Electronic Supplementary Material (ESI) for Green Chemistry.

Metal-Free Approach for Hindered Amide-Bond Formation with Hypervalent Iodine(III) Reagents: Application to Hindered Peptide Synthesis

Hyo-Jun Lee,[1,2] Xiao Huang,[1] Shigeyoshi Sakaki,[3] and Keiji Maruoka*[1,4]

[1]Laboratory of Organocatalytic Chemistry, Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, 606-8501, Japan.

[2]Current address: Department of Chemistry, Kunsan National University, Gunsan 54150, Republic of Korea.

[3]Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto 606-8103, Japan.

[4]Guangdong University of Technology, Guangzhou 510006, China.

Supplementary Information

Table of Contents

1. General Information:

^{1}H NMR spectra were measured on a JEOL JNM-FX400 (400 MHz) or a JEOL JNM-FX500 (500 MHz) spectrometer. Data were reported as follows: chemical shifts in ppm from tetramethylsilane as an internal standard, integration, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, dd = double-doublet, m =multiplet, br = broad and app = apparent), coupling constants (Hz), and assignment. ^{13}C NMR spectra were measured on a JEOL JNM-FX400 (100 MHz) or a JEOL JNM-FX500 (125 MHz) spectrometer with complete proton decoupling. Chemical shifts were reported in ppm from the residual solvent as an internal standard. High performance liquid chromatography (HPLC) was performed on Shimadzu 20A instruments using Daicel Chiralpak IA and IG 4.6 mm x 25cm columns. The high-resolution mass spectra (HRMS) were performed on Thermo Scientific EXACTIVE PLUS. For thin layer chromatography (TLC) analysis throughout this work, Merck precoated TLC plates (silica gel 60 GF254, 0.25 mm) were used. The products were purified by flash column chromatography on silica gel 60N (Kanto Chemical Co. Inc., 40-50). Acetonitrile (MeCN), THF, and dichloromethane (DCM) were purchased from Wako Pure Chemistry Co. Inc. as “Dehydrated” and used as received. $PhI(OPiv)_2$ was purchased from TCI. Py•9HF was purchased from Sigma-Aldrich. All the other chemicals were purchased and used as received.

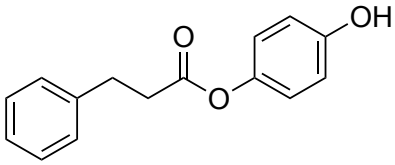
2. Preparation of Ester Substrates

2-1. General Procedures

General Procedure A: To a solution of carboxylic acid (3.0 mmol) in CH_2Cl_2 (10 mL) was added oxalyl chloride (3.5 mmol, 1.2 equiv.), two drops of DMF was then added dropwise. The resulting mixture was stirred at room temperature for 3 h and then concenterated in vacuo. The residue was dissolved in MeCN (10 mL) and treated sequentially with hydroquinone (6.0 mmol, 2 equiv.) and Et_3N (4.5 mmol, 1.5 equiv.) at 0 °C. The reaction mixture was stirred at room temperature for overnight. After quenched with water, the mixture was extracted with ethyl acetate, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel with CH_2Cl_2-ethyl acetate as eluent.

General Procedure B: To a solution of carboxylic acid (2.0 mmol) in CH_2Cl_2 (10 mL) was added 4-((*tert*-butyldimethylsilyl)oxy)phenol (3.0 mmol, 1.5 equiv.) and *N*-(3-dimethylaminopropyl)-*N*′-ethylcarbodiimide hydrochloride (3.0 mmol, 1.5 equiv.). The resulting mixture was stirred at room temperature for 24 h and then filtered through short silica column. After washed with hexane/ethyl acetate mixture (2/1) several times, the filtrate was concentrated in vacuo. The residue was dissolved in THF (9.0 mL) and treaded with Py•9HF (1.0 mL). The mixture was stirred at room temperature for 1 h. After quenched with 1 M aqueous solution of HCl, the mixture was extracted with ethyl acetate, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel with CH_2Cl_2-ethyl acetate as eluent.

2-2. Ester Substrates



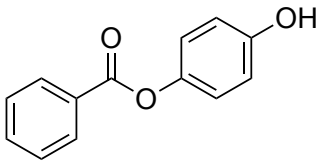
4-Hdroxylpheny 3-phenylpropanate (1a)

White solid. Prepared following general procedure A using 3-phenylpropanoic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.30 (m, 2H), 7.26-7.21 (m, 3H), 5.30 (d, *J* = 7.6 Hz, 1H), 3.06 (t, *J* = 7.6 Hz, 2H), 2.86 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 153.3, 143.9, 140.0, 128.4, 128.3, 126.4, 122.3, 116.0, 35.9, 30.9.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{14}O_3Na$: 265.0835 ($[M + Na]^+$), Found: 265.0838.



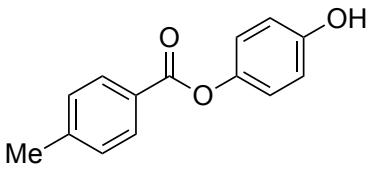
4-Hydroxyphenyl benzoate (6m)

White solid. Prepared following general procedure A using benzoic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.4 Hz, 2H), 7.62(m, 1H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.06-7.02 (m, 2H), 6.84-4.80 (m, 2H), 5.09 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 153.3, 144.3, 133.6, 130.1, 129.4, 128.5, 122.5, 116.0.

HRMS (ESI-TOF) Calcd.for $C_{13}H_{10}O_3Na$: 237.0522 ($[M + Na]^+$), Found: 237.0526.



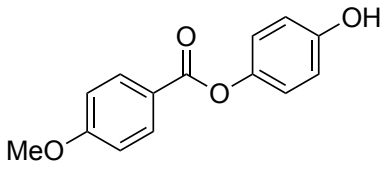
4-Hydroxyphenyl 4-methylbenzoate (6n)

White solid. Prepared following general procedure A using 4-methylbenzoic acid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.01-6.97 (m, 2H), 6.77-6.73 (m, 2H), 5.88 (s, 1H), 2.44 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 153.6, 144.5, 144.0, 130.2, 129.2, 126.5, 122.4, 116.2, 21.7.

HRMS (ESI-TOF) Calcd.for $C_{14}H_{12}O_3Na$: 251.0679 ($[M + Na]^+$), Found: 251.0681.



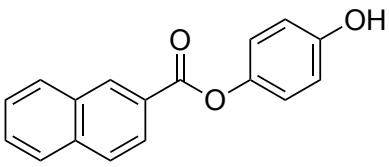
4-Hydroxyphenyl 4-methoxybenzoate (6o)

White solid. Prepared following general procedure A using 4-methoxybenzoic acid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 9.2 Hz, 2H), 7.07-7.02 (m, 2H), 6.97-6.95 (m, 2H), 6.85-6.81 (m, 2H), 4.91 (s, 1H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 163.8, 153.3, 144.3, 132.2, 122.6, 121.7, 116.1, 113.8, 55.5.

HRMS (ESI-TOF) Calcd.for $C_{14}H_{12}O_4Na$: 268.0628 ($[M + Na]^+$), Found: 267.0633.



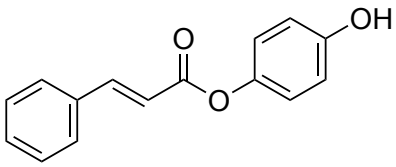
4-Hydroxyphenyl 2-naphthoate (6p)

White solid. Prepared following general procedure A using 2-naphthoic acid.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.51 (s, 1H), 8.77 (s, 1H), 8.15-8.03 (m, 1H), 8.01-7.97 (m, 3H), 7.68-7.58 (m, 2H), 7.08 (d, *J* = 8.8 Hz, 2H), 6.80 (d, *J* = 8.8 Hz, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 165.6, 155.7, 143.3, 135.8, 132.6, 131.8, 130.0, 129.4, 129.0, 128.2, 127.6, 126.9, 125.5, 123.1, 116.2.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{12}O_3Na$: 287.0679 ($[M + Na]^+$), Found: 287.0686.



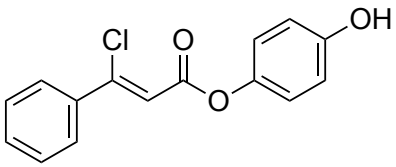
4-Hydroxyphenyl cinnamate (6q)

White solid. Prepared following general procedure A using cinnamic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 16.0 Hz, 1H), 7.58-7.55 (m, 2H), 7.42-7.40 (m, 3H), 7.01 (d, *J* = 8.8 Hz, 2H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.61 (d, *J* = 16.0 Hz, 1H), 4.89 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 153.2, 146.5, 144.2, 134.1, 130.7, 128.9, 128.2, 122.5, 117.2, 116.0.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{12}O_3Na$: 263.0679 ($[M + Na]^+$), Found: 263.0683.



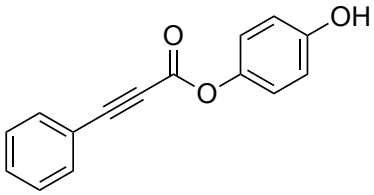
4-Hydroxyphenyl (Z)-3-chloro-3-phenylacrylate (6r)

White solid. Prepared following general procedure A using 3-phenylpropiolic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.72 (m, 2H), 7.49-7.41 (m, 3H), 7.04-7.00 (m, 2H), 6.83-6.79 (m, 2H), 6.75 (s, 1H), 4.82 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 153.3, 148.9, 143.8, 137.0, 131.0, 128.7, 127.3, 122.4, 115.9, 115.3.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{11}O_3ClNa$: 297.0289 ($[M + Na]^+$), Found: 297.0293.



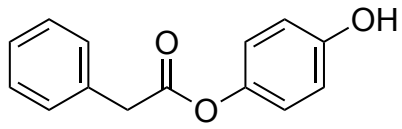
4-Hydroxyphenyl 3-phenylpropiolate (6s)

White solid. Prepared following general procedure B using 3-phenylpropiolic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, J = 7.2 Hz, 2H), 7.47 (t, J = 8.0 Hz, 1H), 7.39 (t, J = 8.0 Hz, 2H), 7.03 (d, J = 8.8 Hz, 2H), 6.81 (d, J = 8.8 Hz, 2H), 5.25 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.1, 153.3, 148.9, 143.8, 137.0, 131.0, 128.7, 127.3, 122.4, 115.9, 115.3.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{10}O_3Na$: 261.0522 ($[M + Na]^+$), Found: 261.0526.



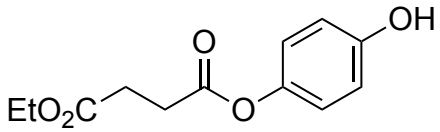
4-Hydroxyphenyl 2-phenylacetate (6t)

White solid. Prepared following general procedure A using phenylacetic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.24 (m, 5H), 6.85 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 8.4 Hz, 2H), 5.33 (s, 1H), 3.83 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 153.4, 143.9, 133.3, 129.2, 128.7, 127.3, 122.4, 115.9, 41.3.

HRMS (ESI-TOF) Calcd.for $C_{14}H_{12}O_2Na$: 251.0679 ($[M + Na]^+$), Found: 251.0681.



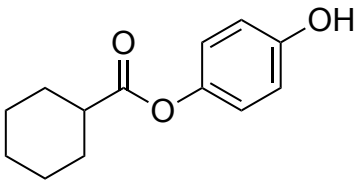
Ethyl (4-hydroxyphenyl) succinate (6u)

White solid. Prepared following general procedure A using 4-ethoxy-4-oxobutanoic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (d, *J* = 8.8 Hz, 2H), 6.71 (d, *J* = 8.8 Hz, 2H), 5.87 (s, 1H), 4.16 (1, *J* = 7.2 Hz, 2H), 2.86-2.83 (m, 2H), 2.73-2.70 (m, 2H), 1.25 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 171.8, 153.6, 143.7, 122.2, 115.9, 61.0, 29.1, 29.1, 14.1.

HRMS (ESI-TOF) Calcd.for $C_{12}H_{14}O_5Na$: 261.0733 ($[M + Na]^+$), Found: 261.0740.



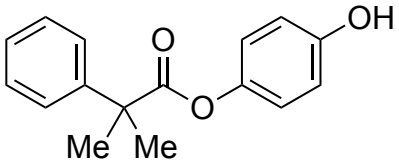
4-Hydroxyphenyl cyclohexanecarboxylate (6v)

White solid. Prepared following general procedure A using cyclohexanecarboxylic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83 (d, *J* = 8.4 Hz, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 5.91 (s, 1H), 2.57-2.48 (m, 1H), 2.05-2.01 (m, 2H), 1.82-1.78 (m, 2H), 1.69-1.65 (m, 1H), 1.60-1.51 (m, 2H), 1.39-1.21 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 153.4, 143.8, 122.2, 116.0, 43.1, 28.9, 25.6, 25.2.

HRMS (ESI-TOF) Calcd.for $C_{13}H_{16}O_3Na$: 243.0992 ($[M + Na]^+$), Found: 243.0995.



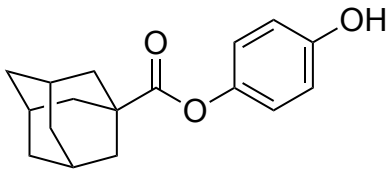
4-Hydroxyphenyl 2-methyl-2-phenylpropanoate (6w)

White solid. Prepared following general procedure A using 2-methyl-2-phenylpropanoic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.42 (m, 2H), 7.39-7.34 (m, 2H), 7.29-7.25 (m, 1H), 5.13 (brs, 1H), 1.70 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.1, 153.2, 144.3, 144.0, 128.5, 126.9, 125.5, 122.1, 115.9, 46.7, 26.3.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{16}O_3Na$: 279.0992 ($[M + Na]^+$), Found: 279.0998.



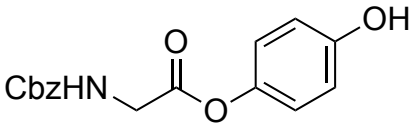
4-Hydroxyphenyl (3r,5r,7r)-adamantane-1-carboxylate (6y)

White solid. Prepared following general procedure A using 1-adamantanecarboxylic acid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83-6.80 (m, 2H), 6.70-6.67 (m, 2H), 5.59 (brs, 1H), 2.06 (s, 3H0, 2.02 (s, 6H), 1.74 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.4, 153.3, 144.1, 122.2, 116.0, 40.9, 38.6, 38.5, 36.3, 36.3, 27.8, 27.7.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{20}O_3Na$: 295.1305 ($[M + Na]^+$), Found: 295.1313.



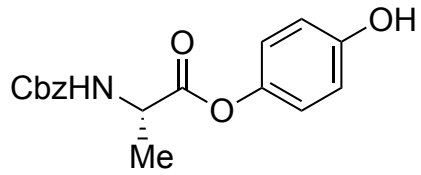
4-Hydroxyphenyl ((benzyloxy)carbonyl)glycinate (10a)

White solid. Prepared following general procedure B using *N*-Cbz-L-Ala-OH.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.31 (m, 5H), 6.95 (d, J = 9.0 Hz, 2H), 6.80 (d, J = 9.0 Hz, 2H), 5.29 (brs, 1H), 5.15 (s, 2H), 4.88 (brs, 1H), 4.22 (d, J = 5.5 Hz, 2H).

^{13}C NMR (100 MHz, CD_3OD) δ 172.3, 156.0, 154.0, 143.6, 136.0, 128.6, 128.4, 128.2, 122.1, 116.1, 67.3, 49.9, 18.5.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{15}NO_5Na$: 324.0842 ($[M + Na]^+$), Found: 324.085.



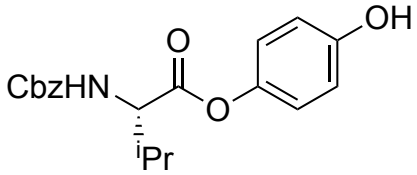
4-Hydroxyphenyl ((benzyloxy)carbonyl)-L-alaninate (10b)

White solid. Prepared following general procedure B using *N*-Cbz-L-Ala-OH.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.30 (m, 5H), 6.86 (d, *J* = 10.5 Hz, 2H), 6.74 (d, *J* = 10.5 Hz, 2H), 6.07 (s, 1H), 5.43 (d, *J* = 9.0 Hz, 1H), 5.13 (s, 2H), 4.58 (t, *J* = 9.0 Hz, 1H), 1.50 (d, *J* = 9.0 Hz, 3H).

^{13}C NMR (100 MHz, CD_3OD) δ 172.2, 155.9, 153.9, 143.5, 135.9, 128.5, 128.2, 128.1, 122.0, 116.0, 67.2, 49.8, 18.3.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{16}NO_5Na$: 338.0999 ($[M + Na]^+$), Found: 338.1006.



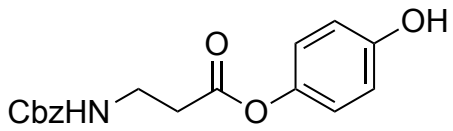
4-Hydroxyphenyl ((benzyloxy)carbonyl)-L-valinate (10c)

White solid. Prepared following general procedure B using *N*-Cbz-Val-OH.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54-7.33 (m, 5H), 6.87 (d, *J* = 10.5 Hz, 2H), 6.75 (d, *J* = 10.5 Hz, 2H), 5.92 (s, 1H), 5.38 (d, *J* = 10.5 Hz, 1H), 5.13 (s, 2H), 4.52-4.48 (m, 1H), 2.34-2.31 (m, 1H), 1.06 (d, *J* = 8.5 Hz, 3H), 0.99 (d, *J* = 8.5 Hz, 3H).

^{13}C NMR (100 MHz, CD_3OD) δ 171.3, 156.6, 154.0, 143.3, 135.8, 128.5, 128.2, 128.0, 122.0, 116.0, 67.3, 59.1, 31.1, 18.9, 17.5.

HRMS (ESI-TOF) Calcd.for $C_{19}H_{21}NO_5Na$: 366.1312 ($[M + Na]^+$), Found: 366.1330.



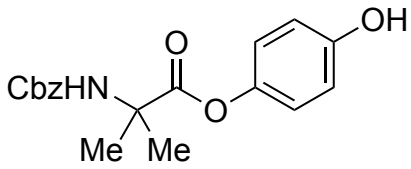
4-Hydroxyphenyl 3-(((benzyloxy)carbonyl)amino)propanoate (10e)

White solid. Prepared following general procedure B using *N*-Cbz-*β*-Ala-OH.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.28 (m, 5H), 6.91 (d, *J* = 8.8 Hz, 2H), 6.78 (d, *J* = 8.8 Hz, 2H), 5.28 (s, 1H), 5.10 (s, 2H), 4.94 (s, 1H), 3.55 (q, *J* = 6.0 Hz, 2H), 2.78 (d, *J* = 6.0 Hz, 2H).

^{13}C NMR (100 MHz, CD_3OD) δ 172.5, 158.7, 156.3, 144.6, 138.3, 129.4, 128.9, 128.7, 123.4, 116.5, 67.4, 37.7, 35.5.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{17}NO_5Na$: 338.0999 ($[M + Na]^+$), Found: 338.1004.



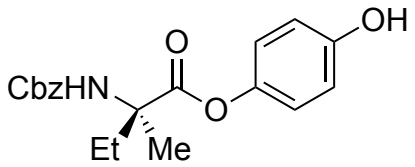
4-Hydroxyphenyl 2-(((benzyloxy)carbonyl)amino)-2-methylpropanoate (10f)

White solid. Prepared following general procedure B using *N*-Cbz-Aib-OH.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.27 (m, 5H), 6.80 (brs, 2H), 6.71 (d, *J* = 8.0 Hz, 2H), 5.85 (s, 1H), 5.37 (s, 1H), 5.11 (s, 2H), 5.13 (s, 2H), 1.64 (s, 6H).

^{13}C NMR (100 MHz, CD_3OD) δ 175.7, 157.6, 156.3, 144.9, 138.3, 129.4, 128.9, 128.7, 123.2, 116.5, 67.3, 57.2, 25.5.

HRMS (ESI-TOF) Calcd.for $C_{18}H_{19}NO_5Na$: 352.1155 ($[M + Na]^+$), Found: 352.1169.



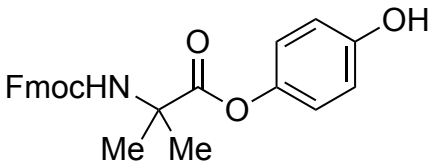
4-Hydroxyphenyl (*R*)-2-amino-2-methylbutanoate (10g)

White solid. Prepared following general procedure B using *N*-Cbz-(*R*)-α-Ethylalanine.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.27 (m, 5H), 6.79-6.70 (m, 4H), 6.47 (s, 1H), 5.59 (s, 1H), 5.11 (s, 2H), 2.22-1.93 (m, 2H), 1.67 (s, 3H), 0.95 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 155.0, 153.9, 143.6, 136.0, 128.5, 128.1, 128.0, 122.0, 116.0, 66.8, 60.3, 30.3, 22.5, 8.2.

HRMS (ESI-TOF) Calcd.for $C_{19}H_{21}NO_5Na$: 366.1312 ($[M + Na]^+$), Found: 366.1328.



4-Hydroxyphenyl 2-((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-2-methylpropanoate (10l)

White solid. Prepared following general procedure B using *N*-Fmoc-Aib-OH.

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.36 (s, 1H), 7.84 (d, *J* = 7.6 Hz, 2H), 7.67 (d, *J* = 7.6 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 2H), 7.26 (d, *J* = 7.2 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 6.69 (d, *J* = 8.8 Hz, 2H), 4.31 (d, *J* = 6.4 Hz, 2H), 4.19 (t, *J* = 7.2 Hz, 1H), 1.42 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 174.9, 155.7, 155.4, 144.2, 143.4, 141.2, 128.1, 127.5, 125.6, 122.6, 120.6, 116.0, 65.8, 55.9, 47.1, 25.4.

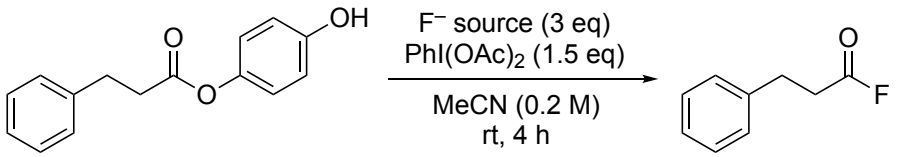
HRMS (ESI-TOF) Calcd.for $C_{25}H_{23}NO_5Na$: 440.1468 ($[M + Na]^+$), Found: 440.1485.

3. Optimization Studies of Acyl Fluoride Generation

3-1. General Procedure for Acyl Fluoride Generation

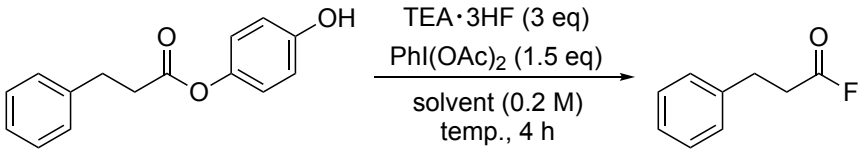
A reaction tube with magnetic stirring bar was charged with **1a** (0.10 mmol) and I(III) reagent (0.15 mmol, 1.5 equiv.) under argon atmosphere. Solvent (0.50 mL) was added at the corresponding temperature and then flouride source (0.15 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at the same temperature for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. The yield of acyl fluoride **5** was determined by ^{19}F NMR with 4,4'-difluorobenzophenone as internal standard.

3-2. Optimization of Reaction Conditions



Entry	F⁻ source	yield	Entry	F⁻ source	yield
1	TBAF (1M THF)	no TM	6	KF	no TM
2	TBAF·3H$_2$O	no TM	7	CsF	no TM
3	TMAF·4H$_2$O	no TM	8	Zn$_2$F	no TM
4	TBA·Ph3SiF	no TM	9	AgF	trace
5	NH$_4$F	no TM	10	KHF$_2$	2%
			11	TEA·3HF	33%

Table S1: Evaluation of Fluoride Source



Entry	temp.	solvent	yield	Entry	temp.	solvent	yield
1	rt	MeCN	33%	6	-10 °C	MeCN	63%
2	40 °C	MeCN	20%	7	0 °C	MeCN	67%
3	-40 °C	MeCN	19%	8	-5 °C	MeCN	68%
4	-30 °C	MeCN	41%	9	-5 °C	DMF	no TM
5	-20 °C	MeCN	56%	10	-5 °C	THF	16%
				11	-5 °C	CH_2Cl_2	43%

Table S2: Evaluation of Solvent & Temperature

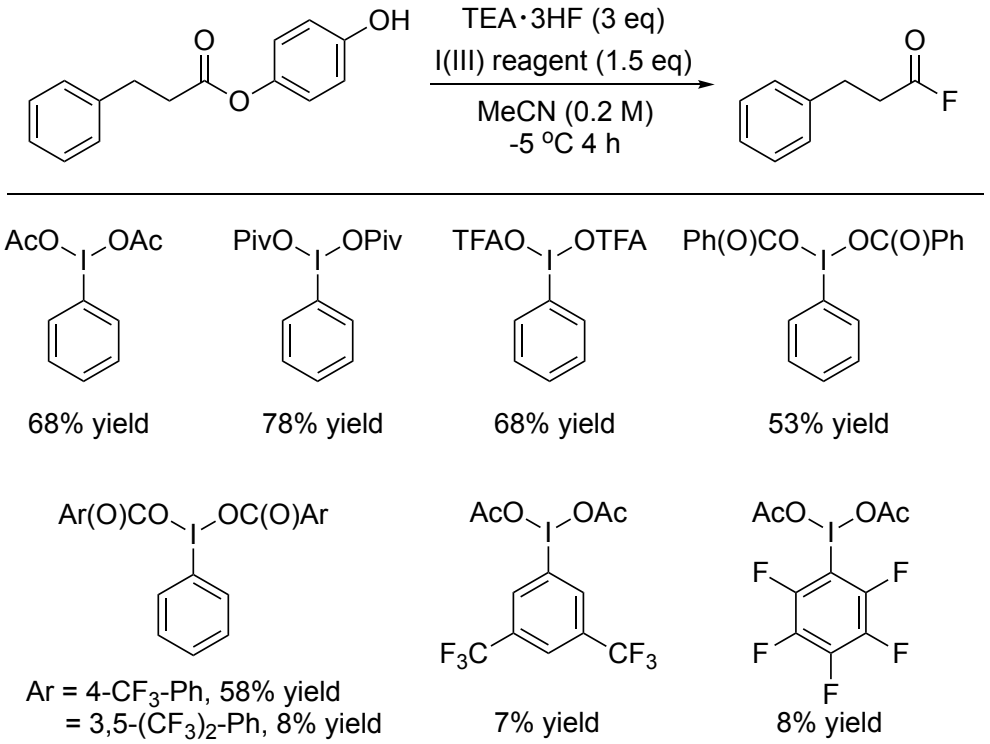
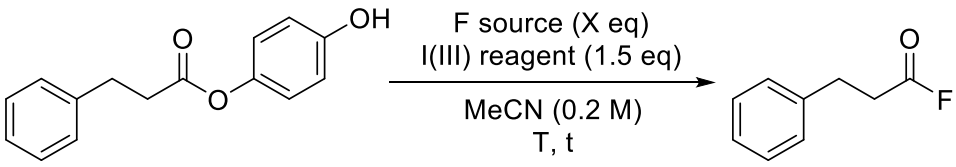


Table S3: Evaluation of Hypervalent I(III) reagent



Entry	F source	I(III) reagent	t (h)	t (°C)	yield
1	TEA•3HF (3 eq)	$PhI(OAc)_2$	4	-5	68%
1	Py•9HF (3 eq)	$PhI(OAc)_2$	4	-5	92%
2	Py•9HF (3 eq)	$PhI(OPiv)_2$	4	-5	99%
3	Py•9HF (3 eq)	$PhI(OPiv)_2$	1	-5	99%
4	Py•9HF (1.5 eq)	$PhI(OPiv)_2$	1	-5	99%
5	Py•9HF (1.5 eq)	-	1	0	no TM
6	Py•9HF (1.5 eq)	-	1	rt	no TM
7	Py•9HF (1.5 eq)	$PhI(OPiv)_2$	1	0	99%
8	Py•9HF (1.5 eq)	$PhI(OPiv)_2$	10 min	0	99%

Table S4: Further Evaluation

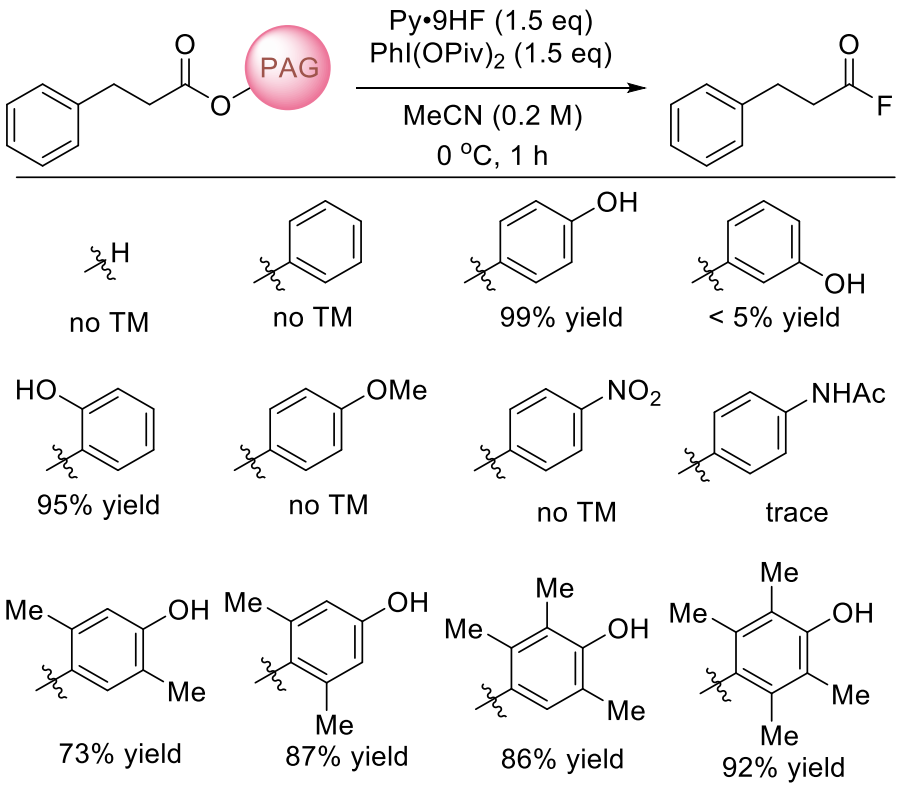
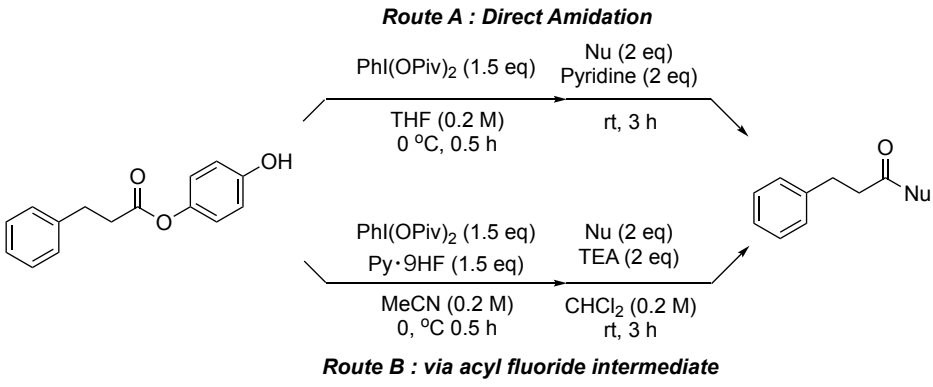


Table S5: Evaluation of PAG

4. Direct Amidation vs Amidation via Acyl Fluoride Intermediate



Route				
A	88% yield	83% yield	no TM	no TM
B	95% yield	95% yield	87% yield	88% yield

Table S5: Transformation of amides with/without a Py·9HF

5. Generation of Acyl Fluoride Intermediate

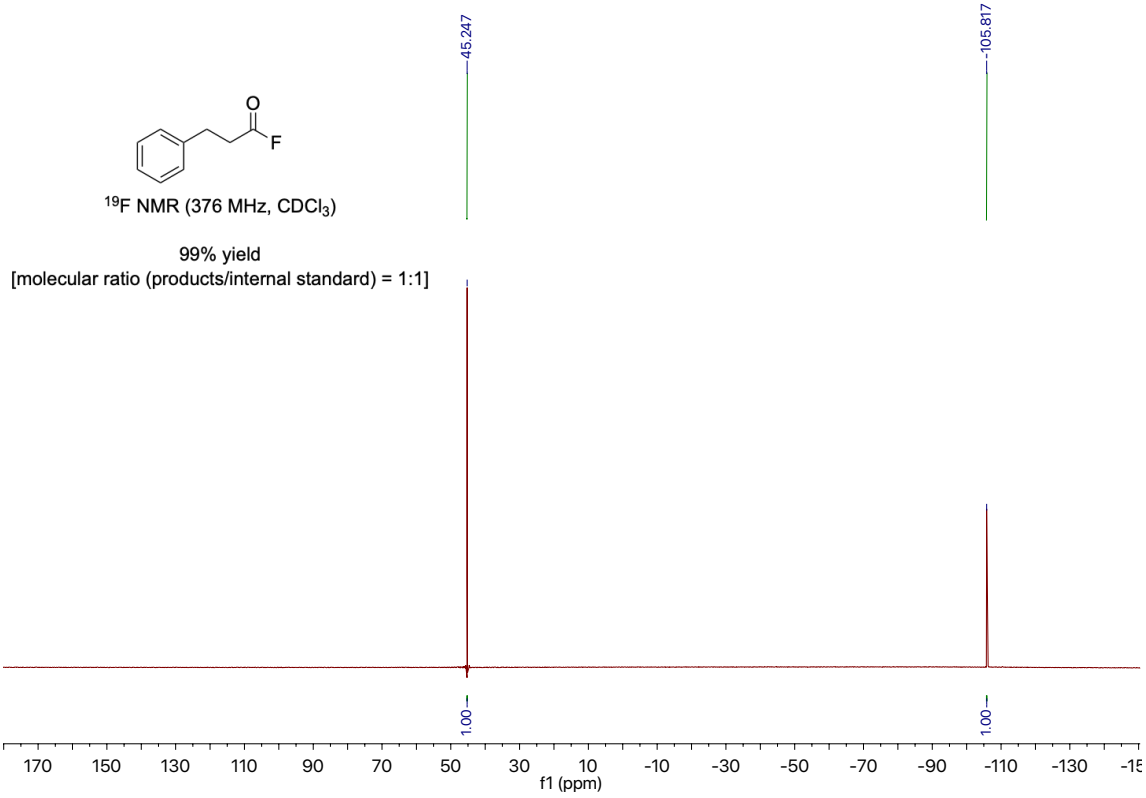
5-1. General Procedures

General Procedure C: A reaction tube with magnetic stirring bar was charged with substrate (0.10 mmol) and $PhI(OPiv)_2$ (0.15 mmol, 1.5 equiv.) under argon atmosphere. MeCN (0.50 mL) was added at 0 °C and then Py•9HF (0.15 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at 0 °C for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. The yield of acyl fluoride was determined by ^{19}F NMR with 4,4'-difluorobenzophenone as internal standard.

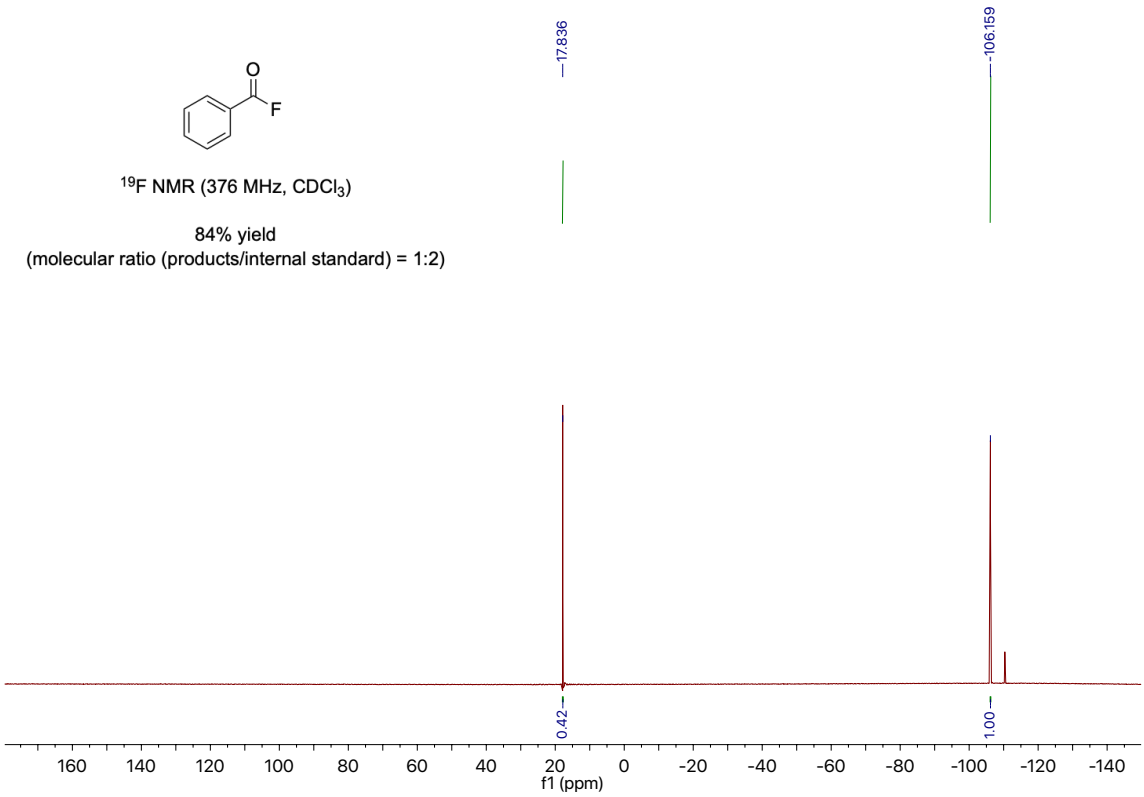
General Procedure D: A reaction tube with magnetic stirring bar was charged with substrate (0.10 mmol) and $PhI(OPiv)_2$ (0.15 mmol, 1.5 equiv.) under argon atmosphere. MeCN (2.0 mL) was added at –10 °C and then Py•9HF (0.15 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at –10 °C for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. The yield of acyl fluoride was determined by ^{19}F NMR with 4,4'-difluorobenzophenone as internal standard.

5.2 Determination of NMR Yield

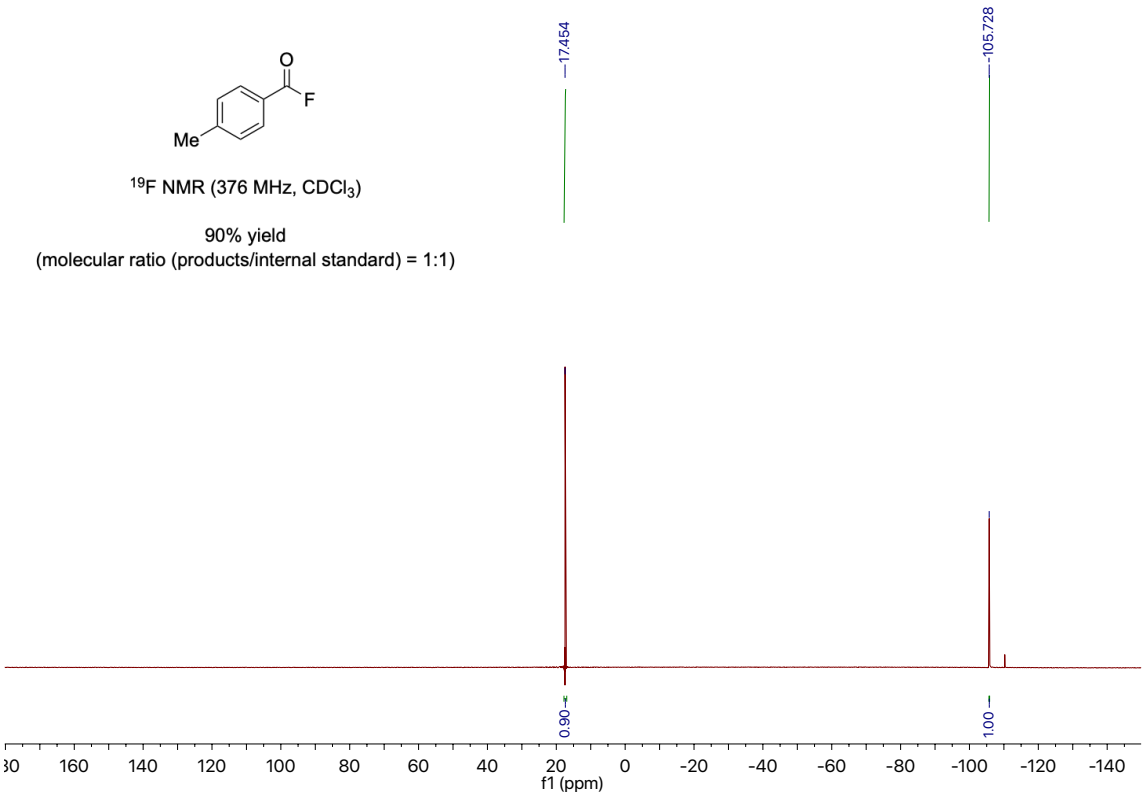
5 (Prepared by the general procedure C)



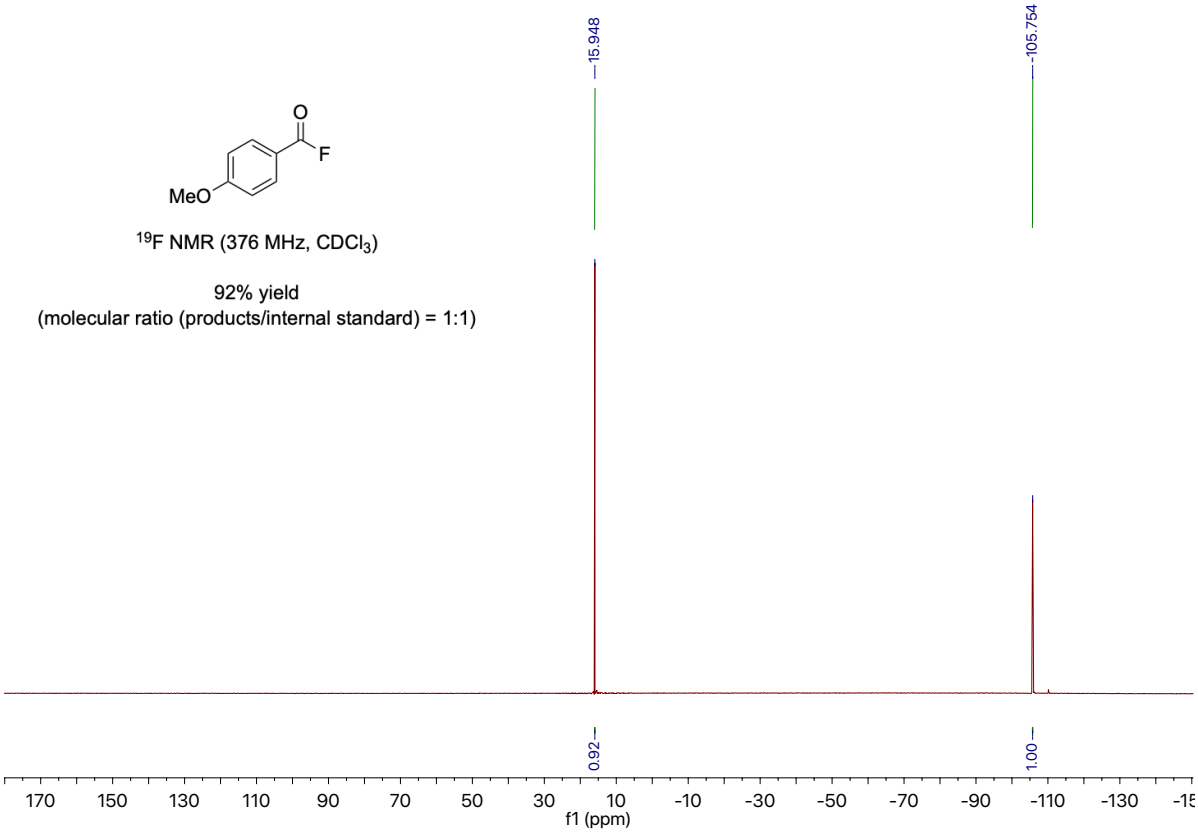
7m (Prepared by the general procedure C)



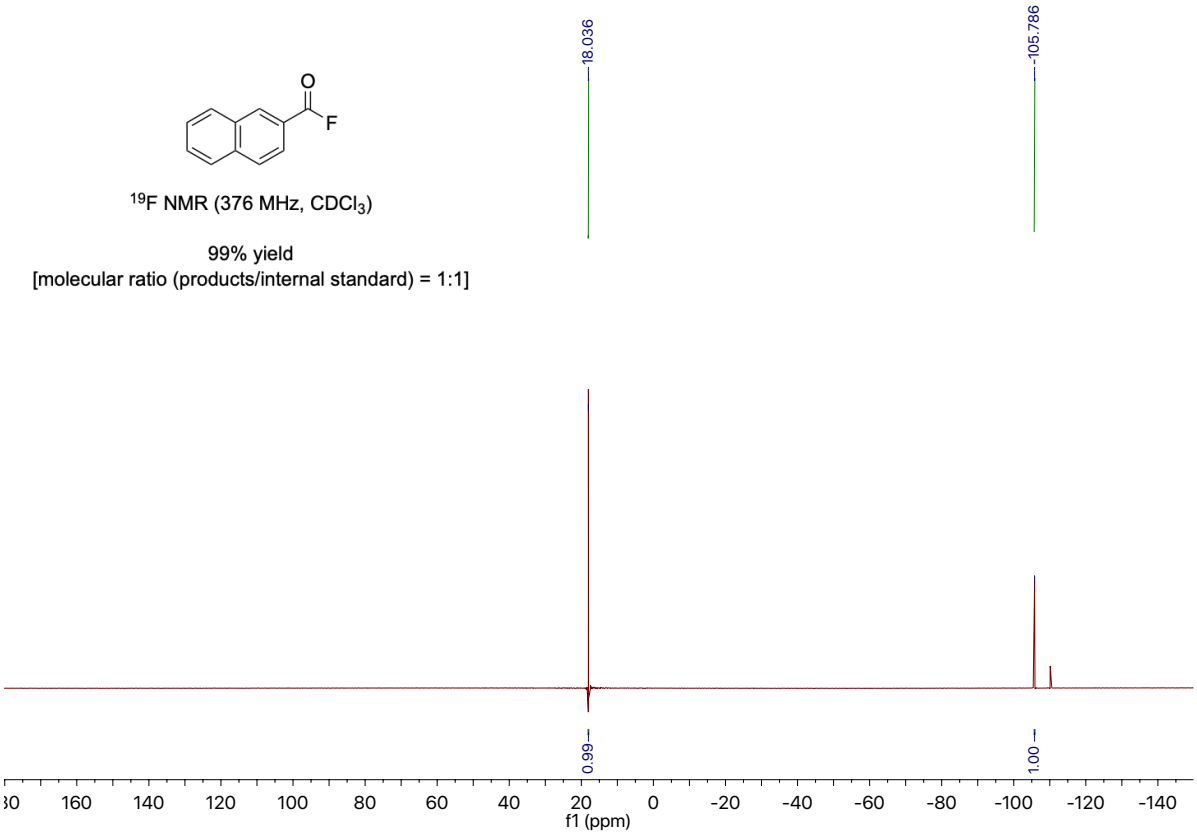
7n (Prepared by the general procedure C)



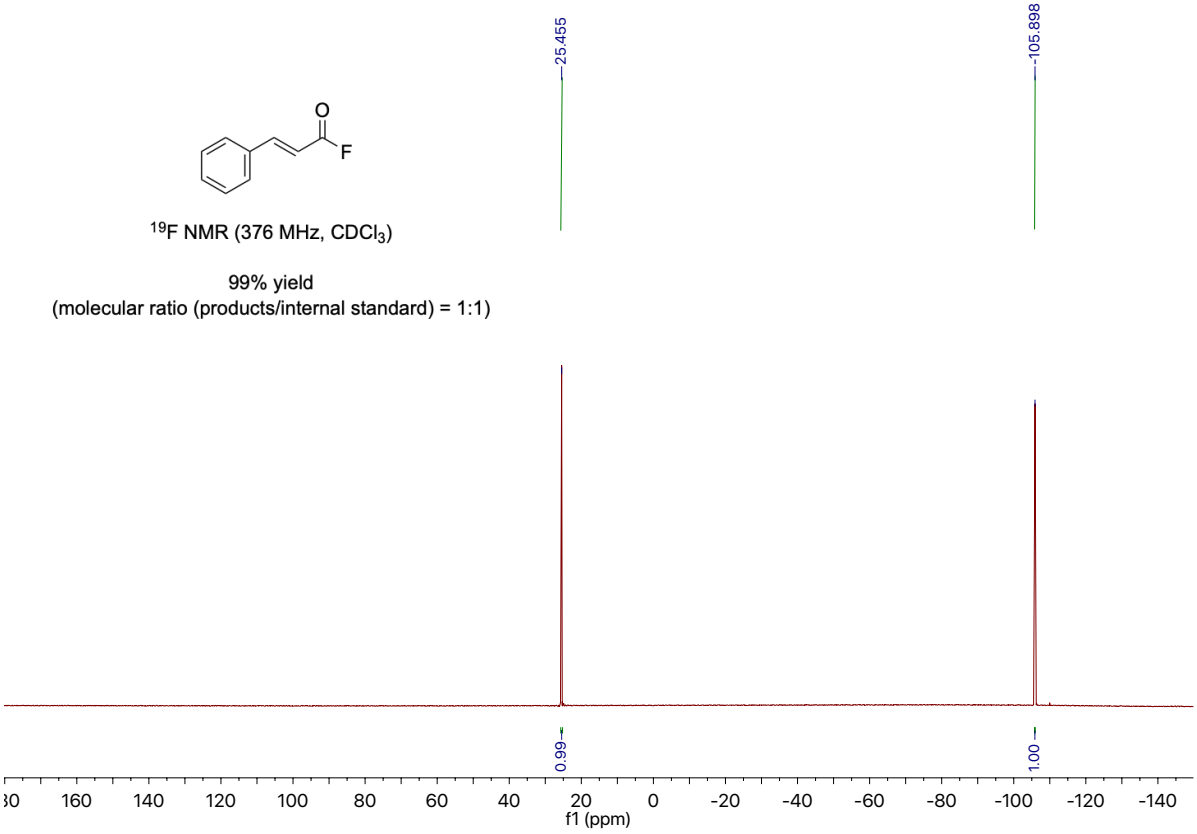
7o (Prepared by the general procedure C)



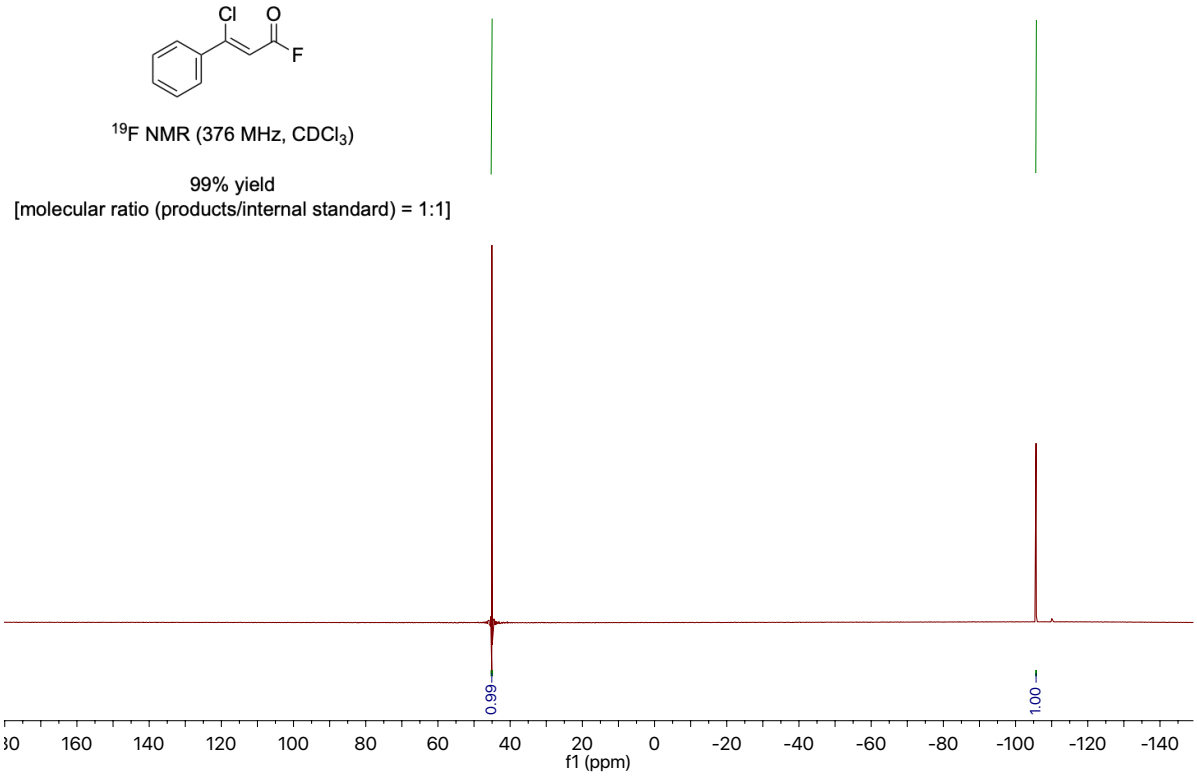
7p (Prepared by the general procedure C)



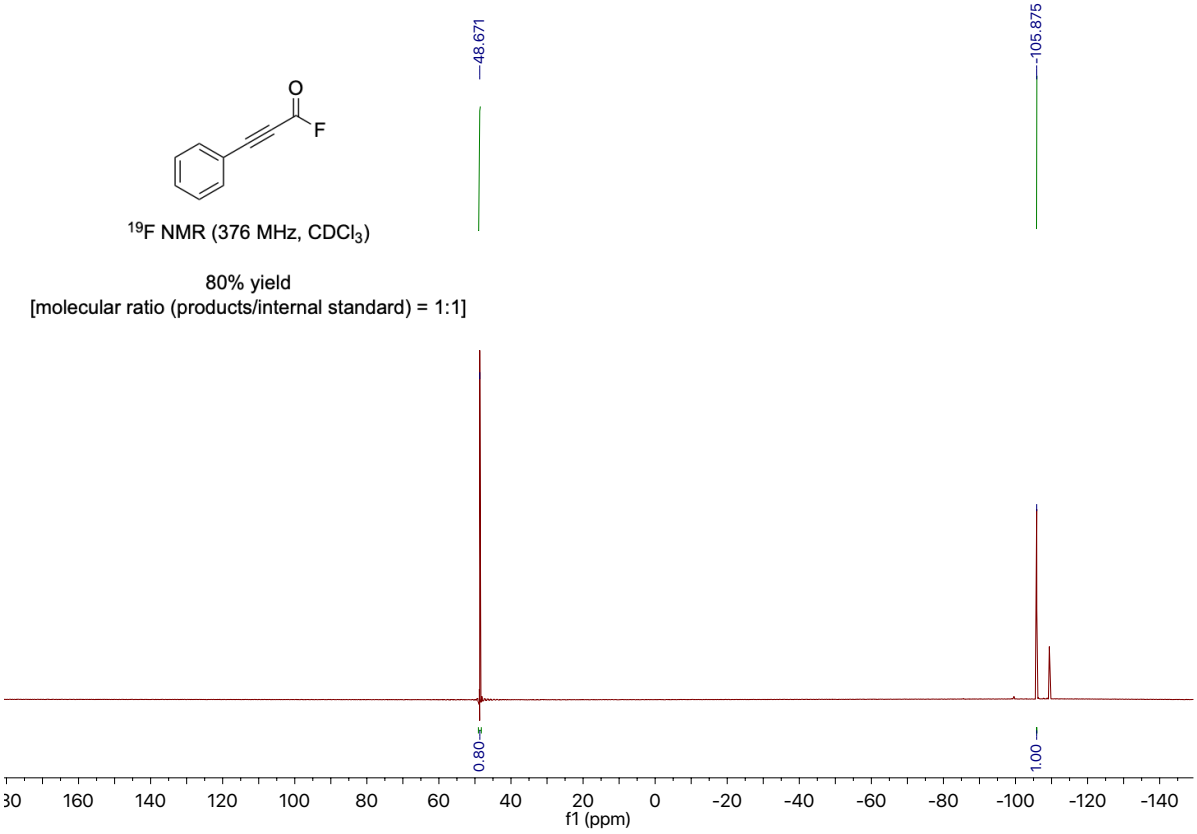
7q (Prepared by the general procedure C)



7r (Prepared by the general procedure C)



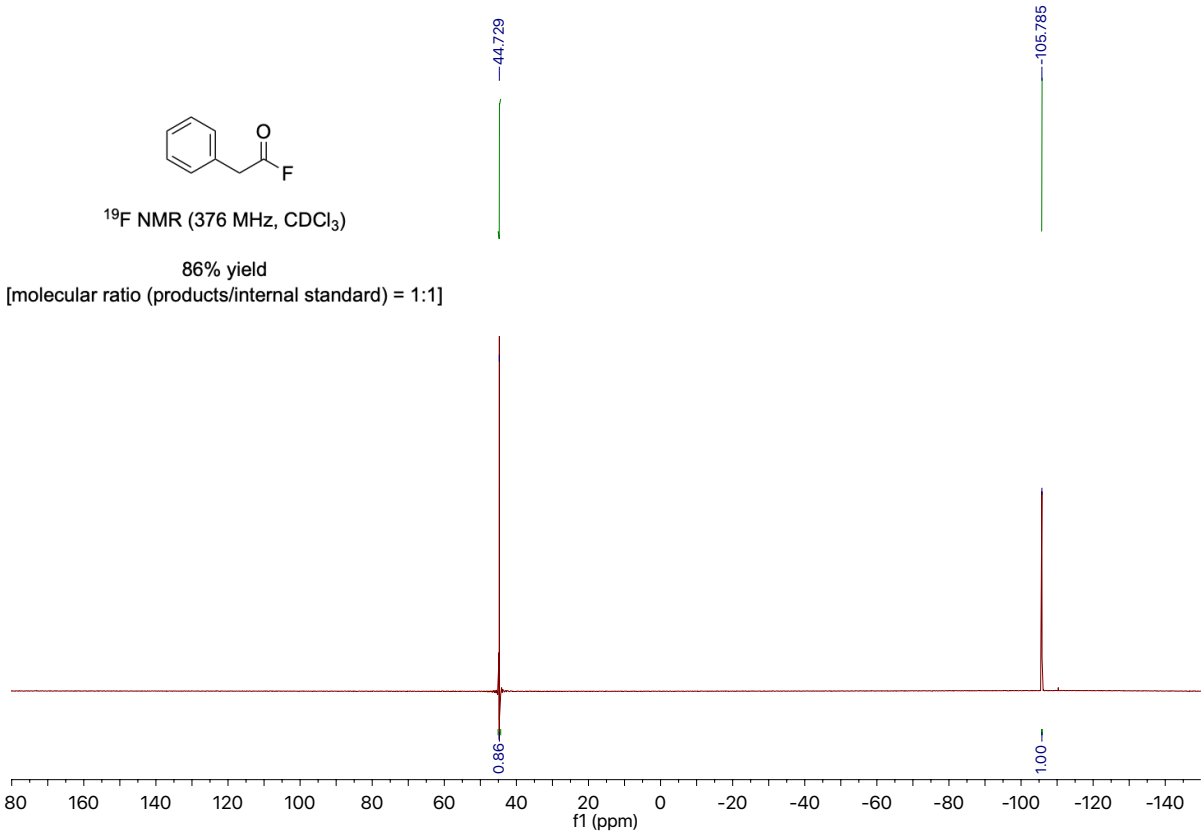
7s (Prepared by the general procedure C)



^{19}F NMR (376 MHz, $CDCl_3$)

80% yield
[molecular ratio (products/internal standard) = 1:1]

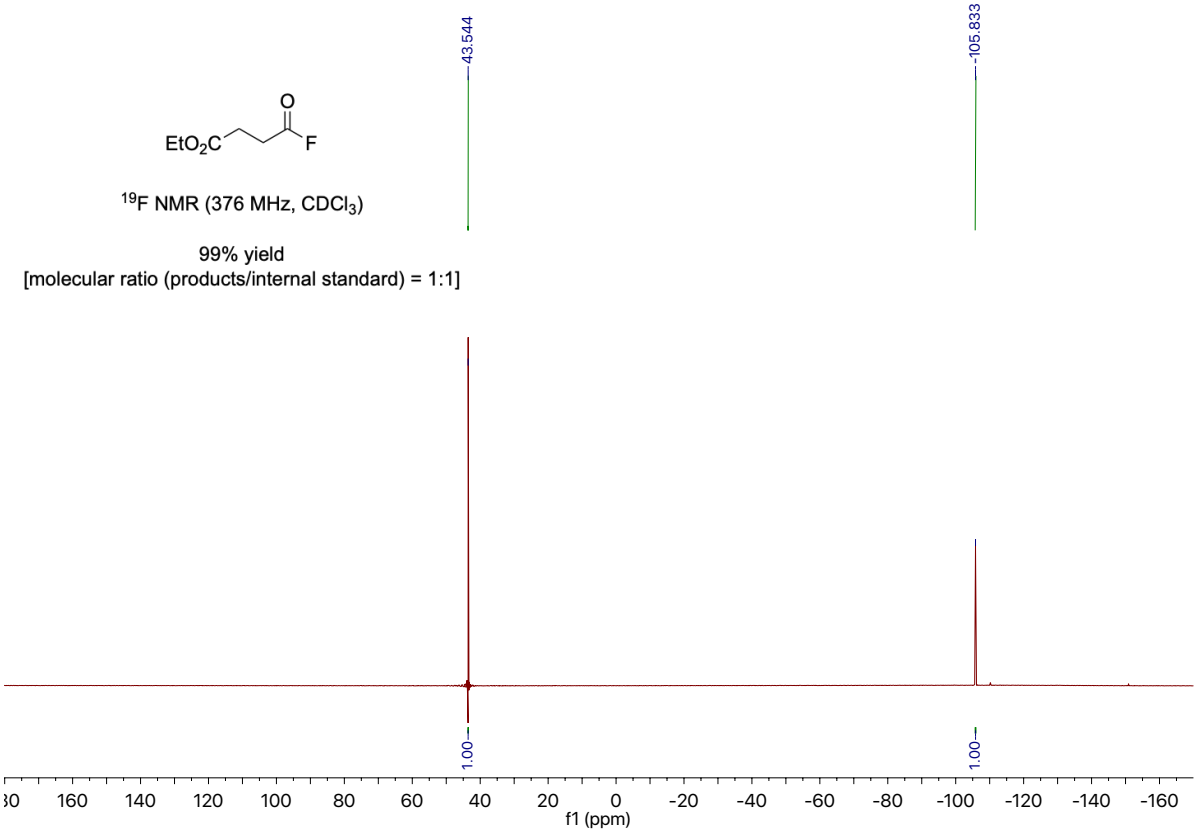
7t (Prepared by the general procedure C)



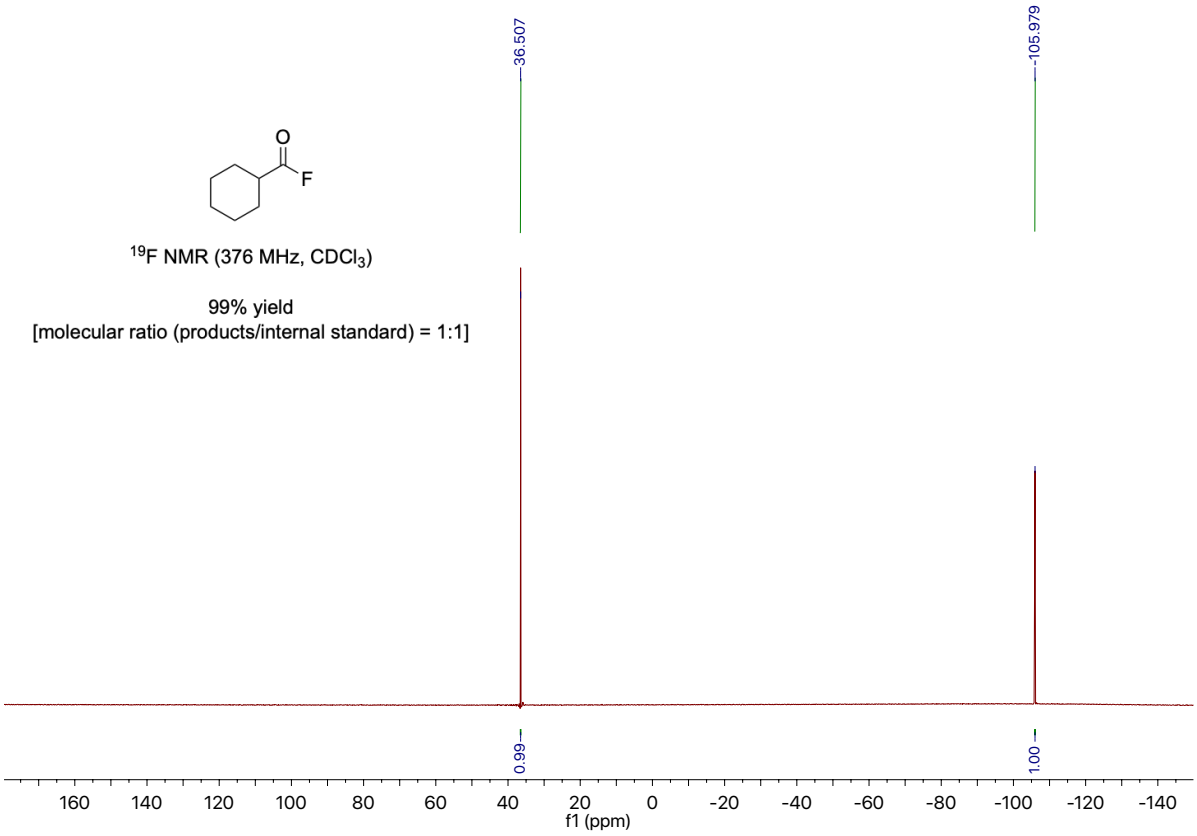
^{19}F NMR (376 MHz, $CDCl_3$)

86% yield
[molecular ratio (products/internal standard) = 1:1]

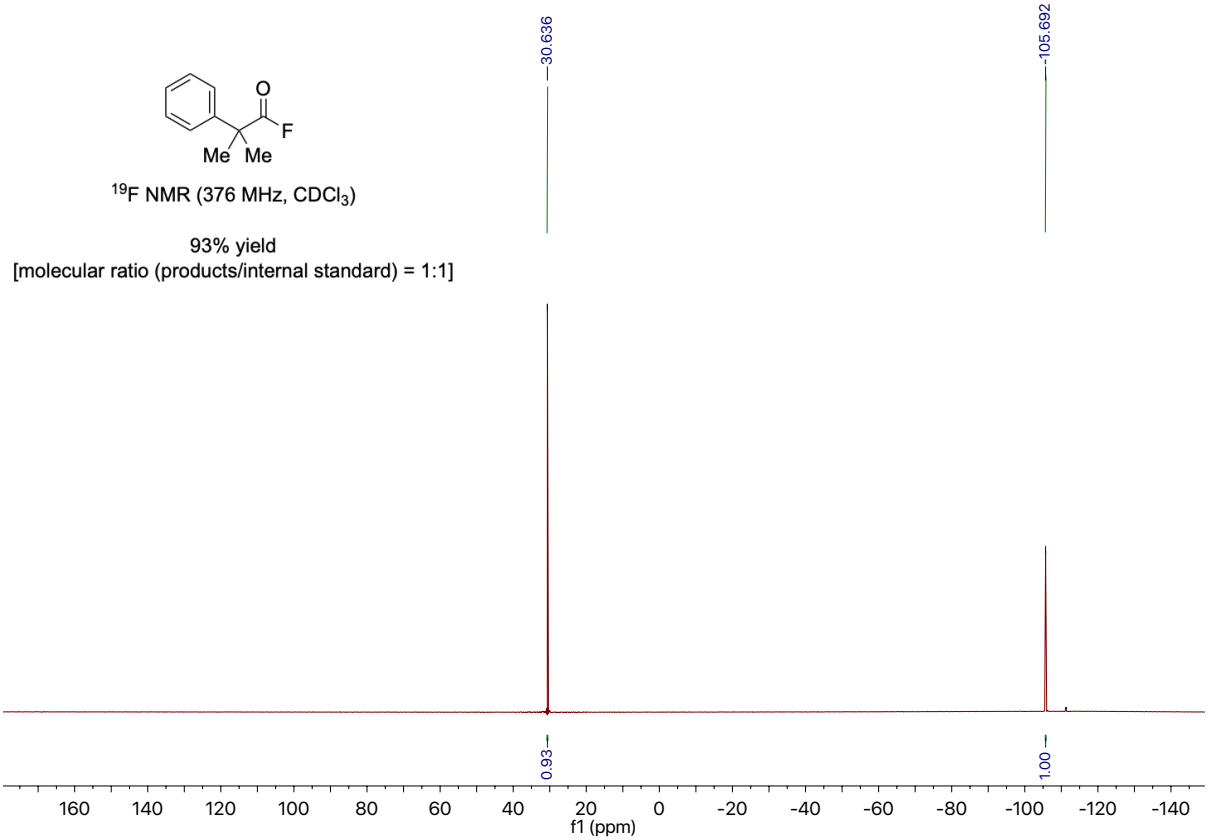
7u (Prepared by the general procedure C)



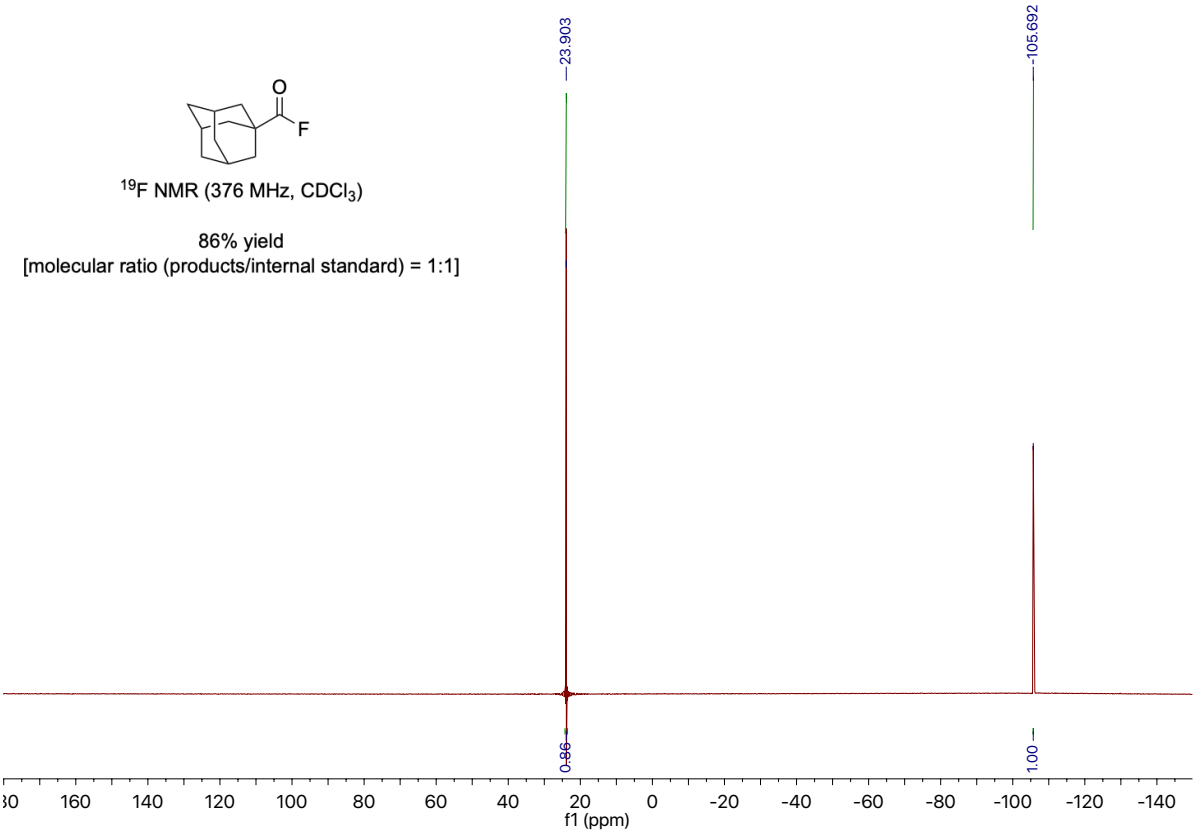
7v (Prepared by the general procedure C)



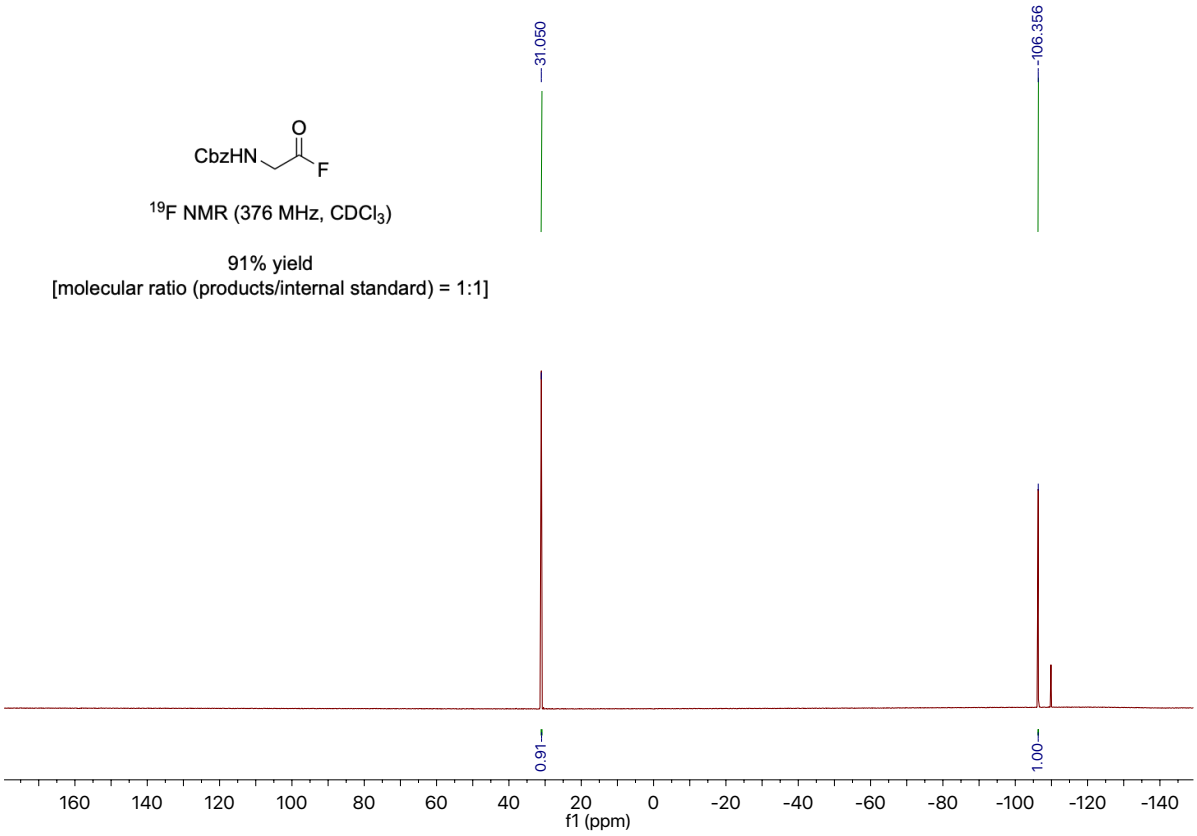
7w (Prepared by the general procedure C)



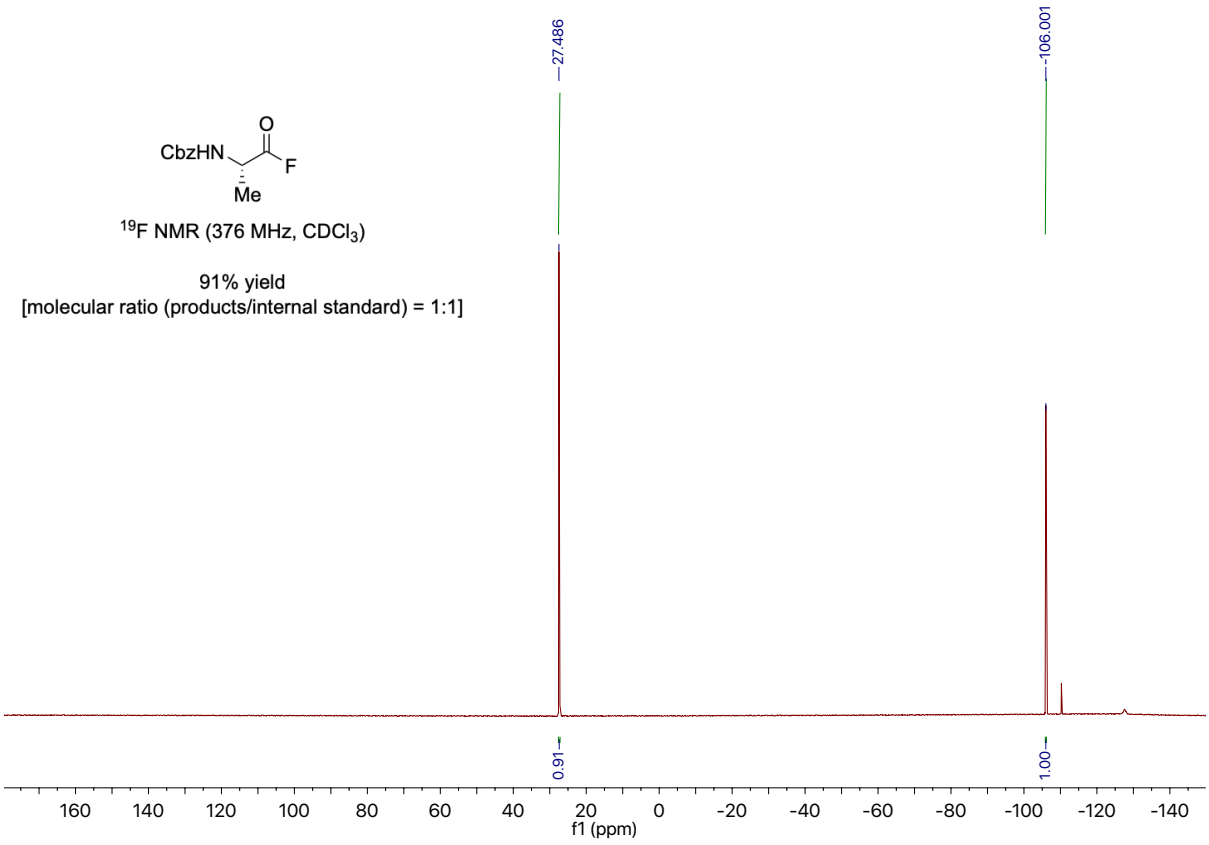
7y (Prepared by the general procedure C)



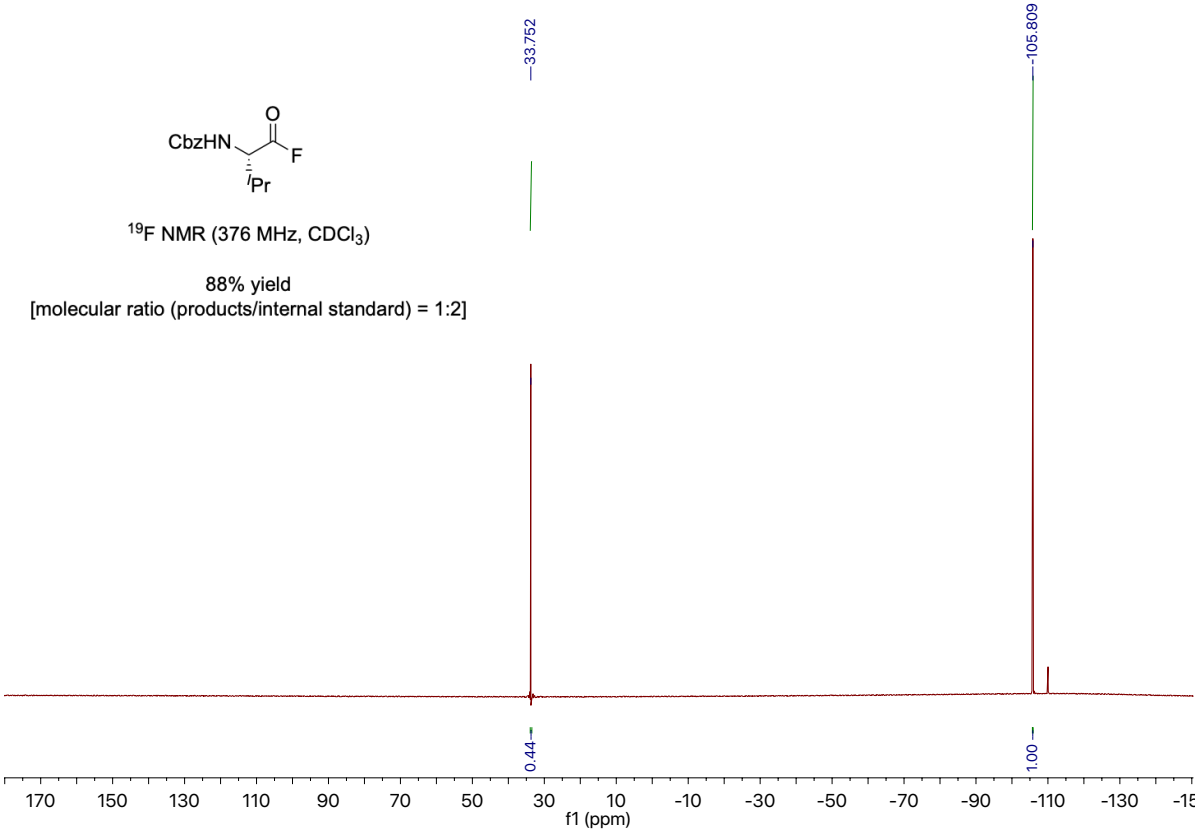
11a (Prepared by the general procedure D)



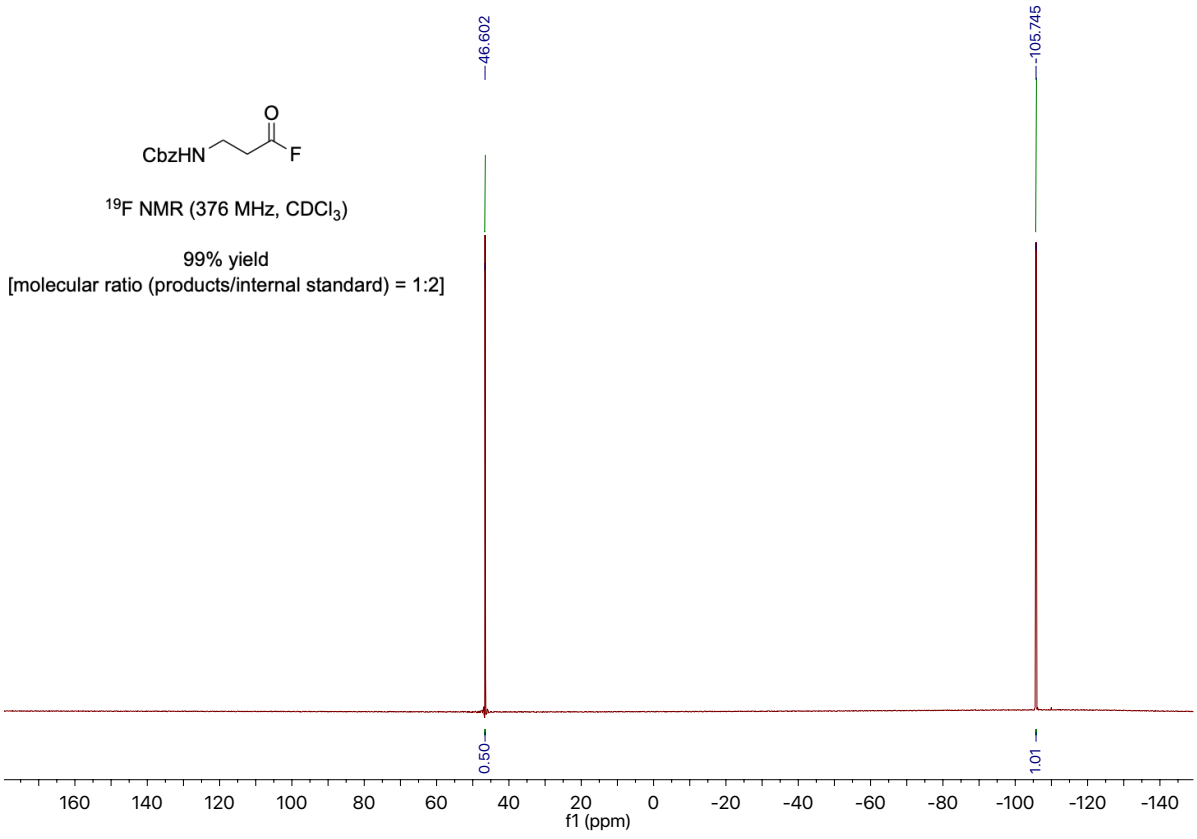
11b (Prepared by the general procedure D)



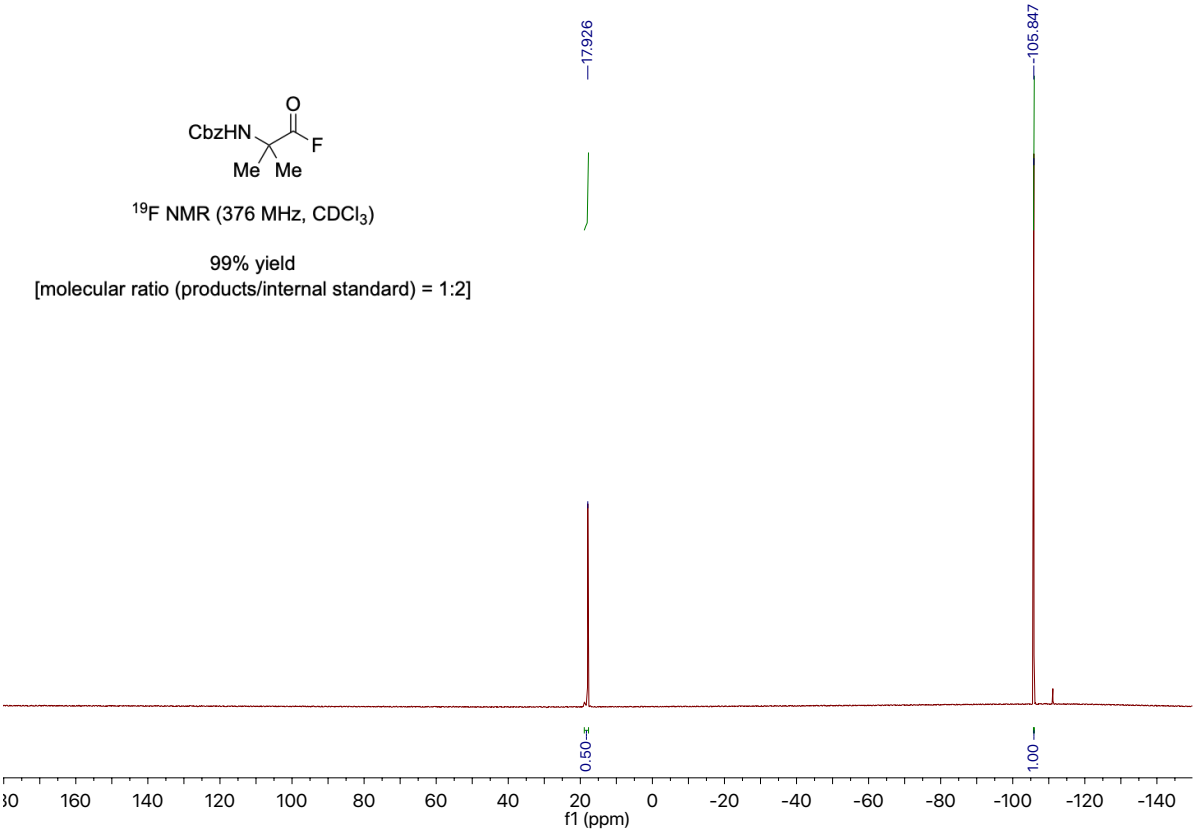
11c (Prepared by the general procedure D)



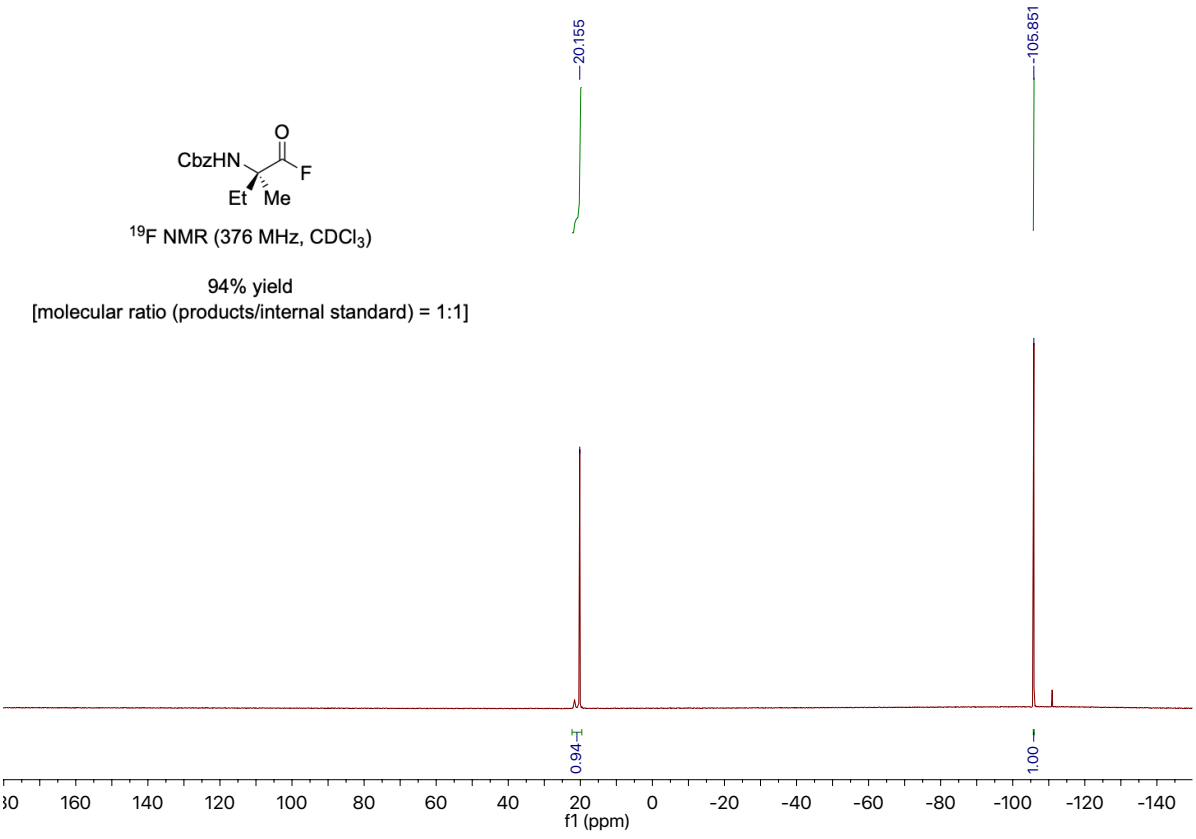
11e (Prepared by the general procedure D)



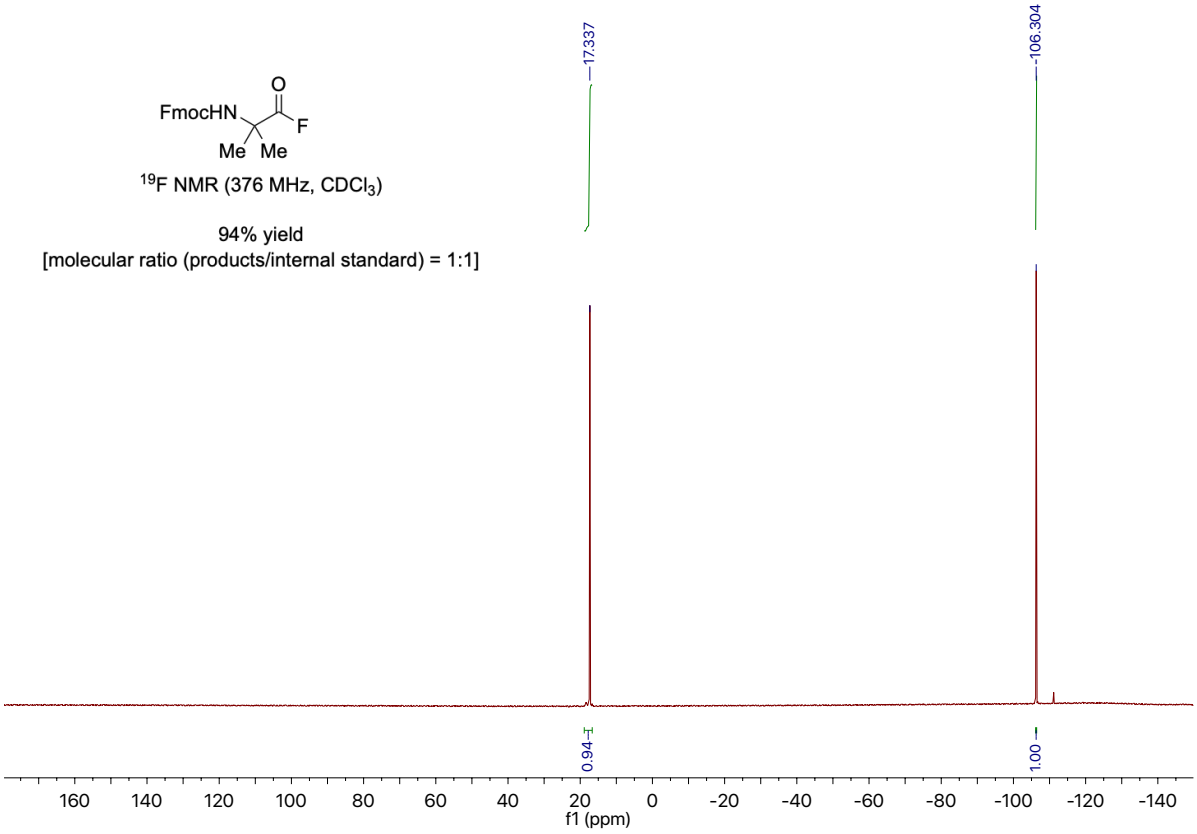
11f (Prepared by the general procedure D)



11g (Prepared by the general procedure D)

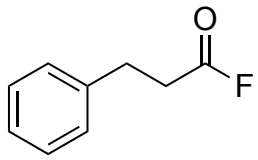


11l (Prepared by the general procedure D)



5-3. Purification of Acyl Fluoride 5

A reaction tube with magnetic stirring bar was charged with 4-hydroxyphenyl cinnamate (**1**) (0.30 mmol) and $PhI(OPiv)_2$ (0.45 mmol, 1.5 equiv.) under argon atmosphere. MeCN (1.50 mL) was added at 0 °C and then Py•9HF (0.45 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at 0 °C for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. Purification by flash column chromatography on silica gel (eluent : only hexane to hexane/CH_2Cl_2 (9/1)) provided **5** in 88% yield (40 mg, 0.26 mmol).



3-Phenylpropanoyl fluoride (5)

Colorless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.25 (m, 2H), 7.25-7.20 (m, 3H), 2.99 (t, J = 7.5 Hz, 2H), 2.83 (t, J = 7.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9 (d, $J_{C\text{-}F}$ = 358.5 Hz), 138.9, 128.8, 128.3, 126.9, 33.9 (d, $J_{C\text{-}F}$ = 50.1 Hz), 30.0, (d, $J_{C\text{-}F}$ = 2.3 Hz).

^{19}F NMR (470 MHz, $CDCl_3$) δ 45.43.

HRMS (ESI-TOF) Calcd.for C_9H_9OFNa: 175.0530 ($[M + Na]^+$), Found: 175.0526.

6. Computational Mechanism Study

6-1. Computational Details

All calculations were performed using the Gaussian 16[S1] program package employing the M06-2X[S2] functional. The reported geometries were fully optimized using the 6-31G* basis sets for C, H, O, and F atoms and Lanl2DZdp basis set[S3] for I atom. The vibrational frequency analysis was made for all the optimized geometries to determine whether it is a stationary structure with no imaginary frequency or a transition state with only one imaginary frequency. Intrinsic reaction coordinate (IRC)[S4] calculations were carried out to make sure if the transition state connects the correct reactant and product. Solvent effects of acetonitrile were evaluated by SMD[S5] model. To evaluate better potential energy, single point calculations were carried out using the 6-311+G** basis sets for C, H, O, and F atoms and def2-QZVP basis set[S6] for I atom, where the optimized geometries in gas phase were employed. CYLView[S7] visualization program was used to describe the 3-dimenstional structure.

The zero-point energy ($E_{gas}^{v_0}$) was calculated in gas phase because it is likely that the vibration is not influenced very much by solvation. Thus, the total energy E_{sol} for each species is defined using the eqn (S1):

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0} \quad \text{(S1)}$$

where E_{sol}^{pot} is a potential energy involving a non-electrostatic term in solution. As for the bimolecular process, the entropy change must be considered because it decreases significantly during the process. In this context, the Gibbs energy (G_{sol}^0) in solution is evaluated by eqn (S2):

$$\begin{aligned} G_{sol}^0 &= H_0 - T(S_r^0 + S_v^0 + S_t^0) \\ &= E^T + P\Delta V - T(S_r^0 + S_v^0 + S_t^0) \\ &= E_{sol} + E_{therm} - T(S_r^0 + S_v^0 + S_t^0) \end{aligned} \quad \text{(S2)}$$

where in solution ΔV is 0, E_{therm} represents the thermal correction by translational, vibrational, and rotational movements, and S_r^0, S_v^0, and S_t^0 represent rotational, vibrational, and translational entropies, respectively. Generally, the Thacker-Tetrode equation is applied to evaluate translational entropy S_t^0. However, owing to the great suppress of translation movement in solution, the usual Thacker-Tetrode equation cannot be directly employed to evaluate S_t^0 in solution.[S8] Hence, the translational entropy should be corrected using the method developed by Whitesides et al.,[S9] while the rotational entropy was estimated in a normal way because the rotation movement would occur in solvation cage. Thermal correction

and entropy contributions of vibration movements to the Gibbs energy were estimated employing the frequency calculations at 298.15 K and 1 atm.

6-2. Discussion of Ligand Exchange Reaction of Hypervalent Iodine Reagent $PhI(OPiv)_2$

Hypervalent iodine reagent $PhI(OPiv)_2$ approaches **1** to induce the ligand exchange of the iodine atom. In this ligand exchange, we investigated two reaction pathways leading to the formation of aromatic intermediate with I-O bond and that of non-aromatic intermediate with $I\text{-}C^{ortho}$ bond because the recent report proposed that the iodine is bound with the ortho carbon atom to afford non-aromatic intermediate;[S10] for brevity, the former is named aromatic pathway and the latter is de-aromatic pathway here. In the de-aromatic pathway, the Gibbs free energy of activation ($\Delta G^{o\ddagger}$) is very large (25.1 kcal/mol), as shown by red line in Figure S1. Also, it is highly endothermic (the Gibbs free energy of reaction ΔG^{o} = 22.4 kcal/mol); geometry changes are shown in Figures S2 and S3. In contrast, the $\Delta G^{o\ddagger}$ value in the aromatic pathway is 16.9 kcal/mol and the ΔG^{o} is 2.8 kcal/mol, as shown by sky blue line in Figure S1. These results indicate that the de-aromatic pathway is much more difficult than the aromatic one. We investigated how much HF molecules influence the energy change using HF to $(HF)_7$, as shown in Figure S1; geometry changes are presented in Figures S4 and S5. The hypervalent iodine reagent interacts with the OH group of the substrate to afford the first intermediate **IM1-N** (**N** = 1-16). The HF clusters interact with the ester moiety and/or the pivalate moiety. Because both the pivalate and ester moieties are polarized, it is likely that both interact with HF cluster. Such interaction structure is found in **TS1-14**, **TS1-15**, and **TS1-16**, where $(HF)_5$, $(HF)_6$, and $(HF)_7$ clusters interact with the pivalate and ester moieties. The $\Delta G^{o\ddagger}$ value is 22.0, 21.2 and 21.5 kcal/mol for them (Figure S1), respectively, indicating that the $\Delta G^{o\ddagger}$ value depends little on the presence of HF cluster.

If acyl fluoride, $PhCH_2CH_2COF$ (**5**), is formed more easily from aromatic intermediate with a smaller $\Delta G^{o\ddagger}$ value than 25.1 kcal/mol, the reaction does not necessarily occur through the de-aromatic intermediate. Thus, the next work is to investigate the reaction of HF molecule with the aromatic intermediate.

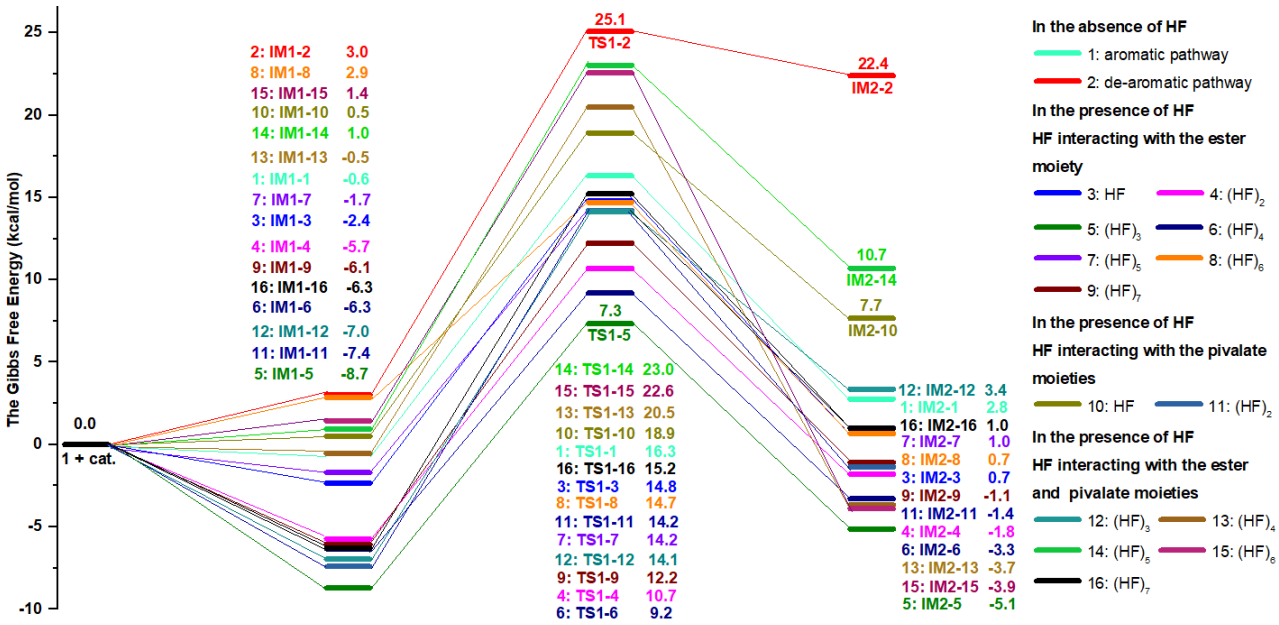


Figure S1: The Gibbs free energy profile (in kcal/mol) in ligand exchange reaction.

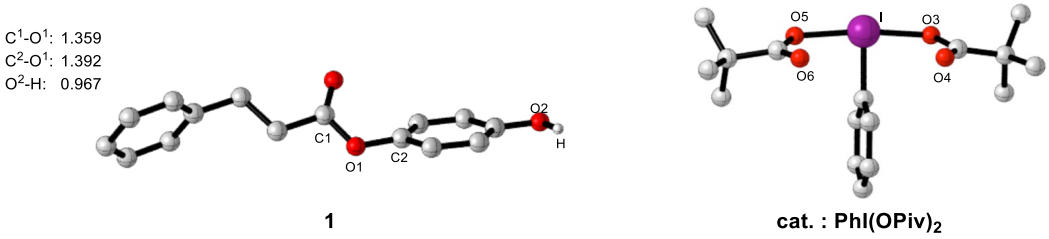
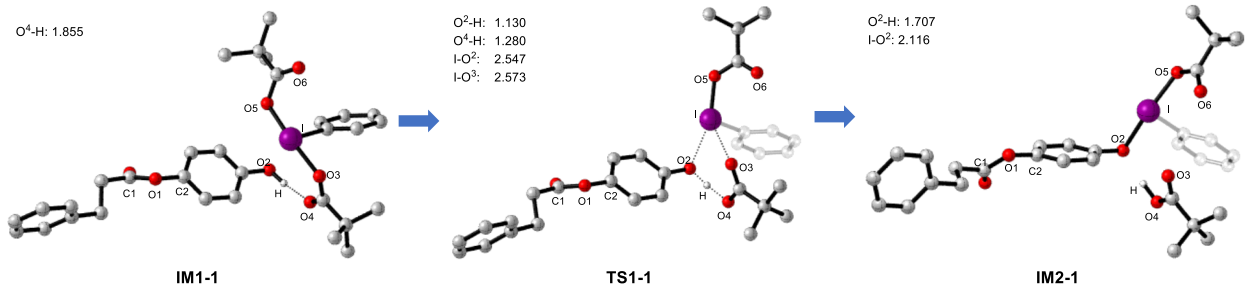


Figure S2: Optimized geometries of 1 and hypervalent iodine reagent $PhI(OPiv)_2$ (Some hydrogen atoms are omitted for clarify. Bond distance is in Å.)

(1) Geometry changes in the reaction with the OH group affording I-O bond in the absence of HF molecule



(2) Geometry changes in the reaction with the OH group affording I-C bond at the ortho position in the absence of HF molecule

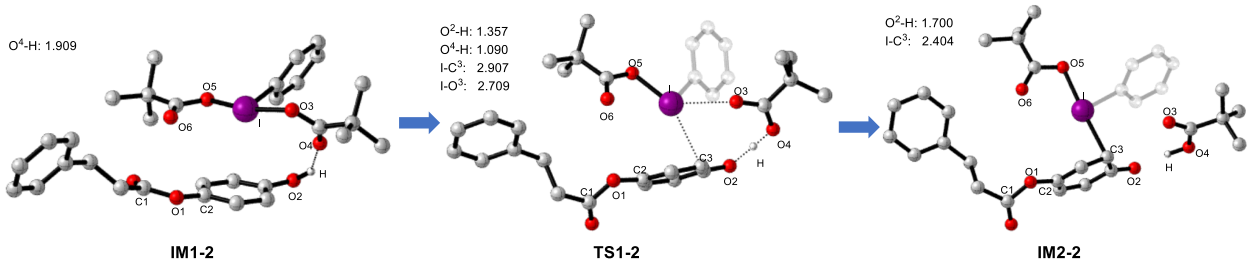
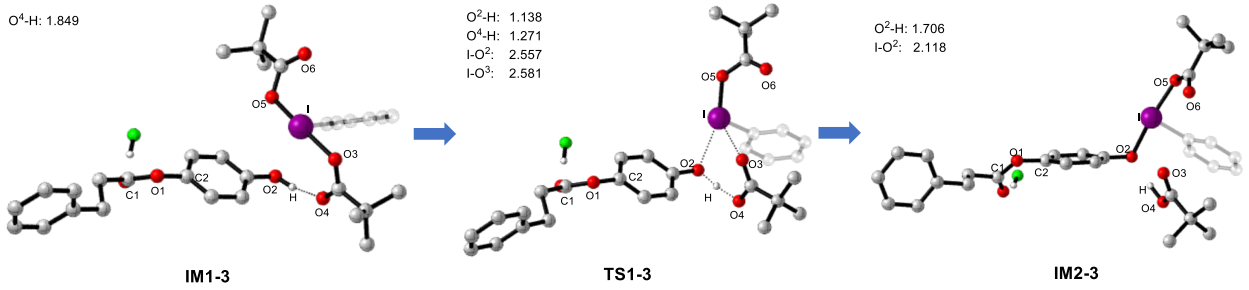


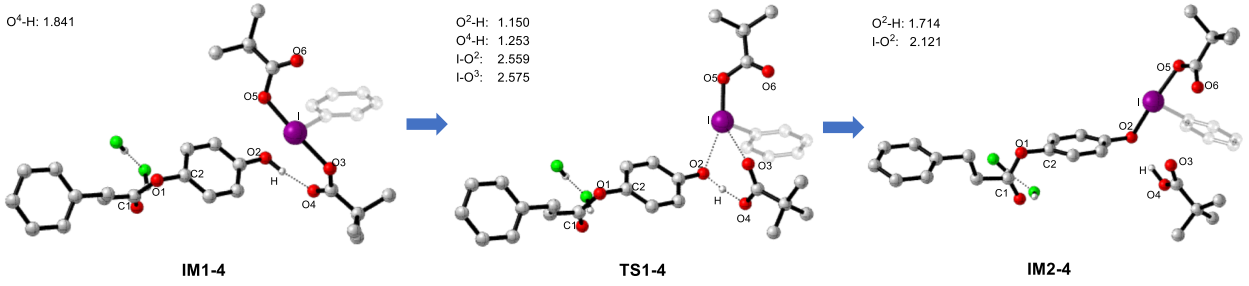
Figure S3: Geometry changes in the reaction of hypervalent iodine reagent $PhI(OPiv)_2$ with substrate ester affording aromatic intermediate with I-O bond and de-aromatic intermediate with I-C bond in the absence of HF molecule

(Some hydrogen atoms are omitted for clarify. Bond distance is in Å.)

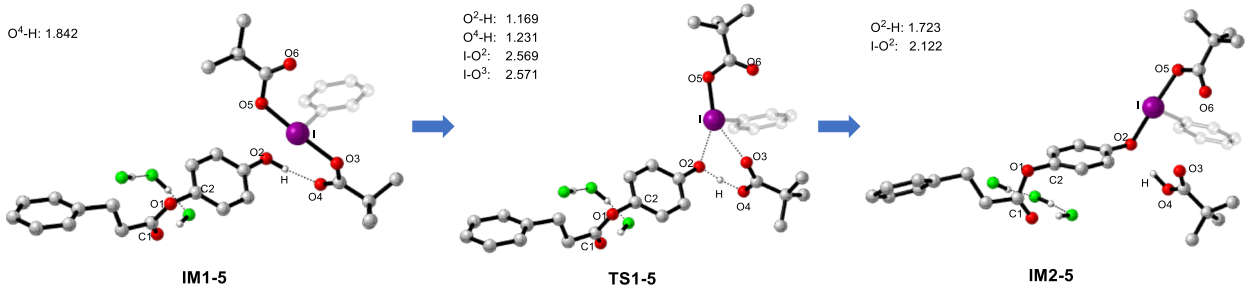
(3) Geometry changes in the presence of HF interacting with the ester moiety



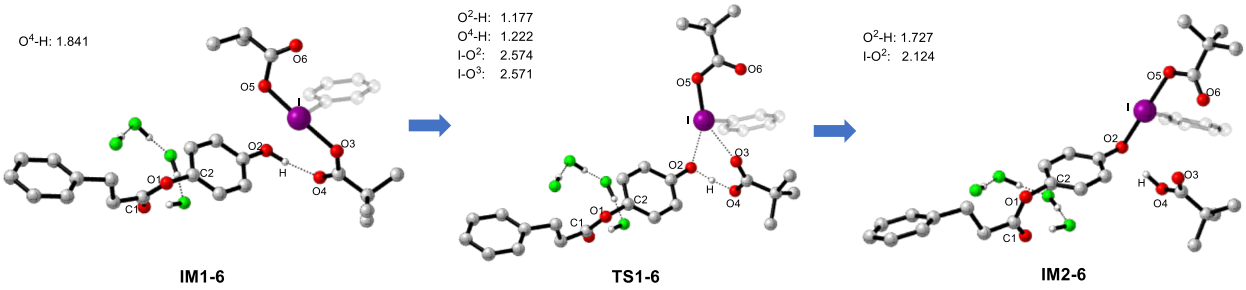
(4) Geometry changes in the presence of $(HF)_2$ interacting with the ester moiety



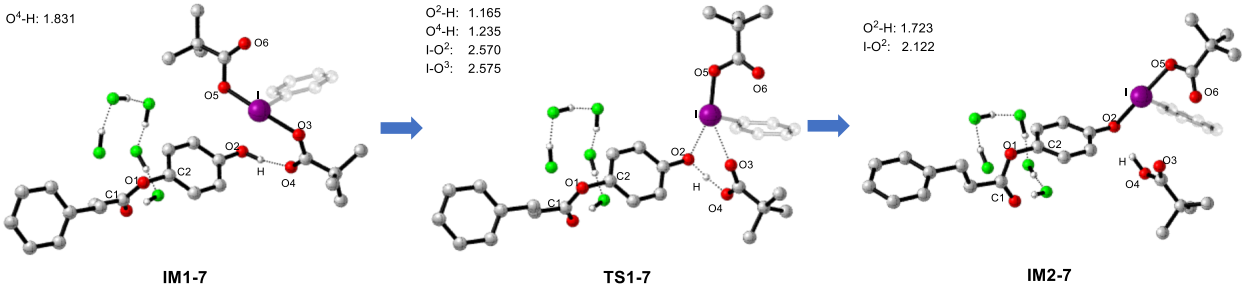
(5) Geometry changes in the presence of $(HF)_3$ interacting with the ester moiety



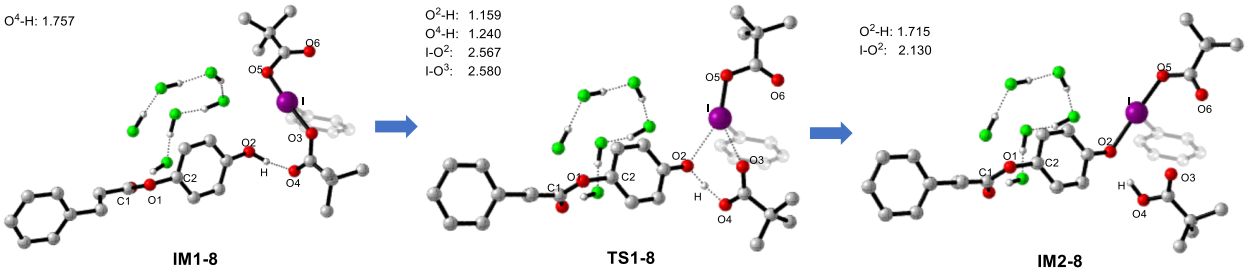
(6) Geometry changes in the presence of $(HF)_4$ interacting with the ester moiety



(7) Geometry changes in the presence of $(HF)_5$ interacting with the ester moiety



(8) Geometry changes in the presence of $(HF)_6$ interacting with the ester moiety



(9) Geometry changes in the presence of $(HF)_7$ interacting with the ester moiety

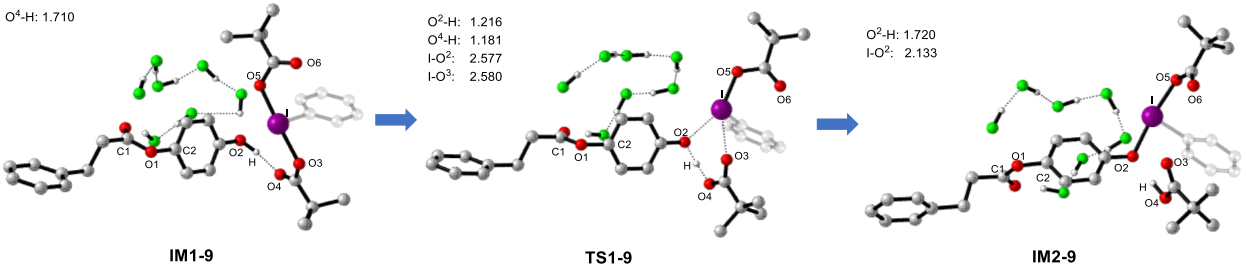
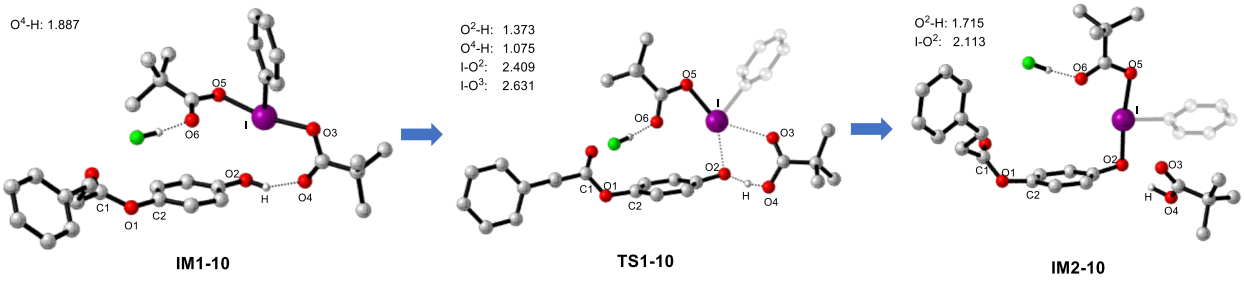
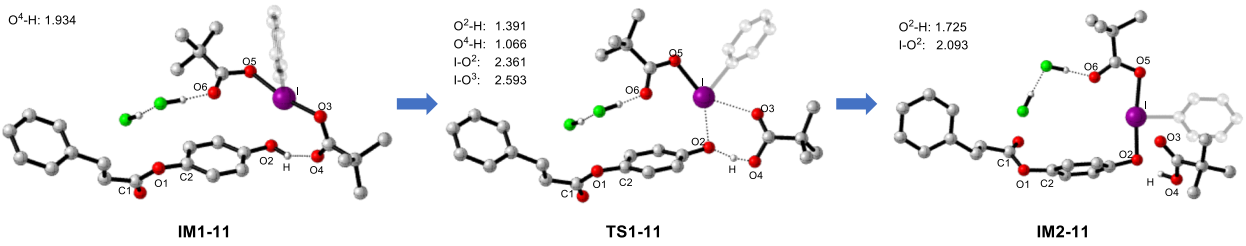


Figure S4: Geometry changes in the ligand exchange affording the aromatic intermediate in the presence of $(HF)_n$ cluster interacting with the ester moiety (n = 1-7)
(Some hydrogen atoms are omitted for clarify. Bond distance is in Å.)

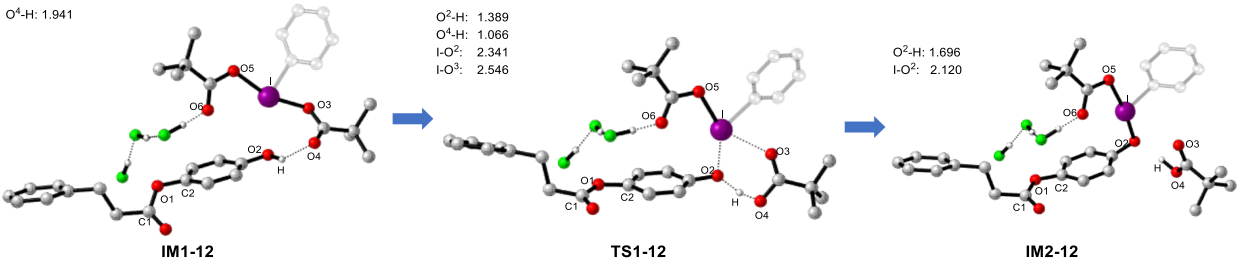
(10) Geometry changes in the presence of HF interacting with the pivalate moiety



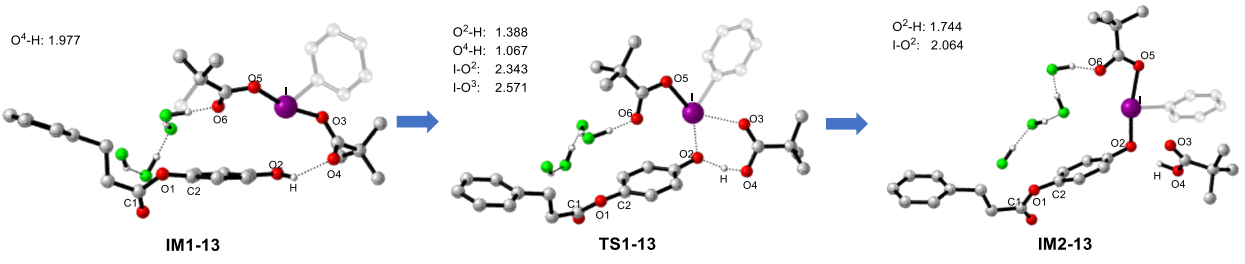
(11) Geometry changes in the presence of $(HF)_2$ interacting with the pivalate moiety



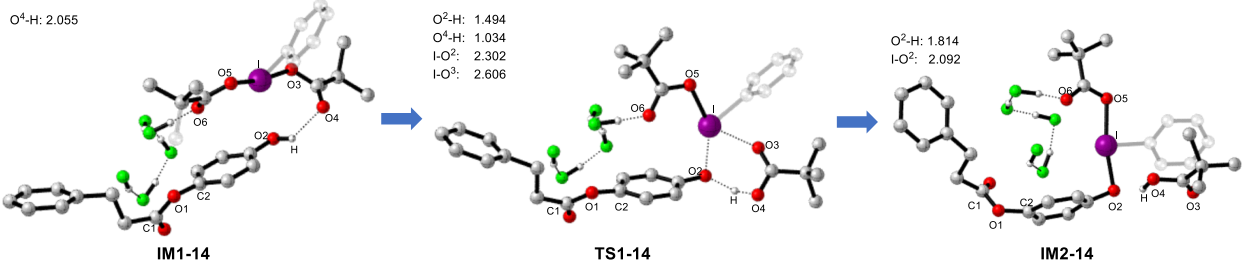
(12) Geometry changes in the presence of $(HF)_3$ interacting with the pivalate and ester moieties



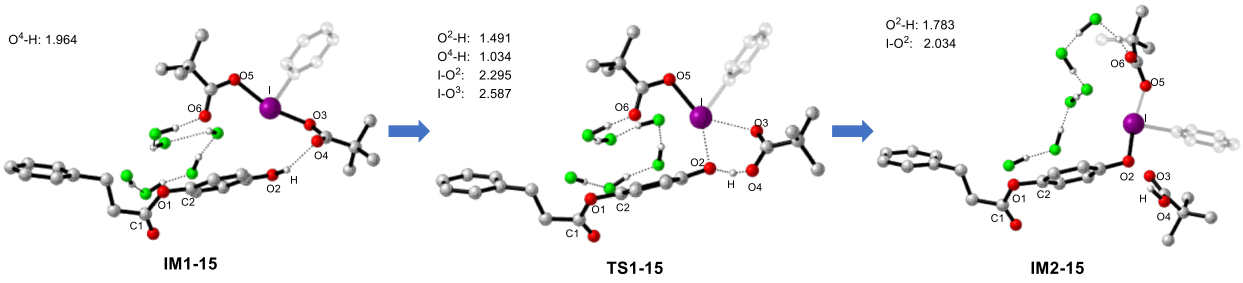
(13) Geometry changes in the presence of $(HF)_4$ interacting with the pivalate and ester moieties



(14) Geometry changes in the presence of $(HF)_5$ interacting with the pivalate and ester moieties



(15) Geometry changes in the presence of $(HF)_6$ interacting with the pivalate and ester moieties



(16) Geometry changes in the presence of $(HF)_7$ interacting with the pivalate and ester moieties

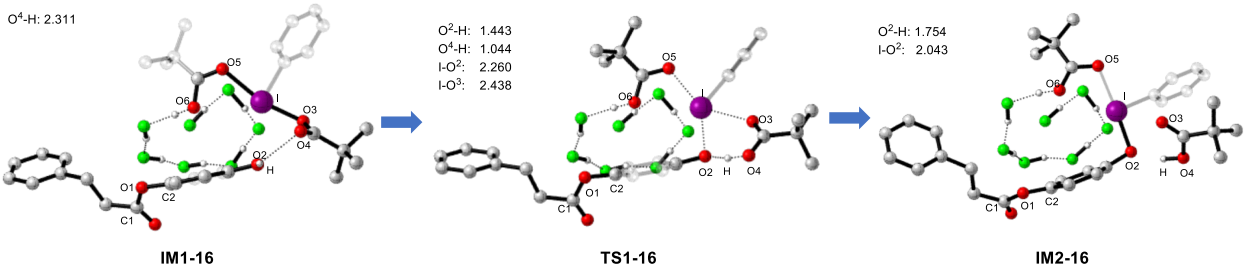


Figure S5: Geometry changes in the ligand exchange affording the aromatic intermediate in the presence of $(HF)_n$ cluster interacting with the pivalate and/or ester moieties (n = 1-7) (Some hydrogen atoms are omitted for clarify. Bond distance is in Å.)

6-3. Discussion of Reaction of HF Molecule with Aromatic Intermediate

We investigated the reaction of HF with the aromatic intermediate using various $(HF)_n$ (n = 1-7) clusters, as shown in Figure S6. When HF molecules participate in this process, the $\Delta G^{o\ddagger}$ value decreases sharply, as clearly shown by comparison of the reaction with one HF molecule and that with two HF molecules in Figure S6; the corresponding geometry changes are displayed in Figures S7 and S8. Because $(HF)_2$ cluster does not simultaneously interact with both the ester and pivalate moieties (Figure S7b), the energy change still somewhat differs from the other energy changes in the presence of $(HF)_3$ to $(HF)_7$ clusters. In the presence of $(HF)_3$ cluster, both the ester and pivalate moieties seem to interact with $(HF)_3$ (Figure S7c). Though the energy changes in the presence of $(HF)_3$ to $(HF)_5$ are moderately different from each other probably because the HF chain is not long enough to induce some strain, the energy changes in the presence of $(HF)_6$ and $(HF)_7$ are similar to each other, indicating that these energy changes are useful for discussing the energy changes in the reaction in the presence of HF molecules. Actually, the $(HF)_6$ and $(HF)_7$ clusters can interact with both the ester and pivalate moieties, as shown in Figures S7f and S7g.

The $\Delta G^{o\ddagger}$ value is 6.4 kcal/mol for **TS1** and 11.7 kcal/mol for **TS2** in the presence of $(HF)_6$. Both are much smaller than the $\Delta G^{o\ddagger}$ value of the ligand exchange via de-aromatization pathway, indicating that the reaction occurs without de-aromatization intermediate. We presented discussion in the main text using the computational results with the $(HF)_6$ cluster.

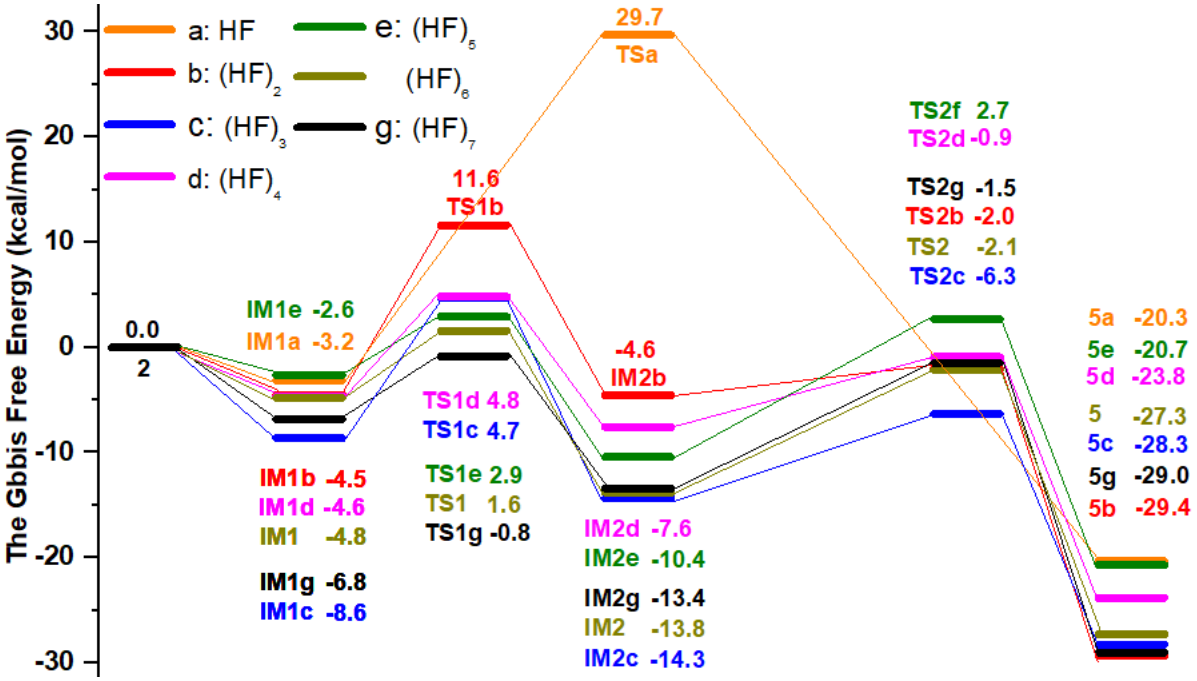
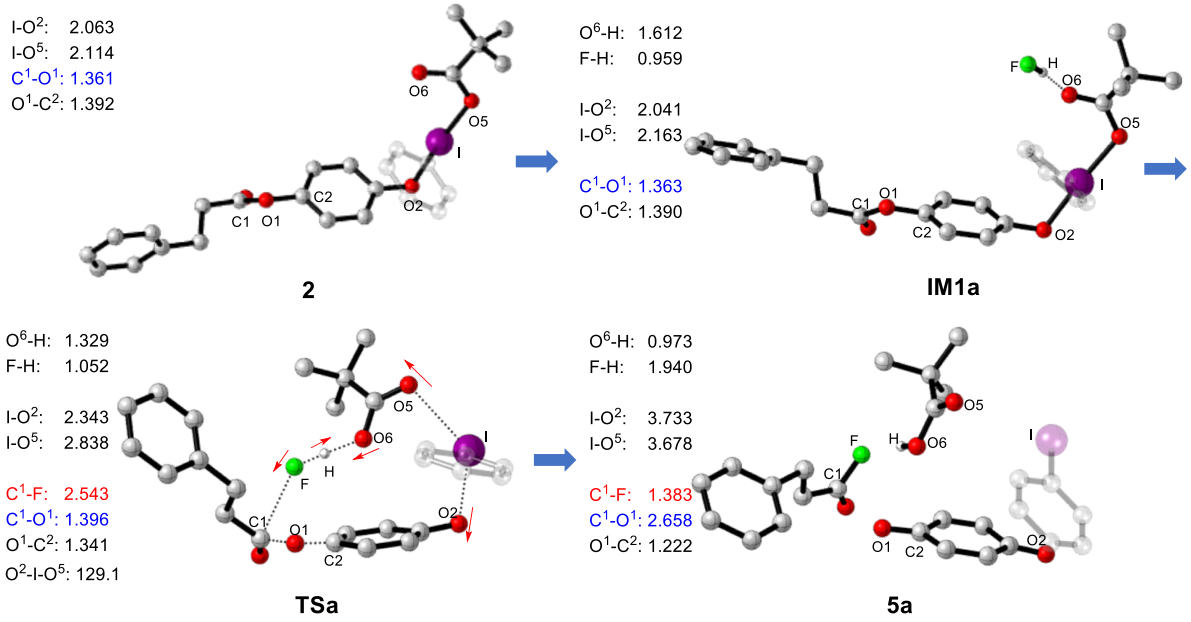
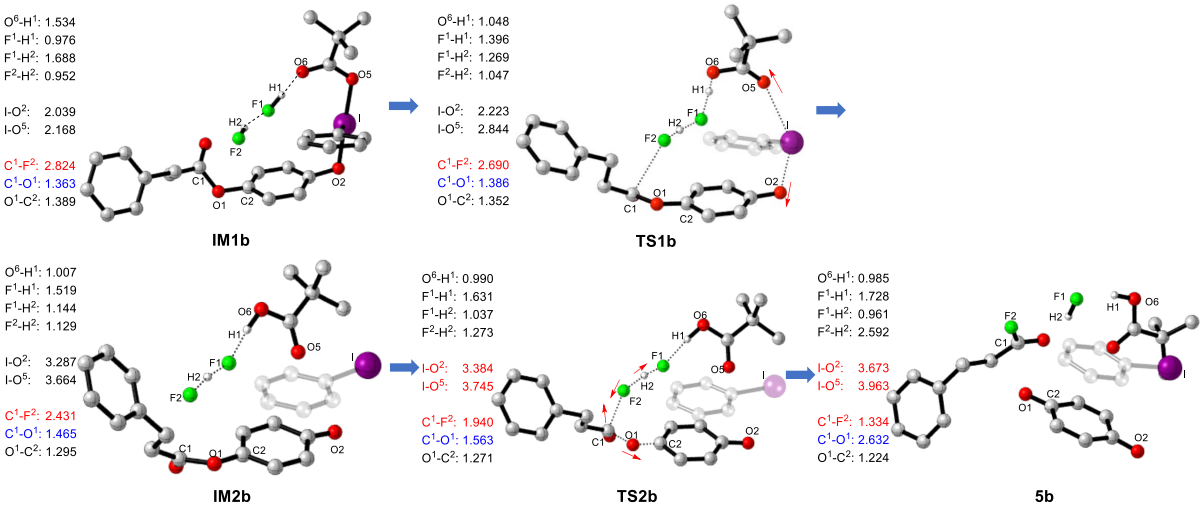


Figure S6: The Gibbs free energy profile (in kcal/mol) for I-O bond cleavage and F^- nucleophilic attack.

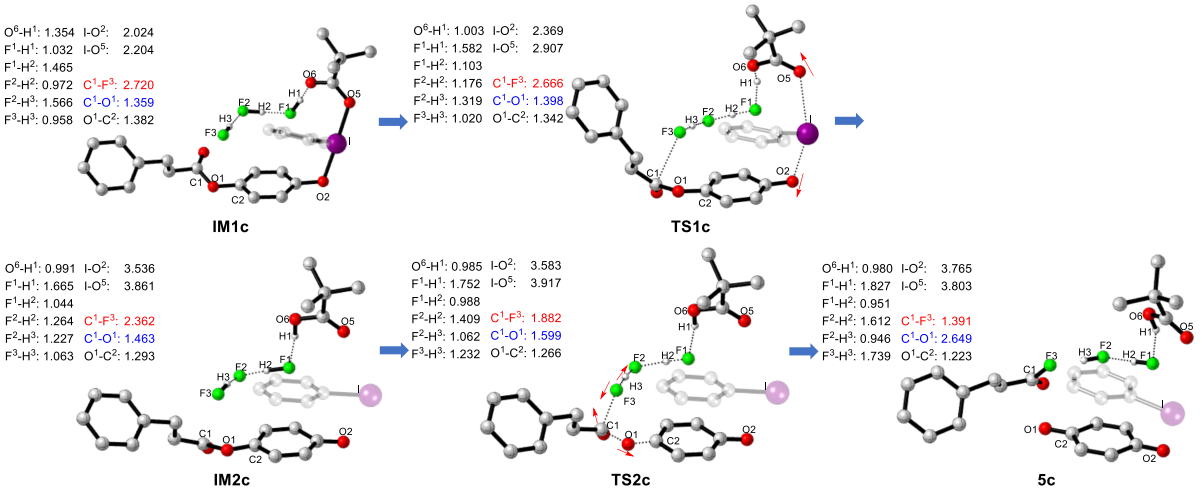
(a) Geometry changes in the reaction of HF with **2**



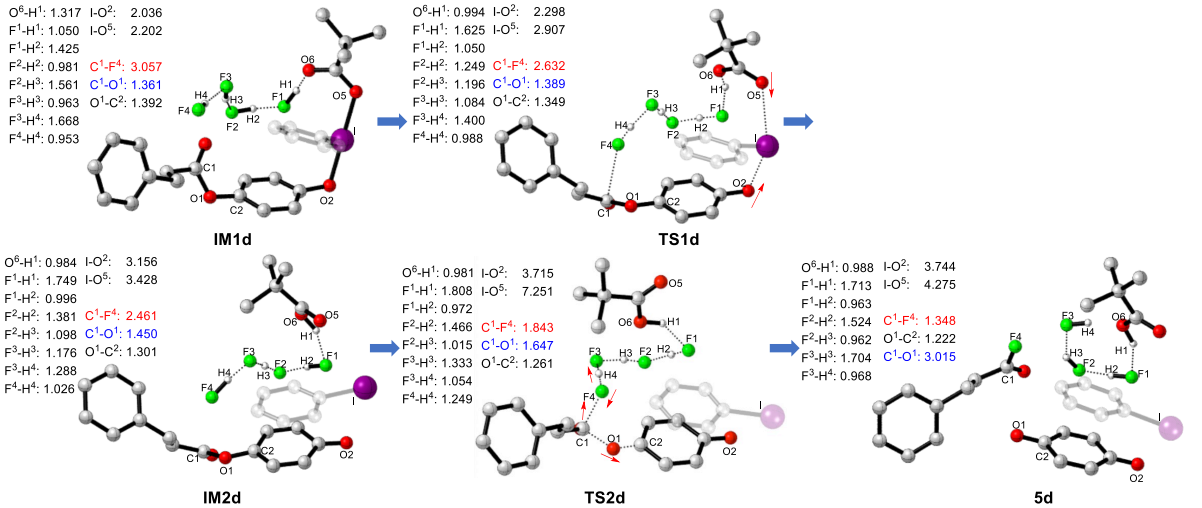
(b) Geometry changes in the reaction of $(HF)_2$ with **2**



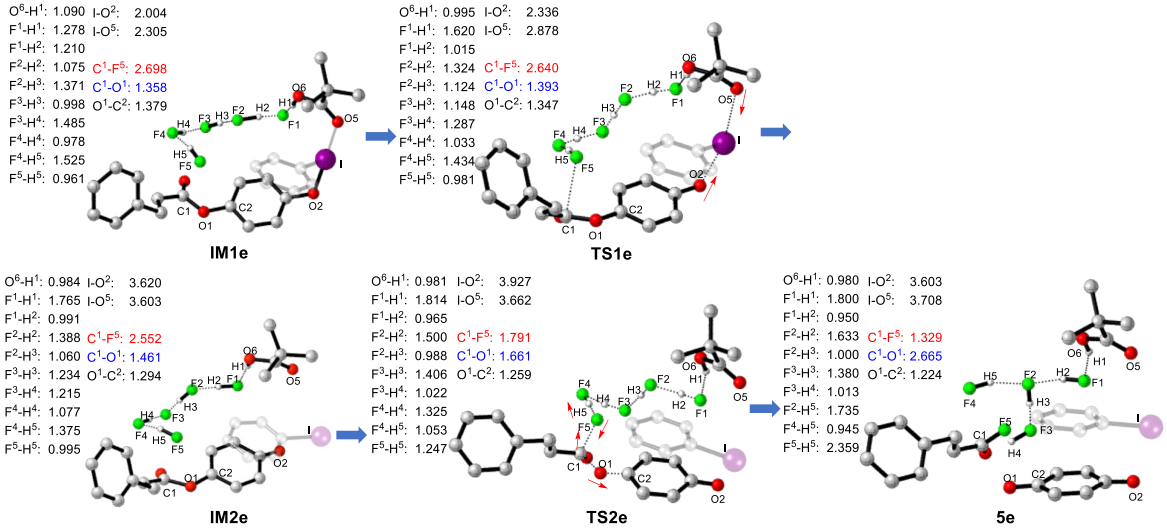
(c) Geometry changes in the reaction of $(HF)_3$ with **2**



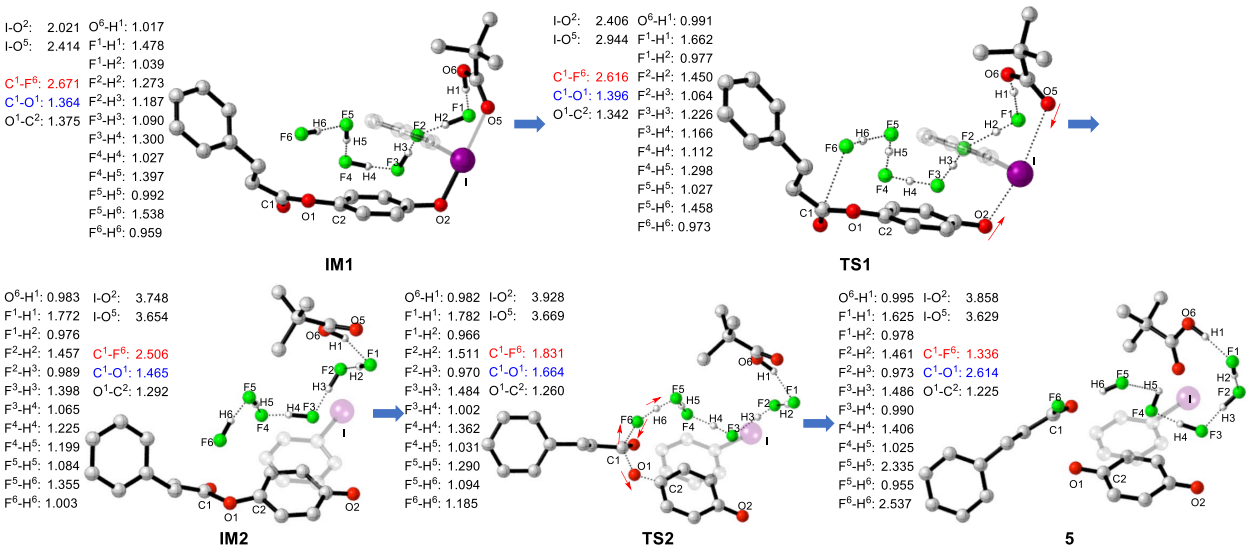
(d) Geometry changes in the reaction of $(HF)_4$ with **2**



(e) Geometry changes in the reaction of $(HF)_5$ with **2**



(f) Geometry changes in the reaction of $(HF)_6$ with **2**



(g) Geometry changes in the reaction of $(HF)_7$ with **2**

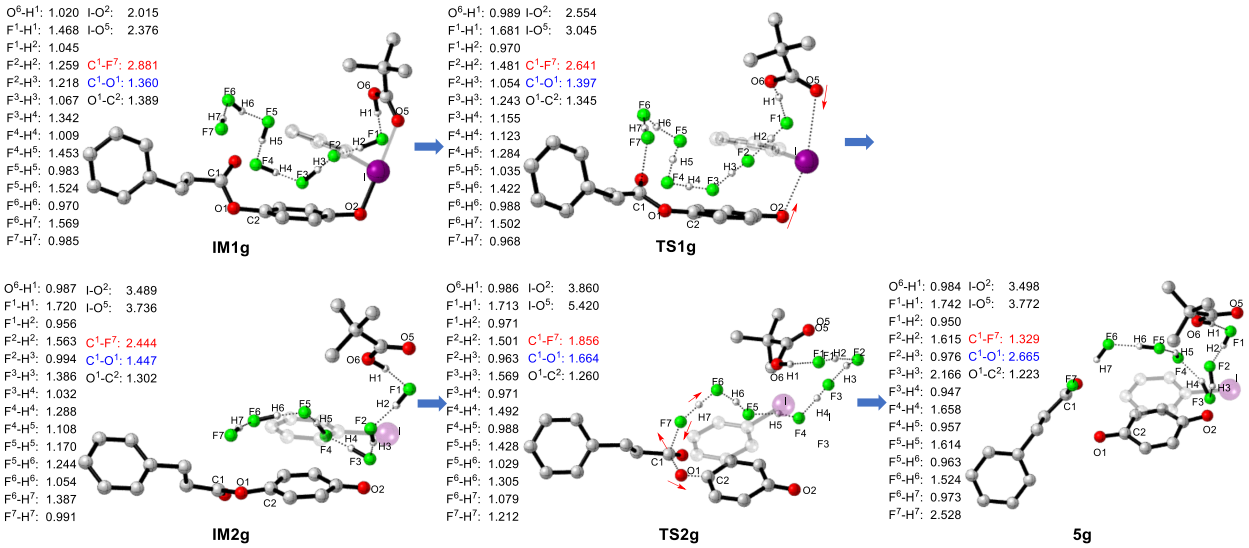


Figure S7. Geometry changes in the reaction of I-O bond cleavage and F^- nucleophilic attack assisted by $(HF)_n$ cluster (n = 1-7)

(Some hydrogen atoms are omitted for clarify. Red arrows in TS represent movements of reaction-center atoms. Bond distance is in Å.)

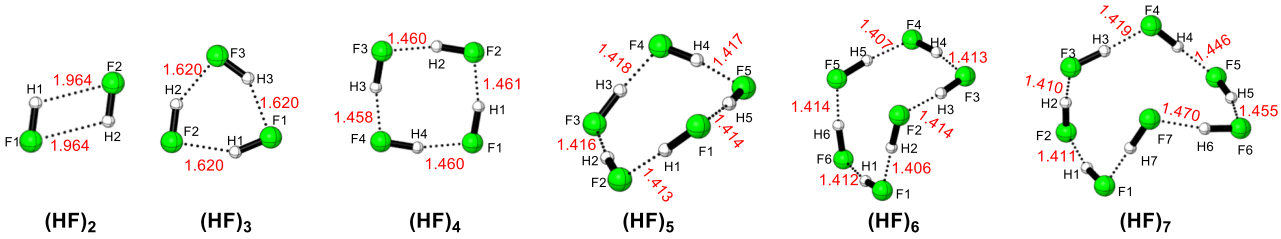


Figure S8. Optimized geometries of $(HF)_n$ cluster (n = 2-7).

(Bond distance is in Å.)

6-4. Cartesian Coordinates

1

C	5.51705300	1.20576400	0.50737300
C	4.24043700	0.82432900	0.91061300
C	3.60398600	-0.27411000	0.32819800
C	4.27507800	-0.98296400	-0.67086600
C	5.55175800	-0.60596300	-1.07802800
C	6.17650300	0.49084800	-0.48938400
H	5.99890000	2.05910900	0.97468300
H	3.72969400	1.38149600	1.69274200
H	3.79186800	-1.84309500	-1.12892500
H	6.06093200	-1.17156100	-1.85235800
H	7.17320600	0.78444600	-0.80317800
C	2.19978000	-0.65179800	0.73122100
H	2.05247100	-1.73318100	0.64497200
H	2.01915900	-0.39701800	1.78022200
C	1.16579400	0.06371000	-0.13889000
H	1.29296700	-0.19097800	-1.19752300
H	1.28658900	1.15185600	-0.07831700
C	-0.24835900	-0.27664900	0.26564400
O	-0.56092300	-0.99379700	1.17743800
O	-1.13038000	0.35086400	-0.55524400
C	-2.49820000	0.21489700	-0.33687000
C	-3.24971000	1.37967100	-0.37496000
C	-3.11235100	-1.02325500	-0.16435400
C	-4.63301900	1.31594500	-0.23733700
H	-2.74560200	2.32919400	-0.51841200
C	-4.49121900	-1.08474100	-0.02180700
H	-2.51601200	-1.92628500	-0.13078000
C	-5.25598100	0.08257600	-0.05707700
H	-5.22441100	2.22758800	-0.26987500
H	-4.99666500	-2.03364700	0.11878300
O	-6.60345300	-0.04880600	0.08684500
H	-7.01435300	0.82643400	0.05478800

Cat.

I	-0.01444700	-1.05155200	-0.48509000
C	0.01905500	1.02989500	-0.31217800
C	0.06445400	1.79168100	-1.47604400
C	0.00892000	1.59524800	0.95882800
C	0.09870800	3.17869600	-1.35635600
H	0.07388900	1.31907000	-2.45219800
C	0.04325100	2.98501000	1.05354600
H	-0.02422900	0.96533700	1.83852100
C	0.08790900	3.77110600	-0.09541100
H	0.13394300	3.79245300	-2.25040300
H	0.03621400	3.44996900	2.03376400
H	0.11506300	4.85261900	-0.00845200
O	-2.10115700	-0.88908100	-0.61988900
O	2.07554500	-0.93447900	-0.61200500
C	-2.74523500	-0.54718200	0.49375400
C	2.71945700	-0.59436900	0.50263900
O	2.16793200	-0.44103200	1.57337500
O	-2.19419900	-0.39240400	1.56467200
C	-4.23913300	-0.31448700	0.26322900
C	4.21195000	-0.35473400	0.27147300
C	4.82826400	-1.55048800	-0.46372200
H	4.33931000	-1.71187400	-1.42725400
H	5.89385500	-1.36596400	-0.63745400
H	4.73619900	-2.46662200	0.12926500
C	4.89822800	-0.13770800	1.61860900
H	5.96466400	0.05720800	1.46362500
H	4.45709000	0.70984800	2.14870100
H	4.79388100	-1.01952200	2.25716800
C	4.32771000	0.90881200	-0.59702500
H	3.85842400	1.76659800	-0.10243600
H	5.38366700	1.14602300	-0.76541800
H	3.84304300	0.76015000	-1.56581500
C	-4.85174400	-1.52496300	-0.45113000
H	-5.91907900	-1.34906100	-0.62304500

H	-4.36599500	-1.69809000	-1.41427300
H	-4.75204700	-2.43141700	0.15537300
C	-4.92216800	-0.08066600	1.60922200
H	-4.48352400	0.77686000	2.12525800
H	-5.98994200	0.10711700	1.45466200
H	-4.81158800	-0.95224000	2.26057900
C	-4.36548200	0.93433400	-0.62440400
H	-5.42345900	1.16125200	-0.79419200
H	-3.90189500	1.80304700	-0.14391600
H	-3.88163500	0.77433900	-1.59170200

HF

F	0.00000000	0.00000000	0.09306600
H	0.00000000	0.00000000	-0.83759200

$(HF)_2$

F	0.00000000	1.23469800	0.00000000
H	0.69279600	0.60309500	0.00000000
F	0.00000000	-1.23469800	0.00000000
H	-0.69279600	-0.60309500	0.00000000

$(HF)_3$

F	-0.95653200	1.06703300	0.00000000
H	0.00000000	1.10621600	0.00000000
F	-0.44581200	-1.36189700	0.00000000
H	-0.95801100	-0.55310800	0.00000000
F	1.40234400	0.29486400	0.00000000
H	0.95801100	-0.55310800	0.00000000

$(HF)_4$

F	1.70600900	0.14176300	0.00192600
H	-0.88036800	1.06127900	-0.00053400
F	-0.14173400	1.70412000	-0.00192600
H	1.06303500	0.87978400	0.00049800
F	0.14133200	-1.70463800	-0.00192900
H	0.88036000	-1.06317700	-0.00047700
F	-1.70558900	-0.14106800	0.00192900
H	-1.06318200	-0.87948000	0.00050300

$(HF)_5$

F	-1.12130300	-1.55824300	-0.43794500
H	1.08810100	1.27060300	-0.09647800
F	1.86794400	0.71216200	0.13445300
H	-0.16515200	-1.64736000	-0.20594800
F	1.19600900	-1.59211300	0.16843500
H	1.52861100	-0.66262500	0.15861900
F	-0.12913000	1.92625300	-0.41159800
H	-0.87850200	1.42035800	-0.01641000
F	-1.80853700	0.51144000	0.54681800
H	-1.61790900	-0.37646700	0.15873600

$(HF)_6$

F	-1.88282200	-1.26905600	-0.32476900
H	0.71783800	1.44988300	0.44290800
F	-0.14699400	1.50310000	0.92001500
H	-2.00336600	-0.30064000	-0.48204800
F	-1.95382300	1.10681300	-0.59335600
H	-1.23396600	1.37753200	0.02487800
F	1.88250400	1.26925900	-0.32456800
H	2.00315600	0.30069800	-0.48209700
F	0.14731700	-1.50399700	0.91962600
H	-0.71753900	-1.45005300	0.44279500
F	1.95380400	-1.10611300	-0.59371500
H	1.23399900	-1.37747000	0.02446500

$(HF)_7$

F	-1.38699400	-1.93647000	-0.00476700
H	1.14703200	1.44317800	-0.31303400
F	0.66329700	2.00464900	0.32763100
H	-1.89323800	-1.25109300	-0.50906300
F	-2.40942400	-0.05059500	-1.04119300
H	-2.13072300	0.59386200	-0.34579400
F	1.85359900	0.60378600	-1.25453900
H	2.24845100	-0.14822000	-0.76840300
F	0.33614900	-0.63993800	1.02059400
H	-0.38535400	-1.21304700	0.65489700
F	2.51805600	-1.21696800	0.18132300
H	1.67449000	-1.12985700	0.66099100
F	-1.57730500	1.25555000	0.76981400
H	-0.63705800	1.52505400	0.63063300

2

C	-9.86609800	-0.60865900	0.24250200
C	-8.66935600	0.08122100	0.07108400
C	-7.45926200	-0.60591600	-0.04822000
C	-7.47213300	-2.00111300	0.01157800
C	-8.66633200	-2.69574500	0.18311500
C	-9.86740100	-2.00032500	0.29888200
H	-10.79857000	-0.05943900	0.32900900
H	-8.67116900	1.16787000	0.02477500
H	-6.53566400	-2.54638400	-0.08192900
H	-8.65945900	-3.78067900	0.22265400
H	-10.79992700	-2.54011500	0.42965000
C	-6.15749300	0.14526600	-0.18181500
H	-5.42897000	-0.45022600	-0.73985600
H	-6.31611500	1.07450900	-0.74063100
C	-5.57140600	0.48181700	1.20100300
H	-5.37800000	-0.45028800	1.74441100
H	-6.27373700	1.07977900	1.78550700
C	-4.28091500	1.25991600	1.10922100
O	-4.07597000	2.34095700	1.58934900
O	-3.36477300	0.55605200	0.38915100
C	-2.10576300	1.09756200	0.14684300
C	-1.31328300	1.62513300	1.16180500
C	-1.63579600	1.01493700	-1.15792800
C	-0.03633800	2.07929500	0.85423300
H	-1.69561700	1.69196000	2.17265800
C	-0.35477600	1.46241700	-1.45830900
H	-2.27733600	0.59025000	-1.92296100
C	0.45244300	2.00511900	-0.45434900
H	0.59388300	2.50423500	1.62992700
H	0.04091200	1.39432500	-2.46666300
O	1.70028700	2.44914500	-0.76684200
I	3.28822000	1.30953700	-0.10593600
C	2.50985700	-0.22018300	-1.29776300
C	1.70208500	-1.18702000	-0.70803200
C	2.71005000	-0.14980200	-2.67365200
C	1.09162000	-2.12722500	-1.53635600
H	1.56734600	-1.20988700	0.36681000
C	2.09273500	-1.10027800	-3.48229200
H	3.32690300	0.62985000	-3.10751900
C	1.28537600	-2.08417100	-2.91410100
H	0.45569300	-2.88852800	-1.09697000
H	2.24209300	-1.06728800	-4.55657000
H	0.80293400	-2.81884400	-3.55079400
C	4.71003900	-0.96946100	1.12929200
O	3.62623700	-1.20573100	1.62962000
C	5.95729200	-1.82336500	1.36931900
O	4.92978000	0.04137100	0.29891400
C	6.35956300	-2.45192500	0.02653300
H	6.59528400	-1.67903000	-0.70947500
H	7.24203300	-3.08559500	0.16575500
H	5.55170600	-3.07567100	-0.37128100
C	7.09169900	-0.92632600	1.88152600
H	6.81914100	-0.45034000	2.82961100
H	7.98974000	-1.52966500	2.05232200
H	7.32848000	-0.14417500	1.15621400
C	5.63132000	-2.91137900	2.39036300
H	5.32012600	-2.47354700	3.34279200
H	4.81627100	-3.54757100	2.03592300
H	6.51552200	-3.53409000	2.56282400

IM1a

C	-8.67381700	2.28847700	1.10929700
C	-7.42377500	1.72558400	0.86705800
C	-7.15351000	1.07906200	-0.34080800
C	-8.16377600	1.00490500	-1.30235100
C	-9.41510400	1.56638600	-1.06510300
C	-9.67340600	2.20992300	0.14280600
H	-8.86607200	2.79192000	2.05175200
H	-6.64332200	1.79156600	1.62168500
H	-7.96360100	0.50533300	-2.24752500
H	-10.18795700	1.50406500	-1.82497800
H	-10.64774300	2.65058800	0.32865900
C	-5.81578200	0.42242300	-0.57828200
H	-5.55762200	0.47137100	-1.64221800
H	-5.02935900	0.94752900	-0.02831100
C	-5.84185100	-1.05039400	-0.13115100
H	-6.61625000	-1.60505400	-0.66516700
H	-6.06438300	-1.09502500	0.94108500
C	-4.52958200	-1.75302500	-0.37919900
O	-4.37234800	-2.73657900	-1.04901100
O	-3.52386500	-1.10140500	0.26986800
C	-2.22286700	-1.58557200	0.20154000
C	-1.61458300	-1.93150400	-1.00202600
C	-1.52136800	-1.63882000	1.39974300
C	-0.28820900	-2.34588200	-0.99261200
H	-2.17461300	-1.89168600	-1.92756400
C	-0.19182100	-2.04433000	1.40267600
H	-2.02469300	-1.35327200	2.31717800
C	0.42729500	-2.41053400	0.20583100
H	0.20213400	-2.63442600	-1.91765300
H	0.38113700	-2.08594900	2.32341300
O	1.72450600	-2.83853100	0.22689100
I	3.14060000	-1.52782400	-0.43902400
C	2.65917100	-0.24824200	1.14093300
C	1.74676300	0.77725800	0.91801900
C	3.28420200	-0.44341500	2.37089600
C	1.47817800	1.65915900	1.96369900
H	1.27640800	0.91259700	-0.04750800
C	2.98702300	0.43715600	3.40677500
H	3.98929500	-1.25456500	2.51671300
C	2.09319600	1.48825400	3.19971700
H	0.80208300	2.48774200	1.78583900
H	3.46439800	0.30654400	4.37241900
H	1.88140100	2.18036300	4.00832000
C	4.29299200	1.11148100	-1.17309500
O	3.16347600	1.30555900	-1.63220600
C	5.26056400	2.25773100	-0.89547500
O	4.69674100	-0.06738900	-0.78908300
C	4.90135100	2.71653700	0.53330900
H	5.02500200	1.89852100	1.25209100
H	5.56125900	3.53987500	0.82672600
H	3.86523300	3.06719500	0.56618600
C	6.71432100	1.78828300	-0.95888300
H	6.96891200	1.42411400	-1.95952700
H	7.37766600	2.62671000	-0.72271100
H	6.89998100	0.98267000	-0.24535800
C	5.00860800	3.40273600	-1.87937400
H	5.17048900	3.08114900	-2.91302200
H	3.98782000	3.77928000	-1.78636800
H	5.69802700	4.22539000	-1.66383400
F	1.88565500	3.30124000	-0.67646200
H	2.34832500	2.61391200	-1.15916400

IM1b

C	-8.28130600	0.86665100	1.23818200
C	-7.00490000	0.34242700	1.05613900
C	-6.10806300	0.93518100	0.16388600
C	-6.51943500	2.06529100	-0.54598900
C	-7.79521900	2.59359000	-0.36788600
C	-8.68011900	1.99514800	0.52559500
H	-8.96406800	0.39613800	1.93915400
H	-6.69438000	-0.53715200	1.61575800
H	-5.82857000	2.53561100	-1.24177700
H	-8.09723300	3.47528100	-0.92487400
H	-9.67425200	2.40710000	0.66781200
C	-4.74380200	0.33595800	-0.06629000
H	-4.02520600	1.10278600	-0.37006500
H	-4.35912600	-0.11184600	0.85606400
C	-4.79696900	-0.75410000	-1.15746500
H	-5.16217300	-0.33279200	-2.09648100
H	-5.46563000	-1.55996500	-0.83970700
C	-3.41337100	-1.29702400	-1.39281300
O	-2.68968500	-1.00040400	-2.30507800
O	-3.06857800	-2.14323000	-0.38092000
C	-1.73235200	-2.46654600	-0.19788200
C	-0.91197600	-2.90329300	-1.23272100
C	-1.24780900	-2.33752300	1.09901700
C	0.43782200	-3.10841200	-0.97446500
H	-1.30794000	-3.02117300	-2.23214900
C	0.09913900	-2.55787400	1.35435500
H	-1.92474100	-2.01109500	1.88111300
C	0.95431000	-2.89150100	0.30232200
H	1.11224000	-3.39202800	-1.77697800
H	0.51479000	-2.41168900	2.34605400
O	2.31145300	-2.91952200	0.51669400
I	3.22563400	-1.23604900	-0.18044400
C	2.42229400	-0.10824600	1.38761600
C	1.12582900	0.37352400	1.25178100
C	3.21121400	0.15665700	2.50448400
C	0.59910500	1.14860400	2.28312900
H	0.52492600	0.14815600	0.38278100
C	2.66861800	0.94062300	3.51897700
H	4.22235100	-0.22883900	2.58055200
C	1.36793700	1.43401500	3.40776000
H	-0.41523600	1.51972000	2.18058400
H	3.26502000	1.16374000	4.39754900
H	0.95521700	2.04306100	4.20572700
C	3.38117100	1.64235200	-1.06084300
O	2.21272300	1.51936600	-1.43776700
C	4.00759300	3.02748700	-0.91705600
O	4.14695000	0.66435700	-0.67210000
F	-1.59382300	0.51376800	-0.21503300
H	-1.06918300	0.23321600	-0.95813300
C	3.96899800	3.32522400	0.59398200
H	4.58955600	2.61303200	1.14590300
H	4.34636300	4.33647500	0.77885800
H	2.94468400	3.26204200	0.98002100
C	5.45680500	3.01952300	-1.41232300
H	5.50595100	2.79309900	-2.48248900
H	5.90251500	4.00718000	-1.25465300
H	6.05090100	2.27689300	-0.87541100
C	3.17774200	4.05803000	-1.68068300
H	3.15205900	3.82703200	-2.74980400
H	2.14786400	4.07896700	-1.31762700
H	3.61849100	5.05197500	-1.55218900
F	0.36179600	-0.13879000	-1.77213700
H	1.10201700	0.49175900	-1.68900700

IM1c

C	-8.41604000	0.91331700	1.48911800
C	-7.12616900	0.44392400	1.25748600
C	-6.35700300	0.95189600	0.20782900
C	-6.91079700	1.94062900	-0.60863500
C	-8.20039200	2.41338400	-0.38186600
C	-8.95704800	1.90057300	0.66892500
H	-8.99814100	0.51048400	2.31243000
H	-6.70476400	-0.32521600	1.90094900
H	-6.32026200	2.34426300	-1.42782900
H	-8.61349800	3.18519200	-1.02412100
H	-9.96180800	2.26970100	0.84908800
C	-4.97860300	0.40843200	-0.07206100
H	-4.34271900	1.17345100	-0.52613800
H	-4.48778000	0.10060900	0.85688100
C	-5.04997200	-0.80663100	-1.01889900
H	-5.52255900	-0.52712300	-1.96295100
H	-5.63867800	-1.60103200	-0.54848400
C	-3.66785400	-1.32002000	-1.32927500
O	-3.09347400	-1.18843900	-2.37655500
O	-3.15478500	-1.93997800	-0.23374100
C	-1.81022900	-2.22481200	-0.09066000
C	-0.91608900	-2.45232000	-1.13758000
C	-1.38658400	-2.30083600	1.23475800
C	0.41790800	-2.71385400	-0.83375400
H	-1.24433400	-2.40188300	-2.16475900
C	-0.05438700	-2.55243600	1.52772100
H	-2.11178500	-2.12407200	2.02152200
C	0.85541700	-2.74463500	0.48850700
H	1.13351900	-2.85734800	-1.63708700
H	0.30407200	-2.56947000	2.55176400
O	2.18766500	-2.90222000	0.79654700
I	3.35885900	-1.35418600	0.22432800

C	2.16487600	-0.00081800	1.28263400
C	0.98495800	0.45845700	0.70482200
C	2.58831900	0.39215600	2.55034700
C	0.20215500	1.34998900	1.43780900
H	0.66632900	0.13442900	-0.27984000
C	1.79919300	1.29448700	3.25692300
H	3.51228300	0.01236300	2.97324800
C	0.61210500	1.76928200	2.70030500
H	-0.73027700	1.68722500	1.00130900
H	2.11239400	1.61980100	4.24359500
H	-0.00238000	2.46666200	3.26063300
C	4.01944200	1.44579500	-0.84232900
O	3.03393200	1.36139400	-1.59887600
C	4.64091900	2.81367600	-0.58129000
O	4.53001900	0.46932800	-0.17435200
F	-1.94705900	0.61673100	-0.49982800
H	0.31609700	-0.00827500	-2.51993700
F	-0.58750200	0.34071500	-2.59632400
H	-1.51293000	0.45200200	-1.33806900
C	4.08703000	3.24306000	0.79101100
H	4.42984000	2.56477700	1.57794300
H	4.43468500	4.25474100	1.02437200
H	2.99059900	3.24475700	0.79003800
C	6.16744500	2.70562800	-0.51912400
H	6.57957100	2.38929800	-1.48287700
H	6.59212700	3.68449400	-0.27422700
H	6.47993600	1.98739400	0.24188600
C	4.20957100	3.80683000	-1.65955900
H	4.54544300	3.48334800	-2.64926500
H	3.12257700	3.90772900	-1.68992500
H	4.64932700	4.78701700	-1.44925400
F	1.69582300	-0.46626600	-2.34169200
H	2.31636100	0.29430100	-2.02283800

IM1d

C	8.54340100	0.35343500	-0.97205300
C	7.31386800	-0.30111300	-0.92553400
C	6.16554800	0.37338900	-0.51172500
C	6.26516000	1.71787700	-0.13882100
C	7.49122100	2.37267900	-0.18478300
C	8.63433800	1.69188300	-0.60211700
H	9.42905800	-0.18287900	-1.29905100
H	7.24396000	-1.34651700	-1.21687800
H	5.36746000	2.23953200	0.18614100
H	7.55590100	3.41766500	0.10292500
H	9.59085600	2.20386000	-0.63953100
C	4.83114600	-0.32332000	-0.41767900
H	4.04705300	0.34034400	-0.79532200
H	4.82480800	-1.23732200	-1.01954200
C	4.49660600	-0.67282200	1.04765600
H	4.65470700	0.20081800	1.68141000
H	5.13072700	-1.49560900	1.39193200
C	3.04744100	-1.04648000	1.16479900
O	2.19202100	-0.37186500	1.67745000
O	2.78651500	-2.23191800	0.54898000
C	1.44925800	-2.55094300	0.33016700
C	0.52429900	-2.59361600	1.36849100
C	1.07493800	-2.80080500	-0.98381800
C	-0.81413900	-2.81518100	1.06736100
H	0.83007900	-2.38274600	2.38486200
C	-0.26414900	-3.02557800	-1.28070900
H	1.82828000	-2.76662200	-1.76369600
C	-1.21231500	-2.99326700	-0.25881200
H	-1.56475500	-2.77541700	1.85117900
H	-0.59852400	-3.16421100	-2.30336300
O	-2.54295400	-3.03076000	-0.59517000
I	-3.48973200	-1.24877700	-0.32623800
C	-1.87076700	-0.22533300	-1.17229500
C	-0.84345900	0.22186200	-0.34454400
C	-1.85355800	-0.06798600	-2.55583200
C	0.24763100	0.85167400	-0.94269200
H	-0.86540800	0.07093200	0.72814000
C	-0.75761600	0.56994000	-3.12954200
H	-2.66916900	-0.43335400	-3.17069700
C	0.28662800	1.02185100	-2.32456700
H	1.06222600	1.20639800	-0.32358700
H	-0.72198300	0.70709000	-4.20537800
H	1.14240000	1.51279000	-2.77688900
C	-3.82602700	1.71796200	0.43654600
O	-3.09641200	1.55004300	1.43390200
C	-4.05831300	3.13114100	-0.08336200
O	-4.35597500	0.77490600	-0.26169700
F	2.98853100	1.95619800	0.59550700
H	-1.04997700	-0.25927100	2.95725000
F	-0.08999900	-0.19032100	3.14670200
H	2.30693900	1.76451900	1.23331900
C	-3.15017400	3.25236200	-1.32298100
H	-3.45306700	2.54239300	-2.09834600
H	-3.22418500	4.26672400	-1.72818800
H	-2.10214300	3.05941400	-1.06558900
C	-5.52443000	3.31223400	-0.48949200
H	-6.18815400	3.21652600	0.37601300
H	-5.66293900	4.31198500	-0.91330900
H	-5.82007900	2.57131600	-1.23548500
C	-3.65304200	4.15936200	0.97171600
H	-4.25324200	4.04900200	1.87975400
H	-2.60191500	4.04777700	1.24678600
H	-3.80907700	5.16767700	0.57524800
F	0.79074100	1.80868000	1.92633900
H	0.60555100	0.98603100	2.39165500
F	-2.40496500	-0.41848700	2.54428100
H	-2.76490300	0.43118500	2.04341400

IM1e

C	8.83053200	1.10226200	-0.81304100
C	7.70293400	0.29641900	-0.96087400
C	6.48064600	0.67511300	-0.40693000
C	6.40419300	1.87762300	0.30395100
C	7.52721000	2.68380300	0.45317000
C	8.74499300	2.29775800	-0.10601700
H	9.77508800	0.79564100	-1.25214000
H	7.77144800	-0.63627200	-1.51580600
H	5.44910600	2.16923700	0.73649000
H	7.45355600	3.61652200	1.00422300
H	9.62186800	2.92730200	0.00890100
C	5.25207200	-0.19241300	-0.52252900
H	4.38431100	0.43292700	-0.74965500
H	5.36219100	-0.91474800	-1.33666300
C	4.97685900	-0.93267800	0.79645300
H	5.11468800	-0.26568800	1.64951000
H	5.67305900	-1.77195100	0.91514500
C	3.56793600	-1.45188300	0.90953200
O	2.89814700	-1.42685000	1.90831600
O	3.13811300	-1.95871300	-0.27864500
C	1.79856700	-2.23481400	-0.49713900
C	0.94890500	-2.79046400	0.45774800
C	1.34278200	-1.93339900	-1.77907700
C	-0.39180800	-2.97537700	0.13390300
H	1.30354700	-3.02473300	1.45026700
C	0.00486900	-2.12155000	-2.09557700
H	2.04052600	-1.51817800	-2.49822500
C	-0.86454600	-2.61692700	-1.12426200
H	-1.08580800	-3.34348800	0.87994700
H	-0.38649100	-1.84998400	-3.07058300
O	-2.21228400	-2.69213600	-1.41964800
I	-3.33964500	-1.20372300	-0.67334900
C	-1.92752500	0.24338600	-1.17144100
C	-0.89203700	0.46501700	-0.26798000
C	-2.00507600	0.85880200	-2.41977200
C	0.12973600	1.33330600	-0.65599800
H	-0.86080800	-0.03602000	0.69448100
C	-0.98721100	1.73963500	-2.77166800
H	-2.82856500	0.65470900	-3.09601600
C	0.07790100	1.96298600	-1.89684500
H	0.97749600	1.48268700	0.00262500
H	-1.02002300	2.23770600	-3.73519400
H	0.87992200	2.63286100	-2.19003200
C	-4.26269100	1.62644300	0.66919200
O	-3.85377400	1.36917000	1.86166800
C	-4.33672300	3.09985100	0.31231600
O	-4.54781200	0.74968400	-0.17720600
H	-2.90448600	-1.25712600	2.35320700
F	-1.77851700	-1.44107800	2.07121600
C	-2.87945400	3.60008800	0.25813100
H	-2.30715800	3.07390400	-0.51417700
H	-2.88089300	4.66712800	0.01320800
H	-2.37881800	3.46090600	1.21981100
C	-5.00256200	3.28096900	-1.05037100
H	-6.02288700	2.88701500	-1.05094600
H	-5.04120400	4.34663600	-1.29585200
H	-4.43805600	2.76469500	-1.83190700
C	-5.10746000	3.85076600	1.40565900
H	-6.14142000	3.49743800	1.47393400
H	-4.63145500	3.72188100	2.38010200
H	-5.12842400	4.91785400	1.16376100
F	0.28569500	-1.66543200	3.14173100
H	-0.64980600	-1.60531000	2.77088600
F	-3.96653200	-0.97960700	2.41936700
H	-3.89747400	0.35130200	2.10434500
F	0.95058700	0.42717100	2.15292200
H	0.86228000	-0.46471200	2.55916300
F	2.99849600	1.23750200	0.96731800
H	2.35093100	0.84257700	1.55263500

IM1

C	8.32104600	2.37485400	-0.31242400
C	7.38177000	1.51287600	-0.87625300
C	6.19963700	1.20949100	-0.20185200
C	5.97313600	1.78348900	1.05379500
C	6.90782700	2.64340400	1.61962100
C	8.08612600	2.94222900	0.93635300
H	9.23605800	2.60335800	-0.85057000
H	7.56712200	1.07230100	-1.85305100
H	5.05037300	1.54320100	1.57859400
H	6.71763200	3.08392200	2.59371300
H	8.81619900	3.61455000	1.37611300
C	5.17607900	0.25666500	-0.76869700
H	4.17309000	0.65546100	-0.59701000
H	5.30415600	0.14995700	-1.85075900
C	5.26710800	-1.11490300	-0.09004700
H	5.38564300	-0.99297900	0.99068100
H	6.14462800	-1.67308900	-0.43608500
C	4.05531400	-2.00313600	-0.24335000
O	3.86645100	-3.01159500	0.37866700
O	3.20337000	-1.52885100	-1.19742900
C	1.87985300	-1.89517400	-1.26631000
C	1.16123300	-2.49915900	-0.23374000
C	1.24459500	-1.50980600	-2.44836100
C	-0.21393000	-2.66698400	-0.37682200
H	1.65220400	-2.83167700	0.66852400
C	-0.12222500	-1.68692000	-2.58789400
H	1.83653200	-1.04558100	-3.22956000
C	-0.85233700	-2.25398000	-1.54288700
H	-0.79626800	-3.09006300	0.43431800
H	-0.64125900	-1.36734500	-3.48610900
O	-2.22253800	-2.34608500	-1.67172000
I	-3.29837100	-0.81537000	-0.90824100
C	-1.72708900	0.53847700	-1.00632200
C	-0.77274400	0.46649900	0.00502300
C	-1.60671600	1.36650600	-2.12178100
C	0.38034900	1.23885300	-0.13972800
H	-0.89458800	-0.18895800	0.86209300
C	-0.46671100	2.15710800	-2.22025800
H	-2.37277300	1.38705300	-2.88987000
C	0.52748900	2.07623700	-1.24255900
H	1.17351000	1.14993100	0.59367700
H	-0.34417900	2.81587900	-3.07365900
H	1.43070700	2.66895100	-1.34704400
C	-4.18682000	1.94833700	0.70463100
O	-4.01715500	1.48628200	1.90517600
C	-4.03169900	3.45197900	0.57797700
O	-4.41703200	1.23028500	-0.28386000
F	0.66806300	-3.13550500	2.72218500
H	-3.43036400	-1.32674500	2.06129100
F	-2.19282000	-1.61245300	1.97923700
H	-0.29369500	-3.48751700	2.64837800
C	-2.54354800	3.75566000	0.84265900
H	-1.89934800	3.26011900	0.10741600
H	-2.38336900	4.83555300	0.76178200
H	-2.24703800	3.43117800	1.84341000
C	-4.41569000	3.90036900	-0.83061000
H	-5.45495200	3.64803300	-1.05947000
H	-4.29503000	4.98487800	-0.91112100
H	-3.77673500	3.42374100	-1.57926100
C	-4.90361500	4.14654000	1.63244000
H	-5.96457500	3.92815500	1.47392100
H	-4.63023400	3.82838000	2.64084200
H	-4.76497000	5.22943200	1.55723800
F	-1.55523200	-3.73996000	2.45895900
H	-1.92412900	-2.73367600	2.26215900
F	-4.40685100	-0.97550800	2.01175300
H	-4.18172800	0.48447200	1.95791200
F	0.78614200	-0.79028000	2.29179600
H	0.70546100	-1.75709600	2.49800400
F	2.93806500	-0.09424600	1.25397600
H	2.16391100	-0.43496200	1.70684900

IM1g

C	8.99410100	0.49330200	-0.59329800
C	7.79813000	-0.19730700	-0.78067600
C	6.57283700	0.43506100	-0.57253500
C	6.56115500	1.77411900	-0.16842300
C	7.75312000	2.46542300	0.01885800
C	8.97397400	1.82617000	-0.19363200
H	9.94107200	-0.01040500	-0.76196900
H	7.81571200	-1.23781600	-1.09625600
H	5.60197300	2.26111800	-0.00608500
H	7.73120300	3.50592300	0.32848000
H	9.90465600	2.36607800	-0.04952000
C	5.26474500	-0.29844200	-0.73457900
H	4.54108200	0.35471100	-1.23024100
H	5.39153700	-1.18902100	-1.35681500
C	4.69024700	-0.70447700	0.63421300
H	4.77251500	0.11682900	1.34848600
H	5.24578400	-1.55911700	1.03823900
C	3.23165100	-1.06247200	0.56624900
O	2.37600700	-0.66557900	1.31412800
O	2.97402700	-1.89996500	-0.47446300
C	1.64451200	-2.14892700	-0.78920200
C	0.76571100	-2.71515300	0.12892400
C	1.23679600	-1.80365300	-2.07186700
C	-0.56613400	-2.88467100	-0.23154100
H	1.10312500	-2.96026200	1.12798900
C	-0.09491700	-1.97252800	-2.42877400
H	1.95756900	-1.37222600	-2.75795000
C	-0.99350800	-2.48634900	-1.49606300
H	-1.27981300	-3.26881500	0.48620900
H	-0.45908700	-1.67052500	-3.40519700
O	-2.33362800	-2.51591600	-1.82624900
I	-3.42074300	-0.99068800	-1.08287500
C	-1.83494400	0.35396300	-1.16270500
C	-0.99358300	0.40897600	-0.05393100
C	-1.60335200	1.06531500	-2.33945600
C	0.15254700	1.19470000	-0.15663400
H	-1.20168800	-0.15181200	0.85208700
C	-0.45611500	1.85127500	-2.40617900
H	-2.28645600	0.99808400	-3.17977400
C	0.42681400	1.89895300	-1.32555600
H	0.83019200	1.24387100	0.68255200
H	-0.24597000	2.41145500	-3.31155100
H	1.34273300	2.47726700	-1.38094900
C	-4.36008800	1.74285000	0.49775900
O	-4.20249800	1.28922600	1.69981600
C	-4.24148400	3.24793400	0.35689600
O	-4.55008000	1.01510400	-0.49603900
F	0.96382700	-2.14609300	3.22097700
H	-3.56600700	-1.46815400	1.93817200
F	-2.31622800	-1.61171900	1.89144200
H	0.10583300	-2.66550800	3.10993600
C	-2.74064100	3.57023700	0.51071700
H	-2.14976700	3.10242000	-0.28455600
H	-2.60559800	4.65441100	0.44214200
H	-2.35859700	3.23084200	1.47741700

C	-4.72794400	3.68313700	-1.02465900
H	-5.78036200	3.42577100	-1.17581900
H	-4.61898300	4.76754400	-1.12078300
H	-4.14290700	3.20306200	-1.81362100
C	-5.04270900	3.93874900	1.46696000
H	-6.10820500	3.69830100	1.39397900
H	-4.68694900	3.63931100	2.45502200
H	-4.93139000	5.02282900	1.36851800
F	-1.05546000	-3.27202400	2.81714200
H	-1.69250400	-2.50498400	2.43630300
F	-4.56273500	-1.16852800	1.84008300
H	-4.34862700	0.28177300	1.76050200
F	0.40266300	0.17743700	2.79868100
H	0.69545700	-0.75675900	2.89172500
F	2.24472200	1.78984100	2.43968500
H	1.63311900	1.05155400	2.58501300
F	3.17786800	1.77988900	0.09764100
H	2.88069800	1.72941600	1.00711000

IM2b

C	7.48913800	0.82245600	-1.98726500
C	6.69440600	-0.05339900	-1.24871700
C	5.47576900	0.37140500	-0.72388900
C	5.05693800	1.68829900	-0.94398500
C	5.84883400	2.56193800	-1.68007600
C	7.06776100	2.13046800	-2.20393300
H	8.43616500	0.48066200	-2.39357100
H	7.02390100	-1.07634700	-1.08238700
H	4.10264700	2.00463500	-0.52630500
H	5.51417900	3.58062400	-1.85004700
H	7.68473900	2.81253500	-2.78049900
C	4.59328500	-0.53762300	0.09704100
H	3.56179900	-0.42732800	-0.24411600
H	4.88731500	-1.58488600	-0.02969900
C	4.63904600	-0.14689800	1.57944500
H	4.69005200	0.93970500	1.68318200
H	5.51991000	-0.56264300	2.08298200
C	3.44222200	-0.52789900	2.39266200
O	3.15406200	-0.24193300	3.50301500
O	2.63332700	-1.53991600	1.71001300
C	1.34114500	-1.56980400	1.78556500
C	0.54888200	-0.50230500	2.32664100
C	0.75328400	-2.77622800	1.23519700
C	-0.79459100	-0.60431100	2.25348400
H	1.02878200	0.40891000	2.64472900
C	-0.58301300	-2.91792200	1.22054800
H	1.43696000	-3.51980200	0.84184000
C	-1.45328400	-1.85333200	1.78521100
H	-1.45054300	0.22369600	2.50246000
H	-1.07848400	-3.80564400	0.84165100
O	-2.65243200	-2.01734800	1.88889600
I	-3.64204000	-1.34267600	-1.17137700
C	-1.56070100	-1.45331100	-1.36353800
C	-0.76422800	-0.41518200	-0.88113000
C	-0.99308600	-2.56193000	-2.01028800
C	0.61828900	-0.48422100	-1.06079200
H	-1.18966300	0.43301600	-0.35351200
C	0.38338600	-2.61324000	-2.18482800
H	-1.62794000	-3.35875700	-2.38371400
C	1.19052900	-1.57496400	-1.71027600
H	1.23548500	0.30919200	-0.65260600
H	0.82624200	-3.46251800	-2.69625400
H	2.26610900	-1.61539200	-1.85792400
C	-2.83555900	2.40586100	0.52264200
O	-1.78178000	3.08431700	0.09959800
C	-4.15564000	3.06008000	0.12705100
O	-2.76207300	1.35785300	1.14178900
F	2.38354600	1.11559900	0.94788400
H	1.34694900	1.56310900	0.92315700
C	-4.23035700	3.08422900	-1.40764200
H	-4.19287500	2.06863000	-1.81732100
H	-5.17315100	3.54466100	-1.72251800
H	-3.40140300	3.65872400	-1.82866800
C	-5.31501000	2.25098300	0.70351300
H	-5.26091700	2.21093500	1.79499400
H	-6.26678400	2.70987900	0.41561500
H	-5.29301300	1.22182500	0.33418100
C	-4.18082600	4.49703100	0.66680400
H	-4.11339000	4.50773400	1.75989100
H	-3.34887900	5.07941300	0.26393100
H	-5.12081500	4.98095400	0.38027600
F	0.23157300	1.81575700	0.93402100
H	-0.93991100	2.62924300	0.41290800

IM2c

C	7.74200000	0.44842200	-2.26189700
C	6.53292700	-0.05817700	-1.79392400
C	5.75610400	0.66853300	-0.88907100
C	6.21605100	1.91458300	-0.45767700
C	7.42506100	2.42507300	-0.92233100
C	8.19100500	1.69272600	-1.82596100
H	8.33154500	-0.12601600	-2.96966300
H	6.18216600	-1.02826700	-2.13987600
H	5.61647600	2.48968300	0.24392200
H	7.76684500	3.39736500	-0.58155100
H	9.13200800	2.09118500	-2.19153100
C	4.46779000	0.09922000	-0.34518400
H	3.76748500	0.89384300	-0.08291600
H	3.99043500	-0.53617100	-1.09884200
C	4.74829300	-0.72310800	0.91835900
H	5.17463800	-0.09740100	1.70670400
H	5.49081000	-1.50340500	0.69879100
C	3.59082700	-1.43433400	1.54807200
O	3.44985000	-1.81420000	2.65828400
O	2.66540700	-1.89987000	0.51468400
C	1.40741700	-2.11130600	0.72648800
C	0.71586700	-1.80524000	1.95693700
C	0.73276400	-2.69949400	-0.41266000
C	-0.59007500	-2.12821600	2.04616200
H	1.21260400	-1.25257600	2.74131200
C	-0.56457300	-3.03963500	-0.32389000
H	1.32379400	-2.84058400	-1.31029200
C	-1.30300400	-2.84496600	0.95218200
H	-1.18011500	-1.85537000	2.91405300
H	-1.11156100	-3.50179800	-1.13949300
O	-2.42697000	-3.27697600	1.10000700
I	-4.03597400	-1.33120200	-1.37591500
C	-2.08460800	-0.58792500	-1.26551400
C	-1.62996600	-0.06602900	-0.05147100
C	-1.27049500	-0.58174400	-2.40659700
C	-0.34199200	0.46039100	0.01894700
H	-2.27225100	-0.05337300	0.82428100
C	0.01536500	-0.06560200	-2.31230800
H	-1.64405300	-0.97172900	-3.34754300
C	0.48936200	0.44095600	-1.09520000
H	0.02105200	0.83703800	0.96525500
H	0.65245500	-0.05791600	-3.19193400
H	1.49708300	0.83430100	-1.01085300
C	-3.26908900	2.39966100	1.06214700
O	-2.08798200	2.61121200	1.64627100
C	-3.59764000	3.45408800	0.01202600
O	-3.96852400	1.44085700	1.31027700
H	-0.20490700	0.65448300	3.14471600
F	1.03771400	0.79066000	3.33399300
C	-2.62753200	3.23569300	-1.16209500
H	-2.75656500	2.23642400	-1.59461800
H	-2.82662000	3.97558200	-1.94517500
H	-1.58828300	3.33875900	-0.83661700
C	-5.03899100	3.26101800	-0.45440100
H	-5.73957000	3.39087500	0.37563500
H	-5.27915600	3.99357100	-1.23226400
H	-5.18418500	2.25500400	-0.85712200
C	-3.39733500	4.85743300	0.59659600
H	-4.06203400	5.02602100	1.45031200
H	-2.36698000	4.99973300	0.93050900
H	-3.62707200	5.60943200	-0.16607300
H	1.73028300	0.71932100	2.32321600
F	-1.20878200	0.47856800	2.91714000
H	-1.87728300	1.84347800	2.23699000
F	2.25885800	0.51209000	1.42459400

IM2d

C	7.62325400	0.80234800	-1.58721100
C	6.66778900	-0.20303100	-1.44615700
C	5.48821000	0.03718200	-0.74436800
C	5.27464100	1.29899900	-0.17986000
C	6.22636100	2.30270300	-0.31922300
C	7.40411100	2.05582200	-1.02435000
H	8.53742900	0.60515400	-2.13852800
H	6.83943200	-1.18115700	-1.88929200
H	4.35015700	1.47606700	0.36664300
H	6.04877800	3.28011300	0.11844200
H	8.14660000	2.83971600	-1.13533500
C	4.44217600	-1.03309000	-0.54613400
H	3.45271400	-0.59916900	-0.70827200
H	4.57751300	-1.84669000	-1.26614800
C	4.49744900	-1.57828700	0.88613500
H	4.65030500	-0.76088000	1.59635700
H	5.33185900	-2.27618700	1.02166900
C	3.26040200	-2.26377900	1.37920700
O	3.00615900	-2.67346200	2.46032900
O	2.34112500	-2.54078300	0.29307400
C	1.04987600	-2.57475900	0.44816900
C	0.36265600	-2.05347000	1.59972400
C	0.35244000	-3.17592800	-0.66178500
C	-0.97899400	-2.20143400	1.65527700
H	0.90599400	-1.53154100	2.37382400
C	-0.98541600	-3.33456800	-0.60778000
H	0.95442700	-3.49597900	-1.50439700
C	-1.73419900	-2.91085700	0.59445200
H	-1.56023600	-1.79752700	2.47370700
H	-1.55294200	-3.81383200	-1.39819400
O	-2.92233000	-3.15158100	0.71751700
I	-4.22028700	-0.73034600	-0.83595900
C	-2.23167100	-0.62795600	-1.43249000
C	-1.27396600	-0.05525500	-0.59201500
C	-1.87450000	-1.11180400	-2.70498700
C	0.04688000	0.02828900	-1.03194900
H	-1.54451700	0.31513200	0.39120700
C	-0.55921100	-1.00626800	-3.13341500
H	-2.63284200	-1.54278300	-3.35051800
C	0.40539200	-0.44175400	-2.29350400
H	0.79289500	0.44724200	-0.36776700
H	-0.28633600	-1.36324700	-4.12165400
H	1.43464400	-0.35556200	-2.63004400
C	-2.32379300	3.03626100	0.38672300
O	-2.23547700	2.64104400	1.65954700
C	-1.46451500	4.25715900	0.08525800
O	-2.97189500	2.43781700	-0.44431100
F	2.36294700	0.02274600	1.23063600
H	-1.97045800	0.15646100	2.87956700
F	-0.71349900	0.08376100	3.44653100
H	1.53595600	0.55544600	1.52320000
C	-0.06132500	3.70572700	-0.22823300
H	-0.09363900	3.06805000	-1.11872100
H	0.62501300	4.53736400	-0.42292900
H	0.31908500	3.11255800	0.60854200
C	-2.03240000	4.97654900	-1.13777500
H	-3.02765200	5.38188100	-0.92856800
H	-1.37487700	5.80609600	-1.41846400
H	-2.11969000	4.29002100	-1.98272400
C	-1.39600800	5.20115100	1.28881400
H	-2.39258200	5.55715600	1.56963400
H	-0.95519600	4.70339200	2.15510800
H	-0.78223300	6.07195200	1.03412700
F	0.40621900	1.12310500	1.76794900
H	-0.15025900	0.63878800	2.68428100
F	-2.78143200	0.12182300	2.30203600
H	-2.70671800	1.78341100	1.76232100

IM2e

C	7.74431600	2.45718000	-0.86993700
C	6.88019100	1.41630200	-1.20512700
C	5.76897600	1.13684200	-0.41165700
C	5.53283800	1.91170900	0.72810400
C	6.39352400	2.95053600	1.06464200
C	7.50235200	3.22547600	0.26475700
H	8.60494200	2.66810600	-1.49707600
H	7.06902200	0.81891200	-2.09395700
H	4.66316600	1.68699600	1.34290200
H	6.19806800	3.54946100	1.94859200
H	8.17328800	4.03777000	0.52545700
C	4.83199400	-0.00322700	-0.72828500
H	3.80059000	0.32092900	-0.56944500
H	4.93328600	-0.30805200	-1.77498200
C	5.10682600	-1.19351100	0.19730400
H	5.23317700	-0.85061300	1.22829500
H	6.03160600	-1.71367700	-0.07849400
C	4.02466200	-2.22560500	0.28015400
O	3.94017200	-3.17442900	0.98300500
O	3.03480300	-2.03427700	-0.76021500
C	1.78138500	-2.35414200	-0.61733500
C	1.16378700	-2.63718300	0.65171000
C	1.05116700	-2.39659300	-1.85837200
C	-0.13180500	-3.01840500	0.65604500
H	1.72550900	-2.53057000	1.56839200
C	-0.24674600	-2.76316700	-1.86098900
H	1.59551000	-2.13447400	-2.75818300
C	-0.91496600	-3.14727300	-0.59761900
H	-0.65471900	-3.23588600	1.57695000
H	-0.83331800	-2.84103400	-2.77011900
O	-2.05639100	-3.57131300	-0.59104000
I	-3.75318700	-0.87821700	-0.73230400
C	-1.83267100	-0.23988300	-1.20236300
C	-0.90410900	-0.01948200	-0.18153500
C	-1.50635500	0.03517900	-2.54402400
C	0.35836300	0.47168100	-0.51153400
H	-1.15806900	-0.22207800	0.85283800
C	-0.25177800	0.54144400	-2.85270400
H	-2.24522900	-0.12541500	-3.32266600
C	0.68551100	0.75281400	-1.83675000
H	1.08386200	0.62300400	0.27826400
H	-0.00501700	0.77273100	-3.88431000
H	1.66539500	1.15449600	-2.07842600
C	-3.82250600	2.58147700	0.61237500
O	-3.00904600	1.88795600	1.41834300
C	-3.13455500	3.79851000	0.00189200
O	-4.97805700	2.28030800	0.42175800
H	-3.34941900	-0.84566200	2.53505600
F	-2.15026900	-1.71616400	2.19935800
C	-1.77807400	3.39524500	-0.58856100
H	-1.89565700	2.63929000	-1.37409900
H	-1.29633800	4.27360700	-1.03274700
H	-1.12035400	2.98655700	0.18239200
C	-4.03892400	4.38723200	-1.07877500
H	-5.01407400	4.65616300	-0.66596400
H	-3.57449400	5.28228900	-1.50613700
H	-4.20783000	3.66372300	-1.88228300
C	-2.91961700	4.81858700	1.13205000
H	-3.87534100	5.11849600	1.57412200
H	-2.28843200	4.39880200	1.91997300
H	-2.43165900	5.71422300	0.73226400
F	-0.15759100	-1.87041400	3.33409200
H	-1.31091100	-1.76024900	2.81349000
F	-4.07184300	-0.22171300	2.66117200
H	-3.52610100	1.15770500	1.83784200
F	0.78542800	0.00174700	2.46981000
H	0.35426900	-0.89987000	2.95038600
F	2.82480300	-0.38246500	1.40869700
H	1.98488100	-0.20554600	1.94001200

IM2

C	7.74789300	2.21940700	-0.20855800
C	7.05767900	1.01056600	-0.28218700
C	5.69067600	0.96129500	-0.01662900
C	5.01885400	2.13868100	0.32736500
C	5.70548200	3.34526000	0.40154600
C	7.07333100	3.38751800	0.13311800
H	8.81221400	2.24723000	-0.42013600
H	7.58572100	0.09935000	-0.55284800
H	3.95122500	2.09198700	0.53476200
H	5.17399000	4.25427200	0.66501600
H	7.60972300	4.32934900	0.18883100

C	4.91536300	-0.33333000	-0.06097900
H	3.96565800	-0.16478400	-0.57305100
H	5.46460200	-1.09627900	-0.62211300
C	4.61754400	-0.83184900	1.35687800
H	4.31621800	0.00541600	1.99363000
H	5.49945600	-1.28272300	1.82522500
C	3.49768000	-1.81594000	1.49633500
O	3.07416200	-2.34869300	2.46166600
O	2.96765900	-2.21616700	0.19063200
C	1.72828100	-2.51872300	-0.01118000
C	0.67535400	-2.31519300	0.95400300
C	1.49159800	-3.12081900	-1.30982000
C	-0.54304700	-2.83074800	0.68653200
H	0.86254500	-1.78780100	1.87888300
C	0.27972600	-3.62256100	-1.59437100
H	2.33196000	-3.16001500	-1.99280700
C	-0.80744900	-3.58650100	-0.57485600
H	-1.36923200	-2.73544800	1.38722700
H	0.05399400	-4.12119900	-2.53083100
O	-1.84629900	-4.18076300	-0.75532800
I	-2.77490700	-0.55060600	-0.68801800
C	-1.02425300	-0.62467200	-1.83890800
C	0.13344500	-0.02901700	-1.34096500
C	-1.01863200	-1.23206900	-3.09840400
C	1.29677200	-0.03180200	-2.11037900
H	0.12702300	0.42553700	-0.35761600
C	0.14741800	-1.21460000	-3.86813500
H	-1.92482800	-1.68876600	-3.48497100
C	1.30365000	-0.61333500	-3.38003800
H	2.18309400	0.45634500	-1.71610500
H	0.14022100	-1.66629400	-4.85565800
H	2.20407400	-0.58995900	-3.98610600
C	-3.81017400	2.91722800	-0.16871500
O	-3.87728900	2.30803900	1.02312800
C	-2.69059400	3.94893200	-0.23213600
O	-4.53146700	2.62807100	-1.09459000
F	-0.43899600	-0.82845300	3.22514600
H	-4.91166100	-0.37205000	1.85982900
F	-4.45410000	-0.70582500	3.20247900
H	-1.52937000	-1.37582900	3.11333400
C	-1.37587300	3.16028800	-0.36852700
H	-1.38747500	2.54756600	-1.27803300
H	-0.53572900	3.86071800	-0.43952400
H	-1.21177200	2.50458000	0.49243700
C	-2.90222200	4.83393600	-1.45913700
H	-3.84182200	5.38971800	-1.38339300
H	-2.07986500	5.55205400	-1.54573000
H	-2.94510200	4.23084200	-2.36906300
C	-2.66050600	4.79212400	1.04722300
H	-3.60155900	5.33536000	1.18301500
H	-2.49568800	4.16612300	1.92681100
H	-1.85045900	5.52679000	0.98234300
F	-2.42247100	-1.92652500	2.92872100
H	-3.60996500	-1.21559700	3.12610500
F	-5.11903700	-0.09961900	0.94614400
H	-4.51711800	1.56654600	0.94451200
F	0.06902000	0.87623900	1.80280600
H	-0.23892200	0.10602300	2.50052800
F	2.13861900	0.20639700	0.91197000
H	1.29948600	0.55477600	1.33650900

IM2g

C	7.77817700	2.69695000	-0.88612500
C	7.11216100	1.74717100	-0.11344500
C	5.73600100	1.57037400	-0.24397800
C	5.02978900	2.35931000	-1.15730700
C	5.69211600	3.30740700	-1.92887100
C	7.06965700	3.47771500	-1.79433300
H	8.85083800	2.82447000	-0.77892000
H	7.66787100	1.13541300	0.59322400
H	3.95502100	2.21628100	-1.25291400
H	5.13536200	3.91129800	-2.63842100
H	7.58798900	4.21594400	-2.39783200
C	4.97732500	0.57166000	0.59600600
H	4.24808400	0.05542800	-0.03144900
H	5.65485700	-0.18104000	1.01196400
C	4.21922500	1.28153100	1.72183900
H	3.73455700	2.18390900	1.33714000
H	4.88941300	1.60138700	2.52755900
C	3.10464800	0.51220400	2.36005500
O	2.36867600	0.82416300	3.22918900
O	3.05082900	-0.86754600	1.86508100
C	1.95173700	-1.53638400	1.74968600
C	0.63787100	-0.95605400	1.86335300
C	2.16376000	-2.95404300	1.51892200
C	-0.42944600	-1.78301700	1.87419600
H	0.50873500	0.11351100	1.94504200
C	1.11142400	-3.78617000	1.51864400
H	3.18732600	-3.28179100	1.38040400
C	-0.26352700	-3.26433500	1.76859900
H	-1.44518600	-1.40794800	1.97660300
H	1.20917400	-4.85903400	1.39213800
O	-1.19677400	-4.02237300	1.90884600
I	-1.89448200	-1.95091500	-1.21415400
C	0.10463600	-2.55751700	-1.38887600
C	1.09829000	-1.57953900	-1.37596600
C	0.44128900	-3.90677000	-1.52322300
C	2.43453200	-1.95665900	-1.51260200
H	0.83210300	-0.53662400	-1.25525200
C	1.78184100	-4.27059000	-1.67573100
H	-0.33712500	-4.66381900	-1.53246600
C	2.77883700	-3.29977800	-1.67458500
H	3.19880900	-1.18508600	-1.52623900
H	2.03793500	-5.31812700	-1.80386100
H	3.81805800	-3.58481800	-1.80579300
C	-4.03698100	2.55341600	-0.59453200
O	-3.08035900	1.61068800	-0.57613500
C	-3.54112500	3.89796600	-0.08443000
O	-5.16319600	2.31584500	-0.96709400
F	-1.16829200	1.20075000	1.40068000
H	-5.24585800	-0.36403500	-0.91913800
F	-6.33037900	-0.06232600	0.02276300
H	-2.21025500	0.55731000	1.41575300
C	-2.23600100	4.26495500	-0.80460600
H	-2.39532600	4.35740500	-1.88438500
H	-1.87429600	5.22943200	-0.43145500
H	-1.46486700	3.50907800	-0.63756300
C	-4.61787100	4.94981100	-0.34133200
H	-5.55139700	4.67920700	0.15825000
H	-4.28284500	5.92163800	0.03622900
H	-4.82758700	5.04378100	-1.41087800
C	-3.27605300	3.76237500	1.42459300
H	-4.18797900	3.47837500	1.95657400
H	-2.50754300	3.00926500	1.61698600
H	-2.92654000	4.72414000	1.81612400
F	-3.04144800	-0.10604100	1.53766600
H	-5.91374200	0.56638300	0.63885600
F	-4.42366300	-0.57031300	-1.40448200
H	-3.48645900	0.78761400	-0.93329900
F	-0.11015200	1.44987500	-0.60962200
H	-0.71073600	1.34793300	0.27198700
F	2.05501500	0.89365300	0.11651400
H	1.15793900	1.21713700	-0.20146800
F	-5.03357600	1.18787800	1.67068900
H	-4.19361600	0.65504900	1.65400600

TSa

C	-7.25234500	-0.92293900	1.76447800
C	-6.11857400	-1.43743500	1.14011400
C	-5.06734000	-0.59967700	0.76412300
C	-5.17476200	0.76959000	1.02300500
C	-6.30555700	1.28816500	1.64639300
C	-7.34838000	0.44235000	2.01913700
H	-8.05935500	-1.58913500	2.05410100
H	-6.04469000	-2.50494900	0.94482900
H	-4.35863600	1.42841100	0.73413400
H	-6.37174900	2.35348600	1.84511900
H	-8.22984100	0.84563200	2.50771100
C	-3.85648200	-1.14077300	0.04445900
H	-2.95874700	-0.58990000	0.33577300
H	-3.70453500	-2.19460200	0.29938700
C	-4.01938100	-0.98926200	-1.47016100
H	-4.23605800	0.05301800	-1.72338900
H	-4.86217000	-1.58501300	-1.84154100
C	-2.81274400	-1.34319400	-2.29716500
O	-2.67561300	-1.14934200	-3.46707800
O	-1.85795800	-2.03783500	-1.55200300
C	-0.54070500	-1.85831900	-1.72625500
C	0.02559000	-0.91331400	-2.61729800
C	0.26595800	-2.64739100	-0.88235700
C	1.37428700	-0.69978700	-2.56154200
H	-0.60945200	-0.32994200	-3.26561800
C	1.61995500	-2.42835900	-0.82861100
H	-0.22240100	-3.37502100	-0.24407800
C	2.21125500	-1.43805500	-1.67098900
H	1.84113200	0.06750000	-3.17113900
H	2.26506100	-2.99184700	-0.16161200
O	3.47253600	-1.16325500	-1.58317500
I	3.73310800	0.60184000	-0.06505500
C	3.21284800	-0.74219700	1.42251300
C	1.88001000	-0.85639700	1.81083500
C	4.21813500	-1.57354400	1.92779200
C	1.55545100	-1.84444000	2.74271600
H	1.12941700	-0.19917800	1.37860100
C	3.86645200	-2.55179300	2.84832300
H	5.24711600	-1.46126400	1.60364200
C	2.53644000	-2.68502800	3.25664300
H	0.52320700	-1.95057300	3.06041400
H	4.63124900	-3.20763900	3.25100200
H	2.27110400	-3.44831700	3.98132100
C	0.76311800	2.12677300	0.39373200
O	0.36172400	0.99208600	-0.07000800
C	-0.01832900	3.38324000	-0.03101100
O	1.74786500	2.23068600	1.14296100
C	-1.43069600	3.29963500	0.56951200
H	-1.38736400	3.25031300	1.66303700
H	-2.00397100	4.19148900	0.29174300
H	-1.95530300	2.41974400	0.19036500
C	0.69229900	4.63679800	0.47346900
H	1.70109500	4.71051200	0.05614200
H	0.12805900	5.52917500	0.18031600
H	0.78708000	4.61973700	1.56202200
C	-0.11468100	3.40285800	-1.56370200
H	0.88335200	3.40461700	-2.01888200
H	-0.66875200	2.53473800	-1.92715700
H	-0.63532700	4.30912900	-1.89268200
F	-1.72316700	0.65824100	-1.16798500
H	-0.80508100	0.84442300	-0.68825200

TS1b

C	-7.36268800	0.88340800	1.65459400
C	-6.15047800	0.27008800	1.35312300
C	-5.42735700	0.63130400	0.21321700
C	-5.94825000	1.62193500	-0.62168600
C	-7.16102200	2.23896600	-0.32511300
C	-7.87181200	1.87112500	0.81430100
H	-7.90896500	0.59334300	2.54703600
H	-5.75327900	-0.49868700	2.01287500
H	-5.39254300	1.91295200	-1.50971800
H	-7.54923900	3.01017700	-0.98335600
H	-8.81600200	2.35287600	1.04803300
C	-4.13640500	-0.06832200	-0.13261200
H	-3.49576800	0.56042100	-0.75447600
H	-3.57243000	-0.29826400	0.77797500
C	-4.41820200	-1.38233000	-0.88117400
H	-4.96639900	-1.19614600	-1.80713300
H	-5.03703600	-2.03390600	-0.25049600
C	-3.18003400	-2.15383800	-1.24994400
O	-2.90885300	-2.60409100	-2.32284700
O	-2.42035100	-2.38703000	-0.11478600
C	-1.09539400	-2.65508600	-0.15033900
C	-0.29206600	-2.58978000	-1.30617100
C	-0.53400400	-2.91711500	1.11136600
C	1.06922800	-2.70881700	-1.16368600
H	-0.72413100	-2.36188600	-2.26716700
C	0.83414600	-3.00606300	1.25122800
H	-1.19695500	-2.96400700	1.96792700
C	1.66059800	-2.91834000	0.10617000
H	1.71612900	-2.56286000	-2.02308100
H	1.30003100	-3.13853100	2.22241000
O	2.97586600	-2.93754100	0.23380300
I	3.78438200	-0.87251700	0.07807400
C	2.21305500	-0.13510900	1.18135000
C	1.01717600	0.09731500	0.50601300
C	2.34246500	-0.00803700	2.57019100
C	-0.09786100	0.47258600	1.25563300
H	0.94302900	-0.01256500	-0.57262600
C	1.22175900	0.38202500	3.29099800
H	3.28734300	-0.20365800	3.06571400
C	0.00797300	0.61841000	2.63462200
H	-1.02705700	0.63189300	0.71857500
H	1.29316500	0.49865000	4.36740900
H	-0.85942000	0.92056000	3.21346100
C	2.33673500	2.44618800	-1.13119700
O	1.14763000	2.33544300	-1.66285000
C	2.52518100	3.73948800	-0.33972800
O	3.21487400	1.59325000	-1.21978100
F	-1.45583500	-0.08983600	-1.31531100
H	-0.58757100	0.01740800	-1.89021100
C	1.57669100	3.68164500	0.86889500
H	1.82491800	2.83798900	1.52493900
H	1.66714100	4.60389700	1.45353100
H	0.53899800	3.57037600	0.54295800
C	3.97240000	3.84456900	0.13535100
H	4.66513800	3.84985700	-0.71091800
H	4.11159100	4.76745700	0.70817800
H	4.23370000	2.99575000	0.77515700
C	2.15807600	4.93513200	-1.22772000
H	2.81359800	4.98949500	-2.10322500
H	1.12586200	4.85566200	-1.57593700
H	2.26955100	5.86578800	-0.66074200
F	0.55772800	0.10527000	-2.42963700
H	0.97453400	1.39212400	-2.08490200

TS1c

C	7.07814100	2.11582600	-0.95299100
C	6.38078500	0.92506200	-1.15186700
C	5.18311600	0.68449800	-0.48106400
C	4.68979700	1.65467000	0.39850800
C	5.38366200	2.84281200	0.59817200
C	6.58081000	3.07670900	-0.07832400
H	8.00953700	2.29133400	-1.48270300
H	6.77019400	0.17614500	-1.83744000
H	3.75577300	1.45754000	0.92214300
H	4.99009100	3.58970100	1.28085900
H	7.12203900	4.00482000	0.07667700
C	4.41095600	-0.60046300	-0.65724700
H	3.35294000	-0.36707600	-0.79891300
H	4.74997200	-1.13700000	-1.54963600
C	4.53924200	-1.49423800	0.58045400
H	4.46398200	-0.88582600	1.48681600
H	5.51106200	-1.99817700	0.61989100
C	3.46868600	-2.53685000	0.75562700
O	3.34160300	-3.27124000	1.68713600
O	2.61221200	-2.60872500	-0.34706200
C	1.29749200	-2.83643900	-0.20754800
C	0.61892500	-2.75870900	1.02862900
C	0.60539600	-3.04097600	-1.42237600
C	-0.74979000	-2.80107300	1.02487000
H	1.15272100	-2.56030500	1.94447600
C	-0.76437100	-3.09666100	-1.42087700
H	1.18393400	-3.09623000	-2.33754600
C	-1.48204700	-3.00555700	-0.18751200
H	-1.31083500	-2.60976300	1.93462700
H	-1.33340300	-3.22244900	-2.33625800
O	-2.77021300	-3.04950700	-0.17365500
I	-3.68226800	-0.86453300	-0.08944700
C	-2.01828400	-0.21198900	-1.10856200
C	-0.83602100	0.01944400	-0.40236900
C	-2.07543000	-0.12727700	-2.50768400
C	0.31383000	0.34642900	-1.12081600
H	-0.80626900	-0.06233900	0.67606600
C	-0.92065300	0.20931200	-3.20083600

H	-3.00519200	-0.31645900	-3.03353000
C	0.27114700	0.44313000	-2.50762900
H	1.22943700	0.51164100	-0.56380800
H	-0.94956100	0.28590000	-4.28286900
H	1.17016600	0.70472000	-3.05734400
C	-2.67575900	2.61440900	0.81371200
O	-1.75239500	2.21715200	1.67114300
C	-2.32754300	3.93650300	0.14033200
O	-3.67795900	1.97246900	0.54309800
F	2.04046700	-0.33413800	1.22177200
H	-0.74806900	-0.36790400	2.69931000
F	0.39843600	-0.56838800	2.86445300
H	1.32848400	-0.36735000	1.95080100
C	-1.19259300	3.62763900	-0.85252000
H	-1.50546400	2.87190500	-1.58370800
H	-0.92235400	4.53938400	-1.39618500
H	-0.30696500	3.25546800	-0.32964900
C	-3.55085000	4.46323100	-0.60724000
H	-4.37990300	4.65221000	0.08100600
H	-3.29895700	5.40062800	-1.11377300
H	-3.89394500	3.74132700	-1.35253800
C	-1.84691800	4.95448000	1.18062500
H	-2.63369000	5.17203700	1.91030800
H	-0.97259400	4.58293000	1.71919700
H	-1.58000600	5.89111700	0.67975200
F	-1.81254400	-0.22180500	2.44981600
H	-1.93647100	1.29656400	2.02424500

TS1d

C	7.99097000	1.47747500	-1.13541300
C	7.06952700	0.43398800	-1.20958900
C	5.83362600	0.53268800	-0.57258300
C	5.53186100	1.69453400	0.14592700
C	6.44895500	2.73656100	0.22203200
C	7.68262900	2.63033700	-0.41990400
H	8.94928300	1.38868600	-1.63812500
H	7.31196400	-0.46533800	-1.77086500
H	4.56540800	1.76258400	0.64184100
H	6.20172600	3.63456800	0.77998400
H	8.39886000	3.44399000	-0.36235700
C	4.82210200	-0.58680900	-0.60577800
H	3.82780700	-0.16828700	-0.77809800
H	5.03780200	-1.28009300	-1.42548200
C	4.79823700	-1.33703300	0.73011800
H	4.82414800	-0.62274500	1.55865200
H	5.67620100	-1.98196200	0.84719700
C	3.57494400	-2.17255700	0.99884400
O	3.33055200	-2.75632400	2.01195900
O	2.74053300	-2.24143100	-0.10969300
C	1.42195300	-2.50190700	0.00581200
C	0.67474100	-2.26732800	1.17575800
C	0.80549700	-2.92604100	-1.18996600
C	-0.68583400	-2.46892400	1.13352400
H	1.14126100	-1.87728200	2.06880900
C	-0.55474100	-3.10950000	-1.23164100
H	1.43149500	-3.07160200	-2.06316100
C	-1.32917600	-2.92359700	-0.05333800
H	-1.30707900	-2.21427300	1.98496400
H	-1.06179400	-3.41698300	-2.14049200
O	-2.61824800	-3.11749800	-0.07823700
I	-3.78810700	-1.16205900	-0.37718400
C	-2.11999500	-0.34421400	-1.24295800
C	-1.09152300	0.09767400	-0.40812300
C	-1.98299400	-0.40188100	-2.63753700
C	0.12229500	0.45698600	-0.99371300
H	-1.21519100	0.14365100	0.66728700
C	-0.77784100	-0.00634700	-3.19873100
H	-2.80214700	-0.74837700	-3.25836700
C	0.27562500	0.40320800	-2.37518600
H	0.94393000	0.75297500	-0.35440500
H	-0.65291100	-0.03531700	-4.27611100
H	1.22484300	0.68686000	-2.81904500
C	-3.35565400	2.44058100	0.50049300
O	-2.73995700	2.12318200	1.62733900
C	-2.92189300	3.79898900	-0.03206300
O	-4.14548600	1.70657700	-0.07286600
F	2.51891600	0.23436500	1.14210600
H	-1.68840100	-0.28339900	2.82336600
F	-0.47738600	-0.26985300	3.12731200
H	1.74336500	0.72138000	1.51253100
C	-1.47653300	3.62425900	-0.53437200
H	-1.44175900	2.92766000	-1.38009400
H	-1.09022400	4.59145000	-0.87366900
H	-0.82673500	3.23971800	0.25839800
C	-3.83760000	4.21375200	-1.18118400
H	-4.87182100	4.32194100	-0.84098200
H	-3.50443200	5.17294200	-1.59036200
H	-3.82391200	3.46748400	-1.97965700
C	-2.95721600	4.83822400	1.09547500
H	-3.96819500	4.94532100	1.50224200
H	-2.28529800	4.55730400	1.90912900
H	-2.64475100	5.81105800	0.70191900
F	0.53058900	1.32918400	1.85995400
H	0.04611600	0.61358500	2.51460100
F	-2.65575100	-0.33057500	2.41716800
H	-2.92811600	1.18881000	1.90879200

TS1e

C	8.09472800	2.23420400	-0.70944100
C	7.17049000	1.27297500	-1.11519300
C	6.01109200	1.04682100	-0.37491500
C	5.78987700	1.79689000	0.78463200
C	6.71003200	2.75637400	1.19222300
C	7.86616900	2.97763200	0.44442300
H	8.99239500	2.40239400	-1.29653500
H	7.34995300	0.69466600	-2.01848600
H	4.88360500	1.61429200	1.35914900
H	6.52511200	3.33515200	2.09195000
H	8.58422400	3.72773300	0.76061200
C	5.00645600	-0.00836800	-0.76776600
H	3.99578500	0.38333700	-0.62925300
H	5.11804700	-0.27484700	-1.82388000
C	5.16029200	-1.25529900	0.10981200
H	5.27438500	-0.96484900	1.15853200
H	6.05871000	-1.82435700	-0.15505300
C	3.99651500	-2.20863500	0.10829900
O	3.86012800	-3.16481000	0.80877300
O	3.06940100	-1.88990600	-0.88554900
C	1.77730100	-2.24100200	-0.80074500
C	1.12175200	-2.57685600	0.40456600
C	1.07801800	-2.16642700	-2.02914000
C	-0.22492700	-2.83663600	0.36297500
H	1.65866100	-2.60199200	1.34192700
C	-0.26556100	-2.42251500	-2.06684100
H	1.63856200	-1.88976300	-2.91501200
C	-0.95678100	-2.79944600	-0.87027200
H	-0.77742800	-3.04716300	1.26881700
H	-0.83278300	-2.36951600	-2.99047100
O	-2.20869600	-3.07877700	-0.90059800
I	-3.60076200	-1.14649600	-0.53996500
C	-1.95676400	-0.01059000	-0.99953300
C	-0.96161500	0.13253000	-0.02784800
C	-1.79448300	0.47062200	-2.30884500
C	0.24164800	0.73576900	-0.39627100
H	-1.10723400	-0.23659100	0.98157600
C	-0.60043400	1.09240500	-2.64343700
H	-2.58946900	0.35490000	-3.03806900
C	0.42179200	1.20391900	-1.69383400
H	1.04093200	0.80241900	0.33103600
H	-0.45840200	1.47472500	-3.64903800
H	1.36282400	1.66992600	-1.96972800
C	-3.83926500	2.36126700	0.44601300
O	-3.31989800	2.05659700	1.62711000
C	-3.41693700	3.73980100	-0.04282800
O	-4.56728800	1.61098200	-0.18071600
H	-3.30891900	-0.84295600	2.57912800
F	-2.18612300	-1.67576900	2.28032000
C	-1.88277200	3.78878700	-0.08861600
H	-1.49040400	3.04606700	-0.79167700
H	-1.55981200	4.77970600	-0.42583000
H	-1.45119600	3.59407700	0.89629000
C	-3.99563100	3.97767400	-1.43551900
H	-5.08691200	3.91606600	-1.42488400
H	-3.70163500	4.96959500	-1.79358800
H	-3.62515000	3.22810800	-2.14184900
C	-3.94312600	4.78754100	0.94963700
H	-5.03608100	4.75905600	1.00925400
H	-3.53604300	4.61658000	1.94924800
H	-3.64646800	5.78761000	0.61655300
F	-0.16695000	-1.99423400	3.25573600
H	-1.25241400	-1.82836100	2.85447600
F	-4.08856400	-0.24822900	2.61366900
H	-3.66377900	1.18118800	1.94488000
F	0.77936600	-0.06020400	2.48400700
H	0.38946000	-0.95408300	2.89169400
F	2.85354300	-0.23529800	1.30367400
H	2.05402500	-0.18450800	1.86836300

TS1

C	8.05911900	2.51273200	-0.34055900
C	7.16873500	1.60818000	-0.91676900
C	6.00631200	1.23196400	-0.24542100
C	5.74777900	1.77339100	1.01805600
C	6.63407800	2.67571600	1.59560400
C	7.79342800	3.04826700	0.91606100
H	8.95955000	2.79934200	-0.87521700
H	7.37723700	1.19279900	-1.89991400
H	4.83979100	1.47492300	1.53877900
H	6.42032800	3.09190500	2.57528800
H	8.48523800	3.75390900	1.36512800
C	5.03704600	0.23125400	-0.82579600
H	4.01414200	0.57101000	-0.64542100
H	5.17109100	0.14575300	-1.90910500
C	5.21103500	-1.13953000	-0.16306000
H	5.30673800	-1.02298900	0.92082500
H	6.12619000	-1.63718600	-0.50325000
C	4.07120600	-2.10626300	-0.33738600
O	3.95631200	-3.17055800	0.18880200
O	3.13557700	-1.64277200	-1.26465600
C	1.84391700	-2.00518800	-1.22458100
C	1.20676200	-2.53788500	-0.08282000
C	1.12778200	-1.72365700	-2.41224600
C	-0.14902900	-2.74667800	-0.12797900
H	1.76200800	-2.75177000	0.81852700
C	-0.21798900	-1.96233800	-2.46609200
H	1.67621200	-1.30994600	-3.25101700
C	-0.89663000	-2.51111200	-1.32948300
H	-0.68658200	-3.10320300	0.74410700
H	-0.79992200	-1.76310600	-3.36012900
O	-2.14988900	-2.77783200	-1.38970000
I	-3.53808500	-0.90214200	-0.80387200
C	-1.87870600	0.27505800	-1.05898400
C	-0.89251600	0.24593600	-0.06783600
C	-1.69953400	0.96152700	-2.27096900
C	0.32166100	0.88444600	-0.32659400
H	-1.05288200	-0.26525700	0.87648300
C	-0.49677600	1.61665800	-2.48953600
H	-2.48937800	0.97672400	-3.01464500
C	0.51909100	1.55747800	-1.52780400
H	1.11815300	0.82341700	0.40518900
H	-0.34212300	2.15816700	-3.41711300
H	1.46741100	2.05110600	-1.71720500
C	-3.89563400	2.43572700	0.60273200
O	-3.54468600	1.95064500	1.78645400
C	-3.39127900	3.85387500	0.37618600
O	-4.53993400	1.80245000	-0.21518300
F	0.67030700	-2.98331700	2.83652800
H	-3.55095800	-0.97937500	2.30047900
F	-2.21730300	-1.51826800	2.11856100
H	-0.37758000	-3.35419600	2.84672600
C	-1.85961000	3.84330600	0.49223900
H	-1.41516600	3.19972900	-0.27475000
H	-1.47675500	4.85916400	0.34631000
H	-1.53958900	3.48464400	1.47371800
C	-3.81159000	4.31973300	-1.01573900
H	-4.89898800	4.30142500	-1.12643900
H	-3.45709500	5.34143100	-1.18591000
H	-3.38542900	3.66989900	-1.78636900
C	-3.99059500	4.76474900	1.45783300
H	-5.08417300	4.77327000	1.40378900
H	-3.69497500	4.43233800	2.45584900
H	-3.63483200	5.78971600	1.30992900
F	-1.51016400	-3.60203700	2.72603600
H	-1.96539500	-2.49898500	2.44403300
F	-4.40415300	-0.50265400	2.28460800
H	-3.93166000	1.04833500	1.91876800
F	0.75749600	-0.72309300	2.31441200
H	0.68275000	-1.70724300	2.59682600
F	2.87655600	-0.35512600	1.19627000
H	2.07308300	-0.51127500	1.72312800

TS1g

C	8.92182800	0.77805700	-0.85977100
C	7.75477100	0.04079900	-1.05319000
C	6.52548100	0.53340700	-0.61805300
C	6.47901700	1.77779100	0.01878500
C	7.64165900	2.51495200	0.21328600
C	8.86736900	2.01585900	-0.22645800
H	9.87274200	0.38485900	-1.20595100
H	7.79908700	-0.92496800	-1.55103700
H	5.51609500	2.15636900	0.35604700
H	7.59301200	3.48147100	0.70531600
H	9.77526800	2.59159700	-0.07682100
C	5.24808800	-0.25285600	-0.78306700
H	4.44897200	0.41798400	-1.10811600
H	5.36462100	-1.02539800	-1.54915100
C	4.83191500	-0.89472500	0.54942700
H	4.99496500	-0.20592100	1.38102600
H	5.43457100	-1.78921800	0.75189500
C	3.38583500	-1.28666900	0.63950800
O	2.71092300	-1.32483700	1.62367000
O	2.88672500	-1.61837500	-0.62234500
C	1.60782800	-1.98043900	-0.82901900
C	0.81483200	-2.65711600	0.12764400
C	1.12608700	-1.67038700	-2.12460900
C	-0.49277300	-2.91962800	-0.18011500
H	1.20747000	-2.90957300	1.10162500
C	-0.17315500	-1.94507400	-2.44099100
H	1.80264700	-1.17799100	-2.81410000
C	-1.03896200	-2.58467700	-1.47705400
H	-1.14696400	-3.39354100	0.54245000
H	-0.59312400	-1.70341000	-3.41170900
O	-2.24163100	-2.83909500	-1.76399300
I	-3.71567700	-0.81321400	-1.27000800
C	-1.95281100	0.23581600	-1.21924300
C	-1.15561200	0.16256300	-0.07058100
C	-1.52974800	0.93519300	-2.36630400
C	0.09968100	0.76591800	-0.09819400
H	-1.49169400	-0.35919200	0.81937700
C	-0.28565100	1.54843100	-2.35708200
H	-2.17393800	0.99192800	-3.23765100
C	0.53890400	1.44637300	-1.23010100
H	0.73358700	0.70113300	0.77412800
H	0.04765900	2.09565500	-3.23307400
H	1.52107100	1.90723300	-1.21280100
C	-4.02958800	2.37218800	0.56487800
O	-3.70246200	1.68786400	1.65808800
C	-3.44770400	3.77941200	0.55964300
O	-4.70613700	1.90897400	-0.33302500
F	0.55439100	-2.83088300	3.08732700
H	-3.95870600	-1.28997400	1.86598200
F	-2.63988900	-1.92017900	1.62819700
H	-0.47779400	-3.25319700	2.95786400
C	-1.91615500	3.66166700	0.56537700
H	-1.56255800	3.14981300	-0.33645300
H	-1.47308200	4.66337700	0.58290800
H	-1.56411600	3.10733900	1.43955000
C	-3.91522000	4.50841400	-0.69802600
H	-5.00581300	4.58004600	-0.72889100
H	-3.49590600	5.51961700	-0.71646300
H	-3.59069500	3.97764700	-1.59776000
C	-3.91835600	4.51726500	1.82102900
H	-5.01045200	4.59197700	1.84897500

H	-3.58349800	4.00115000	2.72381300
H	-3.50814100	5.53261300	1.82447500
F	-1.54898500	-3.61178700	2.71921000
H	-2.18904500	-2.67844300	2.20539300
F	-4.76014000	-0.74372900	1.88001600
H	-4.15418400	0.80782900	1.65722200
F	0.24110800	-0.59440400	2.57710900
H	0.44462000	-1.57768800	2.82810700
F	1.96979700	1.06234600	2.73673000
H	1.32425700	0.31451500	2.72875000
F	3.05535400	1.33139600	0.53839100
H	2.68050200	1.24841500	1.42721600

TS2b

C	8.14219700	-0.52032200	-1.11023200
C	6.89348400	-0.69675200	-0.51981300
C	5.86695500	0.22577700	-0.72996400
C	6.11697700	1.33452600	-1.54248200
C	7.36330500	1.51539600	-2.13463200
C	8.37982500	0.58731800	-1.91979700
H	8.92839100	-1.24951100	-0.94048100
H	6.70952200	-1.56485300	0.10938300
H	5.32267200	2.05748200	-1.71350800
H	7.54015600	2.37949400	-2.76753600
H	9.35136300	0.72554500	-2.38348900
C	4.52625500	0.06277300	-0.05506400
H	3.72429600	0.45558500	-0.68415300
H	4.32653100	-0.99836200	0.12630200
C	4.50007600	0.82436800	1.27268300
H	4.73452700	1.88020000	1.11375500
H	5.25732700	0.42468100	1.95936600
C	3.20732500	0.82387600	2.03330500
O	2.90182500	1.38786000	3.02430300
O	2.53898500	-0.56992400	1.80500000
C	1.29283700	-0.76356100	1.96666700
C	0.34028900	0.28063400	2.29515800
C	0.86824900	-2.14931900	1.78309500
C	-0.96416000	-0.03670700	2.36811400
H	0.68307900	1.29687100	2.39860400
C	-0.42856500	-2.47486200	1.87871100
H	1.64687400	-2.86453900	1.54290400
C	-1.44089600	-1.43834800	2.21494600
H	-1.73123600	0.71591600	2.51399100
H	-0.79409700	-3.48750400	1.74328400
O	-2.60520400	-1.73453300	2.38764200
I	-3.67762400	-1.75225000	-0.82193800
C	-1.58987200	-1.72528800	-1.02273100
C	-0.88896400	-0.53920000	-0.81475000
C	-0.92588100	-2.90141100	-1.39455700
C	0.49475100	-0.53138300	-0.99231500
H	-1.39403700	0.36607000	-0.49261800
C	0.45280000	-2.87696000	-1.57127800
H	-1.48657800	-3.81606400	-1.55634500
C	1.16472900	-1.69305800	-1.36948400
H	1.04450600	0.38165400	-0.79266100
H	0.96912000	-3.78442700	-1.86949900
H	2.24175900	-1.67421000	-1.51013700
C	-3.17924200	2.37325400	-0.09007800
O	-2.22125000	3.00871200	-0.75922100
C	-4.57593200	2.76886000	-0.55258500
O	-2.95286800	1.55402400	0.77966900
F	2.19323400	1.55712300	0.55142200
H	1.01943800	2.03592800	0.44034800
C	-4.71420500	2.38512700	-2.03429200
H	-4.57732500	1.30720300	-2.17439400
H	-5.71585300	2.65130700	-2.38858600
H	-3.97561300	2.91106000	-2.64448100
C	-5.61219300	2.02811100	0.28931300
H	-5.51230600	2.28314000	1.34800700
H	-6.62000800	2.29796400	-0.04303400
H	-5.48735900	0.94563400	0.19678900
C	-4.73938400	4.28764200	-0.39518700
H	-4.62826100	4.58913000	0.65176700
H	-3.99711200	4.82478100	-0.99042300
H	-5.73925500	4.58452600	-0.72923900
F	0.00877700	2.26191300	0.38952400
H	-1.34099900	2.75115600	-0.38534100

TS2c

C	7.50399300	0.18622600	-2.37812600
C	6.28097400	-0.16527400	-1.81475000
C	5.64481800	0.67936800	-0.90203000
C	6.26146900	1.88487300	-0.56130500
C	7.48527600	2.24100300	-1.12176400
C	8.10955600	1.39200300	-2.03200300
H	7.98284200	-0.47894800	-3.09001300
H	5.80809700	-1.10574000	-2.08976000
H	5.77358200	2.55149500	0.14591100
H	7.94949000	3.18384400	-0.84988300
H	9.06199100	1.66972600	-2.47202200
C	4.34176400	0.27297800	-0.25635000
H	3.76025700	1.15064800	0.03183700
H	3.73759500	-0.30923400	-0.96026400
C	4.60804300	-0.56285900	0.99794500
H	5.12660300	0.03078300	1.75628000
H	5.26037300	-1.41225300	0.75639000
C	3.42428700	-1.16015600	1.69827100
O	3.32942900	-1.64004600	2.77143000
O	2.55727200	-1.85311900	0.54723800
C	1.34025800	-2.16287900	0.70925100
C	0.59548400	-1.96739300	1.94938300
C	0.70163500	-2.75081500	-0.46581000
C	-0.69064300	-2.35069800	1.99438600
H	1.07055100	-1.47578600	2.78547300
C	-0.58418000	-3.12666200	-0.42314100
H	1.31550800	-2.83085500	-1.35594200
C	-1.36579400	-3.00026000	0.83659100
H	-1.30343900	-2.17739700	2.87252800
H	-1.10362800	-3.55330200	-1.27560200
O	-2.49767700	-3.42727300	0.92095900
I	-4.05547800	-1.24092600	-1.45219400
C	-2.10040400	-0.51462900	-1.25571800
C	-1.65580600	-0.08618200	-0.00477900
C	-1.26900400	-0.44464900	-2.38019200
C	-0.36025100	0.41345200	0.11814900
H	-2.31006400	-0.12403500	0.86096500
C	0.02334900	0.04656900	-2.23635900
H	-1.63253800	-0.76738100	-3.35005600
C	0.48572600	0.46465800	-0.98410700
H	-0.00532000	0.72828000	1.09071000
H	0.67215600	0.10359000	-3.10543000
H	1.49648700	0.83949700	-0.86080000
C	-3.12866500	2.46388100	1.08638700
O	-1.98363100	2.58892100	1.76986500
C	-3.29514100	3.54728000	0.02928000
O	-3.91190200	1.56136400	1.28095000
H	-0.30901000	0.47187800	3.27903100
F	1.07458400	0.61009900	3.50624300
C	-2.18054800	3.35913900	-1.01363800
H	-2.25464500	2.37799000	-1.49726100
H	-2.27224300	4.12932500	-1.78733400
H	-1.19279500	3.44109600	-0.55156700
C	-4.66495700	3.39120700	-0.62747400
H	-5.46680100	3.50210100	0.10792300
H	-4.79282700	4.15299800	-1.40369000
H	-4.76624300	2.40177500	-1.08225800
C	-3.16090800	4.92688700	0.68785200
H	-3.93360300	5.07580400	1.44933700
H	-2.18302700	5.04194300	1.16164500
H	-3.27715400	5.70813500	-0.07095700
H	1.67821200	0.53526800	2.63555700
F	-1.25902300	0.32505500	3.05063300
H	-1.88850200	1.80852000	2.36245800
F	2.28316400	0.33130700	1.58200000

TS2d

C	6.05063000	-3.91143500	-1.10154000
C	4.85363000	-3.40877400	-0.59989500
C	4.59789700	-2.03573000	-0.60520400
C	5.56756900	-1.17356300	-1.12059700
C	6.76663000	-1.67154700	-1.62328600
C	7.01076500	-3.04246600	-1.61463000
H	6.23242000	-4.98164000	-1.09560300
H	4.10335000	-4.08986800	-0.20386000
H	5.37587200	-0.10296600	-1.13255600
H	7.50858900	-0.98886500	-2.02538400
H	7.94358000	-3.43256400	-2.00897400
C	3.31953300	-1.48612000	-0.01854800
H	3.06511000	-0.53286000	-0.48795800
H	2.49095100	-2.17927400	-0.19870400
C	3.47953900	-1.26459300	1.48658700
H	4.26084200	-0.52497100	1.68718300
H	3.78834400	-2.19575100	1.97829700
C	2.28258000	-0.79094000	2.25399000
O	2.17568100	-0.39298000	3.35576500
O	1.05825700	-1.77426000	1.75612300
C	-0.15403700	-1.46272100	1.90609000
C	-0.61452600	-0.22940300	2.54701600
C	-1.11469500	-2.44095500	1.39625700
C	-1.93216900	0.00770400	2.62597200
H	0.10736600	0.48043300	2.91799000
C	-2.43063400	-2.20164500	1.46909800
H	-0.69596600	-3.32741800	0.93328800
C	-2.94168100	-0.96200200	2.11691000
H	-2.31836600	0.91727100	3.07244600
H	-3.17805400	-2.88709600	1.08142500
O	-4.13071900	-0.76510400	2.24719900
I	-5.05622800	-1.04392700	-1.33976300
C	-2.96218300	-0.88616300	-1.30041500
C	-2.37029000	0.21290200	-0.67635000
C	-2.18676700	-1.88722800	-1.89144700
C	-0.97919500	0.29682600	-0.63025300
H	-2.97131500	0.99357400	-0.22206900
C	-0.80045400	-1.78778500	-1.83770900
H	-2.66114500	-2.72838300	-2.38546900
C	-0.19492100	-0.70325100	-1.19766100
H	-0.50759400	1.13255200	-0.12439800
H	-0.19154500	-2.56010700	-2.29878800
H	0.88583100	-0.62426500	-1.14371900
C	0.55651900	3.88069700	-1.12762100
O	0.22250600	3.33753100	0.06078700
C	2.04424100	3.75686300	-1.42161200
O	-0.26434700	4.37225500	-1.86196600
F	1.66774200	0.48887600	1.07968000
H	-1.50675300	2.70431800	1.90065300
F	-0.56320800	2.71363900	3.02248700
H	1.68191100	1.54434900	1.74736800
C	2.34085400	2.26296000	-1.64114500
H	1.74203600	1.86209800	-2.46702500
H	3.39965600	2.13621100	-1.89599900
H	2.12396100	1.68651900	-0.73710900
C	2.36535500	4.55348800	-2.68411200
H	2.13007600	5.61282500	-2.54772400
H	3.43063500	4.45997900	-2.91931500
H	1.78222200	4.19056400	-3.53420700
C	2.85383300	4.27602300	-0.22575900
H	2.65295100	5.33803800	-0.04954300
H	2.61345000	3.72421200	0.68605100
H	3.92341300	4.16607500	-0.43560100
F	1.66805900	2.36858800	2.40465200
H	0.40680300	2.65278500	2.73015700
F	-2.08628700	2.63836800	1.12355700
H	-0.75448900	3.37074100	0.14514200

TS2e

C	-7.93178900	-0.17672800	0.23441500
C	-6.60663300	-0.50844400	-0.03311400
C	-5.56856800	0.35409200	0.32537200
C	-5.88348300	1.55974400	0.95566600
C	-7.20727800	1.89596500	1.22493600
C	-8.23485500	1.02785700	0.86445100
H	-8.72736100	-0.86017300	-0.04553200
H	-6.37218200	-1.45195800	-0.52134300
H	-5.08216200	2.23669100	1.24256800
H	-7.43580900	2.83446100	1.72013800
H	-9.26712600	1.28717400	1.07660300
C	-4.13486900	0.01709600	-0.00943700
H	-3.45180000	0.47428200	0.70930200
H	-3.98329900	-1.06624800	0.02401500
C	-3.78772700	0.53546200	-1.40677300
H	-3.91330000	1.62162700	-1.45552400
H	-4.46190800	0.10109100	-2.15556900
C	-2.40567700	0.28429100	-1.92591200
O	-1.84105900	0.67558300	-2.87685500
O	-2.12258900	-1.32331800	-1.55280400
C	-0.97152900	-1.83375000	-1.56121600
C	0.24043100	-1.11254900	-1.93930000
C	-0.90884100	-3.24945300	-1.18410200
C	1.42273800	-1.74984900	-1.91224300
H	0.16680300	-0.08848100	-2.26884100
C	0.26703100	-3.88739200	-1.14813800
H	-1.84965900	-3.71782800	-0.91806600
C	1.52733700	-3.18752000	-1.52529100
H	2.34930400	-1.24942200	-2.17818700
H	0.36164900	-4.92937800	-0.86108800
O	2.58598200	-3.77606300	-1.54562700
I	2.97685900	-0.97991100	1.08790500
C	1.19010400	-1.98973300	1.51209500
C	-0.01333200	-1.28976600	1.43264900
C	1.20269700	-3.33981400	1.86777700
C	-1.20869900	-1.94681200	1.72504800
H	-0.01735300	-0.24600400	1.14452300
C	0.00114600	-3.98119300	2.17422800
H	2.14265200	-3.88042100	1.92030900
C	-1.20423300	-3.28804100	2.10759400
H	-2.14123100	-1.39334900	1.66534900
H	0.01596000	-5.02591500	2.47025100
H	-2.13549500	-3.78847200	2.35439000
C	2.43322700	3.14743800	0.78211200
O	3.21478800	2.66258300	-0.20229200
C	1.52038000	4.28696800	0.33904900
O	2.52338000	2.76554900	1.92321000
F	1.89967800	1.29392200	-2.33256400
H	4.82486100	0.53363700	-0.84097200
F	4.08041500	0.29776200	-2.15886000
C	0.18063600	4.15363400	1.06874600
H	0.34148700	4.07586700	2.14661000
H	-0.44073800	5.03220400	0.86406500
H	-0.35535100	3.26104600	0.73515300
C	2.23158500	5.57198100	0.80371500
H	3.20472100	5.67982700	0.31317000
H	1.62076700	6.44464700	0.54910200
H	2.38672900	5.55470400	1.88617500
C	1.31443400	4.33788400	-1.17551100
H	2.26612100	4.43535500	-1.70379100
H	0.81470900	3.43912900	-1.54111900
H	0.68878800	5.20187400	-1.42468100
H	3.24833100	0.81759900	-2.21222700
F	5.10196900	0.72533500	0.06179800
H	3.84996700	2.03643500	0.20691800
F	0.70578600	1.39355100	-0.30938900
H	1.47352100	1.39260800	-1.42307700
F	-1.47922500	0.75764800	-0.40180000
H	-0.34216900	1.13585700	-0.41620400

TS2

C	-8.36606100	0.40772000	0.47275100
C	-7.02680600	0.03841800	0.39006600
C	-6.03915000	0.98863000	0.12078400
C	-6.41989900	2.31851700	-0.06768200
C	-7.75852000	2.69293400	0.01388300
C	-8.73484300	1.73772900	0.28428500
H	-9.12143900	-0.34148600	0.68828400
H	-6.74077000	-1.00020100	0.54227000
H	-5.65862200	3.06708400	-0.27423000
H	-8.03819200	3.73180600	-0.13016300
H	-9.77830100	2.02847700	0.35109700
C	-4.59246200	0.57680800	-0.01586000
H	-3.93004900	1.40947500	0.22917600
H	-4.36502600	-0.24298600	0.67261900
C	-4.30584400	0.12957500	-1.45176000
H	-4.45588400	0.95757100	-2.15147100
H	-4.99737600	-0.66897900	-1.74869800

C	-2.93834300	-0.40132200	-1.75718600
O	-2.38995000	-0.61528400	-2.77412200
O	-2.69248600	-1.52587500	-0.55529400
C	-1.60404900	-2.12800400	-0.35378300
C	-0.41488300	-2.00787000	-1.19349900
C	-1.61199500	-3.03178600	0.80304400
C	0.64732600	-2.78783600	-0.92716600
H	-0.41657300	-1.32329100	-2.02937800
C	-0.53636500	-3.76955500	1.10026000
H	-2.52106700	-3.03893400	1.39361100
C	0.66991100	-3.72924800	0.23005800
H	1.53380600	-2.75752300	-1.55080800
H	-0.49828900	-4.43715300	1.95471800
O	1.62248000	-4.44712200	0.44290500
I	2.90374700	-0.74752300	0.75384400
C	1.10816200	-0.85120300	1.82957300
C	0.00581200	-0.12929200	1.37245800
C	1.01896000	-1.61300400	2.99643100
C	-1.18692300	-0.15923200	2.09609900
H	0.07336300	0.44526800	0.45534000
C	-0.17502400	-1.62472900	3.71979200
H	1.87924300	-2.17441700	3.34718300
C	-1.27575800	-0.89601800	3.27700300
H	-2.03565500	0.40550300	1.72236500
H	-0.23548000	-2.20335600	4.63668000
H	-2.19887100	-0.90180900	3.84839400
C	4.07674600	2.72633200	0.44669400
O	4.06858600	2.21281300	-0.79284100
C	3.01361800	3.80039700	0.63813700
O	4.82121300	2.33085000	1.31230400
F	0.40311500	-0.05185800	-3.70179300
H	5.00363900	-0.42990700	-1.85998700
F	4.48816400	-0.62064200	-3.26698900
H	1.46914300	-0.85830800	-3.43998100
C	1.65857400	3.07470100	0.70954000
H	1.64691200	2.36045700	1.54148300
H	0.86024500	3.80673200	0.87698100
H	1.44731000	2.53440100	-0.21850900
C	3.28558300	4.53687300	1.94841200
H	4.25685500	5.03979500	1.92022000
H	2.50854600	5.28939200	2.11951400
H	3.29662300	3.84006900	2.78985800
C	3.01959800	4.77565400	-0.54447500
H	3.98670900	5.28161500	-0.63283600
H	2.81661500	4.25611600	-1.48356500
H	2.24939400	5.53971400	-0.39281200
F	2.19685100	-1.49110100	-3.16800400
H	3.57756000	-0.95327000	-3.25686800
F	5.24805800	-0.23689600	-0.94594800
H	4.68167600	1.44599600	-0.79570800
F	0.05182500	1.19499300	-1.78089200
H	0.23522700	0.55712600	-2.88682900
F	-1.94740800	0.78474900	-0.77457200
H	-0.93824700	1.04634700	-1.33869800

TS2g

C	-8.51653600	1.48987500	0.11970600
C	-7.25350900	0.96884000	-0.14570600
C	-6.12055100	1.48564900	0.48675800
C	-6.27659700	2.53899500	1.38974800
C	-7.53797100	3.06370100	1.65836900
C	-8.66116100	2.53985800	1.02346900
H	-9.38821900	1.07376800	-0.37568900
H	-7.14367200	0.14568700	-0.84857900
H	-5.40137000	2.94639600	1.89032200
H	-7.64364700	3.87924200	2.36684600
H	-9.64539200	2.94576300	1.23407200
C	-4.74590500	0.95101100	0.16191400
H	-4.06713500	1.08981000	1.00568700
H	-4.79859300	-0.12092300	-0.05369500
C	-4.16853600	1.68427700	-1.05052000
H	-4.05473600	2.75164500	-0.83754200
H	-4.84910500	1.60034200	-1.90736000
C	-2.83300900	1.24485900	-1.56696700
O	-2.09968100	1.72551900	-2.34687300
O	-2.95753400	-0.41243800	-1.64311100
C	-1.95201200	-1.16488800	-1.74034100
C	-0.57818700	-0.68312900	-1.85996200
C	-2.24375300	-2.60133400	-1.75844900
C	0.41819300	-1.57077900	-2.01295200
H	-0.38582900	0.37795500	-1.86411400
C	-1.25039800	-3.49012000	-1.87930600
H	-3.28503800	-2.88184400	-1.64692600
C	0.16030000	-3.03999900	-2.04411400
H	1.45341500	-1.25890400	-2.12074300
H	-1.41831000	-4.56207200	-1.88386400
O	1.05330600	-3.83917100	-2.22157800
I	1.96450600	-2.12374600	1.11458200
C	-0.07121700	-2.61958700	1.20326900
C	-1.00581600	-1.58618700	1.24974900
C	-0.48460600	-3.95262900	1.23755500
C	-2.36235500	-1.89250000	1.34938000
H	-0.68243800	-0.55338900	1.19715600
C	-1.84471700	-4.24613800	1.35459500
H	0.24811800	-4.75231000	1.19380300
C	-2.78392700	-3.22079700	1.41728000
H	-3.07927000	-1.07795800	1.38364100
H	-2.16276800	-5.28330300	1.40224400
H	-3.83957200	-3.45389200	1.51718100
C	4.29401800	2.40721000	0.70758200
O	3.30908500	1.50665100	0.53395500
C	3.90742400	3.80241300	0.24332200
O	5.36754700	2.09388800	1.16875600
F	1.40378100	1.44730100	-1.47267800
H	5.40210200	-0.51164000	1.07965300
F	6.60700000	-0.21319600	0.23581700
H	2.57990100	0.63722300	-1.49231300
C	2.56035900	4.19318700	0.86729000
H	2.62317200	4.20960000	1.96049700
H	2.28143300	5.19652000	0.52803300
H	1.77030300	3.49436800	0.58293600
C	5.00285100	4.78039400	0.66321100
H	5.96491600	4.49591000	0.22992400
H	4.74642100	5.78915200	0.32353300
H	5.11873300	4.79652100	1.75073300
C	3.77916100	3.77410200	-1.28937600
H	4.71992900	3.46897400	-1.75522600
H	2.98941600	3.08602900	-1.60135800
H	3.52114600	4.77665700	-1.64696200
F	3.29034800	-0.01787700	-1.69909800
H	6.26710300	0.46341300	-0.35853800
F	4.52090800	-0.71690300	1.43105900
H	3.64148400	0.65328000	0.90015100
F	0.21159300	1.53305700	0.52095400
H	0.96819200	1.50225000	-0.54247100
F	-1.97184400	1.03654900	0.06334500
H	-0.82907700	1.37908400	0.27940600
F	5.45840900	1.13578100	-1.52277700
H	4.60677600	0.67950400	-1.61506800

5a

C	5.75453700	-2.84517800	-1.07278400
C	4.84769400	-1.92176500	-0.56370800
C	5.13412500	-0.55375300	-0.59108000
C	6.34617100	-0.12868200	-1.13430200
C	7.25671700	-1.05094400	-1.64595600
C	6.96270500	-2.41097300	-1.61597500
H	5.51793500	-3.90451200	-1.05043200
H	3.90101100	-2.25158200	-0.14024500
H	6.57641000	0.93378800	-1.16268100
H	8.19443000	-0.70578100	-2.07039300
H	7.66992800	-3.13032800	-2.01654900
C	4.15082300	0.42155100	0.00845000
H	4.31105400	1.42492200	-0.40064000
H	3.13158900	0.11766400	-0.24926900
C	4.29524300	0.45280800	1.53362100
H	5.24707100	0.91024500	1.82918600
H	4.29745700	-0.56237900	1.94100300
C	3.20489200	1.17384900	2.26912000
O	2.99637300	1.24300000	3.43006000
O	1.78340700	-0.93549400	1.49710400
C	0.57910400	-1.02510500	1.68260600
C	-0.13947500	-0.03616200	2.52771800
C	-0.20711700	-2.12155200	1.07128700
C	-1.44444000	-0.17637700	2.78350800
H	0.45873700	0.77198100	2.94066300
C	-1.51034200	-2.26593600	1.33072900
H	0.33760100	-2.78296900	0.40499200
C	-2.21894400	-1.33074800	2.24708900
H	-2.00109800	0.51560700	3.40825800
H	-2.11524000	-3.05610300	0.89377800
O	-3.38072400	-1.50519700	2.55687000
I	-3.69676500	0.92039900	-0.26256000
C	-3.56515700	-1.10027100	-0.84773800
C	-2.55200100	-1.49376000	-1.71890700
C	-4.48200900	-2.01111800	-0.32858300
C	-2.46673200	-2.83965300	-2.07375700
H	-1.83510100	-0.77161000	-2.09852700
C	-4.38159800	-3.35114300	-0.69914000
H	-5.24762400	-1.68776900	0.36734500
C	-3.37607900	-3.76727100	-1.56963000
H	-1.68071800	-3.15814400	-2.75154400
H	-5.09178600	-4.06779000	-0.29880100
H	-3.30287000	-4.81204500	-1.85486200
C	-0.07265300	1.55841200	-1.40363200
O	0.56535000	0.73746200	-0.54122400
C	0.02809900	3.05840500	-1.12336400
O	-0.66519100	1.08505400	-2.33895900
C	1.48396600	3.49507100	-1.36295700
H	1.79347000	3.27572000	-2.38956700
H	1.57110800	4.57433600	-1.20119600
H	2.17675800	2.99840900	-0.67636600
C	-0.90613000	3.79006300	-2.08567800
H	-1.94267700	3.47406200	-1.93472400
H	-0.83693100	4.86946800	-1.91758600
H	-0.64223900	3.57452000	-3.12355800
C	-0.37558700	3.35463200	0.33030600
H	-1.36935400	2.95382800	0.55452800
H	0.33266000	2.94359800	1.05606600
H	-0.40058900	4.43842000	0.48211700
F	2.37181800	1.87280600	1.41415400
H	1.06259200	1.23305600	0.13303400

5b

C	7.26606900	-0.55985300	1.82385400
C	6.13564400	-0.51574800	1.01429000
C	6.13550100	0.22493800	-0.17083600
C	7.28905400	0.92378300	-0.52785100
C	8.42347800	0.88203100	0.27969200
C	8.41418100	0.14014100	1.45744500
H	7.25364900	-1.14376800	2.73898400
H	5.23786200	-1.06331100	1.29419800
H	7.30051700	1.50056400	-1.44975100
H	9.31549500	1.42693700	-0.01349900
H	9.29810400	0.10468300	2.08629300
C	4.88224700	0.29570400	-1.00817200
H	5.12803500	0.53902700	-2.04664400
H	4.37385200	-0.67199600	-1.00685800
C	3.92318000	1.34922700	-0.44536500
H	4.33826700	2.35898300	-0.55542100
H	3.75552300	1.19540500	0.62430800
C	2.56509700	1.35583300	-1.07628600
O	1.60125700	1.95880600	-0.69331000
O	2.25680800	-0.95642500	0.14209700
C	1.23399300	-1.28686100	0.72701300
C	0.31949500	-0.27857700	1.31462700
C	0.87678700	-2.72009800	0.86322000
C	-0.78386900	-0.65335700	1.97133900
H	0.56447100	0.76582000	1.15219300
C	-0.22648300	-3.09345200	1.51871200
H	1.55461700	-3.42548100	0.39281200
C	-1.12623400	-2.09010800	2.15244200
H	-1.48019800	0.06781800	2.38833200
H	-0.52218100	-4.13201300	1.63224500
O	-2.09742500	-2.43985600	2.79359300
I	-3.97331500	-0.88830000	0.04364700
C	-2.35514000	-1.81897100	-0.92657100
C	-1.33306000	-1.02441900	-1.43810800
C	-2.33660500	-3.20557700	-1.06800400
C	-0.27421900	-1.63355500	-2.10870900
H	-1.35133800	0.05253800	-1.32094800
C	-1.27368300	-3.79961400	-1.74748000
H	-3.14084200	-3.81071900	-0.66289800
C	-0.24364400	-3.01900700	-2.26570400
H	0.52080800	-1.00942200	-2.50512500
H	-1.25666100	-4.87854000	-1.86806400
H	0.58018400	-3.48753300	-2.79498900
C	-2.23422300	2.64600300	-0.14645400
O	-2.50576200	2.88201800	-1.42885600
C	-3.20596900	3.32459700	0.80853600
O	-1.26517200	2.00016100	0.20623200
F	2.48498400	0.64375700	-2.20134100
H	0.23693800	1.81678400	-1.66396900
C	-4.64148200	3.24059900	0.27922700
H	-4.96250500	2.19963700	0.17081200
H	-5.31767700	3.73627800	0.98370700
H	-4.73221000	3.72638000	-0.69469900
C	-3.09555300	2.66936100	2.18449600
H	-2.06793500	2.71295000	2.55500700
H	-3.74854100	3.18602500	2.89516900
H	-3.39895300	1.61769600	2.13957300
C	-2.77039100	4.79932000	0.88863300
H	-1.74455700	4.88364000	1.26151000
H	-2.82638600	5.27626400	-0.09414000
H	-3.43163800	5.33869000	1.57478600
F	-0.30823100	1.71791400	-2.44863900
H	-1.78444300	2.46986500	-1.95837700

5c

C	6.92490800	-1.32492900	-2.02302100
C	5.81613200	-0.90141500	-1.29784100
C	5.52917300	0.46040900	-1.16808400
C	6.37360100	1.39033800	-1.77417200
C	7.48467500	0.96945900	-2.50185100
C	7.76232600	-0.38868400	-2.62734500
H	7.13466200	-2.38554100	-2.12064700
H	5.15592000	-1.62619900	-0.82517900
H	6.15624800	2.45178700	-1.68111100
H	8.13140400	1.70316100	-2.97279800
H	8.62631200	-0.71766900	-3.19585800
C	4.34431700	0.89302000	-0.33961000
H	4.01847600	1.89789100	-0.62865000
H	3.50838100	0.20808100	-0.50678400
C	4.69836400	0.86949300	1.15010900
H	5.44696700	1.63339900	1.39239200
H	5.13359900	-0.09501700	1.42822600
C	3.54913200	1.06806800	2.08795900
O	3.50105300	1.00024700	3.26736200
O	2.84104200	-1.32573000	1.20059100
C	1.69394100	-1.70183300	1.39950700
C	0.95176100	-1.27767400	2.61353200
C	1.00763000	-2.59082200	0.43371100
C	-0.31132000	-1.66826900	2.81746700
H	1.48753400	-0.64031200	3.31166300
C	-0.24961200	-2.99564300	0.64244000
H	1.58029300	-2.86961600	-0.44533000
C	-1.00191400	-2.57857400	1.85832100
H	-0.89588000	-1.36040400	3.67862800
H	-0.78911600	-3.63604100	-0.04951700
O	-2.12774700	-2.97739100	2.07238700
I	-3.77352600	-1.93522900	-1.14955400
C	-1.96267300	-0.88314600	-1.04219400
C	-1.67084100	-0.14550800	0.10394200
C	-1.06557000	-0.93792200	-2.11038700
C	-0.46629400	0.55293000	0.16873200
H	-2.37242200	-0.10705200	0.93022800
C	0.13803800	-0.24334000	-2.02358600
H	-1.30509500	-1.51370600	-2.99799200
C	0.44062700	0.50423900	-0.88486300
H	-0.24836100	1.13417600	1.05729600
H	0.83757300	-0.28078200	-2.85321700
H	1.37177900	1.05760800	-0.82513600
C	-3.53434100	2.34963000	0.22687700

O	-2.55852300	2.80989100	1.02947900
C	-3.59495700	3.09131400	-1.10053600
O	-4.25573000	1.43408100	0.54689900
H	-0.92858800	1.25288300	3.14968000
F	0.58574100	1.74370000	3.40327300
C	-2.25710300	2.89046300	-1.82979700
H	-2.07657100	1.82969600	-2.03809900
H	-2.28078400	3.42762700	-2.78431900
H	-1.42273000	3.27072900	-1.23401000
C	-4.74017600	2.51550700	-1.93070500
H	-5.69697100	2.63507900	-1.41514600
H	-4.79326700	3.02986100	-2.89593700
H	-4.58975900	1.44624000	-2.10683000
C	-3.81780000	4.58545500	-0.82585800
H	-4.75855600	4.75090200	-0.29050400
H	-3.00210300	5.00061800	-0.22837600
H	-3.86747600	5.12864500	-1.77557000
H	1.25945100	1.62264700	2.74989500
F	-1.82483500	0.99421100	2.96556900
H	-2.53066800	2.22876800	1.81841700
F	2.37839600	1.43381000	1.43234700
5d			
C	7.17609800	-1.88394900	-0.64792900
C	5.91926000	-1.30600500	-0.50106900
C	5.68065000	-0.00410900	-0.95082000
C	6.72218000	0.70828300	-1.54547900
C	7.98169000	0.13172200	-1.69369600
C	8.21091700	-1.16586300	-1.24499500
H	7.34879500	-2.89738000	-0.29885300
H	5.10492100	-1.85899600	-0.03771600
H	6.54366000	1.72065900	-1.90051900
H	8.78231200	0.69548800	-2.16248400
H	9.19102400	-1.61745200	-1.36168300
C	4.32320700	0.62014700	-0.74236000
H	4.16203900	1.43927800	-1.44964900
H	3.54595300	-0.13162900	-0.91211700
C	4.18824900	1.14851900	0.69458700
H	4.85929800	2.00498200	0.84079800
H	4.45329600	0.38090100	1.42280600
C	2.79949800	1.59830600	1.02812800
O	2.21134100	1.47771300	2.05728200
O	2.68307500	-1.41325800	0.95539700
C	1.56912200	-1.82790500	1.23856300
C	0.85330000	-1.33742200	2.44457000
C	0.88786200	-2.83039100	0.38213400
C	-0.38438300	-1.75978600	2.72588600
H	1.37628200	-0.60104200	3.04560400
C	-0.34647700	-3.25783400	0.66766900
H	1.44278300	-3.16658100	-0.48835100
C	-1.07823100	-2.75748100	1.86442300
H	-0.94948200	-1.40420400	3.58203600
H	-0.88300200	-3.97444900	0.05234700
O	-2.19508700	-3.15316300	2.13108300
I	-4.01619700	-2.26026100	-1.01614100
C	-2.17035100	-1.26728700	-1.11101100
C	-1.80022800	-0.41383300	-0.07256100
C	-1.32641300	-1.48339500	-2.19957800
C	-0.56473500	0.22958100	-0.12876900
H	-2.45785800	-0.26861900	0.77716400
C	-0.09396200	-0.83681500	-2.24087400
H	-1.62682100	-2.14735600	-3.00291200
C	0.28975100	0.01855000	-1.20917700
H	-0.26839800	0.89749900	0.67629200
H	0.56711500	-1.00069900	-3.08653400
H	1.24218900	0.53468000	-1.25543400
C	-3.08311200	2.71125000	-0.11192000
O	-2.37997600	2.68738000	1.06393500
C	-2.55500700	3.75225900	-1.08377800
O	-3.99427800	1.95282200	-0.29212300
F	2.20263700	2.22175700	-0.00701600
H	-1.45157200	0.94361800	3.04308200
F	-0.04533900	1.42705100	3.37820700
H	-0.87735200	3.04375100	1.30130600
C	-1.23132900	3.21925600	-1.66203200
H	-1.38089700	2.25941600	-2.16676400
H	-0.84776400	3.94023700	-2.39152900
H	-0.47329500	3.08724000	-0.88346300
C	-3.58468000	3.93039600	-2.19896800
H	-4.53396600	4.30113800	-1.80144500
H	-3.20907300	4.65029400	-2.93253900
H	-3.77982900	2.98091800	-2.70291500
C	-2.30231600	5.08045600	-0.35618300
H	-3.20868700	5.44632400	0.13633300
H	-1.51311800	4.98517900	0.39465600
H	-1.98350600	5.83190600	-1.08523400
F	0.06762600	3.12232100	1.49659600
H	0.37929300	1.94596900	2.68882400
F	-2.34658800	0.70931700	2.77574200
H	-2.68485600	1.93689900	1.62946700
5e			
C	7.66062300	-0.26106000	1.26118200
C	6.35550600	-0.20051900	0.78400900
C	6.02557600	0.64023100	-0.28268900
C	7.02606400	1.42166000	-0.86052800
C	8.33459100	1.36322500	-0.38580500
C	8.65420500	0.52201400	0.67610500
H	7.90457200	-0.92211800	2.08698200
H	5.57614500	-0.81242100	1.23411500
H	6.78000100	2.07622500	-1.69335400
H	9.10444900	1.97310500	-0.84815500
H	9.67368400	0.47387900	1.04525300
C	4.59378700	0.72038900	-0.75254500
H	4.54720400	1.09054000	-1.78162700
H	4.13908500	-0.27396000	-0.73467100
C	3.78151800	1.63902500	0.16565600
H	4.11607300	2.68060500	0.08284700
H	3.90456300	1.35369400	1.21447900
C	2.30793400	1.62444700	-0.08625200
O	1.45660100	2.14283100	0.58516800
O	2.39813000	-0.79035200	0.88600000
C	1.43593300	-1.49569100	1.16141200
C	0.19311200	-0.91866700	1.72495400
C	1.49008600	-2.96078800	0.93880100
C	-0.85940000	-1.69576600	2.00496100
H	0.17553500	0.15329200	1.88803200
C	0.43418200	-3.73629200	1.20238700
H	2.41898300	-3.34434400	0.52867800
C	-0.82541500	-3.16367900	1.75145500
H	-1.79049000	-1.30546000	2.40094200
H	0.43094200	-4.80784400	1.02869500
O	-1.78460100	-3.87026500	1.98649000
I	-3.09197400	-1.35236500	-0.71003800
C	-1.29896300	-2.19956900	-1.39806800
C	-0.19136400	-1.37872400	-1.60716400
C	-1.23148500	-3.56996900	-1.65024600
C	0.98975700	-1.94135000	-2.09064700
H	-0.25515000	-0.31719400	-1.39240200
C	-0.04727800	-4.11586200	-2.14484200
H	-2.09521300	-4.20158600	-1.46949600
C	1.06144400	-3.30498500	-2.36998800
H	1.85323900	-1.30230700	-2.24907400
H	0.00173800	-5.18038100	-2.35318000
H	1.98025100	-3.73373500	-2.75783400
C	-3.12142200	2.93048700	-0.59333900
O	-3.45552000	2.26106200	0.54936000
C	-2.29474400	4.18680400	-0.34999400
O	-3.53984600	2.58440700	-1.66354600
F	-1.91257000	1.26860600	2.31899100
H	-4.75591600	-0.02781900	1.61608800
F	-3.83262300	-0.16734500	2.86715100
C	-1.22642700	4.27638000	-1.44404400
H	-1.68793600	4.22566200	-2.43294800
H	-0.68199300	5.22181500	-1.35260200
H	-0.51682300	3.44980100	-1.35521300
C	-3.28847000	5.35450800	-0.50150100
H	-4.07388700	5.30428000	0.25991300
H	-2.75721500	6.30447300	-0.38331600
H	-3.75743100	5.33361200	-1.48887100
C	-1.65971200	4.23720900	1.04119200
H	-2.41276300	4.16062500	1.83039700
H	-0.92825800	3.43868900	1.18354800
H	-1.13647500	5.19127300	1.16032100
H	-3.08244000	0.43447100	2.75365900
F	-5.15175900	0.20284900	0.77085800
H	-4.10038800	1.55024600	0.32202000
F	-0.92156600	1.43156700	-0.10401100
H	-2.20355400	1.61846800	1.46287900
F	1.94654400	1.00588700	-1.21182400
H	-0.04407000	1.73347600	0.14088800
5			
C	-7.94097700	0.18288600	-1.35313500
C	-6.64475000	0.13590100	-0.85065900
C	-6.29862600	0.85728100	0.29537400
C	-7.27413300	1.62898400	0.92673800
C	-8.57367200	1.67796800	0.42702700
C	-8.90945800	0.95519100	-0.71415300
H	-8.19778100	-0.38626300	-2.24117200
H	-5.88554400	-0.46860600	-1.34311100
H	-7.01540500	2.19103900	1.82106200
H	-9.32402700	2.27865000	0.93161700
H	-9.92204700	0.99044600	-1.10326900
C	-4.87534900	0.82551200	0.79565900
H	-4.83534600	1.09709500	1.85534300
H	-4.46569700	-0.18321400	0.69406300
C	-4.00162500	1.78493500	-0.01807000
H	-4.30029500	2.82807400	0.14385000
H	-4.10350800	1.59338300	-1.09017100
C	-2.53697900	1.69185600	0.27160500
O	-1.64859400	2.23859700	-0.32217100
O	-2.70065200	-0.63756200	-0.90306100
C	-1.72113000	-1.30404100	-1.21305800
C	-0.46358400	-0.66354000	-1.66246600
C	-1.77072200	-2.78527500	-1.15327000
C	0.60720700	-1.40000200	-1.98075600
H	-0.44977400	0.41914400	-1.72301300
C	-0.69734800	-3.52190700	-1.45521100
H	-2.71174700	-3.21602900	-0.82600800
C	0.57747400	-2.88640400	-1.88886800
H	1.53823900	-0.96011000	-2.32040200
H	-0.69090100	-4.60600900	-1.39897200
O	1.54946600	-3.56032700	-2.16477900
I	2.78978000	-1.52909400	0.87132400
C	0.92565000	-2.35862400	1.36859500
C	-0.16242800	-1.51586900	1.59419100
C	0.79370600	-3.74239500	1.48849900
C	-1.38762800	-2.07137600	1.96247900
H	-0.05063800	-0.44298500	1.47527900
C	-0.43483000	-4.28265000	1.86712700
H	1.64334000	-4.38966500	1.29664400
C	-1.52394100	-3.45070600	2.10997100
H	-2.23615900	-1.41546900	2.13177800
H	-0.53394100	-5.35890000	1.97172500
H	-2.47800200	-3.87470500	2.40756400
C	3.49861100	2.45993300	0.35830200
O	4.39068200	2.09136300	1.23985000
C	2.87751600	3.81569500	0.63331000
O	3.26098700	1.74492800	-0.62139300
F	1.47358100	1.67327800	-2.18417300
H	5.22676200	0.04445300	-0.72511800
F	5.21857300	0.34469800	-2.15485100
H	2.37336000	0.93429000	-2.97204800
C	4.02827600	4.83649900	0.70273500
H	4.57395500	4.88537400	-0.24539600
H	3.61080100	5.82755100	0.90542800
H	4.73242500	4.58367800	1.49843400
C	1.90824500	4.19871800	-0.48395300
H	1.05211200	3.52379100	-0.51434200
H	1.54003000	5.21316300	-0.30548900
H	2.39624300	4.17972400	-1.46332600
C	2.15374600	3.75657600	1.98838200
H	1.35842400	3.00862900	1.96253700
H	2.85083300	3.50725100	2.79237200
H	1.71496200	4.73724700	2.19906600
F	3.07476600	0.34780100	-3.35058900
H	4.33952700	0.35581200	-2.57117500
F	5.30599500	-0.13542700	0.23317300
H	4.76682900	1.21297600	0.96248100
F	0.70847300	1.41667700	0.43628100
H	2.11348900	1.78737600	-1.39148500
F	-2.23506400	0.95597000	1.34518200
H	-0.14039700	1.75093900	0.15393300
5g			
C	8.27614300	0.44824500	-1.87165900
C	7.01553500	0.51572600	-1.28752400
C	6.79744000	1.30530100	-0.15524500
C	7.86476900	2.02353900	0.38369600
C	9.12845800	1.95898600	-0.19912000
C	9.33639200	1.17096800	-1.32753300
H	8.43137900	-0.16431000	-2.75426400
H	6.18308100	-0.04271300	-1.71123200
H	7.70374600	2.64405800	1.26211200
H	9.94925100	2.52734900	0.22689700
H	10.31976400	1.12209200	-1.78403400
C	5.43202100	1.32768000	0.48743800
H	5.30323200	2.23657000	1.08354000
H	4.65613000	1.32241100	-0.28296800
C	5.24426600	0.09499000	1.37758100
H	5.91981500	0.12316100	2.24201000
H	5.47545900	-0.82440300	0.83194500
C	3.86019000	-0.08321700	1.90947400
O	3.43560100	-1.04374800	2.50098000
O	3.28519400	-0.66576500	-0.62711300
C	2.23320800	-1.23311800	-0.88391900
C	1.65511100	-2.22853900	0.05163000
C	1.49716100	-0.95305700	-2.14133100
C	0.44682400	-2.75800200	-0.15971400
H	2.26268200	-2.49194400	0.91202100
C	0.30180000	-1.50610200	-2.37565700
H	1.96910100	-0.25705800	-2.82715900
C	-0.33399200	-2.38529300	-1.36694900
H	0.00127500	-3.48663300	0.50329200
H	-0.28690900	-1.29831200	-3.26377700
O	-1.48011900	-2.78349200	-1.53622800
I	-3.64921500	-0.06125200	-1.87872600
C	-1.78616200	0.63122300	-1.22423300
C	-1.28479100	0.17945500	-0.00363300
C	-1.08810400	1.56899400	-1.98698500
C	-0.06374300	0.67462700	0.45214500
H	-1.83353900	-0.54606200	0.58683500
C	0.12894100	2.05421800	-1.51969700
H	-1.49779500	1.92187800	-2.92781700
C	0.64570700	1.60610200	-0.30331900
H	0.32805500	0.32633200	1.40283500
H	0.67319100	2.78794300	-2.10658200
H	1.59686400	1.98496500	0.05551500
C	-4.76350900	1.99558000	1.03637500
O	-3.84473200	1.11534500	1.46091100
C	-4.25544300	3.43152400	1.10706500
O	-5.85752500	1.66697800	0.64384500
F	-0.93646900	-4.30938300	2.40263700
H	-3.80726300	-2.06845900	0.97322100
F	-2.53424700	-3.03029700	0.72600800
H	-1.39044400	-5.00130100	0.96602000
C	-3.01732800	3.55494200	0.20683800
H	-3.26116000	3.29417400	-0.82964000
H	-2.65384500	4.58863600	0.22177700
H	-2.21278200	2.89527300	0.54635000
C	-5.35974500	4.36996800	0.62600000
H	-6.25462600	4.26947600	1.24595500
H	-5.01272100	5.40765300	0.67336300
H	-5.64418800	4.14004300	-0.40439400
C	-3.87123500	3.75056100	2.55897200
H	-4.73594900	3.65519000	3.22404900
H	-3.08719700	3.07614000	2.91217400
H	-3.50427800	4.78073900	2.62422800
F	-1.36445200	-5.18449400	0.03686200
H	-2.21310800	-3.20366500	-0.17953900
F	-4.52670700	-1.49762200	1.21574900
H	-4.21845900	0.20970500	1.36889700

F	-0.89821900	-1.78152300	2.33299700
H	-1.14383400	-3.37689100	2.35306500
F	1.09091500	-0.75275200	3.40332800
H	-0.12110100	-1.44435900	2.79172400
F	3.05618900	0.96115900	1.73793200
H	1.98460900	-0.91347000	3.05312700

IM1-1

I	2.07286100	0.10031600	-0.90579100
C	3.95689400	-0.20380900	-0.02493100
C	6.42329400	-0.62518000	1.11105400
C	5.07445600	0.33540800	-0.64875300
C	4.02589300	-0.94741800	1.14465700
C	5.28359900	-1.15599300	1.70929500
C	6.31898500	0.12010300	-0.06157800
H	4.97963900	0.90833000	-1.56461100
H	3.12493700	-1.32770800	1.61307600
H	5.36371700	-1.72716500	2.62850200
H	7.20763000	0.52765100	-0.53255900
H	7.39708700	-0.79179100	1.55993400
O	1.38465600	0.16286000	2.31821600
C	0.08616100	0.09246800	1.93187100
C	-2.56094200	-0.17786700	1.13268500
C	-0.62018300	1.20544800	1.47030700
C	-0.54235800	-1.15393900	1.98601400
C	-1.86489300	-1.29455700	1.58762100
C	-1.94659900	1.06478900	1.07202300
H	-0.12720500	2.17223500	1.42531200
H	0.02708400	-2.00810000	2.33692900
H	-2.35495800	-2.25929900	1.63470900
H	-2.51384300	1.91585400	0.70967300
O	2.71269800	2.11712500	-1.13292800
C	2.76595600	2.85066200	-0.04033700
O	2.42805500	2.45585600	1.06839100
C	3.32256700	4.25447300	-0.27905400
O	1.66180000	-1.87795300	-0.48689500
C	2.35051800	-2.80611900	-1.16558100
O	3.16518300	-2.53572300	-2.01871300
C	2.01357400	-4.22258800	-0.70133600
H	1.76367000	1.02163400	2.03864900
C	2.73423400	-5.22400300	-1.60170100
H	2.51013900	-6.24413400	-1.27299200
H	2.41524000	-5.11412000	-2.64192100
H	3.81594300	-5.07168600	-1.56789300
C	2.50261200	-4.35813300	0.74945900
H	3.57655600	-4.15305200	0.82323300
H	1.96921900	-3.66436700	1.40583000
H	2.32421300	-5.37882600	1.10392800
C	0.49494100	-4.43321400	-0.75751500
H	0.12137200	-4.32894700	-1.78173300
H	0.25171700	-5.44288400	-0.40984300
H	-0.02421000	-3.70812000	-0.12509100
C	2.45643300	4.96188200	-1.33025200
H	1.42396500	5.07011700	-0.98109900
H	2.85555800	5.96379400	-1.52001000
H	2.44891900	4.40437000	-2.26998400
C	4.75795700	4.10222400	-0.80597800
H	5.37920800	3.54033200	-0.09946600
H	4.76565500	3.58158100	-1.76746000
H	5.20598700	5.09206900	-0.94212100
C	3.31672600	5.03420500	1.03433400
H	3.71523700	6.04012700	0.86691400
H	2.30251600	5.12274600	1.43313200
H	3.92896200	4.53503100	1.78979400
O	-3.86279100	-0.25685000	0.64377100
C	-4.82400000	-0.88302600	1.37497200
C	-6.15058100	-0.79708800	0.65918600
H	-6.88580000	-1.33482100	1.26149600
H	-6.05823300	-1.30466100	-0.30778700
C	-6.59591400	0.65726600	0.42211100
H	-6.66709900	1.17291000	1.38643600
H	-5.82957200	1.17019100	-0.16657800
C	-7.92501200	0.70608100	-0.29043600
C	-7.98147600	0.72909000	-1.68571200
C	-9.12200500	0.67557500	0.42833500
C	-9.20515300	0.72507300	-2.34931700
H	-7.05524900	0.75492400	-2.25528200
C	-10.34821400	0.67172800	-0.23055600
H	-9.08992800	0.65886700	1.51537600
C	-10.39269900	0.69647000	-1.62242600
H	-9.23131200	0.74815500	-3.43443500
H	-11.26956900	0.65249800	0.34333700
H	-11.34798500	0.69623300	-2.13768800
O	-4.62828300	-1.41616300	2.43296400

IM1-2

I	1.25731900	-0.02773000	0.67948200
C	2.99800500	1.12560000	0.86794900
C	5.33833500	2.55914900	1.06964900
C	3.83953500	0.88049800	1.94626100
C	3.29248400	2.05826700	-0.11698100
C	4.47743100	2.78175000	-0.00238500
C	5.02213800	1.61095900	2.03979200
H	3.58882400	0.12989500	2.68881400
H	2.62203700	2.20890400	-0.95574900
H	4.73059300	3.51063200	-0.76508000
H	5.69191900	1.43800200	2.87606600
H	6.26159100	3.12408600	1.14737200
O	3.16638900	0.38835900	-2.97824800
C	1.85487600	0.07083400	-2.82252800
C	-0.83168400	-0.47227800	-2.30145100
C	1.41955500	-1.25290300	-2.68922300
C	0.91679700	1.09988600	-2.78452200
C	-0.42935000	0.84144100	-2.52974500
C	0.08705000	-1.51766800	-2.41606500
H	2.14110200	-2.06073200	-2.75182400
H	1.25469700	2.12043400	-2.93787200
H	-1.14071700	1.65065900	-2.48962400
H	-0.26342700	-2.53378000	-2.26686300
O	2.53712400	-1.69830900	1.00296700
C	3.52930100	-1.92875600	0.16713000
O	3.75217700	-1.25810400	-0.82865800
C	4.41526200	-3.10129500	0.59387400
O	0.35527500	1.85966800	0.54731300
C	-0.96385100	1.78877000	0.62621300
O	-1.55172300	0.71806700	0.67833000
C	-1.63211100	3.16305400	0.67808000
H	3.68029600	-0.24735800	-2.44676800
O	-2.09730100	-0.89091400	-1.92306200
C	-3.12497600	-0.06795200	-1.62850300
O	-3.15709300	1.11565800	-1.85595000
C	-4.25311100	-0.86083100	-1.01049200
H	-4.85602300	-1.27994000	-1.82684300
H	-3.83411400	-1.70734500	-0.46041300
C	-5.12304200	0.00988000	-0.10105100
H	-4.49429600	0.39604300	0.70815900
H	-5.48121500	0.87254900	-0.67205900
C	-6.28189100	-0.77597000	0.46005900
C	-7.49435000	-0.85157500	-0.22954100
C	-6.14813600	-1.48488000	1.65618400
C	-8.54937300	-1.61422000	0.26364400
H	-7.61148400	-0.30094900	-1.16025300
C	-7.20007200	-2.24885700	2.15405900
H	-5.20921900	-1.43057800	2.20246200
C	-8.40466400	-2.31566700	1.45822900
H	-9.48658700	-1.65757500	-0.28283400
H	-7.08043600	-2.78950600	3.08803400
H	-9.22715200	-2.90833400	1.84620900
C	-3.12779800	3.00003100	0.93585400
H	-3.31092300	2.45909400	1.86964200
H	-3.59402100	3.98830800	1.01100900
H	-3.59800600	2.45192100	0.11650100
C	-0.97445900	3.97178300	1.80663400
H	0.09089400	4.12031100	1.61508100
H	-1.45926500	4.95071800	1.88134100
H	-1.08551600	3.46475700	2.77139500
C	-1.40701500	3.87065300	-0.66696900
H	-1.96106200	3.36466100	-1.46299400
H	-1.77440200	4.90041000	-0.59979100
H	-0.34367600	3.89813800	-0.92468900
C	5.47175100	-3.35463500	-0.47985600
H	6.09301800	-2.46895600	-0.63532900
H	6.11490300	-4.18701700	-0.17612600
H	5.00566200	-3.60792300	-1.43650900
C	5.08585600	-2.70931400	1.91985200
H	4.33739300	-2.55224400	2.70163600
H	5.76334900	-3.50740600	2.24129400
H	5.67133600	-1.78986900	1.80533700
C	3.54526500	-4.34782800	0.79913400
H	4.17382600	-5.18741700	1.11426000
H	2.78518600	-4.17252200	1.56403100
H	3.04164700	-4.63331900	-0.13079500

IM1-3

I	-2.19756300	-0.23193300	-0.94850200
C	-4.05552400	0.16353200	-0.04644000
C	-6.48736100	0.70601000	1.11319000
C	-5.19203400	-0.42744600	-0.58307400
C	-4.08938500	1.01808500	1.04633000
C	-5.32961100	1.28655500	1.62403000
C	-6.41857800	-0.14958100	0.01571800
H	-5.12541300	-1.08683200	-1.44135300
H	-3.17522700	1.43991300	1.44835800
H	-5.38135400	1.94525800	2.48483800
H	-7.32138800	-0.59581300	-0.38855400
H	-7.44738100	0.92038200	1.57133500
O	-1.46166800	-0.05937500	2.25944200
C	-0.16962600	-0.02926900	1.85247200
C	2.46265800	0.15799400	1.00436000
C	0.52483700	-1.18283800	1.47795800
C	0.46628500	1.21307200	1.79314800
C	1.78385300	1.31701100	1.36593500
C	1.84570800	-1.08362700	1.05270600
H	0.02611700	-2.14665400	1.51953500
H	-0.09124400	2.09866400	2.07882300
H	2.26787600	2.28547000	1.33477700
H	2.40458100	-1.96490400	0.75535600
O	-2.86718900	-2.25498900	-1.00935900
C	-2.89463600	-2.90493100	0.13504100
O	-2.52325100	-2.43228800	1.20229900
C	-3.46555000	-4.31849900	0.01761100
O	-1.74530300	1.76028400	-0.68285500
C	-2.42564000	2.65173400	-1.41938900
O	-3.26002900	2.33503000	-2.23642900
C	-2.04935400	4.09038400	-1.06880300
H	-1.85160700	-0.93376200	2.05130900
C	-2.76242800	5.03683500	-2.03259000
H	-2.51036200	6.07332700	-1.78573900
H	-2.46256400	4.84107400	-3.06587000
H	-3.84660800	4.91282300	-1.97173800
C	-2.51214600	4.34777800	0.37421400
H	-3.58909500	4.17399800	0.47939000
H	-1.98246400	3.69573400	1.07484000
H	-2.30516800	5.38813400	0.64592600
C	-0.52744700	4.26124400	-1.16216700
H	-0.17215600	4.06808900	-2.18001800
H	-0.25698200	5.28907200	-0.89863100
H	-0.01291800	3.57867200	-0.48065500
C	-3.42886200	-4.99752600	1.38526300
H	-4.01693700	-4.43793100	2.11720500
H	-3.83829000	-6.00973700	1.30477100
H	-2.40472300	-5.06452300	1.76233700
C	-2.63206300	-5.10943400	-0.99989900
H	-2.64675000	-4.62409200	-1.97878500
H	-1.59115600	-5.19902300	-0.67101900
H	-3.04168700	-6.11970000	-1.10317500
C	-4.91375400	-4.19577500	-0.48118700
H	-5.37092900	-5.18963100	-0.52911200
H	-5.51259400	-3.57682200	0.19643400
H	-4.94455300	-3.75036800	-1.47934600
O	3.76638800	0.17482100	0.49327500
C	4.75319000	0.82431600	1.12934400
C	6.07056700	0.61558100	0.42644400
H	6.83269800	1.16646400	0.98117900
H	5.99580400	1.04848100	-0.57777200
C	6.44513100	-0.87298100	0.30626400
H	6.49522500	-1.31349600	1.30838200
H	5.65400600	-1.39418300	-0.24081300
C	7.76845800	-1.03890700	-0.39966100
C	7.81820600	-1.17995800	-1.78809100
C	8.96758000	-1.00220800	0.31505200
C	9.03867200	-1.28555400	-2.44926900
H	6.88994500	-1.21197900	-2.35400400
C	10.19041400	-1.1075630	-0.34168500
H	8.94027300	-0.8944980	1.39701400
C	10.22861900	-1.2495990	-1.72669300
H	9.06015300	-1.3997190	-3.52864200
H	11.11367800	-1.0818470	0.22873600
H	11.18111200	-1.3345750	-2.24004000
O	4.60662700	1.47816700	2.13712900
F	3.38716100	3.81702100	2.33661500
H	3.83880200	3.00393800	2.49099000

IM1-4

I	-2.37419700	-0.04603300	-1.05059000
C	-4.13077800	0.56866000	-0.07010100
C	-6.42742700	1.40008400	1.18967500
C	-5.35482100	0.22321500	-0.62809300
C	-4.01169300	1.31727900	1.09214100
C	-5.18444100	1.73429700	1.72031300
C	-6.51229800	0.64533800	0.02167700
H	-5.40720900	-0.35991200	-1.54079000
H	-3.03667700	1.54432600	1.50778200
H	-5.11777400	2.31350400	2.63552300
H	-7.48049700	0.39129300	-0.39741600
H	-7.33399600	1.72813400	1.68765300
O	-1.62673300	-0.30935800	2.15188400
C	-0.33501200	-0.40438400	1.75884300
C	2.31163200	-0.47610600	0.96072000
C	0.19631000	-1.57582100	1.20962400
C	0.47205100	0.72738700	1.90329000
C	1.80186500	0.69477200	1.50660300
C	1.52875700	-1.60955900	0.80918800
H	-0.43828900	-2.45053400	1.10092600
H	0.03787900	1.62556000	2.32916700
H	2.45233800	1.55507000	1.61390600
H	1.96101300	-2.50735400	0.37971000
O	-3.38057000	-1.90884800	-1.29172600
C	-3.49361300	-2.66426300	-0.21939500
O	-3.02337500	-2.37741200	0.87475900
C	-4.29789800	-3.94239900	-0.45780400
O	-1.57580100	1.80167900	-0.60549500
C	-2.09562300	2.86549700	-1.23619200
O	-2.98353000	2.78092500	-2.05370600
C	-1.46475900	4.17526700	-0.76602600
H	-2.12847800	-1.09258000	1.84298700
C	-2.00667800	5.31984800	-1.62000300
H	-1.57171600	6.26748600	-1.28594300
H	-1.75605400	5.17306200	-2.67428700
H	-3.09495200	5.38388800	-1.54265400
C	-1.85977400	4.37211800	0.70629500
H	-2.94927800	4.38262400	0.82389700
H	-1.44831600	3.57207800	1.32874600
H	-1.46774000	5.32881800	1.06715100
C	0.06215000	4.08206400	-0.88350100
H	0.36765000	3.92343000	-1.92315900
H	0.51380600	5.01784000	-0.53763200
H	0.45270300	3.25902600	-0.27904700
C	-4.35490900	-4.75611500	0.83356800
H	-4.82958100	-4.18591200	1.63627000
H	-4.92988900	-5.67255000	0.66575700
H	-3.35103200	-5.03045000	1.16876900
C	-3.62583400	-4.75124500	-1.57586600
H	-3.57234600	-4.17097800	-2.50023700
H	-2.61068300	-5.04790500	-1.29112500
H	-4.20280600	-5.66215800	-1.76657900
C	-5.71210000	-3.52922900	-0.89420600
H	-6.33143800	-4.42277000	-1.02451700
H	-6.18697400	-2.89192000	-0.13973800
H	-5.68312400	-2.98520300	-1.84227100
O	3.63561100	-0.49352400	0.50023400
C	4.59755500	-0.79629500	1.37543100
C	5.97838800	-0.68988500	0.79248300

H	6.60228200	-1.43653400	1.29157500
H	6.33878600	0.29424400	1.11842900
C	6.06583800	-0.80897900	-0.73268800
H	5.65293800	-1.77262900	-1.05052900
H	5.44715400	-0.03077300	-1.18852000
C	7.49707500	-0.68051400	-1.19539200
C	8.06168800	0.58008900	-1.40471800
C	8.29671700	-1.81089500	-1.37354600
C	9.39350700	0.70870200	-1.78726700
H	7.44739700	1.46742500	-1.26933100
C	9.62972500	-1.68753700	-1.75676500
H	7.86759800	-2.79754000	-1.21447300
C	10.18156600	-0.42626600	-1.96480100
H	9.81560200	1.69553700	-1.95037800
H	10.23641600	-2.57708700	-1.89566300
H	11.21968800	-0.32791200	-2.26600300
O	4.38286400	-1.11596400	2.53005100
F	4.63202300	1.79404700	2.17967000
H	4.21726900	1.49339600	2.98397900
F	3.36056800	0.62718500	4.02062700
H	3.52669600	-0.19612300	3.54771300

IM1-5

I	-2.55987500	0.20639800	-1.09695100
C	-4.15252900	0.80411100	0.14068900
C	-6.23486400	1.61509400	1.74049700
C	-5.45033100	0.63242700	-0.32316600
C	-3.85647800	1.36950700	1.37279200
C	-4.92188800	1.77830400	2.17381600
C	-6.49806000	1.04211000	0.49815100
H	-5.64164000	0.19041900	-1.29468300
H	-2.82980700	1.46419500	1.70738600
H	-4.71653400	2.21541400	3.14557200
H	-7.52074500	0.92206100	0.15565800
H	-7.05669000	1.93527400	2.37256800
O	-1.53586300	-0.56964200	1.93140900
C	-0.30898100	-0.74182400	1.38949400
C	2.22115500	-0.98112800	0.30881300
C	0.03441200	-1.88795000	0.66497400
C	0.62382100	0.28562700	1.55811800
C	1.89691500	0.16710800	1.01957700
C	1.31000700	-2.00822700	0.12246700
H	-0.69897500	-2.67877200	0.53838100
H	0.33283600	1.16846400	2.11718800
H	2.64747400	0.93753600	1.15311700
H	1.60017400	-2.89272200	-0.43536700
O	-3.74576300	-1.52142100	-1.47903700
C	-3.83247900	-2.40873700	-0.51029100
O	-3.24780400	-2.31305600	0.56189600
C	-4.76313600	-3.57666500	-0.83699500
O	-1.56266600	1.90765700	-0.49374200
C	-2.04653200	3.08605700	-0.91489900
O	-3.01153800	3.18404500	-1.63799500
C	-1.26454400	4.26597500	-0.33971100
H	-2.14792600	-1.25788900	1.59613200
C	-1.78550800	5.55755000	-0.96704400
H	-1.24115400	6.41360100	-0.55518100
H	-1.65029500	5.54690200	-2.05215500
H	-2.85191800	5.68711100	-0.76607000
C	-1.49974100	4.27596800	1.17919000
H	-2.56839700	4.34525600	1.41178400
H	-1.09960800	3.36834600	1.64063700
H	-0.99655400	5.14127700	1.62322700
C	0.23064000	4.08264900	-0.63069000
H	0.42123900	4.05708900	-1.70882400
H	0.79185900	4.92267800	-0.20803700
H	0.60447000	3.15383100	-0.19170000
C	-4.77325100	-4.56141500	0.33056400
H	-5.12062900	-4.07927500	1.24794500
H	-5.43928000	-5.39905300	0.09950500
H	-3.77094700	-4.95498200	0.52031300
C	-4.26961000	-4.26349700	-2.11784000
H	-4.25088300	-3.56208200	-2.95549400
H	-3.26230800	-4.67162100	-1.98220200
H	-4.93871800	-5.09283300	-2.36983000
C	-6.16953600	-3.00114900	-1.06524100
H	-6.87428400	-3.81810800	-1.25196500
H	-6.51553000	-2.44626000	-0.18586700
H	-6.17959400	-2.32949600	-1.92808800
O	3.51185700	-1.08178500	-0.23002400
C	4.43975500	-1.66702700	0.52481300
C	5.83153100	-1.54077100	-0.02233900
H	6.09767500	-2.49180400	-0.49998700
H	6.47695600	-1.43719200	0.85352800
C	6.03101700	-0.36391100	-0.98520400
H	5.55599100	-0.58199000	-1.94645100
H	5.52994200	0.51145200	-0.56373000
C	7.49992500	-0.07145600	-1.16697600
C	8.18810800	0.61859500	-0.16395100
C	8.20250800	-0.50342200	-2.29133200
C	9.54973100	0.87319700	-0.28521600
H	7.63746500	0.95625400	0.71208400
C	9.56713300	-0.24970300	-2.41668800
H	7.67524400	-1.03822300	-3.07781000
C	10.24342800	0.43882600	-1.41399100
H	10.07076400	1.41448300	0.49856400
H	10.10071400	-0.58833100	-3.29956300
H	11.30579600	0.63915900	-1.51143000
O	4.18927100	-2.27727500	1.55300100
F	4.91641100	0.55911300	1.71222900
H	4.37674700	0.41098800	2.49181200
F	2.32093800	-1.98873800	3.13355300
H	2.95837900	-2.20943700	2.41656200
F	3.31601200	0.18765300	3.60540000
H	2.84613800	-0.65862100	3.48188300

IM1-6

I	-2.56519200	0.06174500	-1.17457400
C	-4.20766500	0.75650600	-0.05872400
C	-6.35450100	1.69195400	1.37969900
C	-5.48555800	0.53356000	-0.55497000
C	-3.96246000	1.43343100	1.12743800
C	-5.06017500	1.90421500	1.84665700
C	-6.56642100	1.00737500	0.18493600
H	-5.63669500	0.00458600	-1.48941000
H	-2.95000900	1.56720200	1.49080400
H	-4.89486400	2.42904100	2.78193500
H	-7.57439800	0.84905400	-0.18455900
H	-7.20177500	2.06116100	1.94825000
O	-1.64777800	-0.42349200	1.94458800
C	-0.41275200	-0.66872300	1.45189200
C	2.13471100	-1.05825200	0.46125600
C	-0.06091000	-1.90307100	0.89667400
C	0.52056200	0.37188600	1.49391200
C	1.80072500	0.17980300	0.99462400
C	1.22475300	-2.10009000	0.40198500
H	-0.79549600	-2.70195700	0.86432100
H	0.22648500	1.32262200	1.92516200
H	2.54396400	0.96775900	1.01979000
H	1.52310300	-3.05381700	-0.02058800
O	-3.72383800	-1.70791500	-1.43555100
C	-3.85193800	-2.49448500	-0.38790700
O	-3.31661600	-2.28832100	0.69465800
C	-4.76407300	-3.69588000	-0.63660100
O	-1.60315600	1.81998200	-0.69441900
C	-2.07593700	2.94992900	-1.24316100
O	-3.01417100	2.97083700	-2.00660600
C	-1.31905000	4.18447100	-0.75630000
H	-2.26155800	-1.13635600	1.66878700
C	-1.82928500	5.40820700	-1.51481300
H	-1.30219000	6.30313200	-1.16838200
H	-1.66259800	5.29890100	-2.59002200
H	-2.90185400	5.54670900	-1.35692000
C	-1.59805400	4.33257900	0.74789600
H	-2.67331000	4.41557600	0.94254900
H	-1.20754500	3.47462700	1.30300900
H	-1.11162200	5.23856100	1.12414000
C	0.18501300	3.98808900	-0.98728300
H	0.40668600	3.86569200	-2.05275100
H	0.72904600	4.86762400	-0.62742100
H	0.55207500	3.10686800	-0.45452900
C	-4.82330900	-4.55933800	0.62197400
H	-5.21253200	-3.99059400	1.47036200
H	-5.47615600	-5.42056700	0.44674700
H	-3.82943300	-4.92497200	0.89408100
C	-4.21287500	-4.50338700	-1.81968700
H	-4.15911300	-3.88864900	-2.72143900
H	-3.21139800	-4.88891400	-1.60044100
H	-4.86800400	-5.35840100	-2.01666400
C	-6.16067300	-3.15595900	-0.98212500
H	-6.85417700	-3.99241900	-1.11752600
H	-6.54677500	-2.51933500	-0.17802300
H	-6.13438900	-2.57306100	-1.90690000
O	3.43285500	-1.24950900	-0.03542100
C	4.39509500	-1.47268400	0.85375100
C	5.77532300	-1.49825200	0.26682600
H	6.09672400	-2.54587200	0.21407500
H	6.41322400	-1.01056200	1.00793400
C	5.90308000	-0.80977200	-1.09721700
H	5.45024800	-1.43210300	-1.87511100
H	5.34389200	0.12856700	-1.06172800
C	7.35087400	-0.52578500	-1.41341800
C	7.98908000	0.54478100	-0.77887000
C	8.08245400	-1.32141700	-2.29410900
C	9.33103400	0.81435100	-1.02353500
H	7.41393000	1.16414700	-0.09326500
C	9.42762700	-1.05369300	-2.54203500
H	7.59360400	-2.15412800	-2.79424400
C	10.05445000	0.01433100	-1.90727900
H	9.81339700	1.65166500	-0.52856000
H	9.98440900	-1.67896700	-3.23331300
H	11.10138200	0.22538300	-2.10138200
O	4.18552600	-1.67478600	2.04274500
F	4.91512300	1.05127000	1.04892400
H	4.47020400	1.45472500	1.79618100
F	2.14538500	-1.65140500	3.38643800
H	2.92943300	-1.70211800	2.76998300
F	3.52249100	2.09868600	2.82809600
H	2.95615300	1.48928900	3.34465100
F	2.05550400	0.63858700	4.08592000
H	2.04910300	-0.30927800	3.79957500

IM1-7

I	-2.49252900	-0.33945700	-1.13384500
C	-4.24095200	0.38883700	-0.21448900
C	-6.52523100	1.37073600	0.95801400
C	-5.47042700	-0.05851600	-0.68056500
C	-4.11127500	1.31280000	0.81265600
C	-5.27725900	1.80392100	1.39773800
C	-6.62113200	0.44173600	-0.07553700
H	-5.53219000	-0.77760700	-1.48965300
H	-3.13292600	1.62226700	1.16087800
H	-5.20095000	2.52136700	2.20821900
H	-7.59317400	0.10975600	-0.42563400
H	-7.42651300	1.75857900	1.42135700
O	-1.82750500	-0.26984800	2.10838000
C	-0.54664500	-0.43108600	1.70361900
C	2.06404600	-0.63381800	0.82696400
C	0.04495500	-1.68992600	1.56691800
C	0.18073200	0.72153400	1.39513100
C	1.48905100	0.62327400	0.94612800
C	1.36286700	-1.79000100	1.12974500
H	-0.53124800	-2.58036000	1.79850900
H	-0.30637300	1.68602000	1.47692400
H	2.06783600	1.49884200	0.68667600
H	1.84473300	-2.75622400	1.02112600
O	-3.49672400	-2.21866100	-1.16240000
C	-3.59481600	-2.87031400	-0.02245500
O	-3.13261400	-2.47267100	1.03924000
C	-4.37182100	-4.18226000	-0.13916300
O	-1.68702800	1.54168000	-0.91235900
C	-2.16354700	2.53118100	-1.68500600
O	-3.05165700	2.37074600	-2.48995100
C	-1.47795600	3.86460600	-1.38760200
H	-2.33075000	-1.09267400	1.93662300
C	-1.94374900	4.89704600	-2.41235500
H	-1.46575500	5.86060600	-2.20800200
H	-1.68172000	4.58587000	-3.42753500
H	-3.02845100	5.02529900	-2.37297200
C	-1.89645700	4.29144700	0.02903600
H	-2.98727700	4.34917300	0.11758100
H	-1.51488600	3.59296700	0.77886700
H	-1.48107100	5.28036600	0.24945900
C	0.04424400	3.68593300	-1.44108300
H	0.37421300	3.39335100	-2.44359700
H	0.53746300	4.63002800	-1.18617800
H	0.37046100	2.92036200	-0.73379300
C	-4.41550900	-4.87061700	1.22366200
H	-4.90471800	-4.23706900	1.96806000
H	-4.97026000	-5.81108500	1.14340900
H	-3.40695600	-5.09031000	1.58429600
C	-3.67996100	-5.07960000	-1.17448300
H	-3.63648200	-4.58909700	-2.14993900
H	-2.65938400	-5.32573700	-0.86235200
H	-4.23683900	-6.01678700	-1.27785300
C	-5.79344400	-3.84335700	-0.61376600
H	-6.39395500	-4.75797500	-0.65673300
H	-6.28320900	-3.14612600	0.07546700
H	-5.77395600	-3.39373300	-1.61032600
O	3.38416900	-0.73149600	0.35996600
C	4.36187200	-0.68436100	1.26045700
C	5.73075500	-0.69647600	0.64757100
H	6.43321400	-1.02252300	1.41818100
H	5.95138200	0.35478200	0.42614800
C	5.85369400	-1.54552200	-0.62505700
H	5.56908600	-2.58042500	-0.40417400
H	5.15084600	-1.17222600	-1.37516900
C	7.26490100	-1.50202100	-1.15911600
C	7.65991600	-0.48891100	-2.03546300
C	8.21256400	-2.44161100	-0.74853100
C	8.97168600	-0.41773700	-2.49523800
H	6.92939300	0.24750300	-2.36251400
C	9.52576100	-2.37483000	-1.20589100
H	7.91555100	-3.23565100	-0.06714900
C	9.90848200	-1.36178100	-2.08127600
H	9.26170100	0.37316800	-3.17994600
H	10.24936500	-3.11600800	-0.88090800
H	10.93109100	-1.30937800	-2.44114200
O	4.17714500	-0.64084900	2.46737200
F	4.31242600	1.93367800	1.16604200
H	3.87828100	2.62338600	0.67383200
F	2.23259500	0.10201900	3.73119900
H	2.97920400	-0.27040800	3.17455200
F	2.85040900	3.61103300	-0.03208600
H	2.10697300	3.70156200	0.58865100
F	2.23402100	2.44772600	3.33776200
H	2.19304900	1.45782200	3.47340000
F	1.05536300	3.58838800	1.62079200
H	1.47752300	3.08089700	2.36839300

IM1-8

I	2.99603100	0.29090800	-1.15016600
C	4.13333100	0.52147100	0.59986200
C	5.64819900	0.77195600	2.87254000
C	5.19547800	1.41488500	0.58875200
C	3.79880000	-0.25864800	1.69813600
C	4.58002800	-0.12085700	2.84534600
C	5.95401500	1.53868200	1.74981600
H	5.42663000	1.99622800	-0.29758000
H	2.94757700	-0.93160100	1.66818400
H	4.33843400	-0.71143900	3.72302900
H	6.79278900	2.22700600	1.76795000
H	6.24657900	0.87101800	3.77239800
O	0.97744000	0.55427900	1.45519800
C	-0.33155800	0.66753400	1.10577700
C	-0.32333300	0.66393000	0.50290200
C	-1.19721600	1.53559700	1.77751000
C	-0.82138900	-0.15012400	0.08664100
C	-2.17521500	-0.15584000	-0.22033900
C	-2.55488500	1.53101700	1.47973700
H	-0.80266400	2.17851500	2.55749500
H	-0.13458000	-0.79569500	-0.44428100
H	-2.57448400	-0.80746100	-0.98641800

H	-3.25024200	2.16686000	2.01806100
O	3.06387400	2.40698600	-1.34157800
C	2.59083900	3.22575700	-0.42634000
O	2.03865100	2.87460900	0.60564700
C	2.84128800	4.69952300	-0.75536400
O	3.12525200	-1.75722900	-0.81857400
C	4.35432800	-2.28191000	-0.97649500
O	5.30921900	-1.61715300	-1.30959400
C	4.41640400	-3.77506500	-0.65879600
H	1.41116300	1.43206900	1.38804900
C	5.84250900	-4.26670900	-0.90313000
H	5.90440200	-5.33653500	-0.67821300
H	6.13856500	-4.10961800	-1.94380500
H	6.55503300	-3.73198200	-0.26982200
C	4.03578500	-3.96188100	0.81801400
H	4.70982400	-3.39221200	1.46809500
H	3.01178200	-3.63468500	1.01088800
H	4.12271700	-5.02079500	1.08416400
C	3.43104500	-4.53188900	-1.55942800
H	3.69879100	-4.41553700	-2.61510900
H	3.46506600	-5.59963300	-1.31824800
H	2.40780600	-4.17600500	-1.42598300
C	2.16735500	5.57573400	0.29897500
H	2.55863600	5.35995100	1.29636300
H	2.34780200	6.63119300	0.07031400
H	1.08774000	5.40280300	0.31939000
C	2.28624600	5.01154700	-2.15095800
H	2.76310700	4.38733500	-2.91021600
H	1.20498700	4.84251000	-2.19094400
H	2.47347600	6.06297400	-2.39319100
C	4.36225500	4.92003000	-0.73902000
H	4.58343400	5.97539500	-0.92979100
H	4.78621800	4.65477400	0.23634900
H	4.85122500	4.31807400	-1.51028900
O	-4.39874200	0.58005500	0.23425500
C	-5.13906200	-0.13098300	1.08637000
C	-6.56716400	-0.27467900	0.64320000
H	-7.16644800	-0.47925400	1.53380500
H	-6.59585600	-1.18417200	0.02791600
C	-7.12281600	0.91332300	-0.15279200
H	-7.04894100	1.82313900	0.45327300
H	-6.50691100	1.07085600	-1.04246300
C	-8.55979000	0.66651000	-0.54411200
C	-8.86913600	0.04486000	-1.75558900
C	-9.60187700	1.00827200	0.32043200
C	-10.19068600	-0.22701200	-2.09851200
H	-8.06556200	-0.22330600	-2.43762300
C	-10.92483700	0.73879300	-0.01810800
H	-9.37256800	1.49510500	1.26572400
C	-11.22234500	0.11973800	-1.22974400
H	-10.41485700	-0.70650400	-3.04628500
H	-11.72379300	1.01517200	0.66289500
H	-12.25343900	-0.08894800	-1.49666100
O	-4.71280400	-0.62804700	2.11371200
F	-3.64611800	-2.48802100	0.48825500
H	-2.94692800	-2.77614000	-0.08718100
F	-2.39623900	-1.33433900	2.65072900
H	-3.29916200	-1.04705300	2.35905200
F	-1.92158000	-2.98981600	-1.35246500
H	-0.98415800	-2.93425500	-1.17083800
F	-1.17695600	-2.81605200	1.25052600
H	-1.76939000	-2.20707300	1.78143000
F	0.60133300	-2.71894800	-1.27584500
H	1.07864000	-2.55178500	-0.44835100
F	1.17619300	-2.31053000	1.08334500
H	0.23549400	-2.45745300	1.31211300

IM1-9

I	2.45819500	0.48587100	-1.18065900
C	4.34833600	0.05676000	-0.36293900
C	6.80855300	-0.51079000	0.71887800
C	5.46145900	0.71178200	-0.87353100
C	4.41746800	-0.87114700	0.66533100
C	5.67238200	-1.15174000	1.20465600
C	6.70311600	0.41794700	-0.31476900
H	5.36660200	1.43065100	-1.67968000
H	3.52823300	-1.36098300	1.04532900
H	5.74879500	-1.86933000	2.01497700
H	7.58945700	0.91125300	-0.70030200
H	7.78057300	-0.73504300	1.14575500
O	1.45312100	0.46564700	2.10365600
C	0.22126500	0.59519900	1.49639500
C	-2.27269500	0.73546000	0.36324100
C	-0.49021800	1.78499200	1.57233900
C	-0.28403000	-0.50808800	0.81288200
C	-1.53652100	-0.43600900	0.22866000
C	-1.76215200	1.85213400	1.00393800
H	-0.06456700	2.63280400	2.09869800
H	0.31336300	-1.40983100	0.74379100
H	-1.96173200	-1.27628000	-0.30386300
H	-2.36678400	2.74892300	1.08243800
O	3.11188600	2.52048800	-1.11410900
C	3.14463200	3.10261900	0.06158600
O	2.79250700	2.56868300	1.10973700
C	3.69606100	4.52753900	0.02397800
O	2.00551800	-1.51169000	-1.00452000
C	2.62982400	-2.37422900	-1.82771500
O	3.42426400	-2.01561800	-2.66537800
C	2.24850600	-3.82298600	-1.53500400
H	2.05559000	1.20110500	1.82366700
C	2.83509500	-4.71141700	-2.63104600
H	2.59534700	-5.75879400	-2.42180300
H	2.42383500	-4.44916900	-3.61014300
H	3.92103000	-4.60114800	-2.68455300
C	2.85695600	-4.18259300	-0.16884900
H	3.94197600	-4.02789000	-0.16759900
H	2.41052900	-3.58358500	0.62851200
H	2.66089500	-5.23775500	0.04862100
C	0.72190300	-3.96817300	-1.47335400
H	0.25148300	-3.63773600	-2.40547300
H	0.46462900	-5.02143500	-1.32070600
H	0.29618200	-3.39815200	-0.64498100
C	3.67232200	5.12299000	1.43039400
H	4.27949000	4.52973500	2.11898700
H	4.06752200	6.14352900	1.40370300
H	2.65344400	5.15435800	1.82602600
C	2.83585000	5.36644800	-0.93139100
H	2.84172500	4.94189700	-1.93819100
H	1.79920500	5.42125100	-0.58236900
H	3.23102100	6.38647400	-0.97870100
C	5.13780200	4.45499000	-0.50313500
H	5.58089300	5.45619000	-0.49618900
H	5.75554600	3.80408700	0.12587800
H	5.15885500	4.07302800	-1.52746000
O	-3.56720400	0.78480500	-0.15157400
C	-4.45498500	-0.08516400	0.36409600
C	-5.78733000	0.00535100	-0.31501000
H	-6.30322700	-0.94461400	-0.16441200
H	-5.63319500	0.15911200	-1.38490600
C	-6.60487900	1.16643100	0.28586700
H	-6.71027200	1.00797500	1.36486900
H	-6.05400600	2.10271300	0.14338700
C	-7.96476200	1.25954900	-0.36091500
C	-8.14693000	2.00666000	-1.52652300
C	-9.05173500	0.55887000	0.16531200
C	-9.38937200	2.05664600	-2.15190500
H	-7.30630900	2.55605100	-1.94419500
C	-10.29618500	0.60600300	-0.45675300
H	-8.92018800	-0.02542600	1.07305600
C	-10.46792400	1.35582400	-1.61765300
H	-9.51610400	2.64532800	-3.05519000
H	-11.13272500	0.05914200	-0.03294000
H	-11.43807800	1.39551400	-2.10267700
O	-4.22323100	-0.78892900	1.32929100
F	-2.51269800	-3.51758800	-0.19396700
H	-2.40996800	-3.24837200	0.73149600
F	-2.48712500	-0.26397800	3.15514400
H	-3.03745500	-0.58969600	2.43052400
F	-2.08086600	-2.74888800	2.10418300
H	-1.13098100	-2.92041500	2.22983000
F	-0.29907500	-1.44467800	3.47981800
H	-1.13937300	-0.99702900	3.35630900
F	0.27638900	-3.44115400	1.95341800
H	0.90444100	-2.79980800	2.32688200
F	2.08969200	-1.88059900	2.52516000
H	1.81550600	-0.92742100	2.47393000
F	-3.92877900	-1.82133400	-1.41122200
H	-3.49912100	-2.54660900	-0.96739500

IM1-10

I	-2.81751500	0.46211800	0.30969700
C	-2.74870000	1.31423200	-1.61055800
C	-2.56536600	2.44060100	-4.12039600
C	-2.57103900	0.47987400	-2.70763100
C	-2.83630000	2.69651800	-1.73278400
C	-2.74144400	3.25596500	-3.00552300
C	-2.48251300	1.05841000	-3.97127100
H	-2.50749300	-0.59492400	-2.58184000
H	-2.96516700	3.32464500	-0.85798600
H	-2.81038800	4.33279500	-3.12005800
H	-2.33761000	0.42277100	-4.83852900
H	-2.49079600	2.88348300	-5.10805700
O	-2.12119900	-0.88645000	2.95064900
C	-0.79292800	-0.97272300	2.64098400
C	1.92082800	-0.99369200	2.02282400
C	-0.31097300	-1.83695400	1.65640100
C	0.08879900	-0.13516200	3.31899200
C	1.45028200	-0.14841800	3.02676000
C	1.04284400	-1.83938100	1.34992800
H	-0.99946600	-2.49228500	1.12954000
H	-0.30352600	0.51828500	4.09182800
H	2.13113800	0.49517000	3.56385300
H	1.44057500	-2.49321700	0.58113300
O	-4.11055700	-0.93306200	-0.65775900
C	-4.20810700	-2.07172100	-0.01433800
O	-3.65350900	-2.28067800	1.06093300
C	-5.08633300	-3.10727300	-0.71371100
O	-1.64889200	2.10471700	0.89352100
C	-0.37003000	2.05826400	0.57554800
O	0.13232400	1.05627500	0.07711000
C	0.41589600	3.34475900	0.81659600
H	-2.61628900	-1.57932700	2.47221200
C	1.07922200	3.70531100	-0.52387100
H	1.64080100	4.63776300	-0.40762600
H	1.77050000	2.91776700	-0.83132700
H	0.33010700	3.85043800	-1.31104600
C	-0.48838800	4.48202700	1.28955300
H	-1.25670100	4.71785800	0.54621400
H	-0.98950200	4.23008200	2.22772900
H	0.11830100	5.37898400	1.44993900
C	1.50352600	3.04852600	1.85869300
H	2.15130700	2.23218700	1.53261100
H	2.11952800	3.94316800	1.99775700
H	1.06209300	2.78254200	2.82490500
C	-4.59989600	-3.27573500	-2.15963600
H	-3.56068900	-3.62174600	-2.18920400
H	-5.21768200	-4.02214500	-2.66934600
H	-4.67032300	-2.33238900	-2.70763000
C	-6.52768100	-2.57347100	-0.71142400
H	-6.89173600	-2.43041400	0.31126100
H	-6.59191500	-1.61990200	-1.24209000
H	-7.18463600	-3.29521000	-1.20773700
C	-5.00685500	-4.43313500	0.04061100
H	-5.64596300	-5.17364500	-0.45087900
H	-3.98218700	-4.81502600	0.05858500
H	-5.33756400	-4.31562200	1.07547000
O	3.24665300	-1.13641200	1.65005900
C	4.16068100	-0.14161700	1.76489900
C	5.42326700	-0.52883400	1.03511800
H	5.75083500	-1.50849600	1.40127000
H	6.18934500	0.20855600	1.28468700
C	5.21827500	-0.60289500	-0.48985800
H	4.40283800	-1.30088700	-0.70218700
H	4.89663300	0.37542200	-0.85553300
C	6.48867300	-1.03946800	-1.17558700
C	7.41932100	-0.09811600	-1.62104200
C	6.78345900	-2.39583900	-1.33551200
C	8.61360500	-0.49938300	-2.21369200
H	7.19970900	0.96050400	-1.50377900
C	7.97543800	-2.80299900	-1.92761900
H	6.06541500	-3.13835000	-0.99432000
C	8.89511400	-1.85432500	-2.36889300
H	9.32363500	0.24680400	-2.55732300
H	8.18543100	-3.86153100	-2.04790600
H	9.82440500	-2.16939700	-2.83311500
O	3.99640400	0.87906200	2.38008800
F	2.64516600	0.81518800	-0.28894300
H	1.69299400	0.84865200	-0.14309400

IM1-11

I	2.88062300	0.41774500	-0.49162000
C	2.84774800	1.91895000	0.97561000
C	2.71322600	3.89074100	2.89674800
C	2.71861800	1.54691200	2.30845200
C	2.91143300	3.24927000	0.57570900
C	2.84050300	4.23860500	1.55430500
C	2.65541800	2.55069500	3.27171900
H	2.67200000	0.50101700	2.59019600
H	3.00538600	3.51082200	-0.47288500
H	2.89104900	5.28223300	1.26160700
H	2.54933800	2.27969600	4.31688200
H	2.65740800	4.66651700	3.65319500
O	2.12053600	-1.75209100	-2.49040200
C	0.87676200	-1.87072400	-1.93333800
C	-1.66252400	-1.93786200	-0.82878100
C	0.67559700	-2.47613100	-0.69350400
C	-0.19860300	-1.31195000	-2.62523400
C	-1.47336400	-1.34324500	-2.07364500
C	-0.60187900	-2.51003700	-0.14325700
H	1.51877500	-2.91006900	-0.16280800
H	-0.01624100	-0.86100200	-3.59569700
H	-2.32422000	-0.91086100	-2.58863200
H	-0.78431900	-2.96970100	0.82207100
O	4.28456400	-0.47033500	0.82873600
C	4.52447900	-1.72359000	0.51644900
O	4.01366400	-2.26783200	-0.45789700
C	5.49885700	-2.42597400	1.45750200
O	1.57914500	1.69568900	-1.56699800
C	0.33559200	1.76957400	-1.17249100
O	-0.09935100	1.04210500	-0.27521500
C	-0.51298500	2.83456400	-1.86403900
H	2.76959600	-2.22704000	-1.93858000
C	-1.17744900	3.67285600	-0.75978700
H	-1.78929300	4.45420400	-1.22122400
H	-1.82118000	3.05435900	-0.13158200
H	-0.42501800	4.15566200	-0.12598600
C	0.34217600	3.72744800	-2.76377100
H	1.11646700	4.24582300	-2.18964100
H	0.83225500	3.14980800	-3.55133900
H	-0.29842300	4.48130300	-3.23193300
C	-1.58845000	2.12436200	-2.69979300
H	-2.25352300	1.51787700	-2.08325600
H	-2.19837700	2.87861400	-3.20742000
H	-1.13577300	1.48285400	-3.46302800
C	5.00161200	-2.25986600	2.90024000
H	4.00851000	-2.70367100	3.02989200
H	5.68950100	-2.76733900	3.58407800
H	4.95134200	-1.20363200	3.17732400
C	6.86973300	-1.74860700	1.30022800
H	7.23861500	-1.84149700	0.27353400
H	6.81354700	-0.68756500	1.55733200
H	7.59247700	-2.23185100	1.96559700
C	5.58684800	-3.90444100	1.08349500
H	6.29486700	-4.40868900	1.74875500
H	4.61304500	-4.39328900	1.17766800
H	5.92519800	-4.02880900	0.05190400
O	-2.89788700	-1.91015800	-0.20389700
C	-3.97720600	-2.40896200	-0.87485700
C	-5.27718100	-2.05919700	-0.19013600
H	-5.85416300	-2.98301200	-0.07988600
H	-5.81401400	-1.44448700	-0.91960400
C	-5.16548100	-1.30515000	1.13975000
H	-4.86317000	-1.99264200	1.93683500

H	-4.37689600	-0.55264000	1.06126900
C	-6.46985200	-0.63103300	1.48842100
C	-6.86068600	0.50565200	0.77196800
C	-7.31250200	-1.12010700	2.48538000
C	-8.06663000	1.13847500	1.05087500
H	-6.20180900	0.88175200	-0.00864700
C	-8.52252600	-0.48805200	2.76783800
H	-7.01704300	-2.00251900	3.04795100
C	-8.90216900	0.64271700	2.05165300
H	-8.35603900	2.02170300	0.48931100
H	-9.16744100	-0.87987600	3.54872700
H	-9.84351300	1.13704500	2.27094200
O	-3.88770200	-3.03494300	-1.89442700
F	-4.09688500	0.27806800	-1.40750000
H	-3.47424800	0.44140000	-0.69721900
F	-2.45625400	0.90560700	0.37424600
H	-1.49788100	0.92911700	0.09797800

IM1-12

I	-2.81718300	0.29296500	0.37238300
C	-4.41775100	1.60275300	-0.00137800
C	-6.55983900	3.25979100	-0.51226000
C	-5.32246100	1.24310200	-0.99395400
C	-4.54920000	2.77174500	0.73781300
C	-5.63516800	3.60295300	0.47090200
C	-6.40328700	2.08486700	-1.24383600
H	-5.18654700	0.33158600	-1.56898100
H	-3.81897700	3.03633300	1.49414700
H	-5.75665900	4.51892900	1.03960100
H	-7.11777400	1.82067300	-2.01656000
H	-7.40371700	3.91201000	-0.71155300
O	-1.74625000	-2.40913900	0.60574200
C	-0.41063800	-2.22415100	0.35573100
C	2.27855300	-1.77845200	-0.06394100
C	0.09977100	-2.24060000	-0.94114300
C	0.42208400	-1.98226800	1.44509600
C	1.77642500	-1.75981200	1.23193500
C	1.45433100	-2.01453200	-1.15759900
H	-0.56683000	-2.42007200	-1.78123600
H	0.00042300	-1.98274700	2.44477000
H	2.46610400	-1.57792700	2.04940900
H	1.86714300	-2.01530000	-2.15801500
O	-4.36577100	-1.07255900	0.66035400
C	-4.57764400	-2.02051900	-0.23809400
O	-3.83776900	-2.22356000	-1.18908600
C	-5.85083400	-2.81897200	0.03686500
O	-1.76244900	2.17107300	0.18916600
C	-0.50533300	2.12140000	-0.09808200
O	0.07382000	1.02963700	-0.24495100
C	0.20679700	3.46503600	-0.24156000
H	-2.20614200	-2.64037700	-0.22329800
C	0.77976800	3.54412400	-1.66675300
H	1.29292900	4.50301000	-1.79001900
H	1.49907800	2.74451200	-1.85063000
H	-0.01764200	3.48760200	-2.41521600
C	-0.76095600	4.62480500	-0.00150300
H	-1.59215200	4.60514100	-0.71183400
H	-1.17750200	4.59139000	1.00930400
H	-0.22291700	5.57038600	-0.12089400
C	1.34539500	3.50776800	0.79043900
H	2.05781500	2.69444300	0.64904900
H	1.88421900	4.45498000	0.68774500
H	0.95295200	3.45067900	1.81111700
C	-7.04653600	-1.86508700	-0.11225300
H	-7.11793000	-1.47878800	-1.13551300
H	-7.97287700	-2.40581600	0.10733200
H	-6.96378000	-1.01882900	0.57556300
C	-5.79335100	-3.36319900	1.47142900
H	-4.91629200	-4.00290900	1.61435900
H	-5.74784700	-2.54925500	2.19844200
H	-6.68839100	-3.96214000	1.66836100
C	-5.95149500	-3.96381400	-0.96967100
H	-6.87111300	-4.52965700	-0.78985200
H	-5.96589200	-3.58627800	-1.99522100
H	-5.10104700	-4.64478300	-0.87611100
O	3.61968700	-1.45736000	-0.18721700
C	4.46392000	-2.23391700	-0.92550400
C	5.88666000	-1.80534100	-0.67540000
H	6.53305400	-2.36750800	-1.35220500
H	6.11602800	-2.09204100	0.35712800
C	6.10930900	-0.29012100	-0.81465000
H	5.92905200	0.01723300	-1.85071800
H	5.38178500	0.23447200	-0.19014400
C	7.50692900	0.09074800	-0.39097200
C	7.83345600	0.10761800	0.96924400
C	8.49465100	0.39634200	-1.32671900
C	9.12255800	0.42966100	1.38000800
H	7.06339100	-0.13877200	1.69730500
C	9.78692700	0.71937100	-0.91689900
H	8.24815700	0.38474600	-2.38581800
C	10.10349700	0.73736200	0.43800000
H	9.36302000	0.44303400	2.43883700
H	10.54480400	0.95812800	-1.65702300
H	11.10903800	0.99026700	0.75987500
O	4.09467000	-3.13295000	-1.63021800
F	4.95633800	-1.05034900	2.17161900
H	4.44511000	-0.38281700	1.73004800
F	3.58697400	0.89851900	1.20319700
H	3.18438000	0.78679200	0.32601400
F	2.39432600	0.91454300	-0.93115900
H	1.41872900	0.93502900	-0.64883300

IM1-13

I	-2.69262700	0.45348600	0.39442100
C	-4.00232900	2.06115500	0.07348100
C	-5.74477300	4.15339400	-0.33548200
C	-4.96566500	1.94105200	-0.92174200
C	-3.88021000	3.19703300	0.86582500
C	-4.76428900	4.25065600	0.64932600
C	-5.84425100	3.00516200	-1.11658100
H	-5.02511400	1.04677000	-1.53386600
H	-3.10907800	3.26637800	1.62516000
H	-4.68638400	5.14564100	1.25764100
H	-6.60181900	2.93391600	-1.89004700
H	-6.43174000	4.97771400	-0.49628000
O	-2.16429600	-2.51967500	-0.58750500
C	-0.88271400	-2.15825100	-0.89903500
C	1.74127300	-1.40732600	-1.37389300
C	-0.58949000	-1.29573700	-1.95352700
C	0.14081700	-2.64912900	-0.08713400
C	1.45399000	-2.27827300	-0.32497300
C	0.73305800	-0.92296500	-2.19269000
H	-1.39099900	-0.92010800	-2.58561500
H	-0.10818000	-3.31801000	0.72970100
H	2.25574500	-2.65664900	0.29224800
H	0.98737100	-0.25558100	-3.00950000
O	-4.39047200	-0.69698900	0.75006400
C	-4.89534400	-1.38718600	-0.26157100
O	-4.50415700	-1.26618700	-1.41440900
C	-5.98762000	-2.36126700	0.16670100
O	-1.25049700	2.03271400	0.07736800
C	-0.03541700	1.70178500	0.35531200
O	0.22443800	0.55802900	0.77931600
C	1.03788300	2.76493100	0.15423500
H	-2.77640000	-2.21828900	-1.28268700
C	2.05227100	2.21438900	-0.86126400
H	2.85281900	2.94920200	-0.99762400
H	2.50065100	1.27901300	-0.51904400
H	1.58019100	2.03817000	-1.83361500
C	0.42723500	4.07054300	-0.35470500
H	-0.07708100	3.92669700	-1.31388800
H	-0.30295000	4.47232300	0.35376500
H	1.22313400	4.80980300	-0.48786600
C	1.72781000	2.99177000	1.51050200
H	2.19385500	2.07486400	1.87624800
H	2.50886900	3.74870400	1.38972000
H	1.01621800	3.35471000	2.25998800
C	-7.06317600	-1.60242100	0.95541200
H	-7.52394200	-0.81978700	0.34274900
H	-7.84925900	-2.30033300	1.26108300
H	-6.64043300	-1.13829800	1.84940700
C	-5.32362800	-3.42028200	1.06327300
H	-4.50947000	-3.92797300	0.53593300
H	-4.91526600	-2.96412600	1.96854800
H	-6.06864500	-4.16869100	1.35234000
C	-6.59036700	-3.01601500	-1.07519700
H	-7.37025800	-3.72225600	-0.77354500
H	-7.03476200	-2.26896100	-1.73894400
H	-5.82923500	-3.55775400	-1.64240800
O	3.02022100	-0.91375100	-1.56852000
C	4.07540100	-1.78272500	-1.55177300
C	5.38780900	-1.04248000	-1.48959100
H	5.76461800	-0.92005500	-2.51257700
H	6.07824500	-1.71288700	-0.97340700
C	5.31137800	0.31460000	-0.77443100
H	4.85678200	1.05632200	-1.43945800
H	4.65480600	0.21074600	0.09458600
C	6.67856600	0.77057300	-0.32946200
C	7.25878600	0.18845500	0.80281800
C	7.39913300	1.73530700	-1.03315500
C	8.52962000	0.56704400	1.22136300
H	6.69393000	-0.56481200	1.34804000
C	8.67325000	2.11725900	-0.61652800
H	6.95635400	2.19375400	-1.91447800
C	9.24128600	1.53424000	0.51213600
H	8.96621000	0.11005400	2.10440400
H	9.22087600	2.87152700	-1.17377100
H	10.23276300	1.83156900	0.83946400
O	3.94734200	-2.97464700	-1.60089300
F	4.51337700	-1.88929800	1.10246800
H	4.32061400	-2.81627700	1.21841100
F	3.41157400	-3.98166200	1.83483200
H	2.85624400	-3.31934700	2.27641300
F	2.11578700	-2.10148700	2.69657000
H	2.36663900	-1.32142100	2.15086900
F	2.45926600	-0.12563500	1.35023500
H	1.51090100	0.15402200	1.08138600

IM1-14

I	-2.68615200	0.44630400	0.45973500
C	-4.13876300	1.94864100	0.19900900
C	-6.09254700	3.85762500	-0.16366400
C	-3.96411800	2.90155000	-0.79725900
C	-5.26170700	1.92087900	1.01828900
C	-6.24401400	2.88980100	0.82582100
C	-4.95709500	3.86316700	-0.96979700
H	-3.07609600	2.90157400	-1.41801600
H	-5.37676700	1.15799000	1.78033400
H	-7.12567900	2.88587900	1.45831500
H	-4.84056800	4.61325200	-1.74499700
H	-6.86157400	4.60933100	-0.30756800
O	-2.15726000	-2.39435700	-0.89445400
C	-0.88757800	-1.96974700	-1.16482200
C	1.71809400	-1.11172300	-1.56351600
C	-0.61059700	-1.02863100	-2.15454600
C	0.14379100	-2.48533100	-0.37706800
C	1.44499700	-2.05485900	-0.57493400
C	0.70277000	-0.60400700	-2.35827000
H	-1.41768200	-0.63545000	-2.76871600
H	-0.08049900	-3.22385100	0.38457300
H	2.25563300	-2.44442500	0.02250300
H	0.94393700	0.11880800	-3.13069000
O	-4.27954700	-0.83211100	0.78661300
C	-4.88726500	-1.32079800	-0.29467100
O	-4.54459200	-1.04119400	-1.42950600
C	-6.02431500	-2.27594300	0.04966500
O	-1.35761900	2.13814400	0.16964500
C	-0.11549900	1.85189000	0.35632500
O	0.21648300	0.70047000	0.70663200
C	0.90102000	2.96740400	0.14691100
H	-2.78633000	-1.99977800	-1.52430300
C	1.88650200	2.50674000	-0.93963400
H	2.64600100	3.28298500	-1.08083100
H	2.39261000	1.57856500	-0.66375800
H	1.37441000	2.35273500	-1.89536300
C	0.21022500	4.26400700	-0.27520400
H	-0.32598400	4.13842700	-1.22039100
H	-0.50610700	4.59934700	0.47979900
H	0.96521000	5.04474700	-0.40953700
C	1.64715900	3.16843400	1.47744700
H	2.16724900	2.25736400	1.77983700
H	2.39037500	3.96181100	1.35208700
H	0.95912200	3.46917600	2.27456200
C	-6.73388700	-2.68983400	-1.23851800
H	-6.04127100	-3.18171100	-1.92602100
H	-7.54524900	-3.38536100	-1.00193600
H	-7.15599500	-1.82166600	-1.75236000
C	-7.00039500	-1.57302300	1.00292100
H	-6.50848700	-1.30870600	1.94275400
H	-7.40655600	-0.66106100	0.55073800
H	-7.83737700	-2.24224200	1.22665800
C	-5.40192900	-3.50134300	0.73934300
H	-6.18803300	-4.22926200	0.96493000
H	-4.66146400	-3.98197400	0.09182400
H	-4.90888900	-3.21686000	1.67226900
O	2.98811500	-0.58096700	-1.71612700
C	4.05653800	-1.43401900	-1.73519000
C	5.35847100	-0.68951600	-1.57753500
H	5.76488500	-0.48618400	-2.57587100
H	6.03982400	-1.39571900	-1.09735900
C	5.25366600	0.60456300	-0.75670200
H	4.84736500	1.40751400	-1.38088900
H	4.54584600	0.43919100	0.06027700
C	6.59639700	0.99805000	-0.19278500
C	7.09972700	0.30246500	0.91205900
C	7.36863900	2.01292800	-0.75677900
C	8.34627300	0.61855100	1.44047200
H	6.49426000	-0.48947500	1.34813200
C	8.61888500	2.33270400	-0.22946100
H	6.98596500	2.55969700	-1.61553800
C	9.11041400	1.63641600	0.87045400
H	8.72274400	0.07308600	2.30063100
H	9.20777600	3.12701500	-0.67844500
H	10.08317300	1.88506000	1.28334800
O	3.94857600	-2.62083800	-1.87359500
F	4.32854400	-1.81578000	0.91894300
H	4.33774800	-2.75729500	0.73089800
F	3.96085400	-4.25973500	0.64604100
H	3.09892700	-4.27770400	1.08177900
F	2.23161700	-1.74026500	2.66279100
H	2.47954200	-1.05837700	1.99096100
F	2.49210900	0.08512200	1.13050800
H	1.51772000	0.34422500	0.92115200
F	1.81533400	-3.93897400	1.80336900
H	1.96382200	-3.03349600	2.16955900

IM1-15

I	-2.86174500	0.30305500	0.65472900
C	-4.14277500	1.77118500	-0.12861400
C	-5.85666700	3.64286700	-1.20211400
C	-3.68113600	2.59423500	-1.14853600
C	-5.43889600	1.85280300	0.36632000
C	-6.29827800	2.80188200	-0.18411300
C	-4.55300800	3.53956100	-1.68216800
H	-2.66710400	2.50288100	-1.52253000
H	-5.77667600	1.18758500	1.15377300
H	-7.31264400	2.88343400	0.19242500
H	-4.21157700	4.18798100	-2.48220000
H	-6.53102900	4.38007900	-1.62500600
O	-1.99141700	-2.46920600	-0.43731700
C	-0.67872100	-2.19435300	-0.70601600
C	2.01344200	-1.69465700	-1.15417900
C	-0.27895700	-1.56620900	-1.88307200
C	0.26585200	-2.54439800	0.25741300
C	1.61306400	-2.28335000	0.04537200
C	1.07393600	-1.32679700	-2.10839700
H	-1.02153000	-1.27810700	-2.62350200
H	-0.06534200	-3.02699300	1.16966500
H	2.34619800	-2.55416200	0.79298500
H	1.41427400	-0.85322700	-3.02297100
O	-4.48409800	-0.96184600	0.47384000
C	-4.78957700	-1.40409500	-0.74451000
O	-4.11170600	-1.15588200	-1.72622900

C	-6.04875900	-2.26301400	-0.76137500
O	-1.57876600	2.04935500	0.86404900
C	-0.32744500	2.01329600	0.58009000
O	0.27479200	0.93917300	0.34268400
C	0.40667900	3.34940200	0.55882500
H	-2.53161000	-2.19801800	-1.20083100
C	1.11380300	3.48864700	-0.79969900
H	1.62810700	4.45407500	-0.83208700
H	1.85689500	2.70361600	-0.94789900
H	0.39468400	3.46165300	-1.62592500
C	-0.56215700	4.51241000	0.77118100
H	-1.32575900	4.54537300	-0.01233000
H	-1.07292100	4.43468000	1.73417100
H	-0.00316400	5.45297100	0.74849100
C	1.44712400	3.30217700	1.69263400
H	2.12941500	2.46073500	1.56243300
H	2.02876100	4.22920200	1.68277200
H	0.95811500	3.21528100	2.66841100
C	-6.37236600	-2.64297700	-2.20536300
H	-5.54754800	-3.19839600	-2.65882000
H	-7.26915200	-3.27008200	-2.22596800
H	-6.55289000	-1.75380600	-2.81570200
C	-7.20380700	-1.46533500	-0.14002800
H	-6.99590400	-1.22575900	0.90618200
H	-7.37719200	-0.53104500	-0.68609800
H	-8.12188700	-2.05991200	-0.18378700
C	-5.76462100	-3.52025400	0.07694300
H	-6.64199700	-4.17478300	0.05837500
H	-4.91256000	-4.07741400	-0.32624200
H	-5.54396400	-3.25822600	1.11466300
O	3.32865100	-1.37358500	-1.42494100
C	4.32474900	-2.23145400	-1.07262800
C	5.68467300	-1.58932400	-1.21105400
H	6.20646400	-2.07839500	-2.04214400
H	6.22476400	-1.87042800	-0.30236300
C	5.68053300	-0.06529300	-1.37841500
H	5.37110300	0.19608100	-2.39562300
H	4.93485100	0.35871900	-0.70154800
C	7.04099700	0.51106800	-1.07403600
C	7.44609700	0.64192900	0.25866500
C	7.92700400	0.88734900	-2.08328700
C	8.70585300	1.13954300	0.57308100
H	6.75406400	0.34661900	1.04484800
C	9.19063600	1.38701200	-1.77285600
H	7.62211300	0.79080700	-3.12272600
C	9.58315400	1.51456200	-0.44386100
H	9.00437300	1.23864100	1.61248000
H	9.86778500	1.67771000	-2.57052700
H	10.56643000	1.90490700	-0.20017300
O	4.13624200	-3.36004500	-0.70715800
F	4.35015300	-0.96095700	1.27738300
H	4.11371500	-1.62446600	1.93393000
F	3.43554900	-2.57348100	2.92042200
H	2.50361700	-2.35006400	3.04128600
F	2.08691500	-0.26027800	2.19900100
H	2.76209200	-0.11793900	1.53852400
F	2.78054200	0.89340600	0.06473600
H	1.80985800	0.88191500	0.06286700
F	0.97697300	-2.38193300	3.22679200
H	0.55761000	-1.60551000	2.85015200
F	-0.47955200	-0.56136500	2.22212700
H	0.03231400	-0.14290000	1.50713600

IM1-16

I	-2.74696900	0.28614900	-0.45011800
C	-4.08176100	1.82170600	0.04201700
C	-5.86643600	3.79298600	0.73079300
C	-5.35316900	1.79196100	-0.51932200
C	-3.67116900	2.79932300	0.94032700
C	-4.58499300	3.79606600	1.27683200
C	-6.25084600	2.79477200	-0.16204400
H	-5.63813900	1.01169300	-1.21903600
H	-2.67030800	2.77716000	1.36153300
H	-4.29233700	4.57050400	1.97818600
H	-7.24862700	2.79577400	-0.58822000
H	-6.57104800	4.57186200	1.00346700
O	-1.98106500	-2.44907400	-0.90737400
C	-0.60727200	-2.36931700	-0.93343700
C	2.13902600	-2.10460000	-0.85168300
C	0.12708500	-2.50522400	-2.10600800
C	0.02362900	-2.09758500	0.27841200
C	1.40296800	-1.96570700	0.32276400
C	1.51325000	-2.37356800	-2.06005300
H	-0.37332300	-2.71239100	-3.04849300
H	-0.57074300	-1.96959200	1.17543000
H	1.89481100	-1.74409000	1.25884600
H	2.11495700	-2.46866500	-2.95713800
O	-4.16759000	-0.97460200	0.25190400
C	-4.73169800	-1.81941100	-0.62299200
O	-4.50478200	-1.79361800	-1.81435700
C	-5.66033500	-2.80826900	0.07275800
O	-1.53598000	2.12049700	-1.04105800
C	-0.29344800	2.07357600	-0.94355200
O	0.25678700	0.90628700	-0.81984900
C	0.53177000	3.34371000	-1.03296900
H	-2.34296400	-2.60905000	-1.79408300
C	1.47797800	3.20995900	-2.24056200
H	2.04438500	4.14048100	-2.34223600
H	2.19105200	2.39385400	-2.10864500
H	0.91705500	3.05144000	-3.16735700
C	-0.40472300	4.53798300	-1.22113100
H	-0.98622000	4.44889700	-2.14261600
H	-1.10444400	4.62379000	-0.38522500
H	0.19312700	5.45262000	-1.27252700
C	1.34463400	3.51296200	0.26345600
H	2.03539200	2.68434500	0.42167000
H	1.92746700	4.43523600	0.17964000
H	0.68315200	3.59091700	1.12966800
C	-6.33051200	-3.68364800	-0.98484100
H	-5.58707300	-4.23653100	-1.56487100
H	-6.99616000	-4.40149000	-0.49547100
H	-6.91901500	-3.08059400	-1.68193500
C	-6.71093100	-2.03050700	0.87806600
H	-6.23892900	-1.40014000	1.63538700
H	-7.31831200	-1.39462700	0.22431800
H	-7.38047400	-2.73739400	1.37843600
C	-4.79816400	-3.66340700	1.01628900
H	-5.42933600	-4.41612100	1.49966700
H	-4.00528900	-4.17834400	0.46464200
H	-4.33190400	-3.04588100	1.78775100
O	3.50522500	-1.88399600	-0.88021000
C	4.29531400	-2.49104000	0.05213900
C	5.70425300	-1.94556400	0.03086300
H	6.38094800	-2.77853700	-0.18975400
H	5.90967700	-1.65232800	1.06515800
C	5.95462400	-0.76323300	-0.91183200
H	5.96530400	-1.10996900	-1.95030600
H	5.12455900	-0.05747500	-0.82621600
C	7.25068100	-0.06974100	-0.57092900
C	7.30508000	0.76954500	0.54683000
C	8.41116000	-0.26730900	-1.31850300
C	8.49220400	1.39804100	0.90616600
H	6.40016500	0.92166300	1.13202100
C	9.60320400	0.36114700	-0.96227100
H	8.37973600	-0.91702500	-2.18992400
C	9.64649400	1.19536900	0.15069000
H	8.51803300	2.04902600	1.77484100
H	10.49767000	0.19906900	-1.55619500
H	10.57375700	1.68654400	0.42884700
O	3.90443100	-3.34767000	0.79531400
F	3.86744700	-0.11654600	1.33485900
H	3.33262600	-0.28305900	2.16944900
F	2.74147000	-0.68513400	3.33468500
H	1.75595900	-0.83728200	3.25242600
F	1.41711700	0.72666100	1.61979500
H	3.12894700	0.43936000	0.21222100
F	2.81529200	0.82358200	-0.63623600
H	1.24710100	0.89147600	-0.66082700
F	-1.42653500	-0.19404500	2.59369700
H	-1.15654500	0.80752100	2.16466300
F	-0.75332000	1.77375400	1.68422500
H	0.57570300	1.22394400	1.64925800
F	0.47475700	-1.34843000	3.24607500
H	-0.35070900	-0.78949400	2.98330400

IM2-1

I	-2.10572400	-0.96663900	-0.74925300
C	-3.66872200	0.41207000	-0.93728800
C	-5.66572000	2.28521000	-1.19422200
C	-4.46417900	0.68663900	0.17032600
C	-3.82811100	1.05347900	-2.16008400
C	-4.83954700	2.00399500	-2.27885300
C	-5.47877200	1.63044800	0.02225800
H	-4.27796700	0.19535100	1.11951900
H	-3.16780800	0.83493900	-2.99218600
H	-4.97871900	2.52054200	-3.22263700
H	-6.11577700	1.86266000	0.87025100
H	-6.45375800	3.02497700	-1.29349700
O	-0.93195000	0.65762000	-1.42927300
C	0.40659800	0.41401700	-1.28221100
C	3.12590200	-0.05717400	-1.02141200
C	0.99610700	0.43157400	-0.01389400
C	1.18303600	0.14025800	-2.41084000
C	2.54811500	-0.09246200	-2.28720400
C	2.36100800	0.19921400	0.11061100
H	0.37261000	0.64016900	0.85144300
H	0.70318000	0.12804900	-3.38405300
H	3.15725300	-0.29005100	-3.15994500
H	2.84600400	0.21085500	1.08101900
O	-1.78665100	1.51966000	1.40918600
C	-2.00454700	2.63157700	0.96489300
O	-1.76604600	2.96146600	-0.30022700
C	-2.51713300	3.79154900	1.80978000
O	-3.52544600	-2.44092000	-0.34673900
C	-3.94742000	-2.59373000	0.90886400
O	-3.61662700	-1.86701500	1.82223700
C	-4.91853600	-3.76665700	1.05782900
H	-1.41664600	2.15150500	-0.76022300
C	-5.29910800	-3.91239200	2.53004100
H	-6.00255600	-4.74312800	2.64870900
H	-4.41680300	-4.10961700	3.14494500
H	-5.76712500	-2.99875800	2.90540100
C	-6.16205400	-3.45482500	0.21093100
H	-6.63722400	-2.52418500	0.54002500
H	-5.90009400	-3.35502000	-0.84543300
H	-6.89136200	-4.26488400	0.31736500
C	-4.24851000	-5.04820000	0.54527600
H	-3.34498400	-5.27662400	1.12061500
H	-4.93934400	-5.89121600	0.65260000
H	-3.97498900	-4.95254400	-0.50823300
C	-1.27022600	4.54023200	2.31317900
H	-0.68177700	4.92517300	1.47470500
H	-1.57602300	5.38544800	2.93890500
H	-0.63606600	3.87862700	2.91154500
C	-3.30307600	3.22730900	2.99350900
H	-4.19463100	2.69308800	2.64730000
H	-2.69367200	2.52511400	3.56622200
H	-3.62407400	4.04251000	3.65026200
C	-3.39059100	4.73692500	0.98044800
H	-3.75499400	5.55034700	1.61720800
H	-2.82792400	5.16751200	0.14922200
H	-4.25558300	4.20871100	0.56640100
O	4.46693900	-0.35172300	-0.80361200
C	5.43030200	0.22516300	-1.57446400
C	6.79483300	-0.21686000	-1.10541700
H	7.53336300	0.23363000	-1.77180600
H	6.86185300	-1.30659800	-1.19982700
C	7.06595200	0.17883300	0.35764800
H	6.96396400	1.26507100	0.46047500
H	6.30649200	-0.28230500	0.99599200
C	8.44636100	-0.25395000	0.78638700
C	8.64975000	-1.50730200	1.36768500
C	9.55248200	0.56872500	0.56180700
C	9.92857500	-1.92944600	1.72044700
H	7.79501000	-2.15492700	1.54917000
C	10.83303600	0.15122900	0.91287300
H	9.40506900	1.54760400	0.11116600
C	11.02422900	-1.10024500	1.49366300
H	10.06900200	-2.90466100	2.17637200
H	11.68171800	0.80473600	0.73595000
H	12.02168900	-1.42624700	1.77089200
O	5.20676300	0.97900700	-2.48167500

IM2-2

I	0.39401600	0.32023300	-0.09228900
C	2.24759300	1.21978400	-0.47347500
C	4.71782100	2.36644200	-0.87174000
C	2.70105200	2.16951300	0.43816100
C	2.98997300	0.83377200	-1.58349300
C	4.24697900	1.41037100	-1.76638700
C	3.94274800	2.75347900	0.22162900
H	2.09584600	2.45042900	1.29298200
H	2.62166400	0.09122300	-2.28107000
H	4.85396500	1.10425300	-2.61201100
H	4.31086600	3.50265500	0.91525700
H	5.69175100	2.82002900	-1.02869800
O	2.71560600	-2.19757900	-1.60488300
C	1.58919800	-2.30309700	-1.09580900
C	-0.96643700	-2.78214400	0.10221600
C	1.28643700	-1.88091000	0.28063500
C	0.45130200	-2.78546500	-1.87679100
C	-0.76066300	-3.00521600	-1.31141700
C	0.05003600	-2.34385500	0.88533100
H	2.15450800	-1.69451200	0.91106700
H	0.62953300	-2.99202000	-2.92665200
H	-1.58444300	-3.37119800	-1.91135100
H	-0.13242800	-2.16276400	1.94025200
O	4.04965000	-0.62654700	1.19206700
C	5.07616400	-0.88266100	0.58984500
O	5.10300400	-1.53075100	-0.56695100
C	6.46897100	-0.56697500	1.12544400
O	-0.32798300	2.37352200	-0.36060800
C	-1.61960700	2.39644800	-0.14312700
O	-2.26542800	1.38818700	0.12919500
C	-2.25403800	3.78585900	-0.26281700
H	4.17402300	-1.75430200	-0.85113100
O	-2.21428400	-2.84204000	0.68473100
C	-3.24709500	-3.56598200	0.15897700
O	-3.10016600	-4.50415800	-0.57508400
C	-4.54303300	-2.91948900	0.56719600
H	-5.35516700	-3.63889000	0.44770600
H	-4.48389400	-2.60127100	1.61119500
C	-4.75144500	-1.68127700	-0.33719800
H	-3.82875100	-1.09046300	-0.34896200
H	-4.93418300	-2.02766200	-1.36165200
C	-5.88356300	-0.80106600	0.13276200
C	-7.20489200	-1.25480600	0.10603600
C	-5.61642000	0.48358600	0.61161800
C	-8.24230500	-0.44189600	0.55205300
H	-7.42363900	-2.25016500	-0.27499100
C	-6.65584700	1.29979000	1.05374900
H	-4.58994100	0.84596200	0.62398600
C	-7.96941700	0.83941000	1.02788300
H	-9.26484100	-0.80585400	0.52360300
H	-6.43571100	2.29964900	1.41699900
H	-8.77864400	1.47553600	1.37282300
C	-3.73784500	3.69875800	0.09044900
H	-3.87409900	3.33618300	1.11439900
H	-4.19662800	4.68981300	0.00754000
H	-4.26388000	3.01273200	-0.57963800
C	-1.52712900	4.74016400	0.69417800
H	-0.46382000	4.79981600	0.44864000
H	-1.96206200	5.74241800	0.61752900
H	-1.62644300	4.40670700	1.73292000
C	-2.07361500	4.26735600	-1.70974100
H	-2.57191800	3.59162000	-2.41289500
H	-2.51527000	5.26299400	-1.82498700
H	-1.01362500	4.32162600	-1.97104000
C	6.99459900	-1.87173400	1.75083900
H	7.05518300	-2.66583500	1.00106800
H	7.99537200	-1.70491400	2.16330900
H	6.33980200	-2.20561500	2.56218000
C	7.40413100	-0.12918400	-0.00612900

H	7.03262500	0.77880700	-0.49195000
H	8.39816500	0.08418100	0.40153000
H	7.49599700	-0.90893200	-0.76526700
C	6.36420000	0.52041600	2.19317200
H	7.35138700	0.71284000	2.62623300
H	5.98584800	1.45238600	1.76115800
H	5.67967100	0.21875500	2.98922000

IM2-3

I	2.21957000	-0.95481400	0.70032200
C	3.76532800	0.44549300	0.86973100
C	5.73778900	2.34750100	1.09982000
C	4.57623100	0.69340400	-0.23294700
C	3.89756500	1.12646400	2.07436500
C	4.89685300	2.09128500	2.17935700
C	5.57816700	1.65270500	-0.09820600
H	4.41194700	0.16955200	-1.16864600
H	3.22624300	0.92685400	2.90240400
H	5.01498900	2.63856200	3.10856900
H	6.22705900	1.86488500	-0.94243600
H	6.51628100	3.09862200	1.18851800
O	1.01974300	0.68546600	1.29763200
C	-0.31357200	0.42919100	1.13977700
C	-3.01970700	-0.06355700	0.85718300
C	-0.88492200	0.40892800	-0.13765400
C	-1.10416400	0.18180300	2.26450400
C	-2.46648600	-0.06616600	2.13221700
C	-2.24621100	0.16495700	-0.27417500
H	-0.25047600	0.59752000	-0.99951800
H	-0.64182900	0.20193000	3.24584000
H	-3.07545800	-0.23527600	3.01117000
H	-2.71879800	0.14695500	-1.25062000
O	1.90886500	1.45773900	-1.55125000
C	2.11858700	2.58429300	-1.14084100
O	1.86349600	2.95478700	0.10961900
C	2.63792700	3.71697700	-2.01803600
O	3.65660900	-2.43058700	0.38349800
C	4.11090200	-2.62313700	-0.85567600
O	3.79702300	-1.93098200	-1.80115700
C	5.09325700	-3.79296600	-0.93957400
H	1.51155000	2.15919300	0.59227900
C	5.51454500	-3.98405900	-2.39542800
H	6.22576300	-4.81349100	-2.46759300
H	4.65044000	-4.20718100	-3.02708900
H	5.98743200	-3.08012500	-2.78781700
C	6.31128500	-3.44524800	-0.06994700
H	6.78983200	-2.52263700	-0.41625300
H	6.02010500	-3.31310700	0.97512900
H	7.04786400	-4.25344700	-0.13016900
C	4.41695400	-5.06166800	-0.40358600
H	3.53092600	-5.31496100	-0.99548900
H	5.11551300	-5.90293000	-0.46433600
H	4.11416800	-4.93364000	0.63842200
C	1.39433600	4.43142900	-2.57645900
H	0.78405200	4.84203000	-1.76616100
H	1.70458900	5.25524700	-3.22796500
H	0.78034100	3.73985000	-3.16178700
C	3.45470300	3.11642300	-3.16254400
H	4.34476900	2.60686600	-2.77750400
H	2.86511700	2.38530600	-3.71960400
H	3.78037700	3.90914800	-3.84401700
C	3.48337500	4.70349000	-1.20798900
H	3.85297800	5.49554900	-1.86821200
H	2.89854400	5.15981200	-0.40631000
H	4.34456500	4.20160200	-0.75515100
O	-4.36364600	-0.36963100	0.62298700
C	-5.34674100	0.24158200	1.30533900
C	-6.69828500	-0.20126000	0.80693100
H	-7.45480700	0.32017900	1.39664600
H	-6.79728900	-1.27683600	0.99336700
C	-6.88993300	0.06903700	-0.69686600
H	-6.75724700	1.13947300	-0.89001500
H	-6.11350400	-0.46272800	-1.25473800
C	-8.25964000	-0.37307700	-1.15022900
C	-8.46804900	-1.67466300	-1.61127500
C	-9.35157300	0.49342700	-1.06750900
C	-9.73910400	-2.10170500	-1.98513200
H	-7.62380100	-2.35673000	-1.68193000
C	-10.62435900	0.07092100	-1.44043800
H	-9.19982200	1.50990300	-0.71152200
C	-10.82102300	-1.22891600	-1.90043500
H	-9.88389500	-3.11507900	-2.34650800
H	-11.46223500	0.75804000	-1.37502700
H	-11.81226100	-1.55909000	-2.19434100
O	-5.16871300	1.04828000	2.18880700
F	-4.14690300	0.70474000	4.60795100
H	-4.50032200	1.04474300	3.80302800

IM2-4

I	2.29914800	-1.02267700	0.72201900
C	3.87475000	0.33225200	0.96689000
C	5.89849400	2.16514600	1.28968700
C	4.76653000	0.52378300	-0.08325200
C	3.95219800	1.03544800	2.16325100
C	4.97821300	1.96558400	2.31488900
C	5.79296000	1.44850300	0.09843300
H	4.64419100	-0.01417500	-1.01746600
H	3.22040900	0.87960300	2.94831500
H	5.05495700	2.52996600	3.23817800
H	6.50399400	1.61720700	-0.70448100
H	6.69722300	2.88931800	1.41482200
O	1.11327900	0.66201000	1.22553500
C	-0.21163100	0.46528600	0.95738500
C	-2.89768000	0.09647100	0.44815200
C	-0.66663800	0.40907800	-0.36614900
C	-1.11043300	0.32260200	2.01797100
C	-2.46628900	0.14544200	1.76622200
C	-2.02120900	0.22596200	-0.61988800
H	0.05241900	0.52670400	-1.17238300
H	-0.73235000	0.37167500	3.03360100
H	-3.19279900	0.04919200	2.56450000
H	-2.40185200	0.18103800	-1.63488100
O	2.22821700	1.36566900	-1.57039800
C	2.44096000	2.49266400	-1.16291400
O	2.11242200	2.88954200	0.06241900
C	3.05095000	3.59723600	-2.01690000
O	3.71073900	-2.53802500	0.50953800
C	4.22210800	-2.76950200	-0.70104900
O	3.96665400	-2.09650100	-1.67718000
C	5.19060800	-3.95356600	-0.70513700
H	1.70663100	2.11262100	0.53155100
C	5.66761800	-4.19968200	-2.13529100
H	6.37138300	-5.03840000	-2.14990500
H	4.82694300	-4.43624900	-2.79320100
H	6.16605800	-3.31486300	-2.53928400
C	6.37683700	-3.58698400	0.20037900
H	6.87896300	-2.68178100	-0.15834500
H	6.04551500	-3.41520700	1.22762400
H	7.10620600	-4.40388000	0.19821300
C	4.47919300	-5.19561400	-0.15283300
H	3.61449900	-5.46081700	-0.77047200
H	5.17004100	-6.04536800	-0.15637900
H	4.13675900	-5.02815200	0.87110200
C	1.86909200	4.35636800	-2.64620400
H	1.23246100	4.79707200	-1.87298200
H	2.24731200	5.16208000	-3.28431000
H	1.26039700	3.68572700	-3.26076300
C	3.90509300	2.95691900	-3.11127500
H	4.75024600	2.41337300	-2.67497800
H	3.31829200	2.24739300	-3.69838400
H	4.30076400	3.73177500	-3.77600100
C	3.88916600	4.55563900	-1.16627200
H	4.32296700	5.32935500	-1.80890500
H	3.28030500	5.03836400	-0.39868500
H	4.70576500	4.02429300	-0.66676600
O	-4.25208900	-0.14561800	0.18831200
C	-5.07144100	0.90736900	0.11496400
C	-6.50919100	0.52171900	-0.08658900
H	-6.97966200	1.31443500	-0.67490500
H	-6.95023300	0.56703300	0.91745500
C	-6.74486700	-0.85869100	-0.70882500
H	-6.24447900	-0.91367200	-1.68174900
H	-6.28852800	-1.62172000	-0.07182200
C	-8.22242700	-1.12286400	-0.87060700
C	-8.97150000	-1.62837400	0.19473700
C	-8.87683700	-0.81960000	-2.06588700
C	-10.34265400	-1.82988400	0.06793000
H	-8.47145400	-1.86922400	1.13016400
C	-10.24845700	-1.02002300	-2.19791700
H	-8.30338000	-0.42707100	-2.90251200
C	-10.98508800	-1.52597700	-1.13023700
H	-10.90966300	-2.22763600	0.90392000
H	-10.74105000	-0.78352000	-3.13602700
H	-12.05392700	-1.68523400	-1.23168300
O	-4.69441600	2.06052200	0.21027300
F	-5.30262700	0.83069000	2.81145100
H	-4.76985400	1.62119000	2.82822000
F	-3.71050400	2.74956000	2.41726300
H	-3.84114100	2.60013800	1.47421300

IM2-5

I	-2.36552800	1.12730600	0.60178300
C	-3.82464100	-0.27149300	1.14266400
C	-5.68150300	-2.17128200	1.85035100
C	-4.82228600	-0.59272900	0.22827900
C	-3.71620400	-0.87740500	2.38888700
C	-4.65909000	-1.84233600	2.73597800
C	-5.76248900	-1.54989100	0.60507400
H	-4.84438000	-0.12787500	-0.75173100
H	-2.90611900	-0.62177000	3.06305700
H	-4.59066800	-2.33274900	3.70119500
H	-6.55323100	-1.81917600	-0.08841800
H	-6.41452200	-2.92228300	2.12736900
O	-1.04003200	-0.46381700	1.06576800
C	0.22923300	-0.22391500	0.62713400
C	2.80958700	0.22480200	-0.22760800
C	0.52264400	-0.25255300	-0.74217700
C	1.23371200	0.05374400	1.55892700
C	2.53800700	0.27236900	1.13240900
C	1.82599400	-0.03021700	-1.17195700
H	-0.27827100	-0.47203900	-1.44303300
H	0.98022100	0.06984500	2.61369400
H	3.34715800	0.45931300	1.82847900
H	2.08433000	-0.05919300	-2.22548400
O	-2.43836500	-1.41806900	-1.51325300
C	-2.55670000	-2.51886600	-1.00713700
O	-2.07683800	-2.81372800	0.19645700
C	-3.21077500	-3.70215200	-1.70938800
O	-3.86211000	2.56654000	0.45993500
C	-4.53769500	2.67403900	-0.68596900
O	-4.38457300	1.92516800	-1.62755600
C	-5.54501000	3.82487800	-0.65994600
H	-1.64583700	-1.99453500	0.55700000
C	-6.22281000	3.92193300	-2.02544700
H	-6.95436700	4.73658800	-2.01662300
H	-5.49035400	4.11723300	-2.81337100
H	-6.73701100	2.99007400	-2.27419500
C	-6.58054900	3.51478200	0.43218200
H	-7.09191200	2.56725500	0.23007100
H	-6.10514600	3.44918100	1.41410700
H	-7.33428500	4.30878800	0.45889200
C	-4.81367700	5.13197600	-0.32700100
H	-4.05304800	5.36035600	-1.08119600
H	-5.53125300	5.95908600	-0.31002300
H	-4.32775900	5.07115400	0.64973000
C	-2.07981800	-4.43667400	-2.45150900
H	-1.32113600	-4.79554700	-1.74931200
H	-2.49091500	-5.29834100	-2.98805900
H	-1.59905200	-3.77389500	-3.17773100
C	-4.23648300	-3.17210700	-2.71188000
H	-5.04962600	-2.65014900	-2.19558800
H	-3.77377500	-2.46777400	-3.40635200
H	-4.66769100	-4.00381600	-3.27857600
C	-3.87329700	-4.64843400	-0.70467500
H	-4.34596500	-5.47782500	-1.24175800
H	-3.14156200	-5.05641400	-0.00394200
H	-4.64345700	-4.12846600	-0.12567200
O	4.12939500	0.44814600	-0.64024300
C	4.91392700	-0.62165300	-0.76607700
C	6.35805400	-0.28777100	-0.99926300
H	6.57179300	-0.42741000	-2.06612900
H	6.92085600	-1.05571000	-0.46249400
C	6.77009000	1.11330500	-0.53131000
H	6.37351800	1.86865300	-1.21640400
H	6.32067300	1.29265600	0.44892400
C	8.27185000	1.21708000	-0.42942600
C	8.92294100	0.64474800	0.66793500
C	9.03540000	1.83515200	-1.41902100
C	10.30862200	0.69238600	0.77369300
H	8.32498600	0.16444400	1.44024200
C	10.42437700	1.88534700	-1.31621800
H	8.53785300	2.28576200	-2.27455000
C	11.06368500	1.31395700	-0.22004500
H	10.80097800	0.24852600	1.63353700
H	11.00607900	2.37347500	-2.09221100
H	12.14526000	1.35440900	-0.13762600
O	4.50039700	-1.77015800	-0.72455100
F	5.49550500	-0.51587200	1.73318100
H	4.87282700	-1.17611500	2.04405100
F	2.52510100	-2.69238300	0.42723900
H	3.20403200	-2.29694100	-0.16553000
F	3.68700500	-2.08306500	2.48460800
H	3.15167700	-2.36291000	1.71866200

IM2-6

I	-2.43154600	1.13195000	0.57691500
C	-3.89181900	-0.28278700	1.07079600
C	-5.74886300	-2.20556300	1.71198600
C	-4.90967800	-0.54721200	0.16050500
C	-3.76381700	-0.95528400	2.28046800
C	-4.70711700	-1.93119800	2.59371900
C	-5.84944000	-1.51737700	0.50373300
H	-4.94796600	-0.02963900	-0.79234800
H	-2.93832400	-0.74223300	2.95072500
H	-4.62362200	-2.47325400	3.52969100
H	-6.65566400	-1.74361500	-0.18731600
H	-6.48188400	-2.96574900	1.96259300
O	-1.11404800	-0.49089600	0.95140900
C	0.15470900	-0.24933900	0.51525500
C	2.73949900	0.17643100	-0.33576200
C	0.43914000	-0.21446000	-0.85561200
C	1.17112700	-0.03935100	1.45272600
C	2.47662200	0.17193400	1.02690100
C	1.74550200	-0.00619100	-1.28442600
H	-0.37100600	-0.38066700	-1.56051700
H	0.92791100	-0.07495400	2.50927500
H	3.28953300	0.31969800	1.72732700
H	1.99778200	0.00589100	-2.33952800
O	-2.54218100	-1.29002000	-1.66431000
C	-2.67173100	-2.41507400	-1.21787200
O	-2.18491900	-2.78194000	-0.03690500
C	-3.34910100	-3.54842700	-1.97803700
O	-3.92161600	2.58198500	0.52666600
C	-4.61074200	2.75269300	-0.60361800
O	-4.46794800	2.05799700	-1.58727200
C	-5.62192700	3.89549400	-0.49848500
H	-1.74232600	-1.98901100	0.36530400
C	-6.29973100	4.08493900	-1.85426500
H	-7.03661200	4.89212900	-1.78816600
H	-5.56820800	4.34105700	-2.62557100
H	-6.80743300	3.16974400	-2.16918900
C	-6.65620400	3.50149600	0.56778700
H	-7.16287000	2.56874000	0.29672500
H	-6.18042300	3.36673000	1.54251300
H	-7.41387100	4.28769400	0.65222500
C	-4.89926500	5.17992100	-0.07233300
H	-4.13829200	5.46546800	-0.80643100
H	-5.62196000	5.99945900	0.00095900
H	-4.41498600	5.05337200	0.89882800
C	-2.23763600	-4.24696400	-2.78183600
H	-1.47135800	-4.65461900	-2.11537100
H	-2.66592600	-5.07085100	-3.36246000
H	-1.76199500	-3.54579400	-3.47460400

C	-4.38518900	-2.94956700	-2.93001000
H	-5.18437600	-2.45162100	-2.37004500
H	-3.92628800	-2.20953900	-3.58894500
H	-4.83421500	-3.74185200	-3.53786600
C	-4.00516800	-4.54729300	-1.02133200
H	-4.49433600	-5.33854500	-1.59959600
H	-3.26680900	-5.00330500	-0.35817100
H	-4.76103300	-4.05622700	-0.39986600
O	4.06137800	0.37386500	-0.75829700
C	4.87650800	-0.67551200	-0.70106700
C	6.31015600	-0.35345700	-1.00090800
H	6.52659300	-0.70671100	-2.01674500
H	6.89395700	-0.97761200	-0.31998400
C	6.68211400	1.12510000	-0.83684200
H	6.27785800	1.70823600	-1.66986800
H	6.21674500	1.49686000	0.07945300
C	8.17972500	1.28654400	-0.74607800
C	8.82910100	0.95368000	0.44714000
C	8.94059400	1.72449800	-1.82915800
C	10.21134000	1.05971000	0.55391300
H	8.23124700	0.61373600	1.29063200
C	10.32632600	1.83243200	-1.72528400
H	8.44381000	1.98856100	-2.75973100
C	10.96425400	1.50011600	-0.53401900
H	10.70290500	0.80308100	1.48733600
H	10.90639500	2.17864400	-2.57526100
H	12.04315200	1.58588600	-0.45111300
O	4.49691900	-1.81369900	-0.45905400
F	5.61822800	-0.08238100	1.70302100
H	5.12113700	-0.56113600	2.36814300
F	2.31876900	-2.73763100	0.14932900
H	3.16561100	-2.30623100	-0.15838900
F	4.10732700	-1.13555800	3.38166600
H	3.42505400	-1.74126400	3.02790700
F	2.35720700	-2.58666600	2.53956200
H	2.30381600	-2.65169100	1.55294000

IM2-7

I	2.55044800	-1.05951800	0.67942500
C	4.04742100	0.39281300	0.84458900
C	5.95488400	2.36137800	1.05119600
C	4.97334600	0.52561700	-0.18474100
C	4.03455200	1.21777800	1.96312000
C	5.00233900	2.21543800	2.05587900
C	5.94049000	1.52135600	-0.06136900
H	4.92089100	-0.11162300	-1.06125000
H	3.27736200	1.10210100	2.73086500
H	5.00804600	2.87512000	2.91706200
H	6.67662400	1.64709700	-0.84943000
H	6.70761100	3.13932900	1.13021800
O	1.26721600	0.60793800	0.95771300
C	-0.03420300	0.31983800	0.66839200
C	-2.68145000	-0.20886900	0.10899900
C	-0.43465900	0.10117600	-0.65553400
C	-0.96506900	0.24592200	1.70862900
C	-2.30151100	-0.01432000	1.42805900
C	-1.76998600	-0.16316300	-0.93634600
H	0.30960600	0.16730600	-1.44455800
H	-0.63672300	0.41220800	2.72857600
H	-3.04819900	-0.05579600	2.21023200
H	-2.10738300	-0.31807200	-1.95591100
O	2.45551800	1.06051200	-1.85663900
C	2.61340800	2.23270500	-1.56868500
O	2.23249200	2.74596100	-0.40354500
C	3.20716000	3.26116800	-2.52308500
O	4.03334600	-2.51960400	0.68101800
C	4.61148400	-2.84506000	-0.47684800
O	4.37934300	-2.28020000	-1.52464400
C	5.61971600	-3.98485500	-0.32125100
H	1.83388700	2.01113800	0.13303400
C	6.18156900	-4.34163600	-1.69622000
H	6.91311600	-5.15029000	-1.59688500
H	5.38639000	-4.66940600	-2.37130600
H	6.67123500	-3.47873200	-2.15478400
C	6.74198000	-3.49232900	0.60561000
H	7.23304800	-2.60566600	0.18986000
H	6.34981100	-3.23961400	1.59395300
H	7.49676300	-4.27792500	0.71725000
C	4.92139600	-5.19806900	0.30699500
H	4.10060400	-5.55128100	-0.32633100
H	5.63952900	-6.01751700	0.41715400
H	4.51897300	-4.95158400	1.29244800
C	2.01874800	3.86806200	-3.29032800
H	1.32137300	4.35897600	-2.60467800
H	2.38432900	4.61284300	-4.00518700
H	1.47858800	3.09338500	-3.84341600
C	4.14626300	2.54471500	-3.49400400
H	4.99802000	2.10963900	-2.95975700
H	3.62710900	1.73574400	-4.01215400
H	4.53089300	3.25533300	-4.23286600
C	3.95094500	4.36201100	-1.76226000
H	4.37548600	5.07576300	-2.47648700
H	3.28036700	4.89841400	-1.08736500
H	4.76809900	3.94320400	-1.16589600
O	-4.03339600	-0.46661600	-0.15249900
C	-4.74866100	0.49982700	-0.72975700
C	-6.20364300	0.15810900	-0.86019400
H	-6.59979200	0.72592200	-1.70598700
H	-6.66732700	0.57314100	0.04460700
C	-6.52126700	-1.33694000	-0.98137400
H	-6.01050300	-1.74911600	-1.85858300
H	-6.12707800	-1.86130100	-0.10638900
C	-8.01055800	-1.55502300	-1.09854000
C	-8.79801200	-1.69997600	0.04570300
C	-8.63403000	-1.56295000	-2.34786400
C	-10.17784600	-1.85294400	-0.05517300
H	-8.32249300	-1.69768400	1.02390100
C	-10.01363500	-1.71607500	-2.45390500
H	-8.03025100	-1.45311400	-3.24587600
C	-10.78933100	-1.86138700	-1.30652100
H	-10.77526400	-1.96925800	0.84373300
H	-10.48243500	-1.72510500	-3.43302700
H	-11.86476800	-1.98348900	-1.38712700
O	-4.28117100	1.56248800	-1.10350300
F	-4.77066700	1.68321500	1.56003300
H	-4.82412900	1.29714500	2.43093300
F	-2.44905100	2.72245500	0.09246200
H	-3.15674800	2.22270500	-0.38703400
F	-4.62442600	0.55628000	3.80472900
H	-3.73271400	0.84871600	4.07248400
F	-2.59881300	3.04611400	2.45391100
H	-2.62036300	2.82292900	1.48562700
F	-2.36869000	1.36783000	4.11360200
H	-2.38832700	2.06007200	3.39590800

IM2-8

I	2.35798200	-0.88768800	-0.22620300
C	3.72434100	0.22280400	0.90368900
C	5.46621900	1.72754700	2.40006800
C	4.82362900	0.78631500	0.26492100
C	3.45870700	0.39047200	2.25774000
C	4.34787900	1.16012500	3.00517100
C	5.70373500	1.53980000	1.03925300
H	4.96864200	0.65972600	-0.80262900
H	2.57636900	-0.05126500	2.70866000
H	4.16200500	1.31147800	4.06328700
H	6.57089300	1.99282300	0.56843200
H	6.15406600	2.32487900	2.99014400
O	1.01025000	0.56716500	0.54986700
C	-0.29151300	0.45774900	0.20975700
C	-3.00520500	0.32321600	-0.31422800
C	-1.00618500	1.62069700	-0.11495000
C	-0.95256700	-0.77774300	0.21098600
C	-2.31368300	-0.84586000	-0.05983600
C	-2.36976100	1.55714700	-0.36198700
H	-0.48040100	2.56963000	-0.13529300
H	-0.42421400	-1.68384300	0.48335700
H	-2.83980800	-1.79088300	-0.02756100
H	-2.94160600	2.45454000	-0.57511200
O	2.72678300	2.15392700	-1.41438200
C	2.72837700	3.08537200	-0.63672900
O	2.07866200	3.05143400	0.52964200
C	3.41880000	4.41804100	-0.89893100
O	3.86216400	-2.25960300	-0.63511800
C	4.68110100	-2.02556200	-1.66330400
O	4.65072400	-1.01228300	-2.32815700
C	5.67707500	-3.16609200	-1.87976200
H	1.66296100	2.15238400	0.60369800
C	6.53098400	-2.85285200	-3.10696000
H	7.25584000	-3.65788800	-3.26659500
H	5.91044000	-2.75744800	-4.00208900
H	7.07267000	-1.91242200	-2.97703000
C	6.55724300	-3.26259000	-0.62390900
H	7.08870300	-2.32157200	-0.44443100
H	5.95492200	-3.49356900	0.25827100
H	7.30240900	-4.05382300	-0.75814900
C	4.90821800	-4.47903600	-2.07829700
H	4.25574500	-4.42381300	-2.95622900
H	5.61742500	-5.29857900	-2.23559400
H	4.29540100	-4.71018800	-1.20374600
C	2.33517600	5.38428800	-1.40789700
H	1.55193700	5.52177000	-0.65617400
H	2.78294600	6.36026900	-1.62342600
H	1.87717600	5.00525800	-2.32715800
C	4.48870600	4.21269400	-1.97051900
H	5.26112000	3.52032500	-1.61865300
H	4.05467000	3.79144400	-2.87982500
H	4.96512100	5.16901000	-2.21009300
C	4.04088200	4.96880600	0.38853100
H	4.54614700	5.91670700	0.17390800
H	3.27949300	5.14160300	1.15235500
H	4.77829400	4.27023200	0.79743400
O	-4.39258900	0.23205500	-0.50820800
C	-5.17893900	0.61646600	0.49428100
C	-6.63639900	0.36760600	0.23311800
H	-7.20154100	1.09307600	0.82393400
H	-6.84790300	-0.62003500	0.66517700
C	-7.04911500	0.39502700	-1.24379200
H	-6.77928600	1.36349100	-1.67905300
H	-6.48738600	-0.36781800	-1.79007100
C	-8.53358700	0.15911500	-1.38477100
C	-9.03857500	-1.13705100	-1.50698600
C	-9.43070700	1.22842100	-1.34409700
C	-10.40999700	-1.36085700	-1.59015500
H	-8.34873000	-1.97715200	-1.54283800
C	-10.80284100	1.00968600	-1.42750500
H	-9.04815700	2.24245400	-1.25208800
C	-11.29587600	-0.28694600	-1.55069300
H	-10.78657900	-2.37407200	-1.69000100
H	-11.48687800	1.85218200	-1.40004400
H	-12.36522800	-0.45945800	-1.61877700
O	-4.77499600	1.11471100	1.53266500
F	-4.05853100	-1.40757400	2.11461500
H	-3.43143900	-2.12053800	2.07158000
F	-2.58510500	0.87105800	2.59843200
H	-3.46117900	0.91591400	2.11133600
F	-2.51710600	-3.39987400	1.59692700
H	-1.57155700	-3.39323500	1.75636800
F	-1.65515100	-1.23320200	3.06663600
H	-2.14253900	-0.37394700	2.83594700
F	-0.00068300	-3.48949200	1.77551900
H	0.39931700	-2.71138000	2.20166300
F	0.68818500	-1.37292300	2.75920800
H	-0.26248600	-1.14082600	2.93014700

IM2-9

I	2.50886600	-0.77772700	-0.15811600
C	3.83739400	0.39745000	0.94870500
C	5.50822600	2.00126200	2.42394200
C	4.84574000	1.08647100	0.28323700
C	3.62871700	0.48718300	2.32028200
C	4.48017200	1.30781000	3.05709500
C	5.69150800	1.88900800	1.04653200
H	4.94697500	1.01393500	-0.79427600
H	2.81453600	-0.05204100	2.79301400
H	4.33617000	1.40021800	4.12845100
H	6.48830400	2.43893800	0.55498600
H	6.16742900	2.63793800	3.00551800
O	1.08614400	0.54600900	0.72120000
C	-0.18814200	0.40779000	0.29260100
C	-2.84166000	0.18293000	-0.44982800
C	-0.90098400	1.54116400	-0.12279600
C	-0.81820900	-0.84400500	0.28820900
C	-2.14953900	-0.96046200	-0.08969400
C	-2.23800600	1.43189500	-0.47827700
H	-0.39846400	2.50261200	-0.13251400
H	-0.27993900	-1.72156900	0.62358100
H	-2.65825300	-1.91489100	-0.08146600
H	-2.81557100	2.30237400	-0.77128400
O	2.53050700	2.32871800	-1.25183400
C	2.55405400	3.21862800	-0.42677300
O	2.01775500	3.08732700	0.78902000
C	3.13362700	4.60409500	-0.68388700
O	4.08366000	-2.02661000	-0.67484400
C	4.84673700	-1.69471600	-1.71917600
O	4.72609700	-0.65772200	-2.33540400
C	5.90420100	-2.75713700	-2.02288100
H	1.65850900	2.16284200	0.84695400
C	6.68837900	-2.33583400	-3.26425300
H	7.45605500	-3.08428100	-3.48664100
H	6.02877000	-2.24216000	-4.13119100
H	7.17404600	-1.36874100	-3.11069700
C	6.83661100	-2.85058000	-0.80508100
H	7.31524900	-1.88611500	-0.60299400
H	6.28438700	-3.15680500	0.08693800
H	7.62356800	-3.58641400	-1.00141300
C	5.21306600	-4.10751800	-2.25379000
H	4.52478400	-4.05683800	-3.10420300
H	5.96632900	-4.87137600	-2.47393200
H	4.65061000	-4.41593400	-1.36928900
C	1.95687300	5.48867600	-1.13226000
H	1.19753300	5.55434200	-0.34662800
H	2.31682900	6.49997400	-1.34935600
H	1.49224800	5.08585300	-2.03792200
C	4.16976300	4.50052900	-1.80287600
H	5.01092500	3.86996900	-1.49460300
H	3.73182200	4.05675000	-2.69939500
H	4.55657900	5.49543100	-2.04663400
C	3.76345200	5.18327400	0.58634000
H	4.18321200	6.17122600	0.36811000
H	3.02386800	5.28460800	1.38367900
H	4.56980100	4.53966300	0.95280100
O	-4.20140500	0.07089100	-0.77189700
C	-5.04219400	-0.09096600	0.24508200
C	-6.46272100	-0.26951300	-0.18789500
H	-6.96748600	-0.87278900	0.56908200
H	-6.48095100	-0.80532300	-1.13838600
C	-7.14238300	1.10864600	-0.32216100
H	-7.07153000	1.63501400	0.63603300
H	-6.60166600	1.70399900	-1.06642600
C	-8.58761000	0.95762800	-0.72825600
C	-8.94492600	0.90430500	-2.07690800
C	-9.58505700	0.81798500	0.23880900
C	-10.27231500	0.71963100	-2.45306400
H	-8.17508800	1.01241300	-2.83751800
C	-10.91359000	0.63302900	-0.13297000
H	-9.31644500	0.85888000	1.29189000
C	-11.26036100	0.58375400	-1.48093200
H	-10.53547300	0.68483600	-3.50565400
H	-11.67865700	0.53062000	0.63033100
H	-12.29616200	0.44223900	-1.77254100
O	-4.71435500	-0.00109200	1.42248400
F	-3.02411800	-4.21465200	-0.35618200
H	-2.48898900	-4.07544500	0.43638500
F	-2.61064200	0.56214600	2.48094600
H	-3.45610000	0.30774500	1.97585400
F	-1.74210000	-3.62230500	1.65538600
H	-0.77018700	-3.66288900	1.63924200
F	-1.31952000	-1.26330400	3.21270100
H	-1.86858300	-0.48832400	2.86209000
F	0.69995600	-3.53027000	1.59681900
H	0.91054100	-2.72086900	2.12755800
F	0.97729000	-1.48240900	2.80233000

H	0.00849500	-1.26206400	2.98965900
F	-4.95122900	-2.61260800	-0.02950900
H	-4.30680800	-3.29203900	-0.20174300

IM2-10

I	1.43499800	0.44160900	-0.88180600
C	3.48404000	0.85203900	-0.75870600
C	6.19160500	1.32734400	-0.58834300
C	3.95059200	1.70378200	0.23744800
C	4.33270100	0.21264400	-1.65467800
C	5.70167500	0.45673800	-1.55739400
C	5.31973700	1.94514200	0.30800000
H	3.26331600	2.16970900	0.93417400
H	3.93983000	-0.46940600	-2.40138300
H	6.38055700	-0.03447200	-2.24640500
H	5.70444300	2.61210500	1.07278000
H	7.25800000	1.51795900	-0.52238700
O	1.94160500	-1.57164300	-1.27735100
C	0.70986100	-2.19138600	-1.23752200
C	-1.95748400	-2.92619100	-1.15049700
C	0.09488700	-2.41847900	-0.00157900
C	0.01244600	-2.42594700	-2.42154800
C	-1.32572200	-2.81219700	-2.38662200
C	-1.24181200	-2.78774000	0.03697700
H	0.65605800	-2.22216500	0.90843800
H	0.51431400	-2.25560100	-3.36870700
H	-1.88567600	-2.95074200	-3.30025100
H	-1.76450600	-2.90886800	0.97985600
O	2.77604900	-0.98359900	1.65485500
C	3.76084700	-1.67247500	1.46330100
O	3.93751600	-2.37893100	0.34982000
C	4.89260000	-1.84739600	2.46610700
O	1.18799800	2.53702100	-0.48295000
C	-0.08348700	2.79597000	-0.36337000
O	-0.92658100	1.90570100	-0.53395200
C	-0.48563600	4.21889700	0.00269900
H	3.17141300	-2.18798700	-0.25371700
C	-1.23384500	4.13730600	1.34484300
H	-1.55653200	5.14141100	1.63797900
H	-2.11802900	3.50219700	1.25034700
H	-0.58949600	3.74106900	2.13681700
C	0.73055200	5.13604200	0.11078800
H	1.42224200	4.78825200	0.88343100
H	1.27707400	5.18503500	-0.83520100
H	0.39986800	6.14601100	0.37287700
C	-1.45596800	4.71338600	-1.08239200
H	-2.33543700	4.06690700	-1.13124900
H	-1.78438000	5.72815100	-0.83614400
H	-0.97468300	4.73952500	-2.06559500
C	4.74348000	-0.80278300	3.57031200
H	3.77570800	-0.89467000	4.06906700
H	5.53842300	-0.93052000	4.31221100
H	4.81207400	0.20868600	3.15665900
C	6.24286100	-1.69046900	1.75620600
H	6.36038300	-2.43461900	0.96503700
H	6.33349200	-0.69553400	1.30787300
H	7.05404900	-1.81638000	2.48138300
C	4.77304600	-3.26598200	3.04798300
H	5.57149800	-3.43054000	3.77916300
H	3.81224800	-3.40185800	3.55512600
H	4.86146100	-4.01918600	2.26023200
O	-3.32120100	-3.12042700	-0.99184700
C	-4.18754400	-2.33613300	-1.71389400
C	-5.40454700	-2.01261600	-0.89100800
H	-5.83133700	-2.93224100	-0.47924200
H	-6.13777300	-1.53611400	-1.54406300
C	-4.98425100	-1.05951600	0.24983500
H	-4.32744500	-1.61062700	0.93343600
H	-4.39714900	-0.23007800	-0.16083000
C	-6.16431400	-0.49103200	1.00236100
C	-6.31825500	0.89201700	1.11795700
C	-7.11319800	-1.32791500	1.59679200
C	-7.40330400	1.42638100	1.80974900
H	-5.57241700	1.54481100	0.67164700
C	-8.19769600	-0.79560500	2.28660000
H	-7.00056200	-2.40745900	1.52509300
C	-8.34708400	0.58584700	2.39286200
H	-7.51014200	2.50380300	1.89178500
H	-8.92591400	-1.45899000	2.74344800
H	-9.19345700	1.00277900	2.92986400
O	-3.94886000	-1.91662400	-2.81165300
F	-3.45860300	2.19706300	-0.19523400
H	-2.52189900	2.04073100	-0.33566900

IM2-11

I	1.83275200	0.54923000	-0.86071500
C	3.91736000	0.50981000	-0.69004400
C	6.65841400	0.37816000	-0.45982300
C	4.52408300	1.10879400	0.40943400
C	4.63781100	-0.17352900	-1.66271700
C	6.02429900	-0.23883600	-1.53426700
C	5.91097500	1.04644200	0.50979000
H	3.92999500	1.61146200	1.16401600
H	4.13218000	-0.65591600	-2.49284500
H	6.60412200	-0.77029000	-2.28139000
H	6.40578400	1.51359900	1.35518400
H	7.73886500	0.32965600	-0.36971600
O	1.89346800	-1.45684900	-1.45595700
C	0.55111800	-1.79912600	-1.46383500
C	-2.20339000	-2.01400000	-1.43946600
C	-0.11797300	-1.97033200	-0.24790500
C	-0.15368500	-1.79932100	-2.66666600
C	-1.54020700	-1.92254900	-2.65963800
C	-1.50234100	-2.07349300	-0.23943900
H	0.45616800	-1.95050100	0.67500000
H	0.39004800	-1.66220300	-3.59586200
H	-2.10666300	-1.88443900	-3.58091100
H	-2.06031600	-2.14039700	0.68787300
O	2.78938500	-1.35566200	1.52111000
C	3.60769500	-2.21762500	1.25950700
O	3.65684800	-2.82558600	0.07695500
C	4.64723400	-2.73823500	2.24189800
O	2.00384500	2.61194200	-0.19782400
C	0.81063600	3.07965100	-0.01910000
O	-0.18191300	2.40133300	-0.34204300
C	0.65715900	4.44914400	0.62628800
H	2.95835500	-2.42063400	-0.50070100
C	0.00533100	4.20475000	2.00018100
H	-0.14778300	5.16525700	2.50207600
H	-0.96500700	3.71453600	1.88444100
H	0.64404700	3.58388100	2.63726500
C	2.00704400	5.14599600	0.78229900
H	2.68529000	4.56018800	1.40859000
H	2.48921100	5.29865400	-0.18749800
H	1.85811300	6.12302300	1.25248200
C	-0.29568100	5.28045900	-0.24568500
H	-1.26846700	4.79081200	-0.33590600
H	-0.44536900	6.26061600	0.21758000
H	0.11541600	5.43576100	-1.24832000
C	4.71418600	-1.79378400	3.44045400
H	3.73925100	-1.70654000	3.92578800
H	5.44076500	-2.16881300	4.16848400
H	5.02276800	-0.79140900	3.12557600
C	6.01447500	-2.83229100	1.55396000
H	5.97825700	-3.50773900	0.69615800
H	6.34236400	-1.84828600	1.20273500
H	6.75674900	-3.20783000	2.26647900
C	4.19152900	-4.13846900	2.68625900
H	4.91319200	-4.54896400	3.40031900
H	3.21315500	-4.09514700	3.17568700
H	4.12414600	-4.81619300	1.83075600
O	-3.58167100	-2.03440000	-1.33802100
C	-4.27607300	-0.97607500	-1.86099300
C	-5.66413200	-0.87551500	-1.27797900
H	-6.38034500	-1.22276800	-2.03242400
H	-5.83608900	0.19707800	-1.15553500
C	-5.87268300	-1.60379500	0.05573500
H	-5.97037800	-2.68052100	-0.11448900
H	-4.98481900	-1.44971500	0.67344700
C	-7.08101600	-1.06199800	0.77842900
C	-6.97875800	0.16592200	1.44115100
C	-8.30635100	-1.72714300	0.77865500
C	-8.07870900	0.71377200	2.09138400
H	-6.01861000	0.67804300	1.43654300
C	-9.41129600	-1.18085400	1.42981100
H	-8.39487900	-2.68323900	0.26807900
C	-9.30003500	0.04050600	2.08739400
H	-7.98434100	1.66544300	2.60582600
H	-10.35866400	-1.71158100	1.42428600
H	-10.15926200	0.46608200	2.59650700
O	-3.82591400	-0.23680800	-2.69193600
F	-3.66304000	0.44396500	0.34352700
H	-3.27237300	1.31172200	0.28610100
F	-2.53045200	2.74730700	0.30361100
H	-1.59380300	2.63631000	0.01328000

IM2-12

I	-2.05272100	0.82663400	0.27271400
C	-3.74947600	1.90842200	0.81690600
C	-5.98199100	3.35268900	1.53505600
C	-4.96772600	1.59965600	0.21515500
C	-3.62067700	2.91908500	1.76912000
C	-4.75248200	3.64638200	2.12264200
C	-6.08990900	2.33553700	0.58985100
H	-5.03335700	0.79867800	-0.51400200
H	-2.65894000	3.13550800	2.22229500
H	-4.67316900	4.43875400	2.85942200
H	-7.05010500	2.11196600	0.13687400
H	-6.86218700	3.92113600	1.81782200
O	-2.40610100	-0.84629900	1.52530300
C	-1.13641700	-1.39465600	1.45117100
C	1.54952200	-1.89397200	0.97263200
C	-0.73598400	-2.04110700	0.27992600
C	-0.18813800	-1.07554400	2.42829900
C	1.15094900	-1.33591700	2.19100000
C	0.61130000	-2.30074600	0.02753600
H	-1.48561600	-2.28173900	-0.47035400
H	-0.51036800	-0.56744000	3.33142400
H	1.92645400	-1.05323600	2.89532000
H	0.92320100	-2.75649500	-0.89987200
O	-4.26583700	-1.23954800	-0.95311400
C	-4.56189500	-2.32369900	-0.48117600
O	-4.15315700	-2.71686500	0.71842300
C	-5.40255800	-3.37156800	-1.19677800
O	-1.39013500	2.58748800	-0.87495100
C	-0.21668000	2.30514600	-1.32343500
O	0.20049100	1.12488000	-1.28102200
C	0.66933400	3.44413200	-1.80137000
H	-3.57061000	-2.00023400	1.09209500
C	1.56430900	2.95105900	-2.94318100
H	2.21482600	3.76799600	-3.26983400
H	2.19671700	2.11984800	-2.62302600
H	0.96888200	2.62428000	-3.80145700
C	-0.17030700	4.64358600	-2.24064900
H	-0.81040000	4.38734800	-3.09045400
H	-0.80912200	4.99725000	-1.42824900
H	0.49369700	5.45868200	-2.54485600
C	1.53713300	3.81259300	-0.58045200
H	2.11346600	2.95347000	-0.22340500
H	2.23678900	4.60561900	-0.86253500
H	0.91558200	4.17988900	0.24269900
C	-5.90772900	-2.79760200	-2.51857300
H	-5.07486000	-2.49418300	-3.15803500
H	-6.49975100	-3.55198500	-3.04646500
H	-6.53645000	-1.91841600	-2.35005200
C	-6.57921600	-3.77161400	-0.29523000
H	-6.22478000	-4.18026500	0.65388100
H	-7.22369000	-2.91185400	-0.08324400
H	-7.18390500	-4.53159200	-0.80087300
C	-4.50671100	-4.59512200	-1.45051400
H	-5.08260600	-5.36895800	-1.96857900
H	-3.65051300	-4.33112500	-2.08059100
H	-4.13268300	-5.00764600	-0.51014600
O	2.91720400	-1.90571500	0.81527000
C	3.59165600	-2.53334200	-0.18654400
C	5.05598400	-2.20198500	-0.05941700
H	5.62082400	-2.91213100	-0.66678500
H	5.34386500	-2.29916200	0.99151000
C	5.34479100	-0.75688000	-0.51184500
H	5.06115900	-0.63828300	-1.56284900
H	4.72292000	-0.07394000	0.07069400
C	6.79880600	-0.41253900	-0.30682500
C	7.25268400	-0.05758500	0.96730800
C	7.71329400	-0.47881300	-1.35812400
C	8.59719400	0.23029200	1.17965400
H	6.53716900	-0.01359700	1.78551100
C	9.05997200	-0.19114700	-1.14663300
H	7.36578400	-0.75443500	-2.35110800
C	9.50459100	0.16502000	0.12340500
H	8.93812000	0.50897800	2.17222400
H	9.76046700	-0.24300200	-1.97469900
H	10.55315000	0.39173800	0.29010700
O	3.08003500	-3.22516400	-1.02492600
F	4.42518700	-0.49841000	2.62560700
H	3.84710100	-0.02441300	2.04282200
F	2.88145700	0.93500600	1.11611300
H	2.70901900	0.55460300	0.23605700
F	2.41161300	0.19098100	-1.15524600
H	1.49205200	0.58980200	-1.30478500

IM1-13

I	-2.06204400	0.61452000	0.37112500
C	-3.98272100	0.04270400	0.96792300
C	-6.49260300	-0.79560700	1.72848100
C	-5.04882400	0.25661200	0.10028800
C	-4.13120500	-0.59379900	2.19392200
C	-5.40525100	-1.01814100	2.56799400
C	-6.31503000	-0.16218300	0.49848300
H	-4.89366700	0.73265600	-0.86130800
H	-3.27399000	-0.77288900	2.83400700
H	-5.54148100	-1.52035100	3.51981300
H	-7.16192000	-0.00191700	-0.16115100
H	-7.48243100	-1.12507800	2.02764600
O	-1.46973800	-1.24578500	1.04021600
C	-0.13208900	-1.42665900	0.73396800
C	2.54633100	-1.67105900	0.11631100
C	0.24503600	-1.72073100	-0.57555200
C	0.82481600	-1.25686500	1.73296000
C	2.17356500	-1.38549000	1.42898200
C	1.59535600	-1.84933300	-0.88160700
H	-0.52511200	-1.83206300	-1.33472100
H	0.50116000	-1.01701400	2.74076300
H	2.93482700	-1.24722100	2.18593400
H	1.92638400	-2.06805900	-1.89084100
O	-3.16265800	-1.71890700	-1.49865300
C	-3.66094000	-2.68840200	-0.95731100
O	-3.24792600	-3.14162200	0.22345700
C	-4.77323100	-3.52980400	-1.56722000
O	-3.08243300	2.51779300	-0.06771900
C	-2.25569900	3.32963000	-0.61986300
O	-1.13976600	2.92065300	-1.00537900
C	-2.63360800	4.79902900	-0.72755500
H	-2.53032700	-2.53709900	0.54159800
C	-2.24910300	5.30653200	-2.12288200
H	-2.48188800	6.37316300	-2.19734300
H	-1.18073200	5.17449100	-2.31326700
H	-2.80602800	4.77982600	-2.90415300
C	-4.12270000	5.01035700	-0.46055600
H	-4.73418800	4.48035700	-1.19698600
H	-4.40152400	4.65068900	0.53272800
H	-4.35582900	6.07778100	-0.52433200
C	-1.78392100	5.51851100	0.33825100
H	-0.71645300	5.33976200	0.17646400
H	-1.96754700	6.59591100	0.28276000
H	-2.04660800	5.17793300	1.34523300
C	-5.45537500	-2.72235100	-2.67050100
H	-4.73404700	-2.40817400	-3.42824900
H	-6.23233400	-3.32802700	-3.14793900
H	-5.92329700	-1.82214200	-2.25751100
C	-5.78611000	-3.93880100	-0.49216400
H	-5.31113400	-4.53309000	0.29150200
H	-6.23859300	-3.05744500	-0.02556800
H	-6.58354500	-4.53384300	-0.94994800

C	-4.10641000	-4.78419800	-2.15853300
H	-4.86872700	-5.42269300	-2.61712300
H	-3.37731500	-4.51262500	-2.92862700
H	-3.59537200	-5.35778800	-1.37997700
O	3.87185800	-1.68281400	-0.26609500
C	4.77989200	-2.34868600	0.51081000
C	6.20019400	-1.97862500	0.15978500
H	6.69588600	-2.87574100	-0.22858000
H	6.67596600	-1.75597300	1.11994000
C	6.36479100	-0.79277500	-0.79606100
H	6.08339800	-1.08540600	-1.81272900
H	5.67802000	-0.00514800	-0.47925100
C	7.77953200	-0.27001500	-0.76277800
C	8.18934800	0.51729700	0.31846600
C	8.70491000	-0.57721300	-1.75964900
C	9.49514700	0.98844000	0.39778200
H	7.46422100	0.75402700	1.09477200
C	10.01469900	-0.10659700	-1.68382000
H	8.39535600	-1.18734500	-2.60494000
C	10.41275500	0.67722900	-0.60512000
H	9.79844500	1.60203500	1.24077200
H	10.72324800	-0.35165800	-2.46935900
H	11.43202400	1.04611200	-0.54551300
O	4.46443400	-3.13826300	1.35658500
F	4.93552000	0.01663300	1.78549800
H	4.17674100	0.58866900	1.84783300
F	2.82684700	1.42248300	2.04910500
H	2.20563400	1.36320000	1.31473000
F	1.20000900	1.50290400	0.16668000
H	1.26133100	2.40181400	-0.22424000
F	1.07869100	3.72836400	-0.80611000
H	0.11066100	3.55486900	-1.01770300

IM1-14

I	-1.46118400	0.29193600	0.65069400
C	-3.51850300	0.66831100	0.71809900
C	-6.24701600	1.03339200	0.75828900
C	-4.11193100	1.38168500	-0.31794500
C	-4.24931700	0.12835300	1.76880600
C	-5.62903700	0.31921700	1.77889500
C	-5.49163300	1.56419700	-0.28588100
H	-3.51295400	1.79071800	-1.12431400
H	-3.76213100	-0.45407600	2.54293700
H	-6.21866700	-0.10792800	2.58267100
H	-5.97507300	2.11730900	-1.08541800
H	-7.32340500	1.16960100	0.76896100
O	-1.96170000	-1.68211700	1.12731800
C	-0.74910300	-2.34157500	1.14325600
C	1.89862300	-3.08977600	1.13963300
C	-0.12916400	-2.67132600	-0.06587400
C	-0.08189300	-2.51705600	2.35219000
C	1.25353300	-2.90777600	2.35614600
C	1.20702900	-3.04334300	-0.06564500
H	-0.67759600	-2.55118500	-0.99636700
H	-0.58370700	-2.25406700	3.27636400
H	1.80956600	-2.96262400	3.28328000
H	1.74401300	-3.21876900	-0.99162900
O	-5.35797300	-1.98995900	-0.25744500
C	-4.67522000	-1.88764100	-1.24925800
O	-3.33374200	-1.94642900	-1.21437100
C	-5.21529000	-1.73551300	-2.66632800
O	-1.34171800	2.41652800	0.15750300
C	-0.18934800	2.71512200	-0.32377700
O	0.62738600	1.80639600	-0.59290800
C	0.14580200	4.18391600	-0.53840400
H	-3.04817800	-2.05803100	-0.27569600
C	0.87402300	4.32603300	-1.88188700
H	1.12326100	5.37883800	-2.04576000
H	1.80256400	3.75000700	-1.89004800
H	0.24690700	3.99013200	-2.71398100
C	-1.12023200	5.03968200	-0.51064300
H	-1.81236400	4.74926700	-1.30726100
H	-1.64128600	4.94219200	0.44449500
H	-0.84998500	6.09007900	-0.65693200
C	1.09365900	4.59325100	0.60399200
H	1.99592800	3.97637900	0.60640400
H	1.39170400	5.63645800	0.45980100
H	0.60571600	4.49627400	1.57709800
C	-4.94440600	-3.05936200	-3.40106000
H	-5.43224700	-3.89627200	-2.89104000
H	-5.34153100	-3.00175200	-4.42005000
H	-3.87163300	-3.26342900	-3.45593400
C	-4.49652200	-0.59098800	-3.39129900
H	-4.69811800	0.36737400	-2.90171500
H	-3.41554500	-0.75123900	-3.40953900
H	-4.85800300	-0.52647400	-4.42320900
C	-6.71640200	-1.46424000	-2.59336100
H	-7.12647200	-1.36291100	-3.60355600
H	-7.23531700	-2.27741500	-2.08016200
H	-6.91514700	-0.54161800	-2.03877300
O	3.28237000	-3.21009900	1.04659100
C	4.00198200	-2.14133900	1.50909900
C	5.26611100	-1.96237800	0.72034600
H	5.77359700	-2.91878100	0.56922500
H	5.91848800	-1.28080600	1.26864700
C	4.85290600	-1.34416300	-0.63768600
H	4.33037700	-2.11223500	-1.21972800
H	4.13438100	-0.53569700	-0.45824400
C	6.03199300	-0.80668600	-1.41074900
C	6.11022400	0.55151800	-1.72300600
C	7.06654000	-1.65346600	-1.81913900
C	7.20313000	1.05447800	-2.42591000
H	5.30060400	1.21148500	-1.42177400
C	8.15915000	-1.15346600	-2.51972300
H	7.01291500	-2.71579900	-1.59112100
C	8.23112200	0.20488900	-2.82356500
H	7.24965100	2.11301600	-2.66282000
H	8.95415700	-1.82393000	-2.83161500
H	9.08321600	0.59662900	-3.37016200
O	3.60357500	-1.38246500	2.35306300
F	1.66170700	-0.09293400	1.00598800
H	1.83669200	-0.42031600	1.88053100
F	1.02035000	-0.08646200	3.47783800
H	0.77754800	0.77925800	3.15642400
F	3.04817300	2.12515800	1.71590600
H	3.11002500	1.95662100	0.73570500
F	2.98047300	1.94836700	-0.64677600
H	1.93390300	1.89910000	-0.71471400
F	0.71311000	2.10475500	2.30947500
H	1.66213800	2.10351700	2.03668600

IM1-15

I	-2.01428300	0.41263600	-0.66163200
C	-3.98968400	-0.26073300	-0.68719900
C	-6.56329300	-1.23151600	-0.74285100
C	-4.49555900	-0.74258100	-1.88890400
C	-4.72657200	-0.25986900	0.49325400
C	-6.03120500	-0.74269900	0.45062700
C	-5.79739100	-1.24023400	-1.90477900
H	-3.88762900	-0.74630200	-2.78779700
H	-4.28938400	0.09374100	1.42030600
H	-6.62723100	-0.74964800	1.35763400
H	-6.20927100	-1.62793300	-2.83031300
H	-7.57839100	-1.61485500	-0.76295900
O	-1.49853700	-1.30962500	-1.61378800
C	-0.11352000	-1.46022900	-1.56003300
C	2.63525500	-1.65564400	-1.43925600
C	0.63444600	-1.25943000	-2.71552300
C	0.50298400	-1.76185800	-0.34518500
C	1.88531500	-1.86133800	-0.28201900
C	2.01983500	-1.37210200	-2.65423500
H	0.12846300	-1.01598400	-3.64391100
H	-0.10571400	-1.89699300	0.54525900
H	2.38065700	-2.07093700	0.65490000
H	2.63677600	-1.21334400	-3.53167500
O	-2.45104400	-2.14864200	1.21527900
C	-3.00432200	-3.12146600	0.73809900
O	-2.92196600	-3.42743900	-0.55596900
C	-3.81421700	-4.12722500	1.54190000
O	-2.87489900	2.15479000	0.51398300
C	-2.59896000	3.31945500	0.15382800
O	-2.32688100	3.53240700	-1.09275100
C	-2.58687900	4.44771800	1.16783600
H	-2.36478600	-2.73800100	-0.99059800
C	-3.22155500	5.70801500	0.56113000
H	-3.26259900	6.48246600	1.33233300
H	-2.63439900	6.10219400	-0.27115200
H	-4.24403700	5.51631400	0.22024000
C	-3.35123200	4.01383600	2.42042400
H	-4.39886500	3.79619000	2.19101100
H	-2.90354600	3.12379700	2.86761600
H	-3.31976500	4.82531800	3.15303200
C	-1.10825400	4.71297700	1.52294800
H	-0.52916600	4.99438200	0.64209200
H	-1.07349700	5.54307300	2.23488000
H	-0.64441800	3.83759600	1.98367600
C	-2.90960600	-5.35335300	1.75819600
H	-2.00223200	-5.07837700	2.30507800
H	-3.44858700	-6.10597100	2.34303400
H	-2.61971200	-5.79824600	0.80211000
C	-5.07227600	-4.54004300	0.76935500
H	-5.71036000	-3.67312600	0.56729400
H	-4.81476900	-5.00447800	-0.18510100
H	-5.64606800	-5.25760400	1.36527200
C	-4.18734300	-3.50014500	2.88429100
H	-4.73913300	-4.22473100	3.49151100
H	-3.29555000	-3.18507900	3.43068900
H	-4.82082000	-2.61865900	2.73700700
O	4.01037700	-1.60323400	-1.41179300
C	4.70276300	-2.47961700	-0.62058000
C	6.11249300	-2.00967300	-0.35930500
H	6.80027500	-2.71294700	-0.84299800
H	6.25042200	-2.13579400	0.71902800
C	6.41692300	-0.56281100	-0.76269900
H	6.49593700	-0.48363000	-1.85170800
H	5.57753900	0.06115800	-0.44791200
C	7.68193700	-0.07777900	-0.09890500
C	7.64530700	0.28632100	1.25132700
C	8.89719600	-0.01400400	-0.77978400
C	8.79897500	0.70720600	1.90349700
H	6.69463000	0.23433700	1.77849600
C	10.05568200	0.40778700	-0.12947900
H	8.93542200	-0.29312100	-1.83016600
C	10.00923600	0.76937100	1.21348200
H	8.75511500	0.99106900	2.95072000
H	10.99409100	0.45559200	-0.67384700
H	10.91022900	1.09997700	1.72092300
O	4.22995300	-3.50141600	-0.20742000
F	4.21883000	-0.66541800	1.32516300
H	3.37614100	-0.41734400	1.69814900
F	1.91062800	-0.21626100	2.25856400
H	1.49842000	0.66461600	2.18520800
F	0.88186200	4.17752800	-1.09947500
H	-0.08102400	4.98776700	-1.48049400
F	-0.94234600	5.50707500	-1.66506200
H	-1.90140500	4.42793300	-1.30207200
F	0.83013300	1.95997000	2.06158700
H	0.49024000	2.12985300	1.12124000
F	-0.05296800	2.36108900	-0.06150800
H	0.47486200	3.30538700	-0.63007000

IM1-16

I	-1.82749200	0.32260100	-0.14048100
C	-3.72252900	1.05651000	0.28032100
C	-6.22418500	2.00256600	0.89750700
C	-4.65858100	1.17432400	-0.74538400
C	-3.99309900	1.39904800	1.60342100
C	-5.27048100	1.86735300	1.90384800
C	-5.92018300	1.66506600	-0.42159000
H	-4.41359900	0.87182200	-1.75742800
H	-3.22836300	1.30094000	2.36910600
H	-5.51328500	2.13386300	2.92692400
H	-6.66844600	1.77348700	-1.20051000
H	-7.21380200	2.37555400	1.14128800
O	-2.14912700	-1.45787600	0.80730100
C	-0.86695400	-2.00374300	0.84384100
C	1.81198500	-2.64875400	0.67070500
C	-0.43214300	-2.82303800	-0.19627000
C	0.01909500	-1.55650500	1.81926900
C	1.36805000	-1.87724300	1.74524000
C	0.91415400	-3.15954900	-0.26729800
H	-1.13770200	-3.13916100	-0.95925200
H	-0.34023500	-0.88598100	2.58909200
H	2.05544900	-1.48467600	2.48012600
H	1.30054500	-3.75843400	-1.08461000
O	-3.84489300	-1.57941500	-1.71147100
C	-4.70794900	-2.17145600	-1.09011800
O	-4.51701000	-2.62648500	0.14493600
C	-6.09589000	-2.48834300	-1.62875900
O	-1.34899800	2.40213200	-1.07168500
C	-0.11659100	2.57035500	-1.10425000
O	0.62994800	1.50303500	-1.01576900
C	0.52530300	3.92439300	-1.32041100
H	-3.61145200	-2.34913600	0.42804200
C	1.30622000	3.83844300	-2.64646900
H	1.74110500	4.81870300	-2.86181700
H	2.12301500	3.11297300	-2.58327100
H	0.65267900	3.56341800	-3.48047400
C	-0.56198600	4.99409600	-1.39094600
H	-1.25179600	4.80744100	-2.21845800
H	-1.13774200	5.01628800	-0.46206000
H	-0.09460300	5.97204800	-1.53890600
C	1.50366400	4.22862500	-0.17008400
H	2.25742200	3.44597900	-0.05246000
H	2.02258900	5.16264000	-0.40602400
H	0.97005200	4.34595300	0.77384500
C	-6.16254800	-4.00480100	-1.87477900
H	-5.98585100	-4.55804400	-0.94853700
H	-7.15417600	-4.27038200	-2.25570400
H	-5.41808100	-4.31513400	-2.61520600
C	-6.31097800	-1.72704500	-2.93509900
H	-6.27732200	-0.64541000	-2.76544500
H	-5.53912500	-1.97525000	-3.66752600
H	-7.29082200	-1.97801400	-3.35355900
C	-7.15046000	-2.08396700	-0.58974900
H	-8.15078900	-2.28348800	-0.98826400
H	-7.02355800	-2.64558300	0.33832100
H	-7.08105600	-1.01587800	-0.35535700
O	3.13923000	-2.83406100	0.35079000
C	4.14591000	-2.61824800	1.24957400
C	5.44032000	-2.28235500	0.54562700
H	6.07817700	-3.17454200	0.54931100
H	5.93218200	-1.54412200	1.18449100
C	5.27416000	-1.73485900	-0.87950200
H	5.00662100	-2.55108400	-1.55830000
H	4.44477000	-1.02307900	-0.89372900
C	6.53185700	-1.04327200	-1.34309400
C	6.64117400	0.34537700	-1.23816500
C	7.61892800	-1.76891700	-1.83507900
C	7.81260200	0.99519100	-1.61733900
H	5.79130700	0.91309800	-0.86669100
C	8.79210200	-1.12266900	-2.21441700
H	7.54163200	-2.85030400	-1.92548200
C	8.89198100	0.26249100	-2.10519200
H	7.88169000	2.07559400	-1.53428500
H	9.62777000	-1.69994300	-2.59839400
H	9.80544800	0.76822300	-2.40223400
O	4.00346900	-2.69942700	2.43711500
F	3.83457100	0.06171500	1.12773300
H	3.47655900	0.25950200	2.03589300
F	3.10390400	0.39442900	3.38004300
H	2.13423200	0.53422400	3.50674000
F	1.68026000	1.39197000	1.46234700
H	3.33485900	0.96851000	0.08224400
F	3.17977400	1.46017200	-0.75228000
H	1.61468100	1.62369600	-0.89056700
F	-1.16505800	1.25503900	3.07003300
H	-0.81146600	2.04407500	2.28927200
F	-0.34305800	2.69206200	1.52132100
H	0.89136700	1.96796100	1.48570800
F	0.80366800	0.45897800	4.04071100
H	-0.04899700	0.84686900	3.63855600

TS1-1

I	2.25557900	-0.69367300	0.00396400
C	3.77875900	0.46008100	0.82641500
C	5.70868000	2.08895800	1.90304100
C	4.71405200	1.03416700	-0.03136700
C	3.75949000	0.69442000	2.19715800
C	4.74638100	1.51932200	2.73238400
C	5.69342500	1.84879500	0.52930800
H	4.67512800	0.84020200	-1.09671500
H	2.97643100	0.27529200	2.81877200
H	4.75115600	1.72318100	3.79776500
H	6.43910200	2.30479400	-0.11386500
H	6.47094600	2.73426000	2.32761800
O	0.82185500	0.79974800	1.48814700
C	-0.47529900	0.50201100	1.24321700
C	-3.11593100	-0.21395500	0.73193900
C	-1.32097000	1.38240800	0.55525800
C	-0.97123500	-0.73815300	1.66406000
C	-2.28845800	-1.10392100	1.40667200
C	-2.63936100	1.02226500	0.31052100
H	-0.94036100	2.34681400	0.23508500
H	-0.31442700	-1.40001300	2.22003800
H	-2.67249700	-2.05795500	1.74498700
H	-3.31228400	1.69214300	-0.21469100
O	1.76523100	1.60406500	-1.04481500
C	1.77770000	2.74293700	-0.52084100
O	1.46954200	2.97507200	0.69455300
C	2.14959300	3.96351400	-1.36825500
O	3.38951600	-2.37711500	-0.05708000
C	4.36792400	-2.43698400	-0.98573000
O	4.62768600	-1.52524000	-1.73174300
C	5.09393400	-3.78061200	-0.94819800
H	1.08980400	1.85542300	1.18586400
C	6.16699300	-3.78350900	-2.03603900
H	6.69915900	-4.73994000	-2.02085800
H	5.72339500	-3.64485100	-3.02550800
H	6.88849200	-2.97794400	-1.87703800
C	5.73314600	-3.94605300	0.43904300
H	6.44060400	-3.13611600	0.64537500
H	4.97329000	-3.95309900	1.22436200
H	6.28125600	-4.89311500	0.47422400
C	4.07548700	-4.90363600	-1.19219600
H	3.58621300	-4.78786600	-2.16493900
H	4.59242400	-5.86867100	-1.18641700
H	3.30800500	-4.91554800	-0.41445700
C	0.86594400	4.78701000	-1.55301700
H	0.46064000	5.08714500	-0.58264400
H	1.07949100	5.68802100	-2.13849700
H	0.10426900	4.20730500	-2.08645800
C	2.70367500	3.53028000	-2.72317300
H	3.61046800	2.92935500	-2.60010400
H	1.97700400	2.92427600	-3.26947100
H	2.95270100	4.41204500	-3.32370600
C	3.18732400	4.79246900	-0.60174500
H	3.44685700	5.68862000	-1.17632500
H	2.79536500	5.09413300	0.37203100
H	4.10378000	4.21455600	-0.43667100
O	-4.42672000	-0.52357600	0.37755200
C	-5.27792800	-1.05216400	1.29644700
C	-6.64823200	-1.22470200	0.68654200
H	-7.28763100	-1.69014900	1.43955200
H	-6.56945900	-1.90423000	-0.16955500
C	-7.24649100	0.11290300	0.21388100
H	-7.28740600	0.80663300	1.06125500
H	-6.58205400	0.55258900	-0.53585100
C	-8.62831800	-0.08488600	-0.35876300
C	-8.80493200	-0.33577700	-1.72112200
C	-9.75135700	-0.07237900	0.47162100
C	-10.07449900	-0.56574300	-2.24420900
H	-7.93752100	-0.34557100	-2.37718900
C	-11.02273300	-0.30158100	-0.04650000
H	-9.62540500	0.12369900	1.53402000
C	-11.18747100	-0.54908600	-1.40725600
H	-10.19494100	-0.75408400	-3.30661900
H	-11.88572500	-0.28358200	0.61198500
H	-12.17842900	-0.72511700	-1.81364400
O	-4.97201600	-1.32649900	2.42508700

TS1-2

I	-0.96429800	-0.19782800	0.07505400
C	-2.55078800	-1.23762100	-0.83832900
C	-4.62863000	-2.56838100	-2.05597500
C	-2.74218900	-2.58372800	-0.54514100
C	-3.37224900	-0.52834300	-1.70842800
C	-4.42531000	-1.21505700	-2.31223200
C	-3.79003300	-3.25034700	-1.17597800
H	-2.08423500	-3.10449500	0.14191200
H	-3.22902500	0.53438200	-1.89458800
H	-5.08486400	-0.67999000	-2.98749000
H	-3.95265900	-4.30331200	-0.96970700
H	-5.44731000	-3.09343000	-2.53728500
O	-3.09632000	2.63944700	-1.24869500
C	-1.85239500	2.63576100	-0.93376800
C	0.91962800	2.53465300	-0.31285600
C	-1.37594400	2.65901700	0.41916400
C	-0.84841900	2.56590100	-1.95435100
C	0.49286500	2.50159200	-1.65893000
C	-0.00444200	2.67084700	0.70673700
H	-2.10150700	2.74995700	1.21907600
H	-1.18994700	2.55201800	-2.98432400
H	1.22731500	2.43153500	-2.45159900
H	0.34688000	2.71170900	1.73331100
O	-3.29164100	0.53502300	1.25154000
C	-4.46177800	0.89818800	1.08446400
O	-4.83925800	1.80038800	0.23795300
C	-5.60111200	0.22389300	1.84648300
O	0.13036300	-1.88745000	-0.44348800
C	1.37549500	-1.80065100	0.01739700
O	1.75373700	-0.84028800	0.66164600
C	2.24230100	-2.99511800	-0.37784200
H	-4.01919900	2.20807100	-0.35234500
O	2.23804400	2.35667400	0.07083400
C	3.27025000	2.88449100	-0.63977500
O	3.14078200	3.61642400	-1.58339700
C	4.56866100	2.35951200	-0.08057000
H	5.38992000	2.91406900	-0.53900000
H	4.58517400	2.52602800	1.00121900
C	4.69619900	0.84739800	-0.35768000
H	3.79741200	0.34645100	0.01852100
H	4.73968400	0.68808800	-1.44205800
C	5.92309800	0.27016900	0.30293900
C	7.17012700	0.32037400	-0.32374700
C	5.83460800	-0.28737500	1.58139700
C	8.30521700	-0.17624200	0.31094200
H	7.24899000	0.75037200	-1.31975900
C	6.96724800	-0.78606400	2.21910400
H	4.86334000	-0.33602100	2.06976200
C	8.20617700	-0.73084200	1.58489100
H	9.26726100	-0.13288600	-0.19035300
H	6.88208300	-1.22048900	3.21044400
H	9.09009800	-1.12073300	2.07969800
C	3.57528100	-2.91045600	0.36354600
H	3.42669300	-2.90340800	1.44738400
H	4.19203500	-3.77631800	0.10266100
H	4.12491200	-2.00481400	0.09422100
C	1.50724700	-4.29587000	-0.02823400
H	0.55970300	-4.37097500	-0.56783600
H	2.13323600	-5.15053700	-0.30359900
H	1.30377400	-4.35809800	1.04604100
C	2.46926400	-2.91145400	-1.89623500
H	2.97156200	-1.97617400	-2.16518500
H	3.10748200	-3.74268700	-2.21268500
H	1.52283500	-2.97077500	-2.44042700
C	-6.68418400	1.24171900	2.21308800
H	-7.07553800	1.73427900	1.32074400
H	-7.50743900	0.73486900	2.72808800
H	-6.28850100	2.01300400	2.88209300
C	-6.17180800	-0.82721100	0.87800800
H	-5.39951800	-1.55222500	0.59577500
H	-6.99439500	-1.36714600	1.35988000
H	-6.54971300	-0.35183700	-0.03231000
C	-5.05808100	-0.46542200	3.09718200
H	-5.87137400	-0.98042800	3.61937700
H	-4.28830200	-1.19539600	2.83517400
H	-4.61253800	0.26048000	3.78457100

TS1-3

I	2.35897900	-0.63992900	-0.10029500
C	3.87826500	0.45305100	0.80727400
C	5.80018600	2.00552700	2.00365200
C	4.81153300	1.09326600	-0.00481700
C	3.85685200	0.58448900	2.19162000
C	4.83971800	1.37204300	2.78742000
C	5.78724100	1.86775300	0.61574200
H	4.77363900	0.97966100	-1.08177400
H	3.07572000	0.11607200	2.77974500
H	4.84283200	1.49626700	3.86499700
H	6.53154100	2.37335900	0.00906800
H	6.55923700	2.62087600	2.47579000
O	0.90573600	0.71418700	1.51055300
C	-0.38468300	0.44629800	1.21560500
C	-3.01206400	-0.20483600	0.59275100
C	-1.22573200	1.40433400	0.63089100
C	-0.88317900	-0.83676400	1.47513600
C	-2.19519900	-1.17459400	1.15755000
C	-2.53965500	1.07512800	0.32860100
H	-0.84404500	2.40101600	0.43515600
H	-0.23577200	-1.56229400	1.95748500
H	-2.56763100	-2.16582600	1.38243900
H	-3.20913500	1.80278300	-0.11842700
O	1.85431900	1.74943500	-0.93612100
C	1.87501300	2.83212000	-0.30632400
O	1.56906000	2.94804500	0.92753100
C	2.25039900	4.12694000	-1.03275600
O	3.50102900	-2.30182700	-0.31135800
C	4.46870000	-2.28017000	-1.25397600
O	4.70944600	-1.31107500	-1.93051800
C	5.20919500	-3.61422200	-1.32436400
H	1.18501300	1.79821400	1.30795300
C	6.26045700	-3.52826800	-2.42990400
H	6.80451000	-4.47617800	-2.48999800
H	5.79573700	-3.32920300	-3.39921100
H	6.97496300	-2.72559700	-2.23005300
C	5.87786300	-3.86514200	0.03617200
H	6.57989400	-3.06204700	0.28374500
H	5.13386300	-3.93586600	0.83344700
H	6.43746000	-4.80521800	-0.00422200
C	4.19969500	-4.73153600	-1.62494900
H	3.68960200	-4.55649100	-2.57792500
H	4.72881400	-5.68735300	-1.69539300
H	3.44821500	-4.80757800	-0.83536900
C	0.96084900	4.95165100	-1.16583400
H	0.53820600	5.16368500	-0.17957000
H	1.17372000	5.90188400	-1.66774100
H	0.21334300	4.41309200	-1.75904000
C	2.83022000	3.82071700	-2.41142800
H	3.74152600	3.21981000	-2.32649100
H	2.11884800	3.25882100	-3.02117300
H	3.07990600	4.75443300	-2.92712200
C	3.26689800	4.89396100	-0.17879300
H	3.52554400	5.84000100	-0.66733700
H	2.85721600	5.10420800	0.81153200
H	4.18674700	4.31213500	-0.05086500
O	-4.32769800	-0.46527300	0.18926800
C	-5.20906300	-1.04192500	1.01991700
C	-6.57755700	-1.10211100	0.38998300
H	-7.24853800	-1.58453500	1.10350100
H	-6.51839500	-1.73013600	-0.50629900
C	-7.10273600	0.29080100	-0.00377600
H	-7.11721300	0.93337700	0.88384600
H	-6.41064300	0.74101300	-0.72144800
C	-8.48770000	0.19607100	-0.59525200
C	-8.66483800	0.04726000	-1.97230500
C	-9.61456900	0.20426600	0.22985900
C	-9.93985900	-0.08702300	-2.51497600
H	-7.79421800	0.04212300	-2.62412900
C	-10.89115900	0.07035300	-0.30803100
H	-9.48772100	0.32168600	1.30372700
C	-11.05680100	-0.07571300	-1.68331200
H	-10.06120800	-0.19652800	-3.58821400
H	-11.75723200	0.08352900	0.34638900
H	-12.05172800	-0.17734700	-2.10493300
O	-4.94785100	-1.44561700	2.13046500
F	-3.36010300	-3.39788800	2.95355500
H	-3.91965200	-2.64397400	2.86477900

TS1-4

I	-2.40625500	-0.69944900	0.11385600
C	-4.01422000	0.29727500	-0.75124400
C	-6.07516900	1.71776900	-1.87803500
C	-5.03682600	0.75047900	0.07882300
C	-3.97361500	0.55270800	-2.11781300
C	-5.02740800	1.27077700	-2.67870500
C	-6.08076600	1.46024100	-0.50743800
H	-5.01435800	0.54493200	1.14252900
H	-3.12743200	0.23279800	-2.71508000
H	-5.01832500	1.48866300	-3.74126800
H	-6.89453600	1.82069400	0.11344900
H	-6.88958000	2.28064900	-2.32256300
O	-1.10476200	0.98256300	-1.30941700
C	0.20895600	0.82902900	-1.04753100
C	2.89461200	0.41716800	-0.49825600
C	0.94360000	1.80339600	-0.35334300
C	0.84539800	-0.35055200	-1.45834600
C	2.19159200	-0.56270000	-1.18178400
C	2.29055300	1.59724700	-0.08665800
H	0.45111100	2.71979100	-0.04478400
H	0.27458200	-1.08216400	-2.02131300
H	2.70736400	-1.46169100	-1.49827700
H	2.87587900	2.34118200	0.44381800
O	-2.19540800	1.61890100	1.21502200
C	-2.32311400	2.75807200	0.71143900
O	-2.01245000	3.04621400	-0.49391000
C	-2.85152900	3.91400200	1.56449800
O	-3.34333700	-2.49750700	0.09579400
C	-4.34836900	-2.68521300	0.97939500
O	-4.73521600	-1.82460600	1.73062500
C	-4.92278500	-4.09705700	0.88094100
H	-1.50828000	2.01045900	-0.98728000
C	-6.03107100	-4.24368900	1.92261500
H	-6.45637500	-5.25050900	1.86302200
H	-5.64387800	-4.08628100	2.93276100
H	-6.82822400	-3.51543200	1.75246300
C	-5.48583400	-4.29107300	-0.53543800
H	-6.26751200	-3.55561300	-0.75256500
H	-4.69939400	-4.19624000	-1.28823900
H	-5.92738200	-5.28966900	-0.61506500
C	-3.80002000	-5.11175000	1.14120500
H	-3.36410200	-4.97125700	2.13580000
H	-4.21032200	-6.12550700	1.09202800
H	-3.00602200	-5.02152500	0.39592100
C	-1.67425400	4.87318900	1.79796500
H	-1.28131900	5.23751600	0.84461000
H	-2.00389100	5.73200400	2.39278800
H	-0.86553700	4.37278400	2.34221300
C	-3.38857300	3.39627600	2.89649500
H	-4.21740000	2.69869300	2.73862700
H	-2.61253500	2.86709500	3.45462400
H	-3.75242400	4.23327300	3.50230600
C	-3.95587000	4.63459400	0.78150300
H	-4.33015200	5.48446300	1.36291500
H	-3.57551700	4.99744800	-0.17587200
H	-4.79634900	3.96031300	0.58149700
O	4.23946200	0.19134400	-0.17144400
C	5.16428100	0.49969500	-1.08337100
C	6.55694500	0.13247800	-0.65491900
H	7.24189400	0.83995700	-1.13017800
H	6.73870300	-0.84633000	-1.11713500
C	6.78564100	0.05589200	0.85856000
H	6.54783900	1.02286500	1.31529900
H	6.09811000	-0.67790300	1.28851100
C	8.21542200	-0.32253800	1.16100300
C	8.59898400	-1.66523300	1.19841300

C	9.18979800	0.65827100	1.35550700
C	9.92472300	-2.02066800	1.42852800
H	7.84780300	-2.43746900	1.04878300
C	10.51742200	0.30785200	1.58648100
H	8.90262100	1.70697700	1.32977700
C	10.88826700	-1.03373800	1.62348600
H	10.20527600	-3.06899800	1.45876500
H	11.26179800	1.08307600	1.74017400
H	11.92222500	-1.30911700	1.80566400
O	4.90976500	1.01458100	-2.15655400
F	4.78392600	-1.91867500	-2.27053600
H	4.36387000	-1.43874600	-2.97930000
F	3.55971600	-0.32161400	-3.79515800
H	3.86545500	0.38711100	-3.21732000

TS1-5

I	-2.38636500	0.77070100	-0.13184000
C	-4.02201700	-0.10774900	0.80769500
C	-6.12939700	-1.38394600	2.01848000
C	-5.16190600	-0.36751200	0.05004300
C	-3.88979200	-0.48793500	2.13900200
C	-4.96774700	-1.13165800	2.74321000
C	-6.22705100	-1.00481800	0.67976700
H	-5.21083000	-0.07129800	-0.99116000
H	-2.96098600	-0.31997700	2.67235300
H	-4.88929400	-1.44422200	3.77893400
H	-7.13064600	-1.21422600	0.11648200
H	-6.96236200	-1.88959000	2.49620000
O	-1.13106400	-1.10518600	1.09477900
C	0.15200100	-1.04964500	0.69633300
C	2.78694700	-0.83831800	-0.13431900
C	0.71876000	-2.04534700	-0.11666600
C	0.93128900	0.05324000	1.07741000
C	2.25237900	0.16392600	0.66003700
C	2.04153100	-1.94204100	-0.52484100
H	0.11725400	-2.90214000	-0.40219500
H	0.49391400	0.79991000	1.73268800
H	2.88059900	0.99351300	0.96260700
H	2.49881800	-2.70878000	-1.14202600
O	-2.51318400	-1.49715000	-1.33545500
C	-2.71582000	-2.63949300	-0.86721700
O	-2.31970400	-3.01908500	0.28847600
C	-3.45129900	-3.68968000	-1.70152900
O	-3.11762700	2.65095000	0.06401100
C	-4.15197600	3.00536700	-0.73050500
O	-4.67784500	2.24650700	-1.50648600
C	-4.56361100	4.45740700	-0.49636600
H	-1.67463700	-2.08534700	0.76419100
C	-5.70869300	4.79687000	-1.44951200
H	-6.01976200	5.83418200	-1.29048100
H	-5.40010100	4.67974900	-2.49172500
H	-6.56781500	4.14293600	-1.27912200
C	-5.01946100	4.59750300	0.96438500
H	-5.86184500	3.93170400	1.17944000
H	-4.20549500	4.36398600	1.65512100
H	-5.34578500	5.62694800	1.14385300
C	-3.35572700	5.36872900	-0.75736100
H	-2.99586600	5.26209400	-1.78599800
H	-3.65181100	6.41221600	-0.60936700
H	-2.53396200	5.14034200	-0.07435300
C	-2.41580000	-4.75310900	-2.09846600
H	-1.96676600	-5.20297700	-1.20853000
H	-2.89764600	-5.54255700	-2.68540800
H	-1.61928700	-4.31335600	-2.70898400
C	-4.06411600	-3.05185600	-2.94587100
H	-4.79231600	-2.28187600	-2.67123600
H	-3.29755600	-2.57773900	-3.56340000
H	-4.57662500	-3.81510800	-3.54133000
C	-4.54063500	-4.32938600	-0.83163600
H	-5.06662500	-5.10180100	-1.40347900
H	-4.10477700	-4.78225900	0.06156500
H	-5.27422400	-3.58068600	-0.51176200
O	4.12400600	-0.71665600	-0.54156800
C	5.04860700	-1.26738700	0.24130200
C	6.45532200	-0.91232400	-0.14353900
H	6.88685500	-1.76484000	-0.68245400
H	7.00006600	-0.82760300	0.80019500
C	6.58195100	0.37896800	-0.96056600
H	6.21503600	0.21499900	-1.97823300
H	5.94327900	1.13779000	-0.50088400
C	8.01252300	0.85766600	-0.97716000
C	8.52726600	1.51457300	0.14489300
C	8.85144900	0.62885100	-2.06742600
C	9.85211500	1.93611100	0.17385100
H	7.87079900	1.69338600	0.99446600
C	10.17963500	1.05004900	-2.04235300
H	8.45937700	0.12125000	-2.94558600
C	10.68267600	1.70438600	-0.92180800
H	10.23736500	2.44958400	1.04946600
H	10.82018400	0.86857400	-2.90006500
H	11.71634100	2.03515500	-0.90181200
O	4.79044300	-2.01616200	1.17158800
F	5.12257100	0.85069800	1.69914500
H	4.53969600	0.54434800	2.39717800
F	2.77096500	-2.14553000	2.57557300
H	3.48860500	-2.20064000	1.90338700
F	3.42376900	0.06440000	3.36788100
H	3.08379700	-0.81328700	3.10724300

TS1-6

I	-2.44932700	0.73016100	-0.25527100
C	-4.07798400	-0.09918600	0.73853900
C	-6.18043100	-1.30394500	2.02778100
C	-5.21741200	-0.40876600	-0.00058200
C	-3.94402500	-0.39440900	2.09118500
C	-5.01971500	-1.00206200	2.73508500
C	-6.27985400	-1.00993400	0.66815900
H	-5.26864700	-0.17628600	-1.05780400
H	-3.01546700	-0.19059200	2.61217900
H	-4.94031500	-1.24818700	3.78850500
H	-7.18312200	-1.25694500	0.11978100
H	-7.01150400	-1.78155800	2.53661500
O	-1.21666800	-1.10458800	1.06297500
C	0.07212800	-1.08773500	0.68594800
C	2.72957500	-0.96840400	-0.09102200
C	0.64534800	-2.14317000	-0.04318900
C	0.85786700	0.03074400	1.00699800
C	2.18845400	0.09677100	0.61178000
C	1.97991500	-2.08721300	-0.42196100
H	0.03916400	-3.01063100	-0.28315600
H	0.42024900	0.82477600	1.60353500
H	2.81403600	0.94581300	0.85974600
H	2.44277900	-2.90240800	-0.96846900
O	-2.56623400	-1.58408200	-1.36944100
C	-2.78254300	-2.70533900	-0.85992000
O	-2.41588600	-3.03681100	0.32110300
C	-3.50014700	-3.78904700	-1.66593700
O	-3.16776300	2.62026100	-0.13436700
C	-4.21472300	2.94098100	-0.92737700
O	-4.75852800	2.14660500	-1.65376100
C	-4.61209300	4.40618800	-0.76182100
H	-1.77480600	-2.09691600	0.76623700
C	-5.77747800	4.70207200	-1.70482700
H	-6.07742400	5.74909000	-1.59589500
H	-5.49492400	4.52521200	-2.74597100
H	-6.63681000	4.06564000	-1.47832700
C	-5.03143000	4.62968300	0.69942600
H	-5.87264300	3.98333100	0.97085600
H	-4.20250400	4.42828000	1.38242200
H	-5.34661000	5.66997400	0.82944800
C	-3.40473000	5.29226600	-1.10123000
H	-3.07042000	5.12650000	-2.13065400
H	-3.69035900	6.34459200	-1.00397800
H	-2.56824800	5.09545000	-0.42628100
C	-2.46530000	-4.88308500	-1.97066100
H	-2.05486900	-5.29273800	-1.04352900
H	-2.93625900	-5.69527100	-2.53491700
H	-1.64128600	-4.48414600	-2.57269400
C	-4.06039200	-3.20896000	-2.96219200
H	-4.78469200	-2.41515000	-2.75371900
H	-3.26581300	-2.77896100	-3.57670900
H	-4.56412700	-3.99529000	-3.53459400
C	-4.62753500	-4.37121300	-0.80391600
H	-5.14172700	-5.16729300	-1.35352000
H	-4.22938700	-4.78095100	0.12696800
H	-5.36351000	-3.59982100	-0.55052300
O	4.07962800	-0.90696900	-0.47160700
C	4.98482500	-1.17141700	0.46353800
C	6.39992800	-0.92026100	0.03343500
H	6.86523500	-1.89253200	-0.17084200
H	6.90070200	-0.51023100	0.91380200
C	6.54543500	0.02635300	-1.16405100
H	6.25149600	-0.48621000	-2.08508500
H	5.85977800	0.86565600	-1.02311200
C	7.96115200	0.53879700	-1.26374600
C	8.38666200	1.53970500	-0.38434800
C	8.87037300	0.01739000	-2.18320200
C	9.69441100	2.01021500	-0.42704300
H	7.67358100	1.94428200	0.33138600
C	10.18190300	0.48693500	-2.22885200
H	8.54746300	-0.75906600	-2.87266700
C	10.59647200	1.48393900	-1.35100700
H	10.01083300	2.79099800	0.25785500
H	10.87847100	0.07437900	-2.95236300
H	11.61700600	1.85211100	-1.38694000
O	4.70769600	-1.61214200	1.57180600
F	5.14310300	1.32032300	1.15919100
H	4.57871500	1.51721600	1.90840500
F	2.58505500	-2.08497100	2.68021100
H	3.41334500	-1.92392900	2.14409200
F	3.46038800	1.83736500	2.92440000
H	2.94458700	1.07699100	3.26434500
F	2.11545200	0.00170900	3.75078200
H	2.26646600	-0.86910800	3.30005500

TS1-7

I	-2.60220900	0.60874200	-0.35858600
C	-4.19435400	-0.27876000	0.64373700
C	-6.23507200	-1.55696700	1.96133300
C	-5.25149700	-0.78650400	-0.10801300
C	-4.10995600	-0.41161200	2.02571600
C	-5.15384000	-1.05876900	2.68332900
C	-6.28468800	-1.42254600	0.57407200
H	-5.26375600	-0.67627700	-1.18599600
H	-3.23932300	-0.05378900	2.56352100
H	-5.11105200	-1.18096600	3.76027400
H	-7.12486500	-1.82223200	0.01552400
H	-7.04157100	-2.06354900	2.48156300
O	-1.26207400	-0.93751000	1.19585200
C	0.03496700	-0.82709200	0.85929300
C	2.69485800	-0.50696400	0.14620700
C	0.74465000	-1.89279700	0.28197500
C	0.68393700	0.39958500	1.06491900
C	2.01653200	0.56407600	0.70312100
C	2.07784800	-1.73210300	-0.06795400
H	0.24457300	-2.84412100	0.13245300
H	0.14083100	1.21307100	1.53360500
H	2.53520800	1.49982800	0.86626000
H	2.64316700	-2.55194900	-0.49944000
O	-2.43401600	-1.81315700	-1.21574700
C	-2.55928900	-2.89158300	-0.59411200
O	-2.22157300	-3.05575000	0.62880400
C	-3.11941700	-4.12494900	-1.30537000
O	-3.51355500	2.41322100	-0.49149200
C	-4.54003700	2.53132900	-1.36300600
O	-4.96067700	1.60809700	-2.01510400
C	-5.08900100	3.95621900	-1.38882700
H	-1.69732500	-1.99945600	0.99424700
C	-6.22296600	4.02069700	-2.41102000
H	-6.63113700	5.03594500	-2.43878200
H	-5.86609900	3.75912600	-3.41068600
H	-7.02613300	3.32675700	-2.14996700
C	-5.60989700	4.29763500	0.01583100
H	-6.39743000	3.60175600	0.32344700
H	-4.80499800	4.26148900	0.75404400
H	-6.03265600	5.30744200	0.00865700
C	-3.95770500	4.91976600	-1.77593800
H	-3.55171700	4.67544300	-2.76310200
H	-4.35059300	5.94081200	-1.81532000
H	-3.14505900	4.88790200	-1.04617300
C	-1.96376100	-5.12772900	-1.44428000
H	-1.56344800	-5.39068400	-0.46119600
H	-2.31844500	-6.04084800	-1.93451000
H	-1.15393700	-4.70831900	-2.05166800
C	-3.66692200	-3.74841800	-2.67978600
H	-4.47899700	-3.01987100	-2.59029200
H	-2.88934900	-3.30201900	-3.30428700
H	-4.05615600	-4.64028400	-3.18266500
C	-4.22521300	-4.73083500	-0.43187900
H	-4.62416200	-5.63240000	-0.90970000
H	-3.83709600	-4.99262400	0.55492500
H	-5.04960300	-4.02139200	-0.29769300
O	4.04173900	-0.33049000	-0.20622300
C	4.96332600	-0.89405600	0.57134500
C	6.36729000	-0.55180500	0.16733100
H	7.01614700	-1.36112000	0.51166300
H	6.61754500	0.33376100	0.76612600
C	6.56842500	-0.25873000	-1.32414000
H	6.27137800	-1.13387500	-1.91243300
H	5.91133400	0.56360800	-1.62076500
C	8.00923500	0.09168700	-1.60760300
C	8.45685300	1.40767700	-1.47063800
C	8.93010200	-0.89669900	-1.96020700
C	9.79366800	1.73053600	-1.68423800
H	7.74742500	2.18592800	-1.19839100
C	10.26841000	-0.57863500	-2.17562300
H	8.59242600	-1.92455000	-2.07163200
C	10.70355400	0.73684600	-2.03782400
H	10.12448200	2.75904400	-1.57811400
H	10.97080400	-1.35819100	-2.45405600
H	11.74589500	0.98716300	-2.20774000
O	4.70745600	-1.60910900	1.52718500
F	4.58757200	1.01669100	2.24629300
H	4.32827400	1.92545700	2.12147800
F	2.74752600	-1.29736900	2.98570000
H	3.50288400	-1.42859100	2.35175000
F	3.65087400	3.31545500	1.79840600
H	2.75892800	3.22607100	2.18337700
F	2.40391100	0.88084400	3.88239000
H	2.59453200	0.01413900	3.42618300
F	1.49798800	2.74973200	2.74685400
H	1.79670500	1.91744000	3.21105900

TS1-8

I	2.62021800	-0.40637900	-0.65879900
C	3.88668400	0.37719200	0.79092300
C	5.51575900	1.48825300	2.69501200
C	4.98964500	1.11357100	0.36732200
C	3.55513900	0.19274900	2.12943600
C	4.39615700	0.75771100	3.08574100
C	5.81134900	1.66772400	1.34455200
H	5.19552600	1.24065400	-0.68946200
H	2.65655000	-0.34613600	2.40949000
H	4.16375300	0.63398300	4.13811300
H	6.67994900	2.24574200	1.04637200
H	6.15962700	1.92977500	3.44893200
O	0.98646500	0.90128600	0.82724000
C	-0.30402700	0.82156500	0.47044100
C	-3.00015600	0.57723700	-0.12041800
C	-1.11293800	1.96648300	0.37080400
C	-0.86583400	-0.43740300	0.20813000
C	-2.21470500	-0.56081200	-0.09340000
C	-2.46664700	1.84125800	0.08902500
H	-0.67213700	2.94107900	0.55380200
H	-0.25202500	-1.32484800	0.29417300
H	-2.66224400	-1.53170700	-0.26219700
H	-3.11176300	2.71350600	0.05376200
O	2.39884200	2.08591700	-1.28892600
C	2.34088000	3.10439100	-0.56528900
O	1.87330800	3.11350300	0.62555800
C	2.86498500	4.44476400	-1.08714400
O	3.65863500	-2.13725800	-0.81542100
C	4.87256800	-2.07872500	-1.40744000

O	5.36287800	-1.05125400	-1.80530600
C	5.52494800	-3.45771100	-1.47718400
H	1.38932600	1.98842400	0.81985600
C	6.87073000	-3.32211000	-2.18798300
H	7.35482100	-4.30236100	-2.24207300
H	6.74143600	-2.93893900	-3.20370300
H	7.52974600	-2.63422500	-1.65201000
C	5.72273700	-3.96817000	-0.04140700
H	6.35440400	-3.28477900	0.53572600
H	4.76478700	-4.07601900	0.47326100
H	6.21621200	-4.94499700	-0.07001200
C	4.59979800	-4.41023400	-2.24830900
H	4.42211800	-4.04882600	-3.26659400
H	5.07182500	-5.39564000	-2.31680600
H	3.63692800	-4.51983100	-1.74348300
C	1.73457100	5.47636500	-0.97683700
H	1.39527100	5.56533800	0.05805300
H	2.08835000	6.45517300	-1.31865400
H	0.87995900	5.18841900	-1.59900300
C	3.33356600	4.31322400	-2.53403500
H	4.12844600	3.56732900	-2.62207400
H	2.51315100	3.99943800	-3.18525000
H	3.71519600	5.27621700	-2.89045600
C	4.03316300	4.86386700	-0.18232900
H	4.41581900	5.84093000	-0.49740700
H	3.71000300	4.92731800	0.85988000
H	4.85446100	4.14092100	-0.24488600
O	-4.37977400	0.41437700	-0.33672200
C	-5.17341200	0.48695500	0.72810400
C	-6.60623900	0.15616200	0.42349200
H	-7.22588800	0.67382800	1.16022100
H	-6.70506700	-0.91814700	0.63120600
C	-7.05746300	0.45825500	-1.01060400
H	-6.91559700	1.52419800	-1.22003500
H	-6.42322000	-0.09174400	-1.71132500
C	-8.50609400	0.07952000	-1.20327400
C	-8.85366000	-1.20909600	-1.61426800
C	-9.52499200	0.99291700	-0.92510200
C	-10.18945700	-1.57720300	-1.74784000
H	-8.06807100	-1.92774200	-1.83630100
C	-10.86229400	0.62972300	-1.05768100
H	-9.26580000	2.00020400	-0.60686300
C	-11.19771200	-0.65763200	-1.46964900
H	-10.44288600	-2.58146500	-2.07296800
H	-11.64248600	1.35321000	-0.84236800
H	-12.23972700	-0.94198300	-1.57615000
O	-4.79343500	0.77656900	1.85136100
F	-3.92796700	-1.76114500	1.85970200
H	-3.25758800	-2.40184400	1.65300600
F	-2.57204600	0.44825300	2.83697300
H	-3.45204100	0.54868200	2.36746700
F	-2.28902200	-3.48634600	0.88444600
H	-1.33789100	-3.44286500	1.00087100
F	-1.51863700	-1.65328000	2.81671800
H	-2.04602900	-0.78681400	2.78120600
F	0.23224600	-3.44495100	0.97406500
H	0.58725800	-2.79245200	1.60571400
F	0.83024300	-1.66892300	2.51651600
H	-0.12703800	-1.49521800	2.72052600

TS1-9

I	2.73317800	-0.26525400	-0.55752500
C	3.92280900	0.63421300	0.88879100
C	5.45915600	1.88060100	2.78687900
C	5.01524700	1.38588100	0.46445400
C	3.56072700	0.49463600	2.22459700
C	4.35357900	1.12925400	3.17825300
C	5.78957700	2.00952900	1.43863700
H	5.25052200	1.47098600	-0.59061400
H	2.67752400	-0.07111700	2.49884400
H	4.09610900	1.04180100	4.22846400
H	6.64896100	2.60089400	1.13983800
H	6.06580400	2.37608900	3.53811900
O	0.98590300	1.00049300	0.85116100
C	-0.27910500	0.86871100	0.44196500
C	-2.93653100	0.53046600	-0.29141400
C	-1.14252100	1.97631200	0.35551900
C	-0.77645200	-0.40289600	0.10559600
C	-2.10195800	-0.57418700	-0.26465900
C	-2.47455600	1.80391900	0.00434200
H	-0.75815600	2.96176400	0.59827200
H	-0.12495800	-1.26317500	0.17087800
H	-2.49970600	-1.55078900	-0.50624200
H	-3.15896600	2.64550400	-0.03077900
O	2.40765200	2.19343700	-1.26910000
C	2.29438100	3.22092100	-0.57155400
O	1.80495500	3.23214600	0.61663300
C	2.76198200	4.57515400	-1.10457600
O	3.83070000	-1.95896600	-0.55426800
C	5.06151600	-1.91236200	-1.11073900
O	5.53504100	-0.91017400	-1.58548500
C	5.75864200	-3.26721100	-1.01242400
H	1.37657500	2.15176700	0.82448400
C	7.06194600	-3.20341700	-1.80722000
H	7.58326400	-4.16290700	-1.73100100
H	6.86804800	-2.99503600	-2.86311500
H	7.71600500	-2.41592200	-1.42477400
C	6.04826600	-3.52654400	0.47540300
H	6.68341200	-2.73945100	0.89514200
H	5.12134500	-3.57325500	1.05303300
H	6.57370600	-4.48123600	0.58059700
C	4.83568200	-4.36277200	-1.56322700
H	4.59376700	-4.18148900	-2.61574300
H	5.34284300	-5.33062500	-1.49498400
H	3.90277100	-4.41403000	-0.99647100
C	1.57347600	5.54493400	-1.05282500
H	1.20089600	5.64376700	-0.03031400
H	1.88387200	6.53186400	-1.41249900
H	0.75366900	5.19392500	-1.68904500
C	3.28109900	4.43674600	-2.53355300
H	4.11688700	3.73296000	-2.58047300
H	2.49886300	4.06602600	-3.20145400
H	3.62242500	5.41080600	-2.90008900
C	3.87735400	5.07746300	-0.17561900
H	4.21629000	6.06581100	-0.50476000
H	3.51966400	5.14920700	0.85464600
H	4.73756300	4.39886200	-0.19512200
O	-4.29310400	0.34358300	-0.60435000
C	-5.05011400	-0.20474400	0.33750300
C	-6.46590200	-0.42500700	-0.09472100
H	-6.83364300	-1.31704600	0.41623300
H	-6.48902600	-0.59955700	-1.17165800
C	-7.32053300	0.80225200	0.28120100
H	-7.24706800	0.96771700	1.36153600
H	-6.91292900	1.68952300	-0.21645700
C	-8.76062400	0.59858500	-0.11978800
C	-9.20394100	0.96898400	-1.39090500
C	-9.66142000	-0.01102100	0.75588400
C	-10.52080500	0.73929700	-1.77904300
H	-8.50991300	1.44475000	-2.08000300
C	-10.97910500	-0.24266400	0.37191200
H	-9.32556500	-0.30270700	1.74829500
C	-11.41212300	0.13252300	-0.89751000
H	-10.85171800	1.03699400	-2.76917200
H	-11.66881900	-0.71358400	1.06548600
H	-12.43991700	-0.04510200	-1.19765400
O	-4.67141700	-0.42175600	1.48328600
F	-2.64136000	-3.62136100	-1.64248100
H	-2.04900600	-3.69035300	-0.88347200
F	-2.57878600	-0.00547700	2.62801900
H	-3.41819600	-0.16327700	2.07447800
F	-1.22282000	-3.61124600	0.37286400
H	-0.25966000	-3.50744800	0.28516800
F	-1.12342400	-1.85136900	2.67407900
H	-1.73563900	-1.04287800	2.61134700
F	1.17764500	-3.16524900	0.28669000
H	1.26678100	-2.59614200	1.09840800
F	1.16573700	-1.73528800	2.19631500
H	0.17772700	-1.68608300	2.43465300
F	-4.69805400	-2.52009800	-0.65854500
H	-3.99763400	-2.98396000	-1.10565000

TS1-10

I	2.15420800	0.35739800	-0.44994200
C	3.84169400	1.59247700	-0.20704300
C	5.96957000	3.32348200	0.09176600
C	4.55329900	1.58509600	0.98921000
C	4.17413800	2.44049500	-1.25768400
C	5.24839400	3.31437000	-1.09819900
C	5.62327200	2.46200000	1.13218600
H	4.28870600	0.89507400	1.78148700
H	3.60818100	2.42699100	-2.18350000
H	5.51943300	3.98322500	-1.90837100
H	6.18960200	2.46789700	2.05787800
H	6.80784200	4.00248600	0.20988400
O	2.00405400	-1.87843200	-1.33336000
C	0.66181100	-1.91258500	-1.35945900
C	-2.10708500	-1.61718100	-1.32190400
C	-0.08347300	-2.32953100	-0.24173300
C	-0.01650700	-1.37389300	-2.46574100
C	-1.39754600	-1.23166200	-2.45398700
C	-1.46284700	-2.18448000	-0.22621100
H	0.44198300	-2.74142400	0.61582000
H	0.57007300	-1.06167100	-3.32420000
H	-1.91997300	-0.79695000	-3.29715900
H	-2.05420800	-2.46044500	0.63989900
O	4.25385900	-1.11274400	0.14167400
C	4.31165700	-2.30504300	0.47377600
O	3.40919800	-3.18287700	0.16772900
C	5.51264000	-2.84690500	1.24289100
O	1.18467000	2.19615600	0.00660000
C	-0.09734000	2.00826400	0.19200700
O	-0.60068000	0.89487600	0.04100400
C	-0.90583000	3.22040300	0.64385600
H	2.70645900	-2.70220600	-0.48901800
C	-1.31290800	2.93782500	2.10173000
H	-1.91450700	3.77371400	2.47322800
H	-1.91066700	2.02454000	2.16034100
H	-0.43379800	2.83682000	2.74734300
C	-0.09025000	4.50899300	0.55052900
H	0.80413500	4.46252700	1.17737600
H	0.22622200	4.70400600	-0.47836500
H	-0.70701900	5.34903500	0.88542900
C	-2.16577900	3.29910300	-0.22930900
H	-2.76367200	2.39049700	-0.13917400
H	-2.76954900	4.15343600	0.09415300
H	-1.91426300	3.43513900	-1.28574500
C	6.29959400	-1.69285600	1.86252200
H	5.69609800	-1.16404200	2.60837500
H	7.19269300	-2.08137400	2.36261900
H	6.60489400	-0.97045600	1.10125900
C	6.38262400	-3.59354700	0.21683800
H	5.81941000	-4.40717100	-0.24837300
H	6.73005800	-2.91447800	-0.56843000
H	7.25923700	-4.01682700	0.71831100
C	5.03793000	-3.82249600	2.32569400
H	5.90460000	-4.22530000	2.86026600
H	4.39269800	-3.32079700	3.05459000
H	4.47854300	-4.65127200	1.88689500
O	-3.48586500	-1.49342400	-1.24229900
C	-4.04532800	-0.26786800	-1.44389400
C	-5.51123800	-0.30966000	-1.09754600
H	-5.97742000	-1.13493800	-1.64731500
H	-5.95974900	0.62885400	-1.43060900
C	-5.74118700	-0.51413500	0.41237400
H	-5.23665600	-1.43442100	0.72266500
H	-5.26784200	0.30567900	0.95826700
C	-7.21556700	-0.58364000	0.72198100
C	-7.92789000	0.56812900	1.06311300
C	-7.90832300	-1.79338800	0.62712400
C	-9.29774100	0.51475200	1.30649400
H	-7.39843600	1.51474400	1.14246600
C	-9.27750100	-1.85284500	0.86966100
H	-7.36357600	-2.69770300	0.36488800
C	-9.97681500	-0.69719000	1.21042500
H	-9.83451700	1.41961600	1.57502500
H	-9.79864000	-2.80261000	0.79657100
H	-11.04419400	-0.74186000	1.40277500
O	-3.44044700	0.68922100	-1.84829400
F	-2.90259500	0.24163700	0.96352500
H	-2.07297400	0.45372500	0.52440000

TS1-11

I	2.23248400	0.37703500	-0.35165200
C	3.86721400	1.70843000	-0.30966600
C	5.91714700	3.55397300	-0.27111600
C	4.65965900	1.81048000	0.82976400
C	4.07971600	2.50259500	-1.43073400
C	5.11552900	3.43516100	-1.40233800
C	5.68992600	2.74481000	0.84165700
H	4.48709300	1.16106600	1.67997600
H	3.45166600	2.40340500	-2.31010700
H	5.29414400	4.06328000	-2.26881500
H	6.31817000	2.83671700	1.72172400
H	6.72526800	4.27806200	-0.25572600
O	2.08169900	-1.87782500	-1.03526200
C	0.75220500	-2.01448200	-0.87730300
C	-2.00573200	-2.05778500	-0.49313200
C	0.20824000	-2.56518200	0.29605100
C	-0.11494100	-1.47532100	-1.84308600
C	-1.49144300	-1.48622600	-1.65303200
C	-1.16538100	-2.60309200	0.47564800
H	0.87996400	-2.96353900	1.05146300
H	0.31690500	-1.05482300	-2.74627700
H	-2.16419300	-1.04962000	-2.38071400
H	-1.60719000	-3.02857300	1.37019900
O	4.42781300	-0.92661700	0.09975200
C	4.63546100	-2.10303000	0.43272200
O	3.78465400	-3.06300200	0.25263800
C	5.96917300	-2.51734100	1.04396500
O	1.20594000	2.25371800	-0.03777500
C	-0.04071000	2.08773800	0.27067100
O	-0.50487800	0.94933600	0.44712100
C	-0.89817600	3.34671800	0.36877900
H	2.96546300	-2.65682400	-0.29612200
C	-1.60449900	3.34236100	1.73315100
H	-2.23146700	4.23607300	1.81086900
H	-2.24320200	2.46489300	1.84681400
H	-0.87929300	3.36478600	2.55322500
C	-0.04898400	4.60812200	0.21283200
H	0.70937000	4.67653200	0.99792100
H	0.46186800	4.62749700	-0.75330200
H	-0.69770600	5.48699400	0.28058000
C	-1.93790700	3.26062900	-0.76337900
H	-2.55587100	2.36345400	-0.68823400
H	-2.59488700	4.13453200	-0.70939400
H	-1.45052600	3.26406000	-1.74409600
C	6.71537400	-1.28464700	1.55293900
H	6.16082600	-0.79796700	2.36262200
H	7.69418800	-1.58196100	1.94267500
H	6.85942100	-0.55256400	0.75422900
C	6.76792800	-3.19543600	-0.08313200
H	6.23132100	-4.06672200	-0.46850900
H	6.94629600	-2.49969100	-0.90927700
H	7.73750400	-3.52524100	0.30409500
C	5.72985700	-3.51586800	2.18221100
H	6.69202400	-3.82644300	2.60238900
H	5.13800100	-3.06544200	2.98592100
H	5.20144800	-4.40098900	1.82212500
O	-3.35432300	-2.02756100	-0.20046100
C	-4.26789400	-2.31586000	-1.17407900
C	-5.66174400	-1.88740300	-0.78118100
H	-6.33511900	-2.72886900	-0.97217400
H	-5.92072200	-1.11175400	-1.50944000
C	-5.83419600	-1.33648700	0.63891500
H	-5.82943000	-2.15719200	1.36394400
H	-4.98101400	-0.69881800	0.88287900
C	-7.10686500	-0.53353600	0.75439600
C	-7.16713800	0.73161300	0.15939200
C	-8.23398600	-1.02185100	1.41318800
C	-8.33011700	1.49023100	0.22599600
H	-6.28544000	1.10665200	-0.35729200
C	-9.40175500	-0.26347900	1.48212400

H	-8.19611700	-2.00342100	1.87950300
C	-9.45241900	0.99407400	0.88905400
H	-8.36244900	2.47180500	-0.23734200
H	-10.27116200	-0.65637100	2.00069600
H	-10.36053300	1.58653900	0.94288300
O	-3.98003900	-2.83051400	-2.21887400
F	-3.99096200	0.44317700	-1.27811600
H	-3.57702800	0.37153200	-0.41736500
F	-2.84485000	0.49357700	0.94134100
H	-1.87510200	0.65556800	0.75124700

TS1-12

I	-2.37588100	0.32572400	0.28796000
C	-3.97842400	1.69131400	0.43962300
C	-5.97870200	3.57963800	0.64974400
C	-4.90910700	1.80316000	-0.58846300
C	-4.02821800	2.49652300	1.57134200
C	-5.04004000	3.45064400	1.66887200
C	-5.91350100	2.75894700	-0.47580500
H	-4.85964600	1.14741700	-1.45019200
H	-3.29389600	2.38998300	2.36327600
H	-5.09228800	4.08766200	2.54563000
H	-6.64812800	2.85879800	-1.26833000
H	-6.76714600	4.32066800	0.73219900
O	-2.14528000	-1.91421800	0.92904500
C	-0.81709200	-2.03426100	0.72905500
C	1.93306800	-2.01159100	0.27412300
C	-0.29738800	-2.31338100	-0.54318300
C	0.07119900	-1.74875900	1.77922200
C	1.43648700	-1.74855200	1.55330400
C	1.07226400	-2.31197800	-0.78335300
H	-0.98942700	-2.52782100	-1.35390400
H	-0.33647400	-1.53425500	2.76199800
H	2.15086600	-1.53520500	2.34097800
H	1.46304500	-2.51990000	-1.76744400
O	-4.59170900	-0.92738500	0.22318500
C	-4.84402400	-2.07596900	-0.17847300
O	-3.96320900	-3.02023400	-0.25282900
C	-6.26634000	-2.46657600	-0.56138700
O	-1.40356200	2.21000100	-0.23415800
C	-0.17236200	2.06308500	-0.58234500
O	0.34249200	0.92812100	-0.63090000
C	0.61544500	3.33119900	-0.90005700
H	-3.07524100	-2.65484600	0.21032300
C	1.31266700	3.14214600	-2.25585400
H	1.87709900	4.04908900	-2.49366200
H	2.01070300	2.30319000	-2.23327500
H	0.58431300	2.97661800	-3.05635300
C	-0.30321300	4.55238800	-0.93896200
H	-1.06830100	4.44943300	-1.71382400
H	-0.80958600	4.70009400	0.01817200
H	0.29394100	5.44285100	-1.15857900
C	1.66626400	3.48946700	0.21345700
H	2.32569500	2.62188200	0.27486900
H	2.27736100	4.37281500	0.00314100
H	1.18786900	3.63036200	1.18814200
C	-7.08150600	-1.21574400	-0.88911000
H	-6.67903700	-0.70593800	-1.77134500
H	-8.11677000	-1.49839300	-1.10484900
H	-7.07314900	-0.50865500	-0.05592800
C	-6.85629700	-3.17728100	0.67019500
H	-6.26721600	-4.06217600	0.92702500
H	-6.87848200	-2.50668800	1.53497300
H	-7.88167400	-3.49264900	0.45169600
C	-6.24299800	-3.42837500	-1.75416900
H	-7.26807000	-3.71892700	-2.00599100
H	-5.79748300	-2.95554200	-2.63553500
H	-5.66958600	-4.32816200	-1.52242600
O	3.30576600	-1.90423100	0.20427900
C	4.06540400	-2.20308300	-0.88378600
C	5.50502100	-1.87925400	-0.57899300
H	6.13005000	-2.40043300	-1.30701100
H	5.73615500	-2.22700400	0.43153700
C	5.76174900	-0.36078900	-0.64573200
H	5.51470600	0.00812000	-1.64701000
H	5.09604800	0.14332000	0.05825500
C	7.19539800	-0.04306600	-0.29997800
C	7.60764300	-0.07188800	1.03619000
C	8.13293600	0.24512800	-1.29170000
C	8.93288800	0.18919600	1.36896400
H	6.87618900	-0.30582600	1.80660600
C	9.46072500	0.50650000	-0.95965000
H	7.81867400	0.26828900	-2.33252700
C	9.86334500	0.47998300	0.37231300
H	9.24077000	0.16766600	2.41004500
H	10.17904700	0.73273800	-1.74193500
H	10.89693400	0.68526500	0.63360100
O	3.63865300	-2.64508500	-1.91687800
F	4.81232100	-1.13976000	2.40750300
H	4.24087100	-0.51466600	1.98150400
F	3.28927700	0.66845500	1.37518400
H	3.07290700	0.50341100	0.43996500
F	2.67284300	0.49928800	-0.97500400
H	1.66511300	0.67381200	-0.89121500

TS1-13

I	-2.41051900	0.33836900	0.15287200
C	-4.05290300	1.66620100	0.17501300
C	-6.11205200	3.50100300	0.21235900
C	-4.88999900	1.76065000	-0.93187300
C	-4.22418200	2.46194700	1.30105900
C	-5.26564000	3.38912100	1.31105300
C	-5.92461100	2.68988700	-0.90640500
H	-4.74672900	1.11145100	-1.78823300
H	-3.56155800	2.36856900	2.15541800
H	-5.41320200	4.01853800	2.18246300
H	-6.58763500	2.77604000	-1.76121800
H	-6.92378300	4.22101800	0.22703900
O	-2.19263300	-1.91336400	0.76262700
C	-0.87553600	-2.05591400	0.51123900
C	1.85279200	-2.11075500	-0.04111100
C	-0.41911300	-2.42232500	-0.76536300
C	0.06119100	-1.71295900	1.49872000
C	1.42293900	-1.74027400	1.23232100
C	0.94058700	-2.46098300	-1.03370300
H	-1.14581400	-2.67579800	-1.53279700
H	-0.30433600	-1.42409900	2.47926900
H	2.14010300	-1.47631100	1.99654200
H	1.31581200	-2.73818900	-2.01292100
O	-4.63111200	-0.94478300	-0.02589800
C	-4.87547200	-2.10171100	-0.40351800
O	-3.99942300	-3.05462200	-0.40934500
C	-6.28070400	-2.49550500	-0.84274100
O	-1.45710600	2.23885900	-0.29999500
C	-0.17391400	2.14804700	-0.40473300
O	0.39494200	1.04338300	-0.32773300
C	0.59219400	3.45659000	-0.58104400
H	-3.12586600	-2.67037500	0.06785100
C	1.67235700	3.25848200	-1.65305200
H	2.22167600	4.19618100	-1.78194000
H	2.38559500	2.48417400	-1.36498600
H	1.22878800	2.98949200	-2.61706400
C	-0.34976200	4.59516600	-0.97399500
H	-0.84500200	4.38896600	-1.92751600
H	-1.12272900	4.75144500	-0.21777500
H	0.22873500	5.51827200	-1.07912000
C	1.24894200	3.75470400	0.77948500
H	1.90430300	2.94012000	1.09289700
H	1.84552100	4.66846800	0.69520000
H	0.49150000	3.90964200	1.55478300
C	-7.08935900	-1.24555200	-1.18825400
H	-6.65370400	-0.72155100	-2.04591600
H	-8.11348100	-1.53093600	-1.44915600
H	-7.11833600	-0.54833000	-0.34725100
C	-6.91443700	-3.22529600	0.35509000
H	-6.33074200	-4.11018500	0.62344900
H	-6.97408900	-2.56644200	1.22719500
H	-7.92909000	-3.54246300	0.09319000
C	-6.20339300	-3.44300800	-2.04510800
H	-7.21517600	-3.74045200	-2.33921700
H	-5.72999200	-2.95524100	-2.90366300
H	-5.63018600	-4.33992200	-1.80161700
O	3.17518500	-2.06247400	-0.43209700
C	4.17228000	-2.41206500	0.42882700
C	5.52294100	-2.07320000	-0.14800300
H	5.88145900	-2.93913900	-0.71838600
H	6.18926400	-1.95491300	0.70874800
C	5.52951600	-0.81043000	-1.02395700
H	5.11077000	-1.04212500	-2.00802100
H	4.87450400	-0.06553900	-0.56445300
C	6.92604400	-0.25594300	-1.15914800
C	7.50068400	0.42406900	-0.07965100
C	7.67785800	-0.42739500	-2.32116100
C	8.79610900	0.92203500	-0.16402400
H	6.91277600	0.55556500	0.82635100
C	8.97682000	0.07056800	-2.40952900
H	7.23991300	-0.95330100	-3.16628600
C	9.53903900	0.74664000	-1.33116700
H	9.22785700	1.45094300	0.68042500
H	9.54828600	-0.06933900	-3.32229200
H	10.55008200	1.13637300	-1.39835800
O	3.97936300	-2.93713500	1.49225800
F	4.66302000	-0.17081200	1.81860000
H	4.40591700	-0.68245300	2.57890000
F	3.34492400	-0.80273700	3.83848500
H	2.87532400	-0.04112000	3.47782700
F	2.29476900	1.00831500	2.54043900
H	2.65026100	0.86024900	1.63663900
F	2.74077600	0.80500100	0.17813600
H	1.76810400	0.88156600	-0.10345000

TS1-14

I	-2.37739900	0.25868800	0.17311100
C	-4.09163700	1.50068800	0.23418200
C	-6.32661400	3.11869200	0.26428400
C	-4.58341600	1.99168500	-0.97009700
C	-4.69545700	1.78929400	1.45213400
C	-5.82068700	2.60957400	1.45892000
C	-5.70982400	2.81232500	-0.94643300
H	-4.09832700	1.74859600	-1.91027800
H	-4.30905900	1.37241800	2.37595300
H	-6.30436400	2.84573200	2.40111100
H	-6.10309900	3.20910800	-1.87682600
H	-7.20598000	3.75429500	0.27716600
O	-2.13784500	-2.03013600	0.21333000
C	-0.83388600	-2.09391200	-0.11874700
C	1.86676100	-1.96160600	-0.78152200
C	-0.43075200	-2.11470100	-1.46430600
C	0.14384200	-2.00025300	0.88742600
C	1.48864200	-1.93768200	0.56006400
C	0.91630500	-2.06160200	-1.79318100
H	-1.19066900	-2.17140400	-2.23921700
H	-0.16819900	-1.97669200	1.92670200
H	2.24628700	-1.86898800	1.32591700
H	1.24810600	-2.07395900	-2.82570800
O	-4.61926500	-1.04382000	0.43058400
C	-5.01373500	-1.87972100	-0.38758500
O	-4.21151000	-2.70195200	-1.00803500
C	-6.47958500	-1.98366100	-0.77853000
O	-1.49731900	2.26481200	-0.02423300
C	-0.21845200	2.22168600	-0.15509800
O	0.37853300	1.12729200	-0.22243800
C	0.52677700	3.55322600	-0.18554100
H	-3.27006600	-2.55972100	-0.60521000
C	1.55286400	3.51632500	-1.32683300
H	2.09134200	4.46868200	-1.35283200
H	2.28288100	2.71744700	-1.18217600
H	1.06340400	3.37618100	-2.29605900
C	-0.44317300	4.71971800	-0.37197700
H	-0.98731800	4.63572800	-1.31742800
H	-1.17591300	4.76031600	0.43747300
H	0.12062300	5.65774000	-0.38076600
C	1.25338400	3.67163900	1.16671300
H	1.93724800	2.83537400	1.32305400
H	1.83074800	4.60135700	1.18180900
H	0.53886200	3.69773100	1.99585300
C	-6.94963800	-3.43203900	-0.59372800
H	-6.87853200	-3.73771000	0.45501900
H	-7.99630300	-3.51844500	-0.90300400
H	-6.34840600	-4.11778800	-1.19540500
C	-6.57371900	-1.58666200	-2.26189000
H	-6.22242200	-0.55924400	-2.41228800
H	-5.97812800	-2.25690900	-2.88686400
H	-7.61796700	-1.63857000	-2.58654700
C	-7.30453600	-1.02229300	0.07578400
H	-8.35683900	-1.07968300	-0.22060400
H	-7.22681900	-1.27368800	1.13728300
H	-6.95854400	0.00898000	-0.04976100
O	3.17735100	-1.79215100	-1.17117500
C	4.17379500	-2.42824000	-0.48451600
C	5.52857800	-1.87696000	-0.85013100
H	5.96254900	-2.51695500	-1.62815800
H	6.14468300	-2.00725900	0.04274500
C	5.51897800	-0.40663600	-1.29417000
H	5.18717300	-0.33586100	-2.33474900
H	4.78809200	0.13480600	-0.68865200
C	6.88317700	0.21551100	-1.12787900
C	7.32322400	0.56173800	0.15445600
C	7.73553700	0.42935900	-2.21059600
C	8.58609500	1.11078800	0.34660500
H	6.65554100	0.39274400	0.99698400
C	9.00228500	0.97990300	-2.02202900
H	7.40238400	0.16496700	-3.21145900
C	9.43050800	1.32198900	-0.74308000
H	8.91287100	1.37822200	1.34707500
H	9.65349600	1.14237800	-2.87574800
H	10.41612500	1.75211000	-0.59424800
O	3.97369500	-3.32101000	0.29190400
F	4.36166700	-0.72195200	1.56233700
H	4.29579200	-1.48514700	2.13989800
F	3.80108800	-2.53273300	3.18450900
H	2.93305900	-2.19399800	3.43502000
F	2.26212600	0.68477300	2.48441900
H	2.63119000	0.60637400	1.56743600
F	2.72103600	0.83344100	0.15145000
H	1.73146900	0.96495200	-0.08606100
F	1.65504000	-1.38433200	3.56356400
H	1.87357600	-0.53077900	3.12646600

TS1-15

I	-2.38239500	0.21979800	0.11978600
C	-4.11802500	1.41207800	-0.09034200
C	-6.37667300	2.96404800	-0.41501500
C	-4.57375700	1.67740700	-1.37701400
C	-4.76927900	1.89464000	1.03856400
C	-5.90577100	2.68069500	0.86574300
C	-5.71303000	2.46499900	-1.53344800
H	-4.05353400	1.28200400	-2.24393400
H	-4.40784500	1.65472800	2.03268700
H	-6.42593700	3.06711400	1.73612800
H	-6.07955800	2.68533500	-2.53091500
H	-7.26545200	3.57359200	-0.54133200
O	-2.09821700	-2.04810000	0.32742600
C	-0.78096200	-2.11129300	0.05223100
C	1.94453600	-2.00679400	-0.50418400
C	-0.32150700	-2.26453100	-1.26589200
C	0.15004800	-1.88847500	1.08064200
C	1.51041200	-1.84046400	0.81036000
C	1.03717400	-2.22518600	-1.53856500
H	-1.04593400	-2.41480300	-2.06182400
H	-0.21350400	-1.77596000	2.09616400
H	2.23043300	-1.68138000	1.60186300
H	1.41602500	-2.34541100	-2.54773400
O	-4.59276900	-1.09483300	0.40411500
C	-4.95509100	-2.00939500	-0.34254700
O	-4.12436200	-2.85939300	-0.88167000
C	-6.41417800	-2.19227300	-0.72963900
O	-1.53053500	2.23323100	-0.14694900
C	-0.26410800	2.23520200	-0.33231700
O	0.37487000	1.16118800	-0.43378100
C	0.42906800	3.59360600	-0.39237000
H	-3.19325200	-2.66411900	-0.47607000
C	1.34287200	3.62699200	-1.62584400

H	1.84813900	4.59676700	-1.66899800
H	2.10807600	2.84913800	-1.57925500
H	0.76768300	3.50274500	-2.54901900
C	-0.59614400	4.72557700	-0.45215900
H	-1.23165500	4.63852400	-1.33811900
H	-1.24261700	4.72171800	0.42873200
H	-0.07018700	5.68429900	-0.49608800
C	1.27535100	3.70796200	0.88820400
H	2.05243000	2.94198300	0.91530700
H	1.76140300	4.68809700	0.91005100
H	0.65286100	3.61026600	1.78370000
C	-6.84871300	-3.62036800	-0.37451600
H	-6.77638800	-3.79672300	0.70344500
H	-7.89098400	-3.76961300	-0.67444600
H	-6.22695100	-4.35727100	-0.88855600
C	-6.50774300	-1.97855300	-2.24990400
H	-6.18385900	-0.96708200	-2.52118500
H	-5.88966100	-2.70183600	-2.78766600
H	-7.54785000	-2.09799600	-2.56996600
C	-7.26968600	-1.15845800	0.00092600
H	-8.31746900	-1.27656300	-0.29347100
H	-7.19556700	-1.28156900	1.08495200
H	-6.94798900	-0.14052800	-0.24307300
O	3.26834200	-1.88430400	-0.86034600
C	4.22955900	-2.50471300	-0.11062000
C	5.61397800	-2.06756700	-0.52055900
H	6.07286200	-2.88636800	-1.08780500
H	6.17451400	-1.98385000	0.41384000
C	5.67705800	-0.75096500	-1.30635400
H	5.37325700	-0.92192700	-2.34406700
H	4.95678000	-0.05150400	-0.87457500
C	7.06313400	-0.15738200	-1.25115900
C	7.49170000	0.46723600	-0.07464400
C	7.94581500	-0.23818200	-2.32768300
C	8.77265800	0.99945900	0.01982800
H	6.80073300	0.52750200	0.76378400
C	9.23079000	0.29460200	-2.23701700
H	7.62224000	-0.72046900	-3.24710400
C	9.64730900	0.91474400	-1.06312600
H	9.09028600	1.48432200	0.93816000
H	9.90553600	0.22547900	-3.08510000
H	10.64728300	1.33124200	-0.99109000
O	3.98051300	-3.31085300	0.74184200
F	4.46581300	-0.36532500	1.43072900
H	4.10381500	-0.61602900	2.27837000
F	3.34426200	-1.08959500	3.59039500
H	2.43149300	-0.80680800	3.64274600
F	2.30665800	0.83397900	2.00661800
H	2.67862400	0.77923600	1.06763400
F	2.73124400	0.95047800	-0.29606700
H	1.70823300	1.05856400	-0.46442400
F	0.85565200	-0.68844900	3.89532200
H	0.38811600	-0.00685700	3.40345800
F	-0.04736400	1.05071300	2.35996000
H	0.87242600	1.04313400	2.01894200

TS1-16

I	-2.42584100	0.08986600	-0.31534400
C	-3.89842900	1.53224200	0.09763600
C	-5.72388100	3.50082700	0.70490300
C	-4.85430500	1.87605500	-0.85434000
C	-3.83855600	2.13402600	1.34963700
C	-4.76660700	3.13229400	1.64516800
C	-5.76938300	2.87551600	-0.54189200
H	-4.88454000	1.37534100	-1.81699400
H	-3.09477900	1.82597200	2.07776500
H	-4.73790800	3.61658500	2.61558700
H	-6.51907100	3.16553400	-1.27105900
H	-6.44302100	4.27792300	0.94306100
O	-2.12251500	-2.10951500	0.10804500
C	-0.77918900	-2.18907800	-0.02541300
C	1.97881100	-2.09170100	-0.28918300
C	-0.18578900	-2.46484500	-1.26565300
C	0.02472400	-1.84153200	1.07037500
C	1.40227700	-1.79254500	0.94512700
C	1.19727600	-2.43312900	-1.38947800
H	-0.81681500	-2.71191800	-2.11503600
H	-0.45262500	-1.57790900	2.00585200
H	2.01757300	-1.50356500	1.78556900
H	1.68651400	-2.65013500	-2.33269200
O	-4.55921600	-1.04040500	0.02531600
C	-4.94624900	-2.10980800	-0.47892300
O	-4.14741600	-3.03399600	-0.91051300
C	-6.43051500	-2.39618900	-0.64602800
O	-1.41758400	2.03319200	-1.07598600
C	-0.17329100	2.04463500	-1.03248800
O	0.43912800	0.92157300	-0.80376100
C	0.60526600	3.31355300	-1.33492300
H	-3.18101600	-2.78950500	-0.59907700
C	1.46247600	3.03158300	-2.58376500
H	1.98936100	3.94984500	-2.85967700
H	2.21018000	2.25789000	-2.39246400
H	0.84199600	2.72733200	-3.43308500
C	-0.37608000	4.45439700	-1.60180000
H	-1.01900800	4.23632700	-2.45882100
H	-1.01446300	4.62811400	-0.73160900
H	0.18832400	5.36772700	-1.81192800
C	1.51706800	3.66832400	-0.14747300
H	2.22188800	2.86718400	0.07963400
H	2.08998500	4.56080000	-0.41747000
H	0.92709900	3.88219700	0.74576100
C	-6.70272800	-2.51606600	-2.15520700
H	-6.11331000	-3.32284100	-2.59780900
H	-7.76448200	-2.72953200	-2.31364500
H	-6.46389200	-1.58140500	-2.67457800
C	-7.25530900	-1.26141500	-0.04130800
H	-7.05921400	-1.15900600	1.02936100
H	-7.02085700	-0.30363300	-0.51476000
H	-8.32003600	-1.47142500	-0.18283800
C	-6.74706000	-3.72937200	0.04731900
H	-7.80925600	-3.95962700	-0.08217300
H	-6.15679200	-4.54341400	-0.37959200
H	-6.53931800	-3.67407100	1.12055700
O	3.33766400	-1.97355500	-0.50035800
C	4.20429200	-2.52113500	0.40538100
C	5.62698500	-2.07638300	0.16225400
H	6.23838200	-2.97669200	0.03800700
H	5.94437200	-1.62036900	1.10567500
C	5.84195100	-1.09310500	-0.99290400
H	5.71467000	-1.60897300	-1.95039900
H	5.07331900	-0.31755000	-0.94995400
C	7.20962800	-0.46114800	-0.90941000
C	7.43949900	0.55515800	0.02358300
C	8.26736700	-0.88623000	-1.71271200
C	8.69733000	1.13480400	0.14728800
H	6.61531200	0.88468400	0.65342400
C	9.52968200	-0.30789500	-1.59240500
H	8.09936900	-1.67545200	-2.44169100
C	9.74752900	0.70421400	-0.66252000
H	8.85944700	1.92525900	0.87383400
H	10.34241700	-0.64822800	-2.22699600
H	10.72968000	1.15690600	-0.56858900
O	3.85885500	-3.26114300	1.28310200
F	4.03808500	0.04248800	1.36135200
H	3.52885800	0.07189800	2.21747500
F	2.96136700	-0.10634300	3.48642000
H	1.96956100	-0.10668900	3.48843000
F	1.70123300	1.09881500	1.59380200
H	3.29681900	0.54766300	0.18751400
F	3.00072700	0.84593500	-0.69721100
H	1.43179000	0.96552800	-0.68947400
F	-1.29530200	0.58235600	2.89691600
H	-0.90164700	1.42494000	2.21817600
F	-0.43337900	2.18947600	1.55223200
H	0.85383900	1.59462000	1.57697700
F	0.61521800	-0.45142300	3.73066500
H	-0.22073700	0.04147100	3.39358600

7. Hypervalent I(III)-Promoted Amide (or ester) Formation

7-1. General Procedures

General Procedure E: A reaction tube with magnetic stirring bar was charged with substrate (0.10 mmol) and $PhI(OPiv)_2$ (0.15 mmol, 1.5 equiv.) under argon atmosphere. MeCN (0.50 mL) was added at 0 °C and then Py•9HF (0.15 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at 0 °C for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. The residue was dissolved in CH_2Cl_2 (0.50 mL) and treaded with corresponding amine (0.20 mmol, 2.0 equiv.) and Et_3N (0.20 mmol, 2.0 equiv.) at 0 °C. The mixture was stirred at room temperature for 3 h. After quenched with water, the mixture was extracted with CH_2Cl_2, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel with hexanes-ethyl acetate as eluent.

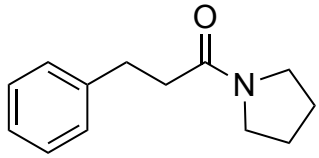
General Procedure F: A reaction tube with magnetic stirring bar was charged with substrate (0.10 mmol) and $PhI(OPiv)_2$ (0.15 mmol, 1.5 equiv.) under argon atmosphere. MeCN (0.50 mL) was added at 0 °C and then Py•9HF (0.15 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at 0 °C for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. The residue was dissolved in CH_2Cl_2 (0.50 mL) and treaded with oxazolidine-2-one (0.10 mmol, 1.0 equiv.), 4-DMAP (0.10 mmol, 1.0 equiv.), and Et_3N (0.20 mmol, 2.0 equiv.) at 0 °C. The mixture was stirred at room temperature for 3 h. After quenched with water, the mixture was extracted with CH_2Cl_2, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel with hexanes-ethyl acetate as eluent.

General Procedure G: A reaction tube with magnetic stirring bar was charged with substrate (0.10 mmol) and $PhI(OPiv)_2$ (0.15 mmol, 1.5 equiv.) under argon atmosphere. MeCN (0.50 mL) was added at 0 °C and then Py•9HF (0.15 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at 0 °C for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. The residue was dissolved in CH_2Cl_2 (0.5 mL) and treaded with corresponding alcohol (1.0 mmol, 10 equiv.), 4-DMAP (0.10 mmol, 1.0 equiv.), and Et_3N (0.20 mmol, 2.0 equiv.) at 0 °C. The mixture was stirred at room temperature for overnight. After quenched with water, the mixture was

extracted with CH_2Cl_2, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel with hexanes-ethyl acetate as eluent.

General Procedure H: A reaction tube with magnetic stirring bar was charged with substrate (0.10 mmol) and $PhI(OPiv)_2$ (0.15 mmol, 1.5 equiv.) under argon atmosphere. MeCN (2.0 mL) was added at –10 °C and then Py•9HF (0.15 mmol, 1.5 equiv.) was added dropwise at the same temperature. The mixture was stirred at –10 °C for 30 min and filtered through silica pad. After washed with CH_2Cl_2 three times, the filtrate was concentrated in vacuo. The residue was dissolved in CH_2Cl_2 (1.0 mL) and treaded with corresponding amine hydrochloride (0.20 mmol, 2.0 equiv.) and DIPEA (0.40 mmol, 4.0 equiv.) at 0 °C. The mixture was stirred at room temperature for 3 h. After quenched with water, the mixture was extracted with CH_2Cl_2, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel with hexanes-ethyl acetate as eluent.

7-2. Amide (or Ester) Products



3-Phenyl-1-(pyrrolidin-1-yl)propan-1-one (4a)

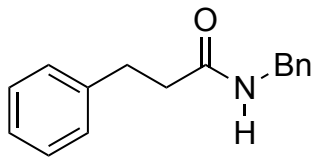
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (48 mg, 0.20 mmol, 1.0 equiv.) and pyrrolidine (32 μL, 0.40 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 39 mg (95% yield) of the title compound.

Colorless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (m, 2H), 7.21-7.15 (m, 3H), 3.42 (t, *J* = 6.4 Hz, 2H), 3.26 (t, *J* = 6.4 Hz, 2H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.54 (t, *J* = 7.6 Hz, 2H), 1.89-1.76 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 141.4, 128.3, 128.3, 126.0, 46.4, 45.5, 36.7, 31.1, 25.9, 24.3.

HRMS (ESI-TOF) Calcd.for $C_{13}H_{17}NONa$: 226.1202 ($[M + Na]^+$), Found: 226.1201.



***N*-Benzyl-3-phenylpropanamide (4b)**

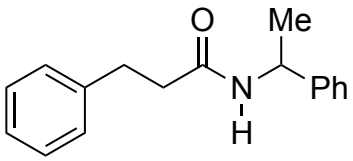
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.) and benzylamine (22 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 22 mg (92% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.17 (m, 10H), 5.93 (brs, 1H), 4.35 (d, *J* = 5.6Hz, 2H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.49 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 140.6, 138.0, 128.5, 128.4, 128.3, 127.5, 127.3, 126.1, 43.3, 38.3, 31.6.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{17}NONa$: 262.1202 ($[M + Na]^+$), Found: 262.1202.



3-Phenyl-*N*-(1-phenylethyl)propenamide (4c)

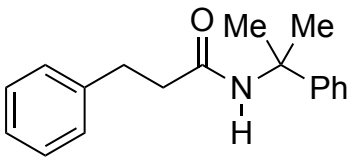
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 23 mg (95% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.16 (m, 10H), 5.59 (d, *J* = 6.4 Hz, 1H), 5.12-5.05 (m, 1H), 2.95 (t, *J* = 7.6 Hz, 2H), 2.46 (t, *J* = 7.6 Hz, 2H), 1.39 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 142.9, 140.7, 128.5, 128.5, 128.3, 127.2, 126.1, 126.1, 48.5, 38.5, 31.6, 21.5.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{19}NONa$: 276.1359 ($[M + Na]^+$), Found: 276.1359.



3-Phenyl-*N*-(2-phenylpropan-2-yl)propenamide (4d)

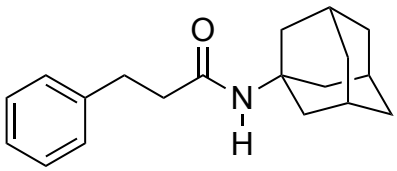
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.) and 2-phenylpropan-2-amine (26 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 4/1) afforded 22 mg (78% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.18 (m, 10H), 5.59 (brs, 1H), 2.94 (t, *J* = 7.6 Hz, 2H), 2.45 (t, *J* = 7.6 Hz, 2H), 1.62 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 146.6, 140.9, 128.5, 128.4, 128.3, 126.5, 126.1, 124.6, 55.8, 39.1, 31.5, 28.9.

HRMS (ESI-TOF) Calcd.for $C_{18}H_{21}NONa$: 290.1515 ($[M + Na]^+$), Found: 290.1515.



***N*-((3*s*,5*s*,7*s*)-adamantan-1-yl)-3-phenylpropanamide (4e)**

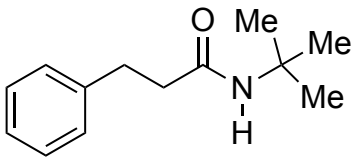
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.) and 1-adamantylamine (30 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 4/1) afforded 25 mg (88% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.25(m, 3H), 7.22-7.17 (m, 2H), 4.97 (brs, 1H), 2.91 (t, *J* = 7.6 Hz, 2H), 2.36 (t, *J* = 7.6 Hz, 2H), 2.02 (s, 3H), 1.91 (s, 6H), 1.63 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 141.0, 128.4, 128.4, 126.0, 51.7, 41.5, 39.5, 39.5, 31.7. 29.3.

HRMS (ESI-TOF) Calcd.for $C_{19}H_{25}NONa$: 306.1828 ($[M + Na]^+$), Found: 306.1830.



***N*-(*tert*-butyl)-3-phenylpropanamide (4f)**

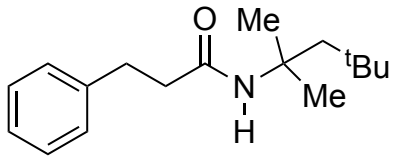
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.) and *tert*-butylamine (21 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 4/1) afforded 19 mg (92% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.22 (m, 3H), 7.19-7.17 (m, 2H), 5.09 (brs, 1H), 2.92 (t, *J* = 7.6 Hz, 2H), 2.36 (t, *J* = 7.6 Hz, 2H), 1.26 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 141.0, 128.4, 128.4, 126.1, 51.0, 39.4, 31.7, 28.6.

HRMS (ESI-TOF) Calcd.for $C_{13}H_{19}NONa$: 228.1359 ($[M + Na]^+$), Found: 228.1357.



3-Phenyl-*N*-(2,4,4-trimethylpentan-2-yl)propenamide (4g)

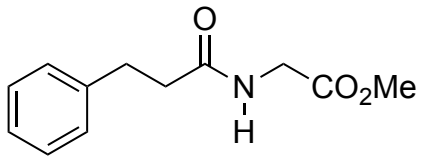
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.) and 2,4,4-trimethylpentan-2-amine (26 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 4/1) afforded 23 mg (88% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (m, 2H), 7.19-7.13 (m, 3H), 5.12 (brs, 1H), 2.91 (t, *J* = 7.6 Hz, 2H), 2.36 (t, *J* = 7.6 Hz, 2H), 1.65 (s, 2H), 1.32 (s, 6H), 0.92 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 141.0, 128.4, 128.4, 126.1, 55.0, 51.5, 39.6, 31.5, 31.5, 31.3, 29.0.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{27}NONa$: 284.1985 ($[M + Na]^+$), Found: 284.1990.



Methyl (3-phenylpropanoyl)glycinate (4h)

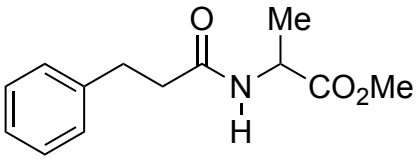
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (48 mg, 0.20 mmol, 1.0 equiv.), glycine methyl ester hydrochloride (50 mg, 0.40 mmol, 2.0 equiv.), and triethylamine (0.11 mL, 0.40 mmol, 4.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 39 mg (88% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.24 (m, 2H), 7.19-7.16 (m, 3H), 5.98 (s, 1H), 4.00 (d, *J* = 5.2 Hz, 2 H), 3.73 (s, 3H), 2.96 (t, *J* = 7.6 Hz, 2H), 2.53 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 170.4, 140.5, 128.4, 128.2, 126.2, 52.3, 41.1, 37.9, 31.3.

HRMS (ESI-TOF) Calcd.for $C_{12}H_{15}NO_3Na$: 244.0944 ($[M + Na]^+$), Found: 244.0943.



Methyl (3-phenylpropanoyl)alaninate (4i)

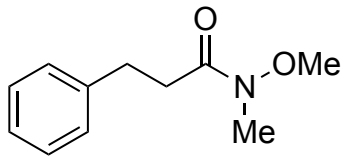
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.), alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.), and triethylamine (56 μg, 0.40 mmol, 4.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 22 mg (94% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.24 (m, 2H), 7.19-7.17 (m, 3H), 5.96 (d, *J* = 5.6 Hz, 1H), 4.60-4.53 (m, 1H), 3.71 (s, 3H), 2.95 (t, *J* = 7.6 Hz, 2H), 2.56-2.45 (m, 2H), 1.32 (d, *J* = 7.2Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 171.4, 140.6, 128.4, 128.3, 126.2, 52.4, 47.8, 38.1, 31.4, 18.4.

HRMS (ESI-TOF) Calcd.for $C_{13}H_{17}NO_3Na$: 258.1101 ($[M + Na]^+$), Found: 258.1102.



***N*-Methoxy-*N*-methyl-3-phenylpropanamide (4j)**

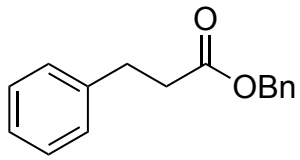
Prepared following general procedure F using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 5/1) afforded 18 mg (93% yield) of the title compound.

Colorless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30-7.17(m, 5H), 3.59 (s, 3H), 3.16 (s, 3H), 2.95 (t, *J* = 7.6 Hz, 2H), 2.73 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 141.3, 128.4, 128.4, 126.0, 61.1, 33.7, 32.1, 30.6.

HRMS (ESI-TOF) Calcd.for $C_{11}H_{15}NO_2Na$: 216.0995 ($[M + Na]^+$), Found: 216.0994.



Benzyl 3-phenylpropanoate (9k)

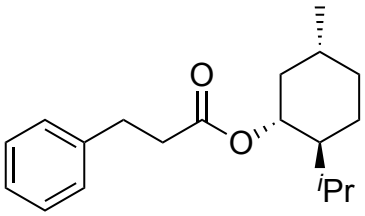
Prepared following general procedure G using 4-hydroxyphenyl 3-phenylpropanoate (48 mg, 0.20 mmol, 1.0 equiv.) and benzyl alcohol (0.20 mL, 2.0 mmol, 10 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 20/1) afforded 46 mg (95% yield) of the title compound.

Colorless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.12(m, 10H), 5.11 (s, 2H), 2.97 (t, *J* = 7.6 Hz, 2H), 2.68 (t, *J* = 7.6 Hz, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 140.3, 135.8, 128.5, 128.4, 128.2, 128.1, 126.2, 66.2, 35.8, 30.8.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{16}NO_2Na$: 263.1043 ($[M + Na]^+$), Found: 263.1042.



(1*R*,2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl 3-phenylpropanoate (9l)

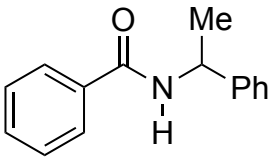
Prepared following general procedure G using 4-hydroxyphenyl 3-phenylpropanoate (24 mg, 0.10 mmol, 1.0 equiv.) and (1*R*,2*S*,5*R*)-(−)-Menthol (156 mg, 1.0 mmol, 10 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 20/1) afforded 21 mg (73% yield) of the title compound.

Colorless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.25(m, 2H), 7.20-7.16 (m, 3H), 4.66 (td, *J* = 10.8, 4.4 Hz, 1H), 2.94 (t, *J* = 7.6 Hz, 2H), 2.60 (t, *J* = 7.6 Hz, 2H), 1.93-1.91 (m, 1H), 1.75-1.61 (m, 3H), 1.50-1.42 (m, 1H), 1.35-1.24 (m, 1H), 1.01 (qd, *J* = 14.0, 4.4 Hz, 1H), 0.88-0.82 (m, 8H), 0.69 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 140.5, 128.4, 128.2, 126.1, 74.1, 46.9, 40.8, 36.1, 34.1, 31.3, 31.0, 26.0, 23.3, 21.9, 20.7, 16.2.

HRMS (ESI-TOF) Calcd.for $C_{19}H_{28}NO_2Na$: 311.1982 ($[M + Na]^+$), Found: 311.1979.



***N*-(1-Phenylethyl)benzamide (8m)**

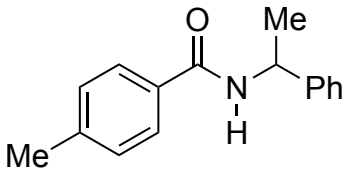
Prepared following general procedure H using 4-hydroxyphenyl benzoate (21 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 7/1) afforded 17 mg (76% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77-7.74(m, 2H), 7.50-7.46 (m, 1H), 7.42-7.32 (m, 6H), 7.29-7.24 (m, 1H), 6.35 (brs, 1H), 5.36.-5.29 (m, 1H), 1.50 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.5, 143.0, 134.5, 131.4, 128.7, 128.4, 127.4, 126.8, 126.2, 49.1, 21.6.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{15}NONa$: 248.1046 ($[M + Na]^+$), Found: 248.1043.



4-Methyl-*N*-(1-phenylethyl)benzamide (8n)

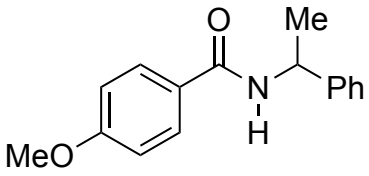
Prepared following general procedure E using 4-hydroxyphenyl 4-methylbenzoate (23 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 7/1) afforded 20 mg (84% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.0 Hz, 2H), 7.39-7.32 (m, 4H), 7.28-7.25 (m, 1H), 7.20 (d, *J* = 8.0 Hz, 2H), 6.37 (d, *J* = 6.8 Hz, 1H), 5.36-5.29 (m, 1H), 2.37 (s, 3H), 1.58 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.4, 143.1, 141.8, 131.6, 129.1, 128.6, 127.3, 126.8, 126.2, 49.0, 21.7, 21.3.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{17}NONa$: 262.1202 ($[M + Na]^+$), Found: 262.1203.



4-Methoxy-*N*-(1-phenylethyl)benzamide (8o)

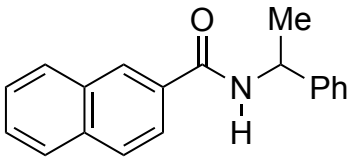
Prepared following general procedure E using 4-hydroxyphenyl 4-methoxybenzoate (24 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 7/1) afforded 23 mg (90% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.8 Hz, 2H), 7.39-7.31 (m, 4H), 7.27-7.24 (m, 1H), 6.88 (d, *J* = 8.8 Hz, 2H), 6.31 (d, *J* = 7.2 Hz, 1H), 5.34-5.27 (m, 1H), 3.82 (s, 3H), 1.57 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.0, 162.1, 143.2, 128.6, 128.6, 127.3, 126.7, 126.2, 113.6, 55.3, 49.0, 21.7.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{17}NO_2Na$: 278.1152 ($[M + Na]^+$), Found: 278.1149.



***N*-(1-Phenylethyl)-2-naphthamide (8p)**

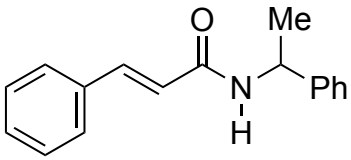
Prepared following general procedure E using 4-hydroxyphenyl 2-naphthoate (26 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 9/1) afforded 24 mg (87% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (s, 1H), 7.89-7.81 (m, 4H), 7.57-7.49 (m, 2H), 7.44-7.25 (m, 5H), 6.55 (d, *J* = 7.2 Hz, 1H), 5.43-5.36 (m, 1H), 1.64 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 143.0, 134.6, 132.5, 131.7, 128.8, 128.7, 128.4, 127.7, 127.6, 127.4, 127.3, 126.7, 126.3, 123.5, 49.3, 21.7.

HRMS (ESI-TOF) Calcd.for $C_{19}H_{17}NONa$: 298.1202 ($[M + Na]^+$), Found: 298.1204.



***N*-(1-Phenylethyl)cinnamamide (8q)**

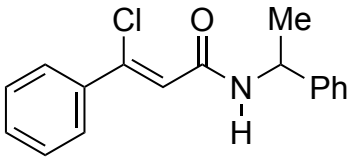
Prepared following general procedure E using 4-hydroxyphenyl cinnamate (24 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 7/1) afforded 24 mg (96% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 15.6 Hz, 1H), 7.48-7.46 (m, 2H), 7.37-7.32 (m, 7H), 7.29-7.27 (m, 1H), 6.39 (d, *J* = 15.6 Hz, 1H), 5.93 (d, *J* = 7.2 Hz, 1H), 5.31-5.24 (m, 1H), 1.56 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 143.0, 141.2, 134.7, 129.6, 128.7, 127.7, 127.4, 126.2, 120.5, 48.9, 21.6.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{17}NONa$: 274.1202 ($[M + Na]^+$), Found: 274.1202.



(*Z*)-3-Chloro-3-phenyl-*N*-(1-phenylethyl)acrylamide (8r)

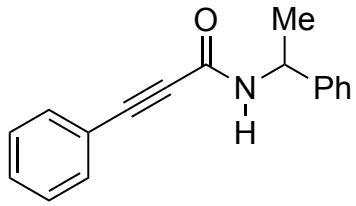
Prepared following general procedure E using 4-hydroxyphenyl (*Z*)-3-chloro-3-phenylacrylate (27 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 7/1) afforded 26 mg (91% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61-7.58 (m, 2H), 7.40-7.33 (m, 7H), 7.29-7.25 (m, 1H), 6.62 (d, *J* = 6.8 Hz, 1H), 6.05 (s, 1H), 5.29-5.22 (m, 1H), 1.58 (d, *J* = 6.8 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 142.7, 138.8, 136.9, 130.1, 128.7, 128.5, 127.4, 126.9, 126.2, 121.1, 49.1, 21.8;

HRMS (ESI-TOF) Calcd.for $C_{17}H_{16}NOClNa$: 308.0813 ($[M + Na]^+$), Found: 308.0817.



3-Phenyl-*N*-(1-phenylethyl)propiolamide (8s)

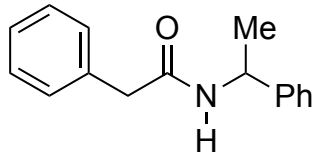
Prepared following general procedure E using 4-hydroxyphenyl 3-phenylpropiolate (24 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 7/1) afforded 20 mg (80% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44-7.42 (m, 2H), 7.39-7.18 (m, 8H), 6.16 (d, *J* = 7.2 Hz, 1H), 5.18-5.11 (m, 1H), 1.48 (d, *J* = 6.8 Hz, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 142.1, 132.4, 130.0, 128.7, 128.4, 127.6, 126.2, 120.1, 84.7, 83.0, 49.3, 21.4.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{15}NONa$: 272.1046 ($[M + Na]^+$), Found: 272.1046.



2-Phenyl-*N*-(1-phenylethyl)acetamide (8t)

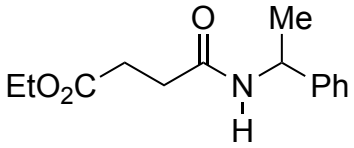
Prepared following general procedure E using 4-hydroxyphenyl 2-phenylacetate (23 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1) afforded 20 mg (84% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.33 (m, 2H), 7.30-7.21 (m, 6H), 7.19-7.17 (m, 2H), 5.67 (brs, 1H), 5.14-5.08 (m. 1H), 3.56 (s, sH), 1.38 (d, J = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 169.9, 143.0, 134.8, 129.3, 128.9, 128.5, 127.3, 127.2, 125.9, 48.6, 43.8, 21.7.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{17}NONa$: 262.1202 ($[M + Na]^+$), Found: 262.1199.



Ethyl 4-oxo-4-((1-phenylethyl)amino)butanoate (8u)

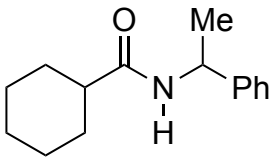
Prepared following general procedure E using ethyl (4-hydroxyphenyl) succinate (24 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 μL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 3/1) afforded 22 mg (88% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.29 (m, 4H), 7.27-7.23 (m, 1H), 7.13-7.11 (m, 2H), 6.02 (d, *J* = 5.2 Hz, 1H), 5.14-5.07 (m, 1H), 4.12 (q, *J* = 7.2 Hz, 2H), 2.72-2.25 (m, 2H), 2.52-2.42 (m, 2H), 1. 47 (d, *J* = 6.8 Hz, 3H), 1.23 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 170.4, 143.1, 128.5, 127.2, 126.0, 60.6, 48.7, 31.1, 29.5, 21.7, 14.1.

HRMS (ESI-TOF) Calcd.for $C_{14}H_{19}NO_3Na$: 272.1257 ($[M + Na]^+$), Found: 272.1257.



***N*-(1-Phenylethyl)cyclohexanecarboxamide (8v)**

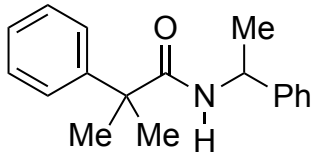
Prepared following general procedure E using 4-hydroxyphenyl cyclohexanecarboxylate (22 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 3/1) afforded 21 mg (91% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.23 (m, 5H), 5.67 (brs, 1H), 5.16-5.09 (m, 1H), 2.10-2.02 (m, 1H), 1.88-1.72 (m, 4H), 1.66-1.65 (m, 1H), 1.47 (d, *J* = 6.8 Hz, 3H), 1.47-1.37 (m, 2H), 1.29-1.17 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 142.1, 132.4, 130.0, 128.7, 128.4, 127.6, 126.2, 120.1, 84.7, 83.0, 49.3, 21.4.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{21}NONa$: 254.1515 ($[M + Na]^+$), Found: 254.1514.



2-Methyl-2-phenyl-N-(1-phenylethyl)propenamide (8w)

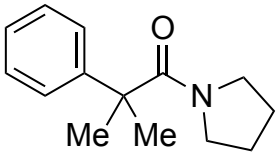
Prepared following general procedure E using 4-Hydroxyphenyl 2-methyl-2-phenylpropanoate (25 mg, 0.10 mmol, 1.0 equiv.) and 1-phenylethylamine (25 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 5/1) afforded 21 mg (79% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.30 (m, 4H), 7.29-7.20 (m, 4H), 7.13-7.11 (m, 2H), 5.32 (brs, 1H), 5.32-5.03 (m. 1H), 1.58 (s, 3H), 1.55 (s, 3H), 1.32 (d, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.4, 145.1, 143.3, 128.6, 128.4, 127.0, 126.9, 126.3, 125.8, 48.6, 46.9, 27.0, 26.9, 21.6.

HRMS (ESI-TOF) Calcd.for $C_{18}H_{21}NONa$: 290.1515 ($[M + Na]^+$), Found: 290.1515.



2-Methyl-2-phenyl-1-(pyrrolidin-1-yl)propan-1-one (8x)

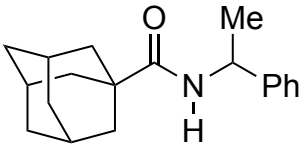
Prepared following general procedure E using 4-hydroxyphenyl 2-methyl-2-phenylpropanoate (25 mg, 0.10 mmol, 1.0 equiv.) and pyrrolidine (16 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 5/1) afforded 17 mg (78% yield) of the title compound.

Colorless oil

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.29 (m, 2H), 7.27-7.20 (m, 3H), 3.51 (t, *J* = 7.2 Hz, 2H), 2.71 (t, *J* = 7.2 Hz, 2H), 1.71-1.65 (m, 2H), 1.59-1.54 (m, 2H), 1.54 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 145.9, 128.6, 126.2, 125.3, 47.3, 47.1, 46.9, 27.3, 26.5, 23.1.

HRMS (ESI-TOF) Calcd.for $C_{14}H_{19}NONa$: 240.1359 ($[M + Na]^+$), Found: 240.1345.



(3*r*,5*r*,7*r*)-*N*-(1-Phenylethyl)adamantane-1-carboxamide (8y)

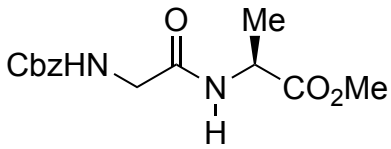
Prepared following general procedure E using 4-hydroxyphenyl (3*r*,5*r*,7*r*)-adamantane-1-carboxylate (27 mg, 0.10 mmol, 1.0 equiv.) and pyrrolidine (16 µL, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 5/1) afforded 23 mg (84% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.23 (m, 5H), 5.79 (d, *J* = 6.4 Hz, 1H), 5.15-5.08 (m, 1H), 2.03 (s, 3H), 1.85 (d, *J* = 0.8 Hz, 6H), 1.75-1.67 (m, 6H), 1.46 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.9, 143.5, 128.5, 127.1, 125.9, 48.0, 40.4, 39.1, 36.4, 28.0, 21.7.

HRMS (ESI-TOF) Calcd.for $C_{19}H_{25}NONa$: 306.1828 ($[M + Na]^+$), Found: 306.1831.



Mthyl ((benzyloxy)carbonyl)glycyl-L-alaninate (12a)

N-Cbz-Gly-L-Ala-OMe

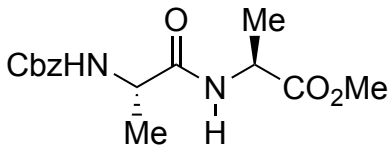
Prepared following general procedure H using 4-hydroxyphenyl ((benzyloxy)carbonyl)glycinate (30 mg, 0.10 mmol, 1.0 equiv.) and L-alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/2) afforded 26 mg (88% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.31 (m, 5H), 6.59 (brs, 1H), 5.47 (brs, 1H), 5.13 (s, 2H), 4.63-4.55 (m, 1H), 3.96-3.84 (m, 2H), 3.74 (s, 3H), 1.40 (d, J = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 168.4, 156.5, 136.0, 128.5, 128.2, 128.1, 67.2, 52.5, 48.0, 44.4, 18.3.

HRMS (ESI-TOF) Calcd.for $C_{14}H_{18}N_2O_4Na$: 317.1108 ($[M + Na]^+$), Found: 317.1106.



Methyl ((benzyloxy)carbonyl)-L-alanyl-L-alaninate (12b)

N-Cbz-L-Ala-L-Ala-OMe

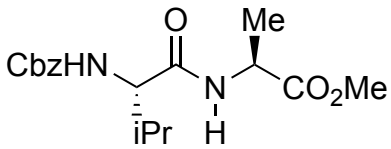
Prepared following general procedure H using 4-hydroxyphenyl ((benzyloxy)carbonyl)-L-alaninate (31 mg, 0.10 mmol, 1.0 equiv.) and L-alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/2) afforded 27 mg (87% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38-7.30 (m, 5H), 6.56 (brs, 1H), 5.36 (brs, 1H), 4.11 (s, 2H), 4.56 (q, *J* = 7.2 Hz, 1H), 4.29-4.23 (m, 1H), 3.75 (s, 3H), 1.39 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 171.1, 155.8, 136.1, 128.5, 128.2, 128.0, 67.0, 52.5, 50.3, 48.0, 18.6, 18.2.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{20}N_2O_5Na$: 331.1264 ($[M + Na]^+$), Found: 331.1267.



Mthyl ((benzyloxy)carbonyl)-L-valyl-L-alaninate (12c)

N-Cbz-L-Val-L-Ala-OMe

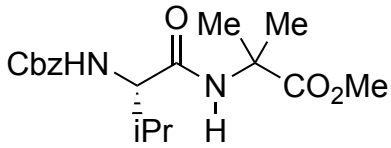
Prepared following general procedure H using 4-hydroxyphenyl ((benzyloxy)carbonyl)-L-valinate (34 mg, 0.10 mmol, 1.0 equiv.) and L-alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 27 mg (80% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.27 (m, 5H), 6.33 (d, *J* = 7.2 Hz, 1H), 5.35 (d, *J* = 7.6 Hz, 1H), 5.09 (s, 2H), 4.60-4.53 (m, 1H), 4.02-3.98 (s, 1H), 3.73 (s, 3H), 2.15-2.06 (m, 1H), 1.39 (d, *J* = 7.2 Hz, 3H), 0.96 (d, *J* = 6.8 Hz, 3H), 0.91 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 170.7, 156.3, 136.1, 128.4, 128.1, 128.0, 66.0, 60.1, 52.4, 47.9, 31.3, 19.0, 18.1, 17.7.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{24}N_2O_5Na$: 359.1577 ($[M + Na]^+$), Found: 359.1588.



Mthyl (*S*)-2-(2-(((benzyloxy)carbonyl)amino)-3-methylbutanamido)-2-methylpropanoate (12d)

N-Cbz-L-Val-Aib-OMe

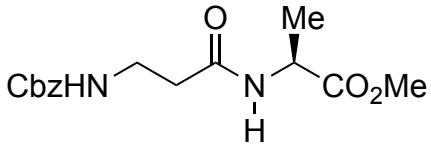
Prepared following general procedure H using 4-hydroxyphenyl ((benzyloxy)carbonyl)-L-valinate (34 mg, 0.10 mmol, 1.0 equiv.) and 2-aminoisobutyric acid methyl ester hydrochloride (31 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 27 mg (77% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37-7.29 (m, 5H), 6.48 (brs, 1H), 5.38 (d, *J* = 8.8 Hz, 1H), 5.10 (s, 2H), 3.98-3.94 (m, 1H), 3.71 (s, 3H), 2.16-2.06 (m, 1H), 1.52 (s, 6H), 0.96 (d, *J* = 6.8 Hz, 3H), 0.92 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 170.2, 156.3, 136.2, 128.5, 128.1, 127.9, 66.9, 60.2, 56.4, 52.5, 31.1, 24.7, 24.5, 19.0, 17.6.

HRMS (ESI-TOF) Calcd.for $C_{18}H_{26}N_2O_5Na$: 373.1734 ($[M + Na]^+$), Found: 373.1737.



Mthyl (3-(((benzyloxy)carbonyl)amino)propanoyl)-L-alaninate (12e)

N-Cbz-β-Ala-L-Ala-OMe

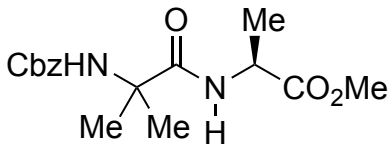
Prepared following general procedure H using 4-hydroxyphenyl 3-(((benzyloxy)carbonyl)amino)propanoate (31 mg, 0.10 mmol, 1.0 equiv.) and L-alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/2) afforded 27 mg (88% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46-7.27 (m, 5H), 6.21 (d, *J* = 7.2 Hz, 1H), 5.49 (brs, 1H), 5.06 (s, 2H), 4.58-4.51 (m, 1H), 3.72 (s, 3H), 3.49-3.41 (m, 2H), 2.43 (d, *J* = 5.6 Hz, 2H), 1.36 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 170.9, 156.4, 136.4, 128.4, 128.0, 127.9, 66.5, 52.5, 47.9, 36.9, 35.7, 18.1.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{20}N_2O_5Na$: 331.1264 ($[M + Na]^+$), Found: 331.1271.



Mthyl (2-(((benzyloxy)carbonyl)amino)-2-methylpropanoyl)-L-alaninate (12f)

N-Cbz-Aib-L-Ala-OMe

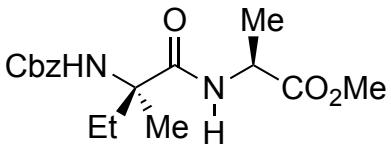
Prepared following general procedure H using 4-hydroxyphenyl 2-(((benzyloxy)carbonyl)amino)-2-methylpropanoate (33 mg, 0.10 mmol, 1.0 equiv.) and L-alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 30 mg (93% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.27 (m, 5H), 6.70 (brs, 1H), 5.33 (brs, 1H), 5.07 (s, 2H), 4.52 (t, *J* = 6.8 Hz, 2H), 3.71 (s, 3H), 1.51 (d, *J* = 5.2 Hz, 3H), 1.33 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 173.4, 154.9, 133.6, 128.5, 128.1, 128.0, 66.7, 56.7, 52.4, 48.1, 25.6, 25.1, 18.1.

HRMS (ESI-TOF) Calcd.for $C_{16}H_{22}N_2O_5Na$: 335.1421 ($[M + Na]^+$), Found: 345.1236.



Methyl ((*R*)-2-(((benzyloxy)carbonyl)amino)-2-methylbutanoyl)-L-alaninate (12g)

N-Cbz-D-Iva-L-Ala-OMe

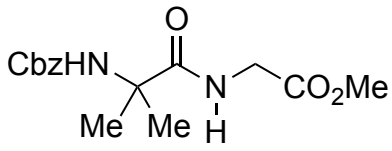
Prepared following general procedure H using 4-hydroxyphenyl (*R*)-2-amino-2-methylbutanoate (34 mg, 0.10 mmol, 1.0 equiv.) and L-alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 28 mg (83% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62-7.27 (m, 5H), 6.62 (brs, 1H), 5.55 (brs, 1H), 5.06 (s, 2H), 4.56-4.52 (m, 1H), 3.72 (s, 3H), 2.08 (brs, 1H), 1.78-1.69 (m, 1H), 1.54 (d, *J* = 3.2 Hz, 3H), 0.83 (d, *J* = 8.8 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 173.0, 154.7, 136.3, 128.5, 128.1, 127.9, 66.5, 60.1, 52.4, 48.1, 30.7, 22.7, 18.1, 8.0.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{24}N_2O_5Na$: 359.1577 ($[M + Na]^+$), Found: 359.1588.



Mthyl (2-(((benzyloxy)carbonyl)amino)-2-methylpropanoyl)glycinate (12h)

N-Cbz-Aib-Gly-OMe

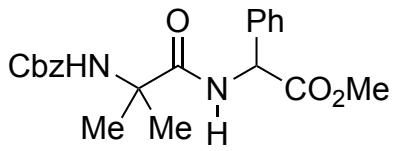
Prepared following general procedure H using 4-hydroxyphenyl 2-(((benzyloxy)carbonyl)amino)-2-methylpropanoate (33 mg, 0.10 mmol, 1.0 equiv.) and glycine methyl ester hydrochloride (25 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 29 mg (93% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.26 (m, 5H), 6.85 (brs, 1H), 5.37 (brs, 1H), 5.09 (s, 2H), 4.02 (brs, 1H), 3.74 (s, 3H), 1.54 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 170.4, 155.0, 136.0, 128.5, 128.1, 128.0, 66.7, 56.8, 56.5, 52.2, 41.3, 25.4.

HRMS (ESI-TOF) Calcd.for $C_{15}H_{20}N_2O_5Na$: 331.1264 ($[M + Na]^+$), Found: 331.1265.



Mthyl 2-(2-(((benzyloxy)carbonyl)amino)-2-methylpropanamido)-2-phenylacetate (12i)

N-Cbz-Aib-Phg-OMe

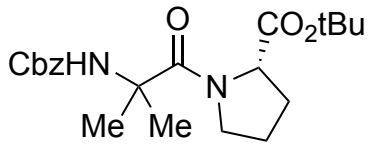
Prepared following general procedure H using 4-hydroxyphenyl 2-(((benzyloxy)carbonyl)amino)-2-methylpropanoate (33 mg, 0.10 mmol, 1.0 equiv.) and 2-phenylglycine methyl ester hydrochloride (40 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 35 mg (91% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.27 (m, 10H), 5.50 (d, *J* = 6.8 Hz, 1H), 5.08 (s, 2H), 3.70 (s, 3H), 1.54 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 171.1, 155.0, 136.3, 136.2, 128.8, 128.5, 128.4, 128.1, 128.0, 127.1, 66.7, 56.8, 56.6, 52.7, 29.6, 25.2.

HRMS (ESI-TOF) Calcd.for $C_{21}H_{24}N_2O_5Na$: 407.1577 ($[M + Na]^+$), Found: 407.1583.



***tert*-Btyl (2-(((benzyloxy)carbonyl)amino)-2-methylpropanoyl)-L-prolinate (12j)**

N-Cbz-Aib-L-Pro-O^{t}Bu

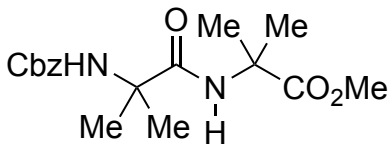
Prepared following general procedure H using 4-hydroxyphenyl 2-(((benzyloxy)carbonyl)amino)-2-methylpropanoate (33 mg, 0.10 mmol, 1.0 equiv.) and L-proline *tert*-butyl methyl ester hydrochloride (40 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1 to 1/1) afforded 36 mg (92% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.27 (m, 5H), 5.77 (brs, 1H), 5.09-4.99 (m, 2H), 4.39 (brs, 1H), 3.67-3.62 (m, 1H), 3.51-3.42 (m, 1H), 2.06-1.89 (m, 2H), 1.85-1.74 (m, 2H), 1.64-1.59 (m, 3H), 1.55-1.51 (m, 3H), 1.41 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 154.1, 136.5, 128.4, 128.1, 128.0, 115.9, 80.9, 66.2, 61.7, 56.6, 47.9, 27.9, 27.7, 25.6, 24.3, 23.9.

HRMS (ESI-TOF) Calcd.for $C_{21}H_{30}N_2O_5Na$: 413.2047 ($[M + Na]^+$), Found: 413.2046.



Mthyl 2-(2-(((benzyloxy)carbonyl)amino)-2-methylpropanamido)-2-methylpropanoate (12k)

N-Cbz-Aib-Aib-OMe

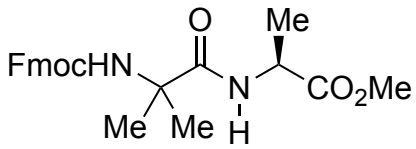
Prepared following general procedure H using 4-hydroxyphenyl 2-(((benzyloxy)carbonyl)amino)-2-methylpropanoate (33 mg, 0.10 mmol, 1.0 equiv.), 2-aminoisobutyric acid methyl ester hydrochloride (31 mg, 0.20 mmol, 2.0 equiv.) and THF instead of CH_2Cl_2 in amidation step for 3 days. Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1) afforded 26 mg (77% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.28 (m, 5H), 6.90 (brs, 1H), 5.30 (s, 2H), 5.08 (brs, 1H), 3.70 (s, 3H), 1.49 (m, 14H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 173.4, 155.0, 136.2, 128.5, 128.1, 128.0, 66.6, 56.9, 56.3, 52.5, 25.3, 24.4.

HRMS (ESI-TOF) Calcd.for $C_{17}H_{24}N_2O_5Na$: 359.1577 ($[M + Na]^+$), Found: 359.1585.



Mthyl (2-((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-2-methylpropanoyl)-L-alaninate (12l)

N-Fmoc-Aib-L-Ala-OMe

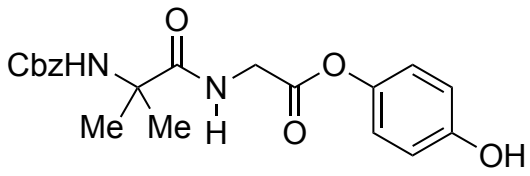
Prepared following general procedure H using 4-hydroxyphenyl 2-((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-2-methylpropanoate (40 mg, 0.10 mmol, 1.0 equiv.) and L-alanine methyl ester hydrochloride (28 mg, 0.20 mmol, 2.0 equiv.). Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 2/1) afforded 37 mg (90% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.59-7.56 (m, 2H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.30 (t, *J* = 7.6 Hz, 2H), 6.75 (brs, 1H), 5.39 (brs, 1H), 4.55-4.50 (m, 1H), 4.18 (d, *J* = 6.0 Hz, 2H), 4.19 (t, *J* = 6.8 Hz, 1H), 3.71 (s, 3H), 1.51 (s, 6H), 1.37 (d, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.8, 173.3, 155.0, 143.7, 143.7, 141.2, 127.6, 127.0, 124.9, 119.9, 66.5, 56.7, 48.2, 47.1, 25.5, 25.0, 18.2.

HRMS (ESI-TOF) Calcd.for $C_{23}H_{26}N_2O_5Na$: 433.1734 ($[M + Na]^+$), Found: 433.1742.



4-Hdroxyphenyl (2-(((benzyloxy)carbonyl)amino)-2-methylpropanoyl)glycinate (13)

N-Cbz-Aib-Gly-OPh(*p*-OH)

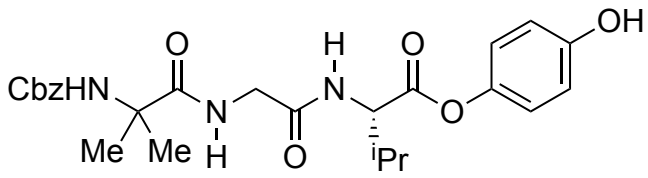
Prepared following general procedure H using 4-hydroxyphenyl 2-(((benzyloxy)carbonyl)amino)-2-methylpropanoate (33 mg, 0.10 mmol, 1.0 equiv.), 4-hydroxyphenyl glycinate (33 mg, 0.20 mmol, 2.0 equiv.), and THF instead of CH_2Cl_2 in amidation step. Purification by flash column chromatography on silica gel (eluent : hexane/ethyl acetate 1/2) afforded 36 mg (93% yield) of the title compound.

White solid

^{1}H NMR (400 MHz, CD_3OD) δ 8.30 (t, *J* = 5.6 Hz, 1H), 7.33-7.26 (m, 5H), 6.92-6.90 (m, 2H), 6.77-6.74 (m, 2H), 5.05 (s, 2H), 4.11 (s, 2H), 1.47 (s, 6H).

^{13}C NMR (100 MHz, CD_3OD) δ 178.2, 170.5, 157.1, 156.4, 144.5, 138.0, 129.4, 128.9, 128.9, 123.2, 116.5, 67.4, 57.6, 42.5, 25.6.

HRMS (ESI-TOF) Calcd.for $C_{20}H_{22}N_2O_6Na$: 409.1370 ($[M + Na]^+$), Found: 409.1376.



Mthyl (2-((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-2-methylpropanoyl)-L-alaninate (14)

N-Cbz-Aib-Gly-L-Val-OPh(*p*-OH)

Prepared following general procedure H using 4-hydroxyphenyl (2-(((benzyloxy)carbonyl)amino)-2-methylpropanoyl)glycinate (38 mg, 0.10 mmol, 1.0 equiv.), 4-hydroxyphenyl L-valinate (41 mg, 0.20 mmol, 2.0 equiv.), and THF instead of CH_2Cl_2 in amidation step. Purification by flash column chromatography on silica gel (eluent : CH_2Cl_2/ethyl acetate 1/2) afforded 43 mg (73% yield) of the title compound.

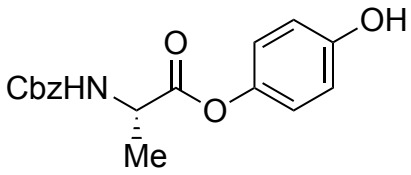
White solid

^{1}H NMR (400 MHz, CD_3OD) δ 7.31 (m, 5H), 6.92-6.87 (m, 2H), 6.78-6.74 (m, 2H), 5.10-4.99 (m, 2H), 4.50 (d, *J* = 7.2 Hz, 1H), 4.20 (d, *J* = 17.2 Hz, 1H), 3.75 (d, *J* = 17.2 Hz, 1H), 2.45-2.36 (m, 1H), 1.46 (s, 3H), 1.40 (s, 3H), 1.09 (d, *J* = 6.8 Hz, 3H), 1.08 (d, *J* = 6.8 Hz, 3H).

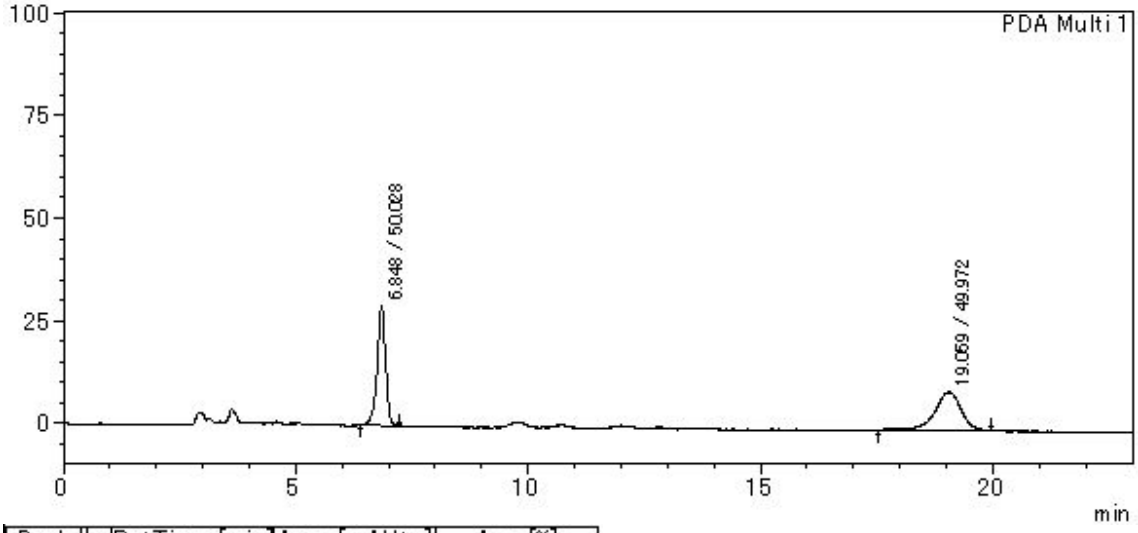
^{13}C NMR (100 MHz, CD_3OD) δ 177.9, 172.5, 172.1, 158.0, 156.5, 144.5, 137.9, 129.4, 128.9, 128.9, 123.2, 116.6, 67.8, 59.7, 57.7, 43.9, 31.6, 26.3, 24.8, 19.6, 19.0.

HRMS (ESI-TOF) Calcd.for $C_{25}H_{31}N_3O_7Na$: 508.2054 ($[M + Na]^+$), Found: 508.2058.

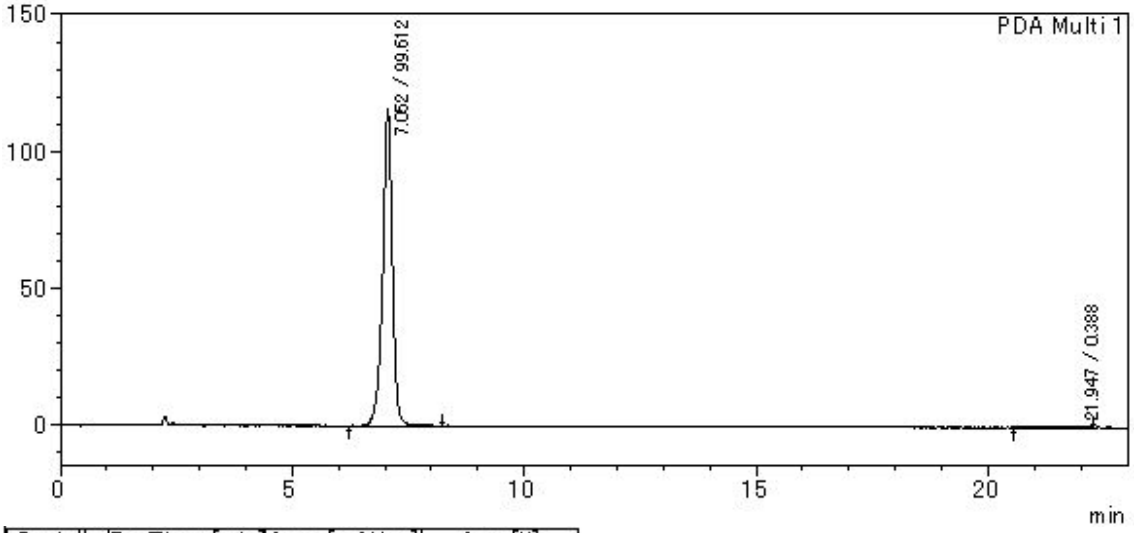
8. Racemization Studies



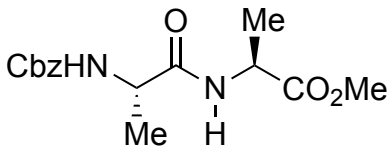
HPLC analysis: 99% ee, Daicel Chiralpak IA, hexane/i-PrOH = 3/1, flow rate = 1.3 mL/min, λ = 210 nm, retention time; t_R (major) = 7.0 min, t_R (minor) = 21.9 min.



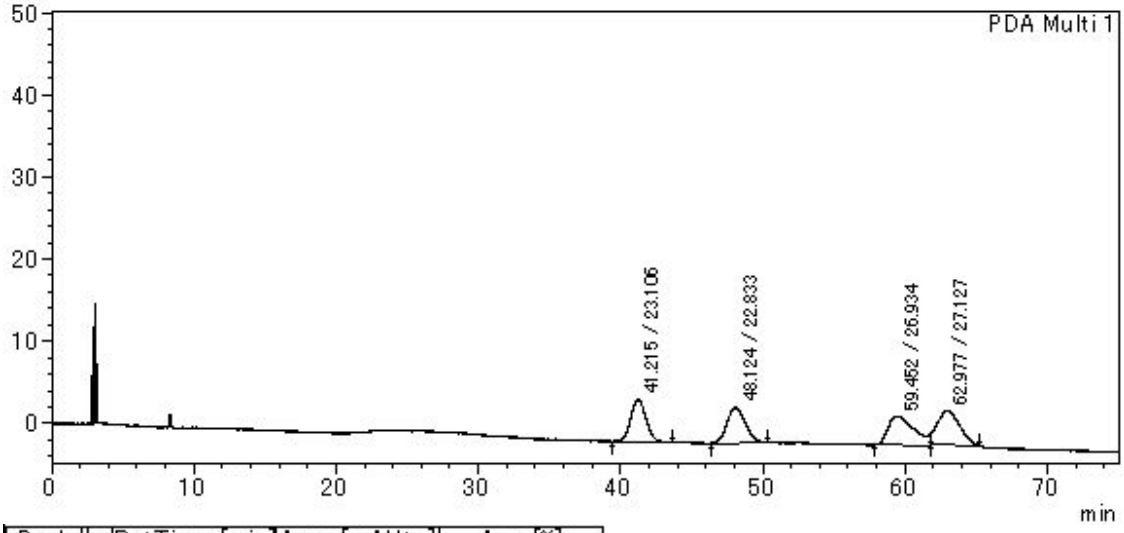
Peak#	RetTime [min]	Area [mAU*s]	Area [%]
1	6.848	362352	50.028
2	19.059	361945	49.972
合計			100.000



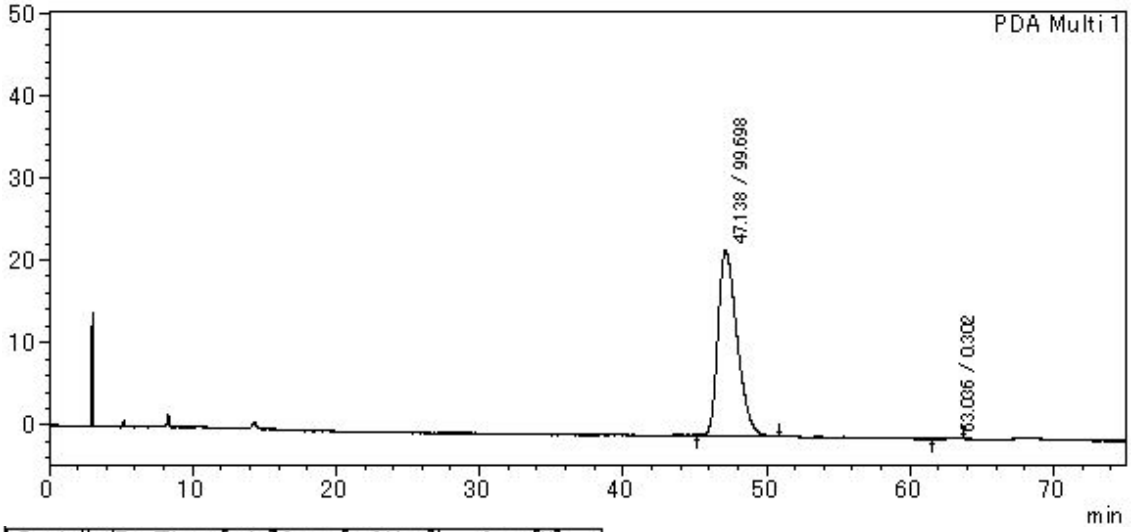
Peak#	RetTime [min]	Area [mAU*s]	Area [%]
1	7.052	1687015	99.612
2	21.947	6565	0.388
合計			100.000



HPLC analysis: 99% ee, Daicel Chiralpak IG, hexane/i-PrOH = 10/1, flow rate = 1.0 mL/min, λ = 210 nm, retention time; t_R (major) = 47.1 min, t_R (minor) = 63.0 min.



Peak#	RetTime [min]	Area [mAU*s]	Area [%]
1	41.215	390409	23.106
2	48.124	385811	22.833
3	59.452	455094	26.934
4	62.977	458359	27.127
合計			100.000



Peak#	RetTime [min]	Area [mAU*s]	Area [%]
1	47.138	2069753	99.698
2	63.036	6276	0.302
合計			100.000

9. References

S1. M. J. Frisch, G. W. Trucks, H. B. *et al. Gaussian 16*, Revision B.01; Gaussian, Inc., Wallingford CT, 2016.

S2. Y. Zhao, & D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215-241.

S3. C. E. Check, T. O. Faust, J. M. Bailey, B. J. Wright, T. M. Gilbert, L. S. Sunderlin, *J. Phys. Chem. A* **2001**, *105,* 8111-8116.

S4. K. Fukui, *Chem. Res.* **1981**, *14,* 363-368.

S5. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B* **2009**, *113*, 6378-6396.

S6. F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7,* 3297-3305.

S7. C. Y. Legault, CYLView, version 1.0b; Université de Sherbrooke: Sherbrooke, Quebec, Canada, 2009.

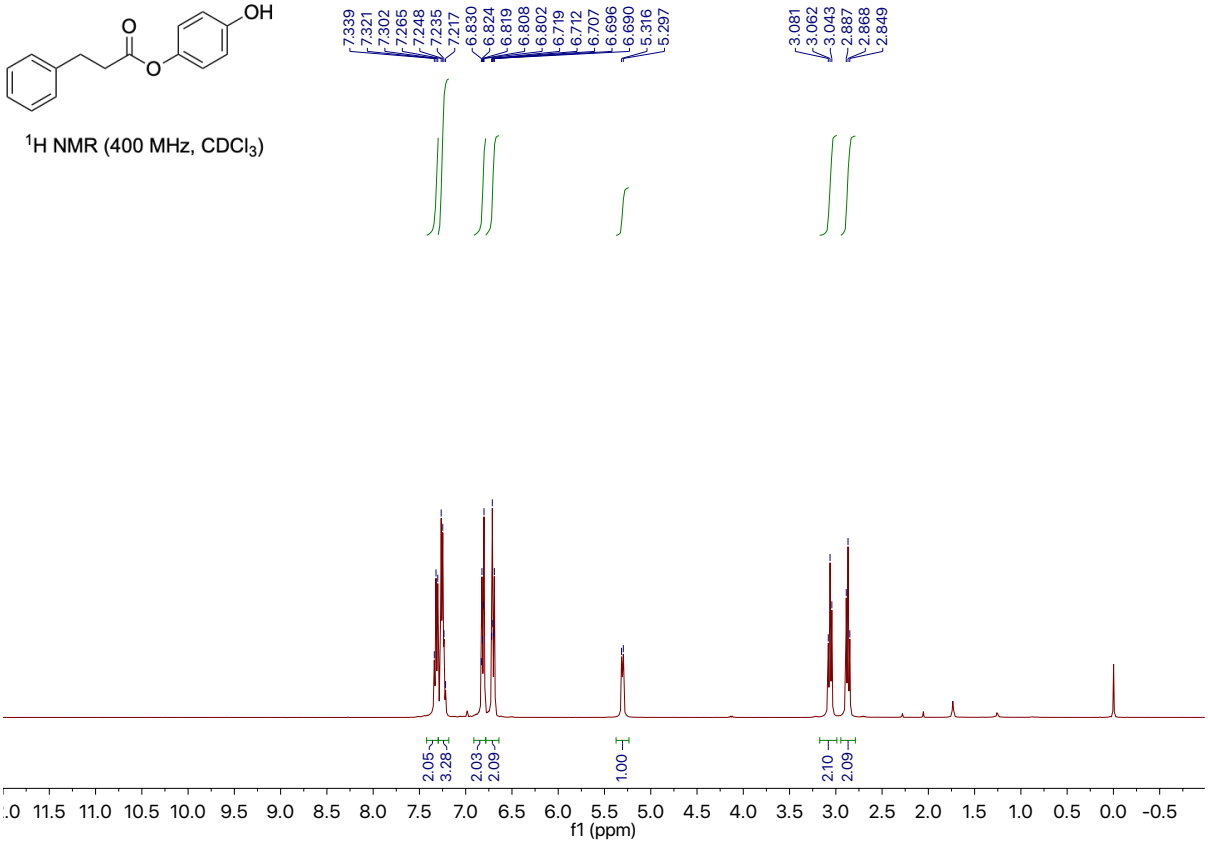
S8. a) S. Sakaki, Y. Ohnishi, H. Sato, *The Chemical Record* **2010***, 10*, 29-45; b) A. Ishikawa, Y. Nakao, H. Sato, S. Sakaki, S. *Dalton Trans.* **2010**, *39,* 3279-3289; c) A. Ishikawa, Y. Nakao, H. Sato, S. Sakaki, S. *Inorg. Chem*. **2009**, *48*, 8154-8163; d) Y. Ohnishi, Y. Nakao, H. Sato, T. Hiyama, S. Sakaki, *Organometallics* **2009**, *28,* 2583-2594.

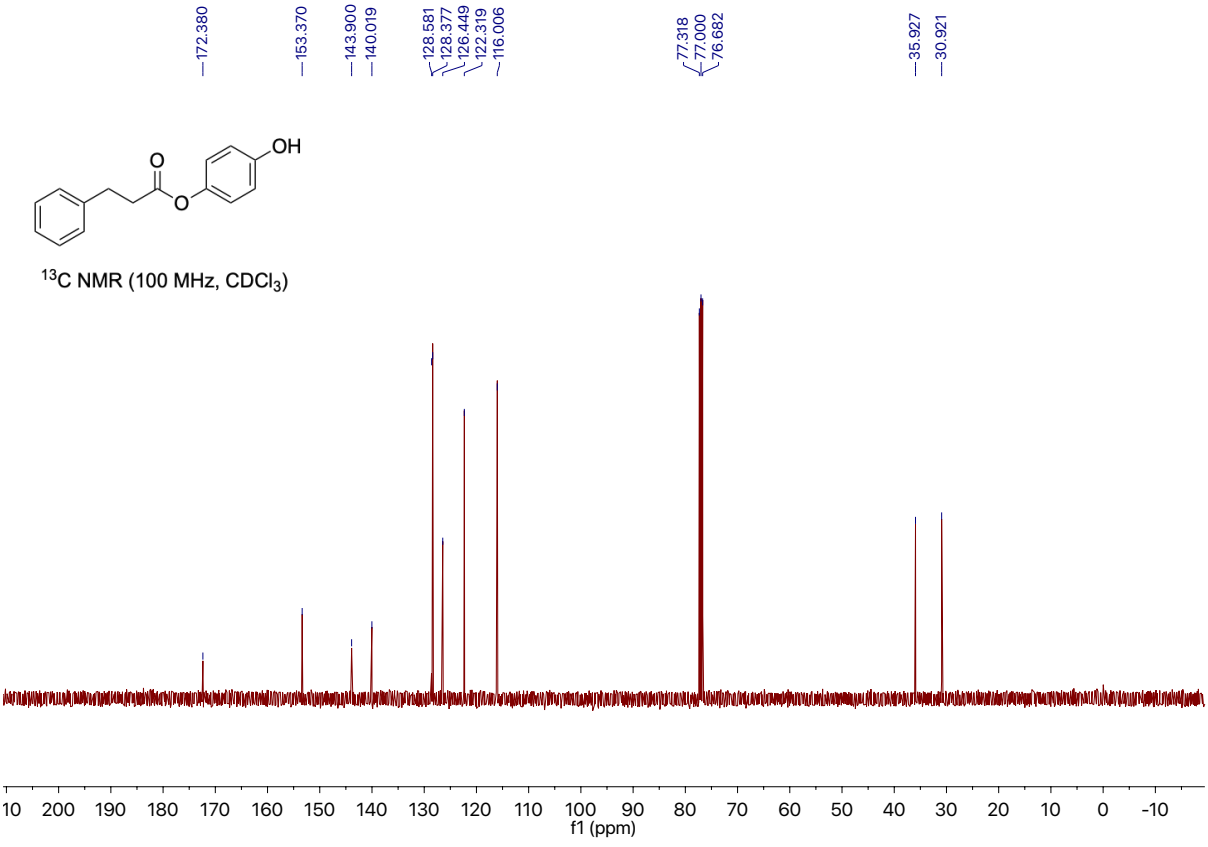
S9. M. Mammen, E. I. Shakhnovich, J. M. Deutch, G. M. Whitesides, *J. Org. Chem.* **1998**, *63*, 3821-3830.

S10. B. Ganji, A. Ariafard, *Org. Biomol. Chem.* **2019**, *17,* 3521-3528.

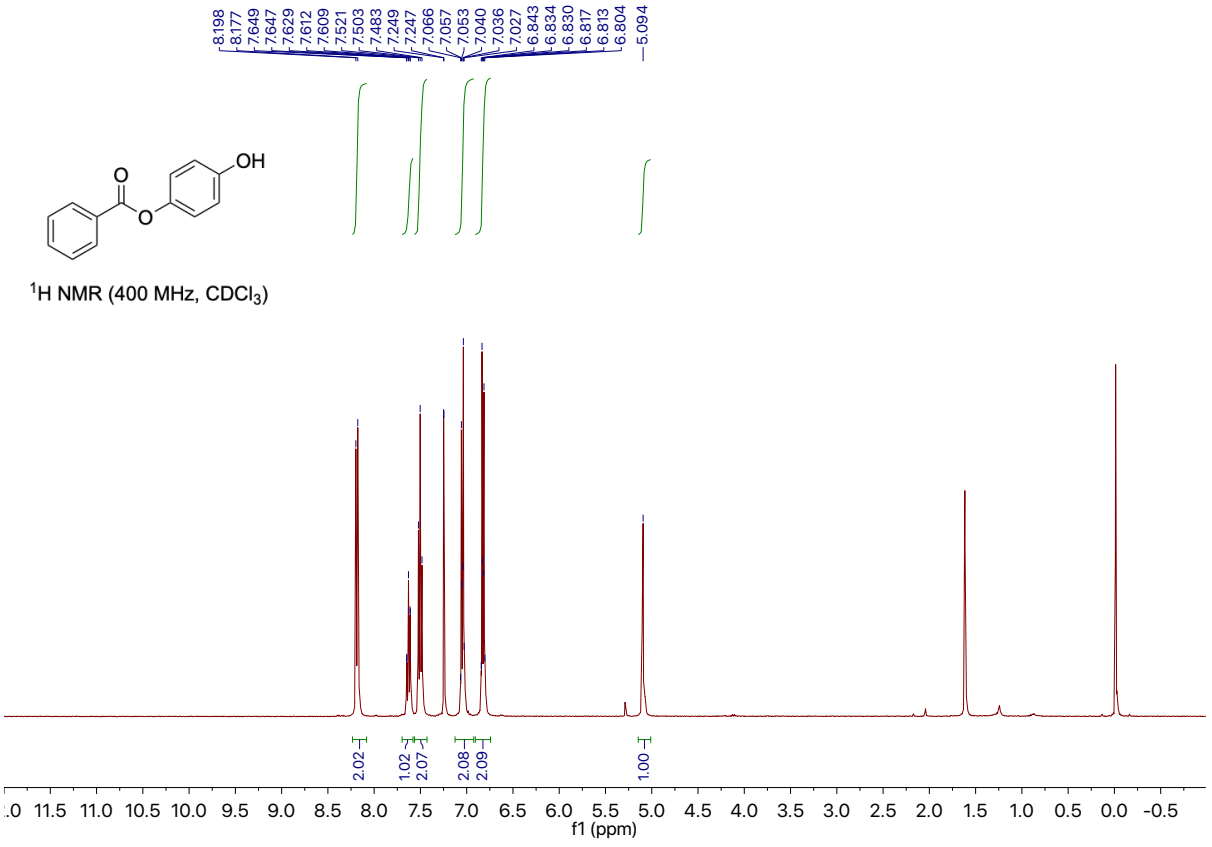
10. Spectral data

^{1}H NMR (400 MHz, $CDCl_3$)

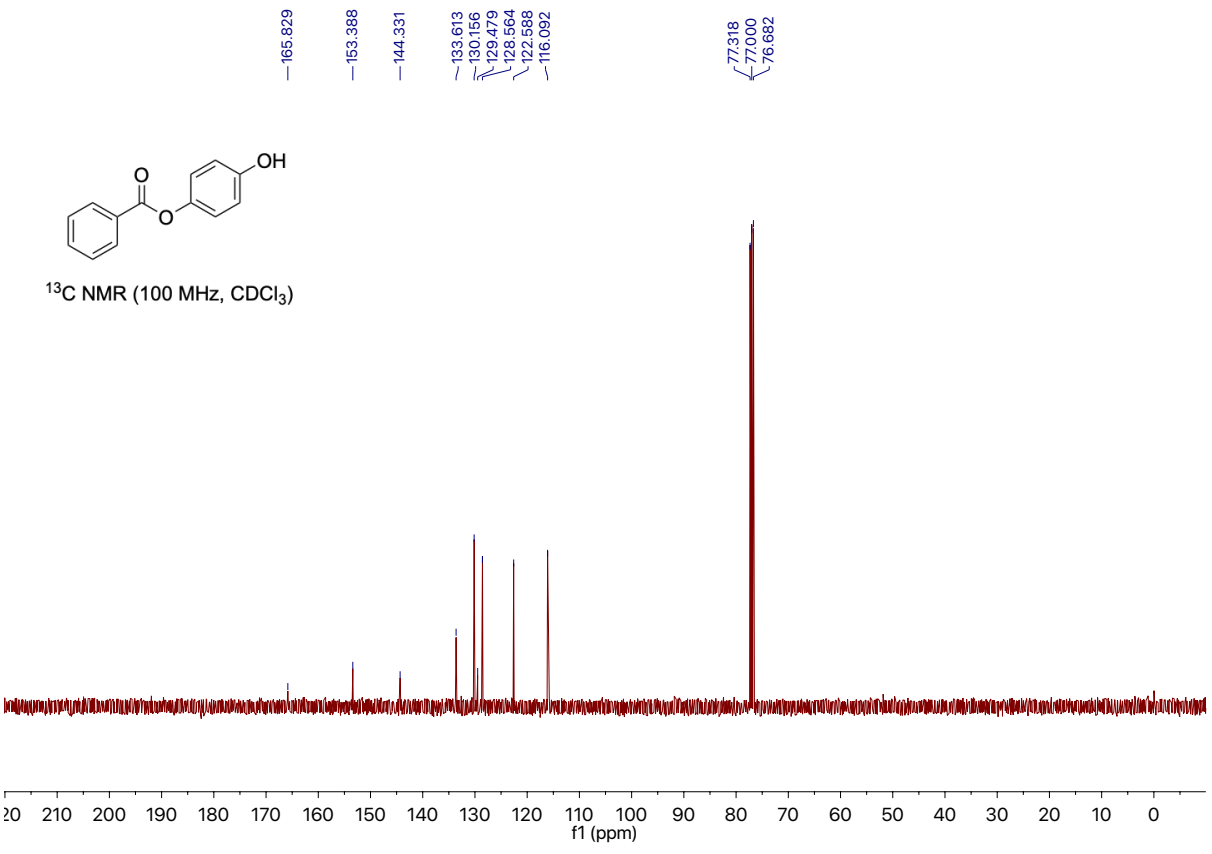




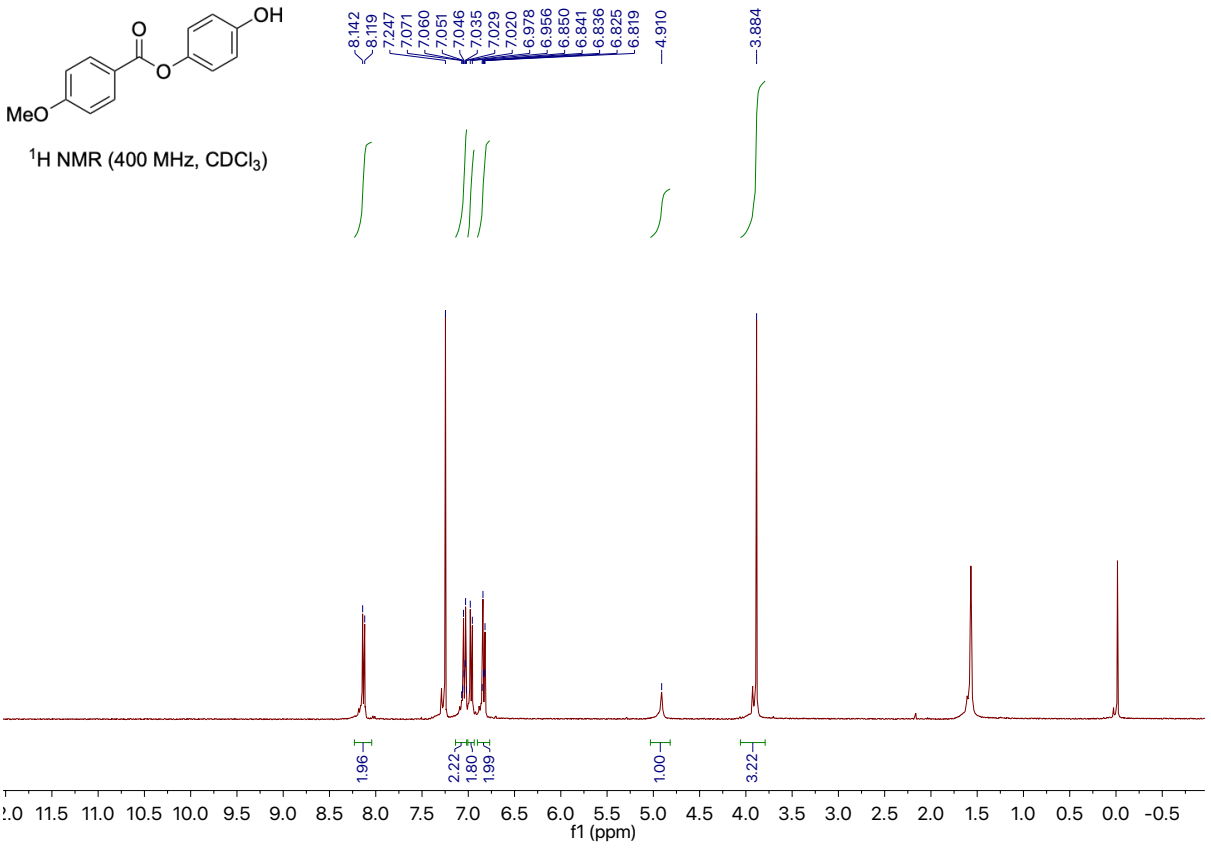
^{13}C NMR (100 MHz, $CDCl_3$)

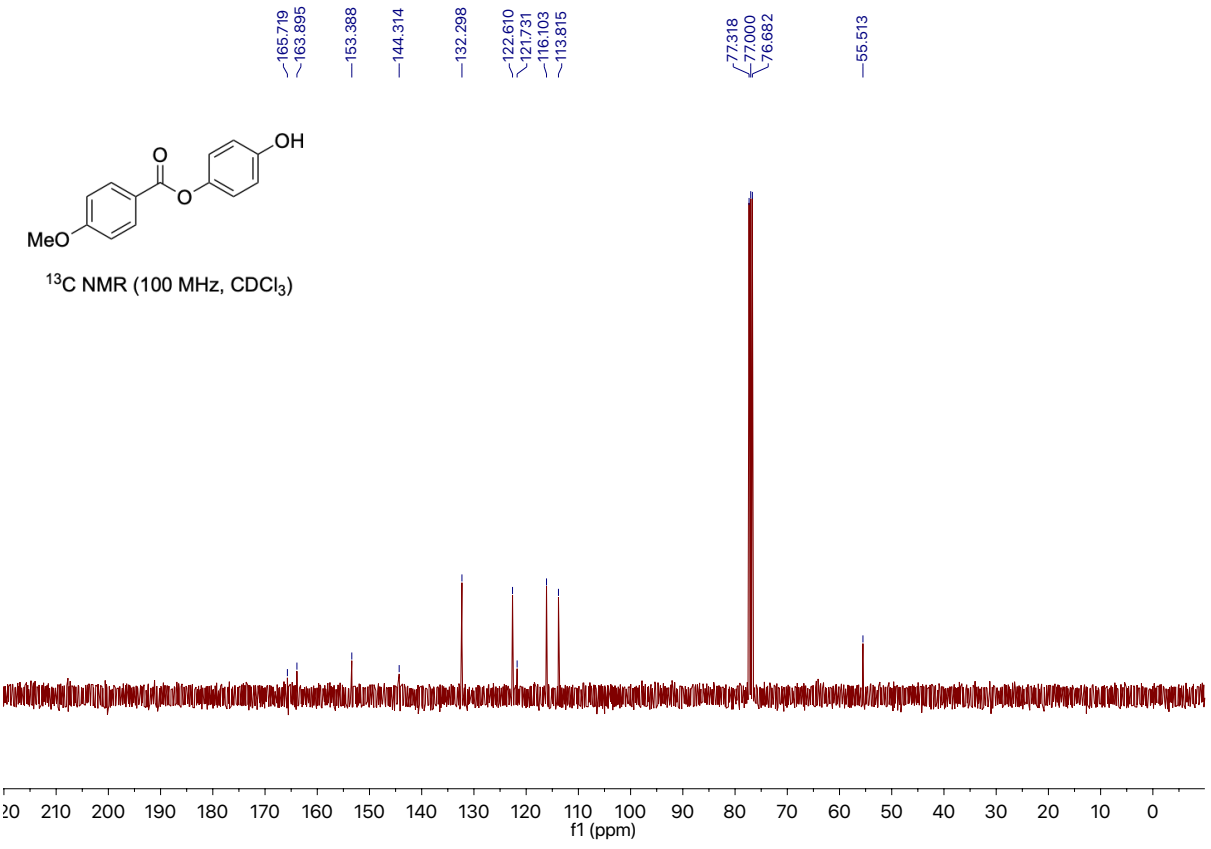


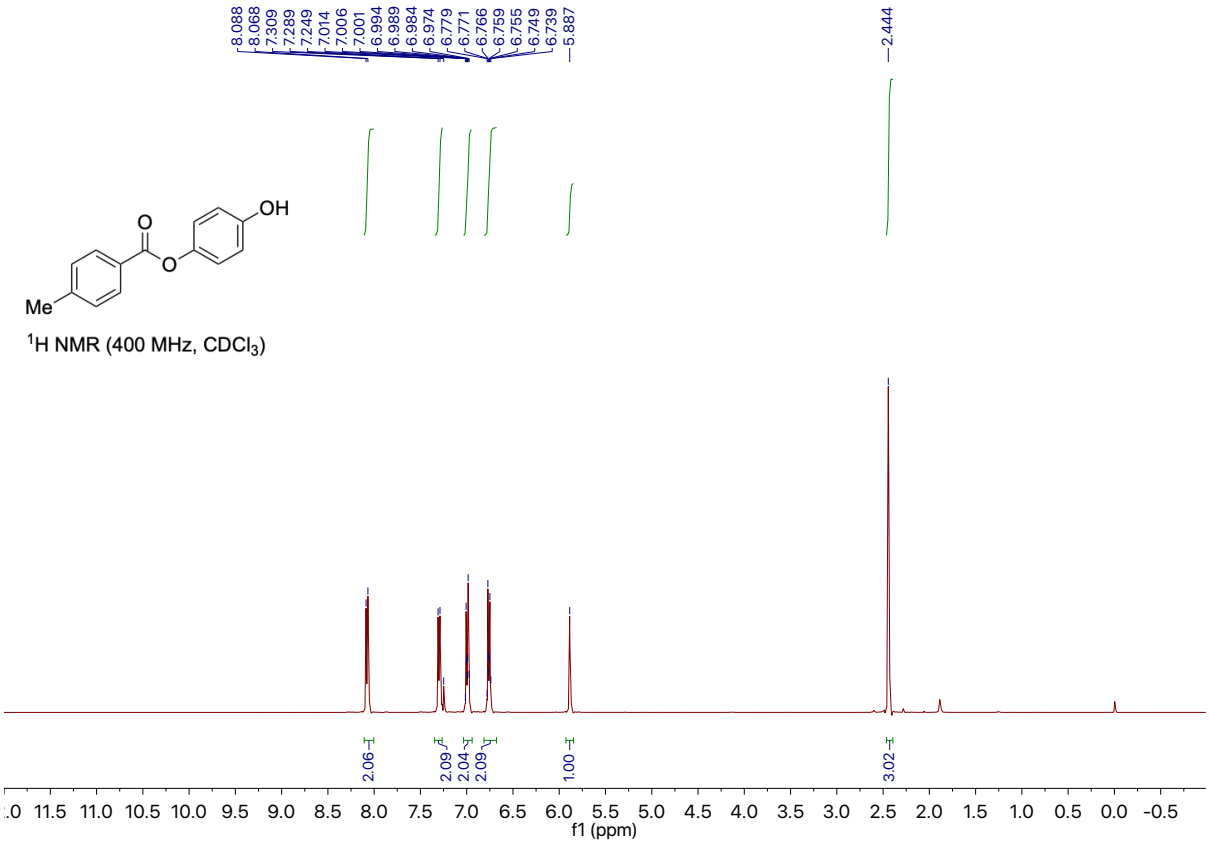
^{1}H NMR (400 MHz, $CDCl_3$)



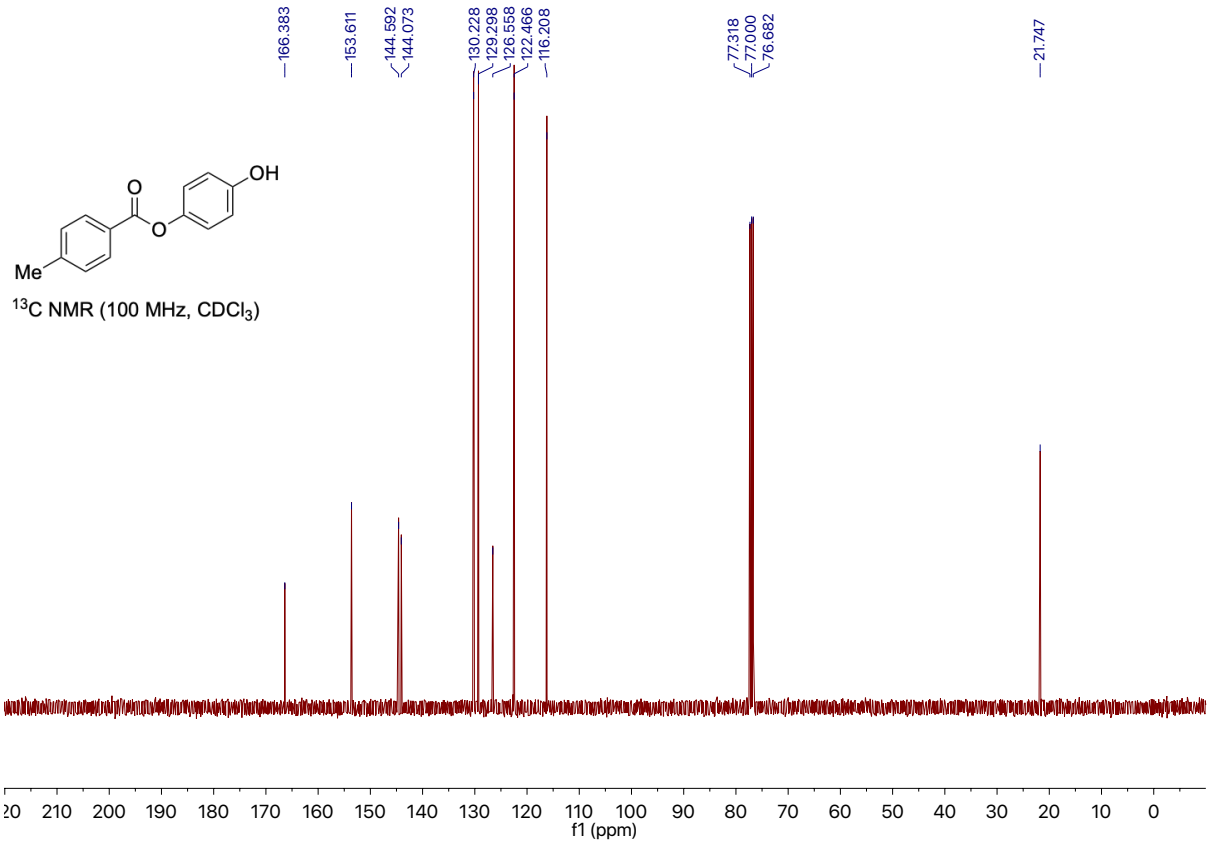
^{13}C NMR (100 MHz, $CDCl_3$)


OH
O
O
MeO
^{1}H NMR (400 MHz, $CDCl_3$)
8.142
8.119
7.247
7.071
7.060
7.051
7.046
7.035
7.029
7.020
6.978
6.956
6.850
6.841
6.836
6.825
6.819
4.910
3.884
1.96
2.22
1.80
1.99
1.00
3.22
f1 (ppm)

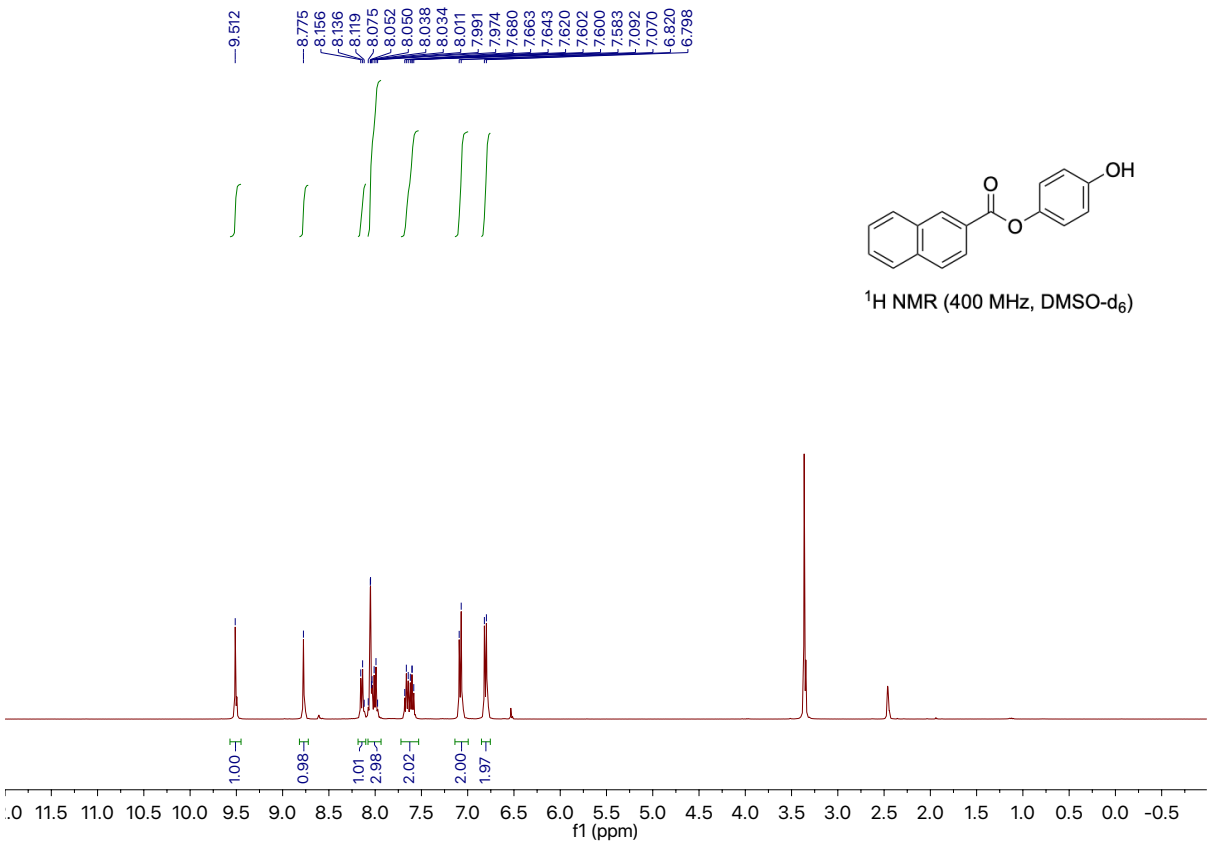

165.719
163.895
153.388
144.314
132.298
122.610
121.731
116.103
113.815
77.318
77.000
76.682
55.513
OH
O
O
MeO
^{13}C NMR (100 MHz, $CDCl_3$)
f1 (ppm)

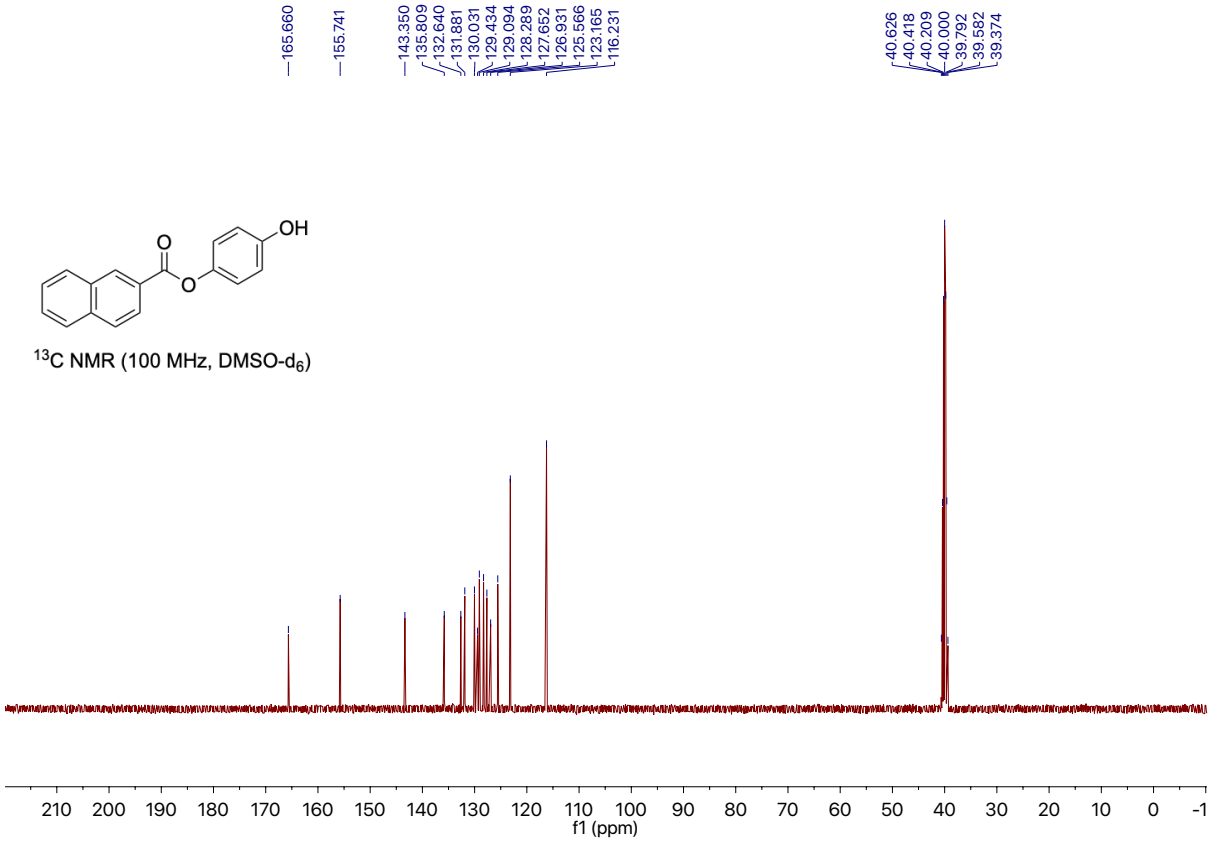


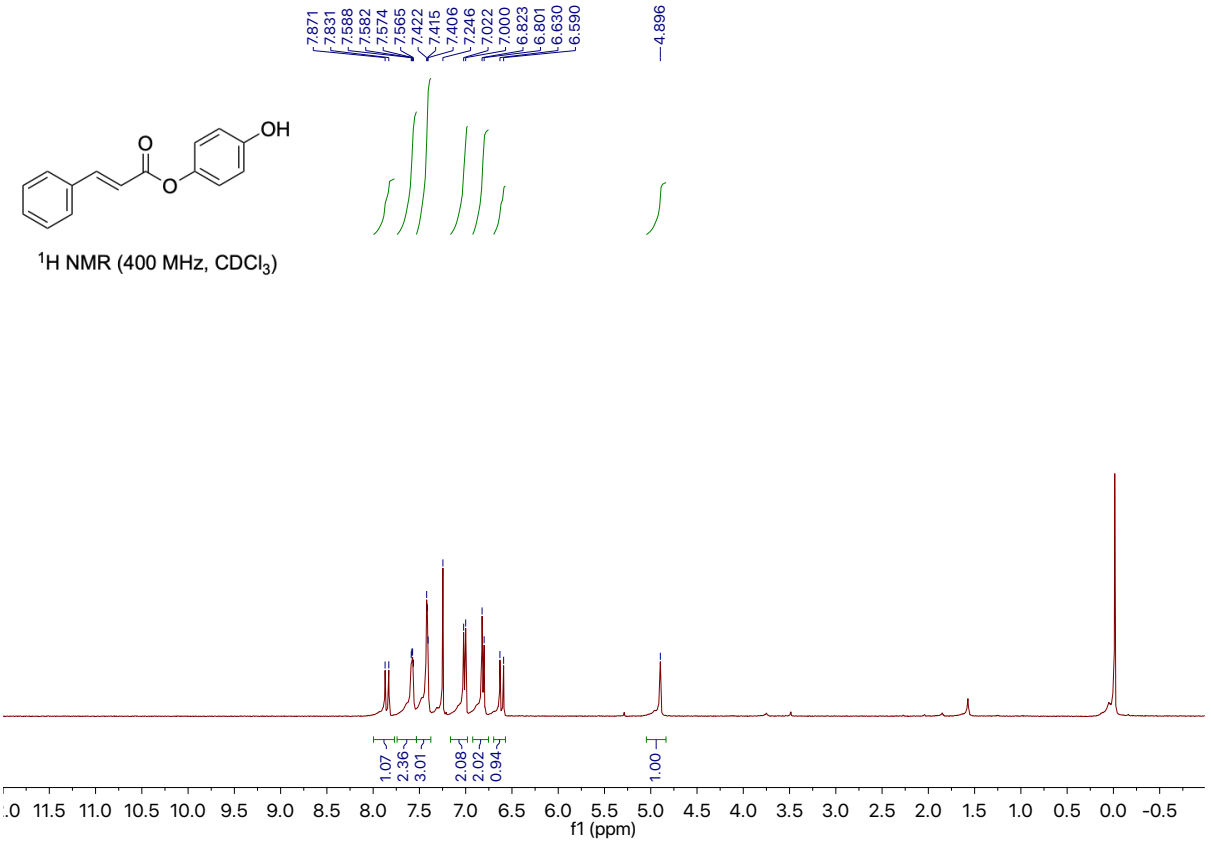
^{1}H NMR (400 MHz, $CDCl_3$)



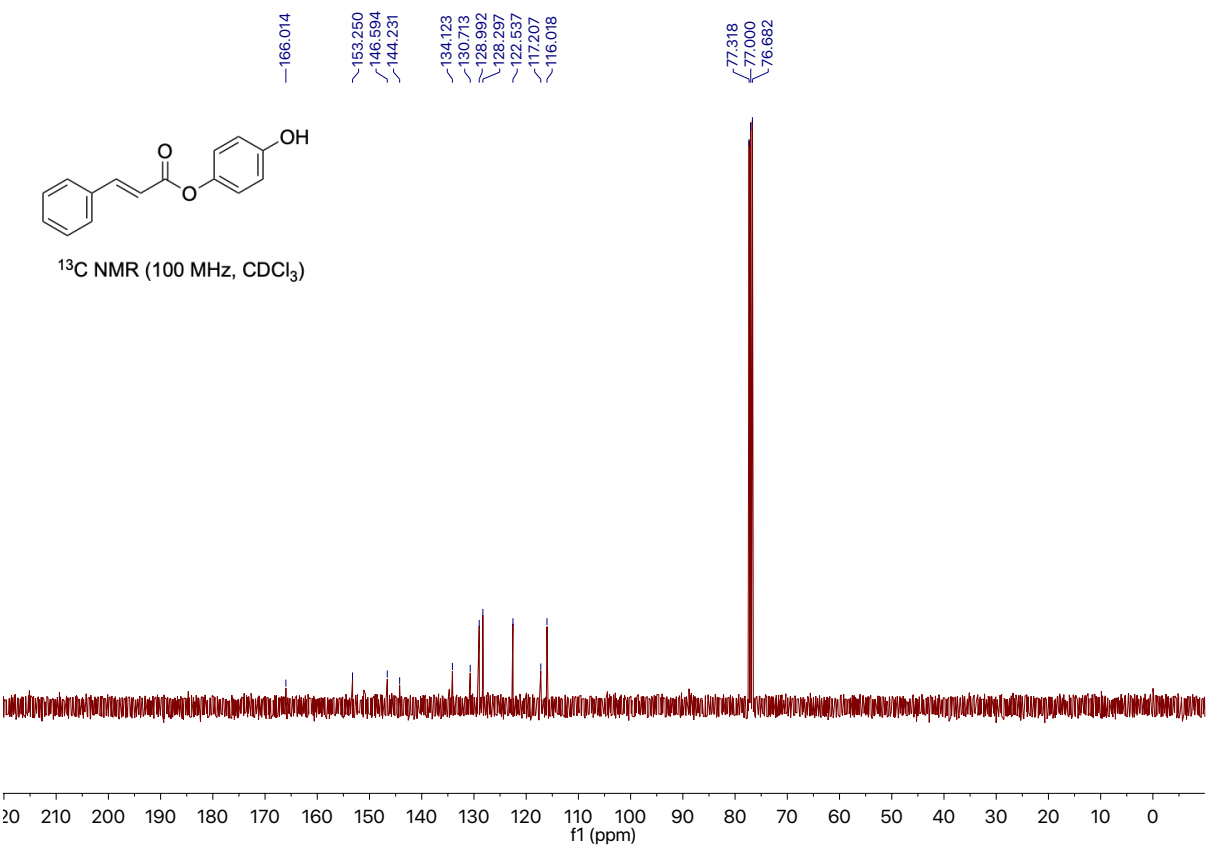
^{13}C NMR (100 MHz, $CDCl_3$)


9.512
8.775
8.156
8.136
8.119
8.075
8.052
8.050
8.038
8.034
8.011
7.991
7.974
7.680
7.663
7.643
7.620
7.602
7.600
7.583
7.092
7.070
6.820
6.798
OH
O
O
1H NMR (400 MHz, DMSO-d6)
1.00
0.98
1.01
2.98
2.02
2.00
1.97
f1 (ppm)

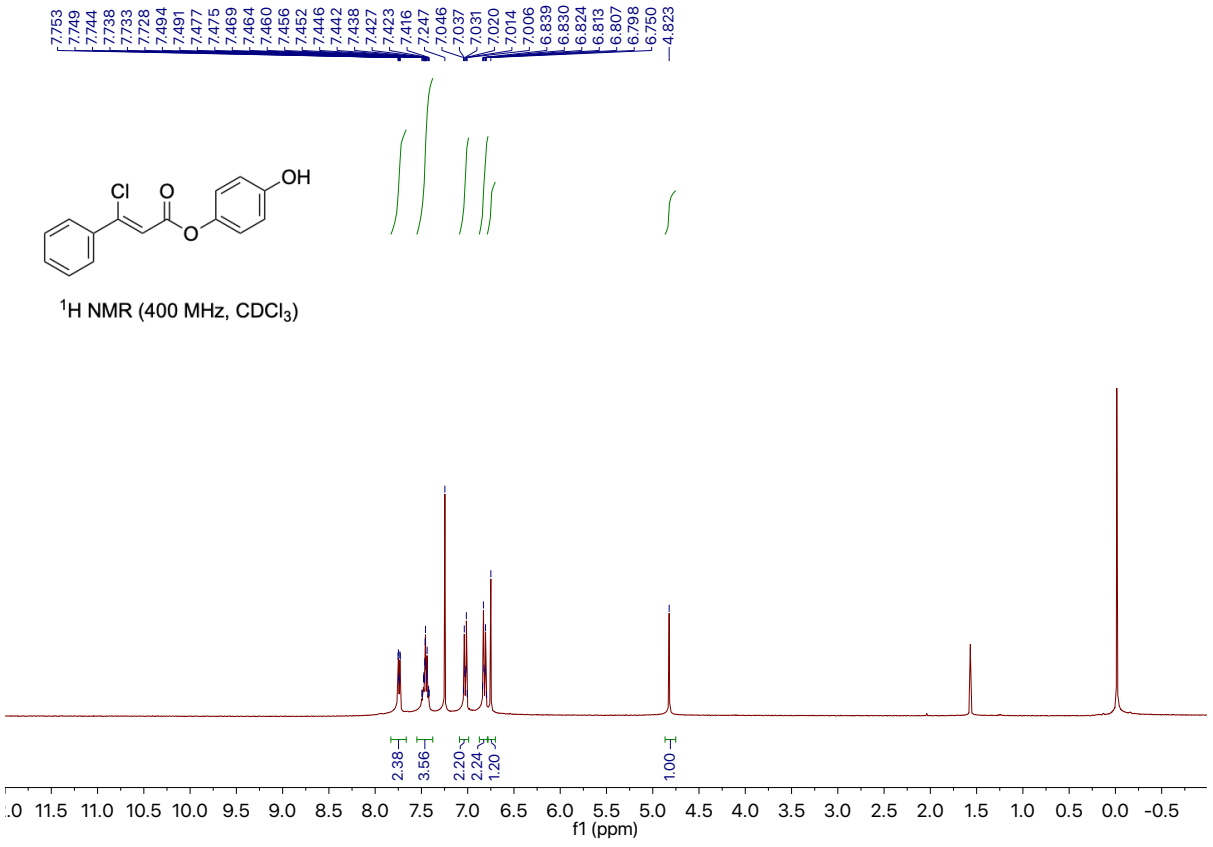

165.660
155.741
143.350
135.809
132.640
131.881
130.031
129.434
129.094
128.289
127.652
126.931
125.566
123.165
116.231
40.626
40.418
40.209
40.000
39.792
39.582
39.374
OH
O
O
13C NMR (100 MHz, DMSO-d6)
f1 (ppm)



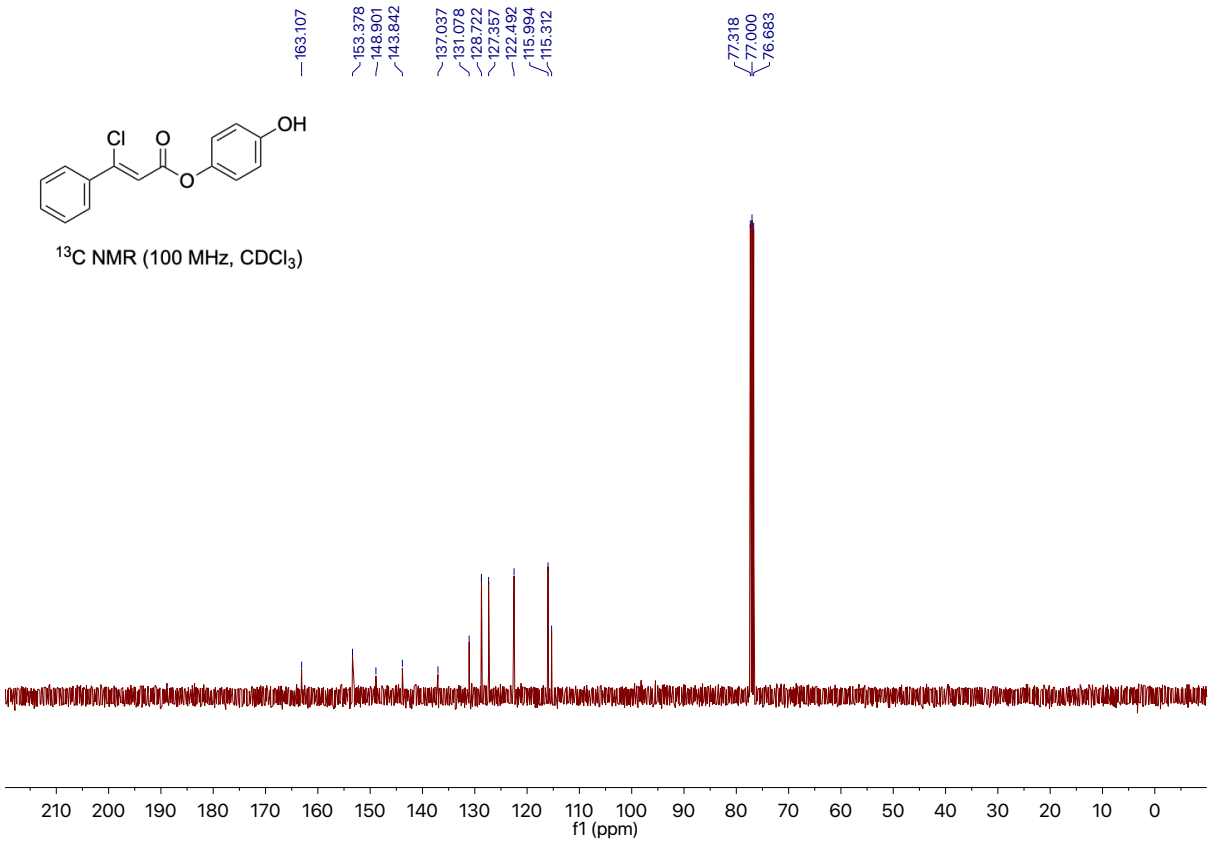
^{1}H NMR (400 MHz, $CDCl_3$)



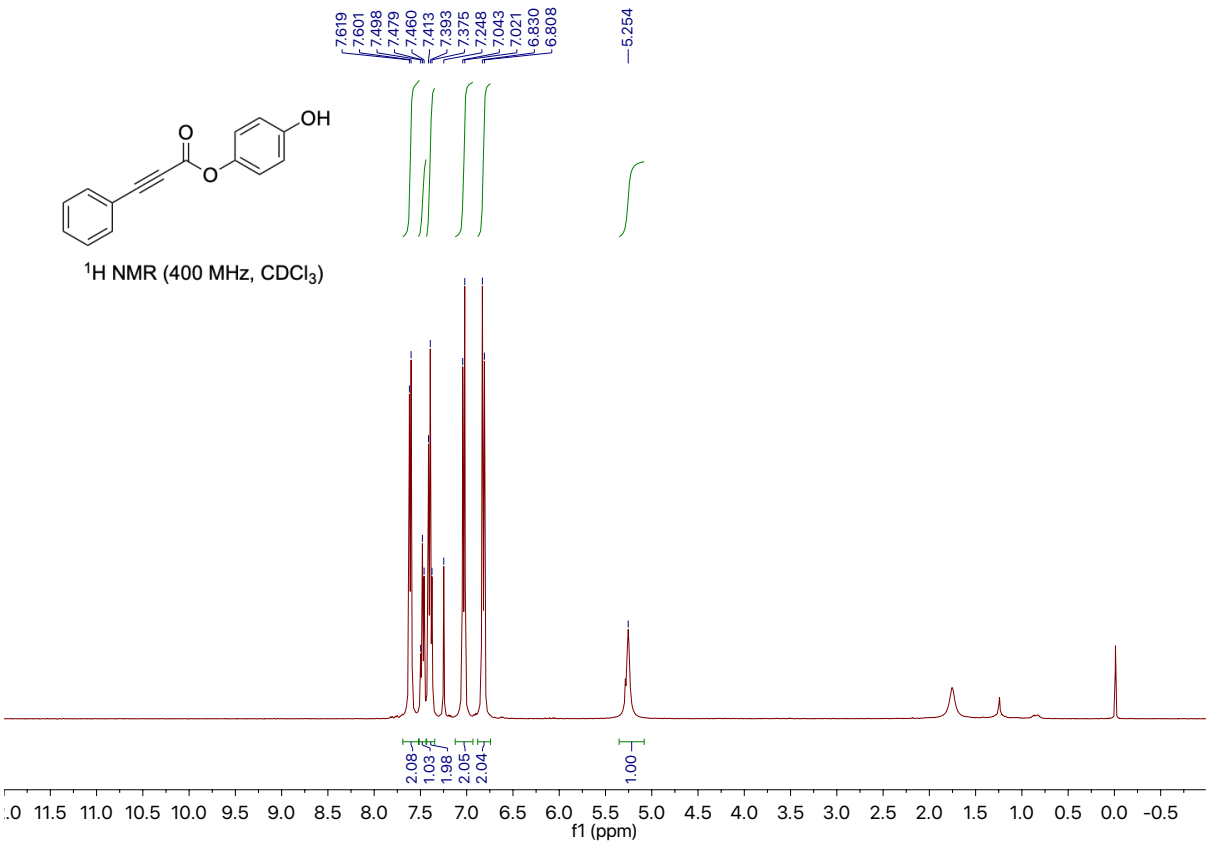
^{13}C NMR (100 MHz, $CDCl_3$)



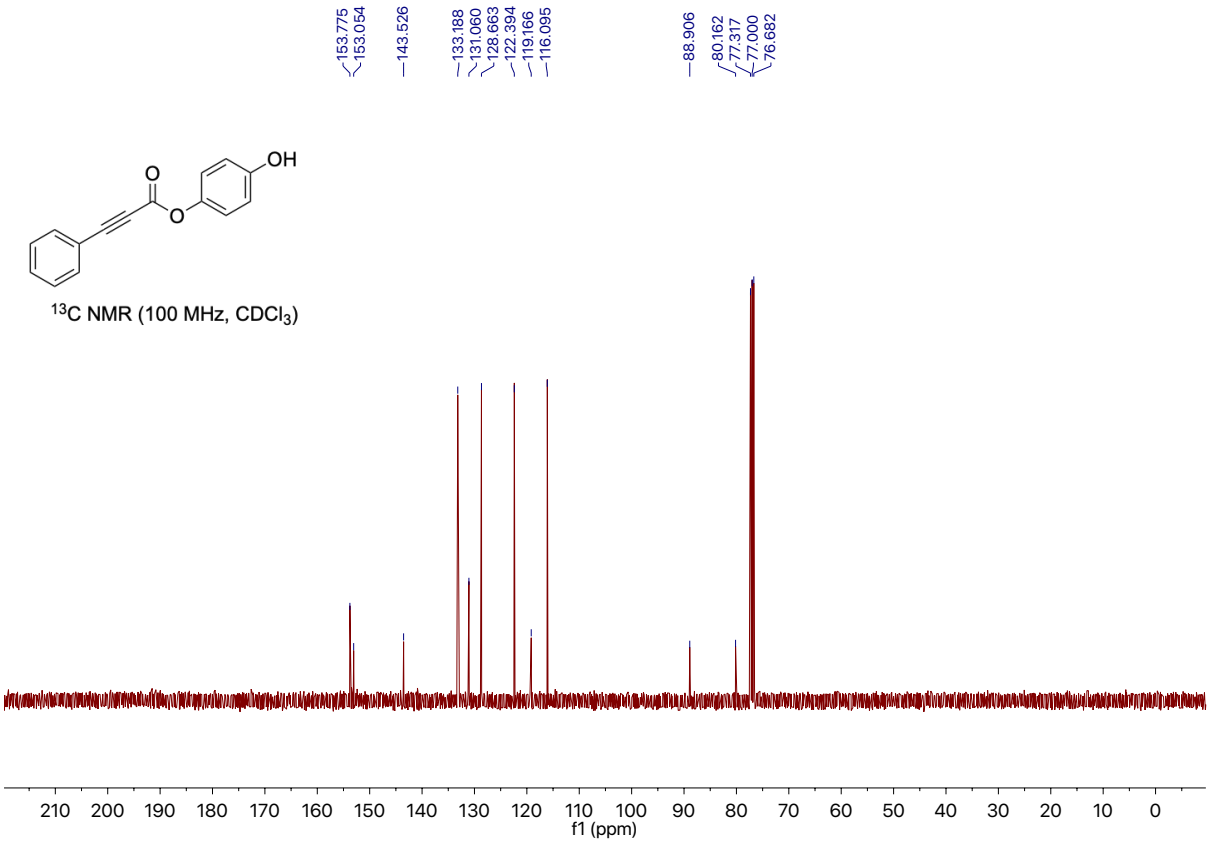
^{1}H NMR (400 MHz, $CDCl_3$)



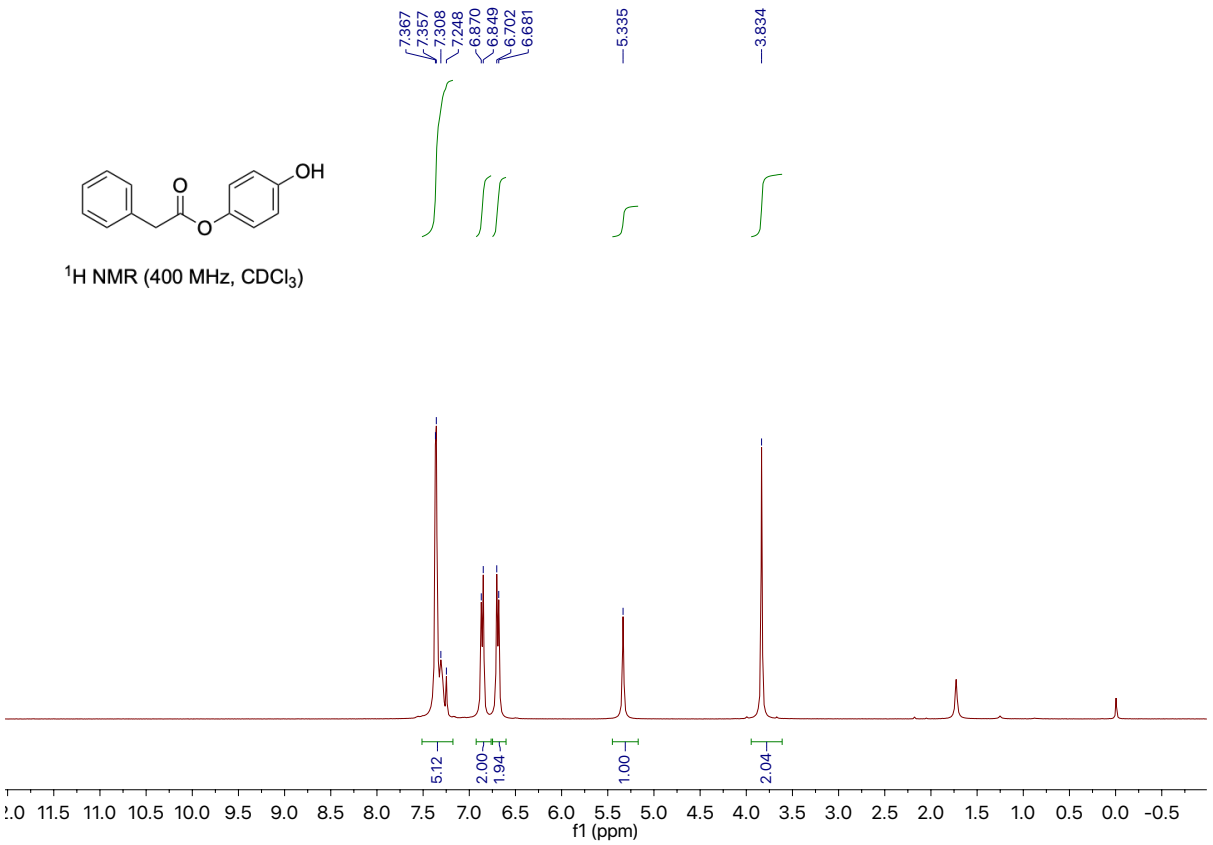
^{13}C NMR (100 MHz, $CDCl_3$)

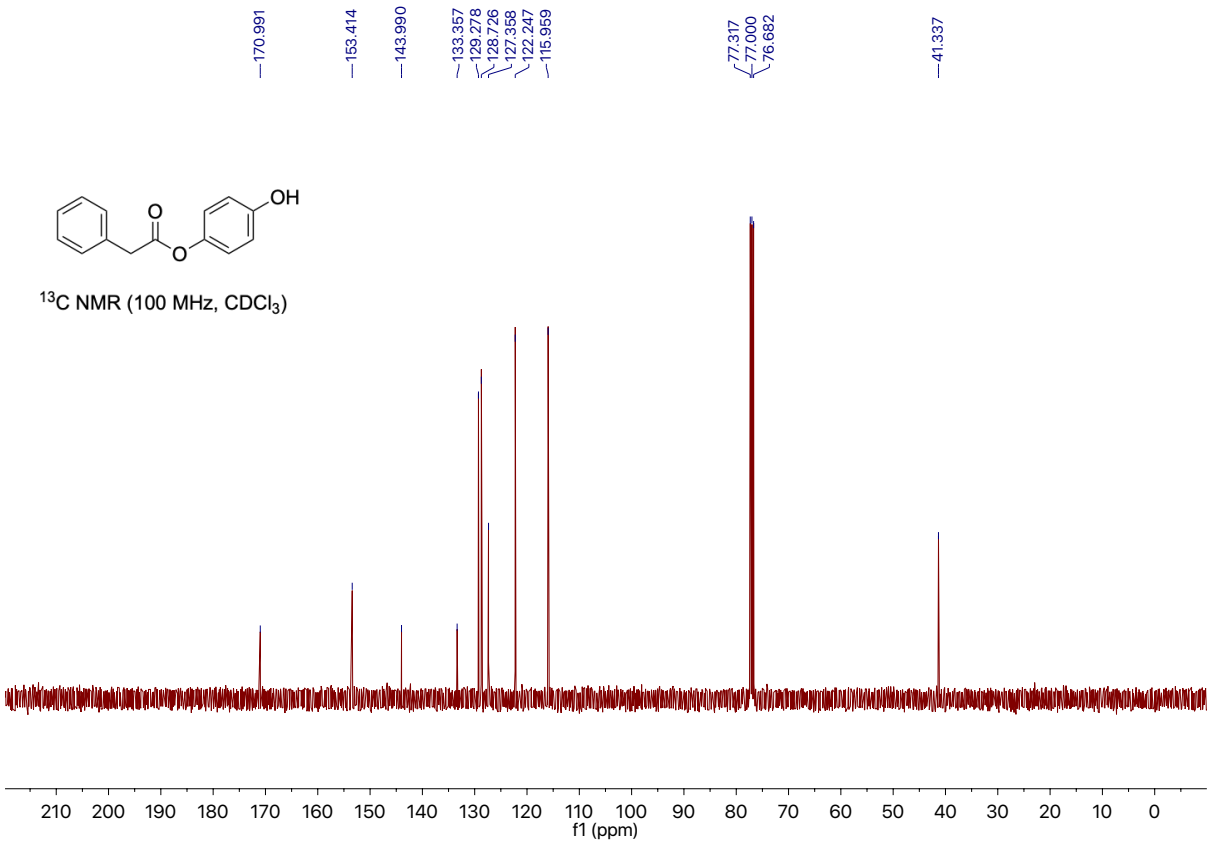


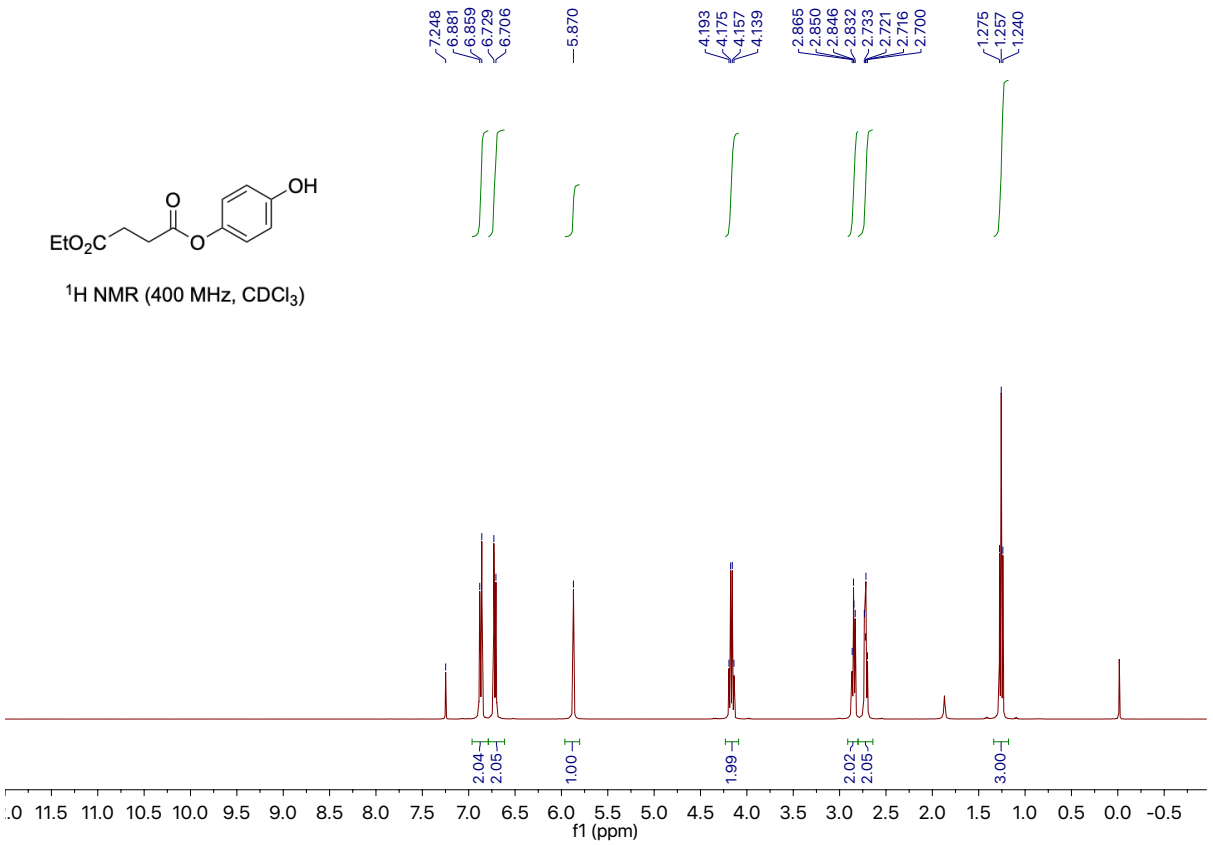
^{1}H NMR (400 MHz, $CDCl_3$)

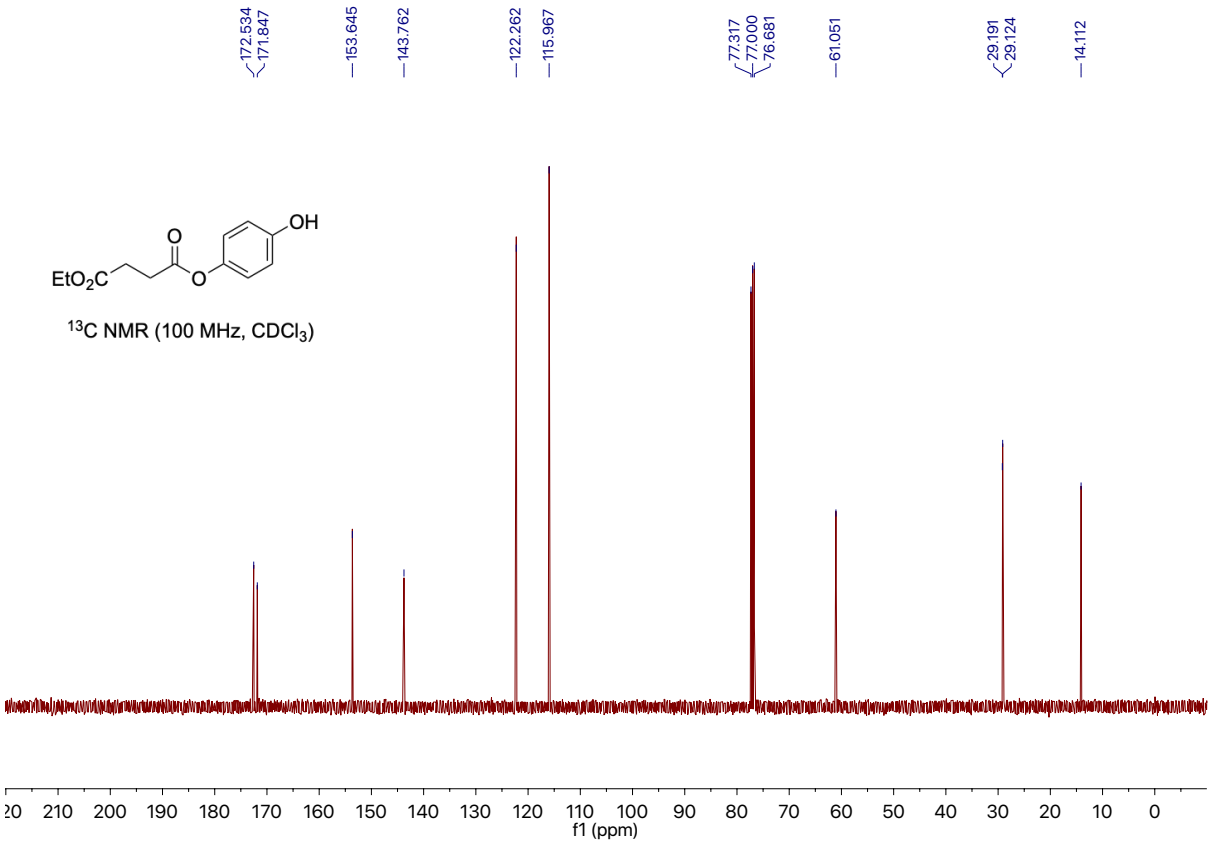


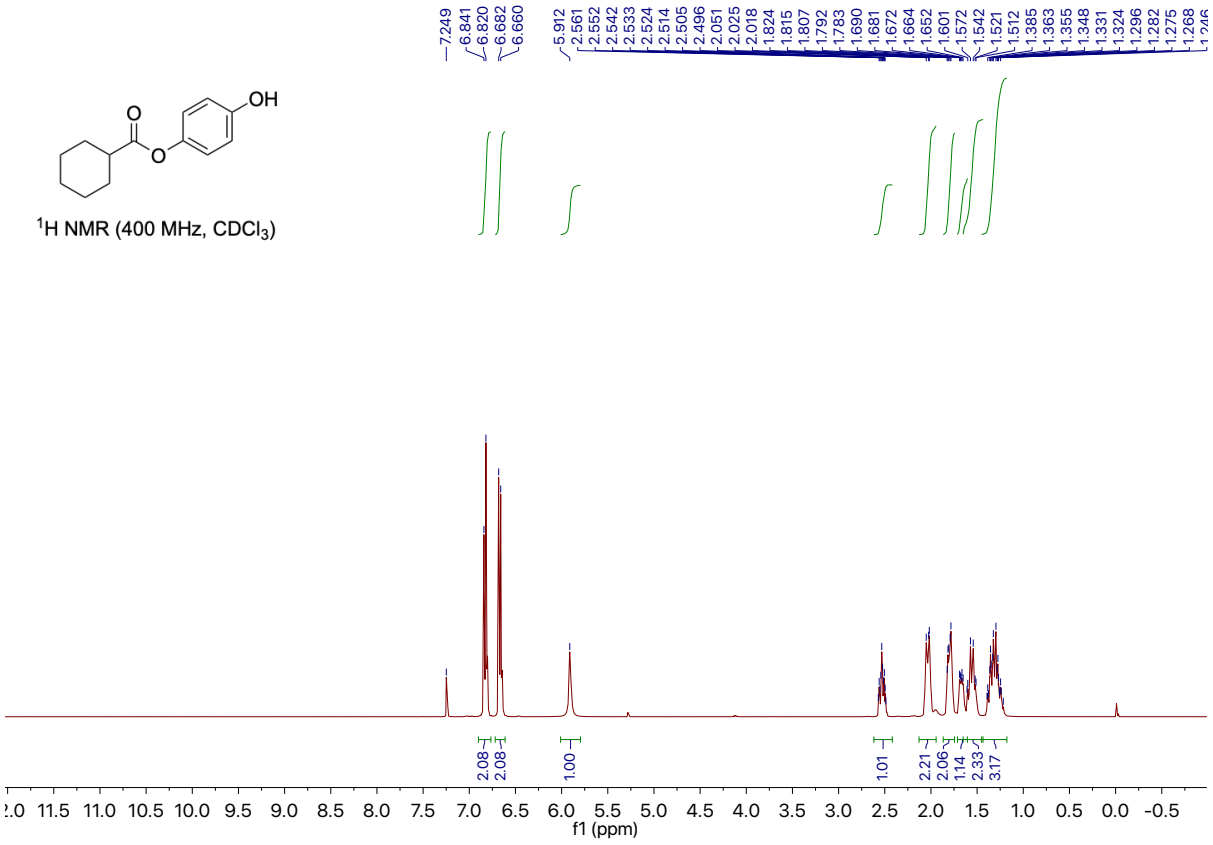
^{13}C NMR (100 MHz, $CDCl_3$)

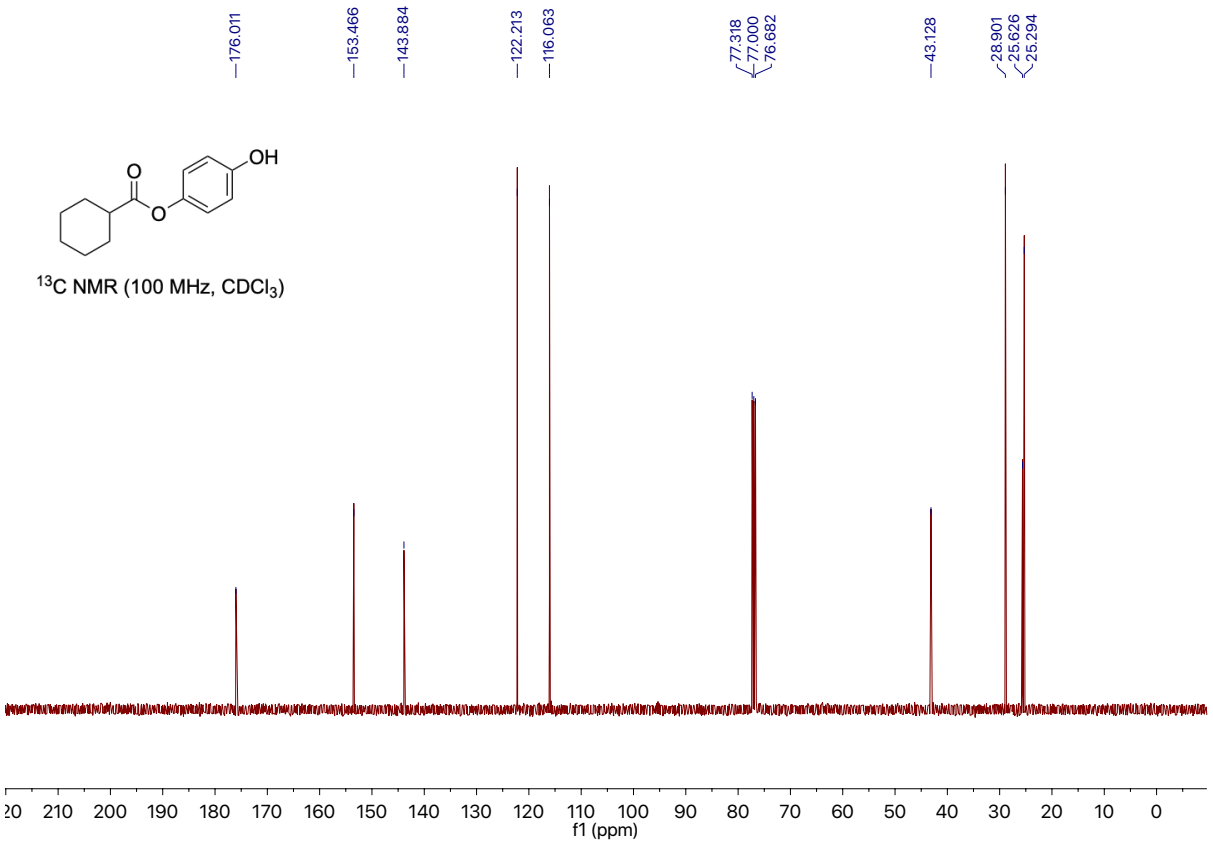

7.367
7.357
7.308
7.248
6.870
6.849
6.702
6.681
5.335
3.834
OH
O
O
^{1}H NMR (400 MHz, CDCl$_3$)
5.12
2.00
1.94
1.00
2.04
f1 (ppm)

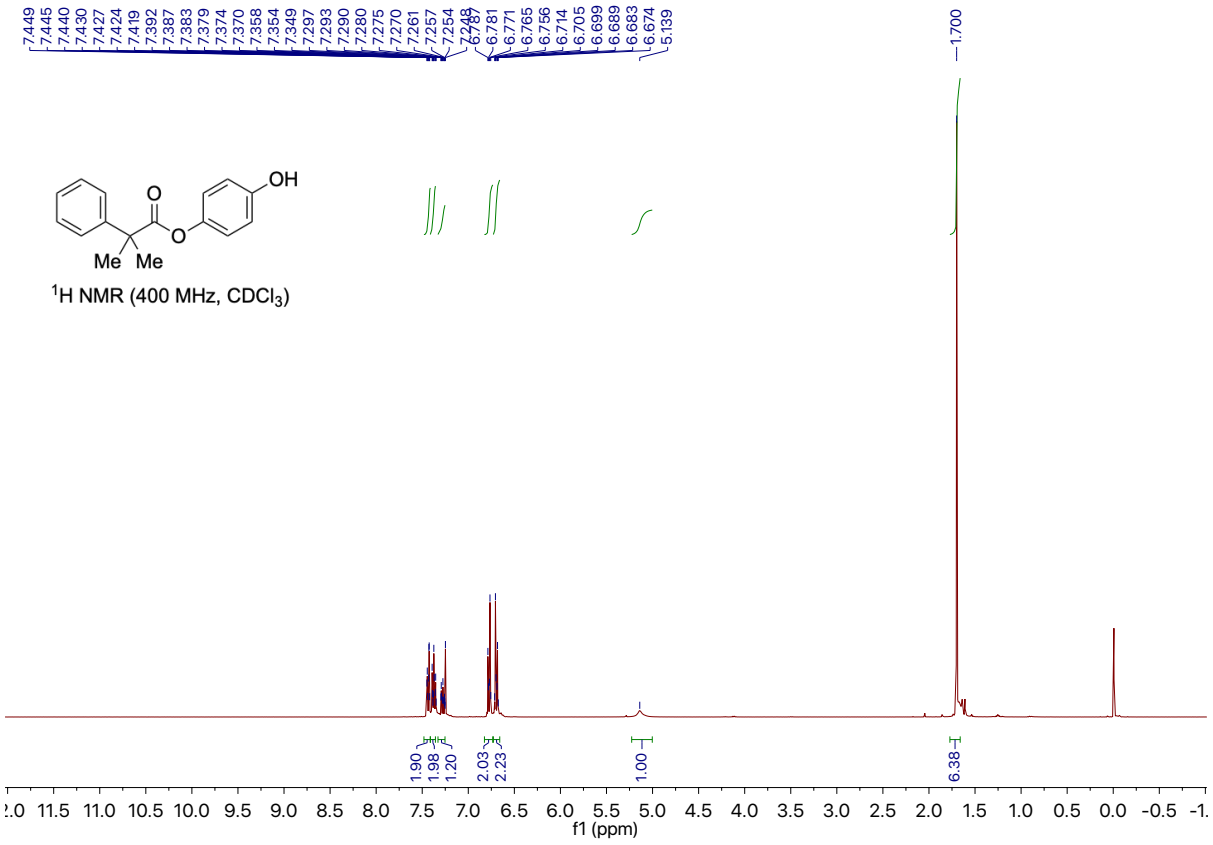

170.991
153.414
143.990
133.357
129.278
128.726
127.358
122.247
115.959
77.317
77.000
76.682
41.337
OH
O
O
^{13}C NMR (100 MHz, CDCl$_3$)
f1 (ppm)

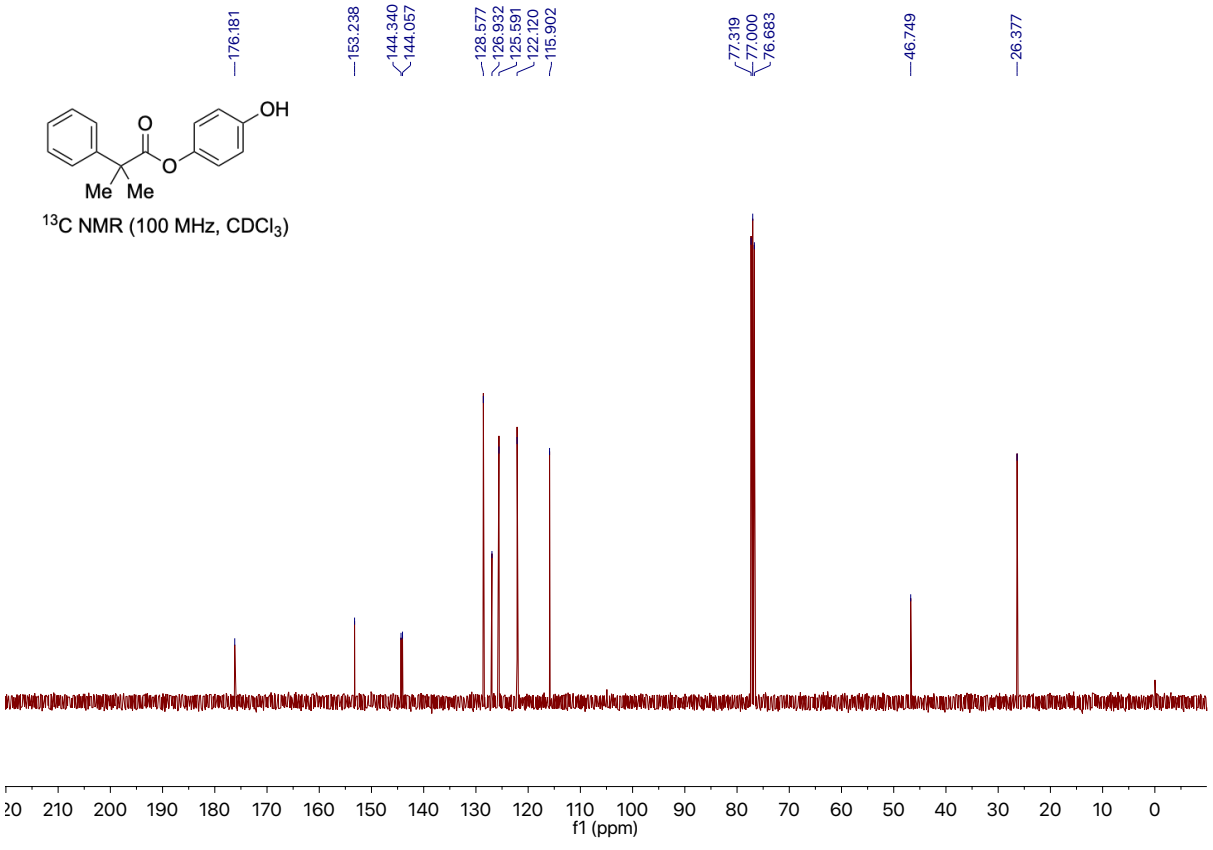

7.248
6.881
6.859
6.729
6.706
5.870
4.193
4.175
4.157
4.139
2.865
2.850
2.846
2.832
2.733
2.721
2.716
2.700
1.275
1.257
1.240
OH
O
O
EtO2C
1H NMR (400 MHz, CDCl3)
2.04
2.05
1.00
1.99
2.02
2.05
3.00
f1 (ppm)

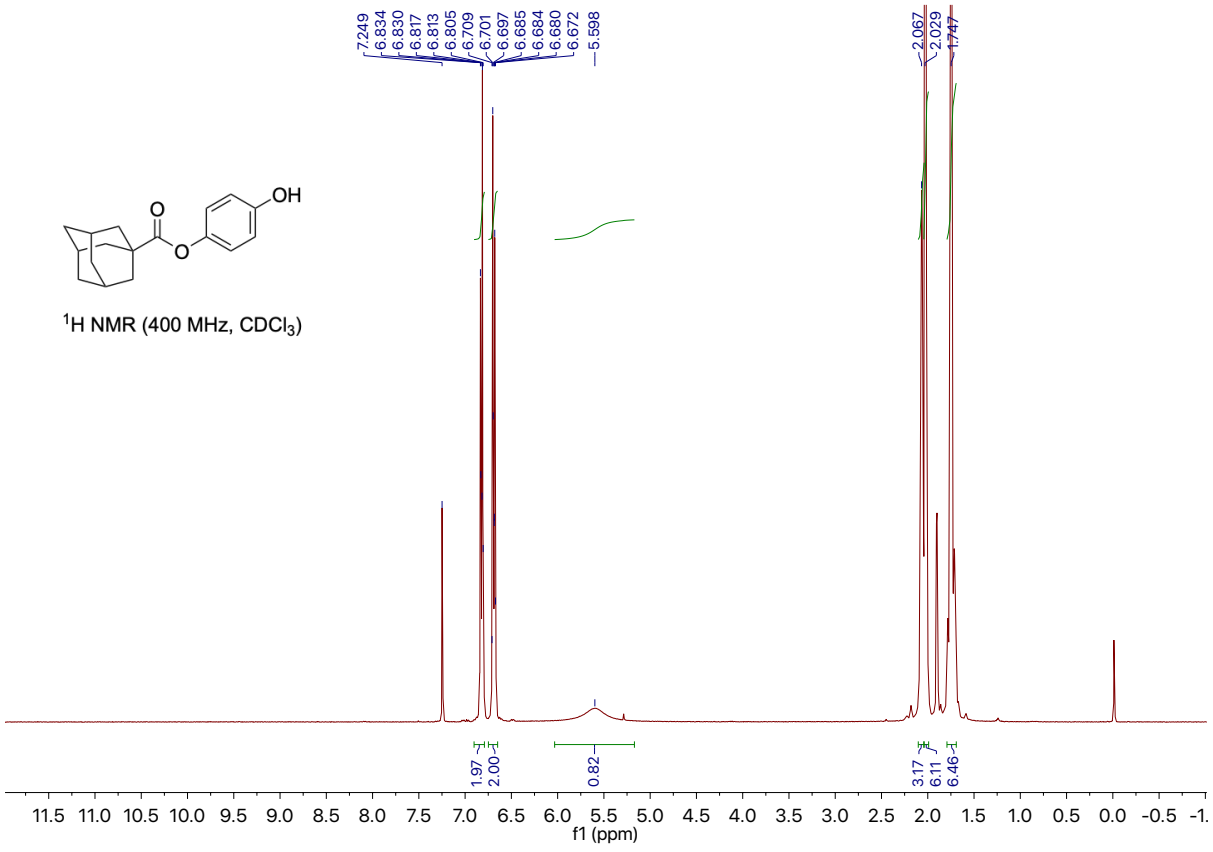

172.534
171.847
153.645
143.762
122.262
115.967
77.317
77.000
76.681
61.051
29.191
29.124
14.112
OH
O
O
EtO2C
13C NMR (100 MHz, CDCl3)
f1 (ppm)

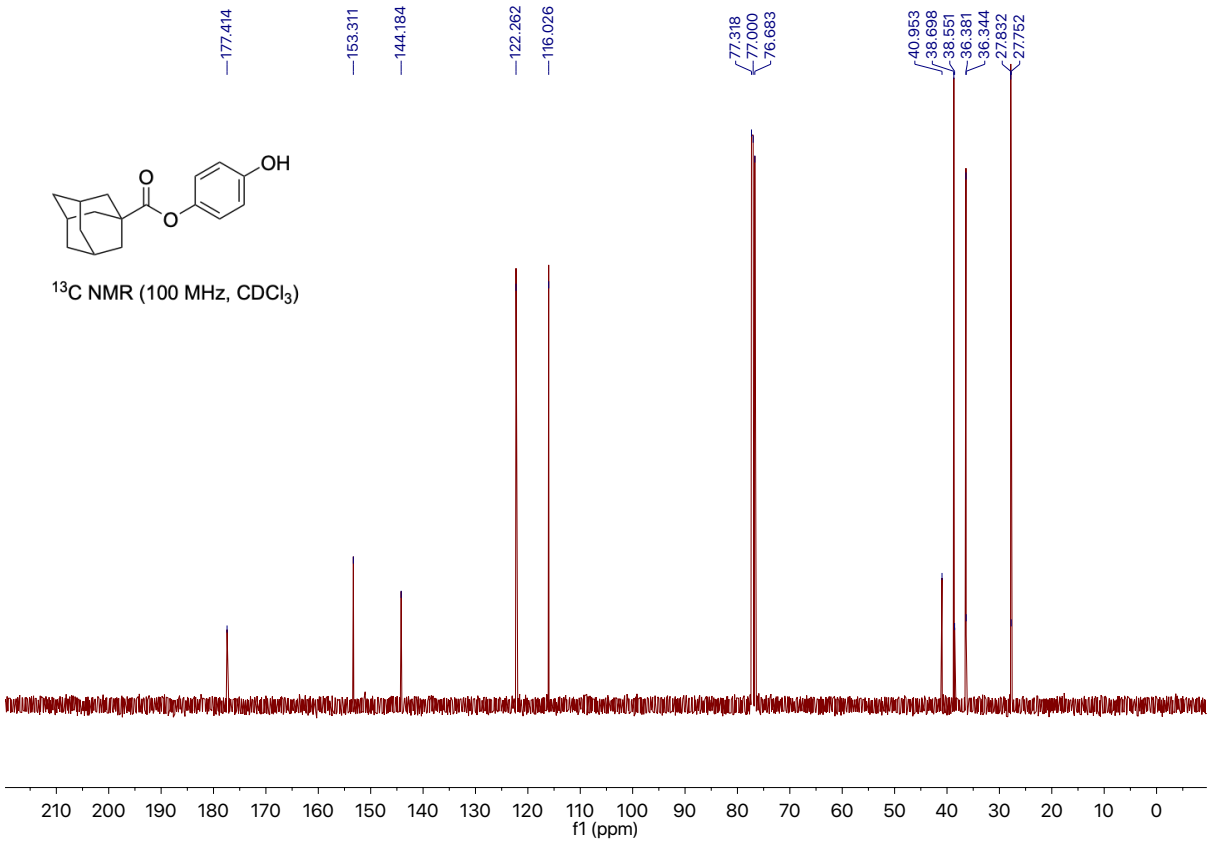

OH
O
O
^{1}H NMR (400 MHz, $CDCl_3$)
7.249
6.841
6.820
6.682
6.660
5.912
2.561
2.552
2.542
2.533
2.524
2.514
2.505
2.496
2.051
2.025
2.018
1.824
1.815
1.807
1.792
1.783
1.690
1.681
1.672
1.664
1.652
1.601
1.572
1.542
1.521
1.512
1.385
1.363
1.355
1.348
1.331
1.324
1.296
1.282
1.275
1.268
2.08
2.08
1.00
1.01
2.21
2.06
1.14
2.33
3.17
f1 (ppm)

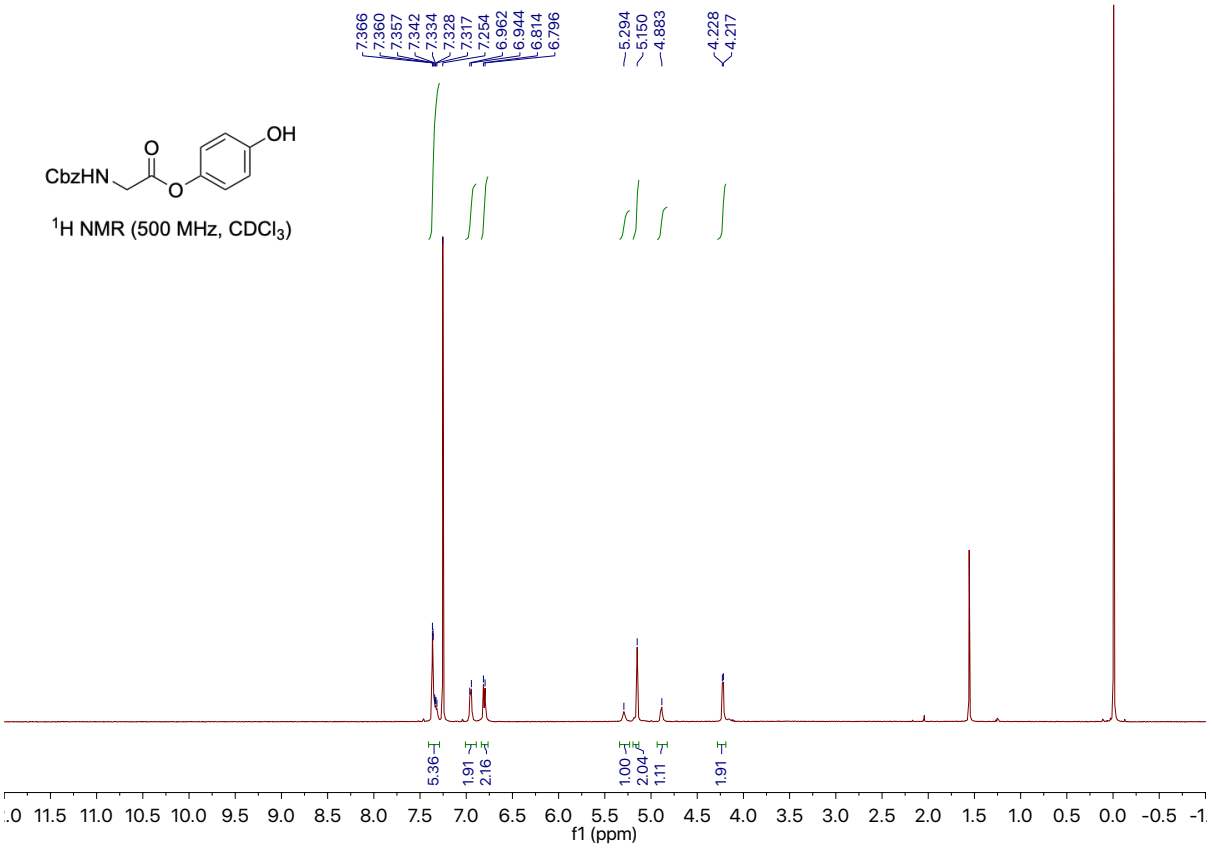

OH
O
O
^{13}C NMR (100 MHz, $CDCl_3$)
176.011
153.466
143.884
122.213
116.063
77.318
77.000
76.682
43.128
28.901
25.626
25.294
f1 (ppm)

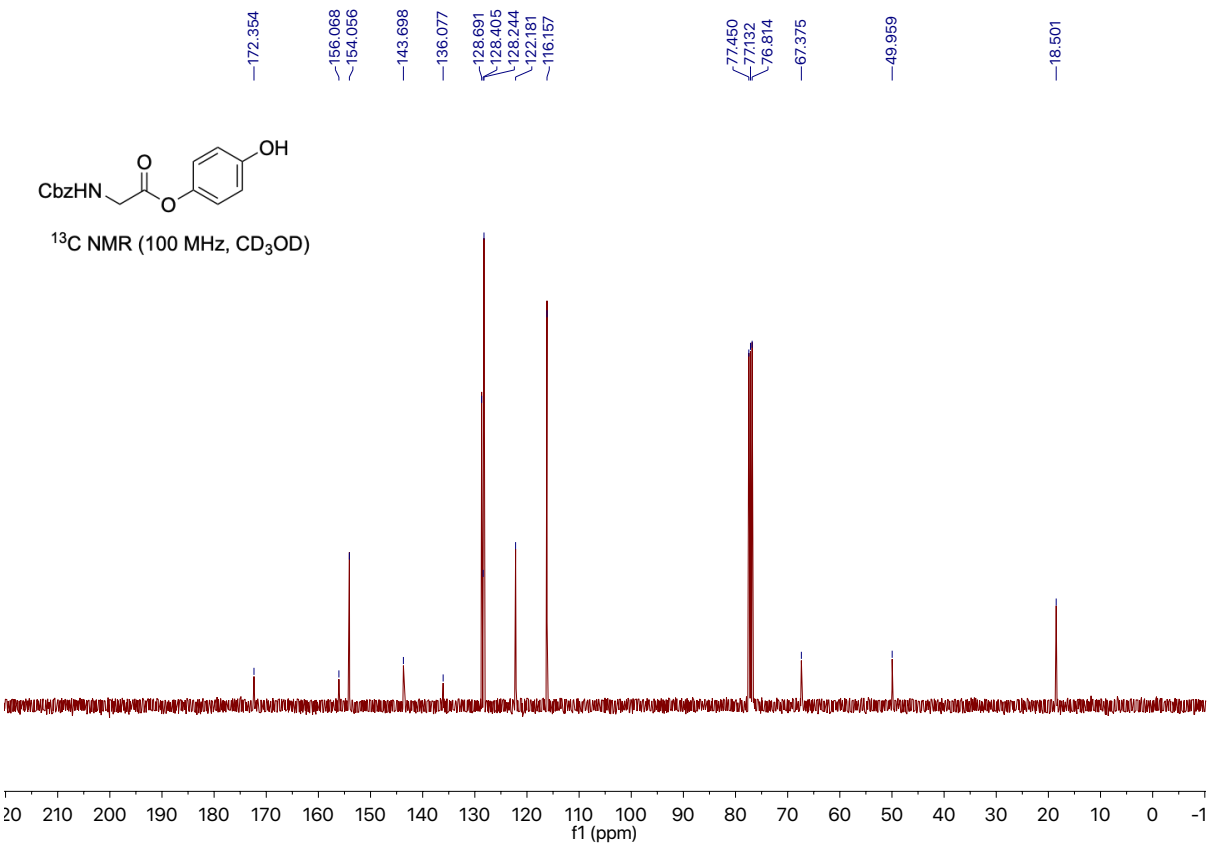

7.449
7.445
7.440
7.430
7.427
7.424
7.419
7.392
7.387
7.383
7.379
7.374
7.370
7.358
7.354
7.349
7.297
7.293
7.290
7.280
7.275
7.270
7.261
7.257
7.254
6.781
6.771
6.765
6.756
6.714
6.705
6.699
6.689
6.683
6.674
5.139
1.700
OH
O
O
Me Me
1H NMR (400 MHz, CDCl3)
1.90
1.98
1.20
2.03
2.23
1.00
6.38
f1 (ppm)

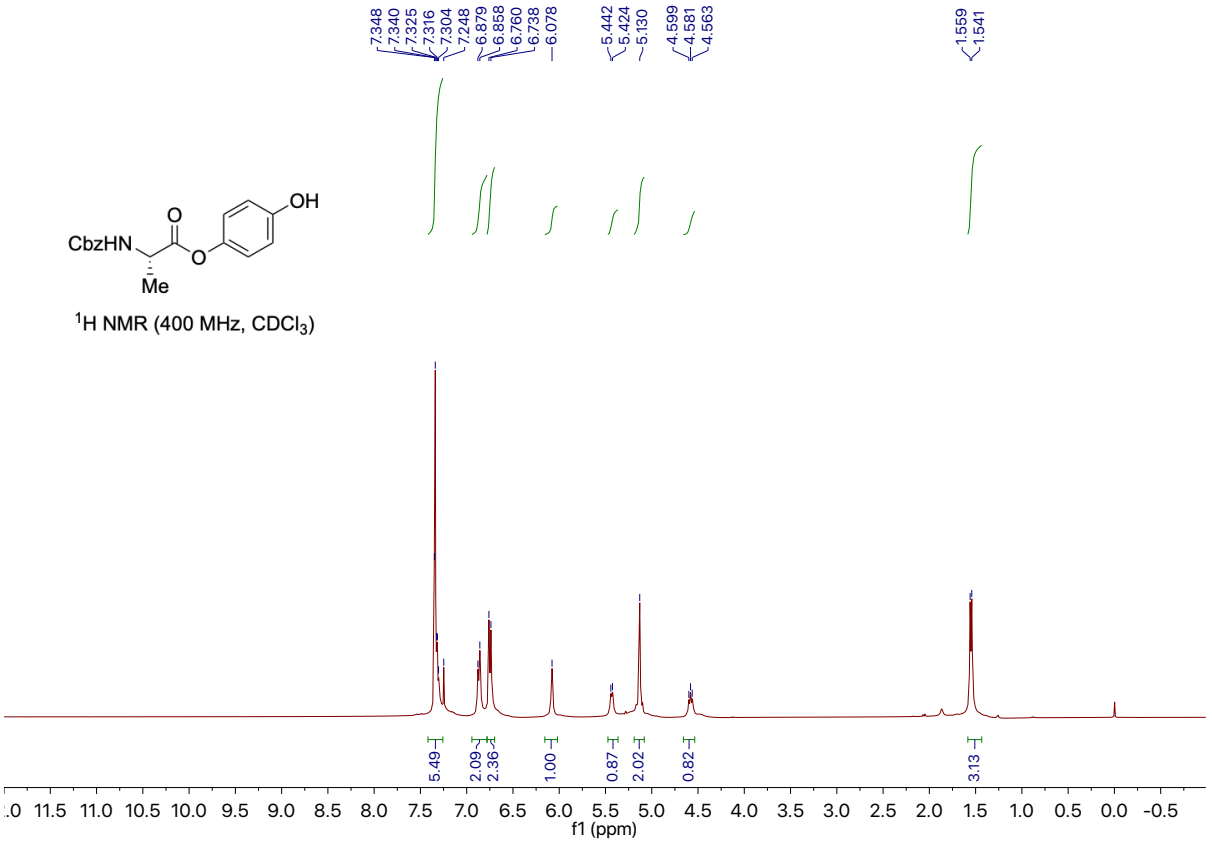

176.181
153.238
144.340
144.057
128.577
126.932
125.591
122.120
115.902
77.319
77.000
76.683
46.749
26.377
OH
O
O
Me Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)


7.249
6.834
6.830
6.817
6.813
6.805
6.709
6.701
6.697
6.685
6.684
6.680
6.672
5.598
2.067
2.029
1.747
OH
O
O
1H NMR (400 MHz, CDCl3)
1.97
2.00
0.82
3.17
6.11
6.46
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)

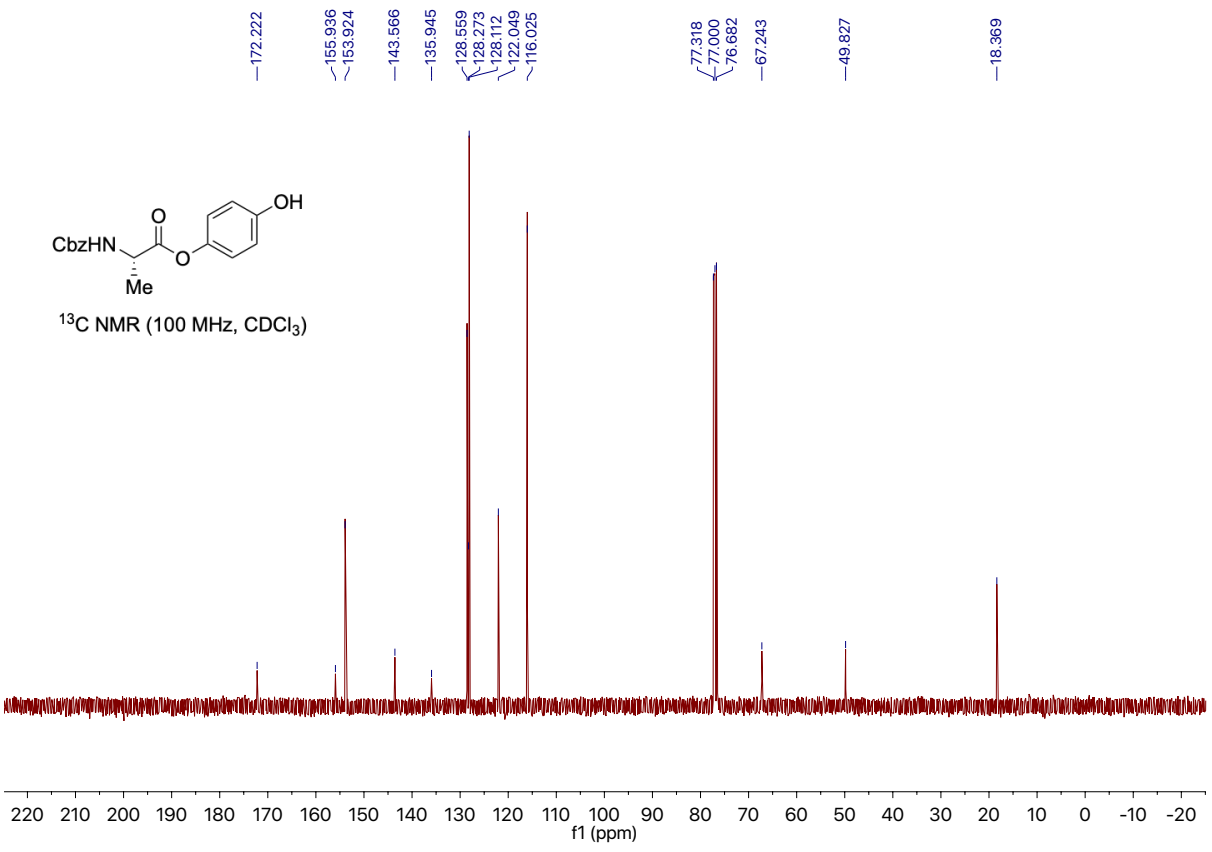

177.414
153.311
144.184
122.262
116.026
77.318
77.000
76.683
40.953
38.698
38.551
36.381
36.344
27.832
27.752
OH
O
O
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.366
7.360
7.357
7.342
7.334
7.328
7.317
7.254
6.962
6.944
6.814
6.796
5.294
5.150
4.883
4.228
4.217
OH
O
CbzHN
O
^{1}H NMR (500 MHz, $CDCl_3$)
5.36
1.91
2.16
1.00
2.04
1.11
1.91
f1 (ppm)

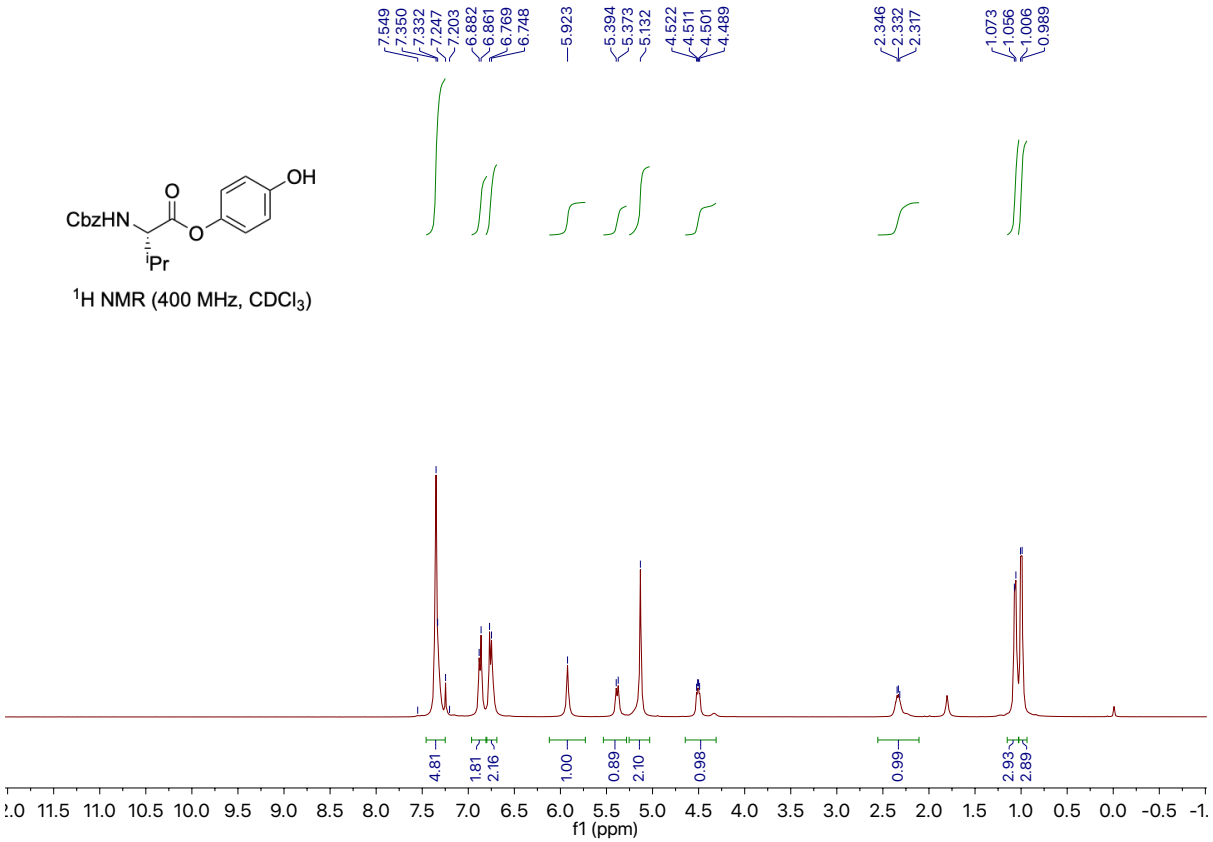

172.354
156.068
154.056
143.698
136.077
128.691
128.405
128.244
122.181
116.157
77.450
77.132
76.814
67.375
49.959
18.501
OH
O
CbzHN
O
^{13}C NMR (100 MHz, CD_3OD)
f1 (ppm)



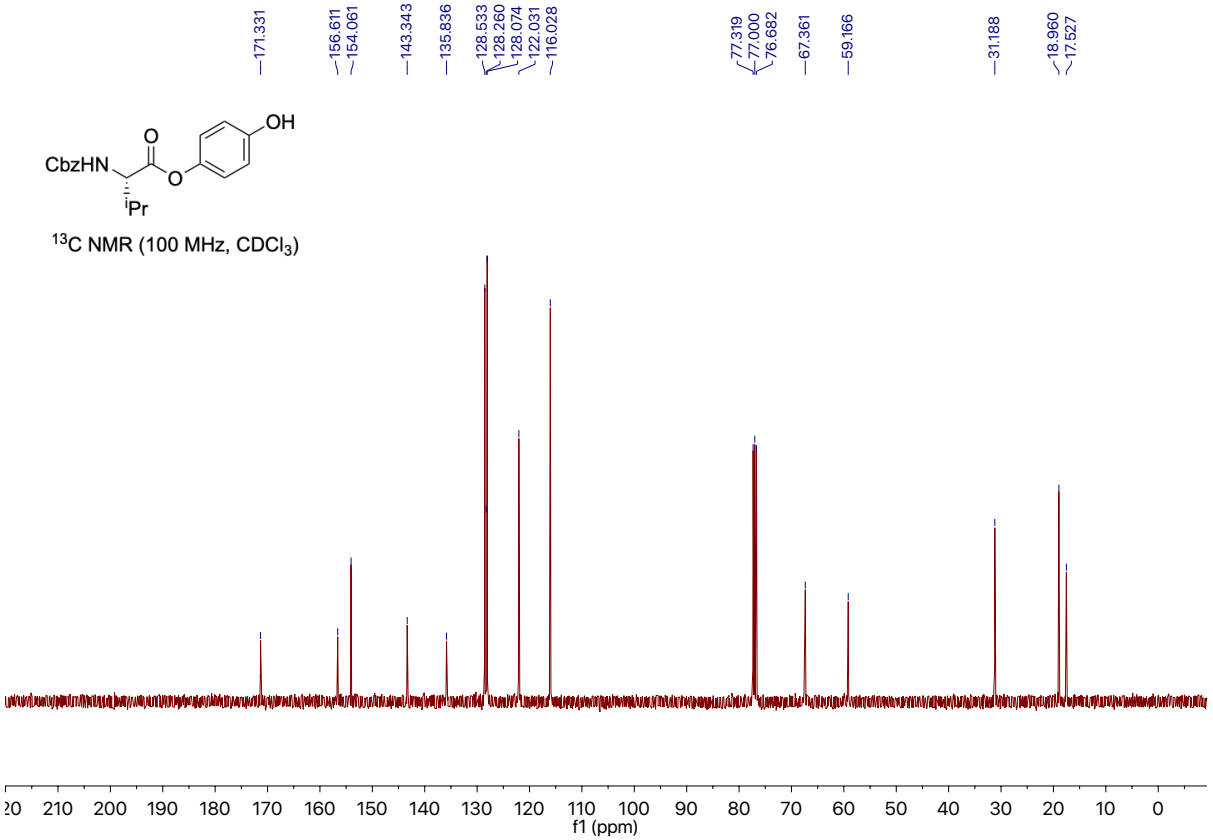
^{1}H NMR (400 MHz, $CDCl_3$)



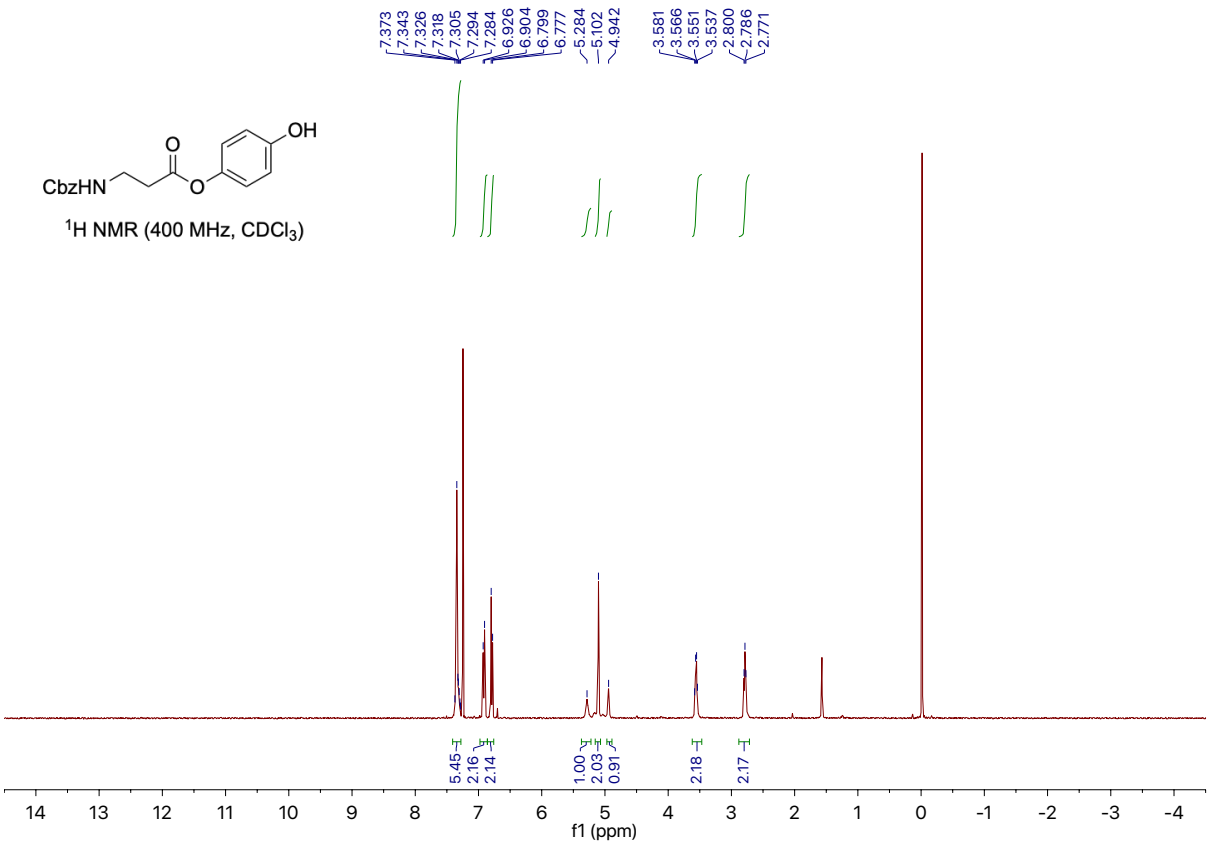
^{13}C NMR (100 MHz, $CDCl_3$)

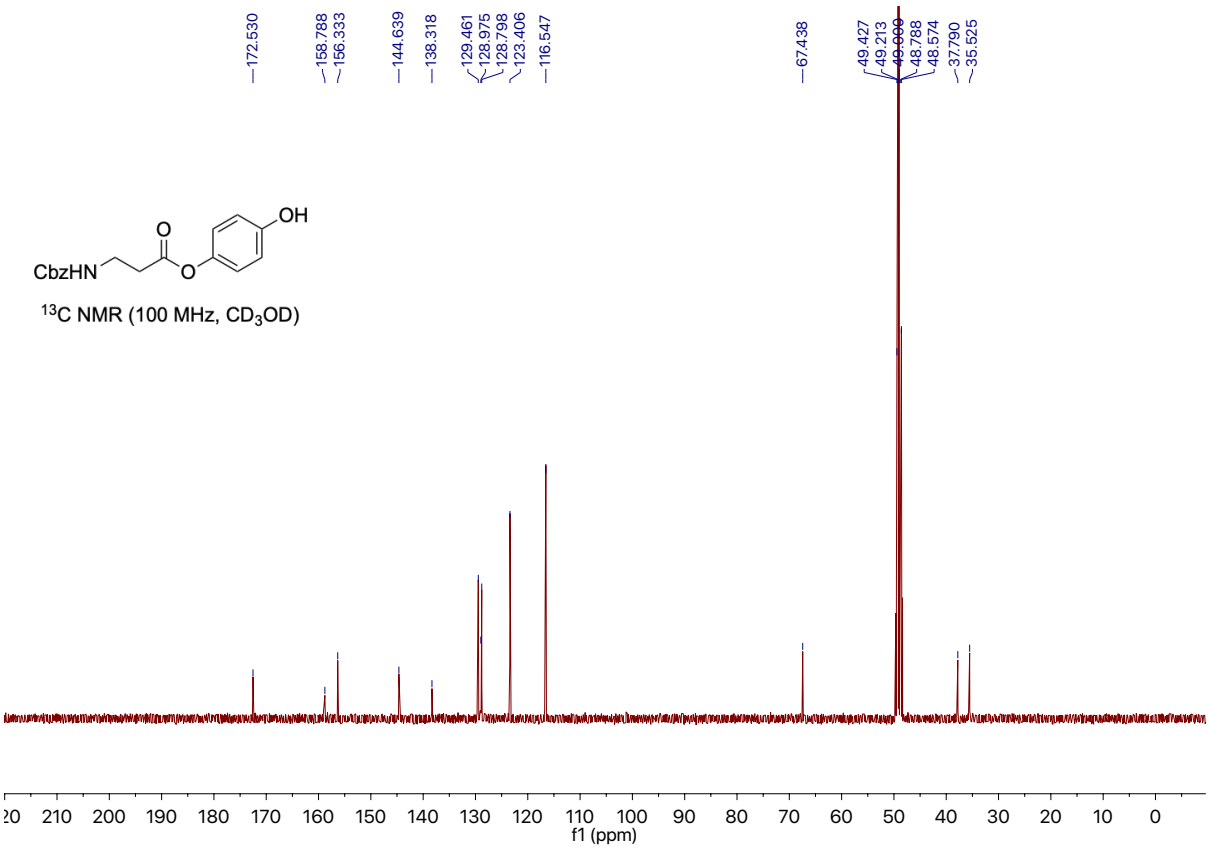


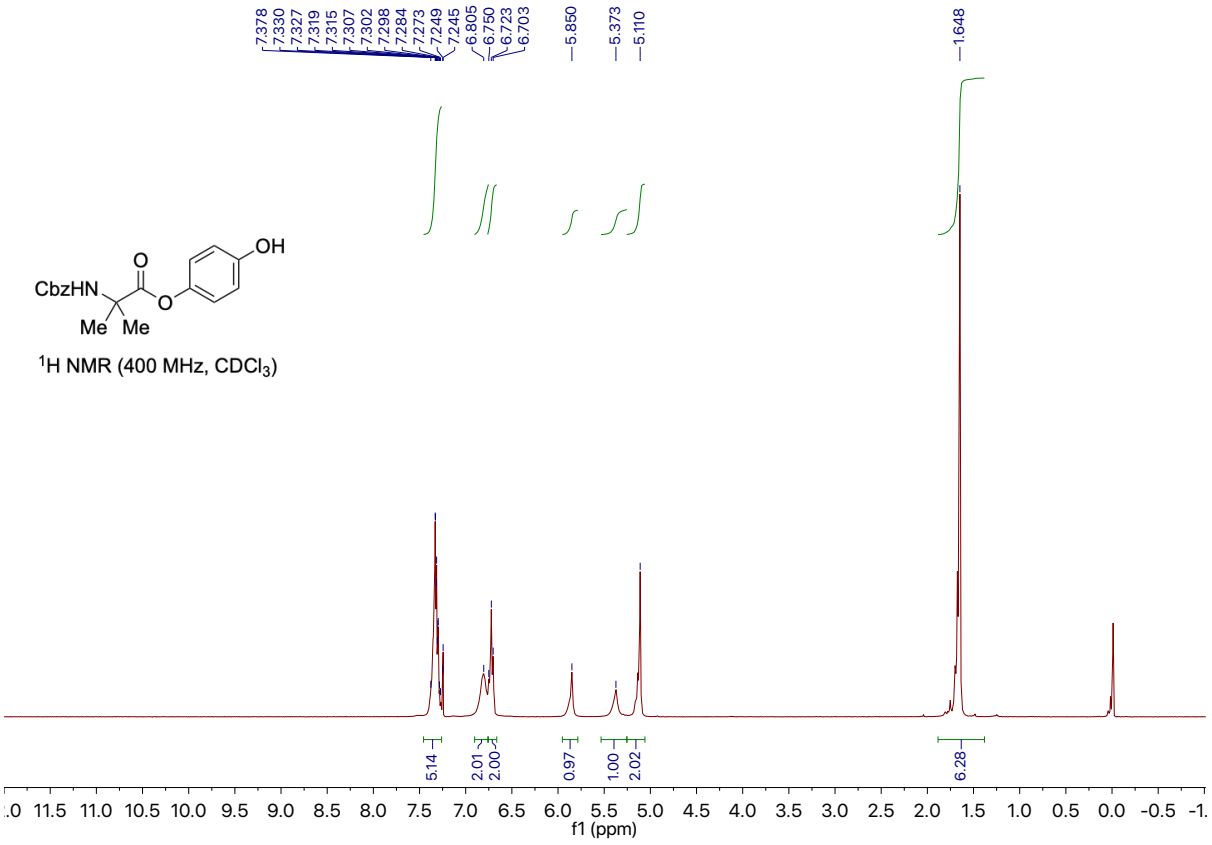
^{1}H NMR (400 MHz, $CDCl_3$)



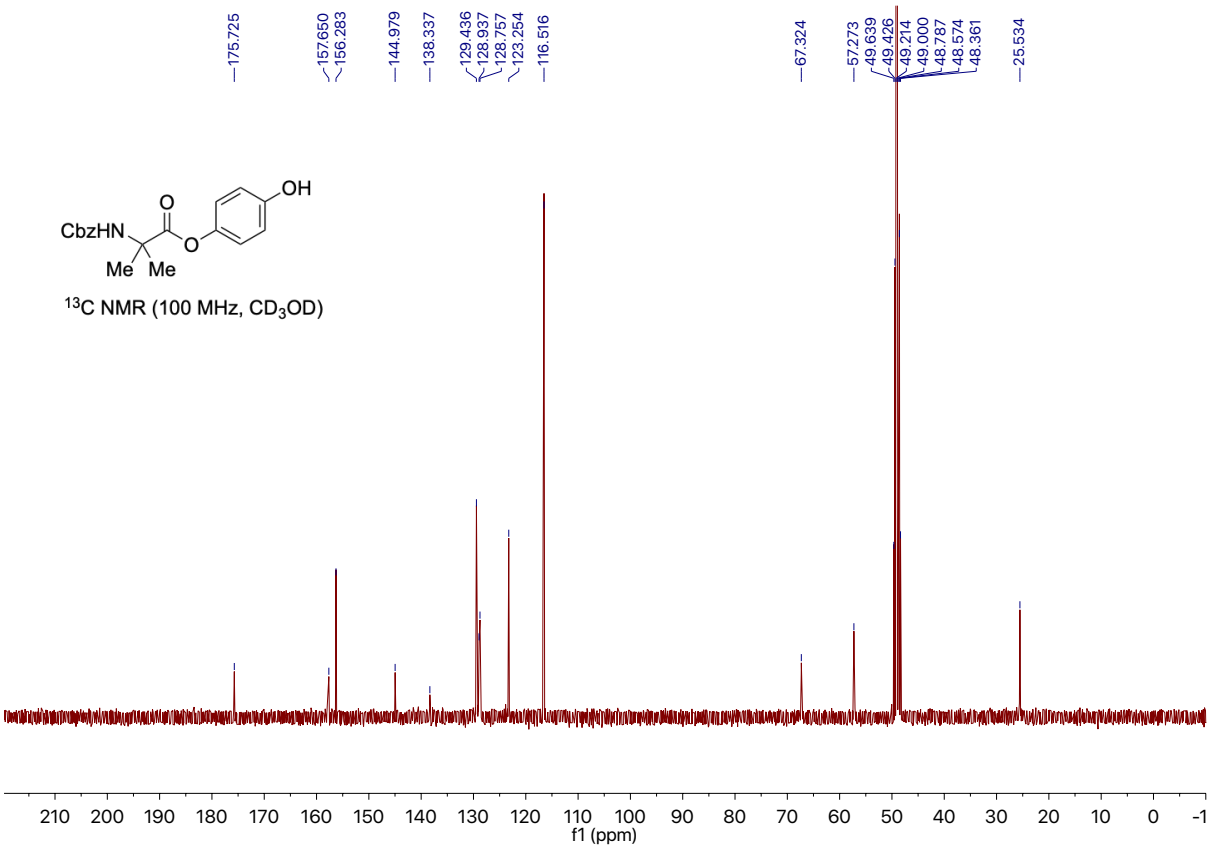
^{13}C NMR (100 MHz, $CDCl_3$)


7.373
7.343
7.326
7.318
7.305
7.294
7.284
6.926
6.904
6.799
6.777
5.284
5.102
4.942
3.581
3.566
3.551
3.537
2.800
2.786
2.771
OH
O
CbzHN
O
1H NMR (400 MHz, CDCl3)
5.45
2.16
2.14
1.00
2.03
0.91
2.18
2.17
f1 (ppm)

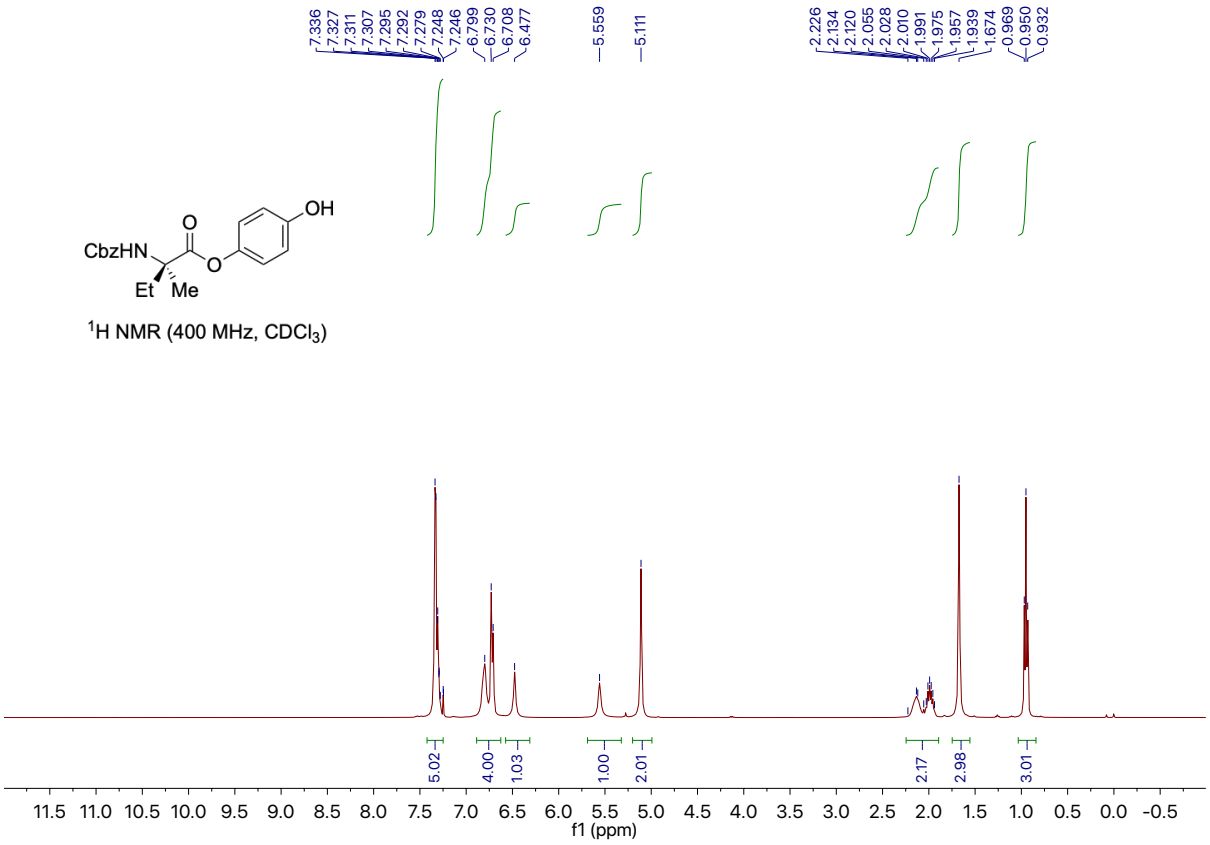

172.530
158.788
156.333
144.639
138.318
129.461
128.975
128.798
123.406
116.547
67.438
49.427
49.213
48.788
48.574
37.790
35.525
OH
O
CbzHN
O
13C NMR (100 MHz, CD3OD)
f1 (ppm)



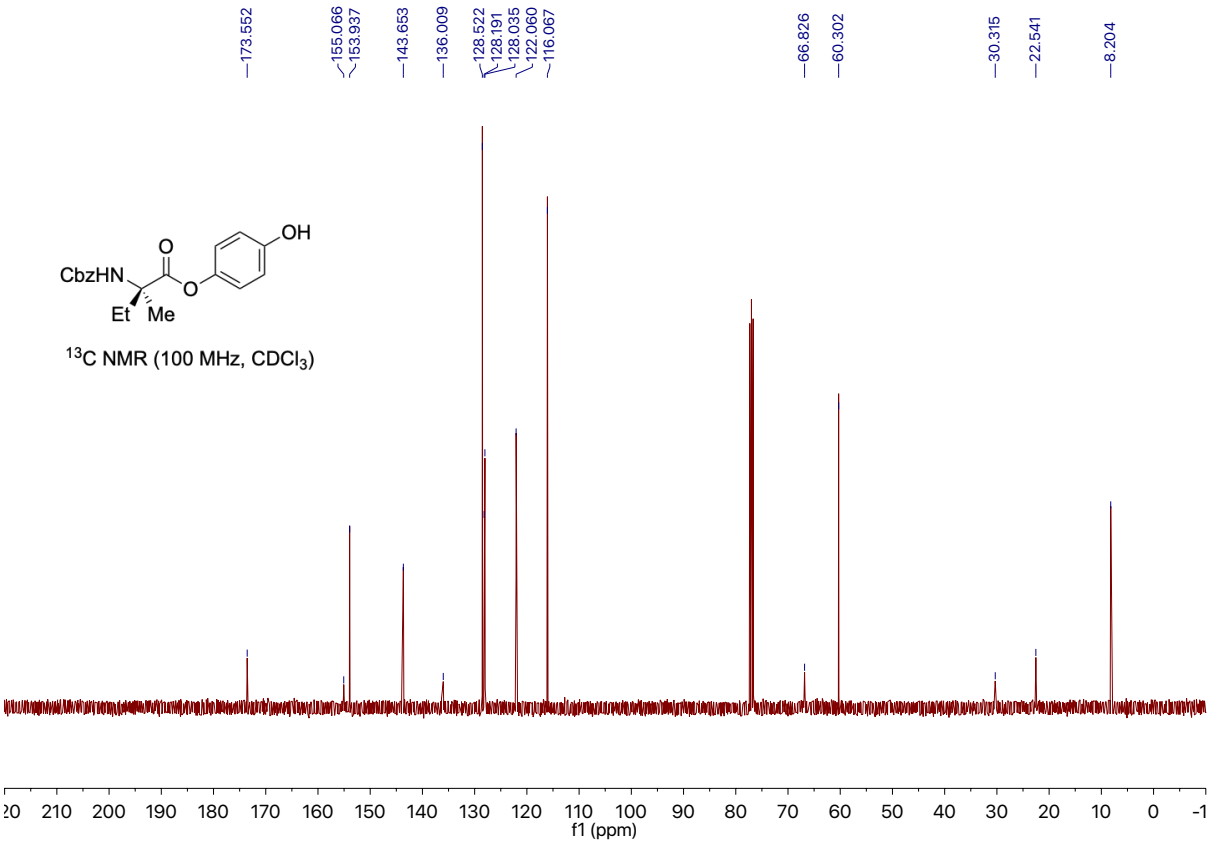
^{1}H NMR (400 MHz, $CDCl_3$)



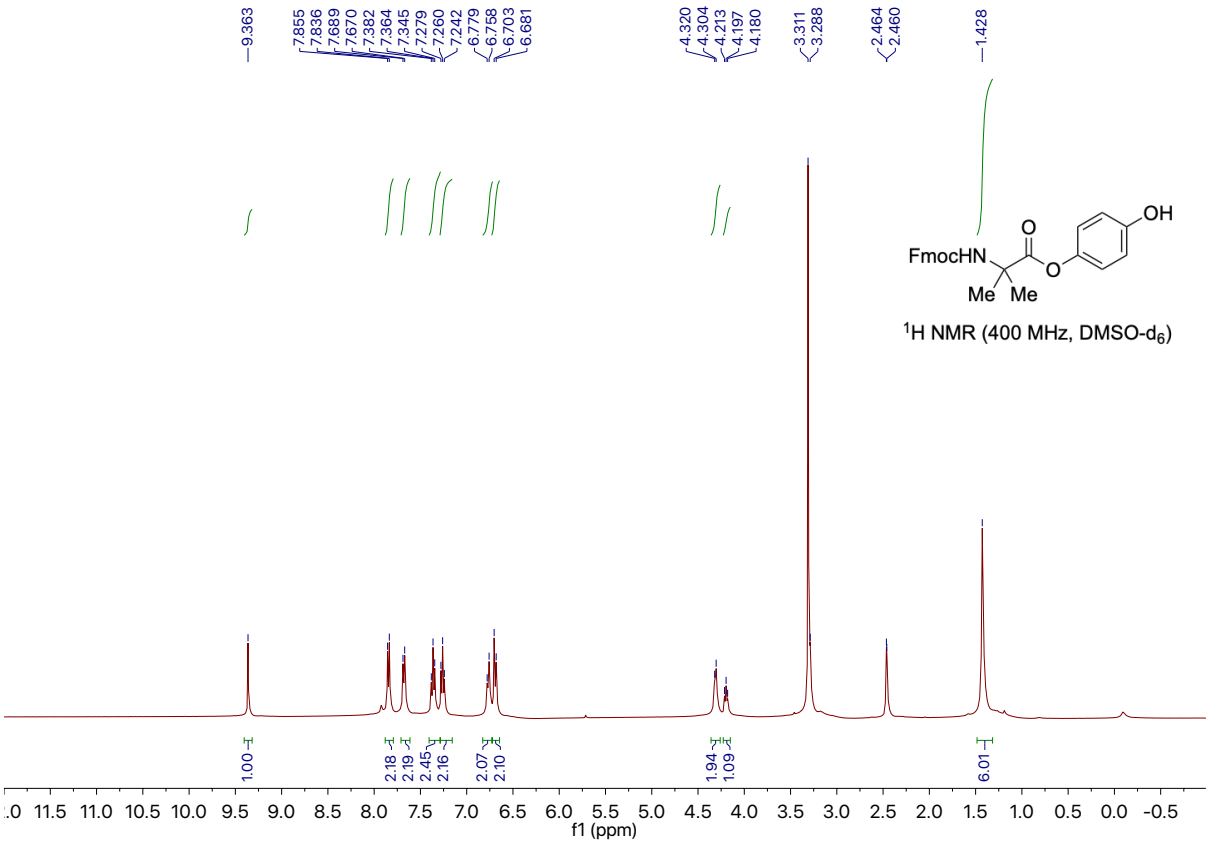
^{13}C NMR (100 MHz, CD_3OD)



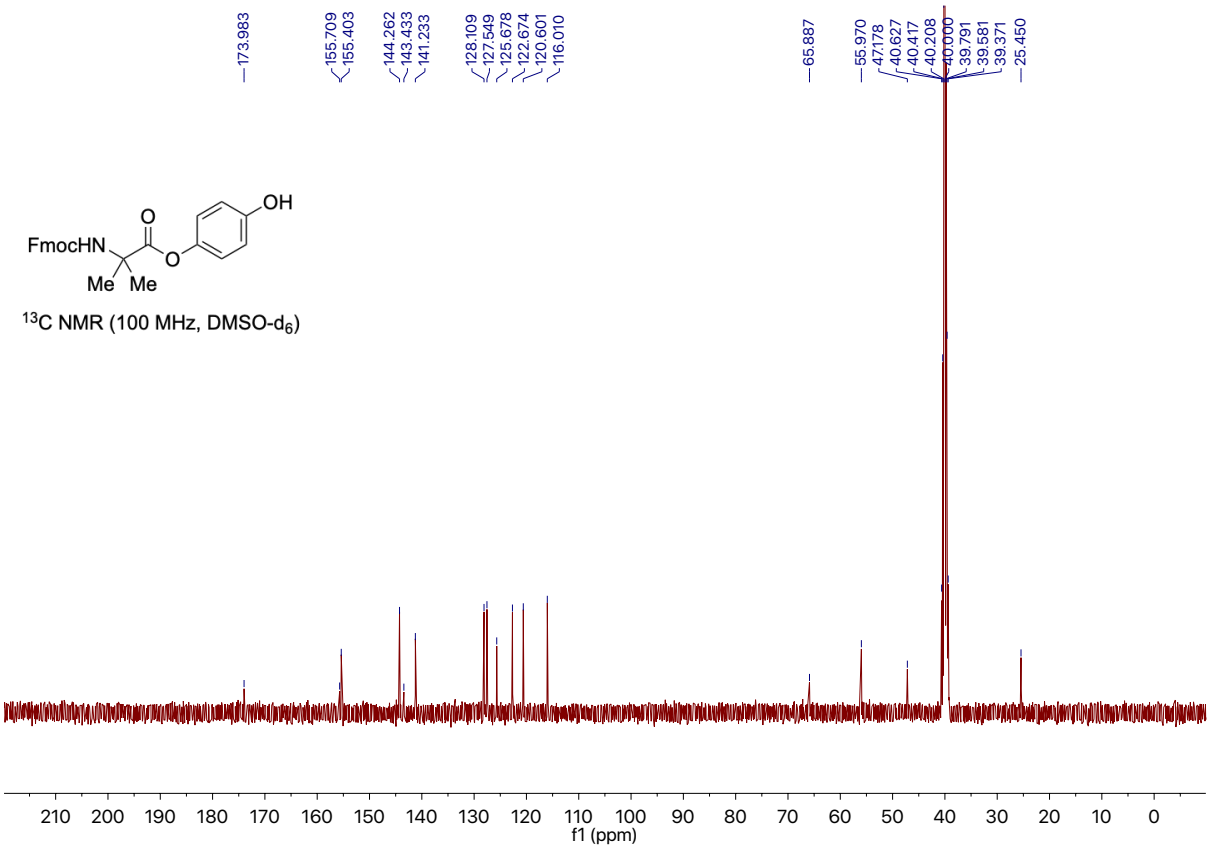
^{1}H NMR (400 MHz, $CDCl_3$)



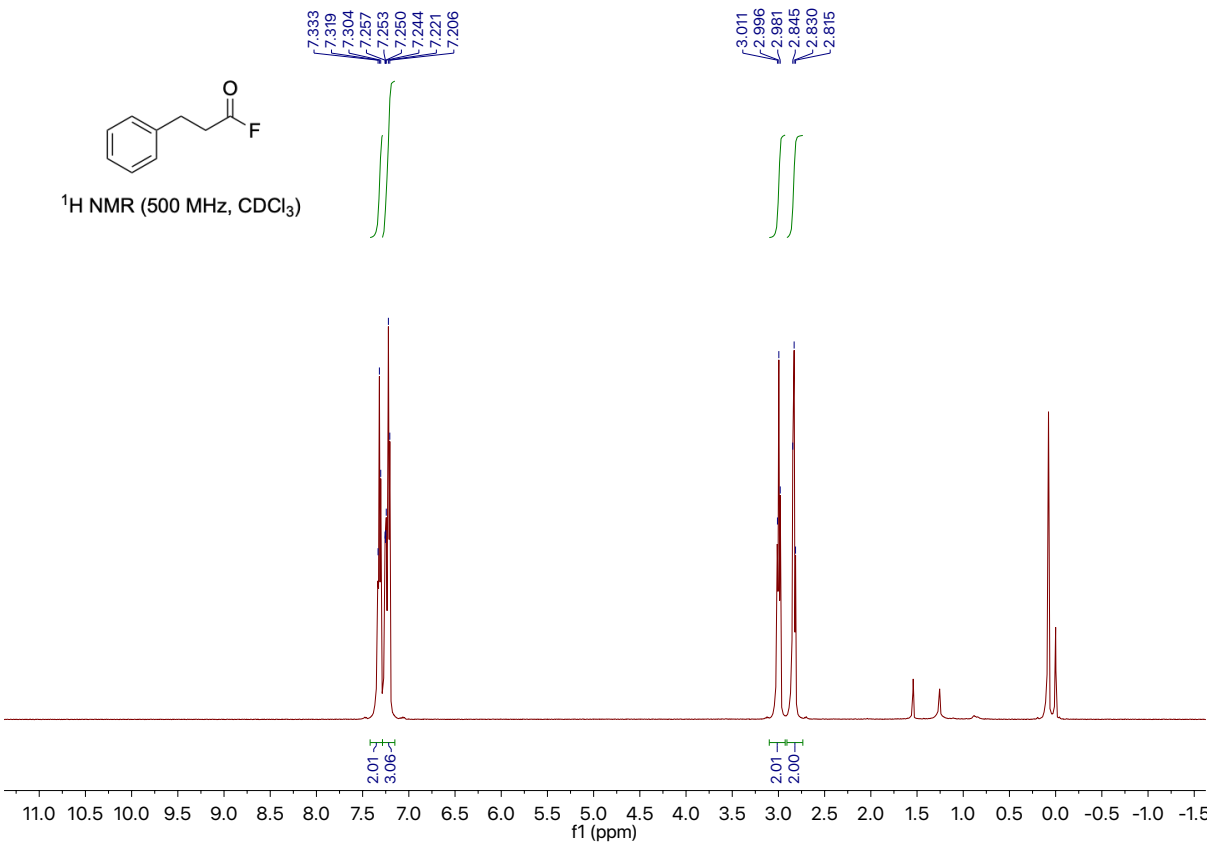
^{13}C NMR (100 MHz, $CDCl_3$)

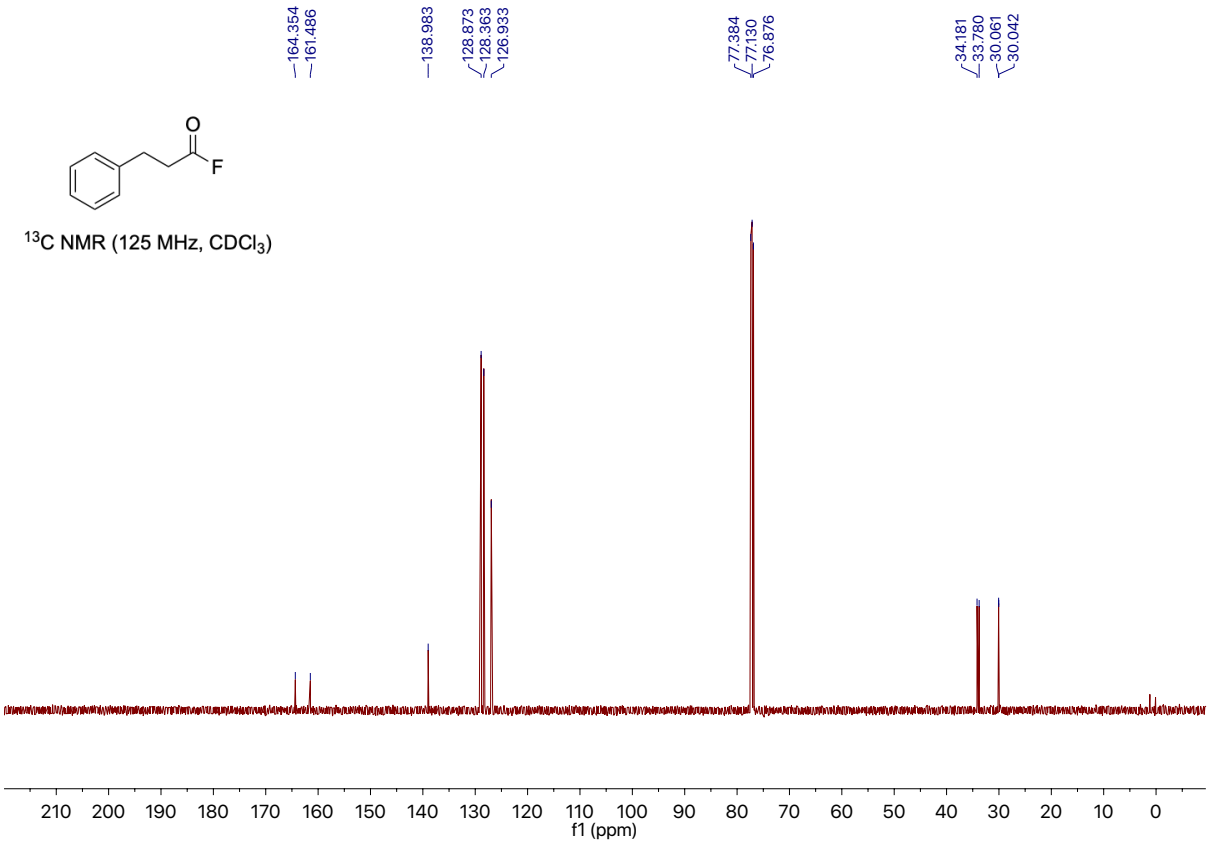


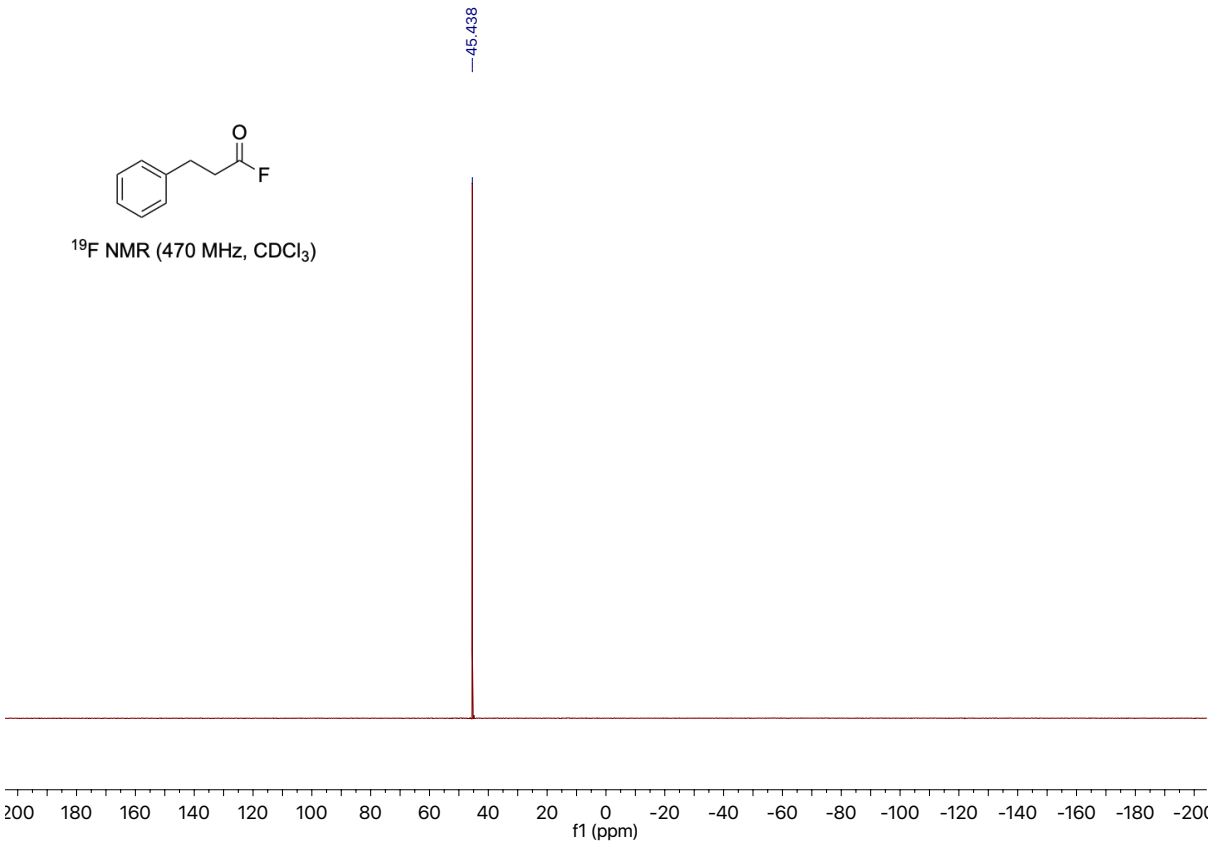
^{1}H NMR (400 MHz, DMSO-d_6)



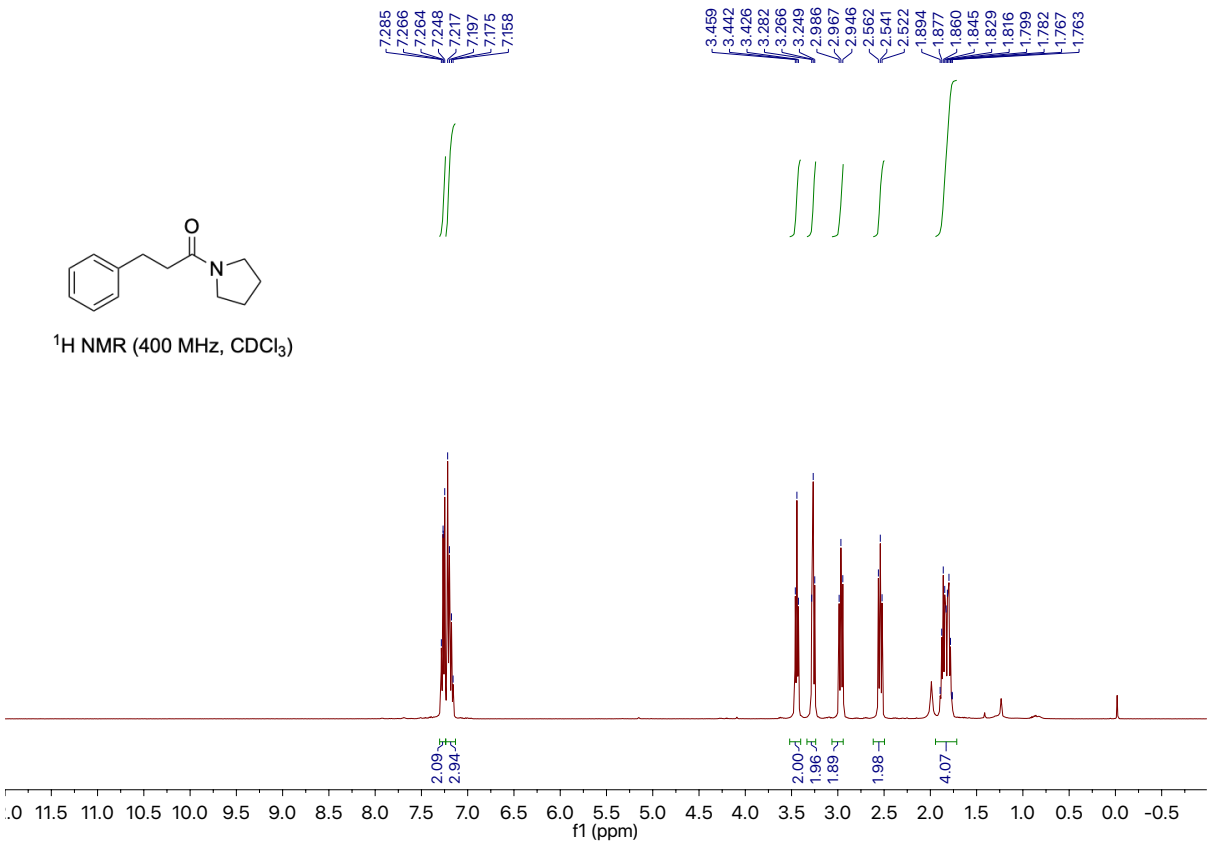
^{13}C NMR (100 MHz, DMSO-d_6)


7.333
7.319
7.304
7.257
7.253
7.250
7.244
7.221
7.206
3.011
2.996
2.981
2.845
2.830
2.815
O
F
^{1}H NMR (500 MHz, $CDCl_3$)
2.01
3.06
2.01
2.00
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 -1.0 -1.5
f1 (ppm)

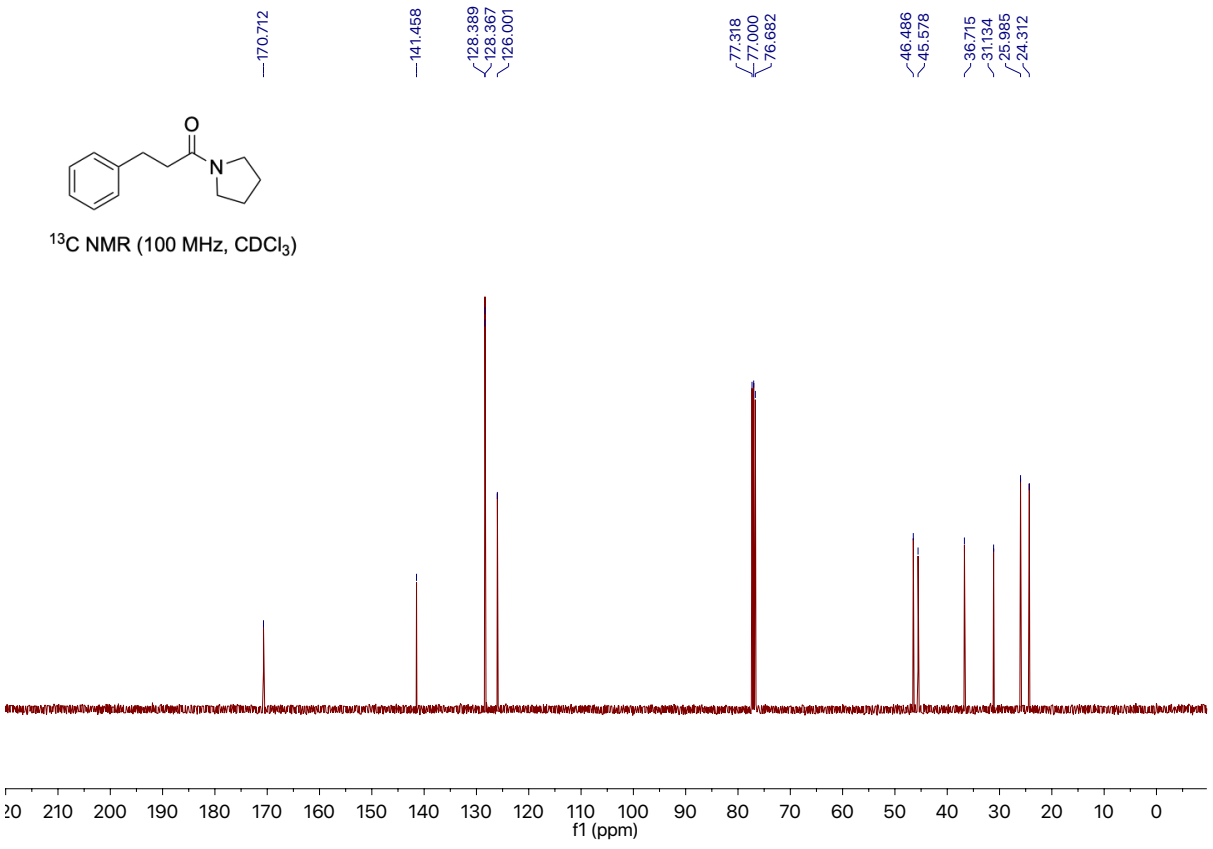

164.354
161.486
138.983
128.873
128.363
126.933
77.384
77.130
76.876
34.181
33.780
30.061
30.042
O
F
^{13}C NMR (125 MHz, $CDCl_3$)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



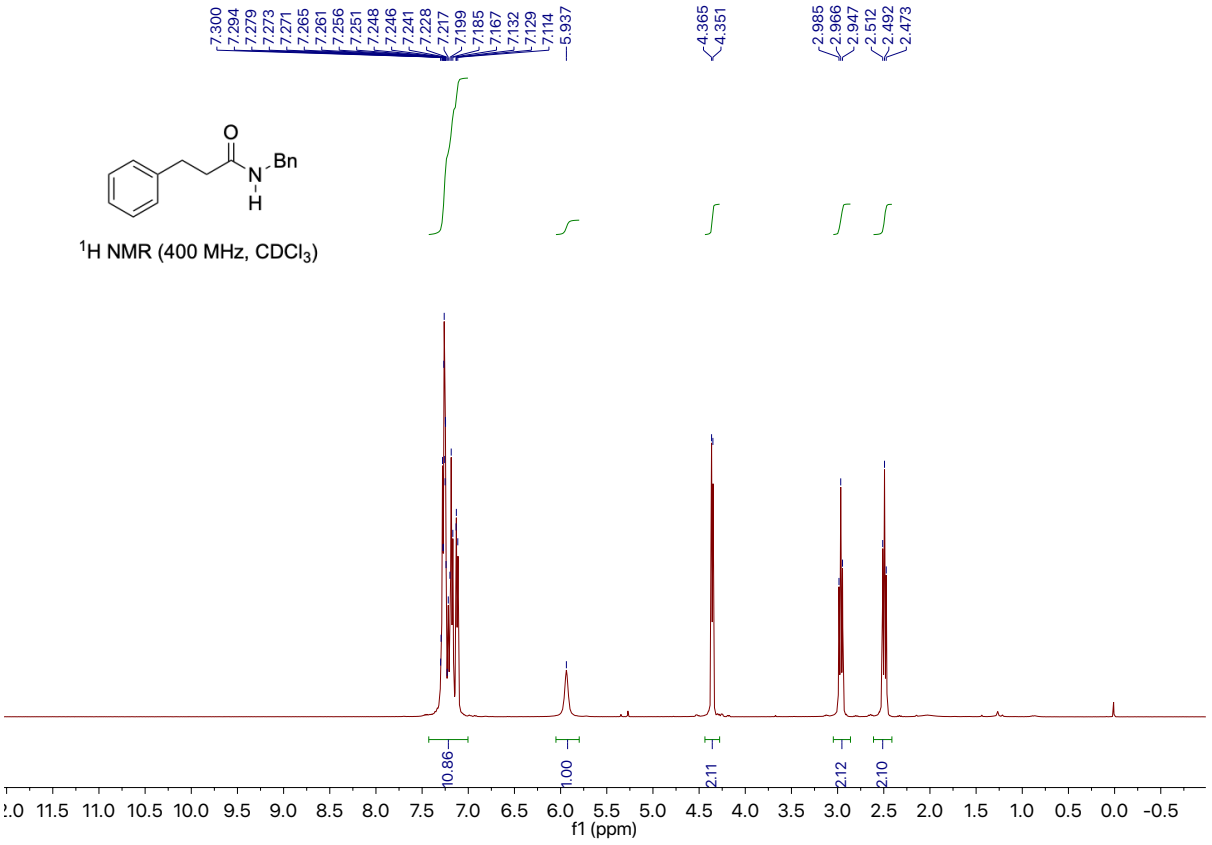
^{19}F NMR (470 MHz, $CDCl_3$)

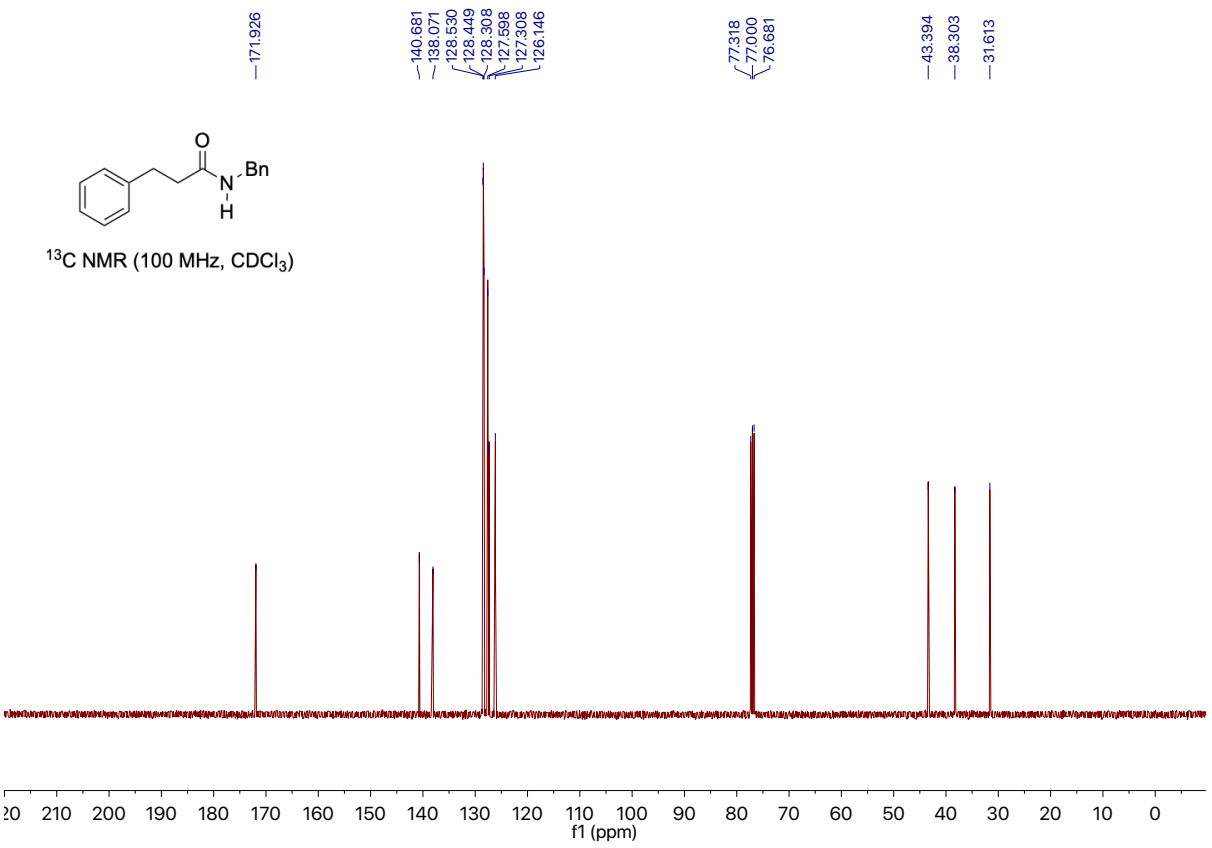


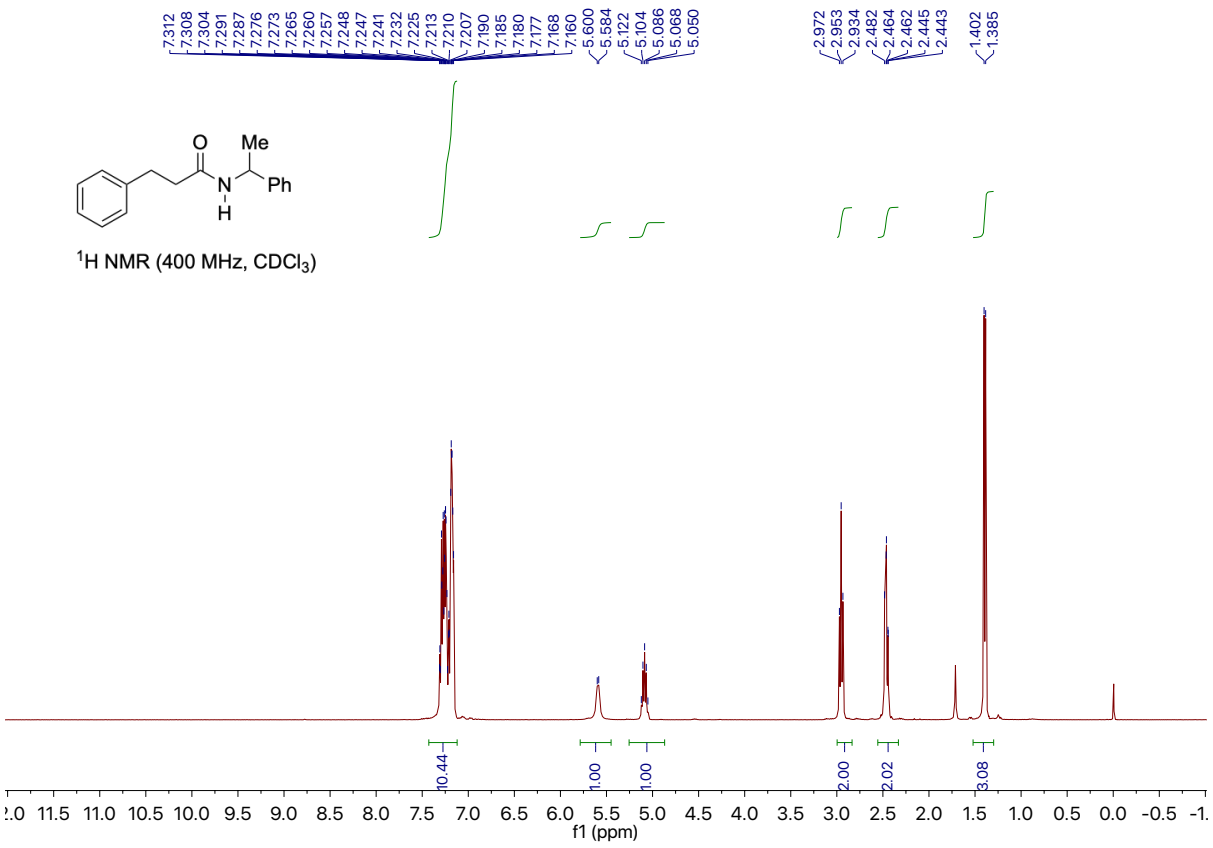
^{1}H NMR (400 MHz, $CDCl_3$)



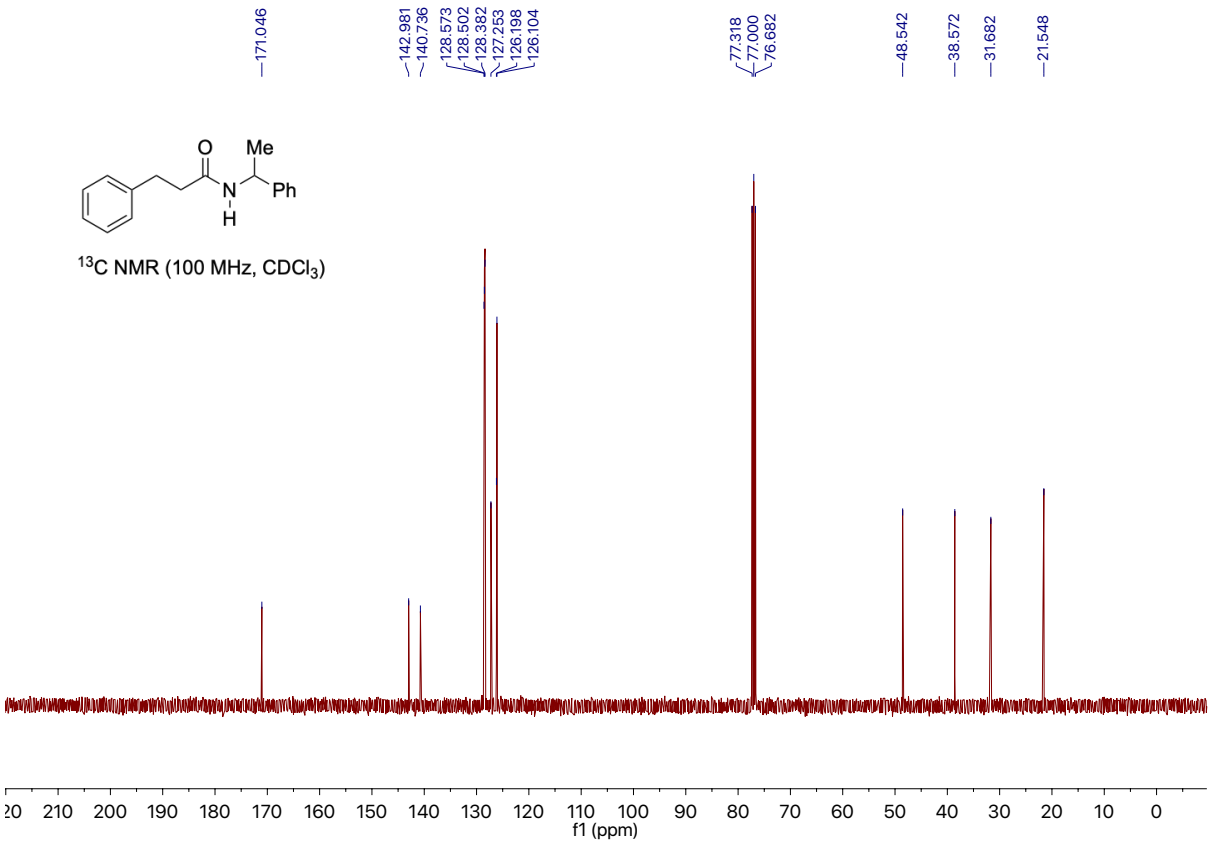
^{13}C NMR (100 MHz, $CDCl_3$)


7.300
7.294
7.279
7.273
7.271
7.265
7.261
7.256
7.251
7.248
7.246
7.241
7.228
7.217
7.199
7.185
7.167
7.132
7.129
7.114
5.937
4.365
4.351
2.985
2.966
2.947
2.512
2.492
2.473
O
N
H
Bn
1H NMR (400 MHz, CDCl3)
10.86
1.00
2.11
2.12
2.10
f1 (ppm)

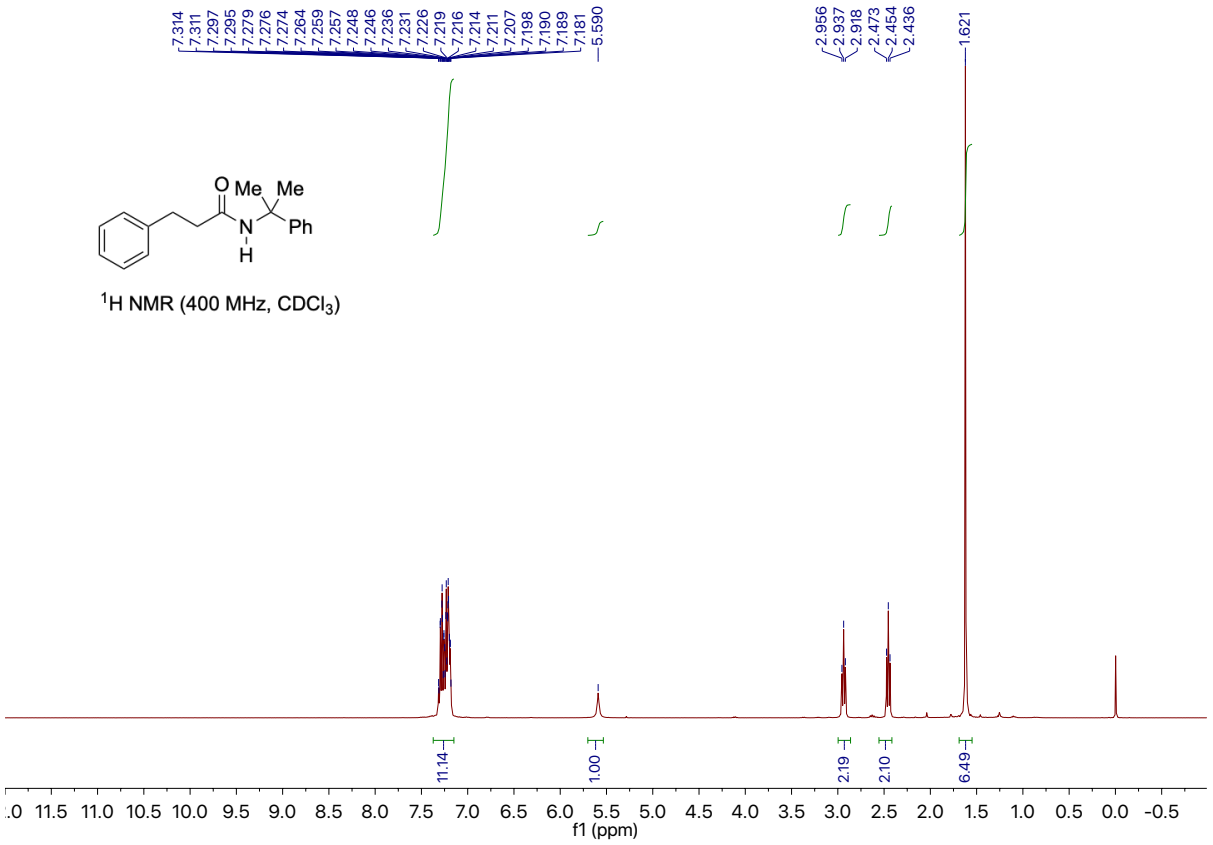

171.926
140.681
138.071
128.530
128.449
128.308
127.598
127.308
126.146
77.318
77.000
76.681
43.394
38.303
31.613
O
N
H
Bn
13C NMR (100 MHz, CDCl3)
f1 (ppm)



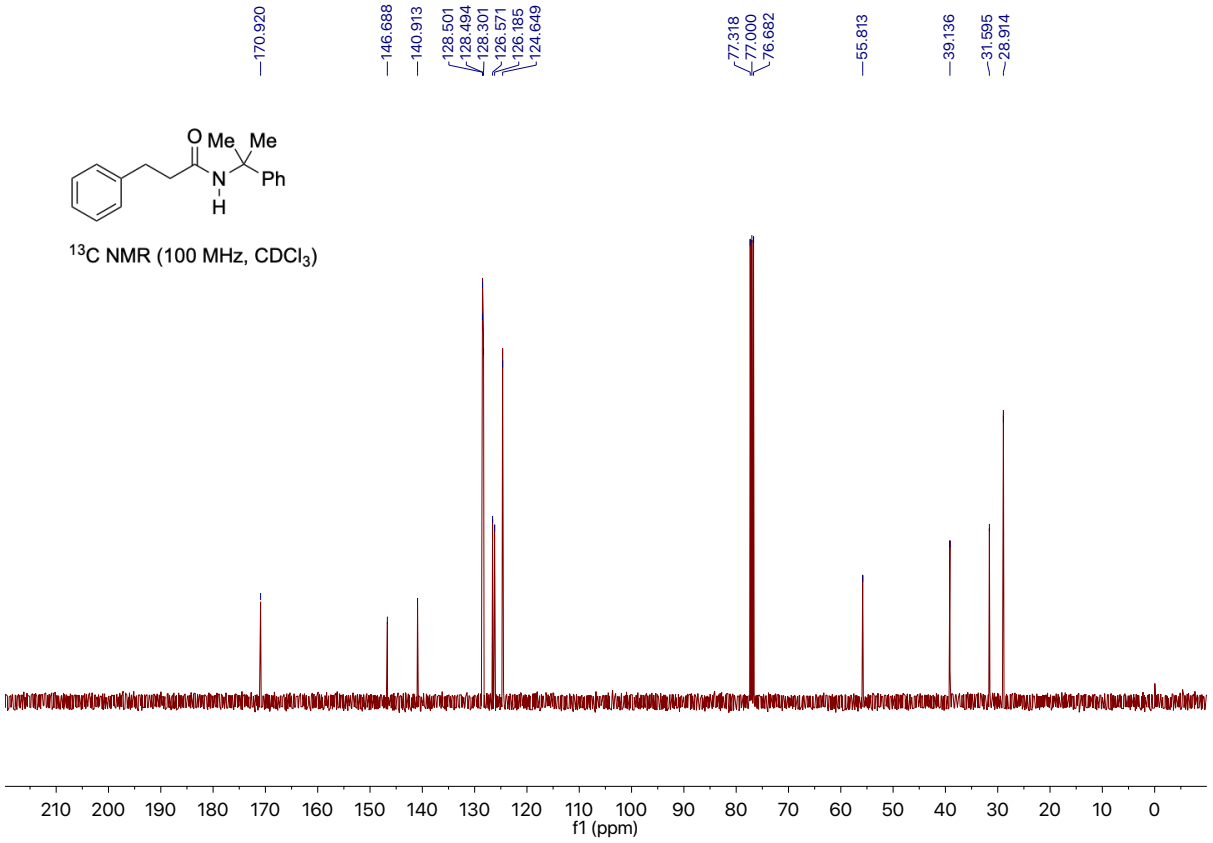
^{1}H NMR (400 MHz, $CDCl_3$)



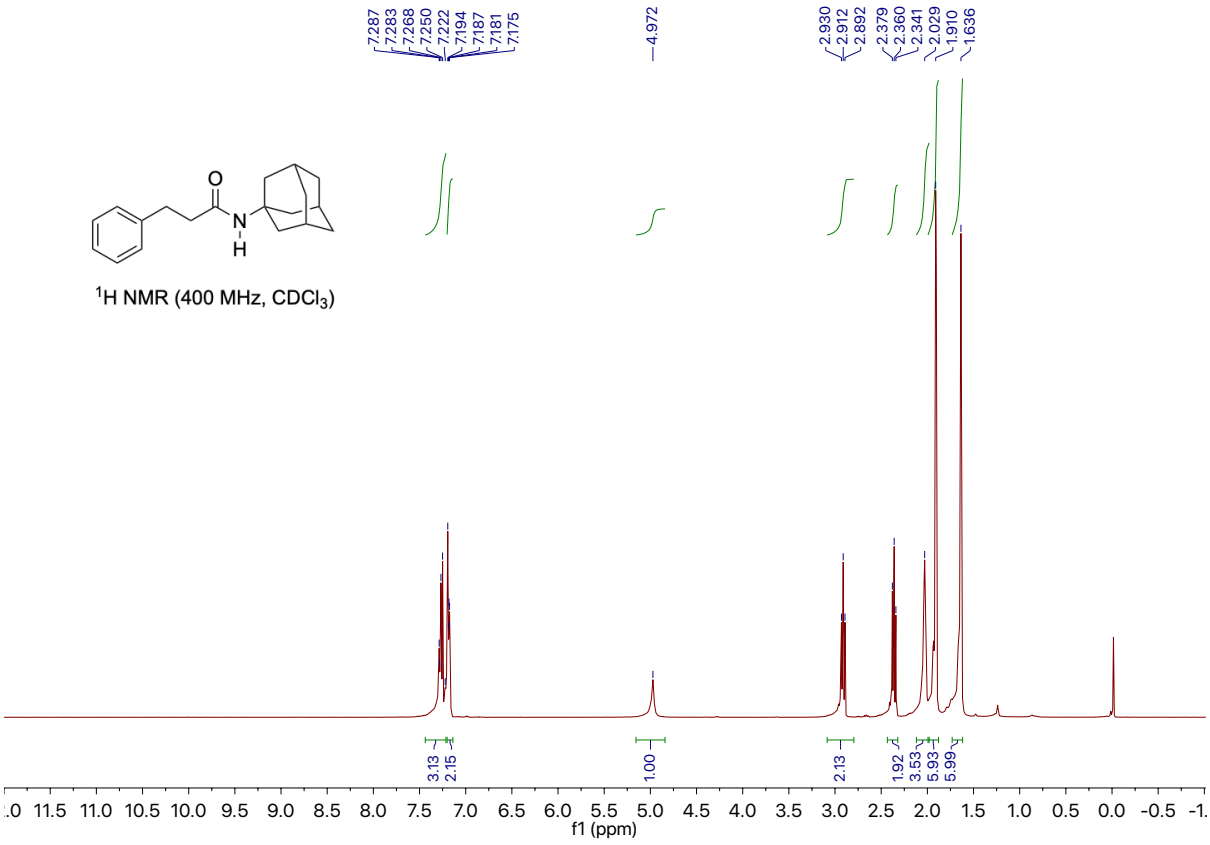
^{13}C NMR (100 MHz, $CDCl_3$)



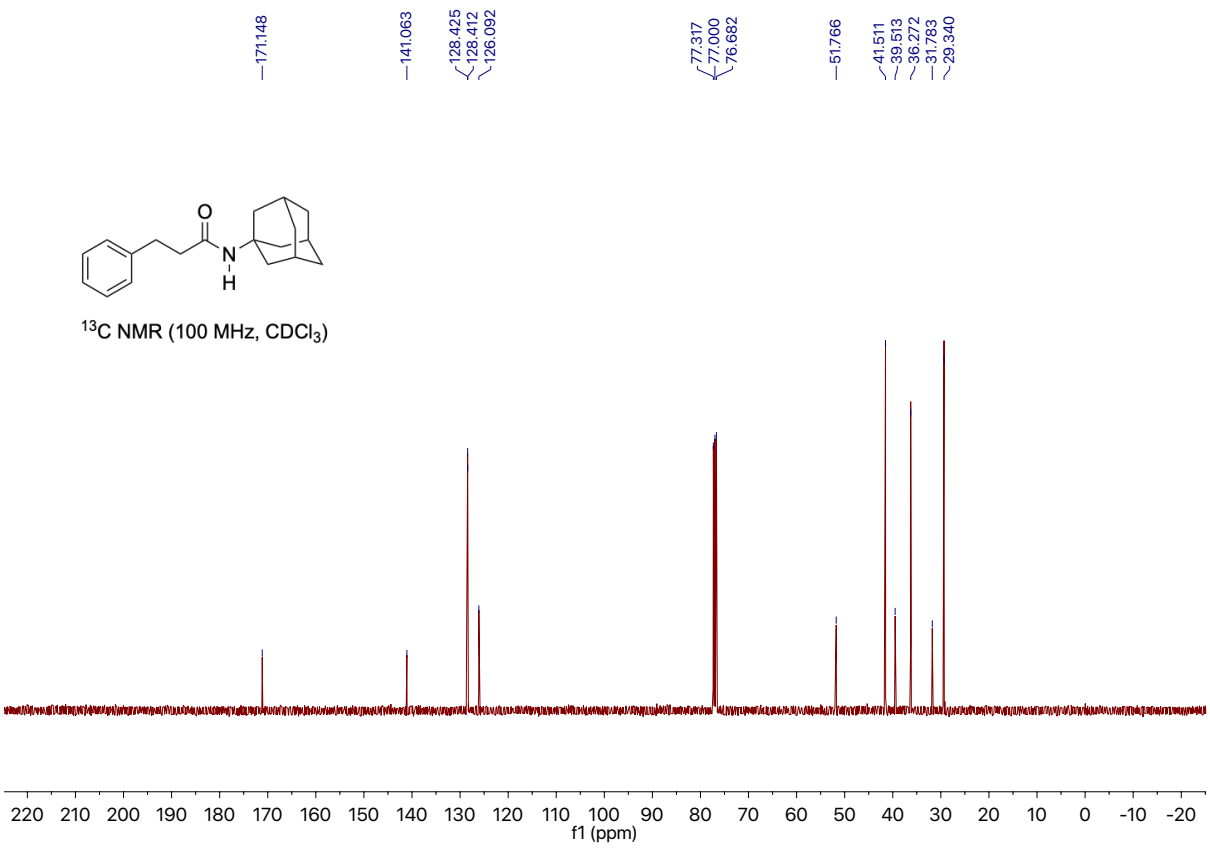
^{1}H NMR (400 MHz, $CDCl_3$)



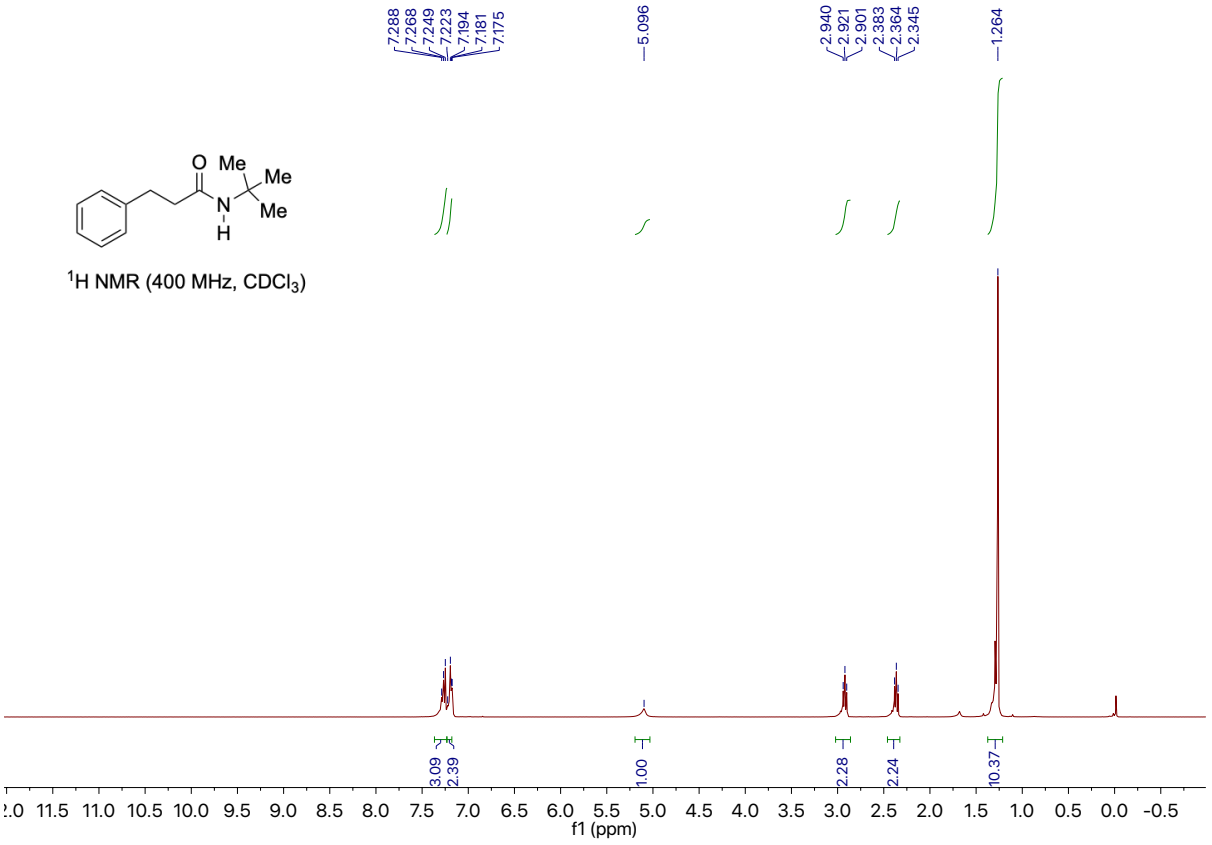
^{13}C NMR (100 MHz, $CDCl_3$)



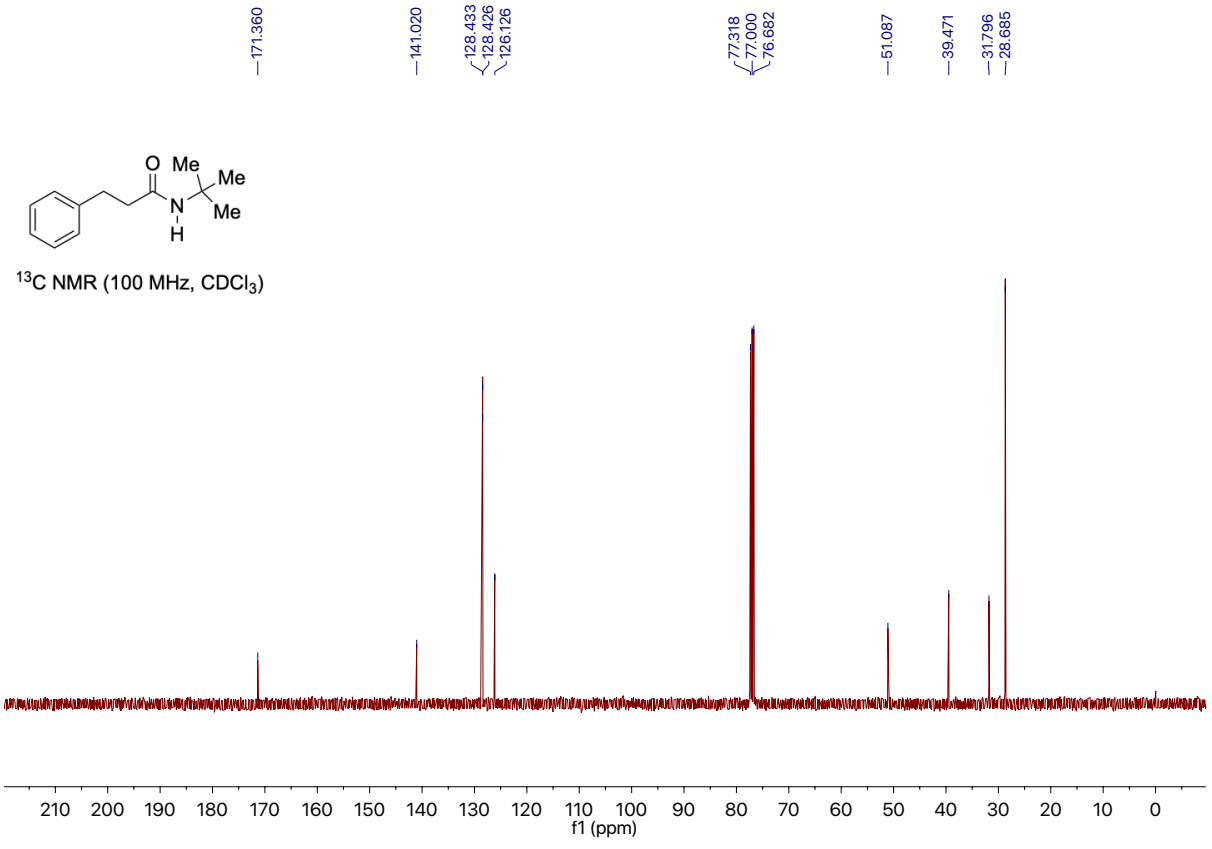
^{1}H NMR (400 MHz, $CDCl_3$)



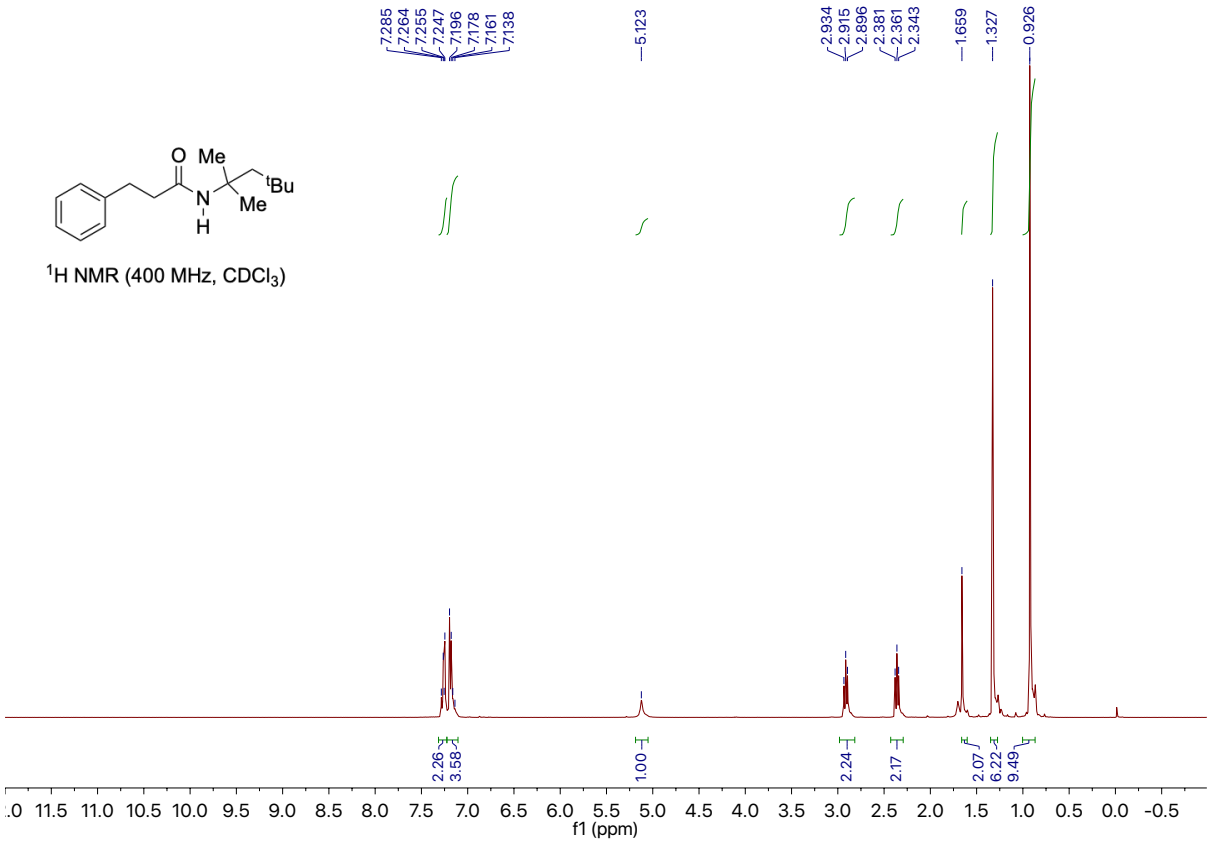
^{13}C NMR (100 MHz, $CDCl_3$)



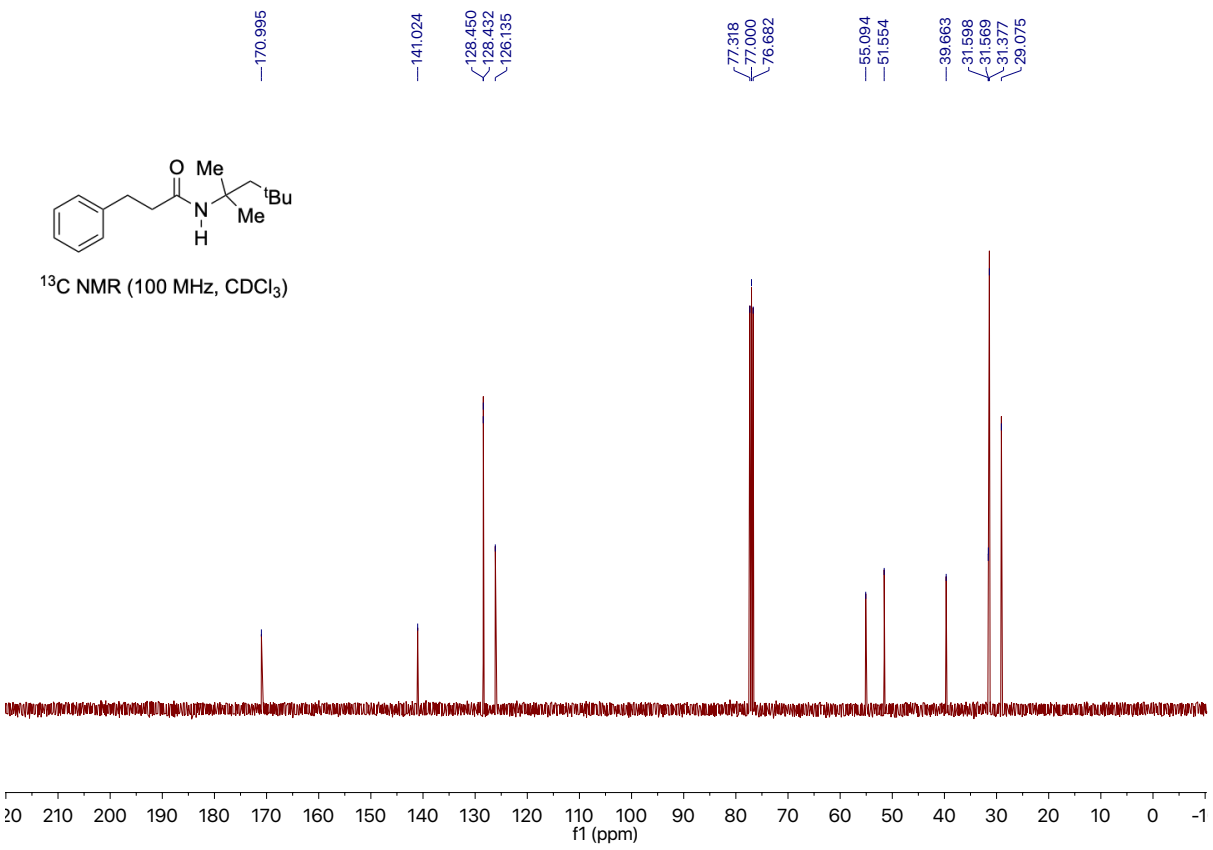
^{1}H NMR (400 MHz, $CDCl_3$)



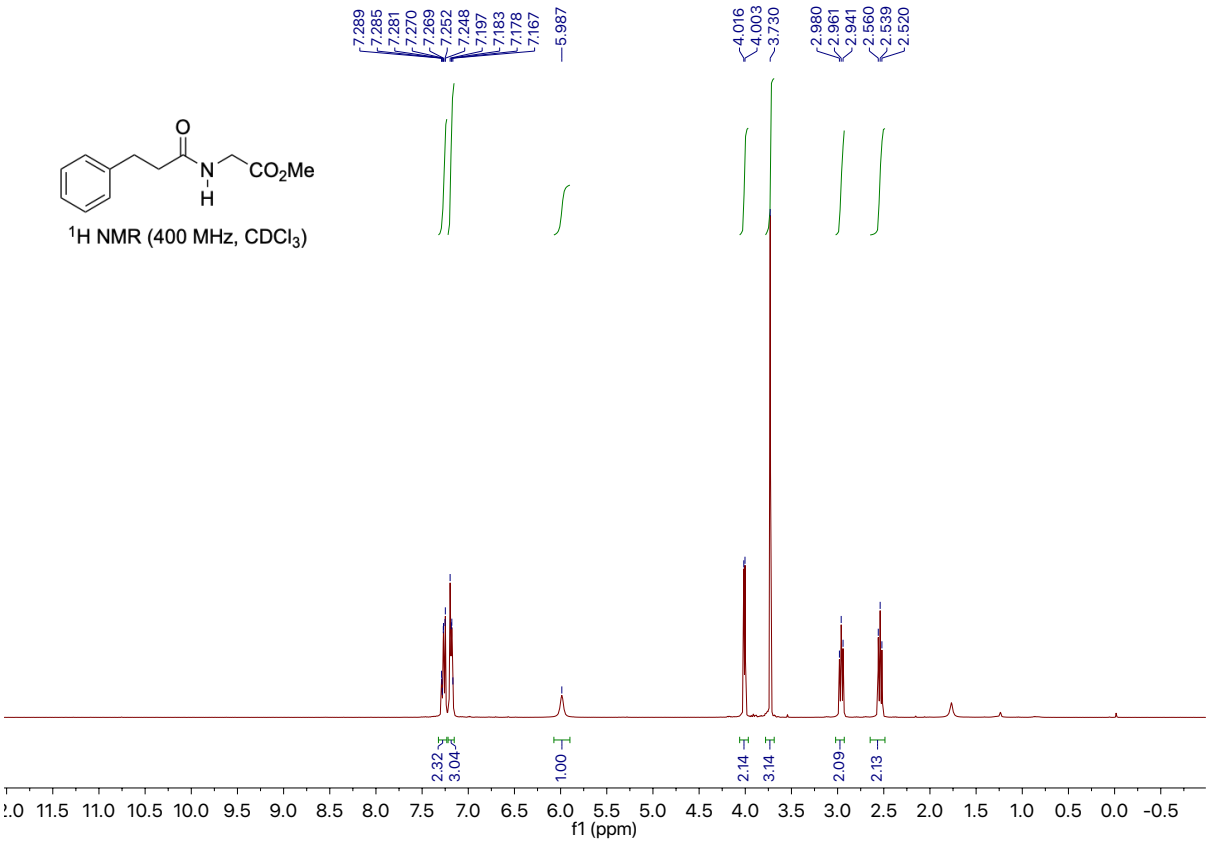
^{13}C NMR (100 MHz, $CDCl_3$)

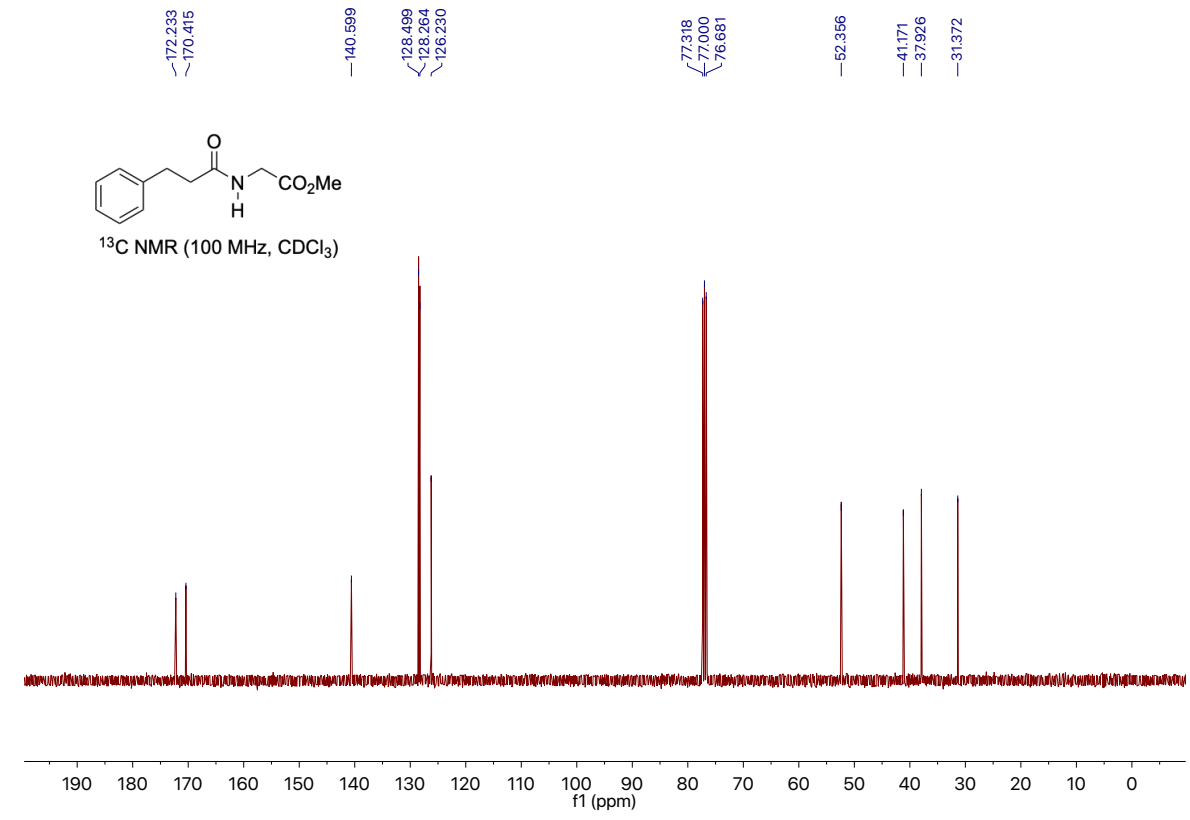


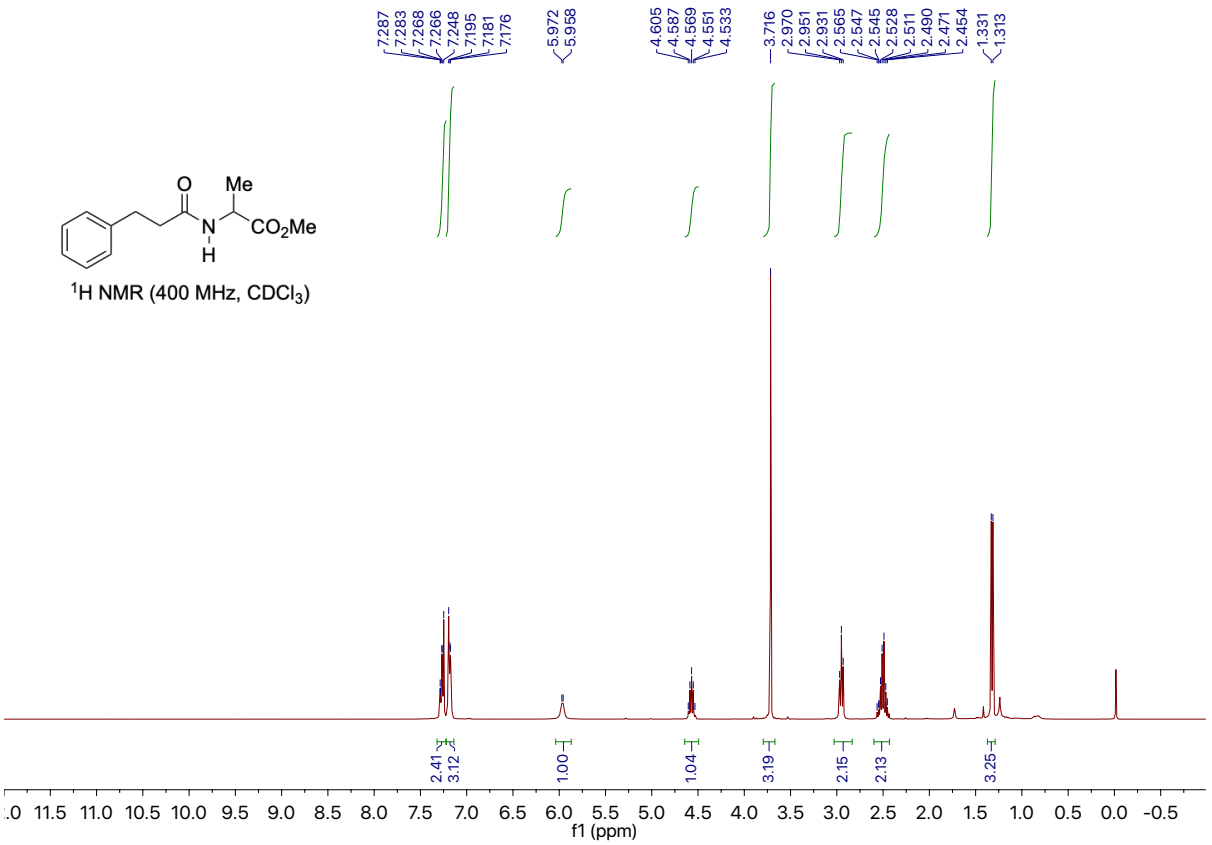
^{1}H NMR (400 MHz, $CDCl_3$)

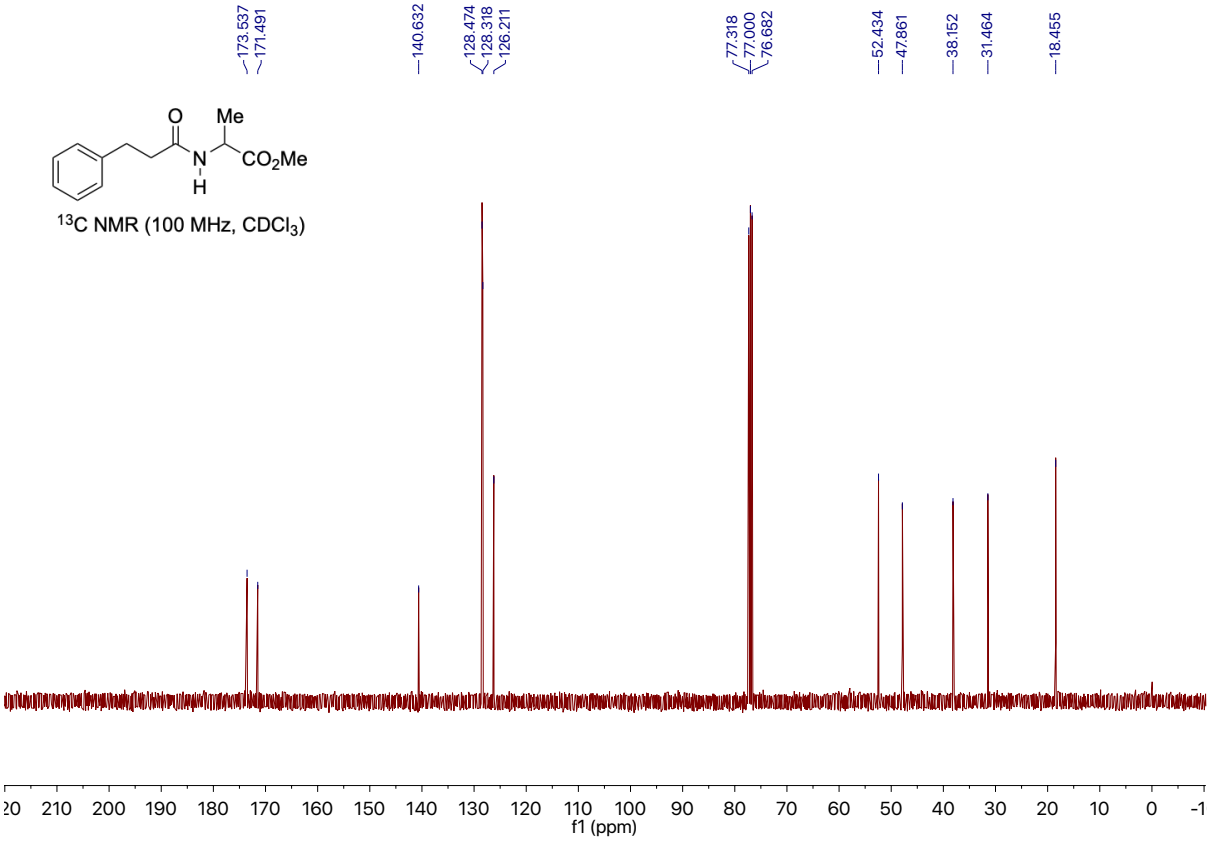


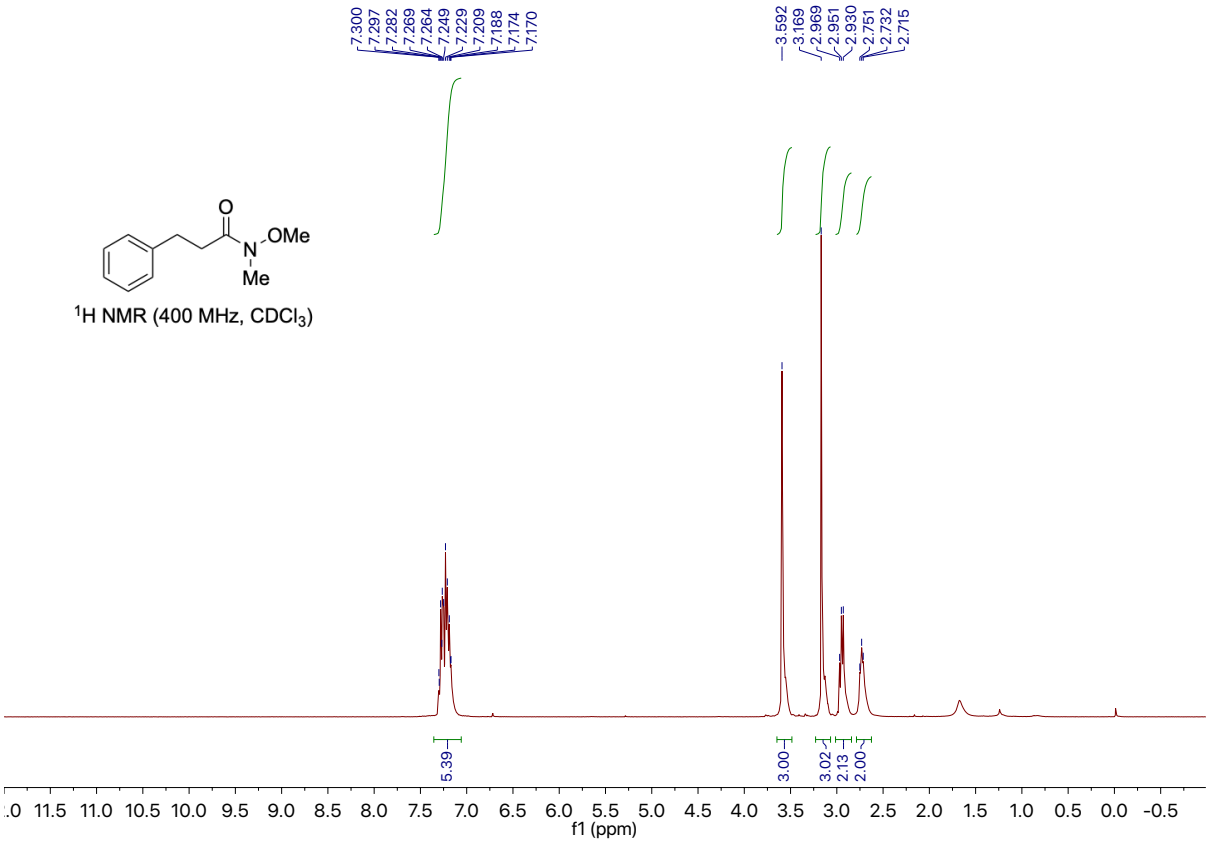
^{13}C NMR (100 MHz, $CDCl_3$)

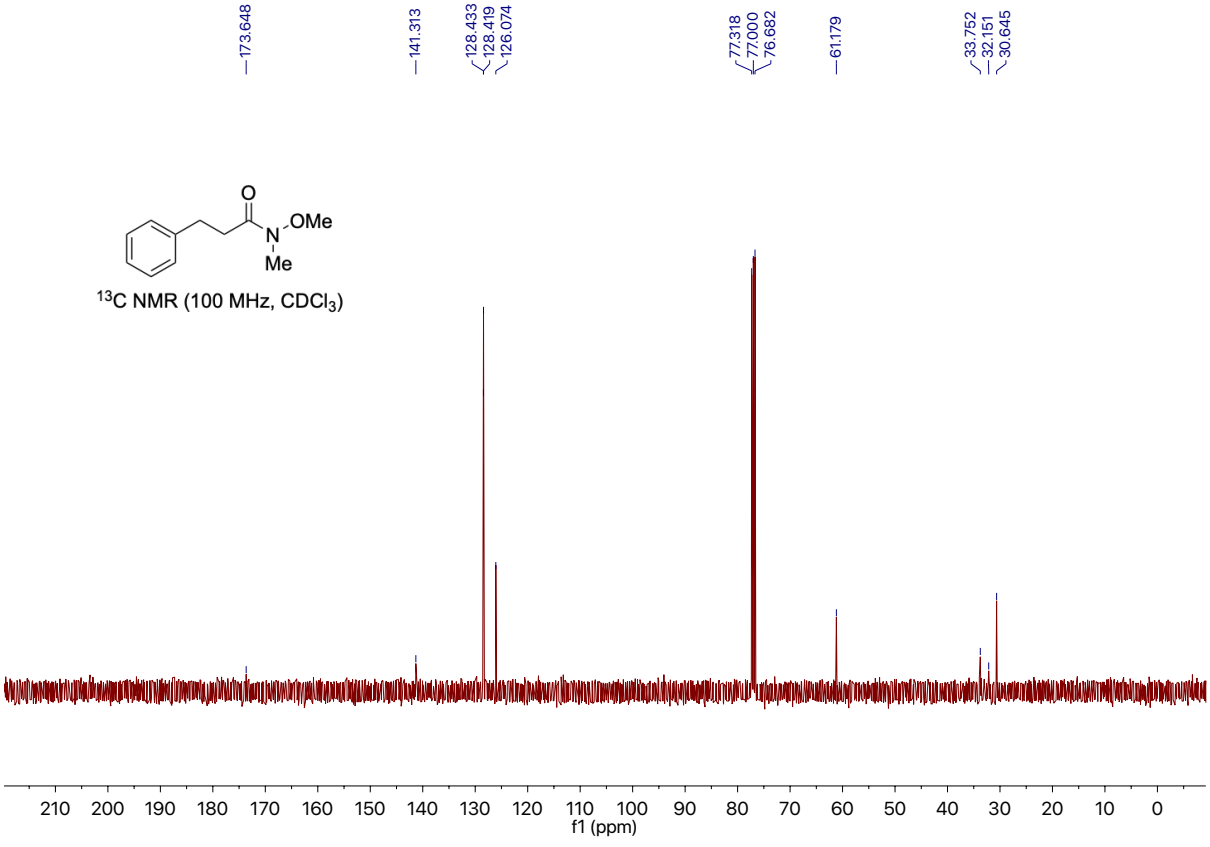

7.289
7.285
7.281
7.270
7.269
7.252
7.248
7.197
7.183
7.178
7.167
5.987
4.016
4.003
3.730
2.980
2.961
2.941
2.560
2.539
2.520
O
N
H
CO2Me
1H NMR (400 MHz, CDCl3)
2.32
3.04
1.00
2.14
3.14
2.09
2.13
f1 (ppm)

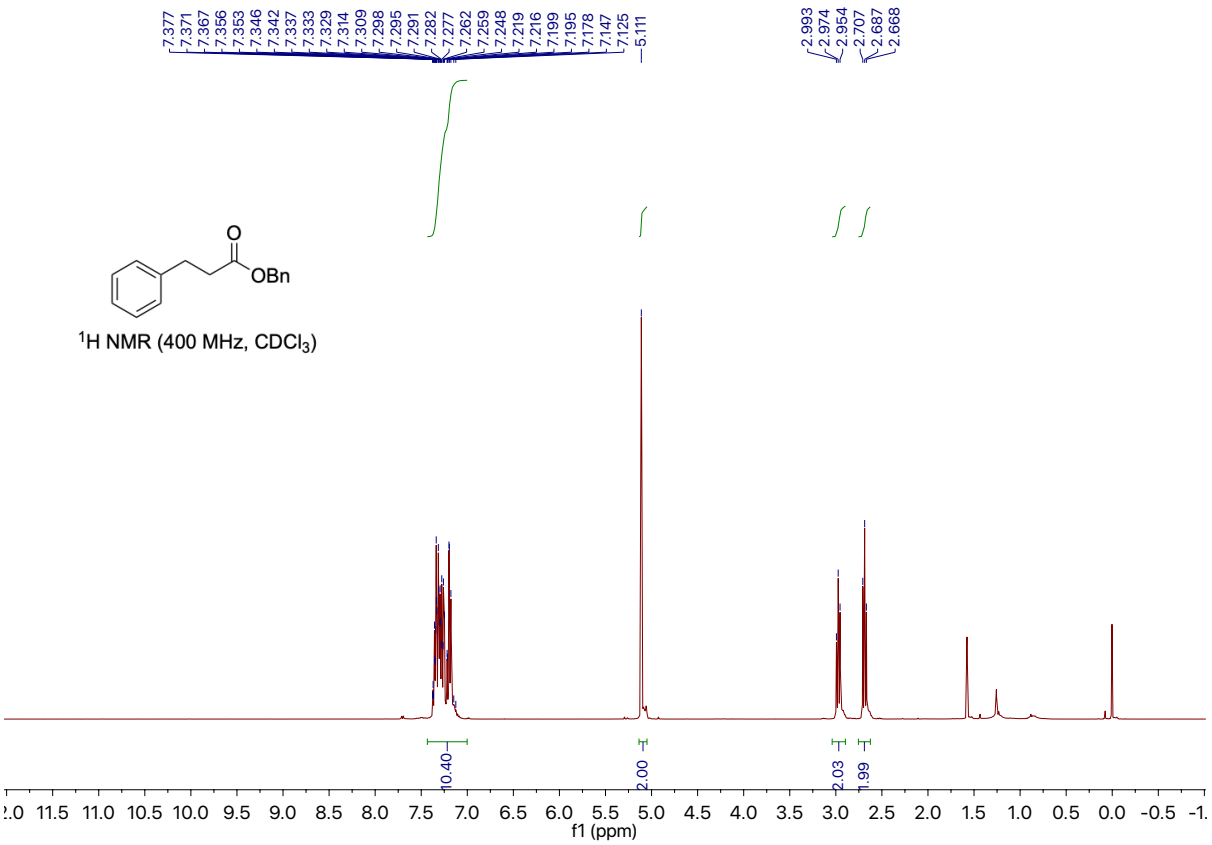

172.233
170.415
140.599
128.499
128.264
126.230
77.318
77.000
76.681
52.356
41.171
37.926
31.372
O
N
H
CO2Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)


7.287
7.283
7.268
7.266
7.248
7.195
7.181
7.176
5.972
5.958
4.605
4.587
4.569
4.551
4.533
3.716
2.970
2.951
2.931
2.565
2.547
2.545
2.528
2.511
2.490
2.471
2.454
1.331
1.313
O
Me
N
H
CO2Me
1H NMR (400 MHz, CDCl3)
2.41
3.12
1.00
1.04
3.19
2.15
2.13
3.25
f1 (ppm)

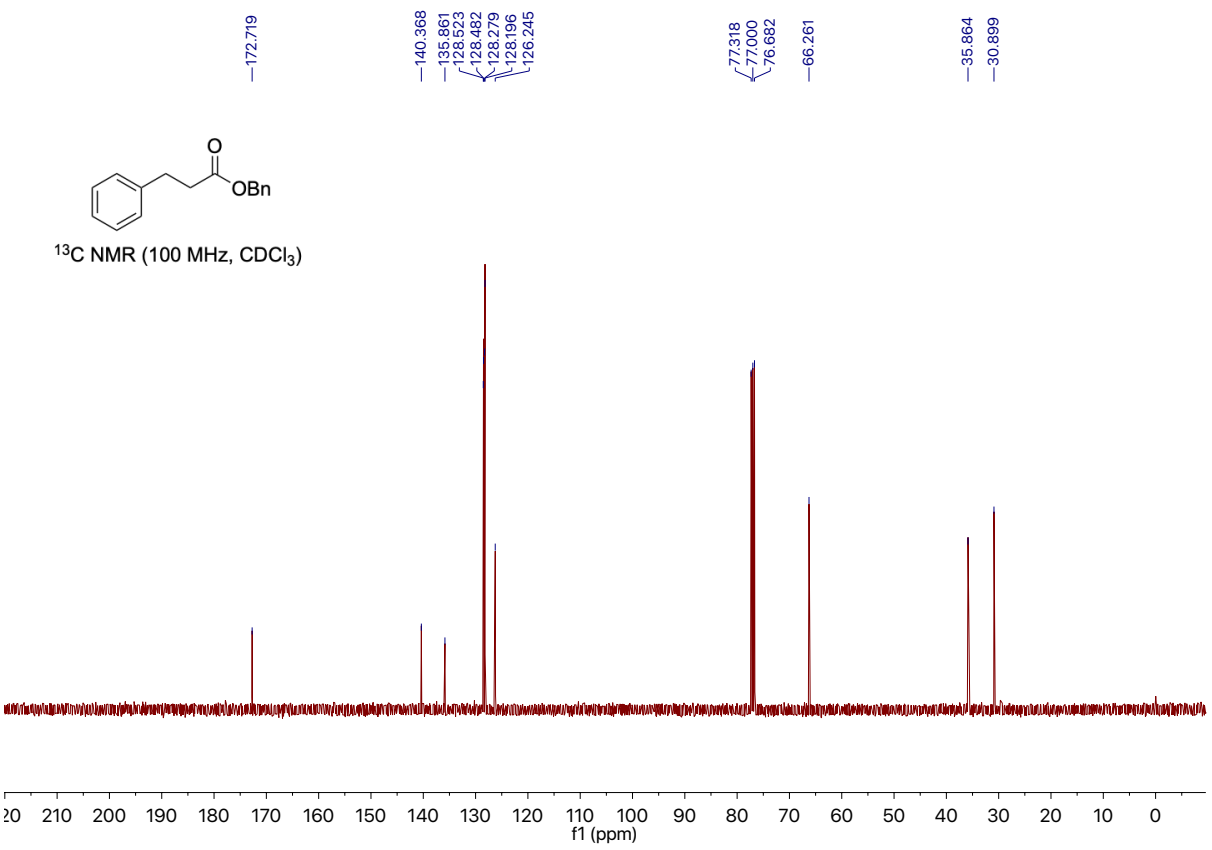

173.537
171.491
140.632
128.474
128.318
126.211
77.318
77.000
76.682
52.434
47.861
38.152
31.464
18.455
O
Me
N
H
CO2Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)


7.300
7.297
7.282
7.269
7.264
7.249
7.229
7.209
7.188
7.174
7.170
3.592
3.169
2.969
2.951
2.930
2.751
2.732
2.715
O
N
OMe
Me
1H NMR (400 MHz, CDCl3)
5.39
3.00
3.02
2.13
2.00
f1 (ppm)

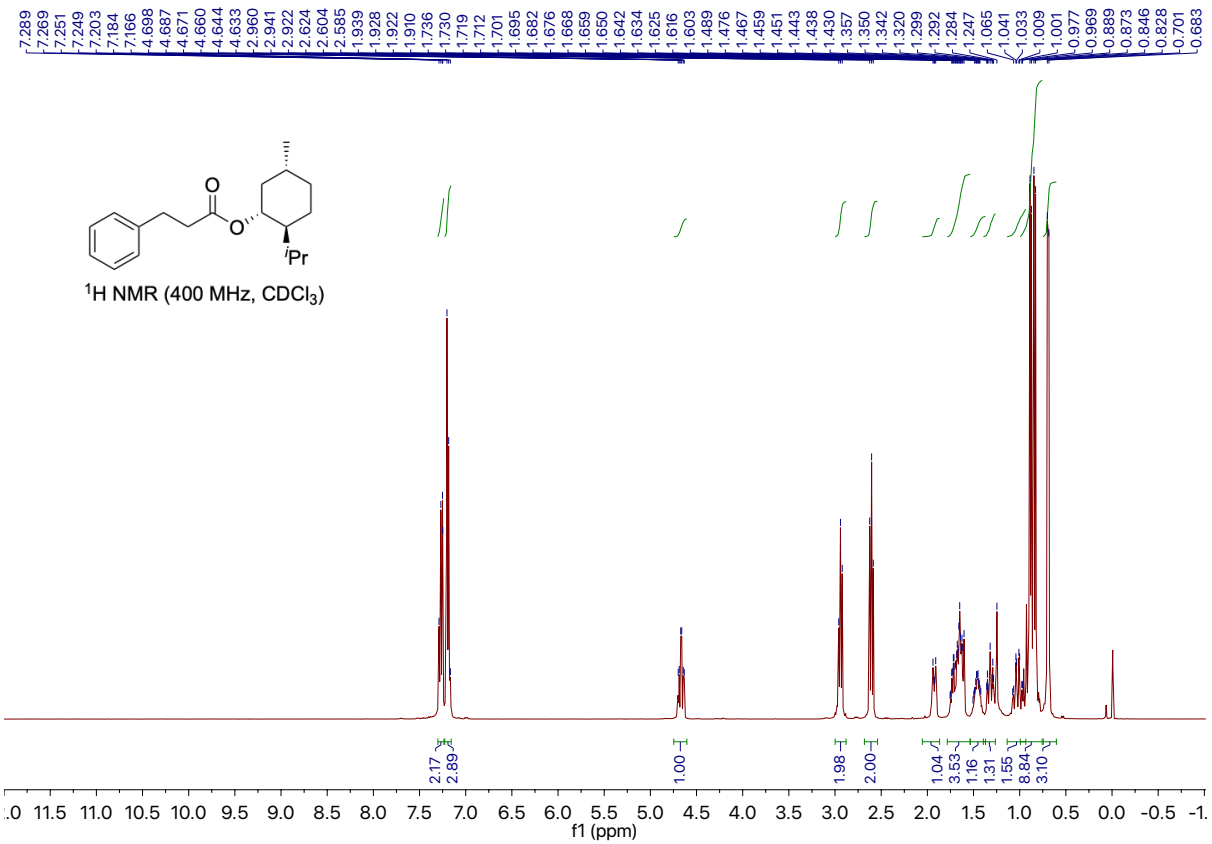

173.648
141.313
128.433
128.419
126.074
77.318
77.000
76.682
61.179
33.752
32.151
30.645
O
N
OMe
Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)

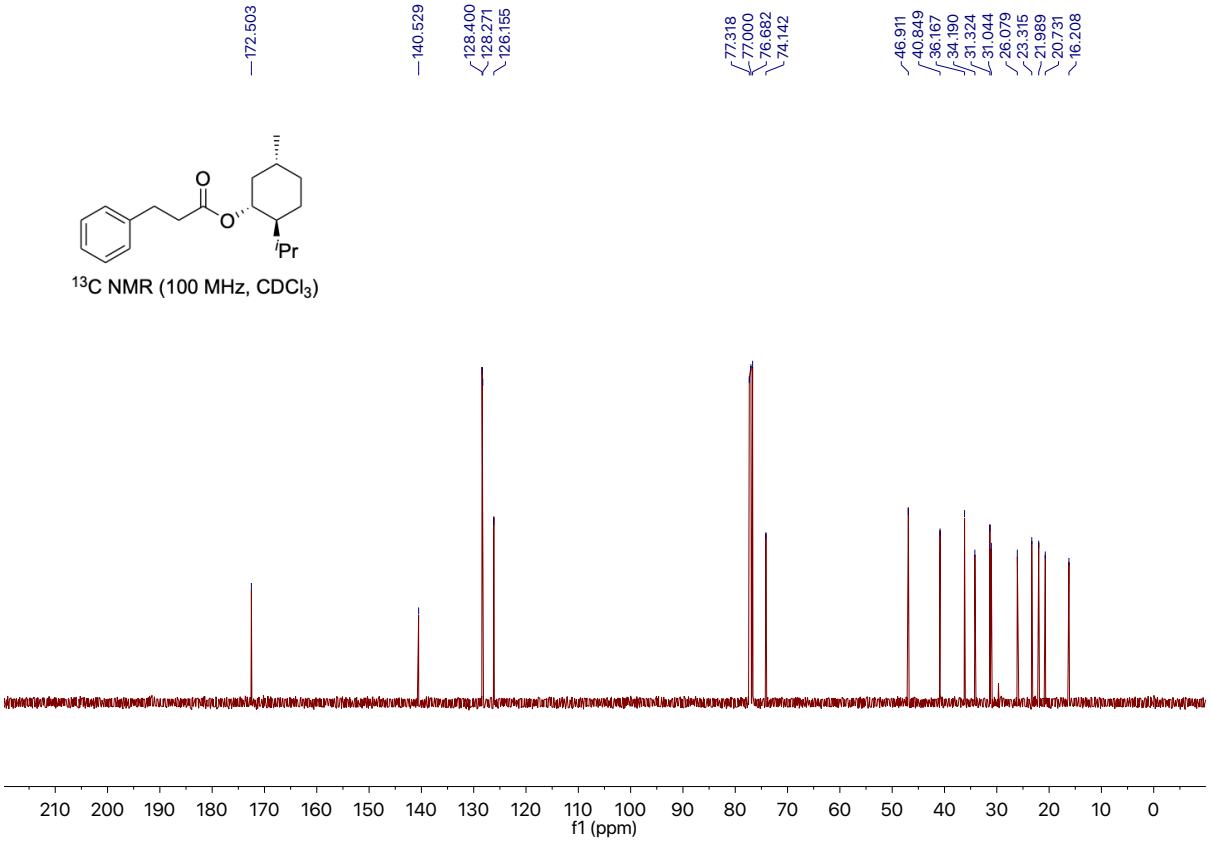


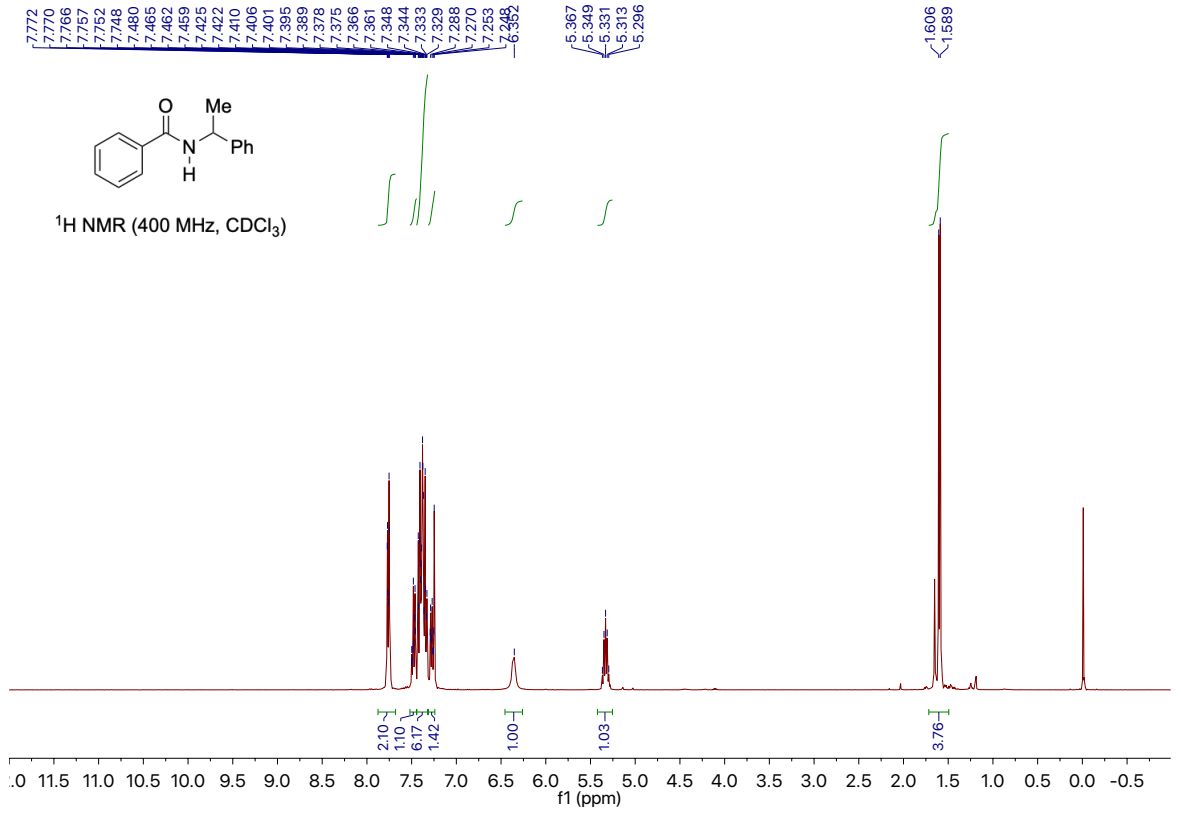
^{1}H NMR (400 MHz, $CDCl_3$)



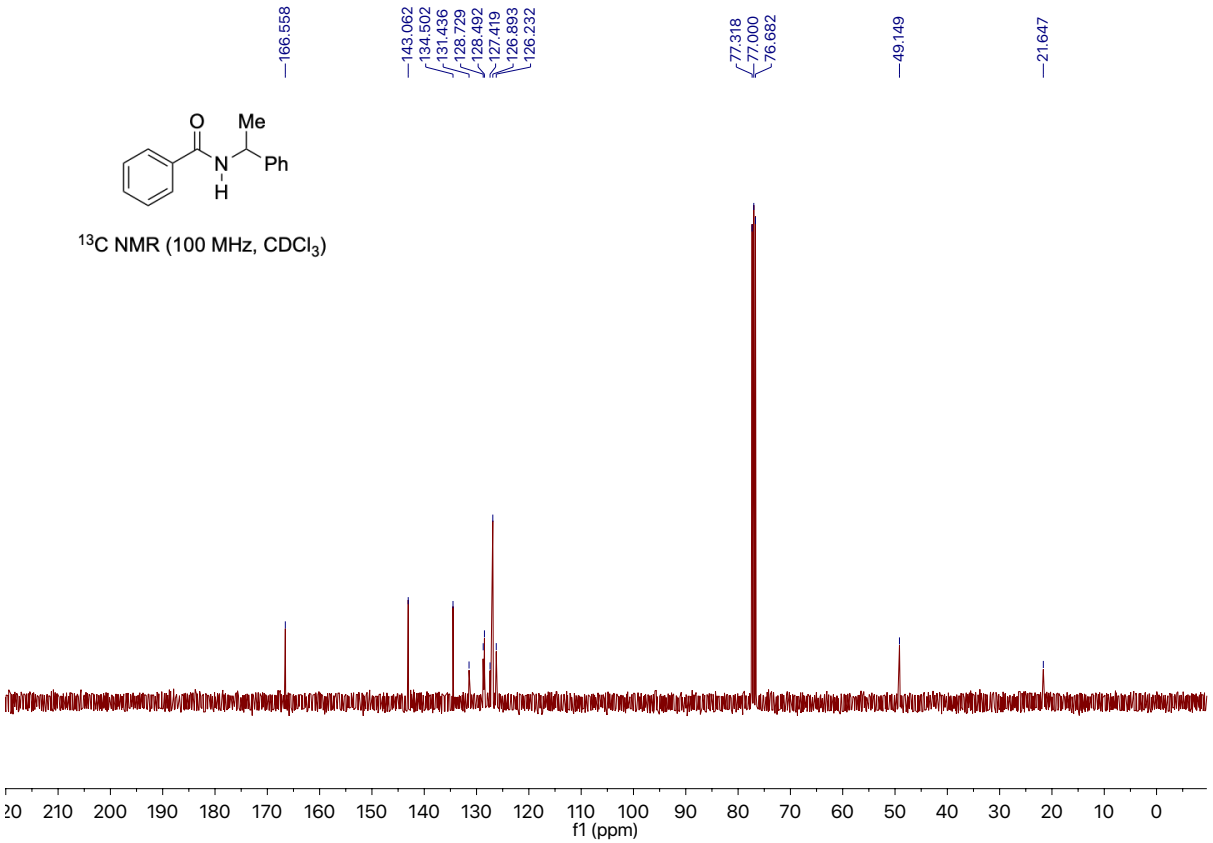
^{13}C NMR (100 MHz, $CDCl_3$)


7.289 7.269 7.251 7.249 7.203 7.184 7.166 4.698 4.687 4.671 4.660 4.644 4.633 2.960 2.941 2.922 2.624 2.604 2.585 1.939 1.928 1.922 1.910 1.736 1.730 1.719 1.712 1.701 1.695 1.682 1.676 1.668 1.659 1.650 1.642 1.634 1.625 1.616 1.603 1.489 1.476 1.467 1.459 1.451 1.443 1.438 1.430 1.357 1.350 1.342 1.320 1.299 1.292 1.284 1.247 1.065 1.041 1.033 1.009 1.001 0.977 0.969 0.889 0.873 0.846 0.828 0.701 0.683
O
O
iPr
1H NMR (400 MHz, CDCl3)
2.17 2.89 1.00 1.98 2.00 1.04 3.53 1.16 1.31 1.55 8.84 3.10
f1 (ppm)

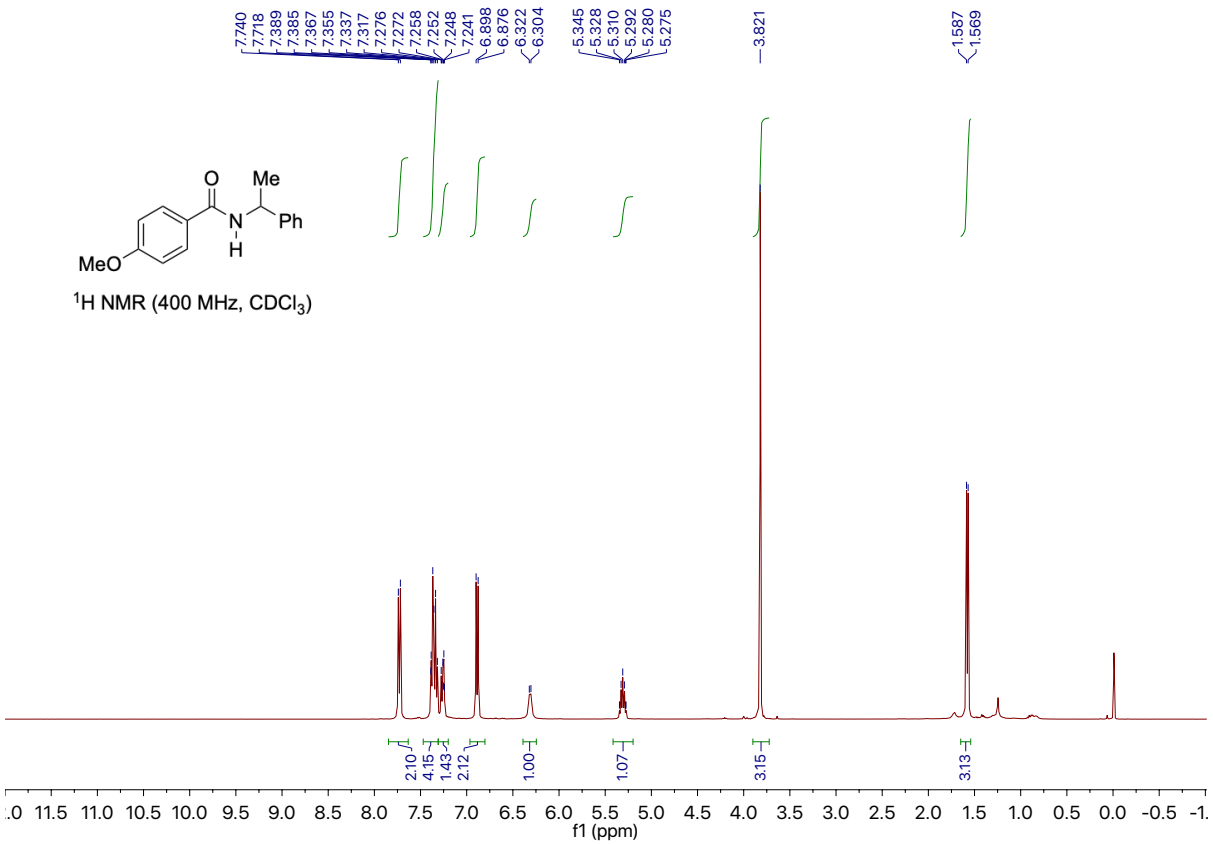

172.503 140.529 128.400 128.271 126.155 77.318 77.000 76.682 74.142 46.911 40.849 36.167 34.190 31.324 31.044 26.079 23.315 21.989 20.731 16.208
O
O
iPr
13C NMR (100 MHz, CDCl3)
f1 (ppm)



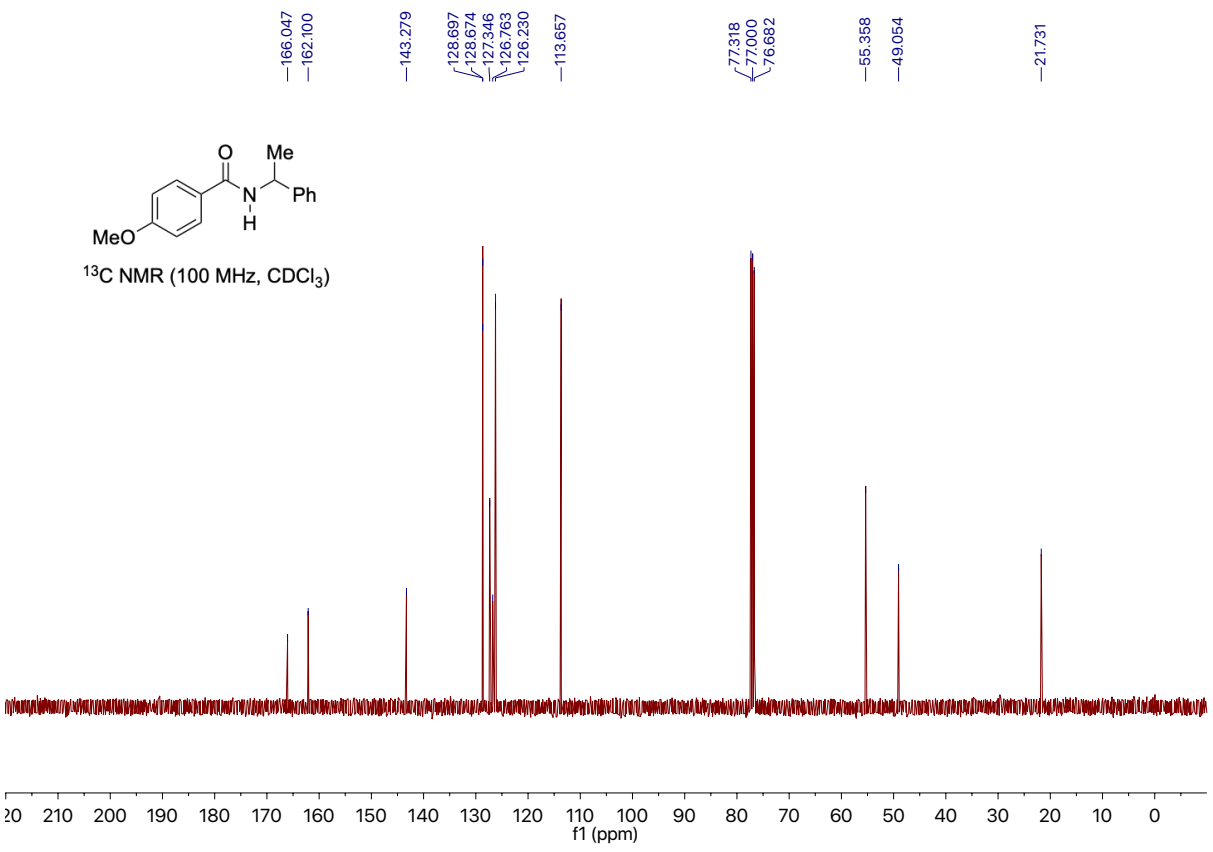
^{1}H NMR (400 MHz, $CDCl_3$)



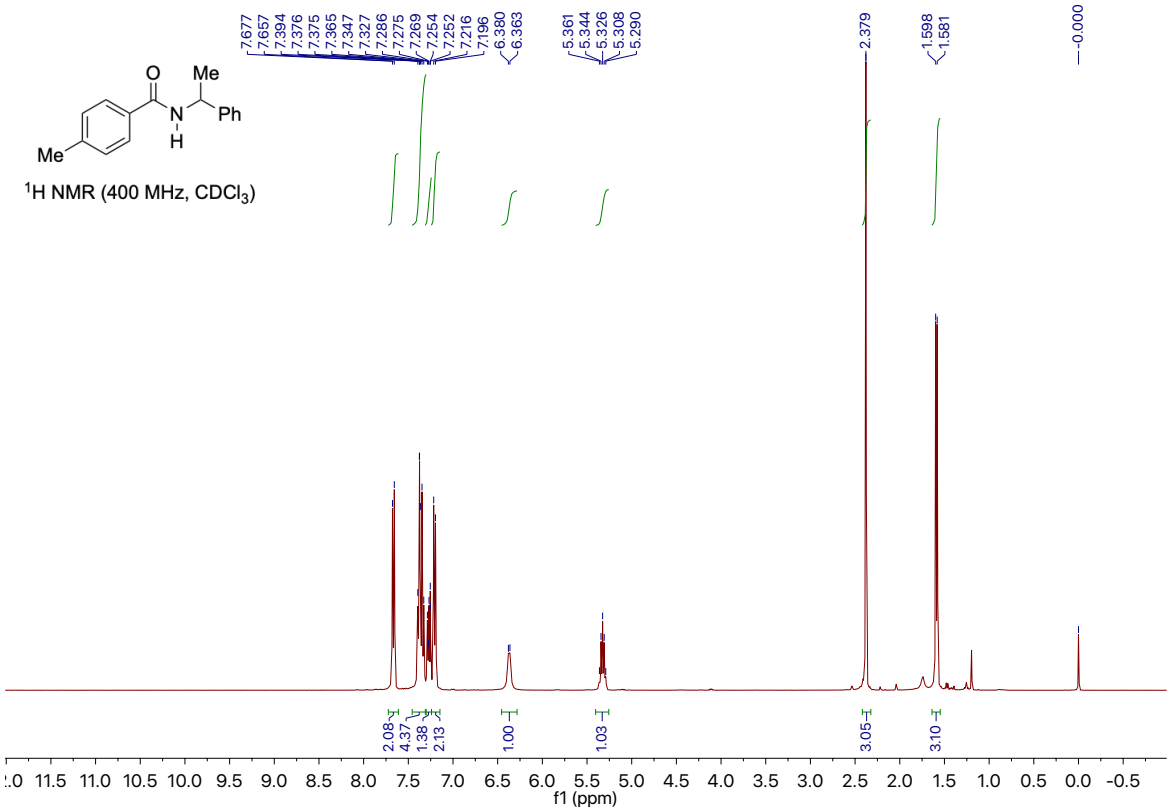
^{13}C NMR (100 MHz, $CDCl_3$)



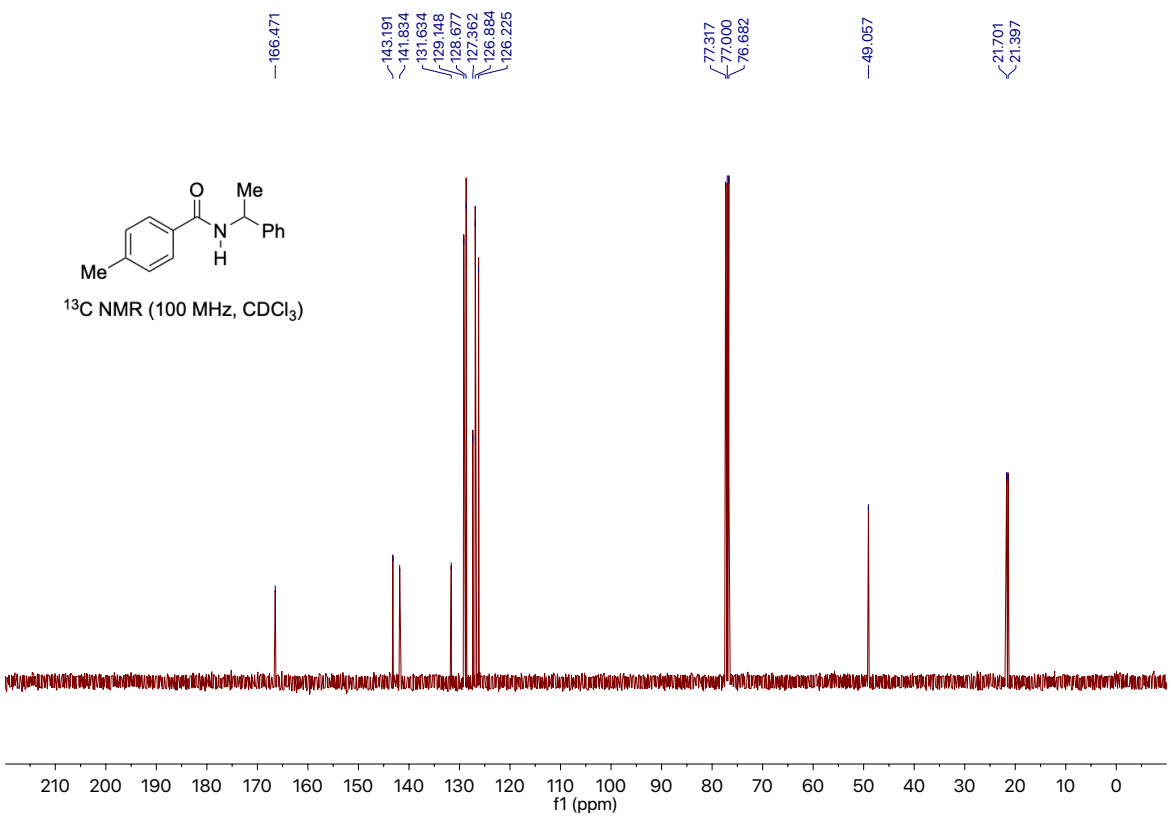
^{1}H NMR (400 MHz, $CDCl_3$)



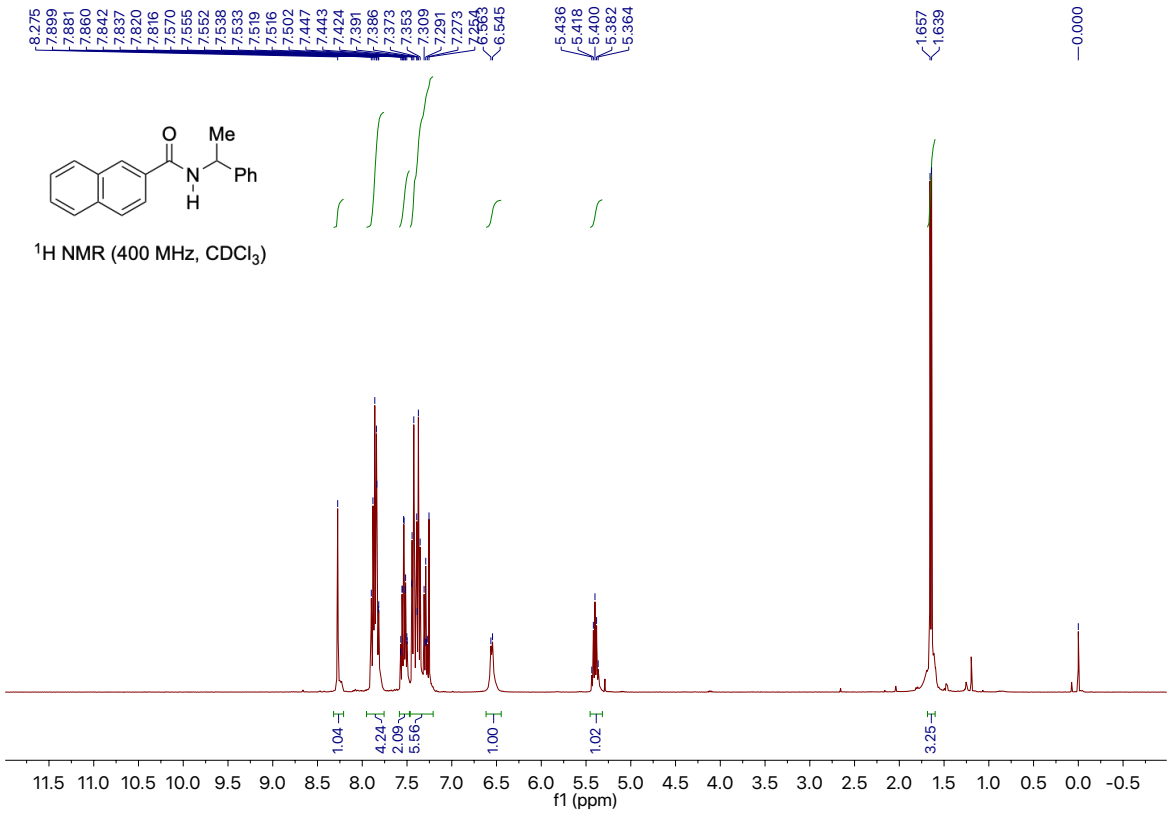
^{13}C NMR (100 MHz, $CDCl_3$)



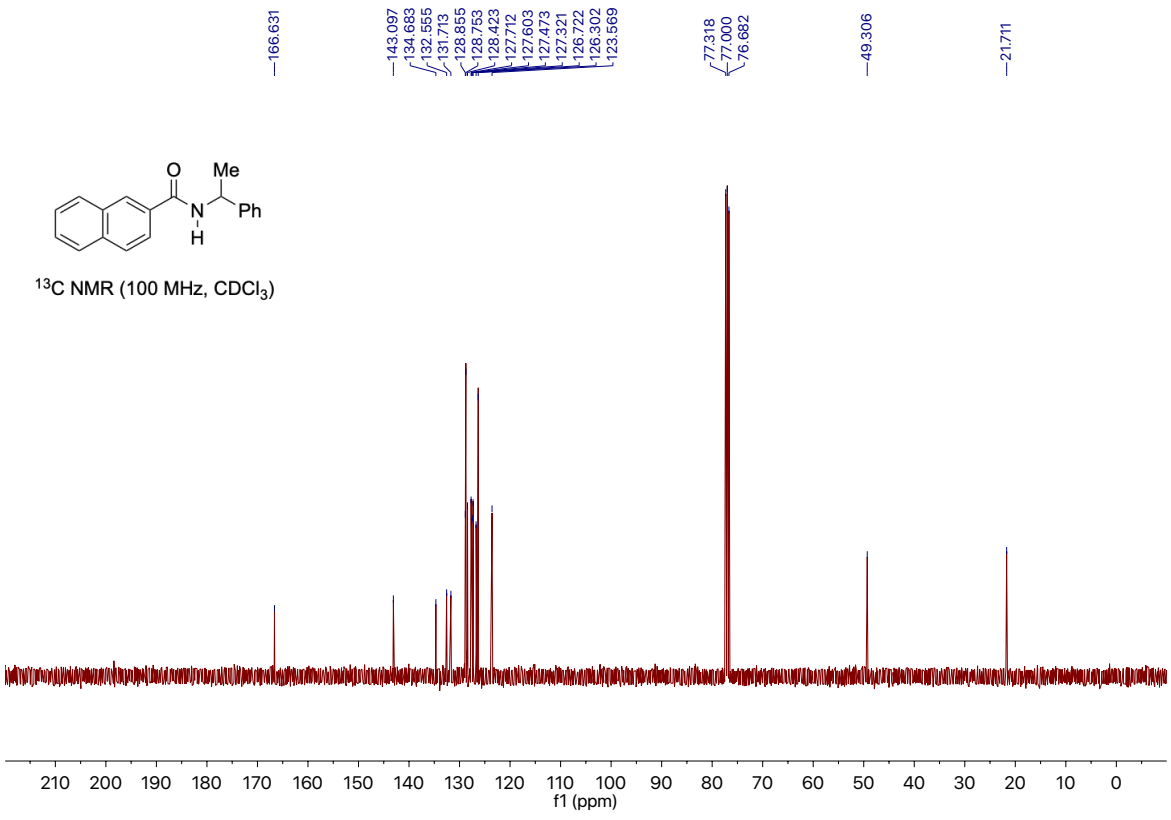
^{1}H NMR (400 MHz, $CDCl_3$)



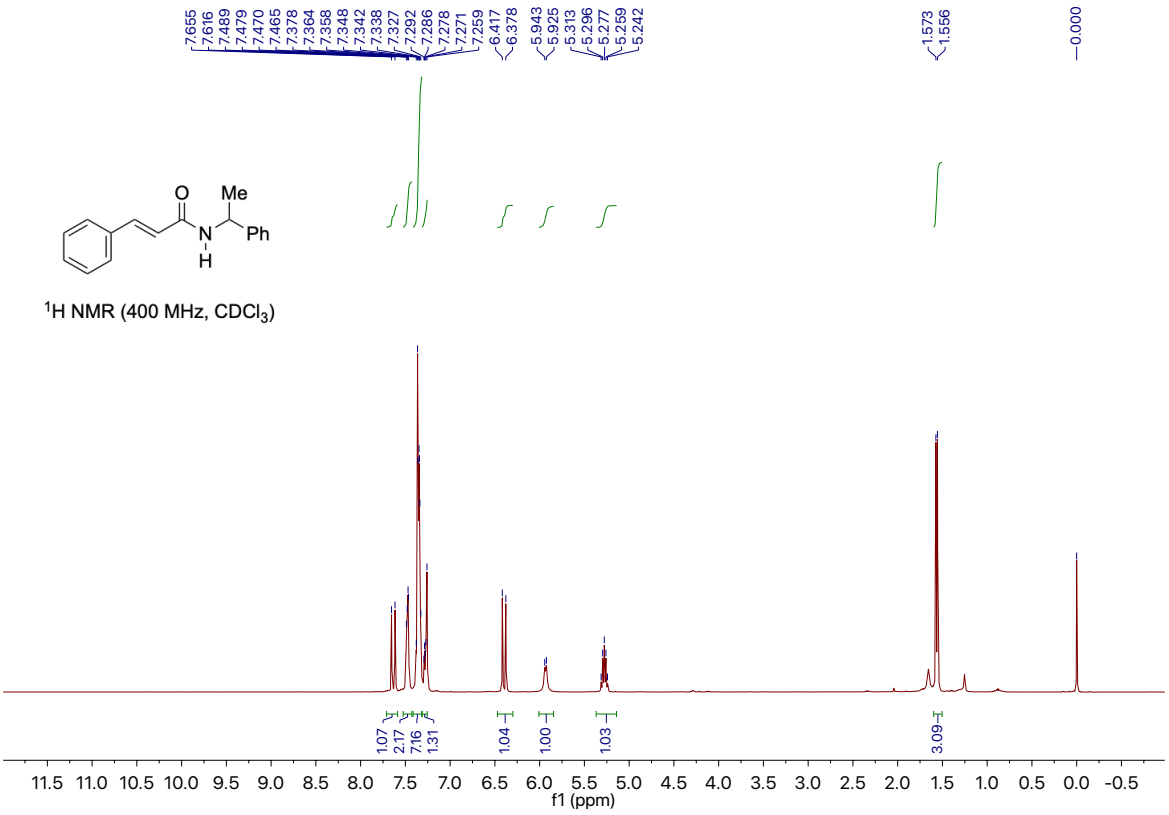
^{13}C NMR (100 MHz, $CDCl_3$)



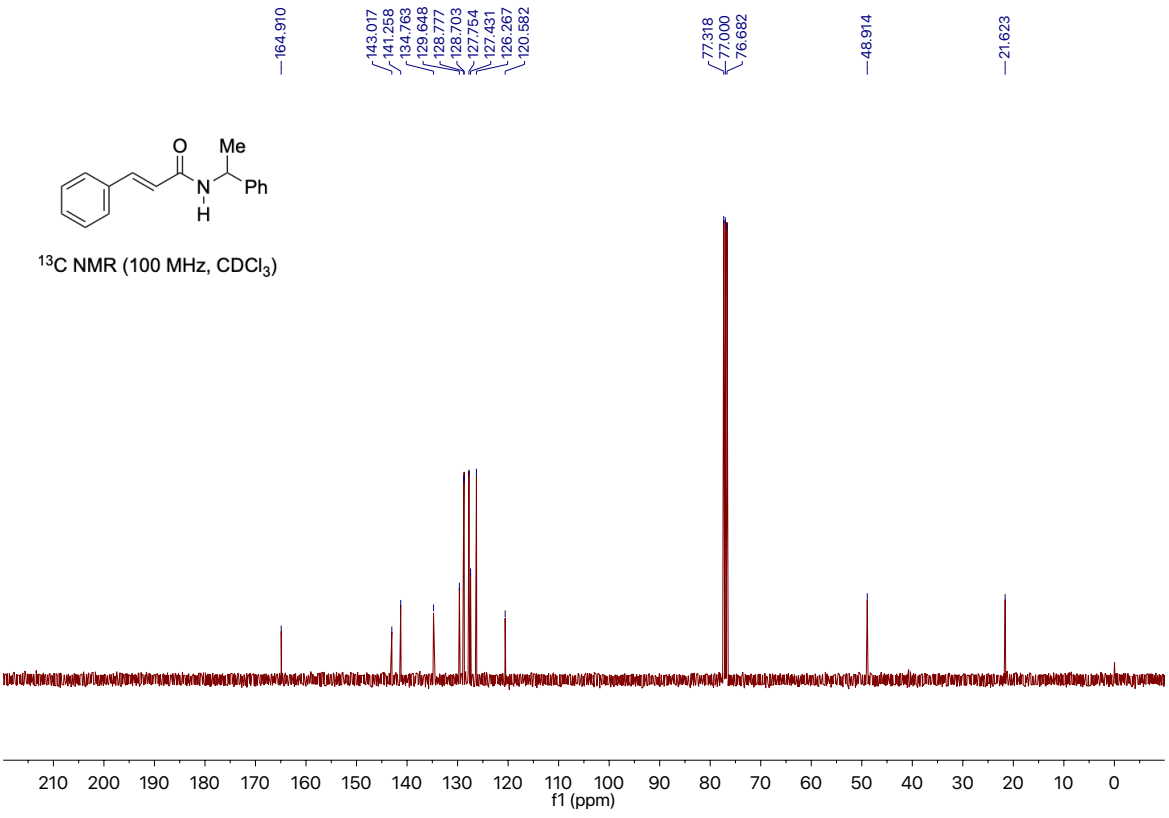
^{1}H NMR (400 MHz, $CDCl_3$)



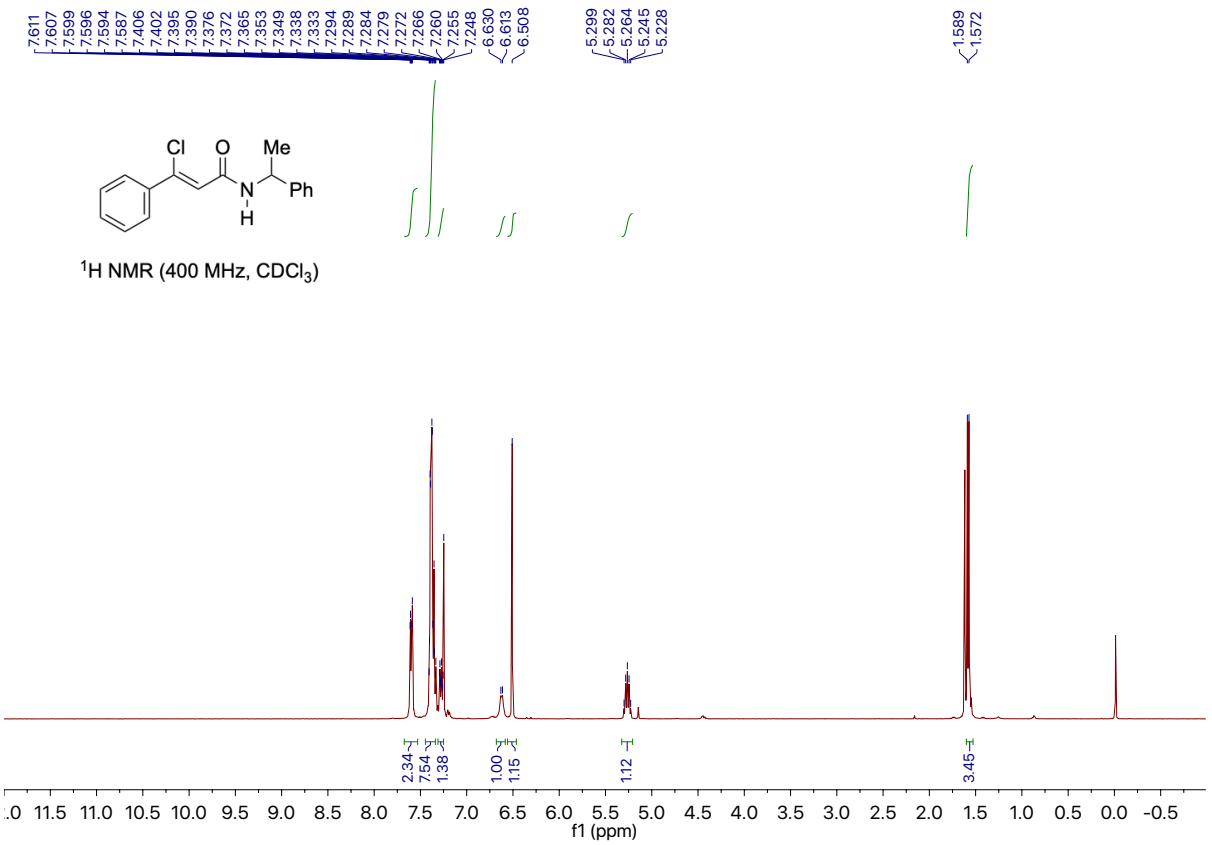
^{13}C NMR (100 MHz, $CDCl_3$)



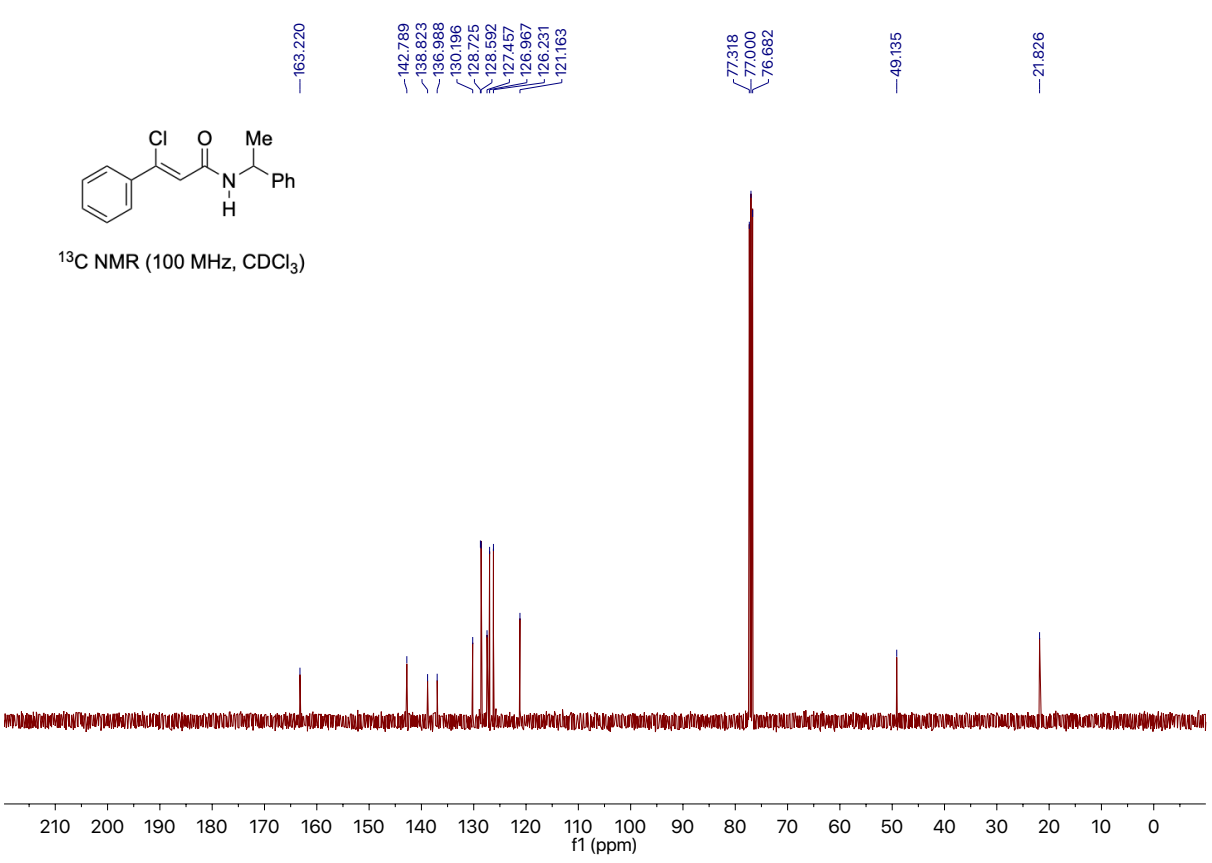
^{1}H NMR (400 MHz, $CDCl_3$)



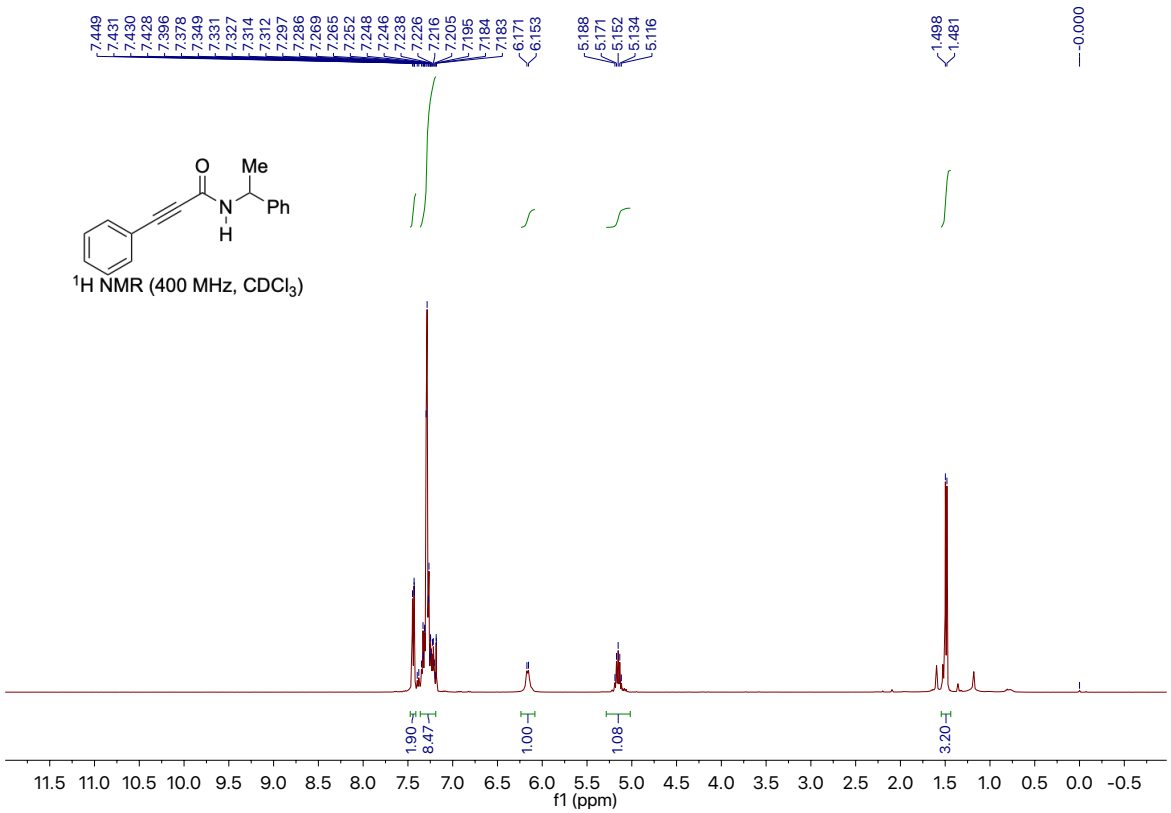
^{13}C NMR (100 MHz, $CDCl_3$)

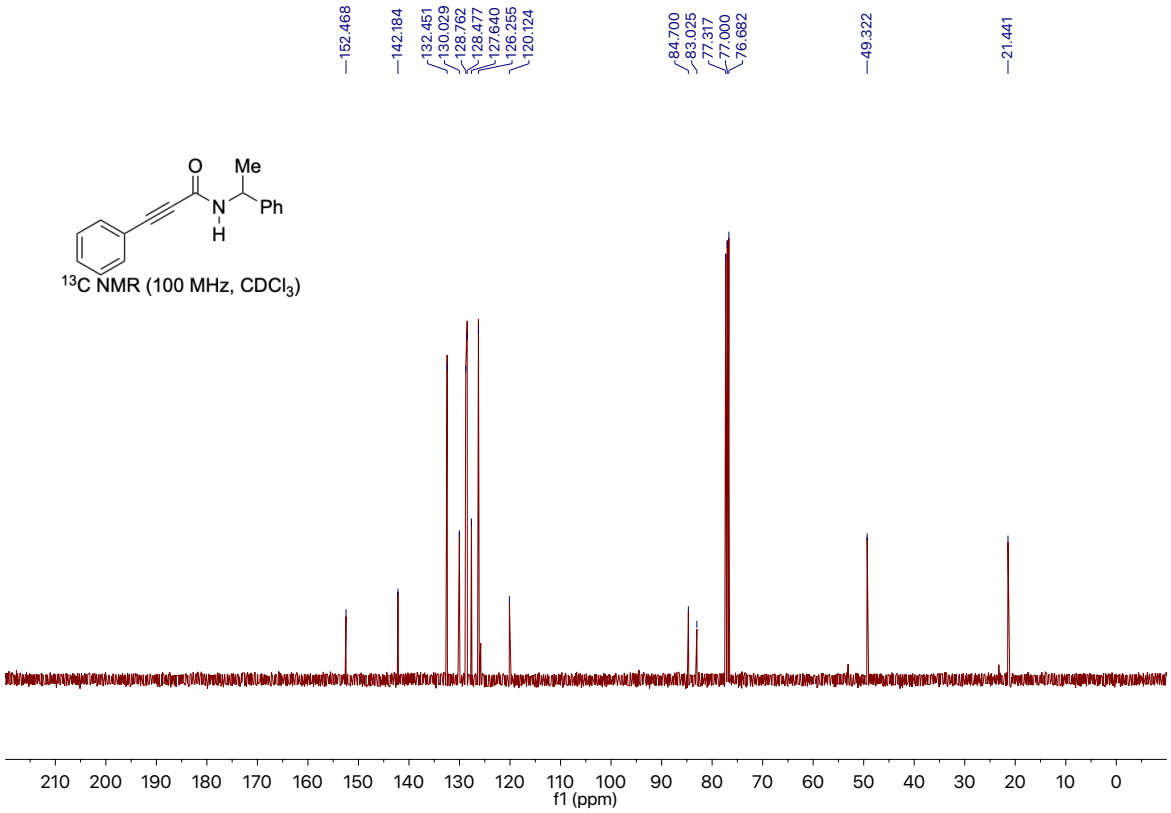


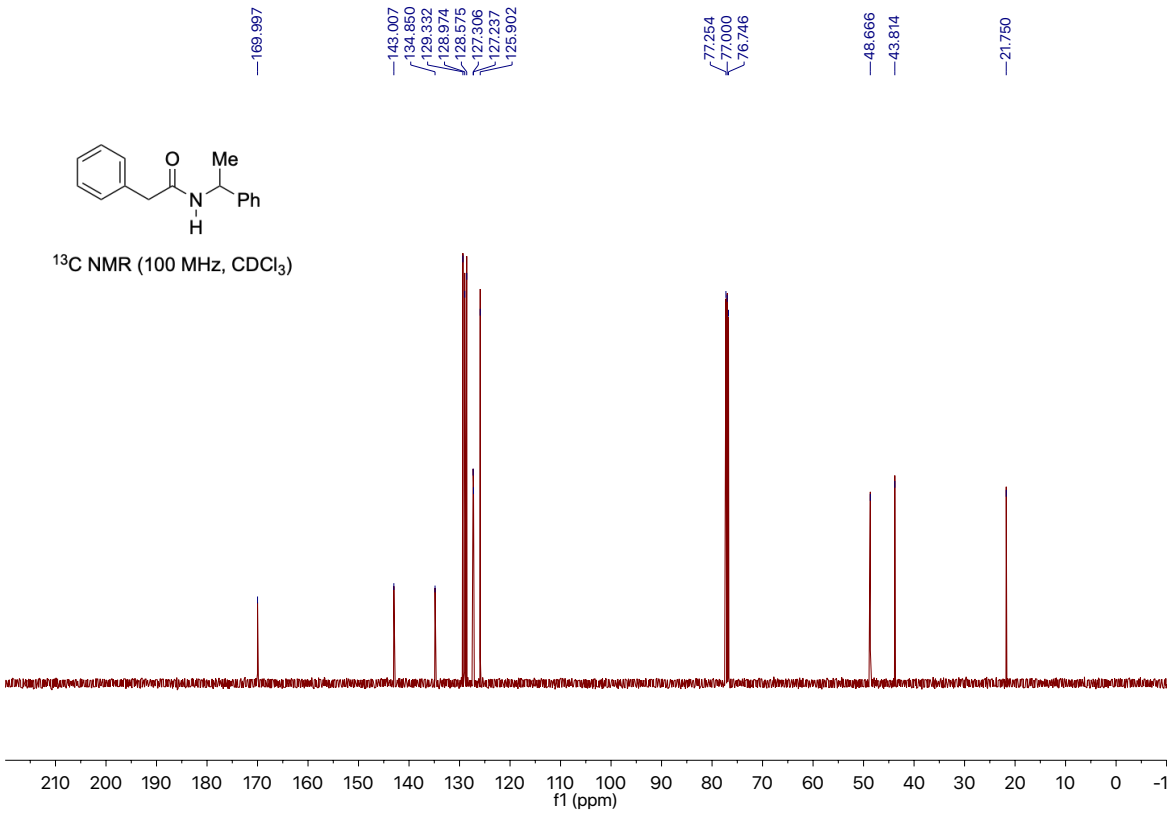
^{1}H NMR (400 MHz, $CDCl_3$)

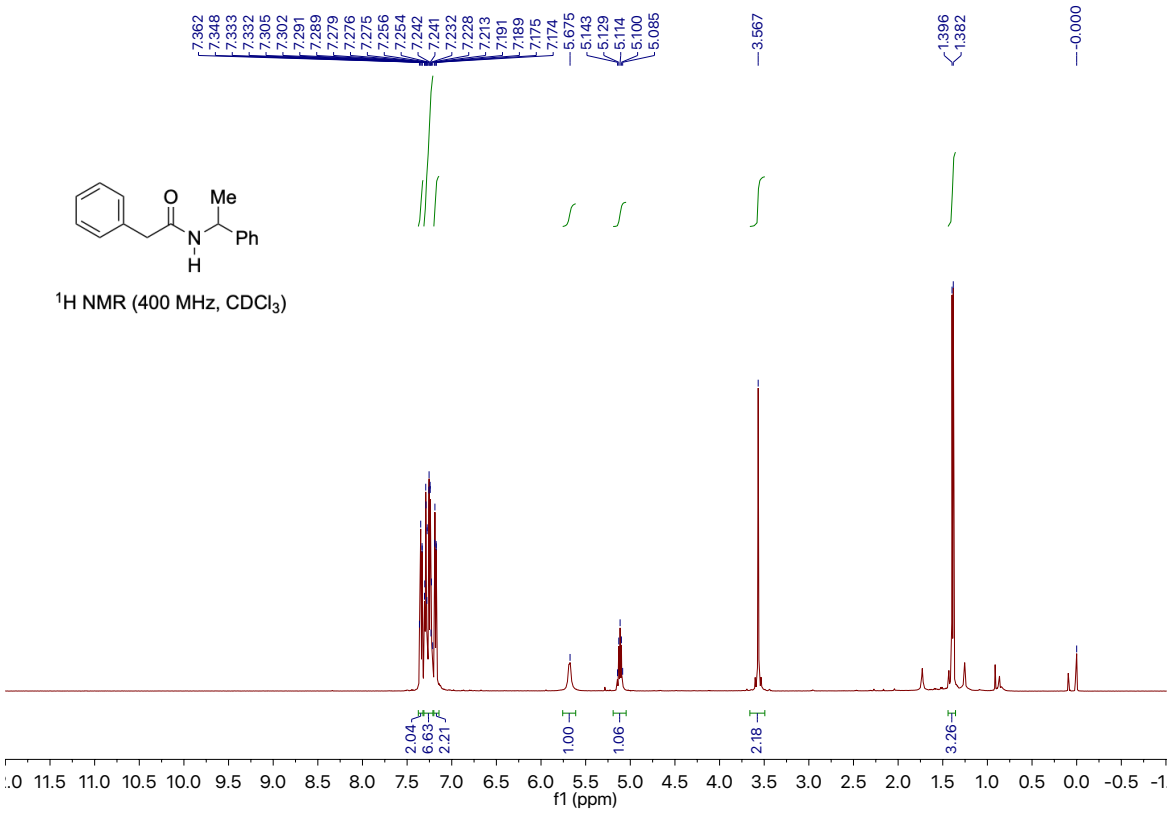


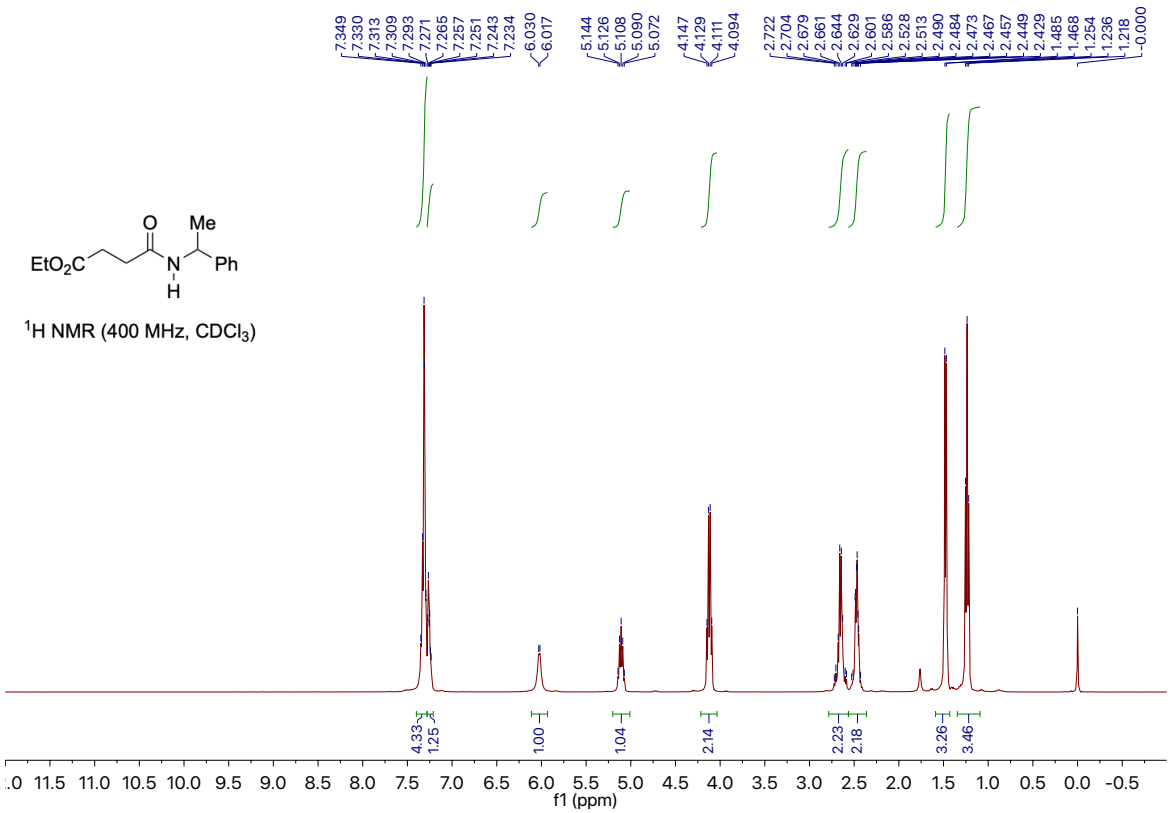
^{13}C NMR (100 MHz, $CDCl_3$)

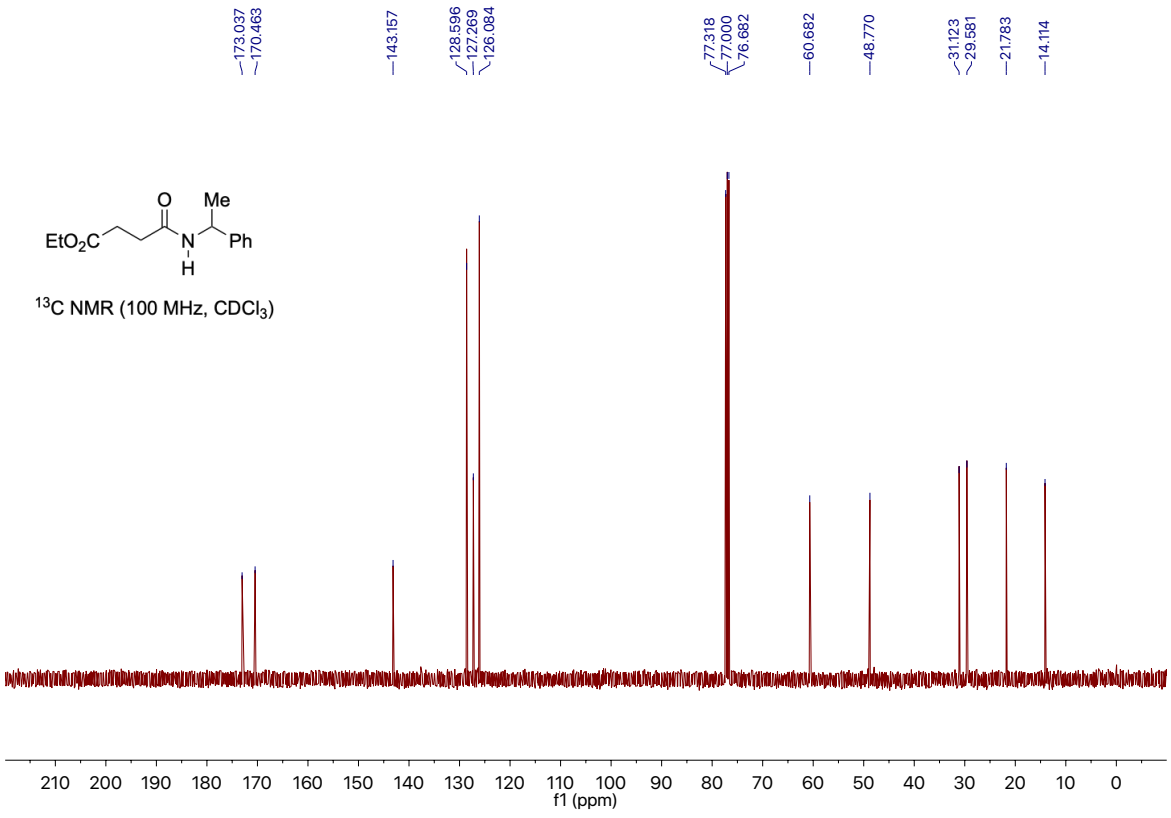

7.449
7.431
7.430
7.428
7.396
7.378
7.349
7.331
7.327
7.314
7.312
7.297
7.286
7.269
7.265
7.252
7.248
7.246
7.238
7.226
7.216
7.205
7.195
7.184
7.183
6.171
6.153
5.188
5.171
5.152
5.134
5.116
1.498
1.481
0.000
O
Me
N
H
Ph
1H NMR (400 MHz, CDCl3)
1.90
8.47
1.00
1.08
3.20
11.5 11.0 10.5 10.0 9.5 9.0 8.5 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)

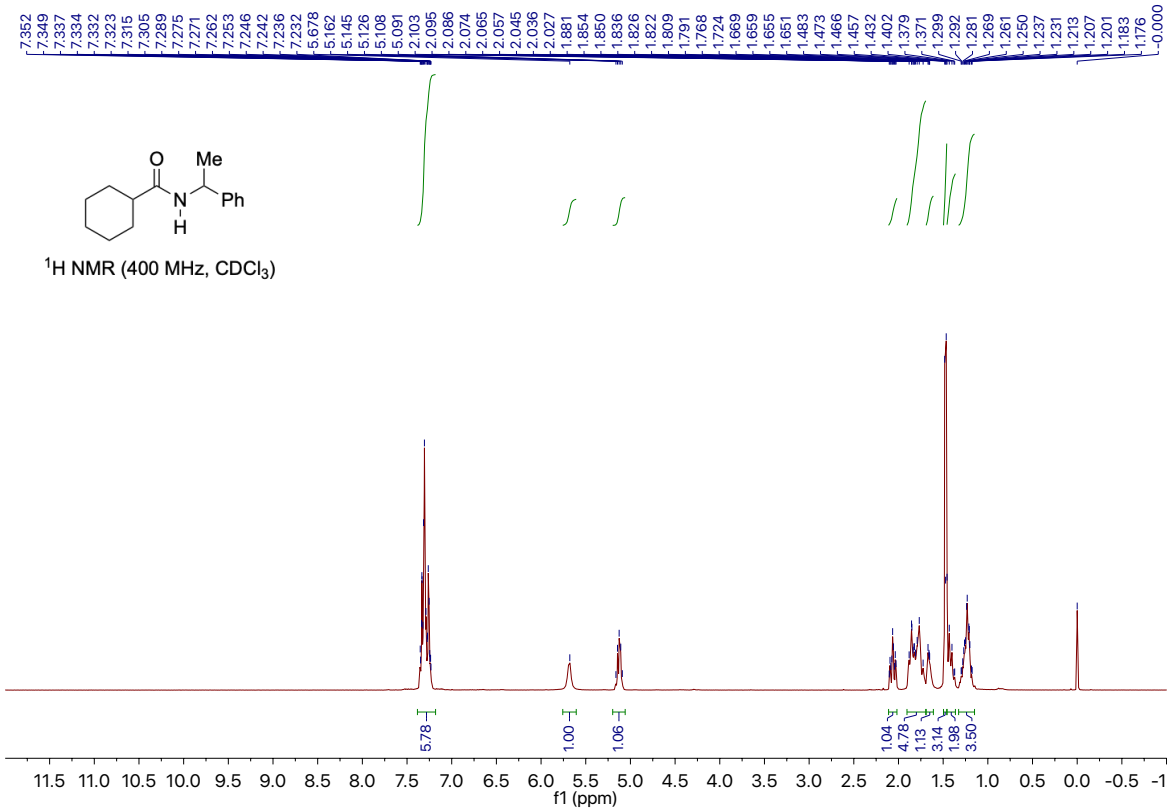

152.468
142.184
132.451
130.029
128.762
128.477
127.640
126.255
120.124
84.700
83.025
77.317
77.000
76.682
49.322
21.441
O
Me
N
H
Ph
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


169.997
143.007
134.850
129.332
128.974
128.575
127.306
127.237
125.902
77.254
77.000
76.746
48.666
43.814
21.750
O
Me
N
H
Ph
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

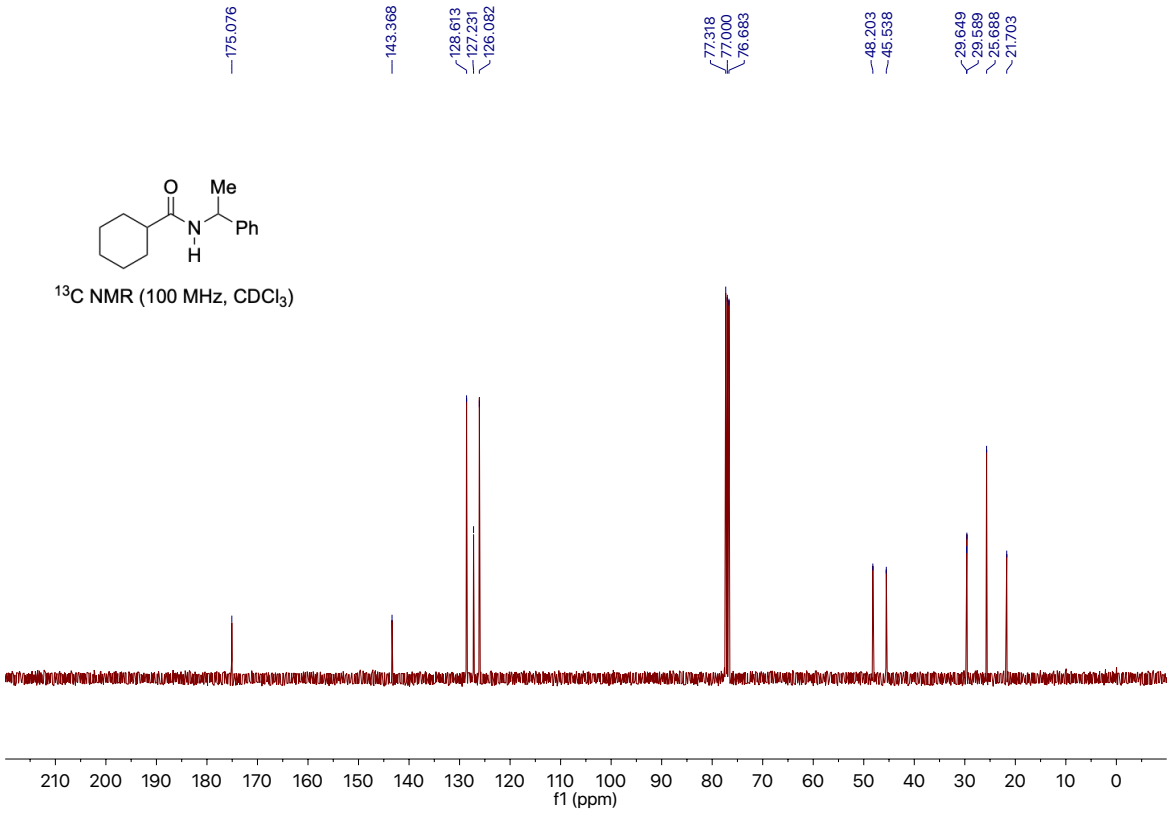

7.362
7.348
7.333
7.332
7.305
7.302
7.291
7.289
7.279
7.276
7.275
7.256
7.254
7.242
7.241
7.232
7.228
7.213
7.191
7.189
7.175
7.174
5.675
5.143
5.129
5.114
5.100
5.085
3.567
1.396
1.382
0.000
O
Me
N
H
Ph
1H NMR (400 MHz, CDCl3)
2.04
6.63
2.21
1.00
1.06
2.18
3.26
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 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)


7.349
7.330
7.313
7.309
7.293
7.271
7.265
7.257
7.251
7.243
7.234
6.030
6.017
5.144
5.126
5.108
5.090
5.072
4.147
4.129
4.111
4.094
2.722
2.704
2.679
2.661
2.644
2.629
2.601
2.586
2.528
2.513
2.490
2.484
2.473
2.467
2.457
2.449
2.429
1.485
1.468
1.254
1.236
1.218
-0.000
O
Me
EtO2C
N
Ph
H
1H NMR (400 MHz, CDCl3)
4.33
1.25
1.00
1.04
2.14
2.23
2.18
3.26
3.46
f1 (ppm)

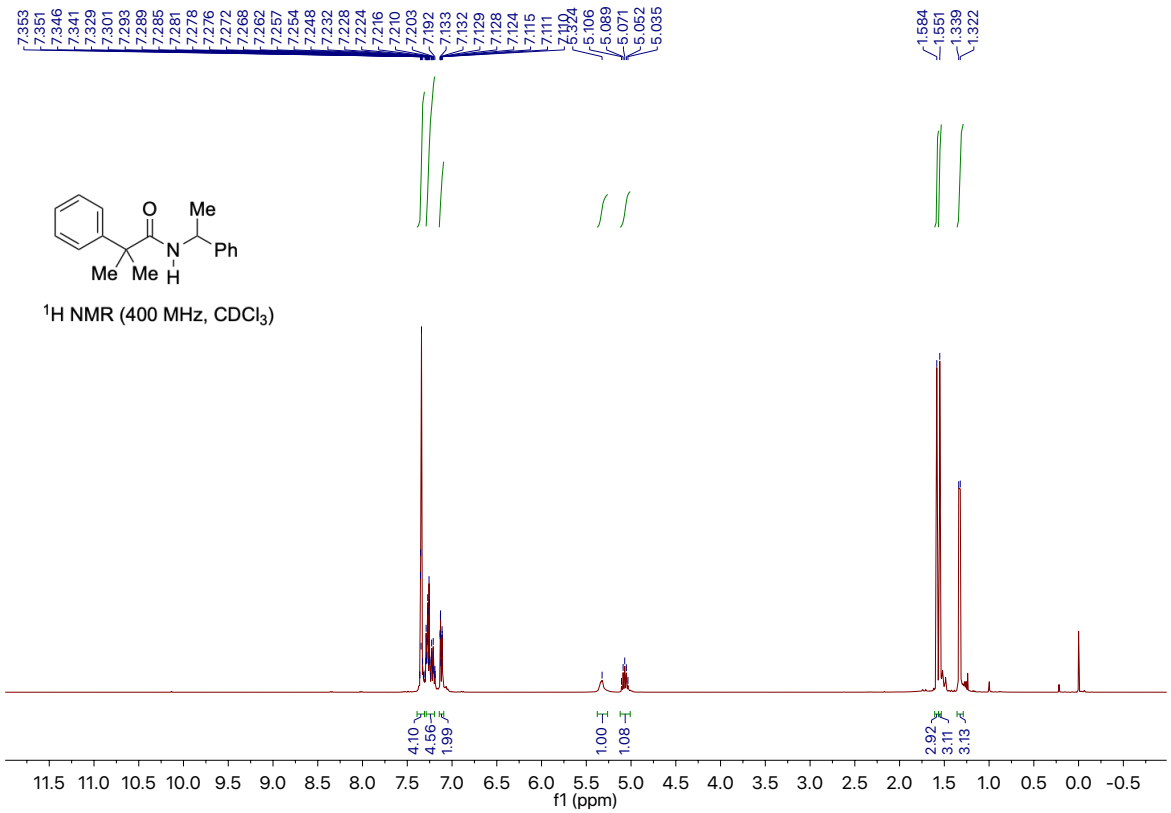

173.037
170.463
143.157
128.596
127.269
126.084
77.318
77.000
76.682
60.682
48.770
31.123
29.581
21.783
14.114
O
Me
EtO2C
N
Ph
H
13C NMR (100 MHz, CDCl3)
f1 (ppm)



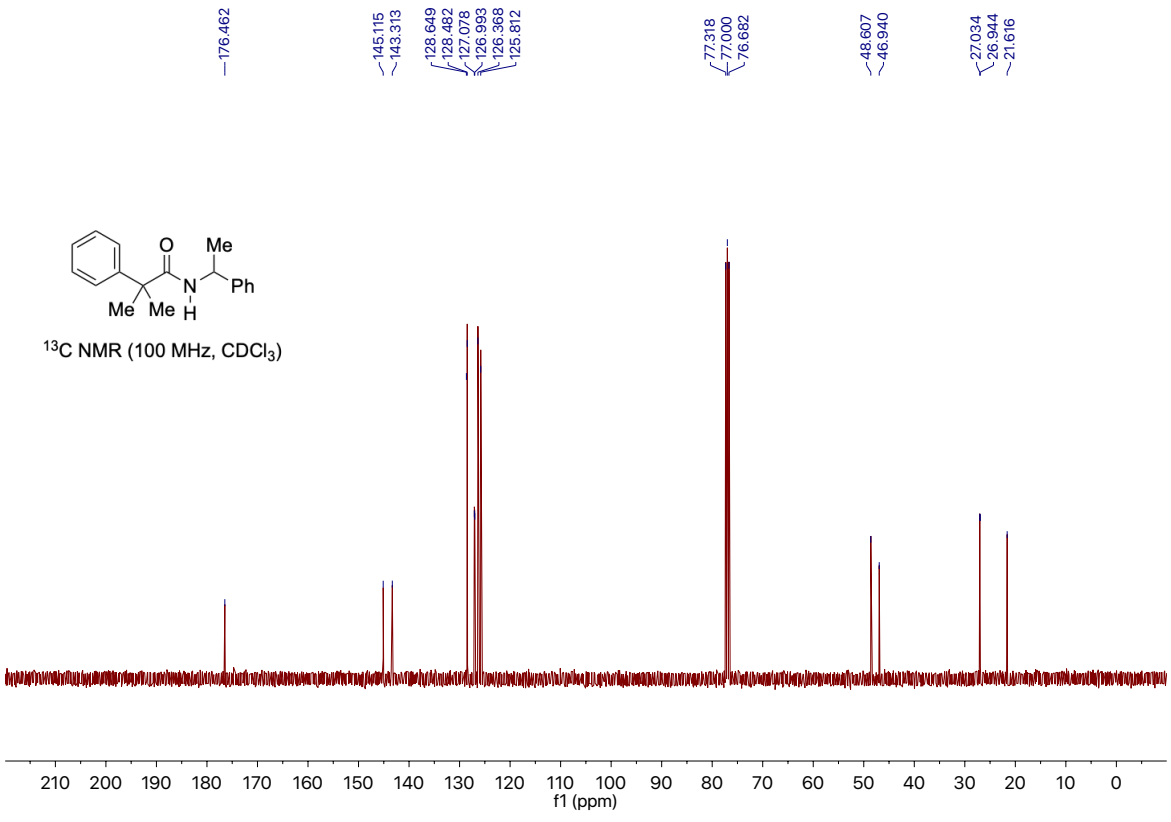
^{1}H NMR (400 MHz, $CDCl_3$)



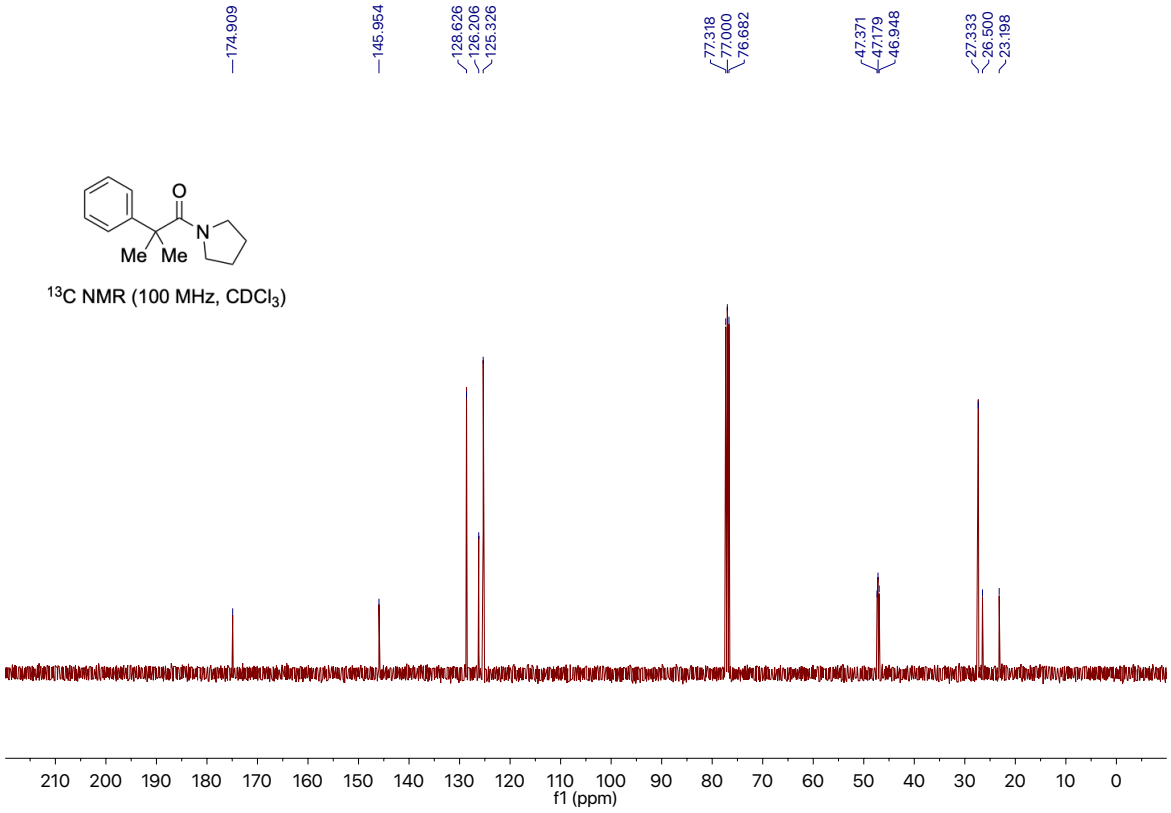
^{13}C NMR (100 MHz, $CDCl_3$)

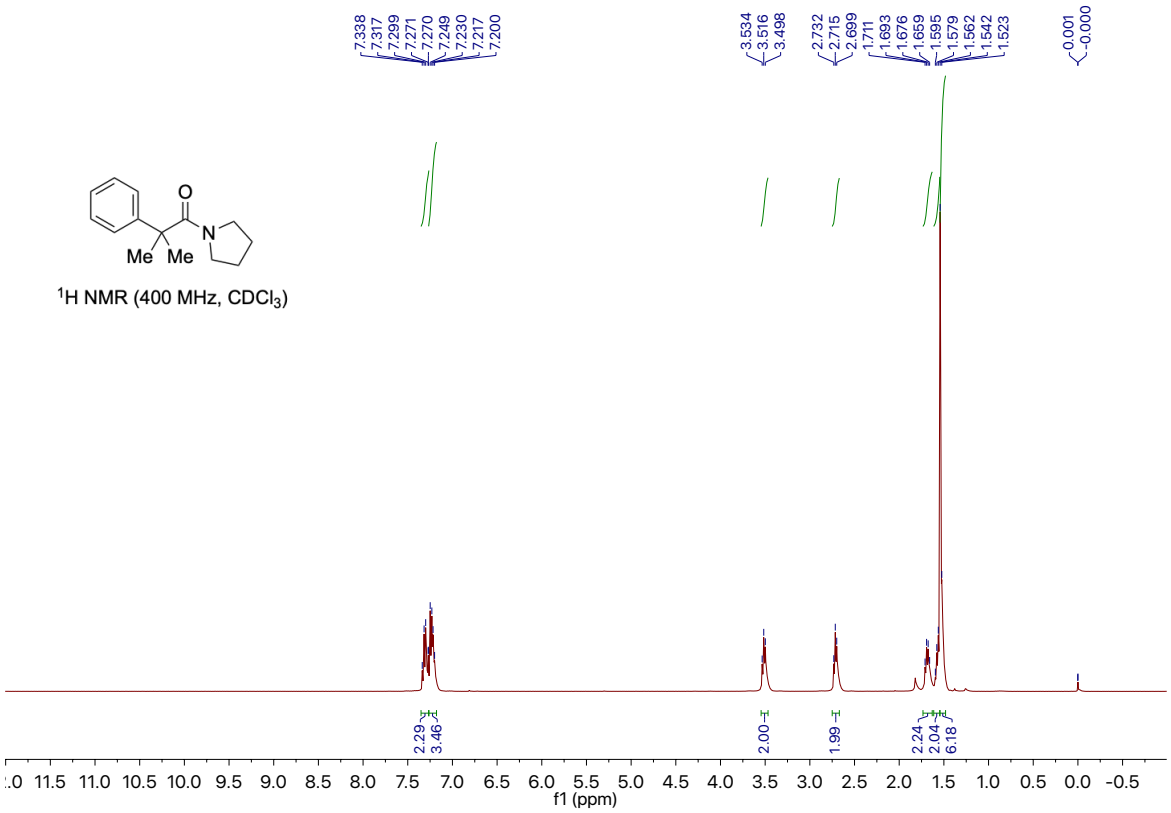


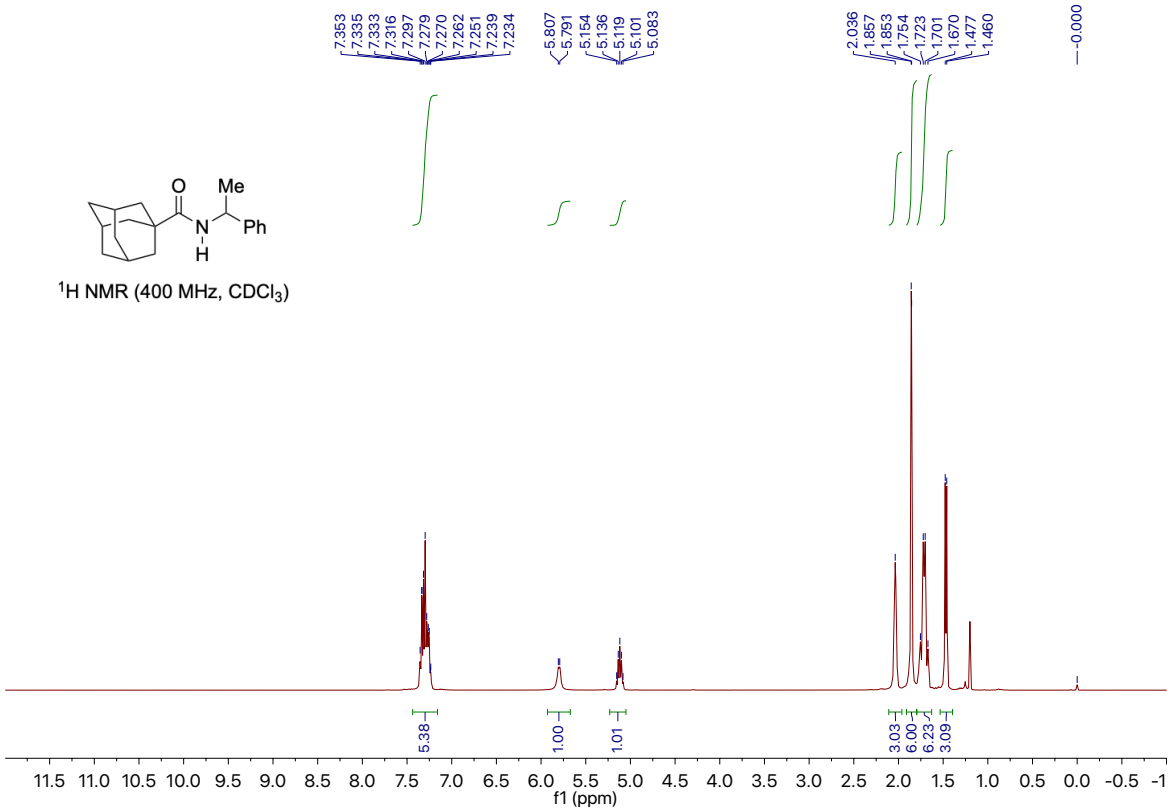
^{1}H NMR (400 MHz, $CDCl_3$)



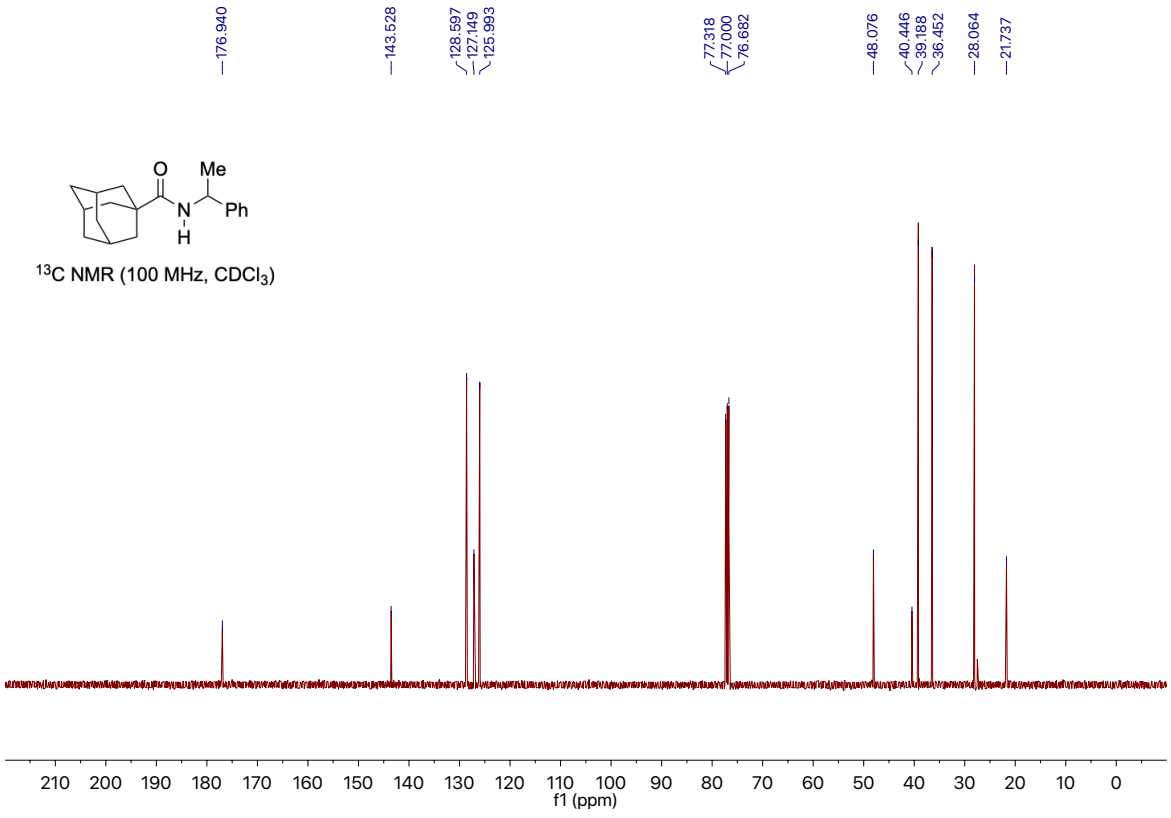
^{13}C NMR (100 MHz, $CDCl_3$)


174.909
145.954
128.626
126.206
125.326
77.318
77.000
76.682
47.371
47.179
46.948
27.333
26.500
23.198
O
N
Me Me
13C NMR (100 MHz, CDCl3)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

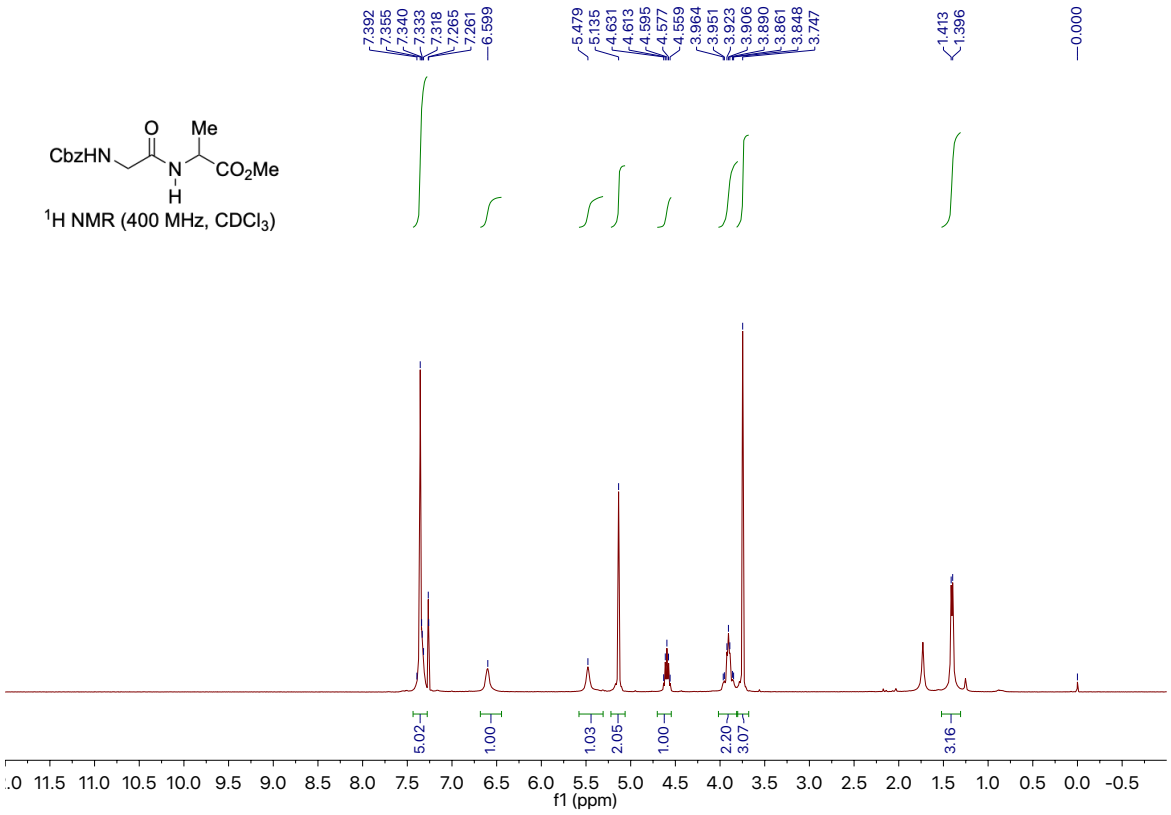

7.338
7.317
7.299
7.271
7.270
7.249
7.230
7.217
7.200
3.534
3.516
3.498
2.732
2.715
2.699
1.711
1.693
1.676
1.659
1.595
1.579
1.562
1.542
1.523
0.001
-0.000
O
N
Me Me
1H NMR (400 MHz, CDCl3)
2.29
3.46
2.00
1.99
2.24
2.04
6.18
.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

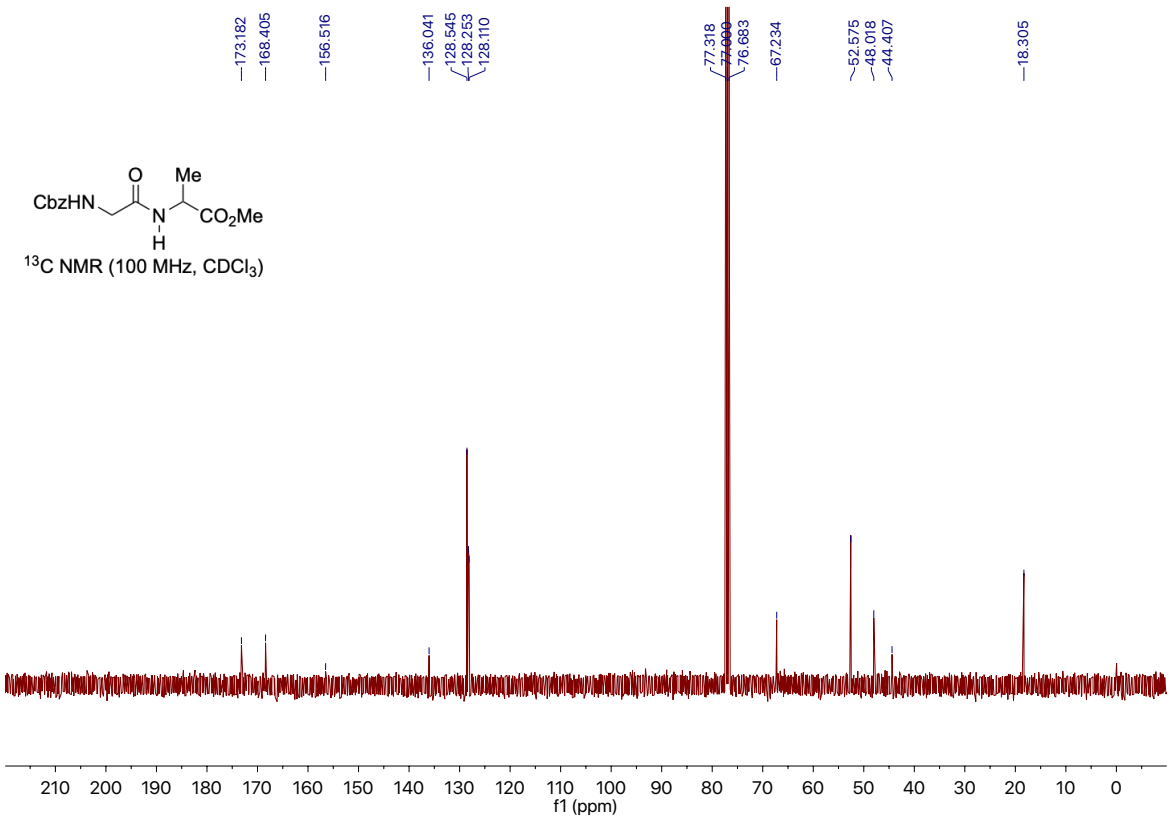


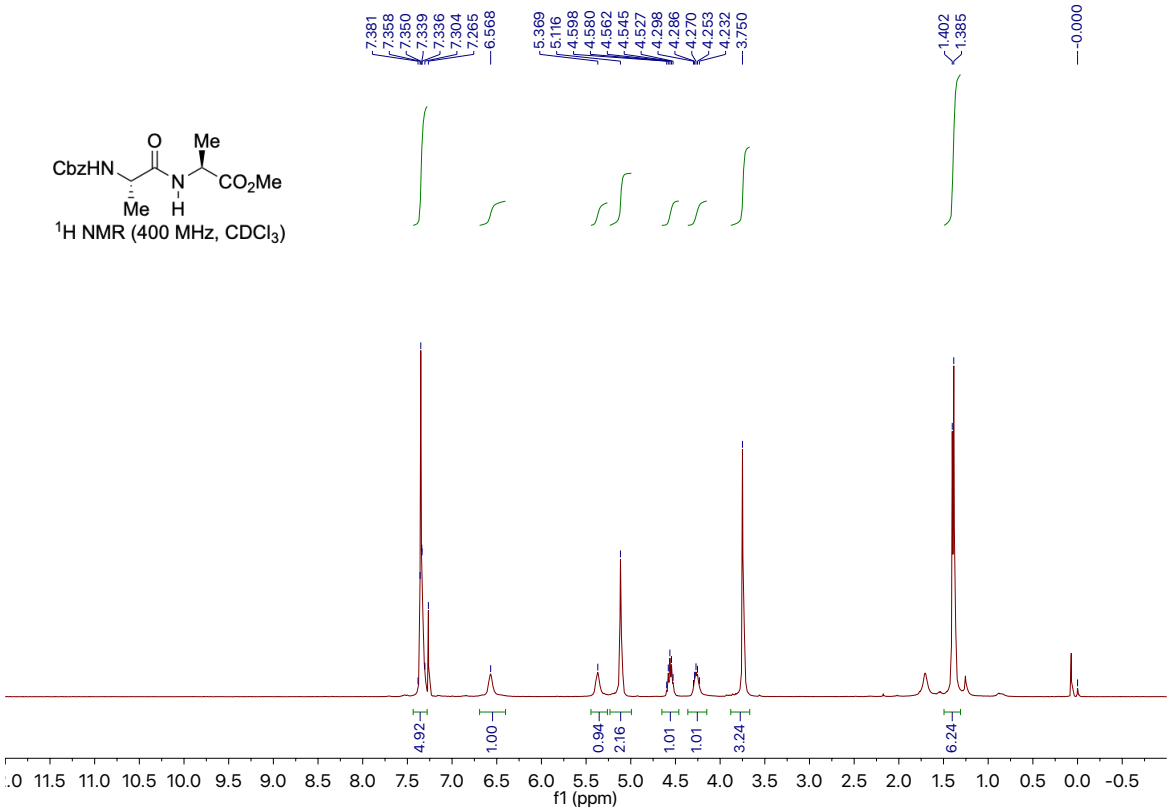
^{1}H NMR (400 MHz, $CDCl_3$)

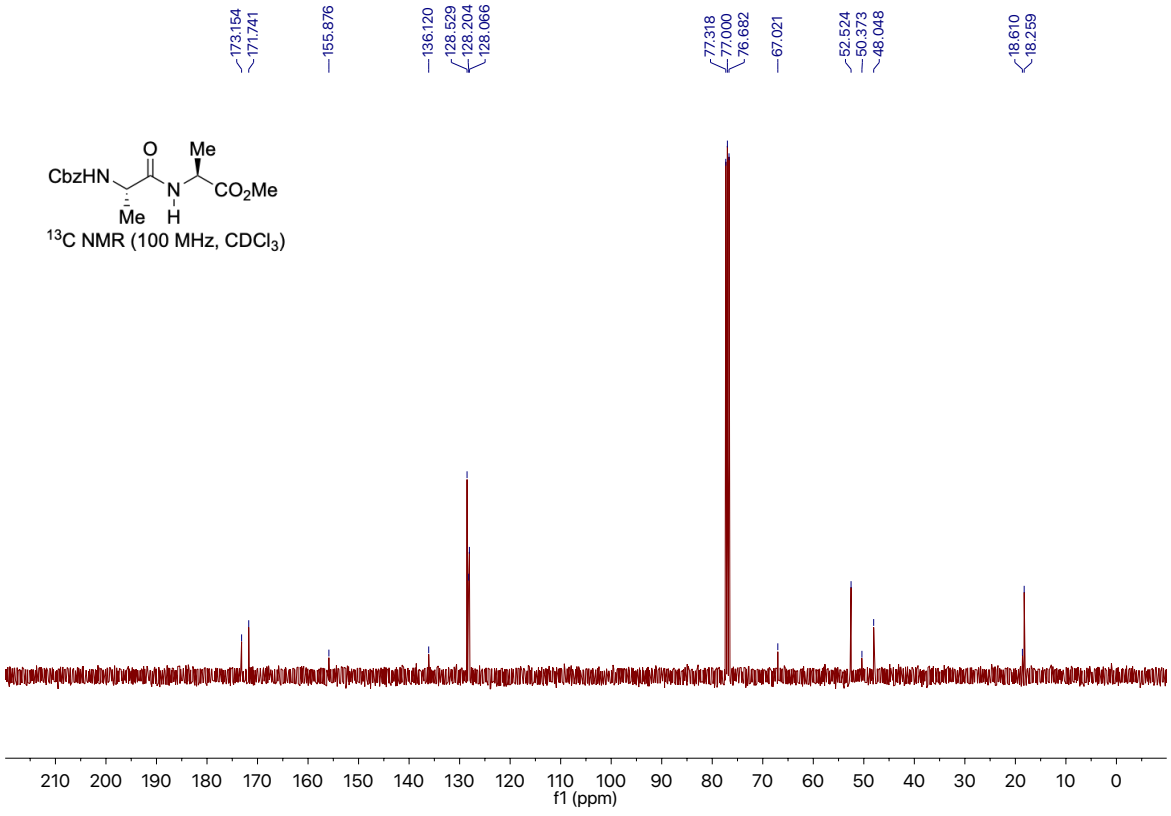


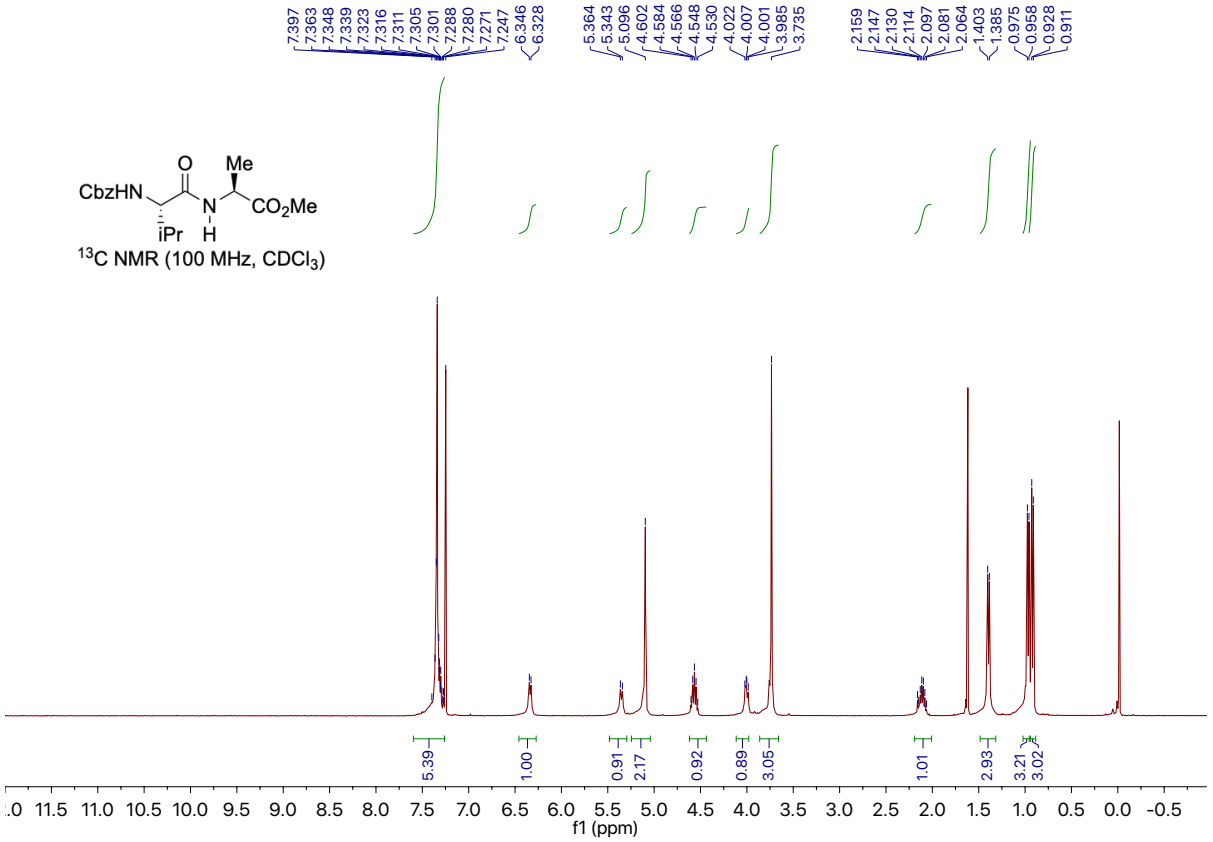
^{13}C NMR (100 MHz, $CDCl_3$)

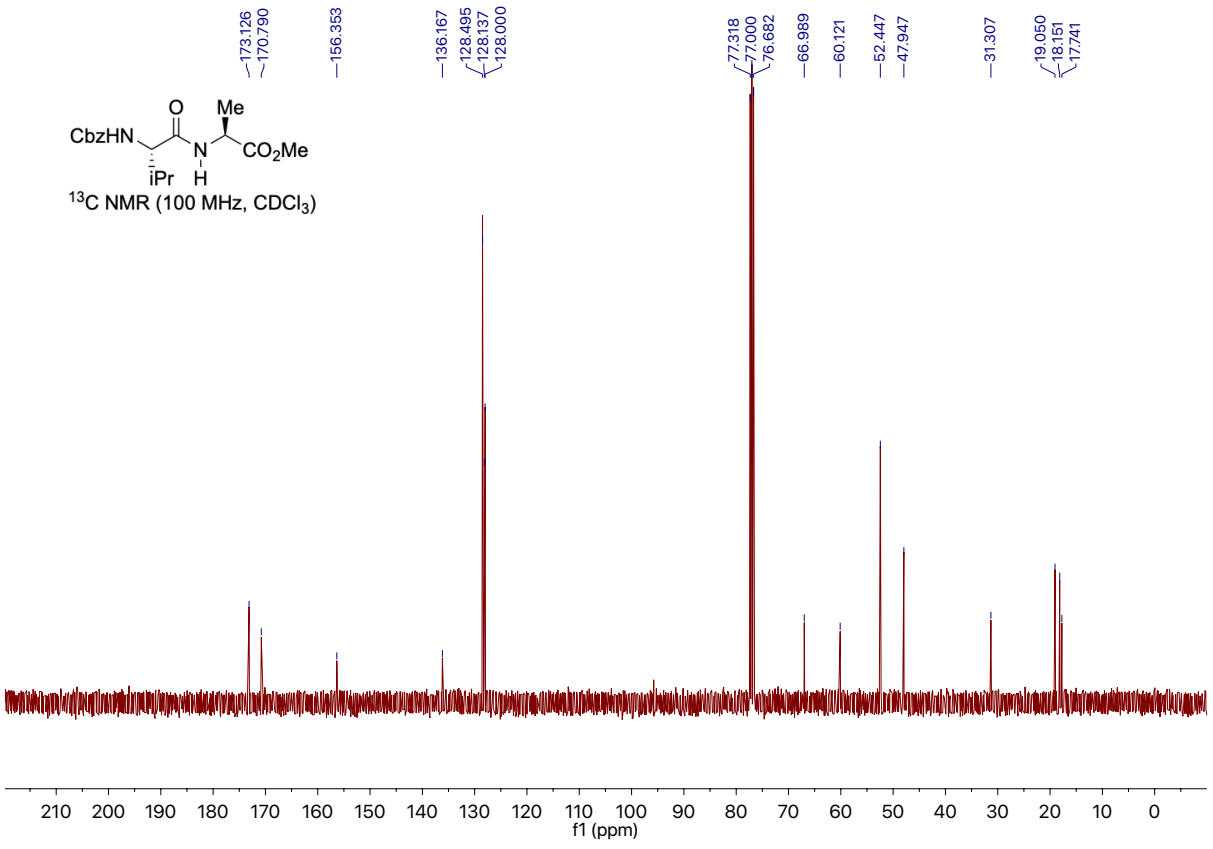

7.392
7.355
7.340
7.333
7.318
7.265
7.261
6.599
5.479
5.135
4.631
4.613
4.595
4.577
4.559
3.964
3.951
3.923
3.906
3.890
3.861
3.848
3.747
1.413
1.396
0.000
O
Me
CbzHN
N
CO2Me
H
1H NMR (400 MHz, CDCl3)
5.02
1.00
1.03
2.05
1.00
2.20
3.07
3.16
f1 (ppm)

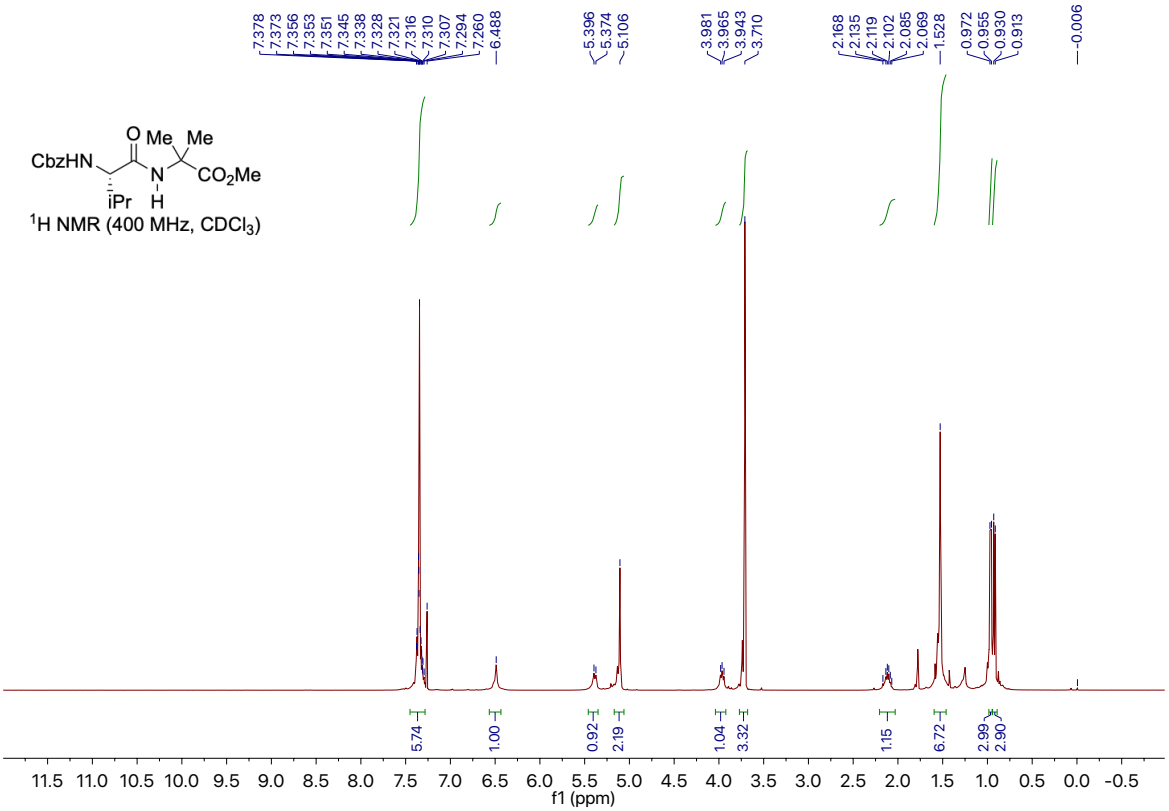

173.182
168.405
156.516
136.041
128.545
128.253
128.110
77.318
77.000
76.683
67.234
52.575
48.018
44.407
18.305
O
Me
CbzHN
N
CO2Me
H
13C NMR (100 MHz, CDCl3)
f1 (ppm)

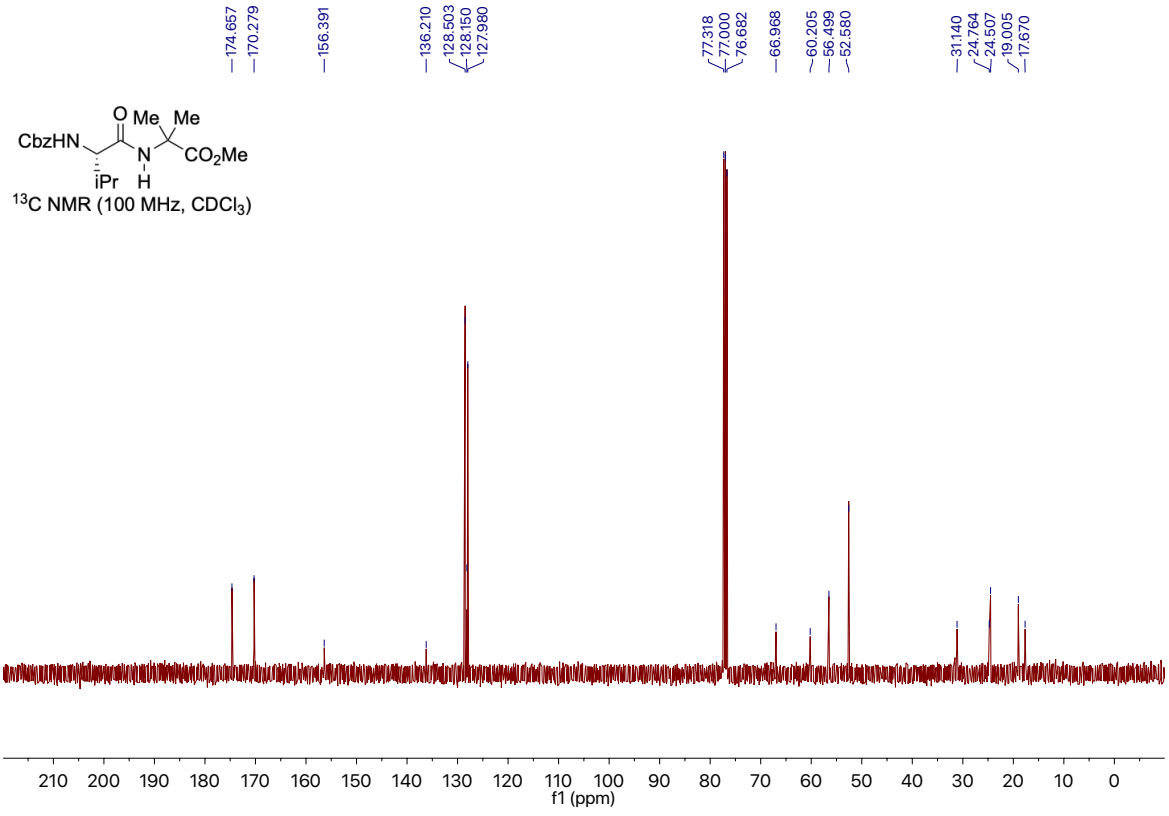

7.381
7.358
7.350
7.339
7.336
7.304
7.265
6.568
5.369
5.116
4.598
4.580
4.562
4.545
4.527
4.298
4.286
4.270
4.253
4.232
3.750
1.402
1.385
0.000
CbzHN
O
Me
N
H
Me
CO2Me
1H NMR (400 MHz, CDCl3)
4.92
1.00
0.94
2.16
1.01
1.01
3.24
6.24
f1 (ppm)

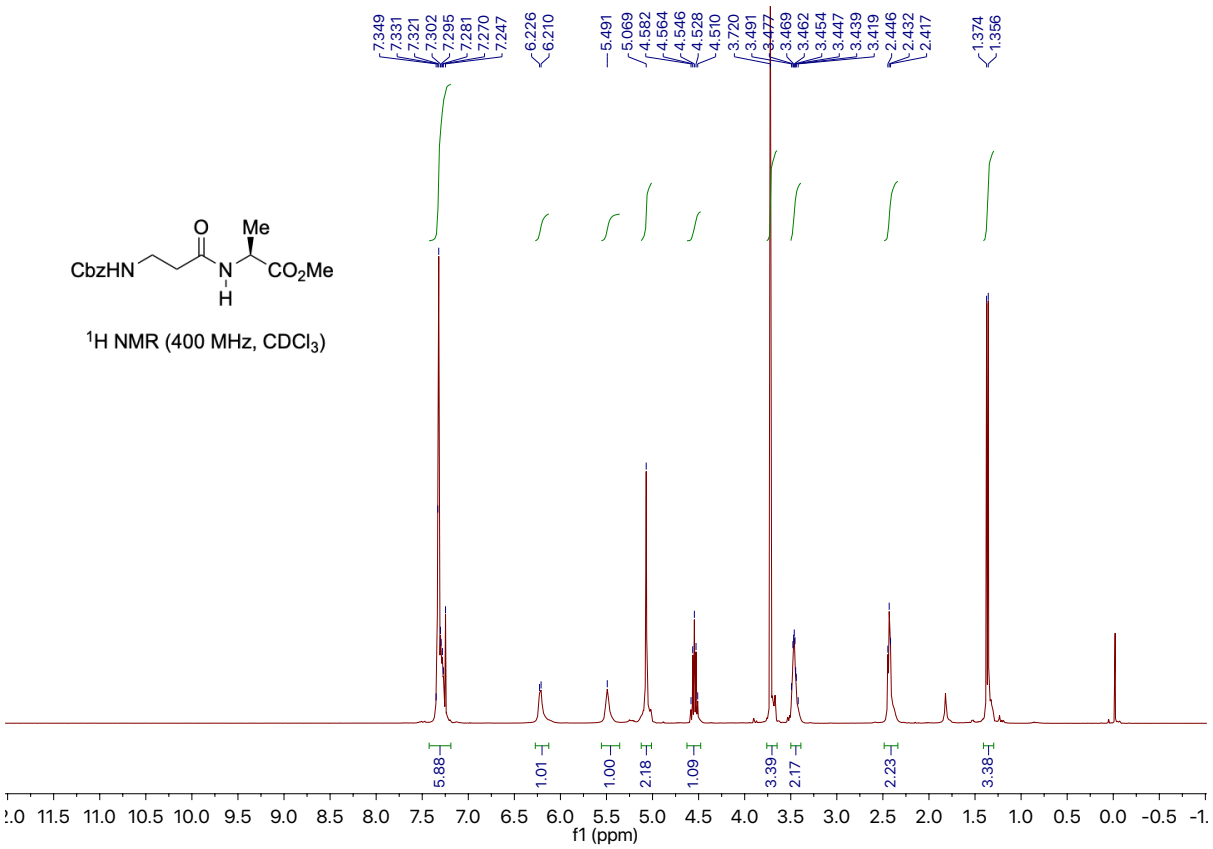

173.154
171.741
155.876
136.120
128.529
128.204
128.066
77.318
77.000
76.682
67.021
52.524
50.373
48.048
18.610
18.259
CbzHN
O
Me
N
H
Me
CO2Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)

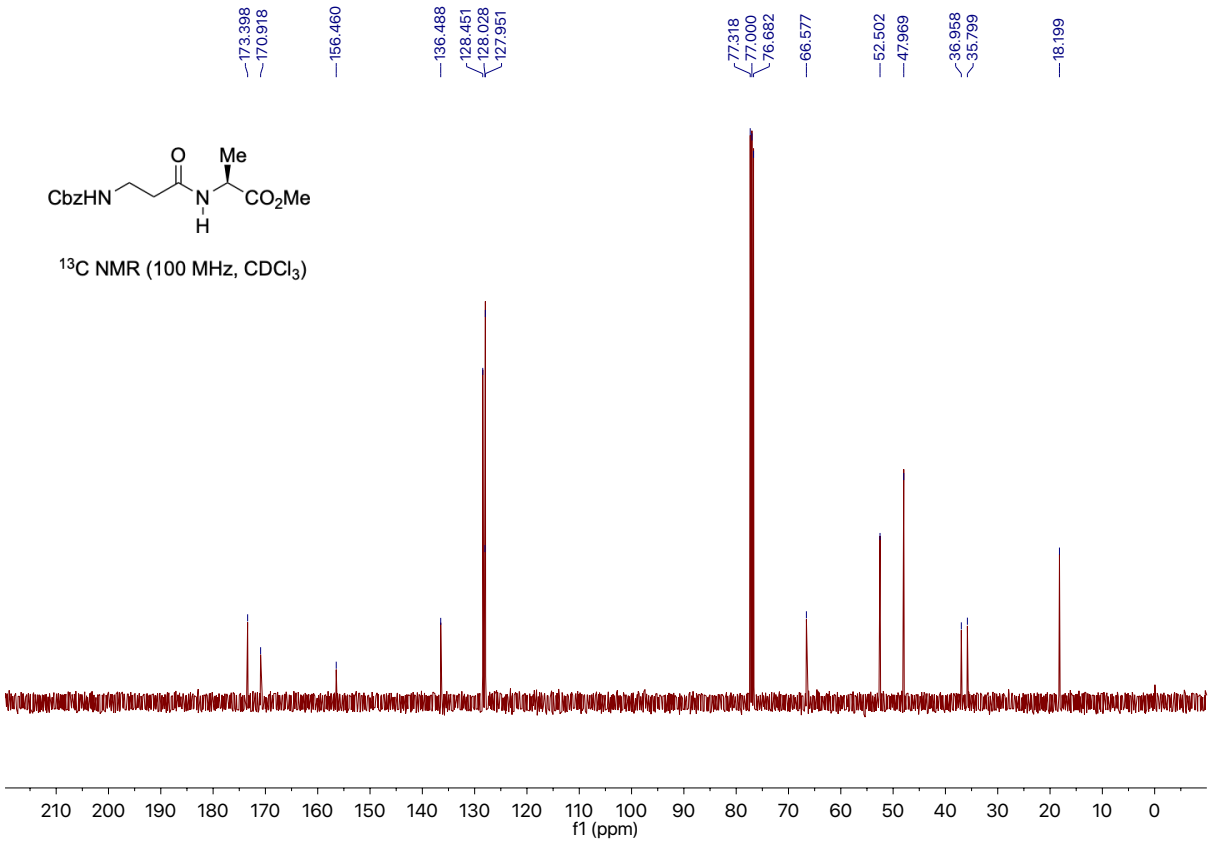

7.397
7.363
7.348
7.339
7.323
7.316
7.311
7.305
7.301
7.288
7.280
7.271
7.247
6.346
6.328
5.364
5.343
5.096
4.602
4.584
4.566
4.548
4.530
4.022
4.007
4.001
3.985
3.735
2.159
2.147
2.130
2.114
2.097
2.081
2.064
1.403
1.385
0.975
0.958
0.928
0.911
CbzHN
O
Me
N
H
iPr
CO2Me
13C NMR (100 MHz, CDCl3)
5.39
1.00
0.91
2.17
0.92
0.89
3.05
1.01
2.93
3.21
3.02
f1 (ppm)

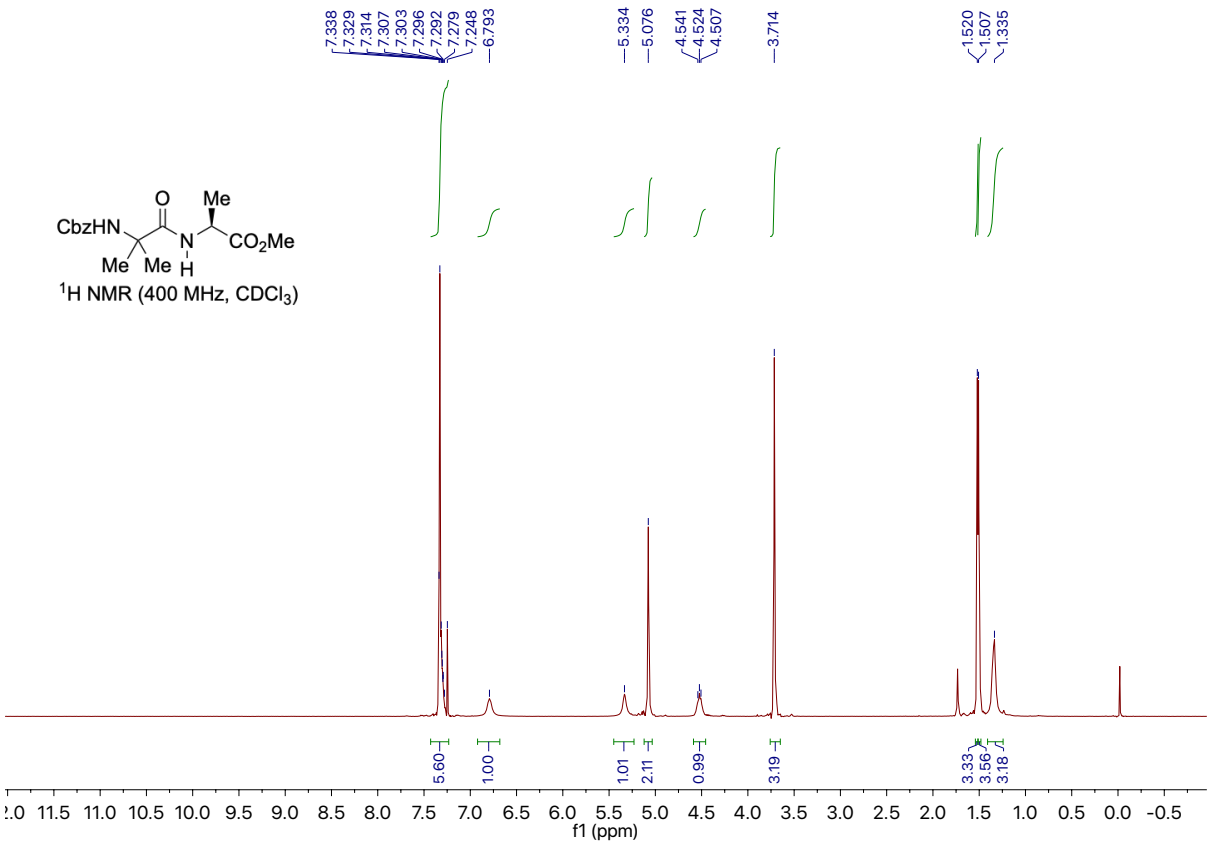

173.126
170.790
156.353
136.167
128.495
128.137
128.000
77.318
77.000
76.682
66.989
60.121
52.447
47.947
31.307
19.050
18.151
17.741
CbzHN
O
Me
N
H
iPr
CO2Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)

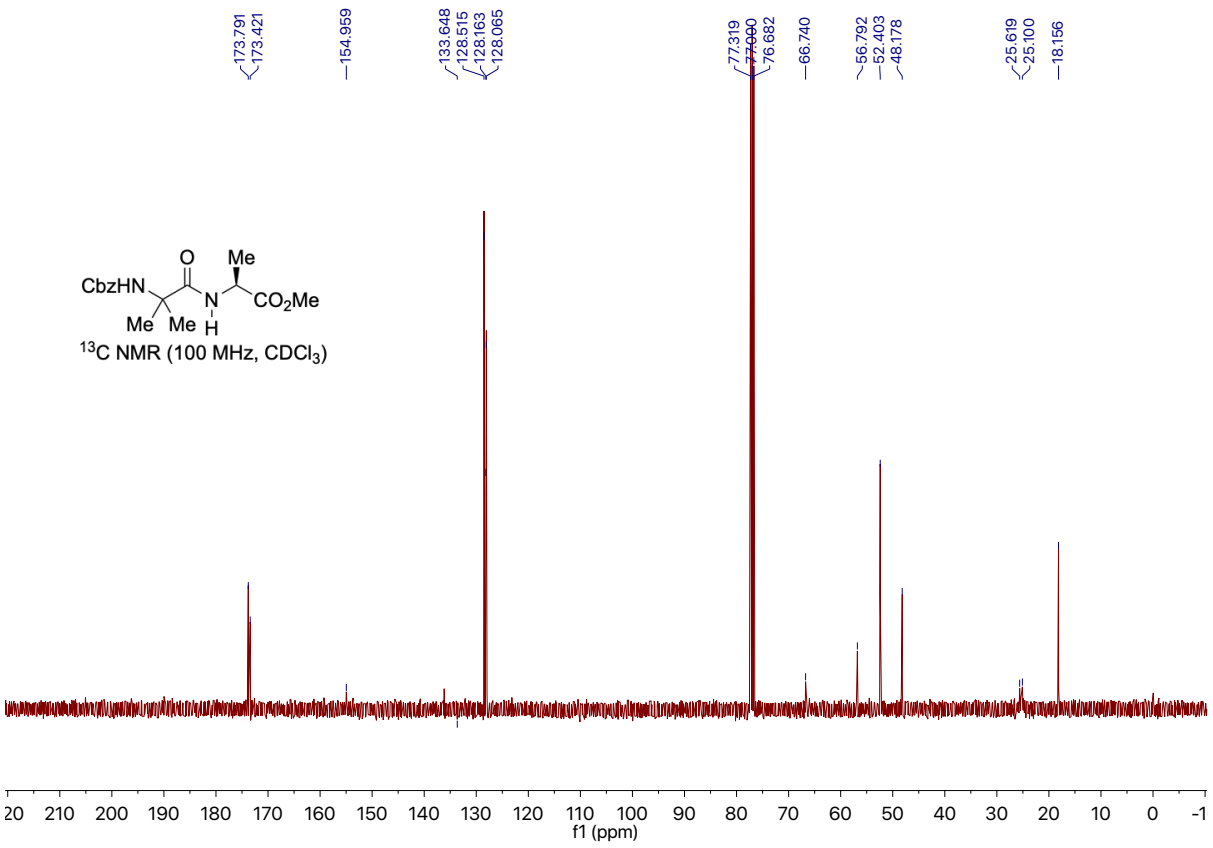

7.378
7.373
7.356
7.353
7.351
7.345
7.338
7.328
7.321
7.316
7.310
7.307
7.294
7.260
6.488
5.396
5.374
5.106
3.981
3.965
3.943
3.710
2.168
2.135
2.119
2.102
2.085
2.069
1.528
0.972
0.955
0.930
0.913
0.006
5.74
1.00
0.92
2.19
1.04
3.32
1.15
6.72
2.99
2.90
f1 (ppm)

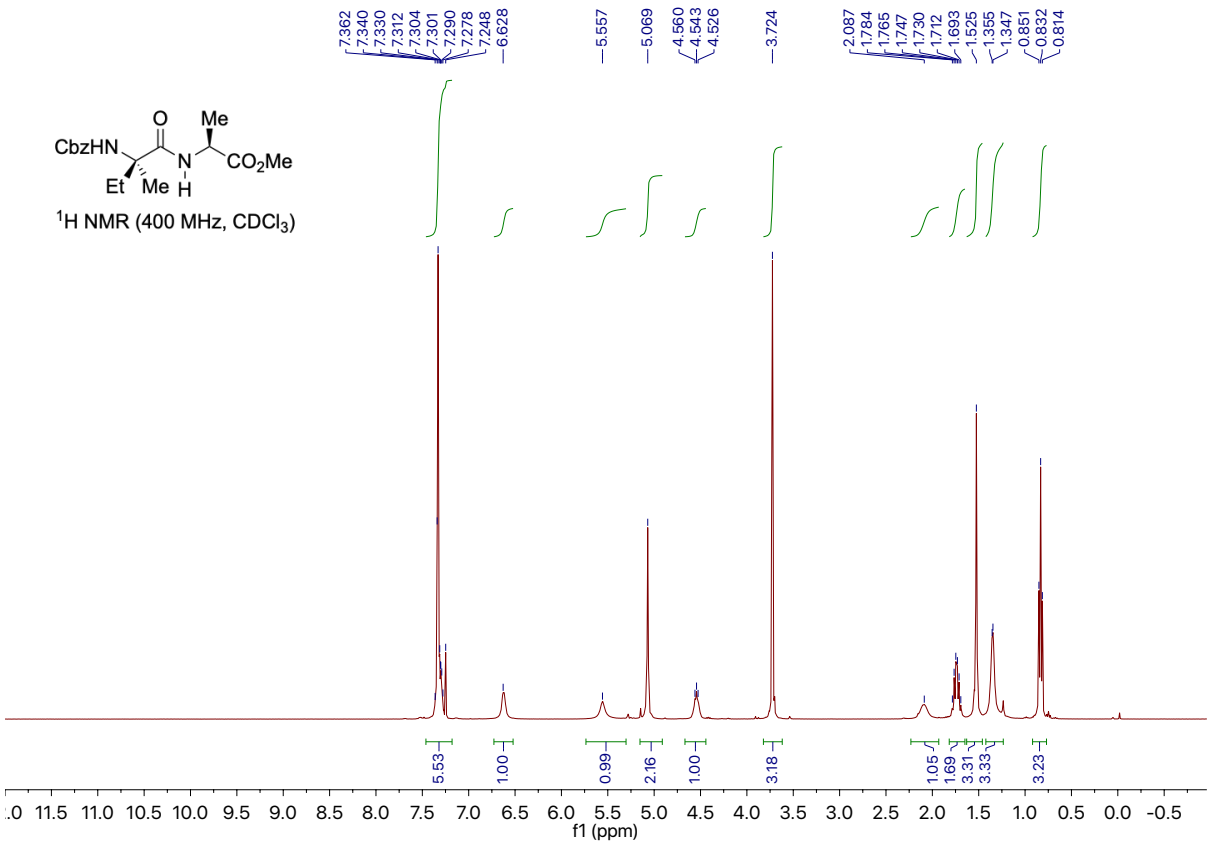

174.657
170.279
156.391
136.210
128.503
128.150
127.980
77.318
77.000
76.682
66.968
60.205
56.499
52.580
31.140
24.764
24.507
19.005
17.670
f1 (ppm)

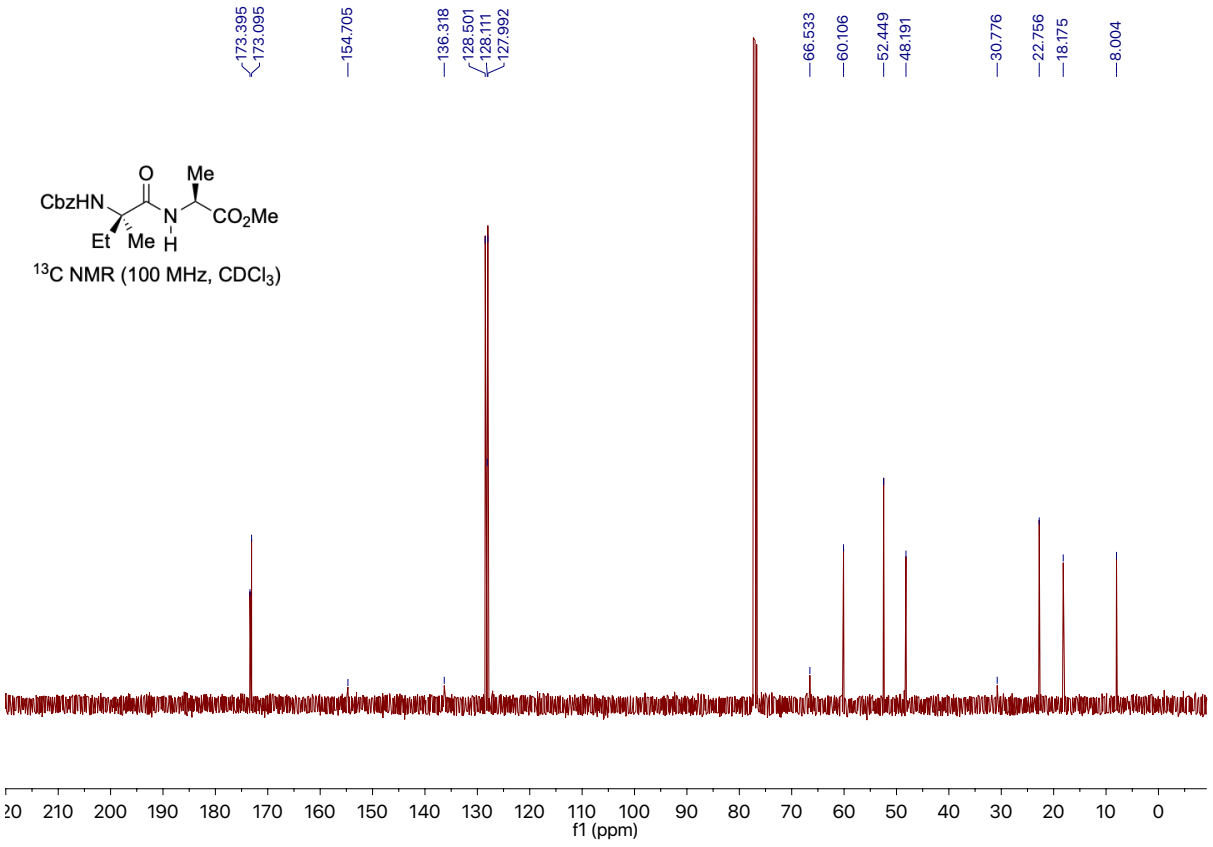

7.349
7.331
7.321
7.302
7.295
7.281
7.270
7.247
6.226
6.210
5.491
5.069
4.582
4.564
4.546
4.528
4.510
3.720
3.491
3.477
3.469
3.462
3.454
3.447
3.439
3.419
2.446
2.432
2.417
1.374
1.356
CbzHN
O
Me
N
H
CO2Me
1H NMR (400 MHz, CDCl3)
5.88
1.01
1.00
2.18
1.09
3.39
2.17
2.23
3.38
f1 (ppm)

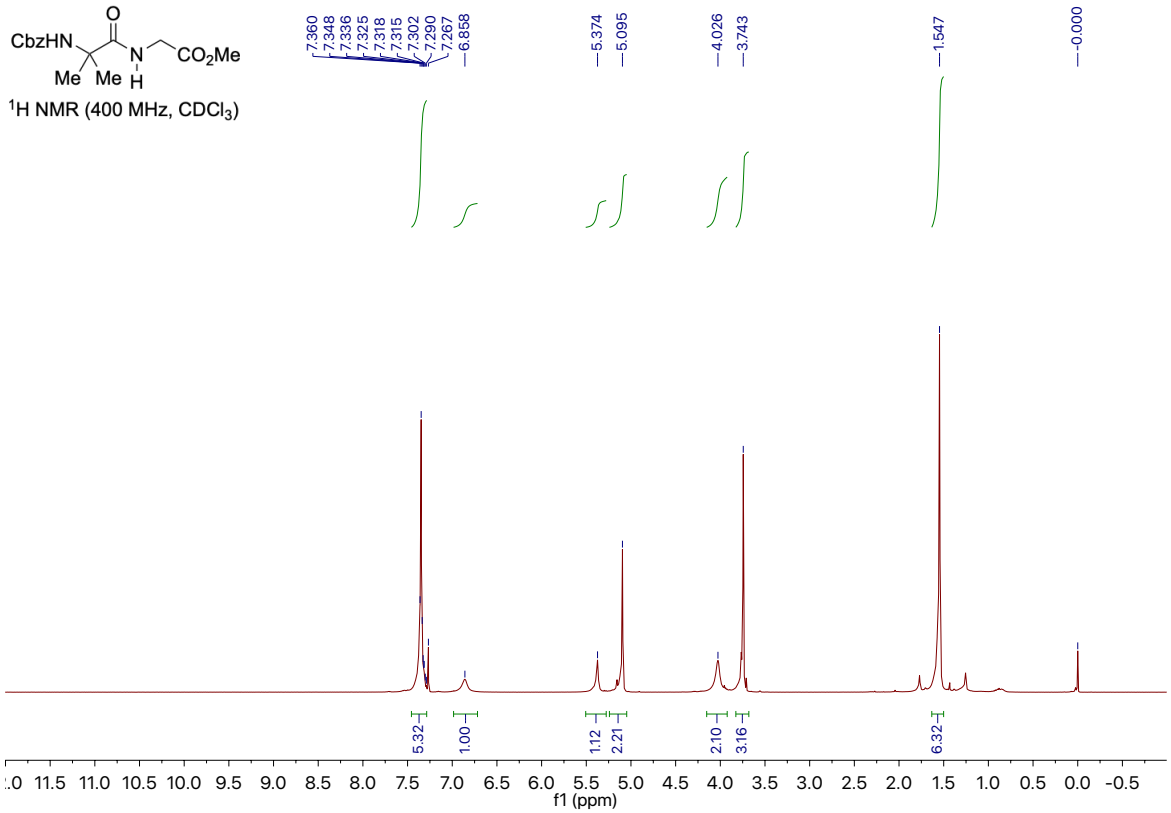

173.398
170.918
156.460
136.488
128.451
128.028
127.951
77.318
77.000
76.682
66.577
52.502
47.969
36.958
35.799
18.199
CbzHN
O
Me
N
H
CO2Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)

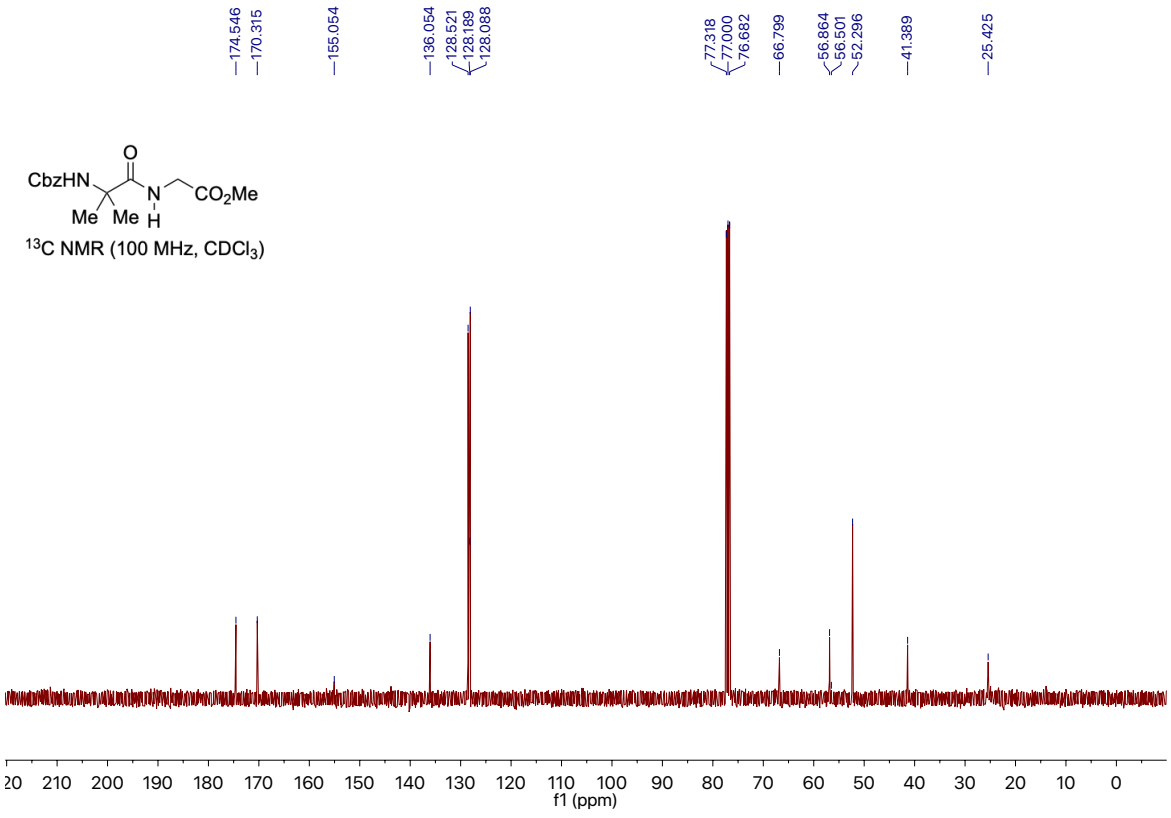

7.338
7.329
7.314
7.307
7.303
7.296
7.292
7.279
7.248
6.793
5.334
5.076
4.541
4.524
4.507
3.714
1.520
1.507
1.335
CbzHN
O
Me
N
H
CO2Me
Me
Me
1H NMR (400 MHz, CDCl3)
5.60
1.00
1.01
2.11
0.99
3.19
3.33
3.56
3.18
f1 (ppm)

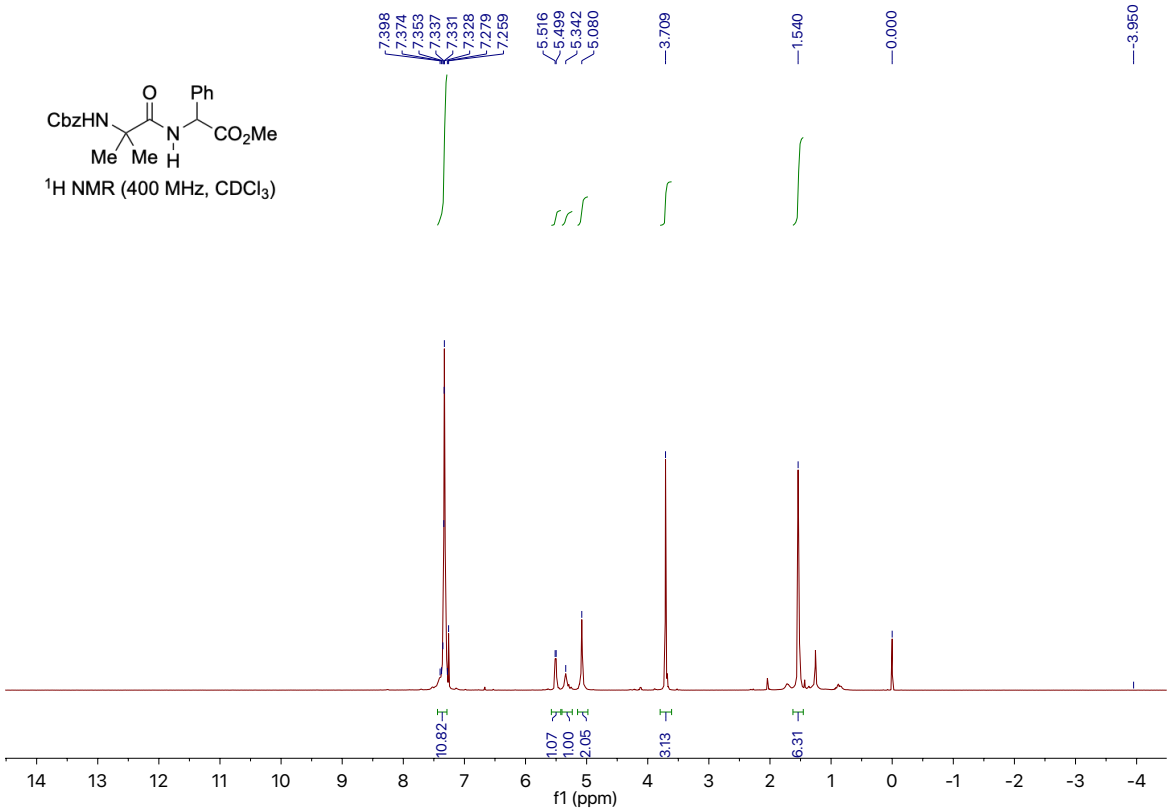

173.791
173.421
154.959
133.648
128.515
128.163
128.065
77.319
77.000
76.682
66.740
56.792
52.403
48.178
25.619
25.100
18.156
CbzHN
O
Me
N
H
CO2Me
Me
Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)

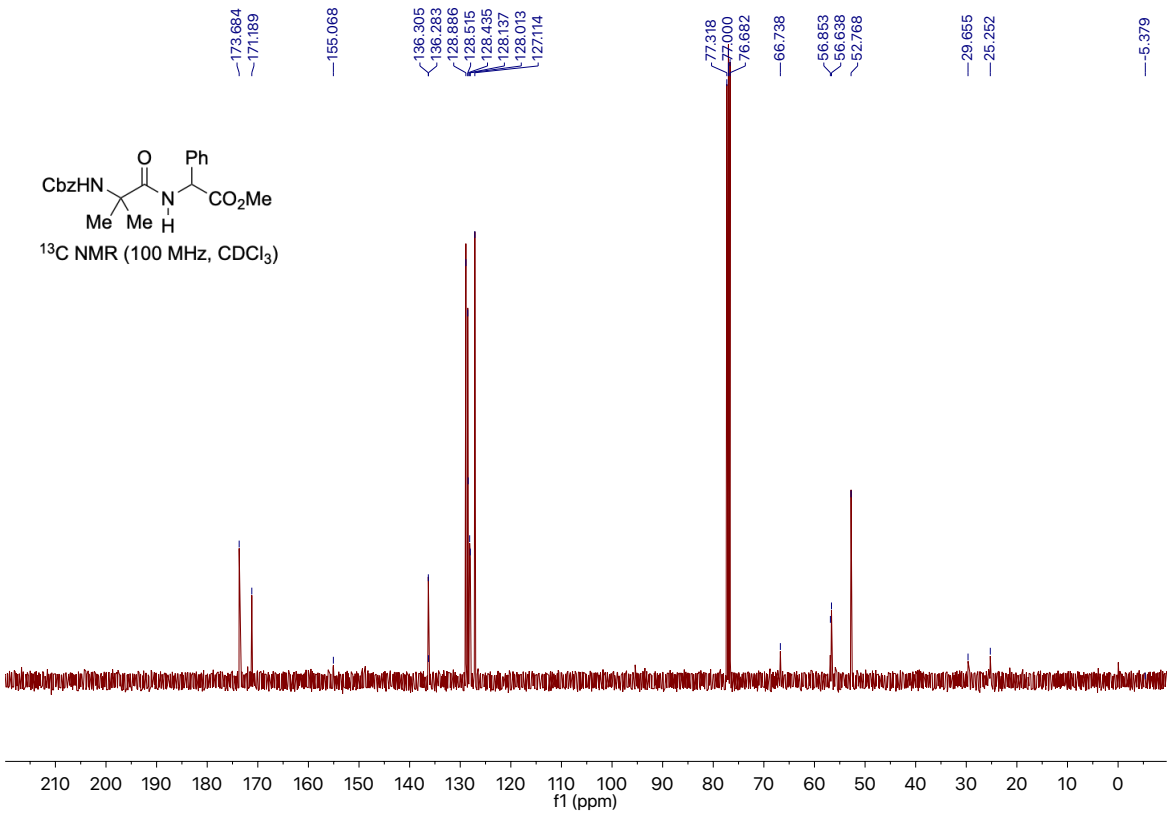

7.362
7.340
7.330
7.312
7.304
7.301
7.290
7.278
7.248
6.628
5.557
5.069
4.560
4.543
4.526
3.724
2.087
1.784
1.765
1.747
1.730
1.712
1.693
1.525
1.355
1.347
0.851
0.832
0.814
CbzHN
O
Me
N
H
Et
Me
CO2Me
1H NMR (400 MHz, CDCl3)
5.53
1.00
0.99
2.16
1.00
3.18
1.05
1.69
3.31
3.33
3.23
f1 (ppm)

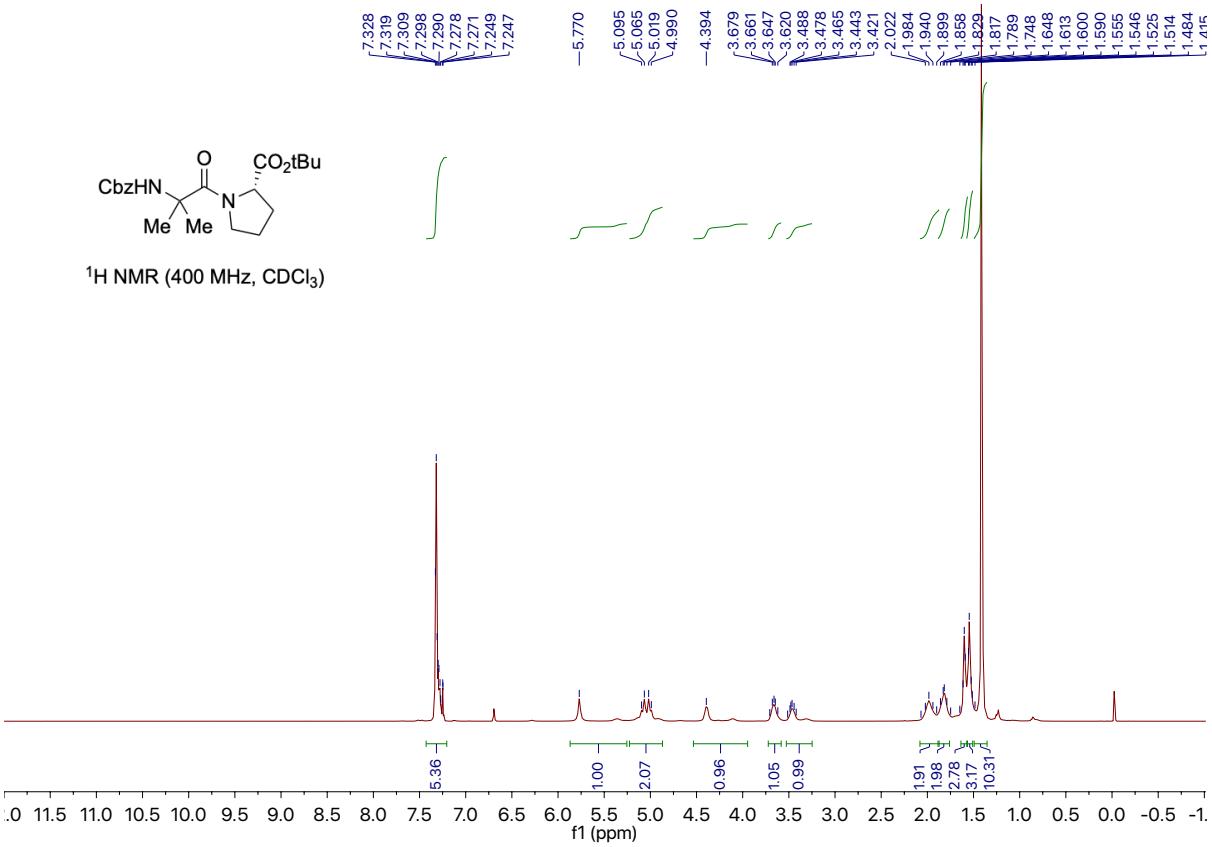

173.395
173.095
154.705
136.318
128.501
128.111
127.992
66.533
60.106
52.449
48.191
30.776
22.756
18.175
8.004
CbzHN
O
Me
N
H
Et
Me
CO2Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)

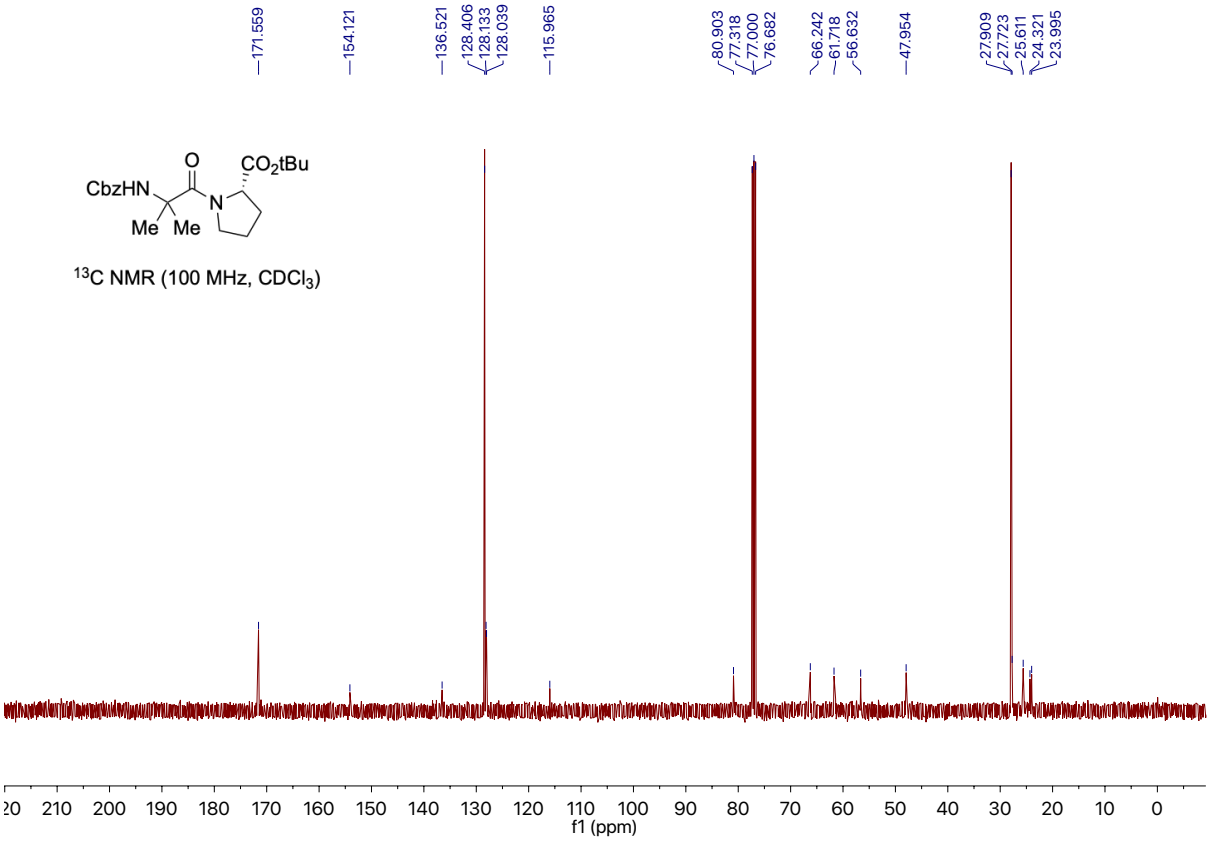

CbzHN
O
N
H
Me
Me
CO2Me
1H NMR (400 MHz, CDCl3)
7.360
7.348
7.336
7.325
7.318
7.315
7.302
7.290
7.267
6.858
5.374
5.095
4.026
3.743
1.547
0.000
5.32
1.00
1.12
2.21
2.10
3.16
6.32
f1 (ppm)

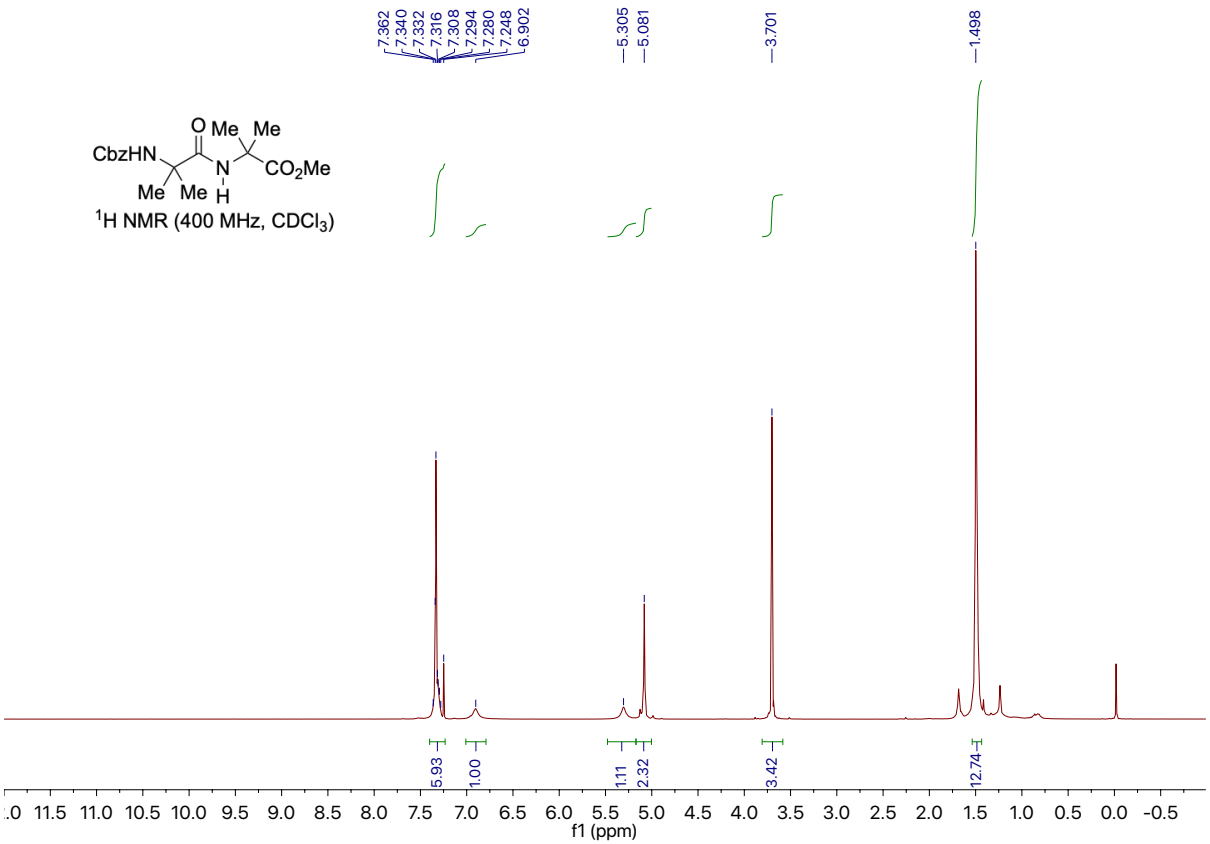

CbzHN
O
N
H
Me
Me
CO2Me
13C NMR (100 MHz, CDCl3)
174.546
170.315
155.054
136.054
128.521
128.189
128.088
77.318
77.000
76.682
66.799
56.864
56.501
52.296
41.389
25.425
f1 (ppm)

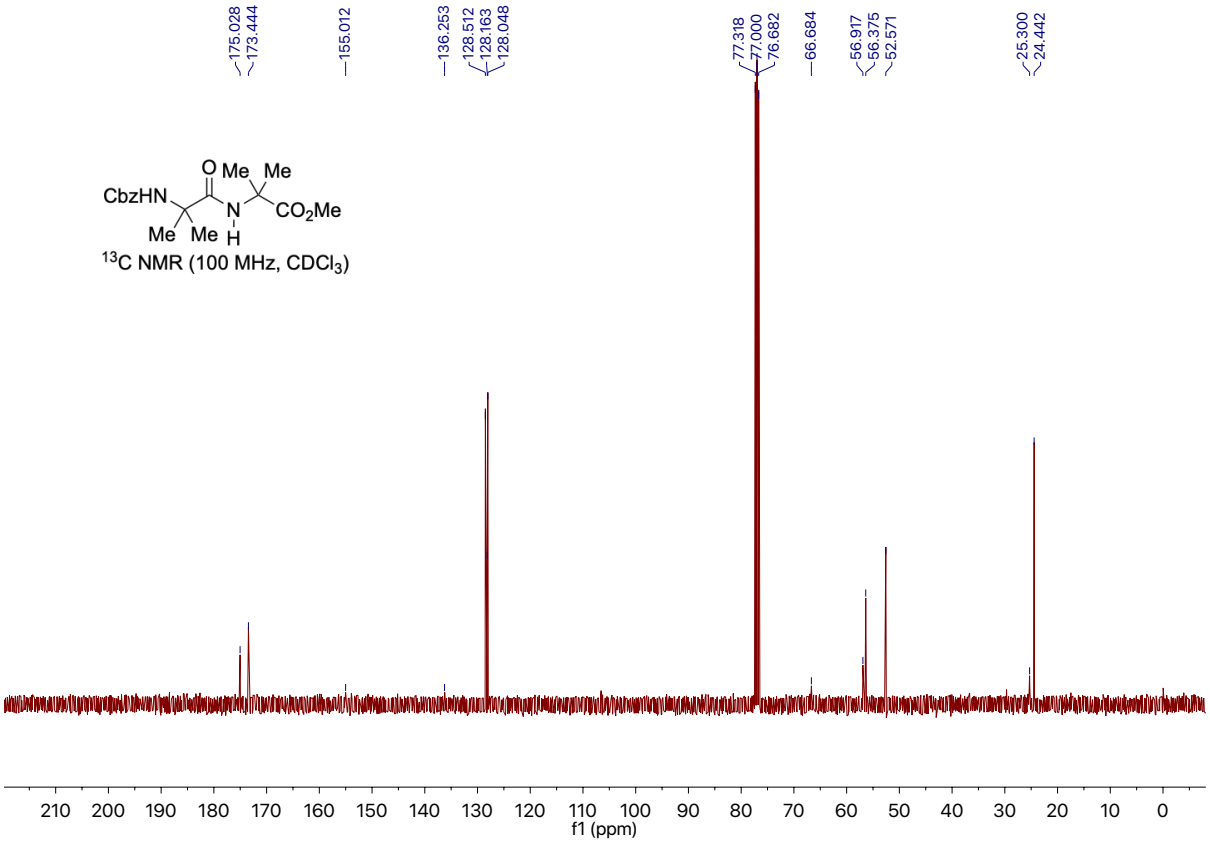

7.398
7.374
7.353
7.337
7.331
7.328
7.279
7.259
5.516
5.499
5.342
5.080
3.709
1.540
0.000
3.950
O
Ph
CbzHN
N
CO2Me
Me
Me
H
1H NMR (400 MHz, CDCl3)
10.82
1.07
1.00
2.05
3.13
6.31
f1 (ppm)

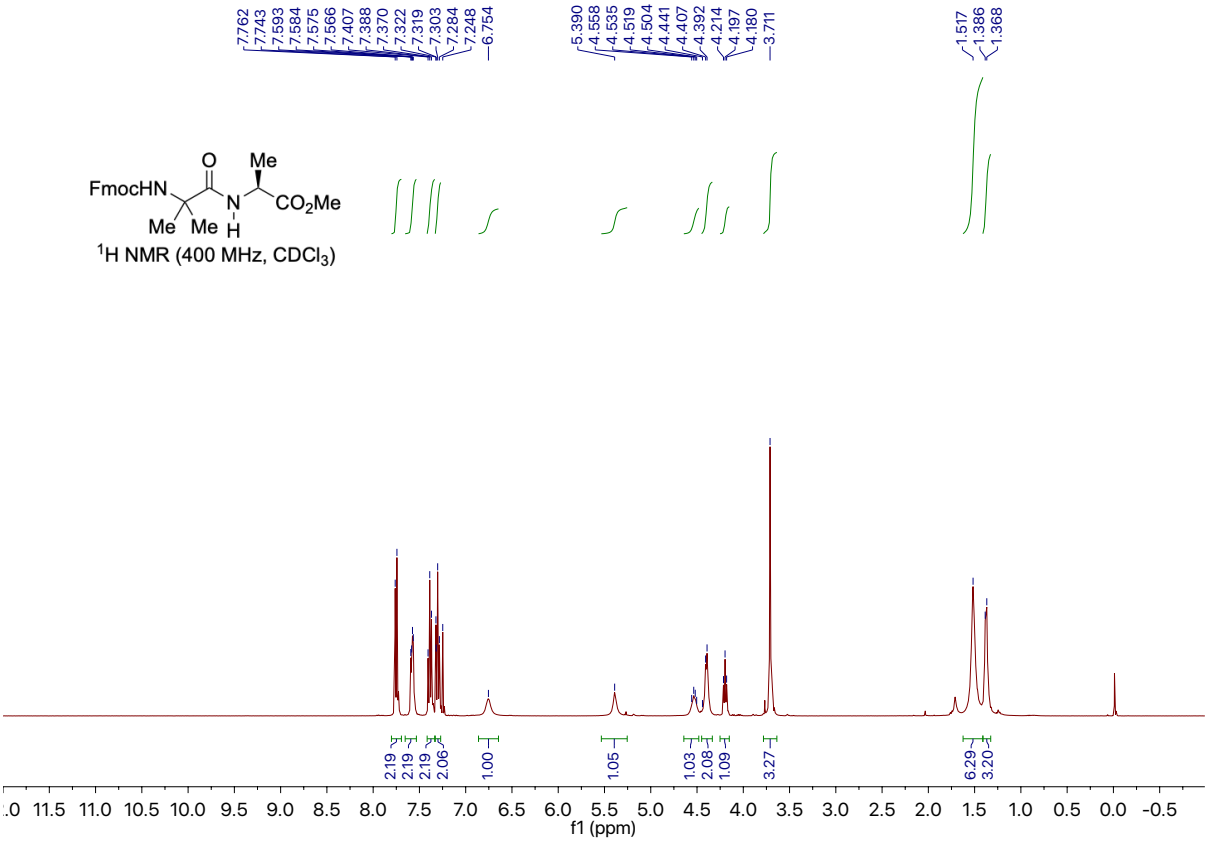

173.684
171.189
155.068
136.305
136.283
128.886
128.515
128.435
128.137
128.013
127.114
77.318
77.000
76.682
66.738
56.853
56.638
52.768
29.655
25.252
5.379
O
Ph
CbzHN
N
CO2Me
Me
Me
H
13C NMR (100 MHz, CDCl3)
f1 (ppm)

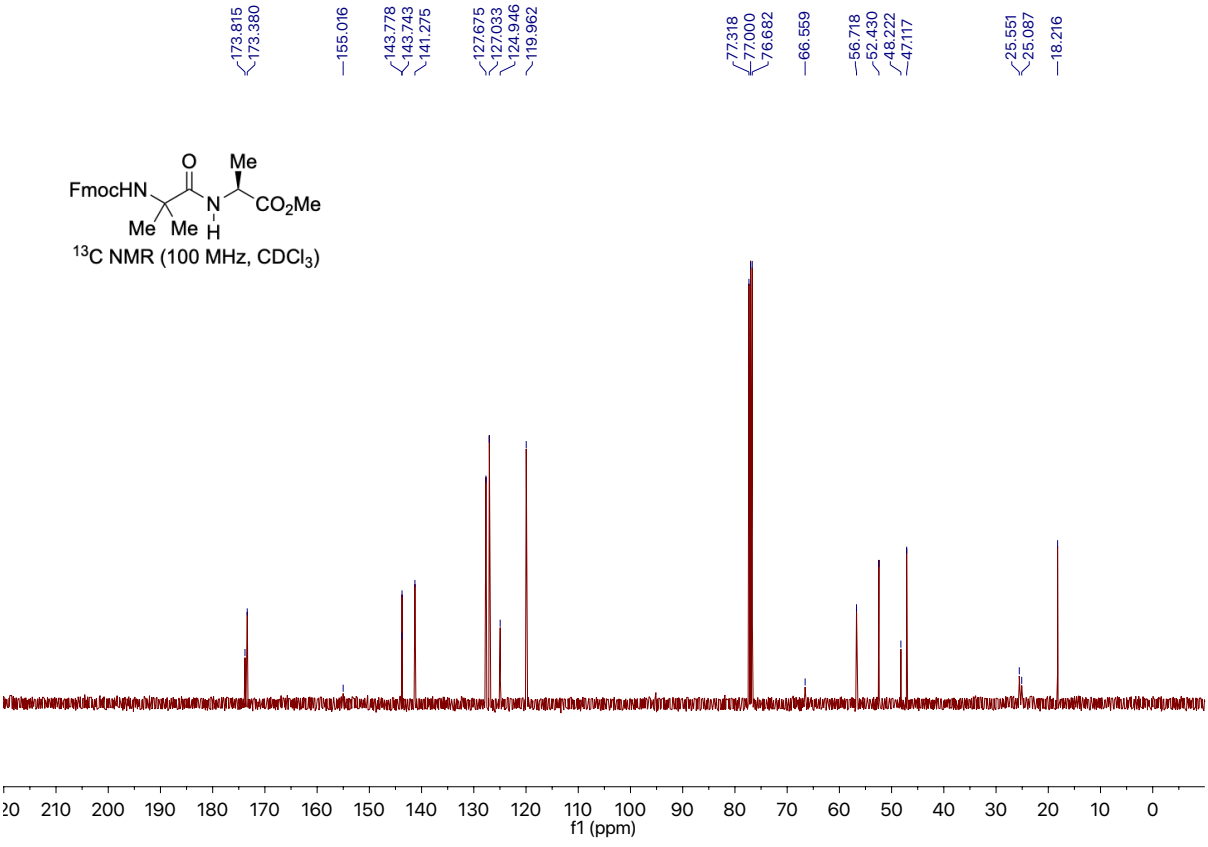

CbzHN
O
CO2tBu
N
Me Me
1H NMR (400 MHz, CDCl3)
f1 (ppm)

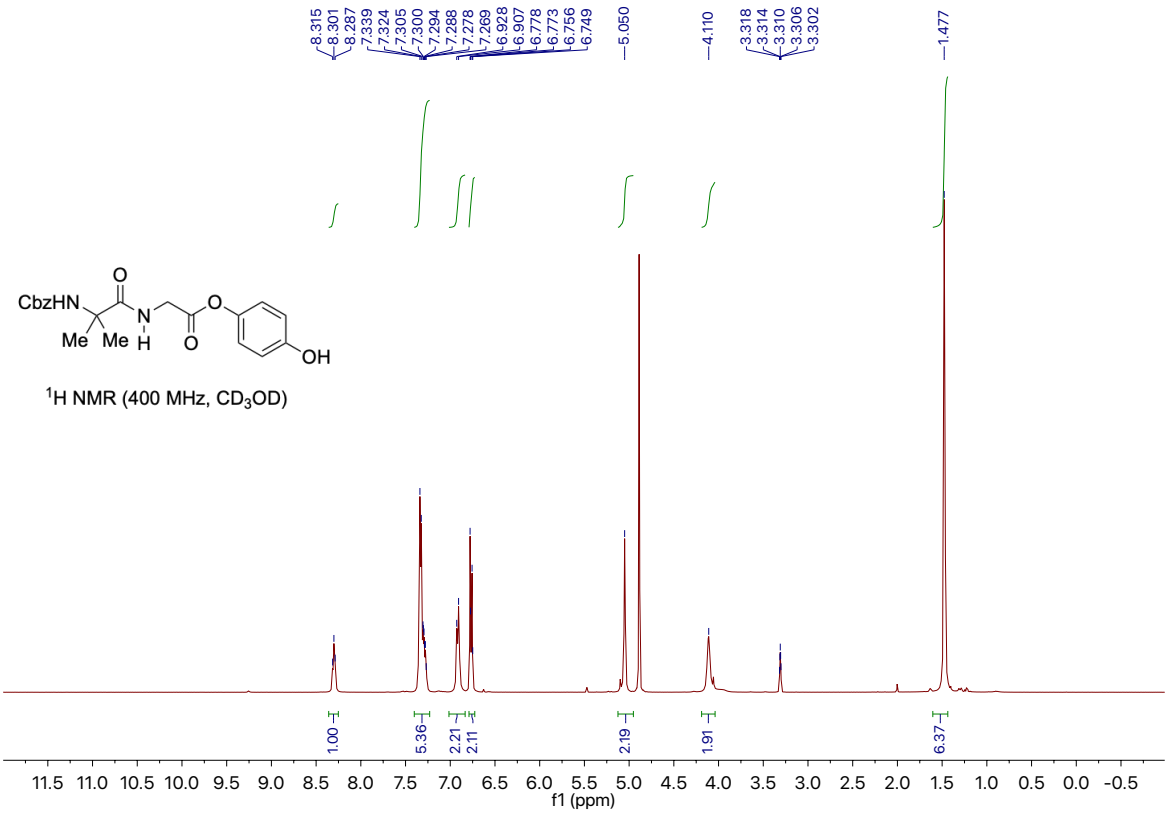

CbzHN
O
CO2tBu
N
Me Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)


7.362
7.340
7.332
7.316
7.308
7.294
7.280
7.248
6.902
5.305
5.081
3.701
1.498
CbzHN
O
Me
Me
N
H
CO2Me
Me
Me
1H NMR (400 MHz, CDCl3)
5.93
1.00
1.11
2.32
3.42
12.74
f1 (ppm)

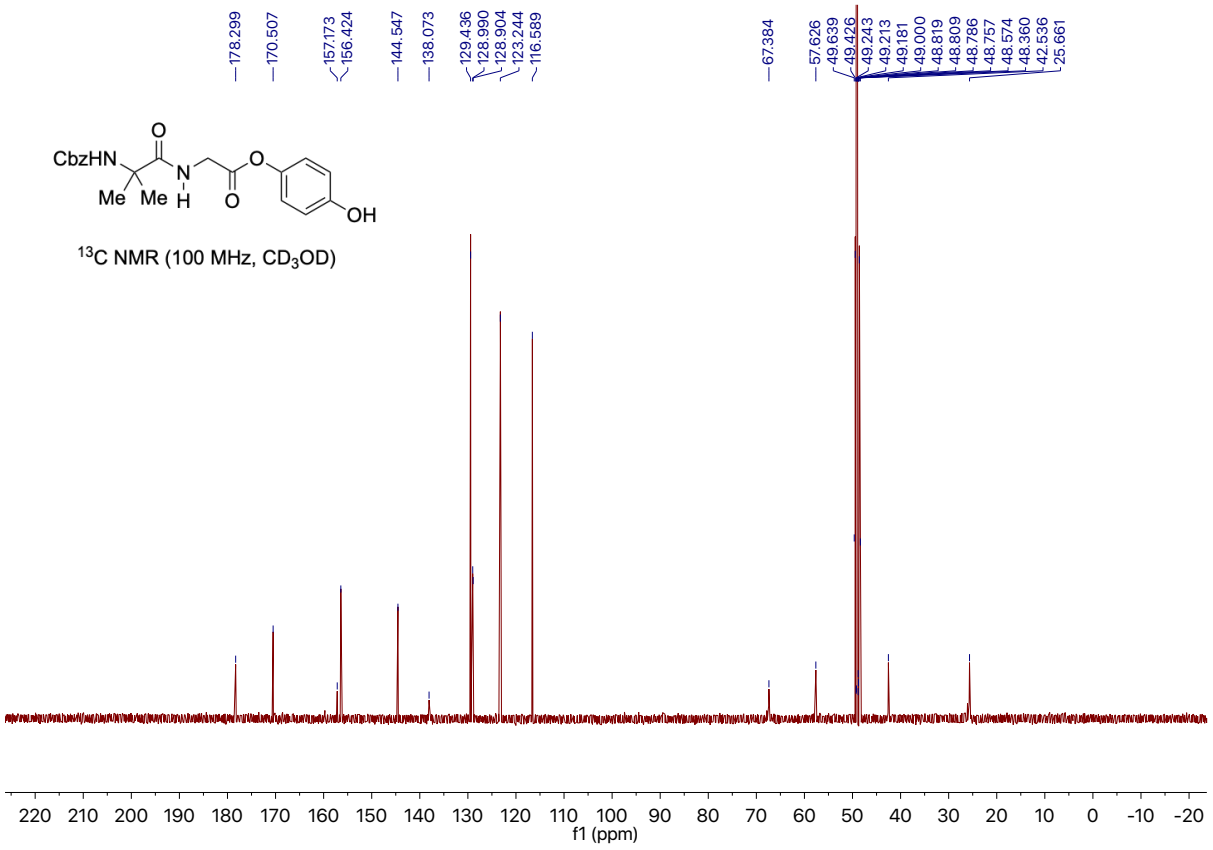

175.028
173.444
155.012
136.253
128.512
128.163
128.048
77.318
77.000
76.682
66.684
56.917
56.375
52.571
25.300
24.442
CbzHN
O
Me
Me
N
H
CO2Me
Me
Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)


7.762
7.743
7.593
7.584
7.575
7.566
7.407
7.388
7.370
7.322
7.319
7.303
7.284
7.248
6.754
5.390
4.558
4.535
4.519
4.504
4.441
4.407
4.392
4.214
4.197
4.180
3.711
1.517
1.386
1.368
FmocHN
O
Me
N
H
CO2Me
Me
Me
1H NMR (400 MHz, CDCl3)
2.19
2.19
2.19
2.06
1.00
1.05
1.03
2.08
1.09
3.27
6.29
3.20
f1 (ppm)

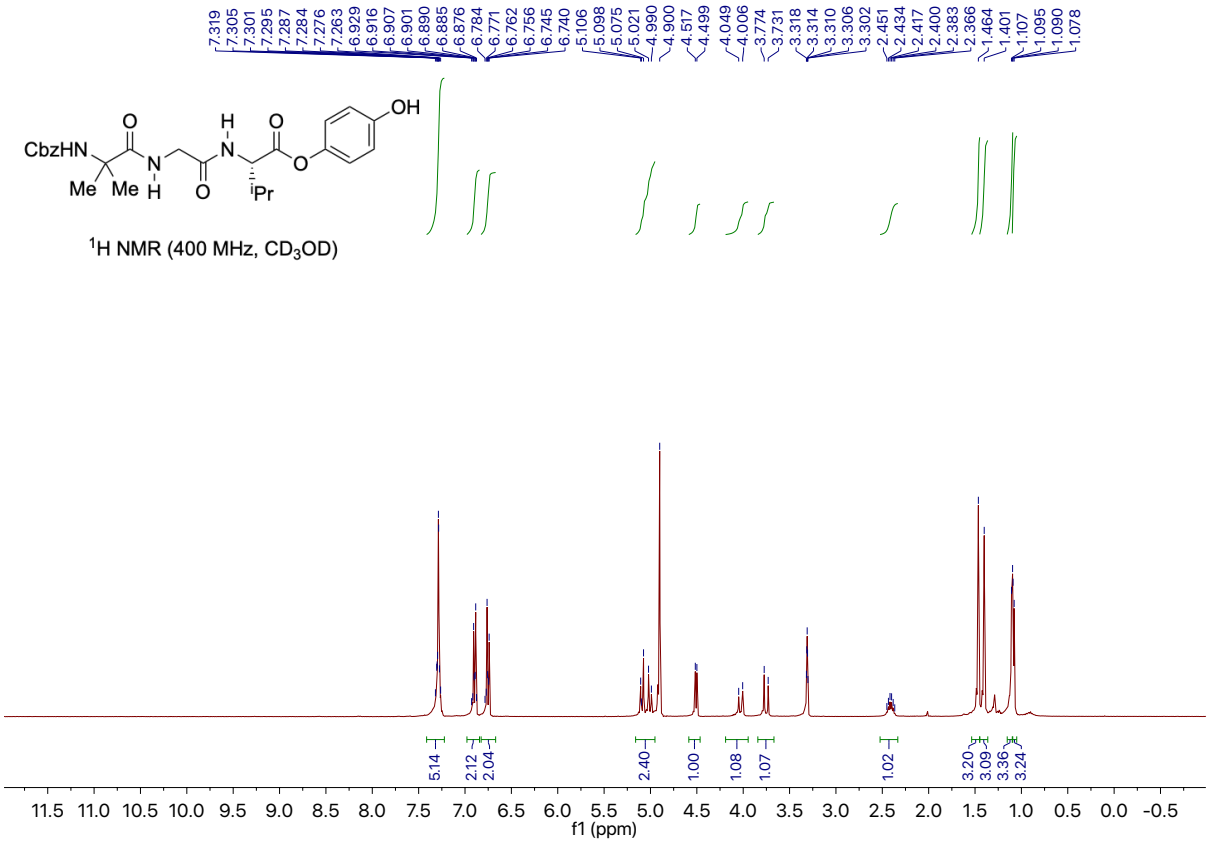

173.815
173.380
155.016
143.778
143.743
141.275
127.675
127.033
124.946
119.962
77.318
77.000
76.682
66.559
56.718
52.430
48.222
47.117
25.551
25.087
18.216
FmocHN
O
Me
N
H
CO2Me
Me
Me
13C NMR (100 MHz, CDCl3)
f1 (ppm)



^{1}H NMR (400 MHz, CD_3OD)



^{13}C NMR (100 MHz, CD_3OD)


7.319
7.305
7.301
7.295
7.287
7.284
7.276
7.263
6.929
6.916
6.907
6.901
6.890
6.885
6.876
6.784
6.771
6.762
6.756
6.745
6.740
5.106
5.098
5.075
5.021
4.990
4.900
4.517
4.499
4.049
4.006
3.774
3.731
3.318
3.314
3.310
3.306
3.302
2.451
2.434
2.417
2.400
2.383
2.366
1.464
1.401
1.107
1.095
1.090
1.078
CbzHN
Me
Me
H
N
O
H
N
O
O
OH
iPr
1H NMR (400 MHz, CD3OD)
5.14
2.12
2.04
2.40
1.00
1.08
1.07
1.02
3.20
3.09
3.36
3.24
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)
177.963
172.511
172.123
158.025
156.568
144.516
137.978
129.417
128.992
128.954
123.284
116.668
67.809
59.722
57.773
49.639
49.425
49.212
49.000
48.786
48.573
48.361
43.983
31.677
26.388
24.857
19.646
19.075
CbzHN
Me
Me
H
N
O
H
N
O
O
OH
iPr
13C NMR (100 MHz, CD3OD)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)