.9 kcal/mol) is added to energies of all species. c_s is the standard molar concentration in solution (1 mol/L), c_g is the standard molar concentration in gas phase (0.0446 mol/L), and R is the gas constant. 3.2 kcal/mol free energy correction on HFIP solvent molecule was included based on the concentration of pure HFIP solvent under the standard state (9.45 mol/L).[10] The 3D diagrams of molecules were generated using CYLView20.[11]

3.1 Exploration of C−H activation transition state with HFIP solvent involvements

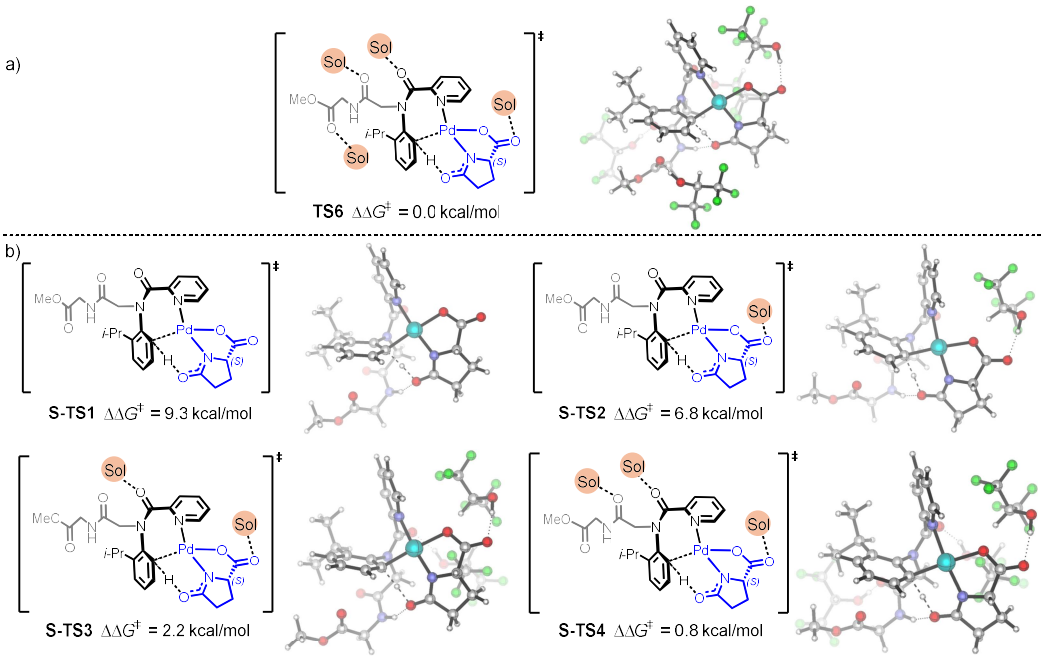


Fig. S1 Pd/L-pGlu-catalyzed C–H bond activation of methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-**1a**) with or without the HFIP involvements.

3.2 Conformers of C−H activation transition state without HFIP involvement

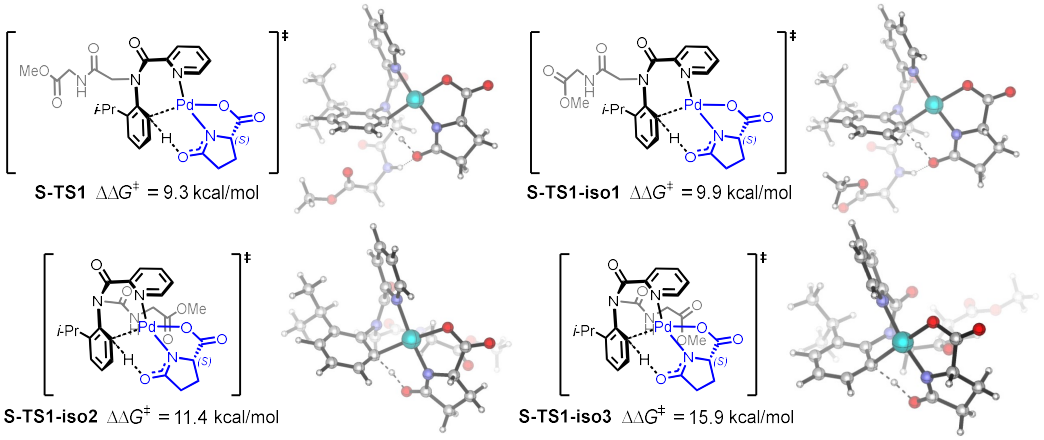


Fig. S2 Conformers of Pd/L-pGlu-catalyzed C−H bond activation transition state of methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-**1a**) with no HFIP solvent involvement. Free energies are compared to **TS6**.

3.3 Conformers of C−H activation transition state with one HFIP involvement

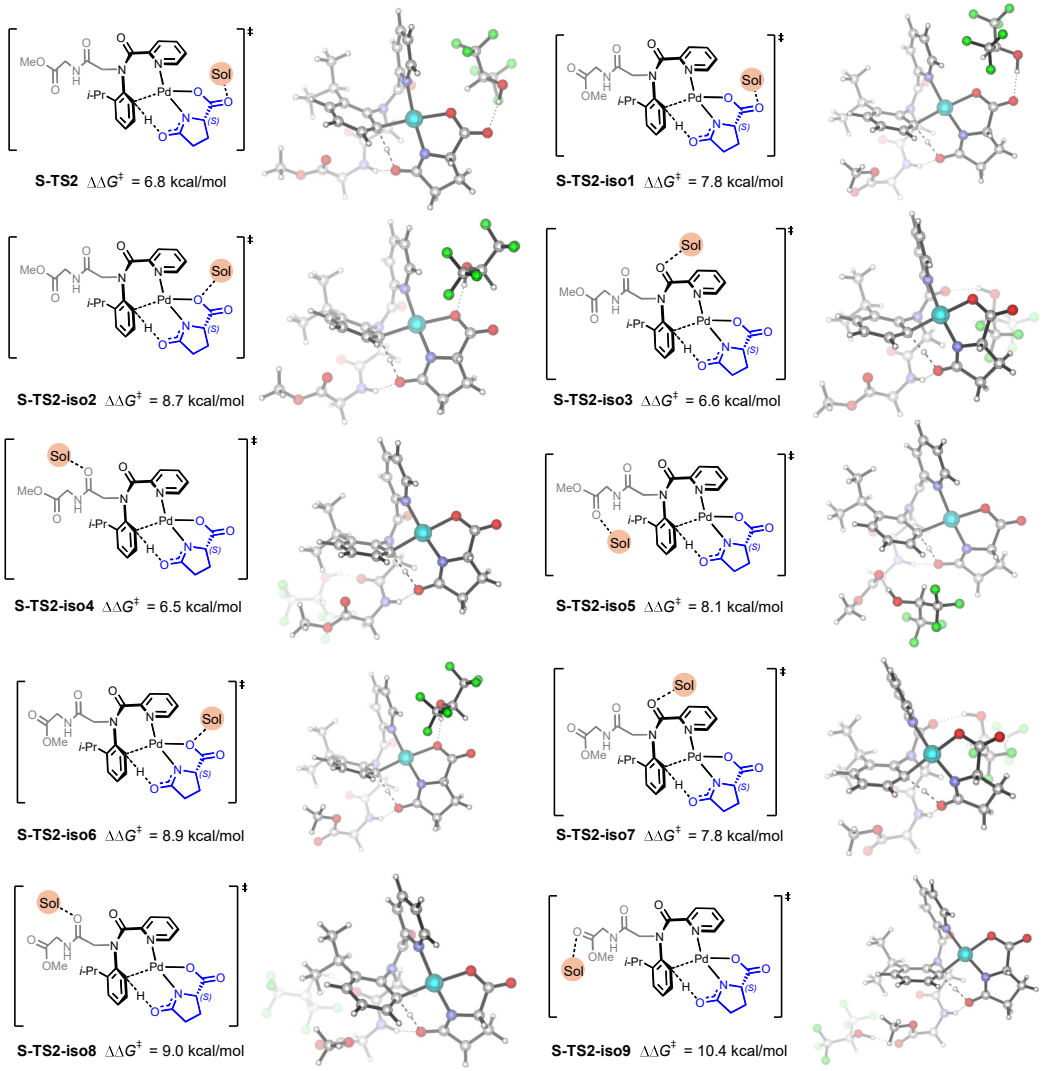


Fig. S3 Conformers of Pd/L-pGlu-catalyzed C−H bond activation transition state of methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-**1a**) with one HFIP solvent involvement. Free energies are compared to **TS6**.

3.4 Conformers of C−H activation transition state with two HFIP involvements

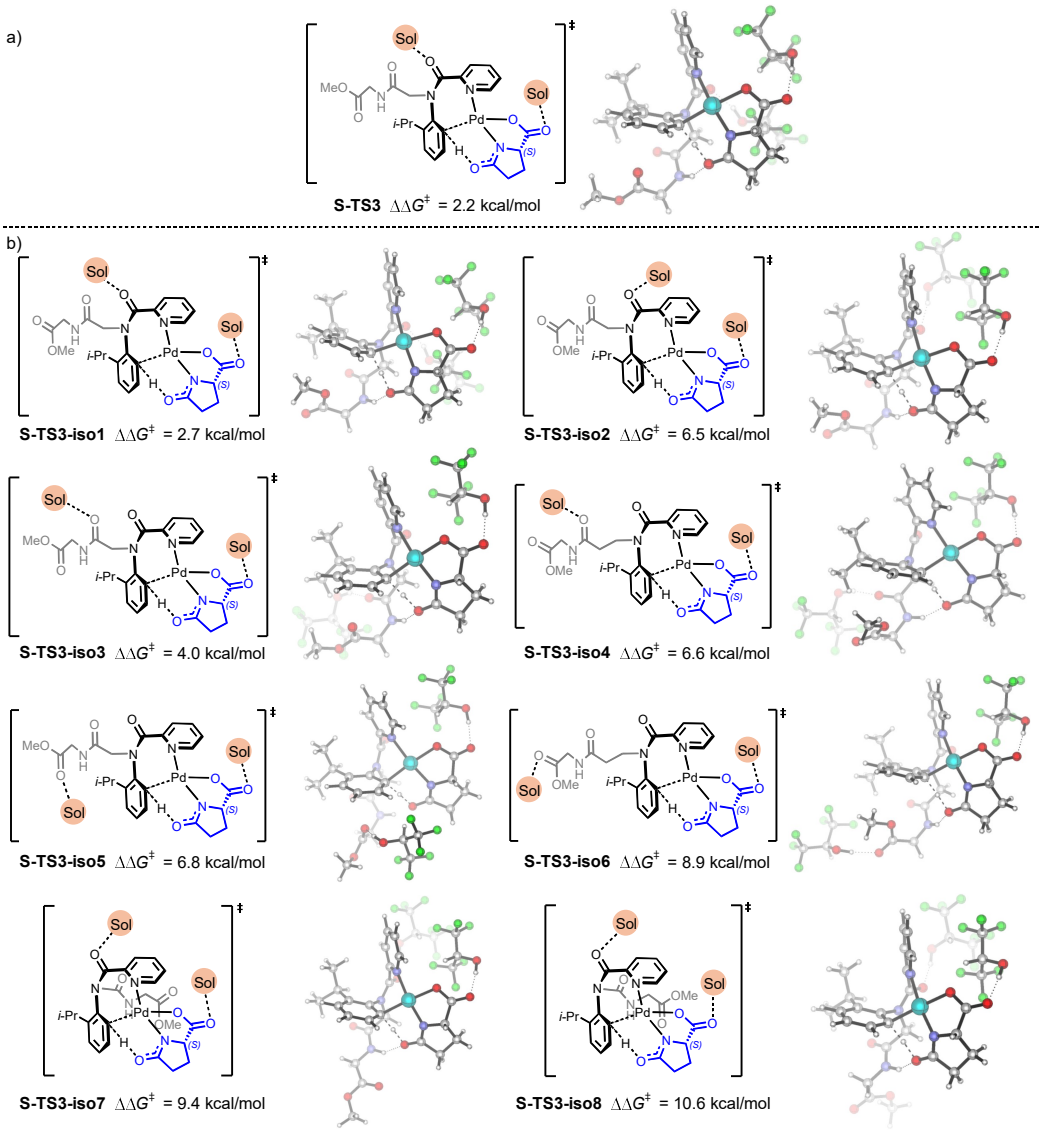


Fig. S4 Conformers of Pd/L-pGlu-catalyzed C−H bond activation transition state of methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-**1a**) with two HFIP solvent involvements. Free energies are compared to **TS6**.

3.5 Conformers of C−H activation transition state with three HFIP involvements

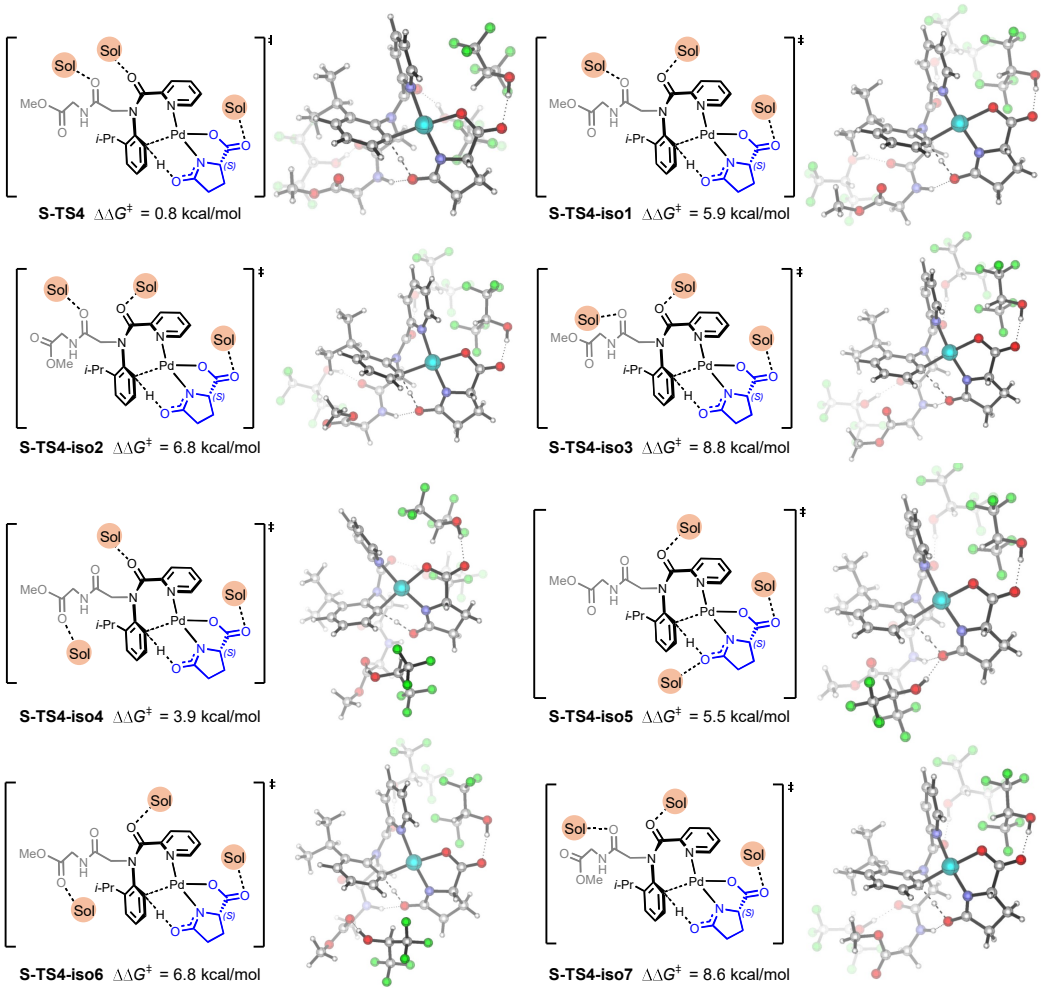


Fig. S5 Conformers of Pd/L-pGlu-catalyzed C−H bond activation transition state of methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-**1a**) with three HFIP solvent involvements. Free energies are compared to **TS6**.

3.6 Conformers of C−H activation transition state with four HFIP involvements

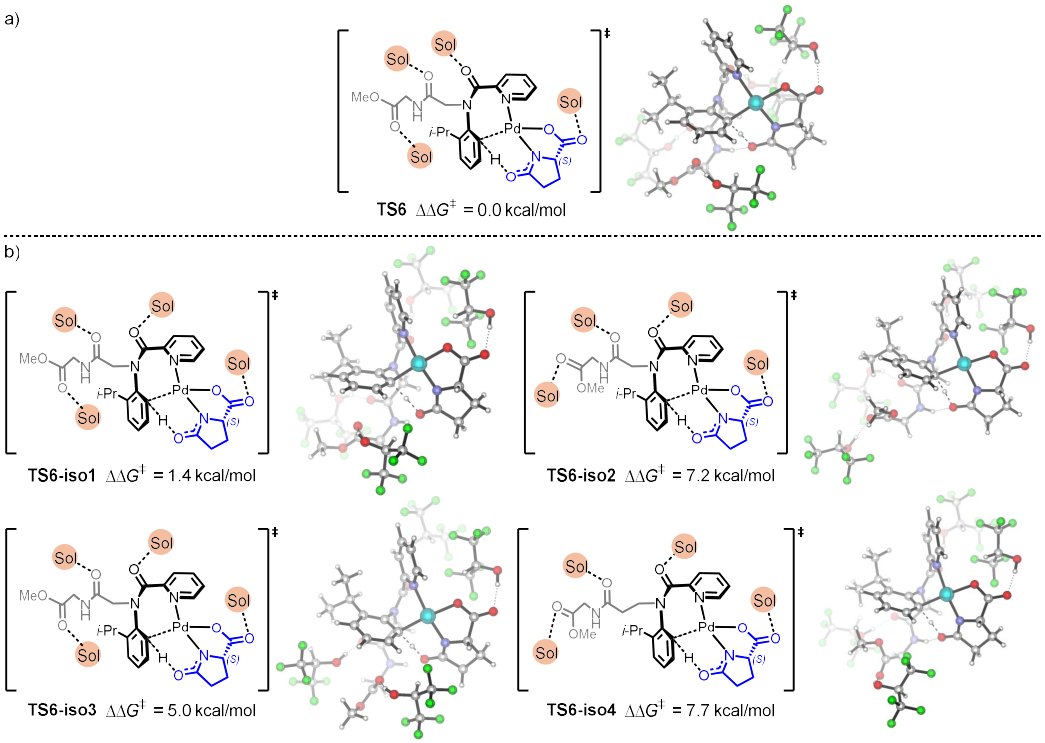


Fig. S6 Conformers of Pd/L-pGlu-catalyzed C−H bond activation transition state of methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-**1a**) with four HFIP solvent involvements. Free energies are compared to **TS6**.

3.7 Conformers of C−H activation transition state leading to (*S*)-axial chirality

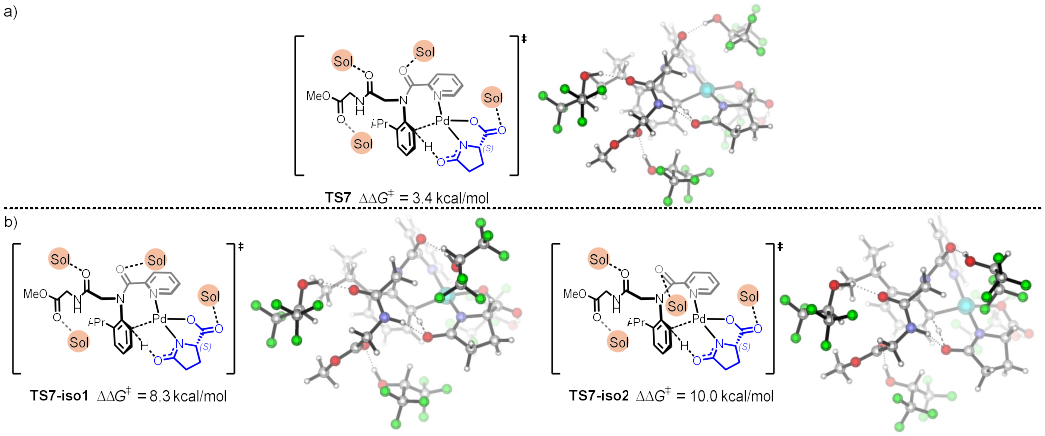


Fig. S7 Conformers of Pd/L-pGlu-catalyzed C−H bond activation transition state of methyl *N*-(2-isopropylphenyl)-*N*-picolinoylglycylglycinate (*rac*-**1a**) leading to (*S*)-axial chirality. Free energies are compared to **TS6**.

3.8 Table of Energies

Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures calculated at the MN15L/def2-TZVPP-SMD (HFIP)//ω-B97XD/6-31G(d)-LANL2DZ level of theory.

Table S11. Energies for all calculated species

Structures	*ZPE*	*tcH*	*tcG*	*E*	*H*	*G*	Imaginary Frequency
TS6	0.782997	0.860324	0.660297	-4999.989365	-4999.129041	-4999.329068	1355.1*i*
TS7	0.782242	0.860046	0.657468	-4999.981121	-4999.121075	-4999.323653	1337.0*i*
TFIP	0.063467	0.073554	0.02832	-789.516565	-789.443011	-789.488245	
S-TS1	0.519575	0.554821	0.453252	-1841.83490308	-1841.280082	-1841.381651	1389.5*i*
S-TS2	0.584642	0.630741	0.500794	-2631.369596	-2630.738855	-2630.868802	1354.5*i*
S-TS3	0.651057	0.707265	0.557055	-3420.916271	-6841.832542	-3420.359216	1355.3*i*
S-TS4	0.716769	0.783715	0.607293	-4210.451947	-4209.668232	-4209.844654	1345.1*i*
S-TS1-iso1	0.519668	0.554892	0.453326	-1841.83399594	-1841.279104	-1841.380670	1391.7*i*
S-TS1-iso2	0.518154	0.554125	0.449906	-1841.82817367	-1841.274049	-1841.378268	1369.4*i*
S-TS1-iso3	0.518793	0.554520	0.450379	-1841.82160309	-1841.267083	-1841.371224	1256.4*i*
S-TS2-iso1	0.584507	0.630699	0.501270	-2631.36848782	-2630.737789	-2630.867218	1394.3*i*
S-TS2-iso2	0.584659	0.630633	0.502086	-2631.36793147	-2630.737298	-2630.865845	1378.6*i*
S-TS2-iso3	0.584336	0.630538	0.501461	-2631.37054376	-2630.740006	-2630.869083	1382.1*i*
S-TS2-iso4	0.584823	0.630877	0.503453	-2631.37277800	-2630.741901	-2630.869325	1383.6*i*
S-TS2-iso5	0.585055	0.630959	0.504466	-2631.37122026	-2630.740261	-2630.866754	1400.1*i*
S-TS2-iso6	0.584552	0.630607	0.501495	-2631.36692738	-2630.736320	-2630.865432	1376.8*i*
S-TS2-iso7	0.585156	0.631132	0.503262	-2631.37043359	-2630.739302	-2630.867172	1380.5*i*
S-TS2-iso8	0.585229	0.631113	0.503387	-2631.36861105	-2630.737498	-2630.865224	1385.6*i*
S-TS2-iso9	0.585358	0.631188	0.502765	-2631.36584638	-2630.734658	-2630.863081	1386.8*i*
S-TS3-iso1	0.651083	0.707359	0.557217	-3420.915749	-6841.831498	-3420.358532	1357.5*i*
S-TS3-iso2	0.650440	0.707139	0.554497	-3420.90689516	-3420.199756	-3420.352398	1388.7*i*
S-TS3-iso3	0.650577	0.707259	0.553473	-3420.90992827	-3420.202669	-3420.356455	1366.1*i*
S-TS3-iso4	0.650606	0.707271	0.553125	-3420.905343	-3420.198072	-3420.352218	1366.3*i*
S-TS3-iso5	0.651106	0.707458	0.554952	-3420.90684786	-3420.199390	-3420.351896	1387.3*i*
S-TS3-iso6	0.650606	0.707112	0.552782	-3420.90140673	-3420.194295	-3420.348625	1370.2*i*
S-TS3-iso7	0.649822	0.706750	0.552469	-3420.90029762	-3420.193548	-3420.347829	1335.9*i*
S-TS3-iso8	0.650031	0.707005	0.551785	-3420.89769105	-3420.190686	-3420.345906	1370.0*i*
S-TS4-iso1	0.717039	0.783888	0.608314	-4210.44478795	-4209.660900	-4209.836474	1376.2*i*
S-TS4-iso2	0.716312	0.783500	0.605870	-4210.44095246	-4209.657452	-4209.835082	1382.4*i*
S-TS4-iso3	0.716974	0.783812	0.606341	-4210.43826054	-4209.654449	-4209.831920	1386.1*i*
S-TS4-iso4	0.717733	0.784085	0.611289	-4210.451062	-4209.666977	-4209.839773	1377.5*i*
S-TS4-iso5	0.716688	0.783656	0.608516	-4210.44561260	-4209.661957	-4209.837097	1386.3*i*
S-TS4-iso6	0.717388	0.784156	0.607995	-4210.44306597	-4209.658910	-4209.835071	1415.1*i*
S-TS4-iso7	0.71734	0.784121	0.608373	-4210.44056285	-4209.656442	-4209.832190	1373.5*i*

TS6-iso1	0.782235	0.860045	0.657766	-4999.98453691	-4999.124492	-4999.326771	1396.2*i*
TS6-iso2	0.782464	0.860345	0.654902	-4999.97024734	-4999.109902	-4999.315345	1385.7*i*
TS6-iso3	0.783345	0.860368	0.662250	-4999.98329276	-4999.122925	-4999.321043	1428.7*i*
TS6-iso4	0.782497	0.860006	0.656146	-4999.97063587	-4999.110630	-4999.314490	1398.9*i*
TS7-iso1	0.782503	0.860181	0.658479	-4999.974365	-4999.114184	-4999.315886	1286.5*i*
TS7-iso2	0.783681	0.860932	0.661444	-4999.975287	-4999.114355	-4999.313843	1331.9*i*

3.9 Cartesian coordinates of the structures

TS6

C	1.18460800	-1.94990700	-0.99609000
O	1.75996300	-2.71903000	-0.23363900
N	0.01056500	-1.33092800	-0.71212800
C	-0.59069800	-0.39861000	-1.63642500
C	-1.52442800	-0.83763500	-2.57246600
C	-0.17566500	0.94781100	-1.55008200
C	-1.99586800	0.11939800	-3.48746800
C	-0.71186500	1.86649500	-2.46337600
H	-0.20580300	1.46643700	-0.27845700
C	-1.60624400	1.44851600	-3.44417800
H	-2.70406600	-0.19584500	-4.24892500
H	-0.43721900	2.91295800	-2.39005700
H	-2.00733000	2.16010400	-4.15941300
C	-0.39934200	-1.31199000	0.69347100
H	0.14846600	-0.53033900	1.22632700
H	-0.13637500	-2.26886300	1.14409100
C	-2.03532400	-2.26408300	-2.65629300
H	-1.67489900	-2.80101900	-1.77534800
C	-3.56889700	-2.30068600	-2.61391900
H	-3.92230800	-3.33063800	-2.52575200
H	-3.93609100	-1.74114300	-1.74948700
H	-4.01058100	-1.87199500	-3.52131500
C	-1.50713300	-2.96671100	-3.91412500
H	-1.87936800	-2.48000300	-4.82358600
H	-0.41339000	-2.95132200	-3.95387700
H	-1.83821600	-4.01045700	-3.93422800
C	1.84018000	-1.67210500	-2.32902600
C	2.14943500	-2.73247100	-3.16876600
C	2.85473100	-2.47973600	-4.33832100

H	1.85090600	-3.73555400	-2.88720000
C	2.95444100	-0.17924200	-3.70113300
C	3.26548100	-1.18071700	-4.60781200
H	3.10034000	-3.28964200	-5.01696900
H	3.29137400	0.84067700	-3.84226300
H	3.84260400	-0.94013400	-5.49266600
N	2.23901600	-0.41557800	-2.59292000
C	0.83849200	2.61367300	1.01624300
C	2.99990500	3.22469200	0.50835200
C	2.80965100	3.48377700	2.01796000
C	1.27805800	3.41712200	2.21311600
H	3.11544600	4.16388300	-0.04923800
H	3.30389600	2.69352900	2.58619200
H	3.23837100	4.43648500	2.33041400
H	0.97128000	2.92987100	3.14064400
H	0.79771300	4.40027800	2.17041400
N	1.75964700	2.57634800	0.10246100
O	-0.29271500	2.01738000	0.87376000
C	4.16060100	2.31254000	0.08569300
O	5.23886600	2.36429200	0.66833300
O	3.91551600	1.53527800	-0.92442900
Pd	1.90804700	1.18205200	-1.27116100
C	-1.89695600	-1.13059000	0.84052900
O	-2.68795800	-1.98940300	0.44754400
N	-2.29048300	0.00275400	1.45238200
H	-1.60684700	0.74406800	1.57485200
C	-3.69062200	0.34154200	1.47976900
H	-4.28876000	-0.47826600	1.88284700
H	-3.83901000	1.21363900	2.12334000
C	-4.17619700	0.71285300	0.08649100
O	-3.44824200	1.13013000	-0.79155100
O	-5.48017100	0.54740200	-0.04496200
C	-6.04968600	0.93680400	-1.30108300
H	-5.57392400	0.38504800	-2.11531600
H	-7.10461900	0.68206800	-1.22460600
H	-5.91483900	2.00995600	-1.45166800
O	1.83377300	-2.54651000	2.52423900
H	2.04995600	-2.68232200	1.58194000
C	2.81863000	-1.80089000	3.15297800
H	3.83531000	-2.14345300	2.93348800
C	2.60263600	-1.96396000	4.65848700
F	2.80480000	-3.23566000	5.00757700
F	3.46235400	-1.20057400	5.34729000
F	1.36295600	-1.62302100	5.02184400

C	2.75365100	-0.33439200	2.70910200
F	3.72966200	0.40653400	3.23047200
F	2.86616400	-0.27885600	1.36528600
F	1.58227100	0.25337500	3.01764400
O	6.79290200	0.24049400	-0.16783100
H	6.34002800	1.06993500	0.10640000
C	5.82257800	-0.73197700	-0.32987500
H	4.80821100	-0.32606900	-0.28230900
C	5.93957600	-1.76974000	0.78764300
F	5.82781700	-1.15455500	1.97876900
F	4.94528400	-2.68161900	0.72550800
F	7.09628200	-2.43064400	0.77903500
C	5.96206000	-1.34813400	-1.72092800
F	5.00620500	-2.27700300	-1.93649300
F	5.81332200	-0.40241600	-2.65941000
F	7.14415200	-1.93421900	-1.91978700
O	-4.92150400	-2.89592900	1.74616500
H	-4.01947000	-2.75430400	1.40022600
C	-5.78301900	-2.67958000	0.68054400
H	-5.39602900	-1.93428400	-0.02374900
C	-7.09118200	-2.10903700	1.22995400
F	-6.84564600	-1.00206500	1.94055600
F	-7.91284000	-1.77305800	0.21900400
F	-7.73745600	-2.96502400	2.02041000
C	-5.98142200	-3.96901100	-0.12803600
F	-6.63535900	-3.71865600	-1.27476800
F	-4.77905800	-4.47273500	-0.44713900
F	-6.65286800	-4.90859800	0.53631200
O	-3.05715400	3.78277300	-1.45641400
H	-3.22875800	2.82669900	-1.51717700
C	-2.59532600	4.02052100	-0.16715300
H	-2.07986800	3.15572800	0.26504000
C	-3.75684800	4.36104700	0.77725800
F	-4.73682200	3.44617900	0.63078600
F	-3.36310200	4.31065100	2.05885600
F	-4.28988600	5.55959300	0.54745200
C	-1.56283800	5.14558900	-0.23551200
F	-1.19939500	5.53630400	0.99900400
F	-0.44951000	4.71308200	-0.85507900
F	-2.00762200	6.20961200	-0.89541800

TS7

C	0.42735800	-2.97756800	0.07864300

O	0.65375700	-3.88651700	-0.71643200
N	-0.66019100	-2.17322600	-0.02731600
C	-0.81113000	-1.02300200	0.82606900
C	-1.57751100	-1.09979600	1.98383700
C	-0.11268300	0.14037300	0.44862400
C	-1.58797300	0.03740600	2.80965900
C	-0.15158600	1.24106200	1.31685900
H	-0.32972600	0.66294900	-0.77287000
C	-0.88696900	1.19251800	2.49493600
H	-2.16859700	0.00740200	3.72771800
H	0.39671800	2.13834600	1.05647200
H	-0.91805800	2.05405700	3.15387300
C	-1.33362900	-2.17681100	-1.32698800
H	-1.44885900	-3.21212400	-1.65197000
H	-0.70330700	-1.65925000	-2.06155700
C	-2.37440900	-2.32989000	2.36944100
H	-2.35787900	-3.01254400	1.51516400
C	-1.74461300	-3.04240700	3.57325500
H	-2.30588500	-3.95108900	3.81524600
H	-0.70467400	-3.32241000	3.37475100
H	-1.75176900	-2.39735400	4.46006700
C	-3.83824000	-1.96428000	2.63769600
H	-3.95471000	-1.41886300	3.58142300
H	-4.22710900	-1.33751900	1.83192200
H	-4.45983500	-2.86163100	2.69359000
C	1.40389500	-2.75450500	1.21607800
C	1.68766800	-3.80704300	2.07373000
C	2.65982900	-3.63349500	3.05284900
H	1.16055800	-4.74656900	1.95500400
C	3.01798300	-1.42415600	2.21353200
C	3.32901500	-2.41940400	3.12862600
H	2.89786000	-4.44068500	3.73722500
H	3.52278800	-0.46853800	2.22566300
H	4.09896600	-2.23600700	3.86852800
N	2.07808500	-1.58984600	1.27446700
C	0.62586700	1.52754300	-2.34498400
C	2.85189600	1.07500400	-2.69866700
C	2.58040500	2.44132700	-3.34547300
C	1.03598500	2.44872500	-3.47279400
H	2.93496600	0.28452600	-3.45791700
H	2.91003000	3.23390400	-2.66743000
H	3.09299300	2.56879500	-4.29956000
H	0.57437700	3.42997700	-3.34695500
H	0.69349800	2.03323000	-4.42847900

N	1.64372200	0.84805300	-1.91739600
O	-0.54552700	1.40766500	-1.82832000
C	4.04081600	0.88725900	-1.75533000
O	5.07074300	1.53240000	-1.90084500
O	3.84752200	-0.01194800	-0.83077700
Pd	1.83160400	-0.21346200	-0.29108200
C	-2.71373200	-1.54354100	-1.24045700
O	-3.63348600	-2.07453700	-0.62548800
N	-2.85821800	-0.38913600	-1.92441200
H	-2.02900300	0.13448700	-2.18919700
C	-4.09607700	0.33679600	-1.84394600
H	-4.93853400	-0.32498300	-2.05261800
H	-4.09806500	1.12837100	-2.59731700
C	-4.27841800	0.99373200	-0.48592900
O	-3.38785100	1.15025100	0.32438900
O	-5.53223400	1.37866600	-0.31235600
C	-5.83304600	2.05541900	0.91738300
H	-6.90449600	2.23945600	0.88744500
H	-5.57940800	1.41523900	1.76557800
H	-5.27516000	2.99292200	0.96924000
O	3.37770500	-4.39028500	-0.84327700
H	2.40723800	-4.28094700	-0.87855000
C	3.99591000	-3.20711400	-1.22521300
H	3.62337000	-2.31738000	-0.70588900
C	3.77434100	-2.93744200	-2.71776800
F	2.45687700	-2.69771600	-2.91209200
F	4.43717400	-1.85923800	-3.15825200
F	4.11382400	-3.97233400	-3.48273800
C	5.46584100	-3.32985300	-0.82943700
F	6.15814800	-2.23871700	-1.16717500
F	5.54742600	-3.46938300	0.50390400
F	6.05297600	-4.38810800	-1.39241800
O	5.85570600	2.73554100	0.43482300
H	5.79755300	2.35303900	-0.46536900
C	5.06786600	1.94007300	1.25073500
H	4.85045800	0.96710000	0.79342400
C	3.71378100	2.61953500	1.48781300
F	3.10287200	2.84484700	0.30904700
F	2.88171300	1.82934800	2.20747500
F	3.80892200	3.78401800	2.12244500
C	5.82687400	1.66289000	2.54716400
F	5.08793600	0.88508500	3.37794200
F	6.95129900	0.99771600	2.28019000
F	6.14144500	2.77106200	3.21564400

O	-6.04243100	-2.99534300	0.39797200
H	-5.14097000	-2.91617300	0.04117500
C	-6.66691700	-1.77657100	0.18419900
H	-5.95952200	-0.94407000	0.12628600
C	-7.57439800	-1.47438500	1.37681600
F	-6.83455100	-1.32268200	2.48559000
F	-8.24172600	-0.32265400	1.18550700
F	-8.46337100	-2.43828200	1.60198400
C	-7.42117800	-1.79080600	-1.15174000
F	-7.92900900	-0.58644500	-1.44781900
F	-6.55430600	-2.11033100	-2.13271100
F	-8.41042200	-2.68154700	-1.17471200
O	-2.62440100	3.72731200	0.96955900
H	-2.87976300	2.78973700	1.02834900
C	-1.81950400	3.85617800	-0.15835500
H	-1.41070300	2.90024000	-0.50099600
C	-0.61896000	4.75080200	0.17145800
F	-0.04267100	4.35264700	1.31324100
F	0.30663100	4.65815300	-0.80120100
F	-0.94698400	6.03547800	0.30814300
C	-2.63986100	4.40395700	-1.32987000
F	-1.88181400	4.57774400	-2.42268200
F	-3.60648400	3.51581900	-1.65026800
F	-3.24211500	5.55617200	-1.04990600

TS8

C	1.55764500	-1.87952700	1.21357900
C	2.79760600	-2.49619200	1.09629000
C	0.68584800	-1.76034100	0.11143000
C	3.19756200	-3.00967400	-0.13861600
C	1.10842400	-2.31388700	-1.11370000
H	-0.57143700	-2.07778800	0.44650400
C	2.35412400	-2.92210000	-1.24634600
H	4.16679800	-3.49132100	-0.23553500
H	0.43917300	-2.26931400	-1.96941000
H	2.66553400	-3.33685200	-2.20072700
C	-2.51764400	-1.57169100	0.33601100
C	-3.10577800	0.47508600	-0.56921800
C	-4.30741600	0.00049200	0.27070500
C	-4.02773600	-1.50456100	0.46304700
H	-3.34211700	0.44538900	-1.64299800
H	-4.30084400	0.51823800	1.23473300
H	-5.26397400	0.20745500	-0.21140800

H	-4.35437400	-1.90694600	1.42428200
H	-4.48018200	-2.11665100	-0.32650600
N	-2.06798100	-0.50246700	-0.27458100
O	-1.77226200	-2.50258400	0.76106100
C	-2.56504200	1.88349400	-0.27754700
O	-3.32221900	2.81715000	-0.09999200
O	-1.25582000	1.97457700	-0.28726500
Pd	-0.24185500	0.20026800	-0.15709700
C	2.78949900	0.73224800	-0.33968200
C	3.96215000	1.46435100	-0.22775700
C	1.52321900	2.51153400	0.42425400
C	3.89657000	2.77122500	0.24311000
H	4.90528000	1.00838600	-0.50677300
C	2.65440500	3.30260900	0.56953700
H	0.52337800	2.88274300	0.62509000
H	4.79834500	3.36666800	0.34693900
H	2.54961500	4.31958000	0.93014000
N	1.59339900	1.24211500	-0.01079000
H	1.24451300	-1.48296400	2.17613900
H	3.45427400	-2.58037900	1.95740100
H	2.79520000	-0.28762800	-0.70482200

TFIP

O	0.04578600	1.85551400	-0.00910600
H	-0.72082800	2.33210800	-0.35062600
C	0.00372500	0.55066800	-0.49675700
H	0.00095300	0.50085300	-1.59448000
C	-1.26934700	-0.16408800	-0.02530900
F	-2.32520200	0.60958000	-0.35597800
F	-1.42463000	-1.34424100	-0.63106700
F	-1.30171900	-0.35467600	1.29143500
C	1.29043700	-0.13484500	-0.03160300
F	2.34467500	0.45171600	-0.60669700
F	1.28521100	-1.42552400	-0.39342100
F	1.44440900	-0.06879600	1.28905700

S-TS1

C	-0.31482700	1.72612800	1.75220800
O	-0.57092700	1.88820700	2.93374700
N	0.56177700	0.79311800	1.28368000
C	0.89264800	0.67638400	-0.11173700
C	1.94476400	1.42142200	-0.64394900

C	0.11113800	-0.20086700	-0.89084600
C	2.16983200	1.29754000	-2.02351700
C	0.40185900	-0.30490300	-2.25825500
H	-0.05969800	-1.46260300	-0.35904700
C	1.41977400	0.45216300	-2.82709900
H	2.97228900	1.87599600	-2.47375200
H	-0.17968900	-0.98893800	-2.87078800
H	1.63724000	0.37680800	-3.88823900
C	0.89295200	-0.30799500	2.18381800
H	0.14288900	-1.10163200	2.07976400
H	0.84880900	0.08011600	3.20274600
C	2.81454100	2.34967000	0.18435400
H	2.56385900	2.18795000	1.23588600
C	4.30347800	2.01695700	0.02502800
H	4.90001200	2.64959300	0.69098200
H	4.48970900	0.97401600	0.29039700
H	4.65187400	2.19382200	-1.00011800
C	2.53589000	3.81721400	-0.17020200
H	2.79668000	4.02718600	-1.21472300
H	1.47845700	4.06786100	-0.03650200
H	3.13071400	4.48315400	0.46454600
C	-1.04221900	2.59517100	0.74783100
C	-1.05357300	3.97164800	0.94428000
C	-1.82714800	4.76783400	0.11173900
H	-0.46894100	4.38924900	1.75558700
C	-2.57287800	2.77740300	-0.97933000
C	-2.60423100	4.15843100	-0.86750200
H	-1.83991100	5.84549700	0.23860400
H	-3.19460100	2.24892200	-1.69242000
H	-3.24215300	4.73618600	-1.52608700
N	-1.79413400	2.01113500	-0.20046500
C	-1.44358100	-2.89049400	-0.07408700
C	-3.66730200	-2.42968700	-0.47920600
C	-3.62881100	-3.67913600	0.42545300
C	-2.16691600	-4.16495200	0.30186100
H	-4.00778100	-2.68795400	-1.49152600
H	-3.84829400	-3.38654500	1.45671100
H	-4.36135500	-4.43136900	0.13055600
H	-1.75504000	-4.59246700	1.21899700
H	-2.03665900	-4.90415500	-0.49788300
N	-2.27681900	-2.00364100	-0.53583500
O	-0.18730500	-2.66614400	0.04706500
C	-4.54402500	-1.25032400	-0.00732100
O	-5.67692800	-1.46591400	0.37771300

O	-3.99098400	-0.06952700	-0.11007100
Pd	-1.96754800	-0.06956700	-0.45536000
C	2.29611800	-0.83759000	1.92857800
O	3.29370000	-0.16331100	2.13542500
N	2.35250600	-2.12514800	1.49518200
H	1.51471100	-2.54015500	1.10060700
C	3.62989000	-2.65187500	1.09807700
H	4.36868600	-2.47402200	1.88198500
H	3.54490700	-3.73238200	0.94879300
C	4.12545700	-2.02026700	-0.19741300
O	3.42381000	-1.47918800	-1.01522900
O	5.44899300	-2.17050200	-0.32099800
C	6.01594100	-1.61096500	-1.50551600
H	5.82298300	-0.53586800	-1.54641900
H	7.08587400	-1.80518500	-1.43924400
H	5.59282300	-2.08366500	-2.39548400

S-TS2

C	-0.14490100	-1.45068600	1.23716600
O	0.42222100	-1.54872900	2.31103800
N	-1.32473000	-0.78677200	1.05768300
C	-1.98797100	-0.72437600	-0.21674200
C	-2.90870300	-1.70599300	-0.57919200
C	-1.65397600	0.35283000	-1.06621000
C	-3.47044700	-1.59957900	-1.86168500
C	-2.26560500	0.41905900	-2.32697600
H	-1.71895300	1.58326500	-0.47640300
C	-3.16578100	-0.56065200	-2.72823000
H	-4.18152000	-2.35670800	-2.18120700
H	-2.03157600	1.25187900	-2.98486700
H	-3.63691700	-0.51250900	-3.70502700
C	-1.71318800	0.15303200	2.10595800
H	-1.24507300	1.12707400	1.91820300
H	-1.33020200	-0.23781200	3.05011900
C	-3.29304900	-2.86722900	0.31921100
H	-2.84217500	-2.69079500	1.29900300
C	-4.81089500	-2.93912400	0.52970400
H	-5.05008700	-3.73881300	1.23858400
H	-5.18431000	-1.99953400	0.94258900
H	-5.33971400	-3.15664200	-0.40657600
C	-2.75245700	-4.19022800	-0.24217900
H	-3.21601600	-4.42775700	-1.20740700
H	-1.66905600	-4.14926700	-0.39470700

H	-2.97255300	-5.01344700	0.44608500
C	0.50833800	-2.07749600	0.02486200
C	0.89688900	-3.40938400	0.08674900
C	1.60168300	-3.95810400	-0.97552900
H	0.65568300	-3.98424900	0.97312700
C	1.55207300	-1.81355200	-2.02523500
C	1.93830700	-3.14393700	-2.04973600
H	1.90697400	-4.99892400	-0.95219500
H	1.83271100	-1.12612300	-2.81404100
H	2.51871600	-3.51636000	-2.88519900
N	0.83326800	-1.29403400	-1.01885200
C	-0.70615400	3.32352800	-0.30625600
C	1.43434600	3.50464500	-1.14435800
C	1.26570700	4.63383300	-0.10677500
C	-0.26447800	4.71748400	0.08108400
H	1.49986200	3.90995000	-2.16368300
H	1.75119600	4.34167600	0.82909300
H	1.71491000	5.57192200	-0.43485400
H	-0.57922900	4.95832800	1.09887000
H	-0.73082800	5.44422200	-0.59472500
N	0.21209900	2.72014800	-1.00959800
O	-1.81409800	2.77057900	0.01204700
C	2.63933500	2.57128900	-0.96308200
O	3.73816700	3.03706700	-0.67688600
O	2.41024300	1.31131900	-1.16164000
Pd	0.41765000	0.76277400	-1.09323800
C	-3.22559800	0.27724100	2.21159800
O	-3.93065700	-0.65666300	2.56183500
N	-3.72228300	1.51057000	1.92497400
H	-3.14132900	2.15469100	1.39857900
C	-5.15040600	1.66471500	1.85422700
H	-5.61489700	1.24046800	2.74618900
H	-5.39933900	2.72932300	1.81237700
C	-5.72920300	0.97966200	0.62195000
O	-5.10594800	0.71583700	-0.37658600
O	-7.03220800	0.72916200	0.78465500
C	-7.66593100	0.07483200	-0.31485300
H	-7.19113200	-0.89189800	-0.50126300
H	-8.70558100	-0.06001900	-0.01889100
H	-7.59899400	0.68642100	-1.21817000
O	5.45328400	0.91978200	-0.14582900
H	4.92259500	1.70954000	-0.39197000
C	4.60416300	0.01138300	0.46418300
H	3.54827400	0.25295900	0.30536300

C	4.83966700	0.01100800	1.97603500
F	4.58850800	1.23820300	2.45747900
F	4.01916000	-0.84598500	2.60586500
F	6.09532100	-0.30837700	2.30460700
C	4.81357700	-1.36005800	-0.17303000
F	3.96220200	-2.27141700	0.34019100
F	4.56984900	-1.29509600	-1.49223400
F	6.05252600	-1.83172000	-0.01396300

S-TS3

C	0.44854600	-0.85546500	-1.61655200
O	-0.33289000	-0.31095700	-2.39291000
N	1.57915700	-0.28385000	-1.14308700
C	2.44831100	-0.97100300	-0.21851400
C	3.50089000	-1.75307900	-0.68824000
C	2.16629900	-0.81813400	1.15625500
C	4.25764200	-2.43292400	0.28027100
C	2.97802000	-1.49608900	2.07670600
H	1.96597600	0.46754700	1.56415000
C	4.01440800	-2.31300900	1.63953700
H	5.07415100	-3.06811700	-0.05232700
H	2.78913100	-1.37038800	3.13941300
H	4.63709800	-2.84654500	2.35094100
C	1.72654700	1.16451700	-1.31244400
H	1.15552400	1.68287100	-0.53700100
H	1.30851100	1.44133600	-2.27977000
C	3.83567800	-1.92609500	-2.15869800
H	3.21329300	-1.22981400	-2.72714400
C	5.29777500	-1.56265700	-2.45009800
H	5.48733300	-1.62854400	-3.52671400
H	5.50744400	-0.54035200	-2.12954100
H	5.99225400	-2.24853100	-1.94957900
C	3.52705800	-3.35795900	-2.61986800
H	4.16623500	-4.08429900	-2.10345600
H	2.48615200	-3.63117900	-2.42020500
H	3.70886400	-3.45977600	-3.69522200
C	0.10992100	-2.25801200	-1.16673600
C	-0.12728100	-3.23408700	-2.12445400
C	-0.53467300	-4.49605000	-1.71240000
H	-0.00103700	-2.98780500	-3.17209200
C	-0.51633200	-3.69214100	0.53708700
C	-0.73336800	-4.72838800	-0.35768200
H	-0.71613200	-5.27841400	-2.44170400

H	-0.70172800	-3.80883900	1.59793300
H	-1.08056900	-5.68685000	0.00940700
N	-0.08545800	-2.48565900	0.14348500
C	0.75610100	1.62103500	2.70127400
C	-1.18559600	0.73355500	3.58009000
C	-1.32684400	2.26866700	3.65881000
C	0.10813500	2.78393300	3.41528400
H	-1.10963100	0.28562900	4.58056100
H	-1.99703900	2.61205300	2.86879500
H	-1.74362900	2.59657400	4.61191800
H	0.15534400	3.68461000	2.80022400
H	0.65116000	2.98235000	4.34656400
N	0.06635300	0.52525200	2.86232700
O	1.83239400	1.66672700	2.01380400
C	-2.29422600	-0.03112300	2.84277900
O	-3.46819400	0.30422300	2.97222300
O	-1.89935000	-1.04011300	2.13089500
Pd	0.09970400	-0.97886400	1.59591100
C	3.18829100	1.58361600	-1.30994700
O	3.95458700	1.26090400	-2.20553100
N	3.55517600	2.38090500	-0.27525200
H	2.96184100	2.41856500	0.54666900
C	4.94321300	2.73047800	-0.14379200
H	5.31961100	3.13660400	-1.08496500
H	5.05043500	3.50087200	0.62550400
C	5.79385700	1.52852900	0.24919500
O	5.37713900	0.53019300	0.78237300
O	7.07892500	1.74133100	-0.05228900
C	7.96645200	0.67291200	0.27698300
H	7.67013100	-0.23980000	-0.24623100
H	8.95316300	0.99877400	-0.05024100
H	7.96086400	0.48616500	1.35388600
O	-0.98947900	2.36394700	-2.41810900
H	-0.92295400	1.39014900	-2.47807100
C	-2.08210300	2.72617900	-1.64689200
H	-2.99336200	2.16774800	-1.88646200
C	-2.36997500	4.19904600	-1.94142500
F	-2.66429300	4.35155000	-3.23410000
F	-3.41550700	4.63234400	-1.22330400
F	-1.32231900	4.97950100	-1.65743100
C	-1.79733500	2.47180800	-0.16192600
F	-2.82003500	2.80372500	0.62634100
F	-1.55125400	1.15706800	0.01744800
F	-0.71007800	3.12839500	0.27857700

O	-5.01933200	-1.06338200	1.15506500
H	-4.54599900	-0.60482300	1.88663500
C	-4.14041600	-1.17091100	0.09246800
H	-3.12061100	-0.87538000	0.35750700
C	-4.58619300	-0.25436700	-1.04849900
F	-4.69791300	1.00513700	-0.59250900
F	-3.67748600	-0.22920600	-2.04633200
F	-5.75999300	-0.59966800	-1.57947300
C	-4.05637500	-2.63556900	-0.33366100
F	-3.21641000	-2.79048100	-1.37889900
F	-3.57697400	-3.38040300	0.67321100
F	-5.23704500	-3.14656700	-0.68766600

S-TS4

C	-0.52411700	-0.75543400	-1.38984900
O	-0.94203800	0.11381600	-2.14742900
N	0.49213700	-0.58367400	-0.50847100
C	0.93615900	-1.65515600	0.35098600
C	1.93555000	-2.52865400	-0.07094200
C	0.30244800	-1.77241000	1.60736800
C	2.25547900	-3.58375300	0.80002300
C	0.68755000	-2.82688100	2.44680500
H	0.22989000	-0.61555400	2.31651500
C	1.65233100	-3.74097600	2.03772600
H	3.01654200	-4.29622300	0.49412000
H	0.22485600	-2.91909700	3.42565000
H	1.94411900	-4.56324000	2.68355100
C	0.87440500	0.78781800	-0.17043600
H	0.23320900	1.15901800	0.63298200
H	0.72001500	1.41898900	-1.04465400
C	2.66637200	-2.40599200	-1.39576600
H	2.37214900	-1.45945500	-1.85669600
C	4.18512400	-2.35230400	-1.18489300
H	4.69103400	-2.14159100	-2.12985900
H	4.44061500	-1.56078600	-0.47639800
H	4.57495300	-3.30271800	-0.80087900
C	2.29191400	-3.55546800	-2.34155400
H	2.61731300	-4.52101600	-1.93589200
H	1.21075900	-3.61082400	-2.50195200
H	2.77831000	-3.42073100	-3.31344800
C	-1.20472400	-2.10345200	-1.43910100
C	-1.31569100	-2.76212400	-2.65521400
C	-2.03475000	-3.94877000	-2.71377500

H	-0.85406600	-2.32860700	-3.53452400
C	-2.53624100	-3.67952600	-0.39331700
C	-2.65575000	-4.41493500	-1.56255000
H	-2.12874900	-4.48668900	-3.65110300
H	-3.04127000	-3.97472200	0.51847200
H	-3.25154800	-5.31989700	-1.56611800
N	-1.80981700	-2.55549800	-0.32663000
C	-1.02020500	0.55247700	3.39828200
C	-3.26946400	0.04168600	3.48747300
C	-3.13202300	1.50767300	3.95099000
C	-1.61957000	1.67062400	4.21803600
H	-3.58891000	-0.61095800	4.31152700
H	-3.45433400	2.17446100	3.14942400
H	-3.74553000	1.72257500	4.82674200
H	-1.21648500	2.63413800	3.90008800
H	-1.35648000	1.52603800	5.27212000
N	-1.92243100	-0.33099200	3.07183300
O	0.20407600	0.45510300	3.04026500
C	-4.22436000	-0.23574300	2.31777300
O	-5.29633600	0.35624000	2.23765900
O	-3.82913700	-1.14044800	1.47647300
Pd	-1.79430800	-1.49014600	1.48704800
C	2.33968600	0.87450900	0.20942000
O	3.22409500	0.66936500	-0.62384800
N	2.59524700	1.21367300	1.48586400
H	1.83324000	1.18566600	2.15720100
C	3.95289800	1.18441900	1.97075400
H	4.61584600	1.72703400	1.29397500
H	3.99452400	1.68033300	2.94447300
C	4.43549000	-0.25304600	2.14058600
O	3.71799500	-1.19524000	2.36817800
O	5.76292100	-0.32606400	2.01714800
C	6.33834300	-1.62729000	2.15585300
H	5.90264500	-2.31211900	1.42391900
H	7.40151400	-1.48998400	1.96830000
H	6.16496400	-2.01632000	3.16190300
O	-1.08966400	2.81854600	-1.66010700
H	-1.23573800	1.90068500	-1.96065100
C	-2.22598700	3.31645200	-1.04204900
H	-3.14874000	3.12055700	-1.59821100
C	-2.06001900	4.83540200	-0.96819000
F	-2.01575200	5.34349700	-2.20122600
F	-3.09303300	5.39589400	-0.32356800
F	-0.93766000	5.18364400	-0.33271600

C	-2.41518700	2.68080100	0.34097100
F	-3.53683600	3.07996500	0.93976100
F	-2.47806900	1.33930000	0.20402500
F	-1.39200200	2.93205500	1.17725600
O	-6.43641000	-0.21153900	-0.20842100
H	-6.13822100	-0.03350900	0.71261700
C	-5.31015500	-0.26094000	-1.00954900
H	-4.38186200	-0.28664500	-0.43081000
C	-5.24438800	0.98420200	-1.89640600
F	-5.28363300	2.08408800	-1.12420900
F	-4.08655800	1.03600600	-2.58985300
F	-6.24459500	1.06681300	-2.77367900
C	-5.33618900	-1.55572100	-1.81930700
F	-4.25551300	-1.64749800	-2.62261600
F	-5.30760900	-2.61322500	-0.99459000
F	-6.42044900	-1.67184200	-2.58763400
O	5.52239300	2.06555700	-1.12204000
H	4.60739000	1.72623900	-1.09794600
C	6.34526200	0.96211700	-0.95011600
H	5.86922500	0.17862400	-0.35059900
C	7.58256900	1.40319900	-0.16828500
F	7.21787000	1.96552400	0.98941400
F	8.36020000	0.34232900	0.11780500
F	8.32569400	2.28771700	-0.83412800
C	6.68354600	0.32193900	-2.30247100
F	7.31261000	-0.85422600	-2.13319400
F	5.54422900	0.07976700	-2.96908000
F	7.45000100	1.09322700	-3.07342300

S-TS1-iso1

C	-0.23089100	1.69830700	1.77517600
O	-0.45987900	1.83466100	2.96478200
N	0.63040800	0.76993700	1.26670900
C	0.93134500	0.69288000	-0.13636900
C	1.95577300	1.47638200	-0.67183400
C	0.14265100	-0.17030700	-0.92230700
C	2.12246300	1.42732800	-2.06398500
C	0.37998100	-0.20672800	-2.30393300
H	-0.02482800	-1.44308100	-0.41637600
C	1.34931600	0.60933200	-2.87778100
H	2.89077700	2.04764400	-2.51869500
H	-0.21220900	-0.87402800	-2.92471800
H	1.51292000	0.60342900	-3.95181700

C	0.95934200	-0.36289300	2.12399200
H	0.20791600	-1.15078200	1.99257400
H	0.91347800	-0.01229300	3.15669900
C	2.85196100	2.36879400	0.16753100
H	2.62307900	2.17387800	1.21841400
C	4.33123900	2.01879000	-0.03857000
H	4.95509100	2.63216100	0.61987600
H	4.51430700	0.97009000	0.20785400
H	4.65354100	2.20866200	-1.07017400
C	2.58596000	3.85053600	-0.13239300
H	2.83759400	4.09601500	-1.17143000
H	1.53340800	4.10894600	0.02313500
H	3.19642700	4.48614000	0.51798500
C	-0.97898200	2.58941200	0.80608900
C	-0.98296700	3.96143800	1.03058900
C	-1.77222900	4.77539700	0.23049500
H	-0.37934700	4.36160800	1.83680000
C	-2.54669300	2.80815300	-0.88298800
C	-2.57197700	4.18685400	-0.74310000
H	-1.77926200	5.85044000	0.37810200
H	-3.18532600	2.29557700	-1.59275200
H	-3.22206000	4.77873900	-1.37677000
N	-1.75258600	2.02510500	-0.13707300
C	-1.39862200	-2.87834400	-0.12170300
C	-3.63392300	-2.41019800	-0.45170300
C	-3.56900700	-3.67460400	0.43023600
C	-2.11179200	-4.15848600	0.25425200
H	-4.00617600	-2.65084500	-1.45703700
H	-3.75766200	-3.40007700	1.47246600
H	-4.31008200	-4.42184300	0.14434000
H	-1.67316300	-4.60091000	1.15163000
H	-2.00622600	-4.88477100	-0.56066700
N	-2.24543400	-1.98354700	-0.54348200
O	-0.13942900	-2.65545000	-0.03329300
C	-4.49354200	-1.23829400	0.06615300
O	-5.61478400	-1.45494700	0.48096800
O	-3.94053200	-0.05538500	-0.03326300
Pd	-1.93307600	-0.05223200	-0.43097300
C	2.36301700	-0.88846100	1.86428500
O	3.35979400	-0.20900800	2.05775700
N	2.41737000	-2.18393300	1.46263600
H	1.58404200	-2.60989500	1.07152700
C	3.70172500	-2.77834400	1.19926700
H	4.36978500	-2.61510400	2.04715000

H	3.57088300	-3.85742300	1.07431300
C	4.43178700	-2.25837800	-0.03225800
O	5.62711800	-2.34300500	-0.17138800
O	3.59623700	-1.76853400	-0.95510200
C	4.22370800	-1.31695100	-2.15487600
H	4.92919900	-2.06454500	-2.52391500
H	3.41557100	-1.15451900	-2.86551200
H	4.75547700	-0.37981300	-1.96907100

S-TS1-iso2

C	1.67815600	1.11599300	-1.14894900
O	1.72475200	2.10842900	-1.85799800
N	1.49310700	1.16364500	0.19884800
C	1.87302400	0.06252200	1.04498900
C	3.22225600	-0.14136900	1.34688800
C	0.85048600	-0.77074600	1.53141400
C	3.53023500	-1.22397000	2.18312100
C	1.21643700	-1.83916500	2.36309900
H	-0.30742400	-0.20647800	1.97170400
C	2.54929800	-2.06472400	2.69228700
H	4.57053000	-1.41046600	2.43770900
H	0.43801600	-2.48891000	2.75407500
H	2.82744800	-2.89181000	3.33861800
C	1.35351400	2.46000700	0.86477300
H	2.33676200	2.88729900	1.08635000
H	0.83924000	2.27095300	1.81418100
C	4.33882400	0.73583200	0.80367500
H	3.89985400	1.48613200	0.13842400
C	5.05051700	1.48995800	1.93539500
H	5.80794900	2.16662400	1.52602300
H	4.34295400	2.08517300	2.52175500
H	5.55387600	0.79694500	2.61951000
C	5.33435800	-0.08094300	-0.03208000
H	5.86316200	-0.81904800	0.58153600
H	4.82591300	-0.61760900	-0.84008900
H	6.08559800	0.58033100	-0.47704600
C	1.82436300	-0.23788200	-1.81414500
C	2.76581800	-0.32359600	-2.83592700
C	2.88476400	-1.50410400	-3.55519400
H	3.37257900	0.54653300	-3.05617400
C	1.08440800	-2.38465800	-2.25543800
C	2.02018800	-2.55248400	-3.26446100
H	3.62498400	-1.59529900	-4.34341900

H	0.35424500	-3.15147000	-2.02417200
H	2.05170400	-3.48583900	-3.81452900
N	1.00304000	-1.26127900	-1.52347400
C	-2.29096700	-0.57530100	2.07743900
C	-3.21535000	-2.13775100	0.63702500
C	-4.39747000	-1.37081400	1.27218000
C	-3.75709300	-0.58991200	2.44241900
H	-3.21366600	-3.19284900	0.94507400
H	-4.81361300	-0.67875400	0.53893800
H	-5.19184300	-2.04437200	1.59789800
H	-4.12755700	0.43213400	2.53734700
H	-3.88164800	-1.09033500	3.40994200
N	-2.03372100	-1.48048800	1.16886300
O	-1.39744500	0.19755700	2.55726700
C	-3.12402000	-2.13966700	-0.90159700
O	-4.11337000	-2.32846500	-1.57953000
O	-1.90987100	-1.98685600	-1.38412500
Pd	-0.51138800	-1.34946600	-0.04181100
C	0.60523500	3.56833300	0.11094400
O	1.10298200	4.67578300	0.03245100
N	-0.65219900	3.30949400	-0.34295400
H	-1.05739000	4.05579200	-0.89081700
C	-1.35575300	2.05203200	-0.30855400
H	-1.07583600	1.38682100	-1.14074000
H	-1.15589300	1.52165700	0.62324600
C	-2.85736200	2.21736400	-0.38999400
O	-3.64307900	1.42264000	0.06875700
O	-3.21423100	3.30761400	-1.07379000
C	-4.62155300	3.49763000	-1.24438200
H	-5.10950700	3.60242200	-0.27271000
H	-4.72450900	4.41274800	-1.82562500
H	-5.05544300	2.64835400	-1.77649500

S-TS1-iso3

C	0.59376600	1.34475700	0.84589000
O	1.72244900	1.35823900	1.32191000
N	0.35834800	1.20560600	-0.48185900
C	-0.90474600	1.53192100	-1.08201400
C	-1.25551000	2.86903200	-1.27833700
C	-1.74969700	0.46080900	-1.41819600
C	-2.52124000	3.11441300	-1.83065300
C	-3.00074300	0.76209400	-1.96946300
H	-1.17779600	-0.58921300	-1.99917300

C	-3.38852200	2.08426800	-2.17115800
H	-2.82982100	4.14276700	-2.00185700
H	-3.66304800	-0.05276000	-2.24869500
H	-4.36005300	2.31516800	-2.59798700
C	1.47308900	0.79028700	-1.31623900
H	2.18512600	1.61197800	-1.44450700
H	1.06796600	0.52236200	-2.29535600
C	-0.33385900	4.02682800	-0.93454600
H	0.57157300	3.61536600	-0.47633300
C	0.09874800	4.77645200	-2.20260400
H	0.81163600	5.56997100	-1.95358900
H	0.57495000	4.09797600	-2.91802900
H	-0.76012400	5.24068900	-2.70093900
C	-0.97201900	4.98194200	0.08305000
H	-1.85365100	5.48061700	-0.33526600
H	-1.28619800	4.44744700	0.98558100
H	-0.25768000	5.75949000	0.37428100
C	-0.59520200	1.45765700	1.77110800
C	-0.52789300	2.37559100	2.81247200
C	-1.56700400	2.43234800	3.73209400
H	0.34330000	3.01539100	2.88980200
C	-2.60347700	0.62790000	2.55573700
C	-2.62228200	1.53759000	3.60357500
H	-1.54335400	3.15051000	4.54522000
H	-3.37911300	-0.11969400	2.43850600
H	-3.44441200	1.52533400	4.30971500
N	-1.62244300	0.60004800	1.64372100
C	-0.88445600	-2.58508100	-2.00332900
C	-1.60230100	-3.84105400	-0.20016700
C	-0.43011500	-4.60549300	-0.84823100
C	-0.33948700	-3.97588100	-2.25183000
H	-2.55158900	-4.37051900	-0.36442600
H	0.48637800	-4.39396400	-0.28970600
H	-0.58654200	-5.68536200	-0.85707700
H	0.67368600	-3.91649600	-2.65390200
H	-0.96972800	-4.49320000	-2.98552600
N	-1.62203600	-2.57127200	-0.91522000
O	-0.65327400	-1.56287700	-2.71512700
C	-1.49610700	-3.59578700	1.31408200
O	-1.27371600	-4.52374000	2.06678100
O	-1.71186200	-2.36080800	1.70218300
Pd	-1.71335800	-0.97764600	0.22051500
C	2.12293500	-0.48477300	-0.75417800
O	1.44714300	-1.46347600	-0.48941200

N	3.48081000	-0.49748500	-0.65805500
H	3.83931900	-1.34706700	-0.24067100
C	4.31775900	0.67701200	-0.51328100
H	4.49057100	1.17852700	-1.47131200
H	3.85371800	1.39827000	0.17177700
C	5.69038500	0.36823600	0.05188200
O	6.59286400	1.16784400	0.04920500
O	5.77408900	-0.86163600	0.57189900
C	7.03463400	-1.20266300	1.15401500
H	7.29178900	-0.49168900	1.94186900
H	6.90613200	-2.20320500	1.56419100
H	7.81721800	-1.19406700	0.39203400

S-TS2-iso1

C	0.85907600	-1.52838500	-1.81750600
O	0.67933100	-1.64820900	-3.01694000
N	1.90958000	-0.84669100	-1.27189500
C	2.15598300	-0.81146100	0.14187400
C	2.88538300	-1.83492100	0.74837400
C	1.61655800	0.27042100	0.86839500
C	2.99771700	-1.78309200	2.14654000
C	1.79257800	0.28909000	2.26048900
H	1.85392200	1.51820900	0.33364800
C	2.46200800	-0.74758100	2.90138000
H	3.53092100	-2.58247000	2.65491100
H	1.39035100	1.12008100	2.83378900
H	2.57515300	-0.74955200	3.98167300
C	2.59203000	0.11613700	-2.12850800
H	2.09893800	1.09223700	-2.04538300
H	2.49092600	-0.23619400	-3.15654700
C	3.51662500	-2.98074000	-0.02097500
H	3.40044100	-2.76736100	-1.08647000
C	5.02320000	-3.07063700	0.25351600
H	5.46679000	-3.86104900	-0.36053400
H	5.51592100	-2.13011400	-0.00448000
H	5.23171500	-3.31131800	1.30356800
C	2.81219500	-4.30710700	0.29675800
H	2.94491200	-4.58420500	1.34958200
H	1.73614900	-4.24768000	0.10198200
H	3.22814000	-5.11416100	-0.31550600
C	-0.17616200	-2.12186400	-0.88558200
C	-0.61826700	-3.41911100	-1.11883100
C	-1.68947600	-3.91323500	-0.38642800

H	-0.13272400	-4.00511100	-1.89036600
C	-1.82685700	-1.79644200	0.70742800
C	-2.31225000	-3.08282700	0.53853200
H	-2.05066100	-4.92237200	-0.55480600
H	-2.30208600	-1.10301000	1.38980700
H	-3.17860700	-3.40116100	1.10439500
N	-0.77538700	-1.32677500	0.01794000
C	0.94179800	3.27258800	-0.05832800
C	-1.34416500	3.46203500	0.18706200
C	-0.89806700	4.61315800	-0.73935400
C	0.62637900	4.68605500	-0.49695600
H	-1.65581800	3.84896100	1.16693400
H	-1.10236300	4.34623900	-1.78081000
H	-1.41813500	5.54742600	-0.52539600
H	1.20802000	4.96190800	-1.37937800
H	0.88928200	5.38249900	0.30809100
N	-0.13762600	2.66098700	0.34285300
O	2.09010500	2.70839600	-0.08068800
C	-2.48945000	2.56458800	-0.30095700
O	-3.54654100	3.07698700	-0.65530100
O	-2.27425800	1.28764100	-0.25753800
Pd	-0.36496800	0.71258700	0.27418000
C	4.07550300	0.21748300	-1.80576500
O	4.83764800	-0.72763400	-1.93845100
N	4.48819000	1.45136600	-1.41884100
H	3.80086700	2.11911800	-1.08868000
C	5.87806000	1.65698100	-1.10567600
H	6.50274200	1.28277400	-1.91915400
H	6.06165700	2.73096400	-1.00597100
C	6.37961100	0.98661900	0.16662100
O	7.54493600	0.74473100	0.36232500
O	5.40244700	0.76451800	1.05356200
C	5.83333100	0.19098500	2.28809200
H	6.69846600	0.72920100	2.68096600
H	4.98285500	0.27193200	2.96222700
H	6.09921100	-0.85906900	2.13962700
O	-5.61544000	1.25391000	-0.65465400
H	-4.89853100	1.92551900	-0.72760300
C	-5.06802200	0.08113100	-0.16571900
H	-3.99791100	-0.00673300	-0.38515100
C	-5.76414800	-1.09319000	-0.84848800
F	-5.52536200	-1.06198200	-2.16278400
F	-5.29094300	-2.27061200	-0.38250200
F	-7.08553000	-1.09226100	-0.66586000

C	-5.19771600	0.04585500	1.36129800
F	-4.61566000	-1.05860200	1.89355000
F	-4.56617500	1.10463900	1.88869100
F	-6.46098600	0.06719000	1.78336400

S-TS2-iso2

C	-1.13374000	1.44064100	-2.11028000
O	-1.07676000	1.49554800	-3.32677000
N	-2.07093600	0.72118500	-1.42477600
C	-2.16097000	0.73729000	0.01081100
C	-2.92555600	1.70710800	0.65649300
C	-1.43803400	-0.25100900	0.71558000
C	-2.91246400	1.68744800	2.06077700
C	-1.48065600	-0.23334700	2.11761500
H	-1.65425400	-1.52891900	0.27267400
C	-2.20942300	0.74057300	2.79000500
H	-3.48533900	2.44069300	2.59526400
H	-0.93871700	-0.99489300	2.67184300
H	-2.23840700	0.76002100	3.87503300
C	-2.77596200	-0.32099800	-2.16583900
H	-2.20317400	-1.25528000	-2.12032000
H	-2.83250200	0.00225800	-3.20659300
C	-3.72077800	2.77330300	-0.07489200
H	-3.68480100	2.54021500	-1.14222900
C	-5.19852900	2.75679800	0.33719300
H	-5.75588100	3.49514100	-0.24906300
H	-5.63725500	1.77495700	0.14673700
H	-5.32738200	3.00964500	1.39703600
C	-3.10324200	4.16108200	0.14889400
H	-3.16563000	4.45575500	1.20357000
H	-2.04740000	4.18368400	-0.13985200
H	-3.63746400	4.91464400	-0.43990800
C	-0.09031600	2.18338900	-1.30550400
C	0.15880500	3.51825200	-1.59408400
C	1.18922000	4.17299500	-0.92972800
H	-0.44853300	4.01487600	-2.34177500
C	1.67315300	2.12246500	0.19676600
C	1.95945900	3.46194000	-0.01882300
H	1.39612400	5.21845200	-1.13383100
H	2.27585100	1.52023800	0.86194700
H	2.79238700	3.91536800	0.50485800
N	0.66594900	1.49647400	-0.42965600
C	-0.66060500	-3.23453400	-0.14576900

C	1.64308400	-3.25257200	-0.12407600
C	1.19637200	-4.49090900	-0.93087500
C	-0.28529500	-4.65170100	-0.52287300
H	2.05901900	-3.55300000	0.84700900
H	1.27138000	-4.27885200	-2.00206500
H	1.80551600	-5.37018700	-0.71799300
H	-0.93303300	-5.03071000	-1.31648700
H	-0.40875600	-5.30350600	0.35037400
N	0.40439700	-2.52091100	0.08733600
O	-1.84521100	-2.75817400	-0.06797400
C	2.69216100	-2.33341700	-0.76685200
O	3.79439600	-2.76939500	-1.04733900
O	2.32624200	-1.08694400	-0.92249800
Pd	0.47908300	-0.56764500	-0.10049400
C	-4.19087800	-0.51392600	-1.64125300
O	-5.03943900	0.36046000	-1.72867500
N	-4.44441100	-1.73787500	-1.10515200
H	-3.65841900	-2.31506600	-0.82521200
C	-5.70788100	-1.93707500	-0.44659600
H	-6.52179800	-1.60862700	-1.09536900
H	-5.84546300	-3.00230000	-0.23841600
C	-5.77925500	-1.16940900	0.86830300
O	-4.82179500	-0.82380900	1.51550500
O	-7.04854700	-0.94976600	1.22519500
C	-7.21892400	-0.22668600	2.44463600
H	-6.74800100	0.75657700	2.36692700
H	-8.29504100	-0.12606500	2.58030100
H	-6.77404600	-0.77117600	3.28129400
O	4.24358200	0.72584700	-0.63572800
H	3.56524200	0.08263200	-0.94983300
C	5.14515500	0.00791800	0.13767200
H	5.20913500	-1.04620700	-0.16316100
C	4.69988200	0.02878200	1.60488100
F	3.48261000	-0.54671400	1.71515800
F	5.53035800	-0.64231400	2.40790500
F	4.57667200	1.27733600	2.08225200
C	6.52728900	0.62861600	-0.06304700
F	7.45206800	0.01304200	0.69046700
F	6.89571600	0.51009600	-1.34097400
F	6.54386900	1.92977000	0.25265400

S-TS2-iso3

C	-0.01522600	0.64138100	1.91329800

O	-0.89475700	0.12871300	2.60694100
N	0.87651600	-0.07925300	1.20320800
C	1.89968900	0.53690900	0.39159500
C	3.15677800	0.80027100	0.93267300
C	1.55227500	0.85114300	-0.93691000
C	4.07618600	1.44497000	0.09066500
C	2.52521700	1.45922900	-1.74028700
H	0.87896800	-0.15257200	-1.61016300
C	3.77939900	1.76880300	-1.22428000
H	5.06101900	1.68403400	0.48275200
H	2.28747000	1.68924900	-2.77542400
H	4.52780200	2.25232700	-1.84484400
C	0.57387100	-1.50111100	1.02028700
H	-0.17262200	-1.60832400	0.22707200
H	0.15318500	-1.87383400	1.95557800
C	3.54643100	0.45997500	2.35985200
H	2.75183100	-0.16043300	2.78312000
C	4.83532200	-0.37018300	2.41056500
H	5.04281000	-0.66939500	3.44353400
H	4.72831600	-1.27477300	1.80844900
H	5.70020600	0.20050700	2.05141400
C	3.67693500	1.73499700	3.20498800
H	4.48939400	2.37199800	2.83490300
H	2.75635400	2.32761600	3.18439300
H	3.89890000	1.48191100	4.24757100
C	0.05951700	2.15080200	1.87635700
C	0.09607400	2.83986700	3.08266500
C	0.04820200	4.22784000	3.06762300
H	0.15062100	2.28046800	4.00929400
C	-0.14903700	4.12402600	0.68778700
C	-0.07979200	4.88124500	1.84777100
H	0.09007600	4.78788100	3.99601000
H	-0.29720500	4.58041700	-0.28358200
H	-0.14603600	5.96121300	1.78655700
N	-0.06248700	2.78661400	0.69946500
C	-0.69002900	-0.51917100	-2.80841300
C	-2.20116300	1.15543500	-3.28190100
C	-2.91592400	-0.18365400	-3.56663500
C	-1.76322400	-1.21086200	-3.61512800
H	-2.01555700	1.70939300	-4.21175600
H	-3.59678600	-0.41334200	-2.74400600
H	-3.50348500	-0.15288100	-4.48501000
H	-2.01011400	-2.17583700	-3.16771700
H	-1.39708200	-1.39232000	-4.63246900

N	-0.92632400	0.75671100	-2.69886900
O	0.32053800	-1.08640300	-2.25848000
C	-2.92741600	2.12723500	-2.32898200
O	-4.10104700	2.37945600	-2.51342200
O	-2.18107800	2.66171700	-1.39410600
Pd	-0.36517400	1.77601600	-1.11541800
C	1.81986700	-2.32496100	0.72565500
O	2.67688200	-2.52124500	1.57406900
N	1.86055200	-2.87260200	-0.51443600
H	1.25322000	-2.49435700	-1.23474600
C	3.03895600	-3.59268100	-0.91073800
H	3.31985900	-4.30460500	-0.13160100
H	2.83112900	-4.15658200	-1.82479300
C	4.21825000	-2.66327800	-1.16969000
O	4.14339800	-1.46968100	-1.31896800
O	5.35706000	-3.36251800	-1.23378900
C	6.53199400	-2.59072300	-1.48286500
H	6.66989300	-1.84488400	-0.69596100
H	7.35613800	-3.30306300	-1.48585400
H	6.45917800	-2.08257400	-2.44776600
O	-3.55889200	-0.45179100	2.24826000
H	-2.72571400	0.00280500	2.46635000
C	-3.22024700	-1.64352300	1.63202600
H	-2.23575800	-2.01390900	1.94098300
C	-3.15324400	-1.46364000	0.10852700
F	-2.39008600	-0.39284000	-0.17550300
F	-2.57202800	-2.52314400	-0.48995000
F	-4.34340900	-1.27544400	-0.45795900
C	-4.23717000	-2.70487800	2.05414000
F	-4.01849800	-3.85709800	1.39648900
F	-4.11004500	-2.95104100	3.36245400
F	-5.49233300	-2.32620200	1.82152200

S-TS2-iso4

C	1.51535500	1.55357300	-1.69880200
O	1.49129100	1.58009700	-2.91727500
N	0.75841300	0.70491100	-0.94345400
C	0.75015700	0.74140600	0.49550500
C	-0.14687800	1.57380600	1.16410100
C	1.67437100	-0.08300000	1.16964700
C	-0.06884800	1.58808300	2.56525100
C	1.68821600	-0.04513700	2.57062500
H	1.70874000	-1.39918800	0.74623900

C	0.82609100	0.79499800	3.26767100
H	-0.74684100	2.23248500	3.11827200
H	2.37991800	-0.68717200	3.10975000
H	0.84295300	0.82742000	4.35281200
C	0.22202900	-0.46924900	-1.62209700
H	0.96835700	-1.27237800	-1.61455300
H	0.02468100	-0.19107800	-2.65911900
C	-1.16753700	2.44340300	0.45381200
H	-1.16162400	2.16208700	-0.60258800
C	-2.58456800	2.19157400	0.98251500
H	-3.32542200	2.65552700	0.32658000
H	-2.78941600	1.11911800	1.01991600
H	-2.72085800	2.60263100	1.99014600
C	-0.79879500	3.92921600	0.56204200
H	-0.80865200	4.26133600	1.60720500
H	0.20052200	4.12537800	0.16027800
H	-1.51882700	4.54153100	0.00856200
C	2.46078600	2.49355700	-0.98243400
C	2.44463100	3.84096000	-1.32373100
C	3.38765800	4.69168200	-0.76403300
H	1.70283200	4.19342600	-2.03080600
C	4.32848600	2.79799400	0.34957700
C	4.34914600	4.15912600	0.08763800
H	3.38361400	5.75028300	-1.00235900
H	5.08237300	2.32604400	0.96855700
H	5.11902900	4.77894600	0.53217200
N	3.39291700	1.98287100	-0.15972700
C	2.95942900	-2.89370600	0.26218300
C	5.21796600	-2.48034400	0.05730200
C	4.93258100	-3.79110300	-0.70510600
C	3.54391700	-4.21720700	-0.17765900
H	5.79793700	-2.67401600	0.96997000
H	4.88540900	-3.58245500	-1.77821200
H	5.70538400	-4.54436400	-0.54725400
H	2.90691800	-4.69819100	-0.92362800
H	3.61060500	-4.88915200	0.68655400
N	3.89235500	-2.00274800	0.42562700
O	1.71454000	-2.63340800	0.43927500
C	5.96277500	-1.37133500	-0.71529200
O	6.96087000	-1.65268900	-1.34880100
O	5.46497400	-0.16850900	-0.58199500
Pd	3.59638000	-0.07101600	0.25002600
C	-1.07899600	-0.93465600	-0.99453300
O	-2.10392200	-0.25818200	-1.04232600

N	-1.04534500	-2.14827900	-0.41064200
H	-0.14453200	-2.56825600	-0.20104900
C	-2.22520100	-2.63896300	0.25378100
H	-3.07501300	-2.63250200	-0.43176300
H	-2.05071200	-3.67225100	0.56608700
C	-2.56271300	-1.80885900	1.48826300
O	-1.76481000	-1.19813600	2.15329300
O	-3.87637600	-1.86586500	1.73801300
C	-4.33434800	-1.10691300	2.86142000
H	-4.13756100	-0.04389600	2.70151500
H	-5.40651900	-1.28659700	2.91393800
H	-3.83483300	-1.43669600	3.77482500
O	-4.48476000	0.99337300	-1.50917500
H	-3.54566500	0.73982800	-1.54986500
C	-5.10809000	0.05047300	-0.70474300
H	-4.43558900	-0.37460300	0.04616500
C	-5.60329900	-1.13333700	-1.54542500
F	-4.57700300	-1.62276600	-2.26283500
F	-6.05696400	-2.13048200	-0.77043400
F	-6.57235500	-0.79459500	-2.39751100
C	-6.23102800	0.74501000	0.06245700
F	-6.93552300	-0.14108100	0.78886000
F	-5.71130500	1.63631600	0.92201100
F	-7.07721400	1.39110200	-0.73674500

S-TS2-iso5

C	3.32504800	0.96559700	-1.24958200
O	3.96092600	0.96393500	-2.29021300
N	2.03257500	1.38929300	-1.15180400
C	1.32201100	1.42722600	0.09798400
C	1.33756300	2.58680500	0.87538100
C	0.63065100	0.26263500	0.48450500
C	0.65084700	2.53700000	2.09829500
C	-0.04604900	0.27465100	1.71175400
H	-0.17309100	-0.27929300	-0.51364500
C	-0.03374200	1.40645000	2.51978500
H	0.65476700	3.41810500	2.73463600
H	-0.58401700	-0.61087000	2.03185900
H	-0.55894500	1.40718200	3.47011500
C	1.27783000	1.47670800	-2.40043500
H	0.88357000	0.48585200	-2.65770700
H	1.97229300	1.78597300	-3.18319800
C	2.08185600	3.84732400	0.47400700

H	2.39466400	3.72708100	-0.56622900
C	1.17741900	5.08457800	0.53102100
H	1.71007500	5.95269300	0.12895900
H	0.27976600	4.92975500	-0.07160800
H	0.88186200	5.32554700	1.55939200
C	3.33047200	4.03791200	1.34659100
H	3.05757000	4.19367200	2.39745800
H	3.99009400	3.16505600	1.30221900
H	3.89764800	4.91449700	1.01465200
C	4.00906800	0.44100000	-0.00371900
C	5.25301700	0.95937400	0.33957100
C	5.95264600	0.39657700	1.39791500
H	5.65407400	1.78453200	-0.23721300
C	4.18267800	-1.19090700	1.63024500
C	5.40889600	-0.70301900	2.05271900
H	6.91647700	0.79774000	1.69385400
H	3.73627000	-2.07260000	2.07485100
H	5.92728800	-1.19152600	2.86953600
N	3.48605000	-0.61867400	0.63614400
C	-0.80793800	-2.03415000	-1.26004400
C	0.24849100	-3.97740400	-0.61850300
C	-0.55741100	-4.30637800	-1.89447400
C	-1.53049800	-3.11196700	-2.03015800
H	-0.18406500	-4.47172400	0.26127300
H	0.12264700	-4.34761400	-2.75044500
H	-1.06623300	-5.26852800	-1.82735200
H	-1.71761400	-2.79986500	-3.06023100
H	-2.49939100	-3.29525600	-1.55432800
N	0.09431100	-2.53782700	-0.47621000
O	-1.01545900	-0.76324100	-1.33529600
C	1.75395300	-4.32009900	-0.63267900
O	2.11538000	-5.40919400	-1.03228600
O	2.54208600	-3.39051500	-0.15396200
Pd	1.67658000	-1.55099900	0.12658900
C	0.16083300	2.50799800	-2.31191900
O	0.38644800	3.70295000	-2.20559200
N	-1.09391600	1.98939100	-2.41303800
H	-1.21762700	0.99133900	-2.27789700
C	-2.23299500	2.83627100	-2.21053000
H	-1.98403800	3.84841700	-2.53974700
H	-3.08461800	2.48688000	-2.80128200
C	-2.66043500	2.88972500	-0.75425400
O	-2.07578000	2.33238900	0.15276500
O	-3.76218100	3.61139200	-0.60950500

C	-4.31366200	3.68075300	0.71072200
H	-3.56309500	4.04152200	1.41782100
H	-5.14330300	4.38232900	0.64250900
H	-4.66859900	2.69482800	1.01886200
O	-3.42969500	0.57406600	1.76882700
H	-2.85120400	1.27500400	1.41141400
C	-3.34692900	-0.50809100	0.89998700
H	-2.42001000	-0.51136700	0.31745200
C	-4.48804100	-0.45835300	-0.12276800
F	-4.33693400	0.62512200	-0.91223900
F	-4.48469600	-1.53476400	-0.92311100
F	-5.68708000	-0.36578400	0.44918300
C	-3.36723600	-1.79966700	1.72236700
F	-3.09050600	-2.86138000	0.94244800
F	-2.43418700	-1.75588300	2.68135300
F	-4.54469600	-2.01778000	2.30955300

S-TS2-iso6

C	1.18114200	1.48204300	2.07333300
O	1.15276400	1.53528000	3.29007600
N	2.10532400	0.76505700	1.36420400
C	2.16004700	0.79856600	-0.07088000
C	2.87813600	1.80327500	-0.72017800
C	1.43840300	-0.19193400	-0.77159500
C	2.78526300	1.83729300	-2.12062300
C	1.40852700	-0.12761400	-2.17313300
H	1.67403700	-1.47195700	-0.34724900
C	2.06088500	0.89991900	-2.84591500
H	3.30647500	2.62680600	-2.65621000
H	0.86087700	-0.88602900	-2.72611900
H	2.01368400	0.97067400	-3.92872700
C	2.81041200	-0.29380800	2.07600200
H	2.24390900	-1.22941600	1.99738500
H	2.85250900	-0.00312100	3.12732500
C	3.70588800	2.84595600	0.00838300
H	3.70189300	2.58887800	1.07070400
C	5.16852100	2.81005800	-0.45370200
H	5.76022000	3.52488500	0.12734900
H	5.59624700	1.81714800	-0.29607500
H	5.26687500	3.08114900	-1.51246500
C	3.10500700	4.24772200	-0.16500500
H	3.14540500	4.57154000	-1.21215400
H	2.05776600	4.28009400	0.15275100

H	3.66747200	4.97560300	0.42925800
C	0.11259000	2.21561600	1.29349900
C	-0.14048800	3.54917000	1.58371700
C	-1.19103800	4.19342700	0.94070200
H	0.48008200	4.05341000	2.31532000
C	-1.68500000	2.13478600	-0.16711800
C	-1.97624900	3.47303200	0.05017900
H	-1.40124900	5.23804700	1.14559500
H	-2.29912400	1.52593500	-0.81573100
H	-2.82359700	3.91879200	-0.45668200
N	-0.65882000	1.51896300	0.43829400
C	0.72231300	-3.19556200	0.09089900
C	-1.58084000	-3.24361800	0.15551100
C	-1.08798800	-4.47903000	0.93903200
C	0.37792300	-4.61986000	0.47066900
H	-2.02736300	-3.54500400	-0.80155300
H	-1.12184200	-4.27133200	2.01318400
H	-1.69421800	-5.36506000	0.74738000
H	1.06109400	-4.99826100	1.23426300
H	0.47286600	-5.26288100	-0.41259900
N	-0.36045700	-2.49440800	-0.09656200
O	1.89686700	-2.70287800	-0.02684000
C	-2.61693300	-2.33947900	0.83778300
O	-3.70311400	-2.78669500	1.15721200
O	-2.26167400	-1.08677900	0.98119800
Pd	-0.45552000	-0.54472800	0.10245100
C	4.23670500	-0.46835600	1.57558300
O	5.07196000	0.41798800	1.66718000
N	4.51523500	-1.70190200	1.08081200
H	3.74683900	-2.29823300	0.79439100
C	5.83854300	-1.97317600	0.58414000
H	6.58090000	-1.64835400	1.31587000
H	5.95358800	-3.05248100	0.44690800
C	6.20822400	-1.30343600	-0.73263300
O	7.34938700	-1.17816000	-1.10336900
O	5.13851300	-0.93278900	-1.44502400
C	5.43793500	-0.34897100	-2.71312100
H	6.11426600	-0.99125400	-3.28160900
H	4.48035600	-0.24543800	-3.21911100
H	5.90347700	0.63056700	-2.57566200
O	-4.21533400	0.68781700	0.67938700
H	-3.52766800	0.06011600	1.00287800
C	-5.11336800	-0.05382500	-0.07587600
H	-5.16698400	-1.10211800	0.24617400

C	-4.67487400	-0.05739100	-1.54539000
F	-3.45351800	-0.62596900	-1.65072600
F	-5.50373900	-0.74932100	-2.33159500
F	-4.56253500	1.18287400	-2.04620400
C	-6.50015200	0.55901600	0.11928700
F	-7.42291200	-0.08048300	-0.61614000
F	-6.86017200	0.46420600	1.40127900
F	-6.52890100	1.85287900	-0.22379200

S-TS2-iso7

C	0.07288700	0.51752000	1.92231300
O	-0.82376700	0.00312000	2.59056800
N	0.92147700	-0.19736600	1.15318500
C	1.95762900	0.42741800	0.36773000
C	3.22899500	0.61434500	0.91108000
C	1.60738400	0.84039500	-0.93178800
C	4.14871800	1.31658500	0.11764700
C	2.58285300	1.49489200	-1.69576900
H	0.87218700	-0.08195500	-1.65078100
C	3.84100700	1.75804700	-1.16220700
H	5.13953100	1.51171700	0.51951000
H	2.34056100	1.80921300	-2.70749700
H	4.58513100	2.29717100	-1.74186800
C	0.54137500	-1.58119300	0.86611900
H	-0.20466900	-1.58977700	0.06630700
H	0.09437900	-1.99464900	1.77161100
C	3.63314400	0.13143000	2.29179600
H	2.82430800	-0.49722900	2.67326200
C	4.88853100	-0.74839400	2.23034700
H	5.10591100	-1.15564800	3.22309900
H	4.73395400	-1.58943900	1.55034900
H	5.76867100	-0.17907000	1.90657600
C	3.83341300	1.31384800	3.24985800
H	4.66852800	1.94750600	2.92738400
H	2.94034500	1.94521200	3.30320500
H	4.05922900	0.95147800	4.25847600
C	0.22111600	2.02068500	1.98455700
C	0.31823100	2.62520000	3.23179400
C	0.33921200	4.01174700	3.30847000
H	0.36487500	2.00318300	4.11817400
C	0.08242400	4.07642800	0.93260600
C	0.21604500	4.75029600	2.13748400
H	0.43119600	4.50665100	4.26955800

H	-0.06570500	4.60167000	-0.00339400
H	0.20307100	5.83392600	2.14970400
N	0.10421800	2.73845200	0.85482500
C	-0.73785000	-0.31663400	-2.83041300
C	-2.18824300	1.44445400	-3.16615500
C	-2.96409700	0.15613600	-3.51780300
C	-1.85830000	-0.91535000	-3.64753300
H	-2.00010600	2.04981200	-4.06280500
H	-3.64326100	-0.09342000	-2.69978600
H	-3.56164100	0.26682600	-4.42333500
H	-2.13877300	-1.89082300	-3.24454100
H	-1.52307100	-1.05966000	-4.68118700
N	-0.91851900	0.95983600	-2.64063300
O	0.26082600	-0.95527300	-2.34095700
C	-2.85061900	2.38139600	-2.13579500
O	-4.01528400	2.69528600	-2.27018400
O	-2.05955900	2.82391200	-1.18737200
Pd	-0.28112000	1.85543400	-1.01215000
C	1.73644700	-2.45846600	0.52168900
O	2.59045800	-2.74028100	1.34940700
N	1.72743300	-2.96013600	-0.73545400
H	1.13567600	-2.52778400	-1.43726600
C	2.77948300	-3.85745300	-1.13719800
H	2.87334600	-4.67014800	-0.41379300
H	2.51707100	-4.29437300	-2.10514100
C	4.16481200	-3.23901900	-1.26917600
O	5.17998400	-3.88412200	-1.17866200
O	4.12110700	-1.93432800	-1.56034300
C	5.39556600	-1.31848500	-1.74578500
H	6.02685200	-1.93007600	-2.39374400
H	5.19116100	-0.35009200	-2.19807000
H	5.88989800	-1.18673400	-0.77929700
O	-3.52537000	-0.43613400	2.25594200
H	-2.67322400	-0.02578000	2.48572800
C	-3.23977400	-1.61063300	1.58196000
H	-2.26460500	-2.02834800	1.85699700
C	-3.19005400	-1.36480300	0.06700300
F	-2.39608000	-0.30704100	-0.18206900
F	-2.65286800	-2.41401600	-0.58768500
F	-4.38111200	-1.11253100	-0.47160200
C	-4.28732000	-2.65394100	1.97343500
F	-4.11521900	-3.78391100	1.26574000
F	-4.15303500	-2.95781900	3.26849900
F	-5.53133000	-2.22367500	1.77302700

S-TS2-iso8

C	1.36095300	1.56451900	-1.68455300
O	1.29332400	1.59383200	-2.90043800
N	0.66175700	0.68388500	-0.90699600
C	0.70867500	0.72435900	0.52996300
C	-0.17332400	1.54832800	1.23283900
C	1.68115800	-0.07106200	1.16789100
C	0.00525100	1.61775800	2.62308000
C	1.78745300	0.00981000	2.56340800
H	1.73547800	-1.38314100	0.74247500
C	0.97066100	0.87250300	3.28771300
H	-0.64325800	2.27274300	3.19928000
H	2.52425800	-0.60476500	3.07409200
H	1.07570100	0.96014000	4.36535100
C	0.17390900	-0.52054900	-1.56532300
H	0.95034900	-1.29404400	-1.54900500
H	-0.03580800	-0.26395700	-2.60590100
C	-1.27521800	2.35511800	0.57062300
H	-1.30968600	2.06425100	-0.48231200
C	-2.64585800	2.02809700	1.17738200
H	-3.44314500	2.48360300	0.58514000
H	-2.82159600	0.94873200	1.18541900
H	-2.73438100	2.40251800	2.20480800
C	-0.98724700	3.86034700	0.65010600
H	-0.96888000	4.20589600	1.69081200
H	-0.02061700	4.10882300	0.20018900
H	-1.76690900	4.42220000	0.12518500
C	2.30240400	2.53064400	-0.99855500
C	2.22407200	3.88105600	-1.31716500
C	3.16476700	4.75526100	-0.79022200
H	1.43779000	4.21842900	-1.98241000
C	4.22359200	2.87867300	0.24410700
C	4.18551400	4.24337200	0.00306100
H	3.11258300	5.81645600	-1.01037000
H	5.02409000	2.42358900	0.81546600
H	4.95589500	4.88295900	0.41774500
N	3.29031100	2.03984300	-0.22996400
C	2.99963500	-2.84907600	0.20569900
C	5.23740700	-2.37944700	-0.09411700
C	4.95283100	-3.69736300	-0.84407200
C	3.60038400	-4.15824400	-0.25526900
H	5.85886800	-2.55876300	0.79385500

H	4.85213200	-3.49099900	-1.91392300
H	5.75052900	-4.43078900	-0.72083000
H	2.94494600	-4.65993800	-0.97090800
H	3.72329000	-4.82402400	0.60747600
N	3.91679500	-1.93397800	0.32749000
O	1.75731800	-2.62080800	0.43363600
C	5.92293900	-1.25257900	-0.89391200
O	6.90469000	-1.50461800	-1.56290200
O	5.39706600	-0.06205400	-0.74329900
Pd	3.56627200	-0.01216500	0.16111300
C	-1.10705000	-1.02265700	-0.93042200
O	-2.13247900	-0.34727800	-0.91310300
N	-1.06011700	-2.26579800	-0.41431700
H	-0.15466400	-2.68232700	-0.21868100
C	-2.24817100	-2.80305300	0.20655900
H	-3.08918300	-2.75098800	-0.48621200
H	-2.06594600	-3.85221700	0.45523600
C	-2.66280200	-2.07506900	1.47844500
O	-3.81241400	-1.87492400	1.79259300
O	-1.61094800	-1.73697000	2.22620700
C	-1.92848100	-1.11917900	3.47576900
H	-2.59705200	-1.75847300	4.05685200
H	-0.97464700	-0.98658100	3.98237200
H	-2.40779300	-0.15157800	3.30929400
O	-4.50122900	0.92557900	-1.36869300
H	-3.58093800	0.61021700	-1.37186700
C	-5.23534500	0.02061400	-0.61124100
H	-4.66295900	-0.42670200	0.21029600
C	-5.70804700	-1.14584800	-1.48703800
F	-4.63768200	-1.70341700	-2.08947800
F	-6.30039700	-2.10451800	-0.76387900
F	-6.55414100	-0.76470000	-2.44639700
C	-6.39121300	0.78704500	0.02843400
F	-7.21403700	-0.03836100	0.69021200
F	-5.91068900	1.67518500	0.91283500
F	-7.11348700	1.45896100	-0.87048500

S-TS2-iso9

C	1.96219400	1.70864900	-1.73485700
O	2.22228600	1.87199100	-2.91436100
N	1.14949400	0.71707000	-1.26546400
C	0.81084600	0.60025200	0.12672900
C	-0.28236700	1.30268200	0.63948900

C	1.63599800	-0.21534200	0.92646400
C	-0.48536900	1.22266200	2.02578800
C	1.36169000	-0.28680800	2.29986100
H	1.90193700	-1.47097700	0.41230800
C	0.31942400	0.44988400	2.85327400
H	-1.30999300	1.77956100	2.46345300
H	1.98167700	-0.91867900	2.93064900
H	0.12556800	0.41807000	3.92182300
C	0.93403700	-0.42261800	-2.14804200
H	1.74063300	-1.15300000	-2.01149400
H	0.97720100	-0.05158600	-3.17395200
C	-1.21335200	2.14593100	-0.21284300
H	-0.94409400	1.98111300	-1.25940000
C	-2.67313100	1.70523400	-0.05280300
H	-3.31476000	2.28341100	-0.72331600
H	-2.79477700	0.65272400	-0.31546600
H	-3.04387100	1.86202900	0.96740200
C	-1.05118400	3.63731900	0.11263500
H	-1.35217500	3.85146700	1.14527400
H	-0.01351400	3.96609800	-0.00556300
H	-1.68139200	4.24075800	-0.54920700
C	2.61214100	2.63681400	-0.73127700
C	2.52129000	4.00899100	-0.93376200
C	3.22799400	4.86338100	-0.09924600
H	1.91063600	4.37924000	-1.74892000
C	4.11491800	2.93773800	1.00354100
C	4.04390300	4.31703700	0.88538400
H	3.15865900	5.93842100	-0.22901800
H	4.77035000	2.46072100	1.72271200
H	4.63475800	4.94263900	1.54413900
N	3.39878200	2.11288200	0.22458800
C	3.37490300	-2.80499000	0.13101500
C	5.56580900	-2.19300400	0.51089100
C	5.60212100	-3.44360200	-0.39177400
C	4.17909700	-4.02911500	-0.24798700
H	5.93251600	-2.42532200	1.52017500
H	5.78750300	-3.13885100	-1.42616700
H	6.38796300	-4.14352100	-0.10553800
H	3.78683500	-4.48829700	-1.15835300
H	4.11026700	-4.77146800	0.55631600
N	4.15020600	-1.86125900	0.57956600
O	2.10407200	-2.66555100	0.02049300
C	6.35492600	-0.95790100	0.02957200
O	7.49546500	-1.09318300	-0.36630400

O	5.72246800	0.18390500	0.13681000
Pd	3.71194900	0.04725000	0.49113800
C	-0.42674900	-1.06196700	-1.93098800
O	-1.47384800	-0.46091100	-2.11316800
N	-0.39093400	-2.37318700	-1.57093700
H	0.45771400	-2.74690700	-1.15814200
C	-1.64275500	-3.04662300	-1.35089800
H	-2.27691800	-2.96956800	-2.23630200
H	-1.44709300	-4.10602500	-1.15953300
C	-2.45804200	-2.50626700	-0.18683200
O	-3.67263600	-2.56456600	-0.16100700
O	-1.70531300	-2.04814300	0.80109200
C	-2.39348600	-1.60406600	1.97633700
H	-3.13507400	-2.34423300	2.28522500
H	-1.62187400	-1.48644900	2.73365600
H	-2.88357500	-0.64678600	1.78594400
O	-5.32094100	-0.68275800	0.94882900
H	-4.72750200	-1.38032200	0.60814000
C	-6.40807200	-0.59035900	0.09089200
H	-6.67519500	-1.55264300	-0.36453400
C	-6.09850000	0.36448800	-1.06950600
F	-4.98383000	-0.04582800	-1.68788100
F	-7.08837200	0.37510000	-1.97364900
F	-5.90318500	1.62151700	-0.65608700
C	-7.61213700	-0.15003500	0.92414200
F	-8.69355000	0.02992000	0.15182100
F	-7.90547700	-1.09643600	1.82452000
F	-7.37827800	0.98682500	1.58247500

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C	0.46387200	-0.84370500	-1.62072700
O	-0.31942700	-0.28971900	-2.38621200
N	1.58997300	-0.27387700	-1.12931300
C	2.46183200	-0.98640100	-0.22996700
C	3.49782700	-1.77414300	-0.73104400
C	2.19545200	-0.86296100	1.14984900
C	4.23148900	-2.51463300	0.20957400
C	2.98864900	-1.59516400	2.04503000
H	1.99541200	0.41071500	1.59044300
C	3.98821500	-2.44010600	1.57453800
H	5.02538400	-3.16550500	-0.14731800
H	2.80786200	-1.49883800	3.11224600
H	4.58429400	-3.03146400	2.26359300

C	1.71697500	1.18083600	-1.21869300
H	1.18813200	1.64340700	-0.38107700
H	1.24029800	1.51402600	-2.13996600
C	3.83693800	-1.88430900	-2.20629700
H	3.21153500	-1.16852400	-2.74593400
C	5.29686200	-1.49143400	-2.46980700
H	5.49661900	-1.50791000	-3.54614000
H	5.49310700	-0.47972500	-2.10807000
H	5.99607300	-2.19018900	-1.99348400
C	3.54560500	-3.29645500	-2.73364400
H	4.19698800	-4.03950000	-2.25781100
H	2.50925100	-3.59336900	-2.54414100
H	3.72438800	-3.34206500	-3.81312300
C	0.13156400	-2.25522000	-1.19429900
C	-0.09984500	-3.21953000	-2.16491400
C	-0.50768200	-4.48706200	-1.77030800
H	0.02954400	-2.95983300	-3.20896400
C	-0.50106700	-3.71096700	0.48907500
C	-0.71268100	-4.73621600	-0.41959400
H	-0.68469000	-5.26074400	-2.50987500
H	-0.69174100	-3.84109800	1.54743500
H	-1.06085800	-5.69942800	-0.06608100
N	-0.06885800	-2.49948300	0.11264700
C	0.79448900	1.55790200	2.74478000
C	-1.16056600	0.67209900	3.59757000
C	-1.29151700	2.20692800	3.69615000
C	0.14950500	2.71454900	3.47174500
H	-1.09252300	0.21084500	4.59247400
H	-1.95216800	2.56637100	2.90530600
H	-1.71369000	2.52468600	4.65022600
H	0.20848200	3.62422000	2.87107000
H	0.68642200	2.89493100	4.41014600
N	0.09371500	0.46534100	2.88344800
O	1.87543000	1.60526100	2.06480600
C	-2.26897800	-0.07677400	2.84491700
O	-3.44282500	0.25446100	2.97795400
O	-1.87379700	-1.07370300	2.11387900
Pd	0.12050900	-1.01484300	1.59025700
C	3.17055800	1.62296400	-1.27535300
O	3.90493300	1.32166900	-2.20460100
N	3.55845000	2.42744800	-0.25687500
H	2.99940000	2.46034400	0.58822500
C	4.90203000	2.94390400	-0.24519100
H	5.12541900	3.42649900	-1.19898000

H	4.98046400	3.69995700	0.54159600
C	6.00402100	1.91920500	-0.01210000
O	7.14529500	2.09427900	-0.36085500
O	5.58130800	0.85141500	0.67558900
C	6.59594200	-0.10813200	0.97024500
H	7.47127700	0.37887100	1.40546800
H	6.14549700	-0.80387200	1.67563000
H	6.89301900	-0.63253200	0.05795700
O	-1.00382300	2.38106900	-2.40646400
H	-0.95031000	1.40753400	-2.47315500
C	-2.07244300	2.75303500	-1.60652500
H	-3.00074100	2.22067600	-1.83948700
C	-2.33064700	4.23769900	-1.86833200
F	-2.66872700	4.41804300	-3.14641000
F	-3.33646200	4.68674800	-1.10445600
F	-1.25228500	4.98446800	-1.61223800
C	-1.76901100	2.46379900	-0.13150100
F	-2.78463400	2.77274400	0.67490400
F	-1.51844700	1.14499600	0.01345200
F	-0.67928800	3.11195300	0.31501300
O	-4.98863700	-1.09131100	1.13300600
H	-4.52146900	-0.64409700	1.87473500
C	-4.10824100	-1.16267400	0.06852600
H	-3.09349200	-0.85590200	0.33924400
C	-4.56974200	-0.22898900	-1.05179600
F	-4.68674000	1.02083700	-0.57075700
F	-3.66842900	-0.17829200	-2.05557900
F	-5.74454200	-0.57317300	-1.57968800
C	-3.99824800	-2.61633100	-0.38840500
F	-3.13692000	-2.73647700	-1.42078200
F	-3.52721600	-3.37730900	0.61032300
F	-5.16499600	-3.13447000	-0.77613600

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C	0.29223800	-1.28647900	-0.33744300
O	-0.43100300	-1.63756900	-1.26368500
N	1.62169300	-1.07227300	-0.49426300
C	2.50127700	-0.82719000	0.61410500
C	3.01468300	-1.89639800	1.34881900
C	2.79160100	0.51681500	0.91645900
C	3.78978600	-1.56607000	2.47168100
C	3.60530800	0.78597200	2.02756800
H	3.13923400	1.31092800	-0.15252500

C	4.08481800	-0.25328900	2.81700500
H	4.17987300	-2.37123100	3.08869500
H	3.84602500	1.81763400	2.26996900
H	4.69006100	-0.04704300	3.69505400
C	2.11457100	-0.84237900	-1.84980600
H	2.08306500	0.23210000	-2.06386300
H	1.43655600	-1.35356200	-2.53489200
C	2.75463700	-3.35289300	1.01004600
H	2.23477600	-3.38483400	0.04925300
C	4.07136600	-4.11876900	0.82556700
H	3.86212000	-5.14692100	0.51337100
H	4.68037000	-3.64976800	0.04903500
H	4.64761300	-4.16815900	1.75799800
C	1.86917100	-4.01524400	2.07452800
H	2.37211100	-4.04132500	3.04878600
H	0.92169700	-3.48159500	2.20299300
H	1.64278600	-5.04790500	1.78955500
C	-0.33598100	-1.03172800	1.01552500
C	-1.26047600	-1.95032400	1.49848100
C	-1.96058100	-1.65924400	2.66229700
H	-1.45942700	-2.85758200	0.93824100
C	-0.81019600	0.43065900	2.74763800
C	-1.73104000	-0.44642900	3.29810000
H	-2.69686300	-2.35785600	3.04138400
H	-0.62987500	1.40700200	3.18272200
H	-2.27181700	-0.16291600	4.19330500
N	-0.11638700	0.14437800	1.63470200
C	2.80989900	3.13782000	-0.92971900
C	1.16193100	4.49346500	-0.05204400
C	1.44881500	5.00444000	-1.47852800
C	2.81607900	4.36788700	-1.80998400
H	1.51826200	5.20814400	0.70272100
H	0.67883300	4.62914900	-2.15941300
H	1.44885500	6.09314000	-1.54170000
H	2.94415300	4.09857000	-2.86050400
H	3.65693800	5.01137000	-1.52447600
N	1.94112700	3.26312200	0.03673300
O	3.52511300	2.08965300	-1.09012900
C	-0.30000900	4.18009600	0.29305700
O	-1.18759100	4.96346900	-0.02358500
O	-0.49509800	3.08137100	0.95677700
Pd	1.05872300	1.72845300	0.89006400
C	3.51075400	-1.41161400	-2.05597600
O	3.74440900	-2.60670400	-1.96763500

N	4.44862500	-0.49595000	-2.40626600
H	4.27023500	0.48537900	-2.22771700
C	5.79648600	-0.93440800	-2.66006800
H	5.79090400	-1.76115900	-3.37333200
H	6.35585900	-0.10846000	-3.10926200
C	6.58156200	-1.41643000	-1.44744300
O	7.54879400	-2.13082700	-1.53972900
O	6.12166600	-0.91267800	-0.29637200
C	6.86165300	-1.30119100	0.86182200
H	7.93110100	-1.14805300	0.70247600
H	6.49228100	-0.67255300	1.66950800
H	6.67855800	-2.35544300	1.08635800
O	-2.70321100	-3.17863900	-1.10992300
H	-1.95538600	-2.58701200	-1.32237200
C	-3.79537900	-2.39115800	-0.76586400
H	-3.52003400	-1.49450700	-0.20053000
C	-4.68591000	-3.23123600	0.14566300
F	-4.01516600	-3.53173700	1.27914300
F	-5.78763000	-2.56058100	0.49964400
F	-5.05364000	-4.38224400	-0.41229100
C	-4.52762300	-1.89867300	-2.02148500
F	-5.46922200	-0.99999800	-1.70941600
F	-3.64307900	-1.31069900	-2.83731100
F	-5.11043800	-2.89289100	-2.69822500
O	-3.64944600	3.66444500	-0.02209800
H	-2.83333700	4.21174100	0.02389100
C	-3.29291500	2.35180400	0.23371700
H	-2.44116400	2.27510000	0.91709900
C	-2.85596000	1.65211400	-1.05748400
F	-1.88909900	2.36230000	-1.65829000
F	-2.33352600	0.43211500	-0.79174600
F	-3.84543100	1.48762200	-1.93243400
C	-4.46790100	1.65662700	0.91416300
F	-4.17546500	0.35502400	1.15881400
F	-4.70618000	2.22790200	2.10043000
F	-5.58957700	1.69033600	0.20140900

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C	-0.70340700	-1.39146700	-0.73894400
O	-0.87260300	-1.77394300	-1.88245900
N	0.27221100	-0.50590700	-0.37546900
C	0.52174700	-0.14643600	0.99307700
C	1.38798500	-0.91412200	1.76972300

C	-0.14624900	0.98917100	1.49655700
C	1.54564400	-0.52556900	3.10935100
C	0.07038200	1.34517800	2.83631300
H	-0.05789400	2.11161200	0.70414200
C	0.90889800	0.58475800	3.64353800
H	2.20344100	-1.11120600	3.74582100
H	-0.42289300	2.22711000	3.23618900
H	1.07264300	0.85580000	4.68182800
C	0.84681700	0.30822800	-1.44059600
H	0.23662400	1.20675800	-1.59072200
H	0.82080100	-0.28453600	-2.35713900
C	2.13533900	-2.12286500	1.23901800
H	1.98628200	-2.15159700	0.15631100
C	3.64281300	-1.99889000	1.48797300
H	4.18829200	-2.76999500	0.93815700
H	4.00414900	-1.02575700	1.14737300
H	3.88856200	-2.10609200	2.55139400
C	1.58414300	-3.42266100	1.84019400
H	1.73516500	-3.44957700	2.92612700
H	0.51135600	-3.53160400	1.65086900
H	2.09872800	-4.28818200	1.40953300
C	-1.64475100	-1.89999600	0.33182200
C	-1.89892000	-3.26529200	0.38706300
C	-2.87657600	-3.73922900	1.24879900
H	-1.34612900	-3.92551700	-0.27056400
C	-3.30577100	-1.47918400	1.88787600
C	-3.59962700	-2.82698500	2.00866500
H	-3.08946300	-4.80125400	1.30820500
H	-3.86411400	-0.72674600	2.43309800
H	-4.39760800	-3.14418100	2.66900500
N	-2.33611900	-1.02192500	1.07922700
C	-1.17323500	3.60904500	-0.05179700
C	-3.46427200	3.58767700	0.18917400
C	-3.14961700	4.53157900	-0.98930700
C	-1.64390500	4.82686100	-0.81394400
H	-3.83671700	4.14874700	1.05743400
H	-3.32831300	4.00625600	-1.93221100
H	-3.77121600	5.42772700	-0.98452700
H	-1.09716100	4.93734500	-1.75302300
H	-1.45916000	5.72467800	-0.21222900
N	-2.17236400	2.99374800	0.51499500
O	0.03515500	3.19144500	0.02997600
C	-4.47561300	2.46178600	-0.06852600
O	-5.50884200	2.69843300	-0.68561800

O	-4.17187700	1.31097400	0.44428400
Pd	-2.17360900	1.06464200	0.91279300
C	2.28893300	0.67710500	-1.14423400
O	3.17976200	-0.16729600	-1.09215600
N	2.53201900	1.99135200	-0.96684400
H	1.74991500	2.61518300	-0.79438200
C	3.85897400	2.41121400	-0.59469700
H	4.59035500	2.02759900	-1.30850100
H	3.90530300	3.50353000	-0.61857000
C	4.21541900	1.94100600	0.81236400
O	3.42072000	1.75138800	1.69836800
O	5.53777500	1.77846200	0.92886200
C	6.00515500	1.31211300	2.19922200
H	5.51089100	0.37363500	2.46018000
H	7.07442900	1.15545200	2.07110100
H	5.80686800	2.05711600	2.97302400
O	5.30536100	-1.87003500	-1.39965000
H	4.41261400	-1.48337400	-1.42283800
C	6.16052100	-0.85852500	-0.98684300
H	5.66606200	-0.11835100	-0.35095900
C	6.70059700	-0.08176600	-2.19391600
F	5.66459300	0.34804800	-2.93595400
F	7.39003700	1.00389400	-1.80960000
F	7.48796100	-0.81938300	-2.97781300
C	7.26548600	-1.48317000	-0.13786800
F	8.18701700	-0.56435600	0.20313700
F	6.74525200	-1.96287300	1.00345400
F	7.88755000	-2.48334100	-0.75761800
O	-6.75338600	0.35351700	-1.47614700
H	-6.37335200	1.21481500	-1.19167900
C	-6.01676900	-0.66094400	-0.88757700
H	-5.45942600	-0.31747300	-0.01022400
C	-4.96689800	-1.18401600	-1.87237600
F	-4.15065900	-0.18104700	-2.22990600
F	-4.20096800	-2.14311600	-1.31392900
F	-5.50224500	-1.69238600	-2.98389800
C	-6.97938000	-1.74325600	-0.40769300
F	-6.31246200	-2.75934600	0.18273500
F	-7.81193300	-1.23435100	0.50916100
F	-7.71558100	-2.26329600	-1.39112600

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C	-0.61888000	-1.40609800	-0.60031100

O	-0.75308000	-1.87307500	-1.71587800
N	0.32065300	-0.46224400	-0.28558600
C	0.53488700	-0.00916500	1.05941800
C	1.39912700	-0.70856800	1.90390500
C	-0.17279200	1.13645900	1.47528900
C	1.47807000	-0.25958600	3.23156700
C	-0.02440600	1.56340300	2.80393400
H	-0.10374600	2.19975600	0.61028400
C	0.78151400	0.85272400	3.68667700
H	2.11664400	-0.80096700	3.92480200
H	-0.55344700	2.45210900	3.13774600
H	0.87659200	1.16396500	4.72294900
C	0.86845100	0.31073400	-1.39254900
H	0.23532600	1.18397800	-1.58827100
H	0.85476300	-0.33053400	-2.27655800
C	2.21741700	-1.90690800	1.46039100
H	2.10405800	-1.99933200	0.37739400
C	3.71008000	-1.69748500	1.74596700
H	4.30198900	-2.48313100	1.27048300
H	4.05451000	-0.74096100	1.34261000
H	3.92407300	-1.71930000	2.82167300
C	1.70740400	-3.19819100	2.11414600
H	1.83049400	-3.16540600	3.20347700
H	0.64566100	-3.36408700	1.90395600
H	2.27124500	-4.05892700	1.74017700
C	-1.56905900	-1.86509500	0.48484600
C	-1.78858700	-3.22960100	0.63102000
C	-2.77977500	-3.66861700	1.49581900
H	-1.20095200	-3.91858200	0.03598600
C	-3.28602300	-1.38175300	1.96026700
C	-3.54908800	-2.72531900	2.16751900
H	-2.96800900	-4.72916700	1.62380200
H	-3.88013100	-0.60841800	2.43384600
H	-4.35909100	-3.01755900	2.82471200
N	-2.30474900	-0.95574100	1.14834400
C	-1.23287800	3.61873000	-0.26958400
C	-3.52898500	3.55286200	-0.07758000
C	-3.20992100	4.42297000	-1.31068700
C	-1.71676100	4.76934600	-1.12269500
H	-3.93724700	4.16150500	0.74106000
H	-3.35385700	3.83138600	-2.21964900
H	-3.85367000	5.30054300	-1.37954500
H	-1.15062700	4.83042700	-2.05478100
H	-1.56918300	5.71054800	-0.58005200

N	-2.23046100	3.01801000	0.31759300
O	-0.01746300	3.23846600	-0.13624100
C	-4.50304900	2.38394700	-0.27954900
O	-5.52785500	2.54469700	-0.93217900
O	-4.18016500	1.27894500	0.31911200
Pd	-2.19281300	1.11991700	0.84080800
C	2.30212000	0.72515900	-1.12662600
O	3.19944400	-0.09907100	-0.97594700
N	2.53667600	2.05134500	-1.09432100
H	1.75494700	2.68781600	-0.97504100
C	3.88354500	2.51175100	-0.84971500
H	4.57127600	2.05354200	-1.56161700
H	3.91083000	3.59639500	-0.98615100
C	4.40217000	2.19202900	0.54607100
O	5.54101300	1.86264600	0.77928100
O	3.46735600	2.37191000	1.48158500
C	3.90686900	2.15691800	2.82508100
H	4.79685800	2.75397900	3.03544700
H	3.07331200	2.46066300	3.45557700
H	4.13487400	1.09988200	2.98213400
O	5.25519200	-1.88658000	-1.20586900
H	4.41011200	-1.40540600	-1.22208600
C	6.24426300	-0.96416100	-0.88555900
H	5.89899000	-0.16734500	-0.21597900
C	6.75280100	-0.26817900	-2.15361300
F	5.70712000	0.29821900	-2.79190200
F	7.62318600	0.70916600	-1.87231600
F	7.33405000	-1.11070400	-3.00946100
C	7.34792300	-1.71423100	-0.14208100
F	8.38718900	-0.91040500	0.12227500
F	6.87696300	-2.16631600	1.03086900
F	7.80042300	-2.76390300	-0.83045500
O	-6.68162100	0.09815300	-1.55544700
H	-6.33075200	0.98797100	-1.32821300
C	-5.90472600	-0.85569800	-0.91969800
H	-5.37351200	-0.45255600	-0.05160300
C	-4.82222700	-1.37207200	-1.87259700
F	-4.04928700	-0.34834800	-2.26783600
F	-4.01849600	-2.26835300	-1.26591400
F	-5.32280500	-1.95248700	-2.96432800
C	-6.82475300	-1.95955500	-0.40601600
F	-6.11947900	-2.92701500	0.22051700
F	-7.68052600	-1.45383300	0.49124600
F	-7.53486100	-2.54133400	-1.37310100

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C	-1.46025200	2.42026900	1.01063100
O	-2.10544500	2.66795200	2.01404400
N	-0.10308300	2.27649300	1.00645000
C	0.65128800	2.04739400	-0.19309800
C	1.17263700	3.12550300	-0.90989500
C	0.83237400	0.70980900	-0.59773000
C	1.87718500	2.82067500	-2.08525100
C	1.55154200	0.46461200	-1.77688800
H	1.25319900	-0.12466200	0.42785900
C	2.07270100	1.51775400	-2.51959600
H	2.28279800	3.63831800	-2.67501800
H	1.70280500	-0.55631600	-2.10885900
H	2.62676900	1.32284400	-3.43276200
C	0.53212300	2.05444300	2.30514000
H	0.44385400	0.99547700	2.57700600
H	-0.01351900	2.64441600	3.04345200
C	0.95973800	4.57378000	-0.50873600
H	0.54801200	4.57934200	0.50337400
C	2.27695500	5.35731900	-0.46320200
H	2.09447800	6.36427700	-0.07368200
H	2.99167800	4.86389300	0.19918800
H	2.72431100	5.46554900	-1.45876300
C	-0.04791200	5.24385700	-1.45434100
H	0.34141100	5.28402200	-2.47896500
H	-0.99847300	4.70109900	-1.48100800
H	-0.24804800	6.27140000	-1.13182800
C	-2.21662300	2.25040100	-0.29149700
C	-3.15286000	3.22164200	-0.62888900
C	-3.98537500	3.01490800	-1.71826800
H	-3.23362700	4.10576100	-0.00777500
C	-2.93709400	0.89285500	-2.02412600
C	-3.88094400	1.82235600	-2.42531900
H	-4.72380500	3.75961600	-1.99523800
H	-2.83806400	-0.06592700	-2.52019400
H	-4.53512400	1.59611100	-3.25855100
N	-2.10872700	1.10632400	-0.98846700
C	1.00062600	-1.98898300	1.15628800
C	-0.68864700	-3.31898100	0.33668700
C	-0.24782300	-3.93655400	1.68151600
C	1.10900800	-3.25493900	1.96783600
H	-0.41399200	-3.96423700	-0.50818900

H	-0.97869100	-3.68076600	2.45385400
H	-0.17926300	-5.02384200	1.63447100
H	1.28439100	-3.03090200	3.02240700
H	1.96234300	-3.83439100	1.60130400
N	0.06911900	-2.07604800	0.25471900
O	1.71582500	-0.92871000	1.30138600
C	-2.17979900	-2.98478400	0.18064100
O	-3.03008800	-3.77119700	0.58402900
O	-2.44020300	-1.86808800	-0.42449500
Pd	-0.88478100	-0.50243000	-0.44926400
C	1.98634300	2.50831000	2.30719800
O	2.29726200	3.68543600	2.22083500
N	2.89250000	1.50373600	2.46030700
H	2.58339000	0.54827800	2.31834900
C	4.29500200	1.77564200	2.34092900
H	4.47609400	2.81430000	2.62981400
H	4.87591500	1.13249200	3.00875500
C	4.80587000	1.56865700	0.92569900
O	4.10256200	1.27578300	-0.02046700
O	6.11834400	1.73609800	0.86535700
C	6.73631200	1.51193300	-0.40781000
H	6.30377600	2.17475900	-1.16095100
H	7.79117400	1.73675900	-0.26062000
H	6.60561500	0.47088100	-0.70964500
O	4.61596100	-0.88482700	-1.64317400
H	4.41201700	0.00018600	-1.28348100
C	4.02927600	-1.81339500	-0.79100600
H	3.18390400	-1.39567900	-0.23556900
C	5.03804400	-2.28462900	0.26360000
F	4.51195400	-3.21951700	1.06991500
F	6.15254100	-2.77541700	-0.27423100
F	5.39216700	-1.24234700	1.04220000
C	3.48959000	-2.97572900	-1.62914200
F	2.77822900	-3.82309500	-0.86097400
F	2.66684100	-2.52087600	-2.58319200
F	4.45649400	-3.67357500	-2.22332400
O	-5.48824900	-2.51055600	0.80724800
H	-4.65240300	-3.01882600	0.70613900
C	-5.30688100	-1.25909800	0.24253100
H	-4.46705400	-1.23553300	-0.45914100
C	-4.97119100	-0.23751600	1.33333400
F	-3.84348800	-0.60649700	1.96075500
F	-4.75676800	0.98754100	0.81302800
F	-5.93120400	-0.12318000	2.25294200

C	-6.55935500	-0.89640900	-0.55057200
F	-6.42694900	0.31121000	-1.14239900
F	-6.75235700	-1.79297600	-1.52587300
F	-7.66229700	-0.85706900	0.19907300

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C	-1.46025200	2.42026900	1.01063100
O	-2.10544500	2.66795200	2.01404400
N	-0.10308300	2.27649300	1.00645000
C	0.65128800	2.04739400	-0.19309800
C	1.17263700	3.12550300	-0.90989500
C	0.83237400	0.70980900	-0.59773000
C	1.87718500	2.82067500	-2.08525100
C	1.55154200	0.46461200	-1.77688800
H	1.25319900	-0.12466200	0.42785900
C	2.07270100	1.51775400	-2.51959600
H	2.28279800	3.63831800	-2.67501800
H	1.70280500	-0.55631600	-2.10885900
H	2.62676900	1.32284400	-3.43276200
C	0.53212300	2.05444300	2.30514000
H	0.44385400	0.99547700	2.57700600
H	-0.01351900	2.64441600	3.04345200
C	0.95973800	4.57378000	-0.50873600
H	0.54801200	4.57934200	0.50337400
C	2.27695500	5.35731900	-0.46320200
H	2.09447800	6.36427700	-0.07368200
H	2.99167800	4.86389300	0.19918800
H	2.72431100	5.46554900	-1.45876300
C	-0.04791200	5.24385700	-1.45434100
H	0.34141100	5.28402200	-2.47896500
H	-0.99847300	4.70109900	-1.48100800
H	-0.24804800	6.27140000	-1.13182800
C	-2.21662300	2.25040100	-0.29149700
C	-3.15286000	3.22164200	-0.62888900
C	-3.98537500	3.01490800	-1.71826800
H	-3.23362700	4.10576100	-0.00777500
C	-2.93709400	0.89285500	-2.02412600
C	-3.88094400	1.82235600	-2.42531900
H	-4.72380500	3.75961600	-1.99523800
H	-2.83806400	-0.06592700	-2.52019400
H	-4.53512400	1.59611100	-3.25855100
N	-2.10872700	1.10632400	-0.98846700
C	1.00062600	-1.98898300	1.15628800

C	-0.68864700	-3.31898100	0.33668700
C	-0.24782300	-3.93655400	1.68151600
C	1.10900800	-3.25493900	1.96783600
H	-0.41399200	-3.96423700	-0.50818900
H	-0.97869100	-3.68076600	2.45385400
H	-0.17926300	-5.02384200	1.63447100
H	1.28439100	-3.03090200	3.02240700
H	1.96234300	-3.83439100	1.60130400
N	0.06911900	-2.07604800	0.25471900
O	1.71582500	-0.92871000	1.30138600
C	-2.17979900	-2.98478400	0.18064100
O	-3.03008800	-3.77119700	0.58402900
O	-2.44020300	-1.86808800	-0.42449500
Pd	-0.88478100	-0.50243000	-0.44926400
C	1.98634300	2.50831000	2.30719800
O	2.29726200	3.68543600	2.22083500
N	2.89250000	1.50373600	2.46030700
H	2.58339000	0.54827800	2.31834900
C	4.29500200	1.77564200	2.34092900
H	4.47609400	2.81430000	2.62981400
H	4.87591500	1.13249200	3.00875500
C	4.80587000	1.56865700	0.92569900
O	4.10256200	1.27578300	-0.02046700
O	6.11834400	1.73609800	0.86535700
C	6.73631200	1.51193300	-0.40781000
H	6.30377600	2.17475900	-1.16095100
H	7.79117400	1.73675900	-0.26062000
H	6.60561500	0.47088100	-0.70964500
O	4.61596100	-0.88482700	-1.64317400
H	4.41201700	0.00018600	-1.28348100
C	4.02927600	-1.81339500	-0.79100600
H	3.18390400	-1.39567900	-0.23556900
C	5.03804400	-2.28462900	0.26360000
F	4.51195400	-3.21951700	1.06991500
F	6.15254100	-2.77541700	-0.27423100
F	5.39216700	-1.24234700	1.04220000
C	3.48959000	-2.97572900	-1.62914200
F	2.77822900	-3.82309500	-0.86097400
F	2.66684100	-2.52087600	-2.58319200
F	4.45649400	-3.67357500	-2.22332400
O	-5.48824900	-2.51055600	0.80724800
H	-4.65240300	-3.01882600	0.70613900
C	-5.30688100	-1.25909800	0.24253100
H	-4.46705400	-1.23553300	-0.45914100

C	-4.97119100	-0.23751600	1.33333400
F	-3.84348800	-0.60649700	1.96075500
F	-4.75676800	0.98754100	0.81302800
F	-5.93120400	-0.12318000	2.25294200
C	-6.55935500	-0.89640900	-0.55057200
F	-6.42694900	0.31121000	-1.14239900
F	-6.75235700	-1.79297600	-1.52587300
F	-7.66229700	-0.85706900	0.19907300

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C	1.29218100	-1.35985000	1.34063700
O	1.75548900	-1.57957700	2.44436900
N	0.22083900	-0.54016200	1.11605400
C	-0.37712100	-0.40970200	-0.18083500
C	-1.34229800	-1.32714400	-0.59972600
C	0.07222300	0.64528600	-1.00016200
C	-1.80099800	-1.19977800	-1.91985500
C	-0.44749100	0.74591300	-2.30045400
H	0.10353100	1.87408900	-0.39230100
C	-1.36411800	-0.18941700	-2.76827800
H	-2.53272000	-1.91497400	-2.28661400
H	-0.11809300	1.55904800	-2.94204400
H	-1.74847400	-0.12913200	-3.78246600
C	-0.09049400	0.43880500	2.14899700
H	0.46557700	1.36430200	1.95763800
H	0.25045300	0.02238600	3.09891700
C	-1.88325600	-2.43313100	0.28709700
H	-1.46347200	-2.28931100	1.28610500
C	-3.40692900	-2.32754900	0.42056200
H	-3.77571100	-3.08792100	1.11675800
H	-3.68895100	-1.35070800	0.81679900
H	-3.91485700	-2.48300500	-0.53822700
C	-1.46178100	-3.81393400	-0.23369900
H	-1.90895300	-4.02154000	-1.21338000
H	-0.37462800	-3.89200300	-0.34058000
H	-1.79615700	-4.59552700	0.45649000
C	1.97247700	-1.99511900	0.14662900
C	2.27691100	-3.34996100	0.20598300
C	3.06028400	-3.91434500	-0.78943800
H	1.92463600	-3.92649200	1.05307000
C	3.21584600	-1.75240700	-1.79086000
C	3.54753700	-3.09668100	-1.80282900
H	3.31061300	-4.96947000	-0.75976400

H	3.59680200	-1.06760500	-2.53997500
H	4.19666500	-3.48104900	-2.58030300
N	2.42851500	-1.21169400	-0.84666700
C	1.25578600	3.51309900	-0.17167000
C	3.42588500	3.51578800	-0.95001500
C	3.33100500	4.63251300	0.10922700
C	1.81005100	4.85376200	0.25532000
H	3.55080200	3.93522700	-1.95802500
H	3.75804400	4.27393300	1.05057500
H	3.87453100	5.53216400	-0.18158900
H	1.48827100	5.10517500	1.26833600
H	1.43284500	5.63174400	-0.41906200
N	2.13563500	2.84034700	-0.86097800
O	0.09359400	3.05580200	0.10781600
C	4.53805200	2.47408300	-0.76688500
O	5.66292300	2.83118800	-0.43399800
O	4.20340000	1.24932700	-1.03041300
Pd	2.17489600	0.87337100	-0.94592900
C	-1.58353800	0.70921800	2.26082800
O	-2.38619800	-0.15758200	2.56584300
N	-1.93514000	2.00890200	2.05895900
H	-1.29216800	2.61616500	1.56202200
C	-3.31793100	2.38426600	2.15363700
H	-3.76501900	1.90727100	3.02917400
H	-3.39850500	3.46658100	2.28990300
C	-4.19590500	2.01313300	0.96937500
O	-5.40094700	2.17673100	1.00789600
O	-3.52269900	1.55574600	-0.07070300
C	-4.28759000	1.21400200	-1.23440300
H	-4.97238700	2.02359600	-1.49386400
H	-3.55256500	1.06110000	-2.02033300
H	-4.85359500	0.29915000	-1.05511300
O	-7.36750700	1.03159100	-0.53478500
H	-6.72715600	1.48727700	0.04873000
C	-8.04337000	0.05935900	0.18395200
H	-8.43313000	0.41941800	1.14643400
C	-7.11440700	-1.12060600	0.50386700
F	-6.11877700	-0.68447900	1.29581000
F	-7.74497700	-2.10642200	1.14811700
F	-6.55290800	-1.63324900	-0.59892600
C	-9.25672400	-0.35141700	-0.65334000
F	-9.99467700	-1.26510300	-0.00669500
F	-10.02986500	0.71362300	-0.88074600
F	-8.89951400	-0.86674100	-1.83253900

O	7.11694900	0.68804200	0.53805100
H	6.66739700	1.47562300	0.15877500
C	6.36746500	-0.43438000	0.22700500
H	5.65583900	-0.25001300	-0.58413200
C	5.52716900	-0.84462200	1.43992700
F	4.64821000	0.12979000	1.72697100
F	4.81692600	-1.96353400	1.19297600
F	6.26247600	-1.06456900	2.52963900
C	7.30837700	-1.53842700	-0.24950800
F	6.61497900	-2.62901700	-0.64342400
F	8.00576400	-1.11199900	-1.30862100
F	8.17486700	-1.93018600	0.68744800

S-TS3-iso7

C	0.09897100	-1.44533500	-0.19876000
O	-0.57026100	-1.71826800	-1.19092500
N	1.45080400	-1.39368000	-0.23100100
C	2.26683800	-1.22009900	0.93832200
C	2.65402800	-2.32577600	1.69745500
C	2.66897900	0.09440800	1.24197900
C	3.47368700	-2.06353300	2.80723900
C	3.50217600	0.29469400	2.35207800
H	3.07235400	0.84316000	0.18127000
C	3.90459100	-0.78395600	3.13264300
H	3.78712400	-2.89663400	3.43048100
H	3.83275500	1.30175200	2.59163000
H	4.54724300	-0.63266500	3.99467200
C	2.09992800	-1.31327000	-1.54424500
H	2.17705800	-0.26079700	-1.83931400
H	1.46565200	-1.83790200	-2.25909900
C	2.19961400	-3.74465100	1.40353300
H	1.73364900	-3.74556300	0.41472100
C	3.37522000	-4.72738200	1.34063700
H	3.00929500	-5.71683800	1.04752700
H	4.10514800	-4.40366400	0.59553900
H	3.87092500	-4.83597800	2.31283400
C	1.16171300	-4.19726200	2.44160100
H	1.60759300	-4.25451900	3.44199200
H	0.31286100	-3.50793800	2.49402000
H	0.77888700	-5.19133900	2.18785100
C	-0.62065600	-1.12607800	1.09436300
C	-1.68740300	-1.93779400	1.46294300
C	-2.45081700	-1.59433600	2.57083300

H	-1.93751800	-2.80178300	0.85695000
C	-1.07313900	0.33749100	2.83123700
C	-2.13631000	-0.43600500	3.26881500
H	-3.29591800	-2.20801700	2.85952500
H	-0.81984200	1.27456200	3.31359000
H	-2.71746000	-0.11245900	4.12428400
N	-0.32119300	-0.00114200	1.77175700
C	2.97377600	2.70113800	-0.59680100
C	1.47587800	4.22737600	0.27657000
C	1.84449300	4.71751600	-1.14028100
C	3.12942100	3.92677700	-1.46753500
H	1.87694800	4.90068300	1.04646400
H	1.04388600	4.44666800	-1.83507900
H	1.97556000	5.79915700	-1.18750700
H	3.23224200	3.64747800	-2.51793900
H	4.03991400	4.46261400	-1.17459900
N	2.12453100	2.92471900	0.37495000
O	3.54989900	1.57794100	-0.76793300
C	-0.02068100	4.05952800	0.56798500
O	-0.81027700	4.93941800	0.24384800
O	-0.35645300	2.96850100	1.18842600
Pd	1.05551000	1.46949500	1.15285400
C	3.46410500	-1.99148100	-1.51956000
O	3.57374000	-3.20619200	-1.42018200
N	4.52745100	-1.16444800	-1.61599900
H	4.42992700	-0.15309900	-1.63166200
C	5.85800200	-1.71039000	-1.55965400
H	6.05262500	-2.18926300	-0.59136100
H	5.99019300	-2.48918100	-2.31888000
C	6.87102600	-0.61037800	-1.78157300
O	6.59722700	0.55195800	-1.96326300
O	8.11227000	-1.09933000	-1.74435900
C	9.15496700	-0.14235400	-1.94529200
H	9.12288000	0.62540700	-1.16869400
H	10.08520100	-0.70595100	-1.88872300
H	9.05232600	0.33326100	-2.92347400
O	-2.98824500	-3.00968300	-1.31362700
H	-2.14896400	-2.52291700	-1.43005400
C	-3.99178700	-2.07857800	-1.07369500
H	-3.65453900	-1.22734600	-0.47316900
C	-5.07977600	-2.78358600	-0.26756900
F	-4.57212600	-3.18954600	0.91611200
F	-6.10001000	-1.96038800	-0.00351800
F	-5.55846900	-3.86296300	-0.88311500

C	-4.51535600	-1.49358700	-2.39192100
F	-5.37892800	-0.49542400	-2.16886200
F	-3.48264100	-1.00404800	-3.09034600
F	-5.12571600	-2.40856000	-3.15120200
O	-3.35067200	3.89080100	-0.10074200
H	-2.50696700	4.36607400	0.07200500
C	-3.12935900	2.54648500	0.14464600
H	-2.36686800	2.38112000	0.91283900
C	-2.60871000	1.85021500	-1.11728900
F	-1.52687100	2.49320400	-1.58357100
F	-2.21905900	0.58343200	-0.84431400
F	-3.50512500	1.79559200	-2.09984500
C	-4.42563900	1.93492800	0.66705300
F	-4.26745400	0.60842900	0.90100100
F	-4.75175100	2.49703600	1.83638900
F	-5.45221400	2.07739900	-0.16565500

S-TS3-iso8

C	-0.35917400	-1.26981700	-0.17472200
O	0.20616800	-1.80098100	0.77649700
N	-1.69162000	-1.03240800	-0.17960700
C	-2.41071400	-0.55475200	-1.32756500
C	-2.91856900	-1.45966300	-2.26105900
C	-2.59658900	0.83754300	-1.43239000
C	-3.62904800	-0.91028100	-3.34059300
C	-3.32721200	1.32822100	-2.52472000
H	-2.98500300	1.46816300	-0.27932000
C	-3.84393300	0.45486200	-3.47598100
H	-4.02939600	-1.58201500	-4.09476600
H	-3.48959500	2.39872700	-2.61701700
H	-4.40783200	0.83233500	-4.32351000
C	-2.39742000	-1.11116300	1.10543000
H	-2.31941900	-0.14086000	1.61015200
H	-1.89929600	-1.86631100	1.71308900
C	-2.69719200	-2.95986200	-2.17733500
H	-2.30412200	-3.18228000	-1.18182300
C	-4.00398900	-3.74853000	-2.32531100
H	-3.80715200	-4.81479500	-2.17464500
H	-4.73187800	-3.43326700	-1.57458800
H	-4.44242900	-3.63385200	-3.32388500
C	-1.66601600	-3.40551800	-3.22505400
H	-2.03881800	-3.22973800	-4.24138200
H	-0.71897300	-2.86657100	-3.11874300

H	-1.46234100	-4.47647300	-3.12244200
C	0.47241500	-0.84457700	-1.36612000
C	1.43857300	-1.72798800	-1.83410800
C	2.30248500	-1.31762800	-2.84109200
H	1.53647200	-2.70661700	-1.37732100
C	1.21951400	0.80885800	-2.80635400
C	2.18893300	-0.02607400	-3.33801600
H	3.06980600	-1.99039900	-3.20508100
H	1.12345100	1.84022600	-3.12568800
H	2.85669400	0.34814800	-4.10498200
N	0.36936500	0.40910200	-1.84707300
C	-2.68899600	3.14630600	0.79725100
C	-0.93545600	4.54888600	0.26814800
C	-1.33554900	4.86141700	1.72567100
C	-2.73750500	4.22641900	1.85387300
H	-1.19095100	5.38125100	-0.40169700
H	-0.63176700	4.37243800	2.40577000
H	-1.32096900	5.93018200	1.94197800
H	-2.94826600	3.79958400	2.83667100
H	-3.54151000	4.93233200	1.61442800
N	-1.74394800	3.38349900	-0.07264700
O	-3.43579400	2.11035200	0.74039300
C	0.54236700	4.21720500	0.02232500
O	1.41593000	4.91057300	0.53068300
O	0.77015900	3.20637000	-0.76050500
Pd	-0.83109500	1.93380800	-1.03905600
C	-3.85110000	-1.52822800	0.91303400
O	-4.16195200	-2.68425900	0.66920800
N	-4.75539900	-0.52600000	1.01210700
H	-4.45303100	0.41331500	1.23574100
C	-6.15677900	-0.80101800	0.84259600
H	-6.68783100	0.14501300	0.70629100
H	-6.31916000	-1.40527300	-0.05401700
C	-6.82485600	-1.54599600	1.99267000
O	-7.92197600	-2.03832000	1.89494600
O	-6.08427000	-1.55604400	3.10256200
C	-6.65255900	-2.26376300	4.20511500
H	-6.82851900	-3.30794400	3.93683700
H	-5.91853200	-2.19392700	5.00703100
H	-7.59825200	-1.80692500	4.50682700
O	2.41884300	-3.42457600	0.75463000
H	1.63759200	-2.86358000	0.92571600
C	3.53954200	-2.60205600	0.76713400
H	3.35036100	-1.61236000	0.33891200

C	4.59886200	-3.26453800	-0.10972100
F	4.14977400	-3.33881900	-1.38077400
F	5.73127800	-2.55375100	-0.12649900
F	4.88588500	-4.50483300	0.28074900
C	4.02056100	-2.36432000	2.20446600
F	5.00036800	-1.45347700	2.24290600
F	2.99545300	-1.90453500	2.93429500
F	4.46892700	-3.48119900	2.78566600
O	3.76453000	3.46722900	0.84139300
H	3.01567400	4.08889500	0.70284700
C	3.37121700	2.23164900	0.35552300
H	2.65057300	2.31510900	-0.46445100
C	2.66388300	1.42840000	1.45232800
F	1.64486200	2.14212500	1.95769500
F	2.12906300	0.29085400	0.95152400
F	3.46290100	1.09014600	2.46125100
C	4.59801600	1.51945600	-0.20547900
F	4.25663700	0.30260800	-0.69816800
F	5.10188300	2.22182500	-1.22565600
F	5.56193000	1.33455300	0.69168600

S-TS4-iso1

C	0.37670600	0.69834100	0.15071800
O	0.69355200	1.49850900	-0.72314400
N	-0.72767300	-0.08232000	0.04969900
C	-1.22500500	-0.88492700	1.13441100
C	-2.05432400	-0.31618900	2.09882200
C	-0.84196300	-2.24012800	1.15748200
C	-2.47595900	-1.16056600	3.13840400
C	-1.31321900	-3.04160900	2.20767800
H	-0.97157500	-2.91487100	-0.03936300
C	-2.12427000	-2.50089700	3.19920400
H	-3.11638600	-0.74973400	3.91400200
H	-1.04028300	-4.09313300	2.23552500
H	-2.48800200	-3.12012000	4.01313900
C	-1.29437900	-0.26909300	-1.28464000
H	-0.81546700	-1.13146300	-1.76231100
H	-1.06929600	0.62465800	-1.86879200
C	-2.49188600	1.13653800	2.07462000
H	-2.20427000	1.55273900	1.10530400
C	-4.01537200	1.26442800	2.18612700
H	-4.33092800	2.28565900	1.95920800
H	-4.50523500	0.59545300	1.47466500

H	-4.37228300	1.01884900	3.19358900
C	-1.78904600	1.94027300	3.17729600
H	-2.06532500	1.56758700	4.17090000
H	-0.69956300	1.87823400	3.08931800
H	-2.07722800	2.99509000	3.12088800
C	1.27642800	0.54241100	1.35718400
C	1.79140900	1.69244100	1.94320500
C	2.73286100	1.57356900	2.95763400
H	1.48982200	2.66521200	1.57033600
C	2.60544000	-0.79604800	2.69975600
C	3.14623300	0.30565000	3.34356100
H	3.15722600	2.46136800	3.41089000
H	2.93032900	-1.80340300	2.93353400
H	3.89692700	0.16215600	4.11172300
N	1.68175900	-0.68653600	1.73208100
C	0.00303700	-4.22301200	-1.21601900
C	2.18315100	-4.80729900	-0.74811600
C	1.93978100	-5.14026300	-2.23455000
C	0.39996000	-5.14043400	-2.34983200
H	2.29216000	-5.72203500	-0.14959900
H	2.36854500	-4.34876200	-2.85648200
H	2.39855400	-6.08380100	-2.53172800
H	0.02079500	-4.76817300	-3.30413700
H	-0.03449200	-6.13301400	-2.18138400
N	0.96795000	-4.10591400	-0.34660100
O	-1.11293600	-3.60402700	-1.10053100
C	3.39691500	-3.92236400	-0.43216500
O	4.47441600	-4.15301700	-0.96980800
O	3.19559300	-2.98022800	0.43661400
Pd	1.21125100	-2.49690100	0.76051500
C	-2.80177900	-0.44158900	-1.23464600
O	-3.54688700	0.46917500	-0.88262400
N	-3.26872200	-1.64302400	-1.62615700
H	-2.62313400	-2.42255800	-1.69989600
C	-4.68403600	-1.90245200	-1.53913700
H	-5.24180200	-1.14481200	-2.09279600
H	-4.89263700	-2.87604000	-1.99070300
C	-5.15443600	-1.92633400	-0.08773800
O	-4.47449000	-2.25059500	0.85306900
O	-6.43366600	-1.54672800	-0.00798700
C	-6.99608700	-1.49415200	1.30742900
H	-6.38987700	-0.85199700	1.95067400
H	-7.98996100	-1.07014900	1.17737900
H	-7.04983300	-2.49614100	1.73896600

O	2.07209500	3.86541800	-0.44773700
H	1.61159300	3.04672900	-0.71403000
C	3.43560600	3.59714200	-0.40479500
H	3.66410400	2.58574600	-0.05348200
C	4.05518400	4.56422900	0.60092100
F	3.51833000	4.35022800	1.82145800
F	5.37482800	4.37446800	0.70619000
F	3.83625900	5.84032400	0.29124700
C	4.05257400	3.71566800	-1.80422500
F	5.33386900	3.32911000	-1.80321500
F	3.37678200	2.91811000	-2.64254700
F	3.99331800	4.96002500	-2.28647300
O	6.04781700	-1.87072700	-1.01041000
H	5.60006600	-2.74572300	-0.97088000
C	5.20343700	-0.94248600	-0.42642800
H	4.57198600	-1.38174100	0.35261000
C	4.23930500	-0.36603700	-1.46849700
F	3.56988500	-1.35910300	-2.07567500
F	3.31037400	0.42520800	-0.88307200
F	4.84579800	0.35112300	-2.41102900
C	6.05451200	0.13038400	0.24650400
F	5.26537900	1.06700200	0.82981500
F	6.78787300	-0.41816900	1.22077100
F	6.87400600	0.75916000	-0.59085500
O	-5.26681700	2.58830800	-0.62964500
H	-4.46396200	2.05337600	-0.75452500
C	-6.33892800	1.70905800	-0.67747500
H	-6.07498100	0.69940000	-0.34903400
C	-6.85257400	1.55957800	-2.11483700
F	-5.82734100	1.19913200	-2.90860100
F	-7.78189200	0.59614200	-2.20622200
F	-7.37102700	2.68680900	-2.60242100
C	-7.40969200	2.21261500	0.28834300
F	-8.52354300	1.46222200	0.20593500
F	-6.96348100	2.11813700	1.55127700
F	-7.74644600	3.48008100	0.06453500

S-TS4-iso2

C	0.30483900	0.66818600	0.18332600
O	0.58625500	1.49548700	-0.67589000
N	-0.77114400	-0.15259700	0.07124700
C	-1.23426300	-0.98396000	1.14752900
C	-2.06146700	-0.44919800	2.13603600

C	-0.81236100	-2.32708600	1.14690300
C	-2.40262900	-1.30671400	3.19398300
C	-1.21508300	-3.14829000	2.21093500
H	-0.92619700	-2.98214700	-0.05801300
C	-1.99091600	-2.63241600	3.24351300
H	-3.02097200	-0.91754200	3.99850900
H	-0.90622900	-4.19016000	2.22370600
H	-2.28206300	-3.25858200	4.08192600
C	-1.32009300	-0.35745800	-1.26561300
H	-0.82386200	-1.21392300	-1.73547400
H	-1.10283500	0.53695300	-1.85245300
C	-2.57780200	0.97798100	2.12187000
H	-2.33275400	1.40967000	1.14828600
C	-4.10518100	1.01781600	2.26243400
H	-4.47896900	2.02503600	2.06492800
H	-4.58070900	0.34663200	1.54141600
H	-4.42816300	0.73113000	3.27066200
C	-1.90232800	1.82105600	3.21204900
H	-2.12819300	1.42884300	4.21087600
H	-0.81351800	1.83372200	3.09696200
H	-2.26310600	2.85356900	3.16693100
C	1.22118600	0.51747200	1.37757900
C	1.70388000	1.67136200	1.98285300
C	2.66329600	1.56283000	2.98158400
H	1.36366600	2.64086600	1.63535100
C	2.61613900	-0.80354600	2.66944200
C	3.12695900	0.30185500	3.33129700
H	3.06345800	2.45455100	3.44892900
H	2.98207000	-1.80319500	2.87393400
H	3.89376400	0.16759400	4.08506800
N	1.67443400	-0.70514800	1.71801700
C	0.06897600	-4.24118600	-1.27338200
C	2.27258800	-4.76601900	-0.84070800
C	2.02170600	-5.07961800	-2.33010400
C	0.48124000	-5.12726700	-2.42678000
H	2.41743100	-5.68781500	-0.26098400
H	2.41698700	-4.26370900	-2.94261500
H	2.50613800	-6.00256300	-2.65022600
H	0.07861400	-4.75213800	-3.37021700
H	0.08071400	-6.13576400	-2.26935100
N	1.04136900	-4.11003900	-0.41272900
O	-1.06293500	-3.65838900	-1.13534800
C	3.46106600	-3.84965000	-0.52086600
O	4.54167000	-4.03754800	-1.06679300

O	3.23686600	-2.92640400	0.36481900
Pd	1.24846500	-2.51233000	0.71566800
C	-2.82380200	-0.54699500	-1.23213800
O	-3.57908500	0.33096800	-0.82557100
N	-3.28200600	-1.72028600	-1.70710000
H	-2.63997000	-2.49921200	-1.80878200
C	-4.70824500	-1.94847700	-1.73170700
H	-5.20665000	-1.14297300	-2.27317200
H	-4.90002200	-2.89130100	-2.25109000
C	-5.34947500	-2.02288300	-0.35232800
O	-6.44325900	-1.57634300	-0.10074400
O	-4.58948200	-2.68407100	0.52356100
C	-5.17325100	-2.85148100	1.81853200
H	-6.15684600	-3.31851200	1.73349800
H	-4.48373800	-3.48859500	2.36879400
H	-5.27495800	-1.88320100	2.31473700
O	1.89623900	3.90401200	-0.36799700
H	1.45008400	3.08389900	-0.65164000
C	3.26503700	3.66079300	-0.34554500
H	3.51579800	2.64745600	-0.01519400
C	3.87877500	4.62109900	0.67028300
F	3.35342500	4.38156400	1.89109400
F	5.20136700	4.44666600	0.76342000
F	3.64124800	5.89843900	0.38108500
C	3.86373400	3.81573300	-1.74940800
F	5.15449300	3.46271800	-1.76767100
F	3.19940100	3.01302000	-2.59232000
F	3.76649700	5.06473800	-2.21198800
O	6.05173100	-1.70353200	-1.07964700
H	5.63339300	-2.59280000	-1.05701100
C	5.17948000	-0.81743400	-0.47132100
H	4.57010500	-1.29459200	0.30276900
C	4.18758500	-0.25529100	-1.49503200
F	3.55430000	-1.26015200	-2.12176200
F	3.23111900	0.48426400	-0.88643400
F	4.75952000	0.50669200	-2.42322400
C	5.99636300	0.27131500	0.21821700
F	5.17766800	1.16843000	0.82225100
F	6.75236400	-0.27019500	1.17910300
F	6.78973600	0.94327200	-0.61015400
O	-5.19619000	2.50647900	-0.48227500
H	-4.45429400	1.89659300	-0.63323400
C	-6.36366500	1.76091400	-0.59958000
H	-6.25342500	0.72303400	-0.26370800

C	-6.80251000	1.69082200	-2.06699000
F	-5.78548600	1.19357600	-2.80223700
F	-7.85042500	0.87569900	-2.23680500
F	-7.11541700	2.88484000	-2.57238000
C	-7.41236500	2.40440200	0.30544600
F	-8.60442400	1.80839700	0.16443400
F	-7.04304900	2.27267400	1.58961700
F	-7.56696900	3.70597700	0.05756500

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C	-0.54792000	-0.87536500	0.02168000
O	-0.97757200	-1.55223800	-0.90811500
N	0.64864500	-0.24142100	-0.04615200
C	1.24817100	0.45673400	1.06042600
C	2.05885300	-0.23326100	1.96056500
C	0.99156300	1.83906900	1.16345900
C	2.60920300	0.51973900	3.00977400
C	1.58467400	2.54141800	2.22348300
H	1.13331200	2.57227500	-0.00481100
C	2.39067900	1.88274200	3.14447700
H	3.24406600	0.01662200	3.73283000
H	1.41106400	3.61036900	2.31363700
H	2.85292300	2.42597400	3.96262900
C	1.20441300	-0.04765600	-1.38638000
H	0.74548700	0.84061000	-1.83621400
H	0.93390200	-0.91631800	-1.98864200
C	2.32440500	-1.72566000	1.86783900
H	2.08207700	-2.03776500	0.84801400
C	3.79609300	-2.07320100	2.11564700
H	3.97744000	-3.12031300	1.85281000
H	4.46677400	-1.45023900	1.52236100
H	4.06856700	-1.95732900	3.17142900
C	1.42688100	-2.49848100	2.84562300
H	1.65218000	-2.21917300	3.88202400
H	0.36496800	-2.30257000	2.67310500
H	1.59485300	-3.57582600	2.74290400
C	-1.41167000	-0.71730500	1.25400300
C	-2.06068300	-1.84537700	1.74327800
C	-2.97226500	-1.70781700	2.78125100
H	-1.88116000	-2.80936400	1.28006900
C	-2.55357500	0.64146200	2.74094600
C	-3.21975100	-0.44050900	3.29279200
H	-3.49959100	-2.57583800	3.15862400

H	-2.74902400	1.65487400	3.07179400
H	-3.94011000	-0.27857700	4.08591000
N	-1.66192300	0.51032600	1.74524200
C	0.24113000	4.05459100	-1.03541200
C	-1.83920400	4.82251400	-0.41062300
C	-1.63104000	5.24142600	-1.88106000
C	-0.10754900	5.08830900	-2.08126300
H	-1.82742000	5.69502900	0.25681000
H	-2.17414600	4.55079100	-2.53300600
H	-1.99722400	6.24844800	-2.08340600
H	0.18198800	4.74995600	-3.07857900
H	0.43840700	6.01554500	-1.87042900
N	-0.68621600	3.97541800	-0.12316600
O	1.28786000	3.31571800	-1.02320700
C	-3.12178800	4.04041800	-0.09658000
O	-4.19268200	4.42050100	-0.55802800
O	-2.98076300	3.01717700	0.68711400
Pd	-1.04021700	2.32136900	0.88300200
C	2.72134400	0.06697200	-1.38511700
O	3.42402500	-0.90600200	-1.10436500
N	3.19383000	1.26062500	-1.78626700
H	2.54916300	2.04417000	-1.80448300
C	4.60186100	1.55818300	-1.81643900
H	5.15292500	0.72979000	-2.26658600
H	4.77078100	2.43907600	-2.44050000
C	5.17431500	1.80257600	-0.42506300
O	4.54140400	1.73989100	0.59964800
O	6.47217900	2.07920600	-0.51948600
C	7.19345200	2.08001900	0.71416100
H	7.14025900	1.08620000	1.16198000
H	8.22176800	2.32507400	0.45173500
H	6.78270800	2.82324600	1.40148900
O	-2.59547800	-3.77419600	-0.81156700
H	-2.06964200	-2.97525200	-1.00982700
C	-3.92691000	-3.39680200	-0.68151600
H	-4.05240300	-2.41383200	-0.21604000
C	-4.59308900	-4.40960100	0.24622300
F	-4.02064000	-4.34444900	1.46798600
F	-5.89490700	-4.14517500	0.40060000
F	-4.46527700	-5.66295000	-0.18323400
C	-4.60339400	-3.30750000	-2.05549800
F	-5.83016400	-2.78186600	-1.95650500
F	-3.87157000	-2.51286700	-2.84776500
F	-4.70840300	-4.49803500	-2.65393300

O	-6.00057900	2.33139800	-0.64741600
H	-5.44822300	3.14314600	-0.57766700
C	-5.24189500	1.26536200	-0.19723700
H	-4.52682500	1.55638800	0.57927300
C	-4.40345600	0.68292600	-1.34058200
F	-3.67497700	1.65178100	-1.91653100
F	-3.52656000	-0.23810500	-0.87681800
F	-5.13361300	0.10334700	-2.29069100
C	-6.18341200	0.23840400	0.42506000
F	-5.49215500	-0.84879200	0.84913100
F	-6.77686100	0.76314900	1.50307700
F	-7.12895000	-0.18541200	-0.40770700
O	5.94670900	-0.85688600	-0.18640200
H	5.03655000	-0.92345800	-0.55790800
C	6.74389800	-1.88586500	-0.65852800
H	6.17049200	-2.75565300	-1.00212700
C	7.61672000	-2.35963800	0.50732300
F	6.84563100	-2.90191900	1.45720300
F	8.49620700	-3.28920000	0.11313800
F	8.29885700	-1.35047000	1.05893600
C	7.56695600	-1.39164500	-1.85477400
F	8.30738700	-2.36793500	-2.39077300
F	6.72591700	-0.95337600	-2.81147800
F	8.37450500	-0.38143200	-1.52818300

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C	-1.25495500	2.10735900	1.06251800
O	-2.18148600	1.81995300	1.81664700
N	0.04924400	1.88620000	1.34540900
C	1.09637300	2.21171900	0.40876800
C	1.75210000	3.44008400	0.48447700
C	1.40218300	1.24220400	-0.56969200
C	2.73112700	3.69016000	-0.49164500
C	2.39738200	1.54410600	-1.50920300
H	1.55272600	-0.02348700	-0.05181800
C	3.05757100	2.76766600	-1.47360600
H	3.24917900	4.64514500	-0.47286000
H	2.65847200	0.81224600	-2.26461400
H	3.82450000	2.99840000	-2.20662700
C	0.34612900	1.01732900	2.49102900
H	0.16577900	-0.02527400	2.21549000
H	-0.33741600	1.27408100	3.30098900
C	1.42144200	4.51185800	1.50811700

H	0.75680200	4.06742000	2.25352900
C	2.67024300	5.00104600	2.25229400
H	2.37710800	5.70249700	3.04032700
H	3.19059500	4.16346300	2.72063000
H	3.36136700	5.52878800	1.58408500
C	0.69531800	5.68590000	0.83449400
H	1.34795200	6.18723900	0.10962000
H	-0.20096000	5.35484400	0.30082400
H	0.39600600	6.42714900	1.58322200
C	-1.60976500	2.76573000	-0.25153800
C	-2.37514100	3.92359000	-0.23201900
C	-2.78253900	4.48254100	-1.43609100
H	-2.64835700	4.35969600	0.72157300
C	-1.71678800	2.66516000	-2.56130500
C	-2.44762300	3.84135200	-2.62146400
H	-3.37125000	5.39375100	-1.44595300
H	-1.47049500	2.10182100	-3.45326700
H	-2.76795600	4.22353900	-3.58331300
N	-1.29012700	2.14696600	-1.40109500
C	1.12464200	-1.97577800	-0.39490600
C	-0.31194300	-2.53994800	-2.10473400
C	-0.17081000	-3.79448800	-1.21321500
C	1.03654500	-3.47621000	-0.30248400
H	0.12683300	-2.69784400	-3.09846900
H	-1.07893200	-3.92135900	-0.62118200
H	-0.02807200	-4.70150000	-1.80145900
H	0.90098900	-3.78720400	0.73483800
H	1.97449800	-3.90631700	-0.66670300
N	0.45004400	-1.51316600	-1.40476400
O	1.78315700	-1.20494900	0.39593200
C	-1.73330200	-1.99747300	-2.32029900
O	-2.67517500	-2.76966300	-2.47094200
O	-1.84037800	-0.70491900	-2.35328500
Pd	-0.28021200	0.31311100	-1.45393800
C	1.76404800	1.22483500	3.00702700
O	2.09549800	2.24862000	3.58399400
N	2.59434900	0.16544600	2.82191300
H	2.31325500	-0.56319000	2.17422000
C	3.98688200	0.27696000	3.14460800
H	4.10450000	1.01789200	3.93964700
H	4.37972200	-0.67661400	3.51068700
C	4.82168000	0.70511200	1.95027400
O	4.36595000	0.95777300	0.85296400
O	6.10811300	0.75552600	2.26008000

C	7.00860200	1.10569800	1.20188700
H	6.73535200	2.07447300	0.77710200
H	7.99280300	1.15497100	1.66417900
H	6.98795400	0.34065700	0.42361800
O	-2.33006500	-0.40341000	3.43724600
H	-2.44221900	0.38584300	2.87078700
C	-2.93385900	-1.50410600	2.84990400
H	-3.93612900	-1.30031100	2.45834900
C	-3.08533900	-2.56723700	3.93869700
F	-3.87729200	-2.10845300	4.90986600
F	-3.63957000	-3.68169000	3.44208400
F	-1.90844200	-2.89717800	4.48035000
C	-2.09696500	-1.99685400	1.66381100
F	-2.61500200	-3.06808600	1.06414600
F	-2.01896200	-1.01106600	0.74459400
F	-0.83317700	-2.29321200	2.01537200
O	-5.04959800	-1.37678900	-2.31272000
H	-4.24916200	-1.92552300	-2.47643900
C	-4.70159100	-0.39391700	-1.40379500
H	-3.62925000	-0.38169200	-1.18761500
C	-5.41873700	-0.63688000	-0.07503500
F	-5.11148700	-1.86299500	0.38187400
F	-5.02031200	0.24230900	0.86937400
F	-6.74628500	-0.55730900	-0.16699200
C	-5.02305300	0.97551400	-2.00073900
F	-4.67698700	1.96780100	-1.15271800
F	-4.32663200	1.16047300	-3.13113100
F	-6.31628000	1.13002400	-2.29180900
O	5.24676300	-0.15029000	-1.50598700
H	4.98401400	0.45203800	-0.78363500
C	4.51005100	-1.31858400	-1.34079700
H	3.57985000	-1.15070800	-0.78871200
C	5.30875000	-2.34085500	-0.52347800
F	5.54511900	-1.83983900	0.70614100
F	4.62818100	-3.48537400	-0.36009700
F	6.48824000	-2.62963200	-1.06951000
C	4.12530900	-1.85337200	-2.72239500
F	3.31671700	-2.92359300	-2.61066900
F	3.45259700	-0.92153200	-3.41259800
F	5.18391300	-2.21201300	-3.44698300

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C	-1.04264800	-1.44927100	-0.27423600

O	-1.84036800	-1.79312700	-1.13972800
N	0.29048400	-1.36363400	-0.50353100
C	1.26133200	-1.20502400	0.54481400
C	1.69785700	-2.31223300	1.27090600
C	1.73541400	0.10009300	0.78478400
C	2.64621300	-2.06511200	2.27665000
C	2.69925100	0.28363200	1.78850600
H	2.15910600	0.83013700	-0.34061200
C	3.15849800	-0.80113200	2.52852000
H	3.00526100	-2.90258800	2.86822100
H	3.10371400	1.27612100	1.96653300
H	3.91438500	-0.66209200	3.29405200
C	0.74500600	-1.25744000	-1.88671400
H	0.93423500	-0.20274800	-2.11933200
H	-0.06313600	-1.61842500	-2.52466000
C	1.17554200	-3.72138400	1.05493400
H	0.56996900	-3.71955800	0.14496000
C	2.31288800	-4.72506300	0.82641600
H	1.89307000	-5.71305600	0.61133800
H	2.92438800	-4.42274700	-0.02611900
H	2.95374200	-4.82294300	1.71094700
C	0.29343900	-4.15039400	2.23685700
H	0.87801600	-4.21361300	3.16270800
H	-0.52419700	-3.44272500	2.40868100
H	-0.14316500	-5.13673700	2.04819800
C	-1.57121300	-1.04404100	1.08421100
C	-2.60006700	-1.79508900	1.64025600
C	-3.19792500	-1.36169300	2.81679200
H	-2.95331000	-2.68241200	1.12618300
C	-1.74179800	0.52905700	2.77461100
C	-2.75796200	-0.17910600	3.39612400
H	-4.01432400	-1.92608600	3.25130600
H	-1.39524700	1.47873500	3.16566800
H	-3.20703800	0.21254800	4.30114400
N	-1.15201200	0.10683400	1.64532700
C	2.00992300	2.67199800	-1.12428000
C	0.55844900	4.21717100	-0.24023400
C	0.88320100	4.68151700	-1.67426200
C	2.14963000	3.86889900	-2.03121600
H	1.02102400	4.87699700	0.50618400
H	0.05643300	4.41140700	-2.33787200
H	1.02918200	5.75983200	-1.74189900
H	2.20942300	3.56502500	-3.07859200
H	3.07615000	4.40184500	-1.78467500

N	1.18019400	2.89901200	-0.15722600
O	2.62102800	1.53609700	-1.25977300
C	-0.92197700	4.08416000	0.14439800
O	-1.71967100	4.95104100	-0.19410800
O	-1.21777400	3.04420500	0.86017800
Pd	0.17255400	1.50346800	0.79112300
C	1.97611400	-2.11462800	-2.14222400
O	1.95446100	-3.32761000	-2.01723900
N	3.08002500	-1.43404700	-2.55820400
H	3.12234500	-0.43439600	-2.40514900
C	4.31906100	-2.15620800	-2.67265700
H	4.15551100	-3.08489200	-3.22268700
H	5.04905100	-1.55629800	-3.22074300
C	4.89569200	-2.48921700	-1.30484300
O	4.51704000	-1.99523200	-0.26621500
O	5.88315900	-3.37206300	-1.39418000
C	6.52899700	-3.69256700	-0.15714500
H	5.81794700	-4.16158300	0.52711100
H	7.32722600	-4.38608800	-0.41665500
H	6.93303200	-2.78809000	0.30141200
O	-4.26598100	-3.05227100	-0.86202400
H	-3.43323500	-2.61527700	-1.12518700
C	-5.19929200	-2.05569700	-0.59965700
H	-4.76008300	-1.17022100	-0.12881500
C	-6.20731100	-2.62787900	0.39328500
F	-5.57662400	-2.94022200	1.54578600
F	-7.15975000	-1.73690500	0.68739600
F	-6.79227600	-3.73837500	-0.05131600
C	-5.85074700	-1.56881200	-1.90011700
F	-6.65348700	-0.52156500	-1.67725900
F	-4.88785400	-1.18283200	-2.74825800
F	-6.56795200	-2.52247800	-2.50141900
O	-4.31219200	3.95511300	-0.17360400
H	-3.44488700	4.41709200	-0.13689600
C	-4.08958300	2.62712500	0.14779100
H	-3.25299000	2.49902200	0.84228400
C	-3.71774800	1.82851800	-1.10592400
F	-2.67046500	2.40156700	-1.72038900
F	-3.33639400	0.57070300	-0.78416400
F	-4.70853800	1.73740100	-1.98978100
C	-5.33185400	2.08552800	0.84832300
F	-5.16495300	0.77846000	1.16940800
F	-5.52652400	2.74317900	1.99660900
F	-6.43826700	2.18325100	0.11763800

O	4.99561600	2.04120200	0.15441300
H	4.24128100	1.88398800	-0.44076700
C	5.70733700	0.84631800	0.22739400
H	5.06107100	-0.03452400	0.32666400
C	6.58078200	0.89543300	1.47666100
F	5.81255400	1.04676700	2.56506700
F	7.26385400	-0.25251500	1.61556200
F	7.45797600	1.89853600	1.45402400
C	6.51404900	0.65350600	-1.06041800
F	7.15677200	-0.52446200	-1.08971100
F	5.65163200	0.66157400	-2.10315000
F	7.40628900	1.61603000	-1.27279600

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C	1.19479400	1.70968600	-0.31090400
O	2.01080000	1.84864600	-1.21790900
N	-0.12329900	1.96036400	-0.49080700
C	-1.08835300	1.89961000	0.57262200
C	-1.37671600	3.04147400	1.32066600
C	-1.71373300	0.65911500	0.79925600
C	-2.32050300	2.89447400	2.34979300
C	-2.65567600	0.57462500	1.83465900
H	-2.14712900	0.02996000	-0.36820300
C	-2.95736400	1.68968000	2.60823200
H	-2.55939100	3.75851300	2.96369800
H	-3.15316100	-0.36793000	2.03106500
H	-3.68754300	1.61906500	3.40866600
C	-0.58942400	2.06556600	-1.87777700
H	-0.71637800	1.05709700	-2.28846600
H	0.18403300	2.57613600	-2.45339800
C	-0.68747200	4.37693800	1.10346600
H	-0.17436000	4.33156900	0.13961200
C	-1.68732400	5.53639600	1.02277700
H	-1.16079400	6.45867100	0.75669100
H	-2.43942000	5.34205200	0.25493300
H	-2.18902600	5.71124600	1.98202300
C	0.35376100	4.62423900	2.20494600
H	-0.12567200	4.69376900	3.18887400
H	1.09411300	3.81918100	2.25126900
H	0.88380800	5.56503800	2.02243800
C	1.69110500	1.22459500	1.03608100
C	2.84054000	1.81321900	1.55173300
C	3.40068500	1.30474100	2.71633600

H	3.31123500	2.62964100	1.01522000
C	1.67804500	-0.34628900	2.73991100
C	2.80683200	0.20606700	3.32281900
H	4.30473600	1.74393300	3.12082000
H	1.20663700	-1.23306200	3.14784100
H	3.22145000	-0.24220800	4.21791900
N	1.12259400	0.15492300	1.62488500
C	-2.30288700	-1.79741000	-1.20617100
C	-1.31118100	-3.61049000	-0.19239700
C	-1.61326000	-4.02279700	-1.65076700
C	-2.60055800	-2.94047200	-2.14240300
H	-1.94233300	-4.15941300	0.51791000
H	-0.68753900	-3.99222200	-2.23248900
H	-2.01765000	-5.03304900	-1.71980500
H	-2.45239000	-2.64015300	-3.18208300
H	-3.64859000	-3.23145100	-2.02224800
N	-1.66066700	-2.19560200	-0.14837000
O	-2.62264000	-0.56319700	-1.38599300
C	0.14437500	-3.76663000	0.27145200
O	0.76585000	-4.78792800	0.00058200
O	0.62409400	-2.77915800	0.96447100
Pd	-0.42357500	-1.00181400	0.81147800
C	-1.87453800	2.87842100	-1.98853900
O	-1.89735300	4.08049200	-1.78087500
N	-2.96173300	2.16694000	-2.39268400
H	-2.92432200	1.15487100	-2.34234300
C	-4.25466100	2.78777200	-2.42453200
H	-4.12787300	3.85563000	-2.61963700
H	-4.86635000	2.36706000	-3.22837400
C	-5.00891800	2.61526200	-1.11762900
O	-4.56647000	2.03695400	-0.14546700
O	-6.21236100	3.16254200	-1.18449100
C	-7.04332300	3.02273500	-0.02506000
H	-6.55512200	3.46709900	0.84540400
H	-7.96272200	3.55531500	-0.26141400
H	-7.24943900	1.96745900	0.16328100
O	4.63778500	2.61211900	-1.03591800
H	3.73400500	2.31333900	-1.25585900
C	5.39865600	1.48486900	-0.74809300
H	4.83355500	0.70599000	-0.22598000
C	6.51930100	1.92171800	0.19180500
F	5.98712000	2.38786400	1.34162100
F	7.31712200	0.89612500	0.50743000
F	7.26917500	2.89594900	-0.32039400

C	5.92115000	0.84233700	-2.03933300
F	6.53941400	-0.31776600	-1.78759400
F	4.88370000	0.59423500	-2.85021300
F	6.77383100	1.63387700	-2.69659600
O	3.48925300	-4.24152200	-0.04192500
H	2.55759900	-4.54793200	0.03222500
C	3.50567100	-2.88189100	0.21813900
H	2.71101300	-2.57886000	0.90730200
C	3.26549500	-2.08781600	-1.07035300
F	2.13342800	-2.50434700	-1.66014700
F	3.10171500	-0.77090100	-0.80526900
F	4.25202400	-2.20222800	-1.95635700
C	4.82979400	-2.53579700	0.89163300
F	4.89939300	-1.20578300	1.15013800
F	4.91523000	-3.16231900	2.07029400
F	5.89564700	-2.86105700	0.16672200
O	-5.82847100	-0.01647200	1.18163200
H	-5.37656300	0.81240000	0.93100000
C	-5.41528300	-0.99009800	0.27912900
H	-4.43770800	-0.76506700	-0.15919400
C	-6.39396200	-1.08066900	-0.89886100
F	-6.44441000	0.11047800	-1.52789300
F	-5.99434200	-1.98743800	-1.80414000
F	-7.63287200	-1.38606000	-0.52000700
C	-5.28556400	-2.31801300	1.02992500
F	-4.84659100	-3.29179000	0.20981400
F	-4.39077400	-2.20739100	2.02215100
F	-6.43830400	-2.71671800	1.56199100

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C	-0.71629200	-0.96830500	-0.67354300
O	-1.45311900	-1.42782400	-1.53992500
N	0.47241500	-0.38929800	-0.97028100
C	1.43424400	-0.00503500	0.02474300
C	2.34863600	-0.93990400	0.51334500
C	1.40790700	1.33546200	0.45473100
C	3.24404400	-0.48501500	1.49486500
C	2.33151000	1.73548800	1.43144700
H	1.31344800	2.27586500	-0.53982600
C	3.24538800	0.82621100	1.95323800
H	3.95974200	-1.18649200	1.91288500
H	2.32512600	2.76703200	1.77473000
H	3.96079600	1.12911300	2.71060300

C	0.68769700	0.03864400	-2.35292400
H	0.30093700	1.05690600	-2.47638000
H	0.12025400	-0.63174700	-2.99968600
C	2.37999700	-2.39209800	0.07212500
H	1.73809200	-2.48620200	-0.80745500
C	3.78735600	-2.83077100	-0.34790500
H	3.75444800	-3.84821200	-0.74990700
H	4.17723000	-2.17909900	-1.13495700
H	4.48245100	-2.84038400	0.49762800
C	1.83625500	-3.30175000	1.18387100
H	2.48037300	-3.26536500	2.07065800
H	0.82714700	-3.00920500	1.49163600
H	1.79967800	-4.34010700	0.83840100
C	-1.17550400	-1.01209300	0.76766300
C	-1.76733500	-2.18259400	1.22767500
C	-2.32295600	-2.20778300	2.50027400
H	-1.82868700	-3.04466300	0.57246400
C	-1.70552600	0.08581900	2.73640800
C	-2.29040700	-1.05190100	3.26889800
H	-2.80173500	-3.10796800	2.86652800
H	-1.69870500	1.02459400	3.27818900
H	-2.73537500	-1.01275900	4.25606300
N	-1.14813700	0.10827300	1.51524200
C	0.39127000	4.00726800	-1.00582000
C	-1.33023600	4.78654700	0.31743700
C	-1.46818600	5.48295900	-1.05287300
C	-0.08587000	5.26030600	-1.70434800
H	-1.02990800	5.49941500	1.09730200
H	-2.24952800	4.98397700	-1.63387000
H	-1.74012100	6.53491200	-0.96041600
H	-0.11826100	5.11574300	-2.78636100
H	0.61358900	6.07865800	-1.49614000
N	-0.26257600	3.81434100	0.10793300
O	1.29419600	3.20526000	-1.42647200
C	-2.57282500	4.05310300	0.83914000
O	-3.67160000	4.59182700	0.77799500
O	-2.35737700	2.88163300	1.35739300
Pd	-0.55391600	2.01799000	0.85504800
C	2.15794000	-0.05258900	-2.73638700
O	2.73685200	-1.12396200	-2.81229100
N	2.74878100	1.14056200	-3.01529200
H	2.28283400	1.99942700	-2.74254700
C	4.15312300	1.17994600	-3.32561600
H	4.43938300	0.23778300	-3.79341300

H	4.35582400	1.99149900	-4.03342700
C	5.06427100	1.39184000	-2.12804800
O	6.20384000	0.97124600	-2.09356200
O	4.50617000	2.13386100	-1.18284100
C	5.34779500	2.52206800	-0.08981100
H	6.24462100	3.01993400	-0.46578700
H	4.74652900	3.20729800	0.50451000
H	5.63663800	1.65769800	0.50913700
O	-3.21328800	-3.53494000	-1.36458300
H	-2.63674200	-2.77911300	-1.58664800
C	-4.39826100	-3.02178900	-0.84864800
H	-4.24840600	-2.11725800	-0.25053900
C	-4.98267200	-4.07755700	0.08628600
F	-4.12260700	-4.30678200	1.10138200
F	-6.13587500	-3.66691000	0.62364500
F	-5.19394900	-5.24234900	-0.52371900
C	-5.35604800	-2.63103900	-1.98123900
F	-6.44490800	-2.01658900	-1.50353700
F	-4.72704700	-1.78290400	-2.80629900
F	-5.75425100	-3.68327200	-2.70175700
O	-5.69991400	2.69007400	0.77749000
H	-5.06875500	3.43960400	0.85404000
C	-4.95678500	1.52182500	0.77711600
H	-4.02732400	1.61804100	1.34746300
C	-4.53232700	1.15742500	-0.64983500
F	-3.89882000	2.19691000	-1.21693900
F	-3.65645100	0.12579200	-0.64592000
F	-5.54992200	0.82095400	-1.43852900
C	-5.77634700	0.42596100	1.45094500
F	-5.08853000	-0.74300600	1.46060900
F	-6.00304900	0.75065300	2.72848000
F	-6.94696200	0.20020800	0.86267500
O	7.70404100	0.19015700	0.06545100
H	7.33756400	0.54503900	-0.76697500
C	6.99145900	-0.95677500	0.38341300
H	5.94599900	-0.92135100	0.04634700
C	6.95212700	-1.05908200	1.90734300
F	6.36209800	0.03884100	2.41599200
F	6.22300500	-2.11826800	2.30611000
F	8.16002700	-1.16245700	2.45072500
C	7.62811900	-2.18073100	-0.28982000
F	6.97697400	-3.31284200	0.02008700
F	7.56432600	-2.02006400	-1.61734400
F	8.90703100	-2.33350500	0.05169500

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C	1.26380500	1.26091000	0.14244600
O	1.80410400	1.93685800	-0.72659200
N	-0.02549000	0.85056200	0.03593800
C	-0.73590700	0.20973000	1.11023300
C	-1.36683600	0.97999500	2.08526200
C	-0.75673700	-1.19813000	1.11832400
C	-2.00120500	0.28059000	3.12501500
C	-1.43255300	-1.84371500	2.16420400
H	-1.06982600	-1.80181800	-0.09960100
C	-2.04496900	-1.10452300	3.17156200
H	-2.48686000	0.84907900	3.91332600
H	-1.48545300	-2.92661500	2.17850100
H	-2.56027300	-1.60756600	3.98404100
C	-0.61008300	0.86510700	-1.30414100
H	-0.35334100	-0.06716600	-1.82089500
H	-0.16523200	1.69766100	-1.85215800
C	-1.39022100	2.49676400	2.07184500
H	-1.02028100	2.82492900	1.09673200
C	-2.82163300	3.02691900	2.21789100
H	-2.86454900	4.09534400	1.99212600
H	-3.48909100	2.51143700	1.52286400
H	-3.20669000	2.88504300	3.23455400
C	-0.47120700	3.07357000	3.15717300
H	-0.81216000	2.78040600	4.15733800
H	0.55946200	2.72318900	3.04041100
H	-0.46793800	4.16746200	3.10994800
C	2.07976500	0.83266200	1.34239000
C	2.91280500	1.77353400	1.93620700
C	3.78455900	1.37005700	2.93975500
H	2.90949800	2.79669700	1.57598300
C	2.96927700	-0.85514800	2.65428900
C	3.81261800	0.03106900	3.30529500
H	4.45372100	2.08803000	3.39857700
H	2.98955100	-1.91704300	2.87125200
H	4.49533600	-0.33689700	4.06200700
N	2.11097700	-0.46636600	1.69812600
C	-0.54770200	-3.37202700	-1.23507000
C	1.34369100	-4.58205100	-0.72817500
C	0.97812100	-4.91694500	-2.18908700
C	-0.48197900	-4.42462800	-2.31336500
H	1.17185500	-5.44098100	-0.06553000

H	1.63103100	-4.35391400	-2.86241200
H	1.09719600	-5.97681300	-2.41559000
H	-0.73131500	-4.00447100	-3.29021500
H	-1.21472600	-5.20642100	-2.08618600
N	0.41608700	-3.51357000	-0.37741000
O	-1.41447900	-2.42300400	-1.14282000
C	2.77176400	-4.08742500	-0.45694400
O	3.72404200	-4.62540100	-1.00925700
O	2.87027100	-3.11803600	0.40146800
Pd	1.12625800	-2.04945500	0.71778400
C	-2.11330400	1.06691100	-1.26069200
O	-2.62175900	2.10487300	-0.84629200
N	-2.85388400	0.04084800	-1.72783700
H	-2.41403300	-0.86429100	-1.85701700
C	-4.28839700	0.11599900	-1.62948000
H	-4.66621800	1.00018800	-2.14605000
H	-4.72691300	-0.76774200	-2.10117500
C	-4.73660700	0.13752900	-0.17503000
O	-4.11348200	-0.36680300	0.73622300
O	-5.89702600	0.75665900	-0.03607700
C	-6.43815100	0.81175400	1.29163700
H	-5.75758400	1.35970700	1.94697700
H	-7.38125900	1.34427700	1.19252900
H	-6.59436200	-0.19925500	1.67281100
O	3.83427100	3.78152800	-0.45179600
H	3.14149900	3.14808200	-0.71888800
C	5.04190000	3.09472400	-0.40030500
H	4.93650600	2.06834400	-0.03376900
C	5.93721400	3.82801300	0.59504100
F	5.36743200	3.79807100	1.81928500
F	7.13346600	3.23911100	0.69625700
F	6.12209400	5.10695800	0.27639500
C	5.66702300	2.98566100	-1.79725800
F	6.73883300	2.18482900	-1.78454700
F	4.76337800	2.46112700	-2.63597000
F	6.03940600	4.17175200	-2.28689700
O	5.90902300	-2.90947600	-1.04282800
H	5.21701900	-3.60737000	-1.00916900
C	5.38699600	-1.77079800	-0.45364600
H	4.64790000	-2.00176000	0.32008900
C	4.64904300	-0.92209300	-1.49410600
F	3.71912800	-1.66459300	-2.11540900
F	3.99220800	0.10462200	-0.90375300
F	5.44921500	-0.40908300	-2.42487900

C	6.52455900	-1.01782400	0.22930000
F	6.06612400	0.12370100	0.80061600
F	7.03342400	-1.76566300	1.21463600
F	7.51177400	-0.68729200	-0.59726400
O	-3.83147100	4.56656200	-0.53565400
H	-3.14703000	3.88895500	-0.66836000
C	-5.05196000	3.91588200	-0.64454900
H	-4.98941200	2.85886900	-0.37276500
C	-5.55051700	3.94786400	-2.09449200
F	-4.59562900	3.43639200	-2.89302800
F	-6.64610200	3.18882400	-2.25260800
F	-5.82799600	5.17805900	-2.52251100
C	-6.03211200	4.54970700	0.34013100
F	-7.25188100	3.99566900	0.21939100
F	-5.61942600	4.32610200	1.59830800
F	-6.15400900	5.86392600	0.17359600
O	-4.37575200	-2.98570700	1.61996000
H	-4.26678300	-2.01864300	1.60675400
C	-4.15644300	-3.42866700	0.32286200
H	-3.45042500	-2.79628600	-0.22732800
C	-5.46275700	-3.44581100	-0.48883300
F	-6.13494500	-2.29604400	-0.29070700
F	-5.20188700	-3.52567800	-1.80506100
F	-6.27665300	-4.44728600	-0.16209100
C	-3.52084600	-4.81752300	0.39946100
F	-3.44217100	-5.37265400	-0.82359600
F	-2.26387400	-4.72728500	0.87114400
F	-4.19285600	-5.64449200	1.19190600

TS6-iso2

C	1.69473200	0.79133400	0.16601700
O	2.12646800	1.56843800	-0.67682100
N	0.49556600	0.16695600	0.02582400
C	-0.11774100	-0.58526900	1.08527300
C	-0.85162100	0.07239900	2.07387300
C	0.06988300	-1.98054400	1.07370600
C	-1.34400500	-0.72449400	3.11975100
C	-0.47749900	-2.73118000	2.12473500
H	-0.13781800	-2.60177300	-0.13739000
C	-1.16389600	-2.10121800	3.15772900
H	-1.89218700	-0.24293000	3.92535700
H	-0.34854700	-3.81022600	2.12870900
H	-1.56260900	-2.67638500	3.98829500

C	-0.05413200	0.06590300	-1.32245300
H	0.29856100	-0.85955300	-1.79134400
H	0.32124600	0.91418400	-1.89769500
C	-1.11906700	1.56609700	2.06887400
H	-0.77217100	1.96155600	1.11072000
C	-2.62193500	1.86056700	2.16262100
H	-2.81612800	2.91701100	1.96238700
H	-3.18129200	1.27987700	1.42379300
H	-3.02007200	1.63045900	3.15830600
C	-0.34909500	2.27337700	3.19238900
H	-0.67872300	1.92346300	4.17800400
H	0.72850400	2.09502400	3.11734900
H	-0.52122400	3.35332800	3.14497200
C	2.55020700	0.46994200	1.37179100
C	3.20909800	1.51464700	2.00825800
C	4.12018100	1.22761100	3.01711000
H	3.04395300	2.53417900	1.67695100
C	3.68313200	-1.09084300	2.65302300
C	4.36131900	-0.09966400	3.34477100
H	4.65475300	2.03093500	3.50965900
H	3.87107700	-2.14153200	2.84183700
H	5.08334800	-0.37551600	4.10406700
N	2.78673300	-0.81740600	1.69209300
C	0.63821200	-3.99977300	-1.36041800
C	2.72469200	-4.88157900	-0.92419300
C	2.42767100	-5.15169300	-2.41360000
C	0.90067600	-4.94033500	-2.51446800
H	2.71692600	-5.81347800	-0.34253300
H	2.95718700	-4.41678600	-3.02723700
H	2.74958400	-6.14425400	-2.73028400
H	0.56893800	-4.50372400	-3.45893900
H	0.33861000	-5.86886400	-2.35921400
N	1.61606900	-4.03386200	-0.49786600
O	-0.38144900	-3.23645100	-1.22036300
C	4.04384000	-4.16797400	-0.59898100
O	5.08165300	-4.51437700	-1.14912300
O	3.96782600	-3.23468000	0.30199700
Pd	2.07491300	-2.50716200	0.65254000
C	-1.56848100	0.13325800	-1.31005000
O	-2.17032200	1.13016600	-0.92129200
N	-2.21179600	-0.95747700	-1.77198000
H	-1.70527900	-1.83148800	-1.87216700
C	-3.65530400	-0.95217200	-1.80477400
H	-4.01507300	-0.09299900	-2.37302000

H	-4.00090500	-1.86648900	-2.29448800
C	-4.29259200	-0.88726300	-0.42595700
O	-5.24863500	-0.18551700	-0.16294800
O	-3.72091100	-1.70512700	0.44198800
C	-4.34168500	-1.77177300	1.73341500
H	-5.37942000	-2.09274900	1.63233800
H	-3.76278600	-2.50465900	2.29059400
H	-4.29577600	-0.79661300	2.22319600
O	3.82400700	3.70988100	-0.27348200
H	3.26663900	2.97653700	-0.59517800
C	5.14158000	3.26681200	-0.23742100
H	5.23618100	2.22169900	0.07477300
C	5.87100100	4.10696000	0.80780200
F	5.31172200	3.90183200	2.02025200
F	7.15879900	3.75958600	0.89774200
F	5.80171100	5.41195000	0.55656800
C	5.78274700	3.35726100	-1.62823400
F	6.99338800	2.78708500	-1.63843800
F	5.00664700	2.70388000	-2.50411300
F	5.91136600	4.61642600	-2.05408100
O	6.98406500	-2.48667000	-1.00006200
H	6.40195100	-3.27823900	-1.03494500
C	6.27061800	-1.46495100	-0.39851000
H	5.55204800	-1.83349000	0.34065600
C	5.44336700	-0.70204300	-1.43913300
F	4.68559000	-1.55894000	-2.14031600
F	4.59310800	0.16453900	-0.83834000
F	6.18243300	-0.00932200	-2.30181500
C	7.25265200	-0.56752700	0.34844300
F	6.60278800	0.47665900	0.92081700
F	7.82807700	-1.25473400	1.34135300
F	8.21057700	-0.07052900	-0.42690000
O	-3.42468900	3.57699400	-0.62591600
H	-2.71665200	2.92174700	-0.74167000
C	-4.61909600	2.88479500	-0.78784600
H	-4.54735600	1.84198000	-0.46981400
C	-5.02085400	2.84772000	-2.26666400
F	-3.99469900	2.35798900	-2.98785000
F	-6.06799100	2.02586600	-2.47092700
F	-5.33264600	4.04313600	-2.76078700
C	-5.68023700	3.52438000	0.10313200
F	-6.86328300	2.91097700	-0.06206100
F	-5.33205700	3.38799600	1.39159900
F	-5.84548800	4.82371400	-0.14135400

O	-7.88011100	-0.09990600	-1.15067900
H	-6.95964400	0.20120600	-1.15677100
C	-8.12907300	-0.63113700	0.10663100
H	-7.41674200	-0.27895400	0.85903800
C	-8.00842500	-2.16284400	0.07717400
F	-6.88488300	-2.52389000	-0.57049000
F	-7.91634600	-2.66041100	1.32530300
F	-9.03078700	-2.76226400	-0.53122000
C	-9.51347800	-0.16047500	0.55738500
F	-9.86468400	-0.75844300	1.70917800
F	-9.48898500	1.15846400	0.77060100
F	-10.45531600	-0.41850100	-0.34864100

TS6-iso3

C	1.48696500	1.51434100	-0.44647300
O	2.21369100	1.83275800	-1.38421300
N	0.15128100	1.37566800	-0.59922100
C	-0.75118600	1.07431000	0.47736400
C	-1.30050900	2.10686900	1.23558100
C	-1.04748800	-0.28557200	0.69149600
C	-2.26780900	1.73820200	2.18336300
C	-1.99455600	-0.59639700	1.67730700
H	-1.21575500	-1.07226500	-0.48046700
C	-2.62898500	0.41492500	2.39199300
H	-2.75123600	2.51467200	2.76815000
H	-2.24340200	-1.63256600	1.87587400
H	-3.38830300	0.17030000	3.12805900
C	-0.34964100	1.34226600	-1.97592000
H	-0.06251400	0.39280100	-2.44088500
H	0.12860600	2.14911300	-2.53720600
C	-0.81493900	3.54445800	1.15179800
H	-0.09476700	3.60894900	0.33058400
C	-1.92377400	4.55969700	0.85719100
H	-1.51173600	5.57406400	0.88432100
H	-2.33702600	4.38790500	-0.13868600
H	-2.72819200	4.50725000	1.59741700
C	-0.08386900	3.90819500	2.45531600
H	-0.78377800	3.94237400	3.29822300
H	0.69553700	3.17864200	2.69754200
H	0.38431100	4.89433000	2.36693800
C	2.09219400	1.27673300	0.91917900
C	3.01866300	2.20001300	1.38770300
C	3.66317800	1.96006900	2.59485500

H	3.25728400	3.07268500	0.78960000
C	2.45408300	-0.09283800	2.75091100
C	3.37154600	0.79506400	3.29112800
H	4.40089600	2.66240000	2.96448500
H	2.22982300	-1.03781200	3.23214400
H	3.86281900	0.55427000	4.22645000
N	1.81862700	0.14281600	1.59281400
C	-0.73958900	-2.88943400	-1.19073200
C	0.67585200	-4.27003500	-0.01171700
C	0.55461000	-4.86677400	-1.43301000
C	-0.64865300	-4.12121200	-2.05369600
H	0.21617700	-4.92251200	0.74002600
H	1.47088800	-4.65690400	-1.99156100
H	0.41716300	-5.94818100	-1.41250300
H	-0.51027900	-3.85028300	-3.10294700
H	-1.58579300	-4.68026700	-1.97224300
N	-0.07567300	-3.02361100	-0.08289800
O	-1.39774100	-1.81709100	-1.46798700
C	2.09821600	-3.94835700	0.46901000
O	3.00740600	-4.74525600	0.26568000
O	2.23724400	-2.82337700	1.10227400
Pd	0.69709900	-1.46690500	0.83491500
C	-1.85575200	1.55659200	-2.04158200
O	-2.36640900	2.61546300	-1.67368900
N	-2.55742500	0.54427700	-2.58910800
H	-2.12278300	-0.37264900	-2.61492300
C	-3.99290200	0.59883400	-2.68856400
H	-4.31005900	1.63362400	-2.82684100
H	-4.32732700	0.02880900	-3.56029000
C	-4.68067400	0.04449100	-1.45156200
O	-4.08163600	-0.45350100	-0.52022100
O	-5.98840200	0.16992700	-1.54245900
C	-6.74452400	-0.19480100	-0.37876600
H	-6.42799300	0.42404700	0.46205500
H	-7.78200400	0.01086900	-0.63341600
H	-6.60540300	-1.25338200	-0.15552800
O	4.49776000	3.34557100	-1.24365700
H	3.74666400	2.75394600	-1.44598400
C	5.57892400	2.55654000	-0.86753300
H	5.28783000	1.67704800	-0.28377400
C	6.46786700	3.40873400	0.03413500
F	5.78669800	3.74485200	1.15105600
F	7.55733200	2.73523400	0.41776800
F	6.85531800	4.54147700	-0.54828900

C	6.31732900	2.02628100	-2.10334500
F	7.25755100	1.13797700	-1.76088200
F	5.43554200	1.41302100	-2.90431100
F	6.90169400	2.99997100	-2.80790700
O	5.43917500	-3.42983800	0.16230400
H	4.64179900	-3.99628800	0.26723400
C	5.04654100	-2.11600300	0.35221300
H	4.18234500	-2.03040900	1.01922800
C	4.61106700	-1.49317900	-0.97802600
F	3.65232500	-2.24445600	-1.54317700
F	4.07693600	-0.26391000	-0.78721700
F	5.60326700	-1.37059500	-1.85640700
C	6.19447700	-1.36073900	1.01492300
F	5.85986100	-0.06025600	1.21121800
F	6.44172900	-1.88163600	2.22118700
F	7.32156400	-1.38295800	0.30978100
O	-4.54768300	2.48856700	-0.01434600
H	-3.75897600	2.59621000	-0.58848900
C	-5.26802700	3.67122500	0.02897700
H	-4.63755200	4.56373300	-0.06776800
C	-5.92782900	3.74767700	1.40777700
F	-4.98774000	3.87023700	2.35864100
F	-6.74008400	4.80546100	1.49986400
F	-6.63859700	2.65045900	1.68552600
C	-6.28841400	3.73470600	-1.11586700
F	-6.87267300	4.93521200	-1.18464700
F	-5.65125900	3.52604100	-2.28129800
F	-7.24751800	2.81152100	-1.00154200
O	-4.58849600	-2.57987000	1.09544700
H	-4.51249300	-1.68061300	0.71895800
C	-3.87708000	-3.41854100	0.24620300
H	-3.10237100	-2.87958100	-0.30956600
C	-4.81232100	-4.02896800	-0.80531600
F	-5.38781200	-3.04017000	-1.51342700
F	-4.13671000	-4.79840400	-1.67669400
F	-5.78342300	-4.76381300	-0.26954000
C	-3.17965900	-4.48140500	1.09811800
F	-2.46207400	-5.32210700	0.32705700
F	-2.32216900	-3.90266200	1.95150900
F	-4.03819200	-5.20754200	1.80827500

TS6-iso4

C	1.49832200	1.28988200	0.10316100

O	2.11644600	1.90605100	-0.75917100
N	0.17420600	1.02168600	-0.02035300
C	-0.60819900	0.41647900	1.02230000
C	-1.18908000	1.21517600	2.00781500
C	-0.74846100	-0.98364500	0.98996000
C	-1.89920300	0.54437800	3.01607900
C	-1.50726500	-1.59510000	1.99865000
H	-1.01368200	-1.53622900	-0.26113300
C	-2.07315000	-0.83320000	3.01532000
H	-2.33746700	1.12894400	3.82085100
H	-1.64726000	-2.67113300	1.98166700
H	-2.64546500	-1.30891100	3.80589900
C	-0.38682700	1.11883000	-1.36815900
H	-0.17118400	0.19190000	-1.91190000
H	0.11348200	1.94233600	-1.88034000
C	-1.04813800	2.72616600	2.04969200
H	-0.65418100	3.04716000	1.08129900
C	-2.39836300	3.42457000	2.24566300
H	-2.27840800	4.50599300	2.12742600
H	-3.13886500	3.08834000	1.51785400
H	-2.80503700	3.25527100	3.24997300
C	-0.05935200	3.14872100	3.14608200
H	-0.43529700	2.87094200	4.13806500
H	0.91866300	2.67557800	3.01659500
H	0.08202400	4.23450500	3.13266300
C	2.25316500	0.78946800	1.31566900
C	3.15718300	1.65644100	1.91855800
C	3.96813900	1.18752100	2.94403300
H	3.25278000	2.67189500	1.54983000
C	2.95964700	-0.95705400	2.66146700
C	3.86471100	-0.14376900	3.32442700
H	4.68996200	1.84762900	3.40990200
H	2.87804500	-2.01412600	2.88698000
H	4.49310600	-0.56342200	4.10104700
N	2.16071700	-0.50306300	1.68231500
C	-0.57418400	-3.14128100	-1.38022100
C	1.12986700	-4.55814300	-0.74582400
C	0.84709700	-4.83518600	-2.23855500
C	-0.53381400	-4.18290100	-2.47088100
H	0.83960400	-5.41078700	-0.11749300
H	1.61097700	-4.34269200	-2.84727700
H	0.86745100	-5.89953500	-2.47479400
H	-0.65354400	-3.72575300	-3.45550000
H	-1.36277000	-4.88406800	-2.32213300

N	0.28169900	-3.41274000	-0.43565500
O	-1.31561900	-2.09681400	-1.35416000
C	2.57860900	-4.20287100	-0.38130400
O	3.50617700	-4.83626800	-0.87097800
O	2.72072600	-3.23633900	0.47511900
Pd	1.07556400	-2.00258600	0.68000900
C	-1.87946600	1.41354300	-1.36396000
O	-2.30697000	2.50518800	-0.98861000
N	-2.64543100	0.42295100	-1.85916500
H	-2.22555600	-0.49296300	-1.98389800
C	-4.07669200	0.52050000	-2.01100100
H	-4.34701700	1.54699500	-2.27747000
H	-4.40027600	-0.13383500	-2.82139500
C	-4.87482400	0.15332200	-0.77093100
O	-5.96537500	-0.38248700	-0.83828700
O	-4.27482900	0.51924800	0.34446000
C	-5.04086100	0.41127500	1.55095800
H	-5.12982200	-0.63781500	1.83934500
H	-4.47825600	0.96944600	2.29554200
H	-6.02548500	0.85768800	1.40216400
O	4.30494700	3.54622100	-0.44896000
H	3.55767800	2.98213700	-0.72570000
C	5.44229900	2.74823800	-0.39853600
H	5.24112300	1.73713600	-0.02981700
C	6.40518600	3.39364500	0.59465100
F	5.84755100	3.39681100	1.82464900
F	7.55088400	2.70959400	0.67633100
F	6.68909500	4.65713600	0.28623400
C	6.05196600	2.58018000	-1.79638200
F	7.04535100	1.68416500	-1.78576500
F	5.10173800	2.13904200	-2.63226000
F	6.53074100	3.72660300	-2.28841200
O	5.80829100	-3.29254500	-0.94923300
H	5.07551000	-3.94544100	-0.89299000
C	5.36013500	-2.11273700	-0.38050000
H	4.59752600	-2.28142200	0.38674000
C	4.69642500	-1.22843500	-1.44156100
F	3.71278600	-1.90762900	-2.05438600
F	4.12001200	-0.14150400	-0.87662800
F	5.53864200	-0.79902600	-2.37723700
C	6.53778200	-1.42943900	0.30839000
F	6.14599000	-0.25996100	0.87328800
F	6.99282900	-2.20370200	1.29901200
F	7.54897800	-1.16211500	-0.51211100

O	-4.83169500	3.14904500	-0.27127500
H	-3.92360100	2.84227300	-0.48750200
C	-4.93004100	4.48250200	-0.64694900
H	-3.95169200	4.97093200	-0.73259200
C	-5.70525200	5.22020100	0.44639800
F	-5.00194300	5.20045200	1.58748600
F	-5.90997000	6.50192600	0.11474100
F	-6.88948600	4.65488400	0.68492100
C	-5.59471100	4.57850700	-2.02484900
F	-5.62771600	5.83620000	-2.47661300
F	-4.87654800	3.85061300	-2.90376200
F	-6.83809600	4.09744100	-2.02280400
O	-6.36487500	-2.59369000	0.74829900
H	-6.42373200	-1.74392400	0.27006500
C	-5.72827300	-3.50717200	-0.07959400
H	-5.82246800	-3.25762600	-1.14363600
C	-6.39710900	-4.87021800	0.11732600
F	-7.66581700	-4.80970500	-0.29370600
F	-5.77227200	-5.81478600	-0.60392900
F	-6.38747800	-5.24959700	1.39508100
C	-4.22512000	-3.53434200	0.22882300
F	-3.54742000	-4.31544200	-0.62703000
F	-3.73423100	-2.28835200	0.10733800
F	-3.95493700	-3.95033000	1.46849000

TS7-iso1

C	-0.38745200	2.19000500	2.29525400
O	-0.57509300	3.39689500	2.13855100
N	0.62449600	1.51527900	1.69582700
C	0.59590700	0.07262700	1.65437600
C	1.37261600	-0.67675500	2.53057900
C	-0.28565100	-0.51142700	0.72110000
C	1.19932500	-2.07106600	2.49287000
C	-0.41871300	-1.90728100	0.73304700
H	-0.15471900	-0.17592200	-0.56416700
C	0.31585000	-2.68669300	1.61919800
H	1.78512200	-2.68557800	3.17098500
H	-1.09915100	-2.37806300	0.03398400
H	0.20757700	-3.76644100	1.61283700
C	1.31959800	2.23924200	0.62687600
H	1.62512100	3.21268200	1.01684000
H	0.62482100	2.40228400	-0.20279700
C	2.37169500	-0.06307100	3.49132800

H	2.45730500	0.99857500	3.24317000
C	1.89618100	-0.18713100	4.94437700
H	2.61637600	0.28266400	5.62263000
H	0.92182300	0.29064900	5.08991400
H	1.79732600	-1.23923600	5.23678200
C	3.75666200	-0.69342300	3.30304000
H	3.79496200	-1.71410300	3.70102200
H	4.01442300	-0.73138100	2.24237100
H	4.52524400	-0.10814000	3.81452500
C	-1.32832100	1.41891400	3.19902900
C	-1.35978600	1.68104500	4.56056300
C	-2.29380700	1.01499300	5.34783600
H	-0.66443700	2.39711100	4.98373100
C	-3.10497000	-0.05724900	3.37036500
C	-3.17657100	0.12832400	4.74397400
H	-2.33367300	1.19269200	6.41749200
H	-3.77319100	-0.73259700	2.85411900
H	-3.92214900	-0.41292500	5.31441800
N	-2.20041000	0.57726800	2.61550300
C	-1.19206400	0.27959300	-2.26053800
C	-3.31072000	1.14770000	-2.05645000
C	-3.22415700	0.55884800	-3.47207300
C	-1.69595400	0.40294500	-3.68070000
H	-3.22492100	2.24201400	-2.07115600
H	-3.71538400	-0.41839200	-3.48936300
H	-3.69573400	1.19472300	-4.22242500
H	-1.40616100	-0.47471100	-4.26221400
H	-1.24639100	1.28603500	-4.14629900
N	-2.11896400	0.60846900	-1.41914800
O	-0.02611600	-0.10852800	-1.88130500
C	-4.48138200	0.81729900	-1.13268300
O	-5.58699600	0.52741900	-1.57724400
O	-4.18366000	0.89551600	0.13355700
Pd	-2.16535500	0.45613500	0.51932500
C	2.56730700	1.50633700	0.16197100
O	3.56836900	1.41247300	0.86766600
N	2.50467000	1.01939100	-1.09206300
H	1.59708600	0.91220900	-1.53834800
C	3.59357000	0.23974400	-1.61212900
H	4.53963600	0.76849800	-1.48441700
H	3.43908000	0.07969700	-2.68213500
C	3.67500300	-1.12767800	-0.95469200
O	2.77108100	-1.64247300	-0.32915200
O	4.85695200	-1.68496100	-1.16605600

C	5.04739500	-3.00448100	-0.63524700
H	6.07774300	-3.26111600	-0.87081000
H	4.89467000	-2.99567700	0.44653000
H	4.35057900	-3.69855100	-1.11015400
O	-1.49021300	3.50791000	-0.48777800
H	-1.34190400	3.62961400	0.46963000
C	-1.06228200	4.63971100	-1.16719000
H	-0.20740200	5.13086000	-0.68452600
C	-2.19963700	5.66847000	-1.22872900
F	-2.53639300	6.00585800	0.02235600
F	-1.82233700	6.77877300	-1.87379200
F	-3.28217400	5.17713000	-1.83342200
C	-0.58684700	4.19435600	-2.55164200
F	-0.07896100	5.21748600	-3.24026700
F	0.37798300	3.26468600	-2.42755700
F	-1.57091400	3.65097600	-3.27841000
O	-6.60953000	-1.68244900	-0.33299600
H	-6.43790300	-0.85035200	-0.82552500
C	-5.70820100	-1.71277800	0.71801700
H	-5.29909300	-0.71903000	0.93912300
C	-4.50898100	-2.59773500	0.35701200
F	-3.94071900	-2.15625000	-0.77788200
F	-3.55130400	-2.54503300	1.31536700
F	-4.82720800	-3.87808100	0.18173200
C	-6.43957100	-2.18766900	1.97098200
F	-5.58787500	-2.26727600	3.02478100
F	-7.39071000	-1.31101200	2.30068900
F	-7.00471600	-3.38464600	1.82604300
O	6.09931200	1.22828400	1.96322500
H	5.18984300	1.49004100	1.73814600
C	6.50857000	0.33410000	0.98614600
H	5.67171900	-0.19453600	0.52037400
C	7.37513900	-0.74074200	1.64156100
F	6.63386700	-1.46341000	2.49549100
F	7.85918700	-1.59130100	0.71938100
F	8.40176700	-0.22979800	2.31615700
C	7.22799000	1.07474900	-0.14873900
F	7.50148200	0.25950300	-1.17679400
F	6.41637500	2.04387400	-0.61414500
F	8.36384300	1.64735800	0.24663500
O	1.55921400	-3.91958600	-1.34220200
H	1.97652000	-3.27148100	-0.74792500
C	0.78638300	-3.19662800	-2.24653900
H	0.55306800	-2.18612400	-1.89476900

C	-0.55543500	-3.90844200	-2.45326700
F	-1.11030700	-4.20631600	-1.27071000
F	-1.40980300	-3.10444600	-3.11013700
F	-0.44233800	-5.04341200	-3.14415100
C	1.54717200	-3.01740000	-3.56385600
F	0.82183000	-2.33708000	-4.46300000
F	2.67294100	-2.30472300	-3.33552800
F	1.91962100	-4.17099000	-4.11191100

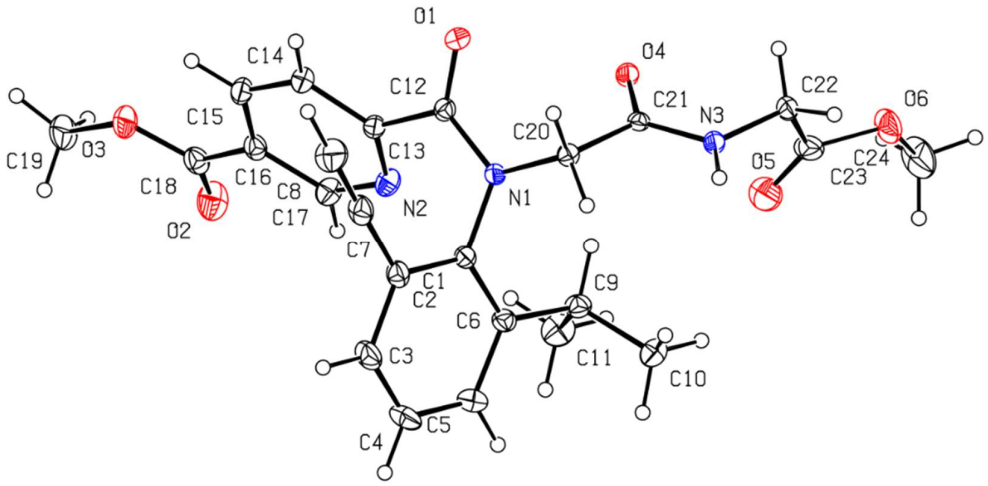
TS7-iso2

C	-0.27463100	2.44702700	2.09503400
O	-0.26159100	3.67282000	1.99898100
N	0.63025500	1.63791200	1.49327700
C	0.50399800	0.20387700	1.56524300
C	1.20496500	-0.51427500	2.52961300
C	-0.38766200	-0.40525100	0.66020900
C	0.93476200	-1.89045900	2.61368300
C	-0.61738900	-1.78285000	0.79299600
H	-0.20095800	-0.20232600	-0.65676500
C	0.03409700	-2.52421800	1.77100600
H	1.45517200	-2.47634600	3.36629100
H	-1.31088800	-2.26934200	0.11816300
H	-0.15064500	-3.58965100	1.86113800
C	1.47674100	2.25196200	0.46491000
H	1.91110700	3.16810500	0.86911100
H	0.86422100	2.52758800	-0.39765300
C	2.22146200	0.11275000	3.46423900
H	2.40234700	1.13413900	3.11765500
C	1.69252600	0.17650600	4.90267200
H	2.42235200	0.66753900	5.55502900
H	0.75017900	0.73087400	4.96042300
H	1.51141700	-0.82915300	5.30025300
C	3.55467000	-0.64224600	3.39473800
H	3.49443400	-1.61491700	3.89675100
H	3.84143300	-0.81321300	2.35500400
H	4.35380200	-0.07026300	3.87357900
C	-1.34410400	1.81692600	2.96447600
C	-1.43791300	2.20629900	4.29370200
C	-2.45413400	1.67668900	5.08126500
H	-0.72070000	2.91632600	4.68922100
C	-3.22557200	0.48137700	3.16158000
C	-3.35902100	0.79307300	4.50673900
H	-2.53891800	1.95475700	6.12661600

H	-3.91016400	-0.19524700	2.67036500
H	-4.16924300	0.35081300	5.07429100
N	-2.24121300	0.98377600	2.40557400
C	-1.22538100	0.06322400	-2.39117000
C	-3.33507400	0.96254700	-2.32852100
C	-3.25854500	0.13741800	-3.62009800
C	-1.72877300	-0.01254900	-3.81546200
H	-3.23804600	2.03488700	-2.55031300
H	-3.71947000	-0.84096000	-3.45567000
H	-3.75698600	0.61824200	-4.46274000
H	-1.41769500	-0.94774900	-4.28410400
H	-1.30250900	0.81799400	-4.39175800
N	-2.14718600	0.52826400	-1.60847000
O	-0.06648100	-0.28623500	-1.95878000
C	-4.51378500	0.82517400	-1.36444800
O	-5.62986300	0.52183100	-1.77405100
O	-4.21275000	1.08065700	-0.12542300
Pd	-2.19727600	0.63491800	0.33677600
C	2.62419400	1.34747200	0.04673100
O	3.61094100	1.17651800	0.75764900
N	2.50686400	0.79403400	-1.17621500
H	1.59666400	0.75809400	-1.62464900
C	3.50921500	-0.12602200	-1.64046600
H	4.50188500	0.32128500	-1.56247600
H	3.32246900	-0.35513100	-2.69272700
C	3.47496400	-1.43785500	-0.87499600
O	2.52797500	-1.82656900	-0.22273200
O	4.60885600	-2.10331000	-1.02772200
C	4.68991700	-3.38688000	-0.39116300
H	5.69397100	-3.74818800	-0.60115300
H	4.54247400	-3.27615400	0.68560900
H	3.93631600	-4.05720900	-0.81001200
O	0.42768600	5.07223100	-0.27817900
H	0.08365300	4.71143900	0.56435400
C	-0.60499900	5.40916900	-1.13645200
H	-1.31748100	6.12863800	-0.70827300
C	-1.42392200	4.16950400	-1.52187100
F	-1.96175800	3.64518700	-0.40807700
F	-2.42375900	4.45340800	-2.36128100
F	-0.66941100	3.21451300	-2.09218400
C	0.03863000	6.08903300	-2.34811200
F	-0.89477900	6.45006100	-3.23925900
F	0.68568600	7.18800400	-1.95776300
F	0.91005000	5.28456400	-2.96245400

O	-6.73652600	-1.49251800	-0.30486400
H	-6.54240300	-0.72993300	-0.89167700
C	-5.83149200	-1.42410500	0.74098400
H	-5.39003700	-0.42416800	0.84070200
C	-4.66467700	-2.38681300	0.48886900
F	-4.06295100	-2.07943200	-0.67442500
F	-3.71984000	-2.28009700	1.45327000
F	-5.03457200	-3.66309200	0.42923200
C	-6.57140700	-1.72028800	2.04385900
F	-5.72309600	-1.67105100	3.10194700
F	-7.51178800	-0.79634300	2.25182100
F	-7.15089600	-2.91930500	2.05530000
O	6.09531100	0.89767600	1.91844900
H	5.21512000	1.22708300	1.66822400
C	6.42232300	-0.09148000	1.00335100
H	5.54072800	-0.56809800	0.56515900
C	7.18130000	-1.19699600	1.73506400
F	6.37063200	-1.78856000	2.62642800
F	7.58726500	-2.14820200	0.87578700
F	8.24878200	-0.74151800	2.38567400
C	7.20958100	0.50663900	-0.16912800
F	7.42364800	-0.39901600	-1.13435500
F	6.48530700	1.50365800	-0.71163100
F	8.38572800	1.00972000	0.20240100
O	1.19560900	-4.12347700	-0.99711800
H	1.64307900	-3.43962600	-0.46766100
C	0.50027300	-3.46119600	-2.00459900
H	0.33712100	-2.40132900	-1.78209800
C	-0.88660500	-4.09458400	-2.16826600
F	-1.47910700	-4.23185900	-0.97522800
F	-1.67158800	-3.30040800	-2.92011800
F	-0.84742400	-5.29678400	-2.74310600
C	1.30404800	-3.49801100	-3.30796300
F	0.64405400	-2.89586700	-4.30901900
F	2.46607800	-2.83073300	-3.13626500
F	1.61385300	-4.73278800	-3.69317000

4. X-Ray Data of 3hb



Bond precision: C-C = 0.0025 A Wavelength=1.54178

Cell: a=9.3386(3) b=10.3729(3) c=24.4089(7)
alpha=90 beta=90 gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	2364.45(12)	2364.45(12)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C24 H25 N3 O6	C24 H25 N3 O6
Sum formula	C24 H25 N3 O6	C24 H25 N3 O6
Mr	451.47	451.47
Dx,g cm-3	1.268	1.268
Z	4	4
Mu (mm-1)	0.764	0.764
F000	952.0	952.0
F000'	955.13	
h,k,lmax	11,12,29	11,12,29
Nref	4335[2484]	4334
Tmin,Tmax	0.746,0.892	0.676,0.753
Tmin'	0.742	

Correction method= # Reported T Limits: Tmin=0.676 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.74/1.00 Theta(max)= 68.241

R(reflections)= 0.0287(4312) wR2(reflections)= 0.0734(4334)

S = 1.071 Npar= 322

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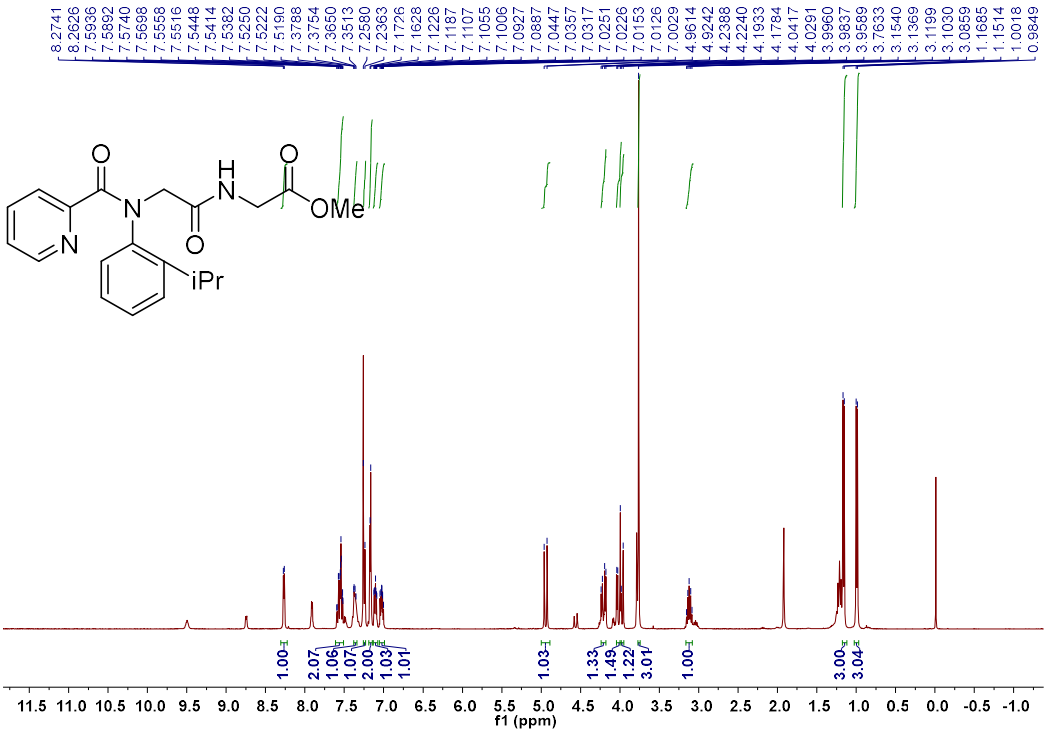
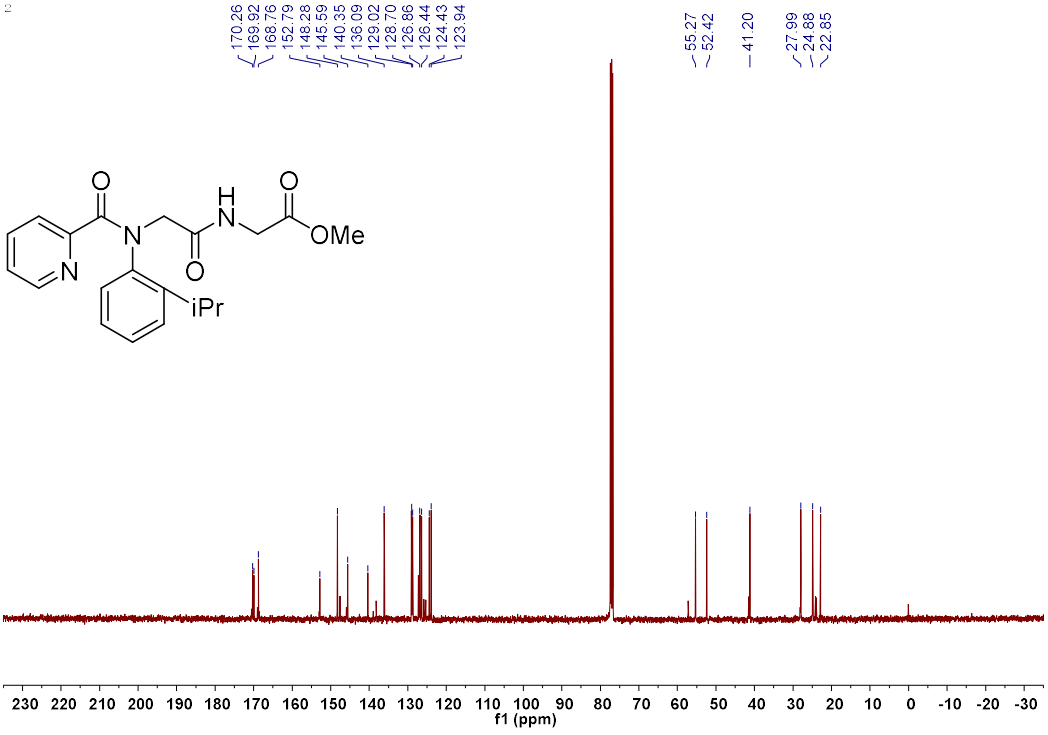
10) Xiang, Y.; Fan, X.; Pei-Jun Cai, P.-J.; Yu, Z.-X. Understanding Regioselectivities of Corey–Chaykovsky Reactions of Dimethylsulfoxonium Methylide (DMSOM) and Dimethylsulfonium Methylide (DMSM) toward Enones: A DFT Study. Eur. *J. Org. Chem.* **2019**, 582.
11) 20 CYLview, C. Y. Legault, Université de Sherbrooke, 2020 (http://www.cylview.org).

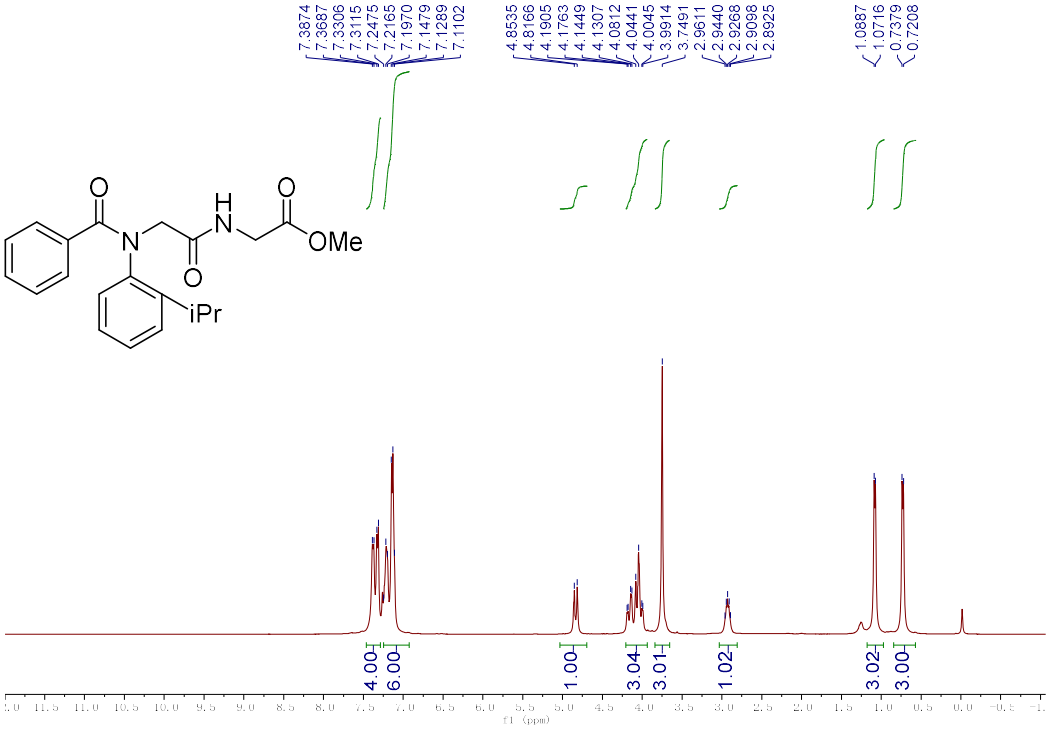
6. NMR Spectra

rac-1a





***rac*-1b**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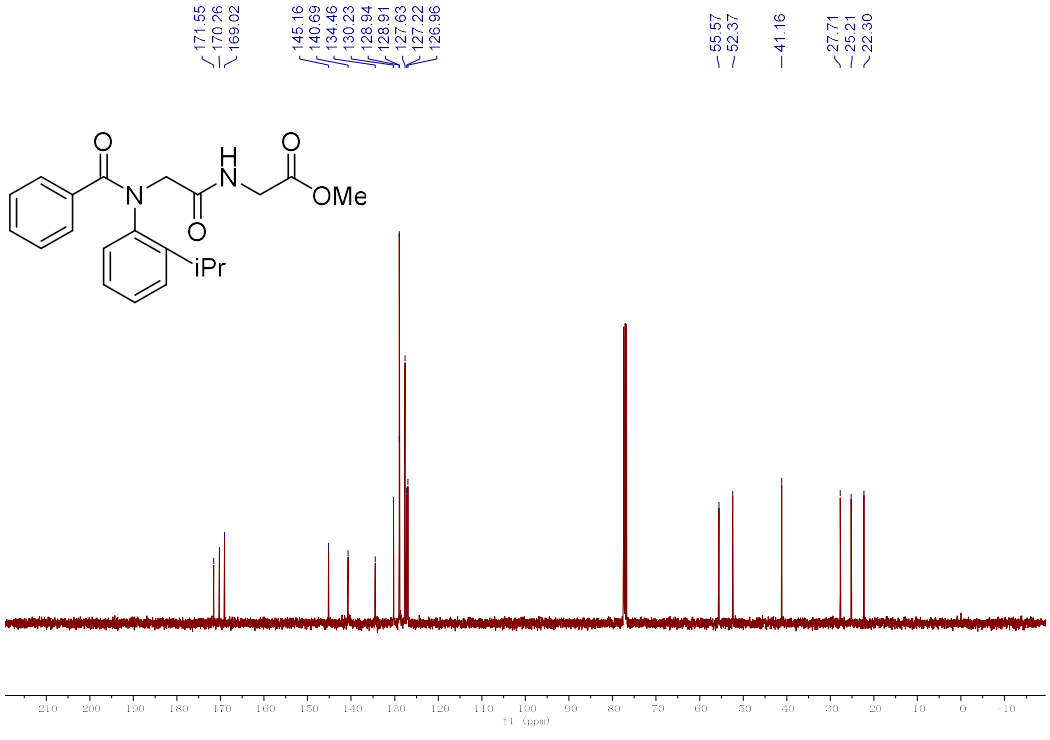
7.3115
7.2475
7.2165
7.1970
7.1479
7.1289
7.1102
4.8535
4.8166
4.1905
4.1763
4.1449
4.1307
4.0812
4.0441
4.0045
3.9914
3.7491
2.9611
2.9440
2.9268
2.9098
2.8925
1.0887
1.0716
0.7379
0.7208
O
H
N
O
N
OMe
O
iPr
4.00
6.00
1.00
3.04
3.01
1.02
3.02
3.00
f1 (ppm)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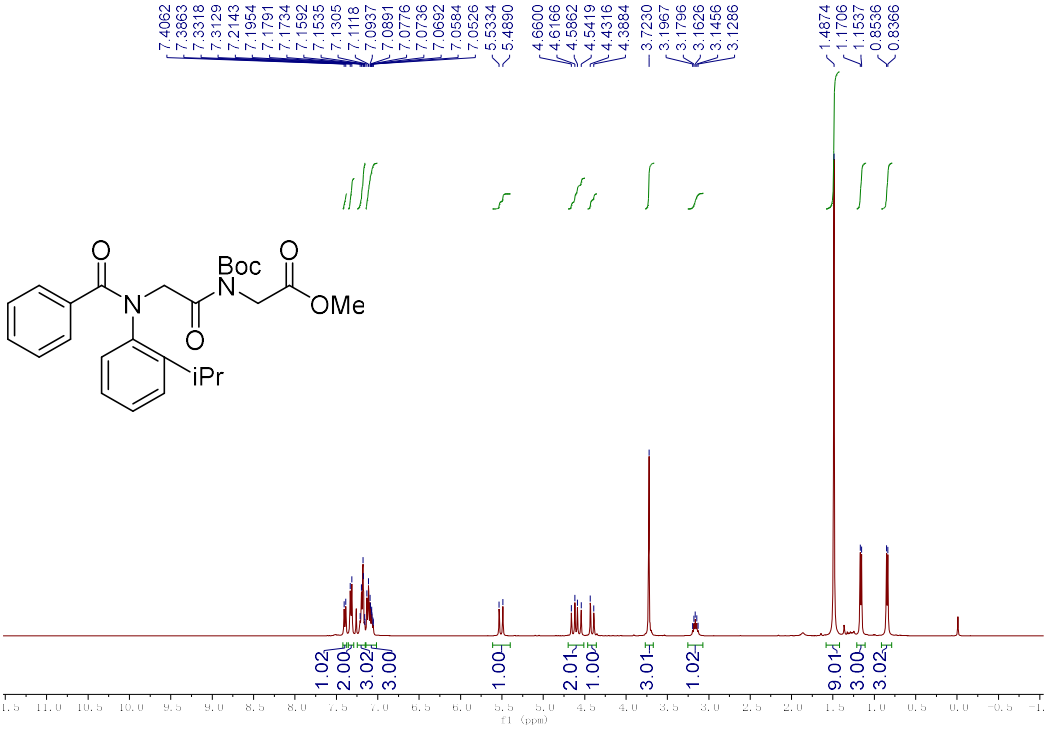
169.02
145.16
140.69
134.46
130.23
128.94
128.91
127.63
127.22
126.96
55.57
52.37
41.16
27.71
25.21
22.30
O
H
N
O
N
OMe
O
iPr
f1 (ppm)

***rac*-1c**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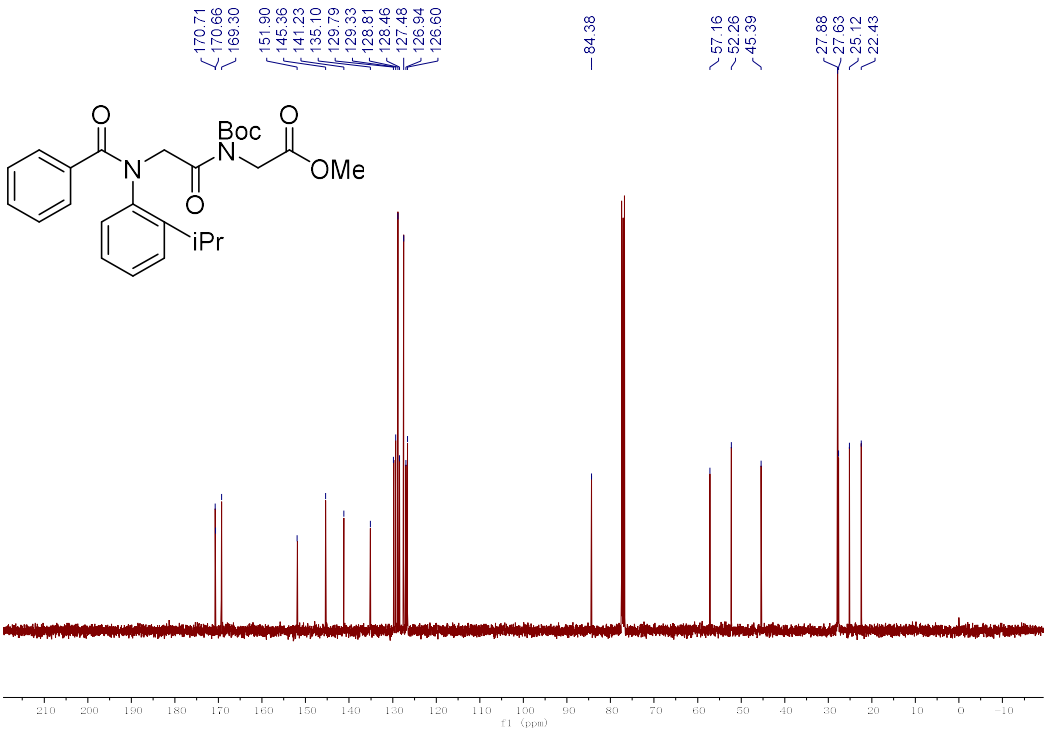
7.3863
7.3318
7.3129
7.2143
7.1954
7.1791
7.1734
7.1592
7.1535
7.1305
7.1118
7.0937
7.0891
7.0776
7.0736
7.0692
7.0584
7.0526
5.5334
5.4890
4.6600
4.6166
4.5862
4.5419
4.4316
4.3884
3.7230
3.1967
3.1796
3.1626
3.1456
3.1286
1.4874
1.1706
1.1537
0.8536
0.8366
Boc
N
O
OMe
iPr
1.02
2.00
3.02
3.00
1.00
2.01
1.00
3.01
1.02
9.01
3.00
3.02
f1 (ppm)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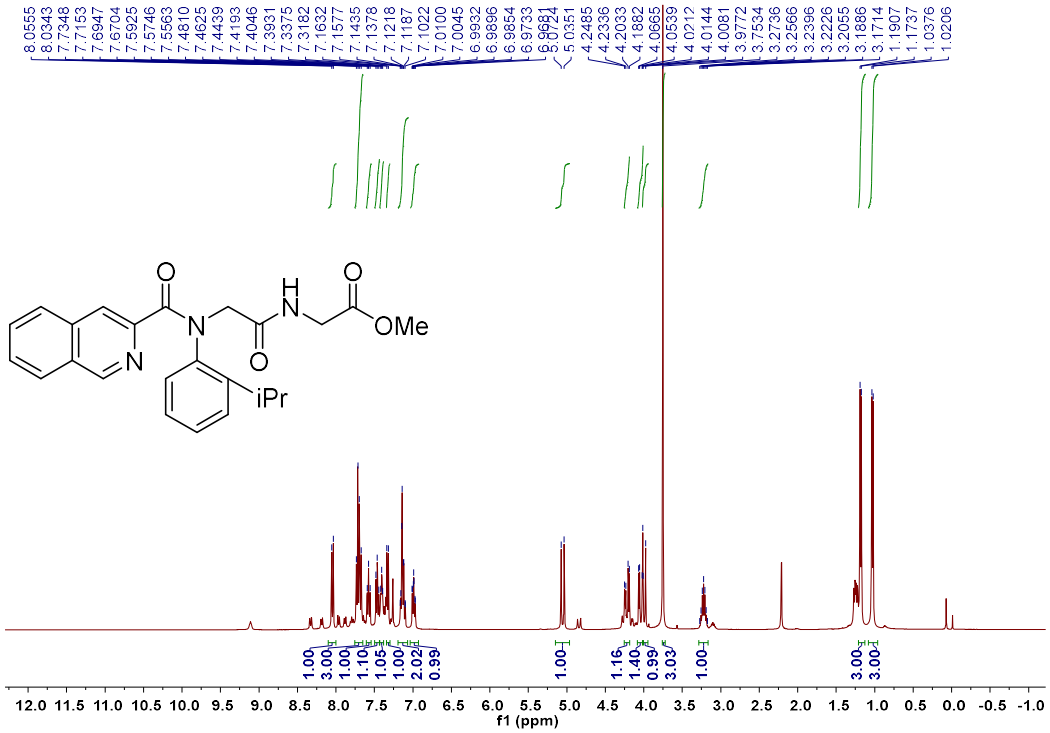
170.66
169.30
151.90
145.36
141.23
135.10
129.79
129.33
128.81
128.46
127.48
126.94
126.60
84.38
57.16
52.26
45.39
27.88
27.63
25.12
22.43
Boc
N
O
OMe
iPr
f1 (ppm)

***rac*-1d**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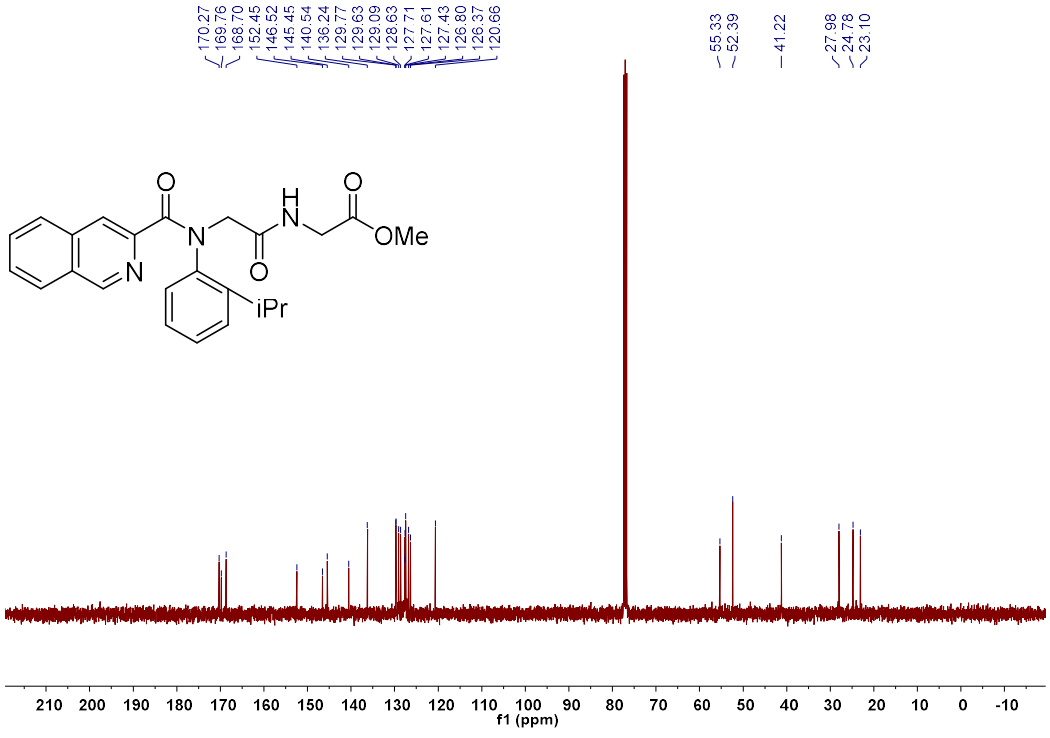
7.4625
7.4439
7.4193
7.4046
7.3931
7.3375
7.3182
7.1632
7.1577
7.1435
7.1378
7.1218
7.1187
7.1022
7.0100
7.0045
6.9932
6.9886
6.9854
6.9733
6.9681
5.0724
5.0351
4.2485
4.2336
4.2033
4.1882
4.0665
4.0539
4.0212
4.0144
4.0081
3.9772
3.7534
3.2736
3.2566
3.2396
3.2226
3.2055
3.1886
3.1714
1.1907
1.1737
1.0376
1.0206
O
N
H
N
O
O
OMe
iPr
1.00
3.00
1.00
1.10
1.05
1.00
2.02
0.99
1.00
1.16
1.40
0.99
3.03
1.00
3.00
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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146.52
145.45
140.54
136.24
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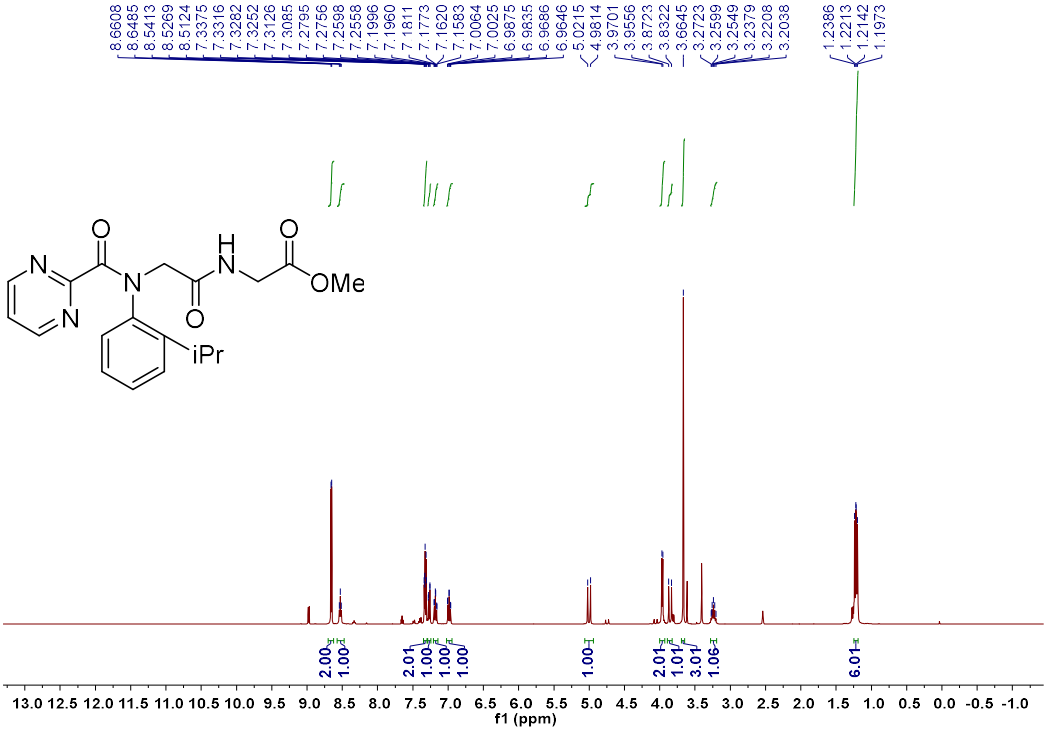
129.09
128.63
127.71
127.61
127.43
126.80
126.37
120.66
55.33
52.39
41.22
27.98
24.78
23.10
O
N
H
N
O
O
OMe
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

***rac*-1e**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7.3316
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7.3126
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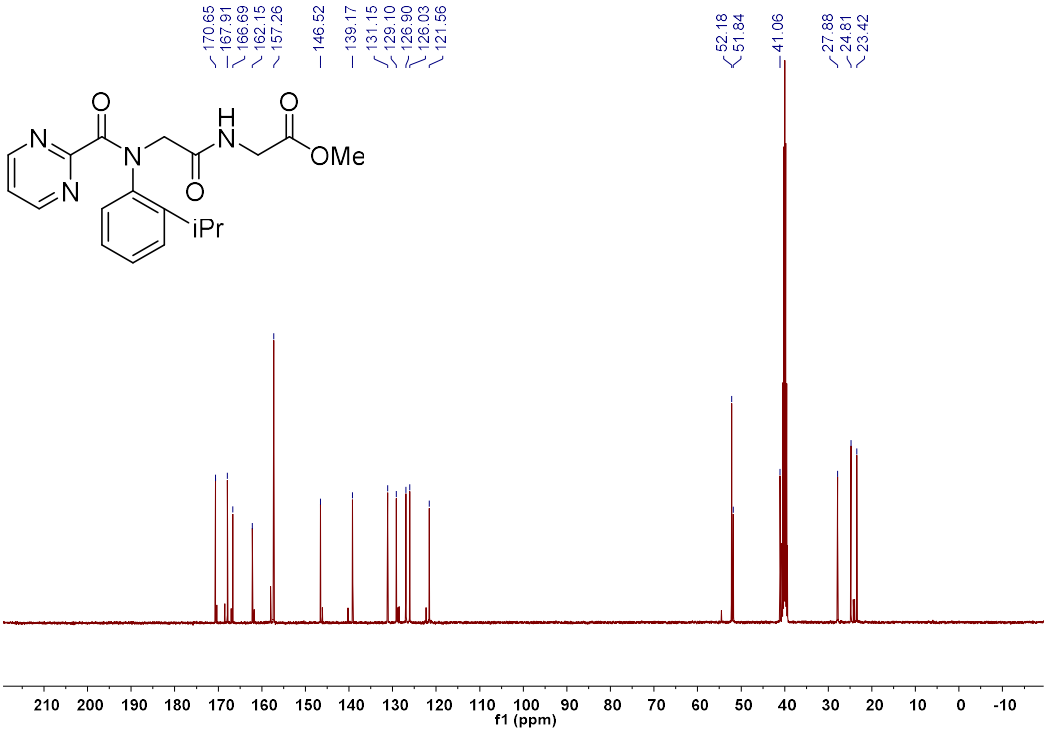
7.2795
7.2756
7.2598
7.2558
7.1996
7.1960
7.1811
7.1773
7.1620
7.1583
7.0064
7.0025
6.9875
6.9835
6.9686
6.9646
5.0215
4.9814
3.9701
3.9556
3.8723
3.8322
3.6645
3.2723
3.2599
3.2549
3.2379
3.2208
3.2038
1.2386
1.2213
1.2142
1.1973
N
O
H
N
O
OMe
N
O
iPr
2.00
1.00
2.01
1.00
1.00
1.00
1.00
2.01
1.01
3.01
1.06
6.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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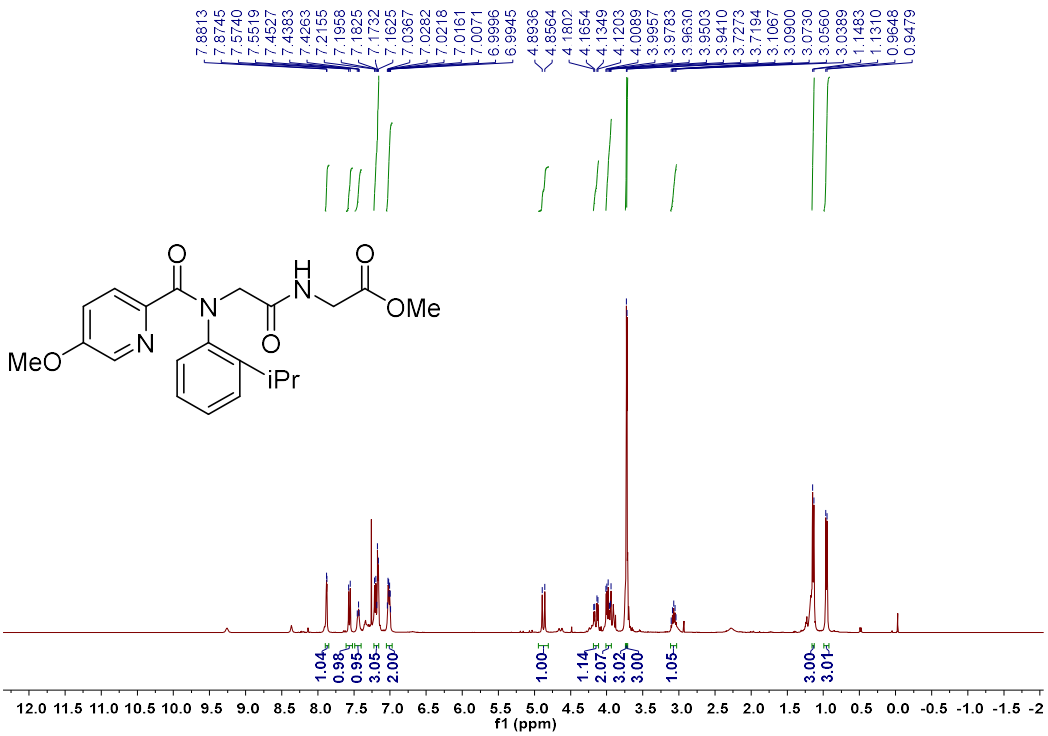
146.52
139.17
131.15
129.10
126.90
126.03
121.56
52.18
51.84
41.06
27.88
24.81
23.42
N
O
H
N
O
OMe
N
O
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

***rac*-1f**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7.4263
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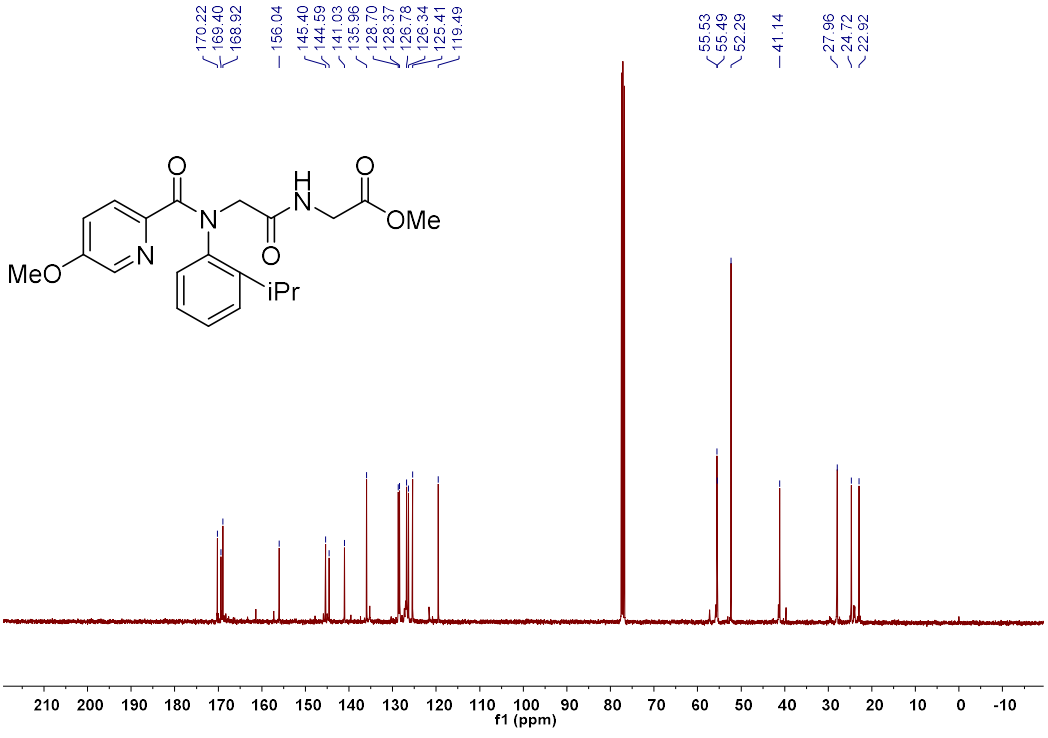
7.1958
7.1825
7.1732
7.1625
7.0367
7.0282
7.0218
7.0161
7.0071
6.9996
6.9945
4.8936
4.8564
4.1802
4.1654
4.1349
4.1203
4.0089
3.9957
3.9783
3.9630
3.9503
3.9410
3.7273
3.7194
3.1067
3.0900
3.0730
3.0560
3.0389
1.1483
1.1310
0.9648
0.9479
O
N
H
N
O
O
OMe
MeO
N
O
iPr
1.04
0.98
0.95
3.05
2.00
1.00
1.14
2.07
3.02
3.00
1.05
3.00
3.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2
f1 (ppm)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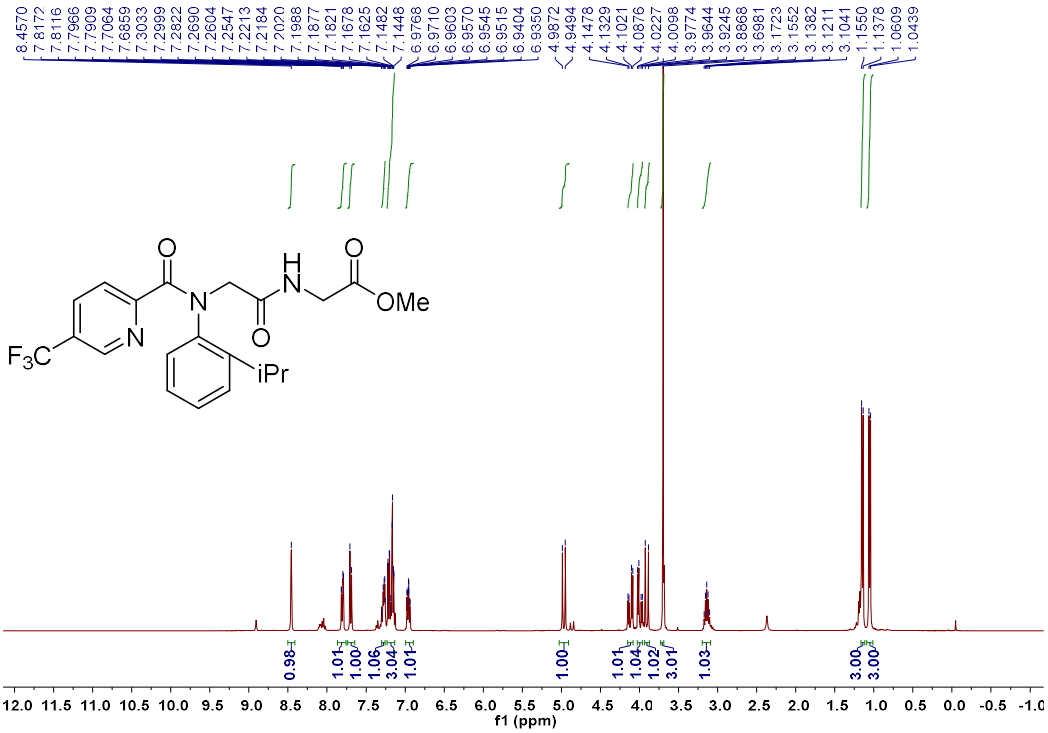
145.40
144.59
141.03
135.96
128.70
128.37
126.78
126.34
125.41
119.49
55.53
55.49
52.29
41.14
27.96
24.72
22.92
O
N
H
N
O
O
OMe
MeO
N
O
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

***rac*-1g**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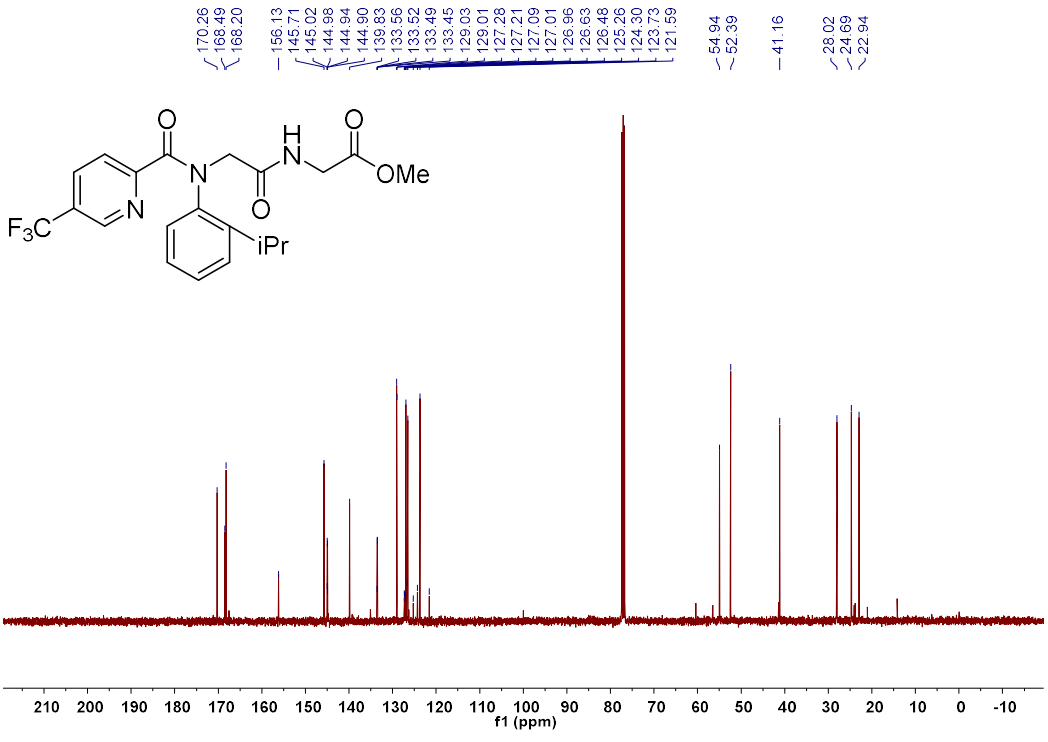
7.3033
7.2999
7.2822
7.2690
7.2604
7.2547
7.2213
7.2184
7.2020
7.1988
7.1877
7.1821
7.1678
7.1625
7.1482
7.1448
6.9768
6.9710
6.9603
6.9570
6.9545
6.9515
6.9404
6.9350
4.9872
4.9494
4.1478
4.1329
4.1021
4.0876
4.0227
4.0098
3.9774
3.9644
3.9245
3.8868
3.6981
3.1723
3.1552
3.1382
3.1211
3.1041
1.1550
1.1378
1.0609
1.0439
O
H
N
O
N
OMe
O
N
F3C
iPr
0.98
1.01
1.00
1.06
3.04
1.01
1.00
1.01
1.04
1.02
3.01
1.03
3.00
3.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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156.13
145.71
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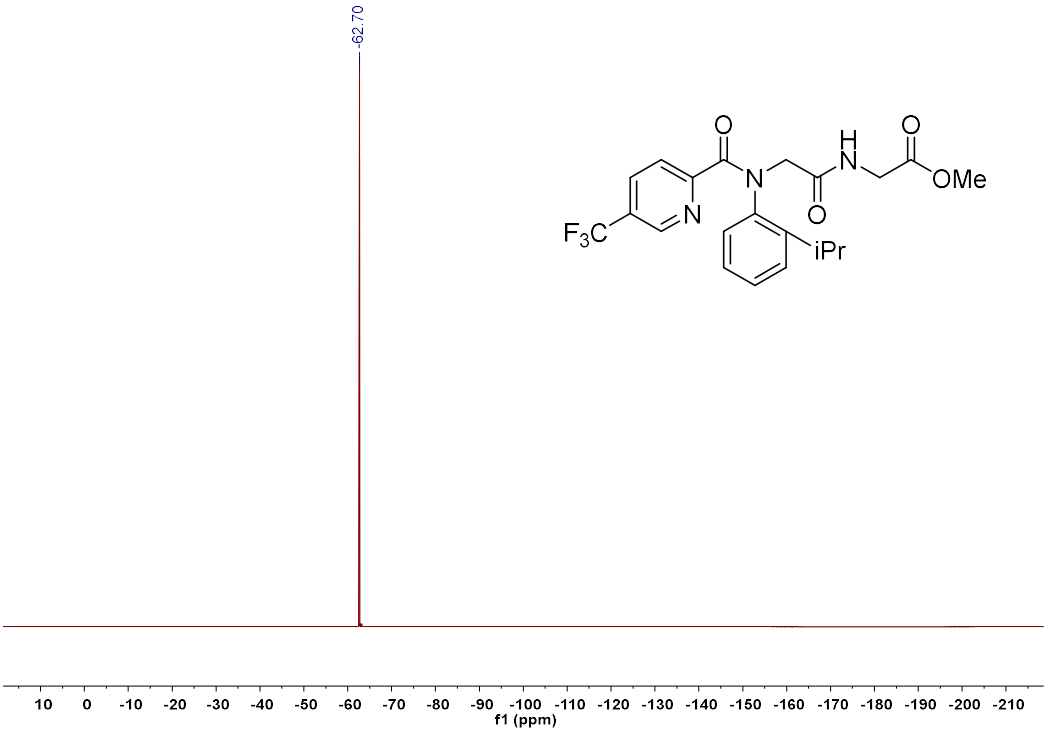
144.94
144.90
139.83
133.56
133.52
133.49
133.45
129.03
129.01
127.28
127.21
127.09
127.01
126.96
126.63
126.48
125.26
124.30
123.73
121.59
54.94
52.39
41.16
28.02
24.69
22.94
O
H
N
O
N
OMe
O
N
F3C
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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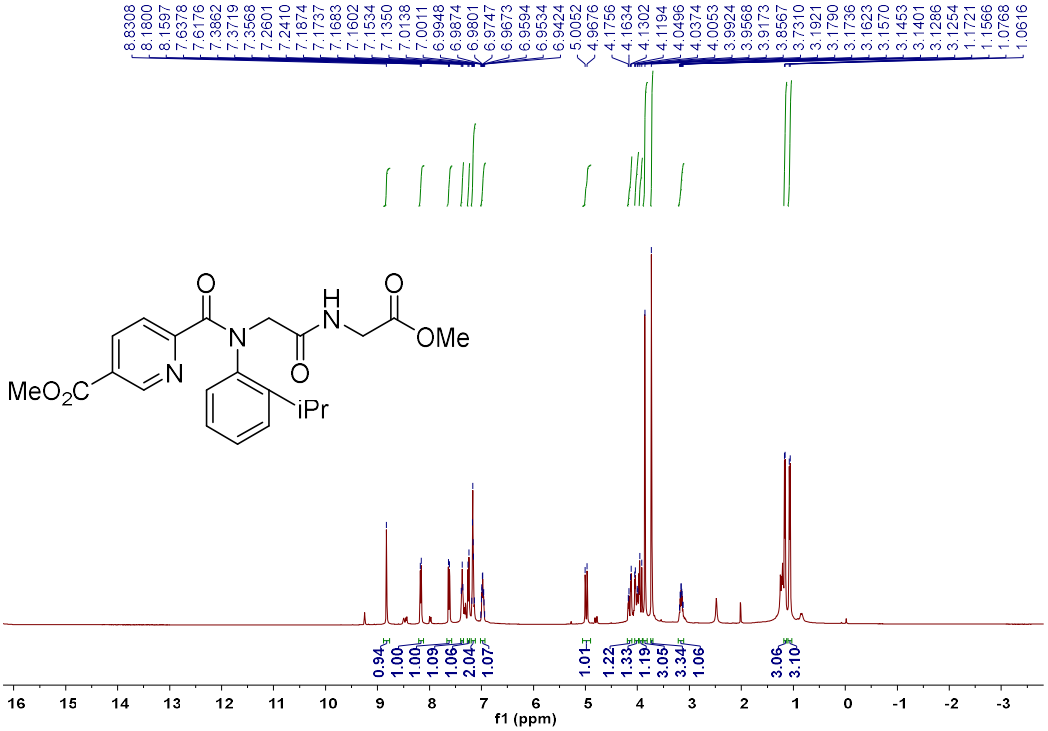
H
N
O
N
N
O
OMe
F3C
iPr
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

***rac*-1h**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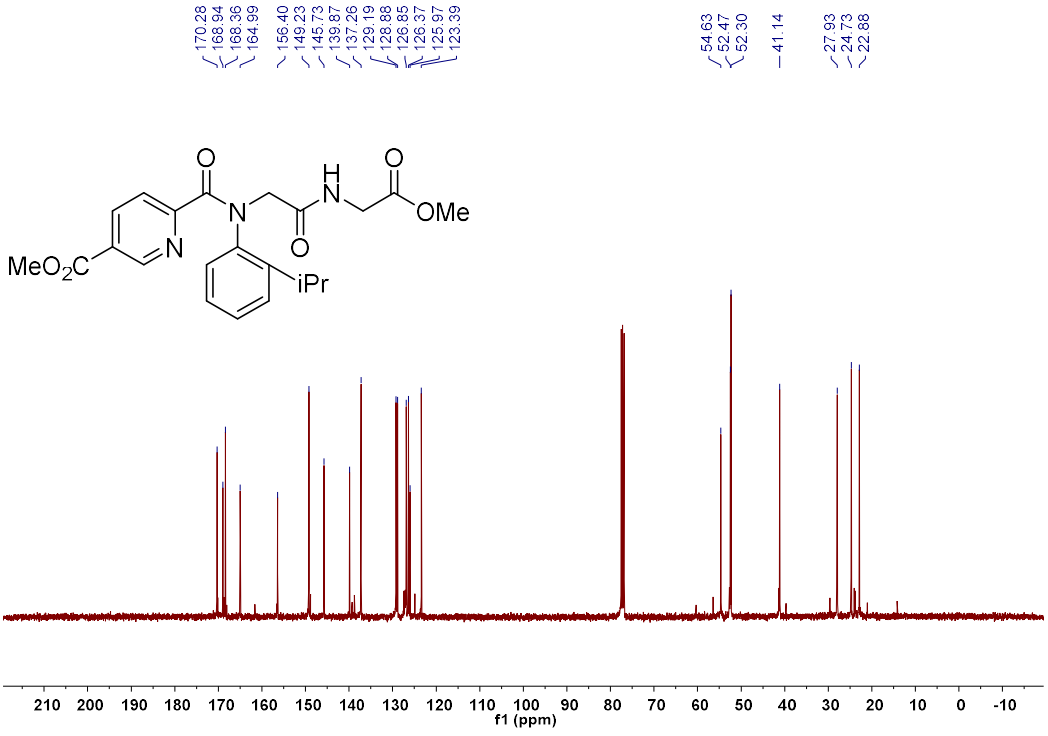
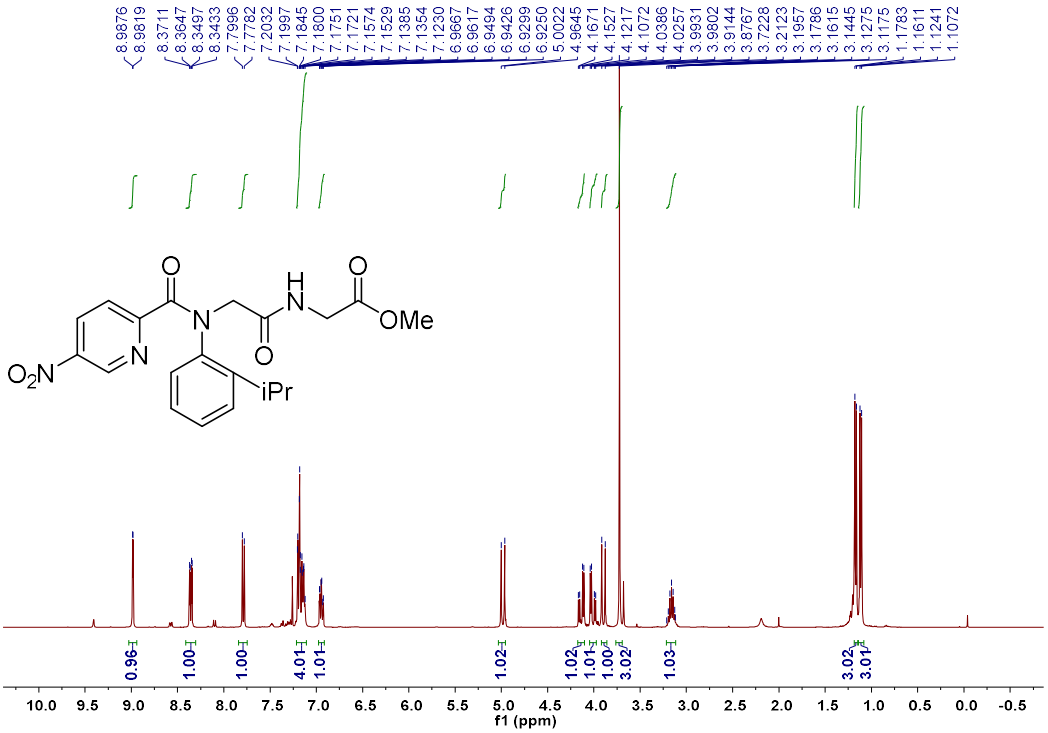
7.3719
7.3568
7.2601
7.2410
7.1874
7.1737
7.1683
7.1602
7.1534
7.1350
7.0138
7.0011
6.9948
6.9874
6.9801
6.9747
6.9673
6.9594
6.9534
6.9424
5.0052
4.9676
4.1756
4.1634
4.1302
4.1194
4.0496
4.0374
4.0053
3.9924
3.9568
3.9173
3.8567
3.7310
3.1921
3.1790
3.1736
3.1623
3.1570
3.1453
3.1401
3.1286
3.1254
1.1721
1.1566
1.0768
1.0616
MeO2C
N
O
N
H
N
O
O
OMe
iPr
0.94
1.00
1.00
1.09
1.06
2.04
1.07
1.01
1.22
1.33
1.19
3.05
3.34
1.06
3.06
3.10
f1 (ppm)


170.28
168.94
168.36
164.99
156.40
149.23
145.73
139.87
137.26
129.19
128.88
126.85
126.37
125.97
123.39
54.63
52.47
52.30
41.14
27.93
24.73
22.88
MeO2C
N
O
N
H
N
O
O
OMe
iPr
f1 (ppm)

***rac*-1i**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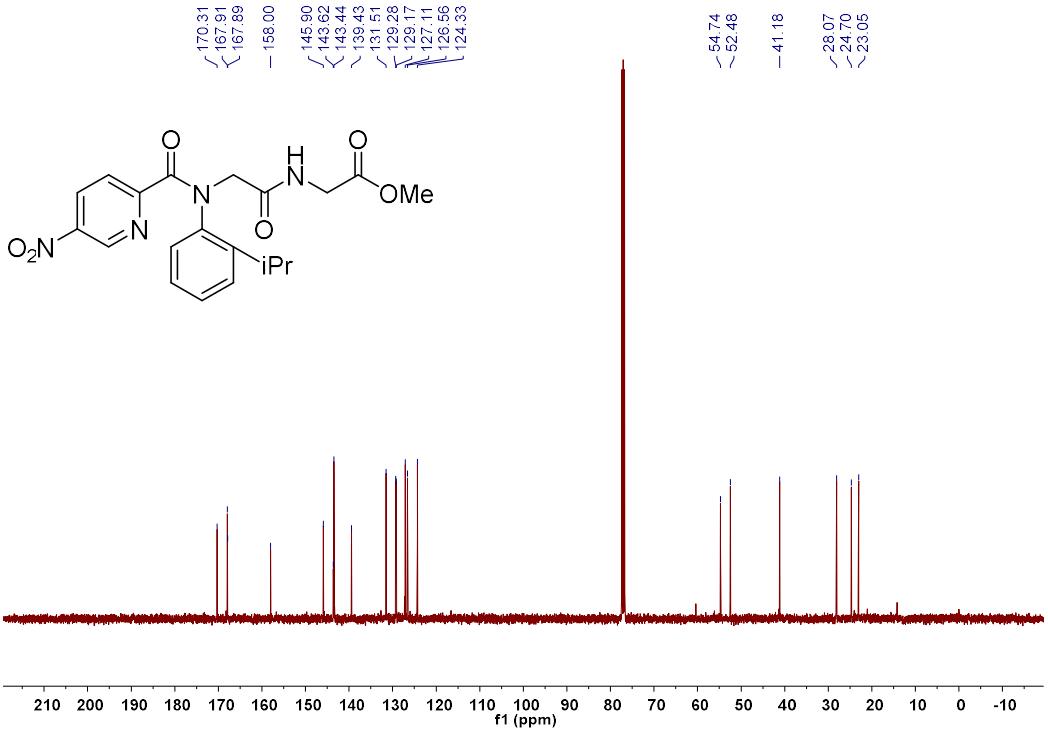
8.3433
7.7996
7.7782
7.2032
7.1997
7.1845
7.1800
7.1751
7.1721
7.1574
7.1529
7.1385
7.1354
7.1230
6.9667
6.9617
6.9494
6.9426
6.9299
6.9250
5.0022
4.9645
4.1671
4.1527
4.1217
4.1072
4.0386
4.0257
3.9931
3.9802
3.9144
3.8767
3.7228
3.2123
3.1957
3.1786
3.1615
3.1445
3.1275
3.1175
1.1783
1.1611
1.1241
1.1072
O
N
O
H
N
O
OMe
O
N
O2N
iPr
0.96
1.00
1.00
4.01
1.01
1.02
1.02
1.01
1.00
3.02
1.03
3.02
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


170.31
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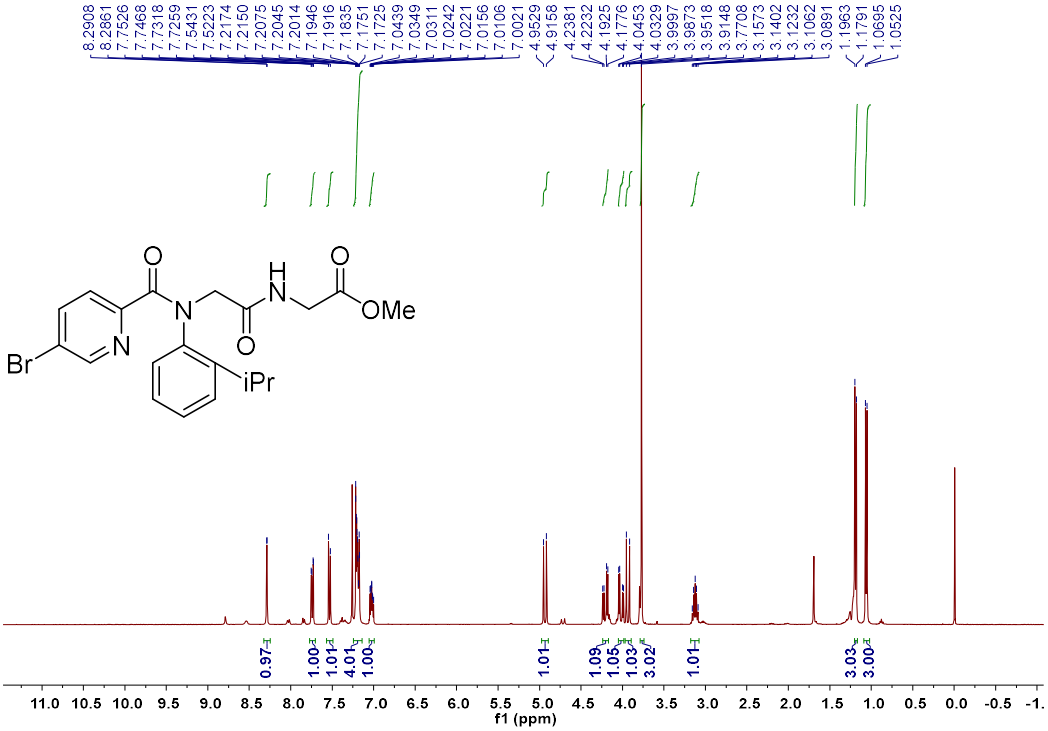
167.89
158.00
145.90
143.62
143.44
139.43
131.51
129.28
129.17
127.11
126.56
124.33
54.74
52.48
41.18
28.07
24.70
23.05
O
N
O
H
N
O
OMe
O
N
O2N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

***rac*-1j**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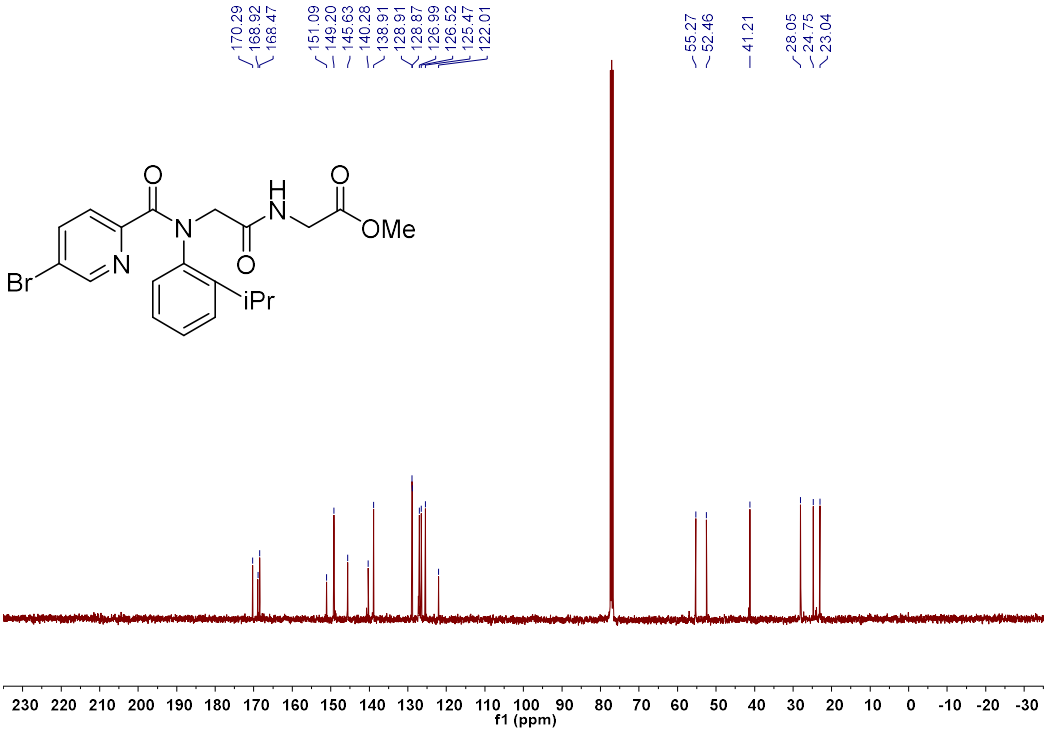
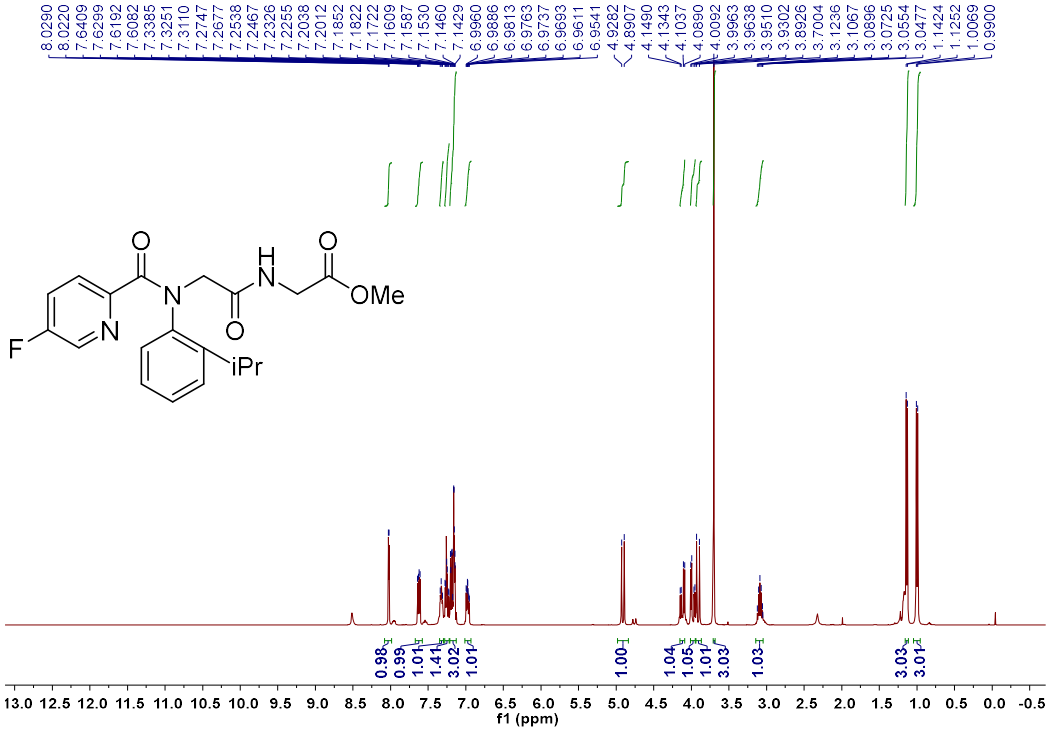
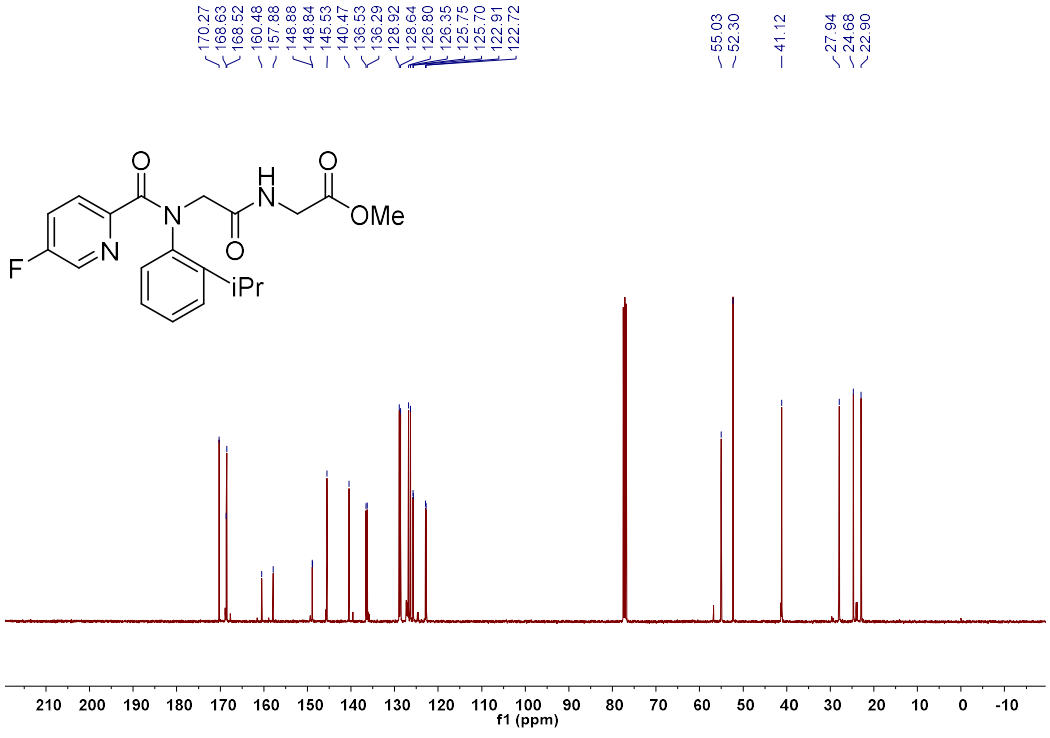
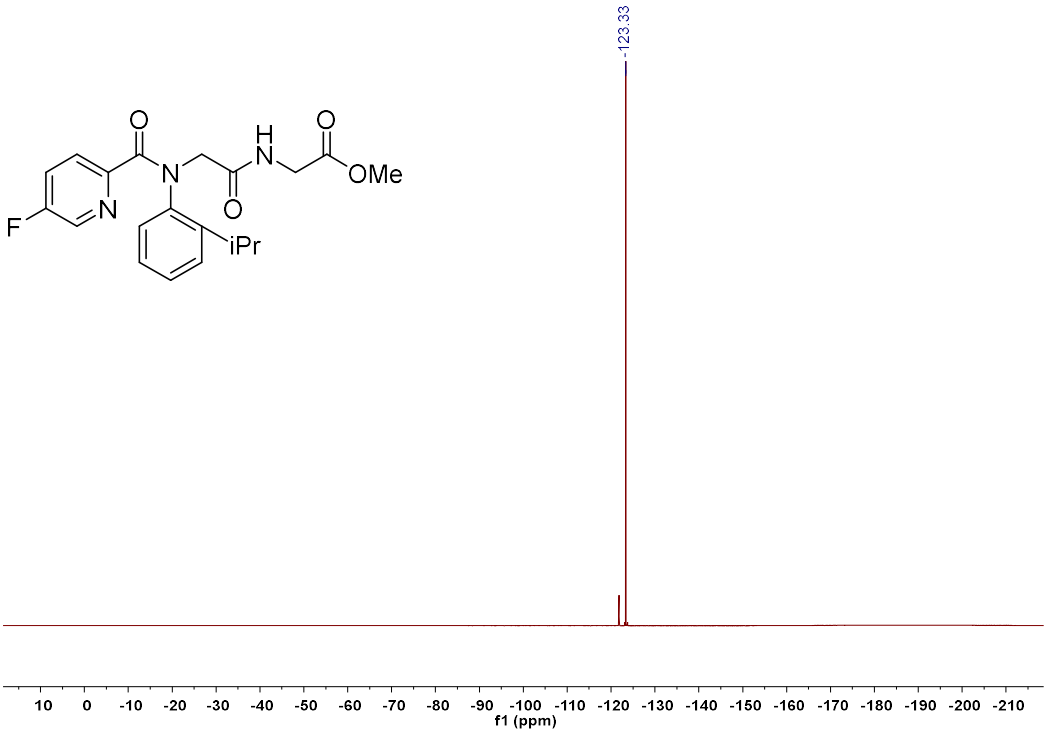
7.7318
7.7259
7.5431
7.5223
7.2174
7.2150
7.2075
7.2045
7.2014
7.1946
7.1916
7.1835
7.1751
7.1725
7.0439
7.0349
7.0311
7.0242
7.0221
7.0156
7.0106
7.0021
4.9529
4.9158
4.2381
4.2232
4.1925
4.1776
4.0453
4.0329
3.9957
3.9873
3.9518
3.9148
3.7708
3.1573
3.1402
3.1232
3.1062
3.0691
1.1963
1.1791
1.0695
1.0525
O
N
H
N
O
OMe
Br
N
O
iPr
0.97
1.00
1.01
4.01
1.00
1.01
1.09
1.05
1.03
3.02
1.01
3.03
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)


170.29
168.92
168.47
151.09
149.20
145.63
140.28
138.91
128.91
128.87
126.99
126.52
125.47
122.01
55.27
52.46
41.21
28.05
24.75
23.04
O
N
H
N
O
OMe
Br
N
O
iPr
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30
f1 (ppm)

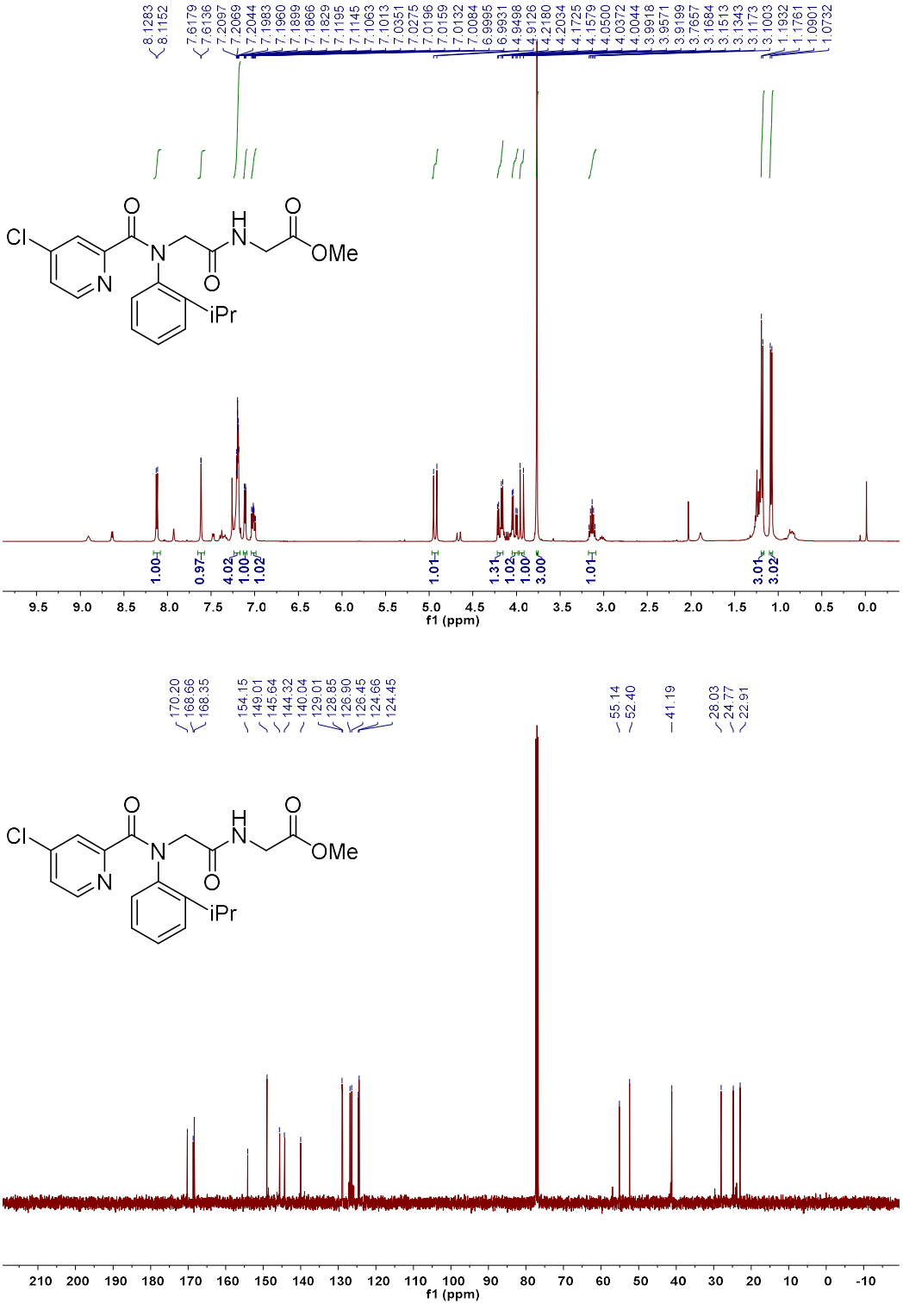
***rac*-1k**


8.0290
8.0220
7.6409
7.6299
7.6192
7.6082
7.3385
7.3251
7.3110
7.2747
7.2677
7.2538
7.2467
7.2326
7.2255
7.2038
7.2012
7.1852
7.1822
7.1722
7.1609
7.1587
7.1530
7.1460
7.1429
6.9960
6.9886
6.9813
6.9763
6.9737
6.9693
6.9611
6.9541
4.9282
4.8907
4.1490
4.1343
4.1037
4.0890
4.0092
3.9963
3.9638
3.9510
3.9302
3.8926
3.7004
3.1236
3.1067
3.0886
3.0725
3.0554
3.0477
1.1424
1.1252
1.0069
0.9900
O
H
N
O
N
O
OMe
F
N
iPr
0.98
0.99
1.01
1.41
3.02
1.01
1.00
1.04
1.05
1.01
3.03
1.03
3.03
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

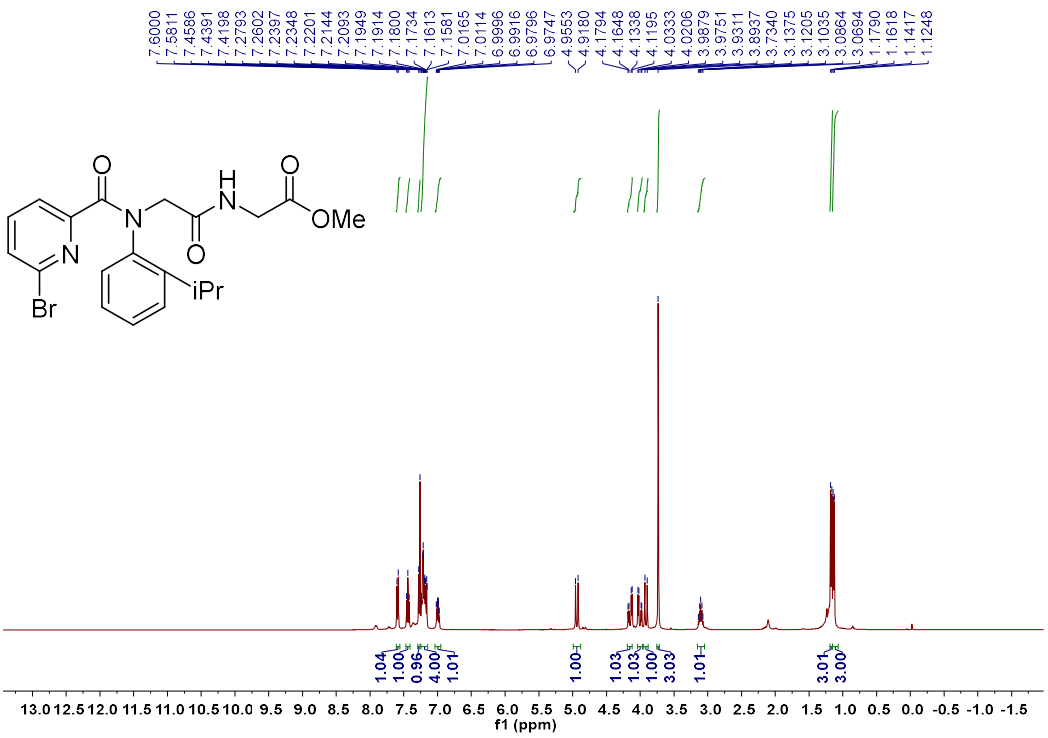

170.27
168.63
168.52
160.48
157.88
148.88
148.84
145.53
140.47
136.53
136.29
128.92
128.64
126.80
126.35
125.75
125.70
122.91
122.72
55.03
52.30
41.12
27.94
24.68
22.90
O
H
N
O
N
O
OMe
F
N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

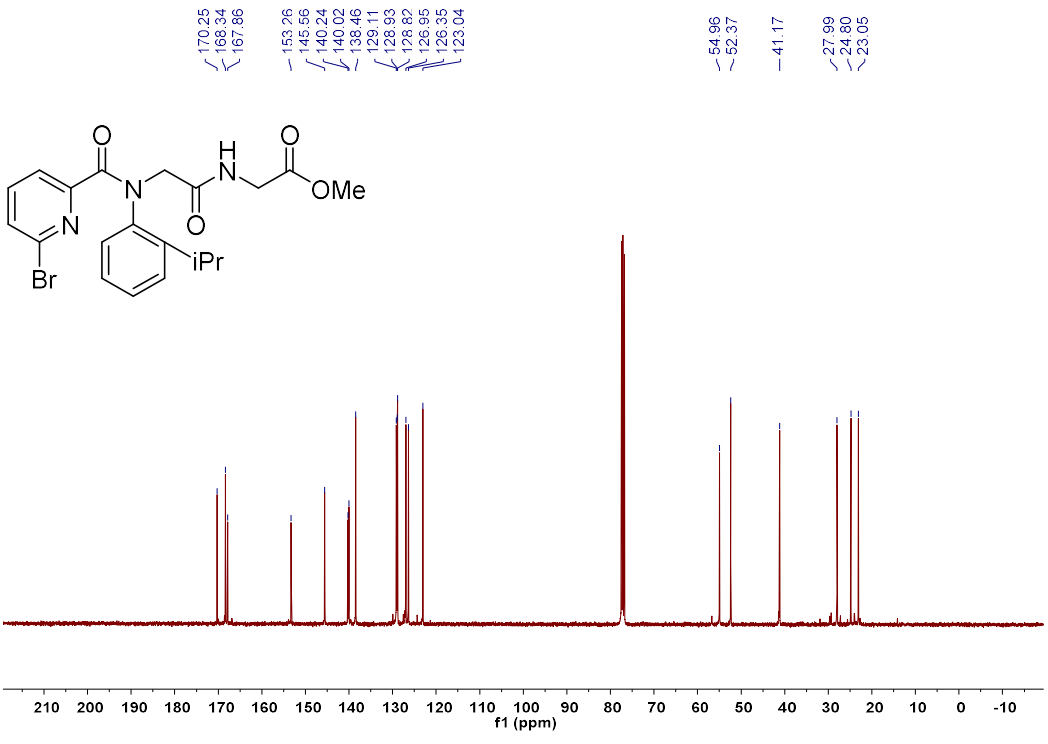

-123.33
O
N
H
N
O
OMe
F
N
iPr
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

***rac*-11**

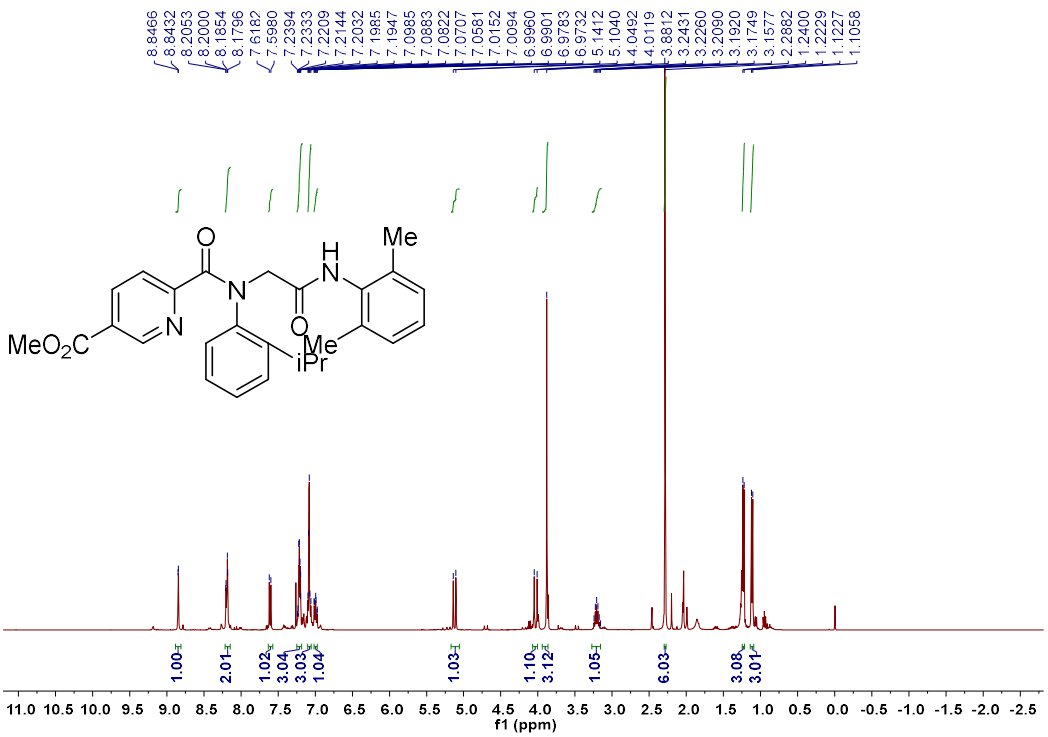

8.1283
8.1152
7.6179
7.6136
7.2097
7.2069
7.2044
7.1983
7.1960
7.1899
7.1866
7.1829
7.1195
7.1145
7.1063
7.1013
7.0351
7.0275
7.0196
7.0159
7.0132
7.0084
6.9995
6.9931
4.9498
4.9126
4.2180
4.2034
4.1725
4.1579
4.0500
4.0372
4.0044
3.9918
3.9571
3.9199
3.7657
3.1684
3.1513
3.1343
3.1173
3.1003
1.1932
1.1761
1.0901
1.0732
Cl
N
O
N
H
N
O
O
OMe
iPr
1.00
0.97
4.02
1.00
1.02
1.01
1.31
1.02
1.00
3.00
1.01
3.01
3.02
f1 (ppm)
170.20
168.66
168.35
154.15
149.01
145.64
144.32
140.04
129.01
128.85
126.90
126.45
124.66
124.45
55.14
52.40
41.19
28.03
24.77
22.91
f1 (ppm)

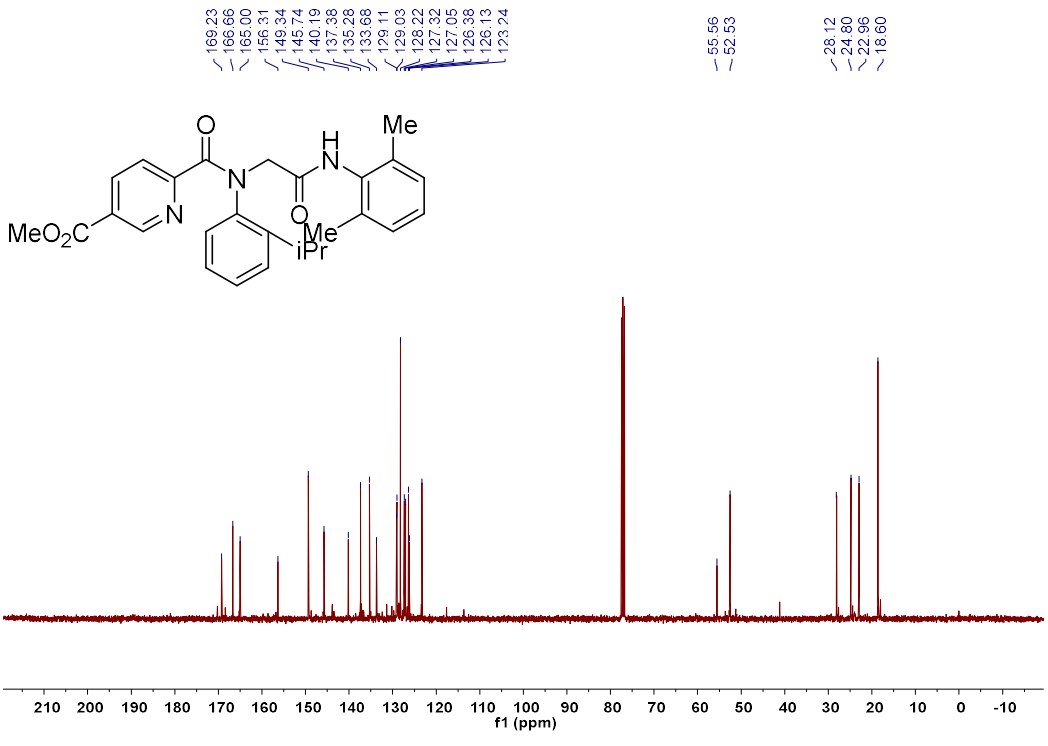
***rac*-1m**


7.6000
7.5811
7.4586
7.4391
7.4198
7.2793
7.2602
7.2397
7.2348
7.2201
7.2144
7.2093
7.1949
7.1914
7.1800
7.1734
7.1613
7.1581
7.0165
7.0114
6.9996
6.9916
6.9796
6.9747
4.9553
4.9180
4.1794
4.1648
4.1338
4.1195
4.0333
4.0206
3.9879
3.9751
3.9311
3.8937
3.7340
3.1375
3.1205
3.1035
3.0864
3.0694
1.1790
1.1618
1.1417
1.1248
O
H
N
O
N
OMe
O
N
Br
iPr
1.04
1.00
0.96
4.00
1.01
1.00
1.03
1.03
1.00
3.03
1.01
3.01
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

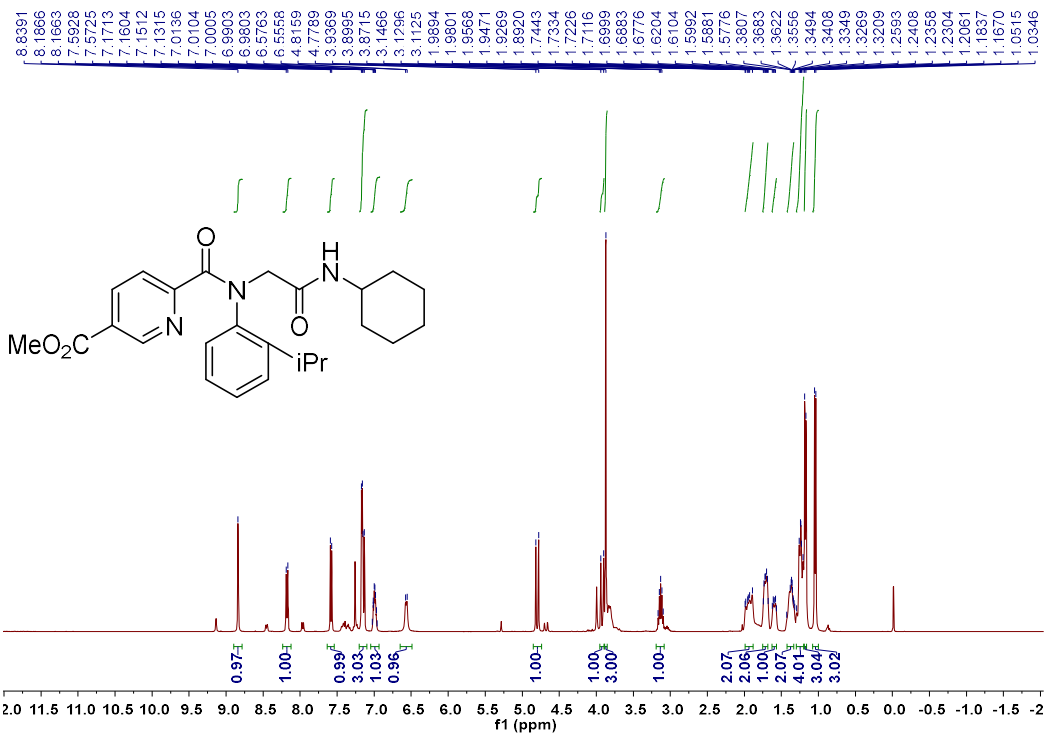

170.25
168.34
167.86
153.26
145.56
140.24
140.02
138.46
129.11
128.93
128.82
126.95
126.35
123.04
54.96
52.37
41.17
27.99
24.80
23.05
O
H
N
O
N
OMe
O
N
Br
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

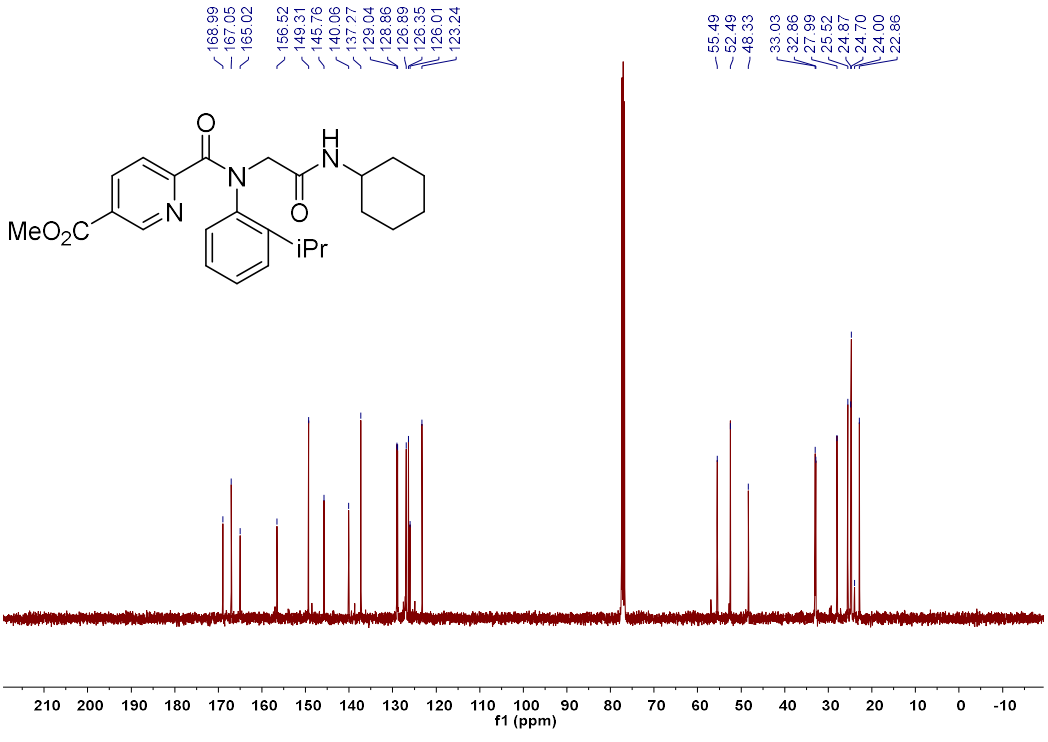
***rac*-4a**


8.8466
8.8432
8.2053
8.2000
8.1854
8.1796
7.6182
7.5980
7.2394
7.2333
7.2209
7.2144
7.2032
7.1985
7.1947
7.0965
7.0883
7.0822
7.0707
7.0581
7.0152
7.0094
6.9960
6.9901
6.9783
6.9732
5.1412
5.1040
4.0492
4.0119
3.8812
3.2431
3.2260
3.2090
3.1920
3.1749
3.1577
2.2882
2.2400
2.2229
1.1227
1.1058
MeO2C
N
O
N
H
N
O
Me
iPr
Me
1.00
2.01
1.02
3.04
3.03
1.04
1.03
1.10
3.12
1.05
6.03
3.08
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2.5
f1 (ppm)

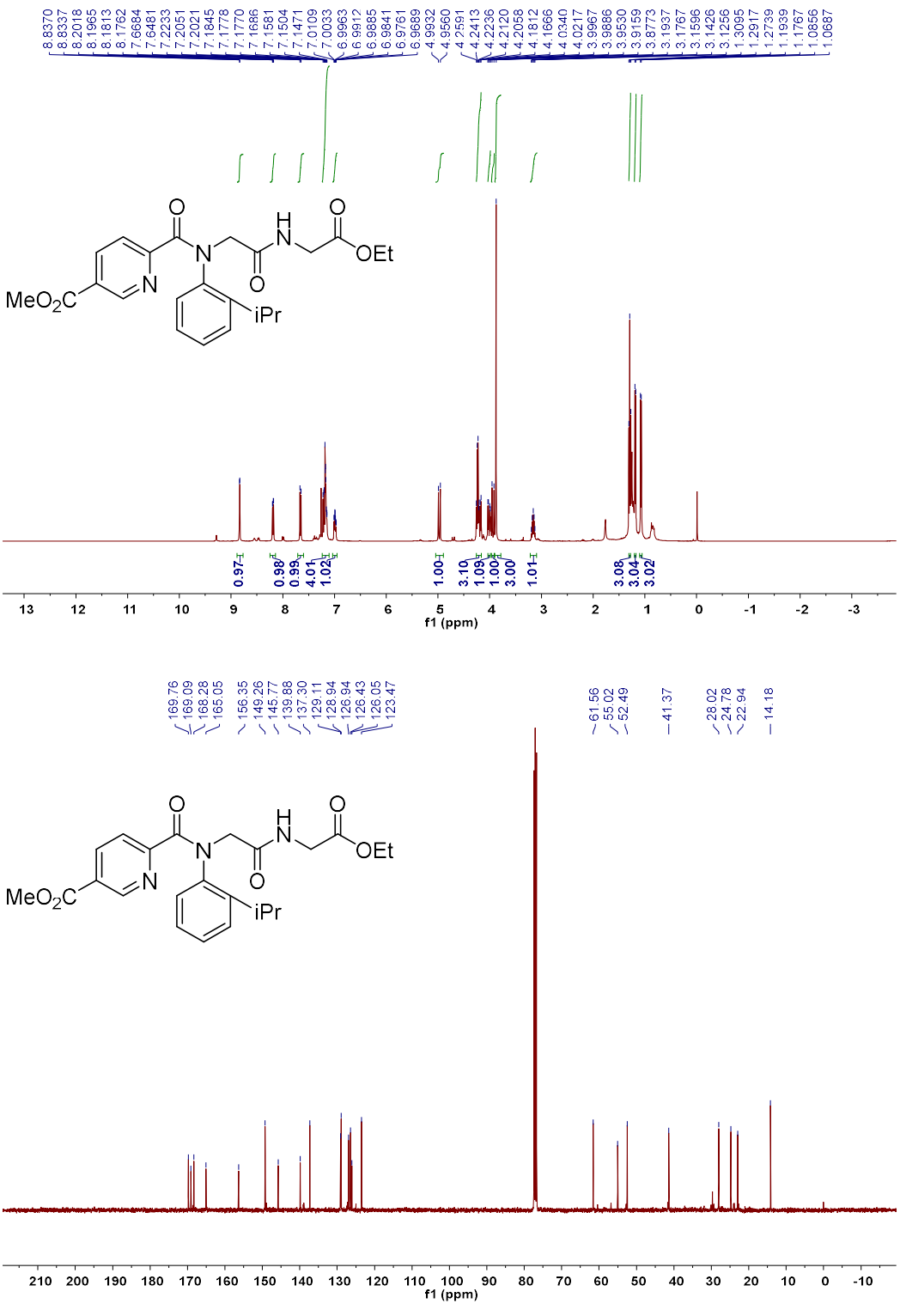

169.23
166.66
165.00
156.31
149.34
145.74
140.19
137.38
135.28
133.68
129.11
129.03
128.22
127.32
127.05
126.38
126.13
123.24
55.56
52.53
28.12
24.80
22.96
18.60
MeO2C
N
O
N
H
N
O
Me
iPr
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

***rac*-4b**

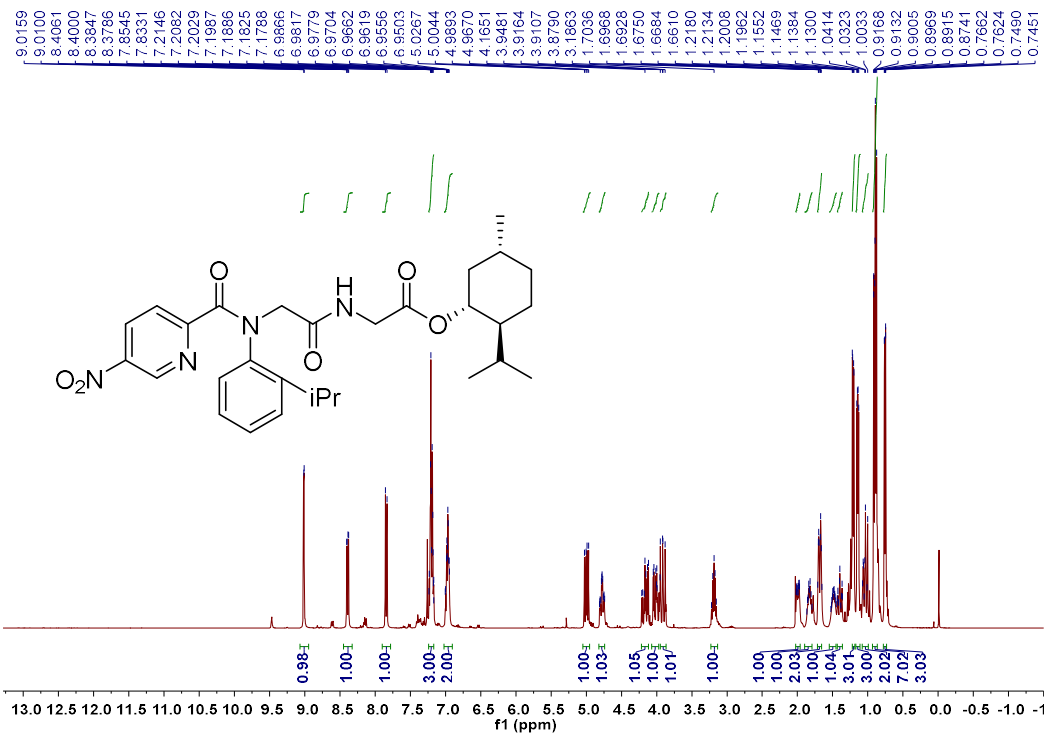

8.8391
8.1866
8.1663
7.5928
7.5725
7.1713
7.1604
7.1512
7.1315
7.0136
7.0104
7.0005
6.9903
6.9803
6.5763
6.5558
4.8159
4.7789
3.9369
3.8995
3.8715
3.1466
3.1296
3.1125
1.9894
1.9801
1.9568
1.9471
1.9269
1.8920
1.7443
1.7334
1.7226
1.7116
1.6999
1.6883
1.6776
1.6204
1.6104
1.5992
1.5881
1.5776
1.3807
1.3683
1.3622
1.3556
1.3494
1.3408
1.3349
1.3269
1.3209
1.2593
1.2408
1.2358
1.2304
1.2061
1.1837
1.1670
1.0515
1.0346
MeO2C
iPr
0.97
1.00
0.99
3.03
1.03
0.96
1.00
1.00
3.00
1.00
2.07
2.06
1.00
2.07
4.01
3.04
3.02
f1 (ppm)

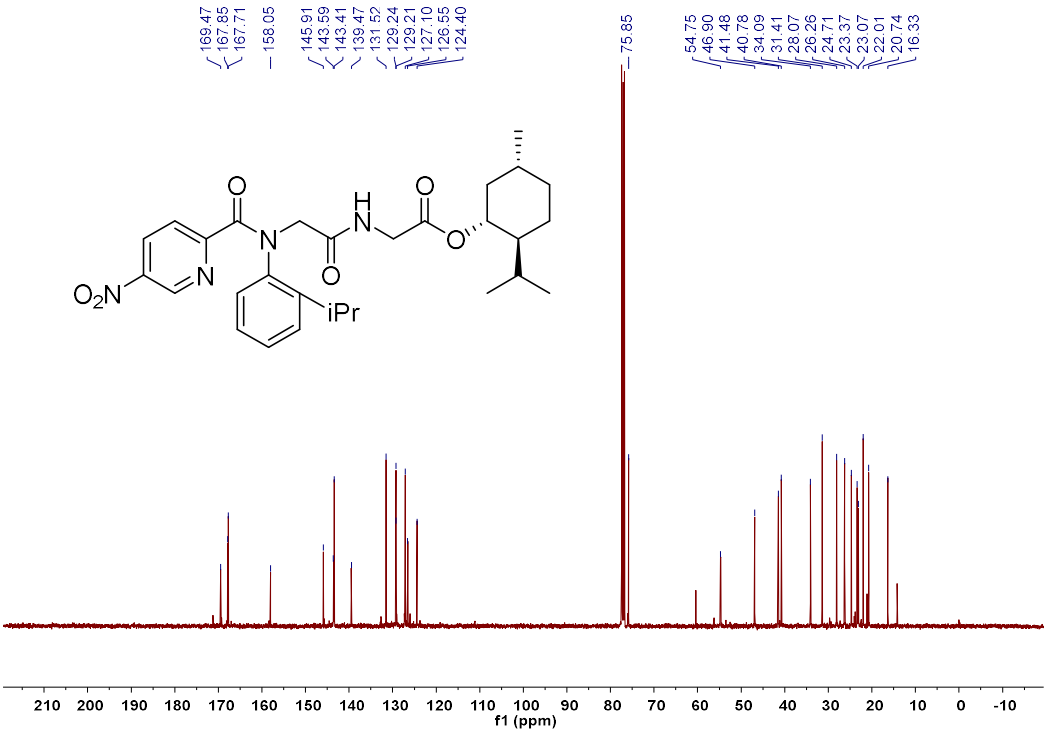

168.99
167.05
165.02
156.52
149.31
145.76
140.06
137.27
129.04
128.86
126.89
126.35
126.01
123.24
55.49
52.49
48.33
33.03
32.86
27.99
25.52
24.87
24.70
24.00
22.86
MeO2C
iPr
f1 (ppm)

***rac*-4c**

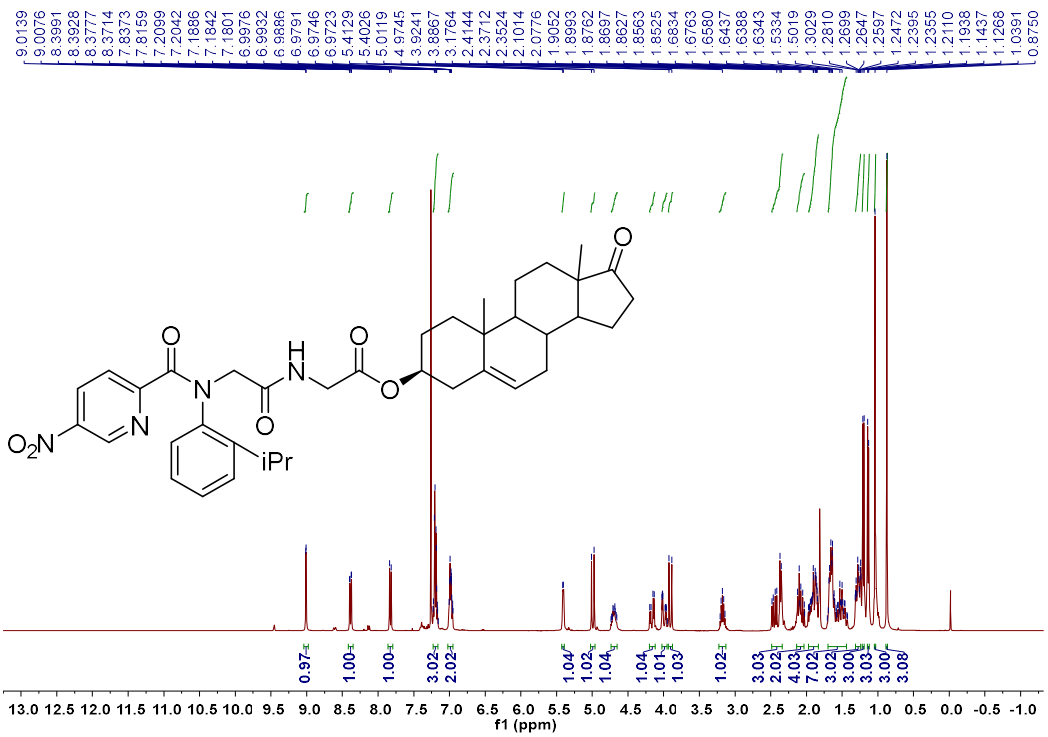

8.8370
8.8337
8.2018
8.1965
8.1813
8.1762
7.6884
7.6481
7.2233
7.2051
7.2021
7.1845
7.1778
7.1770
7.1686
7.1581
7.1504
7.1471
7.0109
7.0033
6.9963
6.9912
6.9885
6.9841
6.9761
6.9689
4.9932
4.9560
4.2591
4.2413
4.2236
4.2120
4.2058
4.1812
4.1666
4.0340
4.0217
3.9967
3.9886
3.9530
3.9159
3.8773
3.1937
3.1767
3.1596
3.1426
3.1256
1.3095
1.2917
1.2739
1.1939
1.1767
1.0856
1.0687
MeO2C
N
O
N
H
O
O
OEt
iPr
0.97
0.98
0.99
4.01
1.02
1.00
3.10
1.09
1.00
3.00
1.01
3.08
3.04
3.02
f1 (ppm)
169.76
169.09
168.28
165.05
156.35
149.26
145.77
139.88
137.30
129.11
128.94
126.94
126.43
126.05
123.47
61.56
55.02
52.49
41.37
28.02
24.78
22.94
14.18
f1 (ppm)

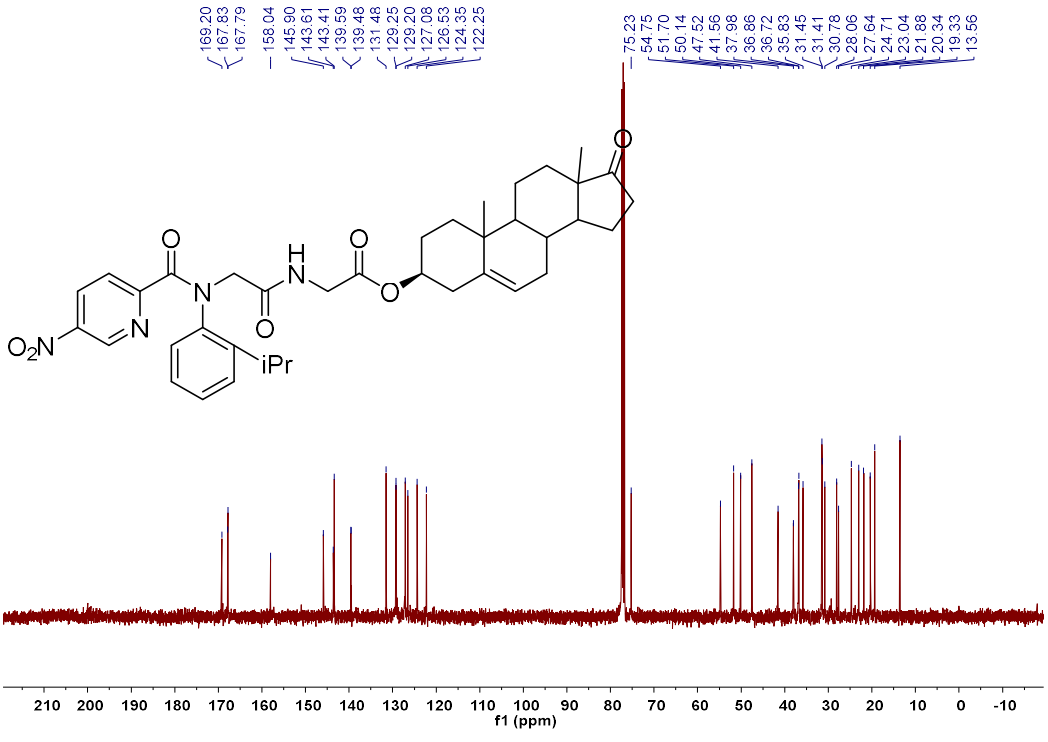
***rac*-4d**


9.0159
9.0100
8.4061
8.4000
8.3847
8.3786
7.8545
7.8331
7.2146
7.2082
7.2029
7.1987
7.1886
7.1825
7.1788
6.9866
6.9817
6.9779
6.9704
6.9662
6.9619
6.9556
6.9503
5.0267
5.0044
4.9893
4.9670
4.1651
3.9481
3.9164
3.9107
3.8790
3.1863
1.7036
1.6968
1.6928
1.6750
1.6684
1.6610
1.2180
1.2134
1.2008
1.1962
1.1552
1.1469
1.1384
1.1300
1.0414
1.0323
1.0033
0.9168
0.9132
0.9005
0.8969
0.8915
0.8741
0.7662
0.7624
0.7490
0.7451
O2N
iPr
0.98
1.00
1.00
3.00
2.00
1.00
1.03
1.05
1.00
1.01
1.00
1.00
1.00
2.03
1.00
1.04
3.01
3.00
2.02
7.02
3.03
f1 (ppm)

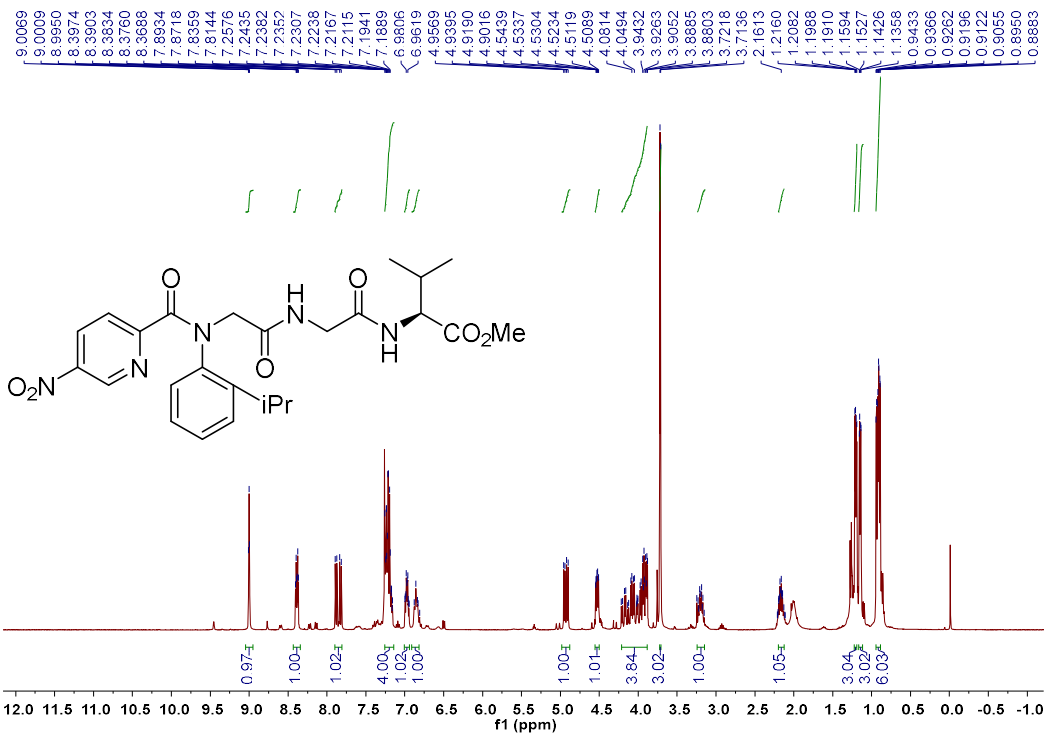

169.47
167.85
167.71
158.05
145.91
143.59
143.41
139.47
131.52
129.24
129.21
127.10
126.55
124.40
75.85
54.75
46.90
41.48
40.78
34.09
31.41
28.07
26.26
24.71
23.37
23.07
22.01
20.74
16.33
O2N
iPr
f1 (ppm)

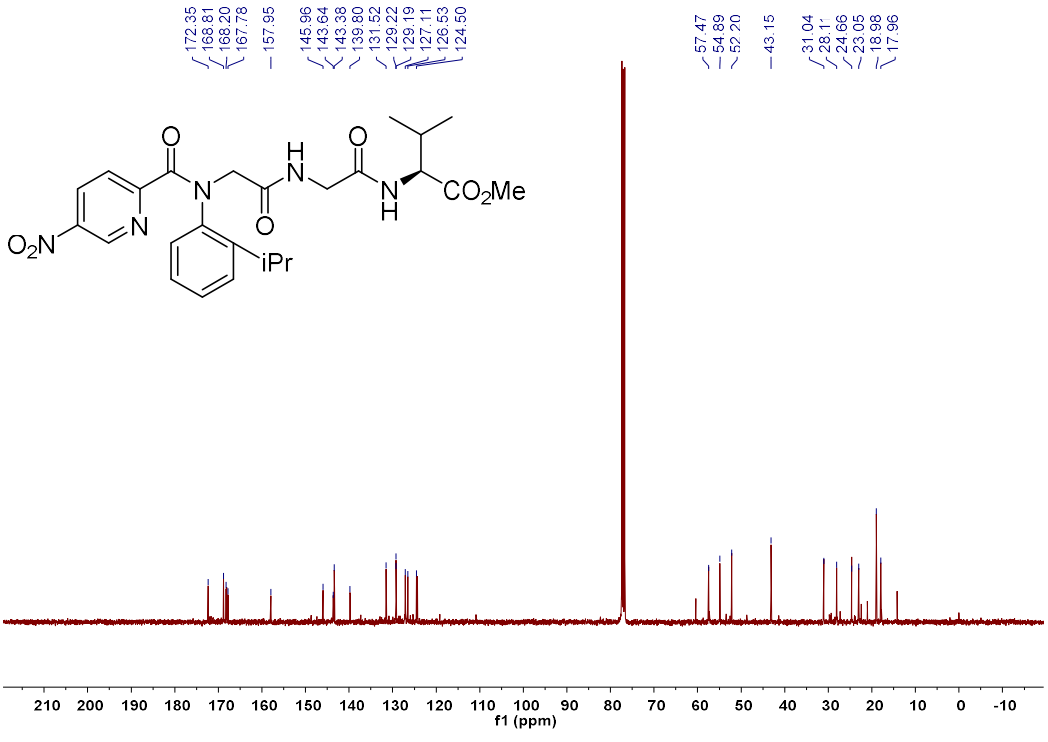
***rac*-4e**


9.0139
9.0076
8.3991
8.3928
8.3777
8.3714
7.8373
7.8159
7.2099
7.2042
7.1886
7.1842
7.1801
6.9976
6.9932
6.9886
6.9791
6.9746
6.9723
5.4129
5.4026
5.0119
4.9745
3.9241
3.8867
3.1764
2.4144
2.3712
2.3524
2.1014
2.0776
1.9052
1.8993
1.8762
1.8697
1.8627
1.8563
1.8525
1.6834
1.6763
1.6580
1.6437
1.6388
1.6343
1.5334
1.5019
1.3029
1.2810
1.2699
1.2647
1.2597
1.2472
1.2395
1.2355
1.2110
1.1938
1.1437
1.1268
1.0391
0.8750
O
O
N
O
H
N
O
O
O2N
N
O
iPr
0.97
1.00
1.00
3.02
2.02
1.04
1.02
1.04
1.04
1.01
1.03
1.02
3.03
2.02
4.03
7.02
3.02
3.00
3.03
3.00
3.08
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

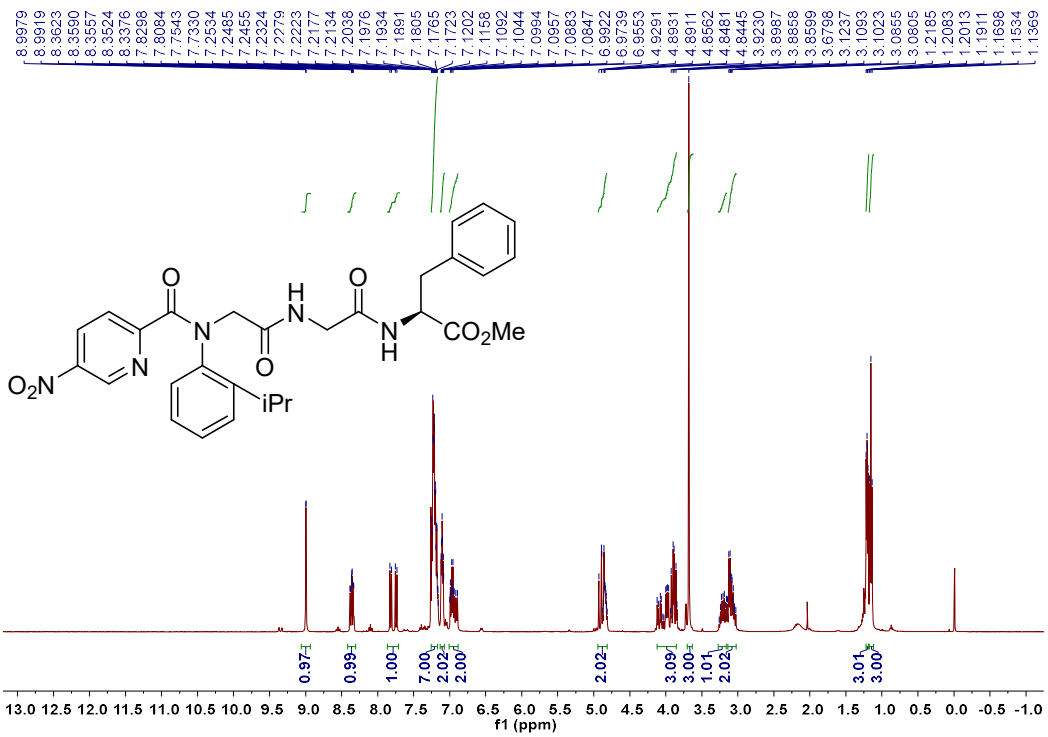

169.20
167.83
167.79
158.04
145.90
143.61
143.41
139.59
139.48
131.48
129.25
129.20
127.08
126.53
124.35
122.25
75.23
54.75
51.70
50.14
47.52
41.56
37.98
36.86
36.72
35.83
31.45
31.41
30.78
28.06
27.64
24.71
23.04
21.88
20.34
19.33
13.56
O
O
N
O
H
N
O
O
O2N
N
O
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

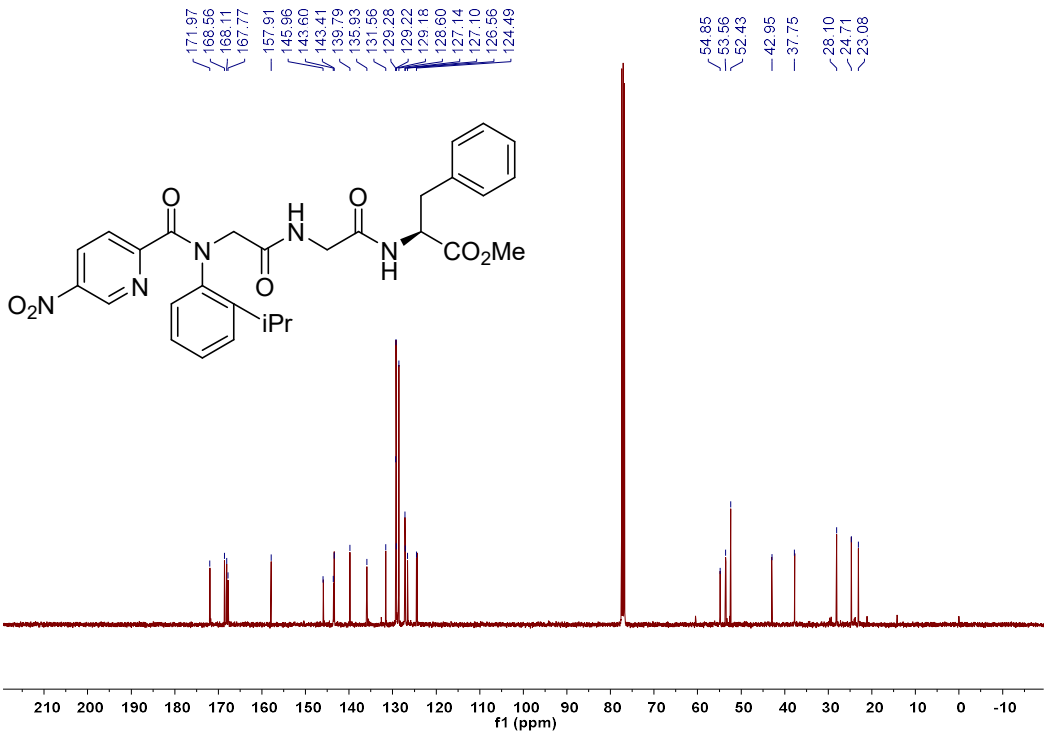
***rac*-4f**


9.0069
9.0009
8.9950
8.3974
8.3903
8.3834
8.3760
8.3688
7.8934
7.8718
7.8359
7.8144
7.2576
7.2435
7.2382
7.2352
7.2307
7.2238
7.2167
7.2115
7.1941
7.1889
6.9806
6.9619
4.9569
4.9395
4.9190
4.9016
4.5439
4.5337
4.5304
4.5234
4.5119
4.5089
4.0814
4.0494
3.9432
3.9263
3.9052
3.8885
3.8803
3.7218
3.7136
2.1613
1.2160
1.2082
1.1988
1.1910
1.1594
1.1527
1.1426
1.1358
0.9433
0.9366
0.9262
0.9196
0.9122
0.9055
0.8950
0.8883
O2N
iPr
CO2Me
0.97
1.00
1.02
4.00
1.02
1.00
1.00
1.01
3.84
3.02
1.00
1.05
3.04
3.02
6.03
f1 (ppm)

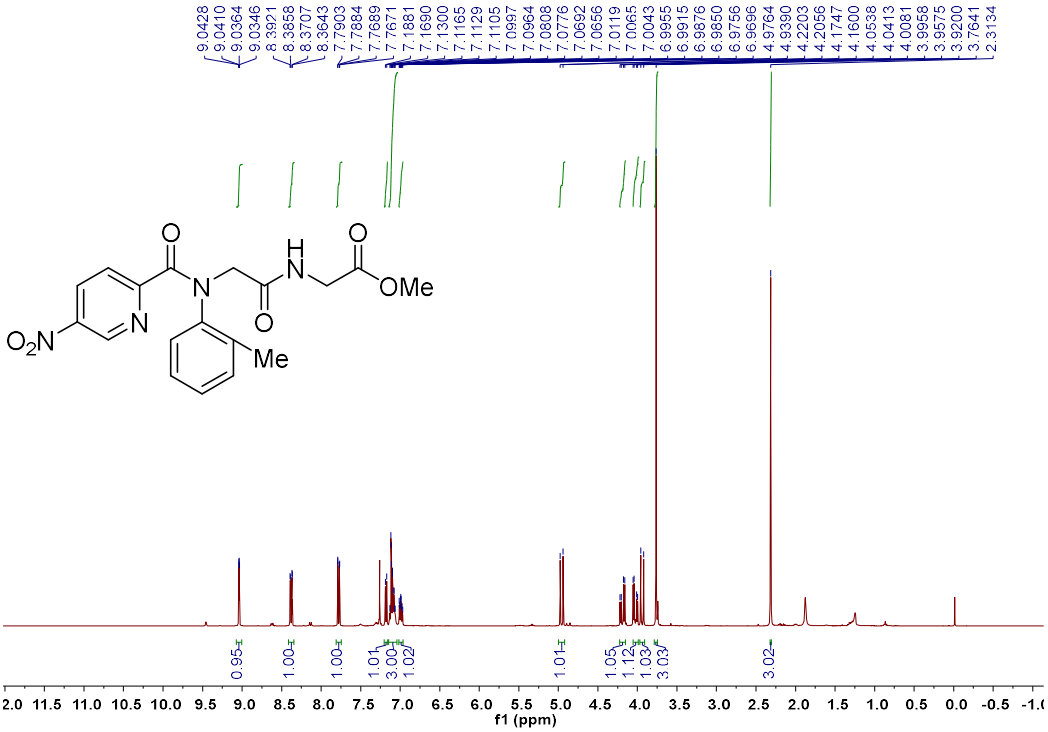

172.35
168.81
168.20
167.78
157.95
145.96
143.64
143.38
139.80
131.52
129.22
129.19
127.11
126.53
124.50
57.47
54.89
52.20
43.15
31.04
28.17
24.66
23.05
18.98
17.96
O2N
iPr
CO2Me
f1 (ppm)

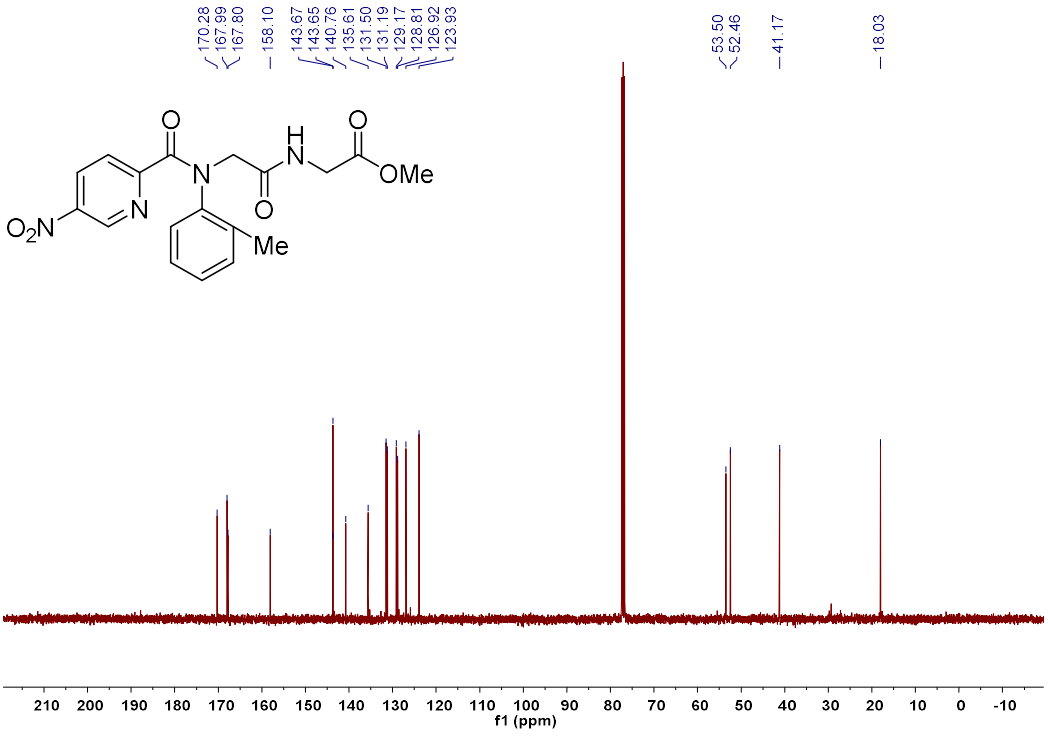
***rac*-4g**


8.9979
8.9919
8.3623
8.3590
8.3557
8.3524
8.3376
7.8298
7.8084
7.7543
7.7330
7.2534
7.2485
7.2455
7.2324
7.2279
7.2223
7.2177
7.2134
7.2038
7.1976
7.1934
7.1891
7.1805
7.1765
7.1723
7.1202
7.1158
7.1092
7.1044
7.0994
7.0957
7.0883
7.0847
6.9922
6.9739
6.9553
4.9291
4.8931
4.8911
4.8562
4.8481
4.8445
3.9230
3.8987
3.8858
3.8599
3.6798
3.1237
3.1093
3.1023
3.0855
3.0805
1.2185
1.2083
1.2013
1.1911
1.1698
1.1534
1.1369
O
N
O
H
N
O
N
H
CO2Me
O2N
N
iPr
0.97
0.99
1.00
7.00
2.02
2.00
2.02
3.09
3.00
1.01
2.02
3.01
3.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

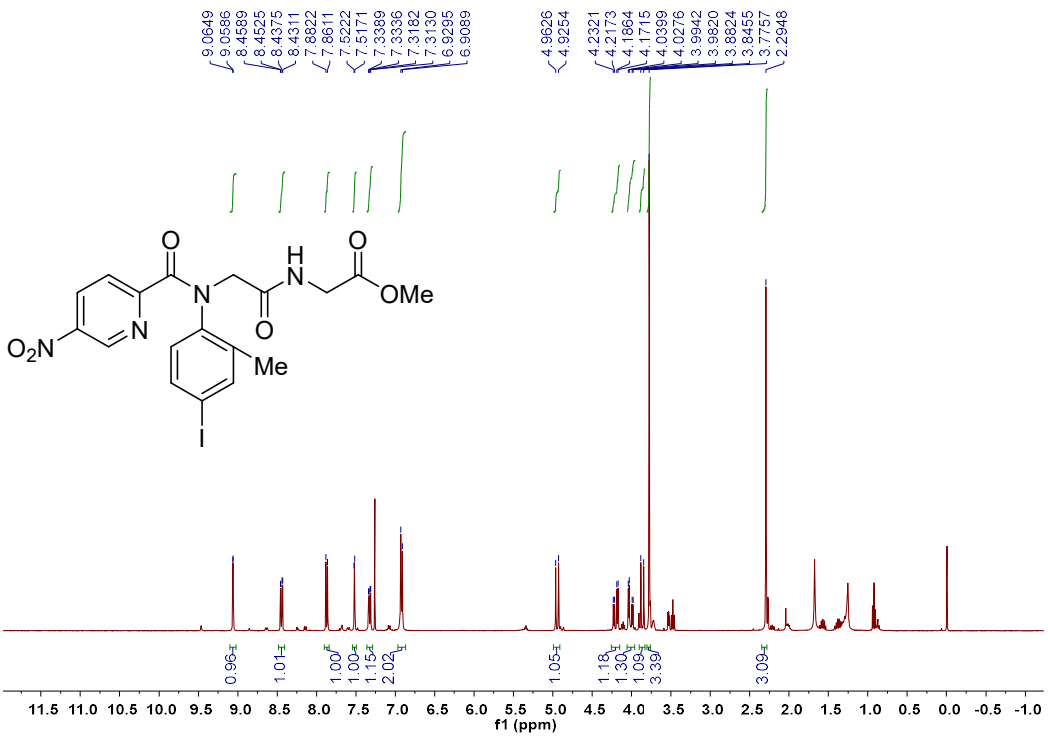

171.97
168.56
168.11
167.77
157.91
145.96
143.60
143.41
139.79
135.93
131.56
129.28
129.22
129.18
128.60
127.14
127.10
126.56
124.49
54.85
53.56
52.43
42.95
37.75
28.10
24.71
23.08
O
N
O
H
N
O
N
H
CO2Me
O2N
N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

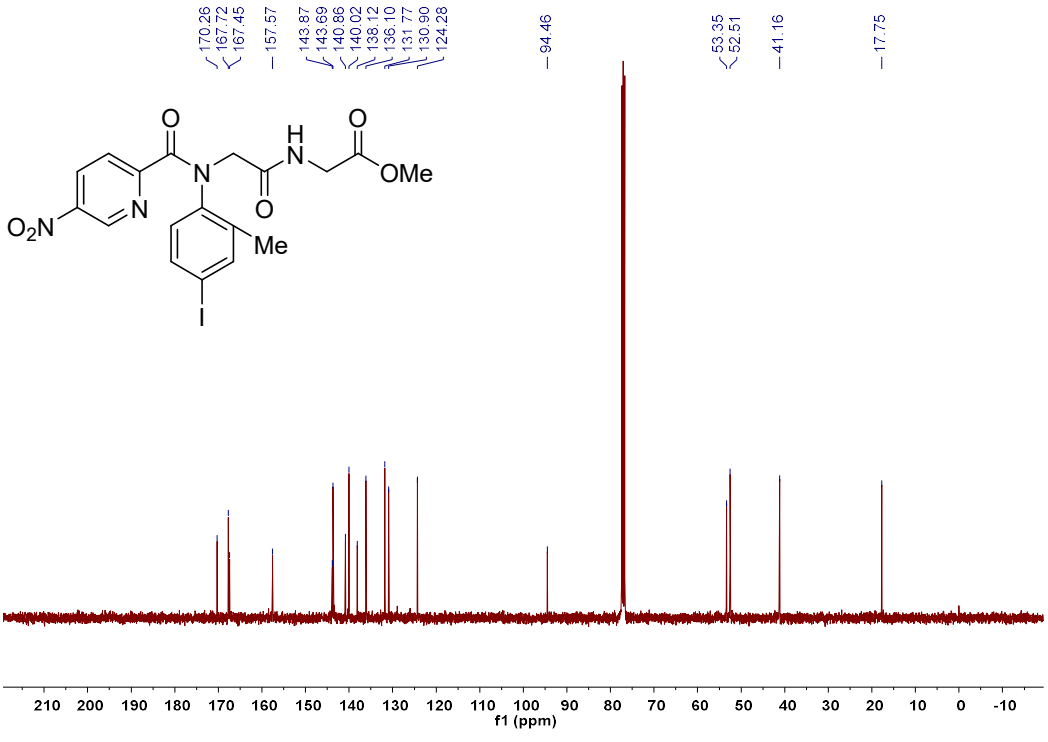
***rac*-4h**


9.0428
9.0410
9.0364
9.0346
8.3921
8.3858
8.3707
8.3643
7.7903
7.7884
7.7689
7.7671
7.1881
7.1690
7.1300
7.1165
7.1129
7.1105
7.0997
7.0964
7.0808
7.0776
7.0692
7.0656
7.0119
7.0065
7.0043
6.9955
6.9915
6.9876
6.9850
6.9756
6.9696
4.9764
4.9390
4.2203
4.2056
4.1747
4.1600
4.0538
4.0413
4.0081
3.9958
3.9575
3.9200
3.7641
2.3134
O
H
N
O
N
OMe
O
N
O2N
Me
0.95
1.00
1.00
1.01
3.00
1.02
1.01
1.05
1.12
1.03
3.03
3.02
f1 (ppm)

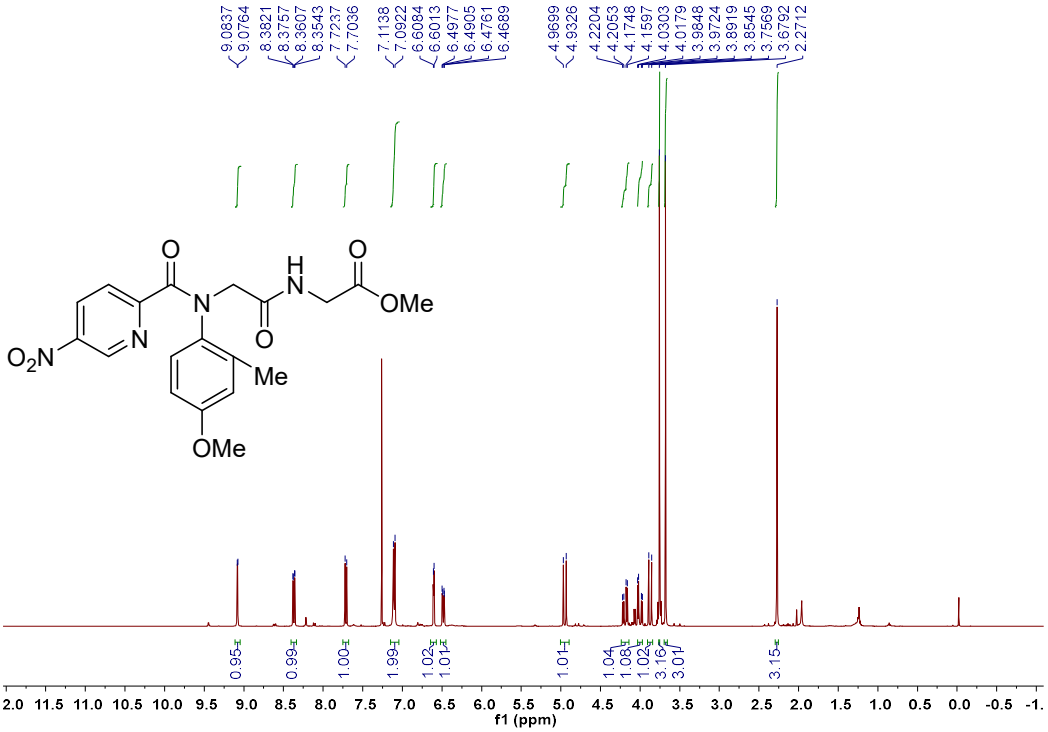

170.28
167.99
167.80
158.10
143.67
143.65
140.76
135.61
131.50
131.19
129.17
128.81
126.92
123.93
53.50
52.46
41.17
18.03
O
H
N
O
N
OMe
O
N
O2N
Me
f1 (ppm)

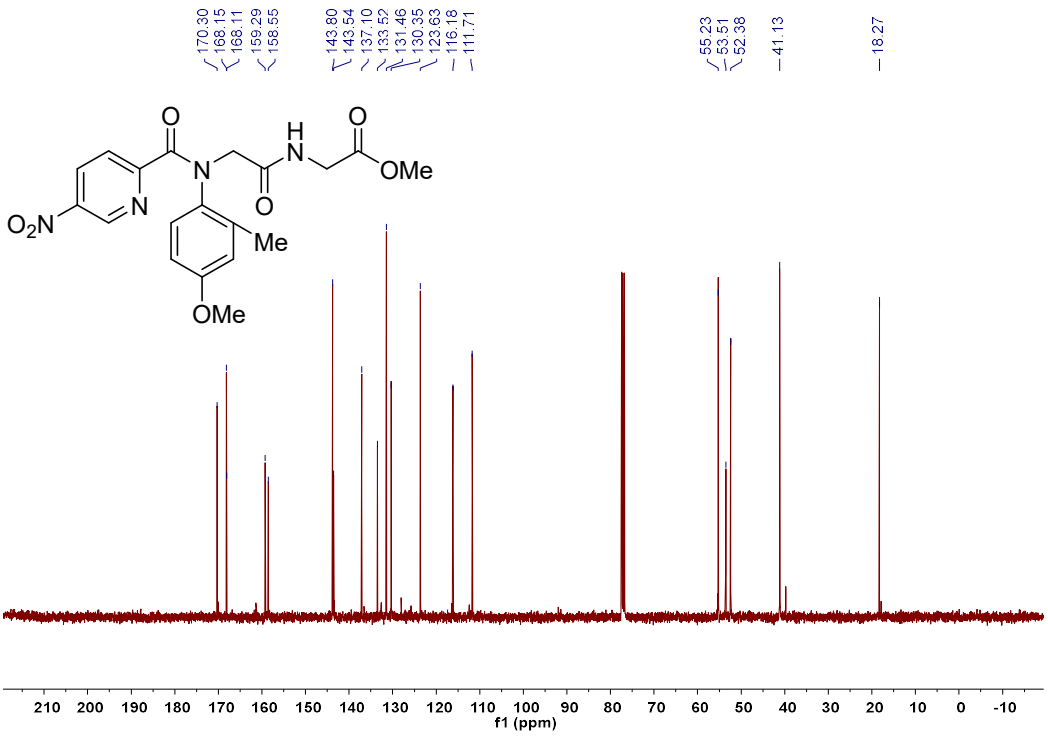
***rac*-4i**


9.0649
9.0586
8.4589
8.4525
8.4375
8.4311
7.8822
7.8611
7.5222
7.5171
7.3389
7.3336
7.3182
7.3130
6.9295
6.9089
4.9626
4.9254
4.2321
4.2173
4.1864
4.1715
4.0399
4.0276
3.9942
3.9820
3.8824
3.8455
3.7757
2.2948
O
H
N
O
N
OMe
O
O2N
N
Me
I
0.96
1.01
1.00
1.00
1.15
2.02
1.05
1.18
1.30
1.09
3.39
3.09
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

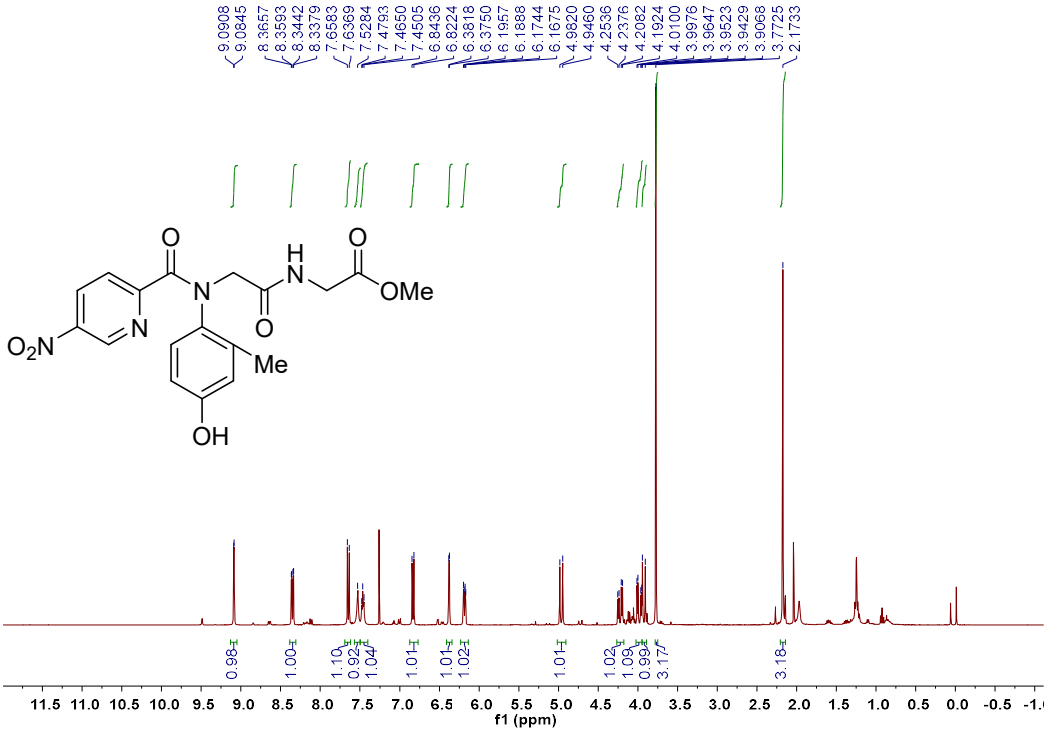

170.26
167.72
167.45
157.57
143.87
143.69
140.86
140.02
138.12
136.10
131.77
130.90
124.28
94.46
53.35
52.51
41.16
17.75
O
H
N
O
N
OMe
O
O2N
N
Me
I
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

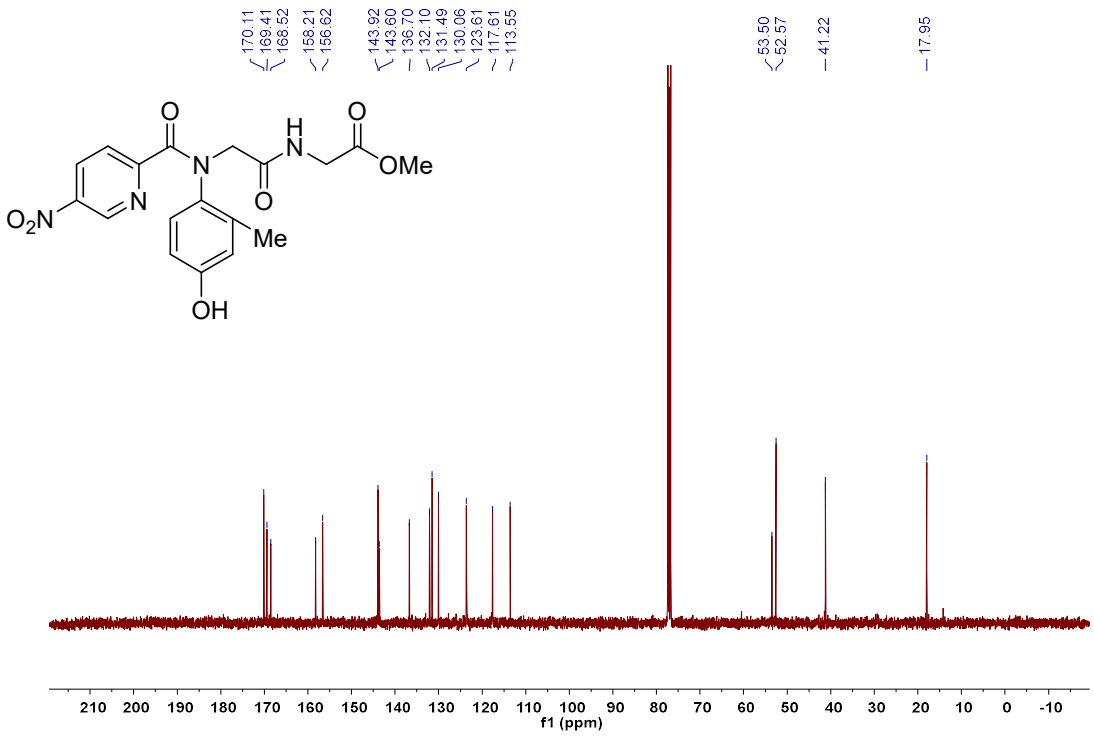
***rac*-4j**


9.0837
9.0764
8.3821
8.3757
8.3607
8.3543
7.7237
7.7036
7.1138
7.0922
6.6084
6.6013
6.4977
6.4905
6.4761
6.4689
4.9699
4.9326
4.2204
4.2053
4.1748
4.1597
4.0303
4.0179
3.9848
3.9724
3.8919
3.8545
3.7569
3.6792
2.2712
O
N
O
H
N
O
OMe
O
N
O2N
Me
OMe
0.95
0.99
1.00
1.99
1.02
1.01
1.01
1.04
1.08
1.02
3.16
3.01
3.15
f1 (ppm)

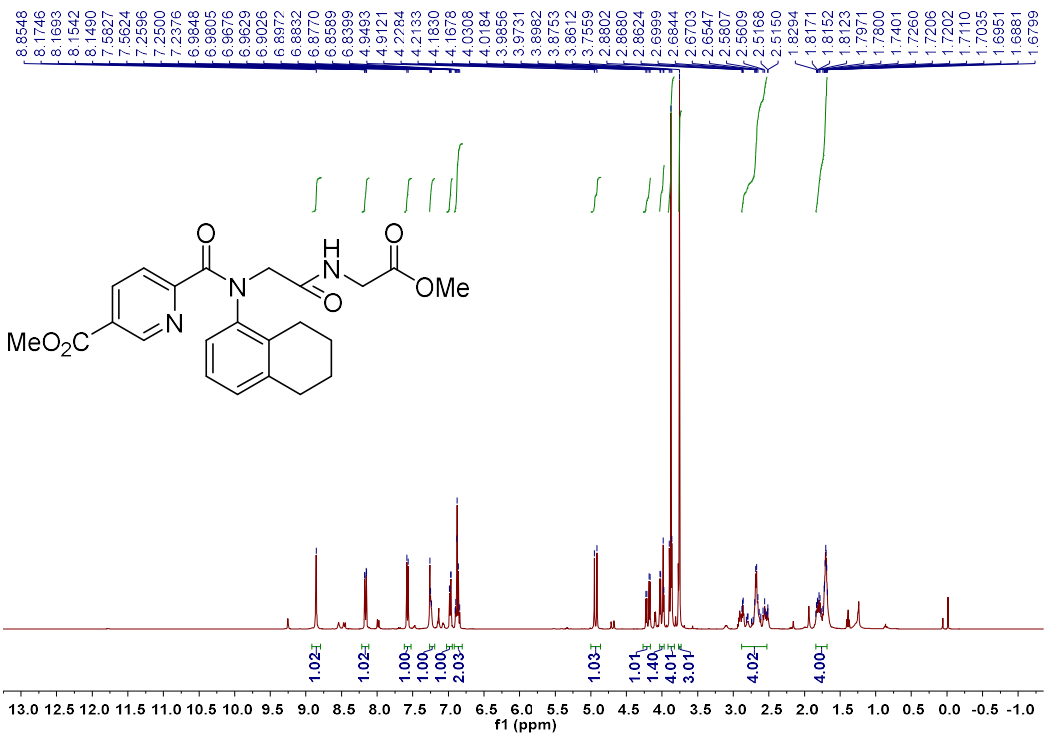

170.30
168.15
168.11
159.29
158.55
143.80
143.54
137.10
133.52
131.46
130.35
123.63
116.18
111.71
55.23
53.51
52.38
41.13
18.27
O
N
O
H
N
O
OMe
O
N
O2N
Me
OMe
f1 (ppm)

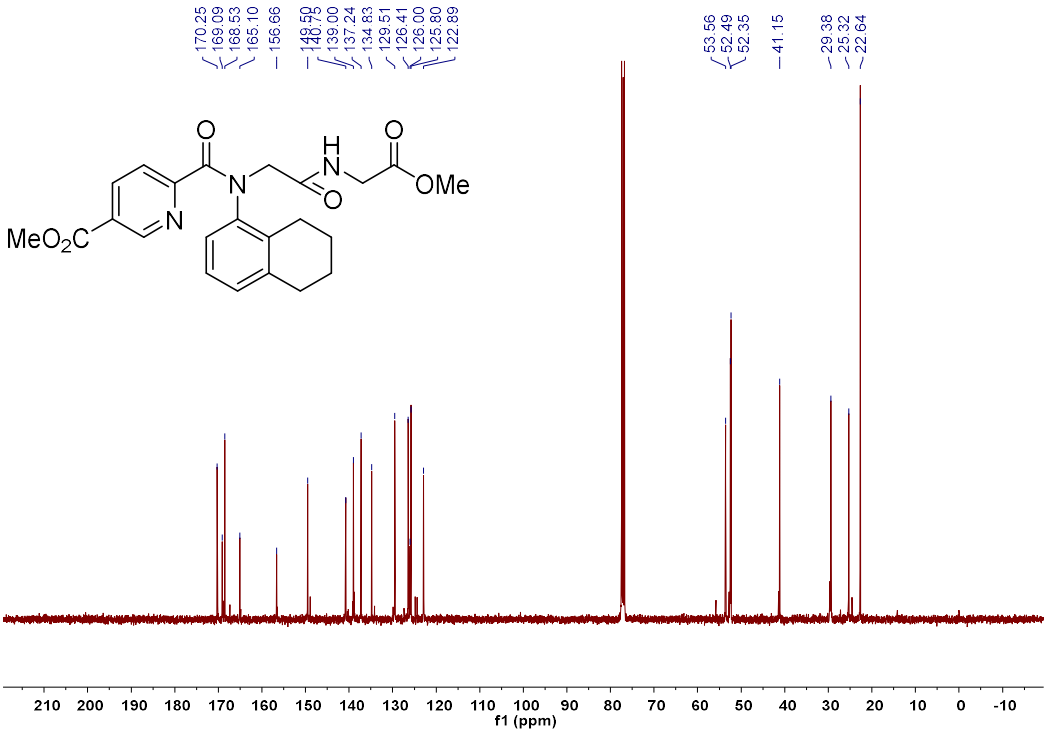
***rac*-4k**


9.0908
9.0845
8.3657
8.3593
8.3442
8.3379
7.6583
7.6369
7.5284
7.4793
7.4650
7.4505
6.8436
6.8224
6.3818
6.3750
6.1957
6.1888
6.1744
6.1675
4.9820
4.9460
4.2536
4.2376
4.2082
4.1924
4.0100
3.9976
3.9647
3.9523
3.9429
3.9068
3.7725
2.1733
O
H
N
O
OMe
N
O
O2N
Me
OH
0.98
1.00
1.10
0.92
1.04
1.01
1.01
1.02
1.01
1.02
1.09
0.99
3.17
3.18
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

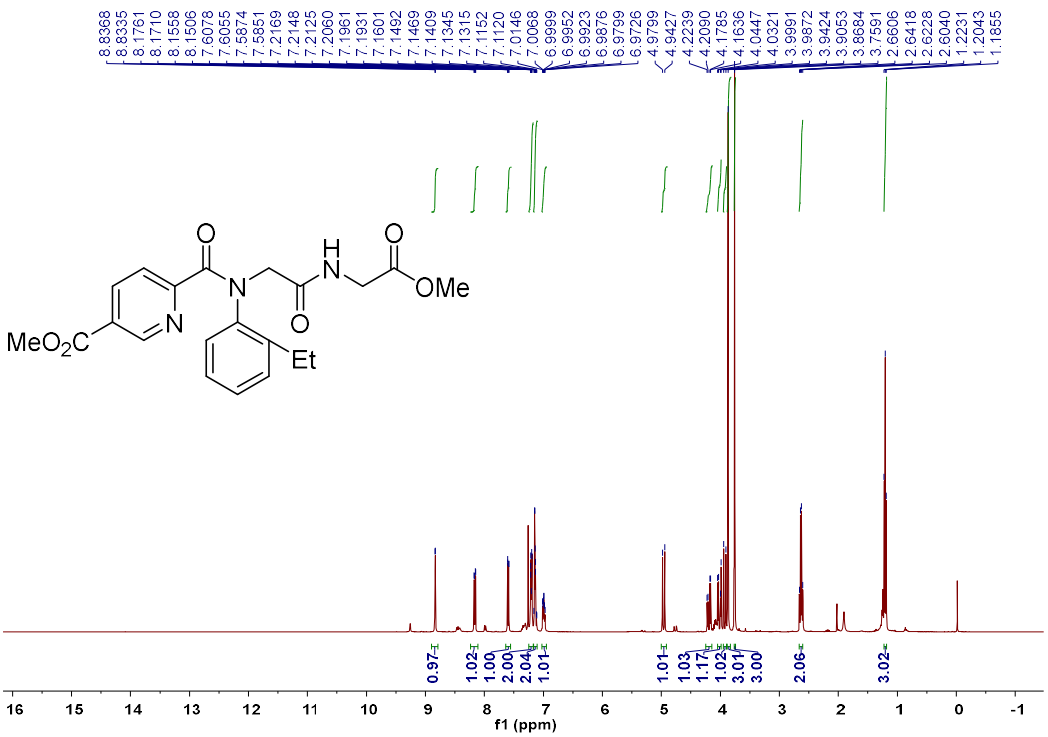

170.11
169.41
168.52
158.21
156.62
143.92
143.60
136.70
132.10
131.49
130.06
123.61
117.61
113.55
53.50
52.57
41.22
17.95
O
H
N
O
OMe
N
O
O2N
Me
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

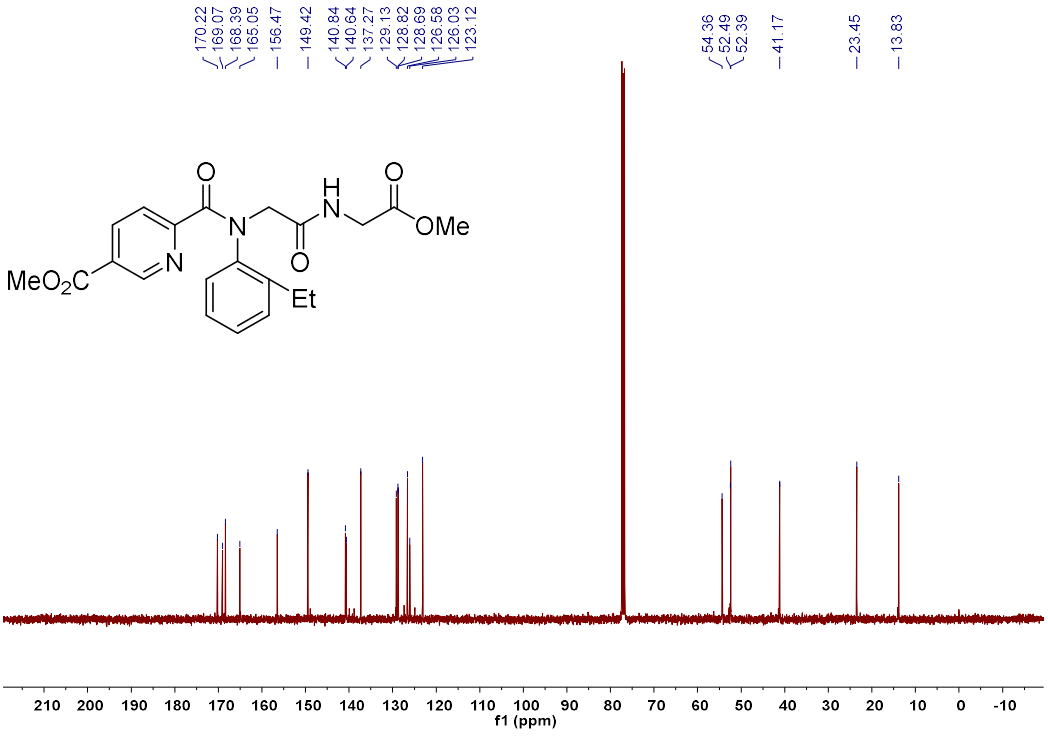
***rac*-4l**


8.8548
8.1746
8.1693
8.1542
8.1490
7.5827
7.5624
7.2596
7.2500
7.2376
6.9848
6.9805
6.9676
6.9629
6.9026
6.8972
6.8832
6.8770
6.8589
6.8399
4.9493
4.9121
4.2284
4.2133
4.1830
4.1678
4.0308
4.0184
3.9856
3.9731
3.8962
3.8753
3.8612
3.7559
2.8802
2.8680
2.8624
2.6999
2.6844
2.6703
2.6547
2.5807
2.5609
2.5168
2.5150
1.8294
1.8171
1.8152
1.8123
1.7971
1.7800
1.7401
1.7260
1.7206
1.7202
1.7110
1.7035
1.6951
1.6881
1.6799
1.02
1.02
1.00
1.00
1.00
2.03
1.03
1.01
1.40
4.01
3.01
4.02
4.00
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)
MeO2C
OMe

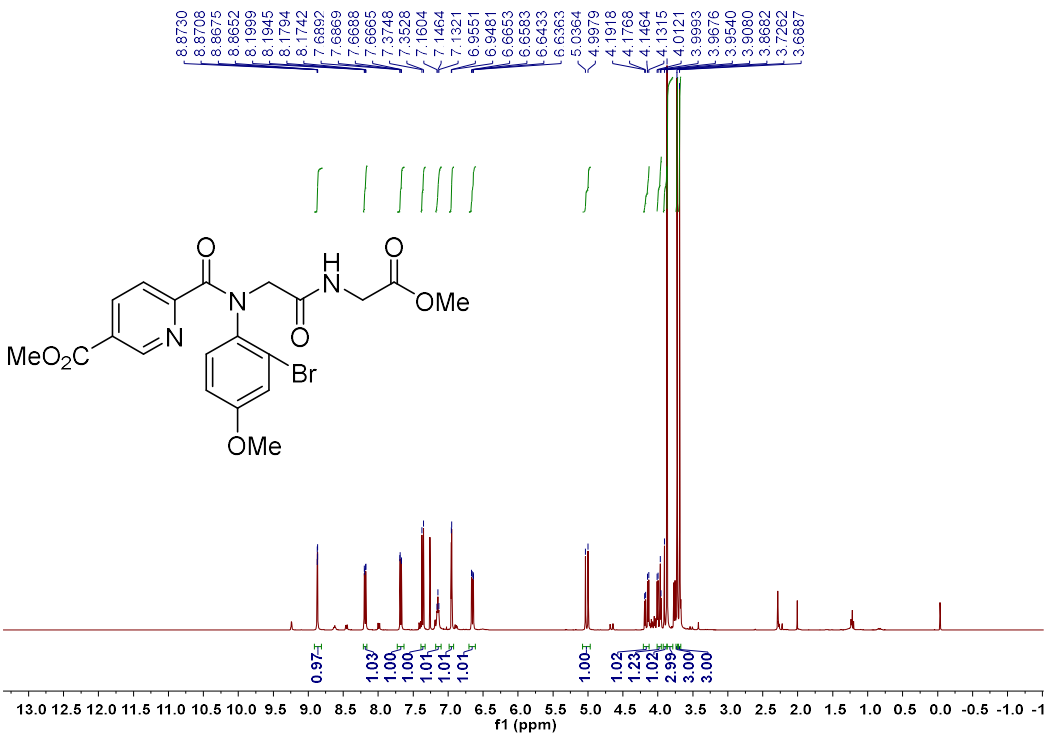

170.25
169.09
168.53
165.10
156.66
148.50
140.75
139.00
137.24
134.83
129.51
126.41
126.00
125.80
122.89
53.56
52.49
52.35
41.15
29.38
25.32
22.64
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
MeO2C
OMe

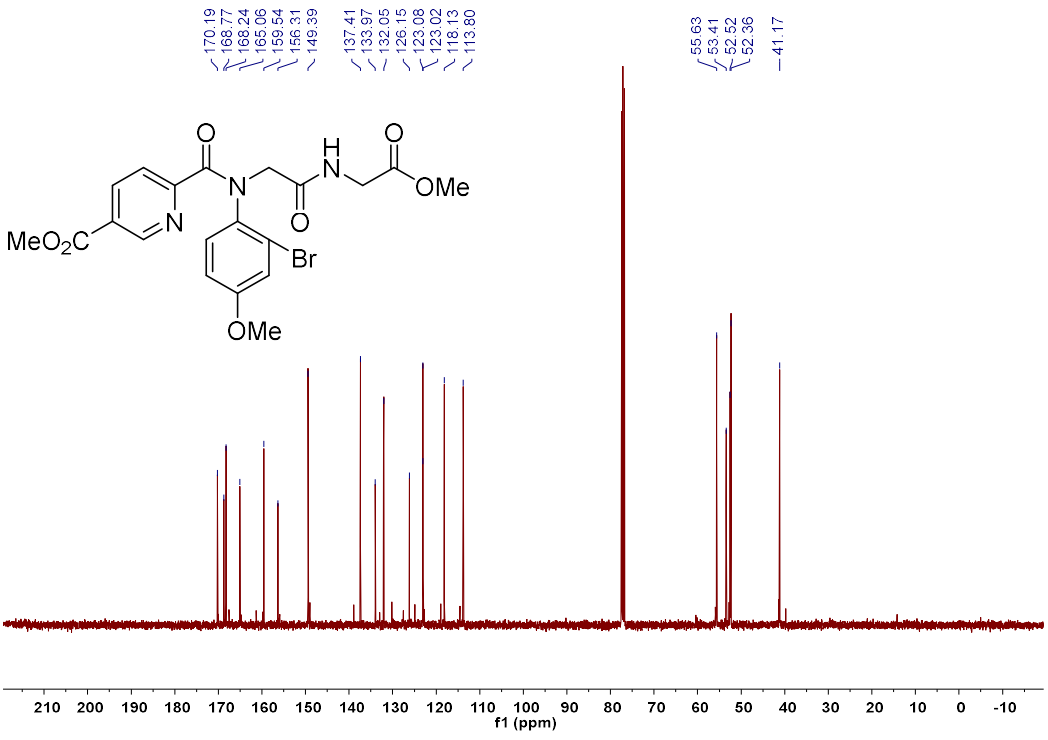
***rac*-4m**


8.8368
8.8335
8.1761
8.1710
8.1558
8.1506
7.6078
7.6055
7.5874
7.5851
7.2169
7.2148
7.2125
7.2060
7.1961
7.1931
7.1601
7.1492
7.1469
7.1409
7.1345
7.1315
7.1152
7.1120
7.0146
7.0068
6.9999
6.9952
6.9923
6.9876
6.9799
6.9726
4.9799
4.9427
4.2239
4.2090
4.1785
4.1636
4.0447
4.0321
3.9991
3.9872
3.9424
3.9053
3.8684
3.7591
2.6606
2.6418
2.6228
2.6040
1.2231
1.2043
1.1655
0.97
1.02
1.00
2.00
2.04
1.01
1.01
1.03
1.17
1.02
3.01
3.00
2.06
3.02
f1 (ppm)

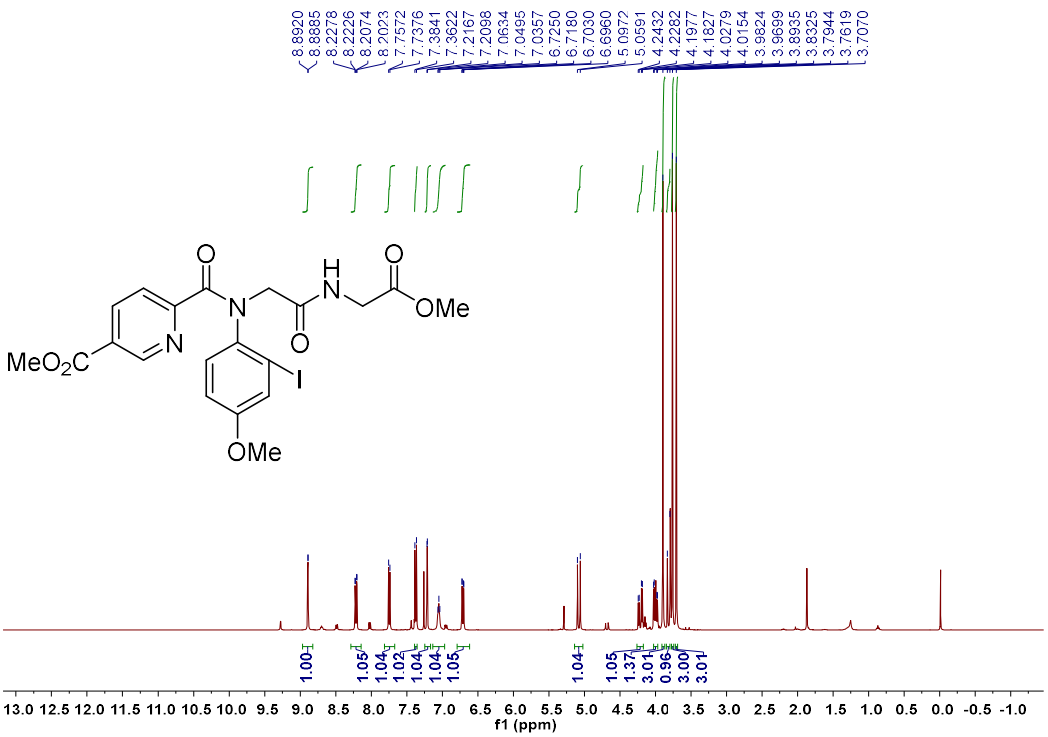

170.22
169.07
168.39
165.05
156.47
149.42
140.84
140.64
137.27
129.13
128.82
128.69
126.58
126.03
123.12
54.36
52.49
52.39
41.17
23.45
13.83
f1 (ppm)

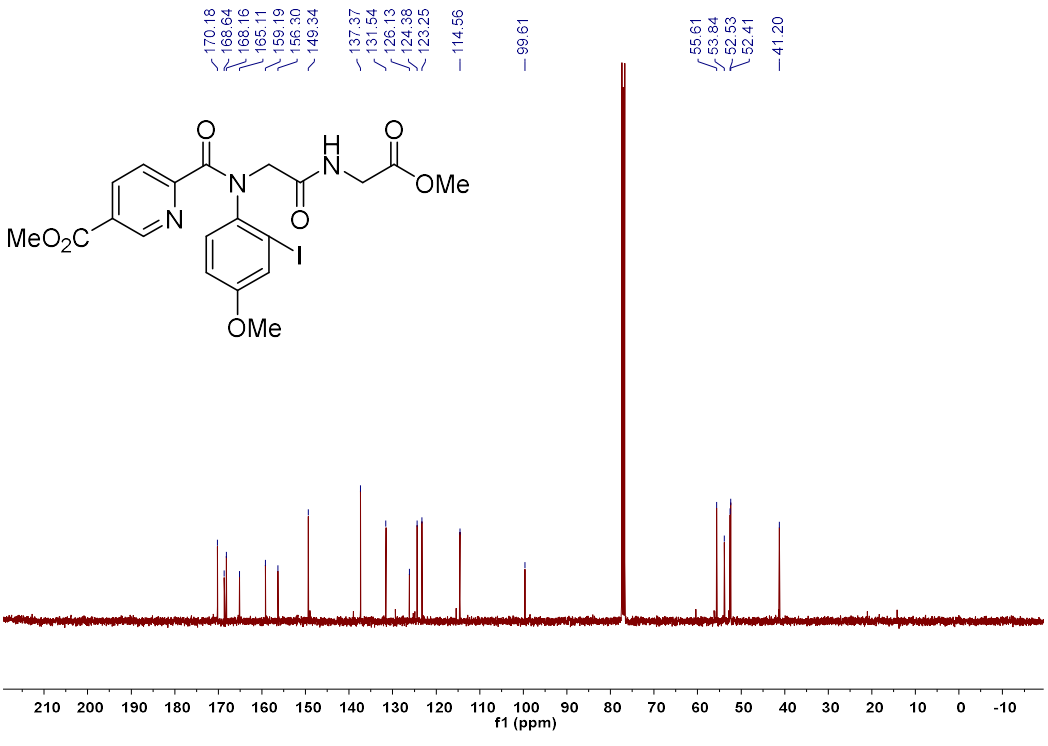
***rac*-4n**


8.8730
8.8708
8.8675
8.8652
8.1999
8.1945
8.1794
8.1742
7.6892
7.6869
7.6688
7.6665
7.3748
7.3528
7.1604
7.1464
7.1321
6.9551
6.9481
6.6553
6.6583
6.6433
6.6363
5.0364
4.9979
4.1918
4.1768
4.1464
4.1315
4.0121
3.9993
3.9676
3.9540
3.9080
3.8682
3.7262
3.6887
0.97
1.03
1.00
1.00
1.01
1.01
1.01
1.00
1.02
1.23
1.02
2.99
3.00
3.00
f1 (ppm)

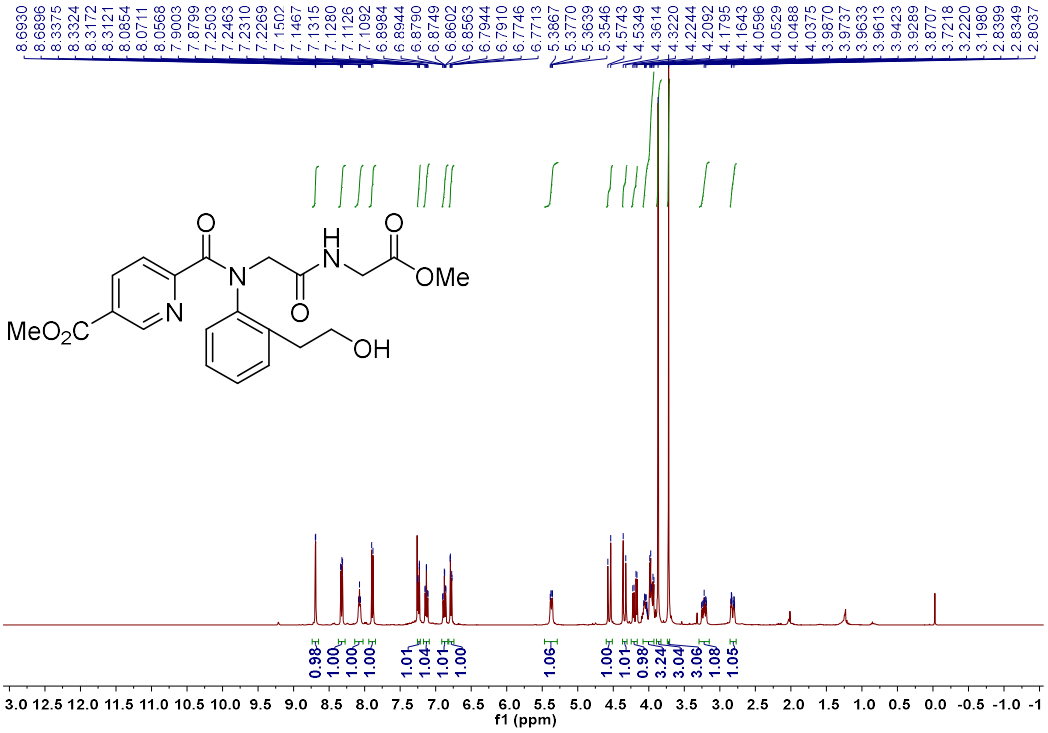

170.19
168.77
168.24
165.06
159.54
156.31
149.39
137.41
133.97
132.05
126.15
123.08
123.02
118.13
113.80
55.63
53.41
52.52
52.36
41.17
f1 (ppm)

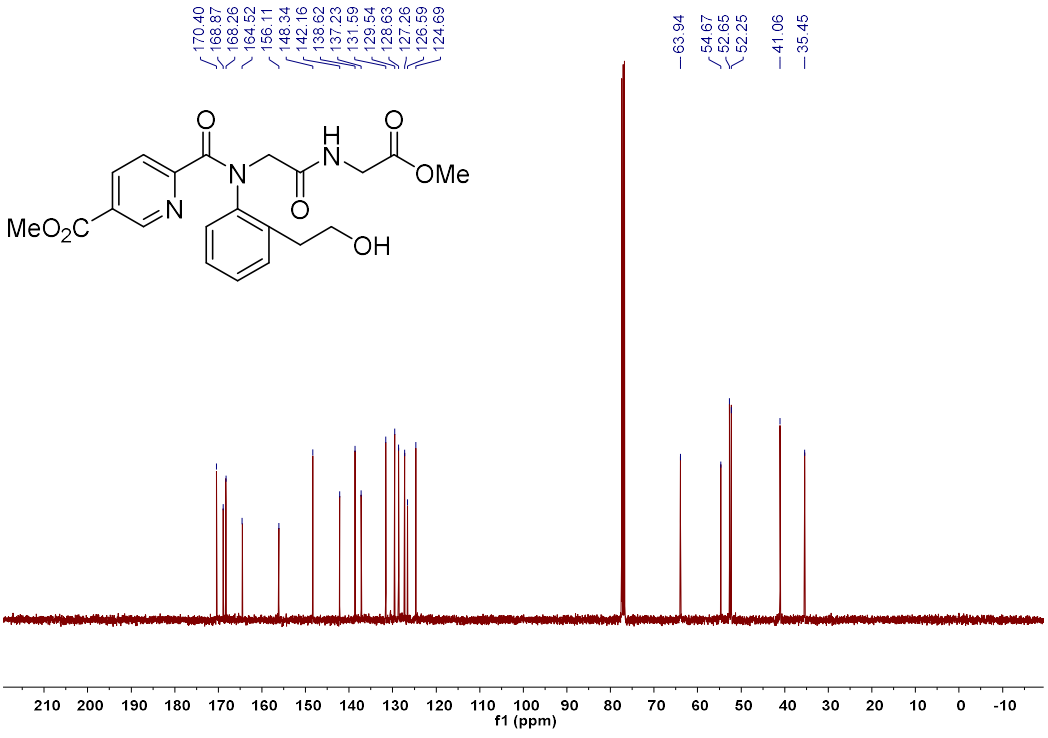
***rac*-4o**


8.8920
8.8885
8.2278
8.2226
8.2074
8.2023
7.7572
7.7376
7.3841
7.3622
7.2167
7.2098
7.0634
7.0495
7.0357
6.7250
6.7180
6.7030
6.6960
5.0972
5.0591
4.2432
4.2282
4.1977
4.1827
4.0279
4.0154
3.9824
3.9699
3.8935
3.8325
3.7944
3.7619
3.7070
1.00
1.05
1.04
1.02
1.04
1.04
1.05
1.04
1.05
1.37
3.01
0.96
3.00
3.01
f1 (ppm)

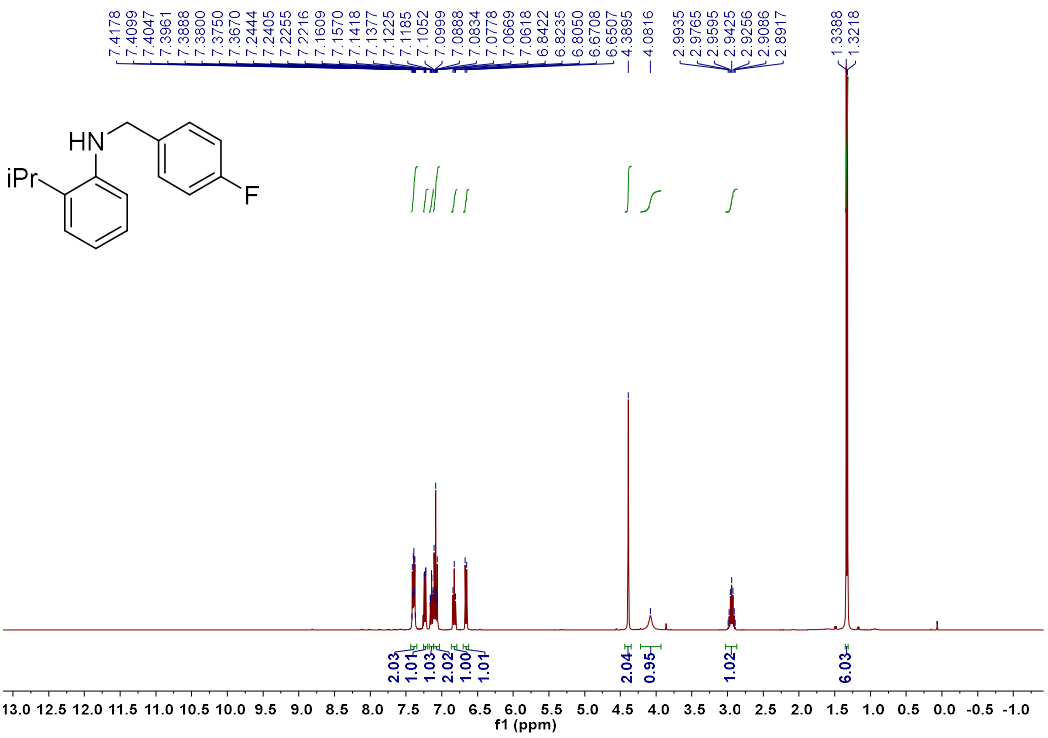

170.18
168.64
168.16
165.11
159.19
156.30
149.34
137.37
131.54
126.13
124.38
123.25
114.56
99.61
55.61
53.84
52.53
52.41
41.20
f1 (ppm)

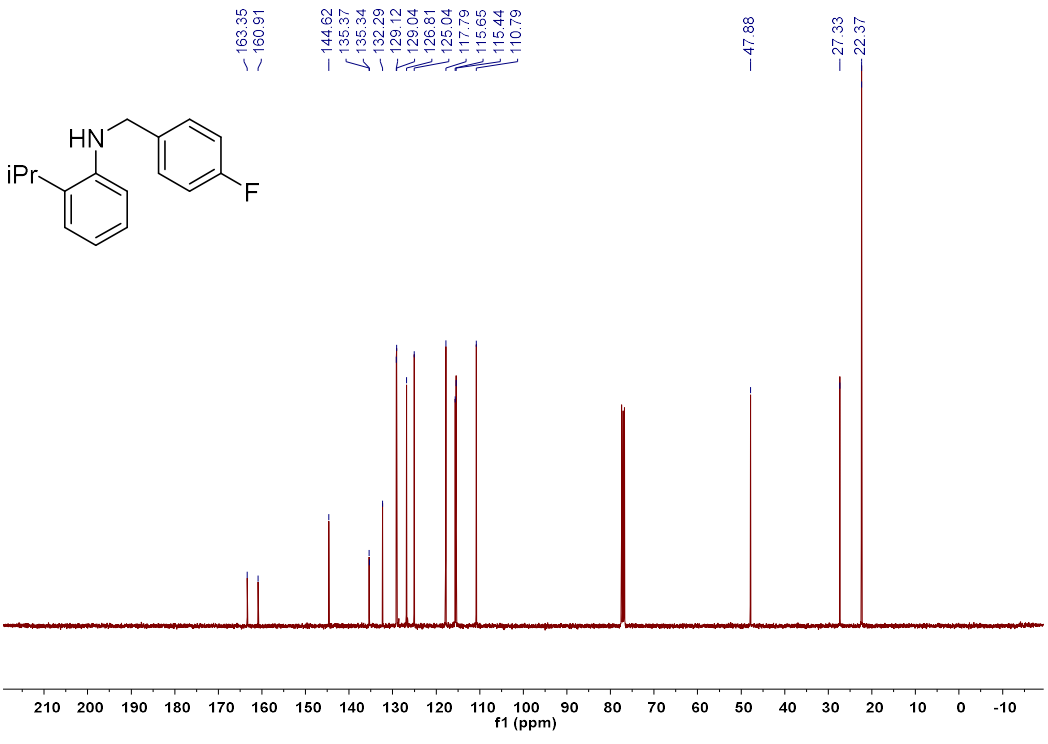
***rac*-4p**

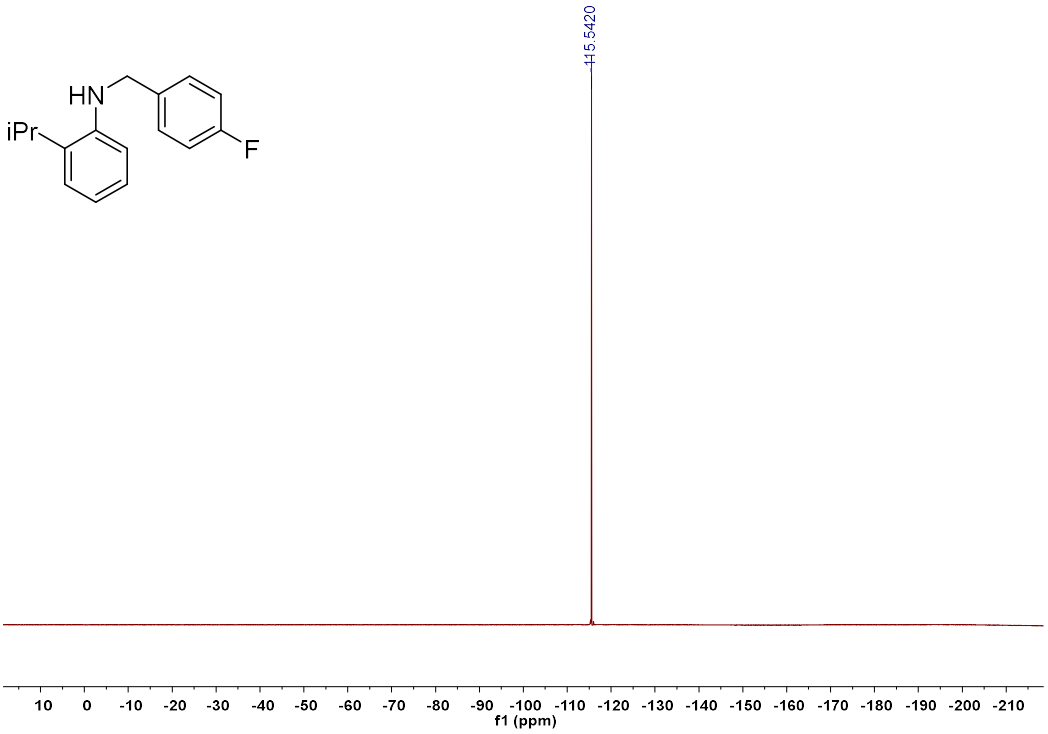

8.6930
8.6896
8.3375
8.3324
8.3172
8.3121
8.0854
8.0711
8.0568
7.9003
7.8799
7.2503
7.2463
7.2310
7.2269
7.1502
7.1467
7.1315
7.1280
7.1126
7.1092
6.8984
6.8944
6.8790
6.8749
6.8602
6.8563
6.7944
6.7910
6.7746
6.7713
5.3867
5.3770
5.3639
5.3546
4.5743
4.5349
4.3614
4.3220
4.2244
4.2092
4.1795
4.1643
4.0596
4.0529
4.0488
4.0375
3.9870
3.9737
3.9633
3.9613
3.9423
3.9289
3.8707
3.7218
3.2220
3.1980
2.8399
2.8349
2.8037
MeO2C
N
O
N
H
N
O
O
OMe
OH
0.98
1.00
1.00
1.00
1.01
1.04
1.01
1.00
1.06
1.00
1.01
0.98
3.24
3.04
3.06
1.08
1.05
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1
f1 (ppm)


170.40
168.87
168.26
164.52
156.11
148.34
142.16
138.62
137.23
131.59
129.54
128.63
127.26
126.59
124.69
63.94
54.67
52.65
52.25
41.06
35.45
MeO2C
N
O
N
H
N
O
O
OMe
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

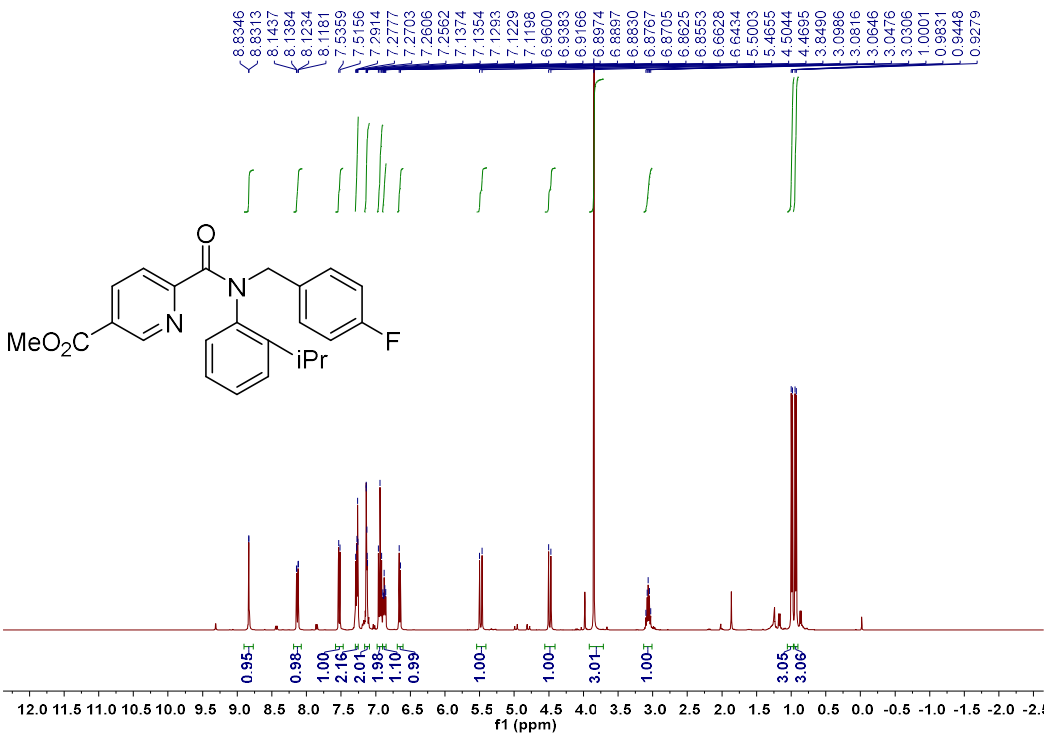
4qq

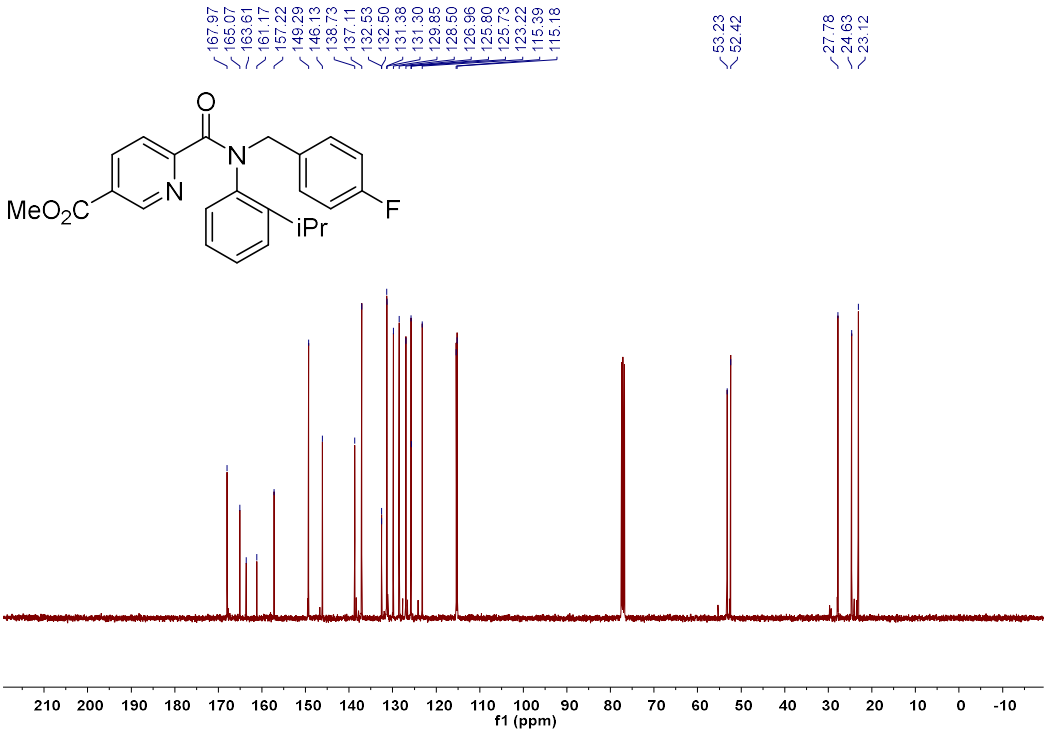

7.4178
7.4099
7.4047
7.3961
7.3888
7.3800
7.3750
7.3670
7.2444
7.2405
7.2255
7.2216
7.1609
7.1570
7.1418
7.1377
7.1225
7.1185
7.1052
7.0999
7.0888
7.0834
7.0778
7.0669
7.0618
6.8422
6.8235
6.8050
6.6708
6.6507
4.3895
4.0816
2.9935
2.9765
2.9595
2.9425
2.9256
2.9086
2.8917
1.3388
1.3218
HN
iPr
F
2.03
1.01
1.03
2.02
1.00
1.01
2.04
0.95
1.02
6.03
f1 (ppm)

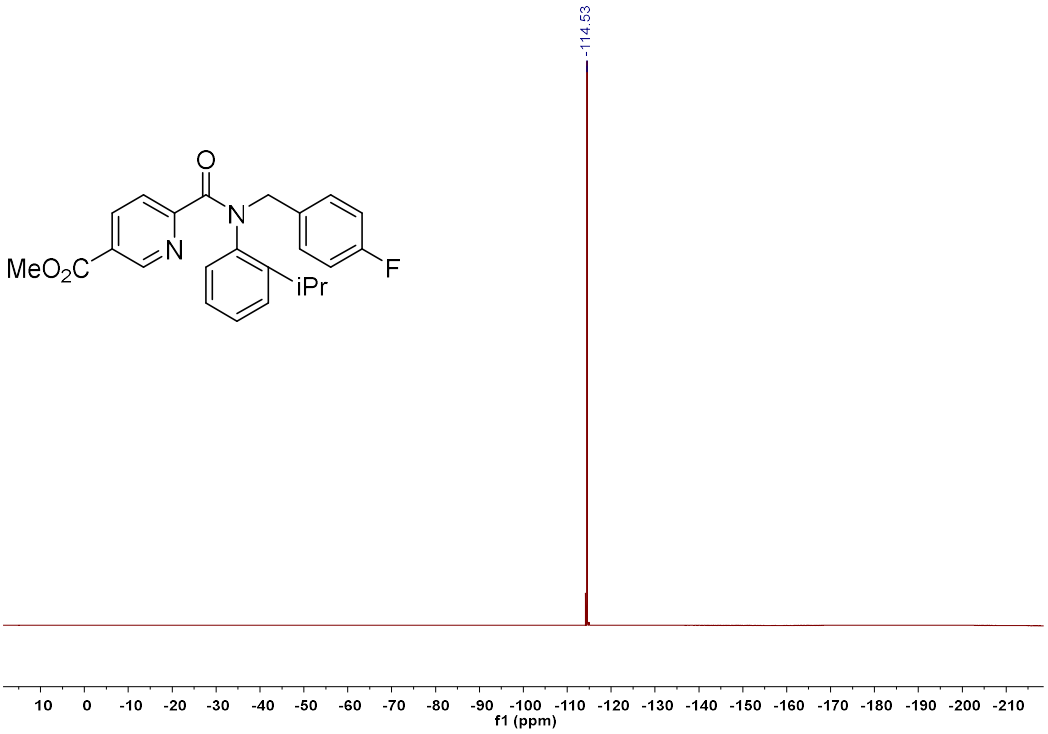

163.35
160.91
144.62
135.37
135.34
132.29
129.12
129.04
126.81
125.04
117.79
115.65
115.44
110.79
47.88
27.33
22.37
HN
iPr
F
f1 (ppm)


HN
iPr
F
-115.5420
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

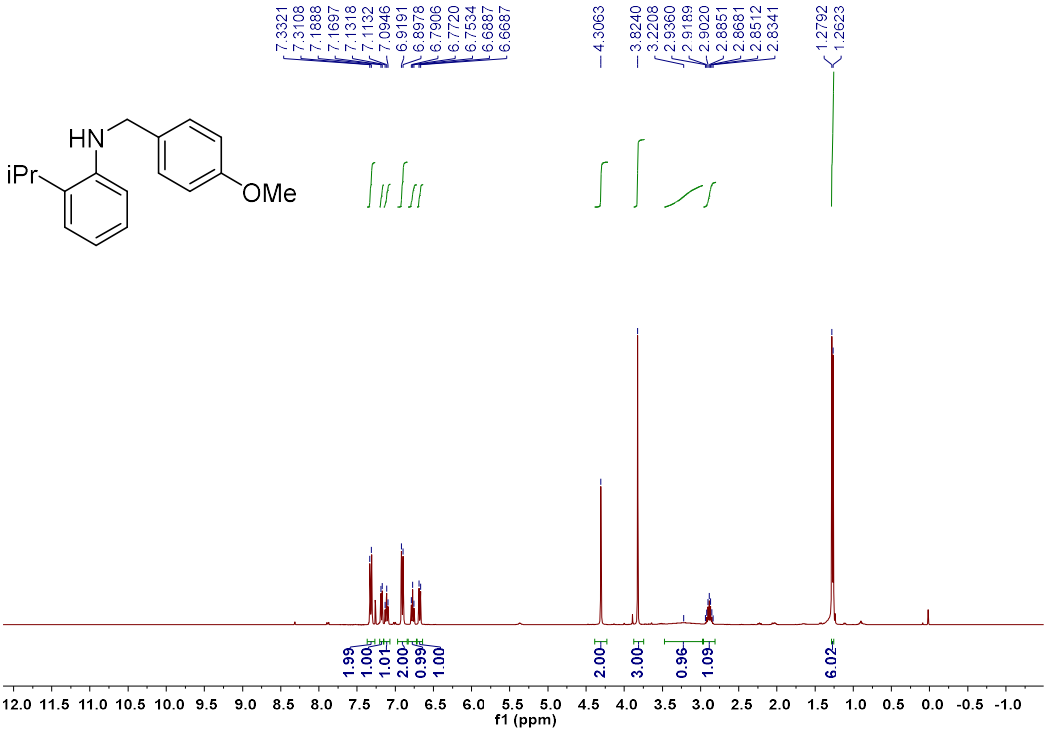
***rac*-4q**

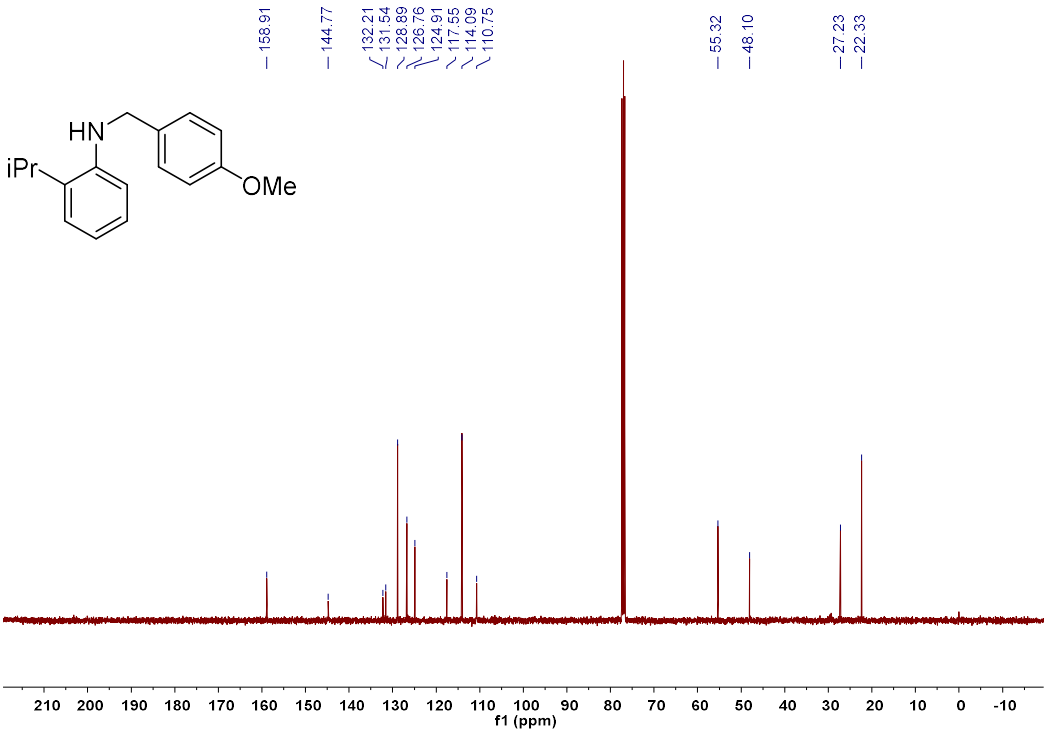

8.8346
8.8313
8.1437
8.1384
8.1234
8.1181
7.5359
7.5156
7.2914
7.2777
7.2703
7.2606
7.2562
7.1374
7.1354
7.1293
7.1229
7.1198
6.9600
6.9383
6.9166
6.8974
6.8897
6.8830
6.8767
6.8705
6.8625
6.8553
6.6628
6.6434
5.5003
5.4655
4.5044
4.4695
3.8490
3.0986
3.0816
3.0646
3.0476
3.0306
1.0001
0.9831
0.9448
0.9279
MeO2C
N
O
N
iPr
F
0.95
0.98
1.00
2.16
2.01
1.98
1.10
0.99
1.00
1.00
3.01
1.00
3.05
3.06
f1 (ppm)


167.97
165.07
163.61
161.17
157.22
149.29
146.13
138.73
137.11
132.53
132.50
131.38
131.30
129.85
128.50
126.96
125.80
125.73
123.22
115.39
115.18
53.23
52.42
27.78
24.63
23.12
MeO2C
N
O
N
iPr
F
f1 (ppm)

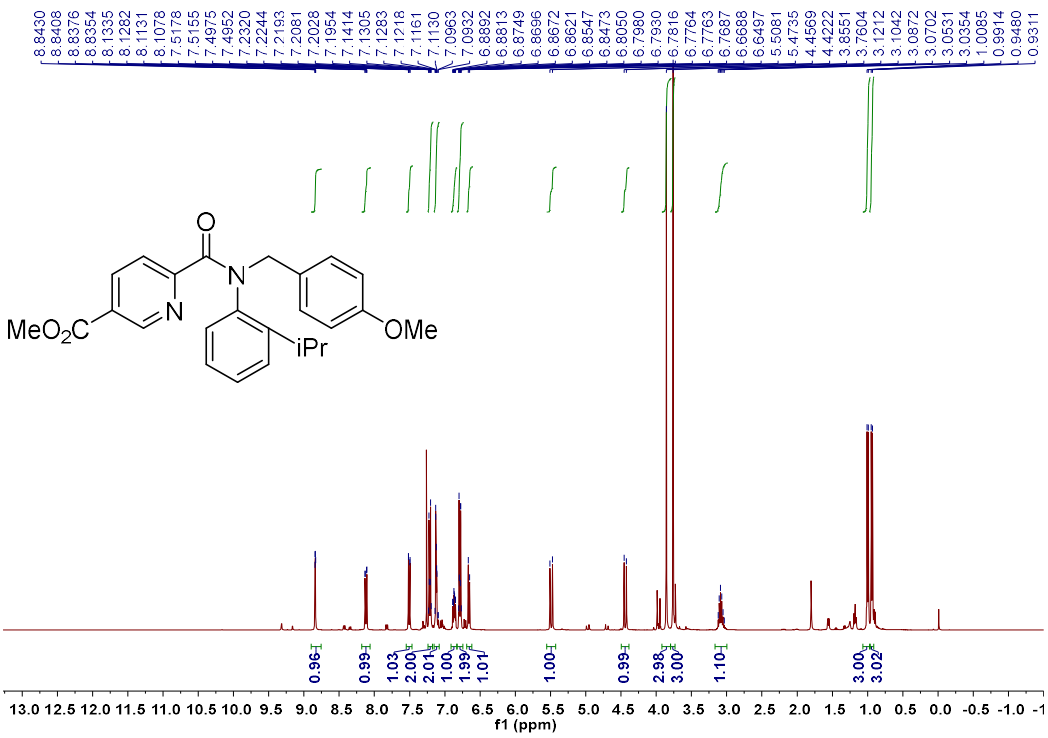

-114.53
O
N
N
MeO2C
iPr
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

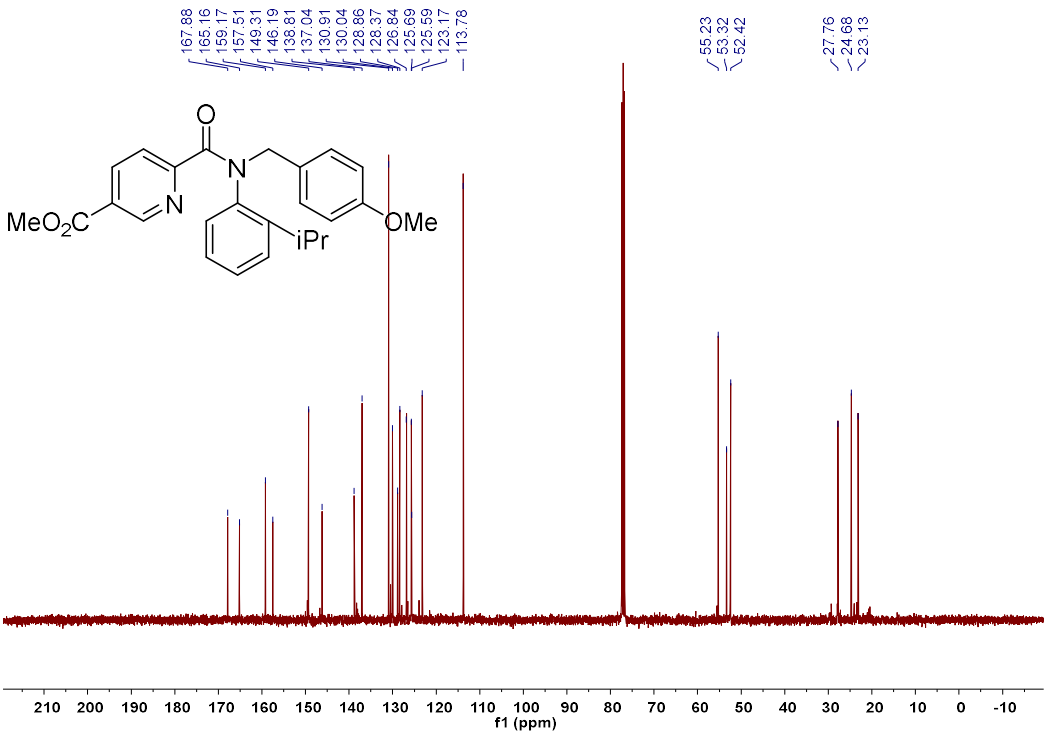
4rr


7.3321
7.3108
7.1888
7.1697
7.1318
7.1132
7.0946
6.9191
6.8978
6.7906
6.7720
6.7534
6.6887
6.6687
4.3063
3.8240
3.2208
2.9360
2.9189
2.9020
2.8851
2.8681
2.8512
2.8341
1.2792
1.2623
HN
iPr
OMe
1.99
1.00
1.01
2.00
0.99
1.00
2.00
3.00
0.96
1.09
6.02
f1 (ppm)

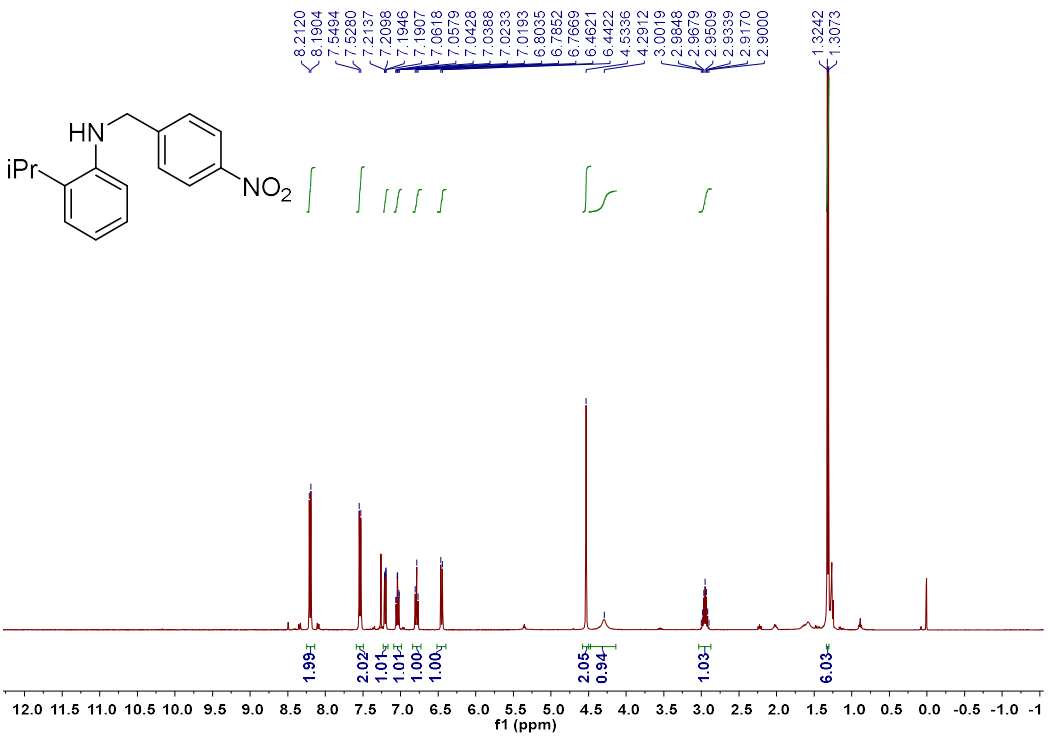

158.91
144.77
132.21
131.54
128.89
126.76
124.91
117.55
114.09
110.75
55.32
48.10
27.23
22.33
HN
iPr
OMe
f1 (ppm)

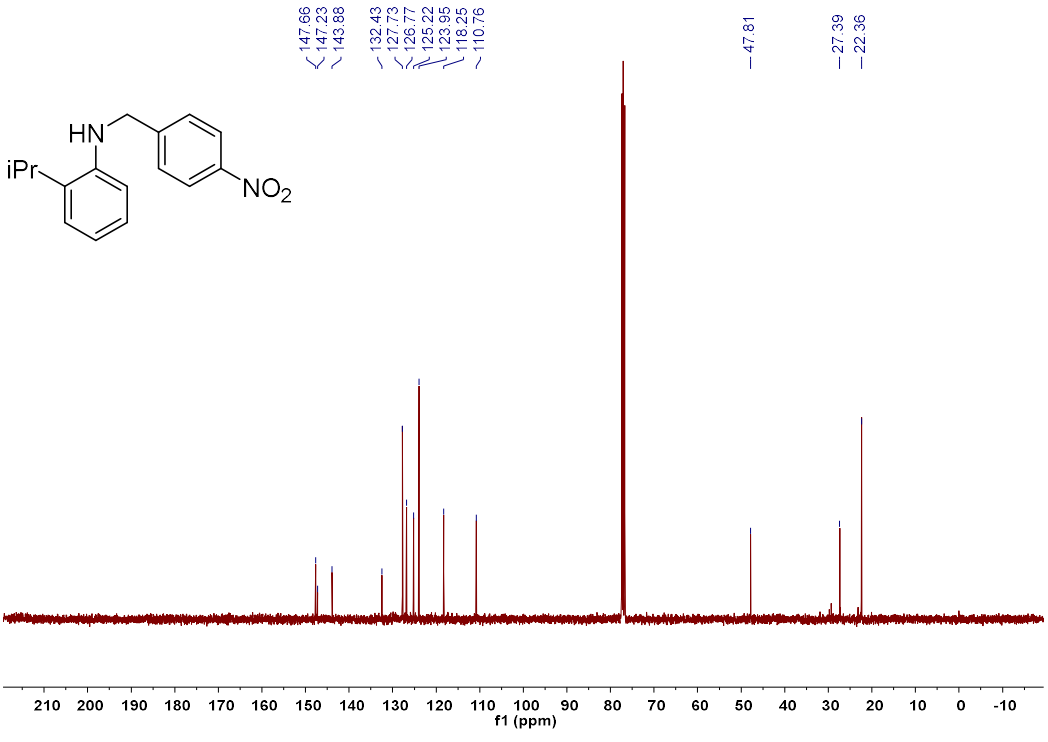
***rac*-4r**


8.8430
8.8408
8.8376
8.8354
8.1335
8.1282
8.1131
8.1078
7.5178
7.5155
7.4975
7.4952
7.2320
7.2244
7.2193
7.2081
7.2028
7.1954
7.1414
7.1305
7.1283
7.1218
7.1161
7.1130
7.0963
7.0932
6.8892
6.8813
6.8749
6.8696
6.8672
6.8621
6.8547
6.8473
6.8050
6.7980
6.7930
6.7816
6.7764
6.7763
6.7687
6.6688
6.6497
5.5081
5.4735
4.4569
4.4222
3.8551
3.7604
3.1212
3.1042
3.0872
3.0702
3.0531
3.0354
1.0085
0.9914
0.9480
0.9311
O
N
N
MeO2C
iPr
OMe
0.96
0.99
1.03
2.00
2.01
1.00
1.99
1.01
1.00
0.99
2.98
3.00
1.10
3.00
3.02
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1
f1 (ppm)

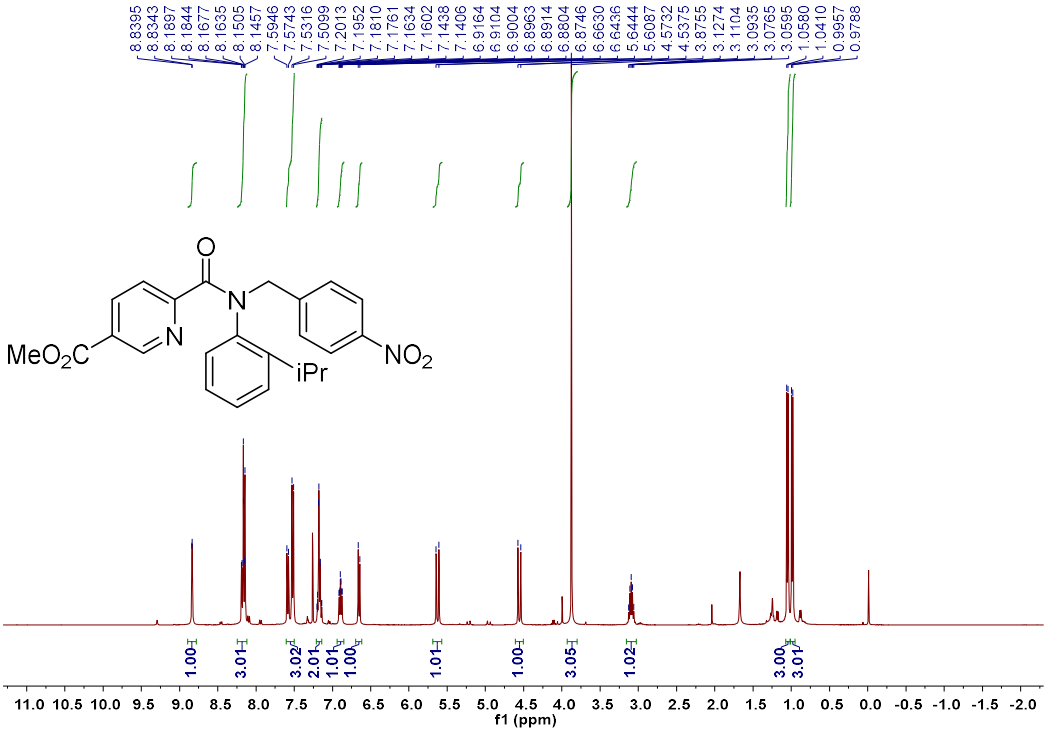

167.88
165.16
159.17
157.51
149.31
146.19
138.81
137.04
130.91
130.04
128.86
128.37
126.84
125.69
125.59
123.17
113.78
55.23
53.32
52.42
27.76
24.68
23.13
O
N
N
MeO2C
iPr
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

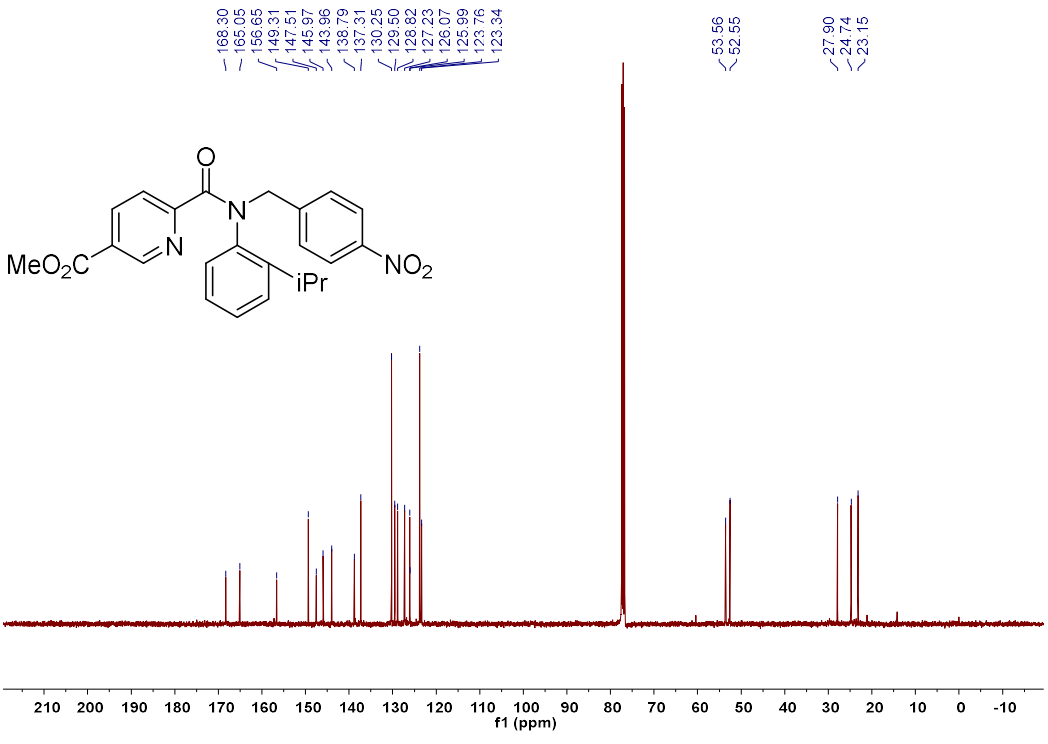
4ss


8.2120
8.1904
7.5494
7.5280
7.2137
7.2098
7.1946
7.1907
7.0618
7.0579
7.0428
7.0388
7.0233
7.0193
6.8035
6.7852
6.7669
6.4621
6.4422
4.5336
4.2912
3.0019
2.9848
2.9679
2.9509
2.9339
2.9170
2.9000
1.3242
1.3073
HN
iPr
NO2
1.99
2.02
1.01
1.01
1.00
1.00
2.05
0.94
1.03
6.03
f1 (ppm)

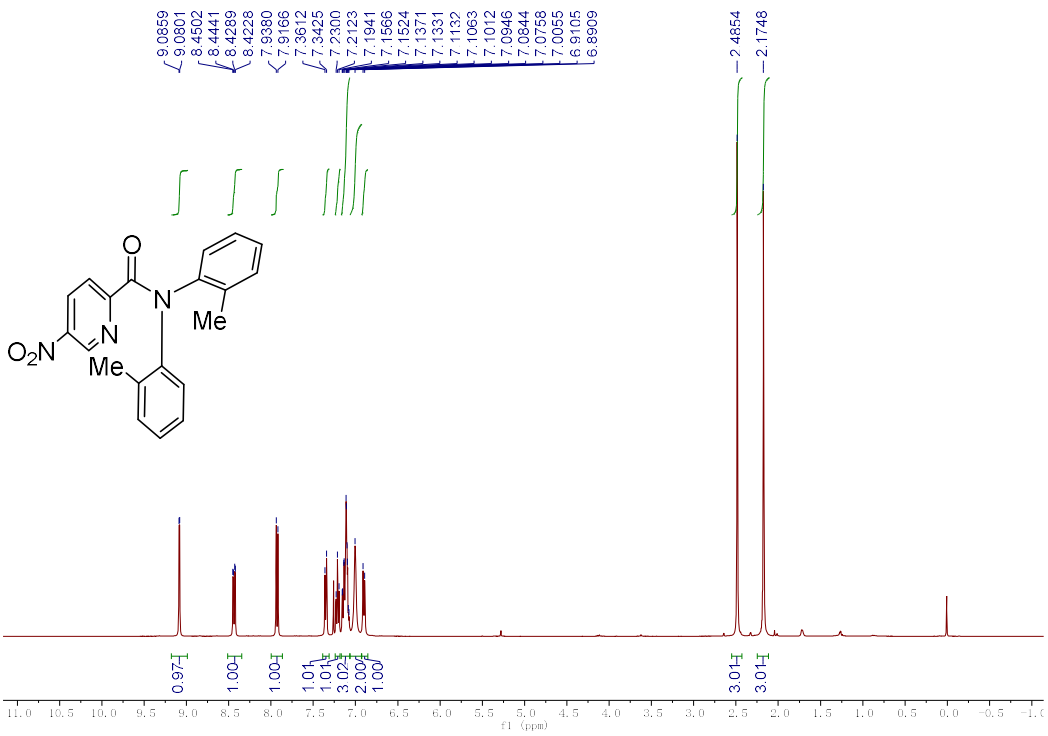

147.66
147.23
143.88
132.43
127.73
126.77
125.22
123.95
118.25
110.76
47.81
27.39
22.36
HN
iPr
NO2
f1 (ppm)

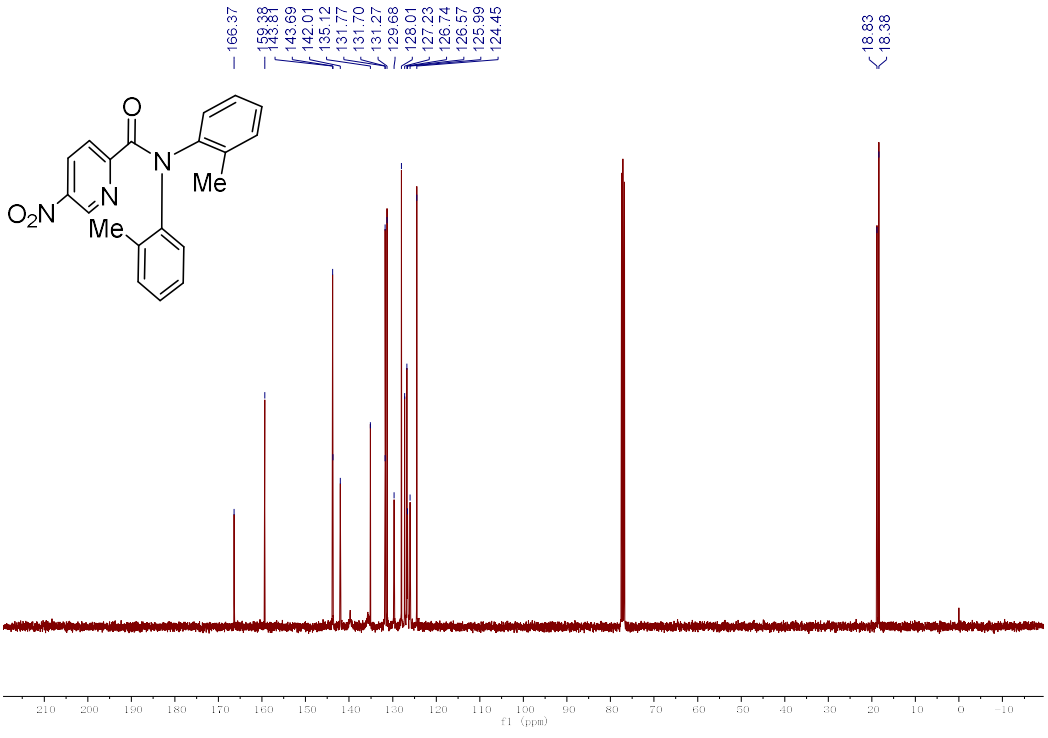
***rac*-4s**


8.8395
8.8343
8.1897
8.1844
8.1677
8.1635
8.1505
8.1457
7.5946
7.5743
7.5316
7.5099
7.2013
7.1952
7.1810
7.1761
7.1634
7.1602
7.1438
7.1406
6.9164
6.9104
6.9004
6.8963
6.8914
6.8804
6.8746
6.6630
6.6436
5.6444
5.6087
4.5732
4.5375
3.8755
3.1274
3.1104
3.0935
3.0765
3.0595
1.0580
1.0410
0.9957
0.9788
O
N
N
MeO2C
iPr
NO2
1.00
3.01
3.02
2.01
1.01
1.00
1.01
1.00
3.05
1.02
3.00
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

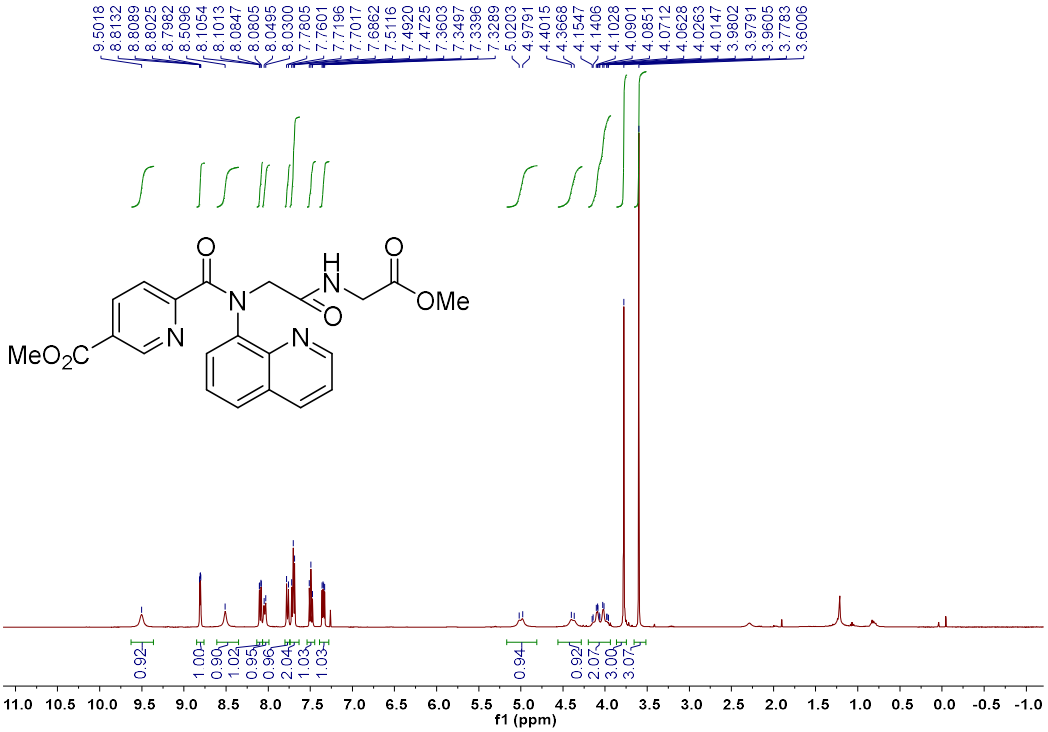

168.30
165.05
156.65
149.31
147.51
145.97
143.96
138.79
137.31
130.25
129.50
128.82
127.23
126.07
125.99
123.76
123.34
53.56
52.55
27.90
24.74
23.15
O
N
N
MeO2C
iPr
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

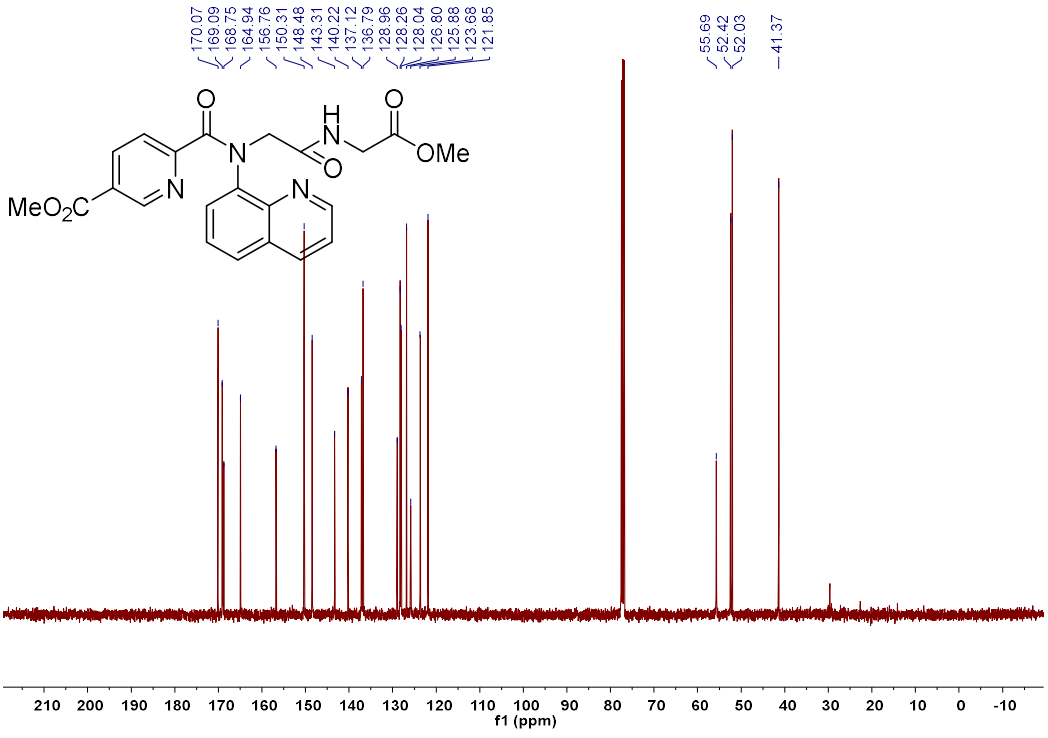
***rac*-4t**


9.0859
9.0801
8.4502
8.4441
8.4289
8.4228
7.9380
7.9166
7.3612
7.3425
7.2300
7.2123
7.1941
7.1566
7.1524
7.1371
7.1331
7.1132
7.1063
7.1012
7.0946
7.0844
7.0758
7.0055
6.9105
6.8909
2.4854
2.1748
0.97
1.00
1.00
1.01
1.01
3.02
2.00
1.00
3.01
3.01
O
N
Me
O2N
N
Me
f1 (ppm)

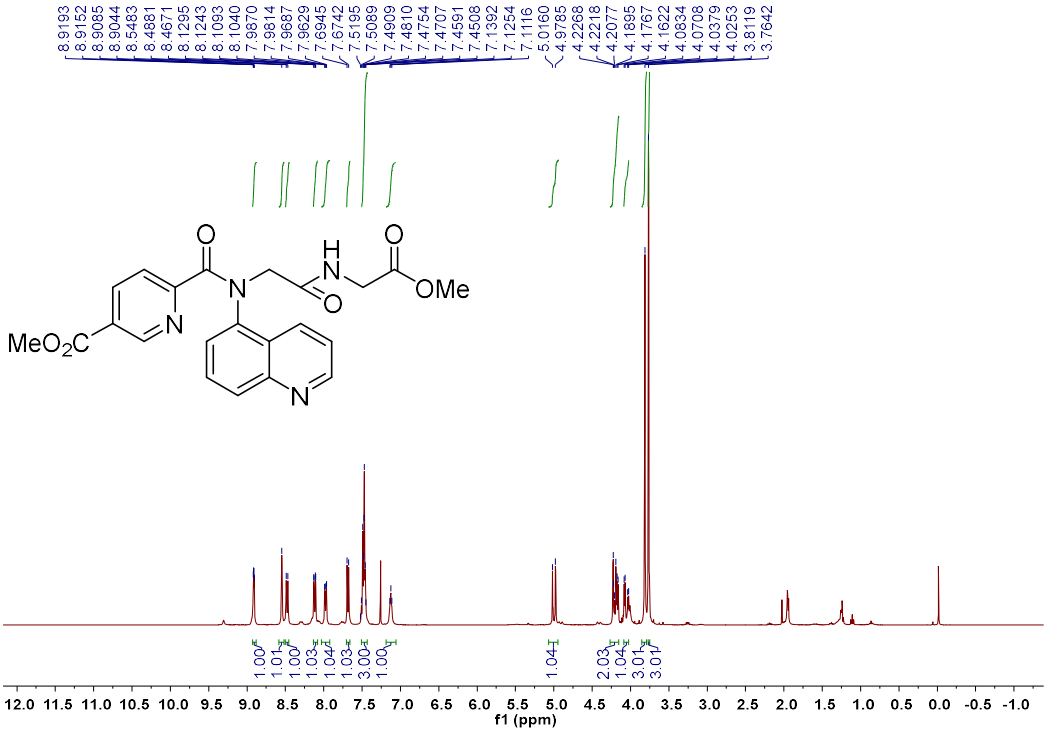

166.37
159.38
143.81
143.69
142.01
135.12
131.77
131.70
131.27
129.68
128.01
127.23
126.74
126.57
125.99
124.45
18.83
18.38
O
N
Me
O2N
N
Me
f1 (ppm)

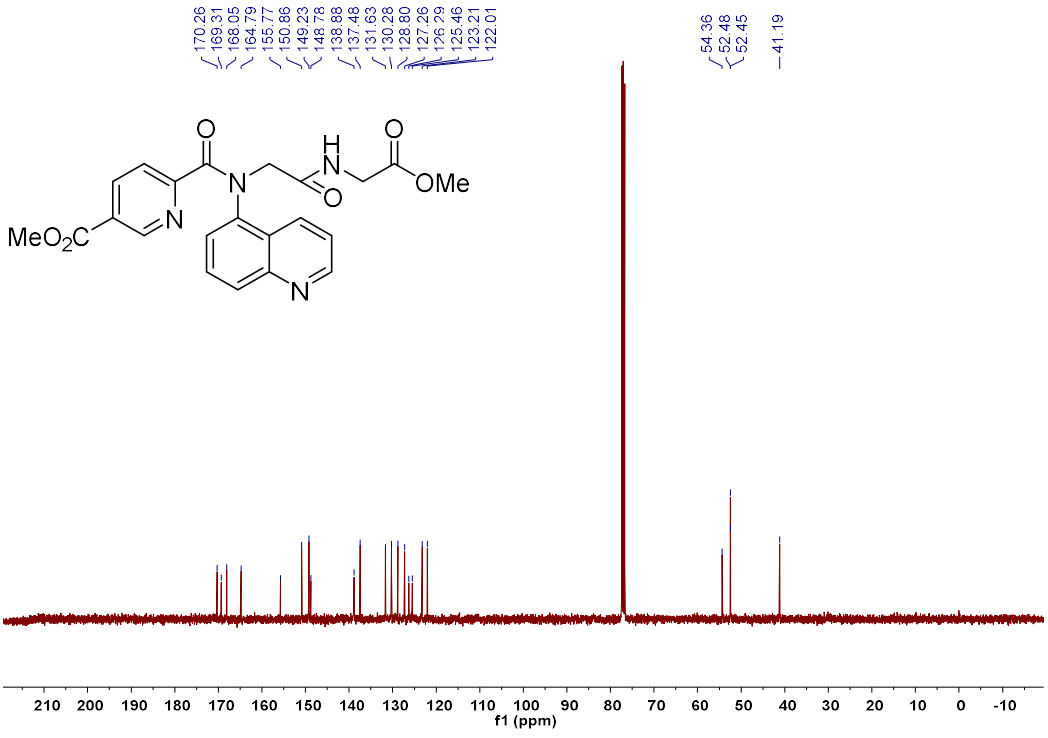
***rac*-4u**


9.5018
8.8132
8.8089
8.8025
8.7982
8.5096
8.1054
8.1013
8.0847
8.0805
8.0495
8.0300
7.7805
7.7601
7.7196
7.7017
7.6862
7.5116
7.4920
7.4725
7.3603
7.3497
7.3396
7.3289
5.0203
4.9791
4.4015
4.3668
4.1547
4.1406
4.1028
4.0901
4.0851
4.0712
4.0628
4.0263
4.0147
3.9802
3.9791
3.9605
3.7783
3.6006
MeO2C
OMe
0.92
1.00
0.90
1.02
0.95
0.96
2.04
1.03
1.03
0.94
0.92
2.07
3.00
3.07
f1 (ppm)

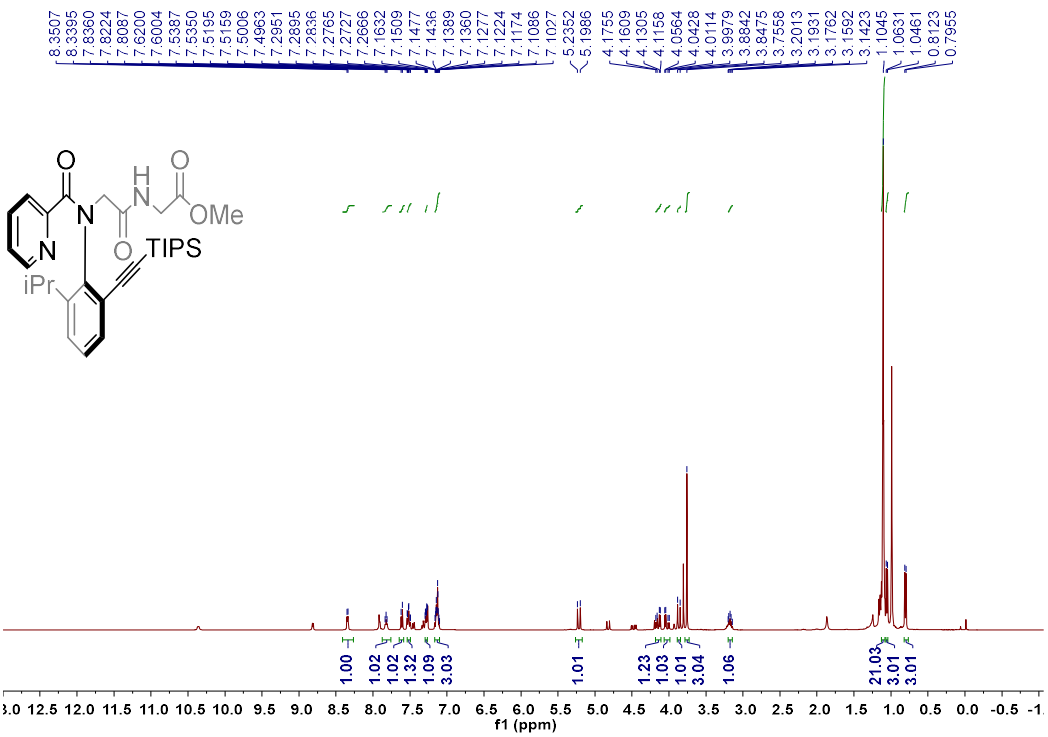

170.07
169.09
168.75
164.94
156.76
150.31
148.48
143.31
140.22
137.12
136.79
128.96
128.26
128.04
126.80
125.88
123.68
121.85
55.69
52.42
52.03
41.37
MeO2C
OMe
f1 (ppm)

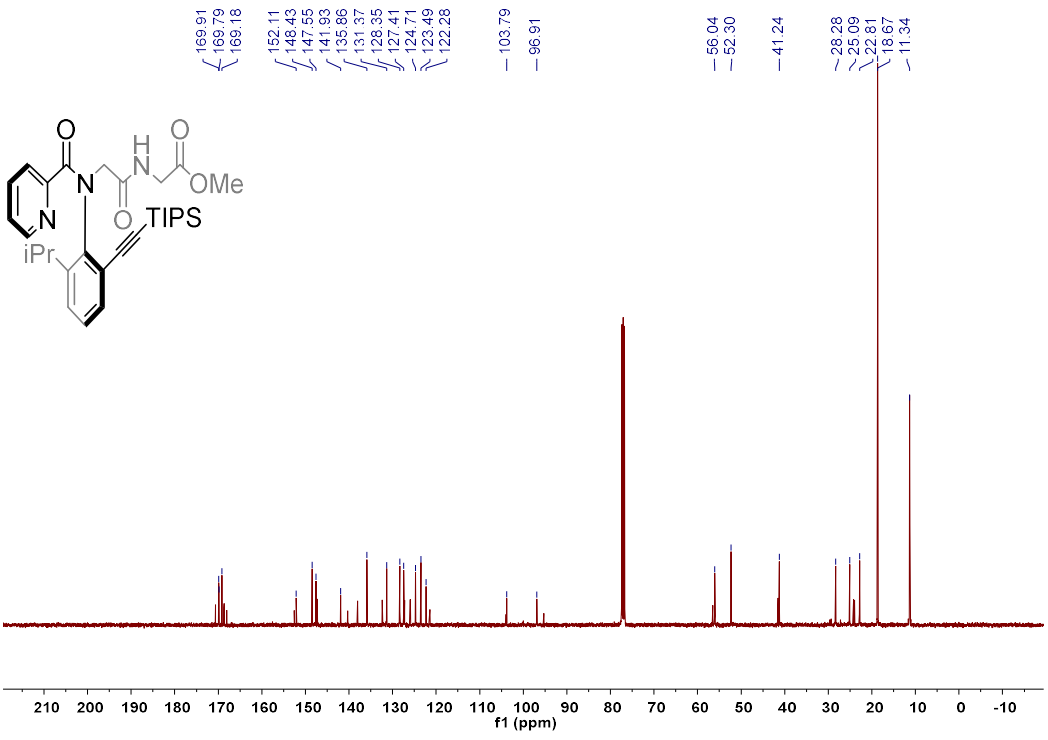
***rac*-4v**


8.9193
8.9152
8.9085
8.9044
8.5483
8.4881
8.4671
8.1295
8.1243
8.1093
8.1040
7.9870
7.9814
7.9687
7.9629
7.6945
7.6742
7.5195
7.5089
7.4909
7.4810
7.4754
7.4707
7.4591
7.4508
7.1392
7.1254
7.1116
5.0160
4.9785
4.2268
4.2218
4.2077
4.1895
4.1767
4.1622
4.0834
4.0708
4.0379
4.0253
3.8119
3.7642
O
H
N
O
N
OMe
O
N
MeO2C
N
1.00
1.01
1.00
1.03
1.04
1.03
3.00
1.00
1.04
2.03
1.04
3.01
3.01
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


170.26
169.31
168.05
164.79
155.77
150.86
149.23
148.78
138.88
137.48
131.63
130.28
128.80
127.26
126.29
125.46
123.21
122.01
54.36
52.48
52.45
41.19
O
H
N
O
N
OMe
O
N
MeO2C
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3a


8.3507
8.3395
7.8360
7.8224
7.8087
7.6200
7.6004
7.5387
7.5350
7.5195
7.5159
7.5006
7.4963
7.2951
7.2895
7.2636
7.2765
7.2727
7.2666
7.1632
7.1509
7.1477
7.1436
7.1389
7.1360
7.1277
7.1224
7.1174
7.1086
7.1027
5.2352
5.1986
4.1755
4.1609
4.1305
4.1158
4.0564
4.0428
4.0114
3.9979
3.8842
3.8475
3.7558
3.2013
3.1931
3.1762
3.1592
3.1423
1.1045
1.0631
1.0461
0.8123
0.7955
O
N
H
N
O
OMe
N
O
TIPS
iPr
1.00
1.02
1.02
1.32
1.09
3.03
1.01
1.23
1.03
1.01
3.04
1.06
21.03
3.01
3.01
f1 (ppm)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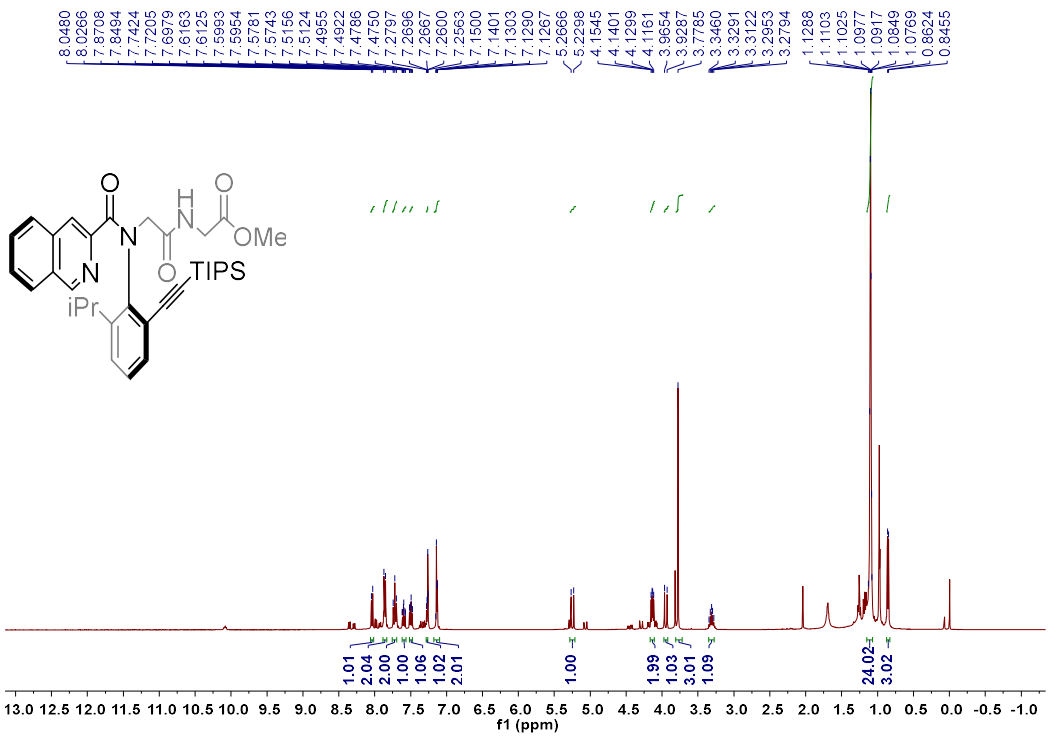
169.79
169.18
152.11
148.43
147.55
141.93
135.86
131.37
128.35
127.41
124.71
123.49
122.28
103.79
96.91
56.04
52.30
41.24
28.28
25.09
22.81
18.67
11.34
O
N
H
N
O
OMe
N
O
TIPS
iPr
f1 (ppm)

3d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7.7424
7.7205
7.6979
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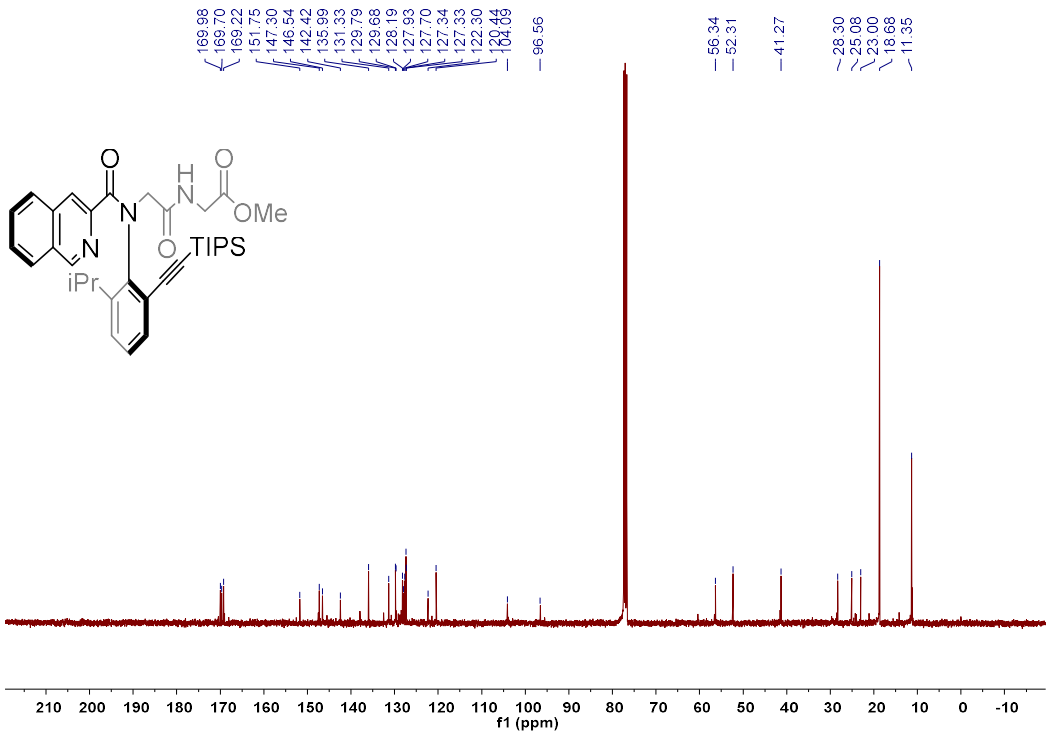
7.6125
7.5993
7.5954
7.5781
7.5743
7.5156
7.5124
7.4955
7.4922
7.4786
7.4750
7.2797
7.2696
7.2667
7.2600
7.2563
7.1500
7.1401
7.1303
7.1290
7.1267
5.2666
5.2298
4.1545
4.1401
4.1299
4.1161
3.9654
3.9287
3.7785
3.3460
3.3291
3.3122
3.2953
3.2794
1.1288
1.1103
1.1025
1.0977
1.0917
1.0849
1.0769
0.8624
0.8455
O
H
N
O
OMe
N
O
TIPS
iPr
1.01
2.04
2.00
1.00
1.06
1.02
2.01
1.00
1.99
1.03
3.01
1.09
24.02
3.02
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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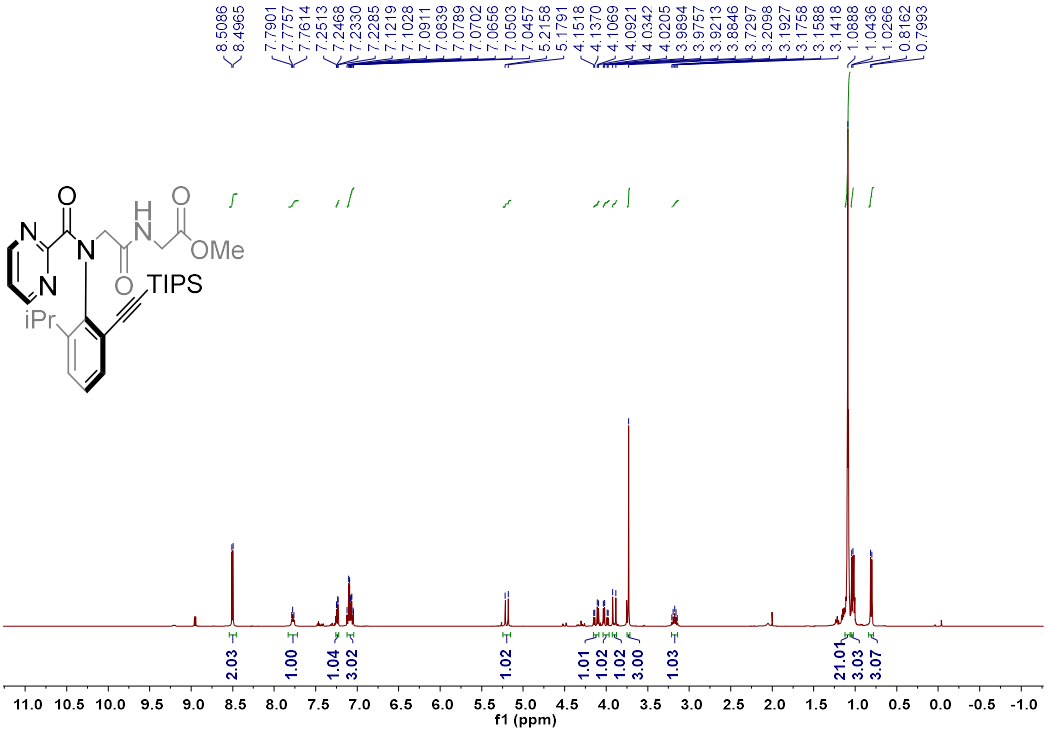
169.22
151.75
147.30
146.54
142.42
135.99
131.33
129.79
129.68
128.19
127.93
127.70
127.34
127.33
122.30
120.44
104.09
96.56
56.34
52.31
41.27
28.30
25.08
23.00
18.68
11.35
O
H
N
O
OMe
N
O
TIPS
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3e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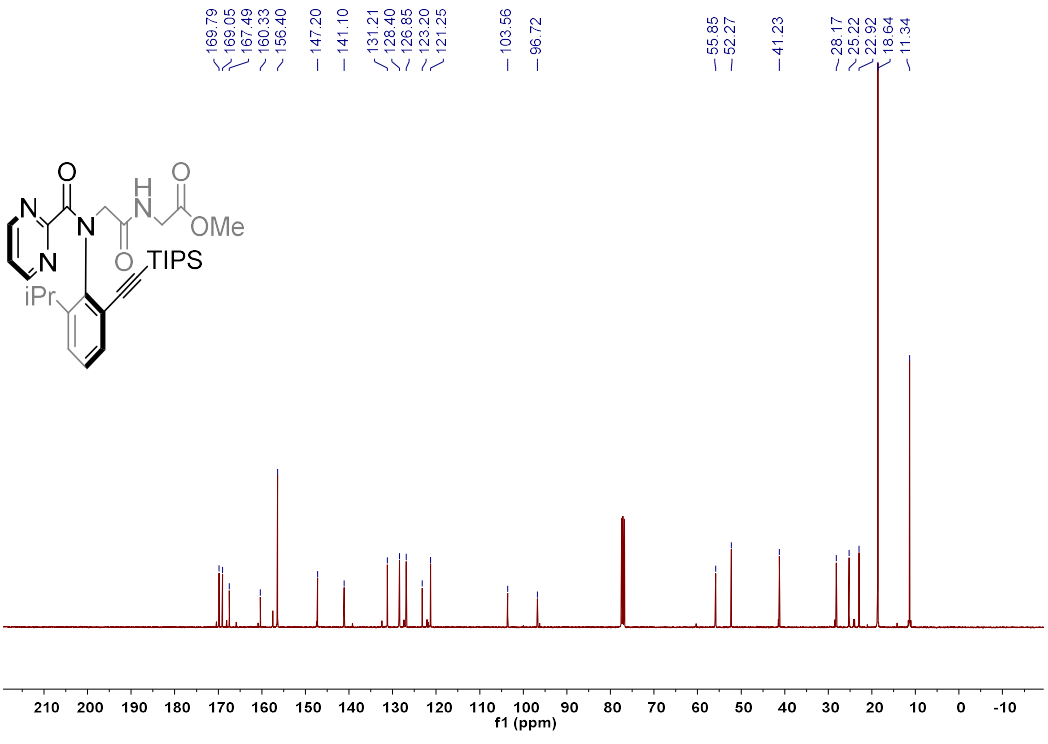
8.4965
7.7901
7.7757
7.7614
7.2513
7.2468
7.2330
7.2285
7.1219
7.1028
7.0911
7.0839
7.0789
7.0702
7.0656
7.0503
7.0457
5.2158
5.1791
4.1518
4.1370
4.1069
4.0921
4.0342
4.0205
3.9894
3.9757
3.9213
3.8846
3.7297
3.2098
3.1927
3.1758
3.1588
3.1418
1.0888
1.0436
1.0266
0.8162
0.7993
O
N
N
H
N
O
OMe
O
TIPS
iPr
2.03
1.00
1.04
3.02
1.02
1.01
1.02
1.02
3.00
1.03
21.01
3.03
3.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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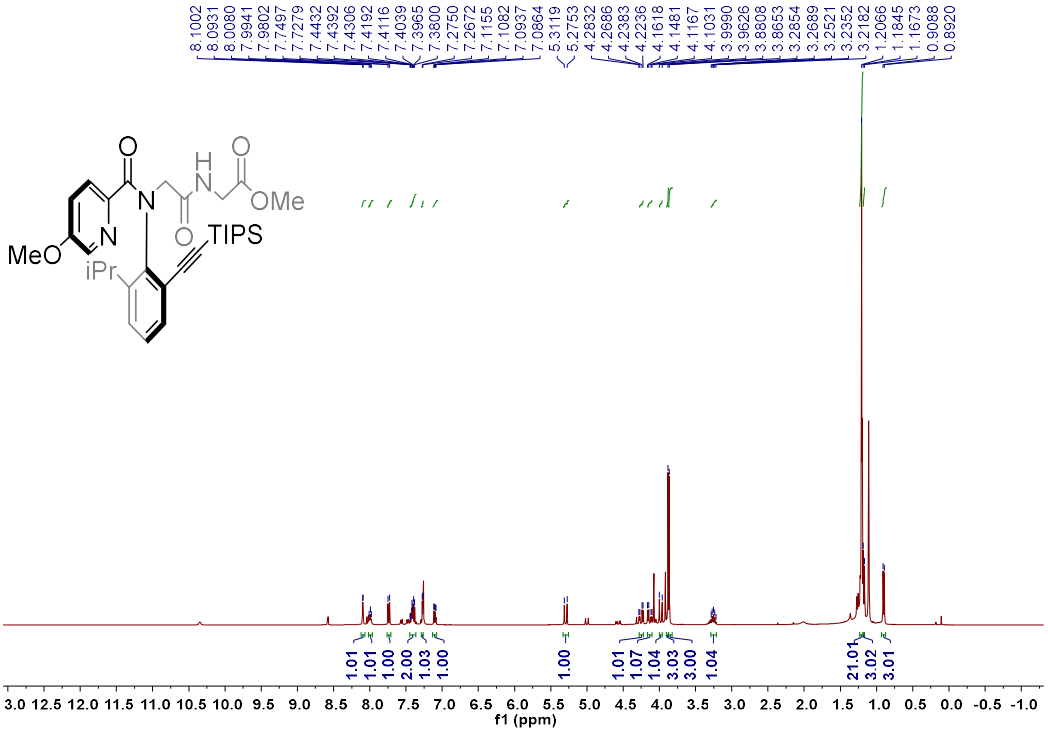
169.05
167.49
160.33
156.40
147.20
141.10
131.21
128.40
126.85
123.20
121.25
103.56
96.72
55.85
52.27
41.23
28.17
25.22
22.92
18.64
11.34
O
N
N
H
N
O
OMe
O
TIPS
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3f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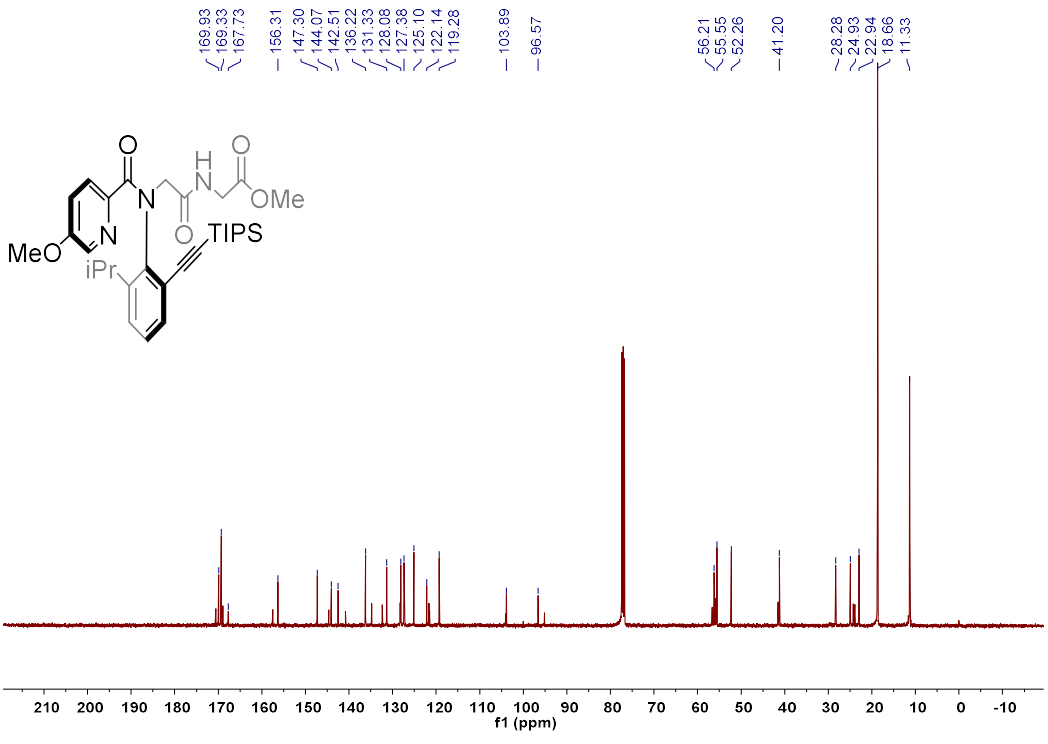
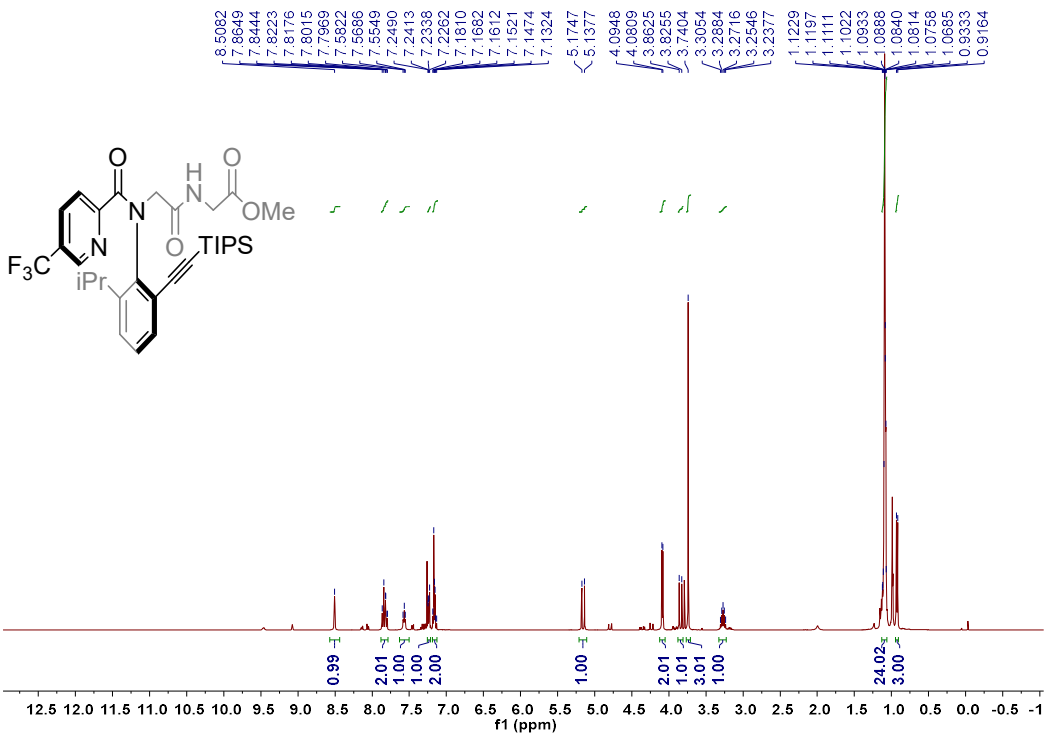
8.0931
8.0080
7.9941
7.9802
7.7497
7.7279
7.4432
7.4392
7.4306
7.4192
7.4116
7.4039
7.3965
7.3800
7.2750
7.2672
7.1155
7.1082
7.0937
7.0864
5.3119
5.2753
4.2832
4.2686
4.2383
4.2236
4.1618
4.1481
4.1167
4.1031
3.9990
3.9626
3.8808
3.8653
3.2854
3.2689
3.2521
3.2352
3.2182
1.2066
1.1845
1.1673
0.9088
0.8920
O
N
H
N
O
OMe
O
TIPS
MeO
N
iPr
1.01
1.01
1.00
2.00
1.03
1.00
1.00
1.01
1.07
1.04
3.03
3.00
1.04
21.01
3.02
3.01
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


169.93
169.33
167.73
156.31
147.30
144.07
142.51
136.22
131.33
128.08
127.38
125.10
122.14
119.28
103.89
96.57
56.21
55.55
52.26
41.20
28.28
24.93
22.94
18.66
11.33
O
N
H
N
O
OMe
O
TIPS
MeO
N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3g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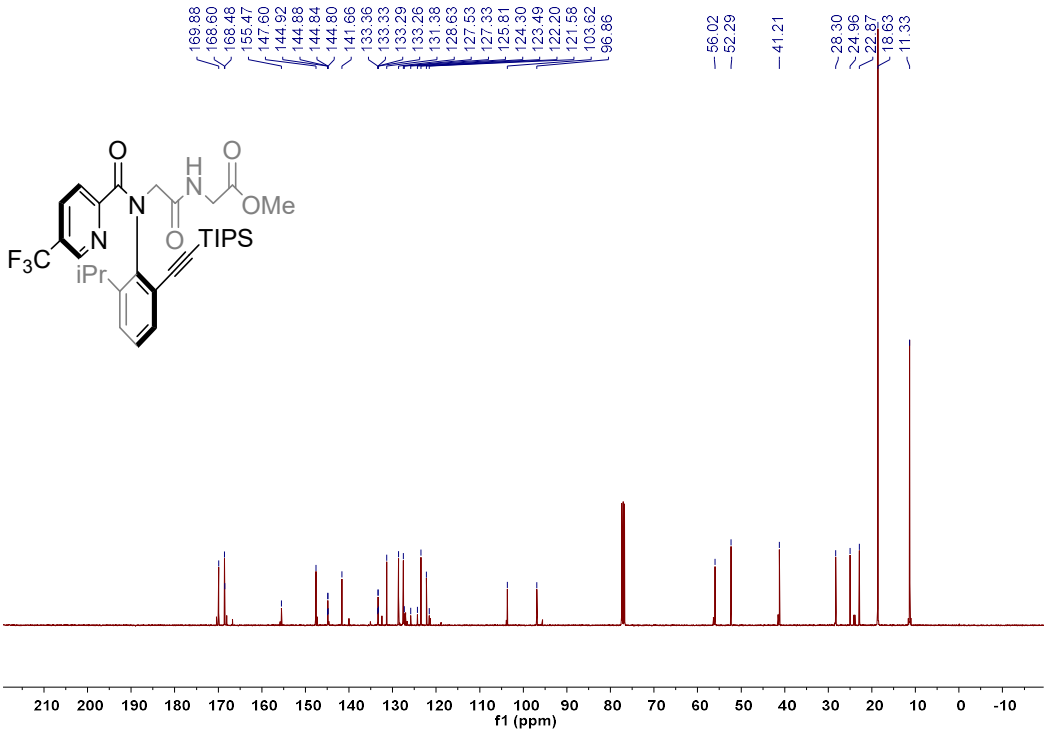
7.8223
7.8176
7.8015
7.7969
7.5822
7.5686
7.5549
7.2490
7.2413
7.2338
7.2262
7.1810
7.1682
7.1612
7.1521
7.1474
7.1324
5.1747
5.1377
4.0948
4.0809
3.8625
3.8255
3.7404
3.3054
3.2884
3.2716
3.2546
3.2377
1.1229
1.1197
1.1111
1.1022
1.0933
1.0888
1.0840
1.0814
1.0758
1.0685
0.9333
0.9164
O
N
H
N
O
OMe
O
TIPS
F3C
N
iPr
0.99
2.01
1.00
1.00
2.00
1.00
2.01
1.01
3.01
1.00
24.02
3.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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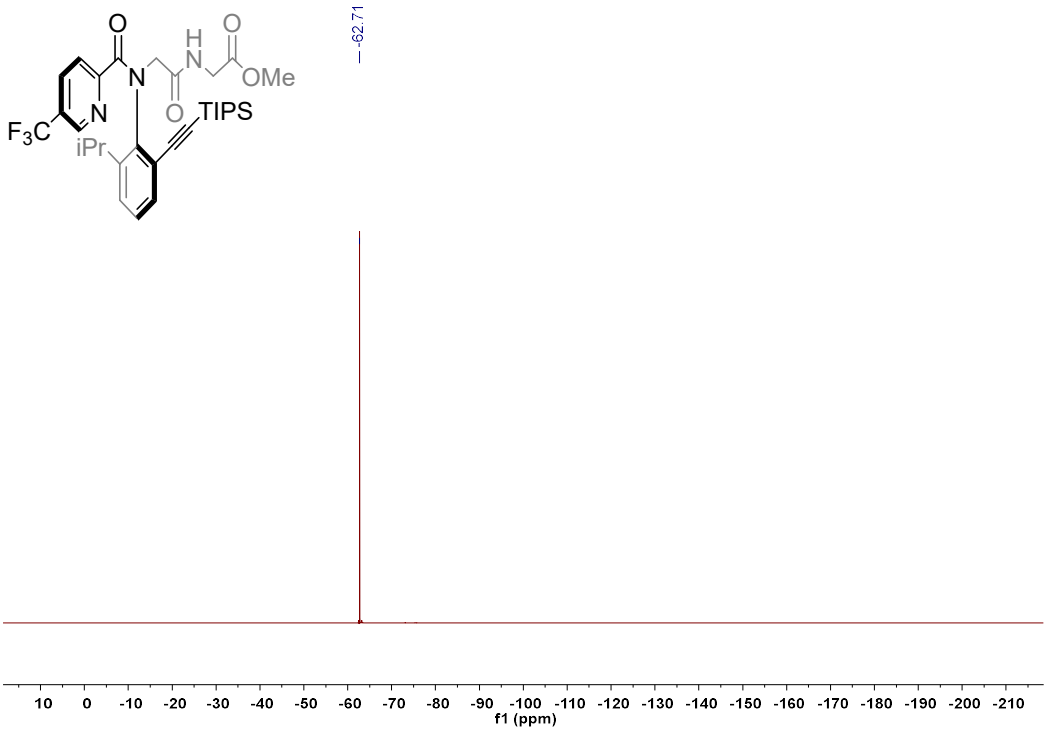
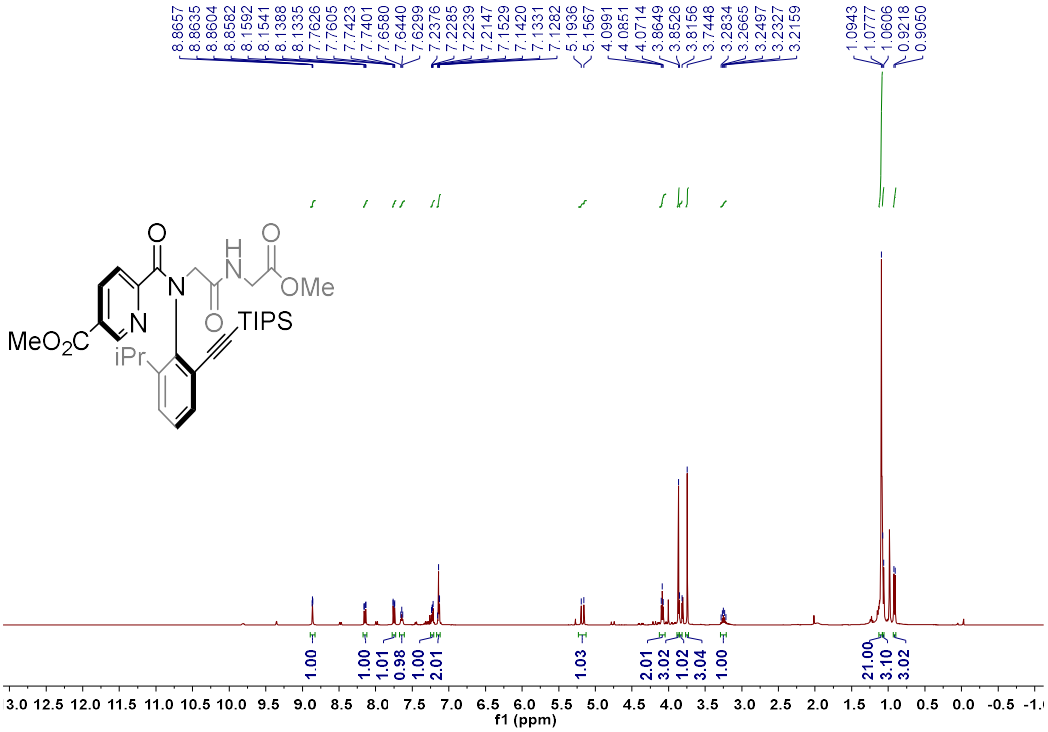
168.48
155.47
147.60
144.92
144.88
144.84
144.80
141.66
133.36
133.33
133.29
133.26
131.38
128.63
127.53
127.33
125.81
124.30
123.49
122.20
121.58
103.62
96.86
56.02
52.29
41.21
28.30
24.96
22.87
18.63
11.33
O
N
H
N
O
OMe
O
TIPS
F3C
N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


O
H
N
O
N
OMe
O
TIPS
N
F3C
iPr
-62.71
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3h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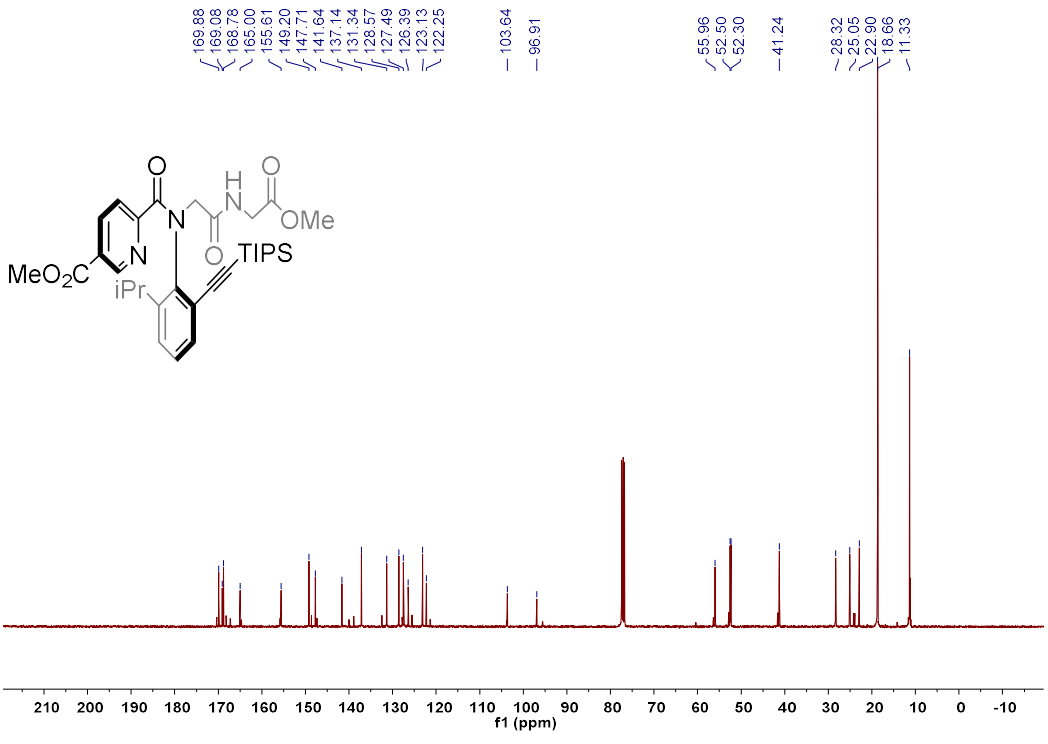
8.8604
8.8582
8.1592
8.1541
8.1388
8.1335
7.7626
7.7605
7.7423
7.7401
7.6580
7.6440
7.6299
7.2376
7.2285
7.2239
7.2147
7.1529
7.1420
7.1331
7.1282
5.1936
5.1567
4.0991
4.0851
4.0714
3.8649
3.8526
3.8156
3.7448
3.2834
3.2665
3.2497
3.2327
3.2159
1.0943
1.0777
1.0606
0.9218
0.9050
MeO2C
iPr
N
O
H
N
O
OMe
O
TIPS
1.00
1.00
1.01
0.98
1.00
2.01
1.03
2.01
3.02
1.02
3.04
1.00
21.00
3.10
3.02
f1 (ppm)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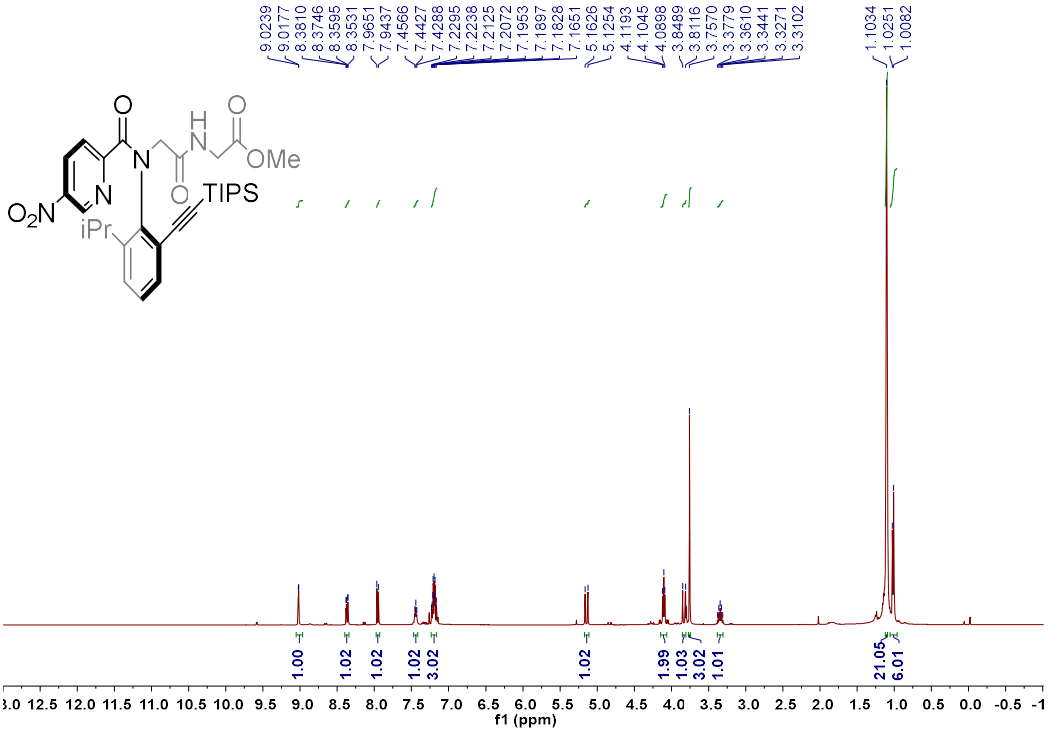
169.08
168.78
165.00
155.61
149.20
147.71
141.64
137.14
131.34
128.57
127.49
126.39
123.13
122.25
103.64
96.91
55.96
52.50
52.30
41.24
28.32
25.05
22.90
18.66
11.33
MeO2C
iPr
N
O
H
N
O
OMe
O
TIPS
f1 (ppm)

3i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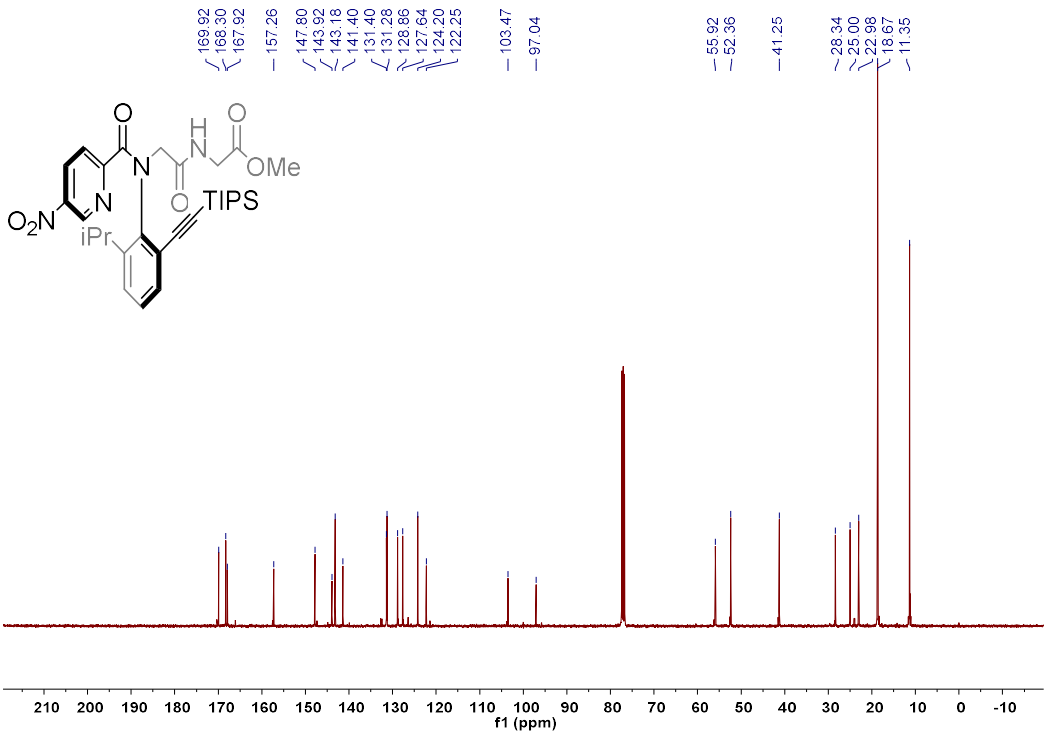
8.3810
8.3746
8.3595
8.3531
7.9651
7.9437
7.4566
7.4427
7.4288
7.2295
7.2238
7.2125
7.2072
7.1953
7.1897
7.1828
7.1651
5.1626
5.1254
4.1193
4.1045
4.0898
3.8489
3.8116
3.7570
3.3779
3.3610
3.3441
3.3271
3.3102
1.1034
1.0251
1.0082
O
N
H
N
O
OMe
O
TIPS
O2N
N
iPr
1.00
1.02
1.02
1.02
3.02
1.02
1.99
1.03
3.02
1.01
21.05
6.01
f1 (ppm)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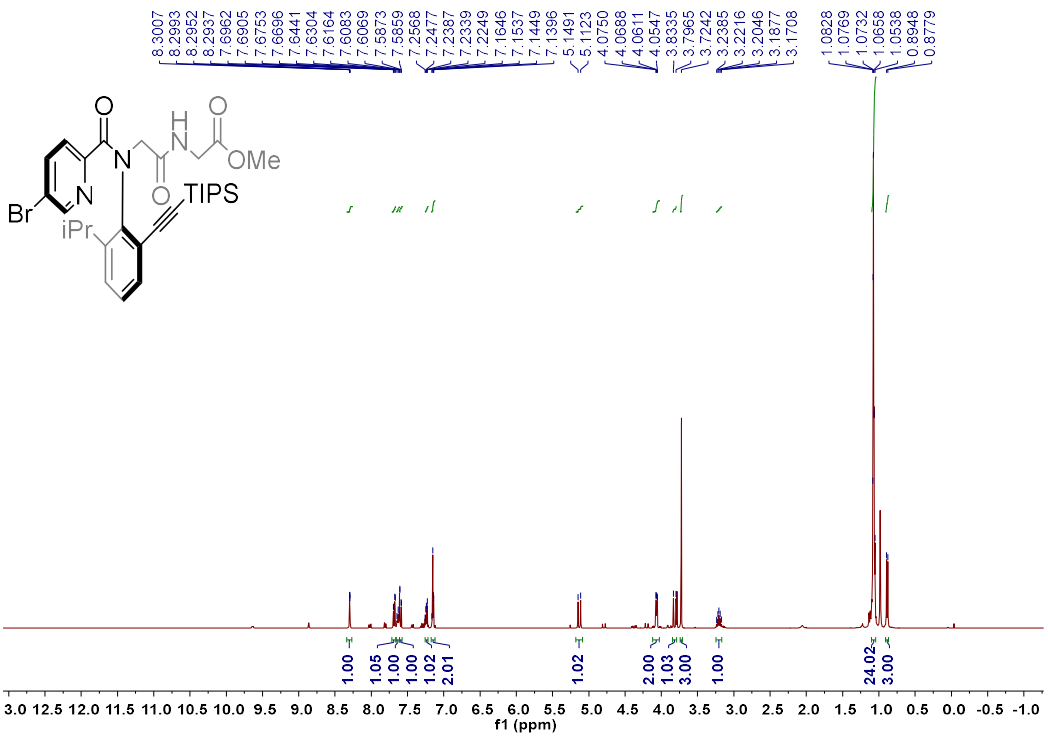
167.92
157.26
147.80
143.92
143.18
141.40
131.40
131.28
128.86
127.64
124.20
122.25
103.47
97.04
55.92
52.36
41.25
28.34
25.00
22.98
18.67
11.35
O
N
H
N
O
OMe
O
TIPS
O2N
N
iPr
f1 (ppm)

3j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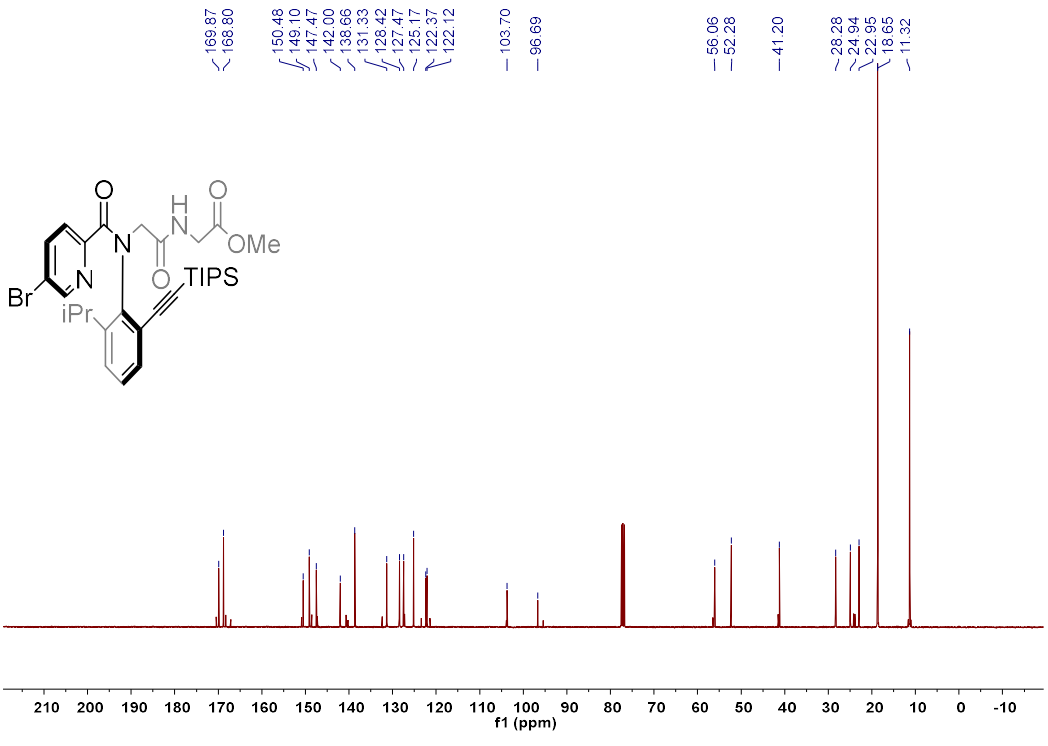
8.2952
8.2937
7.6962
7.6905
7.6753
7.6696
7.6441
7.6304
7.6164
7.6083
7.6069
7.5873
7.5859
7.2568
7.2477
7.2387
7.2339
7.2249
7.1646
7.1537
7.1449
7.1396
5.1491
5.1123
4.0750
4.0688
4.0611
4.0547
3.8335
3.7965
3.7242
3.2385
3.2216
3.2046
3.1877
3.1708
1.0828
1.0769
1.0732
1.0658
1.0538
0.8948
0.8779
O
N
H
N
O
OMe
Br
N
O
TIPS
iPr
1.00
1.05
1.00
1.00
1.02
2.01
1.02
2.00
1.03
3.00
1.00
24.02
3.00
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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142.00
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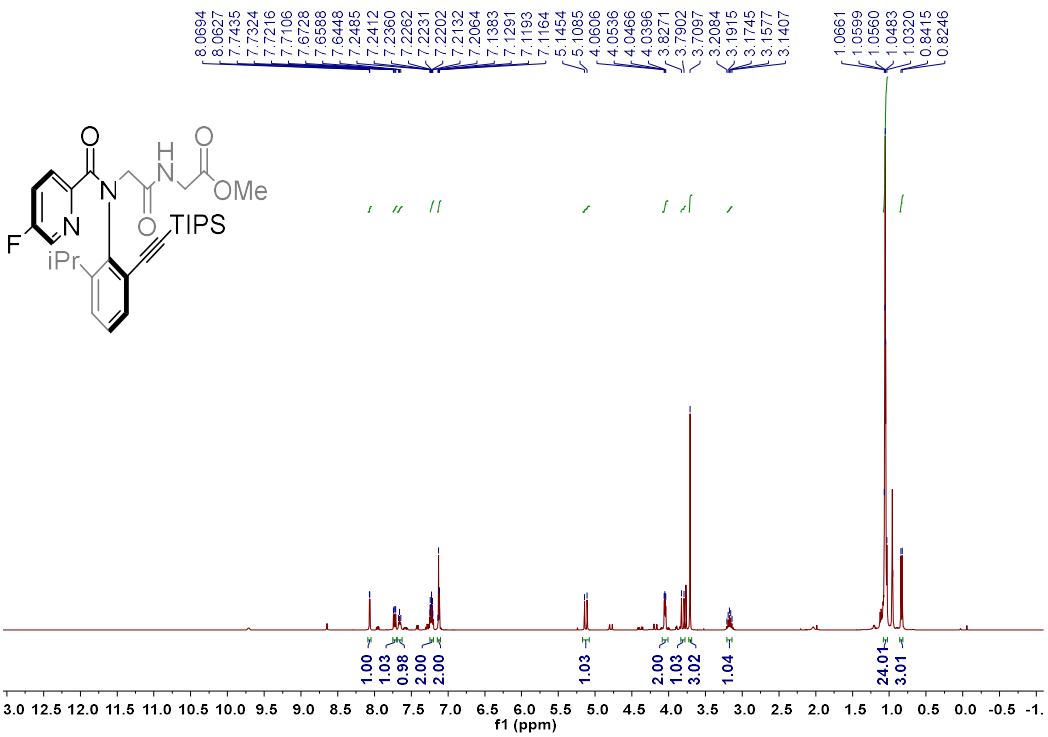
131.33
128.42
127.47
125.17
122.37
122.12
103.70
96.69
56.06
52.28
41.20
28.28
24.94
22.95
18.65
11.32
O
N
H
N
O
OMe
Br
N
O
TIPS
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3k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7.7216
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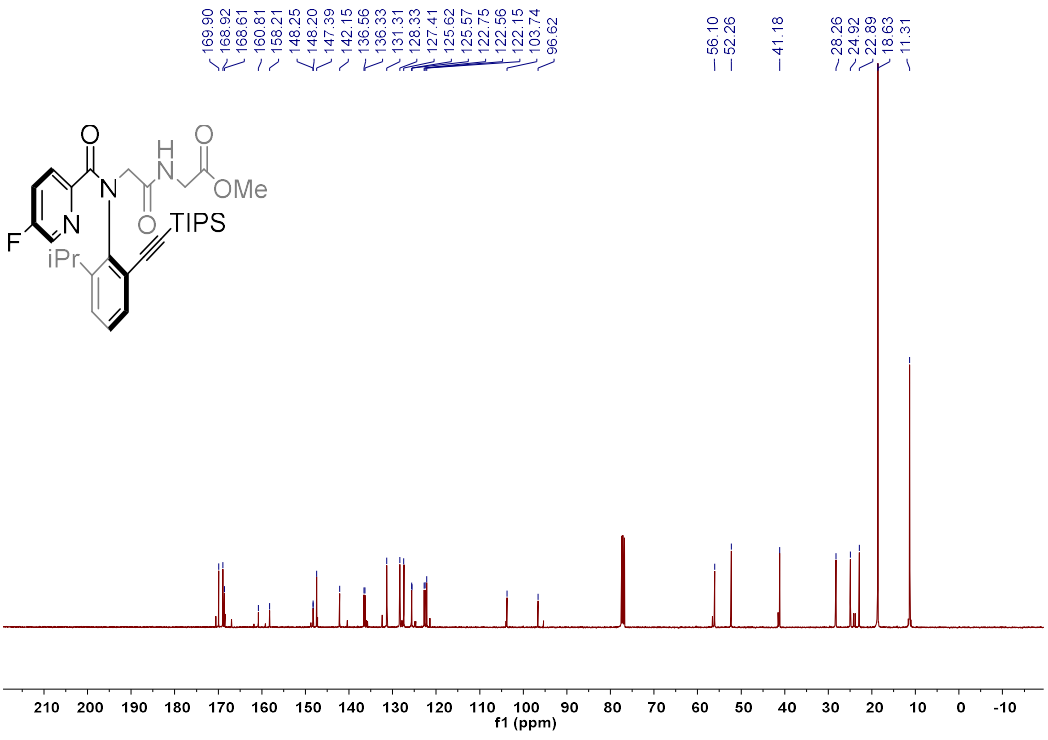
7.6728
7.6588
7.6448
7.2485
7.2412
7.2360
7.2262
7.2231
7.2202
7.2132
7.2064
7.1383
7.1291
7.1193
7.1164
5.1454
5.1065
4.0606
4.0536
4.0466
4.0396
3.8271
3.7902
3.7097
3.2084
3.1915
3.1745
3.1577
3.1407
1.0661
1.0599
1.0560
1.0483
1.0320
0.8415
0.8246
O
H
N
O
OMe
N
O
TIPS
F
N
iPr
1.00
1.03
0.98
2.00
2.00
1.03
2.00
1.03
3.02
1.04
24.01
3.01
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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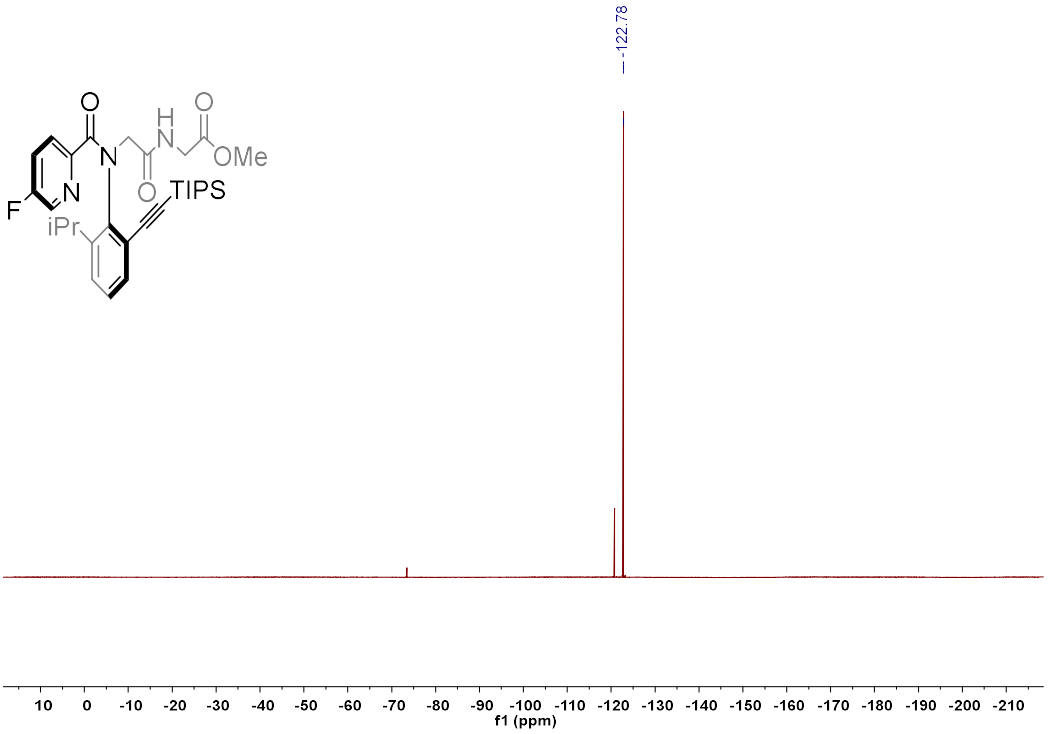
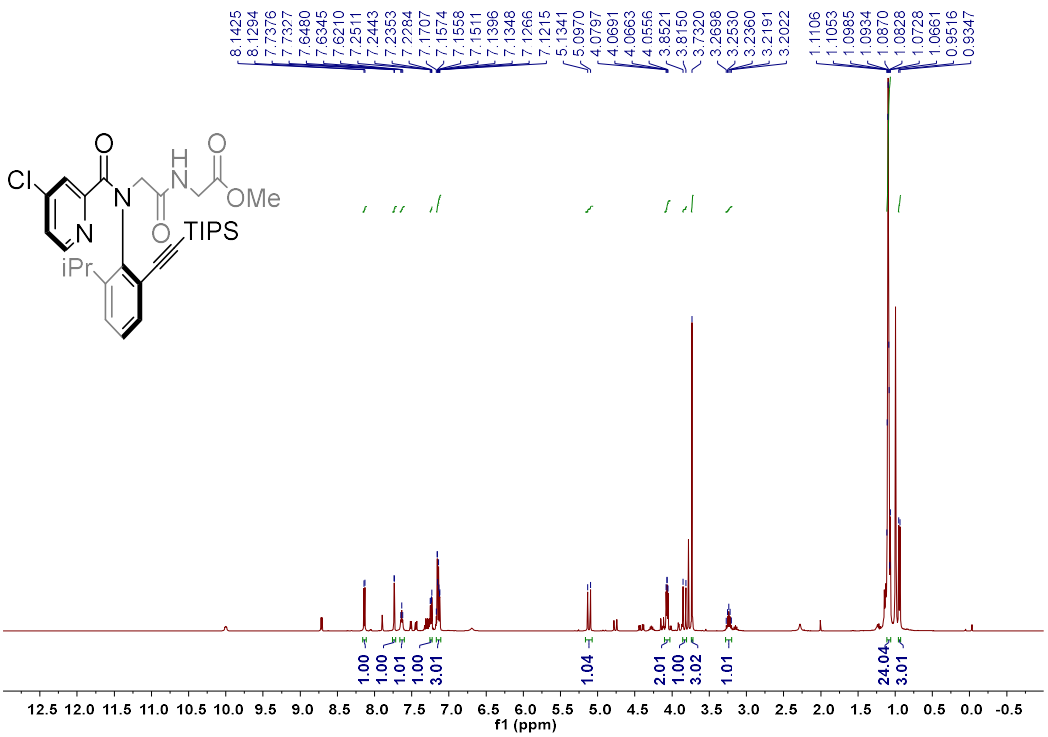
158.21
148.25
148.20
147.39
142.15
136.56
136.33
131.31
128.33
127.41
125.62
125.57
122.75
122.56
122.15
103.74
96.62
56.10
52.26
41.18
28.26
24.92
22.89
18.63
11.31
O
H
N
O
OMe
N
O
TIPS
F
N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-122.78
O
H
N
O
OMe
N
O
TIPS
F
N
iPr
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

3l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7.7327
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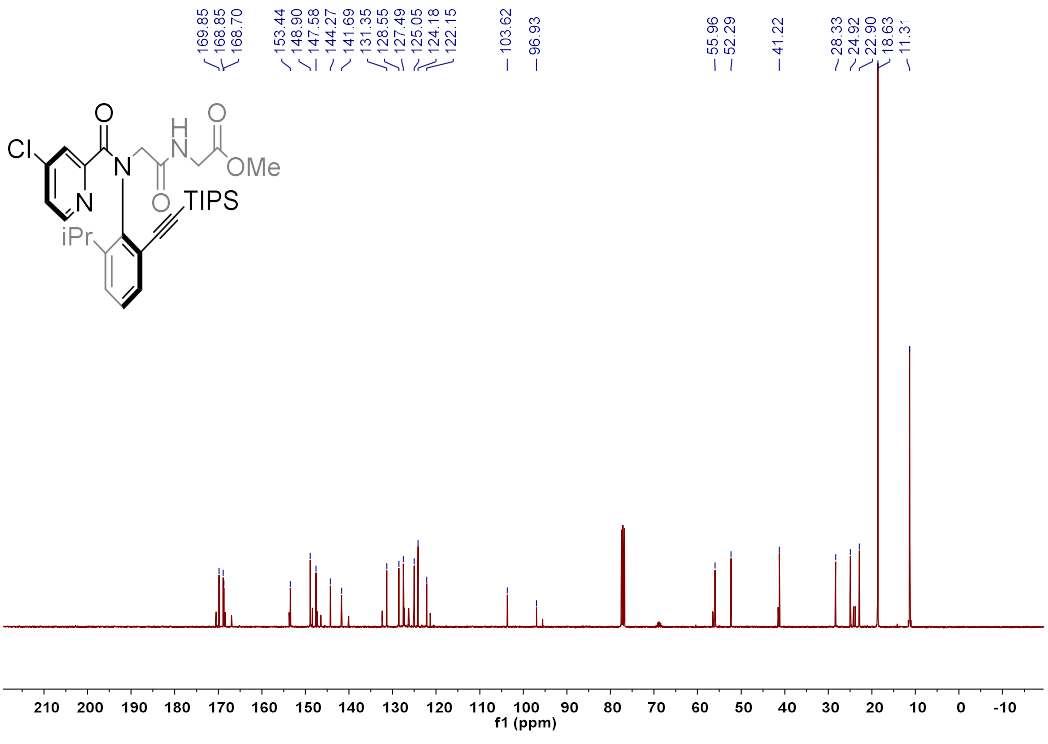
7.6210
7.2511
7.2443
7.2353
7.2284
7.1707
7.1574
7.1558
7.1511
7.1396
7.1348
7.1266
7.1215
5.1341
5.0970
4.0797
4.0691
4.0663
4.0556
3.8521
3.8150
3.7320
3.2698
3.2530
3.2360
3.2191
3.2022
1.1106
1.1053
1.0985
1.0934
1.0870
1.0828
1.0728
1.0661
0.9516
0.9347
Cl
N
O
H
N
O
OMe
O
TIPS
iPr
1.00
1.00
1.01
1.00
3.01
1.04
2.01
1.00
3.02
1.01
24.04
3.01
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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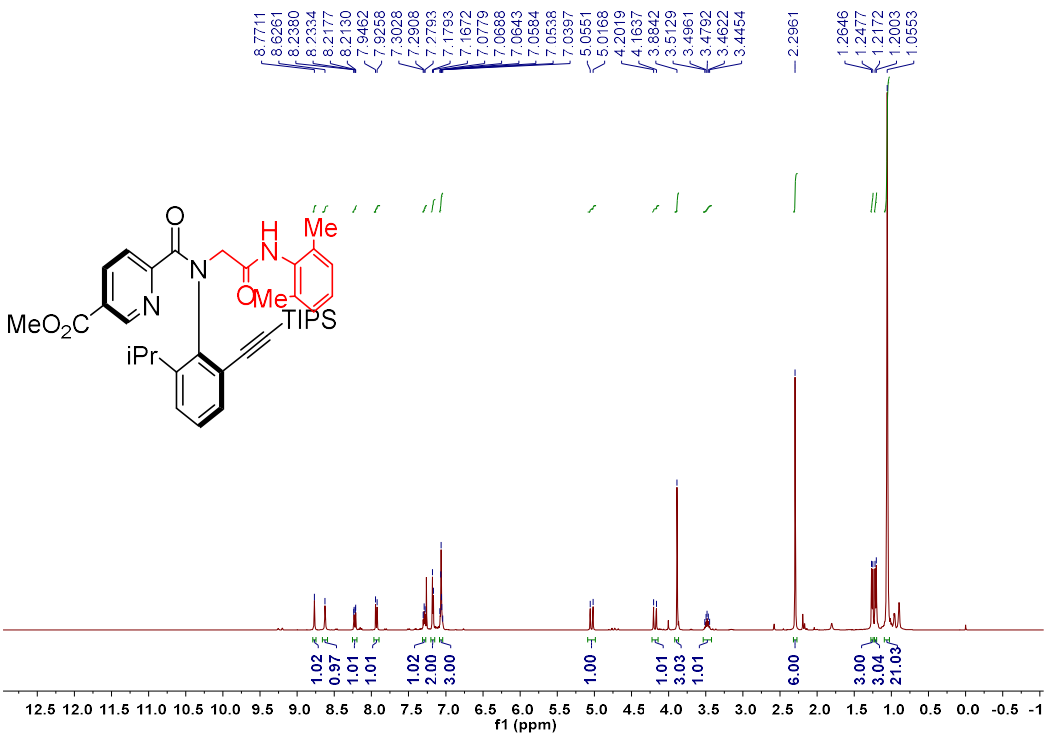
147.58
144.27
141.69
131.35
128.55
127.49
125.05
124.18
122.15
103.62
96.93
55.96
52.29
41.22
28.33
24.92
22.90
18.63
11.3
Cl
N
O
H
N
O
OMe
O
TIPS
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5a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8.2177
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7.9462
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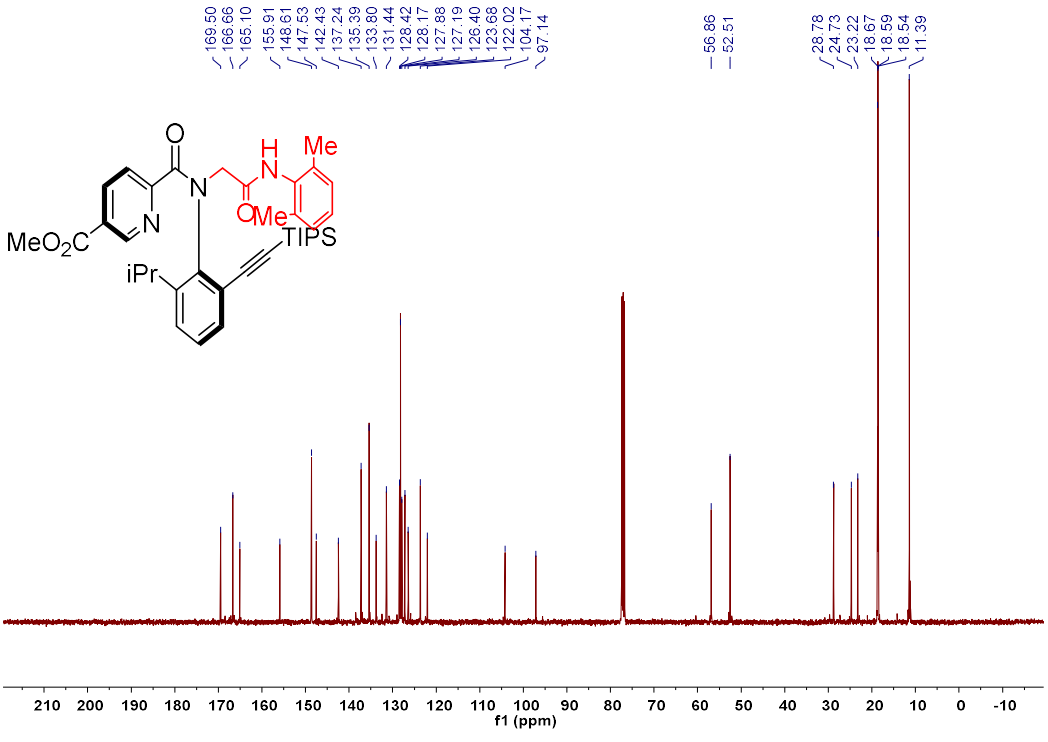
7.3028
7.2908
7.2793
7.1793
7.1672
7.0779
7.0688
7.0643
7.0584
7.0538
7.0397
5.0551
5.0168
4.2019
4.1637
3.8842
3.5129
3.4961
3.4792
3.4622
3.4454
2.2961
1.2646
1.2477
1.2172
1.2003
1.0553
1.02
0.97
1.01
1.01
1.02
2.00
3.00
1.00
1.01
3.03
1.01
6.00
3.00
3.04
21.03
f1 (ppm)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166.66
165.10
155.91
148.61
147.53
142.43
137.24
135.39
133.80
131.44
128.42
128.17
127.88
127.19
126.40
123.68
122.02
104.17
97.14
56.86
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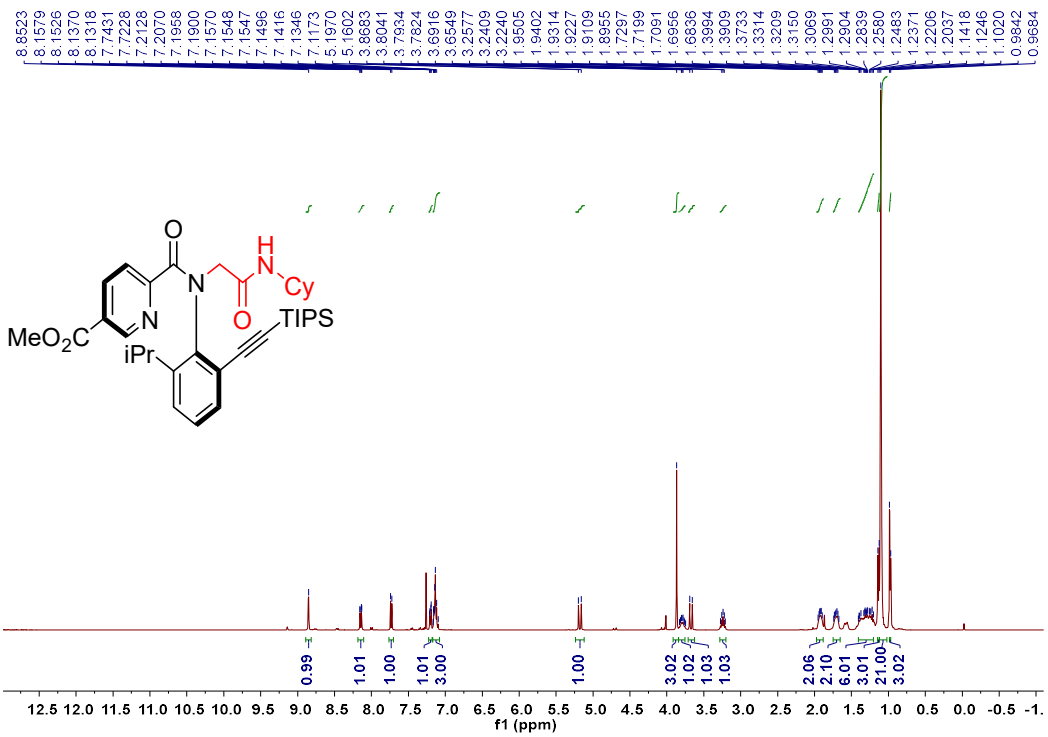
28.78
24.73
23.22
18.67
18.59
18.54
11.39
f1 (ppm)

5b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8.1526
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8.1318
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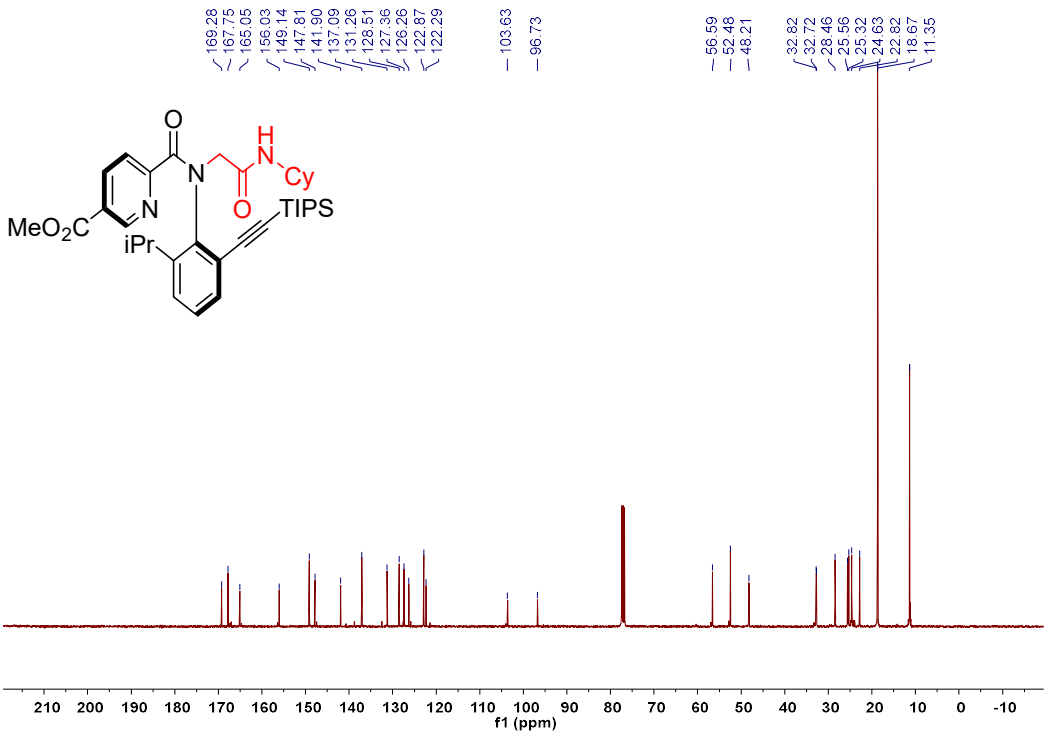
7.2070
7.1958
7.1900
7.1570
7.1548
7.1547
7.1496
7.1416
7.1346
7.1173
5.1970
5.1602
3.8683
3.8041
3.7934
3.7824
3.6916
3.6549
3.2577
3.2409
3.2240
1.9505
1.9402
1.9314
1.9227
1.9109
1.8955
1.7297
1.7199
1.7091
1.6956
1.6836
1.3994
1.3909
1.3733
1.3314
1.3209
1.3150
1.3069
1.2991
1.2904
1.2839
1.2580
1.2483
1.2371
1.2206
1.2037
1.1418
1.1246
1.1020
0.9842
0.9684
O
N
H
N
Cy
O
TIPS
MeO2C
N
iPr
0.99
1.01
1.00
1.01
3.00
1.00
3.02
1.02
1.03
1.03
2.06
2.10
6.01
3.01
21.00
3.02
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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167.75
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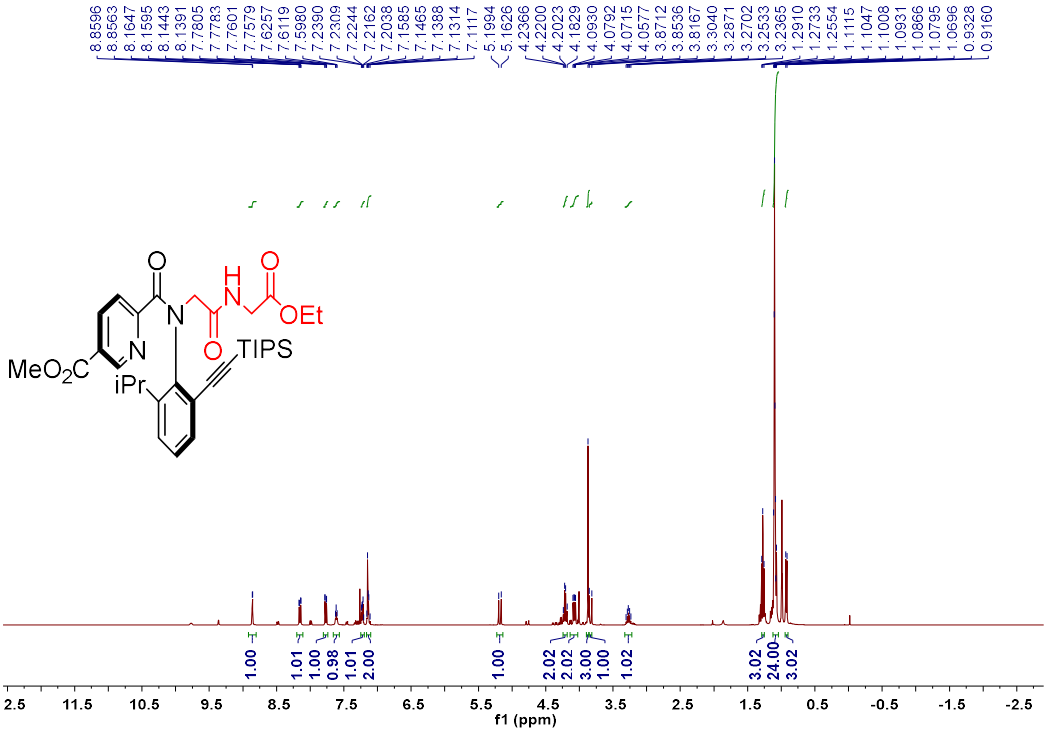
149.14
147.81
141.90
137.09
131.26
128.51
127.36
126.26
122.87
122.29
103.63
96.73
56.59
52.48
48.21
32.82
32.72
28.46
25.56
25.32
24.63
22.82
18.67
11.35
O
N
H
N
Cy
O
TIPS
MeO2C
N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5c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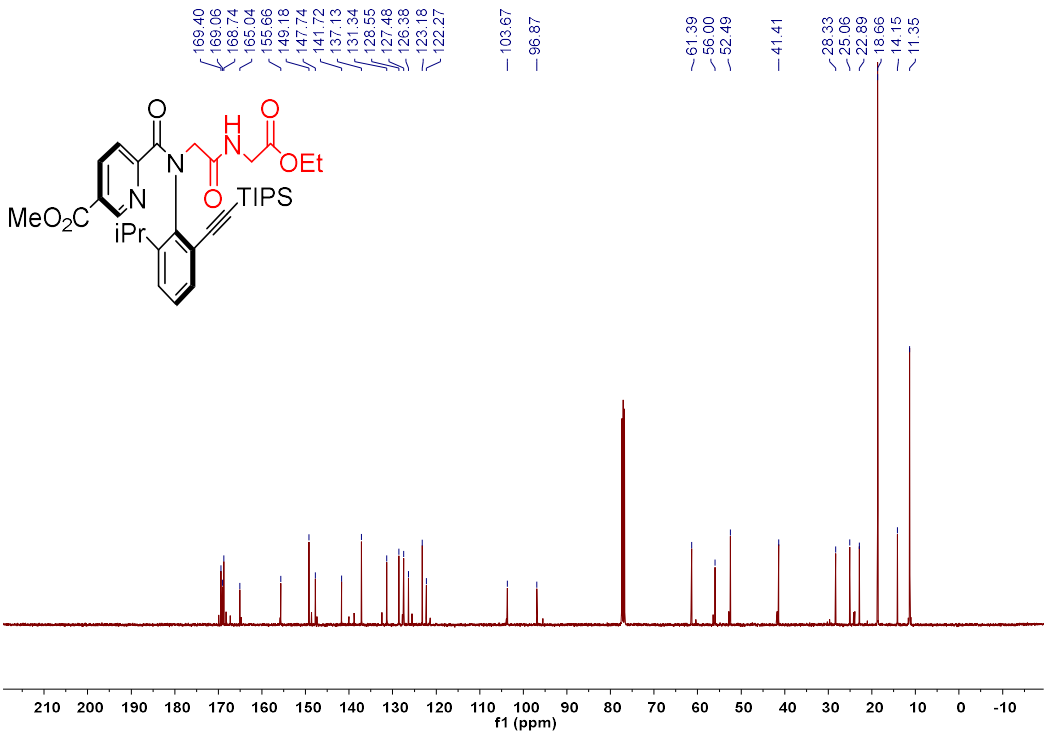
8.1443
8.1391
7.7805
7.7783
7.7601
7.7579
7.6257
7.6119
7.5980
7.2390
7.2309
7.2244
7.2162
7.2038
7.1585
7.1465
7.1388
7.1314
7.1117
5.1994
5.1626
4.2366
4.2200
4.2023
4.1829
4.0930
4.0792
4.0715
4.0577
3.8712
3.8536
3.8167
3.3040
3.2871
3.2702
3.2533
3.2365
1.2910
1.2733
1.2554
1.1115
1.1047
1.1008
1.0931
1.0866
1.0795
1.0696
0.9328
0.9160
MeO2C
iPr
N
O
H
N
O
OEt
O
TIPS
1.00
1.01
1.00
0.98
1.01
2.00
1.00
2.02
2.02
3.00
1.00
1.02
3.02
24.00
3.02
2.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
-2.5
f1 (ppm)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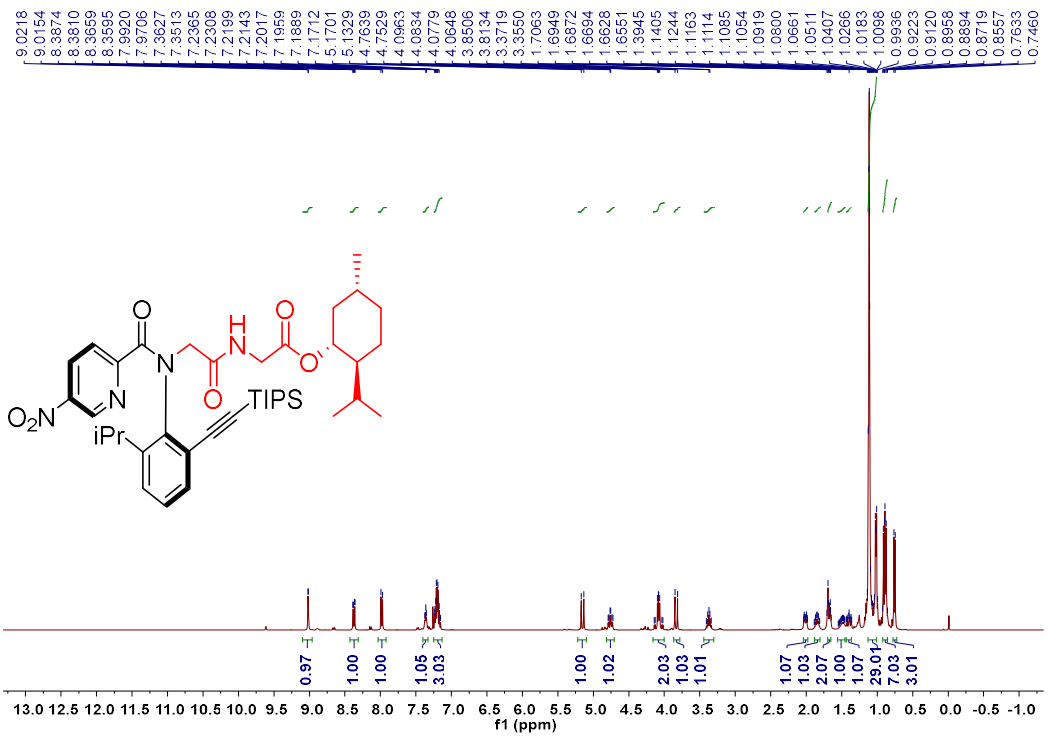
155.66
149.18
147.74
141.72
137.13
131.34
128.55
127.48
126.38
123.18
122.27
103.67
96.87
61.39
56.00
52.49
41.41
28.33
25.06
22.89
18.66
14.15
11.35
MeO2C
iPr
N
O
H
N
O
OEt
O
TIPS
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

5d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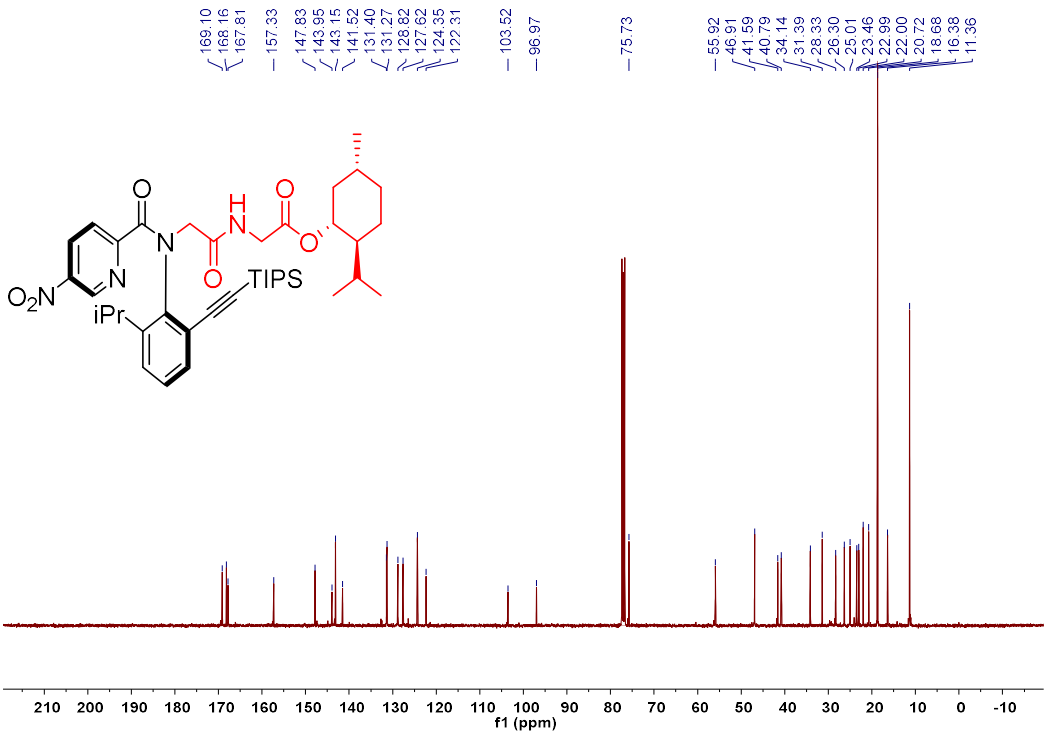
8.3595
7.9920
7.9706
7.3627
7.3513
7.2365
7.2308
7.2199
7.2143
7.2017
7.1959
7.1889
7.1712
5.1701
5.1329
4.7639
4.7529
4.0963
4.0834
4.0779
4.0648
3.8506
3.8134
3.7719
3.3550
1.7063
1.6949
1.6872
1.6694
1.6628
1.6551
1.3945
1.1405
1.1244
1.1163
1.1114
1.1085
1.1054
1.0919
1.0800
1.0661
1.0511
1.0407
1.0266
1.0183
1.0098
0.9936
0.9223
0.9120
0.8958
0.8894
0.8719
0.8557
0.7633
0.7460
O
N
O
H
N
O
O
TIPS
O_2N
iPr
0.97
1.00
1.00
1.05
3.03
1.00
1.02
2.03
1.03
1.01
1.07
1.03
2.07
1.00
1.07
29.01
7.03
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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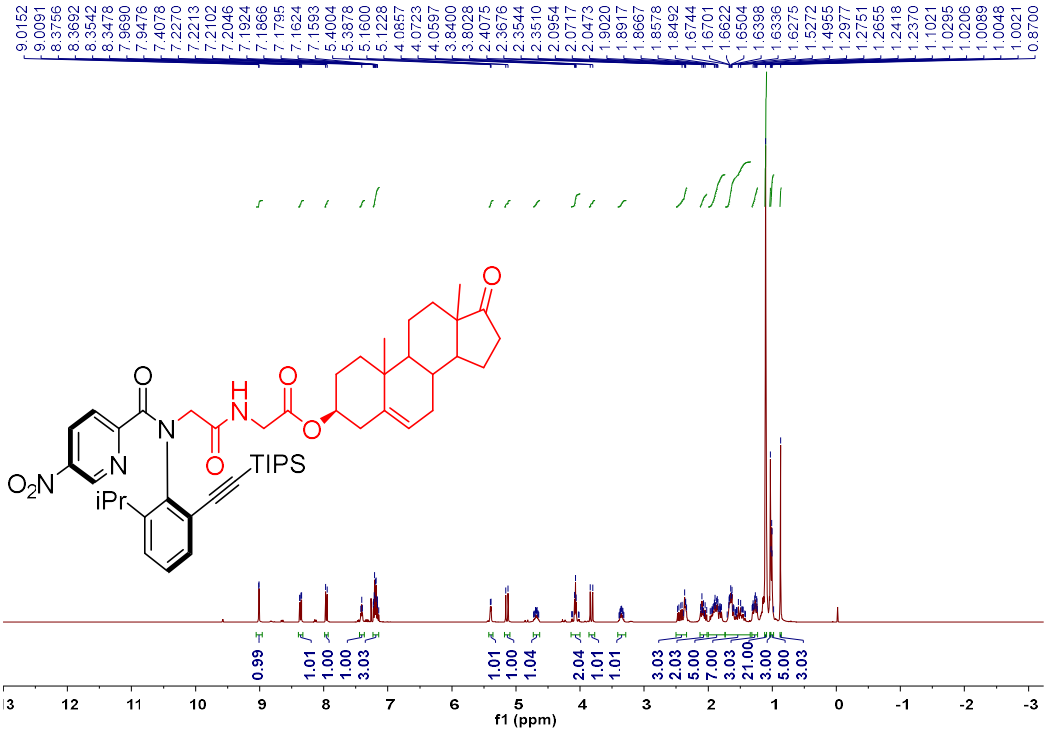
167.81
157.33
147.83
143.95
143.15
141.52
131.40
131.27
128.82
127.62
124.35
122.31
103.52
96.97
75.73
55.92
46.91
41.59
40.79
34.14
31.39
28.33
26.30
25.01
23.46
22.99
22.00
20.72
18.68
16.38
11.36
O
N
O
H
N
O
O
TIPS
O_2N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5e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8.3542
8.3478
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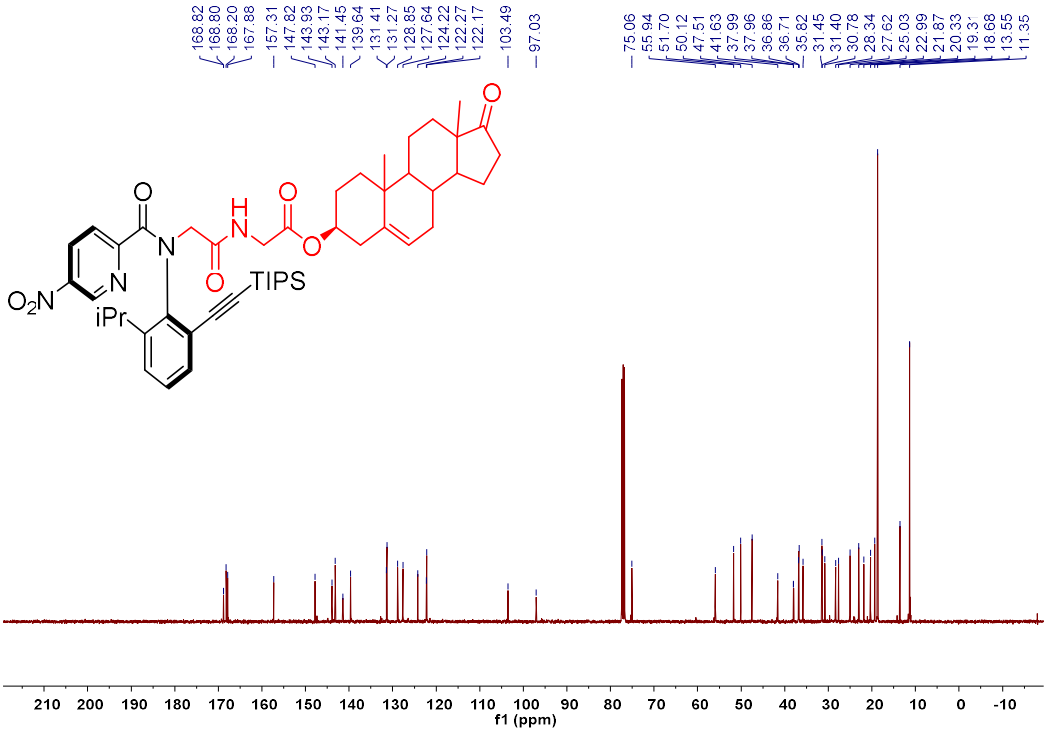
7.4078
7.2270
7.2213
7.2102
7.2046
7.1924
7.1866
7.1795
7.1624
7.1593
5.4004
5.3878
5.1600
5.1228
4.0857
4.0723
4.0597
3.8400
3.8028
2.4075
2.3676
2.3544
2.3510
2.0954
2.0717
2.0473
1.9020
1.8917
1.8867
1.8578
1.8492
1.6744
1.6701
1.6622
1.6504
1.6398
1.6336
1.6275
1.5272
1.4955
1.2977
1.2751
1.2655
1.2418
1.2370
1.1021
1.0295
1.0206
1.0089
1.0048
1.0021
0.8700
O
N
H
O
O
N
O2N
iPr
O
TIPS
0.99
1.01
1.00
1.00
3.03
1.01
1.00
1.04
2.04
1.01
1.01
3.03
2.03
5.00
7.00
3.03
21.00
3.00
5.00
3.03
f1 (ppm)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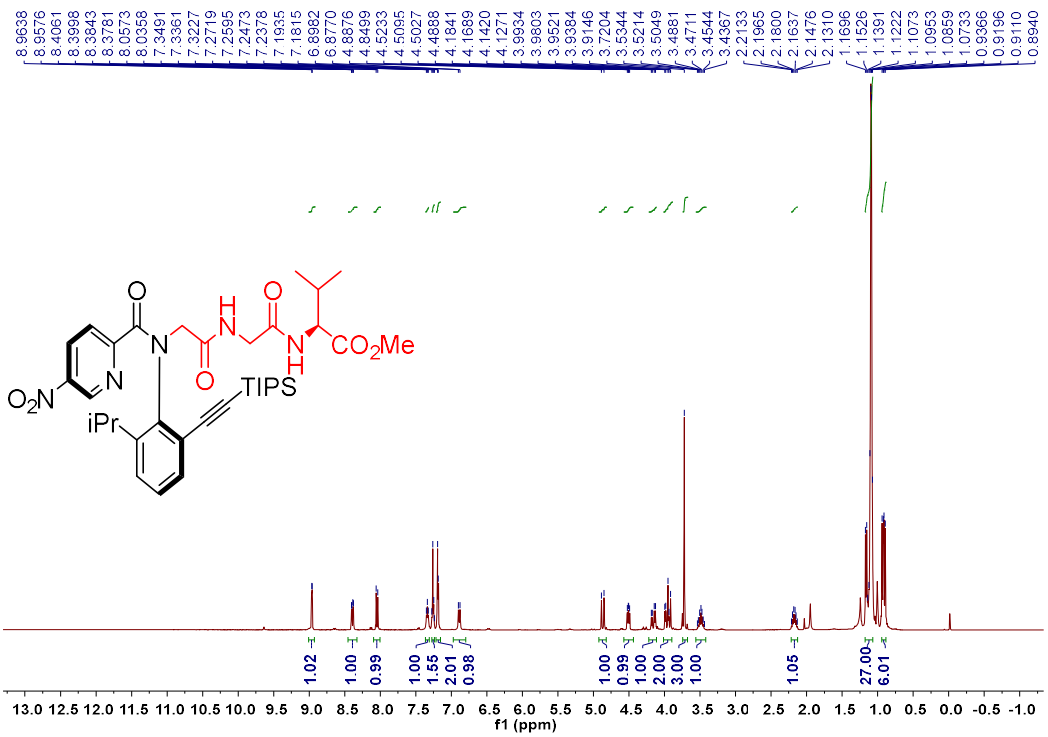
157.31
147.82
143.93
143.17
141.45
139.64
131.41
131.27
128.85
127.64
124.22
122.27
122.17
103.49
97.03
75.06
55.94
51.70
50.12
47.51
41.63
37.99
37.96
36.86
36.71
35.82
31.45
31.40
30.78
28.34
27.62
25.03
22.99
21.87
20.33
19.31
18.68
13.55
11.35
O
N
H
O
O
N
O2N
iPr
O
TIPS
f1 (ppm)

5f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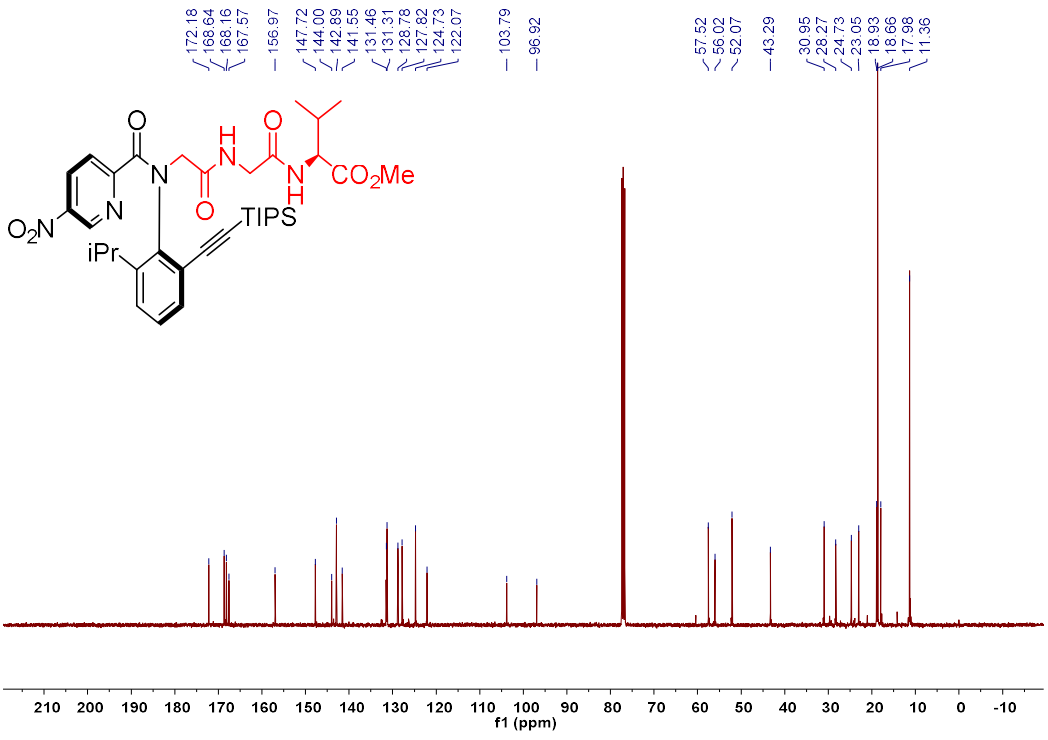
7.3491
7.3361
7.3227
7.2719
7.2595
7.2473
7.2378
7.1935
7.1815
6.8982
6.8770
4.8876
4.8499
4.5233
4.5095
4.5027
4.4888
4.1841
4.1689
4.1420
4.1271
3.9934
3.9803
3.9521
3.9384
3.9146
3.7204
3.5344
3.5214
3.5049
3.4881
3.4711
3.4544
3.4367
2.2133
2.1965
2.1800
2.1637
2.1476
2.1310
1.1696
1.1526
1.1391
1.1222
1.1073
1.0953
1.0859
1.0733
1.0366
0.9196
0.9110
0.8940
O2N
iPr
TIPS
CO2Me
1.02
1.00
0.99
1.00
1.55
2.01
0.98
1.00
0.99
1.00
2.00
3.00
1.00
1.05
27.00
6.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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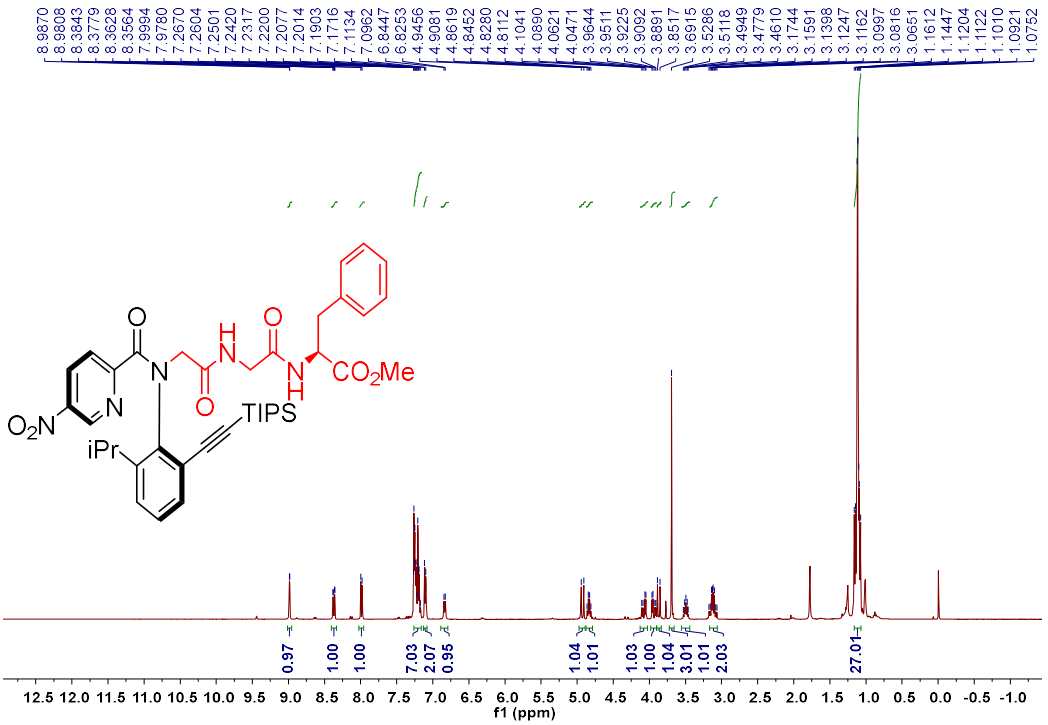
144.00
142.89
141.55
131.46
131.31
128.78
127.82
124.73
122.07
103.79
96.92
57.52
56.02
52.07
43.29
30.95
28.27
24.73
23.05
18.93
18.66
17.98
11.36
O2N
iPr
TIPS
CO2Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5g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7.9994
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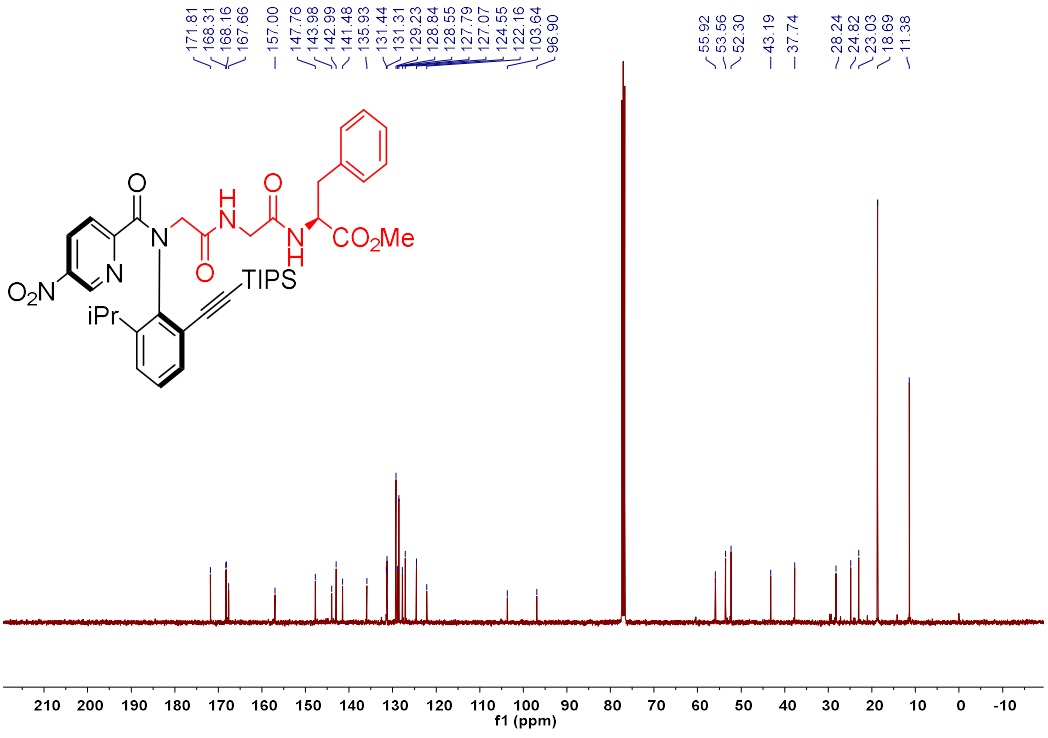
7.2670
7.2604
7.2501
7.2420
7.2317
7.2200
7.2077
7.2014
7.1903
7.1716
7.1134
7.0962
6.8447
6.8253
4.9456
4.9081
4.8619
4.8452
4.8280
4.8112
4.1041
4.0890
4.0621
4.0471
3.9644
3.9511
3.9225
3.9092
3.8891
3.8517
3.6915
3.5286
3.5118
3.4949
3.4779
3.4610
3.1744
3.1591
3.1398
3.1247
3.1162
3.0997
3.0816
3.0651
1.1612
1.1447
1.1204
1.1122
1.1010
1.0921
1.0752
O2N
iPr
TIPS
CO2Me
0.97
1.00
1.00
7.03
2.07
0.95
1.04
1.01
1.03
1.00
1.04
3.01
1.01
2.03
27.01
f1 (ppm)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168.16
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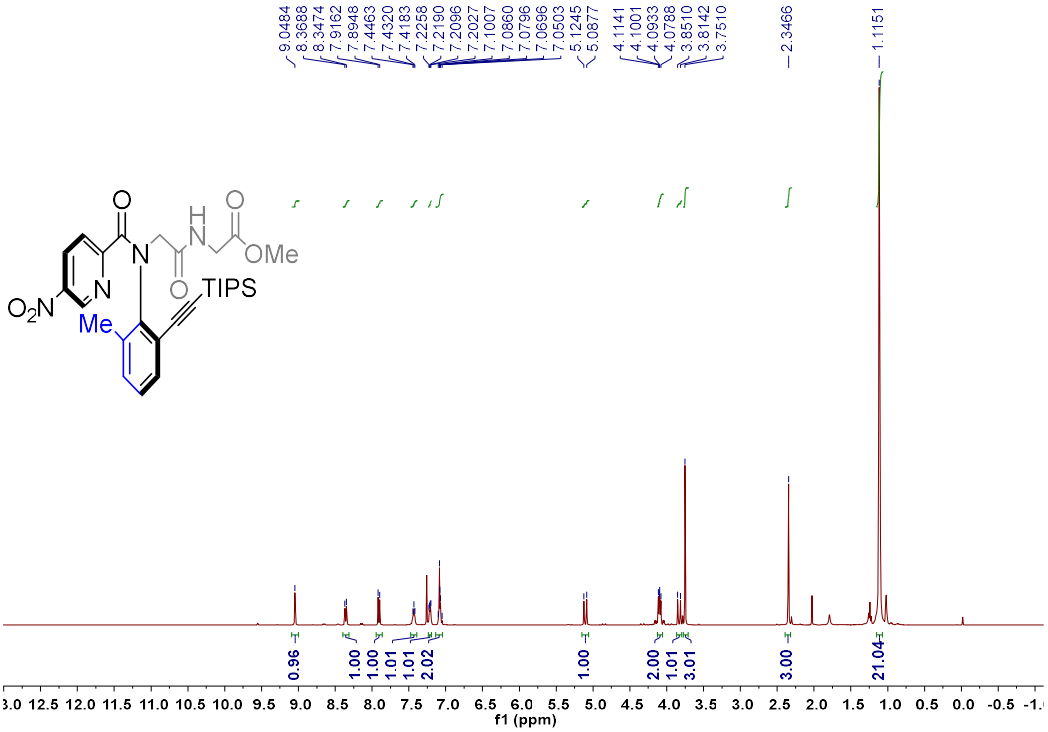
147.76
143.98
142.99
141.48
135.93
131.44
131.31
129.23
128.84
128.55
127.79
127.07
124.55
122.16
103.64
96.90
55.92
53.56
52.30
43.19
37.74
28.24
24.82
23.03
18.69
11.38
O2N
iPr
TIPS
CO2Me
f1 (ppm)

5h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8.3474
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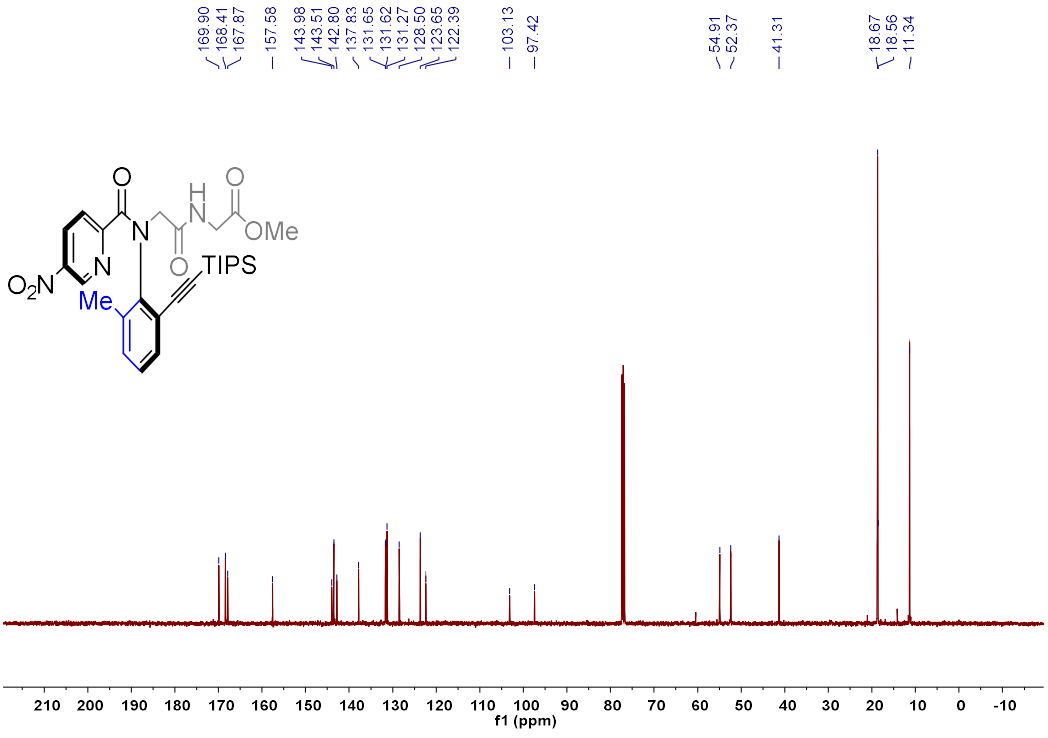
7.8948
7.4463
7.4320
7.4183
7.2258
7.2190
7.2096
7.2027
7.1007
7.0860
7.0796
7.0696
7.0503
5.1245
5.0877
4.1141
4.1001
4.0933
4.0788
3.8510
3.8142
3.7510
2.3466
1.1151
0.96
1.00
1.00
1.01
1.01
2.02
1.00
2.00
1.01
3.01
3.00
21.04
f1 (ppm)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167.87
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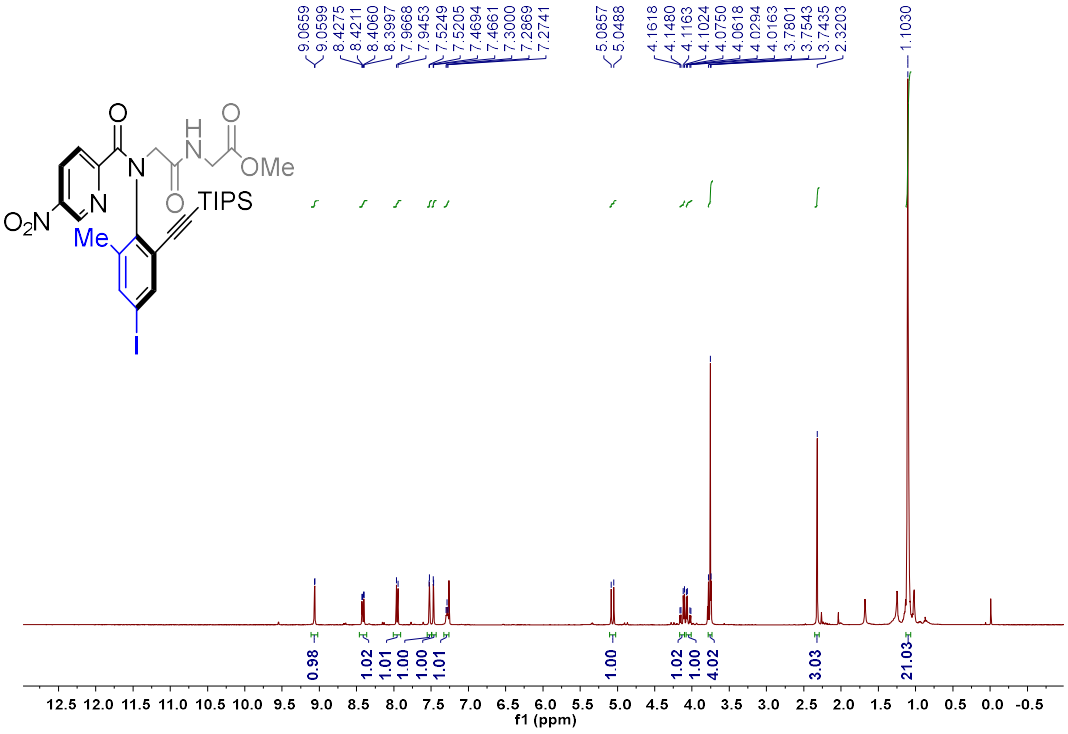
143.51
142.80
137.83
131.65
131.62
131.27
128.50
123.65
122.39
103.13
97.42
54.91
52.37
41.31
18.67
18.56
11.34
f1 (ppm)

5i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8.4060
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7.9668
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7.5249
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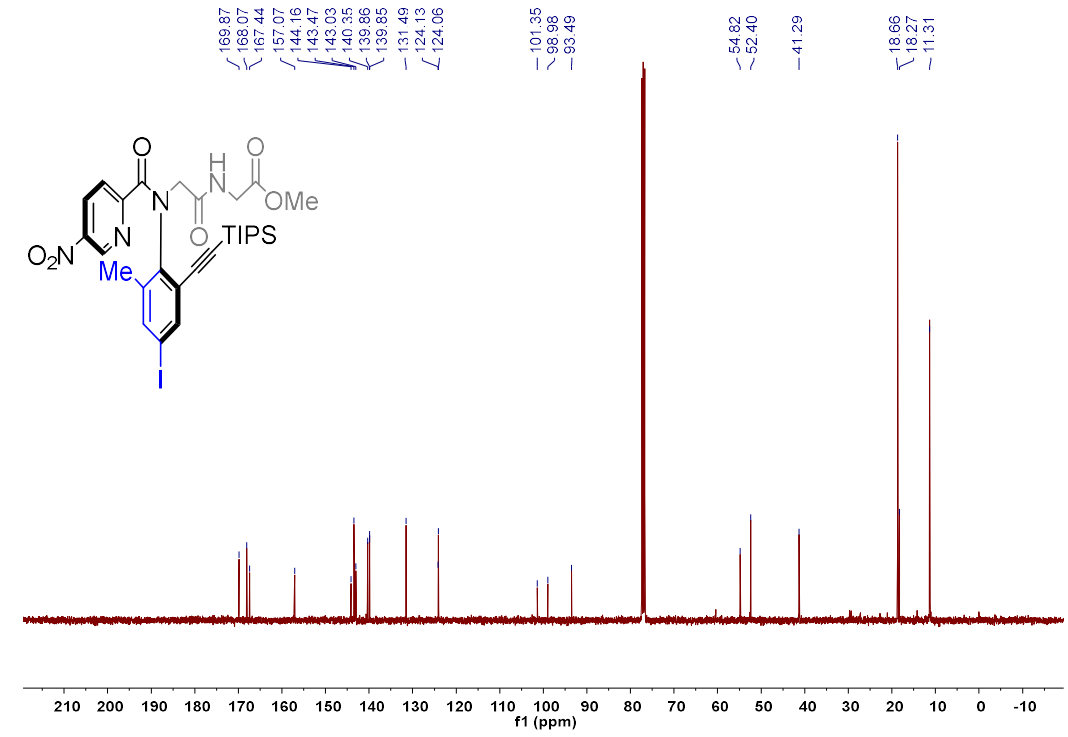
7.4694
7.4661
7.3000
7.2869
7.2741
5.0857
5.0488
4.1618
4.1480
4.1163
4.1024
4.0750
4.0618
4.0294
4.0163
3.7801
3.7543
3.7435
3.7203
1.1030
O2N
Me
I
TIPS
OMe
0.98
1.02
1.01
1.00
1.00
1.01
1.00
1.02
1.00
4.02
3.03
21.03
f1 (ppm)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144.16
143.47
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140.35
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124.06
101.35
98.98
93.49
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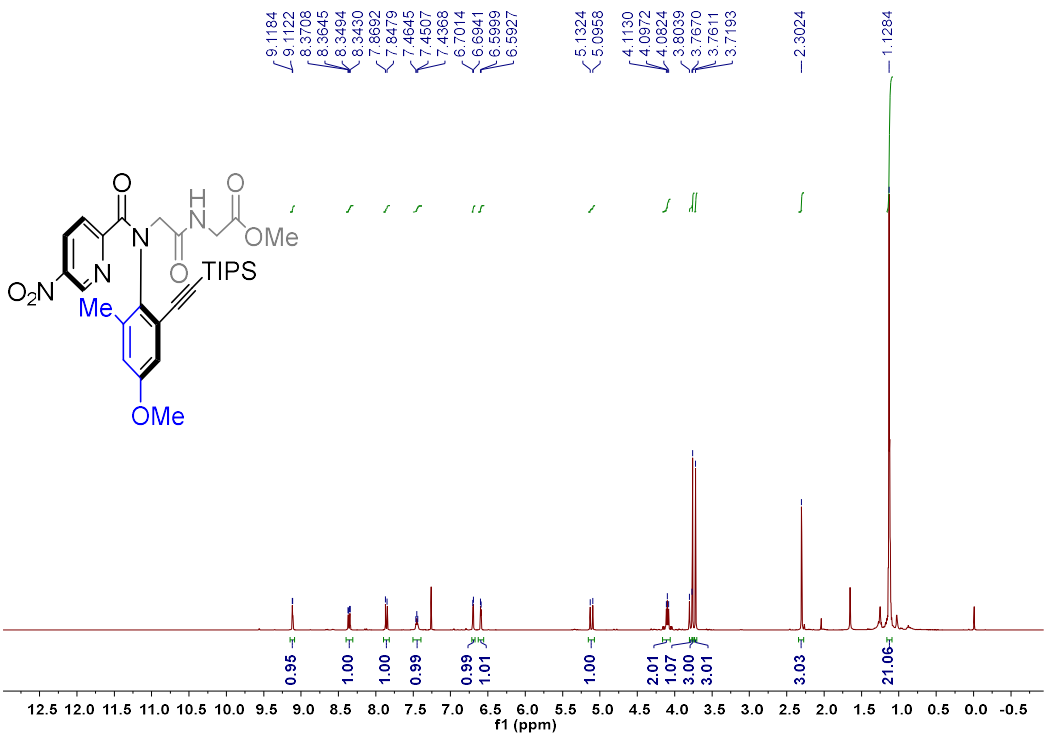
41.29
18.66
18.27
11.31
O2N
Me
I
TIPS
OMe
f1 (ppm)

5j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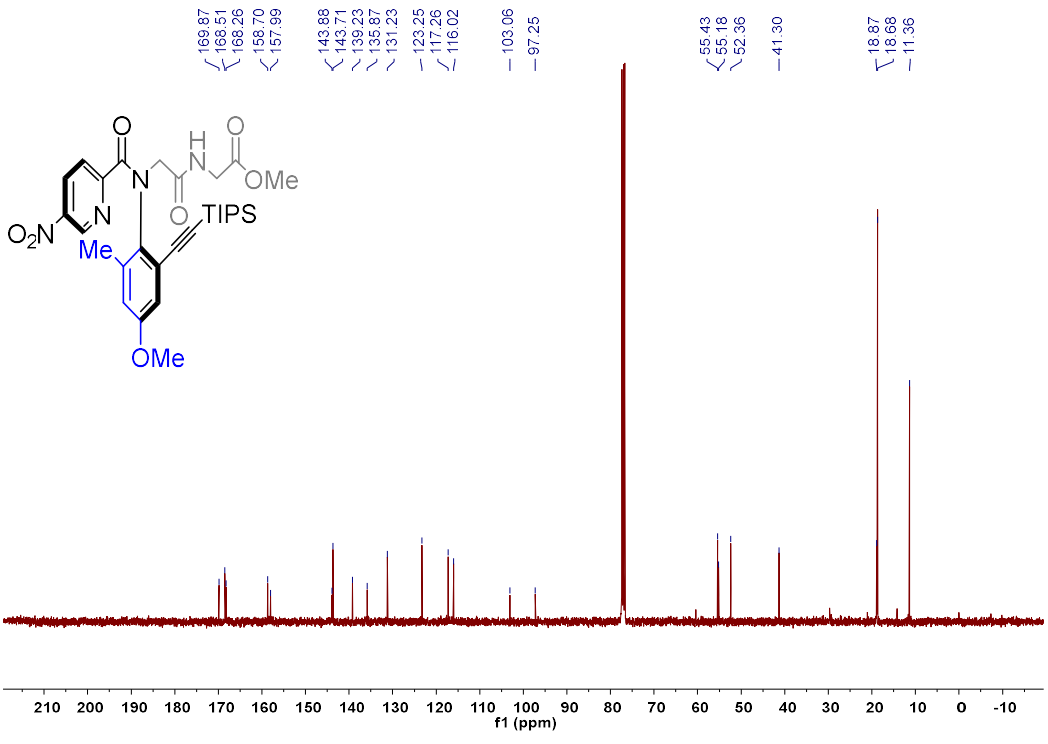
7.4645
7.4507
7.4368
6.7014
6.6941
6.5999
6.5927
5.1324
5.0958
4.1130
4.0972
4.0824
3.8039
3.7670
3.7611
3.7193
2.3024
1.1284
O
N
O
H
N
O
OMe
O
TIPS
O2N
N
Me
OMe
0.95
1.00
1.00
0.99
0.99
1.01
1.00
2.01
1.07
3.00
3.01
3.03
21.06
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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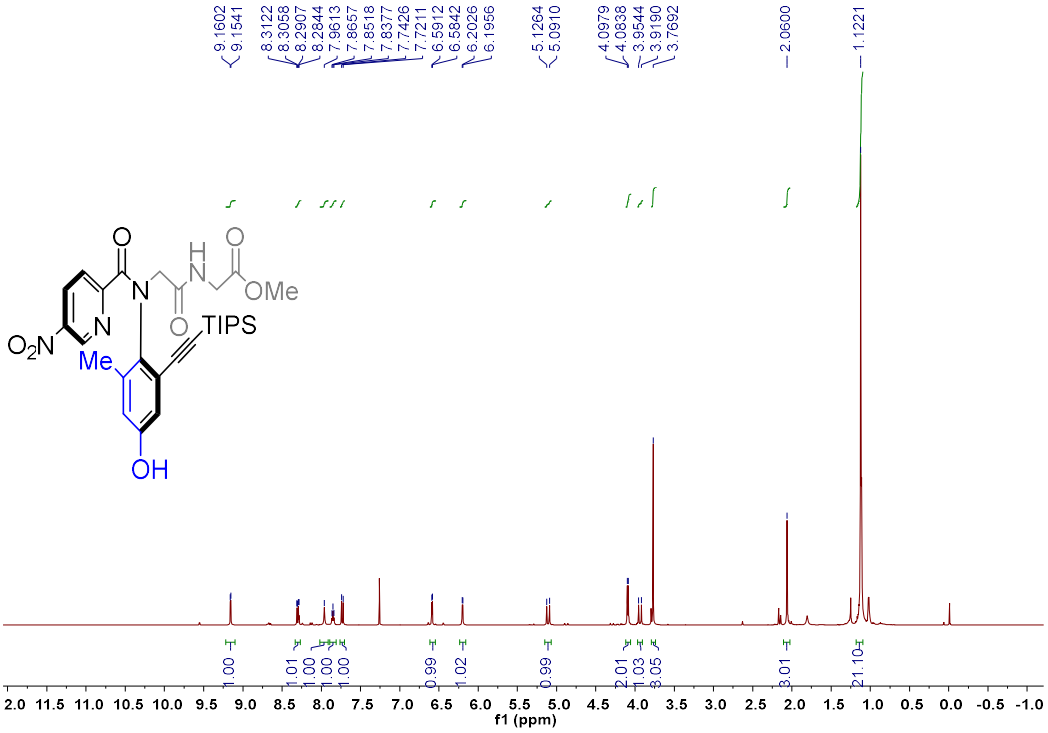
157.99
143.88
143.71
139.23
135.87
131.23
123.25
117.26
116.02
103.06
97.25
55.43
55.18
52.36
41.30
18.87
18.68
11.36
O
N
O
H
N
O
OMe
O
TIPS
O2N
N
Me
OMe
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

5k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8.2907
8.2844
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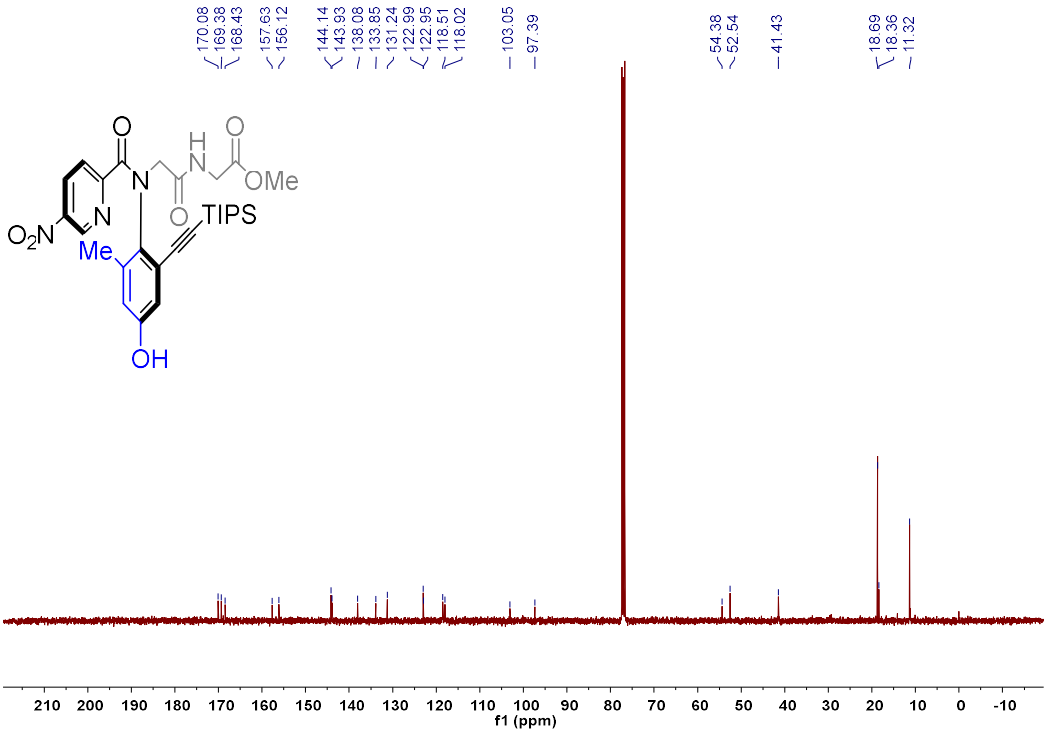
7.8657
7.8518
7.8377
7.7426
7.7211
6.5912
6.5842
6.2026
6.1956
5.1264
5.0910
4.0979
4.0838
3.9544
3.9190
3.7692
2.0600
1.1221
O
N
H
N
O
OMe
O
TIPS
O2N
N
Me
OH
1.00
1.01
1.00
1.00
1.00
0.99
1.02
0.99
2.01
1.03
3.05
3.01
21.10
f1 (ppm)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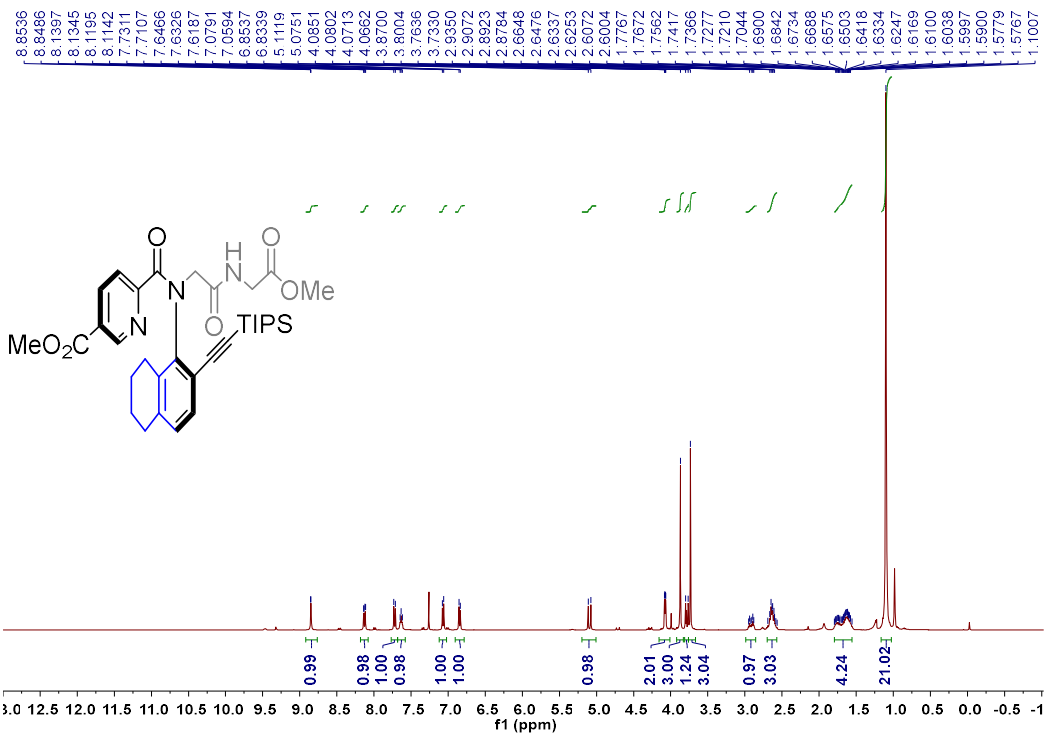
168.43
157.63
156.12
144.14
143.93
138.08
133.85
131.24
122.99
122.95
118.51
118.02
103.05
97.39
54.38
52.54
41.43
18.69
18.36
11.32
O
N
H
N
O
OMe
O
TIPS
O2N
N
Me
OH
f1 (ppm)

5l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8.1345
8.1195
8.1142
7.7311
7.7107
7.6466
7.6326
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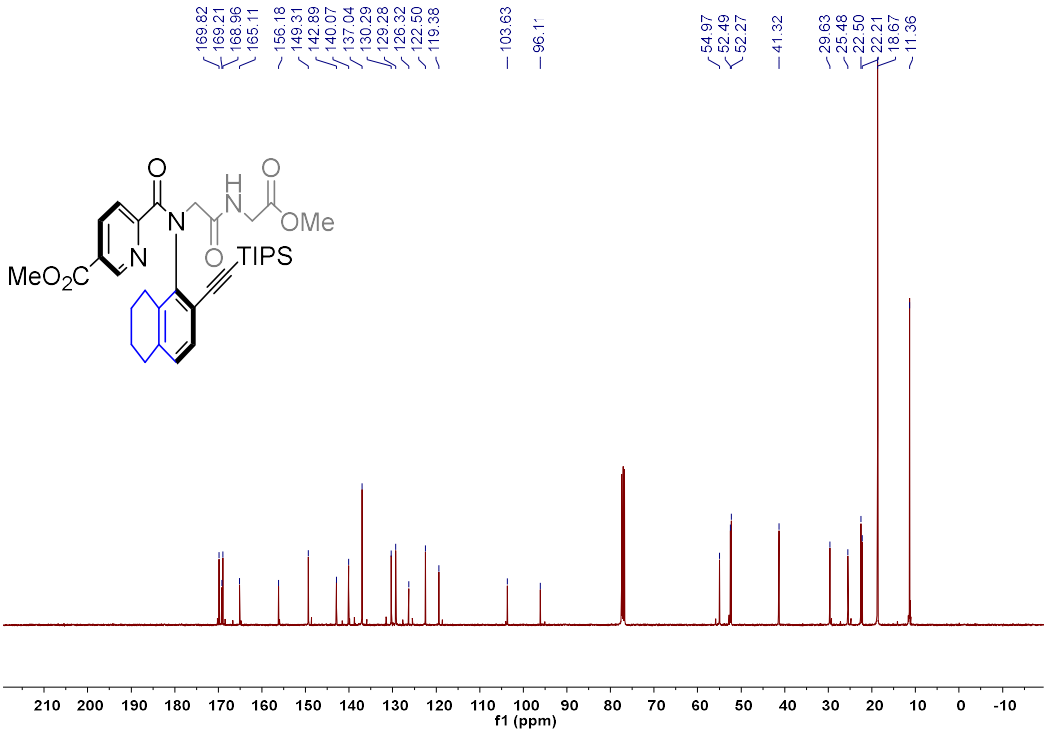
7.0791
7.0594
6.8537
6.8339
5.1119
5.0751
4.0851
4.0802
4.0713
4.0662
3.8700
3.8004
3.7636
3.7330
2.9350
2.9072
2.8923
2.8784
2.6648
2.6476
2.6337
2.6253
2.6072
2.6004
1.7767
1.7672
1.7562
1.7417
1.7366
1.7277
1.7210
1.7044
1.6900
1.6842
1.6734
1.6688
1.6575
1.6503
1.6418
1.6334
1.6247
1.6169
1.6100
1.6038
1.5997
1.5900
1.5779
1.5767
1.1007
O
H
N
N
O
OMe
O
TIPS
MeO2C
0.99
0.98
1.00
0.98
1.00
1.00
0.98
2.01
3.00
1.24
3.04
0.97
3.03
4.24
21.02
f1 (ppm)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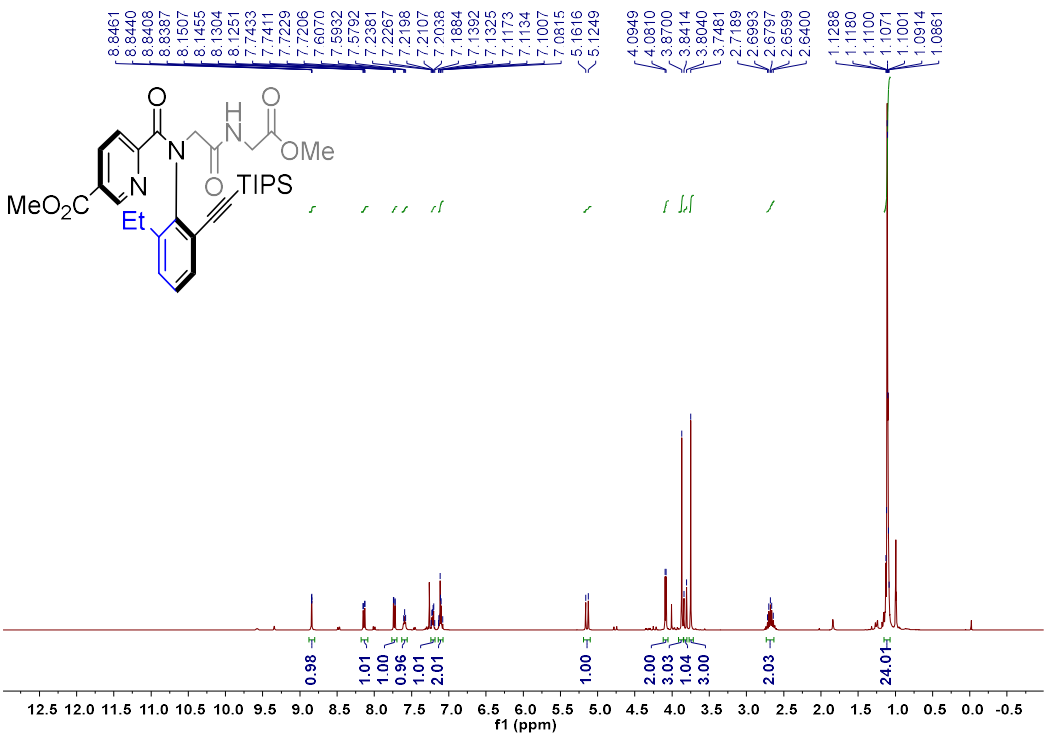
156.18
149.31
142.89
140.07
137.04
130.29
129.28
126.32
122.50
119.38
103.63
96.11
54.97
52.49
52.27
41.32
29.63
25.48
22.50
22.21
18.67
11.36
O
H
N
N
O
OMe
O
TIPS
MeO2C
f1 (ppm)

5m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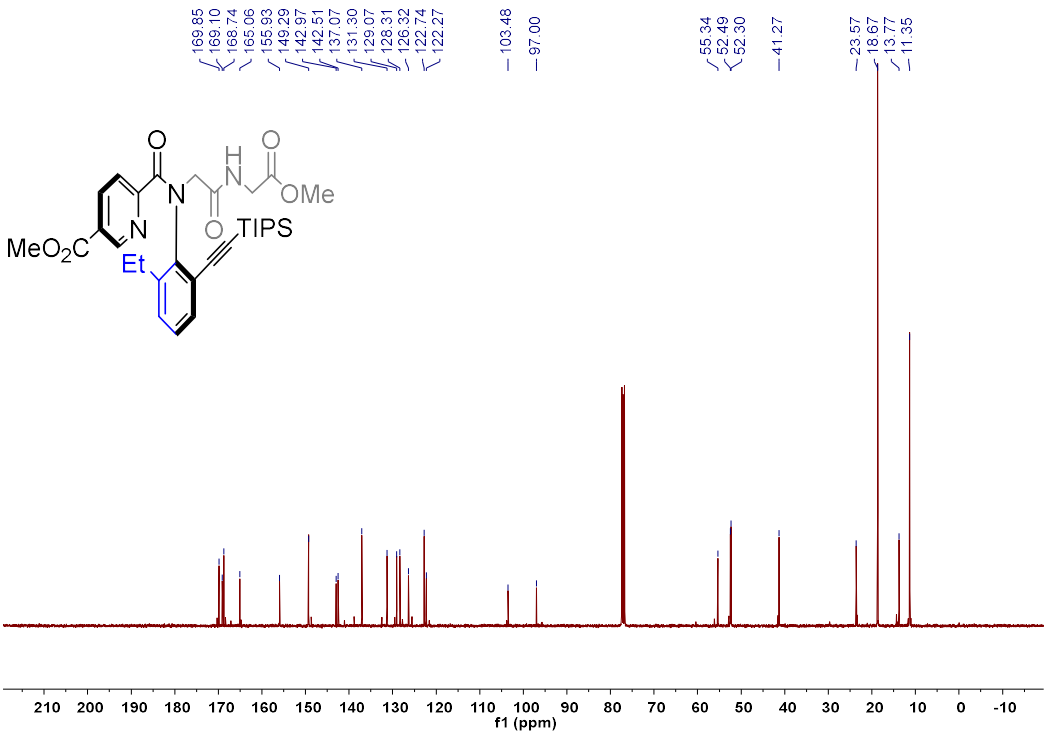
8.8440
8.8408
8.8387
8.1507
8.1455
8.1304
8.1251
7.7433
7.7411
7.7229
7.7206
7.6070
7.5932
7.5792
7.2381
7.2267
7.2198
7.2107
7.2038
7.1884
7.1392
7.1325
7.1173
7.1134
7.1007
7.0815
5.1616
5.1249
4.0949
4.0810
3.8700
3.8414
3.8040
3.7481
2.7189
2.6993
2.6797
2.6599
2.6400
1.1288
1.1180
1.1100
1.1071
1.1001
1.0914
1.0861
MeO2C
Et
N
O
H
N
O
OMe
TIPS
0.98
1.01
1.00
0.96
1.01
2.01
1.00
2.00
3.03
1.04
3.00
2.03
24.01
f1 (ppm)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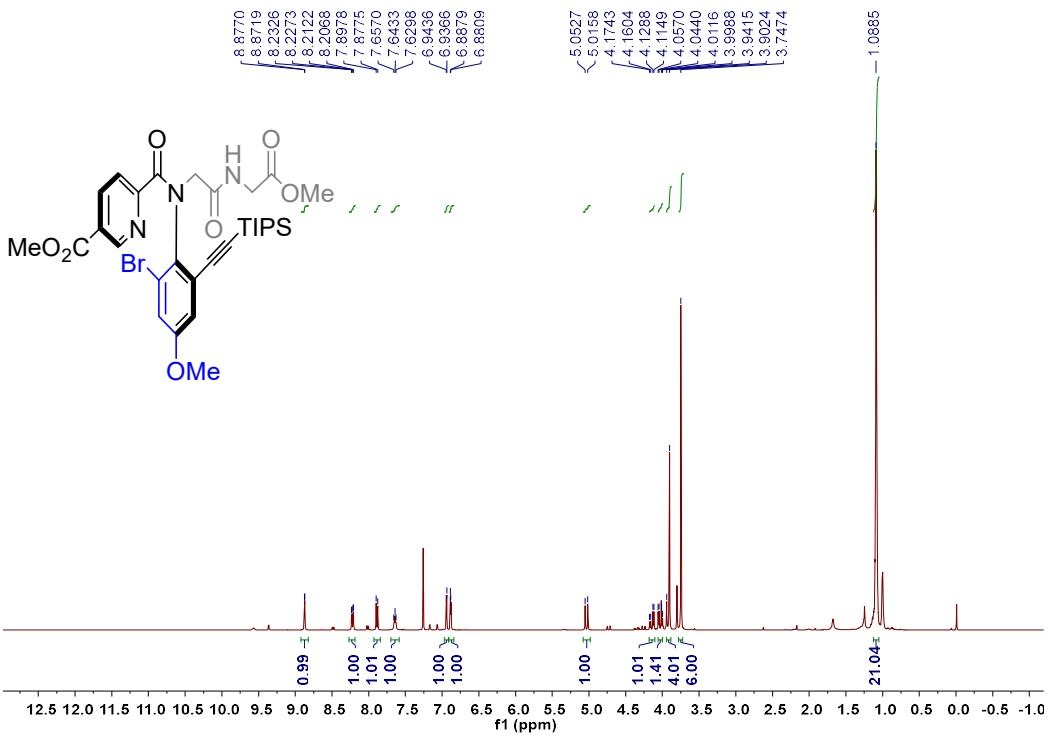
168.74
165.06
155.93
149.29
142.97
142.51
137.07
131.30
129.07
128.31
126.32
122.74
122.27
103.48
97.00
55.34
52.49
52.30
41.27
23.57
18.67
13.77
11.35
MeO2C
Et
N
O
H
N
O
OMe
TIPS
f1 (ppm)

5n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8.2273
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7.8978
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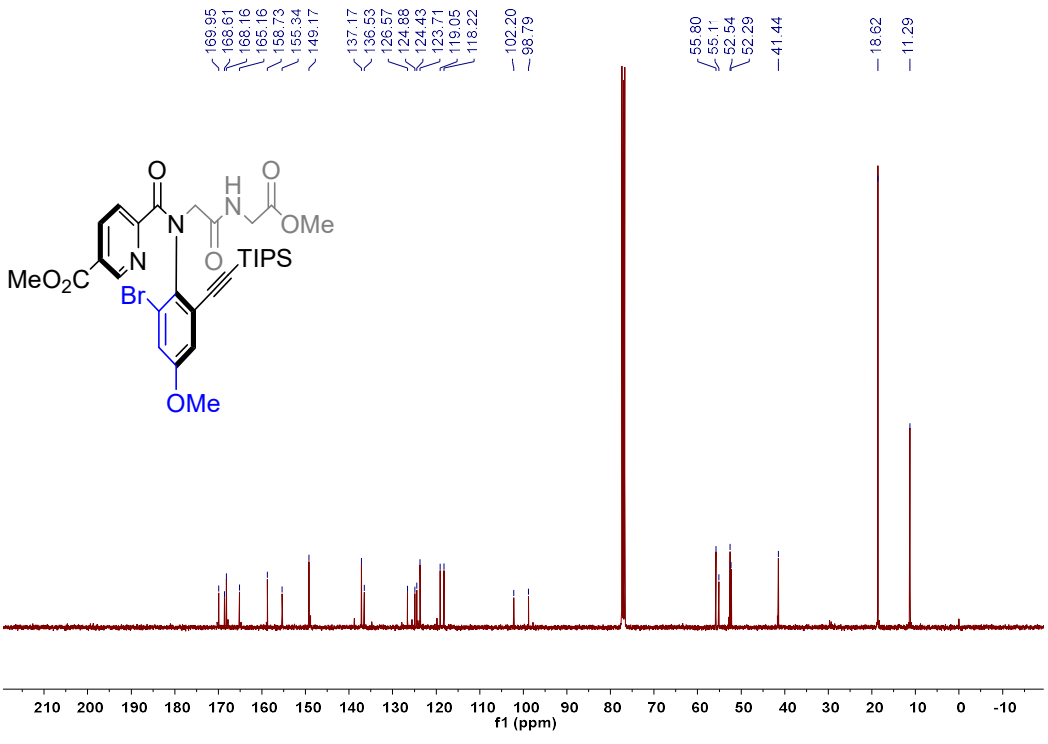
7.6570
7.6433
7.6298
6.9436
6.9366
6.8879
6.8809
5.0527
5.0158
4.1743
4.1604
4.1288
4.1149
4.0570
4.0440
4.0116
3.9988
3.9415
3.9024
3.7474
1.0885
0.99
1.00
1.01
1.00
1.00
1.00
1.00
1.01
1.41
4.01
6.00
21.04
f1 (ppm)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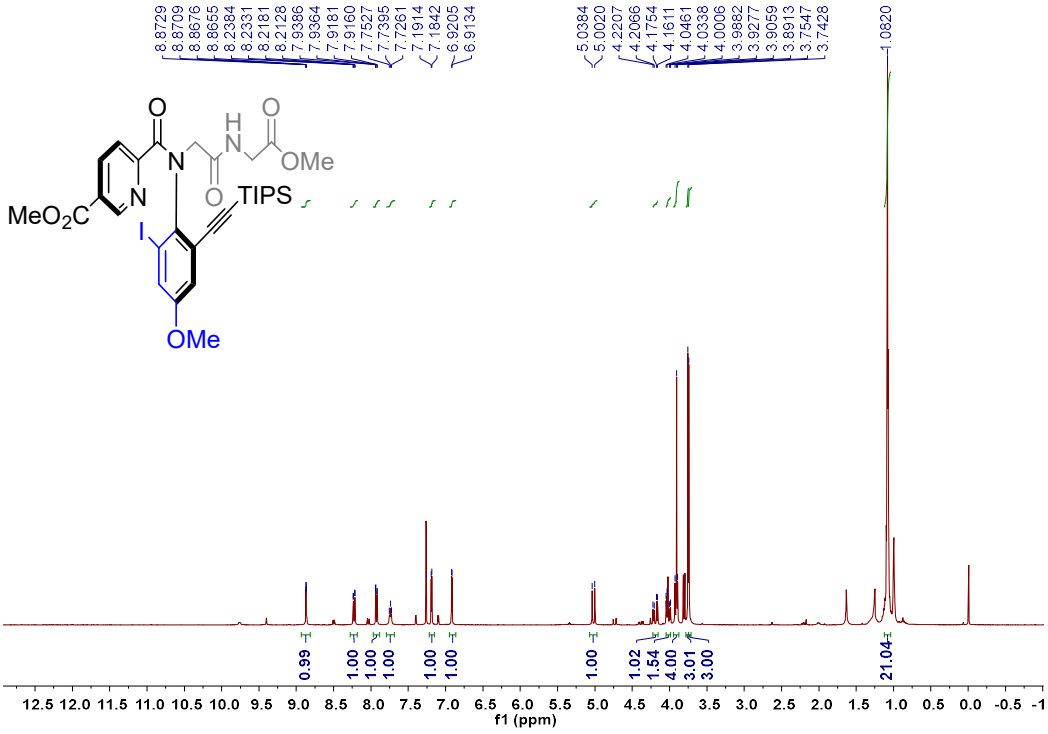
158.73
155.34
149.17
137.17
136.53
126.57
124.88
124.43
123.71
119.05
118.22
102.20
98.79
55.80
55.1
52.54
52.29
41.44
18.62
11.29
f1 (ppm)

5o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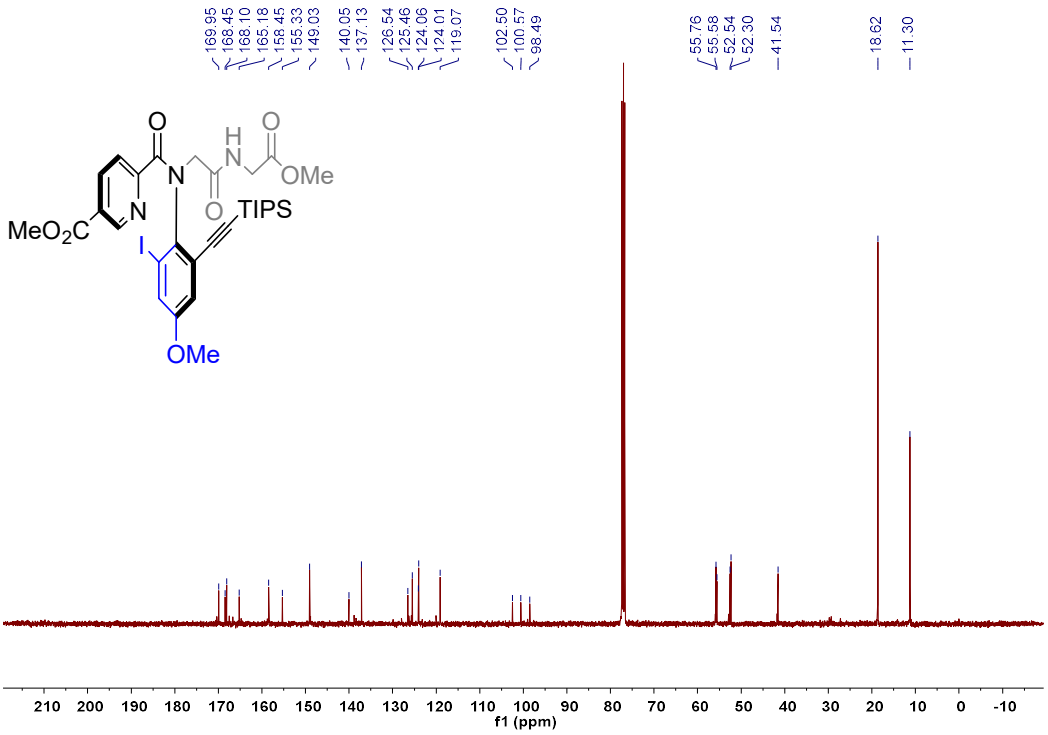
8.8676
8.8655
8.2384
8.2331
8.2181
8.2128
7.9386
7.9364
7.9181
7.9160
7.7527
7.7395
7.7261
7.1914
7.1842
6.9205
6.9134
5.0384
5.0020
4.2207
4.2066
4.1754
4.1611
4.0461
4.0338
4.0006
3.9882
3.9277
3.9059
3.8913
3.7547
3.7428
1.0820
MeO2C
TIPS
OMe
OMe
0.99
1.00
1.00
1.00
1.00
1.00
1.00
1.02
1.54
4.00
3.01
3.00
21.04
f1 (ppm)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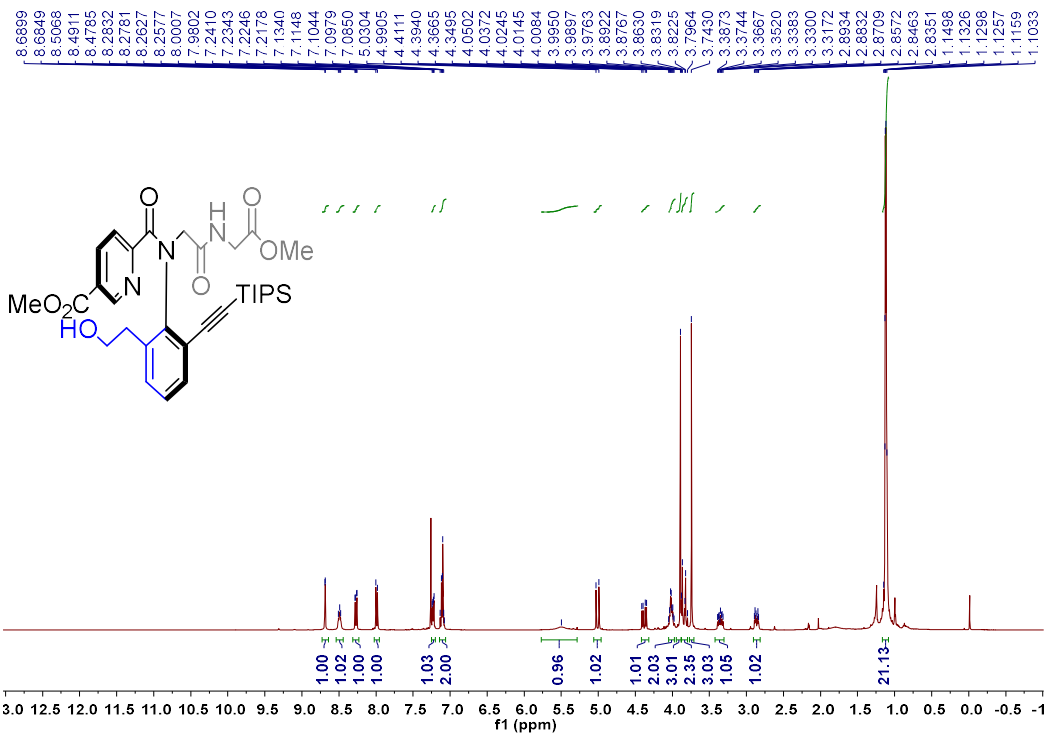
158.45
155.33
149.03
140.05
137.13
128.54
125.46
124.06
124.01
119.07
102.50
100.57
98.49
55.76
55.58
52.54
52.30
41.54
18.62
11.30
MeO2C
TIPS
OMe
OMe
f1 (ppm)

5p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8.2781
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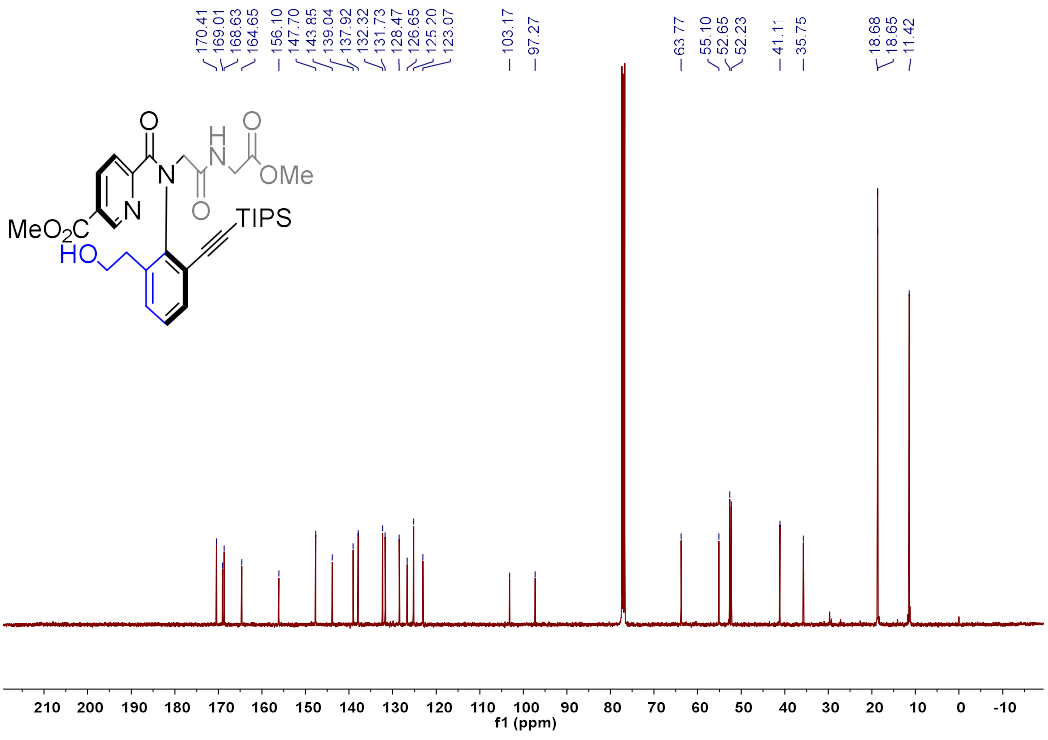
8.2577
8.0007
7.9802
7.2410
7.2343
7.2246
7.2178
7.1340
7.1148
7.1044
7.0979
7.0850
5.0304
4.9905
4.4111
4.3940
4.3665
4.3495
4.0502
4.0372
4.0245
4.0145
4.0084
3.9950
3.9897
3.9763
3.8922
3.8767
3.8630
3.8319
3.8225
3.7964
3.7430
3.3873
3.3744
3.3667
3.3520
3.3383
3.3300
3.3172
2.8934
2.8832
2.8709
2.8572
2.8463
2.8351
1.1498
1.1326
1.1298
1.1257
1.1159
1.1033
O
N
H
N
O
OMe
O
N
TIPS
MeO2C
HO
1.00
1.02
1.00
1.00
1.03
2.00
0.96
1.02
1.01
2.03
3.01
2.35
3.03
1.05
1.02
21.13
f1 (ppm)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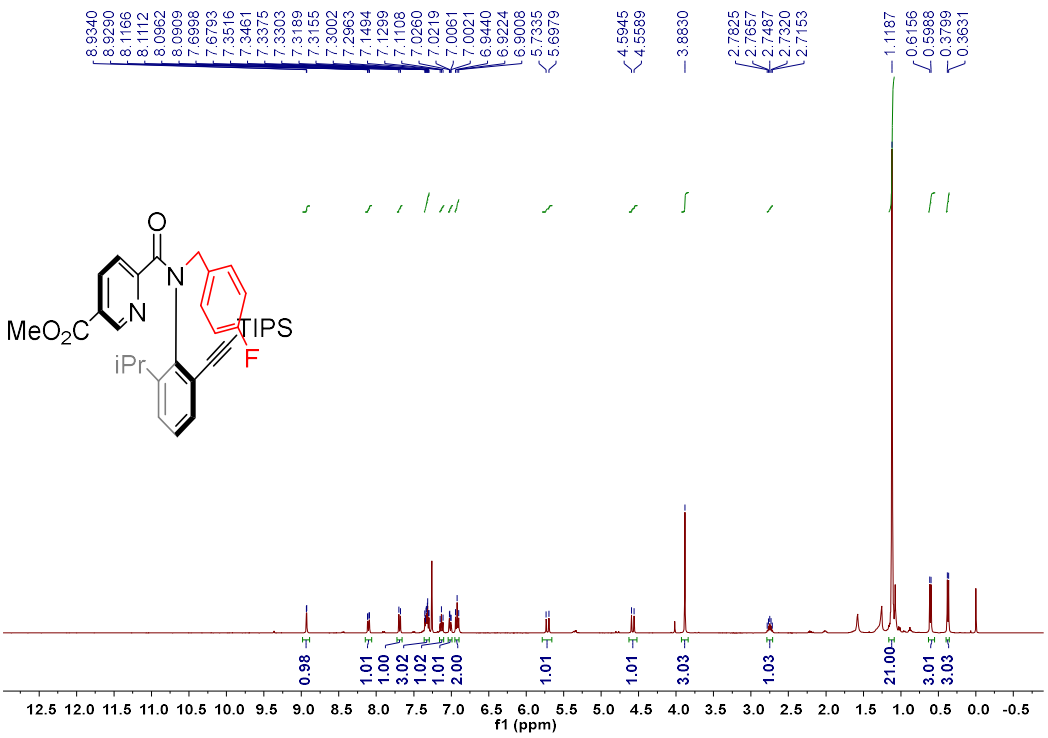
156.10
147.70
143.85
139.04
137.92
132.32
131.73
128.47
126.65
125.20
123.07
103.17
97.27
63.77
55.10
52.65
52.23
41.17
35.75
18.68
18.65
11.42
O
N
H
N
O
OMe
O
N
TIPS
MeO2C
HO
f1 (ppm)

5q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8.1112
8.0962
8.0909
7.6998
7.6793
7.3516
7.3461
7.3375
7.3303
7.3189
7.3155
7.3002
7.2963
7.1494
7.1299
7.1108
7.0260
7.0219
7.0061
7.0021
6.9440
6.9224
6.9008
5.7335
5.6979
4.5945
4.5589
3.8830
2.7825
2.7657
2.7487
2.7320
2.7153
1.1187
0.6156
0.5988
0.3799
0.3631
MeO2C
N
O
N
TIPS
F
iPr
0.98
1.01
1.00
3.02
1.02
1.01
2.00
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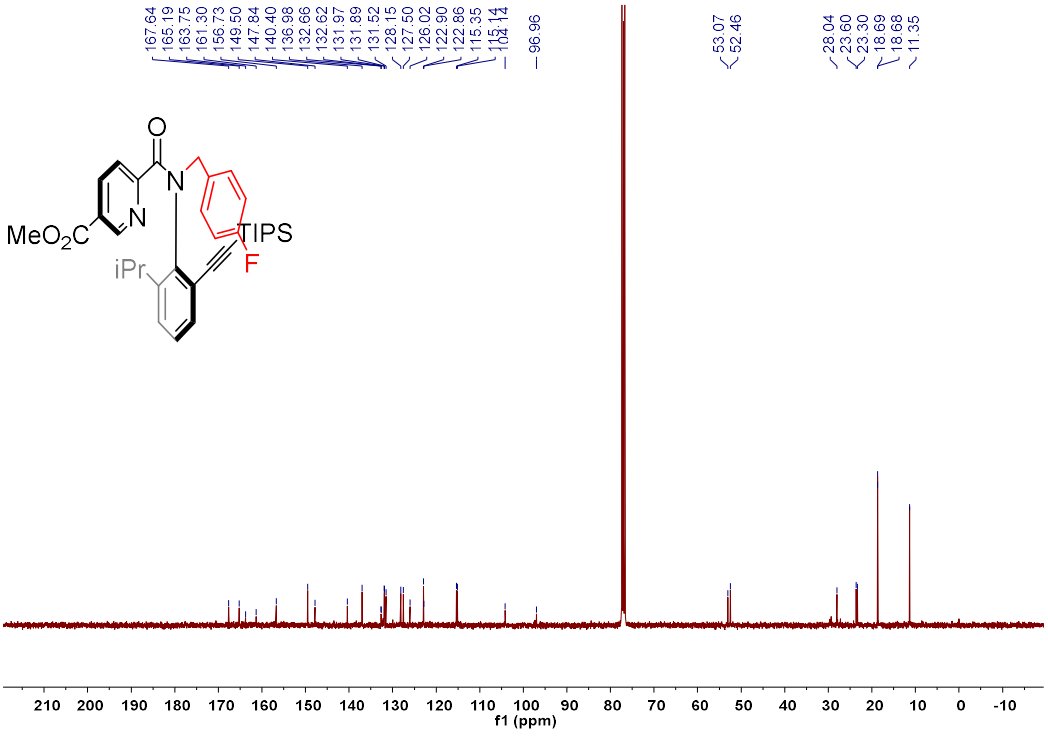
1.03
21.00
3.01
3.03
f1 (ppm)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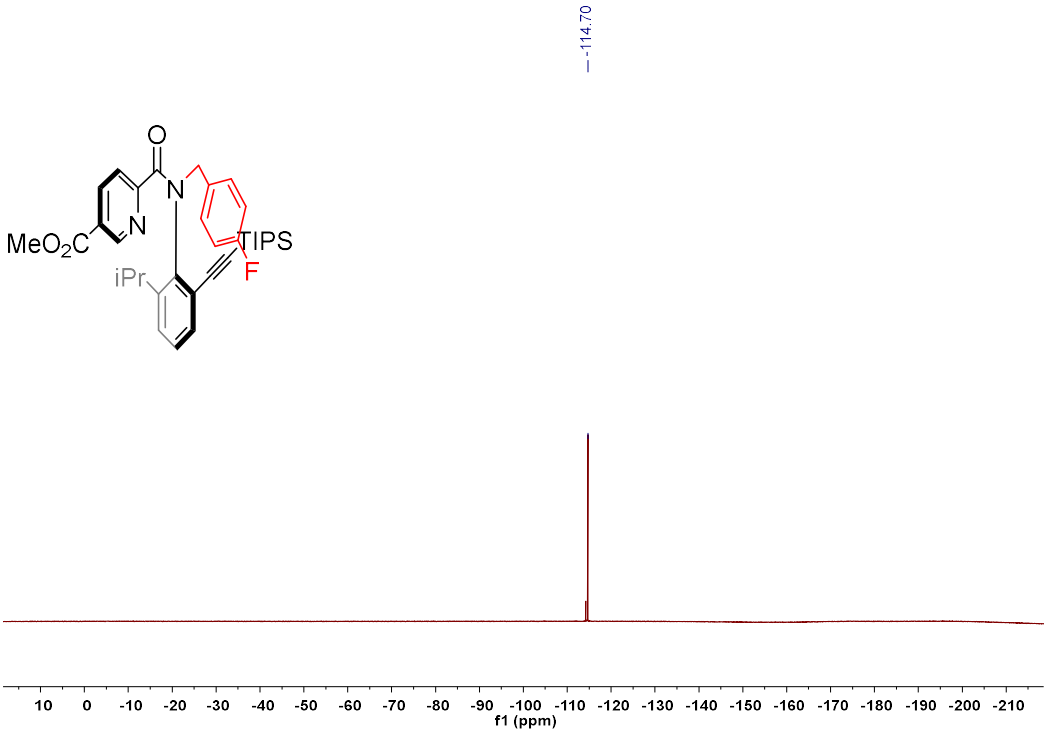
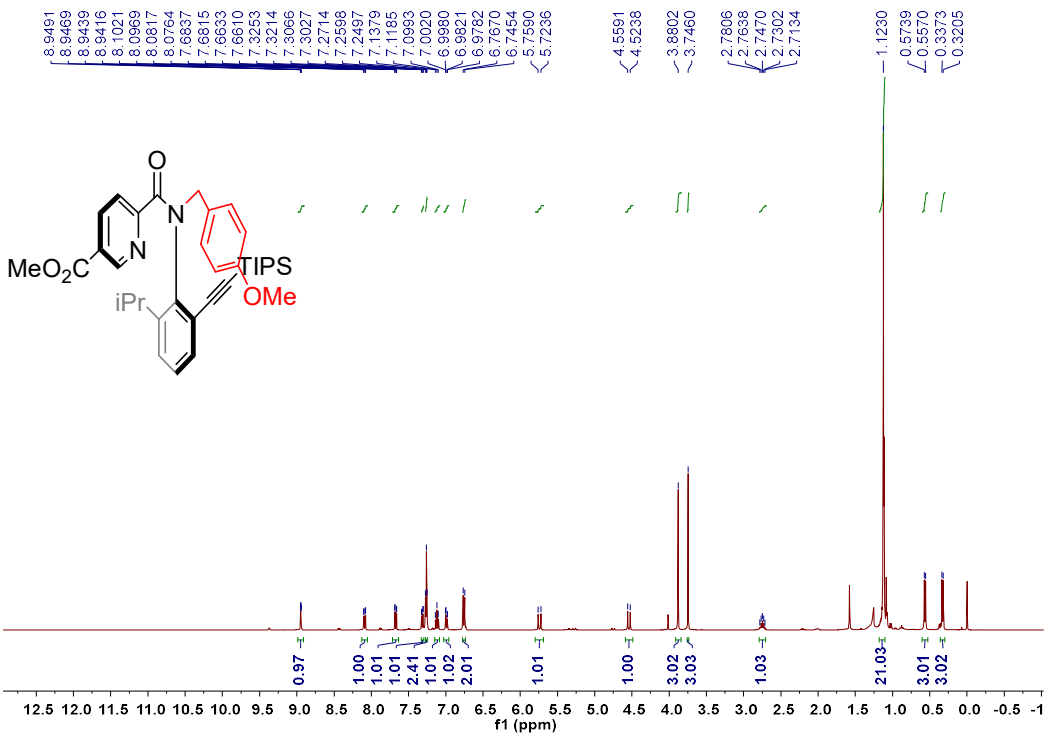
165.19
163.75
161.30
156.73
149.50
147.84
140.40
136.98
132.66
132.62
131.97
131.89
131.52
128.15
127.50
126.02
122.90
122.86
115.35
115.14
104.14
96.96
53.07
52.46
28.04
23.60
23.30
18.69
18.68
11.35
MeO2C
N
O
N
TIPS
F
iPr
f1 (ppm)


-114.70
O
N
N
MeO2C
iPr
TIPS
F
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

5r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7.6610
7.3253
7.3214
7.3066
7.3027
7.2714
7.2598
7.2497
7.1379
7.1185
7.0993
7.0020
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6.9821
6.9782
6.7670
6.7454
5.7590
5.7236
4.5591
4.5238
3.8802
3.7460
2.7806
2.7638
2.7470
2.7302
2.7134
1.1230
0.5739
0.5570
0.3373
0.3205
O
N
N
MeO2C
iPr
TIPS
OMe
0.97
1.00
1.01
1.01
2.41
1.01
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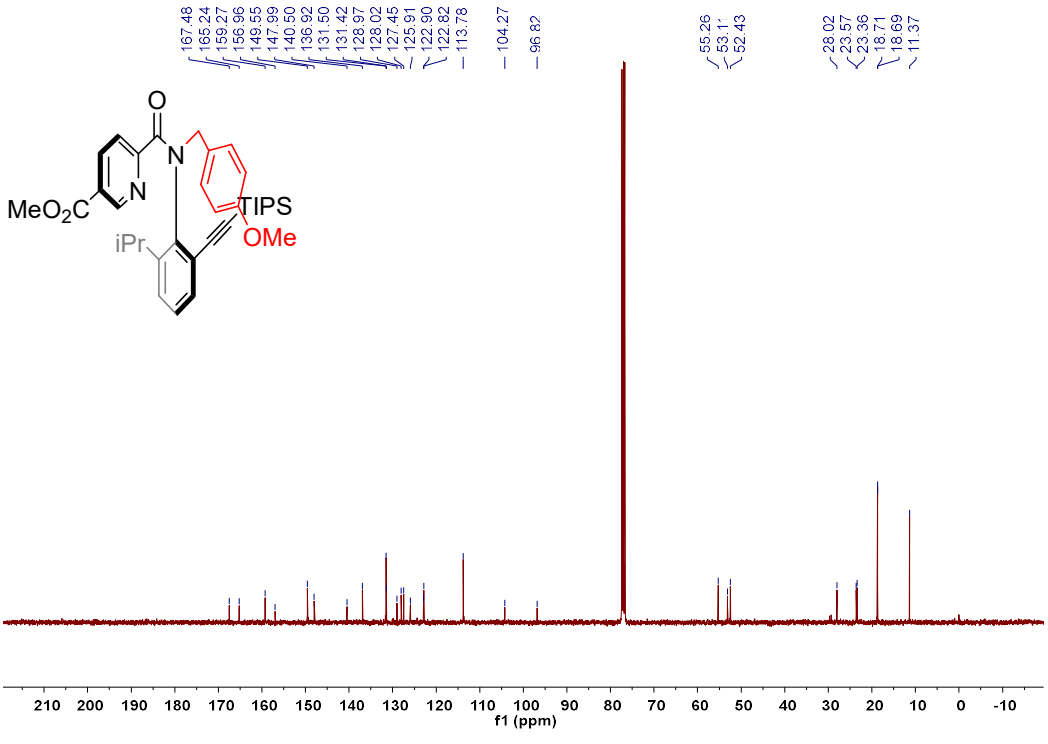
1.03
21.03
3.01
3.02
f1 (ppm)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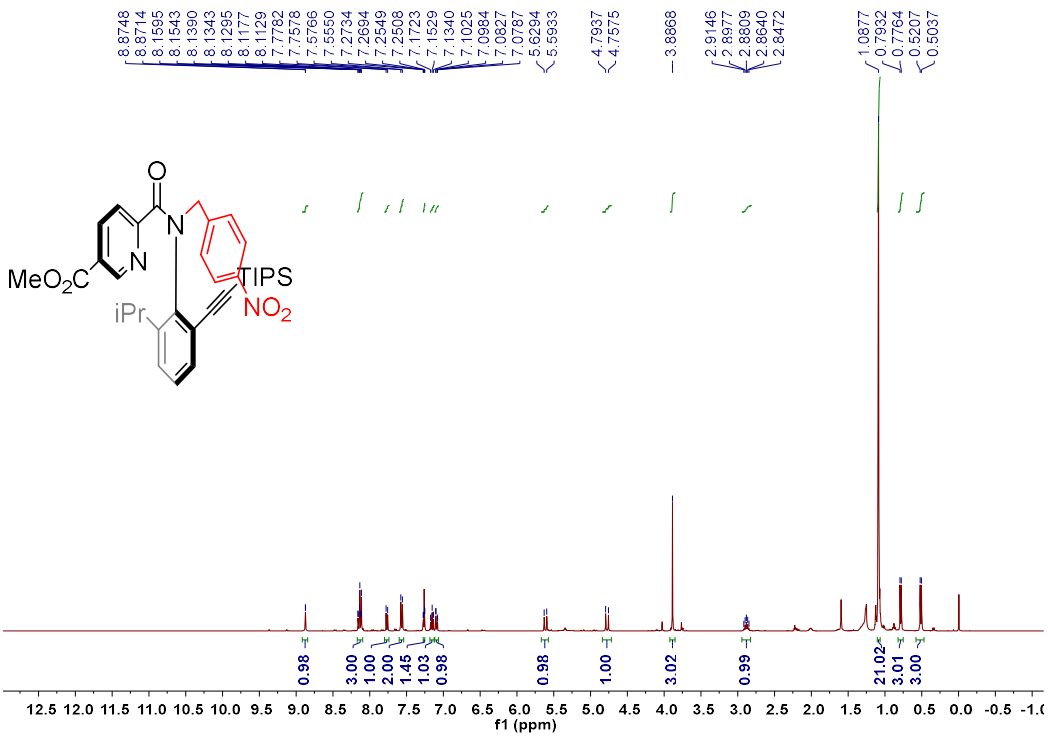
159.27
156.96
149.55
147.99
140.50
136.92
131.50
131.42
128.97
128.02
127.45
125.91
122.90
122.82
113.78
104.27
96.82
55.26
53.11
52.43
28.02
23.57
23.36
18.71
18.69
11.37
O
N
N
MeO2C
iPr
TIPS
OMe
f1 (ppm)

5s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8.1343
8.1295
8.1177
8.1129
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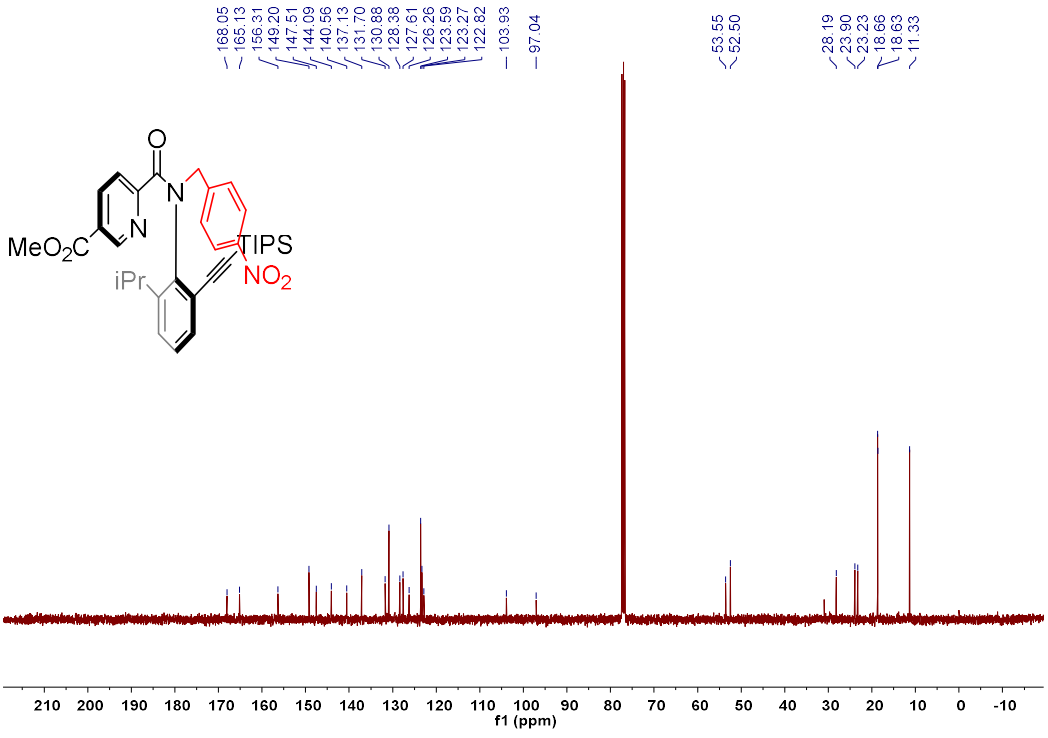
7.7578
7.5766
7.5550
7.2734
7.2694
7.2549
7.2508
7.1723
7.1529
7.1340
7.1025
7.0984
7.0827
7.0787
5.6294
5.5933
4.7937
4.7575
3.8868
2.9146
2.8977
2.8809
2.8640
2.8472
1.0877
0.7932
0.7764
0.5207
0.5037
MeO2C
N
O
N
iPr
TIPS
NO2
0.98
3.00
1.00
2.00
1.45
1.03
0.98
0.98
1.00
3.02
0.99
21.02
3.01
3.00
f1 (ppm)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147.51
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137.13
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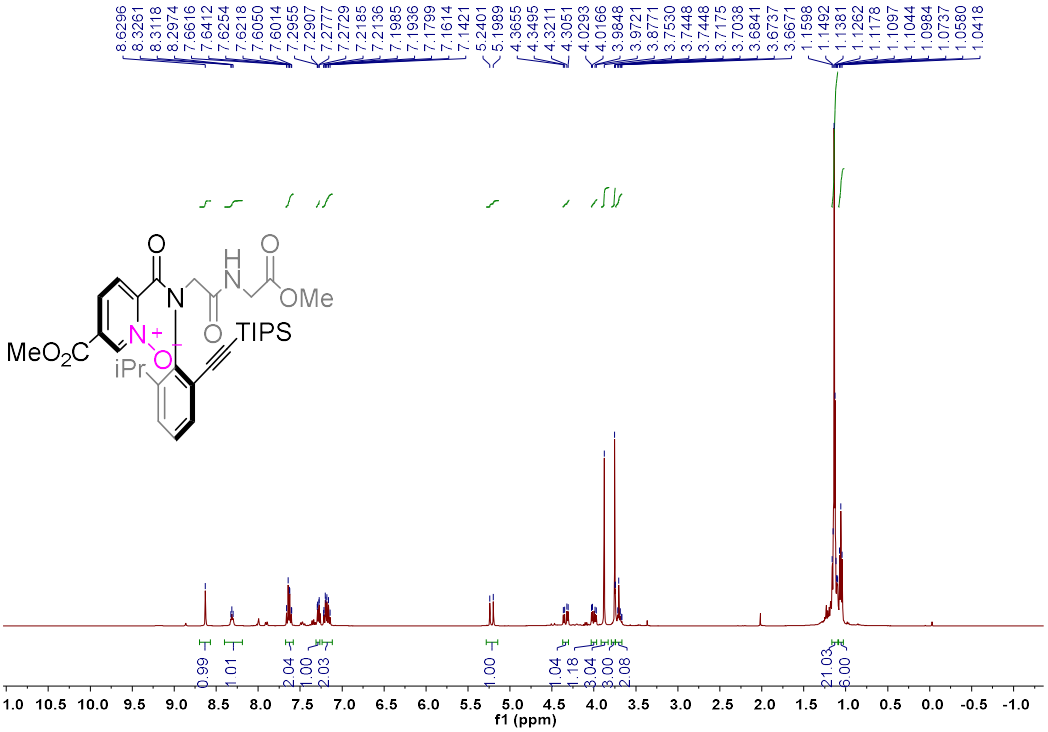
130.88
128.38
127.61
126.26
123.59
123.27
122.82
103.93
97.04
53.55
52.50
28.19
23.90
23.23
18.66
18.63
11.33
MeO2C
N
O
N
iPr
TIPS
NO2
f1 (ppm)

3ha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7.2777
7.2729
7.2185
7.2136
7.1965
7.1936
7.1799
7.1614
7.1421
5.2401
5.1989
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4.3495
4.3211
4.3051
4.0293
4.0166
3.9848
3.9721
3.8771
3.7530
3.7448
3.7448
3.7175
3.7038
3.6841
3.6737
3.6671
1.1598
1.1492
1.1381
1.1262
1.1178
1.1097
1.1044
1.0984
1.0737
1.0580
1.0418
OMe
TIPS
MeO2C
iPr
0.99
1.01
2.04
1.00
2.03
1.00
1.04
1.18
3.04
3.00
2.08
21.03
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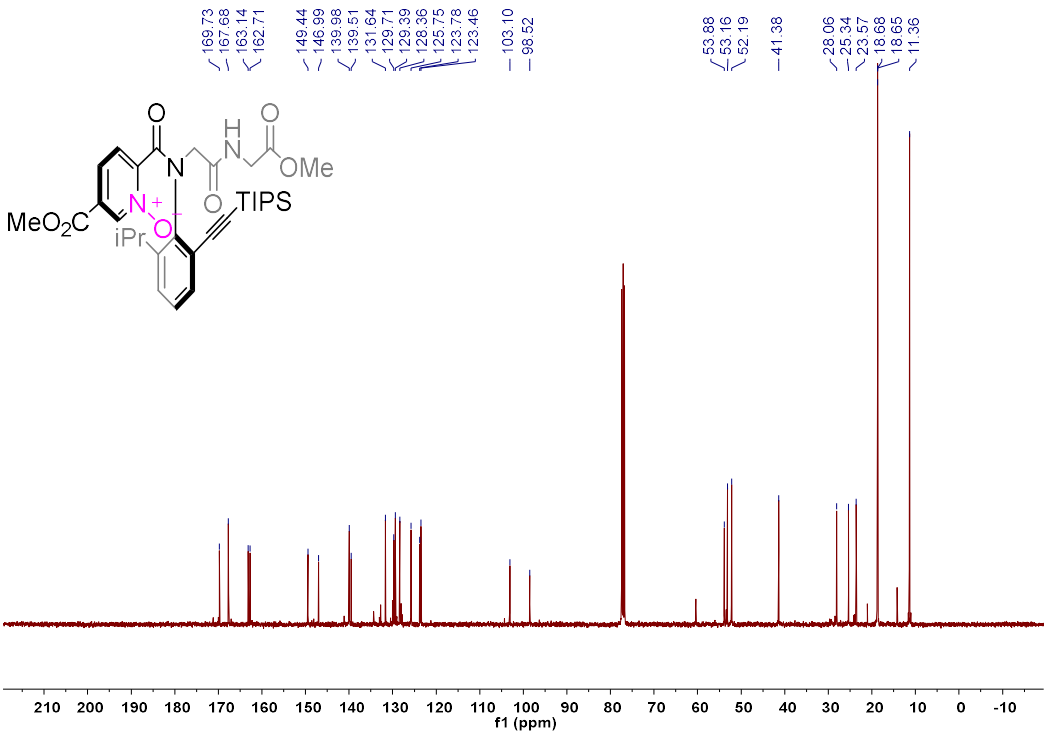
f1 (ppm)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129.71
129.39
128.36
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123.78
123.46
103.10
98.52
53.88
53.16
52.19
41.38
28.06
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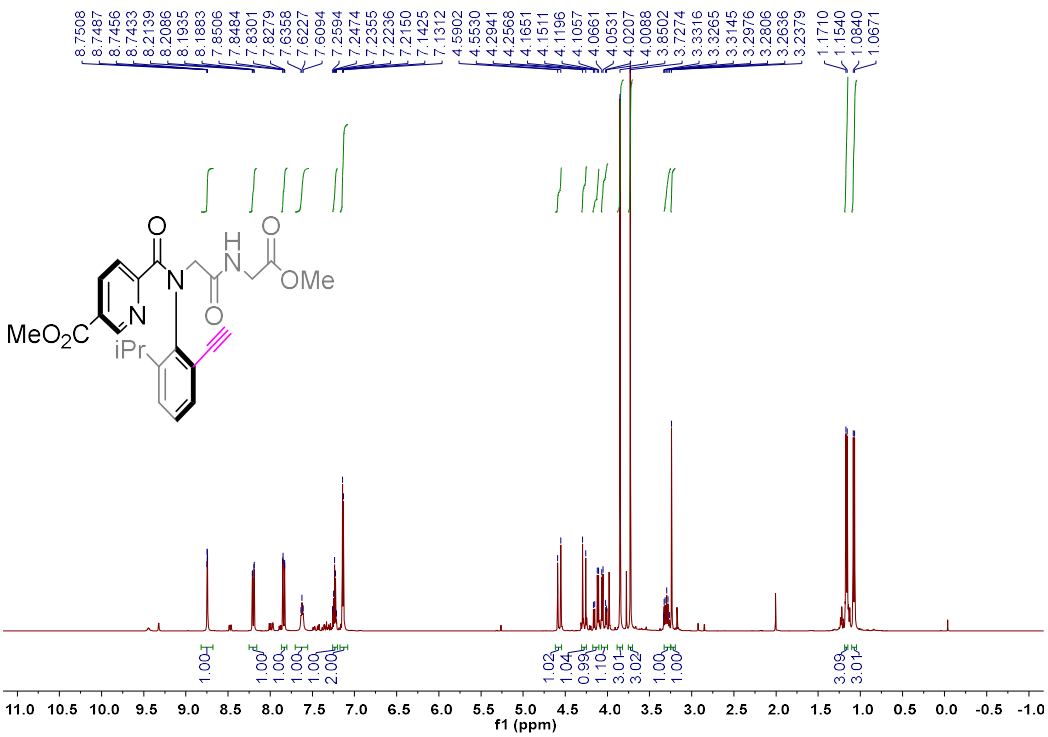
23.57
18.68
18.65
11.36
OMe
TIPS
MeO2C
iPr
f1 (ppm)

3hb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8.1935
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7.8279
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7.2594
7.2474
7.2355
7.2236
7.2150
7.1425
7.1312
4.5902
4.5530
4.2941
4.2568
4.1651
4.1511
4.1196
4.1057
4.0661
4.0531
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3.8502
3.7274
3.3316
3.3265
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3.2976
3.2806
3.2636
3.2379
1.1710
1.1540
1.0840
1.0671
MeO2C
iPr
OMe
1.00
1.00
1.00
1.00
2.00
1.02
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1.10
3.01
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1.00
1.00
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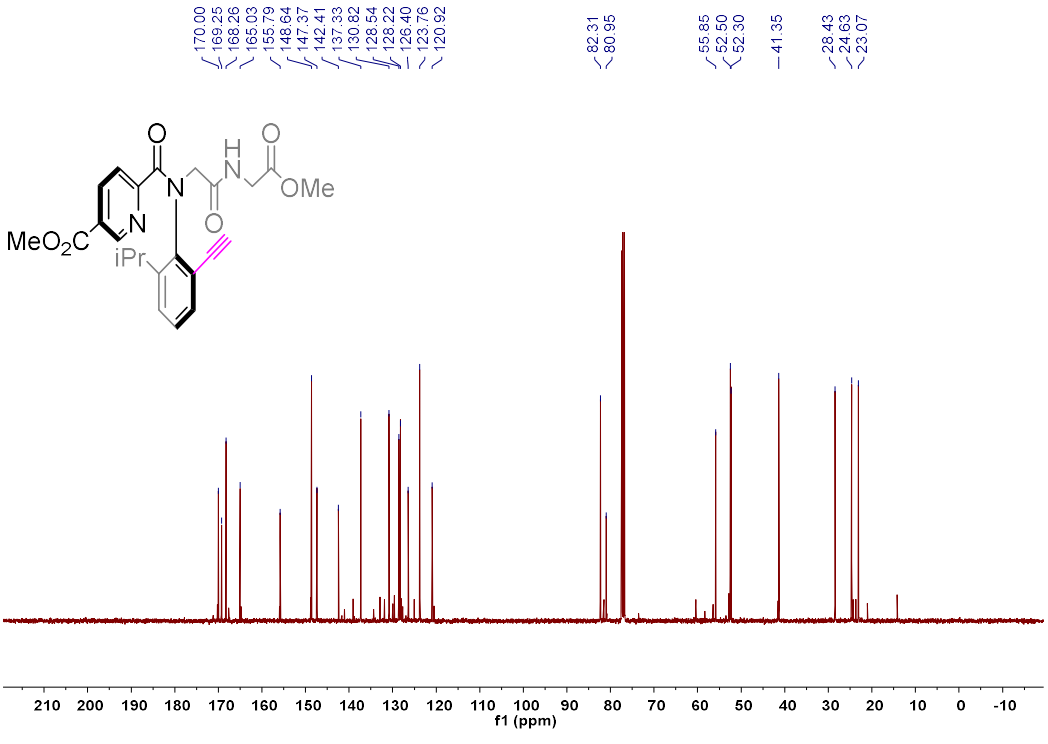
3.01
f1 (ppm)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123.76
120.92
82.31
80.95
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41.35
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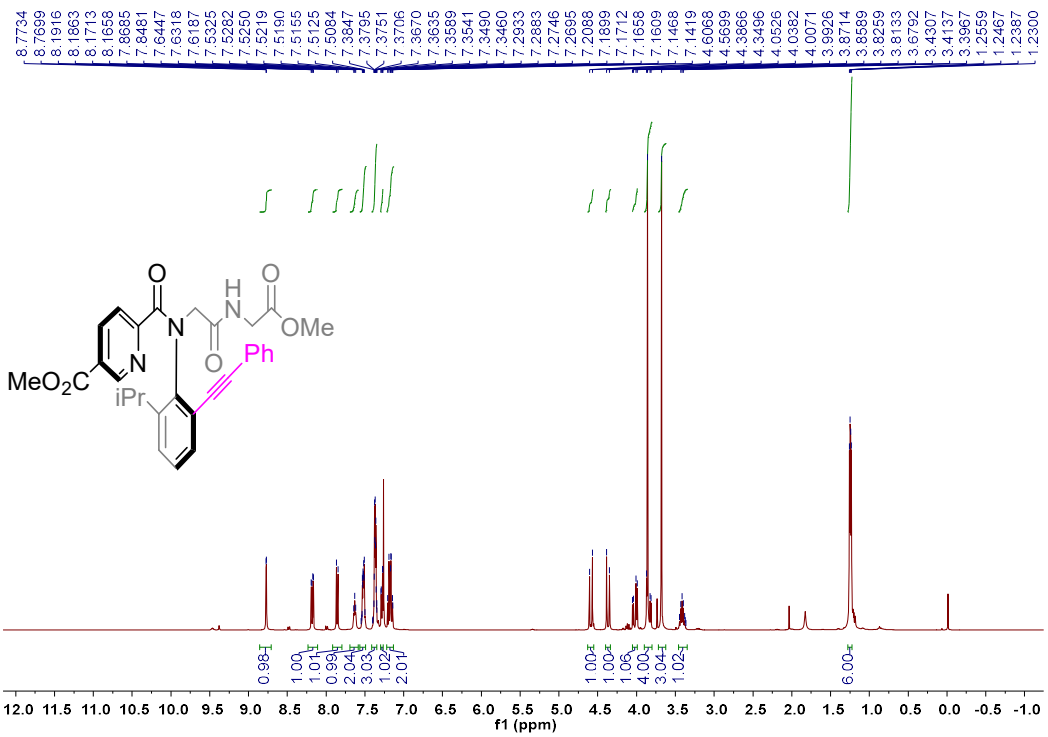
23.07
MeO2C
iPr
OMe
f1 (ppm)

3hc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7.5190
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7.5125
7.5084
7.3847
7.3795
7.3751
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7.3635
7.3589
7.3541
7.3490
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7.1899
7.1712
7.1658
7.1609
7.1468
7.1419
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4.5699
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4.0526
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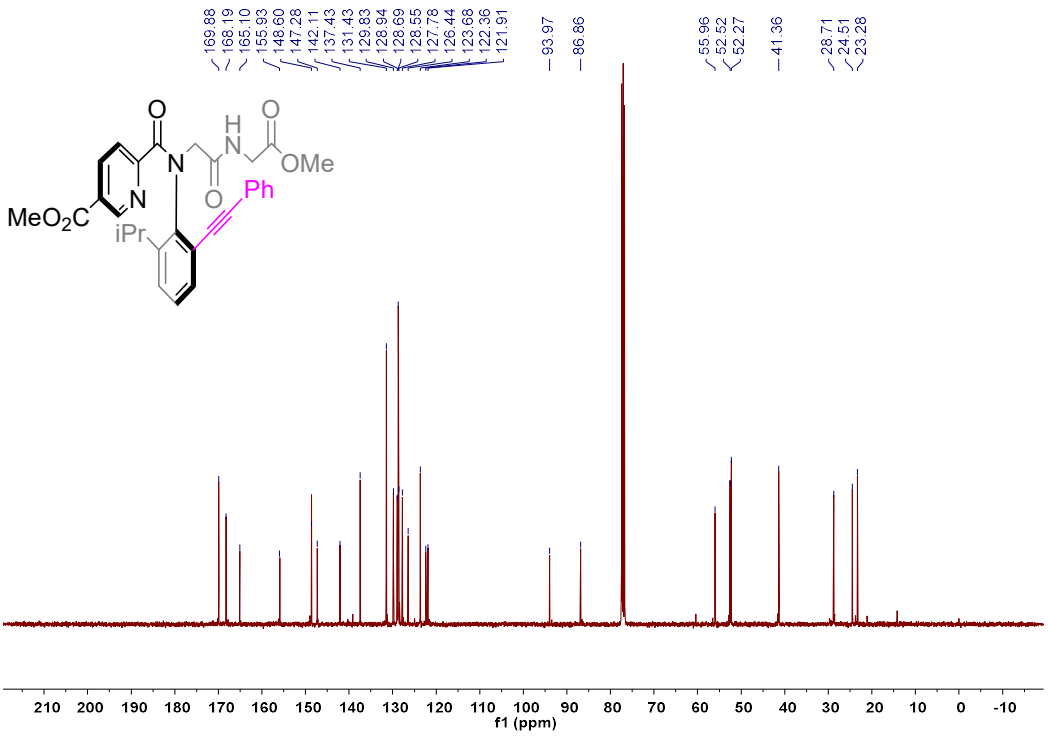
4.0071
3.9926
3.8714
3.8589
3.8259
3.8133
3.6792
3.4307
3.4137
3.3967
1.2559
1.2467
1.2387
1.2300
O
H
N
O
OMe
N
O
Ph
MeO2C
N
iPr
0.98
1.00
1.01
0.99
2.04
3.03
1.02
2.01
1.00
1.00
1.06
4.00
3.04
1.02
6.00
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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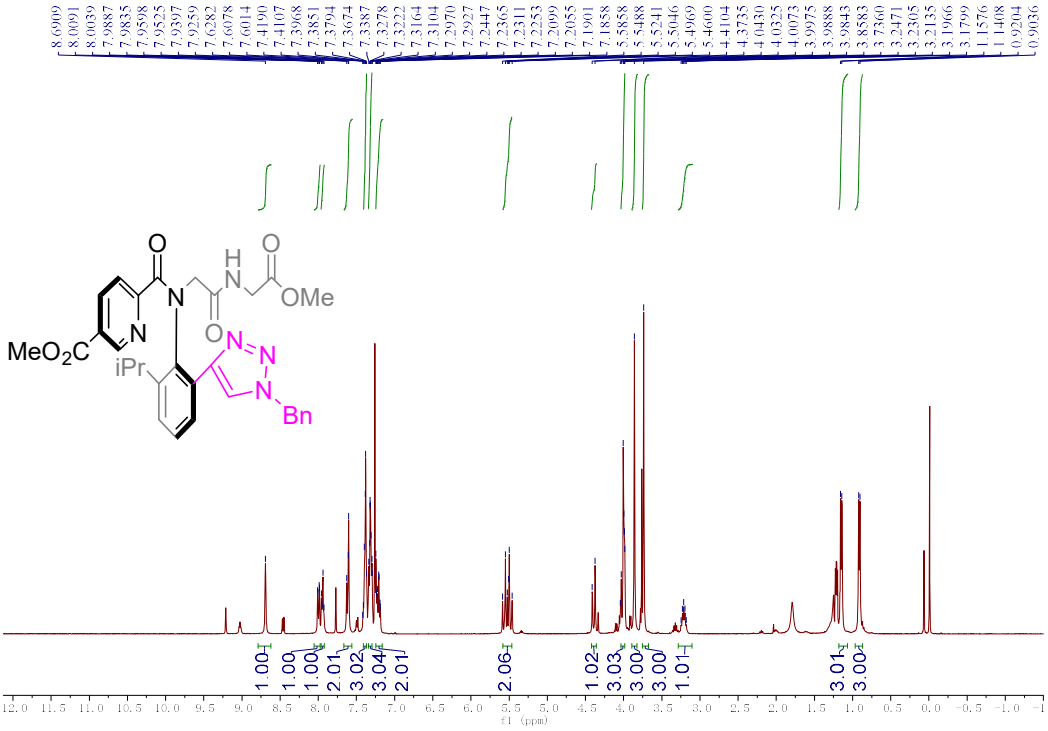
127.78
126.44
123.68
122.36
121.91
93.97
86.86
55.96
52.52
52.27
41.36
28.71
24.51
23.28
O
H
N
O
OMe
N
O
Ph
MeO2C
N
iPr
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3hd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7.6014
7.4190
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7.3851
7.3794
7.3674
7.3387
7.3278
7.3222
7.3164
7.3104
7.2970
7.2927
7.2447
7.2365
7.2311
7.2253
7.2099
7.2055
7.1901
7.1858
5.5858
5.5488
5.5241
5.5046
5.4969
5.4600
4.4104
4.3735
4.0430
4.0325
4.0073
3.9975
3.9888
3.9843
3.8583
3.7360
3.2471
3.2305
3.2135
3.1966
3.1799
1.1576
1.1408
0.9204
0.9036
MeO2C
iPr
N
O
H
OMe
Bn
1.00
1.00
1.00
2.01
3.02
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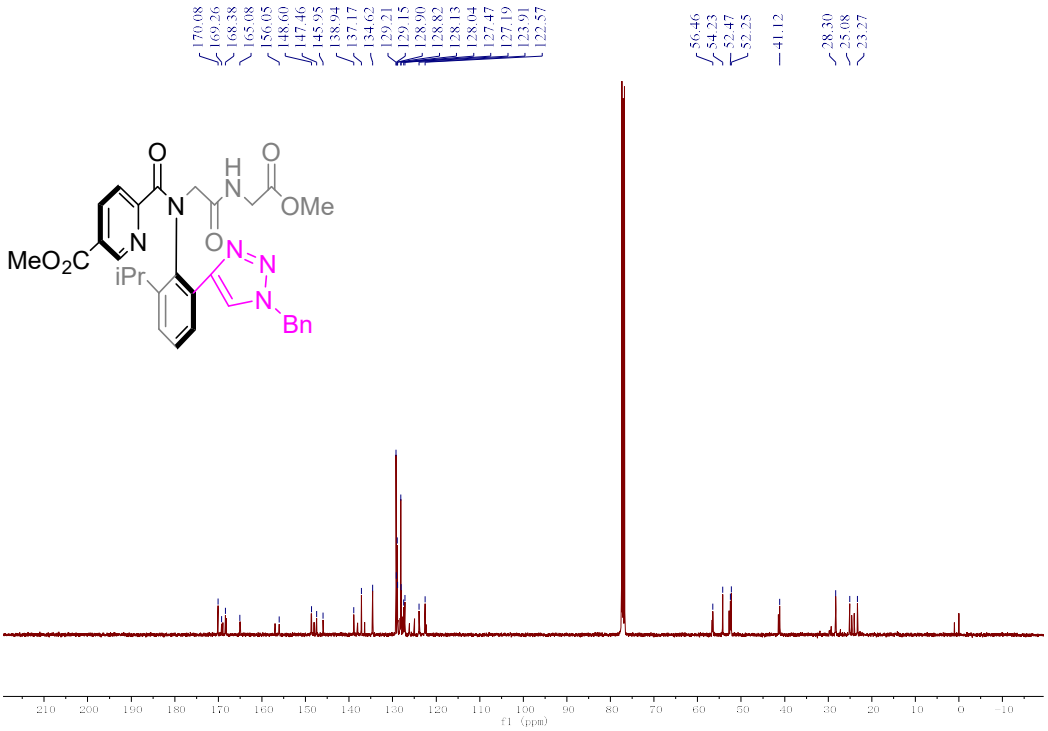
3.00
1.01
3.01
3.00
f1 (ppm)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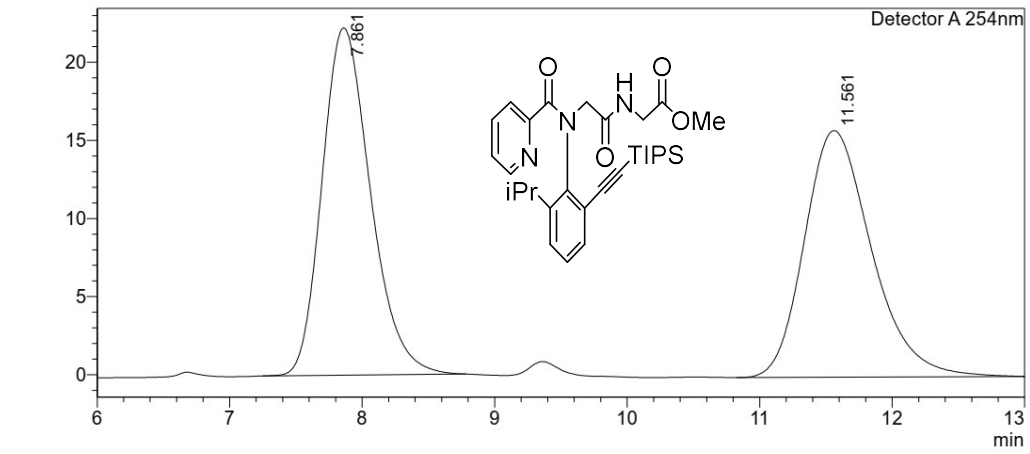
128.82
128.13
128.04
127.47
127.19
123.91
122.57
56.46
54.23
53.47
52.25
41.12
28.30
25.08
23.27
MeO2C
iPr
N
O
H
OMe
Bn
f1 (ppm)

7. Copies of HPLC Analysis

3a: OD-H, *n*-Hexane/*i*-PrOH = 90/10, rate = 0.8 mL/min, 254nm

<Chromatogram>

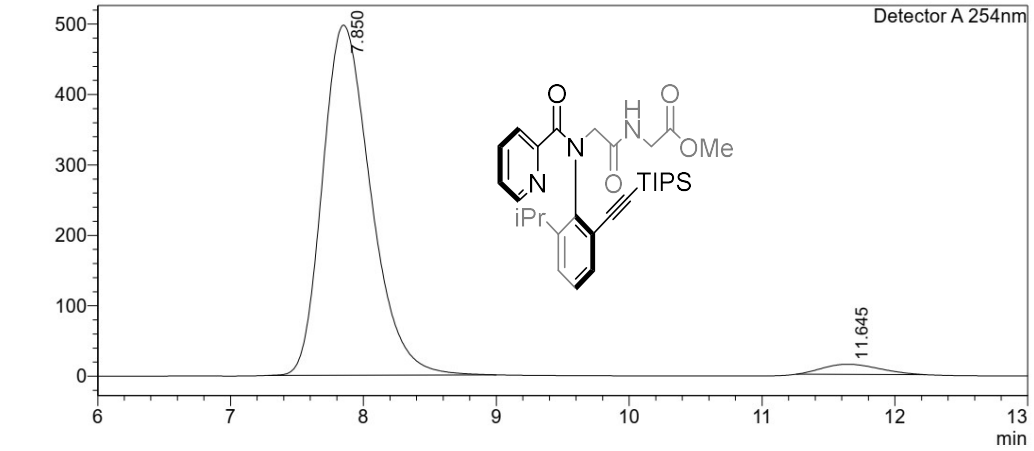


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.861	565418	22227	50.399		M	
2	11.561	556465	15791	49.601		M	
Total		1121883	38018				

<Chromatogram>



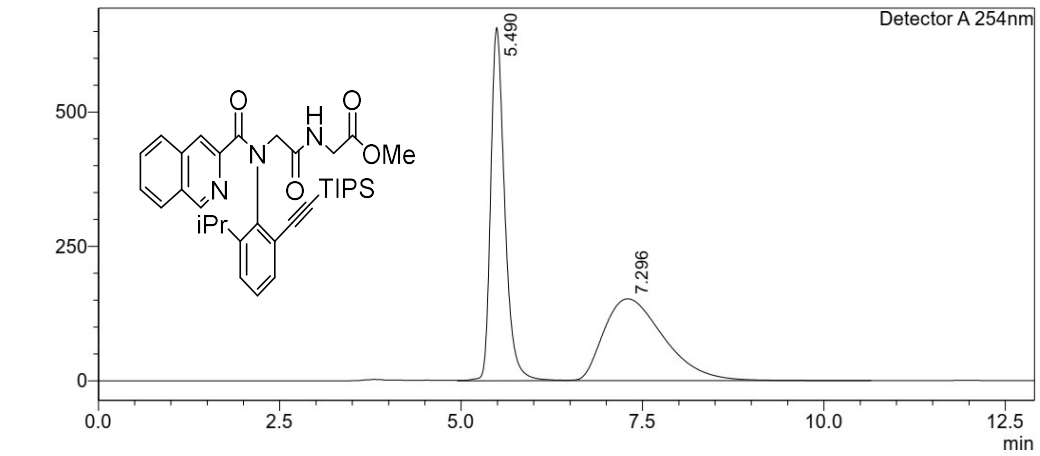
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.850	12540781	497211	96.694		M	
2	11.645	428831	14406	3.306		M	
Total		12969612	511616				

3d: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254 nm

<Chromatogram>

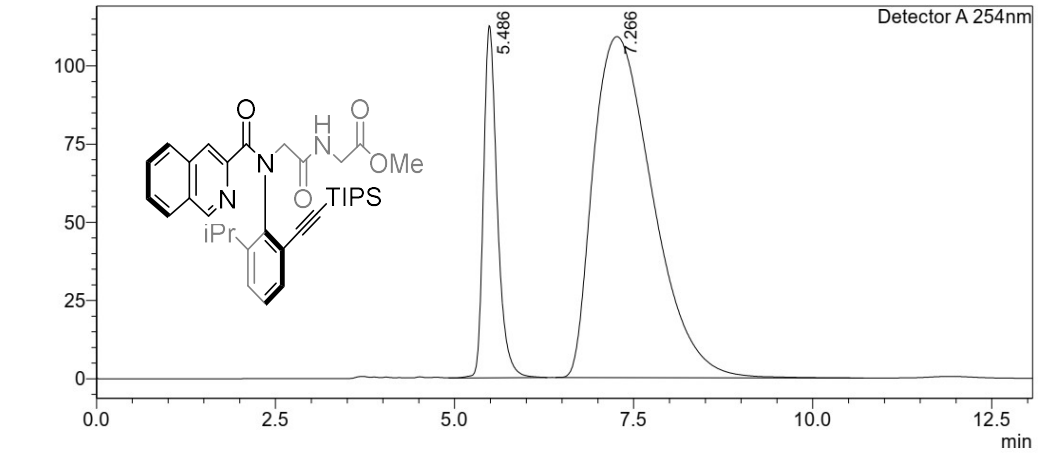


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	5.490	8826544	656434	50.154			
2	7.296	8772395	152303	49.846		SV	
Total		17598939	808737				

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	5.486	1503468	112513	19.269			
2	7.266	6299183	108993	80.731			
Total		7802650	221506				

3e: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254 nm

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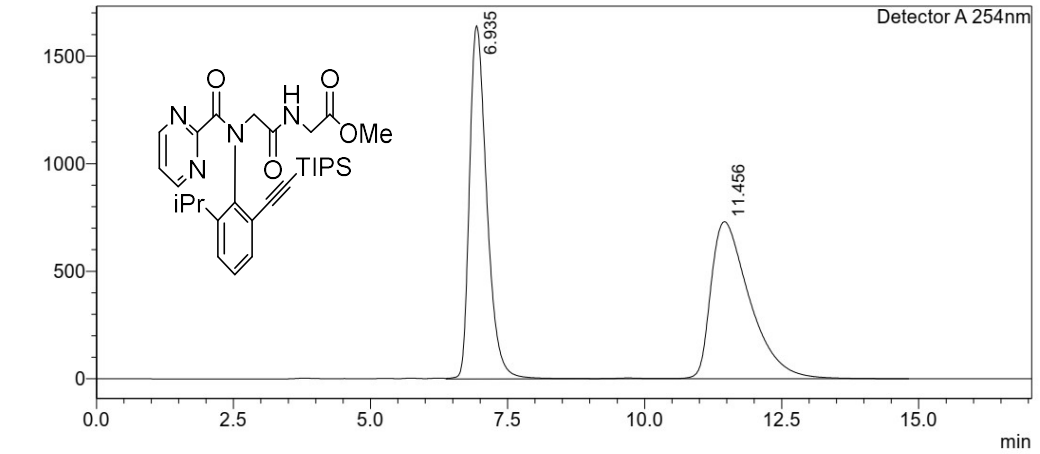
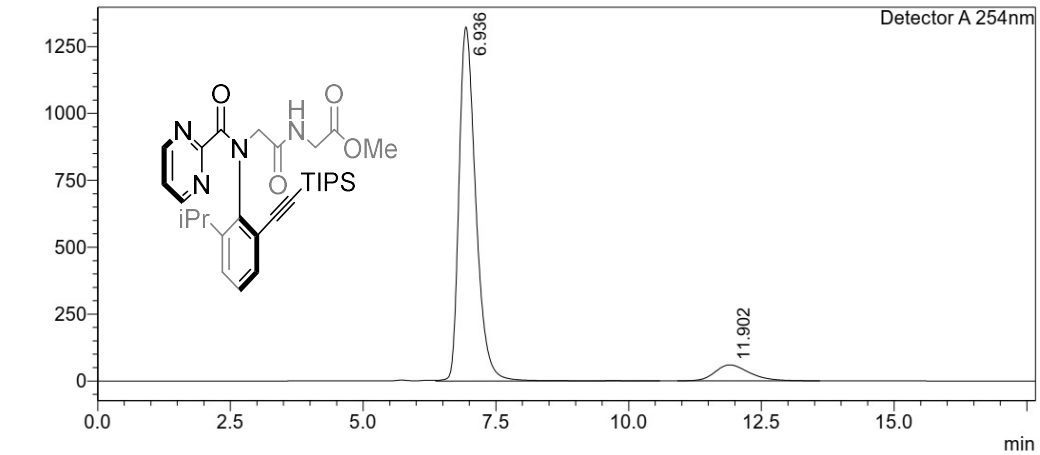


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.935	36139334	1640118	50.055		M	
2	11.456	36059598	730011	49.945		V M	
Total		72198932	2370129				

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.936	29006439	1322905	91.479		M	
2	11.902	2701778	59604	8.521		M	
Total		31708217	1382509				

3f: OD-H, *n*-Hexane/*i*-PrOH = 85/15, rate = 0.8 mL/min, 254 nm

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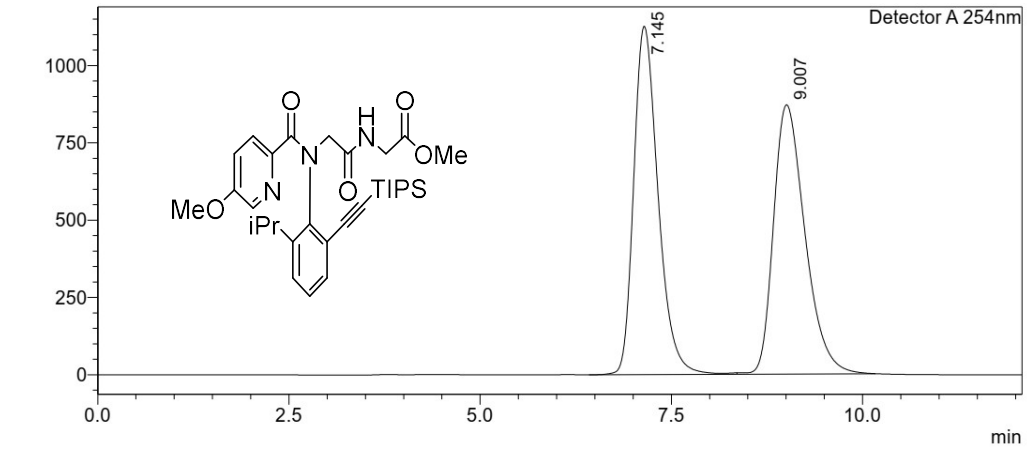

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.145	24989102	1126598	50.082		M	
2	9.007	24907621	871041	49.918		V M	
Total		49896723	1997639				

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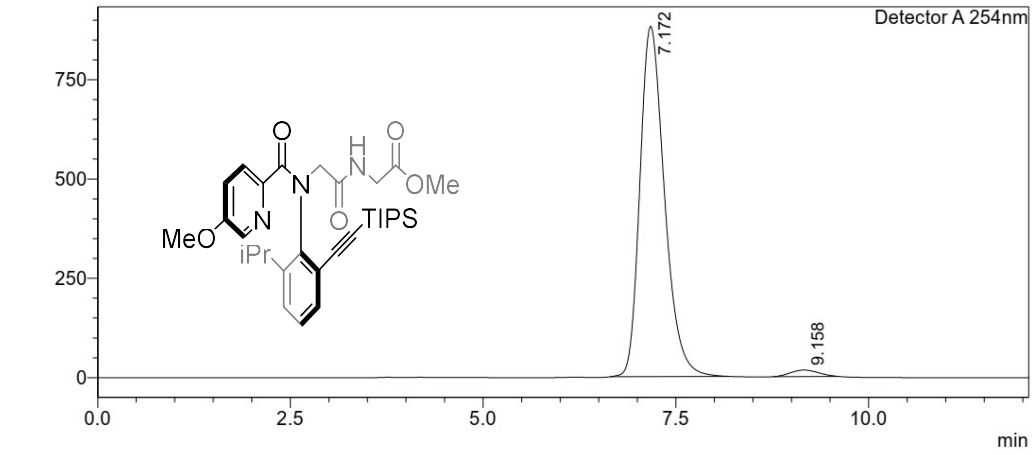

<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.172	19540678	881249	97.922		M	
2	9.158	414690	16397	2.078		M	
Total		19955368	897646				

3g: AD-H, *n*-Hexane/*i*-PrOH = 85/15, rate = 0.8 mL/min, 254nm

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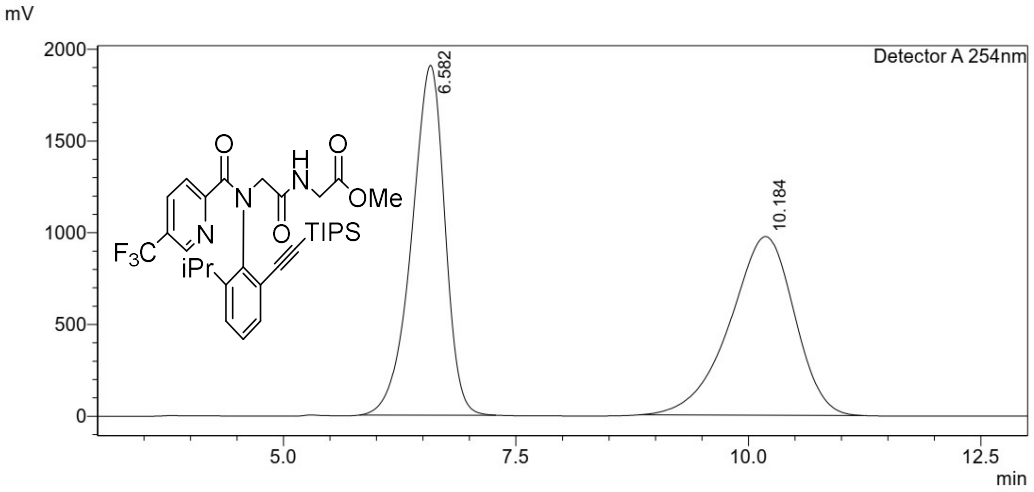
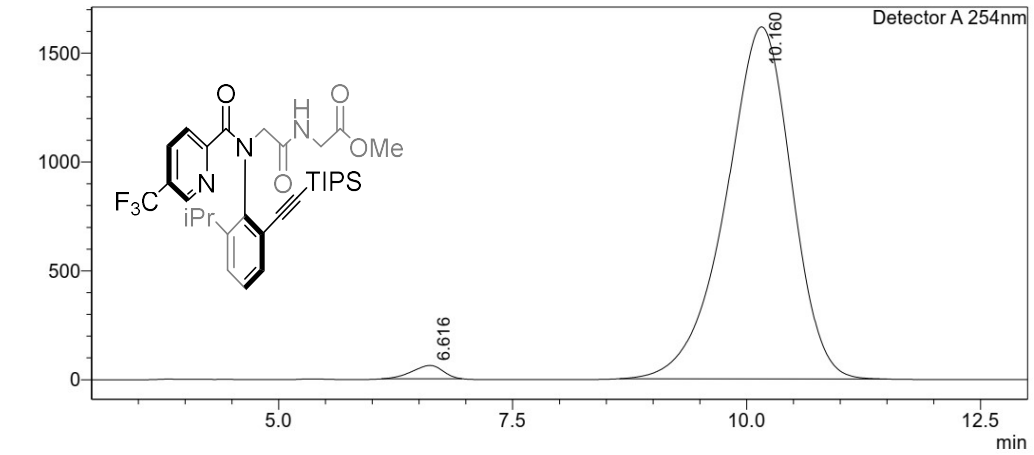


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.582	47323316	1906633	50.060		M	
2	10.184	47209965	973816	49.940		M	
Total		94533281	2880450				

<Chromatogram>



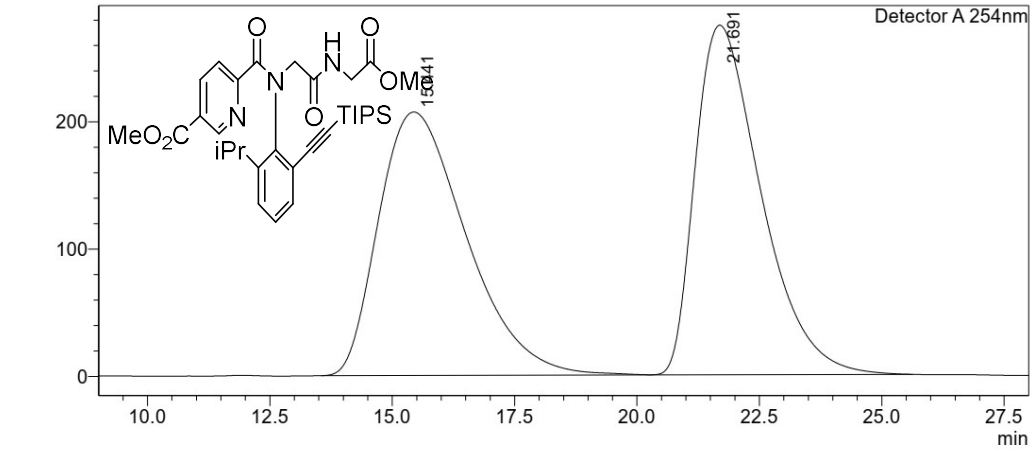
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.616	1409687	61239	1.748		M	
2	10.160	79248148	1617872	98.252		M	
Total		80657836	1679111				

3h: OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, 254 nm

<Chromatogram>

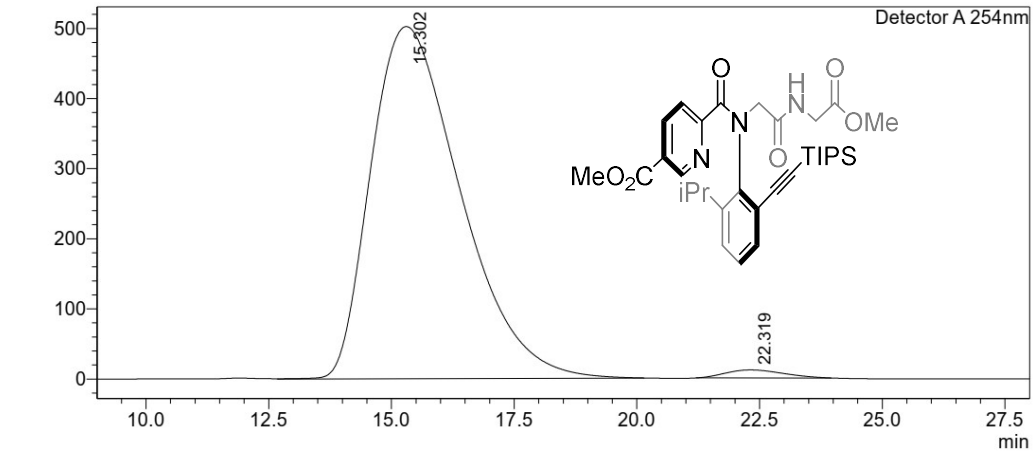


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.441	25822193	207022	50.061		M	
2	21.691	25759122	274743	49.939		V M	
Total		51581315	481766				

<Chromatogram>



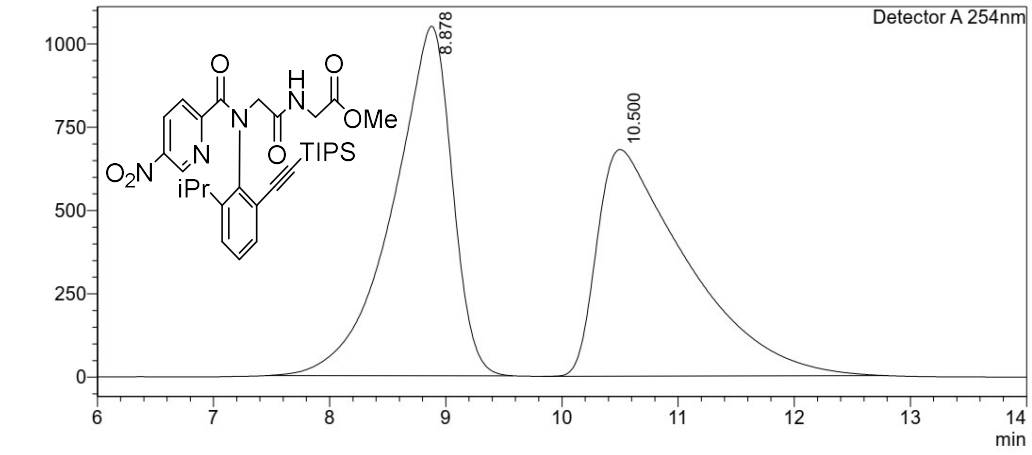
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.302	63858106	502171	98.558		M	
2	22.319	934210	11446	1.442		M	
Total		64792315	513616				

3i: AD-H, *n*-Hexane/*i*-PrOH = 85/15, rate = 0.8 mL/min, 254nm

<Chromatogram>

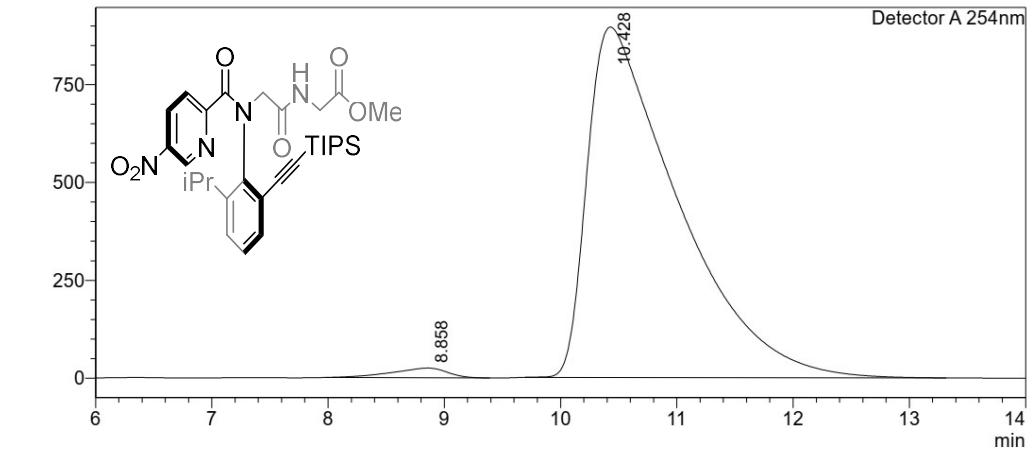


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.878	37210480	1048530	50.239		M	
2	10.500	36856676	679805	49.761		M	
Total		74067156	1728334				

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.858	830027	24955	1.681		M	
2	10.428	48560437	895351	98.319		M	
Total		49390464	920306				

3j: OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, 254 nm

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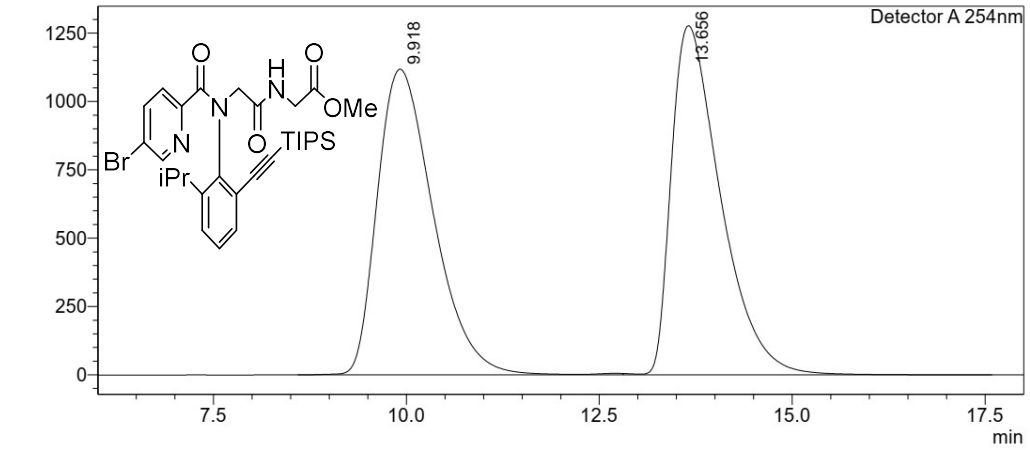
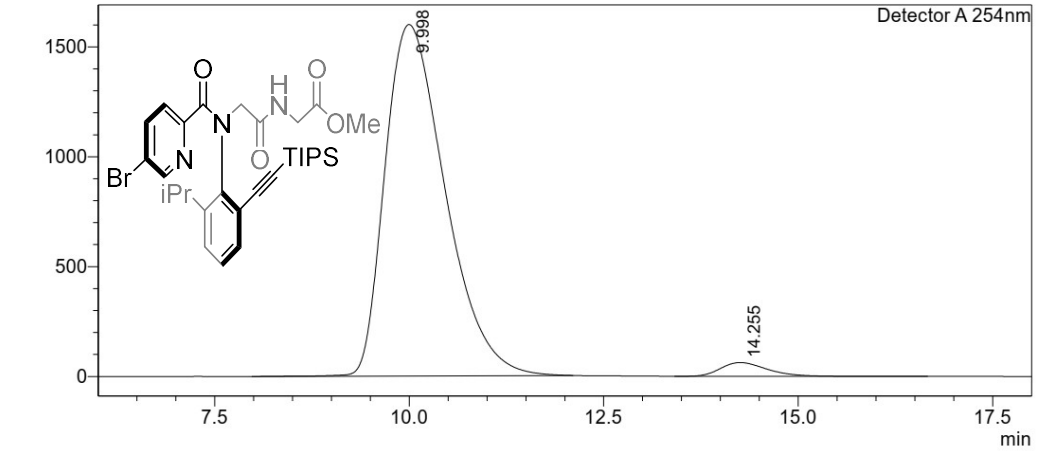


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.918	56725570	1118656	49.952		M	
2	13.656	56834927	1277511	50.048		V M	
Total		113560497	2396167				

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.998	86181163	1599205	97.051		M	
2	14.255	2619036	62731	2.949		M	
Total		88800198	1661936				

3k: OD-H, *n*-Hexane/*i*-PrOH = 90/10, rate = 0.8 mL/min, 254 nm

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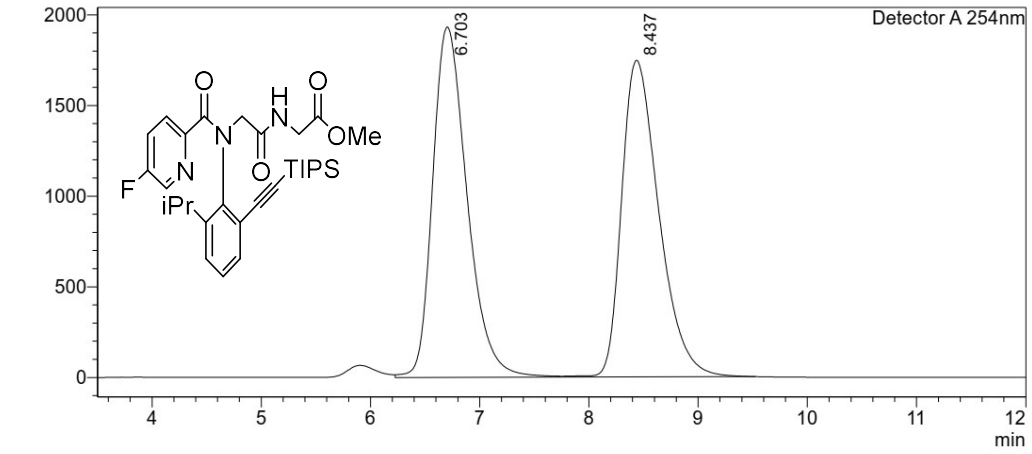
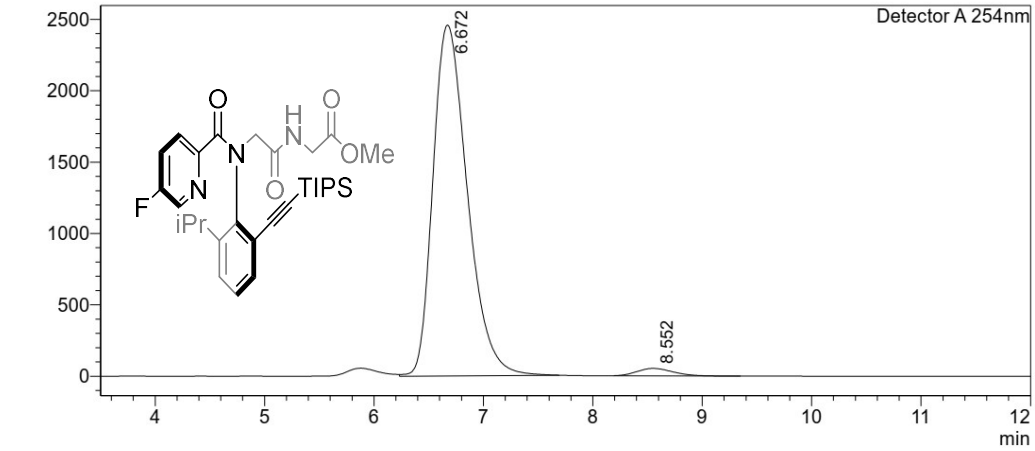


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.703	42317151	1931742	50.565		M	
2	8.437	41372157	1745901	49.435		V M	
Total		83689308	3677642				

<Chromatogram>



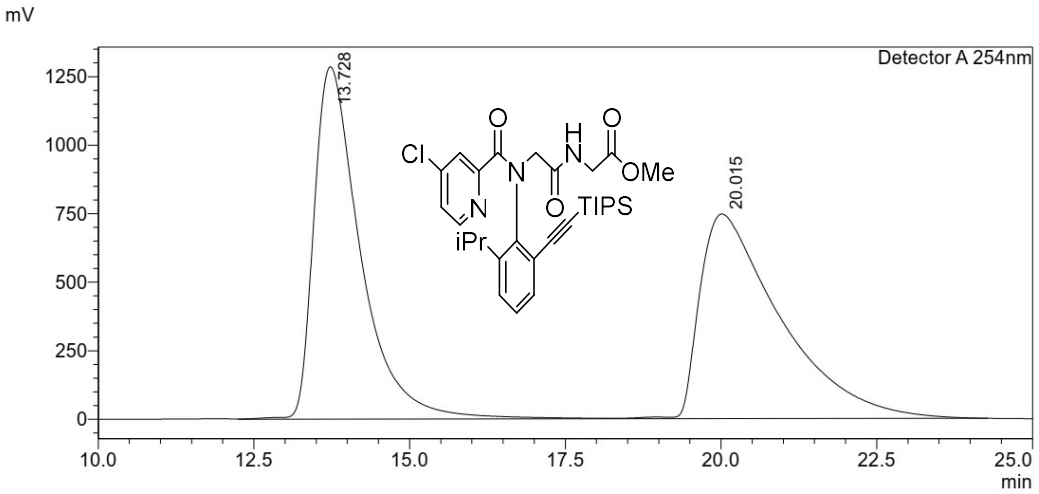
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.672	53734678	2457776	97.848		M	
2	8.552	1181757	52121	2.152		M	
Total		54916434	2509898				

3l: OD-H, *n*-Hexane/*i*-PrOH = 97/3, rate = 0.8 mL/min, 254 nm

<Chromatogram>

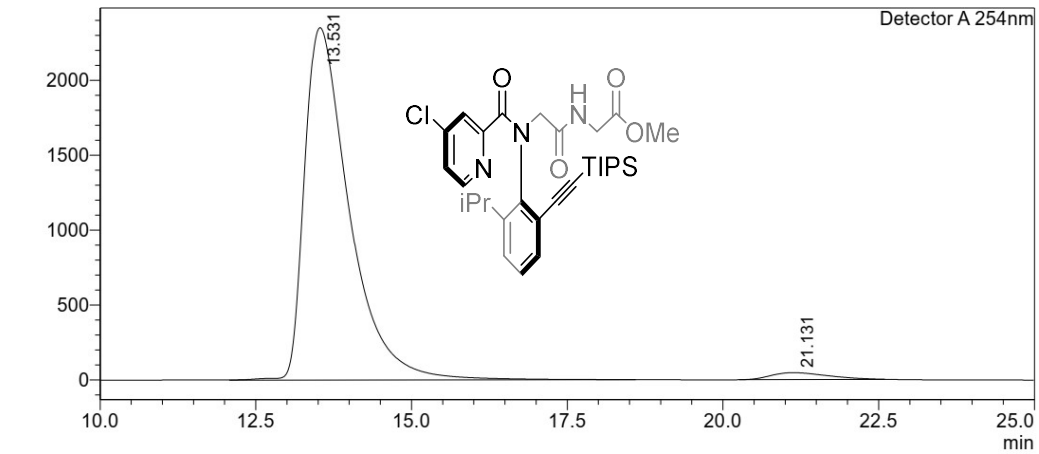


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.728	67027140	1285470	49.915		M	
2	20.015	67255811	746640	50.085		V M	
Total		134282951	2032111				

<Chromatogram>



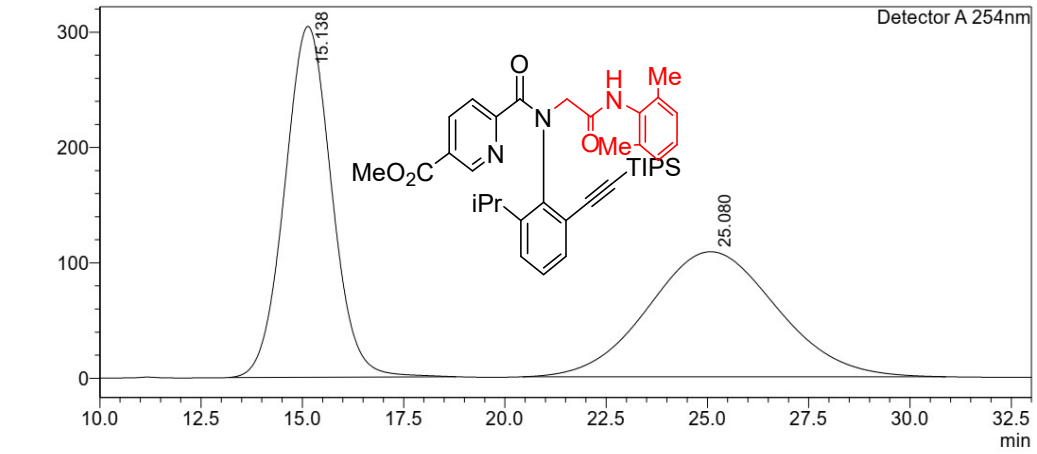
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.531	117863950	2351847	97.571		M	
2	21.131	2934090	46352	2.429		M	
Total		120798040	2398199				

5a: IC, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254 nm

<Chromatogram>

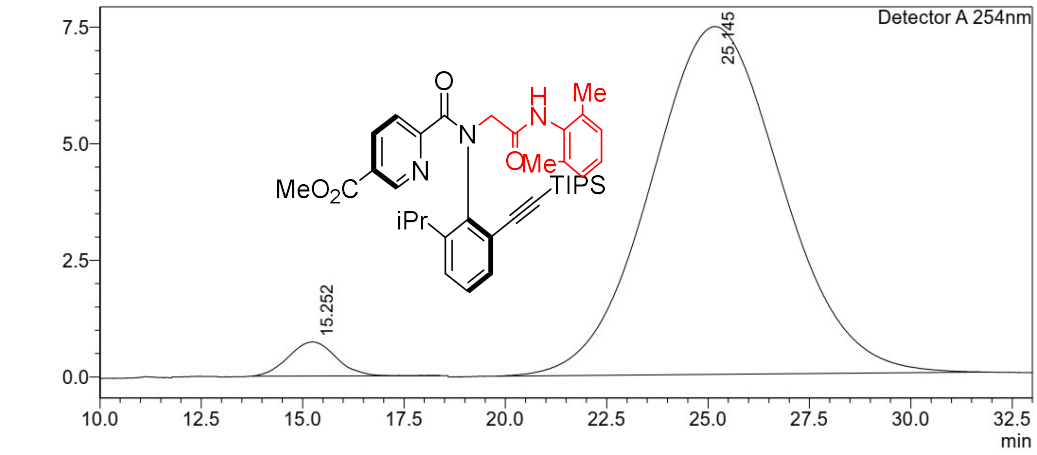


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.138	24481658	304070	50.457		M	
2	25.080	24038573	108389	49.543		M	
Total		48520231	412459				

<Chromatogram>



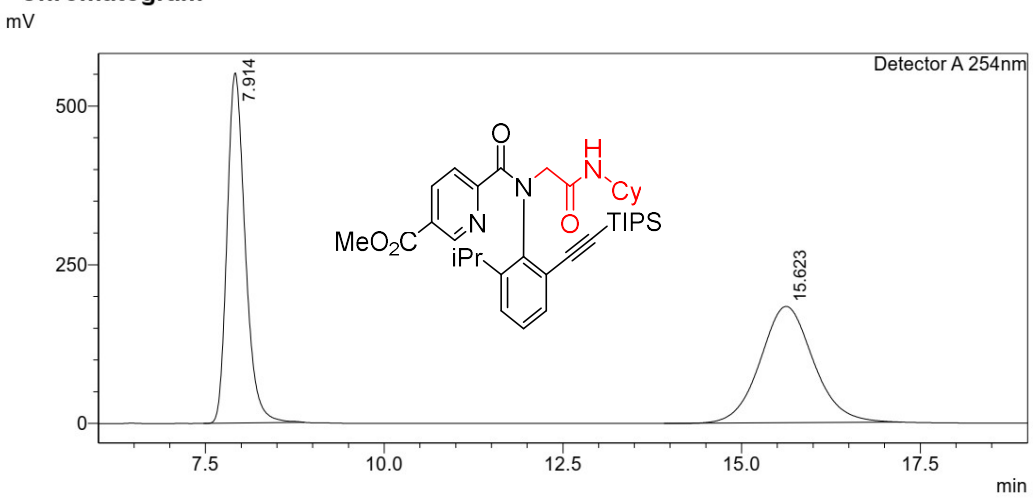
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	15.252	59704	732	3.428		M	
2	25.145	1682116	7459	96.572		M	
Total		1741820	8191				

5b: IC, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254 nm

<Chromatogram>

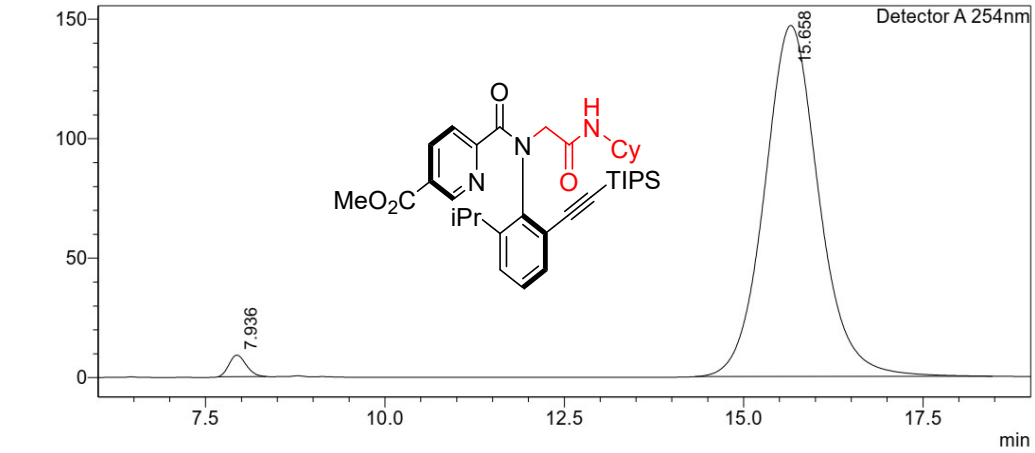


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.914	9731556	551509	50.580		M	
2	15.623	9508451	183369	49.420		M	
Total		19240007	734878				

<Chromatogram>



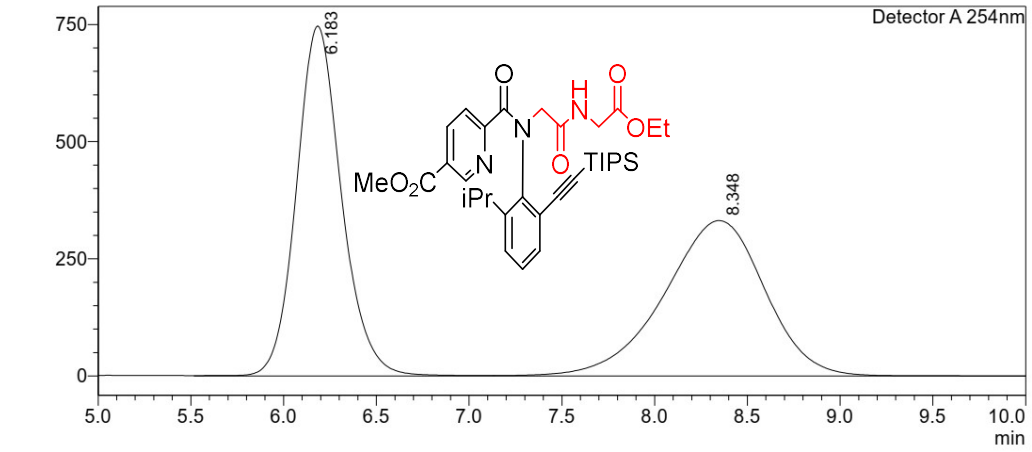
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.936	151237	9065	1.914		M	
2	15.658	7750249	146927	98.086		M	
Total		7901486	155992				

5c: AD-H, *n*-Hexane/*i*-PrOH= 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

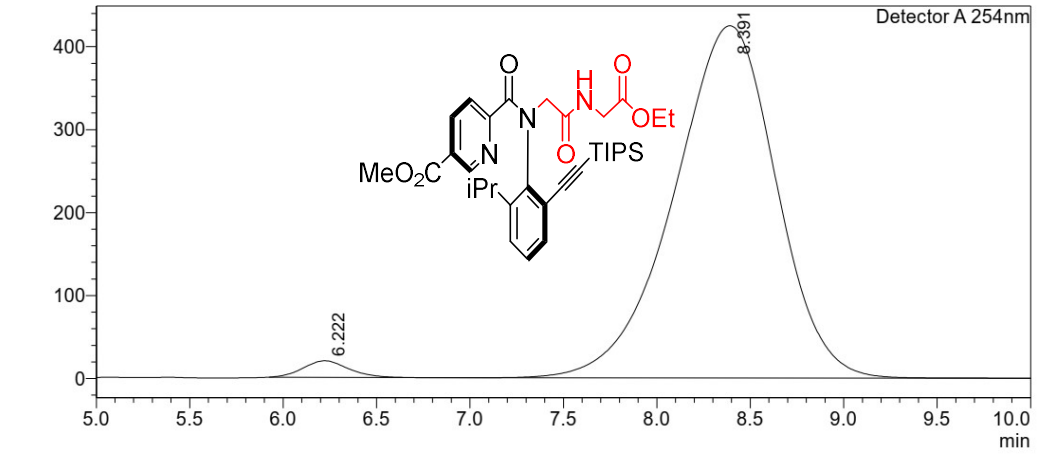


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.183	12640384	746845	50.159			
2	8.348	12560144	331532	49.841		V	
Total		25200528	1078378				

<Chromatogram>



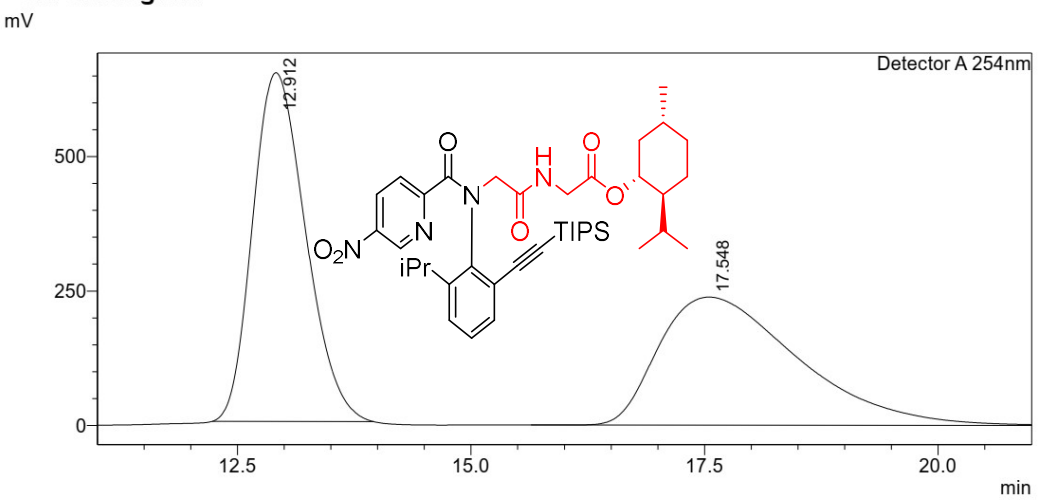
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.222	328831	19877	1.994		S M	
2	8.391	16159450	424514	98.006			
Total		16488281	444392				

5d: AD-H, *n*-Hexane/*i*-PrOH = 97/3, rate = 0.8 mL/min, 254 nm

<Chromatogram>

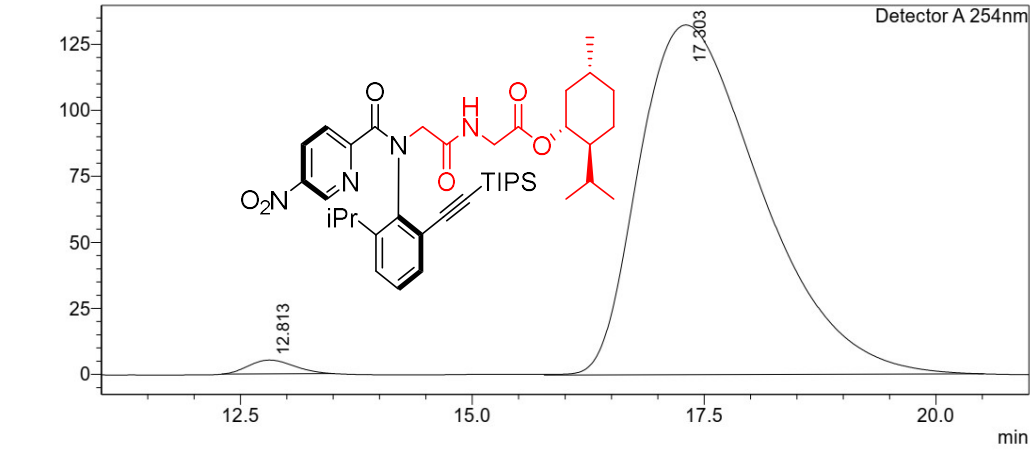


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.912	25572125	648382	50.893		M	
2	17.548	24675053	238003	49.107		M	
Total		50247178	886385				

<Chromatogram>



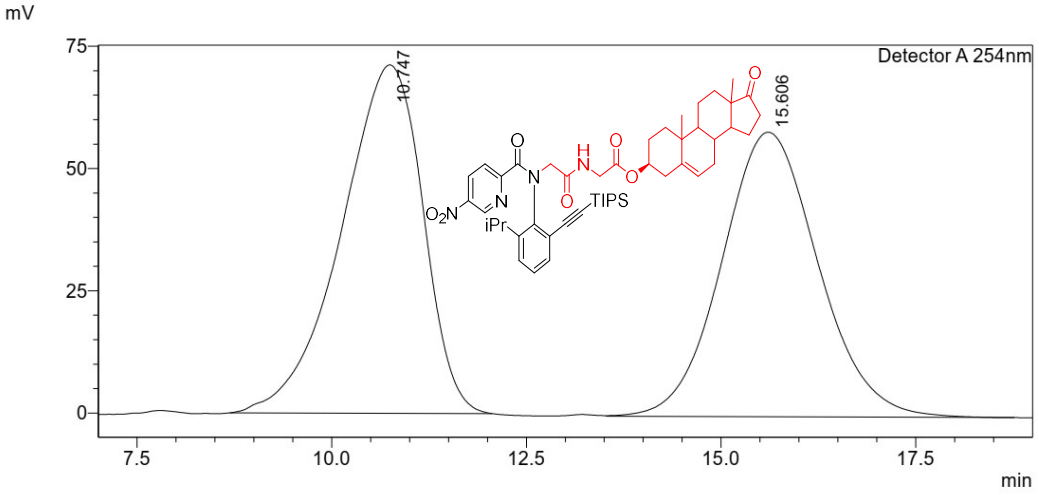
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.813	180517	5251	1.467		M	
2	17.303	12125097	132421	98.533		M	
Total		12305614	137672				

5e: AD-H, *n*-Hexane/ *i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

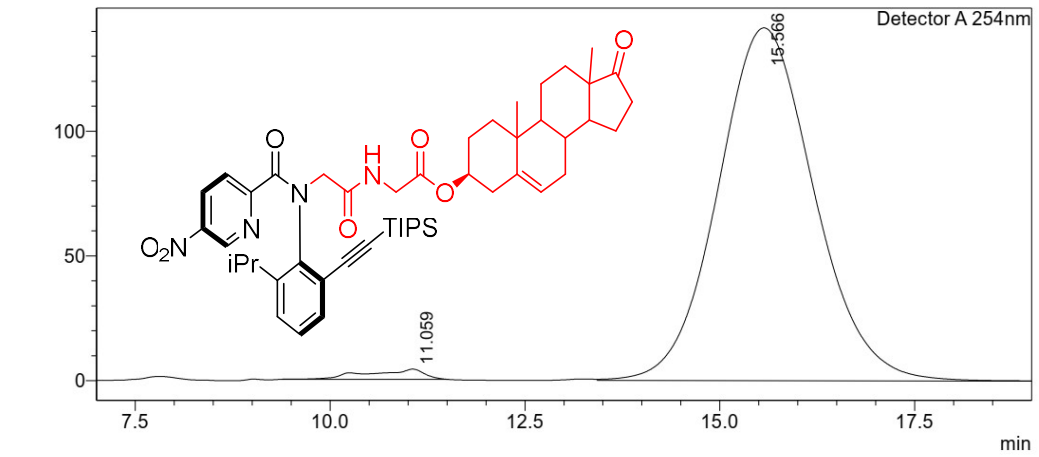


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.747	5182284	71238	50.821		M	
2	15.606	5014916	58194	49.179			
Total		10197200	129432				

<Chromatogram>



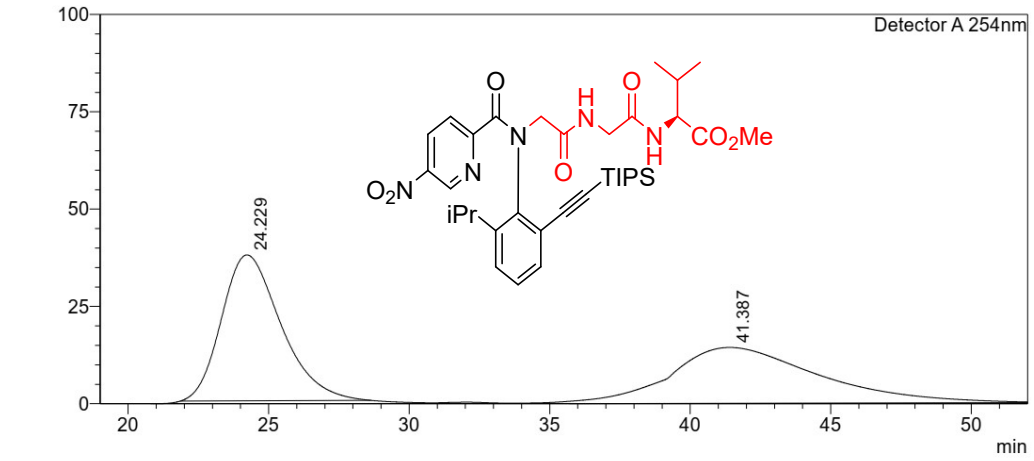
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	11.059	206985	4134	1.675		M	
2	15.566	12147668	141389	98.325			
Total		12354654	145523				

5f: OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, 254 nm

<Chromatogram>

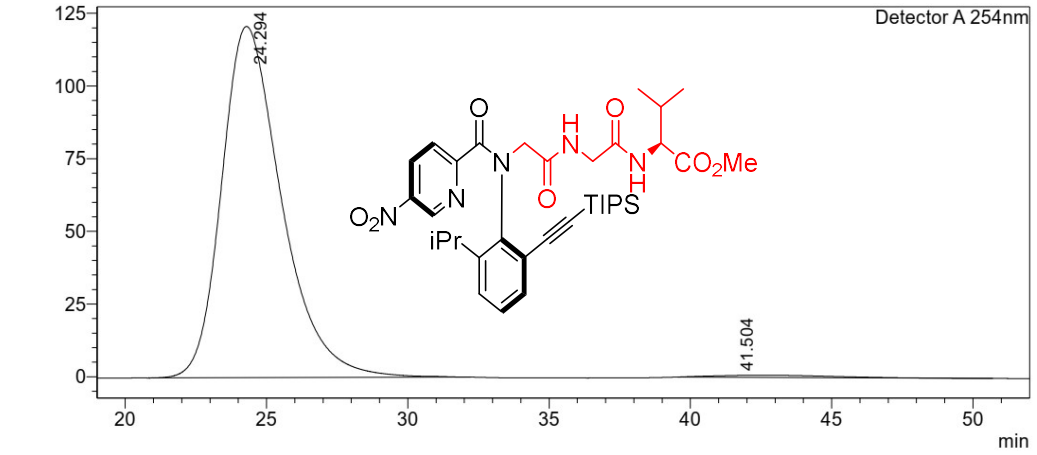


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	24.229	5523831	37500	50.441		M	
2	41.387	5427226	14386	49.559		M	
Total		10951056	51886				

<Chromatogram>



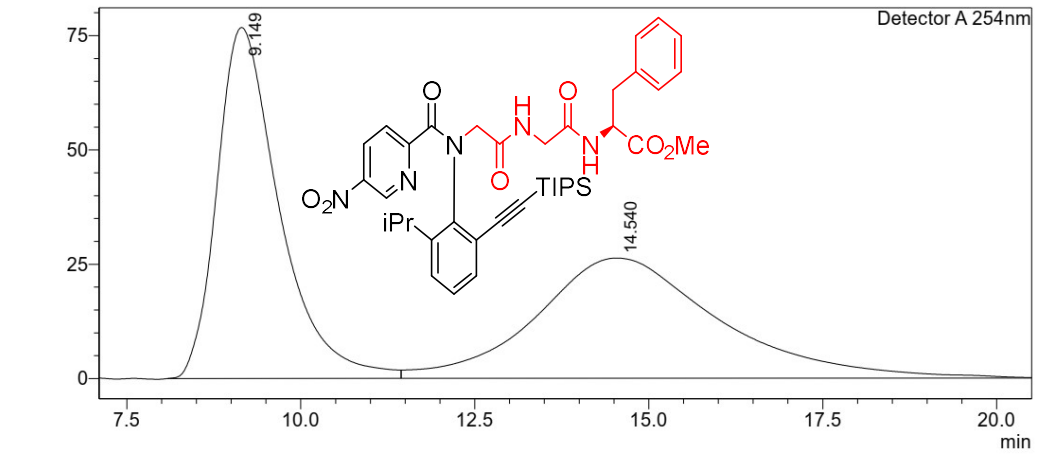
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	24.294	17846584	120801	98.757		M	
2	41.504	224711	618	1.243		M	
Total		18071295	121419				

5g: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254 nm

<Chromatogram>

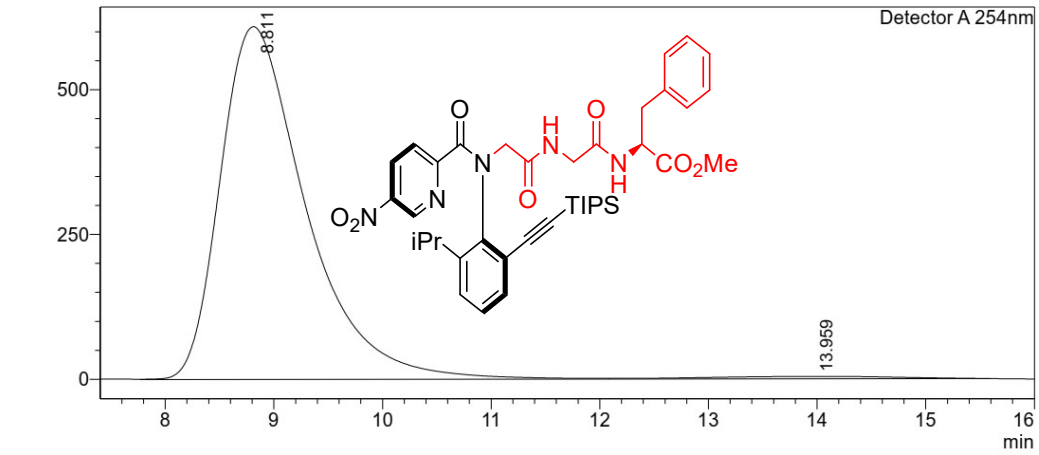


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.149	4778837	76760	49.827		M	
2	14.540	4812068	26286	50.173		V M	
Total		9590904	103046				

<Chromatogram>



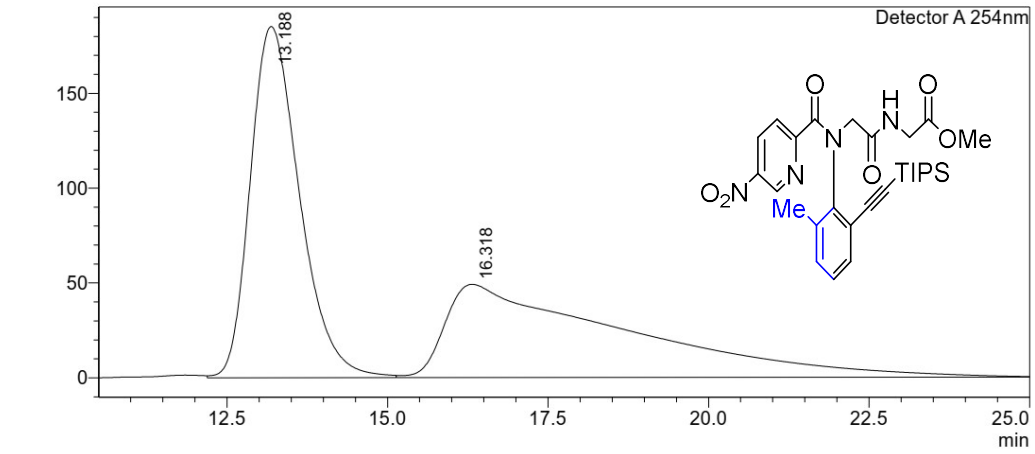
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.811	33415587	608953	98.488			
2	13.959	513068	4015	1.512		V M	
Total		33928655	612968				

5h: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

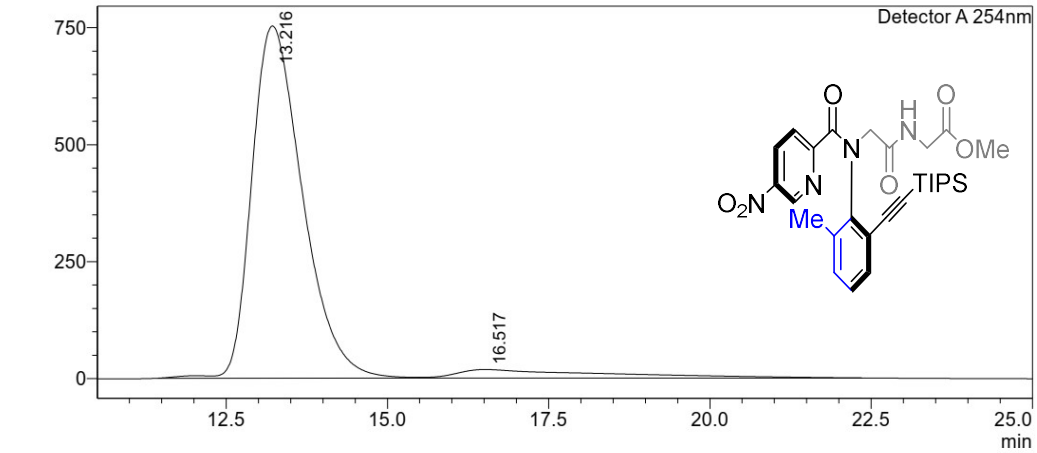


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.188	9889075	185167	50.751		M	
2	16.318	9596218	49178	49.249		V M	
Total		19485293	234344				

<Chromatogram>



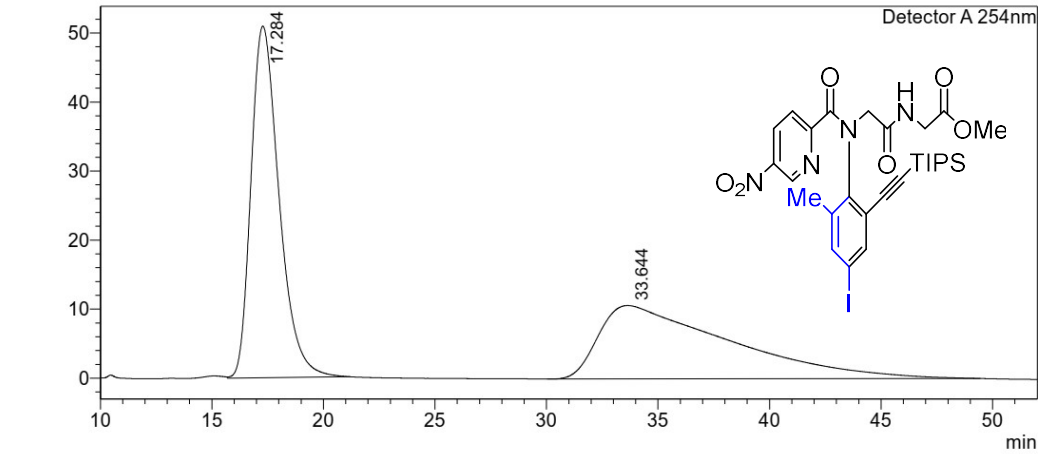
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	13.216	41190281	752920	93.260		M	
2	16.517	2976871	18361	6.740		V M	
Total		44167151	771281				

5i: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254 nm

<Chromatogram>

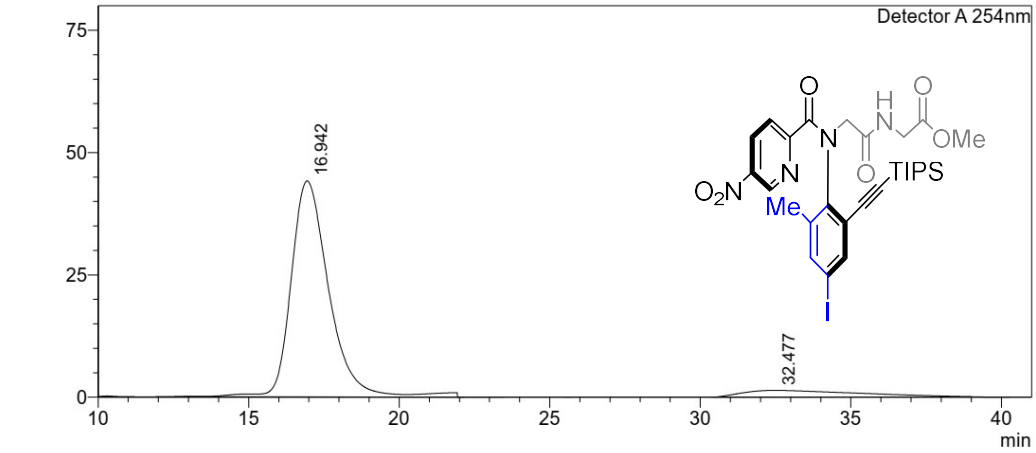


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	17.284	4460947	50938	50.776		M	
2	33.644	4324680	10629	49.224		M	
Total		8785626	61567				

<Chromatogram>



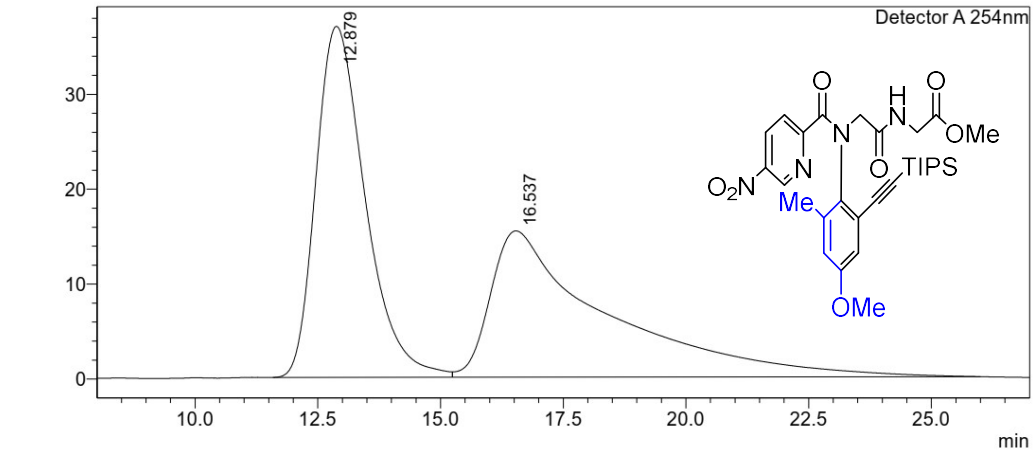
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	16.942	3878017	44147	91.344		M	
2	32.477	367512	1378	8.656		M	
Total		4245529	45525				

5j: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 1.0 mL/min, 254 nm

<Chromatogram>

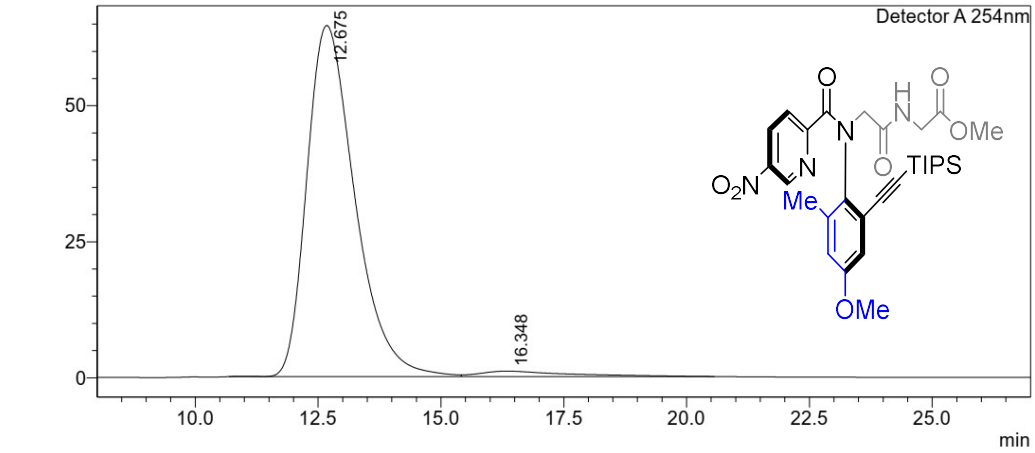


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.879	2582973	36976	50.370			
2	16.537	2545042	15413	49.630		V	
Total		5128016	52389				

<Chromatogram>



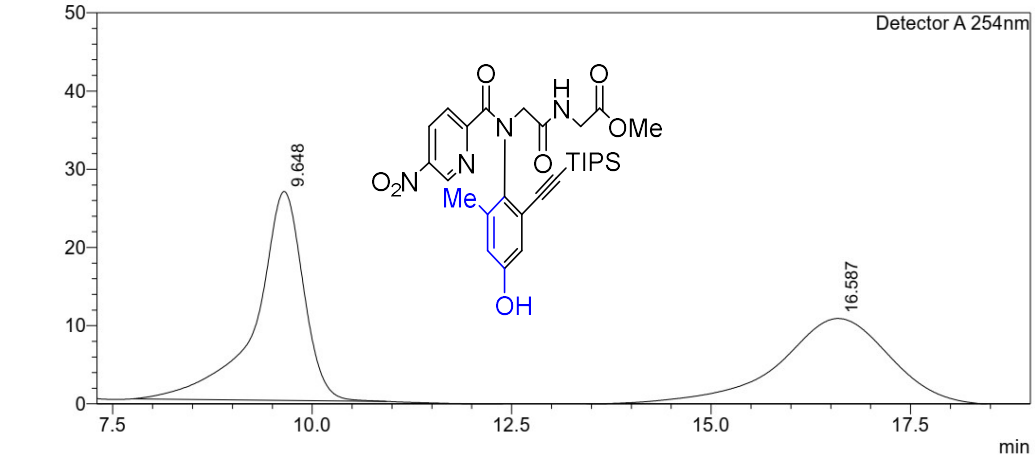
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	12.675	4386526	64532	97.162		M	
2	16.348	128118	1003	2.838		V M	
Total		4514644	65534				

5k: AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

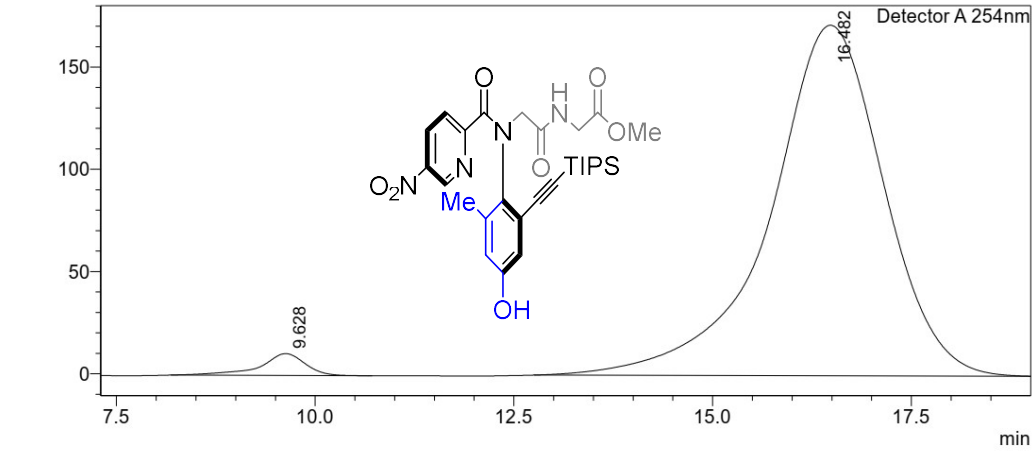


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.648	1111998	26703	50.439		M	
2	16.587	1092632	11062	49.561			
Total		2204631	37764				

<Chromatogram>



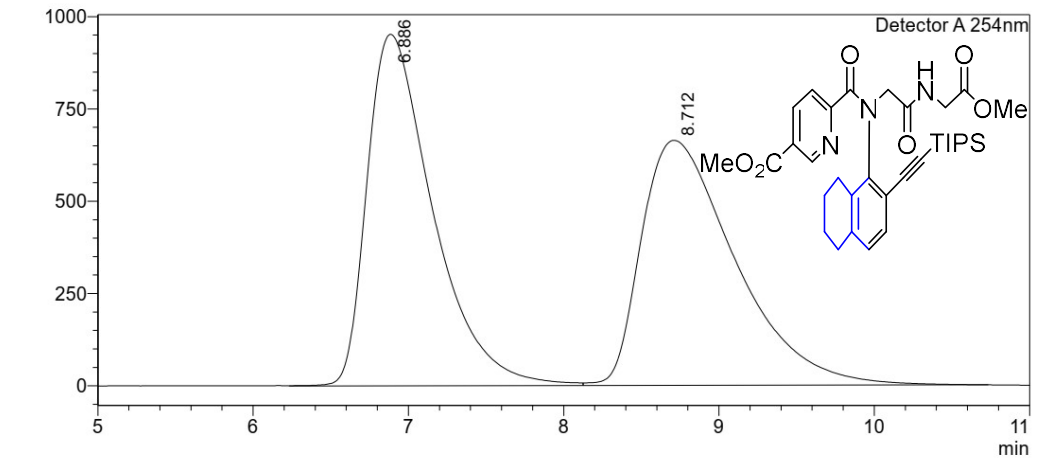
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.628	423331	10681	2.425		M	
2	16.482	17031794	171501	97.575		M	
Total		17455125	182182				

5l: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

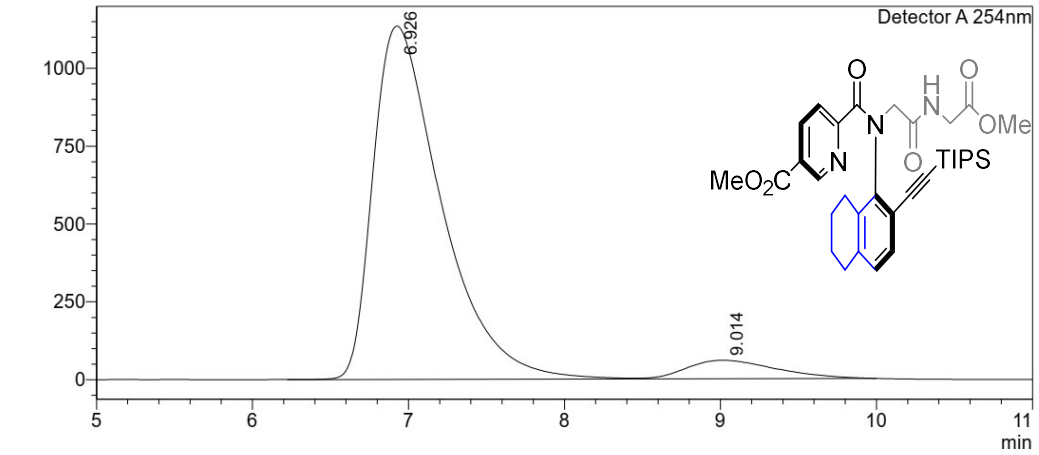


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.886	28005533	952042	50.080			
2	8.712	27916549	663761	49.920		V M	
Total		55922082	1615804				

<Chromatogram>



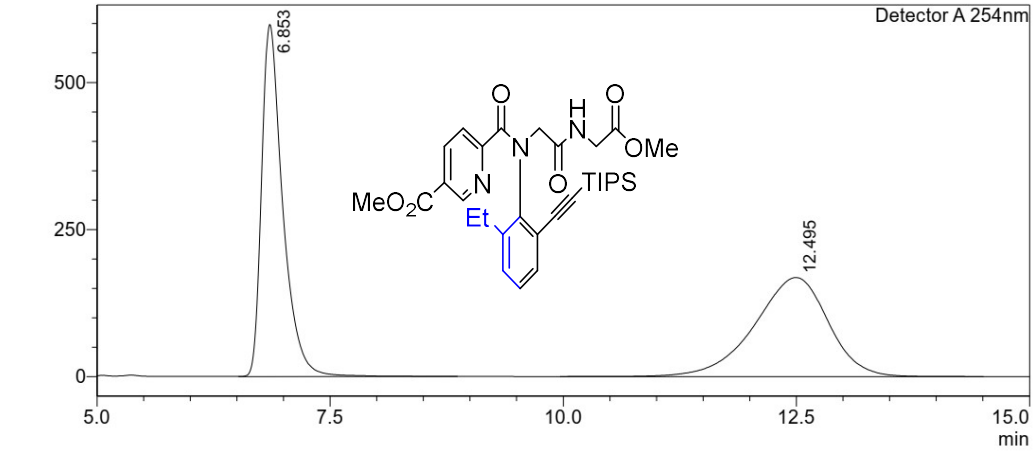
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.926	34663841	1134875	93.587			
2	9.014	2375508	59494	6.413		V M	
Total		37039349	1194369				

5m: AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

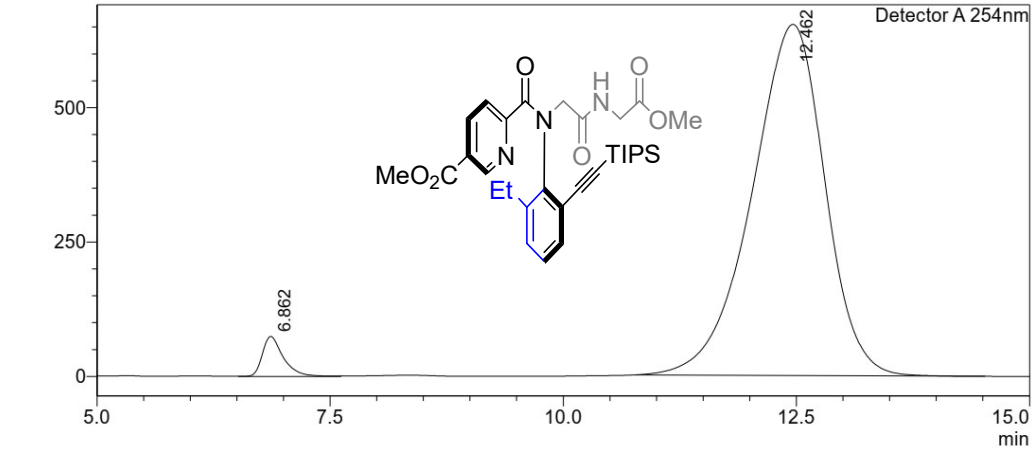


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.853	9424931	598239	50.321		M	
2	12.495	9304737	168259	49.679			
Total		18729669	766498				

<Chromatogram>



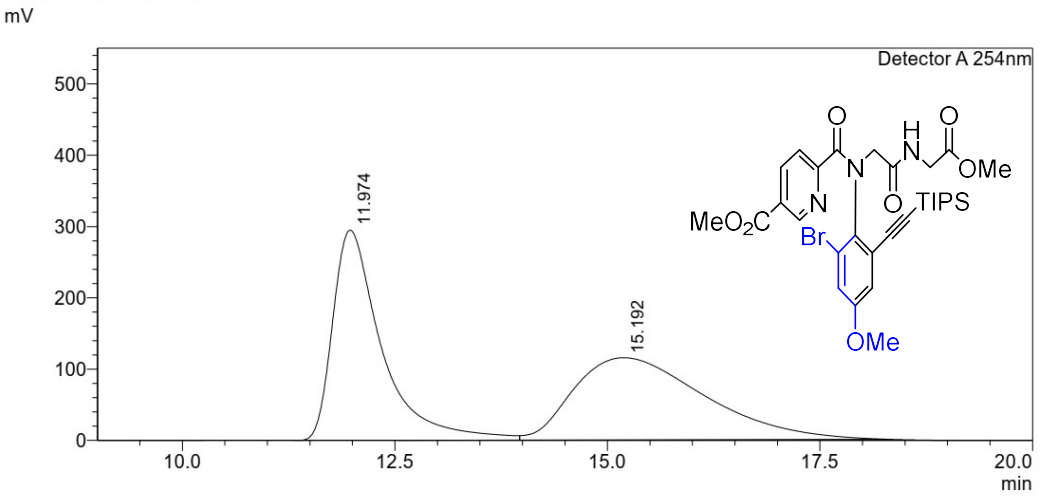
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.862	1155627	74178	3.151			
2	12.462	35518463	653108	96.849		M	
Total		36674090	727286				

5n: AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

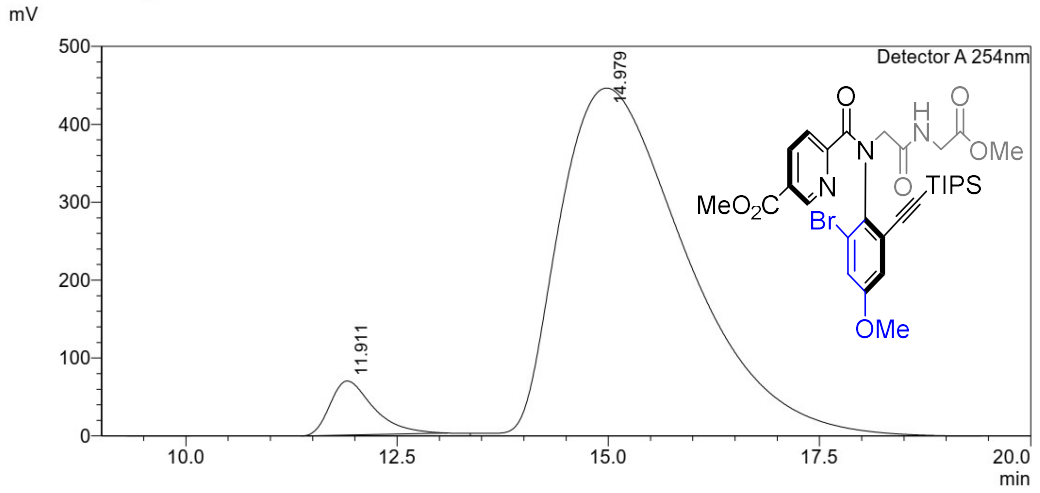


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	11.974	11888348	295069	48.973		M	
2	15.192	12387189	115235	51.027		V M	
Total		24275536	410304				

<Chromatogram>



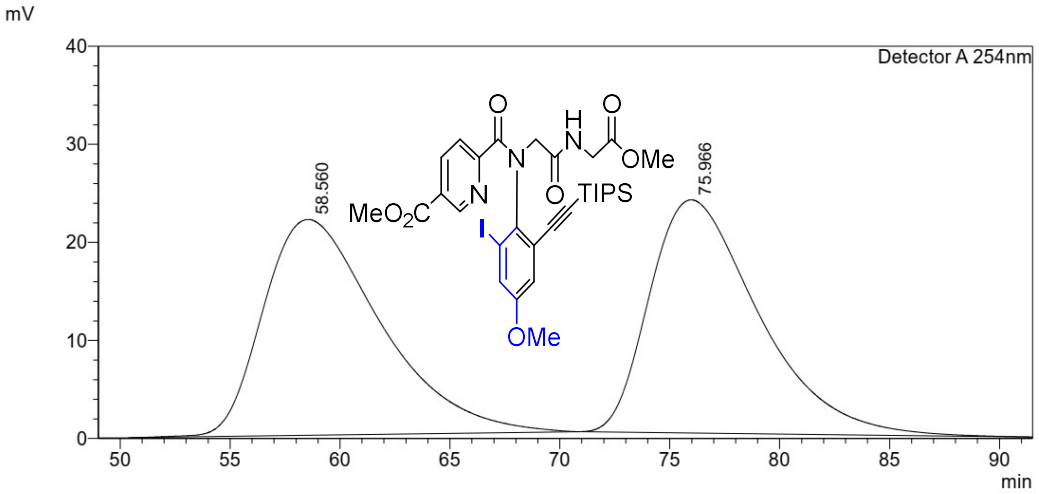
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	11.911	2509754	69695	5.068		M	
2	14.979	47007345	447261	94.932			
Total		49517099	516956				

5o: OD-H, *n*-Hexane/*i*-PrOH = 95/5, rate = 0.8 mL/min, 254 nm

<Chromatogram>

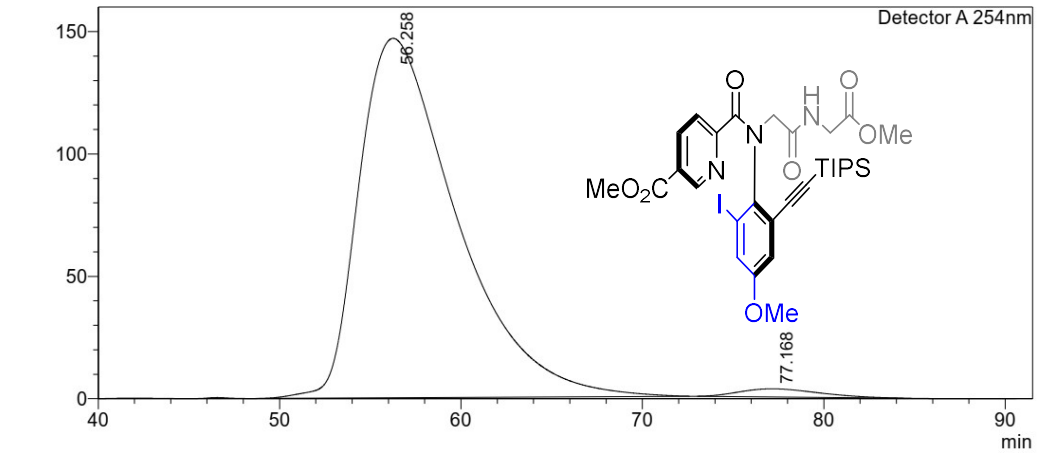


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	58.560	8178240	22016	49.833		M	
2	75.966	8233054	23769	50.167		M	
Total		16411294	45786				

<Chromatogram>



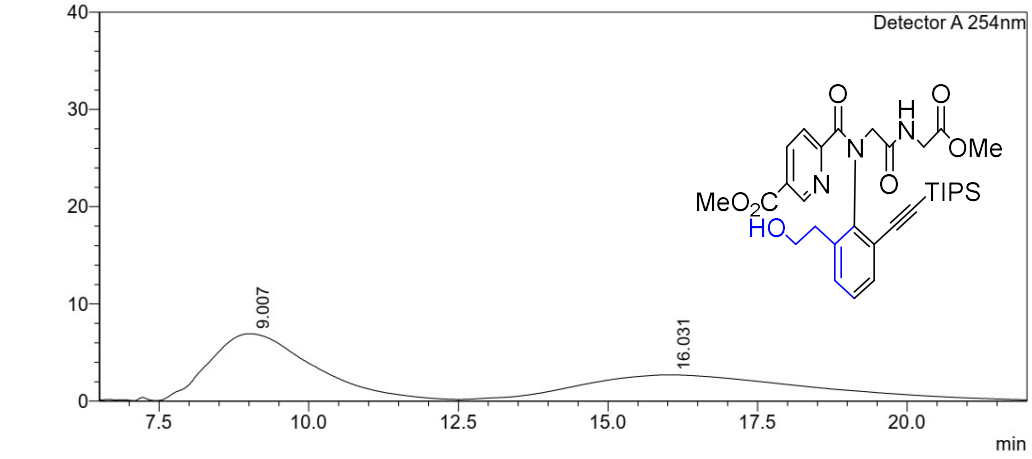
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	56.258	55080278	146846	98.209			
2	77.168	1004577	3308	1.791		M	
Total		56084856	150154				

5p: AS-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

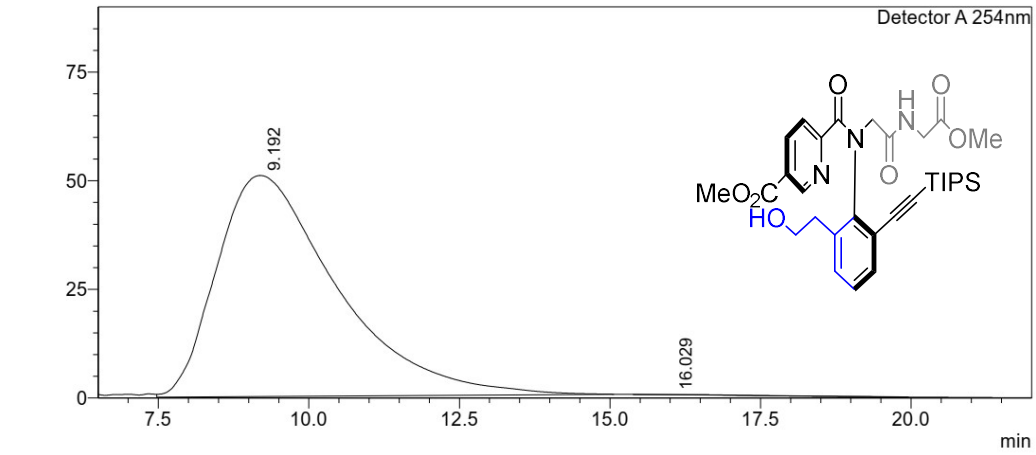


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.007	884493	7024	50.802			
2	16.031	856566	2852	49.198		V M	
Total		1741059	9876				

<Chromatogram>



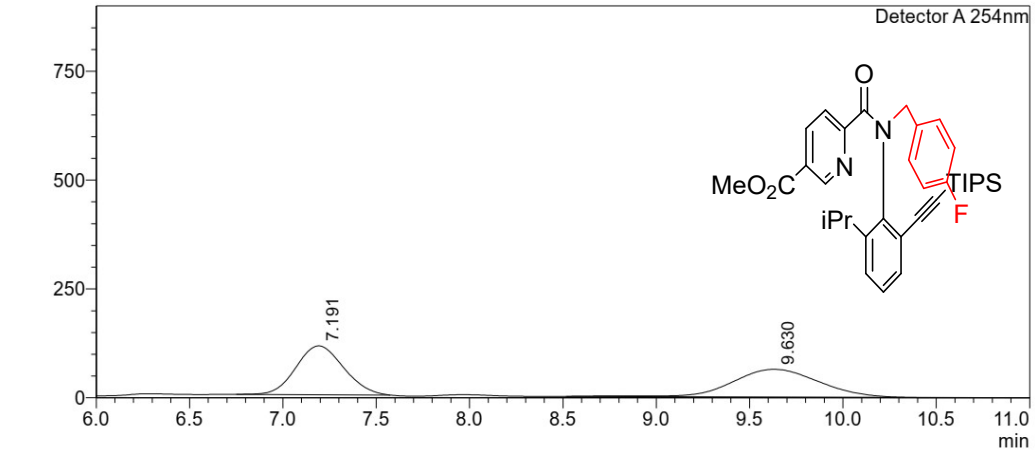
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.192	7072632	50861	99.952		M	
2	16.029	3371	46	0.048		M	
Total		7076002	50907				

5q: AD-H, *n*-Hexane/*i*-PrOH = 90/10, rate = 0.8 mL/min, 254nm

<Chromatogram>

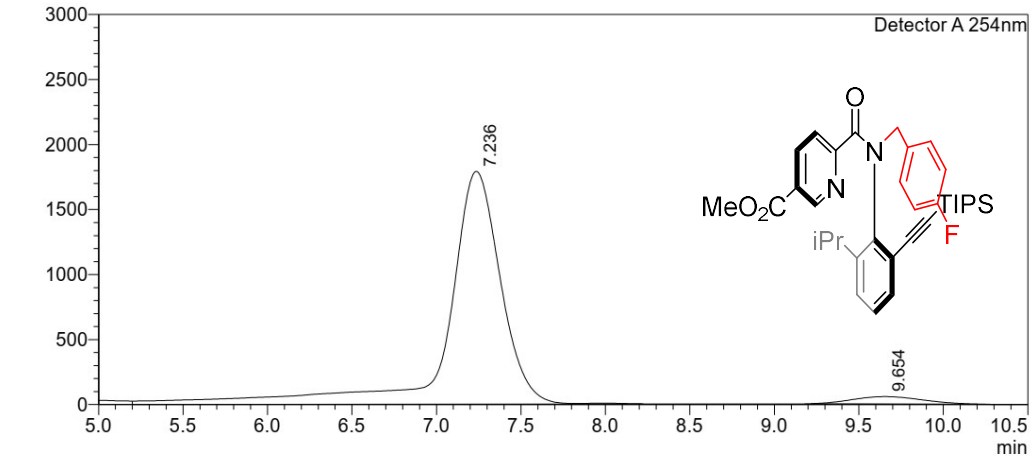


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.191	1995187	112176	49.655		M	
2	9.630	2022930	63511	50.345		M	
Total		4018117	175687				

<Chromatogram>



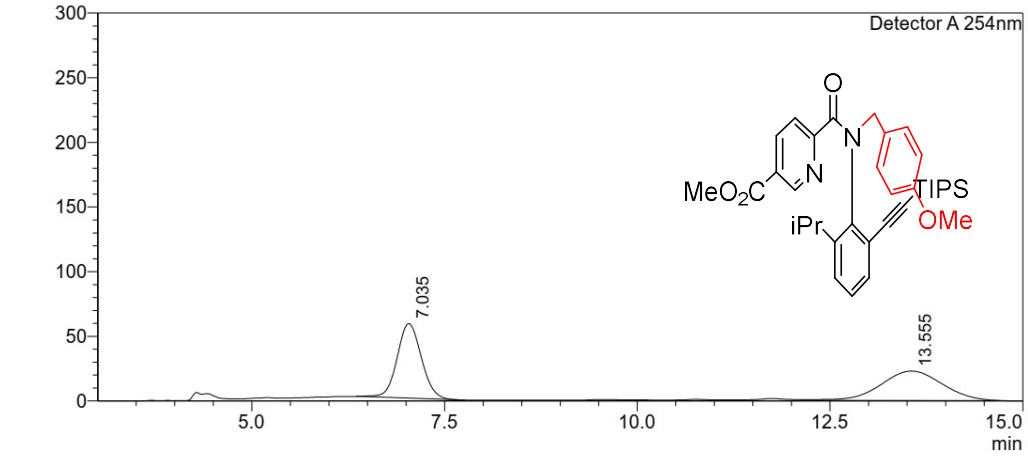
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.236	40027475	1790204	96.102		M	
2	9.654	1623423	56359	3.898		M	
Total		41650898	1846563				

5r: AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

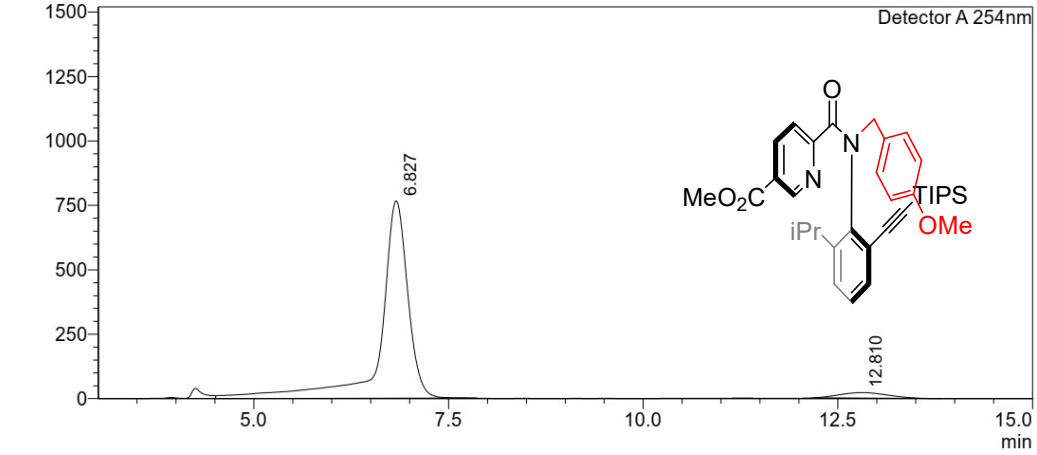


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	7.035	1263608	57692	49.908		M	
2	13.555	1268281	22753	50.092		M	
Total		2531889	80445				

<Chromatogram>



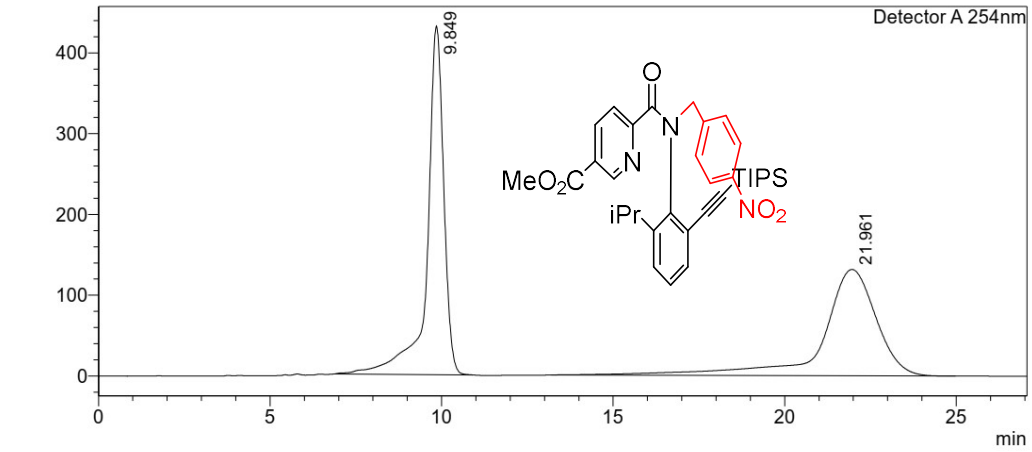
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.827	19180714	766185	95.407		M	
2	12.810	923475	21428	4.593		M	
Total		20104189	787613				

5s: AD-H, *n*-Hexane/*i*-PrOH = 90/10, rate = 0.8 mL/min, 254nm

<Chromatogram>

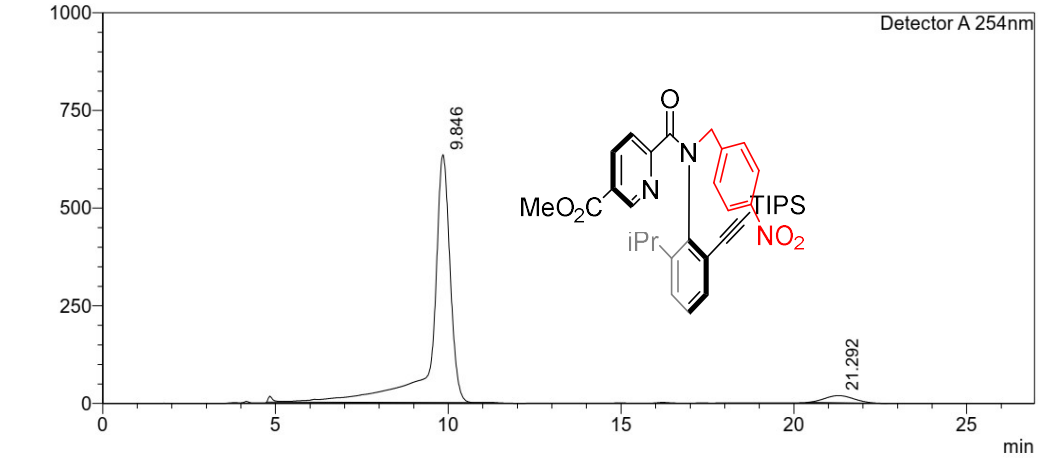


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.849	14631059	431515	50.423		M	
2	21.961	14385785	131635	49.577		M	
Total		29016844	563150				

<Chromatogram>



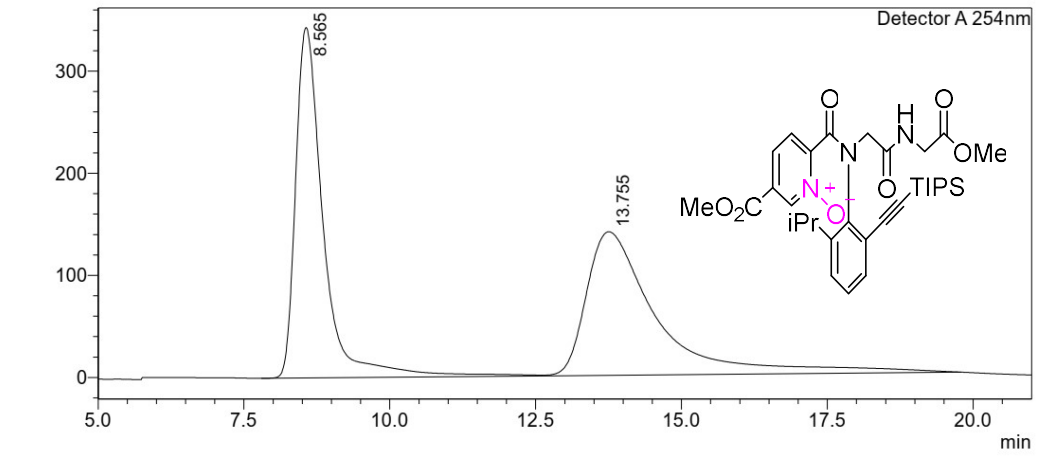
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	9.846	23146664	634254	95.593		M	
2	21.292	1067069	18300	4.407		M	
Total		24213733	652554				

3ha: OD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

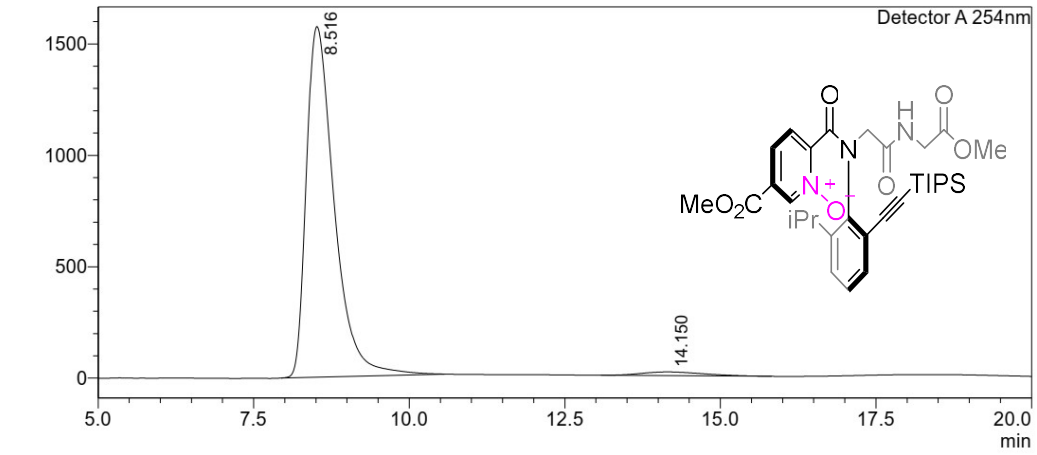


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.565	11385802	343096	49.019		M	
2	13.755	11841728	140546	50.981		V M	
Total		23227529	483642				

<Chromatogram>



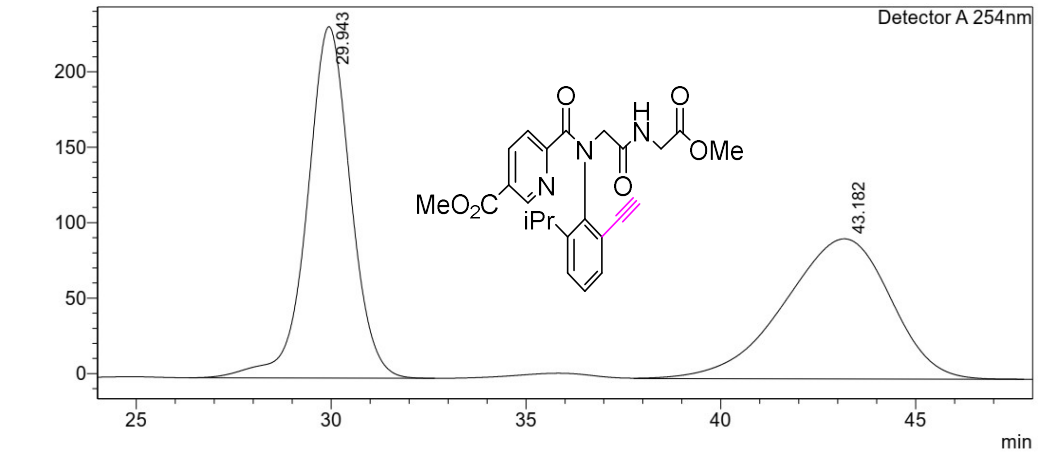
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	8.516	49110573	1573382	97.661		M	
2	14.150	1176155	16755	2.339		M	
Total		50286728	1590137				

3hb: AD-H, *n*-Hexane/*i*-PrOH = 80/20, rate = 0.8 mL/min, 254nm

<Chromatogram>

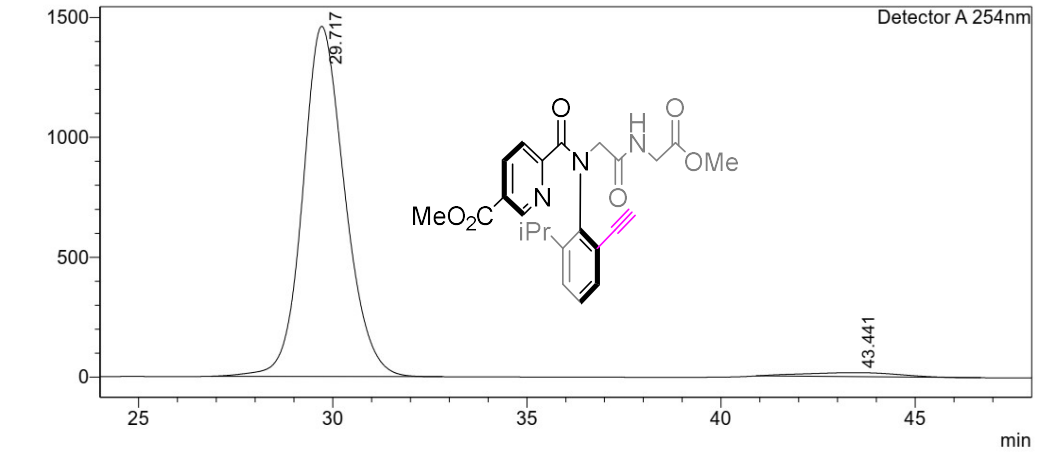


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	29.943	18057778	232900	50.490			
2	43.182	17707339	92843	49.510			
Total		35765117	325743				

<Chromatogram>



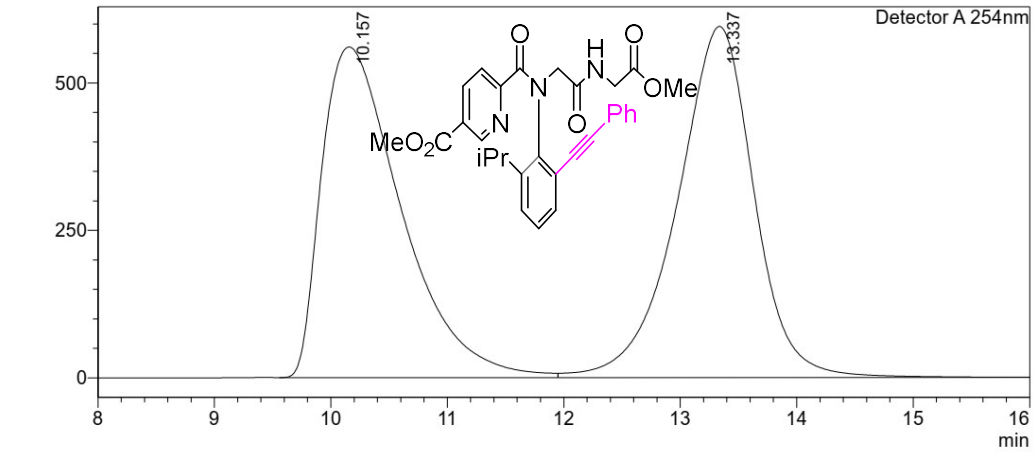
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	29.717	110299012	1460271	97.424		M	
2	43.441	2916876	17180	2.576		M	
Total		113215888	1477452				

3hc: IF-3, *n*-Hexane/*i*-PrOH = 60/40, rate = 0.6 mL/min, 254 nm

<Chromatogram>

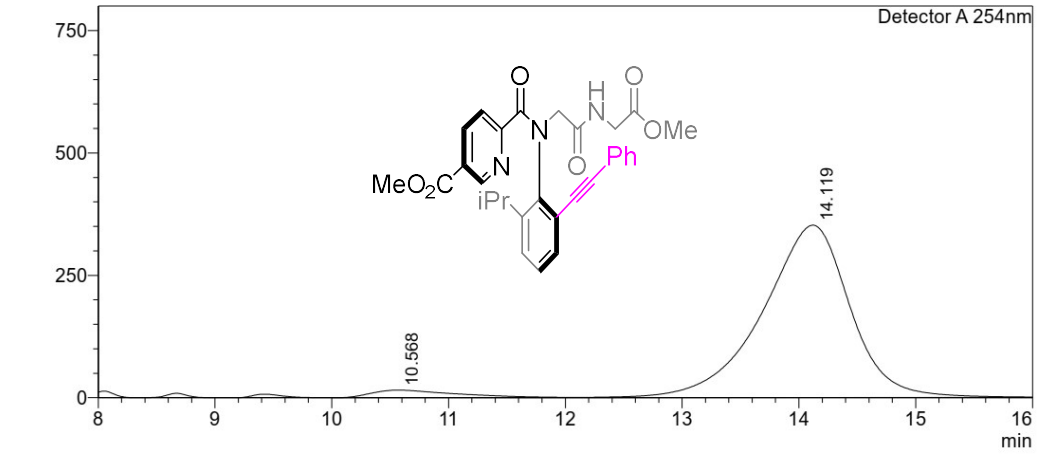


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.157	26714773	560803	49.420			
2	13.337	27342195	595455	50.580		V	
Total		54056968	1156258				

<Chromatogram>



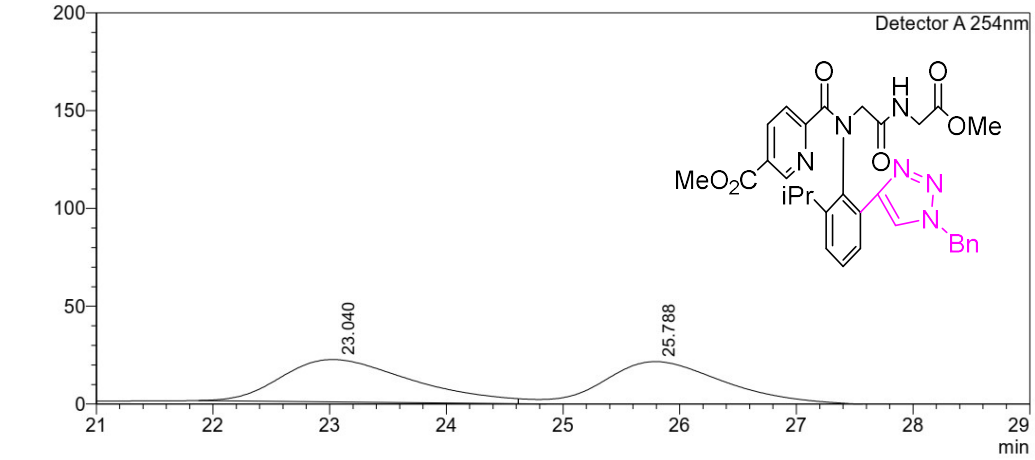
<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	10.568	825817	15828	4.269			
2	14.119	18520846	352443	95.731		V	
Total		19346663	368271				

3hd: IF-3, *n*-Hexane/*i*-PrOH = 50/50, rate = 0.8 mL/min, 254nm

<Chromatogram>

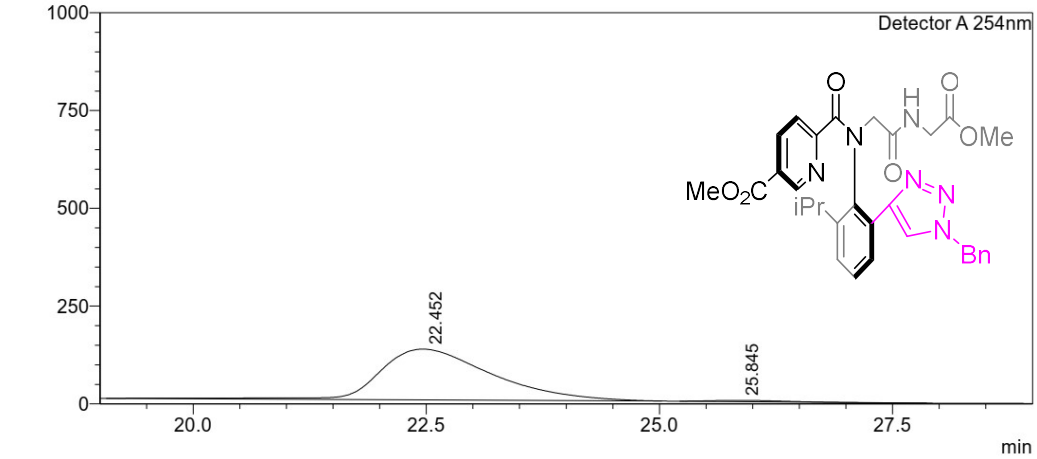


<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	23.040	1686029	21637	49.612		M	
2	25.788	1712367	22124	50.388		V M	
Total		3398396	43761				

<Chromatogram>



<Peak Table>

Detector A 254nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	22.452	10866611	129728	98.429		M	
2	25.845	173433	3259	1.571		M	
Total		11040044	132986				