Rhodium(III)-Catalyzed Chemoselective C–H Functionalization of Benzamides with Methyleneoxetanones Controlled by the Solvent

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I. General

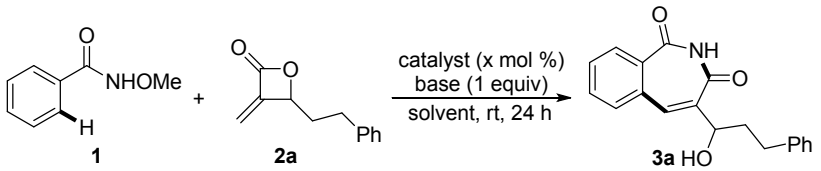
NMR spectra were recorded on JEOL 400 NMR (^{1}H 400 MHz; ^{13}C 100 MHz) in either $CDCl_3$, DMSO-d_6 or CD_3OD. Abbreviations for data quoted are s, singlet; brs, broad singlet; d, doublet; t, triplet; dd, doublet of doublets; m, multiplet. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; d_6-DMSO: δ_H = 2.50 ppm, δ_C = 39.52 ppm; CD_3OD: δ_H = 3.31 ppm, δ_C = 49.00 ppm). Mass spectra and high-resolution mass spectra were measured on an agilent TOF-G6230B mass spectrometer and Thermo-DFS mass spectrometer. Thin-layer chromatographies were done on pre-coated silica gel 60 F254 plates (Merck). Silica gel 60H (200-300 mesh) and preparative TLC (200x200 mm, 0.2-0.25 mm in thickness) manufactured by Qingdao Haiyang Chemical Group Co. (China) were used for general chromatography. $[Cp^*IrCl_2]_2$, $[Cp^*RhCl_2]_2$, $[Ru(p\text{-cymene})Cl_2]_2$ and CsOAc were purchased from Aldrich and used without further purification. Substrates benzamide derivatives and α-methylene-β-lactones were synthesized according to published procedures.[S1,S2] Other chemicals were purchased from commercial suppliers and were dried and purified when necessary. No attempts were made to optimize yields for substrate synthesis.

II. Experimental Information and Characterization Data

Optimization studies:

The mixture of *N*-methoxybenzamide **1a** (0.15 mmol, 1.0 equiv), α-methylene-β-lactone **2a** (0.15 mmol, 1.0 equiv), catalyst (x mol %) and base (0.15 mmol, 1.0 equiv) in the solvent (1.5 mL) was stirred for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC (eluent: PE/EA = 1/1) to afford the corresponding 1*H*-benzo[*c*]azepine-1,3(2*H*)-dione **3a**.

Table S1. Conditions Screening for the Synthesis of 1*H*-benzo[*c*]azepine-1,3(2*H*)-dione **3a**[a]

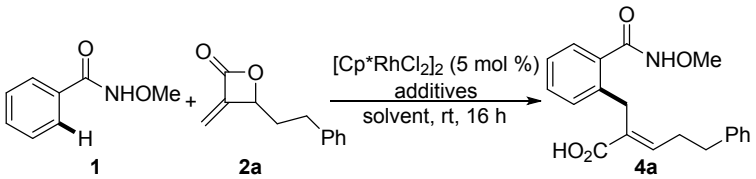


Entry	Catalyst (x mol %)	Base	Solvent	Yield (%)[b]	
				3a	**4a**
1	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	dioxane	68	n.d.
2	$[CyRuCl_2]_2$ (2.5)	CsOAc	dioxane	13	n.d.
3	$[Cp^*IrCl_2]_2$ (2.5)	CsOAc	dioxane	6	n.d.
4	$Cp^*Co(CO)I_2$ (5)	CsOAc	dioxane	NR	n.d.
5	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	MeOH	53	n.d.
6	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	EtOH	54	n.d.
7	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	DCE	70	n.d.
8	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	H_2O	57	n.d.
9	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	CH_3CN	<5	n.d.
10	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	THF	34	n.d.
11	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	TFE	11	36
12	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	HFIP	39	<5
13	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	DCE	43	n.d.
14	$[Cp^*RhCl_2]_2$ (2.5)	AgOAc	DCE	47	n.d.
15	$[Cp^*RhCl_2]_2$ (2.5)	K_2CO_3	DCE	21	n.d.
16	$[Cp^*RhCl_2]_2$ (2.5)	$Cu(OAc)_2$	DCE	<5	n.d.
17[c]	**$[Cp^*RhCl_2]_2$ (2.5)**	**CsOAc**	**DCE**	**88**	n.d.
18[c]	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	DCE/TFE (1/1)	12	<5
19[d]	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	DCE	83	n.d.

[a]Reaction conditions: **1a** (0.15 mmol, 1 equiv), **2a** (0.15 mmol, 1 equiv), catalyst (x mol %) and base (0.15 mmol, 1 equiv) in solvent (1.5 mL) at rt for 24 h without exclusion of air or moisture. [b]Isolated yields were reported. [c]**2a** (0.18 mmol, 1.2 equiv). [d]Under dry N_2 atmosphere. TFE: 2,2,2-Trifluoroethanol; HFIP: 1,1,1,3,3,3-Hexafluoro-2-propanol; n.d.: not detected.

The mixture of *N*-methoxybenzamide **1a** (0.15 mmol, 1.0 equiv), α-methylene-β-lactone **2a** (0.15 mmol, 1.0 equiv), catalyst (x mol %) and base (0.15 mmol, 1.0 equiv) in the solvent (1.5 mL) was stirred for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC (eluent: PE/EA = 1/1) to afford the corresponding *ortho*-allylation product **4a**.

Table S2. Conditions Screening for C-H Allylation[a]

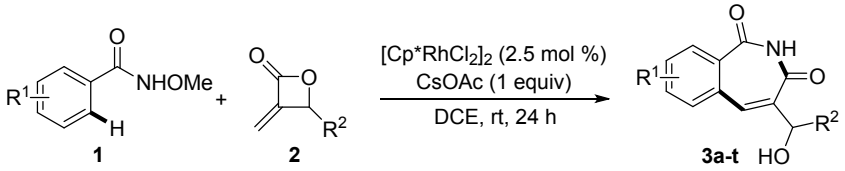


Entry	Base	Solvent	Yield (%)[b]	
			4a	**3a**
1	CsOAc	dioxane	n.d.	70
2	CsOAc	MeOH	n.d.	51
3	CsOAc	EtOH	n.d.	55
4	CsOAc	DCE	n.d.	68
5	CsOAc	CH_3CN	n.d.	<5
6	CsOAc	THF	n.d.	34

7	CsOAc	TFE	41	8
8	CsOAc	HFIP	trace	43
9	NaOAc	TFE	26	11
10	KOPiv	TFE	56	<5
11	$Zn(OAc)_2$	TFE	32	9
12[e]	**KOPiv**	**TFE**	**67**	**<5**
13[c,d]	KOPiv	TFE	60	<5
14[c,e]	KOPiv	TFE	66	<5
15[c]	KOPiv	DCE/TFE (1/1)	<5	<5
16[f]	KOPiv	TFE	63	<5

[a]Reaction conditions: **1a** (0.2 mmol, 1 equiv), **2a** (0.2 mmol, 1 equiv), $[Cp^*RhCl_2]_2$ (5 mol %) and base (0.2 mmol, 1 equiv) in solvent (2.0 mL) at rt for 16 h without exclusion of air or moisture. [b]Isolated yields were reported. [c]**2a** (0.3 mmol, 1.5 equiv). [d]1 equiv of HOAc was added. [e]The reaction was conducted at 60 °C. [f]Under dry N_2 atmosphere. TFE: 2,2,2-Trifluoroethanol; HFIP: 1,1,1,3,3,3-Hexafluoro-2-propanol; n.d.: not detected.

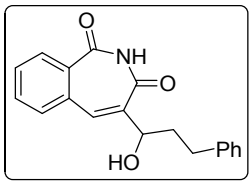
General procedure for C-H annulations:



The mixture of *N*-methoxybenzamides **1** (0.2 mmol, 1.0 equiv), α-methylene-β-lactones **2** (0.24 mmol, 1.2 equiv), $[Cp^*RhCl_2]_2$ (2.5 mol %) and CsOAc (0.2 mmol, 1.0 equiv) in DCE (2.0 mL) was stirred at room temperature for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding 1*H*-benzo[*c*]azepine-1,3(2*H*)-dione **3a**-**t**.

Characterization of products:

4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3a)



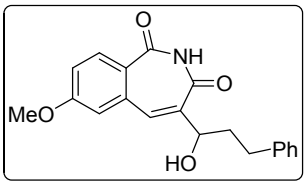
This compound was obtained in 88% yield (54.0 mg) as white solid. m.p.: 73-75 °C. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.04 (s, 1H), 7.65 (s, 1H), 7.63-7.59 (m, 1H), 7.58 (d, *J* = 1.8 Hz, 1H), 7.54-7.50 (m, 2H), 7.50-7.46 (m, 1H), 7.27-7.22 (m, 2H), 7.18-7.13 (m, 1H), 7.13-7.10 (m, 2H), 5.71 (dt, *J* = 8.2, 2.5 Hz, 1H), 2.66 (t, *J* = 8.1 Hz, 2H), 2.23-2.13 (m, 1H), 1.96-1.86 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 169.6, 164.3, 140.6, 137.8, 136.2, 130.19, 130.15, 129.9, 128.9, 128.5, 128.4, 128.2, 126.1, 79.5, 32.6, 30.0.

HRMS (ESI) calculated for $C_{19}H_{18}NO_3$ ($[M+H]^+$): 308.1286; found: 308.1280.

4-(1-hydroxy-3-phenylpropyl)-7-methoxy-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3b)



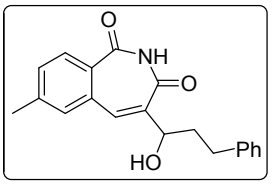
This compound was obtained in 60% yield (40.4 mg) as white solid. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.91 (s, 1H), 7.68 (d, *J* = 1.8 Hz, 1H), 7.62 (d, *J* = 8.6 Hz, 1H), 7.46 (s, 1H), 7.28-7.22 (m, 2H), 7.19-7.14 (m, 1H), 7.12-7.05 (m, 3H), 6.89 (d, *J* = 2.6 Hz, 1H), 5.72 (dt, *J* = 8.4, 2.4 Hz, 1H), 3.76 (s, 3H), 2.72-2.56 (m, 2H), 2.18-2.08 (m, 1H), 1.96-1.84 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 169.1, 164.3, 160.3, 140.5, 136.2, 132.5, 130.3, 129.4, 128.4, 128.3, 128.2, 126.1, 115.5, 113.8, 79.1, 55.6, 32.8, 30.0.

HRMS (ESI) calculated for $C_{20}H_{20}NO_4$ ($[M+H]^+$): 338.1392; found: 338.1388.

4-(1-hydroxy-3-phenylpropyl)-7-methyl-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3c)



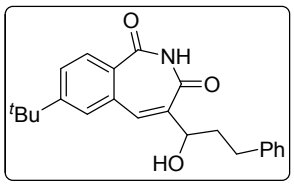
This compound was obtained in 77% yield (49.4 mg) as white solid. m.p.: 92.5-94 °C. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65 (d, *J* = 1.8 Hz, 1H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.31-7.18 (m, 4H), 7.16-7.11 (m, 2H), 6.96 (s, 1H), 6.27 (s, 1H), 5.92 (s, 1H), 5.31 (dt, *J* = 9.1, 2.4 Hz, 1H), 2.88-2.80 (m, 1H), 2.78-2.69 (m, 1H), 2.33 (s, 3H), 2.26-2.17 (m, 1H), 2.07-1.97 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 170.0, 164.3, 141.4, 140.5, 137.7, 133.5, 131.3, 131.0, 129.7, 128.81, 128.78, 128.6, 128.3, 126.5, 78.8, 33.3, 30.8, 29.8.

HRMS (ESI) calculated for $C_{20}H_{20}NO_3$ ([M+H]$^+$): 322.1443; found: 322.1436.

7-(*tert*-butyl)-4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3d)



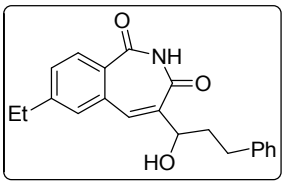
This compound was obtained in 69% yield (50.1 mg) as white solid. Eluent: PE/EA = 1/1, R_f = 0.4.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 1.8 Hz, 1H), 7.55 (d, *J* = 8.1 Hz, 1H), 7.46 (dd, *J* = 8.1, 1.9 Hz, 1H), 7.28-7.22 (m, 3H), 7.21-7.16 (m, 1H), 7.13-7.09 (m, 2H), 6.44 (s, 1H), 5.96 (s, 1H), 5.35 (dt, *J* = 9.4, 2.2 Hz, 1H), 2.88-2.80 (m, 1H), 2.78-2.69 (m, 1H), 2.24-2.15 (m, 1H), 2.07-1.96 (m, 1H), 1.26 (s, 9H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 170.4, 164.4, 154.4, 140.4, 137.3, 133.5, 131.0, 129.4, 128.73, 128.67, 128.2, 127.5, 126.5, 126.1, 79.0, 35.0, 33.7, 31.1, 31.0.

HRMS (ESI) calculated for $C_{23}H_{26}NO_3$ ([M+H]$^+$): 364.1912; found: 364.1902.

7-ethyl-4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3e)



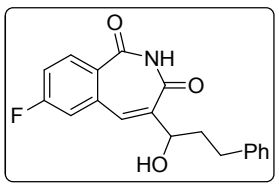
This compound was obtained in 65% yield (43.5 mg) as white solid. Eluent: PE/EA = 1/1, R_f = 0.4.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, *J* = 1.8 Hz, 1H), 7.52 (d, *J* = 7.9 Hz, 1H), 7.30-7.25 (m, 4H), 7.23-7.18 (m, 1H), 7.15-7.11 (m, 2H), 7.01 (d, *J* = 1.2 Hz, 1H), 5.90 (s, 1H), 5.81 (s, 1H), 5.33 (dt, *J* = 9.1, 2.3 Hz, 1H), 2.88-2.81 (m, 1H), 2.79-2.70 (m, 1H), 2.63 (q, *J* = 7.6 Hz, 2H), 2.26-2.16 (m, 1H), 2.08-1.98 (m, 1H), 1.20 (t, *J* = 7.7 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 169.5, 164.3, 146.2, 140.6, 136.0, 135.1, 130.3, 129.6, 128.9, 128.5, 128.2, 128.1, 126.1, 79.3, 32.8, 30.1, 27.8, 15.5.

HRMS (ESI) calculated for $C_{21}H_{22}NO_3$ ([M+H]$^+$): 336.1599; found: 336.1593.

7-fluoro-4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3f)



This compound was obtained in 72% yield (46.8 mg) as light yellow solid. Eluent: PE/EA = 1/1, R_f = 0.4.

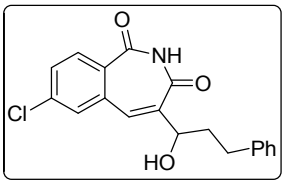
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.65-7.61 (m, 2H), 7.31-7.26 (m, 2H), 7.24-7.13 (m, 4H), 6.88 (dd, *J* = 9.2, 2.5 Hz, 1H), 6.37 (s, 1H), 5.96 (s, 1H), 5.31 (dt, *J* = 9.2, 2.4 Hz, 1H), 2.89-2.81 (m, 1H), 2.78-2.70 (m, 1H), 2.28-2.19 (m, 1H), 2.09-1.99 (m, 1H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 168.6, 164.0, 162.4 (d, *J* = 247.0 Hz), 140.6, 137.5, 133.9 (d, *J* = 3.0 Hz), 133.0 (d, *J* = 8.3 Hz), 130.8 (d, *J* = 9.0 Hz), 128.4, 128.2, 127.8, 126.1, 116.8 (d, *J* = 21.4 Hz), 115.5 (d, *J* = 22.5 Hz), 79.2, 32.6, 29.9.

^{19}F NMR (376 MHz, $CDCl_3$): δ -107.4.

HRMS (ESI) calculated for $C_{19}H_{17}FNO_3$ ($[M+H]^+$): 326.1192; found: 326.1185.

7-chloro-4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3g)



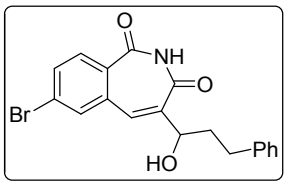
This compound was obtained in 60% yield (40.9 mg) as light yellow solid. Eluent: PE/EA = 1/1, R_f = 0.4.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61-7.53 (m, 2H), 7.42 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.31-7.26 (m, 2H), 7.21 (t, *J* = 7.3 Hz, 1H), 7.18-7.12 (m, 3H), 6.65 (s, 1H), 6.13 (s, 1H), 5.33-5.26 (m, 1H), 2.88-2.81 (m, 1H), 2.78-2.70 (m, 1H), 2.29-2.19 (m, 1H), 2.08-1.98 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 169.4, 164.0, 140.1, 138.8, 137.1, 134.6, 132.9, 130.2, 129.6, 128.9, 128.8, 128.5, 127.4, 126.5, 78.9, 33.1, 30.6.

HRMS (ESI) calculated for $C_{19}H_{17}ClNO_3$ ($[M+H]^+$): 342.0897; found: 342.0890.

7-bromo-4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3h)



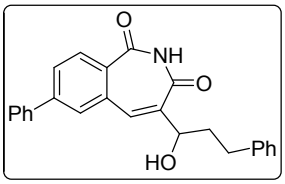
This compound was obtained in 67% yield (51.6 mg) as light yellow solid. m.p.: 103-105 °C. Eluent: PE/EA = 1/1, R_f = 0.4.

^{1}H NMR (400 MHz, DMSO-d_6): δ 8.08 (s, 1H), 7.76-7.68 (m, 2H), 7.60 (d, *J* = 1.6 Hz, 1H), 7.56 (d, *J* = 8.3 Hz, 1H), 7.51 (d, *J* = 1.5 Hz, 1H), 7.27 (t, *J* = 7.4 Hz, 2H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.12 (d, *J* = 7.3 Hz, 2H), 5.76-5.71 (m, 1H), 2.71-2.57 (m, 2H), 2.18-2.07 (m, 1H), 1.95-1.85 (m, 1H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 168.6, 163.9, 140.4, 137.7, 136.4, 132.7, 132.5, 131.1, 130.2, 128.5, 128.1, 127.3, 126.1, 123.4, 79.1, 32.5, 29.9.

HRMS (ESI) calculated for $C_{19}H_{17}BrNO_3$ ($[M+H]^+$): 386.0392; found: 386.0383.

4-(1-hydroxy-3-phenylpropyl)-7-phenyl-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3i)



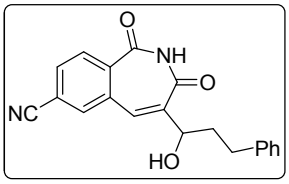
This compound was obtained in 67% yield (51.3 mg) as white solid. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75-7.62 (m, 3H), 7.50-7.42 (m, 5H), 7.38 (s, 1H), 7.22-7.16 (m, 3H), 7.10-7.04 (m, 2H), 6.47 (s, 1H), 6.10 (s, 1H), 5.33 (dt, *J* = 9.3, 2.0 Hz, 1H), 2.86-2.69 (m, 2H), 2.29-2.19 (m, 1H), 2.10-1.99 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 170.0, 164.3, 144.0, 140.2, 139.1, 137.9, 134.8, 131.9, 129.4, 129.0, 128.9, 128.8, 128.74, 128.67, 128.6, 127.7, 127.1, 126.4, 78.9, 33.5, 30.7.

HRMS (ESI) calculated for $C_{25}H_{22}NO_3$ ($[M+H]^+$): 384.1599; found: 384.1592.

4-(1-hydroxy-3-phenylpropyl)-1,3-dioxo-2,3-dihydro-1*H*-benzo[*c*]azepine-7-carbonitrile (3j)



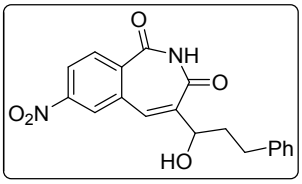
This compound was obtained in 47% yield (31.2 mg) as light yellow solid. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.22 (s, 1H), 8.00 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.93 (d, *J* = 1.4 Hz, 1H), 7.88 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 1.8 Hz, 1H), 7.27-7.23 (m, 2H), 7.19-7.14 (m, 1H), 7.13-7.10 (m, 2H), 5.82 (dt, *J* = 8.8, 2.4 Hz, 1H), 2.67-2.61 (m, 2H), 2.17-2.07 (m, 1H), 1.93-1.83 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 168.2, 163.8, 140.5, 138.5, 133.6, 132.2, 131.2, 129.1, 128.5, 128.4, 128.1, 126.7, 126.1, 117.7, 113.1, 79.3, 32.5, 29.9.

HRMS (ESI) calculated for $C_{20}H_{17}N_2O_3$ ([M+H]$^+$): 333.1239; found: 333.1233.

4-(1-hydroxy-3-phenylpropyl)-7-nitro-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3k)



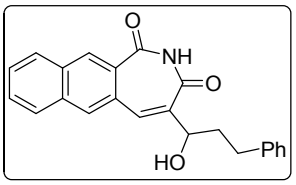
This compound was obtained in 37% yield (26.0 mg) as light yellow solid. m.p.: 63-65 °C. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.35-8.26 (m, 2H), 8.15 (d, *J* = 2.2 Hz, 1H), 7.96 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.49 (d, *J* = 1.8 Hz, 1H), 7.25 (t, *J* = 7.3 Hz, 2H), 7.20-7.12 (m, 3H), 5.77-5.70 (m, 1H), 2.75-2.61 (m, 2H), 2.30-2.19 (m, 1H), 2.04-1.93 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 168.0, 163.7, 148.1, 142.9, 140.3, 138.9, 131.4, 129.7, 128.4, 128.2, 126.3, 126.1, 124.6, 123.3, 79.4, 32.4, 30.0.

HRMS (ESI) calculated for $C_{19}H_{17}N_2O_5$ ([M+H]$^+$): 353.1137; found: 353.1132.

4-(1-hydroxy-3-phenylpropyl)-1*H*-naphtho[2,3-*c*]azepine-1,3(2*H*)-dione (3l)



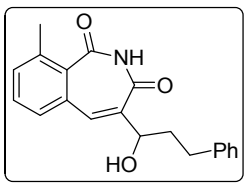
This compound was obtained in 34% yield (24.3 mg) as light yellow solid. m.p.: 112-115 °C. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.31 (s, 1H), 8.11 (s, 1H), 8.04-8.00 (m, 2H), 7.94-7.89 (m, 1H), 7.68-7.62 (m, 2H), 7.52 (d, *J* = 8.7 Hz, 1H), 7.29-7.23 (m, 3H), 7.20-7.14 (m, 3H), 5.87-5.83 (m, 1H), 2.79-2.69 (m, 2H), 2.37-2.26 (m, 1H), 2.08-1.98 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 169.1, 164.3, 140.6, 139.7, 136.9, 133.4, 129.1, 128.9, 128.4, 128.3, 128.2, 128.1, 127.7, 127.1, 126.1, 126.0, 124.9, 124.2, 79.9, 33.2, 30.2.

HRMS (ESI) calculated for $C_{23}H_{20}NO_3$ ([M+H]$^+$): 358.1443; found: 358.1436.

4-(1-hydroxy-3-phenylpropyl)-9-methyl-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3m)



This compound was obtained in 29% yield (18.6 mg) as white solid. Eluent: PE/EA = 1/1, Rf = 0.3.

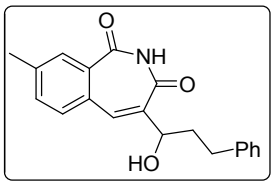
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.00 (s, 1H), 7.80 (s, 1H), 7.39-7.33 (m, 2H), 7.30-7.24 (m, 3H), 7.20-7.15 (m, 3H), 7.10 (d, *J* = 1.7 Hz, 1H), 5.73 (dt, *J* = 8.6, 2.2 Hz, 1H), 2.70 (t, *J* = 8.1 Hz, 2H), 2.30 (s, 3H), 2.29-2.19 (m, 1H), 2.01-1.91 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 169.6, 164.2, 140.6, 140.5, 136.5, 134.4, 132.1, 128.5, 128.4, 128.2, 127.9, 127.3, 126.1, 125.5, 79.7, 32.6,

30.1, 18.9.

HRMS (ESI) calculated for $C_{20}H_{20}NO_3$ ([M+H]$^+$): 322.1443; found: 322.1435.

4-(1-hydroxy-3-phenylpropyl)-8-methyl-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3n)



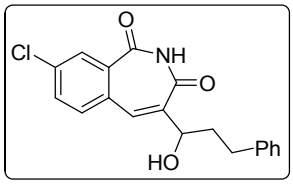
This compound was obtained in 66% yield (42.4 mg) as light yellow oil. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.99 (s, 1H), 7.62 (s, 1H), 7.52 (d, *J* = 1.6 Hz, 1H), 7.42 (s, 1H), 7.38-7.31 (m, 2H), 7.25 (t, *J* = 7.4 Hz, 2H), 7.19-7.11 (m, 3H), 5.71-5.66 (m, 1H), 2.67 (t, *J* = 8.0 Hz, 2H), 2.37 (s, 3H), 2.25-2.16 (m, 1H), 1.97-1.86 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 169.7, 164.4, 140.7, 140.4, 138.0, 135.3, 130.7, 128.9, 128.8, 128.4, 128.3, 128.2, 127.1, 126.1, 79.4, 32.6, 30.1, 20.9.

HRMS (ESI) calculated for $C_{20}H_{20}NO_3$ ([M+H]$^+$): 322.1443; found: 322.1438.

8-chloro-4-(1-hydroxy-3-phenylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3o)



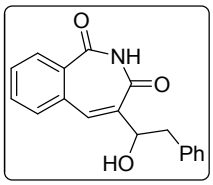
This compound was obtained in 26% yield (17.7 mg) as light yellow oil. Eluent: PE/EA = 1/1, R_f = 0.4.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.13 (s, 1H), 7.77 (s, 1H), 7.66 (d, *J* = 2.1 Hz, 1H), 7.59 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.52-7.47 (m, 2H), 7.28-7.22 (m, 2H), 7.19-7.10 (m, 3H), 5.73-5.67 (m, 1H), 2.65 (t, *J* = 8.0 Hz, 2H), 2.23-2.12 (m, 1H), 1.97-1.85 (m, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 168.1, 164.1, 140.6, 139.3, 136.9, 134.7, 130.7, 130.1, 128.9, 128.4, 128.2, 128.1, 127.3, 126.1, 79.5, 32.5, 30.0.

HRMS (ESI) calculated for $C_{19}H_{17}ClNO_3$ ([M+H]$^+$): 342.0897; found: 342.0892.

4-(1-hydroxy-2-phenylethyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3p)



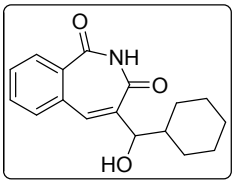
This compound was obtained in 75% yield (43.9 mg) as white solid. m.p.: 81-83 °C. Eluent: PE/EA = 1/1, R_f = 0.2.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.04 (s, 1H), 7.68-7.57 (m, 3H), 7.57-7.52 (m, 3H), 7.27-7.18 (m, 3H), 7.14-7.10 (m, 2H), 5.99-5.95 (m, 1H), 3.22 (dd, *J* = 15.0, 3.4 Hz, 1H), 2.97 (dd, *J* = 15.0, 7.5 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 169.7, 164.1, 137.8, 136.1, 135.3, 130.2, 129.9, 129.5, 129.1, 128.7, 128.2, 126.8, 79.6, 36.5.

HRMS (ESI) calculated for $C_{18}H_{16}NO_3$ ([M+H]$^+$): 294.1130; found: 294.1125.

4-(cyclohexyl(hydroxy)methyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3q)



This compound was obtained in 80% yield (45.6 mg) as light yellow oil. Eluent: PE/EA = 1/1, R_f = 0.5.

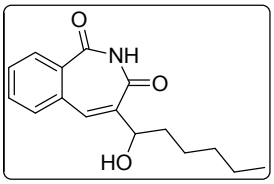
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.04 (s, 1H), 7.64-7.58 (m, 2H), 7.57-7.48 (m, 4H), 5.61 (dd, *J* = 3.9, 1.8 Hz, 1H), 1.83-1.75 (m, 1H), 1.66-

1.48 (m, 5H), 1.18-0.93 (m, 5H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 169.5, 164.6, 137.5, 134.6, 130.5, 130.13, 130.08, 129.2, 129.1, 128.1, 83.6, 38.6, 28.2, 25.5, 25.4, 25.1.

HRMS (ESI) calculated for $C_{17}H_{20}NO_3$ ([M+H]$^+$): 286.1443; found: 286.1437.

4-(1-hydroxyhexyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3r)



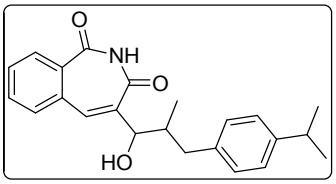
This compound was obtained in 81% yield (44.2 mg) as light yellow oil. Eluent: PE/EA = 1/1, R_f = 0.4.

^{1}H NMR (400 MHz, DMSO-d_6): δ 8.03 (s, 1H), 7.64 (s, 1H), 7.61-7.58 (m, 1H), 7.55-7.48 (m, 4H), 5.73-5.68 (m, 1H), 1.92-1.82 (m, 1H), 1.67-1.57 (m, 1H), 1.37-1.29 (m, 2H), 1.26-1.16 (m, 4H), 0.80 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 169.6, 164.5, 137.8, 136.4, 130.1, 130.0, 129.0, 128.2, 80.1, 30.71, 30.65, 23.6, 21.8, 13.7.

HRMS (ESI) calculated for $C_{16}H_{20}NO_3$ ([M+H]$^+$): 274.1443; found: 274.1437.

4-(1-hydroxy-3-(4-isopropylphenyl)-2-methylpropyl)-1*H*-benzo[*c*]azepine-1,3(2*H*)-dione (3s)

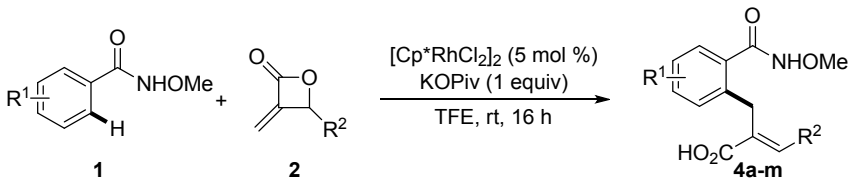


This compound was obtained in 74% yield (53.7 mg) as light yellow oil. Eluent: PE/EA = 1/1, R_f = 0.3. Two inseparable distereoselective isomers were obtained, the ratio was determined as 1:1 by ^{1}H-NMR analysis.

^{1}H NMR (400 MHz, DMSO-d_6): δ 8.06 (s, 0.5H), 8.03 (s, 0.5H), 7.70-7.65 (m, 1H), 7.62-7.40 (m, 5H), 7.16 (d, *J* = 8.1 Hz, 1H), 7.08 (d, *J* = 8.1 Hz, 1H), 7.02 (d, *J* = 8.0 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.71 (dd, *J* = 3.5, 1.9 Hz, 0.5H), 5.64-5.61 (m, 0.5H), 2.88-2.68 (m, 1.5H), 2.62 (d, *J* = 10.7 Hz, 0.5H), 2.48-2.41 (m, 0.5H), 2.26-2.18 (m, 0.5H), 2.17-2.02 (m, 1H), 1.17 (d, *J* = 6.9 Hz, 3H), 1.12 (d, *J* = 6.9 Hz, 3H), 0.77 (d, *J* = 6.5 Hz, 1.5H), 0.66 (d, *J* = 6.8 Hz, 1.5H).

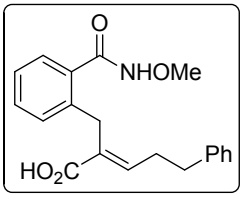
^{13}C NMR (100 MHz, DMSO-d_6): δ 169.5, 169.4, 164.3, 146.2, 145.9, 137.6, 137.1, 136.84, 136.76, 135.1, 134.7, 131.0, 130.33, 130.32, 130.2, 130.11, 130.06, 129.4, 129.2, 128.8, 128.6, 128.5, 128.1, 127.0, 126.3, 126.1, 83.6, 82.4, 38.2, 36.3, 35.22, 35.19, 33.0, 32.9, 23.94, 23.89, 14.7, 12.1.

HRMS (ESI) calculated for $C_{23}H_{26}NO_3$ ([M+H]$^+$): 364.1912; found: 364.1906.



The mixture of *N*-methoxybenzamides **1** (0.2 mmol, 1.0 equiv), α-methylene-β-lactones **2** (0.3 mmol, 1.5 equiv), $[Cp^*RhCl_2]_2$ (5 mol %) and KOPiv (0.2 mmol, 1.0 equiv) in TFE (2.0 mL) was stirred at room temperature for 16 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding allylated benzamides **4a**-**m**.

2-(2-(methoxycarbamoyl)benzyl)-5-phenylpent-2-enoic acid (4a)



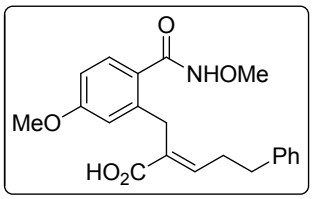
This compound was obtained in 67% yield (45.4 mg) as white solid. Eluent: PE/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-d_6): δ 7.34-7.25 (m, 5H), 7.22-7.18 (m, 2H), 7.14 (td, *J* = 7.4, 0.9 Hz, 1H), 6.79 (d, *J* = 7.3 Hz, 1H), 6.64 (t, *J* = 7.4 Hz, 1H), 3.69 (s, 3H), 3.49 (s, 2H), 2.77 (t, *J* = 7.4 Hz, 2H), 2.61-2.54 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 171.4, 165.4, 141.6, 138.3, 137.9, 135.4, 134.4, 129.3, 128.6, 128.5, 128.4, 128.3, 125.8, 125.4, 62.6, 35.1, 30.2, 29.6.

HRMS (ESI) calculated for $C_{20}H_{22}NO_4$ ([M+H]$^+$): 340.1549; found: 340.1543.

2-(5-methoxy-2-(methoxycarbamoyl)benzyl)-5-phenylpent-2-enoic acid (4b)



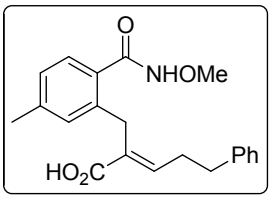
This compound was obtained in 69% yield (50.9 mg) as light yellow oil. Eluent: DCM/EA = 1/1, R_f = 0.2.

^{1}H NMR (400 MHz, CD$_3$OD): δ 7.32 (d, *J* = 8.5 Hz, 1H), 7.27-7.18 (m, 4H), 7.17-7.12 (m, 1H), 6.90 (t, *J* = 7.5 Hz, 1H), 6.77 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.62 (d, *J* = 2.5 Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 3.70 (s, 2H), 2.77 (t, *J* = 7.5 Hz, 2H), 2.57 (q, *J* = 7.5 Hz, 2H).

^{13}C NMR (100 MHz, CD$_3$OD): δ 169.4, 162.8, 142.6, 142.0, 141.9, 135.4, 130.8, 129.5, 129.4, 127.0, 126.5, 115.3, 112.3, 64.3, 55.7, 36.1, 31.9, 30.6.

HRMS (ESI) calculated for $C_{21}H_{24}NO_5$ ([M+H]$^+$): 370.1654; found: 370.1649.

2-(2-(methoxycarbamoyl)-5-methylbenzyl)-5-phenylpent-2-enoic acid (4c)



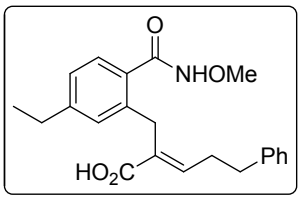
This compound was obtained in 36% yield (25.4 mg) as colorless oil. Eluent: PE/EA/HOAc = 30/20/1, R_f = 0.4.

^{1}H NMR (400 MHz, CD$_3$OD): δ 7.28-7.20 (m, 5H), 7.18-7.12 (m, 1H), 7.01 (d, *J* = 7.7 Hz, 1H), 6.85 (s, 1H), 6.81-6.74 (m, 1H), 3.81 (s, 3H), 3.63 (s, 2H), 2.79 (t, *J* = 7.3 Hz, 2H), 2.62-2.54 (m, 2H), 2.23 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 170.6, 165.5, 141.4, 138.9, 138.2, 137.5, 136.0, 131.5, 128.7, 128.4, 128.3, 128.2, 126.2, 125.9, 62.7, 34.8, 30.1, 29.3, 21.0.

HRMS (ESI) calculated for $C_{21}H_{24}NO_4$ ([M+H]$^+$): 354.1705; found: 354.1701.

2-(5-ethyl-2-(methoxycarbamoyl)benzyl)-5-phenylpent-2-enoic acid (4d)



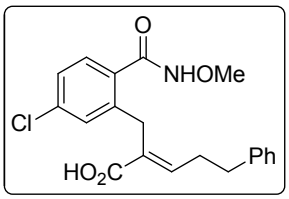
This compound was obtained in 59% yield (43.3 mg) as white solid. Eluent: PE/EA/HOAc = 30/15/1, R_f = 0.3.

^{1}H NMR (400 MHz, CD$_3$OD): δ 7.29-7.22 (m, 3H), 7.20-7.13 (m, 3H), 7.06 (d, *J* = 7.7 Hz, 1H), 7.01-6.83 (m, 2H), 3.82 (s, 3H), 3.74 (s, 2H), 2.76 (t, *J* = 7.2 Hz, 2H), 2.61-2.50 (m, 4H), 1.15 (t, *J* = 7.5 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 170.3, 165.5, 145.2, 141.3, 138.8, 138.2, 134.8, 131.6, 131.5, 128.4, 128.3, 128.2, 127.4, 125.9, 125.0, 124.9, 62.8, 34.6, 30.1, 29.1, 28.0, 15.4.

HRMS (ESI) calculated for $C_{22}H_{26}NO_4$ ([M+H]$^+$): 368.1862; found: 368.1857.

2-(5-chloro-2-(methoxycarbamoyl)benzyl)-5-phenylpent-2-enoic acid (4e)



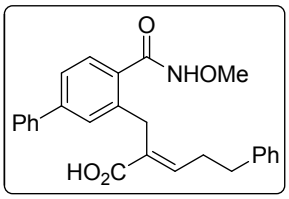
This compound was obtained in 47% yield (35.1 mg) as light yellow solid. Eluent: PE/EA/HOAc = 30/20/1, R_f = 0.4.

^{1}H NMR (400 MHz, CD_3OD): δ 7.35 (d, *J* = 8.2 Hz, 1H), 7.27-7.19 (m, 5H), 7.18-7.12 (m, 1H), 7.02 (d, *J* = 1.9 Hz, 1H), 6.84 (t, *J* = 7.5 Hz, 1H), 3.81 (s, 3H), 3.63 (s, 2H), 2.79 (t, *J* = 7.4 Hz, 2H), 2.56 (q, *J* = 7.4 Hz, 2H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 170.8, 164.4, 141.5, 141.2, 137.2, 136.1, 134.1, 133.3, 130.4, 128.4, 128.3, 128.1, 125.9, 125.7, 62.7, 35.0, 30.0, 29.7.

HRMS (ESI) calculated for $C_{20}H_{21}ClNO_4$ ([M+H]$^+$): 374.1159; found: 374.1156.

2-((4-(methoxycarbamoyl)-[1,1'-biphenyl]-3-yl)methyl)-5-phenylpent-2-enoic acid (4f)



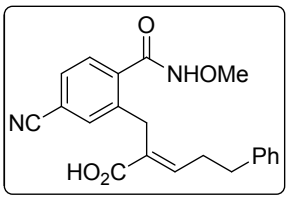
This compound was obtained in 65% yield (53.9 mg) as white solid. Eluent: DCM/EA/HOAc = 50/50/1, R_f = 0.3.

^{1}H NMR (400 MHz, CD_3OD): δ 7.54-7.51 (m, 2H), 7.49-7.40 (m, 4H), 7.37-7.32 (m, 2H), 7.22-7.16 (m, 4H), 7.11-7.06 (m, 1H), 6.91 (t, *J* = 7.4 Hz, 1H), 3.84 (s, 3H), 3.77 (s, 2H), 2.78 (t, *J* = 7.4 Hz, 2H), 2.65-2.57 (m, 2H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 171.2, 165.1, 141.5, 141.0, 139.7, 139.1, 138.2, 135.2, 133.5, 129.3, 129.0, 128.4, 128.3, 127.7, 126.8, 126.6, 125.8, 124.0, 62.6, 35.1, 30.0, 29.8.

HRMS (ESI) calculated for $C_{26}H_{26}NO_4$ ([M+H]$^+$): 416.1862; found: 416.1857.

2-(5-cyano-2-(methoxycarbamoyl)benzyl)-5-phenylpent-2-enoic acid (4g)



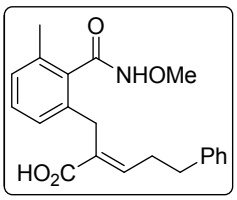
This compound was obtained in 73% yield (53.1 mg) as light yellow solid. Eluent: DCM/EA = 2/1, R_f = 0.3.

^{1}H NMR (400 MHz, CD_3OD): δ 7.56 (d, *J* = 7.9 Hz, 1H), 7.50 (d, *J* = 7.9 Hz, 1H), 7.28-7.20 (m, 4H), 7.19-7.13 (m, 2H), 6.83 (t, *J* = 7.4 Hz, 1H), 3.83 (s, 3H), 3.64 (s, 2H), 2.81 (t, *J* = 7.2 Hz, 2H), 2.58 (q, *J* = 7.2 Hz, 2H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 171.0, 163.7, 141.5, 140.6, 137.4, 135.9, 131.8, 129.4, 129.0, 128.4, 128.3, 125.9, 118.7, 111.3, 67.2, 34.9, 29.9, 29.6.

HRMS (ESI) calculated for $C_{21}H_{21}N_2O_4$ ([M+H]$^+$): 365.1501; found: 365.1500.

2-(2-(methoxycarbamoyl)-3-methylbenzyl)-5-phenylpent-2-enoic acid (4h)



This compound was obtained in 30% yield (21.2 mg) as light yellow oil. Eluent: DCM/EA/HOAc = 50/50/1, R_f = 0.4.

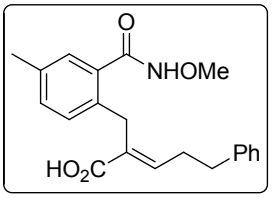
^{1}H NMR (400 MHz, CD_3OD): δ 7.27-7.21 (m, 2H), 7.19-7.11 (m, 4H), 7.07-7.00 (m, 2H), 6.72 (d, *J* = 7.7 Hz, 1H), 3.84 (s, 3H), 3.58 (s, 2H), 2.76 (t, *J* = 7.3 Hz, 2H), 2.53 (q, *J* = 7.4 Hz, 2H), 2.33 (s, 3H).

^{13}C NMR (100 MHz, CD_3OD): δ 171.7, 169.2, 144.8, 142.4, 138.3, 136.6, 134.5, 132.7, 130.7, 129.6, 129.4, 128.8, 127.1, 126.0, 64.4, 35.8, 31.9,

30.0, 19.1.

HRMS (ESI) calculated for $C_{21}H_{24}NO_4$ ([M+H]$^+$): 354.1705; found: 354.1700.

2-(2-(methoxycarbamoyl)-4-methylbenzyl)-5-phenylpent-2-enoic acid (4i)



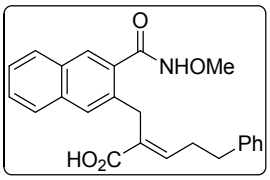
This compound was obtained in 62% yield (43.8 mg) as colorless oil. Eluent: DCM/EA/HOAc = 50/50/1, R_f = 0.4.

^{1}H NMR (400 MHz, CD_3OD): δ 7.28-7.20 (m, 4H), 7.19-7.13 (m, 2H), 7.07 (d, *J* = 7.9 Hz, 1H), 6.84-6.77 (m, 2H), 3.82 (s, 3H), 3.59 (s, 2H), 2.79 (t, *J* = 7.4 Hz, 2H), 2.57 (q, *J* = 7.4 Hz, 2H), 2.28 (s, 3H).

^{13}C NMR (100 MHz, CD_3OD): δ 175.3, 169.5, 142.8, 139.9, 136.7, 136.5, 134.1, 132.1, 129.9, 129.7, 129.5, 129.4, 127.0, 64.3, 36.3, 32.0, 30.2, 20.8.

HRMS (ESI) calculated for $C_{21}H_{24}NO_4$ ([M+H]$^+$): 354.1705; found: 354.1701.

2-((3-(methoxycarbamoyl)naphthalen-2-yl)methyl)-5-phenylpent-2-enoic acid (4j)



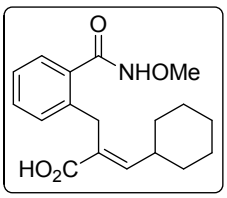
This compound was obtained in 55% yield (42.8 mg) as white solid. Eluent: DCM/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, CD_3OD): δ 7.88 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 8.1 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.53-7.43 (m, 2H), 7.29-7.15 (m, 5H), 7.03 (d, *J* = 8.5 Hz, 1H), 6.86 (t, *J* = 7.2 Hz, 1H), 3.92 (s, 3H), 3.70 (s, 2H), 2.82 (t, *J* = 7.2 Hz, 2H), 2.67-2.61 (m, 2H).

^{13}C NMR (100 MHz, DMSO-*d_6*): δ 170.8, 166.0, 141.5, 136.9, 136.6, 135.8, 131.3, 130.5, 128.8, 128.5, 128.3, 127.8, 126.6, 126.1, 125.9, 125.4, 124.9, 62.8, 34.9, 30.2, 27.2.

HRMS (ESI) calculated for $C_{24}H_{24}NO_4$ ([M+H]$^+$): 390.1705; found: 390.1701.

3-cyclohexyl-2-(2-(methoxycarbamoyl)benzyl)acrylic acid (4k)



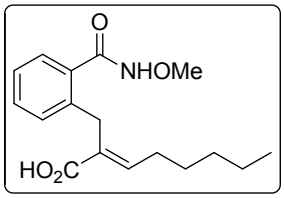
This compound was obtained in 40% yield (25.4 mg) as light yellow oil. Eluent: DCM/EA = 1/1, R_f = 0.3.

^{1}H NMR (400 MHz, CD_3OD): δ 7.39-7.32 (m, 2H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.16 (d, *J* = 7.7 Hz, 1H), 6.70 (d, *J* = 10.0 Hz, 1H), 3.85 (s, 3H), 3.78 (s, 2H), 2.46-2.36 (m, 1H), 1.77-1.64 (m, 5H), 1.39-1.18 (m, 10H).

^{13}C NMR (100 MHz, CD_3OD): δ 169.5, 148.3, 139.9, 134.3, 132.7, 131.5, 129.6, 129.0, 127.0, 64.4, 39.1, 33.5, 30.5, 27.0, 26.6.

HRMS (ESI) calculated for $C_{18}H_{24}NO_4$ ([M+H]$^+$): 318.1705; found: 318.1698.

2-(2-(methoxycarbamoyl)benzyl)oct-2-enoic acid (4l)



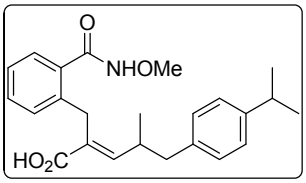
This compound was obtained in 53% yield (32.3 mg) as light yellow oil. Eluent: DCM/EA = 2/3, R_f = 0.4.

^{1}H NMR (400 MHz, CD_3OD): δ 7.39-7.34 (m, 2H), 7.24 (t, *J* = 7.1 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H), 3.84 (s, 3H), 3.80 (s, 2H), 2.25 (q, *J* = 7.4 Hz, 2H), 1.52-1.43 (m, 2H), 1.35-1.29 (m, 4H), 0.90 (t, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, CD_3OD): δ 172.2, 169.5, 145.3, 139.7, 134.3, 132.9, 131.5, 129.6, 128.9, 127.1, 64.4, 32.7, 30.2, 29.8, 29.6, 23.5, 14.3.

HRMS (ESI) calculated for $C_{17}H_{24}NO_4$ ([M+H]$^+$): 306.1705; found: 306.1702.

5-(4-isopropylphenyl)-2-(2-(methoxycarbamoyl)benzyl)-4-methylpent-2-enoic acid (4m)



This compound was obtained in 29% yield (22.9 mg) as light yellow oil. Eluent: DCM/EA = 1/1, R_f = 0.4.

^{1}H NMR (400 MHz, CD_3OD): δ 7.36-7.32 (m, 1H), 7.18-7.14 (m, 2H), 7.13-7.08 (m, 4H), 6.80-6.73 (m, 1H), 6.62 (d, *J* = 10.1 Hz, 1H), 3.81 (s, 3H), 3.49 (d, *J* = 5.1 Hz, 2H), 2.90-2.79 (m, 2H), 2.72-2.59 (m, 2H), 1.23 (d, *J* = 6.9 Hz, 6H), 1.09 (d, *J* = 6.5 Hz, 3H).

^{13}C NMR (100 MHz, CD_3OD): δ 171.7, 169.2, 144.8, 142.4, 138.3, 136.6, 134.5, 132.7, 130.7, 129.6, 129.4, 128.8, 127.1, 126.0, 64.4, 35.8, 31.9, 30.0, 19.1.

HRMS (ESI) calculated for $C_{24}H_{30}NO_4$ ([M+H] +): 396.2175; found: 396.2173.

III. DFT Studies

Computational details:

Density functional theory (DFT) calculations were performed using Gaussian 09.[S3] Geometry optimizations were carried out at the M06-2X[S4] level with a standard 6-31G(d,p) basis set (SDD[S5] basis set for Rh) using SMD[S6] solvation model (solvent = DCE and TFE, respectively). Frequency analyses were computed at the same level of theory to ensure that the optimized structures were at either a minimum or transition state.

Table S3. The compared key geometric structures about the two pathways

Species	the O-C bond (Å)		the N-O bond (Å)	
	TFE	DCE	TFE	DCE
INT-1	1.47	1.47	1.40	1.40
TS-6 (*β*-O elimination pathway)	**2.12**	**2.16**	/	/
TS-3 (*β*-H elimination pathway)	/	/	**1.98**	**1.94**

As shown in Table S3, we compared the geometric structures about the *β*-O elimination pathways both in TFE and DCE (please see above and the Table S3 in revised SI). From the starting-point **INT-1**, the distances of the O-C bond are nearly identical (1.47 Å); however, the distances of the breaking O-C bond of the **TS-6** are 2.12 Å and 2.16 Å in TFE and DCE, respectively. Obviously, the solvent changes the transition-state structure and makes it become more tight (associate) and lower energy barrier in TFE. On the contrary, considering the structures about β-H elimination pathways both in TFE and DCE, the distances of the breaking N-O bond of the **TS-6** (the limiting step of the *β*-H elimination pathway) are 1.98 Å and 1.94 Å in TFE and DCE, respectively. This indicates that TFE makes the transition-state structure become looser and require to overcome higher energy barrier compared to DCE.

As listed in Fig. S1, we calculated and compared the electrostatic potential surfaces of the intermediate **INT-1**, the transition state **TS-6** for the determining step (C-O bond cleavage step) in *β*-O elimination pathways as well as the transition state **TS-3** for the determining step (N-O bond cleavage step) in *β*-H elimination pathways in both of solvents (TFE and DCE, respectively, please see above and the Figure S1 in revised SI). Generally, the higher charge dispersion will help to make transition state become more stable, which can further decrease the barrier and improve the reaction rate. In **INT-1**, the electron densities of the N-O bond are almost the same in both of the solvents; however, there is higher charge dispersion in **TS-6** with TFE than that with DCE. The obvious charge dispersion change indicates that the high-polar solvent decrease the barrier of **TS-6** and makes the *β*-O elimination pathway become a more favorable pathway, compared to the *β*-H elimination pathway. Besides, the electrostatic potential surfaces of **TS-3** for the determining step (N-O bond cleavage step) in *β*-H elimination pathways have been also performed,

unfortunately, it is difficult to distinguish the differences between TFE and DCE, due to the densities of the N-O bond have been shielded by surrounding atoms.

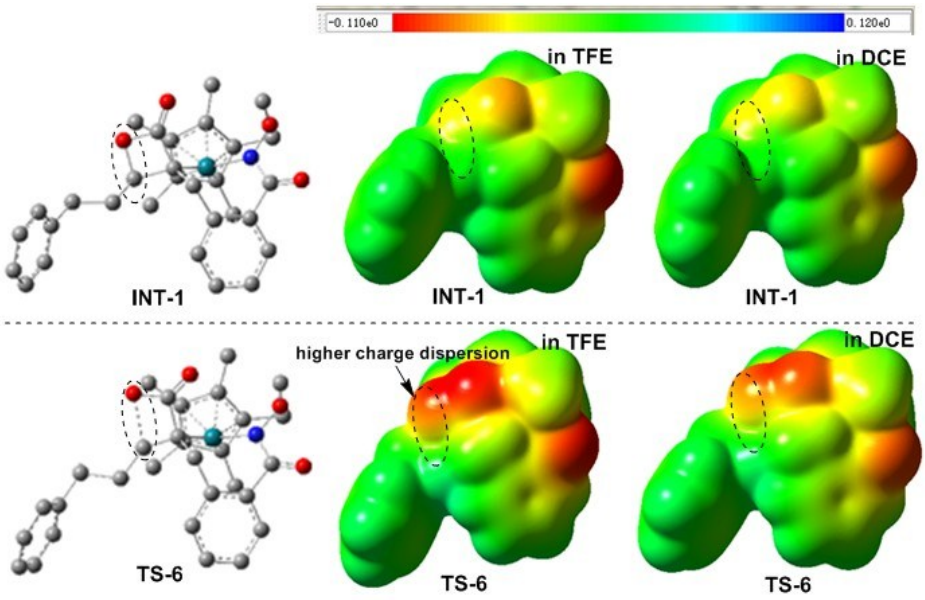


Figure S1. Calculated electrostatic potential surfaces of the transition states and pre-intermediate in rate-determining step (C-O bond cleavage step) in *β*-O elimination pathway.

Various Energy Values For All of The Relevant Species [optimized at the at the level of M06-2X/6-31G(d,p) (SDD for Rh) with SMD atomic radii for experimental solvent DCE and TFE, respectively]

CH_3COOH (in DCE)

Zero-point correction= 0.062522 (Hartree/Particle)
Thermal correction to Energy= 0.067126
Thermal correction to Enthalpy= 0.068071
Thermal correction to Gibbs Free Energy= 0.034689
Sum of electronic and zero-point Energies= -228.934501
Sum of electronic and thermal Energies= -228.929896
Sum of electronic and thermal Enthalpies= -228.928952
Sum of electronic and thermal Free Energies= -228.962333

CH_3OH (in DCE)

Zero-point correction= 0.051895 (Hartree/Particle)
Thermal correction to Energy= 0.055179
Thermal correction to Enthalpy= 0.056123
Thermal correction to Gibbs Free Energy= 0.029191
Sum of electronic and zero-point Energies= -115.615090
Sum of electronic and thermal Energies= -115.611807
Sum of electronic and thermal Enthalpies= -115.610862
Sum of electronic and thermal Free Energies= -115.637794

Cat. (in DCE)

Zero-point correction= 0.328575 (Hartree/Particle)
Thermal correction to Energy= 0.352693
Thermal correction to Enthalpy= 0.353637
Thermal correction to Gibbs Free Energy= 0.274344

Sum of electronic and zero-point Energies= -956.911664
Sum of electronic and thermal Energies= -956.887546
Sum of electronic and thermal Enthalpies= -956.886602
Sum of electronic and thermal Free Energies= -956.965895

INT-1 (in DCE)

Zero-point correction= 0.581603 (Hartree/Particle)
Thermal correction to Energy= 0.617867
Thermal correction to Enthalpy= 0.618811
Thermal correction to Gibbs Free Energy= 0.512546
Sum of electronic and zero-point Energies= -1628.571214
Sum of electronic and thermal Energies= -1628.534951
Sum of electronic and thermal Enthalpies= -1628.534007
Sum of electronic and thermal Free Energies= -1628.640272

INT-2 (in DCE)

Zero-point correction= 0.582207 (Hartree/Particle)
Thermal correction to Energy= 0.617683
Thermal correction to Enthalpy= 0.618627
Thermal correction to Gibbs Free Energy= 0.514778
Sum of electronic and zero-point Energies= -1628.555761
Sum of electronic and thermal Energies= -1628.520285
Sum of electronic and thermal Enthalpies= -1628.519341
Sum of electronic and thermal Free Energies= -1628.623190

TS-1 (in DCE)

Zero-point correction= 0.577445 (Hartree/Particle)
Thermal correction to Energy= 0.612943
Thermal correction to Enthalpy= 0.613888
Thermal correction to Gibbs Free Energy= 0.510233
Sum of electronic and zero-point Energies= -1628.547933
Sum of electronic and thermal Energies= -1628.512435
Sum of electronic and thermal Enthalpies= -1628.511491
Sum of electronic and thermal Free Energies= -1628.615146

INT-3 (in DCE)

Zero-point correction= 0.578723 (Hartree/Particle)
Thermal correction to Energy= 0.614683
Thermal correction to Enthalpy= 0.615627
Thermal correction to Gibbs Free Energy= 0.510929
Sum of electronic and zero-point Energies= -1628.550076
Sum of electronic and thermal Energies= -1628.514117
Sum of electronic and thermal Enthalpies= -1628.513173
Sum of electronic and thermal Free Energies= -1628.617871

TS-2 (in DCE)

Zero-point correction= 0.576987 (Hartree/Particle)
Thermal correction to Energy= 0.612645
Thermal correction to Enthalpy= 0.613589
Thermal correction to Gibbs Free Energy= 0.509169

Sum of electronic and zero-point Energies= -1628.534638
Sum of electronic and thermal Energies= -1628.498980
Sum of electronic and thermal Enthalpies= -1628.498035
Sum of electronic and thermal Free Energies= -1628.602455

INT-4 (in DCE)

Zero-point correction= 0.581628 (Hartree/Particle)
Thermal correction to Energy= 0.617913
Thermal correction to Enthalpy= 0.618857
Thermal correction to Gibbs Free Energy= 0.511401
Sum of electronic and zero-point Energies= -1628.574321
Sum of electronic and thermal Energies= -1628.538037
Sum of electronic and thermal Enthalpies= -1628.537093
Sum of electronic and thermal Free Energies= -1628.644549

INT-5 (in DCE)

Zero-point correction= 0.646026 (Hartree/Particle)
Thermal correction to Energy= 0.688201
Thermal correction to Enthalpy= 0.689145
Thermal correction to Gibbs Free Energy= 0.568489
Sum of electronic and zero-point Energies= -1857.517998
Sum of electronic and thermal Energies= -1857.475823
Sum of electronic and thermal Enthalpies= -1857.474879
Sum of electronic and thermal Free Energies= -1857.595535

TS-3 (in DCE)

Zero-point correction= 0.641067 (Hartree/Particle)
Thermal correction to Energy= 0.682636
Thermal correction to Enthalpy= 0.683580
Thermal correction to Gibbs Free Energy= 0.564269
Sum of electronic and zero-point Energies= -1857.488078
Sum of electronic and thermal Energies= -1857.446509
Sum of electronic and thermal Enthalpies= -1857.445564
Sum of electronic and thermal Free Energies= -1857.564875

INT-6 (in DCE)

Zero-point correction= 0.644476 (Hartree/Particle)
Thermal correction to Energy= 0.686958
Thermal correction to Enthalpy= 0.687902
Thermal correction to Gibbs Free Energy= 0.567985
Sum of electronic and zero-point Energies= -1857.565342
Sum of electronic and thermal Energies= -1857.522860
Sum of electronic and thermal Enthalpies= -1857.521916
Sum of electronic and thermal Free Energies= -1857.641833

TS-4 (in DCE)

Zero-point correction= 0.643803 (Hartree/Particle)
Thermal correction to Energy= 0.685129
Thermal correction to Enthalpy= 0.686073
Thermal correction to Gibbs Free Energy= 0.568738

Sum of electronic and zero-point Energies= -1857.534042
Sum of electronic and thermal Energies= -1857.492716
Sum of electronic and thermal Enthalpies= -1857.491771
Sum of electronic and thermal Free Energies= -1857.609107

INT-7 (in DCE)

Zero-point correction= 0.645091 (Hartree/Particle)
Thermal correction to Energy= 0.686631
Thermal correction to Enthalpy= 0.687575
Thermal correction to Gibbs Free Energy= 0.570305
Sum of electronic and zero-point Energies= -1857.536869
Sum of electronic and thermal Energies= -1857.495329
Sum of electronic and thermal Enthalpies= -1857.494385
Sum of electronic and thermal Free Energies= -1857.611655

TS-5 (in DCE)

Zero-point correction= 0.644507 (Hartree/Particle)
Thermal correction to Energy= 0.685769
Thermal correction to Enthalpy= 0.686713
Thermal correction to Gibbs Free Energy= 0.569580
Sum of electronic and zero-point Energies= -1857.530211
Sum of electronic and thermal Energies= -1857.488949
Sum of electronic and thermal Enthalpies= -1857.488005
Sum of electronic and thermal Free Energies= -1857.605138

INT-8 (in DCE)

Zero-point correction= 0.645678 (Hartree/Particle)
Thermal correction to Energy= 0.687631
Thermal correction to Enthalpy= 0.688575
Thermal correction to Gibbs Free Energy= 0.568935
Sum of electronic and zero-point Energies= -1857.588392
Sum of electronic and thermal Energies= -1857.546439
Sum of electronic and thermal Enthalpies= -1857.545495
Sum of electronic and thermal Free Energies= -1857.665135

PC1 (in DCE)

Zero-point correction= 0.325748 (Hartree/Particle)
Thermal correction to Energy= 0.344837
Thermal correction to Enthalpy= 0.345781
Thermal correction to Gibbs Free Energy= 0.274624
Sum of electronic and zero-point Energies= -1013.999448
Sum of electronic and thermal Energies= -1013.980358
Sum of electronic and thermal Enthalpies= -1013.979414
Sum of electronic and thermal Free Energies= -1014.050572

TS-6 (in DCE)

Zero-point correction= 0.578263 (Hartree/Particle)
Thermal correction to Energy= 0.614589
Thermal correction to Enthalpy= 0.615533
Thermal correction to Gibbs Free Energy= 0.509402

Sum of electronic and zero-point Energies=	-1628.519738
Sum of electronic and thermal Energies=	-1628.483412
Sum of electronic and thermal Enthalpies=	-1628.482468
Sum of electronic and thermal Free Energies=	-1628.588598

INT-9 (in DCE)

Zero-point correction=	0.581442 (Hartree/Particle)
Thermal correction to Energy=	0.617395
Thermal correction to Enthalpy=	0.618339
Thermal correction to Gibbs Free Energy=	0.514922
Sum of electronic and zero-point Energies=	-1628.596637
Sum of electronic and thermal Energies=	-1628.560684
Sum of electronic and thermal Enthalpies=	-1628.559740
Sum of electronic and thermal Free Energies=	-1628.663157

PC2 (in DCE)

Zero-point correction=	0.379253 (Hartree/Particle)
Thermal correction to Energy=	0.402442
Thermal correction to Enthalpy=	0.403387
Thermal correction to Gibbs Free Energy=	0.324326
Sum of electronic and zero-point Energies=	-1129.567269
Sum of electronic and thermal Energies=	-1129.544080
Sum of electronic and thermal Enthalpies=	-1129.543136
Sum of electronic and thermal Free Energies=	-1129.622196

CH_3COOH (in TFE)

Zero-point correction=	0.062141 (Hartree/Particle)
Thermal correction to Energy=	0.065887
Thermal correction to Enthalpy=	0.066832
Thermal correction to Gibbs Free Energy=	0.036133
Sum of electronic and zero-point Energies=	-228.933883
Sum of electronic and thermal Energies=	-228.930136
Sum of electronic and thermal Enthalpies=	-228.929192
Sum of electronic and thermal Free Energies=	-228.959891

CH_3OH (in TFE)

Zero-point correction=	0.052166 (Hartree/Particle)
Thermal correction to Energy=	0.055435
Thermal correction to Enthalpy=	0.056379
Thermal correction to Gibbs Free Energy=	0.029465
Sum of electronic and zero-point Energies=	-115.616894
Sum of electronic and thermal Energies=	-115.613625
Sum of electronic and thermal Enthalpies=	-115.612681
Sum of electronic and thermal Free Energies=	-115.639594

Cat. (in TFE)

Zero-point correction=	0.327537 (Hartree/Particle)
Thermal correction to Energy=	0.352031
Thermal correction to Enthalpy=	0.352975
Thermal correction to Gibbs Free Energy=	0.271837

Sum of electronic and zero-point Energies=	-956.927498
Sum of electronic and thermal Energies=	-956.903004
Sum of electronic and thermal Enthalpies=	-956.902060
Sum of electronic and thermal Free Energies=	-956.983198

INT-1 **(in TFE)**

Zero-point correction=	0.581350 (Hartree/Particle)
Thermal correction to Energy=	0.617513
Thermal correction to Enthalpy=	0.618457
Thermal correction to Gibbs Free Energy=	0.512451
Sum of electronic and zero-point Energies=	-1628.573308
Sum of electronic and thermal Energies=	-1628.537145
Sum of electronic and thermal Enthalpies=	-1628.536200
Sum of electronic and thermal Free Energies=	-1628.642207

INT-2 **(in TFE)**

Zero-point correction=	0.581993 (Hartree/Particle)
Thermal correction to Energy=	0.617444
Thermal correction to Enthalpy=	0.618388
Thermal correction to Gibbs Free Energy=	0.514502
Sum of electronic and zero-point Energies=	-1628.558474
Sum of electronic and thermal Energies=	-1628.523024
Sum of electronic and thermal Enthalpies=	-1628.522079
Sum of electronic and thermal Free Energies=	-1628.625966

TS-1 **(in TFE)**

Zero-point correction=	0.576975 (Hartree/Particle)
Thermal correction to Energy=	0.612577
Thermal correction to Enthalpy=	0.613521
Thermal correction to Gibbs Free Energy=	0.509288
Sum of electronic and zero-point Energies=	-1628.549443
Sum of electronic and thermal Energies=	-1628.513841
Sum of electronic and thermal Enthalpies=	-1628.512897
Sum of electronic and thermal Free Energies=	-1628.617131

INT-3 **(in TFE)**

Zero-point correction=	0.578540 (Hartree/Particle)
Thermal correction to Energy=	0.614396
Thermal correction to Enthalpy=	0.615340
Thermal correction to Gibbs Free Energy=	0.511206
Sum of electronic and zero-point Energies=	-1628.551164
Sum of electronic and thermal Energies=	-1628.515308
Sum of electronic and thermal Enthalpies=	-1628.514364
Sum of electronic and thermal Free Energies=	-1628.618498

TS-2 **(in TFE)**

Zero-point correction=	0.576347 (Hartree/Particle)
Thermal correction to Energy=	0.612087
Thermal correction to Enthalpy=	0.613031
Thermal correction to Gibbs Free Energy=	0.508171

Sum of electronic and zero-point Energies=	-1628.533379
Sum of electronic and thermal Energies=	-1628.497639
Sum of electronic and thermal Enthalpies=	-1628.496695
Sum of electronic and thermal Free Energies=	-1628.601554

INT-4 (in TFE)

Zero-point correction=	0.580914 (Hartree/Particle)
Thermal correction to Energy=	0.617355
Thermal correction to Enthalpy=	0.618300
Thermal correction to Gibbs Free Energy=	0.510568
Sum of electronic and zero-point Energies=	-1628.569427
Sum of electronic and thermal Energies=	-1628.532985
Sum of electronic and thermal Enthalpies=	-1628.532041
Sum of electronic and thermal Free Energies=	-1628.639773

INT-5 (in TFE)

Zero-point correction=	0.645049 (Hartree/Particle)
Thermal correction to Energy=	0.687399
Thermal correction to Enthalpy=	0.688343
Thermal correction to Gibbs Free Energy=	0.565470
Sum of electronic and zero-point Energies=	-1857.520705
Sum of electronic and thermal Energies=	-1857.478355
Sum of electronic and thermal Enthalpies=	-1857.477411
Sum of electronic and thermal Free Energies=	-1857.600284

TS-3 (in TFE)

Zero-point correction=	0.639749 (Hartree/Particle)
Thermal correction to Energy=	0.681474
Thermal correction to Enthalpy=	0.682418
Thermal correction to Gibbs Free Energy=	0.562661
Sum of electronic and zero-point Energies=	-1857.476968
Sum of electronic and thermal Energies=	-1857.435243
Sum of electronic and thermal Enthalpies=	-1857.434299
Sum of electronic and thermal Free Energies=	-1857.554056

INT-6 (in TFE)

Zero-point correction=	0.645411 (Hartree/Particle)
Thermal correction to Energy=	0.687482
Thermal correction to Enthalpy=	0.688426
Thermal correction to Gibbs Free Energy=	0.569060
Sum of electronic and zero-point Energies=	-1857.568182
Sum of electronic and thermal Energies=	-1857.526111
Sum of electronic and thermal Enthalpies=	-1857.525167
Sum of electronic and thermal Free Energies=	-1857.644533

TS-4 (in TFE)

Zero-point correction=	0.642752 (Hartree/Particle)
Thermal correction to Energy=	0.684514
Thermal correction to Enthalpy=	0.685458
Thermal correction to Gibbs Free Energy=	0.567031

Sum of electronic and zero-point Energies= -1857.547615
Sum of electronic and thermal Energies= -1857.505853
Sum of electronic and thermal Enthalpies= -1857.504909
Sum of electronic and thermal Free Energies= -1857.623336

INT-7 (in TFE)

Zero-point correction= 0.646102 (Hartree/Particle)
Thermal correction to Energy= 0.687342
Thermal correction to Enthalpy= 0.688286
Thermal correction to Gibbs Free Energy= 0.572334
Sum of electronic and zero-point Energies= -1857.552985
Sum of electronic and thermal Energies= -1857.511745
Sum of electronic and thermal Enthalpies= -1857.510801
Sum of electronic and thermal Free Energies= -1857.626753

TS-5 (in TFE)

Zero-point correction= 0.644472 (Hartree/Particle)
Thermal correction to Energy= 0.685793
Thermal correction to Enthalpy= 0.686737
Thermal correction to Gibbs Free Energy= 0.570303
Sum of electronic and zero-point Energies= -1857.544079
Sum of electronic and thermal Energies= -1857.502759
Sum of electronic and thermal Enthalpies= -1857.501815
Sum of electronic and thermal Free Energies= -1857.618249

INT-8 (in TFE)

Zero-point correction= 0.645327 (Hartree/Particle)
Thermal correction to Energy= 0.687412
Thermal correction to Enthalpy= 0.688357
Thermal correction to Gibbs Free Energy= 0.568339
Sum of electronic and zero-point Energies= -1857.605672
Sum of electronic and thermal Energies= -1857.563587
Sum of electronic and thermal Enthalpies= -1857.562643
Sum of electronic and thermal Free Energies= -1857.682660

PC1 (in TFE)

Zero-point correction= 0.325640 (Hartree/Particle)
Thermal correction to Energy= 0.344744
Thermal correction to Enthalpy= 0.345688
Thermal correction to Gibbs Free Energy= 0.274871
Sum of electronic and zero-point Energies= -1013.993784
Sum of electronic and thermal Energies= -1013.974681
Sum of electronic and thermal Enthalpies= -1013.973736
Sum of electronic and thermal Free Energies= -1014.044553

TS-6 (in TFE)

Zero-point correction= 0.578283 (Hartree/Particle)
Thermal correction to Energy= 0.614604
Thermal correction to Enthalpy= 0.615548
Thermal correction to Gibbs Free Energy= 0.509349

Sum of electronic and zero-point Energies=	-1628.530467
Sum of electronic and thermal Energies=	-1628.494146
Sum of electronic and thermal Enthalpies=	-1628.493202
Sum of electronic and thermal Free Energies=	-1628.599402

INT-9 (in TFE)

Zero-point correction=	0.581128 (Hartree/Particle)
Thermal correction to Energy=	0.617073
Thermal correction to Enthalpy=	0.618017
Thermal correction to Gibbs Free Energy=	0.514870
Sum of electronic and zero-point Energies=	-1628.606365
Sum of electronic and thermal Energies=	-1628.570420
Sum of electronic and thermal Enthalpies=	-1628.569476
Sum of electronic and thermal Free Energies=	-1628.672622

PC2 (in TFE)

Zero-point correction=	0.379038 (Hartree/Particle)
Thermal correction to Energy=	0.402165
Thermal correction to Enthalpy=	0.403109
Thermal correction to Gibbs Free Energy=	0.323596
Sum of electronic and zero-point Energies=	-1129.564487
Sum of electronic and thermal Energies=	-1129.541359
Sum of electronic and thermal Enthalpies=	-1129.540415
Sum of electronic and thermal Free Energies=	-1129.619929

Cartesian Coordinates For All of The Species

CH_3COOH (in DCE)			
C	-0.09080900	0.12010500	-0.00008200
O	-0.63637200	1.19874100	-0.00003100
O	-0.77929200	-1.03326100	0.00001700
H	-1.72595700	-0.80818100	0.00003100
C	1.39058300	-0.11438700	0.00005300
H	1.66974500	-0.69515500	0.88255900
H	1.66989600	-0.69518300	-0.88238600
H	1.91297900	0.84037400	0.00008400
CH_3OH (in DCE)			
C	-0.65938400	0.01923400	0.00000200
H	-1.02690400	0.54617700	0.89007300
H	-1.08817800	-0.98542900	-0.00008100
H	-1.02690100	0.54629000	-0.89000600
O	0.74623200	-0.12318200	0.00000200
H	1.12843600	0.76301500	-0.00001800
Cat. (in DCE)			
Rh	0.06910100	0.19821800	-0.09951500
C	1.16289300	-1.17135200	1.12646500
C	0.99375100	-1.74760500	-0.17194200
C	1.59135500	-0.86077500	-1.13066100
C	2.20228400	0.23840900	-0.40187300
C	1.93280700	0.05386900	0.97963700
C	-1.13701000	2.45508300	0.03741400
O	-0.51314100	2.12308300	-1.01554600
O	-1.05077600	1.72403300	1.06750100
C	-2.00652400	3.68044900	0.04506800
H	-3.00973000	3.38916100	-0.28167000
H	-2.07706500	4.09410200	1.05149000
H	-1.62043900	4.42697000	-0.64978700
O	-1.83328100	-0.38035000	-0.76793000
C	-2.53090000	-1.14087300	0.01123900
O	-2.16561300	-1.56720200	1.10877800
C	-3.89827500	-1.49655900	-0.54905200
H	-4.46075300	-0.58264500	-0.75680000
H	-3.77797100	-2.03000300	-1.49613400
H	-4.45185900	-2.11851200	0.15434900
C	2.93355300	1.37376500	-1.03685300
H	3.96001800	1.06574200	-1.26292300
H	2.45575400	1.66889500	-1.97374800
H	2.97186300	2.24276700	-0.37817700
C	2.32670700	0.94908100	2.10765600
H	3.23420400	0.56397700	2.58473500
H	2.52477200	1.96456000	1.76060100
H	1.53887400	0.98924800	2.86310200

C	1.64983300	-1.05169300	-2.61028600
H	1.58123800	-0.09314100	-3.12963700
H	2.59903200	-1.52250900	-2.88792400
H	0.83571400	-1.69044900	-2.95723900
C	0.26100000	-3.01062100	-0.48050900
H	-0.15097100	-2.98753300	-1.49130700
H	0.95219800	-3.85746200	-0.41197800
H	-0.55694900	-3.15906700	0.22558100
C	0.69910400	-1.74245300	2.42379500
H	-0.11728000	-2.44618600	2.26702400
H	1.53405300	-2.25419300	2.91532700
H	0.34475600	-0.95240500	3.09029000

INT-1 (in DCE)

N	2.40277200	0.95507500	-1.10914100
C	1.20118600	2.81489900	-0.25032100
C	1.46619400	3.84273900	0.65915400
H	2.48512100	4.20950300	0.74248300
C	0.44759100	4.39187900	1.42993700
H	0.66582200	5.18204600	2.14136500
C	-0.85944100	3.93644900	1.26048000
H	-1.66952800	4.37385600	1.83594900
C	-1.13217300	2.93672300	0.33064900
H	-2.15965300	2.62344300	0.16745000
C	-0.11411800	2.34548900	-0.42849800
C	2.64736600	-2.07870500	0.21829600
C	3.40878800	-1.19540400	1.08974700
C	2.57344000	-0.87499400	2.16839600
C	1.32922700	-1.64444300	2.05461700
C	1.41510000	-2.44934100	0.90354100
Rh	1.48979400	-0.32847600	0.26727900
C	2.36623500	2.29570500	-1.06152900
O	3.16110000	3.08106800	-1.58873200
C	-0.45195500	1.25767900	-1.42762900
C	-0.28927000	-0.15624100	-0.86531300
C	0.49596000	-3.54253300	0.47246800
H	0.85794800	-4.48674200	0.89539700
H	-0.52617100	-3.38421200	0.82149400
H	0.47580400	-3.64700400	-0.61402700
C	3.14005000	-2.67841200	-1.05596100
H	3.61842400	-3.64406300	-0.85413900
H	2.31218100	-2.84161700	-1.75145500
H	3.86763100	-2.01700300	-1.53015600
C	4.78451500	-0.68407300	0.80690500
H	5.52296300	-1.46318600	1.02535400
H	4.87984900	-0.40094300	-0.24276100
H	5.01805000	0.18722900	1.42215100
C	2.82196000	0.10404000	3.26732400
H	2.95622200	-0.42384700	4.21786900
H	3.71052000	0.70766700	3.07749200
H	1.96412700	0.77455000	3.38321500
C	0.23963600	-1.62271400	3.07863800
H	0.59955500	-2.05452900	4.01893100
H	-0.08547800	-0.59903400	3.28898900
H	-0.62578500	-2.20227300	2.75076000
O	3.49729100	0.45643000	-1.82592200
C	3.11648000	0.25886900	-3.17891800
H	3.98114100	-0.18529200	-3.67994800
H	2.25579000	-0.41756500	-3.24566000
H	2.87621600	1.21723900	-3.65437400
H	0.19953500	1.34303800	-2.30143000
H	-1.47973300	1.41409100	-1.77502300
C	-0.37617300	-1.28283300	-1.84022500
O	0.16202100	-1.64382900	-2.85767700
O	-1.37844400	-1.95279900	-1.20012300
C	-1.49976600	-0.87322300	-0.21069400
C	-2.88531900	-0.26898400	-0.26692000
H	-1.30912100	-1.28570400	0.78580800
C	-3.95820100	-1.28696300	0.14503400
H	-2.92222300	0.59411100	0.40762400
H	-3.09576200	0.09234100	-1.28021100
H	-3.89887000	-2.15151300	-0.52470400
H	-3.74512900	-1.64248700	1.16024700
C	-5.34268100	-0.68968600	0.09270900
C	-6.07395600	-0.69260300	-1.09924400
C	-5.90015000	-0.07534600	1.21803100
C	-7.33253500	-0.09926900	-1.16533200
H	-5.65061100	-1.16833400	-1.98084800
C	-7.15918100	0.51862100	1.15696900
H	-5.34144400	-0.06795800	2.15113000
C	-7.87946500	0.50808400	-0.03600400
H	-7.88849500	-0.11413600	-2.09790900
H	-7.57931700	0.98682800	2.04207700
H	-8.86153300	0.96795800	-0.08493500

INT-2 (in DCE)

N	2.35406300	1.31045400	-0.28563700
C	0.79516200	3.08809400	0.49268500
C	0.68924700	4.48179800	0.59385000
H	1.50608600	5.06880900	0.19211600
C	-0.41150300	5.10353000	1.16946800
H	-0.45244000	6.18666900	1.22803800
C	-1.45690900	4.32910800	1.66123700
H	-2.33036300	4.79258300	2.10912400
C	-1.36938500	2.94467500	1.57588000
H	-2.17854700	2.32993600	1.96174400
C	-0.26160900	2.31022100	1.00243000
C	2.95273700	-2.01995900	-0.53785200
C	3.48694000	-1.73705600	0.78381300
C	2.49713400	-2.09571600	1.71319400

C	1.35076100	-2.64917400	0.99094200	C	-7.04162000	-1.58871300	0.89257700
C	1.67677600	-2.67303400	-0.39085300	H	-5.25517800	-2.76481900	0.64269300
Rh	1.57726700	-0.58472200	0.29817000	C	-7.72991200	-0.43731600	0.51475400
C	2.06611500	2.62583200	-0.21926900	H	-7.68827800	1.33320500	-0.71130100
O	2.78798000	3.50580500	-0.71001600	H	-7.48231700	-2.27573100	1.60874600
C	-0.28547200	0.80361900	0.99870300	H	-8.70752900	-0.22288700	0.93507900
C	-0.23749100	0.10292800	-0.34439500				
C	0.91148900	-3.28531100	-1.52144400	**TS-1 (in DCE)**			
H	1.50631800	-4.09114800	-1.96489600	N	2.54990100	1.01860900	-0.46676700
H	-0.03213000	-3.71661800	-1.18316200	C	1.34618600	2.97481200	0.38434600
H	0.70164400	-2.55579200	-2.30998700	C	1.51231500	4.34504200	0.61289900
C	3.73354100	-1.93764600	-1.80631200	H	2.35857600	4.82756800	0.13773200
H	4.31163900	-2.86272700	-1.92224800	C	0.63437700	5.06952700	1.40978100
H	3.08123700	-1.83669900	-2.67612000	H	0.79744000	6.13054200	1.56991300
H	4.43031500	-1.09924300	-1.78195100	C	-0.44965800	4.42629600	2.00031600
C	4.82832200	-1.12697300	1.03780500	H	-1.14557000	4.97471000	2.62703900
H	4.98344700	-0.27285600	0.37359700	C	-0.63576100	3.06679100	1.78155100
H	4.92347400	-0.78617800	2.07068200	H	-1.48177100	2.55640800	2.23417000
H	5.62179800	-1.85793500	0.84658100	C	0.24185200	2.33260100	0.97446800
C	2.54140200	-1.93920600	3.19913600	C	2.64795700	-2.39857400	-0.36811800
H	2.74736200	-2.90822100	3.66733900	C	3.08341500	-1.95985200	0.94620100
H	3.31863800	-1.23791200	3.50695100	C	1.99552000	-2.14008200	1.84621200
H	1.58197400	-1.58603700	3.58650300	C	0.85979400	-2.58932200	1.08014700
C	0.11482300	-3.19127500	1.63900900	C	1.30204200	-2.81397500	-0.27535700
H	0.30881500	-4.17804500	2.07375700	Rh	1.44708600	-0.56129900	0.34203300
H	-0.22709200	-2.53622100	2.44555700	C	2.41331600	2.35478300	-0.50545700
H	-0.69724600	-3.29388700	0.91490100	O	3.12487200	3.11079500	-1.17827400
O	3.53201100	1.09741000	-1.03219700	C	-0.11069600	0.89195600	0.78820000
C	3.23715300	1.18589200	-2.41723700	C	-0.27941400	0.30587400	-0.50383100
H	4.17335800	0.98158600	-2.94470700	C	0.51296800	-3.43342200	-1.38846900
H	2.48325800	0.44056500	-2.70186000	H	0.97210200	-4.38453000	-1.67917900
H	2.87787800	2.18560000	-2.67313100	H	-0.51364600	-3.64541300	-1.08321100
H	-1.14593900	0.44030000	1.56757400	H	0.48793600	-2.79630000	-2.27834800
H	0.57651000	0.48953900	1.66970700	C	3.53877600	-2.54411200	-1.55927800
C	-0.37417600	0.75936200	-1.67793100	H	4.09283200	-3.48775300	-1.48666900
O	0.02133300	1.72161500	-2.27506500	H	2.96594200	-2.56190500	-2.48945900
O	-1.23716600	-0.18719300	-2.17301200	H	4.26235800	-1.72867300	-1.60683100
C	-1.35325700	-0.81477800	-0.85298200	C	4.47220600	-1.50042200	1.26208300
C	-2.73798200	-0.59580900	-0.28125300	H	4.82148900	-0.80346700	0.49524300
H	-1.11770200	-1.87857300	-0.93207500	H	4.51356200	-0.99573100	2.22967200
C	-3.82632400	-1.26524700	-1.13001000	H	5.16339100	-2.35043000	1.29048600
H	-2.76601000	-0.99694700	0.74038500	C	2.01268200	-1.92095500	3.32844900
H	-2.92922200	0.48391500	-0.21382400	H	2.22214800	-2.86581300	3.84188400
H	-3.75356000	-0.88580600	-2.15459400	H	2.78310700	-1.20257400	3.61602600
H	-3.64134700	-2.34518600	-1.16517600	H	1.04953900	-1.55278000	3.68958600
C	-5.20523800	-0.99662800	-0.57987200	C	-0.48819200	-2.93980400	1.63476600
C	-5.90453200	0.15644900	-0.95047100	H	-0.50627700	-3.97765200	1.98607500
C	-5.78842700	-1.86364900	0.34870900	H	-0.74815300	-2.29893100	2.48148700
C	-7.15722300	0.43555600	-0.40913800	H	-1.26942400	-2.83382700	0.87633700
H	-5.46082900	0.83753700	-1.67294400	O	3.57503000	0.57015700	-1.31108000

C	3.10871200	0.49817900	-2.64912100
H	3.94823700	0.13224900	-3.24650700
H	2.26869700	-0.20648300	-2.73070300
H	2.79632900	1.48422200	-3.00156700
H	-0.80040600	0.52147600	1.54687800
H	1.21536300	0.39191800	1.54189100
C	-0.30582100	0.94636700	-1.84913300
O	0.22224900	1.84011900	-2.44598300
O	-1.29556100	0.12599500	-2.32147000
C	-1.43694000	-0.53941100	-1.01888800
C	-2.79330700	-0.27706900	-0.40573200
H	-1.24263500	-1.60667900	-1.14109900
C	-3.92787900	-0.93178000	-1.20317200
H	-2.78660200	-0.66700600	0.62073400
H	-2.95048800	0.80745300	-0.34171300
H	-3.89731300	-0.55670500	-2.23169100
H	-3.75905300	-2.01433800	-1.24268400
C	-5.27602100	-0.64362300	-0.59022200
C	-5.98157500	0.51275900	-0.93694100
C	-5.82072600	-1.49720600	0.37351000
C	-7.20400200	0.80814000	-0.33795300
H	-5.56755500	1.18334400	-1.68627100
C	-7.04340000	-1.20586900	0.97498700
H	-5.28190100	-2.40093600	0.64917000
C	-7.73879400	-0.05128200	0.62043600
H	-7.74111500	1.70808200	-0.62194800
H	-7.45489500	-1.88253300	1.71784800
H	-8.69274000	0.17592800	1.08596600

INT-3 (in DCE)

N	2.57427500	0.89138100	-0.59742300
C	1.56325800	2.91447700	0.31318600
C	1.86799000	4.25574700	0.56507800
H	2.71302000	4.68023400	0.03496300
C	1.12869900	5.02371700	1.45699700
H	1.39799500	6.06016700	1.63359500
C	0.04940100	4.45162600	2.12371600
H	-0.53709300	5.03205500	2.82875300
C	-0.27705500	3.12339500	1.87780400
H	-1.12552500	2.67339900	2.38626400
C	0.45530700	2.34354300	0.97229400
C	2.48578300	-2.54405500	-0.32517200
C	2.91921200	-2.06575000	0.97191900
C	1.79448900	-2.15532700	1.86824200
C	0.65818300	-2.53210300	1.09129600
C	1.11305000	-2.83266900	-0.25678900
Rh	1.45087600	-0.54018200	0.37796500
C	2.51853600	2.23151800	-0.65269100
O	3.22647900	2.93022700	-1.38727500
C	-0.05725900	0.96105700	0.76631500
C	-0.29852800	0.39566600	-0.49360900
C	0.29571700	-3.42937300	-1.36352300
H	0.71702400	-4.39760900	-1.65386800
H	-0.73625000	-3.60209000	-1.05059100
H	0.28442900	-2.79674300	-2.25749100
C	3.38579500	-2.77167700	-1.49612700
H	3.91363300	-3.72489600	-1.37309600
H	2.82266500	-2.81628000	-2.43133700
H	4.13192700	-1.97859800	-1.57318800
C	4.33884700	-1.74167600	1.32032200
H	4.79308400	-1.13367600	0.53314200
H	4.40099600	-1.18656100	2.25871200
H	4.92969500	-2.65873400	1.42504300
C	1.81189500	-1.94358400	3.35195100
H	1.92305900	-2.90697000	3.86173000
H	2.64318900	-1.30319700	3.65332600
H	0.88383700	-1.48554700	3.70192200
C	-0.72145100	-2.77553800	1.62351200
H	-0.81538000	-3.80477200	1.98817400
H	-0.95058100	-2.10564900	2.45639500
H	-1.48120400	-2.63043200	0.85060600
O	3.52311300	0.34958400	-1.46858700
C	2.97811900	0.23189400	-2.77342100
H	3.76130100	-0.21279300	-3.39317600
H	2.09830500	-0.42821300	-2.76988700
H	2.69936200	1.21422400	-3.16327000
H	-0.68948900	0.60053200	1.57719800
H	1.81606200	0.31208500	1.56921100
C	-0.30046400	0.99244200	-1.86198800
O	0.24608700	1.85811400	-2.48112400
O	-1.31417200	0.18882700	-2.30710000
C	-1.46726100	-0.44507500	-0.99006300
C	-2.81999800	-0.14864600	-0.38519300
H	-1.28954300	-1.51648900	-1.09106700
C	-3.95854000	-0.81204900	-1.17012600
H	-2.81934400	-0.51149100	0.65077400
H	-2.96420800	0.93854500	-0.35090000
H	-3.92259100	-0.46119500	-2.20699300
H	-3.79837500	-1.89672900	-1.18471800
C	-5.30592100	-0.49972100	-0.56780700
C	-6.00716700	0.64809200	-0.94968700
C	-5.85446400	-1.32289800	0.41984500
C	-7.22963900	0.96456000	-0.36159600
H	-5.59002900	1.29498500	-1.71786300
C	-7.07712900	-1.01045400	1.01038900
H	-5.31866400	-2.21971200	0.72270500
C	-7.76850400	0.13521700	0.62065700
H	-7.76354600	1.85735000	-0.67285600
H	-7.49193900	-1.66366000	1.77213700
H	-8.72259300	0.37883100	1.07749600

TS-2 (in DCE)

N	2.57114000	1.01443400	-0.60263200
C	1.38675200	2.95584600	0.28503200
C	1.58191500	4.31844200	0.53552900
H	2.36650100	4.82161900	-0.01844600
C	0.81509900	5.00769300	1.46579000
H	0.99457300	6.06292700	1.64395800
C	-0.17373300	4.32841900	2.17285300
H	-0.77828600	4.84554800	2.91131100
C	-0.39177300	2.97947200	1.92275500
H	-1.17826100	2.45391200	2.45743600
C	0.36255600	2.27186200	0.97458100
C	2.62845500	-2.55203200	-0.17838700
C	2.96216300	-1.96338600	1.10828000
C	1.79373100	-1.99872200	1.92968500
C	0.71660100	-2.46894500	1.10642400
C	1.26714700	-2.88729300	-0.17549900
Rh	1.44995800	-0.54948500	0.26560500
C	2.38763100	2.36146700	-0.67975300
O	3.04888700	3.08336300	-1.41958900
C	-0.04178100	0.85905800	0.74514700
C	-0.29184200	0.31752200	-0.54372500
C	0.52590800	-3.57214500	-1.28526200
H	0.91895200	-4.58341600	-1.43522100
H	-0.53728500	-3.66848100	-1.05512000
H	0.62283900	-3.03810500	-2.23612800
C	3.61417300	-2.78996800	-1.27768800
H	4.24651300	-3.65302500	-1.03844600
H	3.11275900	-2.99120300	-2.22747700
H	4.27039300	-1.92462200	-1.40532700
C	4.34932500	-1.56395700	1.51073600
H	4.83902800	-1.00827800	0.70619500
H	4.33996300	-0.93471900	2.40356700
H	4.95762700	-2.45007000	1.72505300
C	1.69356100	-1.62781500	3.37830000
H	1.76552600	-2.52112400	4.00911600
H	2.49538700	-0.94521600	3.66867000
H	0.74023700	-1.14106900	3.60048700
C	-0.68377100	-2.71441200	1.58169000
H	-0.75303600	-3.69141300	2.07363400
H	-0.99641800	-1.95747700	2.30621400
H	-1.39857000	-2.71223300	0.75476700
O	3.64349500	0.54787200	-1.35131000
C	3.19826400	0.24927500	-2.67035200
H	4.07086000	-0.13330000	-3.20459500
H	2.41311700	-0.51880600	-2.64492000
H	2.82033200	1.15244400	-3.15609800
H	-0.67074000	0.46243800	1.54285300
H	2.36356000	0.56880500	0.83481400
C	-0.31099300	0.93752700	-1.89786600
O	0.24556800	1.80065200	-2.51647900
O	-1.32181200	0.13770400	-2.35650300
C	-1.45710300	-0.52354300	-1.05083900
C	-2.80708500	-0.24995300	-0.42919300
H	-1.26759400	-1.59217200	-1.17772600
C	-3.95440700	-0.89382700	-1.21712200
H	-2.79696300	-0.63601100	0.59821900
H	-2.95260900	0.83608700	-0.36745200
H	-3.92462600	-0.52465400	-2.24786400
H	-3.80137200	-1.97894400	-1.25182400
C	-5.29444800	-0.58260000	-0.59775100
C	-5.98548100	0.58189800	-0.94681200
C	-5.84429000	-1.42144600	0.37591500
C	-7.19864100	0.89949700	-0.34041400
H	-5.56708900	1.24159700	-1.70336000
C	-7.05777900	-1.10793900	0.98478500
H	-5.31629400	-2.33081300	0.65401600
C	-7.73869500	0.05452700	0.62783500
H	-7.72430900	1.80567500	-0.62607500
H	-7.47334200	-1.77322800	1.73560900
H	-8.68534400	0.29926500	1.09935800

INT-4 (in DCE)

N	2.75300700	1.08990600	-0.46135200
C	1.32464400	2.95074500	0.32383000
C	1.49509500	4.30601500	0.63769400
H	2.24620100	4.86804700	0.09202500
C	0.74597100	4.91416800	1.63365000
H	0.89982200	5.96121100	1.87126100
C	-0.19600500	4.15654700	2.32788300
H	-0.78838600	4.60931100	3.11695300
C	-0.39258600	2.82104400	2.00200400
H	-1.15237900	2.24876000	2.52702500
C	0.34175200	2.18122200	0.98860700
C	2.79581000	-2.47784500	-0.04768000
C	2.95541700	-1.88025800	1.27618300
C	1.72279400	-1.96301700	1.95442300
C	0.75482500	-2.48950600	1.01427900
C	1.46602500	-2.90498900	-0.18449400
Rh	1.41087600	-0.59678000	0.15542800
C	2.28712800	2.44444400	-0.69480600
O	2.74346500	3.10621700	-1.59013900
C	-0.02938400	0.77458100	0.68368600
C	-0.28347700	0.27300700	-0.64696500
C	0.87149800	-3.65663000	-1.33597700
H	0.92223200	-4.73817500	-1.16266700
H	-0.18235200	-3.40458700	-1.48099500
H	1.39837100	-3.44407200	-2.26997200
C	3.92340700	-2.65849900	-1.01851100

H	4.61194600	-3.43731800	-0.66956000
H	3.55986800	-2.95250900	-2.00607000
H	4.50067400	-1.73529400	-1.12912000
C	4.25906900	-1.35499100	1.79848100
H	4.77972100	-0.76719600	1.03447000
H	4.11354100	-0.71939500	2.67567500
H	4.92849600	-2.17447700	2.08510700
C	1.42529100	-1.56230200	3.36778600
H	1.43406100	-2.43482500	4.03171400
H	2.16323500	-0.84969300	3.74494700
H	0.43796000	-1.09885900	3.45160800
C	-0.66421900	-2.83764800	1.35500400
H	-0.71743200	-3.80927100	1.86071500
H	-1.10448300	-2.09406200	2.02648400
H	-1.29036000	-2.89948000	0.46025100
O	3.76914200	0.74183700	-1.36546600
C	3.20122200	0.28302700	-2.58921800
H	4.05482900	0.01976000	-3.21593000
H	2.57516100	-0.59947000	-2.41276500
H	2.61300100	1.07202000	-3.06428100
H	-0.70149500	0.37101700	1.44351700
H	3.22073500	1.10130700	0.45243100
C	-0.33149300	0.97093200	-1.95147300
O	0.24332700	1.85292100	-2.53512300
O	-1.37573100	0.23401900	-2.43883600
C	-1.48991800	-0.49973800	-1.16827500
C	-2.82065300	-0.24742500	-0.49976400
H	-1.32706200	-1.56363300	-1.36551900
C	-3.99349200	-0.84714600	-1.28522200
H	-2.78639900	-0.68372600	0.50699000
H	-2.95658200	0.83522400	-0.38019000
H	-3.99586500	-0.42288100	-2.29503700
H	-3.84048700	-1.92843500	-1.38404300
C	-5.31511500	-0.57678900	-0.60994600
C	-6.03916400	0.58365900	-0.89963300
C	-5.81554100	-1.45386900	0.35722000
C	-7.23624400	0.86013700	-0.24281200
H	-5.65952600	1.27279300	-1.65032600
C	-7.01233400	-1.18158900	1.01654800
H	-5.26189200	-2.36078400	0.58998700
C	-7.72681200	-0.02270500	0.71772200
H	-7.78809700	1.76376500	-0.48368000
H	-7.38916900	-1.87634300	1.76116700
H	-8.66104200	0.18957400	1.22819200

INT-5 (in DCE)

N	2.39511700	0.34884100	-0.32782300
C	1.53070800	2.25648500	1.01222700
C	2.04843400	3.52043400	1.31415400
H	3.12390100	3.64496400	1.39841000
C	1.19294500	4.60013300	1.48595800
H	1.59434300	5.58330600	1.70742900
C	-0.18405600	4.40603700	1.37763500
H	-0.86355500	5.24079000	1.51870700
C	-0.69413400	3.14196900	1.10059600
H	-1.76921500	2.99270900	1.03981700
C	0.14908400	2.04091700	0.90884300
C	1.69754500	-2.98499000	-0.20370800
C	1.86375500	-2.56571600	1.18703500
C	0.58645100	-2.49600600	1.78416500
C	-0.38521500	-2.75496500	0.74792300
C	0.32683900	-3.15833700	-0.45396100
Rh	0.67900400	-0.92448300	0.12376400
C	2.51356400	1.15368800	0.85974600
O	3.39972200	0.90859900	1.64766600
C	-0.46955400	0.69350300	0.67098100
C	-0.81865300	0.30429600	-0.67157200
C	-0.30852700	-3.66656600	-1.71195700
H	-0.53475100	-4.73619700	-1.62900100
H	-1.25101100	-3.15447100	-1.92550800
H	0.34859900	-3.53167600	-2.57488300
C	2.83941200	-3.21516500	-1.14817700
H	3.32167900	-4.18053500	-0.95430800
H	2.50719200	-3.20893800	-2.18937800
H	3.61037100	-2.44511000	-1.03570300
C	3.19169400	-2.37227000	1.85519500
H	3.90850200	-1.87606800	1.19325100
H	3.10082500	-1.76536000	2.75889000
H	3.62541900	-3.33913400	2.13758100
C	0.26475900	-2.19662800	3.21675800
H	0.10096900	-3.12170900	3.78223900
H	1.07645200	-1.64786500	3.70099800
H	-0.64529400	-1.59568500	3.30214700
C	-1.85857900	-2.90798200	0.98433600
H	-2.07833700	-3.89246400	1.41497600
H	-2.23043200	-2.15386900	1.68433600
H	-2.42918500	-2.82387100	0.05544900
O	2.40047100	1.18366300	-1.47486800
C	2.29239500	0.37390300	-2.64542700
H	3.18484400	-0.25408200	-2.74813400
H	1.39219900	-0.24551200	-2.59441600
H	2.22273900	1.07639300	-3.47510500
H	-1.19905900	0.43109500	1.44191700
H	3.24698500	-0.22776600	-0.38907700
C	-0.81164600	1.13188800	-1.90963000
O	-0.18738100	2.01933300	-2.42442200
O	-1.95076100	0.56430900	-2.42227400
C	-2.13293600	-0.24904300	-1.21358800
C	-3.40155400	0.13014500	-0.48547900
H	-2.12815800	-1.30516300	-1.49748600

C	-4.66164400	-0.24071200	-1.27734700
H	-3.40946100	-0.37875500	0.48660400
H	-3.38492500	1.20977300	-0.28756400
H	-4.62599700	0.25958100	-2.25101800
H	-4.66081500	-1.32142100	-1.46375400
C	-5.91957600	0.15048700	-0.54255600
C	-6.50493500	1.40380100	-0.74495500
C	-6.49393800	-0.71298400	0.39564500
C	-7.63915800	1.78490300	-0.03103300
H	-6.06697200	2.08336800	-1.47223000
C	-7.62793600	-0.33633300	1.11169400
H	-6.04758200	-1.69133400	0.56021100
C	-8.20444000	0.91505900	0.89970900
H	-8.08367400	2.76043200	-0.20392400
H	-8.06405200	-1.02127500	1.83264100
H	-9.09001300	1.20904000	1.45446000
C	5.59316900	1.02327600	-0.61292300
O	5.16771800	-0.07934600	-0.91086400
O	4.92676100	2.14570100	-0.87988800
H	4.07386000	1.91467100	-1.31003500
C	6.88726500	1.27540400	0.09571600
H	7.46435600	0.35440600	0.15163000
H	7.45262500	2.05469600	-0.41895300
H	6.66417400	1.63304100	1.10534300

TS-3 (in DCE)

N	2.09340600	0.67162600	-0.25334400
C	1.03757000	2.76729800	0.71330600
C	1.29785600	4.10663300	1.02675300
H	2.19832400	4.55858300	0.62649400
C	0.44273400	4.83888600	1.83930000
H	0.66778900	5.87415600	2.07238100
C	-0.69308600	4.22549400	2.36074300
H	-1.36674400	4.77614800	3.00973900
C	-0.96695300	2.89851800	2.04770100
H	-1.86089400	2.42457500	2.44361700
C	-0.12262800	2.14951600	1.21813200
C	2.01316100	-2.65755600	0.40669700
C	2.08578400	-2.05185500	1.70974500
C	0.75704500	-1.95663000	2.21896000
C	-0.13851200	-2.50602700	1.22798400
C	0.64432900	-2.97400200	0.12539700
Rh	0.83752300	-0.68688800	0.36823500
C	2.10303000	2.09749400	-0.10371600
O	3.03561100	2.72535500	-0.55388800
C	-0.56859300	0.76790600	0.89863200
C	-0.79633000	0.33856800	-0.43592800
C	0.14277900	-3.70204400	-1.08391100
H	0.23999200	-4.78542900	-0.94902100
H	-0.91294500	-3.48936800	-1.26937800
H	0.70542000	-3.42765700	-1.98062100
C	3.19471200	-2.98156800	-0.45440700
H	3.71555400	-3.86455900	-0.06588900
H	2.89031700	-3.19673300	-1.48110100
H	3.90940500	-2.15306900	-0.46947800
C	3.34770800	-1.66572600	2.41841100
H	4.10832000	-1.32271400	1.71306900
H	3.16707900	-0.86577900	3.14102100
H	3.75377600	-2.52483400	2.96534900
C	0.35260800	-1.45505600	3.57000400
H	0.35496500	-2.27453700	4.29807100
H	1.03733600	-0.68327500	3.93016100
H	-0.65630800	-1.03433000	3.55110000
C	-1.61411200	-2.68565600	1.41995100
H	-1.81127800	-3.55437400	2.05827000
H	-2.06386900	-1.81495100	1.90647100
H	-2.12895400	-2.85069400	0.46978400
O	2.53161100	0.68611400	-2.14416900
C	1.98339500	-0.43326500	-2.71897600
H	2.74827200	-1.14527300	-3.06777800
H	1.35410900	-0.98005400	-1.97249700
H	1.31143700	-0.17076100	-3.54926100
H	-1.23612200	0.34763000	1.65189000
H	3.07909100	0.37169800	-0.11239900
C	-0.68858000	1.11042400	-1.70586300
O	-0.06613600	2.03093300	-2.15199000
O	-1.68781500	0.41423400	-2.32915600
C	-1.95910000	-0.37464800	-1.11568700
C	-3.34405400	-0.09432100	-0.57995200
H	-1.80406600	-1.43396500	-1.33925300
C	-4.44350400	-0.59790000	-1.52339300
H	-3.43983300	-0.58261000	0.39751500
H	-3.44812300	0.98613700	-0.41753200
H	-4.32526400	-0.11053300	-2.49688100
H	-4.31419800	-1.67583600	-1.67760800
C	-5.82002900	-0.32108700	-0.97152600
C	-6.48600800	0.86930200	-1.27746800
C	-6.43299200	-1.22725300	-0.10055800
C	-7.73665600	1.14719200	-0.72966700
H	-6.01903600	1.58079400	-1.95435800
C	-7.68335000	-0.95363500	0.44931400
H	-5.92445700	-2.15754300	0.14292400
C	-8.33920400	0.23569300	0.13557000
H	-8.24246100	2.07445500	-0.98144000
H	-8.14752800	-1.67058400	1.11984100
H	-9.31497700	0.44930900	0.56055100
C	5.49695800	0.29866800	-1.04422100
O	4.83044700	0.01642100	-0.04437400
O	4.98269800	0.63827200	-2.18852700
H	3.91272300	0.67716700	-2.14029800

C	7.00112400	0.27490300	-1.02802300
H	7.36486700	-0.08611800	-0.06736000
H	7.36714000	-0.36281500	-1.83606200
H	7.37482500	1.28609700	-1.21020400

INT-6 (in DCE)

N	-1.50982300	0.71578500	1.42505700
C	-1.08060300	2.95505100	0.48379000
C	-1.80650600	4.14915100	0.40940900
H	-2.52657400	4.35154200	1.19584300
C	-1.63831800	5.04031600	-0.64309800
H	-2.22715800	5.95128100	-0.68375000
C	-0.71686100	4.75232100	-1.64996100
H	-0.58014300	5.43418500	-2.48329900
C	0.04422800	3.59255500	-1.56827100
H	0.79133800	3.37899900	-2.32858400
C	-0.10571200	2.69841100	-0.49611600
C	-3.65517500	-1.70994000	-1.01232800
C	-3.99166900	-0.33831700	-0.66981400
C	-3.16934300	0.52458900	-1.48062500
C	-2.24448100	-0.29529300	-2.18985900
C	-2.57898900	-1.68802500	-1.92651700
Rh	-2.01032100	-0.67755300	-0.05119200
C	-1.44939000	2.03928800	1.63634100
O	-1.70220300	2.57678900	2.72531500
C	0.82373600	1.55109800	-0.44903300
C	1.57181600	1.24490600	0.60580900
C	-1.94822600	-2.89923200	-2.53752900
H	-2.68841600	-3.42333900	-3.15108300
H	-1.10851200	-2.63034500	-3.18000300
H	-1.59789300	-3.59403100	-1.76823200
C	-4.29609600	-2.93596000	-0.45389000
H	-5.12105500	-3.24117700	-1.10709600
H	-3.57973000	-3.75958800	-0.39910100
H	-4.70063700	-2.75154100	0.54305700
C	-5.09490800	0.09369800	0.23882700
H	-5.22515800	-0.61799700	1.05685000
H	-4.88311800	1.07467800	0.66918900
H	-6.03751800	0.15518500	-0.31595900
C	-3.34538600	1.99881200	-1.60430800
H	-4.11916600	2.18114900	-2.35967700
H	-3.68209000	2.44060300	-0.66577800
H	-2.43024000	2.50008600	-1.92237000
C	-1.18487400	0.16948800	-3.13390900
H	-1.54990800	0.09660100	-4.16444700
H	-0.91370500	1.20988900	-2.93954700
H	-0.28770300	-0.45055300	-3.05215400
O	0.08084800	-1.59382900	0.18708400
C	0.98342300	-1.92355200	-0.85454400
H	0.50080600	-2.48526000	-1.66100300
H	1.40076000	-1.00504100	-1.27233300
H	1.81175900	-2.52737700	-0.46256300
H	0.93190900	0.97292900	-1.36593900
H	-1.75501900	0.26548800	2.30587300
C	1.81234600	1.84660700	1.94703000
O	1.46346100	2.78571400	2.60064200
O	2.74500100	0.90665800	2.29152900
C	2.59302300	0.20679800	1.00231900
C	3.89503100	0.14365500	0.23832400
H	2.16430800	-0.78203600	1.18757400
C	4.93584300	-0.73126200	0.94843400
H	3.68417200	-0.26352700	-0.75852500
H	4.28378600	1.15977000	0.10245900
H	5.13648000	-0.30813800	1.93846600
H	4.51648000	-1.73286800	1.09936000
C	6.21631000	-0.82639900	0.15647700
C	7.22941000	0.12340900	0.31882700
C	6.39164200	-1.83623300	-0.79451800
C	8.39120700	0.06457300	-0.44779300
H	7.10473000	0.91258500	1.05657100
C	7.55201100	-1.89951900	-1.56290300
H	5.61082200	-2.58177000	-0.92766800
C	8.55596300	-0.94802300	-1.39144500
H	9.17000800	0.80779700	-0.30584200
H	7.67408100	-2.69393700	-2.29309200
H	9.46217300	-0.99688600	-1.98706400
C	-1.99735800	-3.05960700	1.85031500
O	-2.36434200	-1.84230200	1.74722100
O	-1.14589400	-3.61012700	1.11203700
H	-0.31456200	-2.45933100	0.54186900
C	-2.67790000	-3.87716500	2.92391200
H	-2.02718100	-4.68496900	3.25951000
H	-2.97175200	-3.24602700	3.76315800
H	-3.58332400	-4.31807400	2.49279600

TS-4 (in DCE)

N	0.61062100	0.51093200	-1.25911500
C	1.15034400	2.95223100	-0.78523400
C	2.18053900	3.87280800	-1.03410000
H	2.92616800	3.60287800	-1.77300000
C	2.27086700	5.08910100	-0.37073700
H	3.09243200	5.76477900	-0.58491200
C	1.29558900	5.42803000	0.56380300
H	1.34101000	6.37444200	1.09345100
C	0.26399900	4.53700000	0.82058100
H	-0.49102400	4.78932300	1.56019900
C	0.16016600	3.29603500	0.17041100
C	3.40049400	-1.40179600	1.30416300
C	3.36943100	0.04681100	1.22687300
C	2.21159800	0.49560300	1.94471600

C	1.45071000	-0.64989500	2.32719900	C	-8.14826900	-0.63291900	1.21413100
C	2.21420100	-1.83065200	1.95717000	H	-6.25791500	-1.04315400	2.15975900
Rh	1.69772200	-0.75080200	0.16204600	C	-8.80855400	-0.37196100	0.01497300
C	1.27693700	1.68743600	-1.62438500	H	-8.58856000	-0.11726000	-2.11256400
O	1.97240900	1.72745800	-2.62674000	H	-8.70721400	-0.67959600	2.14397500
C	-0.93142200	2.42510400	0.64711400	H	-9.88255500	-0.21421700	0.00586300
C	-1.44795300	1.42646900	-0.05383100	C	2.89921800	-2.56491200	-1.95647400
C	1.82717600	-3.25248400	2.20109500	O	2.71314100	-1.33721300	-1.66445900
H	2.40108500	-3.64663900	3.04653100	O	2.29594100	-3.52774200	-1.42163500
H	0.76623800	-3.33975400	2.44002100	H	0.99451500	-2.92431400	-0.90020500
H	2.04383300	-3.86924700	1.32438600	C	3.95459500	-2.85606900	-2.99801200
C	4.48295000	-2.27956000	0.77192500	H	4.89523100	-3.06574900	-2.47700200
H	5.21733400	-2.45861000	1.56487400	H	3.68243900	-3.73946100	-3.57675500
H	4.08625300	-3.24229100	0.44343300	H	4.10451400	-1.99768600	-3.65284700
H	4.99691200	-1.80454300	-0.06615000				
C	4.42006500	0.91550100	0.61846000	**INT-7 (in DCE)**			
H	4.85127700	0.44198900	-0.26652800	N	-0.32523100	0.42253200	1.16400100
H	4.00192100	1.88071100	0.32171900	C	-1.10302100	2.80900500	0.79424600
H	5.22568400	1.09486000	1.33874600	C	-2.24522300	3.55713000	1.11440300
C	1.94077300	1.90287300	2.34802600	H	-2.85284100	3.22067300	1.94736100
H	2.44677900	2.06128100	3.30864800	C	-2.61391100	4.68375800	0.39225800
H	2.34248500	2.62313100	1.63393400	H	-3.51346600	5.22972900	0.65643300
H	0.87735300	2.09197900	2.49419800	C	-1.81439700	5.09921900	-0.66997400
C	0.17619400	-0.62554700	3.10497500	H	-2.07973500	5.97798200	-1.24944900
H	0.39746700	-0.59527000	4.17782800	C	-0.66744300	4.38356500	-0.98555300
H	-0.41590900	0.25769500	2.85295100	H	-0.03977400	4.71402100	-1.80868200
H	-0.42641000	-1.51574100	2.91228600	C	-0.27669800	3.23336200	-0.27644100
O	0.28172600	-2.25975200	-0.62065400	C	-3.38696500	-1.09695800	-1.39751400
C	-0.79368500	-2.88292000	0.06531800	C	-2.77252800	0.16959600	-1.72879700
H	-0.59758900	-3.95243900	0.19689000	C	-1.46908500	-0.11622900	-2.26875400
H	-0.93029000	-2.43082700	1.05260900	C	-1.22453500	-1.51328300	-2.14738500
H	-1.71302000	-2.74913400	-0.50953900	C	-2.43595800	-2.13113100	-1.63262900
H	-1.28767500	2.62670600	1.65711500	Rh	-1.67540900	-0.77894500	-0.15035700
H	0.74046900	-0.11141500	-2.06230300	C	-0.92643600	1.60517700	1.68337300
C	-1.14289100	0.89242800	-1.43261300	O	-1.36449600	1.61375300	2.81378400
O	-1.27700700	1.41358600	-2.54110900	C	0.93109700	2.55574800	-0.77396500
O	-1.83668300	-0.33390500	-1.10232200	C	1.51330000	1.49630400	-0.22392600
C	-2.29617900	0.20276900	0.16400100	C	-2.68051800	-3.58601400	-1.38993300
C	-3.80377900	0.38396100	0.18084100	H	-3.49517900	-3.92928900	-2.03561900
H	-1.96646300	-0.42740100	1.00255900	H	-1.79488200	-4.18139300	-1.61424600
C	-4.53204900	-0.95905500	0.05087900	H	-2.97510700	-3.76139400	-0.35045700
H	-4.09338600	0.88270400	1.11405600	C	-4.76193200	-1.29195200	-0.85444100
H	-4.08858800	1.04185300	-0.64897500	H	-5.46386600	-1.39369600	-1.68942100
H	-4.20167200	-1.44101800	-0.87553100	H	-4.81647800	-2.19874900	-0.24731200
H	-4.23859200	-1.60962900	0.88394000	H	-5.07087800	-0.43828800	-0.24831100
C	-6.03083800	-0.78835500	0.03680700	C	-3.43344100	1.50746000	-1.66806200
C	-6.70416300	-0.52367000	-1.16014300	H	-4.09180600	1.57898900	-0.79906400
C	-6.76992400	-0.83771700	1.22245900	H	-2.69445100	2.31048500	-1.60706700
C	-8.08168100	-0.31772600	-1.17340400	H	-4.03908100	1.66250400	-2.56789900
H	-6.13932700	-0.48237300	-2.08851400	C	-0.57308900	0.85379300	-2.95475100

H	-0.77696900	0.77896900	-4.03023100
H	-0.76897800	1.87969000	-2.64264900
H	0.47959100	0.61871900	-2.79360600
C	0.03668500	-2.20115900	-2.55764300
H	0.11333800	-2.21801200	-3.65017800
H	0.90571400	-1.67089700	-2.15683800
H	0.06547400	-3.22998500	-2.19563500
O	-0.78419700	-2.29055800	1.19783200
C	0.14605300	-3.28132100	0.77659400
H	-0.29713600	-3.96471100	0.04430500
H	0.99782500	-2.75977300	0.33713600
H	0.48290000	-3.85905200	1.64326500
H	1.30474600	2.93283900	-1.72528700
H	-0.35263100	-0.23329000	1.95160900
C	1.20907400	0.65934100	1.00394000
O	1.74433000	0.89010700	2.12009500
O	1.76185800	-0.52026400	0.21039900
C	2.42955900	0.39705000	-0.68694600
C	3.90566200	0.55267300	-0.34892500
H	2.30285300	0.09779100	-1.73791200
C	4.66123800	-0.77114500	-0.50672500
H	4.34655700	1.31952000	-0.99809300
H	3.97920400	0.90165100	0.68685500
H	4.16527500	-1.51971000	0.12060200
H	4.58892500	-1.11220200	-1.54661100
C	6.11131700	-0.64342100	-0.11112800
C	6.47844200	-0.65336500	1.23924800
C	7.10958600	-0.46264100	-1.07227900
C	7.80817100	-0.49097800	1.61871400
H	5.70977200	-0.79108500	1.99634500
C	8.44250900	-0.30035800	-0.69732300
H	6.83793700	-0.45211700	-2.12518800
C	8.79595400	-0.31424300	0.65006400
H	8.07472100	-0.50448400	2.67130900
H	9.20505400	-0.16497800	-1.45861700
H	9.83344300	-0.18969000	0.94438300
C	-3.50577600	-1.52242600	2.12410900
O	-2.96950800	-0.52038600	1.54213600
O	-3.15064400	-2.71545700	1.96935800
H	-1.65900500	-2.67408900	1.53181800
C	-4.67446500	-1.21015700	3.02915600
H	-4.79724400	-1.99059200	3.78012400
H	-4.54144100	-0.23700600	3.50327400
H	-5.58046000	-1.17025400	2.41467400

TS-5 (in DCE)

N	0.42204900	0.51562500	-1.26902100
C	1.39563700	2.83009400	-0.92703900
C	2.59830500	3.49567000	-1.20491900
H	3.22457400	3.10244100	-1.99828100
C	2.99899100	4.61074300	-0.48374800
H	3.94261000	5.09614100	-0.70878300
C	2.17212100	5.09406000	0.52908300
H	2.46252200	5.96547600	1.10762300
C	0.96754400	4.45954300	0.79703800
H	0.32177000	4.84647200	1.58042100
C	0.54030400	3.32115100	0.08775000
C	3.25465800	-1.18768300	1.46154900
C	2.70485200	0.11216300	1.75330000
C	1.37254300	-0.09359200	2.27023300
C	1.06542600	-1.47950400	2.20597000
C	2.23986500	-2.17009700	1.70157900
Rh	1.58768200	-0.83074900	0.18971700
C	1.17833800	1.61952900	-1.78008300
O	1.69642800	1.51791800	-2.87055000
C	-0.73687500	2.74397000	0.52482700
C	-1.41409900	1.70985900	0.01898600
C	2.40446300	-3.63984300	1.48790500
H	3.10705000	-4.04015400	2.22621700
H	1.45554100	-4.16604800	1.59911500
H	2.80181800	-3.84022700	0.48852900
C	4.62291600	-1.46602000	0.93934600
H	5.31238000	-1.55945900	1.78564100
H	4.64472400	-2.40152000	0.37541200
H	4.97281100	-0.65511600	0.29799400
C	3.43209100	1.41344200	1.66196000
H	4.11566600	1.42006500	0.80959700
H	2.73562800	2.24833800	1.55219100
H	4.02060400	1.57214000	2.57237900
C	0.47544000	0.93612700	2.85769000
H	0.54637200	0.85889900	3.94963300
H	0.76574500	1.94583100	2.56571300
H	-0.55977600	0.75339900	2.56734000
C	-0.24232200	-2.06949500	2.61702400
H	-0.39609000	-1.90442200	3.68906900
H	-1.04532800	-1.57648700	2.05428500
H	-0.27573300	-3.14324400	2.42679700
O	0.49694400	-2.24729300	-1.10346000
C	-0.55784400	-3.09187100	-0.64914900
H	-0.20464900	-3.79448200	0.11389500
H	-1.33098700	-2.44120700	-0.23756200
H	-0.95755900	-3.65883400	-1.49632400
H	-1.13234400	3.19110400	1.43555900
H	0.44343400	-0.17985100	-2.02154600
C	-1.02927800	0.83050200	-1.13137100
O	-1.69238000	0.68207400	-2.14500700
O	-1.68435700	-0.37555500	0.31603300
C	-2.38973700	0.77747400	0.68348500
C	-3.83217500	0.81083300	0.17270200
H	-2.41786000	0.94831100	1.77835100

C	-4.62486800	-0.37679000	0.72829200
H	-4.31221400	1.75303700	0.46922600
H	-3.82134800	0.76704600	-0.92113700
H	-4.09064300	-1.29078300	0.44759100
H	-4.63421100	-0.32751000	1.82450300
C	-6.04054700	-0.41597400	0.21100700
C	-6.31348300	-0.90177900	-1.07301600
C	-7.10328500	0.07353300	0.97586300
C	-7.61142100	-0.90108500	-1.57707600
H	-5.49559400	-1.28464400	-1.67934200
C	-8.40486300	0.07560300	0.47648000
H	-6.90624600	0.45463500	1.97517300
C	-8.66330500	-0.41219100	-0.80254400
H	-7.80342500	-1.28488100	-2.57470100
H	-9.21735200	0.45691000	1.08801700
H	-9.67616500	-0.41323700	-1.19326100
C	3.29239100	-1.89519900	-2.06369700
O	2.88711900	-0.81339000	-1.51692600
O	2.79222800	-3.02639200	-1.86525600
H	1.30386000	-2.76123500	-1.42124700
C	4.47976900	-1.75382200	-2.98756000
H	4.55912200	-2.61652400	-3.64859500
H	4.39763600	-0.83254200	-3.56658000
H	5.38643700	-1.68850800	-2.37688800

INT-8 (in DCE)

N	-1.15696700	2.56634600	1.99992500
C	-2.32758900	3.68237000	0.07121600
C	-3.36685900	4.58551900	-0.18973800
H	-4.00263300	4.87692800	0.63769900
C	-3.58116600	5.09914000	-1.45942600
H	-4.38870700	5.80262600	-1.63209100
C	-2.75244700	4.69862000	-2.50661800
H	-2.90509900	5.08519400	-3.50914700
C	-1.73127900	3.79396300	-2.26332300
H	-1.09457200	3.47165300	-3.08239500
C	-1.48373600	3.27116200	-0.97937500
C	-2.16776800	-2.37700000	-1.36197300
C	-1.17769800	-1.58694100	-2.08108400
C	0.06669700	-2.30186600	-2.02739500
C	-0.12218300	-3.45615600	-1.20562300
C	-1.53074700	-3.51945300	-0.83448100
Rh	-0.56810000	-1.70680900	-0.03952300
C	-2.24218200	3.25333500	1.49786000
O	-3.11593600	3.56996200	2.29385000
C	-0.39918500	2.29246900	-0.90978000
C	0.22663400	1.67095200	0.10237100
C	-2.20136000	-4.57857800	-0.01614400
H	-2.99334200	-5.05352700	-0.60385200
H	-1.49548200	-5.35355900	0.28680300
H	-2.65938500	-4.14848200	0.88035900
C	-3.60364600	-2.01008800	-1.17866700
H	-4.19928300	-2.41595300	-2.00373400
H	-3.99113200	-2.41553800	-0.24063700
H	-3.73176100	-0.92536600	-1.16831100
C	-1.48258000	-0.34465900	-2.85318300
H	-2.10083300	0.34051700	-2.26645000
H	-0.56862100	0.17733900	-3.14303500
H	-2.03398900	-0.60141200	-3.76455800
C	1.37261100	-1.91087200	-2.63741200
H	1.70923000	-2.69746600	-3.32035500
H	1.29174400	-0.97929300	-3.19930500
H	2.13135000	-1.78373900	-1.85913200
C	0.92918900	-4.47366500	-0.90272700
H	1.00534700	-5.18705300	-1.73093200
H	1.90410700	-3.99599800	-0.77500600
H	0.69586800	-5.03228400	0.00520700
O	-0.33693500	-2.36526900	2.05543000
C	0.21865000	-3.61116700	2.43183800
H	-0.34557100	-4.45797900	2.02431100
H	1.24425000	-3.65043300	2.05639300
H	0.24348300	-3.69772900	3.52354300
H	-0.03914800	2.01609600	-1.89954200
H	-1.20533000	2.51735200	3.01466100
C	0.00314100	1.93839200	1.54115000
O	0.81379500	1.62008500	2.39318600
O	1.08623200	-0.58912800	0.40903700
C	1.29193200	0.61655100	-0.23131700
C	2.71061000	1.13276100	0.07206600
H	1.23670500	0.50471400	-1.33573700
C	3.78356600	0.17246300	-0.45197700
H	2.84482900	2.11831400	-0.39345300
H	2.81516800	1.25408100	1.15330500
H	3.61274000	-0.81123700	-0.00237300
H	3.67051000	0.06226600	-1.53831300
C	5.17775600	0.65343700	-0.13586300
C	5.74359500	0.41601700	1.12190900
C	5.91541000	1.38789000	-1.06912200
C	7.01232400	0.89567400	1.43708400
H	5.17934700	-0.15257300	1.85774300
C	7.18589300	1.86984600	-0.75900300
H	5.48766500	1.58035200	-2.05039500
C	7.73899500	1.62460500	0.49611300
H	7.43615400	0.69838000	2.41729900
H	7.74482300	2.43496700	-1.49906500
H	8.72929900	1.99685800	0.73952400
C	-2.75465200	-0.62822200	1.71633200
O	-1.86260800	-0.23406000	0.89778800
O	-2.76987400	-1.74991700	2.28459200
H	-1.31902700	-2.27484000	2.29022000

C	-3.85477000	0.35911500	2.03974300
H	-3.51773100	1.01091000	2.85210300
H	-4.07737300	0.99055300	1.17772700
H	-4.75066700	-0.16968600	2.36820500

PC1 (in DCE)

N	-2.12849300	1.93651200	-0.54015400
C	-3.70856300	-0.04040600	-0.50375100
C	-4.96145200	-0.44308100	-0.98235100
H	-5.52309500	0.25823600	-1.58731900
C	-5.47893400	-1.69782200	-0.69747500
H	-6.45243200	-1.98261000	-1.08199700
C	-4.73873600	-2.58235400	0.08398400
H	-5.12612500	-3.56825800	0.31883700
C	-3.49731100	-2.19560000	0.56354900
H	-2.92114600	-2.88521600	1.17271500
C	-2.95066000	-0.92851000	0.28704400
C	-3.32670600	1.34123700	-0.91247700
O	-4.07146000	2.01732700	-1.60222200
C	-1.63282400	-0.69625600	0.87265900
C	-0.78009700	0.34252800	0.85436900
H	-1.28026100	-1.55918500	1.43583500
H	-2.07323700	2.87884500	-0.92153200
C	-0.98690700	1.63877200	0.18045400
O	-0.13284400	2.51973100	0.23823200
O	0.82331100	1.26730200	2.44951700
C	0.56860100	0.20168500	1.55628400
C	1.70880600	0.00991800	0.54831800
H	0.51588500	-0.69675600	2.18166400
C	3.05738700	-0.19302500	1.24925400
H	1.48299500	-0.85988300	-0.08002200
H	1.76354400	0.88387900	-0.11117300
H	3.25506300	0.67514900	1.88521300
H	2.99332800	-1.06897800	1.90569900
C	4.17938400	-0.37842300	0.25832400
C	4.81264500	0.73003400	-0.31369800
C	4.57592300	-1.65608700	-0.14733700
C	5.81820500	0.56684300	-1.26342800
H	4.51402400	1.72947800	-0.00560100
C	5.58244900	-1.82476500	-1.09636300
H	4.09217400	-2.52610100	0.29064500
C	6.20675900	-0.71271400	-1.65796900
H	6.30156100	1.43884900	-1.69374700
H	5.88076900	-2.82521900	-1.39529400
H	6.99272200	-0.84173300	-2.39557700
H	0.84380700	2.06719400	1.90218600

TS-6 (in DCE)

N	2.45278700	1.08501800	-0.75663800
C	0.91165600	2.79298000	-0.08988600
C	0.86314800	3.76025400	0.91938300
H	1.80128500	4.14438800	1.30884600
C	-0.35180000	4.23773900	1.39693300
H	-0.37477800	4.97953700	2.18899800
C	-1.53601200	3.77919200	0.82279900
H	-2.49325700	4.16651600	1.15804100
C	-1.49155600	2.83846800	-0.20249700
H	-2.41804100	2.52387500	-0.67406800
C	-0.27998900	2.30560600	-0.66232200
C	2.67994600	-2.02068500	0.42997900
C	3.11270800	-1.12335100	1.47644800
C	1.99958300	-0.93144100	2.33126800
C	0.91180800	-1.80513900	1.90514700
C	1.34647800	-2.51225700	0.76528600
Rh	1.40132900	-0.35618500	0.29820500
C	2.29332700	2.40812000	-0.57101800
O	3.14957900	3.28007000	-0.74529300
C	-0.27755200	1.26143600	-1.76027100
C	-0.14349000	-0.17845400	-1.26216300
C	0.64402500	-3.59908700	0.02042700
H	1.24776700	-4.51122000	0.07346100
H	-0.33344200	-3.81426400	0.45756200
H	0.49979700	-3.35086900	-1.03568200
C	3.47569800	-2.49005800	-0.73988500
H	3.93787000	-3.45765200	-0.51264500
H	2.82545700	-2.60914600	-1.61147600
H	4.25857500	-1.77138700	-0.98750500
C	4.45542200	-0.48046200	1.60126400
H	5.07103200	-1.05029700	2.30548100
H	4.95987500	-0.44721500	0.63639300
H	4.37131200	0.54324600	1.97365700
C	1.90647900	0.00135900	3.49097100
H	1.94073700	-0.56807500	4.42653200
H	2.72669200	0.72100900	3.49316100
H	0.95831400	0.54744600	3.47142900
C	-0.40037100	-1.91876000	2.61332200
H	-0.27073600	-2.45051700	3.56205600
H	-0.80865200	-0.92958600	2.84089300
H	-1.13052600	-2.46551000	2.01284900
O	3.76119800	0.73478200	-1.11067600
C	3.87255900	0.72943600	-2.52837000
H	4.88038200	0.36850400	-2.75271200
H	3.11845100	0.06665700	-2.96548200
H	3.75805400	1.74573800	-2.92385300
H	0.56486400	1.43389700	-2.43527700
H	-1.19624500	1.36702000	-2.35352100
C	0.14707000	-1.18162200	-2.39849100
O	1.12616700	-1.12528100	-3.14025800
O	-0.83834400	-2.00696300	-2.47054800
C	-1.27429400	-0.84160800	-0.70025500

C	-2.63513100	-0.30045800	-0.48627500
H	-1.11027100	-1.82055400	-0.26321500
C	-3.69945000	-1.40354900	-0.39412100
H	-2.60034900	0.26157200	0.46254900
H	-2.88967800	0.42679300	-1.26411400
H	-3.70430600	-1.95984500	-1.33673400
H	-3.42169400	-2.10375100	0.40151200
C	-5.06506300	-0.82410700	-0.12006600
C	-5.88883700	-0.41407400	-1.17233600
C	-5.50712500	-0.63534400	1.19258200
C	-7.12835100	0.16953800	-0.91910100
H	-5.55442900	-0.55756200	-2.19702500
C	-6.74627700	-0.05319700	1.44998600
H	-4.87425000	-0.95282400	2.01833200
C	-7.56041100	0.35144100	0.39346400
H	-7.75825100	0.47976600	-1.74723700
H	-7.07775800	0.08153300	2.47512000
H	-8.52710500	0.80362700	0.59190800

INT-9 (in DCE)

N	2.38128200	0.99986400	-0.41812700
C	0.82081100	2.60093300	0.50663200
C	0.60352000	3.20116500	1.75155900
H	1.44653800	3.28668300	2.43084000
C	-0.64621400	3.69323400	2.10925800
H	-0.79818300	4.14278900	3.08547100
C	-1.68965200	3.62645700	1.18994000
H	-2.66741200	4.02824400	1.43694700
C	-1.47033600	3.06316400	-0.06405300
H	-2.27888400	3.05686600	-0.79000500
C	-0.23073600	2.52312100	-0.42747200
C	2.50764000	-1.97560600	1.10452200
C	1.99812600	-0.92094500	1.95204500
C	0.57993700	-1.03162400	1.97905600
C	0.20845800	-2.22115000	1.22076600
C	1.38453600	-2.80323400	0.69820200
Rh	1.26208800	-0.75055000	-0.07476100
C	2.24618000	2.17034300	0.24501600
O	3.17515300	2.88880600	0.62424400
C	-0.05180000	1.95957700	-1.82790400
C	0.03755300	0.44885800	-1.92029300
C	1.49400500	-4.01070600	-0.17247300
H	1.87560700	-4.85562400	0.41044300
H	0.52502000	-4.28997500	-0.59009000
H	2.18770800	-3.82875600	-0.99725200
C	3.94368600	-2.25340700	0.81185600
H	4.33316500	-2.97675200	1.53704100
H	4.06253100	-2.67546400	-0.18901400
H	4.53357300	-1.33799300	0.87059700
C	2.83898800	0.12252200	2.61019100
H	3.31339800	-0.30496700	3.50013400
H	3.62020700	0.47800600	1.93311800
H	2.23728600	0.98010100	2.91851600
C	-0.38308100	-0.16911000	2.72793800
H	-0.75729000	-0.70872300	3.60496600
H	0.08945800	0.75403200	3.06576200
H	-1.24512600	0.09640700	2.10902600
C	-1.18799100	-2.73139900	1.08493500
H	-1.41059200	-3.39806800	1.92588700
H	-1.91075400	-1.91243200	1.11400000
H	-1.32570800	-3.29586500	0.16041800
O	3.73171600	0.63014200	-0.54962000
C	4.26954100	1.20281000	-1.73120500
H	5.29072300	0.82164200	-1.81523200
H	3.68609600	0.90127800	-2.60745300
H	4.29517500	2.29557900	-1.65347600
H	0.85755600	2.36549600	-2.27882000
H	-0.89590200	2.29745300	-2.44094000
C	1.20218200	-0.13764500	-2.70611900
O	1.49535100	0.33205000	-3.79873900
O	1.77642500	-1.12838900	-2.10601000
C	-0.92497000	-0.41690000	-1.51023900
C	-2.26920200	-0.04710800	-0.94794000
H	-0.77833900	-1.47509000	-1.73635500
C	-3.35264800	-1.05960500	-1.35231600
H	-2.22775600	0.01831700	0.14749700
H	-2.55972000	0.94758900	-1.29894800
H	-3.45589500	-1.04924600	-2.44352500
H	-3.03266200	-2.06786000	-1.06724500
C	-4.67558900	-0.74310000	-0.70012100
C	-5.46478000	0.31302600	-1.16870700
C	-5.11393300	-1.46251500	0.41480800
C	-6.66160900	0.64222000	-0.53795800
H	-5.13752700	0.87709200	-2.03923100
C	-6.31184400	-1.13656900	1.04921400
H	-4.51339200	-2.29144600	0.78293600
C	-7.08838600	-0.08192800	0.57489400
H	-7.26411300	1.46238800	-0.91654100
H	-6.63908200	-1.70883900	1.91201200
H	-8.02213500	0.17268800	1.06645300

PC2 (in DCE)

N	-3.08394500	-0.04298600	-0.83033900
C	-1.76829100	1.84302400	-0.01853200
C	-1.52669500	3.12613000	-0.52266800
H	-2.27097100	3.57516900	-1.17271400
C	-0.36884800	3.81928900	-0.19625800
H	-0.19109700	4.80811000	-0.60588100
C	0.54412800	3.23824600	0.67942100
H	1.44479300	3.77130000	0.96711800

C	0.29262500	1.97472500	1.20332900
H	0.99378000	1.54614800	1.91418300
C	-0.84782000	1.23859500	0.85930600
C	-3.09942500	1.26854600	-0.42326100
O	-4.12469600	1.92536400	-0.38049500
C	-1.07273200	-0.10803500	1.53107100
C	-0.91011700	-1.33242800	0.64898200
O	-4.22642300	-0.49341800	-1.47166300
C	-5.14327700	-1.02307100	-0.51800900
H	-6.02211300	-1.31609600	-1.09525900
H	-4.72428900	-1.89384300	-0.00560900
H	-5.42287500	-0.25927900	0.21302200
H	-2.07997500	-0.13872200	1.95515400
H	-0.37642300	-0.17821200	2.37412900
C	-2.05743700	-2.28220700	0.67835400
O	-2.85153600	-2.35673500	1.59145300
O	-2.13996500	-3.07212500	-0.40476200
C	0.17546300	-1.64911200	-0.07145200
C	1.46436100	-0.88594900	-0.10746400
H	0.14189900	-2.56055600	-0.66669900
C	2.67748900	-1.81572600	-0.27232100
H	1.44842200	-0.16819000	-0.93980400
H	1.58245900	-0.29698100	0.80646400
H	2.68128800	-2.54188400	0.54859200
H	2.57694600	-2.38060200	-1.20538700
C	3.97254000	-1.04071300	-0.27687100
C	4.50934100	-0.55685200	0.92145800
C	4.63458500	-0.74896900	-1.47197700
C	5.68012300	0.19635000	0.92598000
H	4.00424600	-0.78003400	1.85869200
C	5.80827700	0.00351100	-1.47217300
H	4.22762500	-1.11915400	-2.40971700
C	6.33400000	0.47894800	-0.27302700
H	6.08502800	0.56042600	1.86542700
H	6.31266500	0.21678700	-2.40981500
H	7.24872900	1.06341200	-0.27115200
H	-2.24497500	-0.40666500	-1.27236900
H	-2.87632400	-3.69074600	-0.25558100

CH_3COOH (in TFE)

C	-0.08941900	0.11735100	-0.00001100
O	-0.63266100	1.20251400	-0.00009900
O	-0.78109100	-1.02985800	0.00004300
H	-1.73087200	-0.81952500	-0.00000800
C	1.38909400	-0.11716400	0.00005100
H	1.66435700	-0.69960200	0.88289300
H	1.66447400	-0.69958000	-0.88276900
H	1.91400400	0.83634200	0.00008800

CH_3OH (in TFE)

C	-0.66261900	0.01933600	-0.00000100
H	-1.02287500	0.54835900	0.89052800
H	-1.09141900	-0.98516200	-0.00005800
H	-1.02286200	0.54847100	-0.89046700
O	0.74743900	-0.12360500	-0.00000100
H	1.13336200	0.76115100	0.00001000

Cat. (in TFE)

Rh	0.08840500	0.16554100	-0.11297400
C	1.10652800	-1.23481400	1.13968400
C	0.94129900	-1.80409500	-0.16245500
C	1.59130200	-0.93776900	-1.10807400
C	2.21987200	0.14226900	-0.36745300
C	1.91350200	-0.03457200	1.00784000
C	-1.00452100	2.54244800	-0.00378100
O	-0.42148600	2.14043000	-1.05858500
O	-0.98025600	1.82132500	1.03720300
C	-1.75598900	3.84246500	-0.00895900
H	-2.77516100	3.64541800	-0.35651300
H	-1.80636900	4.25878800	0.99755300
H	-1.28856000	4.55027500	-0.69450900
O	-1.86323000	-0.37639100	-0.79803700
C	-2.64076900	-1.00183600	0.01801500
O	-2.36641800	-1.24628700	1.20284300
C	-3.95363800	-1.46048500	-0.58281200
H	-4.43099300	-0.63487700	-1.11539100
H	-3.74964200	-2.25150400	-1.31104700
H	-4.62009200	-1.84397200	0.18969400
C	2.98672000	1.26283900	-0.98445000
H	4.00301300	0.92587000	-1.21504300
H	2.51865000	1.58694500	-1.91714100
H	3.05136400	2.11853400	-0.31047400
C	2.28798200	0.85319000	2.14638200
H	3.16516200	0.44199000	2.65761400
H	2.52810800	1.86166000	1.80580500
H	1.47205000	0.91331500	2.87082300
C	1.66309400	-1.12125500	-2.58648400
H	1.66948800	-0.15548400	-3.09677000
H	2.58507600	-1.65136500	-2.84890500
H	0.81558100	-1.70246700	-2.95415300
C	0.14586200	-3.02322800	-0.49185400
H	-0.26078700	-2.96363400	-1.50335800
H	0.78978800	-3.90696300	-0.43227500
H	-0.68194400	-3.14837600	0.20930700
C	0.60362700	-1.77231800	2.43713000
H	-0.09935600	-2.59181100	2.28487400
H	1.45120800	-2.14248600	3.02418600
H	0.10709400	-0.98888800	3.01580100

INT-1 (in TFE)

N	2.39479600	0.94042900	-1.12168500
C	1.21940900	2.82077700	-0.25730100
C	1.49056200	3.85819200	0.63983800
H	2.51308800	4.21330200	0.73144100
C	0.47291800	4.42839400	1.39607600
H	0.69564300	5.22519000	2.09863600
C	-0.83676700	3.98202100	1.22651200
H	-1.64549500	4.43294200	1.79351600
C	-1.11425500	2.97225000	0.30897000
H	-2.14337700	2.66340000	0.14740100
C	-0.09944400	2.36221000	-0.43811000
C	2.63007100	-2.11686900	0.21386500
C	3.40132700	-1.21505700	1.05476200
C	2.58068300	-0.87061200	2.13887900
C	1.33407200	-1.63672500	2.05909700
C	1.40195000	-2.46328800	0.92070900
Rh	1.48535200	-0.35415800	0.26142800
C	2.38872200	2.27222500	-1.03263500
O	3.24653200	3.04349800	-1.50707800
C	-0.45272200	1.26910400	-1.42666800
C	-0.31477200	-0.14409200	-0.85802200
C	0.46479600	-3.55325600	0.52299200
H	0.82588400	-4.49360900	0.95533800
H	-0.54811000	-3.37853300	0.89158800
H	0.42418800	-3.67742000	-0.56107500
C	3.09422700	-2.75030800	-1.05466600
H	3.60428300	-3.69471600	-0.83112400
H	2.24959900	-2.96535600	-1.71396100
H	3.79072300	-2.09783400	-1.58477600
C	4.77443700	-0.68467400	0.78252500
H	5.47980200	-1.10023000	1.50965600
H	5.11278400	-0.95804900	-0.21693500
H	4.80514900	0.40526000	0.86695000
C	2.86971100	0.13087900	3.20507800
H	3.04313600	-0.37857000	4.15957700
H	3.75292200	0.72529100	2.96353800
H	2.01762600	0.80466800	3.34211700
C	0.25473800	-1.58112100	3.09074500
H	0.62191400	-1.99430000	4.03664600
H	-0.05537200	-0.54856200	3.27922200
H	-0.61989900	-2.15864800	2.78477400
O	3.52075000	0.44707500	-1.79752600
C	3.20549800	0.27197600	-3.17272700
H	4.10039900	-0.14668200	-3.63972700
H	2.36409300	-0.41984200	-3.29304800
H	2.96501900	1.23406400	-3.64015700
H	0.19745400	1.33742500	-2.30356000
H	-1.47879700	1.43916900	-1.77282700
C	-0.39809700	-1.27430600	-1.81241600
O	0.14771700	-1.64920400	-2.82811100
O	-1.39260300	-1.94806200	-1.16857400
C	-1.52350000	-0.84855200	-0.19214500
C	-2.90917600	-0.25083800	-0.27177800
H	-1.33489100	-1.24785800	0.80935200
C	-3.97985700	-1.26797000	0.14781700
H	-2.95271700	0.62218800	0.38972600
H	-3.10982700	0.09418900	-1.29298200
H	-3.91968200	-2.13877300	-0.51433600
H	-3.76594700	-1.61404200	1.16594200
C	-5.36547500	-0.67477100	0.09017400
C	-6.09592600	-0.68651400	-1.10224600
C	-5.92608000	-0.05779900	1.21257000
C	-7.35745300	-0.09953000	-1.17147200
H	-5.67038000	-1.16452100	-1.98170200
C	-7.18804600	0.52966400	1.14823100
H	-5.36775400	-0.04338400	2.14588500
C	-7.90795200	0.51004400	-0.04499000
H	-7.91314500	-0.12146400	-2.10426200
H	-7.61090300	0.99970700	2.03125900
H	-8.89258900	0.96453100	-0.09623800

INT-2 (in TFE)

N	2.38209700	1.29530700	-0.29663500
C	0.87009100	3.10335700	0.48594700
C	0.79305300	4.49968000	0.58796100
H	1.62276800	5.08082000	0.20526500
C	-0.30164500	5.14398600	1.14985600
H	-0.31898300	6.22761400	1.20981400
C	-1.36903800	4.39123300	1.62617200
H	-2.23846300	4.87237300	2.06324500
C	-1.30920300	3.00530900	1.54201800
H	-2.13513500	2.40868300	1.92013300
C	-0.20907900	2.34513200	0.98361500
C	2.92431100	-2.08362500	-0.51161200
C	3.43216100	-1.80363400	0.81847500
C	2.40307100	-2.11747500	1.72447100
C	1.25848600	-2.64119200	0.97870200
C	1.61949800	-2.68594400	-0.39497300
Rh	1.57502300	-0.60418100	0.28985300
C	2.13151700	2.60919300	-0.21218800
O	2.89243400	3.47699400	-0.69334700
C	-0.26824600	0.83869100	0.99434400
C	-0.23765800	0.12573500	-0.34430400
C	0.86020400	-3.26869000	-1.54475700
H	1.45617500	-4.06598900	-2.00164700
H	-0.08718200	-3.70313400	-1.22144800
H	0.65857000	-2.51950300	-2.31748900
C	3.73227600	-2.03514300	-1.76431400
H	4.28361600	-2.97903600	-1.85656300
H	3.10043700	-1.92670300	-2.64808700

H	4.45804900	-1.22106300	-1.73832300
C	4.79243700	-1.25869200	1.11527800
H	5.05058400	-0.45798600	0.41761600
H	4.85035900	-0.86280700	2.13113200
H	5.54561100	-2.04799200	1.01410700
C	2.41303100	-1.94546100	3.20786900
H	2.58491100	-2.91573800	3.68748000
H	3.19897500	-1.25990900	3.52903300
H	1.45141400	-1.56809100	3.56547600
C	-0.00935600	-3.13093800	1.60435900
H	0.15987900	-4.09193200	2.10265100
H	-0.37379800	-2.42663700	2.35793400
H	-0.79315000	-3.26923500	0.85609300
O	3.56453400	1.06314400	-1.03457700
C	3.27142300	1.09618300	-2.42531700
H	4.20781900	0.87180700	-2.94221100
H	2.51851800	0.33967400	-2.67921500
H	2.91364200	2.08619600	-2.72387500
H	-1.14314700	0.50405000	1.55866900
H	0.57695600	0.50669700	1.67068200
C	-0.36056700	0.77661800	-1.67109900
O	0.05095600	1.73677800	-2.27439900
O	-1.23766200	-0.14946400	-2.17433200
C	-1.36549100	-0.77917600	-0.84875300
C	-2.74826100	-0.54650000	-0.28341900
H	-1.14110300	-1.84351000	-0.93643100
C	-3.83526200	-1.21888600	-1.13147300
H	-2.77671800	-0.94404000	0.73946900
H	-2.93354500	0.53469600	-0.22180400
H	-3.76819400	-0.83902100	-2.15669100
H	-3.64506400	-2.29787700	-1.16694200
C	-5.21368900	-0.95735500	-0.57773600
C	-5.92993200	0.18050400	-0.96203100
C	-5.77993200	-1.81776400	0.36756600
C	-7.18360200	0.45123000	-0.41806000
H	-5.49950900	0.85643000	-1.69740100
C	-7.03374200	-1.55108600	0.91397100
H	-5.23293200	-2.70706300	0.67256300
C	-7.73961900	-0.41488000	0.52214000
H	-7.72829600	1.33714400	-0.73092000
H	-7.46133900	-2.23282700	1.64322400
H	-8.71797900	-0.20719400	0.94453500

TS-1 (in TFE)

N	2.55230300	1.04045200	-0.48905600
C	1.34306800	2.98067700	0.36571700
C	1.52107500	4.34715300	0.60797200
H	2.35519400	4.84325600	0.12550100
C	0.66710300	5.06170300	1.43923300
H	0.83878900	6.11946000	1.61103100
C	-0.40229000	4.41229000	2.04835400
H	-1.07968400	4.95345600	2.70120500
C	-0.59833500	3.05612500	1.81684800
H	-1.43266700	2.54191400	2.28597400
C	0.25455300	2.32993800	0.97762900
C	2.67199100	-2.40697200	-0.33655800
C	3.07342300	-1.95821600	0.98610500
C	1.95878100	-2.12237300	1.85629700
C	0.84030000	-2.56250900	1.06021300
C	1.31957900	-2.80417500	-0.28209300
Rh	1.45932300	-0.55684700	0.33886600
C	2.37480100	2.36251800	-0.55636500
O	3.03824100	3.12035500	-1.29373100
C	-0.10365400	0.89153800	0.78793800
C	-0.27940500	0.30847700	-0.50407600
C	0.55352100	-3.41139500	-1.41756200
H	1.03491800	-4.34524700	-1.72720700
H	-0.47144200	-3.65023100	-1.12722500
H	0.52353100	-2.75173700	-2.29111700
C	3.59448600	-2.57078600	-1.50069600
H	4.14449700	-3.51365700	-1.39453500
H	3.04721700	-2.60500400	-2.44543100
H	4.32536000	-1.76096600	-1.54566700
C	4.46072200	-1.53198500	1.34999000
H	4.87592300	-0.86958300	0.58525600
H	4.47633700	-1.00435100	2.30606300
H	5.11971900	-2.40400700	1.43051300
C	1.93887300	-1.90282200	3.33753600
H	2.14743100	-2.84711300	3.85265600
H	2.69460100	-1.17651300	3.64383800
H	0.96284000	-1.54739500	3.67597300
C	-0.52285600	-2.89570100	1.58563700
H	-0.53889000	-3.91323400	1.99254100
H	-0.81672500	-2.21248900	2.38697400
H	-1.27895900	-2.84188000	0.79775900
O	3.56662200	0.60342100	-1.35735400
C	3.05355800	0.40755500	-2.66924200
H	3.88029700	0.00995900	-3.26249200
H	2.22794800	-0.31663600	-2.65579900
H	2.70901400	1.35323900	-3.09702700
H	-0.78685100	0.51773400	1.55053800
H	1.22764800	0.38034400	1.55043000
C	-0.31412100	0.95709300	-1.83842900
O	0.20582000	1.86414500	-2.43326200
O	-1.29982200	0.14185800	-2.32018300
C	-1.43422400	-0.54070500	-1.01885100
C	-2.78931400	-0.28750400	-0.40312200
H	-1.23334300	-1.60378200	-1.16033900
C	-3.92166100	-0.94050200	-1.20462800
H	-2.77750300	-0.68560500	0.61988500

H	-2.94856400	0.79641500	-0.33174900
H	-3.89167200	-0.56213300	-2.23233100
H	-3.75226500	-2.02279000	-1.24634700
C	-5.26881100	-0.65259000	-0.59013900
C	-5.98249000	0.49547500	-0.94747100
C	-5.80349200	-1.49733600	0.38708000
C	-7.20379100	0.79137800	-0.34601800
H	-5.57589900	1.15966200	-1.70667500
C	-7.02486600	-1.20535500	0.99091100
H	-5.25757700	-2.39401200	0.67200800
C	-7.72887800	-0.05918500	0.62553000
H	-7.74731200	1.68508700	-0.63806000
H	-7.42855900	-1.87482800	1.74472400
H	-8.68177600	0.16850200	1.09337900

INT-3 **(in TFE)**

N	2.55387800	0.94510400	-0.62118600
C	1.49285900	2.92891800	0.29999100
C	1.78242900	4.27123200	0.56396200
H	2.60603700	4.72755200	0.02641100
C	1.05383600	5.00978000	1.48916500
H	1.31057600	6.04727300	1.67753200
C	0.00274700	4.40678400	2.17287400
H	-0.57492800	4.96500500	2.90278800
C	-0.30739900	3.07673900	1.91463600
H	-1.13370700	2.60389800	2.43818900
C	0.41485900	2.32435000	0.97939300
C	2.55445300	-2.51659200	-0.30354700
C	2.96413000	-2.01814700	0.99530300
C	1.82916100	-2.11269700	1.87731000
C	0.70768400	-2.50899500	1.08771100
C	1.18524400	-2.82207000	-0.25070200
Rh	1.47529700	-0.52589900	0.37152300
C	2.42316800	2.27103000	-0.69719100
O	3.05935200	2.99126600	-1.49282100
C	-0.06902500	0.93289200	0.76794600
C	-0.30231500	0.37006300	-0.49629700
C	0.38745300	-3.43165400	-1.36347800
H	0.83253400	-4.38855400	-1.65591900
H	-0.64170400	-3.62782700	-1.05559300
H	0.36737100	-2.79370700	-2.25369200
C	3.47241600	-2.74634800	-1.45986400
H	4.01851800	-3.68529100	-1.30941600
H	2.92091600	-2.82319000	-2.39965700
H	4.20810500	-1.94396400	-1.54874200
C	4.37544400	-1.68709800	1.36798900
H	4.86026100	-1.11183200	0.57431500
H	4.41647300	-1.10116300	2.28861900
H	4.95521600	-2.60474000	1.51971100
C	1.82382800	-1.89367500	3.35919200
H	1.93665600	-2.85531600	3.87210600
H	2.64525500	-1.24509600	3.67013700
H	0.88589700	-1.44419000	3.69356200
C	-0.67431100	-2.76332900	1.60595500
H	-0.75127500	-3.78639600	1.99172800
H	-0.92489500	-2.07988000	2.42129800
H	-1.42629600	-2.65044800	0.82064300
O	3.49453400	0.44063700	-1.52802000
C	2.89126800	0.18599500	-2.79105400
H	3.66623200	-0.27232400	-3.40961000
H	2.04794600	-0.50981000	-2.68216500
H	2.54751400	1.11686700	-3.25081700
H	-0.68958100	0.55296600	1.57873300
H	1.81885900	0.33172700	1.56700600
C	-0.32003200	0.98545300	-1.85094800
O	0.21190400	1.87145700	-2.46414000
O	-1.32194300	0.17979300	-2.30947400
C	-1.46124200	-0.48158100	-0.99802100
C	-2.81326100	-0.20402600	-0.38587400
H	-1.27022700	-1.54741200	-1.12647500
C	-3.95091700	-0.85972500	-1.17773900
H	-2.80532100	-0.58309200	0.64402700
H	-2.96124300	0.88225100	-0.33501500
H	-3.91644600	-0.49847700	-2.21145900
H	-3.79205700	-1.94419300	-1.20171200
C	-5.29556200	-0.54861100	-0.56922600
C	-5.99530200	0.60341800	-0.94125300
C	-5.84131300	-1.37568400	0.41682400
C	-7.21402000	0.92026300	-0.34531300
H	-5.57991000	1.25404400	-1.70741600
C	-7.06023900	-1.06278800	1.01504600
H	-5.30587600	-2.27497400	0.71313600
C	-7.75040600	0.08704200	0.63509600
H	-7.74674000	1.81673300	-0.64859100
H	-7.47284400	-1.71872600	1.77587800
H	-8.70139100	0.33113600	1.09853400

TS-2 **(in TFE)**

N	2.57845700	1.01301900	-0.64950800
C	1.42561600	2.94949000	0.26944300
C	1.64855200	4.30605400	0.53093900
H	2.42198400	4.81388900	-0.03467600
C	0.92160500	4.99008600	1.49628600
H	1.12111700	6.03995600	1.68429600
C	-0.05170400	4.31199000	2.22550100
H	-0.62436100	4.82589600	2.99123200
C	-0.29653900	2.96965000	1.96440700
H	-1.07061900	2.44649000	2.51890700
C	0.41557000	2.26610700	0.98172600
C	2.59506000	-2.60474800	-0.14559000

C	2.94223100	-1.98225400	1.12335300
C	1.77279000	-1.95894200	1.94222300
C	0.68395300	-2.42357200	1.12901900
C	1.22641200	-2.90055500	-0.13777700
Rh	1.45599100	-0.55915000	0.24701500
C	2.37970300	2.34947600	-0.72943300
O	3.00203200	3.06830500	-1.51979500
C	-0.01023100	0.86093400	0.74790600
C	-0.28847700	0.33043200	-0.54211500
C	0.46784200	-3.59356100	-1.22990500
H	0.84736200	-4.61210600	-1.36483200
H	-0.59483900	-3.67111300	-0.99054400
H	0.56621500	-3.07676700	-2.19020200
C	3.57275100	-2.89645600	-1.23904200
H	4.18269800	-3.76911400	-0.97724100
H	3.06442600	-3.10959300	-2.18252600
H	4.25574400	-2.05590800	-1.39351000
C	4.33873400	-1.61447000	1.52241700
H	4.86265400	-1.11851400	0.70035600
H	4.34372400	-0.94362000	2.38449800
H	4.90887700	-2.51275400	1.78590900
C	1.67818300	-1.54367100	3.37838700
H	1.72543100	-2.42103600	4.03362400
H	2.49688800	-0.87419600	3.65204300
H	0.73605900	-1.02773800	3.58232400
C	-0.72188600	-2.61463100	1.61125300
H	-0.80603300	-3.55905200	2.16137400
H	-1.02281000	-1.80952800	2.28736300
H	-1.43388100	-2.65147500	0.78307700
O	3.62214000	0.54693100	-1.44115100
C	3.12177100	0.14535500	-2.71585600
H	3.97312500	-0.28115500	-3.24961800
H	2.33753500	-0.61304100	-2.59394800
H	2.72845800	1.00787600	-3.26157600
H	-0.63315400	0.46604500	1.55099100
H	2.41434700	0.55513000	0.76699200
C	-0.31284400	0.95795300	-1.88567700
O	0.24294500	1.82798400	-2.50636300
O	-1.32811200	0.17119500	-2.35102100
C	-1.46319300	-0.50049800	-1.04379900
C	-2.81067400	-0.21975700	-0.42353700
H	-1.27956200	-1.56793800	-1.18443100
C	-3.95622200	-0.86579700	-1.21206600
H	-2.80030900	-0.60392600	0.60418200
H	-2.95238500	0.86716100	-0.36644300
H	-3.92894400	-0.49677700	-2.24327800
H	-3.79933700	-1.95038200	-1.24584700
C	-5.29620300	-0.55870700	-0.59150600
C	-6.00695100	0.58688100	-0.96213700
C	-5.82681200	-1.38382900	0.40465500
C	-7.22156200	0.89936400	-0.35537800
H	-5.60350800	1.23598800	-1.73592000
C	-7.04136500	-1.07531600	1.01376800
H	-5.28285700	-2.27832400	0.70014800
C	-7.74268900	0.06817100	0.63482400
H	-7.76294600	1.79088200	-0.65791100
H	-7.44200600	-1.72976300	1.78227200
H	-8.69043800	0.30870400	1.10669400

INT-4 (in TFE)

N	2.80013200	1.04788600	-0.44750800
C	1.40700000	2.93224300	0.32381300
C	1.61478500	4.28324900	0.63469500
H	2.38642300	4.82439900	0.09602400
C	0.87789200	4.91171200	1.62687700
H	1.06014100	5.95393300	1.86578200
C	-0.08822200	4.18060100	2.31668900
H	-0.67122400	4.65068500	3.10273400
C	-0.32198200	2.85073700	1.99142900
H	-1.10061200	2.30126300	2.51312300
C	0.39919600	2.18981700	0.98283900
C	2.72433900	-2.54412300	-0.02188300
C	2.88052800	-1.93403000	1.29740200
C	1.63477200	-1.97034200	1.95662500
C	0.66563700	-2.47066500	1.00356200
C	1.38390800	-2.92236700	-0.17995400
Rh	1.39536500	-0.61100900	0.15401800
C	2.35581200	2.39594600	-0.68659200
O	2.80632800	3.03753000	-1.60705300
C	-0.00918300	0.79473900	0.67267200
C	-0.27296400	0.31010300	-0.66487800
C	0.78423700	-3.66358000	-1.33498100
H	0.79611300	-4.74443100	-1.14985200
H	-0.25809100	-3.37897200	-1.50123300
H	1.33557600	-3.47902800	-2.26091300
C	3.86136400	-2.77695000	-0.96974600
H	4.48803100	-3.60691200	-0.62151800
H	3.50620100	-3.02502500	-1.97289300
H	4.50444300	-1.89444400	-1.04449100
C	4.19189900	-1.44738000	1.83627300
H	4.72958600	-0.85457200	1.08776100
H	4.05467200	-0.82709900	2.72553900
H	4.84066800	-2.28817100	2.10876700
C	1.32811500	-1.55058900	3.36212900
H	1.31022800	-2.41799900	4.03269300
H	2.07645400	-0.85067600	3.74280600
H	0.34951200	-1.06632500	3.42945500
C	-0.76865200	-2.77165000	1.32184800
H	-0.85733400	-3.73592300	1.83689900
H	-1.19878900	-2.00829800	1.97740600

H	-1.37996000	-2.82642200	0.41656000
O	3.80952600	0.67245100	-1.34770400
C	3.24171200	0.18073200	-2.56187600
H	4.09426500	-0.14622000	-3.15885400
H	2.57398300	-0.66290200	-2.35456300
H	2.69935000	0.97247900	-3.08571400
H	-0.70045200	0.40928500	1.42453000
H	3.25430100	1.03654700	0.47388200
C	-0.30243000	1.02173500	-1.95507500
O	0.28886700	1.90267400	-2.53431800
O	-1.36185100	0.31823100	-2.45957900
C	-1.49499700	-0.43205800	-1.19435500
C	-2.82282100	-0.16226000	-0.53035000
H	-1.35271100	-1.49447200	-1.41093800
C	-4.00202100	-0.71234200	-1.34203900
H	-2.80506800	-0.62996600	0.46237700
H	-2.93327800	0.91960400	-0.38003600
H	-4.01662100	-0.22428500	-2.32281900
H	-3.84817500	-1.78472300	-1.51097900
C	-5.31552200	-0.49182900	-0.63431300
C	-6.03450300	0.69408200	-0.81244300
C	-5.81204500	-1.44877800	0.25617400
C	-7.22321800	0.91757300	-0.12080300
H	-5.65827700	1.44541800	-1.50296400
C	-7.00051400	-1.22977400	0.94937300
H	-5.26159400	-2.37561800	0.40208600
C	-7.71026700	-0.04473600	0.76224700
H	-7.77138300	1.84246500	-0.27414700
H	-7.37458300	-1.98603500	1.63317900
H	-8.63824000	0.12665200	1.29914000

INT-5 (in TFE)

N	2.28539100	0.28984400	-0.53104600
C	1.30419400	2.40204400	0.25943300
C	1.78764500	3.68036200	0.57162700
H	2.63858400	4.06083600	0.01464200
C	1.21813900	4.43152600	1.58805600
H	1.61050900	5.41381100	1.82819500
C	0.14610300	3.89793100	2.30230500
H	-0.31081300	4.46592300	3.10689600
C	-0.35137700	2.64108000	1.98323700
H	-1.20344100	2.24898100	2.53148900
C	0.19721200	1.85861400	0.95276200
C	1.64837300	-3.19918700	-0.00794100
C	1.95821900	-2.58759400	1.28346500
C	0.75209500	-2.40765400	1.99348700
C	-0.32548100	-2.77153700	1.09750200
C	0.25770200	-3.36053100	-0.09899600
Rh	0.66230300	-1.08336100	0.15550000
C	2.10371900	1.69882300	-0.77344500
O	2.67035900	2.24203900	-1.69394200
C	-0.46544700	0.55755500	0.67378100
C	-0.84525200	0.09599700	-0.64347300
C	-0.50844600	-4.01607100	-1.20626900
H	-0.69640400	-5.07182600	-0.97694800
H	-1.48227600	-3.54189300	-1.35679500
H	0.03769000	-3.97271900	-2.15232200
C	2.68881500	-3.63330400	-0.99514900
H	3.18085400	-4.55304100	-0.65651900
H	2.25455600	-3.82932900	-1.97862000
H	3.46719600	-2.87286200	-1.11192200
C	3.35101200	-2.28710000	1.75120000
H	3.94322500	-1.81910000	0.95649200
H	3.34691900	-1.61064200	2.60983200
H	3.87403600	-3.20443700	2.04632100
C	0.57958400	-1.90291300	3.39386800
H	0.47040200	-2.73644200	4.09786400
H	1.43895000	-1.30759100	3.71303800
H	-0.31491900	-1.27964700	3.48509900
C	-1.77671500	-2.81727200	1.47237200
H	-2.00375300	-3.72607200	2.04273900
H	-2.05404500	-1.96043400	2.09402300
H	-2.41831500	-2.81724600	0.58656200
O	3.20325600	-0.26252600	-1.44388300
C	2.55735400	-0.63889200	-2.66384600
H	3.33230500	-1.13442400	-3.24990100
H	1.73685400	-1.33148800	-2.44873000
H	2.18656100	0.24193600	-3.19298100
H	-1.19254900	0.31184200	1.45000800
H	2.79674800	0.24638000	0.36170000
C	-0.76107600	0.75523300	-1.95625600
O	-0.02416200	1.49336900	-2.56802700
O	-1.93486300	0.23631200	-2.43098000
C	-2.19160500	-0.42452300	-1.13419200
C	-3.43197100	0.12842200	-0.47557700
H	-2.25946900	-1.50279000	-1.30554200
C	-4.70878200	-0.20945900	-1.25490600
H	-3.49283300	-0.28730900	0.53852300
H	-3.32346600	1.21647900	-0.37676300
H	-4.61614000	0.18243900	-2.27385100
H	-4.80456800	-1.29911100	-1.32876600
C	-5.93338900	0.37012400	-0.59185300
C	-6.38070500	1.65369600	-0.91908600
C	-6.61245000	-0.34280400	0.40120800
C	-7.48257000	2.21111500	-0.27379900
H	-5.86030500	2.21743800	-1.68996000
C	-7.71480800	0.21066600	1.04905700
H	-6.27446900	-1.34288700	0.66375700
C	-8.15357300	1.49027000	0.71266900
H	-7.81923400	3.20774900	-0.54363600

H	-8.23364000	-0.35872600	1.81462500
H	-9.01418100	1.92201700	1.21436600
C	5.40853600	1.74001100	0.07014200
O	4.55631500	1.30146300	0.82660700
O	5.44951700	1.43346600	-1.22282900
H	4.69406300	0.84352400	-1.44407000
C	6.50119800	2.67799000	0.47723900
H	6.47680600	2.83151300	1.55452600
H	7.46750400	2.27198800	0.16949800
H	6.35881400	3.63081800	-0.04033300

TS-3 (in TFE)

N	-2.17239400	0.33076700	0.19984500
C	-1.25000700	2.49714400	-0.61489500
C	-1.69240600	3.78035800	-0.94951300
H	-2.58974400	4.16210300	-0.47355700
C	-1.01525700	4.53928700	-1.89675100
H	-1.37960100	5.52533700	-2.16444900
C	0.12219900	4.01569700	-2.50544300
H	0.65628000	4.59240500	-3.25408300
C	0.58320000	2.74987400	-2.15418300
H	1.48534300	2.35565200	-2.61326600
C	-0.08666800	1.97074700	-1.20518600
C	-1.47728900	-3.08009500	0.00079200
C	-1.98658700	-2.49687900	-1.21998600
C	-0.87572000	-2.20310800	-2.06941700
C	0.32406600	-2.53488200	-1.33624600
C	-0.05952500	-3.11480500	-0.07987300
Rh	-0.74714600	-0.90442300	-0.25467300
C	-2.11058100	1.75760400	0.35783600
O	-2.79329100	2.33775700	1.17186300
C	0.52869800	0.67149500	-0.83044700
C	0.81906700	0.31291800	0.51078600
C	0.84971000	-3.71091700	0.95023900
H	0.72836100	-4.79982500	0.96969400
H	1.89856000	-3.50156400	0.72916900
H	0.62511200	-3.33754600	1.95433900
C	-2.29950000	-3.59737500	1.13739900
H	-2.53817600	-4.65584400	0.97648100
H	-1.75814000	-3.51974000	2.08420500
H	-3.24203300	-3.05318000	1.23079100
C	-3.43838400	-2.30946200	-1.53678400
H	-4.00121400	-2.01940000	-0.64399500
H	-3.58424700	-1.53564500	-2.29475700
H	-3.87335100	-3.24128500	-1.91462900
C	-0.92667400	-1.67801600	-3.46980800
H	-0.86526300	-2.50198400	-4.19003900
H	-1.85734000	-1.13686800	-3.65639200
H	-0.09279400	-0.99957200	-3.67015800
C	1.72292900	-2.45276600	-1.86413900
H	2.00119800	-3.39688400	-2.34615300
H	1.82632800	-1.65967600	-2.60920300
H	2.44092500	-2.26580500	-1.06100500
O	-3.17236400	-0.27938700	1.79236700
C	-2.25716800	-0.44155200	2.81743200
H	-2.57859400	-1.24976500	3.49292300
H	-1.28079400	-0.76353400	2.39539500
H	-2.09943500	0.47552800	3.40335700
H	1.23080900	0.29794100	-1.57549700
H	-3.09476000	0.12674600	-0.21952900
C	0.67759300	1.06710900	1.77921300
O	-0.03318400	1.91062200	2.26303500
O	1.75911700	0.48441000	2.37142400
C	2.06916300	-0.28153200	1.14468700
C	3.39378100	0.14715000	0.56045000
H	2.03540000	-1.34793200	1.37912300
C	4.57707800	-0.24378500	1.45401300
H	3.49891200	-0.32258900	-0.42529300
H	3.37594100	1.23346100	0.40420100
H	4.46202500	0.24053500	2.42977900
H	4.55577500	-1.32745700	1.61920800
C	5.89227700	0.15296000	0.83097300
C	6.46468600	1.40010300	1.09748000
C	6.53550800	-0.70149200	-0.07010200
C	7.65434300	1.78397000	0.48150400
H	5.97329800	2.07281500	1.79657000
C	7.72481400	-0.32185000	-0.68791200
H	6.09917300	-1.67481300	-0.28387900
C	8.28807100	0.92350400	-0.41320900
H	8.08814000	2.75469700	0.70265300
H	8.21389000	-0.99955100	-1.38141800
H	9.21632800	1.22028100	-0.89177600
C	-5.62781800	1.04277000	0.50807400
O	-4.95111500	0.59139900	-0.41874600
O	-5.27439400	0.97364600	1.76384100
H	-4.32672400	0.48463100	1.84998600
C	-6.94257000	1.73440300	0.28021100
H	-7.21901000	1.68660100	-0.77204500
H	-7.71409600	1.26811100	0.89745100
H	-6.85249400	2.77824900	0.59374200

INT-6 (in TFE)

N	-1.45202000	0.63326800	1.48560400
C	-0.43180700	2.81356200	1.02862000
C	-1.09323700	4.04196000	1.14525100
H	-1.91071300	4.12160300	1.85609700
C	-0.73228500	5.14086900	0.37563000
H	-1.27449100	6.07594300	0.47462200
C	0.33537600	5.03199300	-0.51461900
H	0.63842100	5.88028000	-1.11968900

C	1.00732300	3.82489500	-0.62701900	H	4.79995700	-2.22086600	-0.87117000
H	1.83364100	3.73812300	-1.32737900	C	6.54873300	-1.17792200	-0.19620200
C	0.64832300	2.69545500	0.13531700	C	7.34747600	-0.92136100	0.92216900
C	-3.93556900	-0.55148300	-1.52195800	C	7.09971600	-0.99792000	-1.46876700
C	-3.53329000	0.82915800	-1.34134100	C	8.66693400	-0.49886500	0.77369100
C	-2.21596600	0.97071000	-1.90605800	H	6.92937300	-1.05733300	1.91688000
C	-1.76796600	-0.32039400	-2.30939700	C	8.41863500	-0.57619300	-1.62174900
C	-2.84840600	-1.26424500	-2.09314400	H	6.48826900	-1.19508800	-2.34648200
Rh	-2.26813400	-0.39253200	-0.17627000	C	9.20672000	-0.32534700	-0.49966700
C	-0.92458400	1.74509200	1.96850600	H	9.27479400	-0.30715300	1.65293400
O	-0.83745300	2.01279300	3.19148400	H	8.83222300	-0.44638300	-2.61750900
C	1.45414900	1.49830500	-0.15238600	H	10.23541900	0.00141300	-0.61690500
C	1.75919800	0.37143500	0.50103200	C	-3.85283200	-2.28876000	1.65172600
C	-2.86102900	-2.72068400	-2.43072100	O	-3.60431300	-1.05280200	1.46157400
H	-3.55351300	-2.89766600	-3.26048900	O	-3.18245400	-3.22809900	1.15267200
H	-1.87334700	-3.07010100	-2.73421400	H	-1.70497200	-2.62552500	0.91813900
H	-3.19688200	-3.31908800	-1.57927900	C	-5.05129700	-2.61082800	2.51285600
C	-5.24840200	-1.13974400	-1.13123300	H	-4.98180200	-3.62423600	2.90849300
H	-5.94083900	-1.05392100	-1.97612100	H	-5.14230600	-1.88892900	3.32605000
H	-5.14615200	-2.19933400	-0.88310300	H	-5.95044500	-2.53486500	1.89197900
H	-5.68352000	-0.61342500	-0.27960300				
C	-4.37639800	1.92961600	-0.78864000	**TS-4** **(in TFE)**			
H	-5.02602200	1.55910400	0.00799200	N	0.59824400	0.50104400	-1.23601800
H	-3.75104700	2.72813700	-0.38121200	C	1.10024600	2.93155100	-0.75866000
H	-5.00758700	2.35358900	-1.57720800	C	2.13749900	3.85193900	-0.97294700
C	-1.50991100	2.25485300	-2.16862100	H	2.90991100	3.59111900	-1.68756300
H	-1.90344900	2.66092800	-3.10853100	C	2.20698900	5.06313500	-0.29715700
H	-1.68419700	2.99382200	-1.38437400	H	3.03466300	5.74023800	-0.48140900
H	-0.43692800	2.10399000	-2.29183500	C	1.20521100	5.39478200	0.61097500
C	-0.44896900	-0.60546200	-2.94777600	H	1.23575100	6.33723600	1.14866100
H	-0.45845200	-0.22755800	-3.97633600	C	0.16774900	4.50086700	0.83515500
H	0.36232300	-0.10366900	-2.41176900	H	-0.60573000	4.74619700	1.55770800
H	-0.23993600	-1.67528800	-2.98134800	C	0.08525800	3.26553600	0.17356500
O	-0.91340400	-2.05848800	0.68488600	C	3.43911600	-1.36604500	1.35005200
C	-0.07448500	-2.79489600	-0.19497600	C	3.36805400	0.08158500	1.28585100
H	-0.65783200	-3.48529600	-0.81352700	C	2.18343300	0.49213100	1.97782700
H	0.44519200	-2.09050300	-0.84687300	C	1.44887700	-0.68095500	2.33874400
H	0.66510700	-3.36817700	0.37465500	C	2.25762400	-1.83297400	1.98654100
H	1.97111900	1.57465200	-1.11138300	Rh	1.73544900	-0.74937100	0.19255500
H	-1.69995200	0.03549500	2.27489100	C	1.23267600	1.67492300	-1.59987700
C	1.59586000	-0.35394800	1.79551500	O	1.90216900	1.74066700	-2.63054000
O	1.06015400	-0.24977400	2.86319300	C	-1.01084900	2.38406500	0.62079200
O	2.43227300	-1.37064300	1.42319000	C	-1.53242000	1.40146900	-0.09825000
C	2.72720500	-0.73243400	0.12965100	C	1.91497400	-3.26429300	2.22994000
C	4.18559000	-0.35256200	0.01616100	H	2.48771500	-3.62875100	3.08977800
H	2.41306600	-1.39504600	-0.68146000	H	0.85368400	-3.38662100	2.45009100
C	5.10365300	-1.58013800	-0.03536600	H	2.17244100	-3.88243300	1.36541000
H	4.30583800	0.24217400	-0.89781400	C	4.55458500	-2.20626300	0.82728300
H	4.45508200	0.28752200	0.86481800	H	5.29075000	-2.35266800	1.62559200
H	4.97553300	-2.15844100	0.88610300	H	4.19898100	-3.18716800	0.50536900

H	5.05705700	-1.71766300	-0.01030100
C	4.39670500	0.97888100	0.68408400
H	4.82358800	0.52996300	-0.21623800
H	3.96252300	1.94551400	0.41658400
H	5.20893300	1.15013800	1.39899900
C	1.85412200	1.88655000	2.37825700
H	2.33257900	2.05501400	3.35139700
H	2.24918300	2.62416800	1.67828200
H	0.78167200	2.03670200	2.50439900
C	0.15035100	-0.69558300	3.07417700
H	0.33488800	-0.61030500	4.15109800
H	-0.47694800	0.14571600	2.76809100
H	-0.39699800	-1.62400400	2.89861400
O	0.34856800	-2.28431300	-0.70032100
C	-0.62933900	-3.02407800	0.02120100
H	-0.23506400	-3.99496000	0.33512700
H	-0.93138300	-2.45958900	0.90755300
H	-1.51004700	-3.18489500	-0.60945500
H	-1.36774500	2.55370600	1.63597000
H	0.73401000	-0.12688700	-2.03413200
C	-1.23389000	0.87805500	-1.47276700
O	-1.30255300	1.38535700	-2.59554200
O	-1.90384300	-0.34462900	-1.17651200
C	-2.36371300	0.16401800	0.11778700
C	-3.87010800	0.32432000	0.14329200
H	-2.00976400	-0.48074300	0.93203300
C	-4.59277200	-1.02253300	0.02449500
H	-4.14976900	0.82091900	1.08040800
H	-4.16851600	0.98239000	-0.68194400
H	-4.27762900	-1.51075500	-0.90435800
H	-4.28865200	-1.66889900	0.85638500
C	-6.09072800	-0.84464600	0.02924700
C	-6.78011400	-0.59442400	-1.16144000
C	-6.81033000	-0.86503400	1.22771800
C	-8.15559200	-0.37378000	-1.15631800
H	-6.23027000	-0.57508800	-2.09960800
C	-8.18639900	-0.64551600	1.23750000
H	-6.28517900	-1.05790400	2.16047700
C	-8.86330700	-0.39852300	0.04447900
H	-8.67563400	-0.18416400	-2.09069100
H	-8.73065800	-0.66891400	2.17701300
H	-9.93559800	-0.22846500	0.04999700
C	3.07473800	-2.37955600	-2.04227900
O	2.84732400	-1.17650300	-1.68858200
O	2.47307500	-3.38284100	-1.57646300
H	1.09673000	-2.87523300	-1.02650600
C	4.16824800	-2.60250800	-3.05919400
H	4.36156400	-1.69705800	-3.63455000
H	5.08023100	-2.87615000	-2.51728400
H	3.90655400	-3.42979600	-3.72058300

INT-7 **(in TFE)**

N	-0.43453000	0.51759900	1.25212200
C	-1.19657500	2.89392100	0.75538100
C	-2.33887100	3.67372100	0.99492400
H	-3.01090200	3.36530600	1.78799500
C	-2.63523200	4.79756000	0.23729400
H	-3.53654600	5.36645900	0.43968200
C	-1.76521900	5.17870700	-0.78113900
H	-1.97617200	6.05348900	-1.38832300
C	-0.61945700	4.43240900	-1.01804500
H	0.06169300	4.73397300	-1.80872300
C	-0.29896300	3.28618500	-0.27033700
C	-3.30277000	-1.15253500	-1.46666400
C	-2.69736400	0.12212000	-1.76808000
C	-1.37168400	-0.14109600	-2.27185700
C	-1.11699000	-1.53615900	-2.16038100
C	-2.32910900	-2.17342100	-1.68036700
Rh	-1.64028800	-0.82090600	-0.17098200
C	-1.11296800	1.69447300	1.65788800
O	-1.70089200	1.69424100	2.72609500
C	0.91897800	2.57767800	-0.69030400
C	1.45541200	1.53251000	-0.07439600
C	-2.56457600	-3.63467300	-1.47891900
H	-3.36344700	-3.96534400	-2.15081800
H	-1.66882100	-4.21548200	-1.70146400
H	-2.88011300	-3.84560400	-0.45259500
C	-4.69055100	-1.37579000	-0.97307100
H	-5.34737700	-1.53266600	-1.83620800
H	-4.74278500	-2.26526300	-0.33982400
H	-5.05834100	-0.51301100	-0.41488800
C	-3.37654000	1.44923600	-1.68787500
H	-3.98361800	1.51812900	-0.78104400
H	-2.65098600	2.26660800	-1.68290600
H	-4.03834800	1.57840900	-2.55140900
C	-0.47459200	0.84977400	-2.92429800
H	-0.66058000	0.78707000	-4.00389500
H	-0.69134900	1.86878200	-2.60385800
H	0.57882700	0.62590700	-2.75227500
C	0.14777500	-2.22211800	-2.55238100
H	0.14974000	-2.39313800	-3.63481400
H	1.01683700	-1.60846300	-2.30235100
H	0.24713000	-3.18745400	-2.05414600
O	-0.59544800	-2.27841600	1.23465700
C	0.22179900	-3.35514100	0.78720400
H	-0.32338400	-4.01879100	0.10843800
H	1.08501500	-2.93130700	0.27173400
H	0.57201000	-3.93441900	1.64759800
H	1.34592900	2.91615400	-1.63301800
H	-0.52914500	-0.12198300	2.04846700

C	1.07245800	0.76038700	1.16863900
O	1.55440200	1.07202400	2.31368300
O	1.69206900	-0.44648200	0.51385900
C	2.37653300	0.40495000	-0.44658600
C	3.85441900	0.55490800	-0.12941200
H	2.24413600	0.02999600	-1.47004500
C	4.58816000	-0.78548200	-0.25691000
H	4.28805100	1.28675400	-0.82218700
H	3.96134100	0.95003700	0.88766800
H	4.16266500	-1.48815300	0.46789300
H	4.40771700	-1.19706600	-1.25752400
C	6.07197000	-0.64133200	-0.02944700
C	6.60570000	-0.68505800	1.26239400
C	6.93775300	-0.41127000	-1.10316800
C	7.97104500	-0.50814500	1.47602800
H	5.94240800	-0.86348200	2.10566100
C	8.30392100	-0.23446700	-0.89442400
H	6.53457300	-0.37537500	-2.11274000
C	8.82504000	-0.28278200	0.39734900
H	8.36932700	-0.54942500	2.48553400
H	8.96205500	-0.06184100	-1.74099000
H	9.88967900	-0.14808300	0.56230300
C	-3.51524100	-1.61779500	2.08479400
O	-3.04503900	-0.59455600	1.48323300
O	-3.03867700	-2.77520400	1.99143500
H	-1.45895900	-2.62967700	1.59707900
C	-4.74499800	-1.38334500	2.92910500
H	-4.67964300	-0.41752300	3.43315300
H	-5.61606400	-1.36072800	2.26543500
H	-4.87475300	-2.18566400	3.65544100

TS-5 **(in TFE)**

N	0.42562000	0.55698900	-1.31460500
C	1.26050900	2.91109400	-0.85969100
C	2.41143500	3.67868600	-1.09604200
H	3.09487100	3.35081000	-1.87139100
C	2.69757600	4.81344100	-0.35268000
H	3.60334400	5.37751000	-0.54798100
C	1.80954700	5.21220400	0.64437300
H	2.01265200	6.09625700	1.24065200
C	0.65744700	4.47445100	0.87522900
H	-0.03501900	4.79311200	1.64893200
C	0.34458700	3.31671300	0.14046700
C	3.31453900	-1.11569300	1.46576600
C	2.69364400	0.14813800	1.75998400
C	1.36898000	-0.13018300	2.26372200
C	1.14158400	-1.53245000	2.19329700
C	2.35345700	-2.15259100	1.69683300
Rh	1.64150600	-0.83274600	0.18413600
C	1.17705400	1.69576000	-1.72455600
O	1.81488100	1.61928800	-2.75887800
C	-0.88905100	2.63066500	0.54455100
C	-1.48788200	1.58029300	-0.01707500
C	2.61338900	-3.61005100	1.50648700
H	3.38697600	-3.93061900	2.21238300
H	1.71659100	-4.20250500	1.68920800
H	2.97504600	-3.81453000	0.49452900
C	4.70389800	-1.32382900	0.97194200
H	5.36594800	-1.43524300	1.83825500
H	4.77558000	-2.23332600	0.37016800
H	5.04972100	-0.47249000	0.38314200
C	3.34965600	1.48488000	1.65310800
H	3.95800400	1.54516800	0.74652800
H	2.61117100	2.29013600	1.63121500
H	4.00723900	1.64215200	2.51516500
C	0.42711600	0.85710600	2.85320700
H	0.53624600	0.80612600	3.94365400
H	0.65310700	1.87518300	2.53524900
H	-0.60803000	0.61657200	2.60669600
C	-0.10160900	-2.22934800	2.63222500
H	-0.11775000	-2.27536800	3.72710400
H	-0.98918800	-1.68946500	2.29466500
H	-0.14437200	-3.24882100	2.24619800
O	0.55247900	-2.25444200	-1.21061200
C	-0.26715700	-3.30314600	-0.69981800
H	0.29722600	-3.95773000	-0.02796500
H	-1.09491300	-2.84201200	-0.16015400
H	-0.66298000	-3.89822200	-1.52921900
H	-1.32515600	3.00987700	1.46738400
H	0.52001100	-0.11719400	-2.08134100
C	-1.02631800	0.80156900	-1.20837100
O	-1.66423400	0.68016600	-2.24826300
O	-1.71771200	-0.55317700	0.10537300
C	-2.43060200	0.56904100	0.57114100
C	-3.88022800	0.62360800	0.08790900
H	-2.44724400	0.64646800	1.67465400
C	-4.67774100	-0.56875700	0.62799600
H	-4.34261300	1.56101300	0.42416600
H	-3.89990600	0.61697000	-1.00789100
H	-4.19699800	-1.49145000	0.28579500
H	-4.62972500	-0.56219700	1.72427200
C	-6.11800600	-0.54022600	0.18363300
C	-6.51154500	-1.15428400	-1.00950000
C	-7.08205200	0.14520700	0.93031200
C	-7.83386400	-1.08989700	-1.44419700
H	-5.77149700	-1.69013900	-1.59954700
C	-8.40541400	0.21248800	0.50005900
H	-6.78941200	0.62736900	1.86050000
C	-8.78595000	-0.40616500	-0.68981900
H	-8.12179600	-1.57699700	-2.37126600

H	-9.14092700	0.74555400	1.09553000
H	-9.81735300	-0.35751800	-1.02539200
C	3.48384700	-1.69704800	-2.07957100
O	3.04234700	-0.65758500	-1.48389300
O	2.96529800	-2.83686000	-1.99171900
H	1.40319100	-2.63073100	-1.58248100
C	4.72954800	-1.50521500	-2.91094100
H	4.68808900	-0.54942400	-3.43647400
H	5.59210800	-1.48249000	-2.23639900
H	4.85384500	-2.32503100	-3.61835800

INT-8 (in TFE)

N	-0.84714000	2.66746300	1.98450100
C	-2.01965400	3.75828500	0.03626500
C	-3.05701300	4.65557500	-0.25277000
H	-3.64752400	5.03883600	0.57060500
C	-3.32920900	5.05480800	-1.55201600
H	-4.13711200	5.75194800	-1.74731300
C	-2.55747700	4.55206900	-2.59856100
H	-2.75504800	4.85181100	-3.62271200
C	-1.53463500	3.65798800	-2.32595100
H	-0.94080300	3.25868700	-3.14321300
C	-1.23671500	3.23971200	-1.01466200
C	-2.39557400	-2.19671700	-1.30768300
C	-1.35319700	-1.51519100	-2.06063700
C	-0.17671600	-2.33640900	-2.01370100
C	-0.45495600	-3.45715600	-1.16870500
C	-1.85257200	-3.38350200	-0.76990800
Rh	-0.71425500	-1.65219400	-0.03533000
C	-1.85907100	3.45916300	1.48374000
O	-2.62154900	3.95261700	2.30972700
C	-0.16955800	2.24803700	-0.92189300
C	0.39991800	1.57625600	0.09329200
C	-2.60101600	-4.36651000	0.07314800
H	-3.43011300	-4.78628800	-0.50575200
H	-1.95908900	-5.18939400	0.39074400
H	-3.02335100	-3.88531700	0.96089900
C	-3.79085200	-1.70405200	-1.11279600
H	-4.42901600	-2.08282900	-1.91893500
H	-4.19817800	-2.05248300	-0.16027500
H	-3.83004400	-0.61245200	-1.13353200
C	-1.54910200	-0.24840400	-2.82619400
H	-2.09420500	0.48840400	-2.22878300
H	-0.59333000	0.18470500	-3.12721600
H	-2.13462000	-0.45072200	-3.73004700
C	1.13845100	-2.08004500	-2.67050900
H	1.30028300	-2.82917500	-3.45305300
H	1.17456100	-1.09100500	-3.12927500
H	1.95601700	-2.16435100	-1.94844100
C	0.50759700	-4.55463400	-0.85642800
H	0.52954500	-5.27240400	-1.68412400
H	1.51740000	-4.15700600	-0.72544900
H	0.22424000	-5.09030700	0.05101400
O	-0.45186900	-2.22957700	2.13114300
C	-0.04060400	-3.54363300	2.47824400
H	-0.72423000	-4.30188400	2.08269700
H	0.95598300	-3.70168800	2.05914900
H	0.01400800	-3.64634700	3.56712200
H	0.21110500	1.97530600	-1.90467100
H	-0.89301600	2.63991800	3.00162600
C	0.12317100	1.78087400	1.52833200
O	0.76287600	1.20314500	2.40002000
O	1.12489600	-0.73561400	0.35073700
C	1.41742600	0.48162800	-0.24929200
C	2.85287700	0.91932600	0.08725800
H	1.37772000	0.39427100	-1.35392300
C	3.88600300	-0.09966300	-0.40753100
H	3.04712400	1.88991800	-0.38743500
H	2.95421700	1.05273000	1.16980600
H	3.70737400	-1.05883800	0.08952300
H	3.74448500	-0.25659200	-1.48469700
C	5.29814400	0.35919000	-0.14291200
C	5.90181300	0.12773000	1.09772800
C	6.01485800	1.06955000	-1.11090500
C	7.18877900	0.58995900	1.36319900
H	5.35503100	-0.42338300	1.85969300
C	7.30309100	1.53300900	-0.85063600
H	5.55696600	1.25653000	-2.07968600
C	7.89460600	1.29414600	0.38842800
H	7.64298900	0.39760500	2.33084400
H	7.84613400	2.07842900	-1.61701200
H	8.89909800	1.65208200	0.59266000
C	-2.79782600	-0.28785900	1.75288900
O	-1.91589800	-0.00245700	0.88246500
O	-2.88304500	-1.39453000	2.34983700
H	-1.41221100	-2.06047400	2.36165700
C	-3.78561100	0.80134600	2.10880900
H	-3.38104900	1.37858100	2.94737600
H	-3.94184100	1.48014300	1.26798700
H	-4.73358600	0.36156200	2.42320000

PC1 (in TFE)

N	-2.13262400	1.93321800	-0.54862400
C	-3.70704500	-0.04424200	-0.50288600
C	-4.96081100	-0.44989700	-0.97734700
H	-5.52874900	0.24469400	-1.58433600
C	-5.47578700	-1.70395300	-0.68534000
H	-6.45004600	-1.99124800	-1.06625900
C	-4.73304400	-2.58434700	0.09821900
H	-5.11933700	-3.56954500	0.33820200

C	-3.49077000	-2.19499800	0.57360300
H	-2.91287000	-2.88171100	1.18444800
C	-2.94632100	-0.92885800	0.29030400
C	-3.32504100	1.33228700	-0.91481100
O	-4.07297700	2.00774600	-1.61016600
C	-1.62901700	-0.69356400	0.87291600
C	-0.77795000	0.34708600	0.84674700
H	-1.27462000	-1.55248600	1.44076100
H	-2.07757200	2.87467700	-0.93459200
C	-0.98870700	1.63467600	0.16577100
O	-0.13157600	2.51689000	0.21191800
O	0.80848700	1.28308000	2.45048000
C	0.56921400	0.21370600	1.55008000
C	1.71655000	0.03314600	0.55037000
H	0.52112200	-0.68395900	2.17606600
C	3.06527900	-0.15476800	1.25550300
H	1.50016200	-0.84379800	-0.07130300
H	1.76654900	0.90217300	-0.11592000
H	3.27165000	0.72718600	1.86995500
H	3.00137700	-1.01599100	1.93113100
C	4.18218100	-0.36450800	0.26393800
C	4.82791300	0.72927300	-0.32186500
C	4.55884200	-1.65196500	-0.13007700
C	5.82701400	0.54226300	-1.27436500
H	4.54466700	1.73613000	-0.02319300
C	5.55879000	-1.84416700	-1.08154100
H	4.06467600	-2.51084800	0.31834900
C	6.19599100	-0.74654900	-1.65733800
H	6.32037300	1.40314700	-1.71596000
H	5.84191700	-2.85180700	-1.37151700
H	6.97684200	-0.89400200	-2.39713500
H	0.84705800	2.08939500	1.91253100

TS-6 (in TFE)

N	2.48500800	1.03588400	-0.82411300
C	1.00354900	2.78744500	-0.10115500
C	0.99787700	3.75413200	0.91018400
H	1.94968800	4.10874800	1.29468700
C	-0.19650500	4.26171700	1.40780100
H	-0.18631400	5.00139500	2.20210100
C	-1.40176400	3.83084300	0.85745800
H	-2.34317700	4.23753200	1.21408700
C	-1.39965100	2.88986700	-0.16858000
H	-2.34214700	2.59173500	-0.61858100
C	-0.21027800	2.33280200	-0.65376400
C	2.58278900	-2.12912200	0.44213500
C	3.10195300	-1.21740900	1.43624000
C	2.03312500	-0.91797100	2.31207400
C	0.87223500	-1.72301600	1.94343000
C	1.23023900	-2.51324500	0.82922700
Rh	1.40469600	-0.38970100	0.27792100
C	2.36640300	2.34837100	-0.57920200
O	3.27693800	3.19008900	-0.69558200
C	-0.26121700	1.28760100	-1.74826600
C	-0.16501300	-0.15445300	-1.23927500
C	0.44107400	-3.58906800	0.15941000
H	0.96963200	-4.54015100	0.28487300
H	-0.55203000	-3.69375300	0.60123400
H	0.33002900	-3.41020200	-0.91449500
C	3.33187500	-2.70106500	-0.71255700
H	3.91977800	-3.56397000	-0.37857500
H	2.64378200	-3.03290100	-1.49329700
H	4.01540000	-1.96163000	-1.13741600
C	4.48739000	-0.66037700	1.50774900
H	5.02026800	-1.12316100	2.34509200
H	5.04122700	-0.86610800	0.59157400
H	4.47537700	0.42065800	1.66873300
C	2.04105700	0.06805600	3.42896500
H	2.01406200	-0.46181900	4.38772700
H	2.93461300	0.69397300	3.40141800
H	1.15605900	0.71049700	3.38180100
C	-0.43015900	-1.69829600	2.67512500
H	-0.33443900	-2.23239500	3.62677200
H	-0.72788600	-0.66966700	2.89877500
H	-1.22463300	-2.17124200	2.09372600
O	3.79959100	0.67252600	-1.16100600
C	3.98020600	0.77069200	-2.56928100
H	5.00353900	0.44116100	-2.76469900
H	3.27110400	0.12392900	-3.09469300
H	3.86048000	1.80705000	-2.90425400
H	0.57219700	1.43580800	-2.44048100
H	-1.18664300	1.42120200	-2.32390500
C	0.10252100	-1.15634100	-2.35085800
O	1.11068700	-1.17878400	-3.06605900
O	-0.92192300	-1.93788700	-2.45666100
C	-1.33332900	-0.80062600	-0.70995100
C	-2.68861500	-0.24496800	-0.53357900
H	-1.19020100	-1.76651300	-0.23728700
C	-3.76294900	-1.34134600	-0.48141600
H	-2.65500200	0.28565500	0.43500900
H	-2.91800200	0.50763400	-1.29437500
H	-3.78244100	-1.85298400	-1.44912300
H	-3.47972800	-2.07941000	0.27744300
C	-5.12123300	-0.76857200	-0.16313500
C	-5.97130500	-0.33517300	-1.18414600
C	-5.53254900	-0.61791100	1.16465200
C	-7.20813100	0.23336500	-0.88571600
H	-5.66096200	-0.44895800	-2.22012500
C	-6.76841800	-0.05100900	1.46690900
H	-4.87837800	-0.95419000	1.96617700

C	-7.61008600	0.37645800	0.44106100
H	-7.85950600	0.56189000	-1.69004000
H	-7.07618400	0.05350600	2.50307900
H	-8.57484800	0.81620200	0.67462000

INT-9 (in TFE)

N	2.40341100	0.98683500	-0.43309700
C	0.86893600	2.58394900	0.51466200
C	0.66493300	3.18013300	1.76382700
H	1.51119200	3.26774900	2.43902900
C	-0.58469700	3.65801000	2.14000200
H	-0.72728300	4.10238400	3.11996700
C	-1.64038600	3.57934400	1.23646100
H	-2.61954700	3.96760600	1.49940500
C	-1.43345700	3.02297400	-0.02309600
H	-2.25234100	3.01187700	-0.73698700
C	-0.19352000	2.49939200	-0.40768400
C	2.45846300	-2.00607300	1.15400900
C	1.96107400	-0.92280600	1.96861700
C	0.53668700	-0.99407200	1.96175200
C	0.14964400	-2.18655400	1.21963300
C	1.32237200	-2.80400400	0.72885400
Rh	1.26008300	-0.77033300	-0.06243400
C	2.28387300	2.14418300	0.23751700
O	3.23314300	2.84751700	0.62780800
C	-0.02922500	1.95648800	-1.81952600
C	0.04518300	0.44570300	-1.93698700
C	1.41595200	-4.02107200	-0.12818000
H	1.67963600	-4.88660000	0.48921300
H	0.46760700	-4.22941200	-0.62720200
H	2.19274600	-3.90015700	-0.88767100
C	3.88584000	-2.33097600	0.86673300
H	4.18326900	-3.21175200	1.44632200
H	4.02273500	-2.56041000	-0.19392600
H	4.54205000	-1.50078600	1.13204300
C	2.80918800	0.10486800	2.63967400
H	3.20022000	-0.31240900	3.57392300
H	3.65558300	0.39114100	2.01069800
H	2.23524500	1.00230400	2.87836100
C	-0.42648000	-0.08650100	2.65476000
H	-0.96234600	-0.64597700	3.42911900
H	0.08452600	0.75376000	3.12582000
H	-1.17061400	0.31085100	1.95585900
C	-1.25332000	-2.66760600	1.06590200
H	-1.48779500	-3.34320700	1.89667900
H	-1.96107900	-1.83659500	1.10581200
H	-1.39355400	-3.21705600	0.13279300
O	3.75193200	0.61022800	-0.60174600
C	4.28926200	1.22295900	-1.76920900
H	5.30633100	0.83692800	-1.86901100
H	3.70044000	0.95586800	-2.65241000
H	4.32063900	2.31193000	-1.65647100
H	0.87995100	2.36689100	-2.26765200
H	-0.87507600	2.31326000	-2.41882500
C	1.21009400	-0.13631900	-2.71365000
O	1.52969400	0.36125800	-3.79564300
O	1.78098500	-1.14383100	-2.14602100
C	-0.93092400	-0.41522200	-1.55375300
C	-2.27248000	-0.03210200	-0.99797600
H	-0.78813900	-1.47410700	-1.77982200
C	-3.36517000	-1.03749100	-1.39375600
H	-2.22846400	0.04121100	0.09732600
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H	-3.48178700	-1.02167100	-2.48357600
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C	-4.67630800	-0.71171800	-0.72338800
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H	-4.50041200	-2.25768200	0.76129300
C	-7.06393800	-0.03104600	0.58803300
H	-7.25242900	1.51175800	-0.90368700
H	-6.60459300	-1.65821100	1.92185700
H	-7.98811300	0.23118400	1.09390000

PC2 (in TFE)

N	-3.05481600	0.01228500	-0.89583800
C	-1.75353500	1.84284900	0.05175600
C	-1.50528200	3.12796500	-0.44378500
H	-2.23950000	3.58717400	-1.09899700
C	-0.34323200	3.80923100	-0.10631700
H	-0.15580200	4.79948600	-0.50826600
C	0.56254100	3.21460500	0.76780600
H	1.46674900	3.73897300	1.06077800
C	0.30072800	1.94973000	1.28423700
H	0.99605300	1.50961700	1.99346700
C	-0.84505600	1.22756600	0.93197400
C	-3.07623200	1.27047500	-0.36689700
O	-4.11894900	1.90301100	-0.25340600
C	-1.09354400	-0.12083000	1.58800100
C	-0.93327100	-1.33094000	0.68905300
O	-4.20617800	-0.37591300	-1.55576100
C	-5.06353000	-1.11759200	-0.68656900
H	-5.99846800	-1.22913100	-1.23824900
H	-4.64137300	-2.10160700	-0.46659500
H	-5.24441400	-0.56695200	0.24066300
H	-2.10538500	-0.14055700	2.00302800
H	-0.40532600	-0.21063600	2.43582900

C	-2.09495800	-2.25815500	0.65886500
O	-2.96097100	-2.28661800	1.51343200
O	-2.11619800	-3.07793200	-0.40065000
C	0.16916100	-1.64980700	-0.00497400
C	1.46462200	-0.89711500	0.00153600
H	0.14307700	-2.55117400	-0.61527700
C	2.65551800	-1.80668400	-0.33653100
H	1.41818700	-0.07844000	-0.73097100
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H	2.70486000	-2.61856200	0.39741600
H	2.48757300	-2.26407700	-1.31799800
C	3.95471100	-1.04069000	-0.34243500
C	4.69549700	-0.88363700	0.83306900
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C	5.87229400	-0.13787000	0.83999300
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C	5.59285900	0.31714200	-1.50973900
H	3.84952300	-0.54550900	-2.43282400
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H	6.43790700	-0.02975400	1.76073500
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H	-2.21246000	-0.34103200	-1.34165300
H	-2.85973800	-3.69593600	-0.2941400

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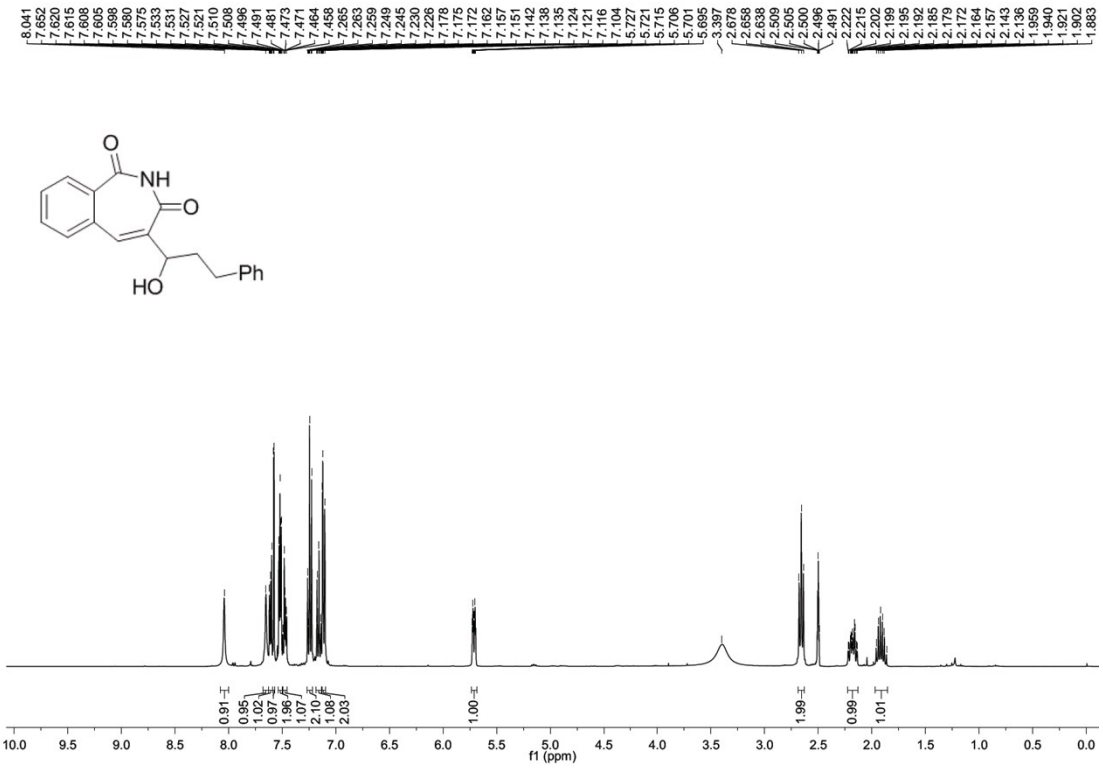
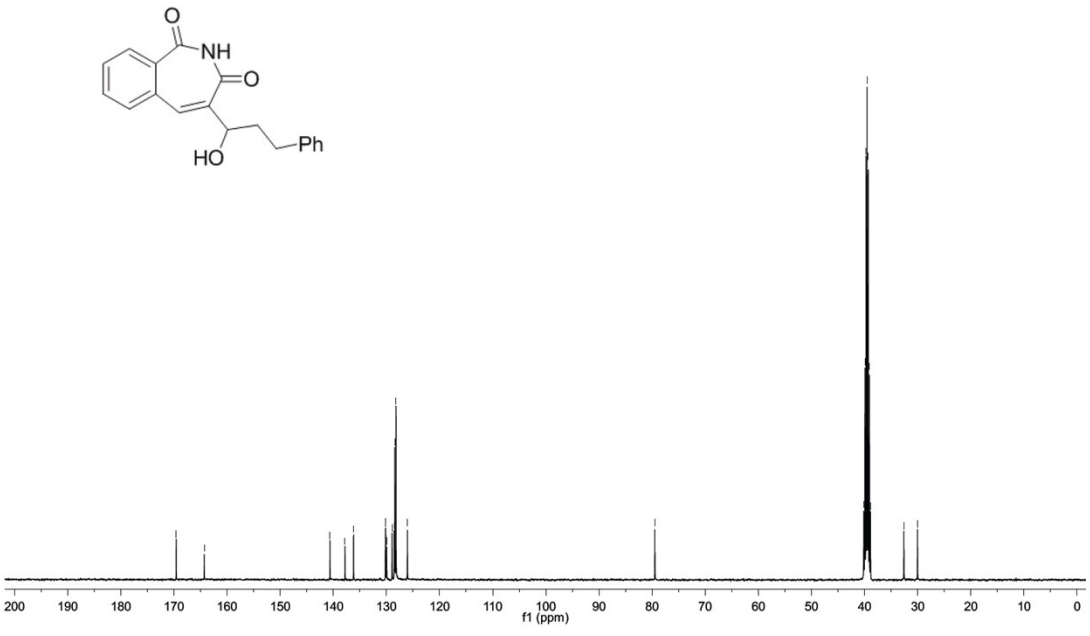
V. Copies of ^{1}H and ^{13}C NMR spectra

3a





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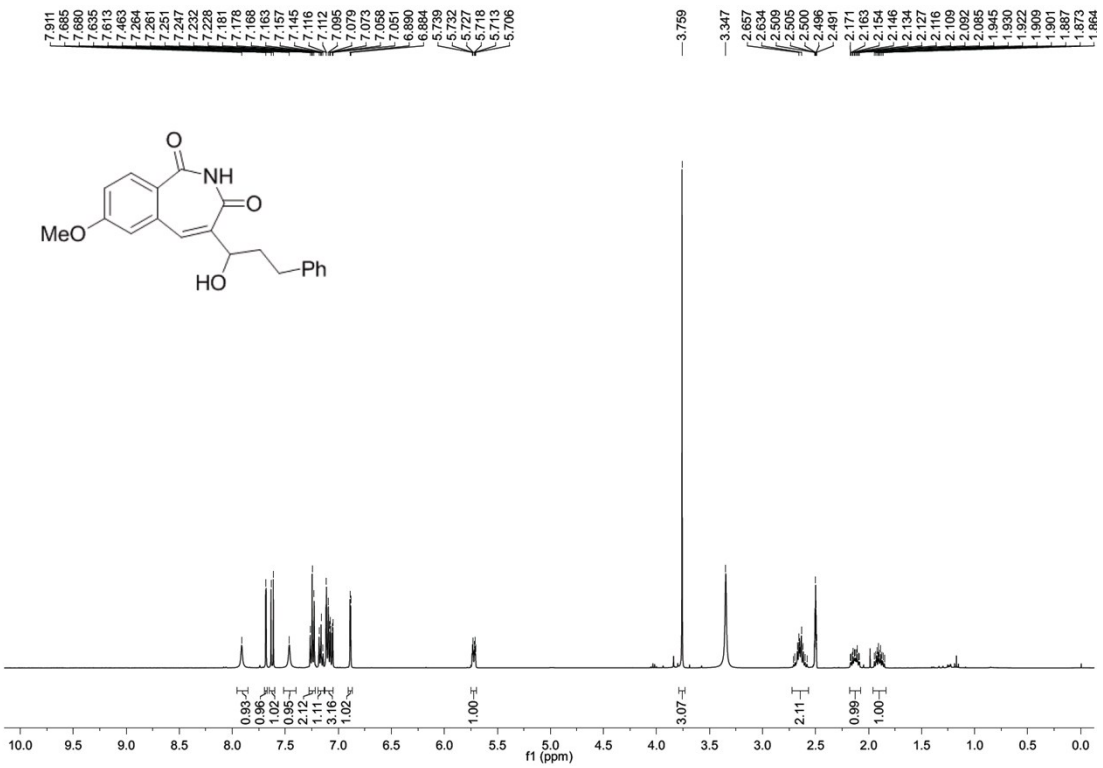
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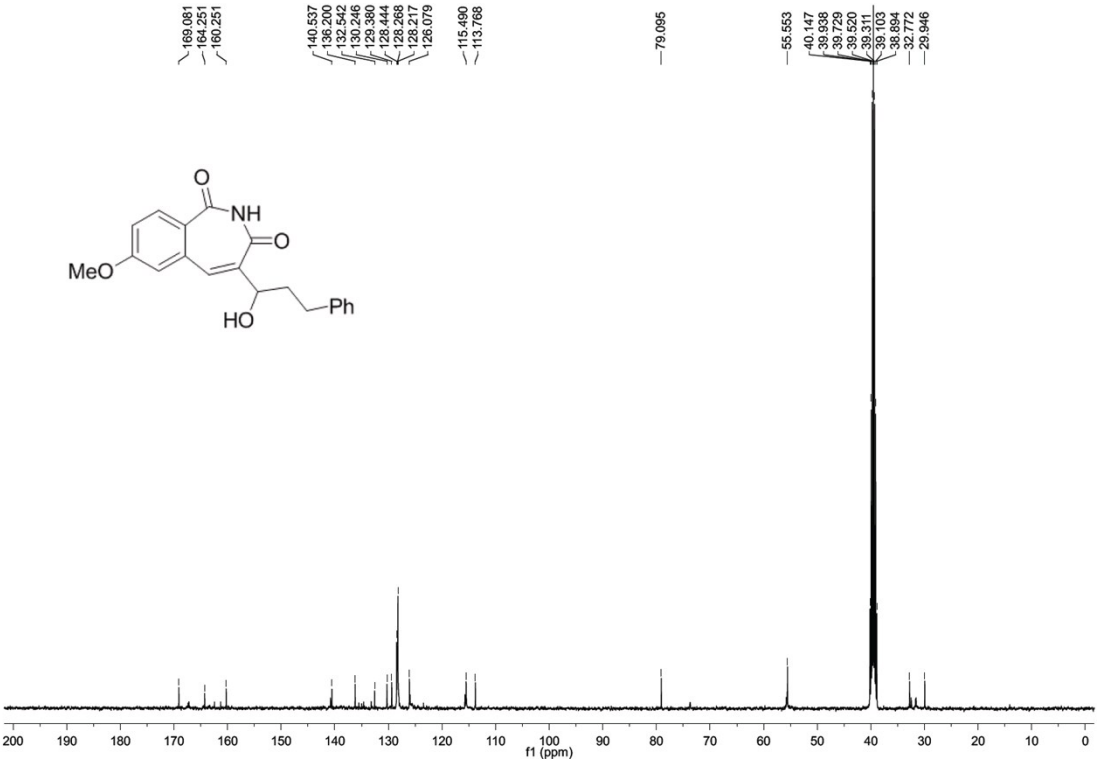
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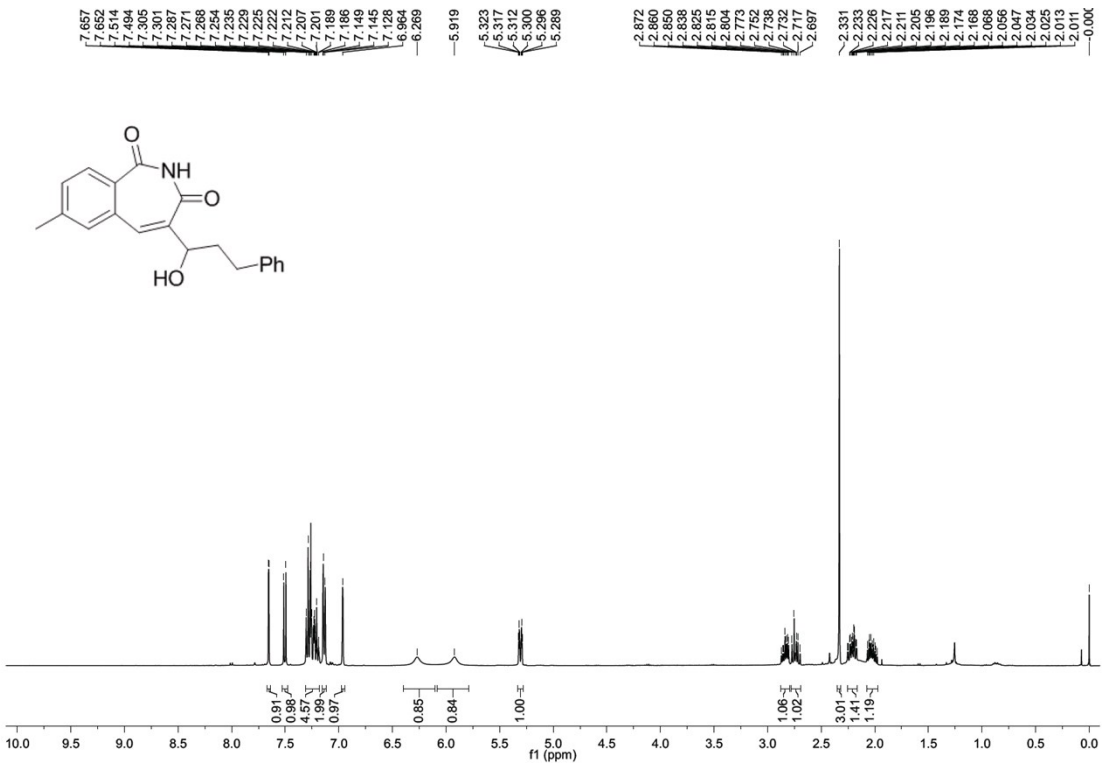
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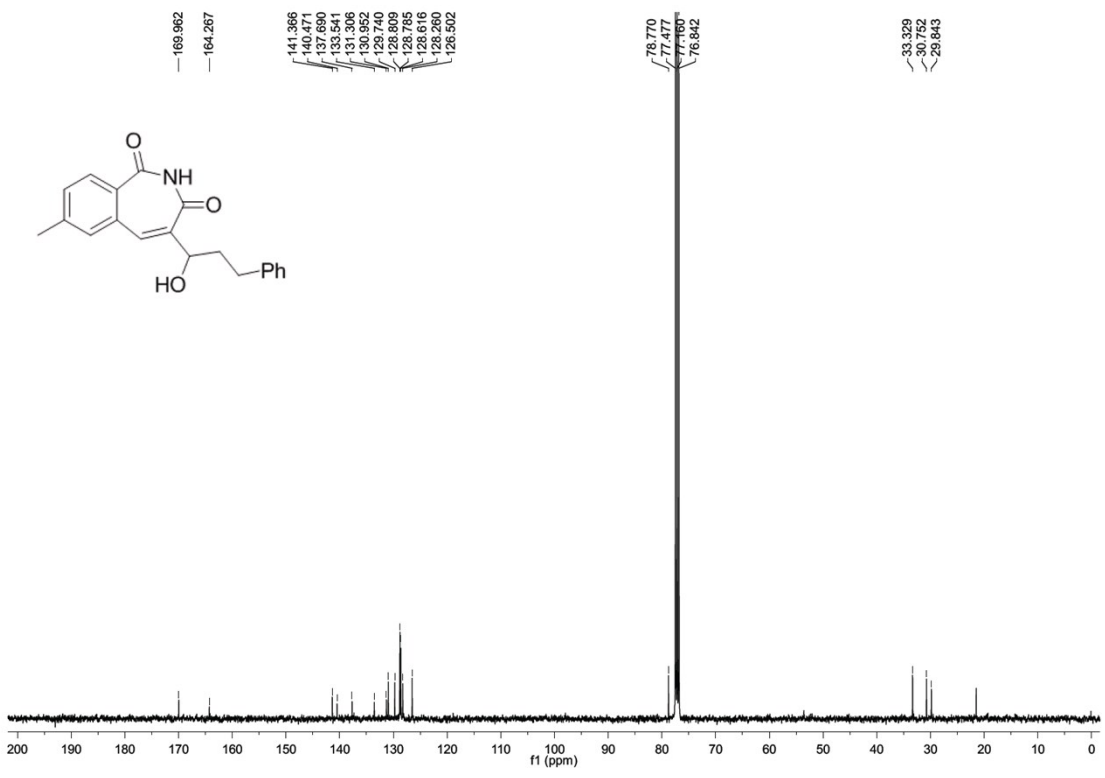
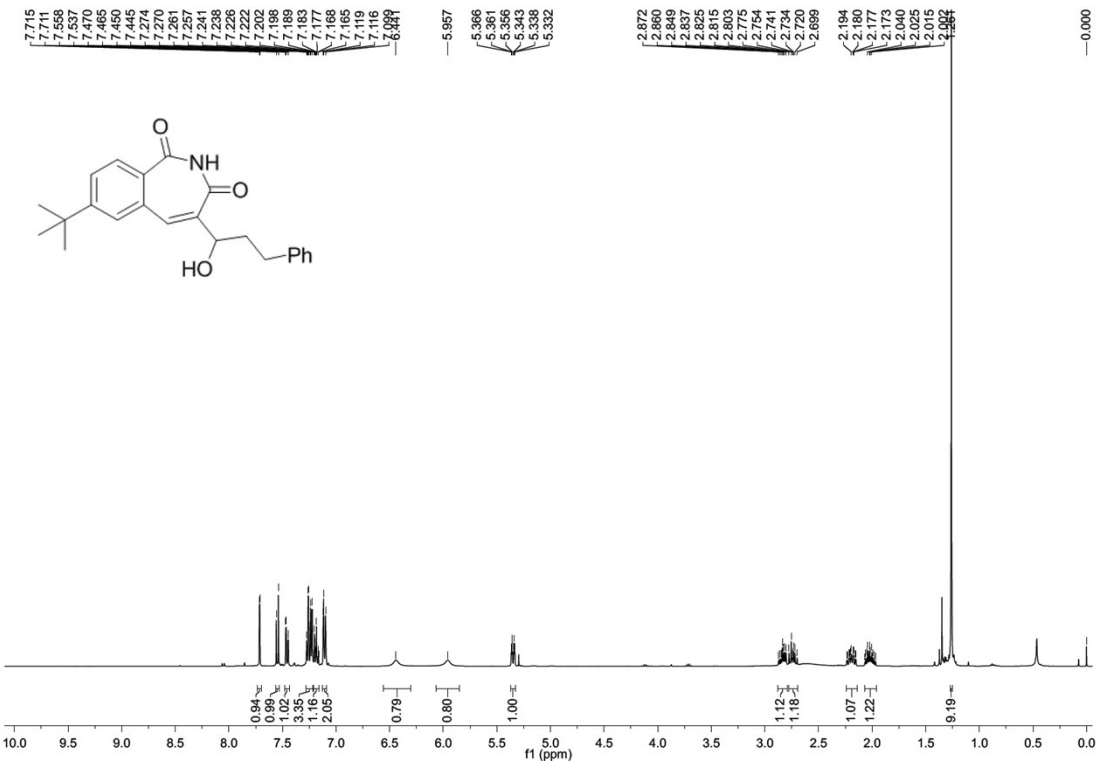
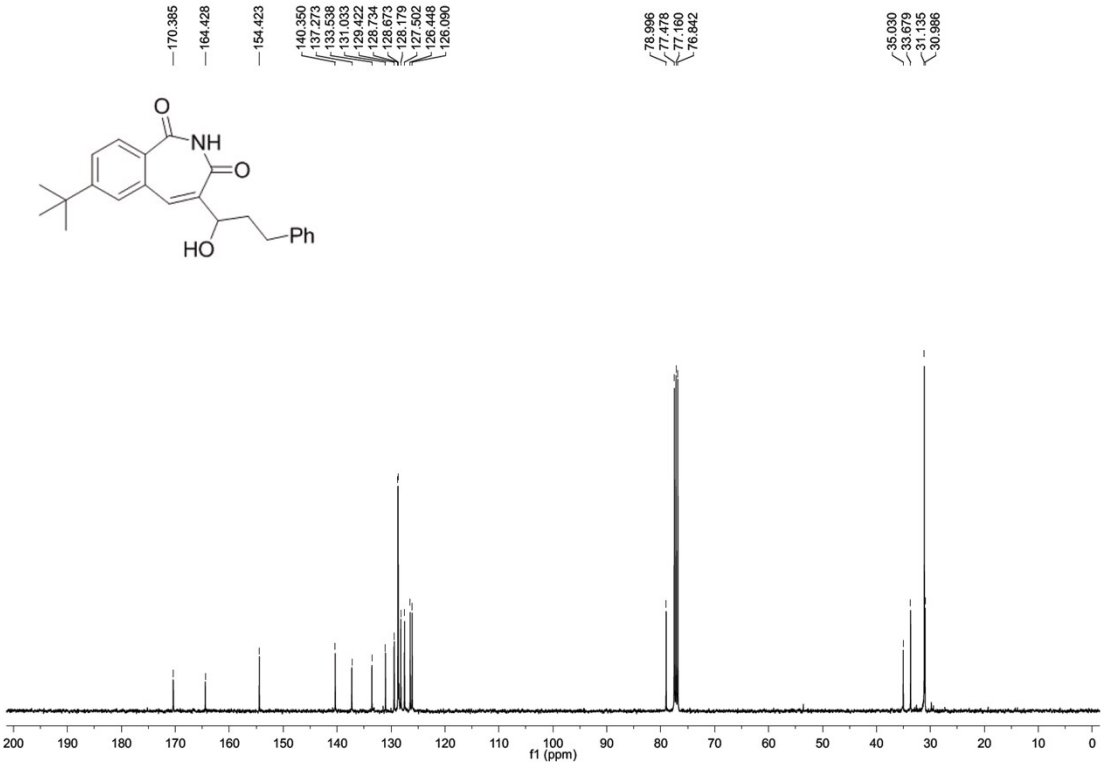
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

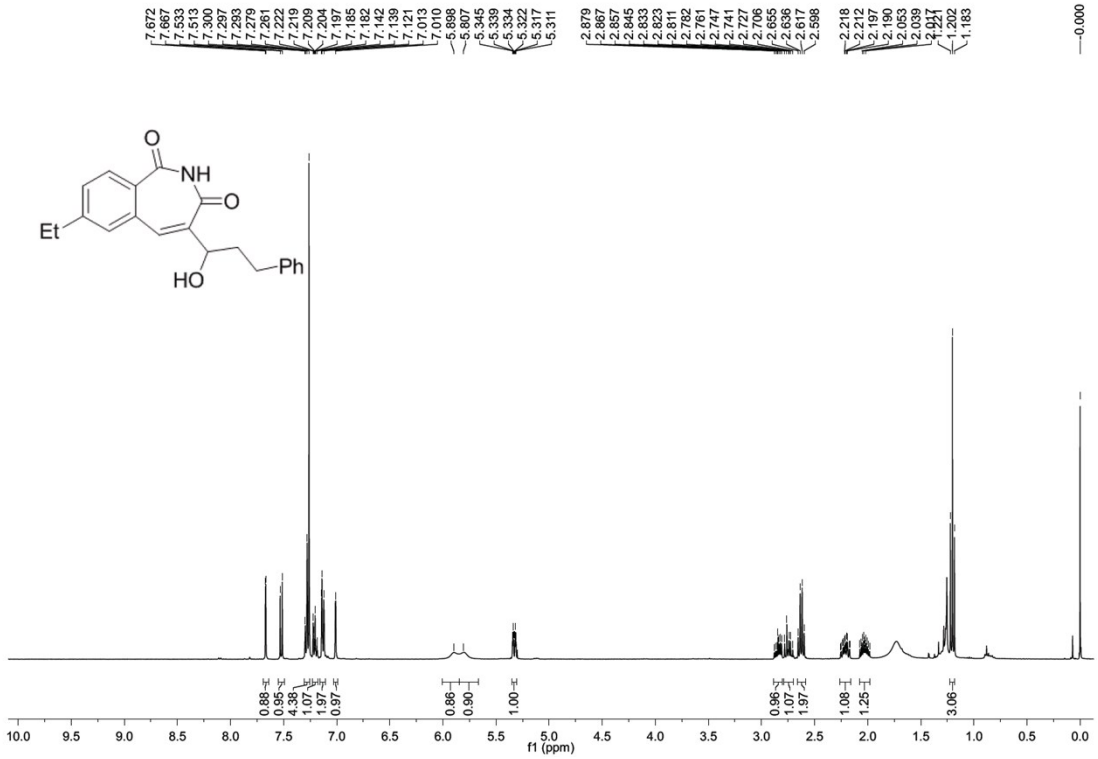

169.962
164.267
141.366
140.471
137.690
133.541
131.306
130.952
129.740
128.809
128.785
128.616
128.260
126.502
78.770
77.477
77.160
76.842
33.329
30.752
29.843
O
NH
O
HO
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3d


7.715
7.711
7.558
7.537
7.470
7.465
7.450
7.445
7.274
7.270
7.261
7.257
7.241
7.238
7.226
7.222
7.202
7.198
7.189
7.183
7.177
7.168
7.165
7.119
7.116
7.099
6.441
5.957
5.366
5.361
5.356
5.343
5.338
5.332
2.872
2.860
2.849
2.837
2.825
2.815
2.803
2.775
2.754
2.741
2.734
2.720
2.699
2.194
2.180
2.177
2.173
2.040
2.025
2.015
1.982
1.261
0.000
O
NH
O
HO
Ph
0.94
0.99
1.02
3.35
1.16
2.05
0.79
0.80
1.00
1.12
1.18
1.07
1.22
9.19
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
f1 (ppm)


170.385
164.428
154.423
140.350
137.273
133.538
131.033
129.422
128.734
128.673
128.179
127.502
126.448
126.090
78.996
77.478
77.160
76.842
35.030
33.679
31.135
30.986
O
NH
O
HO
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3e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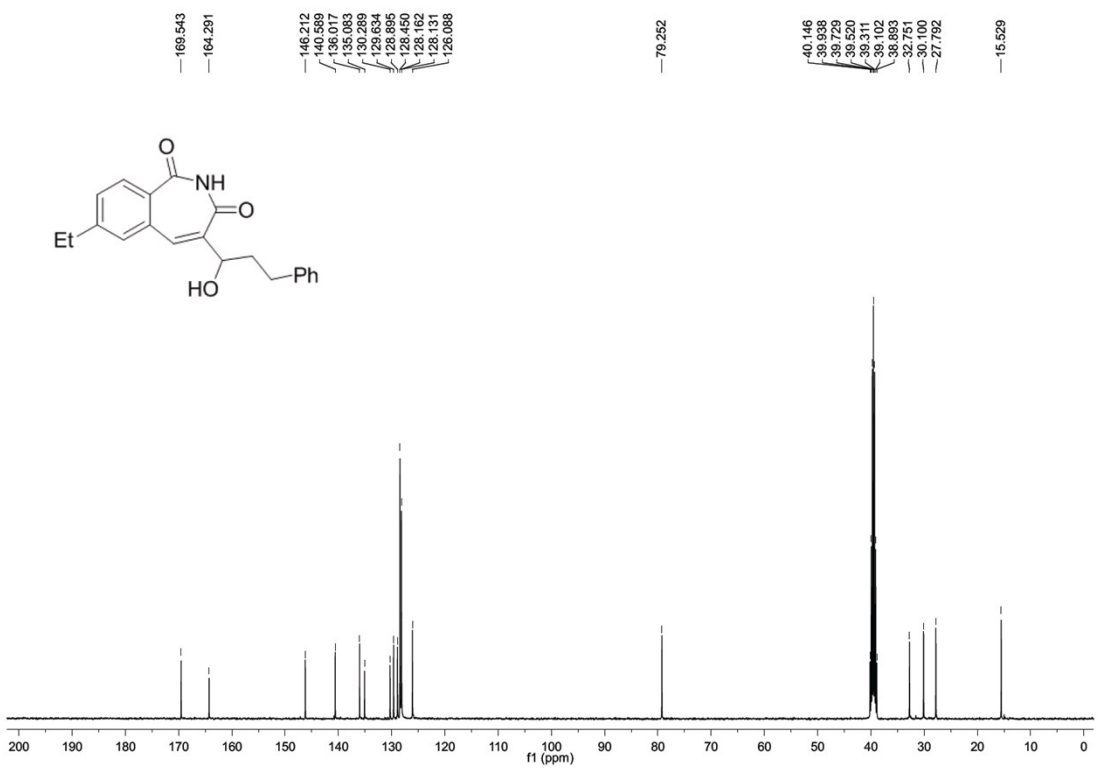
7.667
7.533
7.513
7.300
7.297
7.293
7.279
7.261
7.222
7.219
7.209
7.204
7.197
7.185
7.182
7.142
7.139
7.121
7.013
7.010
5.898
5.807
5.345
5.339
5.334
5.322
5.317
5.311
2.879
2.867
2.857
2.845
2.833
2.823
2.811
2.782
2.761
2.747
2.741
2.727
2.706
2.655
2.636
2.617
2.598
2.218
2.212
2.197
2.190
2.053
2.039
2.021
1.221
1.202
1.183
0.000
O
NH
O
Et
HO
Ph
0.88
0.95
4.38
1.07
1.97
0.97
0.86
0.90
1.00
0.96
1.07
1.97
1.08
1.25
3.06
f1 (ppm)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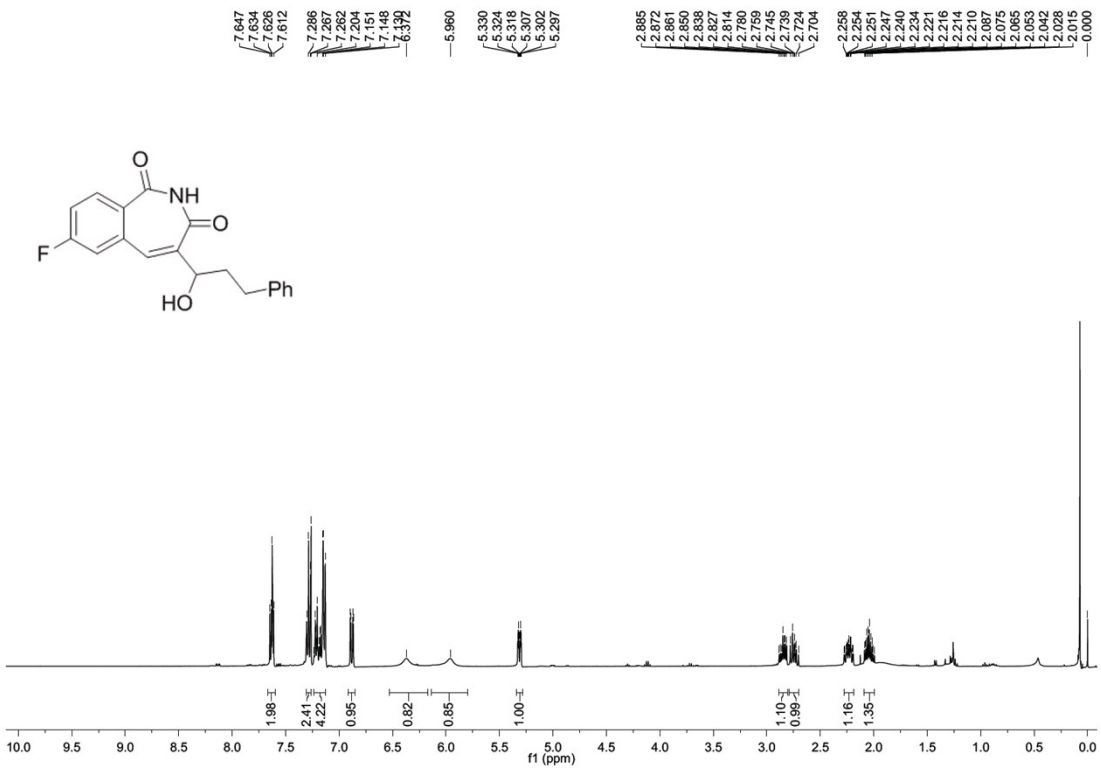
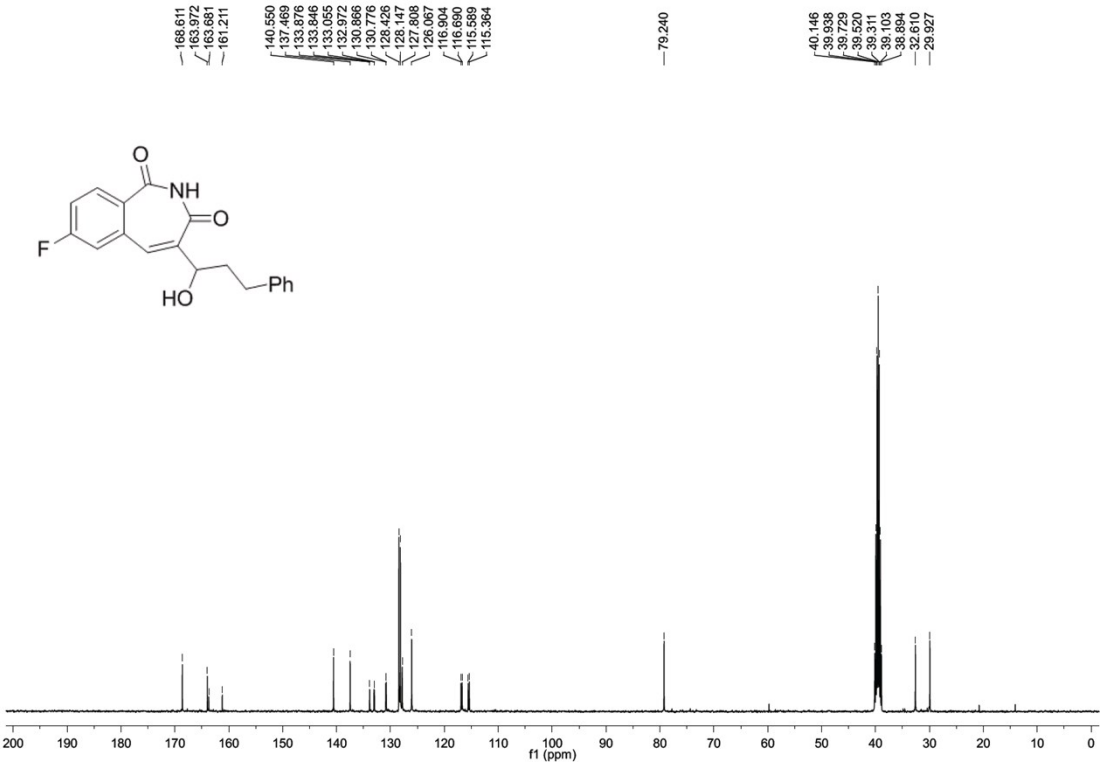
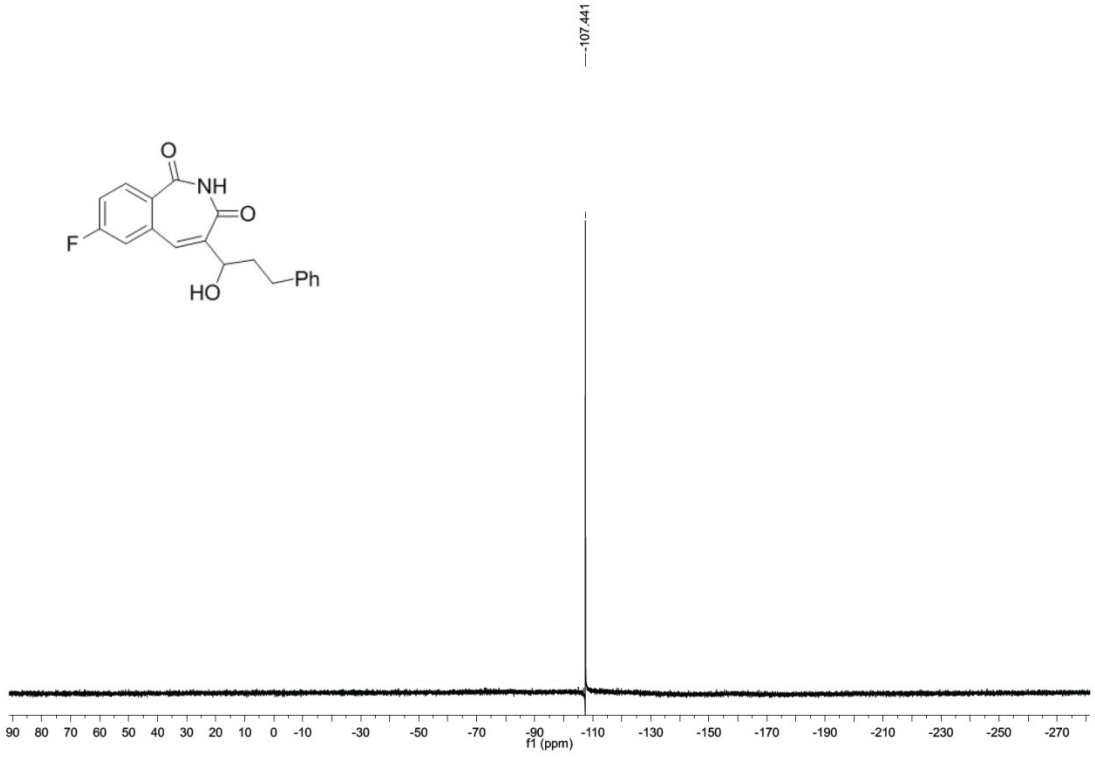
164.291
146.212
140.589
136.017
135.083
130.289
129.634
128.895
128.450
128.162
128.131
126.088
79.252
40.146
39.938
39.729
39.520
39.311
39.102
38.893
32.751
30.100
27.792
15.529
O
NH
O
Et
HO
Ph
f1 (ppm)

3f

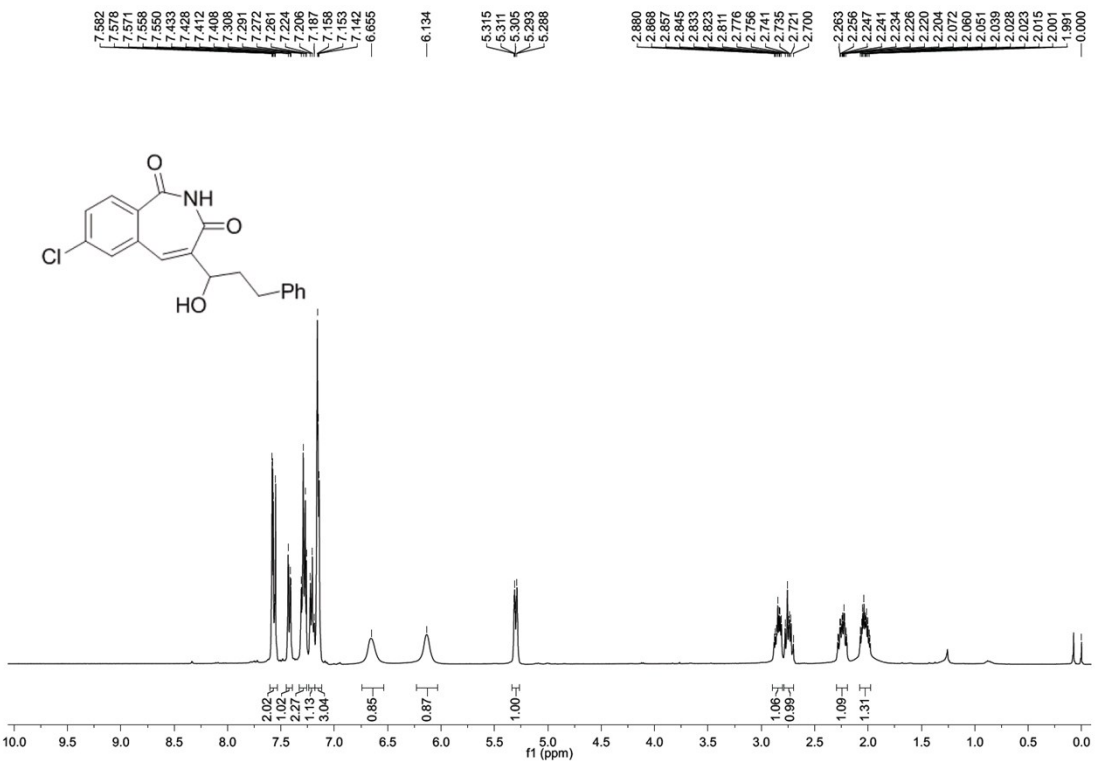

7.647
7.634
7.626
7.612
7.286
7.267
7.262
7.204
7.151
7.148
7.130
6.312
5.960
5.330
5.324
5.318
5.307
5.302
5.297
2.885
2.872
2.861
2.850
2.838
2.827
2.814
2.780
2.759
2.745
2.739
2.724
2.704
2.258
2.254
2.251
2.247
2.240
2.234
2.221
2.216
2.214
2.210
2.087
2.075
2.065
2.053
2.042
2.028
2.015
0.000
O
NH
O
F
HO
Ph
1.98
2.41
4.22
0.95
0.82
0.85
1.00
1.10
0.99
1.16
1.35
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
f1 (ppm)

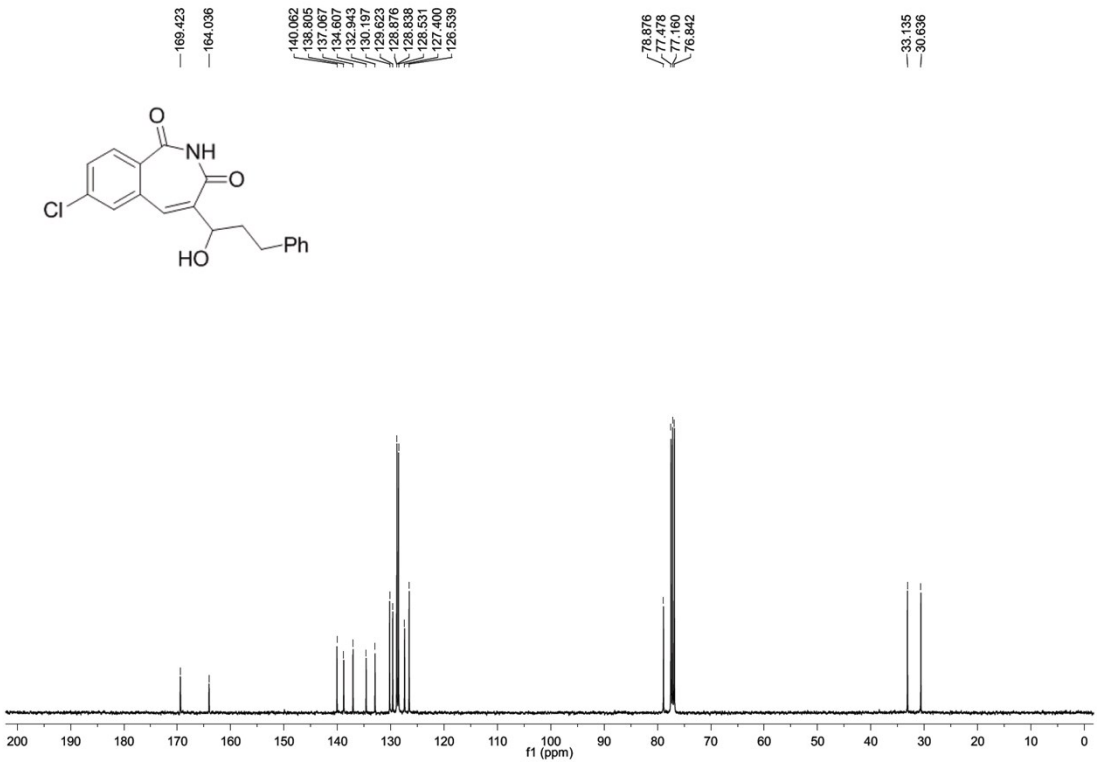

168.611
163.972
163.681
161.211
140.550
137.469
133.876
133.846
133.055
132.972
130.866
130.776
128.426
128.147
127.808
126.067
116.904
116.690
115.589
115.364
79.240
40.146
39.938
39.729
39.520
39.311
39.103
38.894
32.610
29.927
O
NH
O
F
HO
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

^{19}F spectrum of 3f

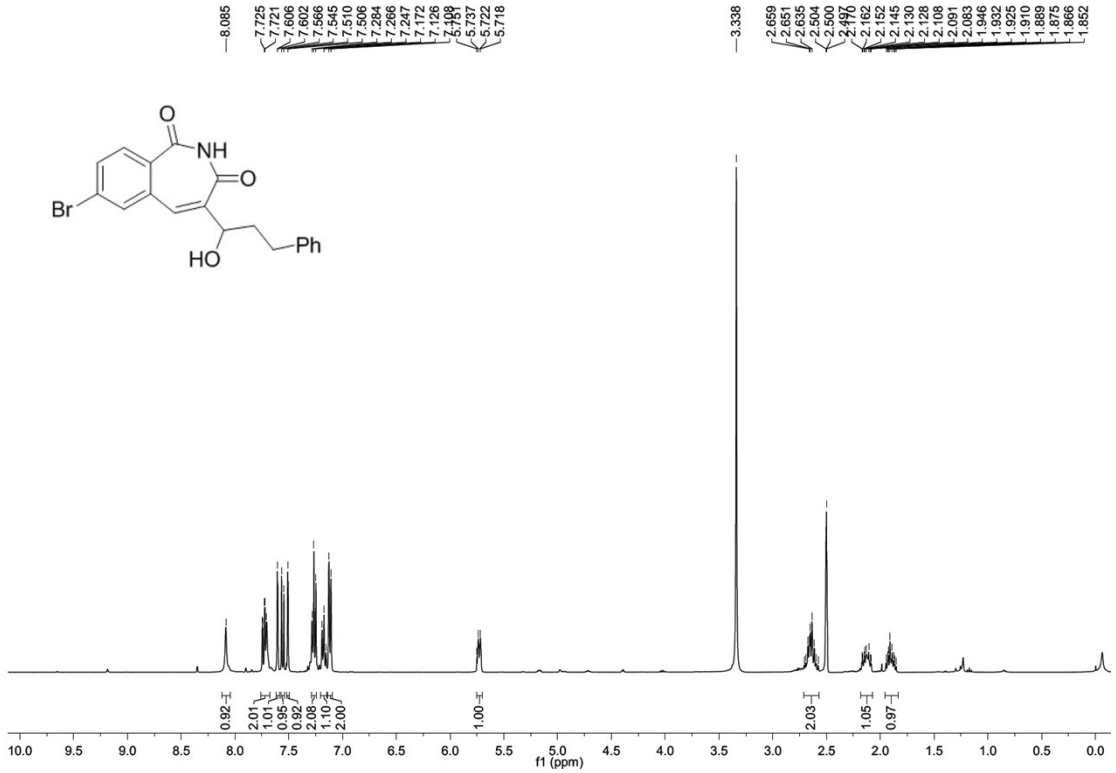


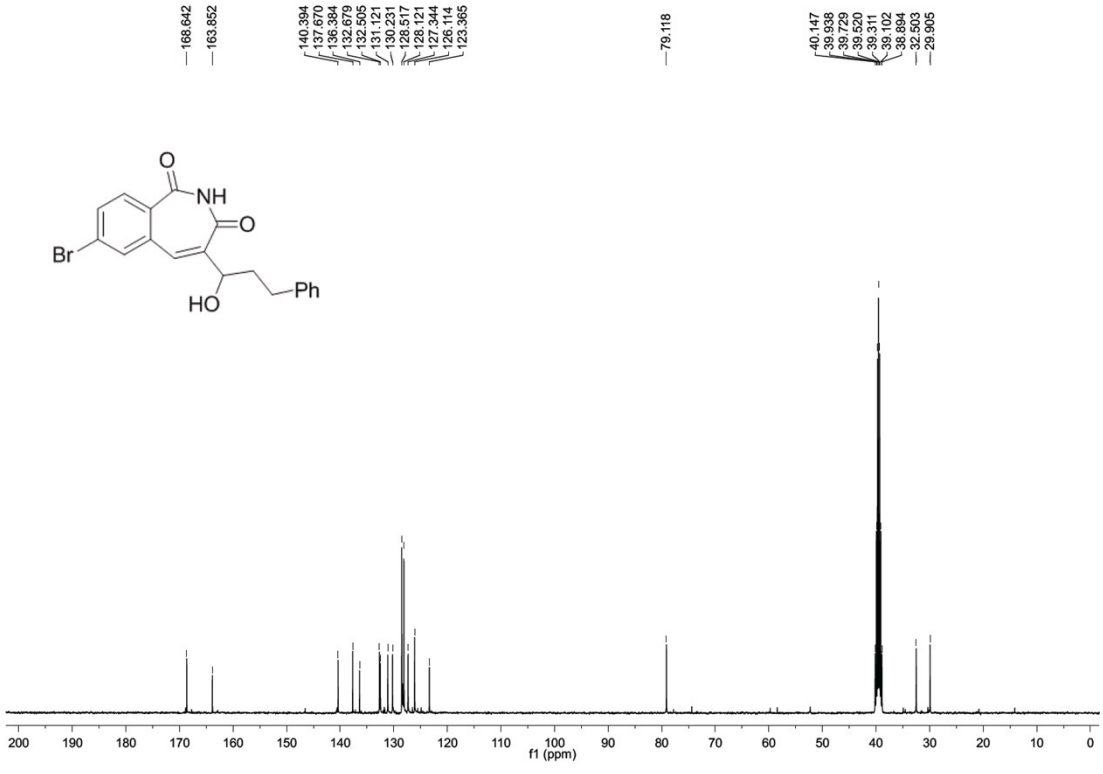
3g


7.582
7.578
7.571
7.558
7.550
7.433
7.428
7.412
7.408
7.308
7.291
7.272
7.261
7.224
7.206
7.187
7.158
7.153
7.142
6.655
6.134
5.315
5.311
5.305
5.293
5.288
2.880
2.868
2.857
2.845
2.833
2.823
2.811
2.776
2.756
2.741
2.735
2.721
2.700
2.263
2.256
2.247
2.241
2.234
2.226
2.220
2.204
2.072
2.060
2.051
2.039
2.028
2.023
2.015
2.001
1.991
0.000
O
NH
O
Cl
HO
Ph
2.02
1.02
2.27
1.13
3.04
0.85
0.87
1.00
1.06
0.99
1.09
1.31
f1 (ppm)

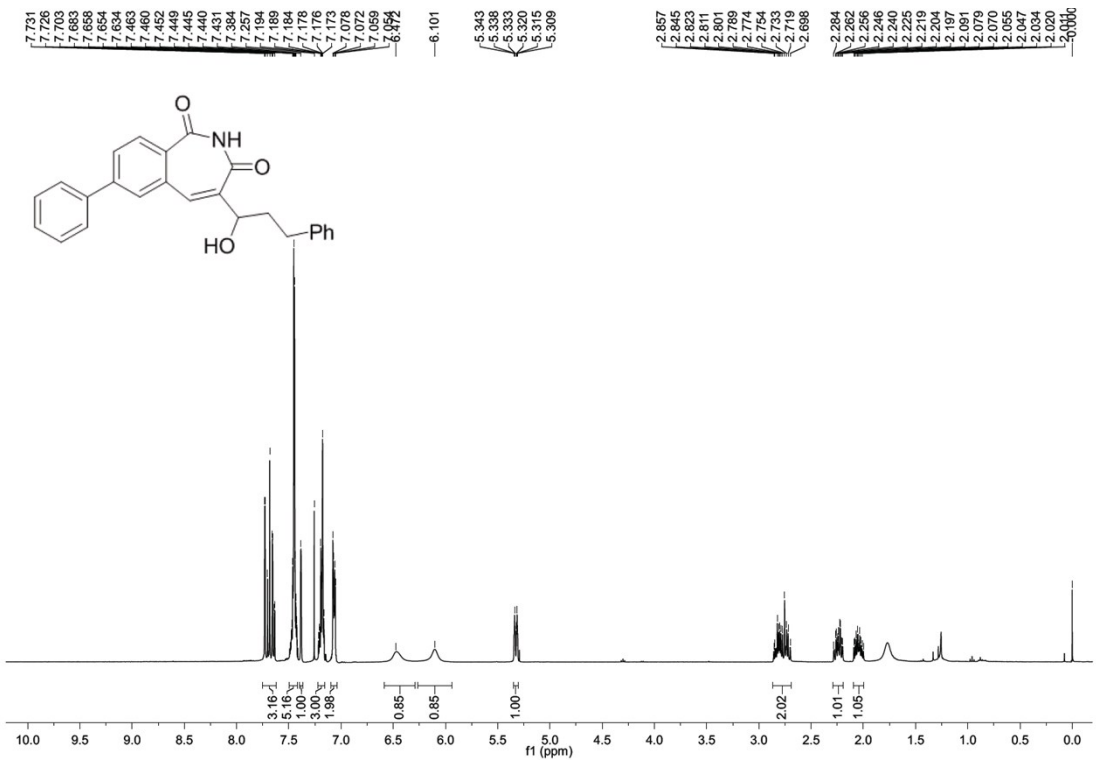

169.423
164.036
140.062
138.805
137.067
134.607
132.943
130.197
129.623
128.876
128.838
128.531
127.400
126.539
78.876
77.478
77.160
76.842
33.135
30.636
O
NH
O
Cl
HO
Ph
f1 (ppm)

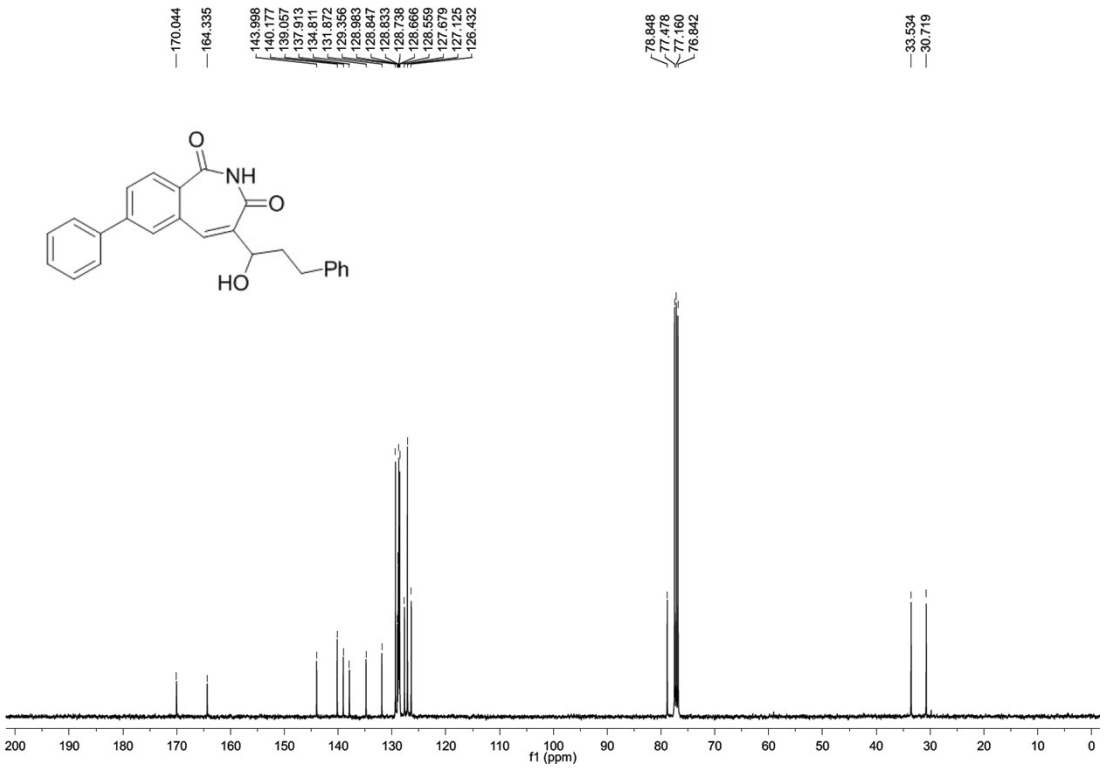
3h


8.085
7.725
7.721
7.606
7.602
7.566
7.545
7.510
7.506
7.284
7.266
7.247
7.172
7.126
5.737
5.722
5.718
3.338
2.659
2.651
2.635
2.504
2.500
2.162
2.152
2.145
2.130
2.128
2.108
2.091
2.083
1.946
1.932
1.925
1.910
1.889
1.875
1.866
1.852
O
NH
O
Br
HO
Ph
0.92
2.01
1.01
0.95
0.92
2.08
1.10
2.00
1.00
2.03
1.05
0.97
f1 (ppm)

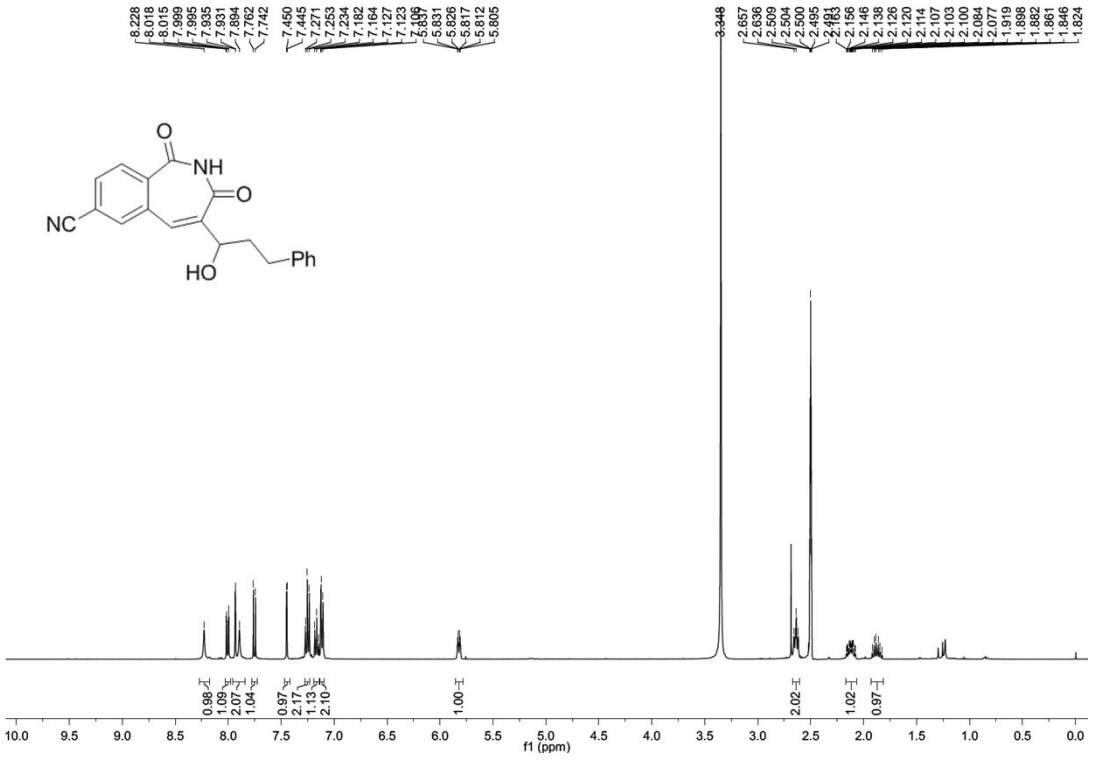

168.642
163.852
140.394
137.670
136.384
132.679
132.505
131.121
130.231
128.517
128.121
127.344
126.114
123.365
79.118
40.147
39.938
39.729
39.520
39.311
39.102
38.894
32.503
29.905
O
NH
O
Br
HO
Ph
f1 (ppm)

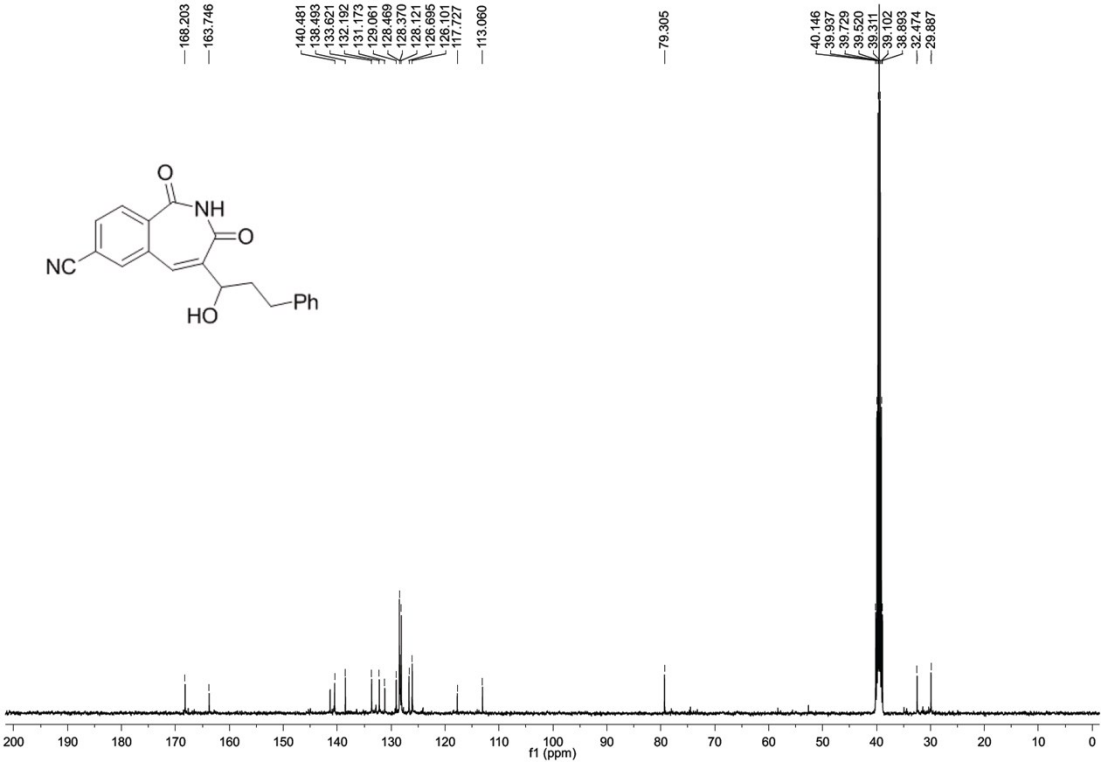
3i


7.731
7.726
7.703
7.683
7.658
7.654
7.634
7.463
7.460
7.452
7.449
7.445
7.440
7.431
7.384
7.257
7.194
7.189
7.184
7.178
7.176
7.173
7.078
7.072
7.059
7.054
6.472
6.101
5.343
5.338
5.333
5.320
5.315
5.309
2.857
2.845
2.823
2.811
2.801
2.789
2.774
2.754
2.733
2.719
2.698
2.284
2.262
2.256
2.246
2.240
2.225
2.219
2.204
2.197
2.091
2.079
2.070
2.055
2.047
2.034
2.020
2.000
O
NH
O
HO
Ph
3.16
5.16
1.00
3.00
1.98
0.85
0.85
1.00
2.02
1.01
1.05
f1 (ppm)

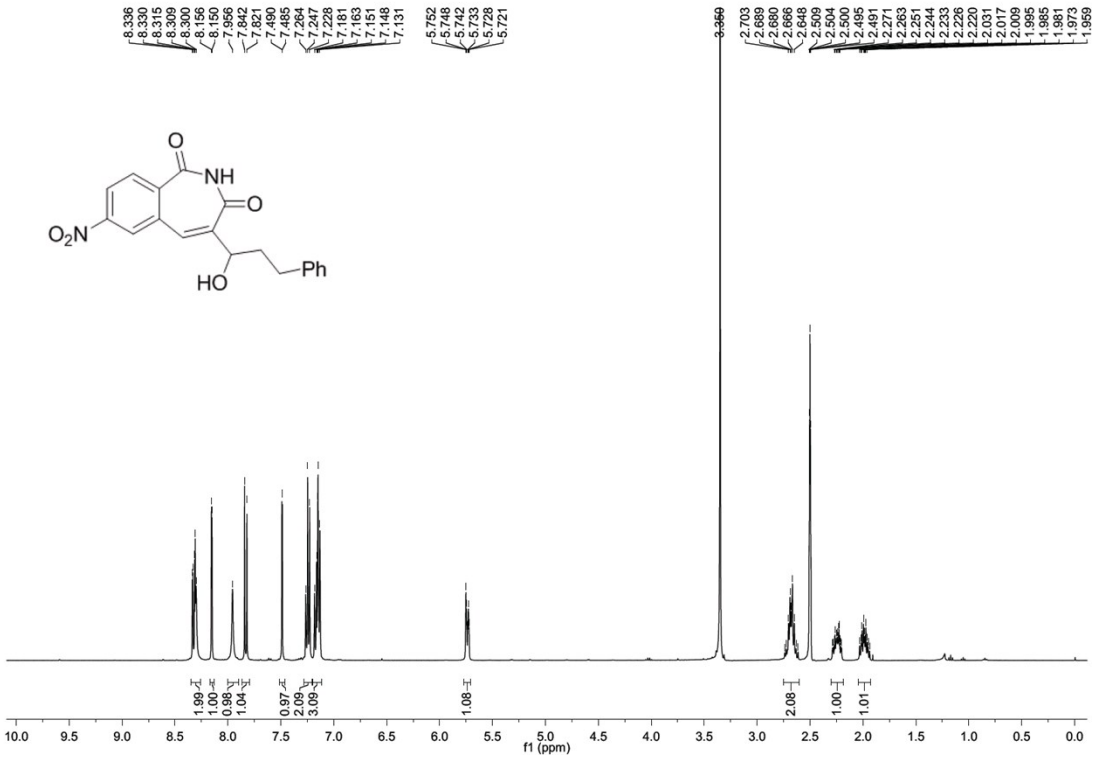

170.044
164.335
143.998
140.177
139.057
137.913
134.811
131.872
129.356
128.983
128.847
128.833
128.738
128.666
128.559
127.679
127.125
126.432
78.848
77.478
77.160
76.842
33.534
30.719
O
NH
O
HO
Ph
f1 (ppm)

3j


8.228
8.018
8.015
7.999
7.996
7.935
7.931
7.894
7.762
7.742
7.450
7.445
7.271
7.253
7.234
7.182
7.164
7.127
7.123
5.831
5.826
5.817
5.812
5.805
3.348
2.657
2.636
2.509
2.504
2.500
2.495
2.156
2.146
2.138
2.126
2.120
2.114
2.107
2.103
2.100
2.084
2.077
1.919
1.898
1.882
1.861
1.846
1.824
O
NH
O
NC
HO
Ph
0.98
1.09
2.07
1.04
0.97
2.17
1.13
2.10
1.00
2.02
1.02
0.97
f1 (ppm)


168.203
163.746
140.481
138.493
133.621
132.192
131.173
129.061
128.469
128.370
128.121
126.695
126.101
117.727
113.060
79.305
40.146
39.937
39.729
39.520
39.311
39.102
38.893
32.474
29.887
O
NH
O
NC
HO
Ph
f1 (ppm)

3k


8.336
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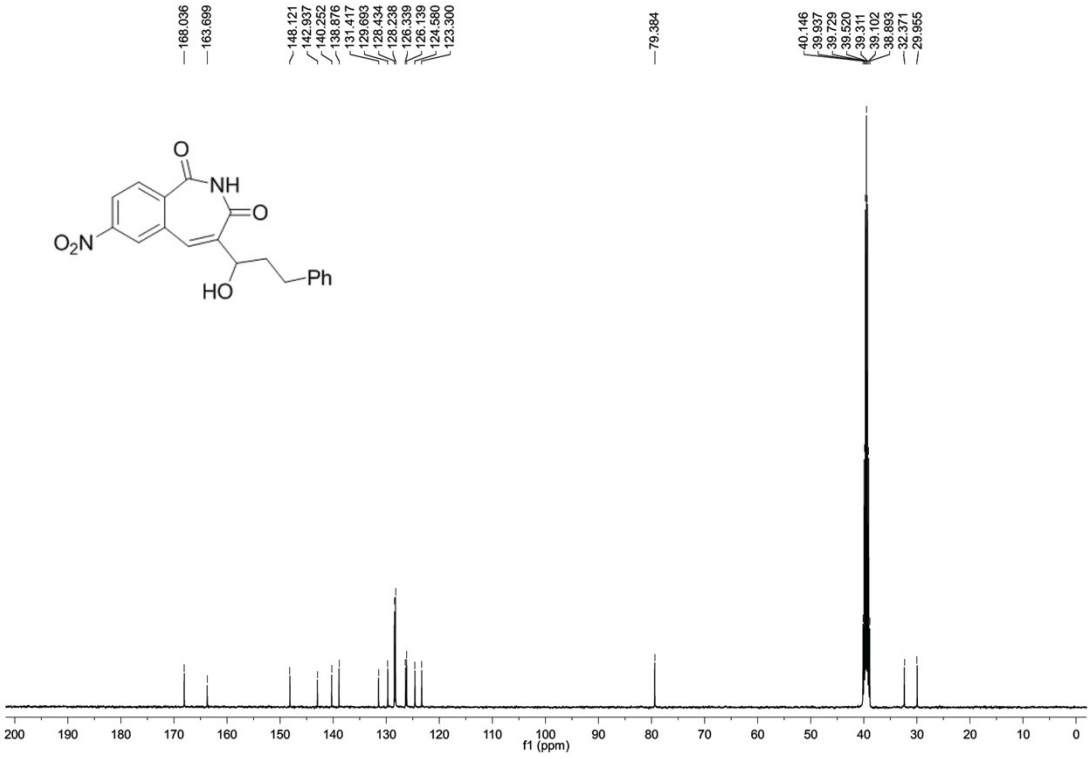
8.315
8.309
8.300
8.156
8.150
7.956
7.842
7.821
7.490
7.485
7.264
7.247
7.228
7.181
7.163
7.151
7.148
7.131
5.752
5.748
5.742
5.733
5.728
5.721
3.360
2.703
2.689
2.680
2.666
2.648
2.509
2.504
2.500
2.495
2.491
2.271
2.263
2.251
2.244
2.233
2.226
2.220
2.031
2.017
2.009
1.995
1.985
1.981
1.973
1.959
O
NH
O
O2N
HO
Ph
1.99
1.00
0.98
1.04
0.97
2.09
3.09
1.08
2.08
1.00
1.01
f1 (ppm)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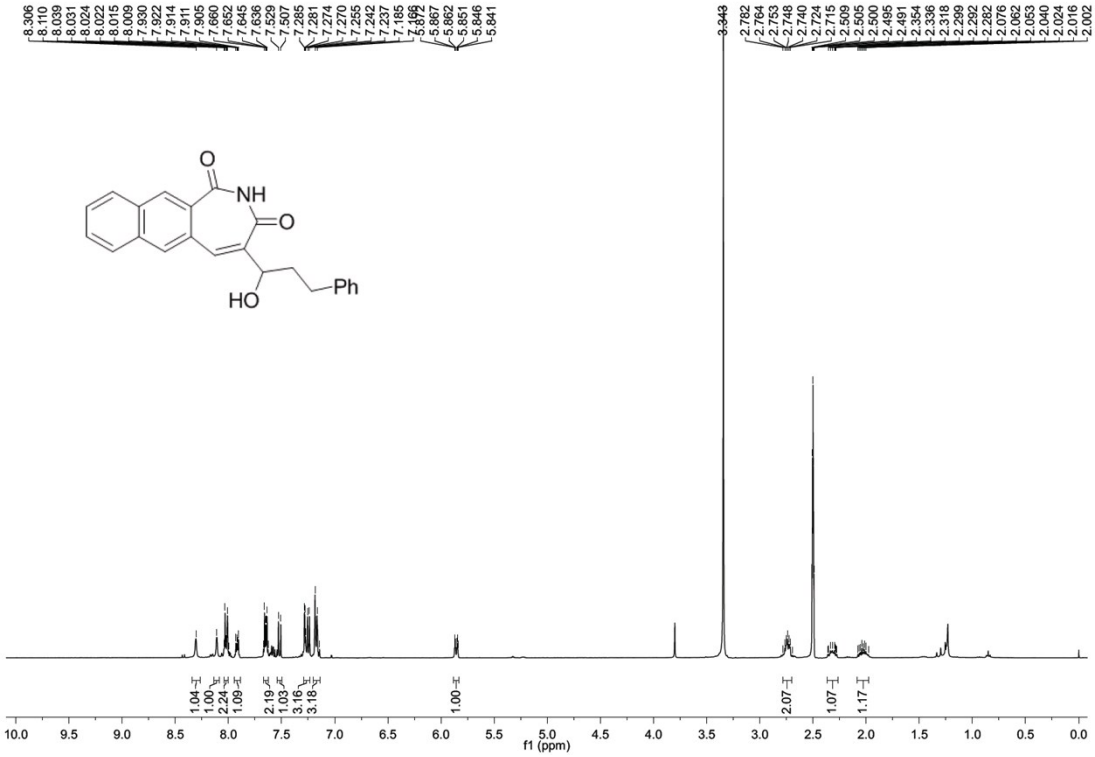
163.699
148.121
142.937
140.252
138.876
131.417
129.693
128.434
128.238
126.339
126.139
124.580
123.300
79.384
40.146
39.937
39.729
39.520
39.311
39.102
38.893
32.371
29.955
O
NH
O
O2N
HO
Ph
f1 (ppm)

3l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8.110
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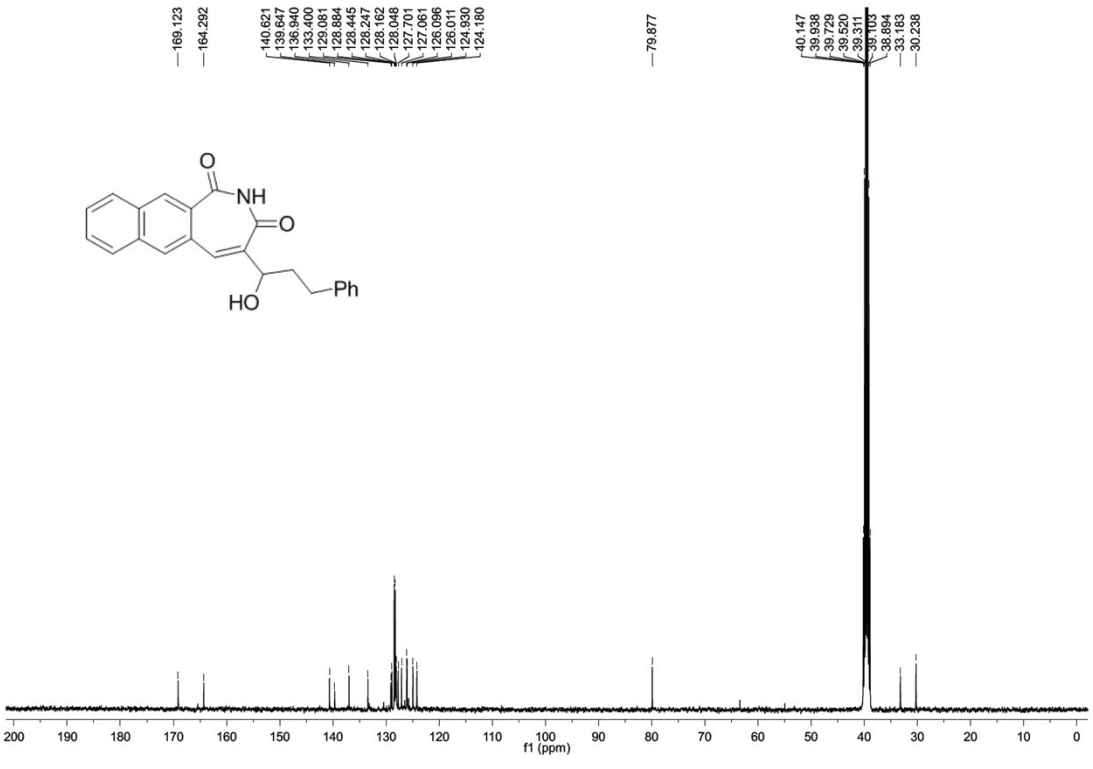
8.031
8.024
8.022
8.015
8.009
7.930
7.922
7.914
7.911
7.905
7.860
7.652
7.645
7.636
7.529
7.507
7.285
7.281
7.274
7.270
7.255
7.242
7.237
7.185
5.867
5.862
5.851
5.846
5.841
3.343
2.782
2.764
2.753
2.748
2.740
2.724
2.715
2.509
2.505
2.500
2.495
2.491
2.354
2.336
2.318
2.299
2.292
2.282
2.076
2.062
2.053
2.040
2.024
2.016
2.002
O
NH
O
HO
Ph
1.04
1.00
2.24
1.09
2.19
1.03
3.16
3.18
1.00
2.07
1.07
1.17
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
f1 (ppm)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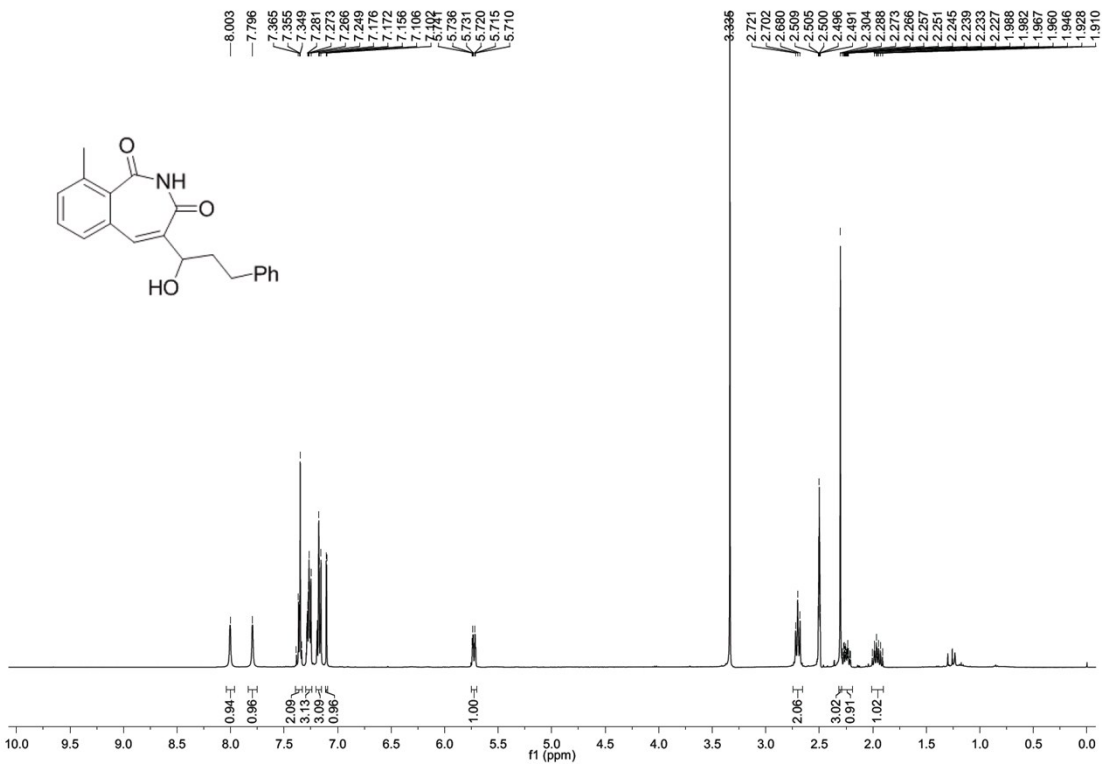
139.647
135.940
133.400
129.081
128.884
128.445
128.247
128.162
128.048
127.701
127.061
126.096
126.011
124.930
124.180
79.877
40.147
39.938
39.729
39.520
39.311
39.103
38.894
33.183
30.238
O
NH
O
HO
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3m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7.355
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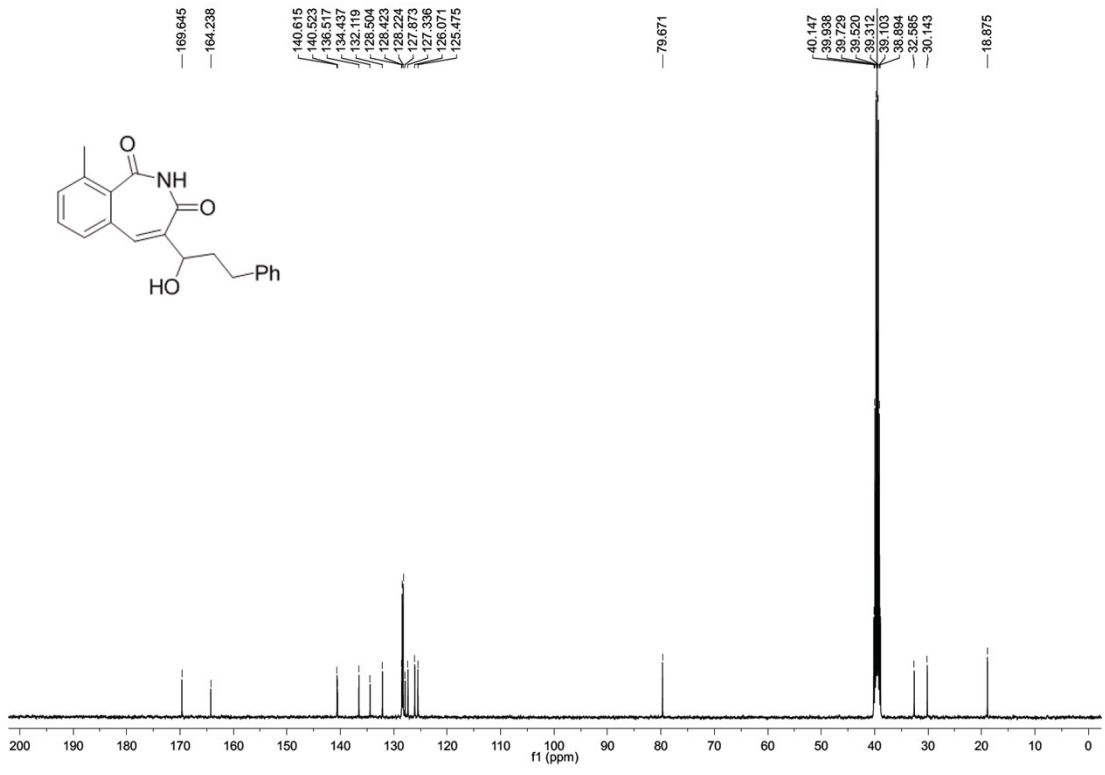
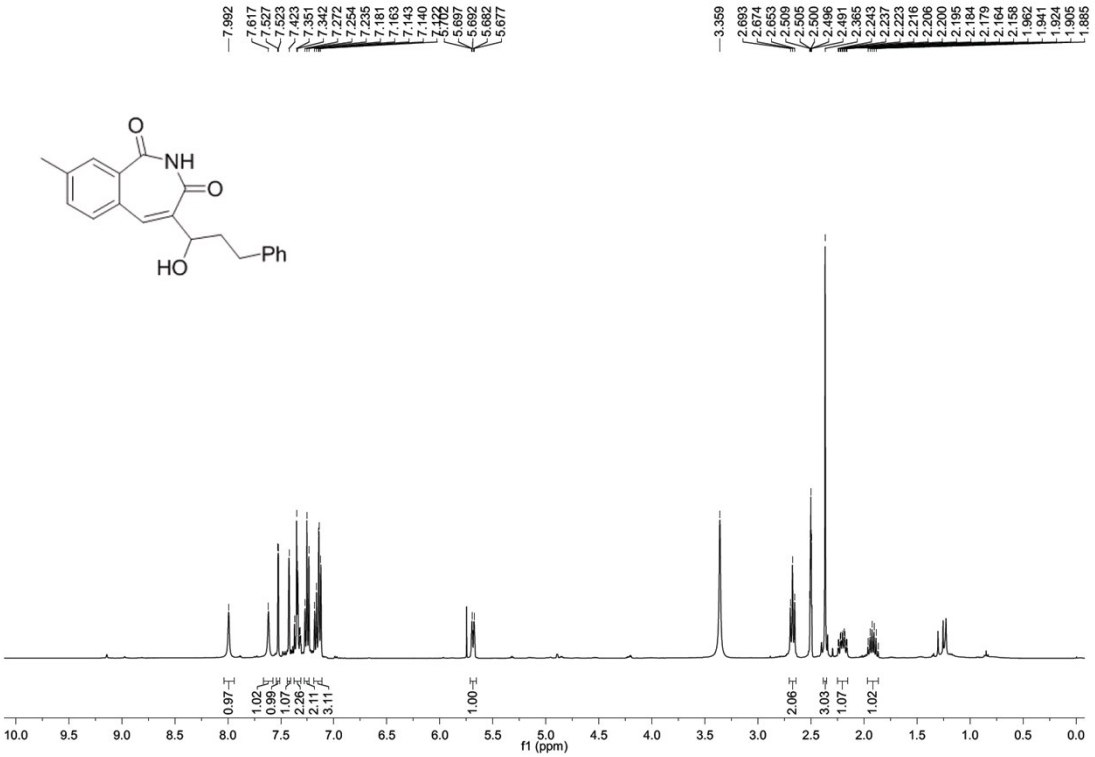
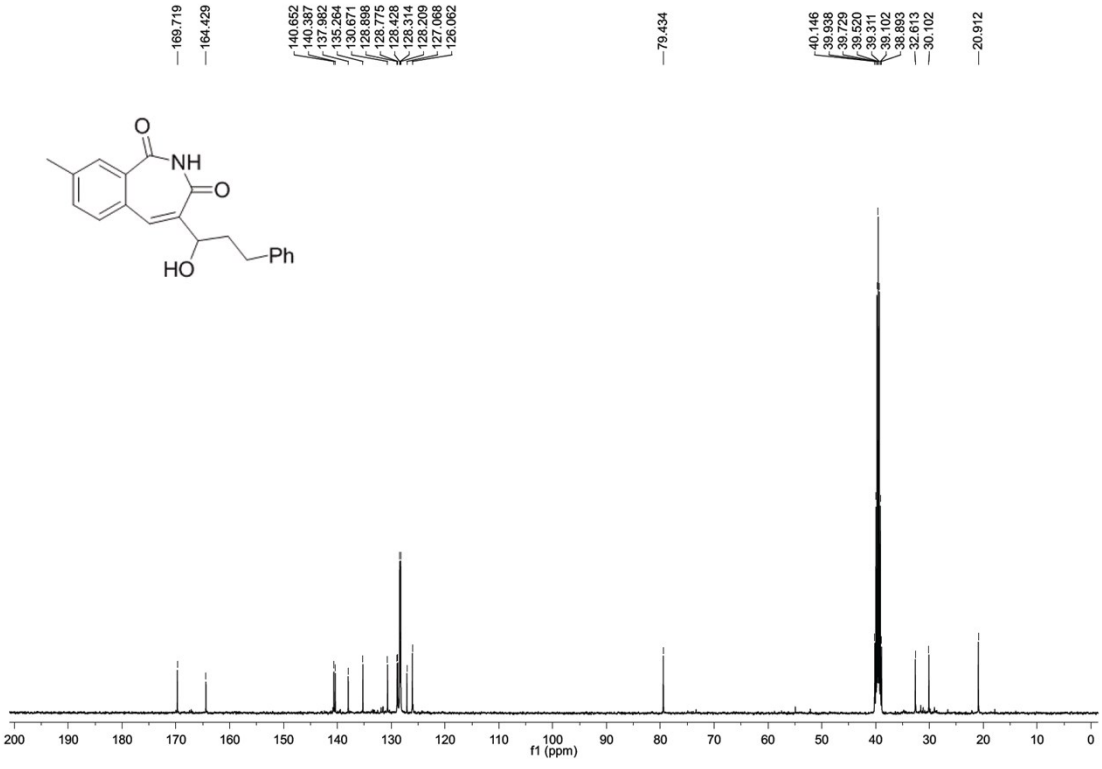
7.281
7.273
7.266
7.249
7.176
7.172
7.156
7.106
5.736
5.731
5.720
5.715
5.710
3.335
2.721
2.702
2.680
2.509
2.505
2.500
2.496
2.491
2.304
2.288
2.273
2.266
2.257
2.251
2.245
2.239
2.233
2.227
1.988
1.982
1.967
1.960
1.946
1.928
1.910
O
NH
O
HO
Ph
0.94
0.96
2.09
3.13
3.09
0.96
1.00
2.06
3.02
0.91
1.02
f1 (ppm)

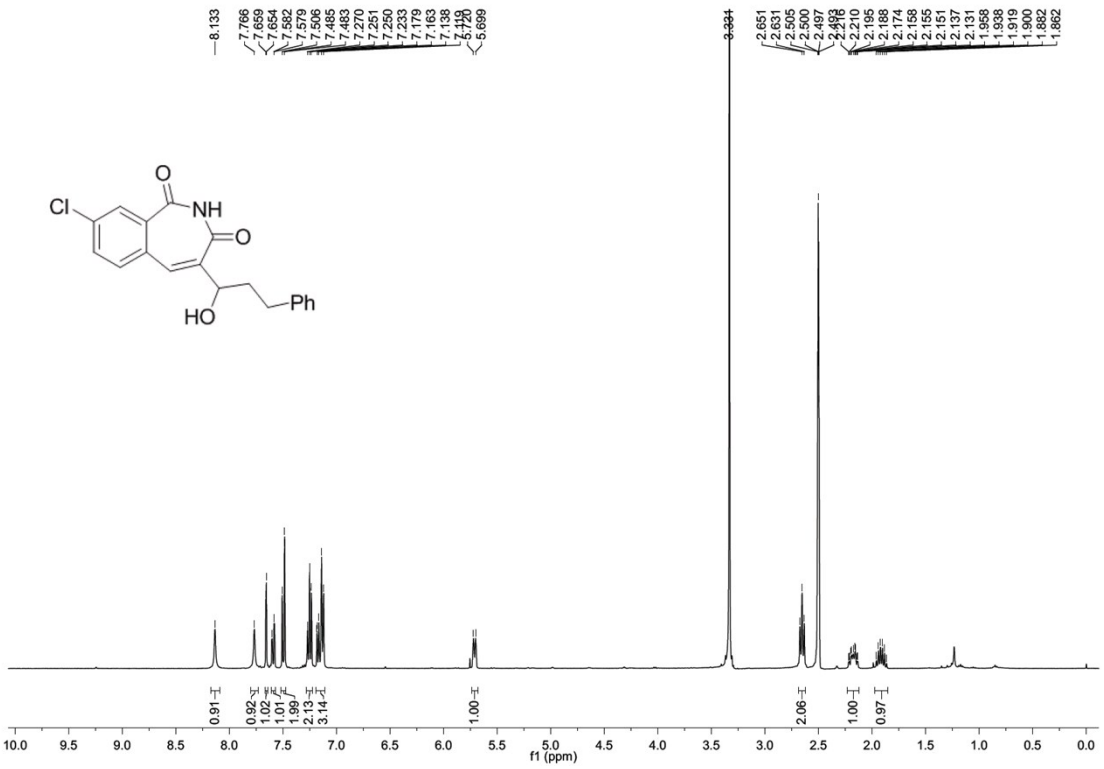

169.645
164.238
140.615
140.523
136.517
134.437
132.119
128.504
128.423
128.224
127.873
127.336
126.071
125.475
79.671
40.147
39.938
39.729
39.520
39.312
39.103
38.894
32.585
30.143
18.875
O
NH
O
HO
Ph
f1 (ppm)

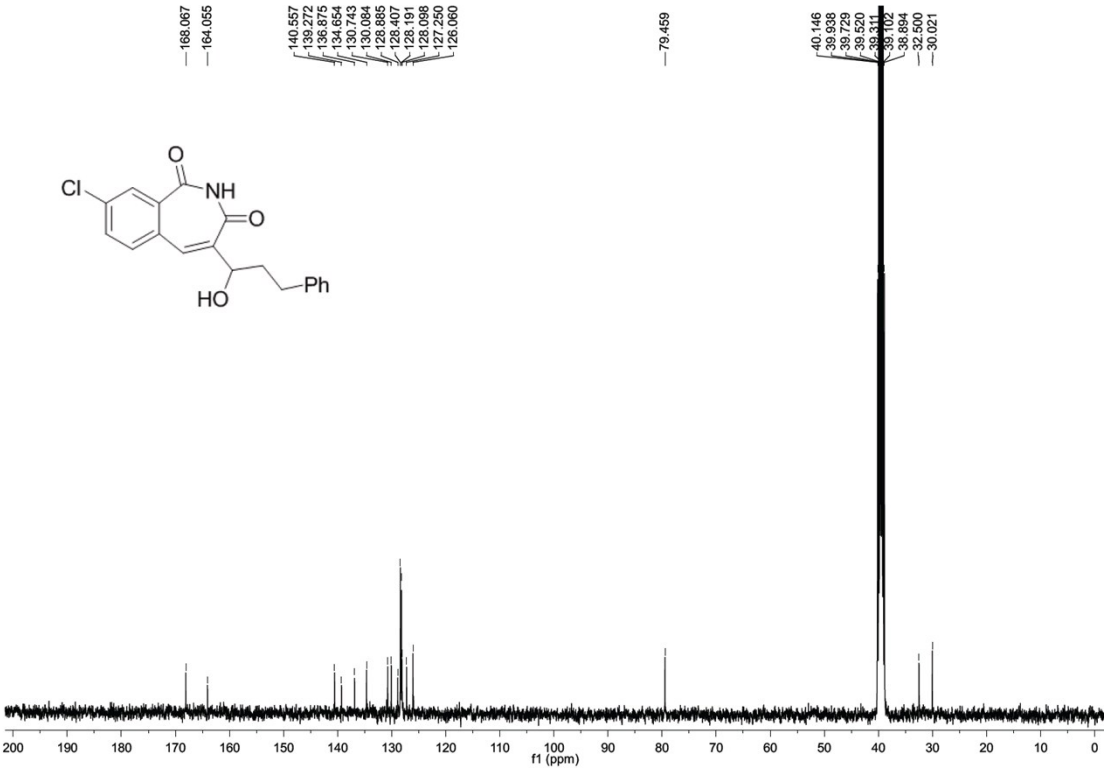
3n


7.992
7.617
7.527
7.523
7.423
7.351
7.342
7.272
7.254
7.235
7.181
7.163
7.143
7.140
5.697
5.692
5.682
5.677
3.359
2.693
2.674
2.653
2.509
2.505
2.500
2.496
2.491
2.365
2.243
2.237
2.223
2.216
2.206
2.200
2.195
2.184
2.179
2.164
2.158
1.962
1.941
1.924
1.905
1.885
O
NH
O
HO
Ph
0.97
1.02
0.99
1.07
2.26
2.11
3.11
1.00
2.06
3.03
1.07
1.02
f1 (ppm)

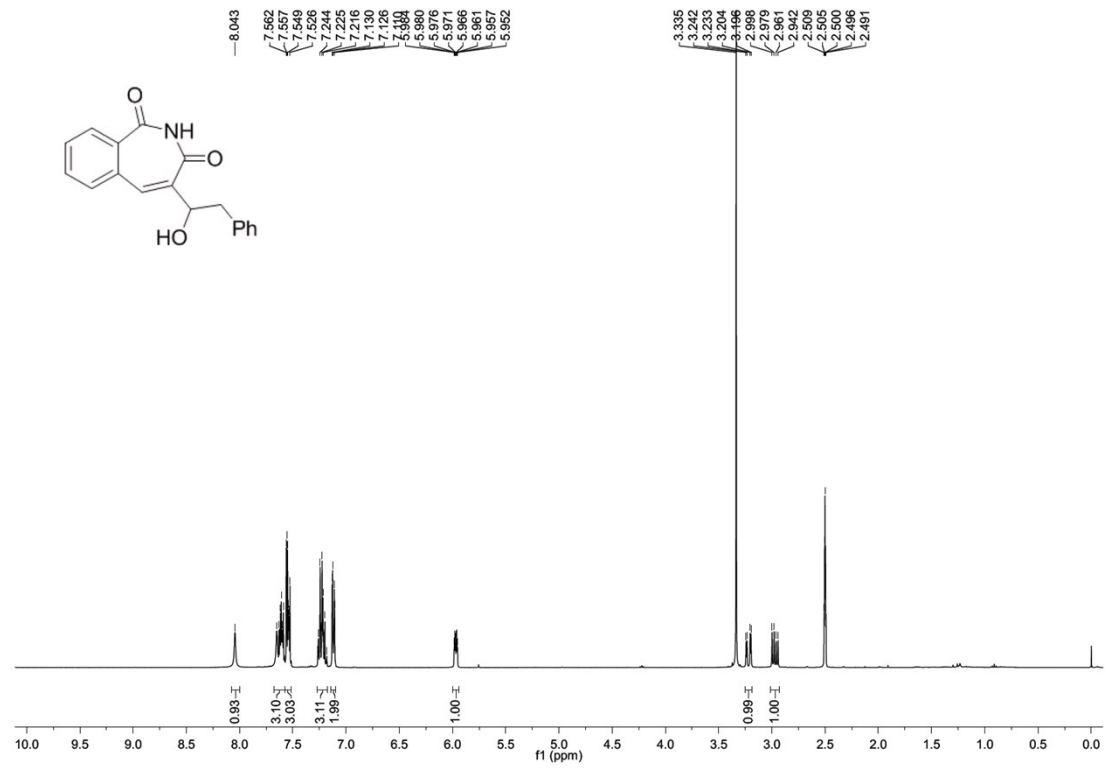

169.719
164.429
140.652
140.387
137.982
135.264
130.671
128.898
128.775
128.428
128.314
128.209
127.668
126.062
79.434
40.146
39.938
39.729
39.520
39.311
39.102
38.893
32.613
30.102
20.912
O
NH
O
HO
Ph
f1 (ppm)

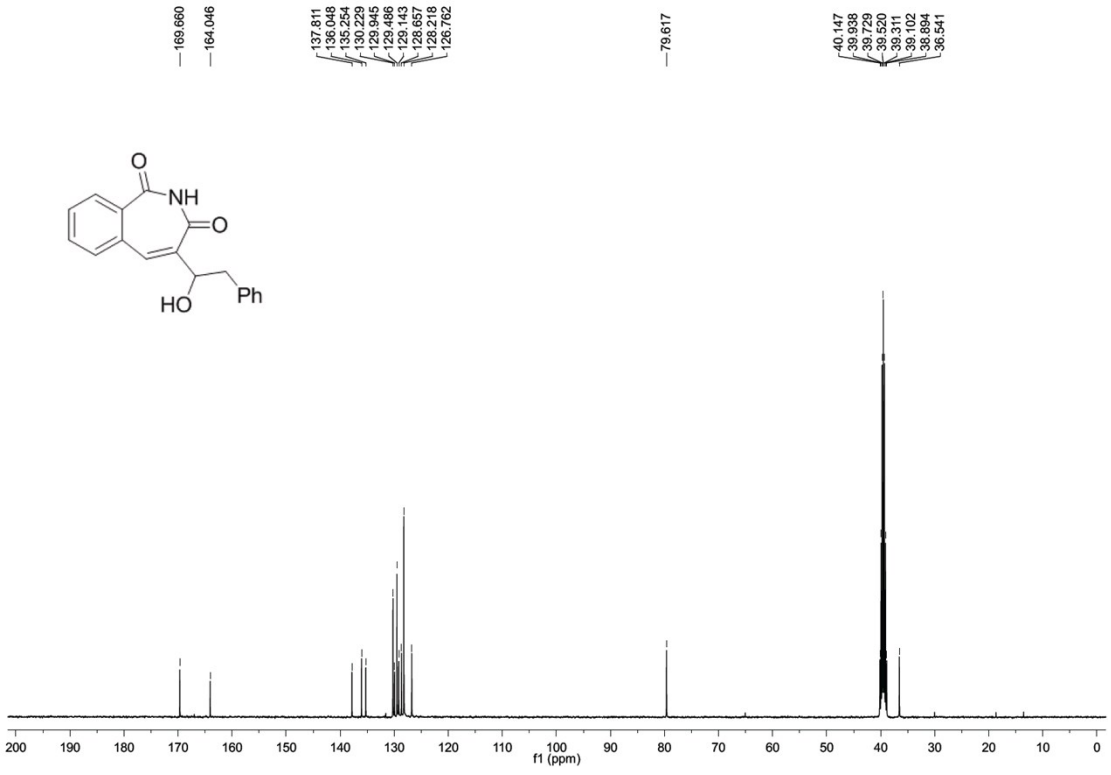
3o


8.133
7.766
7.659
7.654
7.582
7.579
7.506
7.485
7.483
7.270
7.251
7.250
7.233
7.179
7.163
7.138
5.720
5.699
3.334
2.651
2.631
2.505
2.500
2.497
2.210
2.195
2.188
2.174
2.158
2.155
2.151
2.137
2.131
1.938
1.919
1.900
1.882
1.862
O
NH
O
Cl
HO
Ph
0.91
0.92
1.02
1.01
1.99
2.13
3.14
1.00
2.06
1.00
0.97
f1 (ppm)

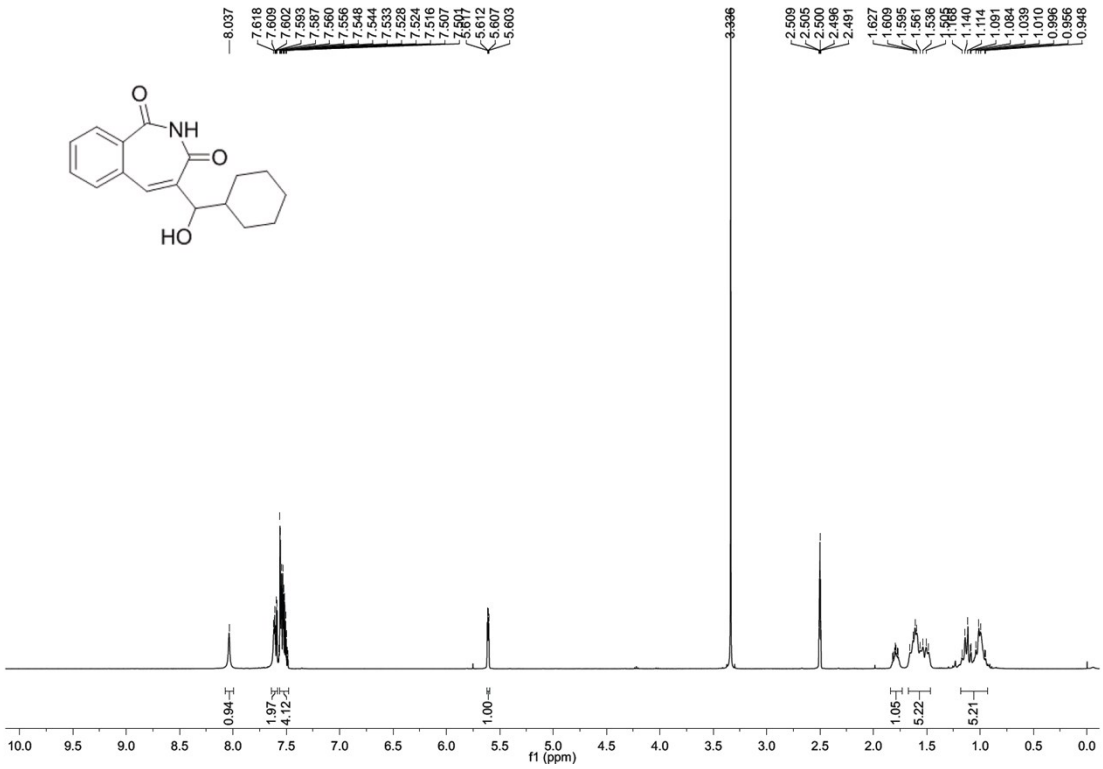

168.067
164.055
140.557
139.272
136.875
134.654
130.743
130.084
128.885
128.407
128.191
128.098
127.250
126.060
79.459
40.146
39.938
39.729
39.520
39.311
39.102
38.894
32.500
30.021
O
NH
O
Cl
HO
Ph
f1 (ppm)

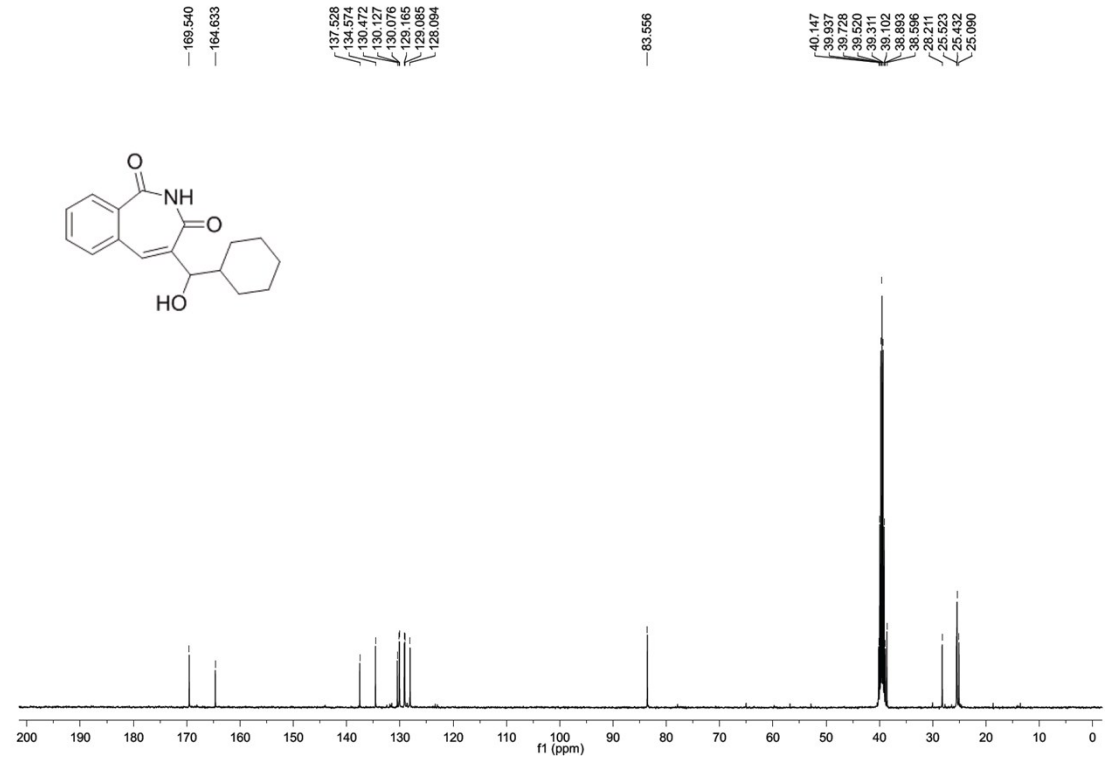
3p


8.043
7.562
7.557
7.549
7.526
7.244
7.225
7.216
7.130
7.126
5.980
5.976
5.971
5.966
5.961
5.957
5.952
3.335
3.242
3.233
3.204
3.196
2.998
2.979
2.961
2.942
2.509
2.505
2.500
2.496
2.491
O
NH
O
HO
Ph
0.93
3.10
3.03
3.11
1.99
1.00
0.99
1.00
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
f1 (ppm)

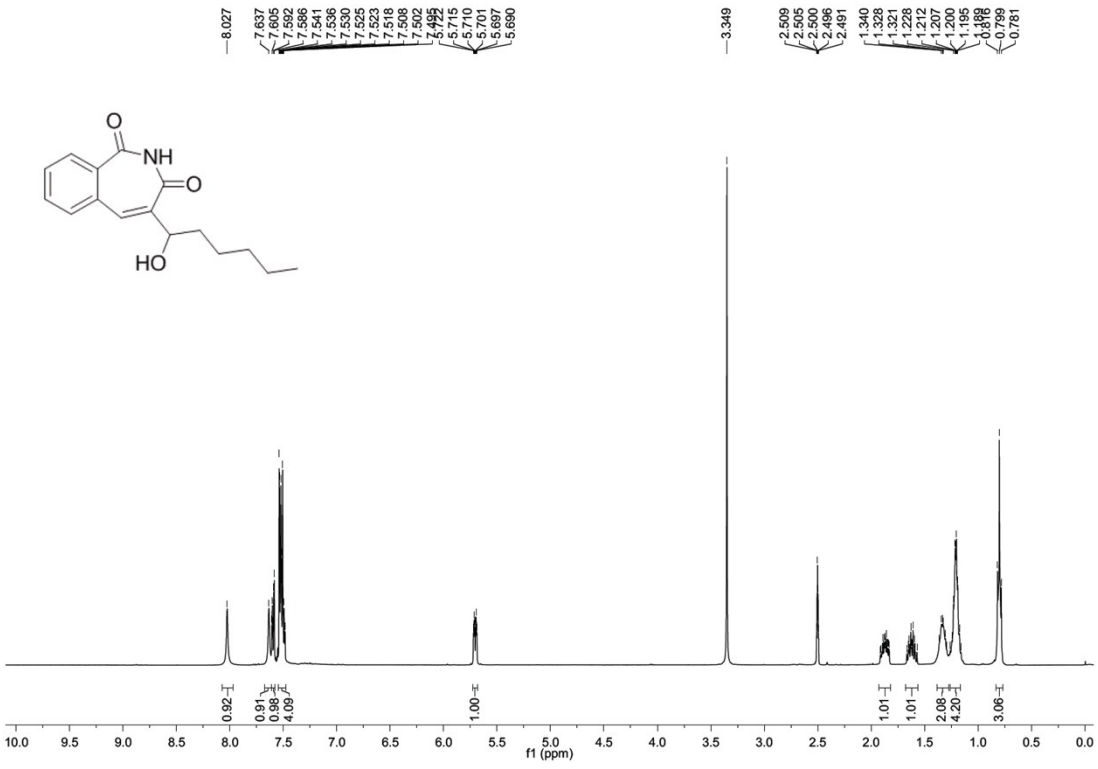

169.660
164.046
137.811
136.048
135.254
130.229
129.945
129.486
129.143
128.657
128.218
126.762
79.617
40.147
39.938
39.729
39.520
39.311
39.102
38.894
36.541
O
NH
O
HO
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

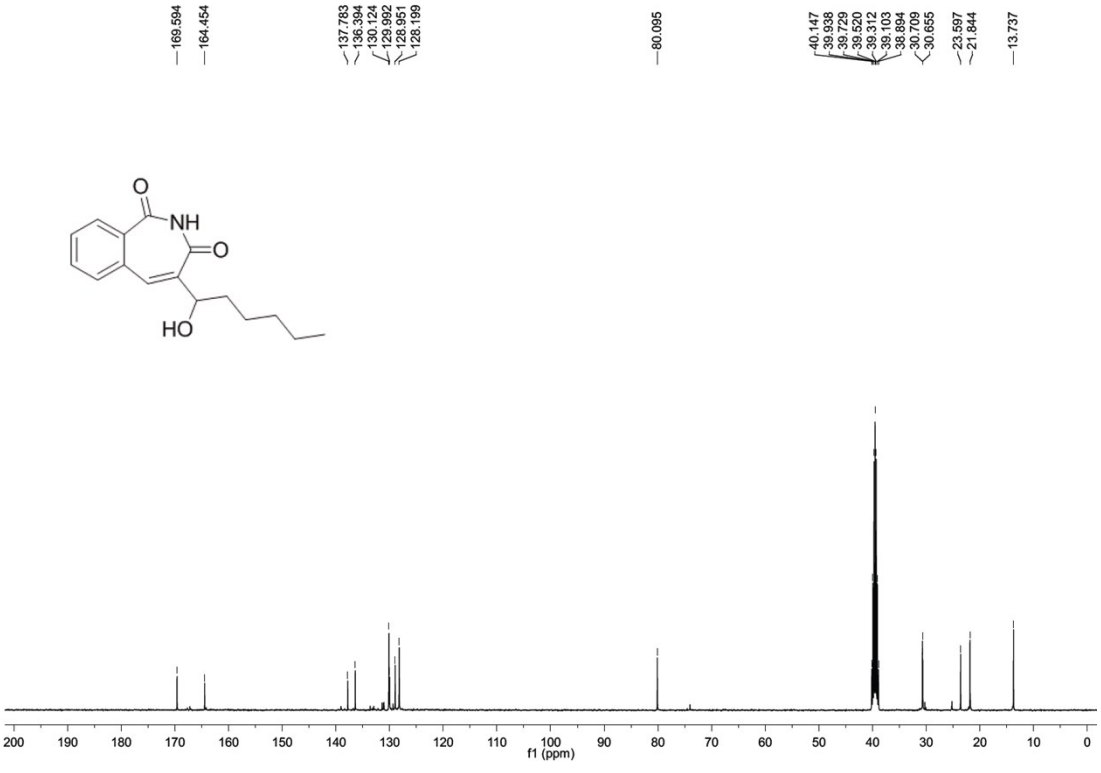
3q


8.037
7.618
7.609
7.602
7.593
7.587
7.560
7.556
7.548
7.544
7.533
7.528
7.524
7.516
7.507
5.612
5.607
5.603
3.336
2.509
2.505
2.500
2.496
2.491
1.627
1.609
1.595
1.561
1.536
1.140
1.114
1.091
1.084
1.039
1.010
0.996
0.956
0.948
NH
O
O
HO
0.94
1.97
4.12
1.00
1.05
5.22
5.21
f1 (ppm)

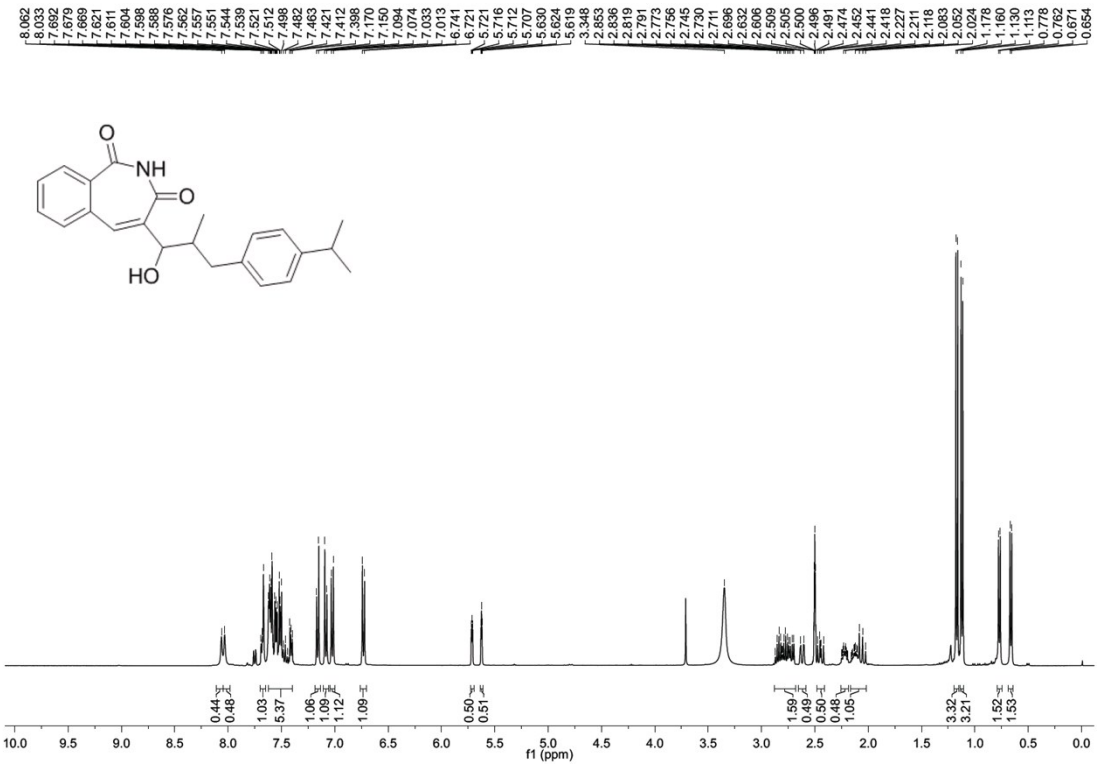

169.540
164.633
137.528
134.574
130.472
130.127
130.076
129.165
129.085
128.094
83.556
40.147
39.937
39.728
39.520
39.311
39.102
38.893
38.596
28.211
25.523
25.432
25.090
NH
O
O
HO
f1 (ppm)

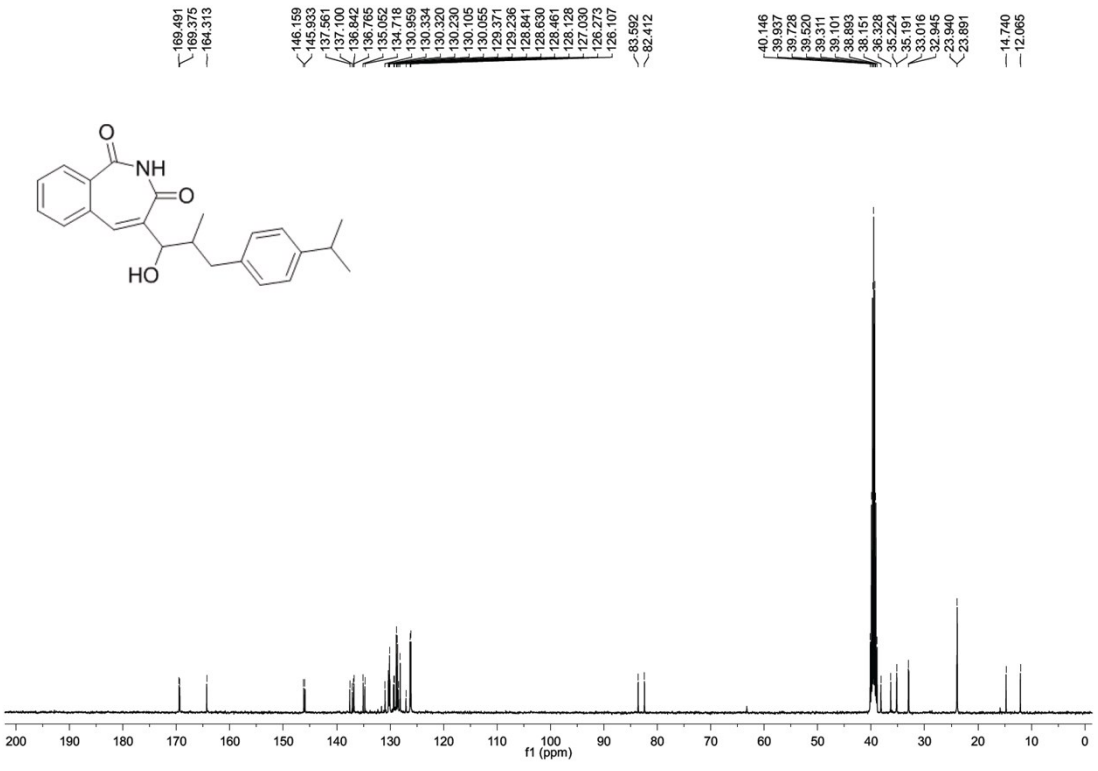
3r


8.027
7.637
7.605
7.592
7.586
7.541
7.536
7.530
7.525
7.523
7.518
7.508
7.502
5.715
5.710
5.701
5.697
5.690
3.349
2.509
2.505
2.500
2.496
2.491
1.340
1.328
1.321
1.228
1.212
1.207
1.200
1.195
0.799
0.781
O
NH
O
HO
0.92
0.91
0.98
4.09
1.00
1.01
1.01
2.08
4.20
3.06
f1 (ppm)

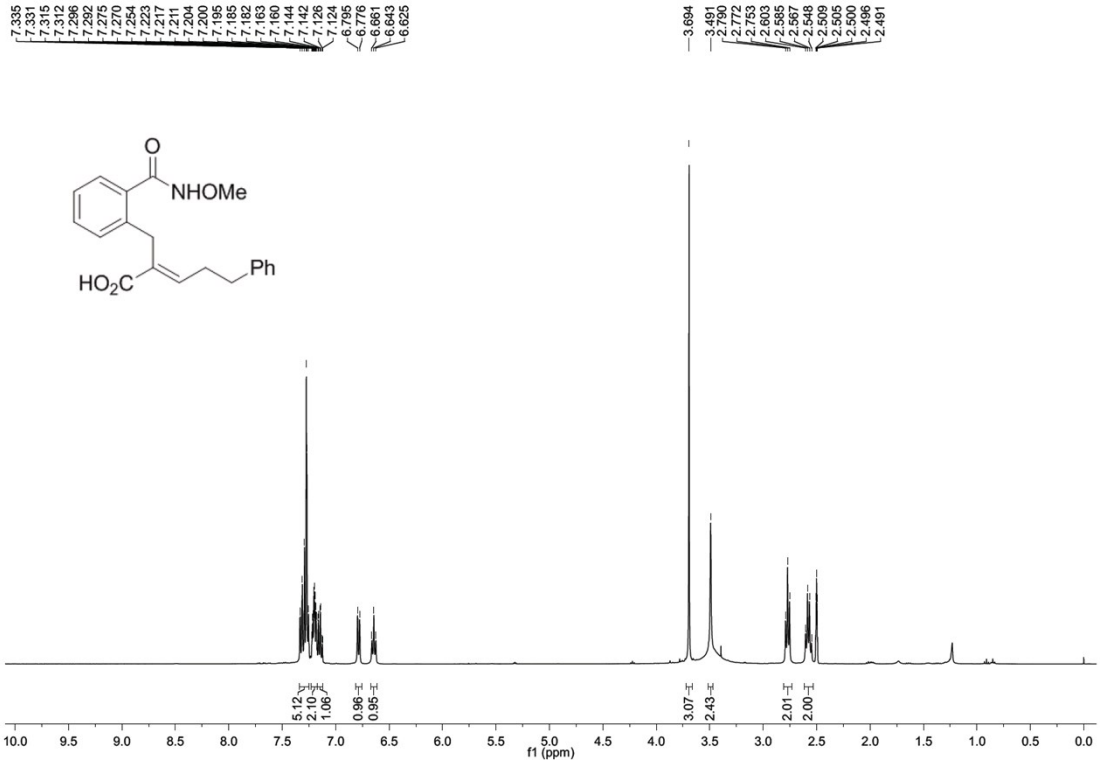

169.594
164.454
137.783
136.394
130.124
129.992
128.951
128.199
80.095
40.147
39.938
39.729
39.520
39.312
39.103
38.894
30.709
30.655
23.597
21.844
13.737
O
NH
O
HO
f1 (ppm)

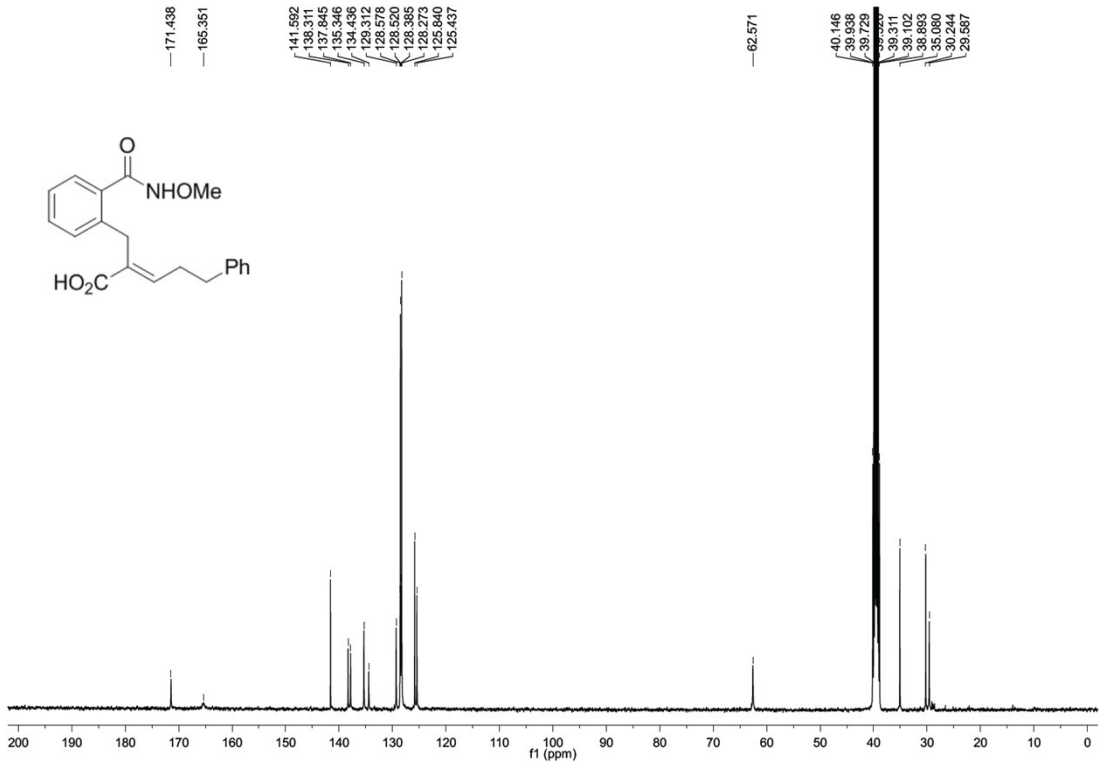
3s


8.062
8.033
7.692
7.679
7.669
7.621
7.611
7.604
7.598
7.588
7.576
7.562
7.557
7.551
7.544
7.539
7.521
7.512
7.498
7.482
7.463
7.421
7.412
7.398
7.170
7.150
7.094
7.074
7.033
7.013
6.741
6.721
5.721
5.716
5.712
5.707
5.630
5.624
5.619
3.348
2.853
2.836
2.819
2.791
2.773
2.756
2.745
2.730
2.711
2.696
2.632
2.606
2.509
2.505
2.500
2.496
2.491
2.474
2.452
2.441
2.418
2.227
2.211
2.118
2.083
2.052
2.024
1.178
1.160
1.130
1.113
0.778
0.762
0.671
0.654
O
NH
O
HO
0.44
0.48
1.03
5.37
1.06
1.09
1.12
1.09
0.50
0.51
1.59
0.49
0.50
0.48
1.05
3.32
3.21
1.52
1.53
f1 (ppm)

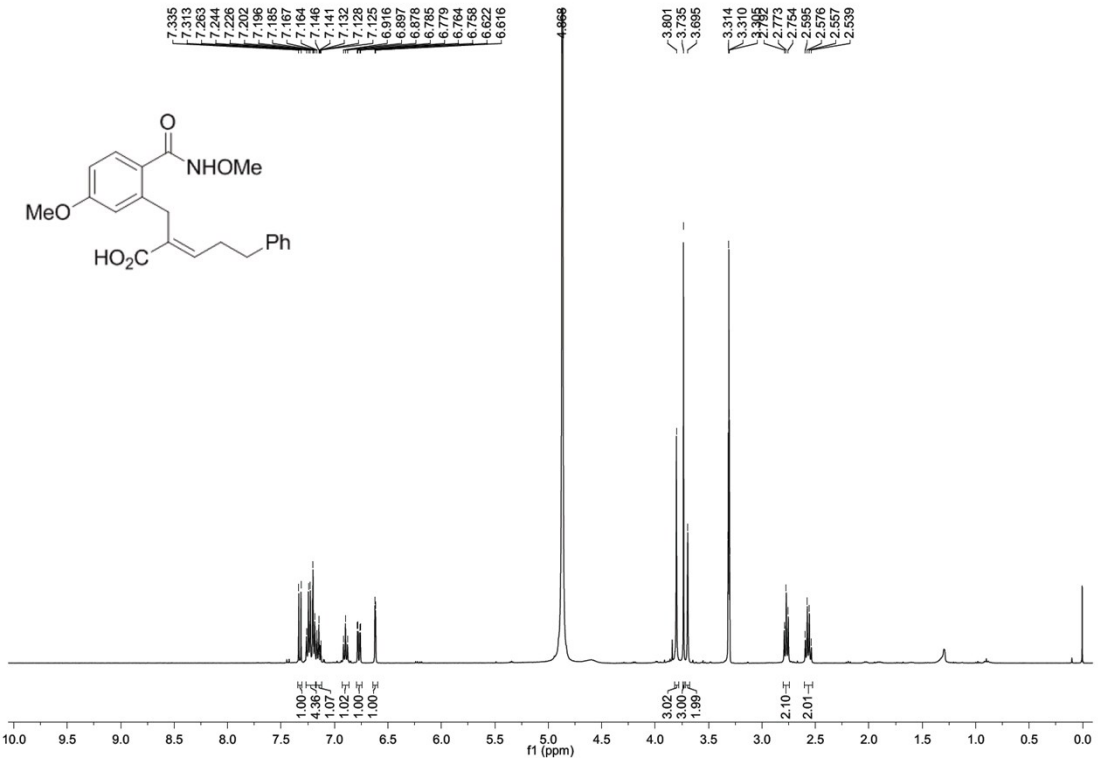

169.491
169.375
164.313
146.159
145.933
137.561
137.100
136.842
136.765
135.052
134.718
130.959
130.334
130.320
130.230
130.105
130.055
129.371
129.236
128.841
128.630
128.461
128.128
127.030
126.273
126.107
83.592
82.412
40.146
39.937
39.728
39.520
39.311
39.101
38.893
38.151
36.328
35.224
35.191
33.016
32.945
23.940
23.891
14.740
12.065
O
NH
O
HO
f1 (ppm)

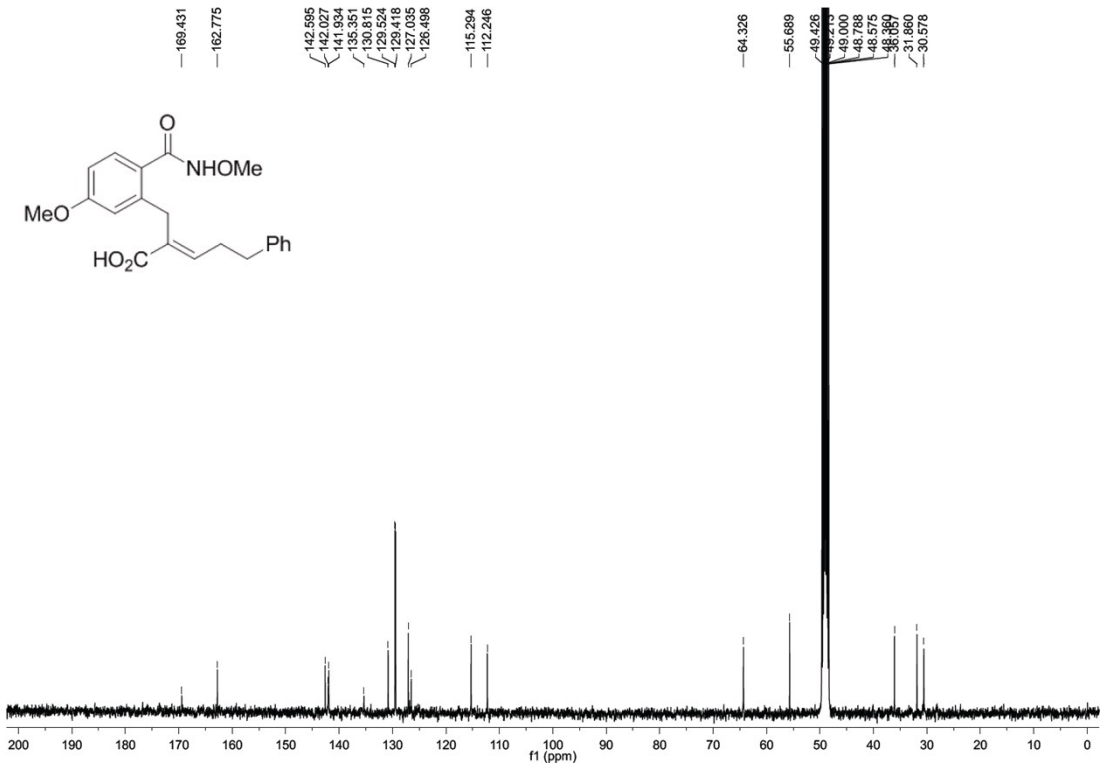
4a


7.335
7.331
7.315
7.312
7.296
7.292
7.275
7.270
7.254
7.223
7.217
7.211
7.204
7.200
7.195
7.185
7.182
7.163
7.160
7.144
7.142
7.126
7.124
6.795
6.776
6.661
6.643
6.625
3.694
3.491
2.790
2.772
2.753
2.603
2.585
2.567
2.548
2.509
2.505
2.500
2.496
2.491
O
NHOMe
HO2C
Ph
5.12
2.10
1.06
0.96
0.95
3.07
2.43
2.01
2.00
f1 (ppm)

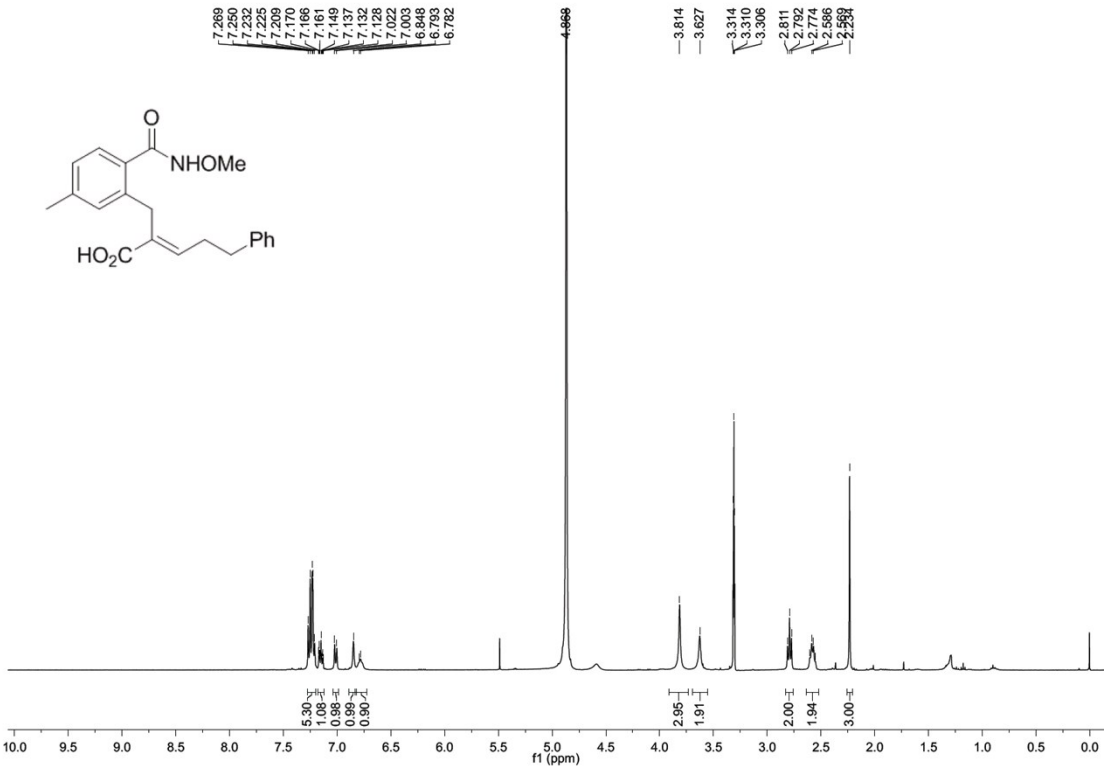

171.438
165.351
141.592
138.311
137.845
135.346
134.436
129.312
128.578
128.520
128.385
128.273
125.840
125.437
62.571
40.146
39.938
39.729
39.311
39.102
38.893
35.080
30.244
29.567
O
NHOMe
HO2C
Ph
f1 (ppm)

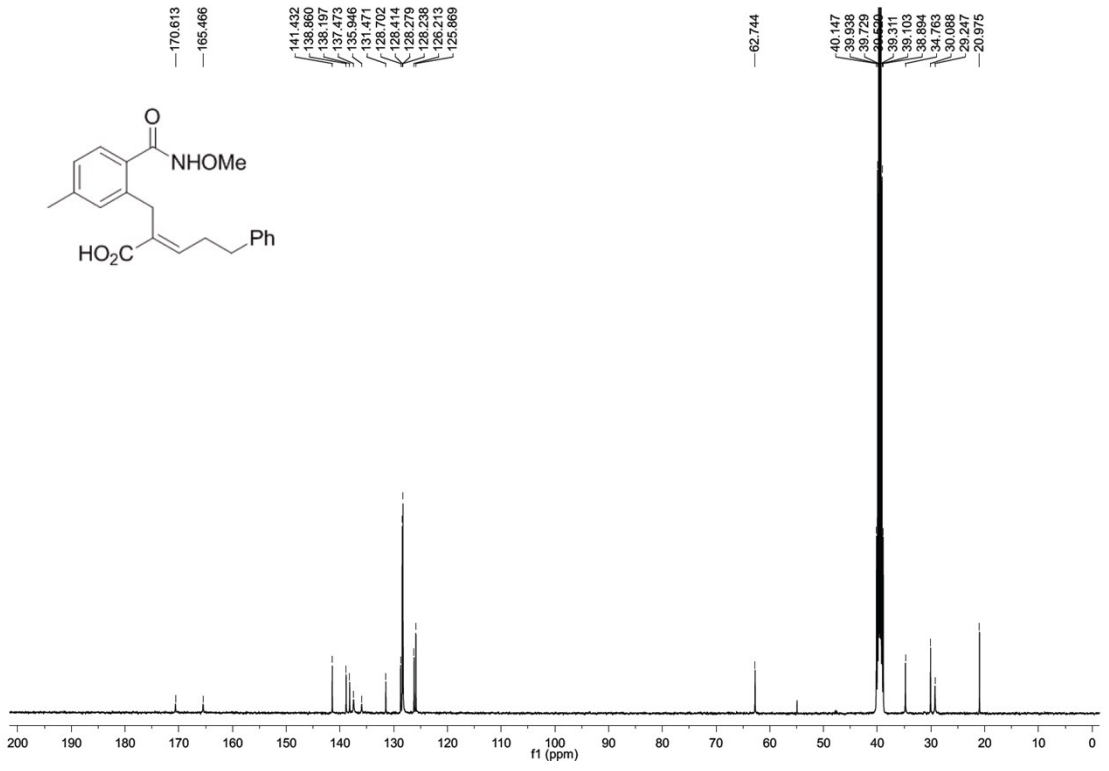
4b


7.335
7.313
7.263
7.244
7.226
7.202
7.196
7.185
7.167
7.164
7.146
7.141
7.132
7.128
7.125
6.916
6.897
6.878
6.785
6.779
6.764
6.758
6.622
6.616
4.868
3.801
3.735
3.695
3.314
3.310
2.773
2.754
2.595
2.576
2.557
2.539
O
NHOMe
MeO
HO2C
Ph
1.00
4.36
1.07
1.02
1.00
1.00
3.02
3.00
1.99
2.10
2.01
f1 (ppm)

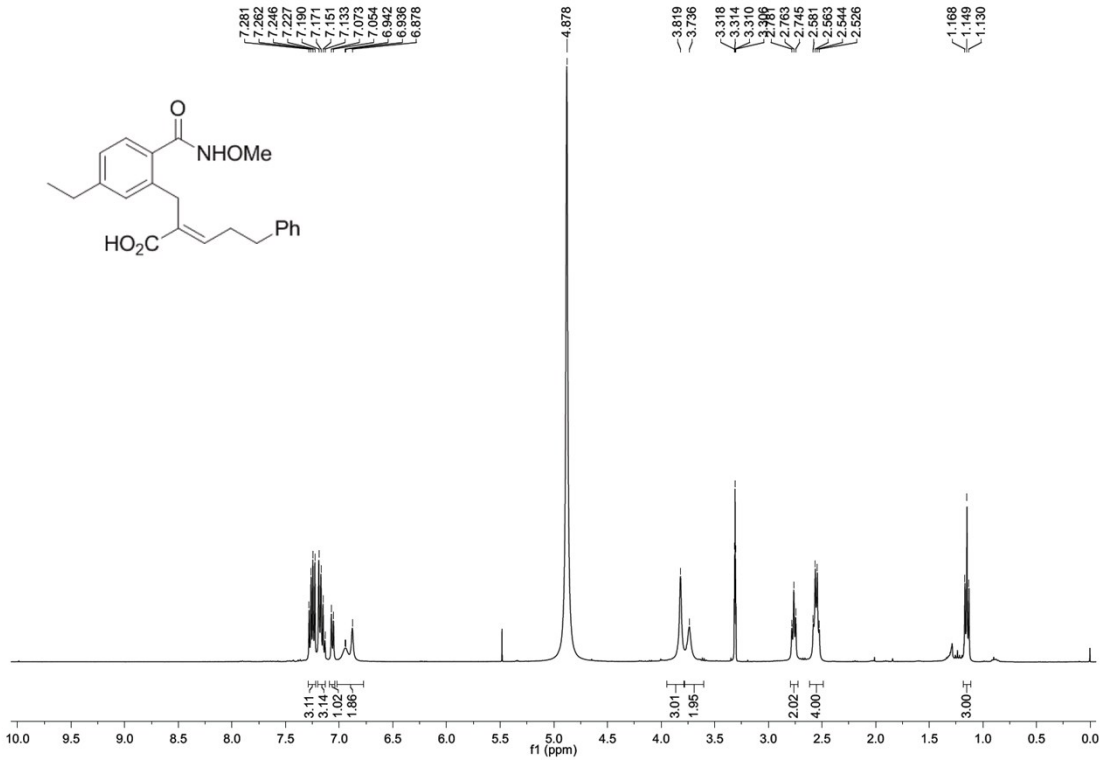

169.431
162.775
142.595
142.027
141.934
135.351
130.815
129.524
129.418
127.035
126.498
115.294
112.246
64.326
55.689
49.426
49.213
49.000
48.788
48.575
31.860
30.578
O
NHOMe
MeO
HO2C
Ph
f1 (ppm)

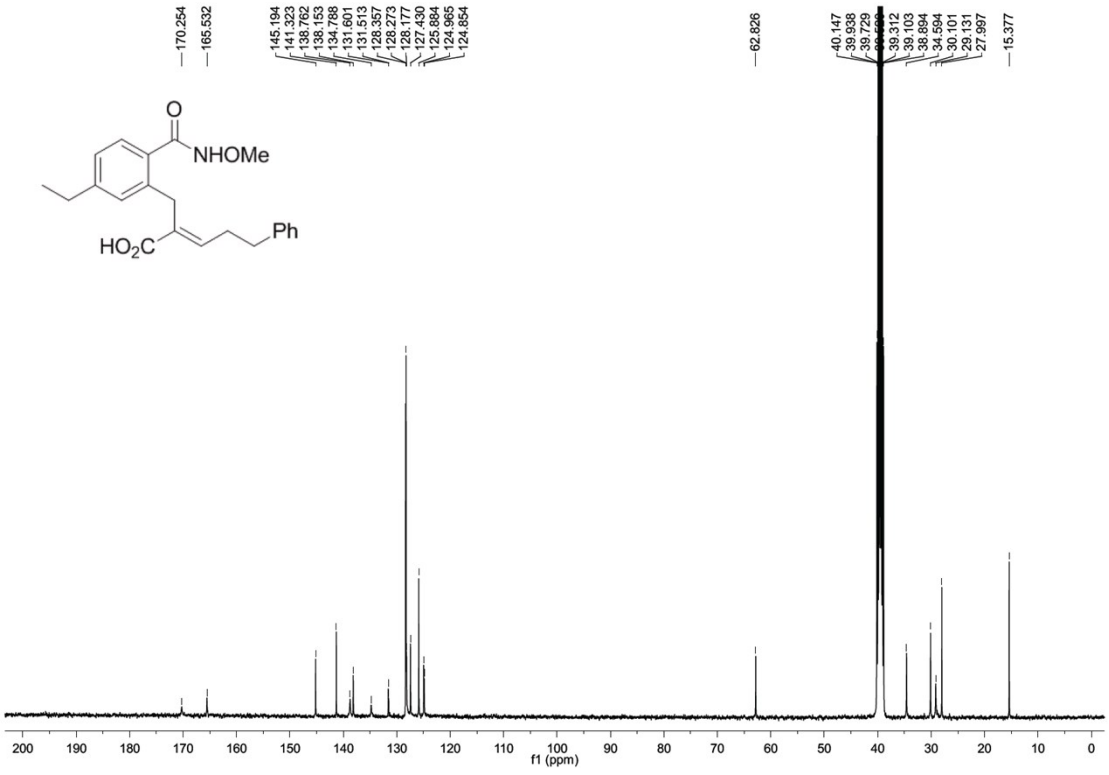
4c


7.269
7.250
7.232
7.225
7.209
7.170
7.166
7.161
7.149
7.137
7.132
7.128
7.022
7.003
6.848
6.793
6.782
4.868
3.814
3.627
3.314
3.310
3.306
2.811
2.792
2.774
2.586
2.569
2.234
O
NHOMe
HO2C
Ph
5.30
1.08
0.98
0.99
0.90
2.95
1.91
2.00
1.94
3.00
f1 (ppm)

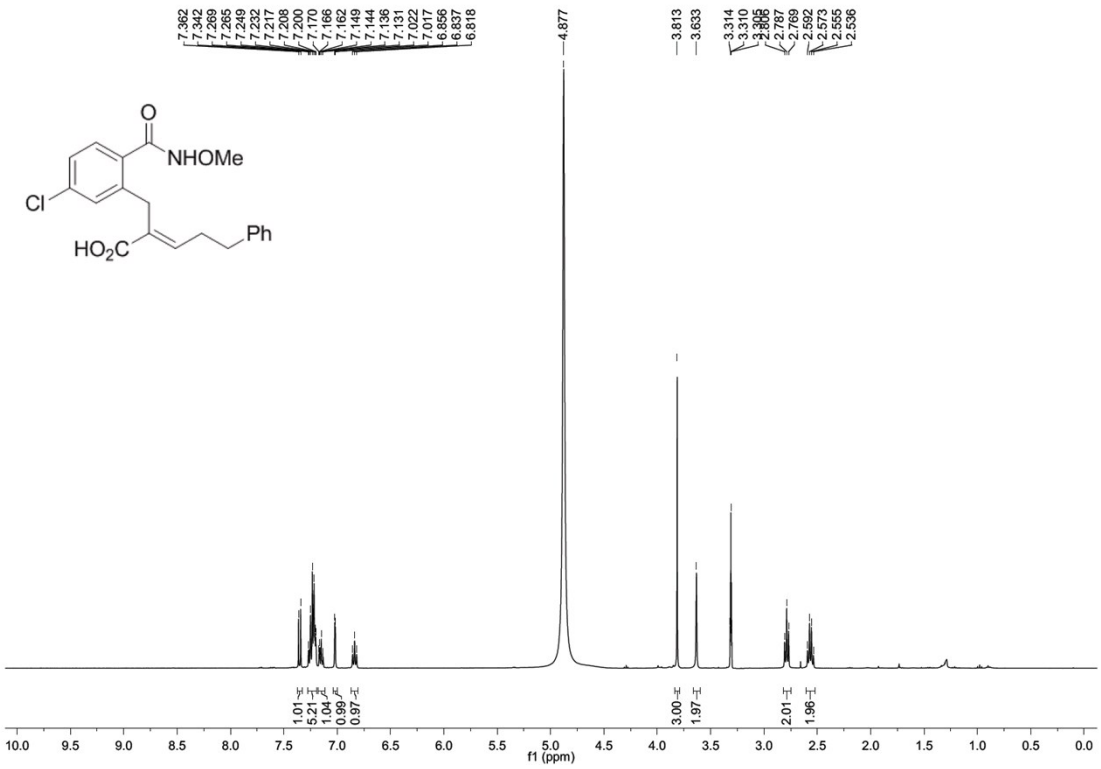

170.613
165.466
141.432
138.860
138.197
137.473
135.946
131.471
128.702
128.414
128.279
128.238
126.213
125.869
62.744
40.147
39.938
39.729
39.520
39.311
39.103
38.894
34.763
30.088
29.247
20.975
O
NHOMe
HO2C
Ph
f1 (ppm)

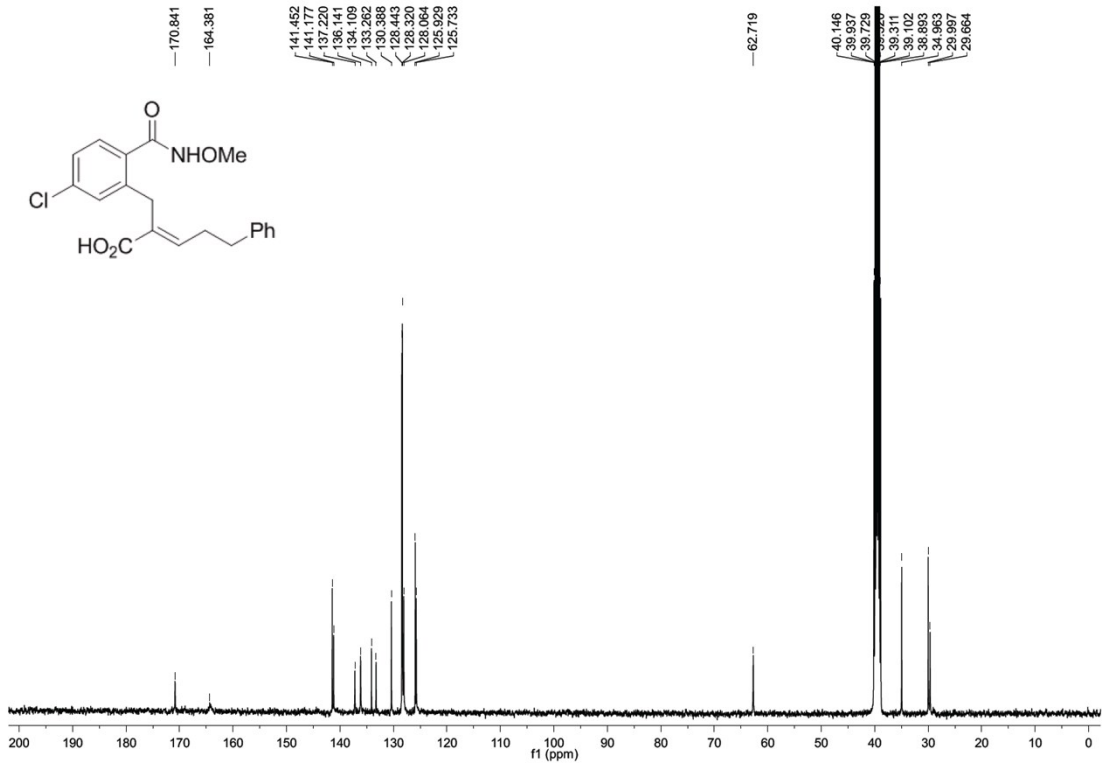
4d


7.281
7.262
7.246
7.227
7.190
7.171
7.151
7.133
7.073
7.054
6.942
6.936
6.878
4.878
3.819
3.736
3.318
3.314
3.310
2.763
2.745
2.581
2.563
2.544
2.526
1.168
1.149
1.130
O
NHOMe
Ph
HO2C
3.11
3.14
1.02
1.86
3.01
1.95
2.02
4.00
3.00
f1 (ppm)


170.254
165.532
145.194
141.323
138.762
138.153
134.788
131.601
131.513
128.357
128.273
128.177
127.430
125.884
124.965
124.854
62.826
40.147
39.938
39.729
39.312
39.103
38.894
34.594
30.101
29.131
27.997
15.377
O
NHOMe
Ph
HO2C
f1 (ppm)

4e


7.362
7.342
7.269
7.265
7.249
7.232
7.217
7.208
7.200
7.170
7.166
7.162
7.149
7.144
7.136
7.131
7.022
7.017
6.856
6.837
6.818
4.877
3.813
3.633
3.314
3.310
2.787
2.769
2.592
2.573
2.555
2.536
O
NHOMe
Cl
HO2C
Ph
1.01
5.21
1.04
0.99
0.97
3.00
1.97
2.01
1.96
f1 (ppm)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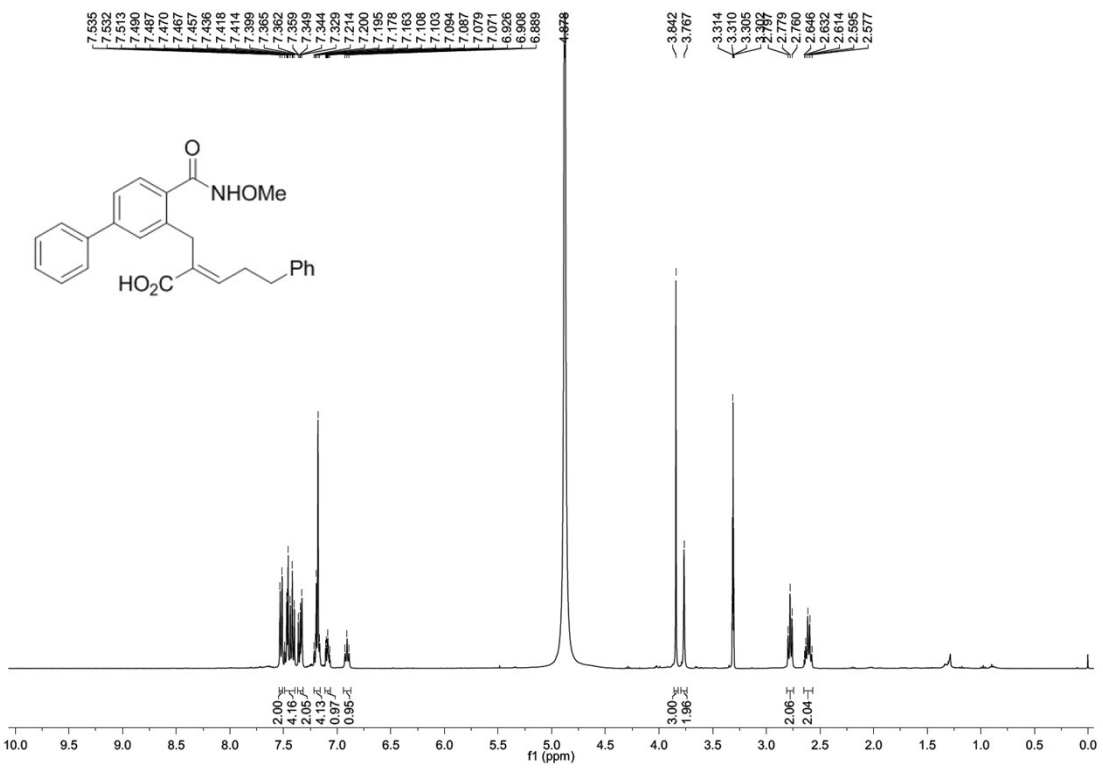
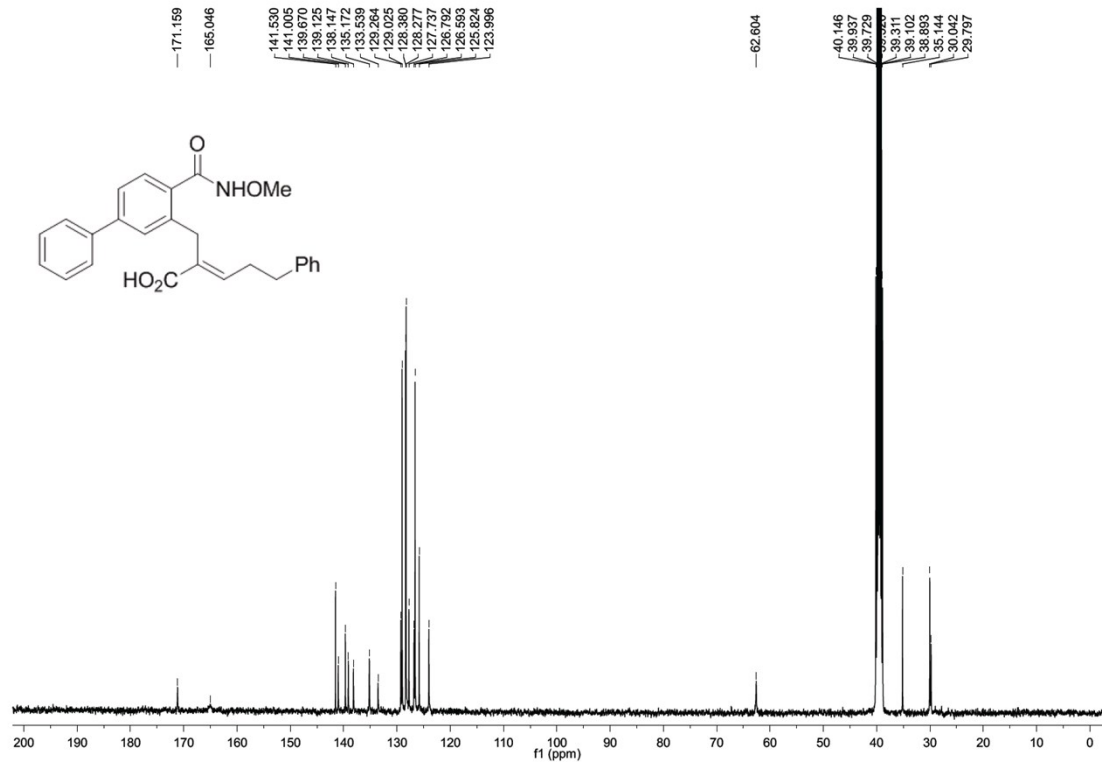
164.381
141.452
141.177
137.220
136.141
134.109
133.262
130.388
128.443
128.320
128.064
125.929
125.733
62.719
40.146
39.937
39.729
39.311
39.102
38.893
34.963
29.997
29.664
O
NHOMe
Cl
HO2C
Ph
f1 (ppm)

4f


7.535
7.532
7.513
7.490
7.487
7.470
7.467
7.457
7.436
7.418
7.414
7.399
7.365
7.362
7.359
7.349
7.344
7.329
7.214
7.200
7.195
7.178
7.163
7.108
7.103
7.094
7.087
7.079
7.071
6.926
6.908
6.889
4.878
3.842
3.767
3.314
3.310
3.305
2.779
2.760
2.646
2.632
2.614
2.595
2.577
O
NHOMe
Ph
HO2C
2.00
4.16
2.05
4.13
0.97
0.95
3.00
1.96
2.06
2.04
f1 (ppm)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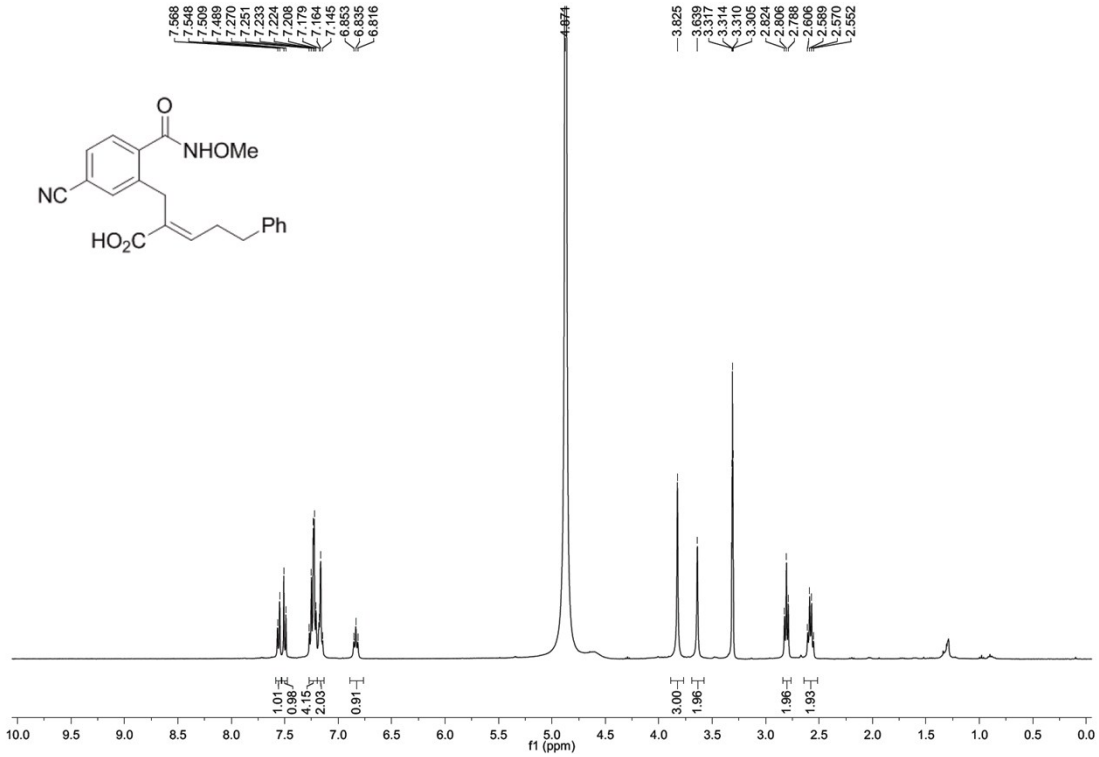
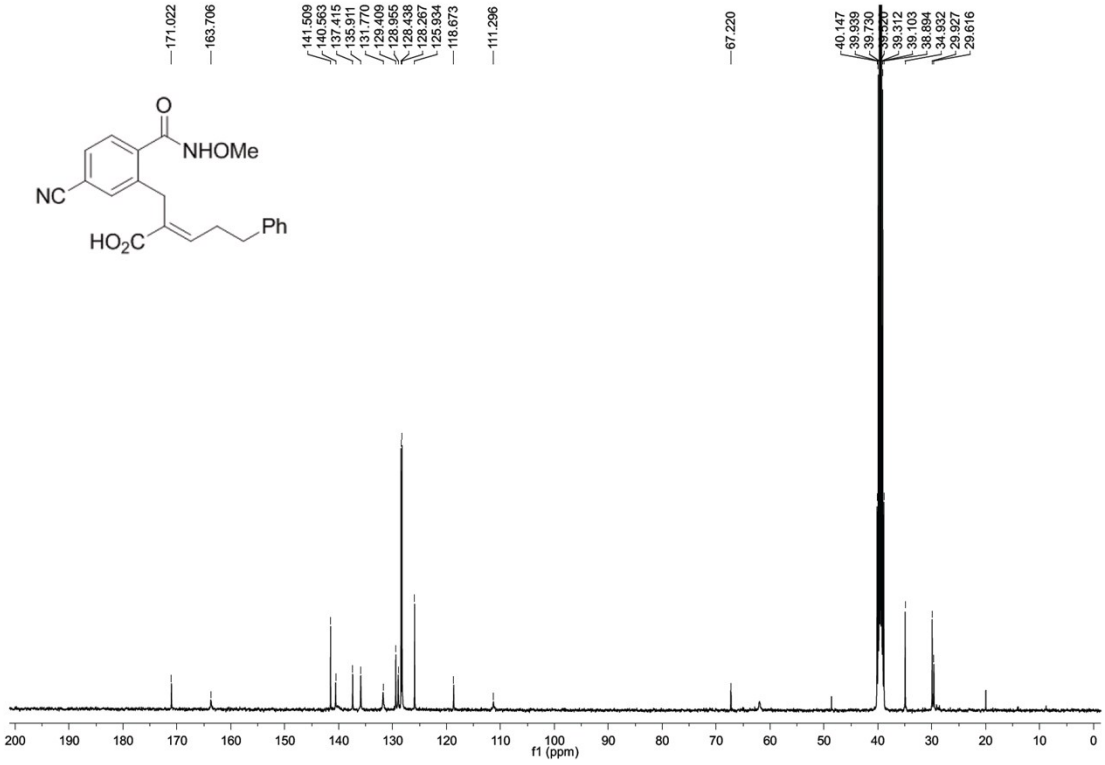
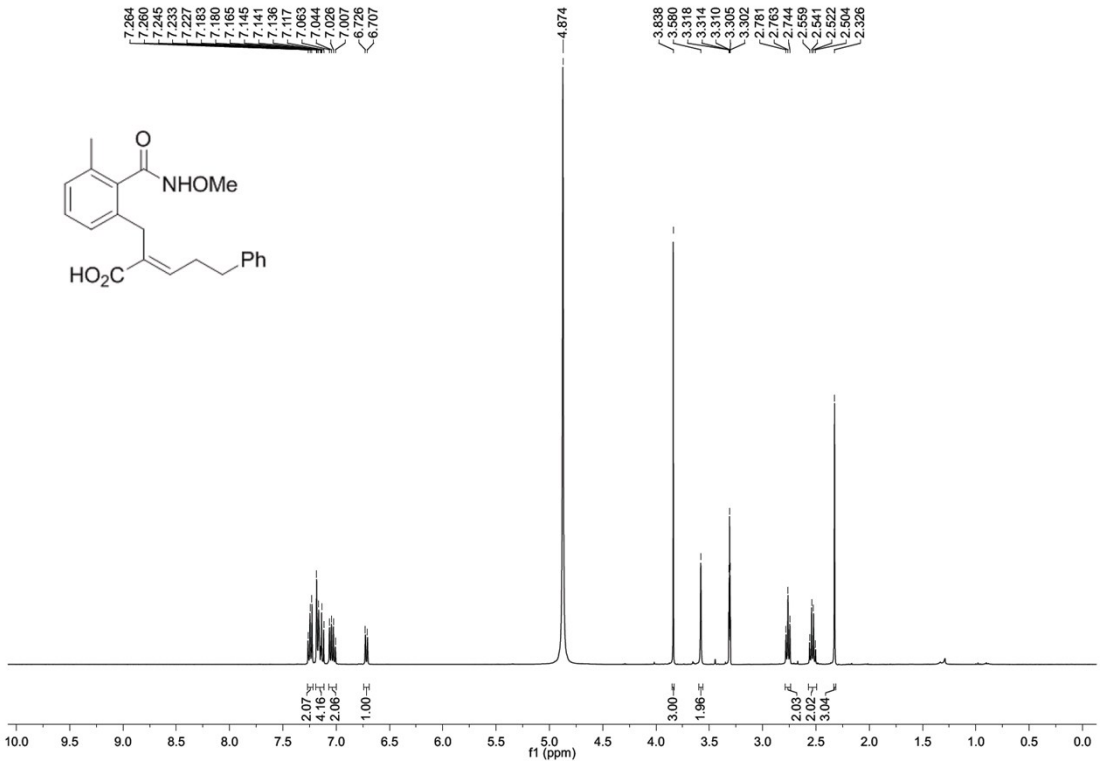
165.046
141.530
141.005
139.670
139.125
138.147
135.172
133.539
129.284
129.025
128.380
128.277
127.737
126.792
126.593
125.824
123.996
62.604
40.146
39.937
39.729
39.311
39.102
38.893
35.144
30.042
29.797
O
NHOMe
Ph
HO2C
f1 (ppm)

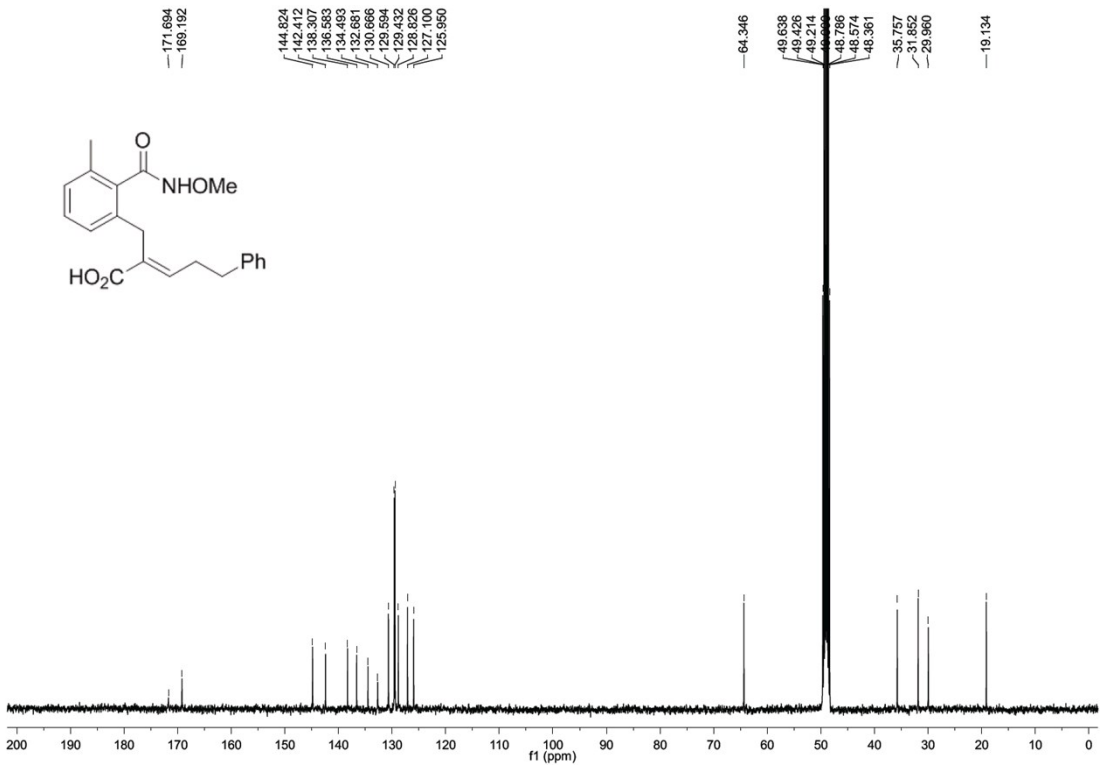
4g


7.568
7.548
7.509
7.489
7.270
7.251
7.233
7.224
7.208
7.179
7.164
7.145
6.853
6.835
6.816
4.674
3.825
3.639
3.317
3.314
3.310
3.305
2.824
2.806
2.788
2.606
2.589
2.570
2.552
O
NHOMe
NC
Ph
HO2C
1.01
0.98
4.15
2.03
0.91
3.00
1.96
1.96
1.93
f1 (ppm)

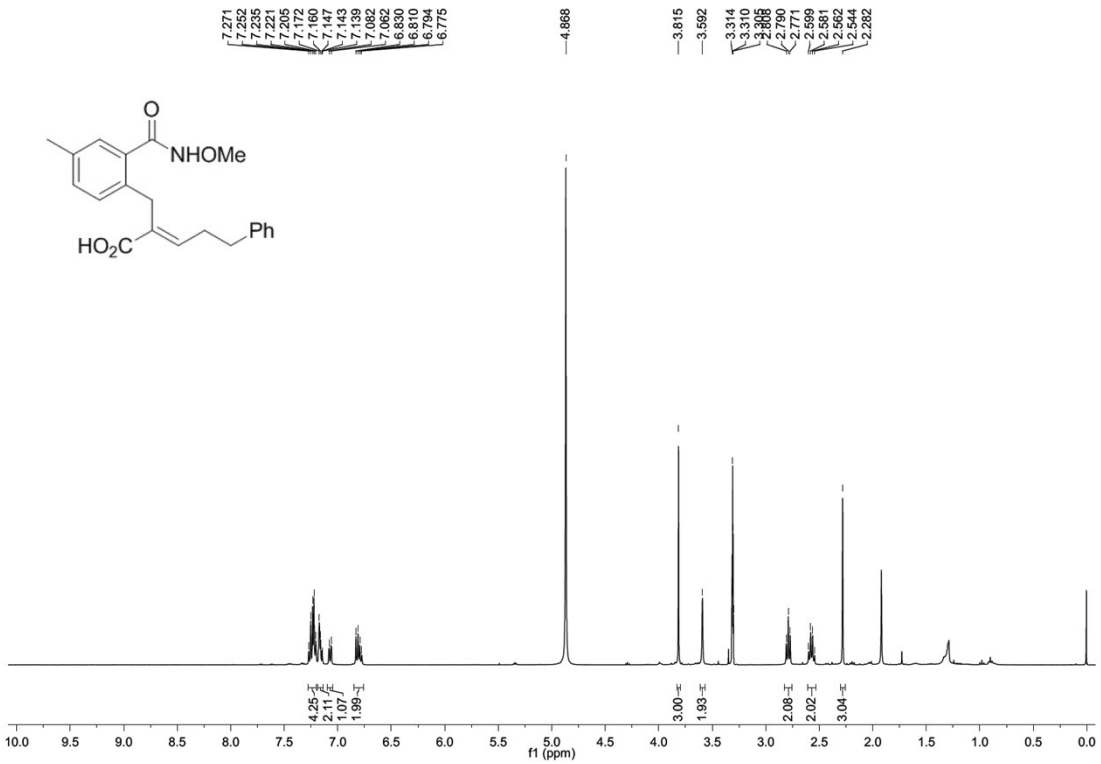

171.022
163.706
141.509
140.563
137.415
135.911
131.770
129.409
128.955
128.438
128.267
125.934
118.673
111.296
67.220
40.147
39.939
39.730
39.520
39.312
39.103
38.894
34.932
29.927
29.616
O
NHOMe
NC
Ph
HO2C
f1 (ppm)

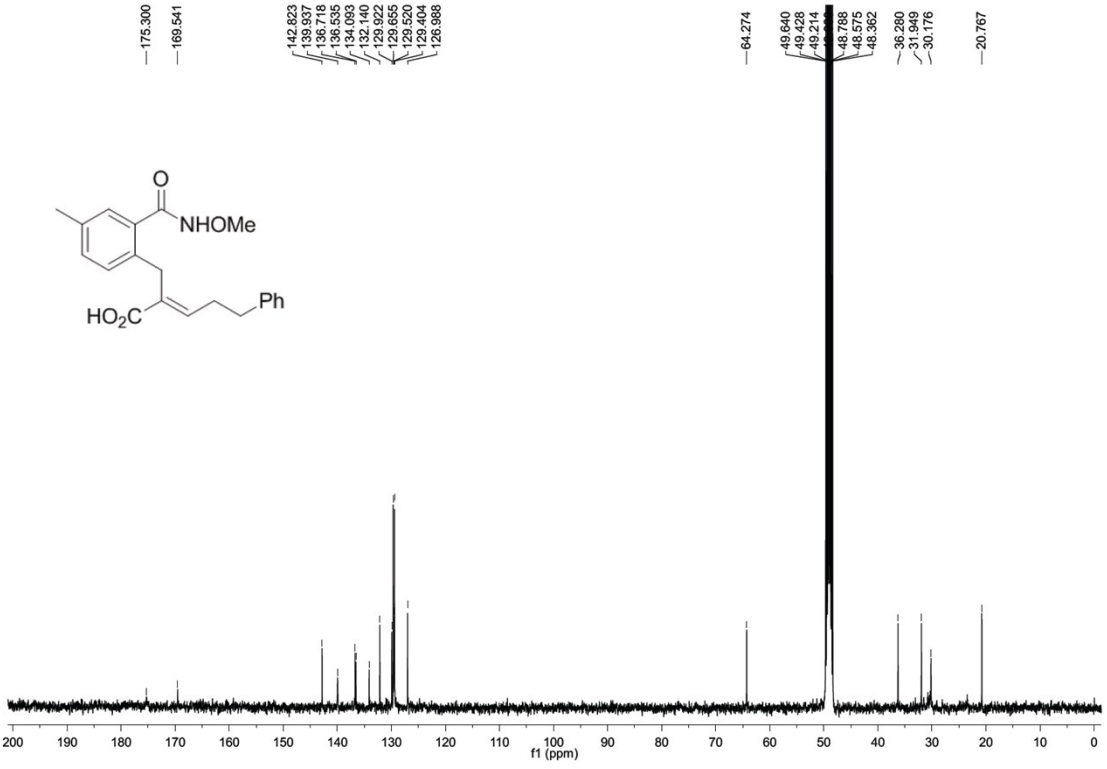
4h


7.264
7.260
7.245
7.233
7.227
7.183
7.180
7.165
7.145
7.141
7.136
7.117
7.063
7.044
7.026
7.007
6.726
6.707
4.874
3.838
3.560
3.318
3.314
3.310
3.305
3.302
2.781
2.763
2.744
2.559
2.541
2.522
2.504
2.326
O
NHOMe
HO2C
Ph
2.07
4.16
2.06
1.00
3.00
1.96
2.03
2.02
3.04
f1 (ppm)

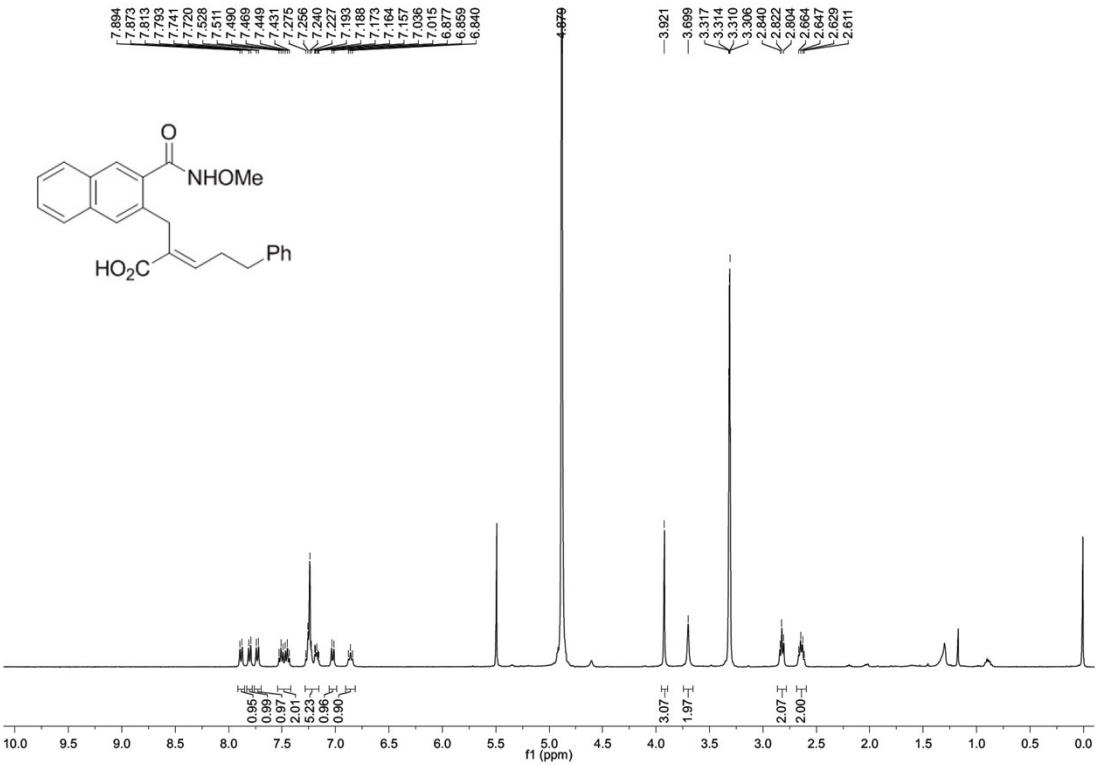

171.694
169.192
144.824
142.412
138.307
136.583
134.493
132.681
130.666
129.594
129.432
128.826
127.100
125.950
64.346
49.638
49.426
49.214
48.786
48.574
48.361
35.757
31.852
29.960
19.134
O
NHOMe
HO2C
Ph
f1 (ppm)

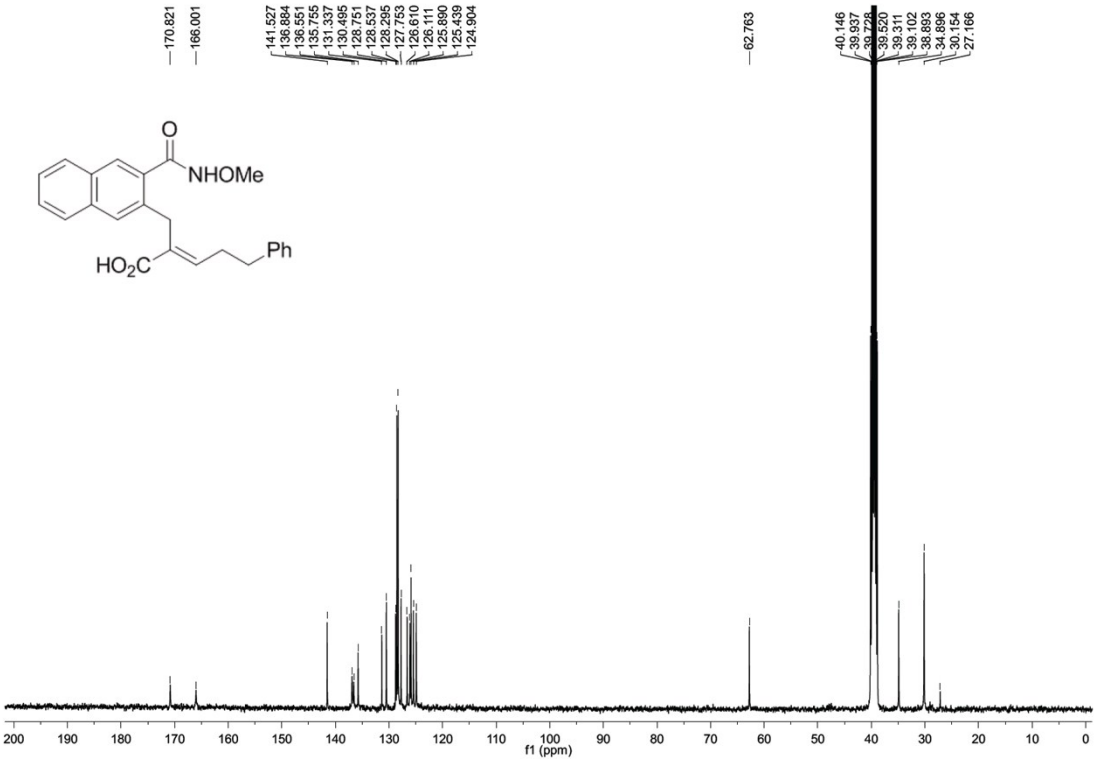
4i


7.271
7.252
7.235
7.221
7.205
7.172
7.160
7.147
7.143
7.139
7.082
7.062
6.830
6.810
6.794
6.775
4.868
3.815
3.592
3.314
3.310
2.790
2.771
2.599
2.581
2.562
2.544
2.282
O
NHOMe
HO2C
Ph
4.25
2.11
1.07
1.99
3.00
1.93
2.08
2.02
3.04
f1 (ppm)


175.300
169.541
142.823
139.937
136.718
136.535
134.093
132.140
129.922
129.655
129.520
129.404
126.988
64.274
49.640
49.428
49.214
48.788
48.575
48.362
36.280
31.949
30.176
20.767
O
NHOMe
HO2C
Ph
f1 (ppm)

4j


7.894
7.873
7.813
7.793
7.741
7.720
7.528
7.511
7.490
7.469
7.449
7.431
7.275
7.256
7.240
7.227
7.193
7.188
7.173
7.164
7.157
7.036
7.015
6.877
6.859
6.840
4.879
3.921
3.699
3.317
3.314
3.310
3.306
2.840
2.822
2.804
2.664
2.647
2.629
2.611
O
NHOMe
HO2C
Ph
0.95
0.99
0.97
2.01
5.23
0.96
0.90
3.07
1.97
2.07
2.00
f1 (ppm)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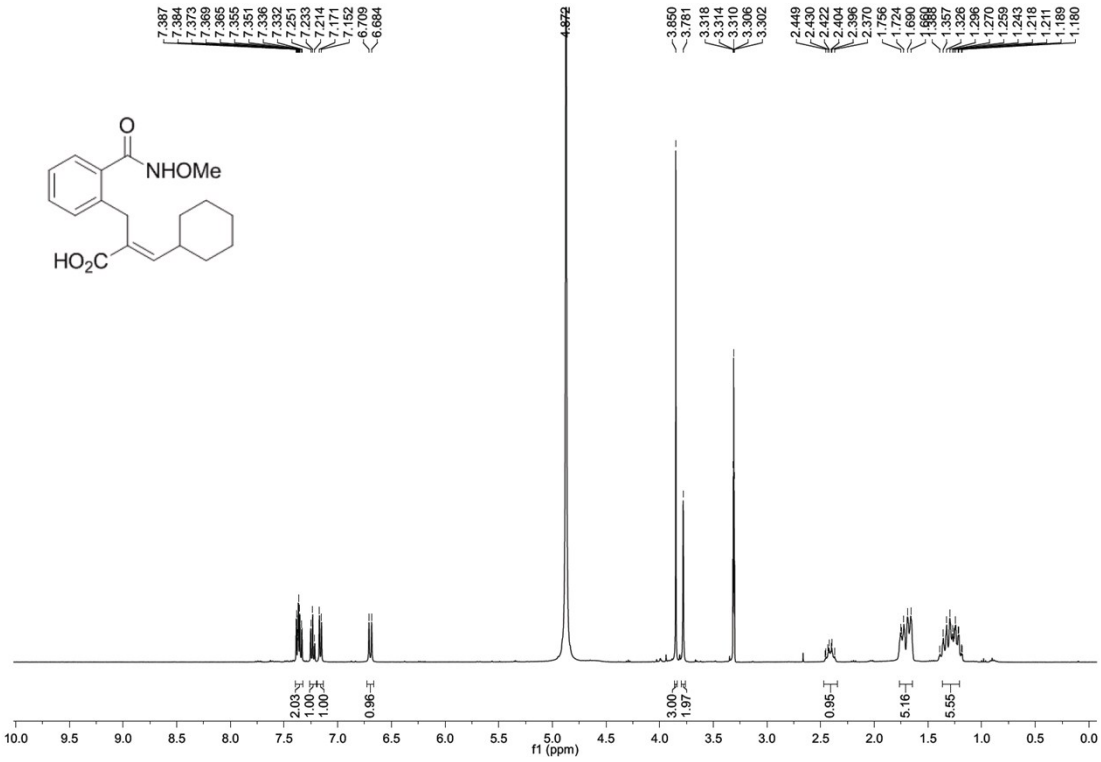
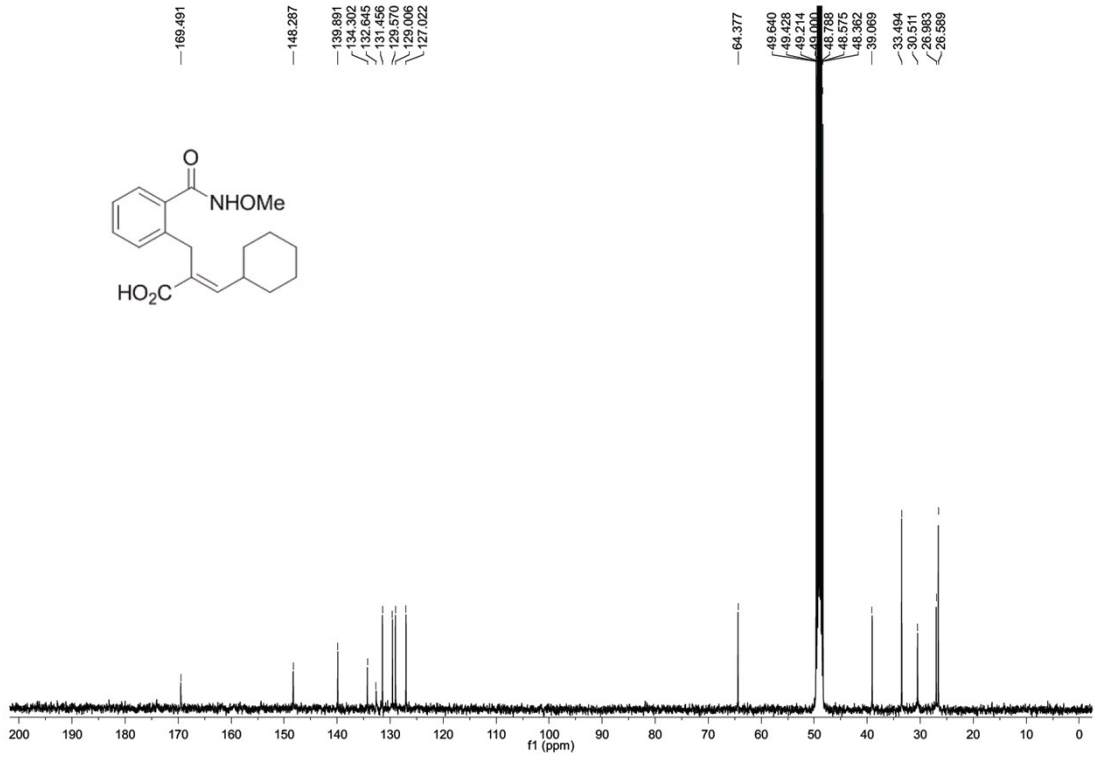
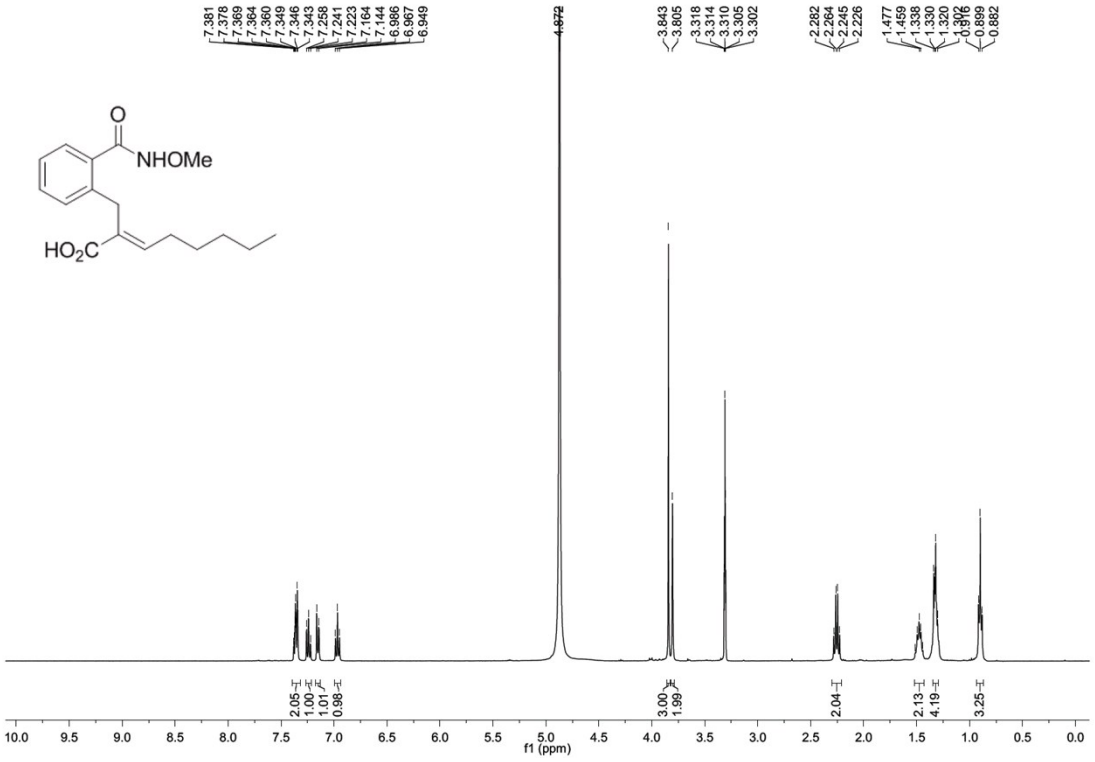
166.001
141.527
136.884
136.551
135.755
131.337
130.495
128.751
128.537
128.295
127.753
126.610
126.111
125.890
125.439
124.904
62.763
40.146
39.937
39.728
39.520
39.311
39.102
38.893
34.896
30.154
27.166
O
NHOMe
HO2C
Ph
f1 (ppm)

4k


7.387
7.384
7.373
7.369
7.365
7.355
7.351
7.336
7.332
7.251
7.233
7.214
7.171
7.152
6.709
6.684
4.872
3.850
3.781
3.318
3.314
3.310
3.306
3.302
2.449
2.430
2.422
2.404
2.396
2.370
1.756
1.724
1.690
1.660
1.357
1.326
1.296
1.270
1.259
1.243
1.218
1.211
1.189
1.180
O
NHOMe
HO2C
2.03
1.00
1.00
0.96
3.00
1.97
0.95
5.16
5.55
f1 (ppm)


169.491
148.287
139.891
134.302
132.645
131.456
129.570
129.006
127.022
64.377
49.640
49.428
49.214
49.000
48.788
48.575
48.362
39.069
33.494
30.511
26.983
26.589
O
NHOMe
HO2C
f1 (ppm)

41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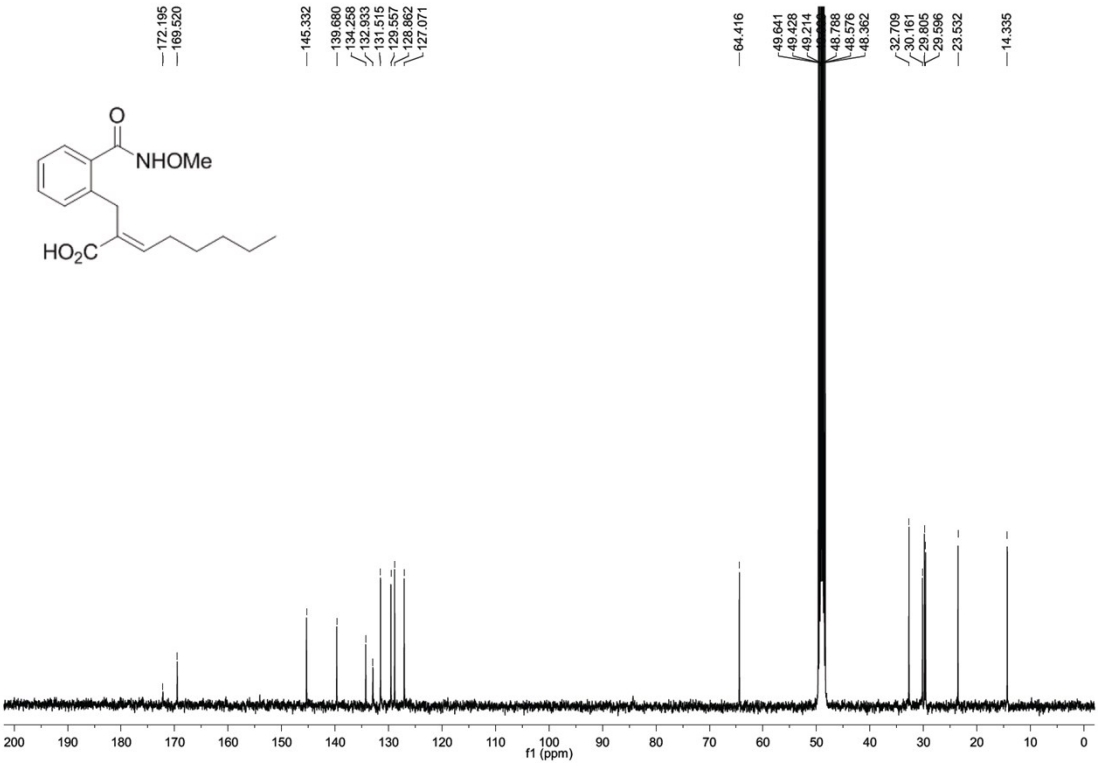
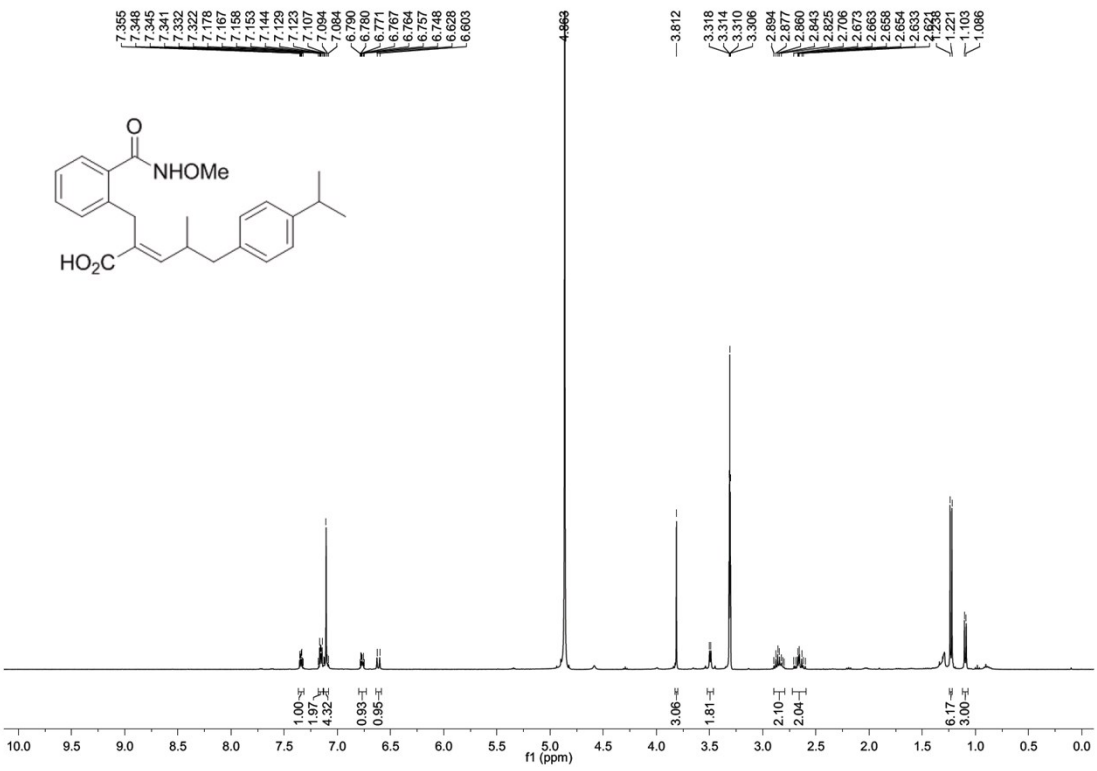
7.378
7.369
7.364
7.360
7.349
7.346
7.343
7.258
7.241
7.223
7.164
7.144
6.986
6.967
6.949
4.872
3.843
3.805
3.318
3.314
3.310
3.305
3.302
2.282
2.264
2.245
2.226
1.477
1.459
1.338
1.330
1.320
0.916
0.899
0.882
O
NHOMe
HO2C
2.05
1.00
1.01
0.98
3.00
1.99
2.04
2.13
4.19
3.25
f1 (ppm)


172.195
169.520
145.332
139.680
134.258
132.933
131.515
129.557
128.862
127.071
64.416
49.641
49.428
49.214
48.788
48.576
48.362
32.709
30.161
29.805
29.596
23.532
14.335
O
NHOMe
HO2C
f1 (ppm)

4m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7.345
7.341
7.332
7.322
7.178
7.167
7.158
7.153
7.144
7.129
7.123
7.107
7.094
7.084
6.790
6.780
6.771
6.767
6.764
6.757
6.748
6.628
6.603
4.863
3.812
3.318
3.314
3.310
3.306
2.894
2.877
2.860
2.843
2.825
2.706
2.673
2.663
2.658
2.654
2.633
1.238
1.221
1.103
1.086
O
NHOMe
HO2C
1.00
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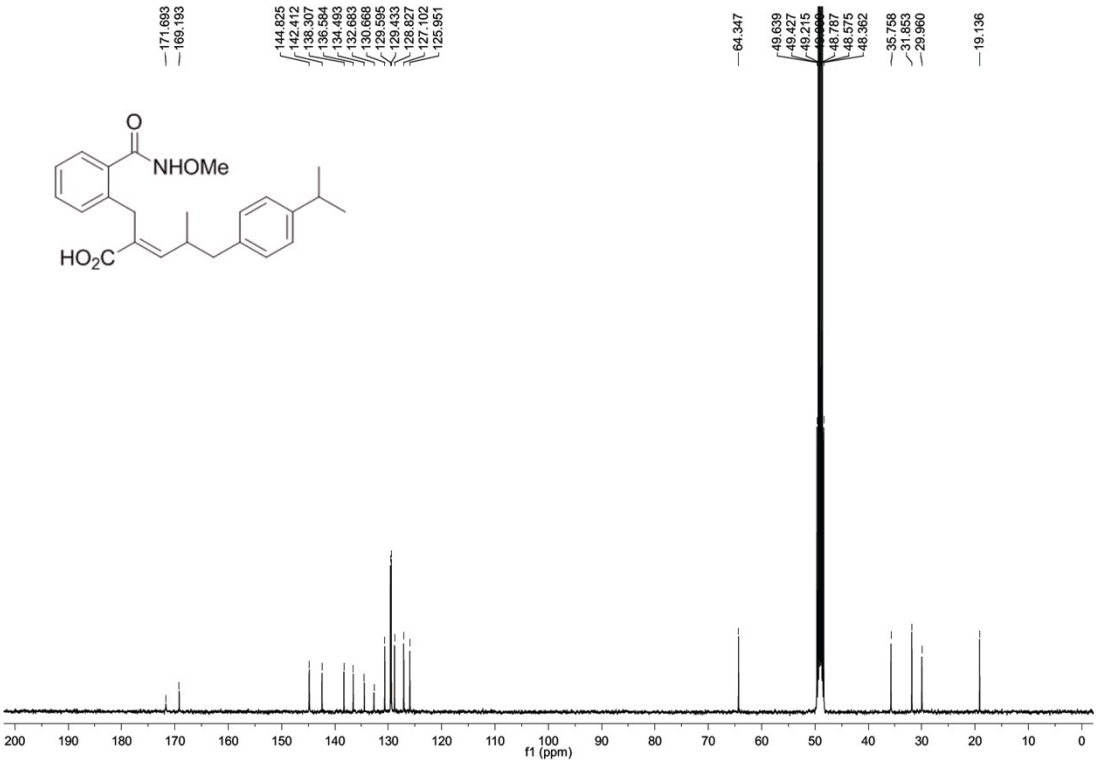
4.32
0.93
0.95
3.06
1.81
2.10
2.04
6.17
3.00
f1 (ppm)


171.693
169.193
144.825
142.412
138.307
136.584
134.493
132.683
130.668
129.595
129.433
128.827
127.102
125.951
64.347
49.639
49.427
49.215
48.787
48.575
48.362
35.758
31.853
29.960
19.136
O
NHOMe
HO2C
f1 (ppm)