Electronic Supplementary Material (ESI) for Chemical Science.

Tetraenamines in Organocatalysis: Application in Asymmetric Synthesis and Insights into the Reaction Mechanism

Julian Stiller, Pernille H. Poulsen, David Cruz Cruz, Jorge Dourado, Rebecca L. Davis and Karl Anker Jørgensen*

[*] Center for Catalysis

Department of Chemistry, Aarhus University

DK-8000 Aarhus C, Denmark

Fax (45) 8919 6199, e-mail: kaj@chem.au.dk

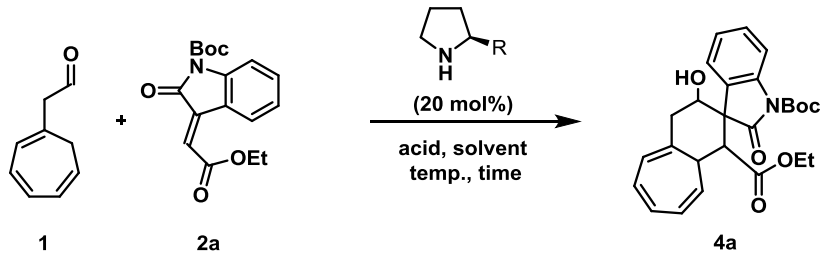
Contents

1. General methods

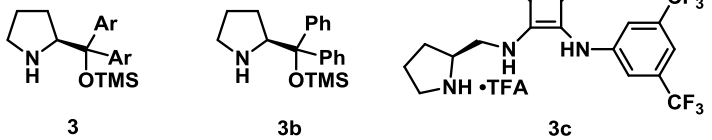
NMR spectra were acquired on a Varian AS 400 spectrometer or a Bruker AVANCE III HD spectrometer, running at 400 MHz for ^{1}H and 100 MHz for ^{13}C, respectively. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CHCl_3$, 7.26 ppm for ^{1}H NMR, $CDCl_3$, 77.0 ppm for ^{13}C NMR). The following abbreviations are used to indicate the multiplicity in NMR spectra: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad resonance. ^{13}C NMR spectra were acquired on a broad band decoupled mode. Mass spectra were recorded on a Bruker MicroTOF-Q High-Performance LC-MS system. Analytical thin layer chromatography (TLC) was performed using pre-coated aluminium-backed plates (Merck Kieselgel 60 F254) and visualized by ultraviolet irradiation, $KMnO_4$ or *p*-anisaldehyde dip. Optical rotations were measured on a Bellingham+Stanley ADP440+ polarimeter. The enantiomeric excess (ee) of the products was determined by Ultraperformance Convergence Chromatography (ACQUITY UPC) using Daicel Chiralpak IA, IB, IC and ID columns as chiral stationary phases (columns were kept at 40 °C during measuring). Unless otherwise noted, analytical grade solvents and commercially available reagents were used without further purification. For FC (FC) Iatrobeads (SRS 8060, 60 μm, Mitsubishi Chemical Medience Corporation) and Merck silica gel 60 (230 - 400 mesh) were used. Racemic samples were prepared using a racemic mixture of enantiomers of **3** (20 mol%) in $CHCl_3$.

2. Synthesis of the cycloadducts

2.1. Optimization



1 2a 4a



3 3b 3c

Ar = 3,5-(CF_3)-C_6H_3

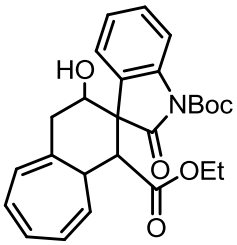
entry[a]	cat	equiv.	acid	solvent	temp.	time[b]	conv. [c]	dr [c]	*ee* [%][d]
1	**3b**	1.2	*o*FBzOH	$CDCl_3$	40 °C	<17	>99% (n.d.)	>95/5	77
2	**3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	20	>99% (n.d.)	>95/5	91
3[e]	**3c**	1.2	*o*FBzOH	$CDCl_3$	40 °C	<17	dec.	-	-
4	***ent*-3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	20	>99% (93%)	>95/5 (>95/5)	94
5	**3**	1.2	*o*FBzOH	$CDCl_3$	4 °C	168	70% (n.d.)	>95/5	96
6	**3**	1.2	*o*FBzOH	$CDCl_3$	20 °C	72	>99% (n.d.)	>95/5	95
7	**3**	1.2	*o*FBzOH	$CDCl_3$	60 °C	<17	>99% (n.d.)	89/11	84
8	**3**	2.0	*o*FBzOH	$CDCl_3$	40 °C	19	>99% (n.d.)	>95/5	92
9	**3**	1.2	-	$CDCl_3$	40 °C	20	90% (n.d.)	>95/5	96
10	**3**	1.2	AcOH	$CDCl_3$	40 °C	20	>99% (n.d.)	>95/5	92
11	**3**	1.2	BzOH	$CDCl_3$	40 °C	20	>99% (n.d.)	>95/5	92
12	**3**	1.2	*o*NO_2BzOH	$CDCl_3$	40 °C	20	>99% (n.d.)	>95/5	82
13[f]	**3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	>48	>99% (n.d.)	>95/5	90
14	**3**	1.2	-	CH_2Cl_2	40 °C	72	40% (n.d.)	>95/5	96
15	**3**	1.2	-	CH_3CN	40 °C	48	20% (n.d.)	n.d.	n.d.
16	**3**	1.2	-	Tol	40 °C	48	70% (n.d.)	>95/5	85
17	**3**	1.2	-	EtOH	40 °C	48	15% (n.d.)	n.d.	n.d.
18[g]	**3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	24	>99% (95%)	>95/5 (>95/5)	94
19[i]	**3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	3	27%[h]	>95/5	n.d.
20[ji]	**3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	3	18%[h]	>95/5	n.d.
21[k]	**3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	3	9%[h]	>95/5	n.d.
22	**3**	1.0	*o*FBzOH	$CDCl_3$	40 °C	2	12%[h]	>95/5	n.d.
23	**3**	2.0	*o*FBzOH	$CDCl_3$	40 °C	2	20%[h]	>95/5	n.d.
24	**3**	3.0	*o*FBzOH	$CDCl_3$	40 °C	2	21%[h]	>95/5	n.d.
25[l]	**3**	1.2	*o*FBzOH	$CDCl_3$	40 °C	2	15%[h]	>95/5	n.d.

[a] Reactions carried out at 0.1 mmol or 0.05 mmol scale of the Oxindole in the solvent (0.25 M). [b] Indicates the approximate time to full conversion. [c] Determined by ^{1}H NMR spectroscopy of the crude reaction mixture. [d] Determined by Chiral Ultraperformance Convergence Chromatography (UPC^2). [e] 4.0 equiv. of DEA employed. [f] c = 0.10 mL. [g] 10 mol% of acid used. [h] Product yield based on comparison with internal standard. [i] 20 mol% of **3** used. [j] 10 mol% of **3** used. [k] 5 mol% of **3** used. [l] 5.0 equiv. Na_2SO_4 added. (We found that the addition of 5 equiv. of Na_2SO_4 was required to obtain high diastereoselectivities (86:14 - >95:5) for all substrates).

2.2. General procedure

In a dry glass vial, a mixture of the oxindole **2** (0.10 mmol, 1.0 equiv.), *o*-FBA (0.02 mmol, 20 mol%), catalyst **3** (0.02 mmol, 20 mol%) and Na_2SO_4 (0.50 mmol, 5.0 equiv.) were dissolved in 0.4 mL of dry $CHCl_3$ before aldehyde **1** (0.12 mmol, 1.2 equiv.) was added. The reaction mixture was heated to the appropriate temperature and stirred for the time indicated. When the reaction was completed, the mixture was plugged over Iatrobeads, concentrated and purified by FC on Iatrobeads to afford the corresponding cycloadduct **4**.

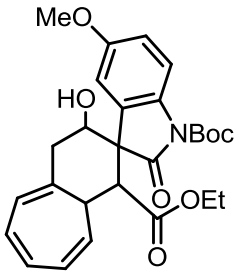
2.3. Results and characterization



4a

Cycloadduct **4a** was obtained after 24 h at 40 °C. FC on Iatrobeads (pentane/EtOAc 15/1 to 10/1) afforded the pure compound in 93% yield, >95/5 dr and 94% ee.

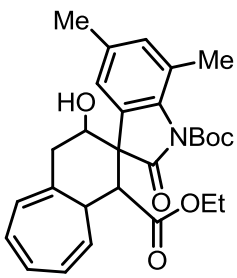
Yellow foam. $[\alpha]_D^{20}$ = −14.6 (*c* 0.51, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.85 (d, *J* = 8.2 Hz, 1H), 7.29 (m, 1H), 7.09 (m, 2H), 6.65 (m, 2H), 6.20 (m, 2H), 5.05 (dd, *J* = 9.2, 5.0 Hz, 1H), 4.03 (m, 1H), 3.96 (d, *J* = 10.3 Hz, 1H), 3.71 (m, 2H), 3.12 (m, 1H), 2.99 (dd, *J* = 16.2, 7.6 Hz, 1H), 2.76 (dd, *J* = 16.4, 3.8 Hz, 1H), 2.51 (dd, *J* = 10.2, 4.9 Hz, 1H), 1.66 (s, 9H), 0.86 (t, *J* = 7.1, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.0, 170.9, 149.1, 140.3, 131.1, 130.5, 130.0, 128.9, 128.5, 125.6, 125.0, 124.8, 124.2, 122.7, 115.0, 84.6, 73.9, 61.0, 55.5, 49.7, 36.7, 35.6, 28.1 (3C), 13.3. **HRMS** (ESI+) *m/z* calcd. for $C_{26}H_{29}NO_6Na$ $[M+Na]^+$: 474.1887; found: 474.1889. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.7 min; t_{minor} = 2.4 min.



4b

Cycloadduct **4b** was obtained after 24 h at 40 °C. FC on Iatrobeads (pentane/EtOAc 10/1 to 5/1) afforded the pure compound in 84% yield, >95/5 dr and 91% ee.

Yellow oil. $[\alpha]_D^{20}$ = −37.8 (*c* 0.66, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.9 Hz, 1H), 6.81 (dd, *J* = 9.0, 2.7 Hz, 1H), 6.70 (d, *J* = 2.6 Hz, 1H), 6.65 (dd, *J* = 10.0, 4.6 Hz, 1H), 6.21 (m, 2H), 5.08 (dd, *J* = 9.2, 5.1 Hz, 1H), 4.04 (dd, *J* = 6.9, 4.3 Hz, 1H), 3.98 (d, *J* = 10.2 Hz, 1H), 3.77 (m, 2H), 3.72 (s, 3H), 2.99 (dd, *J* = 16.5, 7.0 Hz, 1H), 2.81 (dd, *J* = 16.8, 3.8 Hz, 1H), 2.47 (m, 1H), 1.66 (s, 9H), 0.88 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.2, 170.9, 156.8, 149.0, 133.5, 130.8, 130.5, 130.0, 129.5, 125.7, 125.0, 122.6, 115.6, 113.3, 110.9, 84.5, 73.4, 61.0, 55.6, 55.5, 49.6, 36.7, 35.3, 28.1 (3C), 13.4. **HRMS** (ESI+) *m/z* calcd. for $C_{27}H_{31}NO_7Na$ $[M+Na]^+$: 504.1993; found: 504.1991. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.9 min; t_{minor} = 2.9 min.

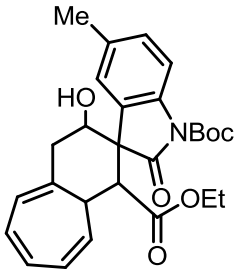


4c

Cycloadduct **4c** was obtained after 24 h at 40 °C. FC on Iatrobeads (pentane/EtOAc 10/1) afforded the pure compound in 66% yield, >95/5 dr and 95% ee.

Yellow oil. $[\alpha]_D^{20}$ = −30.0 (*c* 1.0, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 6.90 (s, 1H), 6.72 (s, 1H), 6.65 (m, 2H), 6.19 (m, 2H), 5.03 (dd, *J* = 9.2, 4.9 Hz, 1H), 4.00 (dd, *J* = 7.9, 3.8 Hz, 1H), 3.93 (d, *J* = 10.4 Hz, 1H), 3.79 (q, *J* = 7.1 Hz, 2H), 3.00

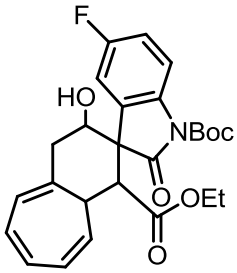
(dd, *J* = 15.8, 8.1 Hz, 2H), 2.74 (dd, *J* = 16.0, 3.7 Hz, 1H), 2.54 (dd, *J* = 10.3, 4.0 Hz, 1H), 2.23 (s, 3H), 2.20 (s, 3H), 1.65 (s, 9H), 0.82 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.7, 170.9, 149.1, 136.4, 134.2, 132.4, 131.6, 130.4, 129.9, 129.7, 125.6, 125.0, 123.2, 122.5, 122.2, 84.7, 74.3, 61.1, 55.9, 49.6, 36.6, 35.7, 27.8 (3C), 21.0, 19.5, 13.3. **HRMS** (ESI+) *m*/*z* calcd. for $C_{28}H_{33}NO_6Na$ $[M+Na]^+$: 502.2200; found: 502.2208. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.4 min; t_{minor} = 1.5 min.



4d

Cycloadduct **4d** was obtained after 24 h at 40 °C. FC on Iatrobeads (pentane/EtOAc 15/1 to 10/1) afforded the pure compound in 86% yield, >95/5 dr and 84% ee.

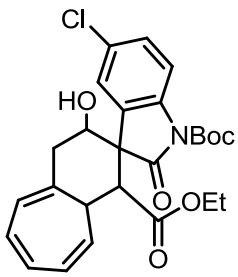
Yellow oil. $[\alpha]_D^{20}$ = −7.8 (*c* 0.49, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.3 Hz, 1H), 7.09 (d, *J* = 8.4 Hz, 1H), 6.88 (s, 1H), 6.65 (m, 2H), 6.21 (m, 2H), 5.03 (dd, *J* = 9.2, 4.9 Hz, 1H), 4.03 (br s, 1H), 3.95 (d, *J* = 10.5 Hz, 1H), 3.73 (m, 2H), 3.01 (dd, *J* = 16.0, 8.0 Hz, 2H), 2.75 (dd, *J* = 16.0, 3.7 Hz, 1H), 2.47 (dd, *J* = 10.3, 4.3 Hz, 1H), 2.26 (s, 3H), 1.66 (s, 9H), 0.88 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.1, 170.8, 149.1, 137.9, 134.4, 131.4, 130.5, 130.0, 129.4, 128.5, 125.5, 125.0, 124.6, 122.6, 114.7, 84.4, 74.3, 60.9, 55.6, 49.9, 36.6, 35.9, 28.1 (3C), 21.1, 13.3. **HRMS** (ESI+) *m*/*z* calcd. for $C_{27}H_{31}NO_6Na$ $[M+Na]^+$: 488.2044; found: 488.2045. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.5 min; t_{minor} = 2.2 min.



4e

Cycloadduct **4e** was obtained after 24 h at rt. FC on Iatrobeads (pentane/EtOAc 15/1 to 10/1) afforded the pure compound in 80% yield, 94/6 dr and 93% ee.

Yellow oil. $[\alpha]_D^{20}$ = −1.6 (*c* 0.49, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 9.0, 4.6 Hz, 1H), 7.01 (td, *J* = 8.9, 2.7 Hz, 1H), 6.85 (dd, *J* = 7.9, 2.7 Hz, 1H), 6.67 (m, 2H), 6.20 (m, 2H), 5.07 (dd, *J* = 9.2, 5.0 Hz, 1H), 4.04 (m, 1H), 3.98 (d, *J* = 10.4 Hz, 1H), 3.77 (m, 2H), 3.04 (m, 2H), 2.78 (dd, *J* = 16.5, 4.1 Hz, 1H), 2.44 (ddd, *J* = 10.3, 5.0, 1.2 Hz, 1H), 1.66 (s, 9H), 0.89 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) 177.6, 170.7, 160.1 (d, *J* = 244.3 Hz), 158.6, 148.9, 136.3 (d, *J* = 2.9 Hz), 130.6, 130.3, 130.2 (d, *J* = 8.1 Hz), 130.0, 125.2, 122.9, 116.3 (d, *J* = 8.1 Hz), 115.4 (d, *J* = 22.7 Hz), 111.7 (d, *J* = 24.9 Hz), 84.9, 73.7, 61.1, 55.7, 49.5, 36.7, 35.5, 28.1 (3C), 13.4. **HRMS** (ESI+) *m*/*z* calcd. for $C_{26}H_{28}FNO_6Na$ $[M+Na]^+$: 492.1793; found: 492.1796. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.3 min; t_{minor} = 1.8 min.

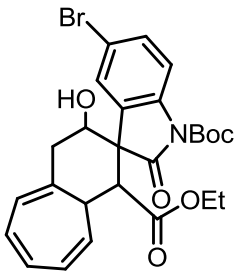


4f

Cycloadduct **4f** was obtained after 24 h at rt. FC on Iatrobeads (pentane/EtOAc 14/1 to 10/1) afforded the pure compound in 71% yield, 88/12 dr and 95% ee.

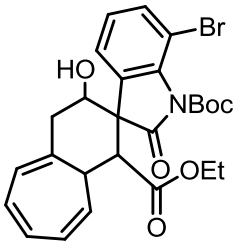
Yellow solid. $[\alpha]_D^{20}$ = −20.6 (*c* = 0.5, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.7 Hz, 1H), 7.28 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.07 (d, *J* = 2.1 Hz, 1H), 6.69 (m, 2H), 6.22 (m, 2H), 5.04 (dd, *J* = 9.3, 5.0 Hz, 1H), 4.04 (m, 1H), 3.97 (d, *J* = 10.8 Hz, 1H), 3.78 (m, 2H), 3.02 (m, 1H), 2.90 (d, *J* = 5.6 Hz, 1H), 2.76 (m, 1H), 2.45 (m, 1H), 1.66 (s, 9H), 0.89 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 177.1, 170.5, 148.8, 138.9, 130.7, 130.6, 130.6, 130.1, 130.0, 129.0, 125.2, 125.1, 124.2, 122.9, 116.2, 85.0, 74.2, 61.1, 55.7, 49.8, 36.6, 35.9, 28.1

(3C), 13.4. **HRMS** (ESI+) *m/z* calcd. for $C_{26}H_{28}ClNNaO_6Na$ $[M+Na]^+$: 508.1497; found: 508.1502. **UPC²**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.6 min; t_{minor} = 2.2 min.



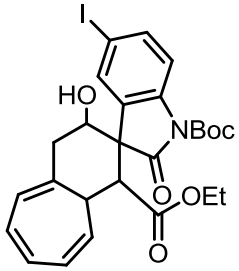
4g

Cycloadduct **4g** was obtained after 24 h at rt. FC on Iatrobeads (pentane/EtOAc 15/1 to 10/1) afforded the pure compound in 93% yield, 89/11 dr and 95% ee. Yellow oil. $[\alpha]_D^{20}$ = −17.2 (*c* 0.69, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.7 Hz, 1H), 7.43 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.20 (d, *J* = 2.0 Hz, 1H), 6.67 (m, 2H), 6.22 (m, 2H), 5.03 (dd, *J* = 9.3, 4.9 Hz, 1H), 4.04 (m, 1H), 3.97 (d, *J* = 10.9 Hz, 1H), 3.77 (m, 2H), 3.02 (dd, *J* = 15.8, 8.5 Hz, 1H), 2.88 (d, *J* = 5.7 Hz, 1H), 2.74 (dd, *J* = 15.8, 3.8 Hz, 1H), 2.44 (dd, *J* = 11.3, 4.3 Hz, 1H), 1.65 (s, 9H), 0.88 (t, *J* = 7.1, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 176.9, 170.5, 148.8, 139.4, 131.9, 131.0, 130.7, 130.0, 126.9, 125.9, 125.1, 125.1, 122.8, 117.6, 116.6, 85.0, 74.4, 61.1, 55.6, 49.9, 36.6, 36.0, 28.1 (3C), 13.4. **HRMS** (ESI+) *m/z* calcd. for $C_{26}H_{28}BrNO_6Na$ $[M+Na]^+$: 552.0992; found: 552,0988. **UPC²**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.6 min; t_{minor} = 2.5 min.



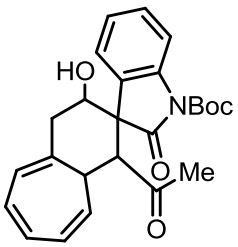
4h

Cycloadduct **4h** was obtained after 24 h at rt. FC on Iatrobeats (pentane/EtOAc 12/1) afforded the pure compound in 72% yield, >95/5 dr and 94% ee. Yellow oil. $[\alpha]_D^{20}$ = +6.2 (*c* 0.47, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.1 Hz, 1H), 7.06 (d, *J* = 7.4 Hz, 1H), 6.95 (t, *J* = 7.8 Hz, 1H), 6.64 (m, 2H), 6.20 (m, 2H), 5.04 (dd, *J* = 9.2, 5.0 Hz, 1H), 4.03 (dd, *J* = 7.6, 4.1 Hz, 1H), 3.95 (d, *J* = 10.3 Hz, 1H), 3.82 (m, 2H), 3.00 (dd, *J* = 16.2, 7.6 Hz, 1H), 2.74 (dd, *J* = 16.4, 3.8 Hz, 1H), 2.50 (dd, *J* = 10.0, 4.6 Hz, 1H), 1.67 (s, 9H), 0.85 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 177.9, 170.6, 147.7, 139.1, 133.6, 132.7, 130.7, 130.5, 129.9, 125.6, 125.4, 125.1, 123.2, 122.7, 106.4, 85.6, 73.7, 61.3, 56.3, 49.1, 36.5, 35.4, 27.7 (3C), 13.3. **HRMS** (ESI+) *m/z* calcd. for $C_{26}H_{28}BrNO_6Na$ $[M+Na]^+$: 552.0992; found: 552,0973. **UPC²**: IC, CO_2/i-PrOH 90/10, 3.0 mL·min^{-1}; t_{major} = 2.1 min; t_{minor} = 2.6 min.



4i

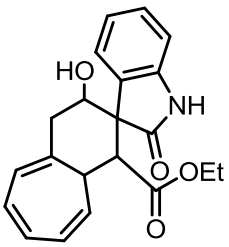
Cycloadduct **4i** was obtained after 24 h at rt. FC on Iatrobeads (pentane/EtOAc 15/1 to 10/1) afforded the pure compound in 77% yield, 86/14 dr and 93% ee. Yellow solid. $[\alpha]_D^{20}$ = −40.4 (*c* = 0.5, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.65 (m, 2H), 7.37 (d, *J* = 1.7 Hz, 1H), 6.68 (m, 2H), 6.22 (m, 2H), 5.03 (dd, *J* = 9.3, 4.9 Hz, 1H), 4.04 (dd, *J* = 8.6, 4.1 Hz, 1H), 3.96 (d, *J* = 10.9 Hz, 1H), 3.78 (qd, *J* = 7.1, 5.2 Hz, 2H), 3.02 (dd, *J* = 15.9, 8.6 Hz, 1H), 2.82 (s, 1H), 2.73 (dd, *J* = 15.9, 4.0 Hz, 1H), 2.44 (m, 1H), 1.65 (s, 9H), 0.88 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 176.7, 170.4, 148.8, 140.2, 137.9, 132.6, 131.4, 130.8, 130.7, 123.0, 125.1, 125.1, 122.8, 116.9, 88.0, 85.0, 74.5, 61.1, 55.5, 50.0, 36.68, 36.1, 28.1 (3C), 13.4. **HRMS** (ESI+) *m/z* calcd. for $C_{26}H_{28}INO_6Na$ $[M+Na]^+$: 600.0854; found: 600.0855. **UPC²**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 1.9 min; t_{minor} = 3.1 min.



4j

Cycloadduct **4j** was obtained after 24 h at rt. FC on Iatrobeads (pentane/EtOAc 14/1 to 10/1) afforded the pure compound in 51% yield, >95/5 dr and 87% ee.

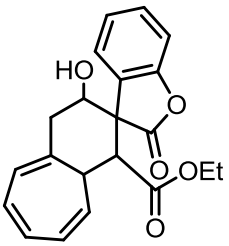
Yellow solid. $[\alpha]_D^{20}$ = −10.8 (*c* = 0.5, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.1 Hz, 1H), 7.30 (td, *J* = 7.9, 1.4 Hz, 1H), 7.10 (m, 2H), 6.73 (m, 2H), 6.34 (dd, *J* = 9.1, 4.9 Hz, 1H), 6.27 (m, 1H), 5.30 (dd, *J* = 9.1, 5.6 Hz, 1H), 4.08 (d, *J* = 10.0 Hz, 1H), 3.94 (t, *J* = 4.2 Hz, 1H), 2.96 (m, 2H), 2.05 (m, 1H), 1.96 (s, 3H), 1.67 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 206.9, 179.2, 148.9, 140.3, 130.6, 130.6, 123.0, 128.6, 127.8, 125.5, 125.5, 124.5, 124.1, 122.9, 115.3, 84.8, 70.8, 56.7, 37.7, 37.6, 33.8, 28.1 (3C). **HRMS** (ESI+) *m*/*z* calcd. for $C_{25}H_{27}NO_5Na$ $[M+Na]^+$: 444.1781; found: 444.1778. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{minor} = 2.5 min; t_{major} = 3.1 min.



4k

Cycloadduct **4k** was obtained after 24 h at 40 °C. FC on Iatrobeads (pentane/EtOAc 3/1 to 2/1) afforded the pure compound in 71% yield, >95/5 dr and 89% ee.

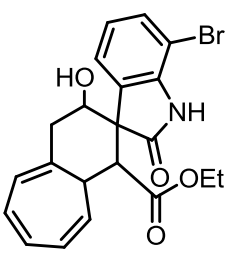
Yellow foam. $[\alpha]_D^{20}$ = −7.1 (*c* =0.5, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.23 (td, *J* = 7.8, 1.1 Hz, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 6.98 (td, *J* = 7.6, 1.0 Hz, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 6.67 (t, *J* = 3.2 Hz, 2H), 6.21 (m, 2H), 5.16 (dd, *J* = 9.3, 5.3 Hz, 1H), 4.01 (t, *J* = 5.1 Hz, 1H), 3.97 (d, *J* = 9.5 Hz, 1H), 3.82 (m, 2H), 3.70 (m, 1H), 2.93 (m, 2H), 2.47 (m, 1H), 0.87 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 181.5, 171.5, 141.0, 130.7, 130.2, 130.1, 129.2, 128.8, 126.0, 125.3, 124.9, 123.0, 122.6, 110.0, 71.7, 61.0, 55.0, 48.0, 37.0, 34.7, 13.6. **HRMS** (ESI+) *m*/*z* calcd. for $C_{21}H_{21}NO_4Na$ $[M+Na]^+$: 374.1363; found: 374.1358. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{minor} = 4.0 min; t_{major} = 4.4 min.



4l

Cycloadduct **4l** was obtained after 24 h at 40 °C. FC on Iatrobeats (pentane/EtOAc 6/1) afforded the pure compound in 59% yield >95/5 dr and 68% ee.

Yellow oil. $[\alpha]_D^{20}$ = −19.6 (*c* 0.70, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.32 (m, 1H), 7.14 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.09 (td, *J* = 7.5, 0.8 Hz, 1H), 6.66 (m, 2H), 6.23 (m, 2H), 5.10 (dd, *J* = 9.2, 5.1 Hz, 1H), 4.11 (m, 1H), 3.98 (d, *J* = 10.4 Hz, 1H), 3.81 (q, *J* = 7.1 Hz, 2H), 3.00 (dt, *J* = 15.8, 7.9 Hz, 1H), 2.93 (d, *J* = 3.3 Hz, 1H), 2.83 (dd, *J* = 16.6, 3.9 Hz, 1H), 2.45 (m, 1H), 0.89 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.6, 170.7, 153.7, 130.6, 130.3, 129.9, 129.7, 127.6, 125.2, 125.1, 124.7, 124.7, 122.9, 110.7, 73.2, 61.3, 54.7, 49.2, 36.7, 35.2, 13.4. **HRMS** (ESI+) *m*/*z* calcd. for $C_{21}H_{20}O_5Na$ $[M+Na]^+$: 375.1208; found: 375,1202. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{major} = 2.1 min; t_{minor} = 2.4 min.

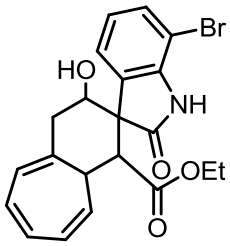


4m

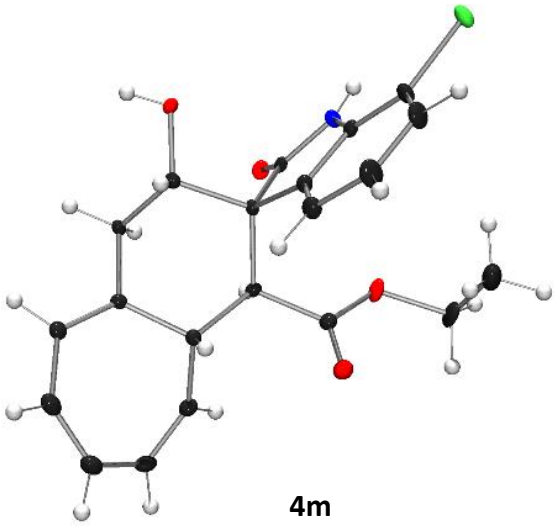
Cycloadduct **4m** was obtained after 24 h at rt. FC on Iatrobeads (pentane/EtOAc 8/1 to 4/1) afforded the pure compound in 74% yield, >95/5 dr and 89% ee (99% ee after crystallization).

Yellow solid. $[\alpha]_D^{20}$ = +26.2 (*c* =0.53, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.18 (s, 1H), 7.35 (d, *J* = 8.3 Hz, 1H), 7.04 (d, *J* = 7.5 Hz, 1H), 6.87 (t, *J* = 7.9 Hz, 1H), 6.67 (m, 2H), 6.22 (m, 2H), 5.13 (dd, *J* = 9.2, 5.2 Hz, 1H), 4.00 (m, 1H), 3.95 (d, *J* = 9.9 Hz, 1H), 3.84 (m, 2H), 3.59 (d, *J* = 3.6 Hz, 1H), 2.99 (dd, *J* = 17.0, 6.0 Hz, 1H), 2.82 (dd, *J* = 17.0, 4.7 Hz, 1H), 2.47 (m, 1H), 0.88 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 180.2, 171.2, 140.7, 131.4, 130.8, 130.5, 130.4, 130.0, 125.7, 125.0, 124.1, 123.9, 122.7, 103.0, 72.2, 61.0, 56.3, 48.2, 36.9, 34.9, 13.5. **HRMS** (ESI+) *m*/*z* calcd. for $C_{21}H_{20}BrNO_4Na$ $[M+Na]^+$: 452.0468; found: 452.0466. **UPC^2**: IC, CO_2/MeOH 80/20, 3.0 mL·min^{-1}; t_{minor} = 3.8 min; t_{major} = 4.6 min.

3. X-Ray structure of cycloadduct 4m



4m

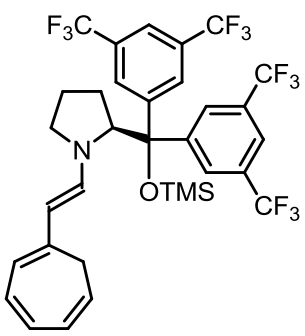


4m

Crystal data for **4m**: $C_{21}H_{20}BrNO_4$, M = 430.29, monoclinic, Space group P 1 21 1 (no. 6), a = 10.3326(5) Å, b = 6.3617(3) Å, c = 14.1521(7) Å, β = 96.731(2)°, V = 923.85(8) Å^3, T = 100 K, Z = 2, d_c = 1.547 g cm^{-3}, μ(Mo Kα, λ = 0.56086 Å) = 1.213 mm^{-1}, 13541 reflections collected, 5045 unique [R_{int} = 0.0341], which were used in all calculations. Refinement on F^2, final R(F) = 0.0384, R_w(F2) = 0.0774. CCDC 974344.

4. Synthesis of intermediates I, III and product V

4.1. Tetraenamine Ia



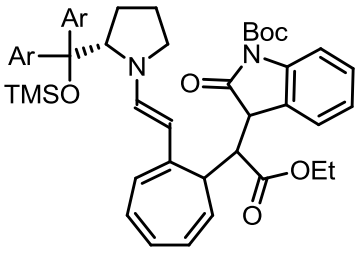
Ia

In a NMR tube aldehyde **1** (0.10 mmol, 1.0 equiv.) and catalyst **3** (Ar = 3,5-$(CF_3)_2C_6H_3$, 0.10 mmol, 1.0 equiv.) or catalyst **3b** (Ar = Ph, 0.10 mmol, 1.0 equiv.) were dissolved in 0.4 mL of $CDCl_3$ and molecular sieves (4 Å) were added. The reaction mixture was shaken for 15 min to obtain **I** as a crude product.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (m, 2H), 7.91 (m, 4H), 6.8 (d, *J* = 13.7 Hz, 1H), 6.47 (dd, *J* = 11.0, 6.3 Hz, 1H), 6.27 (dd, *J* = 11.0, 5.5 Hz, 1H), 6.18 (dd, *J* = 9.2, 5.5 Hz, 1H), 5.86 (d, *J* = 6.3 Hz, 1H), 5.21 (m, 1H), 5.14 (d, *J* = 13.7 Hz, 1H), 4.59 (dd, *J* = 9.2, 1.9 Hz, 1H), 2.92 (m, 1H), 2.45 (m, 2H), 2.31 (m, 1H), 2.23 (m, 1H), 1.83 (m, 1H), 1.61 (m, 1H), 0.42 (m, 1H), −0.11 (m, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 144.5, 143.5, 138.1, 132.9, 131.7 (q, *J* = 34 Hz, 2C), 131.5 (q, *J* = 34 Hz, 2C), 131.3, 129.3 (m, 2C), 129.2 (m, 2C), 127.6, 126.3, 123.1, (q, *J* = 270 Hz, 4C), 122.1 (m, 2C), 120.1, 118.4, 103.8, 83.2, 70.6, 49.1, 29.0, 27.5, 22.5, 1.6 (3C). **HRMS** (ESI+) *m*/*z* calcd. for $C_{33}H_{30}F_{12}NOSi$ $[M-H]^+$: 712.1900; found: 712.1901.

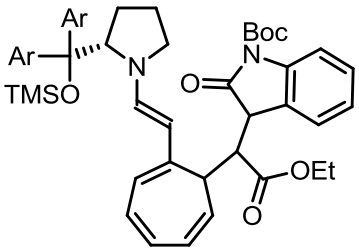
4.2. Intermediate III

In a NMR tube aldehyde **1** (0.10 mmol) and catalyst **3** (Ar = 3,5-$(CF_3)_2C_6H_3$, 0.10 mmol, 1.0 equiv.) or catalyst **3b** (Ar = Ph, 0.10 mmol, 1.0 equiv.) were dissolved in 0.4 mL of $CDCl_3$ and molecular sieves (4 Å) were added. The reaction mixture was shaken for 15 min and oxindole **4a** (0.10 mmol, 1.0 equiv.) was added. After 5 min the reaction mixture was analyzed by NMR spectroscopy. When catalyst **3b** (Ar = Ph) was used the product could be purified by FC (pentane/EtOAc 10/1) affording the pure compound **IIIb**.



IIIa

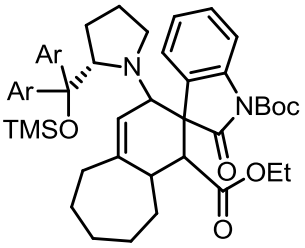
IIIa (Ar = 3,5-$(CF_3)_2C_6H_3$): **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.98 (m, 1H), 7.93 (m, 1H), 7.86 (m, 3H), 7.77 (m, 4H), 7.31 (m, 2H), 7.18 (d, *J* = 7.5 Hz, 1H), 6.57 (dd, *J* = 10.9, 7.1 Hz, 1H), 6.38 (dd, *J* = 10.9, 6.2 Hz, 1H), 6.26 (dd, *J* = 9.8, 6.2 Hz, 1H), 6.00 (d, *J* = 7.0 Hz, 1H), 5.43 (dd, *J* = 9.2, 9.2 Hz, 1H), 4.95 (d, *J* = 10.5 Hz, 1H), 4.26 (m, 1H), 4.10 (m, 3H), 3.60 (s, 1H), 3.27 (d, *J* = 11.0 Hz, 1H), 2.77 (m, 1H), 2.39 (t, *J* = 9.0 Hz, 1H), 2.12 (m, 1H), 1.7 (m, 1H), 1.64 (s, 9H), 1.13 (t, *J* = 6.8 Hz, 3H), 0.36 (m, 1H), −0.10 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.2, 172.3 149.5, 144.4 (2C), 143.8, 142.0, 141.0, 132.9, 131.7 (q, *J* = 33 Hz, 2C), 131.2 (q, *J* = 34 Hz, 2C), 130.3, 129.3 (m, 2C), 129.2 (m, 2C), 127.7, 127.0, 125.8, 125.0, 124.1, 123.6, 123.5, 123.0 (q, *J* = 273 Hz, 4C), 122.2 (m, 1C), 122.0 (m, 1C), 114.6, 103.8, 83.6, 83.0, 70.6, 60.5, 48.7, 45.5, 41.4, 36.4, 28.1 (3C), 27.2, 22.5, 13.9, 1.6 (3C). **HRMS** (ESI+) *m*/*z* calcd. for $C_{50}H_{51}F_{12}N_2O_6Si$ $[M+H]^+$: 1031.3319; found: 1031.3330.



IIIb

IIIb (Ar = Ph): **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.0 Hz, 1H), 7.51 – 7.22 (m, 14H), 6.53 (dd, *J* = 10.7, 7.2 Hz, 1H), 6.28 (dd, *J* = 10.7, 6.2 Hz, 1H), 6.20 (dd, *J* = 8.9, 6.2 Hz, 1H), 5.90 (d, *J* = 7.2 Hz, 1H), 5.24 (dd, *J* = 8.9, 8.9 Hz, 1H), 4.71 (d, *J* = 13.5 Hz, 1H), 4.28 (m, 1H), 4.16 (m, 1H), 4.05 (m, 1H), 3.91 (m, 1H), 3.58 (s, 1H), 3.21 (d, *J* = 11.3 Hz, 1H), 2.68 (m, 1H), 2.41 (t, *J* = 9.1 Hz, 1H), 1.94 (m, 2H), 1.66 (s, 9H), 1.38 (m, 1H), 1.16 (t, *J* = 7.0 Hz, 3H), 0.28 (m, 1H), −0.14 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.3, 172.3 149.5, 142.3 (2C), 141.8, 141.6, 141.0, 132.6, 130.5, 129.9 (2C), 129.2 (2C), 127.8, 127.6, 127.5 (2C), 127.3 (2C), 127.3, 126.8, 126.3, 124.3, 123.6, 123.4, 117.7, 114.6, 100.4, 83.5, 83.2, 69.9, 60.4, 48.2, 45.7, 41.4, 36.4, 28.2 (3C), 27.3, 22.3, 14.0, 1.9 (3C). **HRMS** (ESI+) *m/z* calcd. for $C_{46}H_{55}N_2O_6Si$ $[M+H]^+$: 759.3824; found: 759.3834.

4.3. Product V



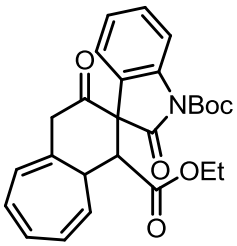
V

In a glass vial a mixture of oxindole **2a** (0.10 mmol, 1.0 equiv.), *o*-FBA (0.02 mmol, 20 mol%) catalyst **3** (0.02 mmol, 20 mol%) were dissolved in 0.4 mL of $CHCl_3$ and aldehyde **5** (0.12 mmol, 1.2 equiv.) was added. The mixture was stirred at rt or 40 °C for 48 h and monitored by ^{1}H NMR spectroscopy. Compound **IV** was the only product detected. For the full characterization of **IV** the reaction was performed with 1 equiv. of **3**.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.94 (s, 2H), 7.90 (s, 1H), 7.80 (s, 2H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.33 (m, 1H), 7.17 (dt, *J* = 14.8, 7.3 Hz, 2H), 5.73 (s, 1H), 4.12 (d, *J* = 9.3 Hz, 2H), 3.93 (m, 2H), 3.49 (dd, *J* = 17.2, 7.3 Hz, 1H), 3.38 (d, *J* = 10.7 Hz, 1H), 3.13 (d, *J* = 9.8 Hz, 1H), 2.51 (m, 4H), 2.01 (m, 1H), 1.92 (dd, *J* = 13.7, 5.0 Hz, 1H), 1.79 (s, 9H), 1.64 (m, 3H), 1.51 (m, 6H), 1.05 (t, *J* = 7.1 Hz, 3H), −0.50 (s, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 176.1, 171.5, 149.1, 145.7, 145.0, 144.4, 137.8, 131.3 (q, *J* = 32.9 Hz, 2C), 130.6, 130.2 (q, *J* = 32.9 Hz, 2C), 130.2 (m, 2C), 128.9 (m, 2C), 128.1, 124.4, 123.8, 123.3 (q, *J* = 271.59 Hz, 2C), 123.0 (q, *J* = 271.59 Hz, 2C) 122.1 (m, 1C), 121.7, 121.2 (m, 1C), 114.0, 85.1, 84.5, 69.1, 62.6, 60.7, 54.4, 49.9, 48.2, 37.2, 35.6, 31.9, 30.7, 29.5, 29.2, 28.1 (3C), 25.3, 22.6, 13.5, 1.0 (3C). **HRMS** (ESI+) *m/z* calcd. for $C_{50}H_{55}F_{12}N_2O_6Si$ $[M+H^+]^+$: 1035.3632; found: 1035.3635.

5. Transformations

5.1. Product 6

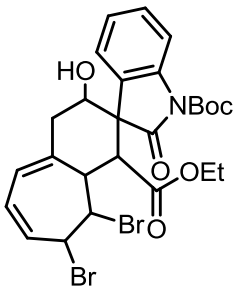


6

In a glass vial cycloadduct **4a** (45.1 mg, 0.1 mmol, 1.0 equiv.) was solved in $CHCl_3$ (1 mL) and cooled to −20 °C. A solution of Dess Martin periodinane (72.0 mg, 0.17 mmol, 1.7 equiv.) in $CHCl_3$ (1 mL) was added to the solution and the reaction mixture was warmed to rt. After 1 h additional 0.5 equiv. of Dess Martin periodinane were added and the reaction mixture was stirred for further 30 min. The reaction mixture was plugged over Iatrobeads, the solvent was removed in vacuum and the product was purified by FC (pentane/EtOAc 15/1) to afford the pure compound **6** in 94% yield and >95/5 dr.

Colourless oil. $[\alpha]_D^{20}$ = −222.4 (*c* 0.53, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.2 Hz, 1H), 7.30 (dd, *J* = 8.2, 7.6 Hz, 1H), 7.02 (dd, *J* = 7.6, 7.8 Hz, 1H), 6.80 (m, 2H), 6.69 (dd, *J* = 11.0, 5.6 Hz, 1H), 6.30 (dd, *J* = 9.2, 5.6 Hz, 1H), 6.21 (d, *J* = 5.6 Hz, 1H), 5.29 (dd, *J* = 9.2, 4.7 Hz, 1H), 4.25 (d, *J* = 12.5 Hz, 1H), 3.87 (m, 2H), 3.79 (d, *J* = 16.8 Hz, 1H), 3.36 (d, *J* = 16.8 Hz, 1H), 2.60 (dd, *J* = 12.5, 4.7 Hz, 1H), 1.65 (s, 9H), 0.93 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 200.8, 172.9, 169.21, 148.7, 141.3, 131.8, 129.5, 129.4, 126.0, 125.4, 124.7, 124.6, 124.5, 123.7, 123.2, 115.5, 84.7, 64.5, 61.4, 49.7, 46.9, 37.9, 28.0 (3C), 13.4. **HRMS** (ESI+) *m/z* calcd. for $C_{26}H_{27}NO_6Na$ $[M+Na]^+$: 472.1731; found: 472.1731.

5.2. Product 7

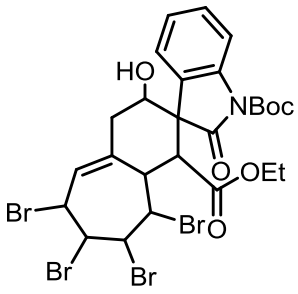


7

In a dry flask under Ar cycloadduct **4a** (45 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry $CDCl_3$ (2 mL) and cooled to −78 °C. A freshly prepared solution of Br_2 (1.0 M in $CDCl_3$, 100 µL, 0.1 mmol, 1.0 equiv.) was added dropwise. The mixture was kept at −78 °C for 2 h. The crude NMR indicates a full conversion of **4a** and a clean formation of **7**, which is stable in solution.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.35 (m, 2H), 7.18 (t, *J* = 7.6 Hz, 1H), 6.05 (d, *J* = 7.7 Hz, 1H), 5.94 (dd, *J* = 11.6, 7.7 Hz, 1H), 5.87 (dd, *J* = 11.6, 5.9 Hz, 1H), 5.17 (m, 1H), 4.68 (d, *J* = 4.3 Hz, 1H), 4.28 (br d, *J* = 11.3 Hz, 1H), 3.99 (d, *J* = 11.3 Hz, 1H), 3.87 (dd, *J* = 6.4, 2.9 Hz, 1H), 3.74 (m, 2H), 2.86 (m, 2H), 1.66 (s, 9H), 0.85 (t, *J* = 7.1 Hz, 3H).

5.3. Product 8



8

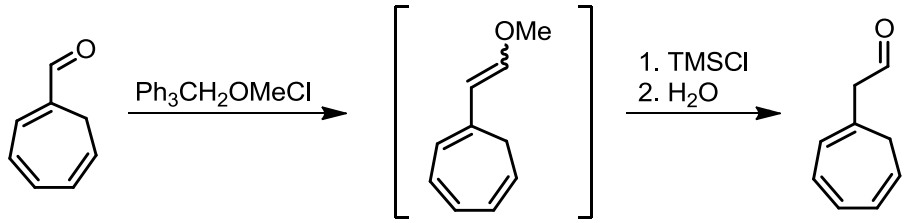
In a dry flask under Ar cycloadduct **4a** (45 mg, 0.1 mmol, 1.0 equiv.) was dissolved in dry $CDCl_3$ (2 mL) and cooled to −78 °C. A freshly prepared solution of Br_2 (1.0 M in $CDCl_3$, 100 µL, 0.1 mmol, 1.0 equiv.) was added dropwise. The mixture was kept at −78 °C for 1 h and again a solution of Br_2 (1.0 M in $CDCl_3$, 200 µL, 0.2 mmol, 2.0 equiv.) was added. After additional 6 h ^{1}H NMR analysis of the crude indicated full conversion of starting material. The reaction was quenched with sat. $Na_2S_2O_3$ solution and extracted with CH_2Cl_2 (3 x 10 mL) giving the clean product **8** in 71 % yield.

Orange oil. $[\alpha]_D^{20}$ = +66.4 (*c* 0.33, CH_2Cl_2). **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.35 (m, 2H), 7.20 (t, *J* = 7.5 Hz, 1H), 6.26 (d, *J* = 3.0 Hz, 1H), 5.46 (m, 1H), 5.17 (dd, *J* = 5.7, 3.3 Hz, 1H), 4.96 (dd, *J* = 7.9, 5.7 Hz, 1H), 4.72 (dd, *J* = 3.3, 1.3 Hz, 1H), 4.29 (br d, *J* = 11.2 Hz, 1H), 3.93 (d, *J* = 11.2 Hz, 1H), 3.84 (m, 1H), 3.74 (m, 2H), 3.13 (br s, 1H), 2.87 (dd, *J* = 14.1, 8.5 Hz, 1H), 2.70 (d, *J* = 14.1 Hz, 1H), 1.66 (s, 9H), 0.86 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 176.5, 169.8, 148.9, 140.0, 138.7, 129.4, 127.7, 127.7, 125.0, 124.5, 115.2, 85.0, 72.4, 61.6, 55.6, 55.6, 55.4, 55.2, 49.1, 48.4, 39.7, 36.7, 28.1 (3C), 13.3. **HRMS** (ESI+) *m*/*z* calcd. for $C_{26}H_{30}Br_4NO_6$ $[M+H]^+$: 767.8801; found: 767.8801.

6. Synthesis of starting materials

6.1. Aldehyde 1

Aldehyde **9** was prepared according to literature procedure in 15 g scale.[2]



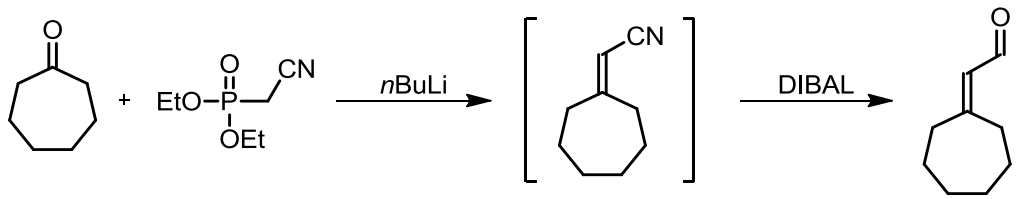
9 **10** **1**

E/Z = 1/1

A solution of (methoxymethyl)triphenylphosphonium chloride (20.3 g, 59.3 mmol, 1.3 equiv.) in dry THF (180 mL) was cooled to 0 °C under Ar and a *n*BuLi solution (1.6 M in hexane, 35.6 mL, 57.0 mmol, 1.25 equiv.) was added dropwise. The mixture was stirred for 2 h at 0 °C. A solution of aldehyde **9** (5.5 g, 45.6 mmol, 1.0 equiv.) in THF (40 mL) was added dropwise. After full addition, the reaction mixture was warmed to rt and stirred for further 12 h. After full conversion of aldehyde (TLC) the reaction mixture was poured into cold pentane (300 mL, −78 °C). The crude mixture was filtrated over Celite and sand and the filtrate was washed with a 1/1 mixture of pentane/Et_2O (500 mL, −20 °C) . The solvent was evaporated carefully (product **10** is volatile!). The crude product **10** was used for the next step without further purification.

A solution of crude product **10** in dry CH_2Cl_2 (50 mL) was cooled to 0 °C under Ar and TMSCl (17.0 mL, 136.8 mmol, 3.0 equiv.) was added dropwise. The reaction mixture was stirred for 15 min at 0 °C and further 2 h at rt. Then the reaction mixture was cooled to 0 °C again and H_2O (8.0 mL, 456.0 mmol, 10 equiv.) was added dropwise. After 45 min H_2O (250 mL) and sat. $NaHCO_3$ solution (60 mL) were added at 0 °C. After extraction with CH_2Cl_2 (3 x 100 mL) the combined organic layer was dried with Na_2SO_4 and the solvent was evaporated. FC on Iatrobeats (pentane/ CH_2Cl_2 4/1 to 2/1) afforded the pure aldehyde **1** in 40% yield over 2 steps. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.60 (t, *J* = 2.3 Hz, 1H), 6.56 (m, 2H), 6.20 (m, 1H), 6.09 (d, *J* = 5.2 Hz, 1H), 5.40 (m, 1H), 3.36 (m, 2H), 2.31 (m, 2H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 198.8, 130.7, 130.2, 127.1, 125.9, 124.9, 120.4, 53.1, 32.5. **HRMS** (APCI+) *m/z* calcd. for $C_9H_{11}O$ $[M+H]^+$: 135.0804; found: 135.0801.

6.2. Aldehyde 5



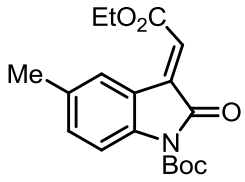
11 **12** **5**

A solution of diethyl cyanomethylphosphonate (1.89 mL, 11.6 mmol, 1.3 equiv.) in dry THF (17.2 mL) was cooled to 0 °C under Ar. *n*BuLi solution (1.6 M in hexane, 11.6 mL, 10.7 mmol, 1.2 equiv.) was added dropwise and the mixture stirred for 1.5 h at the same temperature. A solution of cycloheptanone (1.1 mL, 8.9 mmol, 1.0 equiv.) **11** in dry THF (11.5 mL) was added and the mixture was stirred for 1 h at 0 °C and then allowed to gradually warm up to rt and stirred for additionally 4 h. The reaction mixture was flushed through a plug of silica (pentane/EtOAc 95/5) and the resulting solution concentrated. One quarter of the homologated crude product was solved in dry CH_2Cl_2 (1.3 mL) in a dry flask equipped with a magnetic stirring bar under Ar atmosphere and cooled to −78 °C. DIBAL was added dropwise and the mixture was allowed to warm up to −30 °C within a period of 2 h. The consumption of the starting material was monitored by TLC and after 4 h the reaction was quenched with EtOAc (1 mL) followed by addition of a sat. aq. solution of Rochelle's salt. The suspension was stirred overnight and the phases separated. The aqueous layer was extracted with EtOAc (3 x 20 mL), the combined organic layers were dried over Na_2SO_4, filtered and concentrated. The crude mixture was subjected to FC on silica (pentane/EtOAc 98/2 to 92/8) to give the pure unsaturated aldehyde **5** in 34% yield over 2 steps.

^{1}H NMR (400 MHz, $CDCl_3$) δ δ 9.99 (d, *J* = 8.1 Hz, 1H), 5.85 (d, *J* = 8.1 Hz, 1H), 2.84 (m, 2H), 2.42 (m, 2H), 1.71 (m, 4H), 1.56 (m, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 191.17, 170.22, 127.62, 38.89, 30.53, 29.28, 28.61, 27.41, 27.37. **HRMS** (APCI+) *m*/*z* calcd. for $C_9H_{15}O$ $[M+H]^+$: 139.1117; found: 139.1114.

6.3. Oxindoles

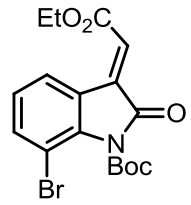
All oxindoles **2** were prepared according to literature procedures.[1] Analytical data for the oxindoles **2i**, **2h** and **2d** not described in literature are given below. For descriptive procedure of product **2l** see below.



2d

Compound **2d** was isolated by FC on silica (pentane/EtOAc 10/1) in 40% yield over two steps.

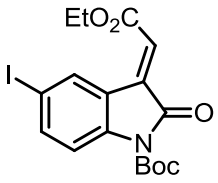
Yellow solid. **Mp**: 123.3 - 124.3 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.49 (m, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.24 (dd, *J* = 8.5, 1.3 Hz, 1H), 6.89 (s, 1H), 4.33 (q, *J* = 7.1 Hz, 2H), 2.38 (s, 3H), 1.64 (s, 9H), 1.38 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.9, 165.5, 148.8, 139.7, 136.6, 134.2, 133.4, 128.6, 122.8, 120.1, 114.7, 84.6, 61.3, 28.1 (3C), 21.1, 14.2. **HRMS** (ESI+) *m*/*z* calcd. for $C_{18}H_{21}NO_5Na$ $[M+Na]^+$: 354.1317; found: 354.1314.



2h

Compound **2h** was isolated by FC on silica (pentane/EtOAc 20/1) in 12% yield over two steps.

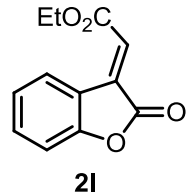
Pale orange solid. **Mp**: 67.7 - 69.7 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 8.1 Hz, 1H), 7.07 (t, *J* = 8.0 Hz, 1H), 6.92 (s, 1H), 4.33 (q, *J* = 7.1 Hz, 2H), 1.65 (s, 9H), 1.37 (dd, *J* = 9.5, 4.7 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 166.6, 165.3, 147.9, 140.7, 137.4, 136.5, 127.8, 125.9, 125.0, 123.7, 107.1, 86.2, 61.9, 28.0 (3C), 14.4. **HRMS** (ESI+) *m*/*z* calcd. for $C_{17}H_{18}BrNO_5Na$ $[M+Na]^+$: 418.0266; found: 418.0268.



2i

Compound **2i** was isolated by FC on silica (pentane/EtOAc 10/1) in 70% yield over two steps.

Yellow solid. **Mp**: 99.4 - 101.0 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 9.02 (d, *J* = 1.7 Hz, 1H), 7.74 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.69 (d, *J* = 8.6 Hz, 1H), 6.91 (s, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 1.63 (s, 9H), 1.39 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 165.0, 164.8, 148.6, 141.4, 141.18, 136.8, 135.0, 124.6, 122.0, 116.9, 88.0, 85.1, 61.6, 28.0 (3C), 14.1. **HRMS** (ESI+) *m*/*z* calcd. for $C_{17}H_{18}INO_5Na$ $[M+Na]^+$: 466.0127; found: 466.0124.



2l

To a solution of benzofuran-2(3*H*)one (1.0 g, 7.46 mmol, 1.0 equiv.) in dry toluene (20 mL) was added ethyl glyoxalate solution (50% in toluene, 1.55 mL, 7.83 mmol, 1.05 equiv.) and triethylamine (155.9 µL, 1.12 mmol, 0.15 equiv.). The mixture was stirred under reflux conditions until TLC analysis indicated full conversion of the starting material. The reaction mixture was then poured into cold water (40 mL) and extracted with Et_2O (3 x 20 mL), the layers were separated and the organic phase was washed with water (4 x 12 mL) and dried with Na_2SO_4. Column chromatography on silica (pentane/EtOAc 10/1) afforded the pure product **2l** in 40% yield as a yellow solid. **Mp**: 84.7 - 85.4 °C. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 7.9 Hz, 1H), 7.48 (td, *J* = 8.0, 1.2 Hz, 1H), 7.22 (t, *J* = 7.7 Hz, 1H), 7.14 (d, *J* = 8.1 Hz, 1H), 6.93 (s, 1H), 4.35 (q, *J* = 7.1 Hz, 2H), 1.38 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 167.7, 1649, 156.1, 133.8, 133.5, 128.9, 125.4, 124.6, 120.6, 111.0, 61.6, 14.1. **HRMS** (ESI+) *m*/*z* calcd. for $C_{12}H_9O_4Na$ $[M+Na]^+$: 241.0471; found: 241.0469.

7. Computational Data

7.1 Methods

All calculations were run using GAUSSIAN09.[3] All structures were optimized in a solvent continuum with IEFPCM-wB97xD/6-31+G(d,p). Solvent effects were estimated with IEFPCM, using chloroform as the solvent. Frequency calculations were performed for all stationary points to identify them as local minima or first order saddle points and to obtain the ZPEs and thermochemical corrections for the free energies. All of the reported values are free energies at 298 K. Intrinsic reaction coordinate (IRC) calculations were used to characterize transition state structures.[4]

7.2 Additional Computational Results

In addition to the data presented in the text we have also examined a variety of other pathways for the reaction of the oxindole **C** with the tetraenamine intermediate. Using the lowest energy conformer of the tetraeneamine intermediate **A** we examined addition of **C** to both the γ- and ζ-carbons of **A** (Figure S1). Addition at the ζ- carbon has a barrier of 32.4 kcal/mol and is highly reactant favored, suggesting that this addition is unlikely to occur.

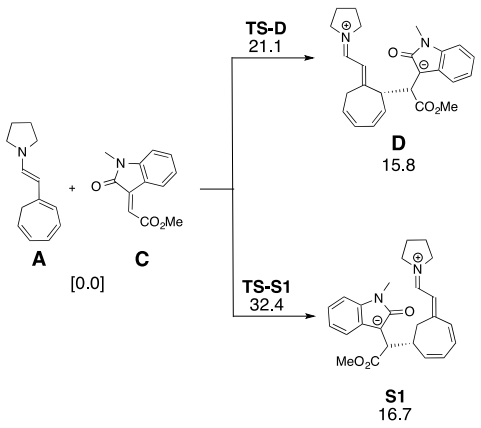


Figure S1: Addition pathways for reaction of tetraeneamine intermediate **A** with **C**. Activation energies are Gibbs free energies (kcal/mol) from IEFPCM-wB97xD6-31+G(d,p) in $CHCl_3$.

We also explored the endo and exo pathways for the addition through the productive conformer of the tetraenamine **B**. Both approaches of the oxindole (**TS-E** and **TS-S2**) were examined. In both the endo and exo pathways, the first addition step is the highest in energy. The approach with the carbonyl of the oxindole over the diene, **TS-E**, is favored by 1.3 kcal/mol.

Additionally we also examined the possibility that intermediate **E** could isomerize to form an intermediate with all three double bonds in the ring system **S4** that would then be able to cyclize. However, our calculations reveal that intermediate **S4** is much higher in energy than **E** and is unlikely to be formed in solution.

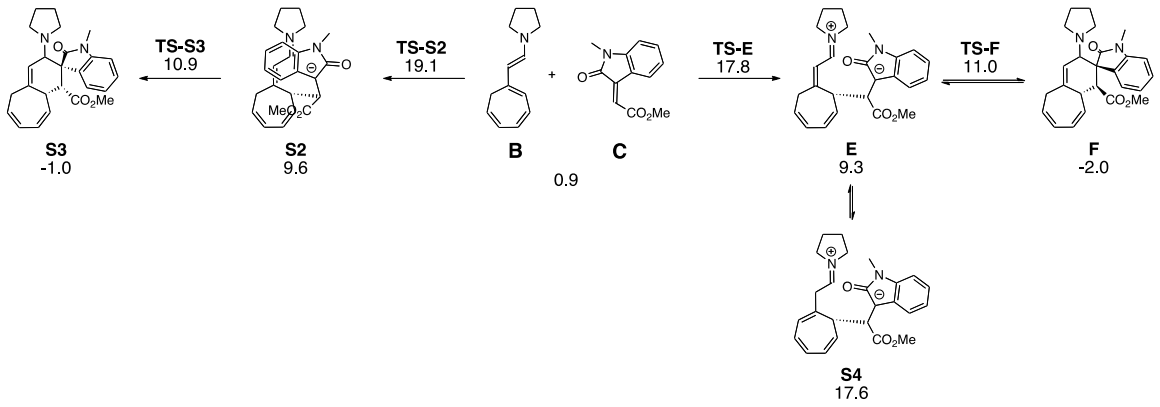


Figure S2: Addition pathways for reaction of tetraeneamine intermediate **B** with **C**. Activation energies are Gibbs free energies (kcal/mol) from IEFPCM-wB97xD/6-31+G(d,p) in $CHCl_3$. All energies are relative to sum of the lowest energy conformers of the reactants (**A** and **C**).

The cross-tetraenamine system was also examined. In this case, the cross tetraenamine intermediate **S5** is 4.5 kcal/mol higher in energy than the lowest energy conformer of the fully conjugated tetraene **A**. Cyclization of the cross tetraenamine with the oxindole **C** occurs in a single, highly asynchronous, step with a barrier of 18.8 kcal/mol and leads to a cyclized product that is 6.6 kcal/mol lower in energy than the reactants (Figure S3). The high asynchronicity of **TS-S6** suggests that the reaction should occur in two steps, however, no zwitterionic intermediate could be located with this method.

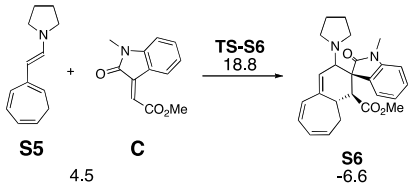


Figure S3: Addition pathways for reaction of cross-tetraenamine intermediate **S5** with **C**. Energies Activation energies are Gibbs free energies (kcal/mol) from IEFPCM-wB97xD/6-31+G(d,p) in $CHCl_3$. All energies are relative to sum of the lowest energy conformers of the reactants (**A** and **C**).

7.3 Coordinates

Prod-H (cyclized product of **H**)

HF = -1167.7136524 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.372304 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.321358 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.392295 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.052325	0.993432	-0.964583
2	6	4.308335	1.271707	-0.566423
3	6	4.926661	0.752032	0.634464
4	6	2.056186	0.259377	-0.100604
5	6	4.649951	-0.462291	1.183632
6	6	2.538135	-1.170276	0.040748
7	6	3.688889	-1.431594	0.705568
8	1	2.718388	1.332834	-1.944626
9	1	4.927215	1.901637	-1.202926
10	1	5.763743	1.313417	1.044204
11	1	2.052983	0.726823	0.894773
12	1	5.287429	-0.791005	2.003010
13	6	1.572233	-2.238382	-0.360335
14	6	0.243472	-2.018453	0.427250
15	1	0.566803	-1.702749	1.454950
16	1	1.355746	-2.229934	-1.436083
17	6	0.652718	0.343959	-0.714681

18	6	-0.412742	-0.644370	-0.150309
19	6	-1.355438	-0.089332	0.877988
20	6	-1.372499	-1.036798	-1.275768
21	6	0.118006	1.761090	-0.640170
22	8	-0.958959	1.910516	-1.424473
23	8	0.555917	2.656147	0.053570
24	6	-1.671203	3.142944	-1.299023
25	6	-2.671155	-0.288738	0.441880
26	7	-2.659406	-0.869862	-0.826622
27	8	-1.072653	-1.411600	-2.402647
28	6	-1.123686	0.501034	2.106546
29	6	-2.216427	0.900147	2.890695
30	6	-3.518087	0.693628	2.441074
31	6	-3.767558	0.090551	1.200924
32	1	-0.107879	0.659635	2.457451
33	1	-2.045563	1.371070	3.853625
34	1	-4.356341	1.002314	3.058735
35	1	-4.782640	-0.071856	0.852809
36	6	-3.837940	-1.188546	-1.591606
37	1	0.736893	0.093423	-1.779952
38	1	-2.503760	3.071499	-1.996840
39	1	-2.039333	3.260095	-0.276788
40	1	-1.028991	3.987555	-1.557375
41	1	-4.423343	-0.285533	-1.798192
42	1	-3.513738	-1.630774	-2.533636
43	1	-4.462495	-1.906059	-1.050754
44	8	-0.594218	-3.049579	0.423035
45	1	1.955288	-3.229998	-0.102311
46	1	3.913666	-2.473968	0.926800

Prod-I (cyclized product of **I**)

HF = -1167.7075691 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.373893 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.323598 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.383971 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.893729	1.217640	1.120901
2	6	4.082365	1.446149	0.537005
3	6	4.793507	0.632027	-0.434836
4	6	1.883418	0.120115	0.875236
5	6	4.565716	-0.671535	-0.701426
6	6	2.416682	-1.253734	0.532072
7	6	3.546410	-1.547177	-0.149125
8	1	2.571158	1.944314	1.861590
9	1	4.602910	2.351711	0.846158
10	1	5.630954	1.111234	-0.936902
11	1	1.342107	0.013120	1.822508
12	1	5.237291	-1.152075	-1.410613
13	6	1.367137	-2.300829	0.723020
14	6	0.279949	-2.121588	-0.400158
15	1	0.872597	-2.076853	-1.347787
16	1	1.767727	-3.312299	0.606990
17	6	0.812338	0.479502	-0.185200
18	6	-0.303587	-0.609678	-0.312718
19	6	-1.414390	-0.489261	0.700165
20	6	-1.055447	-0.415928	-1.632276

21	6	0.155595	1.812925	0.123633
22	8	-0.486210	2.300838	-0.946812
23	8	0.150169	2.373470	1.201337
24	6	-1.278417	3.471395	-0.733565
25	6	-2.626410	-0.325022	0.014976
26	7	-2.394650	-0.298353	-1.361134
27	8	-0.565875	-0.387696	-2.754103
28	6	-1.430362	-0.526786	2.084008
29	6	-2.646352	-0.393433	2.767649
30	6	-3.836869	-0.229227	2.065571
31	6	-3.843571	-0.193080	0.666560
32	1	-0.513386	-0.655659	2.648294
33	1	-2.657352	-0.421628	3.852739
34	1	-4.774401	-0.129063	2.604280
35	1	-4.770905	-0.069671	0.116421
36	6	-3.419049	-0.130910	-2.360490
37	1	1.296753	0.557200	-1.165354
38	1	-1.744532	3.685902	-1.693707
39	1	-2.038800	3.278012	0.026729
40	1	-0.650474	4.307138	-0.417535
41	1	-3.919668	0.836764	-2.243349
42	1	-2.941859	-0.173768	-3.339553
43	1	-4.163107	-0.930015	-2.286868
44	8	-0.674096	-3.045207	-0.392876
45	1	3.688313	-2.600866	-0.386244
46	1	0.880959	-2.235663	1.703763

Prod-G (cyclized product of **G**)

HF = -1167.6960971 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.371785 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.320763 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.375334 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.001337	1.343194	-0.486914
2	6	4.315746	1.480321	-0.246200
3	6	5.132622	0.582613	0.574539
4	6	2.043884	0.361301	0.157983
5	6	4.949367	-0.746494	0.594767
6	6	2.494457	-1.092558	0.197111
7	6	3.897901	-1.433312	-0.239305
8	1	2.551122	2.083510	-1.144856
9	1	4.826126	2.331064	-0.695883
10	1	5.945108	1.024440	1.148255
11	1	1.906766	0.699639	1.197980
12	1	5.585160	-1.365077	1.224444
13	1	4.027837	-1.119866	-1.286696
14	1	4.031624	-2.517664	-0.203107
15	6	1.612564	-2.002460	0.616783
16	6	0.228144	-1.632818	1.109014
17	1	0.399249	-0.938354	1.979226
18	1	1.867778	-3.060143	0.656541
19	6	0.659036	0.422512	-0.535876
20	6	-0.409691	-0.560800	0.036712

21	6	-1.612673	0.041978	0.709402
22	6	-1.050478	-1.349556	-1.102506
23	6	0.075989	1.819391	-0.545716
24	8	-0.860644	1.941415	-1.498397
25	8	0.357783	2.720871	0.217918
26	6	-1.663121	3.123520	-1.446012
27	6	-2.769196	-0.465724	0.106731
28	7	-2.414781	-1.295954	-0.956911
29	8	-0.477148	-1.928003	-2.018299
30	6	-1.727980	0.887025	1.798136
31	6	-3.004485	1.241778	2.259097
32	6	-4.143468	0.736099	1.638319
33	6	-4.041853	-0.136509	0.546729
34	1	-0.840636	1.279564	2.284874
35	1	-3.102410	1.912525	3.107038
36	1	-5.126777	1.012199	2.007617
37	1	-4.929170	-0.542644	0.071780
38	6	-3.353713	-1.989368	-1.802043
39	1	0.819663	0.131111	-1.580084
40	1	-2.386510	3.022994	-2.253378
41	1	-2.174647	3.181614	-0.481849
42	1	-1.050417	4.015632	-1.591116
43	1	-3.983111	-1.280505	-2.351298
44	1	-2.784816	-2.590530	-2.511384
45	1	-3.991744	-2.646177	-1.202934
46	8	-0.581623	-2.652089	1.383618

A

HF = -560.1751663 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.274327 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.233697 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -559.941469 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.714214	1.315123	-0.258567
2	6	4.498044	0.268622	0.137393
3	6	4.003012	-0.961279	0.716514
4	6	2.277092	1.401668	-0.211292
5	6	2.804190	-1.509633	0.431101
6	6	1.394501	0.360548	-0.306622
7	6	1.949734	-0.993830	-0.692922
8	1	4.231863	2.234817	-0.528161
9	1	5.574398	0.425704	0.152548
10	1	4.635977	-1.441924	1.460646
11	1	1.866437	2.402045	-0.080836
12	1	2.448395	-2.361964	1.005296
13	1	2.570297	-0.869267	-1.590837
14	1	1.165908	-1.710115	-0.940706
15	6	-0.024653	0.576818	-0.092116
16	6	-0.995854	-0.370472	-0.208183
17	1	-0.744407	-1.394748	-0.470548
18	7	-2.321040	-0.177484	-0.014790

19	6	-2.904566	1.109819	0.331780
20	6	-3.320425	-1.234347	-0.146244
21	6	-4.385493	0.789495	0.566565
22	1	-2.762281	1.824919	-0.491623
23	1	-2.422757	1.530646	1.222958
24	6	-4.627730	-0.455730	-0.296526
25	1	-3.341061	-1.869233	0.751325
26	1	-3.099513	-1.869431	-1.009502
27	1	-4.552896	0.552064	1.622286
28	1	-5.036008	1.625812	0.302427
29	1	-5.497163	-1.034693	0.022204
30	1	-4.771403	-0.169225	-1.343674
31	1	-0.310903	1.586165	0.194448

B

HF = -560.174567 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.274481 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.234471 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -559.940096 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.329234	-1.379414	-0.559419
2	6	-4.241149	-0.764679	0.253868
3	6	-3.960315	0.363784	1.111003
4	6	-1.944611	-1.033160	-0.742207
5	6	-3.037181	1.314553	0.849353
6	6	-1.399971	0.212758	-0.579641
7	6	-2.345346	1.392814	-0.480939
8	1	-3.650154	-2.305666	-1.034098
9	1	-5.211301	-1.243370	0.369329
10	1	-4.514942	0.418477	2.046347
11	1	-1.285529	-1.848443	-1.033796
12	1	-2.792028	2.052990	1.609199
13	1	-3.091700	1.333069	-1.284375
14	1	-1.802642	2.335250	-0.585505
15	6	0.026943	0.479316	-0.527103
16	6	0.939721	-0.430651	-0.083084
17	1	0.594807	-1.390145	0.297856
18	7	2.278890	-0.264085	-0.038958

19	6	2.944239	0.956272	-0.472146
20	6	3.202576	-1.229158	0.554859
21	6	4.433192	0.645708	-0.286366
22	1	2.623376	1.803477	0.152124
23	1	2.685597	1.191371	-1.511646
24	6	4.442649	-0.384057	0.851073
25	1	3.435334	-2.032539	-0.157860
26	1	2.768364	-1.680289	1.451563
27	1	4.839443	0.198752	-1.199740
28	1	5.016059	1.540834	-0.059705
29	1	5.356985	-0.980520	0.881527
30	1	4.327516	0.118684	1.817166
31	1	0.359493	1.472148	-0.821179

S5

HF = -560.1683258 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.274224 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.233977 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -559.934348 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.227727	-1.176215	-0.739466
2	6	-3.534742	-1.404477	-0.440219
3	6	-4.357822	-0.619464	0.459078
4	6	-1.370494	-0.126150	-0.191949
5	6	-4.218157	0.706739	0.656338
6	6	-1.866159	1.086279	0.171595
7	6	-3.264008	1.523829	-0.171886
8	1	-1.722890	-1.929439	-1.342692
9	1	-3.976992	-2.321363	-0.825643
10	1	-5.125435	-1.157406	1.011965
11	1	-4.813648	1.203661	1.419184
12	1	-3.465690	1.346558	-1.238214
13	1	-3.395436	2.590484	0.021599
14	1	-1.235568	1.771530	0.733860
15	6	0.052936	-0.471814	-0.035538
16	6	1.051540	0.434238	-0.187231
17	1	0.809544	1.449831	-0.497160
18	7	2.377371	0.214980	0.006213

19	6	3.416411	1.185989	-0.327310
20	6	2.915060	-1.060579	0.447936
21	6	4.688849	0.335681	-0.368114
22	1	3.486161	1.964855	0.445506
23	1	3.206772	1.673903	-1.284511
24	6	4.403398	-0.768313	0.658163
25	1	2.758531	-1.834967	-0.319619
26	1	2.411788	-1.395585	1.363267
27	1	4.811970	-0.102991	-1.364192
28	1	5.585659	0.915118	-0.137686
29	1	5.025369	-1.655060	0.519049
30	1	4.569778	-0.390730	1.672690
31	1	0.293983	-1.507713	0.190713

C

HF = -744.1467228 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.212545 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.169596 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -743.977127 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.494705	-0.880798	0.000073
2	6	0.182137	-0.600043	0.000059
3	6	-0.656829	0.600339	0.000010
4	6	-0.784720	-1.774178	0.000069
5	6	2.619312	0.075484	0.000098
6	8	3.782895	-0.587242	-0.000330
7	8	2.546383	1.289610	0.000462
8	6	4.970114	0.214787	-0.000299
9	6	-1.994882	0.155000	-0.000034
10	7	-2.046542	-1.244201	-0.000038
11	8	-0.502414	-2.962179	0.000151
12	6	-0.392674	1.966697	-0.000019
13	6	-1.464913	2.863318	-0.000093
14	6	-2.779457	2.400628	-0.000119
15	6	-3.066360	1.031343	-0.000084
16	1	0.631215	2.315839	0.000038
17	1	-1.269521	3.930287	-0.000118
18	1	-3.599055	3.112201	-0.000162

19	1	-4.090470	0.674401	-0.000091
20	6	-3.264291	-2.023014	0.000123
21	1	1.769357	-1.931905	0.000060
22	1	5.796598	-0.492822	-0.000638
23	1	5.001700	0.843849	-0.892146
24	1	5.001994	0.843330	0.891903
25	1	-3.857509	-1.803158	-0.892123
26	1	-2.989477	-3.077522	-0.000486
27	1	-3.856790	-1.803991	0.893057

TS-D

HF = -1304.3174044 hartrees

Imaginary Frequencies: 1 (-437.7869 1/cm)

Zero-point correction = 0.489619 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.432405 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.884999 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.662536	0.906019	-0.785844
2	6	4.346531	2.065682	-0.660651
3	6	3.781222	3.401563	-0.533802
4	6	2.207587	0.701737	-0.831713
5	6	2.588759	3.688494	0.015144
6	6	1.268877	1.669931	-0.390597
7	6	1.720570	2.643498	0.666045
8	1	4.257479	0.011295	-0.961599
9	1	5.429369	2.010274	-0.748790
10	1	4.385308	4.218608	-0.922645
11	1	1.888847	0.106888	-1.689111
12	1	2.224409	4.712606	-0.001443
13	1	2.300179	2.093302	1.418564
14	1	0.884577	3.112327	1.183917
15	6	-0.051421	1.508071	-0.808175
16	6	-1.161235	1.985980	-0.115868
17	1	-1.037733	2.563111	0.796023
18	7	-2.412424	1.746560	-0.454861

19	6	-2.820065	0.990290	-1.649586
20	6	-3.569104	2.199964	0.330162
21	6	-4.348875	1.080585	-1.638339
22	1	-2.473921	-0.043699	-1.558966
23	1	-2.371049	1.435108	-2.542287
24	6	-4.695303	1.293993	-0.159253
25	1	-3.777390	3.251743	0.101437
26	1	-3.357262	2.108887	1.397533
27	1	-4.683069	1.937979	-2.230924
28	1	-4.804634	0.180329	-2.054158
29	1	-5.678223	1.743951	-0.009657
30	1	-4.666112	0.338867	0.373687
31	1	-0.230842	0.841933	-1.646263
32	6	1.791722	-0.752076	0.479590
33	6	0.411997	-0.979622	0.679748
34	6	-0.609185	-1.674024	-0.073947
35	6	-0.243552	-0.385758	1.833432
36	6	2.618097	-1.837450	-0.133255
37	8	3.615380	-2.191987	0.688238
38	8	2.452510	-2.345433	-1.225077
39	6	4.483920	-3.229680	0.218378
40	6	-1.818273	-1.545546	0.660505
41	7	-1.578867	-0.787873	1.795920
42	8	0.229967	0.336126	2.726542
43	6	-0.647149	-2.338581	-1.302548
44	6	-1.858170	-2.864969	-1.762091
45	6	-3.029451	-2.748923	-1.009288
46	6	-3.018531	-2.086502	0.223337
47	1	0.258488	-2.440870	-1.888483
48	1	-1.885740	-3.377543	-2.719063
49	1	-3.956577	-3.175381	-1.379810
50	1	-3.926240	-1.990560	0.811499
51	6	-2.548947	-0.486599	2.816203

52	1	2.270915	-0.322668	1.357332
53	1	5.232322	-3.356946	0.998241
54	1	3.925388	-4.155763	0.069404
55	1	4.955962	-2.934097	-0.721072
56	1	-2.868054	-1.394646	3.339154
57	1	-2.081796	0.192661	3.530424
58	1	-3.433749	-0.004609	2.386493

D

HF = -1304.3281653 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.492239 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.434771 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.893394 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.437618	1.350991	-0.857604
2	6	3.879330	2.618674	-0.784598
3	6	3.114931	3.826040	-0.471666
4	6	2.047572	0.798396	-0.714040
5	6	1.999212	3.872041	0.270660
6	6	0.983782	1.722795	-0.213483
7	6	1.374914	2.649750	0.900652
8	1	4.175204	0.593918	-1.115521
9	1	4.931972	2.781368	-1.006165
10	1	3.518547	4.759707	-0.856448
11	1	1.746340	0.393875	-1.688091
12	1	1.494966	4.822529	0.421532
13	1	2.100674	2.137678	1.542624
14	1	0.534049	2.931508	1.532893
15	6	-0.266859	1.589047	-0.734205
16	6	-1.432616	2.047628	-0.071498
17	1	-1.359267	2.660377	0.821735
18	7	-2.637140	1.709097	-0.422081

19	6	-2.964855	0.833487	-1.569544
20	6	-3.845297	2.041915	0.355199
21	6	-4.477607	0.620480	-1.458945
22	1	-2.417680	-0.105953	-1.455732
23	1	-2.658984	1.319955	-2.498385
24	6	-4.782806	0.887127	0.019967
25	1	-4.243989	2.995474	-0.007204
26	1	-3.593782	2.133848	1.412408
27	1	-5.014905	1.332845	-2.091873
28	1	-4.750197	-0.389526	-1.768832
29	1	-5.827686	1.141417	0.203424
30	1	-4.523844	0.011179	0.622932
31	1	-0.399200	0.925274	-1.581281
32	6	2.046591	-0.446783	0.277016
33	6	0.693245	-0.964563	0.640579
34	6	-0.290114	-1.599869	-0.175612
35	6	0.087916	-0.626576	1.876227
36	6	2.884573	-1.562855	-0.318101
37	8	3.480120	-2.290008	0.630845
38	8	2.991260	-1.807694	-1.505273
39	6	4.196835	-3.447471	0.187212
40	6	-1.484402	-1.692657	0.605604
41	7	-1.237892	-1.111350	1.830020
42	8	0.533259	0.010274	2.865891
43	6	-0.334291	-2.073935	-1.495628
44	6	-1.514357	-2.642672	-1.988197
45	6	-2.658902	-2.752483	-1.191418
46	6	-2.650153	-2.272408	0.125820
47	1	0.547094	-2.010976	-2.127001
48	1	-1.538041	-3.013133	-3.009618
49	1	-3.559693	-3.207033	-1.592803
50	1	-3.536870	-2.344448	0.750193
51	6	-2.191795	-0.977460	2.896783

52	1	2.524931	-0.135605	1.211293
53	1	4.608805	-3.897724	1.088323
54	1	3.518865	-4.142745	-0.311821
55	1	4.996766	-3.161587	-0.498821
56	1	-2.569937	-1.954481	3.218043
57	1	-1.685104	-0.497290	3.735331
58	1	-3.045707	-0.357103	2.594505

TS-S1

HF = -1304.2948544 hartrees

Imaginary Frequencies: 1 (-654.3325 1/cm)

Zero-point correction = 0.488708 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.427927 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.866928 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.393593	4.064186	-0.213172
2	6	0.832021	3.793198	-0.818287
3	6	1.287827	2.535834	-1.226470
4	6	-1.495727	3.227501	0.042815
5	6	-1.803988	2.015727	-0.565087
6	6	-0.961373	1.537146	-1.726009
7	1	-0.474215	5.058212	0.223320
8	1	1.564163	4.594554	-0.799951
9	1	2.364130	2.427498	-1.337230
10	1	-2.215856	3.606144	0.764713
11	1	-1.057859	2.270152	-2.540131
12	1	-1.325090	0.587949	-2.114393
13	6	-2.952933	1.303427	-0.131304
14	6	-3.421789	0.138474	-0.699904
15	1	-2.916825	-0.308059	-1.549798
16	7	-4.478640	-0.556018	-0.278074
17	6	-5.306609	-0.183800	0.869729
18	6	-4.927247	-1.803758	-0.909104

19	6	-6.222307	-1.395595	1.063134
20	1	-5.870428	0.728828	0.638212
21	1	-4.679693	0.018240	1.744874
22	6	-6.335462	-1.989115	-0.346474
23	1	-4.267534	-2.629387	-0.613976
24	1	-4.901646	-1.709166	-1.997188
25	1	-5.748129	-2.116623	1.737064
26	1	-7.186697	-1.116722	1.490983
27	1	-6.644709	-3.035796	-0.346282
28	1	-7.054015	-1.417462	-0.942655
29	1	-3.485847	1.715672	0.720859
30	6	0.508157	1.378908	-1.380865
31	6	0.910574	0.478394	0.399491
32	6	2.223017	-0.029390	0.402746
33	6	-0.209394	-0.513919	0.494581
34	1	0.774850	1.324938	1.067631
35	6	2.826117	-1.222382	-0.154427
36	6	3.303865	0.797365	0.909567
37	8	-0.771059	-0.448108	1.705569
38	8	-0.559494	-1.302492	-0.360847
39	6	4.222256	-1.115849	0.081111
40	6	2.351499	-2.348121	-0.832620
41	7	4.485218	0.086322	0.722374
42	8	3.249334	1.935981	1.401004
43	6	-1.766768	-1.434052	2.002086
44	6	5.122882	-2.094045	-0.312933
45	6	3.253391	-3.337742	-1.237208
46	1	1.293902	-2.451958	-1.044150
47	6	5.792414	0.557187	1.104397
48	1	-2.150997	-1.172730	2.986287
49	1	-2.564713	-1.411217	1.258591
50	1	-1.313096	-2.427195	2.021693
51	6	4.619829	-3.217520	-0.978770

52	1	6.185898	-1.988640	-0.119319
53	1	2.881406	-4.212713	-1.761991
54	1	6.446731	0.647655	0.230606
55	1	5.670007	1.538680	1.563664
56	1	6.256635	-0.123045	1.826270
57	1	5.303749	-3.996635	-1.301351
58	1	0.979637	0.551313	-1.904400

S1

HF = -1304.3259335 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.492857 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.433998 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.891935 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.148220	3.963561	-0.074491
2	6	1.092275	3.580804	-0.729596
3	6	1.413132	2.376807	-1.239434
4	6	-1.349643	3.335541	0.027676
5	6	-1.763289	2.116918	-0.626907
6	6	-0.931904	1.596366	-1.762413
7	1	-0.072797	4.894239	0.483819
8	1	1.871734	4.336305	-0.696966
9	1	2.434736	2.224380	-1.575760
10	1	-2.082216	3.788569	0.690908
11	1	-0.858512	2.391032	-2.514227
12	1	-1.403353	0.745096	-2.248376
13	6	-2.902176	1.494025	-0.166520
14	6	-3.392969	0.276438	-0.693000
15	1	-2.933135	-0.169754	-1.568230
16	7	-4.382408	-0.408193	-0.190992
17	6	-5.129969	-0.058692	1.032049
18	6	-4.872587	-1.670148	-0.789332

19	6	-5.935502	-1.322890	1.331480
20	1	-5.776204	0.798342	0.815512
21	1	-4.432461	0.212360	1.826853
22	6	-6.187211	-1.923434	-0.056052
23	1	-4.139291	-2.459046	-0.593734
24	1	-4.981117	-1.548215	-1.867650
25	1	-5.339587	-2.008619	1.941402
26	1	-6.855144	-1.096415	1.872306
27	1	-6.431234	-2.985921	-0.022046
28	1	-7.006255	-1.398206	-0.556863
29	1	-3.426390	1.941003	0.672218
30	6	0.494214	1.191338	-1.339784
31	6	0.581765	0.401005	-0.010424
32	6	1.983903	-0.014448	0.316500
33	6	-0.328598	-0.809178	-0.007563
34	1	0.260366	1.046232	0.816582
35	6	2.865077	-0.845668	-0.436082
36	6	2.675268	0.457137	1.457677
37	8	-0.637769	-1.190731	1.237032
38	8	-0.736930	-1.400921	-0.993593
39	6	4.110340	-0.868278	0.264358
40	6	2.764803	-1.582851	-1.625684
41	7	3.978314	-0.087323	1.392659
42	8	2.309364	1.218823	2.391686
43	6	-1.393974	-2.394170	1.370015
44	6	5.209044	-1.580974	-0.193634
45	6	3.872159	-2.299472	-2.091203
46	1	1.828167	-1.611770	-2.176545
47	6	5.007684	0.141169	2.370424
48	1	-1.486262	-2.566449	2.440700
49	1	-2.383936	-2.274999	0.921956
50	1	-0.878154	-3.228619	0.890966
51	6	5.082427	-2.300684	-1.390471

52	1	6.145595	-1.580534	0.357695
53	1	3.787925	-2.866249	-3.014969
54	1	5.894306	0.595833	1.912741
55	1	4.606146	0.823039	3.121675
56	1	5.307963	-0.793465	2.859328
57	1	5.930057	-2.863248	-1.770810
58	1	0.874095	0.544997	-2.136683

TS-E

HF = -1304.3236021 hartrees

Imaginary Frequencies: 1 (-425.7558 1/cm)

Zero-point correction = 0.489881 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.433419 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.890183 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.608929	-0.426981	-0.933638
2	6	-4.584255	-1.363961	-0.885044
3	6	-4.426044	-2.781005	-0.594108
4	6	-2.162866	-0.581944	-0.726956
5	6	-3.457389	-3.302275	0.177542
6	6	-1.597075	-1.703048	-0.072618
7	6	-2.465769	-2.443936	0.914460
8	1	-3.916356	0.559787	-1.275186
9	1	-5.582309	-1.045978	-1.179356
10	1	-5.154808	-3.451075	-1.045246
11	1	-1.590906	-0.130558	-1.535437
12	1	-3.378351	-4.381146	0.285329
13	1	-3.002471	-1.708097	1.529716
14	1	-1.849959	-3.045911	1.584661
15	6	-0.242064	-2.029761	-0.148773
16	6	0.661725	-1.394401	-0.998122
17	1	0.308897	-0.710653	-1.764167
18	7	1.972089	-1.570270	-0.992185

19	6	2.693281	-2.385685	-0.011597
20	6	2.876321	-0.945800	-1.971630
21	6	4.155567	-2.002022	-0.239508
22	1	2.516817	-3.449811	-0.212526
23	1	2.335208	-2.160288	0.996655
24	6	4.203456	-1.665645	-1.734889
25	1	2.961787	0.125120	-1.763642
26	1	2.483947	-1.082286	-2.982080
27	1	4.401900	-1.111410	0.347330
28	1	4.840838	-2.802224	0.045436
29	1	5.057442	-1.041133	-2.003845
30	1	4.249299	-2.585068	-2.327776
31	1	0.136349	-2.775283	0.543305
32	6	-1.533525	0.917356	0.542027
33	6	-0.140508	0.909316	0.718593
34	6	0.983154	1.547289	0.054534
35	6	0.400831	0.195576	1.874822
36	6	-2.198477	2.054322	-0.152601
37	8	-3.190723	2.552590	0.595536
38	8	-1.923643	2.485356	-1.256493
39	6	-3.920443	3.648767	0.031357
40	6	2.138535	1.215822	0.807692
41	7	1.777441	0.401196	1.872086
42	8	-0.200925	-0.453640	2.739841
43	6	1.139599	2.341335	-1.083731
44	6	2.413165	2.800750	-1.432066
45	6	3.533305	2.475980	-0.663555
46	6	3.405415	1.673177	0.474681
47	1	0.276256	2.600108	-1.684179
48	1	2.530620	3.420427	-2.315844
49	1	4.512667	2.848420	-0.947745
50	1	4.271660	1.415532	1.076596
51	6	2.666983	-0.051504	2.911384

52	1	-2.081191	0.580810	1.418569
53	1	-4.662776	3.919299	0.779488
54	1	-3.251765	4.488508	-0.167000
55	1	-4.407132	3.343113	-0.897480
56	1	3.112960	0.796303	3.442154
57	1	2.081143	-0.647161	3.612158
58	1	3.471886	-0.670591	2.500200

E

HF = -1304.33784 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.491579 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.434129 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.903711 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.729095	-0.008878	-0.673387
2	6	-4.757713	-0.865796	-0.802662
3	6	-4.742235	-2.322276	-0.682532
4	6	-2.250627	-0.271804	-0.518491
5	6	-3.886234	-3.001559	0.093683
6	6	-1.855398	-1.604980	0.028271
7	6	-2.834748	-2.312864	0.923603
8	1	-3.972378	1.041229	-0.812362
9	1	-5.725176	-0.427308	-1.040556
10	1	-5.508856	-2.865829	-1.229605
11	1	-1.818614	-0.123525	-1.516176
12	1	-3.931316	-4.086729	0.129769
13	1	-3.310258	-1.563563	1.572617
14	1	-2.312697	-3.026164	1.563185
15	6	-0.612090	-2.116948	-0.155957
16	6	0.377729	-1.462903	-0.945980
17	1	0.088962	-0.737576	-1.699301
18	7	1.648132	-1.774740	-0.943389

19	6	2.288633	-2.669138	0.034358
20	6	2.622609	-1.229461	-1.912157
21	6	3.778533	-2.398975	-0.168668
22	1	2.032105	-3.708648	-0.200098
23	1	1.930598	-2.430799	1.038198
24	6	3.875680	-2.066380	-1.661571
25	1	2.799222	-0.173335	-1.695078
26	1	2.224753	-1.327196	-2.924113
27	1	4.082337	-1.530977	0.424182
28	1	4.392114	-3.252115	0.125187
29	1	4.782782	-1.515406	-1.915648
30	1	3.851088	-2.983916	-2.258401
31	1	-0.325482	-3.011546	0.387796
32	6	-1.568179	0.863354	0.378130
33	6	-0.098286	0.731786	0.596903
34	6	1.032669	1.347867	-0.038977
35	6	0.371848	0.081234	1.780857
36	6	-1.859284	2.228145	-0.214950
37	8	-1.941233	3.166522	0.729762
38	8	-1.968673	2.469930	-1.402009
39	6	-2.090426	4.516514	0.273014
40	6	2.178161	0.998561	0.736031
41	7	1.767132	0.226631	1.806199
42	8	-0.270558	-0.533179	2.659161
43	6	1.233719	2.112751	-1.197104
44	6	2.526174	2.513211	-1.545411
45	6	3.632240	2.160929	-0.765068
46	6	3.462915	1.396106	0.395239
47	1	0.394144	2.391392	-1.824883
48	1	2.672747	3.107030	-2.443147
49	1	4.627280	2.484439	-1.054526
50	1	4.315545	1.116925	1.007890
51	6	2.607509	-0.230066	2.882235

52	1	-2.048364	0.813155	1.361464
53	1	-2.122427	5.125549	1.174270
54	1	-1.239407	4.799488	-0.349685
55	1	-3.015196	4.626527	-0.296906
56	1	3.101179	0.610730	3.381976
57	1	1.970161	-0.749010	3.599590
58	1	3.377412	-0.922834	2.522922

TS-F

HF = -1304.3368478 hartrees

Imaginary Frequencies: 1 (-141.3729 1/cm)

Zero-point correction = 0.491481 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.435821 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.901027 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.790178	0.290384	-0.428884
2	6	-4.904099	-0.435988	-0.623656
3	6	-5.014186	-1.890641	-0.729231
4	6	-2.342004	-0.144390	-0.430476
5	6	-4.210535	-2.743350	-0.078731
6	6	-2.045503	-1.535937	0.046360
7	6	-3.100826	-2.273530	0.825240
8	1	-3.934241	1.366487	-0.374984
9	1	-5.837437	0.115413	-0.723302
10	1	-5.829272	-2.280708	-1.334405
11	1	-2.001312	-0.034298	-1.469543
12	1	-4.348809	-3.814621	-0.199246
13	1	-3.511486	-1.584113	1.578008
14	1	-2.651754	-3.116203	1.354669
15	6	-0.817610	-2.069008	-0.125778
16	6	0.230020	-1.367501	-0.821633
17	1	-0.030347	-0.694976	-1.632733
18	7	1.480260	-1.810028	-0.862652

19	6	2.052867	-2.766209	0.092896
20	6	2.462033	-1.389804	-1.879394
21	6	3.554379	-2.654828	-0.163988
22	1	1.688911	-3.778362	-0.125235
23	1	1.761644	-2.502856	1.112449
24	6	3.624311	-2.359830	-1.666338
25	1	2.775465	-0.357858	-1.704560
26	1	2.014956	-1.460446	-2.874297
27	1	3.966744	-1.810359	0.397703
28	1	4.090806	-3.560128	0.126053
29	1	4.576586	-1.922763	-1.972383
30	1	3.467402	-3.280127	-2.238678
31	1	-0.577552	-3.020221	0.339506
32	6	-1.459815	0.883814	0.396202
33	6	0.007211	0.574339	0.495126
34	6	1.141561	1.236322	-0.117290
35	6	0.488566	-0.005272	1.733874
36	6	-1.631075	2.281695	-0.167261
37	8	-1.484460	3.211899	0.777931
38	8	-1.839244	2.547534	-1.335248
39	6	-1.512734	4.575675	0.338326
40	6	2.281271	0.894465	0.656299
41	7	1.875418	0.139462	1.745211
42	8	-0.155105	-0.556580	2.641213
43	6	1.330164	1.988450	-1.280380
44	6	2.621341	2.383475	-1.641526
45	6	3.728599	2.027542	-0.866963
46	6	3.566895	1.276783	0.302913
47	1	0.486339	2.259922	-1.905796
48	1	2.765291	2.967279	-2.545671
49	1	4.723671	2.339849	-1.168433
50	1	4.422784	0.996284	0.909608
51	6	2.726058	-0.298081	2.822343

52	1	-1.856858	0.883794	1.417256
53	1	-1.368880	5.172069	1.237006
54	1	-0.706836	4.757678	-0.375525
55	1	-2.473775	4.805541	-0.125833
56	1	3.236505	0.551738	3.287745
57	1	2.093074	-0.786688	3.564075
58	1	3.478839	-1.011645	2.469176

F

HF = -1304.3573323 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.492589 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.435510 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.921822 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.735568	0.847784	0.095788
2	6	-4.981511	0.469825	-0.229684
3	6	-5.352451	-0.821620	-0.814017
4	6	-2.448957	0.112739	-0.225769
5	6	-4.763418	-1.972323	-0.457075
6	6	-2.410884	-1.365413	0.135213
7	6	-3.678493	-2.038103	0.589536
8	1	-3.622566	1.829621	0.549612
9	1	-5.789577	1.176267	-0.047829
10	1	-6.172296	-0.834743	-1.528847
11	1	-2.311659	0.192053	-1.316348
12	1	-5.080542	-2.904109	-0.918846
13	1	-4.034936	-1.527704	1.496562
14	1	-3.465067	-3.076190	0.855587
15	6	-1.248053	-2.007407	0.013892
16	6	-0.037699	-1.290593	-0.510468
17	1	-0.250422	-0.996197	-1.549737
18	7	1.130210	-2.110733	-0.554093

19	6	1.567056	-2.970285	0.540250
20	6	2.118793	-2.012078	-1.619564
21	6	3.041381	-3.223281	0.217069
22	1	1.008656	-3.920615	0.557259
23	1	1.436713	-2.504768	1.521918
24	6	3.069564	-3.170459	-1.314456
25	1	2.669216	-1.059309	-1.610173
26	1	1.640774	-2.105601	-2.603887
27	1	3.653155	-2.409600	0.624935
28	1	3.408739	-4.166310	0.629333
29	1	4.069739	-3.009702	-1.724183
30	1	2.673911	-4.104440	-1.729248
31	1	-1.161467	-3.064742	0.246160
32	6	-1.247946	0.815870	0.452773
33	6	0.135410	0.123697	0.230163
34	6	1.196973	0.887935	-0.524920
35	6	0.813779	-0.084558	1.593043
36	6	-1.132783	2.274084	0.055860
37	8	-0.426883	2.956554	0.963807
38	8	-1.574053	2.770113	-0.959353
39	6	-0.077771	4.301974	0.615844
40	6	2.363058	0.907613	0.246014
41	7	2.119882	0.311014	1.488009
42	8	0.292527	-0.529471	2.605878
43	6	1.210219	1.411661	-1.805317
44	6	2.397882	1.966216	-2.299432
45	6	3.551459	1.972982	-1.518688
46	6	3.552772	1.439280	-0.224282
47	1	0.316332	1.395378	-2.420975
48	1	2.419522	2.388646	-3.298449
49	1	4.466872	2.398873	-1.917093
50	1	4.454178	1.440091	0.379538
51	6	3.092432	0.205872	2.550098

52	1	-1.435380	0.784642	1.531161
53	1	0.468990	4.692335	1.471789
54	1	0.554505	4.300338	-0.275390
55	1	-0.975700	4.893977	0.430571
56	1	3.462988	1.195869	2.832728
57	1	2.604966	-0.255730	3.408484
58	1	3.935527	-0.416337	2.234059

TS-S2

HF = -1304.3221068 hartrees

Imaginary Frequencies: 1 (-427.8635 1/cm)

Zero-point correction = 0.490379 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.433895 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.888212 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.474888	1.030702	1.320127
2	6	-4.524512	1.661103	0.745195
3	6	-4.492661	2.493475	-0.450262
4	6	-2.069068	1.027673	0.899170
5	6	-3.634014	2.336765	-1.471932
6	6	-1.647777	1.320021	-0.418899
7	6	-2.661618	1.189736	-1.531026
8	1	-3.664206	0.523730	2.264505
9	1	-5.473852	1.618521	1.274825
10	1	-5.224094	3.297468	-0.497404
11	1	-1.404234	1.332390	1.703975
12	1	-3.638540	3.050369	-2.291956
13	1	-3.206511	0.247761	-1.398841
14	1	-2.160447	1.151733	-2.500769
15	6	-0.316235	1.584953	-0.747495
16	6	0.699183	1.758913	0.190618
17	1	0.465395	1.887778	1.243353
18	7	1.989548	1.858920	-0.097204

19	6	2.562686	1.669842	-1.432945
20	6	3.004576	2.213588	0.904791
21	6	4.067096	1.621410	-1.166915
22	1	2.290959	2.516773	-2.076650
23	1	2.178998	0.748580	-1.880835
24	6	4.243866	2.519902	0.062830
25	1	3.166910	1.367785	1.579170
26	1	2.668025	3.067072	1.498139
27	1	4.361088	0.593426	-0.933993
28	1	4.647434	1.955566	-2.028901
29	1	5.168695	2.321128	0.607870
30	1	4.243726	3.573665	-0.234177
31	1	-0.048894	1.594363	-1.799964
32	6	-1.329270	-0.889902	1.227562
33	6	0.022158	-1.004302	0.868364
34	6	0.748348	-1.425372	-0.320795
35	6	1.023172	-0.792905	1.917669
36	6	-2.437082	-1.711969	0.671176
37	8	-2.395679	-1.883961	-0.651847
38	8	-3.316185	-2.182619	1.368837
39	6	-3.443550	-2.673835	-1.225044
40	6	2.114408	-1.498643	0.045740
41	7	2.256276	-1.129505	1.377909
42	8	0.859271	-0.398756	3.081245
43	6	0.408203	-1.699243	-1.647393
44	6	1.406610	-2.045737	-2.559399
45	6	2.744484	-2.135285	-2.165886
46	6	3.112613	-1.866924	-0.845254
47	1	-0.622469	-1.627201	-1.967331
48	1	1.137537	-2.250772	-3.591198
49	1	3.504738	-2.418206	-2.887153
50	1	4.149325	-1.935866	-0.530424
51	6	3.488711	-1.187017	2.123458

52	1	-1.462152	-0.794477	2.302600
53	1	-3.220149	-2.724192	-2.289531
54	1	-3.449247	-3.673311	-0.787093
55	1	-4.411416	-2.195867	-1.059151
56	1	4.275324	-0.612334	1.622090
57	1	3.305179	-0.759453	3.109867
58	1	3.830221	-2.221319	2.237430

S2

HF = -1304.3382789 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.491811 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.434998 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.903281 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.528961	0.611364	1.289746
2	6	-4.559361	1.390447	0.920753
3	6	-4.549709	2.460257	-0.078143
4	6	-2.075580	0.701378	0.899499
5	6	-3.767375	2.473381	-1.166889
6	6	-1.735488	1.271670	-0.440945
7	6	-2.808896	1.355413	-1.492782
8	1	-3.728787	-0.126063	2.066605
9	1	-5.505094	1.232132	1.435502
10	1	-5.254826	3.274233	0.074555
11	1	-1.619605	1.347507	1.662347
12	1	-3.811175	3.317833	-1.849713
13	1	-3.351202	0.402867	-1.505323
14	1	-2.360320	1.508938	-2.476957
15	6	-0.468690	1.668423	-0.709883
16	6	0.573765	1.674236	0.276881
17	1	0.332889	1.788279	1.328966
18	7	1.841610	1.859975	-0.024822

19	6	2.414676	1.782344	-1.379048
20	6	2.862763	2.169284	0.991986
21	6	3.920268	1.749386	-1.121047
22	1	2.126048	2.674812	-1.947680
23	1	2.048168	0.891557	-1.894121
24	6	4.081717	2.570882	0.162892
25	1	3.053095	1.278832	1.595216
26	1	2.502408	2.963775	1.648982
27	1	4.237910	0.715411	-0.956316
28	1	4.486906	2.152575	-1.962202
29	1	5.016090	2.364653	0.688017
30	1	4.047127	3.641285	-0.064283
31	1	-0.208339	1.962543	-1.722356
32	6	-1.341344	-0.686120	1.175126
33	6	0.107971	-0.748557	0.822711
34	6	0.747557	-1.208953	-0.383440
35	6	1.101343	-0.760602	1.864574
36	6	-2.078751	-1.886784	0.609306
37	8	-2.606376	-1.661008	-0.598617
38	8	-2.166265	-2.956546	1.176372
39	6	-3.259404	-2.767081	-1.230673
40	6	2.119990	-1.400562	-0.074630
41	7	2.312738	-1.131423	1.269750
42	8	0.992237	-0.461744	3.070806
43	6	0.331071	-1.407847	-1.704395
44	6	1.267730	-1.774316	-2.673244
45	6	2.615664	-1.952248	-2.344858
46	6	3.055383	-1.774900	-1.028886
47	1	-0.708150	-1.261387	-1.976338
48	1	0.943005	-1.923517	-3.698972
49	1	3.326890	-2.241764	-3.112327
50	1	4.099092	-1.919811	-0.765550
51	6	3.558846	-1.284824	1.975155

52	1	-1.391914	-0.816753	2.261055
53	1	-3.622911	-2.384989	-2.183266
54	1	-2.549671	-3.581345	-1.390190
55	1	-4.090795	-3.118353	-0.616940
56	1	4.345873	-0.669457	1.522544
57	1	3.400709	-0.963884	3.005816
58	1	3.888254	-2.329428	1.971344

TS-S3

HF = -1304.3382884 hartrees

Imaginary Frequencies: 1 (-40.9774 1/cm)

Zero-point correction = 0.491787 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.437011 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.901278 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.538465	0.592297	1.283066
2	6	-4.578749	1.357241	0.912548
3	6	-4.582151	2.425750	-0.088024
4	6	-2.086387	0.702710	0.892864
5	6	-3.800579	2.446483	-1.177166
6	6	-1.752752	1.264319	-0.453481
7	6	-2.829102	1.339764	-1.502809
8	1	-3.728896	-0.146686	2.060843
9	1	-5.522770	1.187254	1.426768
10	1	-5.296805	3.231549	0.063869
11	1	-1.642763	1.365875	1.648616
12	1	-3.855751	3.289144	-1.861435
13	1	-3.361182	0.381190	-1.515579
14	1	-2.383278	1.498083	-2.487545
15	6	-0.486467	1.657396	-0.724343
16	6	0.557205	1.658916	0.265022
17	1	0.314586	1.800691	1.313501
18	7	1.825130	1.858699	-0.040669

19	6	2.397677	1.777262	-1.394194
20	6	2.842270	2.189395	0.972475
21	6	3.903342	1.754045	-1.136202
22	1	2.105391	2.665316	-1.968347
23	1	2.036889	0.882664	-1.906418
24	6	4.059791	2.588908	0.139737
25	1	3.040058	1.310303	1.590093
26	1	2.476076	2.990985	1.617942
27	1	4.226051	0.723245	-0.961157
28	1	4.468501	2.151764	-1.981031
29	1	4.995144	2.393038	0.667174
30	1	4.019791	3.656735	-0.098507
31	1	-0.224760	1.949930	-1.736963
32	6	-1.328759	-0.667477	1.180312
33	6	0.121440	-0.707596	0.820912
34	6	0.758265	-1.198105	-0.377252
35	6	1.116290	-0.719012	1.865320
36	6	-2.045691	-1.885938	0.626107
37	8	-2.592195	-1.674819	-0.575950
38	8	-2.102409	-2.955772	1.196916
39	6	-3.227750	-2.796541	-1.198150
40	6	2.128699	-1.391142	-0.065691
41	7	2.323785	-1.103793	1.275337
42	8	1.006613	-0.405435	3.066521
43	6	0.338904	-1.417140	-1.693381
44	6	1.272962	-1.804094	-2.656936
45	6	2.620309	-1.981040	-2.326565
46	6	3.062316	-1.783704	-1.014297
47	1	-0.699868	-1.269946	-1.966576
48	1	0.946753	-1.969434	-3.679645
49	1	3.329809	-2.285512	-3.089811
50	1	4.105725	-1.927917	-0.749652
51	6	3.571927	-1.246216	1.979741

52	1	-1.372559	-0.790549	2.267387
53	1	-3.607275	-2.425670	-2.148903
54	1	-2.502801	-3.596704	-1.360680
55	1	-4.046576	-3.162370	-0.576056
56	1	4.355694	-0.632929	1.518846
57	1	3.415120	-0.915206	3.007372
58	1	3.903945	-2.289864	1.985643

S3

HF = -1304.3580435 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.493793 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.437808 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.920235 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.607788	-0.087162	1.203104
2	6	4.791241	-0.655781	0.923608
3	6	5.019066	-1.817529	0.059701
4	6	2.231806	-0.587398	0.830787
5	6	4.295371	-2.097241	-1.034045
6	6	2.020344	-1.175968	-0.548978
7	6	3.168161	-1.220575	-1.519062
8	1	3.620704	0.767727	1.878241
9	1	5.673781	-0.231302	1.398650
10	1	5.853659	-2.464530	0.321763
11	1	2.034267	-1.407193	1.539985
12	1	4.527609	-2.988328	-1.612093
13	1	3.543453	-0.193686	-1.637684
14	1	2.811088	-1.561841	-2.494287
15	6	0.793508	-1.633863	-0.814644
16	6	-0.292805	-1.481415	0.213915
17	1	-0.007597	-2.018929	1.132012
18	7	-1.547596	-2.022087	-0.201521

19	6	-2.115130	-1.879878	-1.541029
20	6	-2.528453	-2.492061	0.766383
21	6	-3.613471	-2.102854	-1.318052
22	1	-1.711738	-2.641809	-2.227475
23	1	-1.917264	-0.900446	-1.983332
24	6	-3.646583	-3.049215	-0.113522
25	1	-2.925765	-1.687461	1.404425
26	1	-2.090214	-3.246509	1.432026
27	1	-4.090309	-1.150621	-1.056166
28	1	-4.114284	-2.504230	-2.202523
29	1	-4.612470	-3.066302	0.397197
30	1	-3.406782	-4.070861	-0.428808
31	1	0.550710	-2.079240	-1.774793
32	6	1.134223	0.466072	1.162407
33	6	-0.289776	0.065160	0.659659
34	6	-0.915955	0.916831	-0.419788
35	6	-1.294844	0.215617	1.806328
36	6	1.455934	1.872655	0.693269
37	8	2.187418	1.898268	-0.421896
38	8	1.064526	2.873240	1.259197
39	6	2.445063	3.188150	-0.987230
40	6	-2.176289	1.329138	0.025311
41	7	-2.383477	0.899351	1.341361
42	8	-1.163945	-0.234192	2.936746
43	6	-0.500713	1.257835	-1.697221
44	6	-1.355075	2.004538	-2.516390
45	6	-2.613676	2.391083	-2.059796
46	6	-3.045932	2.056701	-0.772631
47	1	0.468680	0.937997	-2.061869
48	1	-1.037169	2.275543	-3.517897
49	1	-3.268840	2.965941	-2.706567
50	1	-4.022994	2.362438	-0.413798
51	6	-3.580052	1.152261	2.109064

52	1	1.074728	0.536793	2.252360
53	1	3.012313	2.998748	-1.896647
54	1	1.502062	3.687920	-1.219400
55	1	3.025965	3.799349	-0.294180
56	1	-4.448499	0.703548	1.616279
57	1	-3.449222	0.699892	3.091981
58	1	-3.744847	2.227404	2.224451

S4

HF = -1304.325789 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.492142 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.435247 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.890542 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.446782	-2.219095	-0.932659
2	6	-3.586943	-2.620572	-0.340213
3	6	-3.983396	-2.362604	1.030116
4	6	-1.431554	-1.269985	-0.344171
5	6	-3.142813	-2.143821	2.068414
6	6	-0.905522	-1.784062	0.981800
7	6	-1.693950	-2.108877	2.025961
8	1	-2.261153	-2.546103	-1.952973
9	1	-4.280726	-3.213832	-0.932974
10	1	-5.044696	-2.447716	1.250714
11	1	-0.600810	-1.232123	-1.055632
12	1	-3.581530	-2.058507	3.059407
13	6	0.591870	-1.719496	1.190396
14	6	1.391104	-2.183702	0.027996
15	1	0.958117	-2.869484	-0.697920
16	1	0.859675	-0.676535	1.402520
17	6	-1.910353	0.199581	-0.200155
18	6	-0.799009	1.096604	0.263174

19	6	0.461801	1.327643	-0.361210
20	6	-0.807071	1.773882	1.508755
21	6	-2.448394	0.710689	-1.520316
22	8	-3.387405	1.648725	-1.350783
23	8	-2.058600	0.360278	-2.620261
24	6	-3.859843	2.295936	-2.535463
25	6	1.222349	2.162422	0.519652
26	7	0.453144	2.411841	1.632404
27	8	-1.678643	1.850397	2.409109
28	6	1.069038	0.923719	-1.562659
29	6	2.365588	1.353688	-1.865112
30	6	3.078240	2.185863	-0.996338
31	6	2.505077	2.598526	0.215310
32	1	0.519024	0.314485	-2.274121
33	1	2.819385	1.050895	-2.805710
34	1	4.078193	2.519429	-1.257904
35	1	3.051515	3.245019	0.896526
36	6	0.832477	3.247677	2.740093
37	1	-2.713632	0.254987	0.540435
38	1	-4.605953	3.013521	-2.198896
39	1	-3.037895	2.809660	-3.039169
40	1	-4.307651	1.570145	-3.217773
41	1	1.009481	4.280711	2.418445
42	1	0.010755	3.233759	3.457884
43	1	1.740268	2.871703	3.226505
44	1	-1.203265	-2.339514	2.970413
45	1	0.903393	-2.311108	2.062784
46	7	2.607218	-1.836020	-0.171835
47	6	3.385729	-0.940879	0.716159
48	6	3.422656	-2.268484	-1.328166
49	6	4.766548	-0.860727	0.059485
50	1	3.414563	-1.398497	1.708351
51	1	2.878364	0.026352	0.774972

52	6	4.848095	-2.121510	-0.811238
53	1	3.216116	-1.564717	-2.140698
54	1	3.136854	-3.276459	-1.627878
55	1	4.820115	0.036668	-0.561276
56	1	5.559323	-0.811371	0.806682
57	1	5.564976	-2.026837	-1.627628
58	1	5.122186	-2.994970	-0.211263

TS-S6

HF = -1304.322079 hartrees

Imaginary Frequencies: 1 (-411.4897 1/cm)

Zero-point correction = 0.489712 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.433399 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.888680 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.456094	-2.629298	0.770928
2	6	3.691578	-3.097683	0.474730
3	6	4.483426	-2.734158	-0.691265
4	6	1.653649	-1.719316	-0.054666
5	6	4.466230	-1.512036	-1.250816
6	6	2.218988	-0.584893	-0.662102
7	6	3.719876	-0.371041	-0.620804
8	1	1.940582	-3.077137	1.618176
9	1	4.088231	-3.887959	1.108801
10	1	5.115089	-3.510405	-1.117464
11	1	5.033018	-1.326622	-2.160017
12	1	4.036062	-0.277998	0.428271
13	1	3.973525	0.563766	-1.125126
14	1	1.710579	-0.159177	-1.524062
15	6	0.270756	-2.011036	-0.109187
16	6	-0.652865	-1.346024	-0.896862
17	1	-0.336173	-0.582464	-1.599952
18	7	-1.960755	-1.605067	-0.921104

19	6	-2.900708	-0.973297	-1.853294
20	6	-2.605040	-2.608791	-0.074388
21	6	-4.262293	-1.302132	-1.246750
22	1	-2.793071	-1.419842	-2.850592
23	1	-2.708900	0.099750	-1.922535
24	6	-4.039639	-2.678653	-0.608960
25	1	-2.560364	-2.286696	0.973191
26	1	-2.087020	-3.570342	-0.153800
27	1	-4.510310	-0.560802	-0.481716
28	1	-5.057409	-1.301997	-1.994808
29	1	-4.760074	-2.906512	0.179128
30	1	-4.113699	-3.461986	-1.369941
31	1	-0.085122	-2.811331	0.532048
32	6	1.469302	0.948370	0.608558
33	6	0.079679	0.927395	0.718204
34	6	-1.010949	1.589139	0.016499
35	6	-0.523170	0.218943	1.860070
36	6	2.176172	2.062080	-0.076271
37	8	3.169020	2.532488	0.691460
38	8	1.937005	2.502164	-1.185003
39	6	3.957478	3.587464	0.129406
40	6	-2.196226	1.271279	0.722501
41	7	-1.892232	0.440666	1.793247
42	8	0.035897	-0.420234	2.756146
43	6	-1.105589	2.391026	-1.121703
44	6	-2.356477	2.872092	-1.518687
45	6	-3.508655	2.565425	-0.792082
46	6	-3.439371	1.759738	0.348270
47	1	-0.213951	2.635856	-1.684931
48	1	-2.429906	3.496229	-2.403886
49	1	-4.469802	2.956021	-1.111819
50	1	-4.332271	1.520470	0.917396
51	6	-2.844980	-0.041524	2.760946

52	1	1.986959	0.586030	1.492180
53	1	4.699370	3.831522	0.887098
54	1	4.444682	3.248110	-0.787659
55	1	3.333640	4.456032	-0.089964
56	1	-3.648450	-0.599916	2.267993
57	1	-2.316508	-0.702001	3.449005
58	1	-3.286784	0.786448	3.325513

S6

HF = -1304.3657161 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.493087 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.436570 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1303.929146 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.697655	1.996205	0.433449
2	6	-4.980640	1.730970	0.108965
3	6	-5.484380	0.579922	-0.633346
4	6	-2.472117	1.279468	0.058078
5	6	-4.903750	-0.629442	-0.642148
6	6	-2.414403	-0.197885	-0.295689
7	6	-3.677393	-0.958014	0.156024
8	1	-3.512429	2.931880	0.958432
9	1	-5.721152	2.476025	0.392819
10	1	-6.408930	0.726953	-1.187525
11	1	-5.349378	-1.424458	-1.234998
12	1	-3.853751	-0.707826	1.212802
13	1	-3.495295	-2.032610	0.101160
14	1	-2.306902	-0.310899	-1.383065
15	6	-1.323048	1.970607	0.001477
16	6	-0.064518	1.338771	-0.513165
17	1	-0.250246	1.054723	-1.559792
18	7	1.013041	2.294024	-0.566985

19	6	2.126994	2.112391	-1.486101
20	6	1.571125	2.914986	0.623998
21	6	2.901041	3.436300	-1.353684
22	1	1.758243	1.920717	-2.498949
23	1	2.777813	1.268848	-1.203863
24	6	2.488092	3.995734	0.033714
25	1	2.173617	2.210366	1.222185
26	1	0.786182	3.310939	1.273377
27	1	3.978925	3.271889	-1.429932
28	1	2.615616	4.129891	-2.148647
29	1	3.347525	4.190041	0.680429
30	1	1.938072	4.933606	-0.079632
31	1	-1.291847	3.029846	0.240658
32	6	-1.177528	-0.822730	0.392796
33	6	0.185765	-0.061695	0.195661
34	6	1.263471	-0.814301	-0.550268
35	6	0.826393	0.105705	1.585615
36	6	-0.974414	-2.273321	0.000968
37	8	-0.250046	-2.912887	0.925239
38	8	-1.362654	-2.794498	-1.023255
39	6	0.211677	-4.223619	0.576220
40	6	2.368307	-0.972448	0.291244
41	7	2.089645	-0.422890	1.546463
42	8	0.301651	0.604382	2.569808
43	6	1.321184	-1.267600	-1.855386
44	6	2.494490	-1.883810	-2.308512
45	6	3.587197	-2.030204	-1.457230
46	6	3.541466	-1.574113	-0.134212
47	1	0.470428	-1.155141	-2.520235
48	1	2.551487	-2.247283	-3.329025
49	1	4.492157	-2.505984	-1.821596
50	1	4.395843	-1.685666	0.524921
51	6	3.007933	-0.417874	2.660924

52	1	-1.383799	-0.802536	1.468244
53	1	0.779066	-4.571412	1.437191
54	1	-0.631404	-4.887664	0.378134
55	1	0.852780	-4.164805	-0.306866
56	1	3.903808	0.161092	2.415341
57	1	2.502683	0.041304	3.510266
58	1	3.298758	-1.439766	2.921153

G

HF = -1167.7157392 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.370865 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.316775 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.398965 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.906680	-0.428295	-1.099736
2	6	-3.990686	-0.439792	-0.308503
3	6	-4.045155	-0.560938	1.149842
4	6	-1.464571	-0.517168	-0.657560
5	6	-3.093487	-0.982957	1.997442
6	6	-1.261912	-1.672697	0.302889
7	6	-1.704619	-1.482471	1.727076
8	1	-3.061864	-0.318143	-2.170223
9	1	-4.957487	-0.319312	-0.793630
10	1	-4.993842	-0.266135	1.594150
11	1	-0.870614	-0.689046	-1.554319
12	1	-3.337857	-0.967164	3.058066
13	1	-1.012765	-0.762626	2.197935
14	1	-1.563878	-2.420860	2.275425
15	6	-0.692937	-2.846981	-0.052768
16	6	-0.100165	-3.158434	-1.346434
17	1	-0.063098	-2.359156	-2.105942
18	1	-0.630211	-3.652979	0.675757

19	6	-0.930504	0.803791	-0.039040
20	6	0.497431	0.676817	0.399413
21	6	1.632787	0.315833	-0.389223
22	6	0.910604	0.774591	1.747691
23	6	-1.057286	1.936198	-1.036986
24	8	-1.206288	3.120357	-0.427813
25	8	-0.991632	1.825309	-2.247671
26	6	-1.203550	4.274326	-1.270490
27	6	2.741620	0.204743	0.503708
28	7	2.292852	0.487661	1.775328
29	8	0.257943	1.024448	2.799750
30	6	1.858889	0.066905	-1.751332
31	6	3.139925	-0.286667	-2.186803
32	6	4.209227	-0.390383	-1.291213
33	6	4.015351	-0.139733	0.074070
34	1	1.049916	0.167533	-2.469388
35	1	3.306687	-0.479475	-3.243448
36	1	5.195921	-0.665889	-1.652511
37	1	4.839707	-0.216734	0.778212
38	6	3.095505	0.466893	2.967615
39	1	-1.525490	1.076168	0.838889
40	1	-1.322970	5.124229	-0.600329
41	1	-0.257876	4.347589	-1.811917
42	1	-2.029129	4.232794	-1.984582
43	1	3.899763	1.210950	2.919927
44	1	2.440831	0.703687	3.807940
45	1	3.542986	-0.521500	3.127525
46	8	0.365302	-4.259995	-1.618363

TS-G

HF = -1167.6933278 hartrees

Imaginary Frequencies: 1 (-228.2226 1/cm)

Zero-point correction = 0.370810 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.319441 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.373887 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.074777	1.297493	0.068915
2	6	-4.395194	1.239959	-0.177910
3	6	-5.140498	0.104210	-0.723406
4	6	-1.993808	0.305428	-0.305229
5	6	-4.827008	-1.172677	-0.459480
6	6	-2.340112	-1.165213	-0.172980
7	6	-3.669428	-1.552296	0.425799
8	1	-2.714403	2.232326	0.490237
9	1	-4.979489	2.131933	0.045489
10	1	-6.016181	0.328855	-1.329280
11	1	-1.743079	0.515122	-1.356821
12	1	-5.422003	-1.972922	-0.893669
13	1	-3.780659	-1.035107	1.391721
14	1	-3.677943	-2.626914	0.624825
15	6	-1.417693	-2.075127	-0.507388
16	6	-0.094682	-1.721929	-1.101087
17	1	-0.203000	-0.960753	-1.907434
18	1	-1.594611	-3.136294	-0.339692

19	6	-0.689588	0.551297	0.520331
20	6	0.499275	-0.334139	0.147832
21	6	1.677120	0.155879	-0.587165
22	6	1.064863	-1.120600	1.262653
23	6	-0.231838	1.993619	0.467370
24	8	0.501025	2.313106	1.543937
25	8	-0.442901	2.778881	-0.436694
26	6	1.128328	3.597642	1.520414
27	6	2.806349	-0.510465	-0.071877
28	7	2.417779	-1.272089	1.024560
29	8	0.479885	-1.610368	2.235521
30	6	1.830664	0.979780	-1.695351
31	6	3.105740	1.153146	-2.251507
32	6	4.211007	0.491679	-1.718823
33	6	4.072910	-0.360468	-0.615262
34	1	0.973918	1.490704	-2.122879
35	1	3.230393	1.805959	-3.110525
36	1	5.191003	0.630284	-2.166110
37	1	4.929459	-0.886287	-0.204691
38	6	3.298523	-2.094969	1.811395
39	1	-0.925758	0.323970	1.566193
40	1	1.681172	3.670058	2.455466
41	1	1.808142	3.667063	0.668095
42	1	0.379911	4.390549	1.457815
43	1	4.105637	-1.496522	2.248760
44	1	2.708292	-2.540933	2.612643
45	1	3.735115	-2.890438	1.198457
46	8	0.770581	-2.645309	-1.283263

H

HF = -1167.7179004 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.370606 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.316251 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.401649 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.940716	0.152448	-0.989856
2	6	3.944901	-0.137873	-0.137708
3	6	3.874125	-0.122174	1.308553
4	6	1.500995	0.360340	-0.593739
5	6	3.024627	0.630551	2.051732
6	6	1.386365	1.522273	0.371914
7	6	2.032403	1.562063	1.557020
8	1	3.163264	0.181896	-2.054321
9	1	4.915185	-0.385314	-0.565248
10	1	4.634284	-0.692050	1.838341
11	1	0.948607	0.615135	-1.502530
12	1	3.154790	0.610871	3.131352
13	6	0.445805	2.639729	-0.017876
14	6	0.995280	3.458778	-1.156473
15	1	1.435425	2.887387	-1.998517
16	1	-0.500059	2.198618	-0.369220
17	6	0.812294	-0.902607	-0.010000
18	6	-0.616101	-0.650507	0.371446

19	6	-1.684651	-0.185869	-0.451601
20	6	-1.088008	-0.734682	1.704045
21	6	0.880659	-2.040052	-1.005938
22	8	0.883823	-3.238254	-0.402983
23	8	0.890381	-1.920272	-2.218353
24	6	0.807384	-4.380423	-1.257367
25	6	-2.813330	0.021536	0.401742
26	7	-2.439912	-0.312708	1.684167
27	8	-0.520072	-1.089192	2.770459
28	6	-1.836531	0.099253	-1.818183
29	6	-3.062459	0.574891	-2.296041
30	6	-4.150618	0.770629	-1.439558
31	6	-4.031052	0.489372	-0.070465
32	1	-1.013245	-0.068473	-2.506921
33	1	-3.171785	0.789308	-3.356246
34	1	-5.093099	1.140706	-1.833005
35	1	-4.870833	0.636438	0.603841
36	6	-3.291387	-0.263051	2.840580
37	1	1.333352	-1.218119	0.898293
38	1	0.828652	-5.243468	-0.593490
39	1	-0.122947	-4.365969	-1.830145
40	1	1.655765	-4.407090	-1.945038
41	1	-4.121484	-0.976043	2.760105
42	1	-2.682734	-0.523897	3.708027
43	1	-3.707419	0.741553	2.982841
44	8	0.977964	4.672396	-1.197357
45	1	1.782452	2.375957	2.235765
46	1	0.225946	3.306330	0.819448

TS-H

HF = -1167.7074844 hartrees

Imaginary Frequencies: 1 (-243.1546 1/cm)

Zero-point correction = 0.371234 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.320444 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.387040 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.170342	0.911379	-0.671195
2	6	4.411635	0.907832	-0.149056
3	6	4.844925	0.047861	0.931131
4	6	2.017317	0.155193	-0.059211
5	6	4.365771	-1.205182	1.160060
6	6	2.299888	-1.320201	-0.248682
7	6	3.342921	-1.890518	0.399766
8	1	2.969207	1.503460	-1.563615
9	1	5.161255	1.568245	-0.581171
10	1	5.703678	0.375532	1.513353
11	1	2.003218	0.367588	1.019193
12	1	4.874350	-1.800352	1.916701
13	1	3.428541	-2.975789	0.362360
14	6	1.289806	-2.146528	-0.985995
15	6	-0.018058	-2.210817	-0.174430
16	1	0.170258	-2.083525	0.912506
17	1	1.065860	-1.758574	-1.986388
18	6	0.686557	0.600097	-0.680584

19	6	-0.544666	-0.239995	-0.366197
20	6	-1.366250	-0.059381	0.828782
21	6	-1.500636	-0.397469	-1.465060
22	6	0.396864	2.044271	-0.307015
23	8	-0.493644	2.601187	-1.140075
24	8	0.863307	2.639458	0.644817
25	6	-0.938350	3.916661	-0.803698
26	6	-2.703060	-0.339484	0.468486
27	7	-2.759635	-0.543652	-0.905192
28	8	-1.275414	-0.465564	-2.680871
29	6	-1.069753	0.215584	2.158960
30	6	-2.102490	0.214548	3.106847
31	6	-3.414183	-0.074451	2.732026
32	6	-3.732782	-0.358514	1.396355
33	1	-0.049404	0.434839	2.460008
34	1	-1.876741	0.434979	4.146165
35	1	-4.201149	-0.080207	3.480419
36	1	-4.754319	-0.581188	1.102876
37	6	-3.941807	-0.910761	-1.638923
38	1	0.784069	0.570406	-1.773342
39	1	-1.659395	4.187281	-1.573221
40	1	-1.413722	3.916687	0.179676
41	1	-0.101109	4.618360	-0.802665
42	1	-4.703210	-0.124621	-1.579200
43	1	-3.656246	-1.054044	-2.681674
44	1	-4.362697	-1.843814	-1.250280
45	8	-0.929383	-3.007113	-0.530941
46	1	1.652131	-3.174193	-1.102996

I

HF = -1167.7178596 hartrees

Imaginary Frequencies: none found

Zero-point correction = 0.370604 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.317190 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.400670 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.000021	-0.028786	-1.456560
2	6	-4.094886	-0.341836	-0.736297
3	6	-4.131005	-1.144399	0.470041
4	6	-1.569943	-0.285972	-1.049211
5	6	-3.233572	-2.103117	0.803643
6	6	-1.332252	-1.765490	-0.815686
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9	1	-5.057302	0.014860	-1.100327
10	1	-5.006160	-1.030059	1.105827
11	1	-0.939581	0.024812	-1.886095
12	1	-3.441105	-2.695303	1.692222
13	6	-0.116083	-2.390506	-1.456798
14	6	1.009653	-2.636337	-0.463293
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16	1	-0.352640	-3.375455	-1.882208
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19	6	1.476955	0.679925	-0.383922
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34	1	5.026299	1.173452	-1.939247
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40	1	-2.582125	4.325430	0.523124
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43	1	3.709854	-1.667320	2.085129
44	8	2.149200	-2.873925	-0.805795
45	1	-1.737212	-3.528320	0.225030
46	1	0.287120	-1.780123	-2.269943

TS-I

HF = -1167.7022585 hartrees

Imaginary Frequencies: 1 (-238.3505 1/cm)

Zero-point correction = 0.371672 (Hartree/Particle)

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Thermal correction to Gibbs Free Energy = 0.320429 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -1167.381829 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.074718	0.882174	-1.169972
2	6	-4.248223	0.875840	-0.515115
3	6	-4.698103	-0.053155	0.507753
4	6	-1.854970	0.019796	-0.941280
5	6	-4.215807	-1.297254	0.717117
6	6	-2.116337	-1.448987	-0.700307
7	6	-3.124095	-1.969210	0.033247
8	1	-2.950130	1.634218	-1.944895
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10	1	-5.553082	0.263210	1.101128
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13	6	-0.942452	-2.307126	-1.058399
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23	8	-0.591712	2.587979	-1.051273
24	6	0.328894	3.878034	1.062498
25	6	2.703473	-0.228676	0.056337
26	7	2.397187	-0.415027	1.398649
27	8	0.485493	-0.444420	2.702885
28	6	1.586314	0.225360	-2.026882
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30	6	4.009466	0.087112	-1.914987
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8. References

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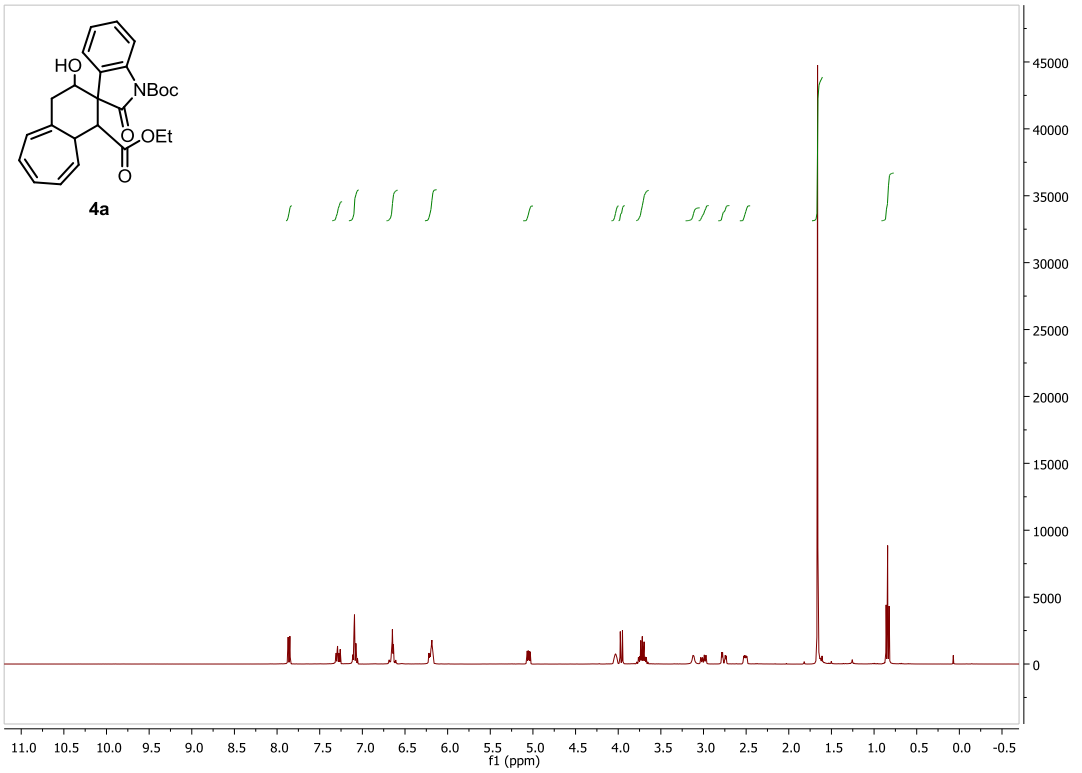
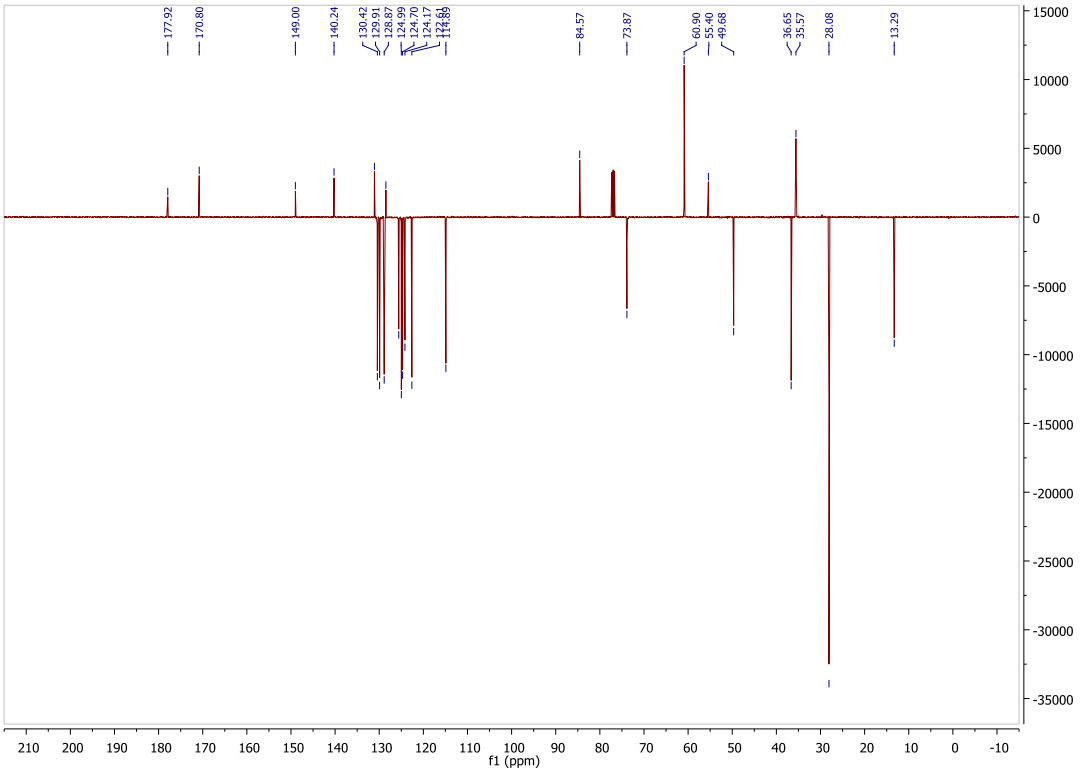
(3) *GAUSSIAN09,* Revision A.02 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. D. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

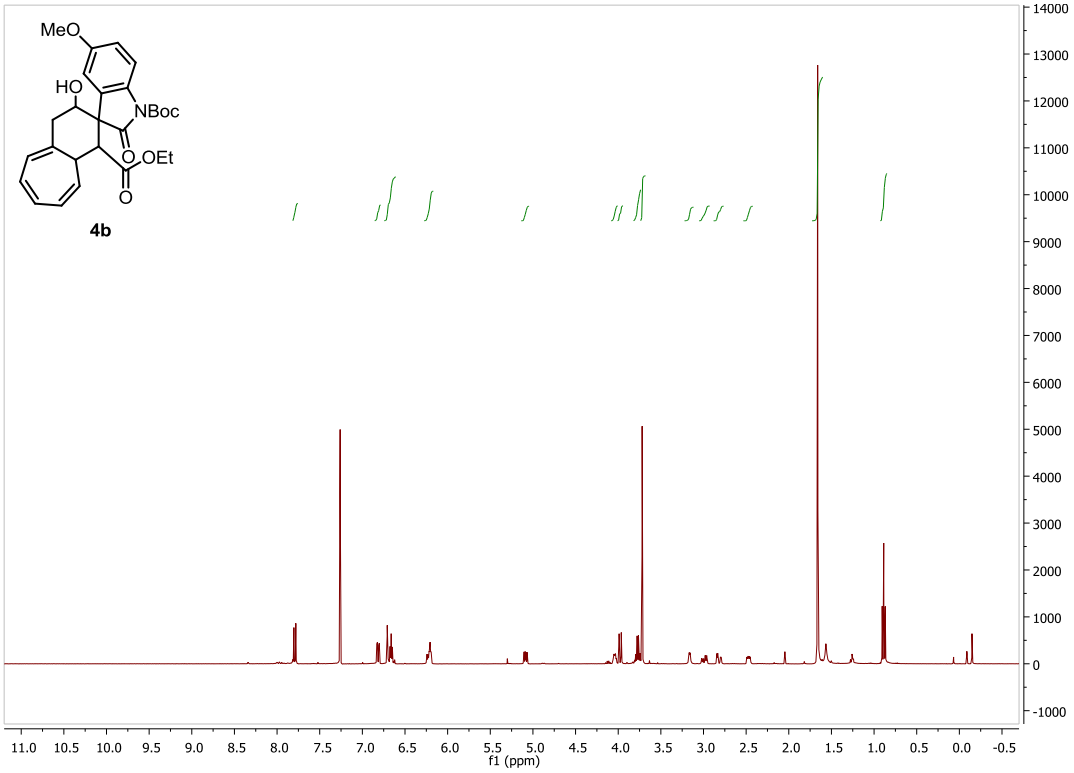
(4) a) C. Gonzalez, H. B. Schlegel, *J. Phys. Chem*. **1990**, 94, 5523. (b) Fukui, K. *Acc. Chem. Res*. **1981**, 14, 363.



^{1}H NMR spectrum of **4a**



^{13}C NMR spectrum of **4a**



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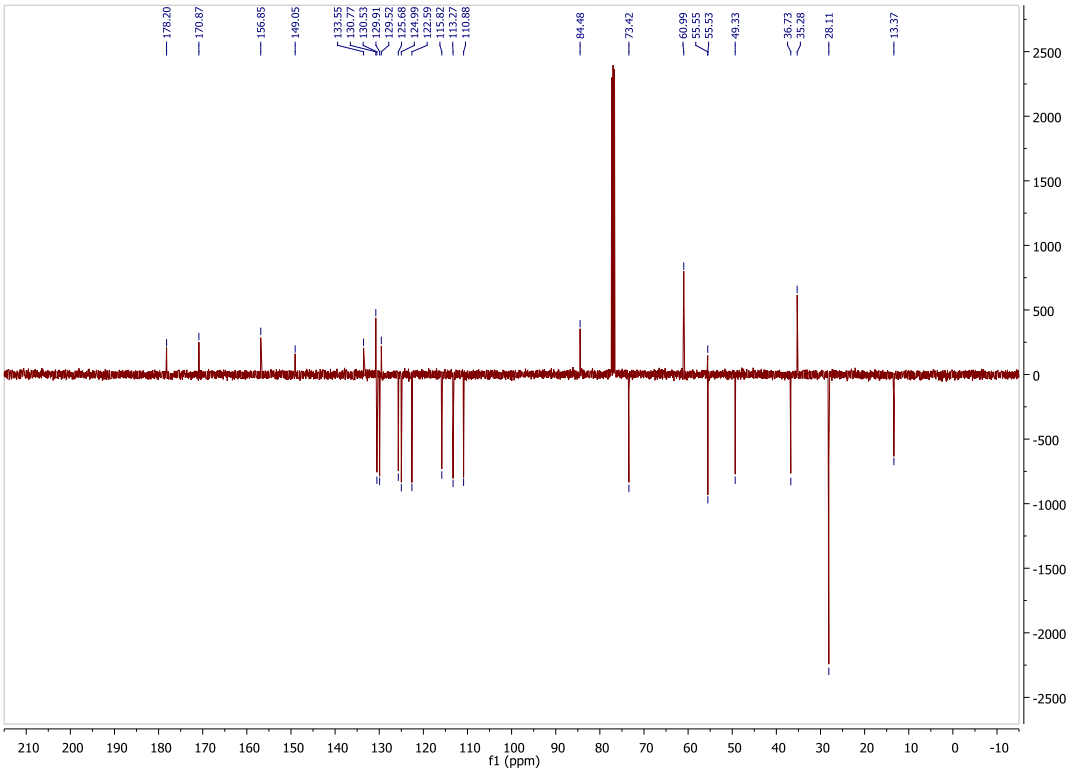
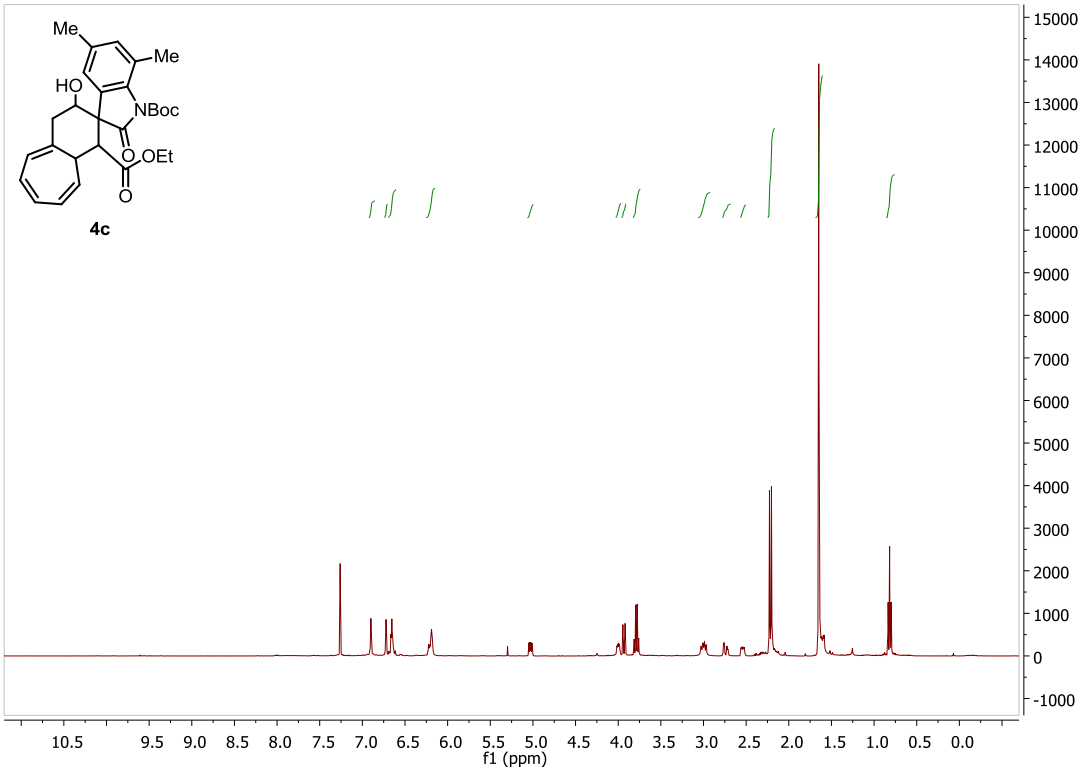


^{13}C NMR spectrum of **4b**



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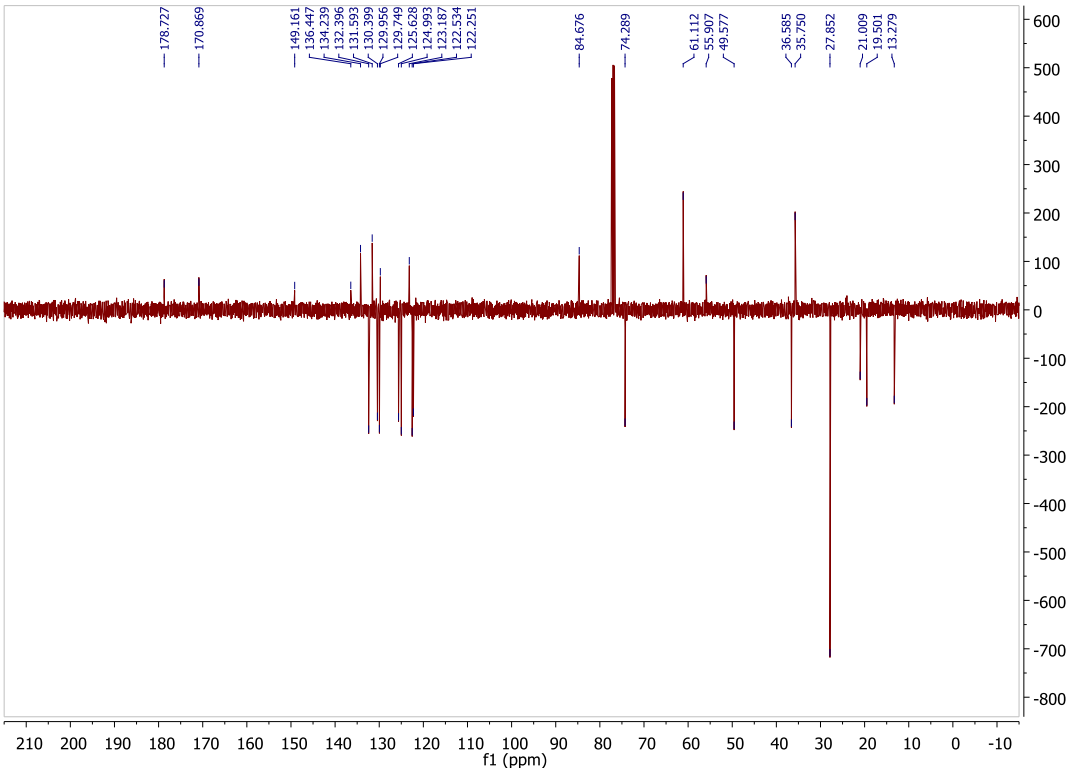

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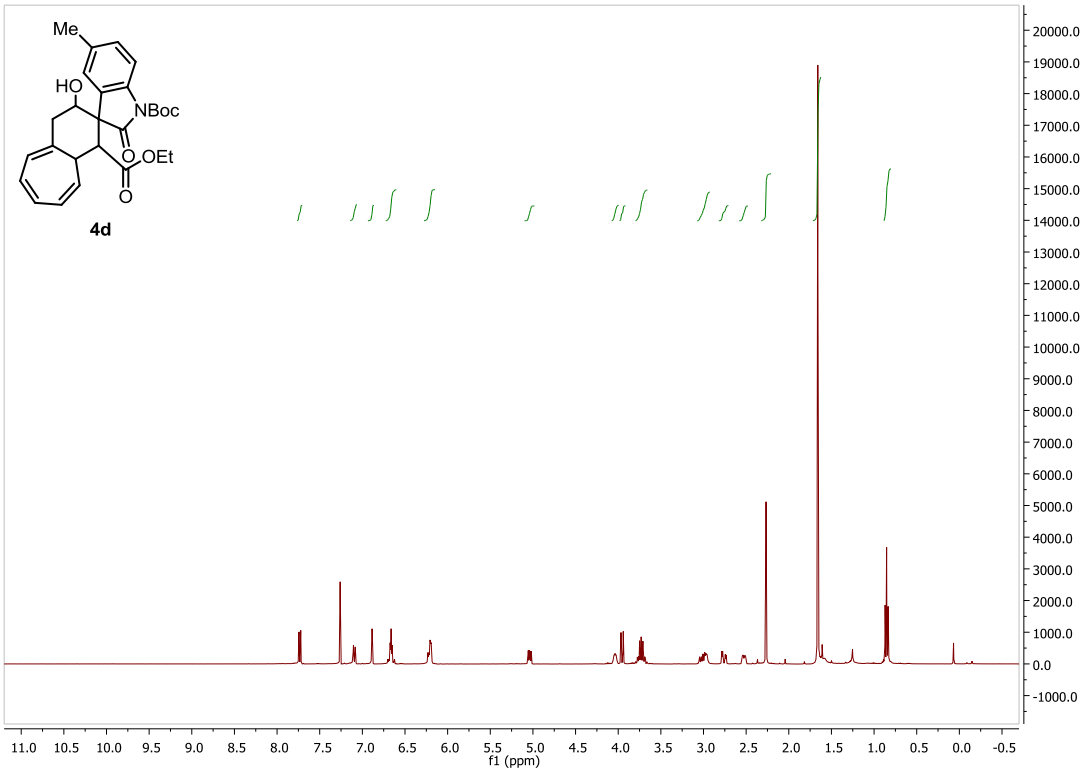
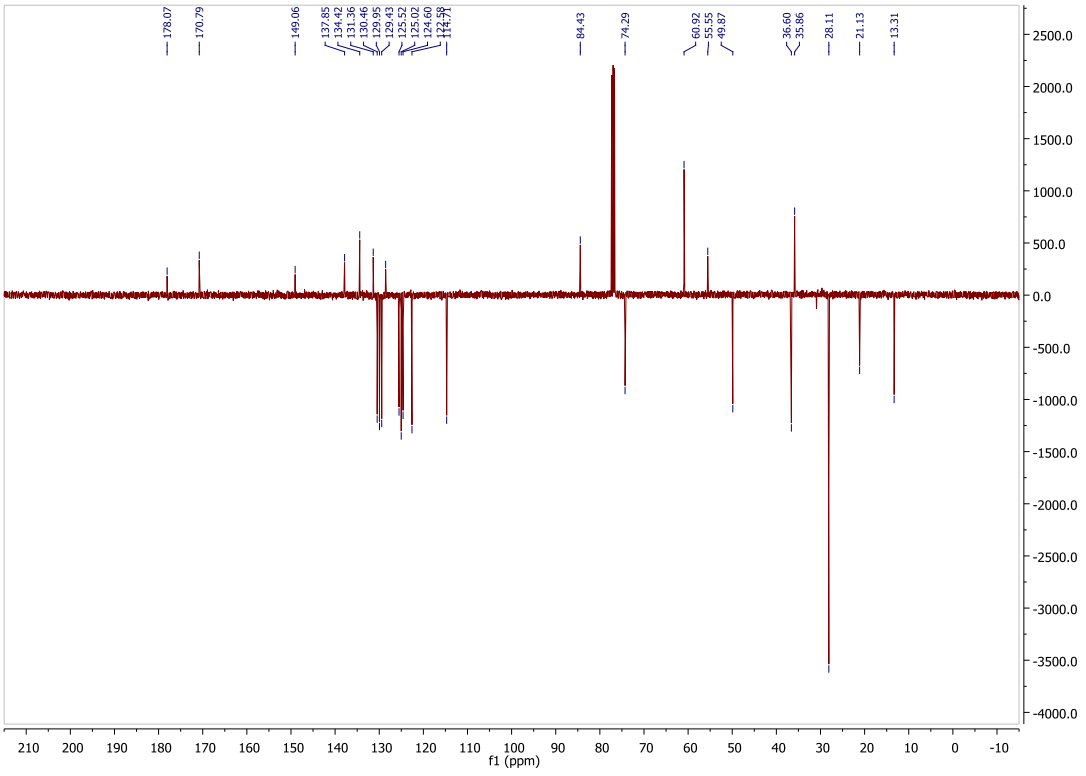


^{1}H NMR spectrum of **4d**



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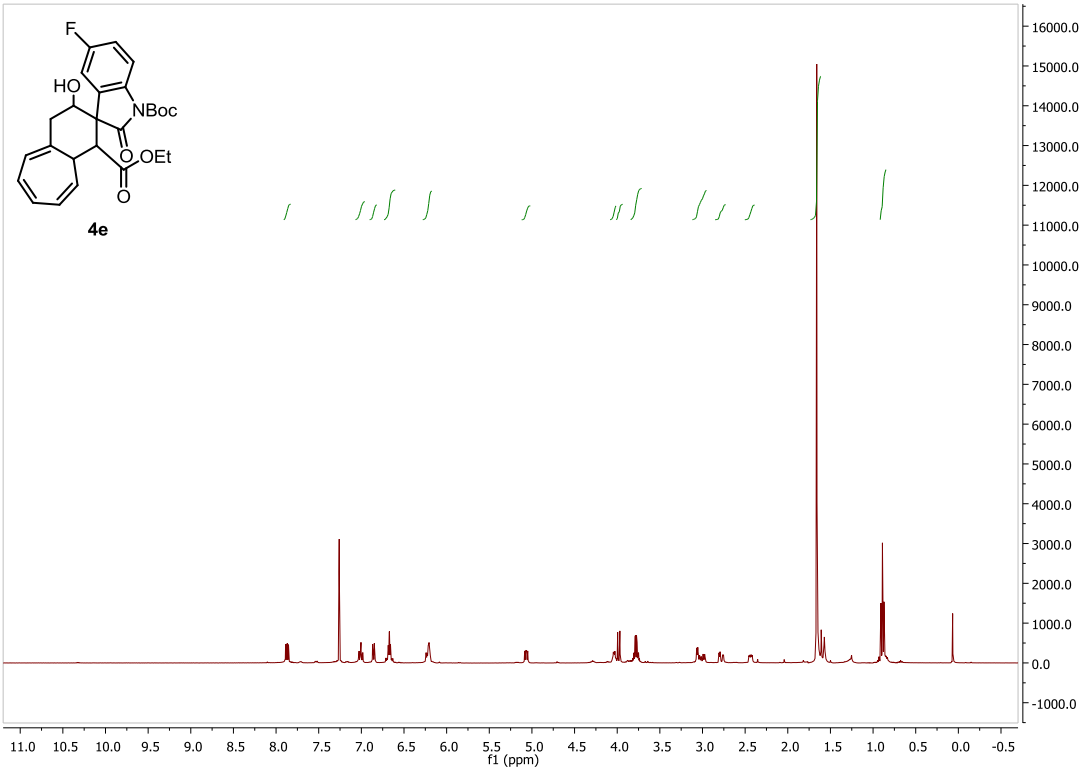
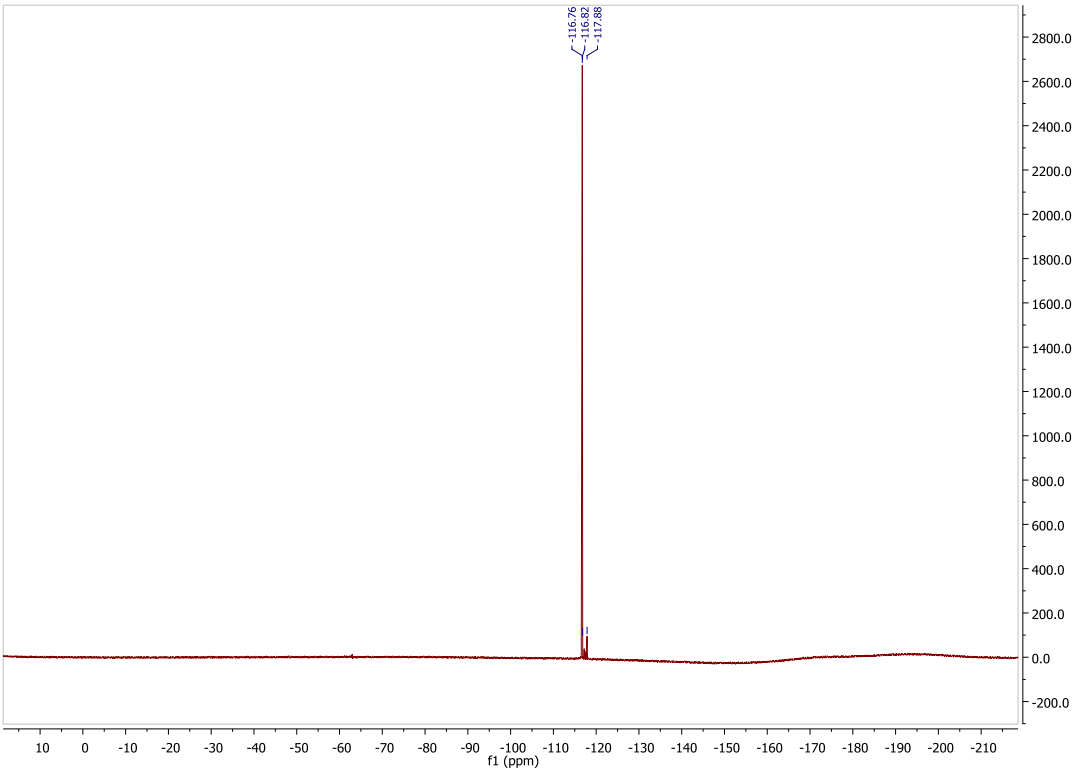
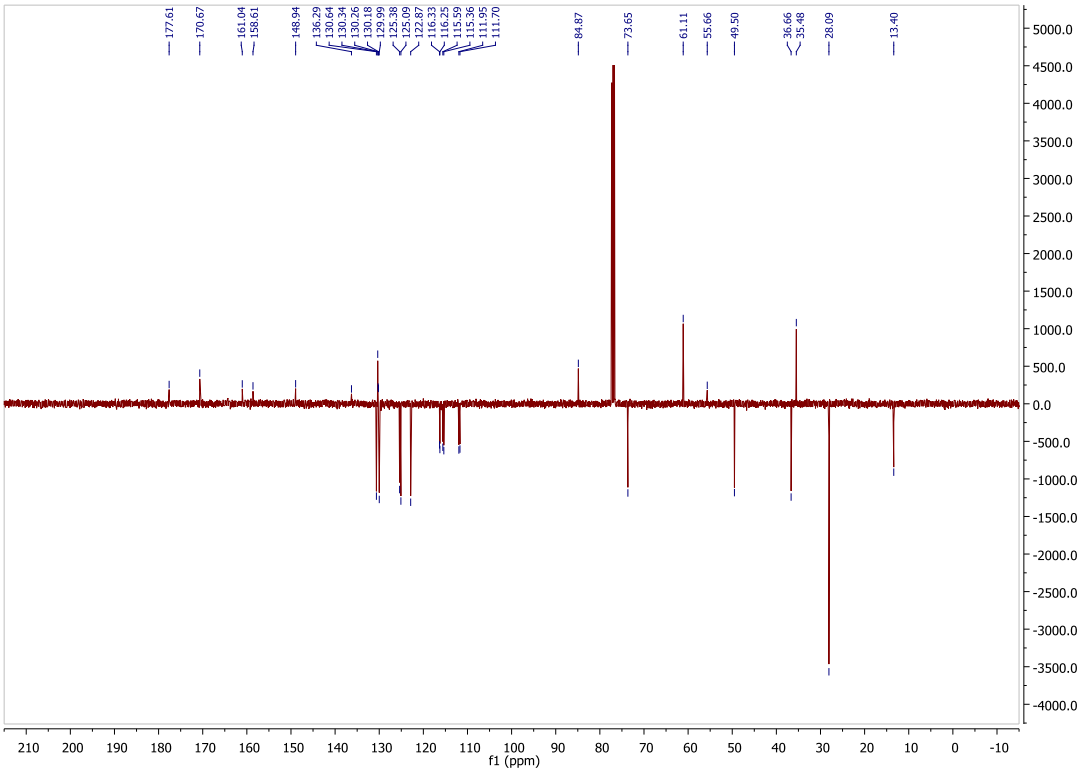


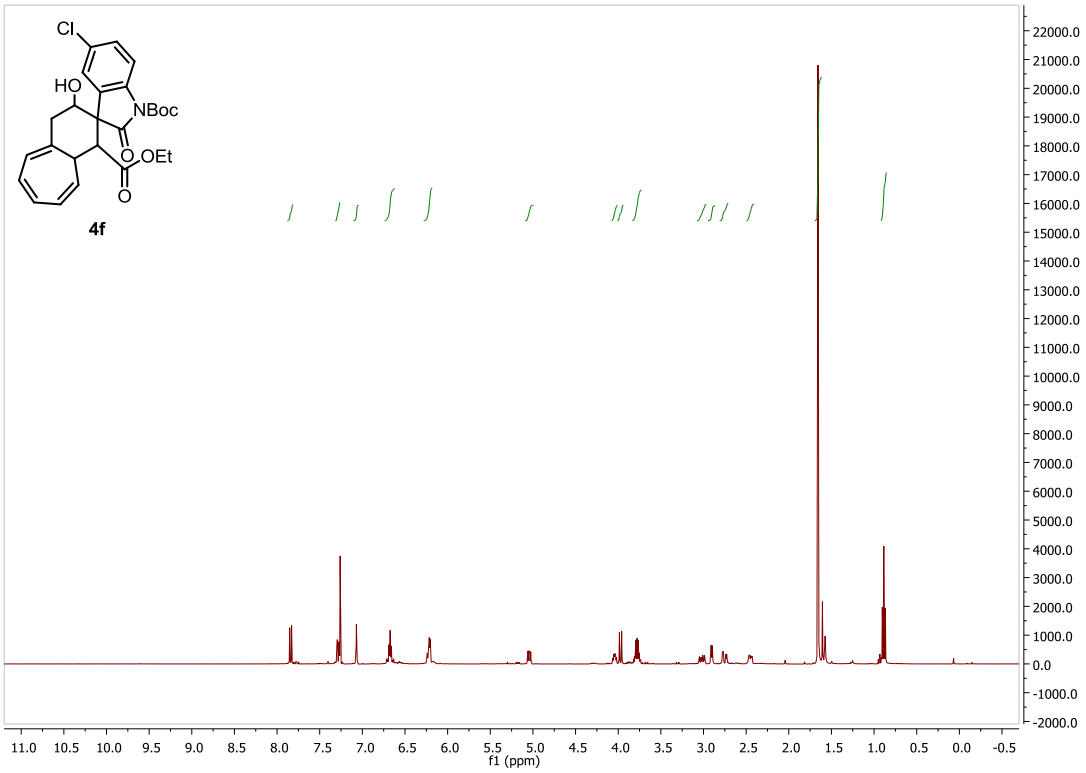
^{1}H NMR spectrum of **4e**



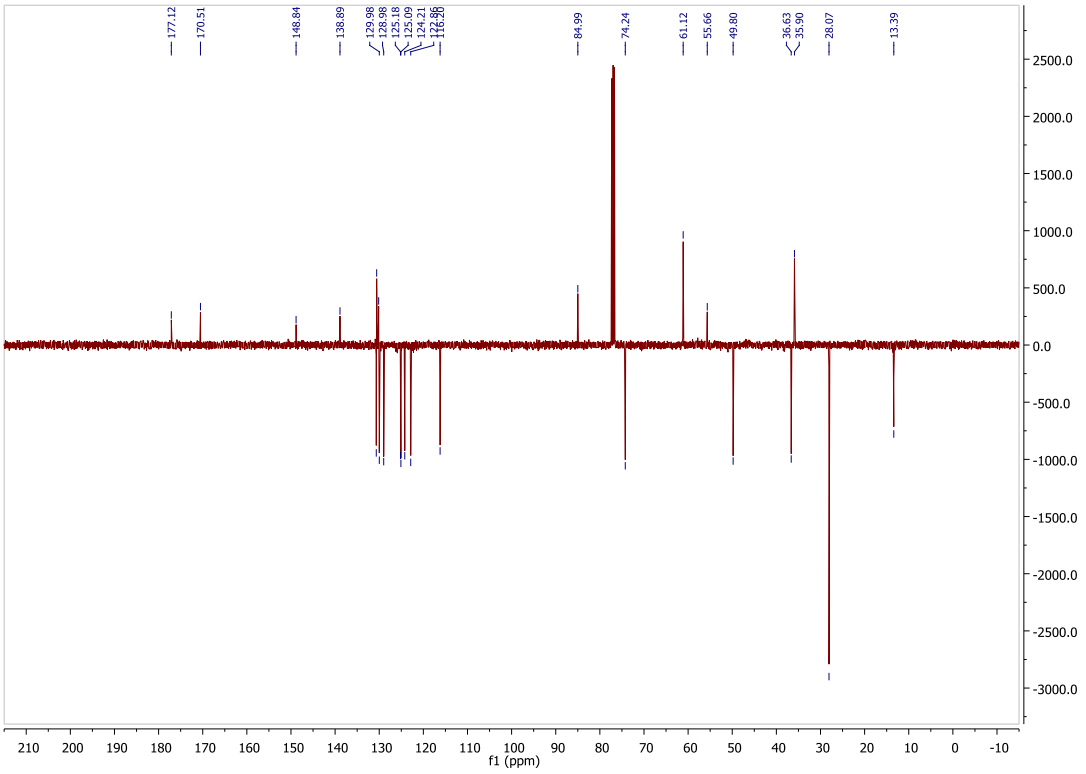
^{19}F NMR spectrum of **4e**



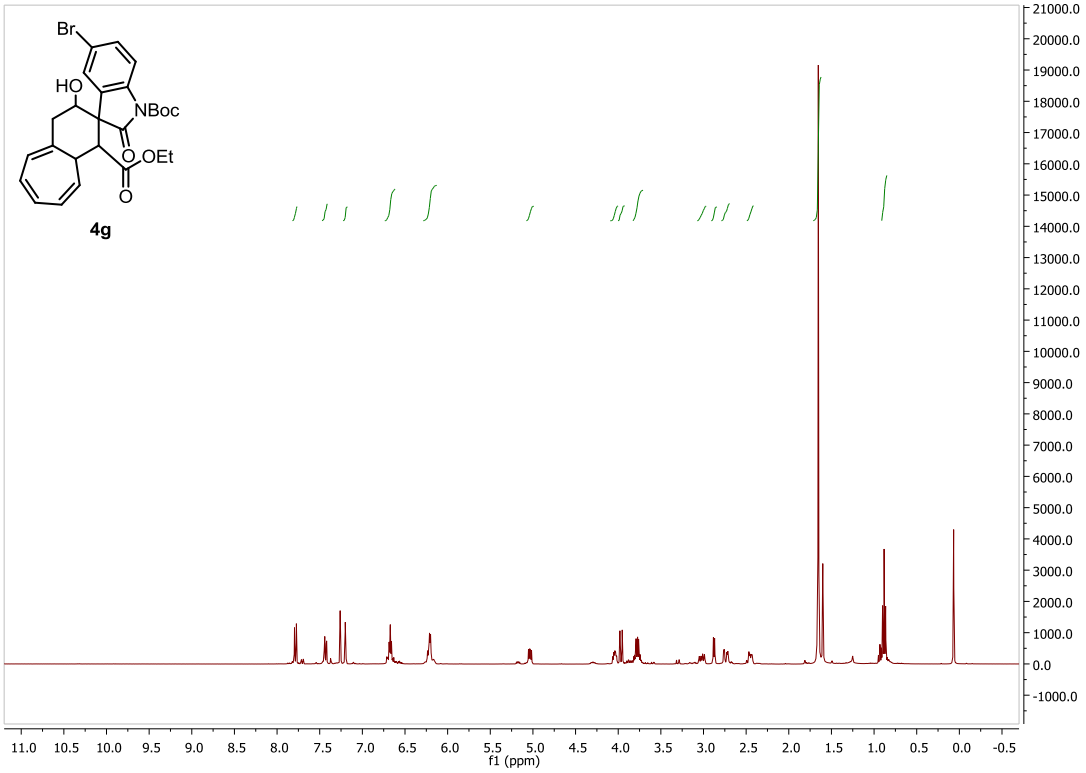
^{13}C NMR spectrum of **4e**



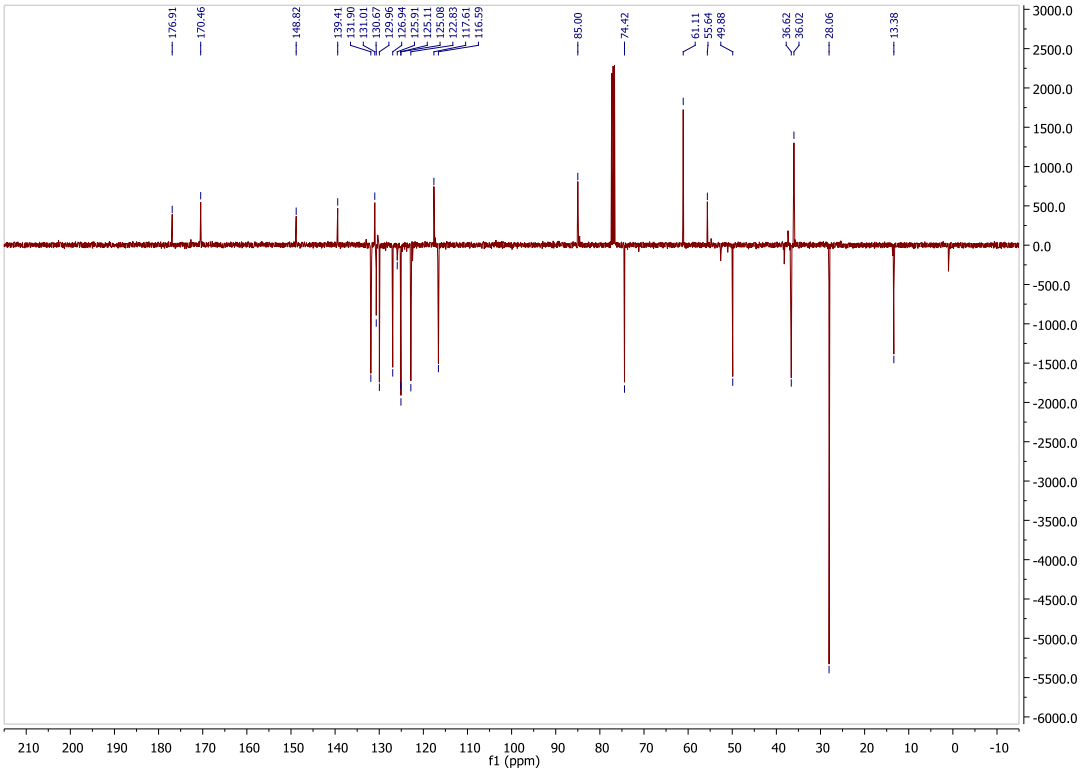
^{1}H NMR spectrum of **4f**



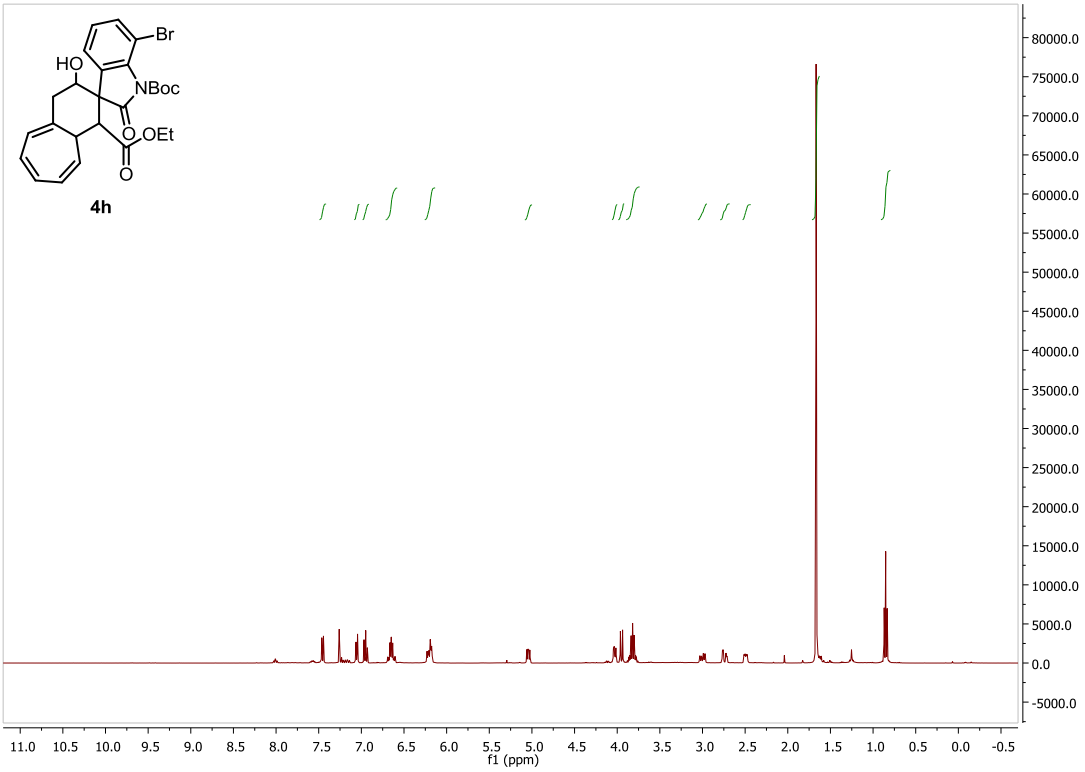
^{13}C NMR spectrum of **4f**



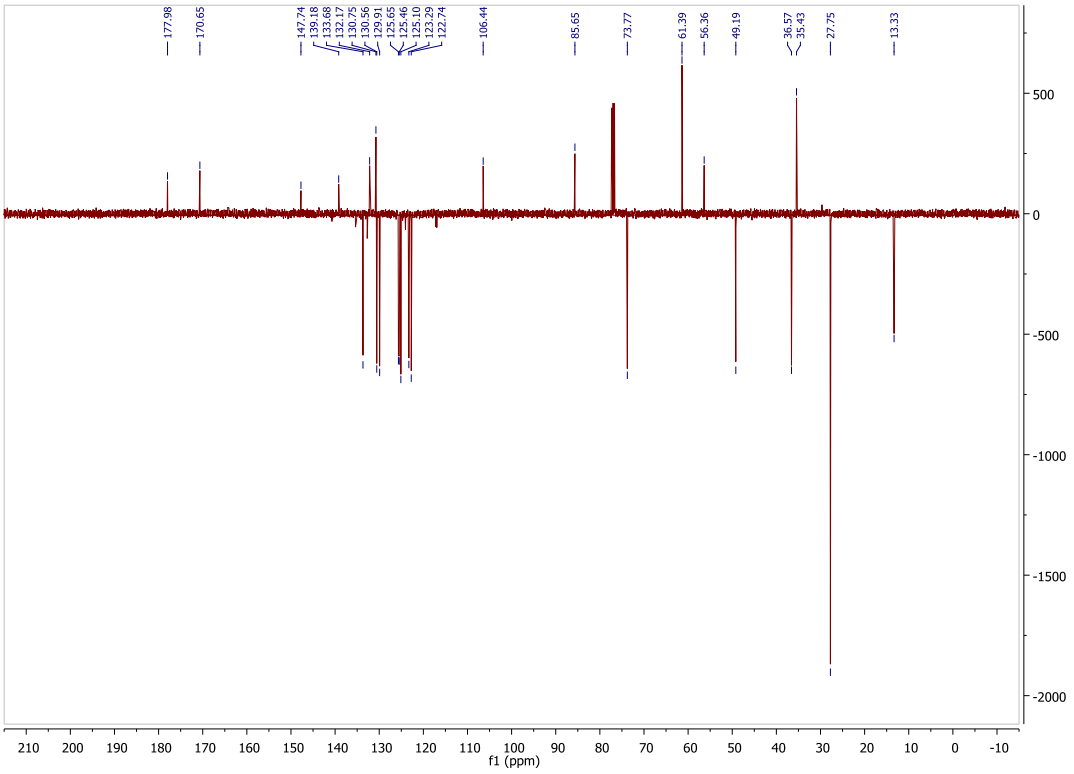
^{1}H NMR spectrum of **4g**



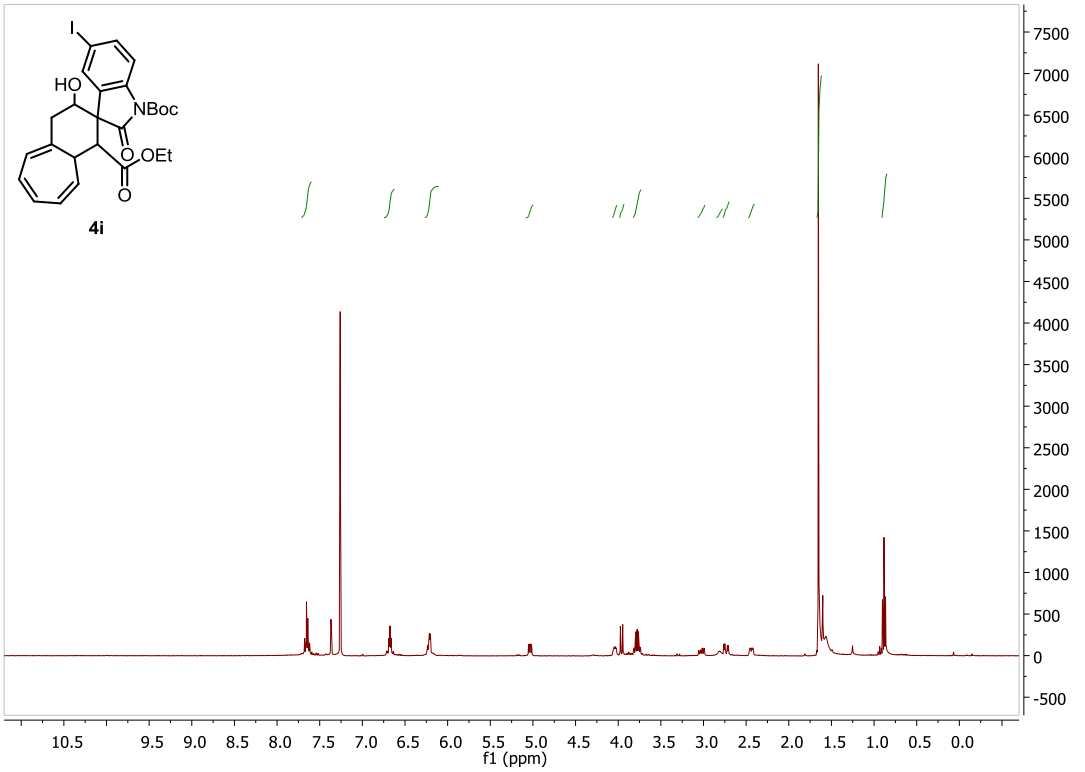
^{13}C NMR spectrum of **4g**



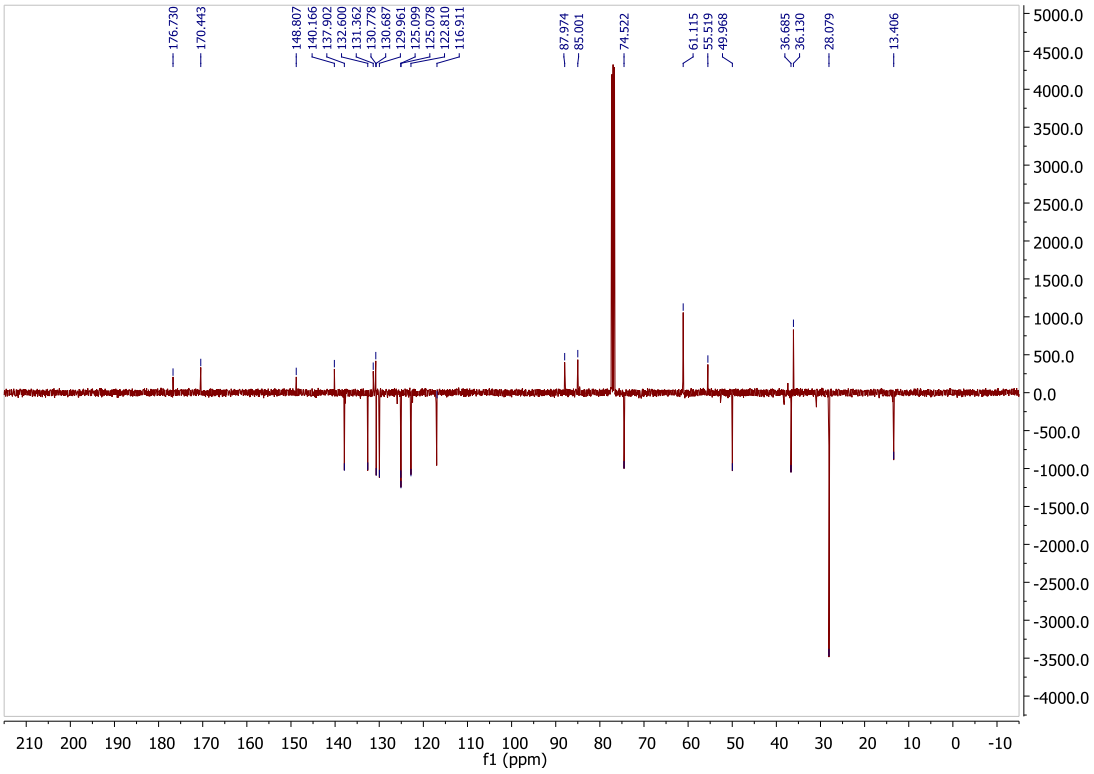
^{1}H NMR spectrum of **4h**



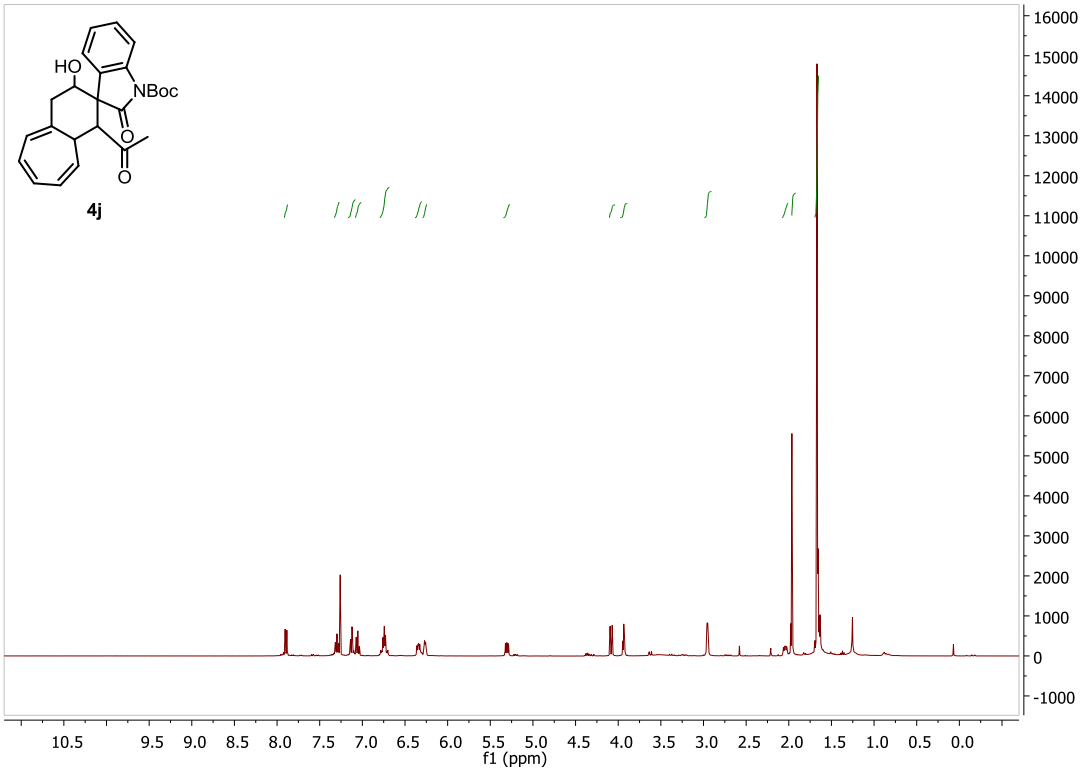
^{13}C NMR spectrum of **4h**



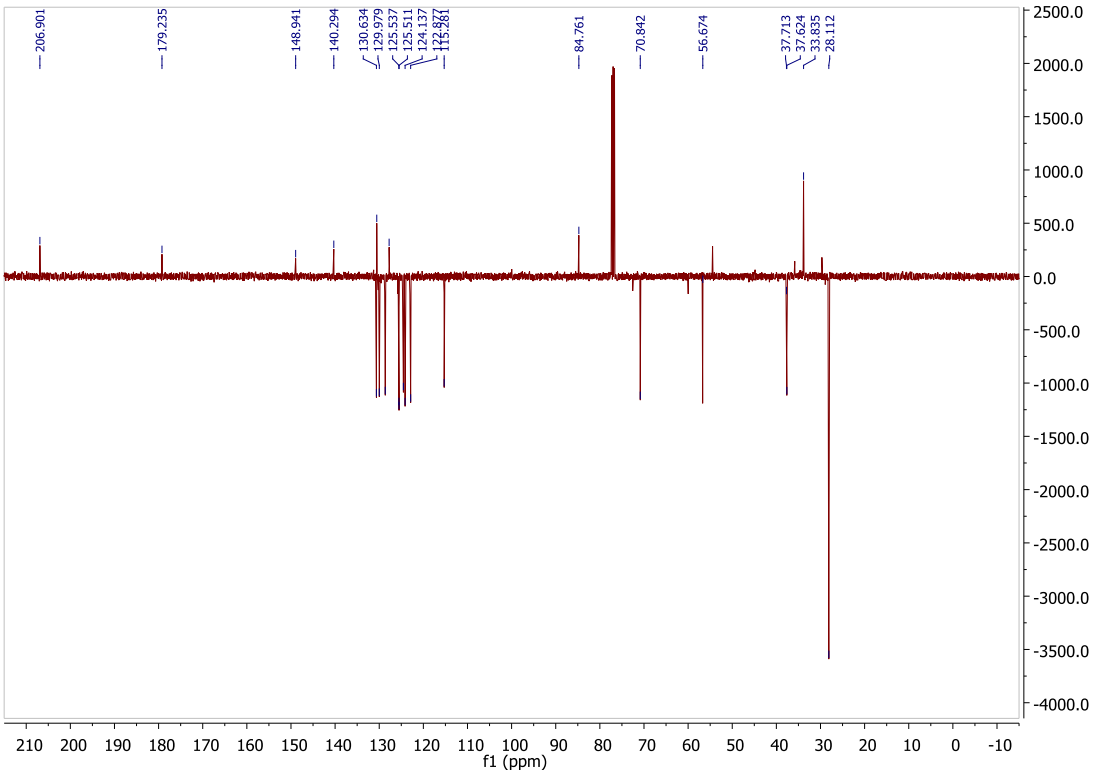
^{1}H NMR spectrum of **4i**



^{13}C NMR spectrum of **4i**



^{1}H NMR spectrum of **4j**



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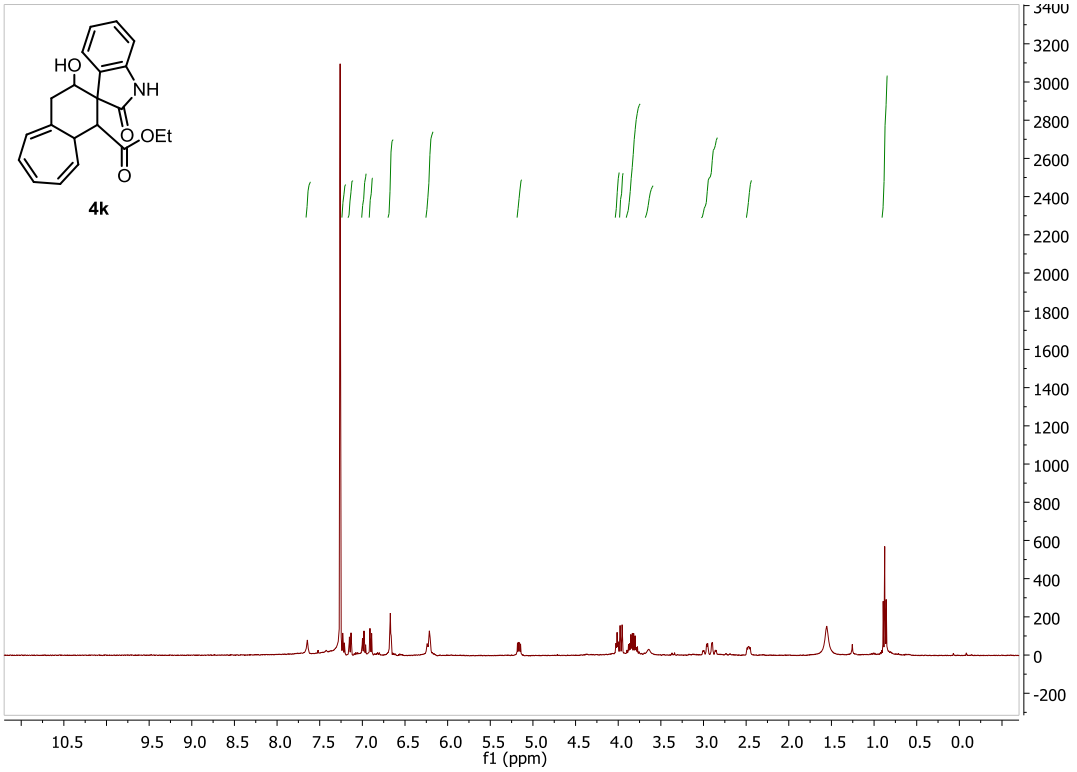

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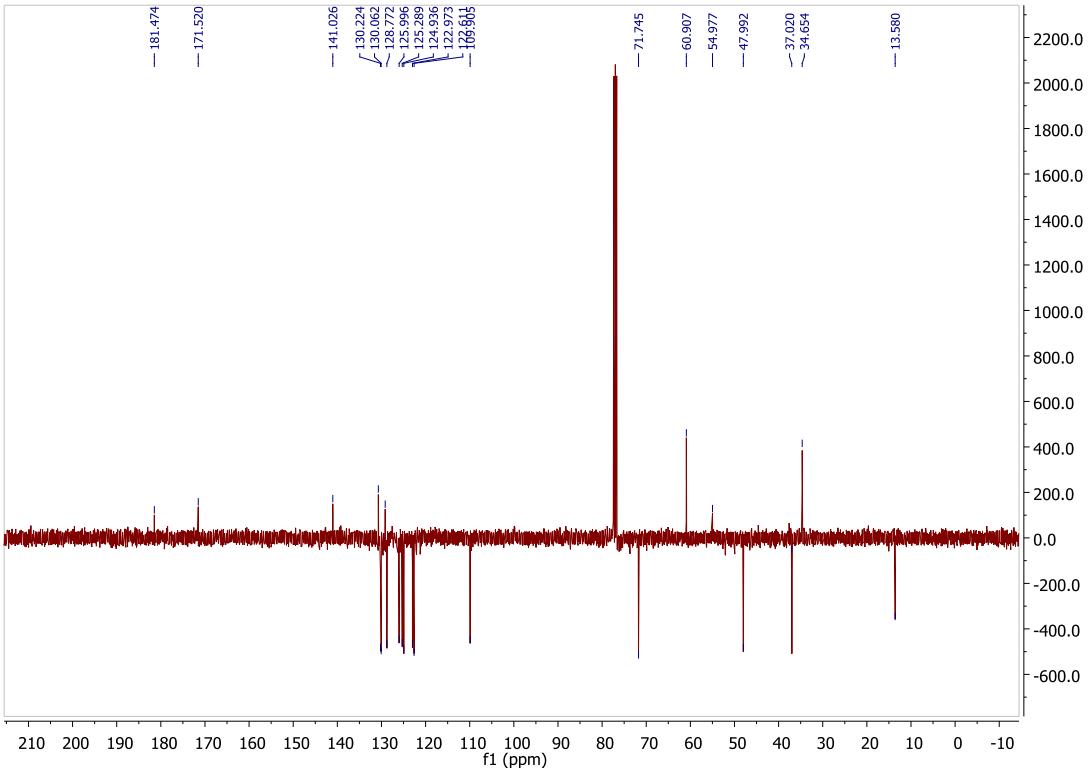

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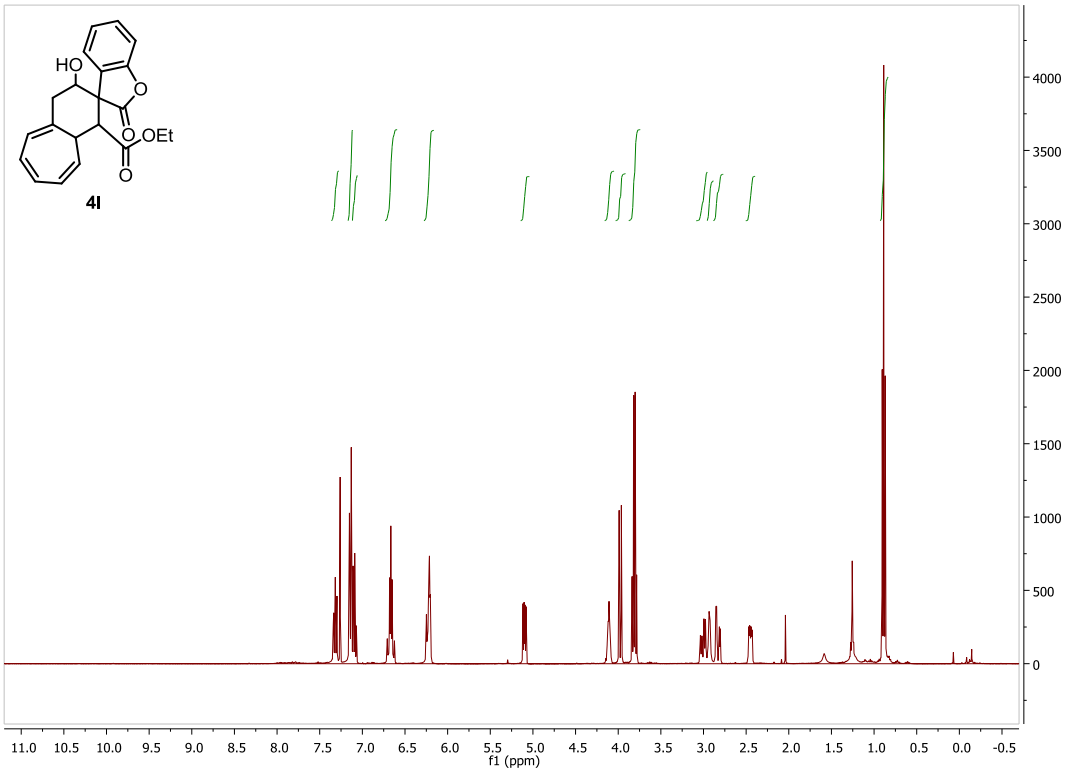

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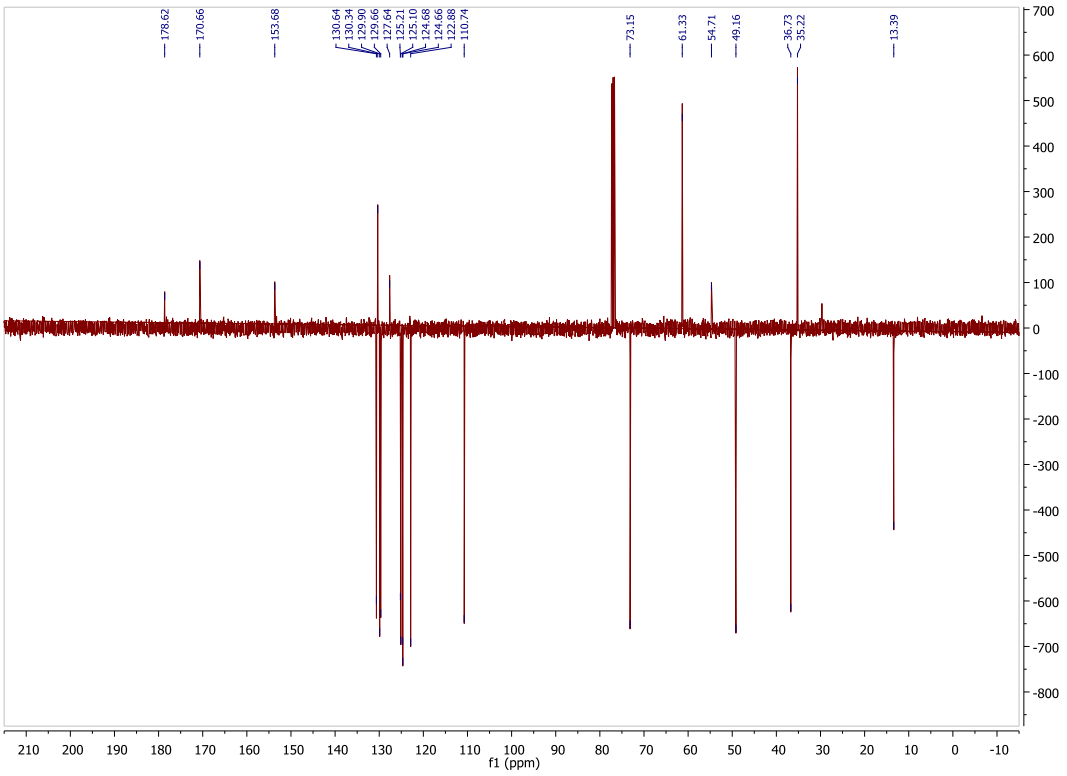

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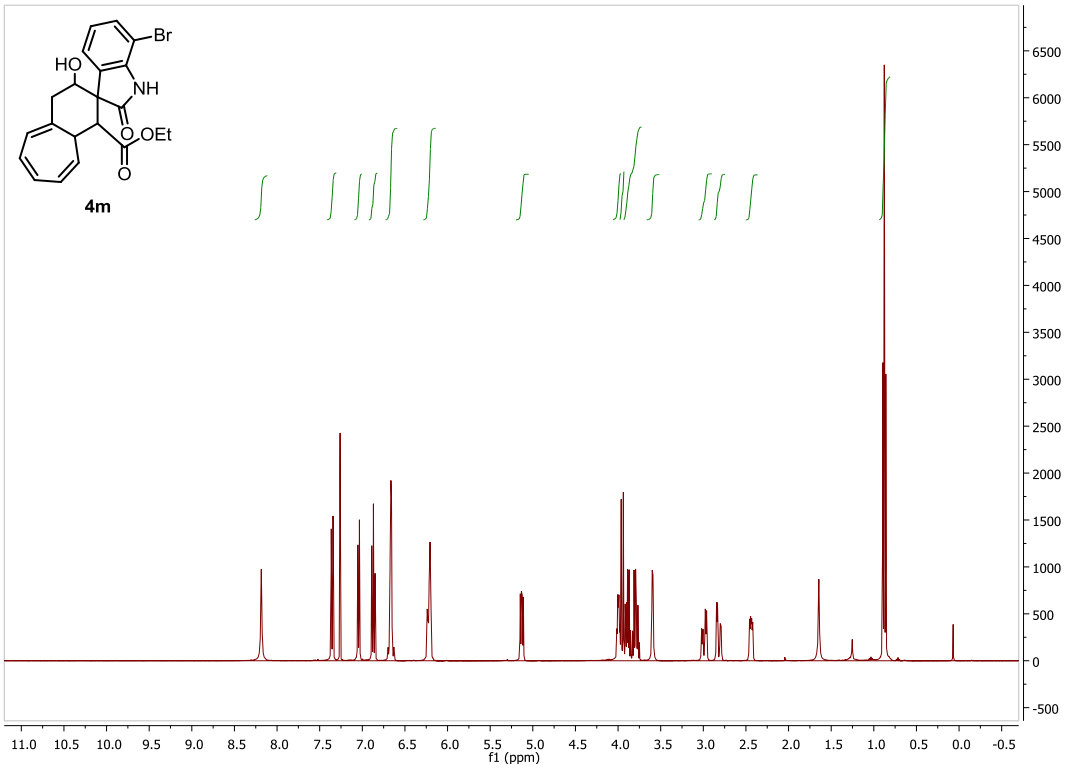

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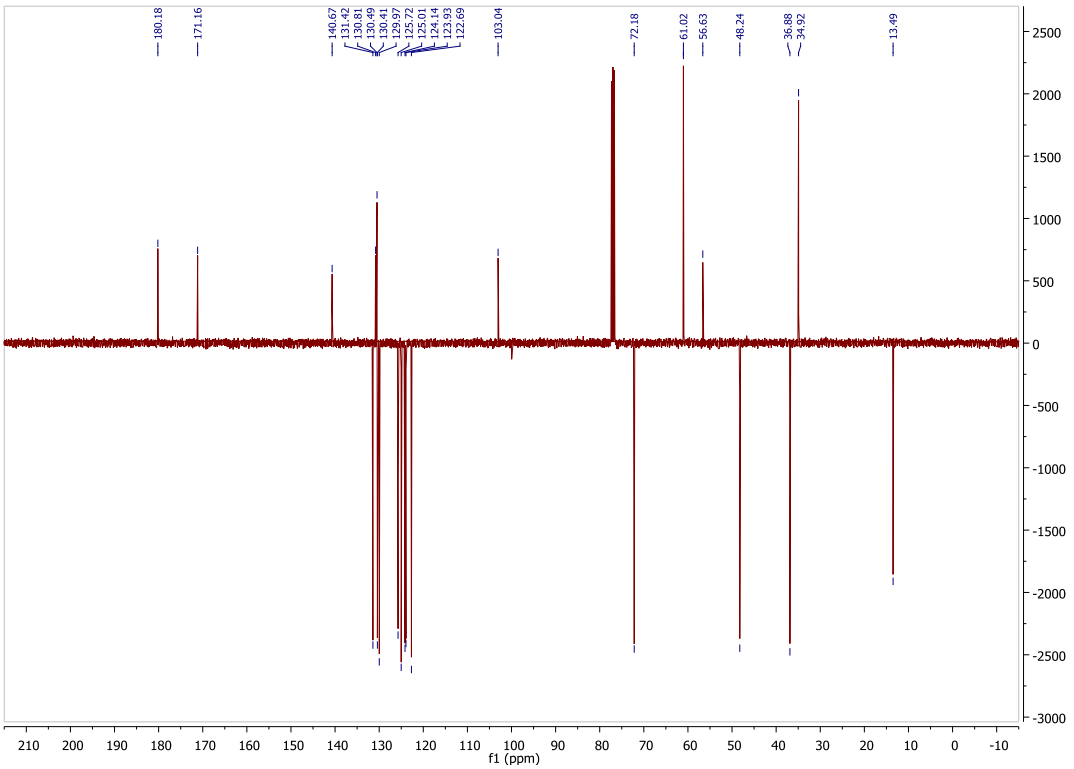

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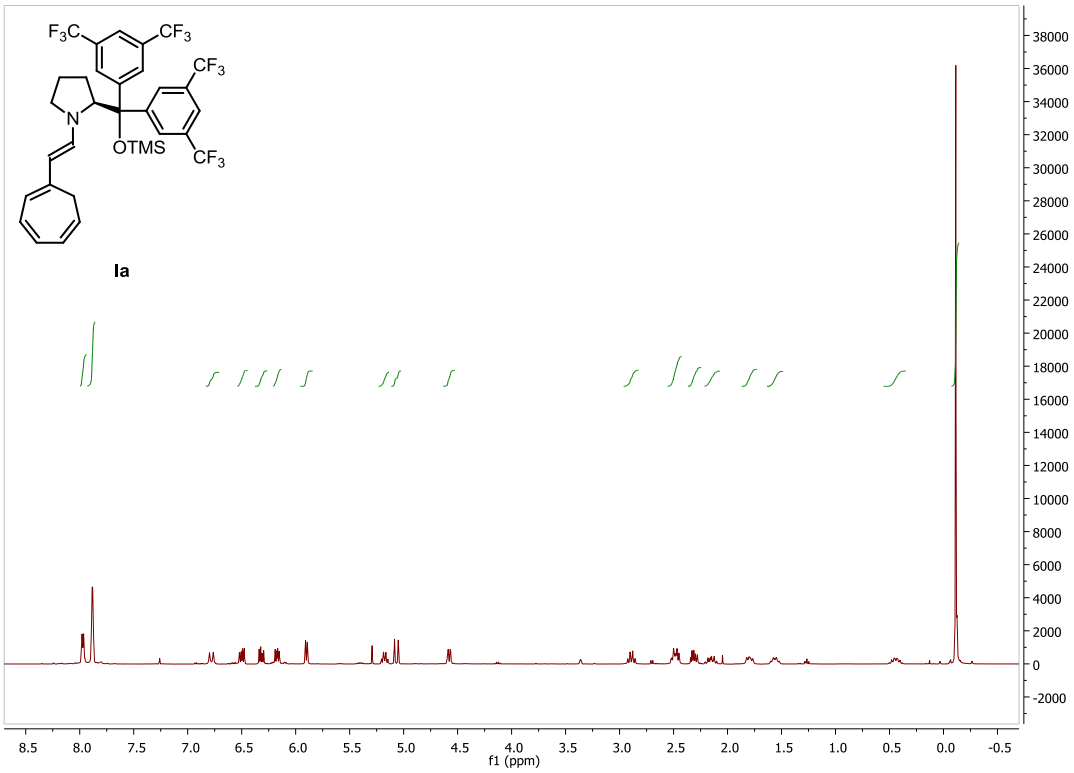

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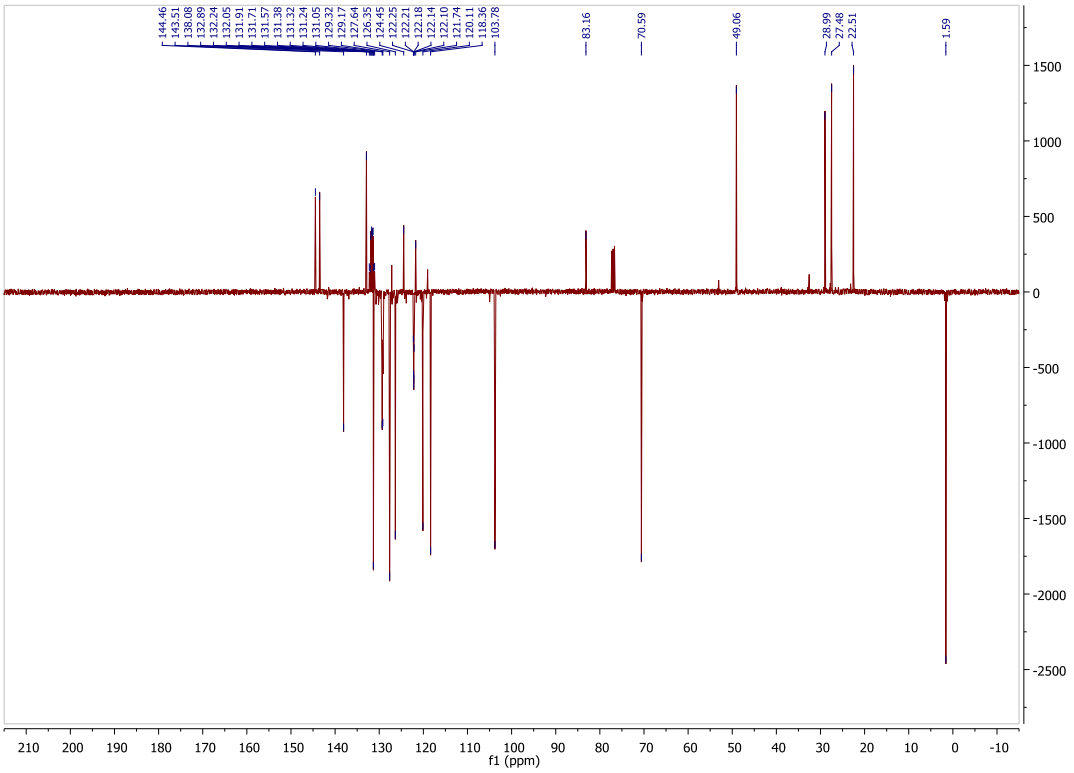

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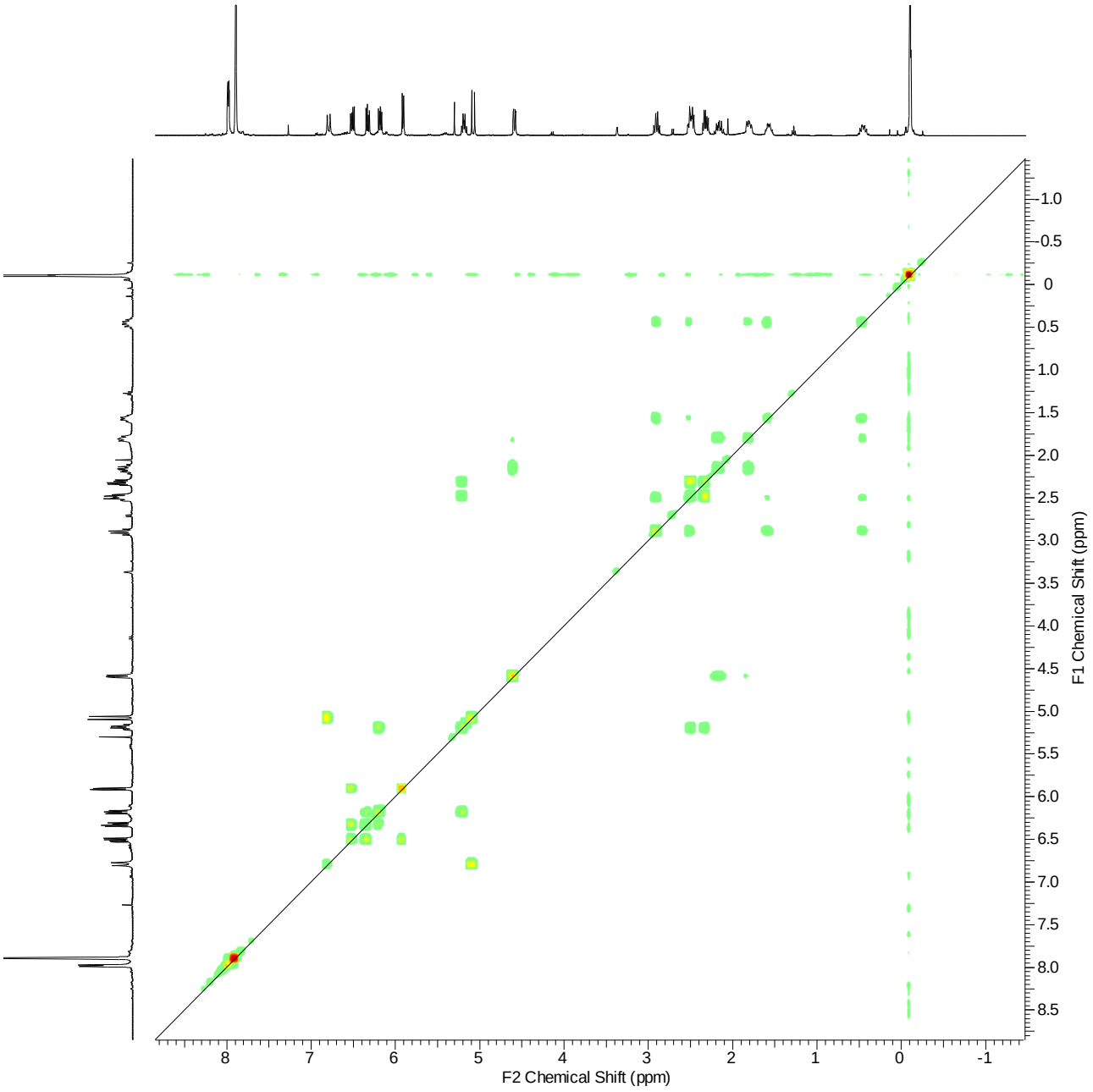

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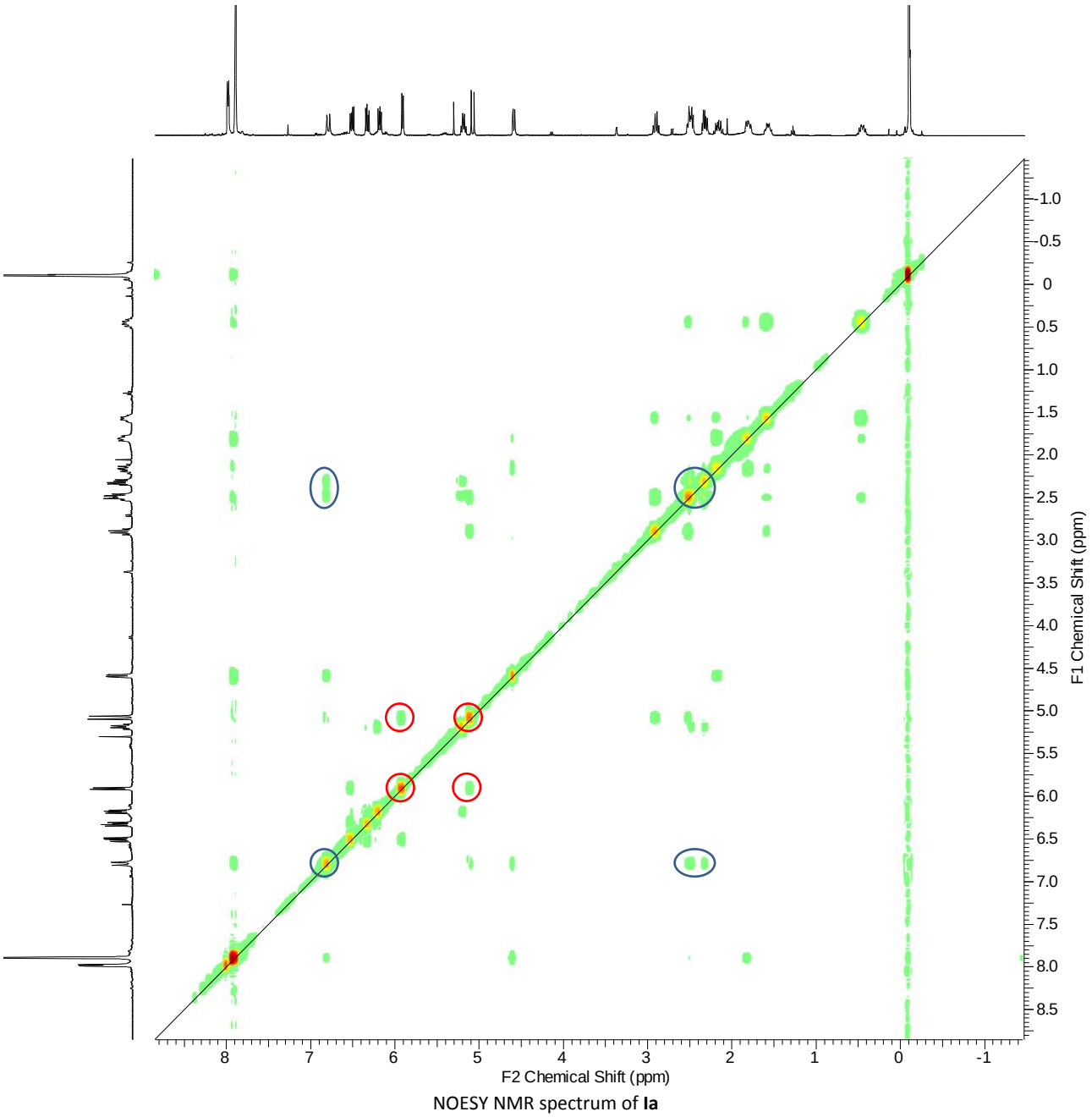

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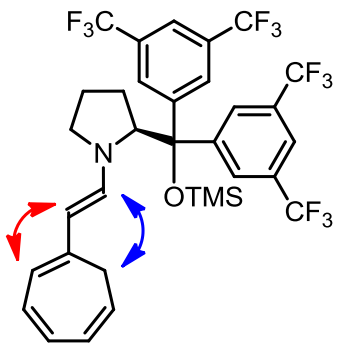
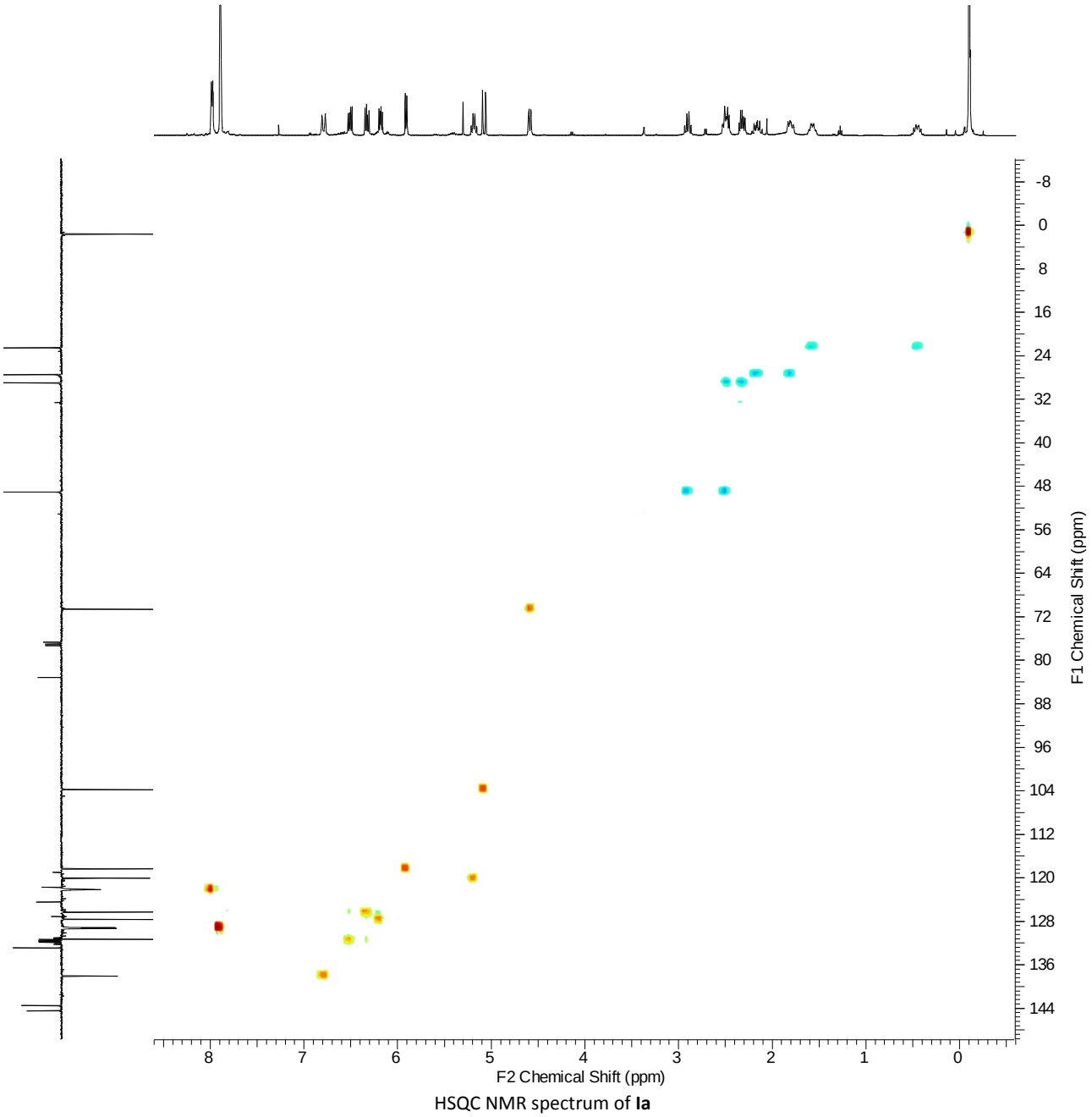


Ia



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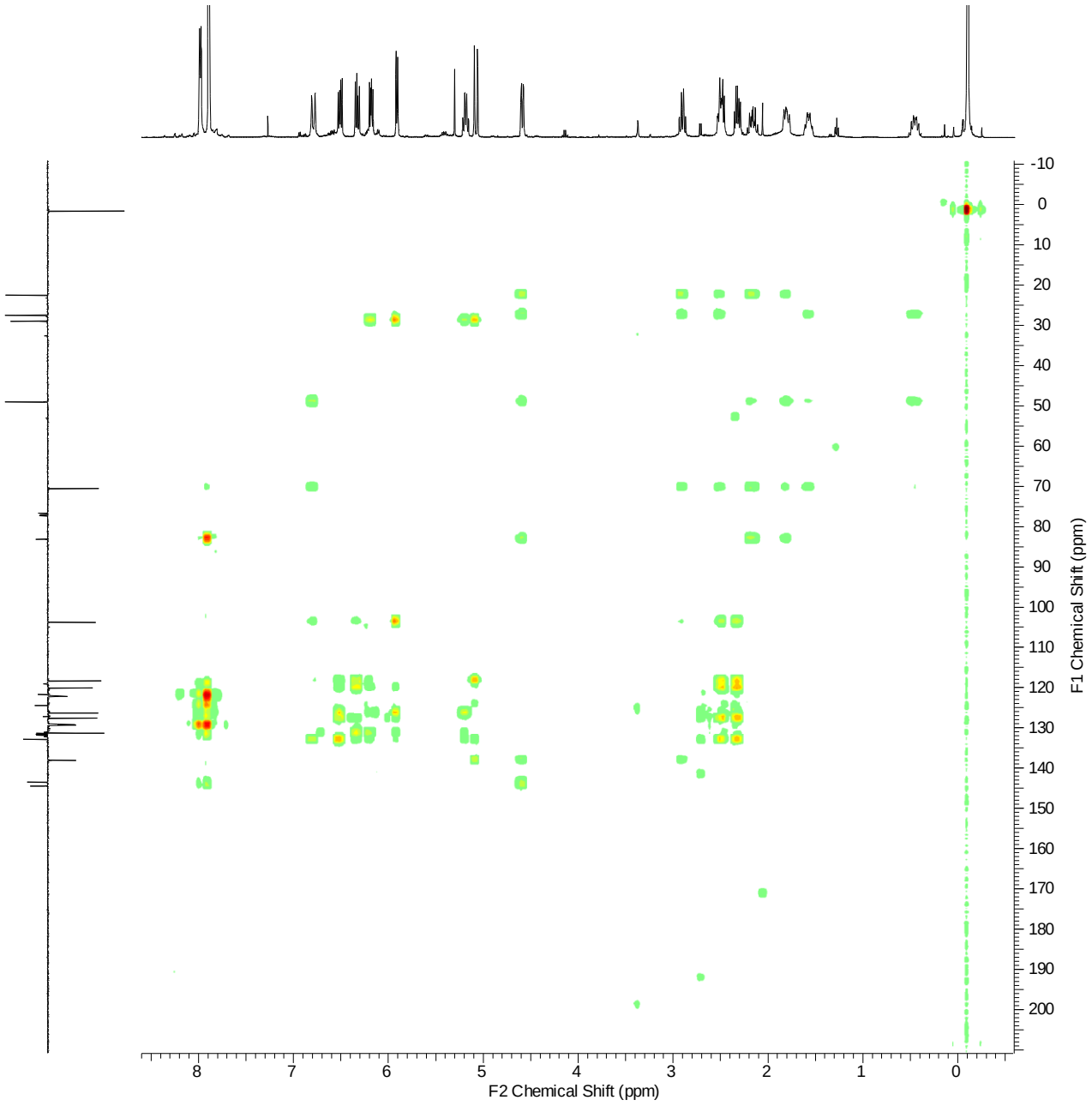

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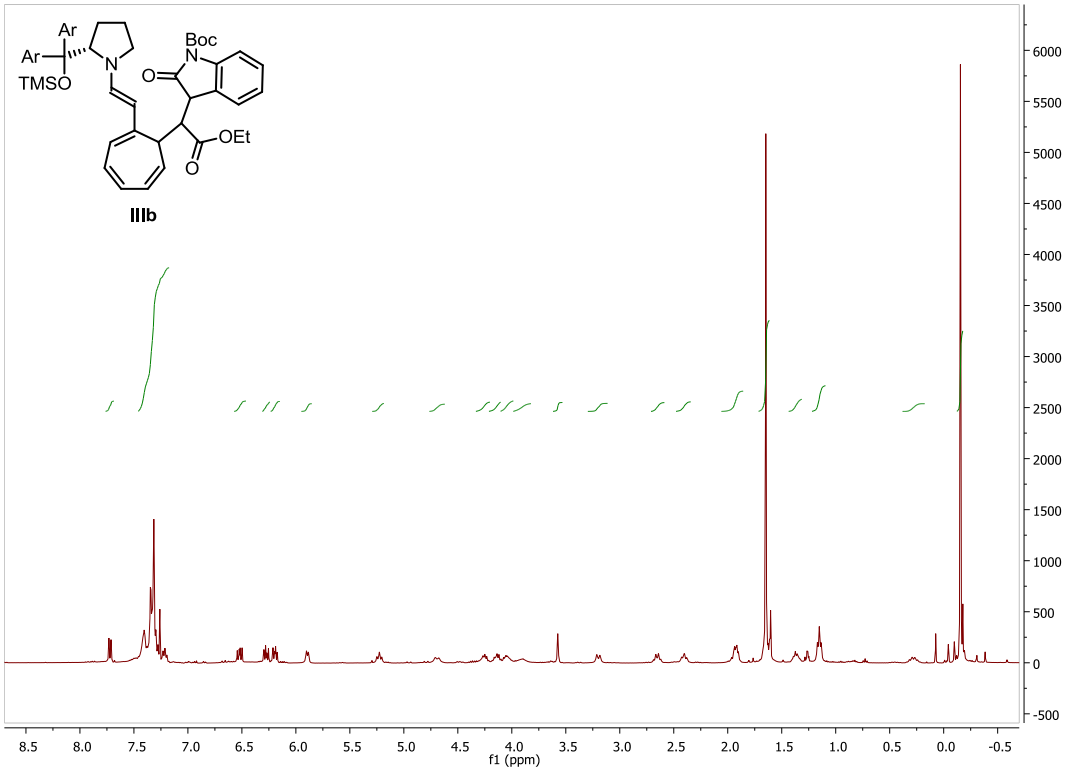
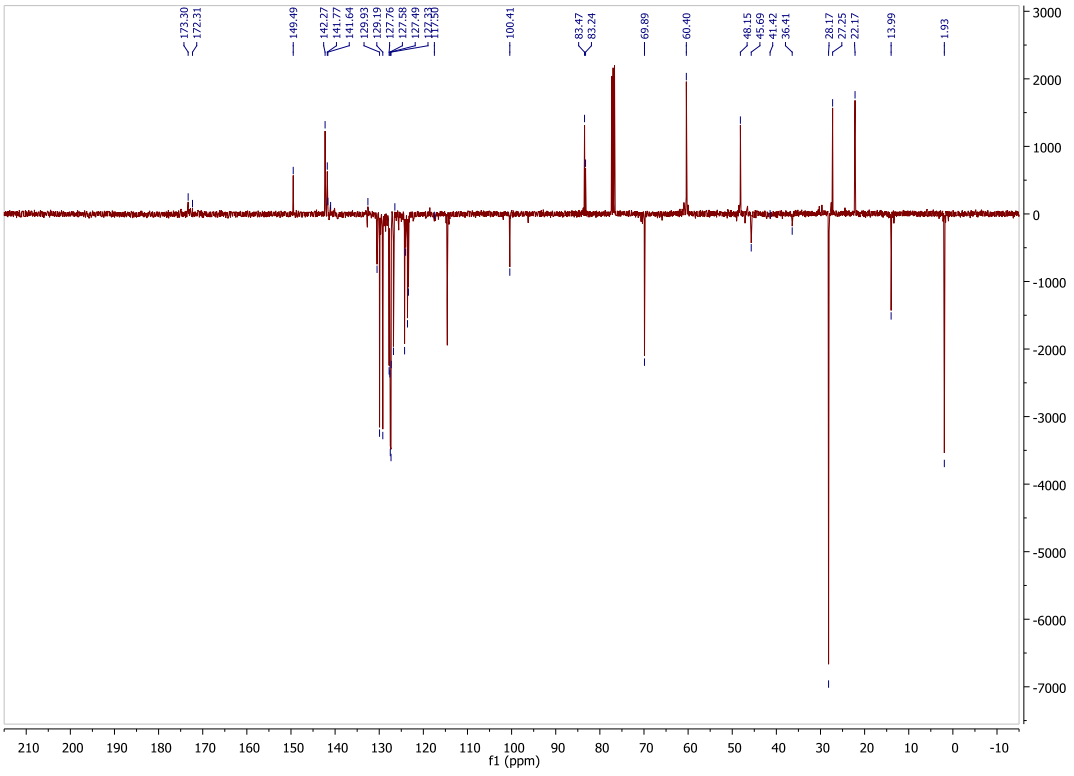
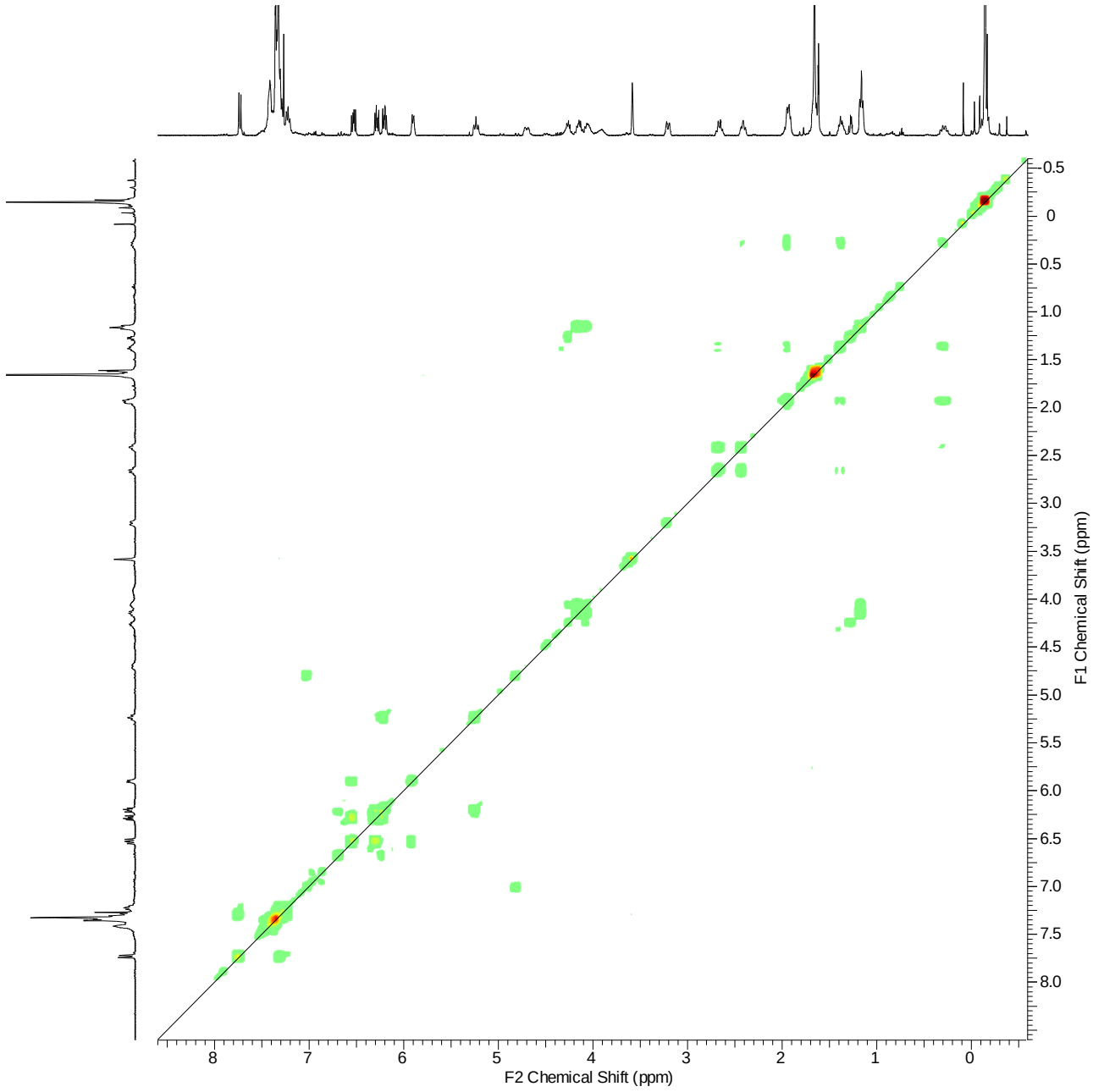


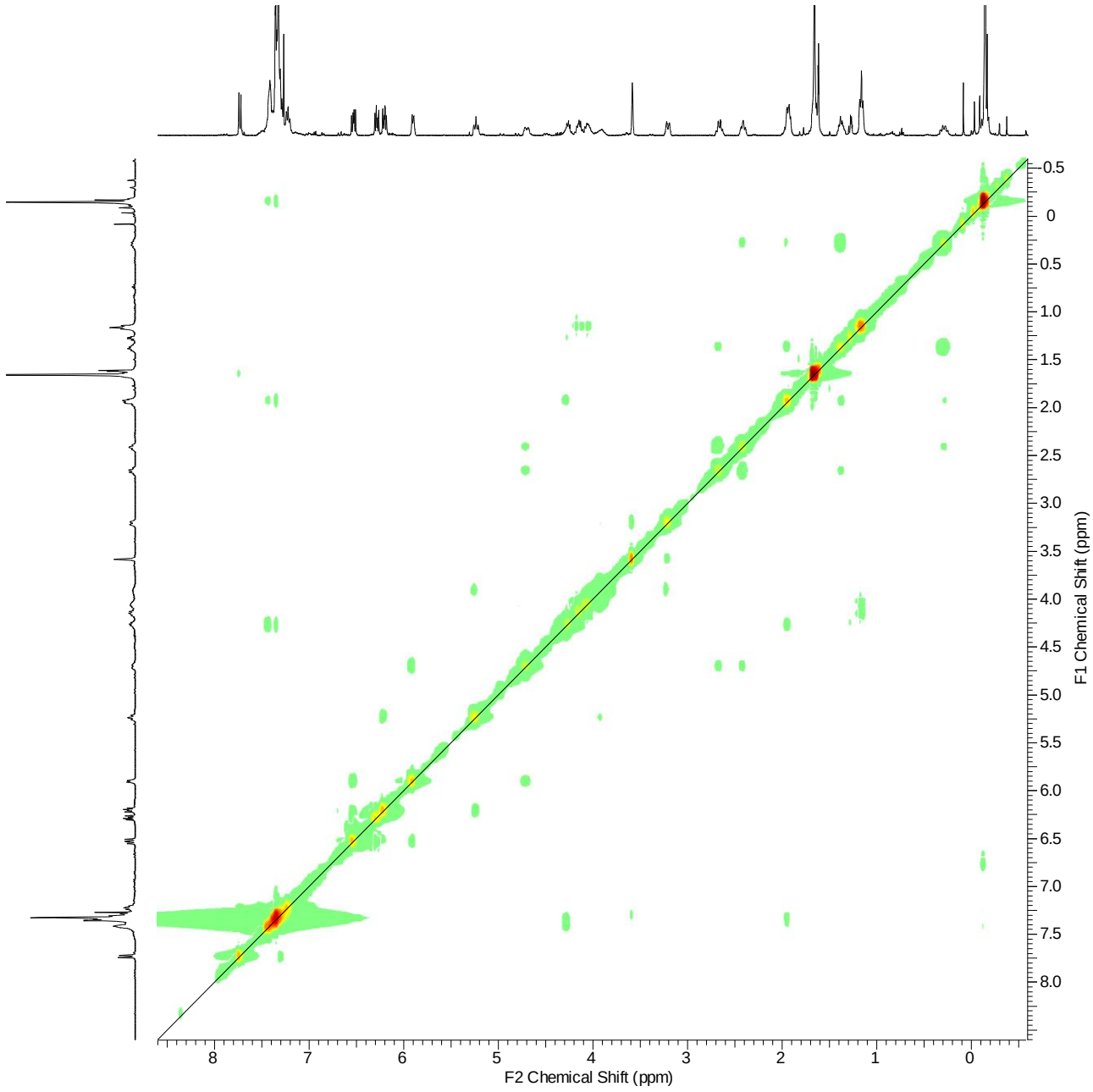
^{1}H NMR spectrum of **IIIb**



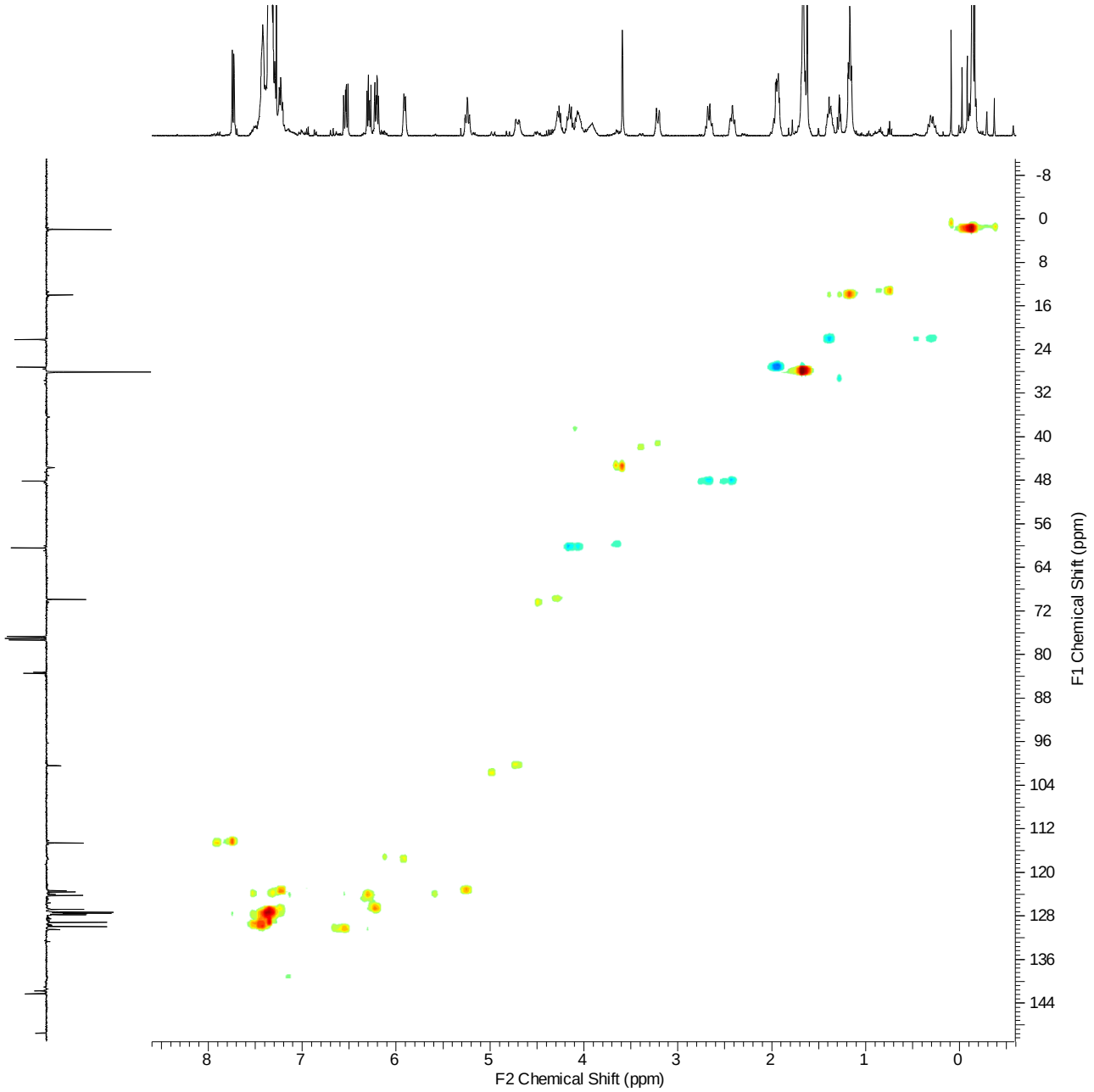
^{13}C NMR spectrum of **IIIb**



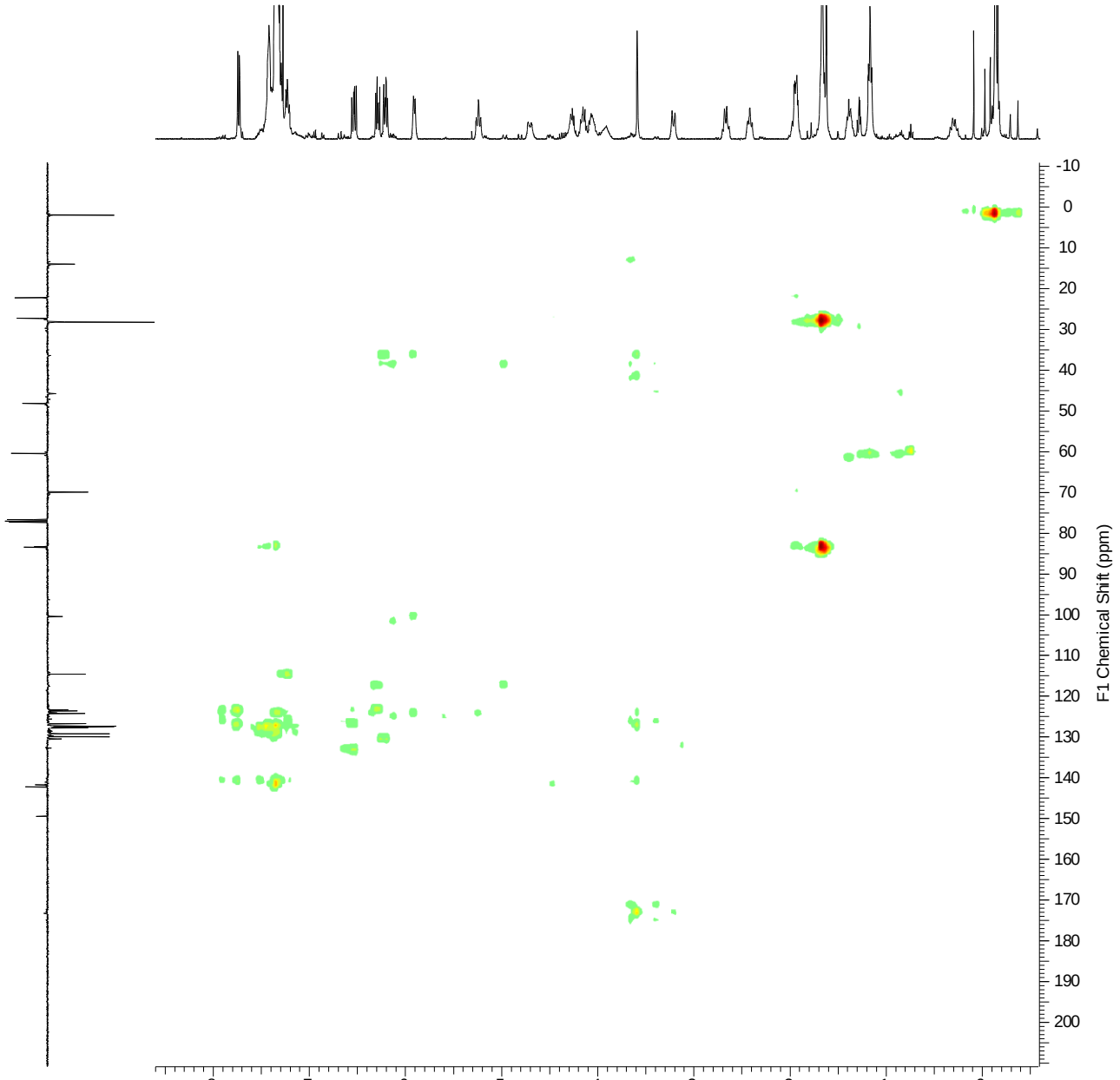
COSY NMR spectrum of **IIIb**



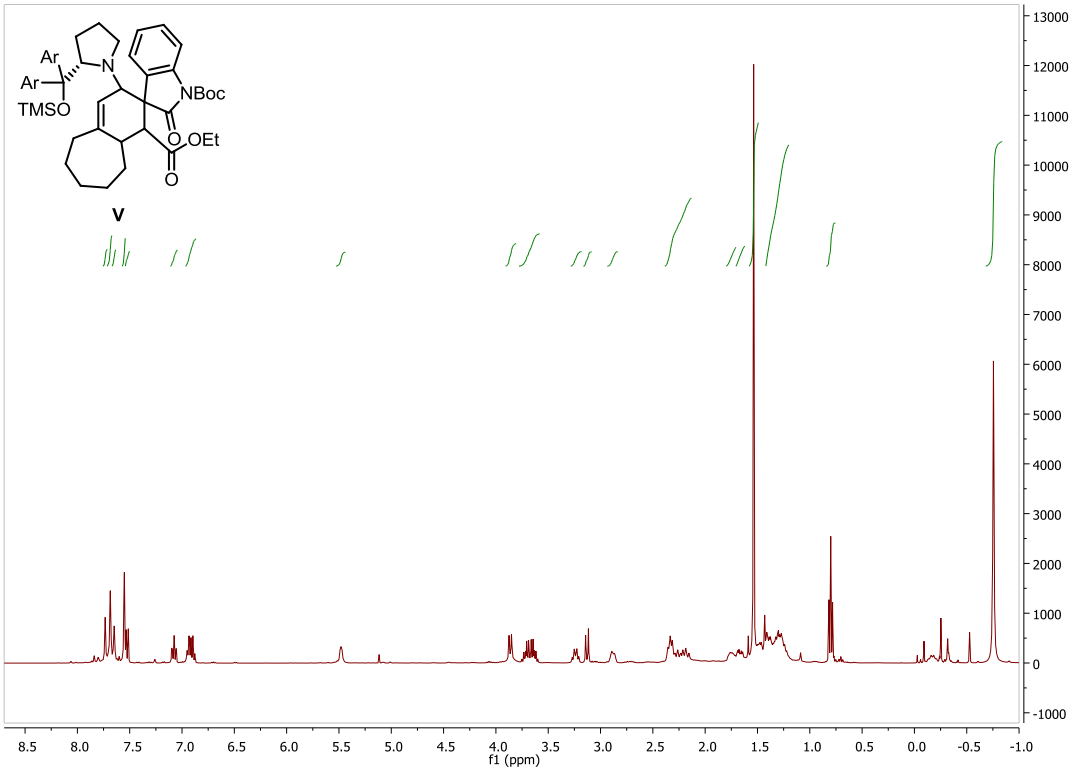
NOESY NMR spectrum of **IIIb**



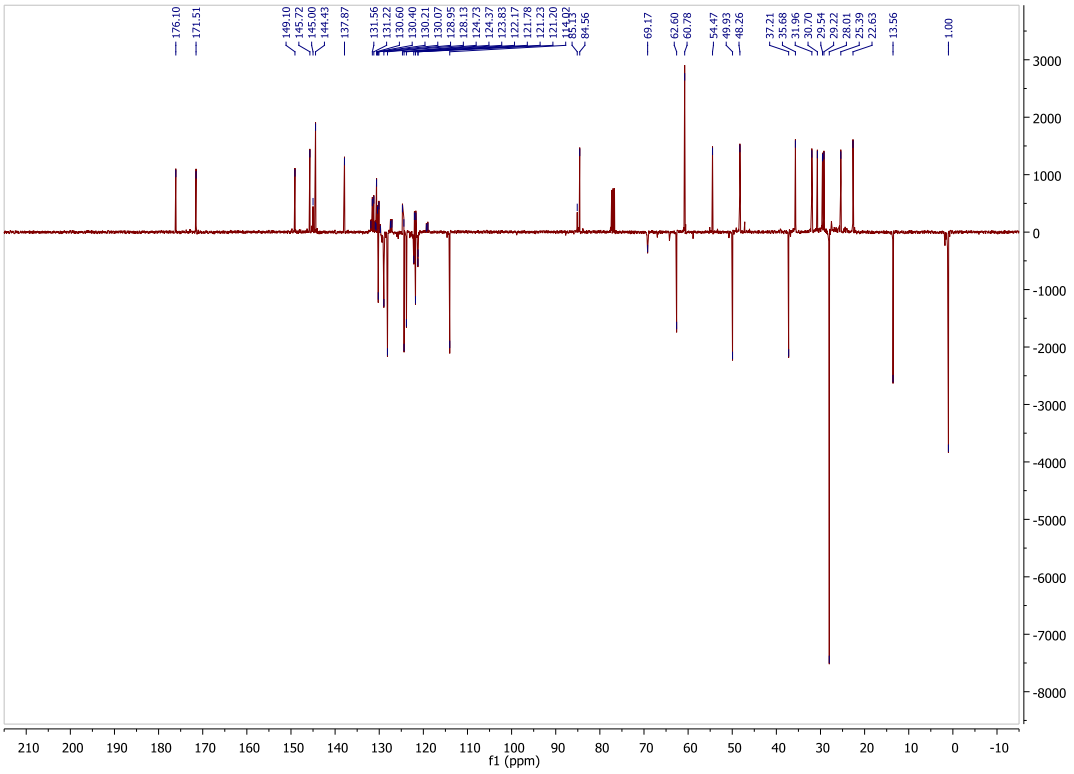
HSQC NMR spectrum of **IIIb**



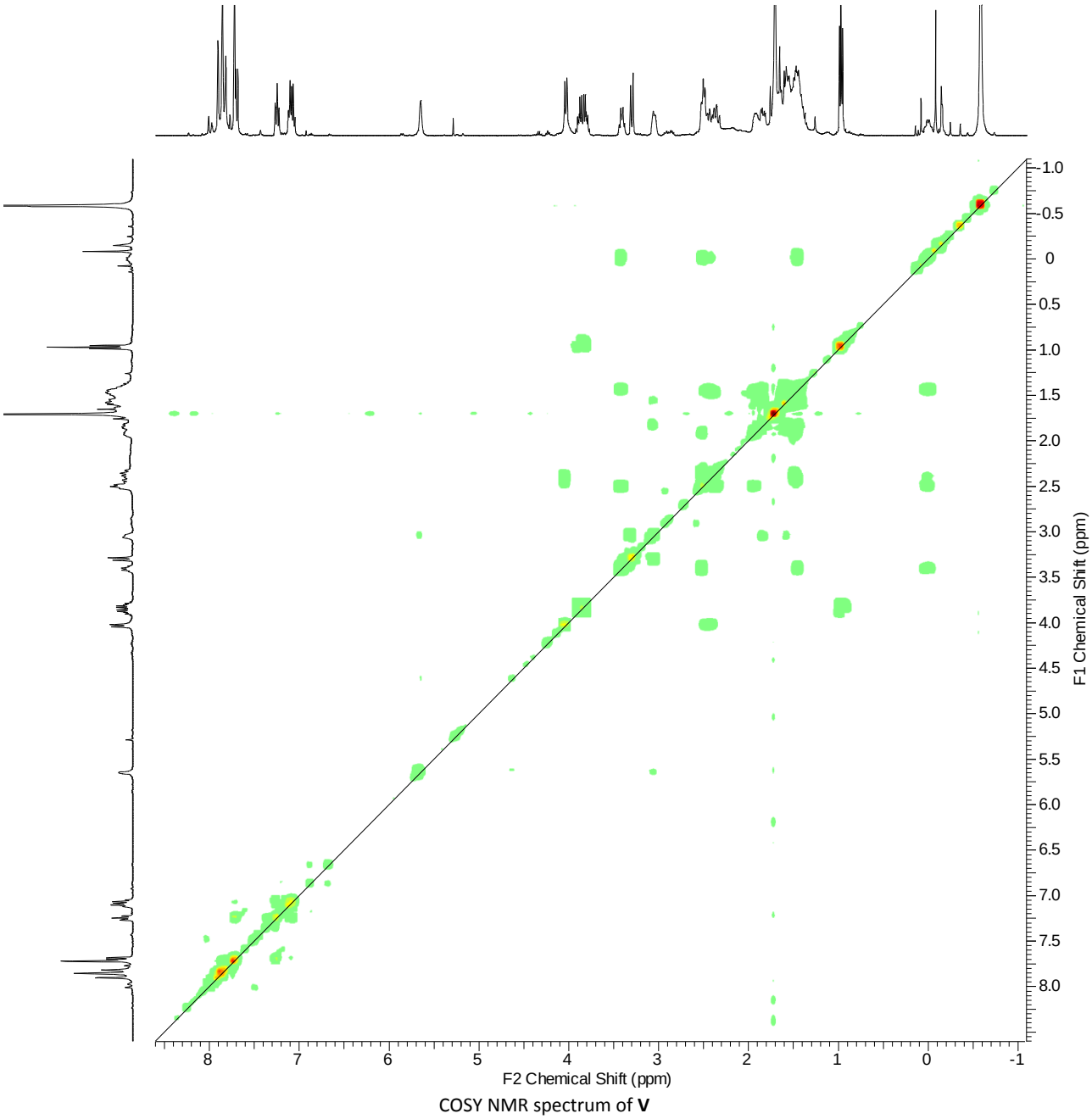
HMBC NMR spectrum of **IIIb**



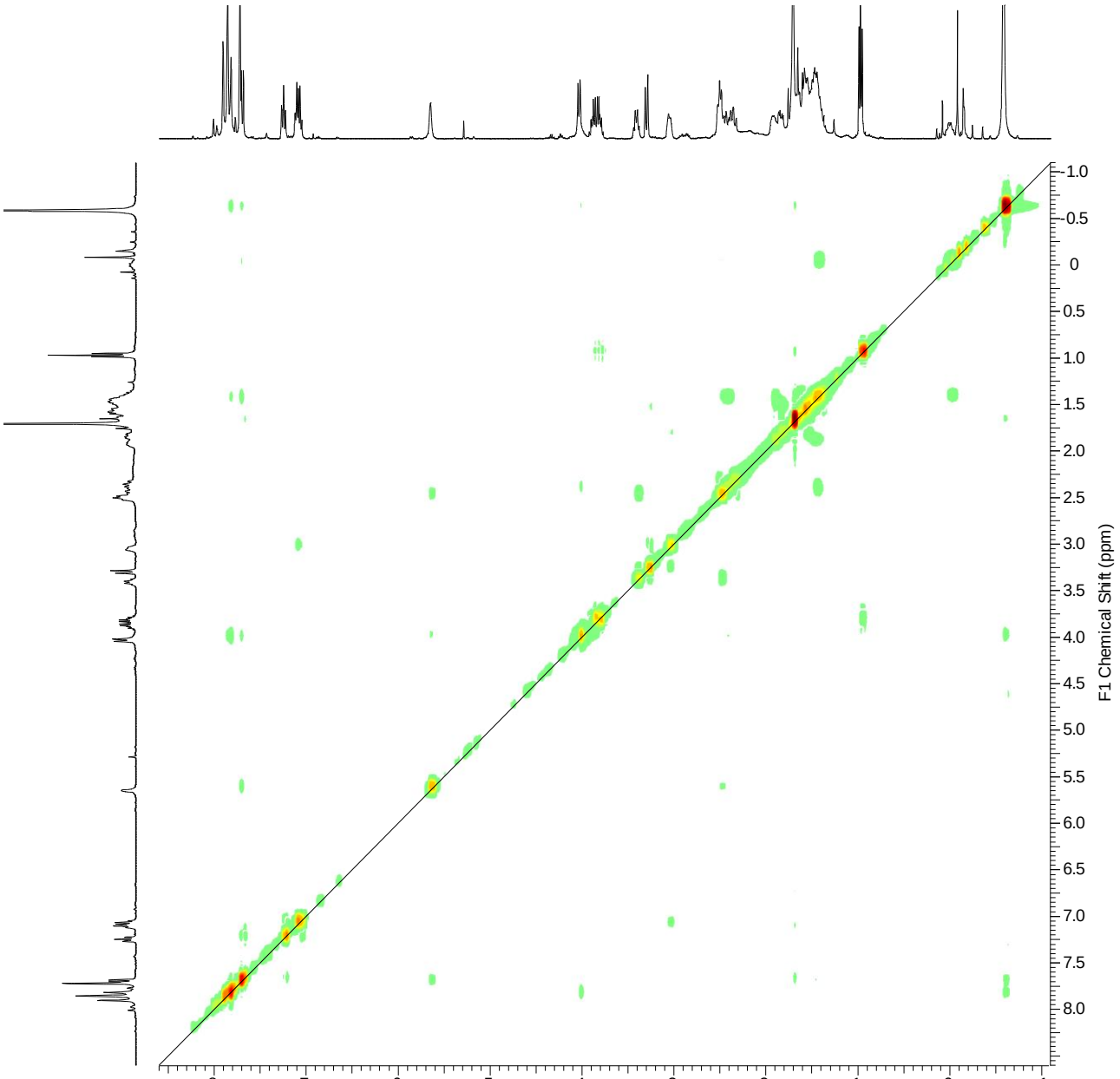
^{1}H NMR spectrum of **V**



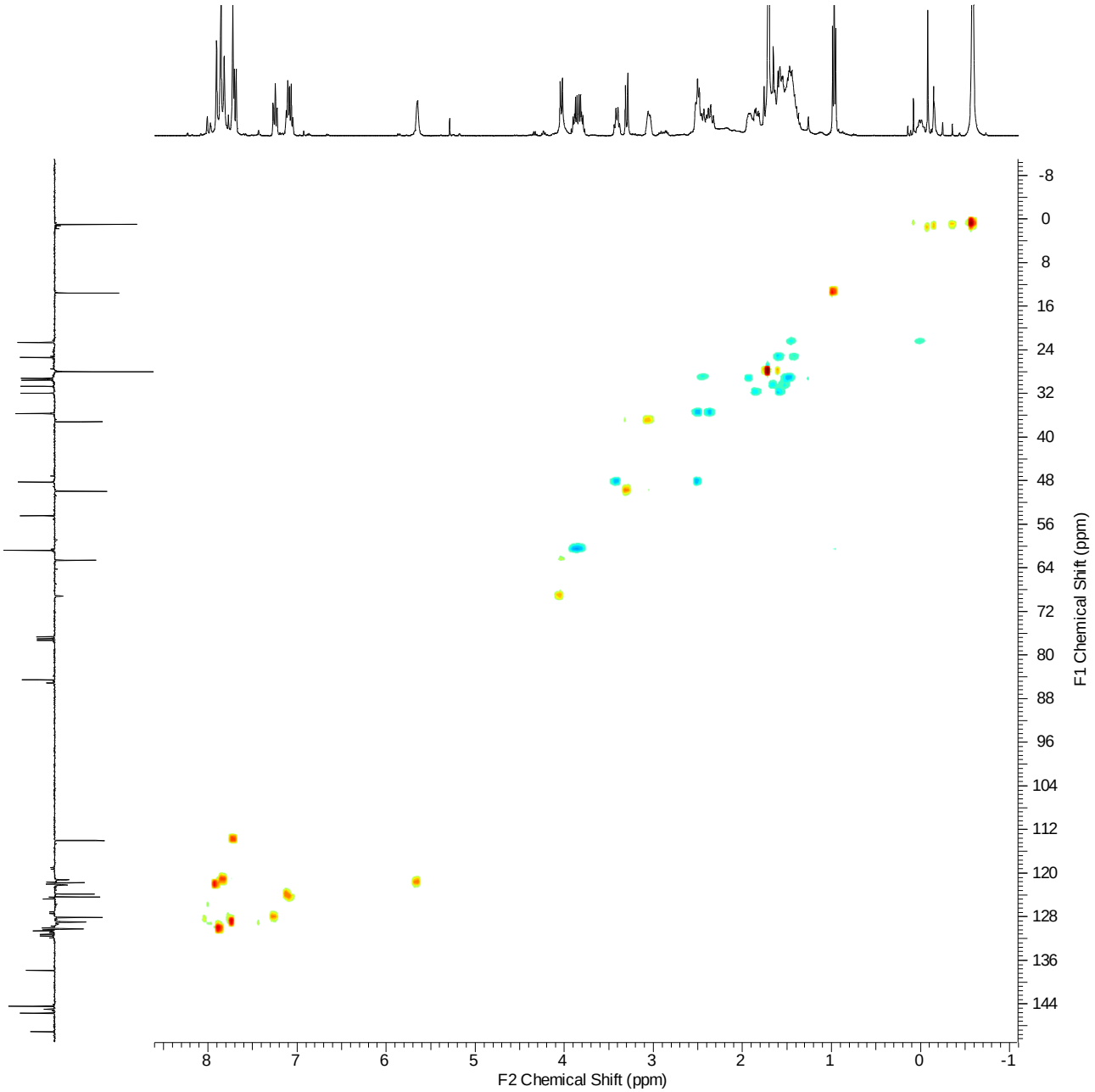
^{13}C NMR spectrum of **V**



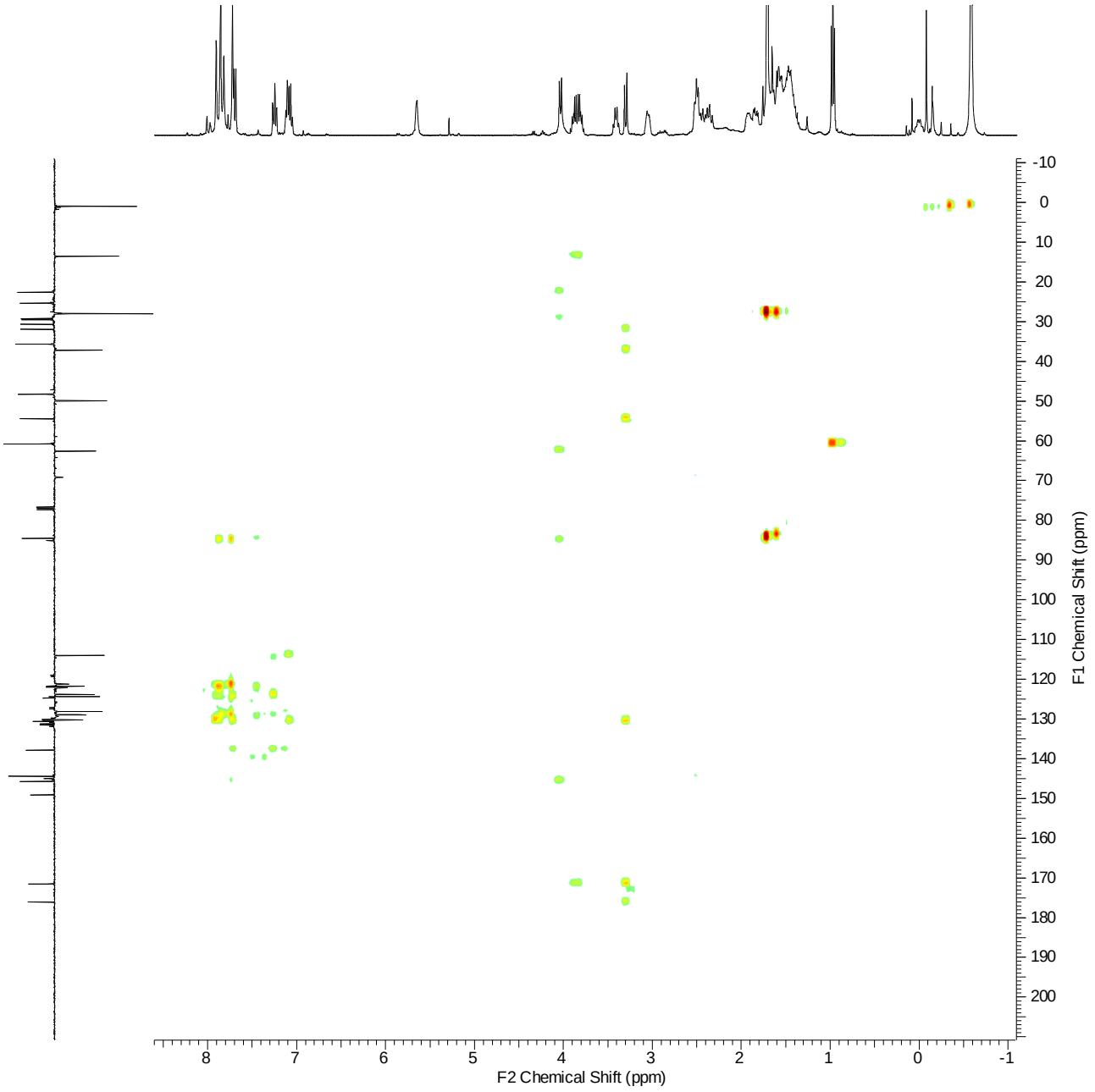
COSY NMR spectrum of **V**



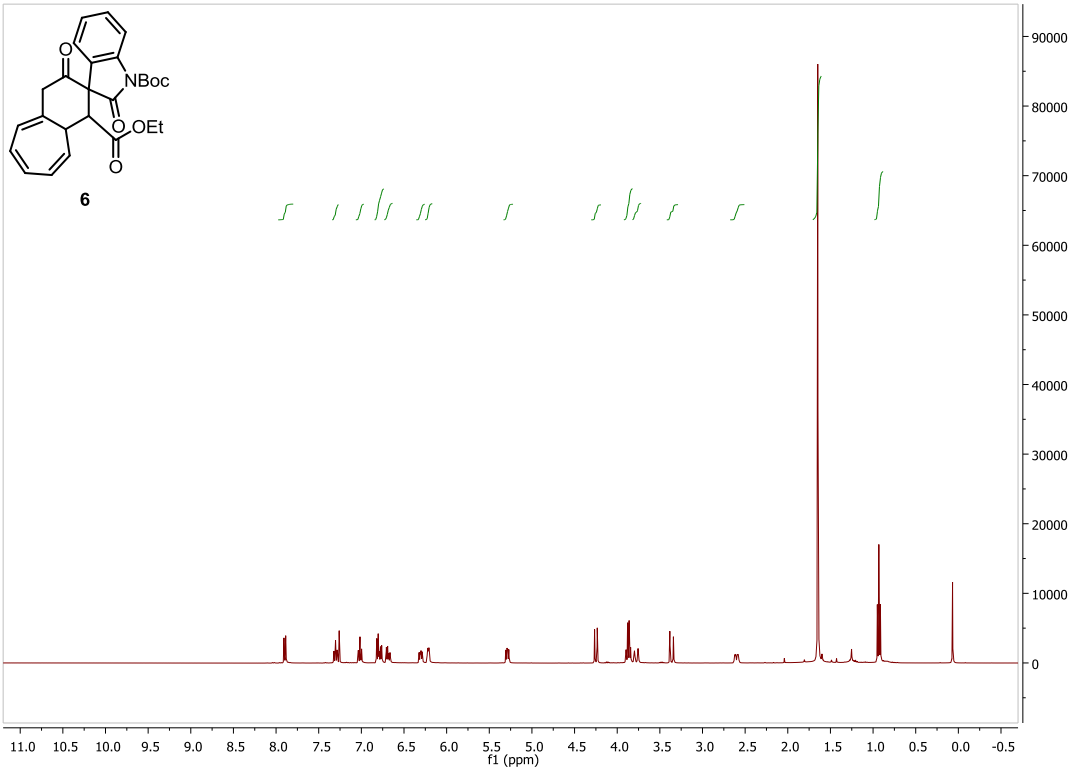
NOESY NMR spectrum of **V**



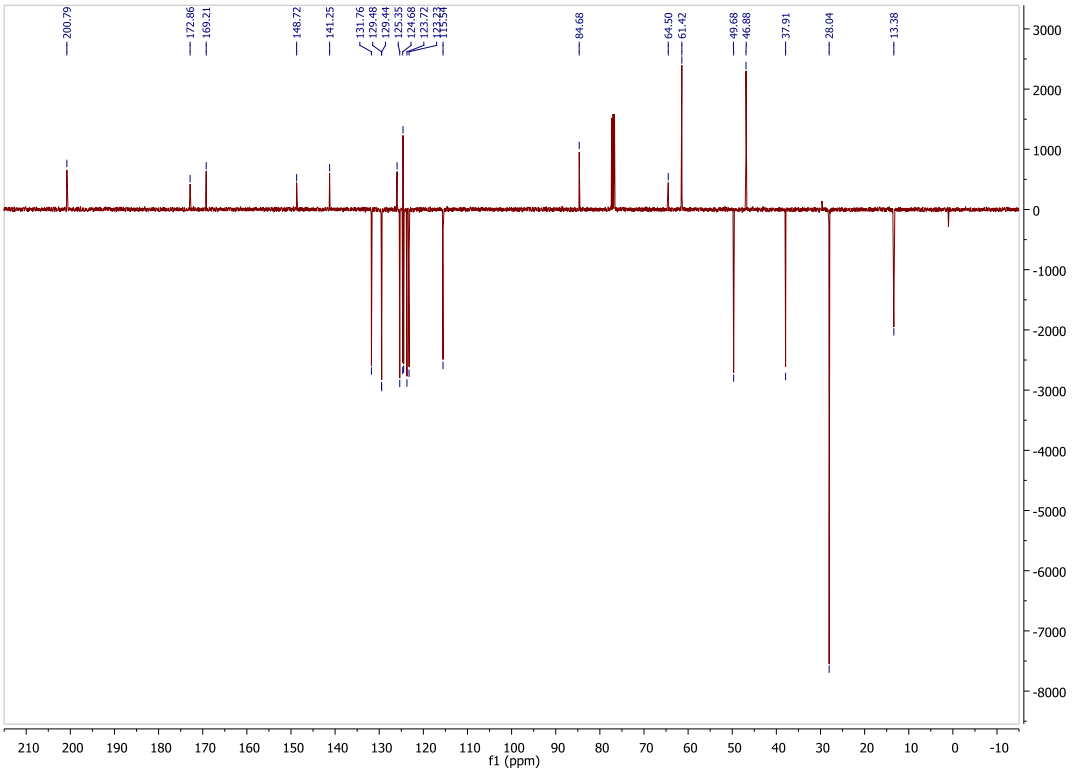
HSQC NMR spectrum of **V**



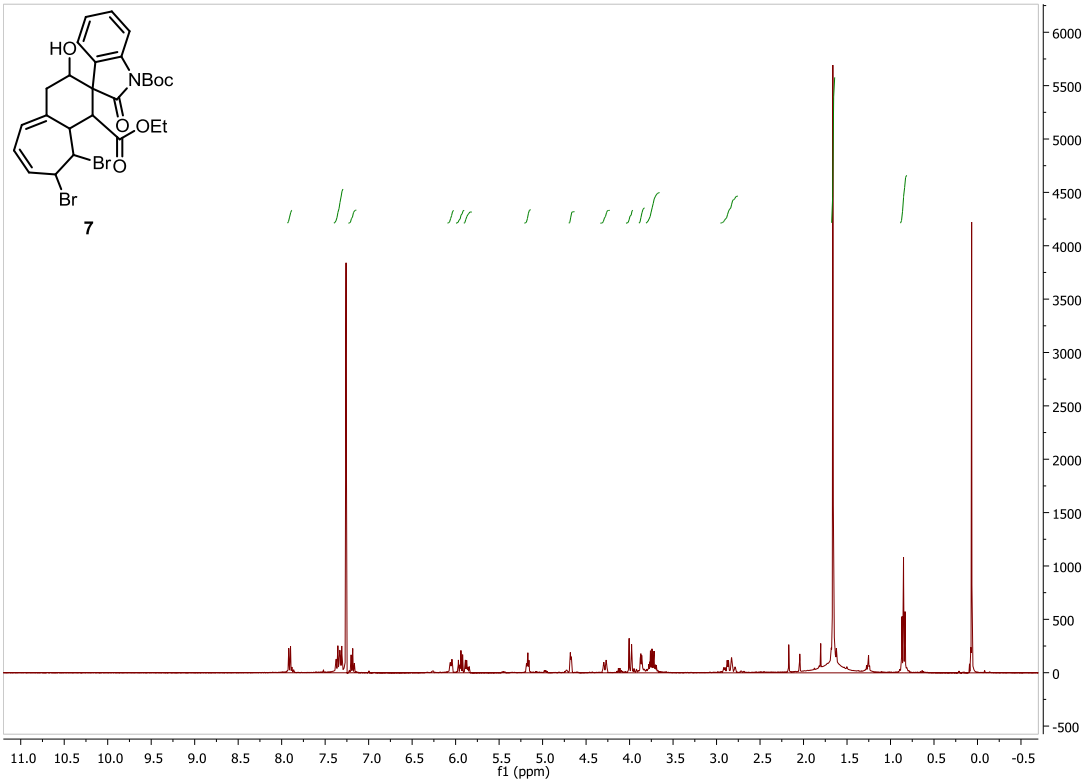
HMBC NMR spectrum of **V**



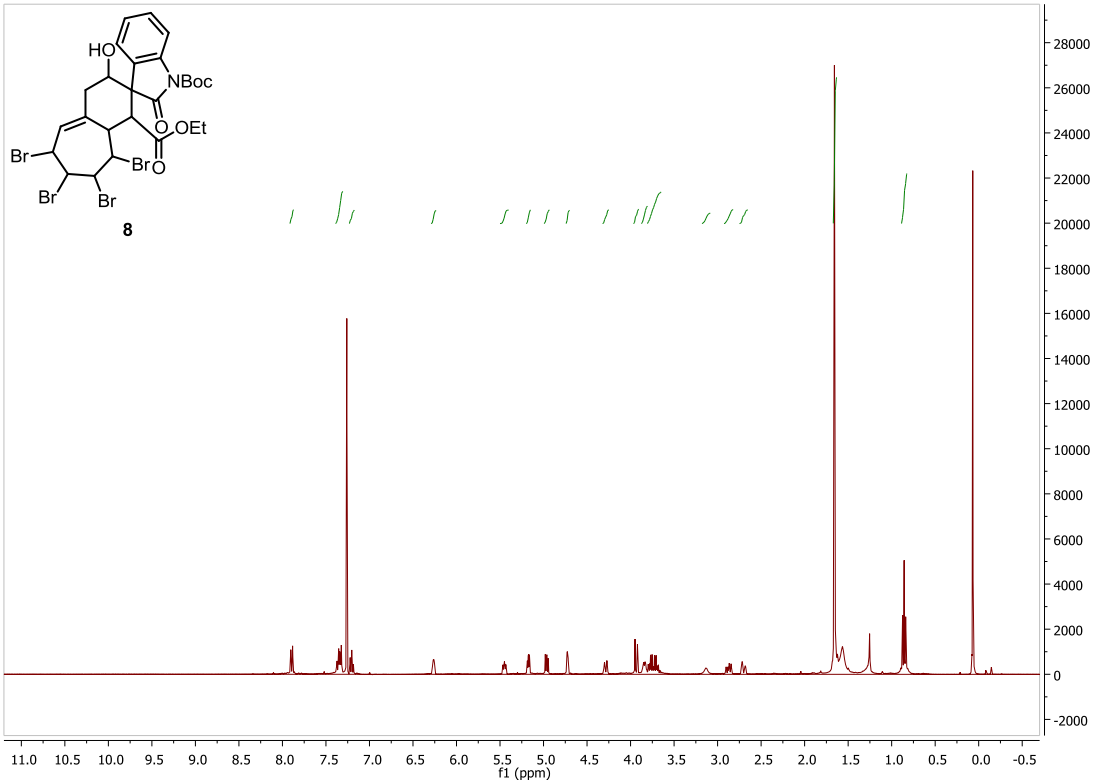
^{1}H NMR spectrum of **6**



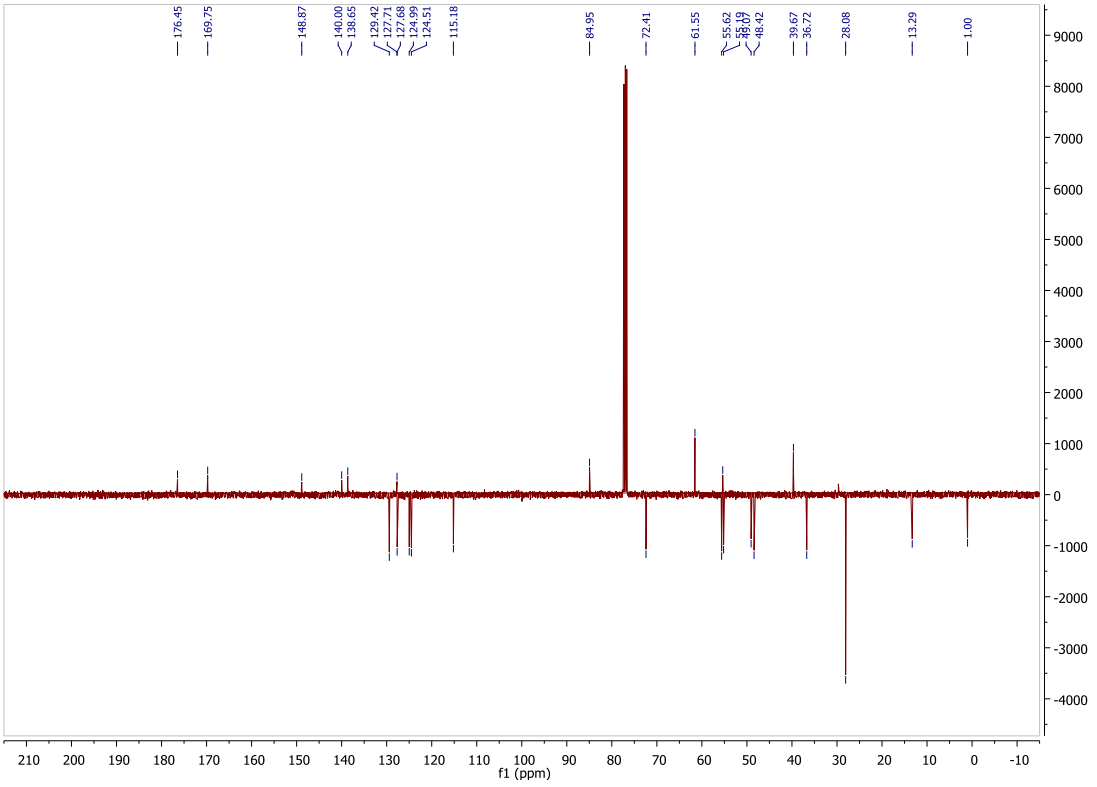
^{13}C NMR spectrum of **6**



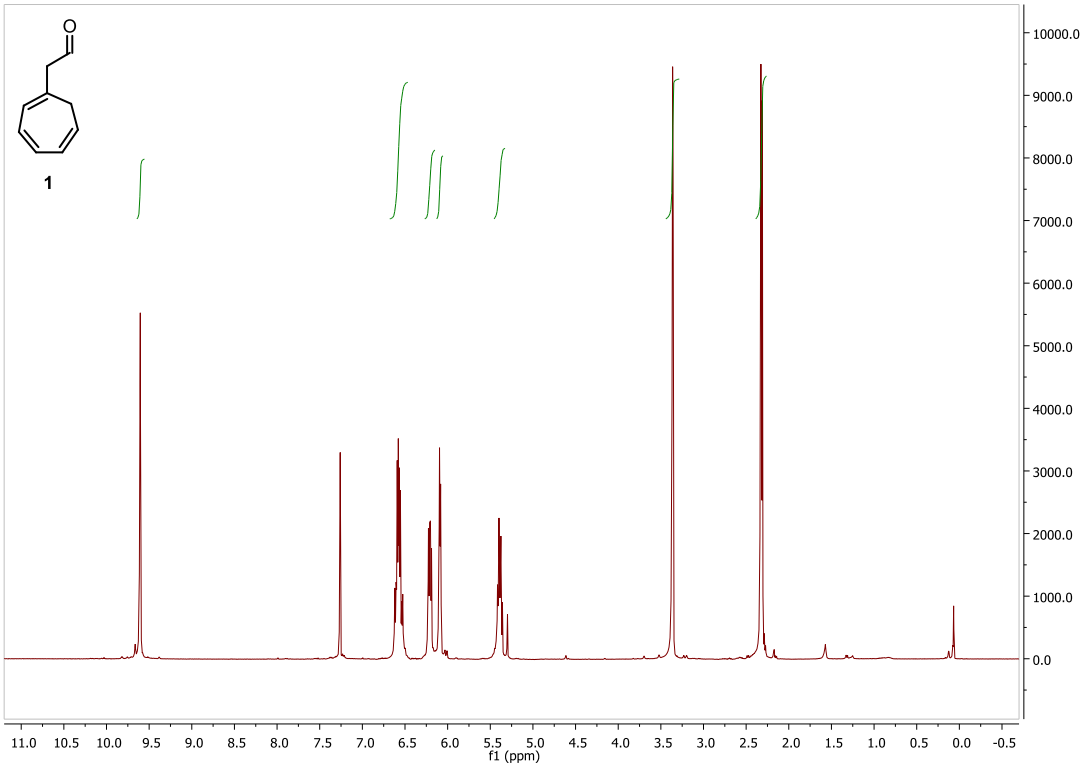
^{1}H NMR spectrum of **7**



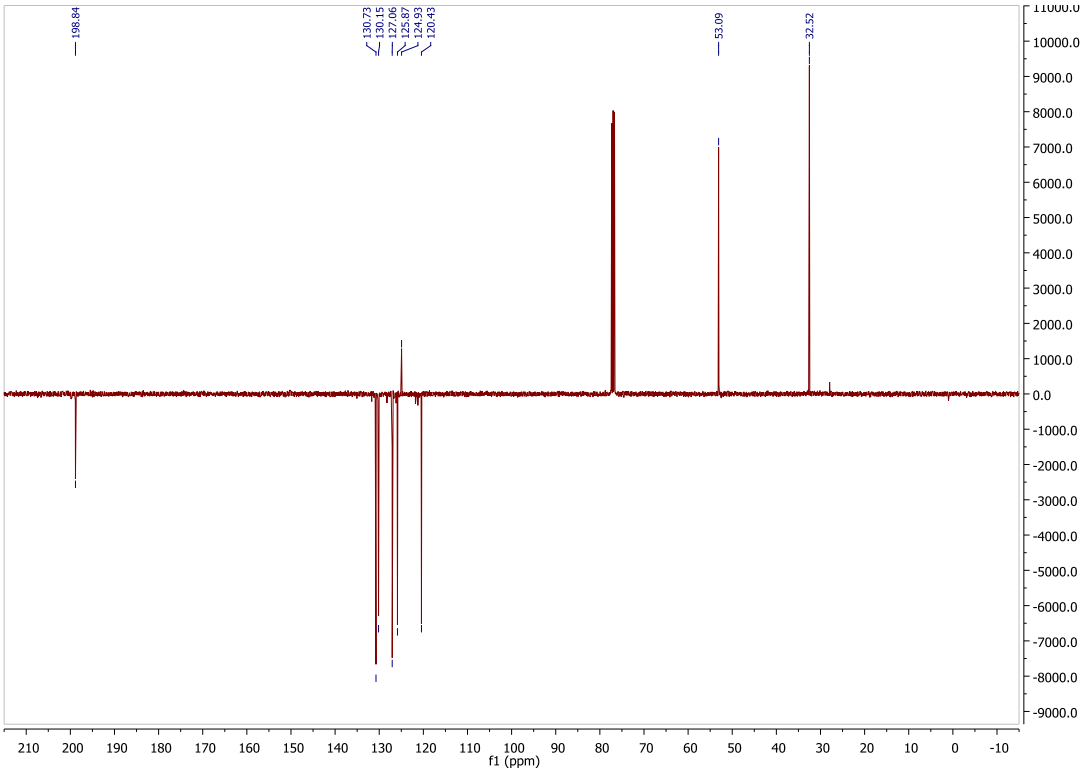
^{1}H NMR spectrum of **8**



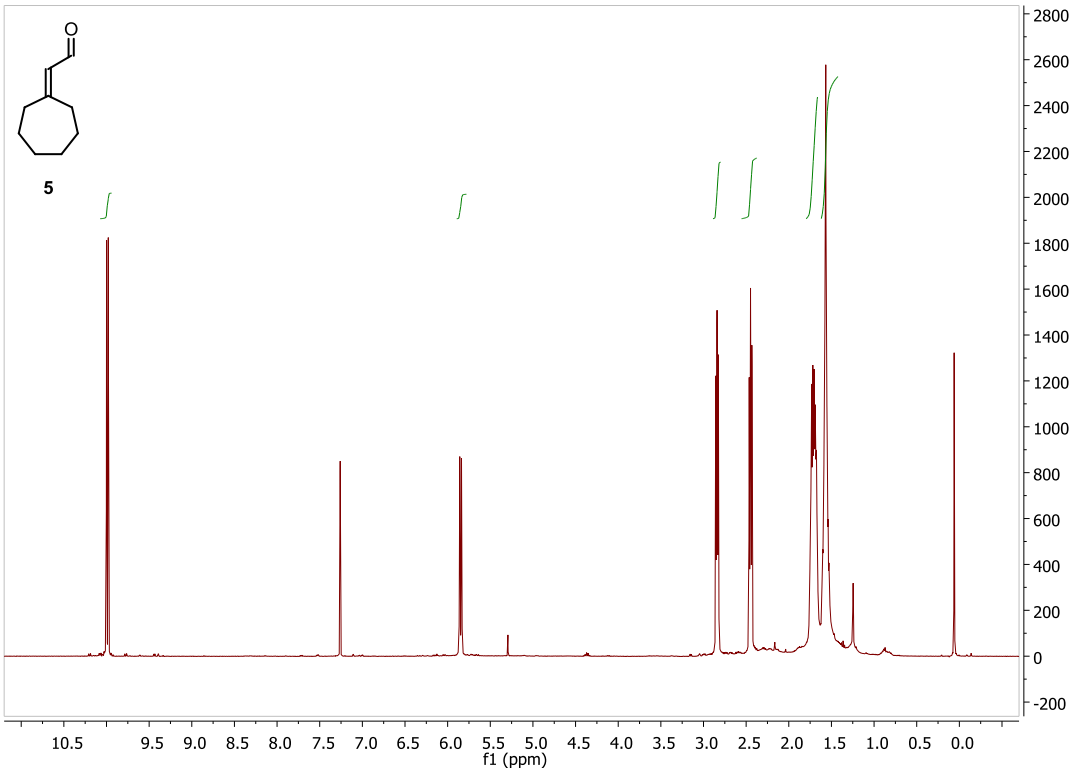
^{13}C NMR spectrum of **8**



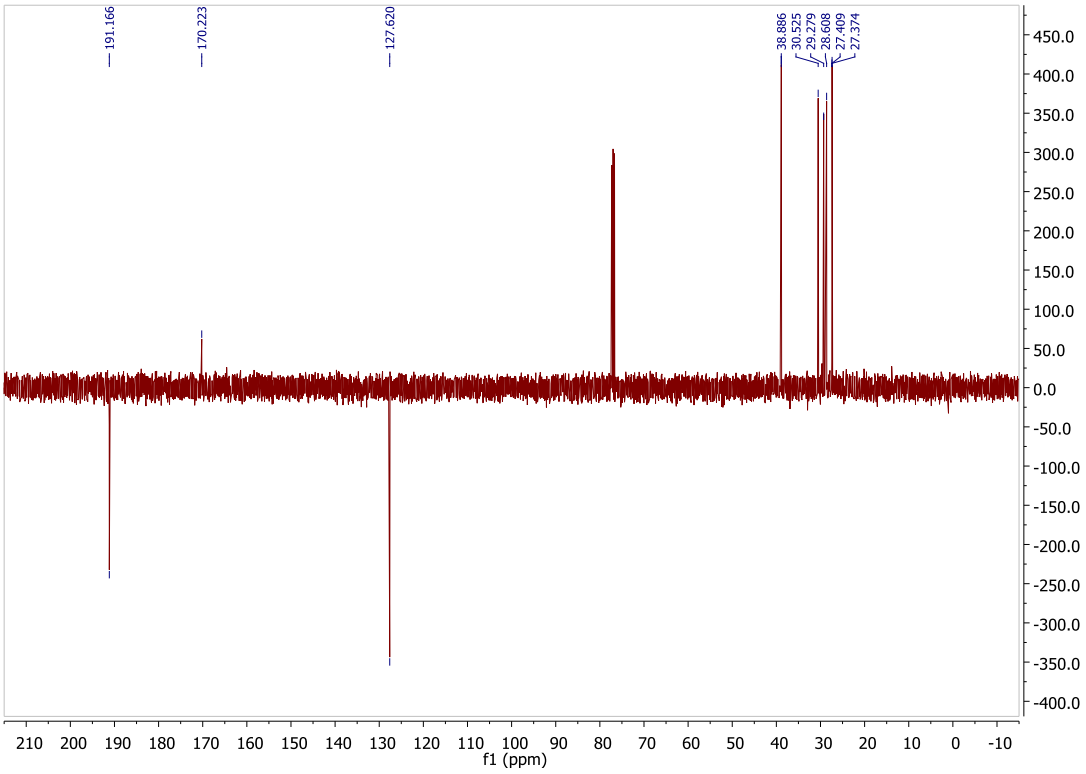
^{1}H NMR spectrum of **1**



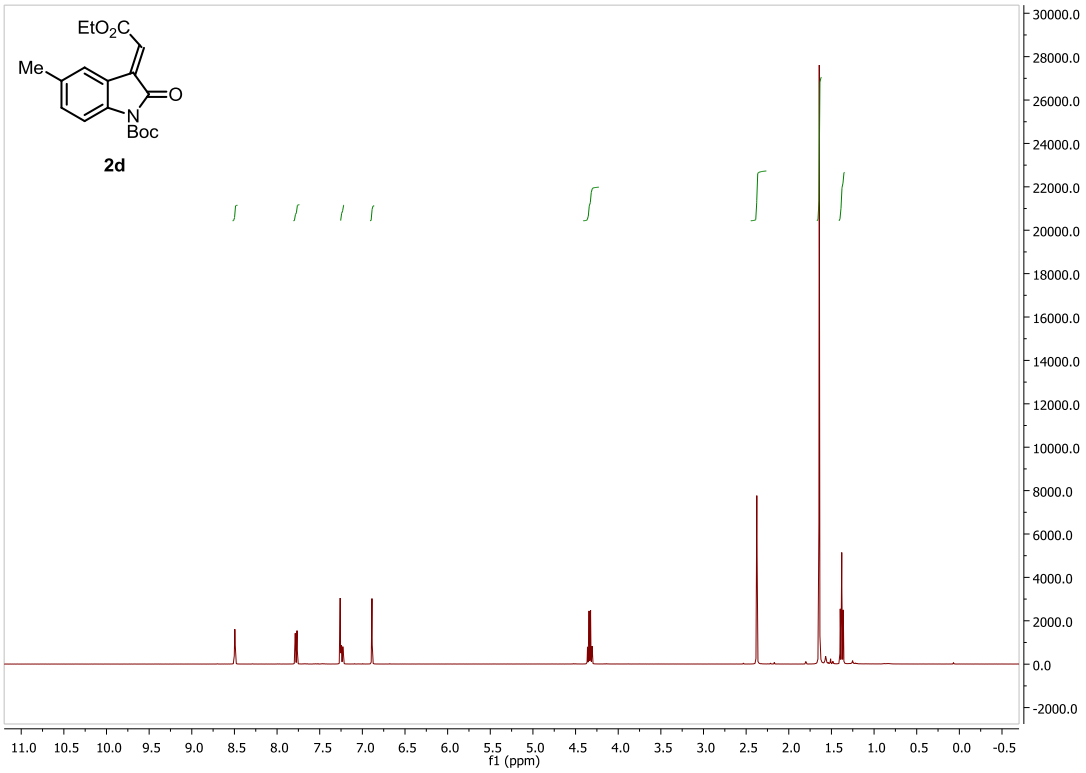
^{13}C NMR spectrum of **1**



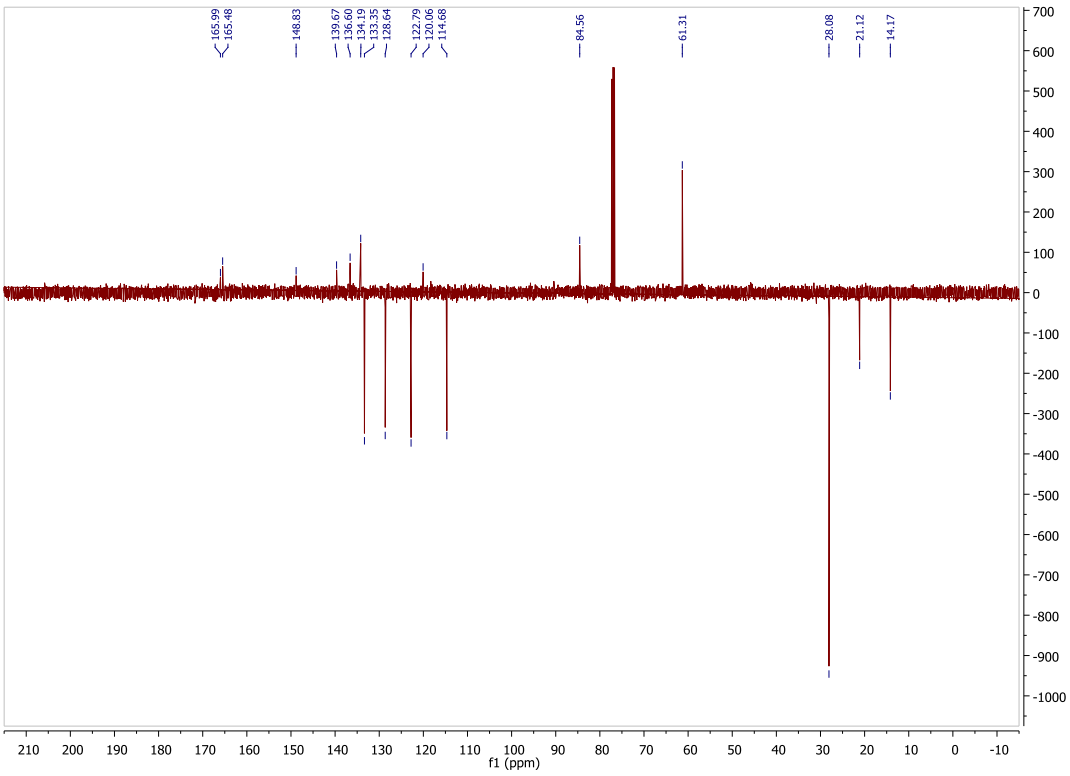
^{1}H NMR spectrum of **5**



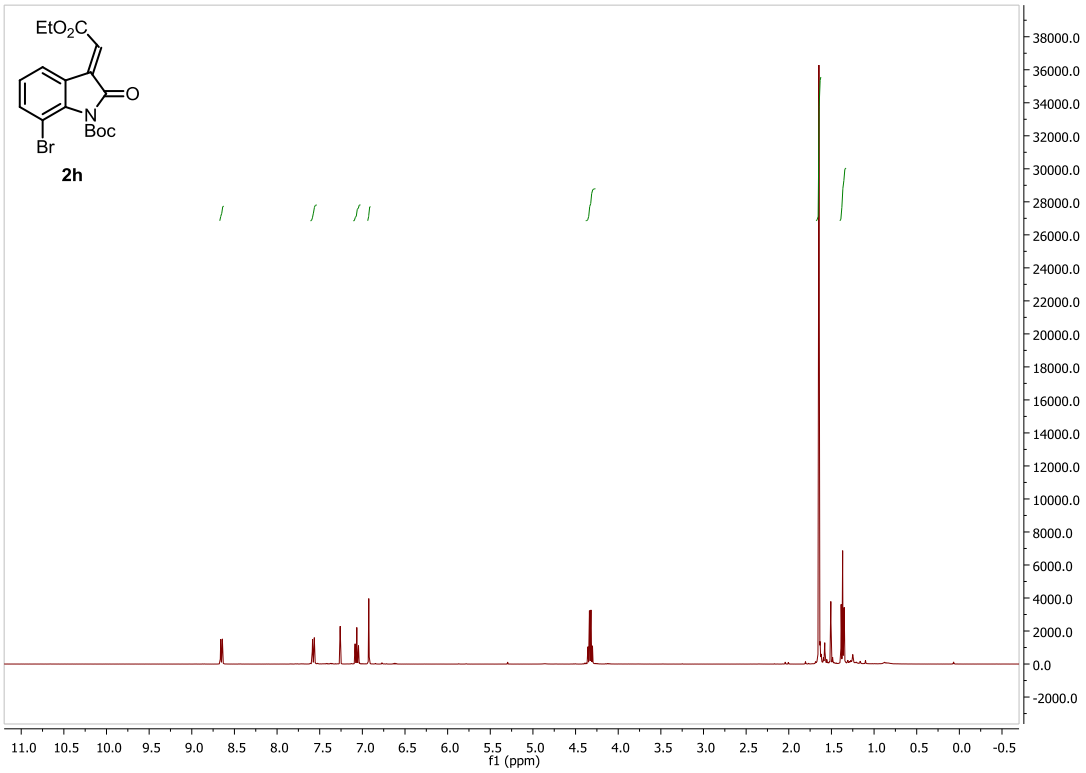
^{13}C NMR spectrum of **5**



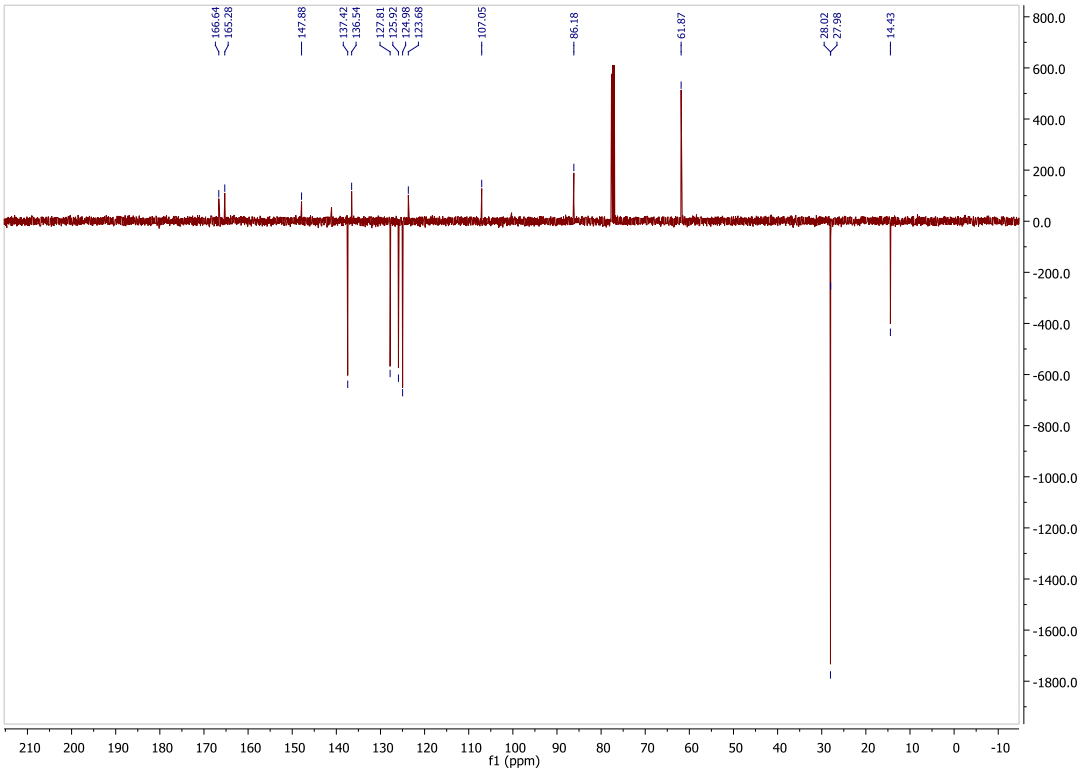
^{1}H NMR spectrum of **2d**



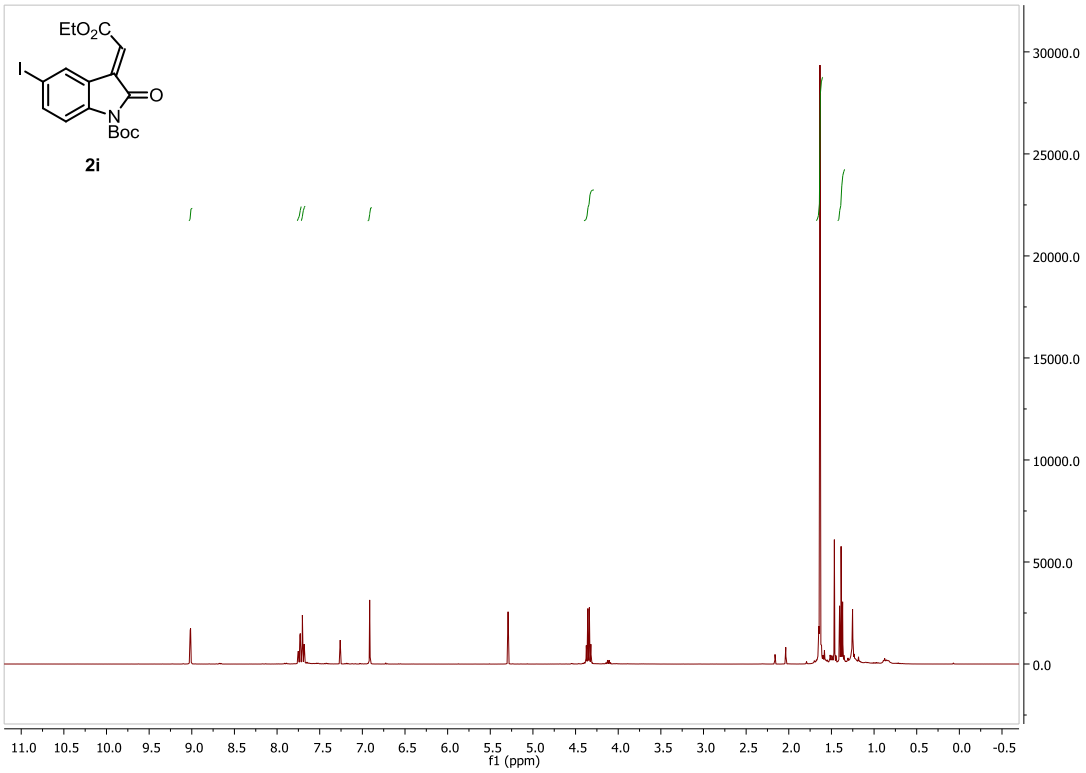
^{13}C NMR spectrum of **2d**



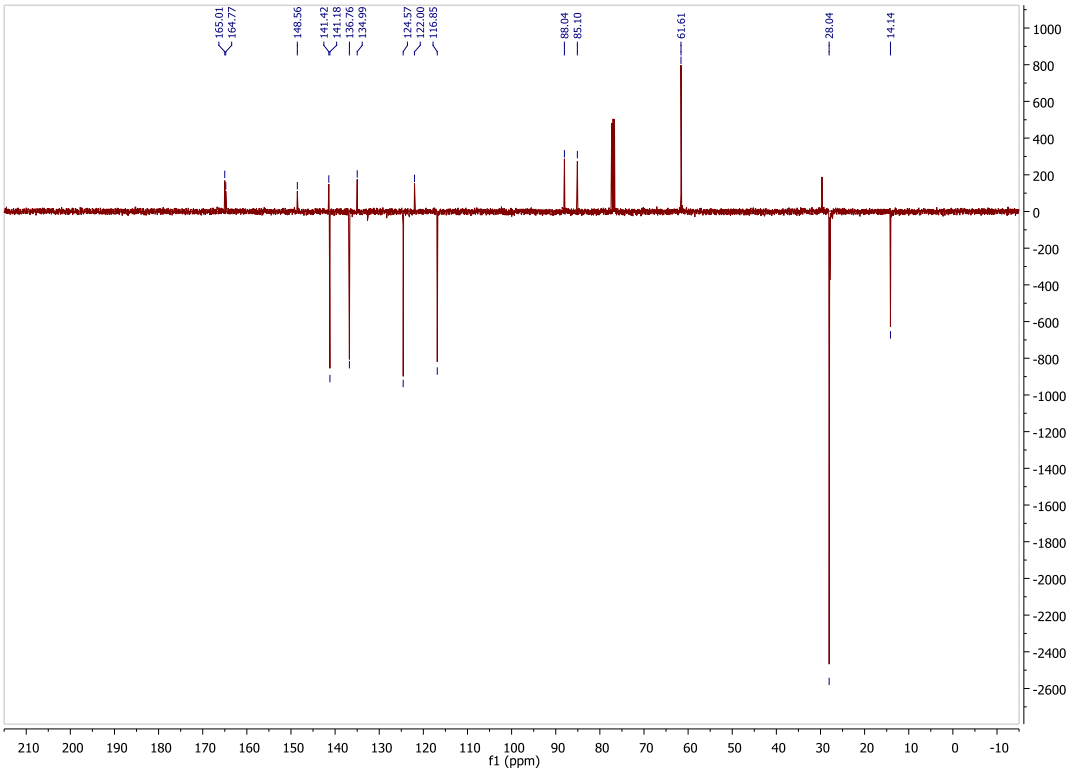
^{1}H NMR spectrum of **2h**



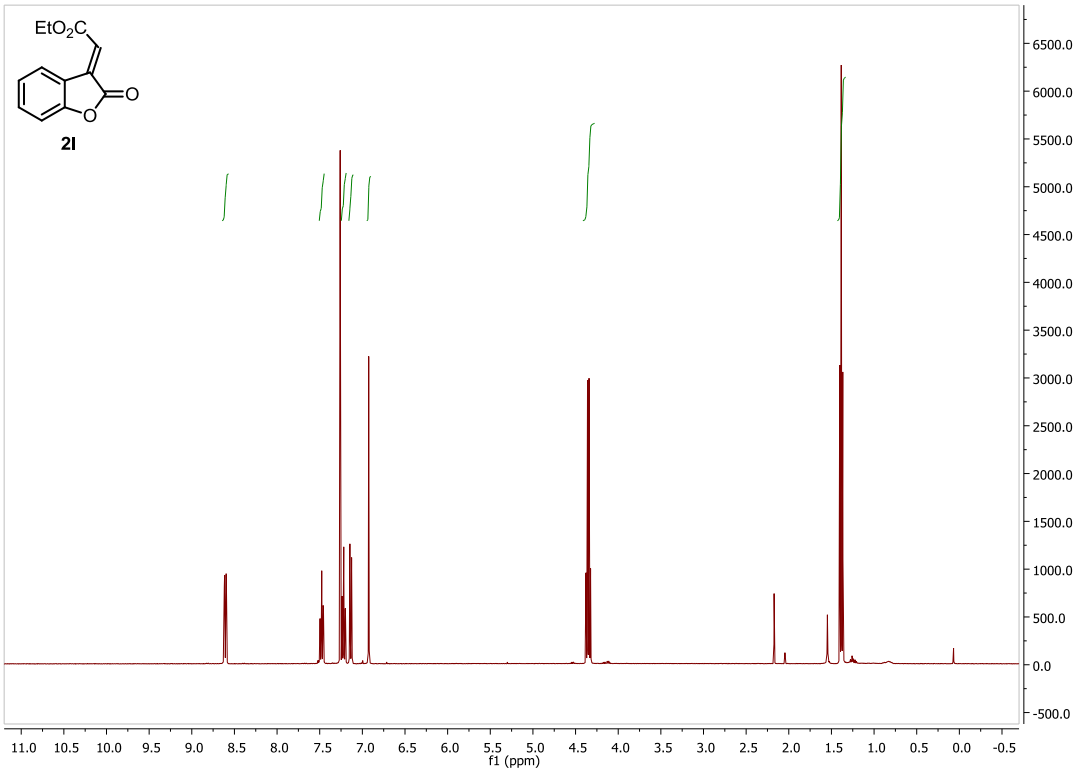
^{13}C NMR spectrum of **2h**



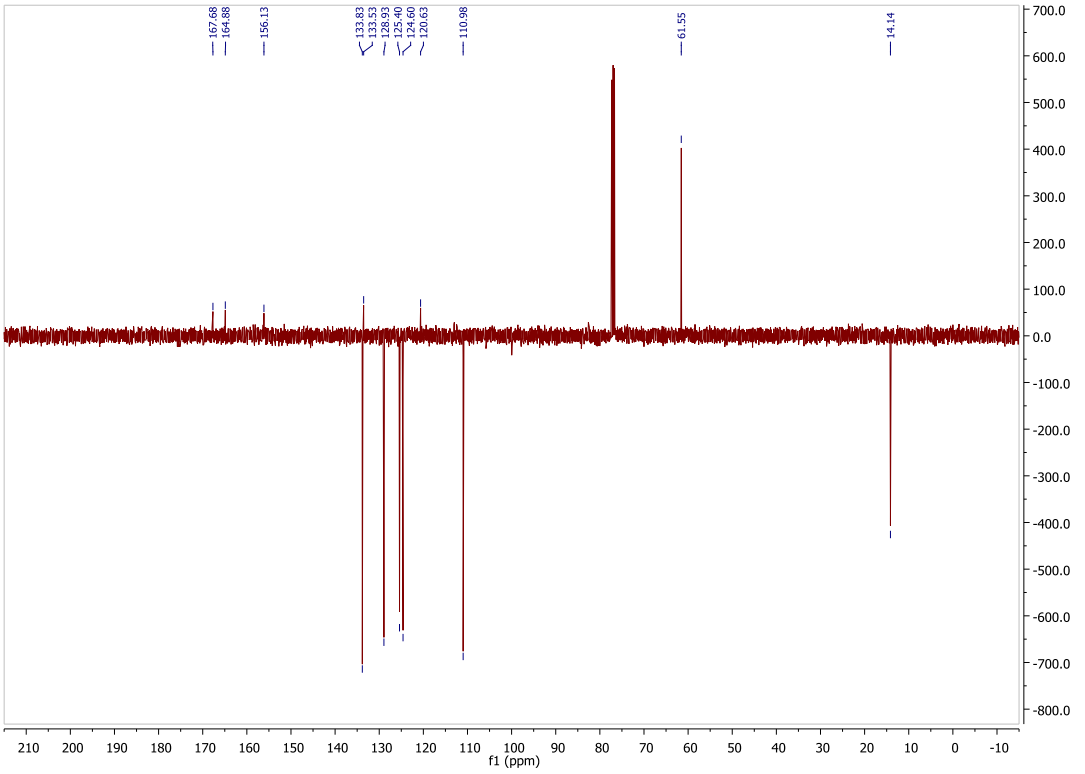
^{1}H NMR spectrum of **2i**



^{13}C NMR spectrum of **2i**



^{1}H NMR spectrum of **2l**



^{13}C NMR spectrum of **2l**