Supporting Information

Enantioselective [2+2] Cycloaddition of 1,2-Dihydroquinolines with 3-Olefinic Oxindoles *via* Brønsted Acid Catalysis

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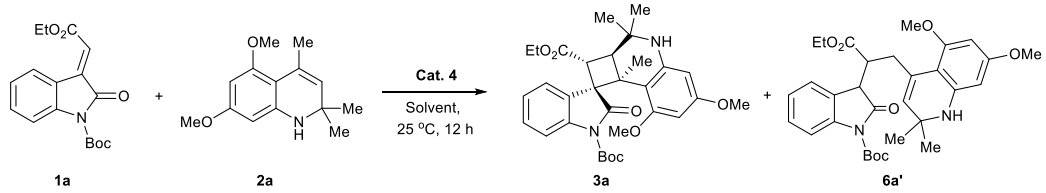
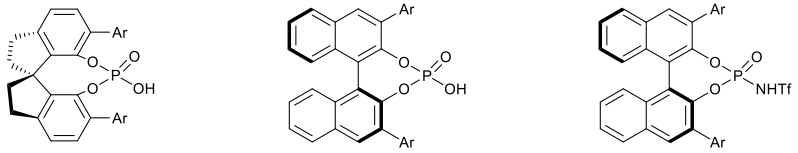
1. General Information

All the 3-ylideneoxindole **1**[1] and 1,2-dihydroquinoline **2**[2] have been synthesized following procedures reported in the literature. Other chemical reagent was obtained from commercial sources and was used without further purification. Catalytic reactions were carried out in Sealing tubes under an air atmosphere with dry solvent. The ^{1}H and ^{13}C NMR spectra were recorded on JEOL at 400 MHz for ^{1}H or at 100 MHz for ^{13}C, respectively. The chemical shifts (δ) for ^{1}H and ^{13}C are given in ppm relative to residual signals of the solvent ($CDCl_3$: δ_H = 7.26 ppm ^{1}H NMR, δ_C = 77.20 ppm ^{13}C NMR; DMSO-d_6: δ_H = 2.50 ppm ^{1}H NMR, δ_C = 39.5 ppm ^{13}C NMR). The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br s = broad singlet, dd = doublet of doublets. ESI high-resolution mass spectra were measured on Thermo-DFS mass spectrometer and Waters SYNAPT G2 (Q-TOF) instrument. The enantiomeric ratio was determined by high-performance liquid chromatography (HPLC) analysis on the chiral column in comparison with authentic racemates, using the Daicel Chiralpak AD-H/OD-H/IE/IC (250 × 4.6 mm). UV detection was monitored at 254 nm. Optical rotation data were examined in CH_2Cl_2 solution at 25 °C and λ = 589 nm. For thin layer chromatography (TLC) analysis throughout this work, Merck precoated TLC plates (silica gel 60 GF_{254}, 0.25 mm) were used, Silica gel 60 H (200-300 mesh) manufactured by Qingdao Haiyang Chemical Group Co. (China) were used for general chromatography, using UV light as the visualizing agent. Melting points were determined on a Mel-Temp apparatus.

2. Reaction optimization

Table S1. Optimization of Reaction Conditions.[a]





4a: Ar = Ph
4b: Ar = 3,5-$(CF_3)_2$Ph
4c: Ar = 2,4,6-$(iPr)_3$Ph
4d: Ar = 2-Naphthyl

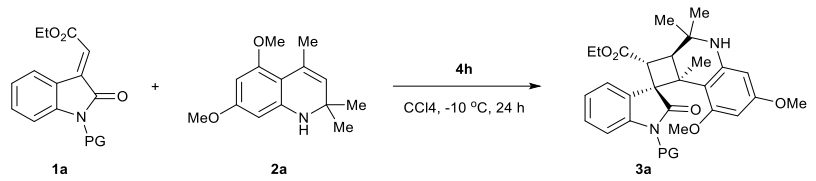
4e: Ar = Ph
4f: Ar = 3,5-$(CF_3)_2$Ph
4g: Ar = 2,4,6-$(iPr)_3$Ph

4h: Ar = Ph
4i: Ar = $SiPh_3$
4j: Ar = 3,5-$(CF_3)_2$Ph
4k: Ar = 2,4,6-$(iPr)_3$Ph

Entry	Catalyst	Solvent	yield (%)[b]		*ee* (%)[c]	
			3a	**6a'**	**3a**	**6a'**
1		CH_2Cl_2	23	20	--	--
2[d]	**CF_3SO_3H**	CH_2Cl_2	<5	33	--	--
3	**4a**	CH_2Cl_2	44	18	25	23
4	**4b**	CH_2Cl_2	29	22	5	28
5	**4c**	CH_2Cl_2	36	22	5	0
6	**4d**	CH_2Cl_2	37	14	19	14
7	**4e**	CH_2Cl_2	44	19	24	33
8	**4f**	CH_2Cl_2	24	25	27	21
9	**4g**	CH_2Cl_2	40	29	12	29
10	**4h**	CH_2Cl_2	58	32	45	26
11	**4i**	CH_2Cl_2	18	24	15	12
12	**4j**	CH_2Cl_2	36	21	11	24
13	**4k**	CH_2Cl_2	50	15	26	15
14	**4h**	DCE	76	<5	49	ND
15	**4h**	CCl_4	80	<5	65	ND
16	**4h**	Toluene	78	<5	58	ND
17[e]	**4h**	CCl_4	86	<5	90	ND
18[f]	**4h**	CCl_4	91	<5	99	ND
19[f]	--	CCl_4	17	<5	--	--

[a] Unless noted otherwise, reactions were performed with **1a** (0.05 mmol), **2a** (0.06 mmol), and **4** (5 mol%) in solvent (1 mL) at rt for 12 hours. [b] Isolated yield of **3a**. [c] Determined by chiral HPLC analysis. [d] (20 mol%) in solvent (1 mL), [e] Reaction performed at 0 °C for 14 hours. [f] Reaction performed at -10 °C for 24 hours.

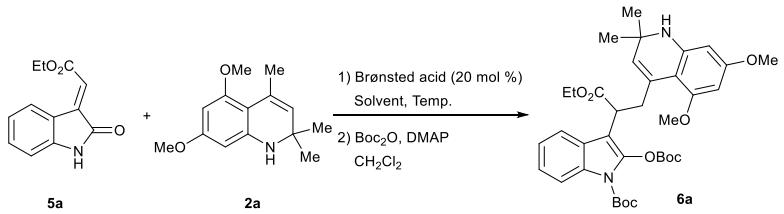
Table S2. Optimization of the reaction conditions for the *N*-PG of 3-ylideneoxindole **1**.[a]



Entry	PG	**1a**	product	yield (%)[b]	*ee* (%)[c]
1	Cbz	**1a**-Cbz	**3a**-Cbz	54	75
2	COOEt	**1a**-COOEt	**3a**-COOEt	53	67
3	H	**1a**-H	**3a**-H	NR	--
4	Me	**1a**-Me	**3a**-Me	NR	--
5	Bn	**1a**-Bn	**3a**-Bn	NR	--

[a] Unless noted otherwise, reactions were performed with **1** (0.05 mmol), **2a** (0.06 mmol), and **4h** (5 mol %) in CCl_4 (2 mL) at -10 °C for 24 hours. [b] Yield of isolated. [c] Determined by chiral HPLC analysis. NR: Not Reaction.

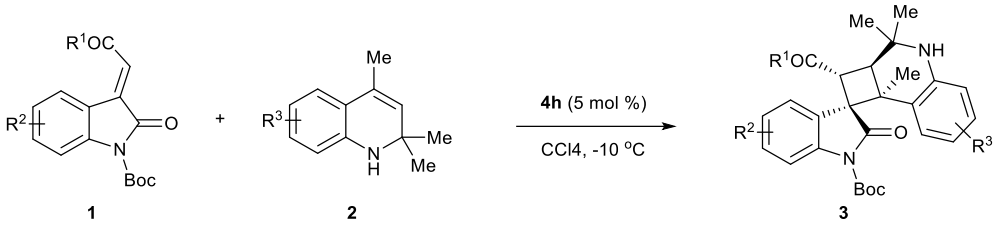
Table S3. Optimization of the ene reaction conditions.[a]



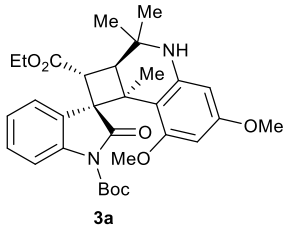
Entry	Brønsted acid	Solvent	Temp. (°C)	yield (%)[b]
1	CF_3CO_2H	Toluene	30	42%
2	CF_3SO_3H	Toluene	30	52%
3	TsOH	Toluene	30	28%
4	CF_3SO_3H	$(CH_2)_2Cl_2$	30	24%
5	CF_3SO_3H	CH_2Cl_2	30	57%
6	CF_3SO_3H	MeCN	30	43%
7	CF_3SO_3H	Acetone	30	28%
8	CF_3SO_3H	CH_2Cl_2	40	63%
9	CF_3SO_3H	CH_2Cl_2	50	60%
10[c]	CF_3SO_3H	CH_2Cl_2	40	70%
11[d]	CF_3SO_3H	CH_2Cl_2	40	76%

[a] Unless noted otherwise, reactions were performed with **5a** (0.05 mmol), **2a** (0.06 mmol), and Brønsted acid (20 mol %) in solvent (1 mL) at 30 °C for 12 hours. [b] Yield was calculated from the isolated major isomer. [c / d] Reaction was performed at 40 °C for 48 / 60 hours, respectively.

3. General Procedure for the Asymmetric Synthesis of [2+2] Cycloadducts 3



The reaction carried out with 3-ylideneoxindole **1** (0.1 mmol), 2,2,4-trimethyl-1,2-dihydroquinoline **2** (0.12 mmol) and chiral *N*-Triflyl Phosphoramides **4h** (3.2 mg, 5 mol %). The mixture was added CCl_4 (1 mL) at -10 °C and continuous stirring for 24 hours. The crude mixture was direct purified by flash chromatography on silica gel with petroleum ether/ethyl acetate to afford the desired spiro[cyclobuta[*c*] quinoline-1,3'-indolin] derivatives **3**, which were dried under vacuum and further analyzed by ^{1}H NMR, ^{13}C NMR, HRMS and HPLC.



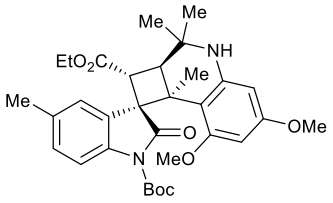
1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3a)

Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-ethoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1a** (33.1 mg, 0.1 mmol) and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydro-quinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 92% yield (50.6 mg) as white solid. The enantiomeric excess was determined to be 99% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 4.44 min, t_{major} = 9.32 min, [α]25 D = -10.00 (*c* 1.0, CH_2Cl_2), m.p. 167 – 170 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 5.80 (dd, *J* = 8.4, 2.4 Hz, 2H), 3.87 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.76 (s, 3H), 3.70 – 3.62 (m, 2H), 3.56 – 3.53 (m, 4H), 2.89 (d, *J* = 10.8 Hz, 1H), 1.60 (s, 9H), 1.35 (s, 3H), 1.27 (s, 3H), 1.19 (s, 3H), 0.63 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 171.3, 160.4, 160.1, 149.7, 144.4, 140.5, 128.2, 127.0, 125.2, 123.1, 114.6, 103.0, 92.2, 89.2, 83.6, 60.2, 57.9, 55.1, 54.7, 50.8, 48.7, 45.4, 42.3, 28.4, 27.4, 25.3, 13.8 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{31}H_{38}N_2O_7$ $[M + H]^+$ 551.2752, found 551.2755.



3b

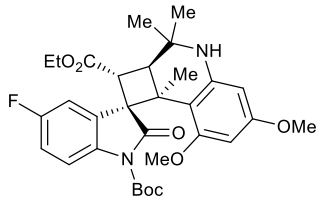
1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-6,8-dimethoxy-3,3,5',8b-tetramethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3b)

Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-ethoxy-2-oxoethylidene)-5-methyl-2-oxoindoline-1-carboxylate **1b** (33.1 mg, 0.1 mmol) and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 62% yield as white solid. The enantiomeric excess was determined to be 85% *ee* by HPLC on Chiralpak IE column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{major} = 13.72 min, t_{minor} = 19.82 min, [α]25 D = -19.00 (*c* 1.0, CH_2Cl_2), m.p. 181 – 183 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 1H), 7.25 (d, *J* = 0.4 Hz, 1H), 7.10 (dd, *J* = 8.4, 0.8 Hz, 1H), 5.80 (dd, *J* = 8.8, 2.4 Hz, 2H), 3.90 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.76 (s, 3H), 3.67 – 3.63 (m, 2H), 3.55 – 3.53 (m, 4H), 2.88 (d, *J* = 11.2 Hz, 1H), 2.38 (s, 3H), 1.59 (s, 9H), 1.36 (s, 3H), 1.28 (s, 3H), 1.19 (s, 3H), 0.62 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 171.3, 160.4, 160.0, 149.8, 144.4, 138.2, 132.6, 128.6, 127.0, 125.8, 114.4, 103.1, 92.2, 89.2, 83.3, 60.2, 57.9, 55.1, 54.6, 50.8, 48.7, 45.2, 42.2, 28.4, 27.5, 25.3, 21.3, 13.7 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{32}H_{40}N_2O_7$ $[M + H]^+$ 565.2908, found 565.2910.



3c

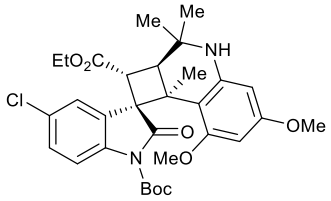
1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-5'-fluoro-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3c)

Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-ethoxy-2-oxoethylidene)-5-fluoro-2-oxoindoline-1-carboxylate **1c** (33.5 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 95% yield as white solid. The enantiomeric excess was determined to be >99% *ee* by HPLC on Chiralpak IE column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{major} = 12.40 min, $[\alpha]_D^{25}$ = -15.00 (*c* 1.0, CH_2Cl_2), m.p. 157 – 160 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 8.8, 4.8 Hz, 1H), 7.20 (dd, *J* = 8.4, 2.68 Hz, 1H), 7.00 (td, *J* = 8.8, 2.8 Hz, 1H), 5.80 (dd, *J* = 7.2, 2.0 Hz, 2H), 3.92 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.76 (s, 3H), 3.72 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.56 – 3.53 (m, 4H), 2.84 (d, *J* = 10.8 Hz, 1H), 1.59 (s, 9H), 1.37 (s, 3H), 1.27 (s, 3H), 1.19 (s, 3H), 0.71 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.23, 170.9, 160.3, 160.2, 159.0 (d, *J* = 241.9 Hz), 149.7, 144.5, 136.5, 128.8 (d, *J* = 8.0 Hz), 115.7 (d, *J* = 7.8 Hz), 114.6 (d, *J* = 22.5 Hz), 112.7 (d, *J* = 24.8 Hz), 102.7, 92.2, 89.3, 60.4, 58.1, 55.1, 54.7, 50.9, 48.7, 45.7, 42.0, 28.4, 28.3, 27.4, 25.4, 13.9 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{31}H_{37}N_2O_7F$ $[M + H]^+$ 569.2658, found 569.2662.



3d

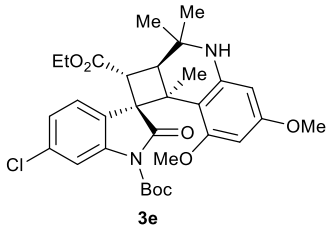
1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-5'-chloro-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3d)

Prepared according to the general procedure using *tert*-butyl (*E*)-5-chloro-3-(2-ethoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1d** (35.2 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 91% yield as white solid. The enantiomeric excess was determined to be 96% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 4.68 min, t_{major} = 7.69 min, $[\alpha]_D^{25}$ = -7.00 (*c* 1.0, CH_2Cl_2), m.p. 164 – 166 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 (d, *J* = 8.8 Hz, 1H), 7.44 (d, *J* = 2.4 Hz, 1H), 7.28 (dd, *J* = 8.8, 2.4 Hz, 1H), 5.80 (dd, *J* = 5.6, 2.4 Hz, 2H), 3.95 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.76 (s, 3H), 3.72 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.67 (br s, 1H), 3.56 – 3.53 (m, 4H), 2.85 (d, *J* = 11.2 Hz, 1H), 1.59 (s, 9H), 1.37 (s, 3H), 1.27 (s, 3H), 1.19 (s, 3H), 0.72 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 170.8, 160.3, 160.2, 149.5, 144.5, 139.0, 128.9, 128.7, 128.1, 125.2, 115.8, 102.6, 92.2, 89.3, 83.9, 60.5, 57.9, 55.1, 54.6, 50.9, 48.7, 45.6, 42.0, 28.32, 28.27, 27.3, 25.4, 13.9 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{31}H_{37}N_2O_7Cl$ $[M + H]^+$ 585.2362, found 585.2361.



3e

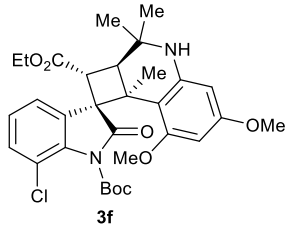
1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-6'-chloro-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3e)

Prepared according to the general procedure using *tert*-butyl (*E*)-6-chloro-3-(2-ethoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1e** (35.2 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 75% yield as white solid. The enantiomeric excess was determined to be 85% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 3.83 min, t_{major} = 5.39 min, $[\alpha]_D^{25}$ = -16.00 (*c* 1.0, CH_2Cl_2), m.p. 162 – 163 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 2.0 Hz, 1H), 7.38 (d, *J* = 8.0 Hz, 1H), 7.13 (dd, *J* = 8.4, 2.0 Hz, 1H), 5.81 (br s, 2H), 3.88 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.77 – 3.68 (m, 5H), 3.55 – 3.51 (m, 4H), 2.85 (d, *J* = 11.2 Hz, 1H), 1.60 (s, 9H), 1.33 (s, 3H), 1.26 (s, 3H), 1.18 (s, 3H), 0.72 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 171.0, 160.3, 160.2, 149.5, 144.4, 141.4, 134.0, 126.0, 125.4, 123.1, 115.4, 102.7, 92.3, 89.3, 84.1, 60.4, 57.6, 55.1, 54.7, 50.8, 48.7, 45.6, 42.1, 28.3, 27.3, 25.3, 13.9 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{31}H_{37}N_2O_7Cl$ $[M + H]^+$ 585.2362, found 585.2364.



3f

1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-7'-chloro-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3f)

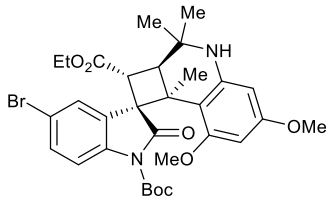
Prepared according to the general procedure using *tert*-butyl (*E*)-7-chloro-3-(2-ethoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1f** (35.2 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 62% yield as white solid. The enantiomeric excess was determined to be 76% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 3.84 min, t_{major} = 4.95 min, $[\alpha]_D^{25}$ = -7.00 (*c* 1.0, CH_2Cl_2), m.p. 151 – 154 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.07 (t, *J* = 8.0 Hz, 1H), 5.83 (d, *J* = 2.4 Hz, 1H), 5.78 (d, *J* = 2.4 Hz, 1H), 3.86 (dd, *J* = 10.4, 7.2 Hz, 1H), 3.76 (s, 3H), 3.68 –

3.62 (m, 2H), 3.60 (s, 3H), 3.50 (d, *J* = 10.8 Hz, 1H), 2.86 (d, *J* = 10.8 Hz, 1H), 1.56 (s, 9H), 1.35 (s, 3H), 1.27 (s, 3H), 1.18 (s, 3H), 0.65 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 171.0, 160.6, 160.1, 148.8, 144.2, 138.1, 130.6, 129.7, 123.7, 123.6, 118.5, 102.6, 92.1, 89.5, 84.5, 60.3, 58.3, 55.1, 55.0, 50.7, 48.6, 45.0, 43.1, 28.3, 27.9, 27.4, 25.3, 13.7 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{31}H_{37}N_2O_7Cl$ $[M + H]^+$ 585.2362, found 585.2367.



3g

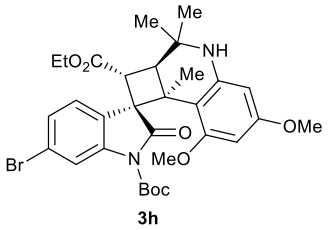
1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-5'-bromo-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3g)

Prepared according to the general procedure using *tert*-butyl (*E*)-5-bromo-3-(2-ethoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1g** (39.6 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 92% yield as white solid. The enantiomeric excess was determined to be 92% *ee* by HPLC on Chiralpak IE column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{major} = 12.68 min, t_{minor} = 18.57 min, $[\alpha]_D^{25}$ = -5.00 (*c* 1.0, CH_2Cl_2), m.p. 168 – 171 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.8 Hz, 1H), 7.57 (d, *J* = 2.0 Hz, 1H), 7.43 (dd, *J* = 8.8, 2.4 Hz, 1H), 5.80 (dd, *J* = 5.2, 2.4 Hz, 2H), 3.96 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.76 (s, 3H), 3.72 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.67 (br s, 1H), 3.55 – 3.53 (m, 4H), 2.84 (d, *J* = 11.2 Hz, 1H), 1.59 (s, 9H), 1.37 (s, 3H), 1.26 (s, 3H), 1.19 (s, 3H), 0.72 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 170.8, 160.3, 160.2, 149.5, 144.5, 139.5, 131.0, 129.3, 128.0, 116.2, 116.1, 102.5, 92.2, 89.3, 83.9, 60.5, 57.8, 55.1, 54.6, 50.9, 48.7, 45.7, 42.0, 28.32, 28.27, 27.3, 25.4, 13.9 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{31}H_{37}N_2O_7Br$ $[M + H]^+$ 629.1857, found 629.1858.



3h

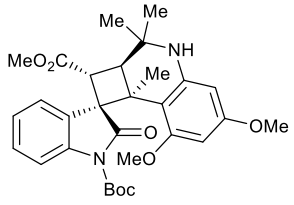
1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-6'-bromo-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3h)

Prepared according to the general procedure using *tert*-butyl (*E*)-6-bromo-3-(2-ethoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1h** (39.6 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 75% yield as white solid. The enantiomeric excess was determined to be 92% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 3.93 min, t_{major} = 5.49 min, $[\alpha]_D^{25}$ = -23.00 (*c* 1.0, CH_2Cl_2), m.p. 163 – 166 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 1.2 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.28 (dd, *J* = 8.4, 2.0 Hz, 1H), 5.81 (br s, 2H), 3.88 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.75 – 3.68 (m, 5H), 3.55 – 3.51 (m, 4H), 2.85 (d, *J* = 10.8 Hz, 1H), 1.60 (s, 9H), 1.33 (s, 3H), 1.26 (s, 3H), 1.18 (s, 3H), 0.72 (t, *J* = 7.2 Hz, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 171.0, 160.3, 160.2, 149.5, 144.4, 141.5, 126.4, 126.1, 125.9, 121.9, 118.1, 102.6, 92.3, 89.3, 84.1, 60.4, 57.6, 55.1, 54.7, 50.8, 48.7, 45.5, 42.0, 28.3, 27.3, 25.3, 13.9 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{31}H_{37}N_2O_7Br$ $[M + H]^+$ 629.1857, found 629.1861.



3i

1'-(*tert*-butyl) 2-methyl (1*S*,2*R*,2a*R*,8b*S*)-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3i)

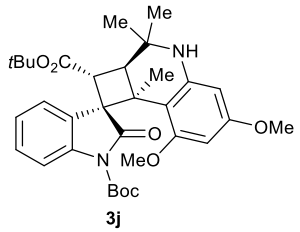
Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-methoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1i** (30.3 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 86% yield as white solid. The enantiomeric excess was determined to be 99% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 4.77 min, t_{major} = 12.91 min, $[\alpha]_D^{25}$ = -17.00 (*c* 1.0, CH_2Cl_2), m.p. 173 – 176 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.0 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 5.80 (dd, *J* = 8.0, 2.4 Hz, 2H), 3.76 (s, 3H), 3.66 (s, 1H), 3.59 (d, *J* = 11.2 Hz,

1H), 3.55 (s, 3H), 3.25 (s, 3H), 2.90 (d, *J* = 10.8 Hz, 1H), 1.60 (s, 9H), 1.34 (s, 3H), 1.27 (s, 3H), 1.18 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 171.8, 160.3, 160.1, 149.7, 144.5, 140.3, 128.2, 126.9, 125.0, 123.2, 114.7, 102.9, 92.2, 89.2, 83.5, 57.9, 55.1, 54.6, 51.5, 50.8, 48.7, 45.6, 42.0, 28.4, 28.3, 27.4, 25.3 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{30}H_{36}N_2O_7$ $[M + H]^+$ 537.2595, found 537.2600.



3j

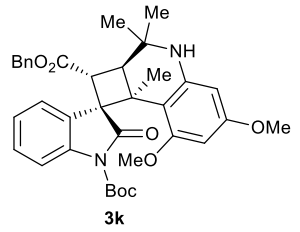
di-*tert*-butyl (1*S*,2*R*,2a*R*,8b*S*)-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3j)

Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-(*tert*-butoxy)-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1j** (34.5 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 85% yield as white solid. The enantiomeric excess was determined to be 99% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 3.29 min, t_{major} = 4.37 min, $[\alpha]_D^{25}$ = -17.00 (*c* 1.0, CH_2Cl_2), m.p. 159 – 161 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 7.2 Hz, 1H), 7.30 (t, *J* = 8.4 Hz, 1H), 7.13 (t, *J* = 7.2 Hz, 1H), 5.80 (dd, *J* = 10.0, 2.4 Hz, 2H), 3.76 (s, 3H), 3.66 (s, 1H), 3.55 (s, 3H), 3.42 (d, *J* = 10.8 Hz, 1H), 2.83 (d, *J* = 10.8 Hz, 1H), 1.58 (s, 9H), 1.38 (s, 3H), 1.27 (s, 3H), 1.20 (s, 3H), 0.94 (s, 9H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 170.3, 160.5, 160.0, 149.9, 144.2, 140.7, 128.0, 127.4, 125.6, 123.1, 114.5, 103.0, 92.1, 89.3, 83.4, 80.5, 57.8, 55.1, 54.6, 50.9, 48.6, 44.7, 43.8, 28.4, 28.3, 27.7 27.6, 25.1 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{33}H_{42}N_2O_7$ $[M + Na]^+$ 601.2884, found 601.2879.



3k

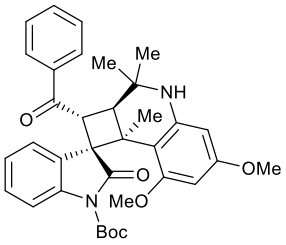
2-benzyl 1'-(*tert*-butyl) (1*S*,2*R*,2a*R*,8b*S*)-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3k)

Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-(benzyloxy)-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1k** (37.9 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 70% yield as white solid. The enantiomeric excess was determined to be 82% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 5.36 min, t_{major} = 7.35 min, $[\alpha]_D^{25}$ = -11.00 (*c* 1.0, CH_2Cl_2), m.p. 148 – 150 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.27 – 7.26 (m, 1H), 7.17 – 7.11 (m, 3H), 7.05 (td, *J* = 7.6, 1.2 Hz, 1H), 6.76 (dd, *J* = 8.0, 1.6 Hz, 2H), 5.82 (br s, 2H), 4.76 (d, *J* = 12.4 Hz, 1H), 4.69 (d, *J* = 12.4 Hz, 1H), 3.75 (s, 3H), 3.63 (d, *J* = 10.8 Hz, 1H), 3.54 (s, 3H), 2.91 (d, *J* = 10.8 Hz, 1H), 1.58 (s, 9H), 1.34 (s, 3H), 1.28 (s, 3H), 1.21 (s, 3H) ppm.

^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 171.1, 160.4, 160.1, 149.7, 140.5, 135.7, 128.4, 128.3, 127.8, 127.7, 127.4, 126.6, 125.1, 123.3, 114.7, 113.6, 92.3, 89.4, 83.4, 66.2, 57.9, 55.1, 54.6, 50.8, 48.8, 45.5, 42.3, 28.3, 27.4, 25.3, 22.8, 14.3 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{40}N_2O_7$ $[M + Na]^+$ 613.2908, found 613.2911.



3l

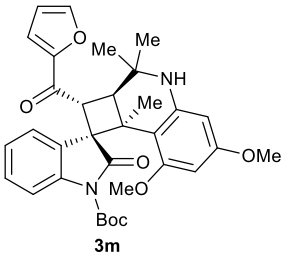
***tert*-butyl (1*S*,2*R*,2a*R*,8b*S*)-2-benzoyl-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1'-carboxylate (3l)**

Prepared according to the general procedure using *tert*-butyl (*E*)-2-oxo-3-(2-oxo-2-phenylethylidene) indoline-1-carboxylate **1l** (34.9 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 87% yield as white solid. The enantiomeric excess was determined to be 96% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 3.97 min, t_{major} = 9.92 min, $[\alpha]_D^{25}$ = -36.00 (*c* 1.0, CH_2Cl_2), m.p. 169 – 171 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 1H), 7.52 (d, *J* = 7.6 Hz, 2H), 7.43 (d, *J* = 7.6 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 7.17 – 7.12 (m, 3H), 7.07 (t, *J* = 7.6 Hz, 1H), 5.85 (s, 2H), 4.37 (d, *J* = 10.4 Hz, 1H), 3.79 (s, 3H), 3.54 (s, 3H), 3.25 (d, *J* = 10.8 Hz, 1H), 1.56 (s, 9H), 1.36 (s, 3H), 1.33 (s, 3H), 1.11 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.1, 173.2, 160.5, 160.0, 149.5, 144.6, 139.9, 135.7, 133.1, 128.4, 128.3, 127.9, 126.2, 125.8, 123.1, 114.1, 103.3, 92.1, 89.2, 83.5, 58.9, 55.1, 54.6, 49.2, 48.8, 45.6, 45.4, 28.4, 28.3, 27.5, 25.2 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{35}H_{38}N_2O_7$ $[M + H]^+$ 599.2752, found 599.2750.



3m

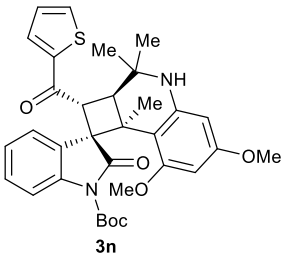
***tert*-butyl (1*S*,2*R*,2a*R*,8b*S*)-2-(furan-2-carbonyl)-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1'-carboxylate (3m)**

Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-(furan-2-yl)-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1m** (33.9 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 86% yield as white solid. The enantiomeric excess was determined to be 98% *ee* by HPLC on Chiralpak AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 4.82 min, t_{major} = 18.56 min, $[\alpha]_D^{25}$ = -48.00 (*c* 1.0, CH_2Cl_2), m.p. 176 – 179 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.47 (d, *J* = 7.6 Hz, 1H), 7.28 (d, *J* = 1.2 Hz, 1H), 7.18 (t, *J* = 8.0 Hz, 1H), 7.07 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 3.6 Hz, 1H), 6.24 (dd, *J* = 3.6, 1.6 Hz, 1H), 5.82 (dd, *J* = 8.0, 2.4 Hz, 2H), 4.12 (d, *J* = 10.4 Hz, 1H), 3.76 (s, 3H), 3.54 (s, 3H), 3.21 (d, *J* = 10.8 Hz, 1H), 1.58 (s, 9H), 1.33 (s, 3H), 1.29 (s, 3H), 1.08 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 185.5, 173.3, 160.5, 160.1, 151.6, 149.7, 146.8, 144.6, 140.0, 128.0, 126.4, 125.8, 123.3, 118.4, 114.2, 112.2, 103.3, 92.2, 89.3, 83.6, 59.2, 55.1, 54.7, 48.8, 48.5, 46.2, 45.4, 28.4, 28.3, 27.5, 25.2 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{33}H_{36}N_2O_7$ $[M + H]^+$ 573.2595, found 573.2599.



3n

***tert*-butyl (1*S*,2*R*,2a*R*,8b*S*)-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2-(thiophene-2-carbonyl)-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1'-carboxylate (3n)**

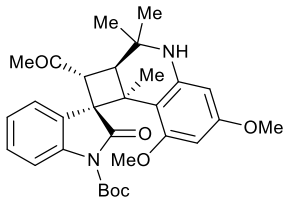
Prepared according to the general procedure using *tert*-butyl (*E*)-2-oxo-3-(2-oxo-2-(thiophen-2-yl)ethylidene)indoline-1-carboxylate **1n** (35.5 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 82% yield as white solid. The enantiomeric excess was determined to be 97% *ee* by HPLC on Chiralpak

AD-H column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 4.19 min, t_{major} = 13.50 min, $[\alpha]_D^{25}$ = -43.00 (*c* 1.0, CH_2Cl_2), m.p. 181 – 184 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 7.2 Hz, 1H), 7.43 – 7.41 (m, 2H), 7.20 (t, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 7.6 Hz, 1H), 6.85 (dd, *J* = 4.8, 4.0 Hz, 1H), 5.84 (dd, *J* = 6.4, 2.4 Hz, 2H), 4.28 (d, *J* = 10.4 Hz, 1H), 3.78 (s, 3H), 3.56 (s, 3H), 3.26 (d, *J* = 10.4 Hz, 1H), 1.58 (s, 9H), 1.35 (s, 3H), 1.31 (s, 3H), 1.09 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 173.5, 160.5, 160.1, 149.5, 144.7, 143.4, 140.0, 134.2, 132.9, 128.2, 128.0, 126.5, 125.8, 123.3, 114.3, 103.3, 92.3, 89.3, 83.6, 59.5, 55.1, 54.7, 48.8, 46.1, 45.7, 28.3, 27.5, 25.3 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{33}H_{36}N_2O_6S$ $[M + H]^+$ 589.2367, found 589.2371.



3o

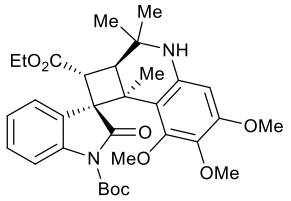
***tert*-butyl (1*S*,2*R*,2a*R*,8b*S*)-2-acetyl-6,8-dimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1'-carboxylate (3o)**

Prepared according to the general procedure using *tert*-butyl (*E*)-2-oxo-3-(2-oxopropylidene)indoline-1-carboxylate **1o** (28.7 mg, 0.1 mmol), and 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol). The title compound was isolated by column chromatography in 60% yield as white solid. The enantiomeric excess was determined to be 79% *ee* by HPLC on Chiralpak IE column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{minor} = 10.96 min, t_{major} = 12.37 min, $[\alpha]_D^{25}$ = -4.00 (*c* 1.0, CH_2Cl_2), m.p. 140 – 143 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 1H), 7.31 (t, *J* = 7.6 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 5.82 (d, *J* = 2.2 Hz, 1H), 5.80 (d, *J* = 1.6 Hz, 1H), 3.76 (s, 3H), 3.65 – 3.62 (m, 2H), 3.56 (s, 3H), 2.92 (d, *J* = 10.4 Hz, 1H), 1.61 (s, 9H), 1.49 (s, 3H), 1.31 (s, 3H), 1.26 (s, 3H), 1.10 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.7, 173.1, 160.4, 160.1, 149.6, 144.7, 140.1, 128.4, 126.1, 125.7, 123.5, 114.8, 103.0, 92.2, 89.2, 83.8, 58.2, 55.1, 54.7, 49.8, 49.1, 48.7, 45.7, 28.4, 28.32, 28.27, 27.7, 25.1 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{30}H_{36}N_2O_6$ $[M + H]^+$ 521.2646, found 521.2647.



3p

1'-(*tert*-butyl) 2-ethyl (1*S*,2*R*,2a*R*,8b*S*)-6,7,8-trimethoxy-3,3,8b-trimethyl-2'-oxo-2a,3,4,8b-tetrahydro-2*H*-spiro[cyclobuta[*c*]quinoline-1,3'-indoline]-1',2-dicarboxylate (3p)

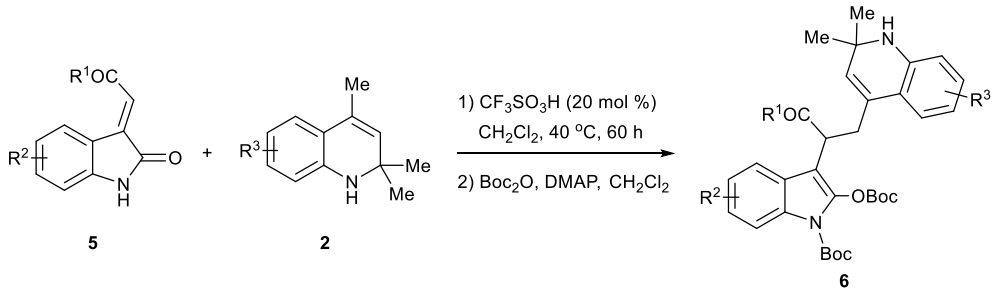
Prepared according to the general procedure using *tert*-butyl (*E*)-3-(2-ethoxy-2-oxoethylidene)-2-oxoindoline-1-carboxylate **1a** (31.7 mg, 0.1 mmol), and 5,6,7-trimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2b** (31.6 mg, 0.12 mmol). The title compound was isolated by column chromatography in 76% yield as white solid. The enantiomeric excess was determined to be 95% *ee* by HPLC on Chiralpak IC column (20% 2-propanol/*n*-hexane, 1 mL/min), UV 254 nm, t_{major} = 7.43 min, t_{minor} = 13.10 min, $[\alpha]_D^{25}$ = -10.00 (*c* 1.0, CH_2Cl_2), m.p. 164 – 167 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 7. 6 Hz, 1H), 7.29 (t, *J* = 8.0 Hz, 1H), 7.12 (t, *J* = 7.6, 1H), 5.88 (s, 1H), 3.84 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.80 (s, 3H), 3.73 (s, 3H), 3.72 (s, 3H), 3.64 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.53 (d, *J* = 11.2 Hz, 1H), 2.86 (d, *J* = 10.8 Hz, 1H), 1.56 (s, 9H), 1.33 (s, 3H), 1.24 (s, 3H), 1.16 (s, 3H), 0.62 (t, *J* = 7.2 Hz, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 171.2, 153.3, 149.9, 140.8, 139.4, 133.8, 128.2, 126.9, 125.1, 123.1, 115.0, 107.4, 93.7, 83.4, 60.8, 60.2, 59.8, 58.3, 55.7, 51.5, 48.6, 45.7, 42.1, 28.3, 28.0, 27.4, 26.7, 13.8 ppm.

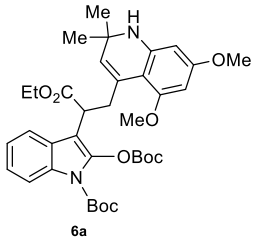
HRMS (ESI – TOF): *m*/*z* calcd for $C_{32}H_{40}N_2O_8$ $[M + H]^+$ 581.2857, found 581.2861.

4. General Procedure for the Synthesis of ene Reaction Products 6



The reaction carried out with 3-ylideneoxindole **5** (0.1 mmol), 2,2,4-trimethyl-1,2-dihydroquinoline **2** (0.12 mmol) and CF_3SO_3H (1.8 μL, 3 mg, 20 mol %). The mixture was added CH_2Cl_2 (2 mL) at 40 °C and continuous stirring for 60 hours. The crude mixture was direct purified by preparative TLC to afford the intermediate.

The protection NH group of the intermediate gave the corresponding easily separable oxindole fused quinoline derivative **6**. To a solution of intermediate in CH_2Cl_2 (2 mL) was added DMAP (2.2 equiv) and di-tert-butyl decarbonate (Boc_2O, 2.5 equiv). The mixture was purified by preparative TLC to give the only major product **6**, which were dried under vacuum and further analyzed by ^1H NMR, ^{13}C NMR and HRMS.



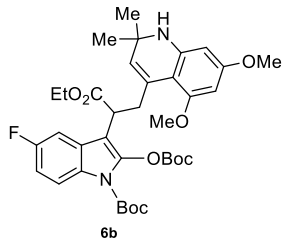
tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-ethoxy-1-oxopropan-2-yl)-1H-indole-1-carboxylate **(6a)**

Prepared according to the general procedure using ethyl (*E*)-2-(2-oxoindolin-3-ylidene)acetate **5a** (21.7 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 77% yield (50.1 mg) as white foam for two steps, m.p. 74 – 76 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 5.85 (d, *J* = 2.0 Hz, 1H), 5.69 (d, *J* = 2.0 Hz, 1H), 5.01 (s, 1H), 4.12 – 4.02 (m, 3H), 3.75 (s, 3H), 3.68 (s, 3H), 3.63 (br s, 1H), 3.48 (dd, *J* = 13.2, 8.0 Hz, 1H), 2.98 (dd, *J* = 13.2, 6.4 Hz, 1H), 1.65 (s, 9H), 1.55 (s, 9H), 1.16 (t, *J* = 7.2 Hz, 3H), 1.13 (s, 3H), 0.95 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 160.5, 158.2, 150.4, 149.1, 146.9, 139.0, 132.1, 129.6, 128.5, 126.9, 123.9, 122.9, 120.5, 115.2, 107.0, 103.1, 91.9, 89.0, 84.6, 84.3, 60.6, 55.3, 55.2, 50.9, 41.4, 37.1, 30.3, 29.7, 28.4, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{46}N_2O_9$ $[M + H]^+$ 651.3276, found 651.3278.



6b

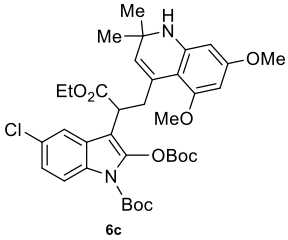
tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-ethoxy-1-oxopropan-2-yl)-5-fluoro-1H-indole-1-carboxylate **(6b)**

Prepared according to the general procedure using ethyl (*E*)-2-(5-fluoro-2-oxoindolin-3-ylidene)-acetate **5b** (23.5 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 72% yield (48.3 mg) as white foam for two steps, m.p. 80 – 83 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 9.2, 4.8 Hz, 1H), 7.26 – 7.23 (m, 1H), 6.95 (td, *J* = 9.2, 2.8 Hz, 1H), 5.85 (d, *J* = 2.3 Hz, 1H), 5.69 (d, *J* = 2.0 Hz, 1H), 4.98 (s, 1H), 4.14 – 4.00 (m, 3H), 3.75 (s, 3H), 3.70 (s, 3H), 3.64 (br s, 1H), 3.47 (dd, *J* = 13.2, 7.6 Hz, 1H), 2.92 (dd, *J* = 13.2, 7.2 Hz, 1H), 1.64 (s, 9H), 1.55 (s, 9H), 1.18 (t, *J* = 7.2 Hz, 3H), 1.13 (s, 3H), 0.94 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 160.6, 159.3 (d, *J* = 238.6 Hz), 158.1, 150.3, 148.8, 146.9, 139.9, 129.5, 128.6, 128.3, 127.9 (d, *J* = 10.3 Hz), 116.3 (d, *J* = 8.9 Hz), 111.6 (d, *J* = 24.8 Hz), 107.0 (d, *J* = 3.6 Hz), 106.32 (d, *J* = 24.7 Hz), 102.9, 91.9, 89.0, 84.8, 84.6, 60.8, 55.3, 55.2, 50.8, 41.3, 37.1, 30.1, 29.6, 28.3, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{45}N_2O_9F$ $[M + H]^+$ 669.3182, found 669.3184.



6c

tert-butyl 2-((tert-butoxycarbonyl)oxy)-5-chloro-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-ethoxy-1-oxopropan-2-yl)-1H-indole-1-carboxylate **(6c)**

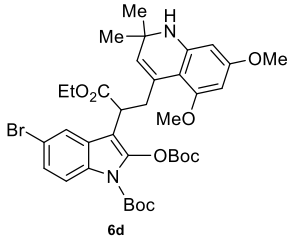
Prepared according to the general procedure using ethyl (*E*)-2-(5-chloro-2-oxoindolin-3-ylidene)-acetate **5c** (25.2 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 73% yield (49.8 mg) as white foam for two steps, m.p. 79 – 81 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.8 Hz, 1H), 7.46 (s, 1H), 7.18 (dd, *J* = 8.8, 2.0 Hz, 1H), 5.86 (d, *J* = 2.0 Hz, 1H), 5.69 (d, *J* = 2.4 Hz, 1H), 4.96 (s, 1H), 4.15 – 4.03 (m, 2H), 3.99 (t, *J* = 7.2 Hz, 1H),

3.76 (s, 3H), 3.71 (s, 3H), 3.63 (br s, 1H), 3.51 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.87 (dd, *J* = 13.2, 7.2 Hz, 1H), 1.64 (s, 9H), 1.55 (s, 9H), 1.18 (t, *J* = 7.2 Hz, 3H), 1.12 (s, 3H), 0.93 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 160.6, 158.1, 150.3, 148.7, 146.9, 139.6, 130.3, 129.5, 128.6, 128.5, 128.2, 124.1, 120.1, 116.3, 106.8, 102.8, 92.0, 89.0, 84.9, 84.8, 60.8, 55.3, 55.2, 50.8, 41.1, 37.3, 30.0, 29.7, 28.3, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{45}N_2O_9Cl$ $[M + H]^+$ 685.2886, found 685.2886.



6d

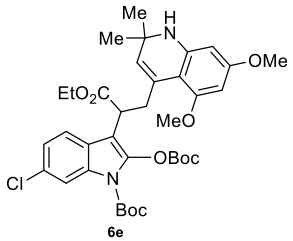
***tert-butyl 5-bromo-2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-ethoxy-1-oxopropan-2-yl)-1H-indole-1-carboxylate* (6d)**

Prepared according to the general procedure using ethyl (*E*)-2-(5-bromo-2-oxoindolin-3-ylidene)-acetate **5d** (29.6 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 70% yield (51.0 mg) as white foam for two steps, m.p. 74 – 76 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.8 Hz, 1H), 7.58 (d, *J* = 1.2 Hz, 1H), 7.32 (dd, *J* = 8.8, 2.0 Hz, 1H), 5.86 (d, *J* = 2.0 Hz, 1H), 5.70 (d, *J* = 2.0 Hz, 1H), 4.96 (s, 1H), 4.15 – 4.03 (m, 2H), 3.97 (t, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 3.71 (s, 3H), 3.63 (br s, 1H), 3.52 (dd, *J* = 13.2, 7.2 Hz, 1H), 2.86 (dd, *J* = 13.2, 7.2 Hz, 1H), 1.64 (s, 9H), 1.55 (s, 9H), 1.18 (t, *J* = 7.2 Hz, 3H), 1.12 (s, 3H), 0.92 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 160.6, 158.1, 150.3, 148.7, 146.9, 139.4, 130.7, 129.5, 128.8, 128.6, 126.8, 123.0, 116.7, 116.3, 106.7, 102.8, 92.1, 89.0, 84.9, 84.8, 60.8, 55.3, 55.2, 50.8, 41.0, 37.3, 30.0, 29.7, 28.3, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{45}N_2O_9Br$ $[M + H]^+$ 729.2381, found 729.2375.



6e

***tert-butyl 2-((tert-butoxycarbonyl)oxy)-6-chloro-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-methoxy-1-oxopropan-2-yl)-1H-indole-1-carboxylate* (6e)**

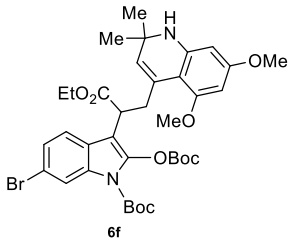
Prepared according to the general procedure using ethyl (*E*)-2-(6-chloro-2-oxoindolin-3-ylidene)-acetate **5e** (25.2 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and

CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 66% yield (45.2 mg) as white foam for two steps, m.p. 75 – 78 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 2.0 Hz, 1H), 7.50 (d, *J* = 8.8 Hz, 1H), 7.15 (dd, *J* = 8.8, 2.0 Hz, 1H), 5.84 (d, *J* = 2.4 Hz, 1H), 5.68 (d, *J* = 2.0 Hz, 1H), 4.97 (s, 1H), 4.13 – 4.02 (m, 3H), 3.75 (s, 3H), 3.69 (s, 3H), 3.63 (br s, 1H), 3.46 (dd, *J* = 13.2, 7.6 Hz, 1H), 2.93 (dd, *J* = 12.8, 6.8 Hz, 1H), 1.65 (s, 9H), 1.55 (s, 9H), 1.16 (t, *J* = 7.2 Hz, 3H), 1.13 (s, 3H), 0.94 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 160.6, 158.1, 150.3, 148.7, 146.9, 139.2, 132.3, 129.8, 129.4, 128.6, 125.4, 123.3, 121.3, 115.6, 106.9, 102.9, 91.9, 89.0, 84.9, 84.8, 60.8, 55.3, 55.2, 50.8, 41.2, 37.1, 30.2, 23.0, 28.3, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{45}N_2O_9Cl$ $[M + H]^+$ 685.2886, found 685.2878.



6f

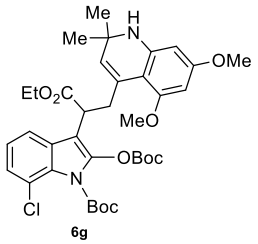
tert-butyl 6-bromo-3-(1-(tert-butoxy)-3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-oxopropan-2-yl)-2-((tert-butoxycarbonyl)oxy)-1H-indole-1-carboxylate **(6f)**

Prepared according to the general procedure using ethyl (*E*)-2-(6-bromo-2-oxoindolin-3-ylidene)-acetate **5f** (29.6 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 60% yield (43.8 mg) as white foam for two steps, m.p. 78 – 81 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20 (d, *J* = 1.6 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, 1H), 7.29 (dd, *J* = 8.8, 2.0 Hz, 1H), 5.84 (d, *J* = 2.4 Hz, 1H), 5.68 (d, *J* = 2.4 Hz, 1H), 4.97 (s, 1H), 4.12 – 4.02 (m, 3H), 3.75 (s, 3H), 3.68 (s, 3H), 3.63 (br s, 1H), 3.46 (dd, *J* = 13.2, 7.6 Hz, 1H), 2.92 (dd, *J* = 13.2, 6.8 Hz, 1H), 1.65 (s, 9H), 1.54 (s, 9H), 1.16 (t, *J* = 7.2 Hz, 3H), 1.13 (s, 3H), 0.94 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 160.6, 158.1, 150.2, 148.7, 146.9, 139.1, 132.7, 129.4, 128.6, 126.0, 125.8, 121.7, 118.4, 117.5, 106.9, 102.9, 91.9, 89.0, 85.0, 84.9, 60.8, 55.3, 55.2, 50.9, 41.2, 37.1, 30.2, 29.7, 28.3, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{45}N_2O_9Br$ $[M + H]^+$ 729.2381, found 729.2388.



6g

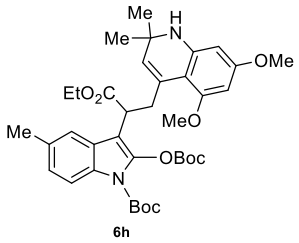
***tert-butyl 3-(1-(benzyloxy)-3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-oxopropan-2-yl)-2-((tert-butoxycarbonyl)oxy)-7-chloro-1H-indole-1-carboxylate* (6g)**

Prepared according to the general procedure using ethyl (*E*)-2-(7-chloro-2-oxoindolin-3-ylidene)-acetate **5g** (25.2 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 66% yield (44.9 mg) as white foam for two steps, m.p. 69 – 72 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.6 Hz, 1H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.08 (t, *J* = 8.0 Hz, 1H), 5.84 (d, *J* = 2.4 Hz, 1H), 5.67 (d, *J* = 2.4 Hz, 1H), 4.93 (s, 1H), 4.14 – 4.03 (m, 3H), 3.75 (s, 3H), 3.70 (s, 3H), 3.45 (dd, *J* = 12.8, 7.2 Hz, 1H), 2.91 (dd, *J* = 13.2, 7.6 Hz, 1H), 1.60 (s, 9H), 1.55 (s, 9H), 1.18 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 3H), 0.87 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 160.5, 158.1, 150.3, 148.0, 146.9, 140.2, 130.5, 129.3, 129.1, 128.7, 125.3, 123.4, 119.9, 119.1, 105.3, 103.0, 91.9, 88.9, 85.1, 84.9, 60.7, 55.3, 55.2, 50.8, 41.3, 37.2, 30.2, 29.5, 27.9, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{45}N_2O_9Cl$ $[M + H]^+$ 685.2886, found 685.2890.



6h

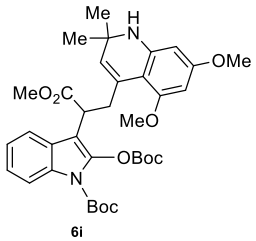
***tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-ethoxy-1-oxopropan-2-yl)-5-methyl-1H-indole-1-carboxylate* (6h)**

Prepared according to the general procedure using ethyl (*E*)-2-(5-methyl-2-oxoindolin-3-ylidene)-acetate **5h** (23.1 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 60% yield (39.8 mg) as white foam for two steps, m.p. 75 – 77 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.4 Hz, 1H), 7.35 (s, 1H), 7.05 (d, *J* = 8.4 Hz, 1H), 5.86 (s, 1H), 5.70 (s, 1H), 5.01 (s, 1H), 4.14 – 4.02 (m, 3H), 3.76 (s, 3H), 3.69 (s, 3H), 3.52 (dd, *J* = 13.2, 7.6 Hz, 1H), 2.94 (dd, *J* = 13.2, 6.8 Hz, 1H), 2.38 (s, 3H), 1.64 (s, 9H), 1.55 (s, 9H), 1.17 (t, *J* = 7.2 Hz, 3H), 1.13 (s, 3H), 0.96 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 160.5, 158.2, 150.4, 149.1, 146.9, 138.8, 132.2, 130.1, 129.7, 128.5, 127.0, 125.2, 120.4, 114.9, 106.8, 103.0, 91.9, 88.9, 84.5, 84.1, 60.6, 55.3, 55.2, 50.9, 41.2, 37.2, 30.2, 29.7, 28.4, 27.8, 21.6, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{37}H_{48}N_2O_9$ $[M + H]^+$ 665.3433, found 665.3432.



6i

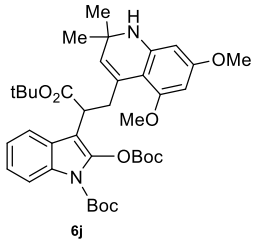
***tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-methoxy-1-oxopropan-2-yl)-1H-indole-1-carboxylate* (6i)**

Prepared according to the general procedure using methyl (*E*)-3-(2-formamidophenyl)acrylate **5i** (20.3 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 71% yield (45.3 mg) as white foam for two steps, m.p. 87 – 90 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.56 (d, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 5.84 (d, *J* = 2.0 Hz, 1H), 5.68 (d, *J* = 2.0 Hz, 1H), 4.99 (s, 1H), 4.14 (t, *J* = 7.2 Hz, 1H), 3.75 (s, 3H), 3.67 (s, 3H), 3.63 (br s, 1H), 3.60 (s, 3H), 3.49 (dd, *J* = 13.2, 7.8 Hz, 1H), 2.98 (dd, *J* = 13.2, 6.8 Hz, 1H), 1.65 (s, 9H), 1.55 (s, 9H), 1.13 (s, 3H), 0.93 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 160.5, 158.2, 150.4, 149.1, 146.9, 139.0, 132.0, 129.5, 128.6, 126.9, 124.0, 122.9, 120.2, 115.3, 106.8, 103.0, 92.0, 89.0, 84.6, 84.4, 55.4, 55.2, 51.9, 50.9, 41.0, 37.0, 30.3, 29.6, 28.4, 27.8 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{35}H_{44}N_2O_9$ $[M + H]^+$ 637.3120, found 637.3123.



6j

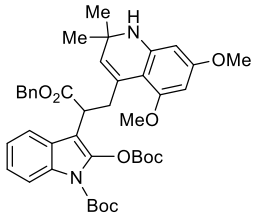
***tert-butyl 3-(1-(tert-butoxy)-3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-oxopropan-2-yl)-2-((tert-butoxycarbonyl)oxy)-1H-indole-1-carboxylate* (6j)**

Prepared according to the general procedure using *tert*-butyl (*E*)-2-(2-oxoindolin-3-ylidene)acetate **5j** (24.5 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 68% yield (46.2 mg) as white foam for two steps, m.p. 80 – 83 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.4 Hz, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.26 – 7.22 (m, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 5.84 (d, *J* = 2.0 Hz, 1H), 5.69 (d, *J* = 2.0 Hz, 1H), 5.06 (s, 1H), 3.99 (dd, *J* = 8.4, 6.0 Hz, 1H), 3.75 (s, 3H), 3.67 (s, 4H), 3.45 (dd, *J* = 13.2, 8.4 Hz, 1H), 2.95 (dd, *J* = 13.2, 6.0 Hz, 1H), 1.65 (s, 9H), 1.55 (s, 9H), 1.35 (s, 9H), 1.16 (s, 3H), 0.98 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 160.4, 158.2, 150.5, 149.1, 146.9, 138.9, 132.1, 129.8, 128.4, 126.9, 123.8, 122.7, 120.8, 115.2, 107.4, 103.2, 91.9, 88.9, 84.4, 84.2, 80.5, 55.3, 55.2, 50.9, 42.3, 37.0, 30.3, 29.6, 28.4, 28.2, 27.8 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{38}H_{50}N_2O_9$ $[M + H]^+$ 679.3589, found 679.3592.



6k

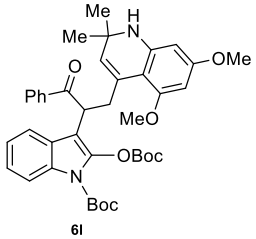
tert-butyl 3-(1-(benzyloxy)-3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-oxopropan-2-yl)-2-((tert-butoxycarbonyl)oxy)-1H-indole-1-carboxylate **(6k)**

Prepared according to the general procedure using benzyl (*E*)-2-(2-oxoindolin-3-ylidene)acetate **5k** (27.9 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 62% yield (44.3 mg) as white foam for two steps, m.p. 73 – 75 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.27 – 7.23 (m, 6H), 7.18 (t, *J* = 7.6 Hz, 1H), 5.83 (d, *J* = 1.6 Hz, 1H), 5.69 (d, *J* = 2.0 Hz, 1H), 5.17 (d, *J* = 12.4 Hz, 1H), 4.98 (d, *J* = 12.4 Hz, 2H), 4.18 (t, *J* = 7.2 Hz, 1H), 3.76 (s, 3H), 3.61 (s, 4H), 3.52 (dd, *J* = 13.2, 8.0 Hz, 1H), 3.01 (dd, *J* = 12.8, 6.4 Hz, 1H), 1.67 (s, 9H), 1.51 (s, 9H), 1.10 (s, 3H), 0.94 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.9, 160.5, 158.2, 150.4, 149.1, 146.9, 139.1, 136.4, 132.1, 129.5, 128.6, 128.4, 128.3, 128.0, 126.8, 124.0, 122.9, 120.5, 115.2, 106.7, 103.0, 91.9, 88.9, 84.6, 84.3, 66.5, 55.3, 55.2, 50.8, 41.4, 37.1, 30.2, 29.5, 28.4, 27.7 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{41}H_{48}N_2O_9$ $[M + H]^+$ 713.3433, found 713.3432.



6l

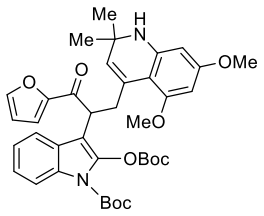
tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-oxo-1-phenylpropan-2-yl)-1H-indole-1-carboxylate **(6l)**

Prepared according to the general procedure using (*E*)-3-(2-oxo-2-phenylethylidene)indolin-2-one **5l** (24.9 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 73% yield (49.6 mg) as white foam for two steps, m.p. 108 – 110 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 2H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 5.83 (d, *J* = 2.0 Hz, 1H), 5.67 (d, *J* = 2.0 Hz, 1H), 5.03 (dd, *J* = 8.0, 5.2 Hz, 1H), 4.84 (s, 1H), 3.76 (s, 3H), 3.68 (dd, *J* = 13.2, 5.2 Hz, 1H), 3.58 (br s, 4H), 2.89 (dd, *J* = 13.2, 8.0 Hz, 1H), 1.62 (s, 9H), 1.52 (s, 9H), 1.01 (s, 3H), 0.78 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 199.4, 160.5, 158.2, 150.2, 149.0, 147.0, 139.1, 137.4, 132.6, 132.1, 129.6, 128.5, 128.5, 126.9, 124.0, 123.0, 120.1, 115.2, 107.0, 103.3, 91.9, 88.9, 84.7, 84.4, 55.4, 55.2, 50.8, 42.7, 37.1, 30.2, 29.6, 28.3, 27.8 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{40}H_{46}N_2O_8$ $[M + H]^+$ 683.3327, found 683.3332.



6m

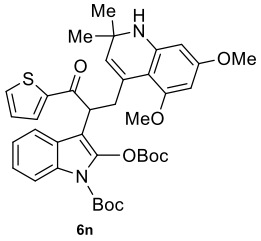
tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-(furan-2-yl)-1-oxopropan-2-yl)-1H-indole-1-carboxylate **(6m)**

Prepared according to the general procedure using (*E*)-3-(2-(furan-2-yl)-2-oxoethylidene)indolin-2-one **5m** (23.9 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 54% yield (36.4 mg) as white foam for two steps, m.p. 143 – 145 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.42 (d, *J* = 1.2 Hz, 1H), 7.25 – 7.16 (m, 2H), 7.03 (d, *J* = 3.6 Hz, 1H), 6.34 (dd, *J* = 3.6, 1.6 Hz, 1H), 5.83 (d, *J* = 2.0 Hz, 1H), 5.66 (d, *J* = 2.0 Hz, 1H), 4.89 (s, 1H), 4.83 (t, *J* = 6.8 Hz, 1H), 3.75 (s, 3H), 3.65 – 3.61 (m, 5H), 2.94 (dd, *J* = 13.2, 7.2 Hz, 1H), 1.63 (s, 9H), 1.53 (s, 9H), 1.01 (s, 3H), 0.87 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 187.8, 160.4, 158.1, 152.6, 150.3, 149.0, 147.0, 146.4, 139.2, 132.1, 129.5, 128.6, 126.8, 124.0, 123.0, 120.4, 117.6, 115.2, 112.1, 106.9, 103.2, 91.9, 89.0, 84.7, 84.4, 55.4, 55.2, 50.8, 43.1, 36.2, 30.0, 29.6, 28.3, 27.8 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{38}H_{44}N_2O_9$ $[M + H]^+$ 673.3120, found 673.3117.



6n

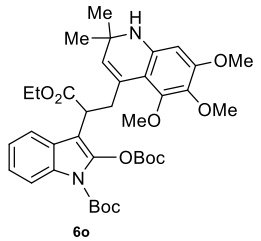
tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(5,7-dimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-oxo-1-(thiophen-2-yl)propan-2-yl)-1H-indole-1-carboxylate **(6n)**

Prepared according to the general procedure using (*E*)-3-(2-oxo-2-(thiophen-2-yl)ethylidene)indolin-2-one **5n** (25.5 mg, 0.1 mmol), 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (28.0 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 58% yield (39.7 mg) as white foam for two steps, m.p. 111 – 114 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 1H), 7.65 (d, *J* = 7.6 Hz, 1H), 7.55 (d, *J* = 3.6 Hz, 1H), 7.47 (d, *J* = 5.2 Hz, 1H), 7.26 – 7.23 (m, 1H), 7.18 (t, *J* = 7.6 Hz, 1H), 6.92 (t, *J* = 4.4 Hz, 1H), 5.84 (d, *J* = 2.0 Hz, 1H), 5.65 (d, *J* = 2.0 Hz, 1H), 4.92 (t, *J* = 6.8 Hz, 1H), 4.88 (s, 1H), 3.75 (s, 3H), 3.67 – 3.61 (m, 4H), 3.57 (br s, 1H), 2.96 (dd, *J* = 13.2, 7.6 Hz, 1H), 1.63 (s, 9H), 1.52 (s, 9H), 0.98 (s, 3H), 0.84 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 192.3, 160.5, 158.2, 150.2, 149.0, 147.0, 144.8, 139.2, 133.3, 132.1, 132.0, 129.4, 128.7, 128.1, 126.8, 124.0, 123.1, 120.4, 115.3, 107.1, 103.1, 91.9, 88.9, 84.8, 84.5, 55.4, 55.2, 50.8, 44.1, 36.9, 30.0, 29.6, 28.4, 27.8 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{38}H_{44}N_2O_8S$ $[M + H]^+$ 689.2891, found 689.2891.



6o

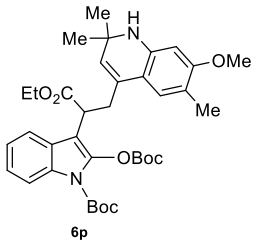
tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(1-ethoxy-1-oxo-3-(5,6,7-trimethoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)propan-2-yl)-1H-indole-1-carboxylate **(6o)**

Prepared according to the general procedure using ethyl (*E*)-2-(2-oxoindolin-3-ylidene)acetate **5a** (21.7 mg, 0.1 mmol), 5,6,7-trimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2b** (31.6 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 44% yield (30.0 mg) as white foam for two steps, m.p. 71 – 73 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 7.6 Hz, 1H), 7.23 (t, *J* = 8.4 Hz, 1H), 7.16 (t, *J* = 7.6 Hz, 1H), 5.81 (s, 1H), 5.05 (s, 1H), 4.19 (t, *J* = 7.6 Hz, 1H), 4.16 – 4.00 (m, 2H), 3.81 (s, 3H), 3.789 (s, 3H), 3.785 (s, 3H) 3.44 (dd, *J* = 13.2, 7.6 Hz, 1H), 2.89 (dd, *J* = 13.6, 7.6 Hz, 1H), 1.65 (s, 9H), 1.55 (s, 9H), 1.16 (t, *J* = 7.2 Hz, 3H), 1.11 (s, 3H), 0.88 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 153.4, 151.7, 150.5, 149.1, 141.5, 139.1, 134.4, 132.0, 130.1, 129.2, 126.9, 123.9, 122.8, 120.3, 115.3, 107.0, 106.7, 93.8, 84.6, 84.3, 61.3, 61.3, 60.7, 55.9, 50.9, 40.7, 36.2, 30.1, 29.3, 28.4, 27.8, 14.4 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{37}H_{48}N_2O_{10}$ $[M + H]^+$ 681.3382, found 681.3379.



6p

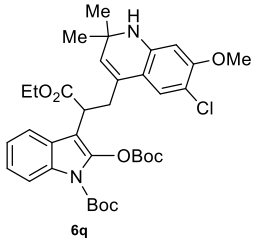
***tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(1-ethoxy-3-(7-methoxy-2,2,6-trimethyl-1,2-dihydroquinolin-4-yl)-1-oxopropan-2-yl)-1H-indole-1-carboxylate* (6p)**

Prepared according to the general procedure using ethyl (*E*)-2-(2-oxoindolin-3-ylidene)acetate **5a** (21.7 mg, 0.1 mmol), 7-methoxy-2,2,4,6-tetramethyl-1,2-dihydroquinoline **2f** (26.1 mg, 0.12 mmol) and CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 57% yield (36.2 mg) as white foam for two steps, m.p. 82 – 83 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 7.2 Hz, 1H), 7.30 – 7.26 (m, 1H), 7.22 (t, *J* = 7.2 Hz, 1H), 6.87 (s, 1H), 5.98 (s, 1H), 5.15 (s, 1H), 4.18 – 4.04 (m, 3H), 3.76 (s, 3H), 3.53 (br s, 1H), 3.38 (dd, *J* = 14.4, 9.2 Hz, 1H), 2.74 (dd, *J* = 14.4, 5.6 Hz, 1H), 2.09 (s, 3H), 1.66 (s, 9H), 1.56 (s, 9H), 1.19 – 1.16 (m, 6H), 1.06 (s, 3H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 158.1, 150.4, 149.0, 143.1, 139.0, 132.1, 129.5, 126.9, 126.4, 125.5, 124.2, 123.0, 120.1, 115.4, 114.9, 112.7, 106.5, 96.5, 84.8, 84.5, 61.0, 55.4, 51.9, 40.2, 33.2, 31.0, 30.6, 28.4, 27.8, 15.7, 14.3 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{36}H_{46}N_2O_8$ $[M + H]^+$ 635.3327, found 635.3325.



6q

***tert-butyl 2-((tert-butoxycarbonyl)oxy)-3-(3-(6-chloro-7-methoxy-2,2-dimethyl-1,2-dihydroquinolin-4-yl)-1-ethoxy-1-oxopropan-2-yl)-1H-indole-1-carboxylate* (6q)**

Prepared according to the general procedure using ethyl (*E*)-2-(2-oxoindolin-3-ylidene)acetate **5a** (21.7 mg, 0.1 mmol), 6-chloro-7-methoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2g** (28.5 mg, 0.12 mmol) and

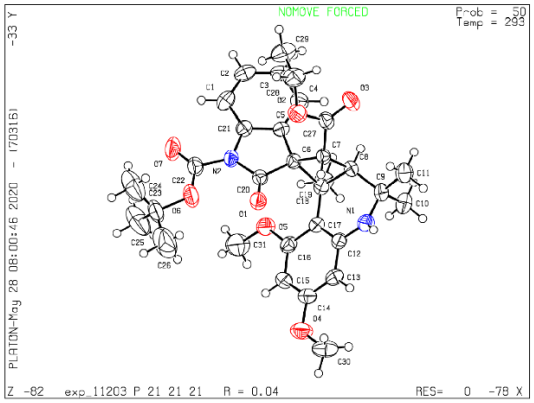
CF_3SO_3H (1.8 μL, 3.0 mg, 20 mol %). The title compound was isolated by preparative TLC in 43% yield (28.4 mg) as white foam for two steps, m.p. 75 – 77 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 7.6 Hz, 1H), 7.29 – 7.19 (m, 2H), 7.08 (s, 1H), 6.01 (s, 1H), 5.10 (s, 1H), 4.16 – 4.03 (m, 3H), 3.82 (br s, 3H), 3.63 (s, 1H), 3.30 (dd, *J* = 14.8, 8.4 Hz, 1H), 2.73 (dd, *J* = 14.8, 7.2 Hz, 1H), 1.65 (s, 9H), 1.56 (s, 9H), 1.21 – 1.17 (m, 6H), 0.96 (s, 3H) ppm.

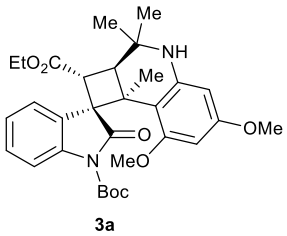
^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 155.0, 150.3, 149.0, 143.7, 139.2, 132.1, 128.5, 128.0, 126.4, 124.7, 124.2, 123.1, 119.9, 115.4, 114.0, 109.8, 106.1, 97.6, 84.9, 84.6, 61.2, 56.1, 52.1, 40.0, 32.9, 31.2, 30.7, 28.4, 27.8, 14.3 ppm.

HRMS (ESI – TOF): *m*/*z* calcd for $C_{35}H_{43}N_2O_9Cl$ $[M + H]^+$ 655.2781, found 655.2780.

5. Crystal Data of 3a



≡

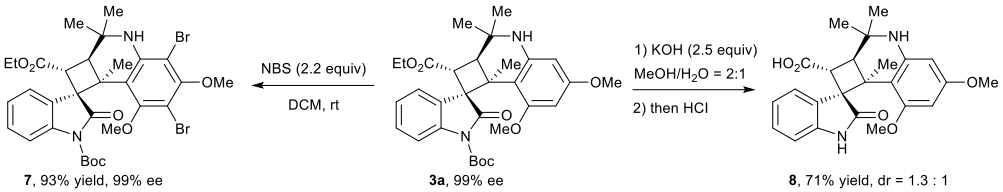


3a

Table S3. Crystal data and structure refinement for **3a**

Empirical formula	$C_{31}H_{38}N_2O_7$
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	11.0073(4)
b/Å	13.7688(6)
c/Å	20.0723(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3042.1(2)
Z	4
ρ_{calc}g/cm^3	1.202
μ/mm^{-1}	0.695
F(000)	1176.0
Crystal size/mm^3	0.120 × 0.110 × 0.110
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.786 to 134.49
Index ranges	-12 ≤ h ≤ 13, -16 ≤ k ≤ 16, -24 ≤ l ≤ 14
Reflections collected	7222
Independent reflections	4791 [R_{int} = 0.0273, R_{sigma} = 0.0497]
Data/restraints/parameters	4791/1356/371
Goodness-of-fit on F^2	1.028
Final R indexes [I>=2σ (I)]	R_1 = 0.0442, wR_2 = 0.1040
Final R indexes [all data]	R_1 = 0.0542, wR_2 = 0.1119
Largest diff. peak/hole / e Å^{-3}	0.20/-0.20
Flack parameter	0.14(15)

6. Product Derivatization

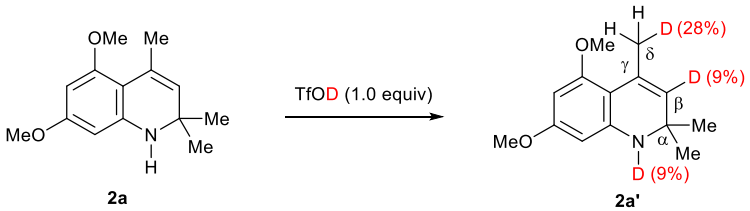


To a solution of **3a** (20.0 mg, 99% *ee*) and NBS (14.2 mg, 2.2 equiv) in CH_2Cl_2 (2 mL) was stirred at room temperature for 30 min. The crude mixture was direct purified by flash chromatography on silica gel with petroleum ether/ethyl acetate to afford the product **7** (23.9 mg, 93% yield, 99% *ee*). The enantiomeric excess was determined by HPLC on Chiralpak OD-H column (5% 2-propanol/*n*-hexane, 1 mL/min, 30 °C), UV 254 nm, t_{major} = 4.13 min, t_{minor} = 4.73 min. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 1H), 7.44 (d, *J* = 7.2 Hz, 1H), 7.33 (t, *J* = 8.0 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 4.63 (s, 1H), 3.89 – 3.82 (m, 4H), 3.72 (s, 3H), 3.67 (dd, *J* = 10.8, 7.2 Hz, 1H), 3.48 (d, *J* = 11.2 Hz, 1H), 2.96 (d, *J* = 11.2 Hz, 1H), 1.62 (s, 9H), 1.39 (s, 3H), 1.28 (s, 3H), 1.25 (s, 3H), 0.64 (t, *J* = 7.1 Hz, 3H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ 172.2, 170.7, 157.8, 154.2, 150.0, 140.9, 128.6, 126.1, 124.9, 123.3, 115.2, 114.7, 100.6, 98.8, 83.6, 61.4, 60.6, 60.4, 58.5, 52.3, 49.0, 45.7, 41.7, 28.23, 28.18, 28.0, 27.0, 13.7 ppm. **HRMS (ESI – TOF)**: *m*/*z* calcd for $C_{31}H_{36}N_2O_7Br_2$ $[M + Na]^+$ 729.0781, found 729.0777.

A solution of the **3a** (20.0 mg) in MeOH (2 mL) was added KOH (2.5 equiv) in H_2O (1 mL) at 65 °C, and continuous stirring overnight. The crude mixture was acidified to pH = 2 with 1 M HCl, extracted with CH_2Cl_2, washed with brine, dried over anhydrous Na_2SO_4, and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (CH_2Cl_2 : MeOH = 10 :1) to afford the product **8** (10.9 mg, 71% yield) with dr = 1.3 : 1, which was determined by integration of ^{1}H NMR signal: δ_{major} 10.13 (s), δ_{minor} 9.96 (s) ppm. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 11.85 (s, 1H), 10.13 (s, 1H *major*), 9.96 (s, 1H, *minor*), 7.42 (d, *J* = 7.6 Hz, 1H, *minor*), 7.14 (t, *J* = 7.6 Hz, 1H, *minor*), 6.98 (t, *J* = 7.6 Hz, 1 H, *major*), 6.90 (t, *J* = 7.6 Hz, 1H, *minor*), 6.79 (d, *J* = 7.6 Hz, 1H, *minor*), 6.71 (d, *J* = 7.6 Hz, 1H, *major*), 6.55 (t, *J* = 7.6 Hz, 1H, *major*), 5.95 (d, *J* = 2.0 Hz, 1H, *major*), 5.83 (d, *J* = 2.4 Hz, 1H, *minor*), 5.74 (d , *J* = 7.6 Hz, 1H, *major*), 5.68 (d, *J* = 2.4 Hz, 1H, *minor*), 5.64 (s, 1H, *major*), 5.54 (s, 1H, *minor*), 5.50 (d, *J* = 2.0 Hz, 1H, *major*), 3.663 (s, 3H, *minor*), 3.660 (s, 3H, *major*), 3.44 (s, 3H, *minor*), 3.06 (d, J = 11.2 Hz, 1H, *minor*), 2.91 (d, J = 10.4 Hz, 1H, *major*), 2.76 (d, J = 10.0 Hz, 2H), 2.70 (s, 3H, *major*), 1.56 (s, 3 H, *major*), 1.23 (s, 3H, *minor*), 1.14 (s, 3H, *minor*), 1.11 (s, 3H, *major*), 1.09 (s, 3H, *major*), 1.05 (s, 3H, *minor*) ppm. 6.98 (t, J = 7.6 Hz, 1H), 6.71 (d, *J* = 7.6 Hz, 1H), 6.55 (t, *J* = 7.6 Hz, 1H), 5.95 (d, *J* = 2.0 Hz, 1H), 5.74 (d, *J* = 7.6 Hz, 1H), 5.64 (s, 1H), 5.50 (d, *J* = 2.0 Hz, 1H), 3.66 (s, 3H), 2.91 (d, *J* = 10.4 Hz, 1H), 2.76 (d, *J* = 10.0 Hz, 1H), 2.70 (s, 3H), 1.56 (s, 3H), 1.11 (s, 3H), 1.09 (s, 3H) ppm. **^{13}C NMR** (100 MHz, DMSO-d_6) δ 178.5, 173.1, 160.5, 159.2, 145.2, 142.5, 131.5, 126.9, 122.6, 119.9, 107.9, 103.4, 91.7, 88.4,

58.6, 54.6, 54.5, 50.1, 49.7, 47.7, 42.5, 41.5, 26.9, 26.8, 24.6 ppm. **HRMS (ESI – TOF)**: *m*/*z* calcd for $C_{24}H_{26}N_2O_5$ $[M + H]^+$ 423.1914, found 423.1909.

7. Deuterium Exchange Experiments



The reaction carried out 5,7-dimethoxy-2,2,4-trimethyl-1,2-dihydroquinoline **2a** (0.2 mmol) and CF_3SO_3D (1.0 equiv). The mixture was added CH_2Cl_2 (1 mL) at rt and continuous stirring for 12 hours. The crude mixture was direct purified by preparative TLC to afford the deuterium product **2a'**, which was dried under vacuum and deuterium incorporation ratio was determined by ^{1}H NMR spectroscopy using DMSO-d_6 as a solvent.

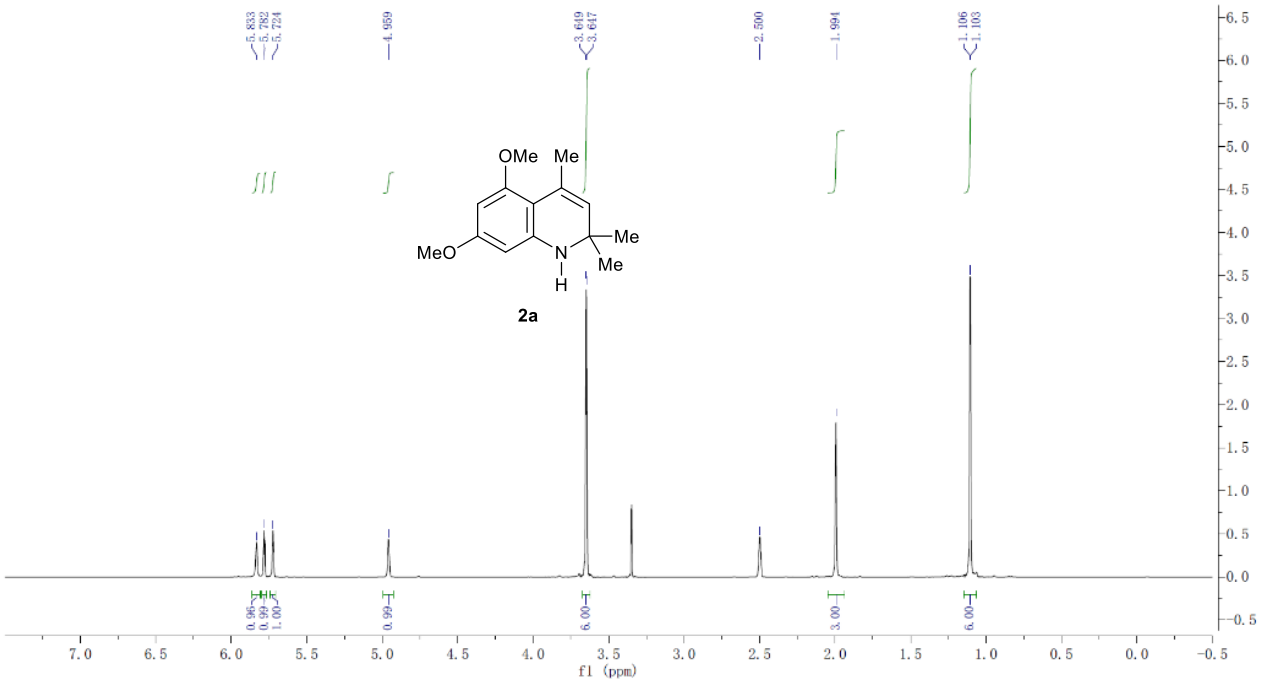


Figure S1. ^{1}H NMR of **2a** in DMSO-d_6.

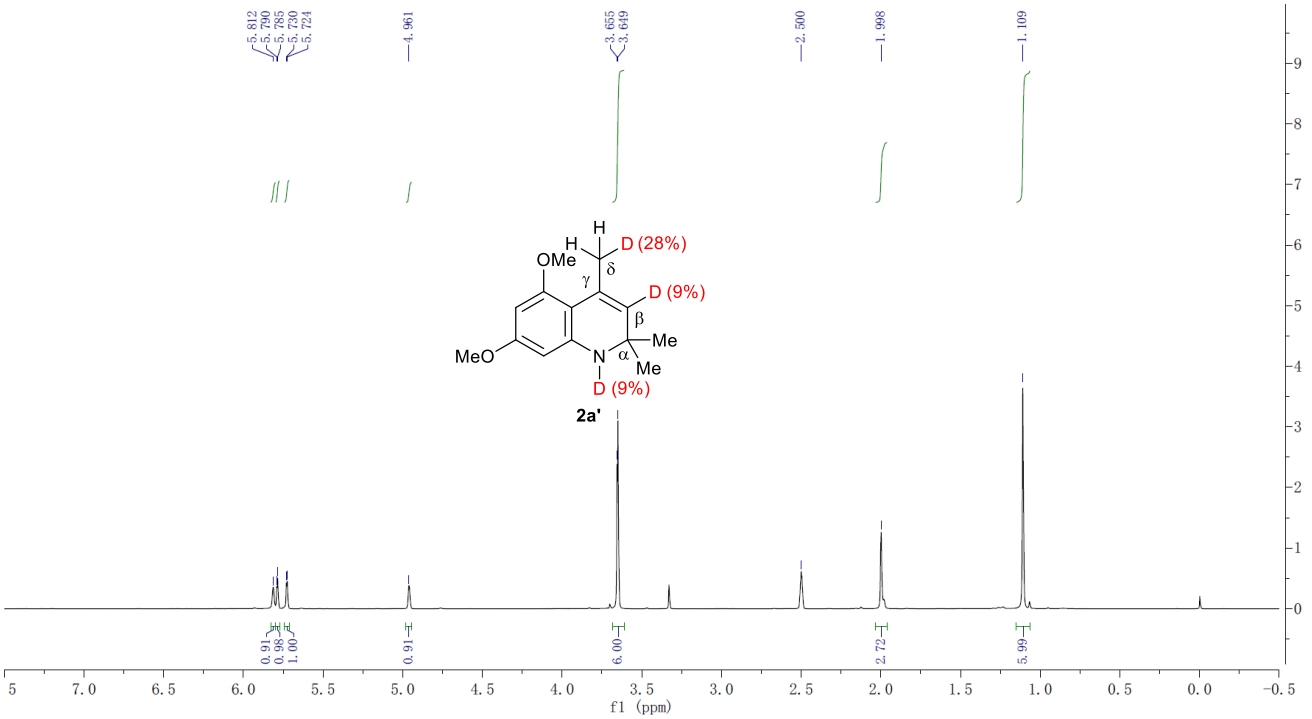


Figure S2. ^{1}H NMR of 2a' after deuterium exchange experiment in DMSO-d_6.

8. Computational Mechanistic Studies

8.1 Computational method

All computations were performed by Gaussian 09 software packages.[3] All optimized geometrics and single-point energies were computed on the dispersion corrected hybrid functional B3LYP[4] /6-31G(d) level. In the calculation level, the dispersion corrected hybrid functional B3LYP was demonstrated as a suitable functional for describe the wreak interactions. Besides, for the single-point energies, the high precision computing level B3LYP-D3/6-311G++(d,p) functional/basis set[5] was applied to all atoms. The optimized structures or transition structures were confirmed by normal vibrational mode analysis. The feature of the optimized structures was no imaginary frequency but transition structure had only one imaginary frequency. Transition structures were also verified by intrinsic reaction coordinate (IRC) calculations.

To estimate the solvent effects, the polarization continuum model (PCM)[6] was applied in this work and the dielectric constant (eps) of CCl_4 was set as 2.23[7]. All energetics reported throughout the article are in kcal/mol, and the bond length unit is angstroms (Å), structures were generated by GaussView 6[8] and CYL view[9].

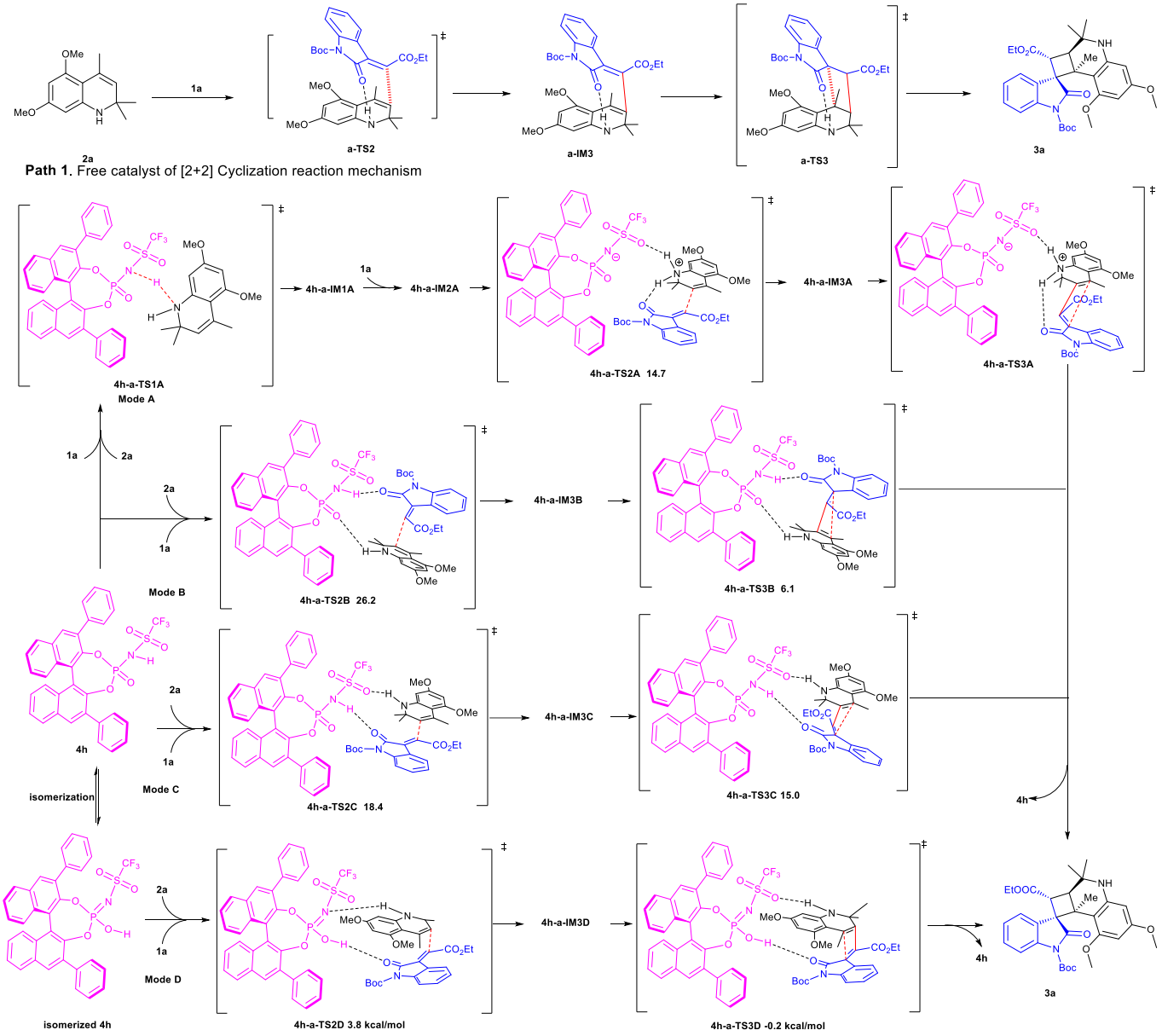
8.2 Reaction Mechanism

The experimental results indicated that the substrate **1a** and **2a** could directly reaction and form the [2+2] cycloaddition reaction products **3a** with free-catalyst/**4h** condition or form the products **6a'** with **TfOH**. The reaction process could be controlled by Brønsted acid. If weak acid **4h** as catalyst, the [2+2] cycloaddition product **3a** was the main product (Table S1, Entry 1). In contrast, when strong acid **TfOH** as catalyst, the ene reaction product **6a'**, as the only product could be obtained (Table S1, Entry 2). Hence, the whole reaction mechanism under the catalysis of **4h/TfOH** was unveiled, the reaction mechanism under free catalyst condition was also discussed.

8.3 The reaction mechanism [2+2] cycloaddition

Firstly, we discussed the [2+2] cyclizaiton reaction. Whole reaction process was shown in **Scheme S1**. Product **3a** could be obtained under the free-catalyst condition or **4h** as the catalyst. According to Woodward-Hoffmann rules[10] the substrate **1a** and **2a** should experience a stepwise process to obtain product **3a**. The whole reaction mechanism under free catalyst condition was given in **Scheme S1** (**path 1)**. Besides, the [2+2] cycloaddition reaction catalysis by **4h** was considered four different reaction modes (**Mode A, B, C and D**). In **mode A**, the NH of **4h** could act as a proton source and combine with N atom of quinoline derivate **2a** to form **4h-a-IM1A.** Then, the carbonyl oxygen of **1a** could form H-bond with NH of **4h-a-IM1A** to afford **4h-a-IM2A**. Finally, **4h-a-IM2A** would experience an intramolecular addition to acquire the final product **3a**. Activating carbonyl of indole derivates in [2+2] cycloaddition reaction was also discussed (**Mode B, C and D**). In this mechanism, the **4h** plays a bridge role via two H-bonds with **1a** and

2a leading to the following [2+2] cycloaddition. It is noted that the **4h** and **2a** could form two types of hydrogen bonds, the O atom of phosphate group (**Mode B**) or O of trifluoromethanesulfonic acid (**Mode C**) could form H-bond with secondary amine moiety of **2a**. In **mode D**, the **4h** experience an isomerization to form isomerized **4h**[11] and act as a activated catalyst was also calculated. The isomerized chiral phosphoramide **4h** act as activated catalyst have been discussed in previous research[11], several calculation results shows that the transition state energy barriere of reaction catalyzed by isomerized chiral phosphoramide were lower than that of chiral phosphoramide. Corresponding energy profile and key transition state structures were given in **Figure S3**.



Path 1. Free catalyst of [2+2] Cyclization reaction mechanism

Path 2. The [2+2] Cyclization reaction mechanism catalyzed by **4h**.

Scheme S1. Reaction mechanism of the [2+2] cycloaddition reaction.

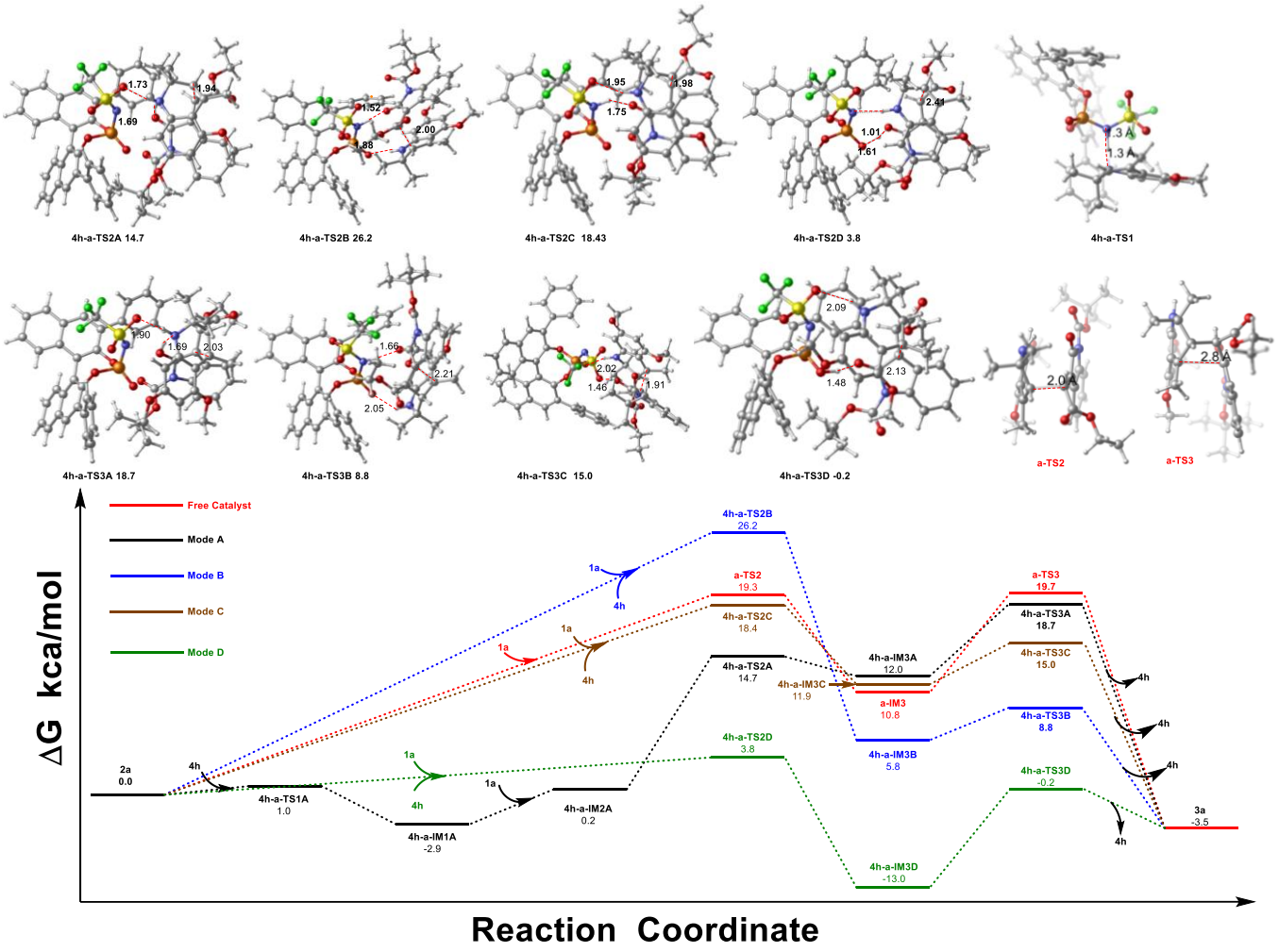


Figure S1. energy profile of [2+2] cycloaddition and corresponding key transition state structures.

Our experimental results show that the [2+2] cycloaddition could slowly happen under catalyst-free condition (ambient temperature). The free energy barrier are predicted to be 19.3 kcal/mol (**a-TS2**) and 19.7 kcal/mol **(a-TS3)**.

When **4h** acting as the catalyst, the proton transfer between **2a** and **4h** leads to the formation of **4h-a-IM1A** with a free energy barrier of 1.0 kcal/mol (**4h-a-TS1A**). Then, substrate **1a** could bind with **4h-a-IM1A** via H-bond interaction to form **4h-a-IM2A,** this step is predicted to be endothermic 3.1 kcal/mol. Then, **4h-a-IM2A** experiences an intramolecular C-C addition with a free energy barrier of 14.5 kcal/mol **(4h-a-TS2A)** to give the intermediate **4h-a-IM3A**. The similar C-C addition were calculated in **mode B, C and D**. However, in **mode D**, the energy barrier of C-C addition is 3.8 kcal/mol **(4h-a-TS2D)** which is lower than that of 14.7, 26.2 and 18.4 kcal/mol **(4h-a-TS2A, 4h-a-TS2B and 4h-a-TS2C).** Besides, starting from the **4h-a-IM3D (4h-a-IM3A , B or C)**, the intramolecular C-C coupling affords the final product **4a**. The free energy of this step is predicted to be 12.8 (6.7, 3.0, 3.1) kcal/mol. Obviously, the energy barrier of **mode D** is lower than that of mode **A**, **B** and **C**. The overall activation free energy of **4h** catalyzed process is determined to be 12.8 kcal/mol (referring to **4h-a-IM3D→4h-a-TS3D**).

With the best reaction mechanism in hand, the chirality selectivity was also calculated. Since the chirality was controlled by C-C addition, the energy barrier of the C-C addition step was discussed and given in **Figure S4**, compare with other 3 transition states, it was noticeable that the dihedral angles of ***RR*-4h-a-TS2D** close to the staggered conformer of Newman projection, and the π-π interaction between two substrates could be find. Hence, less repulsive interaction and π-π interaction might be the reason for ***RR*-4h-a-TS2D** was the lowest transition configuration and **3a** was the main product for the reaction.

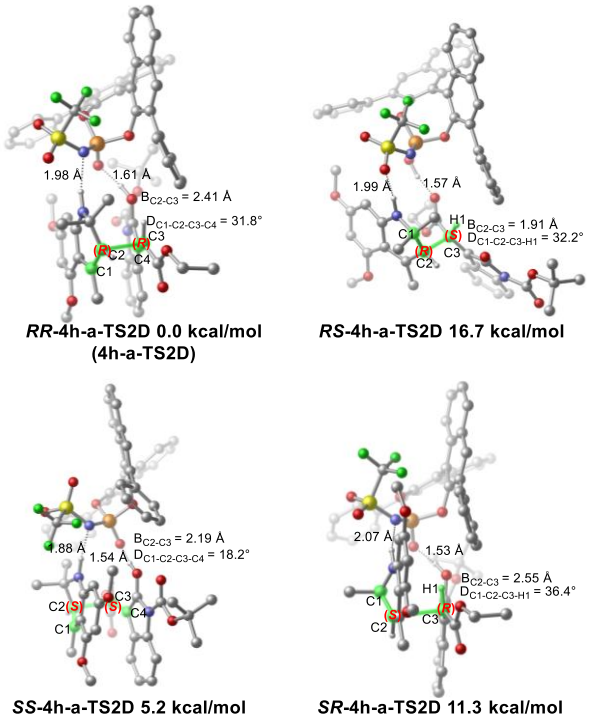


Figure S4. The structures and relative energies of key transition states to form different stereoisomers. Energies are obtained at the B3LYP-D3/6-31++G(d,p) level and are given in kcal/mol.

8.4 The ene reaction mechanism under the catalysis of 4h and TfOH

From the experimental results, when **4h** act as catalyst, product **3a-H** (Table S2, Entry 3) could not be obtained. Both [2+2] cycloaddition product **3a** and ene product **6a'** (major) could be obtained in **TfOH** catalyzed system (Table S1, Entry 2). It suggests that ene reaction needs the assistance of strong Brønsted acid. Here, we will give a reasonable explanation from theoretical analysis.

According to the previous reports,[12] the intermediate **b-IM2** was proposed. Hence, in this reaction, the H migration process may have three different pathways. The corresponding H migration process and energy profiles have shown in **Figure S5.** The first one (**Path 3**) is an intermolecular direct H migration pathway; the H of methyl could transfer to C=C and formation of **b-IM2**. which needs to overcome an energy barrier of 72.6 kcal/mol (**Figure S5, b-TS1**). The second one is acid-mediated direct H migration pathway (**Path 5**). **TfOH** could first combine with the N atom of **2a** and experience a direct H migration process. The energy barrier is predicted to be 62.2 kcal/mol which is difficult to proeed under this reaction condition.

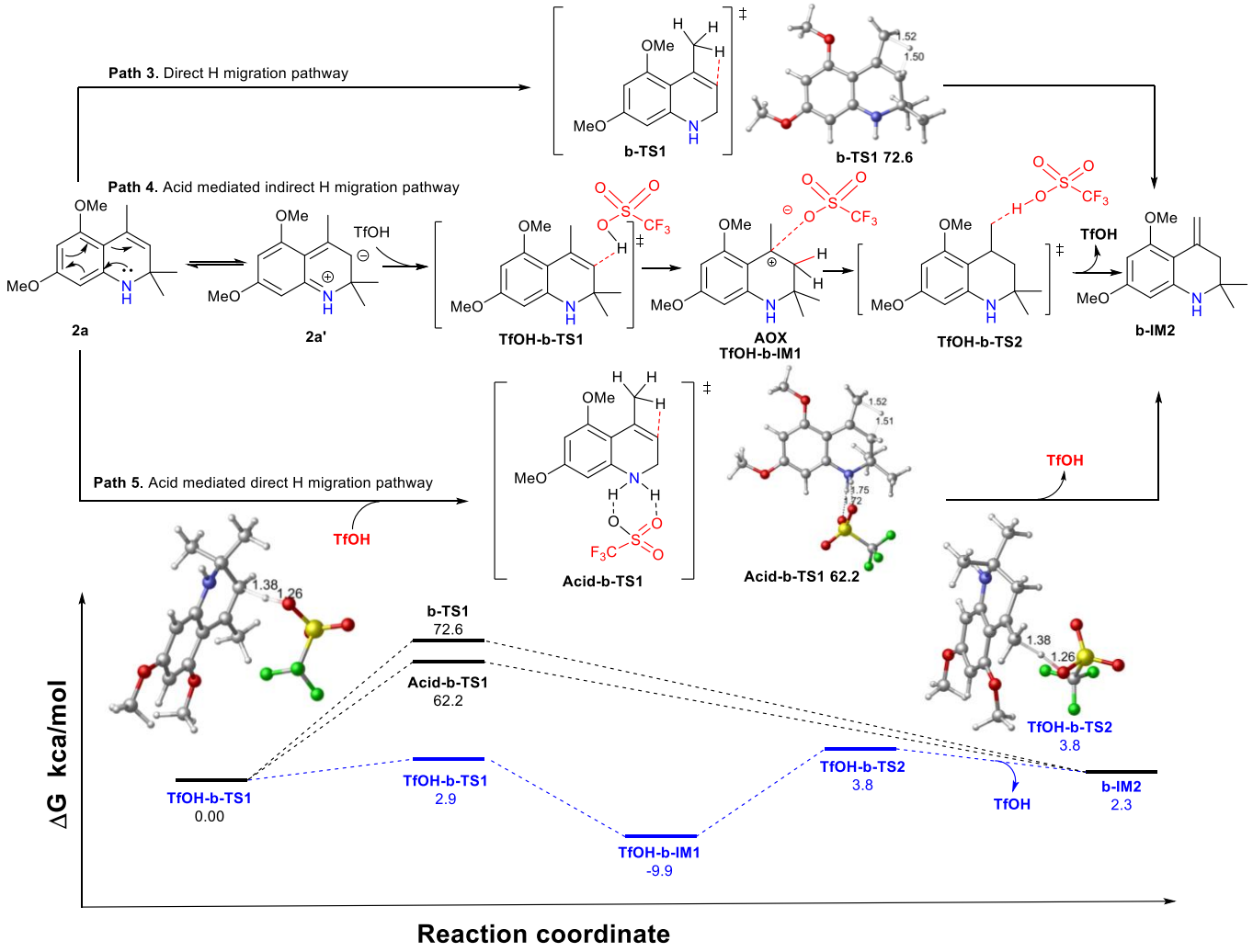


Figure S5. The reaction mechanism and energy profile of H migration process: **Path 3** represents the direct H migration under the free acid condition. **Path 4** represents acid-mediated indirect H migration under the acid condition and **Path 5** represents acid-mediated direct H migration process.

The third pathway is acid-mediated indirect H migration pathway (**Path 4**). We assume that the nonbonding electron pair of N atoms in substrate **2a** could play an electron donor role and enhance the electron density of the C=C bond. Thus, the C=C bond could be easily protonated under **TfOH** as the catalyst to afford the aza-*o*-xylylene (**AOX)** intermediate which has been reported in previous research[2, 12, 13]. The energy barrier of this step is predicted to be 2.92 kcal/mol **(TfOH-b-TS1)**. Then, the methyl of **AOX** intermediate could be easily deprotonated with anion ($\mathbf{CF_3SO_3^-}$) to afford the enamine **b-IM2** and release the acid **TfOH**. The energy barrier of this step is 13.7 kcal/mol which is lower than that of **b-TS1** and **Acid-TS1**. Our calculations are in accord with the experimental results (**Scheme 2**, control experiments) in which **TfOH** will react with substitute **2a**.

Subsequently, the **b-IM2** could along a free catalyst pathway or a **TfOH** mediated pathway to form **6a'** product. The reaction mechanism and corresponding key transition structure of **b-IM2** to **6a'** have shown in **Figure S6**.

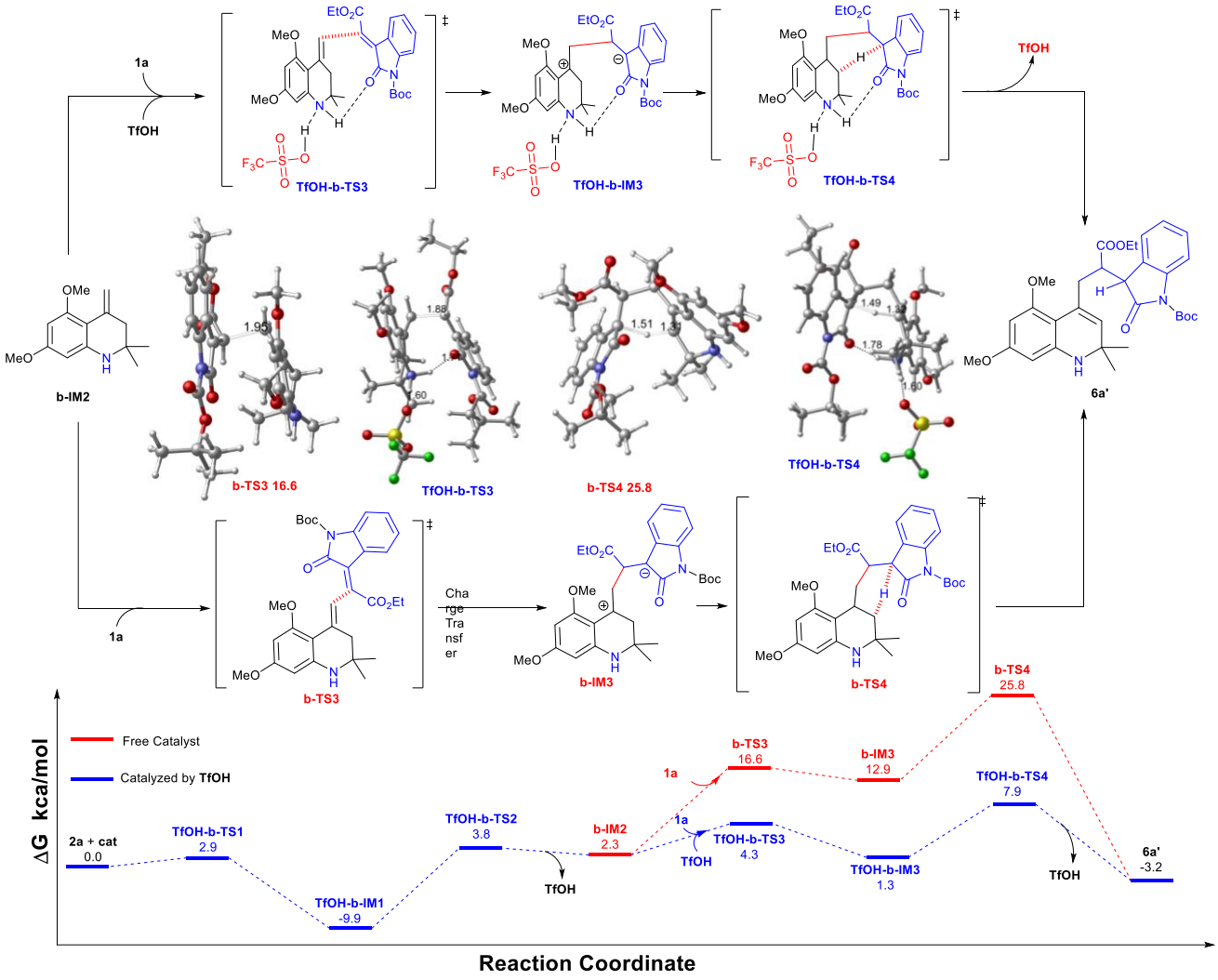


Figure S6. The reaction mechanism of **b-IM2** to **6a'** process.

Firstly, **b-IM2** could generate intermediate **b-IM3** with **1a** under free catalyst condition. Then, an intramolecular H migration process in **b-IM3** could proceed and give the final product **6a'**. The energy barrier of step is as high as 25.8 kcal/mol.

Moreover, **b-IM2** could also form intermediate **TfOH-b-IM3** with **TfOH** and **1a**. In this process, an intramolecular hydrogen bond between **NH** and carbonyl is crucial for decrease the free energy barrier of the reaction system. Subsequently, a similar intramolecular H migration process in **TfOH-b-IM3** could proceed to give the final product **6a'**, the energy barrier is 6.6 kcal/mol. Obviously, the **TfOH** could decrease the activation energy of whole reaction.

Here, the ene reaction catalyzed by **4h** was calculated, the energy profile and key transition state structures were shown in **Figure S7**. We hypothesis that the ene reaction mechanism catalyzed by **4h** was similar with **TfOH**. A reaction mechanism with high energy barrier was obtained. Compare with the [2+2] cycloaddition reaction, the energy barrier of whole **ene** reaction is much higher than that of [2+2] cycloaddition reaction catalyzed by **4h**. Hence, the cycloaddition product **3a** was the main product in whole reaction.

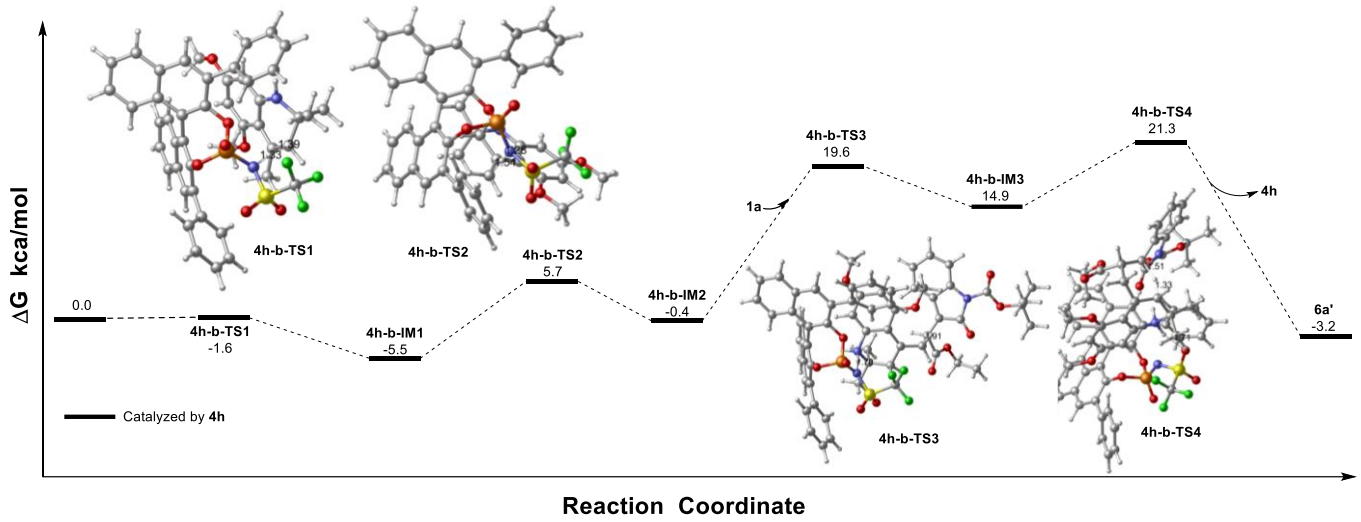


Figure S7. The reaction mechanism of ene reaction catalyze by **4h**.

8.5 The [2+2] cycloaddition reaction catalyzed by TfOH.

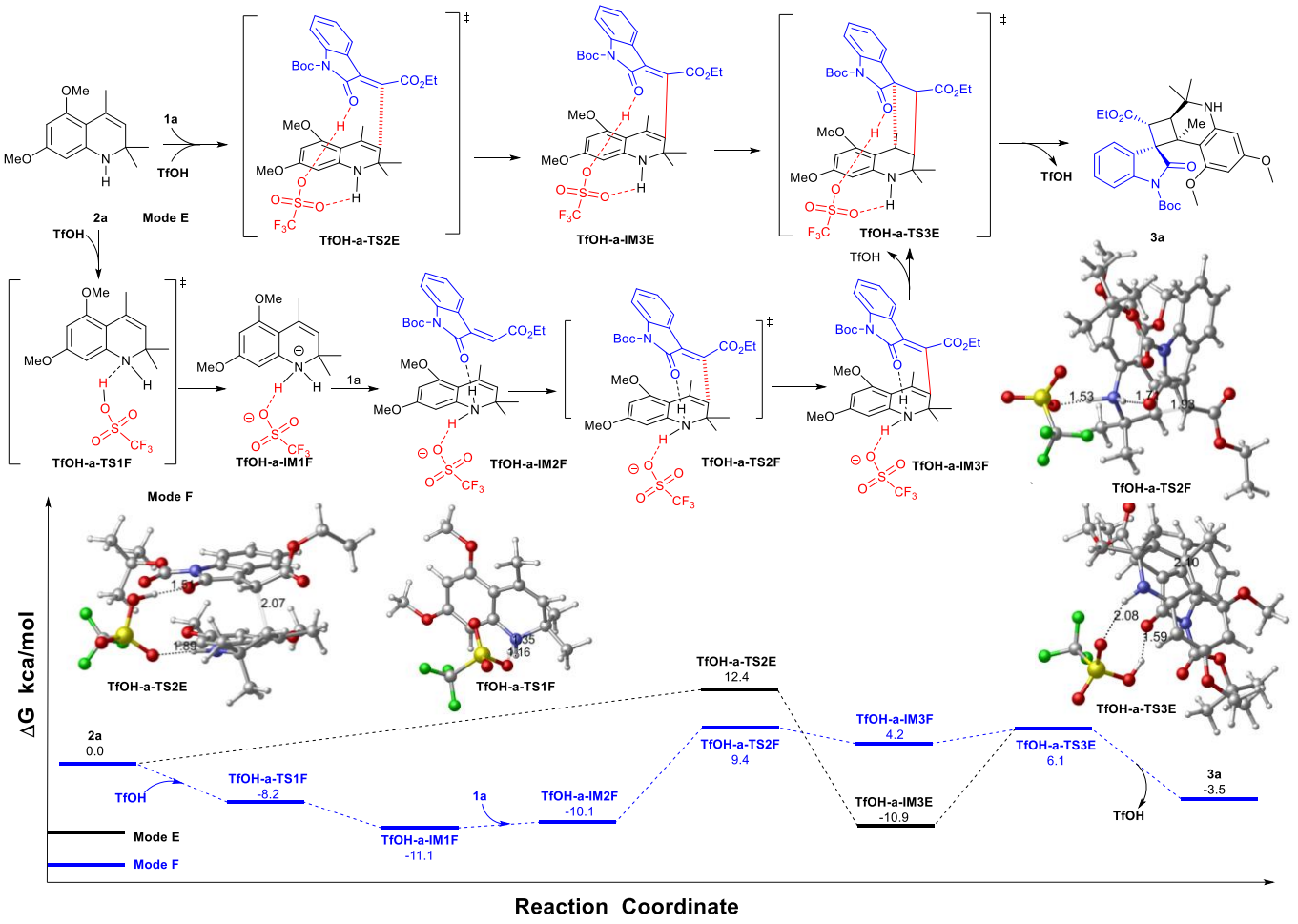


Figure S8. The reaction mechanism, energy profile and key transition structures of [2+2] cycloadditon reaction catalyzed by **TfOH.**

The experimental results shows that the [2+2] product could be obtained when the catalyst is **TfOH**. The [2+2] cycloaddition reaction catalyzed by **TfOH** was also calculated and theoretical analyse results were shown in **Figure S8**, two similar [2+2] cycloaddition reaction mechanism (**Mode E** and **F**) catalyzed by **TfOH** were analyzed. Energy profile shows that the energy barrier of **mode F** is lower than that of **mode E**. Hence, **TfOH** catalyzed [2+2] cycloaddition reaction tends to proceed along **mode F**. Besides, the activation energy of [2+2] reaction is 20.5 kcal/mol (**TfOH-a-IM1F→TfOH-a-TS2F**) which is higher than that of ene activation energy **(**16.8 kcal/mol, **TfOH-b-IM1→TfOH-b-TS4)**. It is in accord with the synchronous observation of **3a** and **6a'** in **TfOH** catalyzed system.

Reaction coordinate

4h-a-TS1A

Zero-point correction=0.781708

Thermal correction to Energy= 0.834524

Thermal correction to Enthalpy= 0.835468

Thermal correction to Gibbs Free Energy= 0.694609

SCF Done: E(Solv) = -3491.35722833

C	-7.768435	-0.212924	1.351035
C	-6.997782	-1.398425	1.391884
C	-5.675283	-1.388546	1.009463
C	-5.053672	-0.191558	0.565552
C	-5.823201	1.016101	0.561689
C	-7.189151	0.967229	0.948312
C	-3.682351	-0.128632	0.152361
C	-3.139655	1.105189	-0.145025
C	-3.871543	2.323845	-0.141291
C	-5.210485	2.237635	0.190987
C	-2.828783	-1.344688	0.066103
C	-3.190734	-2.435758	-0.791648
C	-2.386658	-3.618497	-0.785378
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C	-3.828008	-4.628256	-2.461345

C	-2.741807	-4.709045	-1.622846
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O	-1.208929	-0.323431	1.510734
P	-0.728396	1.056499	0.748714
O	-0.697012	2.156414	1.730431
N	0.714084	0.691748	-0.009906
C	0.339848	-2.739646	1.703448
C	-3.236553	3.626935	-0.449904
C	0.357911	-2.222878	3.010274
C	1.448354	-2.449054	3.850058
C	2.546249	-3.189342	3.405783
C	2.540804	-3.706251	2.109515
C	1.452789	-3.478732	1.267705
C	-3.585281	4.758869	0.303520
C	-3.023924	6.002227	0.023424
C	-2.098437	6.134087	-1.012614
C	-1.740166	5.013692	-1.763303
C	-2.303048	3.769654	-1.488873
S	1.043782	0.833618	-1.611169
O	2.489795	0.936665	-1.774861
O	0.156244	1.749292	-2.319822
C	0.622010	-0.872395	-2.249554
F	1.052085	-0.994921	-3.506120
F	-0.693749	-1.086637	-2.210863
F	1.230716	-1.808553	-1.494936
H	-8.812470	-0.236164	1.649523
H	-7.452391	-2.324236	1.732517
H	-5.093068	-2.301179	1.052173
H	-7.765068	1.888857	0.929899
H	-5.817238	3.138188	0.174654
H	-0.691138	-4.607207	0.099738
H	-4.887552	-1.473126	-1.731163
H	-5.444230	-3.373976	-3.179819
H	-4.087519	-5.464290	-3.104108
H	-2.127594	-5.605494	-1.595370
H	-0.487822	-1.650015	3.369561

H	1.435745	-2.049692	4.860033
H	3.393854	-3.362584	4.061948
H	3.390891	-4.278387	1.748998
H	1.467165	-3.861284	0.252389
H	-4.277159	4.653037	1.133855
H	-3.298596	6.864576	0.624663
H	-1.652462	7.101548	-1.226474
H	-1.013166	5.100325	-2.565496
H	-2.002751	2.910969	-2.074526
C	5.834058	-0.331419	-1.334084
C	5.010015	-1.415098	-1.019667
C	4.033265	-1.292913	-0.032738
C	3.865848	-0.057544	0.580653
C	4.625257	1.076453	0.264561
C	5.647883	0.893571	-0.697576
N	2.762333	0.111172	1.501824
C	3.090046	1.035289	2.649901
C	3.516053	2.334304	2.008642
C	4.251785	2.364331	0.883913
C	4.592687	3.680056	0.231170
C	4.221845	0.415613	3.491614
C	1.842902	1.229291	3.511724
O	6.432821	1.974612	-0.959685
C	7.385544	1.885049	-2.006438
O	5.244437	-2.558767	-1.721332
C	4.307670	-3.616032	-1.582201
H	6.594505	-0.476077	-2.089096
H	3.383527	-2.111600	0.233906
H	5.664461	3.890270	0.267442
H	4.302524	3.669693	-0.824671
H	4.055007	4.491176	0.731202
H	4.470313	1.089084	4.317143
H	3.907455	-0.545917	3.914920
H	5.123154	0.259936	2.893619
H	2.101858	1.866361	4.364016
H	1.031810	1.711096	2.962827

H	1.486845	0.272942	3.905150
H	7.846382	2.871928	-2.071881
H	8.157298	1.137107	-1.784086
H	6.906301	1.639306	-2.961978
H	4.615175	-4.385370	-2.292276
H	4.323205	-4.036038	-0.567357
H	3.292541	-3.276370	-1.818821
H	3.181601	3.254963	2.477363
H	1.717091	0.488965	0.753416
H	2.478819	-0.799751	1.870809

4h-a-IM1=4h-a-IM1A

Zero-point correction=0.786680

Thermal correction to Energy= 0.839771

Thermal correction to Enthalpy= 0.840715

Thermal correction to Gibbs Free Energy= 0.698753

SCF Done: E(Solv) =-3491.36761153

C	-7.810467	-0.187445	1.374725
C	-7.039526	-1.372066	1.431198
C	-5.717050	-1.366772	1.048272
C	-5.094938	-0.176049	0.588117
C	-5.865022	1.031124	0.568556
C	-7.230833	0.987105	0.956037
C	-3.724329	-0.119410	0.172041
C	-3.177358	1.111395	-0.136988
C	-3.913381	2.328980	-0.151811
C	-5.252725	2.247254	0.179742
C	-2.874527	-1.339189	0.090934
C	-3.241476	-2.439106	-0.752982
C	-2.435385	-3.620829	-0.741666
C	-1.288863	-3.668502	0.082883
C	-0.879002	-2.585874	0.837501
C	-1.683715	-1.409491	0.797652
C	-4.352639	-2.392990	-1.636672

C	-4.667703	-3.470057	-2.433767
C	-3.892931	-4.653029	-2.390078
C	-2.798032	-4.721956	-1.561953
O	-1.832260	1.152517	-0.473863
O	-1.255431	-0.305825	1.516179
P	-0.728063	1.046542	0.715710
O	-0.668826	2.151914	1.696442
N	0.669006	0.622797	-0.027988
C	0.330215	-2.699178	1.687412
C	-3.280376	3.627689	-0.484894
C	0.388729	-2.142130	2.977068
C	1.501431	-2.348386	3.793714
C	2.584216	-3.109014	3.344414
C	2.537922	-3.666769	2.065185
C	1.429585	-3.456202	1.245717
C	-3.653646	4.778352	0.227873
C	-3.099692	6.019110	-0.077331
C	-2.155761	6.130875	-1.098926
C	-1.771623	4.992383	-1.808413
C	-2.326504	3.750436	-1.508898
S	1.032296	0.763652	-1.587181
O	2.488479	0.856228	-1.730057
O	0.182104	1.672621	-2.358057
C	0.635936	-0.939489	-2.241020
F	1.050892	-1.058337	-3.505049
F	-0.676063	-1.183720	-2.187980
F	1.269748	-1.879701	-1.501765
H	-8.854551	-0.206627	1.673604
H	-7.493767	-2.293505	1.784253
H	-5.134491	-2.278625	1.103164
H	-7.806773	1.908513	0.925230
H	-5.861658	3.145929	0.146822
H	-0.722966	-4.594421	0.124930
H	-4.947597	-1.489722	-1.687953
H	-5.517067	-3.408595	-3.107897
H	-4.157935	-5.497146	-3.019996

H	-2.181833	-5.617039	-1.530517
H	-0.443295	-1.553137	3.341007
H	1.515047	-1.923475	4.793419
H	3.446184	-3.272186	3.984510
H	3.371795	-4.260885	1.701803
H	1.416581	-3.867198	0.242062
H	-4.360459	4.690417	1.047677
H	-3.395156	6.895506	0.493176
H	-1.715789	7.096547	-1.332970
H	-1.029443	5.062363	-2.598326
H	-2.002457	2.879140	-2.062516
C	5.885857	-0.333883	-1.331516
C	5.077678	-1.422757	-0.994595
C	4.122083	-1.299306	0.015190
C	3.970072	-0.058232	0.610071
C	4.694910	1.085092	0.269198
C	5.702885	0.899144	-0.709835
N	2.865916	0.110627	1.563906
C	3.174159	1.093728	2.687714
C	3.587439	2.370710	2.000490
C	4.306897	2.380191	0.865124
C	4.608157	3.681982	0.167809
C	4.300848	0.494857	3.543295
C	1.904059	1.297247	3.512776
O	6.469712	1.981909	-1.001440
C	7.389401	1.895704	-2.080103
O	5.299994	-2.565202	-1.694514
C	4.347452	-3.612928	-1.561113
H	6.629597	-0.478765	-2.103073
H	3.472827	-2.114022	0.295234
H	5.676194	3.911810	0.171928
H	4.290492	3.631808	-0.878773
H	4.066240	4.496831	0.656179
H	4.533575	1.188382	4.355660
H	3.991725	-0.459651	3.985405
H	5.209035	0.338164	2.956176

H	2.130400	1.997047	4.323698
H	1.087181	1.717366	2.919090
H	1.572257	0.357872	3.962765
H	7.832599	2.888479	-2.169064
H	8.178494	1.161385	-1.875326
H	6.880437	1.634378	-3.015455
H	4.638861	-4.375324	-2.284830
H	4.369221	-4.046861	-0.552644
H	3.336959	-3.253066	-1.783855
H	3.241126	3.298565	2.444291
H	2.001281	0.425401	0.997280
H	2.610961	-0.797588	1.968390

4h-a-IM2=4h-a-IM2A

Zero-point correction=1.128791

Thermal correction to Energy= 1.203685

Thermal correction to Enthalpy= 1.204629

Thermal correction to Gibbs Free Energy= 1.016613

SCF Done: E(Solv) = -4581.97290938

C	-5.672277	3.360061	-2.361255
C	-4.573280	4.221760	-2.319265
C	-3.286228	3.751269	-2.027036
C	-3.134735	2.393948	-1.784086
C	-4.239296	1.505499	-1.816414
C	-5.513175	1.995141	-2.109994
N	-1.945163	1.675792	-1.489136
C	-2.267518	0.340068	-1.222793
C	-3.732572	0.172047	-1.521981
C	-5.084432	-0.715377	1.444394
C	-4.708272	-2.000831	1.599468
C	-4.199771	-1.094105	-1.531627
C	-4.101232	0.357363	1.686809
C	-2.764993	0.015270	1.987092
N	-2.350045	-1.377252	1.779763

C	-3.370593	-2.437451	2.126944
C	-4.364186	1.748973	1.636602
C	-3.354040	2.693623	1.860550
C	-2.064454	2.281344	2.201244
C	-1.769743	0.915404	2.283289
C	-3.417846	-2.549472	3.660743
C	-2.876308	-3.736746	1.486492
O	-1.509996	-0.519470	-0.810714
O	-5.637190	2.125597	1.349708
O	-1.040761	3.119106	2.453132
C	-5.934468	3.507573	1.209280
C	-1.098957	4.430162	1.905910
C	-5.552928	-1.556921	-1.859897
O	-6.507205	-0.880194	-2.202735
O	-5.613585	-2.902755	-1.725330
C	-6.757544	-4.991058	-1.718911
C	-6.897189	-3.506598	-1.990328
O	-0.392555	3.314236	-1.604367
C	0.834549	3.987838	-2.108025
C	0.753214	5.355959	-1.434703
C	0.735632	4.106895	-3.628157
C	2.082429	3.241548	-1.647096
C	-0.636467	2.051071	-1.938544
O	0.038957	1.306544	-2.602148
C	-6.510937	-0.418262	1.051083
H	-6.657956	3.751013	-2.594063
H	-4.710955	5.280685	-2.519715
H	-2.435291	4.417410	-1.992809
H	-6.347786	1.308517	-2.157487
H	-5.426171	-2.796974	1.425633
H	-3.484151	-1.875033	-1.302329
H	-2.056760	-1.440438	0.783263
H	-3.575712	3.746922	1.779848
H	-0.750553	0.611457	2.459055
H	-3.701456	-1.591245	4.106466
H	-2.447540	-2.857169	4.059461

H	-4.172143	-3.290274	3.940629
H	-3.551732	-4.554799	1.755068
H	-2.850252	-3.657504	0.395705
H	-1.870841	-3.979622	1.843305
H	-6.990683	3.551594	0.940580
H	-5.773356	4.045998	2.151604
H	-5.339749	3.961761	0.410359
H	-0.106521	4.850713	2.064360
H	-1.319308	4.384655	0.833933
H	-1.846279	5.050968	2.418660
H	-7.711169	-5.496162	-1.904449
H	-5.998006	-5.436259	-2.369127
H	-6.467856	-5.170196	-0.678468
H	-7.645905	-3.035142	-1.345538
H	-7.177331	-3.298558	-3.027911
H	0.816646	5.249251	-0.348183
H	1.587884	5.979753	-1.769741
H	-0.181563	5.867399	-1.689551
H	0.755183	3.122285	-4.098428
H	1.586803	4.685579	-4.001981
H	-0.185219	4.625104	-3.918441
H	2.965096	3.846629	-1.881389
H	2.035035	3.081175	-0.571072
H	2.180219	2.271778	-2.133541
H	-6.575499	0.185645	0.145978
H	-7.046869	-1.356807	0.880035
H	-7.024822	0.136588	1.841348
C	7.407888	2.192021	-2.827637
C	6.967895	0.910403	-3.234839
C	6.004117	0.239028	-2.516779
C	5.427956	0.814054	-1.353048
C	5.844570	2.128032	-0.964636
C	6.853311	2.785767	-1.718274
C	4.430008	0.151311	-0.568028
C	3.832610	0.845551	0.469334
C	4.195292	2.170613	0.849247

C	5.225470	2.760435	0.140024
C	3.990725	-1.242683	-0.856646
C	4.916087	-2.337886	-0.831828
C	4.439663	-3.651300	-1.142787
C	3.073254	-3.839752	-1.457653
C	2.161227	-2.803457	-1.428429
C	2.650828	-1.509942	-1.090722
C	6.278709	-2.187866	-0.459512
C	7.129795	-3.269678	-0.434803
C	6.666018	-4.560405	-0.780563
C	5.346986	-4.743311	-1.122894
O	2.835316	0.205878	1.178820
O	1.731791	-0.475801	-0.988763
P	1.339984	0.066403	0.507736
O	0.590723	1.340082	0.407634
N	0.661309	-1.175402	1.309851
C	0.740759	-3.050742	-1.779103
C	3.459628	2.920326	1.897981
C	0.050418	-2.210145	-2.664978
C	-1.247878	-2.520622	-3.063358
C	-1.888421	-3.661107	-2.575419
C	-1.216034	-4.491668	-1.676394
C	0.086161	-4.188253	-1.282236
C	3.254556	4.301302	1.731261
C	2.568675	5.047706	2.687241
C	2.054354	4.422652	3.824709
C	2.240461	3.050574	3.995294
C	2.941084	2.304719	3.050403
S	1.006991	-1.740351	2.731372
O	-0.238166	-2.367079	3.269221
O	1.760172	-0.882082	3.653298
C	2.103405	-3.214050	2.416186
F	2.406767	-3.813947	3.571499
F	3.230915	-2.829600	1.813018
F	1.469975	-4.097749	1.628924
H	8.174405	2.707619	-3.399114

H	7.391852	0.453602	-4.124556
H	5.669618	-0.739633	-2.839440
H	7.169574	3.777590	-1.404603
H	5.565874	3.752520	0.421857
H	2.735443	-4.834106	-1.735402
H	6.643640	-1.207389	-0.179300
H	8.166133	-3.131347	-0.140046
H	7.349542	-5.404406	-0.761785
H	4.971308	-5.732339	-1.372986
H	0.519550	-1.302916	-3.025239
H	-1.767426	-1.855567	-3.747780
H	-2.906918	-3.891455	-2.877682
H	-1.705141	-5.377713	-1.279952
H	0.599023	-4.824019	-0.568927
H	3.615474	4.788596	0.830846
H	2.429393	6.115622	2.537385
H	1.507930	4.998344	4.566975
H	1.836630	2.547636	4.868831
H	3.065336	1.241687	3.206109
H	-1.483672	-1.597989	2.323995

4h-a-TS2A

Zero-point correction=1.128434

Thermal correction to Energy= 1.203685

Thermal correction to Enthalpy= 1.204629

Thermal correction to Gibbs Free Energy= 1.016613

SCF Done: E(Solv) = -4581.95232325

C	5.777202	2.789022	1.762658
C	4.729696	3.685474	2.018506
C	3.400286	3.252147	2.037951
C	3.144367	1.911001	1.770992
C	4.196857	0.983717	1.487458
C	5.523388	1.444341	1.502182
N	1.923242	1.212937	1.738253

C	2.169424	-0.121316	1.334733
C	3.587408	-0.287545	1.211424
C	5.132520	-0.715188	-1.338055
C	4.434811	-1.885352	-0.781484
C	4.113861	-1.609144	0.826636
C	4.321343	0.394231	-1.582122
C	2.883883	0.273326	-1.515739
N	2.246981	-1.037671	-1.484853
C	3.154037	-2.237272	-1.568264
C	4.813691	1.753322	-1.705838
C	3.965932	2.841259	-1.649381
C	2.575038	2.639045	-1.516999
C	2.031302	1.348204	-1.519614
C	3.502782	-2.495323	-3.041976
C	2.371029	-3.427363	-1.010217
O	1.278271	-0.928716	0.996954
O	6.149777	1.876887	-1.780883
O	1.684495	3.627666	-1.417819
C	6.730003	3.176267	-1.679674
C	2.130448	4.968237	-1.233882
C	5.374146	-2.070868	1.529145
O	6.414821	-1.454956	1.637506
O	5.219588	-3.340176	1.956440
C	6.023035	-5.397781	2.855137
C	6.381467	-3.954686	2.563053
O	0.511462	2.933973	2.054789
C	-0.657011	3.648740	2.609403
C	-0.487441	5.041221	2.002431
C	-0.534221	3.677490	4.132355
C	-1.965863	3.019802	2.136300
C	0.676437	1.627753	2.271159
O	-0.051391	0.878564	2.876313
C	6.625484	-0.762783	-1.471293
H	6.804991	3.142143	1.788114
H	4.948683	4.729337	2.226127
H	2.587225	3.933823	2.245519

H	6.332103	0.746118	1.337701
H	5.072709	-2.772951	-0.805870
H	3.336975	-2.337816	1.057633
H	1.671028	-1.097340	-0.582170
H	4.366342	3.842906	-1.654029
H	0.958958	1.243377	-1.391005
H	4.001043	-1.637473	-3.501659
H	2.595324	-2.718374	-3.607218
H	4.177103	-3.355357	-3.104955
H	3.017957	-4.309425	-0.972679
H	1.968822	-3.240933	-0.014861
H	1.522430	-3.644287	-1.664004
H	7.807918	3.014733	-1.701763
H	6.434622	3.804008	-2.528138
H	6.438190	3.646994	-0.735270
H	1.221327	5.552040	-1.096853
H	2.764973	5.041930	-0.344928
H	2.670373	5.331118	-2.116889
H	6.877949	-5.911166	3.306176
H	5.180322	-5.457148	3.549354
H	5.750234	-5.923858	1.936030
H	7.224905	-3.866032	1.871192
H	6.635881	-3.397987	3.470340
H	-0.515425	4.974259	0.910759
H	-1.299324	5.695714	2.335764
H	0.464470	5.489727	2.308283
H	-0.610577	2.668842	4.543355
H	-1.340467	4.286902	4.554626
H	0.423422	4.115271	4.435696
H	-2.798469	3.670141	2.427441
H	-1.952267	2.917283	1.052859
H	-2.118263	2.031924	2.569431
H	7.120653	-0.133171	-0.727599
H	6.980584	-1.786801	-1.336046
H	6.944521	-0.400955	-2.453515
C	-7.452965	2.564960	2.608607

C	-7.216157	1.198092	2.886316
C	-6.282825	0.487467	2.165772
C	-5.536538	1.105753	1.127801
C	-5.746536	2.500573	0.875479
C	-6.728923	3.199454	1.626818
C	-4.561431	0.407407	0.344549
C	-3.802185	1.127376	-0.558905
C	-3.946056	2.526090	-0.786563
C	-4.949295	3.168370	-0.085584
C	-4.298038	-1.050793	0.507603
C	-5.331837	-2.022961	0.305819
C	-5.033171	-3.404361	0.530218
C	-3.728911	-3.777842	0.930026
C	-2.703671	-2.860741	1.060810
C	-3.018323	-1.493918	0.810495
C	-6.632875	-1.680941	-0.150851
C	-7.594729	-2.647799	-0.338019
C	-7.308982	-4.008796	-0.078606
C	-6.052572	-4.375182	0.342755
O	-2.832759	0.438172	-1.264577
O	-1.986883	-0.568432	0.889718
P	-1.426130	0.119650	-0.482821
O	-0.631819	1.327925	-0.153522
N	-0.705560	-1.021541	-1.379899
C	-1.353240	-3.312624	1.479734
C	-2.998812	3.277244	-1.647660
C	-0.602863	-2.611801	2.434183
C	0.616368	-3.117962	2.881566
C	1.114406	-4.320416	2.381635
C	0.383731	-5.016219	1.414340
C	-0.835755	-4.514678	0.966944
C	-2.580099	4.555990	-1.243365
C	-1.658387	5.282089	-1.995070
C	-1.125822	4.737196	-3.163990
C	-1.536931	3.469518	-3.578048
C	-2.466945	2.746056	-2.835184

S	-0.901177	-1.383492	-2.891821
O	0.434775	-1.781134	-3.433354
O	-1.709203	-0.497146	-3.735013
C	-1.831736	-2.995132	-2.824668
F	-2.053647	-3.456159	-4.059420
F	-3.001892	-2.816768	-2.205289
F	-1.120139	-3.911733	-2.147068
H	-8.197224	3.112118	3.180176
H	-7.772862	0.705747	3.678572
H	-6.104439	-0.557145	2.390479
H	-6.886967	4.254409	1.416589
H	-5.122056	4.227677	-0.253003
H	-3.532117	-4.824228	1.144368
H	-6.860205	-0.643645	-0.364642
H	-8.580663	-2.363382	-0.694539
H	-8.078833	-4.760995	-0.225272
H	-5.812887	-5.419117	0.528890
H	-0.950615	-1.657395	2.808005
H	1.186058	-2.550528	3.611492
H	2.072900	-4.702061	2.725198
H	0.768801	-5.944317	0.999524
H	-1.385675	-5.039777	0.192943
H	-2.955661	4.968874	-0.312475
H	-1.353885	6.271215	-1.660839
H	-0.398233	5.295342	-3.747601
H	-1.130889	3.030147	-4.484666
H	-2.757618	1.759513	-3.170897
H	1.536599	-1.132706	-2.250392

4h-a-IM3=4h-a-IM3A

Zero-point correction=1.129580

Thermal correction to Energy= 1.204970

Thermal correction to Enthalpy= 1.205914

Thermal correction to Gibbs Free Energy= 1.017200

SCF Done: E(Solv) = -4581.95713629

C	-6.011781	2.363600	-1.282110
C	-5.041121	3.340994	-1.547190
C	-3.689252	3.004602	-1.687098
C	-3.326153	1.670778	-1.529526
C	-4.299636	0.667094	-1.234782
C	-5.651520	1.025984	-1.130647
N	-2.072169	1.038436	-1.631708
C	-2.220120	-0.337881	-1.307774
C	-3.608029	-0.573059	-1.077012
C	-5.036336	-1.251658	1.505059
C	-4.325412	-2.328547	0.770566
C	-4.140831	-1.920770	-0.781186
C	-4.275202	-0.115303	1.764572
C	-2.845816	-0.136841	1.551873
N	-2.138346	-1.407415	1.426922
C	-2.977461	-2.664390	1.451859
C	-4.835361	1.196454	2.040696
C	-4.066253	2.338875	1.977631
C	-2.685911	2.238958	1.690178
C	-2.063726	0.991372	1.558623
C	-3.221580	-3.067862	2.913802
C	-2.159086	-3.751284	0.750243
O	-1.271260	-1.121667	-1.099138
O	-6.162969	1.224681	2.249164
O	-1.878432	3.293424	1.565444
C	-6.827136	2.486079	2.292545
C	-2.426018	4.608602	1.551811
C	-5.456015	-2.168064	-1.512610
O	-6.528337	-2.402666	-0.989170

O	-5.276476	-2.080176	-2.836286
C	-6.042063	-1.954464	-5.088411
C	-6.463774	-2.202085	-3.654576
O	-0.792823	2.864844	-1.907101
C	0.307251	3.682984	-2.457499
C	0.056834	5.033404	-1.786788
C	0.142893	3.767088	-3.974639
C	1.669519	3.130208	-2.043105
C	-0.876928	1.561426	-2.184157
O	-0.120968	0.893664	-2.846952
C	-6.484920	-1.427124	1.843125
H	-7.057916	2.649893	-1.211079
H	-5.340758	4.378354	-1.668440
H	-2.941654	3.755233	-1.903095
H	-6.404985	0.271654	-0.929530
H	-4.924503	-3.240588	0.767495
H	-3.419328	-2.636485	-1.187408
H	-1.580106	-1.383205	0.517173
H	-4.523006	3.309114	2.092511
H	-1.000496	0.967889	1.340420
H	-3.719124	-2.276421	3.480728
H	-2.274767	-3.301676	3.403820
H	-3.860764	-3.956118	2.937170
H	-2.745305	-4.673750	0.690585
H	-1.839604	-3.462169	-0.251424
H	-1.252598	-3.955102	1.327489
H	-7.886774	2.252785	2.398163
H	-6.492660	3.076227	3.153256
H	-6.652154	3.036871	1.362366
H	-1.579127	5.265093	1.358821
H	-3.169734	4.705398	0.754609
H	-2.871845	4.861361	2.521327
H	-6.911082	-2.032219	-5.750322
H	-5.610569	-0.954716	-5.195490
H	-5.296136	-2.688630	-5.408023
H	-6.889323	-3.200213	-3.510301

H	-7.199266	-1.470396	-3.306783
H	0.112760	4.921361	-0.699835
H	0.815114	5.755956	-2.105504
H	-0.929619	5.428616	-2.054434
H	0.283529	2.785716	-4.431821
H	0.889603	4.453821	-4.387673
H	-0.852572	4.143695	-4.235510
H	2.447465	3.841750	-2.342580
H	1.700015	2.998555	-0.962999
H	1.871272	2.165854	-2.508018
H	-7.127536	-0.832514	1.186312
H	-6.773776	-2.471693	1.722443
H	-6.689938	-1.098878	2.865861
C	7.167319	3.250140	-2.538025
C	7.069613	1.880044	-2.877111
C	6.224224	1.044269	-2.182843
C	5.431068	1.534185	-1.111664
C	5.498890	2.930135	-0.796443
C	6.394331	3.760762	-1.521944
C	4.542282	0.704001	-0.354971
C	3.721025	1.299460	0.584376
C	3.723883	2.693427	0.877017
C	4.649324	3.466543	0.201098
C	4.433345	-0.765349	-0.579281
C	5.567235	-1.628712	-0.425618
C	5.414002	-3.023796	-0.704686
C	4.150376	-3.518604	-1.102494
C	3.030863	-2.712207	-1.184052
C	3.204292	-1.329308	-0.890575
C	6.830819	-1.168745	0.032945
C	7.892696	-2.034088	0.169259
C	7.749945	-3.405952	-0.145382
C	6.533717	-3.886978	-0.569155
O	2.830844	0.481879	1.258787
O	2.082129	-0.512781	-0.936026
P	1.459636	0.070299	0.457994

O	0.566116	1.217151	0.165294
N	0.831248	-1.161293	1.302349
C	1.727336	-3.293262	-1.590895
C	2.721314	3.305576	1.784105
C	0.871814	-2.641438	-2.490620
C	-0.289329	-3.269208	-2.938212
C	-0.624248	-4.546634	-2.490908
C	0.204203	-5.191608	-1.568704
C	1.366366	-4.568686	-1.122699
C	2.187735	4.563931	1.458188
C	1.222929	5.166364	2.262860
C	0.758893	4.513812	3.405626
C	1.280168	3.263245	3.739337
C	2.255198	2.664593	2.944781
S	1.043514	-1.565012	2.801679
O	-0.264216	-2.067558	3.325124
O	1.792312	-0.660962	3.679757
C	2.069125	-3.113823	2.680782
F	2.328567	-3.594883	3.900499
F	3.221334	-2.847870	2.058966
F	1.407708	-4.051468	1.982387
H	7.843650	3.896994	-3.089520
H	7.664000	1.484737	-3.695900
H	6.151697	-0.001957	-2.454274
H	6.445236	4.815748	-1.264050
H	4.716843	4.528584	0.418692
H	4.062353	-4.571464	-1.353708
H	6.949852	-0.122887	0.288513
H	8.847674	-1.660794	0.528037
H	8.597606	-4.076818	-0.038729
H	6.403704	-4.942033	-0.796793
H	1.094216	-1.636709	-2.826079
H	-0.940521	-2.741257	-3.628066
H	-1.529932	-5.032541	-2.845828
H	-0.056888	-6.177529	-1.192773
H	1.993238	-5.058873	-0.385244

H	2.510864	5.059240	0.548086
H	0.832136	6.144188	1.990879
H	-0.000904	4.975853	4.030837
H	0.928121	2.740086	4.623773
H	2.634091	1.689620	3.220557
H	-1.410384	-1.503229	2.178387

4h-a-TS3A

Zero-point correction=1.128313 (Hartree/Particle)

Thermal correction to Energy=1.203400

Thermal correction to Enthalpy=1.204344

Thermal correction to Gibbs Free Energy=1.016900

SCF Done: E(Solv) = -4581.94621208

C	-6.27403600	1.94459100	-2.89854400
C	-5.24104500	2.62943100	-3.54709300
C	-3.90446300	2.41406300	-3.19263500
C	-3.65784200	1.49758700	-2.18399000
C	-4.68038800	0.80289600	-1.50088400
C	-6.00539100	1.03662100	-1.87020500
N	-2.41388500	1.07587100	-1.65575200
C	-2.63128900	0.16131500	-0.67797500
C	-4.04593300	0.01380500	-0.44196900
C	-4.39285900	0.78244500	1.40408700
C	-4.64238400	-0.71240700	1.73895800
C	-4.53326800	-1.24137900	0.29659200
C	-3.20036600	1.43113100	1.89402600
C	-2.20894500	0.65319900	2.56323900
N	-2.33587600	-0.75240300	2.49613000
C	-3.67825600	-1.30459900	2.78186600
C	-2.84246400	2.77052100	1.56934400
C	-1.64988300	3.32753500	2.00524000
C	-0.77616900	2.55682400	2.78910200
C	-1.07588500	1.22799700	3.10423700
C	-4.13581100	-0.89430300	4.19337000
C	-3.58391900	-2.83002300	2.69537700

O	-1.63993500	-0.37421200	-0.05811500
O	-3.69876700	3.44394500	0.75339700
O	0.39562500	3.01839400	3.25251300
C	-3.20680000	4.57056400	0.03632600
C	0.97940500	4.14064700	2.59409200
C	-5.83532900	-1.78230800	-0.26891900
O	-6.92265900	-1.69933300	0.26552300
O	-5.62047500	-2.36999100	-1.45775700
C	-7.58109200	-1.97385900	-2.89476900
C	-6.76060600	-2.98497300	-2.11289200
O	-0.87522200	2.68142100	-2.05145200
C	0.31827400	3.33333100	-2.68366400
C	0.27550000	4.72443500	-2.05915900
C	0.08059800	3.37866100	-4.19137600
C	1.60785400	2.60948500	-2.30954600
C	-1.13203000	1.40565100	-2.26231300
O	-0.52423300	0.59857200	-2.91257500
C	-5.68815800	1.54505900	1.26662700
H	-7.30357100	2.12286900	-3.19366500
H	-5.47387000	3.33561000	-4.33798200
H	-3.09561000	2.94044300	-3.68672300
H	-6.81814600	0.52626600	-1.36822300
H	-5.66298900	-0.83973100	2.10861700
H	-3.78698100	-2.03045700	0.17391000
H	-1.87450600	-0.77330200	0.86554600
H	-1.38431700	4.33447100	1.72358400
H	-0.33979800	0.65030700	3.64494500
H	-4.23387000	0.19225600	4.28007000
H	-3.40408300	-1.22947200	4.93550900
H	-5.10385600	-1.34760700	4.43178600
H	-4.57905500	-3.28069600	2.77426000
H	-3.11877500	-3.15826300	1.76232500
H	-2.96641000	-3.20992600	3.51569000
H	-3.98909400	4.82182300	-0.68165300
H	-3.03198600	5.42632100	0.69975000
H	-2.28578600	4.31120500	-0.49479800

H	1.96381200	4.25876000	3.03790800
H	1.07712500	3.92963600	1.52477300
H	0.39104100	5.05296200	2.75737400
H	-8.33234900	-2.50014100	-3.49416500
H	-8.10058200	-1.28957800	-2.21986500
H	-6.94334200	-1.39226000	-3.56673500
H	-6.30823800	-3.72875000	-2.77180000
H	-7.36470900	-3.48900100	-1.35477600
H	0.38213000	4.65030900	-0.97269600
H	1.09984200	5.32887600	-2.44956900
H	-0.66681600	5.23213700	-2.29113700
H	0.04765900	2.37164300	-4.61266500
H	0.90220900	3.92197600	-4.66920000
H	-0.85394400	3.90080600	-4.42611400
H	1.67950900	2.50702900	-1.22664600
H	1.66081000	1.61524500	-2.75151500
H	2.45526000	3.19967000	-2.67485200
H	-5.61064700	2.41778100	0.62589300
H	-6.48587300	0.88912700	0.91340400
H	-5.96471400	1.88450600	2.27472000
C	6.33704500	1.62647400	-4.27791400
C	5.71091800	0.37450000	-4.48776700
C	4.95974400	-0.20861000	-3.49233000
C	4.79065300	0.43474500	-2.23782000
C	5.40159700	1.71182500	-2.03440800
C	6.18395600	2.27794500	-3.07639100
C	4.01202600	-0.12574700	-1.17845200
C	3.77326700	0.63159600	-0.04330400
C	4.40823700	1.88598700	0.20748400
C	5.22569000	2.37581900	-0.79800700
C	3.46041300	-1.50616700	-1.25741900
C	4.32968000	-2.64207500	-1.34750900
C	3.74871100	-3.94960500	-1.37774600
C	2.34172200	-4.08556900	-1.31854100
C	1.49928600	-2.99823400	-1.19836400
C	2.09689700	-1.70832500	-1.14316200

C	5.74631400	-2.53501200	-1.35768400
C	6.54027200	-3.65748800	-1.42840100
C	5.96314600	-4.94737900	-1.49085500
C	4.59552000	-5.08606300	-1.46199400
O	2.90737400	0.11436000	0.90140600
O	1.28787500	-0.60081800	-0.93975600
P	1.29001800	0.07526000	0.56149500
O	0.67628900	1.42500200	0.47010200
N	0.67080900	-1.07011500	1.52000300
C	0.03149300	-3.21227800	-1.17045100
C	4.28467900	2.61957300	1.49417900
C	-0.81827100	-2.52864000	-2.05152400
C	-2.17723400	-2.83435900	-2.09937500
C	-2.70832700	-3.82346900	-1.26740700
C	-1.87258700	-4.49053300	-0.36962400
C	-0.51370200	-4.18514600	-0.32055400
C	4.49029100	4.01178300	1.52484800
C	4.53178300	4.71032200	2.72860100
C	4.33738900	4.03652500	3.93676400
C	4.08127200	2.66523800	3.91851500
C	4.05815700	1.96013300	2.71625700
S	1.13453500	-1.50853500	2.95784500
O	-0.02448000	-2.08980600	3.67820000
O	1.97483000	-0.55343300	3.69893200
C	2.24942300	-2.97682100	2.66003400
F	3.24272100	-2.64779200	1.82727300
F	1.55940200	-3.99351400	2.11958100
F	2.77250700	-3.39106900	3.81904100
H	6.93282900	2.07184600	-5.06957200
H	5.82300100	-0.12914600	-5.44369300
H	4.47877900	-1.16553900	-3.65921300
H	6.65399900	3.24349000	-2.90611300
H	5.77484200	3.29776300	-0.63688700
H	1.91128400	-5.08126300	-1.37760300
H	6.20253100	-1.55464500	-1.29706300
H	7.62140600	-3.55149800	-1.42937300

H	6.60188000	-5.82399700	-1.54950500
H	4.13739100	-6.07143800	-1.49275500
H	-0.41674500	-1.75145900	-2.68951900
H	-2.82829500	-2.29897900	-2.78562900
H	-3.76590600	-4.06110500	-1.31512300
H	-2.27693800	-5.25226600	0.29184400
H	0.13156800	-4.68747400	0.38978000
H	4.61370200	4.55612400	0.59380900
H	4.70437900	5.78342200	2.72135400
H	4.36527700	4.57871600	4.87799700
H	3.89647000	2.12787600	4.84365800
H	3.85912200	0.89824000	2.73861500
H	-1.58656000	-1.23808600	3.00533700

TfOH-a-TS1F

Zero-point correction=0.346294

Thermal correction to Energy= 0.371891

Thermal correction to Enthalpy= 0.372836

Thermal correction to Gibbs Free Energy= 0.289271

SCF Done: E(Solv) = -1712.67070398

C	-2.767576	-1.065187	0.057541
C	-2.165906	-1.389158	-1.159793
C	-1.162833	-0.569435	-1.684226
C	-0.769853	0.544457	-0.964169
C	-1.324203	0.909514	0.275728
C	-2.351852	0.074257	0.760678
N	0.342364	1.326219	-1.441788
C	0.205677	2.807556	-1.223482
C	-0.047393	2.972066	0.256922
C	-0.762297	2.086124	0.973127
C	-0.899228	2.255800	2.464046
C	-0.955454	3.360284	-2.066138
C	1.532749	3.452946	-1.633260
O	-2.931378	0.439909	1.935702

C	-3.867282	-0.433305	2.545693
O	-2.496501	-2.471967	-1.912545
C	-3.475995	-3.366247	-1.407557
H	-3.554881	-1.686123	0.456687
H	-0.692170	-0.839667	-2.623409
H	0.501245	1.133013	-2.431768
H	-0.279135	3.092581	2.798989
H	-1.933332	2.438694	2.765081
H	-0.560716	1.348788	2.973974
H	-1.896803	2.871963	-1.800120
H	-1.064236	4.433679	-1.884145
H	-0.770723	3.213894	-3.138383
H	1.481210	4.533250	-1.466340
H	2.363627	3.048720	-1.049428
H	1.736796	3.289169	-2.698528
H	-4.127244	0.031936	3.497613
H	-4.773984	-0.541618	1.936434
H	-3.429831	-1.422251	2.729645
H	-3.560586	-4.164174	-2.146538
H	-3.168912	-3.791883	-0.443909
H	-4.449587	-2.872062	-1.293108
C	2.493304	-1.985688	-0.005024
F	2.365197	-2.979999	0.877304
F	1.476154	-2.051950	-0.881537
F	3.640461	-2.137829	-0.671049
S	2.452165	-0.348624	0.874735
O	1.160675	-0.323181	1.563434
O	3.694404	-0.251975	1.628566
O	2.481718	0.612092	-0.351220
H	1.448798	0.906743	-0.801555
H	0.400489	3.834865	0.741073

TfOH-a-IM1F

Zero-point correction=0.350296

Thermal correction to Energy= 0.376154

Thermal correction to Enthalpy= 0.377098

Thermal correction to Gibbs Free Energy= 0.292984

SCF Done: E(Solv) = -1712.67889338

C	-2.826627	-0.958671	0.076702
C	-2.256712	-1.316611	-1.146094
C	-1.214777	-0.550260	-1.679656
C	-0.769601	0.536960	-0.956492
C	-1.285266	0.940679	0.282657
C	-2.349244	0.157835	0.778452
N	0.389672	1.273402	-1.450857
C	0.307012	2.775473	-1.245320
C	0.065584	2.956365	0.234119
C	-0.664634	2.096823	0.966133
C	-0.755840	2.262191	2.459912
C	-0.835620	3.336526	-2.101250
C	1.661717	3.352471	-1.663168
O	-2.898632	0.551853	1.955675
C	-3.853488	-0.285748	2.589134
O	-2.648618	-2.379456	-1.893523
C	-3.652459	-3.236754	-1.368990
H	-3.639803	-1.539285	0.484943
H	-0.756416	-0.850159	-2.615517
H	0.534160	1.064593	-2.441606
H	-0.106896	3.082074	2.780737
H	-1.776074	2.464402	2.793041
H	-0.416712	1.342866	2.946762
H	-1.793753	2.891461	-1.820835
H	-0.902716	4.416654	-1.944580
H	-0.658200	3.159439	-3.169960
H	1.662166	4.432348	-1.487759
H	2.470891	2.899535	-1.084627
H	1.848907	3.186979	-2.731157

H	-4.073108	0.190387	3.545547
H	-4.777114	-0.359291	2.000741
H	-3.447702	-1.289286	2.764287
H	-3.778576	-4.031773	-2.104824
H	-3.342991	-3.670865	-0.410267
H	-4.604550	-2.706007	-1.239790
C	2.427590	-2.023188	-0.031930
F	2.199096	-3.040534	0.805856
F	1.437074	-2.005980	-0.952837
F	3.581519	-2.245263	-0.671800
S	2.461401	-0.405240	0.880514
O	1.145957	-0.353529	1.541795
O	3.663450	-0.441827	1.711383
O	2.568163	0.564715	-0.288666
H	1.301279	0.914663	-0.914957
H	0.559510	3.798677	0.708075

TfOH-a-IM2F

Zero-point correction=0.693889

Thermal correction to Energy= 0.743124

Thermal correction to Enthalpy= 0.744068

Thermal correction to Gibbs Free Energy= 0.609849

SCF Done: E(Solv) = -2803.28911826

C	-2.956732	3.956563	-0.074663
C	-1.639404	4.419739	-0.120677
C	-0.592553	3.601846	-0.561411
C	-0.905914	2.308513	-0.952720
C	-2.236663	1.823512	-0.923769
C	-3.266115	2.656181	-0.480265
N	-0.041224	1.292009	-1.439163
C	-0.763820	0.113963	-1.639962
C	-2.213396	0.443430	-1.392457
C	-2.266528	-1.664876	1.374705
C	-1.757489	-2.855959	1.007083

C	-3.108524	-0.534213	-1.642388
C	-1.339437	-0.555245	1.680958
C	0.031879	-0.693076	1.383069
N	0.474670	-1.911639	0.699293
C	-0.289053	-3.179591	1.019997
C	-1.705404	0.684541	2.260232
C	-0.764608	1.697112	2.475146
C	0.574791	1.499056	2.134671
C	0.990715	0.277954	1.591744
C	0.137810	-3.657819	2.417676
C	0.106345	-4.186953	-0.064056
O	-0.298386	-0.984536	-1.899746
O	-3.012773	0.846695	2.592866
O	1.540627	2.435095	2.295663
C	-3.437056	2.075369	3.165191
C	1.173420	3.706791	2.808620
C	-4.569470	-0.473741	-1.479418
O	-5.233280	0.488772	-1.132555
O	-5.107207	-1.680142	-1.753595
C	-6.925495	-3.218097	-1.882866
C	-6.539576	-1.782836	-1.588297
O	1.939307	2.279090	-1.024034
C	3.317082	2.769006	-1.331834
C	3.599841	3.679744	-0.140346
C	3.259994	3.550096	-2.643195
C	4.303711	1.608018	-1.377424
C	1.327186	1.422708	-1.833307
O	1.773893	0.821251	-2.776226
C	-3.765136	-1.511126	1.489937
H	-3.750689	4.615214	0.264187
H	-1.414884	5.437557	0.186255
H	0.427895	3.955127	-0.581486
H	-4.280636	2.282415	-0.466106
H	-2.424904	-3.682535	0.779307
H	-2.707957	-1.482955	-1.984406
H	0.413413	-1.740949	-0.320653

H	-1.084032	2.641147	2.887631
H	2.037582	0.119637	1.344989
H	-0.081352	-2.892872	3.168654
H	1.205649	-3.887965	2.442338
H	-0.432118	-4.555968	2.672620
H	-0.365108	-5.152325	0.142034
H	-0.223877	-3.844549	-1.050660
H	1.191902	-4.324324	-0.079206
H	-4.509550	1.963859	3.330542
H	-2.937058	2.261079	4.123942
H	-3.257303	2.912975	2.482296
H	2.089747	4.297790	2.816912
H	0.428427	4.192099	2.166740
H	0.781450	3.626827	3.830487
H	-8.007769	-3.341531	-1.771271
H	-6.649266	-3.494680	-2.904943
H	-6.426437	-3.905067	-1.192139
H	-6.793259	-1.485350	-0.565914
H	-7.021575	-1.074226	-2.269126
H	3.529127	3.111859	0.790442
H	4.608064	4.095742	-0.228513
H	2.886524	4.511161	-0.102945
H	3.021874	2.893002	-3.482235
H	4.235891	4.009075	-2.831906
H	2.511823	4.348890	-2.588894
H	5.313562	2.018401	-1.490422
H	4.272541	1.028279	-0.452364
H	4.103105	0.944172	-2.217112
H	-4.128955	-0.587506	1.041793
H	-4.258185	-2.360611	1.007998
H	-4.069978	-1.483263	2.541372
S	4.117800	-2.013242	0.809577
O	2.908484	-2.751264	1.330057
O	5.392890	-2.690220	1.037579
C	3.811205	-2.127122	-1.019931
F	3.691624	-3.403601	-1.411648

F	4.791699	-1.552397	-1.724088
F	2.650182	-1.495966	-1.320429
H	1.498813	-2.111937	0.924430
O	4.046120	-0.559947	1.080792

TfOH-a-TS2F

Zero-point correction= 0.693159 (Hartree/Particle)

Thermal correction to Energy= 0.741069

Thermal correction to Enthalpy= 0.742013

Thermal correction to Gibbs Free Energy= 0.611340

SCF Done: E(Solv) = -2803.25954317

C	-2.521026	3.894105	-0.455629
C	-1.250760	4.431374	-0.706978
C	-0.203722	3.619422	-1.150187
C	-0.457320	2.261690	-1.312471
C	-1.737311	1.690621	-1.050528
C	-2.774447	2.534660	-0.628144
N	0.397569	1.244908	-1.779101
C	-0.278280	0.007959	-1.733760
C	-1.632433	0.267288	-1.291585
C	-2.712599	-0.552110	1.497907
C	-2.506476	-1.661854	0.629480
C	-2.496994	-0.858894	-1.123202
C	-1.574345	0.248699	1.753608
C	-0.277419	-0.161517	1.295455
N	-0.054955	-1.510732	0.783533
C	-1.220230	-2.461322	0.857187
C	-1.635343	1.575921	2.309791
C	-0.532057	2.408976	2.328101
C	0.696692	1.955000	1.818407
C	0.836781	0.646155	1.342286
C	-1.254176	-3.057941	2.276777
C	-0.981158	-3.581533	-0.157773
O	0.271876	-1.095380	-1.893175

O	-2.845347	1.976422	2.745864
O	1.803845	2.712832	1.790630
C	-3.023590	3.332278	3.147416
C	1.713853	4.084687	2.167450
C	-3.974283	-0.734838	-1.338525
O	-4.671685	0.231519	-1.102160
O	-4.467401	-1.899825	-1.809371
C	-6.236650	-3.328332	-2.530525
C	-5.896801	-1.938261	-2.032623
O	2.394512	2.222143	-1.400711
C	3.843324	2.475901	-1.608492
C	4.162821	3.463255	-0.488766
C	4.043353	3.111493	-2.983785
C	4.638444	1.182612	-1.431139
C	1.759494	1.329389	-2.167168
O	2.218852	0.657962	-3.056232
C	-4.113027	-0.239035	1.941350
H	-3.328892	4.550580	-0.143094
H	-1.077256	5.496093	-0.576646
H	0.779732	4.023432	-1.351623
H	-3.759693	2.123718	-0.459225
H	-3.356901	-2.334237	0.533635
H	-2.109492	-1.726782	-1.649810
H	0.259836	-1.453480	-0.220441
H	-0.624380	3.417759	2.696626
H	1.806419	0.284140	1.013230
H	-1.358946	-2.279523	3.036972
H	-0.331938	-3.611963	2.470809
H	-2.104114	-3.741325	2.365341
H	-1.850951	-4.245162	-0.175716
H	-0.798963	-3.196859	-1.162112
H	-0.105415	-4.165596	0.136291
H	-4.082810	3.426735	3.387813
H	-2.423549	3.561260	4.035675
H	-2.762841	4.010019	2.328072
H	2.705491	4.500158	1.992187

H	0.978526	4.607370	1.547343
H	1.456135	4.186794	3.228185
H	-7.313229	-3.403234	-2.716043
H	-5.708702	-3.547281	-3.463583
H	-5.960165	-4.086821	-1.791264
H	-6.404197	-1.696865	-1.092995
H	-6.156891	-1.161993	-2.758314
H	3.974923	3.001057	0.483232
H	5.215678	3.756408	-0.545250
H	3.547099	4.365229	-0.578992
H	3.775605	2.414634	-3.779556
H	5.095528	3.390368	-3.104678
H	3.436314	4.018545	-3.082008
H	5.705483	1.429674	-1.396045
H	4.367844	0.678223	-0.499788
H	4.465617	0.492374	-2.256712
H	-4.488156	0.685873	1.497972
H	-4.783174	-1.053328	1.655371
H	-4.156294	-0.112529	3.027563
S	3.268507	-2.416667	1.331904
O	1.941044	-2.667493	2.017230
O	4.432580	-2.859962	2.095373
C	3.143635	-3.564847	-0.121510
F	2.944477	-4.828375	0.282561
F	4.246868	-3.519994	-0.870651
F	2.090691	-3.207169	-0.887579
H	0.783977	-1.954511	1.308248
O	3.318262	-1.079178	0.698091

TfOH-a-IM3F

Zero-point correction= 0.694221 (Hartree/Particle)

Thermal correction to Energy= 0.742309

Thermal correction to Enthalpy= 0.743253

Thermal correction to Gibbs Free Energy= 0.611136

SCF Done: E(Solv) = -2803.26758373

C	-3.782773	2.375164	0.418002
C	-2.869248	3.424650	0.231987
C	-1.636956	3.210138	-0.395490
C	-1.332231	1.917507	-0.807896
C	-2.240200	0.833417	-0.608292
C	-3.480300	1.081287	-0.002483
N	-0.211508	1.417767	-1.490955
C	-0.349287	0.009712	-1.653689
C	-1.605696	-0.354862	-1.089974
C	-2.158269	-1.915840	1.463854
C	-1.715789	-2.638666	0.248469
C	-2.064885	-1.761818	-1.066886
C	-1.359480	-0.834969	1.822745
C	-0.069985	-0.641284	1.196372
N	0.569357	-1.727183	0.467168
C	-0.214084	-3.011840	0.350863
C	-1.806917	0.250477	2.675645
C	-1.083491	1.415432	2.798241
C	0.149744	1.548719	2.123677
C	0.684842	0.496177	1.371974
C	0.041891	-3.843585	1.617038
C	0.315347	-3.771849	-0.868072
O	0.570967	-0.743615	-2.037237
O	-3.012440	0.082240	3.244031
O	0.899006	2.654316	2.201246
C	-3.618766	1.184193	3.917022
C	0.382679	3.804285	2.870490
C	-3.560435	-1.873965	-1.349591
O	-4.381601	-2.412045	-0.632185

O	-3.859717	-1.284100	-2.512653
C	-5.373643	-0.402753	-4.126725
C	-5.260871	-1.247190	-2.874160
O	1.285776	3.032517	-0.997839
C	2.527217	3.824320	-1.182231
C	2.565148	4.673105	0.086193
C	2.383880	4.697600	-2.428308
C	3.740952	2.895966	-1.243200
C	0.963487	2.092228	-1.896677
O	1.557403	1.805953	-2.905914
C	-3.411166	-2.346546	2.161118
H	-4.745614	2.578216	0.879555
H	-3.128263	4.427779	0.559098
H	-0.932519	4.018140	-0.547977
H	-4.189424	0.273119	0.147741
H	-2.276723	-3.567986	0.136702
H	-1.555285	-2.268913	-1.892656
H	0.799223	-1.390863	-0.514214
H	-1.476043	2.239131	3.371855
H	1.677471	0.582498	0.940669
H	-0.265225	-3.317173	2.524383
H	1.106702	-4.075182	1.701962
H	-0.519636	-4.781133	1.557932
H	-0.277054	-4.680341	-1.014447
H	0.289527	-3.167523	-1.776005
H	1.355316	-4.062264	-0.697480
H	-4.601108	0.829042	4.228562
H	-3.035719	1.474538	4.798211
H	-3.722937	2.033139	3.233295
H	1.134462	4.580346	2.734830
H	-0.561683	4.119930	2.416232
H	0.245520	3.609092	3.940062
H	-6.420987	-0.342166	-4.440959
H	-5.005655	0.610792	-3.941016
H	-4.790743	-0.837552	-4.944318
H	-5.610307	-2.273108	-3.027792

H	-5.823150	-0.823550	-2.036594
H	2.651467	4.028850	0.964313
H	3.427963	5.345562	0.054621
H	1.656637	5.279326	0.175057
H	2.319810	4.085567	-3.329071
H	3.256108	5.354489	-2.513742
H	1.488803	5.325856	-2.357192
H	4.651121	3.502782	-1.178584
H	3.737664	2.187961	-0.409606
H	3.763102	2.328855	-2.173497
H	-4.246350	-1.675043	1.937777
H	-3.699793	-3.343977	1.827952
H	-3.278305	-2.337803	3.246135
S	4.017412	-1.439199	0.892979
O	2.905267	-2.251336	1.524468
O	5.298141	-1.532871	1.590317
C	4.245897	-2.336192	-0.716006
F	4.562236	-3.622440	-0.507583
F	5.203008	-1.770767	-1.454130
F	3.090844	-2.304301	-1.416406
H	1.533120	-1.933352	0.919160
O	3.554761	-0.099123	0.465381

TfOH-a-TS3E

Zero-point correction= 0.691712 (Hartree/Particle)

Thermal correction to Energy= 0.740289

Thermal correction to Enthalpy= 0.741233

Thermal correction to Gibbs Free Energy= 4h-a-TS3 0.607535

SCF Done: E(Solv) = -2803.2610395

C	0.28829200	-5.10749600	-0.36114600
C	-1.01835800	-4.95883800	-0.82762800
C	-1.58609600	-3.68887300	-1.00132500
C	-0.80950600	-2.58085400	-0.69578600
C	0.51964000	-2.71340300	-0.21441500
C	1.06306200	-3.98819900	-0.04607800

N	-1.09766200	-1.18570600	-0.81398100
C	0.06780900	-0.45422100	-0.45478000
C	1.02281600	-1.38432200	0.08783300
C	0.92394300	-1.01113900	2.15074600
C	2.38862000	-0.59494900	1.86985500
C	2.42794900	-0.83936500	0.35170500
C	-0.05192400	0.02578500	2.37250400
C	0.33369500	1.39673600	2.18853800
N	1.64788900	1.73006100	2.07630900
C	2.73839100	0.81311000	2.38063400
C	-1.45575300	-0.23668700	2.45323100
C	-2.40556300	0.76701900	2.35677000
C	-1.97619900	2.10056300	2.17990300
C	-0.63134600	2.41510500	2.12144900
C	2.92146600	0.74602400	3.91259700
C	4.01700900	1.34621400	1.72833600
O	0.20274200	0.77044800	-0.51225400
O	-1.80884400	-1.54692700	2.57816400
O	-2.83479500	3.14689000	2.07966500
C	-3.16168800	-1.92408900	2.38185500
C	-4.22910700	2.88909500	2.06483300
C	3.51550400	-1.78416300	-0.10994200
O	4.10510200	-2.57701000	0.59891800
O	3.71649700	-1.65300100	-1.43326700
C	3.92661300	-3.83482200	-2.50687100
C	4.64525600	-2.57486800	-2.05360200
O	-3.30022000	-1.42582000	-1.22216300
C	-4.63483200	-0.99527600	-1.69047100
C	-5.42368200	-2.30325000	-1.67372400
C	-4.52390200	-0.43855800	-3.10982500
C	-5.23589100	0.01646500	-0.71376400
C	-2.29357000	-0.53938100	-1.13530300
O	-2.38716200	0.65953200	-1.28947500
C	0.81577400	-2.38279700	2.76528300
H	0.70835300	-6.10124200	-0.23615100
H	-1.61189000	-5.83643700	-1.06613800

H	-2.59583300	-3.57939800	-1.36775000
H	2.07309700	-4.10402100	0.33057000
H	3.05880000	-1.30292000	2.36461600
H	2.51327200	0.09093900	-0.21241100
H	-0.58178100	2.08854700	-0.93445500
H	-3.45697600	0.53224000	2.41299700
H	-0.33062400	3.44404900	1.97364900
H	2.00942400	0.38054400	4.39568100
H	3.13661400	1.74386600	4.30666800
H	3.74630200	0.07653000	4.18068200
H	4.84163100	0.64130400	1.87388000
H	3.88053100	1.51214000	0.65611900
H	4.30288800	2.30194700	2.18172000
H	-3.17421000	-3.01314500	2.44852700
H	-3.81575400	-1.50483400	3.15664300
H	-3.51304700	-1.61771100	1.39082000
H	-4.70861900	3.86114100	1.94056400
H	-4.50616300	2.23757000	1.22768100
H	-4.56662900	2.43680500	3.00667600
H	4.62111300	-4.48372600	-3.05230000
H	3.53627400	-4.38920900	-1.64976000
H	3.09006300	-3.58643500	-3.16705400
H	5.05427600	-2.01855100	-2.89994400
H	5.44401800	-2.79990100	-1.34369100
H	-5.43825600	-2.73334100	-0.66723600
H	-6.45582300	-2.11953100	-1.98770100
H	-4.97952900	-3.03293900	-2.35806900
H	-3.95570900	0.49233400	-3.12672200
H	-5.52761400	-0.24473500	-3.50251900
H	-4.03596000	-1.16755600	-3.76515200
H	-6.26428300	0.24189500	-1.01555100
H	-5.26349900	-0.39856400	0.29940400
H	-4.65756600	0.94033100	-0.70607700
H	-0.10556100	-2.89925900	2.51248200
H	1.66798100	-2.99927800	2.47188200
H	0.84735300	-2.26555000	3.85799700

S	0.65696500	3.85870700	-1.26239600
O	1.32086700	3.85751800	0.04211800
O	0.40971800	5.10777200	-1.95992600
C	1.77076700	2.82585700	-2.37826400
F	2.51224500	3.65759100	-3.11004300
F	1.04410400	2.05197900	-3.18251100
F	2.58547900	2.05911400	-1.64528400
H	1.85190000	2.61248000	1.62527800
O	-0.69555400	3.04273800	-1.27080300

TfOH-a-TS2E

Zero-point correction= 0.691090 (Hartree/Particle)

Thermal correction to Energy= 0.739118

Thermal correction to Enthalpy= 0.740062

Thermal correction to Gibbs Free Energy= 0.610723

SCF Done: E(Solv) = -2803.25416452

C	-3.207801	3.080192	-0.654804
C	-2.045635	3.856747	-0.710627
C	-0.798651	3.261641	-0.922777
C	-0.741917	1.877697	-1.065166
C	-1.911910	1.074064	-1.025686
C	-3.147490	1.698267	-0.816460
N	0.374160	1.017086	-1.259821
C	-0.092119	-0.334815	-1.323575
C	-1.518397	-0.308702	-1.200954
C	-2.912863	-1.248377	1.390168
C	-2.486537	-2.394252	0.671723
C	-2.232487	-1.537317	-1.189846
C	-1.913111	-0.367241	1.852167
C	-0.521418	-0.745042	1.661165
N	-0.203773	-2.006498	1.332775
C	-1.192964	-3.060707	1.109173
C	-2.152156	0.976411	2.313105
C	-1.133822	1.895179	2.437037

C	0.195353	1.505135	2.135367
C	0.509188	0.203438	1.802782
C	-1.460208	-3.798363	2.443670
C	-0.629705	-4.061623	0.091275
O	0.627132	-1.345241	-1.458643
O	-3.444364	1.286347	2.570020
O	1.233098	2.377849	2.182266
C	-3.772530	2.633188	2.886323
C	0.959652	3.760880	2.373664
C	-3.620163	-1.708637	-1.741296
O	-4.278940	-2.727321	-1.633198
O	-4.039718	-0.632459	-2.434147
C	-6.449071	-0.393790	-2.053267
C	-5.347096	-0.727252	-3.046307
O	1.918169	2.657553	-1.176923
C	3.284687	3.221335	-1.153607
C	3.008094	4.720561	-1.045349
C	3.993790	2.888982	-2.466057
C	4.053402	2.718334	0.069541
C	1.732816	1.333353	-1.226618
O	2.612923	0.498183	-1.247437
C	-4.394741	-0.976314	1.435150
H	-4.171925	3.558833	-0.503618
H	-2.105241	4.936283	-0.604855
H	0.095662	3.861829	-0.980865
H	-4.051969	1.107812	-0.793126
H	-3.254981	-3.099047	0.372421
H	-1.618448	-2.372741	-1.514274
H	0.767230	-2.224192	1.122584
H	-1.347440	2.911866	2.722949
H	1.536957	-0.073514	1.603840
H	-1.823689	-3.101837	3.205085
H	-0.533046	-4.256765	2.803413
H	-2.209223	-4.586744	2.307109
H	-1.407892	-4.768914	-0.212570
H	-0.231294	-3.554198	-0.788556

H	0.192620	-4.625518	0.541876
H	-4.857323	2.651868	2.999943
H	-3.301211	2.943209	3.826879
H	-3.469873	3.304500	2.075307
H	1.922528	4.265154	2.282269
H	0.273110	4.134056	1.606577
H	0.546736	3.953414	3.371282
H	-7.421991	-0.416952	-2.556811
H	-6.466392	-1.123396	-1.239675
H	-6.305788	0.607054	-1.632986
H	-5.309912	-0.004097	-3.863560
H	-5.471903	-1.733511	-3.452009
H	2.481709	4.951401	-0.113607
H	3.951457	5.274996	-1.055351
H	2.395780	5.062606	-1.885675
H	4.161736	1.815057	-2.556933
H	4.962902	3.398834	-2.493133
H	3.401034	3.234078	-3.319726
H	4.925707	3.361154	0.231767
H	3.418732	2.755457	0.959200
H	4.393723	1.693873	-0.065461
H	-4.931216	-1.759584	0.895399
H	-4.745747	-0.966107	2.472938
H	-4.655598	-0.003537	1.016896
H	2.098317	-1.677988	-1.499292
O	2.974676	-2.231392	-1.601348
S	3.538535	-2.781621	-0.250606
O	4.434383	-3.888868	-0.530245
O	2.491366	-2.910078	0.771287
C	4.623993	-1.387687	0.365829
F	5.537127	-1.906083	1.190857
F	3.896260	-0.493711	1.044849
F	5.239724	-0.779224	-0.646169

TfOH-a-IM3E

Zero-point correction= 0.694306 (Hartree/Particle)

Thermal correction to Energy= 0.742621

Thermal correction to Enthalpy= 0.743565

Thermal correction to Gibbs Free Energy= 0.612478

E(Solv)= -2803.29305565

C	3.32220400	2.89996300	0.06731900
C	2.19324800	3.72781500	0.13494900
C	0.95148400	3.22364200	0.53298800
C	0.86473900	1.86957800	0.84658300
C	1.99482200	1.01142400	0.76454000
C	3.23144100	1.54622600	0.38375700
N	-0.22773200	1.07737100	1.27769000
C	0.23829900	-0.25057500	1.44020400
C	1.57055700	-0.32048600	1.11161600
C	2.79822100	-1.33917000	-1.40905000
C	2.43117500	-2.34092300	-0.34192700
C	2.34054200	-1.60571000	1.06530200
C	1.77325400	-0.57580300	-1.91149700
C	0.38501500	-0.93650300	-1.57027200
N	0.12255400	-2.14383800	-1.08870300
C	1.16222200	-3.12018400	-0.75361900
C	1.95391300	0.69347800	-2.61322900
C	0.92555500	1.58658400	-2.73442400
C	-0.37749500	1.23444800	-2.26022300
C	-0.66248200	-0.01724000	-1.76226700
C	1.46557300	-3.97380600	-2.00367200
C	0.61227100	-4.03100500	0.35157600
O	-0.47420900	-1.26687800	1.87368900
O	3.20601200	0.94372700	-3.03948500
O	-1.40605100	2.10315700	-2.30503200
C	3.50972800	2.24713500	-3.53004500
C	-1.16660100	3.46292900	-2.65987600
C	3.73557500	-1.46589400	1.67637500
O	4.76416000	-1.90956400	1.20232000
O	3.67155500	-0.81366700	2.84569300

C	5.68143100	0.57906300	3.00141300
C	4.91940700	-0.61405000	3.55438500
O	-1.75377700	2.72882300	1.16912700
C	-3.10175500	3.33620400	1.27831700
C	-2.83140200	4.78299200	0.86857200
C	-3.57859400	3.25702200	2.72754600
C	-4.06358900	2.65864400	0.30366100
C	-1.57416400	1.43319700	1.43254000
O	-2.42115700	0.63319300	1.76535100
C	4.24993900	-1.19401700	-1.76006000
H	4.28296600	3.32011900	-0.21811900
H	2.28272700	4.78476100	-0.09906700
H	0.08909200	3.86851000	0.60921300
H	4.11142700	0.91438000	0.34101600
H	3.23948400	-3.06682900	-0.23686000
H	1.82082100	-2.30329900	1.73046600
H	-0.86872300	-2.40833700	-0.93168400
H	1.09444500	2.56054100	-3.16396800
H	-1.67253100	-0.27478700	-1.47447300
H	1.82702500	-3.36013600	-2.83456500
H	0.55460000	-4.48496900	-2.32700900
H	2.22614200	-4.72860000	-1.77469300
H	1.38958000	-4.72148000	0.69498500
H	0.22484800	-3.45953600	1.19603200
H	-0.22010800	-4.61893100	-0.04689800
H	4.57578700	2.23281100	-3.75800500
H	2.94121600	2.46431100	-4.44164000
H	3.29782000	2.99911100	-2.76265300
H	-2.12053600	3.97070400	-2.51623800
H	-0.40805300	3.90744300	-2.00750600
H	-0.86382300	3.55446300	-3.70932000
H	6.55354400	0.78565900	3.63174300
H	6.03284800	0.37389800	1.98670400
H	5.04428500	1.46832200	2.98243700
H	4.60958700	-0.44958700	4.58817800
H	5.51079600	-1.53070700	3.49176700

H	-2.46140900	4.83144500	-0.16063300
H	-3.75587700	5.36499400	0.93012400
H	-2.08884600	5.24168900	1.52936400
H	-3.73909600	2.22160800	3.03029900
H	-4.52439000	3.80043700	2.82582000
H	-2.84647800	3.71938900	3.39811400
H	-4.96173900	3.27780500	0.20231100
H	-3.59686500	2.55642600	-0.68093400
H	-4.35689300	1.66882600	0.64781100
H	4.84807600	-1.92234800	-1.21592600
H	4.38886100	-1.32345800	-2.83863700
H	4.62155000	-0.19245800	-1.52976500
H	-1.46390800	-1.26508900	1.70995400
O	-2.83632800	-2.23832400	1.47824900
S	-3.46012400	-2.73558800	0.22391500
O	-4.39488200	-3.85055700	0.37673000
O	-2.49674700	-2.85512300	-0.91583200
C	-4.51708300	-1.30665000	-0.32609500
F	-5.31026400	-1.65954100	-1.34384500
F	-3.74330000	-0.27670600	-0.74741500
F	-5.28124900	-0.85160700	0.67547200

4h-a-TS2B

Zero-point correction= 1.125784 (Hartree/Particle)

Thermal correction to Energy= 1.201705

Thermal correction to Enthalpy= 1.202649

Thermal correction to Gibbs Free Energy= 1.012878

E(Solv) = -4581.93023909

C	6.971028	-1.149203	1.884618
C	7.260499	0.190651	1.611651
C	6.252368	1.072044	1.198005
C	4.965212	0.571904	1.056926
C	4.653578	-0.790353	1.309582
C	5.673353	-1.644083	1.744754

N	3.764636	1.223933	0.674643
C	2.706411	0.262107	0.616049
C	3.250620	-0.998194	1.015505
C	4.000311	-3.073425	-1.025374
C	2.732543	-3.472116	-0.501746
C	2.443519	-2.177685	0.999782
C	4.016184	-1.872279	-1.757328
C	2.741614	-1.227640	-2.058891
N	1.587445	-1.887517	-1.855347
C	1.546694	-3.291615	-1.437245
C	5.204861	-1.108104	-2.054378
C	5.140112	0.203557	-2.472254
C	3.872747	0.803576	-2.681967
C	2.698819	0.091772	-2.536699
C	1.719163	-4.197109	-2.680682
C	0.201420	-3.637247	-0.790067
O	1.568206	0.580504	0.212383
O	6.377261	-1.745843	-1.856411
O	3.738888	2.099375	-3.053236
C	7.583073	-0.988333	-1.858548
C	4.897047	2.926107	-3.091650
C	2.517678	-3.181710	2.102491
O	3.511800	-3.582682	2.676934
O	1.276457	-3.645940	2.357735
C	-0.273939	-5.151869	3.342340
C	1.143075	-4.616692	3.414362
O	4.622621	3.285533	0.348730
C	4.690002	4.742166	0.580847
C	6.123938	5.079722	0.173227
C	4.468770	5.039470	2.065047
C	3.684509	5.467965	-0.313435
C	3.511971	2.601337	0.705844
O	2.450634	3.092628	1.009260
C	5.198671	-3.899061	-0.643026
H	7.761044	-1.813588	2.224178
H	8.273253	0.565299	1.733169

H	6.471324	2.109162	0.989496
H	5.435454	-2.668442	1.995704
H	2.727819	-4.437957	-0.000757
H	1.414522	-1.930447	0.783394
H	0.171351	0.072853	0.525201
H	6.043029	0.771909	-2.625262
H	1.747795	0.583432	-2.698759
H	2.635088	-3.948309	-3.224094
H	0.865514	-4.066516	-3.354009
H	1.767373	-5.251305	-2.384745
H	0.213206	-4.688020	-0.486594
H	-0.026745	-3.045242	0.094699
H	-0.611524	-3.500216	-1.505283
H	8.369872	-1.694032	-1.590007
H	7.786643	-0.574597	-2.853734
H	7.535243	-0.188848	-1.112357
H	4.533547	3.924163	-3.339668
H	5.389848	2.946388	-2.114965
H	5.599102	2.595621	-3.866622
H	-0.452050	-5.857456	4.161057
H	-0.994933	-4.332809	3.410022
H	-0.437615	-5.673568	2.393354
H	1.896549	-5.398642	3.278285
H	1.346318	-4.118093	4.367723
H	6.304494	4.813930	-0.873173
H	6.299951	6.153698	0.289508
H	6.844638	4.542849	0.798184
H	3.446669	4.808059	2.366486
H	4.658873	6.101304	2.254439
H	5.162449	4.452667	2.676586
H	3.826952	6.549790	-0.213815
H	3.843486	5.199918	-1.362717
H	2.659646	5.216583	-0.044056
H	6.049126	-3.304824	-0.323867
H	4.924708	-4.598492	0.150811
H	5.524826	-4.483693	-1.515030

C	-8.742277	0.400318	-2.661215
C	-8.167612	1.586508	-2.149689
C	-6.958869	1.555143	-1.491251
C	-6.257730	0.333826	-1.307114
C	-6.819918	-0.859796	-1.866232
C	-8.076180	-0.794501	-2.525346
C	-4.994137	0.249939	-0.624763
C	-4.341404	-0.966008	-0.629749
C	-4.867948	-2.164329	-1.180756
C	-6.111173	-2.082674	-1.774046
C	-4.374381	1.456234	-0.006952
C	-5.077459	2.240960	0.968355
C	-4.540849	3.509770	1.354571
C	-3.342989	3.971289	0.753739
C	-2.607046	3.183457	-0.106459
C	-3.119751	1.887906	-0.400426
C	-6.263229	1.785167	1.600783
C	-6.897981	2.554572	2.549884
C	-6.383167	3.821381	2.910910
C	-5.228119	4.284858	2.325139
O	-3.082590	-1.047253	-0.035554
O	-2.339121	1.073531	-1.220067
P	-1.796434	-0.368830	-0.720410
O	-1.128490	-1.019064	-1.869420
N	-0.856315	-0.213749	0.661940
C	-1.426602	3.720658	-0.831903
C	-4.113141	-3.440386	-1.132096
C	-1.579277	4.915981	-1.552864
C	-0.528418	5.428248	-2.311552
C	0.686539	4.744037	-2.368368
C	0.853160	3.566674	-1.638823
C	-0.190864	3.063298	-0.866126
C	-4.028875	-4.242120	-2.280181
C	-3.352353	-5.460603	-2.249166
C	-2.752540	-5.897178	-1.067478
C	-2.827659	-5.103846	0.078717

C	-3.496877	-3.883107	0.049123
S	-1.087907	-0.820608	2.197823
O	0.163598	-0.579249	2.903694
O	-1.725510	-2.133123	2.198361
C	-2.348008	0.346986	2.956424
F	-2.244572	0.238975	4.281514
F	-3.581740	0.008569	2.583912
F	-2.094784	1.601152	2.589107
H	-9.699980	0.438786	-3.171950
H	-8.681612	2.534090	-2.282081
H	-6.528386	2.474286	-1.115350
H	-8.494430	-1.711625	-2.931903
H	-6.562220	-2.981206	-2.185123
H	-2.979784	4.965216	0.998689
H	-6.657985	0.810621	1.338238
H	-7.797923	2.182292	3.030657
H	-6.895734	4.420111	3.658156
H	-4.813790	5.249962	2.604756
H	-2.539816	5.423554	-1.540417
H	-0.666774	6.349125	-2.871733
H	1.501542	5.128212	-2.976181
H	1.796516	3.035372	-1.663885
H	-0.014068	2.179504	-0.271206
H	-4.477310	-3.892814	-3.205711
H	-3.288638	-6.064198	-3.150280
H	-2.223021	-6.845649	-1.042316
H	-2.358884	-5.428718	1.002515
H	-3.531436	-3.272215	0.942161
H	0.697099	-1.419255	-2.024611

4h-a-IM3B

Zero-point correction=1.128406 (Hartree/Particle)

Thermal correction to Energy=1.204276

Thermal correction to Enthalpy=1.205220

Thermal correction to Gibbs Free Energy= 1.014535

E(Solv) = -4581.96433916

C	7.182965	0.627171	0.252764
C	6.770783	1.962053	0.159343
C	5.424722	2.308824	0.337527
C	4.511812	1.294366	0.596830
C	4.907002	-0.072655	0.668584
C	6.264000	-0.391677	0.505371
N	3.108088	1.333303	0.753033
C	2.612114	-0.013222	0.919373
C	3.731382	-0.867004	0.864760
C	4.469132	-2.767980	-1.338041
C	3.479889	-3.231379	-0.313853
C	3.609599	-2.342759	1.018988
C	4.146210	-1.588000	-1.975517
C	2.780813	-1.064213	-1.834190
N	1.806617	-1.880918	-1.439792
C	2.049649	-3.222361	-0.899642
C	5.104905	-0.707459	-2.626057
C	4.791719	0.592830	-2.921739
C	3.478740	1.085029	-2.648668
C	2.477816	0.268551	-2.177145
C	1.944418	-4.251688	-2.042976
C	0.963250	-3.520714	0.141121
O	1.405162	-0.309002	1.080086
O	6.332990	-1.230996	-2.812700
O	3.144290	2.380399	-2.859530
C	7.391308	-0.359947	-3.198020
C	4.149633	3.299083	-3.275637
C	4.737905	-2.886056	1.883675
O	5.652153	-3.593123	1.501955

O	4.596025	-2.464006	3.151600
C	6.737762	-1.693873	4.018519
C	5.668960	-2.773406	4.070476
O	2.908985	3.547155	1.018783
C	2.370888	4.899968	0.796740
C	3.340712	5.766895	1.599649
C	0.949235	5.040798	1.339549
C	2.454150	5.220438	-0.694038
C	2.283036	2.440705	0.583013
O	1.160911	2.384083	0.122388
C	5.744247	-3.538086	-1.516017
H	8.235344	0.379299	0.137718
H	7.500325	2.745401	-0.026259
H	5.108159	3.341860	0.294230
H	6.593623	-1.421975	0.570157
H	3.707954	-4.256021	-0.013840
H	2.689100	-2.513195	1.581747
H	-0.076898	0.213761	0.824992
H	5.546385	1.259676	-3.305225
H	1.490538	0.668858	-1.984973
H	2.679165	-4.054498	-2.829685
H	0.944457	-4.208279	-2.484600
H	2.109179	-5.265553	-1.660278
H	1.193569	-4.447676	0.673973
H	0.853852	-2.703164	0.855488
H	-0.000042	-3.653735	-0.357608
H	8.288376	-0.979852	-3.216243
H	7.213707	0.057128	-4.196626
H	7.504940	0.445357	-2.464303
H	3.652105	4.266769	-3.336421
H	4.962370	3.347371	-2.542483
H	4.549529	3.034638	-4.261563
H	7.508445	-1.893978	4.771742
H	7.212015	-1.665932	3.034134
H	6.301101	-0.710335	4.215670
H	5.184712	-2.814212	5.048742

H	6.076121	-3.756352	3.822920
H	4.368362	5.629598	1.248378
H	3.074061	6.823058	1.491400
H	3.301551	5.503495	2.660875
H	0.228815	4.501005	0.728844
H	0.681797	6.103268	1.352580
H	0.897729	4.661595	2.363852
H	2.092266	6.238131	-0.875159
H	3.491354	5.156836	-1.038476
H	1.839736	4.531014	-1.272581
H	5.671002	-4.506622	-1.021079
H	5.966369	-3.676497	-2.577891
H	6.597922	-3.009528	-1.083420
C	-8.522056	-2.644033	-2.451110
C	-8.388781	-1.246721	-2.279270
C	-7.287259	-0.718615	-1.644426
C	-6.257243	-1.560413	-1.146615
C	-6.375264	-2.971893	-1.357189
C	-7.531599	-3.485163	-2.002248
C	-5.090700	-1.051464	-0.478436
C	-4.085393	-1.945239	-0.163282
C	-4.182793	-3.351744	-0.342479
C	-5.337115	-3.832858	-0.926488
C	-4.952209	0.402365	-0.187039
C	-5.919973	1.102381	0.605734
C	-5.803930	2.522497	0.737889
C	-4.757569	3.203032	0.069708
C	-3.778491	2.534098	-0.637832
C	-3.877243	1.115162	-0.680364
C	-6.960097	0.440155	1.308111
C	-7.854615	1.148403	2.078309
C	-7.757667	2.555381	2.184690
C	-6.750437	3.224226	1.529887
O	-2.900031	-1.469701	0.397702
O	-2.844127	0.414254	-1.310818
P	-1.877215	-0.545132	-0.439521

O	-0.906486	-1.195063	-1.347232
N	-1.140671	0.293926	0.809056
C	-2.772485	3.274158	-1.443060
C	-3.111593	-4.277646	0.101186
C	-3.214014	4.334496	-2.252619
C	-2.326243	5.025492	-3.074959
C	-0.981639	4.654090	-3.118631
C	-0.530563	3.609330	-2.311653
C	-1.412276	2.936679	-1.468373
C	-2.704395	-5.327242	-0.735810
C	-1.762771	-6.260137	-0.302974
C	-1.216059	-6.159376	0.976278
C	-1.602101	-5.109097	1.811464
C	-2.535544	-4.171026	1.377864
S	-1.767507	0.485846	2.356271
O	-1.102214	-0.405218	3.297417
O	-3.218458	0.603692	2.304110
C	-1.143179	2.205888	2.727620
F	-1.665552	2.577178	3.898953
F	-1.544223	3.053257	1.780401
F	0.186519	2.214845	2.819278
H	-9.399832	-3.047229	-2.947634
H	-9.160780	-0.582222	-2.656291
H	-7.194760	0.353768	-1.527961
H	-7.611219	-4.560045	-2.142689
H	-5.459051	-4.904583	-1.054070
H	-4.712697	4.286299	0.136129
H	-7.034225	-0.638864	1.246065
H	-8.636786	0.620786	2.616386
H	-8.472129	3.102029	2.793317
H	-6.654620	4.303535	1.615991
H	-4.269029	4.592856	-2.258348
H	-2.691109	5.837697	-3.697908
H	-0.291991	5.174190	-3.778215
H	0.508546	3.298687	-2.336248
H	-1.023539	2.173251	-0.813385

H	-3.122959	-5.400534	-1.735389
H	-1.456282	-7.063593	-0.967001
H	-0.485373	-6.887670	1.317010
H	-1.173648	-5.015480	2.805071
H	-2.827781	-3.359853	2.035103
H	0.853238	-1.518143	-1.371796

4h-a-TS3B

Zero-point correction= 1.127776 (Hartree/Particle)

Thermal correction to Energy= 1.203169

Thermal correction to Enthalpy= 1.204113

Thermal correction to Gibbs Free Energy= 1.016485

E(Solv) = -4581.96161268

C	6.325419	2.521287	-1.889367
C	6.858088	1.240587	-2.060767
C	6.181780	0.106288	-1.594697
C	4.962105	0.291405	-0.959115
C	4.416265	1.583993	-0.754285
C	5.106889	2.703930	-1.231094
N	4.075527	-0.649984	-0.376684
C	2.925596	0.043942	0.120130
C	3.182032	1.443920	-0.012552
C	3.348006	2.171729	2.065472
C	2.523168	3.269575	1.360865
C	2.076621	2.479419	0.132143
C	2.607916	1.261062	2.881019
C	1.219265	1.519727	3.146686
N	0.656670	2.726213	2.834361
C	1.408901	3.836835	2.249114
C	3.110338	-0.017534	3.296386
C	2.328883	-0.937149	3.976184
C	0.970032	-0.638371	4.202287
C	0.420465	0.563168	3.781255
C	2.027190	4.670572	3.387604

C	0.430993	4.687543	1.435445
O	1.908094	-0.519722	0.558096
O	4.383447	-0.291093	2.917053
O	0.124348	-1.473812	4.850590
C	4.895623	-1.603673	3.118175
C	0.646704	-2.653858	5.444519
C	1.887387	3.251716	-1.156168
O	2.199261	4.411719	-1.340927
O	1.382655	2.430721	-2.093639
C	2.642269	2.365086	-4.162874
C	1.393766	2.882776	-3.467736
O	4.811200	-2.426155	-1.540633
C	4.995804	-3.857376	-1.853576
C	5.832061	-3.804053	-3.130919
C	3.634777	-4.502311	-2.118817
C	5.763427	-4.546952	-0.725216
C	4.127203	-2.043799	-0.453009
O	3.605543	-2.781571	0.357639
C	4.802666	2.472852	2.269007
H	6.863167	3.384785	-2.269928
H	7.808896	1.114460	-2.570169
H	6.589556	-0.883825	-1.745199
H	4.687886	3.697101	-1.107521
H	3.185159	4.084345	1.054437
H	1.145310	1.951206	0.354356
H	0.518613	-0.171669	-0.285317
H	2.731645	-1.896958	4.258271
H	-0.623672	0.768259	3.982766
H	2.676336	4.053054	4.016943
H	1.236050	5.080411	4.022622
H	2.619683	5.500402	2.985684
H	0.955019	5.501361	0.928839
H	-0.084146	4.090628	0.679312
H	-0.331995	5.117188	2.094576
H	5.896198	-1.592767	2.682738
H	4.967235	-1.841074	4.186809

H	4.277624	-2.340367	2.598498
H	-0.196891	-3.126226	5.950035
H	1.037137	-3.340080	4.687690
H	1.428681	-2.415444	6.176850
H	2.629994	2.657477	-5.219119
H	3.545468	2.771838	-3.698473
H	2.685767	1.274388	-4.103768
H	0.486452	2.461795	-3.900432
H	1.349296	3.973418	-3.477355
H	6.796513	-3.320648	-2.944798
H	6.018116	-4.818562	-3.497002
H	5.307525	-3.242146	-3.909400
H	3.023166	-4.523372	-1.216406
H	3.784939	-5.529109	-2.469032
H	3.096671	-3.951610	-2.896517
H	6.020291	-5.566263	-1.032601
H	6.695113	-4.009817	-0.516831
H	5.167552	-4.594537	0.186632
H	5.267036	2.841397	1.350114
H	4.862240	3.288164	3.006934
H	5.364364	1.622423	2.645760
C	-8.652827	1.350668	1.394079
C	-8.264990	-0.008912	1.433736
C	-7.039112	-0.403643	0.947442
C	-6.135082	0.541507	0.394869
C	-6.509972	1.924319	0.396834
C	-7.789396	2.294585	0.890674
C	-4.849359	0.178513	-0.131144
C	-4.003990	1.194087	-0.524909
C	-4.325485	2.577157	-0.496770
C	-5.595316	2.903780	-0.061718
C	-4.404559	-1.240374	-0.219246
C	-5.179269	-2.198702	-0.953715
C	-4.805262	-3.576697	-0.896069
C	-3.672194	-3.954926	-0.140915
C	-2.860790	-3.035702	0.496667

C	-3.239062	-1.665797	0.400621
C	-6.282998	-1.833701	-1.769937
C	-6.995980	-2.786302	-2.461945
C	-6.645473	-4.154110	-2.375573
C	-5.568521	-4.536820	-1.611837
O	-2.716201	0.838589	-0.945673
O	-2.420417	-0.724394	1.036893
P	-1.678109	0.471531	0.232314
O	-1.258863	1.530235	1.168505
N	-0.435926	-0.115975	-0.728269
C	-1.677314	-3.523920	1.251499
C	-3.334435	3.619682	-0.858037
C	-1.806532	-4.663763	2.063342
C	-0.693978	-5.225297	2.686339
C	0.569118	-4.654989	2.512104
C	0.708117	-3.503016	1.736321
C	-0.408526	-2.947392	1.116755
C	-3.246534	4.781947	-0.075237
C	-2.328823	5.784179	-0.382487
C	-1.475776	5.639892	-1.476955
C	-1.557637	4.490403	-2.263610
C	-2.474086	3.486382	-1.960628
S	-0.644256	-0.681765	-2.296897
O	-0.696358	0.404162	-3.270181
O	-1.642866	-1.744745	-2.319909
C	1.025848	-1.504366	-2.534745
F	0.997954	-2.114411	-3.719801
F	1.250247	-2.402867	-1.579554
F	2.002063	-0.593191	-2.532651
H	-9.626206	1.646770	1.774154
H	-8.938959	-0.748539	1.856022
H	-6.751173	-1.446608	0.989437
H	-8.065966	3.345582	0.873915
H	-5.901699	3.945705	-0.054083
H	-3.400180	-5.005382	-0.104983
H	-6.554248	-0.788627	-1.856297

H	-7.830830	-2.483337	-3.087232
H	-7.219502	-4.895301	-2.924002
H	-5.273799	-5.581291	-1.551760
H	-2.788150	-5.106011	2.207292
H	-0.814551	-6.111488	3.303977
H	1.440692	-5.109115	2.977626
H	1.674167	-3.036881	1.581386
H	-0.275479	-2.081118	0.493597
H	-3.882807	4.881610	0.799096
H	-2.267103	6.668453	0.245567
H	-0.742767	6.406919	-1.707904
H	-0.905684	4.373575	-3.121924
H	-2.513957	2.597319	-2.578214
H	-0.323747	2.668345	2.588248

4h-a-TS2C

Zero-point correction= 1.125997 (Hartree/Particle)

Thermal correction to Energy= 1.202054

Thermal correction to Enthalpy= 1.202998

Thermal correction to Gibbs Free Energy= 1.012878

SCF Done: E(Solv) = -4581.94257494

C	-5.80365000	2.59463100	-2.34310500
C	-4.77562700	3.52223600	-2.53851700
C	-3.44553700	3.18062500	-2.26286800
C	-3.18293900	1.90520300	-1.78187600
C	-4.21348100	0.95100100	-1.55939400
C	-5.53326400	1.31417200	-1.85779800
N	-1.94211900	1.30371300	-1.45946300
C	-2.17565600	-0.01910800	-0.96948500
C	-3.59677100	-0.25314000	-1.04460000
C	-5.40526200	-0.37338700	1.38785700
C	-4.87674900	-1.68090700	1.16268600
C	-4.10740100	-1.52717600	-0.65367500
C	-4.46743600	0.63550300	1.67525800
C	-3.10402200	0.24422600	1.99462900

N	-2.80257000	-1.05593000	2.18408900
C	-3.76769500	-2.14573000	2.09913700
C	-4.70230100	2.05140100	1.51912200
C	-3.67215900	2.96673600	1.55261900
C	-2.35499500	2.52449600	1.83514000
C	-2.08438500	1.19652500	2.10726800
C	-4.37660000	-2.40858500	3.49679700
C	-3.04459800	-3.41796100	1.62694700
O	-1.27969400	-0.77063600	-0.55508000
O	-5.98421800	2.40701500	1.28937800
O	-1.30638900	3.36620600	1.89419500
C	-6.26764700	3.75601000	0.93620700
C	-1.37456500	4.59081700	1.17117400
C	-5.24823000	-2.15243900	-1.38035300
O	-6.28252900	-1.62815100	-1.74473700
O	-5.00790500	-3.47934900	-1.55229800
C	-5.57640900	-5.66704800	-2.29872600
C	-6.05417200	-4.23154300	-2.20080400
O	-0.54089200	3.01235100	-1.92323900
C	0.58287000	3.67861800	-2.61123500
C	0.39966900	5.13965200	-2.20187100
C	0.42219500	3.51171100	-4.12336200
C	1.92575000	3.15217500	-2.10162700
C	-0.72095800	1.69015500	-2.05361300
O	0.00347800	0.92331200	-2.64453800
C	-6.87188100	-0.14907500	1.13469900
H	-6.82903500	2.86838300	-2.57761900
H	-5.00070600	4.51416900	-2.92102100
H	-2.64267500	3.88826800	-2.41899900
H	-6.32427300	0.58670300	-1.74239700
H	-5.62716700	-2.45871500	1.03043000
H	-3.29725400	-2.23513900	-0.53635600
H	-0.19041800	-1.26491600	0.71760300
H	-3.85796200	4.01203800	1.36295900
H	-1.06056400	0.90484200	2.29805500
H	-4.87929700	-1.51290000	3.87334900

H	-3.58526300	-2.68831000	4.20089500
H	-5.10668700	-3.22549600	3.45550800
H	-3.77173700	-4.17573200	1.31766000
H	-2.37186900	-3.21705400	0.79171000
H	-2.44065900	-3.82763400	2.44186100
H	-7.34177700	3.78831000	0.74944200
H	-6.01714800	4.43765300	1.75819500
H	-5.72716300	4.03746700	0.02679900
H	-0.36050200	4.98838700	1.19358300
H	-1.68042300	4.40767800	0.13723200
H	-2.05664400	5.30596000	1.64948900
H	-6.34231000	-6.28537300	-2.77888600
H	-4.65836800	-5.73256500	-2.89157200
H	-5.37328500	-6.07796700	-1.30450200
H	-6.97265100	-4.14049000	-1.61137300
H	-6.24947500	-3.79245100	-3.18391900
H	0.49471800	5.24571500	-1.11747100
H	1.16669700	5.75772500	-2.67944300
H	-0.58354900	5.51274500	-2.50763400
H	0.53935200	2.46748300	-4.41565000
H	1.18275600	4.10792200	-4.63902500
H	-0.56478900	3.86231400	-4.44438000
H	2.73091200	3.75478200	-2.53786600
H	1.97103300	3.23315600	-1.01450000
H	2.07566700	2.10906400	-2.37818500
H	-7.05352900	0.56774900	0.33595100
H	-7.35604900	-1.09314000	0.87694000
H	-7.34863200	0.25891200	2.03398200
C	7.75533900	2.22181500	-2.44252300
C	7.39186200	0.90440800	-2.80882100
C	6.37710100	0.24795600	-2.14994800
C	5.67375300	0.87496200	-1.08762800
C	6.01240600	2.22416900	-0.74634000
C	7.07542300	2.86621000	-1.43630100
C	4.61541400	0.23215400	-0.36732500
C	3.92084700	0.96658300	0.57468700

C	4.18920200	2.32678900	0.89017900
C	5.26160300	2.90863800	0.23923500
C	4.19203800	-1.16712900	-0.65064800
C	5.08883400	-2.27453000	-0.49910000
C	4.61235500	-3.59141900	-0.79636200
C	3.27329500	-3.77126300	-1.21729900
C	2.38185900	-2.72051400	-1.31725400
C	2.87764500	-1.42415300	-1.00472200
C	6.41466600	-2.12994500	-0.01049100
C	7.23665900	-3.22412200	0.13769100
C	6.77746800	-4.52066100	-0.19332900
C	5.49142700	-4.69689900	-0.64648700
O	2.85246700	0.33370200	1.22186800
O	1.97058300	-0.35774700	-1.03442400
P	1.47308600	0.26236900	0.37526800
O	0.69208100	1.50066800	0.26304100
N	0.72135900	-1.04742700	1.16951300
C	0.97519000	-2.95438700	-1.72709500
C	3.31385600	3.11461200	1.79162400
C	0.36521000	-2.16341800	-2.70932800
C	-0.94188600	-2.42269600	-3.11131800
C	-1.66472300	-3.46664000	-2.53599400
C	-1.06929000	-4.25513800	-1.54951700
C	0.24149800	-4.00252500	-1.14870300
C	3.00617400	4.44184300	1.44962200
C	2.16718100	5.21118000	2.25296600
C	1.60440600	4.66076300	3.40522600
C	1.90184700	3.34305000	3.75320000
C	2.75409900	2.57743800	2.96204700
S	0.92749100	-1.57588500	2.71485700
O	-0.29919600	-2.29439200	3.07795100
O	1.48548600	-0.54675400	3.57961600
C	2.23430800	-2.90398300	2.55767300
F	2.42028600	-3.43765800	3.76527500
F	3.37473400	-2.38519600	2.11665400
F	1.81309100	-3.84832000	1.71629300

H	8.56252200	2.72506900	-2.96673100
H	7.91534500	0.40811100	-3.62076100
H	6.10198300	-0.75795700	-2.44290900
H	7.33120500	3.88569900	-1.15938900
H	5.52886900	3.93484800	0.47330000
H	2.93358900	-4.77266400	-1.46544600
H	6.77384200	-1.14357800	0.25697300
H	8.24536800	-3.09134200	0.51791400
H	7.43867100	-5.37442400	-0.07703900
H	5.11998900	-5.68946700	-0.88787400
H	0.89754500	-1.32384900	-3.13569300
H	-1.40467400	-1.77981700	-3.85392100
H	-2.69527800	-3.64753500	-2.82451300
H	-1.63108600	-5.06024900	-1.08356800
H	0.69474300	-4.60289100	-0.36667900
H	3.40389700	4.86072700	0.53028400
H	1.94367100	6.23667200	1.96998000
H	0.93308500	5.25090900	4.02248500
H	1.46453900	2.90098000	4.64331500
H	2.96737200	1.55604800	3.24812200
H	-1.88546400	-1.29559200	2.54224400

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Zero-point correction=1.127526 (Hartree/Particle)

Thermal correction to Energy=1.203574

Thermal correction to Enthalpy=1.204518

Thermal correction to Gibbs Free Energy=1.014807

E(Solv) = -4581.95491110

C	-5.982690	2.070578	-1.962782
C	-5.030232	3.061824	-2.224936
C	-3.662709	2.806465	-2.045959
C	-3.281909	1.555559	-1.578924
C	-4.238251	0.540383	-1.284456
C	-5.597518	0.811049	-1.498897

N	-2.001052	1.014881	-1.336588
C	-2.145846	-0.330508	-0.828677
C	-3.530734	-0.606834	-0.800716
C	-5.383487	-0.845723	1.510496
C	-4.663621	-2.091544	1.101021
C	-4.087317	-1.923212	-0.393496
C	-4.570240	0.228189	1.815305
C	-3.138670	-0.012470	2.029918
N	-2.716366	-1.261780	2.264739
C	-3.561098	-2.447709	2.119704
C	-4.979644	1.624060	1.751648
C	-4.055727	2.635595	1.698660
C	-2.666374	2.331878	1.820982
C	-2.222322	1.046341	2.054981
C	-4.196183	-2.791806	3.482130
C	-2.676090	-3.618579	1.665862
O	-1.182111	-1.033133	-0.446638
O	-6.307301	1.828030	1.653291
O	-1.718160	3.279547	1.764505
C	-6.771345	3.133809	1.322140
C	-2.006663	4.518477	1.123590
C	-5.153052	-2.375417	-1.383595
O	-6.333845	-2.545871	-1.145656
O	-4.613294	-2.559206	-2.601604
C	-4.719030	-2.915050	-4.950317
C	-5.530424	-2.875346	-3.670633
O	-0.750044	2.809586	-1.874298
C	0.295055	3.546358	-2.605837
C	0.046431	4.988512	-2.164103
C	0.066665	3.383303	-4.109570
C	1.694222	3.101271	-2.175091
C	-0.839995	1.474511	-1.983568
O	-0.082390	0.755330	-2.595044
C	-6.882785	-0.826824	1.445884
H	-7.036617	2.277426	-2.131796
H	-5.344412	4.034975	-2.592188

H	-2.921190	3.562244	-2.268093
H	-6.342726	0.043684	-1.323927
H	-5.361733	-2.929187	1.062915
H	-3.266460	-2.636938	-0.492642
H	-0.083611	-1.302626	0.773742
H	-4.365766	3.656926	1.543394
H	-1.157643	0.869437	2.126326
H	-4.813733	-1.967297	3.850763
H	-3.410930	-2.989780	4.218382
H	-4.825925	-3.685026	3.398499
H	-3.298514	-4.472508	1.377641
H	-2.033738	-3.343490	0.827112
H	-2.026156	-3.930496	2.488242
H	-7.854990	3.045272	1.237195
H	-6.522673	3.850385	2.113990
H	-6.345473	3.455671	0.365935
H	-1.044301	5.021926	1.040171
H	-2.426417	4.346475	0.128290
H	-2.689179	5.133652	1.723742
H	-5.370778	-3.142922	-5.800578
H	-4.238113	-1.948501	-5.129184
H	-3.940072	-3.682507	-4.896408
H	-6.013754	-3.833630	-3.453727
H	-6.308743	-2.106792	-3.698991
H	0.188439	5.080036	-1.083079
H	0.750935	5.659579	-2.666117
H	-0.971340	5.306264	-2.414648
H	0.220978	2.347121	-4.414410
H	0.769206	4.018952	-4.659466
H	-0.952056	3.684605	-4.377240
H	2.435079	3.761240	-2.641430
H	1.788923	3.171524	-1.090913
H	1.895908	2.073640	-2.474822
H	-7.249037	-0.141808	0.678552
H	-7.263443	-1.823709	1.224258
H	-7.299955	-0.472562	2.394997

C	7.548359	2.715513	-2.510246
C	7.305146	1.361780	-2.841747
C	6.359985	0.631157	-2.157862
C	5.610080	1.216093	-1.103448
C	5.825031	2.599212	-0.797843
C	6.819070	3.319074	-1.513279
C	4.620953	0.496138	-0.357982
C	3.873827	1.186085	0.576780
C	4.011075	2.574551	0.850464
C	5.018006	3.237952	0.174425
C	4.314377	-0.939542	-0.610961
C	5.304169	-1.962892	-0.452302
C	4.940146	-3.319494	-0.728016
C	3.617952	-3.619096	-1.132301
C	2.635271	-2.652274	-1.235251
C	3.022150	-1.312898	-0.946211
C	6.617466	-1.697829	0.019589
C	7.532388	-2.714911	0.171931
C	7.183503	-4.050537	-0.138173
C	5.913039	-4.343023	-0.574692
O	2.874915	0.472732	1.250977
O	2.030314	-0.325358	-0.983666
P	1.498601	0.285429	0.417771
O	0.630107	1.462813	0.287177
N	0.825708	-1.045731	1.236071
C	1.250431	-3.022129	-1.620924
C	3.051322	3.298334	1.719407
C	0.529220	-2.279675	-2.565185
C	-0.757408	-2.665122	-2.931823
C	-1.346464	-3.794295	-2.366057
C	-0.636731	-4.542025	-1.423896
C	0.650090	-4.157974	-1.052751
C	2.582050	4.556503	1.308252
C	1.636993	5.248549	2.062689
C	1.133349	4.688072	3.236956
C	1.598101	3.441829	3.658301

C	2.552537	2.754052	2.913606
S	1.064204	-1.529726	2.786648
O	-0.134648	-2.279141	3.182007
O	1.597877	-0.468130	3.627659
C	2.414296	-2.812933	2.634141
F	2.661215	-3.300462	3.850449
F	3.518219	-2.263313	2.138589
F	2.005234	-3.799325	1.836252
H	8.301820	3.277986	-3.053897
H	7.866072	0.895966	-3.646729
H	6.176630	-0.402589	-2.424390
H	6.981377	4.364434	-1.263528
H	5.183154	4.292825	0.373413
H	3.366068	-4.649262	-1.366541
H	6.892543	-0.680519	0.270613
H	8.529689	-2.490701	0.539144
H	7.917179	-4.842475	-0.018917
H	5.626332	-5.367034	-0.799792
H	0.951832	-1.376905	-2.983835
H	-1.315836	-2.052268	-3.632419
H	-2.361635	-4.068985	-2.636390
H	-1.088675	-5.418384	-0.966398
H	1.187754	-4.726245	-0.301109
H	2.935261	4.976022	0.371259
H	1.287089	6.220804	1.724878
H	0.380993	5.215162	3.816786
H	1.211341	2.993454	4.568558
H	2.891126	1.783407	3.251786
H	-1.756934	-1.415353	2.555136

4h-a-TS3C

Zero-point correction=1.126871 (Hartree/Particle)

Thermal correction to Energy=1.202078

Thermal correction to Enthalpy=1.203022

Thermal correction to Gibbs Free Energy=1.015507

E(Solv) = -4581.95073599

C	7.592408	0.901464	-0.762217
C	7.272523	0.448618	-2.046635
C	5.973768	0.033042	-2.360749
C	5.032232	0.085285	-1.345805
C	5.328926	0.520481	-0.040050
C	6.626313	0.940077	0.247311
N	3.647391	-0.244571	-1.395711
C	3.089194	0.024256	-0.182340
C	4.101863	0.416520	0.771589
C	4.077036	-0.890199	2.169343
C	3.791249	0.339502	3.074220
C	3.695853	1.348351	1.928068
C	2.991802	-1.856719	2.007534
C	1.710574	-1.592159	2.581937
N	1.505612	-0.489193	3.367887
C	2.595677	0.206519	4.028364
C	3.066092	-2.949724	1.097249
C	1.992300	-3.795149	0.858323
C	0.766930	-3.535499	1.502191
C	0.628579	-2.449162	2.350616
C	3.040609	-0.619327	5.254922
C	2.099958	1.582637	4.480885
O	1.857248	-0.082975	0.127634
O	4.243042	-3.068618	0.413119
O	-0.327926	-4.319464	1.359693
C	4.398640	-4.147977	-0.497799
C	-0.300036	-5.389873	0.422123
C	4.585568	2.562985	2.113171
O	5.146099	2.857579	3.149022

O	4.705326	3.270817	0.977669
C	5.822011	4.829439	-0.434597
C	5.618354	4.392103	1.001998
O	3.105453	-0.406358	-3.576258
C	2.587460	-1.035198	-4.831663
C	2.834011	0.066942	-5.856966
C	1.098717	-1.340152	-4.685466
C	3.417512	-2.280632	-5.135624
C	3.041835	-1.055995	-2.426552
O	2.597680	-2.148502	-2.190731
C	5.497922	-1.398561	2.317594
H	8.604645	1.228486	-0.545080
H	8.036989	0.426670	-2.817078
H	5.708661	-0.291459	-3.360001
H	6.884927	1.298739	1.238598
H	4.675477	0.561951	3.675811
H	2.670849	1.691288	1.746990
H	1.184235	-0.342020	-0.624451
H	2.072179	-4.598370	0.143686
H	-0.327970	-2.254651	2.817217
H	3.382997	-1.612935	4.946219
H	2.197017	-0.751324	5.938744
H	3.857055	-0.122584	5.791334
H	2.920495	2.161145	4.914891
H	1.678308	2.148650	3.643894
H	1.313486	1.469219	5.234722
H	5.405731	-4.041909	-0.905944
H	4.312812	-5.113076	0.016866
H	3.664643	-4.086906	-1.305761
H	-1.294625	-5.836140	0.467283
H	-0.113974	-5.012160	-0.585856
H	0.450201	-6.141018	0.702095
H	6.511373	5.679616	-0.471162
H	6.245812	4.010688	-1.024710
H	4.874652	5.133701	-0.890351
H	5.183764	5.181939	1.623065

H	6.551268	4.071183	1.473569
H	3.897328	0.321343	-5.910055
H	2.507155	-0.270591	-6.845111
H	2.271979	0.968300	-5.594979
H	0.914623	-2.138360	-3.967004
H	0.710416	-1.649084	-5.661947
H	0.551335	-0.451826	-4.361356
H	3.116751	-2.681992	-6.108732
H	4.483862	-2.034346	-5.185074
H	3.260702	-3.053791	-4.381707
H	5.820805	-2.010587	1.480209
H	6.198063	-0.571145	2.454083
H	5.530994	-2.010370	3.228789
C	-5.959483	5.758034	1.206246
C	-6.690901	4.547808	1.230913
C	-6.091169	3.358603	0.882265
C	-4.727124	3.315777	0.490619
C	-3.976665	4.537592	0.499911
C	-4.630801	5.747940	0.851746
C	-4.061588	2.099615	0.121595
C	-2.704091	2.152978	-0.121742
C	-1.936897	3.348637	-0.133572
C	-2.598185	4.521616	0.167470
C	-4.778072	0.796441	0.009263
C	-5.885662	0.647658	-0.890865
C	-6.615164	-0.582992	-0.892196
C	-6.223822	-1.621976	-0.014831
C	-5.110196	-1.523880	0.795763
C	-4.372489	-0.305729	0.748366
C	-6.266850	1.656562	-1.815698
C	-7.329227	1.468964	-2.670990
C	-8.069109	0.263640	-2.648306
C	-7.713190	-0.740245	-1.778689
O	-2.044394	0.965113	-0.378816
O	-3.237686	-0.207742	1.544946
P	-1.761262	-0.071182	0.857455

O	-0.806184	0.402643	1.886245
N	-1.487048	-1.464434	0.059668
C	-4.789111	-2.623054	1.745800
C	-0.488270	3.309196	-0.448540
C	-5.815616	-3.104543	2.574326
C	-5.582444	-4.146124	3.470792
C	-4.314962	-4.723057	3.554392
C	-3.288959	-4.254382	2.732283
C	-3.519938	-3.214536	1.832437
C	0.425585	4.014889	0.346487
C	1.791202	3.968202	0.071090
C	2.266695	3.215807	-1.005281
C	1.363114	2.520288	-1.809538
C	-0.000938	2.563324	-1.533988
S	-0.856652	-1.620984	-1.352832
O	-0.517963	-3.012531	-1.657520
O	0.203219	-0.592330	-1.674322
C	-2.168019	-1.183445	-2.643932
F	-1.971441	-1.940417	-3.731866
F	-2.101134	0.099709	-3.014285
F	-3.382726	-1.434195	-2.151507
H	-6.446303	6.690153	1.478265
H	-7.734371	4.555747	1.532581
H	-6.658014	2.435954	0.912093
H	-4.053119	6.668854	0.844542
H	-2.053411	5.461683	0.150076
H	-6.802063	-2.541484	-0.002996
H	-5.701160	2.579639	-1.851860
H	-7.597439	2.251963	-3.374611
H	-8.907980	0.130402	-3.325402
H	-8.261273	-1.678874	-1.761256
H	-6.796392	-2.639471	2.526578
H	-6.388618	-4.498263	4.108981
H	-4.128198	-5.530696	4.257403
H	-2.295055	-4.687548	2.780864
H	-2.716743	-2.882037	1.187363

H	0.061450	4.573649	1.203884
H	2.488328	4.502605	0.707733
H	3.332437	3.157820	-1.197795
H	1.723274	1.920871	-2.641326
H	-0.687604	1.996540	-2.148199
H	0.596096	-0.048881	3.267991

4h-a-TS2D (RR-4h-a-TS2D)

Zero-point correction= 1.127692 (Hartree/Particle)

Thermal correction to Energy= 1.203072

Thermal correction to Enthalpy= 1.204017

Thermal correction to Gibbs Free Energy= 1.017731

E(Solv) = -4581.9708206

C	-6.82046000	1.86966800	-2.13281100
C	-6.16482000	3.10539900	-2.19298000
C	-4.78383500	3.19565700	-2.00078900
C	-4.10107800	2.01470600	-1.74519400
C	-4.73835600	0.75491300	-1.66348600
C	-6.12039900	0.69233600	-1.87233500
N	-2.70114200	1.81582400	-1.56104100
C	-2.48435800	0.47572900	-1.31072200
C	-3.70934800	-0.24191700	-1.35959100
C	-4.95728100	-0.99633700	1.37705000
C	-4.13483500	-2.11277200	1.23970500
C	-3.70545900	-1.61551800	-1.07910900
C	-4.33922400	0.26126100	1.61336000
C	-2.89446200	0.30576100	1.73691200
N	-2.18374500	-0.83441100	1.75909000
C	-2.78212700	-2.15896800	1.89986300
C	-5.02260100	1.53049700	1.61274900
C	-4.33420100	2.71968600	1.64487700
C	-2.91703700	2.71478200	1.71326300
C	-2.20322600	1.53393600	1.78825500
C	-3.00228600	-2.47202400	3.40524600
C	-1.82773900	-3.20317500	1.30959600

O	-1.32737800	-0.06866600	-1.08090200
O	-6.37455100	1.46967800	1.55484100
O	-2.35889800	3.93845800	1.71194500
C	-7.10262500	2.68417100	1.42900300
C	-0.93191500	4.02765700	1.76952900
C	-4.75475300	-2.56474600	-1.48042200
O	-5.89755100	-2.30671800	-1.81848900
O	-4.27279200	-3.83522800	-1.43040400
C	-5.20140700	-5.05491300	-3.33400500
C	-5.18551200	-4.88257300	-1.82360100
O	-1.97794500	3.99444100	-1.74156600
C	0.57328700	3.05304300	-2.68663200
C	1.05295700	3.92041700	-1.52799000
C	0.18424100	3.86892800	-3.91740300
C	1.59870000	1.97634000	-3.02718800
C	-1.72788900	2.81514900	-1.84683900
O	-0.61041900	2.24375500	-2.26894600
C	-6.43773200	-1.19226400	1.16668900
H	-7.89332000	1.82257400	-2.29612400
H	-6.73000600	4.00992800	-2.39830500
H	-4.26065700	4.14084000	-2.03620700
H	-6.61935900	-0.26604100	-1.85044800
H	-4.60277000	-3.07910800	1.08179800
H	-2.72959200	-2.06231100	-0.95507100
H	-0.61154500	0.56726400	-0.74482000
H	-4.82917300	3.67885500	1.60248500
H	-1.12474500	1.51979200	1.83761300
H	-3.66039500	-1.72466100	3.85870000
H	-2.03717600	-2.46093700	3.91745300
H	-3.46249200	-3.45956000	3.52581300
H	-2.32966300	-4.17238900	1.23521300
H	-1.47715900	-2.91867400	0.31818400
H	-0.95098500	-3.31247700	1.95160100
H	-8.15122100	2.39077300	1.36247200
H	-6.95458800	3.32533600	2.30629900
H	-6.81099400	3.21951100	0.51947800

H	-0.55305000	3.65525900	2.72664600
H	-0.46655500	3.46584900	0.95743200
H	-0.69960400	5.08692300	1.67187700
H	-5.84232000	-5.90033800	-3.60799100
H	-5.59233900	-4.15483400	-3.81566100
H	-4.19258500	-5.25019200	-3.71261800
H	-4.80459200	-5.77428700	-1.32002000
H	-6.18177700	-4.64622400	-1.44196500
H	1.23019300	3.30047500	-0.64875900
H	2.00040700	4.38873400	-1.81466500
H	0.33177800	4.70288100	-1.28670500
H	-0.20426700	3.21430300	-4.70450700
H	1.07428700	4.37597300	-4.30463900
H	-0.56765000	4.62173300	-3.67365700
H	2.53522600	2.44617200	-3.34270900
H	1.80034400	1.35131600	-2.15712700
H	1.23577700	1.33964300	-3.84051200
H	-6.64064000	-2.22832000	0.88733900
H	-6.97716400	-0.96701500	2.09294300
H	-6.84122800	-0.53481900	0.39964900
C	6.41502500	2.85331500	-3.59620200
C	6.23648700	1.46203100	-3.78108700
C	5.56111700	0.71114600	-2.84532700
C	5.02326000	1.31441400	-1.67810300
C	5.17560700	2.72791500	-1.50692900
C	5.89435500	3.46951100	-2.48252100
C	4.29348200	0.57865700	-0.68828400
C	3.67752300	1.28277000	0.32888100
C	3.81708200	2.68483800	0.53463800
C	4.59525500	3.36550900	-0.38408800
C	4.15628900	-0.90440000	-0.75966200
C	5.30951600	-1.75562400	-0.73085200
C	5.12532800	-3.16815100	-0.87153200
C	3.82010600	-3.68840300	-1.03799100
C	2.69565400	-2.88631500	-1.00588700
C	2.90397400	-1.49130000	-0.81972000

C	6.62630100	-1.26327500	-0.52976800
C	7.70394100	-2.11938200	-0.49915300
C	7.52408300	-3.51193200	-0.67028700
C	6.25992400	-4.02180300	-0.84980100
O	2.86957800	0.57047900	1.20862900
O	1.78215400	-0.67905100	-0.72078800
P	1.41348600	0.08839700	0.68142300
O	0.49999500	1.19974500	0.23948700
N	0.80738400	-0.92502900	1.76057800
C	1.34945000	-3.47307400	-1.21692200
C	3.15428600	3.39319600	1.65834100
C	0.39944700	-2.85495000	-2.04691200
C	-0.81163800	-3.48432300	-2.32792900
C	-1.10213700	-4.73540700	-1.78172700
C	-0.17547800	-5.34809600	-0.93847500
C	1.03615700	-4.72120900	-0.65634700
C	2.71541100	4.71714500	1.47940100
C	2.12583100	5.42643300	2.52285500
C	1.94684200	4.82121100	3.76814000
C	2.36566000	3.50350800	3.95553800
C	2.96794500	2.79510400	2.91738800
S	1.35033200	-1.35265400	3.20321300
O	0.25173100	-1.99871600	3.92930500
O	2.16378700	-0.34223200	3.88744400
C	2.52780400	-2.74697800	2.82061200
F	3.00750900	-3.26077200	3.95564700
F	3.55129100	-2.30576900	2.07708800
F	1.89194800	-3.71448800	2.14288400
H	6.95588500	3.43229000	-4.33906200
H	6.63308800	0.98255600	-4.67126900
H	5.42396300	-0.35250100	-2.99848900
H	6.01357200	4.53990300	-2.33517000
H	4.76632900	4.42946300	-0.25194900
H	3.70480100	-4.75477600	-1.20771800
H	6.77622800	-0.20019300	-0.38539000
H	8.70145300	-1.72205800	-0.33546700

H	8.38391100	-4.17504900	-0.64808100
H	6.10529800	-5.09122100	-0.96764100
H	0.61155300	-1.88427000	-2.47777900
H	-1.53295000	-2.99439600	-2.97551900
H	-2.05471200	-5.20986700	-1.99032800
H	-0.39946600	-6.31084900	-0.48757600
H	1.74175400	-5.18855800	0.02223300
H	2.81737000	5.18830100	0.50728300
H	1.79543100	6.44851200	2.35825800
H	1.47812800	5.36940800	4.58061200
H	2.22622000	3.01271400	4.91408400
H	3.27839200	1.77452000	3.09411500
H	-1.16678100	-0.78380700	1.85448300

4h-a-IM2D

Zero-point correction= 1.131330 (Hartree/Particle)

Thermal correction to Energy= 1.206752

Thermal correction to Enthalpy= 1.207696

Thermal correction to Gibbs Free Energy= 1.021147

SCF Done: E(Solv) = -4582.00094150

C	6.81105700	-1.39149700	-1.47898500
C	6.23293500	-2.64262400	-1.73649300
C	4.84600200	-2.79439500	-1.82223900
C	4.06426000	-1.66099600	-1.63084800
C	4.62577200	-0.38931800	-1.34338900
C	6.01906300	-0.26071900	-1.28518800
N	2.65925200	-1.49977200	-1.67663700
C	2.37349600	-0.15351200	-1.35776600
C	3.53598000	0.53783900	-1.13082700
C	4.87299700	1.20060200	1.41241100
C	3.90513600	2.22997300	0.87142900
C	3.58211000	1.96730400	-0.66331900
C	4.35119800	-0.01900400	1.76284000
C	2.88245300	-0.17641300	1.74733200
N	2.11412000	0.90543400	1.78327900

C	2.64892800	2.27148000	1.76358700
C	5.12139100	-1.25052800	1.96990000
C	4.51493300	-2.46965500	1.91651800
C	3.09615700	-2.56537000	1.74591100
C	2.28569700	-1.45092400	1.71033100
C	3.01814500	2.69754200	3.19998000
C	1.55685700	3.20912700	1.23906000
O	1.14564400	0.33385500	-1.26670800
O	6.44995400	-1.09349700	2.14043400
O	2.64920100	-3.82100600	1.65959700
C	7.27736300	-2.25272200	2.07969200
C	1.24055000	-4.02745000	1.46608300
C	4.52808100	2.75204700	-1.56309100
O	5.61947700	3.19010300	-1.25302400
O	3.99517200	2.88344800	-2.79220100
C	5.72309800	2.31777600	-4.41163800
C	4.85998300	3.42133100	-3.82269900
O	2.07801400	-3.68645200	-2.07092700
C	-0.53435500	-2.84263100	-2.87757100
C	-0.92238500	-3.80742900	-1.75972800
C	-0.14595600	-3.55847300	-4.16978200
C	-1.64052600	-1.81821300	-3.11649500
C	1.76629400	-2.51228600	-2.07213500
O	0.60374800	-1.98672700	-2.44984400
C	6.30280900	1.63562500	1.47972500
H	7.89288300	-1.29827900	-1.43532200
H	6.86884600	-3.51046600	-1.88612300
H	4.38821700	-3.75367300	-2.01859900
H	6.47376500	0.70450100	-1.09715500
H	4.37716000	3.21409700	0.92052100
H	2.59075900	2.38229900	-0.85118300
H	0.50172900	-0.36237700	-0.97272500
H	5.06547000	-3.39692700	1.97914000
H	1.21221900	-1.51849200	1.60162100
H	3.78292100	2.04781500	3.63566100
H	2.12399500	2.64994300	3.82499000

H	3.39833800	3.72562200	3.19838100
H	1.98208700	4.19389200	1.02552500
H	1.07893100	2.82969000	0.33612800
H	0.77738600	3.32426800	1.99428000
H	8.30055300	-1.88653800	2.17008800
H	7.05662200	-2.93558700	2.90797100
H	7.14314600	-2.76440000	1.12087200
H	0.67258800	-3.66843300	2.32854400
H	0.89612700	-3.52078500	0.56384700
H	1.11702700	-5.10413600	1.36414500
H	6.33038200	2.71493300	-5.23260300
H	6.39411200	1.90645300	-3.65248100
H	5.09955700	1.50629900	-4.79880700
H	4.17180200	3.83758200	-4.56123000
H	5.46473300	4.22293500	-3.39331400
H	-1.07689600	-3.25492900	-0.83159800
H	-1.86493700	-4.29519400	-2.03077100
H	-0.15966100	-4.57312000	-1.60955600
H	0.16535200	-2.83356700	-4.92924600
H	-1.01508900	-4.10320900	-4.55391700
H	0.66550000	-4.26798600	-3.99900700
H	-2.55034900	-2.32627800	-3.45078900
H	-1.86447500	-1.27552500	-2.19761400
H	-1.33985300	-1.09784200	-3.88417000
H	6.50078800	2.36625600	0.69334300
H	6.44451700	2.14962400	2.44376200
H	7.01121000	0.81502000	1.43812400
C	-6.42340500	-2.92215800	-3.51569700
C	-6.31320200	-1.51795600	-3.64815000
C	-5.64089400	-0.77475800	-2.70405800
C	-5.03864800	-1.39840100	-1.57972300
C	-5.12054700	-2.82342800	-1.46395800
C	-5.83789900	-3.55769300	-2.44601800
C	-4.30907800	-0.67085400	-0.58330900
C	-3.63582000	-1.38588600	0.38831400
C	-3.69319000	-2.80126900	0.52991100

C	-4.46807300	-3.47992600	-0.39274900
C	-4.21239200	0.81677800	-0.61703900
C	-5.38257700	1.64009400	-0.53692800
C	-5.23652900	3.05828500	-0.66446500
C	-3.95120100	3.61025100	-0.87903200
C	-2.80830400	2.83448200	-0.89970900
C	-2.97579300	1.43325000	-0.70874100
C	-6.67925000	1.11273600	-0.29847500
C	-7.77511200	1.94195200	-0.21652100
C	-7.63391400	3.34085900	-0.37163100
C	-6.38940100	3.88374700	-0.58879400
O	-2.83772700	-0.67051200	1.27492400
O	-1.83334500	0.64879000	-0.65011700
P	-1.40373000	-0.15012800	0.71938700
O	-0.47068700	-1.21778900	0.23165200
N	-0.79693000	0.85783600	1.80876200
C	-1.48705600	3.44838800	-1.18218000
C	-2.94475900	-3.52473900	1.58818900
C	-0.56958200	2.83551800	-2.05027500
C	0.62488500	3.46926800	-2.38735400
C	0.92398800	4.72955800	-1.86849500
C	0.02499900	5.34544600	-0.99552100
C	-1.16479700	4.70772900	-0.65039900
C	-2.43406600	-4.80693300	1.31851900
C	-1.76258300	-5.53433700	2.29810200
C	-1.57052800	-4.98771000	3.56828400
C	-2.05790400	-3.70957200	3.84438700
C	-2.74253000	-2.98421700	2.87060100
S	-1.31555400	1.26763100	3.26439800
O	-0.20782800	1.92628200	3.96741700
O	-2.09688600	0.24078600	3.96063100
C	-2.52219100	2.64672000	2.91573000
F	-2.96467300	3.16505900	4.06382600
F	-3.56675900	2.18809200	2.21439500
F	-1.92342800	3.61644800	2.20650700
H	-6.96235400	-3.49522500	-4.26451700

H	-6.76004200	-1.02187400	-4.50482400
H	-5.55617100	0.29904000	-2.81849700
H	-5.90272000	-4.63762800	-2.34017100
H	-4.57748000	-4.55669600	-0.30687900
H	-3.86800600	4.67972600	-1.04844000
H	-6.79760200	0.04387500	-0.16658300
H	-8.75672200	1.51847200	-0.02462500
H	-8.50771000	3.98277700	-0.30848000
H	-6.26481700	4.95815000	-0.69670600
H	-0.78444800	1.85671500	-2.45859400
H	1.33098000	2.97003500	-3.04314400
H	1.85996900	5.21636400	-2.12874900
H	0.25606000	6.31753600	-0.56860200
H	-1.84368200	5.17441200	0.05591400
H	-2.54665000	-5.22907800	0.32531000
H	-1.37938400	-6.52399200	2.06410200
H	-1.03922900	-5.54954200	4.33150300
H	-1.91010000	-3.26468100	4.82394400
H	-3.10634700	-1.99522500	3.11454000
H	1.09153900	0.80379200	1.82401900

4h-a-TS3D

Zero-point correction= 1.127087 (Hartree/Particle)

Thermal correction to Energy= 1.202352

Thermal correction to Enthalpy= 1.203297

Thermal correction to Gibbs Free Energy= 1.015503

SCF Done: E(Solv) = -4581.97486333

C	7.17296600	-1.10156600	-2.45586200
C	6.62076800	-2.27990100	-2.96749900
C	5.28113000	-2.61473300	-2.73358600
C	4.52190600	-1.73624200	-1.97335800
C	5.06471200	-0.54969300	-1.42845000
C	6.40105200	-0.23180800	-1.68175000
N	3.13711100	-1.76998900	-1.66236800
C	2.81027400	-0.62311800	-0.89275100

C	4.03058300	0.09514300	-0.64258400
C	4.33299300	-0.20803900	1.44196000
C	4.42593500	1.33359600	1.36151300
C	3.98293500	1.51631400	-0.09662500
C	3.16340900	-0.76952700	2.04796300
C	2.20759700	0.08257400	2.68227200
N	2.32794800	1.43681300	2.59279400
C	3.63243500	2.08094600	2.44566400
C	2.84943800	-2.17085700	2.01308300
C	1.80132200	-2.70395100	2.73277200
C	0.99530800	-1.83947200	3.50797200
C	1.16183500	-0.46535600	3.45164800
C	4.40060500	1.99343000	3.78173700
C	3.40246600	3.54749700	2.07031100
O	1.69264400	-0.33981900	-0.43097800
O	3.62511200	-2.91555000	1.17965600
O	0.09328900	-2.46139700	4.29674600
C	3.30961000	-4.29072700	1.00034900
C	-0.62946000	-1.66196600	5.23378300
C	4.83092000	2.50464000	-0.87091900
O	5.60898400	3.29813700	-0.38003600
O	4.63981300	2.37774300	-2.19763000
C	5.41417800	2.54797900	-4.44044700
C	5.47429000	3.17787600	-3.06321000
O	2.71356200	-3.95350800	-2.22015600
C	-0.05161300	-3.37309000	-2.46531200
C	-0.22489100	-4.35751100	-1.31015800
C	0.25409900	-4.06275100	-3.79606000
C	-1.26900700	-2.46552400	-2.60711600
C	2.29102700	-2.83118600	-2.01271400
O	1.02839800	-2.41882100	-2.11456200
C	5.66183200	-0.90877800	1.54371600
H	8.21343900	-0.86204000	-2.65540600
H	7.23601700	-2.95115500	-3.55929500
H	4.84907300	-3.52560000	-3.12533600
H	6.83565200	0.67904500	-1.27949700

H	5.47235300	1.63474300	1.45724100
H	2.93829500	1.84603700	-0.14429000
H	0.46647700	-0.98755600	0.08221000
H	1.57209200	-3.76004500	2.74225100
H	0.53553200	0.20253200	4.02329600
H	4.55703300	0.94927300	4.07295400
H	3.83026700	2.48503000	4.57691100
H	5.37796600	2.48257900	3.70445400
H	4.35504900	4.04717900	1.87832900
H	2.77513400	3.63396700	1.17916700
H	2.89044300	4.06639100	2.88915900
H	3.96194700	-4.63939300	0.20069700
H	3.49023000	-4.85929600	1.92086400
H	2.26582800	-4.41493800	0.69286200
H	0.06329500	-1.10334600	5.87489800
H	-1.30557700	-0.96787200	4.72870100
H	-1.19909500	-2.36678400	5.83935200
H	6.03399300	3.11843000	-5.14052200
H	5.78299300	1.51845000	-4.40152800
H	4.38759400	2.53497200	-4.82035100
H	5.09646000	4.20625800	-3.05845500
H	6.48859000	3.19117000	-2.65608500
H	-0.39977200	-3.81621600	-0.37558400
H	-1.09345800	-4.99594500	-1.50582700
H	0.65491600	-4.99619600	-1.20469100
H	0.47190300	-3.31528800	-4.56638100
H	-0.63187300	-4.62405500	-4.11207700
H	1.09867000	-4.74609900	-3.71621200
H	-2.14619500	-3.06051300	-2.87666600
H	-1.47447100	-1.94763500	-1.67317200
H	-1.10318100	-1.71722300	-3.38804500
H	6.02181000	-0.77441300	2.57488200
H	5.59550400	-1.97372600	1.33517600
H	6.40429900	-0.46072900	0.88057700
C	-5.91025500	-2.81480900	-4.14574900
C	-5.66539500	-1.44072000	-4.37641000

C	-5.06982700	-0.66226300	-3.40983400
C	-4.68552700	-1.21890500	-2.16118300
C	-4.90497600	-2.61671300	-1.94043300
C	-5.53546400	-3.38757200	-2.95319400
C	-4.04144200	-0.45083700	-1.13639800
C	-3.58590700	-1.11204100	-0.01108200
C	-3.80537200	-2.49177100	0.24397300
C	-4.47681100	-3.20827100	-0.72790700
C	-3.79366500	1.00957500	-1.29823800
C	-4.86270100	1.95141400	-1.44200500
C	-4.53640900	3.33500100	-1.61661300
C	-3.17969100	3.73857100	-1.64219700
C	-2.14069100	2.84624800	-1.45935800
C	-2.49783300	1.48595900	-1.26749400
C	-6.23100000	1.57896600	-1.37597400
C	-7.22517700	2.52225300	-1.50525500
C	-6.90346900	3.88498000	-1.70759500
C	-5.58735200	4.27957300	-1.75904300
O	-2.85010100	-0.38799200	0.93802000
O	-1.47795600	0.56286000	-0.99112000
P	-1.36324300	0.10370100	0.55484800
O	-0.46727600	-1.16711100	0.49659700
N	-0.90408300	1.32221900	1.43784700
C	-0.72805000	3.28899400	-1.48029500
C	-3.35206400	-3.14236700	1.49494000
C	0.25401800	2.54493400	-2.15178900
C	1.56731000	2.99905200	-2.21269300
C	1.92662400	4.19803200	-1.59298100
C	0.96032700	4.94036200	-0.91284200
C	-0.35697500	4.49019100	-0.85880400
C	-2.75282300	-4.40947100	1.44576600
C	-2.37666300	-5.06517100	2.61614900
C	-2.61384200	-4.47140200	3.85531800
C	-3.21816100	-3.21493300	3.91341800
C	-3.56845200	-2.54392300	2.74573900
S	-1.42484600	1.82484700	2.85422300

O	-0.35046300	2.55826500	3.54082700
O	-2.19941000	0.83562200	3.61718000
C	-2.67201200	3.12856700	2.37878700
F	-3.26041000	3.60349100	3.47854900
F	-3.60362800	2.59542300	1.57821300
F	-2.07512700	4.13756100	1.73572200
H	-6.38587800	-3.41554700	-4.91538800
H	-5.94574300	-0.99677400	-5.32709100
H	-4.87922400	0.38693200	-3.60032100
H	-5.70617400	-4.44496700	-2.76837800
H	-4.68513200	-4.26049400	-0.55758100
H	-2.95152400	4.78624700	-1.81454200
H	-6.48736500	0.53909600	-1.21172000
H	-8.26622700	2.21858000	-1.44583700
H	-7.69830100	4.61767800	-1.81168200
H	-5.32784000	5.32552100	-1.89987300
H	-0.00965800	1.60785900	-2.62732200
H	2.31805500	2.41023500	-2.72654100
H	2.95462400	4.54674600	-1.62884200
H	1.23335500	5.86625100	-0.41459400
H	-1.09940600	5.05478000	-0.30650700
H	-2.56391500	-4.86991600	0.48143900
H	-1.89774600	-6.03860300	2.55858200
H	-2.32352900	-4.98098100	4.76947000
H	-3.41490800	-2.74749800	4.87298000
H	-4.01535500	-1.55841100	2.80516900
H	1.59616300	1.97698400	3.04675600

RS-4h-a-TS2D

Zero-point correction= 1.125625 (Hartree/Particle)

Thermal correction to Energy= 1.202061

Thermal correction to Enthalpy= 1.203005

Thermal correction to Gibbs Free Energy= 1.008086

SCF Done: E(Solv) = -4581.93458119

C	5.76609900	1.83850800	4.04327200

C	6.87839500	1.00572300	4.18685000
C	7.13898700	-0.00272900	3.25241700
C	6.25841600	-0.15355300	2.18995300
C	5.10617700	0.66965500	2.02663400
C	4.88390100	1.68039200	2.97461300
N	6.29829300	-1.09214500	1.13065900
C	5.19694000	-0.83616800	0.23715700
C	4.41029600	0.21444500	0.84292200
C	3.54835700	2.85935000	-1.12759300
C	3.49962000	1.47892800	-1.49246000
C	3.20256400	0.53405400	0.14051600
C	2.37358100	3.64173600	-1.23429900
C	1.16576500	2.99426200	-1.70084000
N	1.23641700	1.77479800	-2.25485700
C	2.49161900	1.09445600	-2.57241800
C	2.22839300	4.99638600	-0.76404900
C	0.99043200	5.58632000	-0.62460600
C	-0.17658500	4.85698600	-0.96687000
C	-0.09933100	3.59026000	-1.51858200
C	3.02546900	1.58961900	-3.93587200
C	2.19347900	-0.40727500	-2.66053900
O	5.02295000	-1.37750200	-0.85718300
O	3.38423500	5.64304100	-0.46772700
O	-1.33378600	5.50188100	-0.72148200
C	3.31244000	6.97698600	0.01456700
C	-2.55618900	4.78219500	-0.90776100
C	2.05471300	1.18986200	0.81935500
O	0.91355800	0.73269800	0.75556300
O	2.34833700	2.31752600	1.45805200
C	0.84524200	2.43568800	3.40029900
C	1.27053200	3.06270100	2.08340400
O	8.29130200	-2.12495100	1.64053100
C	7.67830400	-4.16025800	-0.24198900
C	8.01287600	-5.05476800	0.95279900
C	8.92930000	-3.60193000	-0.92243100
C	6.79194000	-4.89327600	-1.24889200

C	7.24282400	-2.11319500	1.02043700
O	6.80738000	-3.05945300	0.18445200
C	4.81958400	3.31655500	-0.47330300
H	5.58573900	2.62814500	4.76827100
H	7.55890900	1.14385400	5.02205500
H	8.00612300	-0.64241500	3.33554500
H	4.04168100	2.34761200	2.86484700
H	4.46279800	1.00806200	-1.67226300
H	2.83462700	-0.34767100	-0.37061400
H	0.86164100	6.59419500	-0.25660700
H	-0.98369700	3.05023900	-1.82755500
H	3.22030000	2.66627600	-3.91487500
H	2.28761900	1.38312900	-4.71818400
H	3.95694800	1.07186800	-4.19046500
H	3.12117400	-0.98320800	-2.64647000
H	1.56267700	-0.73835900	-1.83374500
H	1.64754700	-0.61985100	-3.58523200
H	4.34481000	7.28516300	0.18433900
H	2.84478400	7.63971300	-0.72323300
H	2.75209300	7.02983400	0.95614200
H	-2.69694400	4.49253200	-1.95453900
H	-2.58301200	3.88602300	-0.27897800
H	-3.34645300	5.46431500	-0.60319800
H	0.10389600	3.07826700	3.88731600
H	0.39663200	1.45155500	3.24560300
H	1.70458300	2.32616100	4.06877000
H	1.70040300	4.05478200	2.22593700
H	0.44802100	3.15015100	1.37027500
H	7.09215400	-5.38519100	1.44521100
H	8.55293600	-5.94275600	0.60576500
H	8.63073100	-4.52333100	1.67760000
H	8.64433400	-2.92493200	-1.73451100
H	9.51096100	-4.42599900	-1.34971700
H	9.55617400	-3.06129800	-0.21178700
H	7.33014500	-5.74598400	-1.67559300
H	5.88315000	-5.26081800	-0.76175900

H	6.49807000	-4.21519600	-2.05531400
H	5.42482300	2.44750300	-0.20368900
H	5.40330100	3.93649500	-1.16559300
H	4.63660600	3.91687800	0.41689200
C	-6.83979100	-2.26762800	4.90979300
C	-6.05033500	-3.26776600	4.29506900
C	-5.31765300	-2.98696900	3.16403200
C	-5.33359300	-1.68777000	2.59162700
C	-6.10868100	-0.66853100	3.23104900
C	-6.86478300	-0.99591400	4.38787700
C	-4.58215100	-1.35046500	1.41741000
C	-4.55263200	-0.02653400	1.02265300
C	-5.35299000	0.99608100	1.59875300
C	-6.12177500	0.63963600	2.69108300
C	-3.86274400	-2.39668300	0.63702700
C	-4.57103200	-3.49149000	0.04111000
C	-3.81987300	-4.48107400	-0.66951300
C	-2.41487500	-4.35518300	-0.77263700
C	-1.72272700	-3.27357500	-0.25796500
C	-2.50144500	-2.30280300	0.42543000
C	-5.98487900	-3.61484300	0.08379600
C	-6.61793800	-4.67930700	-0.51703700
C	-5.87243800	-5.67636700	-1.18889700
C	-4.50363800	-5.57502500	-1.26415100
O	-3.72913200	0.34390400	-0.05075600
O	-1.86194400	-1.13545700	0.89171800
P	-2.13749500	0.17649000	0.00508200
O	-1.56868400	1.34353400	0.88782300
N	-1.51582100	0.03619000	-1.43475100
C	-0.25077800	-3.18481200	-0.40240600
C	-5.44485200	2.36070700	1.02421800
C	0.57225400	-2.74626200	0.64726200
C	1.95962800	-2.78632800	0.52232900
C	2.55418000	-3.26282000	-0.64765900
C	1.74228100	-3.67605200	-1.70549700
C	0.35567600	-3.63039000	-1.58846900

C	-5.56931600	3.47103600	1.87387700
C	-5.80164000	4.74402100	1.35695500
C	-5.91274000	4.92913200	-0.02170100
C	-5.75865300	3.83706300	-0.87841200
C	-5.51922100	2.56465500	-0.36485200
S	-2.14548200	0.43719300	-2.84590500
O	-1.04537200	0.62763000	-3.80289000
O	-3.20241500	1.45526100	-2.77564600
C	-2.98400900	-1.14813000	-3.36277700
F	-3.54648400	-0.98759700	-4.56099700
F	-3.92953700	-1.46784900	-2.46994800
F	-2.09192700	-2.14012400	-3.42246800
H	-7.41738800	-2.50563700	5.79806900
H	-6.01890700	-4.26583200	4.72193500
H	-4.71122300	-3.75836700	2.70485500
H	-7.45810200	-0.21566100	4.85728100
H	-6.77627700	1.38039100	3.14027100
H	-1.86058100	-5.14188500	-1.27468900
H	-6.56836200	-2.85329400	0.58636100
H	-7.70090000	-4.75149400	-0.47929400
H	-6.38532300	-6.51343900	-1.65323900
H	-3.92016300	-6.32528700	-1.79106900
H	0.12635200	-2.38668400	1.56706900
H	2.58324000	-2.43701500	1.34015000
H	3.63387000	-3.25745500	-0.74529300
H	2.19204700	-4.01634200	-2.63398100
H	-0.26880900	-3.92006700	-2.42775100
H	-5.47775700	3.33228300	2.94713900
H	-5.89717700	5.58999900	2.03172400
H	-6.10662100	5.91867200	-0.42645300
H	-5.82679900	3.97092900	-1.95404500
H	-5.40147800	1.73104500	-1.04589000
H	0.39120500	1.36594800	-2.64434900
H	-0.55495100	1.27520900	0.92012400

SS-4h-a-TS2D

Zero-point correction= 1.127856 (Hartree/Particle)

Thermal correction to Energy= 1.202993

Thermal correction to Enthalpy= 1.203937

Thermal correction to Gibbs Free Energy= 1.016441

SCF Done: E(Solv) = -4581.96120771

C	-6.68388000	2.32663400	-2.02208800
C	-7.09212000	1.01016900	-2.25344300
C	-6.18101700	-0.04725800	-2.18988300
C	-4.85684700	0.24981300	-1.87986100
C	-4.43081100	1.57299300	-1.61405800
C	-5.35802900	2.61672200	-1.70739200
N	-3.72290600	-0.60468400	-1.74417700
C	-2.62187700	0.18329100	-1.38470700
C	-3.01225100	1.53633500	-1.26731900
C	-3.73182300	2.43769400	1.50912100
C	-2.42863200	2.97534900	1.36518000
C	-2.12510000	2.52794700	-0.76068700
C	-3.84403900	1.03694900	1.60864000
C	-2.61845800	0.24810700	1.60701200
N	-1.42644000	0.85662800	1.66463000
C	-1.29170200	2.26075400	2.05748500
C	-5.08466500	0.29089500	1.56849200
C	-5.09516900	-1.07801800	1.46889100
C	-3.86814500	-1.79779800	1.44317500
C	-2.64992100	-1.15735000	1.50974800
C	0.09073900	2.80518200	1.69805400
C	-1.45013200	2.35985700	3.59720600
O	-1.46682200	-0.39227200	-1.25858800
O	-6.21433700	1.03114000	1.61940700
O	-4.01025800	-3.13456700	1.36854300
C	-7.46194600	0.38362800	1.39985900
C	-2.81120700	-3.92092100	1.33579100
C	-2.19007300	3.96897200	-1.11502100
O	-3.17868100	4.63138500	-1.37718100
O	-0.94403000	4.48978400	-1.06771600

C	-1.10686400	6.66267000	0.02791200
C	-0.83047900	5.91538700	-1.26641200
O	-2.64925400	-2.65835000	-1.76734900
C	-5.01431500	-3.88805300	-2.69723800
C	-4.16891700	-4.19172700	-3.93326300
C	-6.50624200	-3.95539500	-3.02047100
C	-4.67494000	-4.79533200	-1.51463900
C	-3.65078400	-2.00269500	-1.93667300
O	-4.84094600	-2.46592500	-2.33084200
C	-4.88252500	3.40782300	1.45253100
H	-7.40369900	3.13692800	-2.09467600
H	-8.12782000	0.79680400	-2.50234900
H	-6.49873700	-1.05936300	-2.37944300
H	-5.02991300	3.63248900	-1.54181000
H	-2.34948800	4.05892700	1.36301600
H	-1.10140500	2.19597100	-0.65004100
H	-6.01123700	-1.64900500	1.42132800
H	-1.71346900	-1.69325300	1.47910700
H	0.31078300	2.77209000	0.63362500
H	0.86039100	2.23936000	2.22825300
H	0.15935400	3.84546700	2.02563500
H	-1.39960100	3.40492500	3.92181900
H	-2.40524300	1.93936500	3.92462500
H	-0.63637800	1.80493700	4.07477300
H	-8.21000800	1.17685000	1.41924500
H	-7.47227400	-0.10938000	0.42229200
H	-7.67412500	-0.34313100	2.19306700
H	-2.21310200	-3.66695700	0.45947800
H	-2.22092100	-3.76932300	2.24463500
H	-3.14455800	-4.95665500	1.27623800
H	-0.93733000	7.73608100	-0.11476600
H	-2.14625100	6.52098900	0.33809100
H	-0.44010100	6.30889600	0.81977100
H	0.19967200	6.05442300	-1.59667200
H	-1.51735800	6.21941500	-2.05935400
H	-3.10445200	-4.09353700	-3.71421700

H	-4.36387300	-5.21725400	-4.26428200
H	-4.42910600	-3.51188800	-4.75104700
H	-7.10360900	-3.71060500	-2.13625600
H	-6.77076500	-4.96564100	-3.34731100
H	-6.76047000	-3.25427100	-3.82147400
H	-3.59917100	-4.84584100	-1.34987100
H	-5.15031000	-4.42543600	-0.60179800
H	-5.04936100	-5.80389700	-1.72076300
H	-4.53097900	4.37200700	1.07779200
H	-5.70628200	3.05963500	0.83773500
H	-5.27629100	3.55553000	2.46716300
C	7.14659800	1.58981100	-4.41016700
C	7.02009000	0.21205000	-4.11489500
C	6.23956700	-0.21121900	-3.06289300
C	5.54003300	0.72210500	-2.25289200
C	5.64308500	2.11287900	-2.57242500
C	6.46934600	2.51750600	-3.65424500
C	4.71071700	0.32314900	-1.15285100
C	3.94729000	1.28782900	-0.52048600
C	4.07893100	2.68193800	-0.77553500
C	4.93435900	3.05825500	-1.79351700
C	4.67129800	-1.08850600	-0.68459100
C	5.86170700	-1.74931200	-0.23220200
C	5.77346800	-3.12027600	0.16731200
C	4.52022300	-3.77499900	0.14027900
C	3.35627600	-3.12689900	-0.22106200
C	3.47133500	-1.76955800	-0.62331800
C	7.11892300	-1.09711800	-0.12733400
C	8.23388600	-1.77594400	0.31020000
C	8.15319500	-3.14223700	0.66643300
C	6.94549700	-3.79564500	0.59908500
O	3.02752500	0.89271500	0.44977100
O	2.30945500	-1.08782200	-0.98261300
P	1.69830400	0.05006900	0.01216600
O	0.71135900	0.83563700	-0.80527400
N	1.08626900	-0.54170800	1.37436100

C	2.06167700	-3.84534400	-0.17830400
C	3.41752700	3.71324000	0.06050900
C	1.12570200	-3.75377500	-1.22031900
C	-0.02659500	-4.53567400	-1.20705700
C	-0.26483700	-5.41869600	-0.15178900
C	0.63742500	-5.48660700	0.91073600
C	1.78814800	-4.70133100	0.89965900
C	2.92608500	4.88870600	-0.52856400
C	2.43694700	5.93037900	0.25709900
C	2.41688800	5.81103000	1.64758800
C	2.88134200	4.63683900	2.24245200
C	3.37371500	3.59513900	1.45978200
S	1.90243200	-0.84910900	2.72426900
O	2.06485200	0.34738800	3.56611600
O	3.03939200	-1.76265600	2.56702300
C	0.58060700	-1.84127300	3.58686200
F	-0.48510100	-1.06972800	3.86441600
F	1.07270700	-2.31928900	4.73134300
F	0.16647200	-2.87103100	2.83208100
H	7.77123400	1.91000200	-5.23906900
H	7.54089300	-0.51908500	-4.72644900
H	6.14361900	-1.26881100	-2.84859000
H	6.54769600	3.57843200	-3.87781400
H	5.08796500	4.11474500	-1.99258000
H	4.47489800	-4.82174900	0.42564700
H	7.19406100	-0.04800300	-0.38523700
H	9.18355200	-1.25450900	0.38894400
H	9.04187500	-3.66662200	1.00564300
H	6.86295000	-4.83967100	0.89012000
H	1.30792100	-3.07847200	-2.04779400
H	-0.74284100	-4.44461400	-2.01635300
H	-1.15524900	-6.04213200	-0.15335400
H	0.44514000	-6.14792100	1.75135700
H	2.47525000	-4.72582600	1.73915200
H	2.92848100	4.98064700	-1.61070700
H	2.07613800	6.83932500	-0.21628700

H	2.04293400	6.62612500	2.26119300
H	2.86211900	4.52657700	3.32282700
H	3.72751300	2.68897600	1.93733800
H	-0.57725300	0.27973400	1.66594800
H	-0.66580300	0.21463100	-1.08787300

SR-4h-a-TS2D

Zero-point correction= 1.126114 (Hartree/Particle)

Thermal correction to Energy= 1.201921

Thermal correction to Enthalpy= 1.202865

Thermal correction to Gibbs Free Energy= 1.014046

E(Solv) = -4581.94909951

C	-4.77593000	6.10416800	-0.42799900
C	-3.63106300	6.89403100	-0.28137600
C	-2.34907300	6.33844200	-0.35578300
C	-2.26567700	4.97305000	-0.58614800
C	-3.40816600	4.15514100	-0.74370800
C	-4.67854800	4.73140600	-0.65887700
N	-1.10463000	4.14415100	-0.70821500
C	-1.52048000	2.84096700	-0.87402500
C	-2.94332700	2.78394400	-0.89912000
C	-5.30817800	0.23114200	1.11706500
C	-4.32275100	1.13772400	1.47209900
C	-3.56407500	1.53889400	-0.92426100
C	-4.94848400	-1.15330600	0.98252000
C	-3.55867200	-1.50751000	1.11222500
N	-2.64947400	-0.53870300	1.40036800
C	-3.07190400	0.64041500	2.15580100
C	-5.84230400	-2.21041900	0.61299600
C	-5.39785700	-3.50327200	0.42006200
C	-4.02797100	-3.80584800	0.60084500
C	-3.11087200	-2.82436600	0.92019800
C	-1.92765000	1.65113800	2.21039800
C	-3.42777400	0.23607800	3.61351800
O	-0.75785000	1.80060500	-0.99932500

O	-7.15343900	-1.86383000	0.47168700
O	-3.71452400	-5.11638600	0.45668400
C	-8.08828800	-2.87412100	0.12909500
C	-2.40867100	-5.52945100	0.86526800
C	-4.88148700	1.28567100	-1.53610600
O	-5.75213500	2.10249900	-1.77801900
O	-4.96785600	-0.02507900	-1.86675100
C	-5.91427200	-0.33458400	-4.08418000
C	-6.14356600	-0.45363300	-2.58668200
O	0.50321200	5.76221000	-0.40082100
C	2.48630000	3.96934700	-1.47085900
C	3.07072100	4.12356900	-0.07129400
C	2.74474100	5.17705700	-2.36834200
C	2.95201600	2.67601700	-2.13007500
C	0.22710700	4.65049100	-0.78938600
O	1.01169600	3.75341000	-1.35862000
C	-6.70024900	0.76612700	0.89661000
H	-5.75730600	6.56470900	-0.36369500
H	-3.73067600	7.96012500	-0.10086900
H	-1.45902800	6.93751100	-0.22782600
H	-5.55619600	4.11378800	-0.79680800
H	-4.59118900	2.18146300	1.60732200
H	-2.91368900	0.67373800	-0.87612700
H	0.10691900	1.80670900	-0.43386300
H	-6.06543600	-4.31789900	0.17756900
H	-2.06303600	-3.03880000	1.06362200
H	-1.48073700	1.80106500	1.23591400
H	-1.13421100	1.28665300	2.86855500
H	-2.28461600	2.61017800	2.59899800
H	-3.72868100	1.11581200	4.19304000
H	-4.24508400	-0.48954400	3.63166800
H	-2.54917000	-0.21761100	4.08368400
H	-9.05607500	-2.37379700	0.06935800
H	-7.84875700	-3.32833400	-0.84071700
H	-8.12580200	-3.65857900	0.89451800
H	-1.63962300	-5.11560700	0.20962600

H	-2.20478600	-5.21593100	1.89492600
H	-2.41072500	-6.61823300	0.79639300
H	-6.78139000	-0.72384600	-4.62931700
H	-5.77386900	0.71327300	-4.36548000
H	-5.02987200	-0.90350900	-4.38851900
H	-6.28770300	-1.48960900	-2.27312300
H	-6.99745300	0.14589300	-2.26640200
H	2.75178500	3.29258200	0.56109800
H	4.16254400	4.10143100	-0.14446400
H	2.76728600	5.06601500	0.38865700
H	2.24859800	5.04880800	-3.33612600
H	3.82205000	5.25893400	-2.54755100
H	2.39506700	6.10133900	-1.90617100
H	4.03700500	2.70241500	-2.26494000
H	2.70130800	1.81514600	-1.51001400
H	2.48126500	2.55093200	-3.11045200
H	-6.69502400	1.85651000	0.96069600
H	-7.12507800	0.47482900	-0.06345300
H	-7.37251600	0.37125100	1.66572000
C	7.54283900	1.56296900	-2.62040700
C	6.80758800	0.53670400	-3.25885900
C	5.78738500	-0.10996300	-2.59800800
C	5.44335900	0.24127400	-1.26600600
C	6.16529000	1.30289900	-0.63217300
C	7.22578000	1.93515000	-1.33499700
C	4.36991300	-0.38372300	-0.54987500
C	4.00307900	0.14854700	0.67315100
C	4.70921200	1.19233100	1.33748900
C	5.79852500	1.72074400	0.66968000
C	3.64255500	-1.55979300	-1.10888300
C	4.34235100	-2.76825500	-1.43431800
C	3.61388400	-3.84058700	-2.04041100
C	2.22651400	-3.69800900	-2.27366600
C	1.51974000	-2.57397700	-1.88775700
C	2.26968600	-1.52210900	-1.28718700
C	5.72079200	-2.96382800	-1.15336400

C	6.35054500	-4.14134900	-1.48763900
C	5.63815800	-5.18558600	-2.12273900
C	4.29780600	-5.03590800	-2.38860400
O	2.87989800	-0.37689900	1.30139200
O	1.58622400	-0.38282000	-0.88318300
P	1.41137500	-0.02508700	0.70620100
O	1.07309100	1.44283200	0.69708600
N	0.37266000	-1.03651900	1.39237000
C	0.05286000	-2.49633200	-2.09976600
C	4.29261200	1.70918800	2.66458500
C	-0.59673500	-1.30338700	-2.45703100
C	-1.97412200	-1.28185100	-2.66891700
C	-2.73213400	-2.44363100	-2.53210400
C	-2.09745400	-3.64001300	-2.19957800
C	-0.72289500	-3.66247300	-1.98131400
C	4.44845200	3.07503400	2.95743700
C	4.07708200	3.58998300	4.19662100
C	3.53690500	2.74907800	5.17047900
C	3.37837800	1.39110300	4.89322600
C	3.75457700	0.87157100	3.65682300
S	0.58111300	-2.02698800	2.62708400
O	-0.74713000	-2.45957500	3.08553100
O	1.57618900	-1.61118400	3.62011700
C	1.29848500	-3.56054000	1.83981900
F	1.41878600	-4.52714700	2.75372600
F	2.49909500	-3.31162900	1.30710200
F	0.48480800	-3.99959600	0.86042100
H	8.34983200	2.06019000	-3.15066900
H	7.04743900	0.25913600	-4.28114600
H	5.22504300	-0.88896100	-3.09847700
H	7.77364200	2.73169400	-0.83794000
H	6.39122300	2.49378400	1.14939500
H	1.70383700	-4.50730700	-2.77421900
H	6.27570000	-2.17658000	-0.65806800
H	7.40359900	-4.27200900	-1.25593800
H	6.14939300	-6.10685300	-2.38638000

H	3.73321100	-5.83680000	-2.85913700
H	-0.02939500	-0.38876500	-2.56388600
H	-2.45893300	-0.34952800	-2.93782900
H	-3.80897600	-2.41244000	-2.65878400
H	-2.67998400	-4.54717300	-2.06995300
H	-0.24237700	-4.58850900	-1.68272000
H	4.83780100	3.74501900	2.19805500
H	4.19704500	4.65152900	4.39487400
H	3.23588600	3.15103600	6.13396500
H	2.95201900	0.72323400	5.63572000
H	3.61037900	-0.18299400	3.46775400
H	-1.68166500	-0.83425100	1.52736300

4h-b-TS1

Zero-point correction= 0.780053 (Hartree/Particle)

Thermal correction to Energy= 0.832877

Thermal correction to Enthalpy= 0.833821

Thermal correction to Gibbs Free Energy= 0.694729

E(Solv)= -3491.36146458

C	-3.00408900	0.41558400	2.83214700
C	-3.34211600	-0.78868600	2.18302400
C	-2.38050200	-1.73332800	1.85985400
C	-1.03422000	-1.48876200	2.16118600
C	-0.62804700	-0.21656700	2.70552700
C	-1.66719200	0.69656800	3.06828000
N	-0.10023700	-2.42785000	1.89852600
C	1.25788200	-2.37892200	2.45156700
C	1.69145700	-0.92255500	2.39414300
C	0.76741600	0.07793200	2.73453600
C	1.31315500	1.46458700	2.93789200
C	2.14992200	-3.28357400	1.60073500
C	1.24265200	-2.87938200	3.91072900
O	-1.26597300	1.83193600	3.68668300
C	-2.24645000	2.75940200	4.13567100
O	-4.61700500	-1.11855700	1.85459500

C	-5.67925400	-0.29115400	2.31051700
H	-3.76717000	1.12953500	3.09418400
H	-2.68500400	-2.67033200	1.41213800
H	-0.39232900	-3.26877900	1.41726700
H	2.72716000	-0.73617300	2.68244100
H	2.36142800	1.49935800	2.63456200
H	0.74499900	2.20042400	2.36370900
H	1.22966600	1.75291300	3.99112700
H	2.18781600	-2.94437100	0.56461200
H	3.16558400	-3.29873400	2.00052500
H	1.76411600	-4.30891900	1.60819100
H	2.24588000	-2.81799500	4.34744800
H	0.56521100	-2.27080200	4.51833600
H	0.90825700	-3.92253500	3.95660100
H	-1.68675900	3.56605200	4.61146600
H	-2.82529200	3.15926700	3.29847600
H	-2.91627000	2.29513200	4.86989700
H	-6.59601900	-0.77095300	1.96504800
H	-5.68961400	-0.22582500	3.40552700
H	-5.61258200	0.71592200	1.88677600
C	-5.30451000	-0.13117100	-4.06900700
C	-4.74247400	1.13581900	-3.78551900
C	-3.61086400	1.24347800	-3.00940900
C	-2.97810700	0.08900000	-2.47581000
C	-3.51981300	-1.19342500	-2.80492600
C	-4.69911600	-1.26986600	-3.59235700
C	-1.80211900	0.15833700	-1.65549400
C	-1.12713500	-1.01975900	-1.37630200
C	-1.65041800	-2.30513400	-1.69010100
C	-2.85445900	-2.36149400	-2.36169400
C	-1.31606800	1.44456400	-1.08686000
C	-2.18037300	2.29511800	-0.31306700
C	-1.65783000	3.52792700	0.19577800
C	-0.29809300	3.85483800	-0.02089300
C	0.54648900	3.03737900	-0.74417800
C	0.00224400	1.83175100	-1.26799000

C	-3.54088300	1.98747000	-0.03797600
C	-4.35862700	2.89135400	0.60265900
C	-3.85316900	4.13206000	1.05518100
C	-2.52185500	4.42746000	0.87627900
O	0.07931900	-0.96328900	-0.68646800
O	0.83441800	1.03615200	-2.04345700
P	1.39750200	-0.38759000	-1.47599300
O	1.92117200	-1.20693200	-2.58586600
N	2.31659700	-0.12472100	-0.11830400
C	1.95446100	3.43543500	-0.98105700
C	-0.97696200	-3.55718600	-1.25893900
C	2.49176700	3.46893200	-2.27572000
C	3.79448900	3.91019600	-2.48362500
C	4.58388300	4.30786400	-1.40386500
C	4.06254400	4.26527500	-0.11198700
C	2.75300200	3.83844700	0.09740600
C	0.35126300	-3.84533200	-1.60553200
C	0.93823500	-5.04105100	-1.19463900
C	0.22061800	-5.96108500	-0.42736900
C	-1.10394900	-5.68611100	-0.08347300
C	-1.69954400	-4.49554900	-0.50379200
S	3.87924100	0.34019300	-0.17279900
O	4.19896900	0.98103000	1.10506300
O	4.23880900	0.94118800	-1.45167600
C	4.82485700	-1.27674400	-0.10859400
F	6.08528300	-1.06007100	-0.48531400
F	4.27297000	-2.19050500	-0.90940100
F	4.82718200	-1.74953000	1.14976200
H	-6.20143000	-0.20128600	-4.67744600
H	-5.20320300	2.03177400	-4.19142300
H	-3.18257200	2.21809000	-2.80819100
H	-5.10381700	-2.25158800	-3.82445100
H	-3.27832200	-3.33138000	-2.60618400
H	0.08154200	4.79922300	0.35841400
H	-3.94057700	1.03075300	-0.34643300
H	-5.40608500	2.65005100	0.76061100

H	-4.51185600	4.84006900	1.55031500
H	-2.10854700	5.36613800	1.23633300
H	1.89161000	-0.50909000	1.08252400
H	1.88685600	3.14455600	-3.11502200
H	4.20028600	3.92781200	-3.49080800
H	5.60722000	4.63306600	-1.56798300
H	4.67852100	4.54673200	0.73689000
H	2.35322700	3.78383000	1.10520100
H	0.92143100	-3.13865300	-2.19866300
H	1.96765500	-5.24890100	-1.47202400
H	0.68768900	-6.88722900	-0.10445600
H	-1.67586900	-6.39628300	0.50734800
H	-2.73290600	-4.28302000	-0.24380400

4h-b-IM1

Zero-point correction=0.785594

Thermal correction to Energy= 0.838924

Thermal correction to Enthalpy= 0.839868

Thermal correction to Gibbs Free Energy= 0.697443

SCF Done: E(Solv) = -3491.37044477

C	7.222321	2.441795	-1.370776
C	7.056493	1.037653	-1.417189
C	5.864631	0.459635	-1.042155
C	4.773850	1.255016	-0.600733
C	4.930910	2.678439	-0.588546
C	6.178403	3.241245	-0.968036
C	3.516754	0.695380	-0.200320
C	2.471534	1.556801	0.086560
C	2.606330	2.973227	0.121150
C	3.842384	3.498025	-0.202868
C	3.300941	-0.775263	-0.101768
C	4.085897	-1.589535	0.779040
C	3.836337	-2.998534	0.817703
C	2.805479	-3.546750	0.019496

C	1.994015	-2.762839	-0.777709
C	2.270304	-1.366724	-0.812322
C	5.072975	-1.057498	1.650948
C	5.800830	-1.878803	2.482091
C	5.581901	-3.276329	2.488212
C	4.616088	-3.819875	1.674753
O	1.232265	1.021493	0.384515
O	1.456096	-0.555988	-1.587096
P	0.328325	0.364493	-0.819094
O	-0.195604	1.333003	-1.815539
N	-0.689815	-0.664654	-0.098071
C	0.886166	-3.372254	-1.552203
C	1.480384	3.855453	0.513724
C	0.579296	-2.966564	-2.861754
C	-0.430364	-3.598958	-3.584215
C	-1.147410	-4.656527	-3.021933
C	-0.851059	-5.067793	-1.721368
C	0.143895	-4.422290	-0.989889
C	1.274291	5.067500	-0.163766
C	0.272424	5.950013	0.236699
C	-0.541404	5.635611	1.325637
C	-0.357610	4.424136	1.994484
C	0.636421	3.536221	1.591025
S	-1.215911	-0.641276	1.391886
O	-2.431471	-1.464979	1.510496
O	-1.226577	0.681691	2.042102
C	0.041170	-1.634392	2.354106
F	-0.335110	-1.712520	3.637493
F	1.257369	-1.081044	2.298224
F	0.118984	-2.881576	1.860130
H	8.169974	2.884728	-1.663564
H	7.875770	0.409949	-1.756112
H	5.745072	-0.616268	-1.088190
H	6.287076	4.322681	-0.942594
H	3.992519	4.572890	-0.155467
H	2.647864	-4.620965	0.045395

H	5.242855	0.011953	1.664573
H	6.546401	-1.448197	3.144461
H	6.167282	-3.913260	3.145135
H	4.421668	-4.889450	1.683595
H	-2.059210	1.839651	-2.662195
H	1.136326	-2.155350	-3.313219
H	-0.648219	-3.270992	-4.597050
H	-1.926819	-5.155423	-3.591561
H	-1.399304	-5.891093	-1.270070
H	0.336435	-4.717388	0.035698
H	1.895768	5.307390	-1.021568
H	0.127845	6.881602	-0.304095
H	-1.319813	6.324679	1.643142
H	-0.996647	4.156368	2.830982
H	0.745831	2.590731	2.106144
C	-5.489925	-1.452991	0.545752
C	-6.194993	-0.348237	1.066798
C	-5.965831	0.953002	0.623608
C	-4.990633	1.186211	-0.349955
C	-4.244318	0.077303	-0.942459
C	-4.534791	-1.257452	-0.422245
N	-4.768494	2.444907	-0.785057
C	-3.479243	2.837167	-1.392989
C	-3.117815	1.748161	-2.404700
C	-3.353306	0.335791	-1.962861
C	-2.615263	-0.695903	-2.748417
C	-2.425522	2.979374	-0.287452
C	-3.677802	4.173869	-2.110131
O	-3.826111	-2.245147	-0.960452
C	-3.824129	-3.526505	-0.321724
O	-7.086992	-0.663053	2.019512
C	-7.824413	0.379602	2.654963
H	-5.690832	-2.425943	0.968925
H	-6.497716	1.795345	1.046947
H	-5.222585	3.173806	-0.246014
H	-3.698976	1.876495	-3.334451

H	-1.903114	-1.197398	-2.082405
H	-3.280440	-1.474730	-3.129113
H	-2.061693	-0.229822	-3.565057
H	-1.454622	3.244300	-0.709856
H	-2.725463	3.768271	0.410273
H	-2.294542	2.056990	0.282099
H	-2.741966	4.476113	-2.589110
H	-4.459704	4.104831	-2.873909
H	-3.951564	4.961256	-1.397238
H	-3.092624	-4.111051	-0.875382
H	-3.505185	-3.407597	0.715506
H	-4.814048	-3.992592	-0.387651
H	-8.460741	-0.116973	3.387439
H	-7.152222	1.079140	3.163614
H	-8.446352	0.918986	1.931548

4h-b-TS2

Zero-point correction=0.779953

Thermal correction to Energy= 0.832909

Thermal correction to Enthalpy= 0.833853

Thermal correction to Gibbs Free Energy= 0.690110

SCF Done: E(Solv) = -3491.34517200

C	-5.119581	1.464146	1.152871
C	-5.147502	2.866378	1.186061
C	-3.982919	3.600813	1.380699
C	-2.754686	2.948940	1.527729
C	-2.675103	1.516503	1.495078
C	-3.901361	0.808113	1.318011
N	-1.624714	3.716296	1.702136
C	-0.364123	3.135063	2.175623
C	-0.216777	1.824968	1.401686
C	-1.379009	0.889586	1.629578
C	-1.094426	-0.442501	1.851468
C	-0.389298	2.889561	3.694551

C	0.775330	4.086558	1.804110
O	-3.808074	-0.536452	1.300694
C	-4.964524	-1.318481	1.017401
O	-6.283829	3.595383	1.043822
C	-7.510762	2.908497	0.840097
H	-6.024739	0.897693	1.003273
H	-4.043474	4.683562	1.410577
H	-1.800648	4.669778	1.993862
H	0.729054	1.339619	1.637301
H	-0.076209	-0.689359	2.140483
H	-1.867558	-1.151541	2.116806
H	-0.905556	-0.950175	0.407650
H	-1.230943	2.248025	3.972872
H	0.535759	2.400417	4.018717
H	-0.486247	3.837805	4.235886
H	1.731734	3.675279	2.140274
H	0.818121	4.237240	0.720900
H	0.641483	5.063455	2.285599
H	-4.610001	-2.346422	0.995055
H	-5.725867	-1.186030	1.795320
H	-5.378809	-1.054783	0.038624
H	-8.272925	3.683633	0.749364
H	-7.486788	2.311244	-0.079693
H	-7.751545	2.258326	1.690303
H	-0.218616	2.076326	0.335644
C	6.973858	2.191298	-0.809427
C	6.752922	1.215031	0.190203
C	5.502893	0.667877	0.372031
C	4.405872	1.070342	-0.435415
C	4.639820	2.028946	-1.473099
C	5.938498	2.583294	-1.624874
C	3.087303	0.529699	-0.280364
C	2.112212	0.890730	-1.193406
C	2.322518	1.833295	-2.236858
C	3.580703	2.392402	-2.340028
C	2.749696	-0.439124	0.796592

C	2.889160	-0.104517	2.184323
C	2.519799	-1.077457	3.167950
C	2.020577	-2.335941	2.752203
C	1.827191	-2.648559	1.420025
C	2.198881	-1.664609	0.460371
C	3.313938	1.176944	2.629750
C	3.389485	1.471753	3.972928
C	3.049852	0.499811	4.943869
C	2.625660	-0.746033	4.545363
O	0.850455	0.307644	-1.087955
O	1.965096	-1.941127	-0.882010
P	0.668564	-1.239718	-1.599908
O	0.644130	-1.498232	-3.045656
N	-0.679085	-1.584344	-0.677043
C	1.200649	-3.929242	1.017986
C	1.245594	2.185821	-3.192564
C	1.706693	-4.699512	-0.040321
C	1.099477	-5.902169	-0.388018
C	-0.023686	-6.351813	0.307451
C	-0.537276	-5.591482	1.356571
C	0.071500	-4.389955	1.710423
C	1.504176	2.184814	-4.569919
C	0.507276	2.535476	-5.478709
C	-0.761933	2.892823	-5.023360
C	-1.028585	2.899346	-3.652853
C	-0.033276	2.547274	-2.746038
S	-1.766534	-2.762935	-1.011992
O	-2.505406	-3.045626	0.218623
O	-1.204969	-3.830906	-1.826933
C	-2.982571	-1.848195	-2.100656
F	-4.106702	-2.570883	-2.199357
F	-2.473518	-1.647412	-3.310462
F	-3.285847	-0.662133	-1.550604
H	7.964164	2.618009	-0.938811
H	7.578936	0.888917	0.815539
H	5.348181	-0.087632	1.133071

H	6.099227	3.317449	-2.410099
H	3.768220	3.130382	-3.114867
H	1.759318	-3.069773	3.509010
H	3.573970	1.929748	1.895852
H	3.713036	2.459261	4.289325
H	3.118339	0.743099	6.000011
H	2.348408	-1.497200	5.280227
H	2.571165	-4.350288	-0.592608
H	1.497364	-6.483354	-1.214522
H	-0.506670	-7.281117	0.019770
H	-1.428757	-5.917154	1.883970
H	-0.356333	-3.778695	2.498957
H	2.483257	1.878157	-4.925610
H	0.719533	2.516662	-6.543880
H	-1.540911	3.159184	-5.732112
H	-2.013412	3.177488	-3.288237
H	-0.240013	2.561170	-1.682366

4h-b-IM2

Zero-point correction=0.785376

Thermal correction to Energy= 0.838640

Thermal correction to Enthalpy= 0.839584

Thermal correction to Gibbs Free Energy= 0.697309

SCF Done: E(Solv) = -3491.36209216

C	-4.218968	-1.477654	-1.587265
C	-4.010183	-2.856888	-1.495926
C	-2.758464	-3.399444	-1.757778
C	-1.680353	-2.564396	-2.070624
C	-1.833045	-1.148841	-2.138233
C	-3.140931	-0.650022	-1.909623
N	-0.442408	-3.154625	-2.269529
C	0.598273	-2.449345	-3.023002
C	0.673509	-1.050515	-2.405839
C	-0.653182	-0.313479	-2.422427
C	-0.621005	1.019992	-2.650796

C	0.259300	-2.378621	-4.522569
C	1.913818	-3.199274	-2.805264
O	-3.294718	0.696378	-1.999537
C	-4.602368	1.254286	-1.977608
O	-4.981085	-3.748445	-1.146409
C	-6.272907	-3.246324	-0.842631
H	-5.189228	-1.050531	-1.390103
H	-2.624732	-4.474261	-1.692403
H	-0.492884	-4.148587	-2.460342
H	1.434603	-0.458869	-2.918776
H	0.336399	1.493787	-2.850903
H	-1.500978	1.644819	-2.678003
H	-0.913170	1.282716	-0.518340
H	-0.697771	-1.873556	-4.683011
H	1.032527	-1.824887	-5.067064
H	0.193921	-3.385375	-4.951753
H	2.732110	-2.696634	-3.327813
H	2.155377	-3.246248	-1.738577
H	1.844502	-4.225073	-3.189704
H	-4.461057	2.324076	-2.121494
H	-5.216148	0.833562	-2.783064
H	-5.093328	1.089237	-1.014025
H	-6.876526	-4.115888	-0.577859
H	-6.243208	-2.550933	0.005859
H	-6.722060	-2.742074	-1.707899
H	0.997852	-1.169198	-1.368744
C	6.204580	-2.655378	2.404595
C	6.357895	-1.453643	1.673994
C	5.259179	-0.794214	1.171441
C	3.948579	-1.303426	1.371668
C	3.791191	-2.496530	2.148107
C	4.947232	-3.159939	2.638884
C	2.777676	-0.649184	0.866121
C	1.539691	-1.149396	1.232826
C	1.353070	-2.323889	2.008910
C	2.491163	-2.981931	2.431647

C	2.845301	0.556222	-0.004785
C	3.508617	0.537021	-1.277508
C	3.452147	1.707529	-2.100834
C	2.746079	2.848674	-1.649842
C	2.083550	2.871481	-0.438743
C	2.156552	1.699109	0.361751
C	4.163997	-0.613285	-1.791584
C	4.754565	-0.597605	-3.035200
C	4.719138	0.567264	-3.836663
C	4.078611	1.693019	-3.375883
O	0.388737	-0.455583	0.830847
O	1.460405	1.697264	1.573814
P	0.038913	0.911896	1.637600
O	-0.512249	0.848968	2.995580
N	-0.976017	1.582991	0.467715
C	1.292037	4.054063	-0.024911
C	-0.001312	-2.800689	2.379931
C	1.424401	4.617915	1.252308
C	0.690281	5.747598	1.601274
C	-0.193891	6.323161	0.687973
C	-0.341800	5.762398	-0.579753
C	0.398621	4.637012	-0.935218
C	-0.277704	-3.126395	3.715028
C	-1.539275	-3.589496	4.084161
C	-2.539040	-3.733879	3.122047
C	-2.272359	-3.414255	1.789211
C	-1.012873	-2.948619	1.418797
S	-2.170083	2.694091	0.803221
O	-2.664954	3.178269	-0.479325
O	-1.755319	3.579292	1.876242
C	-3.531475	1.606802	1.526010
F	-4.708362	2.180156	1.235713
F	-3.400643	1.507985	2.838244
F	-3.494233	0.389960	0.975584
H	7.080501	-3.168485	2.790555
H	7.351005	-1.044157	1.513945

H	5.386381	0.130964	0.621943
H	4.814758	-4.070884	3.216685
H	2.387389	-3.894403	3.011761
H	2.719885	3.731991	-2.281328
H	4.183969	-1.519160	-1.200238
H	5.247724	-1.491653	-3.405861
H	5.190175	0.566339	-4.815146
H	4.030623	2.591696	-3.985149
H	2.101813	4.167628	1.969216
H	0.799494	6.171819	2.594940
H	-0.778582	7.193709	0.970536
H	-1.048930	6.185469	-1.286830
H	0.260061	4.181399	-1.911154
H	0.493363	-2.986372	4.466952
H	-1.742941	-3.826034	5.124749
H	-3.524017	-4.091254	3.409908
H	-3.040209	-3.533482	1.031814
H	-0.806986	-2.717682	0.381262

4h-b-TS3

Zero-point correction=1.128358

Thermal correction to Energy= 1.203983

Thermal correction to Enthalpy= 1.204927

Thermal correction to Gibbs Free Energy= 1.010588

SCF Done: E(Solv) = -4581.93844499

C	-0.720660	-2.675224	-0.252927
C	0.515649	-2.733421	-0.897101
C	1.160546	-1.549225	-1.278230
C	0.565751	-0.348987	-0.988671
C	-0.733127	-0.207087	-0.428200
C	-1.328604	-1.443440	-0.002325
N	1.331224	0.868395	-1.246740
C	0.514609	1.929773	-1.975661
C	-0.626684	2.263437	-1.013280

C	-1.369678	1.082432	-0.430503
C	-2.711527	1.331920	-0.070486
C	0.037926	1.338060	-3.303810
C	1.417294	3.136462	-2.210450
O	-2.505269	-1.364814	0.642791
C	-3.136265	-2.556762	1.119899
O	1.191996	-3.870909	-1.157128
C	0.755715	-5.075047	-0.529637
H	-1.202560	-3.581586	0.077103
H	2.142949	-1.604857	-1.720052
H	2.173449	0.634805	-1.785882
H	-1.343061	2.920267	-1.515284
H	-2.947900	2.376316	0.107807
H	-3.195450	0.646507	0.604821
H	-0.616799	0.474063	-3.162619
H	-0.519635	2.103938	-3.850318
H	0.888854	1.029784	-3.923043
H	0.827999	3.930678	-2.679089
H	1.809470	3.519916	-1.267015
H	2.242118	2.879857	-2.882781
H	-4.061834	-2.221130	1.586001
H	-3.372510	-3.233380	0.294636
H	-2.498603	-3.051711	1.860894
H	1.510594	-5.821730	-0.775923
H	0.703430	-4.944450	0.556710
H	-0.218421	-5.394967	-0.918507
H	-0.214165	2.853369	-0.184061
C	-3.905953	-3.477230	-2.420263
C	-5.016714	-4.062831	-1.797021
C	-5.955371	-3.288341	-1.101210
C	-5.747870	-1.916061	-1.041379
C	-4.631868	-1.303346	-1.672463
C	-3.712262	-2.098469	-2.366012
N	-6.508997	-0.906774	-0.405999
C	-5.834768	0.369743	-0.566089
C	-4.693887	0.103893	-1.424395

C	-3.720728	1.097638	-1.670489
O	-6.139145	1.417789	-0.015635
C	-4.200163	2.508526	-1.995360
O	-3.609146	3.533975	-1.717421
O	-5.323340	2.463507	-2.721623
C	-6.783581	4.186988	-1.799583
C	-5.966566	3.734232	-2.998225
O	-8.336140	-0.025310	0.542178
C	-9.486944	0.027986	1.457543
C	-9.828831	1.517086	1.448600
C	-9.057086	-0.426330	2.853001
C	-10.637092	-0.809196	0.897066
C	-7.670182	-1.157276	0.332143
O	-7.995511	-2.275784	0.689882
H	-3.192042	-4.101272	-2.950548
H	-5.159804	-5.138154	-1.851230
H	-6.804245	-3.737807	-0.605864
H	-2.844082	-1.645804	-2.837301
H	-2.959564	0.801953	-2.392300
H	-7.355098	5.084978	-2.060822
H	-7.473444	3.399339	-1.485440
H	-6.129760	4.420857	-0.956051
H	-5.201997	4.465982	-3.269815
H	-6.596478	3.524641	-3.865430
H	-10.106868	1.839519	0.440408
H	-10.667950	1.714338	2.123488
H	-8.964413	2.105038	1.769640
H	-8.792040	-1.484855	2.859856
H	-9.880458	-0.266504	3.557272
H	-8.197496	0.161298	3.191685
H	-11.530725	-0.659136	1.512810
H	-10.870084	-0.493749	-0.125350
H	-10.384122	-1.870169	0.891642
C	6.742461	-5.179460	-1.095438
C	7.079531	-3.945547	-1.700359
C	6.357780	-2.807185	-1.420002

C	5.260255	-2.843664	-0.520037
C	4.944883	-4.082925	0.122137
C	5.700221	-5.241797	-0.200693
C	4.461522	-1.695817	-0.215751
C	3.499917	-1.793713	0.779192
C	3.182008	-3.009561	1.454503
C	3.899564	-4.130299	1.073845
C	4.620594	-0.406774	-0.948006
C	4.450433	-0.324524	-2.374497
C	4.564487	0.957556	-3.007902
C	4.866441	2.100895	-2.227584
C	4.980023	2.046819	-0.852303
C	4.826480	0.767284	-0.237508
C	4.097487	-1.441157	-3.184380
C	3.867255	-1.298011	-4.534704
C	3.991283	-0.034294	-5.157698
C	4.338143	1.065373	-4.407399
O	2.744954	-0.675363	1.060016
O	4.835713	0.706792	1.141475
P	3.360553	0.615977	1.886338
O	3.529337	0.452034	3.338031
N	2.357982	1.720042	1.191302
C	5.191817	3.274132	-0.050690
C	2.130861	-3.106809	2.502164
C	6.041956	3.290638	1.066342
C	6.217241	4.459000	1.801009
C	5.545120	5.627167	1.441331
C	4.701735	5.624082	0.331755
C	4.531041	4.458939	-0.409868
C	2.256582	-4.073446	3.517254
C	1.266826	-4.243135	4.481721
C	0.124489	-3.441340	4.465850
C	-0.006258	-2.463749	3.480062
C	0.981927	-2.295534	2.512705
S	1.991927	3.122832	1.897286
O	1.373547	3.988570	0.877534

O	3.021579	3.662596	2.781058
C	0.553398	2.664044	2.999537
F	-0.415262	2.085436	2.260780
F	0.054025	3.764005	3.568700
F	0.928791	1.806209	3.945836
H	7.317867	-6.070503	-1.328568
H	7.919989	-3.894880	-2.386399
H	6.630472	-1.864413	-1.880121
H	5.446097	-6.178945	0.288227
H	3.661537	-5.091601	1.518453
H	4.990229	3.054654	-2.731738
H	3.998672	-2.417246	-2.725401
H	3.587518	-2.165251	-5.125311
H	3.813351	0.064333	-6.224359
H	4.437826	2.043138	-4.871694
H	6.557263	2.385846	1.363572
H	6.871152	4.451398	2.667864
H	5.666322	6.530322	2.032099
H	4.155619	6.520987	0.055565
H	3.848279	4.457345	-1.252313
H	3.156765	-4.677124	3.572023
H	1.398457	-4.991276	5.258290
H	-0.642697	-3.564241	5.224947
H	-0.875267	-1.811408	3.463598
H	0.859977	-1.525227	1.769430
H	1.694682	1.263237	-0.301341

4h-b-IM3

Zero-point correction= 1.130592

Thermal correction to Energy= 1.205422

Thermal correction to Enthalpy= 1.206366

Thermal correction to Gibbs Free Energy= 1.018447

SCF Done: E(Solv) = -4581.95381673

C	0.696056	-2.826638	-2.832398
C	1.307403	-2.026160	-1.856063
C	0.672772	-1.766207	-0.621702
C	-0.591004	-2.250766	-0.432350
C	-1.324695	-2.969139	-1.432570
C	-0.590915	-3.309487	-2.621878
N	-1.318427	-1.848377	0.760256
C	-2.316139	-2.881097	1.268321
C	-3.289847	-3.121809	0.116214
C	-2.697846	-3.213105	-1.238258
C	-3.712127	-3.283696	-2.295363
C	-3.041295	-2.259908	2.461717
C	-1.564207	-4.154437	1.665393
O	-1.194459	-4.162833	-3.461880
C	-0.692383	-4.294803	-4.791848
O	2.510248	-1.463491	-2.002702
C	3.224298	-1.588887	-3.230688
H	1.222577	-3.068853	-3.743297
H	1.176309	-1.168833	0.133705
H	-1.874120	-0.988811	0.479672
H	-4.062074	-2.322536	0.055410
H	-4.597779	-3.822963	-1.950744
H	-3.350676	-3.693140	-3.231824
H	-3.549814	-1.335265	2.168582
H	-3.799965	-2.961751	2.822036
H	-2.342363	-2.043883	3.271585
H	-2.287127	-4.880599	2.049960
H	-1.050259	-4.605960	0.812475
H	-0.832296	-3.940134	2.445193

H	-1.412256	-4.926519	-5.311965
H	-0.644583	-3.313666	-5.271308
H	0.288959	-4.782701	-4.794687
H	4.136217	-1.009976	-3.087587
H	3.479682	-2.635437	-3.431438
H	2.640065	-1.175294	-4.059998
H	-3.872901	-4.031173	0.314104
C	-8.584394	-0.925402	-1.269224
C	-8.654130	0.023625	-0.242668
C	-7.496554	0.603729	0.289902
C	-6.271187	0.209709	-0.230384
C	-6.179617	-0.752481	-1.272590
C	-7.352486	-1.317986	-1.788671
N	-4.950690	0.619143	0.090785
C	-4.022704	-0.126489	-0.715647
C	-4.792244	-0.950277	-1.585741
C	-4.246554	-1.781806	-2.669638
O	-2.780875	-0.076577	-0.558610
C	-3.161127	-1.128604	-3.540432
O	-2.456687	-1.764894	-4.305071
O	-3.116285	0.190745	-3.403732
C	-0.706149	0.568182	-3.250858
C	-1.983685	0.872786	-4.010455
O	-5.469246	2.142354	1.663035
C	-5.444636	3.477894	2.306582
C	-6.664034	3.416422	3.224775
C	-5.615843	4.560792	1.241180
C	-4.161351	3.648347	3.116801
C	-4.587265	1.831648	0.705224
O	-3.611923	2.475628	0.386373
H	-9.498045	-1.360784	-1.663409
H	-9.620844	0.316873	0.155616
H	-7.553951	1.326133	1.091319
H	-7.302803	-2.053860	-2.587389
H	-5.066548	-2.014707	-3.360675
H	0.102822	1.205605	-3.615440

H	-0.849689	0.764845	-2.186632
H	-0.422653	-0.475771	-3.387017
H	-1.921631	0.579071	-5.061934
H	-2.248734	1.927280	-3.936547
H	-6.573096	2.583423	3.928405
H	-6.744910	4.346219	3.796240
H	-7.584249	3.286588	2.645872
H	-4.747055	4.610618	0.583534
H	-5.739152	5.532308	1.731066
H	-6.509671	4.365533	0.638971
H	-4.215874	4.587220	3.678579
H	-4.041912	2.829118	3.830906
H	-3.280853	3.672546	2.475708
C	6.634918	4.748886	-2.547720
C	5.372854	5.238862	-2.136584
C	4.458053	4.403104	-1.537098
C	4.754963	3.031725	-1.314917
C	6.053737	2.551807	-1.679352
C	6.966138	3.434523	-2.317209
C	3.826500	2.122943	-0.708148
C	4.279151	0.857939	-0.355451
C	5.583625	0.371463	-0.665241
C	6.420422	1.221068	-1.365660
C	2.406162	2.484786	-0.437641
C	1.533204	2.964746	-1.473724
C	0.169869	3.254582	-1.143179
C	-0.318869	2.962092	0.151591
C	0.497607	2.451824	1.142117
C	1.877197	2.275899	0.828712
C	1.942718	3.157000	-2.822017
C	1.086288	3.695651	-3.757780
C	-0.240449	4.042282	-3.408651
C	-0.691164	3.802767	-2.131555
O	3.426774	0.014336	0.327801
O	2.730452	1.873202	1.841048
P	3.179847	0.293205	1.937390

O	4.347791	0.137570	2.821751
N	1.809477	-0.577115	2.087946
C	-0.078178	2.033813	2.444145
C	6.056785	-0.962622	-0.213393
C	0.567049	2.253205	3.670973
C	-0.006323	1.810382	4.860504
C	-1.239693	1.158569	4.852041
C	-1.895838	0.950855	3.639413
C	-1.318298	1.374848	2.445002
C	7.387686	-1.107361	0.211395
C	7.876791	-2.340251	0.636414
C	7.041239	-3.457051	0.656751
C	5.714590	-3.325960	0.245903
C	5.226189	-2.096254	-0.188160
S	1.433928	-1.515177	3.287081
O	-0.008145	-1.872697	3.126203
O	1.888991	-1.175389	4.631995
C	2.267950	-3.130447	2.855427
F	1.832004	-3.552336	1.645971
F	1.960544	-4.073957	3.754575
F	3.591453	-2.989194	2.795296
H	7.345174	5.416951	-3.026398
H	5.126336	6.285820	-2.288498
H	3.498061	4.789990	-1.216804
H	7.943486	3.051877	-2.600708
H	7.407473	0.874545	-1.658116
H	-1.371600	3.123879	0.354478
H	2.950160	2.888258	-3.112294
H	1.433062	3.849183	-4.776101
H	-0.902436	4.474771	-4.153887
H	-1.719317	4.015903	-1.851019
H	1.525910	2.754905	3.691518
H	0.520742	1.966135	5.796765
H	-1.677374	0.804465	5.780943
H	-2.857359	0.445761	3.621548
H	-1.819895	1.192523	1.500913

H	8.032441	-0.234727	0.244830
H	8.906550	-2.422113	0.973076
H	7.416276	-4.415490	1.004715
H	5.046291	-4.182333	0.276034
H	4.192067	-2.009044	-0.488622
H	-0.670855	-1.624819	1.559683

4h-b-TS4

Zero-point correction=1.126763

Thermal correction to Energy= 1.201190

Thermal correction to Enthalpy= 1.202135

Thermal correction to Gibbs Free Energy= 1.015215

SCF Done: E(Solv) = -4581.94043002

C	-0.792748	2.557075	-3.001563
C	-1.359503	1.781619	-1.982689
C	-0.709088	1.634952	-0.743833
C	0.529189	2.206864	-0.594137
C	1.209265	2.909825	-1.624045
C	0.466617	3.129735	-2.819850
N	1.272721	1.906226	0.630015
C	2.296516	2.954015	1.047539
C	3.175489	3.190525	-0.163408
C	2.581923	3.297497	-1.439561
C	3.590161	3.301549	-2.522251
C	3.100293	2.364417	2.208172
C	1.558624	4.232403	1.464071
O	1.029062	3.950278	-3.730682
C	0.537108	3.930624	-5.068672
O	-2.534228	1.138965	-2.093852
C	-3.251872	1.171536	-3.322116
H	-1.325818	2.711095	-3.927884
H	-1.172621	1.062221	0.052246
H	1.779611	1.011929	0.429548
H	3.940796	2.146315	-0.448584

H	4.444323	3.927156	-2.248872
H	3.212240	3.584303	-3.497682
H	3.620537	1.449648	1.904518
H	3.855397	3.091397	2.522699
H	2.448537	2.139678	3.054114
H	2.299707	4.996155	1.718396
H	0.938887	4.616584	0.649558
H	0.926908	4.046257	2.333989
H	1.226558	4.551256	-5.641527
H	0.546858	2.909987	-5.461085
H	-0.469789	4.360557	-5.126414
H	-4.139015	0.562342	-3.149264
H	-3.553418	2.194268	-3.577427
H	-2.653166	0.742526	-4.134054
H	4.016728	3.859859	0.031271
C	8.366854	1.303320	-0.871419
C	8.468639	0.205892	-0.012191
C	7.340205	-0.535253	0.357271
C	6.110900	-0.142982	-0.156468
C	5.988211	0.965061	-1.023535
C	7.125016	1.688805	-1.380986
N	4.819894	-0.713041	0.009521
C	3.858107	0.050448	-0.704578
C	4.579204	1.142441	-1.372054
C	4.154097	1.793380	-2.659203
O	2.638764	-0.111644	-0.588373
C	3.185261	1.011919	-3.558424
O	2.523718	1.544796	-4.430119
O	3.199531	-0.296357	-3.322730
C	0.792250	-0.756879	-3.345169
C	2.145069	-1.082228	-3.950990
O	5.316258	-2.230445	1.594642
C	5.332094	-3.572245	2.235022
C	6.419419	-3.407666	3.294524
C	5.727230	-4.619837	1.194932
C	3.980673	-3.866097	2.882694

C	4.510883	-1.978084	0.561257
O	3.638389	-2.690733	0.120512
H	9.257612	1.862038	-1.142347
H	9.438713	-0.082156	0.381562
H	7.421432	-1.379202	1.027519
H	7.046088	2.543673	-2.047937
H	5.059115	1.914503	-3.267032
H	0.036362	-1.433884	-3.749653
H	0.824712	-0.885684	-2.261975
H	0.504640	0.269245	-3.575427
H	2.172296	-0.896066	-5.028055
H	2.437056	-2.112264	-3.745974
H	6.161296	-2.601031	3.987066
H	6.522644	-4.335570	3.865237
H	7.385519	-3.177206	2.833685
H	4.956874	-4.728488	0.429993
H	5.863354	-5.586348	1.691066
H	6.672990	-4.346735	0.714550
H	4.060979	-4.793273	3.460479
H	3.689642	-3.060692	3.561510
H	3.195198	-3.986266	2.137002
C	-6.709187	-4.708497	-2.278043
C	-5.448618	-5.213222	-1.880761
C	-4.505426	-4.381198	-1.321296
C	-4.770756	-2.999171	-1.127265
C	-6.066920	-2.502119	-1.478618
C	-7.009502	-3.382197	-2.074540
C	-3.812431	-2.095471	-0.559917
C	-4.234227	-0.814732	-0.228331
C	-5.529238	-0.305562	-0.538400
C	-6.398689	-1.154453	-1.197567
C	-2.392312	-2.475365	-0.315695
C	-1.556065	-2.995792	-1.363011
C	-0.192215	-3.311192	-1.060181
C	0.337331	-2.990298	0.211171
C	-0.439528	-2.432400	1.207350

C	-1.825490	-2.244764	0.930550
C	-2.003599	-3.210345	-2.695679
C	-1.186777	-3.800291	-3.635846
C	0.137785	-4.176845	-3.309447
C	0.628470	-3.912107	-2.052370
O	-3.359515	0.026304	0.427263
O	-2.643110	-1.811164	1.958946
P	-3.081546	-0.226436	2.034928
O	-4.228786	-0.046909	2.941686
N	-1.699621	0.629919	2.143279
C	0.188144	-1.971811	2.470693
C	-5.951122	1.058764	-0.130840
C	-0.408813	-2.132332	3.730200
C	0.216749	-1.645135	4.875651
C	1.454248	-1.006043	4.790531
C	2.062650	-0.854954	3.544528
C	1.432207	-1.324843	2.394832
C	-7.257921	1.260525	0.340723
C	-7.693142	2.525771	0.728551
C	-6.825857	3.616266	0.661987
C	-5.522613	3.428202	0.200459
C	-5.088477	2.166271	-0.196432
S	-1.314414	1.637970	3.278772
O	0.124537	1.988760	3.073631
O	-1.744405	1.376222	4.649218
C	-2.158440	3.224058	2.765900
F	-1.769588	3.553257	1.512625
F	-1.809273	4.227843	3.581525
F	-3.483401	3.089318	2.770904
H	-7.442366	-5.373840	-2.724923
H	-5.225676	-6.268335	-2.011314
H	-3.546697	-4.779169	-1.010851
H	-7.984641	-2.987018	-2.348308
H	-7.382048	-0.792049	-1.483631
H	1.392068	-3.167121	0.387548
H	-3.009902	-2.920226	-2.968762

H	-1.563236	-3.971378	-4.640763
H	0.767951	-4.648570	-4.058460
H	1.657395	-4.144653	-1.790857
H	-1.370975	-2.621792	3.810241
H	-0.273123	-1.755412	5.838209
H	1.931073	-0.616950	5.685533
H	3.026793	-0.359910	3.464903
H	1.888039	-1.179449	1.421963
H	-7.924160	0.408976	0.439116
H	-8.704732	2.654365	1.103531
H	-7.158393	4.600267	0.980691
H	-4.830827	4.265247	0.160300
H	-4.073737	2.032831	-0.543702
H	0.641094	1.756922	1.460792

TfOH-b-TS1

Zero-point correction=0.344470

Thermal correction to Energy= 0.370265

Thermal correction to Enthalpy= 0.371209

Thermal correction to Gibbs Free Energy= 0.287682

SCF Done: E(Solv) = -1712.65130054

C	3.043368	-0.804163	0.220011
C	3.227054	-0.141368	-1.008069
C	2.398202	0.904940	-1.391996
C	1.348214	1.306979	-0.560679
C	1.099835	0.640180	0.692212
C	1.995701	-0.417263	1.045959
N	0.516942	2.303566	-0.968939
C	-0.358885	3.036685	-0.045074
C	-0.929336	1.984545	0.893662
C	-0.088298	0.986879	1.411493
C	-0.569375	0.245652	2.626004
C	-1.465643	3.709092	-0.863796
C	0.448348	4.092571	0.735525

O	1.775019	-1.011705	2.240841
C	2.559199	-2.136284	2.615241
O	4.214839	-0.454829	-1.878616
C	5.093902	-1.527972	-1.565668
H	3.707985	-1.599755	0.516282
H	2.575943	1.396565	-2.342202
H	0.779536	2.787064	-1.817969
H	-1.720206	2.339051	1.553934
H	-1.556980	0.603813	2.916842
H	-0.630338	-0.826727	2.437603
H	0.135052	0.389419	3.452023
H	-2.035314	2.969062	-1.430378
H	-2.150622	4.244970	-0.199024
H	-1.038387	4.442548	-1.559206
H	-0.195131	4.616707	1.450856
H	1.264745	3.619082	1.290426
H	0.877322	4.836396	0.052920
H	2.156372	-2.467777	3.572855
H	2.469105	-2.942738	1.878398
H	3.614271	-1.862631	2.736626
H	5.779565	-1.603042	-2.410385
H	5.663819	-1.323813	-0.650984
H	4.546674	-2.471685	-1.454573
H	-1.649765	1.158409	0.050577
O	-2.299580	0.567992	-0.854356
S	-3.089127	-0.648291	-0.314282
O	-3.213275	-0.601439	1.146842
O	-4.252229	-0.950094	-1.139889
C	-1.872336	-2.016079	-0.643389
F	-1.585397	-2.099874	-1.944391
F	-2.373848	-3.184581	-0.231793
F	-0.725655	-1.786989	0.029434

TfOH-b-IM1

Zero-point correction=0.350616

Thermal correction to Energy= 0.376658

Thermal correction to Enthalpy= 0.377602

Thermal correction to Gibbs Free Energy= 0.295114

SCF Done: E(Solv) = -1712.67918116

C	-0.719984	2.050004	0.794015
C	-0.531826	2.368542	-0.568589
C	0.613565	1.987878	-1.267946
C	1.513473	1.107906	-0.680205
C	1.290357	0.624474	0.682770
C	0.190923	1.231412	1.420730
N	2.557601	0.625539	-1.382810
C	3.596186	-0.235336	-0.807994
C	2.886425	-1.193279	0.150724
C	1.900585	-0.544449	1.074707
C	1.576115	-1.323133	2.307362
C	4.635872	0.625768	-0.067206
C	4.255802	-1.014386	-1.947783
O	0.156075	0.946570	2.722108
C	-1.065576	1.166032	3.439596
O	-1.424698	3.081760	-1.267898
C	-2.767917	3.168909	-0.776615
H	-1.581587	2.419832	1.326282
H	0.711266	2.278402	-2.307758
H	2.684778	0.962186	-2.327382
H	3.629914	-1.750138	0.730746
H	2.003804	-2.326266	2.237589
H	1.984518	-0.827193	3.195641
H	0.492395	-1.392081	2.429575
H	4.166439	1.198576	0.738496
H	5.417185	-0.005962	0.369482
H	5.110777	1.330868	-0.757390
H	5.023796	-1.685465	-1.551506
H	3.515806	-1.613099	-2.487482

H	4.743920	-0.332894	-2.655467
H	-0.897788	0.739525	4.428448
H	-1.271341	2.238451	3.533075
H	-1.876894	0.641288	2.931187
H	-3.339558	3.626869	-1.583999
H	-3.155419	2.169014	-0.561370
H	-2.826110	3.804863	0.113596
C	-2.431798	-1.002996	-1.083237
F	-3.570695	-0.535456	-0.532336
F	-1.769806	0.066928	-1.583116
F	-2.756800	-1.792426	-2.113291
S	-1.400115	-1.912990	0.177674
O	-1.475854	-1.006920	1.357630
O	-2.086872	-3.202326	0.327121
O	-0.056143	-1.953120	-0.454514
H	2.285170	-1.930909	-0.403745

TfOH-b-TS2

Zero-point correction=0.344922

Thermal correction to Energy= 0.370302

Thermal correction to Enthalpy= 0.371246

Thermal correction to Gibbs Free Energy= 0.289139

SCF Done: E(Solv) = -1712.65127158

C	-1.150084	-2.359829	0.561952
C	-2.152118	-2.372704	-0.422740
C	-2.701863	-1.189315	-0.904414
C	-2.253447	0.042736	-0.421566
C	-1.245831	0.108493	0.602839
C	-0.713137	-1.139438	1.060749
N	-2.785950	1.189936	-0.944863
C	-2.623575	2.493547	-0.294670
C	-1.165054	2.557632	0.168058
C	-0.774982	1.388841	1.040239
C	0.095881	1.639889	2.104330

C	-3.595256	2.630143	0.892511
C	-2.892050	3.582496	-1.335775
O	0.269304	-1.058094	1.979512
C	1.105023	-2.185979	2.223623
O	-2.650387	-3.509900	-0.962436
C	-2.121309	-4.759478	-0.536299
H	-0.713902	-3.278993	0.920397
H	-3.469051	-1.240776	-1.669440
H	-3.635695	1.069029	-1.481458
H	-0.983823	3.498816	0.692979
H	0.213036	2.684175	2.389105
H	0.168970	0.922165	2.914309
H	1.315736	1.313477	1.545841
H	-3.433376	1.833354	1.625206
H	-3.457501	3.592526	1.397716
H	-4.633682	2.572641	0.547241
H	-2.763062	4.574526	-0.891741
H	-2.206628	3.484590	-2.182657
H	-3.921370	3.517034	-1.710328
H	1.917597	-1.810599	2.845390
H	0.560728	-2.974776	2.756311
H	1.511930	-2.571610	1.285158
H	-2.660397	-5.517565	-1.105594
H	-1.049121	-4.832769	-0.754149
H	-2.289657	-4.919483	0.535585
C	2.758181	-0.611263	-0.868468
F	3.523942	-1.392300	-0.093036
F	1.503597	-1.096730	-0.839116
F	3.206185	-0.675315	-2.124105
S	2.787781	1.149713	-0.269500
O	2.477270	0.951410	1.229751
O	4.154086	1.607040	-0.494006
O	1.675127	1.803408	-0.970742
H	-0.502573	2.532824	-0.706366

TfOH-b-TS3

Zero-point correction= 0.694028 (Hartree/Particle)

Thermal correction to Energy= 0.742064

Thermal correction to Enthalpy= 0.743008

Thermal correction to Gibbs Free Energy= 0.609292

E(Solv) = -2803.26564601

C	-0.57892500	4.44209900	-0.49383000
C	0.76176600	4.12221000	-0.74647100
C	1.27471300	2.86745000	-0.38203700
C	0.43185100	1.97968400	0.24315300
C	-0.92690600	2.24651200	0.56069300
C	-1.41357700	3.52023300	0.13899400
N	0.92087700	0.64004800	0.52140500
C	0.55622100	0.14253400	1.91256300
C	-0.97569000	0.13398900	1.96083000
C	-1.68357900	1.25636700	1.27326200
C	-3.08825100	1.10017400	1.21735900
C	1.17315100	1.09331400	2.94174400
C	1.10952000	-1.27369100	2.06263000
O	-2.71294500	3.79484400	0.41029200
C	-3.25598600	5.05309400	0.03068000
O	1.63493500	4.95464300	-1.34813900
C	1.19377100	6.24715300	-1.74613700
H	-0.96793400	5.40542400	-0.78642200
H	2.30622400	2.60936800	-0.59247800
H	1.97489100	0.60919600	0.37906800
H	-1.30075600	0.08231400	3.00749500
H	-3.53251400	0.48012800	1.99366300
H	-3.67666800	1.97064400	0.96041700
H	0.73358900	2.09343800	2.88737300
H	0.98761400	0.69433000	3.94353400
H	2.25594500	1.17901000	2.80624000
H	0.75395400	-1.69382800	3.00883500
H	0.75894800	-1.91712800	1.25215700
H	2.20238300	-1.28254500	2.06331100

H	-4.29997100	5.02679800	0.34478700
H	-2.74129900	5.87758700	0.53794000
H	-3.20316800	5.19518400	-1.05509800
H	2.06276700	6.72972300	-2.19344500
H	0.38894400	6.18043100	-2.48849300
H	0.85303300	6.83262600	-0.88345700
H	-1.36968500	-0.80054300	1.51182600
C	-4.61391100	-4.34134200	1.33512800
C	-3.58226600	-5.24946600	1.07586000
C	-2.40126200	-4.84799500	0.44187800
C	-2.28776600	-3.51380600	0.07420000
C	-3.33003600	-2.57631600	0.31545800
C	-4.49856800	-3.00408600	0.96187400
N	-1.19453600	-2.83717800	-0.53400600
C	-1.54451500	-1.47034100	-0.70363900
C	-2.89113900	-1.29979200	-0.19508800
C	-3.43584600	0.01437700	-0.27982700
O	-0.81571100	-0.56984400	-1.15146900
C	-4.92241000	0.21723700	-0.32473100
O	-5.73694400	-0.26028700	0.43831200
O	-5.23283600	1.08178300	-1.31322900
C	-6.93818200	2.59477900	-0.44178800
C	-6.62570000	1.46688100	-1.41188200
O	0.91892800	-2.56942500	-1.27758200
C	2.24196400	-2.99004400	-1.82598700
C	2.84384300	-1.66184600	-2.27398500
C	2.02775600	-3.92060200	-3.01953200
C	3.06765000	-3.62875200	-0.71231600
C	0.01507100	-3.46751500	-0.90390000
O	0.15262600	-4.67235300	-0.84548800
H	-5.51659400	-4.67964000	1.83554000
H	-3.69010800	-6.28852200	1.37296500
H	-1.60058700	-5.54426800	0.24154500
H	-5.29063600	-2.29488200	1.16159800
H	-2.92926100	0.60799700	-1.03600500
H	-7.97295100	2.92907800	-0.57442300

H	-6.81672200	2.25571600	0.59073700
H	-6.27482300	3.44849900	-0.61816800
H	-6.74539200	1.77985700	-2.45101600
H	-7.24892700	0.59107900	-1.21945100
H	2.95634000	-0.96970800	-1.43749800
H	3.84010000	-1.83558200	-2.69235500
H	2.21639300	-1.19695900	-3.04148100
H	1.62206700	-4.88539800	-2.71402200
H	2.99096300	-4.08408200	-3.51409700
H	1.34875500	-3.45925400	-3.74489700
H	4.04751500	-3.90776500	-1.11492200
H	3.23983600	-2.91930800	0.10144100
H	2.58158000	-4.52921800	-0.33147600
S	4.53340600	0.27414500	1.01562100
O	4.77930500	1.22157200	2.11262700
O	3.52437500	0.77391600	0.00475700
C	6.08066900	0.25701000	-0.01004200
F	7.11860400	-0.15731800	0.72541300
F	6.34860700	1.48181800	-0.48056100
F	5.93470400	-0.57707400	-1.05176100
H	0.47496700	-0.00240600	-0.18451700
O	4.31882800	-1.13955300	1.38529500

TfOH-b-IM3

Zero-point correction= 0.694864 (Hartree/Particle)

Thermal correction to Energy= 0.743100

Thermal correction to Enthalpy= 0.744044

Thermal correction to Gibbs Free Energy= 0.609429

E(Solve) = -2803.2705702

C	-0.00364100	4.54437600	0.53380100
C	-1.30706400	4.08394000	0.77145800
C	-1.69144600	2.78726400	0.38419900
C	-0.76886200	2.00546200	-0.26155600
C	0.56063100	2.42162700	-0.58030400
C	0.92299800	3.72719900	-0.11103300

N	-1.09337000	0.62161500	-0.53832000
C	-0.71361600	0.18575200	-1.94482600
C	0.80417500	0.37937100	-2.03454200
C	1.39039100	1.53961900	-1.31637800
C	2.85129000	1.51931100	-1.30525200
C	-1.47875600	1.05429200	-2.94624800
C	-1.07961300	-1.29046800	-2.09082800
O	2.18771700	4.13168600	-0.36028200
C	2.59520800	5.44174600	0.02194900
O	-2.25913000	4.80857800	1.38476100
C	-1.95503300	6.13004700	1.82035700
H	0.28452200	5.53429500	0.85291400
H	-2.68642400	2.41664400	0.60341400
H	-2.12712500	0.45307300	-0.35509300
H	1.10740900	0.41930700	-3.08933500
H	3.26099200	1.02845800	-2.19002000
H	3.30950500	2.49450600	-1.18457100
H	-1.17579800	2.10418300	-2.88928500
H	-1.26769700	0.69430900	-3.95778400
H	-2.55930400	0.99202200	-2.78248000
H	-0.70424900	-1.65468900	-3.05247100
H	-0.62043300	-1.88524600	-1.29757700
H	-2.16121100	-1.44313100	-2.05509700
H	3.63541100	5.52596400	-0.29279400
H	1.99358600	6.20521700	-0.48447300
H	2.52727400	5.57388200	1.10787300
H	-2.87181200	6.50755500	2.27271800
H	-1.15192000	6.12432700	2.56691200
H	-1.67211900	6.76867800	0.97514700
H	1.34512600	-0.51097100	-1.64377500
C	5.16861300	-3.52056200	-1.45922300
C	4.30820300	-4.58228300	-1.15086500
C	3.07986300	-4.36682600	-0.51587200
C	2.73788600	-3.05898500	-0.19546100
C	3.60422600	-1.96703900	-0.49003200
C	4.82701500	-2.21090300	-1.13397300

N	1.56390600	-2.54402500	0.41091500
C	1.70620800	-1.12380400	0.53697200
C	2.96726300	-0.77294900	-0.02242400
C	3.37520100	0.63835900	-0.03056400
O	0.85639000	-0.32590300	0.99248900
C	4.88954500	0.79970500	0.01632300
O	5.58441500	1.19011800	-0.89951200
O	5.35408900	0.42912300	1.21967100
C	7.27382800	1.85641300	1.75089100
C	6.79245800	0.45958500	1.39596500
O	-0.54695200	-2.58348200	1.20205800
C	-1.77932400	-3.19065900	1.77864000
C	-2.56809400	-1.96317400	2.22466000
C	-1.40873400	-4.06377800	2.97752600
C	-2.52052100	-3.96030400	0.68796900
C	0.47613600	-3.34141100	0.81622700
O	0.51667200	-4.55502600	0.77540800
H	6.11196800	-3.72021800	-1.95931300
H	4.59304500	-5.59762800	-1.41017200
H	2.41382300	-5.18341300	-0.27862200
H	5.48762800	-1.38831600	-1.38739000
H	2.94632400	1.12365000	0.85110400
H	8.34947400	1.83729700	1.95853000
H	7.09569500	2.54512000	0.92072600
H	6.75783900	2.22836000	2.64194000
H	6.97403800	-0.25008600	2.20538700
H	7.26400200	0.09545500	0.48026500
H	-2.79436300	-1.30489100	1.38432900
H	-3.52178700	-2.27827000	2.65941800
H	-2.00700000	-1.40030500	2.97782100
H	-0.86763700	-4.96007100	2.67333000
H	-2.32787200	-4.36349000	3.49189700
H	-0.79390100	-3.49673000	3.68498300
H	-3.43603200	-4.38505500	1.11397000
H	-2.81865600	-3.29177200	-0.12393500
H	-1.90819700	-4.77679900	0.30020100

S	-4.63145700	-0.20607400	-0.90517100
O	-5.01675100	0.66364000	-2.02679100
O	-3.67751700	0.45415800	0.06616700
C	-6.14677600	-0.38535400	0.15210600
F	-7.13404100	-0.95583300	-0.54773700
F	-6.56311700	0.81169100	0.58553100
F	-5.87789800	-1.15460900	1.21832500
H	-0.51999800	0.03860100	0.14042000
O	-4.24106200	-1.59169700	-1.23366900

TfOH-b-TS4

Zero-point correction= 0.691314 (Hartree/Particle)

Thermal correction to Energy= 0.739036

Thermal correction to Enthalpy= 0.739980

Thermal correction to Gibbs Free Energy= 0.607042

E(Solv) = -2803.25757534

C	0.23294200	4.58428600	-0.57407000
C	1.48063000	3.99298100	-0.80543100
C	1.73820500	2.67686100	-0.38351100
C	0.73326500	2.00770100	0.27199800
C	-0.55160200	2.54566500	0.54719100
C	-0.77080300	3.87312900	0.08899100
N	0.93342600	0.60427800	0.60791400
C	0.40671000	0.22764500	1.98617400
C	-1.06750300	0.58976000	1.96762000
C	-1.49863600	1.76217600	1.30800600
C	-2.96634100	1.80516200	1.13365200
C	1.19998800	1.02129500	3.03090000
C	0.61190700	-1.27706100	2.17698200
O	-1.98113900	4.42072200	0.36482800
C	-2.24055500	5.76509200	-0.01983400
O	2.50046500	4.60888700	-1.43464200
C	2.32409600	5.94363900	-1.89135200
H	0.04667900	5.59592500	-0.90088000
H	2.70886700	2.22515600	-0.57664700
H	1.95302300	0.30120300	0.57006200

H	-1.60385400	0.32609100	2.88245700
H	-3.49285800	1.49818200	2.04063600
H	-3.35277700	2.76503600	0.80733300
H	1.04110100	2.09779700	2.92540700
H	0.86744200	0.72369200	4.02968600
H	2.27011500	0.80868800	2.94271500
H	0.16658800	-1.57626700	3.13065200
H	0.12745600	-1.85207200	1.38459100
H	1.67614900	-1.51802200	2.18644000
H	-3.25648400	5.97441400	0.31632300
H	-1.54342100	6.45782800	0.46619100
H	-2.18274800	5.88593200	-1.10816100
H	3.27026500	6.22292500	-2.35485900
H	1.51900700	6.00618100	-2.63404100
H	2.10998900	6.62335600	-1.05729200
H	-1.75066900	-0.25471500	1.22176400
C	-4.84074600	-3.42243900	1.81877400
C	-4.05570200	-4.48700300	1.36816300
C	-2.92659900	-4.27338200	0.56821100
C	-2.61349500	-2.96197800	0.23562300
C	-3.39829300	-1.87109800	0.68158800
C	-4.51606600	-2.10589400	1.48388500
N	-1.53071700	-2.45761500	-0.54174900
C	-1.66196900	-1.04916900	-0.66171500
C	-2.76741300	-0.64464500	0.20123500
C	-3.34724500	0.72399800	0.00248000
O	-0.90176100	-0.28366900	-1.26315100
C	-4.86388000	0.66213100	-0.09370800
O	-5.63244800	0.96871900	0.79512400
O	-5.23635700	0.18801100	-1.29242200
C	-7.35193500	1.26792300	-1.89882100
C	-6.65756900	-0.02088100	-1.49246600
O	0.57029800	-2.44500400	-1.33511600
C	1.84776500	-2.97266300	-1.88757300
C	2.52767400	-1.69770000	-2.38013300
C	1.56117700	-3.92379200	-3.04823300

C	2.63231100	-3.63025200	-0.75522600
C	-0.42007900	-3.23676900	-0.95013600
O	-0.42935600	-4.44902000	-0.89506700
H	-5.71124300	-3.61788100	2.43808700
H	-4.32130200	-5.50459500	1.63878500
H	-2.31584900	-5.09192800	0.21554600
H	-5.12194300	-1.27864700	1.83746400
H	-2.95350600	1.10654800	-0.94337000
H	-8.40563900	1.06710900	-2.12224400
H	-7.30510700	2.00043200	-1.08875200
H	-6.88548500	1.69332100	-2.79319200
H	-6.70452300	-0.77344300	-2.28198200
H	-7.08046500	-0.43147200	-0.57274700
H	2.71700300	-1.01445600	-1.55079500
H	3.49153200	-1.94519500	-2.83336400
H	1.90177500	-1.19859300	-3.12615800
H	1.08116400	-4.84251500	-2.71007100
H	2.50864700	-4.17832600	-3.53462100
H	0.91949700	-3.43669700	-3.79038200
H	3.61322900	-3.94095300	-1.12938000
H	2.80016100	-2.91533600	0.05428100
H	2.10655300	-4.50966300	-0.37567600
S	4.58350900	0.22458000	0.71544500
O	4.58683400	1.17744700	-0.41264200
O	3.28832900	-0.55519100	0.79589300
C	5.76679400	-1.11898700	0.21662800
F	7.00902800	-0.63407900	0.11726900
F	5.41652100	-1.63951900	-0.97297500
F	5.75833400	-2.10552700	1.12279000
H	0.42422800	0.05366200	-0.12391500
O	5.05702900	0.70724000	2.01853500

6a′

Zero-point correction= 0.580526 (Hartree/Particle)

Thermal correction to Energy= 0.692236

Thermal correction to Enthalpy= 0.693181

Thermal correction to Gibbs Free Energy= 0.580526

SCF Done: E(Solv) = -1841.01025594

C	-0.40613100	-3.89442000	1.89694500
C	-1.78754000	-3.79348600	1.74021400
C	-2.36453300	-2.73449100	1.03211200
C	-1.52149900	-1.76574100	0.49171700
C	-0.12809800	-1.84227700	0.66471500
C	0.42854100	-2.91284400	1.35621800
N	-1.83061900	-0.62389500	-0.30438000
C	-0.61191500	-0.00607700	-0.74203500
C	0.52908700	-0.66657600	0.01293600
C	1.43426000	0.28740400	0.96871400
C	2.68155100	-0.42040100	0.36103800
C	1.82396200	-0.90144000	-0.82069300
C	1.36117700	1.73978100	0.55401000
C	2.39528000	2.35722400	-0.18122800
N	3.48819600	1.62057800	-0.63307100
C	3.92381400	0.42635300	0.09063200
C	0.20993800	2.50619700	0.80965100
C	0.10072000	3.84998400	0.44969800
C	1.17233500	4.44501300	-0.22641500
C	2.30918000	3.70914400	-0.53885200
C	4.60207700	0.80609600	1.42208700
C	4.90509700	-0.33772600	-0.80462600
O	-0.51555000	0.84793000	-1.58478600
O	-0.81670800	1.82814200	1.41132500
O	1.18398300	5.75191100	-0.62356000
C	-2.08918900	2.45461200	1.49201100
C	0.02548900	6.53056200	-0.38352500
C	1.95526100	-2.28410700	-1.40021000
O	1.25187300	-2.71403800	-2.28799800

O	2.91465500	-3.01588600	-0.78685100
C	4.12247200	-5.03358300	-0.40079700
C	3.02671200	-4.38771900	-1.22482500
O	-4.06285400	-0.93596700	-0.27991400
C	-5.47604000	-0.56424300	-0.47703900
C	-6.21538800	-1.77593200	0.08941400
C	-5.76531400	-0.39800800	-1.96913100
C	-5.80029900	0.69469400	0.32909800
C	-3.08003400	-0.09150800	-0.64101200
O	-3.22984100	0.98850000	-1.16871800
C	1.25538000	0.09094000	2.47564100
H	0.02308300	-4.73282000	2.43730100
H	-2.43710800	-4.55479800	2.16277700
H	-3.43298200	-2.68135000	0.89703900
H	1.50463600	-2.99310300	1.46411200
H	2.96764600	-1.26587100	0.99077400
H	1.82803900	-0.17416000	-1.63835300
H	4.25470000	2.19705800	-0.96018800
H	-0.79990800	4.40421800	0.66319700
H	3.10967400	4.18891100	-1.09309000
H	3.93749500	1.42528000	2.03133000
H	5.51736900	1.37891400	1.23135800
H	4.87347500	-0.08412700	2.00095500
H	5.22806500	-1.26408500	-0.32064200
H	4.44151800	-0.59066000	-1.76230600
H	5.79562600	0.27097000	-1.00637200
H	-2.75832900	1.70386100	1.91684700
H	-2.06189600	3.32862700	2.15521700
H	-2.44656000	2.73810000	0.49784700
H	0.23995200	7.52072700	-0.78984900
H	-0.85348800	6.11204100	-0.89094100
H	-0.18731400	6.61858100	0.69044400
H	4.24750400	-6.08004600	-0.69858900
H	5.07639800	-4.51666900	-0.54698100
H	3.87565400	-5.00612300	0.66563700
H	2.05774200	-4.87621900	-1.08332000

H	3.25150700	-4.39885700	-2.29560600
H	-5.98088400	-1.91191600	1.15021000
H	-7.29604500	-1.63385900	-0.01022900
H	-5.93379500	-2.68537600	-0.45045400
H	-5.22595900	0.45503100	-2.38156500
H	-6.83999000	-0.24427600	-2.11556900
H	-5.47157000	-1.30146400	-2.51344800
H	-6.87920400	0.88019600	0.29457000
H	-5.51242600	0.55679000	1.37717800
H	-5.28054400	1.56465200	-0.07305200
H	1.42770600	-0.94886900	2.76405600
H	1.97957300	0.71566800	3.00876200
H	0.25501900	0.37895700	2.79834600

3a

Zero-point correction= 0.578612 (Hartree/Particle)

SCF Done: E(Solv) = -1841.01419545

C	0.60976400	3.46105400	0.59489400
C	0.24026300	4.03828500	-0.62837600
C	-0.96449900	3.70900700	-1.24194100
C	-1.79143800	2.73969400	-0.64639700
C	-1.40267500	2.06601100	0.53482500
C	-0.21965200	2.50493200	1.17659200
N	-2.98334800	2.37737200	-1.24440100
C	-4.09399300	1.87188100	-0.41854800
C	-3.49773800	0.83967900	0.51322300
C	-2.23277300	0.92799600	0.96058900
C	-1.58991200	-0.27598900	1.61593700
C	-5.09744000	1.19688800	-1.36169300
C	-4.76569900	3.01487500	0.37112100
C	-0.99231300	-1.17469500	0.50331500
C	0.00445100	-2.23432400	1.08301200
C	1.33898700	-1.50364800	1.27436000
N	2.20438200	-1.95414500	0.23656900

C	1.65259400	-3.11755900	-0.38209600
C	0.36336400	-3.33527600	0.12221700
C	2.22419900	-3.97160500	-1.31964000
C	1.46389400	-5.06740700	-1.74366100
C	0.18622600	-5.30762800	-1.23781300
C	-0.37114600	-4.43643000	-0.29654100
O	1.60991500	-0.68755600	2.12226700
O	0.02658500	1.97610800	2.40584600
C	1.28060300	2.22824900	3.02318800
O	1.12722900	4.95158000	-1.12341300
C	0.81295000	5.58293200	-2.35205400
C	-2.09339000	-1.82302700	-0.31807500
O	-2.25452500	-1.68358900	-1.50846600
O	-2.90122800	-2.58919000	0.45692600
C	-4.76430800	-4.03816000	0.79361700
C	-3.99724600	-3.22798500	-0.23205300
O	3.50248500	-0.10933900	0.27258300
C	4.65442500	0.73680500	-0.10870200
C	4.34303200	2.05333500	0.59852200
C	4.66778100	0.93166900	-1.62558300
C	5.94887800	0.12095800	0.42200600
C	3.40851300	-1.35684200	-0.17988900
O	4.20159800	-1.93587800	-0.89637200
H	1.51567200	3.80740100	1.07210500
H	-1.28204600	4.18113900	-2.16406300
H	-3.27557600	2.98057100	-2.00379200
H	-4.10769300	-0.02713200	0.75634100
H	-0.79461700	0.01172400	2.29854400
H	-2.33343200	-0.85595200	2.17083200
H	-4.61024000	0.37898400	-1.90093200
H	-5.94476500	0.79640100	-0.79438900
H	-5.49475100	1.91417800	-2.09105300
H	-5.56791100	2.62678700	1.00900400
H	-4.02979700	3.51192300	1.01047700
H	-5.19841700	3.75947200	-0.31002600
H	-0.44843800	-0.54816300	-0.20982200

H	-0.37269800	-2.59660400	2.04339600
H	3.22096800	-3.79356700	-1.69491700
H	1.88990500	-5.74702600	-2.47604800
H	-0.37718700	-6.17323900	-1.57300700
H	-1.36196600	-4.61414700	0.10741500
H	1.26695200	1.66182500	3.95467300
H	2.10078100	1.86652900	2.39879000
H	1.40681200	3.29627500	3.24175500
H	1.64903400	6.24988700	-2.57013600
H	0.70785900	4.85206300	-3.16457200
H	-0.11105900	6.17156000	-2.27775700
H	-5.61402500	-4.53772900	0.31627400
H	-4.12499100	-4.80308200	1.24656000
H	-5.14576700	-3.39404600	1.59230100
H	-4.61681300	-2.45325000	-0.69481900
H	-3.59193200	-3.85031900	-1.03606400
H	4.30674800	1.90776400	1.68232100
H	5.12218300	2.78818500	0.37218100
H	3.37984400	2.44967500	0.26456600
H	4.87817600	-0.00371800	-2.14508500
H	5.44051100	1.66230100	-1.88767000
H	3.70183000	1.32131300	-1.96332300
H	6.77518000	0.82118700	0.25854200
H	5.86502400	-0.06304100	1.49815300
H	6.17871700	-0.81786700	-0.08302800

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b-TS1

Zero-point correction= 0.302282 (Hartree/Particle)

Thermal correction to Energy= 0.318953

Thermal correction to Enthalpy= 0.319897

Thermal correction to Gibbs Free Energy= 0.259449

SCF Done: E(Solv)= -750.278160399 A.U.

C	2.241643	0.157518	0.013672
C	2.036164	-1.229416	-0.085450
C	0.757617	-1.763075	-0.205135
C	-0.354271	-0.912576	-0.238559
C	-0.184155	0.506567	-0.173554
C	1.134569	1.003602	-0.033256
N	-1.621527	-1.439259	-0.348270
C	-2.820455	-0.711092	0.107365
C	-2.650129	0.697680	-0.469709
C	-1.368990	1.313104	-0.271567
C	-1.625190	2.717914	-0.236611
C	-2.878657	-0.668236	1.643034
C	-4.050756	-1.417457	-0.460206
O	1.244742	2.358904	0.029444
C	2.526547	2.928698	0.226394
O	3.051733	-2.139246	-0.058362
C	4.378379	-1.665808	0.098195
H	3.238471	0.560185	0.104692
H	0.640593	-2.841109	-0.247855
H	-1.676443	-2.449658	-0.304514
H	-2.111021	3.067087	0.674064
H	-3.019247	2.153669	-0.437885
H	-0.918339	3.451324	-0.630977
H	-1.984437	-0.182252	2.045651
H	-3.753200	-0.096703	1.973385
H	-2.942274	-1.679563	2.063557
H	-4.958883	-0.880366	-0.169892
H	-4.003920	-1.457350	-1.553438
H	-4.130911	-2.443755	-0.078601

H	2.366965	4.006760	0.281687
H	2.983641	2.578456	1.160915
H	3.199011	2.703289	-0.611501
H	5.013473	-2.553304	0.103932
H	4.674990	-1.013643	-0.733650
H	4.504066	-1.123219	1.044221
H	-2.997546	0.773147	-1.502232

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b-IM2

Zero-point correction= 0.308856 (Hartree/Particle)

Thermal correction to Energy= 0.325859

Thermal correction to Enthalpy= 0.326803

Thermal correction to Gibbs Free Energy= 0.265436

E(Solv) = -750.399448214

C	2.20431300	0.11105500	0.04075700
C	1.98961900	-1.26206200	-0.11714800
C	0.70058900	-1.76631000	-0.25887000
C	-0.39104000	-0.89397200	-0.26267100
C	-0.21797200	0.51188500	-0.13540300
C	1.10253800	0.97606000	0.03404900
N	-1.66765100	-1.39454700	-0.45910400
C	-2.82213600	-0.70054000	0.12747100
C	-2.63238000	0.77258500	-0.14787900
C	-1.42290200	1.35637100	-0.23756600
C	-1.33960600	2.84250900	-0.49610000
C	-2.90916700	-0.95343100	1.64967800
C	-4.08460400	-1.22378200	-0.56865200
O	1.25805000	2.32408900	0.20709800
C	2.56358400	2.85485000	0.32861600
O	2.99246400	-2.18935600	-0.12520600
C	4.32444700	-1.73400500	0.02885300
H	3.20177600	0.49912100	0.17494900
H	0.56073500	-2.83757100	-0.36277600
H	-1.72388500	-2.40399000	-0.38417800
H	-0.91560500	3.37989400	0.35648800

H	-2.33971300	3.23971500	-0.69721600
H	-0.69822400	3.06438700	-1.35530100
H	-1.98750000	-0.62169300	2.13750800
H	-3.74810300	-0.40198700	2.08928000
H	-3.05305000	-2.02148600	1.86121600
H	-4.97547100	-0.72302200	-0.17451000
H	-4.02670500	-1.04529900	-1.64623000
H	-4.20559000	-2.30132400	-0.39915200
H	2.43715800	3.93501300	0.42318100
H	3.07525000	2.47120800	1.22117400
H	3.17371300	2.63663400	-0.55767700
H	4.95312800	-2.62536400	-0.01139300
H	4.61343800	-1.04964000	-0.77985300
H	4.47053400	-1.23082600	0.99403200
H	-3.53413600	1.37291400	-0.24176900

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b-TS3

Zero-point correction= 0.651598 (Hartree/Particle)

Thermal correction to Energy= 0.690798

Thermal correction to Enthalpy= 0.691743

Thermal correction to Gibbs Free Energy= 0.581171

E(Solv)= -1840.98406162

C	0.99310600	-0.49602600	2.26372000
C	2.19871100	0.16700900	1.98695100
C	2.21210600	1.48455600	1.53650600
C	1.01449500	2.15475700	1.29079400
C	-0.25271500	1.48589300	1.47090300
C	-0.20743700	0.16179200	2.02812200
N	1.06219800	3.45513000	0.86826400
C	-0.05331300	4.16141800	0.22251700
C	-1.35392600	3.64246100	0.85770700
C	-1.43238900	2.14795100	1.04681300
C	-2.61999500	1.48300800	0.67473600
C	-0.02645700	3.92944500	-1.29594000
C	0.10189200	5.65738800	0.52560100

O	-1.39148000	-0.38018600	2.39125700
C	-1.39010200	-1.60831500	3.11465200
O	3.41118200	-0.40624200	2.15810700
C	3.47758200	-1.79858800	2.46902000
H	0.99747500	-1.50445900	2.64310200
H	3.16631400	1.96273300	1.34395900
H	1.97626500	3.75506100	0.55087400
H	-2.20322400	3.99486300	0.26493800
H	-3.46464900	2.13100600	0.44324600
H	-2.89426100	0.56783000	1.17915500
H	-0.04331000	2.86547100	-1.53936000
H	-0.87588600	4.43111400	-1.77457500
H	0.89235000	4.35049100	-1.72274900
H	-0.72143900	6.22369200	0.07755600
H	0.11018100	5.83963100	1.60486900
H	1.03741000	6.04331100	0.10282600
H	-2.43905600	-1.82715500	3.31394900
H	-0.96320500	-2.42209400	2.52387300
H	-0.84425600	-1.49373700	4.05919800
H	4.54089300	-2.03869900	2.49192100
H	3.03646400	-2.00317200	3.45171300
H	2.98575800	-2.39418600	1.69449400
H	-1.45266600	4.09945600	1.85451800
C	-2.20331500	-3.83387000	0.55840900
C	-0.91512500	-4.37187300	0.52495700
C	0.16599700	-3.62021700	0.04226100
C	-0.08124300	-2.32862500	-0.40551200
C	-1.38698000	-1.76228900	-0.38618100
C	-2.44504900	-2.53304500	0.11337700
N	0.82232100	-1.36783200	-0.92083300
C	0.08840500	-0.16283600	-1.26237300
C	-1.29958900	-0.41783500	-0.89952900
C	-2.21677300	0.65712600	-1.04105700
O	0.57403400	0.83040600	-1.78710900
C	-3.61898800	0.49348500	-1.54525200
O	-4.06027800	1.12704800	-2.48206300

O	-4.35935000	-0.39207100	-0.84521700
C	-6.34227100	-1.65846200	-0.44771000
C	-5.71054700	-0.58974500	-1.31768900
O	2.82261600	-0.44656200	-1.36107700
C	4.22687100	-0.44679600	-1.78987100
C	4.44489700	1.02825200	-2.12611800
C	4.36927900	-1.32484900	-3.03345500
C	5.15252100	-0.89086700	-0.65656300
C	2.19748700	-1.56676700	-1.00943800
O	2.73052000	-2.63967700	-0.76436400
H	-3.02863900	-4.42965800	0.93958800
H	-0.73953600	-5.38724100	0.86900400
H	1.16404100	-4.03074700	0.00039400
H	-3.43885000	-2.11269100	0.15281800
H	-1.76827900	1.48108700	-1.58756800
H	-7.37923800	-1.82574900	-0.75772600
H	-5.79956300	-2.60487600	-0.53687700
H	-6.34141100	-1.35569700	0.60445500
H	-6.24551300	0.36325500	-1.25589000
H	-5.67515200	-0.88183900	-2.37113300
H	4.31769200	1.64170800	-1.22844400
H	5.45555000	1.18232500	-2.51783100
H	3.71453500	1.35760100	-2.87024700
H	4.16347400	-2.37091600	-2.79719300
H	5.39061800	-1.24975000	-3.42204900
H	3.67760800	-0.99170400	-3.81396900
H	6.19207800	-0.70415700	-0.94906200
H	4.93704700	-0.32273600	0.25202500
H	5.02996600	-1.95341100	-0.44423100

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b-IM3

Zero-point correction= 0.653379 (Hartree/Particle)

Thermal correction to Energy= 0.692592

Thermal correction to Enthalpy= 0.693536

Thermal correction to Gibbs Free Energy= 0.582912

E(Solv) = -1840.99163473

C	1.00164100	-0.40940600	2.22476000
C	2.19781100	0.28247500	1.97475400
C	2.19718400	1.61561400	1.55484400
C	0.99856100	2.26395500	1.28779000
C	-0.26895200	1.55784000	1.41478700
C	-0.20751400	0.22444200	1.98427700
N	1.01454700	3.56354200	0.87474800
C	-0.08092700	4.20467400	0.12737600
C	-1.40603900	3.64357900	0.67004000
C	-1.42352000	2.16132500	0.93034300
C	-2.60376000	1.40582200	0.49356600
C	0.07739500	3.92402200	-1.37493100
C	-0.01130300	5.71261700	0.39568500
O	-1.37536800	-0.30455300	2.39213600
C	-1.35520700	-1.51774200	3.14632600
O	3.41210600	-0.26774000	2.15475800
C	3.50584900	-1.66077300	2.47277500
H	1.02170000	-1.41951400	2.59894800
H	3.14817800	2.10808400	1.38439400
H	1.93340100	3.89892800	0.60827100
H	-2.21026700	3.91492400	-0.02058700
H	-3.45100800	2.07259500	0.31101900
H	-2.90939700	0.60994500	1.16458000
H	0.08959800	2.85105200	-1.58419200
H	-0.73477300	4.39968000	-1.93758700
H	1.02293700	4.34691100	-1.73655100
H	-0.82490400	6.22800000	-0.12525100
H	-0.08735800	5.92482200	1.46684900
H	0.93363500	6.12903600	0.02647500
H	-2.39918800	-1.73135000	3.37250300

H	-0.94058300	-2.34472700	2.56624500
H	-0.78822800	-1.37318800	4.07397500
H	4.57400800	-1.87366300	2.51196000
H	3.05507400	-1.86664200	3.45019900
H	3.03935800	-2.26923300	1.69316500
H	-1.63489600	4.14381300	1.62484500
C	-2.24836000	-3.77997100	0.68761300
C	-0.97513700	-4.35447500	0.65221100
C	0.12266000	-3.64146900	0.14186200
C	-0.09116100	-2.35115800	-0.32143700
C	-1.38144200	-1.74138600	-0.28440600
C	-2.45976600	-2.47793100	0.23038600
N	0.81983700	-1.41812000	-0.86995000
C	0.09422800	-0.19172100	-1.21203700
C	-1.26040000	-0.41339300	-0.79911100
C	-2.23214800	0.68627600	-0.92332500
O	0.59770900	0.79453600	-1.74786500
C	-3.51962400	0.28585700	-1.62603100
O	-3.71674600	0.42206200	-2.81268700
O	-4.43426400	-0.24502700	-0.78102500
C	-6.51801100	-1.29961300	-0.29634400
C	-5.65207200	-0.71945900	-1.39687000
O	2.82778700	-0.52076900	-1.31638500
C	4.21961500	-0.54766800	-1.77454000
C	4.44292800	0.91348000	-2.16482600
C	4.33329700	-1.46748600	-2.99086700
C	5.16474100	-0.96106900	-0.64531300
C	2.18744100	-1.63064100	-0.94716000
O	2.71683000	-2.70032600	-0.67230400
H	-3.08604000	-4.35005800	1.08182900
H	-0.82557000	-5.36977900	1.00832800
H	1.10755000	-4.08314400	0.09276100
H	-3.44394700	-2.02988500	0.27257600
H	-1.78126200	1.44023100	-1.57147400
H	-7.46560900	-1.65425800	-0.71568900
H	-6.01970000	-2.14515500	0.18871700

H	-6.73805400	-0.54490100	0.46553800
H	-6.13745700	0.11855800	-1.90659600
H	-5.39273000	-1.46403500	-2.15529800
H	4.33438200	1.55810700	-1.28661900
H	5.44776300	1.04724200	-2.57867300
H	3.70106600	1.22205800	-2.90636000
H	4.12882800	-2.50424300	-2.71597700
H	5.34609600	-1.40882000	-3.40402600
H	3.62544500	-1.15750900	-3.76637800
H	6.20110900	-0.81068100	-0.96852000
H	4.98358400	-0.34596100	0.24035300
H	5.02408400	-2.01035100	-0.38354200

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b-TS4

Zero-point correction= 0.647858 (Hartree/Particle)

Thermal correction to Energy= 0.686820

Thermal correction to Enthalpy= 0.687764

Thermal correction to Gibbs Free Energy= 0.575481

E(Solv) = -1840.9636323

C	-4.30342300	-0.10680200	0.49732200
C	-4.76646600	0.60501300	-0.62137000
C	-4.05448500	0.60822700	-1.81937700
C	-2.86806700	-0.11749600	-1.92395700
C	-2.39379500	-0.91590600	-0.83073100
C	-3.12713100	-0.84439100	0.38840200
N	-2.16110500	-0.13219300	-3.10561200
C	-0.69722400	-0.27335000	-3.06503000
C	-0.41130800	-1.48149800	-2.16654600
C	-1.27494300	-1.76441900	-1.08145500
C	-0.78661300	-2.90648700	-0.25328500
C	-0.04649500	1.01060700	-2.51212600
C	-0.20541600	-0.54109900	-4.48916000
O	-2.59917400	-1.52584000	1.42216100
C	-3.21365900	-1.47194900	2.69977800
O	-5.90156700	1.35111500	-0.61469300

C	-6.66102000	1.42223100	0.58292900
H	-4.83765100	-0.07201400	1.43403100
H	-4.42347900	1.20240200	-2.64869600
H	-2.49467400	0.52593300	-3.80055400
H	-0.01244300	-2.35744300	-2.68697600
H	-0.62214700	-3.74935900	-0.93279400
H	-1.47729000	-3.21375000	0.52478300
H	-0.36627000	1.20002100	-1.48430800
H	1.04550000	0.92517500	-2.52124300
H	-0.32361100	1.87111200	-3.13376900
H	0.87835100	-0.69473100	-4.49096100
H	-0.68870500	-1.43101600	-4.90460000
H	-0.42214000	0.31127300	-5.14491500
H	-2.57101700	-2.07180700	3.34215500
H	-3.25818500	-0.43926300	3.06725500
H	-4.22565000	-1.89578200	2.67352500
H	-7.51405500	2.06333500	0.35593700
H	-7.02063600	0.43179700	0.88863100
H	-6.07907400	1.86582500	1.40049100
C	4.96405500	-2.41958900	-1.42620200
C	5.47840700	-1.12097800	-1.39676000
C	4.70077900	-0.04182100	-0.95603300
C	3.39967700	-0.30530600	-0.54806000
C	2.85811900	-1.61300500	-0.58059000
C	3.65031800	-2.67193500	-1.02219100
N	2.41293000	0.57531100	-0.02464900
C	1.22378400	-0.17889600	0.29489400
C	1.46837400	-1.53905100	-0.16161000
C	0.63959700	-2.63407500	0.43917000
O	0.18055300	0.25907700	0.76295100
C	0.44700100	-2.48413500	1.95610600
O	-0.45618000	-2.98439400	2.59412300
O	1.47067500	-1.81209300	2.51195800
C	0.55977300	-0.14576500	4.02749900
C	1.33599800	-1.44832700	3.90325200
O	1.59134300	2.49352400	0.79397500

C	1.39185100	3.94603000	0.85291000
C	0.11357700	4.05530400	1.68367400
C	1.17371000	4.49398500	-0.55873100
C	2.57202500	4.61071600	1.56278800
C	2.57551700	1.95798800	0.06857600
O	3.50406500	2.55551400	-0.44562400
H	5.58814000	-3.24036100	-1.76874500
H	6.49924300	-0.93706000	-1.71893900
H	5.09158200	0.96557900	-0.93443400
H	3.24987600	-3.68241400	-1.04965200
H	1.19887500	-3.57210800	0.33420700
H	0.51986700	0.16579400	5.07785500
H	1.02942600	0.64367900	3.43448000
H	-0.46066000	-0.27301000	3.65693900
H	0.84855800	-2.26589100	4.43960700
H	2.36396100	-1.34218200	4.25727500
H	0.26995700	3.63436500	2.68172800
H	-0.18081300	5.10485600	1.78683100
H	-0.69689500	3.49953000	1.20363300
H	2.07613700	4.39387700	-1.16385500
H	0.90408400	5.55410800	-0.50188800
H	0.35419200	3.95679700	-1.04800900
H	2.35355400	5.67279100	1.72037900
H	2.73226800	4.14593600	2.54138500
H	3.48525900	4.51853000	0.97385900
H	0.65097000	-1.31450600	-1.41213200

Acid-b-TS1

Thermal correction to Energy= 0.371024

Thermal correction to Enthalpy= 0.371968

Thermal correction to Gibbs Free Energy= 0.289350

SCF Done: E(Solv) = -1712.55844741

C	-3.513843	-1.353569	0.031062
C	-2.340528	-2.014076	-0.351930
C	-1.130062	-1.311131	-0.465236
C	-1.130661	0.037348	-0.180200
C	-2.279063	0.758443	0.213397
C	-3.480838	0.016910	0.309624
N	0.151080	0.743787	-0.270516
C	0.115388	2.211758	-0.679744
C	-0.899653	2.846091	0.267175
C	-2.160261	2.186440	0.411385
C	-3.106471	3.208002	0.708122
C	-0.331358	2.282078	-2.140676
C	1.529341	2.756477	-0.496849
O	-4.574097	0.717305	0.695629
C	-5.831542	0.056539	0.750493
O	-2.273636	-3.332596	-0.639587
C	-3.455527	-4.115913	-0.539234
H	-4.440082	-1.901019	0.120611
H	-1.815720	4.003585	0.562747
H	-3.345361	3.869599	-0.123597
H	-3.955382	3.051809	1.374917
H	-1.337984	1.874768	-2.272303
H	-0.346542	3.328338	-2.458155
H	0.359974	1.733660	-2.790280
H	1.530992	3.823674	-0.737809
H	1.874980	2.631004	0.533497
H	2.241159	2.246570	-1.151194
H	-6.552792	0.821046	1.040937
H	-6.108166	-0.356463	-0.227233
H	-5.826653	-0.744057	1.500042

H	-3.160335	-5.130720	-0.806647
H	-3.851700	-4.107702	0.483722
H	-4.227126	-3.763328	-1.235142
C	4.431199	-0.197928	0.172160
F	5.149064	-0.865876	-0.736047
F	4.290502	1.073707	-0.250709
F	5.099498	-0.183447	1.329481
S	2.766275	-0.989175	0.393655
O	2.159093	-0.870002	-0.977865
O	3.035193	-2.351265	0.849901
O	2.088793	-0.082198	1.377124
H	0.679143	0.630342	0.633660
H	-0.453893	3.163839	1.211094

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a-TS2

Zero-point correction= 0.650939 (Hartree/Particle)

Thermal correction to Energy= 0.690054

Thermal correction to Enthalpy= 0.690998

Thermal correction to Gibbs Free Energy= 0.582309

C	0.320451	-3.278176	0.713403
C	-1.075737	-3.260828	0.621383
C	-1.737172	-2.227732	-0.050462
C	-0.976488	-1.208774	-0.619629
C	0.444472	-1.221774	-0.553239
C	1.080136	-2.269312	0.125670
N	-1.377829	-0.037643	-1.312671
C	-0.198010	0.717582	-1.680420
C	0.939989	-0.045811	-1.226448
C	2.648845	0.890360	1.190731
C	2.925520	1.669778	0.037224
C	2.245942	0.476754	-1.420467
C	1.327343	0.936926	1.692186
C	0.373708	1.817787	1.044807
N	0.794740	2.830597	0.234658

C	2.225759	3.019117	-0.050260
C	0.783609	-0.009491	2.632072
C	-0.574292	-0.167823	2.804005
C	-1.466337	0.637562	2.057627
C	-1.005784	1.649465	1.237364
C	2.823222	3.937974	1.039067
C	2.370546	3.707696	-1.411569
O	-0.214503	1.812636	-2.242299
O	1.688569	-0.771824	3.291951
O	-2.813565	0.493883	2.135652
C	1.218418	-1.872132	4.059675
C	-3.344227	-0.621595	2.841099
C	3.444189	-0.407834	-1.656357
O	4.604796	-0.041656	-1.617701
O	3.088385	-1.661508	-1.985121
C	3.525485	-3.938838	-2.506410
C	4.164811	-2.592057	-2.230773
O	-3.592287	-0.411051	-1.109943
C	-5.020219	-0.054691	-1.131847
C	-5.681118	-1.329099	-0.605682
C	-5.444281	0.226057	-2.573730
C	-5.306897	1.125717	-0.200101
C	-2.659099	0.511534	-1.416294
O	-2.882752	1.657845	-1.737377
C	3.719661	-0.061187	1.659122
H	0.819769	-4.094042	1.230071
H	-1.660521	-4.063068	1.063123
H	-2.813116	-2.222051	-0.130187
H	2.159964	-2.296332	0.187843
H	3.959261	1.690670	-0.292944
H	2.251574	1.282400	-2.152040
H	0.169660	3.021115	-0.547670
H	-0.956852	-0.922774	3.471280
H	-1.711238	2.269908	0.697201
H	2.682017	3.506055	2.033960
H	2.326964	4.913588	1.011015

H	3.897137	4.083576	0.875417
H	3.423213	3.736801	-1.710210
H	1.786962	3.202032	-2.183333
H	2.009321	4.739584	-1.343666
H	2.112690	-2.386701	4.414336
H	0.628897	-1.532274	4.920057
H	0.618459	-2.546674	3.438565
H	-4.421892	-0.588293	2.674081
H	-2.939266	-1.560444	2.449790
H	-3.144991	-0.546364	3.917254
H	4.300529	-4.691730	-2.685590
H	2.914257	-4.258148	-1.656657
H	2.879778	-3.887318	-3.388294
H	4.758394	-2.229901	-3.075837
H	4.818373	-2.612577	-1.352559
H	-5.365425	-1.531822	0.423208
H	-6.770103	-1.219409	-0.617261
H	-5.411483	-2.188494	-1.227588
H	-4.925941	1.103749	-2.962636
H	-6.523897	0.408485	-2.610832
H	-5.218491	-0.634434	-3.212356
H	-6.387942	1.199065	-0.036666
H	-4.813531	0.975517	0.763743
H	-4.947997	2.062364	-0.625667
H	4.594297	0.016826	1.010622
H	4.020639	0.178791	2.685066
H	3.378329	-1.097886	1.679685

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a-IM3

Zero-point correction= 0.652843 (Hartree/Particle)

Thermal correction to Energy= 0.692059

Thermal correction to Enthalpy= 0.693003

Thermal correction to Gibbs Free Energy= 0.583620

SCF Done: E(Solv) = -1840.97195158 A.U.

C	0.31518100	-0.05997500	-3.32880400
C	-1.08106100	0.03301600	-3.29348900
C	-1.74625800	0.46958700	-2.13951000
C	-0.99018900	0.79209600	-1.01630300
C	0.43468100	0.70702200	-1.04103900
C	1.07827600	0.27926300	-2.21273000
N	-1.37115800	1.22272200	0.27807300
C	-0.16816700	1.40215300	1.08865300
C	0.92809700	1.06982100	0.24784800
C	2.71877400	-1.36536700	0.45838100
C	2.97186500	-0.20569900	1.35861400
C	2.32493700	1.13928200	0.73858200
C	1.42512800	-1.86291300	0.48630600
C	0.51056300	-1.38775800	1.52560200
N	0.99785400	-0.83609000	2.66919300
C	2.43321400	-0.50855600	2.77674500
C	0.82784200	-2.63512000	-0.59108200
C	-0.53169600	-2.76128200	-0.71264600
C	-1.38232300	-2.17760300	0.26803100
C	-0.87506200	-1.56793800	1.39716200
C	3.17272600	-1.72974400	3.35620000
C	2.58395500	0.66691500	3.74871500
O	-0.17073600	1.70384100	2.28979400
O	1.69216800	-3.11492500	-1.50911500
O	-2.72997500	-2.23345000	0.17099000
C	1.17010300	-3.62730600	-2.73045900
C	-3.31861300	-2.67474500	-1.04910500
C	3.25639600	1.71097600	-0.31992500
O	4.13617800	1.10451600	-0.90171200
O	2.96905700	3.00592800	-0.53841000

C	2.97639900	3.44819900	-2.93635900
C	3.68502600	3.66417100	-1.60919200
O	-3.58710600	1.07562100	-0.11096000
C	-5.00954300	1.04547600	0.25654300
C	-5.68729000	0.76482800	-1.08517400
C	-5.42217300	2.41505900	0.79789800
C	-5.29592400	-0.08228500	1.25206000
C	-2.64416200	1.22264100	0.84563000
O	-2.86462800	1.33535600	2.03174600
C	3.81877200	-1.83665100	-0.44640400
H	0.81250600	-0.38185700	-4.24061300
H	-1.66459500	-0.21413200	-4.17616500
H	-2.82183200	0.55929700	-2.12521900
H	2.15943600	0.20753200	-2.24417800
H	4.04382600	-0.01122700	1.43073500
H	2.31996600	1.86103200	1.55935700
H	0.37649400	-0.12187900	3.05903300
H	-0.96013600	-3.25379500	-1.57029300
H	-1.55033900	-1.15726300	2.13871800
H	3.04435600	-2.61446300	2.72639900
H	2.78032500	-1.95982600	4.35108000
H	4.24564100	-1.52264500	3.44251100
H	3.62298200	1.01159700	3.76972800
H	1.92685900	1.49747300	3.48408600
H	2.31766000	0.33948500	4.75970900
H	2.03988700	-3.86485900	-3.34405900
H	0.58423100	-4.53828500	-2.55836500
H	0.55293600	-2.87029300	-3.22685700
H	-4.39048100	-2.51249600	-0.93049100
H	-2.94726700	-2.08628700	-1.89351600
H	-3.13304300	-3.74211200	-1.21909100
H	3.47899400	4.01974200	-3.72506600
H	2.98686800	2.39097700	-3.21301200
H	1.93451700	3.77611000	-2.87477400
H	3.68998600	4.71811900	-1.32230600
H	4.71024300	3.28777000	-1.63429200

H	-5.37514700	-0.20762600	-1.48026400
H	-6.77492000	0.75537900	-0.96223700
H	-5.42656500	1.53582500	-1.81707700
H	-4.89960900	2.63395600	1.73011400
H	-6.50143300	2.42668900	0.98642600
H	-5.19218400	3.19767600	0.06720200
H	-6.37825100	-0.24247700	1.31351500
H	-4.82119400	-1.00977000	0.92066300
H	-4.91487100	0.15997400	2.24358400
H	4.76583300	-1.38290500	-0.15360300
H	3.90327100	-2.92683500	-0.41647500
H	3.63166100	-1.56447800	-1.48892800

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a-TS3

Zero-point correction= 0.650358 (Hartree/Particle)

Thermal correction to Energy= 0.689928

Thermal correction to Enthalpy= 0.690873

Thermal correction to Gibbs Free Energy= 0.579242

SCF Done: E(Solv) = -1840.97195158 A.U.

C	0.72817300	-3.94734400	1.24023300
C	-0.66281400	-4.07120600	1.20436400
C	-1.44410800	-3.11701800	0.53590200
C	-0.81151800	-2.04526000	-0.08067500
C	0.61139800	-1.90448900	-0.06009300
C	1.36924800	-2.88054800	0.61071700
N	-1.33483500	-0.94466000	-0.80871400
C	-0.20649700	-0.07505500	-1.24441400
C	0.96331300	-0.70224400	-0.74703800
C	1.62975600	0.80120900	1.53235900
C	2.79194900	0.68909000	0.59292600
C	2.25018700	0.05530100	-0.79403600
C	0.68849000	1.75517000	1.21594100
C	1.04292400	2.79685400	0.25007500
N	2.34776700	2.98291200	-0.04923100
C	3.42798900	2.07811500	0.38002600

C	-0.72481600	1.62453000	1.55139100
C	-1.68172300	2.30468900	0.84006700
C	-1.27593400	3.25305800	-0.13715400
C	0.06343500	3.58386400	-0.33213000
C	4.03313400	2.60111200	1.69745700
C	4.50767500	2.06733300	-0.70718800
O	-0.37213900	0.98560900	-1.85164100
O	-1.00543600	0.73303100	2.51286100
O	-2.14818600	3.92981000	-0.88394200
C	-2.35288800	0.28251400	2.67832200
C	-3.48222200	3.41945700	-1.03401900
C	3.34344700	-0.73308700	-1.49296600
O	3.62061800	-0.63165400	-2.66934100
O	3.98060100	-1.59578600	-0.66274300
C	5.44406100	-3.42589700	-0.21949700
C	4.93764600	-2.47755400	-1.28820600
O	-3.47367000	-1.32150100	-0.20239200
C	-4.92757900	-1.27524600	-0.37549300
C	-5.41747800	-2.30178800	0.64714200
C	-5.30578800	-1.70437200	-1.79446300
C	-5.46446700	0.11703500	-0.03105700
C	-2.64914800	-0.59640600	-1.01578400
O	-3.04560500	0.26225500	-1.78190700
C	1.49760000	-0.21934300	2.61603700
H	1.32268200	-4.69363600	1.76250000
H	-1.15165500	-4.91085200	1.69024300
H	-2.51903600	-3.21510200	0.51042600
H	2.44782500	-2.78831800	0.64637200
H	3.54626300	0.02140600	1.00885000
H	2.03343400	0.89675100	-1.45631700
H	2.56391000	3.66818800	-0.75989600
H	-2.73067200	2.10681300	0.99509100
H	0.31070200	4.31943100	-1.08858000
H	3.26898800	2.68696000	2.47583900
H	4.47783900	3.59006800	1.54507600
H	4.81544700	1.92281000	2.05558600

H	5.31744800	1.38916700	-0.42137600
H	4.12111400	1.74766400	-1.67682200
H	4.93770800	3.07060300	-0.81529800
H	-2.31006300	-0.45902800	3.47596800
H	-3.00627900	1.11007600	2.97773800
H	-2.71562000	-0.18520300	1.75977100
H	-3.93838800	4.04188800	-1.80403600
H	-3.44049200	2.37610500	-1.35707000
H	-4.04998400	3.52519600	-0.10209600
H	6.19048600	-4.10480500	-0.64566500
H	5.91015300	-2.87479100	0.60412800
H	4.62351600	-4.02603200	0.18594000
H	4.44222700	-3.00581800	-2.10757400
H	5.74193000	-1.87385600	-1.72143800
H	-5.09011800	-2.02908600	1.65580800
H	-6.51115400	-2.35009600	0.63775900
H	-5.02460800	-3.29628600	0.41472200
H	-4.95280000	-0.98141000	-2.53045000
H	-6.39511000	-1.79046100	-1.87342000
H	-4.86761400	-2.68218700	-2.01988700
H	-6.55969900	0.09530200	-0.01442800
H	-5.11887500	0.42300800	0.96322100
H	-5.13653800	0.85198000	-0.76509300
H	2.42681800	-0.78229900	2.72338200
H	1.24078100	0.25844000	3.56619500
H	0.69878800	-0.92933200	2.39079700

***RR*-4h-a-TS2A (4h-a-TS2A)**

Zero-point correction= 1.128434 (Hartree/Particle)

Thermal correction to Energy= 1.203685

Thermal correction to Enthalpy= 1.204629

Thermal correction to Gibbs Free Energy= 1.016613

SCF Done: E(Solv) = -4581.95232325

C	5.777202	2.789022	1.762658
C	4.729696	3.685474	2.018506
C	3.400286	3.252147	2.037951
C	3.144367	1.911001	1.770992
C	4.196857	0.983717	1.487458
C	5.523388	1.444341	1.502182
N	1.923242	1.212937	1.738253
C	2.169424	-0.121316	1.334733
C	3.587408	-0.287545	1.211424
C	5.132520	-0.715188	-1.338055
C	4.434811	-1.885352	-0.781484
C	4.113861	-1.609144	0.826636
C	4.321343	0.394231	-1.582122
C	2.883883	0.273326	-1.515739
N	2.246981	-1.037671	-1.484853
C	3.154037	-2.237272	-1.568264
C	4.813691	1.753322	-1.705838
C	3.965932	2.841259	-1.649381
C	2.575038	2.639045	-1.516999
C	2.031302	1.348204	-1.519614
C	3.502782	-2.495323	-3.041976
C	2.371029	-3.427363	-1.010217
O	1.278271	-0.928716	0.996954
O	6.149777	1.876887	-1.780883
O	1.684495	3.627666	-1.417819
C	6.730003	3.176267	-1.679674
C	2.130448	4.968237	-1.233882
C	5.374146	-2.070868	1.529145
O	6.414821	-1.454956	1.637506

O	5.219588	-3.340176	1.956440
C	6.023035	-5.397781	2.855137
C	6.381467	-3.954686	2.563053
O	0.511462	2.933973	2.054789
C	-0.657011	3.648740	2.609403
C	-0.487441	5.041221	2.002431
C	-0.534221	3.677490	4.132355
C	-1.965863	3.019802	2.136300
C	0.676437	1.627753	2.271159
O	-0.051391	0.878564	2.876313
C	6.625484	-0.762783	-1.471293
H	6.804991	3.142143	1.788114
H	4.948683	4.729337	2.226127
H	2.587225	3.933823	2.245519
H	6.332103	0.746118	1.337701
H	5.072709	-2.772951	-0.805870
H	3.336975	-2.337816	1.057633
H	1.671028	-1.097340	-0.582170
H	4.366342	3.842906	-1.654029
H	0.958958	1.243377	-1.391005
H	4.001043	-1.637473	-3.501659
H	2.595324	-2.718374	-3.607218
H	4.177103	-3.355357	-3.104955
H	3.017957	-4.309425	-0.972679
H	1.968822	-3.240933	-0.014861
H	1.522430	-3.644287	-1.664004
H	7.807918	3.014733	-1.701763
H	6.434622	3.804008	-2.528138
H	6.438190	3.646994	-0.735270
H	1.221327	5.552040	-1.096853
H	2.764973	5.041930	-0.344928
H	2.670373	5.331118	-2.116889
H	6.877949	-5.911166	3.306176
H	5.180322	-5.457148	3.549354
H	5.750234	-5.923858	1.936030
H	7.224905	-3.866032	1.871192

H	6.635881	-3.397987	3.470340
H	-0.515425	4.974259	0.910759
H	-1.299324	5.695714	2.335764
H	0.464470	5.489727	2.308283
H	-0.610577	2.668842	4.543355
H	-1.340467	4.286902	4.554626
H	0.423422	4.115271	4.435696
H	-2.798469	3.670141	2.427441
H	-1.952267	2.917283	1.052859
H	-2.118263	2.031924	2.569431
H	7.120653	-0.133171	-0.727599
H	6.980584	-1.786801	-1.336046
H	6.944521	-0.400955	-2.453515
C	-7.452965	2.564960	2.608607
C	-7.216157	1.198092	2.886316
C	-6.282825	0.487467	2.165772
C	-5.536538	1.105753	1.127801
C	-5.746536	2.500573	0.875479
C	-6.728923	3.199454	1.626818
C	-4.561431	0.407407	0.344549
C	-3.802185	1.127376	-0.558905
C	-3.946056	2.526090	-0.786563
C	-4.949295	3.168370	-0.085584
C	-4.298038	-1.050793	0.507603
C	-5.331837	-2.022961	0.305819
C	-5.033171	-3.404361	0.530218
C	-3.728911	-3.777842	0.930026
C	-2.703671	-2.860741	1.060810
C	-3.018323	-1.493918	0.810495
C	-6.632875	-1.680941	-0.150851
C	-7.594729	-2.647799	-0.338019
C	-7.308982	-4.008796	-0.078606
C	-6.052572	-4.375182	0.342755
O	-2.832759	0.438172	-1.264577
O	-1.986883	-0.568432	0.889718
P	-1.426130	0.119650	-0.482821

O	-0.631819	1.327925	-0.153522
N	-0.705560	-1.021541	-1.379899
C	-1.353240	-3.312624	1.479734
C	-2.998812	3.277244	-1.647660
C	-0.602863	-2.611801	2.434183
C	0.616368	-3.117962	2.881566
C	1.114406	-4.320416	2.381635
C	0.383731	-5.016219	1.414340
C	-0.835755	-4.514678	0.966944
C	-2.580099	4.555990	-1.243365
C	-1.658387	5.282089	-1.995070
C	-1.125822	4.737196	-3.163990
C	-1.536931	3.469518	-3.578048
C	-2.466945	2.746056	-2.835184
S	-0.901177	-1.383492	-2.891821
O	0.434775	-1.781134	-3.433354
O	-1.709203	-0.497146	-3.735013
C	-1.831736	-2.995132	-2.824668
F	-2.053647	-3.456159	-4.059420
F	-3.001892	-2.816768	-2.205289
F	-1.120139	-3.911733	-2.147068
H	-8.197224	3.112118	3.180176
H	-7.772862	0.705747	3.678572
H	-6.104439	-0.557145	2.390479
H	-6.886967	4.254409	1.416589
H	-5.122056	4.227677	-0.253003
H	-3.532117	-4.824228	1.144368
H	-6.860205	-0.643645	-0.364642
H	-8.580663	-2.363382	-0.694539
H	-8.078833	-4.760995	-0.225272
H	-5.812887	-5.419117	0.528890
H	-0.950615	-1.657395	2.808005
H	1.186058	-2.550528	3.611492
H	2.072900	-4.702061	2.725198
H	0.768801	-5.944317	0.999524
H	-1.385675	-5.039777	0.192943

H	-2.955661	4.968874	-0.312475
H	-1.353885	6.271215	-1.660839
H	-0.398233	5.295342	-3.747601
H	-1.130889	3.030147	-4.484666
H	-2.757618	1.759513	-3.170897
H	1.536599	-1.132706	-2.250392

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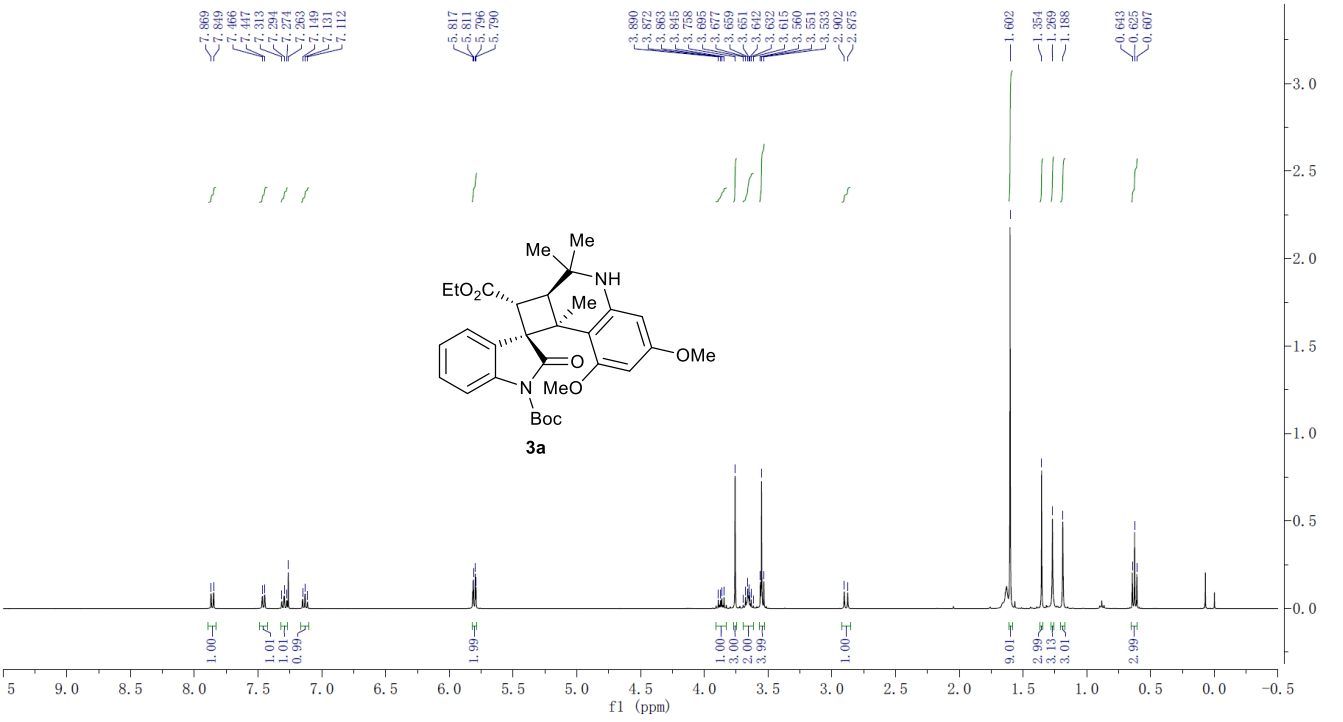
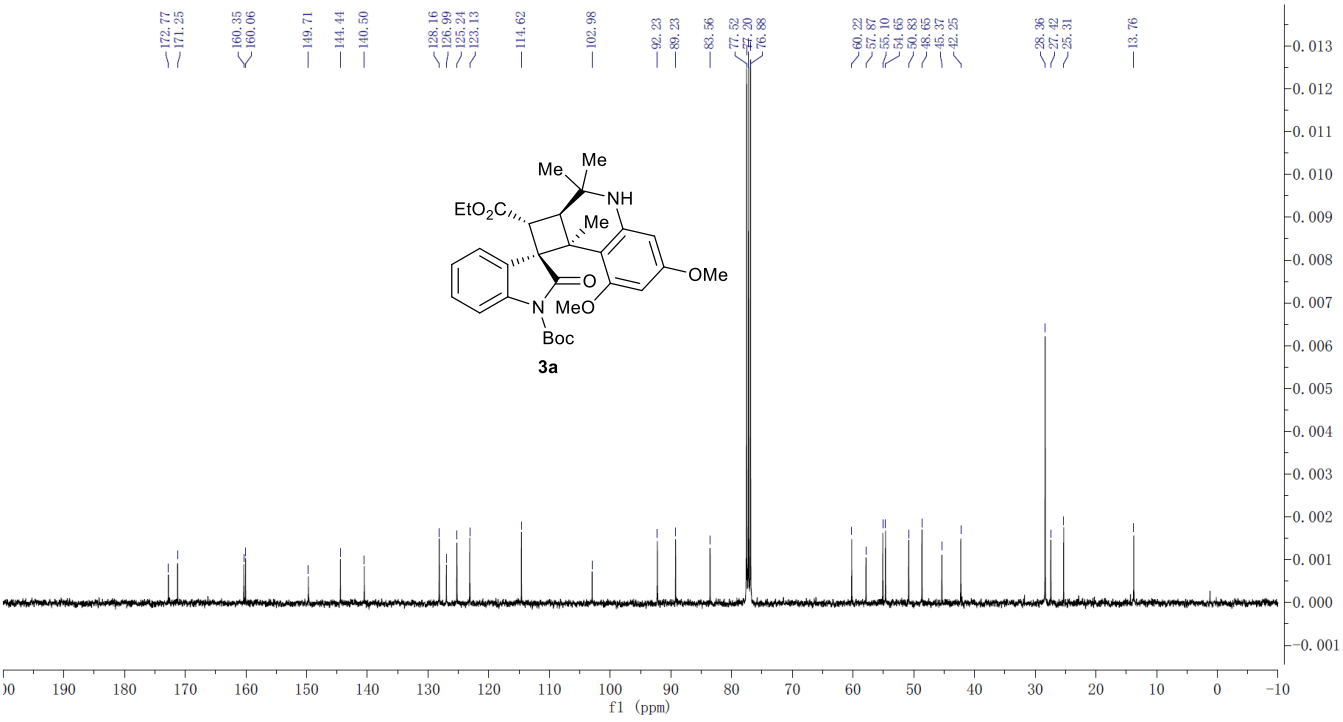
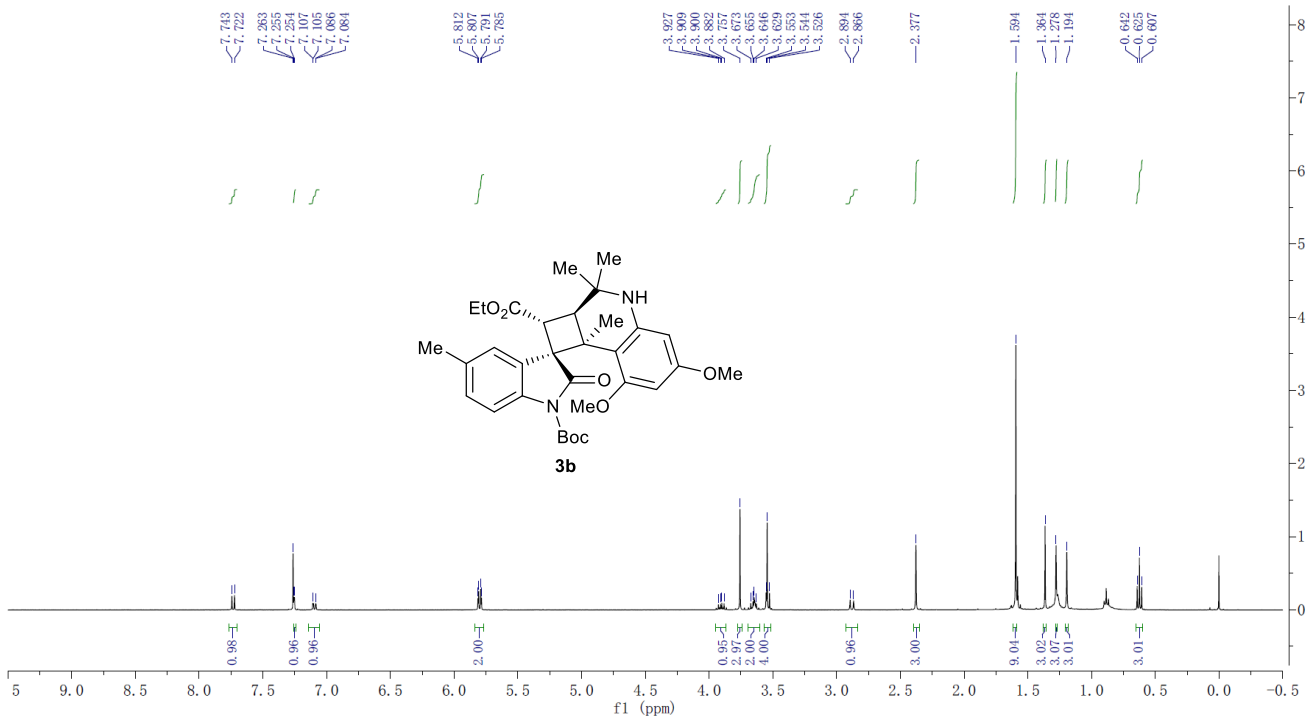
10. NMR Spectra of [2+2] Cycloadducts



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Me
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OMe
N
MeO
Boc
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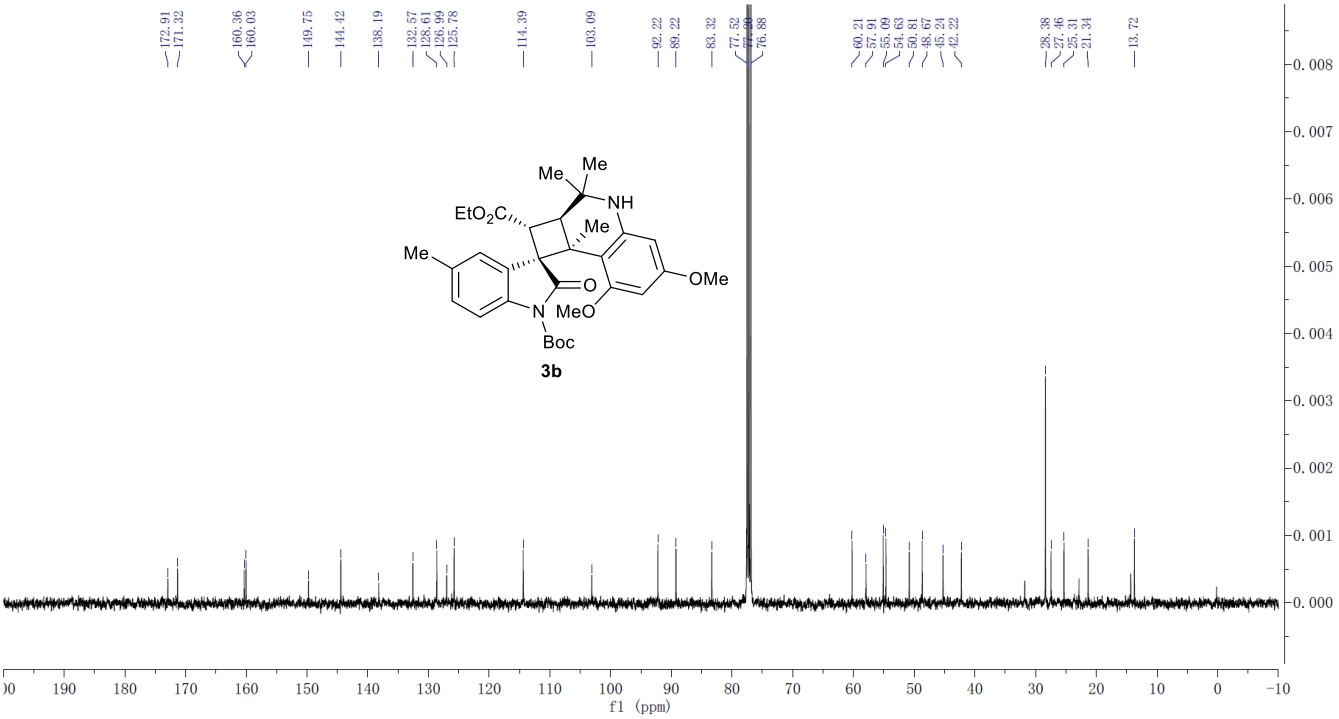
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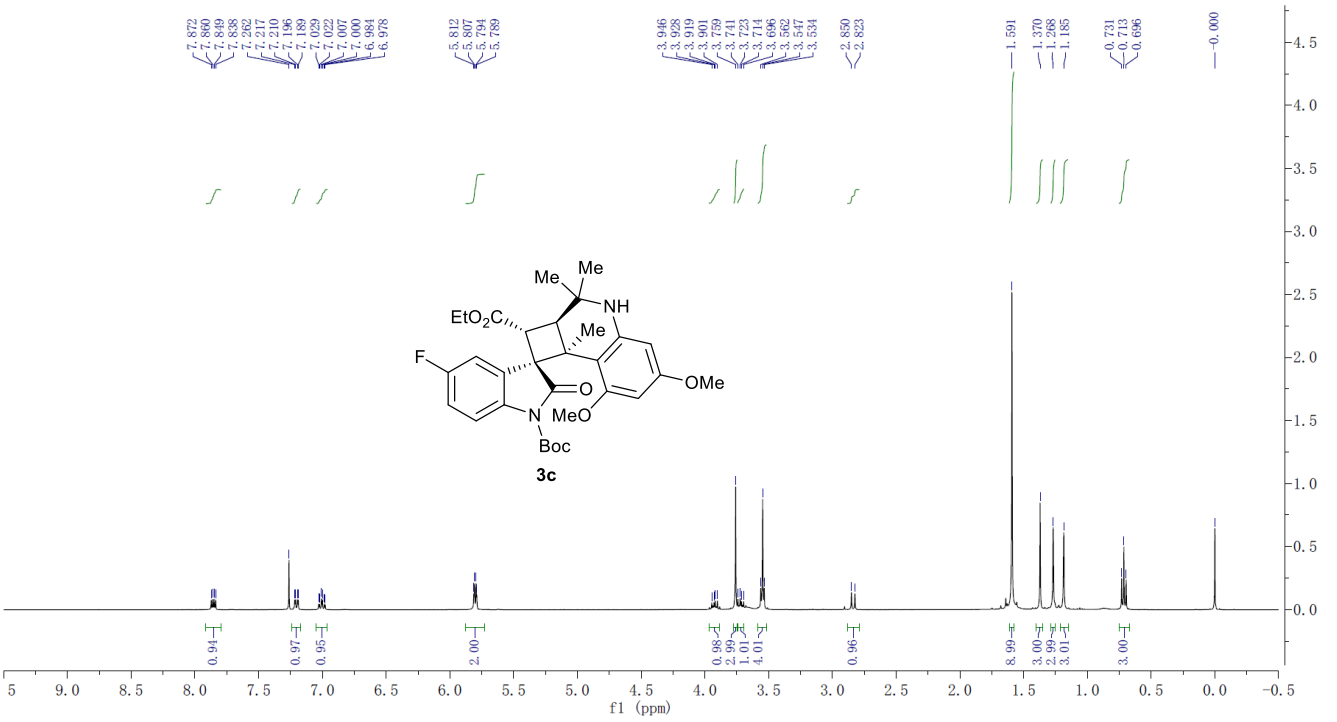
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Boc
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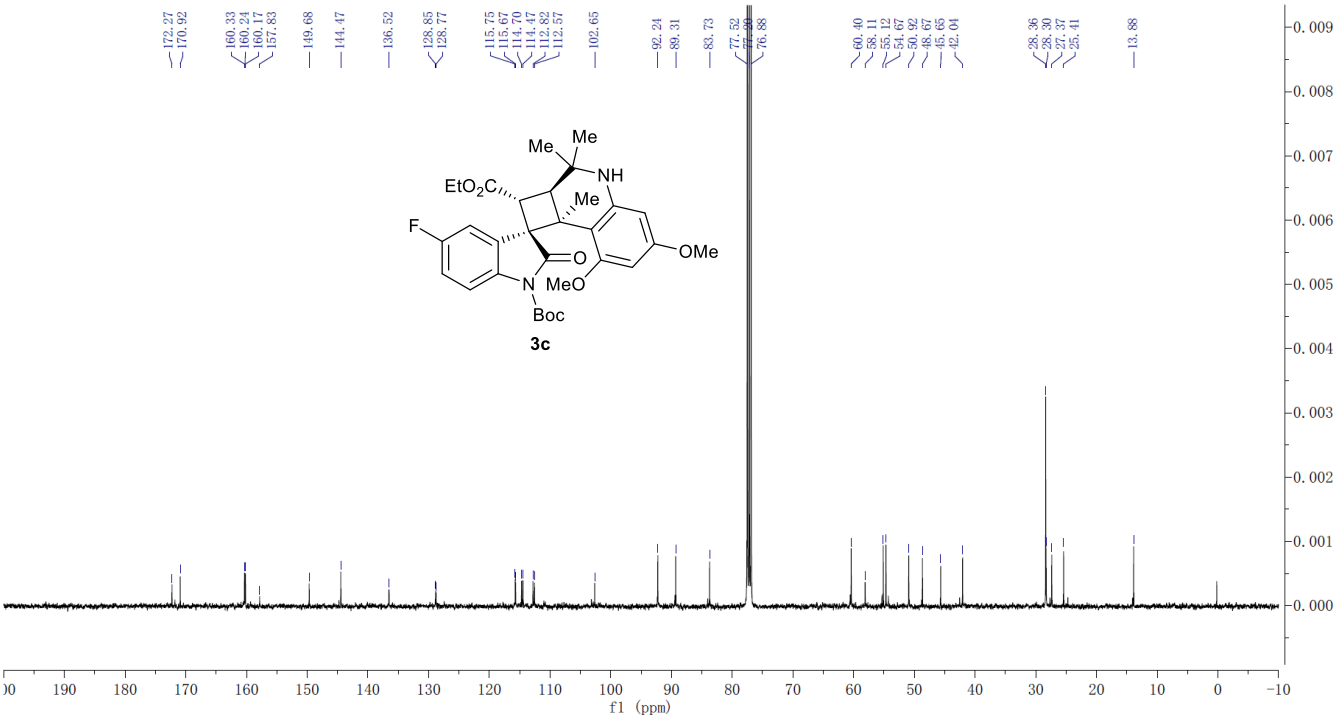
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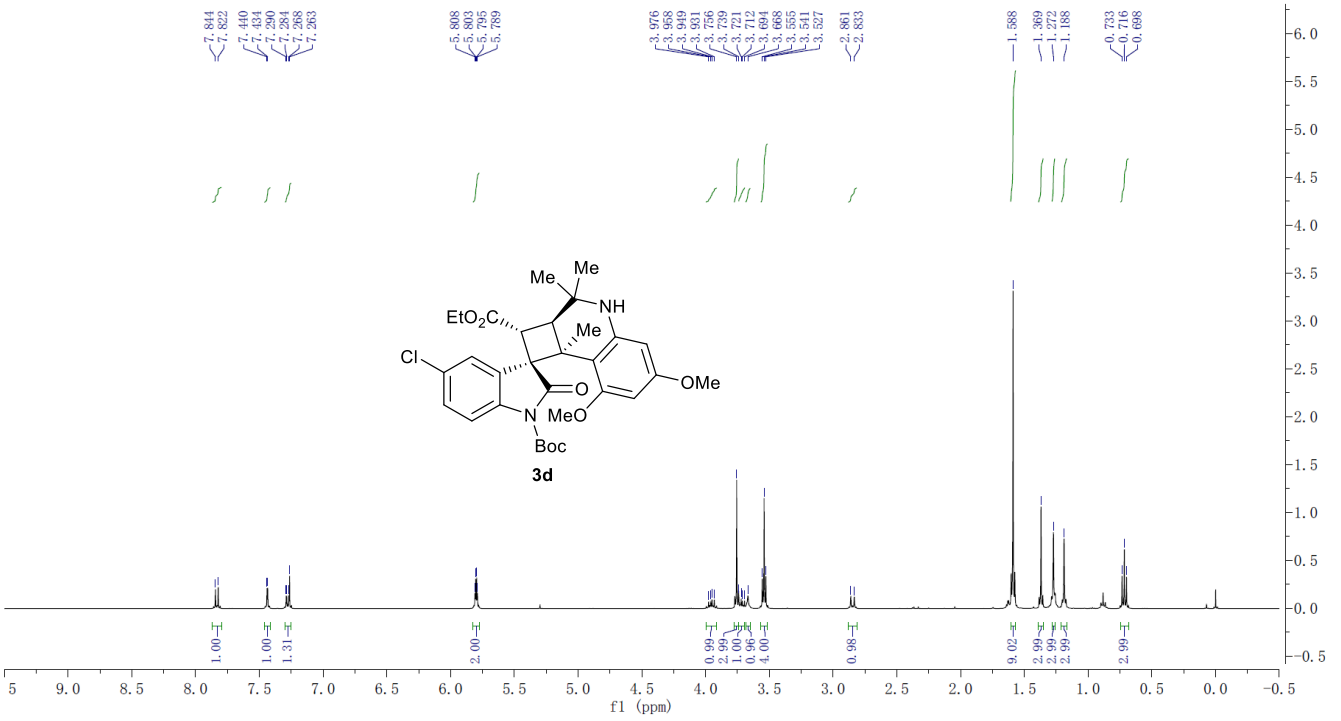
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N
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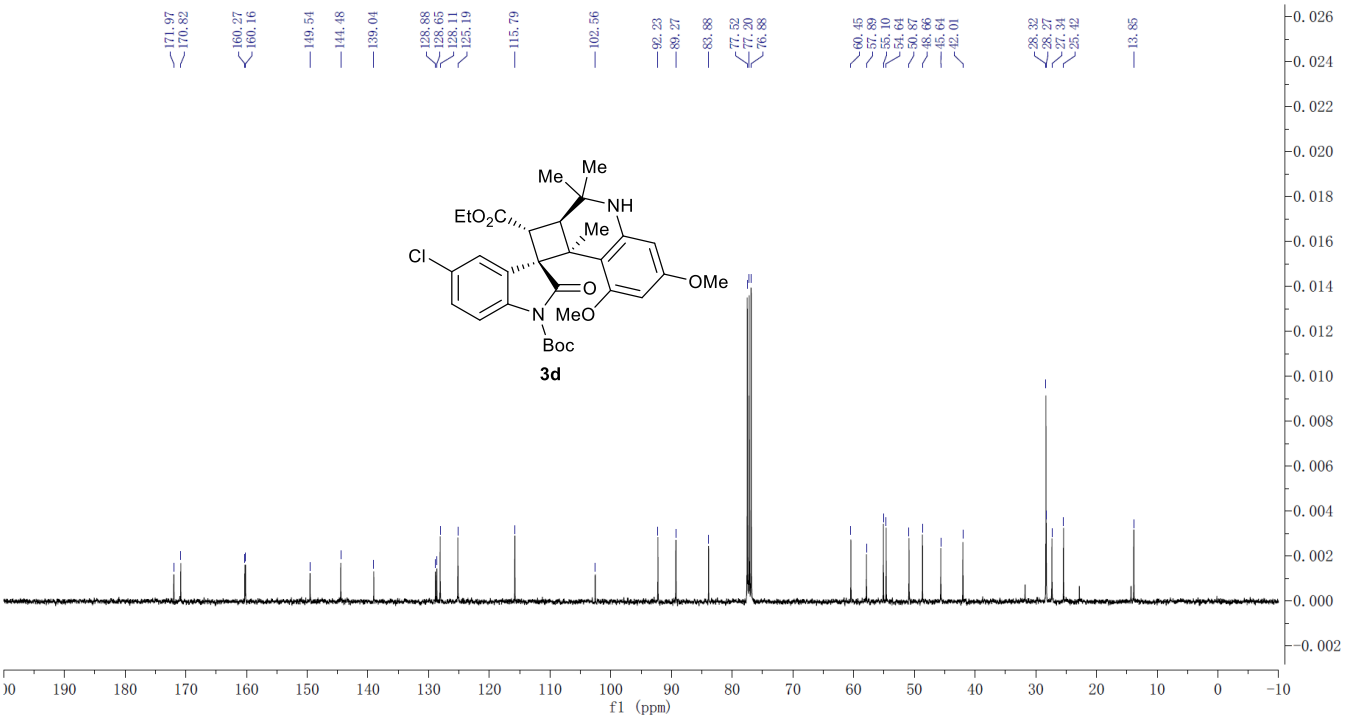
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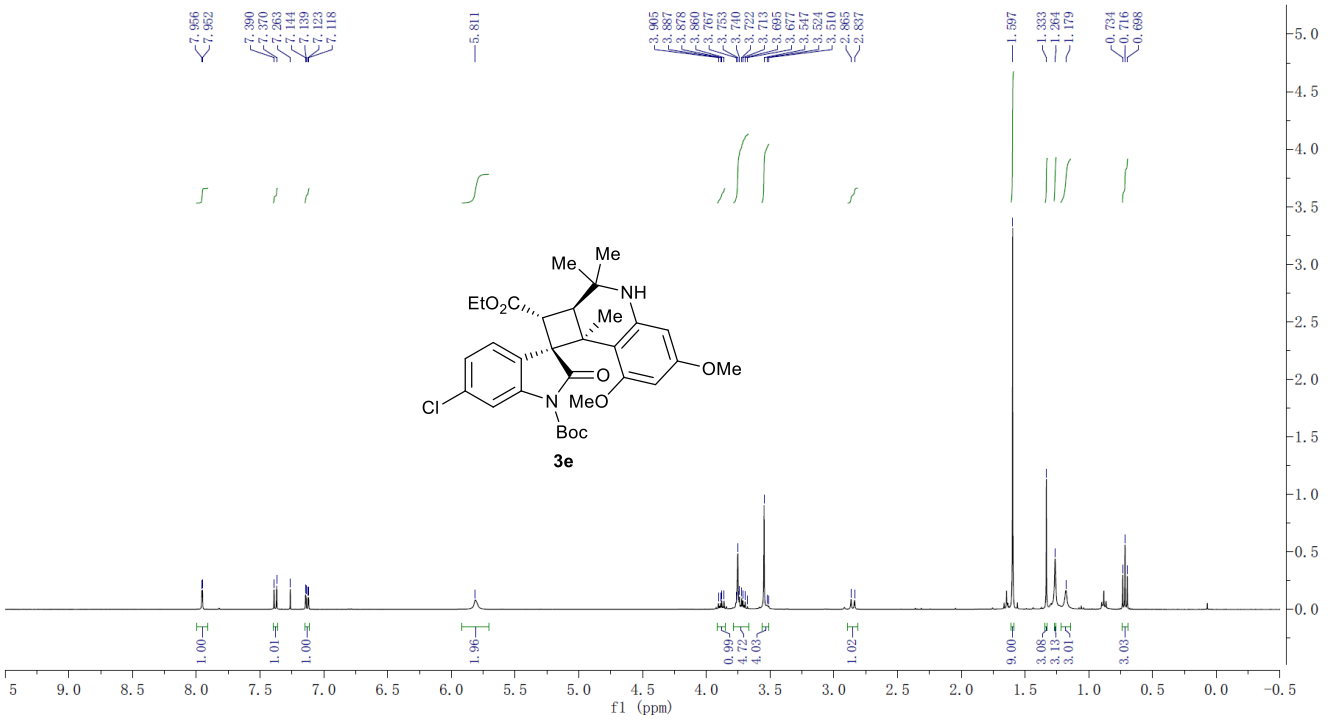
f1 (ppm)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OMe
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Cl
N
MeO
Boc
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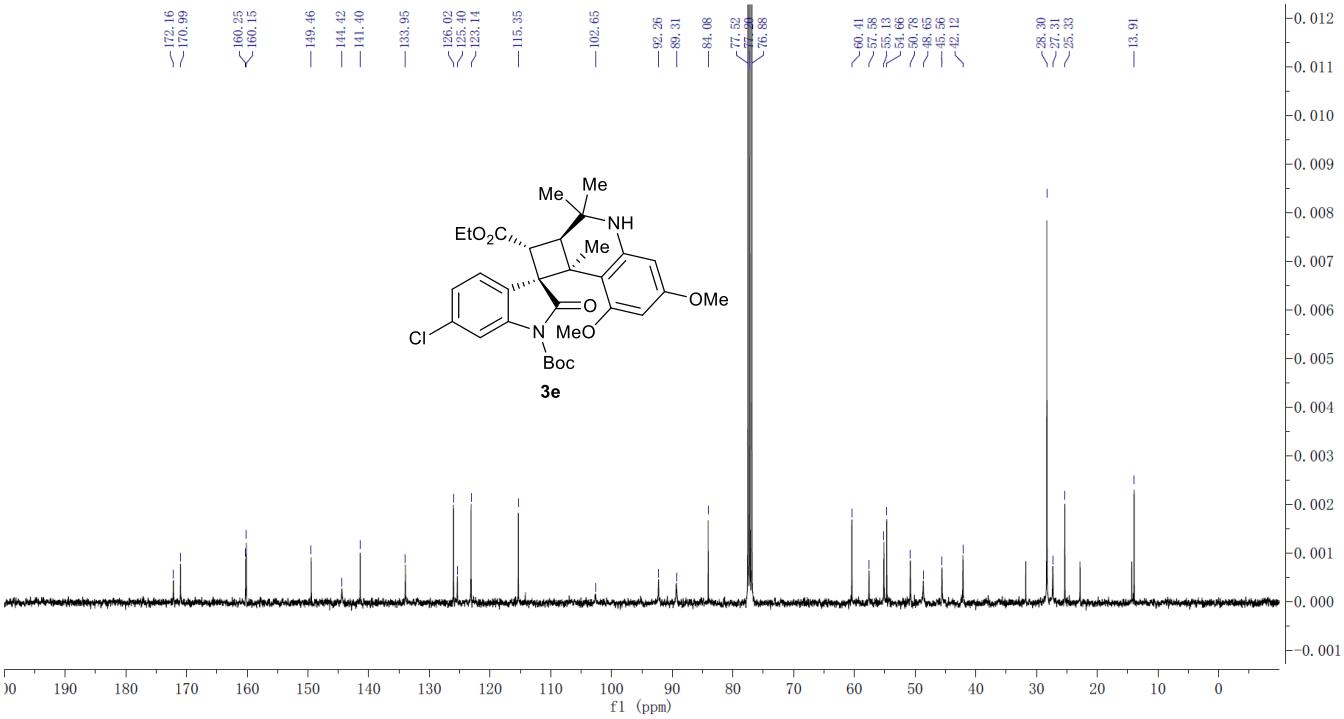
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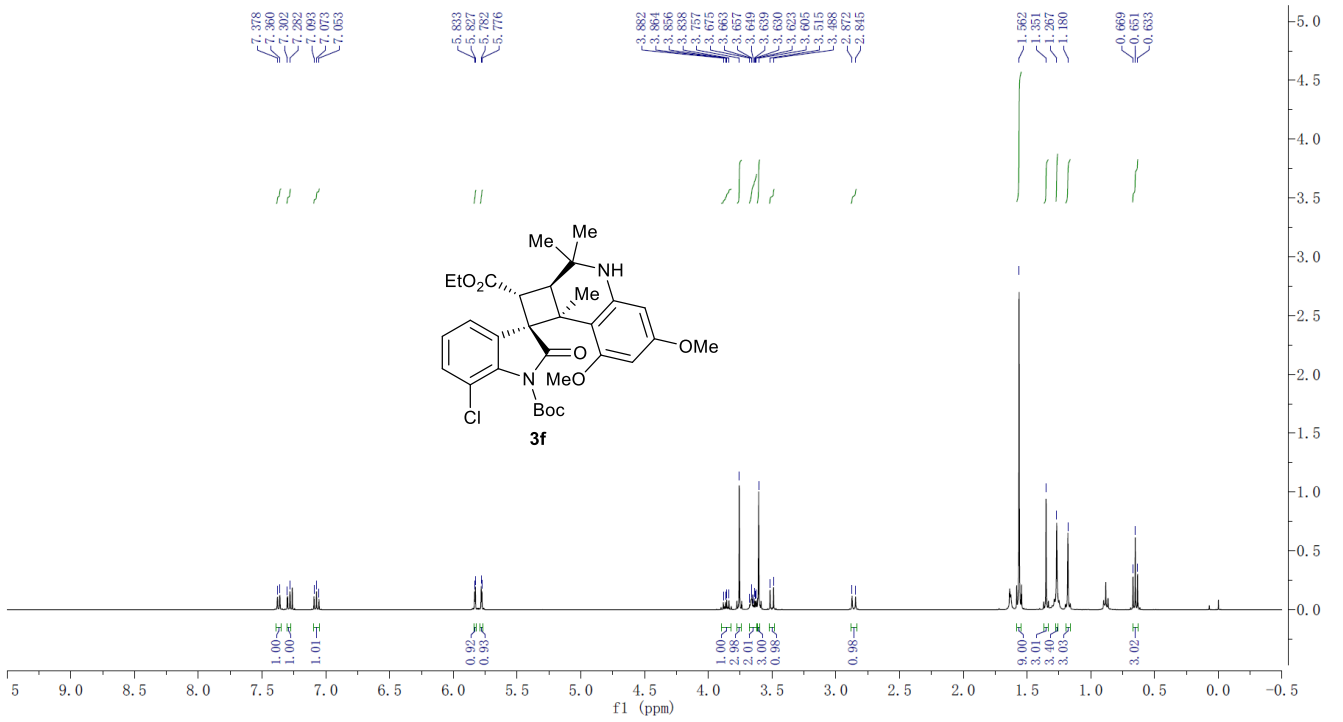
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Cl
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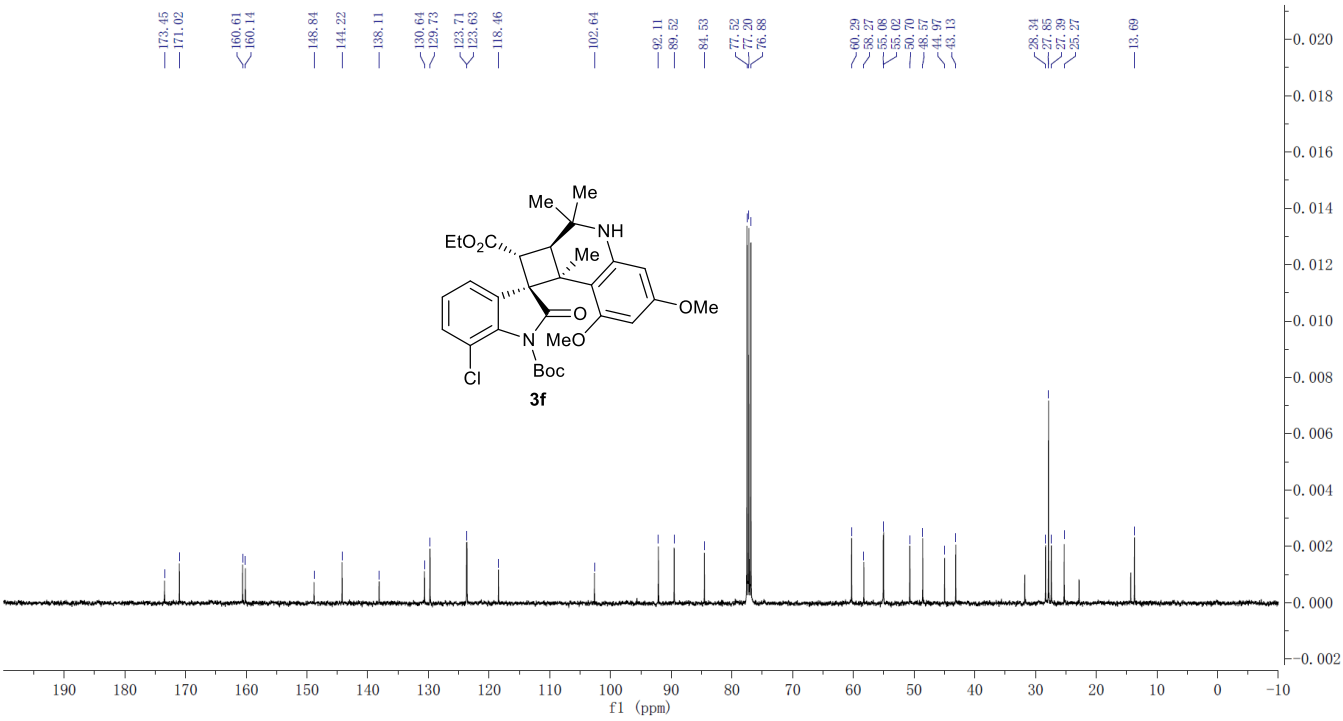
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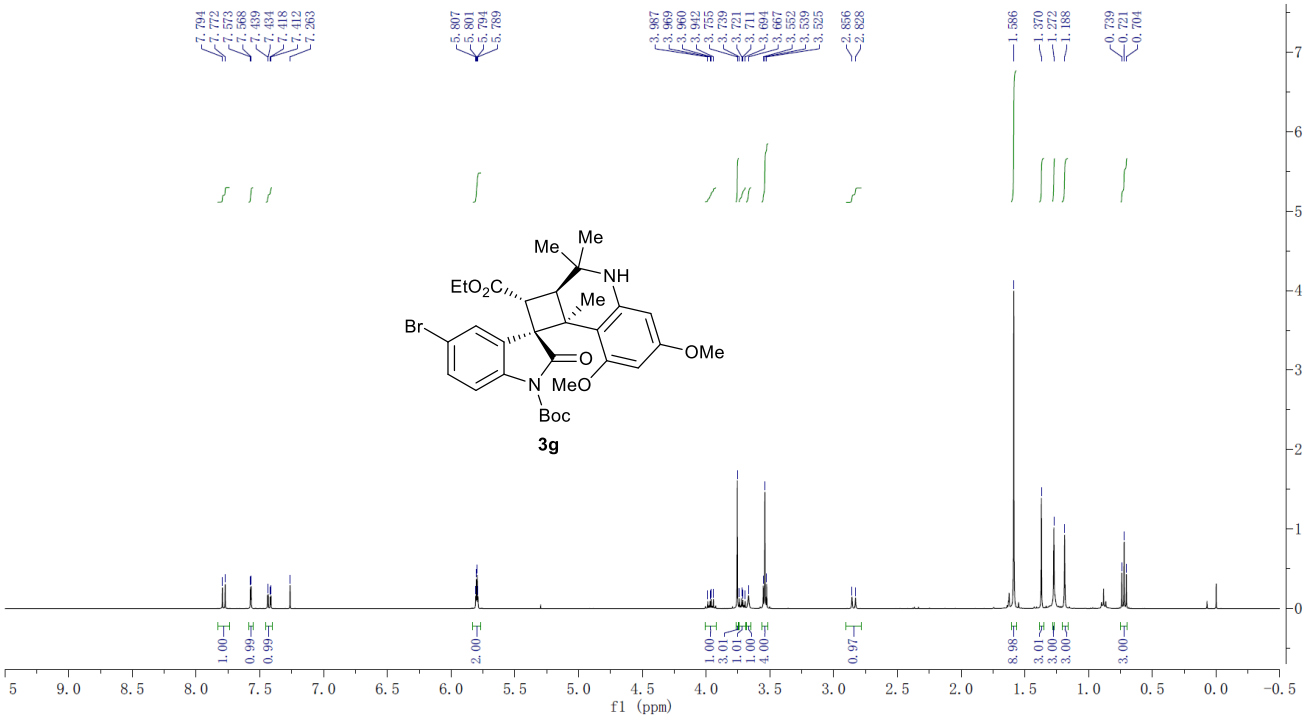
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Br
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OMe
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MeO
Boc
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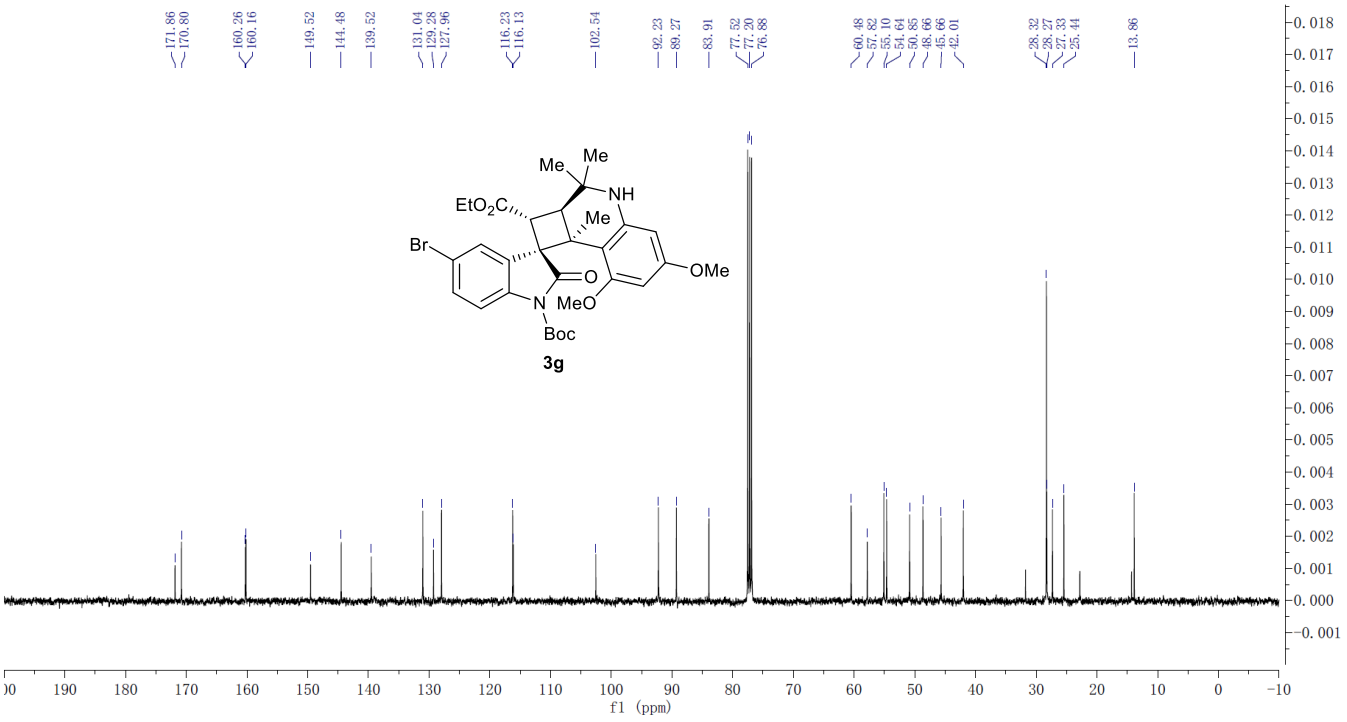
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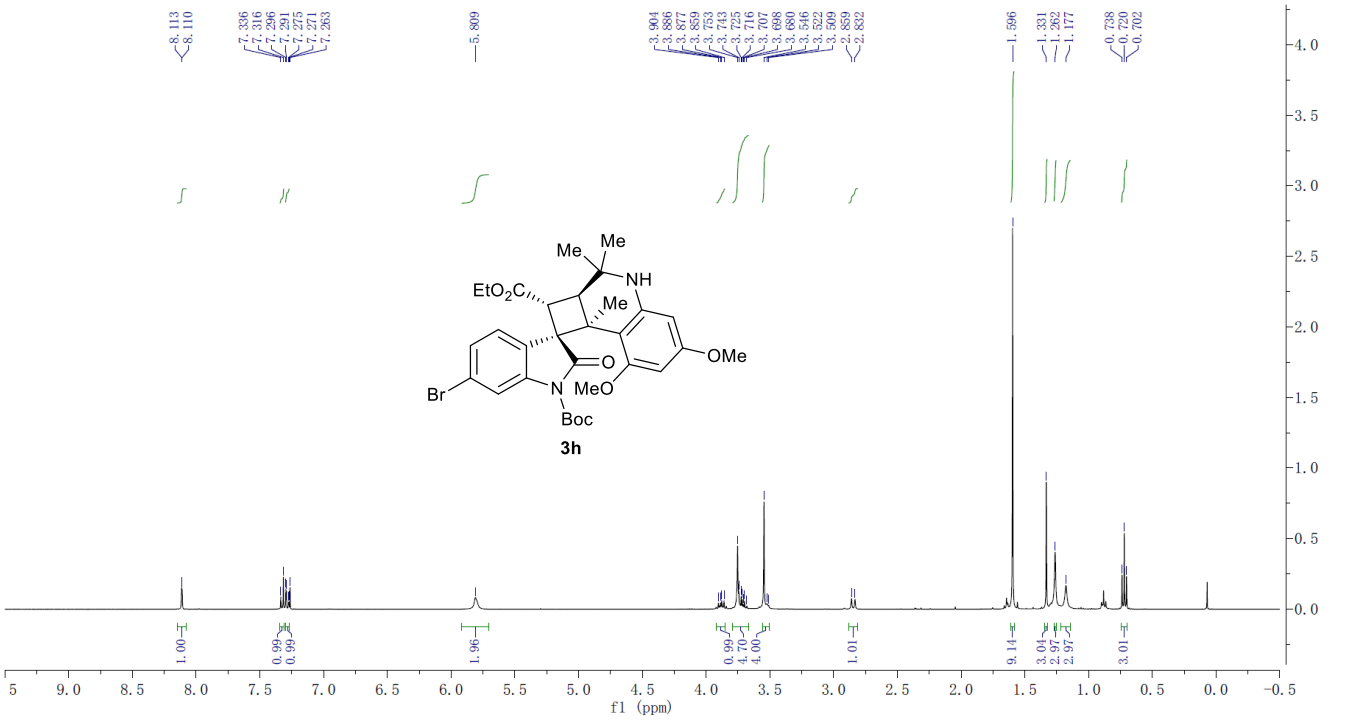
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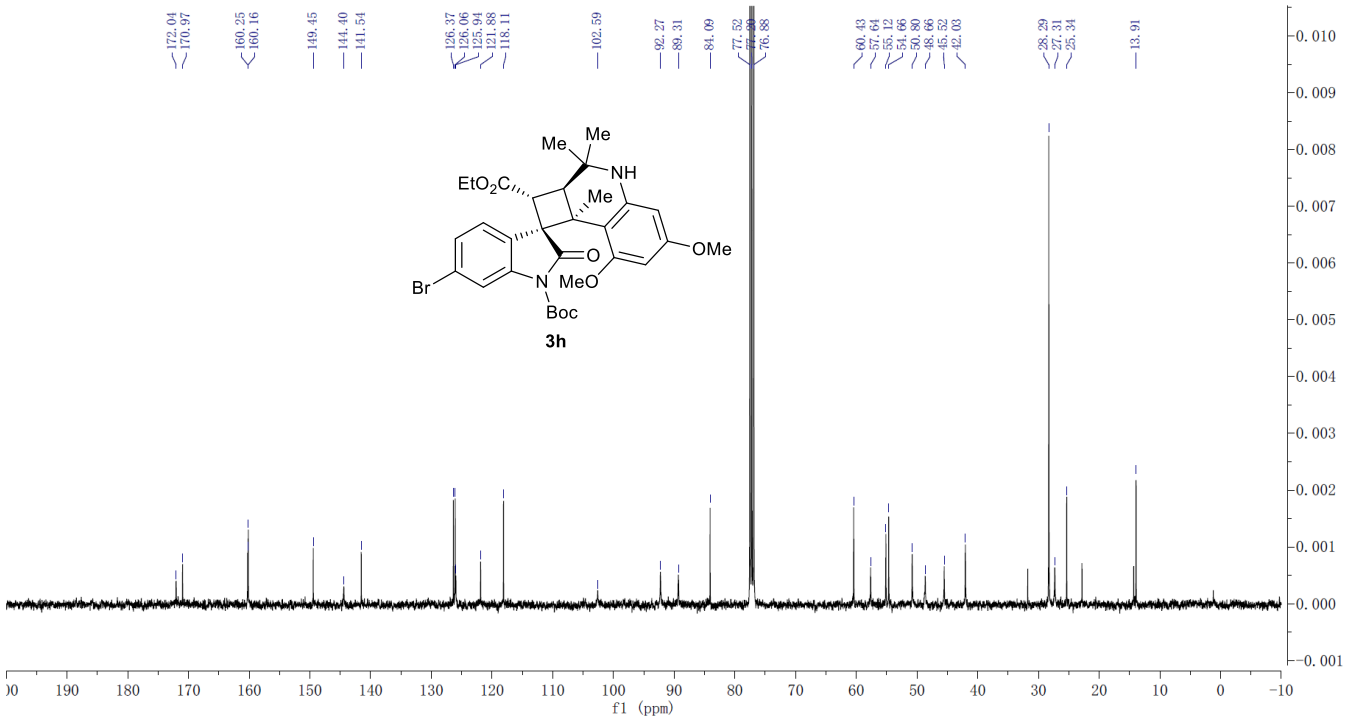
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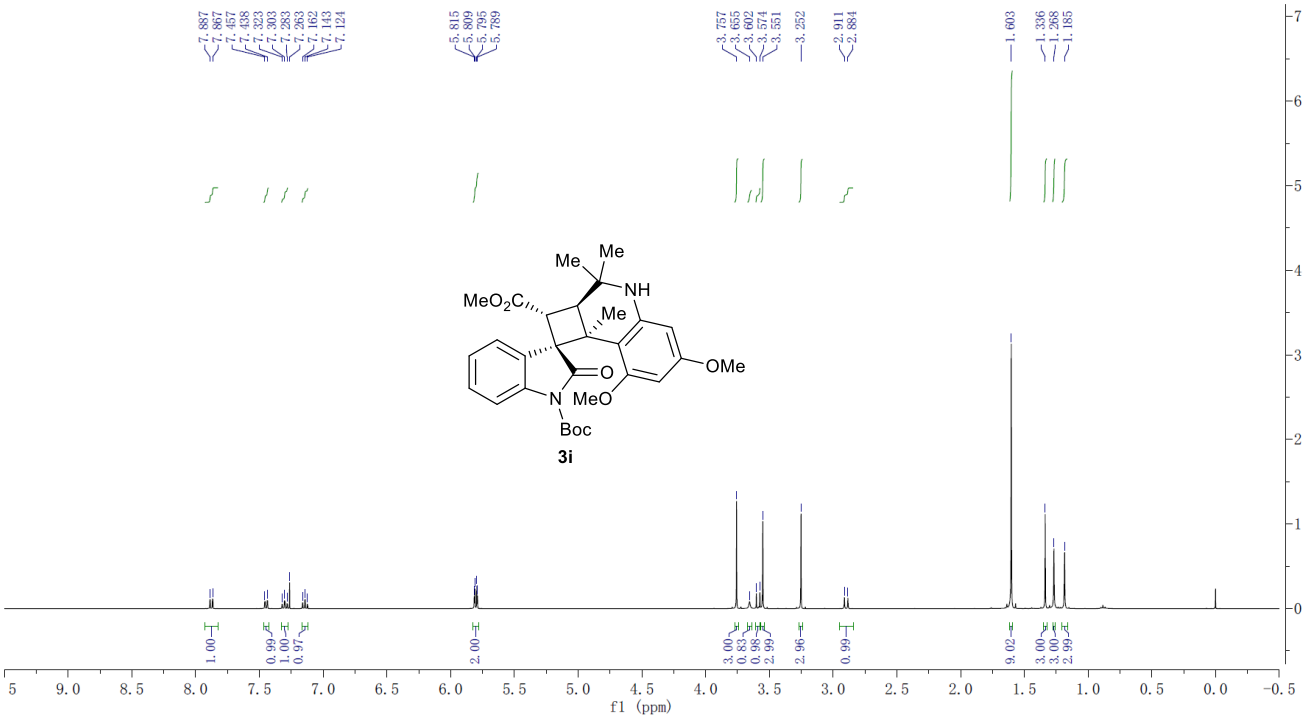
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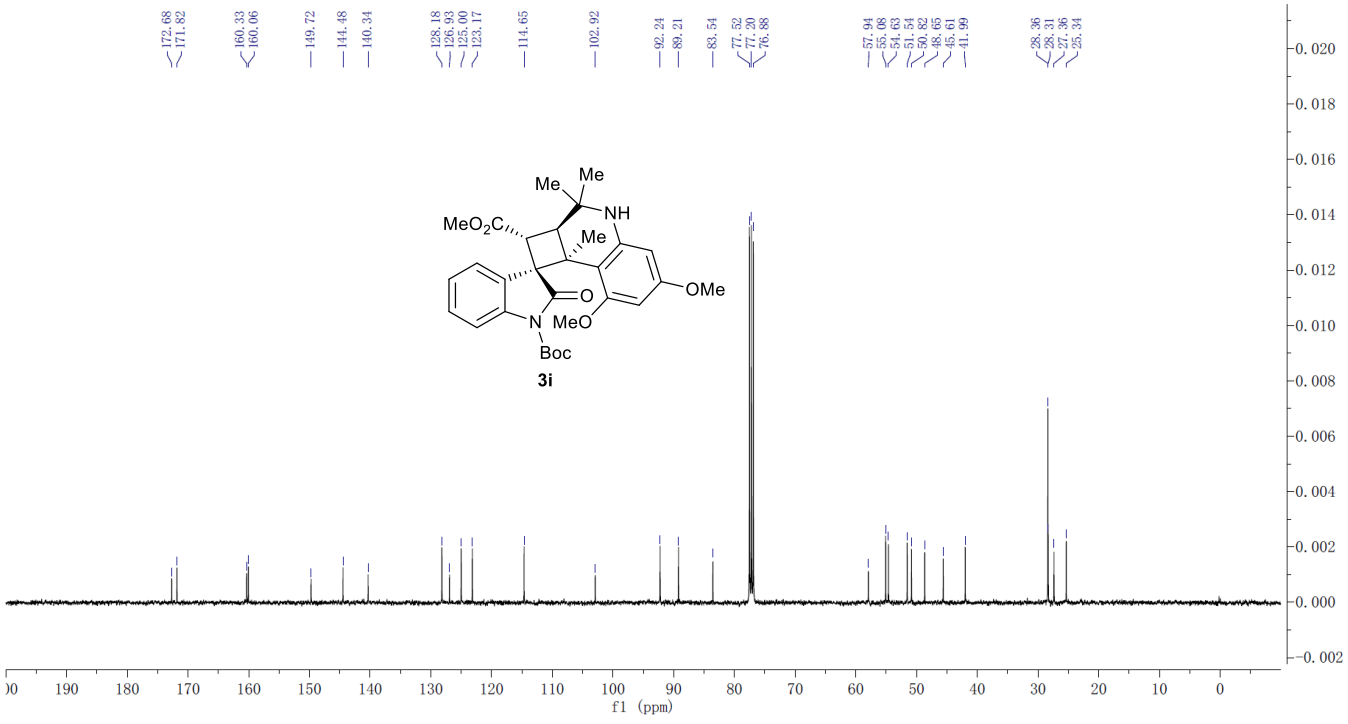
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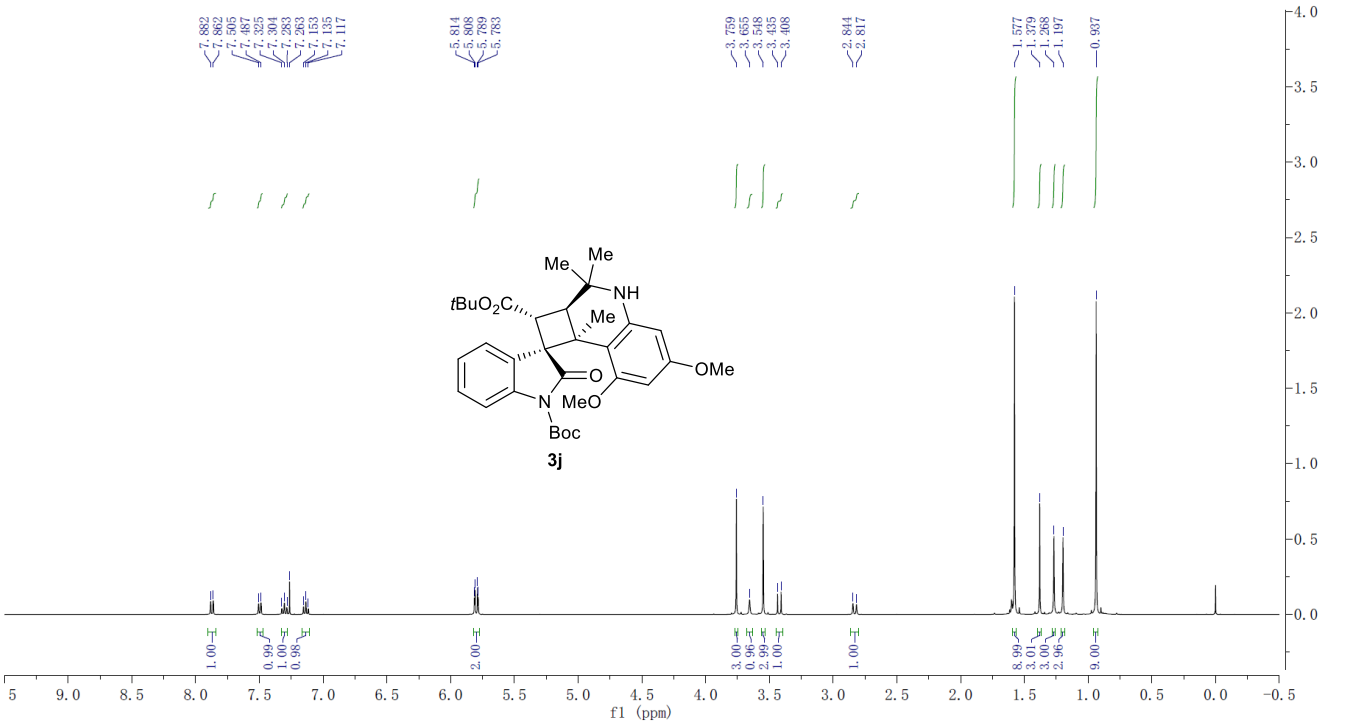
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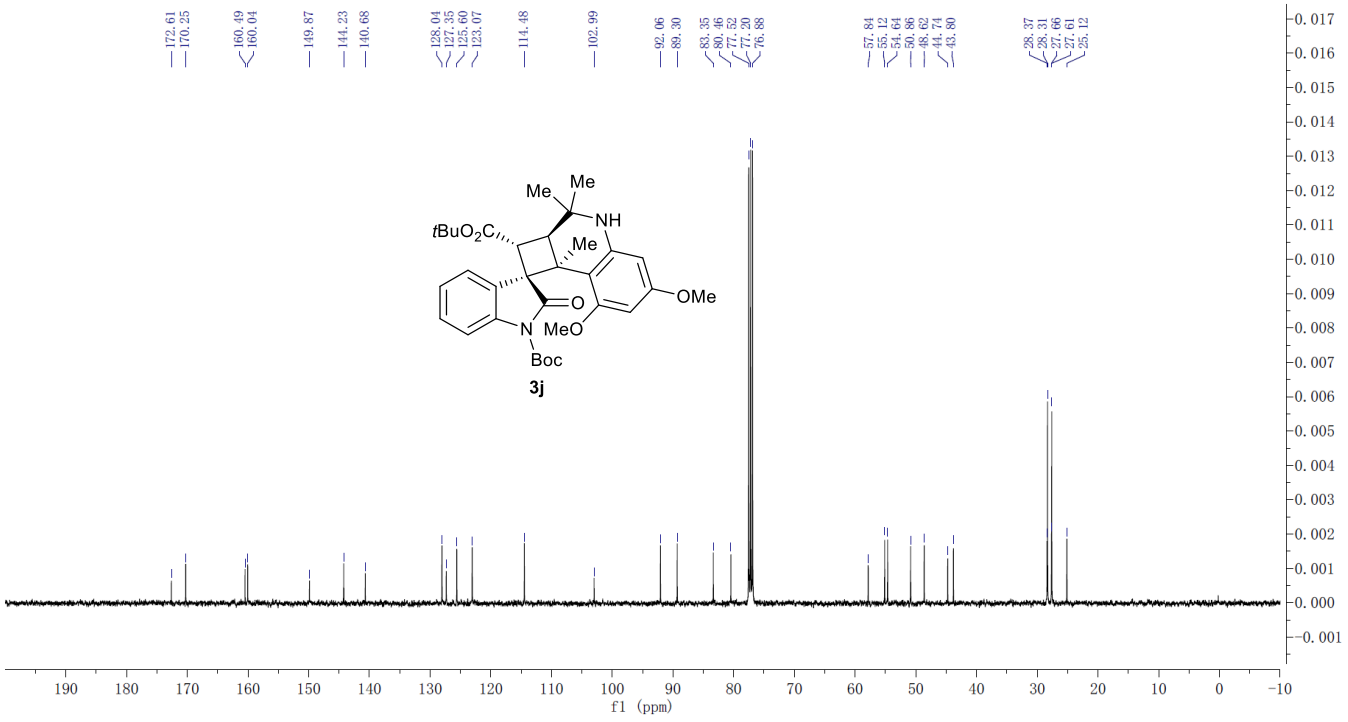
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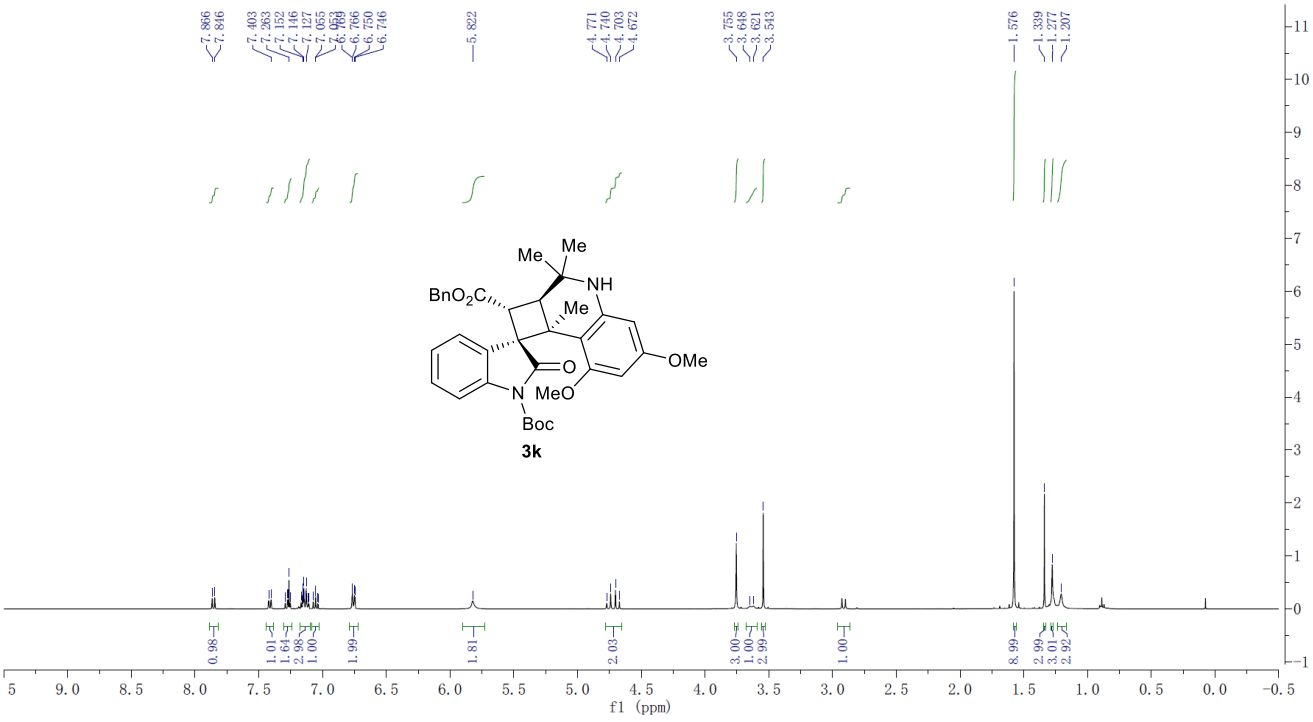
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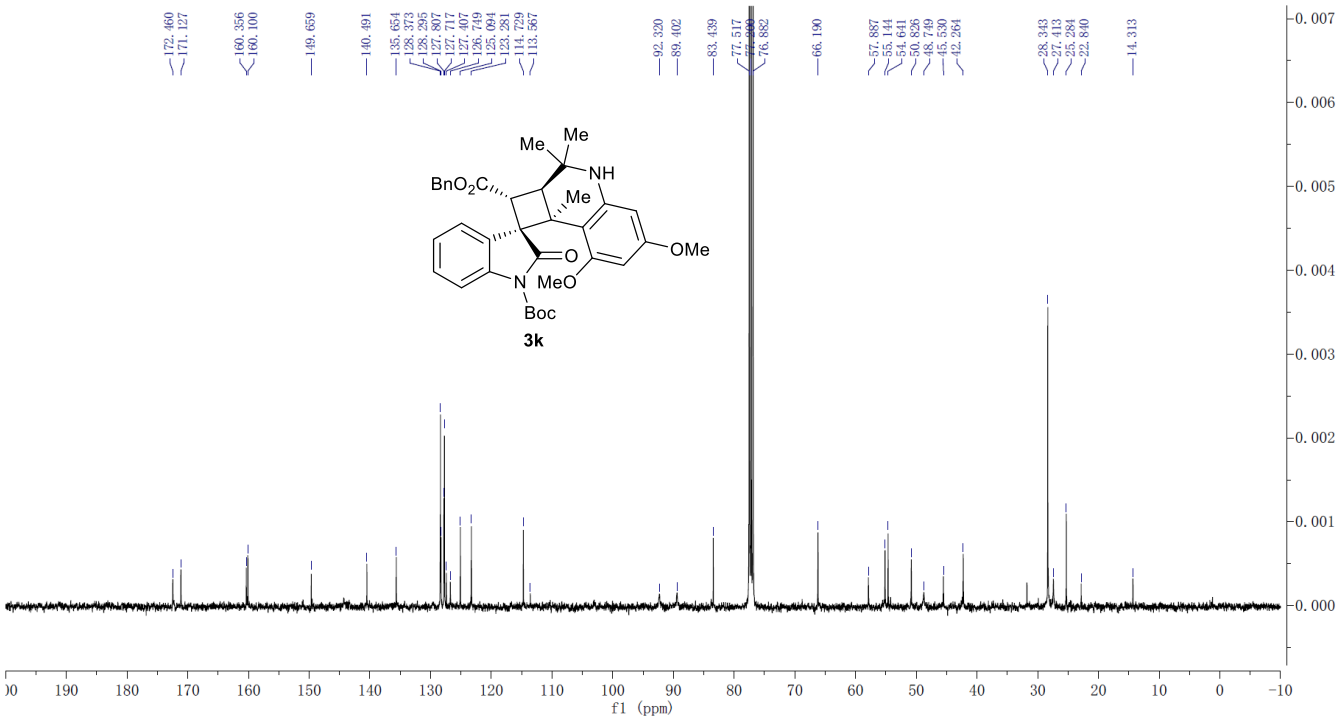
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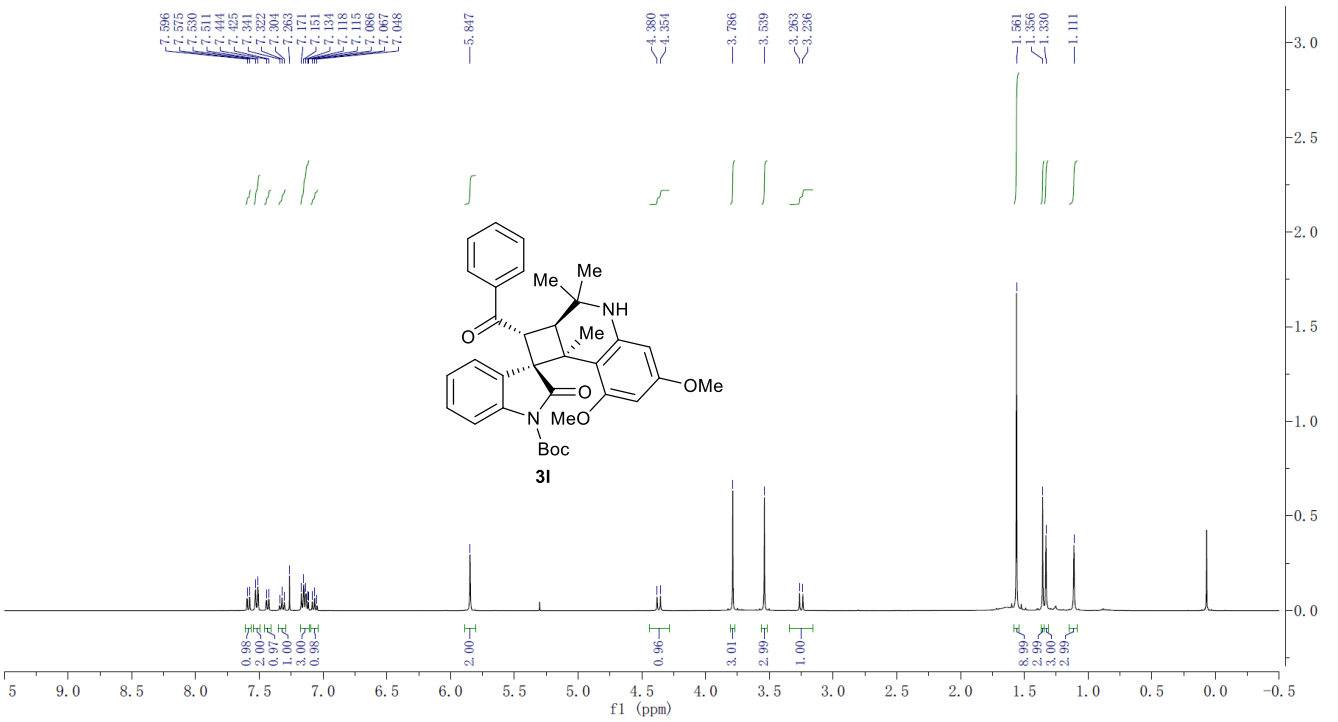
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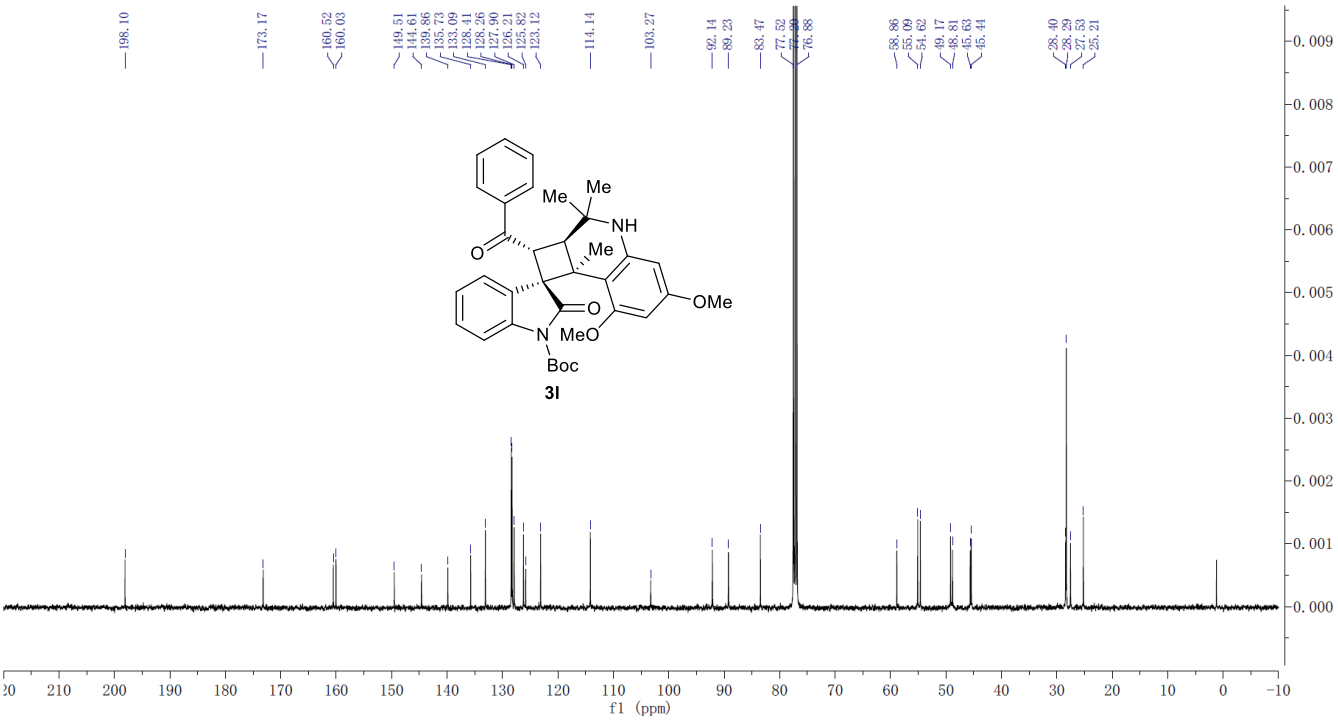
7.048
5.847
4.380
4.354
3.786
3.539
3.263
3.236
1.561
1.356
1.330
1.111
Me
Me
NH
Me
O
O
OMe
N
MeO
Boc
3l
f1 (ppm)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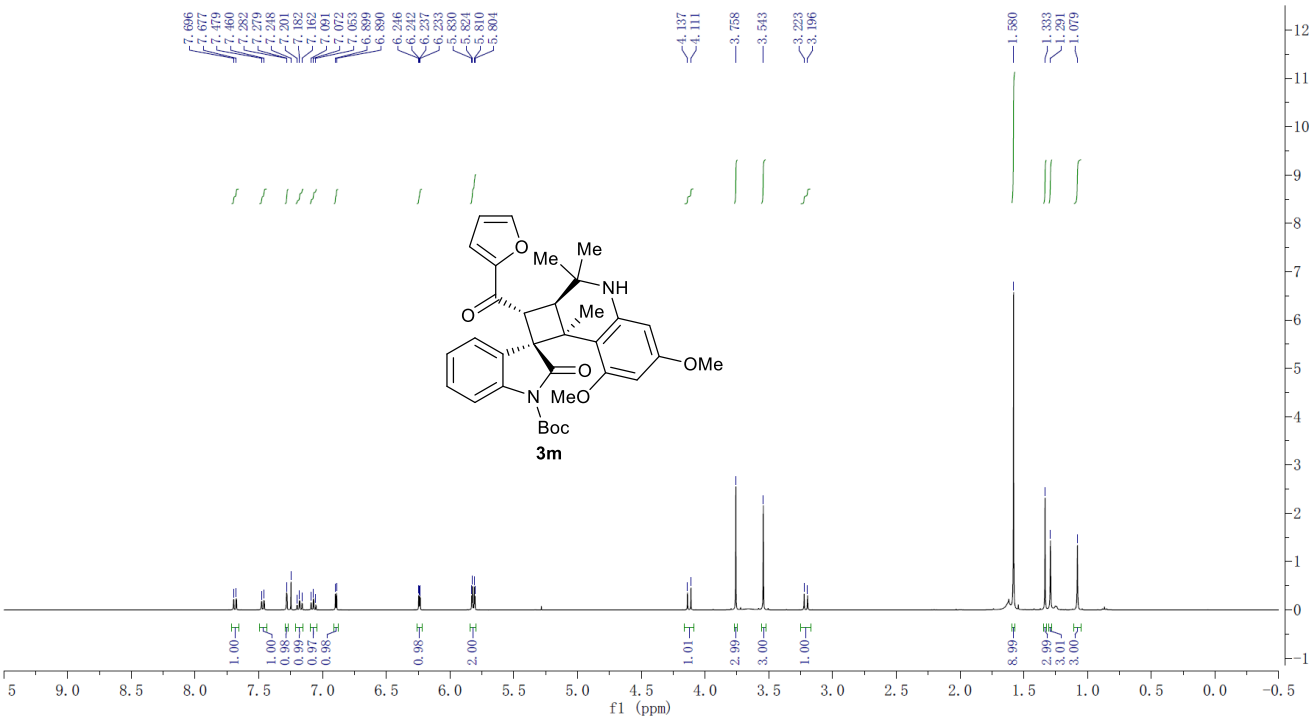
173.17
160.52
160.03
149.51
144.61
139.86
135.73
133.09
128.41
128.26
127.90
126.21
125.82
123.12
114.14
103.27
92.14
89.23
83.47
77.52
76.88
58.86
55.09
54.62
49.17
48.81
45.63
45.44
28.40
28.29
27.53
25.21
Me
Me
NH
Me
O
O
OMe
N
MeO
Boc
3l
f1 (ppm)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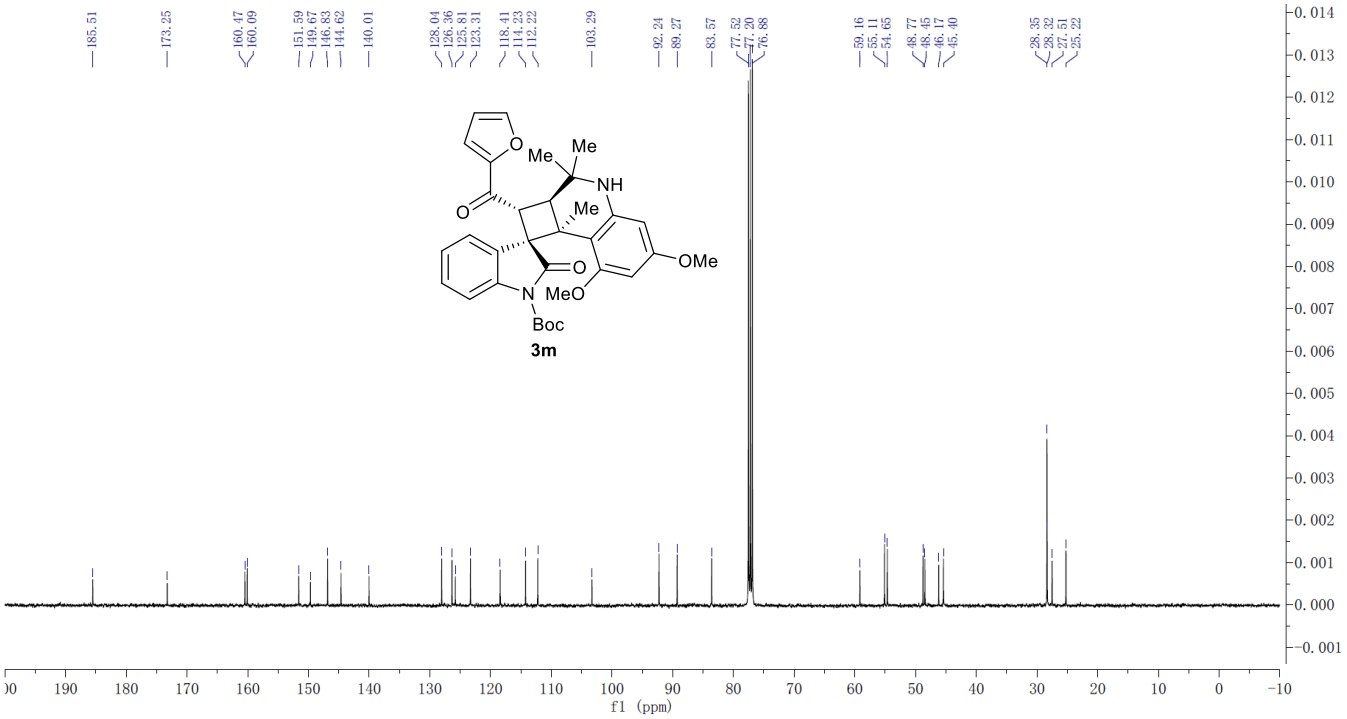
7.201
7.182
7.162
7.091
7.072
7.063
6.899
6.890
6.246
6.242
6.237
6.233
5.830
5.824
5.810
5.804
4.137
4.111
3.758
3.543
3.223
3.196
1.580
1.333
1.291
1.079
Me
Me
NH
Me
O
O
OMe
N
MeO
Boc
3m
1.00
1.00
0.98
0.99
0.97
0.98
0.98
2.00
1.01
2.99
3.00
1.00
8.99
2.99
3.01
3.00
f1 (ppm)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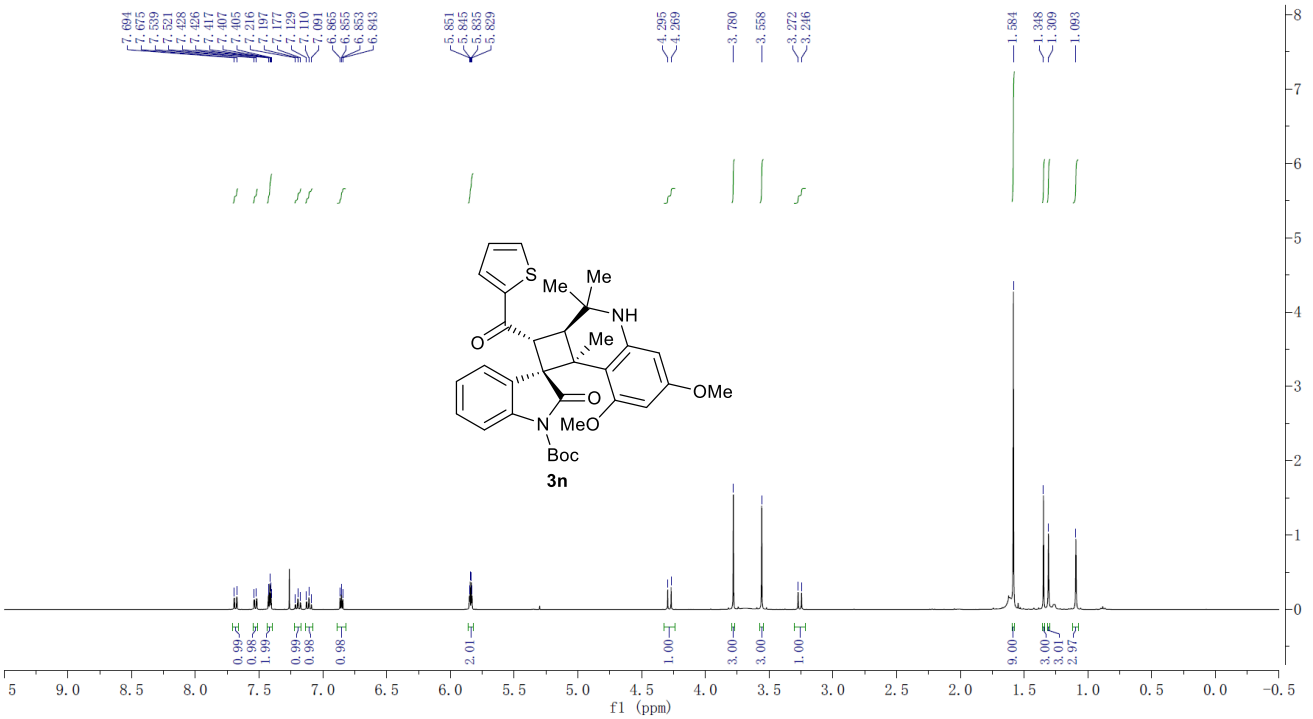
160.47
160.09
151.59
149.67
146.83
144.62
140.01
128.04
126.36
125.81
123.31
118.41
114.23
112.22
103.29
92.24
89.27
83.57
77.52
77.20
76.88
59.16
55.11
54.65
48.77
48.45
46.17
45.40
28.35
28.32
27.51
25.22
Me
Me
NH
Me
O
O
OMe
N
MeO
Boc
3m
f1 (ppm)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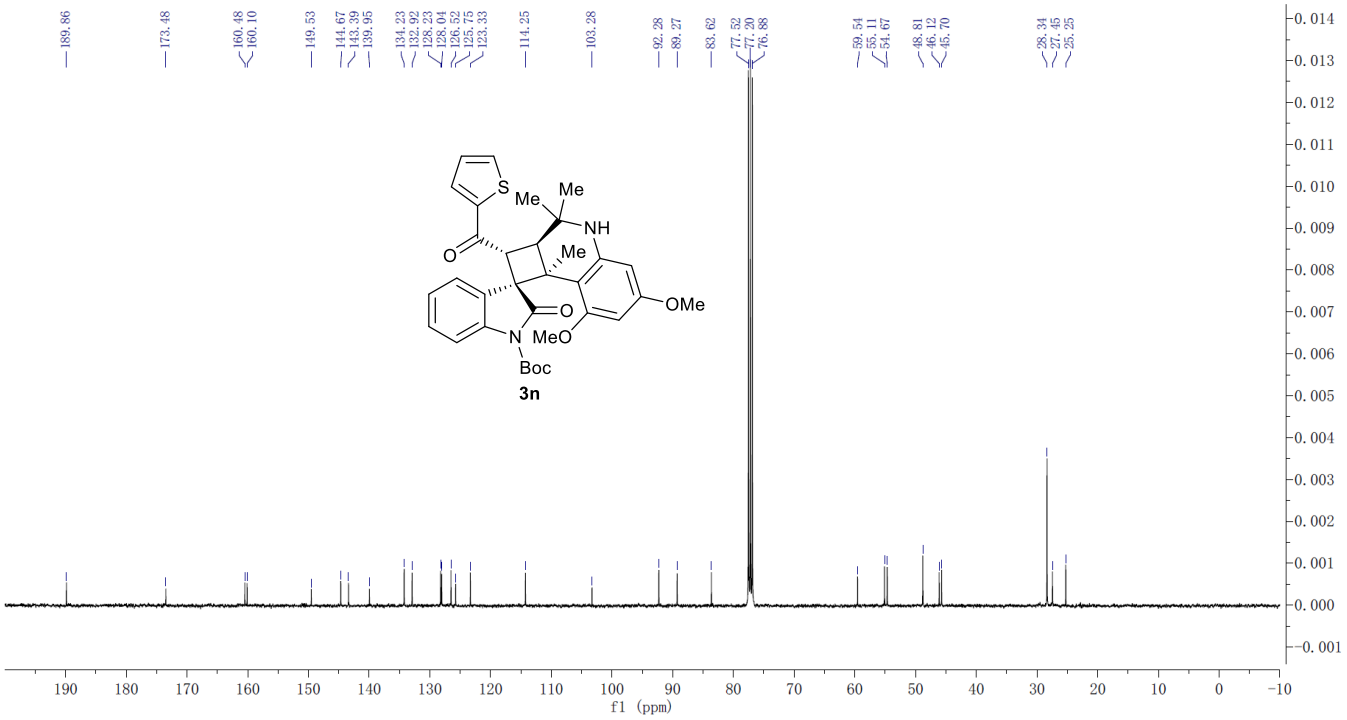
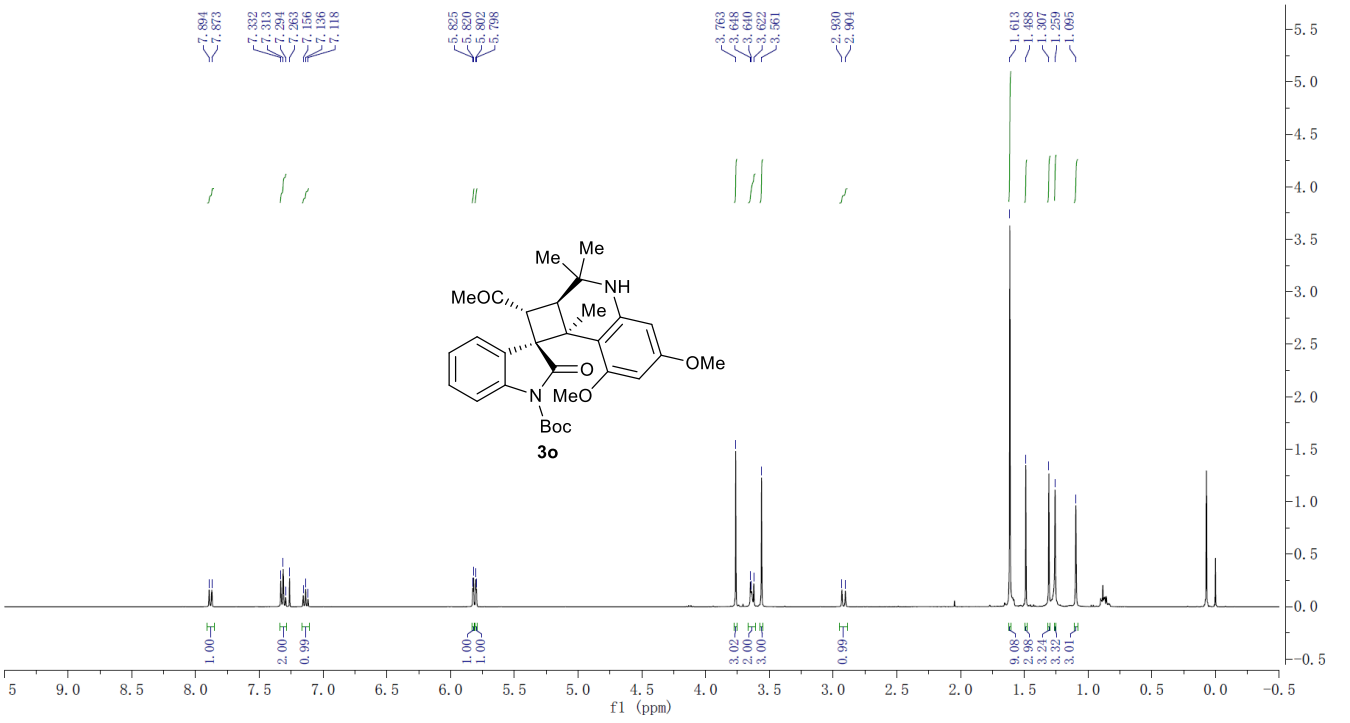
7.426
7.417
7.407
7.405
7.216
7.197
7.177
7.129
7.110
7.091
6.865
6.855
6.853
6.843
5.851
5.845
5.835
5.829
4.295
4.269
3.780
3.558
3.272
3.246
1.584
1.348
1.309
1.093
S
Me
Me
NH
Me
O
O
OMe
N
MeO
Boc
3n
f1 (ppm)


189.86
173.48
160.48
160.10
149.53
144.67
143.39
139.95
134.23
132.92
128.23
128.04
126.52
125.75
123.33
114.25
103.28
92.28
89.27
83.62
77.52
77.20
76.88
59.54
55.11
54.67
48.81
46.12
45.70
28.34
27.45
25.25
S
Me
Me
NH
Me
O
O
OMe
N
MeO
Boc
3n
f1 (ppm)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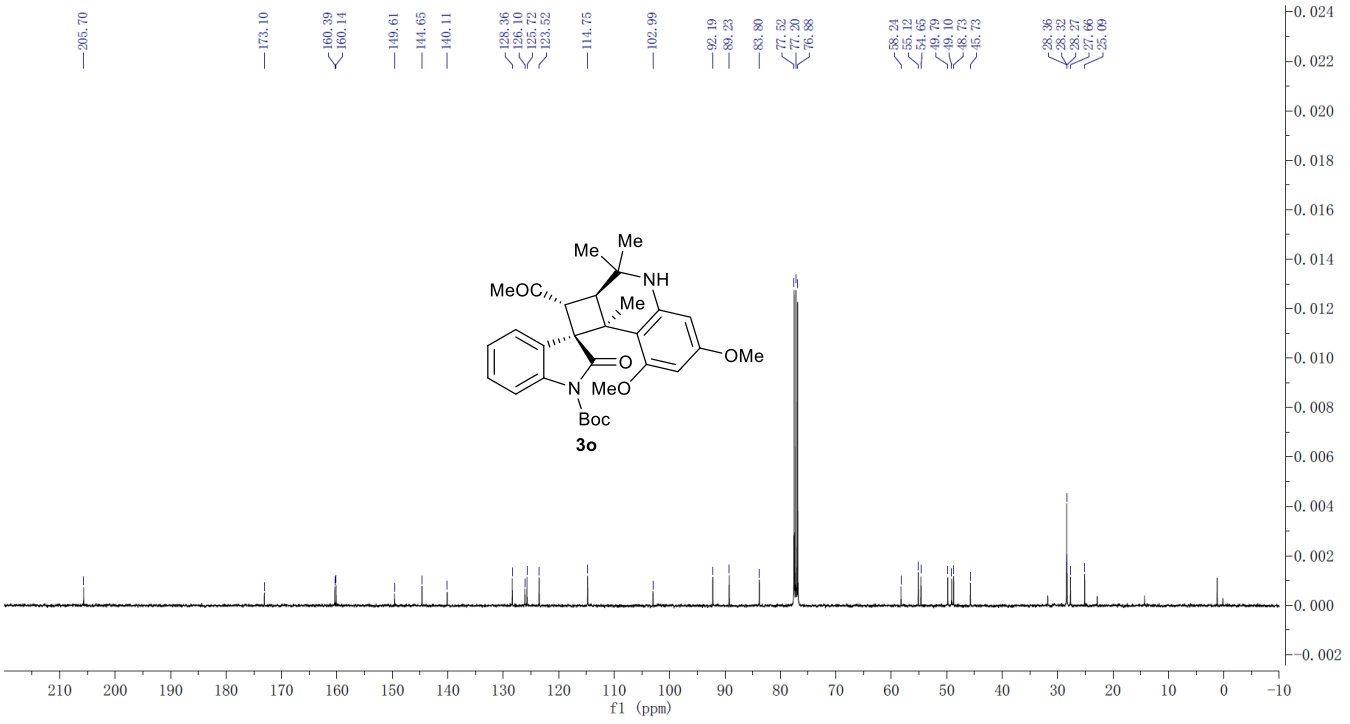
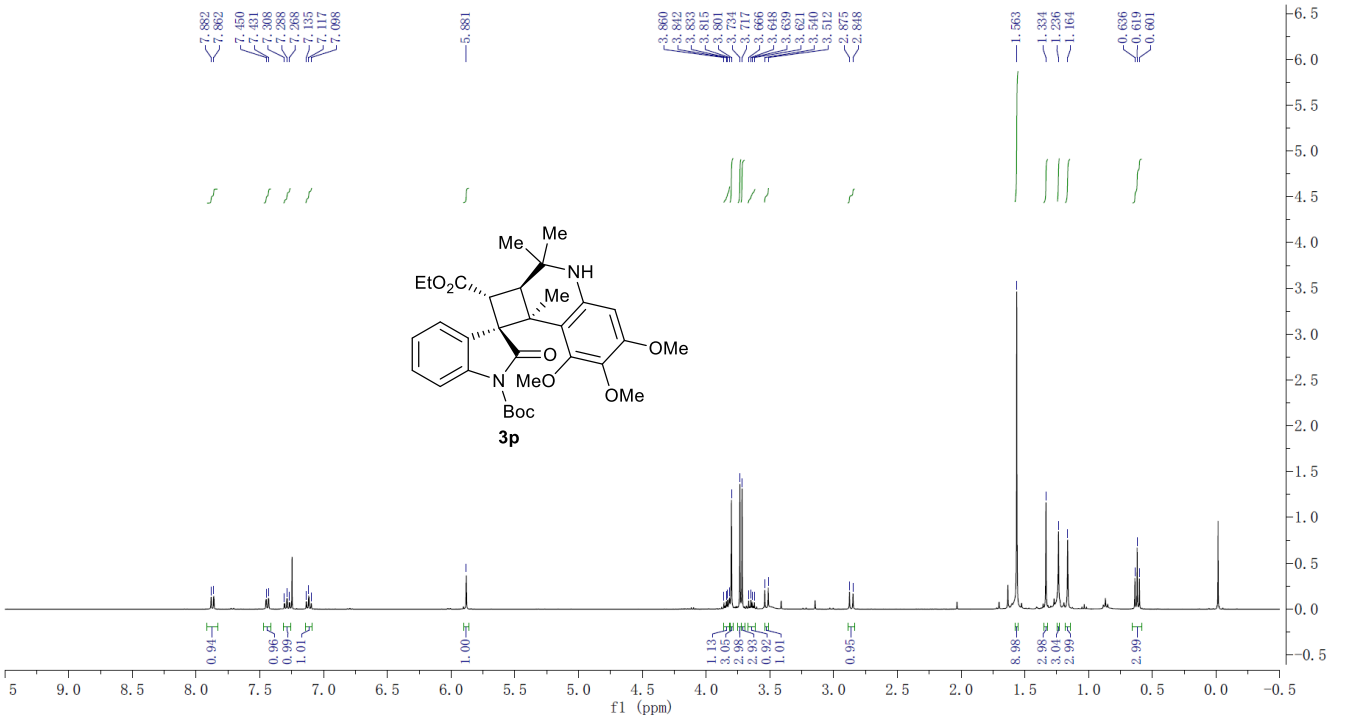
7.332
7.313
7.294
7.263
7.156
7.136
7.118
5.825
5.820
5.802
5.798
3.763
3.648
3.640
3.622
3.561
2.930
2.904
1.613
1.488
1.307
1.259
1.095
Me
Me
NH
MeOC
Me
OMe
O
N
MeO
Boc
3o
1.00
2.00
0.99
1.00
1.00
3.02
2.00
3.00
0.99
9.08
2.98
3.24
3.32
3.01
f1 (ppm)


205.70
173.10
160.39
160.14
149.61
144.65
140.11
128.36
126.10
125.72
123.52
114.75
102.99
92.19
89.23
83.80
77.52
77.20
76.88
58.24
55.12
54.65
49.79
49.10
48.73
45.73
28.36
28.32
28.27
27.66
25.09
Me
Me
NH
MeOC
Me
OMe
O
N
MeO
Boc
3o
f1 (ppm)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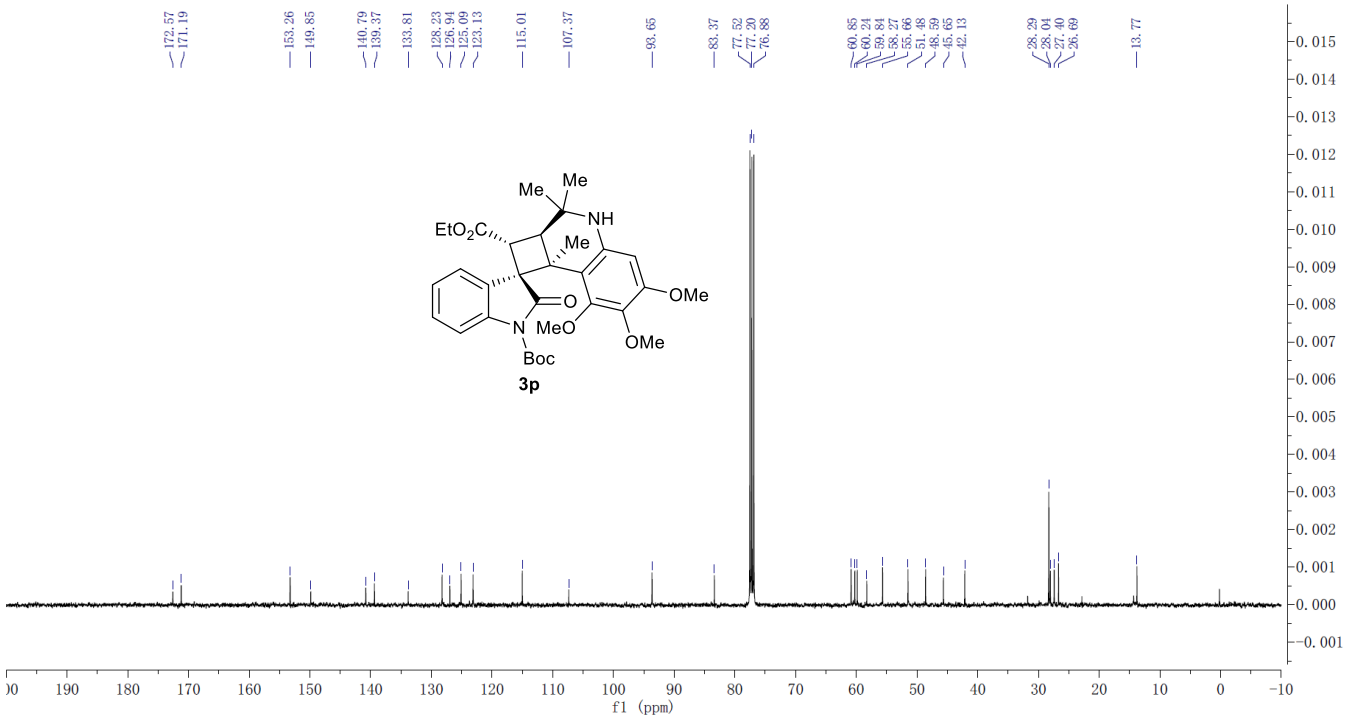
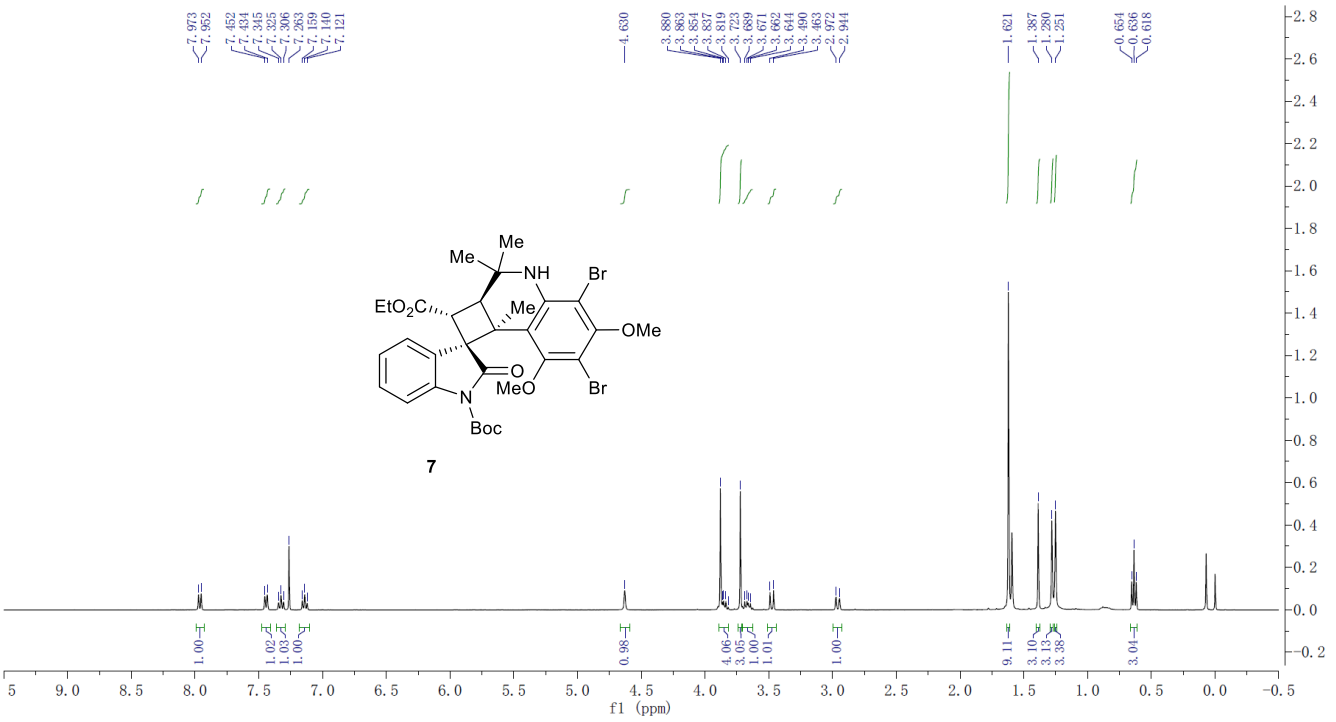
7.431
7.308
7.288
7.268
7.135
7.117
7.098
5.881
3.860
3.842
3.833
3.815
3.801
3.754
3.717
3.666
3.648
3.639
3.621
3.540
3.512
2.875
2.848
1.563
1.334
1.236
1.164
0.636
0.619
0.601
Me
Me
NH
EtO2C
Me
O
OMe
N
MeO
OMe
Boc
3p
0.94
0.96
0.99
1.01
1.00
1.13
3.05
2.98
2.93
0.92
1.01
0.95
8.98
2.98
3.04
2.99
2.99
f1 (ppm)


172.57
171.19
153.26
149.85
140.79
139.37
133.81
128.23
126.94
125.09
123.13
115.01
107.37
93.65
83.37
77.52
77.20
76.88
60.85
60.24
59.84
58.27
55.66
51.48
48.59
45.65
42.13
28.29
28.04
27.40
26.69
13.77
Me
Me
NH
EtO2C
Me
O
OMe
N
MeO
OMe
Boc
3p
f1 (ppm)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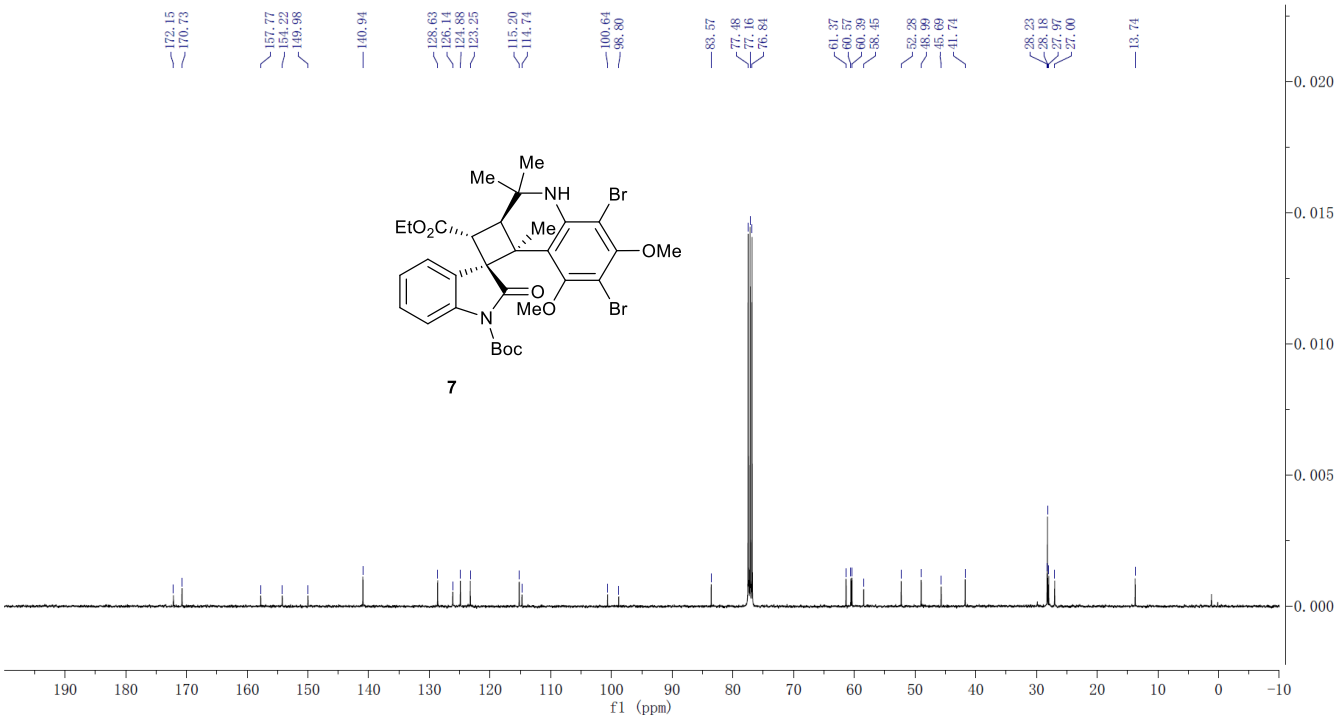
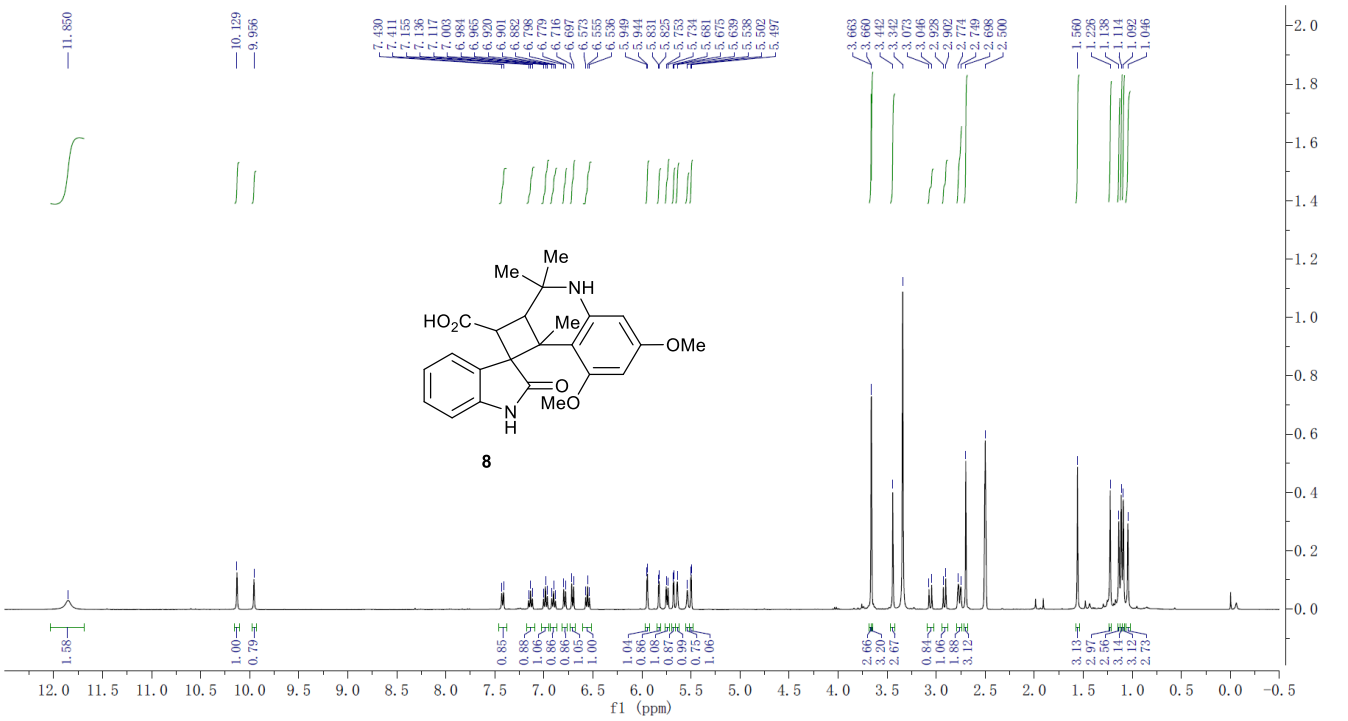
7.345
7.325
7.306
7.263
7.159
7.140
7.121
4.630
3.880
3.863
3.854
3.837
3.819
3.723
3.689
3.671
3.662
3.644
3.490
3.463
2.972
2.944
1.621
1.387
1.280
1.251
0.654
0.636
0.618
Me
Me
NH
Br
EtO2C
Me
OMe
O
MeO
Br
N
Boc
7
1.00
1.02
1.03
1.00
0.98
4.06
3.05
1.00
1.01
1.00
9.11
3.10
3.13
3.38
3.04
f1 (ppm)


172.15
170.73
157.77
154.22
149.98
140.94
128.63
126.14
124.88
123.25
115.20
114.74
100.64
96.80
83.57
77.48
77.16
76.84
61.37
60.57
60.39
58.45
52.28
48.99
45.69
41.74
28.23
28.18
27.97
27.00
13.74
Me
Me
NH
Br
EtO2C
Me
OMe
O
MeO
Br
N
Boc
7
f1 (ppm)


11.850
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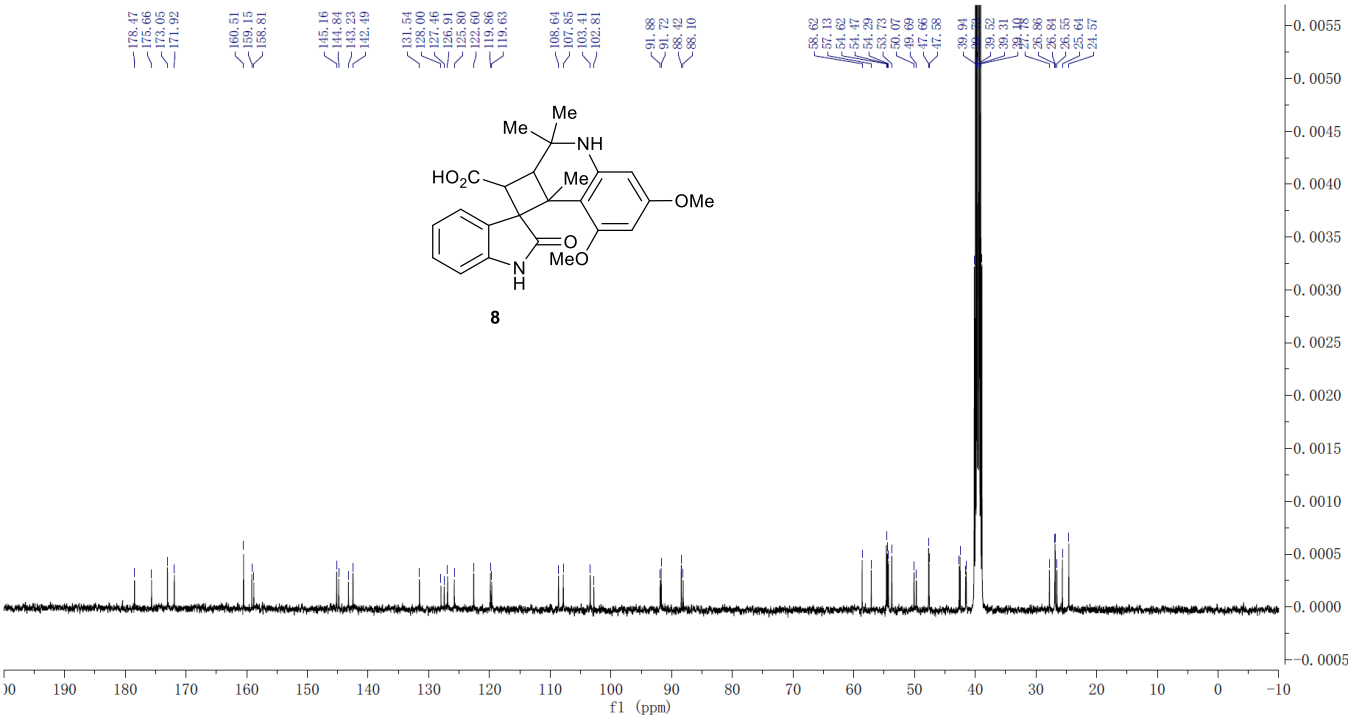
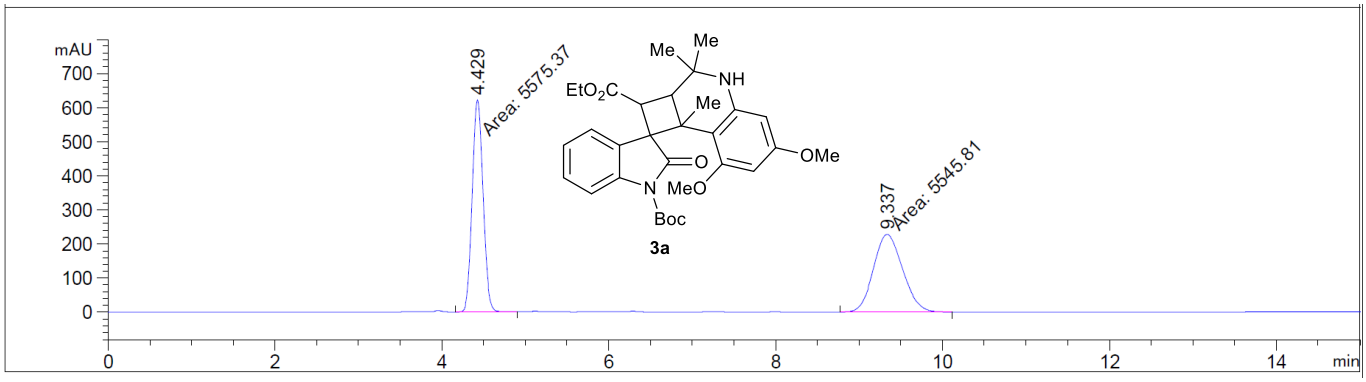
9.956
7.430
7.411
7.155
7.136
7.117
7.003
6.984
6.965
6.920
6.901
6.882
6.798
6.779
6.716
6.697
6.573
6.555
6.536
5.949
5.944
5.831
5.825
5.753
5.734
5.681
5.675
5.639
5.538
5.502
5.497
3.663
3.660
3.442
3.342
3.073
3.046
3.028
2.972
2.774
2.749
2.698
2.500
1.560
1.226
1.138
1.114
1.092
1.046
Me
Me
NH
HO2C
Me
OMe
O
MeO
N
H
8
f1 (ppm)

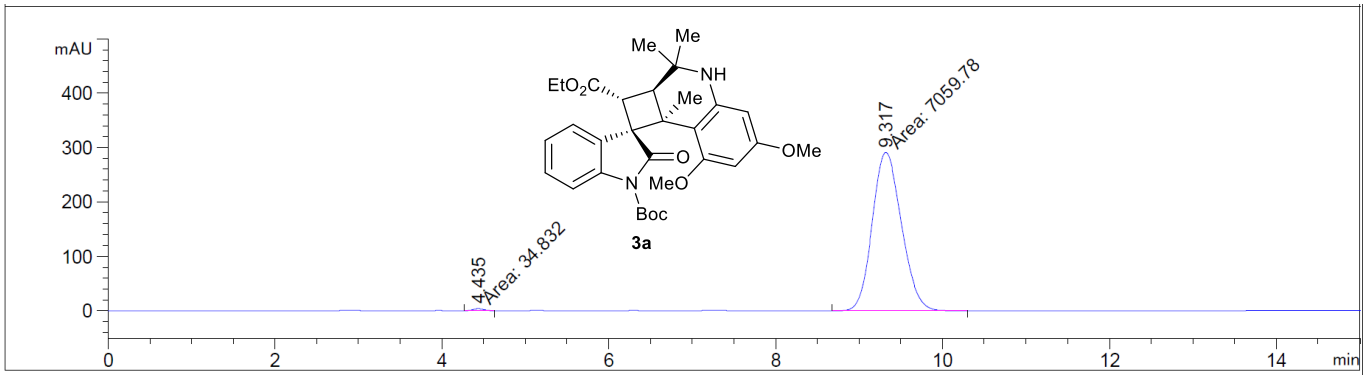

178.47
175.66
173.05
171.92
160.51
159.15
158.81
145.16
144.84
143.23
142.49
131.54
128.00
127.46
126.91
125.80
122.60
119.98
119.63
108.64
107.85
103.41
102.81
91.88
91.72
88.42
88.10
58.62
57.13
54.62
54.47
54.29
53.73
50.67
49.69
47.66
47.38
39.94
39.73
39.52
39.31
27.78
26.86
26.84
26.55
25.64
24.57
Me
Me
NH
HO2C
Me
OMe
O
MeO
N
H
8
f1 (ppm)

11. HPLC trace of [2+2] Cycloadducts



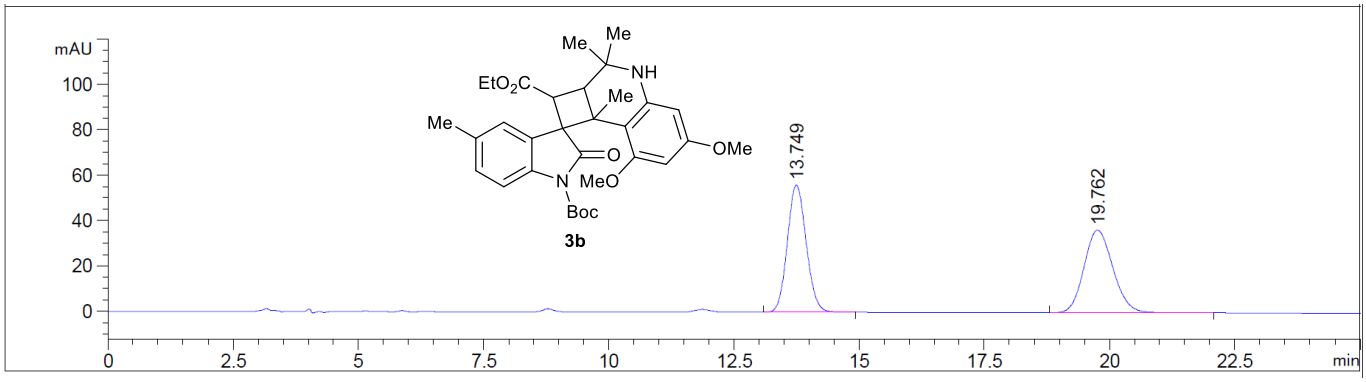
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.429	MM	0.1492	5575.36523	622.78418	50.1329
2	9.337	MM	0.4056	5545.81250	227.91183	49.8671



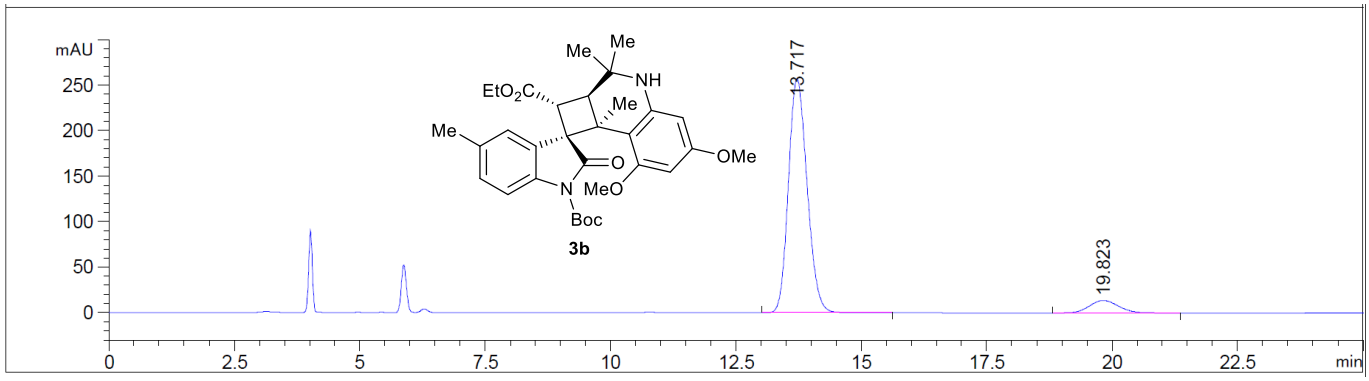
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.435	MM	0.1531	34.83197	3.79203	0.4910
2	9.317	MM	0.4044	7059.78418	290.96979	99.5090



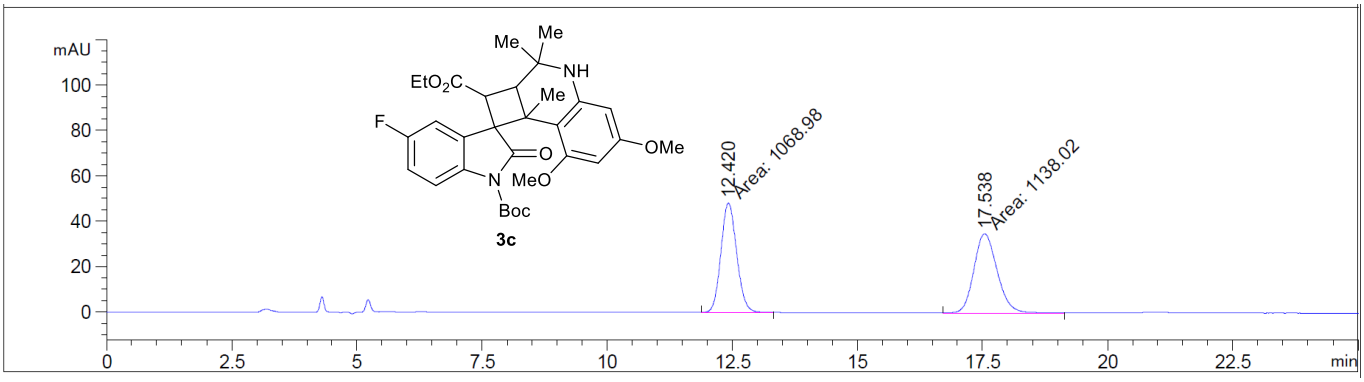
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.749	BB	0.4102	1470.05200	56.01229	50.2007
2	19.762	BB	0.6218	1458.29907	36.36905	49.7993



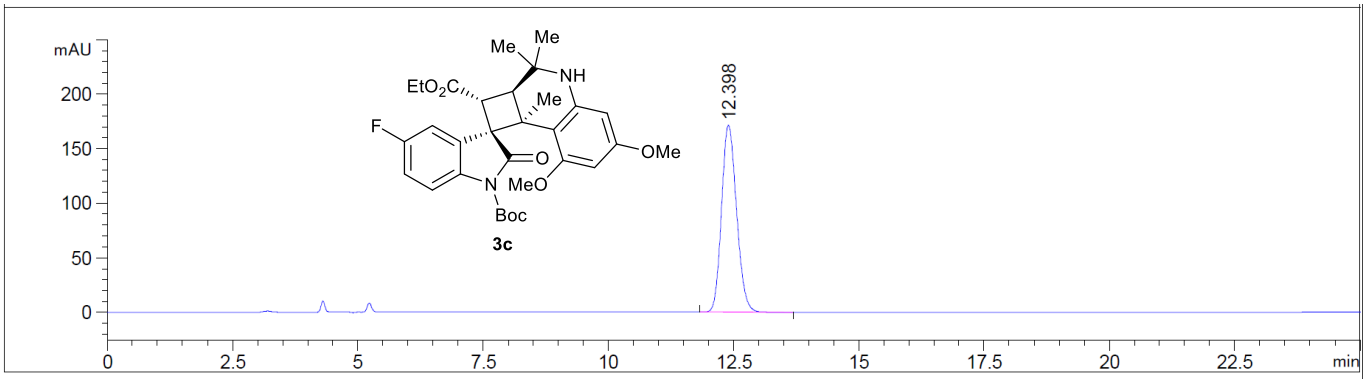
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.717	BB	0.4046	6668.15527	257.11426	92.3514
2	19.823	BB	0.6192	552.26099	13.73085	7.6486



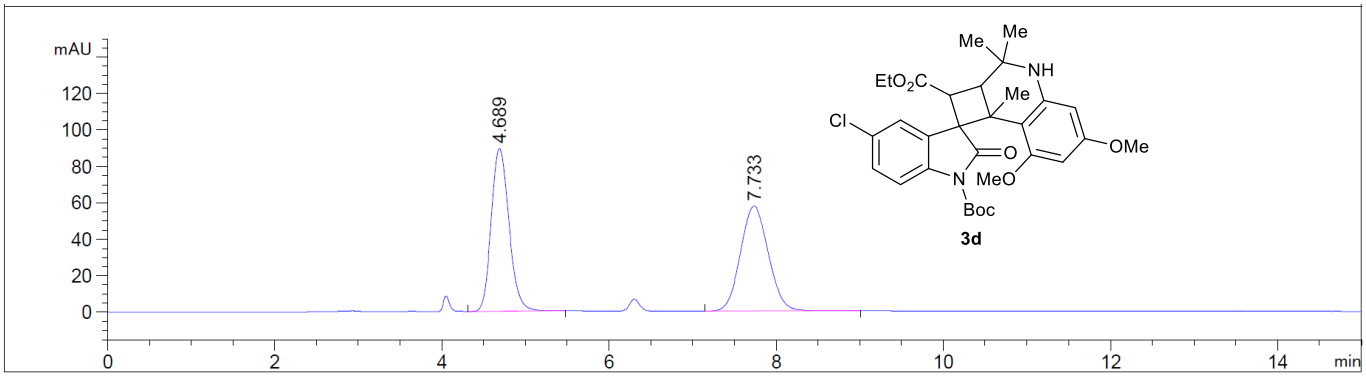
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.420	MM	0.3689	1068.98376	48.29454	48.4359
2	17.538	MM	0.5422	1138.02405	34.98321	51.5641



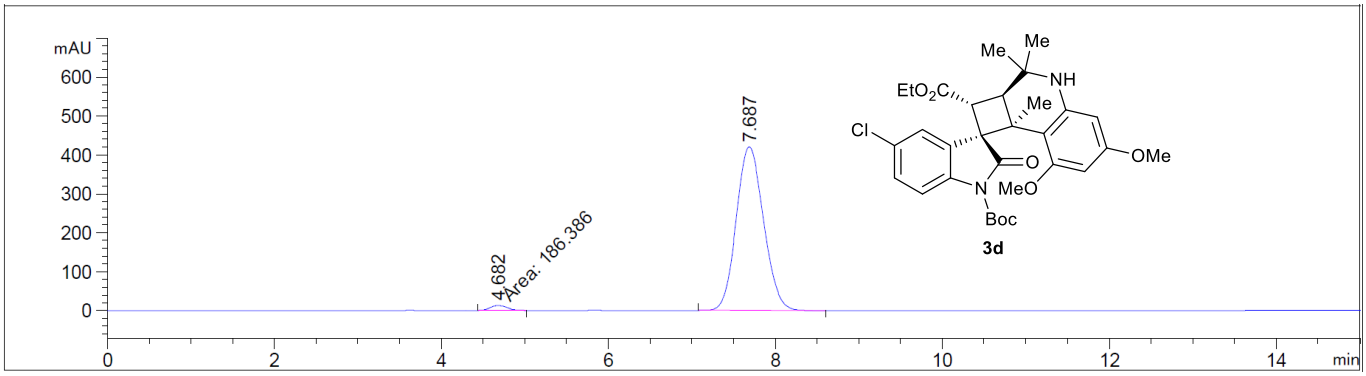
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.398	BB	0.3257	3580.68970	171.43013	100.0000



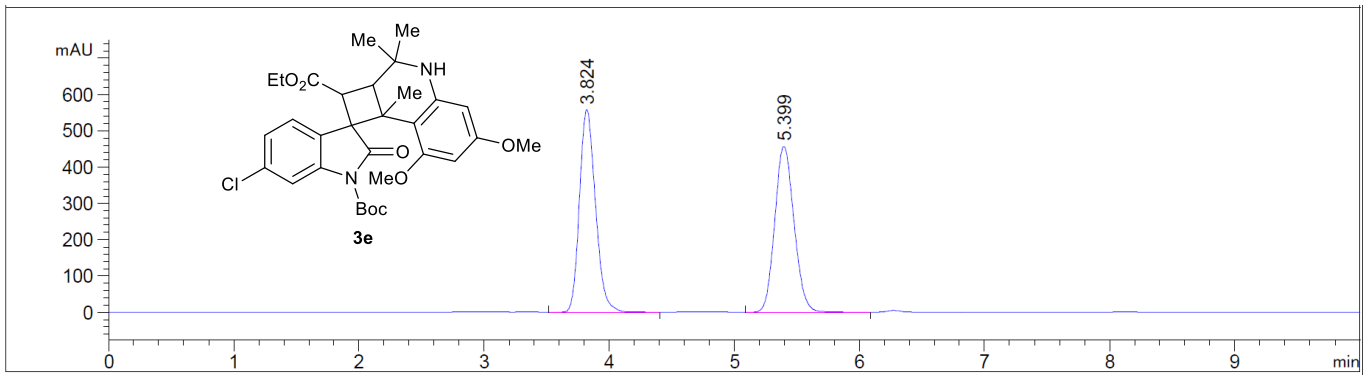
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.689	BB	0.2279	1317.12598	89.40259	49.7229
2	7.733	BB	0.3597	1331.80786	57.60474	50.2771



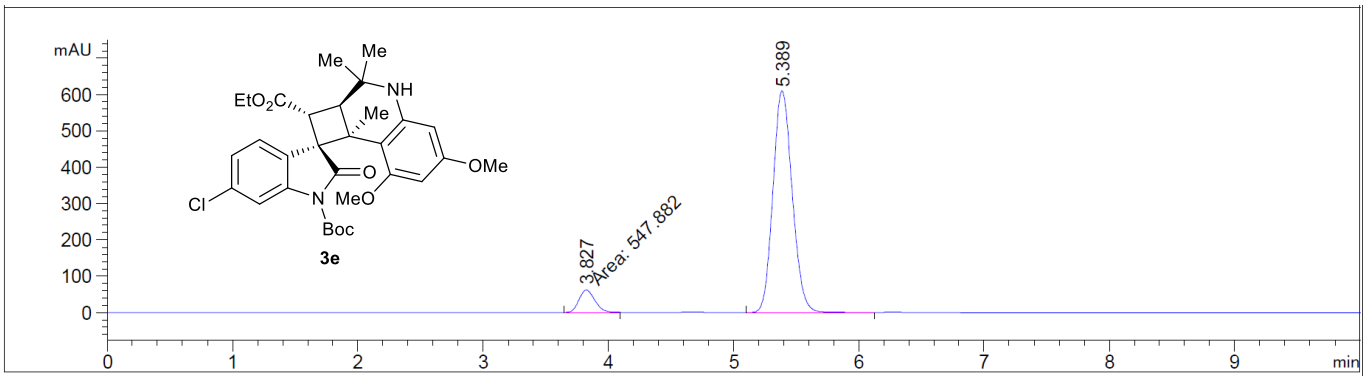
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.682	MM	0.2418	186.38609	12.84492	1.9172
2	7.687	BB	0.3550	9535.25293	419.84015	98.0828



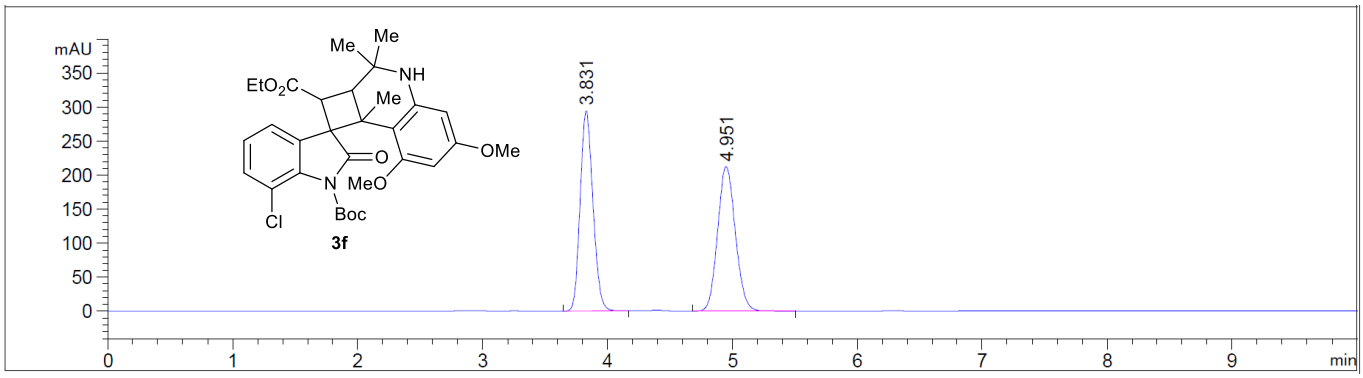
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.824	BB	0.1380	4976.32227	558.11774	50.3920
2	5.399	BB	0.1651	4898.89893	456.90936	49.6080



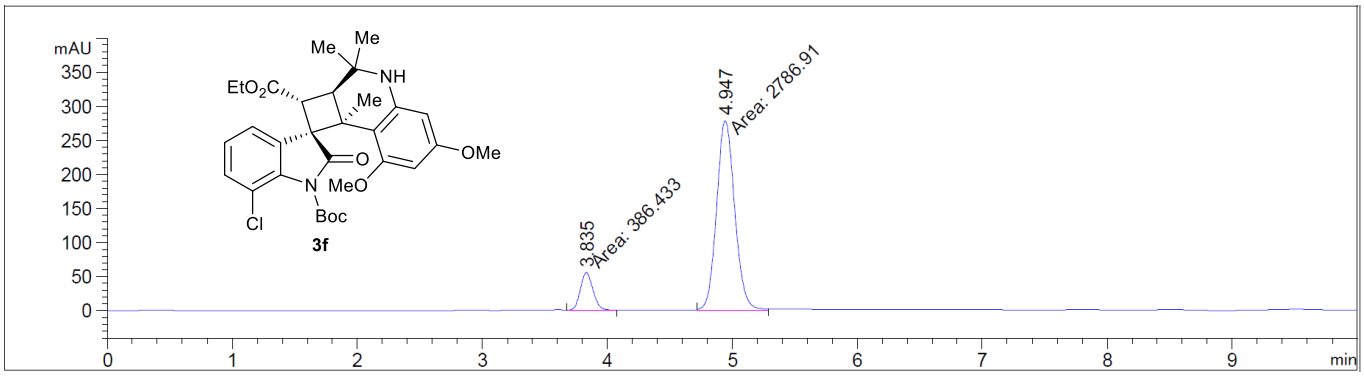
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.827	MM	0.1473	547.88239	61.97501	7.7444
2	5.389	BB	0.1668	6526.63770	610.13306	92.2556



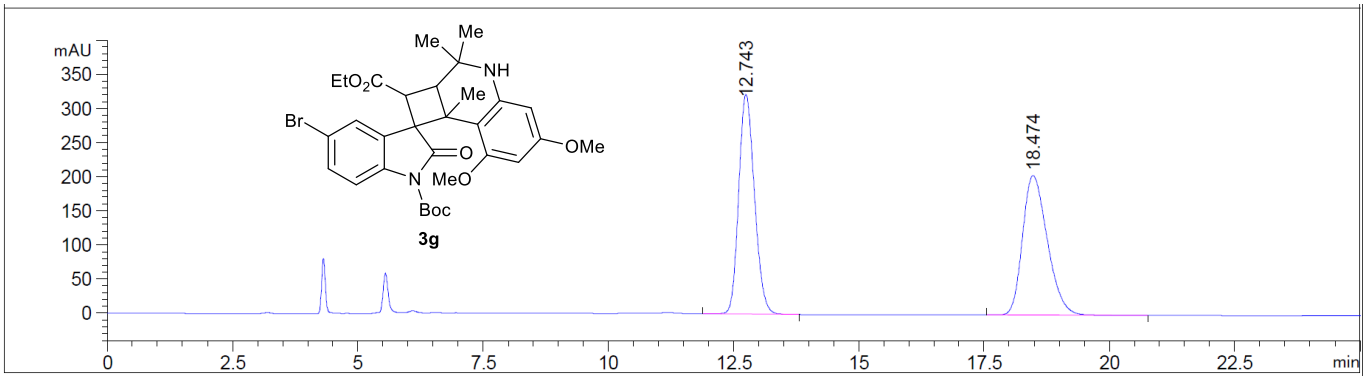
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.831	BB	0.1110	2093.17969	294.37811	49.9362
2	4.951	BB	0.1552	2098.52856	212.47514	50.0638



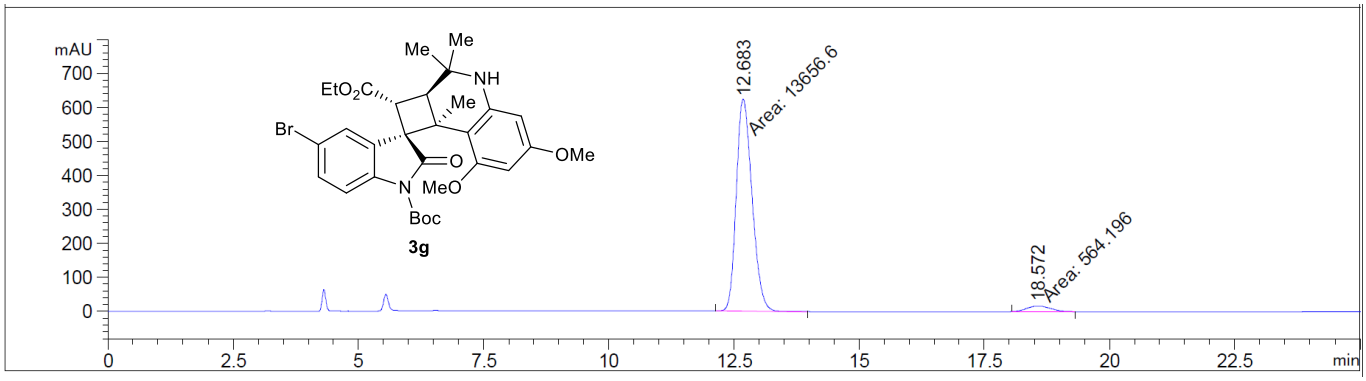
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.835	MM	0.1163	386.43317	55.35588	12.1775
2	4.947	MM	0.1669	2786.90576	278.32953	87.8225



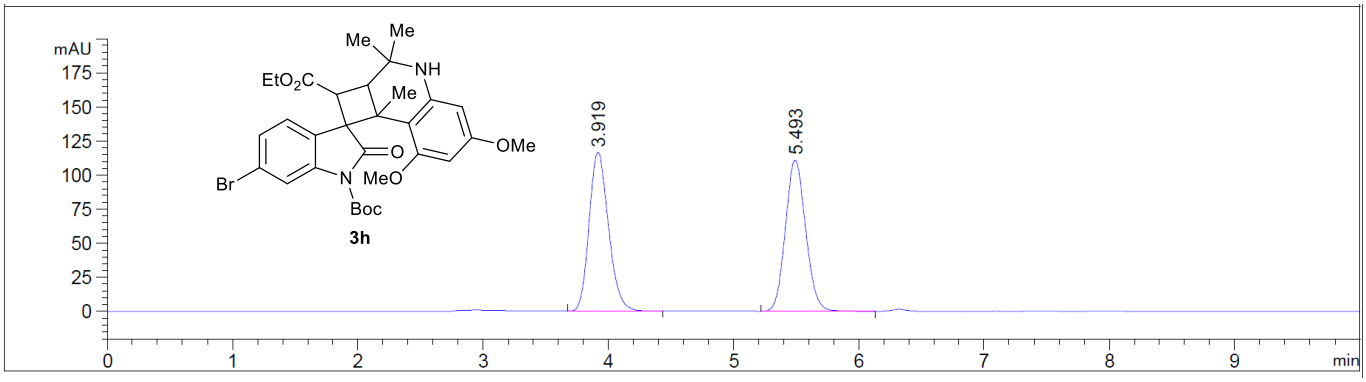
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.743	BB	0.3393	7043.16748	321.90463	49.9554
2	18.474	BBA	0.5339	7055.74121	204.82663	50.0446



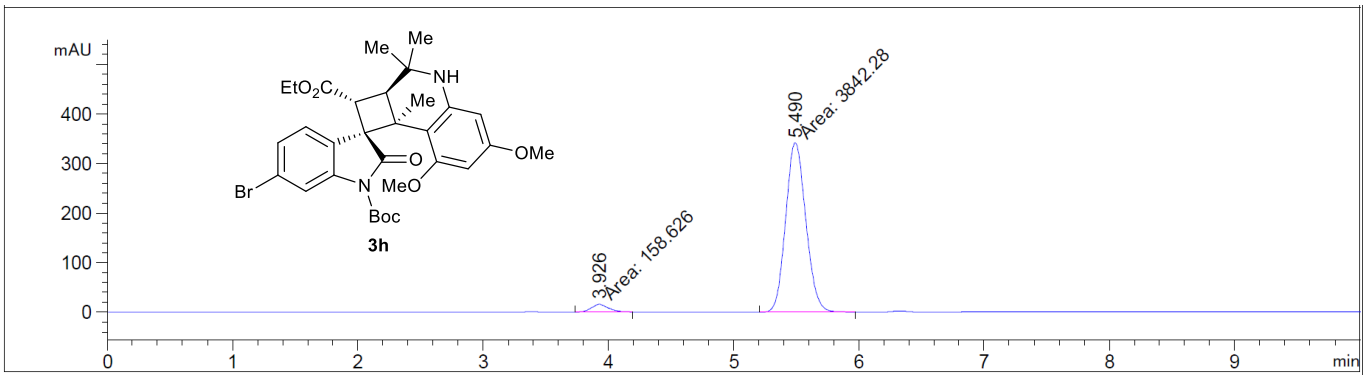
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.683	MM	0.3645	1.36566e4	624.49585	96.0326
2	18.572	MM	0.5541	564.19611	16.97123	3.9674



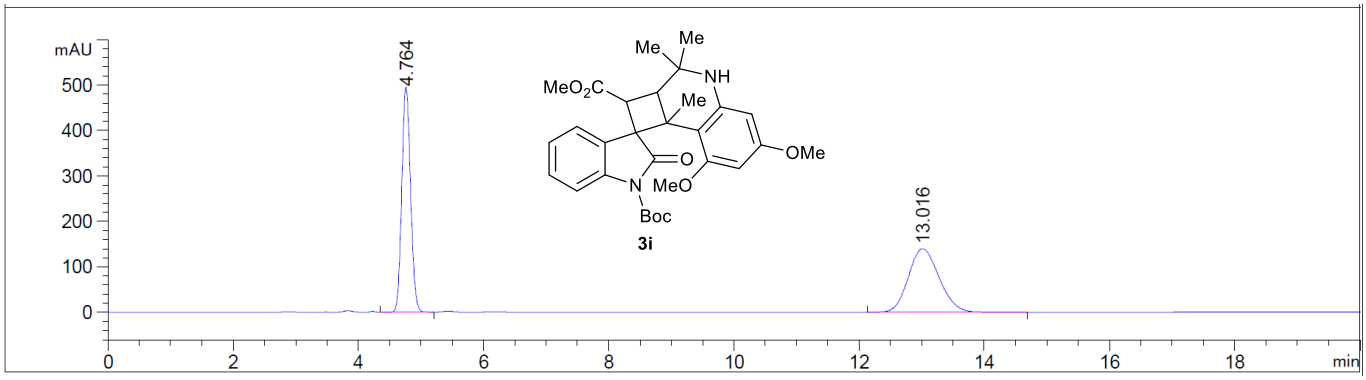
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.919	BB	0.1652	1251.54871	116.60801	50.1065
2	5.493	BB	0.1751	1246.22864	110.87313	49.8935



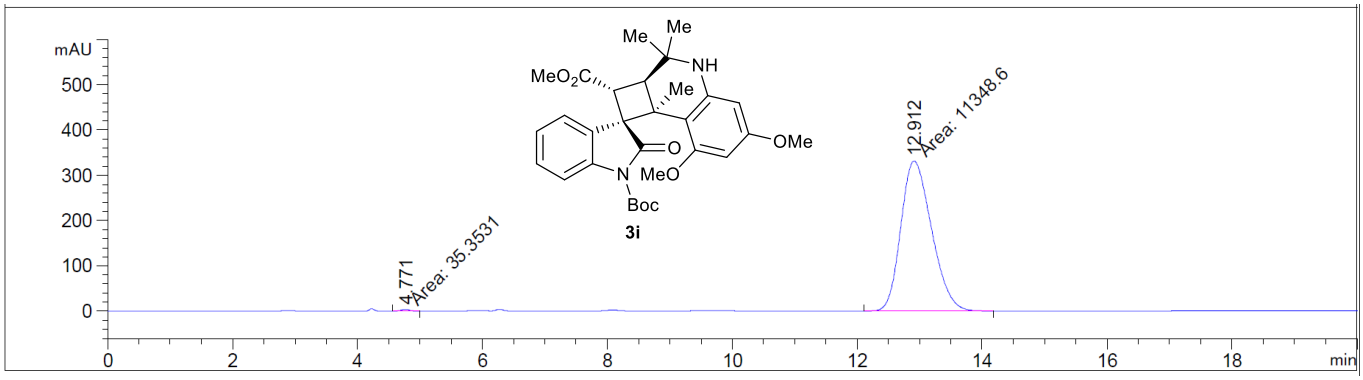
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.926	MM	0.1665	158.62590	15.87540	3.9648
2	5.490	MM	0.1870	3842.27783	342.35974	96.0352



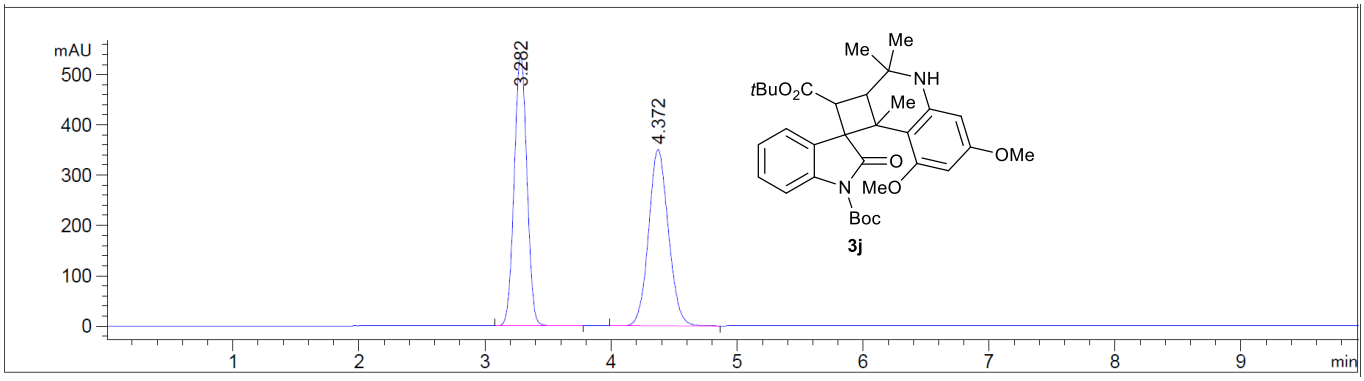
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.764	BB	0.1518	4827.64844	495.06659	50.2961
2	13.016	BB	0.5323	4770.81348	139.73715	49.7039



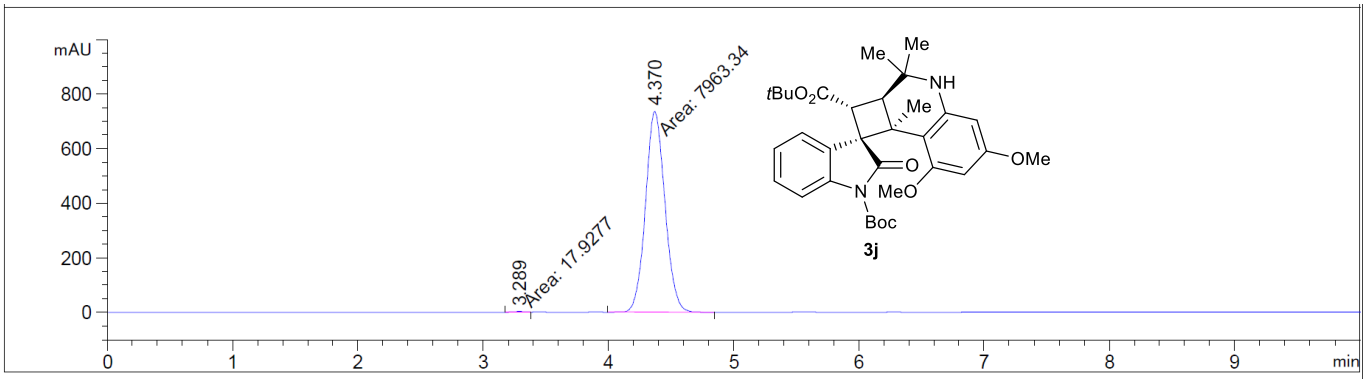
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.771	MM	0.1565	35.35314	3.76433	0.3106
2	12.912	MM	0.5709	1.13486e4	331.30826	99.6894



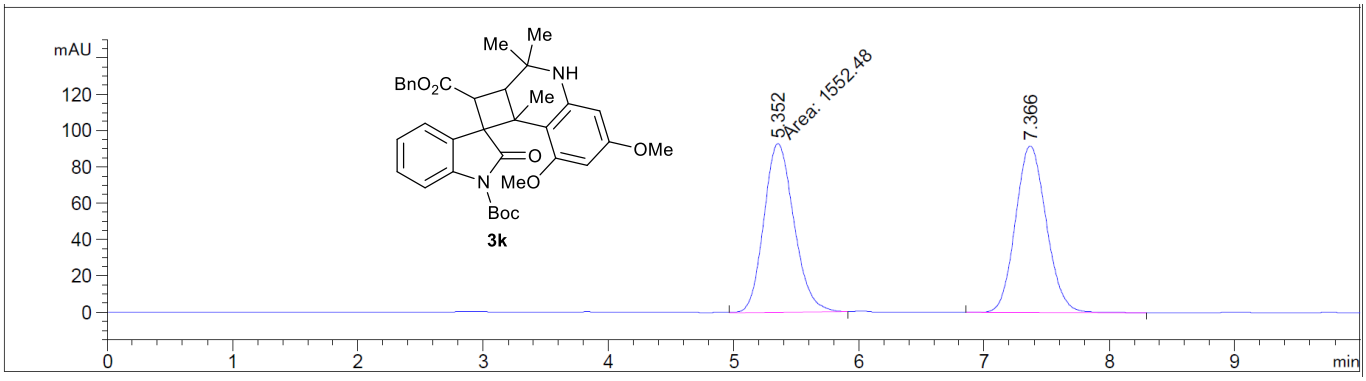
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.282	BB	0.1117	3794.10254	541.60059	49.7203
2	4.372	BB	0.1676	3836.78857	350.66995	50.2797



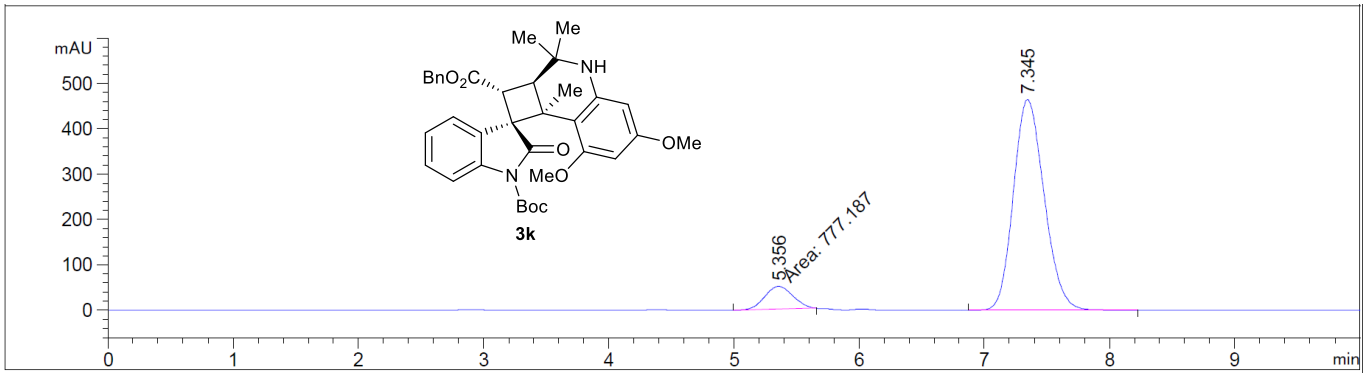
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.289	MM	0.1067	17.92773	2.80023	0.2246
2	4.370	MM	0.1799	7963.33643	737.65466	99.7754



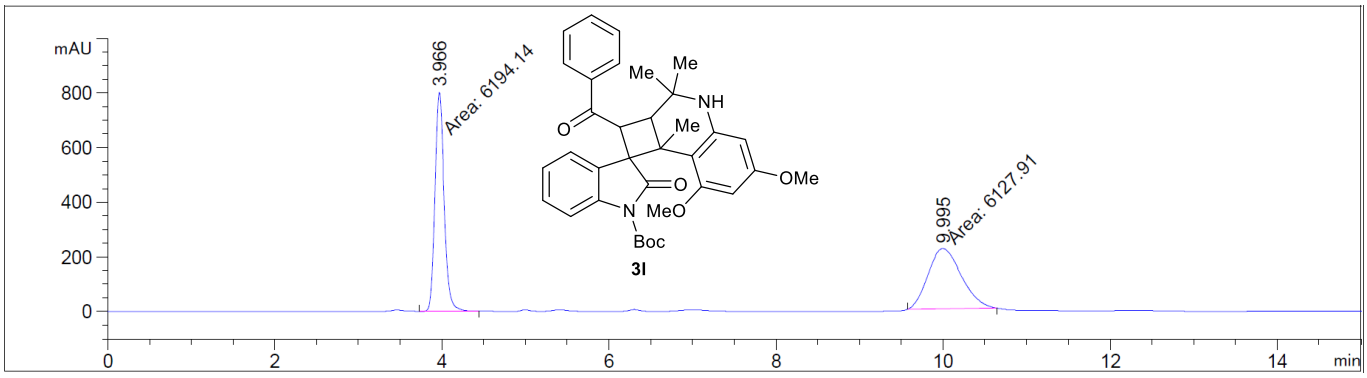
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.352	MM	0.2783	1552.47925	92.98612	49.7712
2	7.366	BB	0.2652	1566.75049	91.76111	50.2288



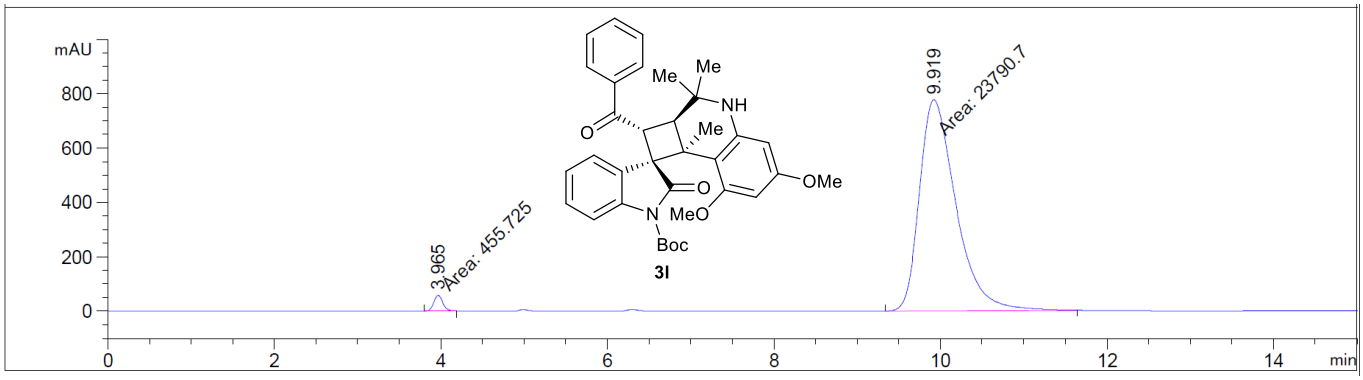
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.356	MM	0.2586	777.18719	50.08448	8.9344
2	7.345	BB	0.2652	7921.64453	464.00839	91.0656



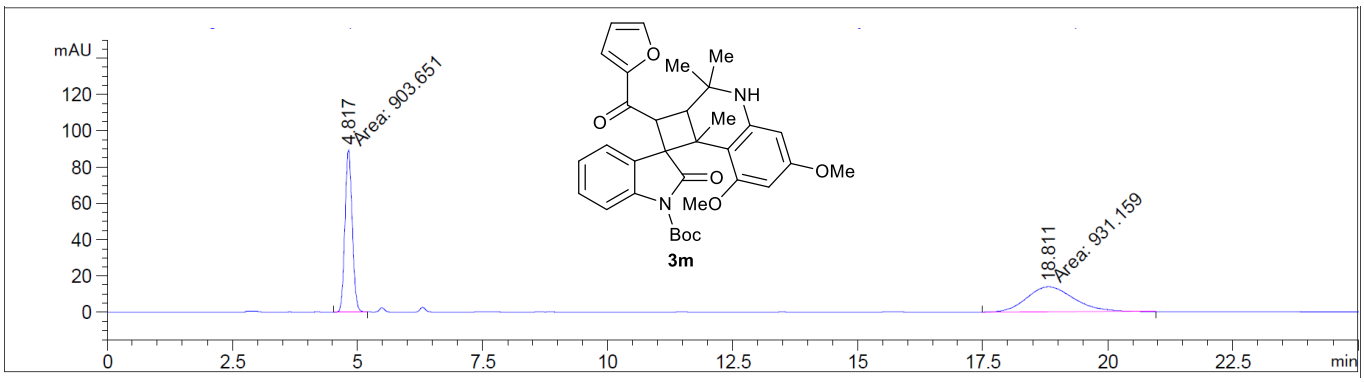
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.966	MM	0.1286	6194.13770	802.94312	50.2688
2	9.995	MM	0.4620	6127.90576	221.05638	49.7312



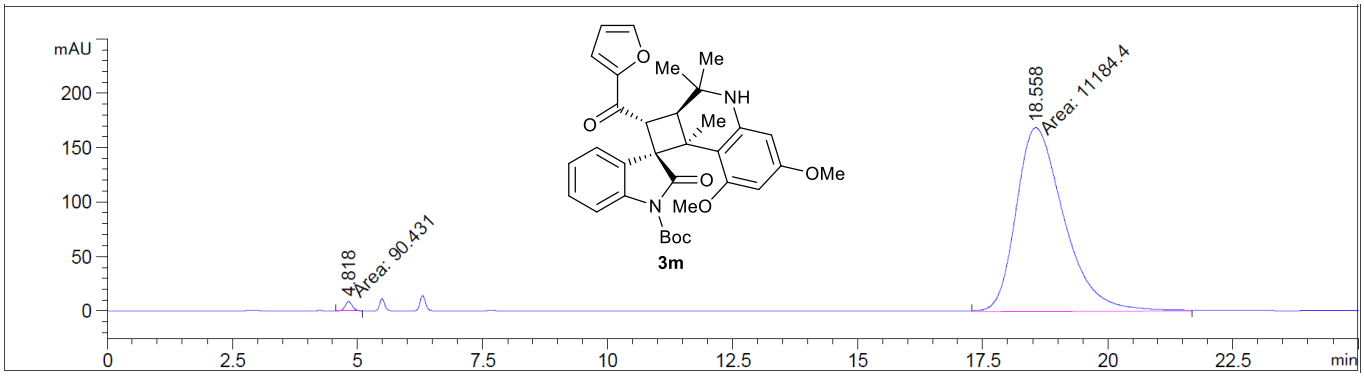
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.965	MM	0.1297	455.72458	58.57633	1.8796
2	9.919	MM	0.5091	2.37907e4	778.84979	98.1204



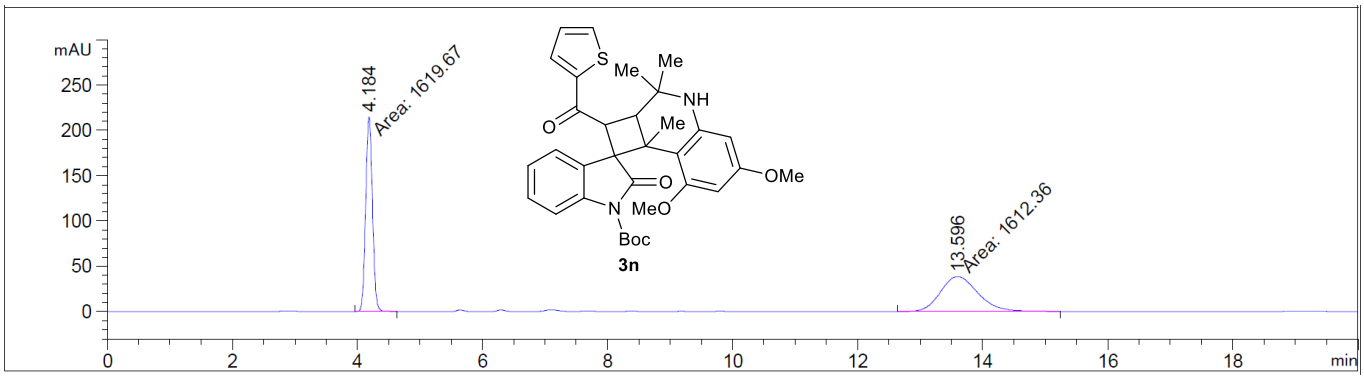
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.817	MM	0.1685	903.65125	89.38818	49.2504
2	18.811	MM	1.1118	931.15887	13.95850	50.7496



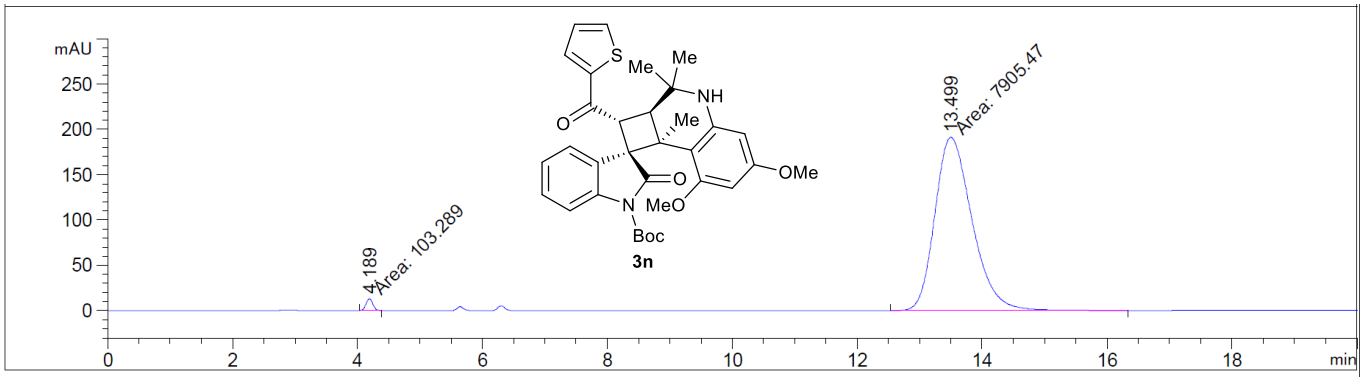
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.818	MM	0.1718	90.43102	8.77059	0.8021
2	18.558	MM	1.1060	1.11844e4	168.54739	99.1979



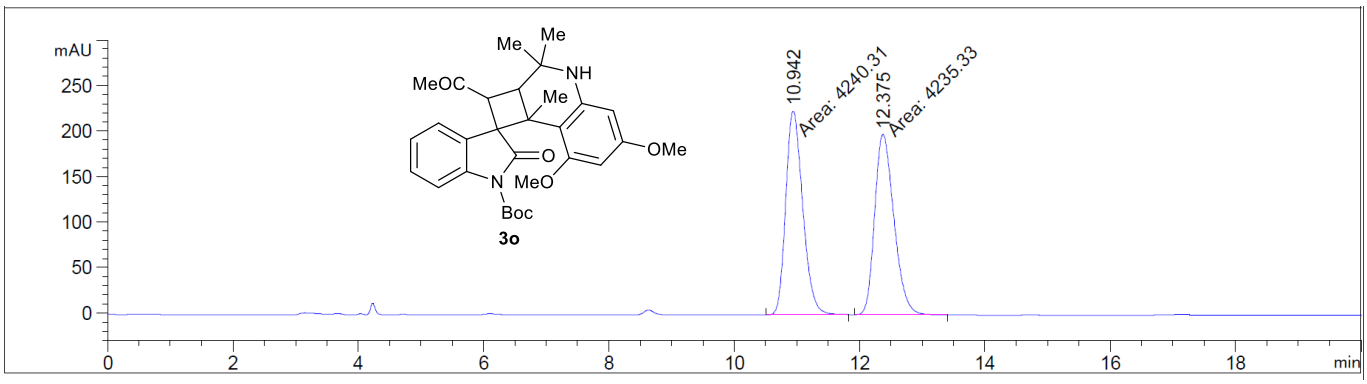
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.184	MM	0.1258	1619.66650	214.64124	50.1130
2	13.596	MM	0.6974	1612.36414	38.53364	49.8870



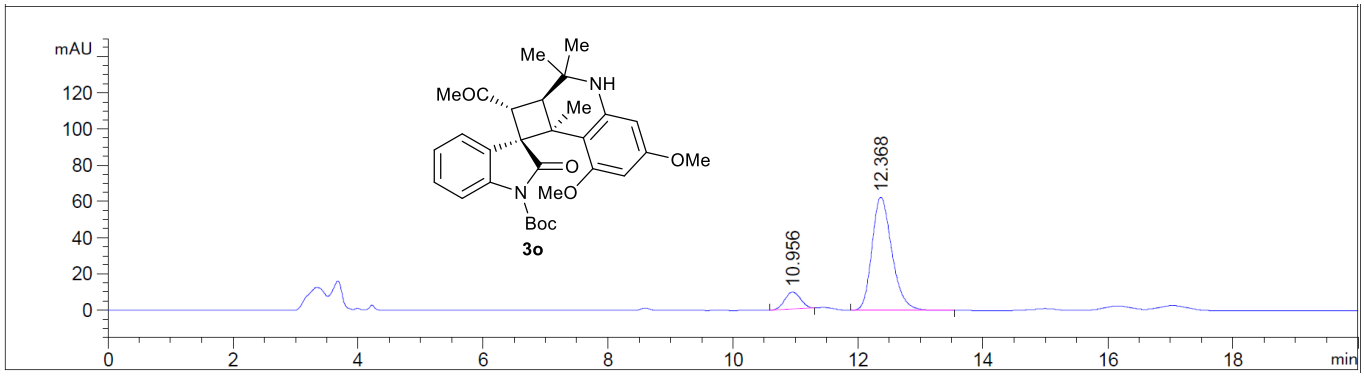
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.189	MM	0.1302	103.28886	13.21878	1.2897
2	13.499	MM	0.6893	7905.46582	191.15170	98.7103



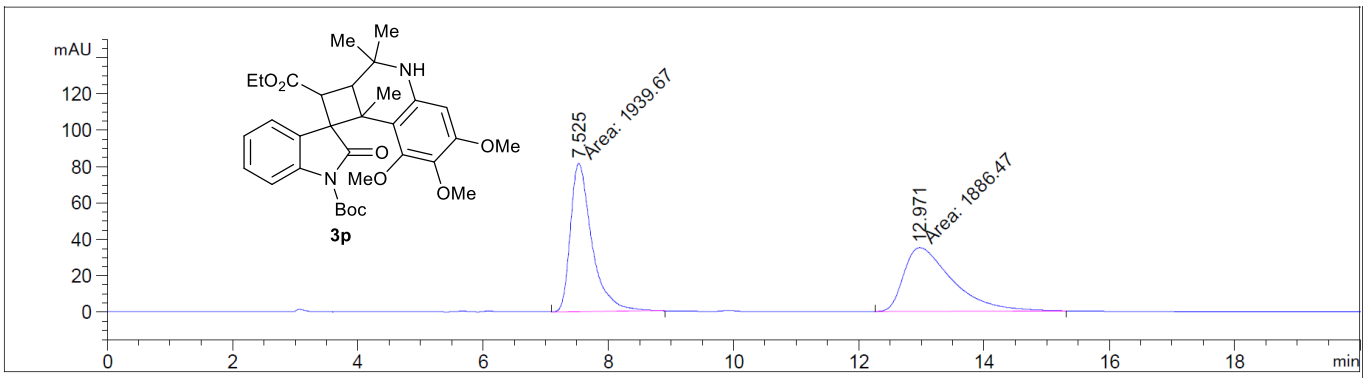
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.942	MM	0.3154	4240.30908	224.07547	50.0293
2	12.375	MM	0.3562	4235.33447	198.15526	49.9707



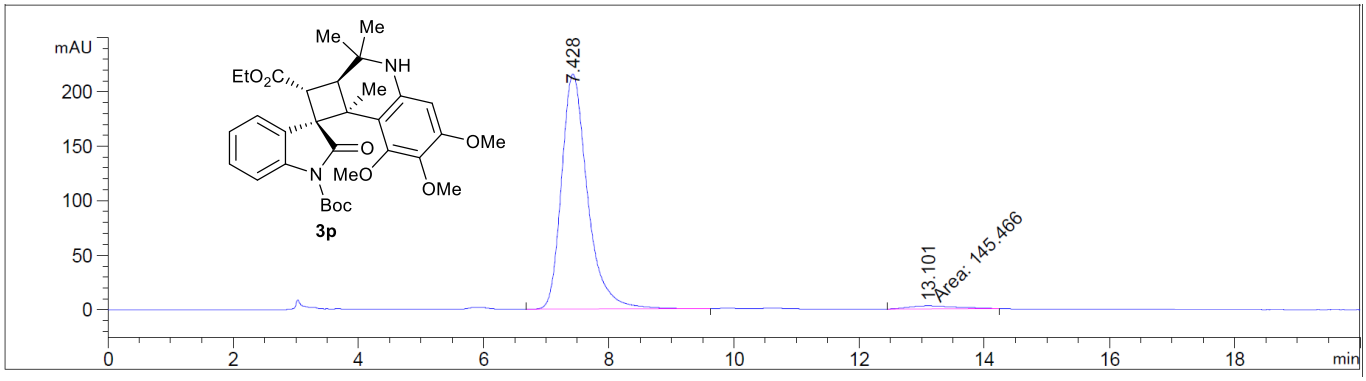
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.956	BB	0.2761	165.82074	9.47789	10.7048
2	12.368	BB	0.3403	1383.20667	62.47532	89.2952



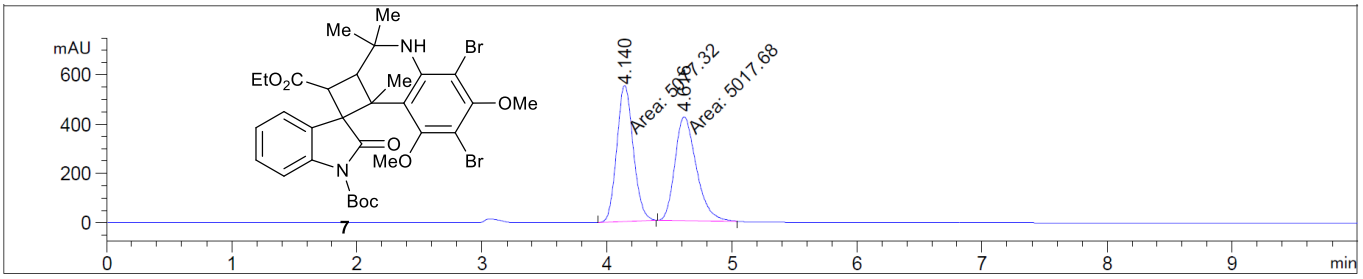
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.525	MM	0.3967	1939.66589	81.49080	50.6952
2	12.971	MM	0.8964	1886.46863	35.07522	49.3048



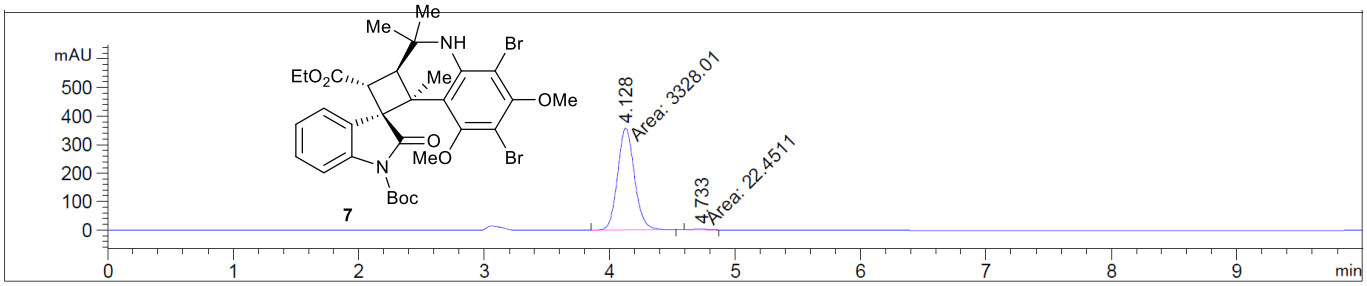
Signal 2: DAD1 B, Sig=254,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.428	BB	0.4369	6231.76465	215.78960	97.7190
2	13.101	MM	0.9081	145.46585	2.66986	2.2810



Signal 2: DAD1 B, Sig=254,4 Ref=off

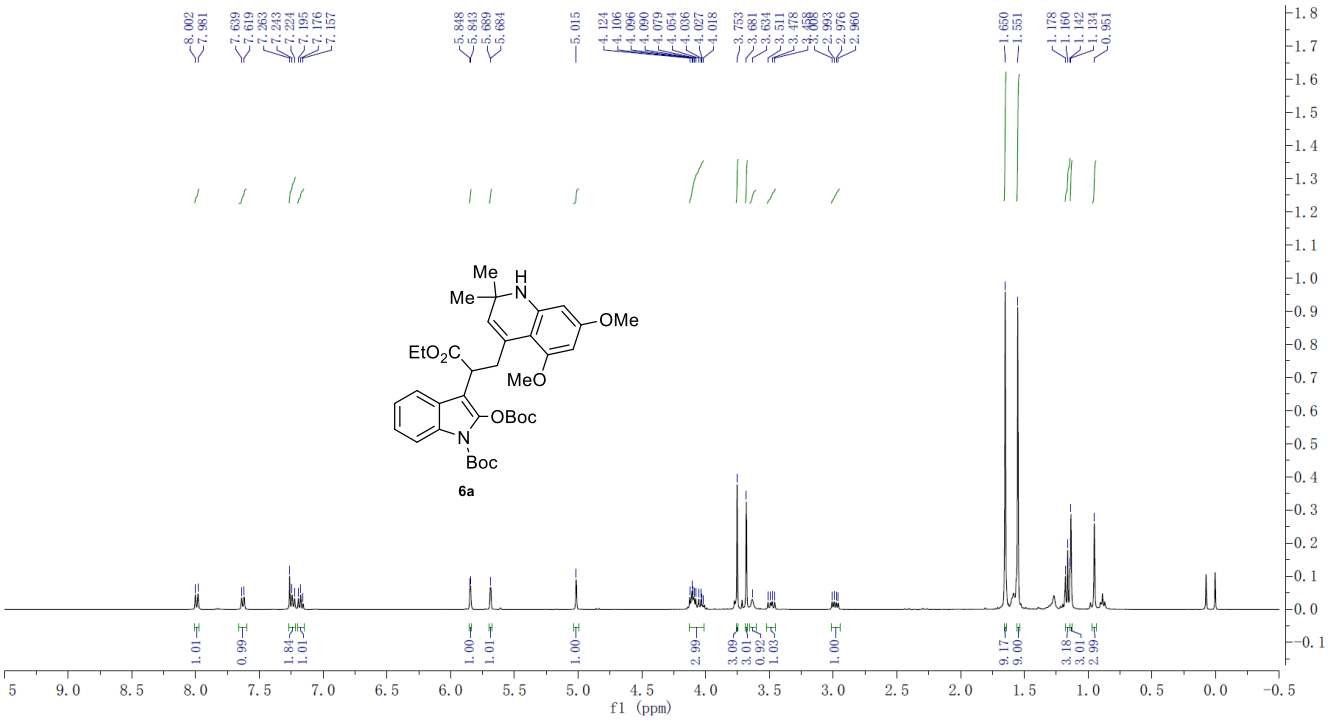
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.140	MM	0.1528	5077.31738	553.67682	50.2954
2	4.616	MM	0.1982	5017.67969	421.85556	49.7046

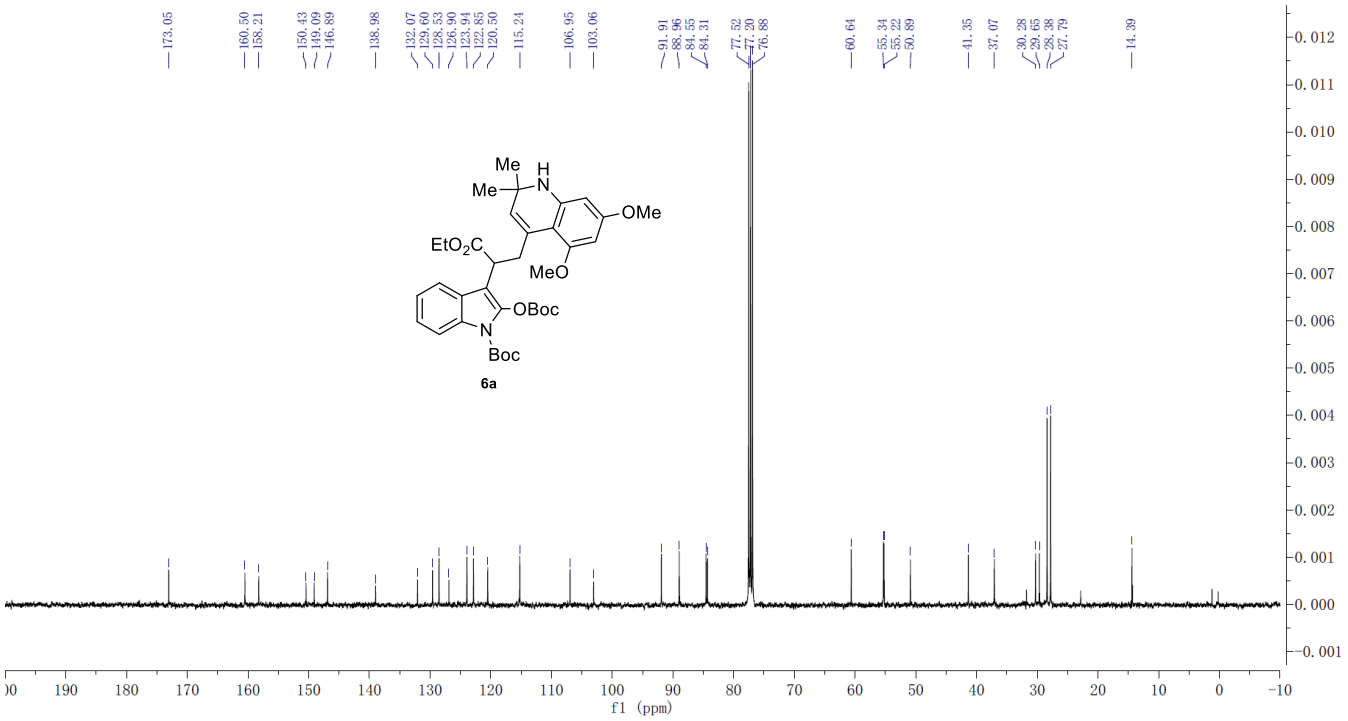


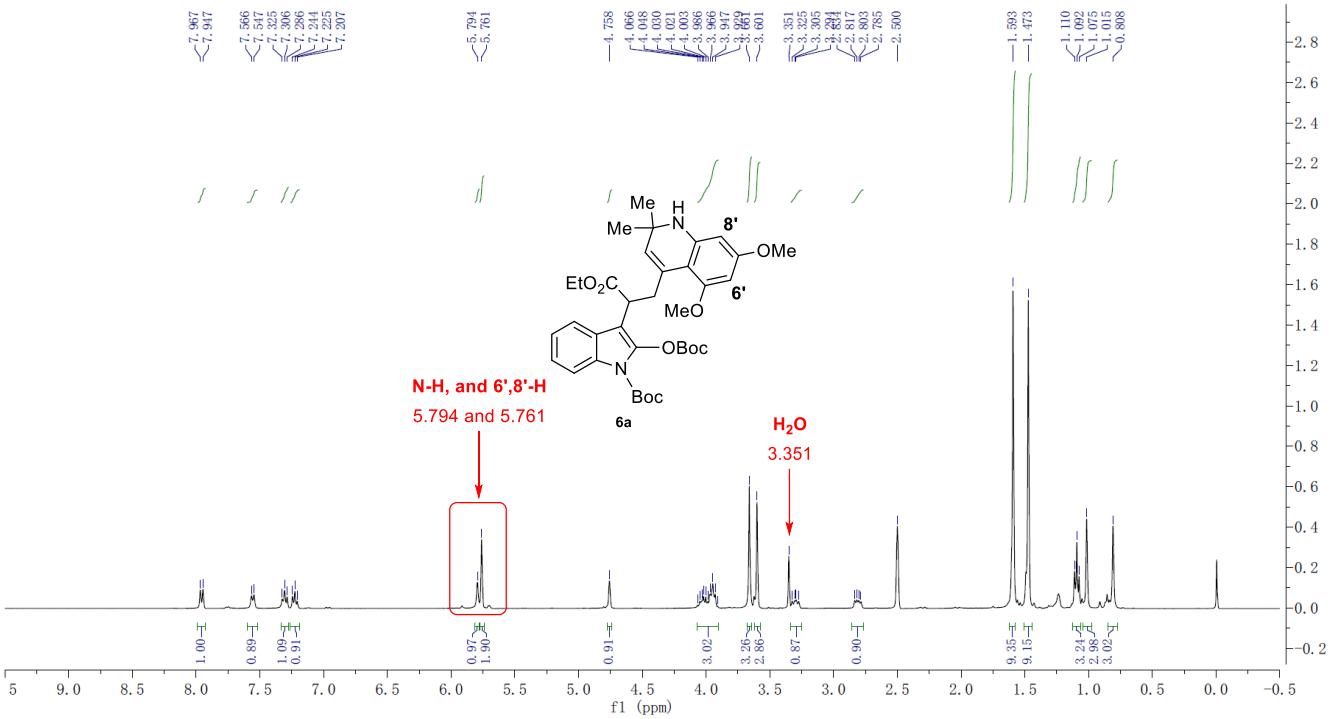
Signal 2: DAD1 B, Sig=254,4 Ref=off

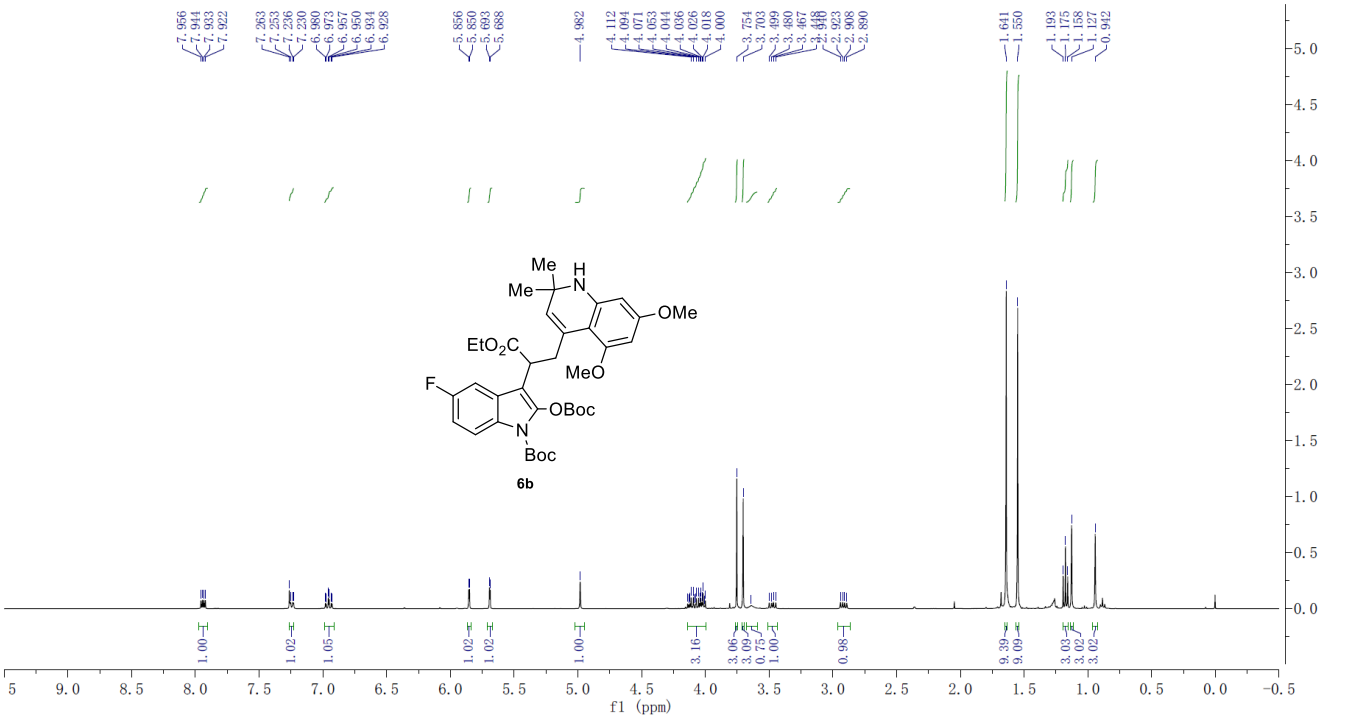
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.128	MM	0.1552	3328.01270	357.47141	99.3299
2	4.733	MM	0.1641	22.45109	2.28001	0.6701

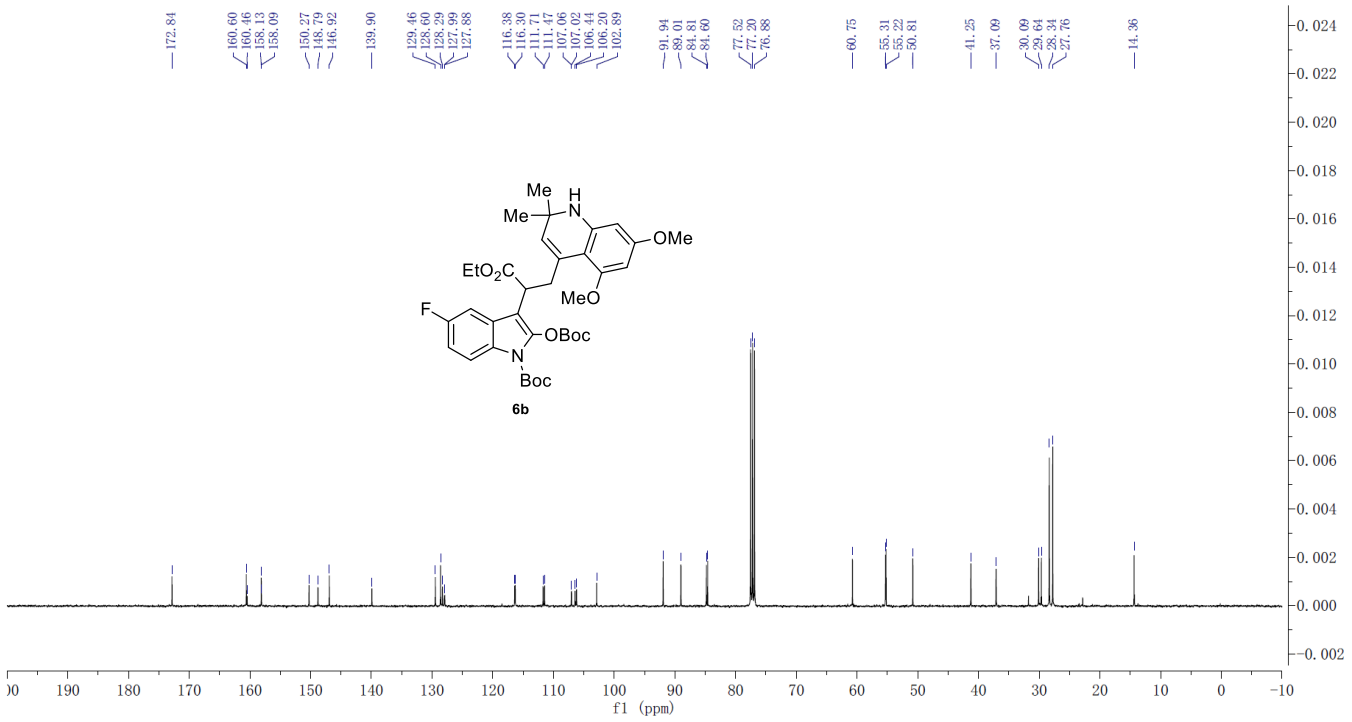
12. NMR Spectra of ene Reaction Products

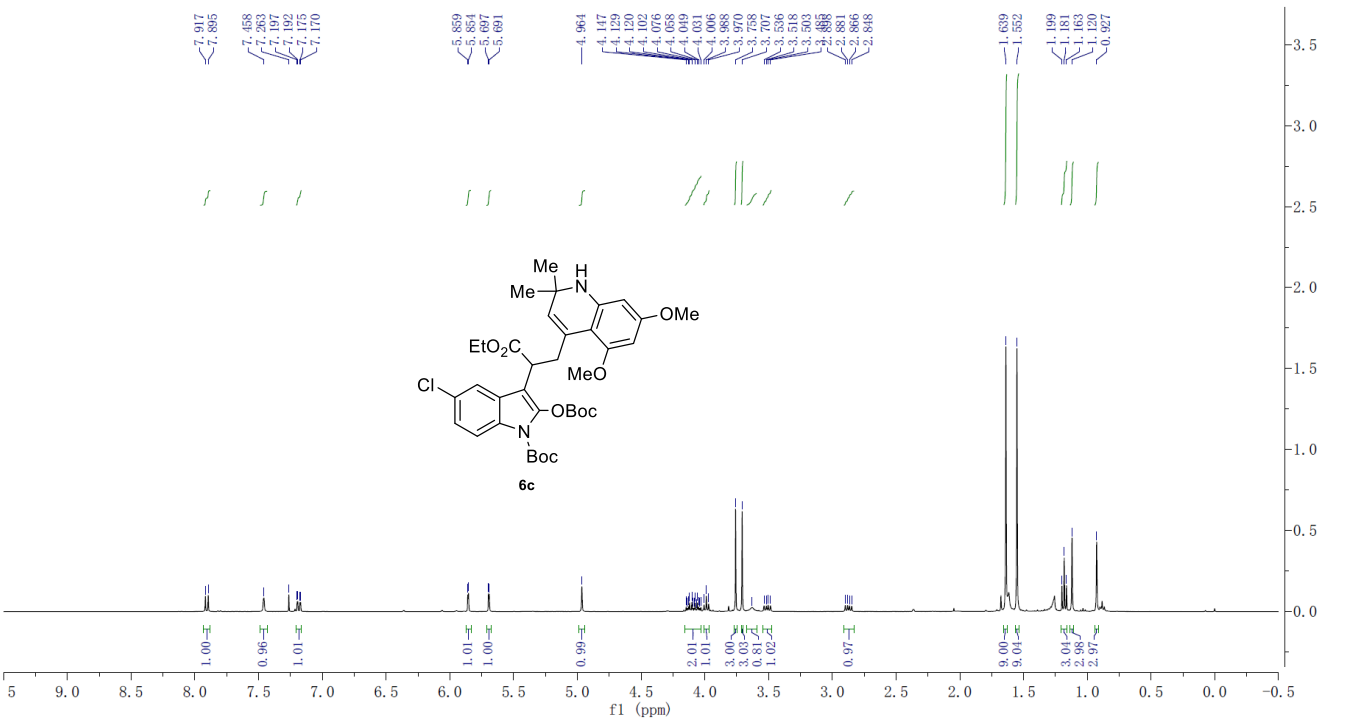


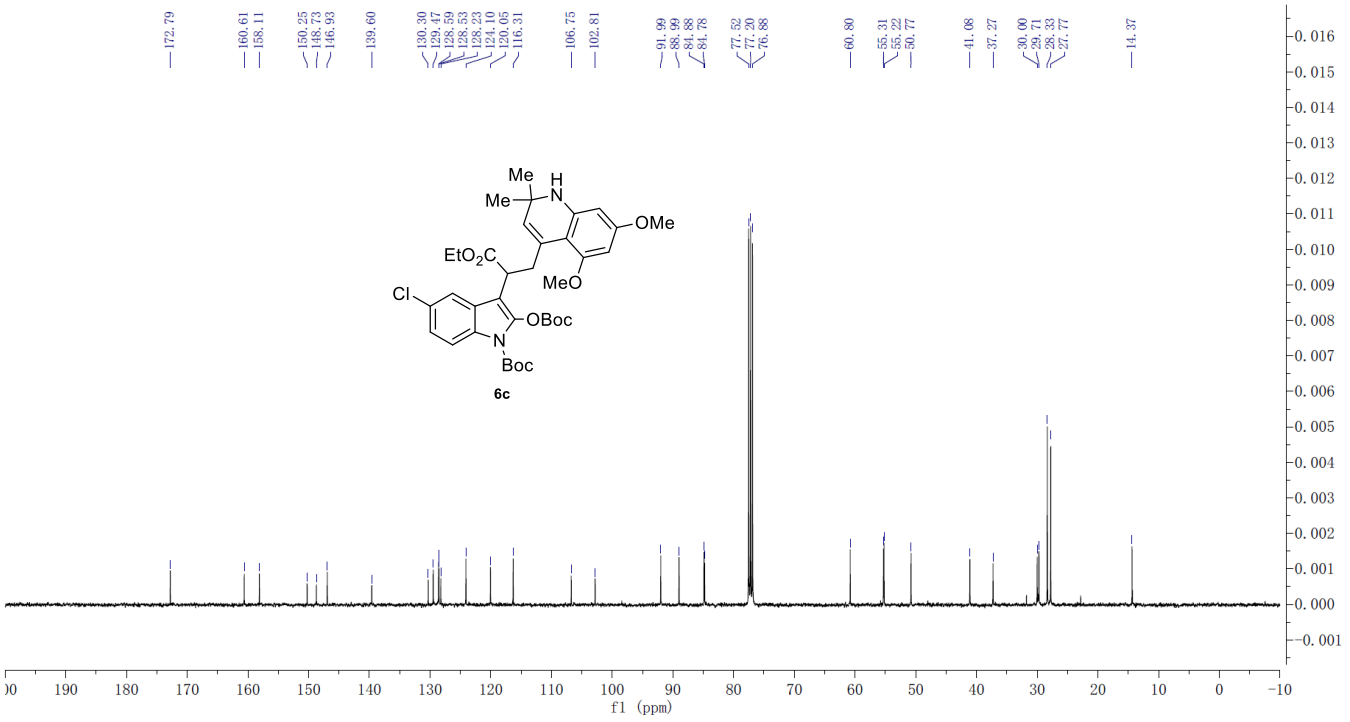


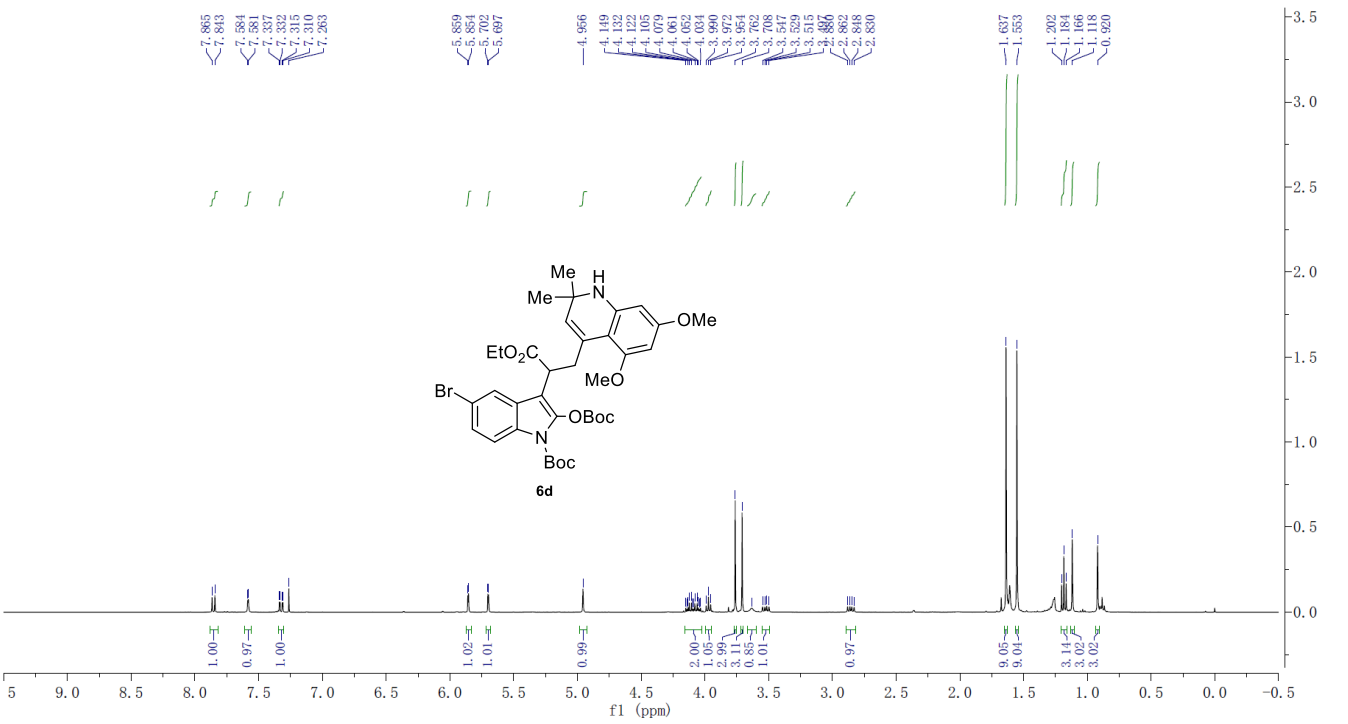

N-H, and 6',8'-H
5.794 and 5.761
H2O
3.351
6a
f1 (ppm)

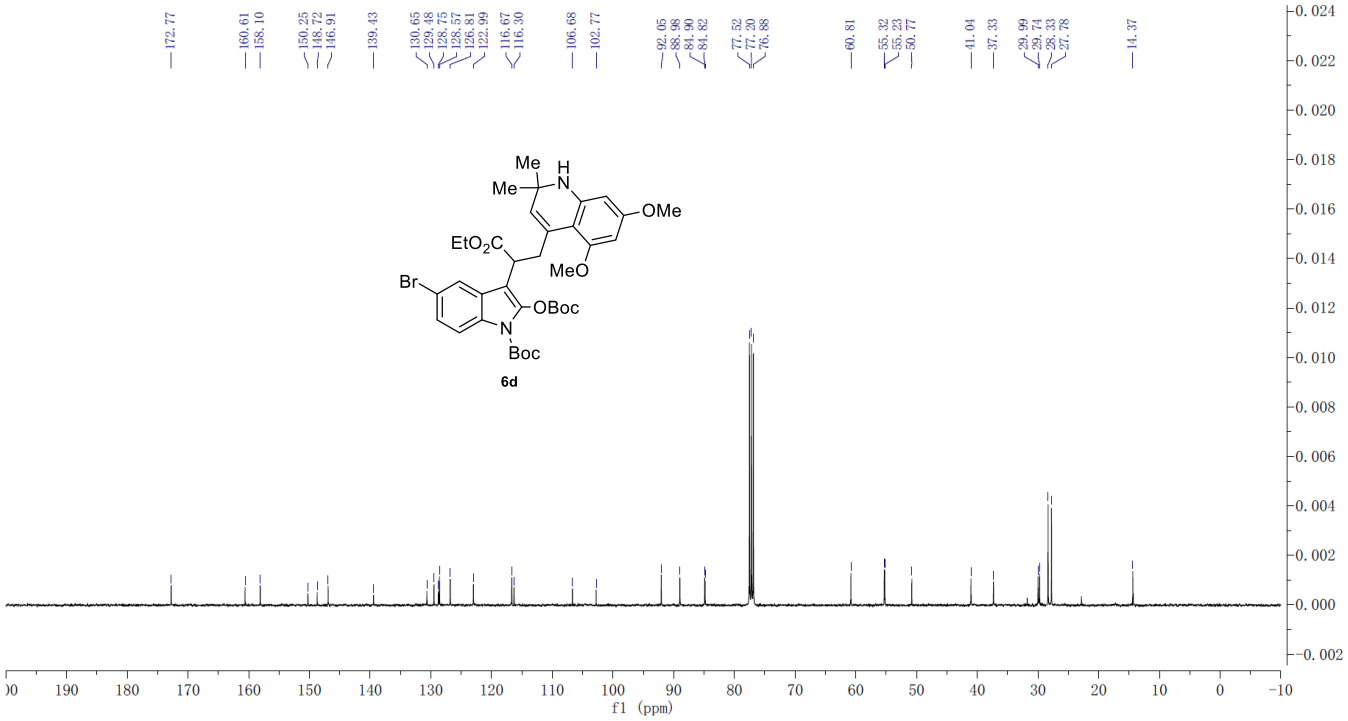

7.956
7.944
7.933
7.922
7.263
7.253
7.236
7.230
6.980
6.973
6.957
6.950
6.934
6.928
5.856
5.850
5.693
5.688
4.962
4.112
4.094
4.071
4.053
4.044
4.036
4.026
4.018
4.000
3.754
3.703
3.499
3.480
3.467
2.923
2.908
2.890
1.641
1.550
1.193
1.175
1.158
1.127
0.942
Me
H
N
Me
OMe
EtO2C
MeO
F
OBoc
N
Boc
6b
1.00
1.02
1.05
1.02
1.02
1.00
3.16
3.06
3.09
0.75
1.00
0.98
9.39
9.09
3.03
3.02
3.02
f1 (ppm)

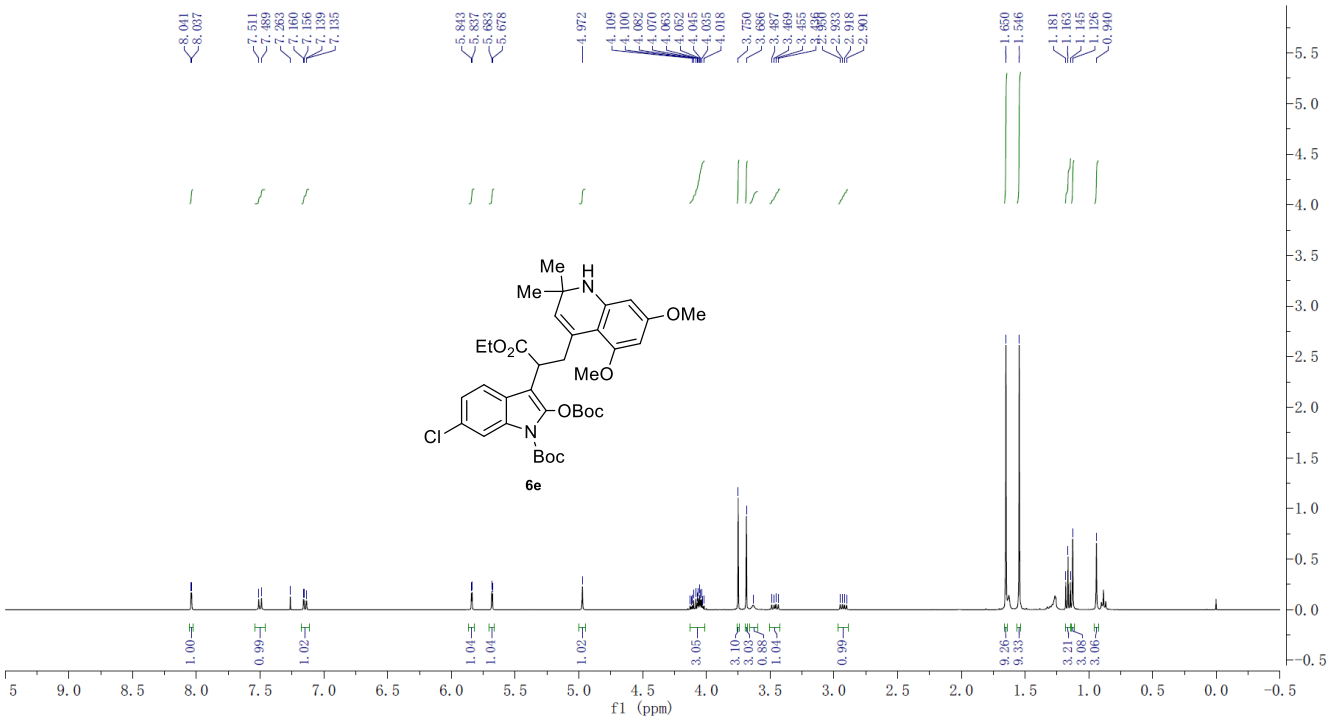

172.84
160.60
160.46
158.13
158.09
150.27
148.79
146.92
139.90
129.46
128.60
128.29
127.99
127.88
116.38
116.20
111.71
111.47
107.06
107.02
106.44
106.20
102.89
91.94
89.01
84.81
84.60
77.52
77.20
76.88
60.75
55.31
55.22
50.81
41.25
37.09
30.09
29.64
28.34
27.76
14.36
Me
H
N
Me
OMe
EtO2C
MeO
F
OBoc
N
Boc
6b
f1 (ppm)


7.917
7.895
7.458
7.263
7.197
7.192
7.175
7.170
5.859
5.854
5.697
5.691
4.964
4.147
4.129
4.120
4.102
4.076
4.058
4.049
4.031
4.006
3.988
3.970
3.758
3.707
3.536
3.518
3.503
2.881
2.866
2.848
1.639
1.552
1.199
1.181
1.163
1.129
0.927
Me
H
N
Me
OMe
EtO2C
MeO
Cl
OBoc
N
Boc
6c
1.00
0.96
1.01
1.01
1.00
0.99
2.01
1.01
3.00
3.03
0.81
1.02
0.97
9.00
9.04
3.04
2.98
2.97
f1 (ppm)


172.79
160.61
158.11
150.25
148.73
146.93
139.60
130.30
129.47
128.59
128.53
128.23
124.10
120.05
116.31
106.75
102.81
91.99
88.99
84.88
84.78
77.52
77.20
76.88
60.80
55.31
55.22
50.77
41.08
37.27
30.00
29.71
28.33
27.77
14.37
Me
H
N
Me
OMe
EtO2C
MeO
Cl
OBoc
N
Boc
6c
f1 (ppm)


7.865
7.843
7.684
7.681
7.337
7.332
7.315
7.310
7.263
5.859
5.854
5.702
5.697
4.966
4.149
4.132
4.122
4.105
4.079
4.061
4.052
4.034
3.990
3.972
3.964
3.762
3.708
3.547
3.529
3.515
2.862
2.848
2.830
1.637
1.553
1.202
1.184
1.166
1.118
0.920
Me
Me
H
N
OMe
EtO2C
MeO
Br
OBoc
N
Boc
6d
1.00
0.97
1.00
1.02
1.01
0.99
2.00
1.05
2.99
3.11
0.85
1.01
0.97
9.05
9.04
3.14
3.02
3.02
f1 (ppm)


172.77
160.61
158.10
150.25
148.72
146.91
139.43
130.65
129.48
128.75
128.57
126.81
122.99
116.67
116.30
106.68
102.77
92.05
86.98
84.90
84.82
77.52
77.20
76.88
60.81
55.32
55.23
50.77
41.04
37.33
29.99
29.74
28.33
27.78
14.37
Me
Me
H
N
OMe
EtO2C
MeO
Br
OBoc
N
Boc
6d
f1 (ppm)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4.109
4.100
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4.070
4.063
4.052
4.045
4.035
4.018
3.750
3.686
3.487
3.469
3.455
2.933
2.918
2.901
1.650
1.546
1.181
1.163
1.145
1.126
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Me
Me
H
N
OMe
EtO2C
MeO
OBoc
Cl
N
Boc
6e
1.00
0.99
1.02
1.04
1.04
1.02
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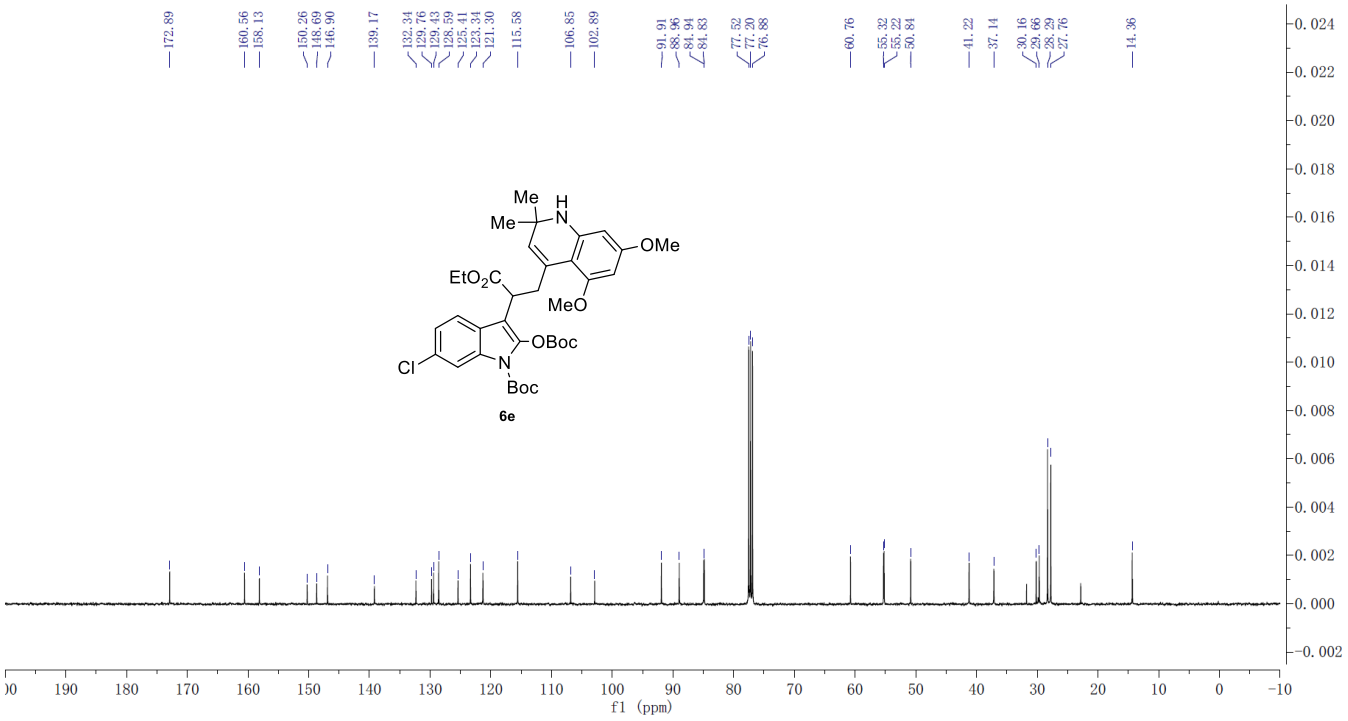
f1 (ppm)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123.34
121.30
115.58
106.85
102.89
91.91
88.96
84.94
84.83
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77.20
76.88
60.76
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55.22
50.84
41.22
37.14
30.16
29.66
28.29
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Me
H
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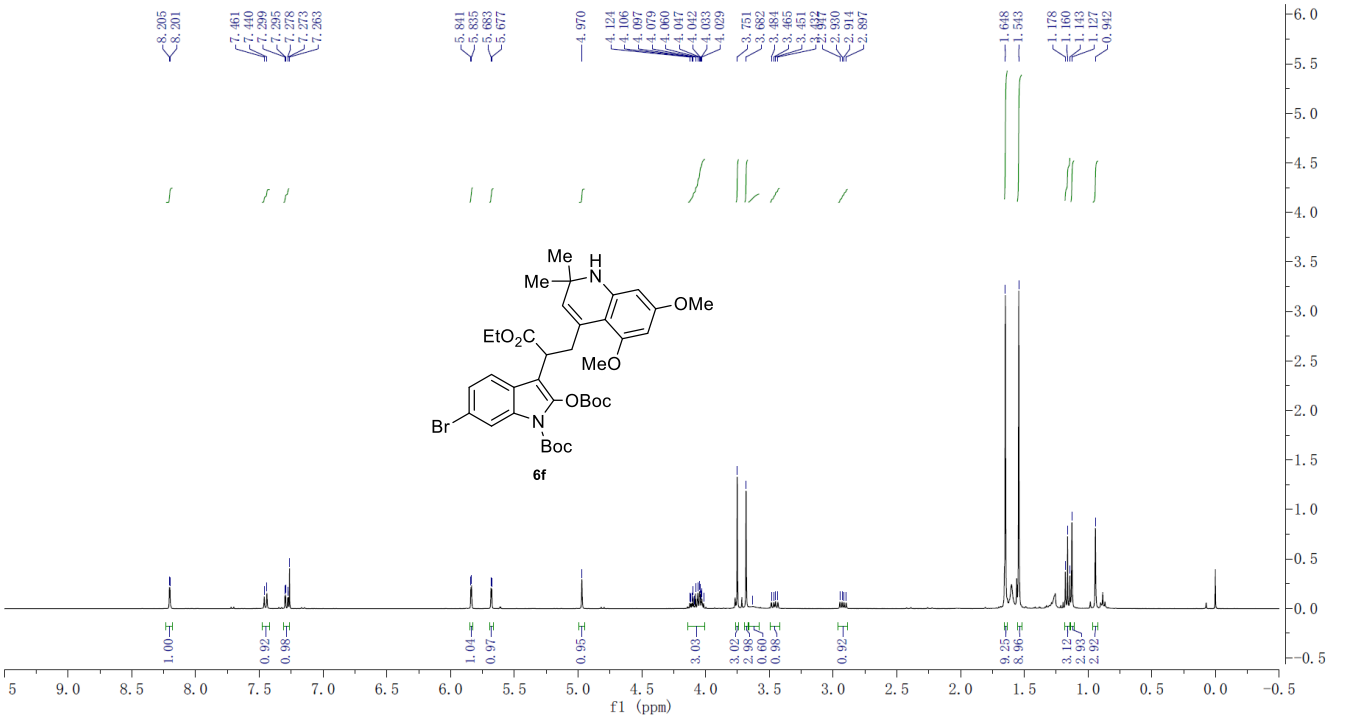
OMe
EtO2C
MeO
OBoc
Cl
N
Boc
6e
f1 (ppm)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4.124
4.106
4.097
4.079
4.060
4.047
4.042
4.033
4.029
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3.484
3.465
3.451
2.930
2.914
2.897
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1.543
1.178
1.160
1.143
1.127
0.942
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Me
H
N
OMe
EtO2C
MeO
OBoc
Br
N
Boc
6f
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0.92
0.98
1.04
0.97
0.95
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3.12
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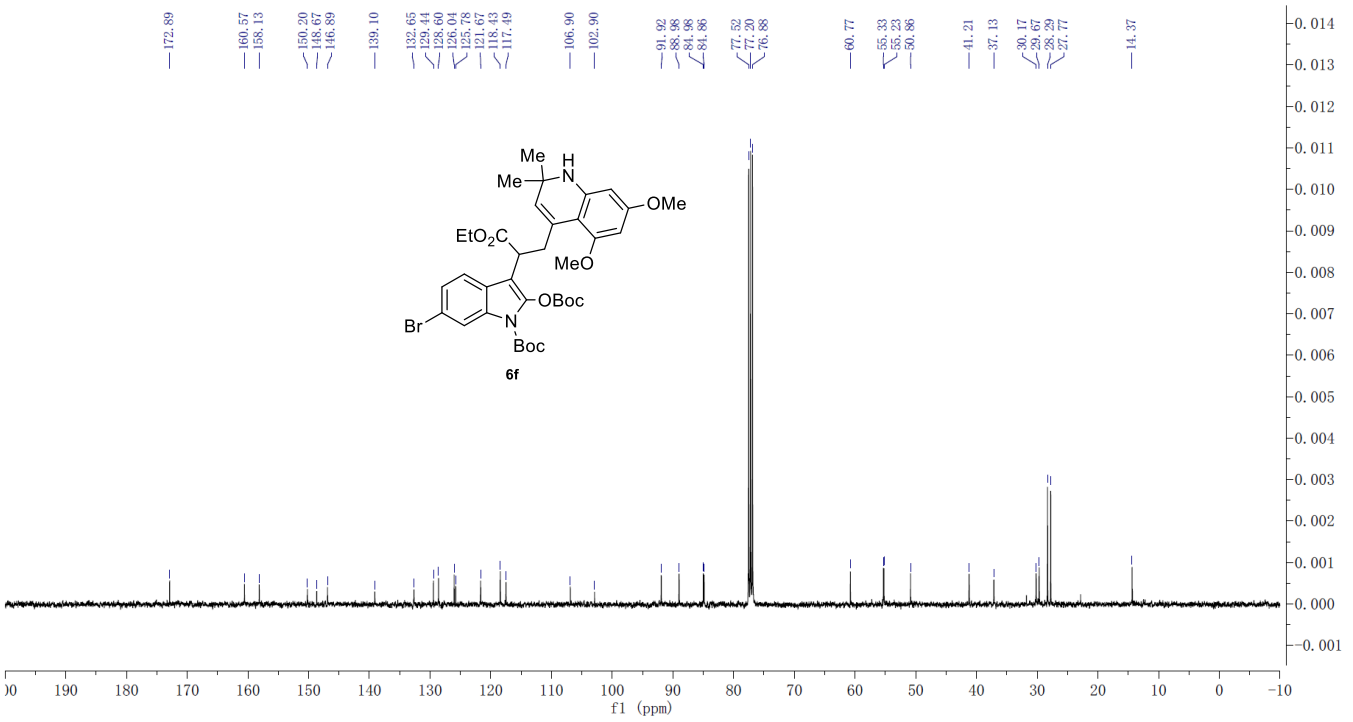
2.92
f1 (ppm)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76.88
60.77
55.33
55.23
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41.21
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29.67
28.29
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EtO2C
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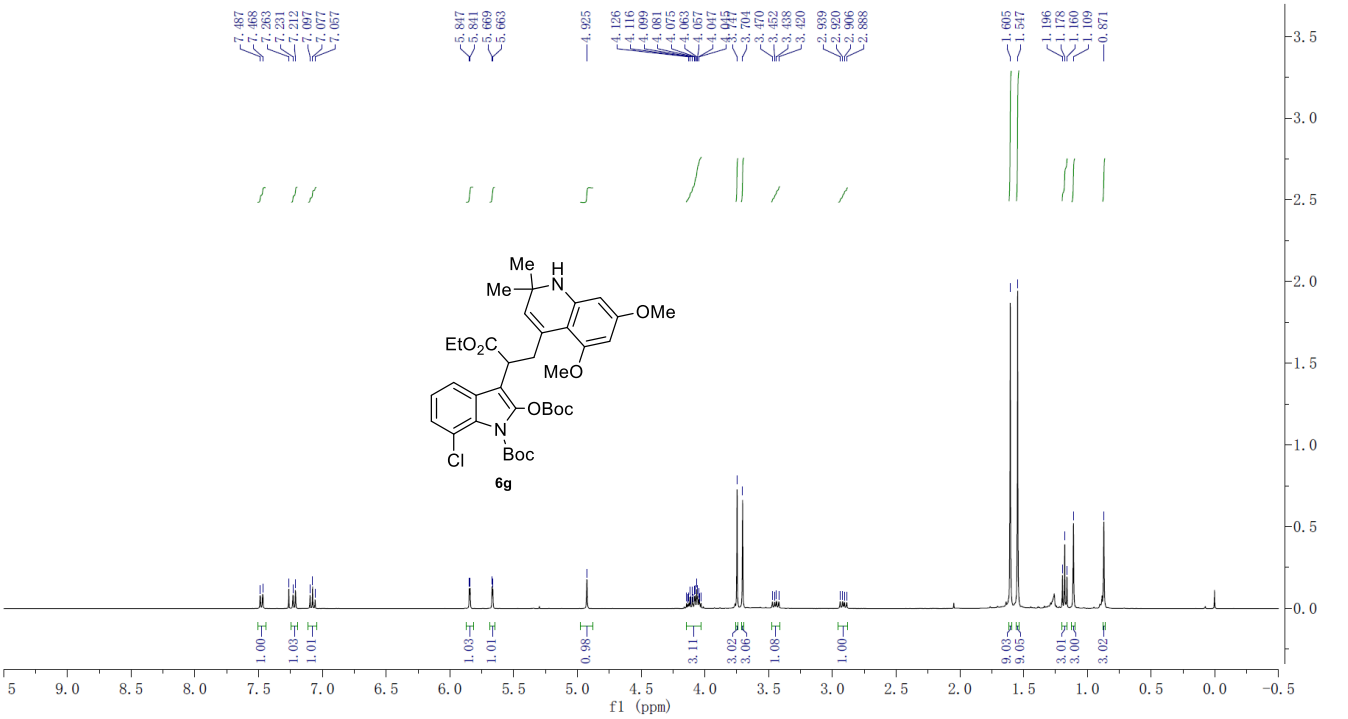
OBoc
Br
N
Boc
6f
f1 (ppm)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4.126
4.116
4.099
4.081
4.075
4.063
4.057
4.047
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3.470
3.452
3.438
3.420
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2.920
2.906
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1.605
1.547
1.196
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1.160
1.109
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Me
OMe
EtO2C
MeO
OBoc
N
Cl
Boc
6g
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1.03
1.01
1.03
1.01
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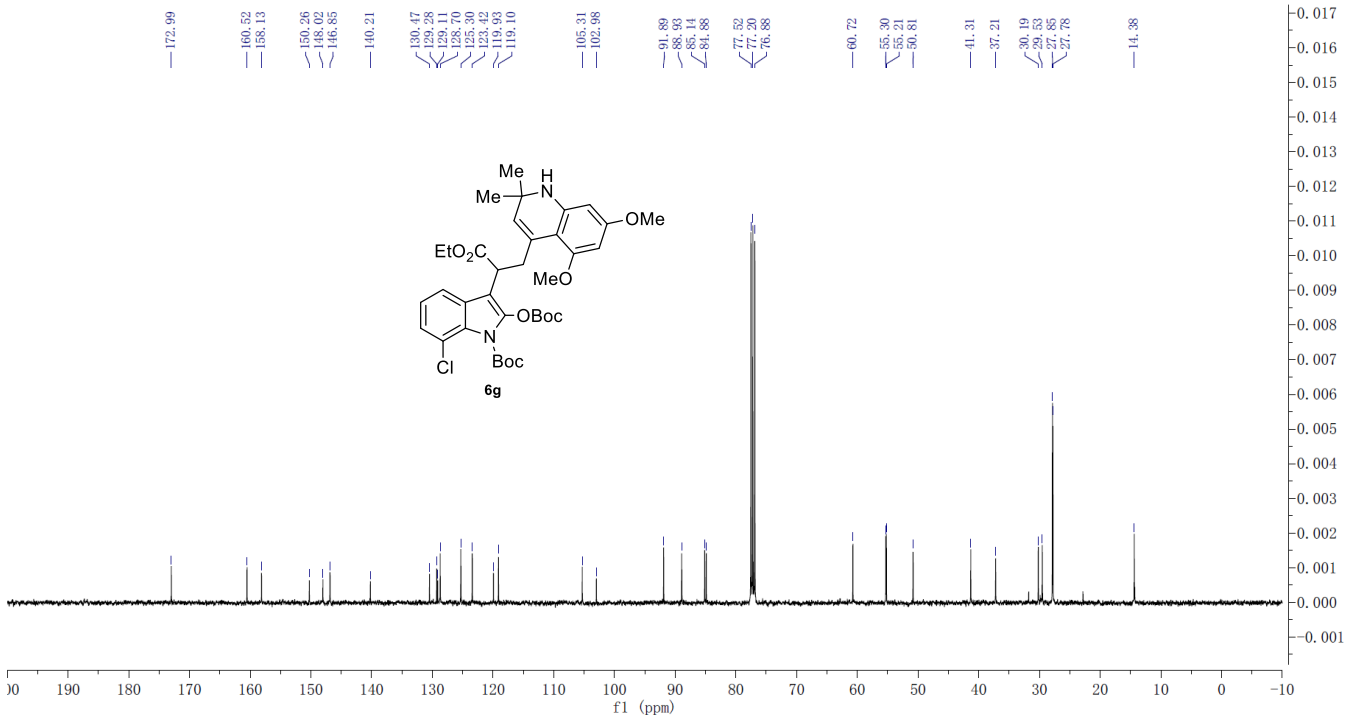
3.01
3.00
3.02
f1 (ppm)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119.10
105.31
102.98
91.89
88.93
85.14
84.88
77.52
77.20
76.88
60.72
55.30
55.21
50.81
41.31
37.21
30.19
29.53
27.85
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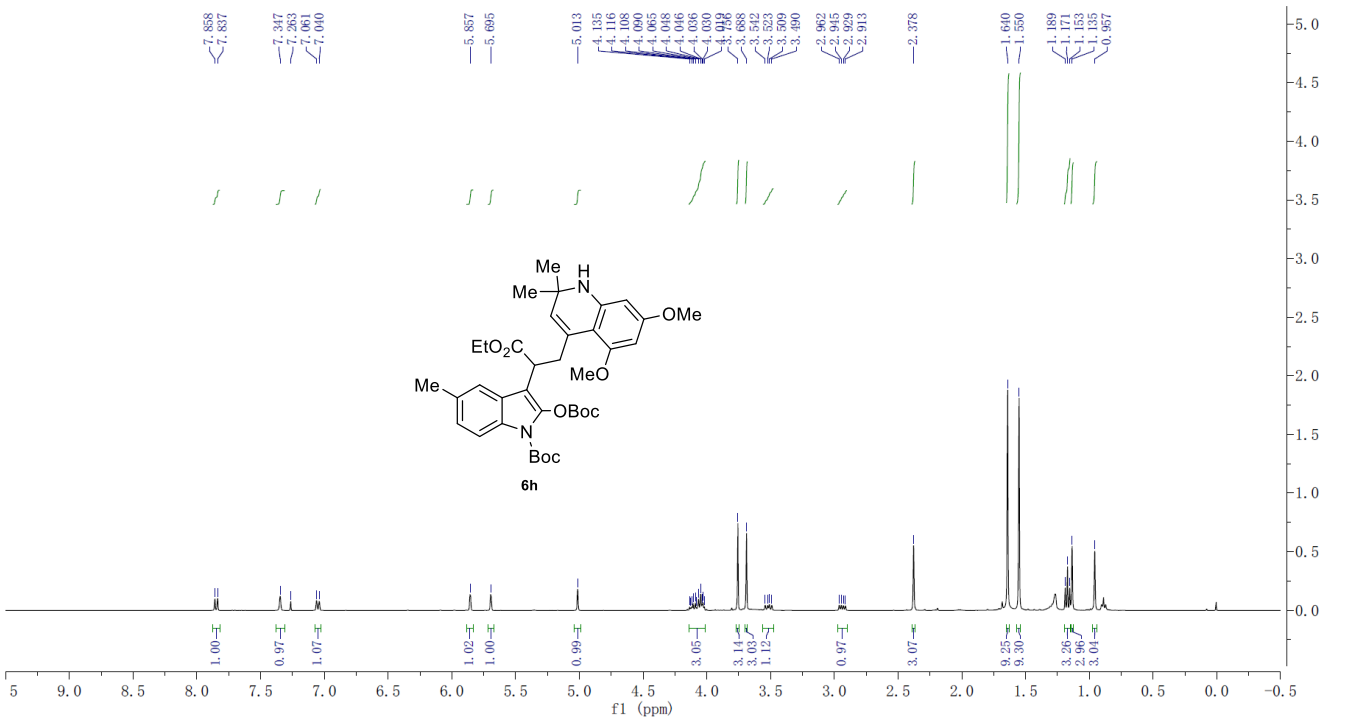
N
Me
OMe
EtO2C
MeO
OBoc
N
Cl
Boc
6g
f1 (ppm)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4.090
4.065
4.048
4.046
4.036
4.030
3.688
3.542
3.523
3.509
3.490
2.962
2.945
2.929
2.913
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1.550
1.189
1.171
1.153
1.135
0.957
Me
H
N
Me
OMe
EtO2C
MeO
Me
OBoc
N
Boc
6h
1.00
0.97
1.07
1.02
1.00
0.99
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1.12
0.97
3.07
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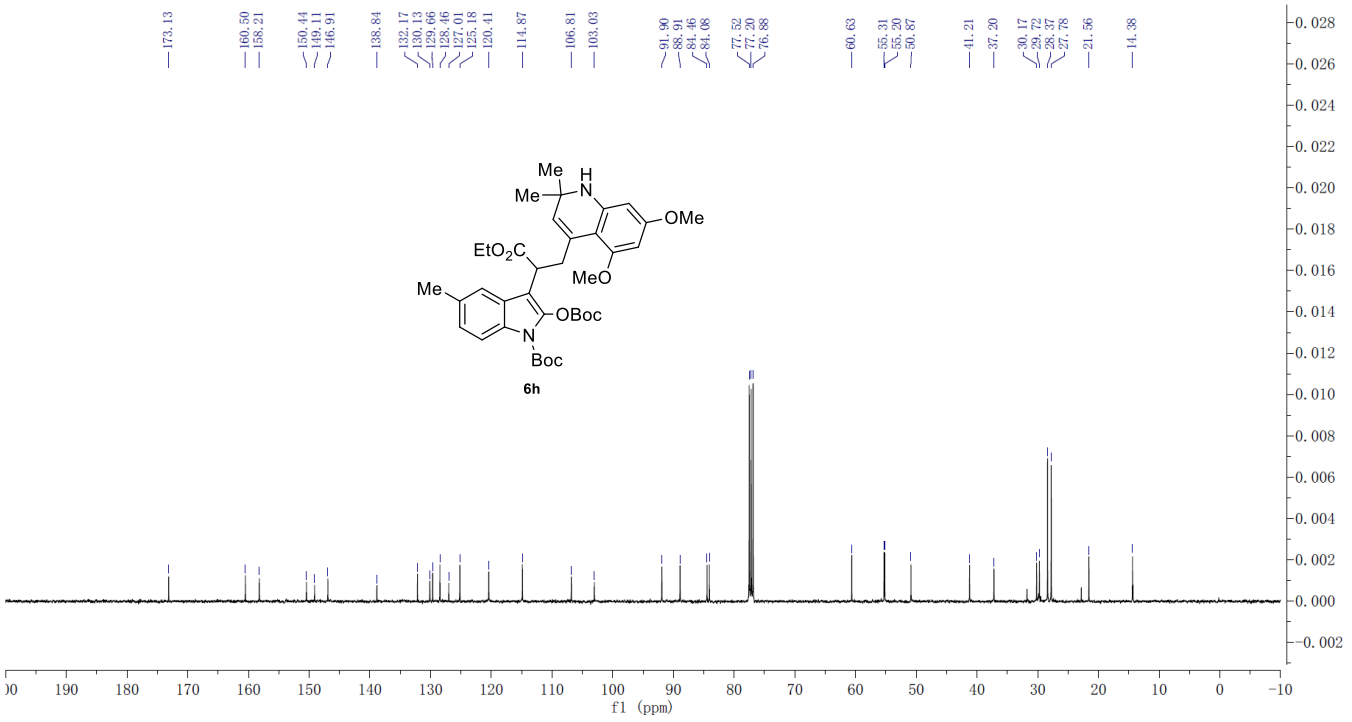
3.26
2.96
3.04
f1 (ppm)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114.87
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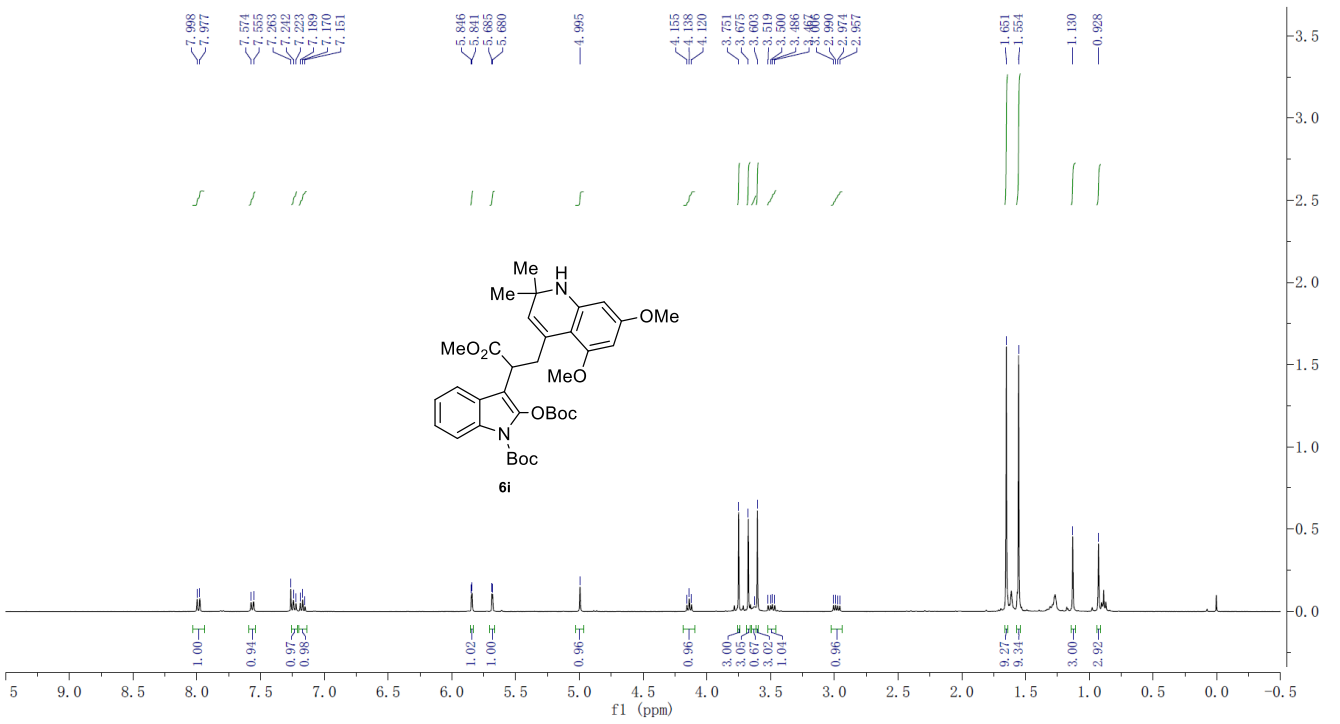
103.03
91.90
88.91
84.46
84.08
77.52
77.20
76.88
60.63
55.31
55.20
50.87
41.21
37.20
30.17
29.72
28.37
27.78
21.56
14.38
Me
H
N
Me
OMe
EtO2C
MeO
Me
OBoc
N
Boc
6h
f1 (ppm)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4.155
4.138
4.120
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3.675
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3.519
3.500
3.486
3.467
3.456
2.969
2.974
2.957
1.651
1.554
1.130
0.928
Me
Me
H
N
OMe
MeO2C
MeO
OBoc
N
Boc
6i
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0.94
0.97
0.98
1.02
1.00
0.96
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3.00
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1.04
0.96
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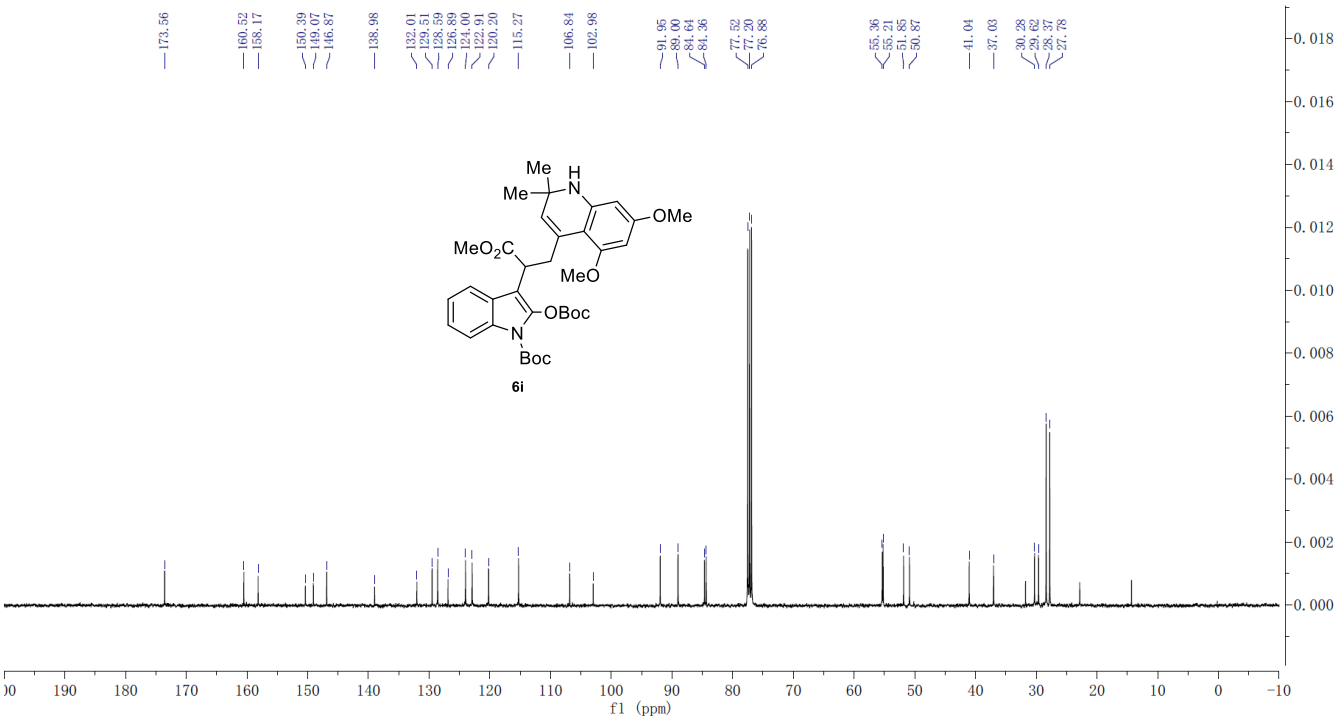
9.34
3.00
2.92
f1 (ppm)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120.20
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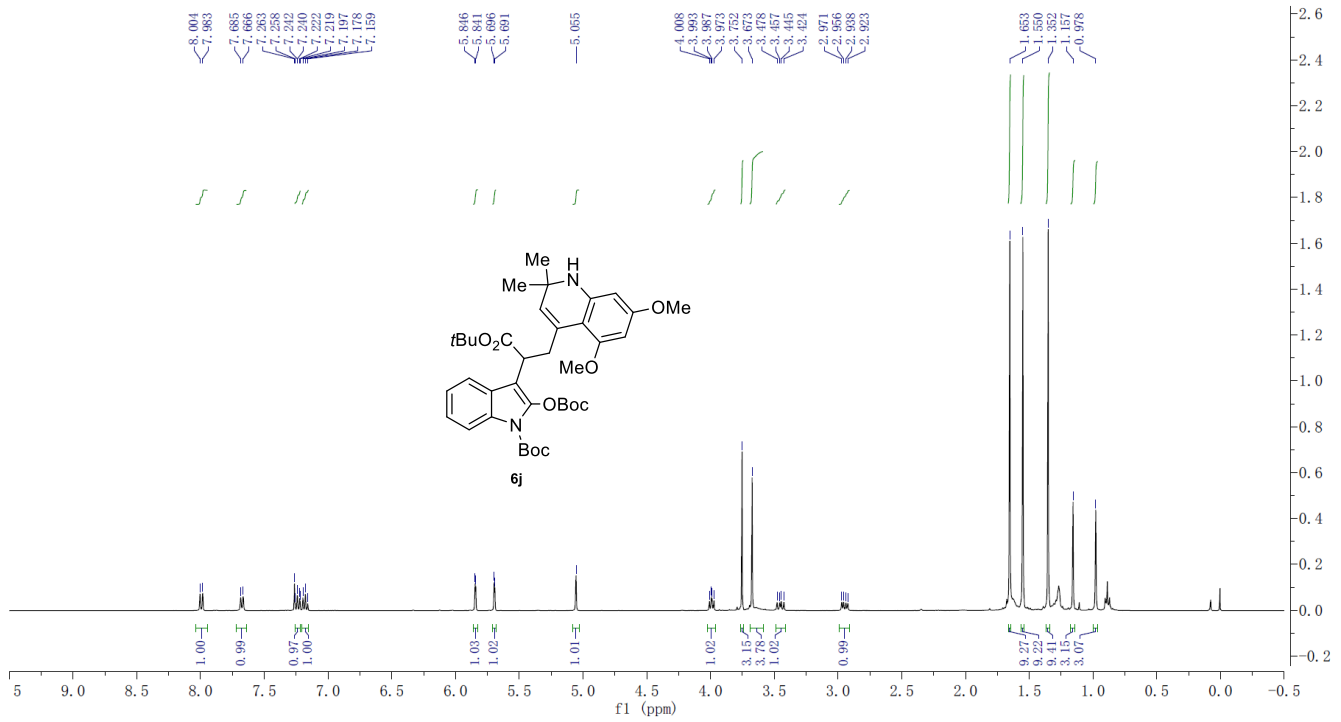
106.84
102.98
91.95
89.00
84.64
84.36
77.52
77.20
76.88
55.36
55.21
51.85
50.87
41.04
37.03
30.28
29.62
28.37
27.78
Me
Me
H
N
OMe
MeO2C
MeO
OBoc
N
Boc
6i
f1 (ppm)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7.159
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5.841
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5.691
5.055
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3.987
3.973
3.752
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3.478
3.457
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3.424
2.971
2.956
2.938
2.923
1.653
1.550
1.382
1.157
0.978
Me
Me
H
N
OMe
tBuO2C
MeO
OBoc
N
Boc
6j
1.00
0.99
0.97
1.00
1.03
1.02
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9.41
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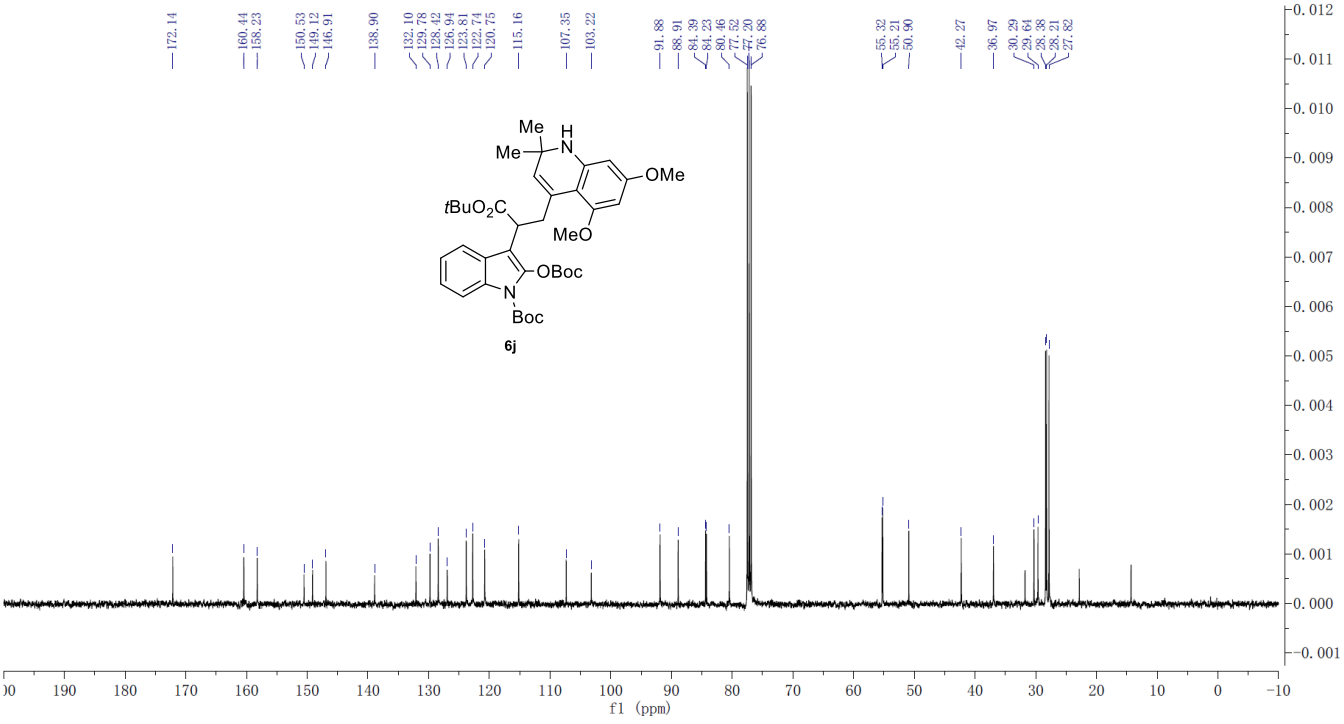
3.07
f1 (ppm)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77.20
76.88
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55.21
50.90
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36.97
30.29
29.64
28.38
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H
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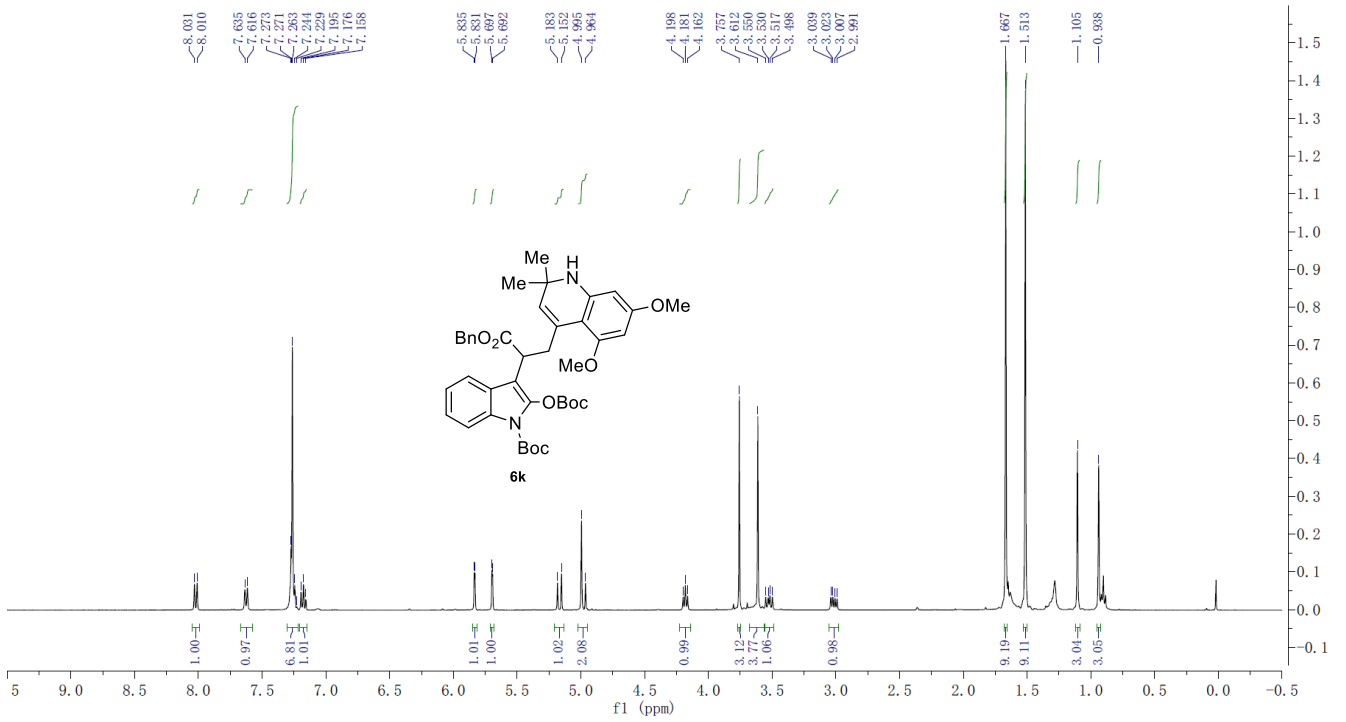
OMe
tBuO2C
MeO
OBoc
N
Boc
6j
f1 (ppm)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5.697
5.692
5.183
5.152
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4.964
4.198
4.181
4.162
3.757
3.612
3.550
3.530
3.517
3.498
3.039
3.023
3.007
2.991
1.667
1.513
1.105
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Me
Me
H
N
OMe
BnO2C
MeO
OBoc
N
Boc
6k
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6.81
1.01
1.01
1.00
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9.11
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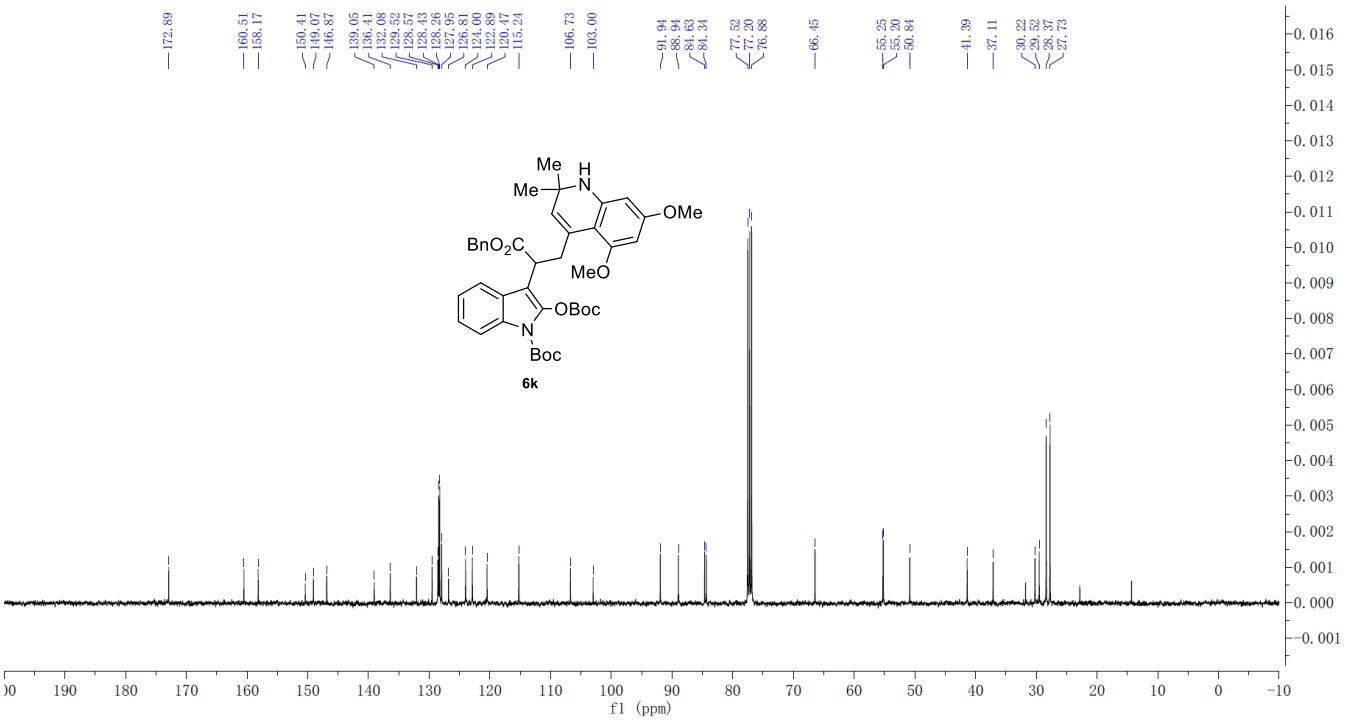
3.05
f1 (ppm)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76.88
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55.20
50.84
41.39
37.11
30.22
29.52
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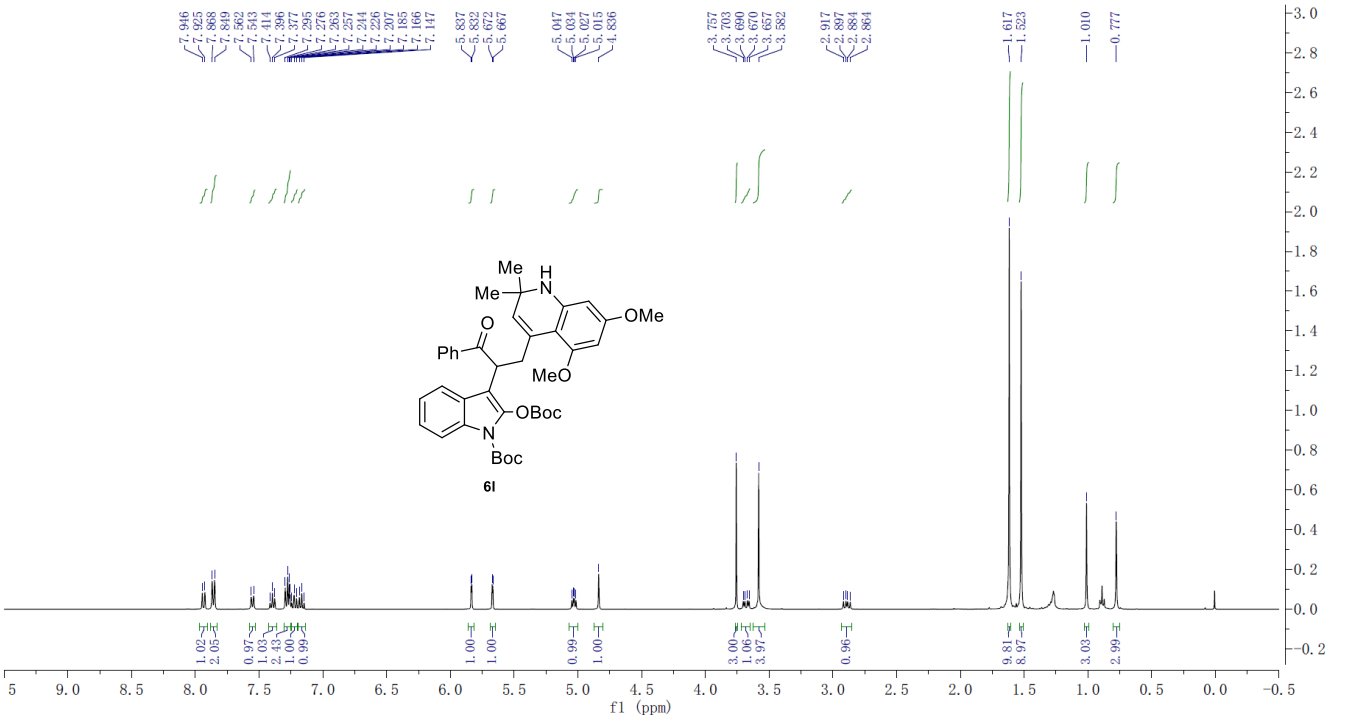
N
OMe
BnO2C
MeO
OBoc
N
Boc
6k
f1 (ppm)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Me
H
N
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O
Ph
MeO
OBoc
N
Boc
6l
1.02
2.05
0.97
1.03
2.43
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1.00
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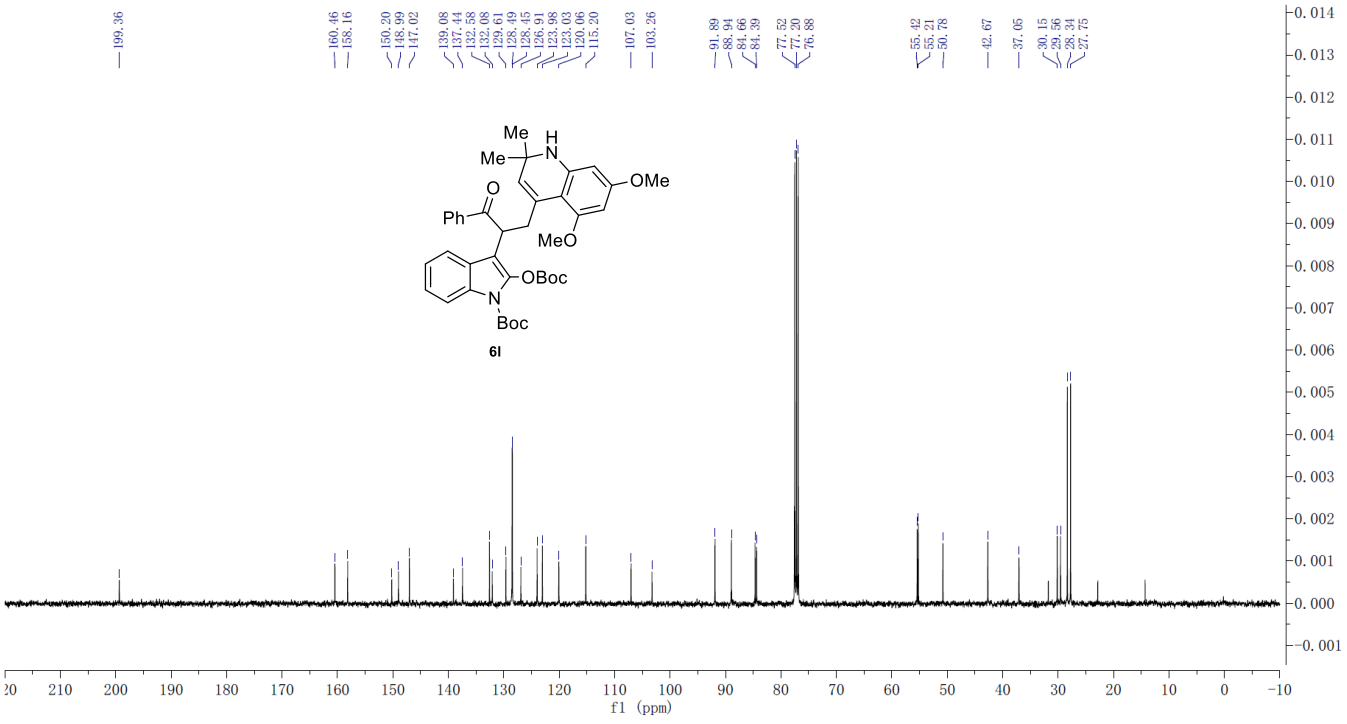
f1 (ppm)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123.98
123.03
120.06
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88.94
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84.39
77.52
77.20
76.88
55.42
55.21
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42.67
37.05
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H
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MeO
OBoc
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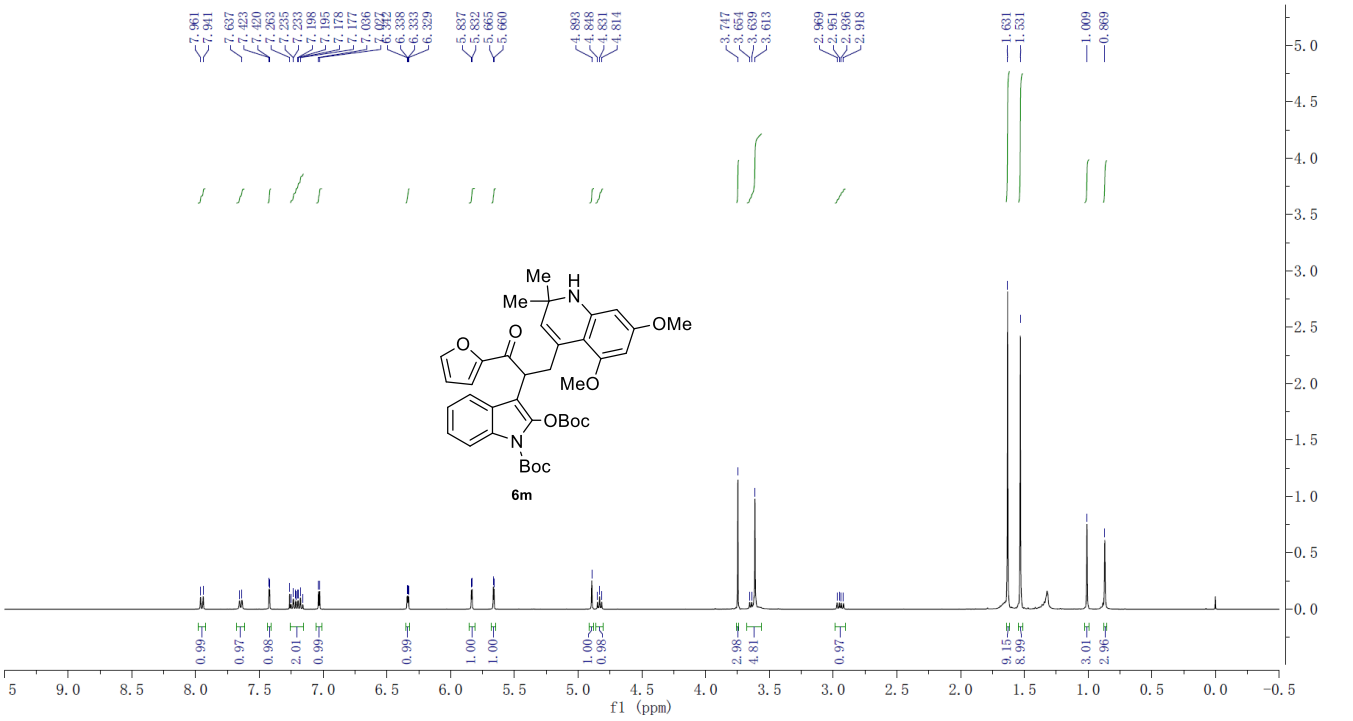
Boc
6l
f1 (ppm)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7.177
7.036
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6.942
6.338
6.333
6.329
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4.893
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4.831
4.814
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2.918
1.631
1.531
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0.869
Me
Me
H
N
OMe
O
O
MeO
OBoc
N
Boc
6m
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0.97
0.98
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0.99
0.99
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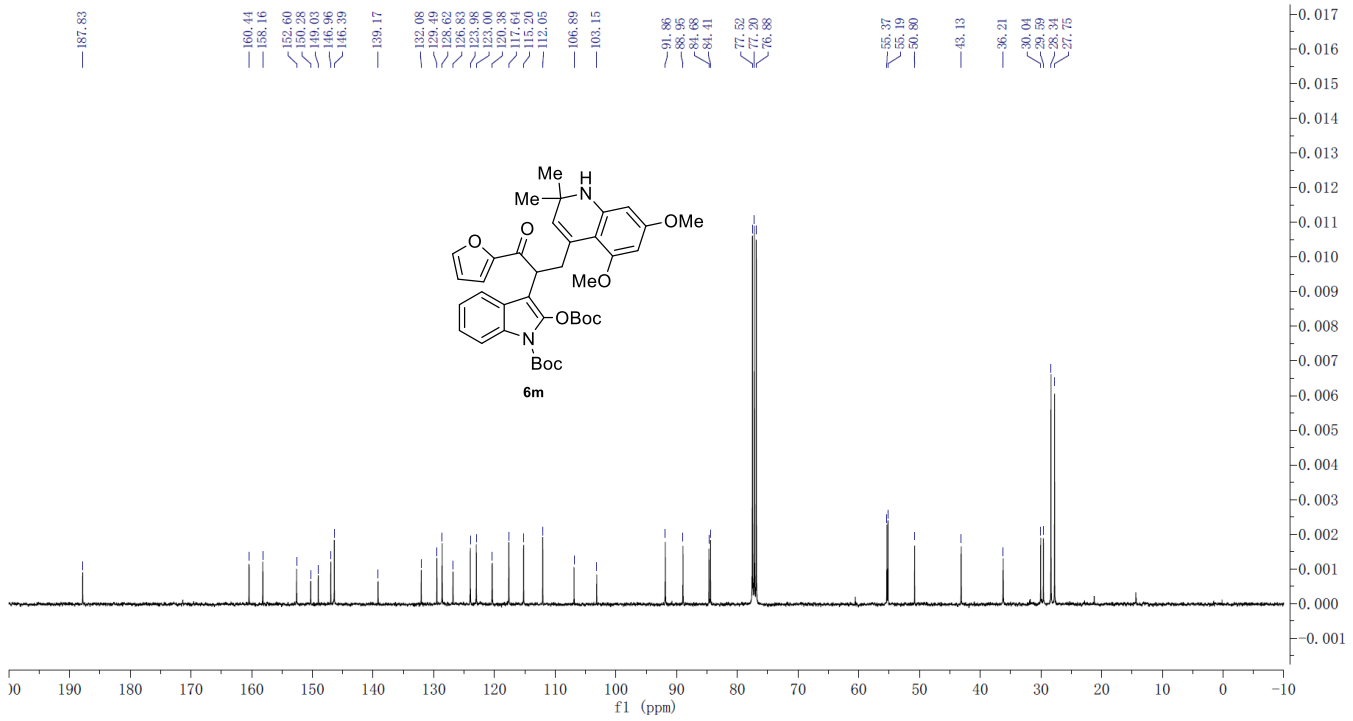
f1 (ppm)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123.00
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117.64
115.20
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91.86
88.95
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84.41
77.52
77.20
76.88
55.37
55.19
50.80
43.13
36.21
30.04
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Me
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MeO
OBoc
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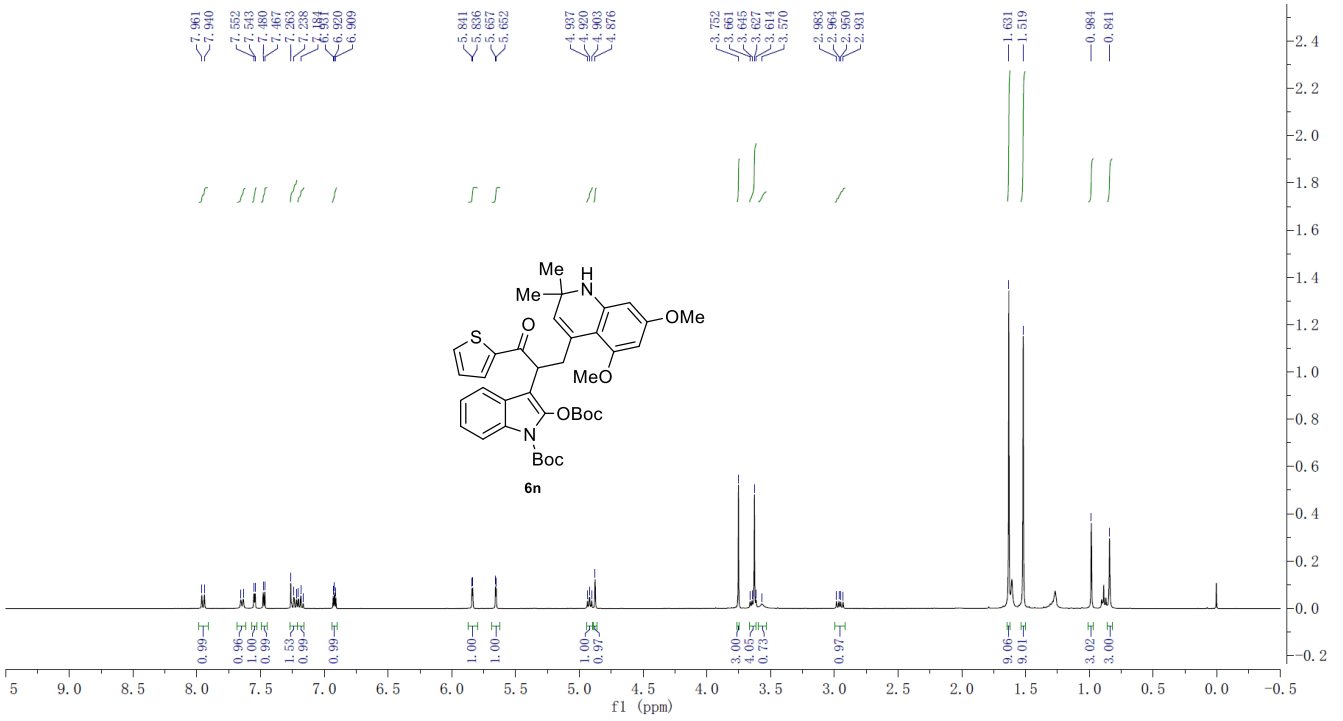
Boc
6m
f1 (ppm)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3.645
3.627
3.614
3.570
2.983
2.964
2.950
2.931
1.631
1.519
0.984
0.841
Me
Me
H
N
O
S
OMe
MeO
OBoc
N
Boc
6n
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0.96
1.00
0.99
1.53
0.99
0.99
1.00
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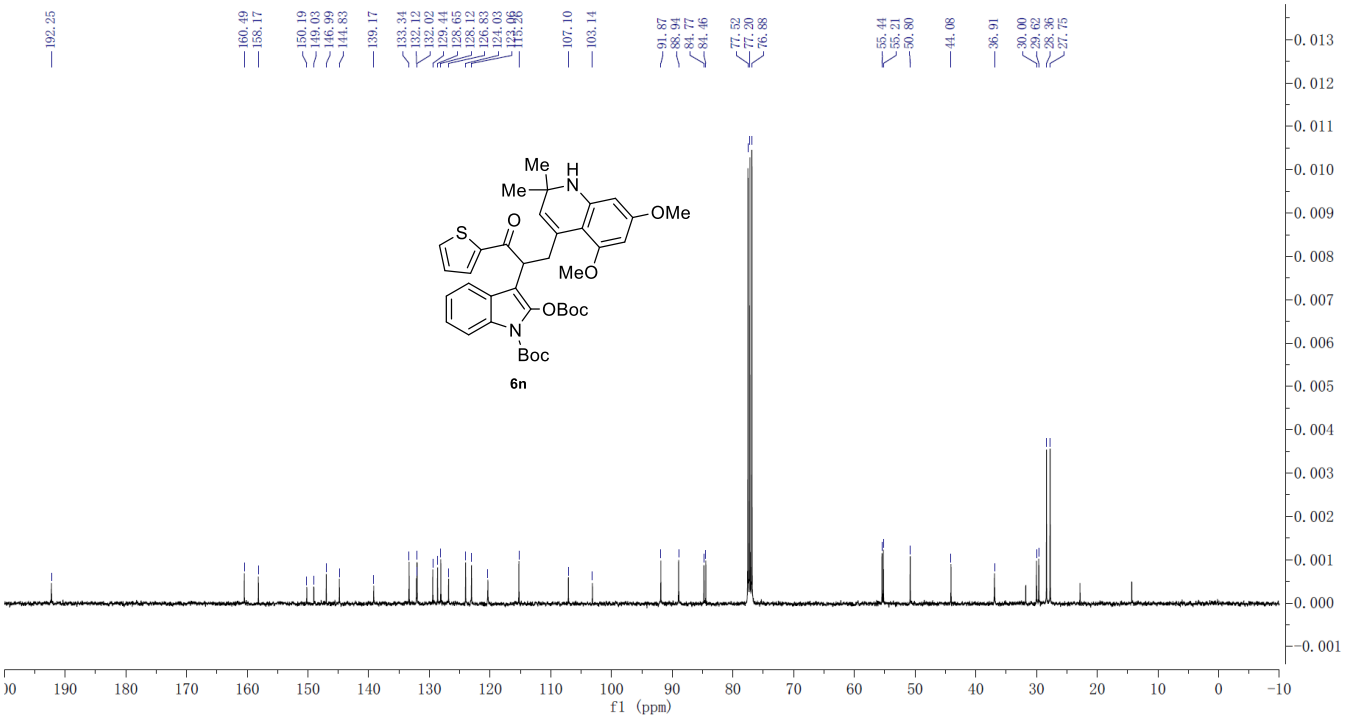
3.00
f1 (ppm)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77.20
76.88
55.44
55.21
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28.36
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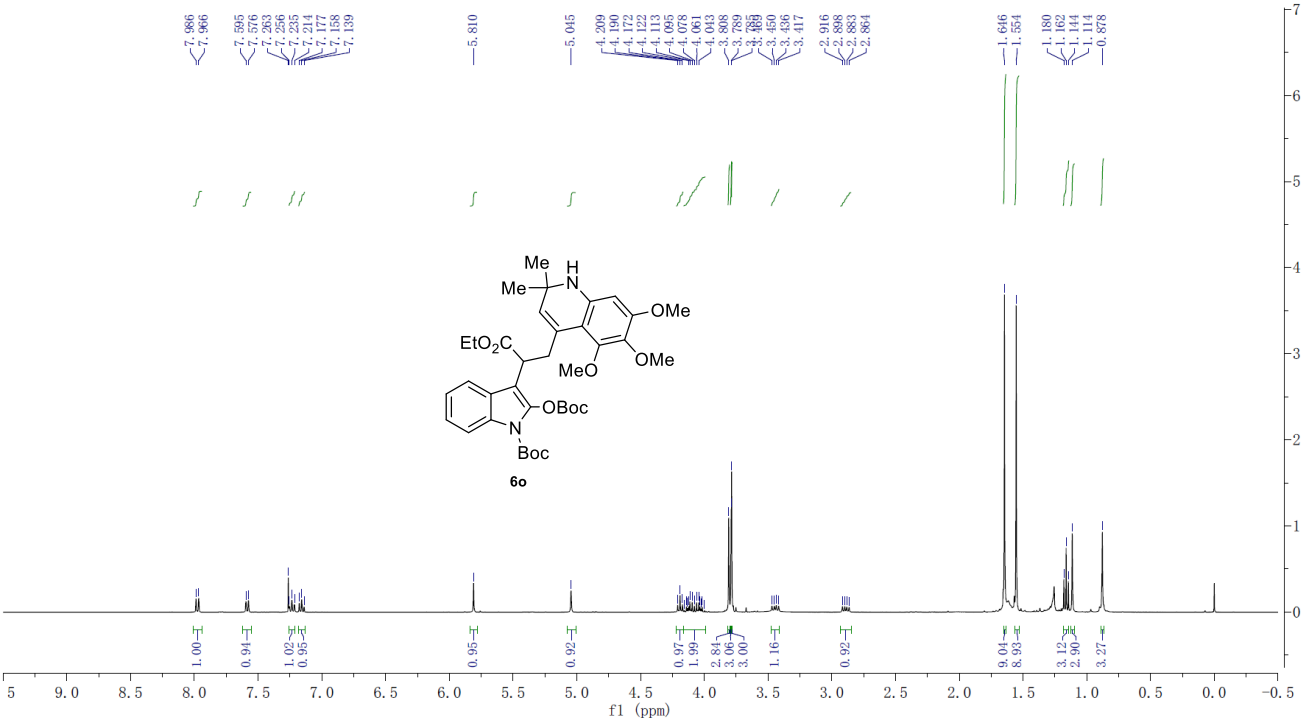
Me
Me
H
N
O
S
OMe
MeO
OBoc
N
Boc
6n
f1 (ppm)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7.214
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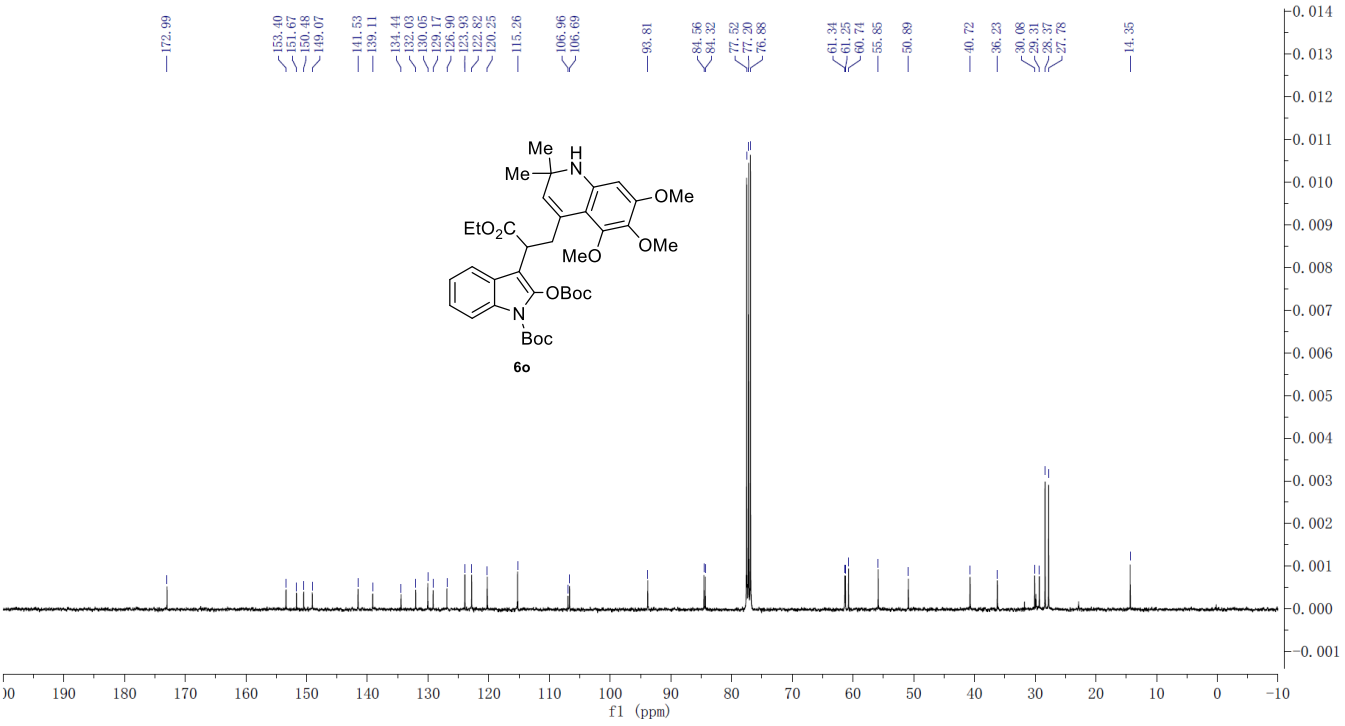
7.158
7.139
5.810
5.045
4.209
4.190
4.172
4.122
4.113
4.095
4.078
4.061
4.043
3.808
3.789
3.450
3.436
3.417
2.916
2.898
2.883
2.864
1.646
1.554
1.180
1.162
1.144
1.114
0.878
Me
Me
H
N
OMe
EtO2C
MeO
OMe
OBoc
N
Boc
6o
1.00
0.94
1.02
0.95
0.95
0.92
0.97
1.99
2.84
3.06
3.00
1.16
0.92
9.04
8.93
3.12
2.90
3.27
f1 (ppm)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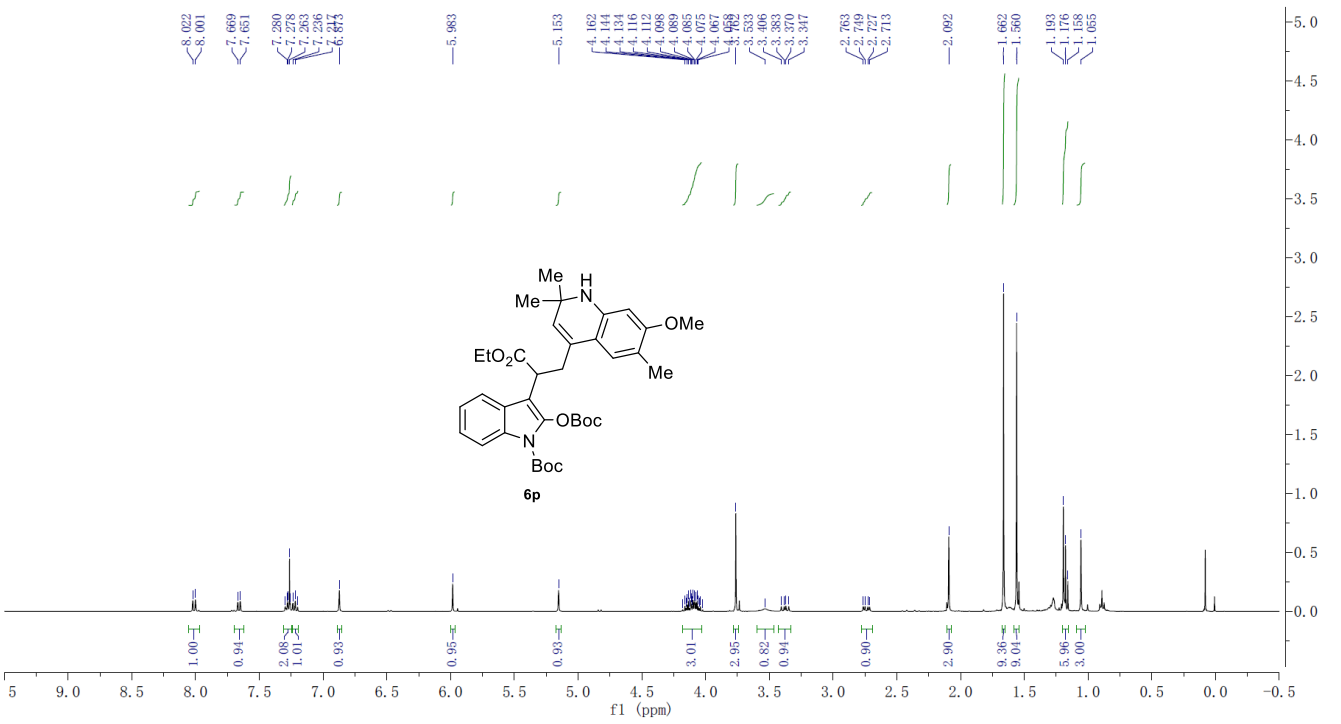
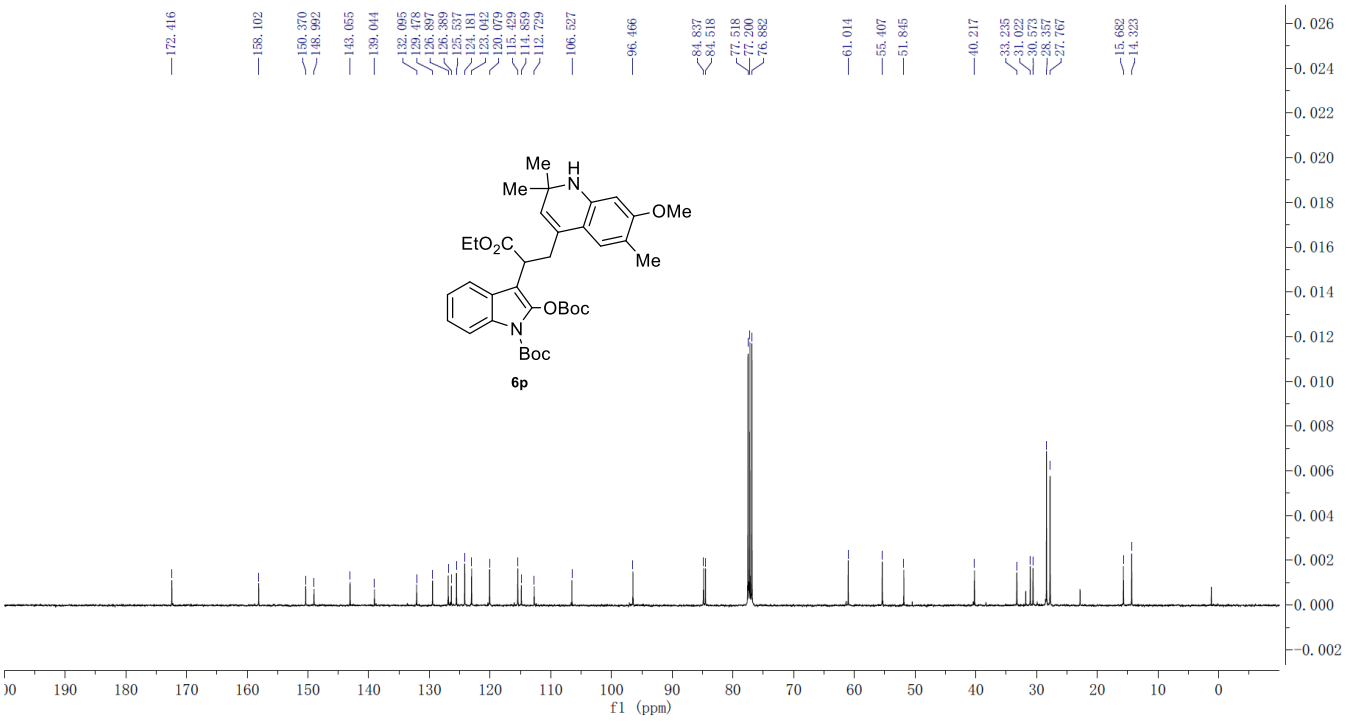
153.40
151.67
150.48
149.07
141.53
139.11
134.44
132.03
130.05
129.17
126.90
123.93
122.82
120.25
115.26
106.96
106.69
93.81
84.56
84.32
77.52
77.20
76.88
61.34
61.25
60.74
55.85
50.89
40.72
36.23
30.08
29.31
28.37
27.78
14.35
Me
Me
H
N
OMe
EtO2C
MeO
OMe
OBoc
N
Boc
6o
f1 (ppm)


8.022
8.001
7.669
7.651
7.280
7.278
7.263
7.236
7.217
6.813
5.983
5.153
4.162
4.144
4.134
4.116
4.112
4.098
4.089
4.055
4.075
4.067
3.762
3.533
3.406
3.383
3.370
3.347
2.763
2.749
2.727
2.713
2.092
1.662
1.560
1.193
1.176
1.158
1.055
Me
H
N
Me
OMe
EtO2C
Me
OBoc
N
Boc
6p
1.00
0.94
2.08
1.01
0.93
0.95
0.93
3.01
2.95
0.82
0.94
0.90
2.90
9.36
9.04
5.96
3.00
f1 (ppm)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139.044
132.095
129.478
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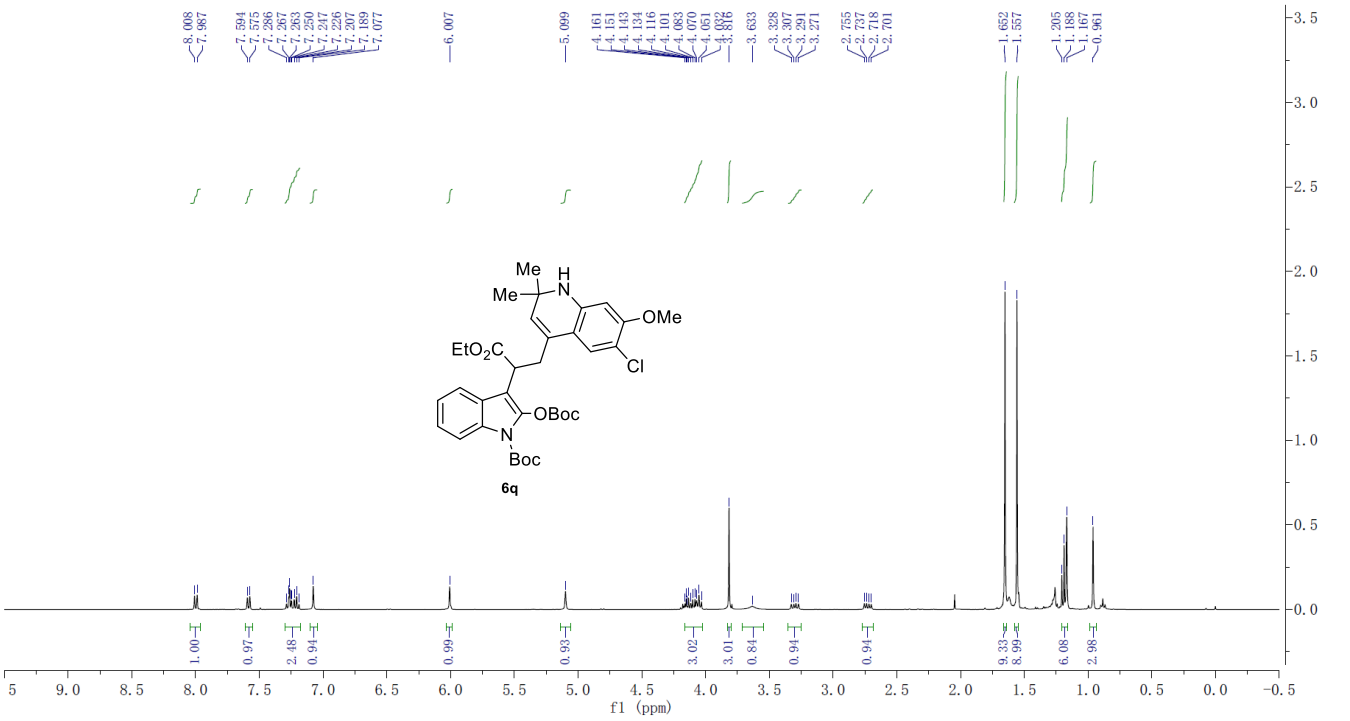
126.389
125.537
124.181
123.042
120.079
115.429
114.859
112.729
106.527
96.466
84.837
84.518
77.518
77.200
76.882
61.014
55.407
51.845
40.217
33.235
31.022
30.573
28.357
27.767
15.682
14.323
Me
H
N
Me
OMe
EtO2C
Me
OBoc
N
Boc
6p
f1 (ppm)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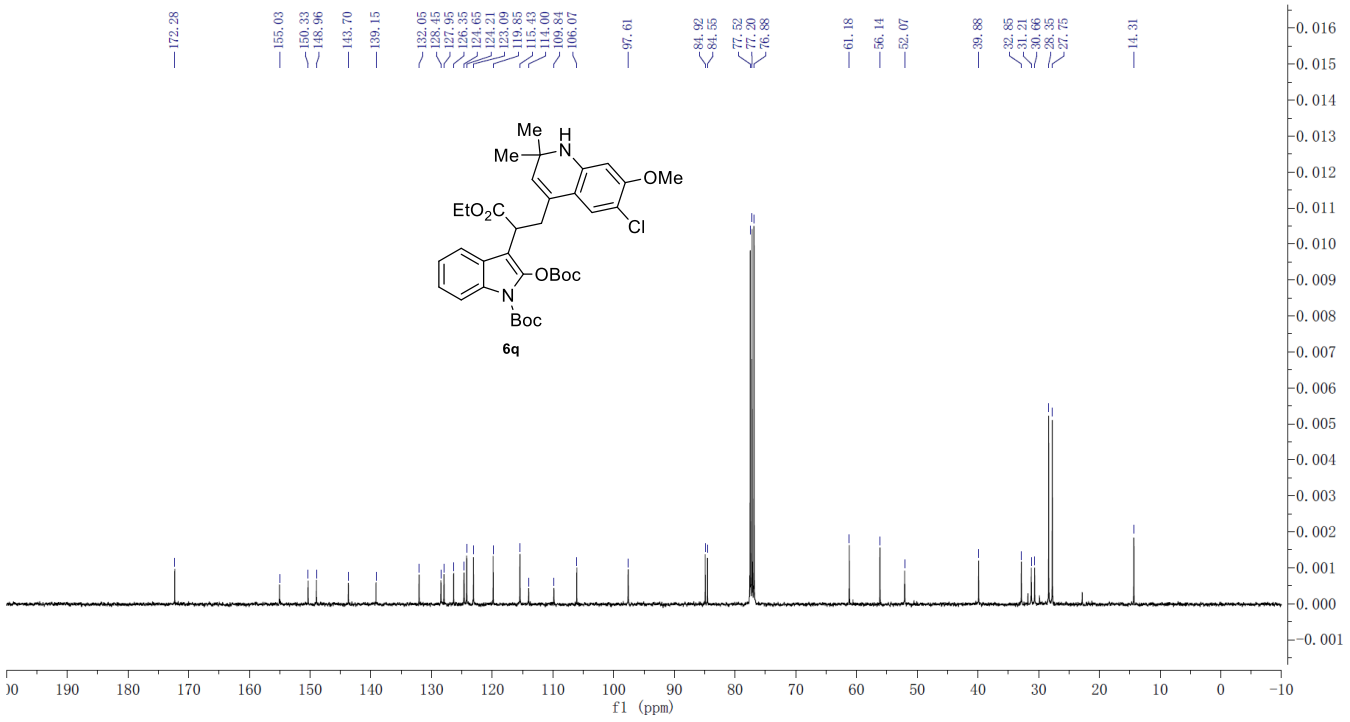
7.594
7.575
7.286
7.267
7.263
7.250
7.247
7.226
7.207
7.189
7.077
6.007
5.099
4.161
4.151
4.143
4.134
4.116
4.101
4.083
4.070
4.051
3.816
3.633
3.328
3.307
3.291
3.271
2.755
2.737
2.718
2.701
1.652
1.557
1.205
1.188
1.167
0.961
Me
Me
H
N
OMe
Cl
EtO2C
OBoc
N
Boc
6q
1.00
0.97
2.48
0.94
0.99
0.93
3.02
3.01
0.84
0.94
0.94
9.33
8.99
6.08
2.98
f1 (ppm)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155.03
150.33
148.96
143.70
139.15
132.05
128.45
127.95
126.65
124.71
123.69
119.85
115.43
114.00
109.84
106.07
97.61
84.92
84.55
77.52
77.20
76.88
61.18
56.14
52.07
39.88
32.85
31.21
30.66
28.35
27.75
14.31
Me
Me
H
N
OMe
Cl
EtO2C
OBoc
N
Boc
6q
f1 (ppm)