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Supplementary Information

Rh(III)-Catalysed Cascade C-H Imidization/Cyclization of *N*-Methoxybenzamides with Isoxazolones for the Assembly of Dihydroquinazolin-4(1*H*)-one Derivatives

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Contents

I. General

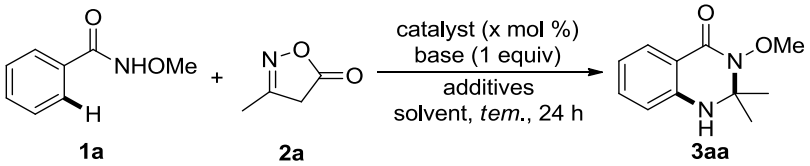
NMR spectra were recorded on JEOL 400 NMR (^{1}H 400 MHz; ^{13}C 100 MHz) in either $CDCl_3$, CD_3OD or DMSO-*d*$_6$. Abbreviations for data quoted are s, singlet; brs, broad singlet; d, doublet; t, triplet; dd, doublet of doublets; m, multiplet. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm; CD_3OD: δ_H = 3.31 ppm, δ_C = 49.00 ppm; *d*$_6$-DMSO: δ_H = 2.50 ppm, δ_C = 39.52 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. *N*-methoxybenzamides[S1] and isoxazolones[S2] were synthesized according to published procedures. 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** (0.2 mmol, 1.0 equiv), 3-methylisoxazol-5(4*H*)-one **2a**, catalyst (x mol %), base (1 equiv) and additives in the solvent was stirred at 100 ^{o}C in an oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC (eluent: PE/EA = 2/1) to afford the corresponding product **3aa**.

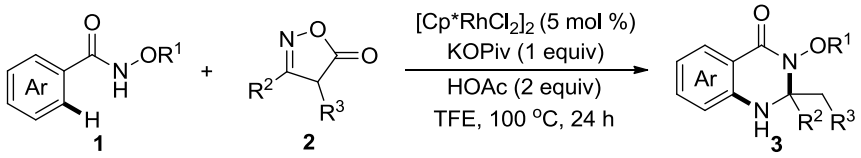
Table S1. Conditions Screening for the Synthesis of **3aa**.[a]



Entry	Catalyst (x mol %)	Base	Additive (y equiv)	Solvent	Yield (%)[b]
1	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	MeOH	23
2	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	THF	n.d.
3	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	TFE	29
4	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	CH_3CN	trace
5	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	toluene	trace
6	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	dioxane	n.d.
7	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	DCE	trace
8	$[Cp^*RhCl_2]_2$ (2.5)	NaOAc	-	HFIP	21
9	$[Cp^*RhCl_2]_2$ (2.5)	CsOAc	-	TFE	38
10	$[Cp^*RhCl_2]_2$ (2.5)	K_2CO_3	-	TFE	18
11	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	-	TFE	48
12	$[Cp^*RhCl_2]_2$ (2.5)	AgOAc	-	TFE	11
13	$[Cp^*RhCl_2]_2$ (2.5)	Cs_2CO_3	-	TFE	9
14	$[Cp^*RhCl_2]_2$ (2.5)	K_3PO_4	-	TFE	15
15	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	HOAc (2)	TFE	65
16	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	PivOH (2)	TFE	57
17	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	H_2O (2)	TFE	39
18	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	$Zn(OAc)_2$ (2)	TFE	56
19	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	$Cu(OAc)_2$ (2)	TFE	n.d.
20	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	$ZnCl_2$ (2)	TFE	n.d.
21	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	AgF (2)	TFE	n.d.
22	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	TfOH (2)	TFE	n.d.
23	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	TsOH (2)	TFE	n.d.
24	$[Cp^*IrCl_2]_2$ (2.5)	KOPiv	HOAc (2)	TFE	trace
25	$[Ru(p\text{-cymene})Cl_2]_2$ (2.5)	KOPiv	HOAc (2)	TFE	n.d.
26	$Cp^*Co(CO)I_2$ (5)	KOPiv	HOAc (2)	TFE	n.d.
27	$Cp^*Rh(CH_3CN)_2(SbF_6)_2$ (5)	-	HOAc (2)	TFE	n.d.
28[c]	$[Cp^*RhCl_2]_2$ (2.5)	KOPiv	HOAc (2)	TFE	70
29	$[Cp^*RhCl_2]_2$ (5)	KOPiv	HOAc (2)	TFE	86
30[d]	$[Cp^*RhCl_2]_2$ (5)	KOPiv	HOAc (2)	TFE	70
31[e]	$[Cp^*RhCl_2]_2$ (5)	KOPiv	HOAc (2)	TFE	66
32[f]	$[Cp^*RhCl_2]_2$ (5)	KOPiv	HOAc (2)	TFE	34
33[g]	$[Cp^*RhCl_2]_2$ (5)	KOPiv	HOAc (2)	TFE	trace
34	$[Cp^*RhCl_2]_2$ (5)	KOPiv	HOAc (1)	TFE	76
35	$[Cp^*RhCl_2]_2$ (5)	KOPiv	K_2CO_3 (1)	TFE	18

[a]Reaction Conditions: **1a** (0.2 mmol), **2a** (0.2 mmol), catalyst (x mol %), base (1 equiv), and additive in the solvent (0.1 M) at 100 °C for 24 h under air. [b]Isolated yield. [c]**2a** (0.24 mmol). [d]TFE (0.2 M). [e]The reaction was conducted at 80 °C. [f]The reaction was conducted at 60 °C. [g]The reaction was conducted at 40 °C. TFE: 2,2,2-Trifluoroethanol; HFIP: 1,1,1,3,3,3-Hexafluoro-2-propanol; n,d.: not detected.

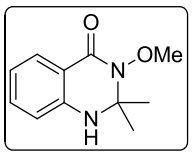
General procedure for the synthesis of dihydroquinazolin-4(1*H*)-ones:



The mixture of *N*-methoxybenzamides **1** (0.2 mmol, 1.0 equiv), isoxazol-5(*4H*)-one **2** (0.24 mmol, 1.2 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), KOPiv (1 equiv) and HOAc (2 equiv) in TFE (2.0 mL) was stirred at 100 °C in an oil bath for 24 h without exclusion of air or moisture. Afterwards, it was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by preparative TLC to afford the corresponding product **3**.

Characterization of products:

3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3aa)



This compound was obtained in 86% yield (35.5 mg) as white solid, m.p.: 160-162 °C. Eluent: PE/EA = 2/1, R_f = 0.5.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.63 (d, *J* = 7.9 Hz, 1H), 7.30-7.23 (m, 1H), 7.08 (s, 1H), 6.70-6.66 (m, 2H), 3.75 (s, 3H), 1.45 (s, 6H).

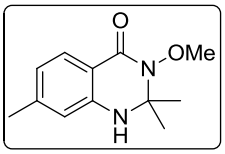
^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 164.0, 145.9, 133.9, 127.3, 117.1, 114.4, 112.8, 75.7, 64.0, 24.5.

HRMS (ESI) calculated for $C_{11}H_{15}N_2O_2$ ($[M+H]^+$): 207.1128; found: 207.1126.

Scale-up synthesis of 3aa: The mixture of *N*-methoxybenzamides **1** (2 mmol, 1.0 equiv), isoxazol-5(*4H*)-one **2a** (2.4 mmol, 1.2 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), KOPiv

(1 equiv) and HOAc (2 equiv) in TFE (20.0 mL) was stirred at 100 ^{o}C in an oil bath for 24 h without exclusion of air or moisture. Afterwards, the mixture was diluted with EtOAc and filtered through a short silica gel column to remove the metal residues. Then, the reaction mixture was concentrated and purified by column chromatography (eluent: PE/EtOAc = 5/1) to afford the desired product **3aa** (0.329 g, 80%).

3-methoxy-2,2,7-trimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3ba)



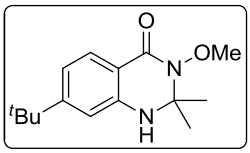
This compound was obtained in 81% yield (35.6 mg) as white solid, m.p.: 214-215 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.5.

^{1}H NMR (400 MHz, CD_3OD): δ 7.59 (d, *J* = 8.0 Hz, 1H), 6.57 (d, *J* = 8.0 Hz, 1H), 6.49 (s, 1H), 3.84 (s, 3H), 2.26 (s, 3H), 1.53 (s, 6H).

^{13}C NMR (100 MHz, CD_3OD): δ 167.4, 147.5, 146.7, 128.7, 120.3, 115.8, 111.8, 77.7, 65.3, 24.9, 21.8.

HRMS (ESI) calculated for $C_{12}H_{17}N_2O_2$ ($[M+H]^+$): 221.1285; found: 221.1283.

7-(*tert*-butyl)-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3ca)



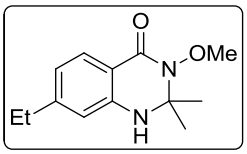
This compound was obtained in 82% yield (43.0 mg) as white solid, m.p.: 217-218 ^{o}C. Eluent: PE/EA = 3/1, R_f = 0.7

^{1}H NMR (400 MHz, CD_3OD): δ 7.63 (d, *J* = 8.4 Hz, 1H), 6.82 (dd, *J* = 8.4, 1.5 Hz, 1H), 6.70 (d, *J* = 1.4 Hz, 1H), 3.84 (s, 3H), 1.53 (s, 6H), 1.27 (s, 9H).

^{13}C NMR (100 MHz, CD_3OD): δ 167.4, 159.7, 147.4, 128.4, 116.9, 112.0, 111.6, 77.7, 65.3, 35.9, 31.4, 25.0.

HRMS (ESI) calculated for $C_{15}H_{23}N_2O_2$ ($[M+H]^+$): 263.1754; found: 263.1750.

7-ethyl-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3da)



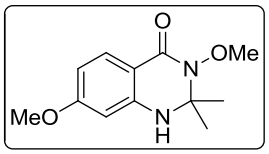
This compound was obtained in 78% yield (36.5 mg) as white solid, m.p.: 202-204 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

^{1}H NMR (400 MHz, CD_3OD): δ 7.62 (d, *J* = 8.1 Hz, 1H), 6.60 (d, *J* = 8.1 Hz, 1H), 6.51 (s, 1H), 3.84 (s, 3H), 2.55 (q, *J* = 7.6 Hz, 2H), 1.53 (s, 6H), 1.20 (t, *J* = 7.6 Hz, 3H).

^{13}C NMR (100 MHz, CD_3OD): δ 167.4, 153.0, 147.6, 128.8, 119.2, 114.6, 112.0, 77.7, 65.3, 30.1, 24.9, 15.5.

HRMS (ESI) calculated for $C_{13}H_{19}N_2O_2$ ($[M+H]^+$): 235.1441; found: 237.1439.

3,7-dimethoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3ea)



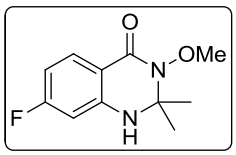
This compound was obtained in 78% yield (36.8 mg) as white solid, m.p.: 194-196 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

^{1}H NMR (400 MHz, CD_3OD): δ 7.63 (d, *J* = 8.8 Hz, 1H), 6.33 (dd, *J* = 8.8, 2.2 Hz, 1H), 6.17 (d, *J* = 2.1 Hz, 1H), 3.84 (s, 3H), 3.78 (s, 3H), 1.53 (s, 6H).

^{13}C NMR (100 MHz, CD_3OD): δ 167.5, 166.6, 149.4, 130.6, 107.4, 107.1, 98.7, 77.6, 65.3, 55.8, 24.9.

HRMS (ESI) calculated for $C_{12}H_{17}N_2O_3$ ($[M+H]^+$): 237.1234; found: 237.1232.

7-fluoro-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3fa)



This compound was obtained in 70% yield (31.4 mg) as white solid, m.p.: 182-184 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

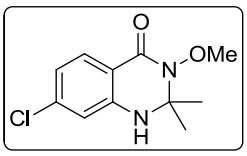
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (dd, *J* = 8.6, 6.4 Hz, 1H), 6.51 (td, *J* = 8.6, 2.2 Hz, 1H), 6.33 (dd, *J* = 10.0, 2.2 Hz, 1H), 4.87 (brs, 1H), 3.90 (s, 3H), 1.60 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$): δ 166.9 (d, *J* = 250.5 Hz), 164.6, 146.6 (d, *J* = 12.4 Hz), 131.2 (d, *J* = 11.3 Hz), 110.8, 106.7 (d, *J* = 22.9 Hz), 101.0 (d, *J* = 25.4 Hz), 76.5, 64.9, 25.3.

^{19}F NMR (376 MHz, $CDCl_3$): -106.0.

HRMS (ESI) calculated for $C_{11}H_{14}FN_2O_2$ ($[M+H]^+$): 225.1034; found: 225.1032.

7-chloro-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3ga)



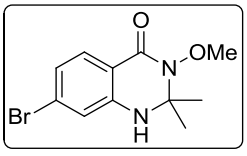
This compound was obtained in 75% yield (36.0 mg) as white solid, m.p.: 239-241 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.65

^{1}H NMR (400 MHz, DMSO-d_6): δ 7.61 (d, *J* = 8.8 Hz, 1H), 7.38 (s, 1H), 6.71-6.69 (m, 2H), 3.75 (s, 3H), 1.45 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 163.1, 146.7, 138.5, 129.3, 117.2, 113.4, 111.6, 75.7, 64.1, 24.7.

HRMS (ESI) calculated for $C_{11}H_{14}ClN_2O_2$ ($[M+H]^+$): 241.0738; found: 241.0735.

7-bromo-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3ha)



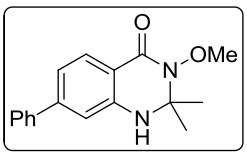
This compound was obtained in 78% yield (44.3 mg) as white solid, m.p.: 220-222 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.65

^{1}H NMR (400 MHz, DMSO-d_6): δ 7.53 (d, *J* = 8.1 Hz, 1H), 7.37 (s, 1H), 6.87-6.82 (m, 2H), 3.75 (s, 3H), 1.45 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.2, 146.8, 129.4, 127.6, 120.0, 116.4, 111.9, 75.8, 64.1, 24.7.

HRMS (ESI) calculated for $C_{11}H_{14}BrN_2O_2$ ([M+H]$^+$): 285.0233; found: 285.0231.

3-methoxy-2,2-dimethyl-7-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3ia)



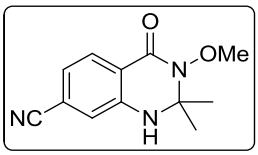
This compound was obtained in 90% yield (50.7 mg) as white solid, m.p.: 180-182 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

^{1}H NMR (400 MHz, CD$_3$OD): δ 7.78 (d, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 7.3 Hz, 2H), 7.41 (t, *J* = 7.4 Hz, 2H), 7.34 (t, *J* = 7.3 Hz, 1H), 6.99 (dd, *J* = 8.2, 1.4 Hz, 1H), 6.90 (d, *J* = 1.1 Hz, 1H), 3.86 (s, 3H), 1.56 (s, 6H).

^{13}C NMR (100 MHz, CD$_3$OD): δ 167.1, 148.7, 147.8, 141.6, 129.9, 129.3, 129.2, 128.0, 118.0, 113.8, 113.1, 77.7, 65.3, 25.1.

HRMS (ESI) calculated for $C_{17}H_{19}N_2O_2$ ([M+H]$^+$): 283.1441; found: 283.1438.

3-methoxy-2,2-dimethyl-4-oxo-1,2,3,4-tetrahydroquinazoline-7-carbonitrile (3ja)



This compound was obtained in 71% yield (32.8 mg) as yellow-green solid, m.p.: 227-229 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.4

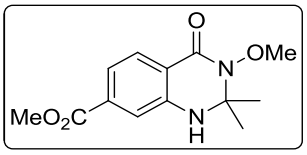
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.75 (d, *J* = 7.9 Hz, 1H), 7.61 (s, 1H), 7.09-7.00 (m, 2H), 3.77 (s, 3H), 1.48 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 162.2, 145.6, 128.6, 119.7, 118.4, 117.8, 116.0, 115.9, 75.8, 64.2, 24.8.

HRMS (ESI) calculated for $C_{12}H_{14}N_3O_2$ ([M+H]$^+$): 232.1081; found: 232.1076.

methyl

3-methoxy-2,2-dimethyl-4-oxo-1,2,3,4-tetrahydroquinazoline-7-carboxylate (3ka)



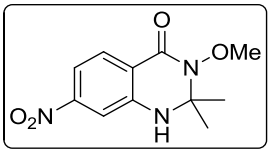
This compound was obtained in 64% yield (33.8 mg) as white solid, m.p.: 223-225 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.4

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.73 (d, *J* = 8.1 Hz, 1H), 7.41 (s, 1H), 7.30 (s, 1H), 7.22 (dd, *J* = 8.2, 1.2 Hz, 1H), 3.83 (s, 3H), 3.77 (s, 3H), 1.47 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 165.8, 162.9, 145.7, 134.3, 127.9, 117.2, 116.1, 115.3, 75.8, 64.1, 52.4, 24.7.

HRMS (ESI) calculated for $C_{13}H_{17}N_2O_4$ ($[M+H]^+$): 265.1183; found: 265.1182.

3-methoxy-2,2-dimethyl-7-nitro-2,3-dihydroquinazolin-4(1*H*)-one (3la)



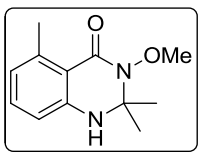
This compound was obtained in 76% yield (38.2 mg) as yellow-green solid, m.p.: 260-261 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.86-7.83 (m, 2H), 7.49 (d, *J* = 1.8 Hz, 1H), 7.44 (dd, *J* = 8.5, 2.0 Hz, 1H), 3.79 (s, 3H), 1.50 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 162.0, 151.2, 146.1, 129.3, 117.1, 111.1, 108.9, 75.9, 64.2, 24.9.

HRMS (ESI) calculated for $C_{11}H_{14}N_3O_4$ ($[M+H]^+$): 252.0979; found: 252.0975.

3-methoxy-2,2,5-trimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3ma)



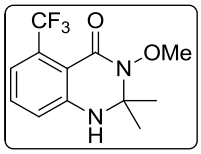
This compound was obtained in 41% yield (18.0 mg) as yellow solid, m.p.: 215-216 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.8

^{1}H NMR (400 MHz, DMSO-d_6): δ 7.10 (t, *J* = 7.7 Hz, 1H), 7.00 (s, 1H), 6.53 (d, *J* = 8.1 Hz, 1H), 6.45 (d, *J* = 7.3 Hz, 1H), 3.73 (s, 3H), 2.52 (s, 3H), 1.42 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 165.3, 147.2, 141.0, 132.9, 120.7, 112.9, 110.6, 74.6, 63.9, 24.4, 22.6.

HRMS (ESI) calculated for $C_{12}H_{17}N_2O_2$ ($[M+H]^+$): 221.1285; found: 221.1281.

3-methoxy-2,2-dimethyl-5-(trifluoromethyl)-2,3-dihydroquinazolin-4(1*H*)-one (3na)



This compound was obtained in 31% yield (17.0 mg) as white solid, m.p.: 239-241 °C. Eluent: PE/EA = 2/1, R_f = 0.5

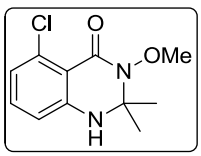
^{1}H NMR (400 MHz, DMSO-d_6): δ 7.63 (s, 1H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 7.00 (d, *J* = 8.2 Hz, 1H), 3.75 (s, 3H), 1.46 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 161.1, 147.9, 133.2, 128.5 (q, *J* = 31.6 Hz), 123.7 (q, *J* = 272.8 Hz), 120.0, 116.5 (q, *J* = 7.3 Hz), 108.4, 74.4, 64.1, 24.4.

^{19}F NMR (376 MHz, DMSO-d_6): -58.2.

HRMS (ESI) calculated for $C_{12}H_{14}F_3N_2O_2$ ($[M+H]^+$): 275.1002; found: 275.0999.

5-chloro-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3oa)



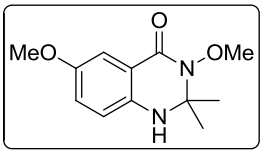
This compound was obtained in 38% yield (18.2 mg) as white solid, m.p.: 198-200 °C. Eluent: PE/EA = 2/1, R_f = 0.5

^{1}H NMR (400 MHz, DMSO-d_6): δ 7.45 (s, 1H), 7.22-7.16 (m, 1H), 6.68 (dd, *J* = 7.6, 1.2 Hz, 1H), 6.65 (dd, *J* = 8.4, 0.8 Hz, 1H), 3.73 (s, 3H), 1.44 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6): δ 162.1, 148.3, 133.9, 133.8, 120.1, 113.9, 108.5, 74.5, 64.0, 24.5.

HRMS (ESI) calculated for $C_{11}H_{14}ClN_2O_2$ ([M+H] $^+$): 241.0738; found: 241.0736.

3,6-dimethoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3pa)



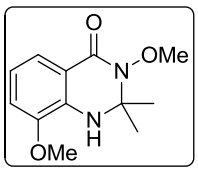
This compound was obtained in 25% yield (11.8 mg) as yellow solid, m.p.: 148-150 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.14 (d, *J* = 3.0 Hz, 1H), 6.96 (dd, *J* = 8.8, 3.1 Hz, 1H), 6.67-6.64 (m, 2H), 3.76 (s, 3H), 3.69 (s, 3H), 1.43 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.7, 151.2, 140.1, 122.2, 116.1, 113.2, 109.1, 75.8, 63.8, 55.1, 24.1.

HRMS (ESI) calculated for $C_{12}H_{17}N_2O_3$ ([M+H] $^+$): 237.1234; found: 237.1233.

3,8-dimethoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3pa')



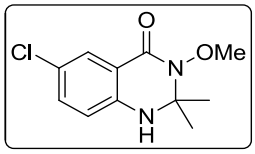
This compound was obtained in 38% yield (17.9 mg) as green solid, m.p.: 154-156 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.7

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.25 (dd, *J* = 8.0, 1.1 Hz, 1H), 6.98 (dd, *J* = 7.9, 1.1 Hz, 1H), 6.66 (t, *J* = 8.0 Hz, 1H), 6.42 (s, 1H), 3.81 (s, 3H), 3.75 (s, 3H), 1.48 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.9, 146.3, 135.9, 118.7, 116.8, 114.0, 112.8, 76.2, 64.0, 55.7, 24.3.

HRMS (ESI) calculated for $C_{12}H_{17}N_2O_3$ ([M+H] $^+$): 237.1234; found: 237.1232.

6-chloro-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3qa)



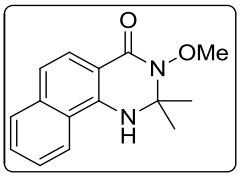
This compound was obtained in 59% yield (28.4 mg) as yellow solid, m.p.: 176-178 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.54 (d, *J* = 2.6 Hz, 1H), 7.31 (s, 1H), 7.31-7.28 (m, 1H), 6.70 (d, *J* = 8.7 Hz, 1H), 3.75 (s, 3H), 1.45 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 162.7, 144.6, 133.7, 126.2, 120.8, 116.5, 113.9, 75.8, 64.1, 24.6.

HRMS (ESI) calculated for $C_{11}H_{14}ClN_2O_2$ ([M+H] $^{+}$): 241.0738; found: 241.0736.

3-methoxy-2,2-dimethyl-2,3-dihydrobenzo[*h*]quinazolin-4(1*H*)-one (3ra)



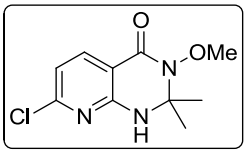
This compound was obtained in 50% yield (25.5 mg) as yellow solid, m.p.: 190-192 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

^{1}H NMR (400 MHz, CD$_3$OD): δ 9.33 (d, *J* = 8.7 Hz, 1H), 7.73 (d, *J* = 8.9 Hz, 1H), 7.62 (d, *J* = 8.0 Hz, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 6.84 (d, *J* = 8.9 Hz, 1H), 3.85 (s, 3H), 1.56 (s, 6H).

^{13}C NMR (100 MHz, CD$_3$OD): δ 169.3, 148.9, 137.1, 134.3, 129.7, 129.6, 129.3, 125.5, 123.8, 117.8, 102.0, 76.6, 65.3, 24.4.

HRMS (ESI) calculated for $C_{15}H_{17}N_2O_2$ ([M+H] $^{+}$): 257.1285; found: 257.1281.

7-chloro-3-methoxy-2,2-dimethyl-2,3-dihydropyrido[2,3-d]pyrimidin-4(1*H*)-one (3sa)



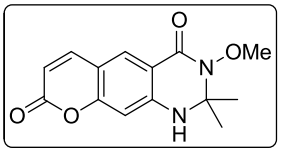
This compound was obtained in 74% yield (35.7 mg) as white solid, m.p.: 219-200 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.47 (s, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 6.76 (d, *J* = 7.9 Hz, 1H), 3.76 (s, 3H), 1.49 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 161.9, 155.4, 153.6, 139.4, 113.1, 106.2, 75.3, 64.2, 25.1.

HRMS (ESI) calculated for $C_{10}H_{13}ClN_3O_2$ ([M+H] $^{+}$): 242.0691; found: 242.0691.

3-methoxy-2,2-dimethyl-2,3-dihydro-4*H*-pyrano[3,2-*g*]quinazoline-4,8(1*H*)-dione (3ta)



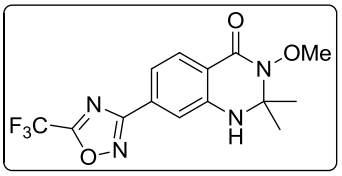
This compound was obtained in 70% yield (38.4 mg) as yellow solid, m.p.: 261-263 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.3.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.01 (s, 1H), 7.96 (d, *J* = 9.7 Hz, 1H), 7.93 (s, 1H), 6.48 (s, 1H), 6.14 (d, *J* = 9.5 Hz, 1H), 3.77 (s, 3H), 1.49 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 162.6, 159.9, 158.0, 148.4, 144.7, 129.3, 110.8, 110.4, 110.3, 99.3, 75.7, 64.2, 25.1.

HRMS (ESI) calculated for $C_{14}H_{15}N_2O_4$ ([M+H] $^{+}$): 275.1026; found: 275.1024.

3-methoxy-2,2-dimethyl-7-(5-(trifluoromethyl)-1,2,4-oxadiazol-3-yl)-2,3-dihydro quinazolin-4(1*H*)-one (3ua)



This compound was obtained in 71% yield (48.6 mg) as yellow solid, m.p.: 190-192 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.7.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.81 (d, *J* = 8.1 Hz, 1H), 7.53 (s, 1H), 7.41 (s,

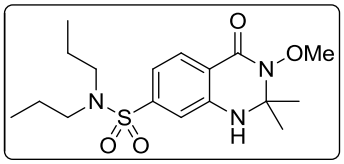
1H), 7.33 (d, *J* = 8.1 Hz, 1H), 3.79 (s, 3H), 1.49 (s, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): 166.0, 165.1 (q, *J* = 43.7 Hz), 162.8, 146.1, 129.0, 128.7, 115.8 (q, *J* = 271.8 Hz), 115.5, 115.4, 113.2, 75.8, 64.1, 24.7.

^{19}F NMR (376 MHz, DMSO-*d*$_6$): -64.9.

HRMS (ESI) calculated for $C_{14}H_{14}F_3N_4O_3$ ([M+H] $^+$): 343.1013; found: 343.1007.

3-methoxy-2,2-dimethyl-4-oxo-*N*,*N*-dipropyl-1,2,3,4-tetrahydroquinazoline-7-sulfonamide (3va)



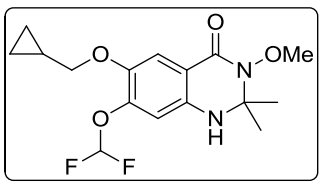
This compound was obtained in 73% yield (53.9 mg) as yellow solid, m.p.: 166-168 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.7.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.79 (d, *J* = 8.2 Hz, 1H), 7.58 (s, 1H), 7.10 (s, 1H), 7.02 (d, *J* = 8.2 Hz, 1H), 3.77 (s, 3H), 3.02 (t, *J* = 7.5 Hz, 4H), 1.52-1.42 (m, 10H), 0.80 (t, *J* = 7.3 Hz, 6H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 162.5, 145.8, 144.2, 128.7, 115.2, 114.4, 112.5, 75.8, 64.1, 49.6, 24.7, 21.6, 11.0.

HRMS (ESI) calculated for $C_{17}H_{28}N_3O_4S$ ([M+H] $^+$): 370.1795; found: 370.1791.

6-(cyclopropylmethoxy)-7-(difluoromethoxy)-3-methoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3wa)



This compound was obtained in 76% yield (52.2 mg) as yellow solid, m.p.: 145-147 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.7

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.26 (s, 1H), 7.15 (t, *J* = 74.0 Hz, 1H), 6.96 (s,

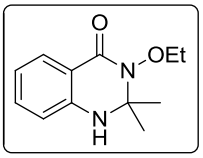
1H), 6.49 (s, 1H), 3.78 (d, *J* = 6.9 Hz, 2H), 3.74 (s, 3H), 1.43 (s, 6H), 1.22-1.16 (m, 1H), 0.57-0.52 (m, 2H), 0.33-0.30 (m, 2H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.3, 145.5, 141.5, 140.9, 116.4 (t, *J* = 258.1 Hz), 113.0, 109.6, 106.0, 76.0, 73.8, 64.1, 24.4, 10.1, 3.0.

^{19}F NMR (376 MHz, DMSO-*d*$_6$): -81.68 (d, *J* = 76.5 Hz).

HRMS (ESI) calculated for $C_{16}H_{21}F_2N_2O_4$ ([M+H]$^+$): 343.1464; found: 343.1460.

3-ethoxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3xa)



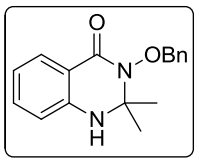
This compound was obtained in 76% yield (33.5 mg) as yellow solid, m.p.: 175-178 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.7.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.61 (d, *J* = 7.7 Hz, 1H), 7.31-7.24 (m, 1H), 7.07 (s, 1H), 6.70-6.66 (m, 2H), 3.97 (q, *J* = 7.1 Hz, 2H), 1.44 (s, 6H), 1.19 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 164.2, 145.8, 133.9, 127.3, 117.0, 114.4, 112.9, 75.5, 71.6, 24.6, 13.4.

HRMS (ESI) calculated for $C_{12}H_{17}N_2O_2$ ([M+H]$^+$): 221.1285; found: 221.1284.

3-(benzyloxy)-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one (3ya)



This compound was obtained in 63% yield (35.5 mg) as yellow oil. Eluent: PE/EA = 2/1, R_f = 0.75.

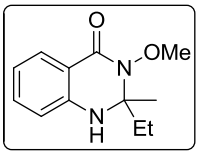
^{1}H NMR (400 MHz, CD$_3$OD): δ 7.78-7.73 (m, 1H), 7.49 (dd, *J* = 7.3, 1.3 Hz, 2H), 7.40-7.34 (m, 3H), 7.31-7.26 (m, 1H), 6.74 (t, *J* = 7.5 Hz, 1H), 6.69 (d, *J* = 8.2 Hz, 1H), 5.02 (s, 2H), 1.52 (s, 6H).

^{13}C NMR (100 MHz, CD$_3$OD): δ 167.4, 147.5, 136.6, 135.5, 130.6, 129.7, 129.4,

128.6, 118.8, 115.8, 114.3, 80.0, 77.6, 25.2.

HRMS (ESI) calculated for $C_{17}H_{19}N_2O_2$ ([M+H] $^+$): 283.1441; found: 283.1441.

2-ethyl-3-methoxy-2-methyl-2,3-dihydroquinazolin-4(1*H*)-one (3ab)



This compound was obtained in 65% yield (28.6 mg) as yellow solid, m.p.: 105-107 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6.

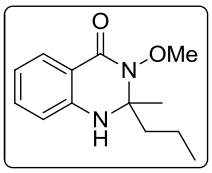
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.28-7.22 (m, 1H), 7.06 (s, 1H), 6.70-6.61 (m, 2H), 3.77 (s, 3H), 1.87 (dq, *J* = 14.6, 7.3 Hz, 1H), 1.67 (dq, *J* = 14.7, 7.4 Hz, 1H), 1.46 (s, 3H), 0.87 (t, *J* = 7.4 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.9, 145.9, 133.9, 127.1, 116.7, 114.0, 112.5, 78.3, 63.9, 29.7, 23.2, 8.4.

HRMS (ESI) calculated for $C_{12}H_{17}N_2O_2$ ([M+H] $^+$): 221.1285; found: 221.1285.

Another reaction was conducted using 3,4-dimethylisoxazol-5(4*H*)-one as the coupling partner to react with *N*-methoxybenzamide **1a** under the standard conditions, affording the desired product 3ab in 29% (12.8 mg) isolated yield.

3-methoxy-2-methyl-2-propyl-2,3-dihydroquinazolin-4(1*H*)-one (3ac)



This compound was obtained in 63% yield (29.5 mg) as yellow solid, m.p.: 181-183 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.5.

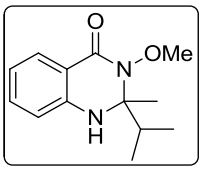
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.58 (d, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.06 (s, 1H), 6.68-6.61 (m, 2H), 3.76 (s, 3H), 1.85-1.75 (m, 1H), 1.68-1.58 (m, 1H), 1.47 (s, 3H), 1.41-1.28 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.8, 145.9, 133.9, 127.1, 116.7, 113.9, 112.5,

77.9, 63.8, 23.8, 16.9, 14.1.

HRMS (ESI) calculated for $C_{13}H_{19}N_2O_2$ ([M+H] $^+$): 235.1441; found: 235.1441.

2-isopropyl-3-methoxy-2-methyl-2,3-dihydroquinazolin-4(1*H*)-one (3ad)



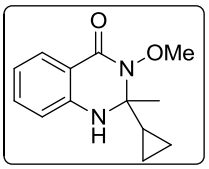
This compound was obtained in 61% yield (28.5 mg) as yellow solid, m.p.: 143-145 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.65.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.55 (d, *J* = 7.8 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 6.99 (s, 1H), 6.70 (d, *J* = 8.3 Hz, 1H), 6.61 (t, *J* = 7.5 Hz, 1H), 3.77 (s, 3H), 2.25-2.15 (m, 1H), 1.50 (s, 3H), 0.92 (d, *J* = 6.9 Hz, 3H), 0.82 (d, *J* = 6.8 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 162.2, 145.8, 133.7, 126.9, 116.3, 113.5, 112.6, 80.4, 63.9, 35.4, 21.2, 17.8, 16.8.

HRMS (ESI) calculated for $C_{13}H_{19}N_2O_2$ ([M+H] $^+$): 235.1441; found: 235.1441.

2-cyclopropyl-3-methoxy-2-methyl-2,3-dihydroquinazolin-4(1*H*)-one (3ae)



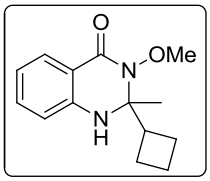
This compound was obtained in 60% yield (27.8 mg) as yellow solid, m.p.: 163-165 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.6.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.57 (d, *J* = 7.7 Hz, 1H), 7.23 (t, *J* = 7.7 Hz, 1H), 6.83 (s, 1H), 6.67-6.61 (m, 2H), 3.78 (s, 3H), 1.47 (s, 3H), 1.41-1.35 (m, 1H), 0.52-0.42 (m, 2H), 0.34-0.24 (m, 2H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.2, 146.0, 133.9, 127.0, 116.7, 113.6, 112.4, 77.5, 63.9, 23.5, 18.4, 1.7, 1.2.

HRMS (ESI) calculated for $C_{13}H_{17}N_2O_2$ ([M+H] $^+$): 233.1285; found: 233.1284.

2-cyclobutyl-3-methoxy-2-methyl-2,3-dihydroquinazolin-4(1*H*)-one (3af)



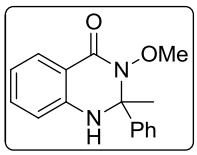
This compound was obtained in 55% yield (27.2 mg) as yellow solid, m.p.: 194-196 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.7.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.27-7.21 (m, 1H), 7.05 (s, 1H), 6.75 (d, *J* = 8.2 Hz, 1H), 6.61 (t, *J* = 7.4 Hz, 1H), 3.72 (s, 3H), 2.97-2.84 (m, 1H), 2.09-1.97 (m, 1H), 1.89-1.85 (m, 1H), 1.81-1.73 (m, 1H), 1.73-1.64 (m, 2H), 1.59-1.51 (m, 1H), 1.38 (s, 3H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.2, 146.2, 133.8, 126.9, 116.4, 113.7, 112.4, 78.4, 63.8, 42.7, 23.4, 22.7, 21.2, 16.6.

HRMS (ESI) calculated for $C_{14}H_{19}N_2O_2$ ([M+H] $^{+}$): 247.1441; found: 247.1438.

3-methoxy-2-methyl-2-phenyl-2,3-dihydroquinazolin-4(1*H*)-one (3ag)



This compound was obtained in 23% yield (12.3 mg) as yellow solid, m.p.: 212-214 ^{o}C. Eluent: PE/EA = 2/1, R_f = 0.7.

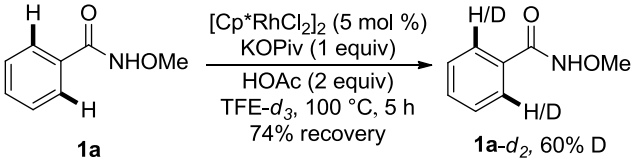
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.96 (s, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 2H), 7.31-7.19 (m, 4H), 6.72 (d, *J* = 8.1 Hz, 1H), 6.65 (t, *J* = 7.5 Hz, 1H), 3.77 (s, 3H), 1.89 (s, 3H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 163.7, 145.8, 144.1, 133.9, 128.1, 127.7, 127.3, 125.6, 117.5, 114.4, 113.7, 79.0, 64.3, 26.2.

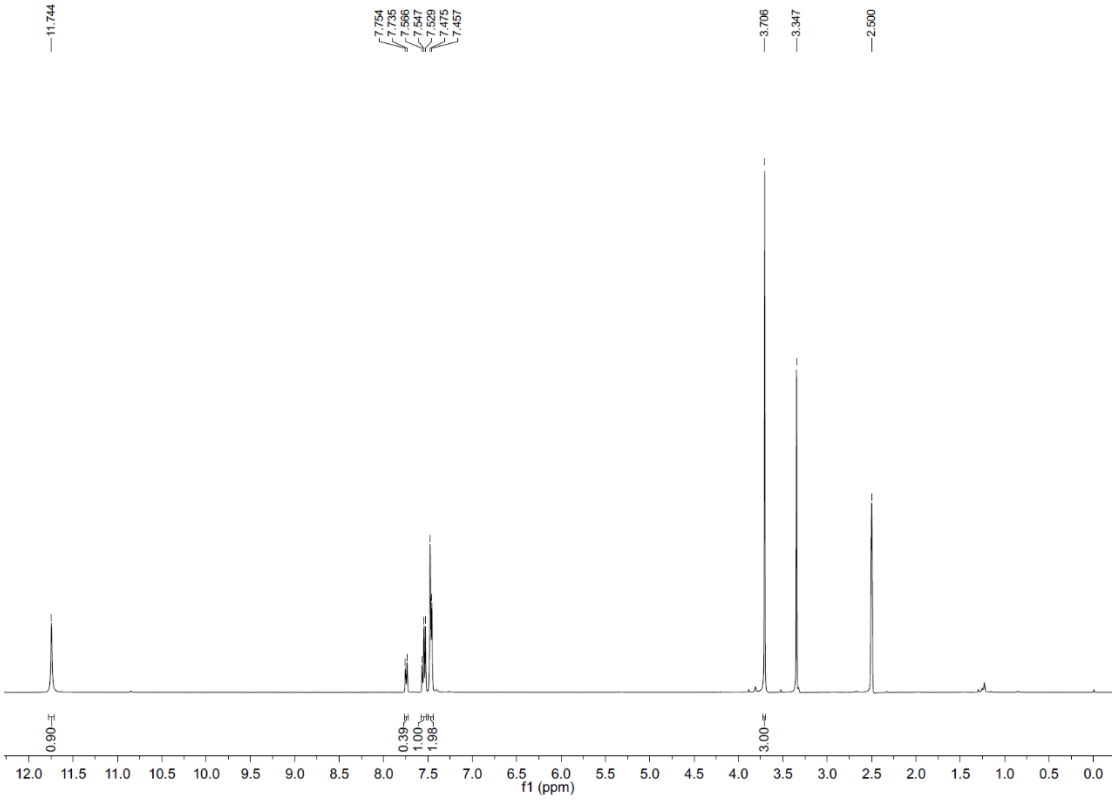
HRMS (ESI) calculated for $C_{16}H_{17}N_2O_2$ ([M+H] $^{+}$): 269.1285; found: 269.1281.

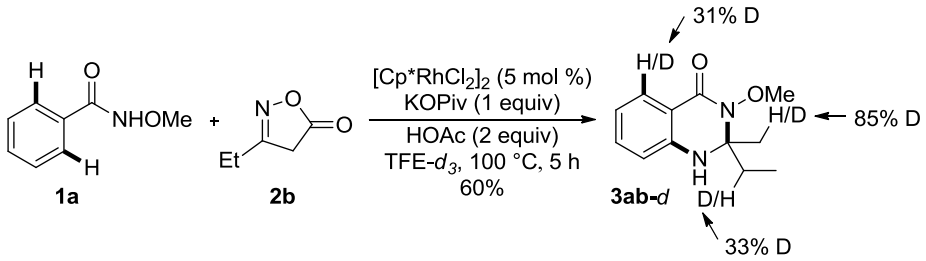
III. Experimental Mechanistic Studies

Deuterium-labeling experiment:

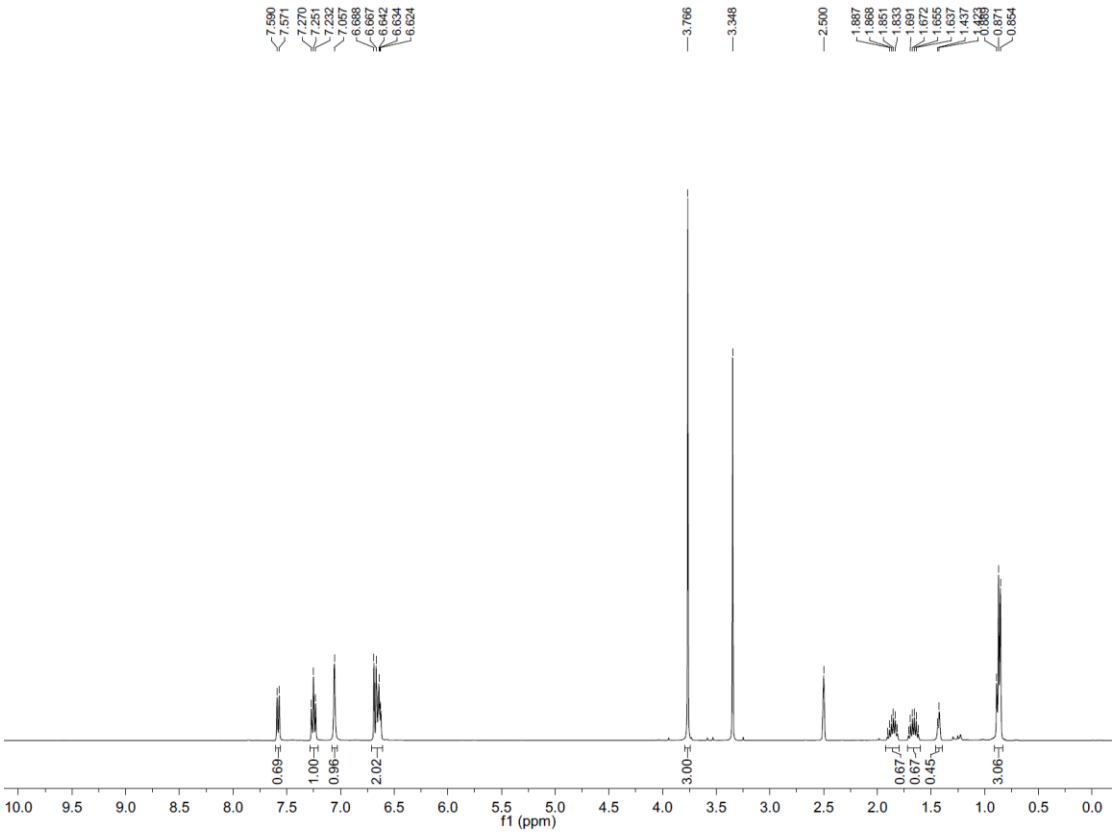


1a (0.1 mmol, 1 equiv) was dissolved in TFE-d_3 (1.0 mL) in the presence of $[Cp^*RhCl_2]_2$ (5 mol %), KOPiv (1 equiv) and HOAc (2 equiv). The mixture was stirred at 100 ^oC in an oil bath for 5 h. Afterwards, the mixture was diluted with EtOAc and transferred to a round bottom flask. The solvent was evaporated under reduced pressure and the recovered **1a** was purified by preparative TLC. The deuterium incorporation was analyzed by ^{1}H-NMR and approximate 60% deuteration was detected at the *ortho* position of the DG.

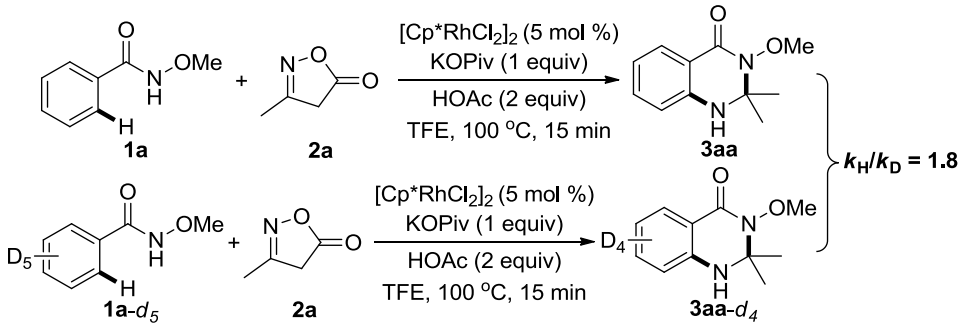




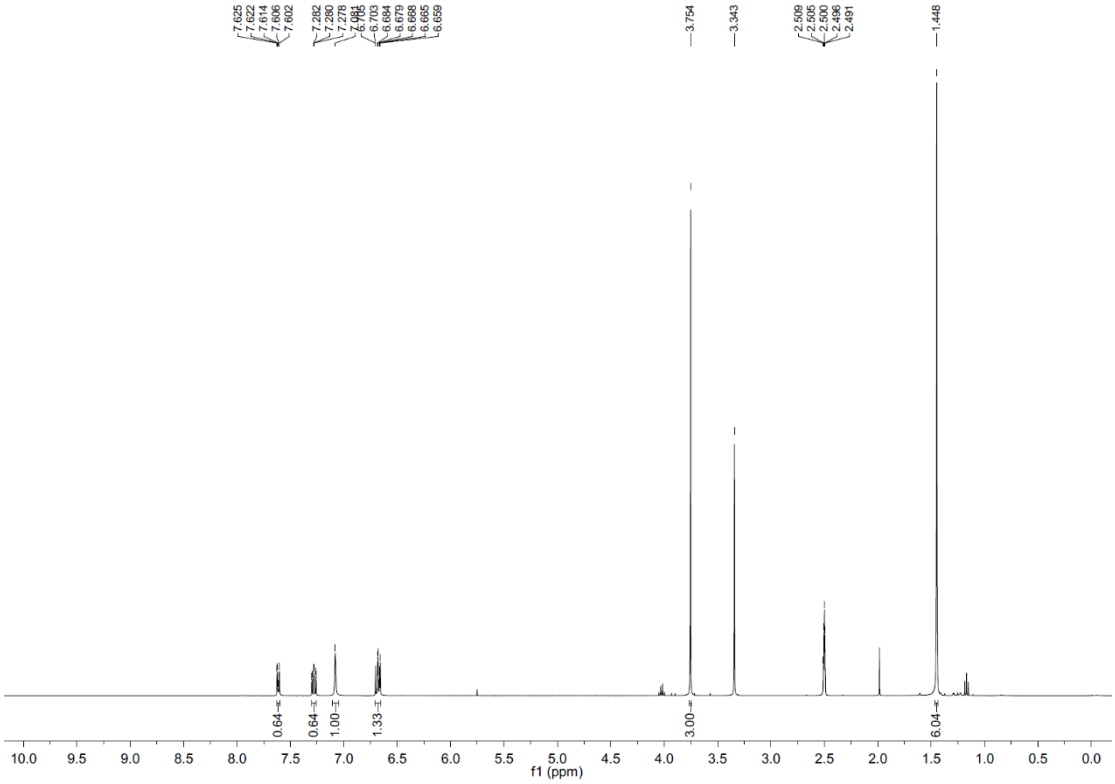
The mixture of *N*-methoxybenzamide **1a** (0.1 mmol, 1 equiv), 3-ethylisoxazol-5(4*H*)-one **2b** (1.2 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), KOPiv (1 equiv) and HOAc (2 equiv) in TFE-d_3 (1.0 mL) was stirred at 100 ^oC in an oil bath for 5 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure, and the resulted mixture was purified by preparative TLC to afford the corresponding product **3ab**. The deuterium incorporation was analyzed by ^1H-NMR.



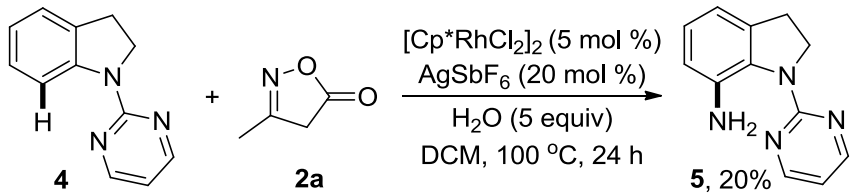
Kinetic isotope study:



The mixture of *N*-methoxybenzamide **1a** or **1a**-d_5 (0.1 mmol, 1 equiv), 3-methylisoxazol-5(4*H*)-one **2a** (1.2 equiv), [Cp*$RhCl_2$]$_2$ (5 mol %), KOPiv (1 equiv) and HOAc (2 equiv) in TFE (1.0 mL) was stirred at 100 ^{o}C in an oil bath for 15 min without exclusion of air or moisture. Afterwards, the two reactions were mixed and the solvent was removed under reduce pressure, the resulted mixture was purified by preparative TLC to afford the corresponding product **3aa**/**3aa**-d_4. The singlet and doublet at δ 3.75 (3H) and 7.61 (0.64H) were selected to measure the KIE, and the primary KIE value was determined to be k_H/k_D = 1.8.



Preliminary investigation on the C-NH_2 formation:



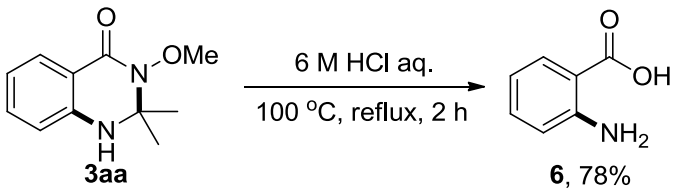
The mixture of 1-(pyrimidin-2-yl)indoline **4** (0.2 mmol, 1 equiv), 3-methylisoxazol-5(4*H*)-one **2a** (1.2 equiv), $[Cp^*RhCl_2]_2$ (5 mol %), $AgSbF_6$ (20 mol %) and H_2O (5 equiv) in DCM (2.0 mL) was stirred at 100 ^oC in an oil bath for 24 h without exclusion of air or moisture. Afterwards, the solvent was removed under reduce pressure; the resulted mixture was purified by preparative TLC (eluent: PE/EA = 2/1, R_f = 0.6) to afford the corresponding product **5** in 20% isolated yield (8.5 mg) as a brown oil.

^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 8.50 (d, *J* = 4.8 Hz, 2H), 6.86-6.76 (m, 2H), 6.64-6.57 (m, 2H), 5.25 (brs, 2H), 4.28 (t, *J* = 7.9 Hz, 2H), 2.95 (t, *J* = 7.8 Hz, 2H).

^{13}C NMR (100 MHz, DMSO-*d*$_6$): δ 159.1, 158.1, 138.0, 135.3, 129.8, 124.6, 116.2, 113.5, 111.0, 51.8, 28.8.

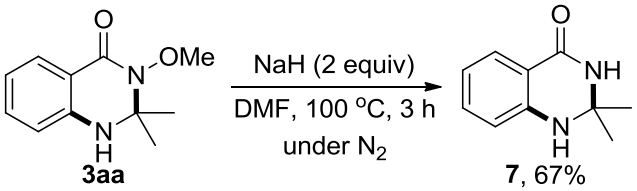
HRMS (ESI) calculated for $C_{12}H_{13}N_4$ ($[M+H]^+$): 213.1135; found: 213.1137.

Derivatization of compound 3aa:



The mixture of 2,3-dihydroquinazolin-4(1*H*)-one **3aa** (0.2 mmol) in 6M HCl aqueous solution (1 mL) was stirred at 100 ^oC in an oil bath, the resulted mixture was allowed to reflux for 2 h without exclusion of air or moisture. Afterwards, the mixture was neutralized by adding the Na_2CO_3 aqueous solution. The resulted mixture was extracted by EA for three times and the organic solvent was combined and dried over $MgSO_4$. The organic solvent was removed under reduce pressure and the resulted mixture was purified by preparative TLC (eluent: DCM/MeOH = 10/1, R_f = 0.4) to afford the corresponding product **6** in 78% isolated yield (21.5 mg) as a white solid.

The compound **6** was a known compound and the characterization data was in agreement with literature precedent.[S3] **^{1}H NMR (400 MHz, DMSO-d_6):** δ 8.54 (brs, 2H), 7.68 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.4 Hz, 1H), 6.73 (d, *J* = 8.2 Hz, 1H), 6.49 (*t*, J = 7.3 Hz, 1H). **^{13}C NMR (100 MHz, $CDCl_3$):** δ 173.9, 151.2, 135.3, 132.3, 116.9, 116.6, 109.7.



2,3-Dihydroquinazolin-4(1*H*)-one **3aa** (0.2 mmol) was added to a solution of 60% NaH (0.4 mmol, 2 equiv) in dry DMF (2 mL) under the nitrogen atmosphere, the resulted mixture was stirred at 100 °C in an oil bath for 3 h. Afterwards, the mixture was diluted with EA and washed with water. The aqueous phase was extracted with EA for three times and the organic solvent was combined and dried over $MgSO_4$. The organic solvent was removed under reduce pressure and the resulted mixture was purified by preparative TLC (eluent: PE/EA = 1/1, R_f = 0.5) to afford the corresponding product **7** in 67% isolated yield (23.5 mg) as a white solid.

The compound **7** was a known compound and the characterization data was in agreement with literature precedent.[S4] **^{1}H NMR (400 MHz, DMSO-d_6):** δ 7.96 (s, 1H), 7.56 (d, *J* = 7.8 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 6.66 (s, 1H), 6.64-6.59 (m, 2H), 1.37 (s, 6H).

IV. DFT Calculations

Computational details:

Gaussian 09 program[S5] has been used to perform all the theoretical calculations. Geometry optimizations and frequency analyses were calculated using the B3LYP functional[S6] with a standard 6-31G(d) basis set (Lanl2dz basis set for Rh) in gas phase. Single point energies were further calculated at the M06 functional[S7] with a standard 6-311++G(d,p) basis set (SDD[S8] basis set for Rh) level using SMD solvation model[S9]

(solvent = 2,2,2-TriFluoroEthanol). Throughout the paper, the energies presented are the M06-calculated Gibbs free energies in TFE solvent with B3LYP-calculated thermodynamic corrections.

Various energy values for all of the relevant species [gas phase results optimized at the level of B3LYP/6-31G(d) (Lanl2dz for Rh)] as well as the single-point results with SMD atomic radii for experimental solvent TFE at the M06/6-311++G(d,p) (SDD for Rh) (SMD)]:

2a

Zero-point correction= 0.089828 (Hartree/Particle)
Thermal correction to Energy= 0.096064
Thermal correction to Enthalpy= 0.097009
Thermal correction to Gibbs Free Energy= 0.059750
Sum of electronic and zero-point Energies= -360.494685
Sum of electronic and thermal Energies= -360.488449
Sum of electronic and thermal Enthalpies= -360.487504
Sum of electronic and thermal Free Energies= -360.524763

SCF Done: E(RM06) = -360.481898677 A.U. after 14 cycles
NFock= 14 Conv=0.20D-08 -V/T= 2.0036
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.45
(included in total energy above)

CH_3COOH

Zero-point correction= 0.062045 (Hartree/Particle)
Thermal correction to Energy= 0.066610
Thermal correction to Enthalpy= 0.067554
Thermal correction to Gibbs Free Energy= 0.034805
Sum of electronic and zero-point Energies= -229.015563
Sum of electronic and thermal Energies= -229.010998
Sum of electronic and thermal Enthalpies= -229.010054
Sum of electronic and thermal Free Energies= -229.042803

SCF Done: E(RM06) = -229.038360949 A.U. after 11 cycles
NFock= 11 Conv=0.68D-08 -V/T= 2.0034
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.16
(included in total energy above)

CO_2

Zero-point correction= 0.011619 (Hartree/Particle)

Thermal correction to Energy= 0.014260
Thermal correction to Enthalpy= 0.015204
Thermal correction to Gibbs Free Energy= -0.009098
Sum of electronic and zero-point Energies= -188.565952
Sum of electronic and thermal Energies= -188.563311
Sum of electronic and thermal Enthalpies= -188.562367
Sum of electronic and thermal Free Energies= -188.586668

SCF Done: E(RM06) = -188.549356609 A.U. after 8 cycles
NFock= 8 Conv=0.76D-08 -V/T= 2.0031
SMD-CDS (non-electrostatic) energy (kcal/mol) = 8.91
(included in total energy above)

Cp*(OAc)$_2$

Zero-point correction= 0.327358 (Hartree/Particle)
Thermal correction to Energy= 0.351522
Thermal correction to Enthalpy= 0.352466
Thermal correction to Gibbs Free Energy= 0.273528
Sum of electronic and zero-point Energies= -956.300107
Sum of electronic and thermal Energies= -956.275943
Sum of electronic and thermal Enthalpies= -956.274999
Sum of electronic and thermal Free Energies= -956.353937

SCF Done: E(RM06) = -957.390074159 A.U. after 17 cycles
NFock= 17 Conv=0.80D-08 -V/T= 2.0831
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.91
(included in total energy above)

PC

Zero-point correction= 0.240077 (Hartree/Particle)
Thermal correction to Energy= 0.253935
Thermal correction to Enthalpy= 0.254880
Thermal correction to Gibbs Free Energy= 0.200126
Sum of electronic and zero-point Energies= -687.253122
Sum of electronic and thermal Energies= -687.239264
Sum of electronic and thermal Enthalpies= -687.238320
Sum of electronic and thermal Free Energies= -687.293073

SCF Done: E(RM06) = -687.242530171 A.U. after 17 cycles
NFock= 17 Conv=0.45D-08 -V/T= 2.0041
SMD-CDS (non-electrostatic) energy (kcal/mol) = 3.44
(included in total energy above)

INT-1

Zero-point correction= 0.360910 (Hartree/Particle)
Thermal correction to Energy= 0.385074
Thermal correction to Enthalpy= 0.386018
Thermal correction to Gibbs Free Energy= 0.307459
Sum of electronic and zero-point Energies= -1013.475833
Sum of electronic and thermal Energies= -1013.451669
Sum of electronic and thermal Enthalpies= -1013.450725
Sum of electronic and thermal Free Energies= -1013.529284

SCF Done: E(RM06) = -1014.50646657 A.U. after 19 cycles
NFock= 19 Conv=0.42D-08 -V/T= 2.0786
SMD-CDS (non-electrostatic) energy (kcal/mol) = 3.76
(included in total energy above)

INT-2

Zero-point correction= 0.452404 (Hartree/Particle)
Thermal correction to Energy= 0.484246
Thermal correction to Enthalpy= 0.485190
Thermal correction to Gibbs Free Energy= 0.389167
Sum of electronic and zero-point Energies= -1373.983709
Sum of electronic and thermal Energies= -1373.951867
Sum of electronic and thermal Enthalpies= -1373.950923
Sum of electronic and thermal Free Energies= -1374.046946

SCF Done: E(RM06) = -1375.00891857 A.U. after 18 cycles
NFock= 18 Conv=0.36D-08 -V/T= 2.0579
SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.09
(included in total energy above)

INT-3

Zero-point correction= 0.450837 (Hartree/Particle)
Thermal correction to Energy= 0.483114
Thermal correction to Enthalpy= 0.484058
Thermal correction to Gibbs Free Energy= 0.387230
Sum of electronic and zero-point Energies= -1373.945270
Sum of electronic and thermal Energies= -1373.912993
Sum of electronic and thermal Enthalpies= -1373.912049
Sum of electronic and thermal Free Energies= -1374.008877

SCF Done: E(RM06) = -1374.99731117 A.U. after 23 cycles
NFock= 23 Conv=0.17D-08 -V/T= 2.0581
SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.48
(included in total energy above)

INT-4

Zero-point correction= 0.436055 (Hartree/Particle)
Thermal correction to Energy= 0.465667
Thermal correction to Enthalpy= 0.466611
Thermal correction to Gibbs Free Energy= 0.376647
Sum of electronic and zero-point Energies= -1185.403237
Sum of electronic and thermal Energies= -1185.373625
Sum of electronic and thermal Enthalpies= -1185.372681
Sum of electronic and thermal Free Energies= -1185.462644

SCF Done: E(RM06) = -1186.42611411 A.U. after 22 cycles
NFock= 22 Conv=0.62D-08 -V/T= 2.0674
SMD-CDS (non-electrostatic) energy (kcal/mol) = 4.13
(included in total energy above)

INT-5

Zero-point correction= 0.439370 (Hartree/Particle)
Thermal correction to Energy= 0.467858
Thermal correction to Enthalpy= 0.468802
Thermal correction to Gibbs Free Energy= 0.381923
Sum of electronic and zero-point Energies= -1185.467882
Sum of electronic and thermal Energies= -1185.439394
Sum of electronic and thermal Enthalpies= -1185.438449
Sum of electronic and thermal Free Energies= -1185.525328

SCF Done: E(RM06) = -1186.50853215 A.U. after 18 cycles
NFock= 18 Conv=0.88D-08 -V/T= 2.0672
SMD-CDS (non-electrostatic) energy (kcal/mol) = 2.95
(included in total energy above)

INT-6

Zero-point correction= 0.503515 (Hartree/Particle)
Thermal correction to Energy= 0.537978
Thermal correction to Enthalpy= 0.538922
Thermal correction to Gibbs Free Energy= 0.438737
Sum of electronic and zero-point Energies= -1414.517352
Sum of electronic and thermal Energies= -1414.482890
Sum of electronic and thermal Enthalpies= -1414.481946
Sum of electronic and thermal Free Energies= -1414.582130

SCF Done: E(RM06) = -1415.58786199 A.U. after 18 cycles
NFock= 18 Conv=0.77D-08 -V/T= 2.0564
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.08
(included in total energy above)

INT-7

Zero-point correction= 0.237700 (Hartree/Particle)
Thermal correction to Energy= 0.252893
Thermal correction to Enthalpy= 0.253837
Thermal correction to Gibbs Free Energy= 0.194694
Sum of electronic and zero-point Energies= -687.244126
Sum of electronic and thermal Energies= -687.228934
Sum of electronic and thermal Enthalpies= -687.227990
Sum of electronic and thermal Free Energies= -687.287133

SCF Done: E(RM06) = -687.221433371 A.U. after 18 cycles
NFock= 18 Conv=0.19D-08 -V/T= 2.0040
SMD-CDS (non-electrostatic) energy (kcal/mol) = 4.36
(included in total energy above)

TS-1

Zero-point correction= 0.450783 (Hartree/Particle)
Thermal correction to Energy= 0.482196
Thermal correction to Enthalpy= 0.483140
Thermal correction to Gibbs Free Energy= 0.389227
Sum of electronic and zero-point Energies= -1373.945118
Sum of electronic and thermal Energies= -1373.913705
Sum of electronic and thermal Enthalpies= -1373.912761
Sum of electronic and thermal Free Energies= -1374.006674

SCF Done: E(RM06) = -1374.99684731 A.U. after 23 cycles
NFock= 23 Conv=0.47D-08 -V/T= 2.0581
SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.53
(included in total energy above)

TS-2

Zero-point correction= 0.447856 (Hartree/Particle)
Thermal correction to Energy= 0.480743
Thermal correction to Enthalpy= 0.481687
Thermal correction to Gibbs Free Energy= 0.382354
Sum of electronic and zero-point Energies= -1373.940332
Sum of electronic and thermal Energies= -1373.907445
Sum of electronic and thermal Enthalpies= -1373.906501
Sum of electronic and thermal Free Energies= -1374.005834

SCF Done: E(RM06) = -1374.96881771 A.U. after 24 cycles
NFock= 24 Conv=0.14D-08 -V/T= 2.0581
SMD-CDS (non-electrostatic) energy (kcal/mol) = 9.19

(included in total energy above)

TS-3

Zero-point correction= 0.435108 (Hartree/Particle)
Thermal correction to Energy= 0.464156
Thermal correction to Enthalpy= 0.465100
Thermal correction to Gibbs Free Energy= 0.377184
Sum of electronic and zero-point Energies= -1185.379420
Sum of electronic and thermal Energies= -1185.350372
Sum of electronic and thermal Enthalpies= -1185.349428
Sum of electronic and thermal Free Energies= -1185.437344

SCF Done: E(RM06) = -1186.40760142 A.U. after 23 cycles
NFock= 23 Conv=0.82D-08 -V/T= 2.0673
SMD-CDS (non-electrostatic) energy (kcal/mol) = 3.89
(included in total energy above)

TS-4

Zero-point correction= 0.498210 (Hartree/Particle)
Thermal correction to Energy= 0.532337
Thermal correction to Enthalpy= 0.533281
Thermal correction to Gibbs Free Energy= 0.433271
Sum of electronic and zero-point Energies= -1414.489765
Sum of electronic and thermal Energies= -1414.455639
Sum of electronic and thermal Enthalpies= -1414.454694
Sum of electronic and thermal Free Energies= -1414.554704

SCF Done: E(RM06) = -1415.54759044 A.U. after 18 cycles
NFock= 18 Conv=0.74D-08 -V/T= 2.0563
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.59
(included in total energy above)

INT-2a

Zero-point correction= 0.451827 (Hartree/Particle)
Thermal correction to Energy= 0.484228
Thermal correction to Enthalpy= 0.485172
Thermal correction to Gibbs Free Energy= 0.385388
Sum of electronic and zero-point Energies= -1373.982960
Sum of electronic and thermal Energies= -1373.950559
Sum of electronic and thermal Enthalpies= -1373.949615
Sum of electronic and thermal Free Energies= -1374.049399

SCF Done: E(RM06) = -1375.00103759 A.U. after 18 cycles
NFock= 18 Conv=0.64D-08 -V/T= 2.0579

SMD-CDS (non-electrostatic) energy (kcal/mol) = 7.94
(included in total energy above)

INT-3a

Zero-point correction= 0.452367 (Hartree/Particle)
Thermal correction to Energy= 0.483919
Thermal correction to Enthalpy= 0.484864
Thermal correction to Gibbs Free Energy= 0.391898
Sum of electronic and zero-point Energies= -1373.973940
Sum of electronic and thermal Energies= -1373.942387
Sum of electronic and thermal Enthalpies= -1373.941443
Sum of electronic and thermal Free Energies= -1374.034409

SCF Done: E(RM06) = -1375.01093627 A.U. after 20 cycles
NFock= 20 Conv=0.39D-08 -V/T= 2.0580
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.05
(included in total energy above)

TS-1a

Zero-point correction= 0.449955 (Hartree/Particle)
Thermal correction to Energy= 0.481643
Thermal correction to Enthalpy= 0.482588
Thermal correction to Gibbs Free Energy= 0.388107
Sum of electronic and zero-point Energies= -1373.926857
Sum of electronic and thermal Energies= -1373.895169
Sum of electronic and thermal Enthalpies= -1373.894225
Sum of electronic and thermal Free Energies= -1373.988706

SCF Done: E(RM06) = -1374.95236383 A.U. after 22 cycles
NFock= 22 Conv=0.86D-08 -V/T= 2.0579
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.72
(included in total energy above)

INT-3b

Zero-point correction= 0.454642 (Hartree/Particle)
Thermal correction to Energy= 0.484961
Thermal correction to Enthalpy= 0.485906
Thermal correction to Gibbs Free Energy= 0.396182
Sum of electronic and zero-point Energies= -1373.941006
Sum of electronic and thermal Energies= -1373.910687
Sum of electronic and thermal Enthalpies= -1373.909743
Sum of electronic and thermal Free Energies= -1373.999467

SCF Done: E(RM06) = -1374.97451040 A.U. after 19 cycles

NFock= 19 Conv=0.30D-08 -V/T= 2.0579
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.64
(included in total energy above)

TS-1b

Zero-point correction= 0.451819 (Hartree/Particle)
Thermal correction to Energy= 0.482059
Thermal correction to Enthalpy= 0.483003
Thermal correction to Gibbs Free Energy= 0.393893
Sum of electronic and zero-point Energies= -1373.907357
Sum of electronic and thermal Energies= -1373.877118
Sum of electronic and thermal Enthalpies= -1373.876174
Sum of electronic and thermal Free Energies= -1373.965283

SCF Done: E(RM06) = -1374.93399775 A.U. after 19 cycles
NFock= 19 Conv=0.94D-08 -V/T= 2.0579
SMD-CDS (non-electrostatic) energy (kcal/mol) = 6.49
(included in total energy above)

INT-6c

Zero-point correction= 0.504150 (Hartree/Particle)
Thermal correction to Energy= 0.538492
Thermal correction to Enthalpy= 0.539436
Thermal correction to Gibbs Free Energy= 0.439140
Sum of electronic and zero-point Energies= -1414.496073
Sum of electronic and thermal Energies= -1414.461731
Sum of electronic and thermal Enthalpies= -1414.460787
Sum of electronic and thermal Free Energies= -1414.561083

SCF Done: E(RM06) = -1415.57009460 A.U. after 18 cycles
NFock= 18 Conv=0.72D-08 -V/T= 2.0564
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.18
(included in total energy above)

TS-4c

Zero-point correction= 0.500366 (Hartree/Particle)
Thermal correction to Energy= 0.533459
Thermal correction to Enthalpy= 0.534403
Thermal correction to Gibbs Free Energy= 0.437747
Sum of electronic and zero-point Energies= -1414.463367
Sum of electronic and thermal Energies= -1414.430274
Sum of electronic and thermal Enthalpies= -1414.429330
Sum of electronic and thermal Free Energies= -1414.525986

SCF Done: E(RM06) = -1415.52540381 A.U. after 19 cycles
NFock= 19 Conv=0.32D-08 -V/T= 2.0564
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.51
(included in total energy above)

TS-5c

Zero-point correction= 0.495776 (Hartree/Particle)
Thermal correction to Energy= 0.529943
Thermal correction to Enthalpy= 0.530888
Thermal correction to Gibbs Free Energy= 0.431033
Sum of electronic and zero-point Energies= -1414.394138
Sum of electronic and thermal Energies= -1414.359971
Sum of electronic and thermal Enthalpies= -1414.359026
Sum of electronic and thermal Free Energies= -1414.458881

SCF Done: E(RM06) = -1415.46078871 A.U. after 18 cycles
NFock= 18 Conv=0.74D-08 -V/T= 2.0564
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.17
(included in total energy above)

TS-6c

Zero-point correction= 0.503671 (Hartree/Particle)
Thermal correction to Energy= 0.536563
Thermal correction to Enthalpy= 0.537507
Thermal correction to Gibbs Free Energy= 0.442878
Sum of electronic and zero-point Energies= -1414.467368
Sum of electronic and thermal Energies= -1414.434476
Sum of electronic and thermal Enthalpies= -1414.433532
Sum of electronic and thermal Free Energies= -1414.528161

SCF Done: E(RM06) = -1415.53728967 A.U. after 18 cycles
NFock= 18 Conv=0.69D-08 -V/T= 2.0564
SMD-CDS (non-electrostatic) energy (kcal/mol) = 4.61
(included in total energy above)

INT-6d

Zero-point correction= 0.437994 (Hartree/Particle)
Thermal correction to Energy= 0.466813
Thermal correction to Enthalpy= 0.467757
Thermal correction to Gibbs Free Energy= 0.379796
Sum of electronic and zero-point Energies= -1185.467873
Sum of electronic and thermal Energies= -1185.439053
Sum of electronic and thermal Enthalpies= -1185.438109
Sum of electronic and thermal Free Energies= -1185.526071

SCF Done: E(RM06) = -1186.50280442 A.U. after 18 cycles
NFock= 18 Conv=0.67D-08 -V/T= 2.0672
SMD-CDS (non-electrostatic) energy (kcal/mol) = 2.76
(included in total energy above)

INT-7d

Zero-point correction= 0.439219 (Hartree/Particle)
Thermal correction to Energy= 0.467215
Thermal correction to Enthalpy= 0.468159
Thermal correction to Gibbs Free Energy= 0.381772
Sum of electronic and zero-point Energies= -1185.447166
Sum of electronic and thermal Energies= -1185.419170
Sum of electronic and thermal Enthalpies= -1185.418226
Sum of electronic and thermal Free Energies= -1185.504613

SCF Done: E(RM06) = -1186.48148285 A.U. after 18 cycles
NFock= 18 Conv=0.72D-08 -V/T= 2.0672
SMD-CDS (non-electrostatic) energy (kcal/mol) = 2.74
(included in total energy above)

INT-8d

Zero-point correction= 0.505411 (Hartree/Particle)
Thermal correction to Energy= 0.538681
Thermal correction to Enthalpy= 0.539625
Thermal correction to Gibbs Free Energy= 0.442845
Sum of electronic and zero-point Energies= -1414.514561
Sum of electronic and thermal Energies= -1414.481290
Sum of electronic and thermal Enthalpies= -1414.480346
Sum of electronic and thermal Free Energies= -1414.577127

SCF Done: E(RM06) = -1415.58025889 A.U. after 18 cycles
NFock= 18 Conv=0.51D-08 -V/T= 2.0564
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.29
(included in total energy above)

TS-4d

Zero-point correction= 0.437543 (Hartree/Particle)
Thermal correction to Energy= 0.465970
Thermal correction to Enthalpy= 0.466914
Thermal correction to Gibbs Free Energy= 0.378939
Sum of electronic and zero-point Energies= -1185.451239
Sum of electronic and thermal Energies= -1185.422812
Sum of electronic and thermal Enthalpies= -1185.421868

Sum of electronic and thermal Free Energies= -1185.509843

SCF Done: E(RM06) = -1186.48948042 A.U. after 19 cycles
NFock= 19 Conv=0.60D-08 -V/T= 2.0672
SMD-CDS (non-electrostatic) energy (kcal/mol) = 3.52
(included in total energy above)

TS-5d

Zero-point correction= 0.438307 (Hartree/Particle)
Thermal correction to Energy= 0.465836
Thermal correction to Enthalpy= 0.466780
Thermal correction to Gibbs Free Energy= 0.382193
Sum of electronic and zero-point Energies= -1185.444055
Sum of electronic and thermal Energies= -1185.416525
Sum of electronic and thermal Enthalpies= -1185.415581
Sum of electronic and thermal Free Energies= -1185.500168

SCF Done: E(RM06) = -1186.47627529 A.U. after 18 cycles
NFock= 18 Conv=0.66D-08 -V/T= 2.0672
SMD-CDS (non-electrostatic) energy (kcal/mol) = 2.37
(included in total energy above)

TS-6d

Zero-point correction= 0.499149 (Hartree/Particle)
Thermal correction to Energy= 0.532135
Thermal correction to Enthalpy= 0.533079
Thermal correction to Gibbs Free Energy= 0.435582
Sum of electronic and zero-point Energies= -1414.468207
Sum of electronic and thermal Energies= -1414.435222
Sum of electronic and thermal Enthalpies= -1414.434278
Sum of electronic and thermal Free Energies= -1414.531775

SCF Done: E(RM06) = -1415.52799750 A.U. after 18 cycles
NFock= 18 Conv=0.60D-08 -V/T= 2.0564
SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.90
(included in total energy above)

Cartesian coordinates for all of the species:

2a

C	-0.84891200	0.78967500	0.09190600
H	-0.38349400	0.19684500	-0.70447600
H	-0.49966900	0.37892100	1.04676500
N	-2.77041200	2.06870800	-0.16672700

O	-1.65097100	2.95948600	-0.18532000
C	-0.47321200	2.25908500	-0.03547600
O	0.60097000	2.79377400	-0.02008800
C	-2.33987200	0.86765700	-0.01431500
C	-3.29184800	-0.28244900	0.04193900
H	-3.08013000	-1.00126800	-0.75924800
H	-3.19719900	-0.81880200	0.99418100
H	-4.31928400	0.07443500	-0.06380800

CH_3COOH

C	0.69578900	-2.04102800	-0.00944700
O	1.90407800	-2.10956900	-0.00979500
O	0.03294500	-0.85534600	-0.00879200
H	0.72212500	-0.16432800	-0.00876800
C	-0.26202200	-3.20636200	-0.00919700
H	-0.90836700	-3.16070500	0.87355400
H	-0.91071700	-3.15932900	-0.89013000
H	0.30083900	-4.13989100	-0.01059500

CO_2

C	4.60923600	0.73712300	0.00000000
O	3.43965300	0.73712300	0.00000000
O	5.77881900	0.73712300	0.00000000

$Cp^*(OAc)_2$

Rh	0.02853700	0.19160100	-0.11016000
C	1.11476900	-1.26404900	1.11946200
C	0.99748900	-1.80515800	-0.20687600
C	1.62475400	-0.88855100	-1.11919200
C	2.22325800	0.18816700	-0.33366800
C	1.90702600	-0.04131400	1.03441900
C	-1.05228200	2.49254000	-0.02735000
O	-0.46456500	2.09978400	-1.08538300
O	-0.98528400	1.77089900	1.01969800
C	-1.85036600	3.77090000	-0.02290700
H	-2.88262400	3.54102600	-0.31191200
H	-1.86453400	4.20996200	0.97761200
H	-1.44199500	4.47975800	-0.74733200
O	-1.88737300	-0.27975800	-0.72021300
C	-2.61574000	-1.13178600	-0.05316100
O	-2.24932100	-1.82886500	0.89581700
C	-4.05557500	-1.18935700	-0.56123000
H	-4.58597300	-0.28478600	-0.24151800
H	-4.08270100	-1.21488000	-1.65474200

H	-4.56327000	-2.06354600	-0.14804100
C	3.00451700	1.32863800	-0.91290300
H	3.98199800	0.98078900	-1.27209100
H	2.47500300	1.77891300	-1.75831700
H	3.17858600	2.11476500	-0.17436400
C	2.28235100	0.80977500	2.20945200
H	3.06801600	0.32084400	2.80014900
H	2.65427700	1.78872200	1.89814000
H	1.42154400	0.97314700	2.86455700
C	1.76400300	-1.05014900	-2.60240000
H	1.73993900	-0.08166000	-3.11061000
H	2.71847200	-1.53483600	-2.85071300
H	0.95881700	-1.66320700	-3.01488600
C	0.32688100	-3.09641300	-0.56015500
H	0.03657800	-3.12200200	-1.61373600
H	1.01736600	-3.93226100	-0.38159800
H	-0.56976500	-3.24018900	0.04562800
C	0.60502100	-1.90400700	2.37358600
H	-0.43343700	-2.21412200	2.23281500
H	1.21302700	-2.78177300	2.63287100
H	0.64358900	-1.20894300	3.21654100

PC

C	-3.84917800	-1.32566400	-0.79680900
C	-3.06853100	-0.68945400	0.16452200
C	-2.60991400	0.61885500	-0.05935400
C	-2.94704600	1.26871200	-1.26275000
C	-3.72984600	0.61445800	-2.21878500
C	-4.18956700	-0.67913000	-1.99175400
H	-4.19957500	-2.33735100	-0.60886300
H	-2.80777700	-1.20076700	1.08855600
H	-3.95256800	1.14591400	-3.13850100
H	-4.79876000	-1.18461700	-2.73473000
C	-2.41161100	2.62362900	-1.55373400
O	-2.48947500	3.16068900	-2.65502000
N	-1.81803000	3.23593000	-0.46906200
O	-1.23039900	4.48532100	-0.65641200
C	-2.18697000	5.52853200	-0.91652700
H	-1.57870500	6.43255600	-1.00042000
H	-2.71318400	5.33695000	-1.85284500
H	-2.89697000	5.63898600	-0.08852000
N	-1.77220200	1.27353200	0.83621200
C	-1.80957000	2.73958900	0.92416400
C	-3.06360800	3.22604500	1.68541900

H	-3.08734600	4.31873700	1.74481900
H	-3.97304800	2.88290600	1.18254600
H	-3.06284500	2.83394200	2.70983900
C	-0.52745200	3.19250100	1.63324100
H	0.34993700	2.87403700	1.06547900
H	-0.50239400	4.27686000	1.75005000
H	-0.48967200	2.73671000	2.62960700
H	-1.70037500	0.83393500	1.74640600

INT-1

Rh	-0.18071000	0.25154000	0.04186900
C	1.01585800	-1.32346900	1.12512300
C	0.80875200	-1.74689800	-0.21088900
C	1.38606200	-0.73051200	-1.07098800
C	2.12214200	0.21934800	-0.23983100
C	1.85563200	-0.11295400	1.09794100
C	2.92751300	1.36959100	-0.76940900
H	3.71979600	1.01542200	-1.44082800
H	2.29581800	2.07278100	-1.32258700
H	3.40515600	1.92627600	0.04127000
C	2.33321900	0.59757500	2.32834000
H	3.14071300	0.03211200	2.81372500
H	2.71245300	1.59624800	2.09852900
H	1.52729100	0.70578600	3.06151500
C	1.43828000	-0.77265300	-2.56709700
H	1.46861300	0.23552000	-2.99008500
H	2.34162900	-1.30378900	-2.90135700
H	0.57147100	-1.29156000	-2.98461000
C	0.17332500	-3.01988100	-0.68575700
H	-0.50571000	-2.84692300	-1.52567200
H	0.94421200	-3.72849500	-1.01823900
H	-0.39696900	-3.50762700	0.10890500
C	0.60938800	-2.04227700	2.37717200
H	-0.23127100	-2.71777300	2.19877400
H	1.44238800	-2.64113500	2.77191000
H	0.30891300	-1.34070700	3.16151200
C	-4.25669800	-1.42255000	-0.30939400
C	-2.87023900	-1.35851500	-0.09800800
C	-2.18248200	-0.15141300	-0.25364900
C	-2.92798900	0.98274800	-0.61738200
C	-4.30350600	0.93251600	-0.83183100
C	-4.97414000	-0.28429700	-0.68034900
H	-4.77506200	-2.37086000	-0.18235800
H	-2.34821000	-2.26607100	0.19351600

H	-4.82635400	1.84254900	-1.11442500
H	-6.04652300	-0.34335600	-0.84713000
C	-2.17065800	2.26387600	-0.75335600
O	-2.63043700	3.33085400	-1.13542300
N	-0.84912900	2.05871500	-0.34802800
O	0.01744400	3.12562700	-0.63389300
C	-0.01903500	4.10562600	0.40389500
H	0.71734200	4.86155300	0.11615400
H	-1.01128100	4.56135400	0.47175400
H	0.26124300	3.66190100	1.36928100

INT-2

Rh	-0.69257800	0.48267700	-0.00373200
C	0.27450700	-1.54858600	0.17429700
C	0.08098900	-1.27884100	-1.23354300
C	0.92857200	-0.17911800	-1.57437000
C	1.68901400	0.20622100	-0.39952300
C	1.29400200	-0.63859200	0.67036200
C	2.74283000	1.26904000	-0.33459200
H	3.74107800	0.81875500	-0.43453100
H	2.62447600	1.99234000	-1.14507100
H	2.69475400	1.80351900	0.61806800
C	1.87434800	-0.61609000	2.05048900
H	2.87382800	-1.07205500	2.04021800
H	1.96682900	0.41521600	2.40943700
H	1.26317000	-1.18435600	2.75739200
C	1.12114100	0.39945300	-2.94183100
H	1.14928600	1.49034300	-2.90649700
H	2.07428800	0.04429900	-3.35678700
H	0.32577300	0.10064600	-3.62822700
C	-0.74667500	-2.09791200	-2.17966100
H	-1.07152200	-1.51140700	-3.04257200
H	-0.16179200	-2.94953900	-2.55287900
H	-1.64355900	-2.49037600	-1.69444100
C	-0.29102100	-2.71960700	0.92125500
H	-1.27753000	-3.00172900	0.54499000
H	0.36725900	-3.59206500	0.80407500
H	-0.37725100	-2.51618600	1.99186400
C	-4.73987400	-1.08905900	-0.52281200
C	-3.45600100	-0.89578100	0.00771400
C	-2.63519100	0.08664200	-0.54100800
C	-3.09981600	0.88120000	-1.59051300
C	-4.37398800	0.67893600	-2.12887200
C	-5.19462500	-0.31273400	-1.59356100

H	-5.38758200	-1.84774400	-0.08968400
H	-3.12579100	-1.50238200	0.84637600
H	-4.69484300	1.30748100	-2.95515500
H	-6.18900900	-0.47653600	-1.99939900
C	-2.20251100	1.96188400	-2.09268000
O	-2.40453900	2.66448800	-3.07200900
N	-1.13641500	2.08491900	-1.20990900
O	-0.12906700	2.93683700	-1.60023000
C	0.09490700	3.96048100	-0.61247200
H	0.86840200	4.59895000	-1.04580900
H	-0.82322500	4.53692500	-0.45994200
H	0.44984100	3.52658200	0.32970400
N	-1.21074500	1.17284500	1.65771100
O	1.38827500	2.51601100	2.32840700
C	0.79459900	2.95888300	3.34189000
O	1.18889100	3.41826300	4.41768900
C	-1.27393300	1.57108300	2.84313300
C	-1.73149100	0.66809000	3.97637300
H	-0.96239200	0.67643900	4.75690200
H	-2.65625700	1.06346400	4.41040900
H	-1.90317600	-0.35372300	3.63209500
C	-0.81330000	2.96610200	3.20048100
H	-1.28751800	3.28715500	4.13108100
H	-1.05338900	3.66820200	2.39763200

INT-3

Rh	-0.69257800	0.48267700	-0.00373200
C	0.27450700	-1.54858600	0.17429700
C	0.08098900	-1.27884100	-1.23354300
C	0.92857200	-0.17911800	-1.57437000
C	1.68901400	0.20622100	-0.39952300
C	1.29400200	-0.63859200	0.67036200
C	2.74283000	1.26904000	-0.33459200
H	3.74107800	0.81875500	-0.43453100
H	2.62447600	1.99234000	-1.14507100
H	2.69475400	1.80351900	0.61806800
C	1.87434800	-0.61609000	2.05048900
H	2.87382800	-1.07205500	2.04021800
H	1.96682900	0.41521600	2.40943700
H	1.26317000	-1.18435600	2.75739200
C	1.12114100	0.39945300	-2.94183100
H	1.14928600	1.49034300	-2.90649700
H	2.07428800	0.04429900	-3.35678700
H	0.32577300	0.10064600	-3.62822700

C	-0.74667500	-2.09791200	-2.17966100
H	-1.07152200	-1.51140700	-3.04257200
H	-0.16179200	-2.94953900	-2.55287900
H	-1.64355900	-2.49037600	-1.69444100
C	-0.29102100	-2.71960700	0.92125500
H	-1.27753000	-3.00172900	0.54499000
H	0.36725900	-3.59206500	0.80407500
H	-0.37725100	-2.51618600	1.99186400
C	-4.73987400	-1.08905900	-0.52281200
C	-3.45600100	-0.89578100	0.00771400
C	-2.63519100	0.08664200	-0.54100800
C	-3.09981600	0.88120000	-1.59051300
C	-4.37398800	0.67893600	-2.12887200
C	-5.19462500	-0.31273400	-1.59356100
H	-5.38758200	-1.84774400	-0.08968400
H	-3.12579100	-1.50238200	0.84637600
H	-4.69484300	1.30748100	-2.95515500
H	-6.18900900	-0.47653600	-1.99939900
C	-2.20251100	1.96188400	-2.09268000
O	-2.40453900	2.66448800	-3.07200900
N	-1.13641500	2.08491900	-1.20990900
O	-0.12906700	2.93683700	-1.60023000
C	0.09490700	3.96048100	-0.61247200
H	0.86840200	4.59895000	-1.04580900
H	-0.82322500	4.53692500	-0.45994200
H	0.44984100	3.52658200	0.32970400
N	-1.21074500	1.17284500	1.65771100
O	1.38827500	2.51601100	2.32840700
C	0.79459900	2.95888300	3.34189000
O	1.18889100	3.41826300	4.41768900
C	-1.27393300	1.57108300	2.84313300
C	-1.73149100	0.66809000	3.97637300
H	-0.96239200	0.67643900	4.75690200
H	-2.65625700	1.06346400	4.41040900
H	-1.90317600	-0.35372300	3.63209500
C	-0.81330000	2.96610200	3.20048100
H	-1.28751800	3.28715500	4.13108100
H	-1.05338900	3.66820200	2.39763200

INT-4

Rh	-0.28464900	0.63755000	-0.03454000
C	0.57830900	-1.44995500	0.34869400
C	0.22076700	-1.44517500	-1.06256300
C	1.07407400	-0.52522100	-1.71059900

C	2.00751800	0.00797100	-0.72992400
C	1.73366400	-0.59823500	0.51897900
C	3.09799900	0.98552200	-1.05602700
H	3.87625900	0.51505200	-1.67279400
H	2.69849300	1.83352500	-1.62073800
H	3.57691400	1.37435300	-0.15351500
C	2.40843900	-0.33418600	1.82827500
H	3.36288300	0.18193700	1.69261000
H	1.76344000	0.30204200	2.45405800
H	2.60453700	-1.26471500	2.37331300
C	1.09367600	-0.17700400	-3.16975500
H	1.18965500	0.90252100	-3.31580600
H	1.94339200	-0.66157600	-3.67068600
H	0.18117800	-0.50192300	-3.67610500
C	-0.80095900	-2.33994800	-1.70034800
H	-1.12440000	-1.95370500	-2.67060100
H	-0.38640400	-3.34463700	-1.86310400
H	-1.69306000	-2.44482500	-1.07605200
C	0.04699400	-2.40163600	1.38124500
H	-0.99199500	-2.67697500	1.17980900
H	0.63409400	-3.33172100	1.38875800
H	0.09618300	-1.97056700	2.38528500
C	-4.46789900	-0.58179300	0.21726400
C	-3.10380100	-0.47855700	0.52038700
C	-2.29368400	0.38608400	-0.21958600
C	-2.86487400	1.14730800	-1.25014400
C	-4.22477800	1.04139200	-1.55542900
C	-5.02794000	0.16951900	-0.82174300
H	-5.09646100	-1.25091900	0.80095800
H	-2.69330900	-1.06263600	1.34009000
H	-4.62401500	1.64708400	-2.36477000
H	-6.08642500	0.07766300	-1.05018700
C	-1.97613900	2.09999800	-1.97937600
O	-2.30555800	2.82124800	-2.91530100
N	-0.73475400	2.07607300	-1.37216700
O	0.26441700	2.83984600	-1.97079400
C	0.32851300	4.13845500	-1.37358000
H	1.16839200	4.64286000	-1.85924900
H	-0.59760500	4.69055800	-1.56457200
H	0.51006900	4.05958900	-0.29462800
N	-0.31430100	1.42383900	1.65550200
C	-1.27386900	2.13096600	2.31819100
C	-1.21996500	2.00129900	3.83270800
H	-1.96927900	2.63681500	4.31480800

H	-1.40886700	0.96317500	4.12996100
H	-0.22693700	2.27224800	4.20733500
C	-2.12377200	3.00671900	1.70823000
H	-2.72876000	3.69295800	2.29422100
H	-2.15357800	3.09812900	0.63083500

INT-5

Rh	-0.05953000	0.95506200	-0.65867400
C	1.79072200	-0.06676000	0.30705500
C	1.30079800	-0.80733700	-0.81723300
C	1.43623200	0.02269100	-2.00456300
C	1.97701800	1.27815000	-1.59439700
C	2.15841700	1.23736400	-0.16280800
C	2.40763000	2.40041900	-2.48899800
H	3.49215200	2.35078700	-2.66040900
H	1.90626100	2.34853100	-3.45551300
H	2.18758200	3.37800400	-2.04979300
C	2.75544800	2.33983600	0.65782800
H	2.46461800	3.32332900	0.27837900
H	2.45079300	2.27820700	1.70588400
H	3.85322800	2.28625600	0.62907000
C	1.13002500	-0.38478800	-3.41456500
H	0.65548900	0.43670800	-3.95777300
H	2.04986600	-0.66875900	-3.94435900
H	0.45122900	-1.24129000	-3.44509700
C	0.85134300	-2.23594100	-0.78867600
H	0.14914500	-2.45412600	-1.59778600
H	1.71176900	-2.91058400	-0.90393700
H	0.36228400	-2.47802100	0.15872900
C	2.02392100	-0.61370200	1.68259300
H	1.21359700	-1.27486200	1.99872200
H	2.95863600	-1.19091100	1.70381200
H	2.11394000	0.18147700	2.42752000
C	-5.20240000	1.33732100	1.37025600
C	-3.86748100	1.00573800	1.51175500
C	-2.92690300	1.17329100	0.45122200
C	-3.42450500	1.71185100	-0.77207700
C	-4.79258000	2.02153100	-0.88712100
C	-5.68412500	1.84947100	0.15799300
H	-5.87672800	1.18758900	2.21028900
H	-3.53276200	0.57989700	2.44876300
H	-5.11685900	2.41034700	-1.84591300
H	-6.73257100	2.10691200	0.03887400
C	-2.63693600	2.00492200	-1.99765800

O	-3.19004800	2.33832000	-3.05160100
N	-1.26044600	1.98164000	-1.86435000
O	-0.61152300	2.36310700	-3.06187300
C	-0.69624500	3.77555400	-3.26830500
H	-0.09026700	3.97122700	-4.15788300
H	-1.73019800	4.07771400	-3.44695300
H	-0.27906600	4.31714000	-2.40856600
N	-1.60525000	0.80053100	0.62403100
C	-1.25763600	0.24466500	1.89573400
C	-0.77604700	1.24238200	2.92315200
H	0.08734100	1.80293900	2.54699400
H	-1.56250300	1.97949800	3.12873000
H	-0.50154500	0.75475000	3.86395500
C	-1.38222100	-1.06560400	2.14827300
H	-1.11923800	-1.47984800	3.11782600
H	-1.77794600	-1.74669500	1.40092000

INT-6

Rh	0.01642300	1.22658600	-1.04040200
C	1.20818500	-0.73492500	-1.23969000
C	-0.16096900	-0.99338300	-1.54507400
C	-0.55614000	-0.16970400	-2.66392700
C	0.61655700	0.56374300	-3.09513300
C	1.68545400	0.24599700	-2.20175800
C	0.69682600	1.44924000	-4.30093600
H	0.95697300	0.85073600	-5.18541400
H	-0.25319000	1.95153300	-4.49424100
H	1.45328600	2.22621100	-4.17772700
C	3.09912600	0.73071400	-2.30413000
H	3.15572200	1.68740000	-2.83004400
H	3.53797400	0.85251100	-1.31194700
H	3.70135500	0.00355200	-2.86731600
C	-1.86737000	-0.22822200	-3.39108100
H	-2.11049800	0.73246000	-3.85234800
H	-1.83086900	-0.98217400	-4.19000700
H	-2.69163700	-0.49125100	-2.72293000
C	-1.05330300	-1.97517000	-0.84733100
H	-2.08372500	-1.61303000	-0.79219500
H	-1.06683400	-2.92635300	-1.39655100
H	-0.70765300	-2.18426100	0.16845000
C	2.06498000	-1.45798200	-0.24373100
H	1.45917700	-1.98153100	0.50217500
H	2.68459700	-2.21149500	-0.75056200
H	2.71373300	-0.75218300	0.27700600

C	-5.07052300	0.39854900	-0.27955400
C	-3.79596400	0.43201000	0.28355500
C	-2.84009000	1.36473400	-0.15213100
C	-3.15151500	2.24911500	-1.20243600
C	-4.45163000	2.22448400	-1.72516300
C	-5.40566400	1.31233100	-1.28011800
H	-5.79492200	-0.33231100	0.06946100
H	-3.52836900	-0.26916100	1.06891200
H	-4.67857200	2.95115300	-2.49809800
H	-6.40067000	1.30863600	-1.71628200
C	-2.20902300	3.24547600	-1.84738800
O	-2.67977000	4.20755100	-2.47022900
N	-0.89554800	2.96955900	-1.70149700
O	-0.04365200	3.82306500	-2.41738100
C	0.13779700	5.07078200	-1.73775400
H	0.88137700	5.61153400	-2.33183100
H	-0.80141700	5.63228100	-1.72107400
H	0.51484400	4.89490200	-0.72747100
N	-1.53980700	1.33851500	0.45022200
C	-1.40538600	1.47410900	1.72929700
C	-2.52372100	1.90988900	2.65161300
H	-2.11919200	2.63965500	3.36239500
H	-3.36691700	2.35287400	2.12153900
H	-2.89133100	1.06384200	3.24549800
C	-0.10203100	1.20623300	2.42005900
H	-0.29354300	0.55573600	3.28453300
H	0.31001200	2.14167400	2.81564700
C	2.26277000	2.45553000	0.67088800
O	1.11847200	2.65521400	0.09886800
O	2.82963500	1.36830600	0.84285100
H	0.64505000	0.75366500	1.77060200
C	2.91825300	3.74875000	1.16449400
H	3.75116300	3.51846900	1.83249000
H	3.29670300	4.31482300	0.30501900
H	2.18944700	4.38600200	1.67542000

INT-7

C	-5.62445200	0.74479000	-0.92875100
C	-4.48438300	0.87144700	-0.14017500
C	-3.42935200	1.72305800	-0.51434000
C	-3.52181500	2.43265800	-1.73861300
C	-4.69000700	2.30401400	-2.50396600
C	-5.73577100	1.47391500	-2.11414300
H	-6.42210600	0.07620800	-0.61557900

H	-4.38305300	0.28909800	0.77088500
H	-4.73647800	2.87217800	-3.42666200
H	-6.62272900	1.38558000	-2.73469600
C	-2.46313800	3.32190700	-2.35282400
O	-2.65619000	3.90699400	-3.41151300
O	-0.17978000	3.93305600	-2.34389300
C	-0.10983800	5.35817600	-2.29497800
H	0.81557500	5.61262300	-2.81893000
H	-0.96407000	5.80682000	-2.81066700
H	-0.06174800	5.71740200	-1.25875600
N	-2.25401200	1.76636400	0.26411200
C	-2.23566100	2.06997000	1.51011700
C	-3.41052700	2.53918000	2.34148100
H	-3.12094000	3.42967000	2.91233000
H	-4.28690500	2.77092700	1.73430600
H	-3.69026500	1.77353200	3.07679500
C	-0.91382100	1.99500000	2.23410400
H	-0.99538000	1.35055200	3.11905600
H	-0.61660100	2.98860400	2.59466400
H	-0.13506400	1.60263500	1.57686900
N	-1.29758900	3.47752300	-1.63048800
H	-1.04224800	2.73755100	-0.97790000

TS-1

Rh	-0.61602500	0.47363000	0.00234100
C	0.32001200	-1.59307300	0.12855800
C	0.10556800	-1.28418000	-1.27020600
C	0.95885900	-0.18427800	-1.60258700
C	1.71688200	0.18280500	-0.42650500
C	1.32563400	-0.68699400	0.63734300
C	2.76632000	1.24790500	-0.34059900
H	3.76662800	0.79872200	-0.42465500
H	2.66036400	1.97316900	-1.15101300
H	2.70150600	1.77856000	0.61328900
C	1.91001000	-0.67577200	2.01636500
H	2.91883200	-1.10998500	1.99744800
H	1.98090500	0.35146800	2.39097200
H	1.31058800	-1.26640700	2.71487600
C	1.13517100	0.42529700	-2.95912000
H	1.14835900	1.51567800	-2.89924300
H	2.08835100	0.09160200	-3.39087500
H	0.33654700	0.13302000	-3.64454000
C	-0.73467300	-2.08065700	-2.22430500
H	-1.06714000	-1.47505500	-3.07097200

H	-0.15591000	-2.92534300	-2.62202800
H	-1.62694000	-2.48194800	-1.73779600
C	-0.24257700	-2.77902200	0.85317800
H	-1.23138200	-3.05156900	0.47629900
H	0.41330200	-3.64965800	0.71239400
H	-0.32188900	-2.59990400	1.92873800
C	-4.66560100	-1.14312300	-0.38835300
C	-3.36477600	-0.93955700	0.09477000
C	-2.57595000	0.05745700	-0.47543900
C	-3.08748700	0.85352300	-1.50095800
C	-4.37768200	0.63964000	-1.99460400
C	-5.16760800	-0.36419400	-1.43594500
H	-5.28862600	-1.91220400	0.06232800
H	-2.99464700	-1.55090100	0.91315000
H	-4.73450300	1.26852400	-2.80574900
H	-6.17426900	-0.53657100	-1.80653000
C	-2.21822900	1.94595800	-2.02913100
O	-2.45088700	2.63223800	-3.01380500
N	-1.14626200	2.09983900	-1.16157600
O	-0.14725100	2.94599300	-1.58930900
C	0.10298800	3.97477500	-0.61451600
H	0.87727100	4.60169800	-1.06328000
H	-0.80639100	4.56259300	-0.45233200
H	0.46508300	3.54375500	0.32629800
N	-1.05446700	1.25583500	1.64427800
O	1.38423300	2.47774600	2.31531900
C	0.85244100	2.93094900	3.36231800
O	1.31346100	3.37985800	4.41450600
C	-1.31084200	1.67542600	2.79463100
C	-2.13536400	0.84394100	3.76783500
H	-1.54580000	0.68532300	4.67792400
H	-3.03967100	1.39690800	4.04302000
H	-2.41872700	-0.11743300	3.33560800
C	-0.75136800	2.99260700	3.28811200
H	-1.18423700	3.24464000	4.25856500
H	-0.98668200	3.78619800	2.57124000

TS-2

Rh	-0.39347600	0.51814400	-0.13729000
C	0.59933300	-1.51556400	0.23340800
C	0.17358300	-1.45493400	-1.14958600
C	0.95514200	-0.44266400	-1.79455800
C	1.90252700	0.07967100	-0.83672200
C	1.69403200	-0.58875200	0.40411200

C	2.93012000	1.12735400	-1.14440100
H	3.69874400	0.72956400	-1.82063700
H	2.46614400	1.98820000	-1.63488900
H	3.42943500	1.48088400	-0.23919800
C	2.43436600	-0.36801700	1.68804000
H	3.35894800	0.19072800	1.52237500
H	1.83387500	0.19609600	2.41416500
H	2.70083200	-1.32550200	2.15047100
C	0.89372000	-0.05296000	-3.24055800
H	1.05983400	1.01977200	-3.36670300
H	1.66686900	-0.58659700	-3.81061200
H	-0.07537200	-0.29623300	-3.68282600
C	-0.77588800	-2.39987600	-1.82168800
H	-1.24796700	-1.94478100	-2.69590000
H	-0.23397400	-3.29404400	-2.15971100
H	-1.57240500	-2.72699800	-1.14933600
C	0.16738900	-2.53028100	1.25207800
H	-0.85670800	-2.87146300	1.07831000
H	0.81656400	-3.41634000	1.20654500
H	0.22718100	-2.12969600	2.26768500
C	-4.55161600	-0.85983100	-0.23883900
C	-3.18887900	-0.79101500	0.08365800
C	-2.40564600	0.23772000	-0.43899800
C	-2.99583100	1.19232600	-1.27306900
C	-4.35526500	1.13007400	-1.59094600
C	-5.13578300	0.09724000	-1.07398800
H	-5.15767300	-1.66362600	0.17275400
H	-2.76272200	-1.53766000	0.74811000
H	-4.77139600	1.89786000	-2.23771500
H	-6.19357700	0.03741500	-1.31469000
C	-2.12870400	2.28673600	-1.79495700
O	-2.49978900	3.24704400	-2.46148000
N	-0.83551800	2.04702000	-1.38397200
O	0.13579500	2.97759200	-1.71560500
C	0.05807300	4.14551900	-0.88093900
H	0.90783300	4.76680400	-1.17436800
H	-0.88071900	4.67391400	-1.06714800
H	0.14238000	3.86740600	0.17638100
N	-0.63097500	1.21026900	1.60082700
O	1.15097300	1.44277300	4.38917900
C	0.07681600	1.80899200	4.81404500
O	-0.64124600	1.85525100	5.78892700
C	-1.33580200	1.54655200	2.62060500
C	-2.54764500	0.77020600	3.10599300

H	-2.65780000	0.91414000	4.18380600
H	-3.44625500	1.13154900	2.59438800
H	-2.44419700	-0.29467600	2.88844800
C	-0.86908700	2.67384400	3.39576300
H	-1.65201800	3.24535600	3.89183400
H	-0.08474400	3.27056800	2.93349500

TS-3

Rh	-0.13133700	0.43493700	-0.00346900
C	0.75748900	-1.67623400	0.28600000
C	0.35612300	-1.56916900	-1.10814400
C	1.10076900	-0.51960700	-1.70681800
C	1.97329100	0.04452000	-0.69406700
C	1.78669400	-0.71114100	0.51920000
C	2.98886300	1.11991300	-0.94564200
H	3.83582200	0.73109000	-1.52850100
H	2.54171000	1.94676100	-1.50505300
H	3.38890400	1.52307600	-0.01061000
C	2.55348200	-0.54003700	1.79768500
H	2.92511300	0.48178500	1.91209200
H	1.93622200	-0.77082400	2.67053900
H	3.42229600	-1.21278000	1.81714000
C	1.04661900	-0.05871500	-3.13480500
H	1.03318900	1.03316100	-3.19131600
H	1.92206000	-0.42061900	-3.69145000
H	0.15299600	-0.42822000	-3.64469500
C	-0.64195700	-2.46294200	-1.78417000
H	-1.01994300	-2.01849000	-2.70825000
H	-0.18308800	-3.42762400	-2.04145900
H	-1.50166400	-2.66604800	-1.13899100
C	0.29601800	-2.72740500	1.25332700
H	-0.71254800	-3.07666800	1.01358300
H	0.95879200	-3.60409700	1.23170800
H	0.28335800	-2.35049900	2.28091400
C	-4.36570800	-0.81043300	0.53619400
C	-2.99655600	-0.68798700	0.80003400
C	-2.25895200	0.28652600	0.12545300
C	-2.88079600	1.17032000	-0.76612300
C	-4.24767800	1.04439800	-1.02203700
C	-4.98865400	0.05525300	-0.37032400
H	-4.94769200	-1.57326700	1.04785600
H	-2.51588500	-1.33216500	1.52999900
H	-4.69872700	1.72329800	-1.74081700
H	-6.05438200	-0.03842700	-0.56239800

C	-2.04878200	2.18014300	-1.50238700
O	-2.50704900	2.94245700	-2.35942200
N	-0.76735300	2.12327700	-1.04459200
O	0.18147300	2.89566200	-1.73653200
C	-0.00591000	4.30280600	-1.54990900
H	0.85147100	4.77144000	-2.04246400
H	-0.94070500	4.62648200	-2.01323200
H	-0.00868100	4.55651300	-0.48247500
N	-0.91963800	1.03156200	1.65383400
C	-1.31750100	2.28129600	2.01349100
C	-2.62279800	2.40711000	2.77172300
H	-2.72386200	3.39749600	3.22560300
H	-3.46304000	2.25492300	2.08470800
H	-2.69106000	1.64058900	3.55044000
C	-0.43528700	3.31744800	1.90524200
H	-0.57272100	4.22754900	2.48344600
H	0.49102400	3.19399400	1.35827600

TS-4

Rh	-0.12820300	1.39893900	-1.22398500
C	0.40823400	-0.78241400	-1.57503900
C	-0.76063500	-0.33916300	-2.33736100
C	-0.30094100	0.61864800	-3.33099100
C	1.06820300	0.88063300	-3.07600100
C	1.51161800	-0.01358100	-1.99848500
C	1.95807800	1.83992700	-3.80504300
H	2.68339600	1.30608300	-4.43409200
H	1.37646800	2.50616300	-4.44631900
H	2.51277700	2.46098900	-3.09494500
C	2.92239400	-0.07103700	-1.49770600
H	3.30036800	0.93515900	-1.29070400
H	3.00864800	-0.66233700	-0.58272200
H	3.57879600	-0.52354600	-2.25324000
C	-1.14041800	1.24631800	-4.40283100
H	-0.94470600	2.31794500	-4.47946300
H	-0.92431300	0.77579400	-5.37141600
H	-2.20666200	1.12277700	-4.20042100
C	-2.10787500	-0.99535800	-2.30127300
H	-2.89710800	-0.31491000	-2.63029800
H	-2.12183100	-1.87511900	-2.96014500
H	-2.36377400	-1.32615000	-1.29136200
C	0.38529200	-1.87101600	-0.54375000
H	-0.46512700	-1.75613700	0.13462800
H	0.29501500	-2.85283300	-1.02781100

H	1.29438400	-1.87814100	0.06219100
C	-4.63659100	-0.03261100	1.10138200
C	-3.25636700	0.12006600	1.20082100
C	-2.56413400	1.11216000	0.47379800
C	-3.30556000	1.91704300	-0.42779400
C	-4.69524400	1.74977700	-0.50712500
C	-5.36913600	0.79513100	0.24889500
H	-5.13316400	-0.80675300	1.68137900
H	-2.68847500	-0.54609500	1.84270000
H	-5.22564200	2.40708900	-1.18799900
H	-6.44698400	0.68918900	0.16426400
C	-2.73854200	2.95834500	-1.36166500
O	-3.49152200	3.72965800	-1.96628300
N	-1.37593800	2.99433800	-1.46860800
O	-0.93751600	3.81254200	-2.53662100
C	-0.81482400	5.16799400	-2.11484500
H	-0.38636800	5.69962200	-2.97045000
H	-1.79786800	5.58341800	-1.87314000
H	-0.14315400	5.25154600	-1.25296100
N	-1.16563600	1.22493700	0.60029000
C	-0.54743800	1.18849200	1.79372500
C	-1.32613600	1.45956000	3.07583200
H	-0.68581900	2.02612200	3.75834100
H	-2.24032100	2.02910400	2.89606400
H	-1.60132300	0.53029300	3.58655400
C	0.83995500	1.06249400	1.92531200
H	1.22765200	0.88296400	2.92609100
H	1.40269500	0.60386900	1.11536100
C	1.90188200	3.72875600	0.21558100
O	1.49633900	2.99248200	-0.70360100
O	1.71512600	3.53329000	1.48249000
H	1.27498400	2.52409100	1.67771400
C	2.70166800	4.97563900	-0.10653700
H	2.16292000	5.85581900	0.26081000
H	3.66364500	4.94461400	0.41521900
H	2.85797400	5.06524800	-1.18252300

INT-2a

Rh	0.00252400	0.24505700	-0.03928300
C	1.40988500	-1.29127300	0.84335600
C	1.04846400	-1.69348000	-0.46572500
C	1.45316100	-0.62577700	-1.36137900
C	2.25377900	0.33789700	-0.60203600
C	2.19238300	-0.04351200	0.74538700

C	2.92807000	1.53948500	-1.19766000
H	3.53989500	1.25452600	-2.06212000
H	2.19437500	2.28457600	-1.52493100
H	3.58541000	2.02411700	-0.47072400
C	2.81416700	0.64045500	1.92473200
H	3.58018700	-0.00393500	2.37740700
H	3.29074800	1.58101900	1.63787700
H	2.07279500	0.86685800	2.69781800
C	1.31585100	-0.63088800	-2.85273700
H	1.24341300	0.38652200	-3.24745300
H	2.19370100	-1.10747100	-3.31337800
H	0.42895900	-1.18450300	-3.17213300
C	0.42494100	-2.98953300	-0.89115000
H	-0.33959300	-2.84165300	-1.65924200
H	1.19029900	-3.65943900	-1.30645500
H	-0.04193300	-3.50941400	-0.05045900
C	1.21473600	-2.05861500	2.11667400
H	0.44672700	-2.82941700	2.01019500
H	2.14972700	-2.55804500	2.40821200
H	0.91681100	-1.40637500	2.94258200
C	-4.01312400	-1.60722200	-0.20565300
C	-2.62263400	-1.48270900	-0.05593500
C	-1.99634300	-0.24149000	-0.21032000
C	-2.81191700	0.86751600	-0.49964600
C	-4.19323700	0.75838500	-0.65385600
C	-4.79982700	-0.49389200	-0.51186200
H	-4.48033500	-2.58240500	-0.08418800
H	-2.04441300	-2.36931100	0.18827500
H	-4.76927100	1.64991800	-0.88886100
H	-5.87385700	-0.60095300	-0.64103700
C	-2.12354500	2.19328200	-0.61392000
O	-2.66109200	3.24636000	-0.93136400
N	-0.78506300	2.04288100	-0.25578100
O	0.01528700	3.16551000	-0.51631200
C	-0.01493800	4.07930300	0.58488600
H	0.72633500	4.84692700	0.34488500
H	-1.00497300	4.53916600	0.67270500
H	0.25508600	3.57250600	1.51910100
C	-2.32411700	1.52632500	3.30749000
H	-2.70863400	2.41609500	3.81951500
H	-2.37319500	1.71681900	2.22932700
N	-2.21444400	-0.60745800	4.22468300
O	-0.88864600	-0.04120200	4.24979000
C	-0.89768900	1.22345700	3.71776100

O	0.10543200	1.88627300	3.62718200
C	-3.01031700	0.25756700	3.70547900
C	-4.46054600	-0.04944400	3.52632300
H	-5.07992900	0.70361400	4.02846800
H	-4.71893700	-0.03727500	2.46069500
H	-4.69098000	-1.03496000	3.93844400

INT-3a

Rh	-0.36543400	0.32993900	0.77496200
C	0.84727200	-1.68752300	0.74780000
C	0.50120500	-1.33587700	-0.60963000
C	1.24780900	-0.14818900	-0.97022400
C	1.96923200	0.27861600	0.17585100
C	1.70391100	-0.66103000	1.24839200
C	2.83721300	1.48683700	0.31716000
H	3.83132400	1.20897300	0.68888400
H	2.95636100	2.01237300	-0.63196200
H	2.38626200	2.17929200	1.03989600
C	2.29193400	-0.57610200	2.62100500
H	3.35249500	-0.86250000	2.60733800
H	2.22394700	0.44843100	3.00076500
H	1.76889500	-1.23484900	3.31804000
C	1.28065800	0.47048500	-2.33399300
H	1.48913100	1.53950300	-2.28078100
H	2.05543300	-0.01097400	-2.94704500
H	0.32667500	0.35079700	-2.85440500
C	-0.26044000	-2.19406400	-1.57270700
H	-0.75769700	-1.59509200	-2.33969800
H	0.42898800	-2.88327300	-2.08003600
H	-1.02601500	-2.78759100	-1.06913300
C	0.39210300	-2.88242800	1.51786800
H	-0.15151100	-3.59015900	0.88722600
H	1.24524300	-3.40756800	1.96254300
H	-0.27035900	-2.55538100	2.33369300
C	-4.14678600	-1.79075600	-0.04440100
C	-2.93282800	-1.44215300	0.56083200
C	-2.25332500	-0.30353300	0.12543100
C	-2.79497500	0.47280400	-0.89990000
C	-4.00476400	0.12221800	-1.50859700
C	-4.68389300	-1.01447900	-1.07783300
H	-4.67769000	-2.67556800	0.29992100
H	-2.53815600	-2.04735600	1.36947500
H	-4.38162000	0.75120600	-2.31068900
H	-5.62630000	-1.29756400	-1.53884400

C	-2.02595000	1.67155900	-1.32390300
O	-2.26397900	2.37483500	-2.29941700
N	-1.02627800	1.89562700	-0.39577100
O	-0.05885400	2.81731400	-0.77322400
C	-0.37993400	4.14258200	-0.32147100
H	0.44249000	4.76491600	-0.68486400
H	-1.32002600	4.47097600	-0.77522400
H	-0.42663900	4.19145600	0.76859800
C	-1.97525400	1.85548800	3.05153200
H	-2.49043500	2.36067100	3.87099400
H	-2.58443000	1.94732500	2.14247400
N	-1.13470800	-0.40101900	2.54797100
O	0.19973900	1.92761200	2.00731500
C	-0.63371400	2.55834100	2.79873700
O	-0.37063100	3.63427100	3.31630700
C	-1.74287100	0.38517400	3.33475000
C	-2.23941700	-0.15305000	4.66438800
H	-1.78409100	0.40803400	5.49001400
H	-3.32629700	-0.02080700	4.73887900
H	-1.99840000	-1.21300100	4.77035600

TS-1a

Rh	-0.19784300	0.34339500	0.58623700
C	1.11771100	-1.60623700	0.95833400
C	0.62796300	-1.54857200	-0.37069800
C	1.16651600	-0.34020000	-0.98232000
C	2.11026400	0.25598800	-0.04705300
C	2.01978500	-0.47356900	1.15386400
C	2.98400400	1.43577900	-0.34858500
H	3.73072600	1.17803500	-1.11170500
H	2.38615200	2.27043500	-0.72480500
H	3.52158700	1.77569300	0.54055900
C	2.72123000	-0.19426000	2.44736000
H	3.42774000	-1.00016200	2.68761900
H	3.27681100	0.74521600	2.41358500
H	2.00143200	-0.12847900	3.27013000
C	1.01959200	0.06271400	-2.41980200
H	1.05916300	1.14991600	-2.52467300
H	1.83198400	-0.37043600	-3.02054200
H	0.07149700	-0.28240200	-2.84037500
C	-0.17488300	-2.58798400	-1.09380100
H	-0.87972800	-2.13589000	-1.79538900
H	0.49636900	-3.24387300	-1.66513900
H	-0.74937400	-3.21427800	-0.40747300

C	0.83703300	-2.65077200	1.99005400
H	0.28882500	-3.49790900	1.56838700
H	1.76648600	-3.03676000	2.42679900
H	0.23818200	-2.22748700	2.81002400
C	-4.15139400	-1.42585300	-0.04450100
C	-2.84308400	-1.24182600	0.42489000
C	-2.12211700	-0.10170400	0.05429200
C	-2.73492400	0.84206300	-0.77841700
C	-4.03635000	0.66075300	-1.25443500
C	-4.74836500	-0.48020900	-0.88524300
H	-4.70342900	-2.31798800	0.24461900
H	-2.40085800	-1.99430300	1.07383300
H	-4.46183400	1.41831000	-1.90731600
H	-5.76119300	-0.63562900	-1.24735000
C	-1.92255700	2.04038000	-1.13717000
O	-2.23437100	2.88991700	-1.96557800
N	-0.78917100	2.05873800	-0.34364600
O	0.19051400	2.96135300	-0.77050000
C	0.02041500	4.24403700	-0.14579900
H	0.88283300	4.83317700	-0.47183700
H	-0.90320600	4.70997500	-0.50260300
H	0.00762900	4.15281400	0.94377400
C	-2.54622500	1.59542900	3.06878800
H	-3.16461700	2.00528600	3.87159100
H	-3.12523400	1.64422900	2.13528700
N	-0.97450600	-0.19432400	2.85232700
O	-0.24283800	1.62274200	2.52523800
C	-1.25645100	2.39793100	2.87188800
O	-1.16487400	3.59967100	3.03936300
C	-2.09652300	0.18654400	3.30642600
C	-2.92053700	-0.79136400	4.11492500
H	-3.16450900	-0.35568100	5.09110500
H	-3.85868800	-0.99188800	3.58445300
H	-2.38564100	-1.73221500	4.26065400

INT-3b

Rh	-0.37764800	0.46740900	0.24867100
C	0.69244600	-1.54633200	0.01841600
C	0.33452700	-1.17364000	-1.36326700
C	0.94196300	0.04422700	-1.66810000
C	1.64915100	0.49585200	-0.45703900
C	1.60507800	-0.58544200	0.51571200
C	2.53062800	1.70614400	-0.40569100
H	3.43987300	1.54843200	-1.00324200

H	2.00146400	2.57431700	-0.80867200
H	2.84006100	1.93665600	0.61794900
C	2.48173300	-0.70180000	1.72630200
H	3.46238200	-1.10105500	1.43106300
H	2.65882700	0.26588700	2.20464000
H	2.06494100	-1.38022200	2.47453300
C	0.88693300	0.82141300	-2.95013500
H	0.54008900	1.84366800	-2.77209600
H	1.88396700	0.87512500	-3.40848100
H	0.21280600	0.35733200	-3.67492500
C	-0.56168900	-2.00173100	-2.23410500
H	-0.73166000	-1.52868400	-3.20417300
H	-0.12280900	-2.99230000	-2.41335200
H	-1.54057900	-2.15987700	-1.76551200
C	0.31087100	-2.85033900	0.65686100
H	-0.74184600	-3.09150000	0.47502300
H	0.90971200	-3.67678900	0.24844000
H	0.46802100	-2.83262500	1.73892900
C	-4.27819300	-1.59838700	0.55257600
C	-3.59233200	-0.79966800	1.45980200
C	-2.97106700	0.39649600	1.05487000
C	-3.07512500	0.81480100	-0.29995500
C	-3.83028000	0.02065300	-1.18290200
C	-4.41160900	-1.17416900	-0.77576100
H	-4.74652000	-2.52017100	0.88627800
H	-3.54782000	-1.05770600	2.51308600
H	-3.94498600	0.38474800	-2.19871500
H	-4.98457300	-1.76718900	-1.48359600
C	-2.42091800	2.03693200	-0.93434900
O	-2.93754900	2.60639800	-1.89424800
N	-1.22140600	2.29851900	-0.34679300
O	-0.39612900	3.18459800	-1.09323600
C	-0.79953400	4.55152400	-0.93311000
H	-0.04191600	5.12988700	-1.47092200
H	-1.78279100	4.71560000	-1.38143000
H	-0.81408500	4.84203400	0.12175900
C	-0.51326600	2.58298300	2.50350200
H	0.27951400	3.00354200	1.88246200
H	-0.21573300	2.70616100	3.55533500
N	-2.36349800	1.14590500	2.13915500
O	-2.82967600	2.51769700	2.08178500
C	-1.78925100	3.37231000	2.29170200
O	-1.95973300	4.56425800	2.34623200
C	-0.87264100	1.13551100	2.17909900

C	-0.44245100	0.15575000	3.27083000
H	0.64291200	0.16534100	3.39510400
H	-0.89684900	0.44395300	4.22969200
H	-0.75516000	-0.87030100	3.05049100

TS-1b

Rh	-0.37947000	0.47229500	0.39858800
C	0.71730700	-1.56661800	0.21359600
C	0.20527700	-1.25644600	-1.10981300
C	0.77295100	-0.03015900	-1.51960000
C	1.68782700	0.42380300	-0.46338700
C	1.69468400	-0.57301900	0.55848600
C	2.60546800	1.60330400	-0.58362700
H	3.42690800	1.38954600	-1.28242500
H	2.06287500	2.47754400	-0.95253800
H	3.05149900	1.86447300	0.38082800
C	2.64452900	-0.63730000	1.71859500
H	3.57426600	-1.13687300	1.41250600
H	2.91761700	0.35722600	2.08406700
H	2.23430700	-1.20663400	2.55673400
C	0.57245900	0.68591700	-2.82278000
H	0.43377300	1.75934400	-2.66468400
H	1.44852300	0.54748900	-3.47186100
H	-0.30259200	0.31256700	-3.36081100
C	-0.74716900	-2.11711000	-1.88605000
H	-1.14199700	-1.59096300	-2.75862500
H	-0.24292600	-3.02519200	-2.24404100
H	-1.60110900	-2.43192200	-1.27738100
C	0.44716700	-2.84302700	0.95819700
H	-0.57979300	-3.18682800	0.80305200
H	1.11542400	-3.64636000	0.61607200
H	0.60343900	-2.72922900	2.03540100
C	-4.24817700	-1.57432600	-0.03974500
C	-3.17294400	-1.12731400	0.72621700
C	-2.55169600	0.08681700	0.40659200
C	-3.04246800	0.88390300	-0.64495700
C	-4.13601600	0.43312700	-1.39072100
C	-4.74078100	-0.78647500	-1.09025100
H	-4.72779200	-2.51872700	0.20509500
H	-2.84288500	-1.68644100	1.59712500
H	-4.47002200	1.05103800	-2.21951500
H	-5.59834700	-1.12464900	-1.66536000
C	-2.28503300	2.09741700	-1.10309500
O	-2.63474600	2.78308700	-2.06394400

N	-1.18499500	2.28742700	-0.29914300
O	-0.24810900	3.23287800	-0.79157800
C	-0.72594200	4.58707000	-0.73193800
H	0.13786200	5.19538200	-1.01675400
H	-1.54715100	4.73623100	-1.43541500
H	-1.04692500	4.84977100	0.28074000
C	-0.68145300	2.69433900	2.55794500
H	0.04060500	3.19741900	1.91156700
H	-0.44932500	2.95497400	3.60051800
N	-2.13507100	0.85949100	2.11975300
O	-2.87652300	2.04303600	2.03624700
C	-2.08049000	3.16819700	2.24619200
O	-2.56348800	4.26532400	2.24888900
C	-0.77559200	1.19431700	2.35693600
C	-0.16146100	0.31800000	3.43777500
H	0.91766800	0.47629700	3.49620100
H	-0.59238400	0.57528100	4.41669300
H	-0.35399200	-0.74258300	3.25592000

INT-6c

Rh	0.01154400	1.28148500	-1.18032200
C	0.89100000	-0.82159800	-1.49555200
C	-0.40766900	-0.71215100	-2.15677700
C	-0.30894300	0.29758200	-3.16209400
C	1.01584900	0.87428900	-3.08432500
C	1.76384900	0.12186900	-2.09110300
C	1.56676900	1.91589500	-4.01063800
H	1.89843300	1.46365900	-4.95600900
H	0.80897900	2.67036000	-4.23437500
H	2.42466800	2.42730100	-3.56583900
C	3.21709800	0.30442000	-1.77999700
H	3.52690300	1.34342900	-1.92202300
H	3.44136500	0.02675900	-0.74971100
H	3.82035700	-0.31649700	-2.45741800
C	-1.36518500	0.70082600	-4.14677200
H	-1.40136000	1.78662200	-4.26672700
H	-1.15067900	0.25377400	-5.12719000
H	-2.35871100	0.36725700	-3.83793300
C	-1.57782600	-1.62186900	-1.92589600
H	-2.51676600	-1.16241300	-2.24360500
H	-1.45095900	-2.55534800	-2.49130700
H	-1.68559900	-1.89105100	-0.87127800
C	1.25855900	-1.78230700	-0.40275200
H	0.37022900	-2.23705700	0.04744300

H	1.87996300	-2.60173900	-0.78810800
H	1.81712100	-1.26235700	0.38133300
C	-4.51909700	-0.48156100	0.94220600
C	-3.18975200	-0.13786100	1.18376800
C	-2.55001300	0.83775600	0.41219100
C	-3.24314200	1.50862800	-0.61211500
C	-4.58894100	1.16493400	-0.81699500
C	-5.22332500	0.18029100	-0.06393200
H	-4.99804700	-1.24914300	1.54370600
H	-2.64005500	-0.61852900	1.99025500
H	-5.11507300	1.70948300	-1.59357100
H	-6.26342900	-0.06569700	-0.25898000
C	-2.71416800	2.58950700	-1.55295500
O	-3.52295200	3.23412900	-2.22658300
N	-1.36674800	2.77932300	-1.55291900
O	-0.96350600	3.64919800	-2.58987100
C	-0.61359600	4.92459400	-2.05636600
H	-0.26366600	5.51042700	-2.91226700
H	-1.49071600	5.41445800	-1.61610400
H	0.18575800	4.82594100	-1.31483000
N	-1.15217200	1.13384600	0.73274500
C	-1.00341000	2.12706800	1.80192700
C	-1.61105400	3.48077700	1.58391200
H	-1.49344400	4.08178600	2.48962400
H	-1.11987200	3.98368100	0.74838300
H	-2.67957400	3.41922700	1.35091200
C	-0.34889600	1.77805400	2.91309700
H	-0.21398200	2.49286300	3.71790800
H	0.12186800	0.80769400	3.03605100
C	2.01414700	2.28728100	0.69519500
O	1.19992900	2.73013900	-0.21896200
O	2.13364700	1.10959300	1.05636900
H	-0.72596300	0.28097300	1.09208200
C	2.83652900	3.39313600	1.35321700
H	3.69299700	2.96360600	1.87792300
H	3.17241100	4.12796900	0.61569500
H	2.20676200	3.91928700	2.08037700

TS-4c

Rh	-0.02797400	1.45931100	-1.23523800
C	0.58484200	-0.75768800	-1.51644500
C	-0.55423300	-0.37482000	-2.33885000
C	-0.08854800	0.58497600	-3.32486900
C	1.25768000	0.90031900	-3.01694300

C	1.68185200	0.03917800	-1.90556000
C	2.15203000	1.86361100	-3.73899300
H	2.82126800	1.33759500	-4.43414300
H	1.57054500	2.58942000	-4.31273000
H	2.77734800	2.42288600	-3.03572200
C	3.08365600	-0.02439200	-1.37804700
H	3.53697800	0.97077200	-1.33117000
H	3.12275000	-0.46456100	-0.37933400
H	3.71176800	-0.63393600	-2.04226100
C	-0.90963000	1.09643400	-4.46977800
H	-0.46712700	1.98684300	-4.91872500
H	-0.97739500	0.31822400	-5.24303900
H	-1.92371600	1.35967000	-4.15975100
C	-1.86126300	-1.10637200	-2.40101900
H	-2.65985900	-0.47398200	-2.79536500
H	-1.76658700	-1.97808000	-3.06483200
H	-2.17493100	-1.46689100	-1.41848600
C	0.55274500	-1.81012400	-0.44978900
H	-0.36643900	-1.74470900	0.14156800
H	0.58479300	-2.81334200	-0.89612600
H	1.40009200	-1.71950600	0.23462600
C	-3.87411800	-0.79655000	1.35955800
C	-2.60659700	-0.21791700	1.43635800
C	-2.22057800	0.80787600	0.56150900
C	-3.13619100	1.25555400	-0.42346600
C	-4.41285100	0.67741900	-0.46758600
C	-4.78780700	-0.33818600	0.40920300
H	-4.14632400	-1.59352500	2.04716600
H	-1.89707000	-0.53928000	2.19360100
H	-5.09662700	1.05085800	-1.22292900
H	-5.78261600	-0.77106100	0.34783700
C	-2.85773700	2.28646900	-1.50903900
O	-3.77739300	2.67351900	-2.23935100
N	-1.57247300	2.75120900	-1.59049400
O	-1.35066000	3.53040800	-2.75499400
C	-1.57644000	4.90961400	-2.48716500
H	-1.38041800	5.42261100	-3.43396800
H	-2.61471500	5.08372900	-2.18549700
H	-0.88921400	5.28696700	-1.71874200
N	-0.91914400	1.40021300	0.72676800
C	-1.03083000	2.55417500	1.62226900
C	-1.64213900	3.86282900	1.18498200
H	-1.68885500	4.54799100	2.03774800
H	-1.05619500	4.32429200	0.38801200

H	-2.65784000	3.72991900	0.79980300
C	-0.62747100	2.39812400	2.89367700
H	-0.73785800	3.20574200	3.61211100
H	-0.19609100	1.47226100	3.25843700
C	1.98208900	2.16451400	0.86036600
O	1.46883400	2.75524900	-0.11188700
O	1.52301400	1.05492200	1.37782100
H	0.46100400	0.94707000	1.12409300
C	3.20737800	2.72335400	1.53862600
H	2.89737300	3.19230200	2.47993500
H	3.90558300	1.91869000	1.78653900
H	3.68928000	3.47179100	0.90783600

TS-5c

Rh	-0.01961400	1.24360900	-1.11430000
C	0.99577600	-0.78055700	-1.39496700
C	-0.32224000	-0.79168100	-1.99972200
C	-0.34974500	0.19346800	-3.04174400
C	0.95112900	0.82694100	-3.08827300
C	1.77630500	0.19453800	-2.09070400
C	1.38146000	1.84299100	-4.10314600
H	1.56353600	1.36594600	-5.07649000
H	0.61618600	2.61239700	-4.23135900
H	2.30600100	2.34199100	-3.80086400
C	3.22714100	0.47792000	-1.84919000
H	3.50403500	1.47832000	-2.19243800
H	3.47247000	0.39982100	-0.78905400
H	3.83999800	-0.24439800	-2.40659000
C	-1.48157800	0.48000300	-3.98332000
H	-1.53994000	1.54562000	-4.22026400
H	-1.34025800	-0.07099600	-4.92347300
H	-2.44517400	0.18053500	-3.56306200
C	-1.42475400	-1.74671500	-1.65727600
H	-2.40492100	-1.35252100	-1.93482400
H	-1.27841100	-2.69525000	-2.19207200
H	-1.44677800	-1.97048800	-0.58721100
C	1.48682500	-1.68286500	-0.30155100
H	0.65272900	-2.08461000	0.28179300
H	2.04527100	-2.53719800	-0.70914800
H	2.13810900	-1.13105300	0.38095100
C	-4.77194600	-0.32396600	0.64062100
C	-3.42034500	-0.12398600	0.91763400
C	-2.67613000	0.85904300	0.24893500
C	-3.30345200	1.65591100	-0.73493700

C	-4.66691600	1.44338400	-0.99131400
C	-5.40091100	0.46971300	-0.31897200
H	-5.32405300	-1.09534500	1.17098900
H	-2.92103500	-0.74082500	1.66120900
H	-5.12389200	2.08004000	-1.74157400
H	-6.45402900	0.32861500	-0.54606600
C	-2.65658800	2.73608800	-1.59123800
O	-3.37618800	3.47305800	-2.27323800
N	-1.29965400	2.82919900	-1.51418100
O	-0.78114200	3.70276300	-2.49917800
C	-0.52079600	4.98520100	-1.93775900
H	-0.08252100	5.57542500	-2.74904300
H	-1.45262200	5.46077400	-1.60816200
H	0.18985700	4.90579000	-1.10768900
N	-1.28703100	0.99644900	0.61781900
C	-1.01545500	1.93602500	1.64936700
C	-1.62164400	3.28539200	1.73100200
H	-1.37875600	3.78211900	2.67238600
H	-1.22060000	3.85774400	0.88629400
H	-2.70808300	3.24150400	1.59209700
C	-0.28196000	1.26462300	2.63034000
H	-0.18971700	1.66313100	3.63924500
H	0.62901500	0.76854800	2.25443600
C	2.06418000	2.35714900	0.79566300
O	1.06733500	2.69449300	0.03874900
O	2.37029500	1.20294100	1.13763800
H	-0.93729500	0.31044700	1.87968500
C	2.88476000	3.54950200	1.28648600
H	3.63102300	3.22431000	2.01433700
H	3.38896700	4.02496800	0.43723000
H	2.23021800	4.30450000	1.73460000

TS-6c

Rh	0.00184500	1.34101300	-0.71444500
C	1.00022000	-0.58553300	-1.17102200
C	-0.33031500	-0.69800900	-1.73844300
C	-0.48273100	0.31275300	-2.72790800
C	0.77243600	1.04416500	-2.81600100
C	1.69401300	0.44179500	-1.90471900
C	1.08807700	2.08094700	-3.85114500
H	1.40350400	1.59932800	-4.78781200
H	0.21627500	2.70014100	-4.07948300
H	1.89883900	2.74003700	-3.53021600
C	3.14471600	0.78212300	-1.77102900

H	3.33435500	1.83475200	-1.99604300
H	3.50795700	0.57288400	-0.76409500
H	3.72434900	0.17730600	-2.48264600
C	-1.64403800	0.52466200	-3.65131400
H	-1.95356900	1.57492600	-3.68774300
H	-1.36398500	0.22722300	-4.67117800
H	-2.51273000	-0.06514800	-3.35470800
C	-1.30016500	-1.78748100	-1.40807700
H	-2.31344900	-1.55827700	-1.74075300
H	-0.98077400	-2.71667300	-1.90045000
H	-1.33767700	-1.98190800	-0.33326300
C	1.61132300	-1.50508200	-0.15722000
H	0.83968000	-2.01398900	0.42693700
H	2.22233300	-2.27542300	-0.64930600
H	2.23553600	-0.93833600	0.53733800
C	-4.59666800	-0.74788900	0.01423900
C	-3.42585200	-0.36780300	0.67846600
C	-2.71607400	0.76413600	0.26878700
C	-3.20673000	1.53061200	-0.81759800
C	-4.37784500	1.14322800	-1.47189100
C	-5.07288800	0.00149900	-1.06396100
H	-5.13981500	-1.62919900	0.34616700
H	-3.05302300	-0.93370100	1.52729500
H	-4.73431100	1.75708100	-2.29321200
H	-5.98563000	-0.29181800	-1.57489600
C	-2.53371500	2.81320200	-1.23864400
O	-2.98172500	3.51080800	-2.14124700
N	-1.37333000	3.12602500	-0.50121500
O	-0.99691900	4.47216000	-0.63951700
C	-0.16672000	4.72757700	-1.77179800
H	0.06324200	5.79536200	-1.71210500
H	0.75649400	4.14600500	-1.70027000
H	-0.70242900	4.52071400	-2.70350600
N	-1.53129000	1.16888300	0.94474600
C	-1.60800700	2.46513300	1.35911300
C	-2.91709200	3.11282300	1.80017900
H	-2.78467300	4.19853400	1.82406700
H	-3.77998100	2.87381200	1.18084300
H	-3.13004200	2.77796000	2.82367600
C	2.34933100	2.30030300	0.93673500
O	1.42016700	2.67515700	0.10549000
O	2.48883900	1.17394100	1.41953600
C	3.28695200	3.44270100	1.32967700
H	4.21035100	3.04010700	1.75228100

H	3.50829200	4.08826800	0.47476300
H	2.79548000	4.06141400	2.09037000
C	-0.45408400	3.01289800	2.16523800
H	-0.03466300	3.89867400	1.68331700
H	-0.83110600	3.30783600	3.15186100
H	0.31916700	2.25816300	2.29458400

INT-6d

Rh	0.24671000	1.03718800	-0.14733100
C	1.47930600	-0.82681100	0.16285400
C	0.69446800	-1.06893900	-1.03949900
C	1.04354700	-0.08368200	-1.99367700
C	2.05464000	0.78833900	-1.40183700
C	2.36062300	0.27476800	-0.09594800
C	2.77002900	1.88643000	-2.13110900
H	3.50015600	1.47670100	-2.84369700
H	2.05801900	2.50557900	-2.68221800
H	3.31199900	2.53752600	-1.43869500
C	3.43909500	0.77735000	0.81909500
H	3.61780200	1.84739100	0.68121000
H	3.19027500	0.61256400	1.87195000
H	4.38517400	0.25489000	0.62077100
C	0.50333500	0.07774900	-3.38445200
H	0.20024300	1.11240400	-3.56959900
H	1.26937100	-0.18961100	-4.12533000
H	-0.36546800	-0.56237400	-3.55865600
C	-0.30160200	-2.18041600	-1.20207100
H	-0.95974100	-2.00714700	-2.05719500
H	0.20380000	-3.14331000	-1.35911900
H	-0.93534500	-2.28412500	-0.31487600
C	1.48457100	-1.70770900	1.37917200
H	0.48541400	-2.09869300	1.59515300
H	2.15072000	-2.57051300	1.23656600
H	1.83085600	-1.17086800	2.26746300
C	-4.91699200	-0.38006400	0.74989800
C	-3.67342200	-0.03543900	1.28143000
C	-2.79384500	0.76031300	0.54211600
C	-3.13376200	1.21208100	-0.75163500
C	-4.38742900	0.85121400	-1.26017400
C	-5.27329900	0.06428700	-0.52456100
H	-5.59997900	-0.99502600	1.33003900
H	-3.37222600	-0.37620300	2.26818600
H	-4.64116700	1.21792800	-2.24905100
H	-6.23933300	-0.20119100	-0.94527300

C	-2.26139400	2.07939100	-1.65573500
O	-2.75020700	2.50172500	-2.71091400
N	-1.00773200	2.39327900	-1.20096400
O	-0.27635500	3.13657900	-2.17200200
C	-0.59716400	4.51881100	-2.09663300
H	0.05726500	5.01245700	-2.82250100
H	-1.64340800	4.69282500	-2.36793700
H	-0.39322500	4.91799400	-1.09251200
N	-1.50852200	1.07698300	1.04582600
C	-1.19342200	2.21653000	1.59929400
C	-2.15907800	3.29632800	1.98658700
H	-2.04707700	4.12767400	1.27933900
H	-3.19597400	2.95406900	1.95940200
H	-1.92138100	3.67883700	2.98534900
C	0.26270600	2.38067500	1.53709800
H	0.62078700	3.40999900	1.48658700
H	0.81356100	1.78919600	2.27129400

INT-7d

Rh	0.29972600	0.95295900	-0.09668200
C	1.46542500	-0.80997100	0.34130400
C	0.63791500	-1.25176800	-0.78624800
C	0.94879800	-0.44004000	-1.88817600
C	2.00838700	0.49336700	-1.48813400
C	2.38715000	0.19422600	-0.14887800
C	2.66301800	1.47734000	-2.41331100
H	3.34292800	0.96885600	-3.11171300
H	1.92183200	2.01891400	-3.00980000
H	3.24729400	2.21886500	-1.86179700
C	3.53063900	0.78814000	0.62019200
H	3.77050500	1.79721300	0.27339700
H	3.30534600	0.84975000	1.68858500
H	4.43443600	0.17313700	0.50603300
C	0.33487800	-0.47182800	-3.25753600
H	0.11495100	0.53792300	-3.62046600
H	1.01719400	-0.93655800	-3.98270700
H	-0.60083000	-1.03683500	-3.26997900
C	-0.37334000	-2.35737200	-0.71187900
H	-0.97414100	-2.41631600	-1.62320300
H	0.12021500	-3.32897800	-0.57375400
H	-1.06408800	-2.21700400	0.12708700
C	1.52682400	-1.49616700	1.67407200
H	0.53136900	-1.80658800	2.00524500
H	2.15842800	-2.39517200	1.62418200

H	1.94270800	-0.84004000	2.44390900
C	-4.53253300	-0.74934200	0.13817000
C	-3.39937200	-0.32957000	0.82961300
C	-2.64160800	0.76383500	0.36640400
C	-3.05046000	1.38931000	-0.83815200
C	-4.19519900	0.96481700	-1.52399800
C	-4.94519400	-0.10044000	-1.03549500
H	-5.11233100	-1.58558200	0.52208600
H	-3.09113800	-0.81193200	1.75278600
H	-4.46605900	1.47323600	-2.44450900
H	-5.83627800	-0.43133800	-1.56081800
C	-2.18759300	2.43256900	-1.42613300
O	-2.35384500	2.93782600	-2.52483600
N	-1.06075800	2.77373900	-0.60970100
O	-0.28008900	3.83442900	-1.11935300
C	-0.92861200	5.11662200	-1.13373400
H	-0.25811300	5.74346600	-1.72681700
H	-1.90304400	5.06634200	-1.62249100
H	-1.01724500	5.53618000	-0.12611400
N	-1.51283500	1.17961000	1.07417800
C	-1.16346800	2.58964900	0.93827700
C	-2.10520400	3.56922700	1.63861400
H	-1.71532600	4.59089900	1.61981100
H	-3.10748600	3.56272000	1.19507600
H	-2.19330100	3.25810900	2.68432800
C	0.30558200	2.50893100	1.30051300
H	0.92243600	3.36538900	1.02655400
H	0.46143600	2.16717700	2.32398400

INT-8d

Rh	0.54033600	0.42315300	0.61312600
C	2.11971100	-0.95362300	-0.19539800
C	1.03638400	-0.76574400	-1.16252300
C	1.04386700	0.60541300	-1.58241400
C	2.01302400	1.29995100	-0.78207900
C	2.71009700	0.30998700	0.03987500
C	2.42419800	2.73330300	-0.93978400
H	3.19852500	2.81993200	-1.71543900
H	1.58196700	3.36562400	-1.23211600
H	2.84480000	3.13244900	-0.01191100
C	3.83429500	0.63397100	0.97649300
H	3.58085700	1.48636700	1.61489800
H	4.07479000	-0.20910000	1.62851100
H	4.73964600	0.89511800	0.41286900

C	0.24075900	1.17903200	-2.70608900
H	0.13573400	2.26307400	-2.63730400
H	0.74173900	0.94877900	-3.65714200
H	-0.76240400	0.74954300	-2.75257600
C	0.20205200	-1.86518200	-1.74488300
H	-0.76518200	-1.49432700	-2.09122000
H	0.71841500	-2.32356300	-2.60025800
H	0.01257500	-2.65187600	-1.00900900
C	2.48176500	-2.26933300	0.42375800
H	1.59106000	-2.78959100	0.78944100
H	2.97066900	-2.91922800	-0.31419000
H	3.16505900	-2.14574400	1.26752100
C	-3.64160200	-1.31720200	-0.58475000
C	-2.67448400	-0.67691900	0.17690900
C	-2.31787900	0.66977500	-0.08649400
C	-2.95469900	1.31414300	-1.18476700
C	-3.93231300	0.65084200	-1.94192900
C	-4.28855500	-0.65729400	-1.64513600
H	-3.91411700	-2.34231000	-0.34288400
H	-2.19504900	-1.17779200	1.01110600
H	-4.37570800	1.18563700	-2.77665200
H	-5.05098700	-1.16723900	-2.22722400
C	-2.45830000	2.63281400	-1.64794000
O	-2.64088300	3.07600100	-2.78431700
N	-1.70901200	3.28747800	-0.70069500
O	-0.86107300	4.30314700	-1.15879900
C	-1.56450300	5.54233300	-1.32539400
H	-0.80671600	6.25164400	-1.66975100
H	-2.34893000	5.43170200	-2.07710900
H	-1.98595500	5.88696200	-0.37289000
N	-1.39474500	1.32788500	0.71803100
C	-1.55984400	2.78318700	0.70276000
C	-2.86046100	3.12851700	1.47720700
H	-3.02262400	4.21229200	1.47687000
H	-3.73356900	2.64988900	1.02731800
H	-2.77068300	2.78319300	2.51171500
C	-0.40129000	3.50629800	1.38847100
H	0.54301300	3.35268000	0.86745700
H	-0.59705600	4.58095100	1.43766200
C	0.10948300	-0.04964100	3.09738600
O	-0.21943900	-0.90876000	2.21925900
O	0.73697300	0.99753700	2.73711500
H	-0.30055700	3.11059200	2.39936500
C	-0.27366000	-0.24948500	4.54226400

H	0.43108200	0.26238000	5.20204500
H	-1.27041100	0.17800500	4.70438000
H	-0.31783900	-1.31466600	4.78249300

TS-4d

Rh	0.15062500	1.12816000	-0.52891500
C	1.42148200	-0.69785100	0.09905900
C	0.69837300	-0.83334700	-1.15801800
C	1.30784200	0.07796400	-2.13086900
C	2.24471300	0.86692000	-1.43498600
C	2.32233400	0.37331500	-0.04978600
C	3.09777500	1.95841500	-2.00870000
H	4.04206100	1.55602000	-2.40174500
H	2.58240300	2.46797700	-2.82711600
H	3.35055500	2.70778800	-1.25241800
C	3.27913600	0.91644100	0.96760600
H	3.16947100	2.00017000	1.08351900
H	3.13539800	0.46034400	1.94950600
H	4.31406300	0.72309400	0.65520800
C	0.97465300	0.15332000	-3.58940000
H	1.00835300	1.18325000	-3.95012500
H	1.68720700	-0.44768200	-4.17090400
H	-0.02913400	-0.22874700	-3.79134300
C	-0.29507400	-1.91170500	-1.46354400
H	-0.96948300	-1.62057000	-2.27306400
H	0.22248000	-2.83203300	-1.77110000
H	-0.90456000	-2.14612300	-0.58667800
C	1.15497300	-1.52927700	1.31905700
H	0.10371300	-1.45709900	1.61876800
H	1.38137300	-2.58567100	1.12574500
H	1.76357300	-1.20862300	2.16834200
C	-4.81348200	-0.13859700	1.14293600
C	-3.50080900	0.18551300	1.46187600
C	-2.64692200	0.82160900	0.53246600
C	-3.17284500	1.14148000	-0.74447900
C	-4.49936700	0.79080900	-1.05113700
C	-5.31998800	0.15525900	-0.12863500
H	-5.43803600	-0.63751300	1.88041100
H	-3.09117300	-0.06891000	2.43593800
H	-4.86539500	1.05937000	-2.03653200
H	-6.34188600	-0.10420400	-0.39050800
C	-2.45042300	1.90571700	-1.81470700
O	-3.02448800	2.25180300	-2.84622500
N	-1.12009300	2.24297600	-1.56374800

O	-0.50588500	2.79238700	-2.72160900
C	-0.65970400	4.20935500	-2.72458100
H	-0.10845600	4.55920400	-3.60283200
H	-1.71465400	4.48433300	-2.81989600
H	-0.23249300	4.65363700	-1.81537600
N	-1.31960600	1.06231200	0.91216100
C	-1.06146900	1.98686000	1.93864900
C	-2.11654200	3.03271100	2.24581800
H	-2.37438300	3.59303000	1.33861100
H	-3.04342700	2.58019100	2.61259100
H	-1.75598300	3.73428600	3.00308600
C	0.11813000	2.00785100	2.60603600
H	0.32810800	2.78004100	3.33763000
H	0.88289000	1.25997200	2.43543400

TS-5d

Rh	0.29776300	0.96748600	-0.05068900
C	1.49615700	-0.84121700	0.29302600
C	0.65375900	-1.19280600	-0.84982300
C	0.95281300	-0.30252300	-1.89853900
C	2.00548300	0.60650600	-1.43902800
C	2.39281300	0.20851000	-0.12169900
C	2.66187300	1.64594200	-2.30043800
H	3.36931800	1.18267200	-3.00318100
H	1.92292600	2.19986400	-2.88714000
H	3.21725000	2.37210200	-1.70037600
C	3.53245100	0.76219400	0.68285700
H	3.75842000	1.79530300	0.40442100
H	3.31220900	0.74731400	1.75419900
H	4.44314400	0.16792200	0.52306200
C	0.31950500	-0.22673800	-3.25802200
H	-0.06306800	0.77914700	-3.46588500
H	1.04714700	-0.47147200	-4.04340100
H	-0.51902300	-0.92156300	-3.35249700
C	-0.35876300	-2.30117800	-0.84235400
H	-0.96036900	-2.30508900	-1.75498300
H	0.13356000	-3.27982300	-0.76285000
H	-1.04836000	-2.21072100	0.00449300
C	1.56892200	-1.62182300	1.57304000
H	0.57730600	-1.95999200	1.88910200
H	2.20207200	-2.51338100	1.45564500
H	1.98979800	-1.02304600	2.38610600
C	-4.70218600	-0.60682200	0.36990600
C	-3.55664000	-0.19483100	1.05354600

C	-2.69418800	0.75335300	0.48759300
C	-2.99573300	1.26783800	-0.79640400
C	-4.14499400	0.84816200	-1.47240400
C	-5.00410200	-0.08462700	-0.89138700
H	-5.36383300	-1.33919800	0.82606500
H	-3.31459100	-0.59133500	2.03533000
H	-4.33927700	1.25637500	-2.45925100
H	-5.89655300	-0.40779400	-1.41962500
C	-2.07183800	2.22823600	-1.47771600
O	-2.25668100	2.61979300	-2.62381100
N	-0.97654400	2.64545700	-0.69088400
O	-0.17696000	3.64206500	-1.29912600
C	-0.82753000	4.91151800	-1.42746300
H	-0.08363700	5.54858600	-1.91313900
H	-1.71830900	4.84088900	-2.05575800
H	-1.07931300	5.33515300	-0.44829900
N	-1.51302000	1.13056900	1.15697600
C	-1.17955200	2.47400400	1.14388800
C	-2.14814800	3.53435100	1.62808500
H	-1.74178600	4.53701000	1.47556200
H	-3.12419600	3.45892800	1.13949000
H	-2.29325100	3.38757400	2.70592200
C	0.29114800	2.47954400	1.40369300
H	0.82649200	3.39417700	1.14804700
H	0.54604800	2.08336500	2.38760200

TS-6d

Rh	0.40991200	0.60208800	0.52001600
C	2.23828000	-0.68346800	0.11044700
C	1.13225300	-1.06705400	-0.76413600
C	0.85830800	0.03496700	-1.63696000
C	1.67982800	1.14038300	-1.22430600
C	2.57261300	0.66285300	-0.16877000
C	1.78751000	2.46569200	-1.92169500
H	2.46718200	2.38864800	-2.78195000
H	0.82093800	2.82163400	-2.28808800
H	2.18804200	3.23778800	-1.25906400
C	3.66657500	1.47425100	0.46047900
H	3.35852100	2.51291300	0.61264600
H	3.96357800	1.07032700	1.43189000
H	4.55641300	1.48734200	-0.18369600
C	-0.08959100	0.02395500	-2.79466700
H	-0.40068300	1.03095200	-3.08099600
H	0.40311100	-0.43371000	-3.66397400

H	-0.99079600	-0.55574500	-2.57846800
C	0.51810700	-2.43319300	-0.83589000
H	-0.50416700	-2.38550400	-1.22134300
H	1.09792900	-3.09130400	-1.49843400
H	0.48216000	-2.90173400	0.15195900
C	2.86707600	-1.59436100	1.12162100
H	2.10419900	-2.06305700	1.75211200
H	3.42884600	-2.39575700	0.62344400
H	3.56103500	-1.05806500	1.77420000
C	-3.85712500	-0.82909900	-1.54934900
C	-2.95365300	-0.45901300	-0.56047700
C	-2.44367500	0.85958300	-0.51143200
C	-2.84424600	1.76782700	-1.52089400
C	-3.75865300	1.38247900	-2.50884500
C	-4.27661900	0.09195000	-2.52435700
H	-4.25542800	-1.84122100	-1.55736800
H	-2.64255100	-1.15768800	0.21114000
H	-4.02566100	2.11146500	-3.26795000
H	-4.99046700	-0.20479700	-3.28737200
C	-2.18576900	3.09620800	-1.61238200
O	-2.21427700	3.79772500	-2.62640300
N	-1.53233100	3.46861200	-0.46592700
O	-0.77500700	4.64380900	-0.50631400
C	-1.60044400	5.81827200	-0.50042100
H	-0.89237000	6.65107800	-0.48072300
H	-2.20839500	5.86061700	-1.40666500
H	-2.23537600	5.85328300	0.39270500
N	-1.58155700	1.23046100	0.50166300
C	-1.41098700	2.65127400	0.78081700
C	-2.46287900	3.11715700	1.80246200
H	-2.33942600	4.18474300	2.01961100
H	-3.47381400	2.94979800	1.41639100
H	-2.34173600	2.55397800	2.73287400
C	0.02812000	2.72663100	1.33494000
H	0.72497600	3.17718200	0.63239200
H	0.08016800	3.35683900	2.23422300
C	-0.11095300	-0.03319900	3.36513700
O	-0.13102900	-0.62330700	2.25060700
O	0.16117000	1.20603100	3.50838700
H	0.25619600	1.73580900	2.34837100
C	-0.43933100	-0.81878200	4.61663100
H	0.30333100	-0.61217200	5.39283400
H	-1.41228000	-0.48796400	4.99698500
H	-0.48125800	-1.88845300	4.40507200

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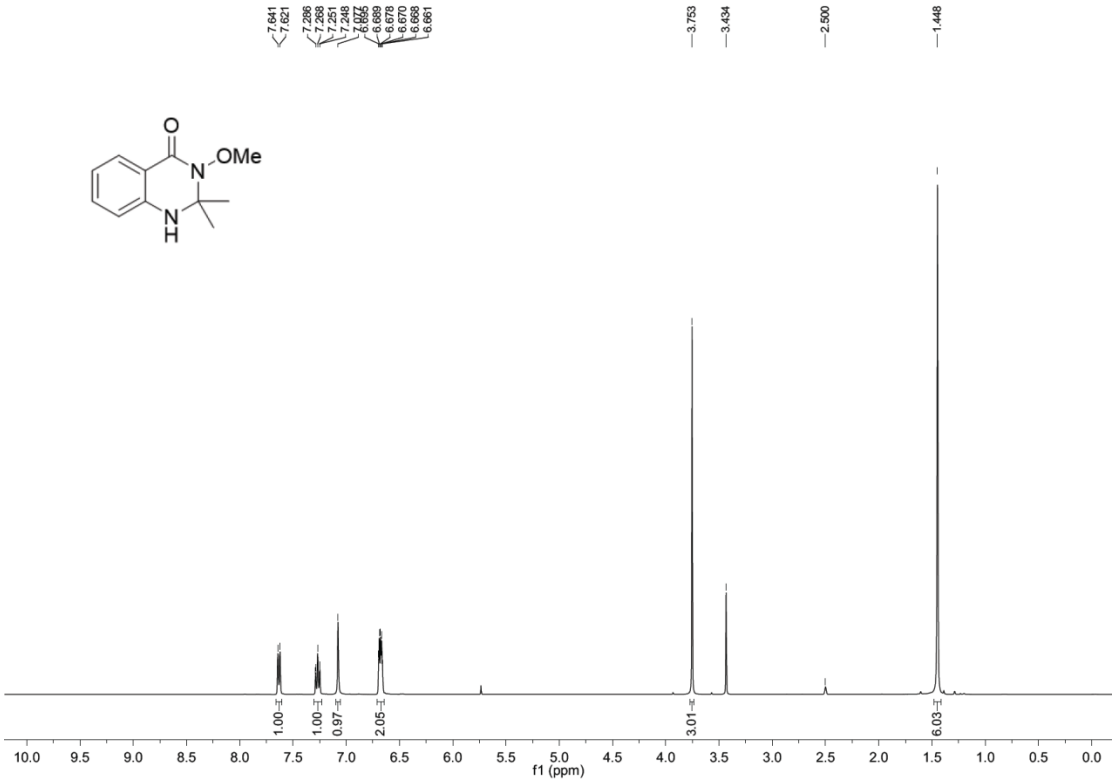
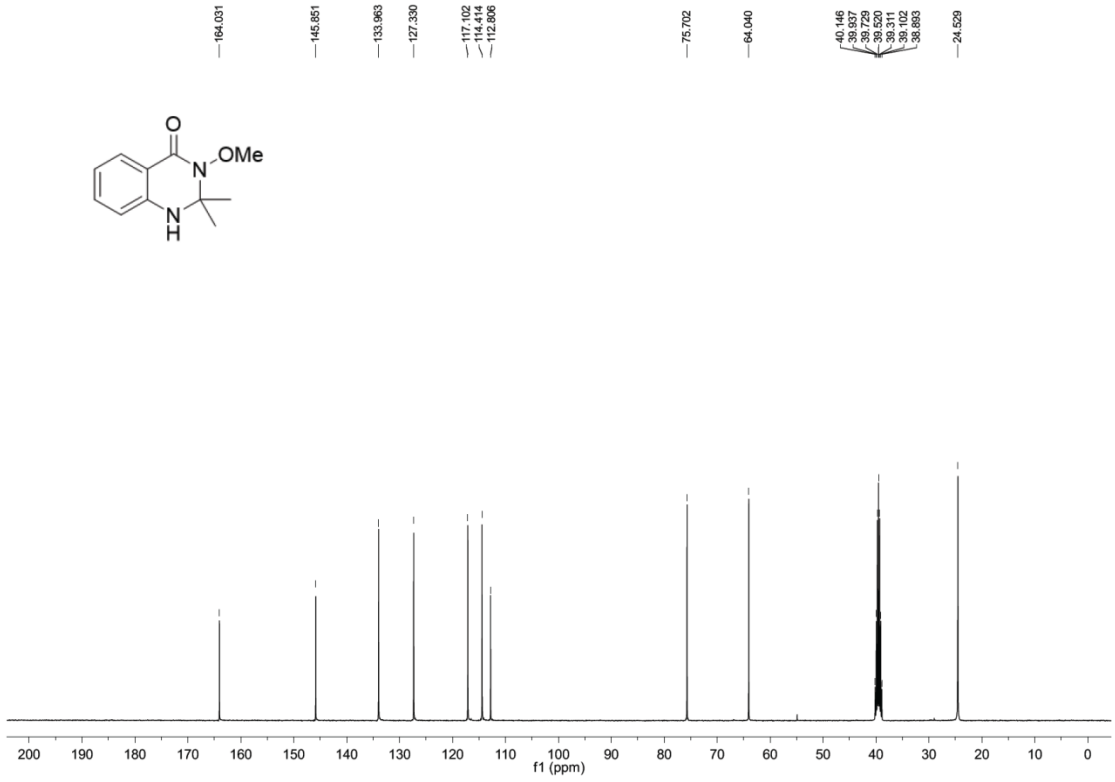
VI. Copies of ^{1}H, ^{13}C and ^{19}F NMR spectra

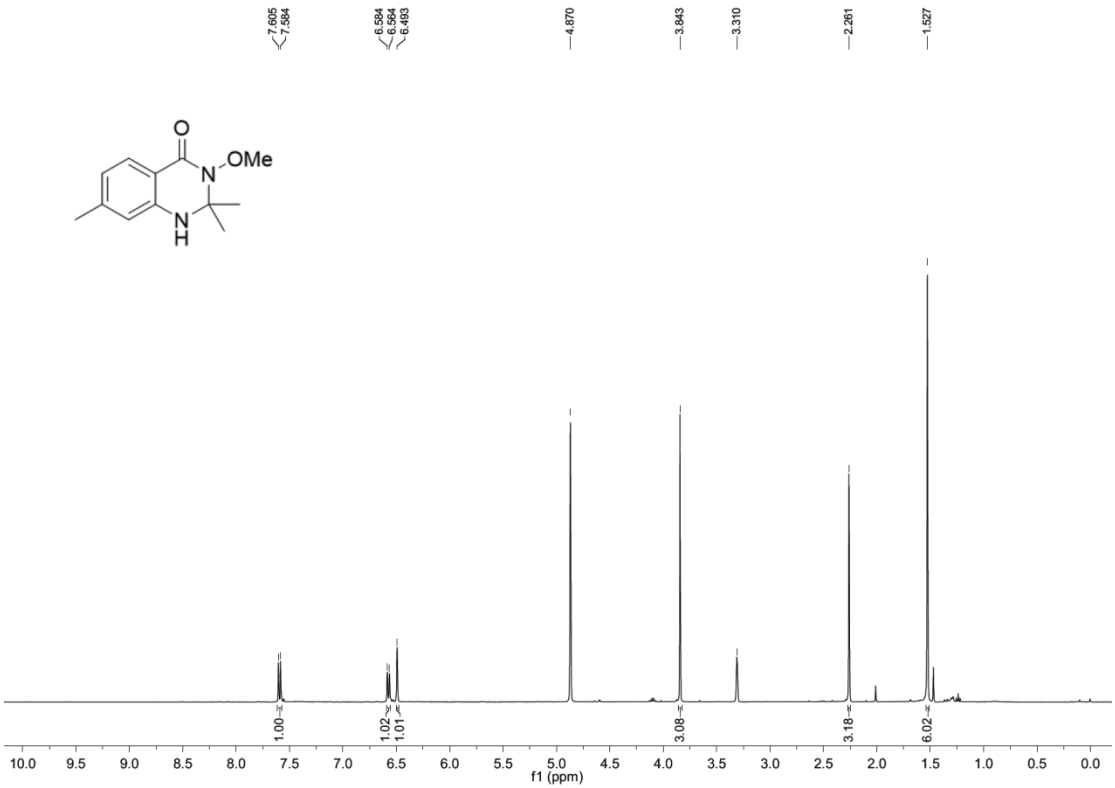
3aa-^{1}H NMR (400 MHz, DMSO-d_6)



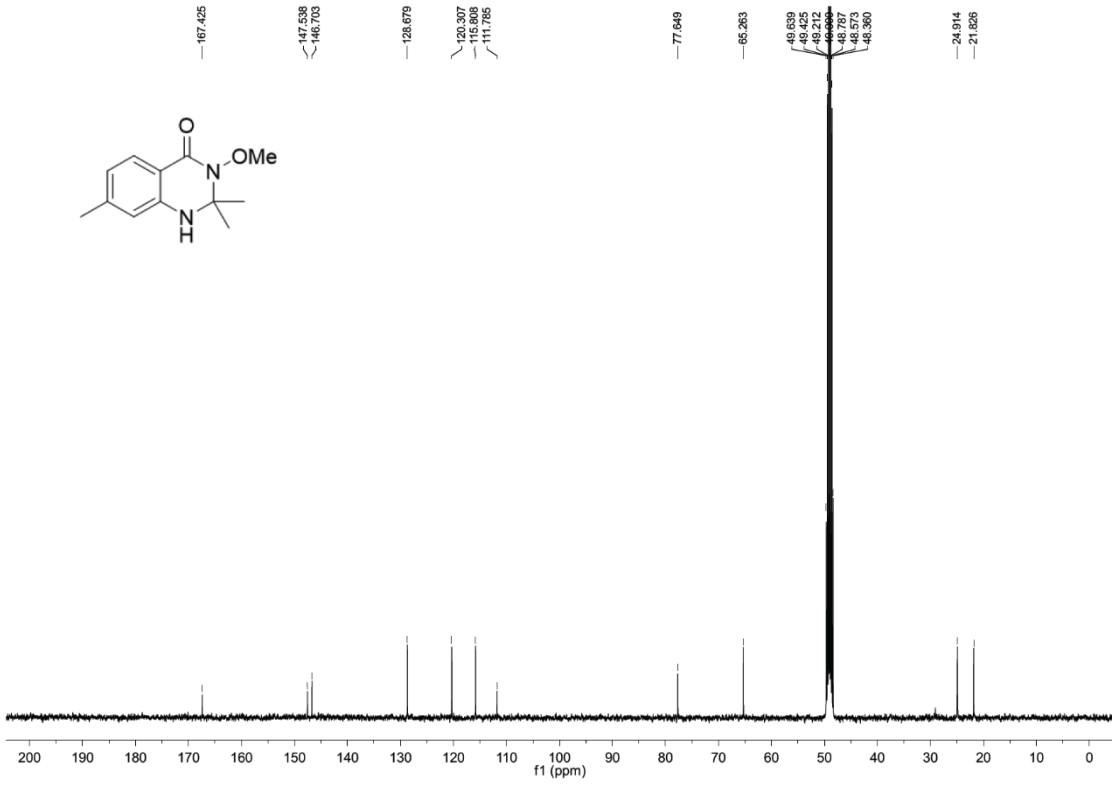
3aa-^{13}C NMR (100 MHz, DMSO-d_6)



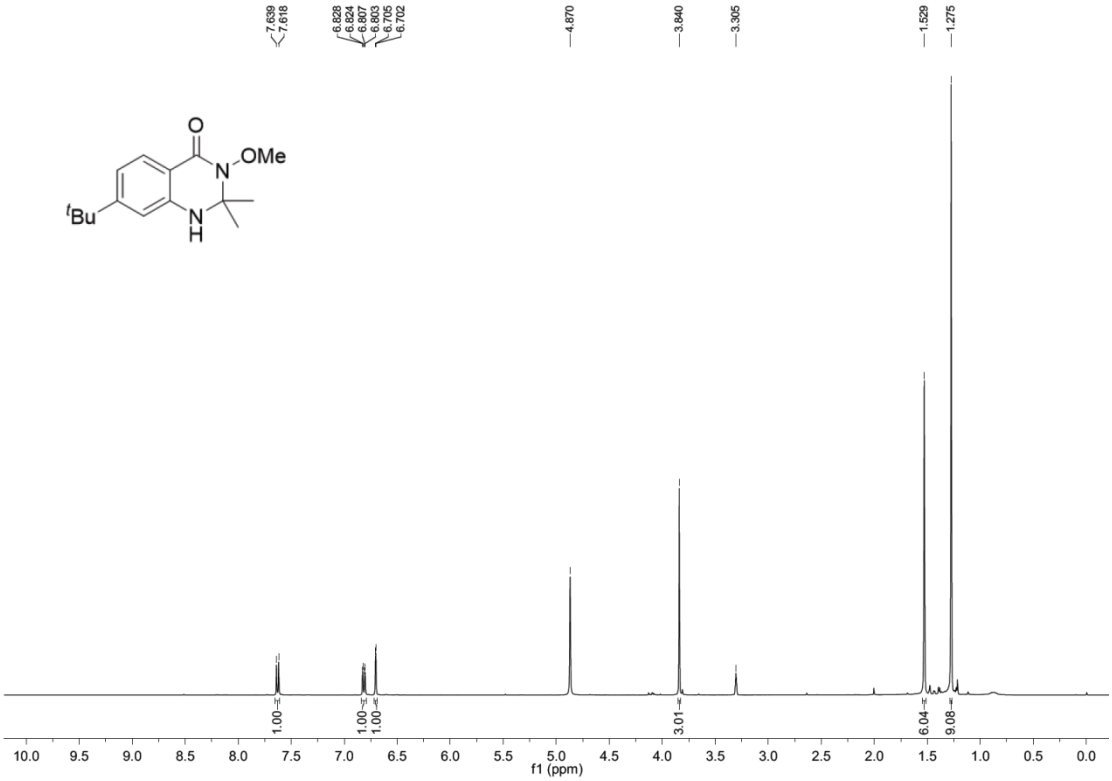
3ba-^{1}H NMR (400 MHz, CD_3OD)



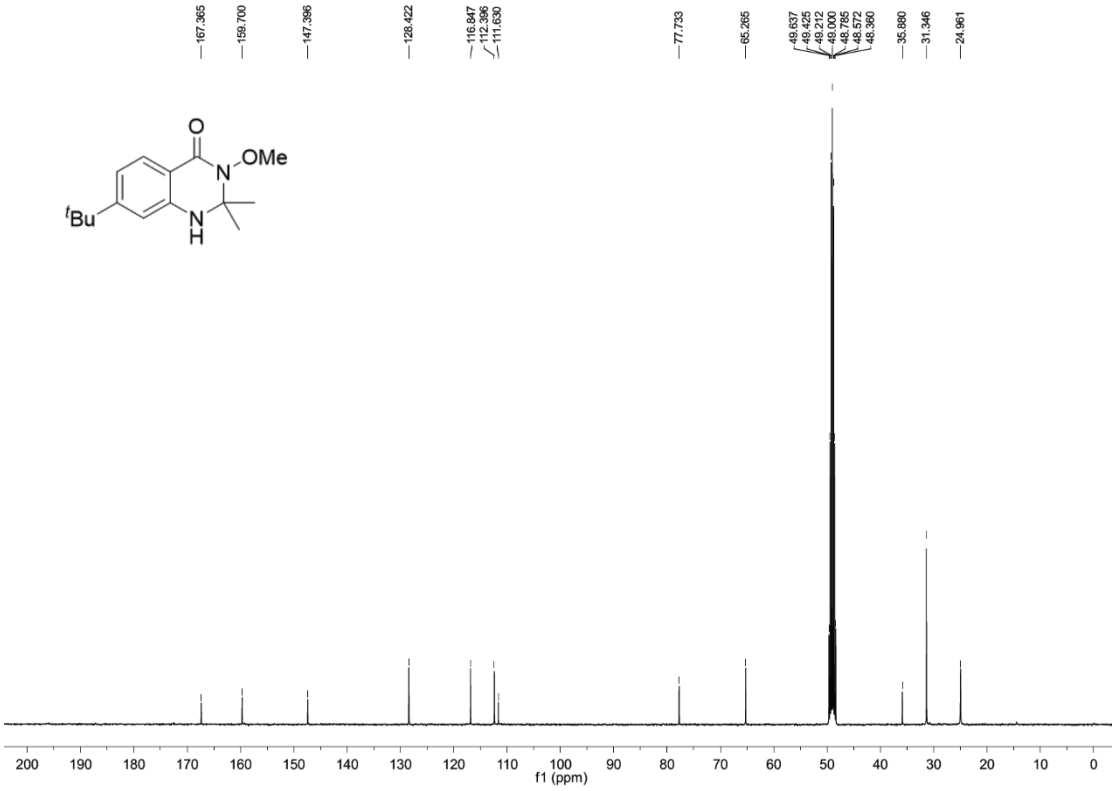
3ba-^{13}C NMR (100 MHz, CD_3OD)



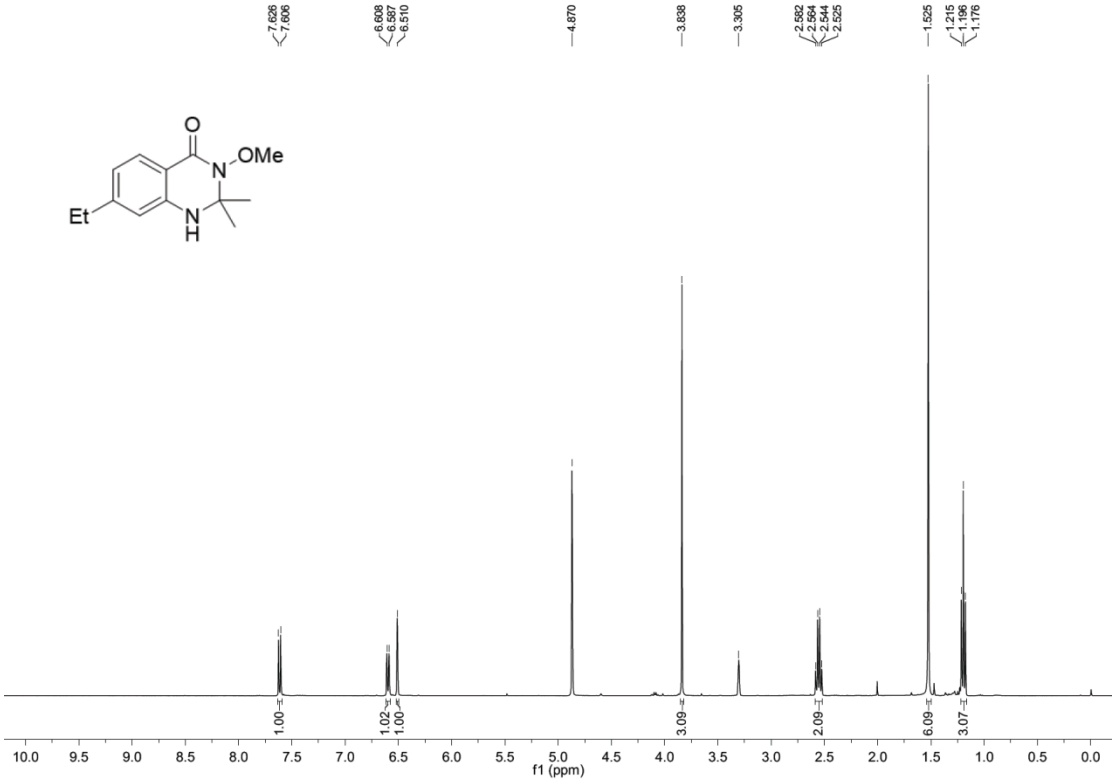
3ca-^{1}H NMR (400 MHz, CD_3OD)



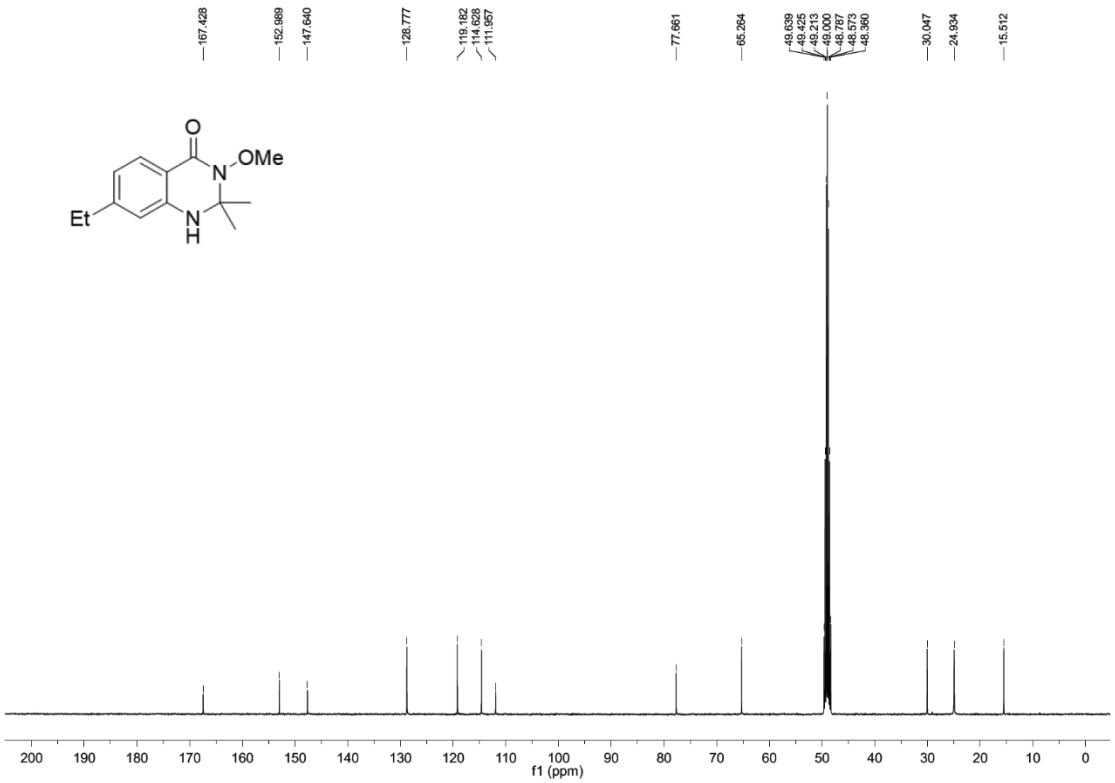
3ca-^{13}C NMR (100 MHz, CD_3OD)



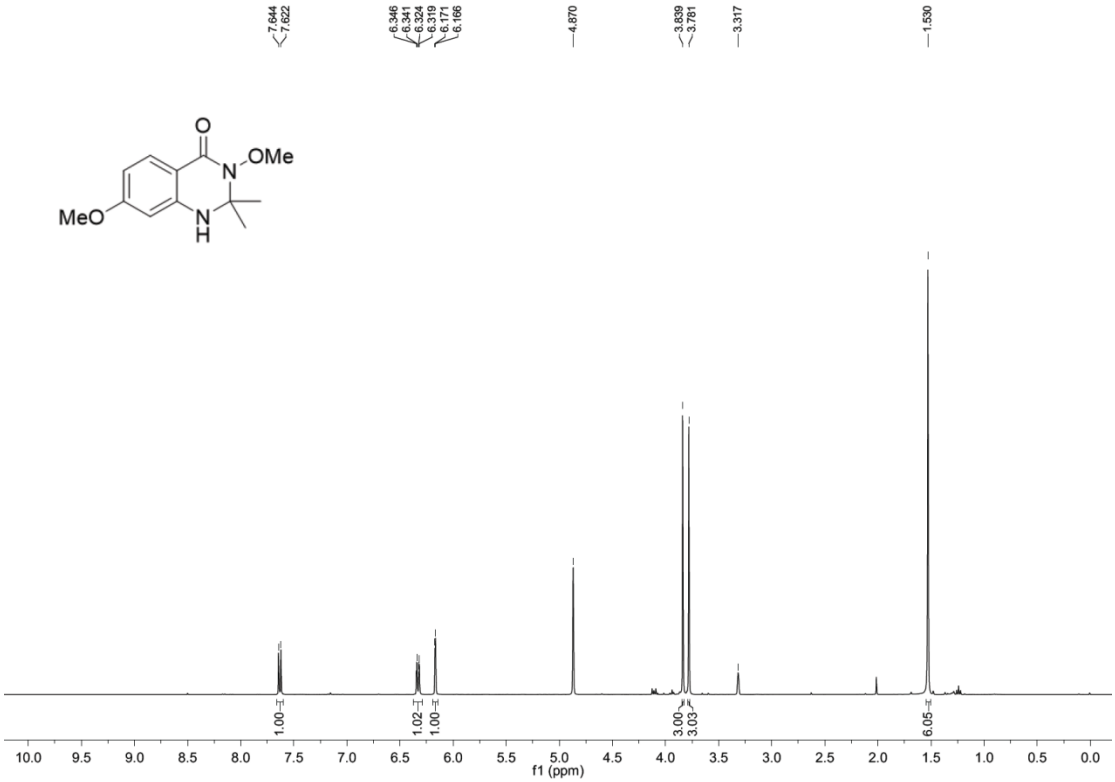
3da-^{1}H NMR (400 MHz, CD_3OD)



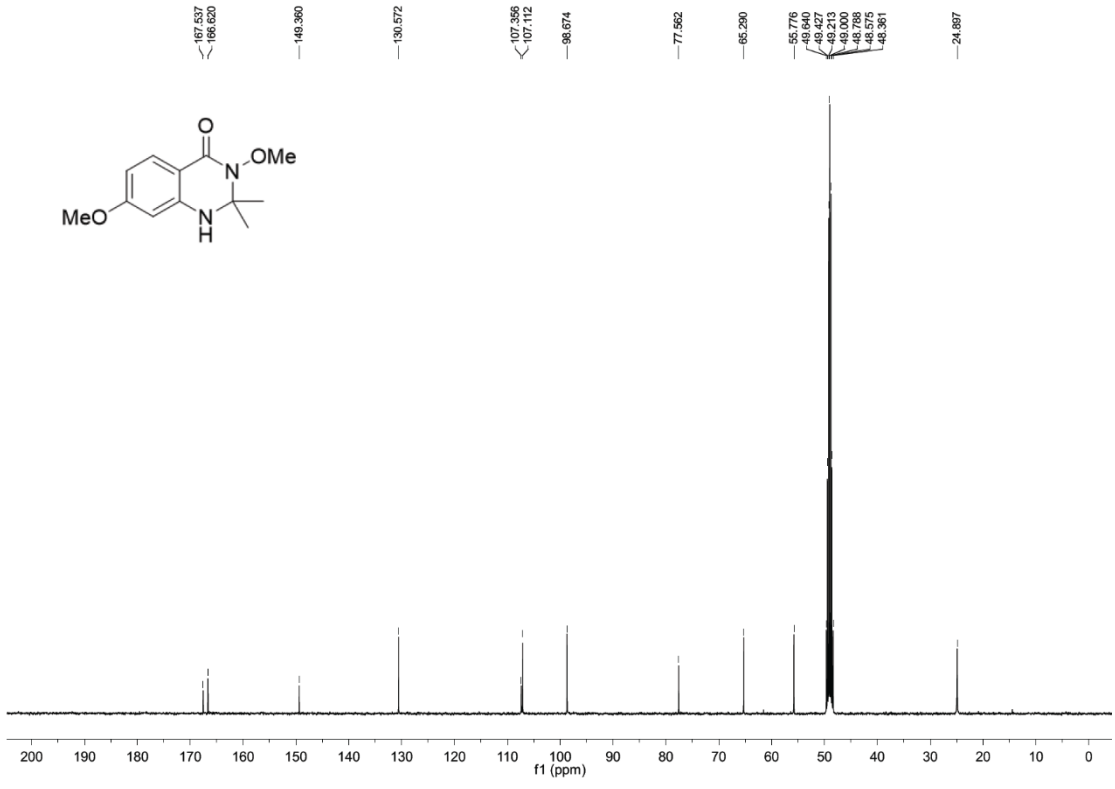
3da-^{13}C NMR (100 MHz, CD_3OD)



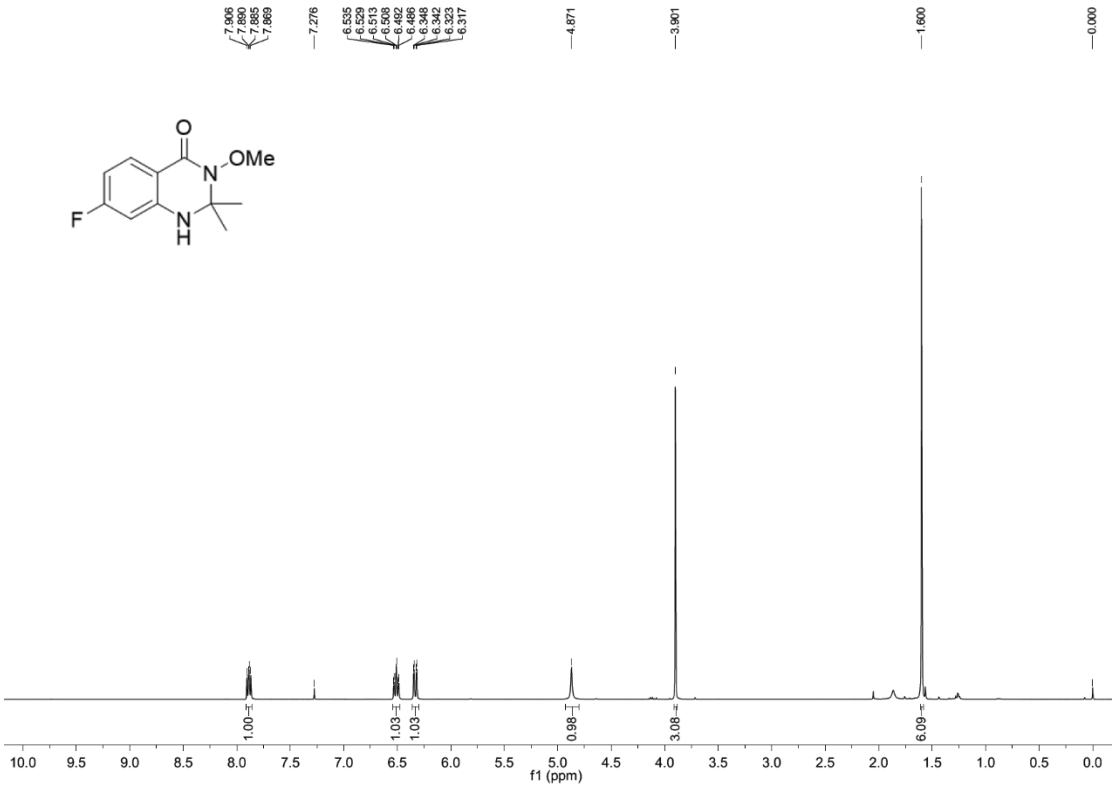
3ea-^{1}H NMR (400 MHz, CD_3OD)



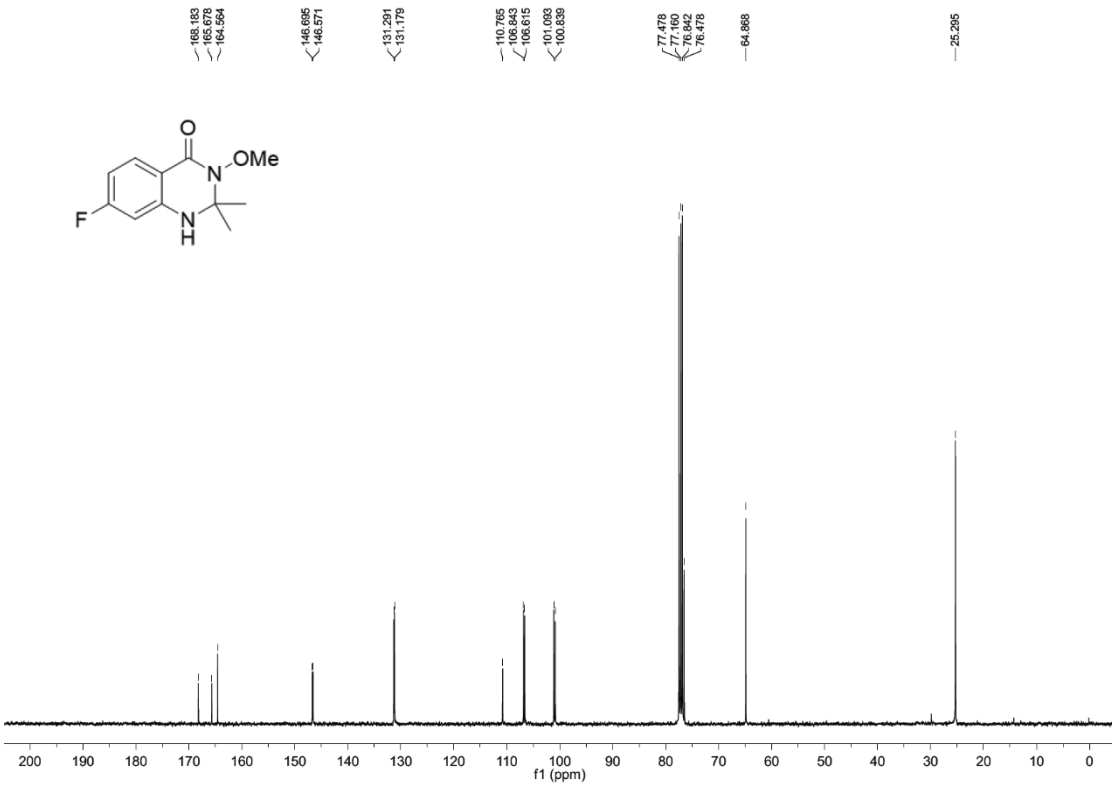
3ea-^{13}C NMR (100 MHz, CD_3OD)



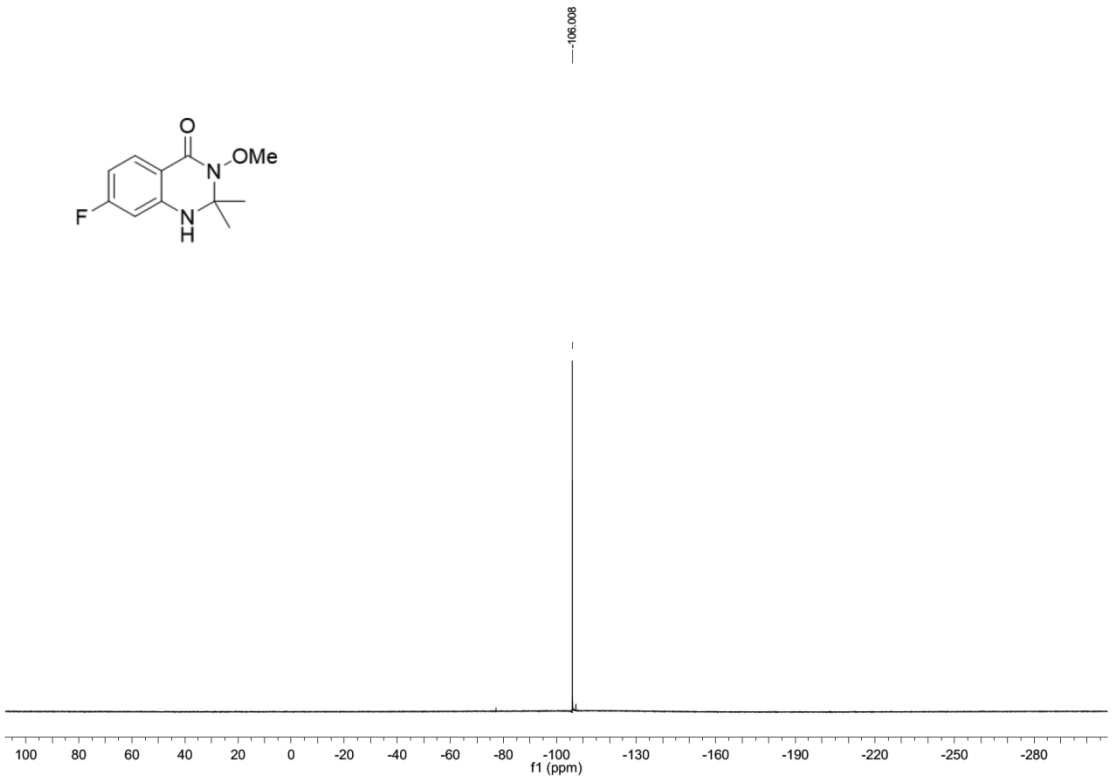
3fa-^{1}H NMR (400 MHz, $CDCl_3$)



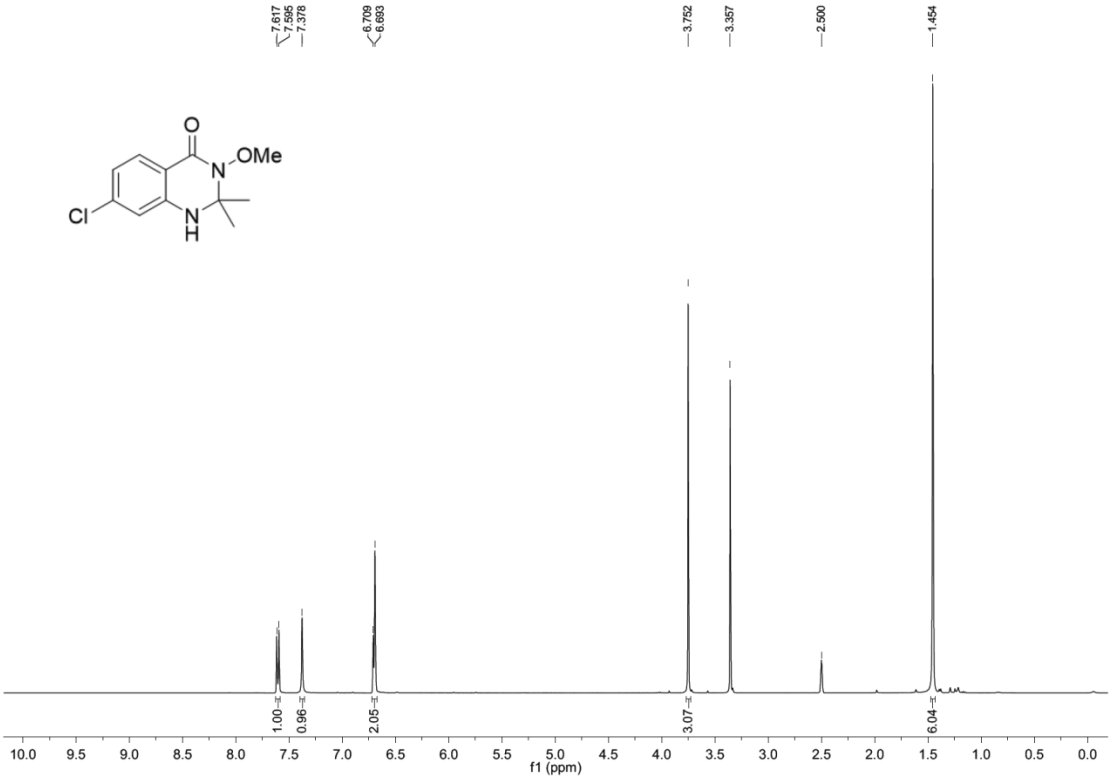
3fa-^{13}C NMR (100 MHz, $CDCl_3$)



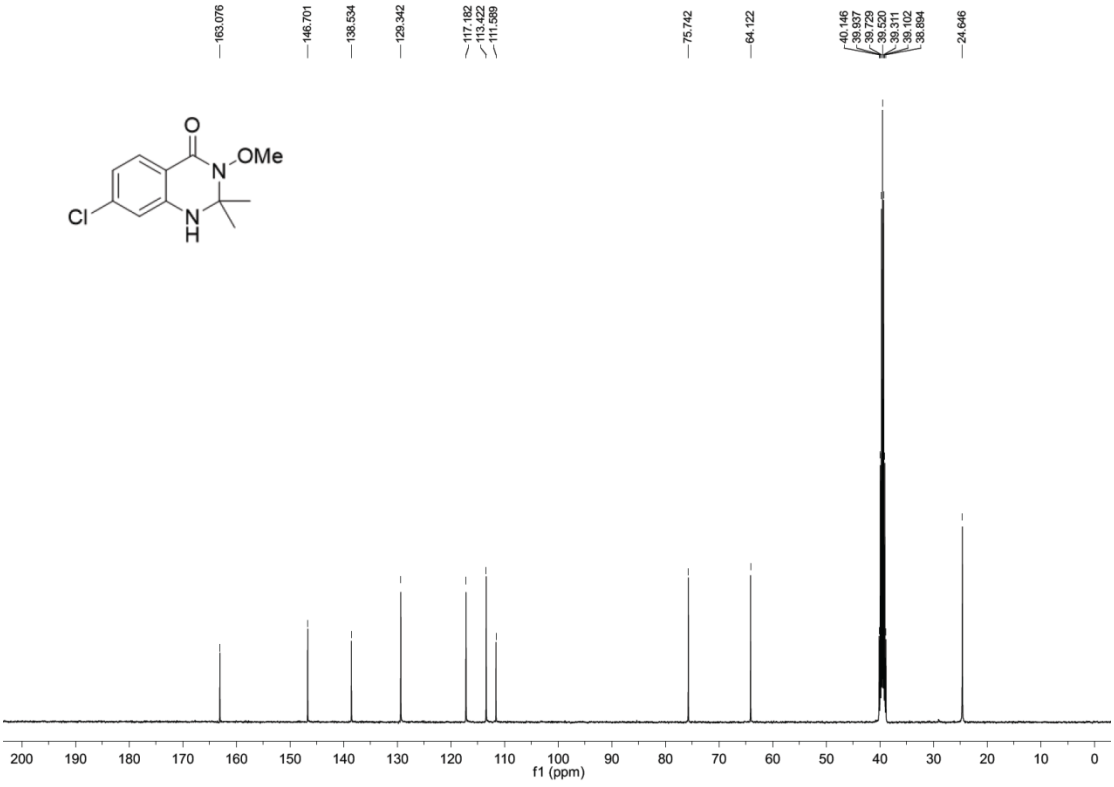
3fa-^{19}F NMR (376 MHz, $CDCl_3$)



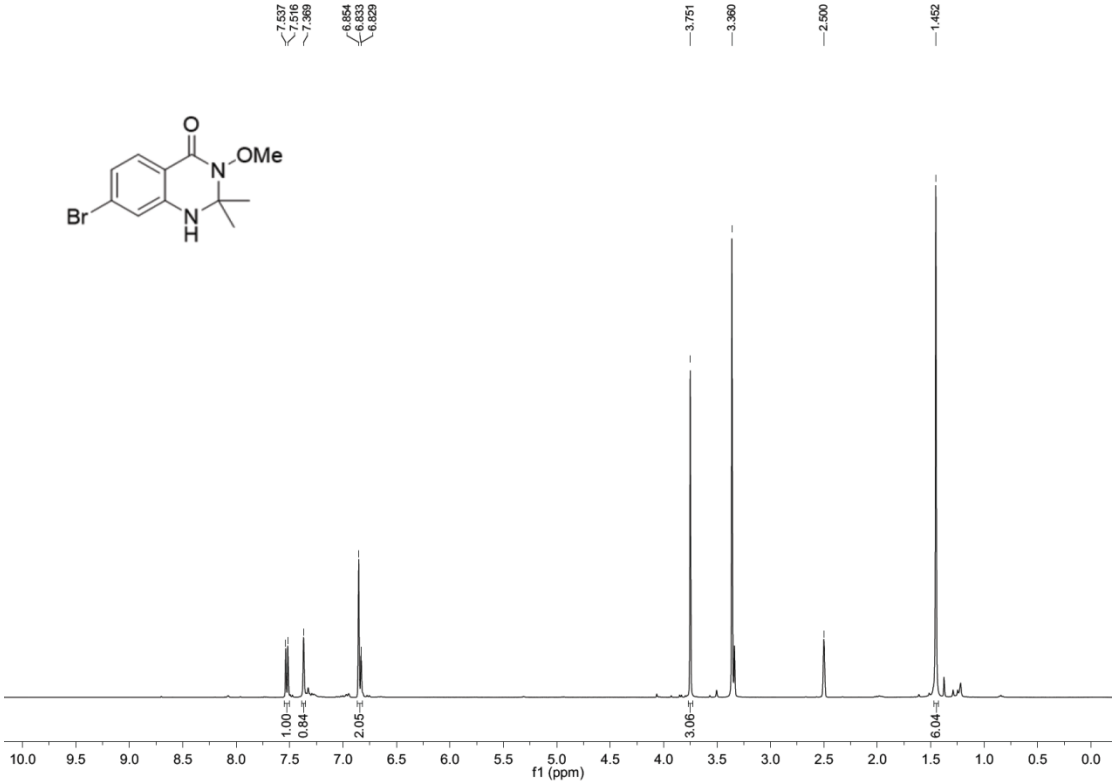
3ga-^{1}H NMR (400 MHz, DMSO-d_6)



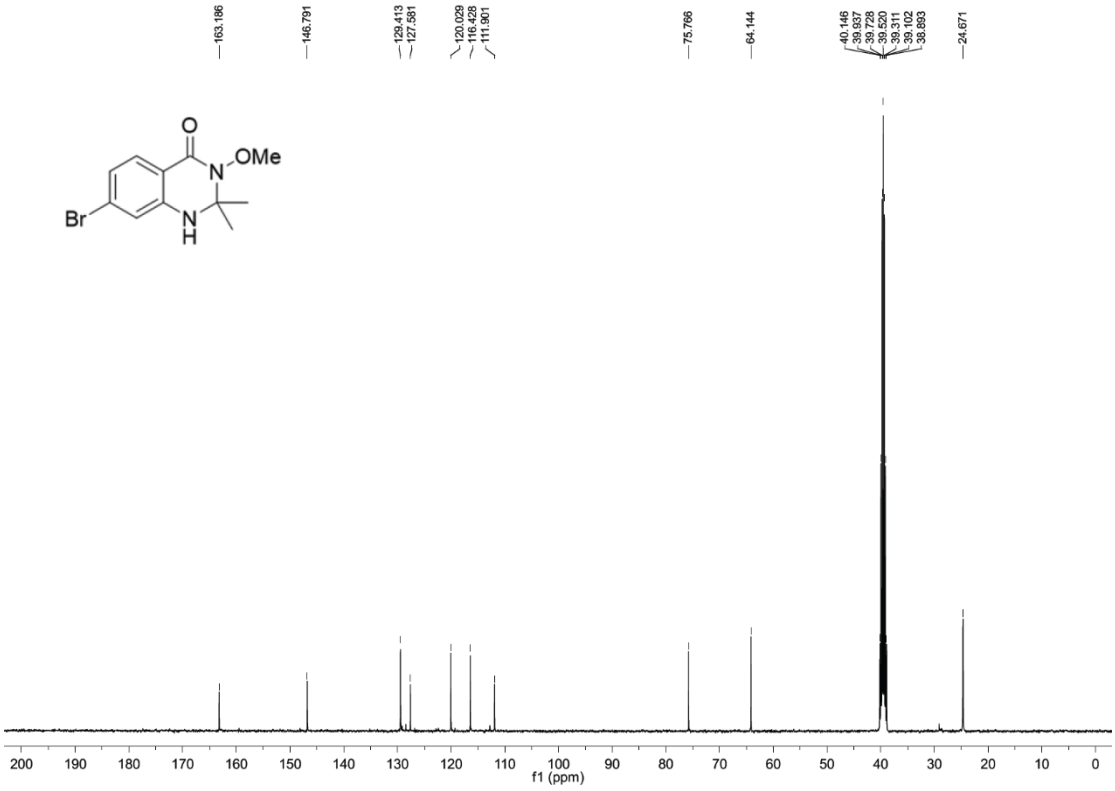
3ga-^{13}C NMR (100 MHz, DMSO-d_6)



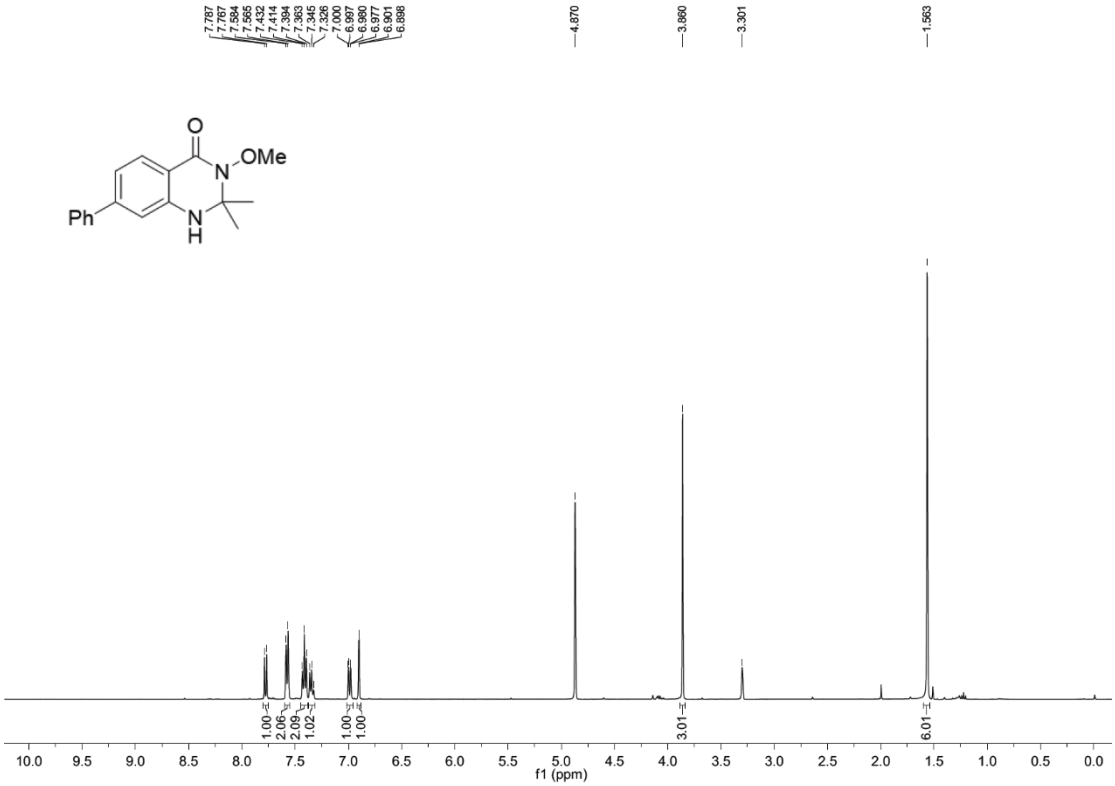
3ha-^{1}H NMR (400 MHz, DMSO-d_6)



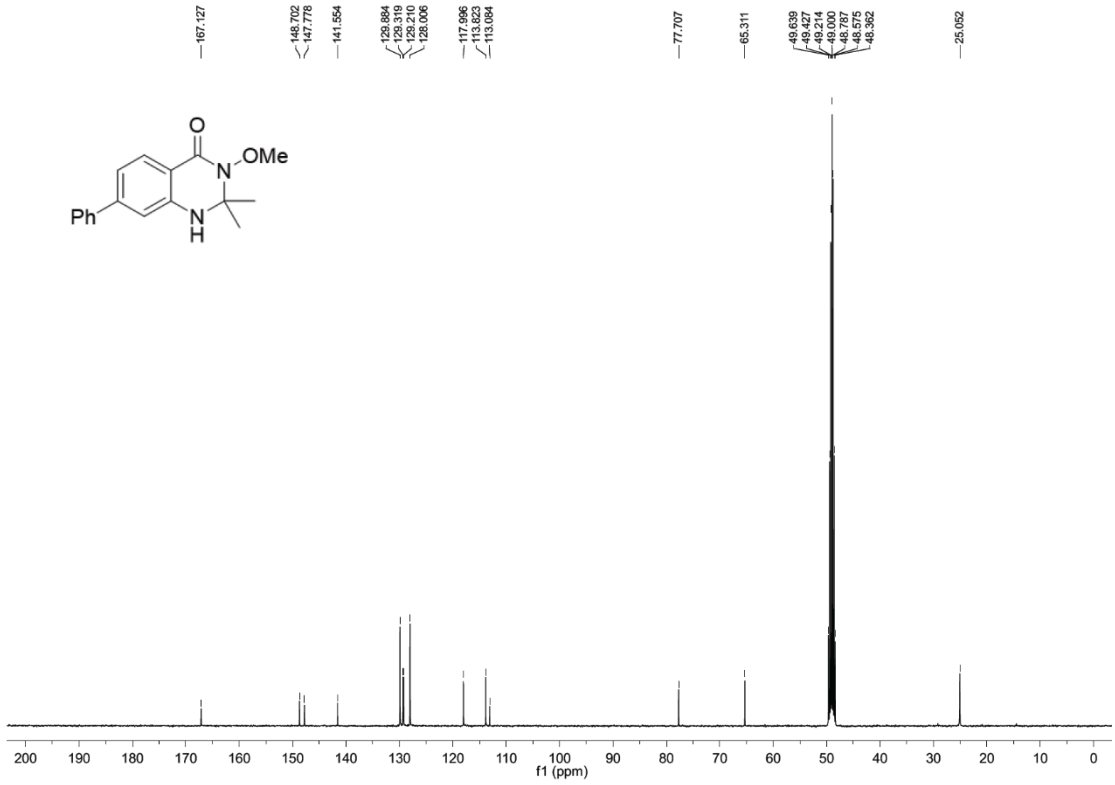
3ha-^{13}C NMR (100 MHz, DMSO-d_6)



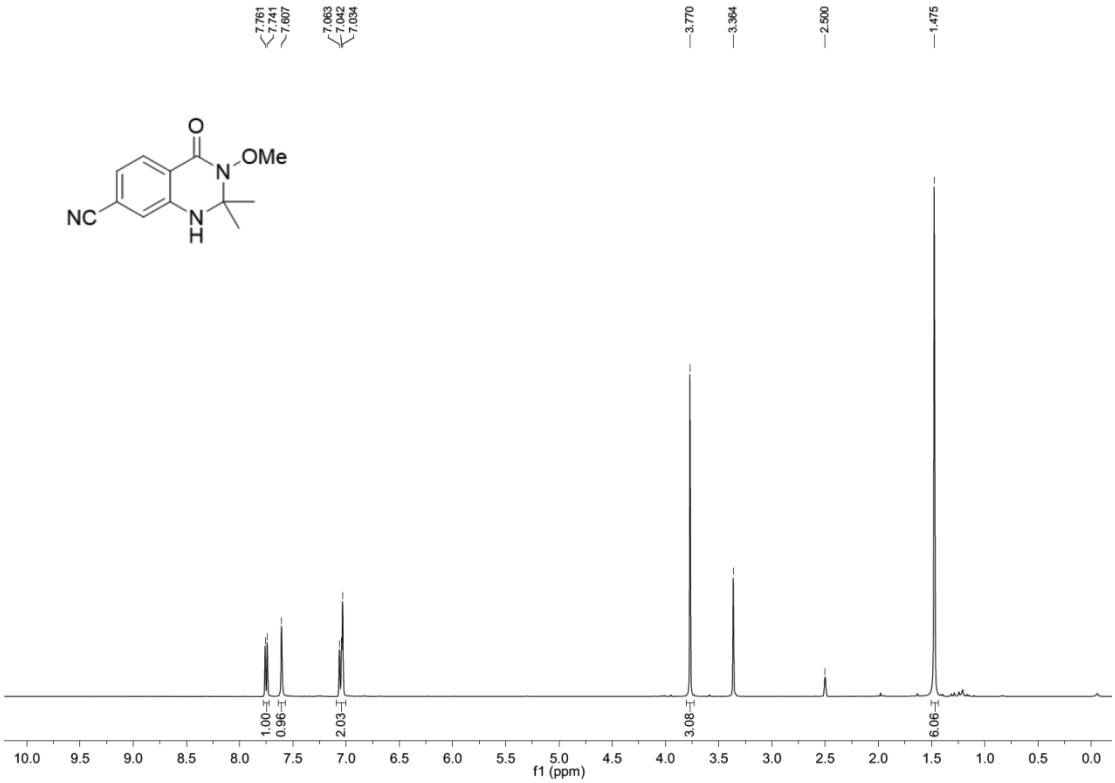
3ia-^{1}H NMR (400 MHz, CD_3OD)



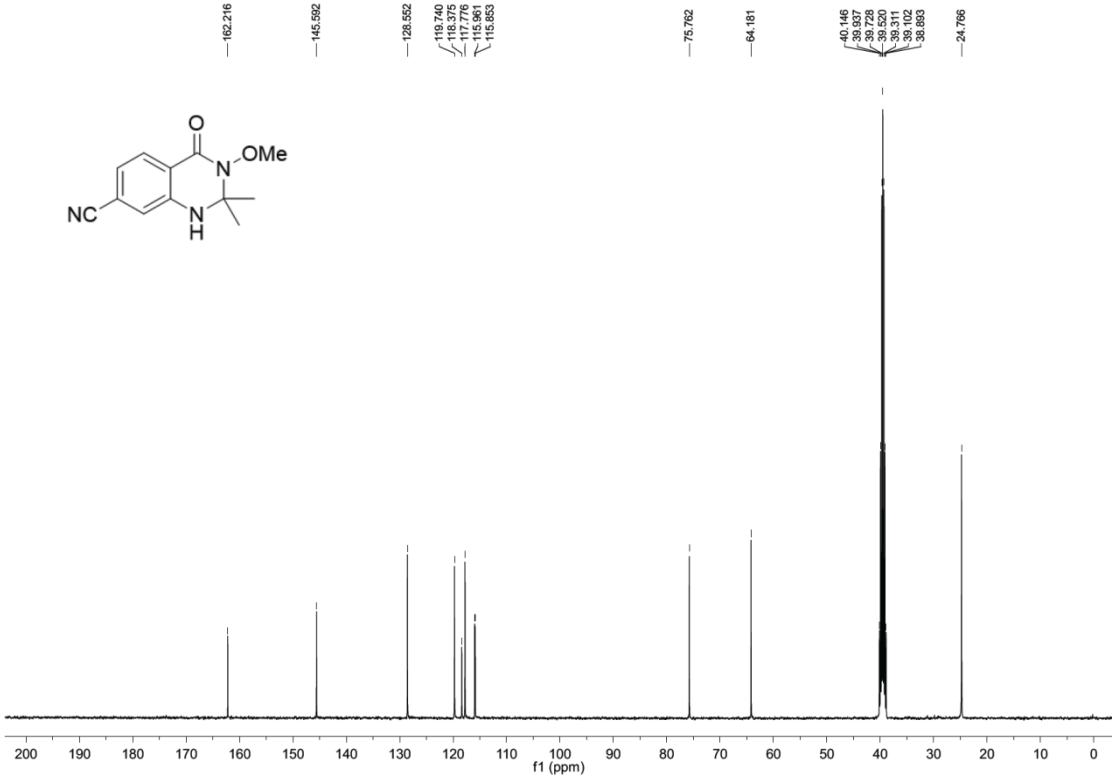
3ia-^{13}C NMR (100 MHz, CD_3OD)



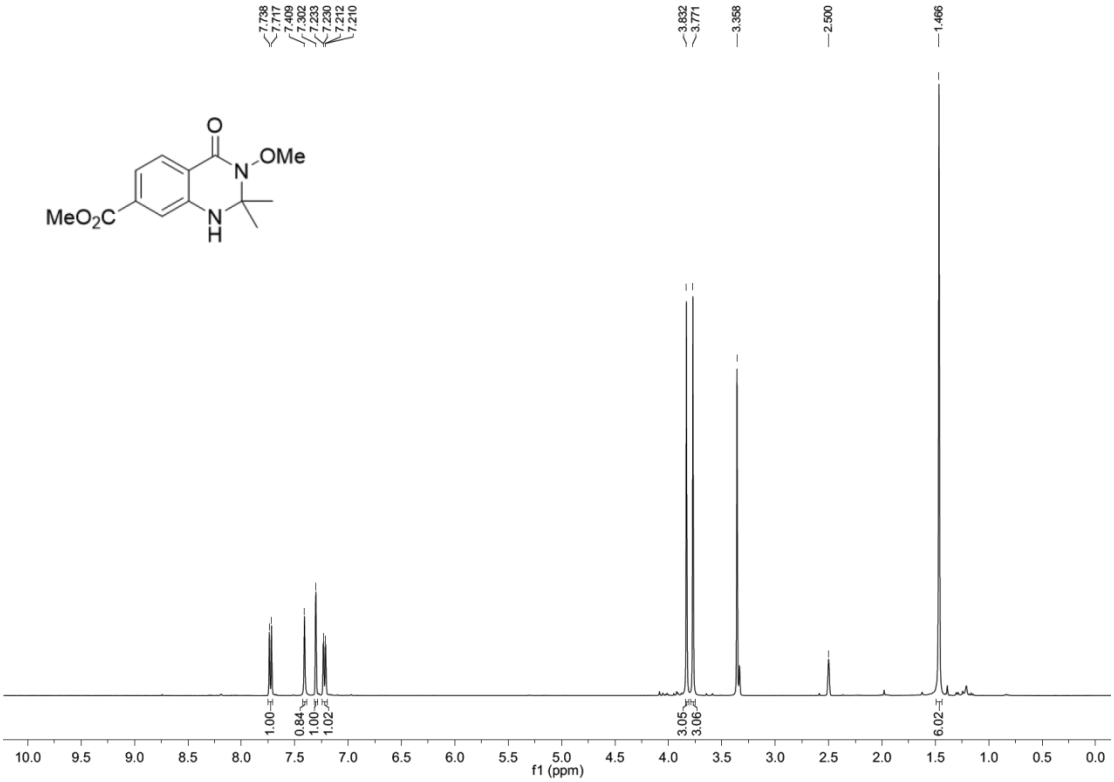
3ja-^{1}H NMR (400 MHz, DMSO-d_6)



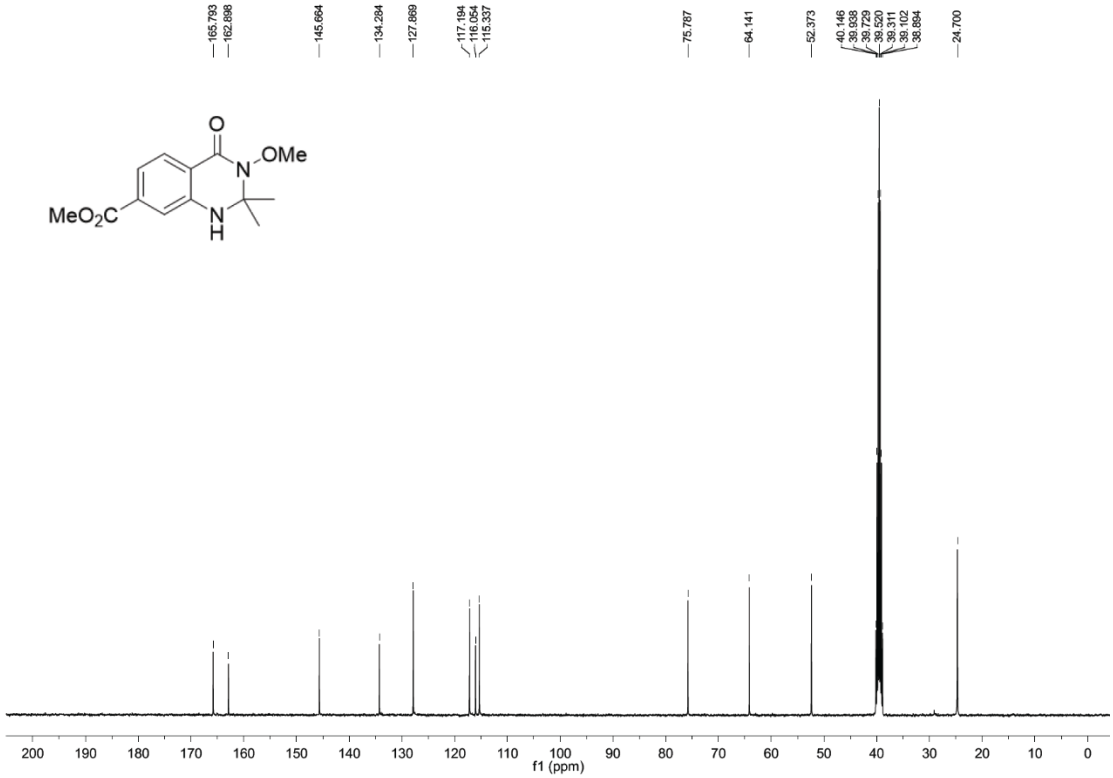
3ja-^{13}C NMR (100 MHz, DMSO-d_6)



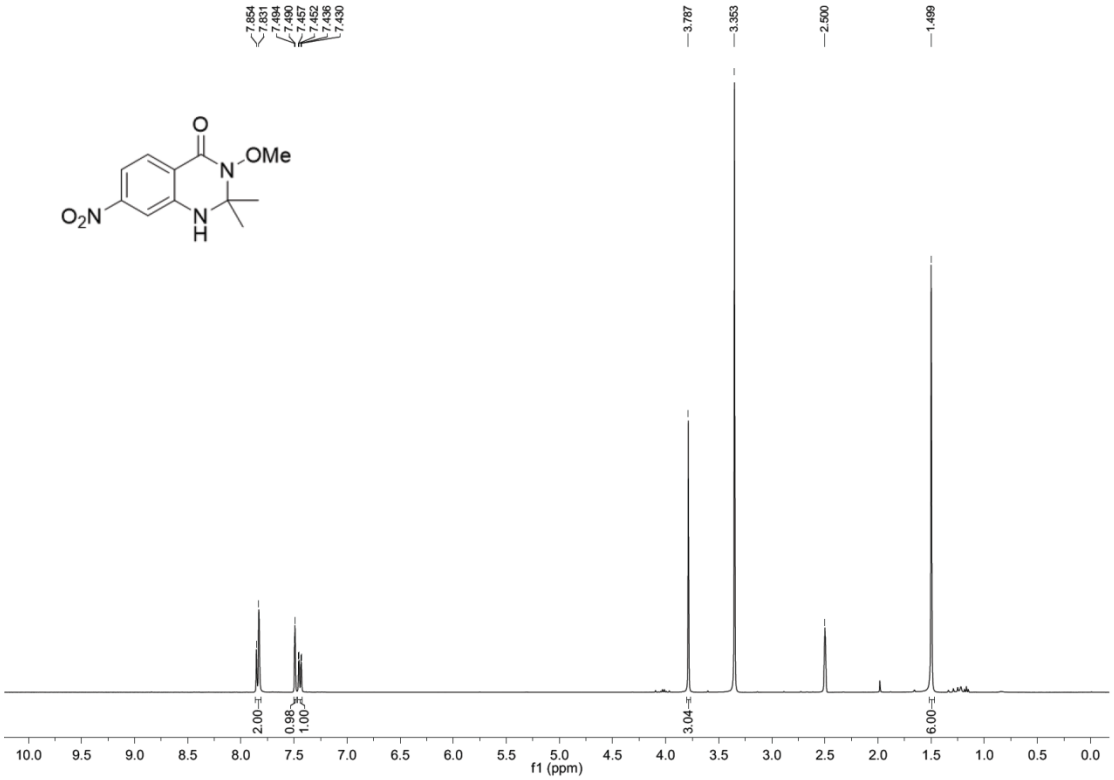
3ka-^{1}H NMR (400 MHz, DMSO-d_6)



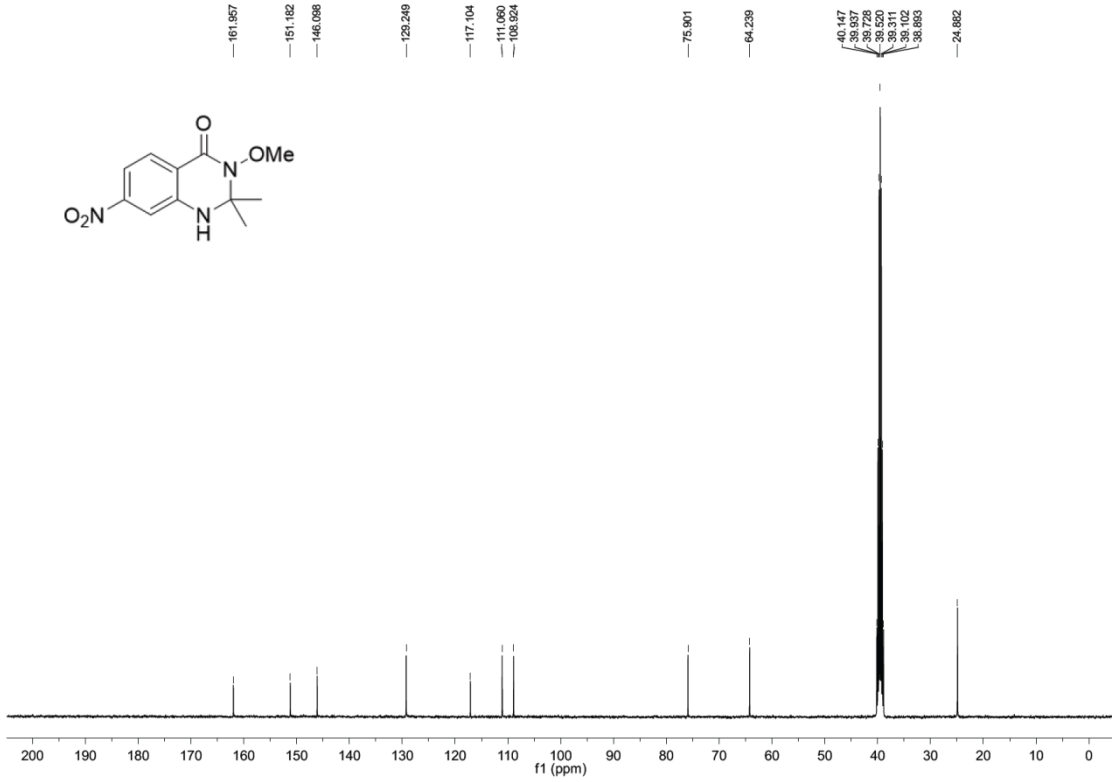
3ka-^{13}C NMR (100 MHz, DMSO-d_6)



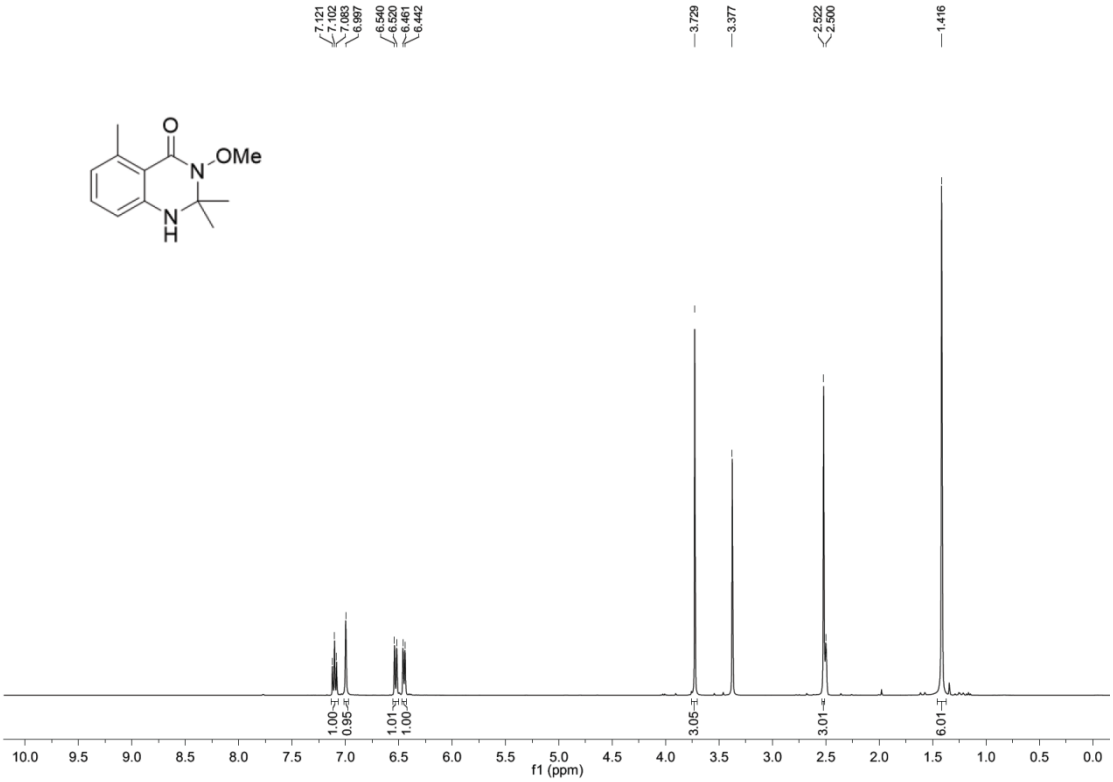
3la-^{1}H NMR (400 MHz, DMSO-d_6)



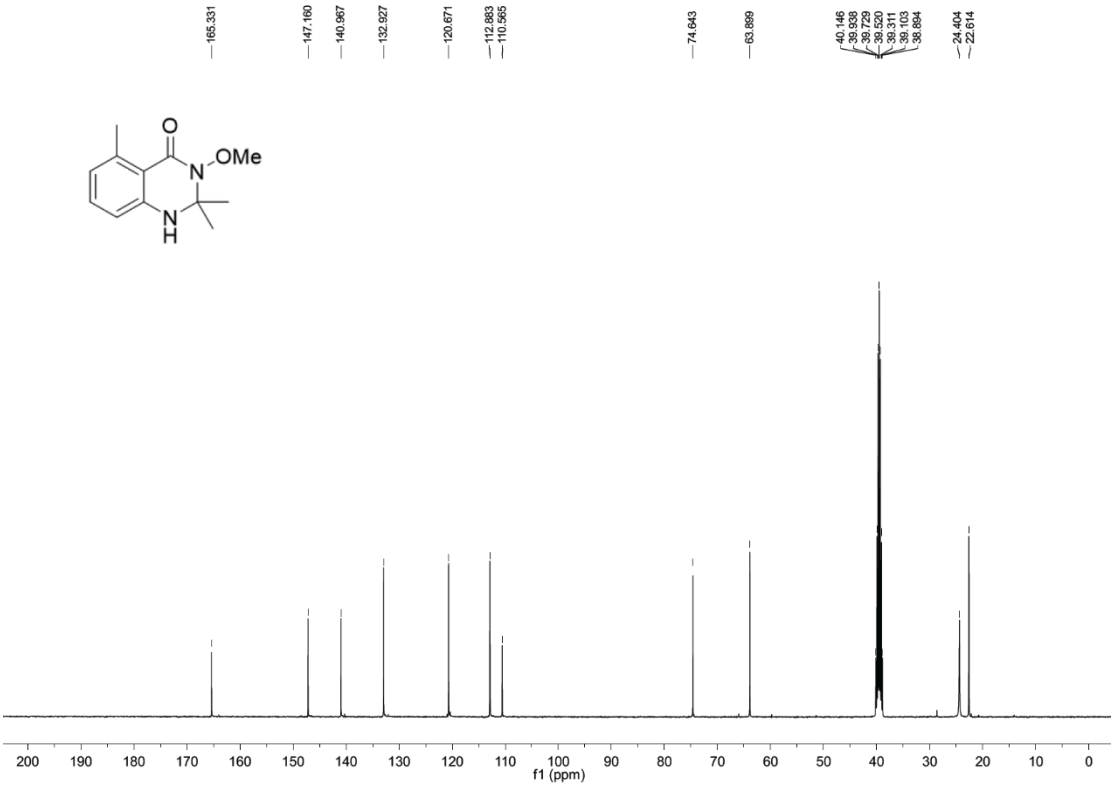
3la-^{13}C NMR (100 MHz, DMSO-d_6)



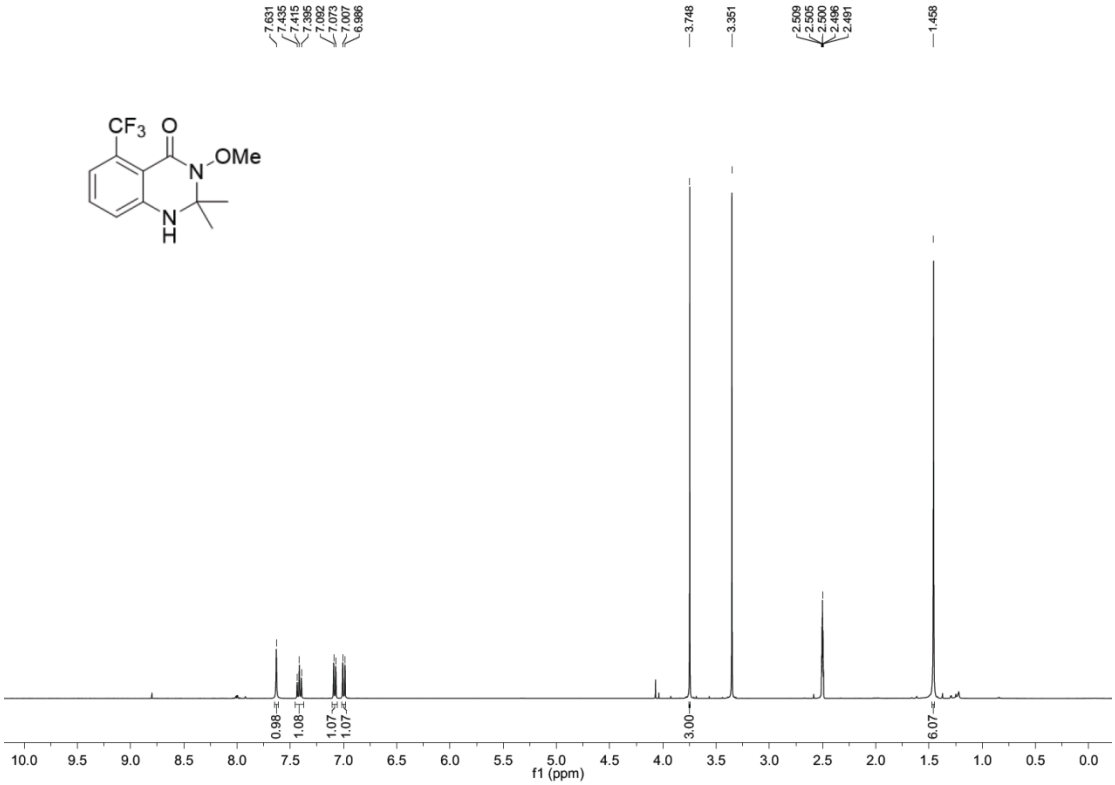
3ma-^{1}H NMR (400 MHz, DMSO-d_6)



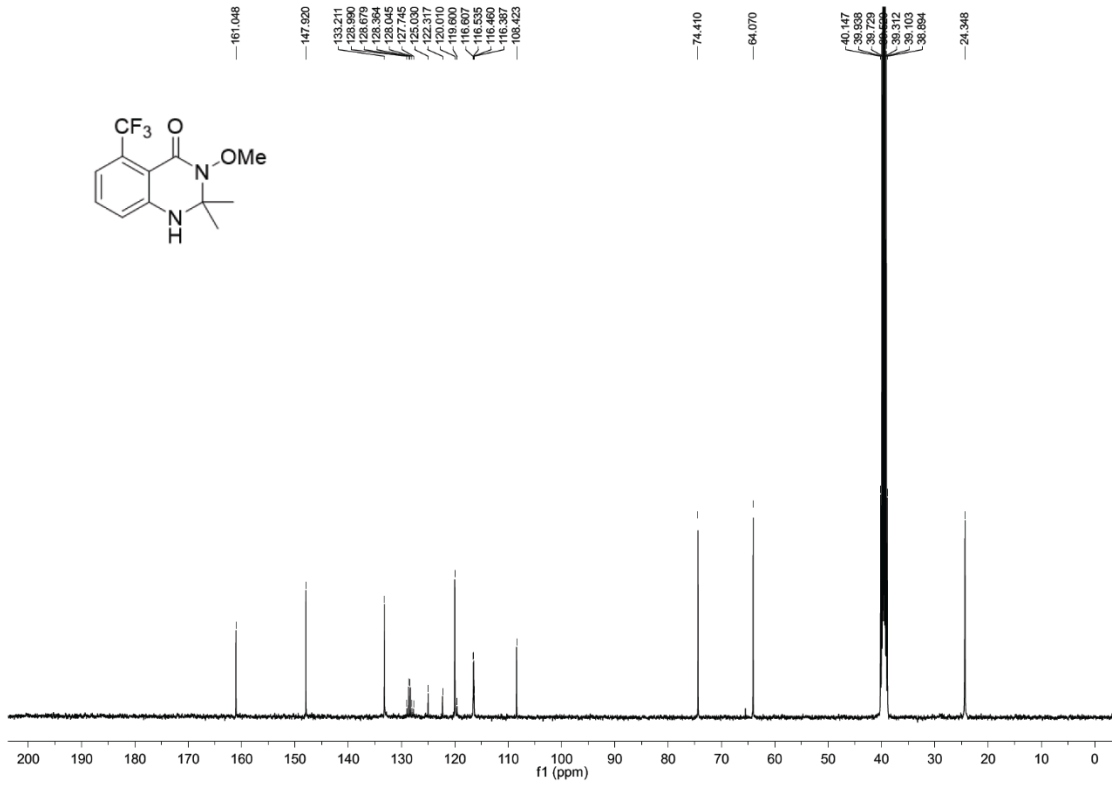
3ma-^{13}C NMR (100 MHz, DMSO-d_6)



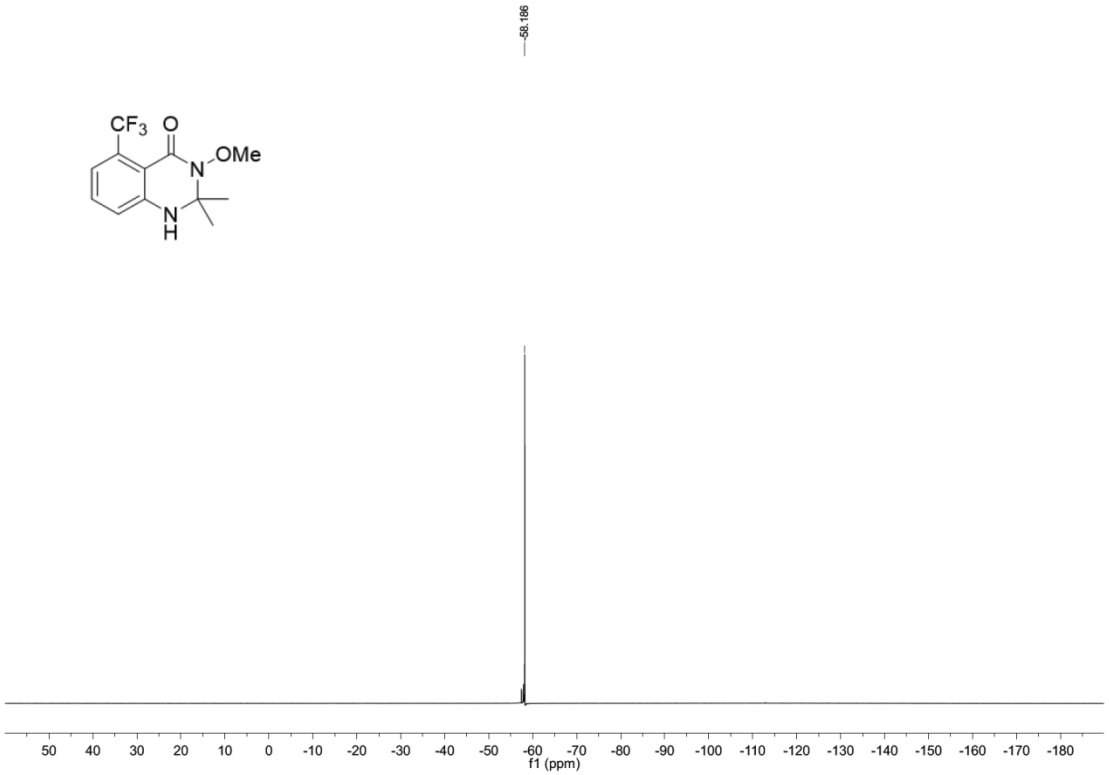
3na-^{1}H NMR (400 MHz, DMSO-d_6)



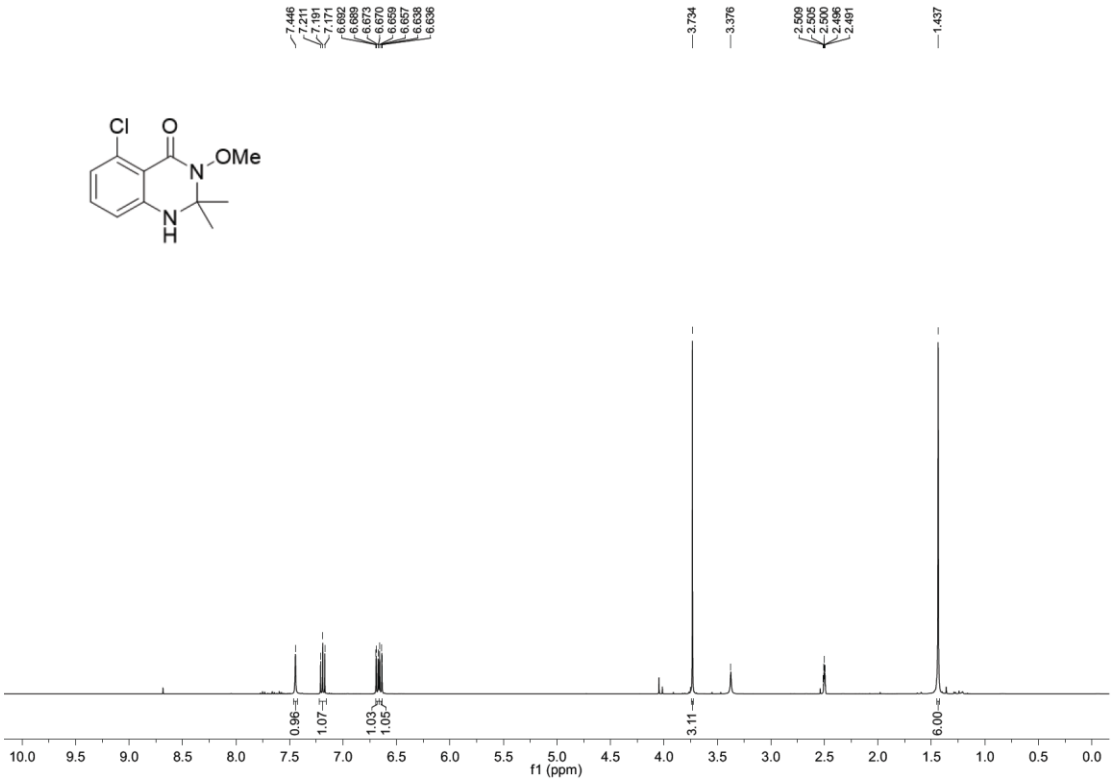
3na-^{13}C NMR (100 MHz, DMSO-d_6)



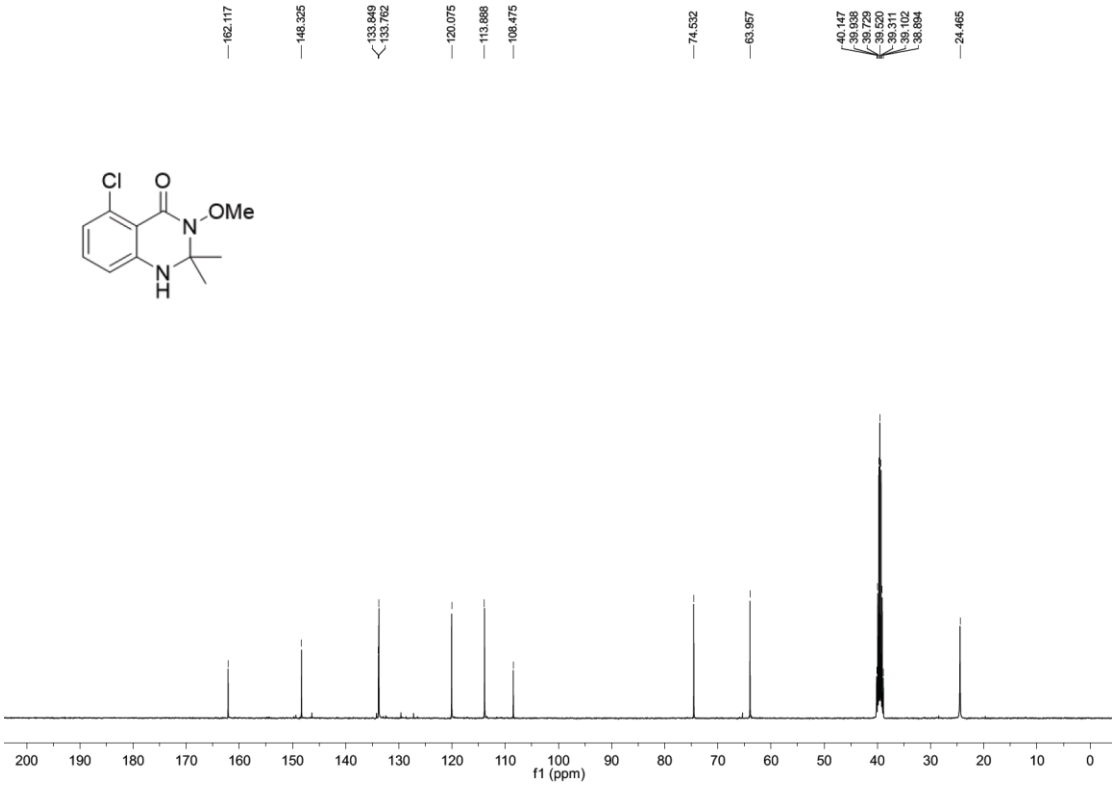
3na-^{19}F NMR (376 MHz, DMSO-d_6)



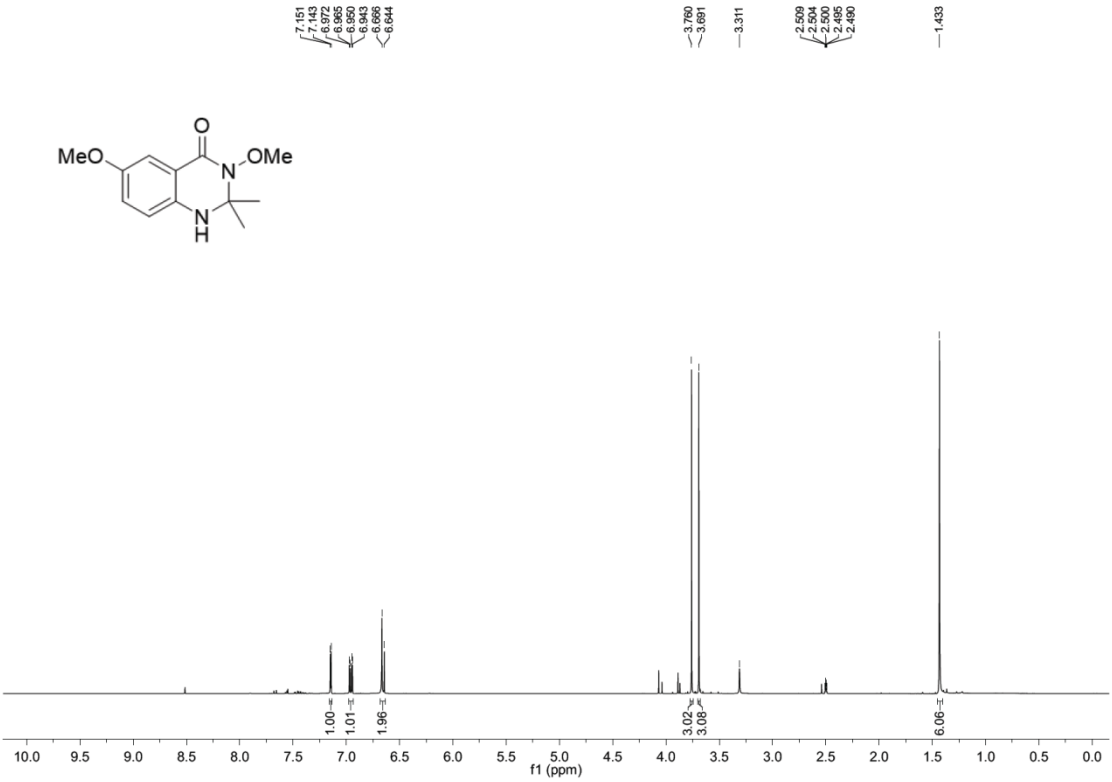
3oa-^{1}H NMR (400 MHz, DMSO-d_6)



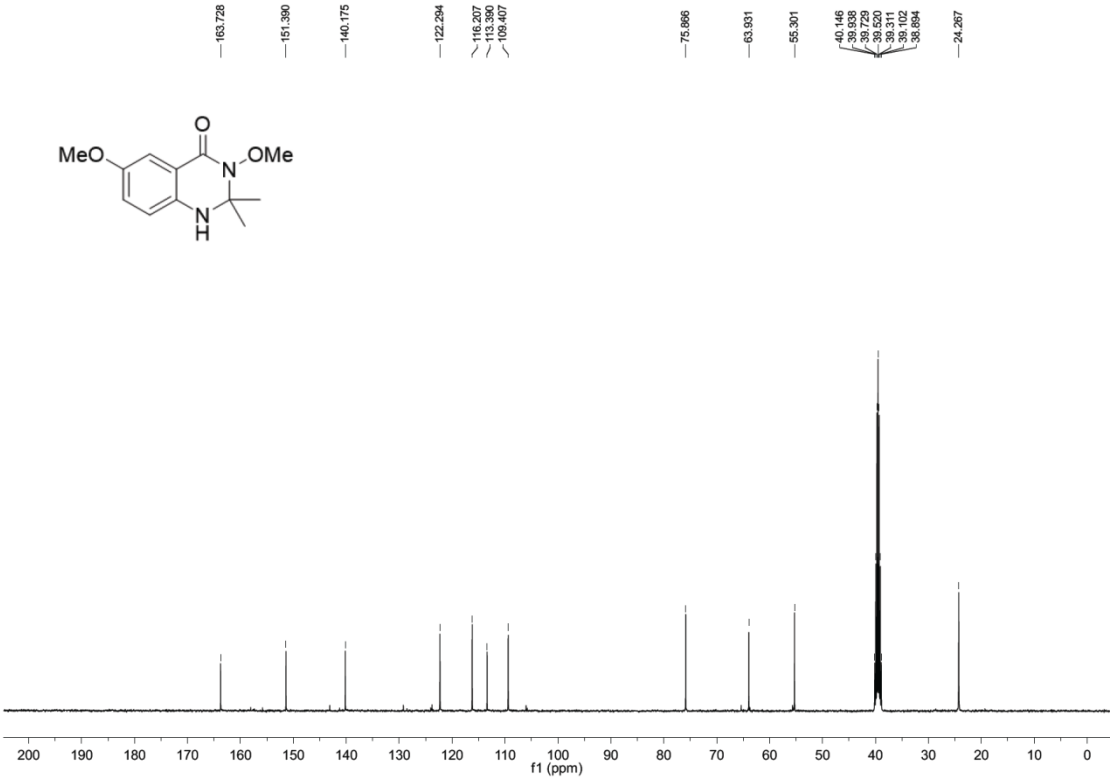
3oa-^{13}C NMR (100 MHz, DMSO-d_6)



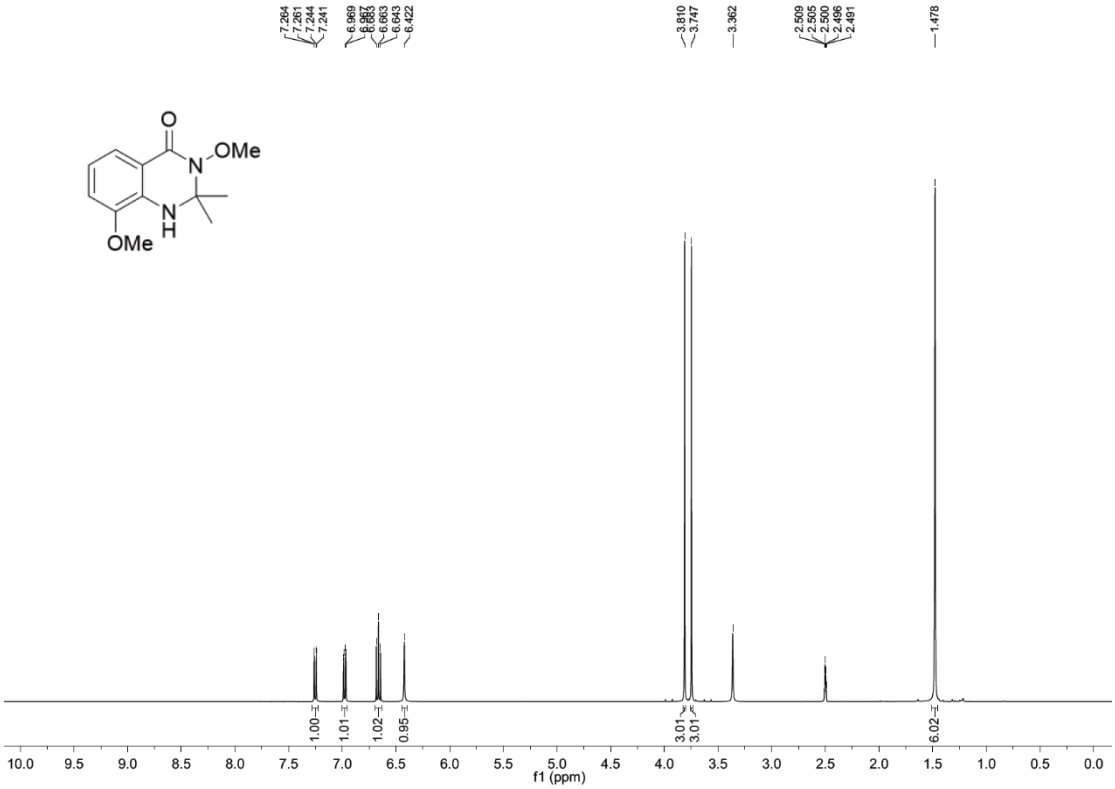
3pa-^{1}H NMR (400 MHz, DMSO-d_6)



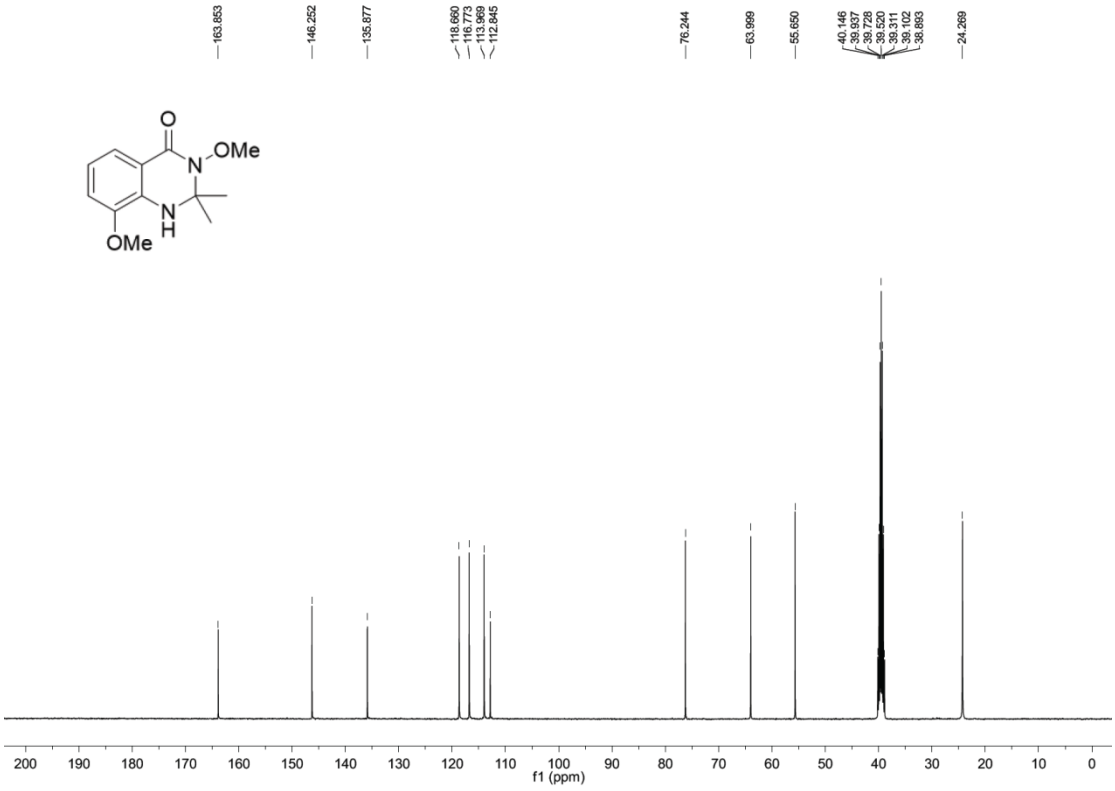
3pa-^{13}C NMR (100 MHz, DMSO-d_6)



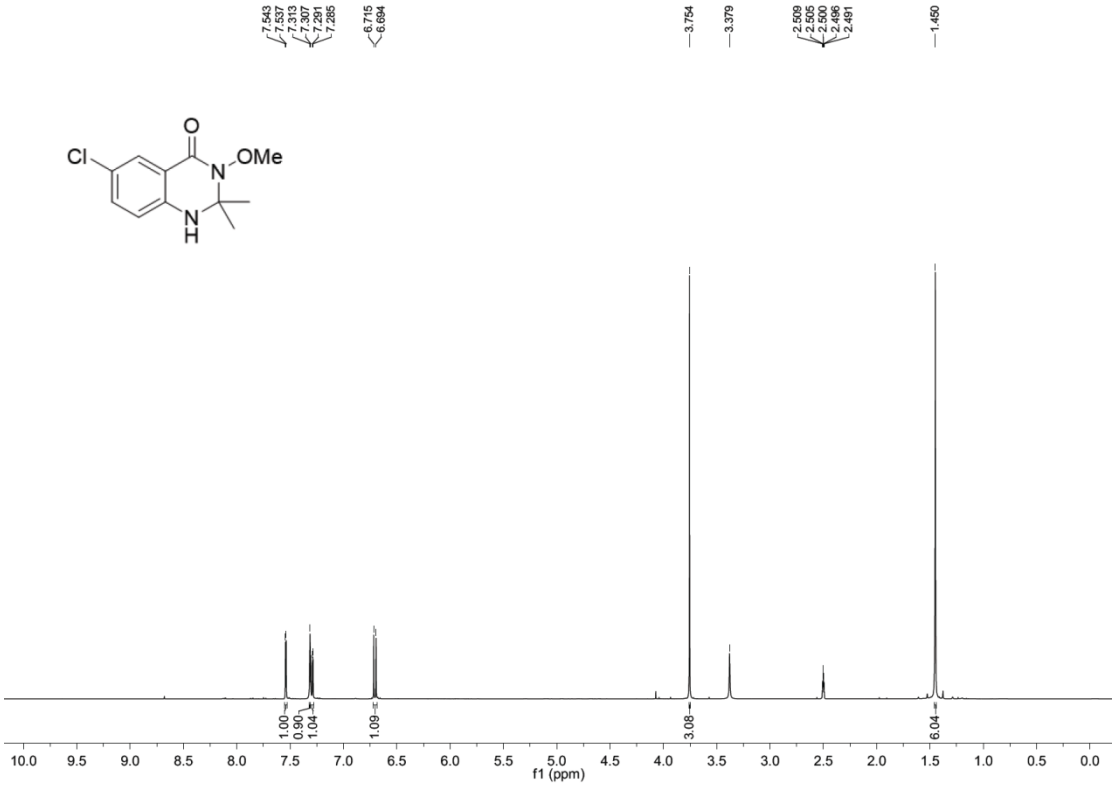
3pa'-^{1}H NMR (400 MHz, DMSO-d_6)



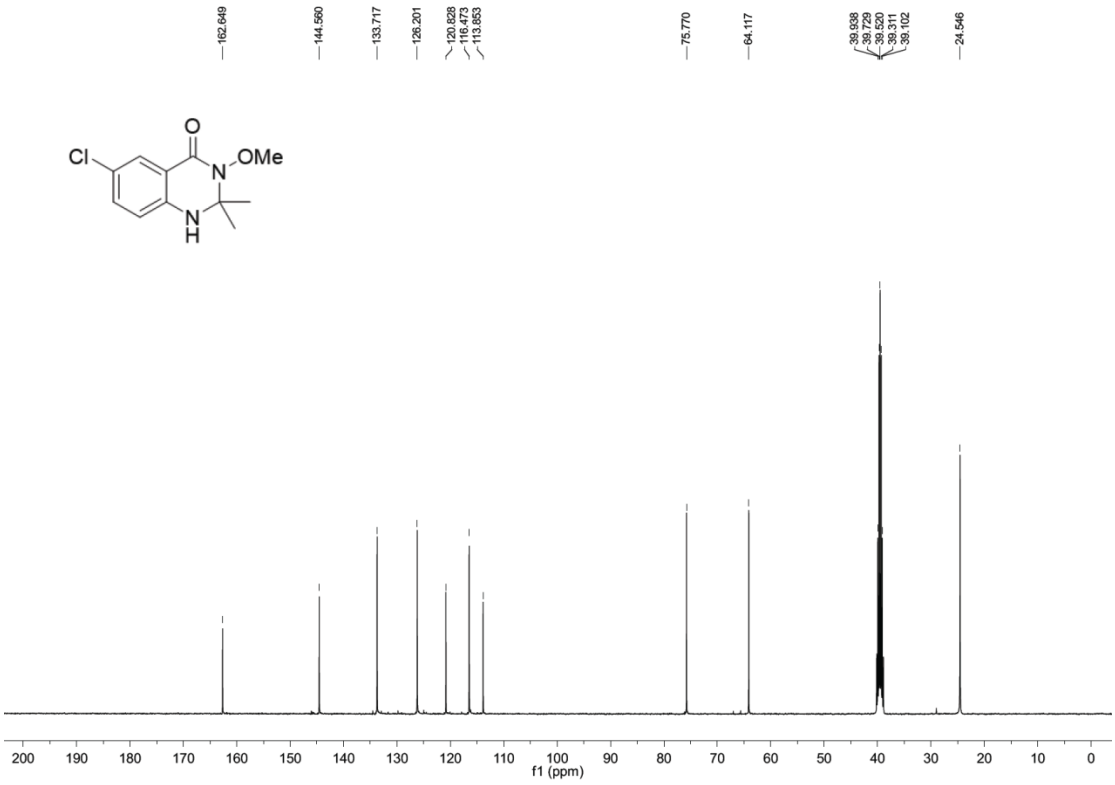
3pa'-^{13}C NMR (100 MHz, DMSO-d_6)



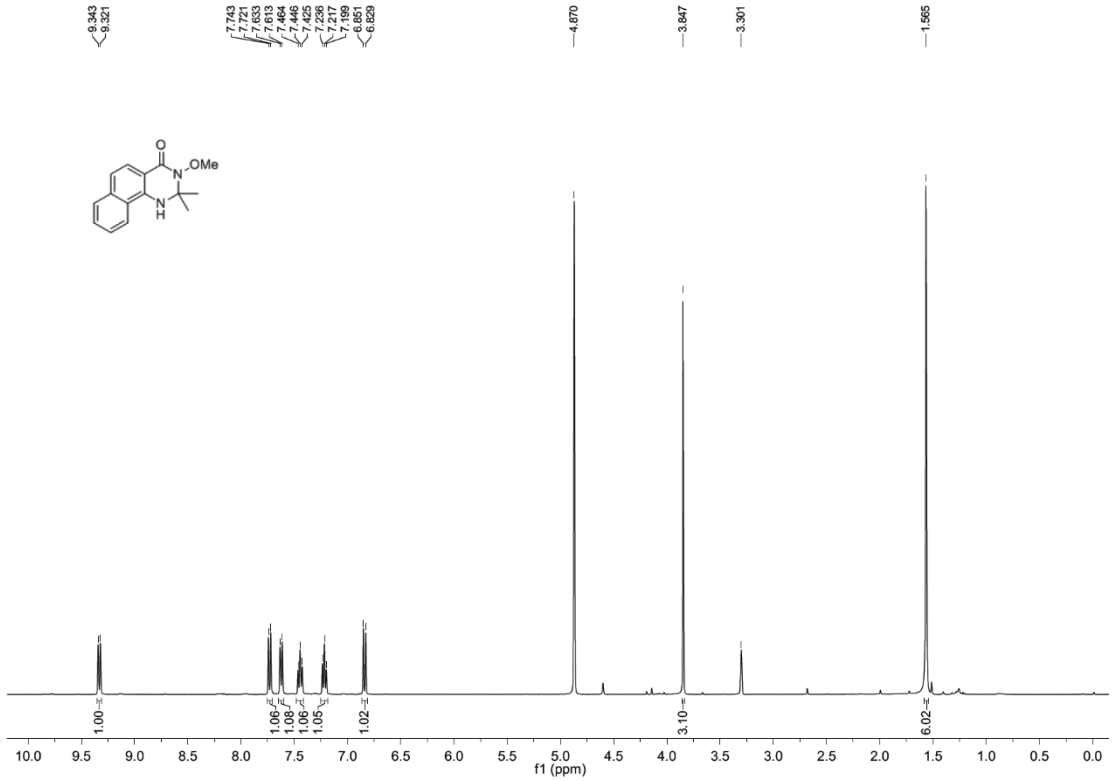
3qa-^{1}H NMR (400 MHz, DMSO-d_6)



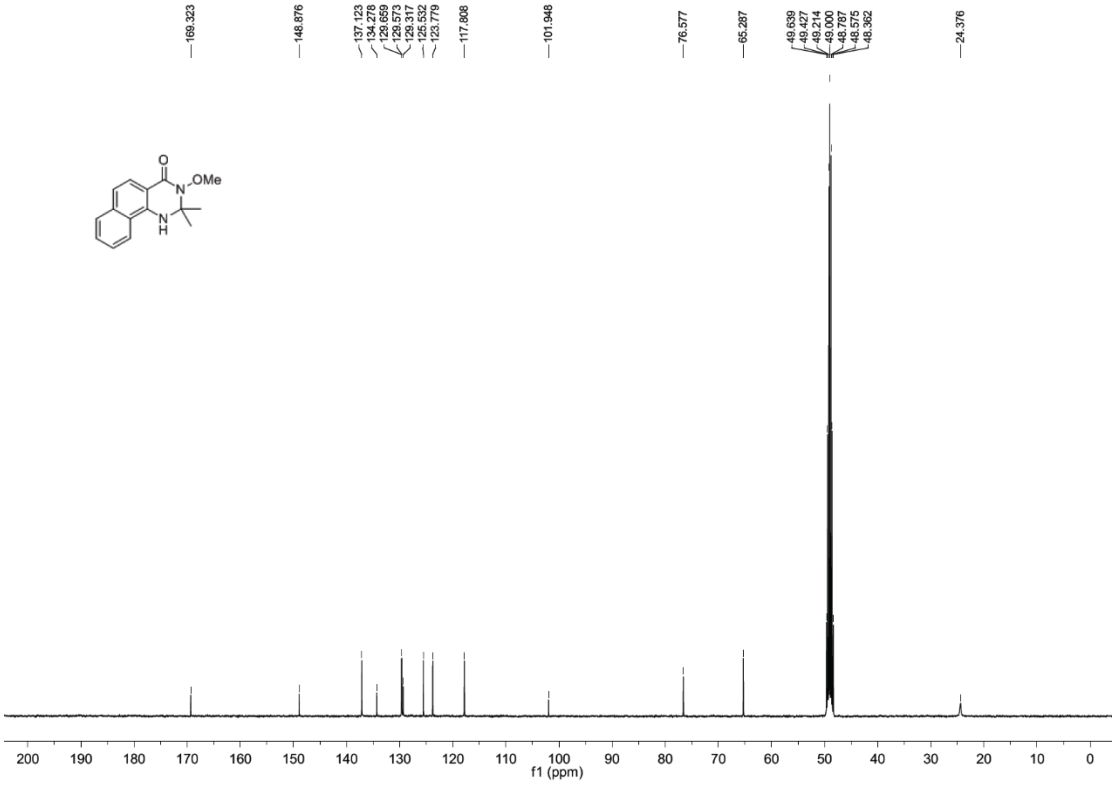
3qa-^{13}C NMR (100 MHz, DMSO-d_6)



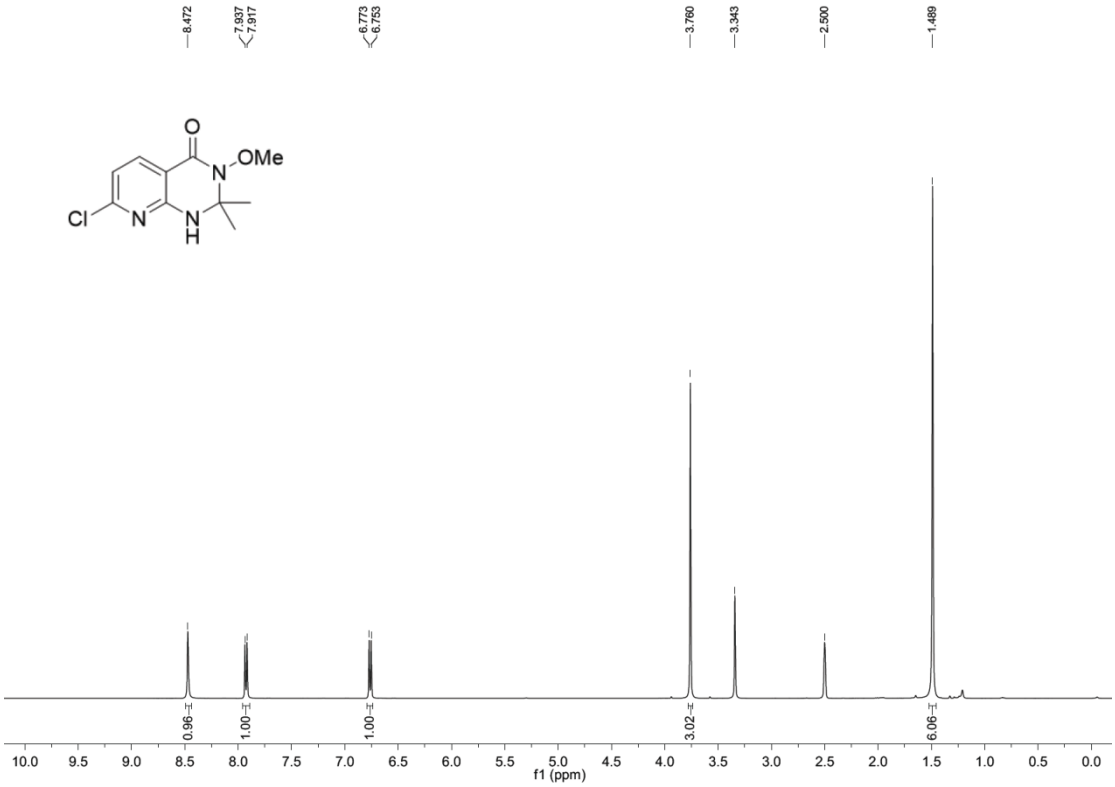
3ra-^{1}H NMR (400 MHz, CD_3OD)



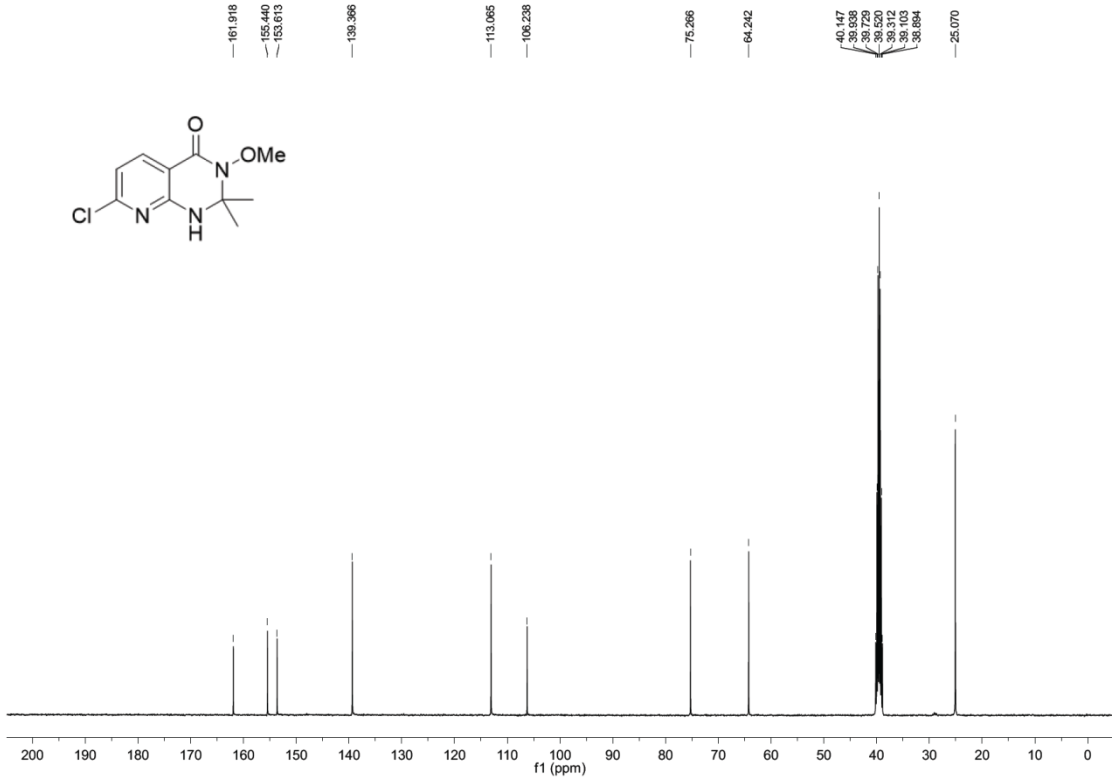
3ra-^{13}C NMR (100 MHz, CD_3OD)



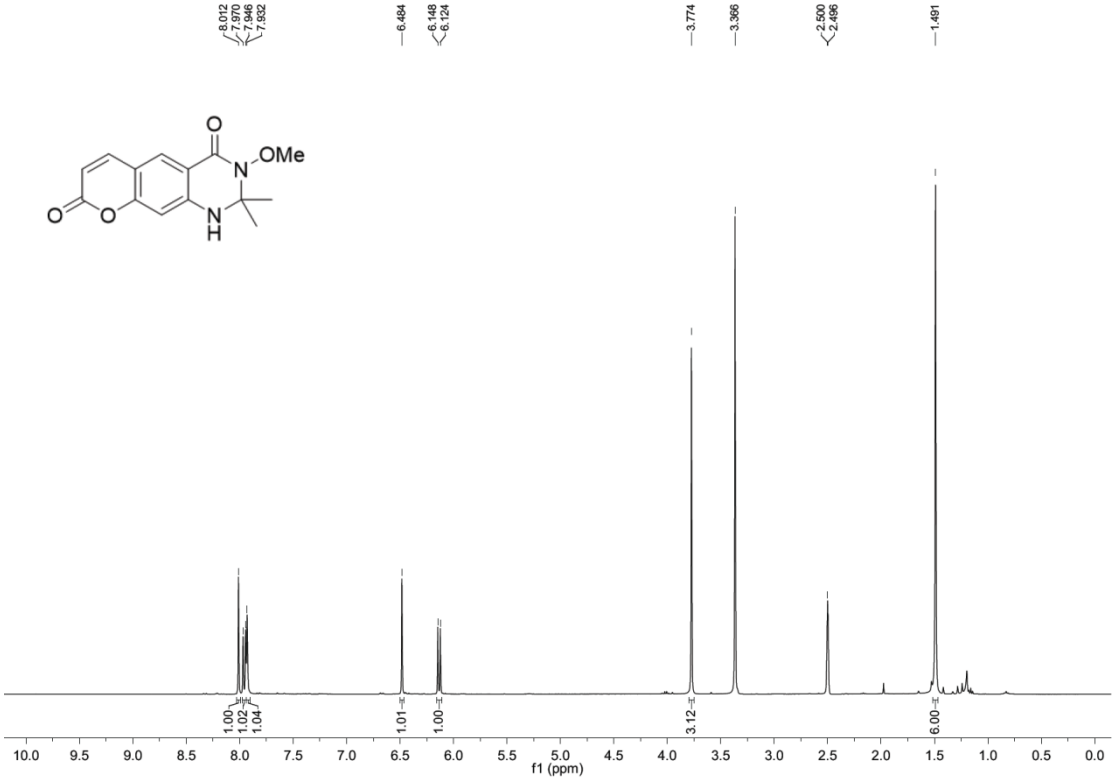
3sa-^{1}H NMR (400 MHz, DMSO-d_6)



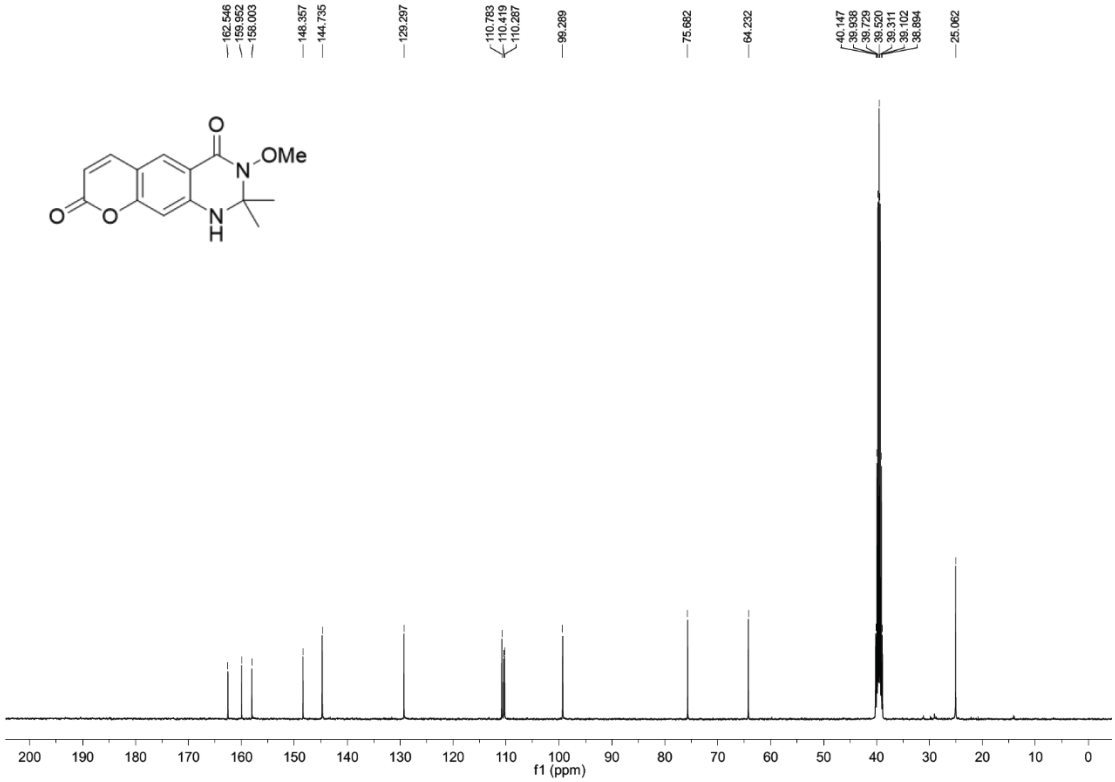
3sa-^{13}C NMR (100 MHz, DMSO-d_6)



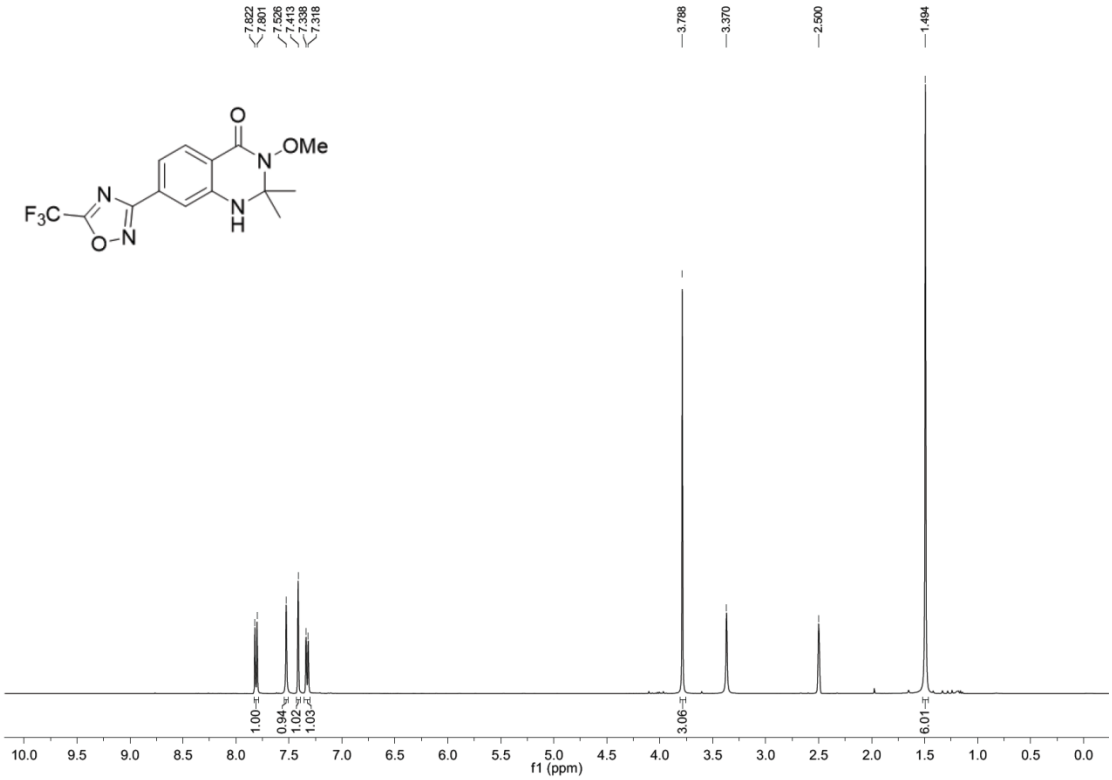
3ta-^{1}H NMR (400 MHz, DMSO-d_6)



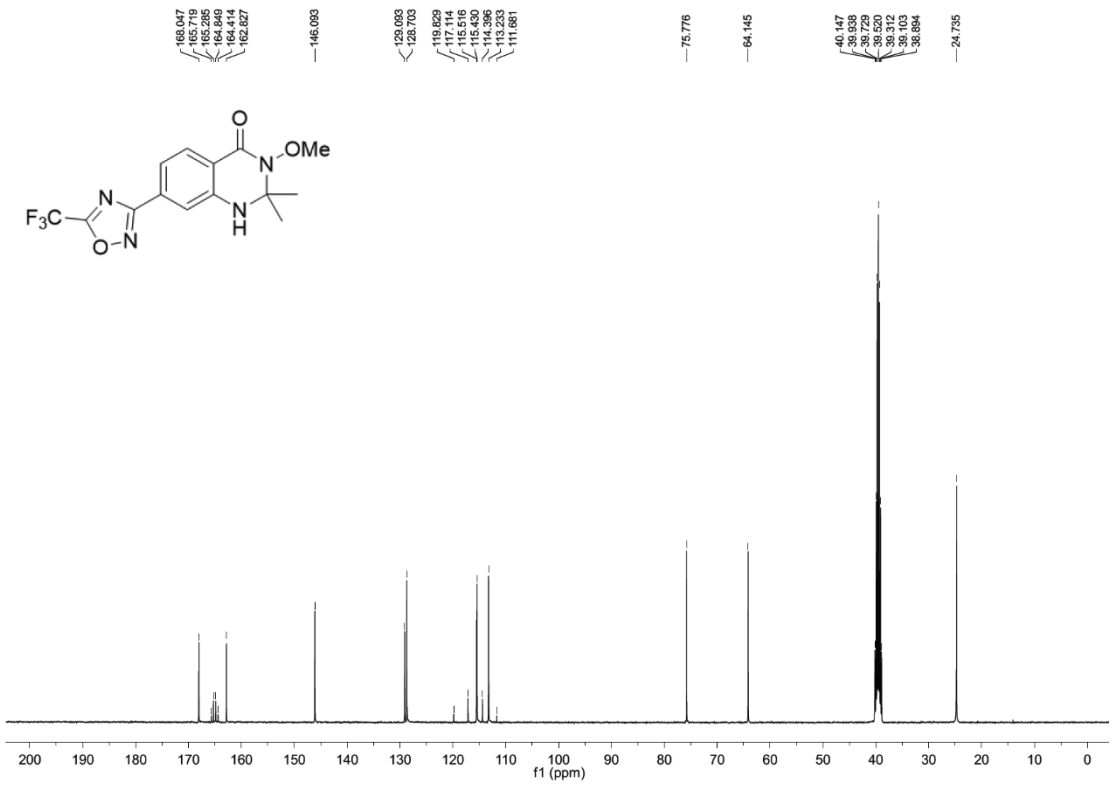
3ta-^{13}C NMR (100 MHz, DMSO-d_6)



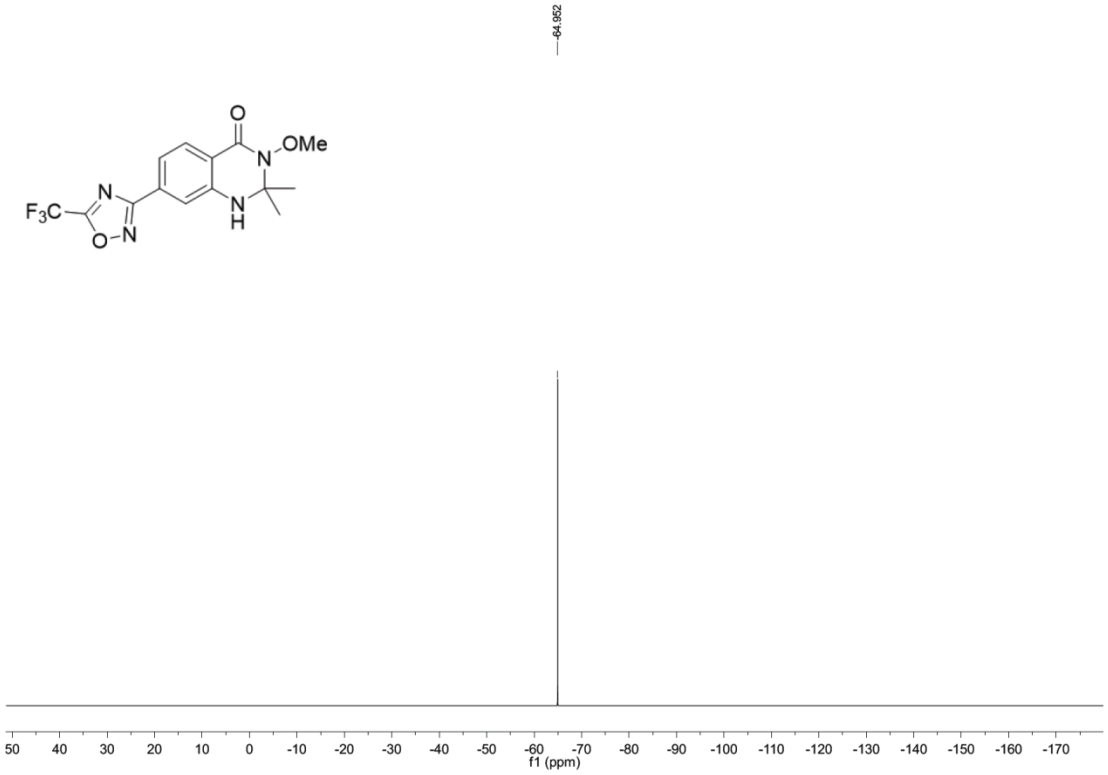
3ua-^{1}H NMR (400 MHz, DMSO-d_6)



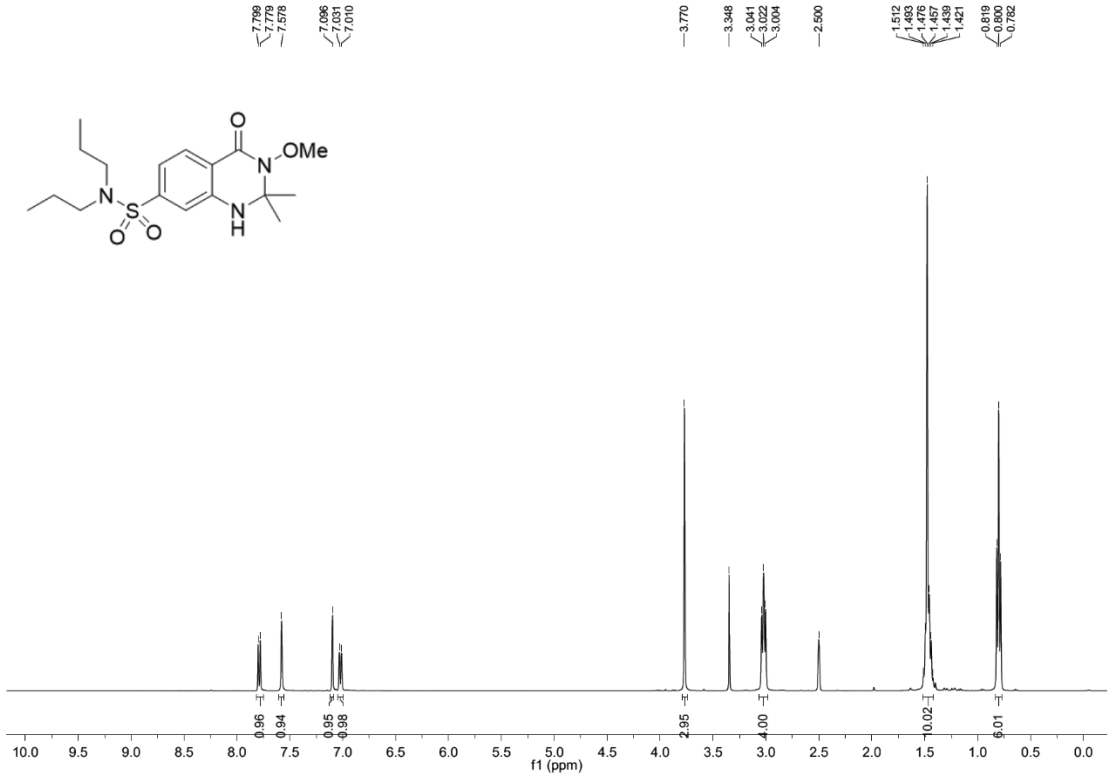
3ua-^{13}C NMR (100 MHz, DMSO-d_6)



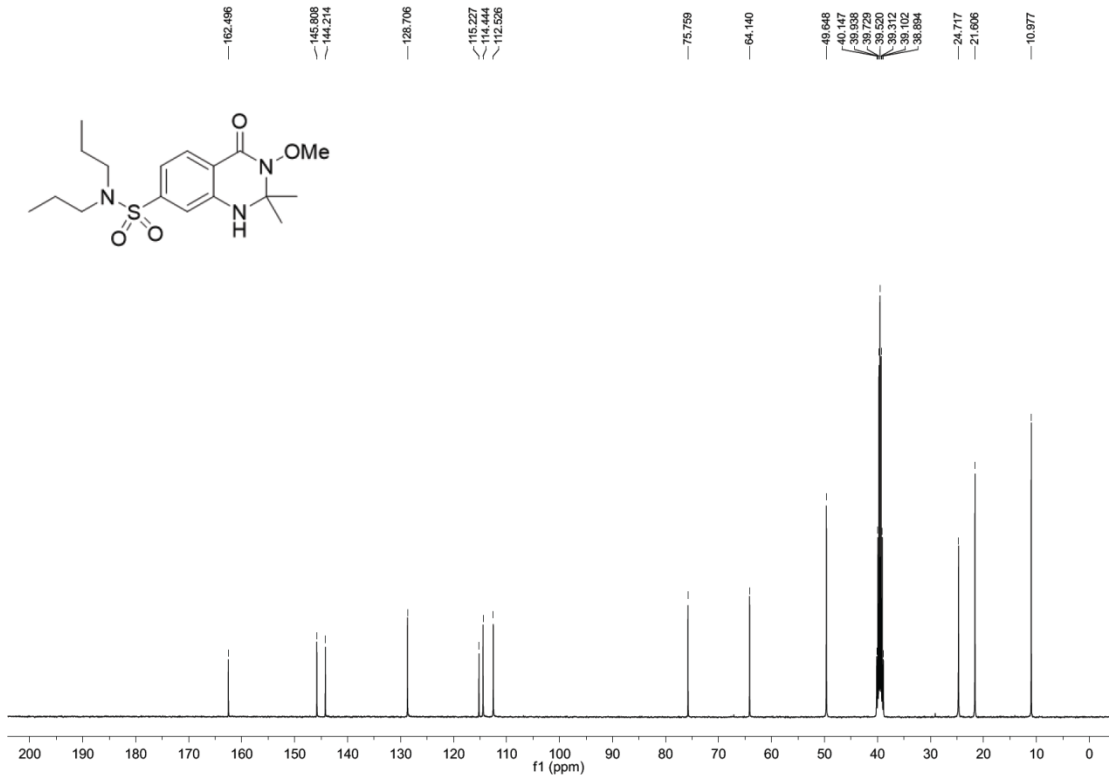
3ua-^{19}F NMR (376 MHz, DMSO-d_6)



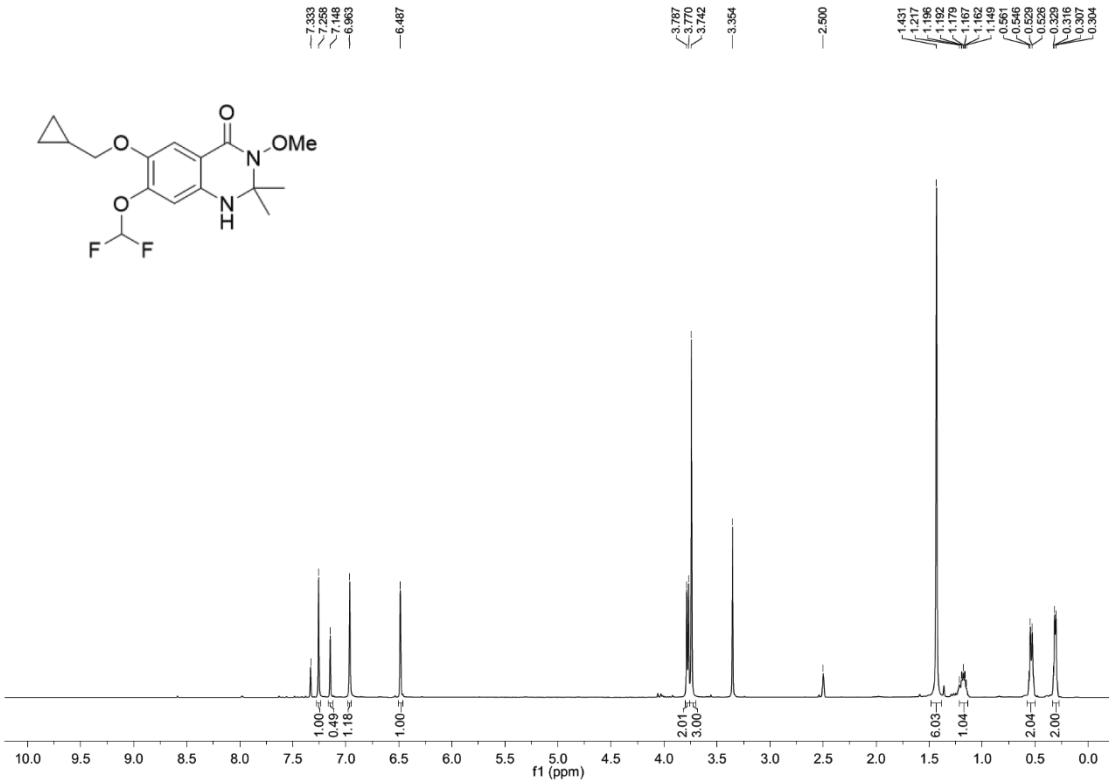
3va-^{1}H NMR (400 MHz, DMSO-d_6)



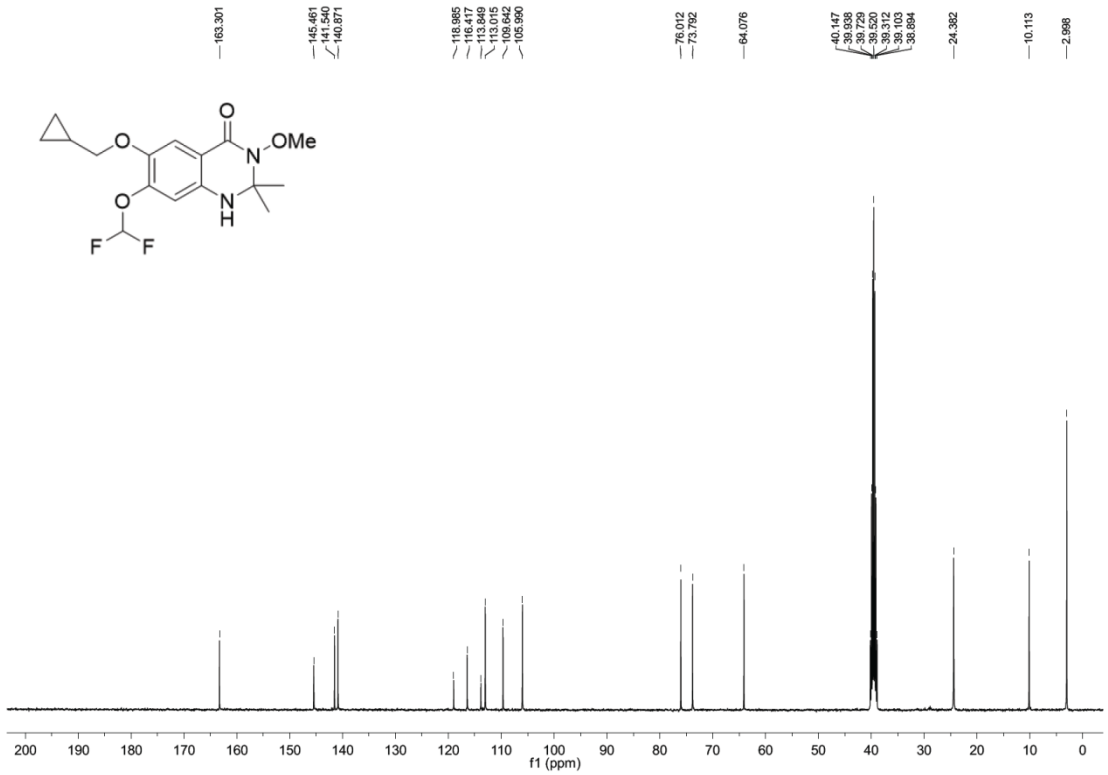
3va-^{13}C NMR (100 MHz, DMSO-d_6)



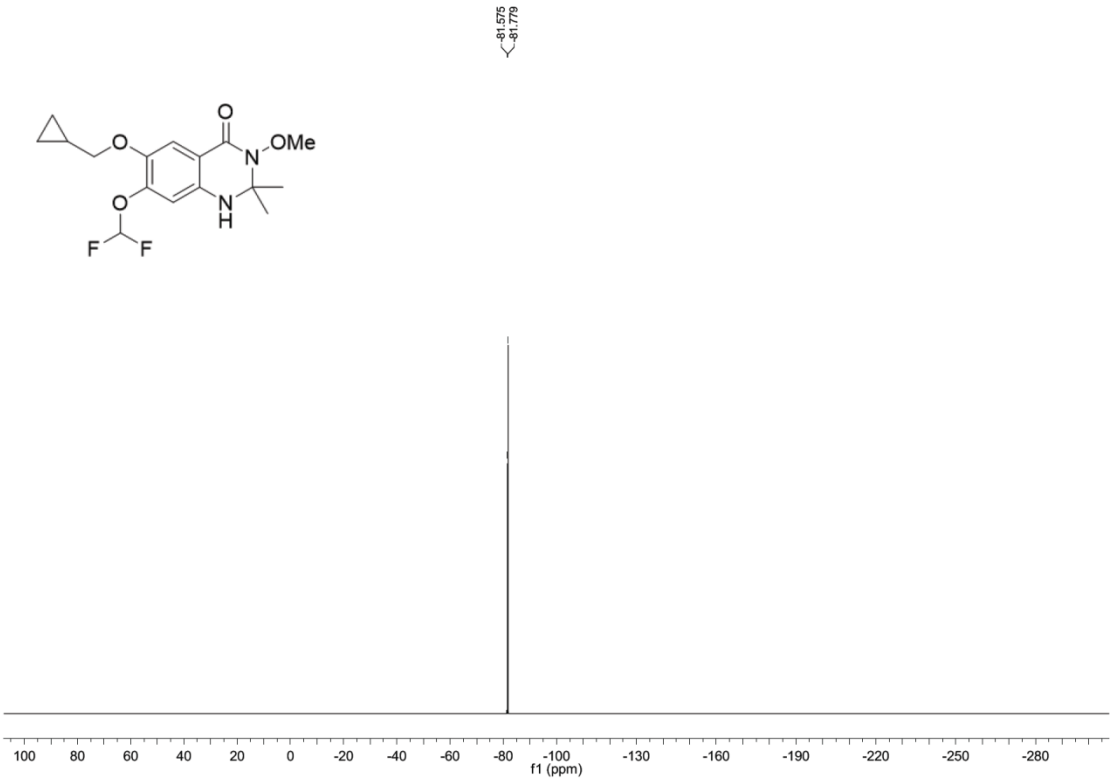
3wa-^{1}H NMR (400 MHz, DMSO-d_6)



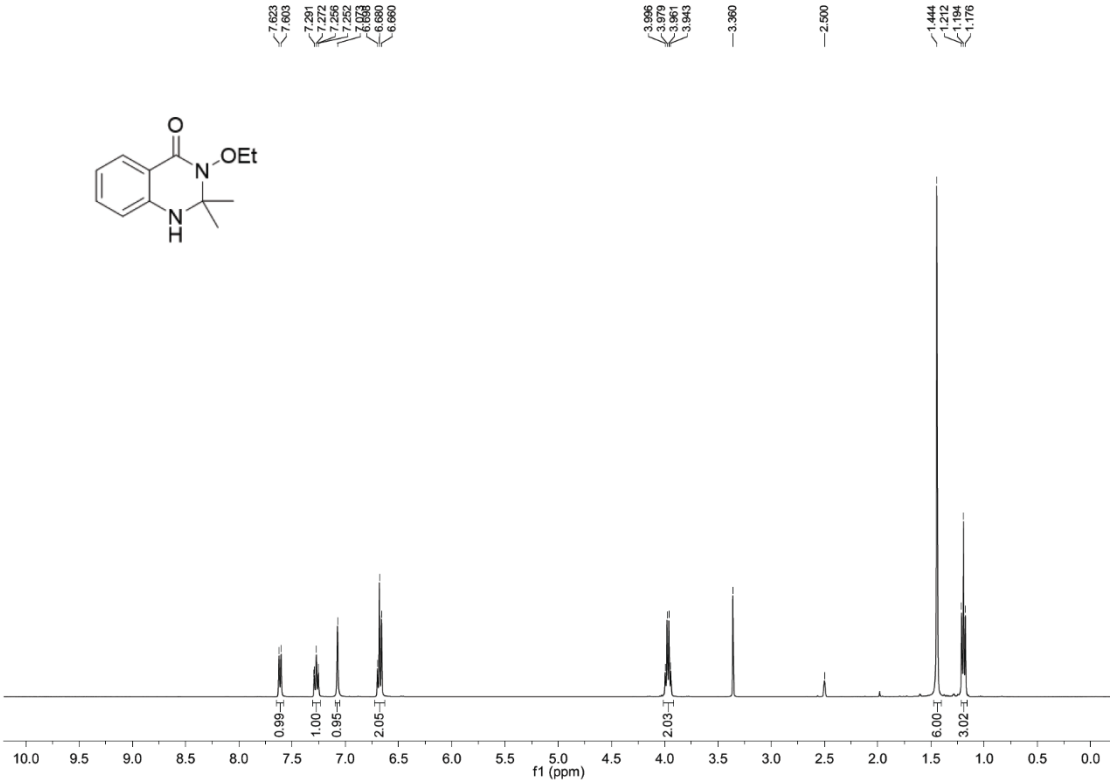
3wa-^{13}C NMR (100 MHz, DMSO-d_6)



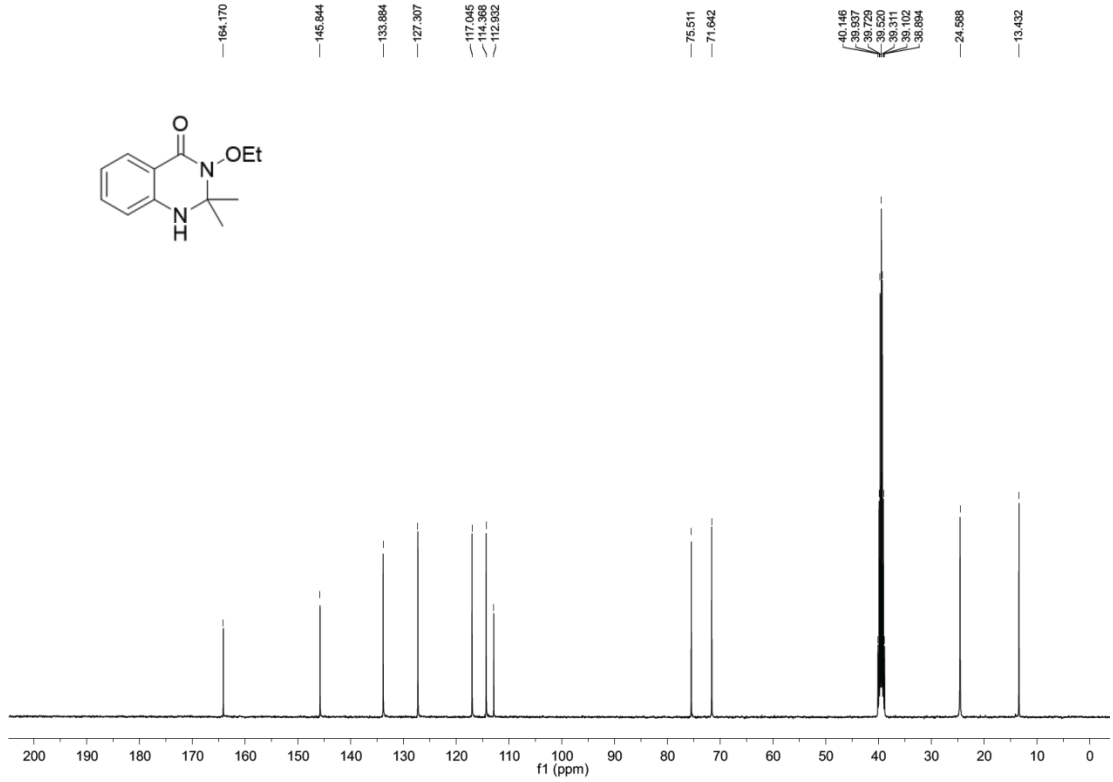
3wa-^{19}F NMR (376 MHz, DMSO-d_6)



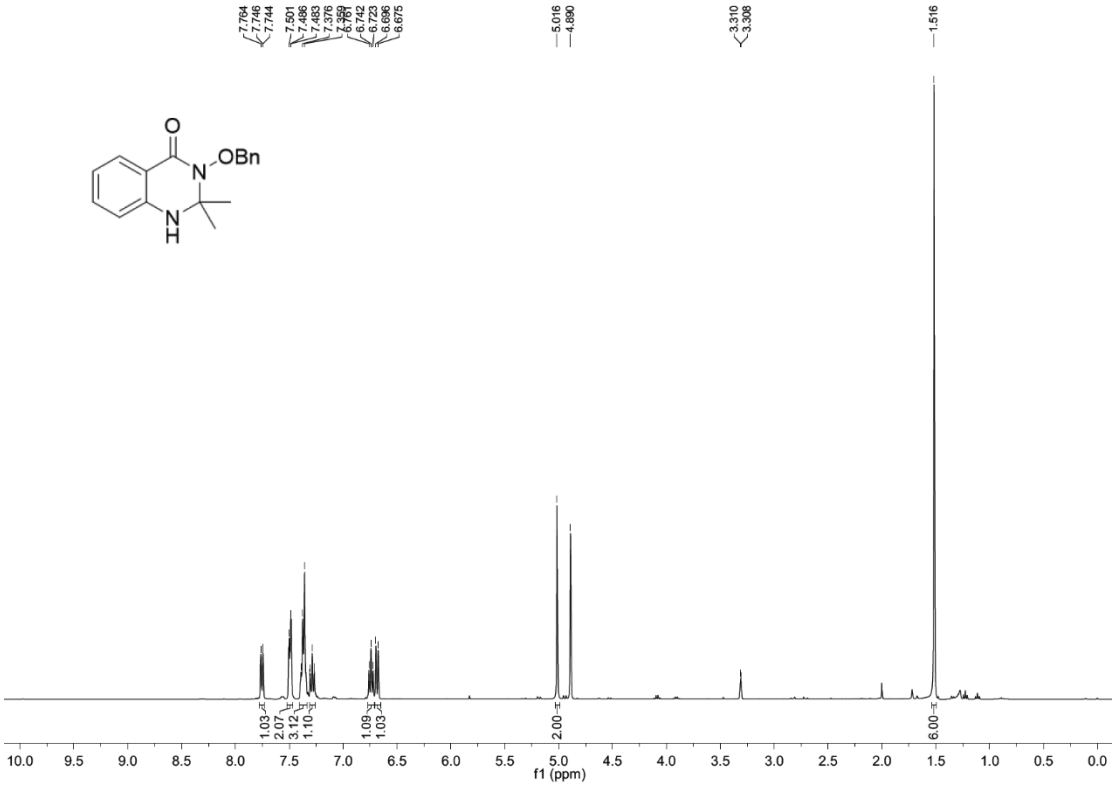
3xa-^{1}H NMR (400 MHz, DMSO-d_6)



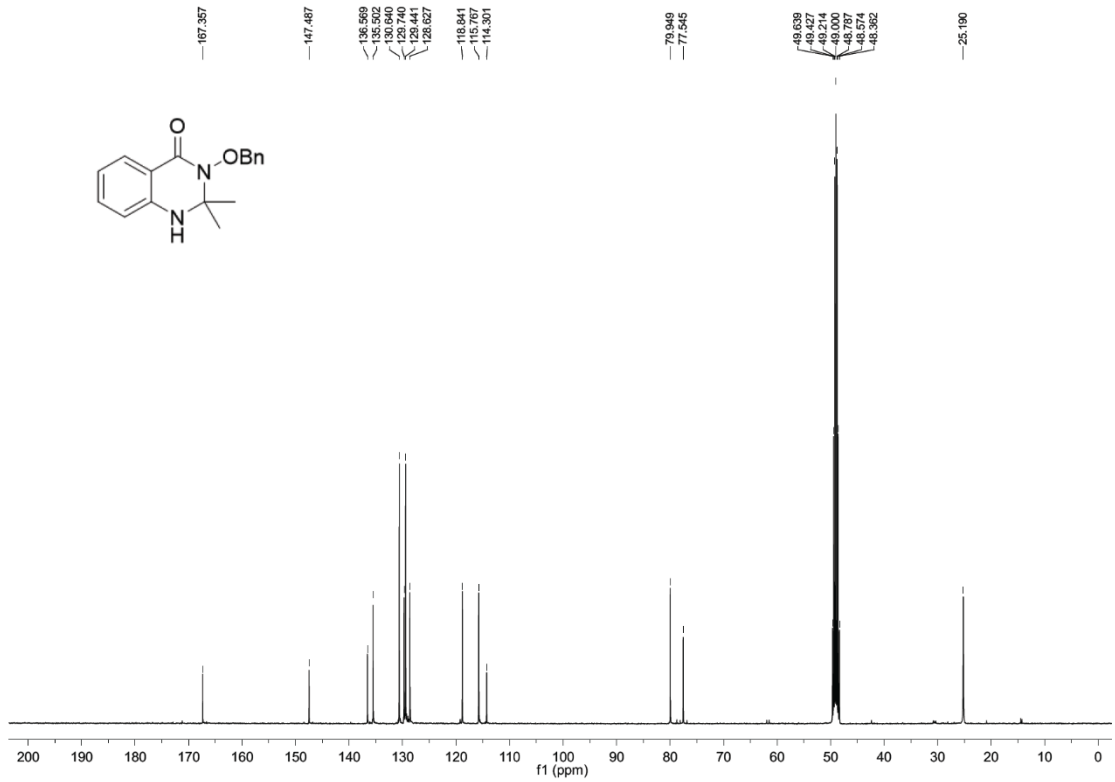
3xa-^{13}C NMR (100 MHz, DMSO-d_6)



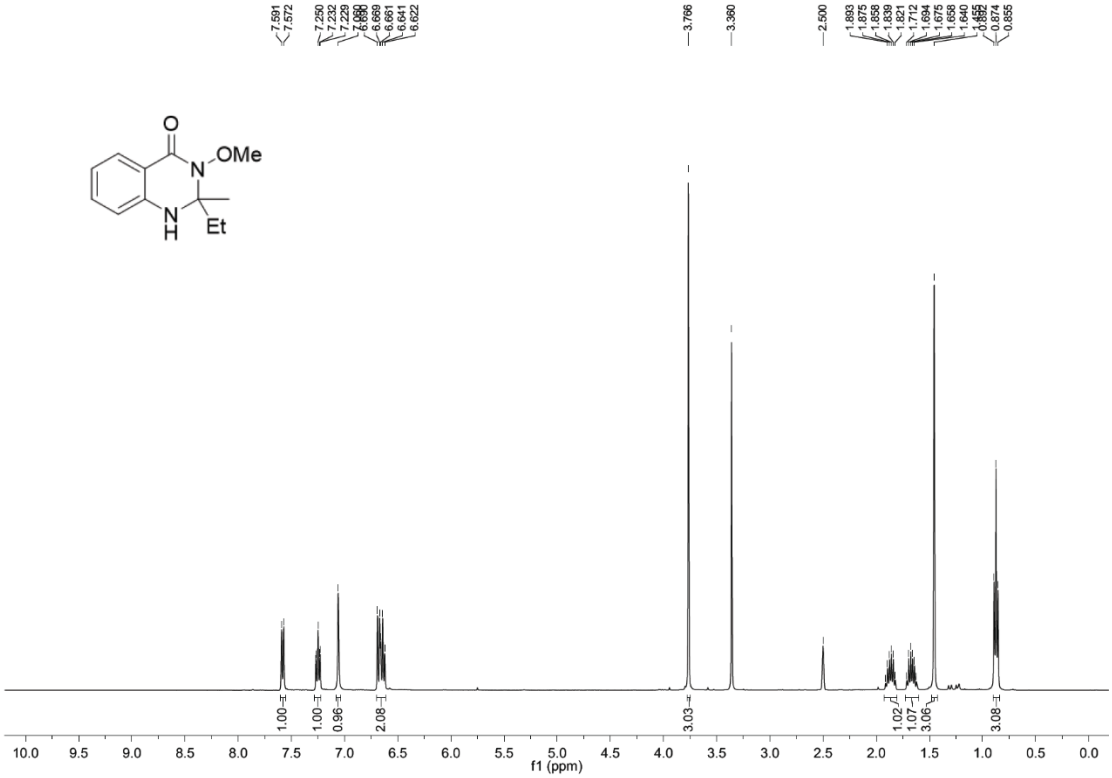
3ya-^{1}H NMR (400 MHz, CD_3OD)



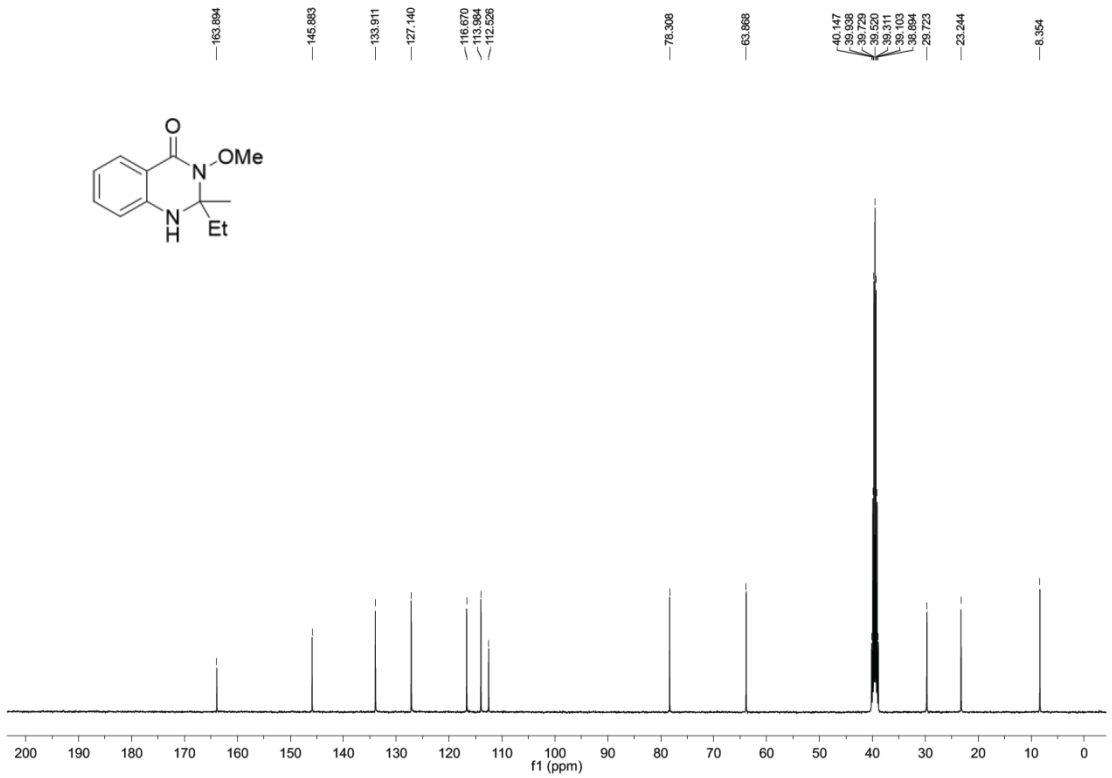
3ya-^{13}C NMR (100 MHz, CD_3OD)



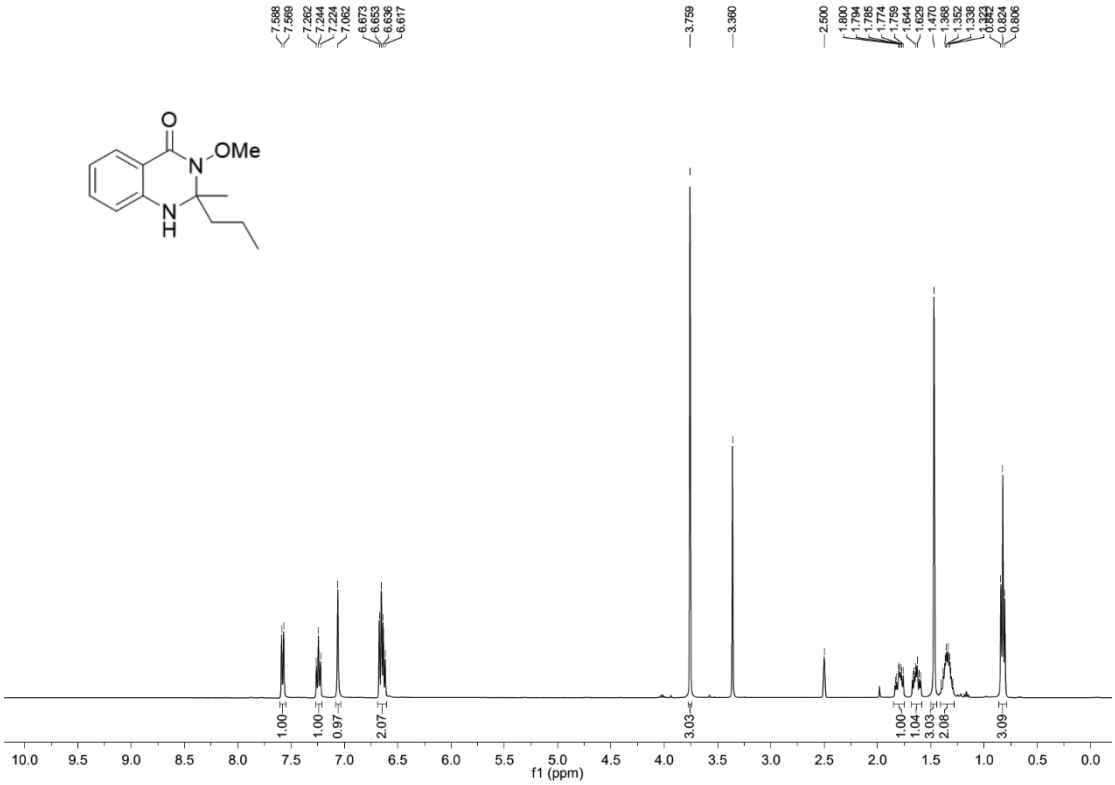
3ab-^{1}H NMR (400 MHz, DMSO-d_6)



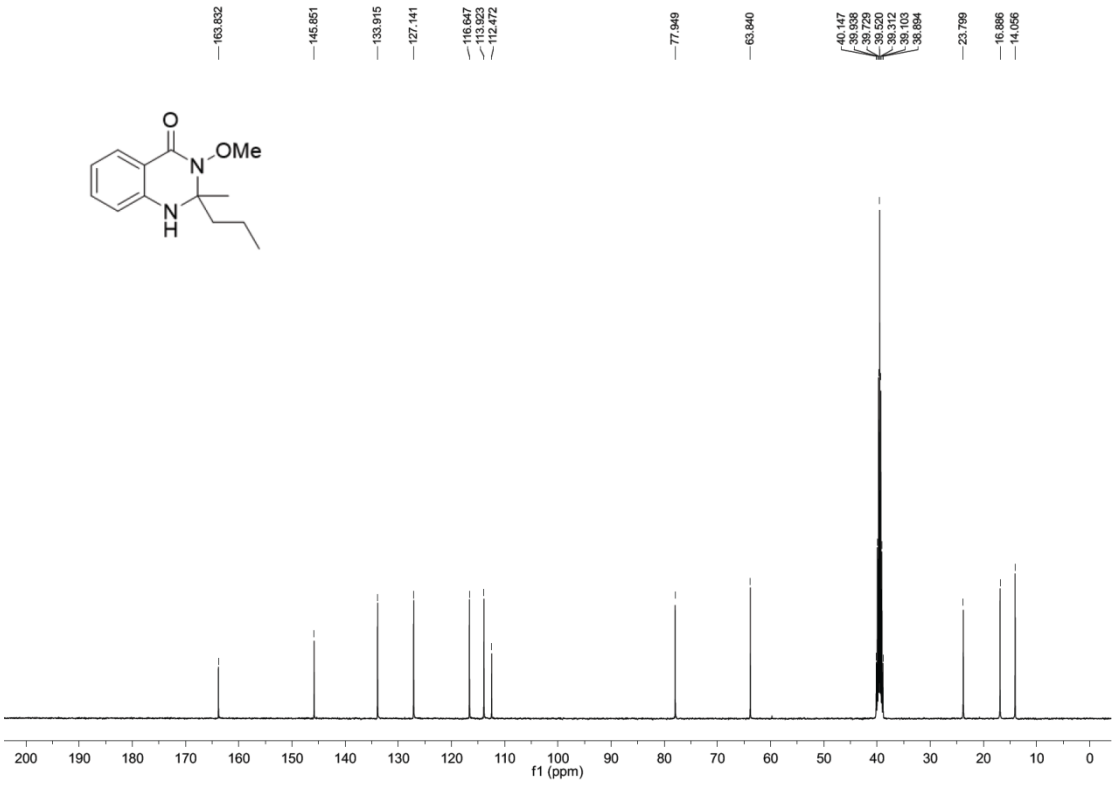
3ab-^{13}C NMR (100 MHz, DMSO-d_6)



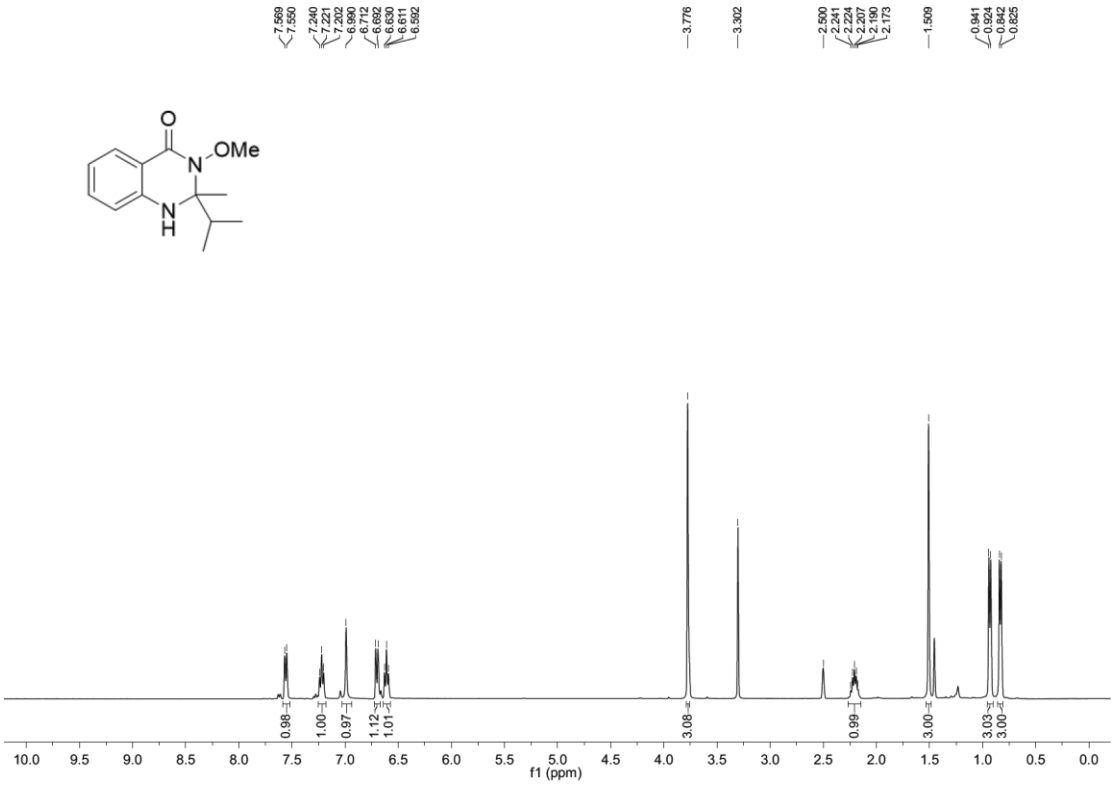
3ac-^{1}H NMR (400 MHz, DMSO-d_6)



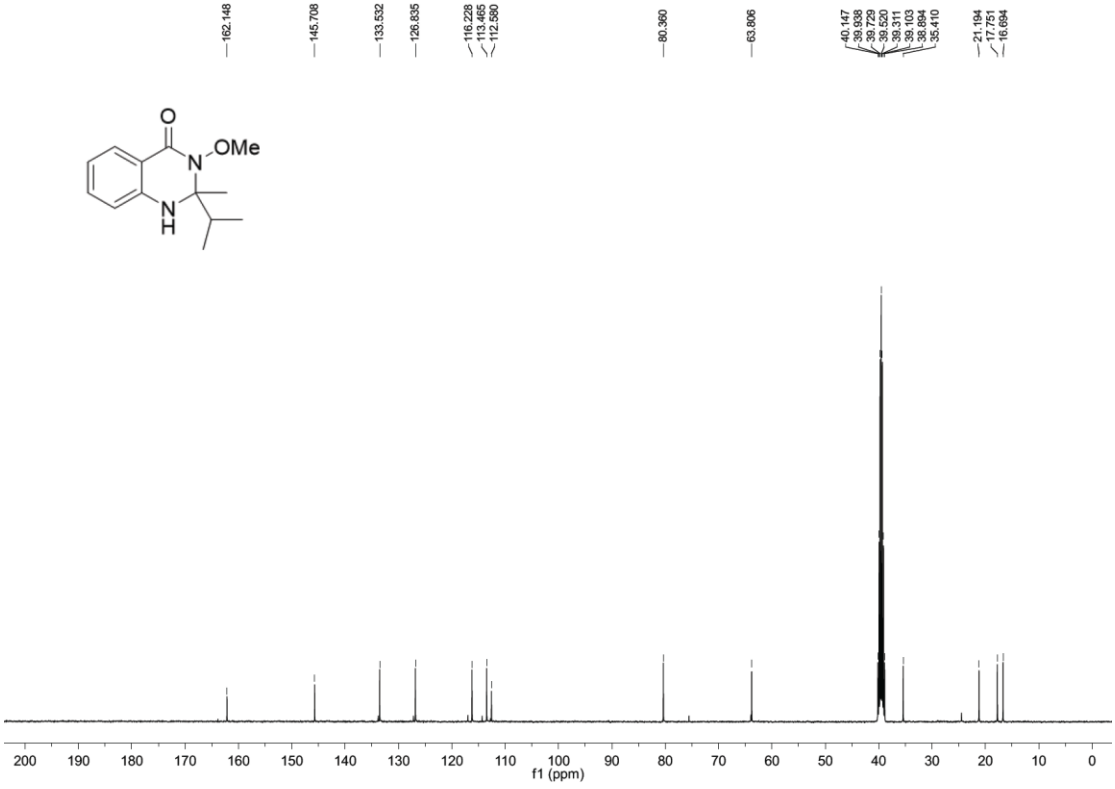
3ac-^{13}C NMR (100 MHz, DMSO-d_6)



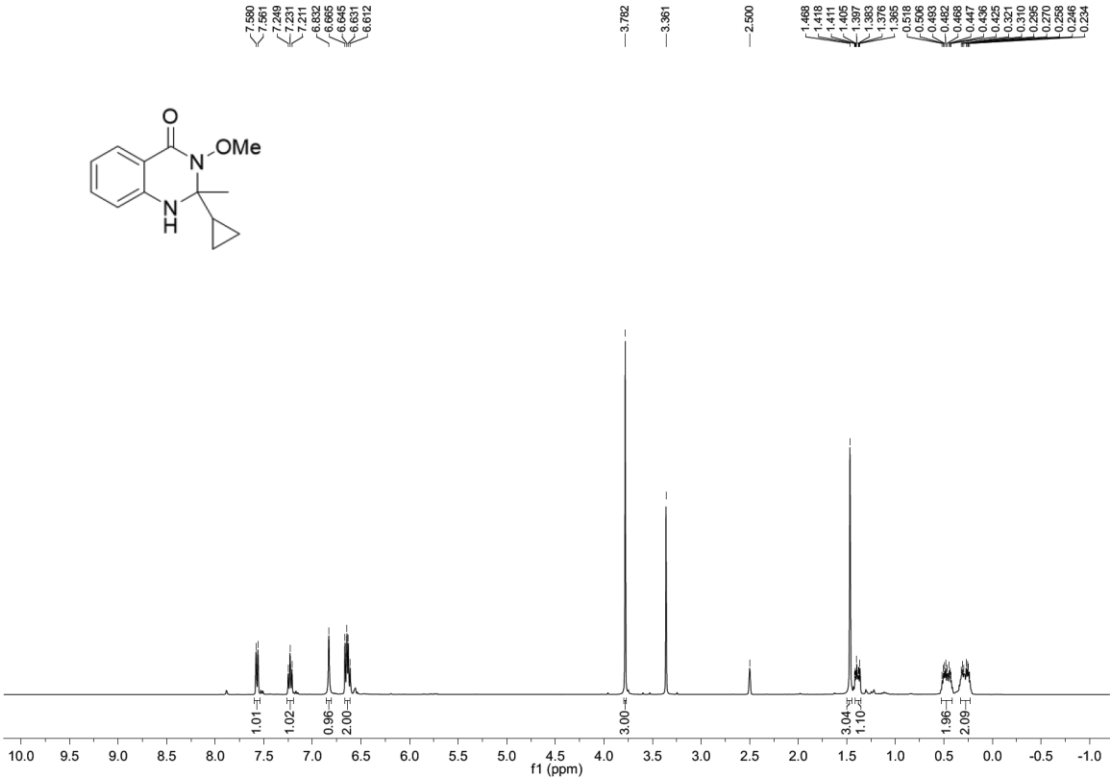
3ad-^{1}H NMR (400 MHz, DMSO-d_6)



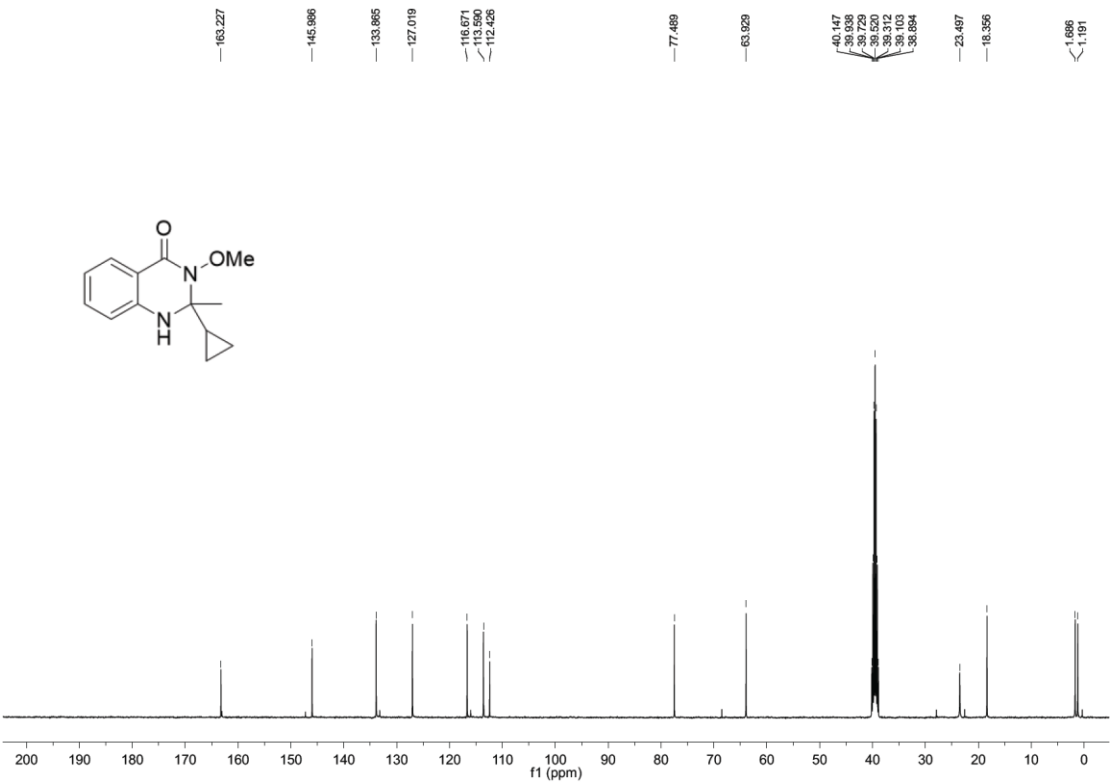
3ad-^{13}C NMR (100 MHz, DMSO-d_6)



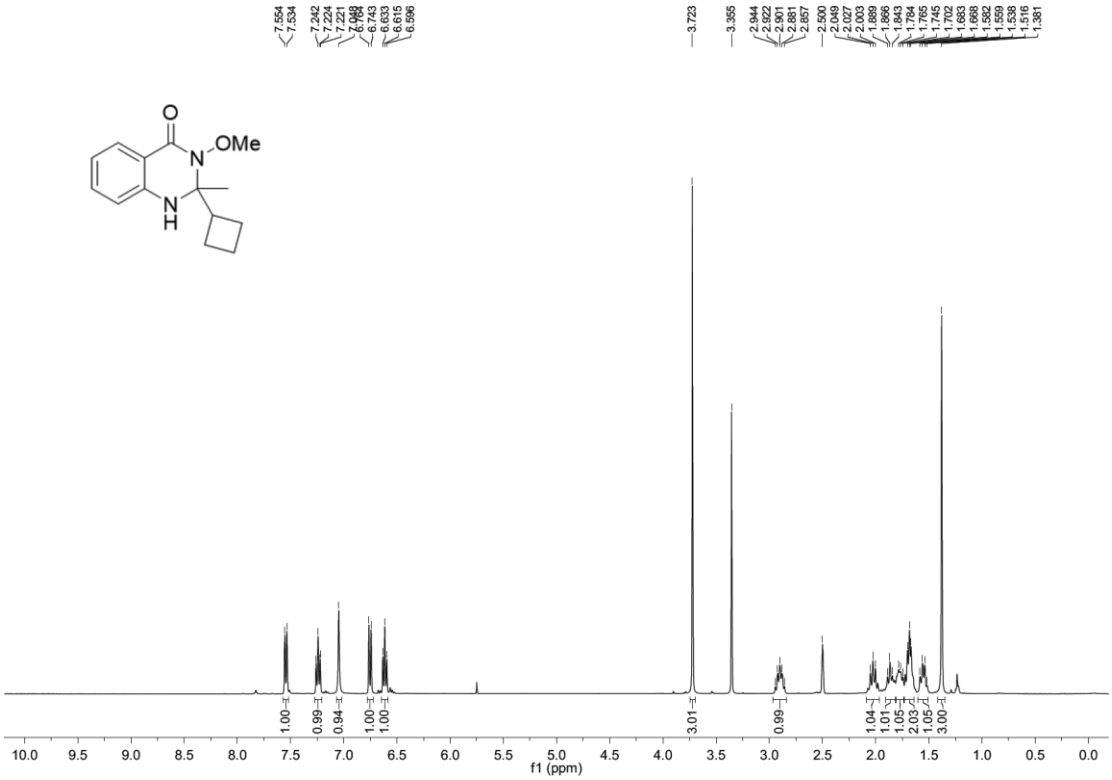
3ae-^{1}H NMR (400 MHz, DMSO-d_6)



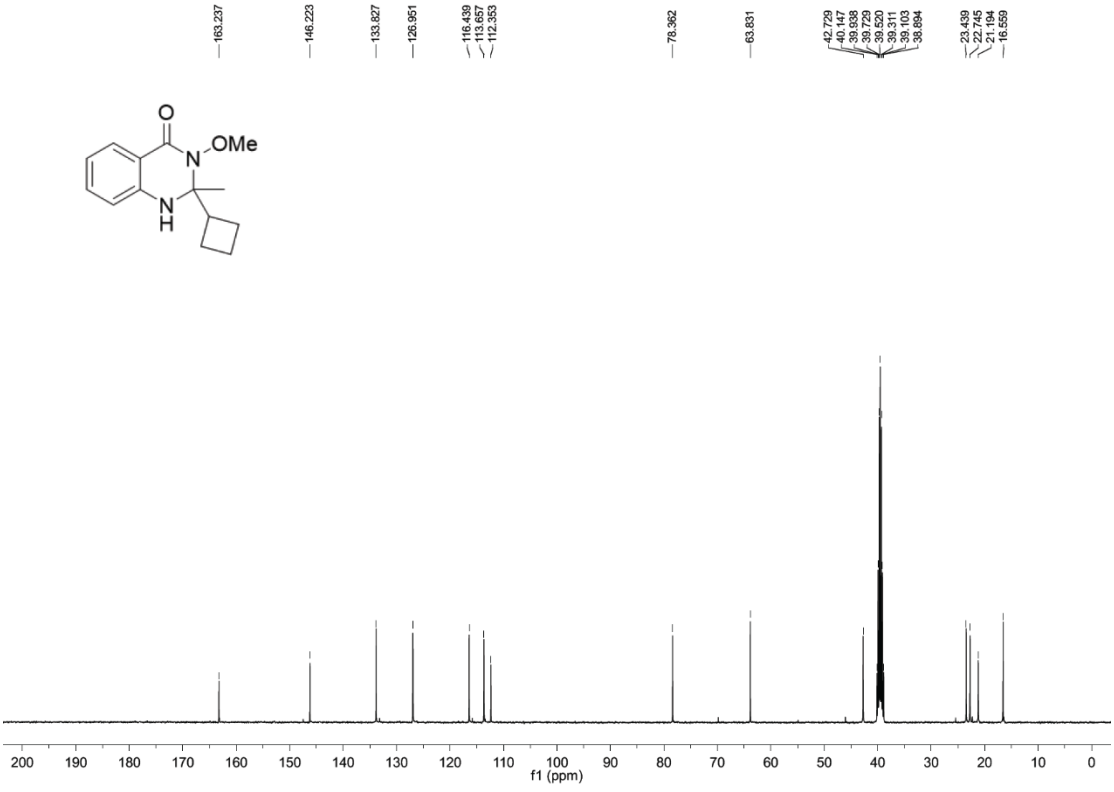
3ae-^{13}C NMR (100 MHz, DMSO-d_6)



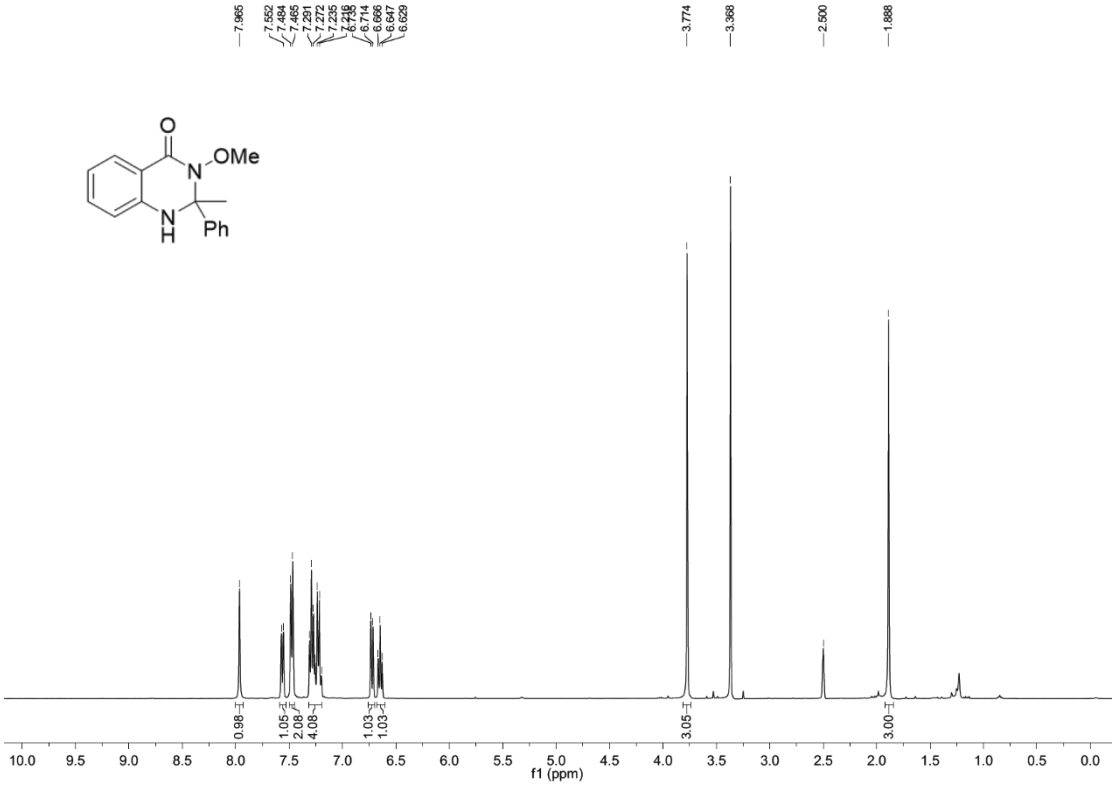
3af-^{1}H NMR (400 MHz, DMSO-d_6)



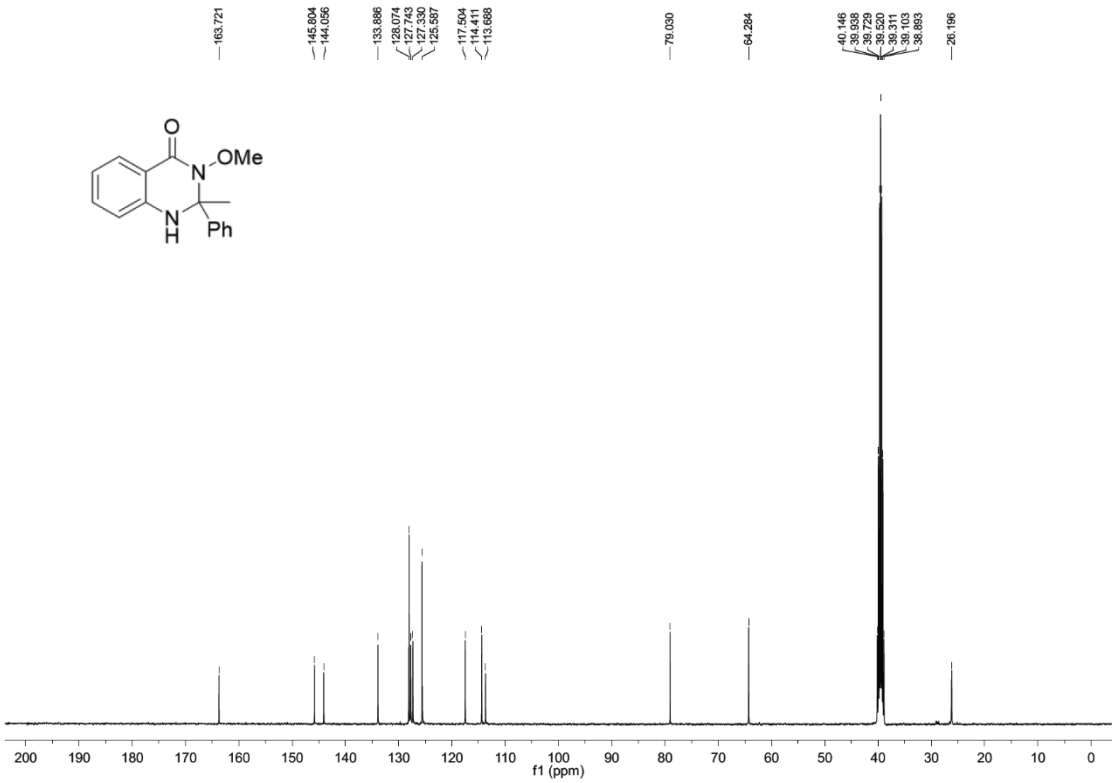
3af-^{13}C NMR (100 MHz, DMSO-d_6)



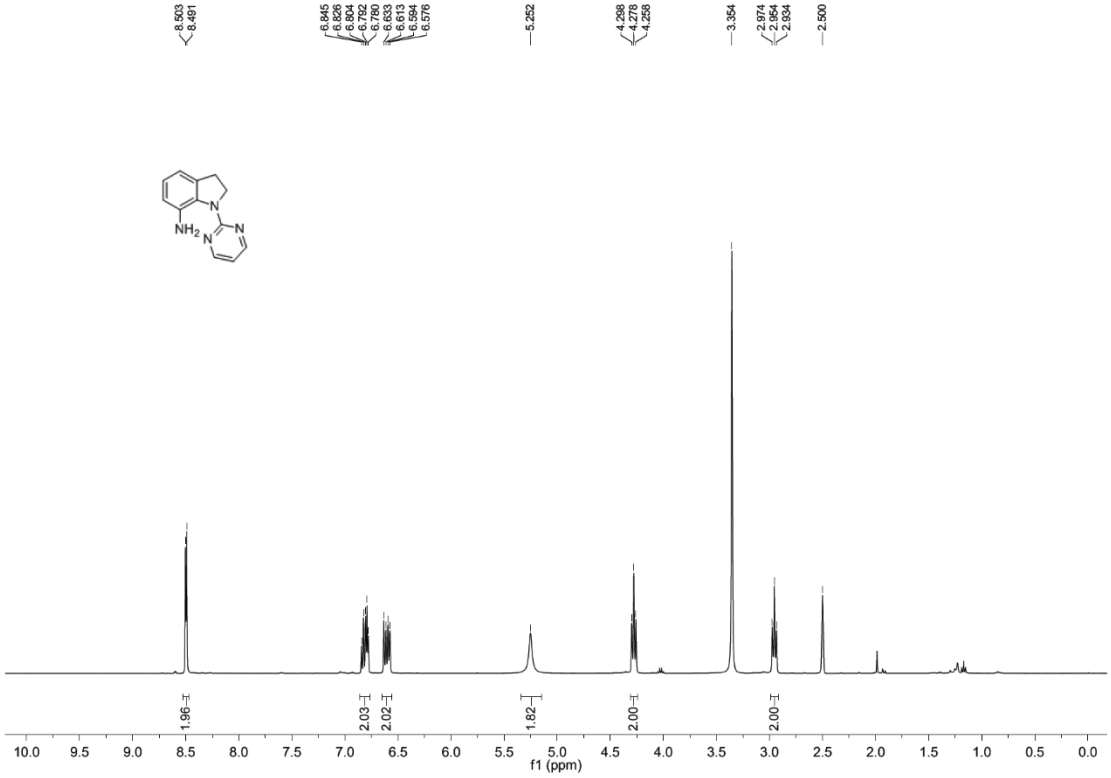
3ag-^{1}H NMR (400 MHz, DMSO-d_6)



3ag-^{13}C NMR (100 MHz, DMSO-d_6)



5-^{1}H NMR (400 MHz, DMSO-d_6)



5-^{13}C NMR (100 MHz, DMSO-d_6)