Electronic Supplementary Information (ESI)

Bismuth nitrate–Promoted Disproportionative Condensation of Indoles with Cyclohexanone: A New-Type Azafulvenium Reactivity of Indole

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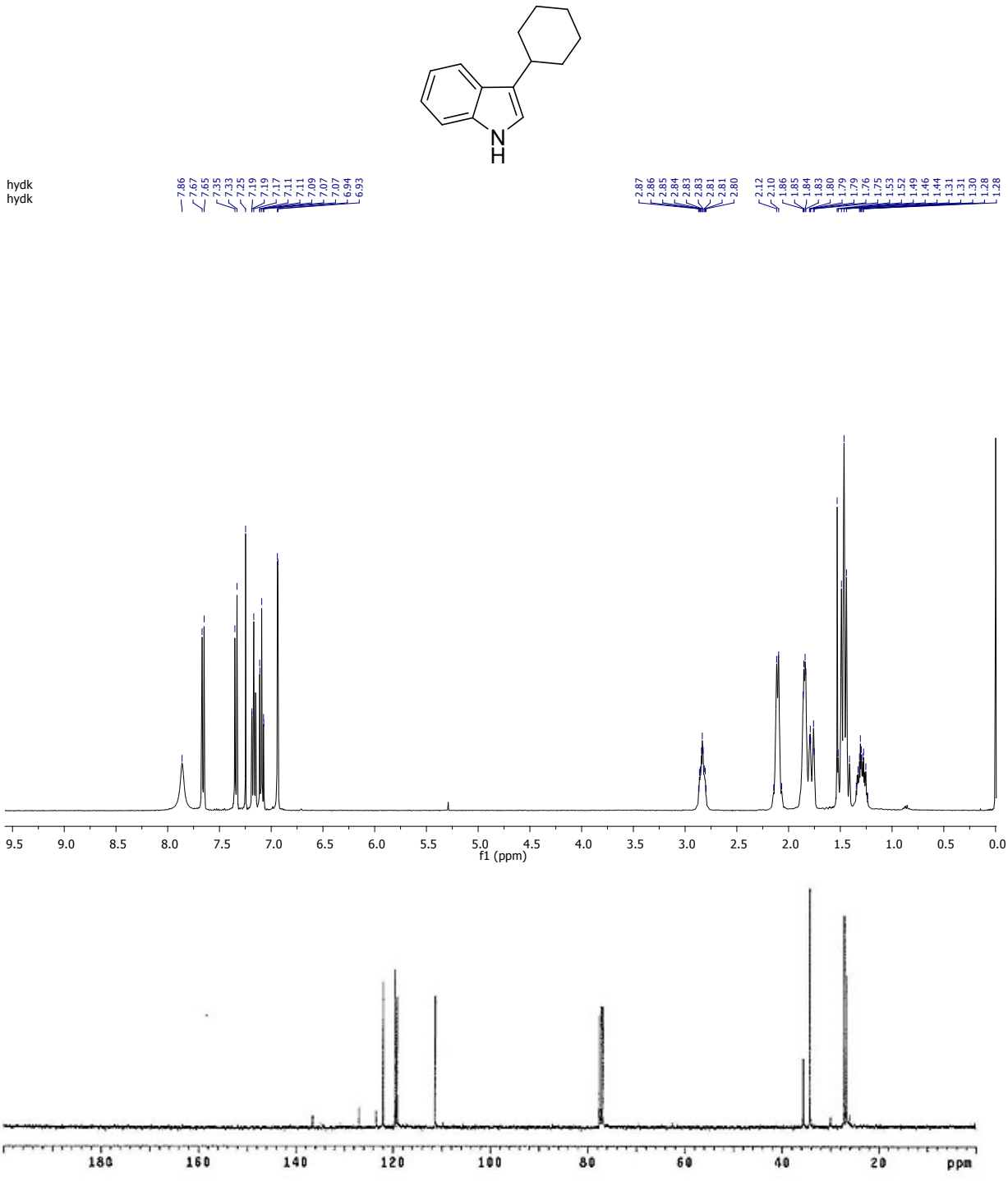
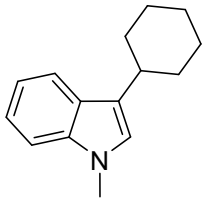
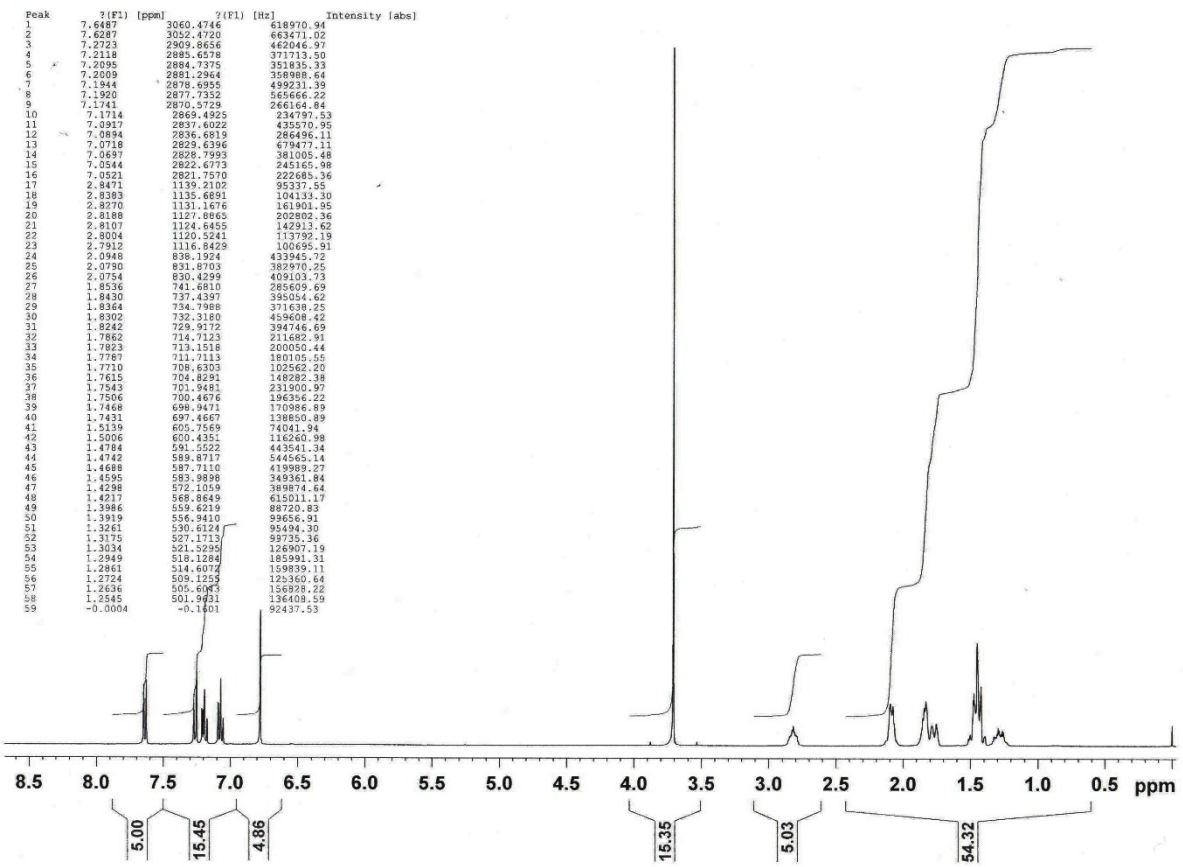


Figure S1. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 3-cyclohexyl-1*H*-indole (**12a**) ($CDCl_3$)



Peak	?(F1) [ppm]	?(F1) [Hz]	Intensity [abs]
1	7.6487	3060.4746	618970.94
2	7.6287	3052.4720	663471.02
3	7.2723	2909.8656	462046.97
4	7.2118	2885.6578	371713.50
5	7.2095	2884.7375	351835.33
6	7.2009	2881.2964	358988.64
7	7.1944	2878.6955	499231.39
8	7.1920	2877.7352	565666.22
9	7.1741	2870.5729	266164.84
10	7.1714	2869.4925	234797.53
11	7.0917	2837.6022	435570.95
12	7.0894	2836.6819	286496.11
13	7.0718	2829.6396	679477.11
14	7.0697	2828.7993	381005.48
15	7.0544	2822.6773	245165.98
16	7.0521	2821.7570	222685.36
17	2.8471	1139.2102	95337.55
18	2.8383	1135.6891	104133.30
19	2.8270	1131.1676	161901.95
20	2.8188	1127.8865	202802.36
21	2.8107	1124.6455	142913.62
22	2.8004	1120.5241	113792.19
23	2.7912	1116.8429	100695.91
24	2.0948	838.1924	433945.72
25	2.0780	831.8703	382970.25
26	2.0754	830.4299	409103.73
27	1.8536	741.6810	285609.69
28	1.8430	737.4397	395054.62
29	1.8364	734.7988	371638.25
30	1.8302	732.3180	459608.42
31	1.8242	729.9172	394746.69
32	1.7862	714.7123	211682.91
33	1.7823	713.1518	200050.44
34	1.7787	711.7113	180105.55
35	1.7710	708.6303	102562.20
36	1.7615	704.8291	148282.38
37	1.7543	701.9481	231900.97
38	1.7506	700.4676	196356.22
39	1.7468	698.9471	170986.89
40	1.7431	697.4667	138850.89
41	1.5139	605.7569	74041.94
42	1.5006	600.4351	116260.98
43	1.4784	591.5522	443541.34
44	1.4742	589.8717	544565.14
45	1.4688	587.7110	419989.27
46	1.4595	583.9898	349361.84
47	1.4298	572.1059	389874.64
48	1.4217	568.8649	615011.17
49	1.3986	559.6219	88720.83
50	1.3919	556.9410	99656.91
51	1.3261	530.6124	95494.30
52	1.3175	527.1713	98735.36
53	1.3034	521.5295	126907.19
54	1.2949	518.1284	185991.31
55	1.2861	514.6072	159839.11
56	1.2724	509.1255	125360.64
57	1.2636	505.6043	156828.22
58	1.2545	501.9031	136408.59
59	-0.0004	-0.1601	92437.53



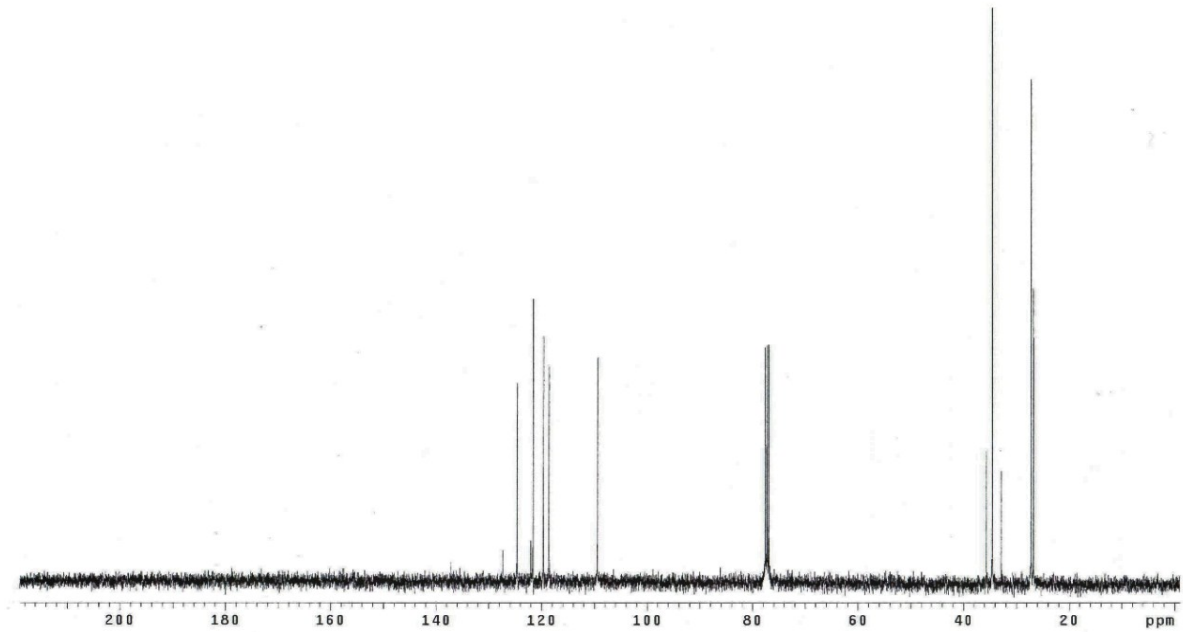


Figure S2. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 3-cyclohexyl-1-methyl-1*H*-indole (**12b**) ($CDCl_3$)

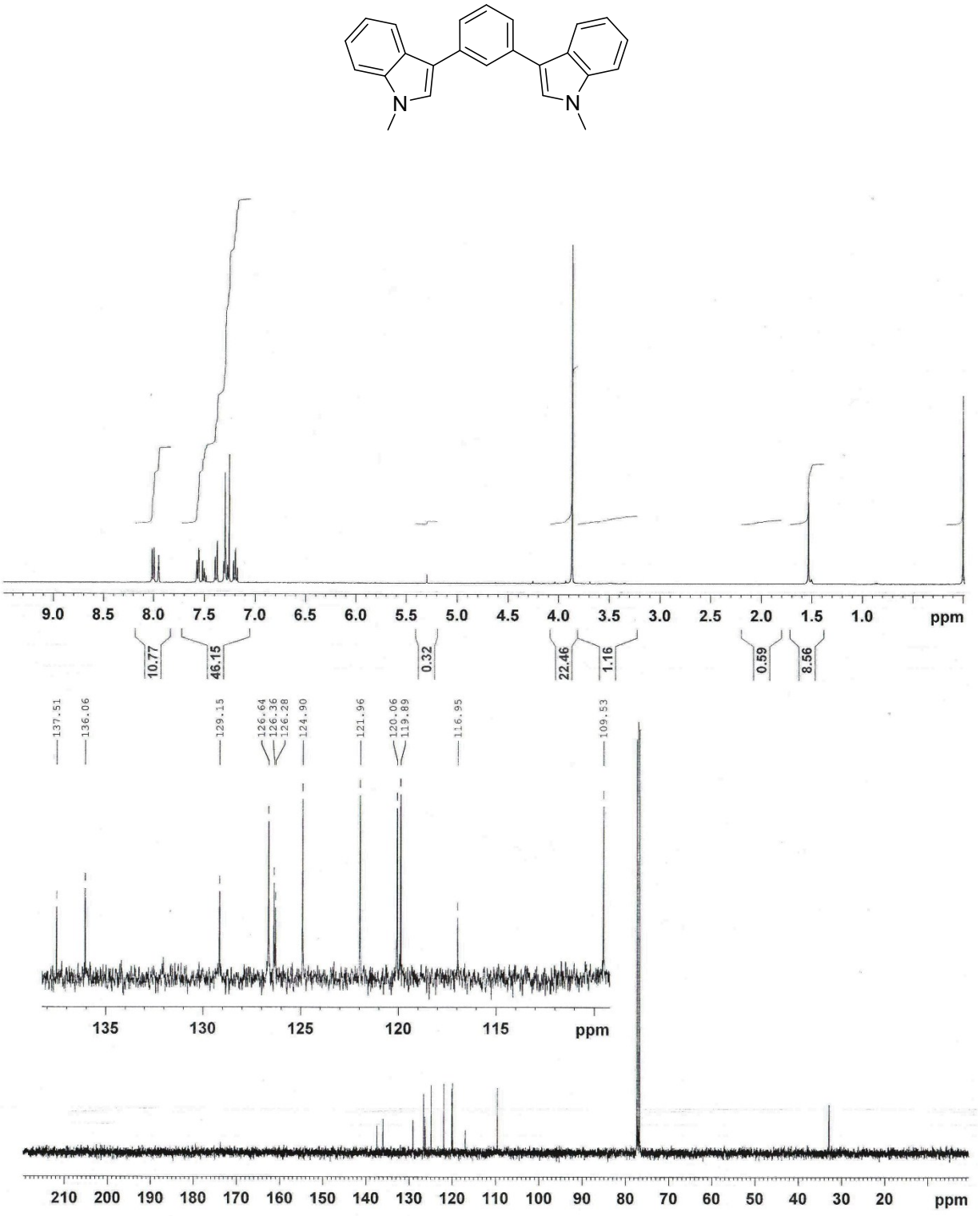


Figure S3. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(1-methyl-1*H*-indol-3-*yl*)benzene (**7b**) ($CDCl_3$)

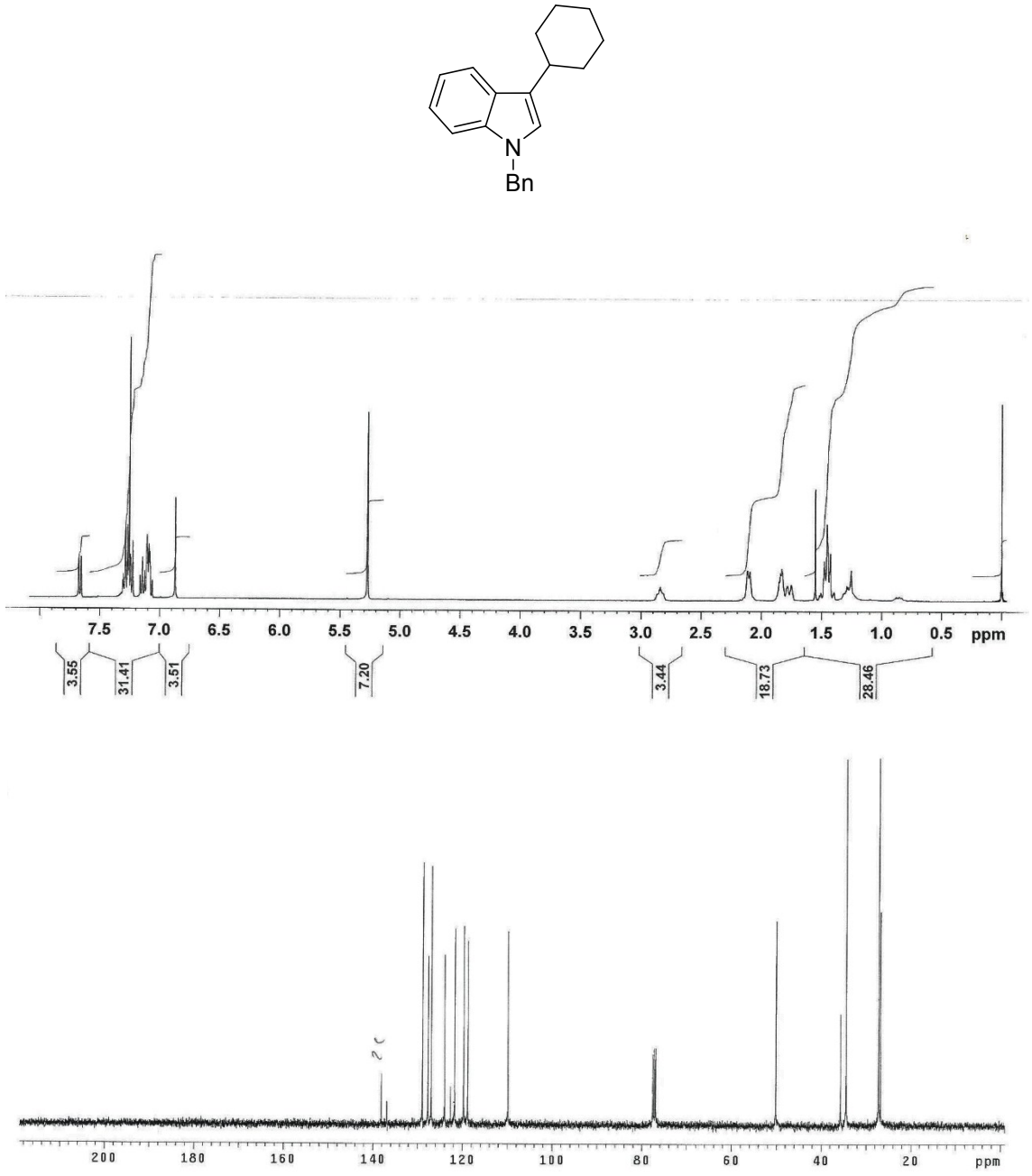


Figure S4. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1-benzyl-3-cyclohexyl-1*H*-indole (**12c**) ($CDCl_3$)

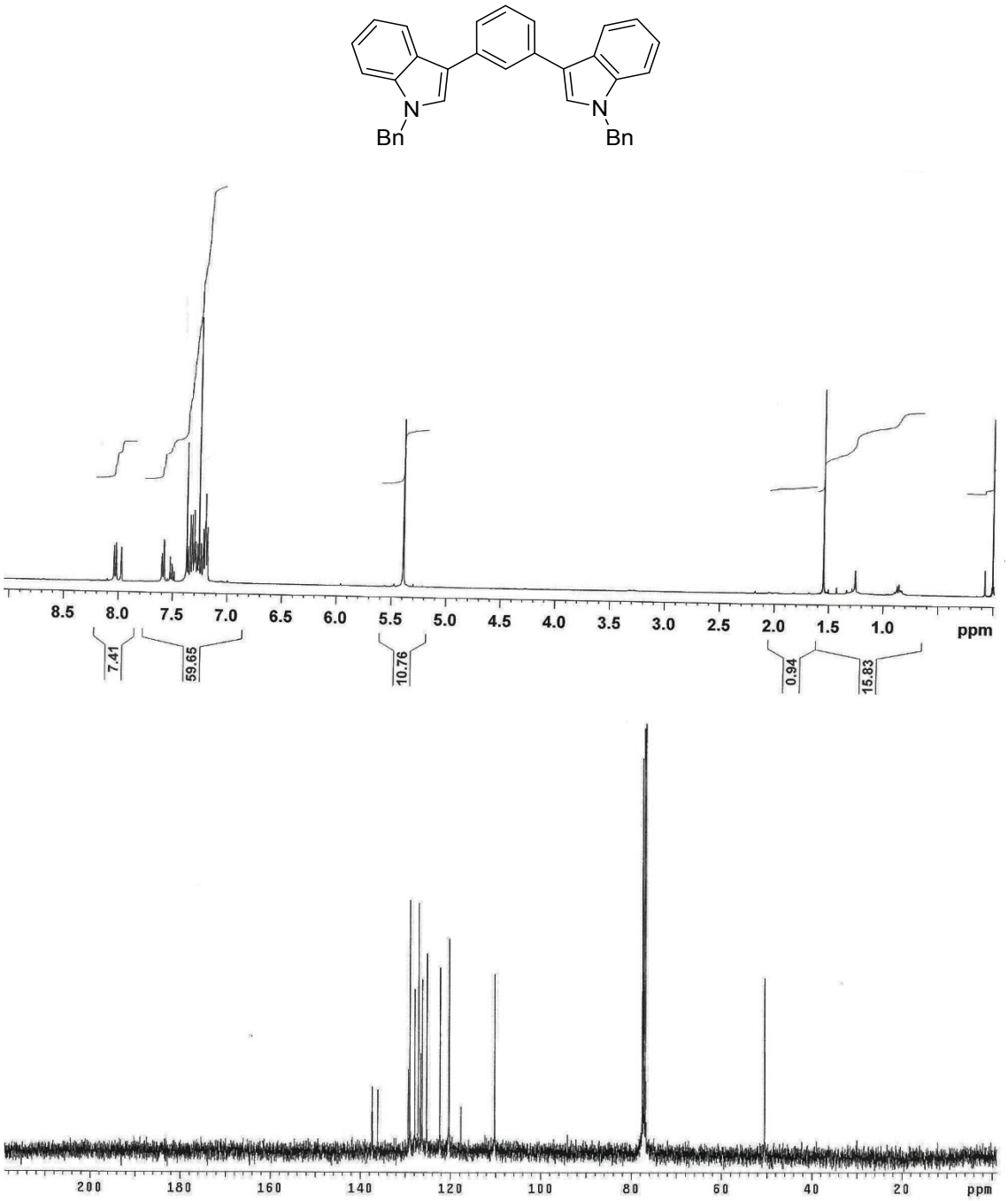


Figure S5. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(1-benzyl-1*H*-indol-3-*yl*)benzene (**7c**) ($CDCl_3$)

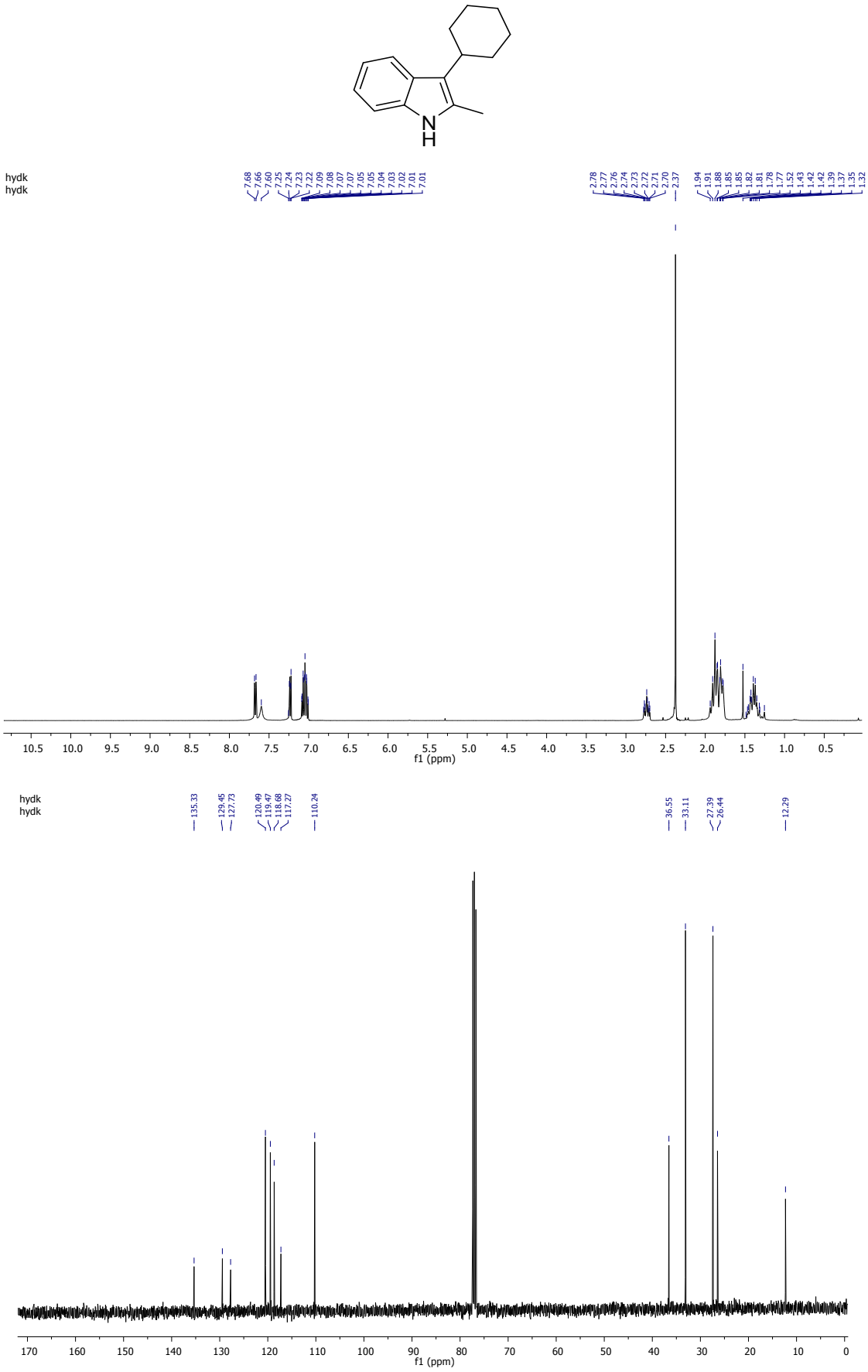


Figure S6. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 3-cyclohexyl-2-methyl-1*H*-indole (**12d**) ($CDCl_3$)

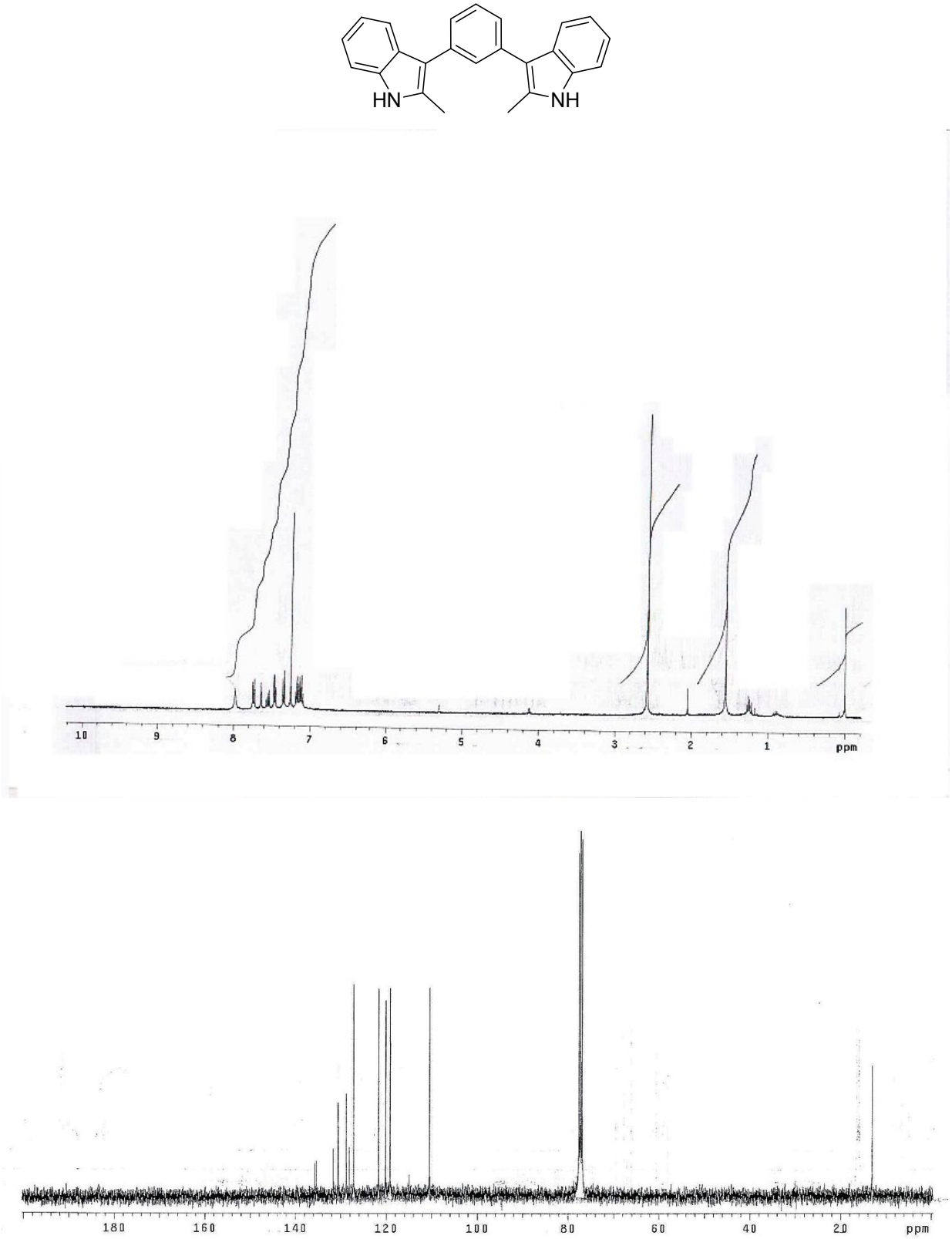


Figure S7. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(2-methyl-1*H*-indol-3-yl)benzene (**7d**) ($CDCl_3$)

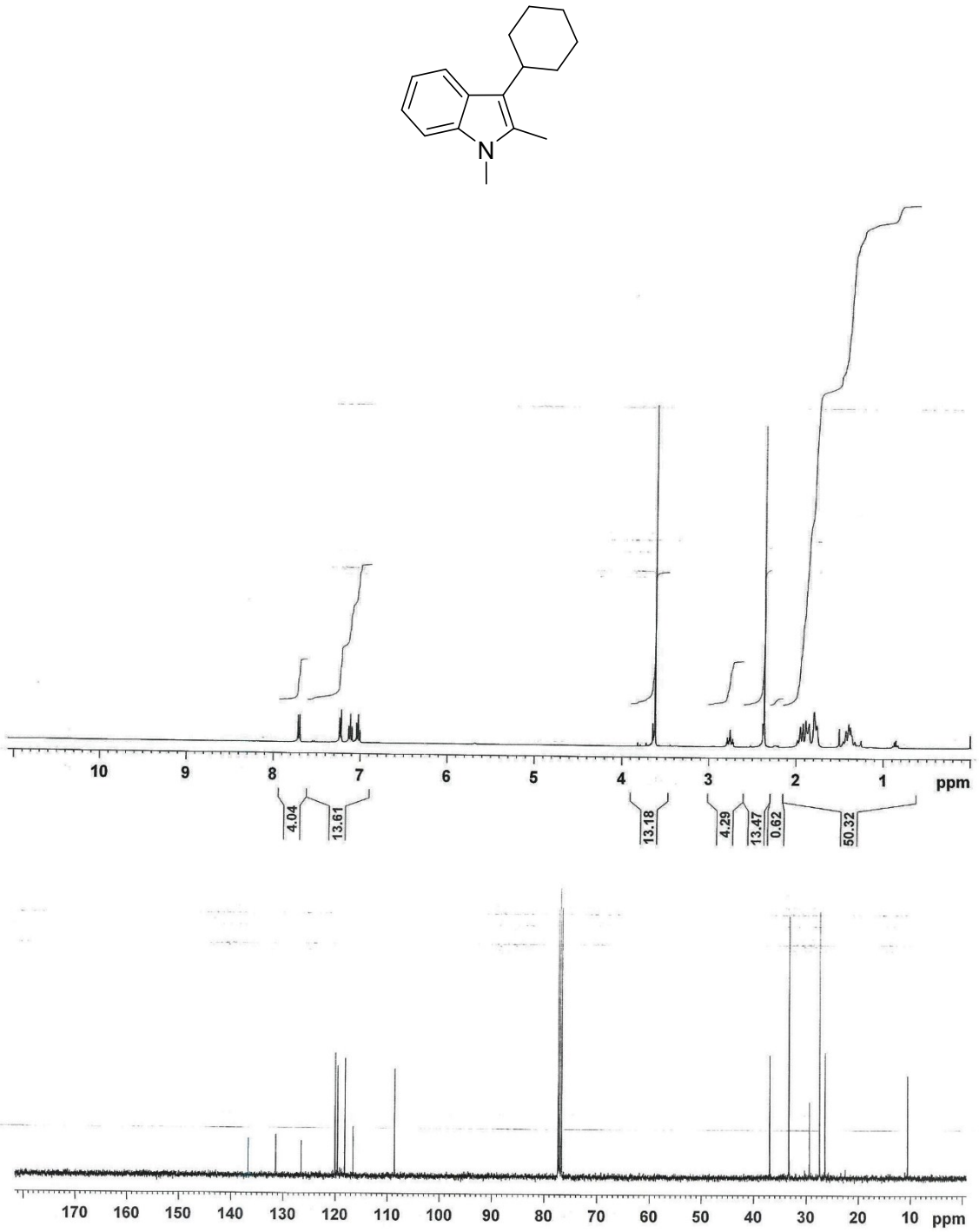


Figure S8. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 3-cyclohexyl-1,2-dimethyl-1*H*-indole (**12e**) ($CDCl_3$)

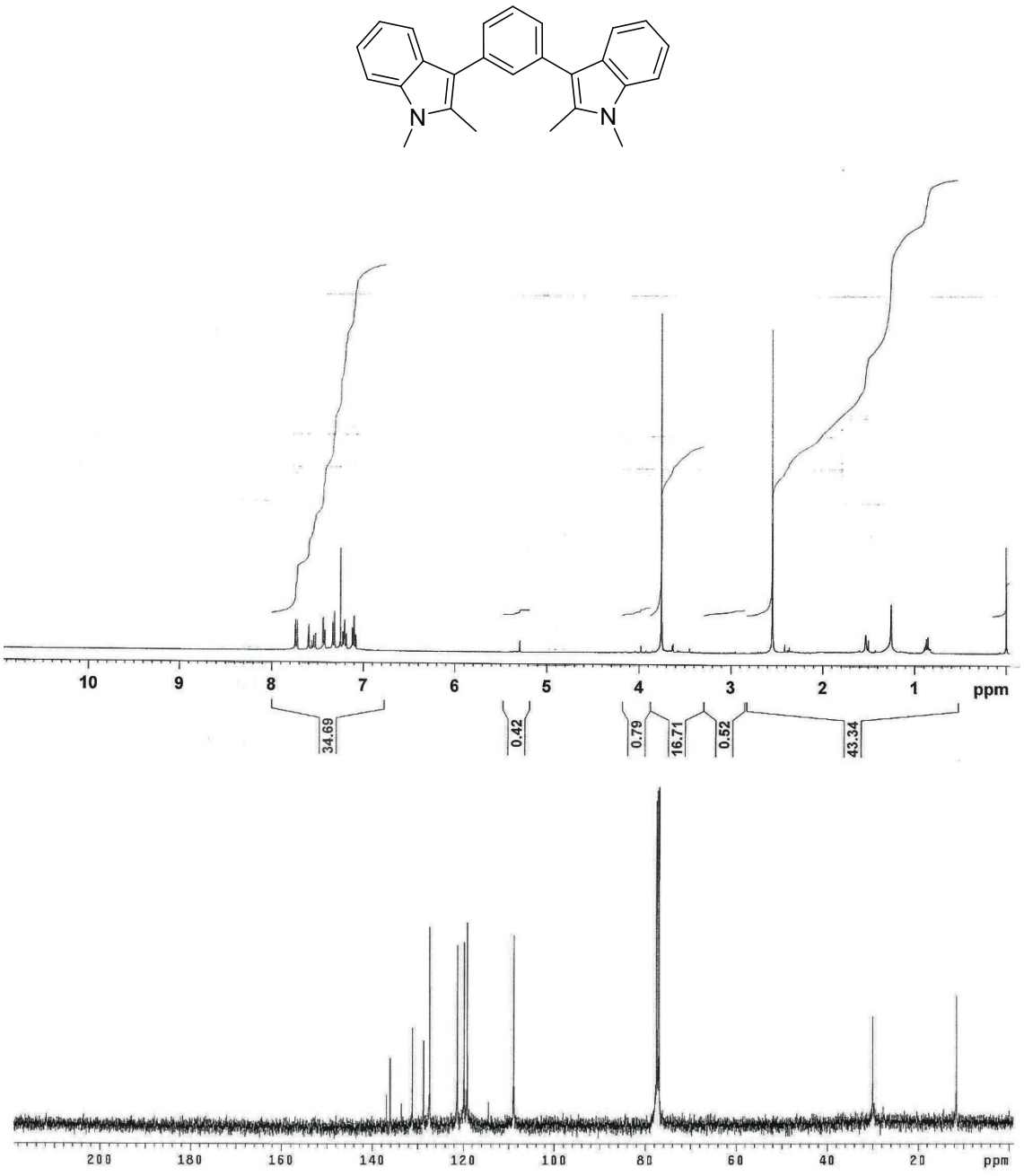


Figure S9. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(1,2-dimethyl-1*H*-indol-3-yl)benzene (**7e**) ($CDCl_3$)

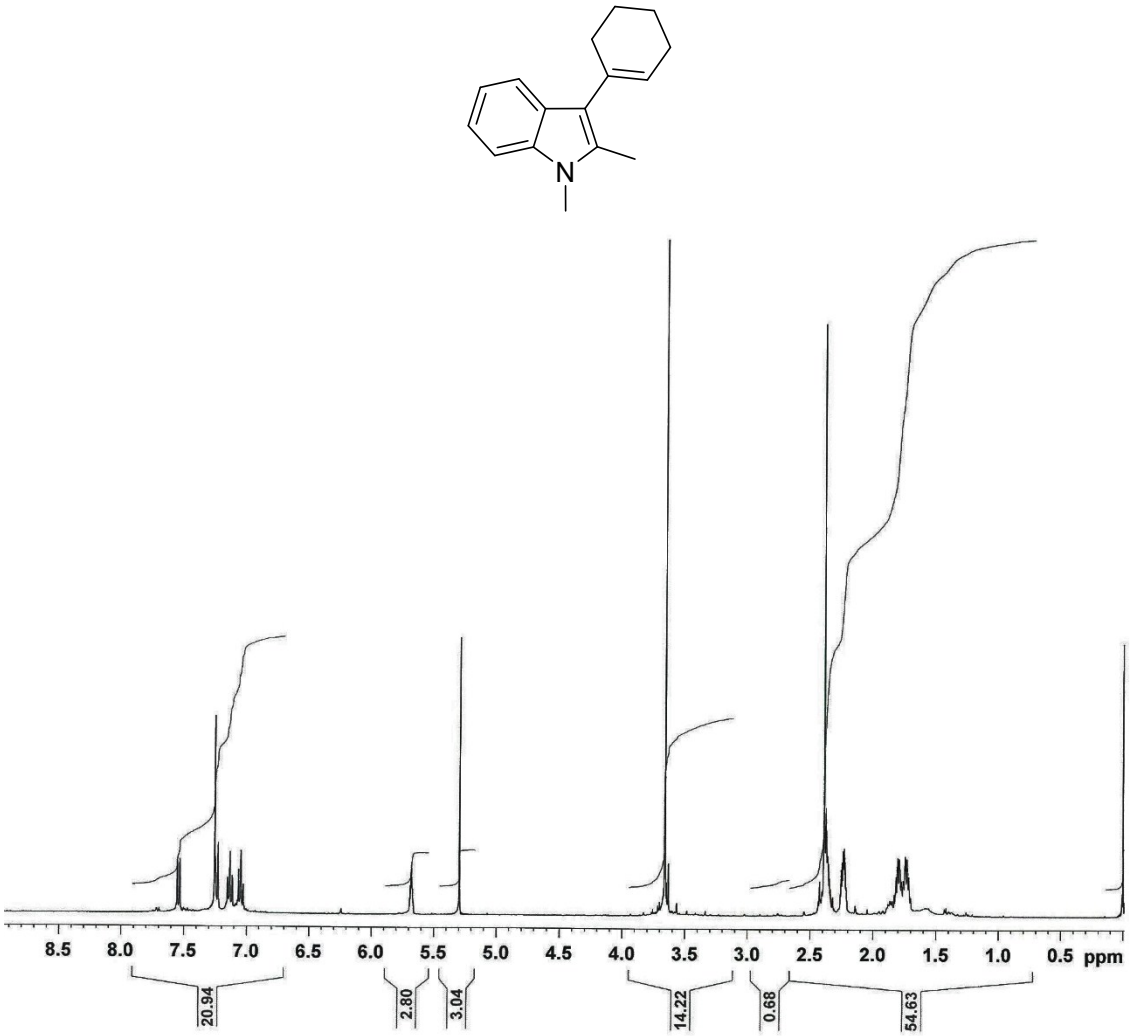


Figure S10. ^{1}H NMR (400 MHz) spectrum of 3-(cyclohex-1-en-1-*yl*)-1,2-dimethyl-1*H*-indole (**22e**) ($CDCl_3$)

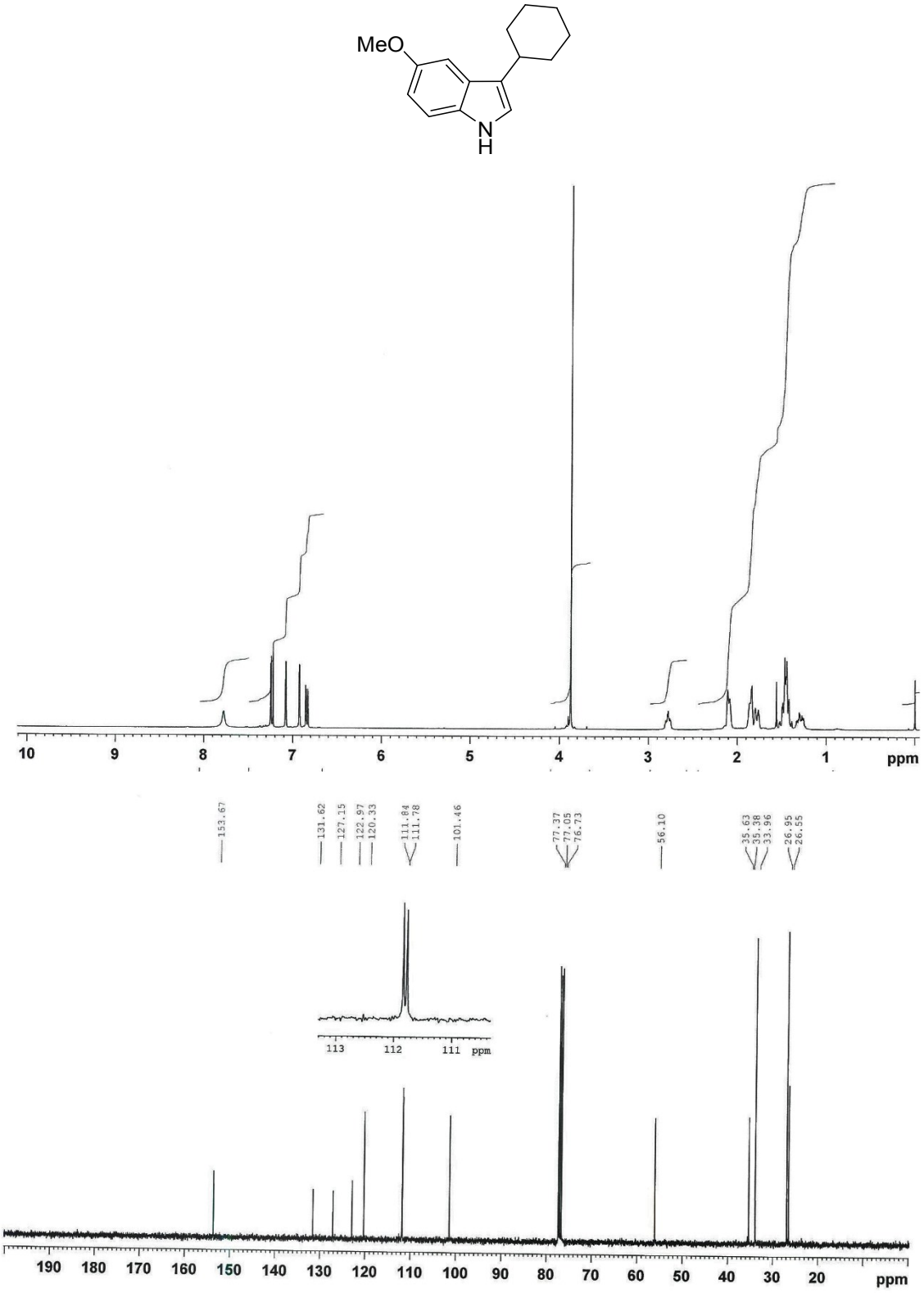


Figure S11. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 3-cyclohexyl-5-methoxy-1*H*-indole (**12f**) ($CDCl_3$)

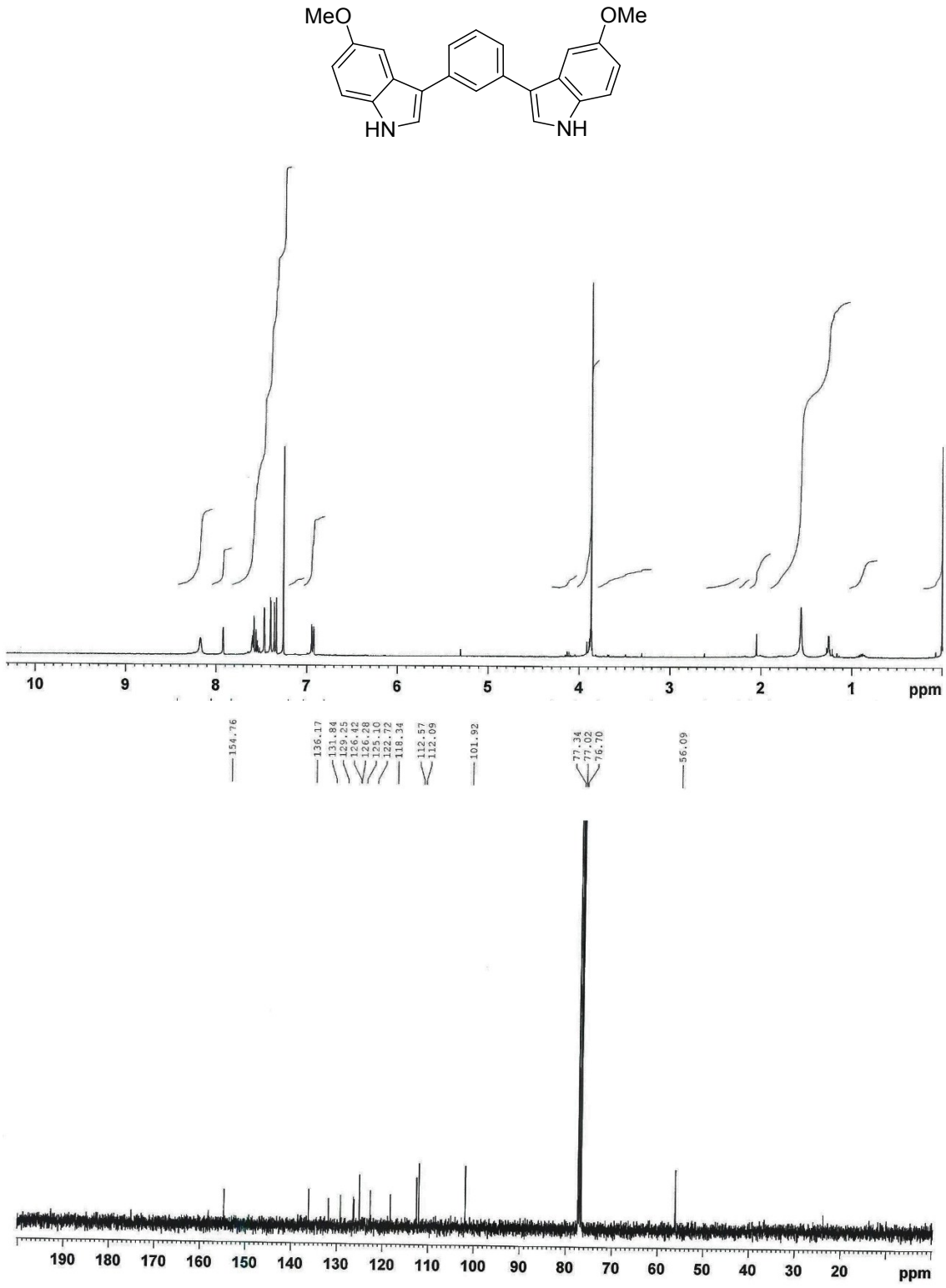


Figure S12. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(5-methoxy-1*H*-indol-3-*yl*)benzene (**7f**) ($CDCl_3$)

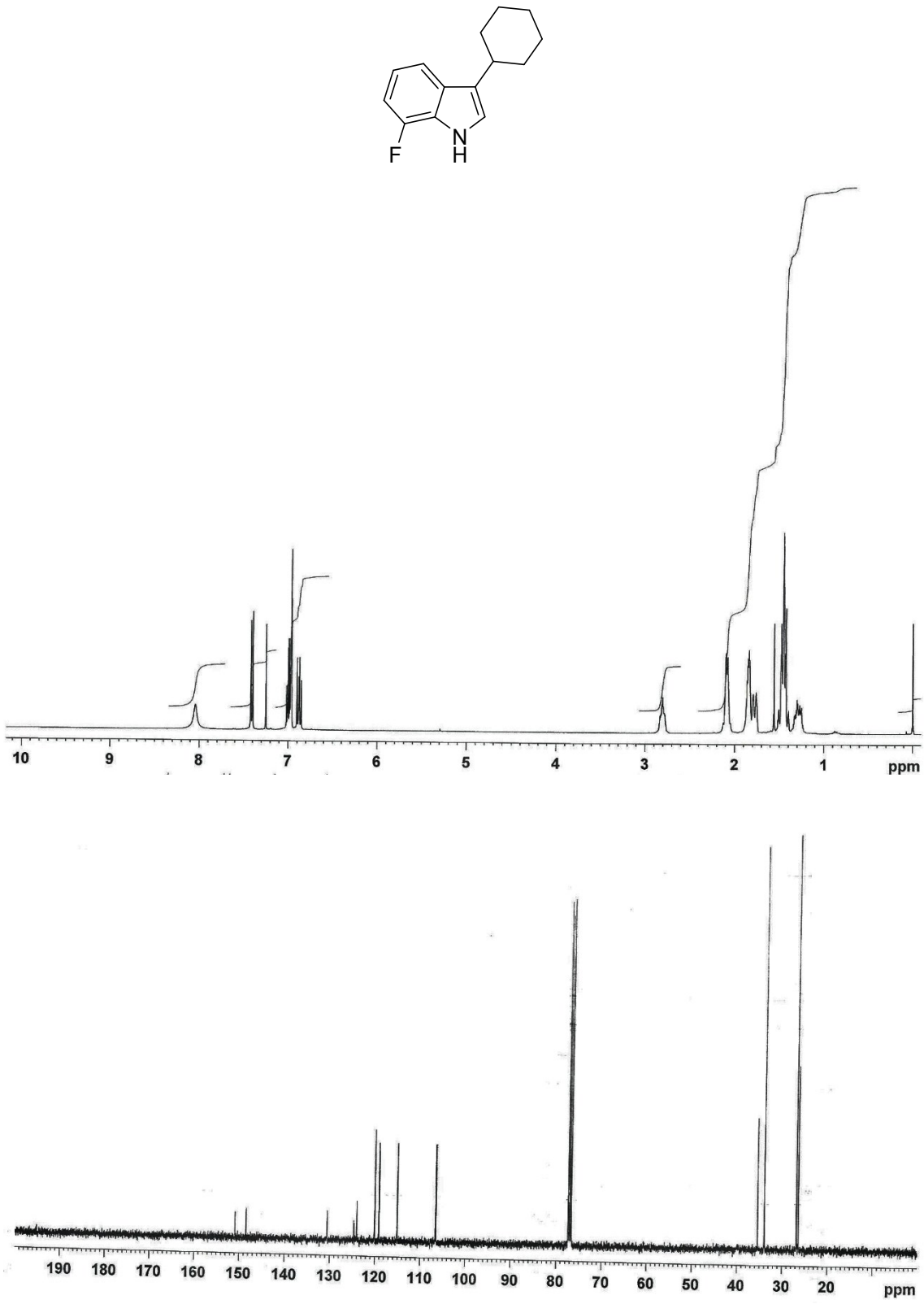


Figure S13. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 3-cyclohexyl-7-fluoro-1*H*-indole (**12g**) ($CDCl_3$)

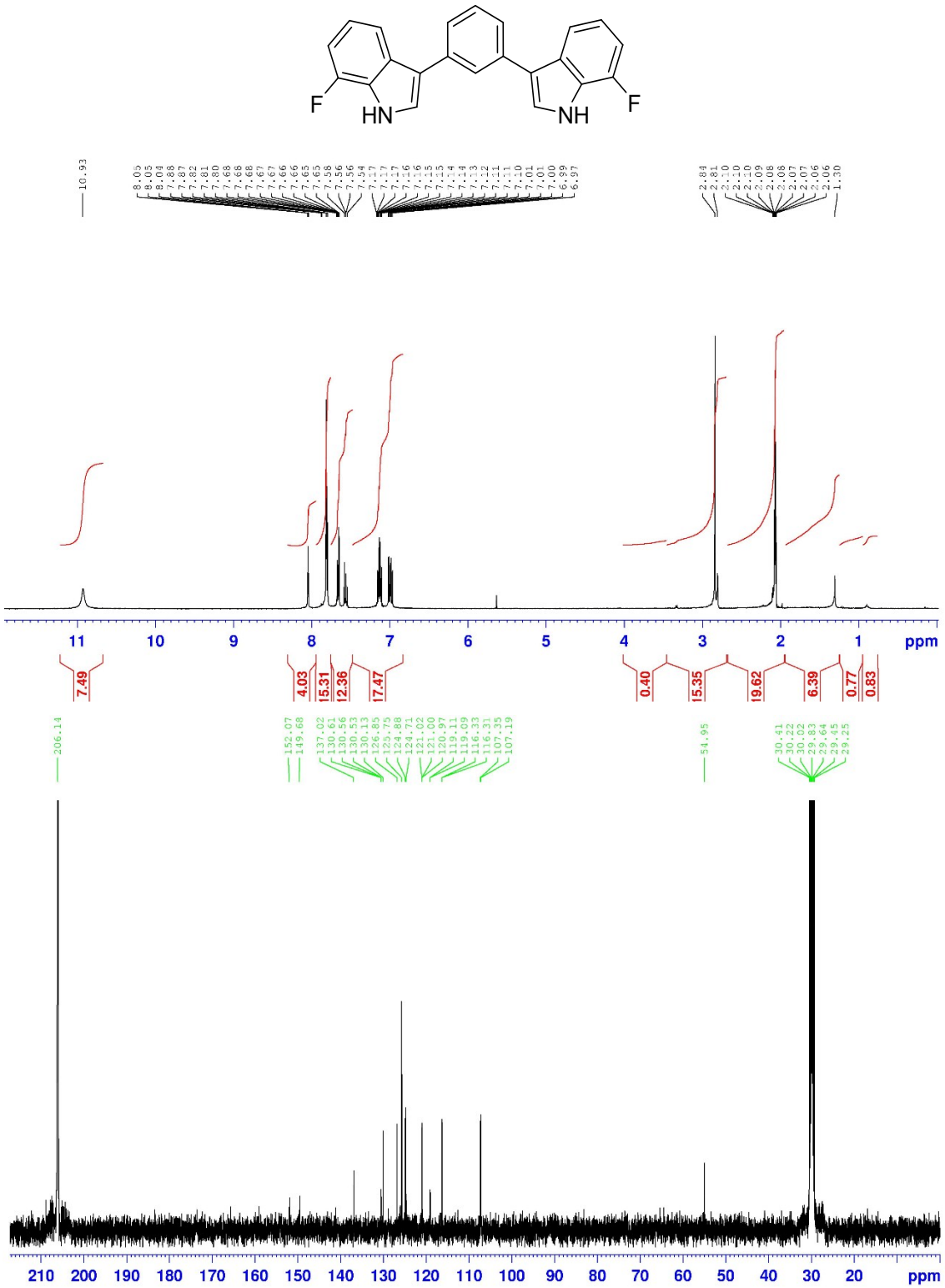


Figure S14. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(7-fluoro-1*H*-indol-3-*yl*)benzene (**7g**) (Acetone-*d6*)

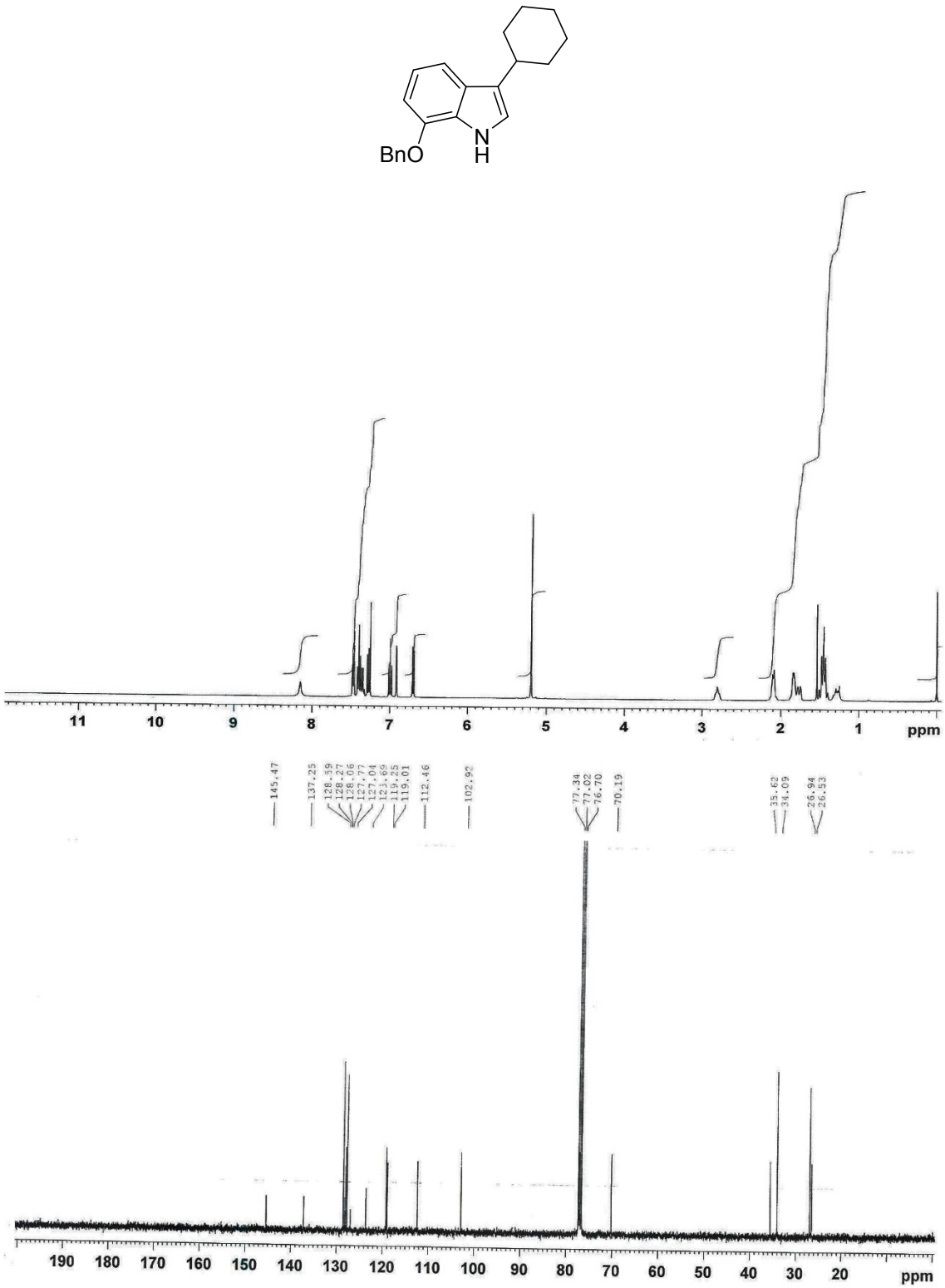


Figure S15. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 7-(benzyloxy)-3-cyclohexyl-1*H*-indole (**12h**) ($CDCl_3$)

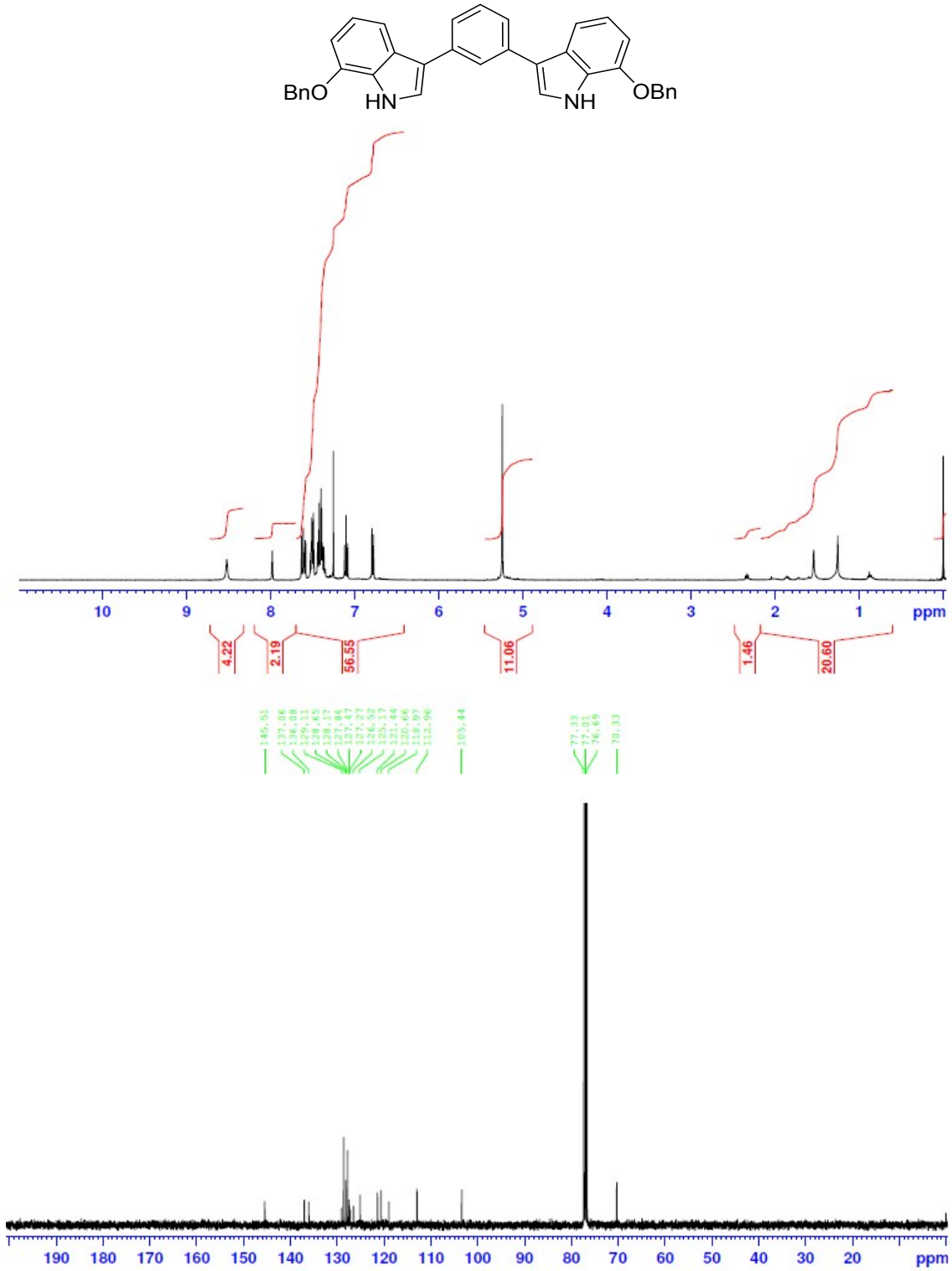


Figure S16. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(7-(benzyloxy)-1*H*-indol-3-*yl*)benzene (**7h**) ($CDCl_3$)

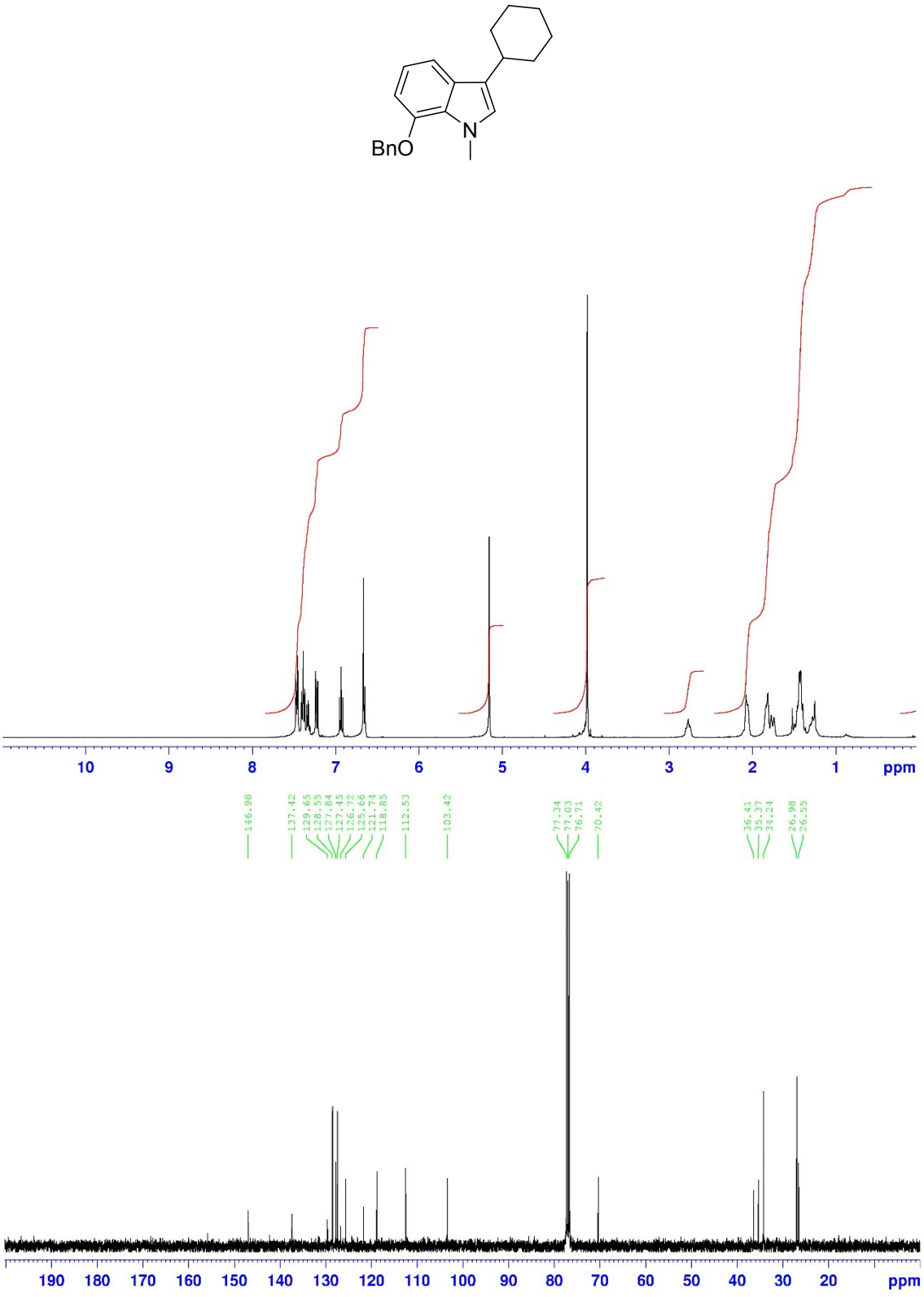


Figure S17. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 7-(benzyloxy)-3-cyclohexyl-1-methyl-1*H*-indole (**12i**) ($CDCl_3$)

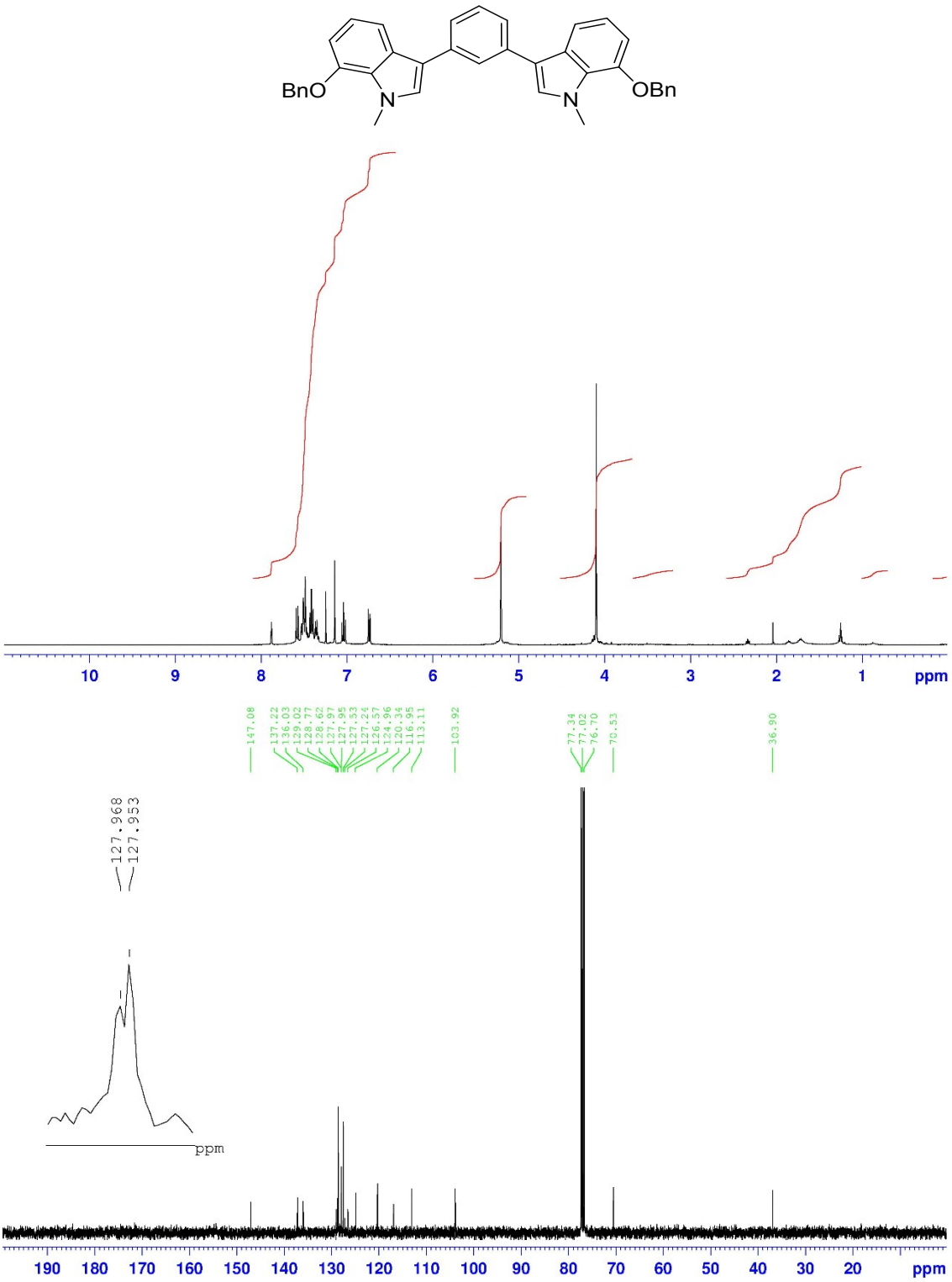


Figure S18. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(7-(benzyloxy)-1-methyl-1*H*-indol-3-*yl*)benzene (**7i**) ($CDCl_3$)

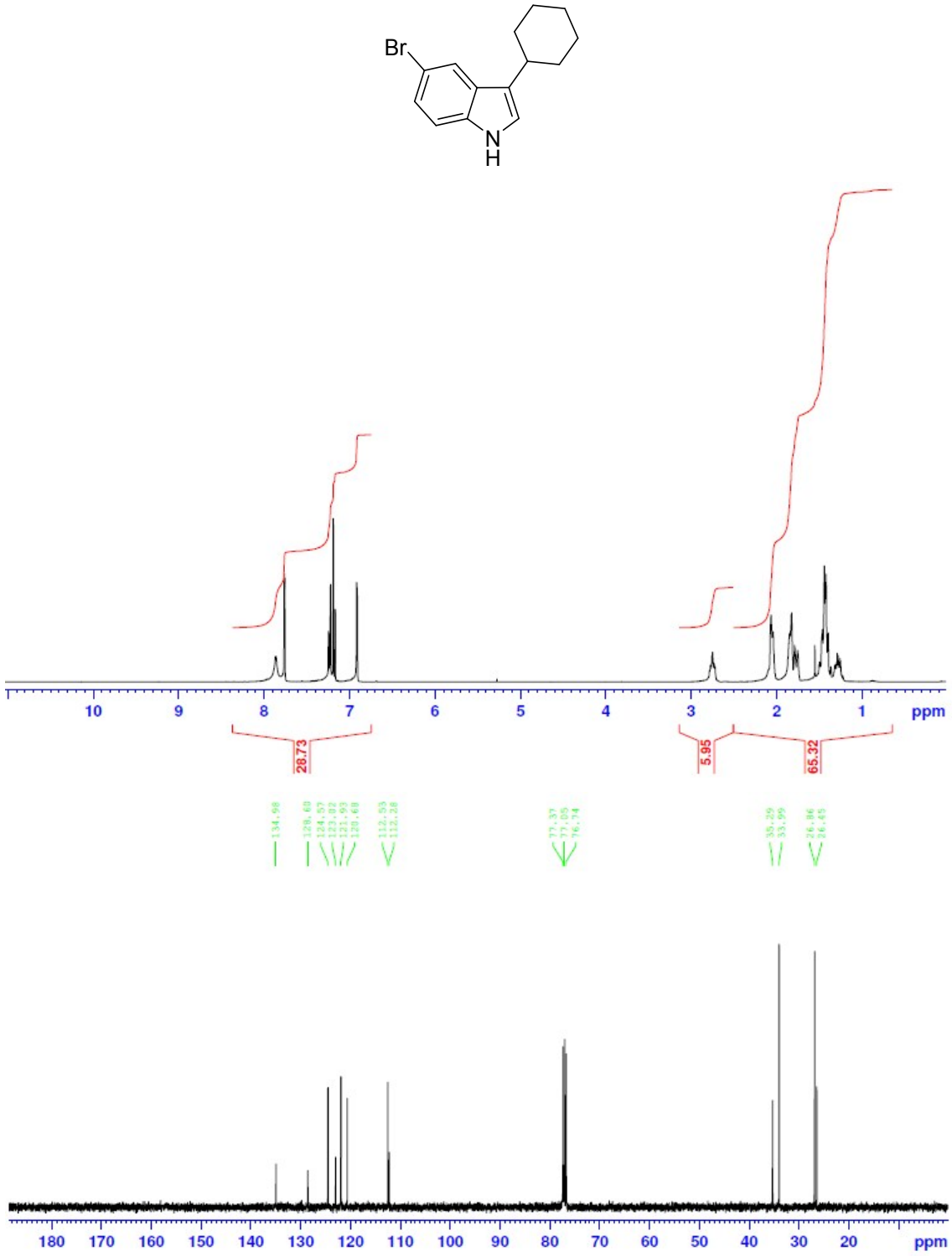


Figure S19. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 5-bromo-3-cyclohexyl-1*H*-indole (**12j**) ($CDCl_3$)

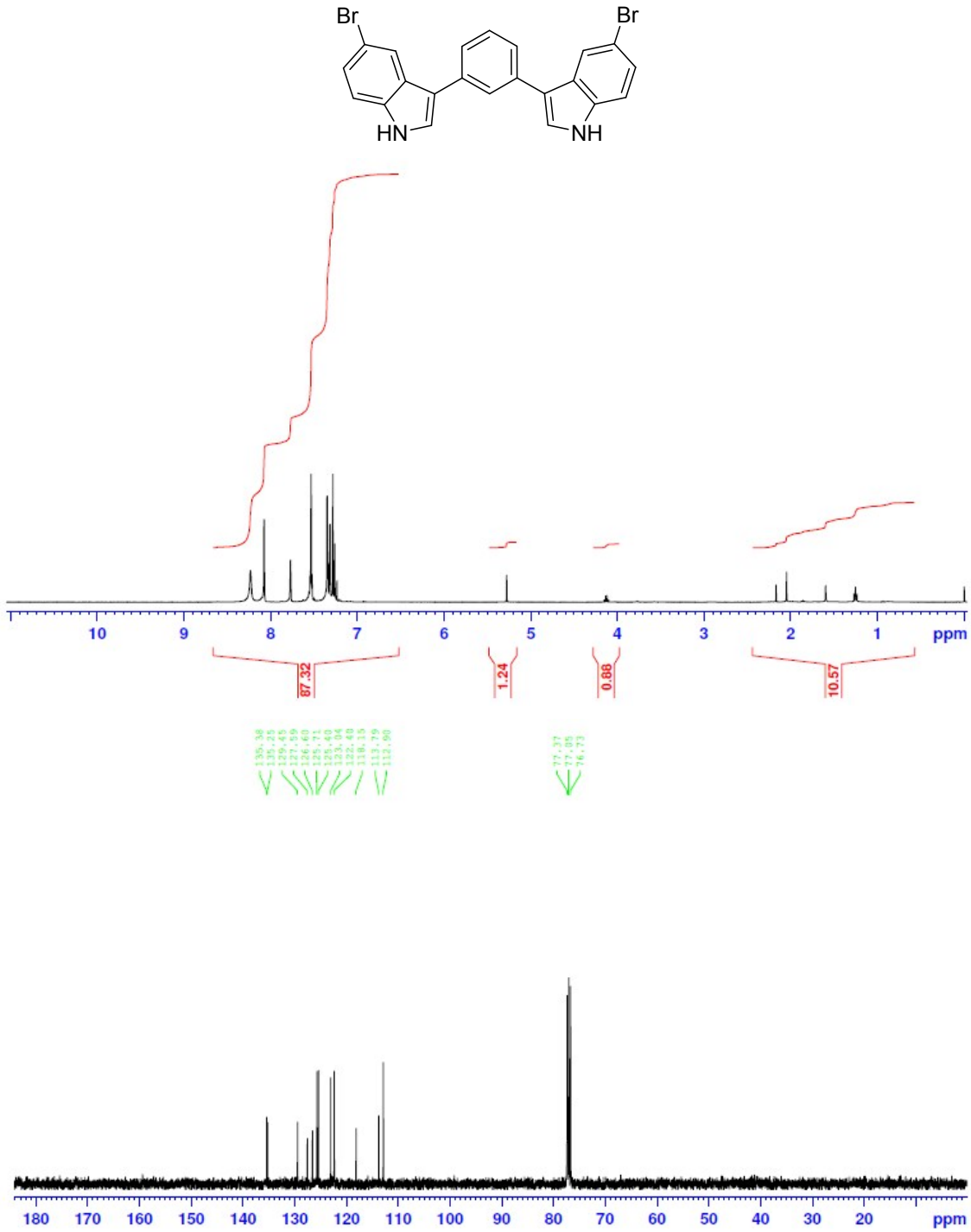


Figure S20. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(5-bromo-1*H*-indol-3-*yl*)benzene (**7j**) ($CDCl_3$)

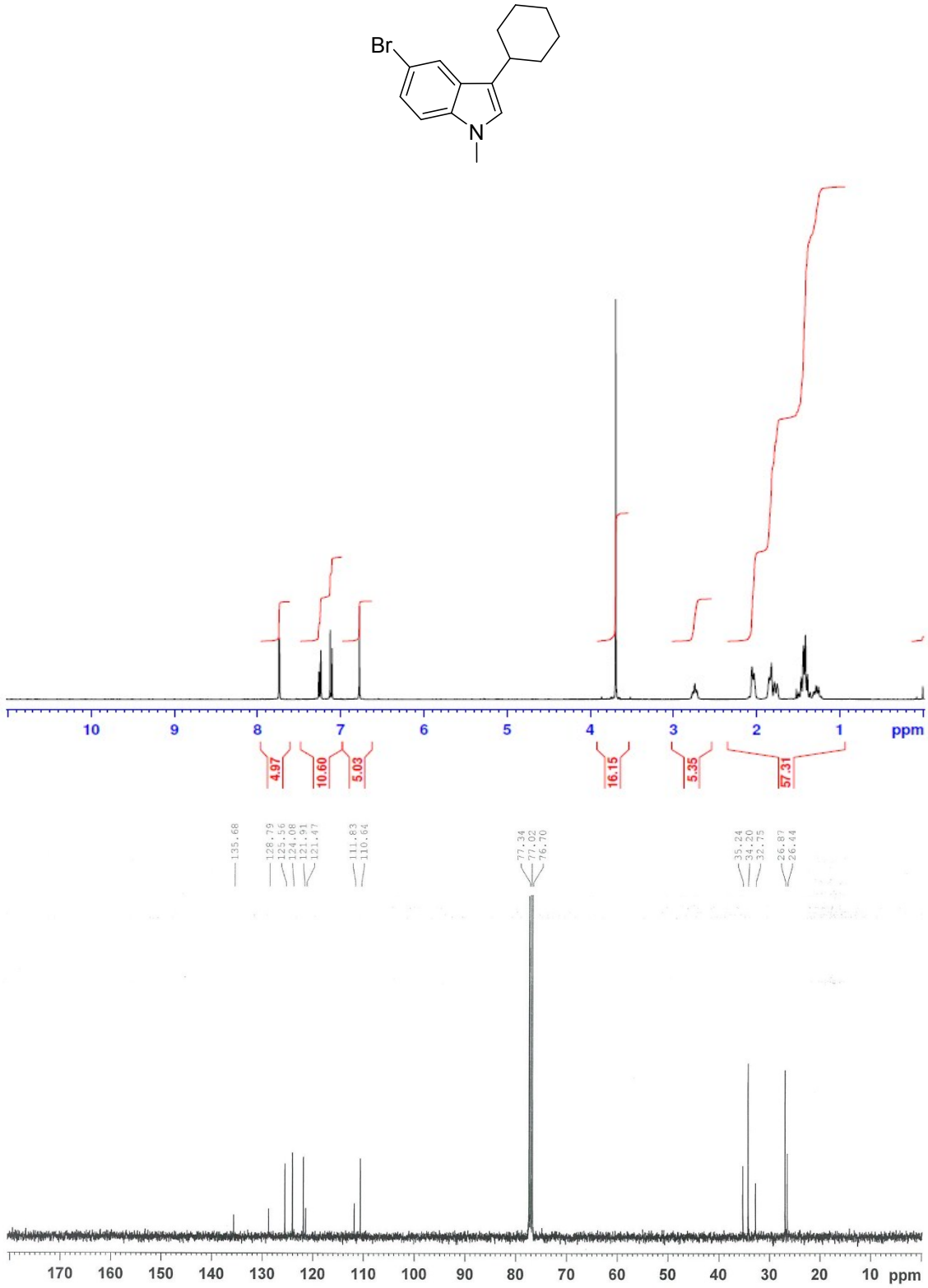


Figure S21. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 5-bromo-3-cyclohexyl-1-methyl-1*H*-indole (**12k**) ($CDCl_3$)

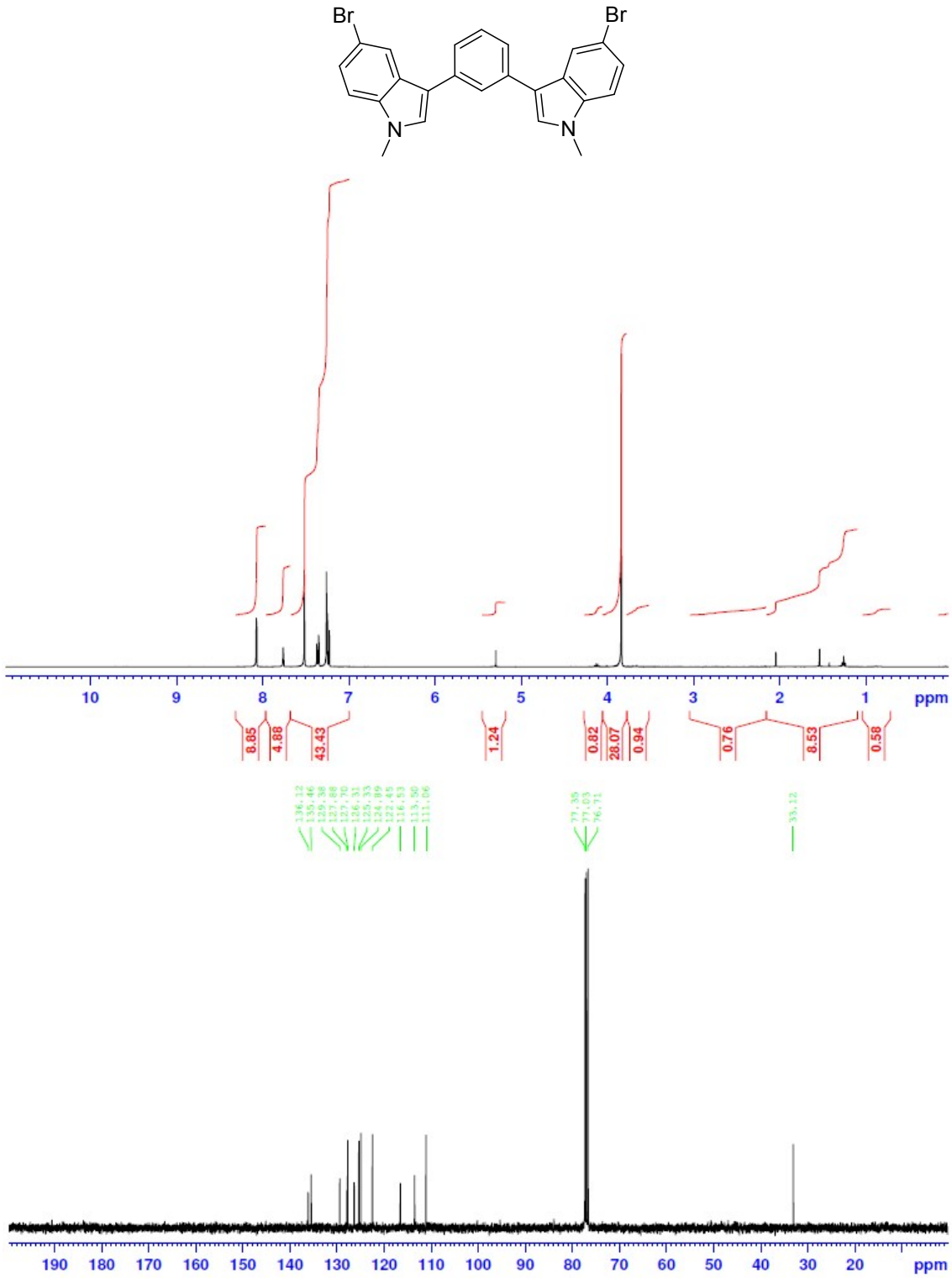


Figure S22. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 1,3-bis(5-bromo-1-methyl-1*H*-indol-3-*yl*)benzene (**7k**) ($CDCl_3$)

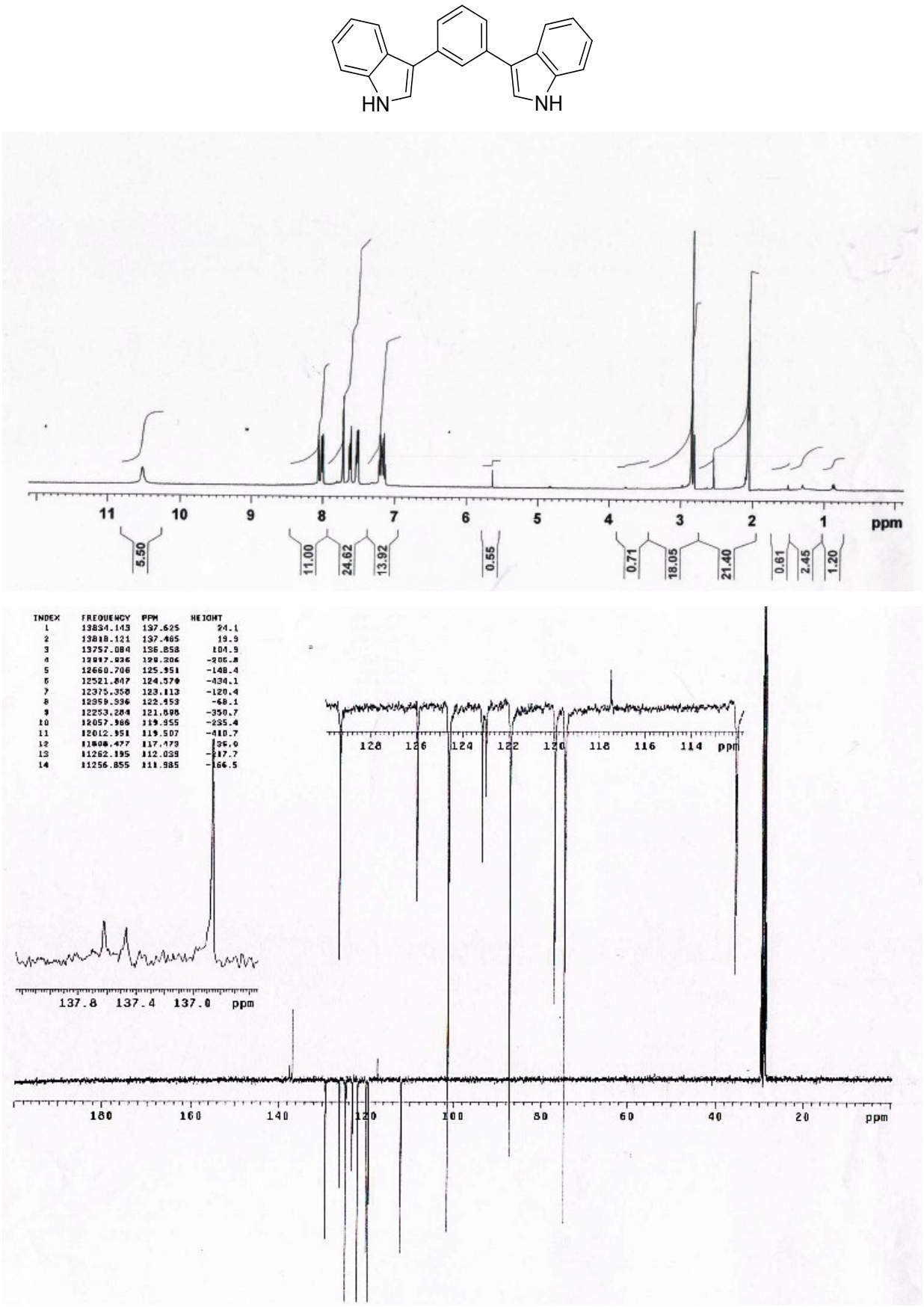


Figure S23. ^{1}H NMR (400 MHz) and APT NMR (100 MHz) spectra of 1,3-di(1*H*-indol-3-*yl*)benzene (**7a**) (Acetone-*d6*)

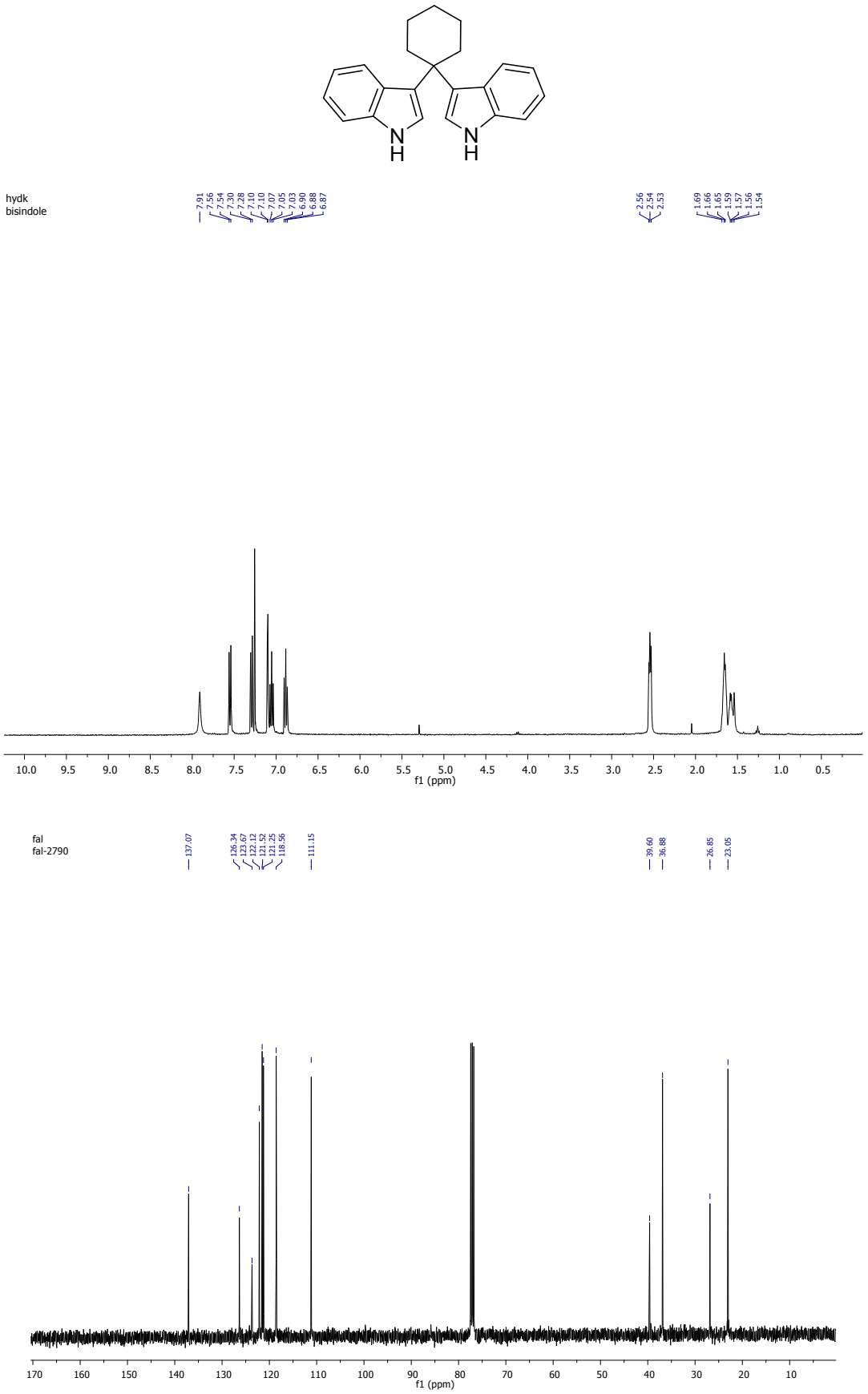


Figure S24. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of 3,3'-(cyclohexane-1,1-*diyl*)bis(1*H*-indole) (**13a**) ($CDCl_3$)

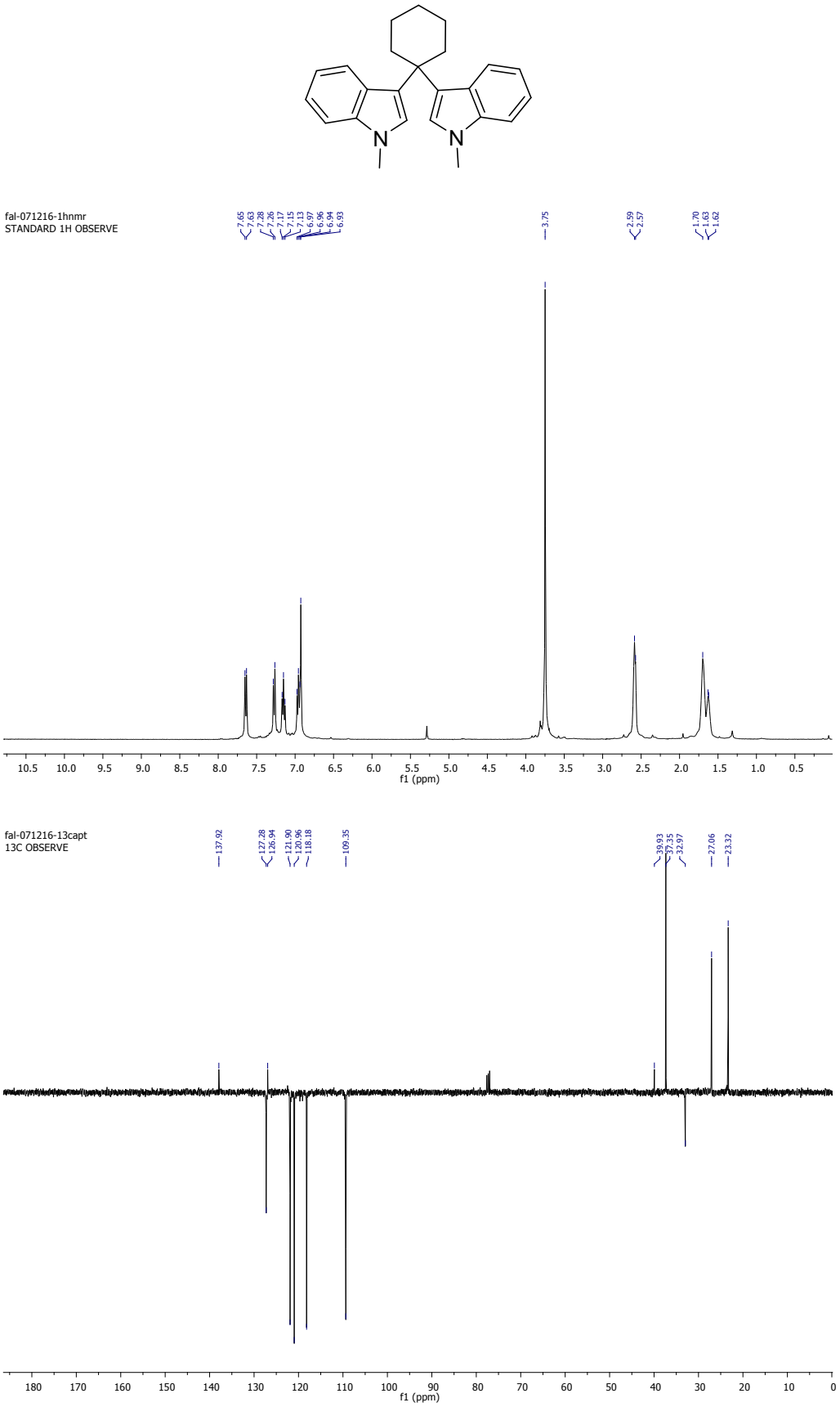


Figure S25. ^{1}H NMR (400 MHz) and APT NMR (100 MHz) spectra of 3,3'-(cyclohexane-1,1-*diyl*)bis(1-methyl-1*H*-indole) (**13b**) ($CDCl_3$)

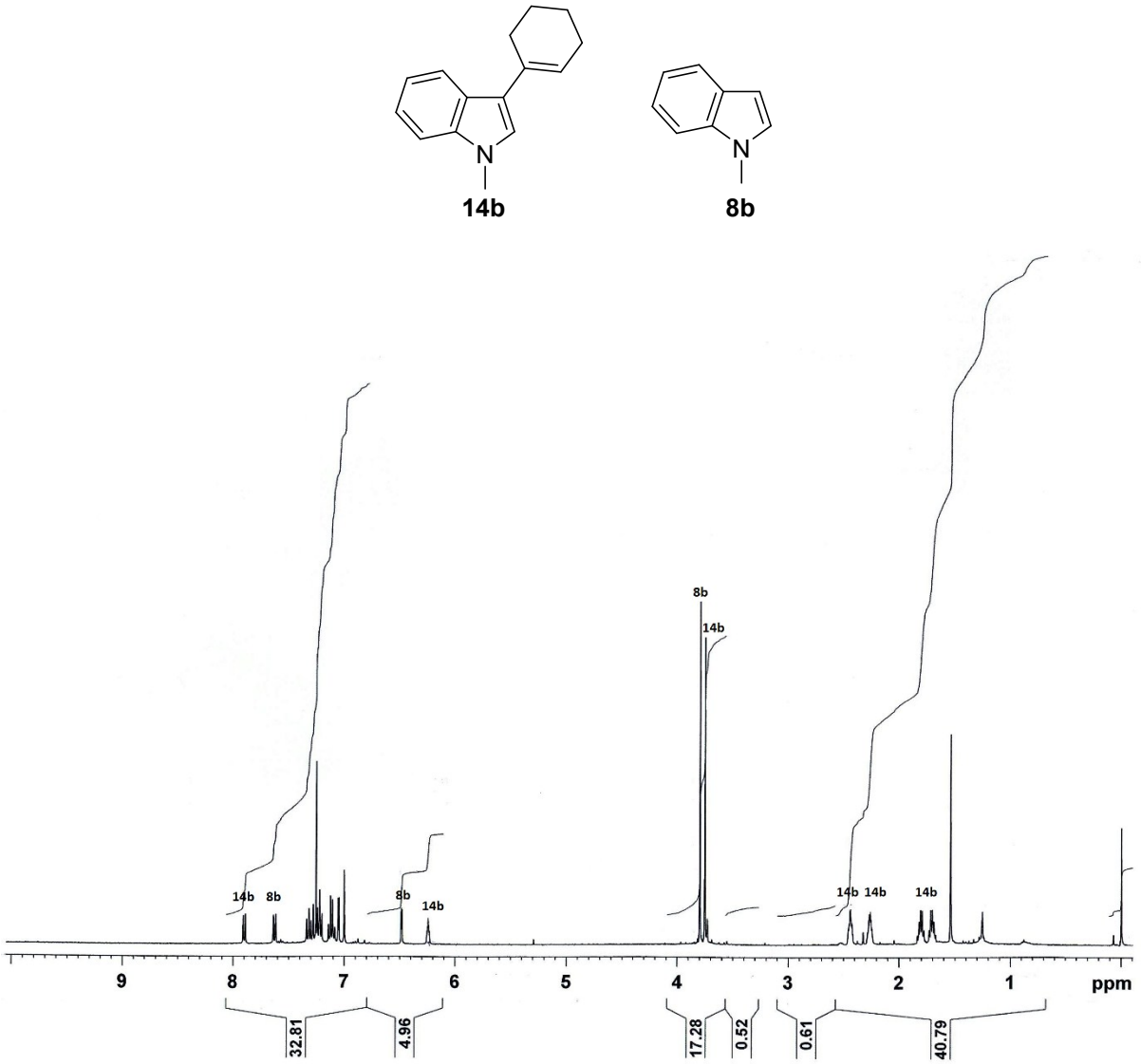


Figure S26. ^{1}H NMR (400 MHz) of the mixture of **14b** and **8b** after thin layer chromatography.

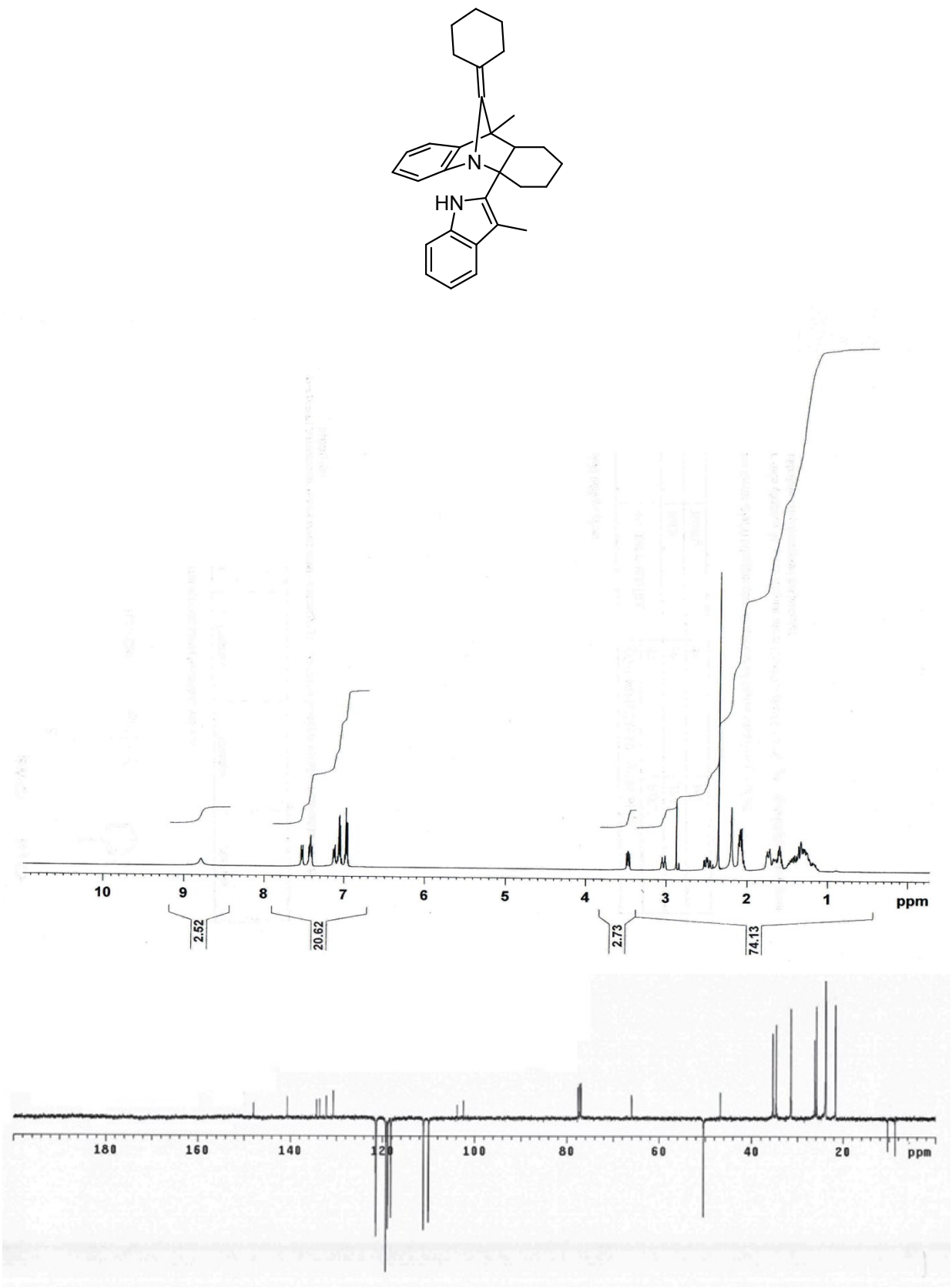
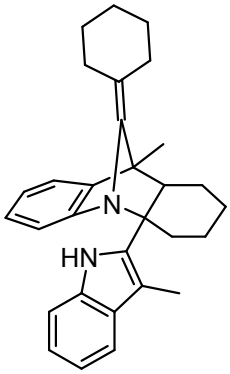


Figure S27. ^{1}H NMR (400 MHz) and APT NMR (100 MHz) spectra of (4aR,9S,10R)-11-cyclohexylidene-9-methyl-4a-(3-methyl-1*H*-indol-2-*yl*)-2,3,4,4a,9,9a-hexahydro-1*H*-9,10-methanoacridine (**27**) ($CDCl_3$)



INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3055.208	7.643	6.6	40	2806.233	7.020	6.4	79	575.235	1.439	3.9
2	3053.375	7.638	8.7	41	2802.873	7.011	5.5	80	568.514	1.422	4.6
3	3049.098	7.627	5.5	42	2800.429	7.005	3.7	81	565.154	1.414	6.6
4	3047.570	7.623	7.2	43	1375.010	3.440	5.1	82	561.488	1.405	5.6
5	3046.654	7.621	7.9	44	1369.205	3.425	5.7	83	555.073	1.389	6.2
6	3009.690	7.529	6.6	45	1364.928	3.414	6.0	84	552.934	1.383	6.3
7	3007.551	7.523	6.9	46	1359.124	3.400	5.2	85	544.075	1.361	5.6
8	3004.191	7.515	4.6	47	1234.789	3.089	4.1	86	540.104	1.351	5.1
9	3001.441	7.508	7.9	48	1235.400	3.090	4.2	87	531.245	1.329	5.6
10	3000.830	7.507	7.6	49	1219.820	3.051	4.6	88	524.829	1.313	7.1
11	2991.055	7.482	8.2	50	1010.254	2.527	88.6	89	517.803	1.295	5.1
12	2988.916	7.477	5.9	51	989.175	2.474	2.8	90	513.221	1.284	7.6
13	2984.334	7.465	9.4	52	956.487	2.393	5.6	91	509.860	1.275	7.0
14	2982.501	7.461	8.3	53	949.767	2.376	107.0	92	500.695	1.252	11.3
15	2901.241	7.257	6.5	54	943.657	2.361	7.2	93	490.003	1.226	13.6
16	2881.384	7.208	3.6	55	942.129	2.357	5.9	94	480.839	1.203	6.1
17	2880.162	7.205	4.6	56	939.074	2.349	6.6	95	477.784	1.195	6.7
18	2874.357	7.190	10.0	57	928.382	2.322	4.6	96	473.812	1.185	6.3
19	2873.135	7.187	9.5	58	923.800	2.311	4.0	97	464.648	1.162	3.2
20	2869.469	7.178	10.2	59	844.372	2.112	3.0	98	461.593	1.155	3.0
21	2867.331	7.173	15.3	60	830.014	2.076	9.3	99	388.580	0.972	5.3
22	2865.498	7.168	10.0	61	827.570	2.070	10.7	100	377.277	0.944	3.9
23	2861.832	7.159	8.7	62	824.516	2.063	8.7	101	11.605	0.029	5.4
24	2859.999	7.154	8.9	63	815.045	2.039	8.7				
25	2854.500	7.141	5.1	64	811.685	2.030	8.1				
26	2852.973	7.137	4.9	65	801.298	2.004	3.1				
27	2847.169	7.122	8.7	66	797.938	1.996	2.8				
28	2835.866	7.094	4.1	67	705.680	1.765	5.3				
29	2834.033	7.089	4.8	68	702.014	1.756	5.5				
30	2829.450	7.078	8.6	69	693.155	1.734	7.9				
31	2827.312	7.072	11.0	70	683.684	1.710	7.8				
32	2826.395	7.070	8.9	71	680.935	1.703	7.7				
33	2823.340	7.063	13.1	72	672.076	1.681	8.1				
34	2819.980	7.054	12.2	73	667.493	1.670	8.1				
35	2818.453	7.050	12.9	74	616.171	1.541	4.3				
36	2816.925	7.047	13.5	75	608.839	1.523	12.5				
37	2812.037	7.034	8.3	76	596.314	1.492	2.8				
38	2810.204	7.030	14.6	77	593.259	1.484	2.8				
39	2808.371	7.025	9.2	78	578.596	1.447	3.5				

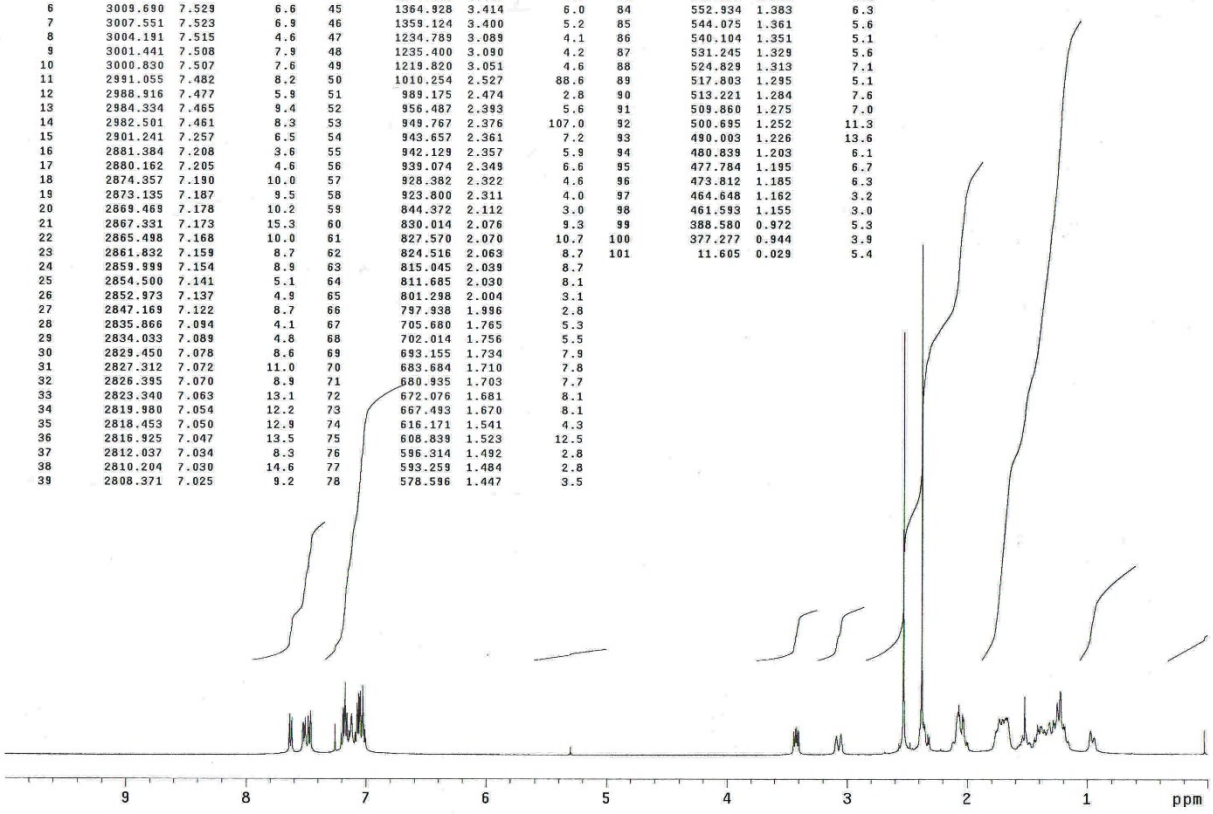


Figure S28. ^{1}H NMR (400 MHz) spectrum of (4aR,9S,10R)-11-cyclohexylidene-9-methyl-4a-(3-methyl-1*H*-indol-2-*yl*)-2,3,4,4a,9,9a-hexahydro-1*H*-9,10-methanoacridine (**27**) (Acetone-d6)

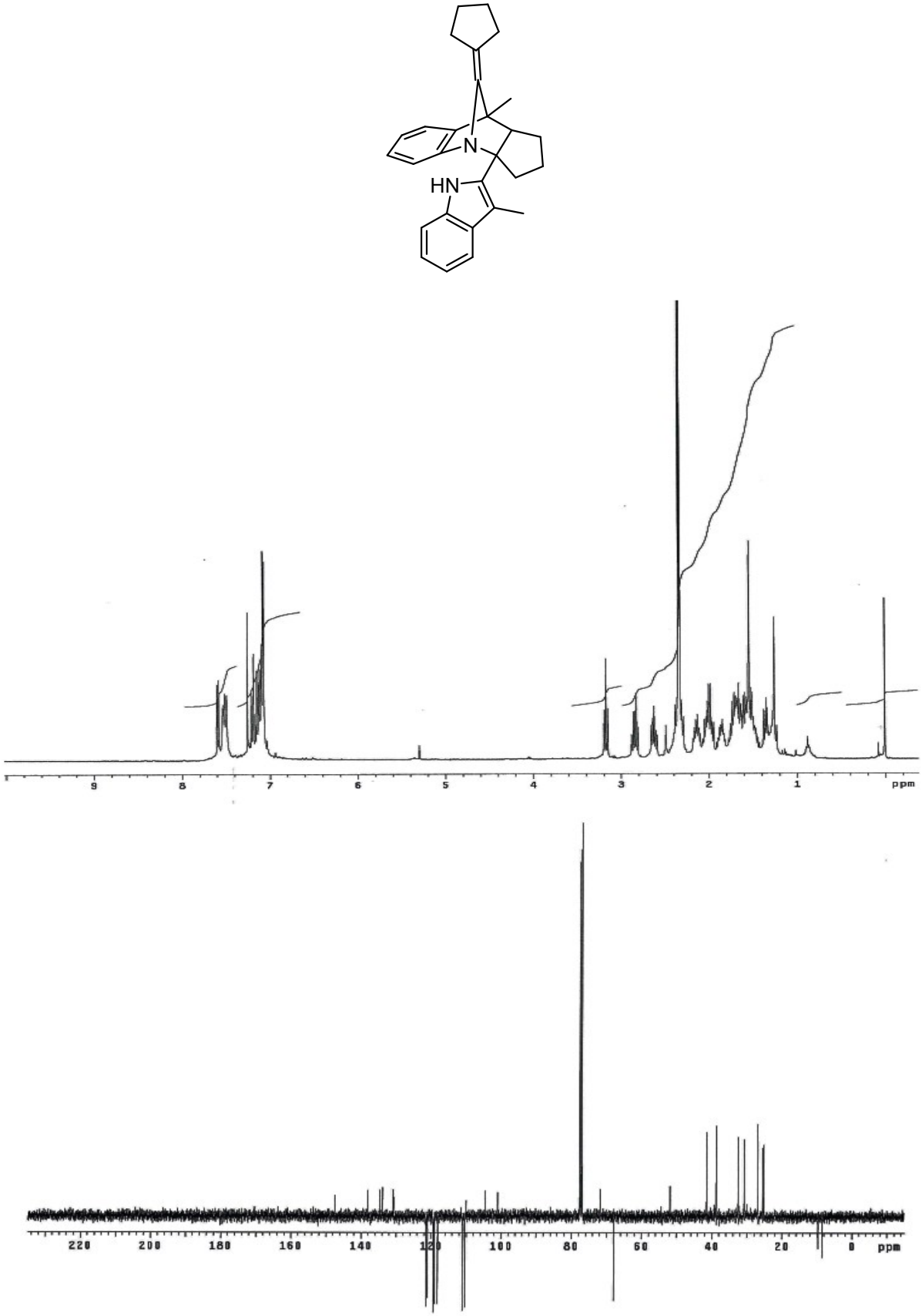


Figure S29. ^{1}H NMR (400 MHz) and APT NMR (100 MHz) spectra of (3aR,4R,9S,9aS)-10-cyclopentylidene-9-methyl-3a-(3-methyl-1*H*-indol-2-*yl*)-1,2,3,3a,9,9a-hexahydro-4,9-methanocyclopenta[b]quinolone (**35**) ($CDCl_3$)

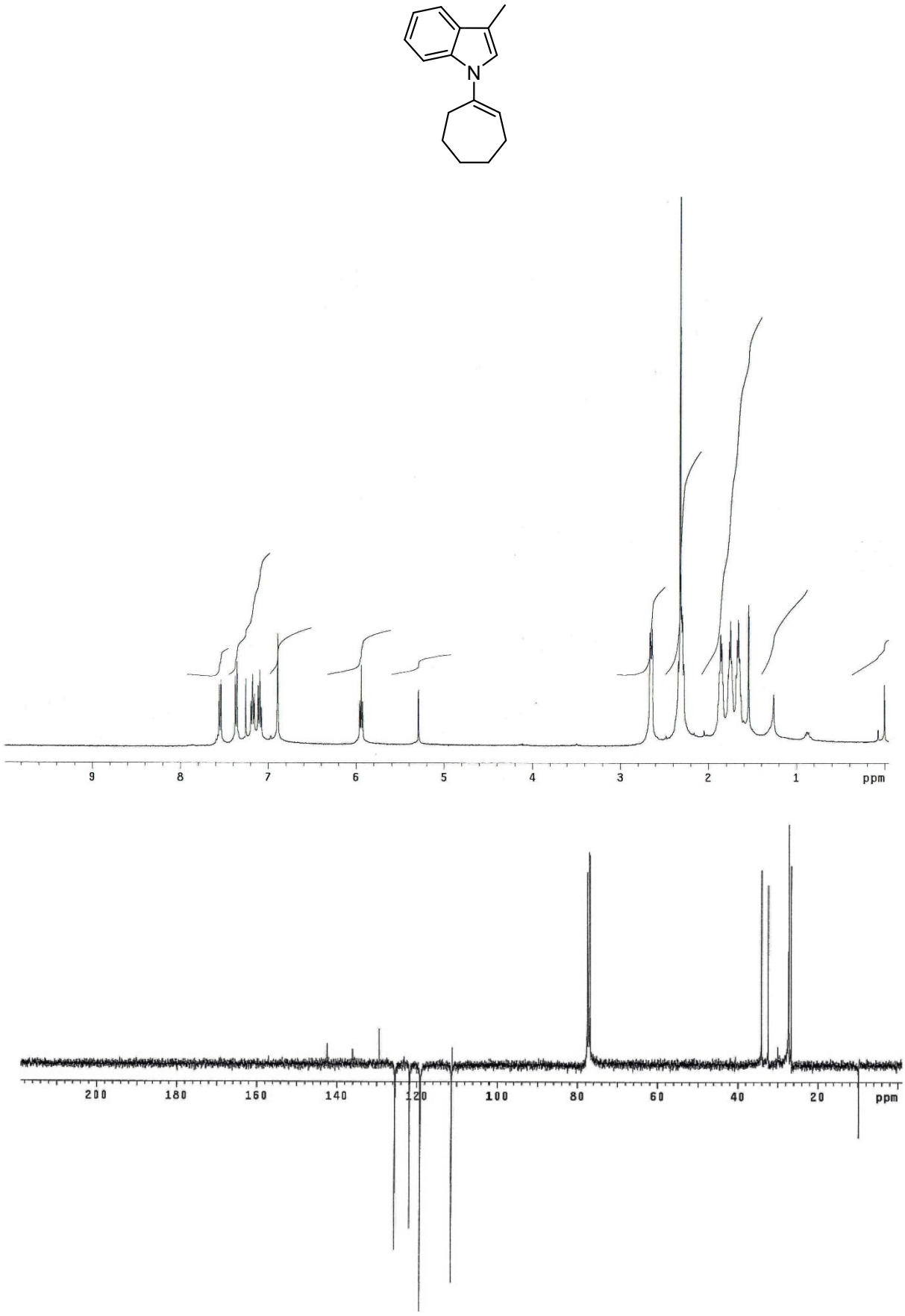
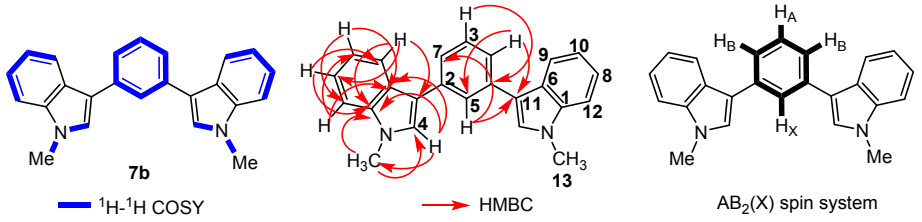


Figure S30. ^{1}H NMR (400 MHz) and APT NMR (100 MHz) spectra of 1-(cyclohept-1-en-1-*yl*)-3-methyl-1*H*-indole (**36**) ($CDCl_3$)

Full analysis for 7b.

Selected 2D NMR correlations for **7b**: The symmetrical structure of this molecule was further constructed by the ^{1}H-^{1}H COSY (H-7/H-3 ; H-9/H-10 ; H-10/H-8 ; H-8/H-12 ; H-13/H-4) and HMBC correlations from H-3 to C-2 (H-5/C-11; H-5/C-7; H-7/C-5; H-7/C-11) and from H-13 to C-4 (H-4/C-1; H-4/C-2; H-4/C-6; H-4/C-13; H-7/C-5; H-7/C-11; H-8/C-1; H-8/C-9; H-9/C-1; H-9/C-8; H-9/C-11; H-10/C-6; H-10/C-12; H-12/C-6; H-12/C-10; H-13/C-1) and ^{13}C NMR (DEPT-135) data.



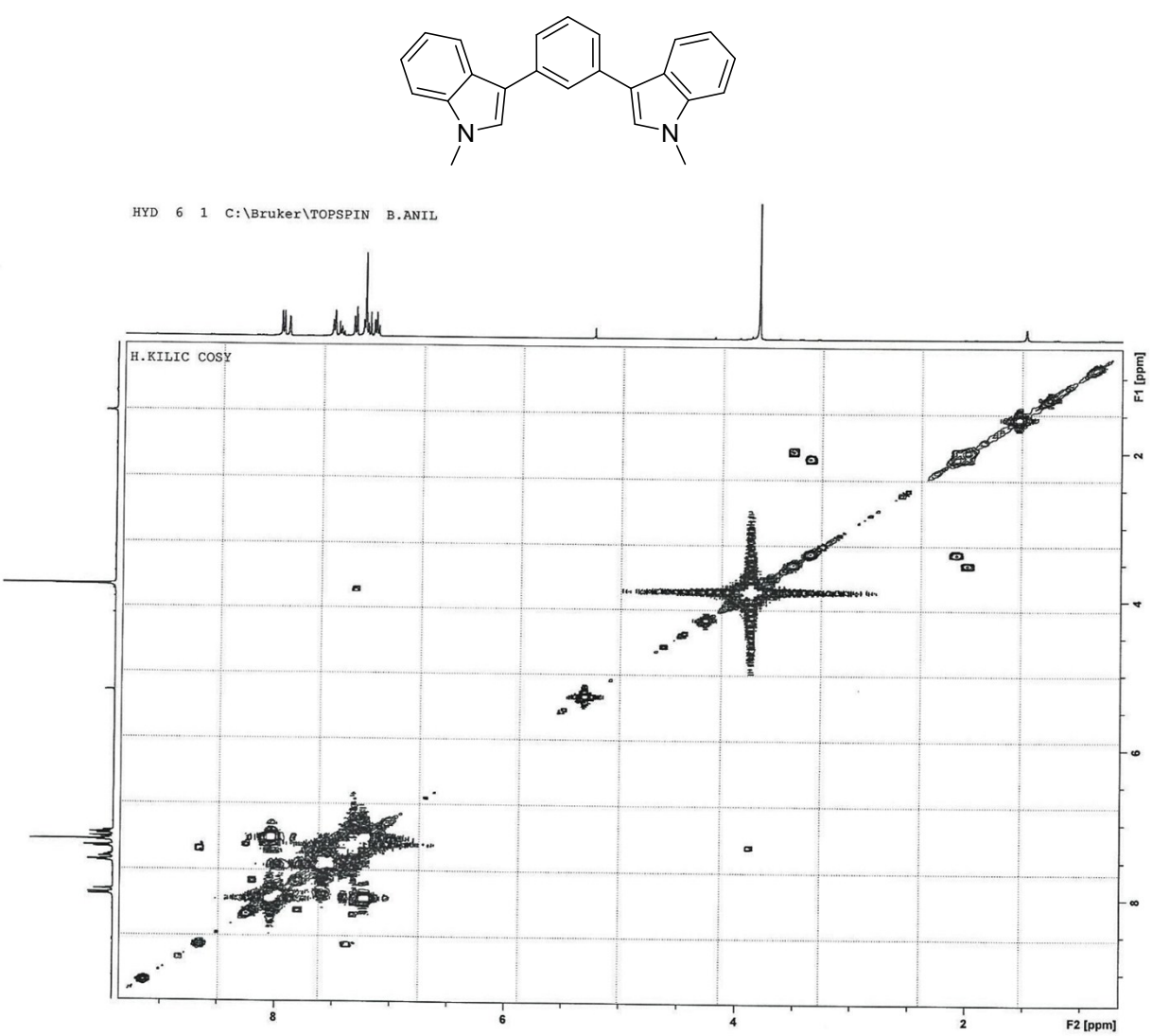


Figure S31. COSY spectrum of 1,3-bis(1-methyl-1*H*-indol-3-*yl*)benzene (**7b**) ($CDCl_3$)

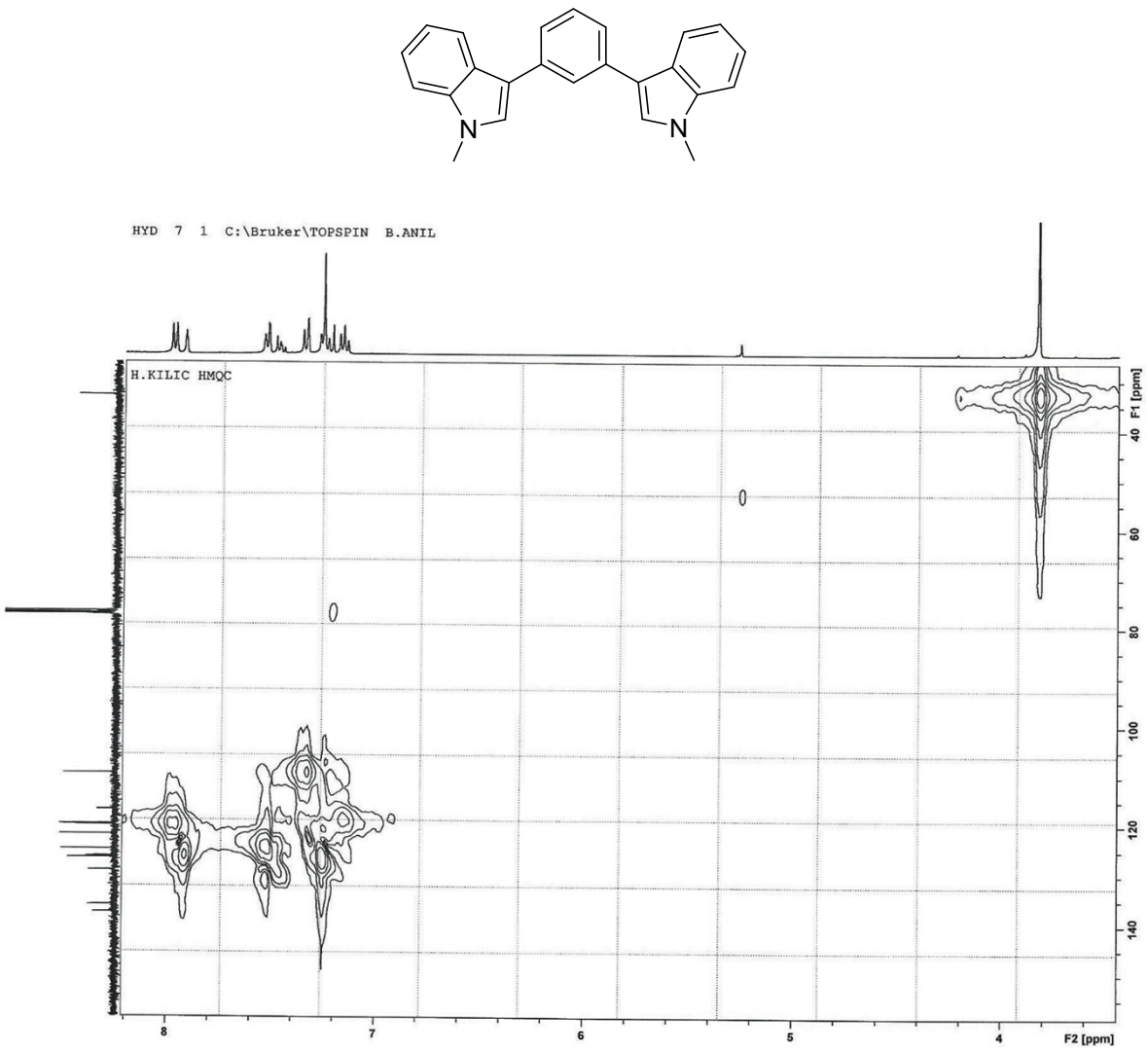
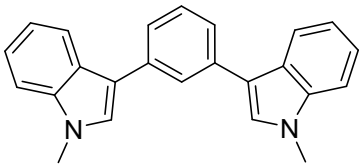


Figure S32. HMQC spectrum of 1,3-bis(1-methyl-1*H*-indol-3-*yl*)benzene (**7b**) ($CDCl_3$)



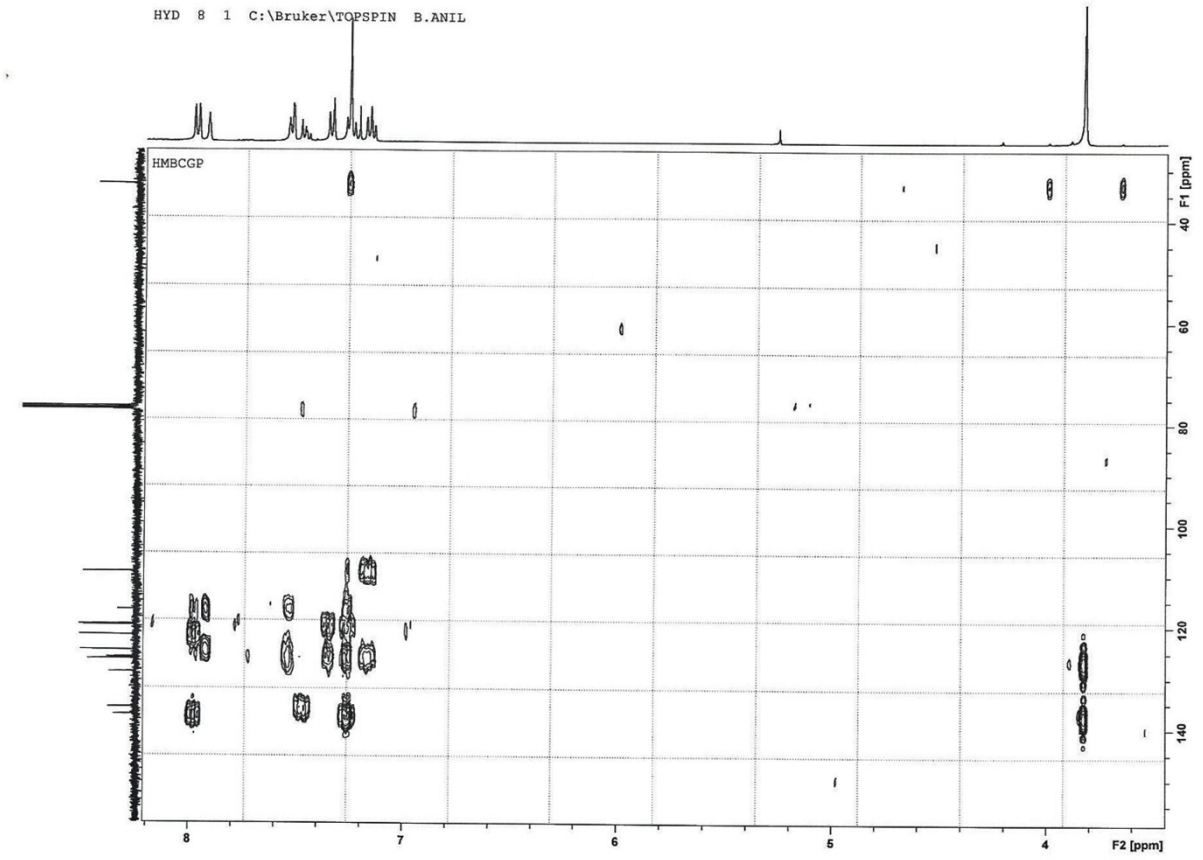
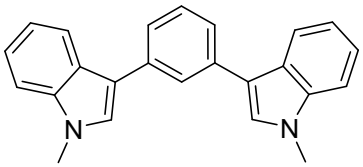


Figure S33. HMBC spectrum of 1,3-bis(1-methyl-1*H*-indol-3-*yl*)benzene (**7b**) ($CDCl_3$)



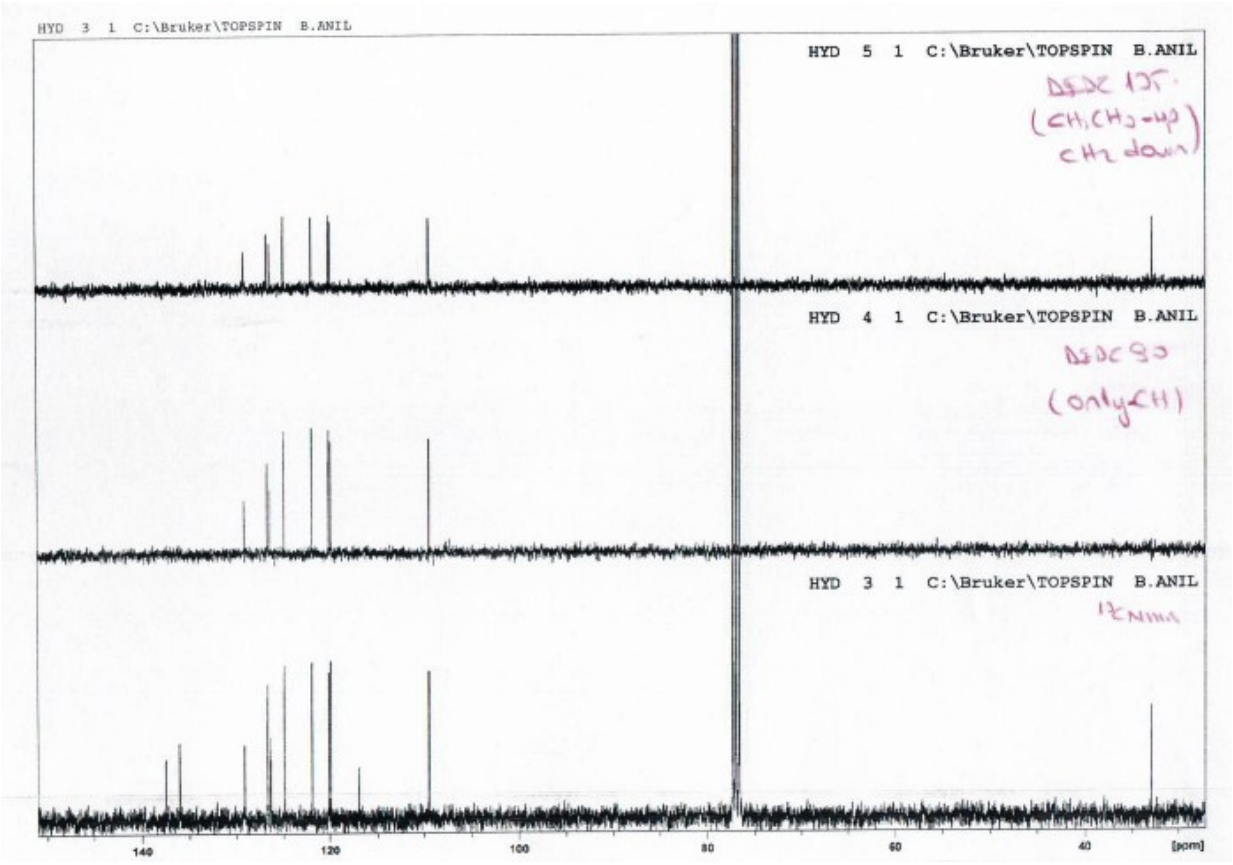


Figure S34. DEPT135, DEPT90 and ^{13}C NMR spectra of 1,3-bis(1-methyl-1*H*-indol-3-*yl*)benzene (**7b**) ($CDCl_3$)

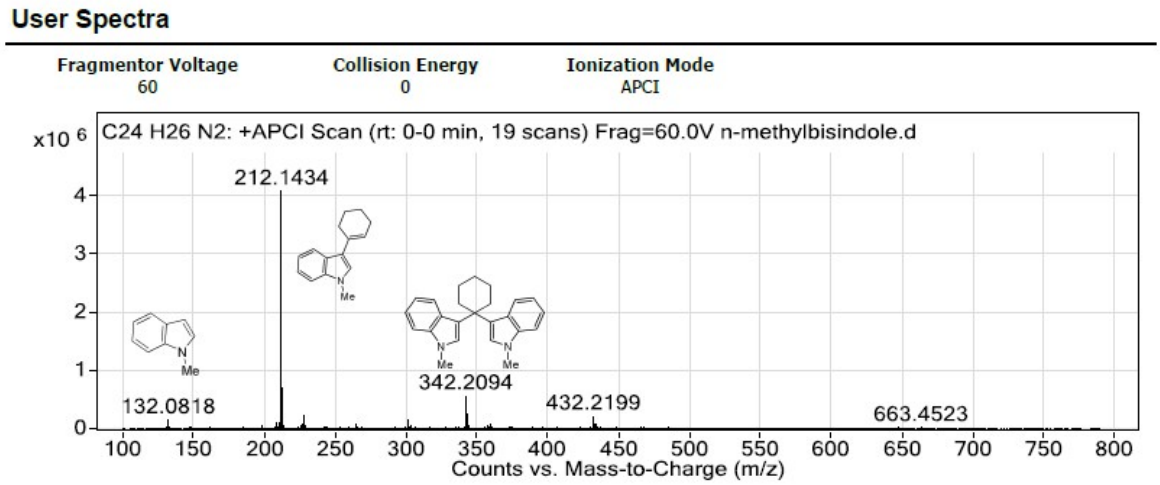


Figure S35. Mass spectrum of 3,3'-(cyclohexane-1,1-*diyl*)bis(1-methyl-1*H*-indole) (**13b**)

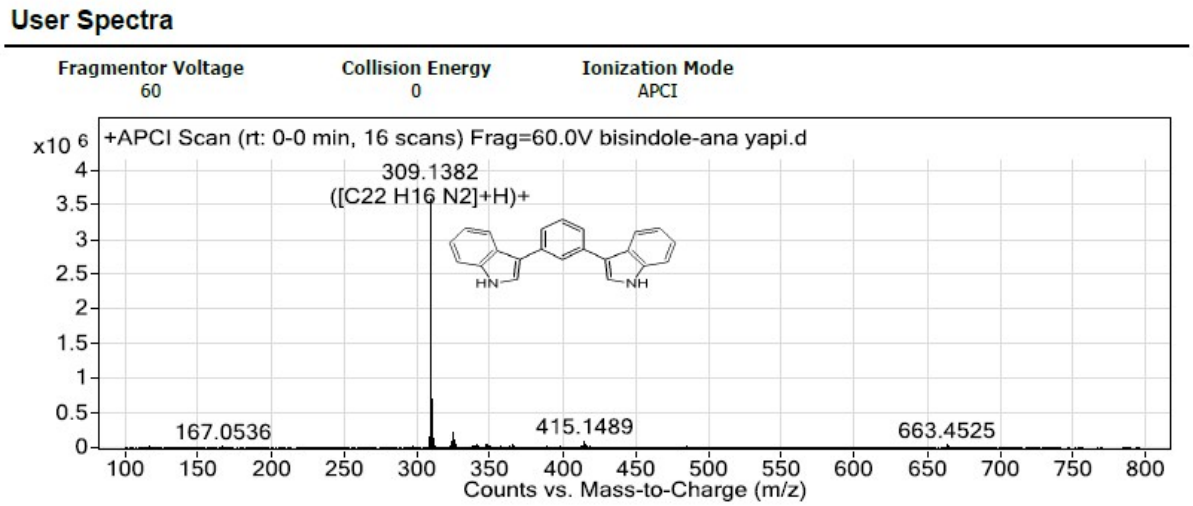


Figure S36. Mass spectrum of 1,3-di(1*H*-indol-3-*yl*)benzene (**7a**)

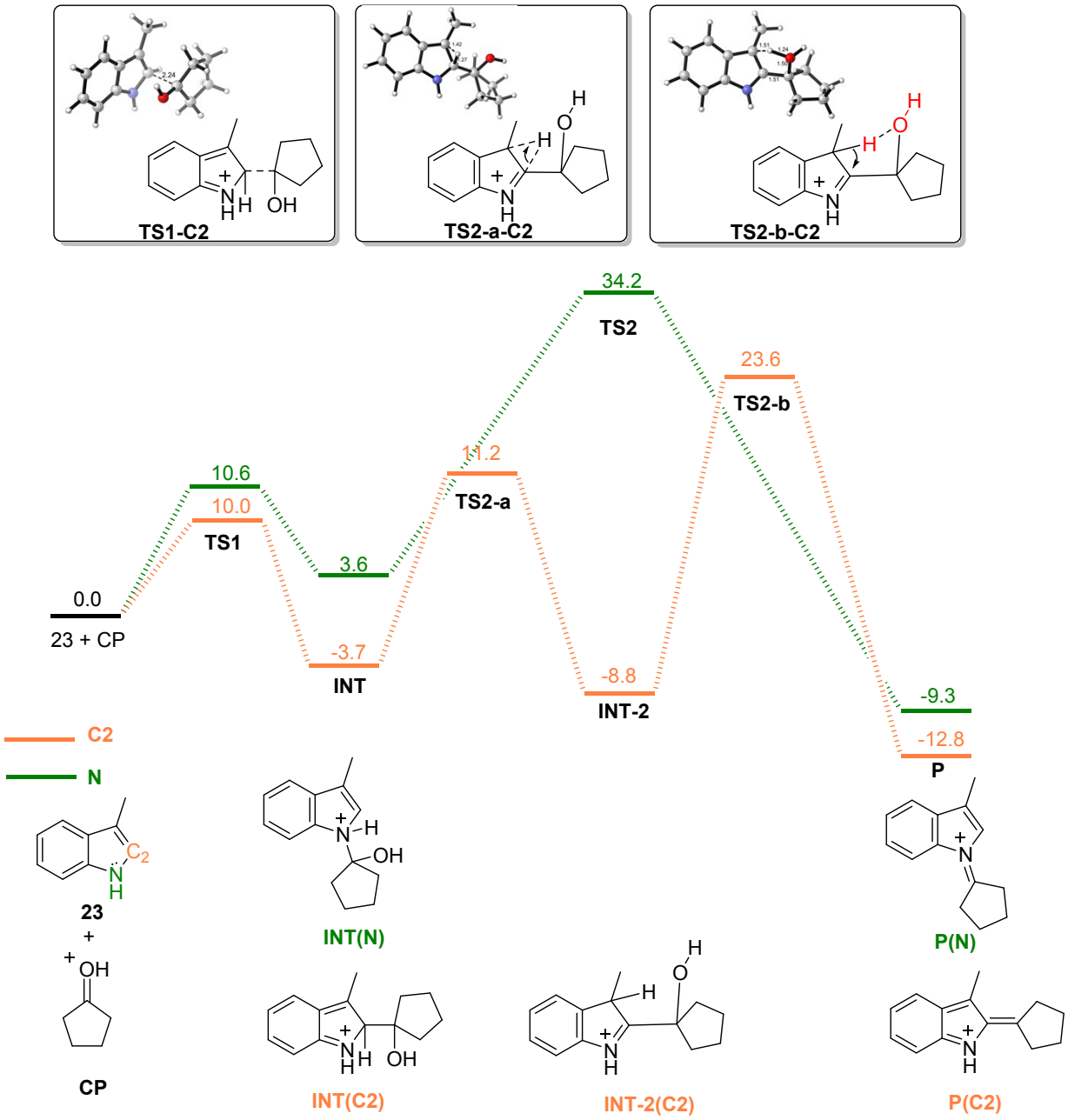


Figure S37. Gibbs Free energy profile for reaction between **23** and cyclopentanone (M06-2X/6-31+G(d,p) in cyclohexanone)

COMPUTATIONAL CALCULATIONS USING GAUSSIAN 09

Optimized geometries and energetics calculated with M062X/6-31+G(d,p) in cyclohexanone (ε = 18.2, IEFPCM) are given below.

8b

Electronic Energy= -402.9789228

Sum of electronic and thermal Free Energies= -402.851931

H	2.22047200	2.13730100	0.00001900
C	1.78658400	1.14126800	0.00002500
C	0.66575500	-1.47558400	-0.00001700
C	0.38995400	0.97726000	0.00000200
C	2.59712700	0.01690200	0.00002600
C	2.03876200	-1.27949400	0.00000800
C	-0.15205600	-0.33624100	-0.00002600
H	3.67661900	0.13085400	0.00003200
H	2.69660200	-2.14294600	0.00000900
H	0.25127700	-2.47854900	-0.00002800
C	-0.72267800	1.88304700	-0.00006600
H	-0.68726500	2.96283500	-0.00011700
C	-1.85485900	1.11123700	0.00004500
H	-2.89638500	1.40444200	0.00007400
N	-1.52448200	-0.22414700	-0.00006400
C	-2.48393000	-1.31288600	0.00004700
H	-3.11442700	-1.26782500	-0.89106400
H	-3.11387800	-1.26815700	0.89156500
H	-1.94960400	-2.26197300	-0.00030400

11

Electronic Energy= -310.1726807

Sum of electronic and thermal Free Energies= -310.037783

C	1.04147400	-0.03087200	0.12005600
C	-1.07944900	-1.23827300	-0.30118400
C	-1.02176600	1.27703300	-0.29148500
C	-1.82266500	0.03530500	0.09347400
C	0.38220500	1.26610300	0.36694200
C	0.32240600	-1.29559200	0.35661400
H	-0.96375200	-1.28520700	-1.38906600
H	-0.90190300	1.32701400	-1.37858200
H	-2.01721900	0.03612700	1.17295600
H	0.25945300	1.33674200	1.45737500
H	0.19417400	-1.37211000	1.44608900
H	-1.62563300	-2.13162200	0.00770400
H	-1.52578400	2.19209600	0.02518200
H	-2.79363600	0.06098200	-0.40885400
H	1.00489400	2.10146600	0.03894400
H	0.92426600	-2.13838100	0.01531000
O	2.23087400	-0.11919000	-0.32288000
H	2.66491400	0.74419100	-0.47052800

8b-TS1-C2

Electronic Energy= -713.1541244

Sum of electronic and thermal Free Energies= -712.868432

H	2.65736400	-2.76707800	-0.57515200
C	2.74615400	-1.71178800	-0.33891600
C	2.97513000	1.08836400	0.28670800
C	1.66273200	-0.82607300	-0.60031900
C	3.88954900	-1.19313000	0.20896500
C	3.99722300	0.19890600	0.51722300
C	1.79234000	0.56395100	-0.28187300
H	4.73422400	-1.83975300	0.41971500
H	4.92323700	0.56188600	0.95189900
H	3.06912500	2.14045800	0.53160400
C	0.38482300	-0.99387600	-1.13700300
H	-0.05667800	-1.91084000	-1.50412500
C	-0.28522400	0.24752500	-1.03093000
H	-1.12416200	0.56892100	-1.63462200
N	0.65134000	1.20001100	-0.62248600
H	-1.20883700	-2.33194900	0.45305100
C	-1.92804700	-1.52213500	0.59382000
C	-2.15775200	0.98976800	0.88962500
C	-4.00036800	-0.35188700	-0.22112300
C	-3.30563900	1.00896400	-0.12318900
C	-3.00462800	-1.48317900	-0.49275500
C	-1.22773900	-0.19409400	0.76018600
H	-2.57794500	0.86486000	1.89930300
H	-4.52232200	-0.55860600	0.72207800
H	-2.94778800	1.31736700	-1.11203200
H	-2.54579300	-1.35579800	-1.48135400
H	-2.41607100	-1.69133800	1.56601000
H	-1.59551400	1.92450300	0.91047800
H	-4.75972400	-0.32333400	-1.00758400
H	-4.02017300	1.77558100	0.18875800
H	-3.51936100	-2.44724000	-0.51047800
O	-0.22558300	-0.13109500	1.63338500
H	0.22019400	-0.98769100	1.74144400
C	0.43040100	2.63253000	-0.50157500
H	0.43150600	2.93810700	0.54877200
H	1.21910400	3.16695300	-1.03508400
H	-0.52883400	2.88059300	-0.95542200

8b-INT(C2)

Electronic Energy= -713.169103

Sum of electronic and thermal Free Energies= -712.888764

H	-0.59450000	-2.60323200	1.54318500
C	-1.21254900	-1.94950500	0.93394200
C	-2.85058100	-0.25414100	-0.67423300
C	-1.05577000	-0.55278500	1.00201200
C	-2.16035100	-2.47507700	0.06931100
C	-2.96592000	-1.63609900	-0.73206100
C	-1.89401200	0.27201300	0.20732700
H	-2.28787400	-3.55069000	0.00211500
H	-3.69455200	-2.08057500	-1.40209700
H	-3.47789100	0.39048300	-1.28234900
C	-0.17016500	0.32761400	1.71034300
H	0.57597700	0.05806500	2.44421400
C	-0.51296500	1.60863500	1.34140100
H	-0.09546000	2.55447700	1.66058000
N	-1.54738500	1.58383500	0.44434400
H	0.55245500	-1.64660900	-1.06562400
C	1.52151200	-1.13770400	-1.02205500
C	2.42449600	1.25577200	-0.67122200
C	3.64415000	-0.74007300	0.30054200
C	3.27361200	0.73008400	0.49595900
C	2.39535600	-1.60917300	0.14933500
C	1.34151000	0.32884000	-1.06110200
H	3.05210700	1.31294800	-1.57737800
H	4.28076700	-0.84663500	-0.58702000
H	2.71343400	0.85458400	1.42827300
H	1.80099900	-1.57596200	1.06808700
H	2.04203400	-1.35037400	-1.97241700
H	2.01100100	2.25304300	-0.50546900
H	4.22853300	-1.08697500	1.15689300
H	4.16893000	1.35101800	0.56976600
H	2.66308300	-2.65310900	-0.02710300
O	0.30498800	0.85466200	-1.58684500
H	-0.37673600	0.19987600	-1.84629400
C	-2.15393500	2.73274100	-0.20425500
H	-1.97353400	2.70476400	-1.28294900
H	-3.23038400	2.74379800	-0.01842900
H	-1.71291900	3.64012700	0.20690000

8b-TS2-C2

Electronic Energy= -713.1137111

Sum of electronic and thermal Free Energies= -712.830954

H	2.85960000	-2.72276500	-0.74144800
C	2.91873500	-1.70779100	-0.36287400
C	3.05972800	0.98620000	0.62668500
C	1.76913900	-0.87209200	-0.37845100
C	4.08489300	-1.19527700	0.14086700
C	4.14678400	0.14492200	0.63005400
C	1.84570000	0.46024500	0.12456500
H	4.98079800	-1.80529400	0.17107000
H	5.09076100	0.51024200	1.02195500
H	3.13008900	1.99618500	1.01353300
C	0.45860000	-1.06062400	-0.82071800
H	0.04651900	-1.96689000	-1.24380000
C	-0.24581400	0.15367400	-0.63739700
H	-0.55947900	0.67225800	-1.87607000
N	0.64144000	1.06176900	-0.00631500
H	-1.94528700	2.05330000	0.64633100
C	-2.41592200	1.08550500	0.48199000
C	-2.50373600	-0.97749300	-0.92897800
C	-3.12277700	-1.09741900	1.52346400
C	-2.54226300	-1.85576000	0.32811500
C	-2.38183900	0.22203900	1.74769900
C	-1.76999700	0.33447900	-0.67032000
H	-3.53025300	-0.71493300	-1.21648300
H	-4.18431700	-0.88566600	1.34091800
H	-1.52788500	-2.19443800	0.57297600
H	-1.33646900	0.02169000	2.02336800
H	-3.45578700	1.28163100	0.19220900
H	-2.05932300	-1.50838700	-1.77734600
H	-3.06919600	-1.72092200	2.42066900
H	-3.13131400	-2.75128000	0.11197300
H	-2.82857900	0.78062800	2.57459900
O	-1.77132800	1.17063600	-1.91756500
H	-2.43533200	0.89320700	-2.57490600
C	0.43928000	2.49424600	0.19736500
H	-0.32107100	2.85822600	-0.49254800
H	0.14144400	2.70283600	1.22762400
H	1.37255100	3.01378000	-0.02229300

8b-P(C2)

Electronic Energy= -636.496340

Sum of electronic and thermal Free Energies= -636.496340

H	2.91488200	-2.83634000	0.12444000
C	2.98791100	-1.75451700	0.15333800
C	3.15204100	1.12126600	0.22306200
C	1.82803200	-0.95496500	-0.06753600
C	4.17335400	-1.11772500	0.38876500
C	4.24548400	0.31247200	0.42003200
C	1.91695100	0.47611800	-0.01224200
H	5.07926100	-1.68865400	0.55792400
H	5.20813000	0.77455700	0.61522000
H	3.23629100	2.20030800	0.27261300
C	0.51347100	-1.26142000	-0.37284800
H	0.08746600	-2.25053300	-0.46374300
C	-0.21794700	-0.03514200	-0.44251200
N	0.69689700	1.01525000	-0.22643700
H	-1.77438400	2.07158000	0.25492200
C	-2.39071800	1.24669900	-0.09149800
C	-2.41596800	-1.11784200	-0.93401800
C	-4.24636400	-0.34701900	0.62644700
C	-3.39747100	-1.53453100	0.18223600
C	-3.36018600	0.82177600	1.04381700
C	-1.59268800	0.05647300	-0.51172900
H	-3.00266800	-0.78383700	-1.80183200
H	-4.90295400	-0.03587400	-0.19607500
H	-2.82276400	-1.92408800	1.03147800
H	-2.76891400	0.54625100	1.92515300
H	-2.98594700	1.58859700	-0.94888600
H	-1.80641400	-1.95819800	-1.26280500
H	-4.89072500	-0.63876500	1.46147300
H	-4.02169900	-2.35014000	-0.19207100
H	-3.95738400	1.69653600	1.31382500
C	0.49668200	2.43807500	-0.49887000
H	-0.28213800	2.55866700	-1.25018400
H	0.23318900	2.98145300	0.41056000
H	1.42298100	2.84342300	-0.90562100

8b-TS1-C3

Electronic Energy= -713.1618557

Sum of electronic and thermal Free Energies= -712.877376

H	1.86500000	-2.61804400	-0.95448700
C	2.13252600	-1.66059700	-0.51702800
C	2.88094200	0.85397800	0.60178800
C	1.34597700	-0.52351100	-0.74922700
C	3.27395800	-1.52869700	0.26669000
C	3.64187900	-0.28849600	0.82005200
C	1.74037600	0.70836700	-0.18750400
H	3.89860900	-2.39635500	0.45224600
H	4.53907200	-0.22234400	1.42633800
H	3.16253300	1.81123400	1.02862300
C	0.08288400	-0.29454200	-1.41631900
H	-0.38104900	-0.93918700	-2.14918800
C	-0.14376700	1.08317000	-1.32184000
H	-0.93268000	1.68060800	-1.76018100
N	0.80134800	1.66766100	-0.56466900
H	-2.41785600	-1.82361900	-1.50277300
C	-2.58711500	-1.33328800	-0.54150800
C	-1.17470800	-0.24868000	1.34833200
C	-3.46371700	0.65883500	0.71547700
C	-2.07371800	0.98982600	1.26149800
C	-3.36930900	-0.02754100	-0.64831200
C	-1.30282400	-1.21724800	0.21502900
H	-1.47282100	-0.84652400	2.22456900
H	-3.99044700	-0.00102700	1.41733800
H	-1.60975200	1.75272200	0.63045500
H	-2.89637700	0.63955800	-1.37689400
H	-3.16630300	-2.04743100	0.06655100
H	-0.12007100	0.01122100	1.50766100
H	-4.05268500	1.57652900	0.63561800
H	-2.14659100	1.42176700	2.26298300
H	-4.36557600	-0.25572000	-1.03550800
O	-0.65185900	-2.35089300	0.29331700
H	0.11091100	-2.30189700	0.89772000
C	0.85023000	3.06778700	-0.17005300
H	0.74567500	3.15504400	0.91436400
H	1.80088600	3.50366400	-0.48302800
H	0.03326100	3.59715200	-0.65871600

8b-INT(C3)

Electronic Energy= -713.1835761

Sum of electronic and thermal Free Energies= -712.895590

H	1.57187800	-2.71624900	-0.51775700
C	1.97521500	-1.74948400	-0.23940700
C	3.10761000	0.77796300	0.42201000
C	1.24936800	-0.58175600	-0.44220200
C	3.25717700	-1.64532000	0.30838100
C	3.81278800	-0.40590500	0.64023400
C	1.84010900	0.63884800	-0.11890700
H	3.83692100	-2.54734300	0.47310800
H	4.81061000	-0.35935600	1.06221200
H	3.53538700	1.74596900	0.65877000
C	-0.13308200	-0.31219000	-0.98234800
H	-0.23172400	-0.64483300	-2.02539400
C	-0.16250100	1.17794000	-0.96788600
H	-0.94514000	1.83086900	-1.33380600
N	0.92647800	1.67610800	-0.47763200
H	-2.56921500	-0.99323000	-1.95655500
C	-2.66557100	-0.84379100	-0.87520600
C	-1.35552800	-0.67772100	1.27952400
C	-3.41170200	0.74352300	0.95001900
C	-2.01081000	0.67742100	1.55970000
C	-3.37047500	0.47935700	-0.55645400
C	-1.30023100	-1.05175800	-0.20624900
H	-1.95878000	-1.45577100	1.76574100
H	-4.04376600	-0.01466100	1.43130200
H	-1.39717500	1.50127600	1.17054900
H	-2.89588100	1.32428300	-1.06748200
H	-3.28974000	-1.66284200	-0.49879600
H	-0.35040400	-0.73000700	1.71704000
H	-3.86863800	1.71735700	1.15064100
H	-2.05530100	0.82792400	2.64250600
H	-4.38640400	0.43001200	-0.96011800
O	-1.00284300	-2.43303200	-0.35516100
H	-0.53964100	-2.75185100	0.43054100
C	1.23268600	3.09510400	-0.30209400
H	1.39273000	3.28337900	0.76051200
H	2.13680100	3.32879400	-0.86519700
H	0.39456600	3.68439200	-0.66779100

8b-TS2-C3

Electronic Energy= -713.1327195

Sum of electronic and thermal Free Energies= -712.851078

H	2.85960000	-2.72276500	-0.74144800
C	2.91873500	-1.70779100	-0.36287400
C	3.05972800	0.98620000	0.62668500
C	1.76913900	-0.87209200	-0.37845100
C	4.08489300	-1.19527700	0.14086700
C	4.14678400	0.14492200	0.63005400
C	1.84570000	0.46024500	0.12456500
H	4.98079800	-1.80529400	0.17107000
H	5.09076100	0.51024200	1.02195500
H	3.13008900	1.99618500	1.01353300
C	0.45860000	-1.06062400	-0.82071800
H	0.04651900	-1.96689000	-1.24380000
C	-0.24581400	0.15367400	-0.63739700
H	-0.55947900	0.67225800	-1.87607000
N	0.64144000	1.06176900	-0.00631500
H	-1.94528700	2.05330000	0.64633100
C	-2.41592200	1.08550500	0.48199000
C	-2.50373600	-0.97749300	-0.92897800
C	-3.12277700	-1.09741900	1.52346400
C	-2.54226300	-1.85576000	0.32811500
C	-2.38183900	0.22203900	1.74769900
C	-1.76999700	0.33447900	-0.67032000
H	-3.53025300	-0.71493300	-1.21648300
H	-4.18431700	-0.88566600	1.34091800
H	-1.52788500	-2.19443800	0.57297600
H	-1.33646900	0.02169000	2.02336800
H	-3.45578700	1.28163100	0.19220900
H	-2.05932300	-1.50838700	-1.77734600
H	-3.06919600	-1.72092200	2.42066900
H	-3.13131400	-2.75128000	0.11197300
H	-2.82857900	0.78062800	2.57459900
O	-1.77132800	1.17063600	-1.91756500
H	-2.43533200	0.89320700	-2.57490600
C	0.43928000	2.49424600	0.19736500
H	-0.32107100	2.85822600	-0.49254800
H	0.14144400	2.70283600	1.22762400
H	1.37255100	3.01378000	-0.02229300

8b-P(C3) / 15b

Electronic Energy= -636.7781253

Sum of electronic and thermal Free Energies= -636.517516

H	-0.29966400	-2.60499400	0.18824600
C	-1.13774000	-1.92645000	0.10135900
C	-3.40760400	-0.24500800	-0.21995500
C	-0.98206200	-0.53783200	0.14558500
C	-2.41503300	-2.45397400	-0.08145400
C	-3.53700600	-1.63070000	-0.23376000
C	-2.12687700	0.25635500	-0.03449500
H	-2.53900900	-3.53116300	-0.11163300
H	-4.51603600	-2.07538900	-0.37409900
H	-4.26454300	0.40652100	-0.35293200
C	0.14845000	0.39936800	0.28741700
C	-0.43971100	1.70571300	0.15608100
H	0.03770800	2.67455900	0.21408000
N	-1.73599500	1.61425300	-0.01116600
C	2.49883100	1.29965200	0.47952300
C	2.08089500	-1.13874800	0.79937200
C	4.10897600	-0.39920700	-0.51343300
C	3.04379600	-1.48413100	-0.36266800
C	3.47444800	0.98040100	-0.68174400
C	1.48125600	0.20412600	0.54581800
H	2.66994900	-1.07091900	1.72330400
H	4.75242200	-0.39776300	0.37566700
H	2.46592700	-1.57764100	-1.29036400
H	1.33148500	-1.91214600	0.94441100
H	4.74819400	-0.62110400	-1.37358400
H	3.49871700	-2.45769100	-0.16131800
C	-2.67552500	2.72254900	-0.14929900
H	-2.12496400	3.65939100	-0.09396700
H	-3.40715700	2.66989300	0.65831300
H	-3.17908800	2.64270400	-1.11381600
H	3.06469300	1.30822900	1.41889200
H	2.06194900	2.28768500	0.33861200
H	2.92237800	1.02527400	-1.62842700
H	4.23844600	1.76209200	-0.71330900

8b-TS3-C3

Electronic Energy= -713.1513212

Sum of electronic and thermal Free Energies= -712.874979

H	-0.42392600	-2.54321200	0.14471800
C	-1.29990400	-1.90633100	0.09901100
C	-3.64947800	-0.30086400	0.01266800
C	-1.18626500	-0.51723200	-0.09512000
C	-2.56255500	-2.46551400	0.23362600
C	-3.72744000	-1.67378000	0.18915000
C	-2.37309700	0.25308300	-0.12367600
H	-2.65608000	-3.53703300	0.37844500
H	-4.69861700	-2.14508300	0.29891800
H	-4.54049400	0.31830400	-0.01456200
C	-0.09154500	0.42089600	-0.25022400
C	-0.67704300	1.67493900	-0.36955800
H	-0.20809300	2.63502200	-0.54248200
N	-2.02485900	1.58024900	-0.29857900
H	1.88189100	2.11936800	0.32027700
C	2.25183300	1.12061300	0.08220100
C	1.80792300	-1.20883700	-0.71420700
C	4.17355500	-0.48110300	-0.27451400
C	3.24195600	-1.20220700	-1.24587200
C	3.74533500	0.97784400	-0.11449900
C	1.33559700	0.16702500	-0.29921400
H	1.73834500	-1.87617300	0.15716600
H	4.14370600	-0.98763300	0.69948800
H	3.26482600	-0.69410900	-2.21806800
H	4.02421500	1.54894600	-1.01011700
H	1.90746000	0.51549700	1.40854800
H	1.11202800	-1.60279000	-1.46071600
H	5.20879600	-0.52614700	-0.62397100
H	3.57114000	-2.23170400	-1.41169500
H	4.27140300	1.44881600	0.72262200
C	-2.97722900	2.67092300	-0.42403600
H	-2.42939000	3.60283400	-0.55648500
H	-3.58841200	2.73759100	0.47900700
H	-3.62386100	2.50531300	-1.28894700
O	1.72818800	0.18648700	2.54219900
H	2.44088800	0.47051600	3.13945800
H	0.88282400	0.51130700	2.89643900

16b+H_3O^+

Electronic Energy= -713.1519566

Sum of electronic and thermal Free Energies= -712.872672

H	-0.35370300	-2.51276600	0.03581800
C	-1.24220200	-1.89134700	0.01281500
C	-3.61871200	-0.32310200	-0.02706700
C	-1.15128600	-0.49319200	-0.12758000
C	-2.49475600	-2.47702500	0.11935200
C	-3.67321300	-1.70235900	0.09823400
C	-2.35139900	0.26039800	-0.13612000
H	-2.57150900	-3.55479700	0.22202600
H	-4.63685300	-2.19389300	0.18462100
H	-4.52087100	0.28045400	-0.03837400
C	-0.07045100	0.46213300	-0.24402400
C	-0.66855000	1.70700700	-0.32449500
H	-0.21016800	2.67797000	-0.46103700
N	-2.02322200	1.59342200	-0.26150700
H	1.87229000	2.07317200	0.59860500
C	2.25928800	1.12978200	0.20947300
C	1.86489400	-1.09172900	-0.86805500
C	4.19939100	-0.42606700	-0.23100700
C	3.31762700	-1.00466900	-1.33593100
C	3.75830900	0.99863000	0.10803000
C	1.37411500	0.21663200	-0.27901500
H	1.77118800	-1.88275700	-0.11071900
H	4.12283800	-1.06218200	0.66148400
H	3.37496200	-0.36061500	-2.22261400
H	4.10427300	1.69343400	-0.66979700
H	1.68216000	0.22475700	1.56617600
H	1.19994000	-1.37328000	-1.69071500
H	5.25099000	-0.42609100	-0.53129900
H	3.66669400	-1.99737200	-1.63381600
H	4.22095100	1.33913800	1.04094500
C	-2.98629200	2.67680700	-0.35154200
H	-2.44758200	3.61926000	-0.44202500
H	-3.60651700	2.70351200	0.54767300
H	-3.62540400	2.54248200	-1.22785600
O	1.39721400	-0.17234100	2.52923600
H	2.06241600	0.01438800	3.21748100
H	0.52818600	0.16857500	2.81166400

8b-TS4-C3

Electronic Energy= -1273.1161745

Sum of electronic and thermal Free Energies= -1272.586080

H	2.20756000	2.76097100	1.32048200
C	2.88469800	1.94932300	1.08256100
C	4.69985200	-0.18135500	0.57083100
C	2.63343400	1.06822700	0.01341600
C	4.01793400	1.76226500	1.86155500
C	4.91851500	0.70825700	1.61290100
C	3.55704100	0.01651600	-0.20977700
H	4.21184100	2.44089700	2.68616600
H	5.79300600	0.59040500	2.24445300
H	5.38590700	-0.99831600	0.37040900
C	1.58006500	0.90330000	-0.97181700
C	1.93902300	-0.21408800	-1.72027000
H	1.42556300	-0.68013900	-2.55158900
N	3.10964600	-0.72926900	-1.28392800
H	-0.58741000	0.27220800	-2.44096800
C	-0.68249800	1.20703100	-1.89483400
C	0.23816500	3.00230800	-0.43963700
C	-2.14596500	3.17881000	-1.20692600
C	-0.79665100	3.88897300	-1.12888200
C	-1.99453500	1.78753300	-1.81280200
C	0.35709700	1.65599400	-1.12069700
H	-0.02917800	2.86487100	0.61850500
H	-2.56135000	3.10563800	-0.19328500
H	-0.44626200	4.12301700	-2.14073200
H	-2.67257800	1.54305100	-2.63286500
H	1.21647000	3.49144000	-0.45612800
H	-2.86379500	3.75653900	-1.79474500
H	-0.90024900	4.83407100	-0.58894800
H	-2.53013400	1.01511900	-0.93582700
C	3.81465600	-1.86610100	-1.84840700
H	3.19466100	-2.31096900	-2.62644700
H	4.00078900	-2.61154600	-1.07113400
H	4.76639900	-1.54389600	-2.27861600
H	-1.78340900	-2.43008000	-1.82532900
C	-0.95018300	-2.43650400	-1.13407800
C	1.28849900	-2.55862000	0.61361800
C	-0.85668500	-1.51950200	-0.07249800
C	0.05307000	-3.38339800	-1.30590200
C	1.15398900	-3.45715500	-0.43484400
C	0.28575600	-1.59874100	0.75781800
H	-0.02415800	-4.09076400	-2.12530500
H	1.90763400	-4.22299800	-0.58732600
H	2.14147600	-2.59341000	1.28492700
C	-1.66583900	-0.42132200	0.44370900
C	-0.92541400	0.10522100	1.51526600
H	-1.16457700	0.93235800	2.17116400
N	0.20707600	-0.58662900	1.70529300

H	-3.10255700	1.62263100	1.56778700
C	-3.73087200	0.94876200	0.97956500
C	-3.84039300	-0.74725300	-0.85304500
C	-5.39869700	-0.96372500	1.11014200
C	-4.58820000	-1.73206100	0.06339100
C	-4.52400100	0.00506200	1.90888600
C	-2.92669000	0.10870000	0.00384800
H	-4.57351200	-0.09289100	-1.34045600
H	-6.19027400	-0.39768400	0.60146400
H	-3.86090100	-2.39071500	0.55565000
H	-3.81429500	-0.55856800	2.52741200
H	-4.43589800	1.56993500	0.41357700
H	-3.29599300	-1.26288700	-1.64334000
H	-5.89409700	-1.66304800	1.79128400
H	-5.24369700	-2.36398400	-0.54349300
H	-5.13851300	0.60792100	2.58451700
C	1.17208600	-0.39642800	2.77746700
H	2.18234600	-0.39861300	2.36126800
H	1.07084100	-1.19725300	3.51415500
H	0.98776100	0.56780500	3.25041900

12b

Electronic Energy= -637.5649843

Sum of electronic and thermal Free Energies= -637.295384

H	-0.23039200	2.25477000	-0.00025400
C	0.76050800	1.80978900	-0.00014000
C	3.38165600	0.70101600	0.00024000
C	0.92176300	0.41092500	-0.00015200
C	1.88439100	2.62330900	0.00009100
C	3.18436300	2.07369400	0.00029300
C	2.24210900	-0.11469900	-0.00000400
H	1.76452200	3.70225600	0.00014500
H	4.04401300	2.73660800	0.00049200
H	4.38057900	0.27486700	0.00038500
C	0.02209300	-0.71895300	-0.00018200
C	0.82329100	-1.83286700	-0.00051200
H	0.53865200	-2.87778700	-0.00074100
N	2.15630200	-1.48353400	-0.00017400
H	-1.66727500	-0.56502900	2.15203000
C	-2.06473400	-0.06120900	1.26333800
C	-2.06473300	-0.06046400	-1.26323600
C	-4.16269800	0.55655800	0.00024200
C	-3.59470800	-0.09878200	-1.26083200
C	-3.59470800	-0.09952000	1.26093100
C	-1.48066500	-0.71735500	-0.00014700
H	-1.72859400	0.98467000	-1.31431300
H	-3.89906800	1.62385100	0.00055600
H	-3.92795900	-1.14561800	-1.30270100
H	-3.92797000	-1.14637500	1.30220100
H	-1.72861300	0.98389500	1.31503500
H	-1.66728000	-0.56376700	-2.15222400
H	-5.25682300	0.49865300	0.00022800
H	-3.98545600	0.39440200	-2.15780100
H	-3.98544300	0.39315900	2.15818500
C	3.28678600	-2.38948400	0.00008300
H	3.90210700	-2.23647500	0.89161100
H	3.90321400	-2.23545800	-0.89049700
H	2.91489300	-3.41398000	-0.00074800
H	-1.80549600	-1.76966200	-0.00045100

17b

Electronic Energy= -635.5631308

Sum of electronic and thermal Free Energies= -635.326643

H	0.25840000	-2.57297300	-0.21058000
C	1.11612900	-1.91803800	-0.12796600
C	3.43800100	-0.27869000	0.00736700
C	0.98170000	-0.52888000	-0.02515900
C	2.39669200	-2.46726000	-0.14302200
C	3.54272000	-1.66444800	-0.07068800
C	2.15332900	0.24794900	0.02348600
H	2.50715700	-3.54378100	-0.21910100
H	4.52419200	-2.12568000	-0.08656200
H	4.31788300	0.35453100	0.04591200
C	-0.13850300	0.41773400	-0.00682100
C	0.46893800	1.71180000	0.03563600
H	0.00122500	2.68678000	0.07383800
N	1.78079200	1.60589600	0.06721100
C	-2.44279700	1.29164600	-0.13794700
C	-2.05611000	-1.19487000	0.08194100
C	-4.38874300	-0.28840600	-0.20334900
C	-3.49876100	-1.24357600	0.58389800
C	-3.76772600	1.06727000	-0.28432300
C	-1.50706000	0.20076000	-0.00039400
H	-1.98950200	-1.62956300	-0.92835800
H	-4.54480500	-0.65543100	-1.22926600
H	-3.51762900	-0.95840900	1.64175800
H	-1.41433400	-1.79740100	0.72857400
H	-5.38354500	-0.20944000	0.24431900
H	-3.87271000	-2.26748700	0.51455900
C	2.73882400	2.70370000	0.13470000
H	2.19359400	3.64535800	0.13762800
H	3.39471000	2.65794200	-0.73594900
H	3.32725700	2.61145700	1.04893500
H	-4.41621000	1.91601800	-0.48835900
H	-2.07103000	2.30666700	-0.21198100

23

Electronic Energy= -402.9895174

Sum of electronic and thermal Free Energies= -402.863996

H	0.25024000	-2.51502200	0.00016400
C	0.66952900	-1.51221300	0.00007800
C	1.78770600	1.10755000	0.00003000
C	-0.17472400	-0.38797300	-0.00002300
C	2.04303700	-1.32022300	0.00007100
C	2.59531900	-0.02056800	0.00002400
C	0.40130800	0.90776000	-0.00001900
H	2.70739200	-2.17871700	0.00011400
H	3.67438500	0.09884300	0.00001300
H	2.21216700	2.10691100	0.00006100
C	-1.60575900	-0.22330600	-0.00007700
C	-1.83103400	1.12812100	-0.00018300
H	-2.76788100	1.66834300	-0.00024300
N	-0.63208800	1.81210300	0.00015500
H	-0.53513500	2.81557800	-0.00198300
C	-2.62498900	-1.32043100	0.00013800
H	-2.52093600	-1.96096800	0.88261400
H	-2.52012200	-1.96200800	-0.88148400
H	-3.63784800	-0.90997200	-0.00056900

23+11 (pre-reactive complex)

Electronic Energy= -713.1769517

Sum of electronic and thermal Free Energies= -712.896089

H	2.03022300	-0.36036600	-2.47794700
C	1.95890100	-0.66018000	-1.43621800
C	1.76743000	-1.46567100	1.29149100
C	1.76877700	0.30495400	-0.43004400
C	2.06067300	-1.99644300	-1.07874200
C	1.96194700	-2.39676400	0.27440600
C	1.68256200	-0.11473300	0.92391400
H	2.20982500	-2.75155200	-1.84313800
H	2.04947100	-3.44854900	0.52747100
H	1.70552100	-1.77453800	2.33078200
C	1.65948600	1.74035200	-0.44214200
C	1.52391300	2.11913100	0.86818300
N	1.52357200	1.01079700	1.69036600
H	1.46383200	1.03537500	2.69751300
H	-3.02751500	-1.44536200	-1.81264100
C	-3.08200500	-0.91265800	-0.86311200
C	-1.77556700	-0.59005700	1.29816400
C	-3.06439700	1.35469800	0.29007900
C	-1.81648200	0.95105900	1.07133800
C	-3.12359700	0.63278600	-1.05433600
C	-1.90286000	-1.21405800	-0.03199500
H	-2.64984800	-0.88175000	1.89120600
H	-3.96300000	1.12526000	0.87551900
H	-0.91453000	1.25258000	0.52577700
H	-2.27789600	0.93385900	-1.68308800
H	-3.97701300	-1.22203700	-0.31167800
H	-0.86542600	-0.90590400	1.81101200
H	-3.05398200	2.43550600	0.12289300
H	-1.77947400	1.42682300	2.05405700
H	-4.03915600	0.87047800	-1.59970900
O	-0.98042200	-1.90676600	-0.56170000
H	-0.16947000	-2.02953500	-0.00572100
C	1.69749900	2.62262200	-1.65123900
H	0.88508800	2.37987400	-2.34444800
H	2.63954600	2.50577900	-2.19663100
H	1.59839100	3.67297200	-1.36778600
H	1.41610000	3.10939800	1.28910500

23-TS1-C2

Electronic Energy= -713.1652345

Sum of electronic and thermal Free Energies= -712.880158

H	-2.90645700	2.31391100	0.55057600
C	-2.91210500	1.25270200	0.32123000
C	-2.92709900	-1.55140500	-0.28418600
C	-1.77871600	0.64006700	-0.26802100
C	-4.01084300	0.47174700	0.58837500
C	-4.01184000	-0.91977900	0.28448100
C	-1.80147800	-0.75131000	-0.56413900
H	-4.89473100	0.91073500	1.03790900
H	-4.89990200	-1.50080400	0.51220000
H	-2.93705500	-2.61151000	-0.51204300
C	-0.52281400	1.14017800	-0.67501000
C	0.23400300	0.03055800	-1.10469200
N	-0.60595600	-1.08457400	-1.11775200
H	-0.37188900	-1.98807200	-1.50411700
H	1.32935200	1.69103200	1.28120000
C	2.00802500	0.85377300	1.11040300
C	2.06647600	-1.57699700	0.32088600
C	4.03403400	-0.04712200	-0.09544100
C	3.23177400	-1.24312500	-0.61322800
C	3.13469100	1.17131900	0.12438900
C	1.24427700	-0.38776000	0.75569600
H	2.47761400	-1.95256600	1.27146800
H	4.51769200	-0.31603700	0.85258400
H	2.86771300	-1.03992000	-1.62638700
H	2.72490900	1.49978100	-0.83792300
H	2.45176300	0.61433500	2.08977600
H	1.42645900	-2.37263200	-0.07134200
H	4.83024500	0.19822800	-0.80366900
H	3.86942800	-2.12780900	-0.68897600
H	3.71365300	2.01068500	0.51850500
O	0.22642700	-0.62942900	1.56332200
H	-0.09705000	-1.54222500	1.48721500
C	-0.10660100	2.57110100	-0.65253500
H	-0.24327700	3.01093300	0.34096900
H	-0.73992100	3.13834000	-1.34275000
H	0.92991000	2.70484800	-0.96243400
H	1.09111500	0.06252500	-1.76432000

23-INT(C2)

Electronic Energy= -713.1814083

Sum of electronic and thermal Free Energies= -712.895386

H	-3.36310300	2.23142300	-0.03052800
C	-3.24922400	1.15381600	-0.07435700
C	-2.93816300	-1.71929800	-0.18671100
C	-1.94556500	0.56690000	-0.19635600
C	-4.32358300	0.32216500	-0.01105200
C	-4.15703100	-1.10762400	-0.07257000
C	-1.80470700	-0.86864900	-0.24222100
H	-5.32559800	0.72377000	0.08334200
H	-5.04831000	-1.72582500	-0.02761800
H	-2.83409700	-2.79665600	-0.23227800
C	-0.69246200	1.11815800	-0.30457700
C	0.31173600	0.00894900	-0.40353100
N	-0.52010600	-1.18289500	-0.35042400
H	-0.17495900	-2.12155900	-0.50489600
H	1.95554500	2.09749400	0.53979500
C	2.43837900	1.11899600	0.52544200
C	2.16110700	-1.34329900	0.72948500
C	3.99035900	-0.42711400	-0.73854700
C	2.98795100	-1.56753600	-0.54050400
C	3.29684800	0.93763500	-0.73040500
C	1.41432800	-0.00262900	0.72249400
H	2.83319200	-1.30810300	1.59575600
H	4.72554100	-0.45823600	0.07628200
H	2.33297500	-1.64407300	-1.41960000
H	2.68714400	1.04832500	-1.63762100
H	3.08316500	1.08283600	1.41190200
H	1.46855800	-2.17290700	0.91326300
H	4.54132100	-0.56584700	-1.67368000
H	3.51019900	-2.52556100	-0.46371700
H	4.03988000	1.73979200	-0.76834100
O	0.77687800	0.22987900	1.96505700
H	0.34716300	-0.58137000	2.27015300
C	-0.37129400	2.56595300	-0.32291200
H	-0.05836600	2.87654200	0.68171300
H	-1.24735500	3.15328100	-0.60033200
H	0.44421000	2.78989500	-1.01390100
H	0.79652900	0.05949100	-1.38925800

23-TS2a-C2

Electronic Energy= -713.1565458

Sum of electronic and thermal Free Energies= -712.873161

H	3.54241000	1.86846900	0.72891500
C	3.29944300	0.85313200	0.43352000
C	2.65208800	-1.82707300	-0.35475300
C	1.98423400	0.50162400	0.06986800
C	4.25693900	-0.13738400	0.40882500
C	3.93127400	-1.45981900	0.01257400
C	1.67349400	-0.82216200	-0.30225800
H	5.27909500	0.09083000	0.68933100
H	4.71744800	-2.20783400	-0.00241500
H	2.41047400	-2.83919200	-0.65902800
C	0.77590700	1.26634700	-0.00438700
C	-0.24298600	0.35750500	-0.48249900
N	0.33833800	-0.88617700	-0.60510800
H	-0.10213300	-1.66923200	-1.06974400
H	-1.68851400	1.63238200	1.38369200
C	-2.28104000	0.84923100	0.90163200
C	-2.52300200	-0.55047100	-1.18930400
C	-3.22367600	-1.46766900	1.07633000
C	-2.71743700	-1.80794200	-0.32596900
C	-2.31926300	-0.42887800	1.73996800
C	-1.75411600	0.60125400	-0.52049200
H	-3.51431400	-0.13850100	-1.41681300
H	-4.24356800	-1.06554800	1.01345000
H	-1.78784500	-2.37916400	-0.22428600
H	-1.30383000	-0.83524800	1.85356800
H	-3.30399700	1.23642400	0.79769900
H	-2.06283400	-0.78611600	-2.15614800
H	-3.27339800	-2.37706700	1.68253900
H	-3.42118000	-2.46959200	-0.83953500
H	-2.67618300	-0.18923700	2.74558800
O	-1.85612100	1.78308900	-1.30970100
H	-2.76217100	2.11743300	-1.26309800
C	0.60179100	2.69158500	0.40488900
H	-0.32408700	3.10866500	0.01172200
H	1.45012600	3.28977800	0.06743100
H	0.57383100	2.72646000	1.49892700
H	0.28938100	1.10914100	-1.33610700

23-INT-2(C2)

Electronic Energy= -713.1938102

Sum of electronic and thermal Free Energies= -712.906538

H	3.79425600	1.83618300	-0.03958000
C	3.44236900	0.80959900	-0.03317500
C	2.54706500	-1.89583800	-0.01425300
C	2.09054400	0.51311000	-0.13618200
C	4.34251400	-0.25397300	0.07567500
C	3.90349000	-1.58267200	0.08415900
C	1.68408300	-0.81775900	-0.12003700
H	5.40431100	-0.04659900	0.15536300
H	4.62796600	-2.38494100	0.17101800
H	2.19360900	-2.92078600	-0.00740300
C	0.87187700	1.38898800	-0.24694600
C	-0.23571600	0.37289200	-0.31100600
N	0.26411500	-0.82438500	-0.23565100
H	-0.28498800	-1.67933700	-0.28239700
H	-1.70188200	1.35775900	1.64557600
C	-2.31711800	0.73359600	0.99146700
C	-2.48547200	-0.27296900	-1.33879400
C	-3.45147300	-1.48948500	0.67254200
C	-2.84586000	-1.63256600	-0.72426700
C	-2.55145400	-0.65522400	1.58490400
C	-1.70146400	0.69634300	-0.42915700
H	-3.42291000	0.25098800	-1.56373900
H	-4.42945900	-0.99722200	0.59192700
H	-1.98296000	-2.31006700	-0.68563200
H	-1.59449500	-1.16986100	1.75039400
H	-3.28487200	1.24089700	0.87991600
H	-1.95308000	-0.38676900	-2.28854600
H	-3.62447500	-2.47810900	1.10728200
H	-3.55241500	-2.12771900	-1.39690100
H	-3.00643600	-0.54184200	2.57289100
O	-1.68823700	1.99423500	-1.00376300
H	-2.58573500	2.35257300	-0.99061900
C	0.72424400	2.40610100	0.90158700
H	-0.18112800	2.99890900	0.77045900
H	1.58926300	3.07145400	0.88410700
H	0.70045400	1.89570400	1.86756000
H	0.84629400	1.93473100	-1.20111900

23-TS2b-C2

Electronic Energy= -713.1414866

Sum of electronic and thermal Free Energies= -712.859053

H	-3.57695300	1.98284600	-0.27104900
C	-3.35037200	0.92414500	-0.19464300
C	-2.78362300	-1.86737400	-0.01789500
C	-2.03084000	0.47698400	-0.04844700
C	-4.36422100	-0.02232200	-0.22961300
C	-4.08434100	-1.40029700	-0.13715600
C	-1.77591100	-0.90266200	0.01531100
H	-5.39474000	0.30162600	-0.33069200
H	-4.90319200	-2.11128500	-0.16747100
H	-2.56171100	-2.92728400	0.04117500
C	-0.74891100	1.17185100	0.00673100
C	0.21255800	0.12836300	0.07184600
N	-0.39580400	-1.06552000	0.11558900
H	0.05730900	-1.93430300	0.37283500
H	1.98716800	1.91858900	-0.94204700
C	2.51513200	1.09063600	-0.46334400
C	2.32842700	-0.77954500	1.22025700
C	3.74428600	-1.07806300	-0.85333300
C	2.86506600	-1.77758300	0.18367000
C	2.98822300	0.07589100	-1.51091200
C	1.62201400	0.40387000	0.56912800
H	3.17116000	-0.36454100	1.78525700
H	4.64641900	-0.68807900	-0.36419700
H	2.04296900	-2.28450500	-0.33774400
H	2.11960600	-0.31368600	-2.06014200
H	3.38615600	1.50068500	0.06352300
H	1.66429600	-1.25821400	1.94731600
H	4.07252600	-1.79585600	-1.61047900
H	3.42367200	-2.55733900	0.70813000
H	3.61926400	0.59108300	-2.23974000
O	1.21417700	1.35380200	1.63982200
H	1.77527500	2.14733600	1.70025000
C	-0.59664500	2.58615200	-0.52459000
H	0.30295600	3.08794100	-0.16677500
H	-1.45208600	3.18118100	-0.19923300
H	-0.57719200	2.57855900	-1.61782900
H	0.00925800	1.39320800	1.23915600

23-P(C2)

Electronic Energy= =-713.1887178

Sum of electronic and thermal Free Energies= -712.909964

H	-3.26717200	-2.62154100	0.18102200
C	-3.18566200	-1.53978100	0.18044700
C	-2.98860400	1.33368700	0.17802000
C	-1.92119600	-0.90470700	-0.00984500
C	-4.28682800	-0.75066000	0.35712000
C	-4.18116700	0.67989800	0.35478600
C	-1.84181200	0.52566100	-0.00502700
H	-5.26276500	-1.20007400	0.50192700
H	-5.08563500	1.26247500	0.50009500
H	-2.91692800	2.41531000	0.17837700
C	-0.63565000	-1.40182400	-0.21861600
C	0.23503800	-0.25153000	-0.34071500
N	-0.56862500	0.89205700	-0.19237600
H	-0.26672900	1.86863300	-0.24532500
H	1.97646400	-2.28103000	-0.81951200
C	2.49919500	-1.33880700	-0.69206000
C	2.32112900	1.13981900	-0.50196300
C	4.21003900	-0.07592000	0.68533300
C	3.26267300	1.12107200	0.73132800
C	3.44182700	-1.38787000	0.53799600
C	1.59122200	-0.16431300	-0.54432800
H	2.93757200	1.21679800	-1.40622400
H	4.89865900	0.03732700	-0.16186400
H	2.65155400	1.08297500	1.64120900
H	2.84368000	-1.57896600	1.43769700
H	3.11300000	-1.17289200	-1.58659100
H	1.66735400	2.01087700	-0.46632500
H	4.81971900	-0.10153600	1.59391300
H	3.81862100	2.06235800	0.75125300
H	4.12544900	-2.23219400	0.41477000
O	-0.03485300	3.68302600	-0.30459900
H	-0.15513100	4.23573500	0.47693400
C	-0.29334800	-2.85311400	-0.26632700
H	0.08490900	-3.13955400	-1.25214300
H	-1.18163500	-3.45073300	-0.06026500
H	0.46639600	-3.10841200	0.47758200
H	-0.36932700	4.19615600	-1.05000100

23-TS3-C2

Electronic Energy= -713.1546508

Sum of electronic and thermal Free Energies= -712.879697

H	3.60887400	2.21812100	-0.33187800
C	3.50007000	1.14609600	-0.19578000
C	3.23816400	-1.67383000	0.17369500
C	2.22101500	0.55083900	-0.16578000
C	4.60954100	0.33948500	-0.03956400
C	4.47575100	-1.05946600	0.14601900
C	2.11182300	-0.85095100	0.00860700
H	5.60244300	0.77668200	-0.05625600
H	5.37021400	-1.66270200	0.26614300
H	3.13733800	-2.74519700	0.31224000
C	0.89731500	1.07846300	-0.28484900
C	0.03554600	-0.00880700	-0.18154900
N	0.78631900	-1.17004900	-0.02535200
H	0.41080000	-2.09467700	0.12734900
H	-1.38425900	-1.86285800	-1.42700500
C	-2.03004600	-1.39087100	-0.68072800
C	-2.21106000	0.98573500	0.10288800
C	-4.30161200	-0.38360800	-0.27481000
C	-3.70621300	1.01794200	-0.14117000
C	-3.45294700	-1.23076600	-1.21945700
C	-1.40741300	-0.07521200	-0.27080200
H	-2.04420300	0.34809300	1.34942900
H	-4.34563300	-0.86894700	0.70941700
H	-3.88448500	1.59088700	-1.06031700
H	-3.41152900	-0.74906800	-2.20385500
H	-2.03440500	-2.05502100	0.19706700
H	-1.73238600	1.93147300	0.35006600
H	-5.33003200	-0.31346400	-0.63888600
H	-4.19010000	1.57455100	0.66760000
H	-3.89533400	-2.22001800	-1.36174700
O	-2.01430700	-0.06898400	2.55553300
H	-1.27680000	0.30929000	3.06239400
C	0.57614300	2.51748100	-0.54742900
H	-0.29703000	2.62484200	-1.19590500
H	1.42092600	3.00207700	-1.04241400
H	0.38025600	3.06736700	0.37938200
H	-2.83088400	0.09560300	3.05463700

26+water

Electronic Energy= -713.1798001

Sum of electronic and thermal Free Energies= -712.899941

H	3.51547700	2.32496000	0.25779800
C	3.39584200	1.25766000	0.10216700
C	3.10034500	-1.54531100	-0.30336500
C	2.13190400	0.68975000	-0.03840300
C	4.50610300	0.41336300	0.03959000
C	4.36470300	-0.96350700	-0.16012600
C	2.02430900	-0.68465500	-0.23270000
H	5.50039200	0.83353600	0.14839600
H	5.24630500	-1.59337000	-0.20306900
H	2.97793200	-2.61144600	-0.45989400
C	0.78410500	1.27293300	-0.02574600
C	-0.11577300	0.28284100	-0.19284200
N	0.60368900	-1.01369300	-0.34753400
H	0.39199100	-1.45764200	-1.25022000
H	-1.75684400	-0.58140500	-2.17098300
C	-2.24482300	-0.69487800	-1.19493400
C	-2.27624600	0.95284400	0.70211300
C	-4.37979000	-0.25793100	0.05736000
C	-3.77622900	0.93769700	0.79494300
C	-3.74154500	-0.40476600	-1.32311200
C	-1.57887600	0.22314300	-0.18671000
H	-1.40019900	-1.72892300	1.96996900
H	-4.19721300	-1.17263700	0.63709100
H	-4.16647600	1.87719500	0.37849200
H	-3.88229100	0.52635700	-1.88637800
H	-2.09889400	-1.74083500	-0.88634000
H	-1.73558000	1.57604800	1.41231800
H	-5.46382100	-0.13912500	-0.02732300
H	-4.06794400	0.93343400	1.85064300
H	-4.22249600	-1.20466500	-1.89313100
O	-0.78993400	-2.34419500	1.54075800
H	-0.45680900	-2.92953200	2.23252700
C	0.51890300	2.73245300	0.13588200
H	-0.50365600	2.98254900	-0.15126700
H	1.21258600	3.30810500	-0.48354300
H	0.67202900	3.03882400	1.17596700
H	0.25157700	-1.66182600	0.41091600

23-TS1-N

Electronic Energy= -713.171337

Sum of electronic and thermal Free Energies= -712.885863

H	-4.08103300	0.35073700	0.61574200
C	-3.25712400	-0.27631400	0.28871200
C	-1.11503000	-1.92882800	-0.59285200
C	-2.05930700	0.28766400	-0.15290400
C	-3.37450400	-1.66457600	0.28253000
C	-2.32274500	-2.47833200	-0.16207000
C	-1.00825300	-0.54360600	-0.56676700
H	-4.29871000	-2.12600900	0.61478700
H	-2.44937400	-3.55566100	-0.17598400
H	-0.30825200	-2.56147400	-0.95022700
C	-1.62665500	1.67090100	-0.35017100
C	-0.37414200	1.61780200	-0.85862900
H	0.27140000	2.42157800	-1.18555000
N	0.10207700	0.27768500	-0.88481500
H	0.67513900	0.00203400	-1.67903700
C	1.34611400	0.19986200	0.92140500
C	1.76924500	-1.22786900	0.88603400
H	0.89626000	-1.87762500	0.98320700
H	2.34325400	-1.34431800	1.81892700
C	2.66740000	-1.56709900	-0.30632200
H	3.08742000	-2.56341900	-0.14951200
H	2.07237600	-1.62789900	-1.22558100
C	3.78472000	-0.53535600	-0.47652000
H	4.38944800	-0.78588000	-1.35198400
H	4.44950000	-0.57527300	0.39560000
C	3.22924200	0.88363300	-0.62079900
H	2.66306600	0.97689900	-1.55531900
H	4.04368900	1.60904900	-0.68406400
C	2.34455200	1.25595800	0.57171000
H	2.96815700	1.31936500	1.47783800
H	1.85994500	2.23000400	0.46151000
O	0.40269500	0.46501000	1.77649800
H	0.24672500	1.42056000	1.88238300
C	-2.45773000	2.88163000	-0.07868500
H	-2.73787100	2.92892500	0.97829200
H	-3.38356400	2.84703100	-0.66097900
H	-1.91836800	3.79468100	-0.33636600

23-INT(N)

Electronic Energy= -713.1754874

Sum of electronic and thermal Free Energies= -712.888260

H	3.45741900	1.72277300	0.83896200
C	3.02192300	0.77372700	0.54312000
C	1.90853000	-1.71229500	-0.27894000
C	1.78085500	0.72003000	-0.08238300
C	3.69713200	-0.42776800	0.76592900
C	3.15574500	-1.64741900	0.35193100
C	1.24602700	-0.51194800	-0.45417200
H	4.66661900	-0.41371000	1.25248800
H	3.71223300	-2.56432600	0.51191100
H	1.50949400	-2.65615000	-0.62972800
C	0.86199300	1.77742700	-0.53011900
C	-0.18982800	1.18970200	-1.11099000
H	-1.04000900	1.61419400	-1.61990700
N	-0.08096000	-0.27888100	-1.04685000
C	-1.27350200	-1.04581600	-0.31507700
C	-1.20217700	-0.87458800	1.20011100
H	-0.17653100	-1.02834600	1.55010900
H	-1.79967500	-1.70734000	1.59326500
C	-1.80150100	0.42698300	1.73903400
H	-1.77566500	0.38380200	2.83148800
H	-1.19554800	1.28972300	1.44108600
C	-3.23485600	0.59479600	1.23743800
H	-3.67675600	1.50758000	1.64718800
H	-3.84357300	-0.24771200	1.59200400
C	-3.26371700	0.64710100	-0.28949300
H	-2.78763700	1.57483400	-0.61809600
H	-4.29494000	0.68979400	-0.65193100
C	-2.60635300	-0.58960800	-0.91970300
H	-3.26462500	-1.44876500	-0.75226900
H	-2.50874800	-0.49025600	-2.00770800
O	-1.04923800	-2.36261400	-0.70639500
H	-0.68279400	-2.87977900	0.02439200
C	1.10599500	3.23847500	-0.36822200
H	0.30410600	3.82392700	-0.81943800
H	2.05523800	3.51759300	-0.83463800
H	1.17242300	3.49007100	0.69495900
H	-0.10799200	-0.67762700	-1.99580400

23-TS2-N

Electronic Energy= -713.1304303

Sum of electronic and thermal Free Energies= -712.847535

H	3.79815900	1.08337300	0.89894800
C	3.14043000	0.27646500	0.59117200
C	1.45065900	-1.82337100	-0.29427800
C	1.88263800	0.55122000	0.05478500
C	3.53624000	-1.05338600	0.70304900
C	2.70565400	-2.08733400	0.25509300
C	1.04459400	-0.49497100	-0.34718500
H	4.50907700	-1.29285800	1.11937300
H	3.04485000	-3.11551200	0.31939200
H	0.85160400	-2.64054100	-0.67888400
C	1.22140200	1.81357500	-0.26567600
C	0.03769600	1.51432400	-0.82604900
H	-0.71084400	2.18032700	-1.22590700
N	-0.15203700	0.08482100	-0.92518600
C	-1.52790100	-0.52429800	-0.72223500
C	-1.66333200	-1.53073800	0.40031500
H	-0.87789100	-2.28420000	0.37219100
H	-2.62087200	-2.04391000	0.25153200
C	-1.67690000	-0.79351600	1.74536500
H	-1.74484500	-1.53307000	2.54704800
H	-0.72417000	-0.26227200	1.88091100
C	-2.84427700	0.19174000	1.80917900
H	-2.83848100	0.72114300	2.76609100
H	-3.78792600	-0.36585200	1.75380500
C	-2.77102200	1.19794600	0.65963200
H	-1.91075200	1.85882200	0.81438600
H	-3.66037400	1.83340400	0.64264100
C	-2.65653400	0.49230400	-0.69822700
H	-3.56641200	-0.08767800	-0.89060200
H	-2.55803700	1.19629300	-1.52866300
O	-1.51949600	-1.14073300	-2.08208200
H	-1.48023900	-2.11522200	-2.08861600
C	1.80331600	3.16851600	-0.03502200
H	1.12185300	3.95064500	-0.37329400
H	2.75152400	3.27521300	-0.57064300
H	2.00731300	3.31872800	1.02941400
H	-0.47928600	-0.53557400	-2.08567000

23-P(N)

Electronic Energy= -713.1783452

Sum of electronic and thermal Free Energies= -712.899959

H	-4.34239800	0.57982400	-0.50930700
C	-3.48478300	-0.08125300	-0.43473800
C	-1.25056000	-1.80763700	-0.12605900
C	-2.20658600	0.43268200	-0.24156200
C	-3.63706000	-1.46596900	-0.49709800
C	-2.53819200	-2.31188400	-0.32558500
C	-1.10332400	-0.42621900	-0.14672800
H	-4.62252900	-1.89390900	-0.64691700
H	-2.68224400	-3.38676200	-0.32938100
H	-0.43184200	-2.48540300	0.07218600
C	-1.74493600	1.80322600	-0.01532400
C	-0.42504300	1.74952500	0.22979000
H	0.27212100	2.55493900	0.38889800
N	0.05085400	0.39905400	0.10153800
C	1.31277200	0.04356800	0.15361700
C	1.81895100	-1.22348100	-0.44782300
H	1.04216300	-1.75193600	-0.99259300
H	2.18360800	-1.86265500	0.36474800
C	2.97991300	-0.89304600	-1.41990400
H	3.36859700	-1.84389200	-1.79292800
H	2.57489400	-0.35060000	-2.28249700
C	4.07824600	-0.06603500	-0.76107800
H	4.86411900	0.15171800	-1.49012100
H	4.53938600	-0.64100100	0.05212700
C	3.50283300	1.23321800	-0.20546500
H	3.13806300	1.86552200	-1.02322500
H	4.26053100	1.80437800	0.33621900
C	2.34358000	0.93297400	0.76314300
H	2.72921900	0.33266800	1.60017700
H	1.92202200	1.83798800	1.19437200
O	0.75075400	-1.28315700	2.46754800
H	1.27900200	-1.79186300	3.09430100
C	-2.61246300	3.01499800	-0.05290200
H	-2.03793100	3.91745600	0.16038000
H	-3.41516300	2.92844000	0.68580900
H	-3.07957700	3.11798300	-1.03688100
H	-0.12413300	-1.21902000	2.86977300

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Electronic Energy= -636.3560396

Sum of electronic and thermal Free Energies= -636.110210

H	-2.95307900	-2.73737900	-0.44545700
C	-3.05452000	-1.66985600	-0.27563300
C	-3.31245100	1.12982200	0.17302400
C	-1.93038500	-0.84468000	-0.15546300
C	-4.30173400	-1.07052100	-0.16707000
C	-4.43063000	0.31698600	0.05752600
C	-2.03498800	0.55174800	0.06264900
H	-5.19539200	-1.68089500	-0.25376100
H	-5.42239900	0.75098400	0.13926400
H	-3.42203300	2.19799200	0.34092500
H	-0.21153900	-2.06082000	-0.39779900
N	-0.59341600	-1.14672200	-0.20651100
C	0.15620800	0.01182600	-0.05030300
C	-0.69950700	1.08007900	0.13410400
C	-0.35170700	2.50990200	0.41469400
H	-0.31734800	3.11655800	-0.49782300
H	0.62447300	2.59028400	0.90116400
H	-1.09876400	2.95915500	1.07657800
H	1.70351800	-1.62127600	1.40952500
C	2.25398300	-1.31656100	0.51185300
C	2.36820600	0.95111900	-0.54129000
C	4.45362300	-0.44509100	-0.32993200
C	3.87355500	0.94941800	-0.57094100
C	3.73533400	-1.12141500	0.83643600
C	1.62420400	-0.05862500	-0.05782000
H	4.32146600	-1.05477300	-1.23360200
H	4.24781500	1.64806600	0.19154700
H	3.82911300	-0.49229200	1.73146300
H	2.14659300	-2.13927300	-0.21095500
H	1.86692000	1.82398100	-0.95443100
H	5.52935000	-0.37844100	-0.13982900
H	4.21585800	1.34730100	-1.53300800
H	4.19422000	-2.08702100	1.07076500

29+water

Electronic Energy= -712.733261

Sum of electronic and thermal Free Energies= -712.467429

H	-2.89837300	2.40449100	0.23778300
C	-2.97254900	1.32146300	0.21565400
C	-3.17101100	-1.55679100	0.16439500
C	-1.79196800	0.52642700	0.01776100
C	-4.16053600	0.67444300	0.37565000
C	-4.26607400	-0.76902000	0.35052500
C	-1.89430700	-0.92460200	-0.01220200
H	-5.06854600	1.25024500	0.52962900
H	-5.24485700	-1.21801200	0.48468800
H	-3.26099800	-2.63911900	0.14662500
N	-0.55587600	0.95058100	-0.14929000
C	0.22729000	-0.20937200	-0.30879000
C	-0.61941100	-1.40557600	-0.22155700
C	-0.25620000	-2.85573200	-0.29546200
H	-1.14161700	-3.46845500	-0.11330100
H	0.49472400	-3.12504700	0.45376500
H	0.13931900	-3.12792300	-1.27908400
H	2.00014500	-2.22001300	-0.79688200
C	2.51252000	-1.26934300	-0.68371600
C	2.29402000	1.20606700	-0.43531600
C	4.25986900	0.00545100	0.63173700
C	3.29015900	1.18092500	0.74627500
C	3.50889200	-1.31871400	0.49631100
C	1.58060100	-0.11171200	-0.49857300
H	4.89969600	0.14822600	-0.24959200
H	2.72369000	1.10490700	1.68316500
H	2.95487900	-1.52929200	1.42022900
H	3.08332700	-1.09063300	-1.60553100
H	2.86472200	1.33440600	-1.36552300
H	4.91926700	-0.02434700	1.50539800
H	3.83165000	2.13144200	0.77255800
H	4.20542400	-2.14770800	0.33876100
H	-0.36929900	2.74551600	-0.27797500
H	1.59880100	2.03823900	-0.33891900
O	-0.32778200	3.73115100	-0.31482300
H	-0.46632200	3.96631800	-1.23833200

30+water

Electronic Energy= -712.7395053

Sum of electronic and thermal Free Energies= -712.473270

H	2.75386000	-2.74059900	-0.30502400
C	2.86779700	-1.66724600	-0.41914500
C	3.16454000	1.13487400	-0.70143900
C	1.80522800	-0.79987600	-0.18032800
C	4.08406600	-1.10657700	-0.81075100
C	4.23806800	0.27846700	-0.94916200
C	1.94274300	0.58666700	-0.32249700
H	4.92739500	-1.76033900	-1.01130100
H	5.19570200	0.68535900	-1.25637400
H	3.27894500	2.20928000	-0.81614000
N	0.51338800	-1.11379700	0.26525200
C	-0.30551500	0.05923900	0.15966100
C	0.64862900	1.20209700	0.03067700
H	-1.76071500	-2.09277000	0.64817500
C	-2.41710800	-1.22652900	0.53473000
C	-2.51866900	1.24423900	-0.03776500
C	-4.44476500	-0.31111400	-0.63841400
C	-3.64472500	0.92699900	-1.03838200
C	-3.52091800	-1.51945600	-0.48970100
C	-1.65145000	0.03582400	0.21358300
H	-1.92847900	2.07544900	-0.42594800
H	-4.95245300	-0.12512800	0.31859700
H	-3.19800400	0.76019700	-2.02769100
H	-3.06319600	-1.75127600	-1.46066500
H	-2.89356000	-1.07722800	1.51638800
H	-5.22421500	-0.51351800	-1.38071200
H	-4.30114200	1.79924400	-1.12641400
H	-4.08640300	-2.40390400	-0.17813000
C	0.46565100	2.49635400	0.34585300
H	1.29302500	3.19505500	0.26606300
H	0.89131700	0.75915400	2.68371900
H	-0.47590000	2.88495000	0.71196100
H	0.12047300	-1.99441800	-0.04255600
H	-2.96820700	1.57720400	0.91060400
O	0.96487400	-0.12080900	3.07511800
H	0.79741300	-0.72743600	2.33622500

TS(1-5) step I

Electronic Energy= -712.6720617

Sum of electronic and thermal Free Energies= -712.408532

H	3.17968200	-2.81301300	0.53171300
C	3.22681300	-1.75539000	0.29705400
C	3.36645800	1.03766900	-0.31955100
C	2.05818200	-1.00098900	0.07531000
C	4.42770800	-1.08546400	0.20800000
C	4.50626200	0.30296700	-0.09746600
C	2.11173200	0.38391300	-0.23710700
H	5.34952200	-1.63380700	0.37643600
H	5.48060700	0.77512800	-0.15629700
H	3.42174600	2.09519900	-0.55724600
N	0.76430200	-1.38780500	0.10561400
C	-0.07199700	-0.29666400	-0.19952800
C	0.78724500	0.84603900	-0.43002300
H	-1.47666500	-2.50892100	0.21833700
C	-2.07929700	-1.62388900	0.43546900
C	-2.32072400	0.79780500	-0.39784800
C	-4.36795500	-0.60963100	0.13527000
C	-3.77646000	0.47486900	-0.75697200
C	-3.52694700	-1.87389600	0.00203400
C	-1.44592100	-0.37454800	-0.11770900
H	-1.88198200	1.42105300	-1.17687700
H	-4.37420500	-0.27453000	1.18122900
H	-3.82908700	0.14062600	-1.80100200
H	-3.54136700	-2.20972600	-1.04225900
H	-2.05350100	-1.49511800	1.53015400
H	-5.40568900	-0.81181700	-0.14733300
H	-4.35564700	1.40033100	-0.69030400
H	-3.93187500	-2.69000700	0.60717900
C	0.41749000	2.24079500	-0.65020700
H	1.30575100	2.86151300	-0.78094900
H	-0.19990300	2.59935500	0.28294800
H	-0.24956900	2.38546800	-1.50417600
H	0.45734500	-2.33139500	0.28057500
H	-2.26762700	1.42878600	0.51717500
O	-1.23983500	2.89279200	1.46502700
H	-0.93448500	3.45165700	2.19084200

TS(1-5) step II

Electronic Energy= =-712.6512741

Sum of electronic and thermal Free Energies= -712.387538

H	-2.96734700	-2.70716000	0.17294000
C	-3.02354400	-1.63749400	-0.00610800
C	-3.19609400	1.16587700	-0.46418200
C	-1.83183500	-0.87448500	-0.12945800
C	-4.23989100	-0.99432500	-0.11780400
C	-4.34410200	0.40305600	-0.34585300
C	-1.94805800	0.52778800	-0.38776100
H	-5.15380600	-1.57662800	-0.03130600
H	-5.32308400	0.86241800	-0.43099300
H	-3.25677700	2.23878100	-0.63254500
N	-0.55505700	-1.31326700	0.00839000
C	0.24526700	-0.20125500	-0.35504900
C	-0.60122000	1.03185600	-0.32048100
H	1.67468100	-2.36509800	-0.16529700
C	2.33446900	-1.55826600	-0.48810200
C	2.41751200	0.86433200	-1.13353400
C	4.36179400	-0.15179800	0.11375900
C	3.54913600	1.12496000	-0.12235700
C	3.46713000	-1.32209900	0.53118300
C	1.56327000	-0.27924300	-0.66196800
H	4.88518600	-0.41631800	-0.81574300
H	3.11302600	1.46219200	0.82856100
H	3.01995600	-1.10879600	1.51212000
H	2.78507800	-1.84632400	-1.44946900
H	5.13163700	0.02397700	0.87295500
H	4.19698000	1.93049300	-0.48473500
H	4.06102900	-2.23591000	0.64183600
C	-0.22394100	2.24145700	0.24226300
H	-0.95817800	3.03817700	0.33555000
H	0.82183400	2.52386700	0.31979000
H	-0.44762700	-0.41452900	1.78910200
H	1.83660000	1.76665400	-1.33101900
H	2.87998300	0.56567300	-2.08634400
H	0.28736200	0.45085600	2.93243200
O	-0.44180300	0.45598000	2.29120600
H	-0.34606200	1.31053700	1.50649400

TS(1-7)

Electronic Energy= -712.6936564

Sum of electronic and thermal Free Energies= -712.432090

H	2.95458900	-2.63370200	-0.17988500
C	3.08057500	-1.55561200	-0.13342400
C	3.41668700	1.27948700	-0.01967600
C	1.95021800	-0.70125700	-0.13602700
C	4.33149600	-0.98047700	-0.08546900
C	4.50345500	0.43328000	-0.03189000
C	2.11534900	0.71983900	-0.06027900
H	5.21300400	-1.61508700	-0.09167600
H	5.50909500	0.84090200	0.00209400
H	3.55807900	2.35633700	0.02763700
N	0.64264300	-1.03349600	-0.19290700
C	-0.05673000	0.16373300	-0.11197900
C	0.81369900	1.27396400	-0.02066600
C	0.50907000	2.74097700	0.04210800
H	1.42534100	3.31793200	-0.10553700
H	0.08870700	3.03490500	1.00999200
H	-0.20152000	3.05093000	-0.73018200
H	-1.73557500	1.70646900	1.31091900
C	-2.24756500	1.31966100	0.42516300
C	-2.18016600	-1.00471100	-0.56756100
C	-4.35402300	0.31036200	-0.47676400
C	-3.70284500	-1.05942200	-0.66494300
C	-3.71894500	1.02394300	0.71331200
C	-1.49169600	0.14397800	-0.12946000
H	-4.20637800	0.91839100	-1.37932300
H	-4.09819100	-1.74846900	0.09251700
H	-3.80084000	0.39187700	1.60707100
H	-2.18411300	2.11376700	-0.33454400
H	-1.63802300	-1.57292000	-1.32703400
H	-5.43300800	0.19771600	-0.33479700
H	-3.98032200	-1.48116700	-1.63567500
H	-4.23455100	1.96271800	0.93458100
H	-0.05102800	-2.11101000	0.51178800
H	-1.70773400	-1.79825400	0.37698100
O	-0.85457100	-2.60373700	1.05046300
H	-0.95093700	-3.51342600	0.73704700

water

Electronic Energy= -76.402724

Sum of electronic and thermal Free Energies= -76.398851

O	0.00000000	0.00000000	0.11688500
H	0.00000000	0.76617500	-0.46754000
H	0.00000000	-0.76617500	-0.46754000

TS-27

Electronic Energy= -1272.6573315

Sum of electronic and thermal Free Energies= -1272.137511

H	4.49626600	1.54216200	0.91782800
C	4.06721800	1.21477100	-0.02653100
C	2.97684600	0.33072000	-2.50368100
C	2.68958500	1.02840900	-0.16956600
C	4.88838600	0.97190700	-1.12177800
C	4.34055100	0.51114000	-2.34017100
C	2.12428000	0.64004300	-1.41686200
H	5.95976900	1.12586000	-1.04200100
H	5.00846300	0.30688800	-3.17243800
H	2.55978200	-0.00632400	-3.44852700
C	1.57279400	1.08570800	0.76569900
C	0.39168100	1.12895800	-0.16198300
N	0.77239400	0.60145600	-1.38887700
C	1.73813100	1.94434600	2.00564500
H	1.14793200	1.59241100	2.85487100
H	1.45037000	2.97806800	1.79053200
H	2.78523500	1.95447400	2.32024300
H	-2.21256300	3.98321600	2.06250100
C	-1.80406700	3.56024900	1.13829100
C	-0.90316300	1.48909200	0.08858400
C	-2.30987000	3.01389700	-1.28076100
C	-1.91913000	1.54524800	-1.01938300
C	-2.81682600	3.68631000	-0.00262000
C	-1.42220000	2.08433600	1.36671700
H	-1.43006900	3.55325000	-1.65661100
H	-2.82092300	0.99900400	-0.70276200
H	-3.75766100	3.20725000	0.30344400
H	-2.33649100	1.53776100	1.64674300
H	-0.89746300	4.12880400	0.89146800
H	-3.07533500	3.05821400	-2.06334600
H	-1.53335200	1.07407300	-1.92497800
H	-3.04281700	4.74129500	-0.19267400
H	-0.72367300	1.99169700	2.19742800
H	-3.21397200	-2.03599100	-2.95670600
C	-3.47760100	-1.82248300	-1.92556700
C	-4.17065900	-1.25966900	0.78187400
C	-2.49792800	-1.72173200	-0.93181600
C	-4.79822300	-1.63764800	-1.53977100
C	-5.14545700	-1.36211400	-0.19912200
C	-2.82288000	-1.42891600	0.41571100
H	-5.58336400	-1.70907600	-2.28621700
H	-6.19044000	-1.22677700	0.06082700
H	-4.44041400	-1.03721900	1.81085400
H	-0.61570000	-1.69259900	-1.86839900
N	-1.13518300	-1.85426800	-1.01467400
C	-0.56489300	-1.56368600	0.22406500
C	-1.59310000	-1.32544900	1.14375000

C	-1.52640700	-1.19066700	2.63568600
H	-1.42896600	-0.14801600	2.95973500
H	-0.68616700	-1.75190100	3.05326800
H	-2.44423200	-1.58309700	3.08285100
H	1.11050800	-3.16358800	-0.97258200
C	1.72514600	-2.41069700	-0.47036800
C	1.42565900	-0.69061200	1.39191500
C	3.63147100	-1.98635000	1.07818100
C	2.76260400	-1.12025000	1.99710000
C	2.80647800	-3.07151700	0.39478900
C	0.85363100	-1.51747700	0.37030600
H	4.09934500	-1.36541300	0.30599400
H	2.52778900	-1.69945300	2.90049100
H	2.33618500	-3.72151100	1.14459100
H	2.23729600	-1.82908400	-1.25308800
H	0.70662000	-0.41413800	2.15860100
H	4.44112400	-2.42745800	1.66979200
H	3.32974700	-0.24569000	2.33548500
H	3.44434400	-3.70260400	-0.23236100

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Electronic Energy= -1272.7028354

Sum of electronic and thermal Free Energies= -1272.177601

H	5.04264400	0.76436100	0.86454800
C	4.50632600	0.50392700	-0.04426100
C	3.12479600	-0.19220300	-2.42547000
C	3.12211900	0.47815100	-0.08428900
C	5.20592900	0.18309600	-1.21842200
C	4.52686200	-0.16060800	-2.38801500
C	2.45111300	0.13354800	-1.26307100
H	6.29134700	0.20583400	-1.21828700
H	5.09149500	-0.40181100	-3.28323800
H	2.58571300	-0.46129000	-3.32888700
C	2.03372400	0.73757200	0.94520000
C	0.98180800	1.27235700	-0.03120700
N	1.02241200	0.18566000	-1.03394700
C	2.48025900	1.48107200	2.18666600
H	1.65777500	1.60304000	2.89740400
H	2.88829900	2.46584100	1.94023800
H	3.26988900	0.91058200	2.68832400
H	-2.99837400	2.67926400	-1.39349600
C	-2.26001800	2.51807200	-0.59963100
C	0.17028900	2.32823500	-0.08696100
C	-1.34357500	3.39707200	1.58114100
C	0.07362800	3.38973100	0.98317900
C	-2.40212800	3.58190200	0.49139400
C	-0.84132400	2.51979900	-1.19195800
H	-1.51373500	2.44020600	2.09510800
H	0.26199200	4.36925800	0.51996800
H	-2.28440200	4.57891700	0.04348000
H	-0.65976800	3.49453500	-1.66878800
H	-2.45898000	1.52726500	-0.16917400
H	-1.42497900	4.18891400	2.33383600
H	0.81675200	3.25590400	1.76752000
H	-3.40600300	3.54460600	0.92866000
H	-0.73099600	1.74987300	-1.95731800
H	-3.70578400	-0.49523200	-3.08277600
C	-3.90459900	-0.71767500	-2.03864000
C	-4.41387100	-1.29109600	0.70321500
C	-2.86015000	-0.88262600	-1.12113100
C	-5.20096900	-0.84697200	-1.56002500
C	-5.45468800	-1.13320600	-0.20118000
C	-3.09010900	-1.16116000	0.24794000
H	-6.03550200	-0.72553100	-2.24382900
H	-6.48156900	-1.22759900	0.13829300
H	-4.62226400	-1.50415300	1.74843300
H	-1.01204900	-0.48940200	-2.11251000
N	-1.50432500	-0.80234300	-1.28755800
C	-0.86224700	-0.99011200	-0.07583400
C	-1.80534600	-1.23484200	0.90056100
C	-1.64671400	-1.54800700	2.36125500

H	-2.48910100	-2.15773300	2.70162500
H	-1.63078700	-0.64140700	2.97785700
H	-0.73609100	-2.11039300	2.57151500
H	0.60179100	-2.58115100	-1.58892500
C	1.13660900	-2.34328500	-0.66274000
C	1.35124500	-0.64748700	1.24667200
C	1.68135900	-3.14319500	1.70630100
C	2.30708500	-1.73995700	1.73135600
C	0.92010500	-3.43856200	0.38787100
C	0.65227700	-0.98979900	-0.11892300
H	2.20137800	-2.28166500	-0.90932000
H	0.59322000	-0.45355500	2.01171300
H	-0.15428600	-3.52979800	0.58394800
H	1.24126300	-4.39794700	-0.02767600
H	1.00715300	-3.26171500	2.56089300
H	2.47931800	-3.87818200	1.85157300
H	2.64802000	-1.50616400	2.74628600
H	3.20124700	-1.73935400	1.09757500

TS-31

Electronic Energy= -1272.6405166

Sum of electronic and thermal Free Energies= -1272.120776

H	3.05130900	-0.75724600	2.96078000
C	3.35247100	-0.28107900	2.03136400
C	4.16693900	0.96990900	-0.40164900
C	2.39688700	0.27213100	1.15390700
C	4.68896800	-0.17979600	1.69057200
C	5.09205600	0.44341100	0.48360400
C	2.80277100	0.89577200	-0.05805400
H	5.44743100	-0.57485300	2.35930200
H	6.15155400	0.51457800	0.25700000
H	4.47734100	1.45804000	-1.32099100
C	0.97488100	0.32742600	1.17934700
C	0.64137600	1.30622500	0.13613600
N	1.72588600	1.29997300	-0.80404600
C	0.18107800	-0.11917000	2.36292700
H	0.09789300	0.68313700	3.10573900
H	0.68713100	-0.96079900	2.84766700
H	-0.82602000	-0.44240000	2.08798900
H	-2.69214600	3.73593400	1.97103200
C	-1.80928100	3.66817400	1.32702100
C	-0.44411800	2.09028600	-0.05277100
C	-0.75796000	4.45295100	-0.82597200
C	-0.56512200	2.98897600	-1.25729400
C	-1.95228300	4.59366000	0.11790400
C	-1.60546300	2.20396500	0.89589900
H	-2.87262100	4.33740400	-0.42550500
H	-2.51073600	1.86458000	0.36682100
H	-0.94557200	3.98281700	1.92762300
H	-2.05503600	5.63286500	0.44817200
H	-1.49087000	1.56575300	1.77036600
H	-4.18753400	0.56679900	-1.78797800
C	-4.17889700	-0.26357700	-1.08759100
C	-4.14074600	-2.43818000	0.74962300
C	-2.97780900	-0.85048300	-0.67358500
C	-5.35585800	-0.78366600	-0.56592400
C	-5.33620500	-1.86226600	0.34433300
C	-2.93047000	-1.93065200	0.23991900
H	-6.30720700	-0.35413400	-0.86425900
H	-6.27536200	-2.24578300	0.73116100
H	-4.14248700	-3.27044400	1.44828100
H	-1.42017200	0.20745700	-1.61271900
N	-1.68582700	-0.55667400	-1.01290500
C	-0.79946300	-1.39137400	-0.33709300
C	-1.54844500	-2.26187800	0.45040500
C	-1.11271000	-3.34565700	1.39618300
H	-0.93306000	-4.29941000	0.88680400
H	-1.89904300	-3.51795500	2.13723500
H	-0.20567400	-3.08678900	1.94401200
H	1.63025500	-2.39008300	1.05722500

C	1.50072800	-2.42479900	-0.03221500
C	1.12794000	-0.45293200	-1.60801900
C	2.73898700	-2.32605700	-2.20536700
C	2.29055900	-0.88970500	-2.47881100
C	2.87353200	-2.52490400	-0.70072700
C	0.65361000	-1.25445000	-0.51682200
H	2.00305700	-3.03618900	-2.60527500
H	3.14734700	-0.22457700	-2.31715400
H	3.55670000	-1.76856200	-0.29683700
H	0.95105400	-3.35049800	-0.24689400
H	0.37553300	0.07944200	-2.17917100
H	3.68794000	-2.51858400	-2.71620200
H	1.99904700	-0.76533200	-3.52683700
H	3.30637200	-3.50341000	-0.46723900
H	0.30274700	2.88052200	-1.90886000
H	-1.46112500	2.68484900	-1.82418000
H	0.15402700	4.79486300	-0.31901700
H	-0.89019500	5.08135400	-1.71293600

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Electronic Energy= -1272.6917374

Sum of electronic and thermal Free Energies= -1272.166630

H	2.73515300	-1.22087700	2.89979600
C	3.12212700	-0.94026600	1.92334600
C	4.14566600	-0.22328000	-0.62747500
C	2.29927100	-0.41153800	0.94378200
C	4.48123600	-1.11107400	1.61640600
C	4.98305300	-0.75995900	0.36302500
C	2.80962100	-0.06159500	-0.31087600
H	5.15366300	-1.51748300	2.36557400
H	6.03919000	-0.89715000	0.15270900
H	4.53060300	0.05633900	-1.60363700
C	0.80930600	-0.13441800	0.87297500
C	0.88527100	1.04261000	-0.10240100
N	1.73186500	0.44035100	-1.14057500
C	0.11722700	-0.05039100	2.21710700
H	-0.95236200	0.14641500	2.11716600
H	0.57152300	0.73092200	2.83438700
H	0.22986300	-1.00205000	2.74978000
H	-0.61978100	4.67952400	2.08095300
C	0.07160300	4.21279600	1.37126600
C	0.37543800	2.27359700	-0.18094000
C	1.30054800	4.51119800	-0.81342200
C	0.69438700	3.19821100	-1.33361900
C	0.38630000	5.17115500	0.22071900
C	-0.53103400	2.89680000	0.85301300
H	2.27387900	4.29404100	-0.35301900
H	-0.24233700	3.43353200	-1.86221500
H	-0.55352000	5.46638500	-0.26719500
H	-1.49532300	3.12029100	0.37034300
H	0.99543100	3.98613500	1.92068800
H	1.48533700	5.19172500	-1.65157800
H	1.36501500	2.70813100	-2.04146300
H	0.84638800	6.08739400	0.60642900
H	-0.73786700	2.21946100	1.68051400
H	-4.00373300	1.67244300	-1.62805100
C	-4.24413700	0.81770000	-1.00279400
C	-4.85813500	-1.42617200	0.63758900
C	-3.24647400	-0.05685300	-0.55458400
C	-5.54810900	0.54909100	-0.61290800
C	-5.85340200	-0.56530600	0.19889900
C	-3.52536300	-1.17512100	0.26299300
H	-6.34856700	1.20600500	-0.93904900
H	-6.88565900	-0.74834100	0.48111100
H	-5.10931900	-2.28136700	1.25904800
H	-1.39728400	0.69905500	-1.23059000
N	-1.89599500	-0.05361300	-0.77886000
C	-1.29039500	-1.12057900	-0.12456400
C	-2.27418600	-1.83290600	0.54271900
C	-2.19021600	-3.01102600	1.47572400

H	-1.30836000	-2.97488200	2.11795700
H	-2.18114500	-3.97142300	0.94814900
H	-3.06621100	-3.01140400	2.13063100
H	1.25729900	-1.63366900	-3.43427800
C	1.61854000	-1.74304800	-2.40750700
C	0.22543400	-1.24931000	-0.12972900
C	1.81804200	-3.29472400	-0.47027600
C	0.64114700	-2.68350100	0.29205800
C	1.53796600	-3.20262900	-1.96507100
C	0.85931700	-0.74855000	-1.50817200
H	2.76520700	-2.79230800	-0.23627100
H	-0.20379100	-3.35210000	0.11380500
H	0.54069100	-3.61475000	-2.17066200
H	2.67448600	-1.45452800	-2.41967500
H	1.92219000	-4.33879100	-0.15560500
H	0.83580600	-2.70563800	1.37132400
H	2.25441800	-3.79385300	-2.54441300
H	0.05773300	-0.31983000	-2.11031500

TS-32

Electronic Energy= -1272.6521513

Sum of electronic and thermal Free Energies= -1272.132392

H	1.05476100	3.48099400	1.43095500
C	1.20667900	2.88578600	0.53305900
C	1.64942500	1.30539200	-1.79866500
C	0.18678000	2.06812600	0.02517400
C	2.42400800	2.91603500	-0.12979400
C	2.63847900	2.11625800	-1.28166300
C	0.38433100	1.28863600	-1.15429400
H	3.22743300	3.54839000	0.23542000
H	3.61448200	2.13944200	-1.76008100
H	1.82526300	0.68318800	-2.67204400
C	-1.10999100	1.68624200	0.53878400
C	-1.71999200	0.95953400	-0.62854600
N	-0.69425900	0.55887900	-1.48835400
C	-1.80766600	2.63811800	1.48361500
H	-1.07187900	3.08840300	2.15689300
H	-2.57245300	2.17010700	2.10075600
H	-2.27879500	3.44556900	0.91344900
H	-4.65204200	-1.69096100	-2.84600900
C	-4.35737800	-1.23384900	-1.89516500
C	-3.02482900	0.67037200	-0.90367000
C	-5.17687100	-0.07969200	0.18055000
C	-4.22080700	1.09549200	-0.09166000
C	-5.58917700	-0.77527700	-1.11561600
C	-3.39672800	-0.06537300	-2.16893100
H	-4.68085400	-0.80842300	0.83761600
H	-4.77266100	1.84621000	-0.67984500
H	-6.16911300	-0.07518400	-1.73326700
H	-3.90815000	0.64571500	-2.83741300
H	-3.83088400	-2.00752800	-1.31899900
H	-6.05664900	0.28881400	0.71882500
H	-3.94304800	1.57561600	0.84432100
H	-6.24290500	-1.62673600	-0.89758800
H	-2.49694400	-0.40739000	-2.68146800
H	4.77616600	0.77406600	1.98692800
C	4.70263800	0.12162700	1.12218300
C	4.49353900	-1.57951600	-1.15862100
C	3.46701000	-0.40148800	0.71254000
C	5.81593800	-0.21748200	0.37157600
C	5.71286500	-1.05833600	-0.76319300
C	3.34107600	-1.26049700	-0.41073700
H	6.78867300	0.17185400	0.65602800
H	6.60942400	-1.29796400	-1.32624000
H	4.42694200	-2.22618900	-2.02919300
H	2.01481700	0.34235700	2.03961900
N	2.22201700	-0.22471200	1.23258700
C	1.28318300	-0.93846600	0.49189800
C	1.95960500	-1.58460600	-0.55124400
C	1.36106200	-2.31769400	-1.70960700

H	1.10071500	-3.35484000	-1.47065000
H	2.07098500	-2.34199700	-2.54120300
H	0.45418700	-1.80220100	-2.04621500
H	-1.92193300	-1.49400500	-0.08501300
C	-1.07111200	-1.96666400	0.42963900
C	-0.64595200	0.12627900	1.66075100
C	-1.78297000	-1.73349900	2.87950100
C	-1.91279900	-0.28006900	2.40114400
C	-1.61779900	-2.69169200	1.68791600
C	-0.11198000	-0.88071900	0.80677100
H	-0.91166700	-1.79942600	3.54134600
H	-2.78278600	-0.19667300	1.73809900
H	-2.58320600	-3.13814200	1.42443000
H	-0.63433200	-2.68990700	-0.25660000
H	0.05777300	0.68077000	2.28033700
H	-2.65759800	-2.01070100	3.47618600
H	-2.08392200	0.38348500	3.25193700
H	-0.94750600	-3.51375600	1.95689300

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Electronic Energy= -1272.7016983

Sum of electronic and thermal Free Energies= -1272.178340

H	-0.41533300	4.08730500	1.52885600
C	-0.07823400	3.54805400	0.64744600
C	0.82751600	2.15434300	-1.65661500
C	-0.53192000	2.27095300	0.35978700
C	0.83390100	4.13713200	-0.24302800
C	1.28044600	3.45130200	-1.37331900
C	-0.08194800	1.59428800	-0.77911000
H	1.19633200	5.14250700	-0.05116900
H	1.98666100	3.92931400	-2.04529100
H	1.17478400	1.60631600	-2.52775600
C	-1.46218300	1.29953000	1.07256700
C	-1.98095700	0.58685900	-0.17788900
N	-0.69470900	0.28098500	-0.82913800
C	-2.36760800	1.92796000	2.11175300
H	-1.75605200	2.39418700	2.89290200
H	-3.01519500	1.19256300	2.59428000
H	-2.99386600	2.70557500	1.66416900
H	-4.17572200	-2.27757600	-2.82290500
C	-4.04389500	-1.80495400	-1.84349000
C	-3.16653800	0.24605900	-0.68522100
C	-5.23525800	-0.86124000	0.16956600
C	-4.49608600	0.47644600	-0.00692200
C	-5.39889400	-1.58581400	-1.16815500
C	-3.28151500	-0.48153900	-2.00589600
H	-4.66054100	-1.49563700	0.85929200
H	-5.10817100	1.12932000	-0.64651400
H	-6.03631100	-0.97952900	-1.82719200
H	-3.84404100	0.15825000	-2.70267100
H	-3.44344000	-2.49386600	-1.23400400
H	-6.21230300	-0.68452900	0.63208800
H	-4.38353800	0.97852600	0.95391800
H	-5.91037500	-2.54329700	-1.02116900
H	-2.29032600	-0.64990700	-2.43193900
H	4.94109700	0.07003200	2.27142300
C	4.88519900	-0.26097000	1.23881200
C	4.73203100	-1.12506000	-1.47087200
C	3.65317900	-0.44165700	0.59882200
C	6.03124800	-0.51937100	0.49996800
C	5.95631700	-0.94775200	-0.84337300
C	3.55371100	-0.87226700	-0.74582100
H	7.00425100	-0.38942700	0.96359300
H	6.87471100	-1.14140700	-1.38908700
H	4.68292000	-1.45718300	-2.50465400
H	2.13570500	0.02033200	1.99811800
N	2.37238400	-0.26540400	1.06109800
C	1.46674000	-0.57459200	0.05995900
C	2.15562000	-0.95566200	-1.07005700
C	1.61245300	-1.36922800	-2.40516400

H	1.75531700	-2.44256200	-2.57983800
H	2.13315900	-0.83978200	-3.21165600
H	0.54773400	-1.14227500	-2.48514400
H	-1.66087300	-1.92737400	0.19487900
C	-0.56768900	-1.97077200	0.21450800
C	-0.51205500	0.17156300	1.61099600
C	-0.30986500	-2.05273700	2.75390700
C	-1.18511200	-0.80893800	2.57419400
C	-0.02745400	-0.53306900	0.27867900
H	-2.17453600	-1.09336900	2.18933500
H	-0.24454500	-2.43213100	-0.72334900
H	0.31270400	0.65842100	2.14350100
H	-0.75163300	-2.71933200	3.50034100
H	-1.34898500	-0.32000600	3.54012700
H	0.65856600	-1.73527800	3.16208200
H	-0.65140000	-3.74601900	1.41798700
C	-0.09935500	-2.80111500	1.41464700
H	0.95874700	-3.05773500	1.28965400

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Electronic Energy= -1272.6413877

Sum of electronic and thermal Free Energies= -1272.122893

H	-1.43386000	1.97279200	-2.08018200
C	-1.08074000	2.19694900	-1.07705500
C	-0.20564300	2.74285300	1.58635100
C	0.05088200	1.53995700	-0.54314800
C	-1.73232800	3.12277800	-0.28977600
C	-1.29981600	3.38725200	1.03768500
C	0.49826900	1.82333700	0.77827400
H	-2.59951500	3.64960900	-0.67579200
H	-1.84409300	4.11660300	1.63053800
H	0.11765100	2.94106700	2.60426600
C	0.85516900	0.47492300	-1.01857600
C	1.98476700	0.44235800	-0.08142600
N	1.53429200	1.01090900	1.15263700
C	0.70179300	-0.11314700	-2.38422300
H	1.07294000	-1.13909400	-2.43703100
H	1.22766600	0.47933700	-3.14274300
H	-0.36195000	-0.12227400	-2.64693200
H	-4.39810100	1.75135300	1.64152600
C	-4.55084500	1.02572500	0.84790100
C	-4.93107400	-0.87651000	-1.23503800
C	-3.51829000	0.17622400	0.43711200
C	-5.77346500	0.90568700	0.19987100
C	-5.96241100	-0.04085300	-0.82967400
C	-3.67695600	-0.76878100	-0.60568700
H	-6.59876500	1.54769500	0.49195900
H	-6.93296100	-0.11395000	-1.31095600
H	-5.09350400	-1.59748100	-2.03162500
H	-1.80419700	0.73561300	1.51278300
N	-2.23386800	0.06254500	0.89274700
C	-1.53880900	-0.88547500	0.14867100
C	-2.41413100	-1.43474300	-0.78404500
C	-2.20920600	-2.54045700	-1.78397000
H	-1.97035900	-3.49683600	-1.30623500
H	-1.41778600	-2.32116600	-2.50670700
H	-3.13007300	-2.68843900	-2.35401500
H	1.59099300	-2.15335800	-0.32678100
C	0.54271100	-2.38591400	-0.09520900
C	0.45038100	-0.66246600	1.64413500
C	0.96062600	-2.98258800	2.35689900
C	1.49981100	-1.54009300	2.27109600
C	0.51309100	-3.50242700	0.96939000
C	-0.12687100	-1.13874700	0.43490100
H	1.73168700	-3.63242600	2.78210100
H	1.77737800	-1.16145300	3.25804300
H	-0.50351200	-3.90681500	1.02892400
H	0.09170600	-2.73681400	-1.02142800
H	-0.16794500	-0.11770200	2.35220400
H	0.11706200	-2.99752200	3.05515800

H	2.40564400	-1.53512100	1.65282900
H	1.16047800	-4.32097400	0.63771400
C	3.26695200	0.03125900	-0.23990700
C	4.29283500	0.17615100	0.85516400
C	3.85215700	-0.46243800	-1.53602200
C	5.41909900	1.12344800	0.40395200
H	4.73398900	-0.81294000	1.04894300
H	3.82593700	0.52908600	1.77543500
C	4.98481300	0.47770400	-1.99402900
H	4.27821200	-1.46166400	-1.36255900
H	3.10570400	-0.55743700	-2.32239000
C	6.04634200	0.64549400	-0.90646900
H	6.17643400	1.19228300	1.19184700
H	5.00156700	2.12960900	0.26663500
H	5.43140400	0.08399100	-2.91293500
H	4.55126500	1.45670700	-2.23789700
H	6.81779200	1.34856100	-1.23842400
H	6.54346100	-0.31976800	-0.73686700

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Electronic Energy= -1272.7014712

Sum of electronic and thermal Free Energies= -1272.176372

H	-1.41925600	1.92629800	-2.38350600
C	-1.04212700	2.30906700	-1.43861400
C	-0.11899300	3.27632400	1.06947300
C	-0.03995900	1.65432500	-0.74320200
C	-1.58330900	3.47261700	-0.87057400
C	-1.13510300	3.94271900	0.36483200
C	0.41993200	2.14439600	0.48462600
H	-2.36881100	4.00942200	-1.39327600
H	-1.57389400	4.84195000	0.78583600
H	0.23215800	3.63448700	2.03227900
C	0.68217500	0.33603200	-0.95401600
C	1.97848000	0.70483900	-0.22902500
N	1.41173900	1.23567400	1.02322300
C	0.62563900	-0.18975400	-2.37298700
H	-0.42292400	-0.34467000	-2.65324900
H	1.14932100	-1.14113300	-2.48877300
H	1.05527900	0.53379300	-3.07214600
H	6.06582500	0.17442900	1.52202800
C	5.27895300	-0.15588000	0.83517900
C	3.28508600	0.60858700	-0.47906600
C	4.80144400	-1.13689900	-1.43834600
C	3.86978900	0.04378500	-1.75163000
C	5.89070900	-0.72862800	-0.44507500
C	4.33154700	1.01678500	0.53325100
H	4.20765500	-1.95737900	-1.01138500
H	4.46282900	0.83383200	-2.23583600
H	6.53302400	0.03244200	-0.91042200
H	4.92448900	1.84187800	0.11091500
H	4.71687600	-0.94727300	1.34961900
H	5.24764900	-1.51166400	-2.36578400
H	3.09889000	-0.25727600	-2.45974000
H	6.53103200	-1.58533600	-0.20841800
H	3.85496000	1.38018100	1.44592900
H	-4.58316200	1.58251100	1.50392100
C	-4.66769900	0.71122400	0.86111300
C	-4.87283400	-1.57104500	-0.82725400
C	-3.53362900	-0.00091500	0.45146400
C	-5.89999300	0.26015100	0.41107500
C	-6.00205600	-0.87394100	-0.42381800
C	-3.60811300	-1.13148700	-0.39427500
H	-6.80166400	0.78824700	0.70545000
H	-6.98236600	-1.20175600	-0.75560800
H	-4.96866300	-2.44033500	-1.47219900
H	-1.85486400	1.02914900	1.19200100
N	-2.21080400	0.19768500	0.74123800
C	-1.42530100	-0.73676300	0.07673400
C	-2.26028200	-1.58723800	-0.62826400
C	-1.94918100	-2.77729300	-1.49523400

H	-1.21674200	-2.55266000	-2.27534000
H	-2.86122300	-3.10692700	-1.99933400
H	-1.57315500	-3.62986300	-0.91889900
C	0.08439000	-0.65551900	0.15737800
C	0.45400700	-2.93749400	1.24162100
C	0.73176600	-2.04421300	0.02679600
C	0.62158200	0.03784300	1.48437600
H	1.81271500	-1.89644700	-0.08029200
H	1.09640600	-3.82158800	1.17386000
H	0.40504700	-2.54575300	-0.88392300
H	-0.58067100	-3.29628500	1.20248500
H	1.24217600	-2.83450900	3.27883900
C	0.70142300	-2.19468100	2.57571800
H	-0.25752100	-1.95128500	3.05062200
H	-0.19661000	0.39965900	2.11321900
C	1.46669500	-0.88907800	2.34913800
H	2.43098400	-1.08118300	1.86373100
H	1.67743600	-0.38567200	3.29780000