Supporting Information

Effect of Extended Benzannelation Orientation on Bergman and Related Cyclizations of Isomeric Quinoxalenediynes

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Table S1. Computed cyclization free energies (25 °C, gas phase, kcal/mol).

Substrate	C^1–C^5		C^1–C^6		(C^1–C^5) – (C^1–C^6)	
	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta\Delta G^{\ddagger}$	$\Delta\Delta G_{rxn}$
linear						
1 (R = H)	40.48	33.27	32.94	14.62	7.54	18.65
3 (R = Ph)	41.18	33.76	46.62	31.88	-5.44	1.88
angular						
2 (R = H)	41.65	34.38	32.05	7.85	9.60	26.53
4 (R = Ph)	42.46	34.89	45.61	25.24	-3.15	9.65
linear–angular						
1 – **2**	-1.17	-1.11	0.89	6.77		
3 – **4**	-1.28	-1.13	1.01	6.64		

Table S2. Computed free energy (25 °C, gas phase, kcal/mol) difference between the singlet and triplet states for the cyclization transition states and diradical products. All values tabulated as singlet minus triplet.

Substrate	C^1–C^5			C^1–C^6		
	transition state	diradical product	diradical product (including sum correction)[a]	transition state	diradical product	diradical product (including sum correction)[a]
linear						
1 (R = H)	-52.65	-4.43	-9.26	-49.92	-2.17	-4.83
3 (R = Ph)	-40.38	-1.16	-4.13	-35.68	-1.00	-2.55
angular						
2 (R = H)	-41.39	-4.23	-8.88	-43.26	-1.39	-3.27
4 (R = Ph)	-36.68	-2.05	-4.76	-29.78	-0.39	-1.33

[a] The sum correction accounts for triplet contamination in the broken-symmetry unrestricted wave function for the singlet diradical product. (Ref: Graefenstein, J.; Hjerpe, A. M.; Kraka, E.; Cremer, D. J. Phys. Chem. A 2000, 104, 1748-1761 and Cramer, C. J. Essentials of Computational Chemistry: Theories and Models; 2nd ed.; John Wiley & Sons, Ltd.: West Sussex, England, 2004.)

Table S3. Relative free energies (25 °C, gas phase, kcal/mol) for C^1–C^5 cyclization of **1**-**4** and corresponding Boltzmann percentages. (Cf. structures in Figure 3.)

Substrate	Products					
linear	Isomer **1**-***Z***	Isomer **1**-***E***	**3**-**Lin**			
1 (R=H)	0 (95.97%)	1.88 (4.03%)	n/a			
3 (R=Ph)	n/a	n/a	0 (100%)			
angular	Isomer **2**-***Z***	Isomer **2**-***E***	**4**-**Lin**	Isomer **2'**-***Z***	Isomer **2'**-***E***	**4'**-**Lin**
2 (R=H)	-0.29 (54.84%)	1.87 (1.43%)	n/a	0 (33.77%)	0.72 (9.97%)	n/a
4 (R=Ph)	n/a	n/a	-0.52 (70.71%)	n/a	n/a	0 (29.29%)

Table S4. Calculated NICS values[a] for the 5- and 6-membered rings formed in the cyclization reactions of **1**-**4**.

Substrate	C^1–C^5		C^1–C^6	
	transition state	product	transition state	product
1 (R = H)	-2.4	-2.6	-15.5	-14.9
2 (R = H)	-2.7	-2.6	-15.3	-16.0
3 (R = Ph)	-2.4	-2.3	-12.7	-12.7
4 (R = Ph)	-2.4	-2.1	-12.8	-14.4

[a]The NICS value for the *p*-benzyne diradical singlet at the same level of theory is -15.9.

Table S5. Mulliken charge populations and Mulliken spin populations for selected atoms in the cyclization transition states and diradical products.

(a) Angularly-fused case.

	Mulliken charge populations				Mulliken spin populations			
	N Proximal to Radical	**C Radical Proximal to N**	**C Radical Distal to N**	Δ (C Radicals)[a]	**N Proximal to Radical**	**C Radical Proximal to N**	**C Radical Distal to N**	Δ (C Radicals)
R=H (**2**)								
C^1-C^5 TS	-0.482	0.006	-0.309	0.315	-0.002	-0.620	0.629	-0.009
C^1-C^5 PRD	-0.487	0.016	-0.221	0.237	0.001	-1.091	1.165	-0.074
C^1-C^6 TS	-0.482	0.077	-0.012	0.089	-0.006	0.289	-0.286	0.003
C^1-C^6 PRD	-0.489	0.025	-0.036	0.061	-0.017	1.083	-1.085	-0.002
R=Ph (**4**)								
C^1-C^5 TS	-0.482	-0.091	0.000	-0.091	0.000	-0.617	0.476	0.141
C^1-C^5 PRD	-0.488	-0.059	0.028	-0.087	0.003	-1.068	0.836	0.231
C^1-C^6 TS	-0.486	0.001	-0.081	0.082	0.012	-0.589	0.583	0.005
C^1-C^6 PRD	-0.492	-0.007	-0.066	0.059	-0.018	1.093	-1.094	-0.001

[a] Proximal C radical – Distal C radical.

(b) Linearly-fused case.

	Mulliken charge populations				Mulliken spin populations			
	N Proximal to Radical	**C Radical Proximal to N**	**C Radical Distal to N**	Δ (C Radicals)	**N Proximal to Radical**	**C Radical Proximal to N**	**C Radical Distal to N**	Δ (C Radicals)
R=H (**1**)								
C^1-C^5 TS	-0.489	-0.032	-0.302	0.271	0.000	0.598	-0.620	-0.022
C^1-C^5 PRD	-0.491	-0.013	-0.225	0.212	-0.003	-1.090	1.178	-0.089
C^1-C^6 TS	-0.486	0.013	0.013	0.000	0.007	0.319	-0.319	0.000
C^1-C^6 PRD	-0.482	-0.012	-0.012	0.000	0.031	-1.104	1.104	0.000
R=Ph (**3**)								
C^1-C^5 TS	-0.493	-0.126	0.015	-0.141	0.002	0.572	-0.455	0.118
C^1-C^5 PRD	-0.494	-0.088	0.033	-0.121	0.006	1.052	-0.843	0.209
C^1-C^6 TS	-0.488	-0.063	-0.063	0.000	-0.014	-0.600	0.600	0.000
C^1-C^6 PRD	-0.483	-0.052	-0.052	0.000	-0.032	-1.111	1.111	0.000

Table S5. (continued)

(c) Angularly-fused case vs. Linearly-fused case

	Mulliken charge populations				Mulliken spin populations			
	Δ N Proximal to Radical	**Δ C Radical Proximal to N**	**Δ C Radical Distal to N**	**Δ Δ (C** Radicals)	**Δ N Proximal to Radical**	**Δ C Radical Proximal to N**	**Δ C Radical Distal to N**	**Δ Δ (C** Radicals)
2 vs. **1**								
C^1-C^5 TS	0.008	0.038	-0.006	0.044	-0.002	0.022	0.008	0.014
C^1-C^5 PRD	0.004	0.029	0.004	0.025	0.004	0.001	-0.013	0.014
C^1-C^6 TS	0.003	0.064	-0.025	0.089	-0.013	-0.030	-0.033	0.003
C^1-C^6 PRD	-0.007	0.037	-0.023	0.061	-0.049	-0.021	-0.020	-0.002
4 vs. **3**								
C^1-C^5 TS	0.010	0.035	-0.015	0.050	-0.002	0.044	0.021	0.023
C^1-C^5 PRD	0.006	0.029	-0.005	0.035	-0.002	0.016	-0.007	0.022
C^1-C^6 TS	0.002	0.063	-0.019	0.082	0.026	-0.012	-0.017	0.005
C^1-C^6 PRD	-0.008	0.044	-0.015	0.059	0.014	-0.018	-0.017	-0.001

Table S6. Activation enthalpies for cyclization reactions of **1**-**4** at 180 °C and ratios of first order rate constants for cyclization between angular and linear analogs at 180 °C.

	Activation enthalpies (kcal/mol) at 180 °C			
	C^1-C^5 pathway		C^1-C^6 pathway	
	R=H	R=Ph	R=H	R=Ph
angular	39.88	39.84	29.90	42.02
linear	38.71	37.89	30.66	42.73
k_l ratio (angular : linear)	1 : 3.70	1 : 8.76	2.32 : 1	2.20 : 1

Table S7. Activation enthalpies for cyclization reactions of **1**-**4** at 25 °C and ratios of first order rate constants for cyclization between angular and linear analogs at 25 °C.

	Activation enthalpies (kcal/mol) at 25 °C			
	C^1-C^5 pathway		C^1-C^6 pathway	
	R=H	R=Ph	R=H	R=Ph
angular	40.26	40.16	30.32	42.36
linear	39.07	38.21	31.16	43.07
k_l ratio (angular : linear)	1 : 7.41	1 : 26.8	4.12 : 1	3.30 : 1

Table S8. Relative enthalpies and free energies (25 °C, gas phase, kcal/mol) and Boltzmann ratios of C^1-C^5 product isomers from cyclization of **3**. (Isomers are designated as in Figure S1).

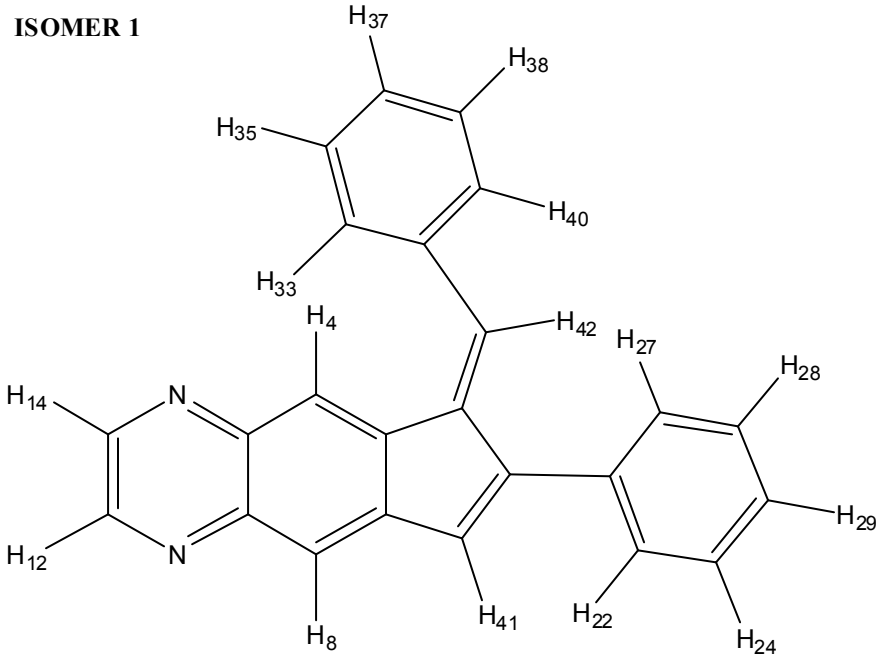
	relative ΔH	relative ΔG	Boltzmann ratio
isomer 1	0.00	0.00	76.90%
isomer 2	0.85	0.71	23.10%

Table S9. Relative enthalpies and free energies (25 °C, gas phase, kcal/mol) and Boltzmann ratios of C^1-C^5 product isomers from cyclization of **4**. (Isomers are designated as in Figure S3).

	relative ΔH	relative ΔG	Boltzmann ratio
isomer 1	0.00	0.00	1.23%
isomer 2	2.23	2.44	0.02%
isomer 3	-2.51	-2.48	80.58%
isomer 4	-1.51	-1.59	18.17%

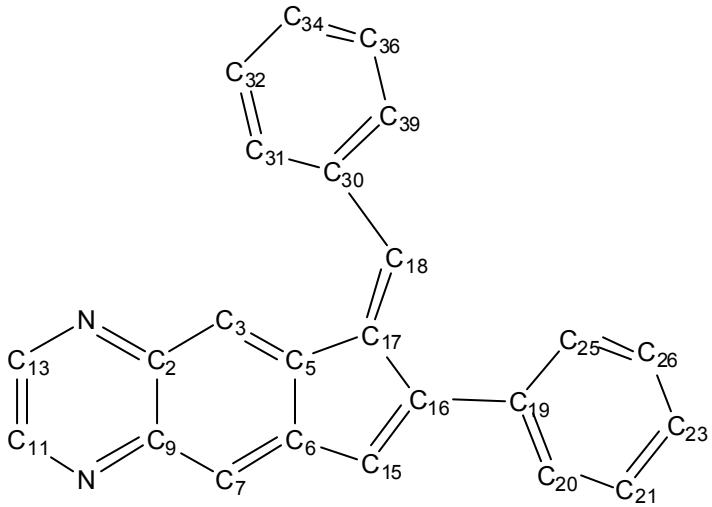
Figure S1. Calculated NMR chemical shifts for C^1-C^5 product isomers from cyclization of **3**.

ISOMER 1



Proton	Chemical Shift (ppm)
4	8.73
8	7.87
12	8.65
14	8.59
22	7.76
24	7.57
27	7.51
28	7.54
29	7.42
33	7.37
35	7.53
37	7.51
38	7.62
40	8.22
41	7.16
42	7.43

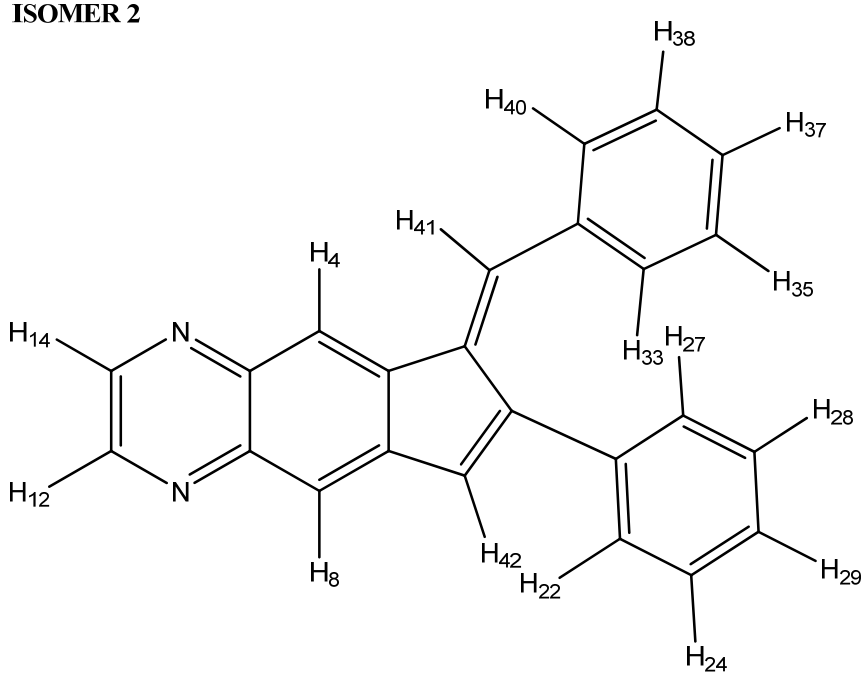
ISOMER 1



Carbon	Chemical Shift (ppm)
2	140.72
3	120.40
5	135.30
6	142.46
7	115.89
9	142.66
11	141.53
13	139.87
15	127.00
16	150.44
17	135.92
18	137.01
19	135.99
20	126.72
21	126.60
23	125.26
25	128.06
26	124.97
30	135.01
31	128.63
32	126.58
34	127.16
36	125.29
39	127.81

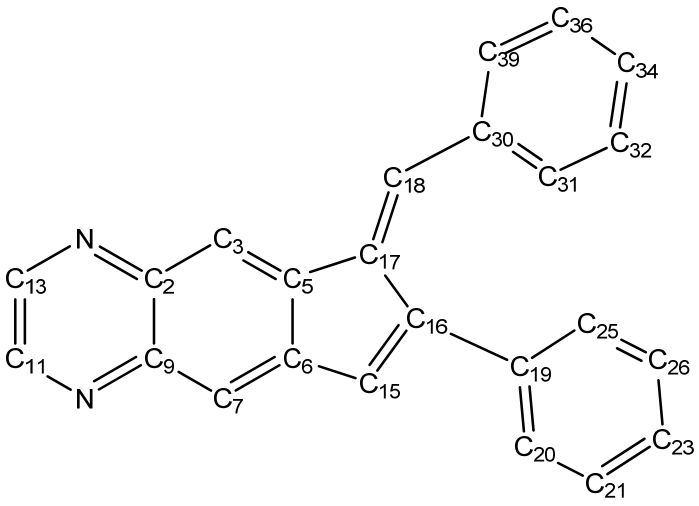
Figure S1. (continued)

ISOMER 2



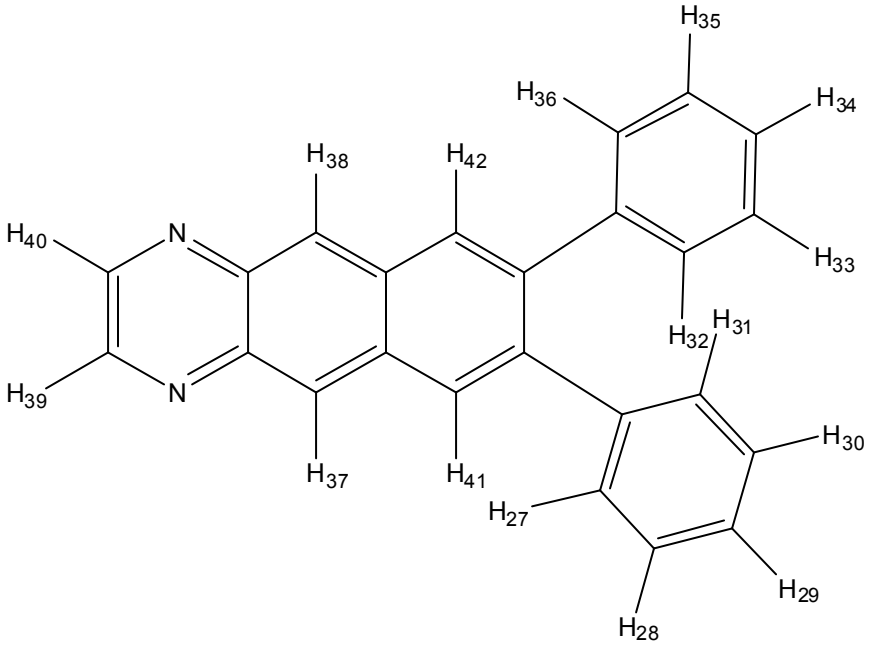
Proton	Chemical Shift (ppm)
4	8.41
8	7.92
12	8.70
14	8.63
22	7.85
24	7.53
27	6.82
28	6.90
29	7.25
33	6.76
35	6.80
37	7.22
38	7.39
40	7.63
41	8.13
42	7.25

ISOMER 2

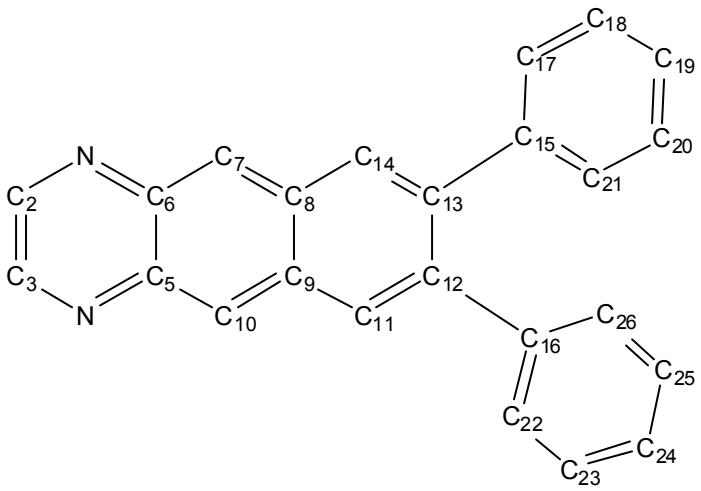


Carbon	Chemical Shift (ppm)
2	141.13
3	116.69
5	142.02
6	140.42
7	116.29
9	142.87
11	141.07
13	139.90
15	133.95
16	147.11
17	132.82
18	132.34
19	135.05
20	125.80
21	125.33
23	124.71
25	128.30
26	124.40
30	133.51
31	130.20
32	124.03
34	126.16
36	125.20
39	129.42

Figure S2. Calculated NMR chemical shifts for C^1-C^6 product from cyclization of **3**.



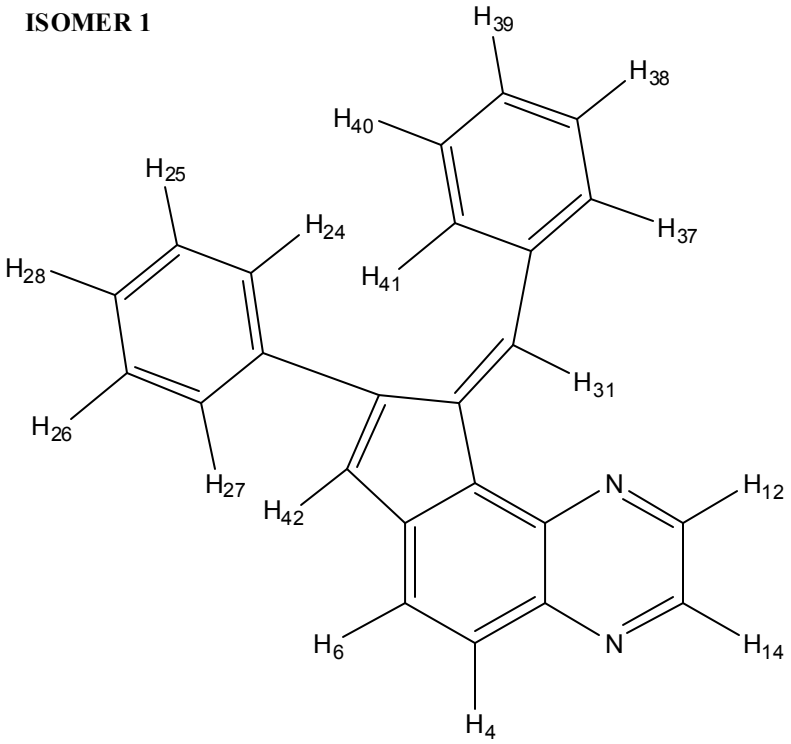
Proton	Chemical Shift (ppm)
27	7.75
28	7.60
29	7.27
30	7.12
31	6.94
32	6.94
33	7.13
34	7.27
35	7.60
36	7.74
37	8.83
38	8.83
39	8.78
40	8.78
41	8.30
42	8.29



Carbon	Chemical Shift (ppm)
2	143.11
3	143.11
5	138.02
6	138.02
7	125.62
8	131.17
9	131.21
10	125.62
11	128.89
12	140.18
13	140.25
14	128.92
15	142.25
16	142.12
17	127.09
18	127.03
19	123.67
20	125.04
21	128.38
22	127.07
23	126.98
24	123.65
25	125.00
26	128.43

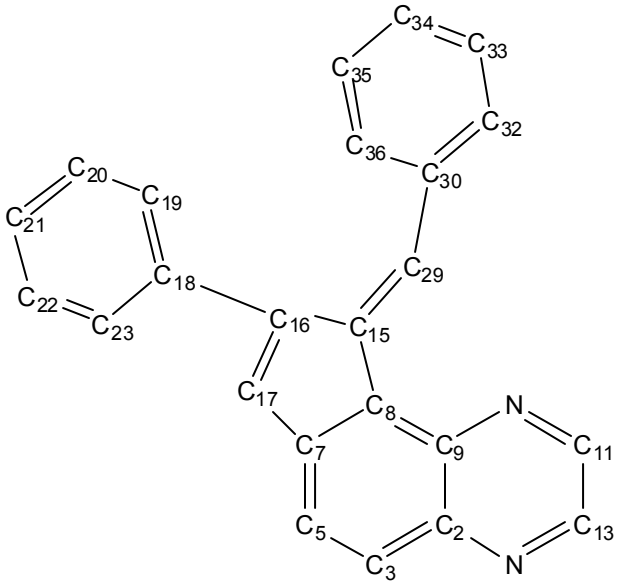
Figure S3. Calculated NMR chemical shifts for C^1-C^5 product isomers from cyclization of **4**.

ISOMER 1



Proton	Chemical Shift (ppm)
4	7.93
6	7.77
12	8.67
14	8.59
24	6.87
25	6.93
26	7.38
27	7.74
28	7.08
31	10.09
37	7.78
38	7.44
39	7.19
40	6.84
41	6.94
42	6.99

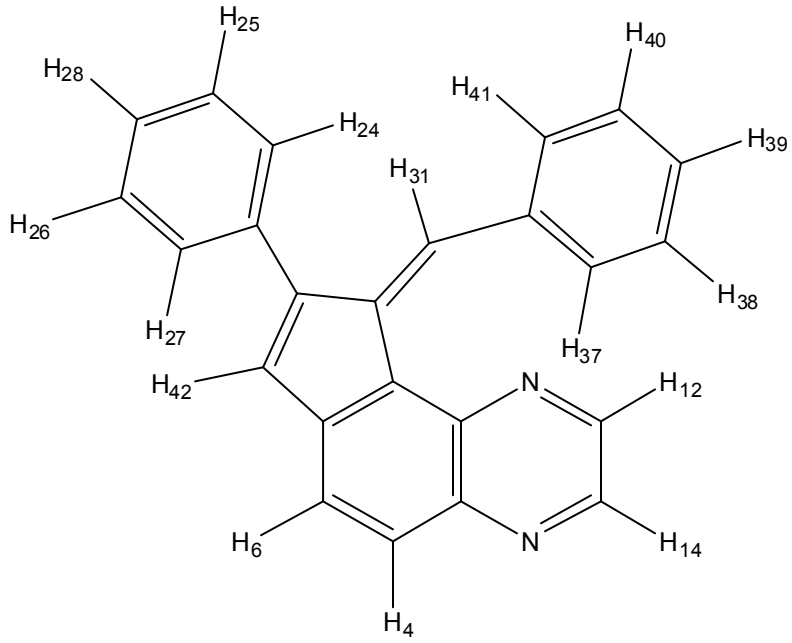
ISOMER 1



Carbon	Chemical Shift (ppm)
2	140.88
3	126.71
5	121.69
7	141.12
8	129.54
9	138.76
11	140.76
13	139.33
15	135.86
16	143.78
17	132.12
18	137.77
19	127.26
20	124.88
21	123.53
22	126.02
23	125.47
29	146.43
30	134.35
32	130.27
33	124.87
34	126.41
35	124.22
36	131.26

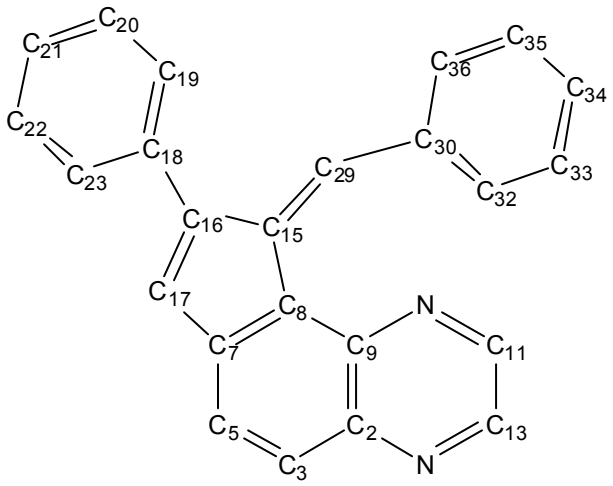
Figure S3. (continued)

ISOMER 2



Proton	Chemical Shift (ppm)
4	7.97
6	7.78
12	8.09
14	8.49
24	7.66
25	7.62
26	7.50
27	7.70
28	7.39
31	7.38
37	7.37
38	7.05
39	7.38
40	7.48
41	7.49
42	6.90

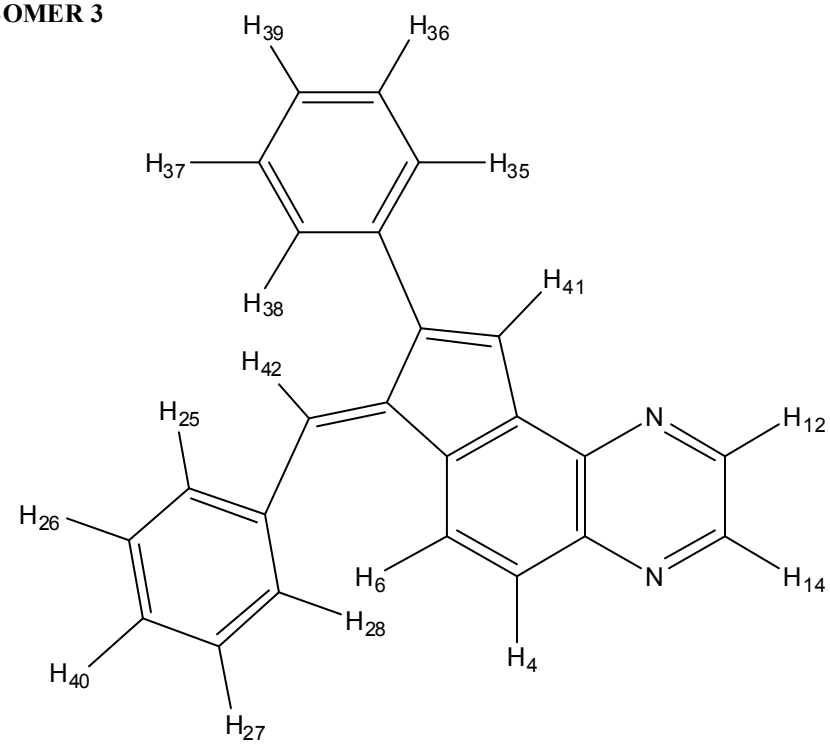
ISOMER 2



Carbon	Chemical Shift (ppm)
2	139.40
3	128.61
5	121.94
7	145.37
8	129.17
9	138.15
11	139.44
13	139.97
15	136.16
16	151.45
17	123.51
18	136.13
19	128.01
20	125.25
21	124.77
22	126.58
23	125.48
29	144.93
30	136.33
32	130.97
33	124.07
34	127.07
35	124.71
36	129.66

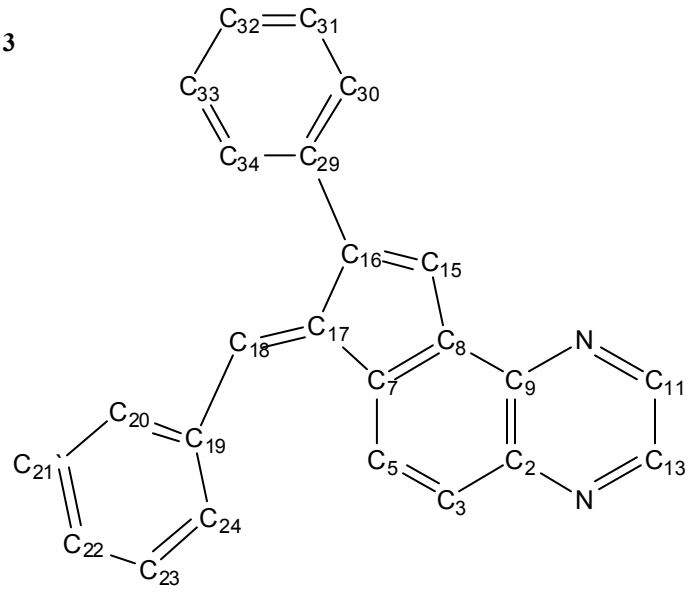
Figure S3. (continued)

ISOMER 3



Proton	Chemical Shift (ppm)
4	7.73
6	8.27
12	8.75
14	8.70
25	7.53
26	7.53
27	7.69
28	8.06
35	7.78
36	7.54
37	7.49
38	7.33
39	7.48
40	7.59
41	7.84
42	7.71

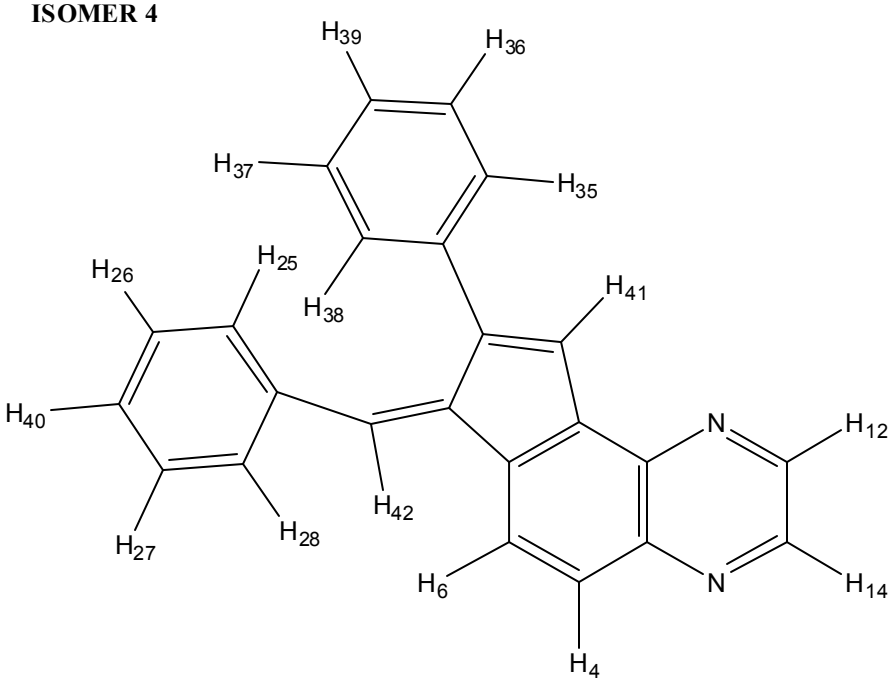
ISOMER 3



Carbon	Chemical Shift (ppm)
2	141.98
3	122.09
5	122.62
7	131.74
8	139.99
9	134.95
11	141.19
13	141.51
15	124.84
16	144.78
17	137.78
18	142.71
19	134.67
20	129.05
21	126.10
22	127.70
23	125.55
24	128.48
29	134.82
30	127.24
31	126.18
32	124.54
33	124.79
34	129.32

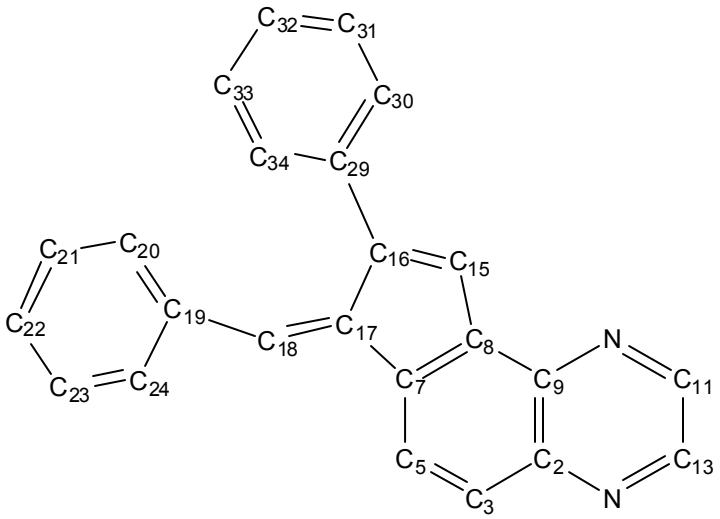
Figure S3. (continued)

ISOMER 4



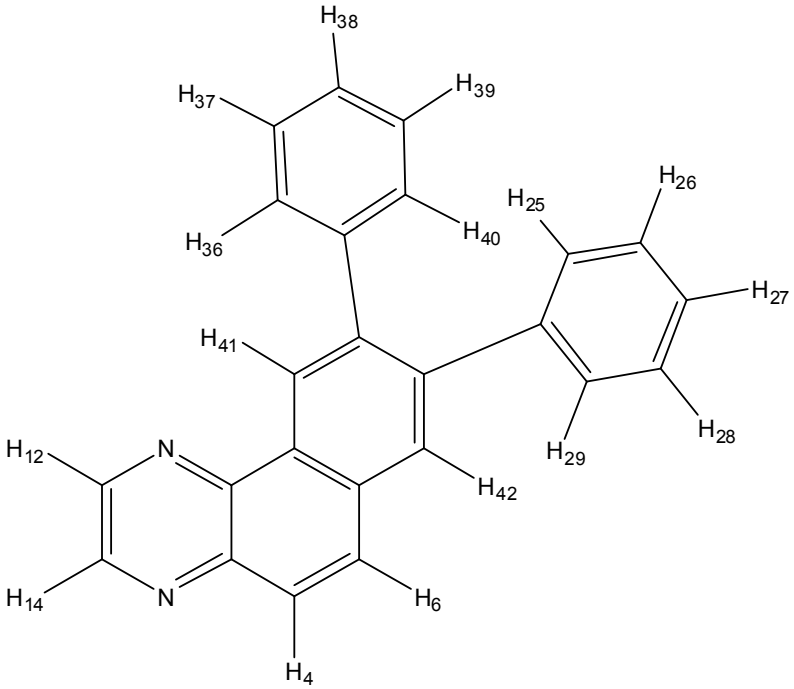
Proton	Chemical Shift (ppm)
4	7.91
6	8.17
12	8.72
14	8.71
25	7.08
26	6.84
27	7.46
28	7.65
35	7.80
36	7.47
37	6.93
38	6.98
39	7.09
40	7.21
41	7.86
42	8.22

ISOMER 4

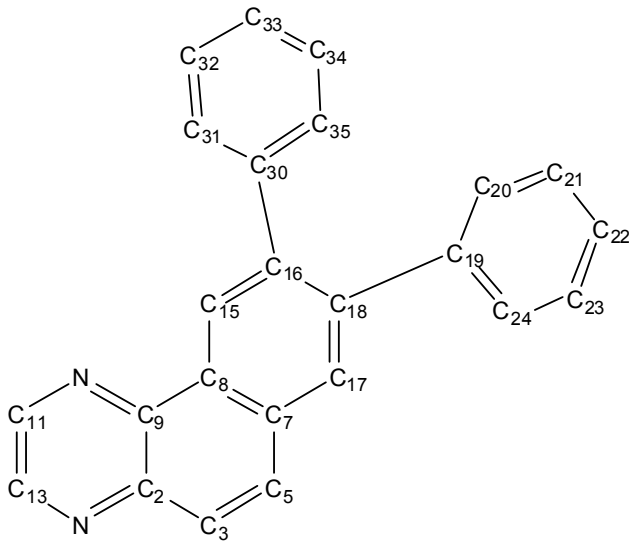


Carbon	Chemical Shift (ppm)
2	141.86
3	123.02
5	118.91
7	137.89
8	136.44
9	135.35
11	141.19
13	141.11
15	131.51
16	140.60
17	134.72
18	138.04
19	133.20
20	131.04
21	124.33
22	127.21
23	125.40
24	130.47
29	138.96
30	125.85
31	127.04
32	123.34
33	125.77
34	126.76

Figure S4. Calculated NMR chemical shifts for C^1-C^6 product from cyclization of **4**.

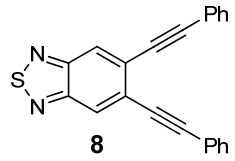


Proton	Chemical Shift (ppm)
4	8.06
6	8.23
12	8.80
14	8.85
25	6.91
26	7.16
27	7.36
28	7.56
29	7.79
36	7.86
37	7.56
38	7.40
39	7.09
40	6.87
41	9.33
42	7.98



Carbon	Chemical Shift (ppm)
2	141.85
3	125.37
5	130.58
7	129.55
8	126.43
9	140.32
11	140.36
13	141.91
15	124.71
16	140.52
17	127.77
18	141.45
19	139.84
20	129.31
21	124.34
22	124.25
23	125.55
24	127.69
30	139.61
31	127.92
32	125.67
33	124.39
34	124.09
35	129.53

^{1}H NMR Spectrum of **8** (500 MHz, $CDCl_3$)



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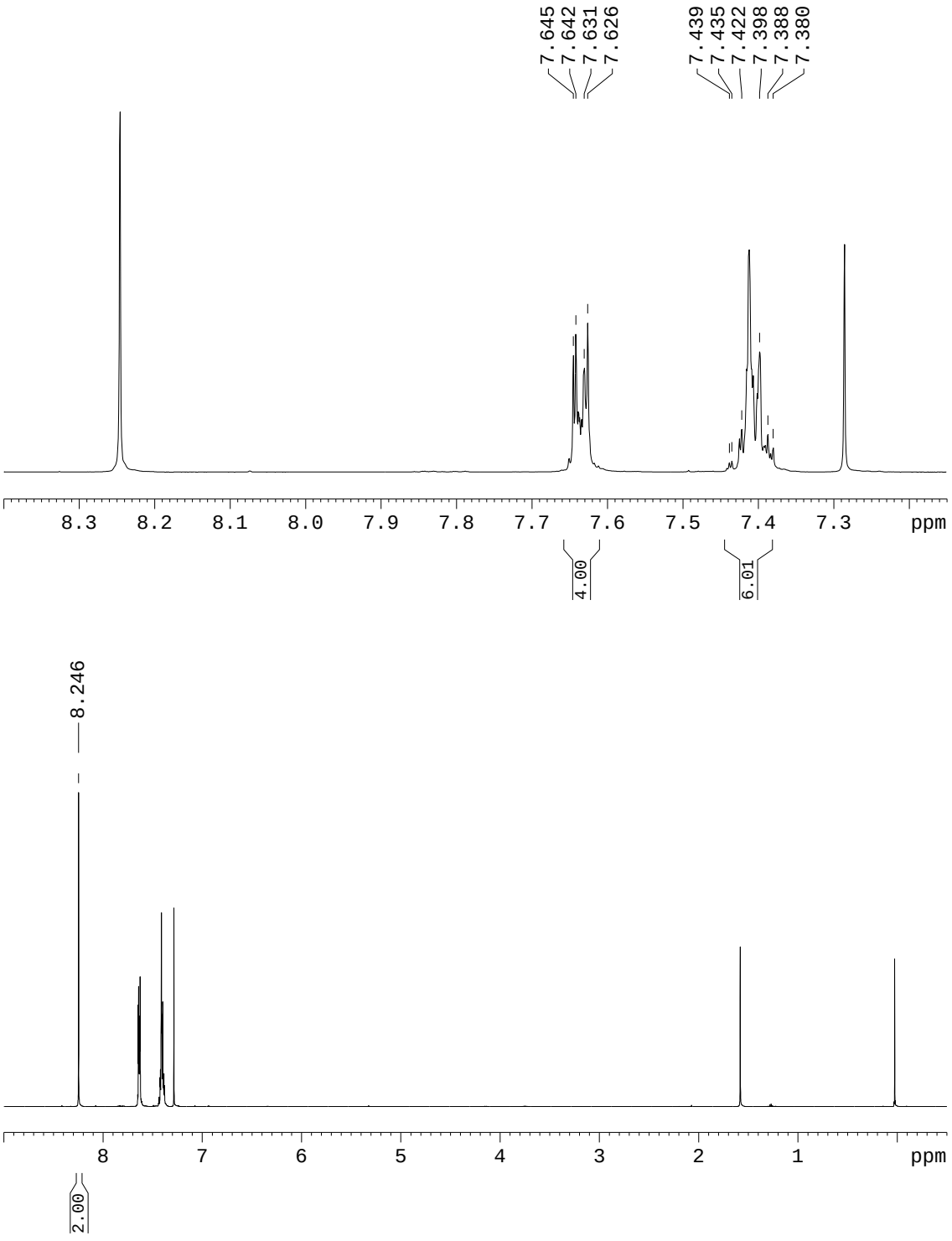
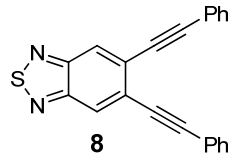
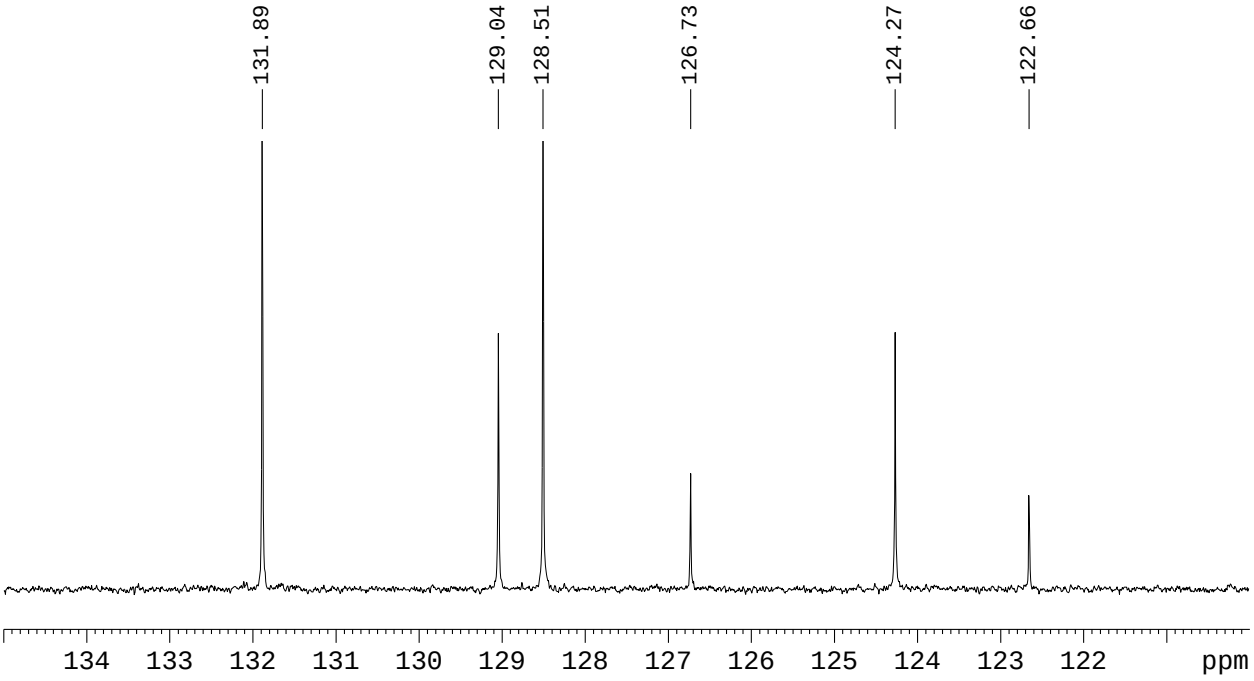
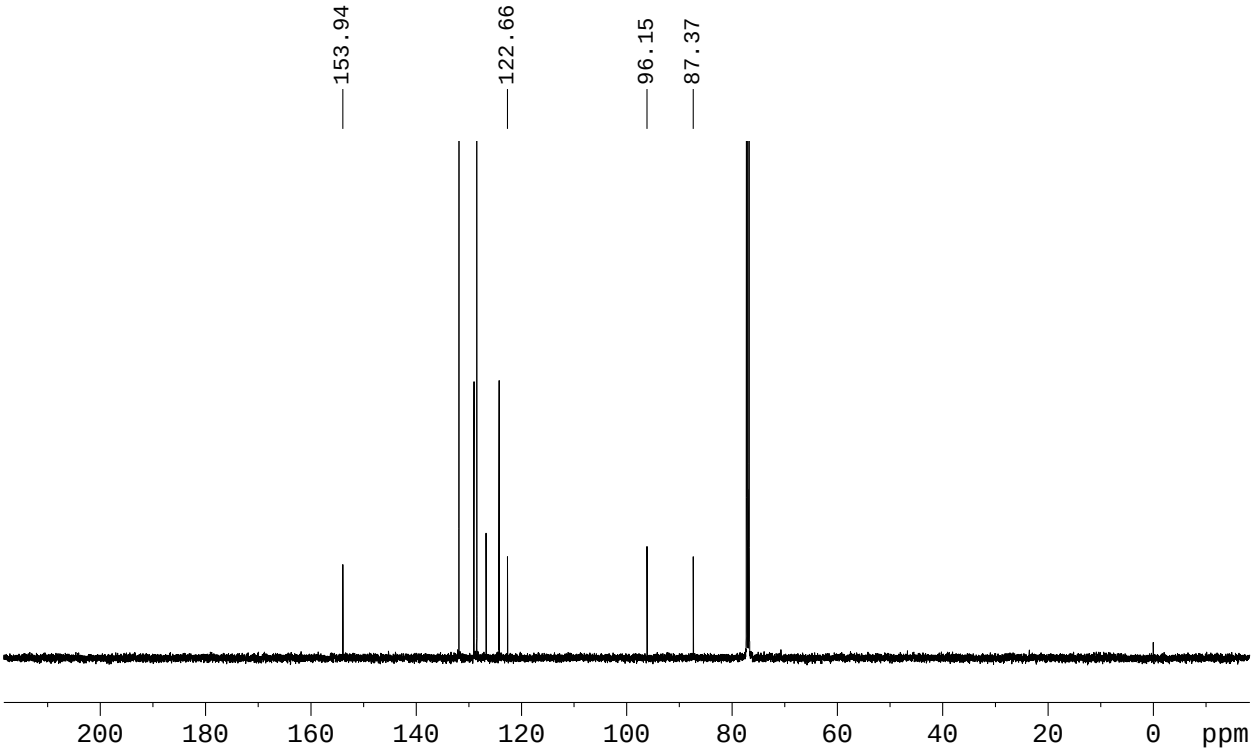


^{13}C NMR Spectrum of **8** (125 MHz, $CDCl_3$)

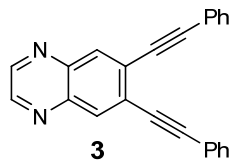


8

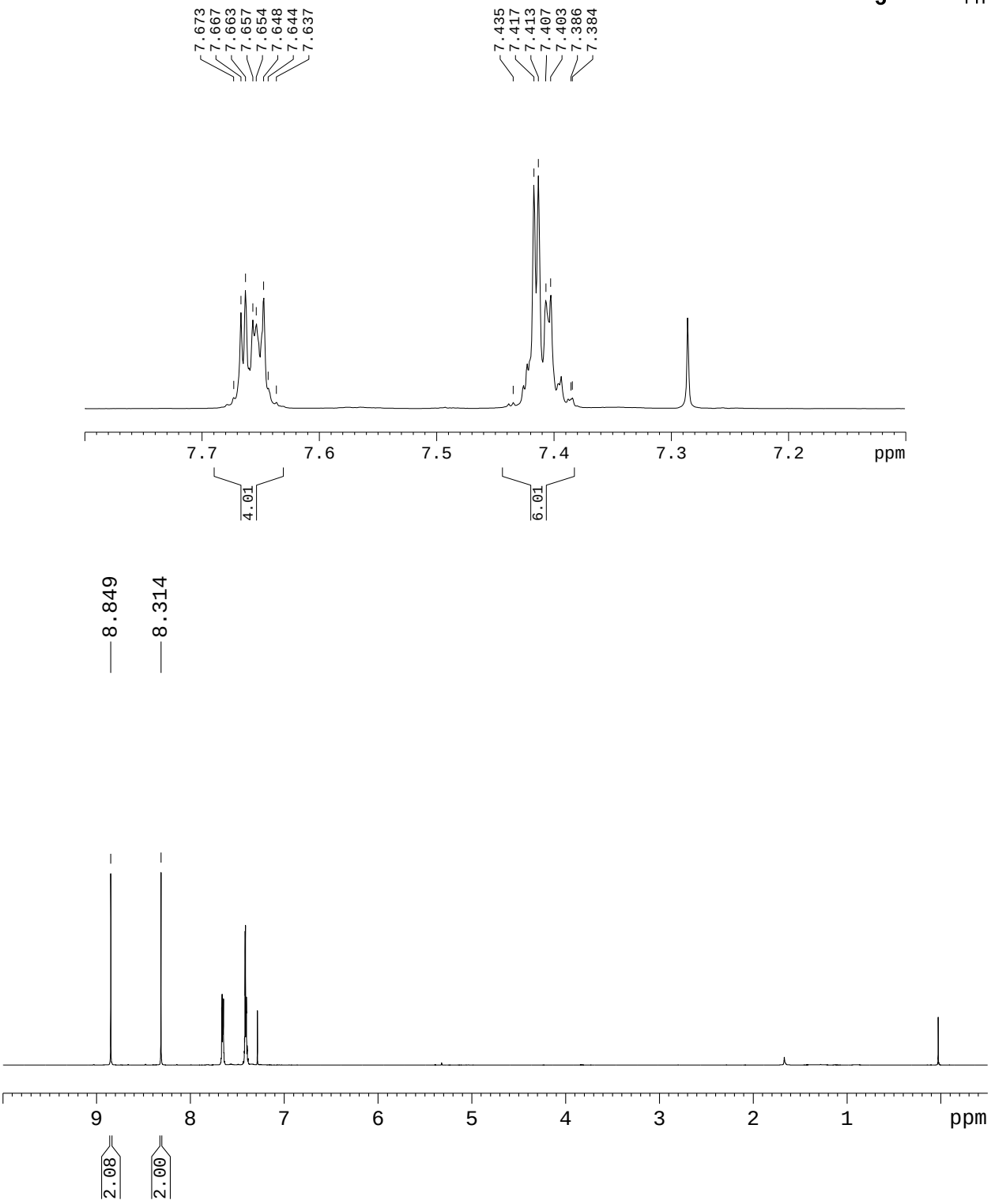




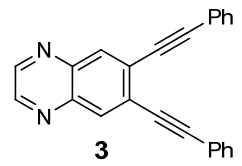
^{1}H NMR Spectrum of **3** (500 MHz, $CDCl_3$)



3



^{13}C NMR Spectrum of **3** (125 MHz, $CDCl_3$)



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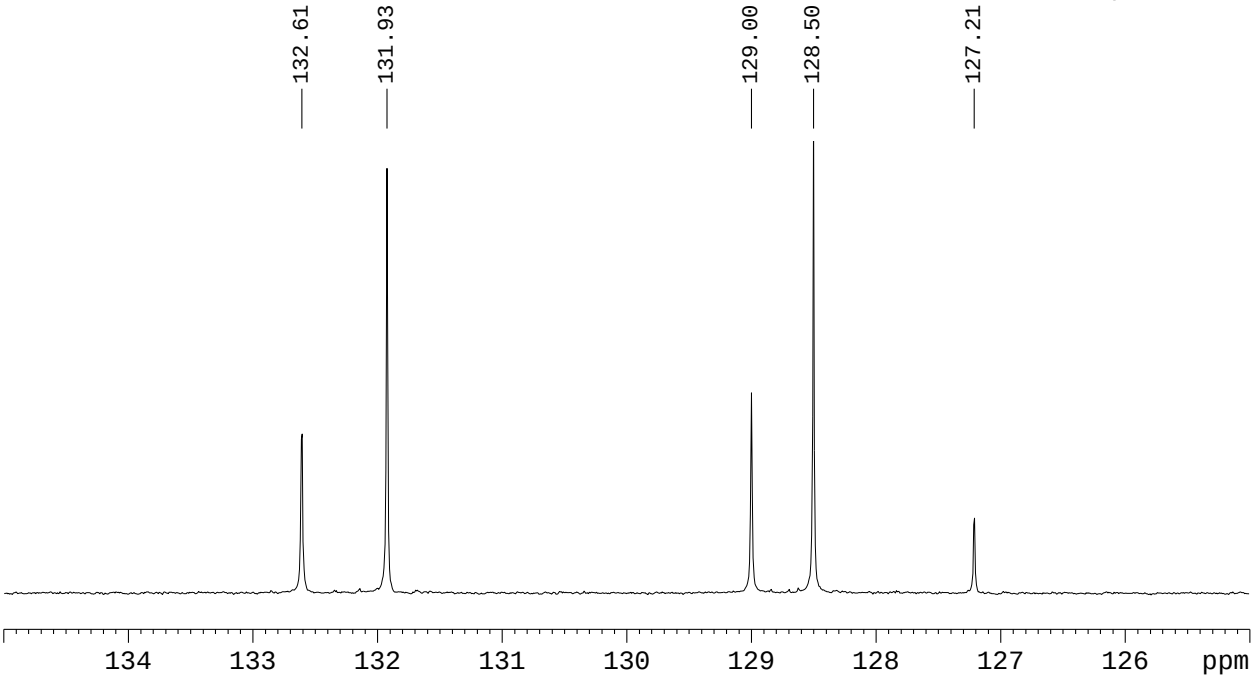
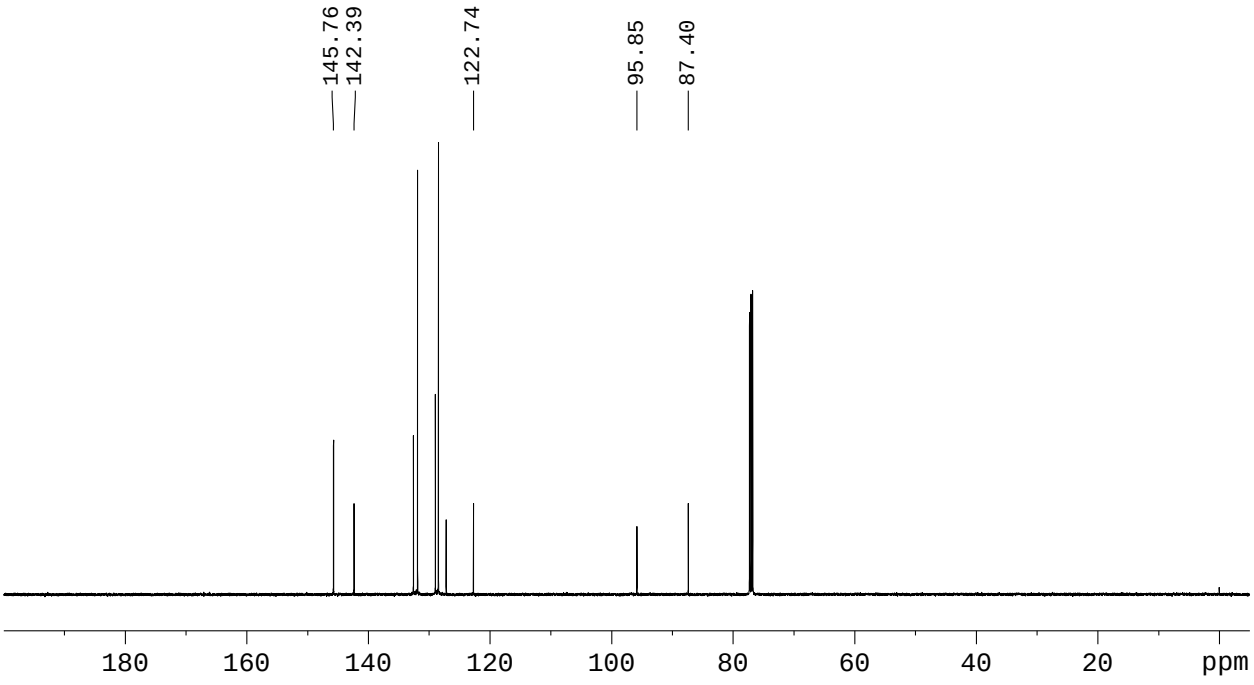
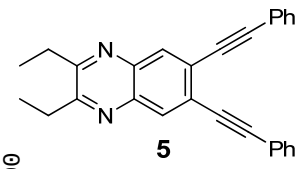
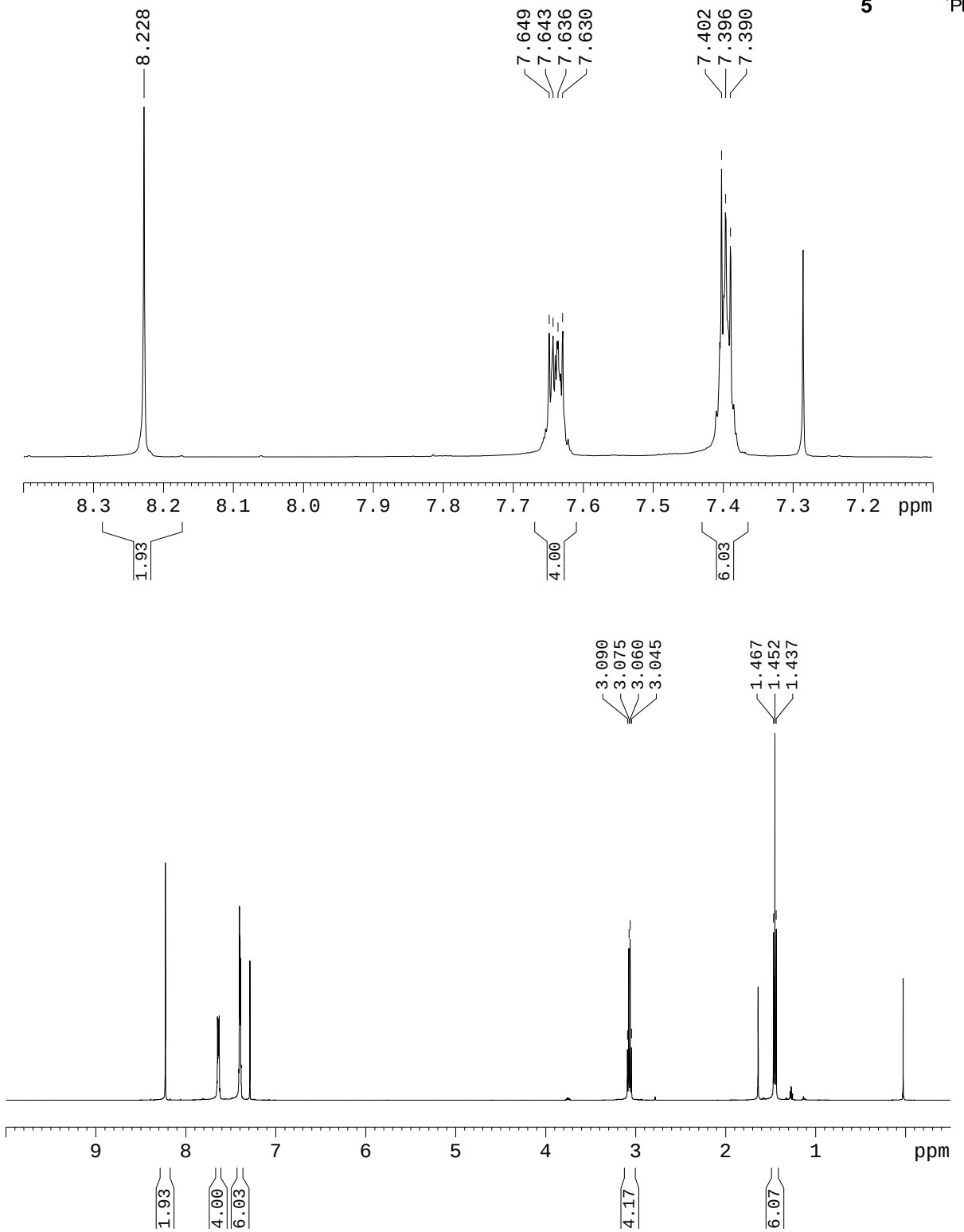




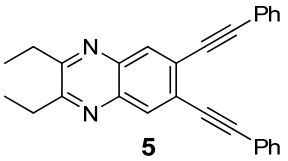
^{1}H NMR Spectrum of **5** (500 MHz, $CDCl_3$)



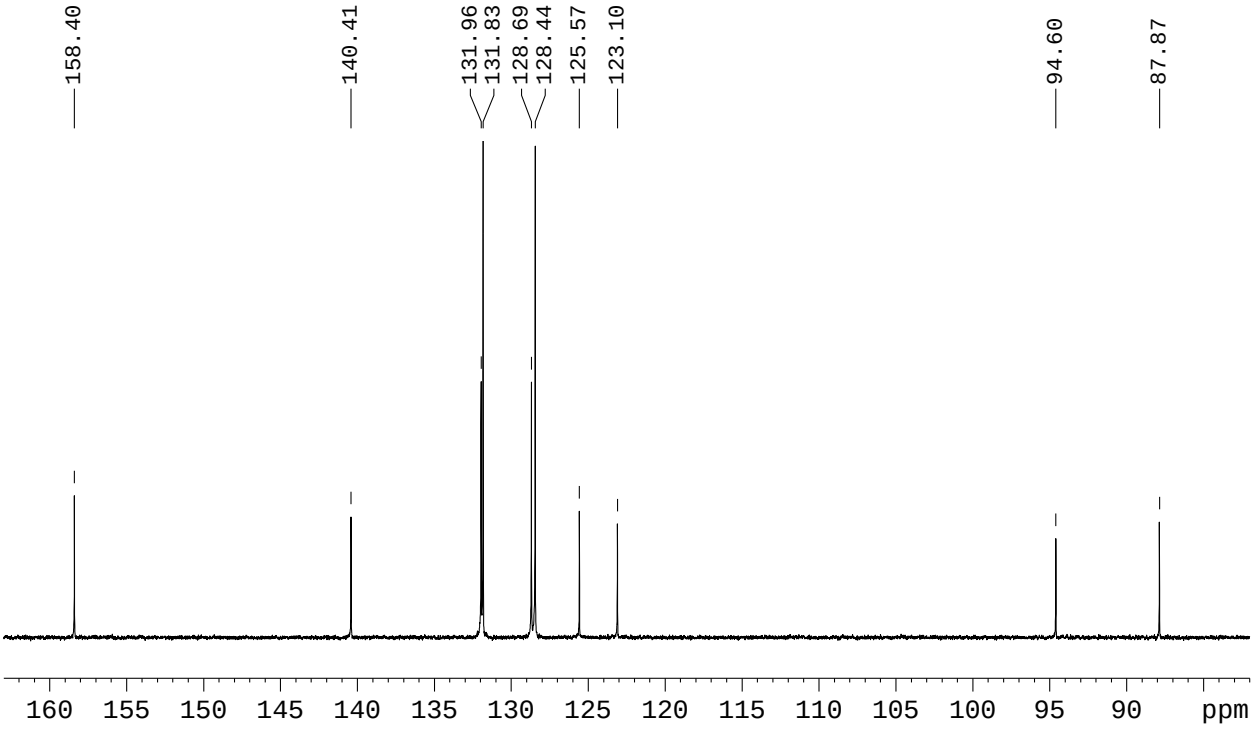
5

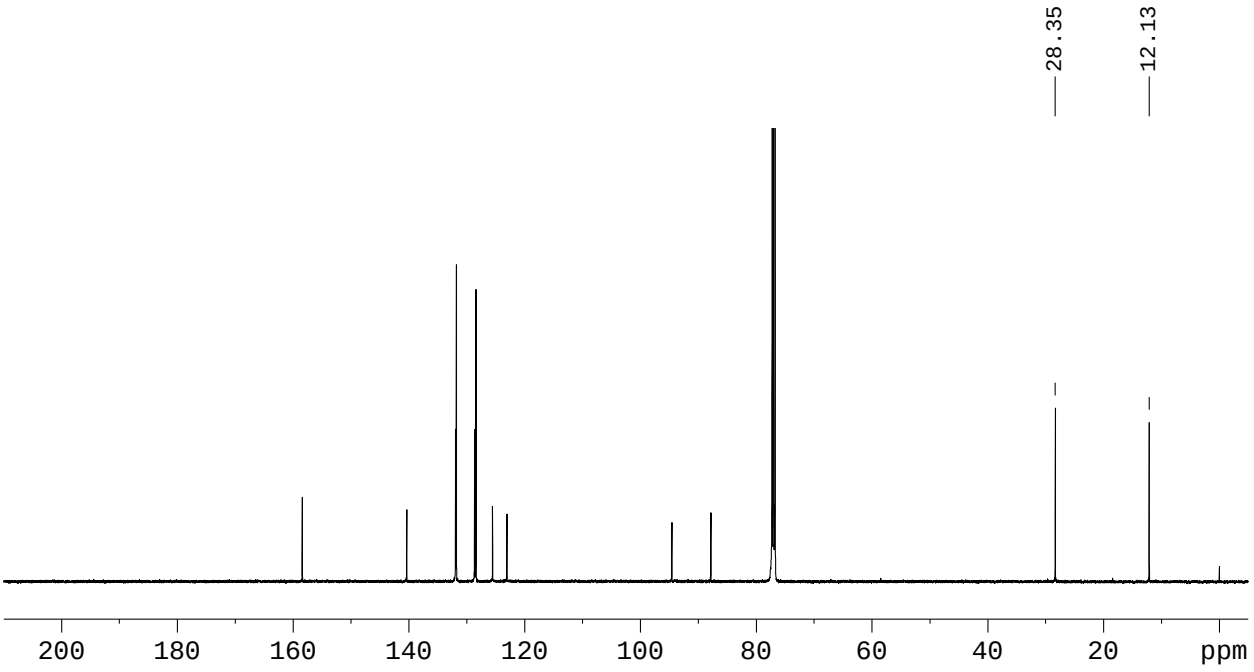


^{13}C NMR Spectrum of **5** (125 MHz, $CDCl_3$)

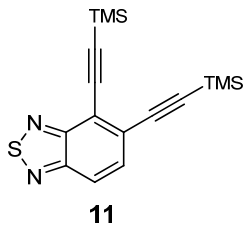


5

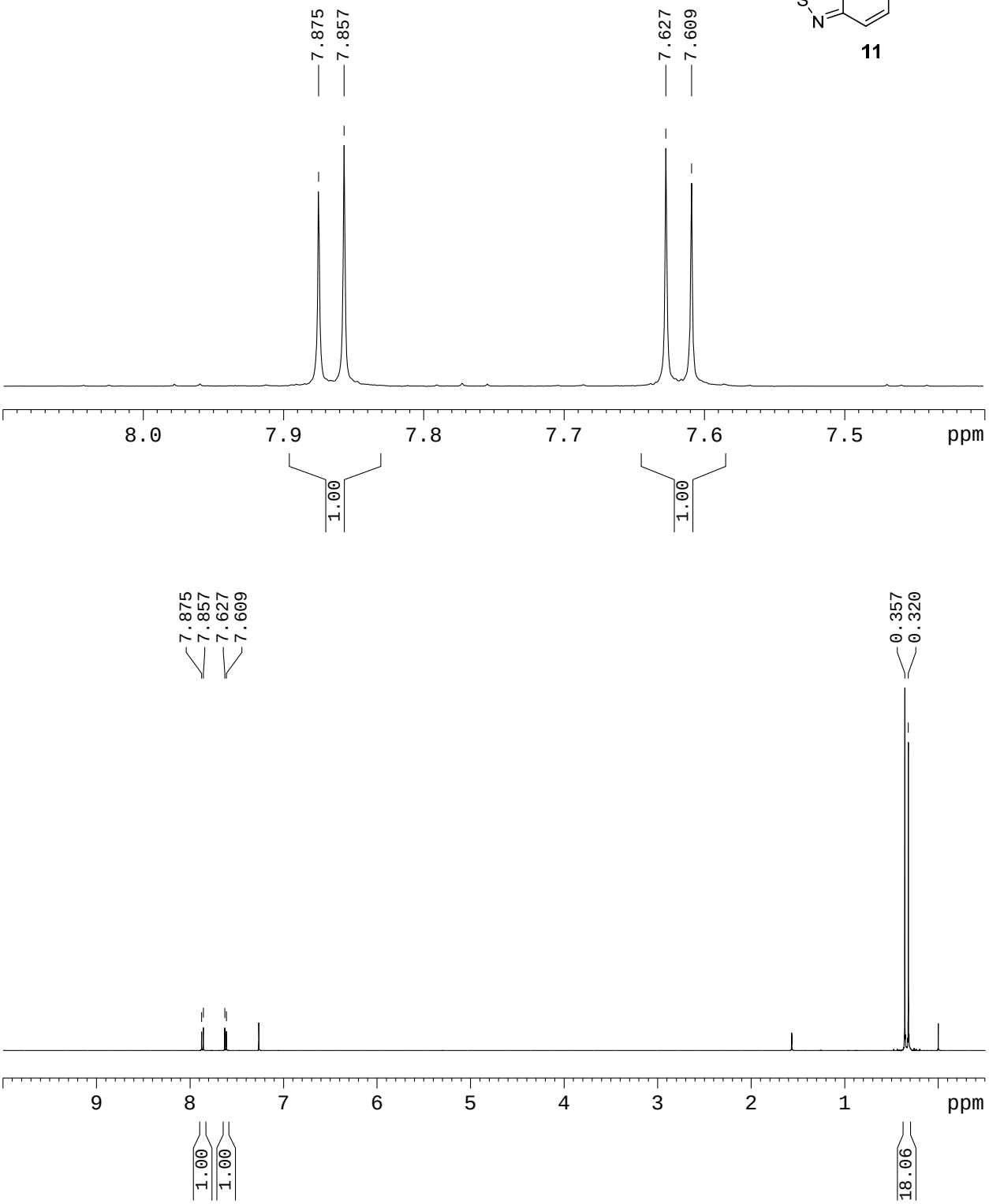




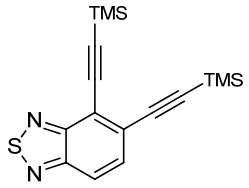
^{1}H NMR Spectrum of **11** (500 MHz, $CDCl_3$)



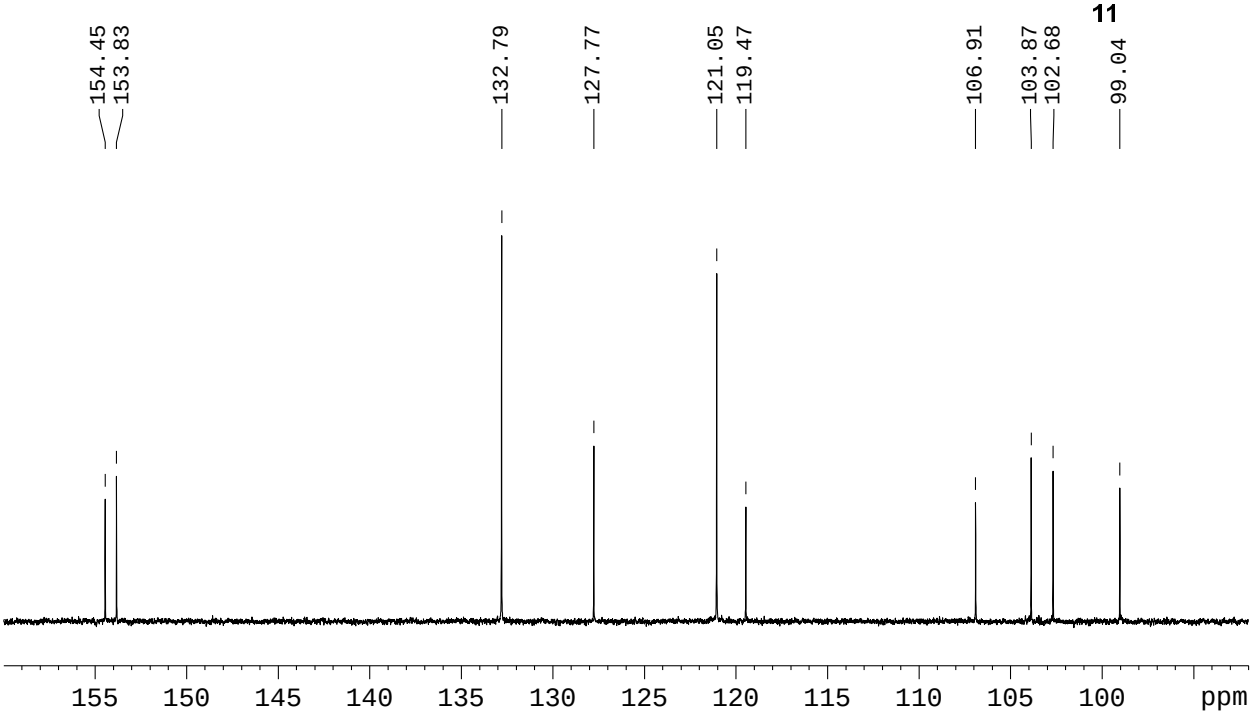
11

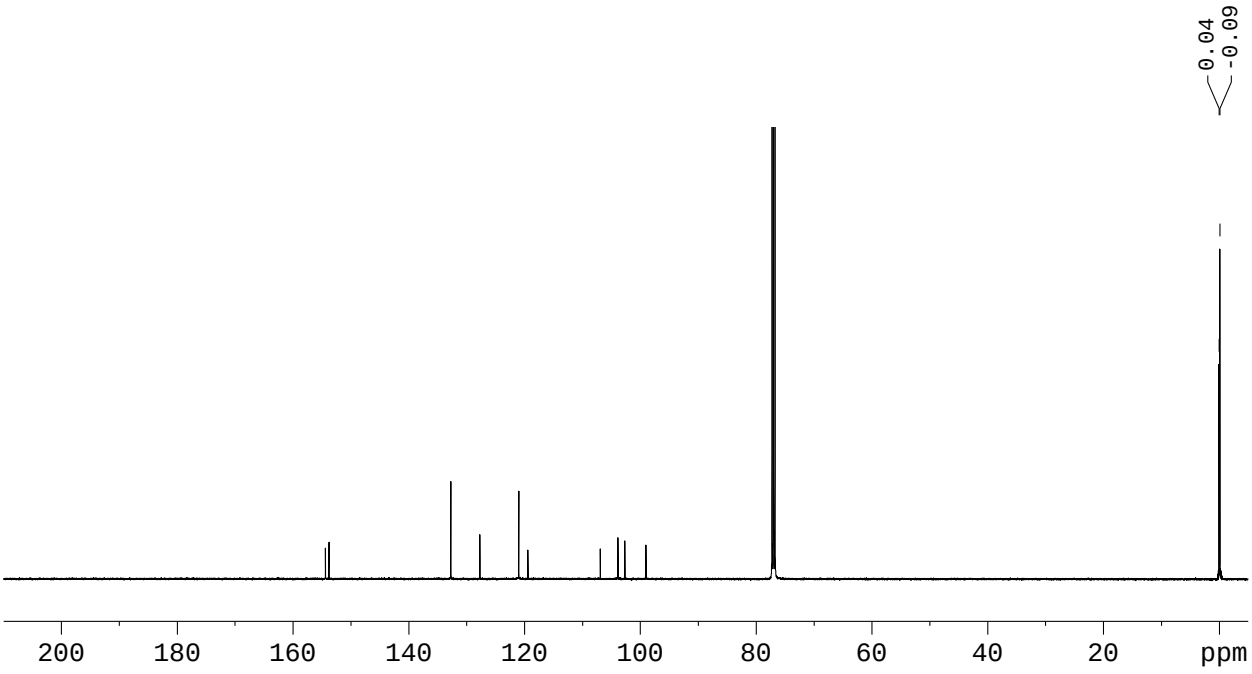


^{13}C NMR Spectrum of **11** (125 MHz, $CDCl_3$)

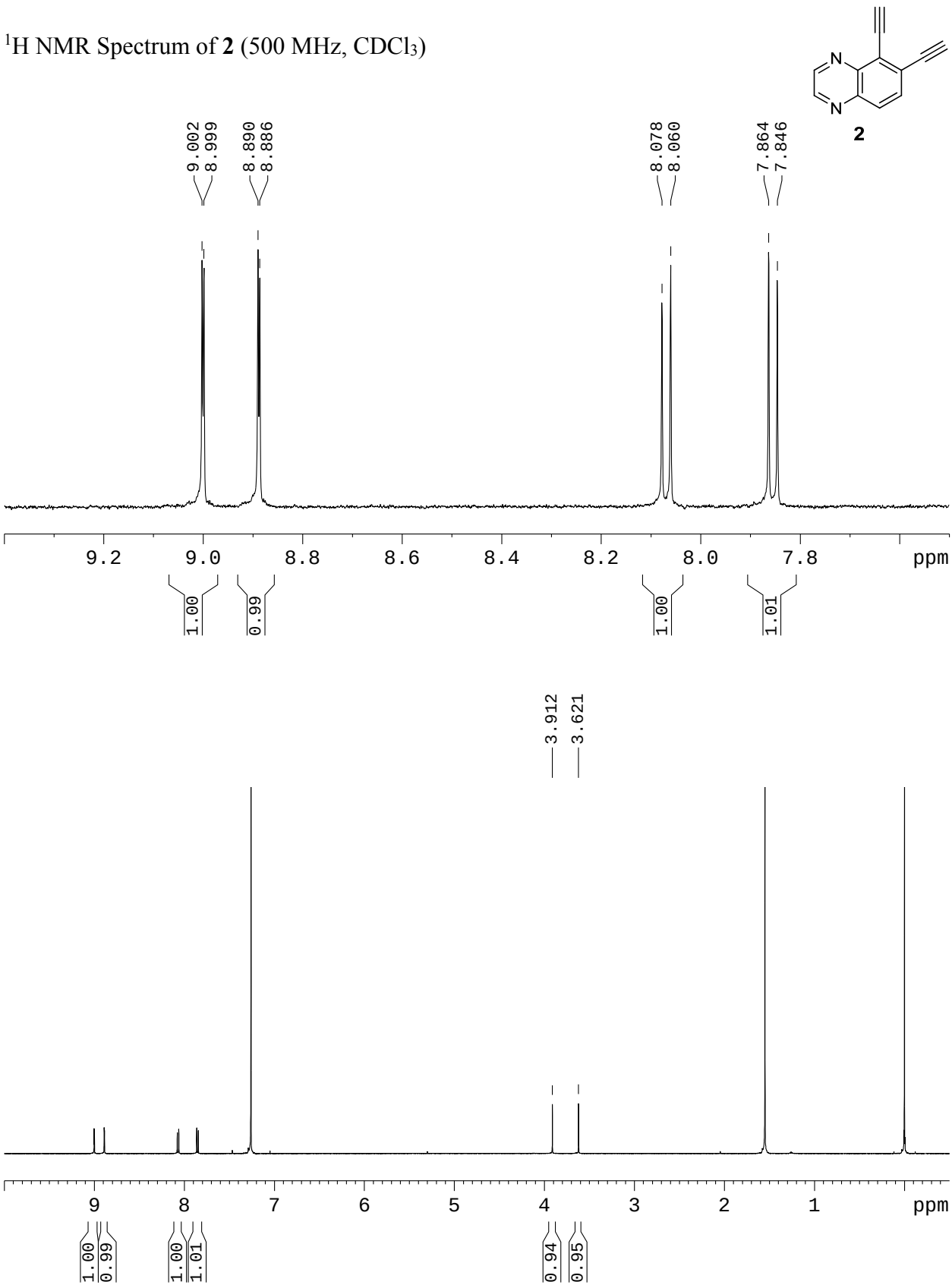


11

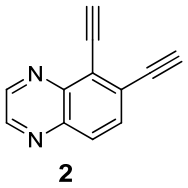




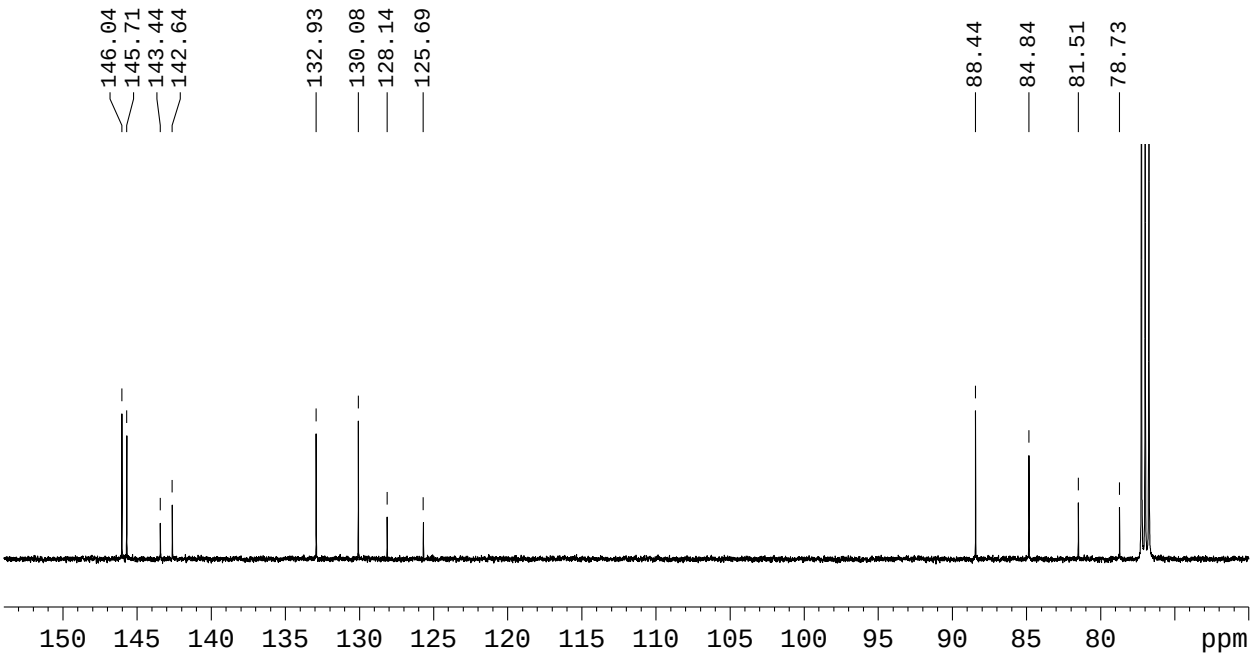
^{1}H NMR Spectrum of **2** (500 MHz, $CDCl_3$)

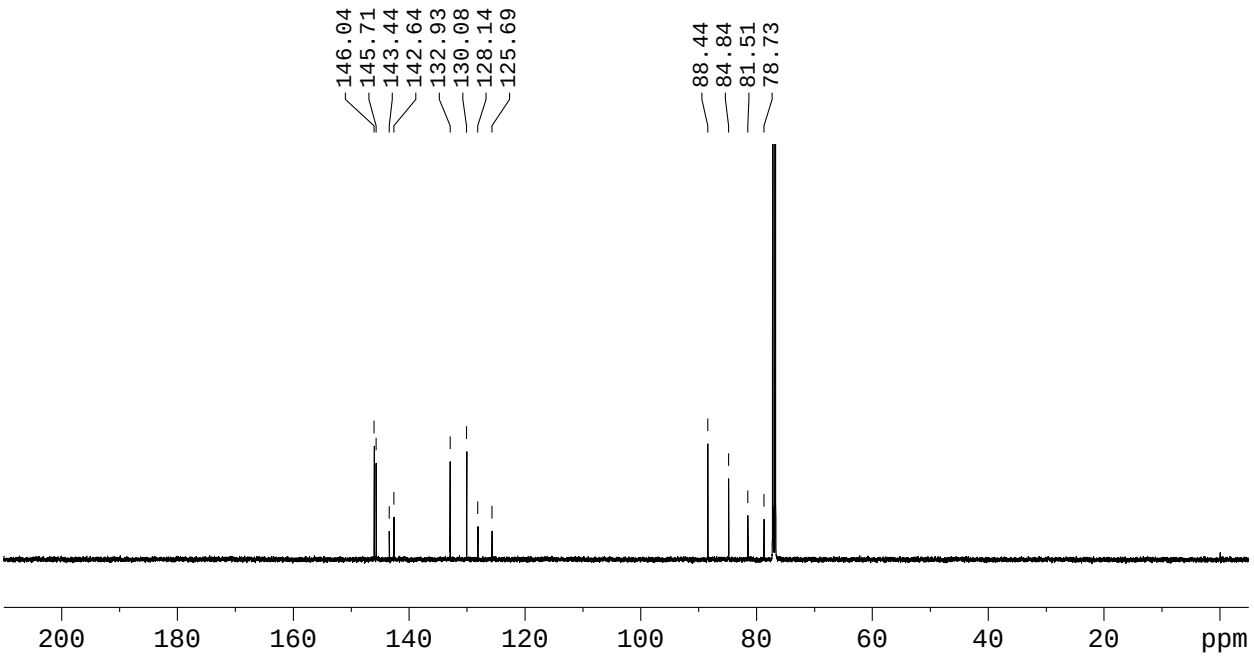


^{13}C NMR Spectrum of **2** (125 MHz, $CDCl_3$)

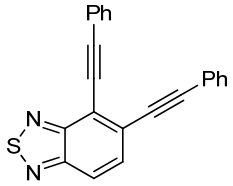


2

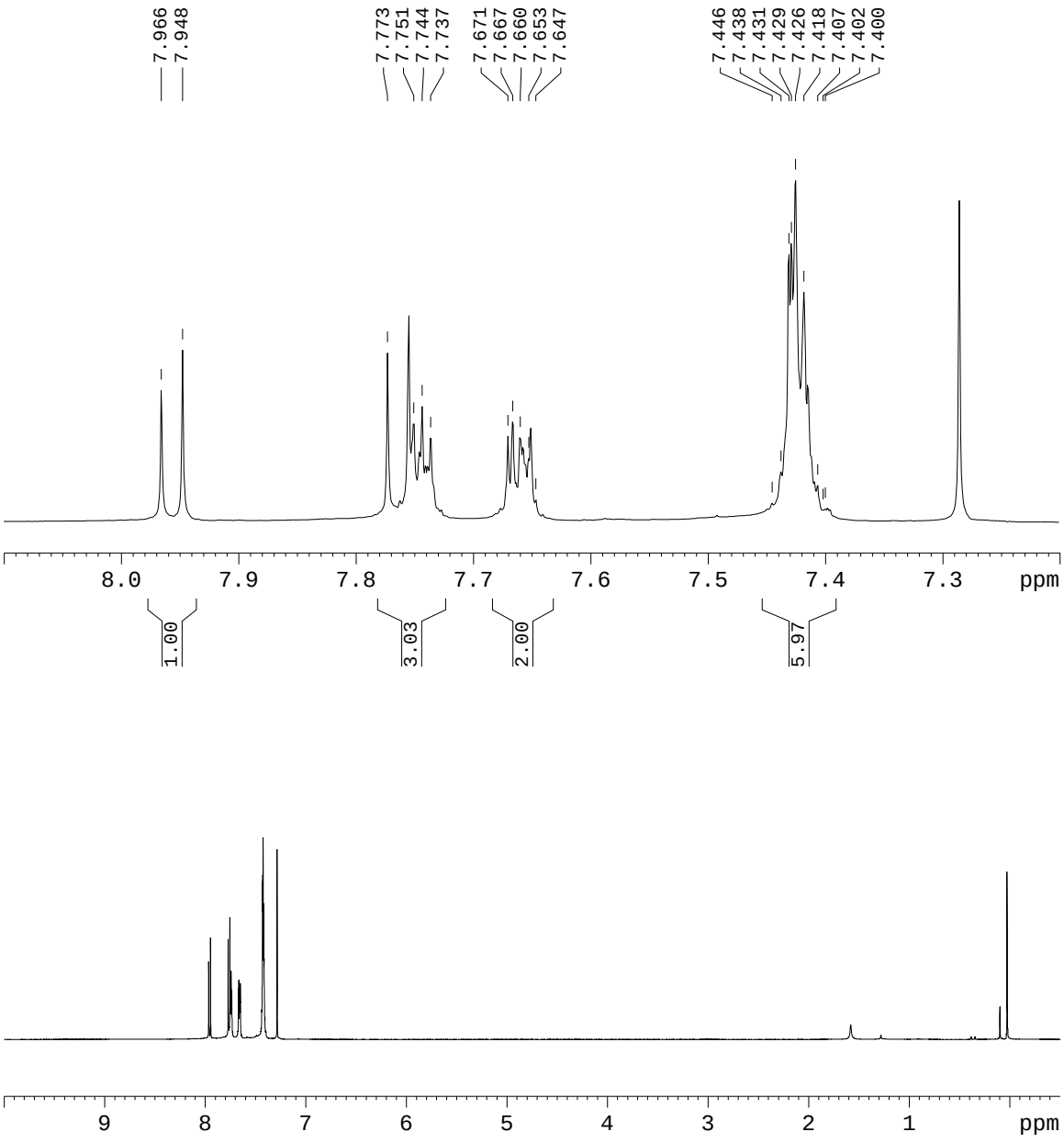




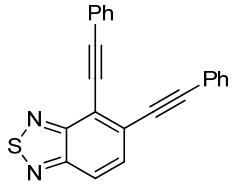
^{1}H NMR Spectrum of **13** (500 MHz, $CDCl_3$)



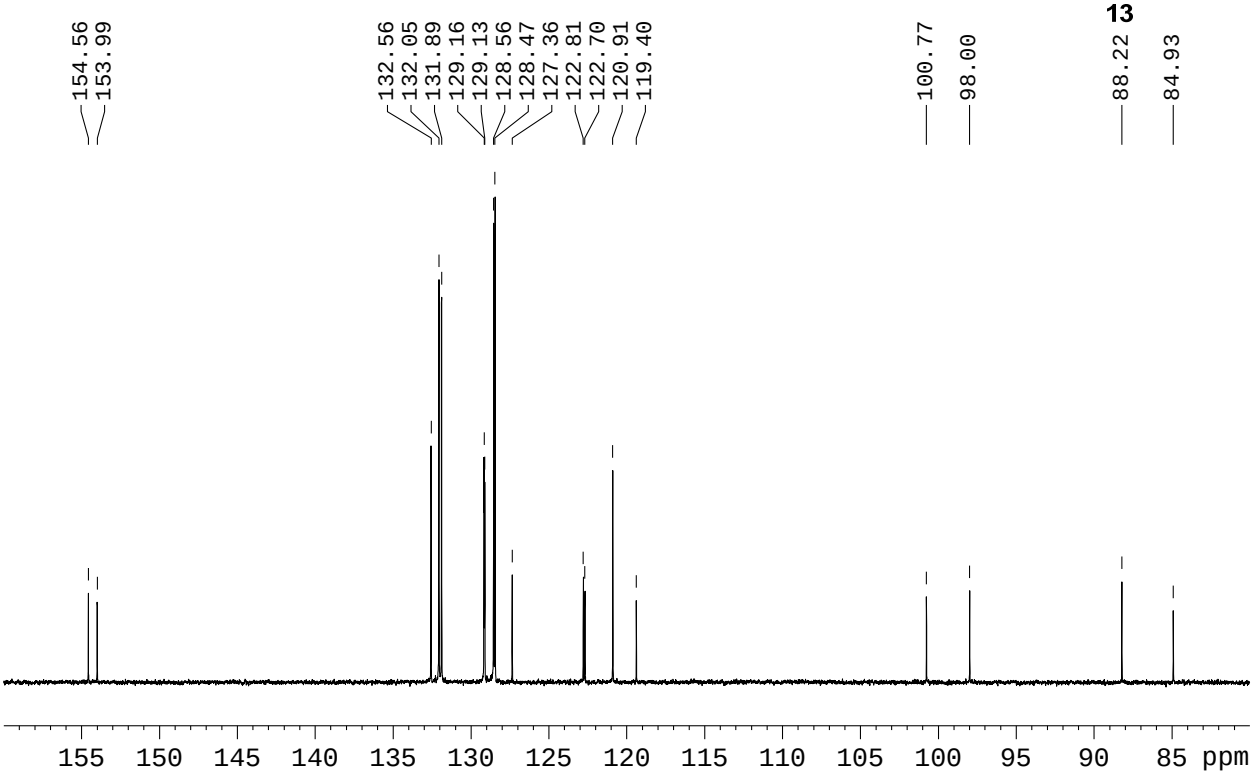
13

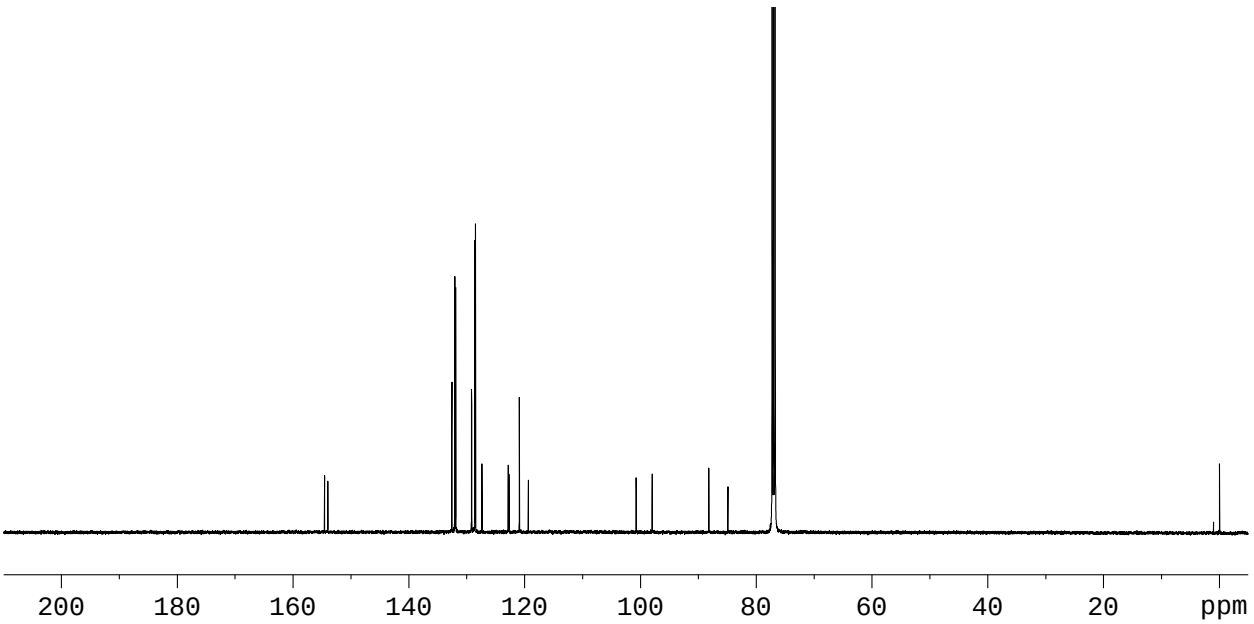


^{13}C NMR Spectrum of **13** (125 MHz, $CDCl_3$)

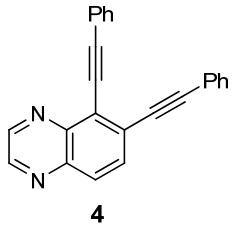


13

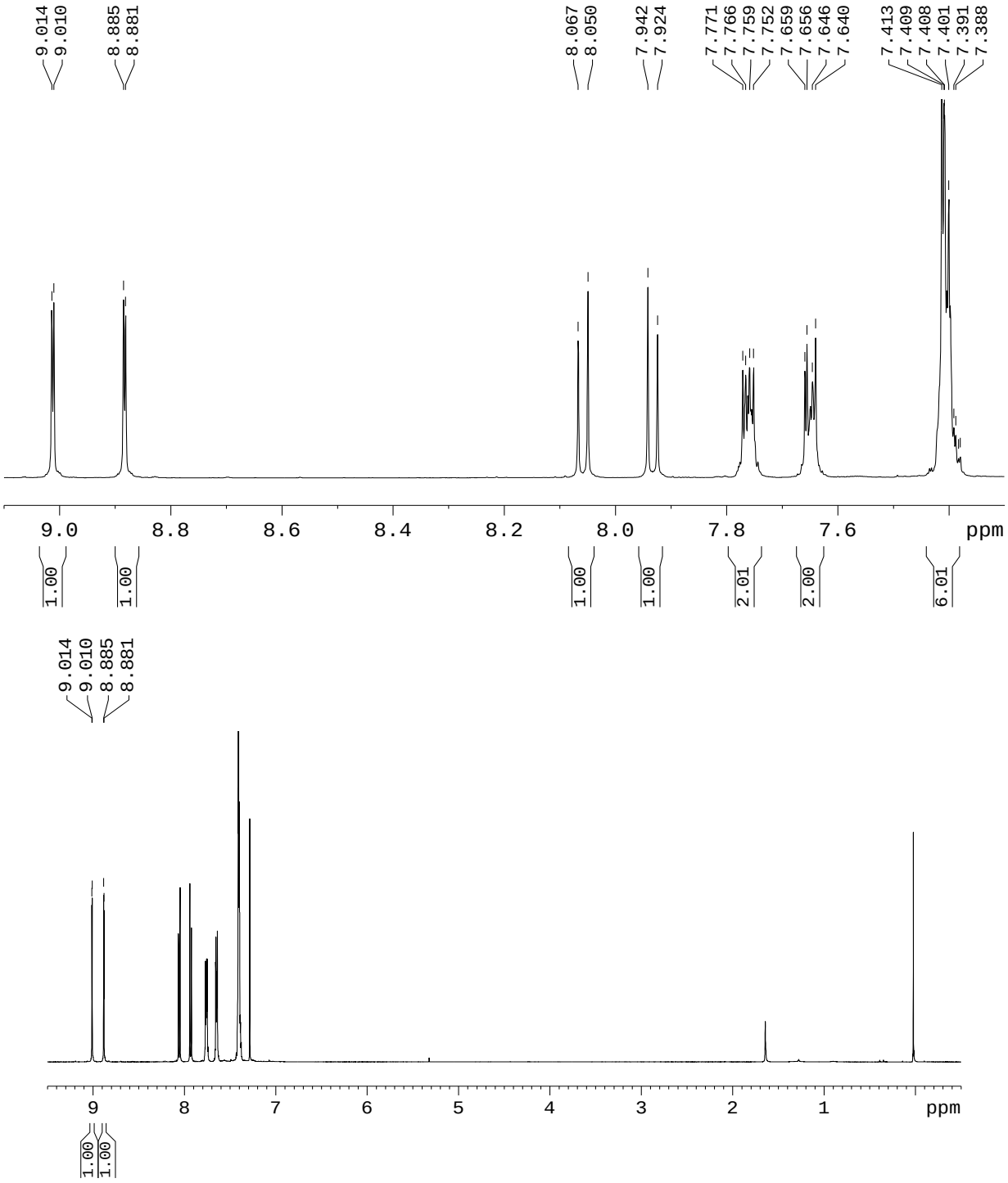




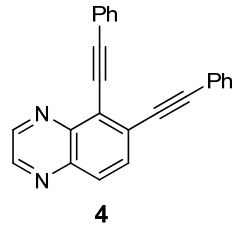
^{1}H NMR Spectrum of **4** (500 MHz, $CDCl_3$)



4



^{13}C NMR Spectrum of **4** (125 MHz, $CDCl_3$)



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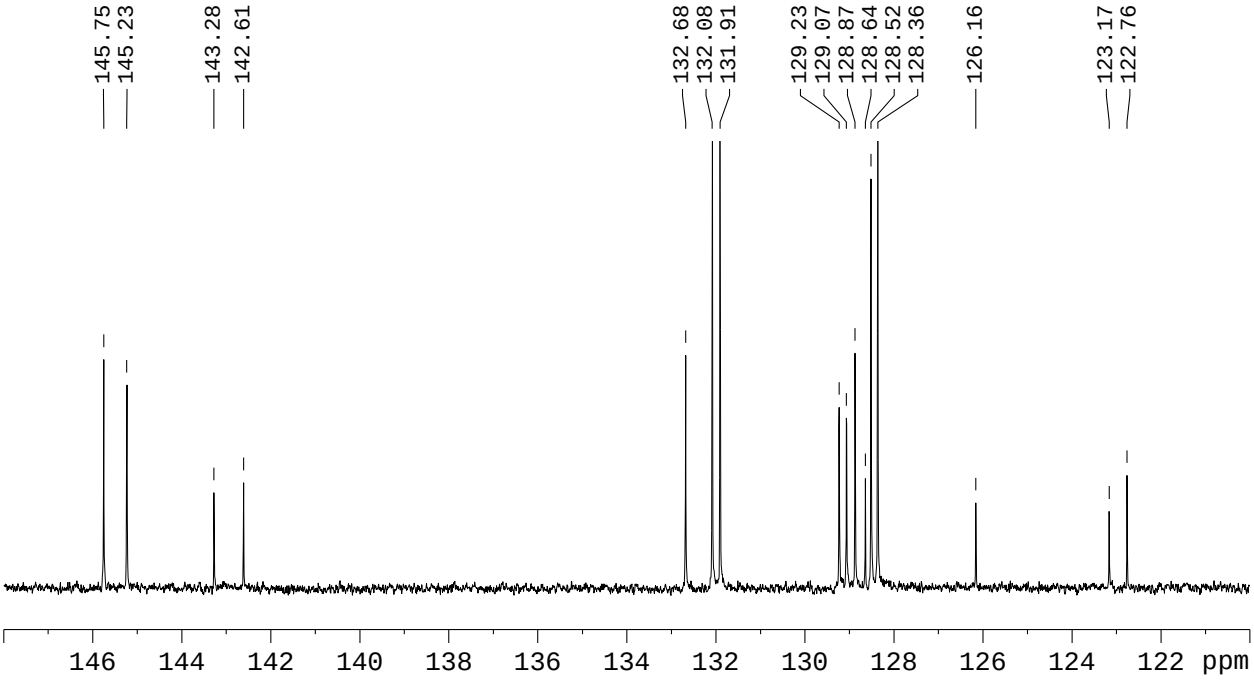
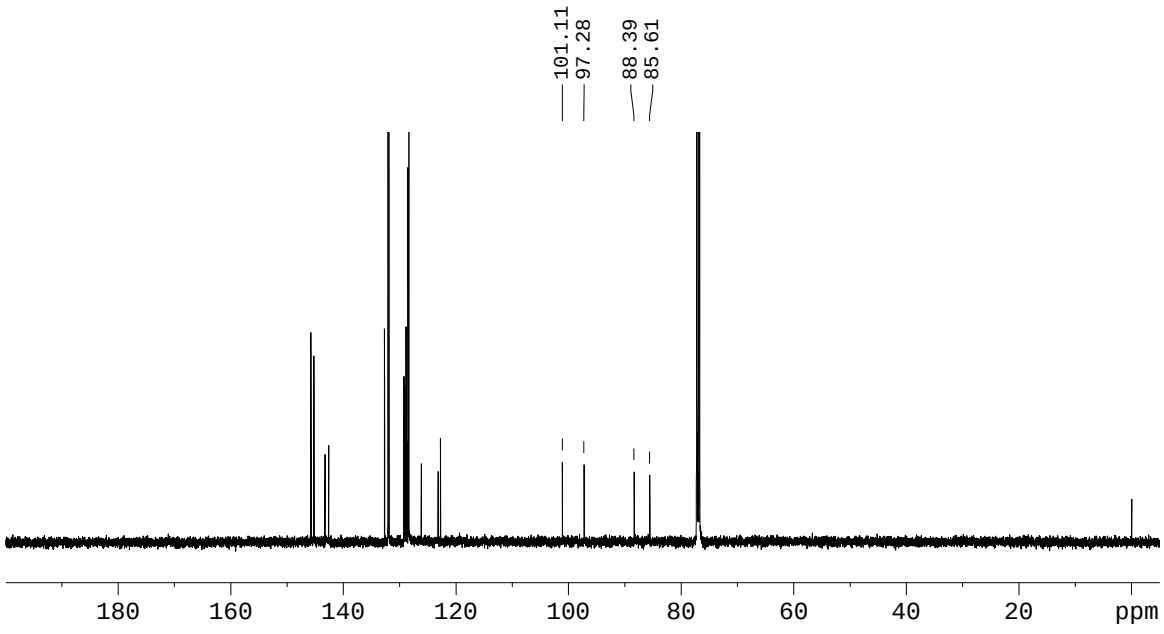
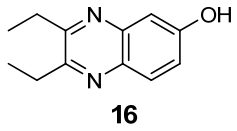
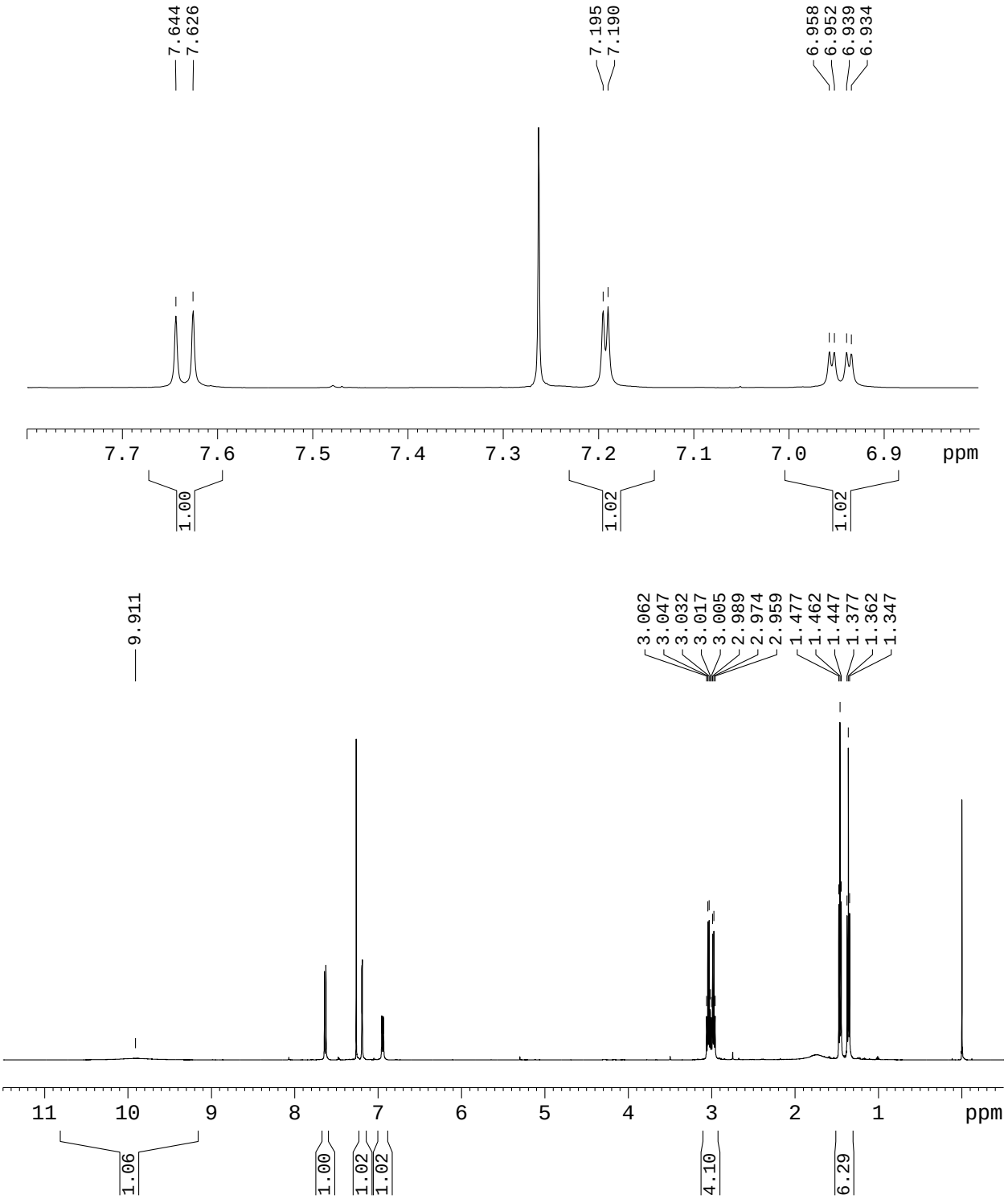




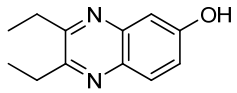
^{1}H NMR Spectrum of **16** (500 MHz, $CDCl_3$)



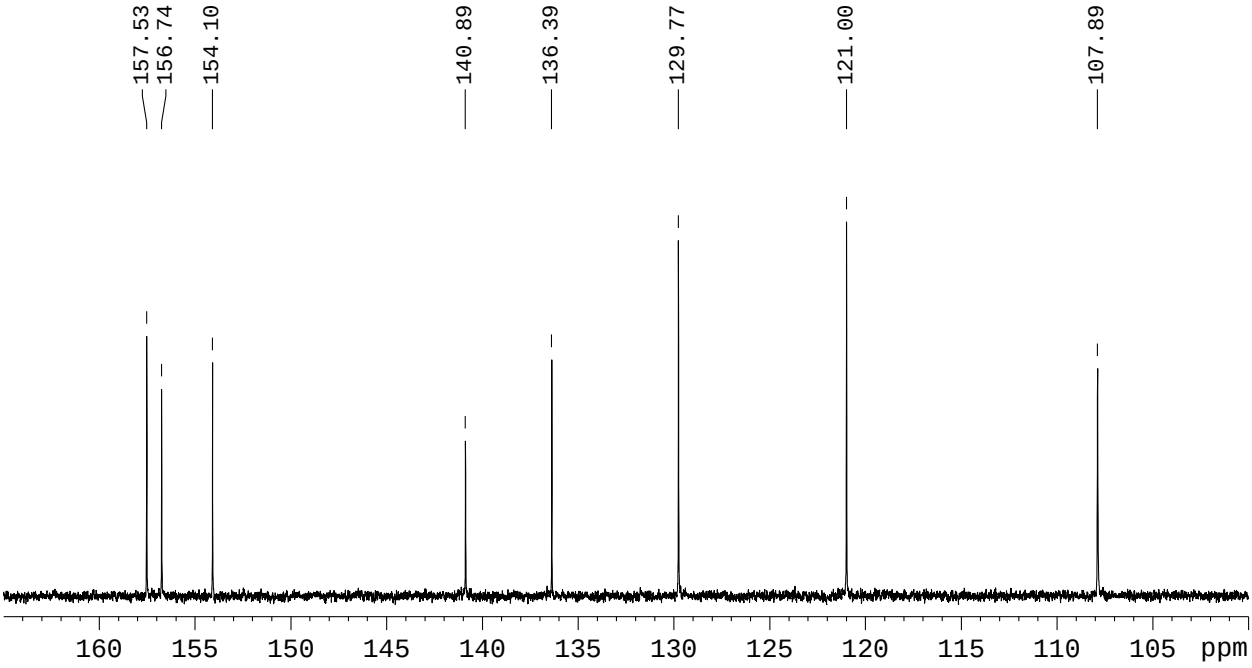
16

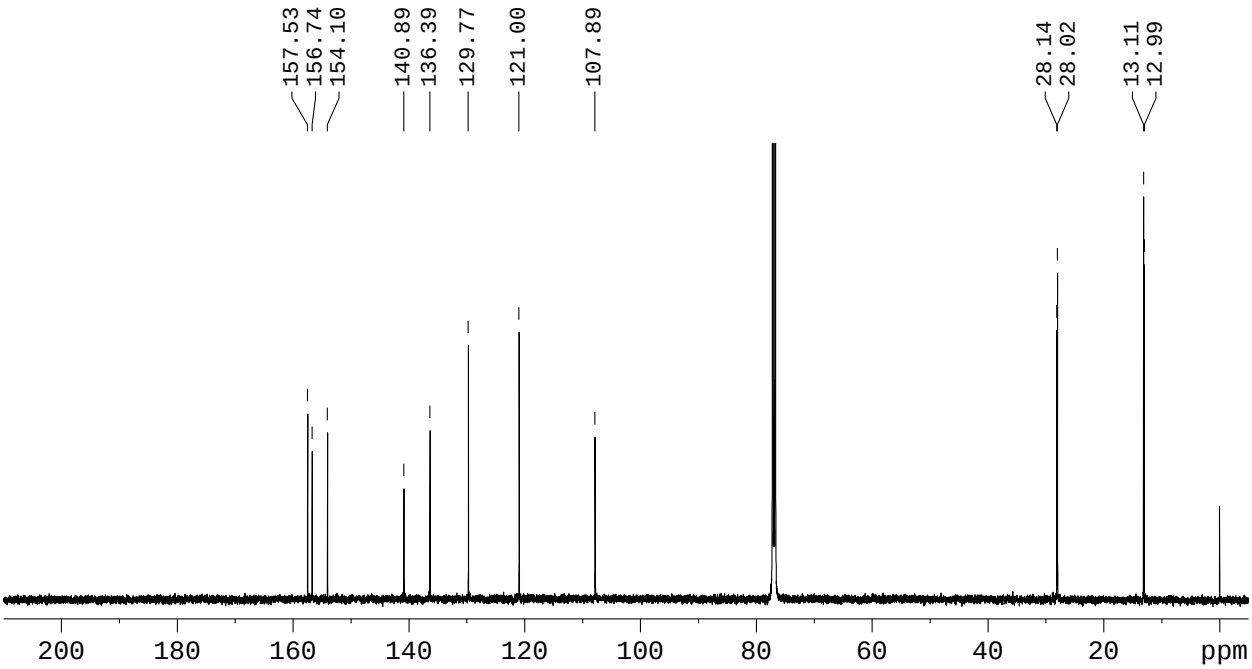


^{13}C NMR Spectrum of **16** (125 MHz, $CDCl_3$)

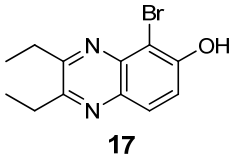


16

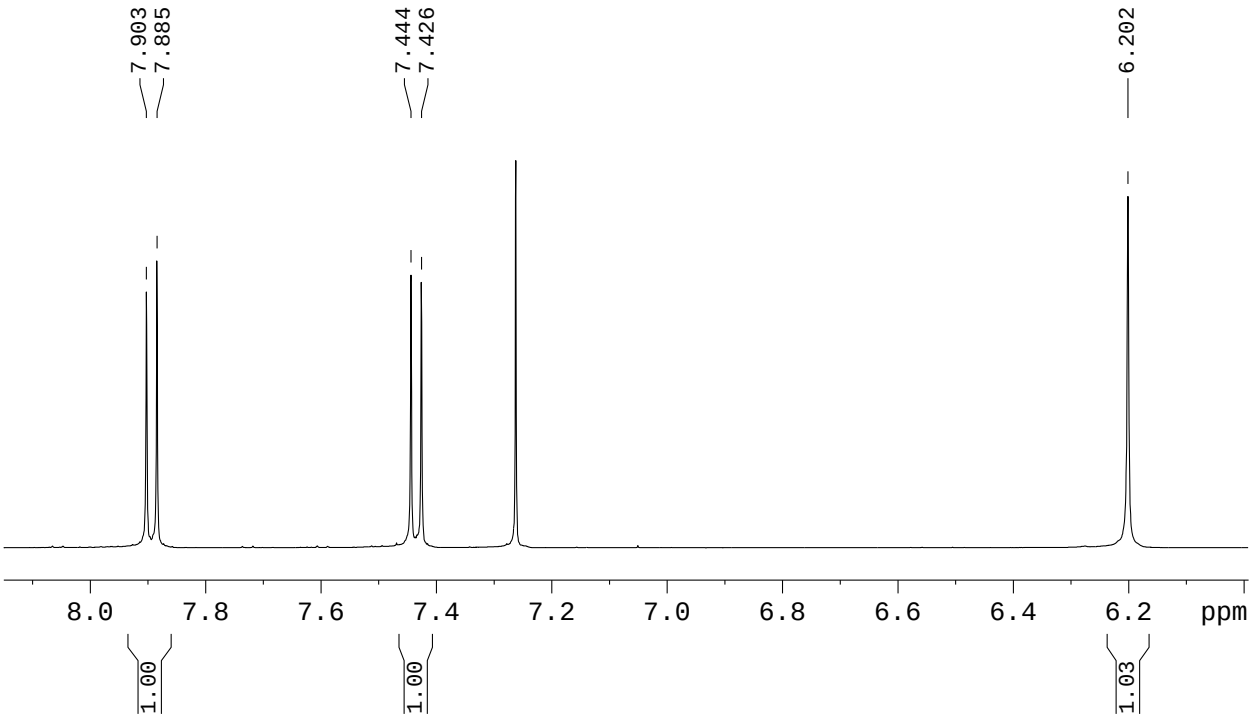


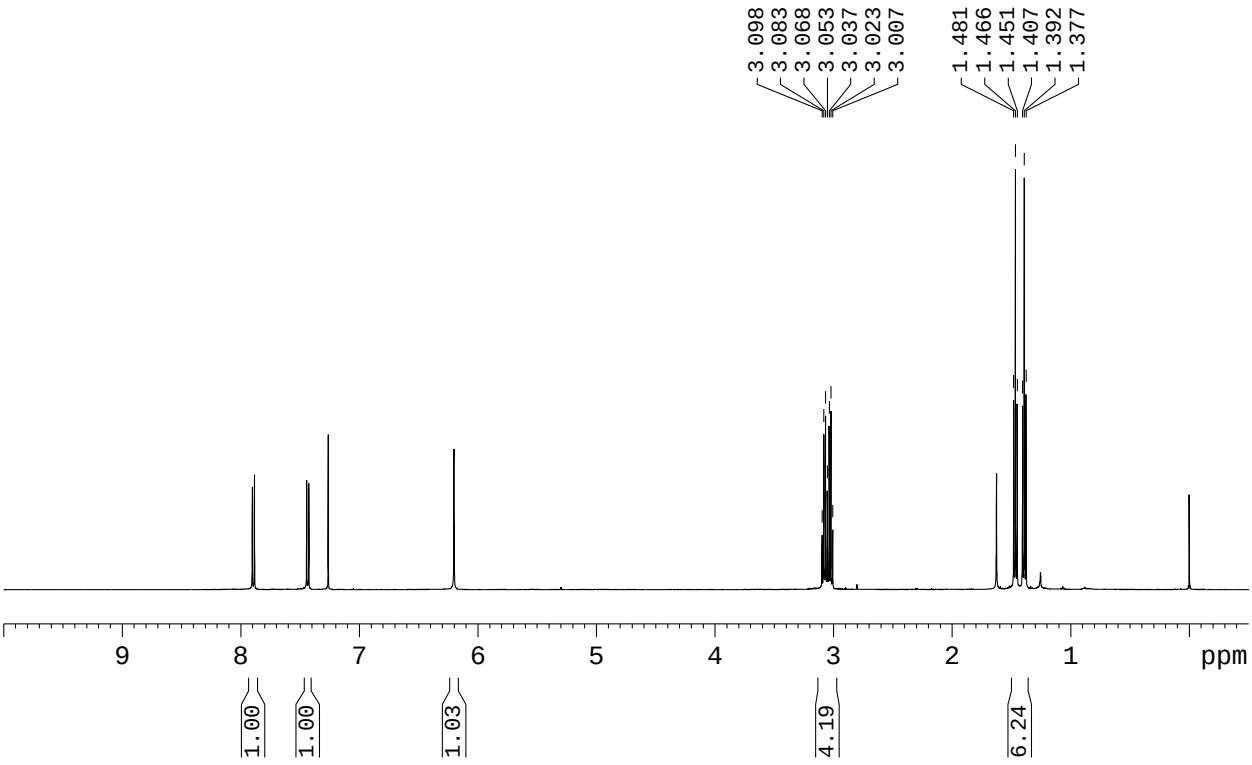


^{1}H NMR Spectrum of **17** (500 MHz, $CDCl_3$)

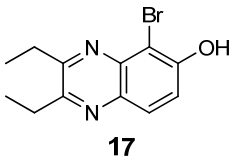


17

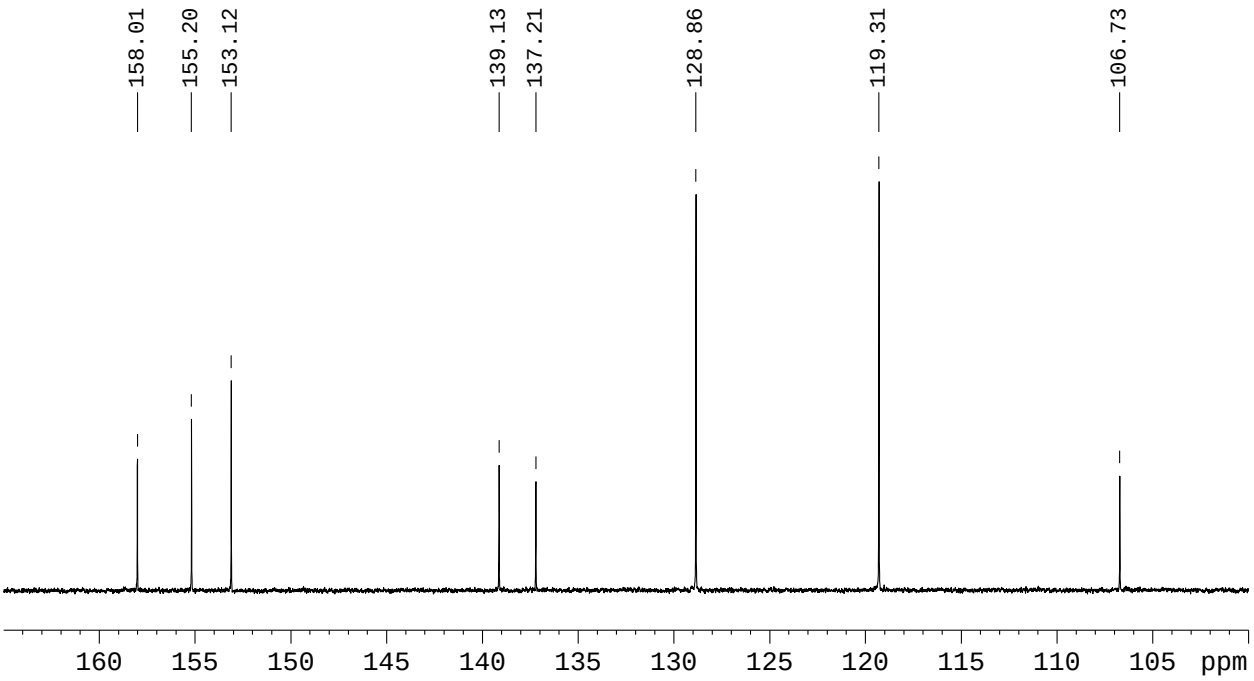


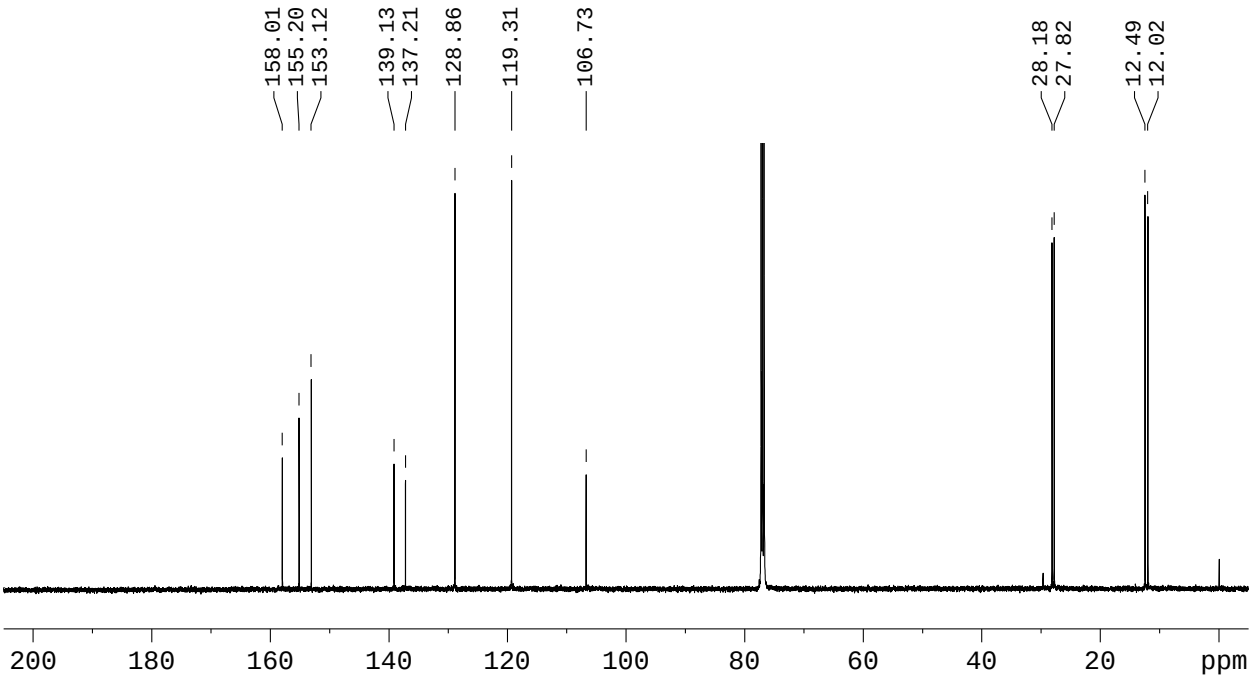


^{13}C NMR Spectrum of **17** (125 MHz, $CDCl_3$)

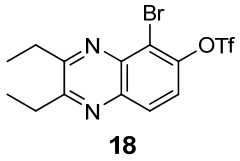


17

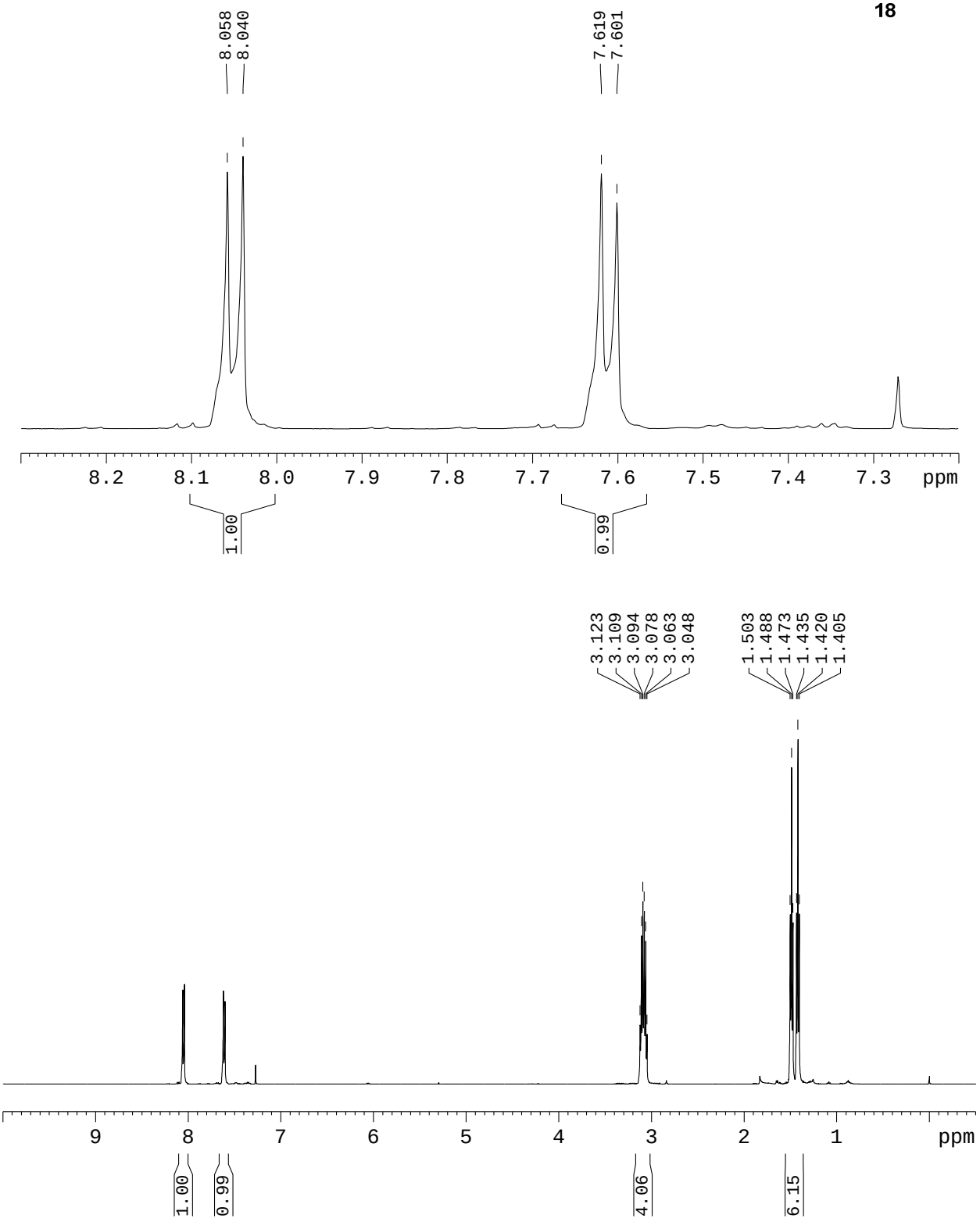




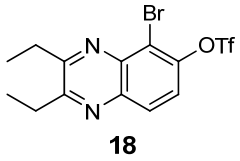
^{1}H NMR Spectrum of **18** (500 MHz, $CDCl_3$)



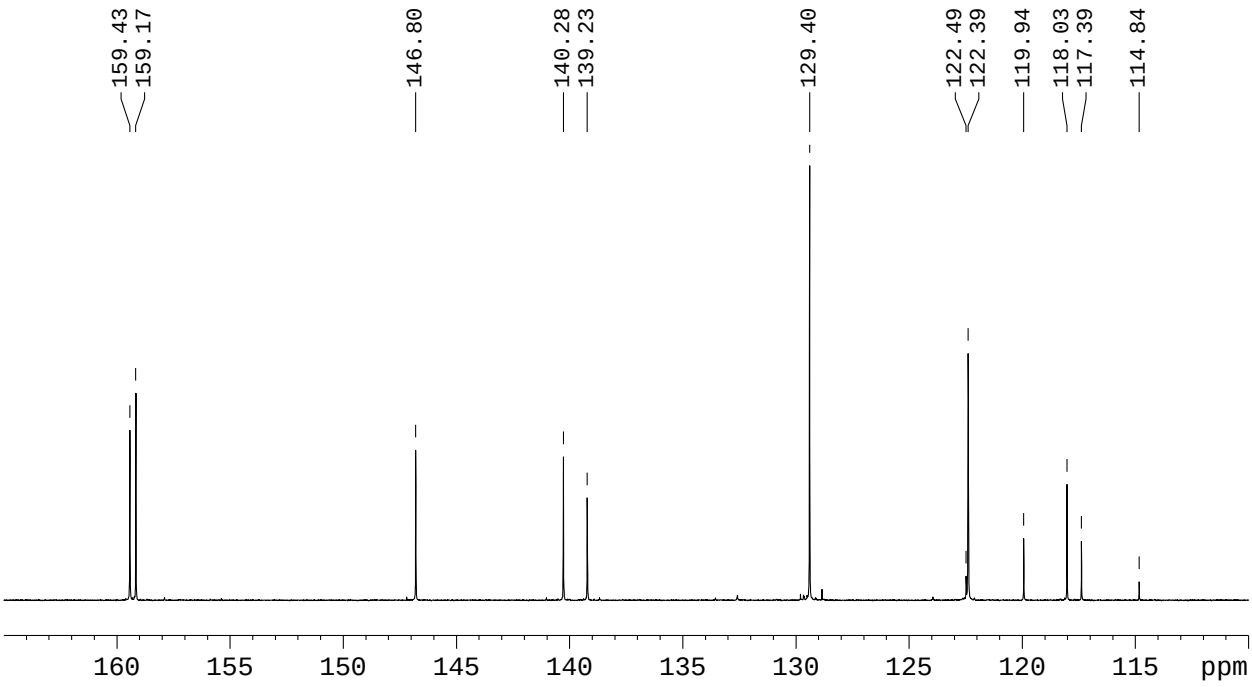
18

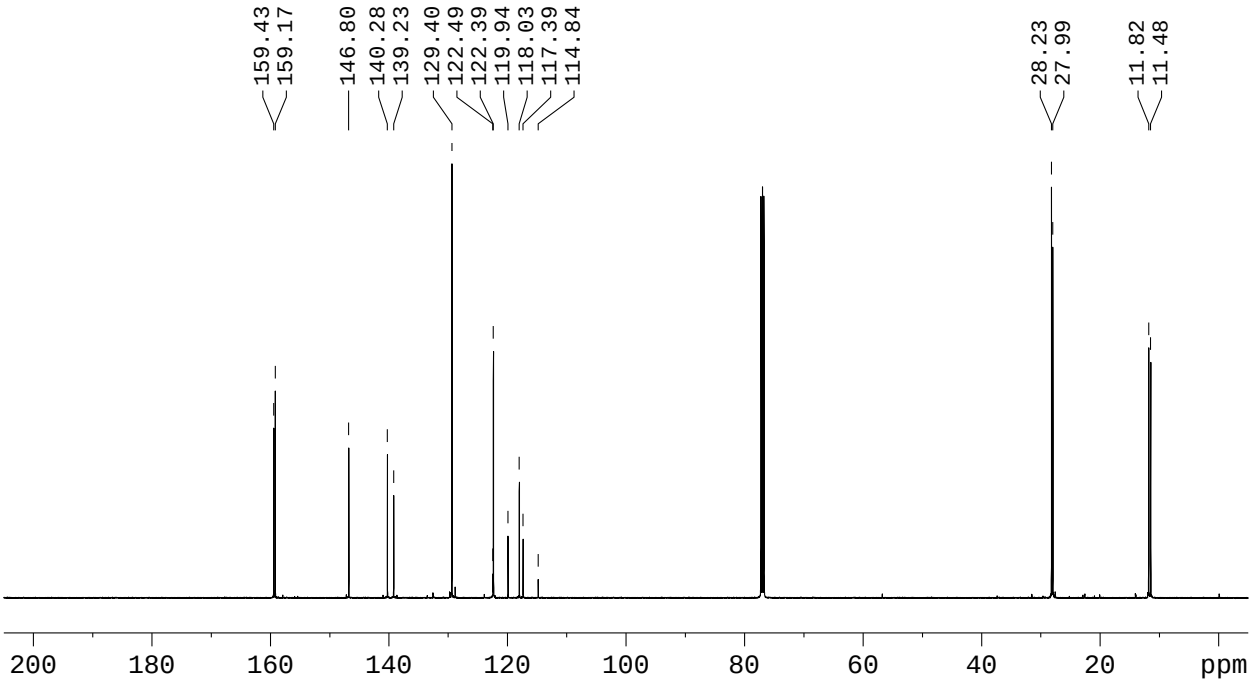


^{13}C NMR Spectrum of **18** (125 MHz, $CDCl_3$)

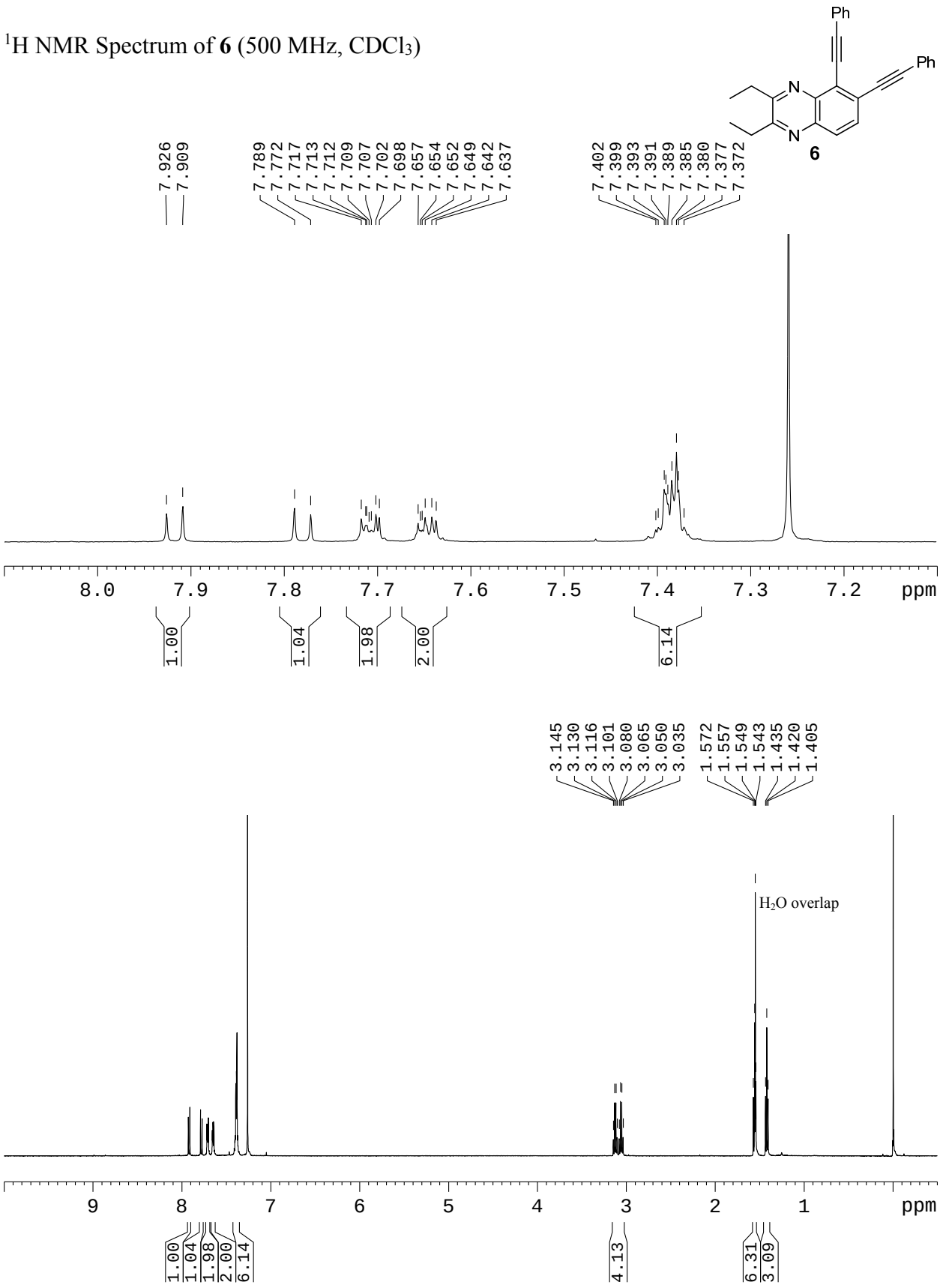


18

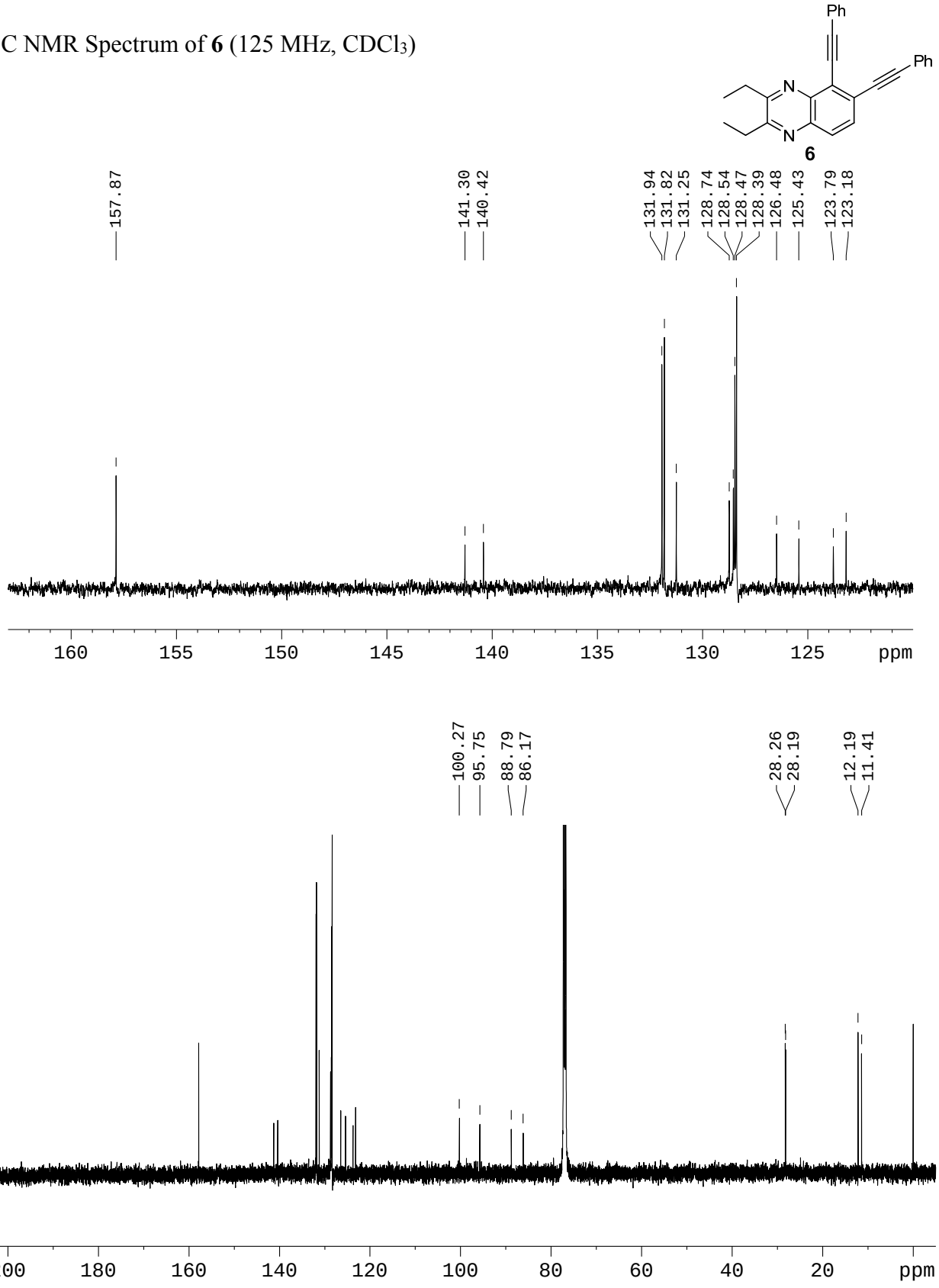




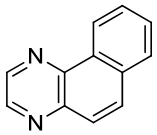
^{1}H NMR Spectrum of **6** (500 MHz, $CDCl_3$)



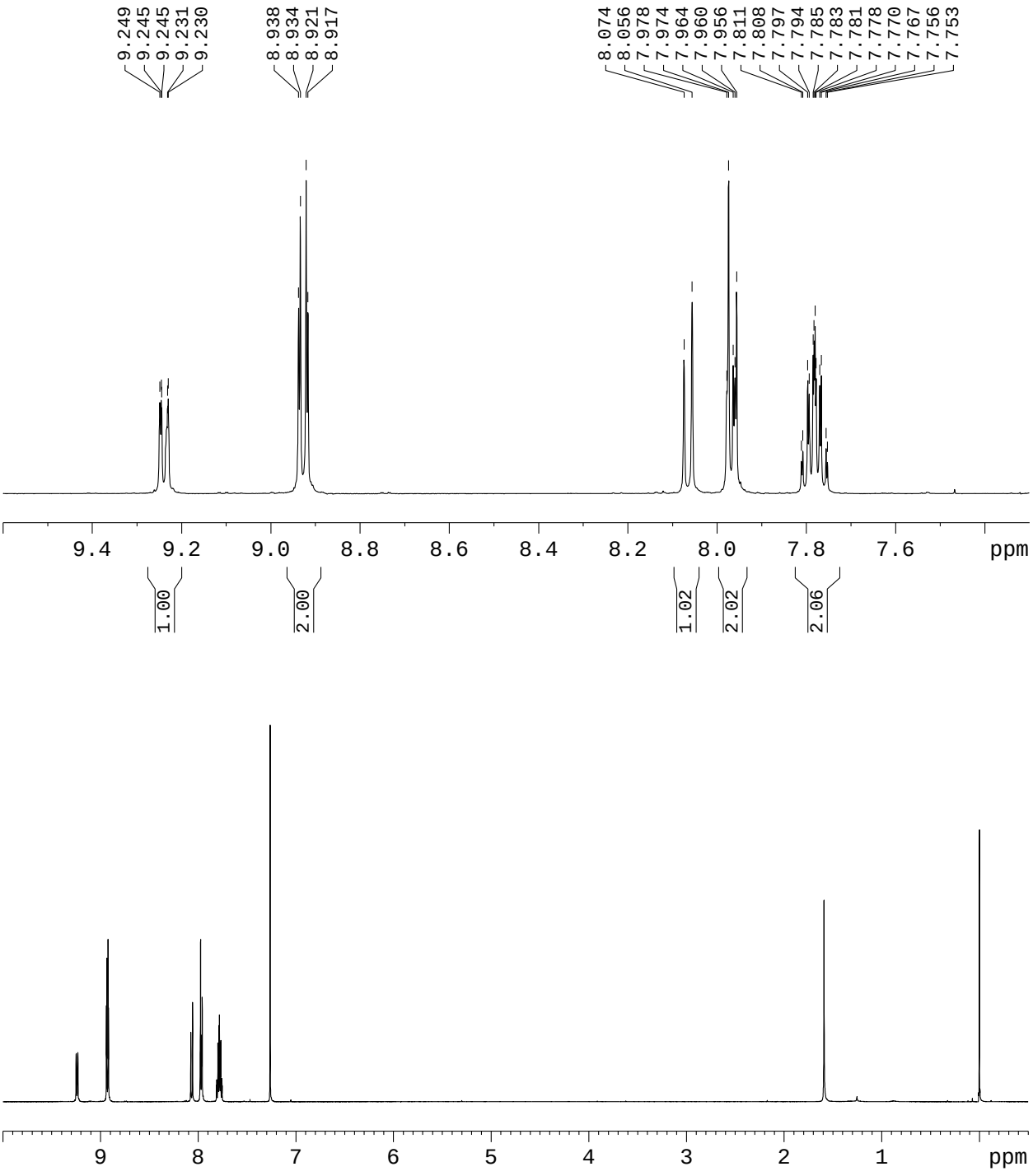
^{13}C NMR Spectrum of **6** (125 MHz, $CDCl_3$)



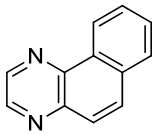
^{1}H NMR Spectrum of **21** (500 MHz, $CDCl_3$)



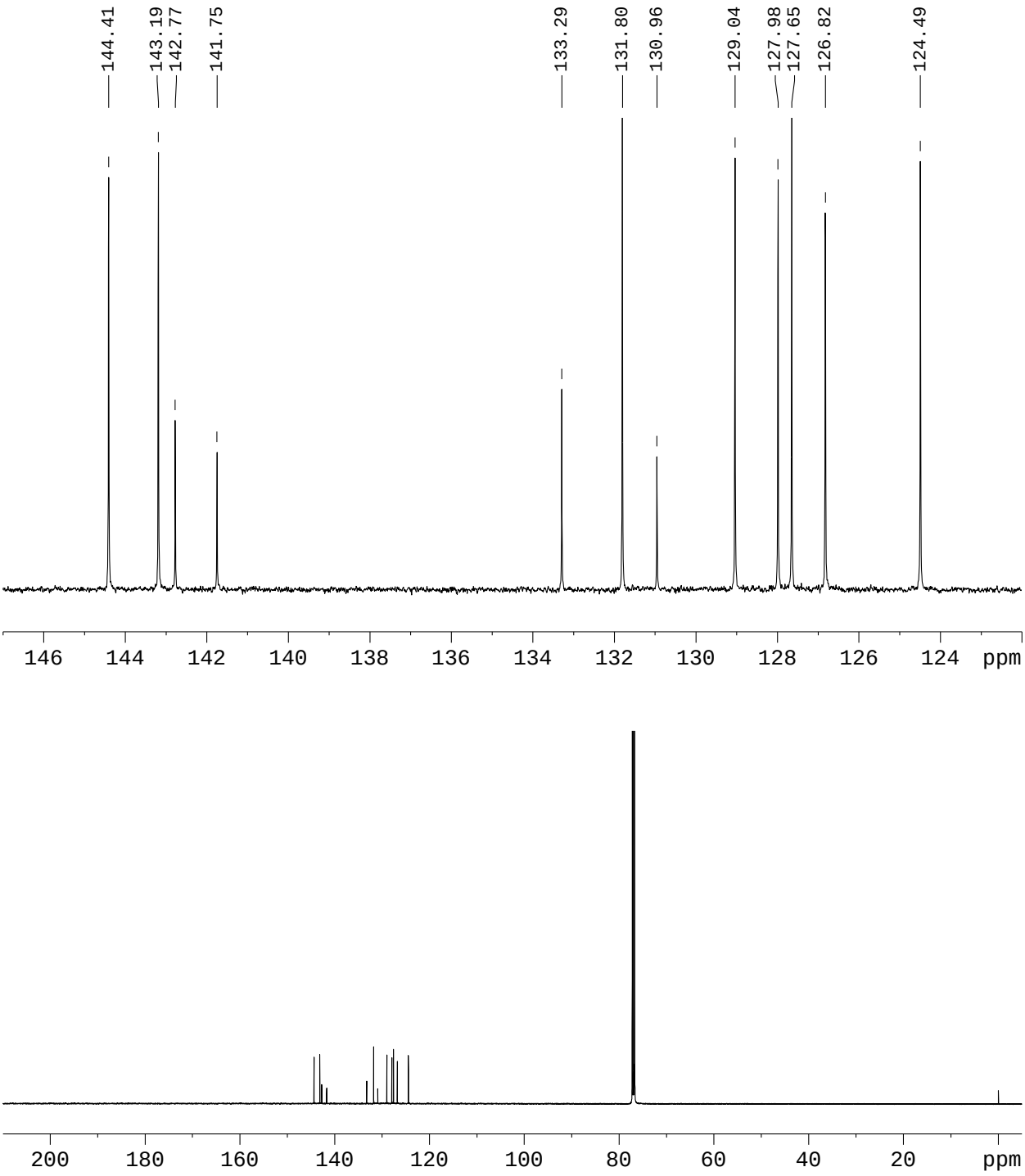
21



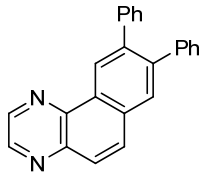
^{13}C NMR Spectrum of **21** (125 MHz, $CDCl_3$)



21



^{1}H NMR Spectrum of **22** (500 MHz, CD_2Cl_2)



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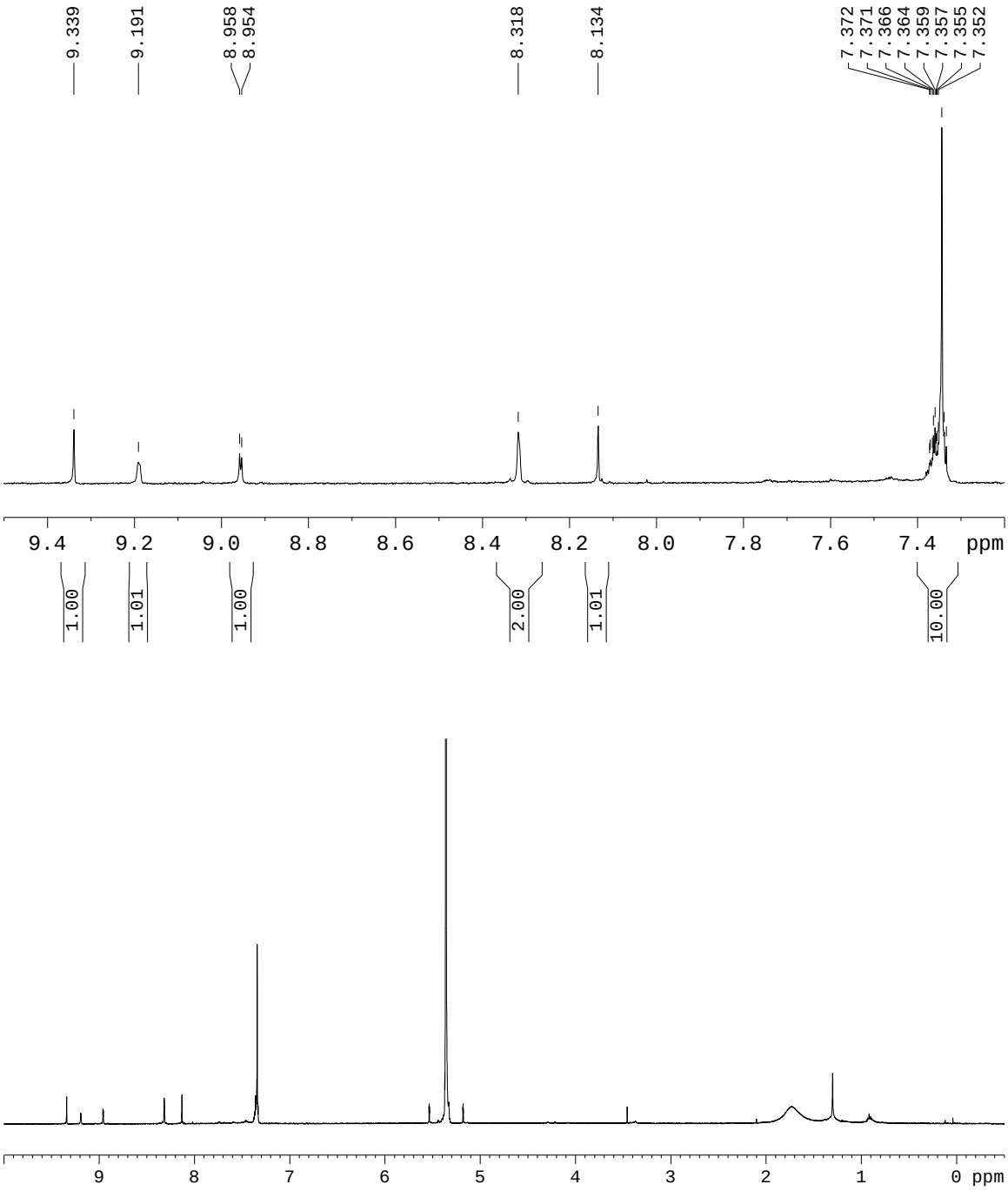
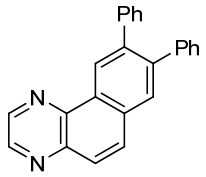


^{1}H NMR Spectrum of **22** (500 MHz, $CDCl_3$)



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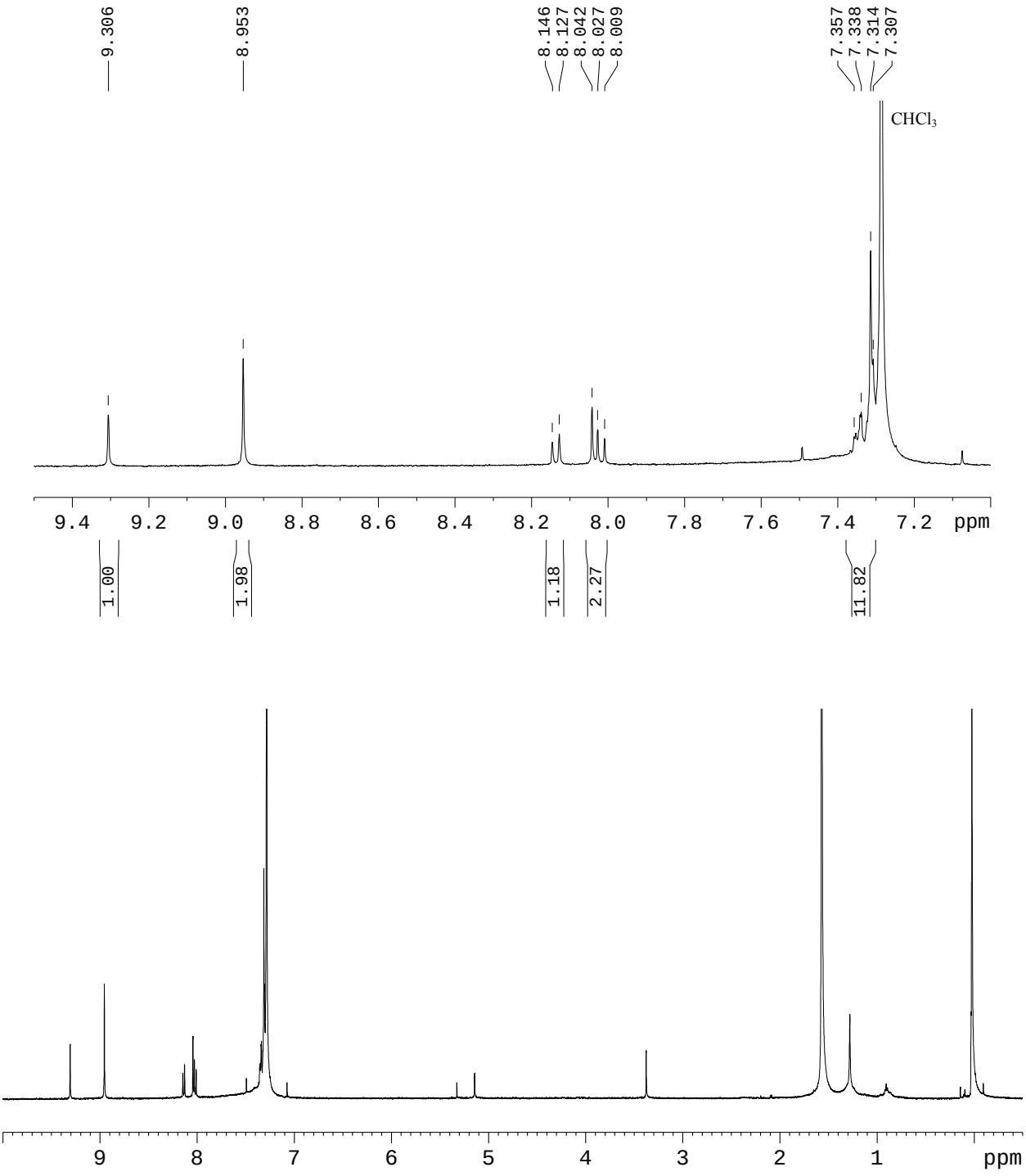
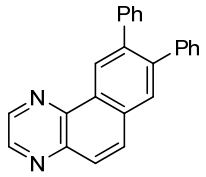
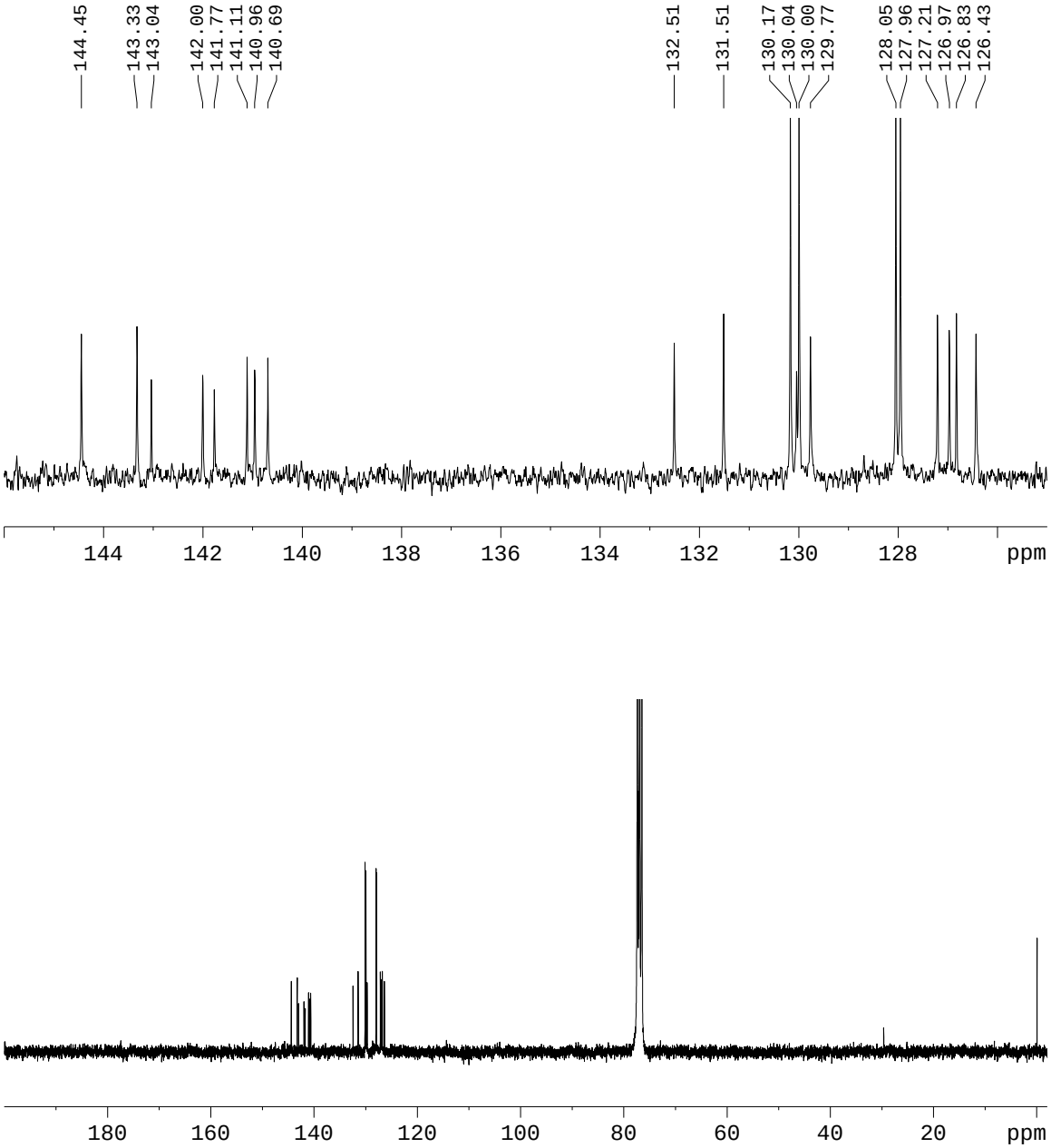


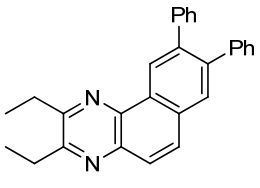
^{13}C NMR Spectrum of **22** (125 MHz, $CDCl_3$)



22



^{1}H NMR Spectrum of **23** (500 MHz, $CDCl_3$)



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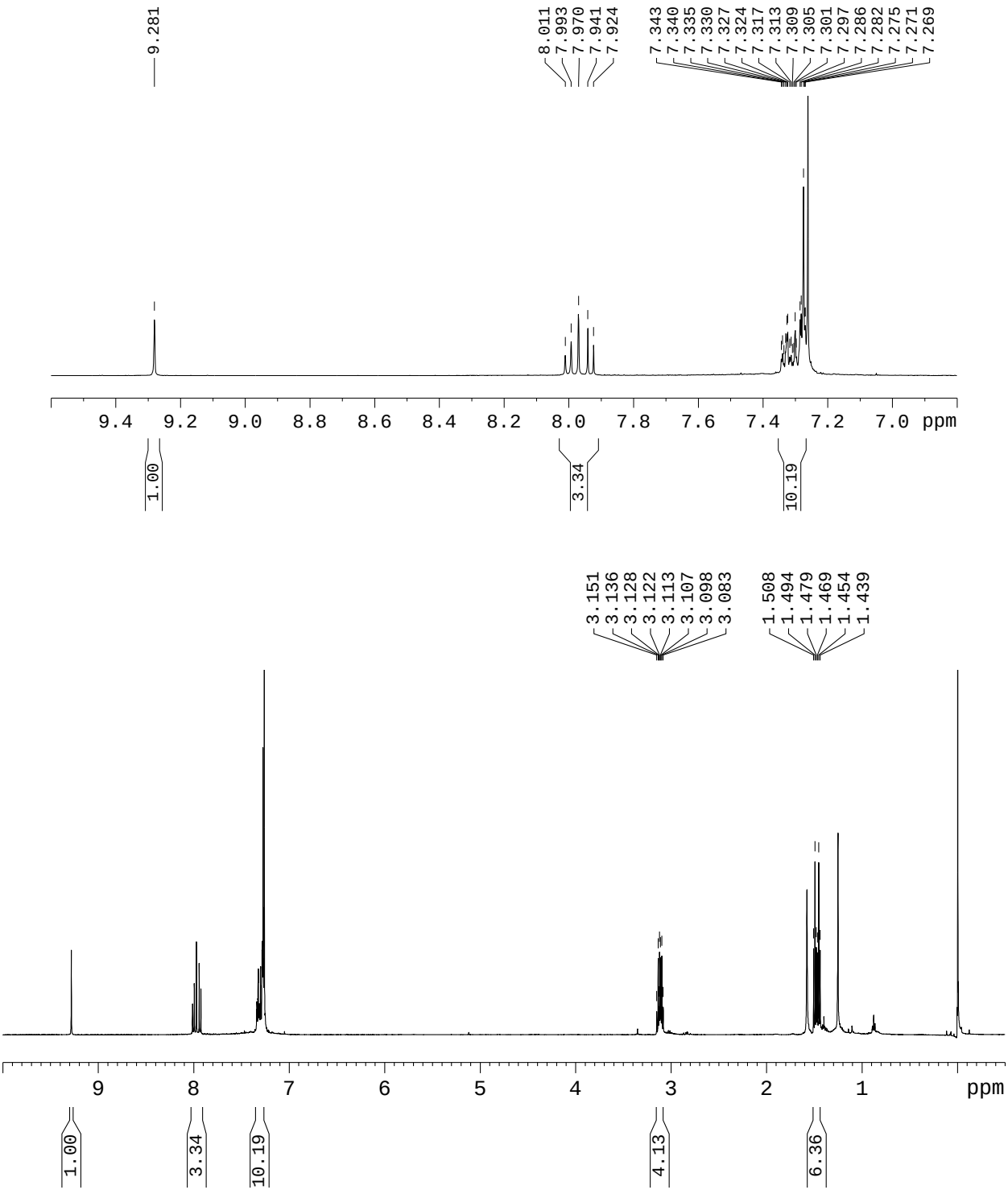
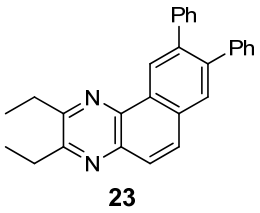


^{13}C NMR Spectrum of **23** (125 MHz, $CDCl_3$)



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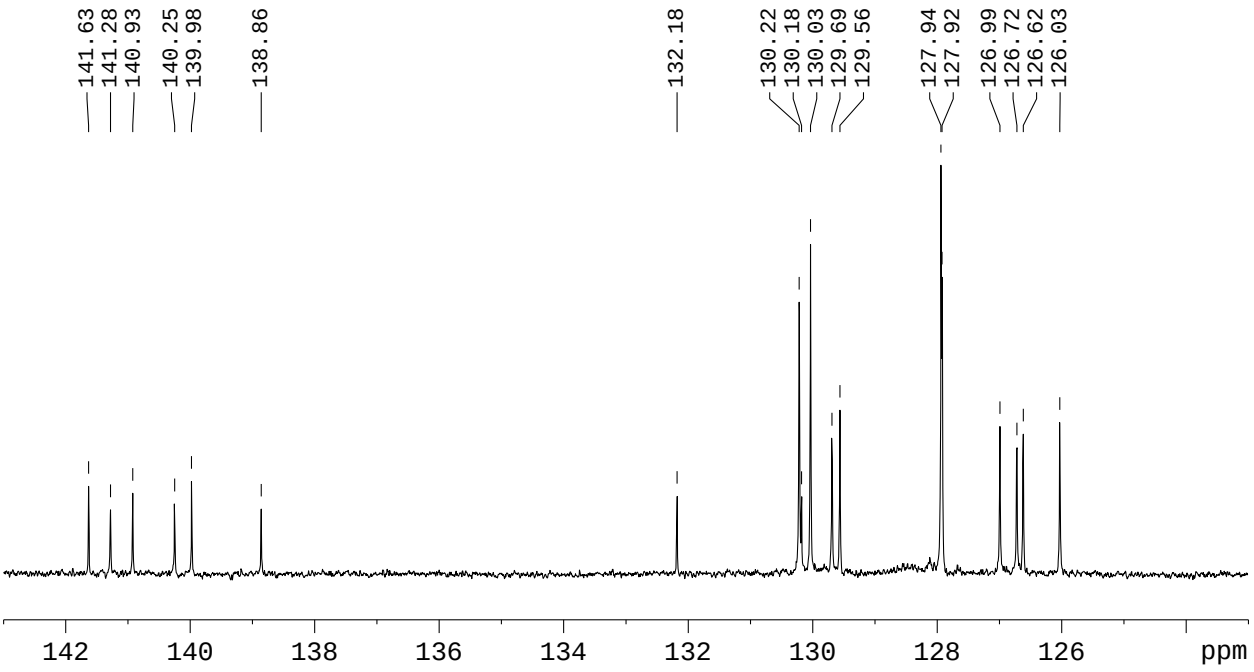
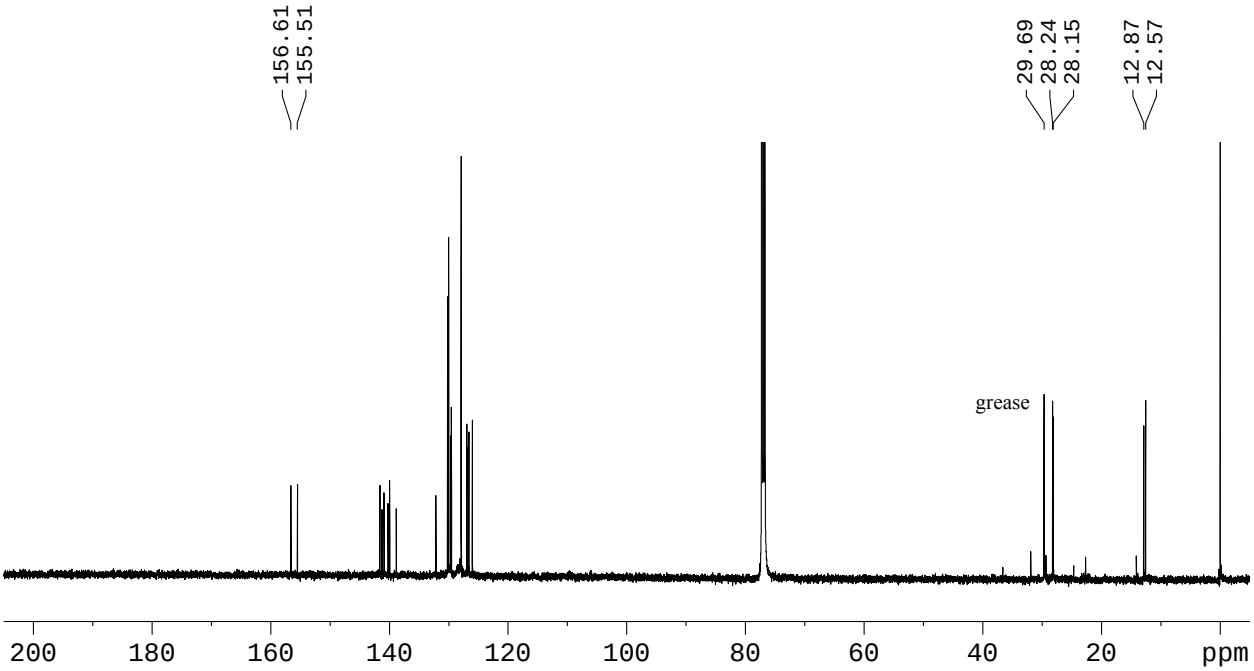
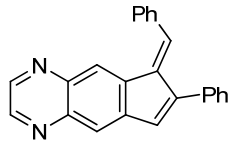
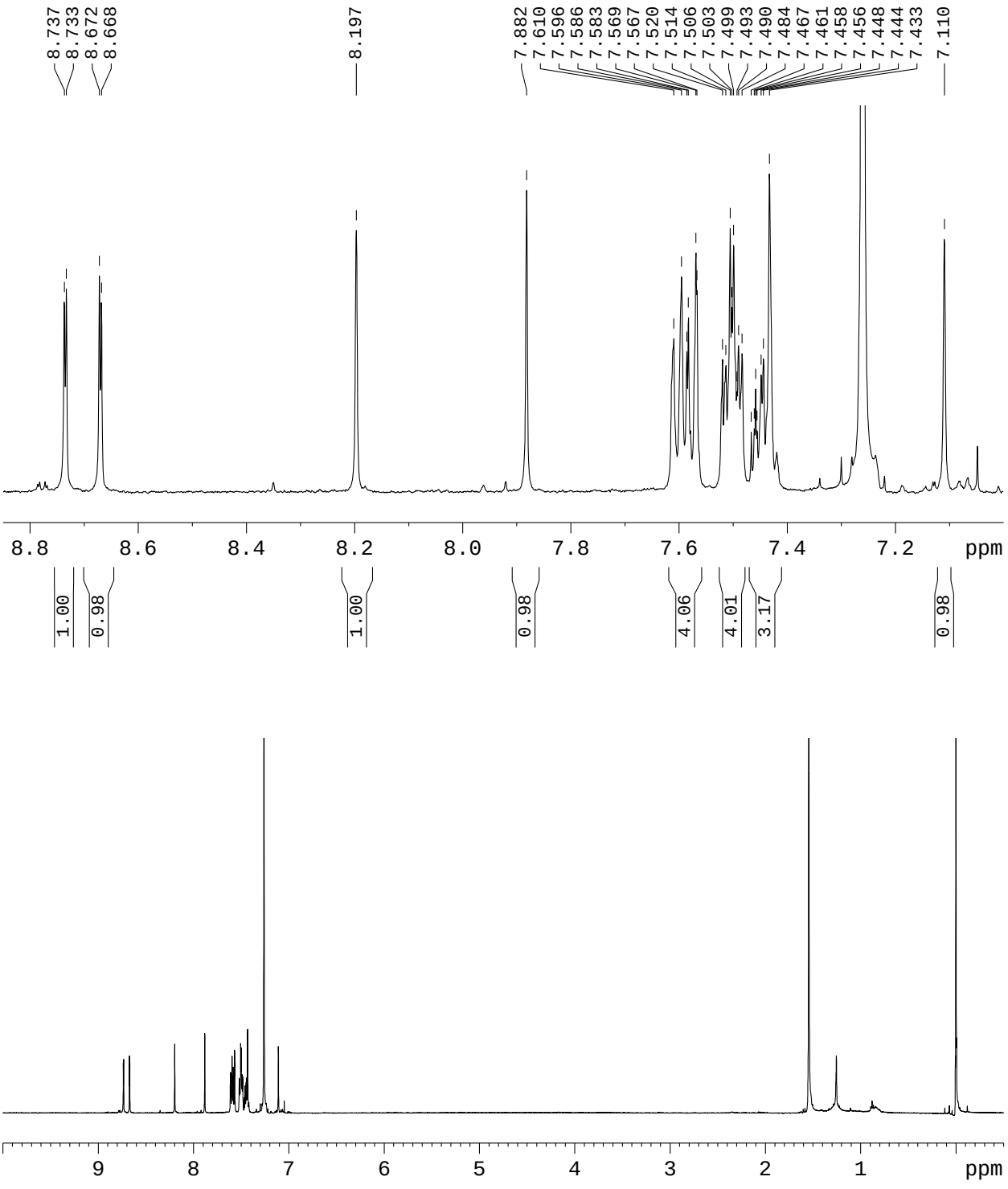




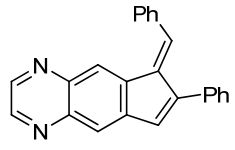
^{1}H NMR Spectrum of **24-*E*** (500 MHz, $CDCl_3$)



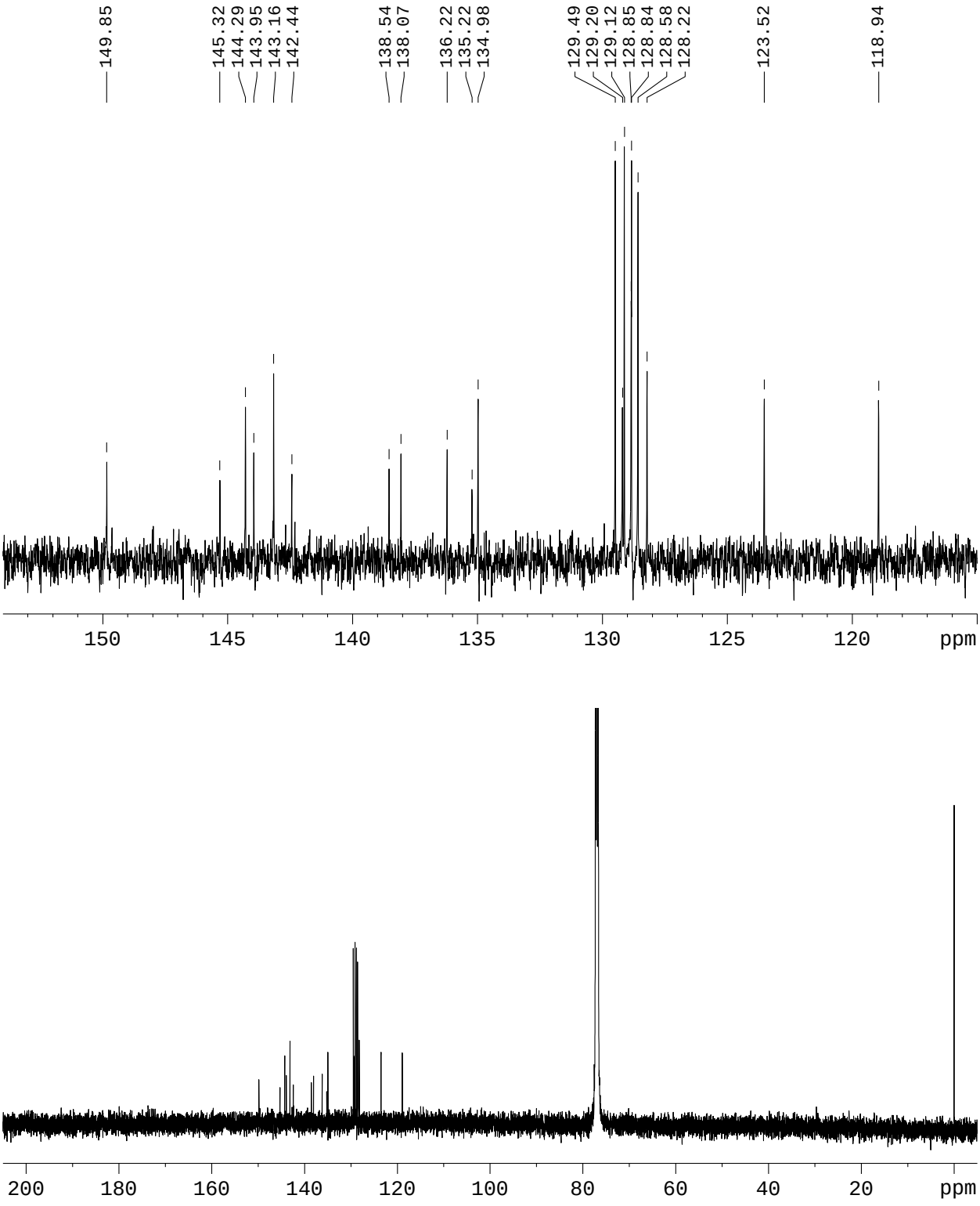
24-*E*



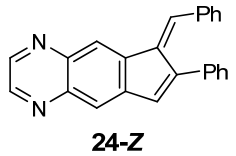
^{13}C NMR Spectrum of **24-*E*** (125 MHz, $CDCl_3$)



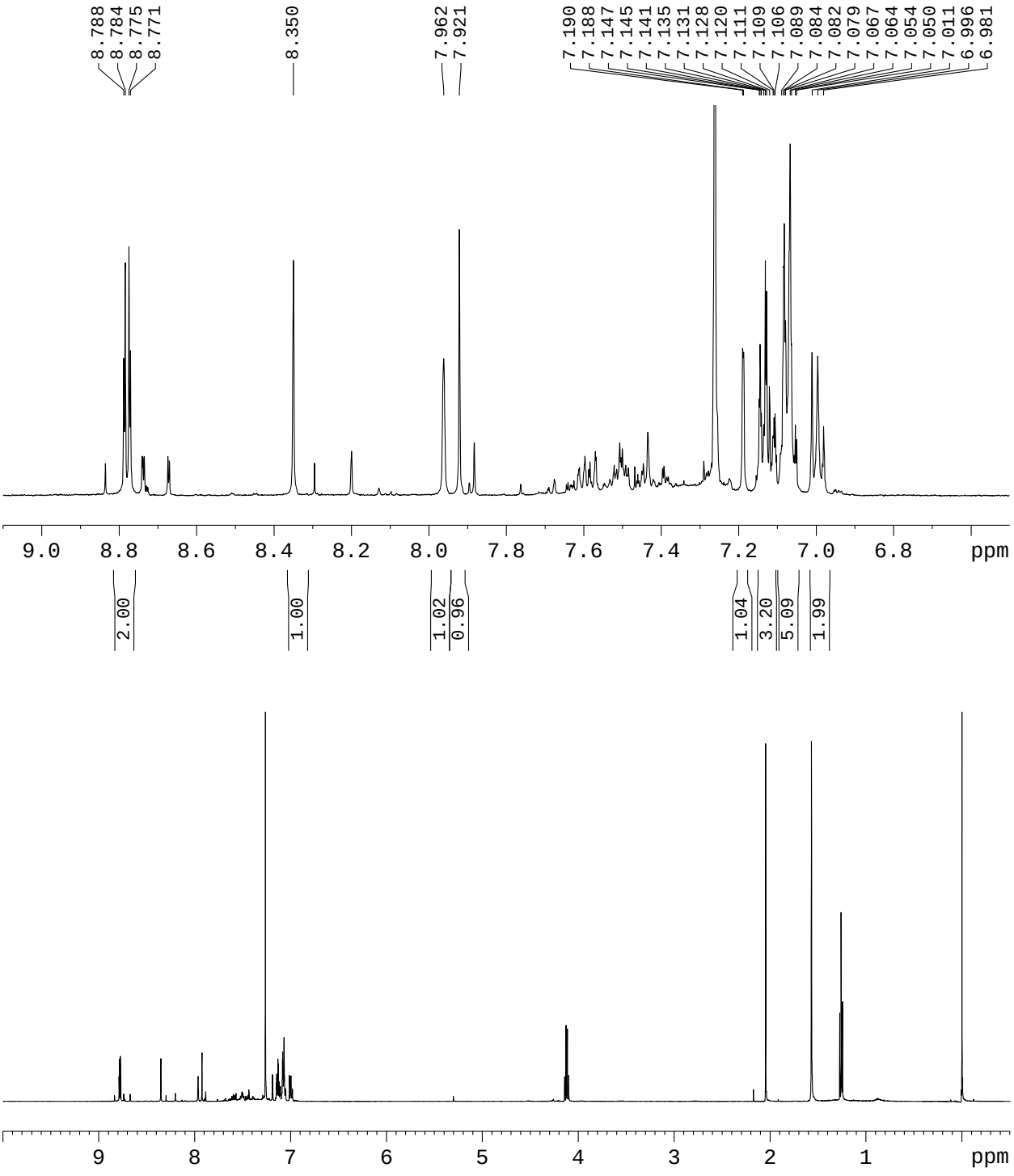
24-*E*



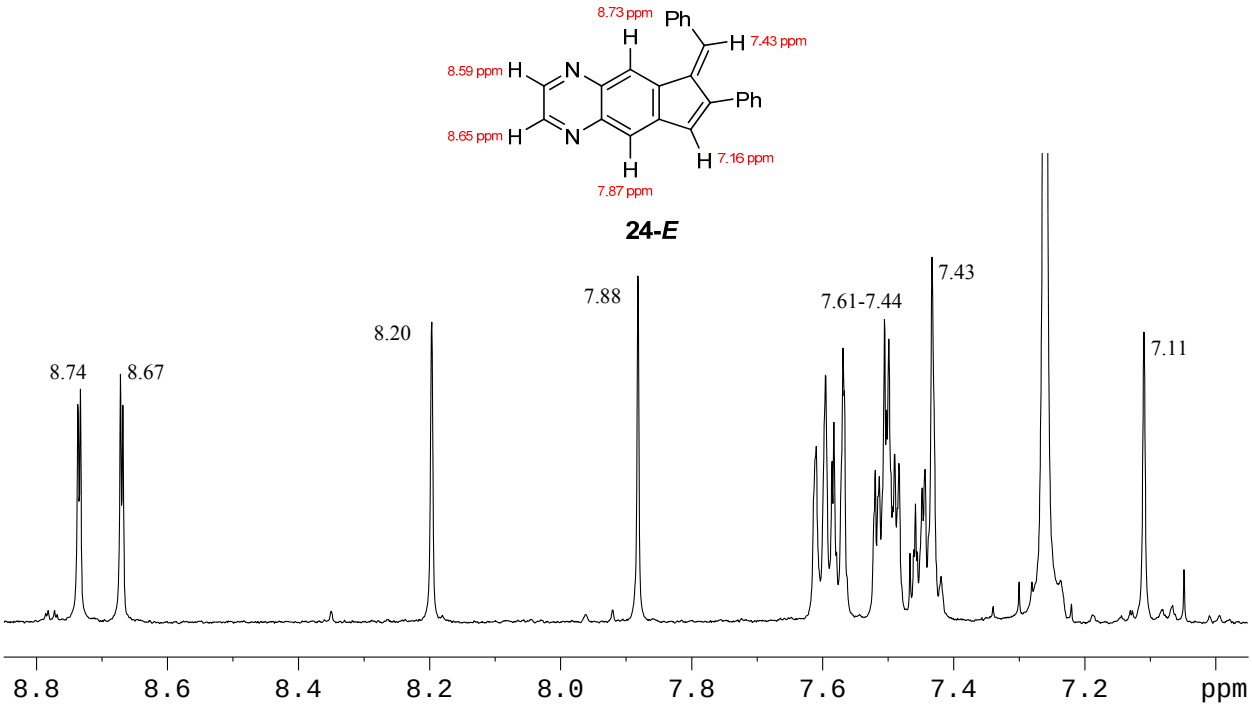
^{1}H NMR Spectrum of **24-*Z*** (500 MHz, $CDCl_3$)

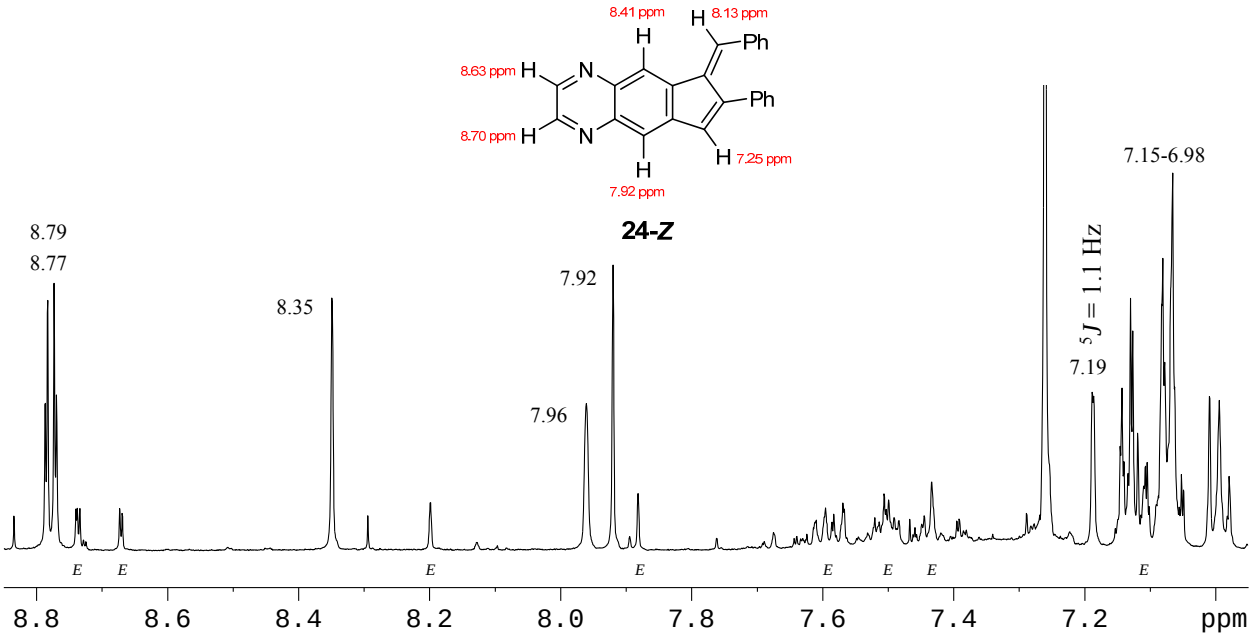


24-*Z*

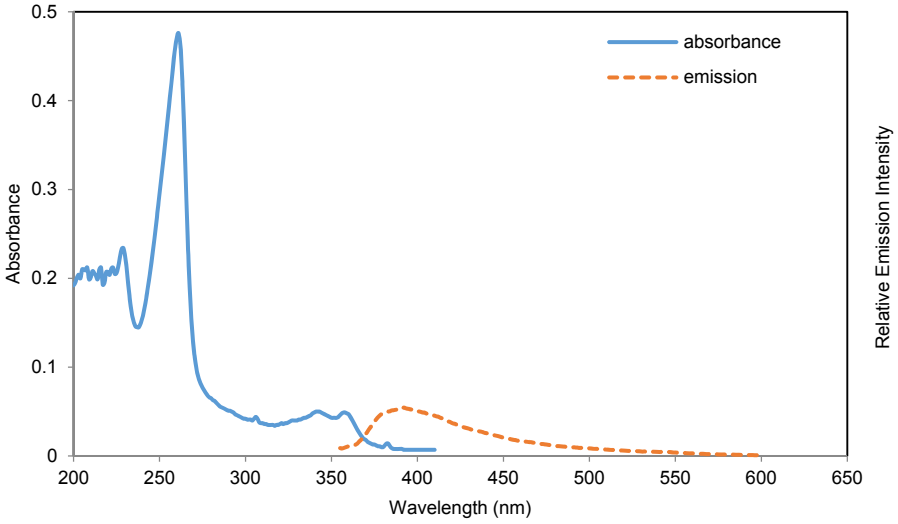


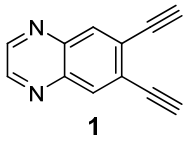
Comparison of fulvene isomers **24-*E*** and **24-*Z*** with calculated ^{1}H NMR shifts (calculated values shown in red on structure)





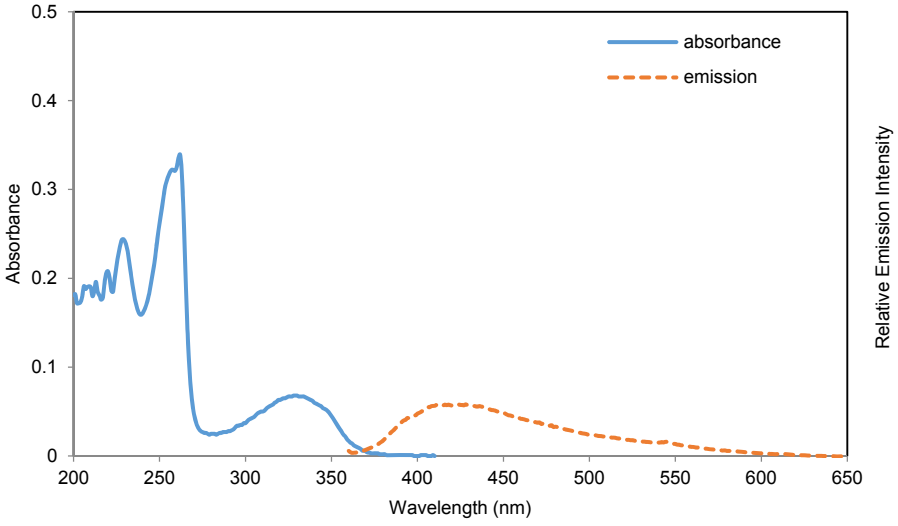
Absorbance and emission spectra of **1**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 350 nm). Absorbance spectra 1.0×10^{-5} M in CH_2Cl_2, emission spectra 1.0×10^{-4} M in CH_2Cl_2.

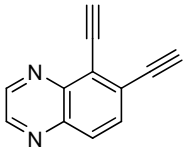




1

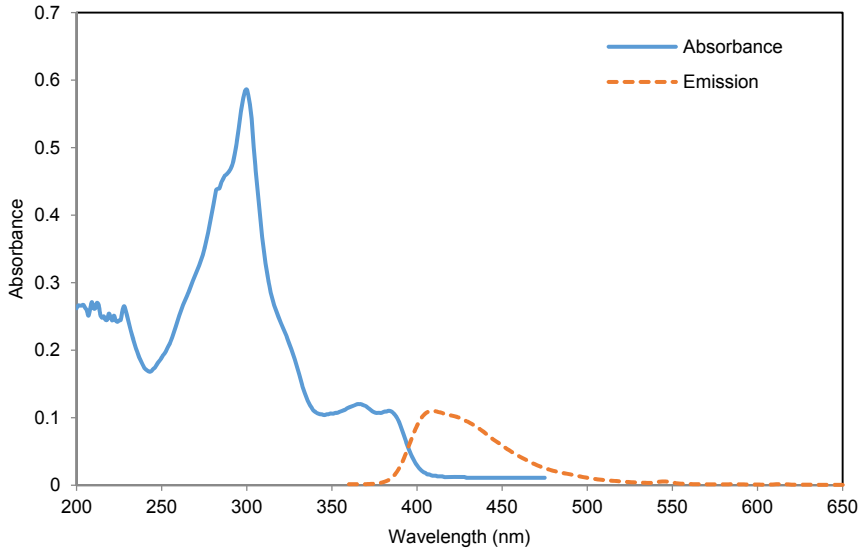
Absorbance and emission spectra of **2**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 350 nm). Absorbance spectra 1.0×10^{-5} M in CH_2Cl_2, emission spectra 1.0×10^{-4} M in CH_2Cl_2.

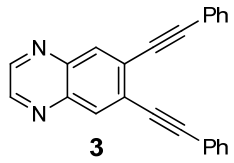




2

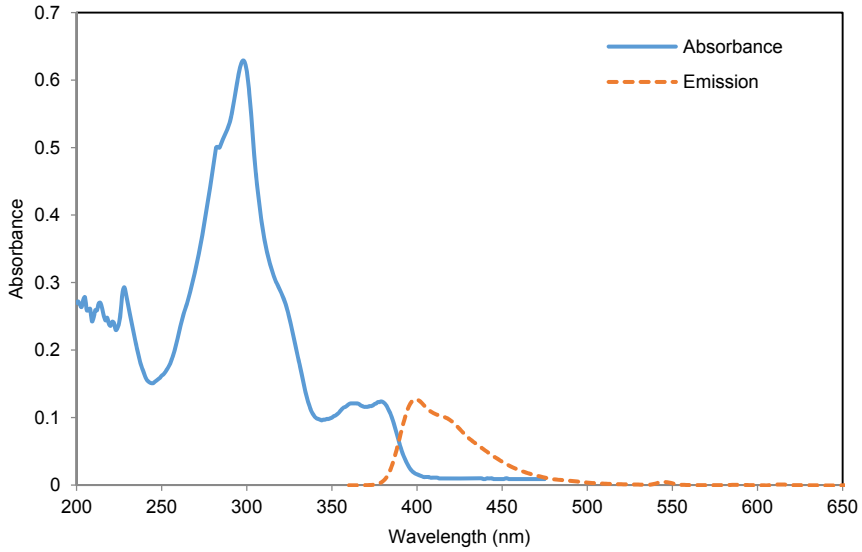
Absorbance and emission spectra of **3**. Fluorescence spectra normalized to facilitate comparison (excitation $\lambda = 350$ nm). Absorbance and emission spectra 1.0×10^{-5} M in CH_2Cl_2.

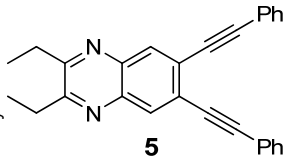




3

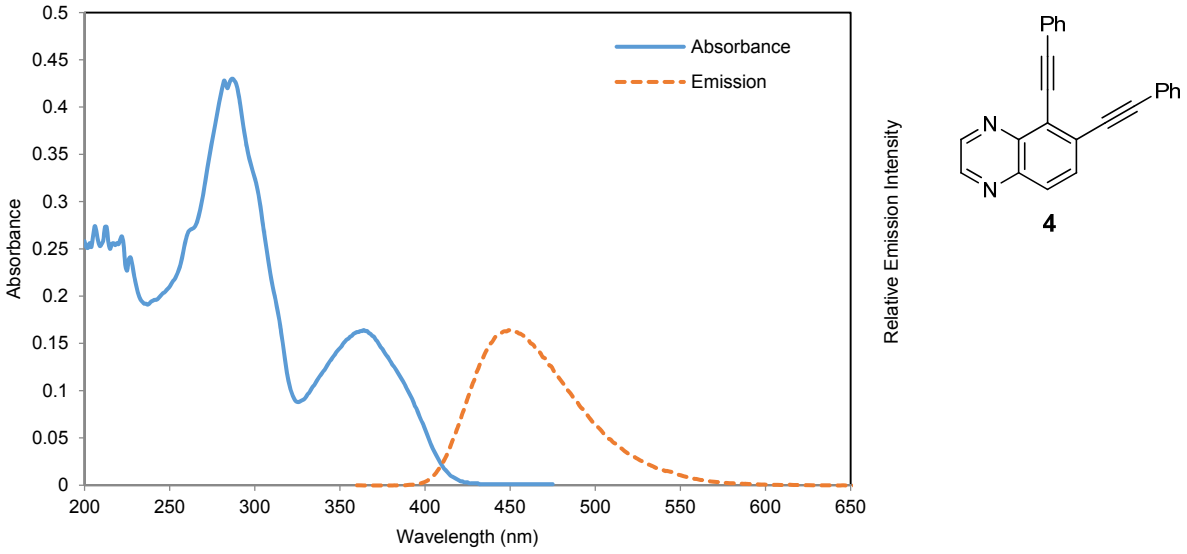
Absorbance and emission spectra of **5**. Fluorescence spectra normalized to facilitate comparison (excitation $\lambda = 350$ nm). Absorbance and emission spectra 1.0×10^{-5} M in CH_2Cl_2.





5

Absorbance and emission spectra of **4**. Fluorescence spectra normalized to facilitate comparison (excitation $\lambda = 350$ nm). Absorbance and emission spectra 1.0×10^{-5} M in CH_2Cl_2.



Absorbance and emission spectra of **6**. Fluorescence spectra normalized to facilitate comparison (excitation $\lambda = 350$ nm). Absorbance and emission spectra 1.0×10^{-5} M in CH_2Cl_2.

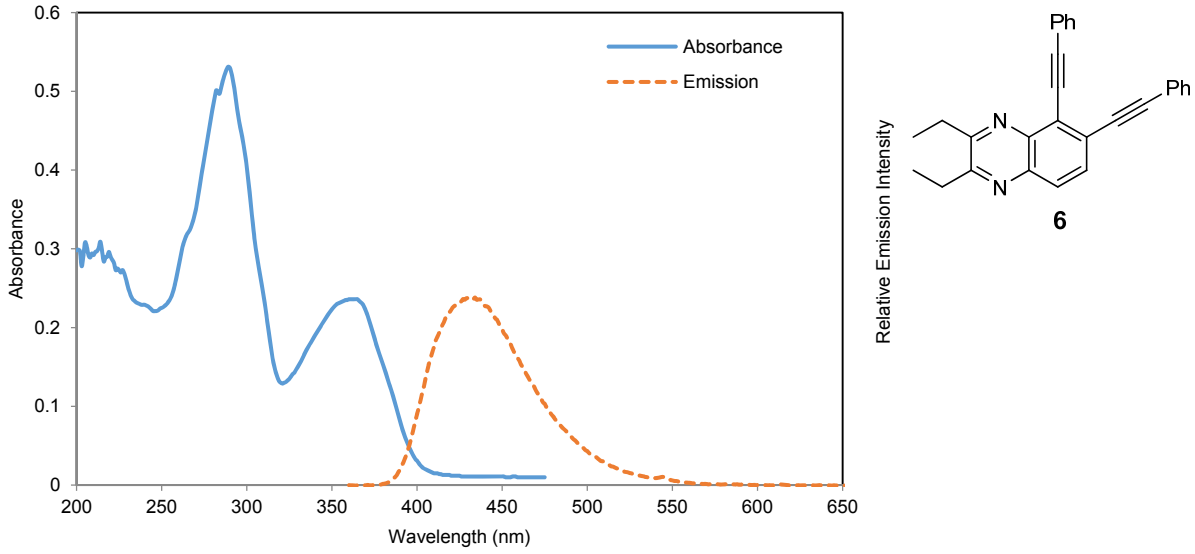
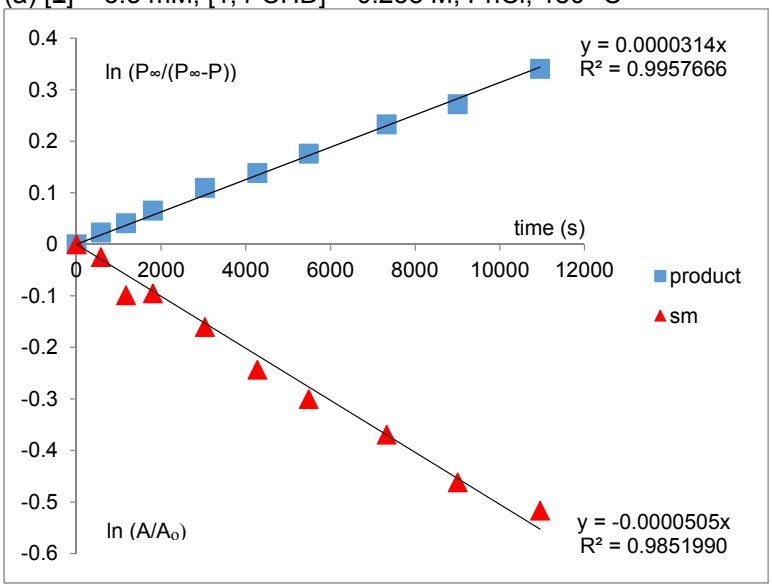
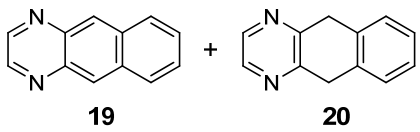
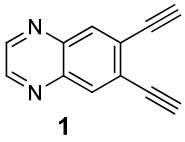


Figure S5. First-order rate constants at different 1,4-CHD concentrations for the disappearance of linear quinoxalenediyne **1** and formation of benzo[*g*]quinoxaline **19** and 5,10-dihydrobenzo[*g*]quinoxaline **20** at 180 °C.

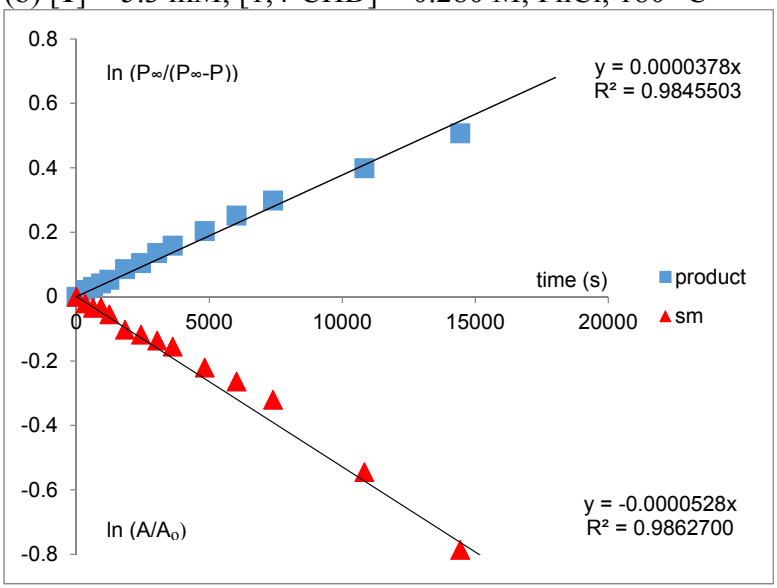
(a) [**1**] = 5.3 mM; [1,4-CHD] = 0.258 M; PhCl, 180 °C

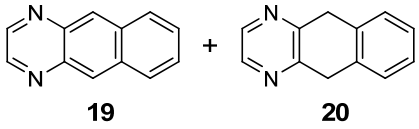






(b) [**1**] = 5.3 mM; [1,4-CHD] = 0.280 M; PhCl, 180 °C





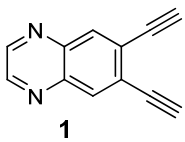
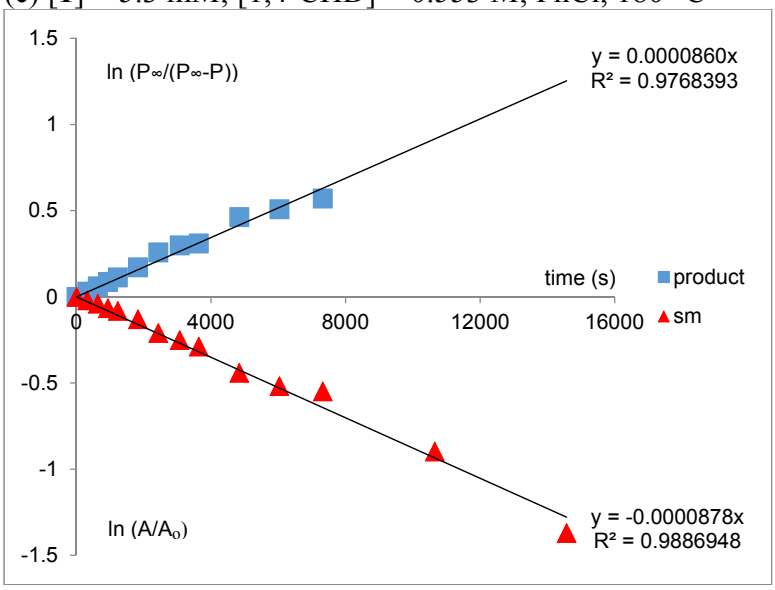
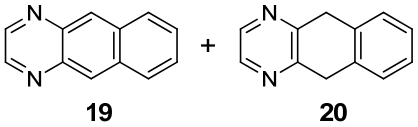


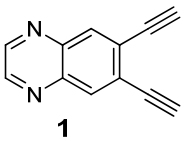
Figure S5 continued.

(c) [**1**] = 5.3 mM; [1,4-CHD] = 0.553 M; PhCl, 180 °C



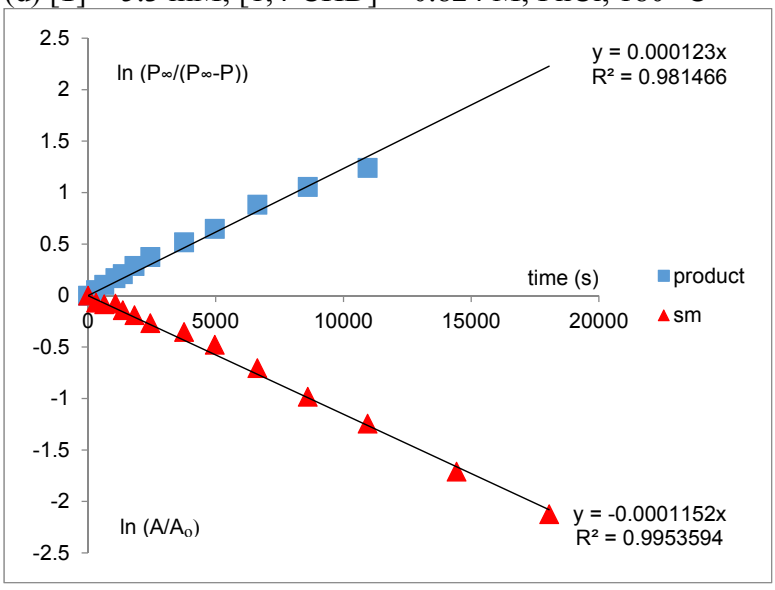


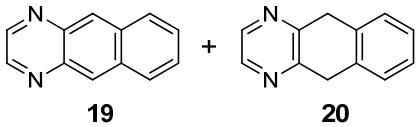
19 **20**



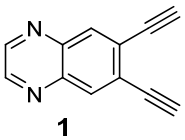
1

(d) [**1**] = 5.3 mM; [1,4-CHD] = 0.824 M; PhCl, 180 °C





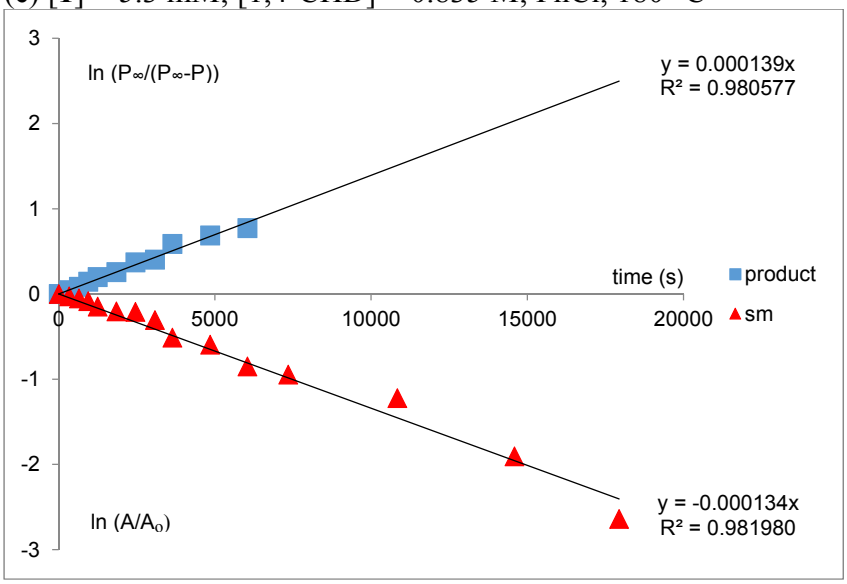
19 **20**

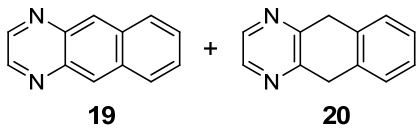


1

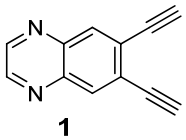
Figure S5 continued.

(e) [**1**] = 5.3 mM; [1,4-CHD] = 0.835 M; PhCl, 180 °C



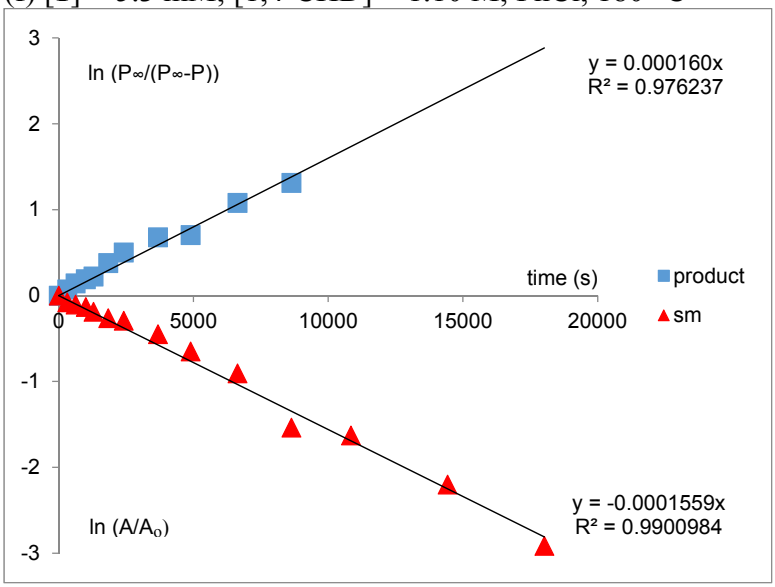


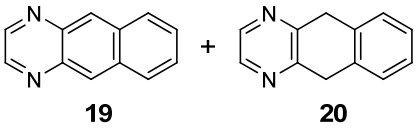
19 + **20**



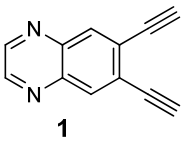
1

(f) [**1**] = 5.3 mM; [1,4-CHD] = 1.10 M; PhCl, 180 °C





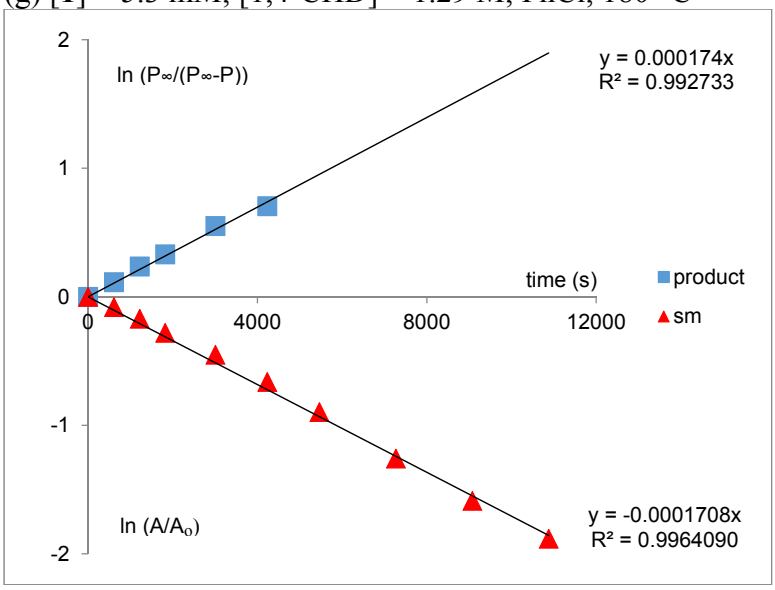
19 + **20**

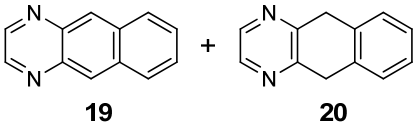


1

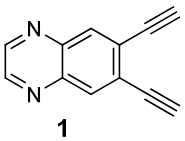
Figure S5 continued.

(g) [**1**] = 5.3 mM; [1,4-CHD] = 1.29 M; PhCl, 180 °C



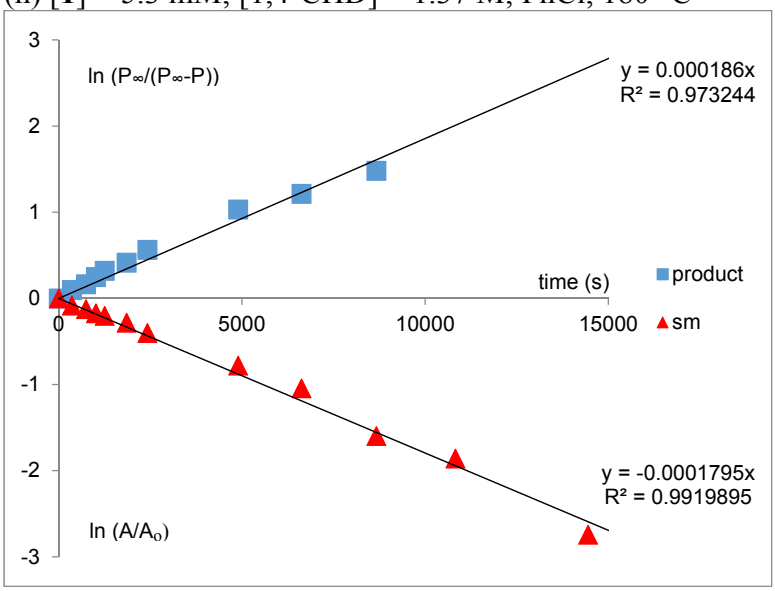


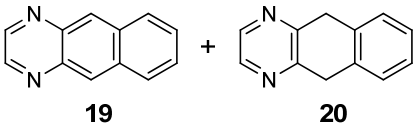
19 **20**



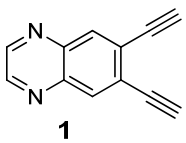
1

(h) [**1**] = 5.3 mM; [1,4-CHD] = 1.37 M; PhCl, 180 °C



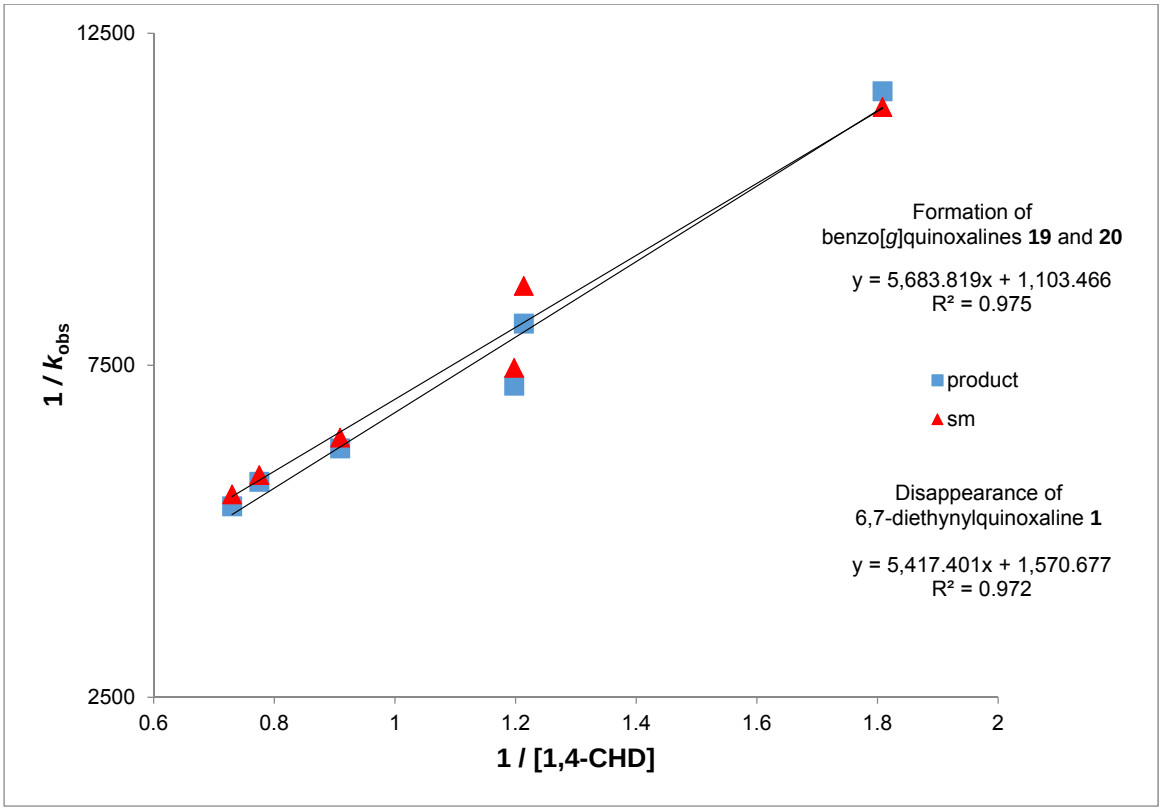


19 **20**



1

Figure S6. Dependence of observed rate constant, k_{obs}, on 1,4-CHD concentration for disappearance of linear quinoxalenediyne **1** and formation of benzo[*g*]quinoxaline **19** and 5,10-dihydrobenzo[*g*]quinoxaline **20** at 180 °C.



SM Disappearance

$k_1 = 6.37 \times 10^{-4}$

$k_{-1}/k_2 = 3.45$

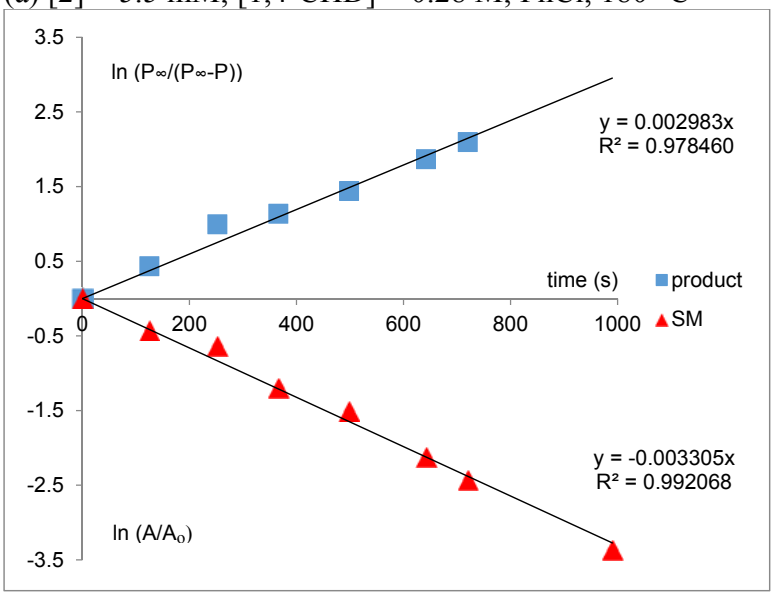
PDT Formation

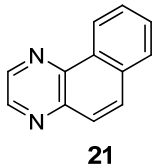
$k_1 = 9.07 \times 10^{-4}$

$k_{-1}/k_2 = 5.15$

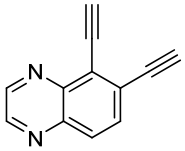
Figure S7. First-order rate constants at different 1,4-CHD concentrations for the disappearance of angular quinoxalenediyne **2** and formation of benzo[*f*]quinoxaline **21** at 180 °C.

(a) [**2**] = 5.5 mM; [1,4-CHD] = 0.28 M; PhCl, 180 °C



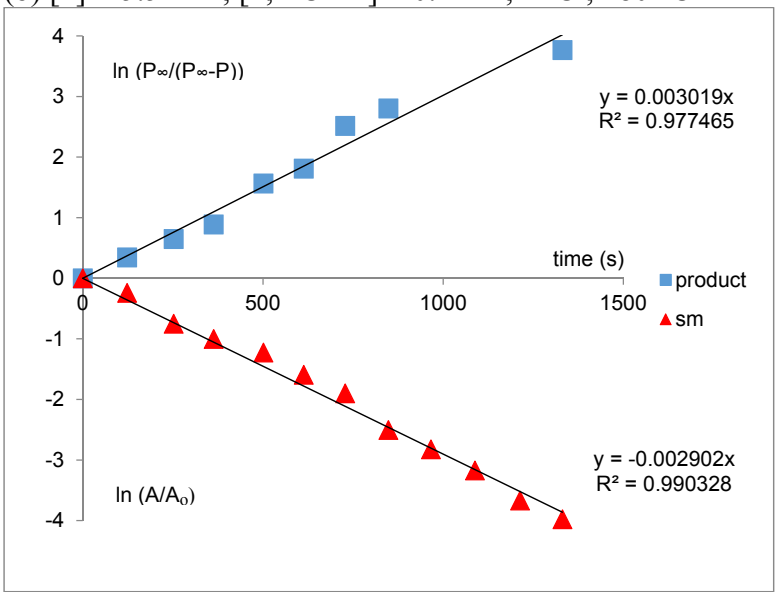


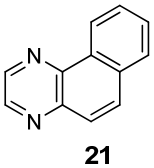
21



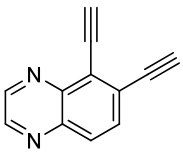
2

(b) [**2**] = 5.5 mM; [1,4-CHD] = 0.41 M; PhCl, 180 °C





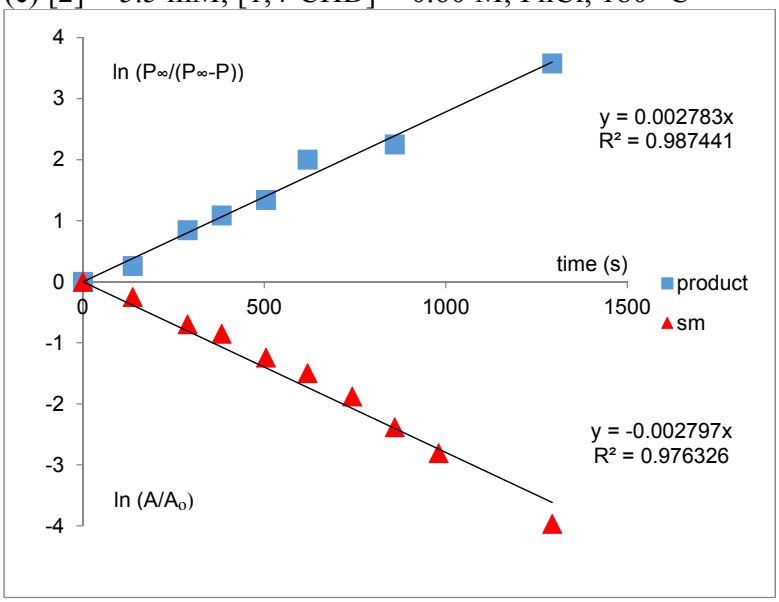
21

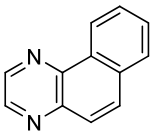


2

Figure S7 continued.

(c) [**2**] = 5.5 mM; [1,4-CHD] = 0.60 M; PhCl, 180 °C





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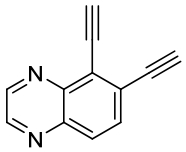

2

Table S10. Raw computational data used to calculate the thermodynamics of the cyclization reactions. Imaginary frequencies (cm^{-1}) when present are given in parentheses.

a) Compound **1** diradical C^1-C^5 product isomers

singlets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
1-*Z*	-570.24156	90.354	6.563	95.583	0
1-*E*	-570.23850	90.325	6.573	95.657	0

triplets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
1-*Z*	-570.23368	90.529	6.581	97.942	0
1-*E*	-570.23514	90.558	6.567	97.873	0

b) Compound **2** diradical C^1-C^5 product isomers

singlets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
2'-*Z*	-570.23787	90.420	6.577	95.623	0
2'-*E*	-570.23702	90.554	6.549	95.347	0
2-*E*	-570.23472	90.352	6.599	95.814	0
2-*Z*	-570.23829	90.412	6.583	95.687	0

triplets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
2'-*Z*	-570.23057	90.592	6.597	97.990	0
2'-*E*	-570.23433	90.754	6.544	97.529	0
2-*E*	-570.23180	90.574	6.593	98.020	0
2-*Z*	-570.23068	90.560	6.607	98.095	0

c) Compound **3** diradical C^1-C^5 product isomers

singlets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
3-Lin	-1032.41497	192.962	12.668	148.573	0

triplets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
3-Lin	-1032.41013	193.059	12.696	155.294	0

d) Compound **4** diradical C^1-C^5 product isomers

singlets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
4'-Lin	-1032.41110	193.009	12.686	148.173	0
4-Lin	-1032.41146	192.998	12.703	149.020	0

triplets	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
4'-Lin	-1032.40598	193.006	12.728	151.682	0
4-Lin	-1032.40718	193.133	12.696	151.709	0

e) Compound **1** cyclization reactivity

C^1-C^5 Cyclization 1-Z	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-570.29170	89.556	7.363	101.655	15.725	123.988	0
singlet transition state	-570.22680	88.477	6.784	96.923	14.782	118.267	1 (-886.63)
triplet transition state	-570.13761	86.556	7.273	103.251	15.491	125.197	1 (-1429.75)
singlet diradical product	-570.24156	90.354	6.563	95.583	14.458	116.634	0
triplet diradical product	-570.23368	90.529	6.581	97.942	14.454	118.936	0

C^1-C^6 Cyclization 1-BC	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-570.29170	89.556	7.363	101.655	15.725	123.988	0
singlet transition state	-570.23974	88.766	6.624	95.667	14.565	116.855	1 (-978.33)
triplet transition state	-570.15223	85.118	7.280	102.380	15.696	124.853	1 (-705.74)
singlet diradical product	-570.27362	91.475	6.289	93.766	13.970	114.234	0
triplet diradical product	-570.26948	91.717	6.298	96.063	13.952	116.462	0

f) Compound **2** cyclization reactivity

C^1-C^5 Cyclization 2-Z	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-570.29021	89.589	7.372	101.600	15.727	123.912	0
singlet transition state	-570.22347	88.543	6.795	96.932	14.777	118.233	1 (-890.68)
triplet transition state	-570.15063	85.427	7.339	102.806	15.700	125.135	1 (-791.40)
singlet diradical product	-570.23829	90.41171	6.583	95.687	14.461	116.696	0
triplet diradical product	-570.23068	90.560	6.607	98.095	14.469	119.060	0

C^1-C^6 Cyclization 2-BC	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-570.29021	89.589	7.372	101.600	15.727	123.912	0
singlet transition state	-570.23946	88.784	6.647	95.802	14.579	116.965	1 (-994.96)
triplet transition state	-570.16512	86.453	7.047	100.667	15.271	122.625	1 (-955.76)
singlet diradical product	-570.28323	91.809	6.269	93.709	13.892	114.025	0
triplet diradical product	-570.28025	91.996	6.276	95.976	13.881	116.242	0

g) Compound **3** cyclization reactivity

C^1-C^5 Cyclization 3-Lin	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-1032.46578	193.310	13.288	158.094	28.767	199.370	0
singlet transition state	-1032.40203	192.140	12.664	148.124	27.824	188.535	1 (-746.53)
triplet transition state	-1032.33237	190.319	13.097	154.649	28.531	195.805	1 (-529.09)
singlet diradical product	-1032.41497	192.962	12.668	148.573	27.942	189.280	0
triplet diradical product	-1032.41013	193.059	12.696	155.294	27.939	195.918	0

C^1-C^6 Cyclization 3-BC	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-1032.46578	193.310	13.288	158.094	28.767	199.370	0
singlet transition state	-1032.39408	192.126	12.548	146.170	27.688	186.523	1 (-827.53)
triplet transition state	-1032.33185	190.756	13.036	154.514	28.403	195.488	1 (-500.13)
singlet diradical product	-1032.42152	193.939	12.306	143.133	27.403	183.350	0
triplet diradical product	-1032.41923	194.145	12.301	145.286	27.379	185.460	0

h) Compound **4** cyclization reactivity

C^1-C^5 Cyclization 4-Lin	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-1032.46503	193.347	13.282	156.564	28.749	197.808	0
singlet transition state	-1032.39816	192.118	12.708	148.828	27.863	189.223	1 (-754.29)
triplet transition state	-1032.33434	190.687	13.103	156.659	28.433	197.534	1 (-654.16)
singlet diradical product	-1032.41147	192.9923	12.705	149.159	27.966	189.832	0
triplet diradical product	-1032.40718	193.1324	12.696	151.725	27.928	192.321	0

C^1-C^6 Cyclization 4-BC	E (gas phase, cc-pVTZ basis, a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	H (thermal, 180°C, kcal/mol)	S (thermal, 180°C, cal/mol*K)	# of imaginary frequencies
enediyne	-1032.46503	193.347	13.282	156.564	28.749	197.808	0
singlet transition state	-1032.39450	192.177	12.557	145.678	27.682	185.989	1 (-848.15)
triplet transition state	-1032.34268	190.434	12.841	149.975	28.183	190.878	1 (-1009.06)
singlet diradical product	-1032.43125	194.261	12.278	142.707	27.325	182.796	0
triplet diradical product	-1032.42982	194.409	12.277	144.910	27.312	184.967	0

i) C^1-C^5 product isomers from cyclization of **3**

	E (a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
isomer #1 (**24-*E***)	-1033.97510	207.568	12.492	144.862	0
isomer #2 (**24-*Z***)	-1033.97340	207.290	12.548	145.313	0

j) C^1-C^5 product isomers from cyclization of **4**

	E (a.u.)	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)	# of imaginary frequencies
isomer #1	-1033.96861	207.396	12.543	145.041	0
isomer #2	-1033.96498	207.376	12.509	144.329	0
isomer #3	-1033.97287	207.594	12.507	144.923	0
isomer #4	-1033.97101	207.368	12.561	145.314	0

Cartesian coordinates of optimized geometries from DFT calculations

1 – reactant

```
C 1.584274 -2.715254 0.509138
C 1.584171 -4.078580 0.903956
N 2.679169 -4.795866 0.972521
C 3.832408 -4.156994 0.640984
C 3.832457 -2.789828 0.244799
N 2.679341 -2.072473 0.183740
C 5.051439 -2.166285 -0.091095
C 5.051354 -4.863522 0.690906
C 6.242135 -2.863722 -0.040198
C 6.242052 -4.247146 0.360629
C 7.462761 -2.215923 -0.383100
C 7.462570 -4.978132 0.416885
C 8.489681 -1.650629 -0.674162
C 8.488269 -5.614158 0.464395
H 0.648934 -2.162249 0.468257
H 0.648684 -4.567887 1.164290
H 5.031508 -1.125579 -0.390243
H 5.031381 -5.902883 0.994689
H 9.398072 -1.157858 -0.931696
H 9.396340 -6.169031 0.507306
```

1 – singlet C^1-C^5 transition state

```
 N    -2.160007     1.521746     0.000002
 C    -1.090933     0.686163     0.000003
 C     0.211133     1.246279     0.000003
 H     0.308878     2.324516     0.000003
 C     1.293020     0.405323     0.000005
 C     1.122369    -1.029068     0.000005
 C    -0.130573    -1.584140     0.000003
 H    -0.287506    -2.655522     0.000000
 C    -1.261898    -0.732053     0.000001
 N    -2.501156    -1.286338    -0.000004
 C    -3.513512    -0.451229    -0.000005
 H    -4.513289    -0.878809    -0.000011
 C    -3.343445     0.954132    -0.000001
 H    -4.211655     1.608656     0.000001
 C     2.424257    -1.639116     0.000002
 C     3.487931    -0.935563    -0.000003
 H     4.560222    -0.955158    -0.000017
 C     2.700087     0.774173     0.000000
 C     3.490408     1.749176    -0.000005
 H     4.438422     2.244001    -0.000010
```

1 – triplet C^1-C^5 transition state

```
 N    -2.217500     1.485726    -0.124609
 C    -1.115596     0.689201    -0.071720
 C     0.159700     1.282328    -0.144893
 H     0.228043     2.358520    -0.248035
 C     1.299366     0.484435    -0.064002
 C     1.152706    -0.957573     0.027429
 C    -0.079664    -1.544313     0.101706
 H    -0.203192    -2.617725     0.176605
 C    -1.242850    -0.730786     0.060112
 N    -2.456396    -1.324225     0.127484
```

C	-3.500915	-0.526179	0.075104
H	-4.484182	-0.985988	0.132178
C	-3.378199	0.878559	-0.049604
H	-4.269398	1.500560	-0.088095
C	2.444803	-1.563916	-0.017011
C	3.603787	-1.184945	-0.242645
H	4.666471	-1.204374	-0.350755
C	2.626137	0.951973	-0.119376
C	3.423076	1.826946	0.462163
H	4.425436	2.184121	0.254391

1 – singlet C^1-C^6 transition state

N	-2.323276	1.712332	-0.000041
N	-2.556046	-1.112868	-0.000145
H	0.110325	2.589062	-0.000107
H	-4.374922	1.715976	-0.000103
C	0.054182	1.507989	-0.000113
C	-0.177203	-1.300401	-0.000194
C	-1.338639	-0.505242	-0.000081
C	-1.221736	0.913647	-0.000029
H	4.521764	-1.539755	0.000693
C	2.514995	1.269936	-0.000413
H	4.728975	0.975069	0.001008
C	1.208557	0.750737	0.000105
H	-4.580623	-0.780669	-0.000191
C	3.673728	0.780274	0.000713
C	-3.480122	1.098077	-0.000092
C	2.289388	-1.468337	-0.000423
C	3.512624	-1.174885	0.000658
C	1.085547	-0.742304	0.000120
H	-0.298758	-2.376083	-0.000223
C	-3.596758	-0.317556	-0.000144

1 – triplet C^1-C^6 transition state

N	-2.395679	1.419372	0.000598
N	-2.357592	-1.426106	-0.000999
H	-0.035815	2.491409	0.000362
H	-4.464767	1.221687	0.000279
C	-0.017312	1.409334	0.000597
C	0.023883	-1.397925	0.001641
C	-1.242106	-0.714922	0.000300
C	-1.250671	0.721640	0.000666
H	4.763595	-1.262375	0.003072
C	2.493186	1.364508	-0.000437
H	4.747655	1.282259	-0.000718
C	1.270937	0.722755	0.000782
H	-4.439503	-1.268579	-0.002861
C	3.709910	1.013018	-0.001780
C	-3.527815	0.673261	-0.000069
C	2.515493	-1.353346	0.000165
C	3.722634	-1.007790	-0.001400
C	1.268295	-0.721233	0.001253
H	0.000963	-2.480108	0.002594
C	-3.516306	-0.698826	-0.001703

1 – singlet C^1-C^5 diradical product – **1-*Z***

N	2.122545	1.531252	0.000000
C	1.067538	0.679026	0.000003
C	-0.245067	1.219052	0.000001
H	-0.359062	2.296653	0.000001
C	-1.308182	0.360657	0.000001
C	-1.108807	-1.068855	-0.000001
C	0.148757	-1.612073	-0.000001
H	0.326639	-2.680539	-0.000004
C	1.263770	-0.737452	0.000001
N	2.512721	-1.269059	-0.000002
C	3.511002	-0.416695	-0.000003
H	4.517947	-0.827161	0.000014
C	3.316429	0.984665	-0.000002
H	4.172831	1.654573	0.000016
C	-2.434755	-1.639669	-0.000008
C	-3.420291	-0.738850	0.000014
H	-4.489482	-0.885963	0.000012
C	-2.765386	0.610908	-0.000004
C	-3.393083	1.770594	-0.000006
H	-4.407288	2.139235	-0.000003

1 – triplet C^1-C^5 diradical product – **1-*Z***

N	2.115010	1.532705	0.000000
C	1.062914	0.676919	0.000004
C	-0.252019	1.210911	0.000002
H	-0.374878	2.288318	0.000002
C	-1.311320	0.348881	0.000001
C	-1.106514	-1.075337	-0.000001
C	0.151552	-1.617488	-0.000001
H	0.332108	-2.685573	-0.000004
C	1.263757	-0.739269	0.000001
N	2.514716	-1.266472	-0.000003
C	3.509987	-0.410657	-0.000004
H	4.518375	-0.817560	0.000017
C	3.310709	0.990119	-0.000002
H	4.164935	1.662777	0.000020
C	-2.436213	-1.644987	-0.000005
C	-3.415048	-0.729591	0.000013
H	-4.483417	-0.892694	0.000011
C	-2.773585	0.604952	-0.000006
C	-3.369067	1.786476	-0.000006
H	-4.376113	2.175537	-0.000003

1 – singlet C^1-C^5 diradical product – **1-*E***

N	2.110600	1.523188	-0.000004
C	1.056644	0.670476	-0.000003
C	-0.256704	1.209491	-0.000002
H	-0.365177	2.288141	-0.000002
C	-1.321116	0.353853	-0.000001
C	-1.121840	-1.077310	0.000002
C	0.136335	-1.619191	0.000003
H	0.313594	-2.687778	0.000009
C	1.252216	-0.745532	0.000000
N	2.500951	-1.277007	0.000003
C	3.499269	-0.424446	0.000002
H	4.506105	-0.835073	-0.000003

C	3.304847	0.976744	-0.000003
H	4.160994	1.646881	-0.000009
C	-2.446999	-1.648761	0.000020
C	-3.427298	-0.737108	-0.000034
H	-4.496480	-0.886718	-0.000029
C	-2.785048	0.604128	0.000008
C	-3.421692	1.759915	0.000012
H	-3.211588	2.817728	0.000021

1 – triplet C^1-C^5 diradical product – **1-*E***

N	2.107580	1.521815	-0.000003
C	1.053664	0.668701	-0.000002
C	-0.259432	1.207008	-0.000001
H	-0.368838	2.286046	-0.000003
C	-1.322083	0.349181	0.000001
C	-1.121775	-1.075876	0.000000
C	0.134825	-1.621918	0.000002
H	0.310307	-2.690934	0.000003
C	1.250197	-0.748370	0.000000
N	2.499545	-1.278762	0.000002
C	3.497009	-0.425482	0.000002
H	4.504238	-0.835353	0.000001
C	3.301810	0.975767	-0.000002
H	4.157811	1.646210	-0.000004
C	-2.451338	-1.645061	0.000004
C	-3.430678	-0.732420	-0.000011
H	-4.499566	-0.889309	-0.000008
C	-2.792238	0.600287	0.000002
C	-3.399929	1.775592	0.000006
H	-3.114026	2.817521	0.000008

1 – singlet C^1-C^6 diradical product – **1-BC**

C	3.744911	0.720238	0.002062
C	1.286979	0.732101	0.000841
C	1.285806	-0.737044	0.003796
C	2.549732	-1.350774	0.005953
C	2.551805	1.343942	0.000098
C	3.743700	-0.728875	0.005078
H	4.688375	-1.261720	0.005971
H	4.690110	1.252124	0.001964
C	-3.408140	-0.712880	0.000325
C	-3.406997	0.715552	-0.002797
C	-1.138016	0.717081	-0.001051
C	-1.139164	-0.718041	0.002058
C	0.067863	-1.417119	0.004360
C	0.070150	1.414196	-0.001591
H	-4.353427	-1.251099	0.000855
H	-4.351420	1.255279	-0.004671
H	0.038696	-2.500046	0.006600
H	0.042768	2.497166	-0.004054
N	-2.310727	1.421663	-0.003508
N	-2.313005	-1.420744	0.002713

1 – triplet C^1-C^6 diradical product – **1-BC**

C	-3.694791	-0.718995	0.000093
C	-1.217710	-0.726200	0.000126
C	-1.217694	0.726361	0.000006
C	-2.491732	1.332728	-0.000078
C	-2.491672	-1.332690	0.000161
C	-3.694748	0.718906	-0.000297
H	-4.628674	1.272084	-0.000423
H	-4.628589	-1.272350	0.000552
C	3.470267	0.714567	0.000011
C	3.470248	-0.714639	-0.000089
C	1.200617	-0.718720	-0.000056
C	1.200634	0.718718	0.000096
C	-0.005523	1.417776	0.000081
C	-0.005582	-1.417713	-0.000046
H	4.415390	1.253152	0.000082
H	4.415354	-1.253250	-0.000109
H	0.019356	2.501160	0.000098
H	0.019214	-2.501097	-0.000133
N	2.375269	-1.421592	-0.000128
N	2.375311	1.421553	0.000111

2 – reactant

N	-14.938744	1.879468	-2.565947
C	-13.610211	2.113247	-2.718377
C	-12.730603	1.013920	-2.854229
H	-13.153579	0.016649	-2.831353
C	-11.388842	1.228791	-3.008857
H	-10.704805	0.395222	-3.113902
C	-10.848050	2.543783	-3.036969
C	-11.689372	3.652870	-2.905366
C	-13.093226	3.438655	-2.743348
N	-13.912819	4.510261	-2.615453
C	-15.190510	4.255050	-2.469704
H	-15.860419	5.105203	-2.365803
C	-15.706017	2.936141	-2.444752
H	-16.773214	2.768467	-2.321683
C	-11.173071	4.975163	-2.930338
C	-10.713565	6.091796	-2.954261
H	-10.315157	7.079067	-2.974361
C	-9.443753	2.702344	-3.200726
C	-8.247243	2.793968	-3.341472
H	-7.194100	2.893736	-3.464801

2 – singlet C^1-C^5 transition state

N	2.690560	1.076667	0.000003
C	1.346856	0.874473	0.000010
C	0.485473	1.999086	0.000045
H	0.943843	2.980956	0.000078
C	-0.879087	1.838480	0.000012
H	-1.539189	2.697182	0.000005
C	-1.420707	0.536489	-0.000045
C	-0.596888	-0.595896	-0.000019
C	0.807478	-0.447741	-0.000018
N	1.610846	-1.541460	-0.000028
C	2.900771	-1.309137	-0.000009
H	3.563722	-2.171059	0.000005

C	3.441381	0.001917	-0.000006
H	4.519315	0.145317	-0.000030
C	-1.407827	-1.781149	0.000034
C	-2.681082	-1.709113	0.000050
C	-2.824810	0.172627	0.000009
C	-3.993689	0.637969	-0.000024
H	-3.604597	-2.253531	0.000109
H	-5.060154	0.546661	-0.000225

2 – triplet C^1-C^5 transition state

N	2.652896	1.123735	-0.000028
C	1.349132	0.868035	0.000072
C	0.423324	1.987084	0.000212
H	0.866152	2.976043	0.000415
C	-0.954400	1.817041	0.000079
H	-1.607193	2.681715	0.000204
C	-1.491994	0.537425	-0.000038
C	-0.572214	-0.655817	0.000292
C	0.851555	-0.471271	0.000056
N	1.671973	-1.523132	-0.000036
C	2.984835	-1.242895	-0.000190
H	3.662995	-2.091228	-0.000340
C	3.468936	0.052472	-0.000143
H	4.536052	0.251914	-0.000156
C	-1.336961	-1.799382	0.000292
C	-2.640898	-1.752831	-0.000116
C	-2.869591	0.176222	-0.000631
C	-4.056862	0.602691	0.000227
H	-3.536621	-2.344558	0.001470
H	-5.124638	0.609256	-0.001818

2 – singlet C^1-C^6 transition state

N	-2.783845	0.827916	-0.000057
C	-1.426626	0.827527	0.000011
C	-0.738931	2.064828	-0.000008
H	-1.330017	2.972866	-0.000078
C	0.627367	2.094832	0.000018
H	1.152555	3.041809	-0.000040
C	1.410092	0.908472	0.000114
C	0.735474	-0.369962	0.000162
C	-0.690214	-0.388365	0.000070
N	-1.322985	-1.588744	0.000045
C	-2.634265	-1.557576	-0.000032
H	-3.154987	-2.512058	-0.000057
C	-3.367600	-0.346786	-0.000075
H	-4.454710	-0.365734	-0.000127
C	1.532042	-1.519610	0.000078
C	2.763118	-1.768892	-0.000046
C	2.814959	0.896635	-0.000042
C	3.684802	-0.014259	-0.000120
H	3.547482	-2.499799	-0.000269
H	4.726179	-0.272341	-0.000117

2 – triplet C^1-C^6 transition state

N	-2.749024	0.857470	0.020784
C	-1.412453	0.812216	0.063737
C	-0.685291	2.051969	0.218988
H	-1.278178	2.954278	0.309433
C	0.682583	2.094990	0.178812
H	1.200002	3.047727	0.192392
C	1.441657	0.917077	0.005444
C	0.726511	-0.414087	0.088882
C	-0.713779	-0.423743	-0.028523
N	-1.364158	-1.587663	-0.143488
C	-2.691841	-1.518730	-0.195511
H	-3.229499	-2.457624	-0.293824
C	-3.378772	-0.308211	-0.117048
H	-4.464001	-0.280697	-0.156181
C	1.536208	-1.480748	0.350267
C	2.767993	-1.781745	0.420418
C	2.774655	0.827337	-0.343642
C	3.695981	-0.022543	-0.493337
H	3.516378	-2.359068	0.930401
H	4.586860	-0.315965	-1.014202

2 – singlet C^1-C^5 diradical product – **2'-*Z***

N	2.717921	0.733533	0.000003
C	1.365060	0.845282	0.000002
C	0.788770	2.140915	-0.000002
H	1.467649	2.985765	-0.000002
C	-0.574805	2.305899	-0.000006
H	-1.015456	3.296271	-0.000010
C	-1.400911	1.164817	-0.000005
C	-0.862749	-0.128830	0.000000
C	0.533141	-0.319633	0.000001
N	1.069914	-1.566770	0.000003
C	2.379240	-1.635248	0.000006
H	2.826915	-2.626544	-0.000002
C	3.205544	-0.484331	0.000003
H	4.287781	-0.590637	-0.000003
C	-1.975222	-1.091041	-0.000011
C	-3.234779	-0.274146	0.000036
C	-2.839056	1.001524	-0.000012
C	-1.921639	-2.410257	-0.000022
H	-4.228050	-0.695331	0.000045
H	-2.629253	-3.226565	-0.000013

2 – triplet C^1-C^5 diradical product – **2'-*Z***

N	2.712833	0.736024	-0.000003
C	1.360450	0.850605	-0.000002
C	0.783495	2.146371	0.000006
H	1.460851	2.992275	0.000008
C	-0.580608	2.310135	0.000011
H	-1.022028	3.300149	0.000013
C	-1.403953	1.167067	0.000007
C	-0.867616	-0.122974	0.000001
C	0.527920	-0.312630	-0.000004
N	1.060527	-1.559854	-0.000005
C	2.369536	-1.632865	-0.000009
H	2.815044	-2.624924	-0.000001

C	3.197832	-0.483028	-0.000006
H	4.279664	-0.591688	0.000001
C	-1.975853	-1.098043	0.000022
C	-3.220690	-0.292324	-0.000046
C	-2.843988	0.994333	0.000003
C	-1.874135	-2.418636	0.000030
H	-4.218942	-0.705206	-0.000059
H	-2.562458	-3.251856	0.000018

2 – singlet C^1-C^5 diradical product – **2'-*E***

N	-2.682135	0.797774	-0.000164
C	-1.327870	0.878324	-0.000277
C	-0.720469	2.159594	-0.000413
H	-1.378041	3.021035	-0.000803
C	0.646711	2.291343	-0.000056
H	1.110487	3.271095	0.000344
C	1.447057	1.131639	0.000169
C	0.876969	-0.148647	-0.000174
C	-0.522378	-0.305296	0.000001
N	-1.089700	-1.539832	0.000263
C	-2.400905	-1.577935	0.000471
H	-2.871822	-2.558226	0.000694
C	-3.199226	-0.408195	0.000212
H	-4.283510	-0.488604	0.000231
C	1.970407	-1.142463	-0.000573
C	3.234055	-0.359903	0.000211
C	2.881103	0.932309	0.000815
C	1.870453	-2.460599	-0.000507
H	4.217481	-0.804385	0.000536
H	1.072811	-3.187535	-0.000976

2 – triplet C^1-C^5 diradical product – **2'-*E***

N	-2.678362	0.801957	-0.000109
C	-1.324401	0.880700	-0.000210
C	-0.714753	2.161811	-0.000274
H	-1.371326	3.024031	-0.000569
C	0.652359	2.291516	0.000057
H	1.118544	3.270242	0.000540
C	1.448239	1.128371	0.000184
C	0.878904	-0.147980	-0.000178
C	-0.520888	-0.304224	-0.000016
N	-1.089729	-1.536942	0.000112
C	-2.401292	-1.574170	0.000291
H	-2.873219	-2.553942	0.000438
C	-3.197530	-0.403530	0.000146
H	-4.281925	-0.482110	0.000140
C	1.974632	-1.146376	-0.000660
C	3.233277	-0.369768	-0.000142
C	2.883717	0.923457	0.000656
C	1.846782	-2.465192	-0.000053
H	4.219048	-0.810558	0.000526
H	1.011245	-3.150464	0.000104

2 – singlet C^1-C^5 diradical product – **2-*E***

N	-2.652089	1.122113	-0.000010
C	-1.315087	0.876657	0.000055
C	-0.418125	1.972492	0.000113
H	-0.845017	2.968365	0.000198
C	0.943216	1.766981	0.000074
H	1.624301	2.611135	0.000188
C	1.439685	0.453714	-0.000005
C	0.577702	-0.649684	0.000090
C	-0.820137	-0.464298	0.000059
N	-1.658884	-1.531369	-0.000019
C	-2.940490	-1.255927	-0.000119
H	-3.632013	-2.095126	-0.000169
C	-3.437365	0.072461	-0.000094
H	-4.510089	0.250842	-0.000124
C	1.409191	-1.830597	0.000032
C	2.718986	-1.548491	0.000229
C	2.830651	-0.065030	-0.000089
C	3.957560	0.621752	-0.000257
H	4.298233	1.645536	-0.000464
H	3.566669	-2.216147	0.000046

2 – triplet C^1-C^5 diradical product – **2-*E***

N	-2.648157	1.124877	-0.000045
C	-1.312208	0.876321	-0.000022
C	-0.411897	1.970569	0.000155
H	-0.836975	2.967224	0.000076
C	0.948591	1.761934	0.000328
H	1.632695	2.604137	0.000302
C	1.439762	0.446651	0.000206
C	0.577441	-0.650970	0.000027
C	-0.820719	-0.465996	-0.000050
N	-1.661132	-1.530787	-0.000057
C	-2.942600	-1.252433	-0.000099
H	-3.635954	-2.090085	-0.000258
C	-3.436081	0.076629	-0.000099
H	-4.508334	0.257699	-0.000198
C	1.411319	-1.833663	0.000313
C	2.721412	-1.551604	0.000028
C	2.834484	-0.077370	-0.000234
C	3.945984	0.640276	-0.000459
H	4.216392	1.686763	-0.000605
H	3.564264	-2.226421	0.000831

2 – singlet C^1-C^5 diradical product – **2-*Z***

N	2.672948	1.099004	0.000000
C	1.333352	0.870921	0.000001
C	0.450234	1.979265	0.000001
H	0.892875	2.968468	0.000000
C	-0.913252	1.794266	0.000000
H	-1.587453	2.643403	-0.000002
C	-1.425289	0.485777	0.000001
C	-0.579143	-0.629049	0.000000
C	0.821479	-0.464285	0.000002
N	1.645928	-1.541848	-0.000002
C	2.931461	-1.282403	-0.000007
H	3.612137	-2.130597	0.000004

C	3.444876	0.038764	0.000003
H	4.519887	0.203683	0.000007
C	-1.429195	-1.796053	-0.000007
C	-2.734202	-1.508282	0.000011
C	-2.816672	-0.009222	-0.000002
C	-3.930667	0.697304	-0.000005
H	-3.592540	-2.161545	0.000014
H	-4.994926	0.514479	-0.000003

2 – triplet C^1-C^5 diradical product – **2-*Z***

N	2.667086	1.107249	0.000000
C	1.328584	0.871997	-0.000001
C	0.439294	1.975688	-0.000001
H	0.875216	2.967689	-0.000001
C	-0.923042	1.780829	-0.000002
H	-1.606342	2.623599	0.000000
C	-1.426163	0.470008	0.000000
C	-0.575377	-0.636042	0.000000
C	0.824274	-0.465793	-0.000002
N	1.654450	-1.538839	0.000003
C	2.938502	-1.272781	0.000010
H	3.623922	-2.116988	-0.000005
C	3.444790	0.051455	-0.000004
H	4.518797	0.222021	-0.000013
C	-1.425774	-1.807455	0.000002
C	-2.732951	-1.505400	-0.000011
C	-2.823800	-0.026308	0.000004
C	-3.917237	0.718263	0.000007
H	-3.581697	-2.173386	-0.000014
H	-4.987238	0.571424	0.000004

2 – singlet C^1-C^6 diradical product – **2-BC**

N	-2.779542	0.814106	0.000021
C	-1.428320	0.811426	0.000284
C	-0.737606	2.063383	0.000289
H	-1.340675	2.963701	0.000637
C	0.619809	2.107732	0.000026
H	1.142497	3.057282	-0.000059
C	1.404690	0.908398	-0.000229
C	0.742252	-0.369852	0.000157
C	-0.697807	-0.403432	0.000211
N	-1.323029	-1.597600	-0.000155
C	-2.640714	-1.569686	-0.000347
H	-3.158330	-2.525454	-0.000107
C	-3.368524	-0.364485	-0.000287
H	-4.455448	-0.378375	-0.000015
C	1.552836	-1.496807	0.000524
C	2.912465	-1.500594	0.000282
C	2.795117	0.878109	-0.000550
C	3.574905	-0.235012	-0.000271
H	3.496520	-2.414610	0.000523
H	4.658820	-0.193168	-0.000575

2 – triplet C^1-C^6 diradical product – **2-BC**

N	-2.782105	0.809508	0.000610
C	-1.431502	0.809456	0.000091
C	-0.742078	2.064286	-0.000063
H	-1.348262	2.962631	0.000201
C	0.615192	2.112648	-0.000448
H	1.138161	3.062511	-0.000910
C	1.394524	0.909319	-0.000232
C	0.740184	-0.359871	0.000148
C	-0.699873	-0.405115	-0.000110
N	-1.320784	-1.599982	-0.000268
C	-2.639192	-1.574682	-0.000164
H	-3.155214	-2.531316	-0.002339
C	-3.368599	-0.371061	0.000474
H	-4.455517	-0.386883	-0.001033
C	1.562853	-1.483040	0.000298
C	2.926878	-1.496706	0.000088
C	2.788621	0.869939	0.000001
C	3.582913	-0.238289	0.000189
H	3.495107	-2.421528	0.000018
H	4.666439	-0.173404	0.000044

3 – reactant

N	-0.181273	-1.672703	0.169008
C	1.172282	-1.792254	0.147347
C	1.755071	-3.067309	0.291650
H	1.099543	-3.919578	0.421379
C	3.127876	-3.228398	0.276411
C	3.979275	-2.074858	0.101322
C	3.411473	-0.821937	-0.034814
H	4.032543	0.055437	-0.166712
C	2.012453	-0.652959	-0.013936
N	1.490432	0.594103	-0.152442
C	0.181871	0.677030	-0.127617
H	-0.258534	1.665260	-0.236456
C	-0.654627	-0.457259	0.033162
H	-1.735269	-0.337197	0.047236
C	5.387991	-2.233032	0.056279
C	3.701489	-4.514590	0.444885
C	6.593578	-2.366911	0.000407
C	4.189740	-5.614612	0.606276
C	8.002697	-2.541184	-0.072912
C	8.870633	-1.460605	0.152863
C	10.244783	-1.641130	0.078919
C	10.773668	-2.894195	-0.221539
C	9.919883	-3.971034	-0.449585
C	8.544398	-3.801188	-0.376933
H	8.453718	-0.487856	0.386565
H	10.906586	-0.800275	0.256022
H	11.848053	-3.030762	-0.279320
H	10.328056	-4.947284	-0.687959
H	7.874133	-4.632929	-0.560976
C	4.776807	-6.894138	0.803630
C	6.115170	-7.001749	1.216800
C	6.688002	-8.250879	1.410659
C	5.940934	-9.407088	1.197029
C	4.612778	-9.309278	0.788883

C	4.030293	-8.064764	0.593268
H	6.688327	-6.097954	1.388734
H	7.721262	-8.323147	1.732596
H	6.391996	-10.381527	1.349686
H	4.027865	-10.207411	0.622692
H	2.997343	-7.982854	0.275493

3 – singlet C^1-C^5 transition state

N	-4.688422	1.769979	-0.007054
C	-3.784393	0.759110	-0.015287
C	-2.403451	1.078458	-0.048244
H	-2.118359	2.123164	-0.064003
C	-1.484631	0.061784	-0.058109
C	-1.904930	-1.322441	-0.036015
C	-3.238661	-1.643903	-0.001129
H	-3.581664	-2.670809	0.017421
C	-4.202266	-0.607241	0.009420
N	-5.519859	-0.933176	0.042451
C	-6.368802	0.068198	0.049413
H	-7.428200	-0.176064	0.075682
C	-5.954051	1.420529	0.024471
H	-6.692835	2.218288	0.031227
C	-0.743504	-2.156886	-0.060686
C	0.442123	-1.663445	-0.115455
C	-0.036750	0.178241	-0.079518
C	0.877982	1.038107	-0.019397
C	1.836901	-2.042315	-0.122490
C	2.246722	-3.137722	0.654694
C	3.572668	-3.547058	0.647781
H	1.510091	-3.655442	1.258052
C	4.511883	-2.871518	-0.128470
H	3.875106	-4.394844	1.253268
C	2.786886	-1.374076	-0.904316
C	4.113537	-1.786921	-0.904275
H	2.476033	-0.542124	-1.523589
H	4.837549	-1.261446	-1.517590
H	5.548419	-3.191123	-0.130066
C	2.021458	1.845470	0.070623
C	2.665332	2.038924	1.312451
C	3.783344	2.852188	1.398037
H	2.274752	1.538846	2.190679
C	4.282806	3.487556	0.261274
H	4.272068	2.991537	2.356073
C	3.653960	3.306788	-0.970570
H	5.158659	4.122613	0.335269
H	4.039633	3.802587	-1.854685
C	2.534130	2.497793	-1.072488
H	2.036945	2.359483	-2.025804

3 – triplet C^1-C^5 transition state

N	-4.719235	1.568405	0.376258
C	-3.761277	0.622888	0.191972
C	-2.405902	0.976642	0.372958
H	-2.170710	1.997120	0.651675
C	-1.417498	0.033040	0.170600
C	-1.777076	-1.323533	-0.175774
C	-3.088807	-1.680216	-0.363173

H	-3.375044	-2.690184	-0.629435
C	-4.106601	-0.712430	-0.185853
N	-5.400058	-1.077380	-0.366288
C	-6.301351	-0.139810	-0.180583
H	-7.343767	-0.414002	-0.323415
C	-5.960045	1.183211	0.189706
H	-6.740374	1.927163	0.331620
C	-0.613934	-2.144922	-0.241629
C	0.600142	-1.999194	0.017850
C	-0.012789	0.266709	0.310852
C	0.872641	1.187839	0.137100
C	1.983268	-2.325890	0.134675
C	2.493960	-3.441837	-0.551522
C	3.833911	-3.779530	-0.431386
H	1.827452	-4.031538	-1.170003
C	4.683625	-3.011657	0.362427
H	4.218096	-4.644042	-0.961879
C	2.844414	-1.558976	0.933243
C	4.185026	-1.902708	1.040974
H	2.450113	-0.697854	1.458827
H	4.843286	-1.301499	1.658462
H	5.731623	-3.276733	0.450326
C	1.830370	2.110955	-0.070206
C	2.120916	3.133277	0.921794
C	3.109486	4.054275	0.700957
H	1.535333	3.146558	1.833368
C	3.870340	4.035145	-0.487351
H	3.311365	4.810964	1.451970
C	3.608295	3.054995	-1.467701
H	4.650027	4.770382	-0.646799
H	4.194327	3.043264	-2.380796
C	2.623042	2.120962	-1.288877
H	2.418402	1.367810	-2.040024

3 – singlet C^1-C^6 transition state

N	-5.342648	1.415641	-0.071194
C	-6.445252	0.709060	-0.035963
C	-6.445207	-0.709209	0.035545
N	-5.342557	-1.415711	0.070923
C	-4.178647	-0.711891	0.035923
C	-4.178692	0.711907	-0.036008
C	-2.956131	1.407717	-0.070164
C	-1.745862	0.741106	-0.038291
C	-1.745824	-0.740912	0.038706
C	-2.956045	-1.407621	0.070253
C	-0.486819	-1.365664	0.042078
C	0.728981	-0.980770	-0.026249
C	0.728859	0.980946	0.026910
C	-0.486903	1.365985	-0.041602
C	2.058590	1.557865	0.147482
C	2.058683	-1.557696	-0.147129
C	2.926293	1.185432	1.181328
C	4.172426	1.786454	1.300670
C	4.572647	2.760985	0.390521
C	3.715168	3.138041	-0.639921
C	2.466484	2.542467	-0.763895
C	2.926468	-1.184757	-1.180726

C	4.172440	-1.786024	-1.300498
C	4.572387	-2.761360	-0.391089
C	3.714857	-3.138859	0.639142
C	2.466354	-2.543002	0.763582
H	2.616153	-0.425715	-1.888795
H	4.833451	-1.491644	-2.108344
H	5.547293	-3.227179	-0.485903
H	4.017739	-3.901720	1.348395
H	1.791058	-2.835257	1.559621
H	1.791118	2.834594	-1.559922
H	4.018242	3.900318	-1.349718
H	5.547724	3.226531	0.484922
H	4.833323	1.492547	2.108781
H	2.615784	0.426972	1.889938
H	-2.985625	-2.488997	0.115279
H	-2.985764	2.489082	-0.115430
H	-7.387762	-1.250919	0.062997
H	-7.387842	1.250701	-0.063547

3 – triplet C^1-C^6 transition state

N	-5.408362	1.402991	0.106916
C	-6.506115	0.689231	0.060491
C	-6.497358	-0.726471	-0.038879
N	-5.388996	-1.424256	-0.089965
C	-4.230372	-0.714704	-0.046387
C	-4.237901	0.710819	0.052510
C	-3.020081	1.418171	0.082416
C	-1.815947	0.741499	0.019801
C	-1.817462	-0.697696	-0.026346
C	-3.000763	-1.403512	-0.078516
C	-0.527919	-1.289720	0.040110
C	0.706892	-1.251672	0.111621
C	0.725714	1.151044	-0.068681
C	-0.559534	1.426771	-0.069979
C	2.008246	1.665754	-0.176492
C	2.064965	-1.686326	0.180818
C	2.622744	2.332634	0.929934
C	3.923783	2.783915	0.844080
C	4.672631	2.587451	-0.322982
C	4.092199	1.928535	-1.415860
C	2.794091	1.469691	-1.354380
C	2.556568	-2.585152	-0.780262
C	3.870105	-3.027771	-0.713584
C	4.710702	-2.578141	0.302265
C	4.231802	-1.682453	1.255094
C	2.919265	-1.235645	1.198561
H	1.895777	-2.929500	-1.567356
H	4.239862	-3.725160	-1.457441
H	5.737490	-2.924293	0.350060
H	4.884317	-1.329107	2.045806
H	2.541974	-0.537555	1.935385
H	2.345598	0.958776	-2.198284
H	4.669332	1.779284	-2.322382
H	5.695229	2.942554	-0.381068
H	4.366947	3.302082	1.688288
H	2.037227	2.490841	1.828607
H	-3.011235	-2.486439	-0.116751

H	-3.050423	2.500285	0.136266
H	-7.435953	-1.274444	-0.074233
H	-7.452177	1.224034	0.102348

3 – singlet C^1-C^5 diradical product – **3-Lin**

N	-4.476764	1.652136	-0.056755
C	-3.589806	0.627523	-0.038257
C	-2.201693	0.925158	-0.058185
H	-1.897206	1.965099	-0.087916
C	-1.307447	-0.106791	-0.041743
C	-1.753483	-1.480069	-0.002053
C	-3.090094	-1.789060	0.018119
H	-3.453571	-2.808969	0.047759
C	-4.032832	-0.732483	-0.000307
N	-5.356291	-1.033809	0.019168
C	-6.188059	-0.017943	0.000931
H	-7.251743	-0.243765	0.016261
C	-5.749306	1.325703	-0.037294
H	-6.473473	2.136640	-0.051678
C	-0.558800	-2.271867	0.004185
C	0.590137	-1.574967	-0.041585
C	0.173110	-0.112824	-0.049601
C	0.954565	0.934552	-0.014303
C	1.956612	-2.091541	-0.054677
C	2.209331	-3.366577	0.475499
C	3.488872	-3.901324	0.460547
H	1.386857	-3.925429	0.909284
C	4.546356	-3.173320	-0.081492
H	3.664216	-4.886675	0.879069
C	3.026305	-1.372152	-0.601422
C	4.308343	-1.909733	-0.612282
H	2.852713	-0.395913	-1.036708
H	5.123525	-1.338426	-1.043302
H	5.547981	-3.589466	-0.089730
C	1.822179	2.002074	0.047320
C	2.272196	2.504959	1.302618
C	3.136421	3.581306	1.353064
H	1.926773	2.026907	2.211475
C	3.584795	4.193091	0.178494
H	3.470330	3.951536	2.316401
C	3.153271	3.713549	-1.061598
H	4.263895	5.036520	0.229335
H	3.498023	4.187728	-1.974247
C	2.286861	2.640089	-1.139712
H	1.946080	2.271798	-2.100487

3 – triplet C^1-C^5 diradical product – **3-Lin**

N	-4.385664	0.772387	-0.002148
C	-3.338194	-0.087604	-0.001369
C	-2.020313	0.440896	-0.001275
H	-1.894562	1.518012	-0.001792
C	-0.966450	-0.426827	-0.000686
C	-1.175432	-1.849181	-0.000005
C	-2.438252	-2.386352	-0.000010
H	-2.622405	-3.453831	0.000476
C	-3.545649	-1.504190	-0.000731
N	-4.799536	-2.024615	-0.000813

C	-5.790641	-1.163449	-0.001554
H	-6.800992	-1.565781	-0.001622
C	-5.584814	0.235580	-0.002246
H	-6.435423	0.912896	-0.002884
C	0.142526	-2.415636	0.000372
C	1.156270	-1.520080	-0.000420
C	0.502322	-0.177477	-0.000446
C	1.054938	1.019235	0.001095
C	2.586214	-1.816967	-0.000870
C	3.006472	-3.157398	0.015518
C	4.353716	-3.481306	0.014485
H	2.258397	-3.943659	0.029522
C	5.317195	-2.473543	-0.002586
H	4.656003	-4.523059	0.027387
C	3.564262	-0.815085	-0.018075
C	4.915609	-1.142285	-0.018760
H	3.263288	0.226636	-0.031497
H	5.657062	-0.350564	-0.032228
H	6.371950	-2.726486	-0.003137
C	1.100442	2.403923	0.002219
C	1.157115	3.131747	1.224946
C	1.247883	4.510706	1.213133
H	1.121745	2.586166	2.160635
C	1.294208	5.211512	0.004580
H	1.281489	5.051107	2.153050
C	1.248144	4.512738	-1.205142
H	1.366462	6.293187	0.005489
H	1.281920	5.054698	-2.144154
C	1.157342	3.133787	-1.219271
H	1.121994	2.589819	-2.155913

3 – singlet C^1-C^6 diradical product – **3-BC**

N	-5.234160	1.419445	0.061301
C	-6.330524	0.713334	0.030733
C	-6.330513	-0.713407	-0.030759
N	-5.234138	-1.419502	-0.061318
C	-4.060940	-0.716828	-0.031548
C	-4.060952	0.716789	0.031541
C	-2.852408	1.414816	0.064764
C	-1.637914	0.730615	0.037114
C	-1.637901	-0.730620	-0.037100
C	-2.852386	-1.414839	-0.064760
C	-0.369435	-1.329500	-0.053665
C	0.846496	-0.736295	-0.000443
C	0.846485	0.736320	0.000483
C	-0.369453	1.329512	0.053689
C	2.074745	1.559341	-0.101617
C	2.074762	-1.559297	0.101642
C	2.201399	2.708986	0.687548
C	3.316712	3.530056	0.570447
C	4.321559	3.217139	-0.340175
C	4.201693	2.079556	-1.134204
C	3.089441	1.254883	-1.016858
C	2.201591	-2.708704	-0.687840
C	3.316896	-3.529790	-0.570766
C	4.321561	-3.217125	0.340144
C	4.201518	-2.079781	1.134488

C	3.089274	-1.255095	1.017174
H	1.418197	-2.947090	-1.399328
H	3.401346	-4.414088	-1.193383
H	5.192909	-3.856503	0.432293
H	4.976249	-1.834016	1.852823
H	2.999383	-0.375988	1.644599
H	2.999686	0.375584	-1.644030
H	4.976570	1.833592	-1.852314
H	5.192910	3.856508	-0.432345
H	3.401032	4.414542	1.192818
H	1.417863	2.947570	1.398812
H	-2.878605	-2.496961	-0.109197
H	-2.878641	2.496938	0.109200
H	-7.275521	-1.251659	-0.053843
H	-7.275540	1.251572	0.053809

3 – triplet C^1-C^6 diradical product – **3-BC**

N	-5.227474	1.419051	0.076182
C	-6.323046	0.713423	0.038290
C	-6.323040	-0.713465	-0.038302
N	-5.227462	-1.419083	-0.076190
C	-4.052875	-0.717438	-0.038955
C	-4.052881	0.717415	0.038952
C	-2.845897	1.416082	0.078495
C	-1.635323	0.724274	0.042261
C	-1.635316	-0.724280	-0.042255
C	-2.845885	-1.416097	-0.078493
C	-0.359260	-1.316772	-0.058982
C	0.863522	-0.731562	-0.002462
C	0.863516	0.731576	0.002481
C	-0.359271	1.316778	0.058993
C	2.079094	1.571883	-0.098955
C	2.079102	-1.571858	0.098968
C	2.179627	2.733752	0.675911
C	3.281463	3.572501	0.556837
C	4.299599	3.264160	-0.340513
C	4.206695	2.113457	-1.119265
C	3.107511	1.271692	-1.000479
C	2.179743	-2.733590	-0.676088
C	3.281574	-3.572347	-0.557028
C	4.299600	-3.264152	0.340497
C	4.206588	-2.113584	1.119438
C	3.107409	-1.271813	1.000668
H	1.386783	-2.967123	-1.378725
H	3.345980	-4.466070	-1.168497
H	5.160893	-3.916876	0.433700
H	4.992189	-1.871184	1.827056
H	3.037842	-0.383036	1.617035
H	3.038028	0.382805	-1.616694
H	4.992384	1.870944	-1.826747
H	5.160893	3.916882	-0.433727
H	3.345792	4.466332	1.168158
H	1.386579	2.967398	1.378410
H	-2.869810	-2.498023	-0.133736
H	-2.869828	2.498008	0.133737
H	-7.268329	-1.251051	-0.067128
H	-7.268340	1.251002	0.067112

4 – reactant

N	-14.052299	3.260865	-2.568025
C	-12.697065	3.237214	-2.627815
C	-12.029406	1.989728	-2.591204
H	-12.631243	1.091843	-2.516828
C	-10.664154	1.944506	-2.645870
H	-10.142897	0.995132	-2.613469
C	-9.883066	3.130579	-2.740574
C	-10.512977	4.383248	-2.789639
C	-11.942015	4.439497	-2.727474
N	-12.555881	5.646507	-2.766757
C	-13.866409	5.639461	-2.706510
H	-14.372423	6.601510	-2.736214
C	-14.617562	4.444424	-2.607039
H	-15.703172	4.482567	-2.559955
C	-9.766877	5.576806	-2.909757
C	-9.115509	6.594780	-3.028685
C	-8.381462	7.802558	-3.166020
C	-9.010202	9.038707	-2.941101
C	-8.294604	10.220248	-3.072386
C	-6.948536	10.190439	-3.430500
C	-6.318263	8.969404	-3.659457
C	-7.024699	7.781822	-3.529224
H	-10.058072	9.051205	-2.664820
H	-8.788659	11.169577	-2.895644
H	-6.392821	11.116253	-3.532831
H	-5.271502	8.943166	-3.942706
H	-6.542471	6.828715	-3.713847
C	-8.471196	3.021842	-2.771503
C	-7.262950	2.894853	-2.778444
C	-5.847098	2.773348	-2.779188
C	-5.041258	3.875449	-2.447547
C	-3.658740	3.754935	-2.447366
C	-3.059116	2.541374	-2.776572
C	-3.850474	1.443180	-3.105146
C	-5.233956	1.553041	-3.106700
H	-5.514905	4.814256	-2.184476
H	-3.045578	4.611012	-2.187287
H	-1.978294	2.451360	-2.775640
H	-3.387063	0.496520	-3.361002
H	-5.854426	0.701867	-3.362178

4 – singlet C^1-C^5 transition state

N	5.512858	-1.247435	0.045277
C	4.161208	-1.113131	0.004564
C	3.358296	-2.279329	-0.022242
H	3.864479	-3.237309	-0.009419
C	1.987702	-2.184927	-0.061621
H	1.372754	-3.076849	-0.080136
C	1.378509	-0.913832	-0.076864
C	2.144123	0.261755	-0.054053
C	3.555492	0.180310	-0.010638
N	4.303567	1.312085	0.016372
C	5.603350	1.145285	0.055439
H	6.221453	2.039764	0.077536
C	6.208688	-0.136317	0.069581
H	7.292065	-0.225768	0.102316

C	1.287176	1.404772	-0.081700
C	0.008177	1.277508	-0.138804
C	-0.041590	-0.625868	-0.101391
C	-1.159808	-1.200446	-0.034174
C	-2.484749	-1.647281	0.069578
C	-3.144192	-1.646305	1.318714
C	-4.445078	-2.111018	1.420094
C	-5.116672	-2.583943	0.292758
C	-4.475465	-2.591824	-0.945910
C	-3.173702	-2.133022	-1.064148
H	-2.619638	-1.272570	2.189971
H	-4.942480	-2.102563	2.383794
H	-4.994889	-2.961114	-1.823503
H	-2.668859	-2.144280	-2.023406
C	-1.220286	2.036677	-0.139424
C	-1.295071	3.207593	0.632792
C	-2.451185	3.974959	0.635388
C	-3.553105	3.587753	-0.124316
C	-3.486663	2.430834	-0.894972
C	-2.329784	1.661385	-0.907155
H	-0.435239	3.498982	1.224836
H	-2.494211	4.877194	1.236243
H	-4.337186	2.127710	-1.496063
H	-2.272999	0.773644	-1.524395
H	-4.457276	4.186949	-0.117600
H	-6.135168	-2.945851	0.379302

4 – triplet C^1-C^5 transition state

N	5.547378	-1.207622	0.093771
C	4.193322	-1.125272	0.042962
C	3.427767	-2.316955	0.074380
H	3.959760	-3.259064	0.134038
C	2.058743	-2.260050	0.031452
H	1.464467	-3.166403	0.065925
C	1.389704	-1.014421	-0.060944
C	2.118093	0.178901	-0.104391
C	3.537361	0.136650	-0.042960
N	4.240941	1.295094	-0.073406
C	5.546901	1.183143	-0.015910
H	6.128515	2.101724	-0.036120
C	6.200999	-0.070059	0.065275
H	7.286751	-0.116549	0.104697
C	1.337351	1.378400	-0.200362
C	0.015966	1.410015	-0.173408
C	-0.043868	-0.934529	-0.060150
C	-1.180095	-1.430352	-0.011164
C	-2.533681	-1.800910	0.061167
C	-3.215187	-1.786817	1.297814
C	-4.546021	-2.164987	1.365958
C	-5.228995	-2.557588	0.214784
C	-4.566700	-2.574773	-1.012939
C	-3.233500	-2.208055	-1.095839
H	-2.682550	-1.472777	2.187670
H	-5.058632	-2.149189	2.321712
H	-5.094743	-2.881089	-1.909577
H	-2.712961	-2.226973	-2.046369
C	-1.131831	2.201967	-0.149129

C	-1.332686	3.156336	0.886708
C	-2.491701	3.908017	0.932790
C	-3.487414	3.735980	-0.033362
C	-3.312323	2.793820	-1.052623
C	-2.163555	2.029286	-1.111490
H	-0.554700	3.285370	1.630184
H	-2.625478	4.639734	1.722634
H	-4.086578	2.657465	-1.800147
H	-2.027068	1.291147	-1.893016
H	-4.395273	4.327386	0.009998
H	-6.271654	-2.849574	0.274100

4 – singlet C^1-C^6 transition state

N	5.690387	-0.345081	-0.000728
C	4.381856	-0.701781	-0.000084
C	4.044518	-2.078245	0.000828
H	4.854686	-2.797645	-0.000011
C	2.734861	-2.466941	0.001213
H	2.475279	-3.518522	-0.003454
C	1.671102	-1.522954	0.003005
C	1.980973	-0.120031	0.001629
C	3.351516	0.278432	-0.000307
N	3.645948	1.601948	-0.000648
C	4.920037	1.917332	-0.001202
H	5.171022	2.975330	-0.001889
C	5.945102	0.942697	-0.001089
H	6.989131	1.246406	-0.001446
C	0.907987	0.775718	0.020497
C	-0.365090	0.691609	0.057849
C	0.314837	-1.880266	-0.014053
C	-0.793211	-1.243640	-0.049367
C	-2.219792	-1.503291	-0.144954
C	-2.828004	-2.350594	0.792615
C	-4.180617	-2.649839	0.693488
C	-4.944132	-2.109407	-0.338108
C	-4.346052	-1.269565	-1.273909
C	-2.994477	-0.964794	-1.179617
H	-2.225371	-2.772814	1.588671
H	-4.638894	-3.309372	1.422727
H	-6.000432	-2.343830	-0.413851
H	-4.934297	-0.849851	-2.082648
H	-2.528700	-0.310854	-1.907155
C	-1.537419	1.544431	0.149412
C	-2.483444	1.386177	1.169615
C	-3.569524	2.247217	1.257027
C	-3.730197	3.272574	0.328909
C	-2.792786	3.438022	-0.687533
C	-1.703252	2.581836	-0.779779
H	-2.358901	0.587957	1.891482
H	-4.292909	2.117037	2.054588
H	-4.580735	3.941989	0.399355
H	-2.908064	4.238855	-1.410109
H	-0.964913	2.709057	-1.563145

4 – triplet C^1-C^6 transition state

N	5.573403	-0.422227	-0.012436
C	4.273185	-0.642665	-0.267915
C	3.915594	-1.755359	-1.107822
H	4.729577	-2.349455	-1.505960
C	2.612061	-2.073811	-1.347537
H	2.357499	-2.959445	-1.918988
C	1.555176	-1.313196	-0.774251
C	1.887724	-0.045656	-0.079802
C	3.264987	0.209779	0.262155
N	3.576500	1.275220	1.017824
C	4.864674	1.466203	1.263405
H	5.128746	2.322709	1.878161
C	5.857731	0.621764	0.754406
H	6.906578	0.807720	0.969327
C	0.839489	0.811905	0.097334
C	-0.431703	0.869733	-0.077916
C	0.236014	-1.694378	-0.687324
C	-0.892563	-1.265197	-0.260655
C	-2.176637	-1.644700	0.229894
C	-2.807418	-0.963712	1.288497
C	-4.045255	-1.383153	1.751190
C	-4.688723	-2.471159	1.163291
C	-4.080088	-3.145922	0.105222
C	-2.840502	-2.740632	-0.362383
H	-2.308336	-0.116421	1.742508
H	-4.514076	-0.855517	2.574643
H	-5.660486	-2.789131	1.524728
H	-4.575543	-3.993590	-0.355957
H	-2.358995	-3.260380	-1.182546
C	-1.526459	1.745639	-0.317208
C	-1.545752	3.005156	0.323576
C	-2.585485	3.890910	0.095166
C	-3.629556	3.545134	-0.763462
C	-3.625338	2.301695	-1.395027
C	-2.593328	1.404155	-1.172594
H	-0.728693	3.262784	0.987338
H	-2.584194	4.857308	0.587718
H	-4.444146	4.239876	-0.936388
H	-4.434983	2.030202	-2.063580
H	-2.589247	0.437191	-1.660152

4 – singlet C^1-C^5 diradical product – **4'-Lin**

N	5.106874	-0.150256	0.013541
C	3.922833	-0.812775	0.008891
C	3.935025	-2.230395	-0.020643
H	4.901863	-2.719600	-0.038629
C	2.762283	-2.944204	-0.026577
H	2.770799	-4.027771	-0.049845
C	1.534807	-2.250184	-0.002749
C	1.490285	-0.848497	0.027812
C	2.682208	-0.098234	0.033639
N	2.654941	1.259375	0.065294
C	3.817944	1.864489	0.068492
H	3.813954	2.951878	0.093671
C	5.046783	1.160213	0.041965
H	5.987811	1.704944	0.045646

C	0.078326	-0.430632	0.041825
C	-0.742297	-1.714988	0.045528
C	0.170434	-2.700726	-0.001398
C	-2.198700	-1.825782	0.067375
C	-3.018560	-0.854185	0.654810
C	-4.400020	-1.009367	0.671295
C	-4.989255	-2.137218	0.109143
C	-4.183740	-3.114730	-0.471565
C	-2.805485	-2.959871	-0.495000
H	-2.573794	0.018030	1.117359
H	-5.017308	-0.246163	1.133173
H	-4.632582	-3.997390	-0.914827
H	-2.177386	-3.711834	-0.960754
H	-6.067408	-2.255222	0.123430
C	-0.387608	0.791116	-0.008600
C	-1.003318	2.020260	-0.070141
C	-1.281660	2.756604	1.116850
C	-1.890964	3.994617	1.041792
C	-2.237767	4.545517	-0.195041
C	-1.965481	3.837852	-1.369481
C	-1.359855	2.597022	-1.322296
H	-1.001387	2.333478	2.074375
H	-2.097252	4.542805	1.954878
H	-2.714349	5.518007	-0.243577
H	-2.232923	4.263124	-2.330893
H	-1.150067	2.046457	-2.231406

4 – triplet C^1-C^5 diradical product – **4'-Lin**

N	4.876105	-0.969121	0.026963
C	3.604509	-1.441271	0.014880
C	3.398411	-2.844507	-0.019857
H	4.278659	-3.476432	-0.036339
C	2.129926	-3.368376	-0.031781
H	1.969609	-4.440139	-0.058549
C	1.027447	-2.488864	-0.009514
C	1.194854	-1.101373	0.023821
C	2.488867	-0.543922	0.037577
N	2.671387	0.800063	0.075579
C	3.913424	1.220053	0.086537
H	4.075822	2.295092	0.117322
C	5.018803	0.335174	0.061186
H	6.032655	0.727993	0.070718
C	-0.144632	-0.466292	0.033257
C	-1.138081	-1.588322	0.029689
C	-0.392792	-2.714985	-0.013575
C	-2.595116	-1.488784	0.047418
C	-3.265685	-0.353989	0.521726
C	-4.654978	-0.306581	0.535933
C	-5.401899	-1.390117	0.085069
C	-4.746874	-2.527344	-0.383827
C	-3.361083	-2.574473	-0.406277
H	-2.697916	0.490275	0.893539
H	-5.154993	0.581356	0.907962
H	-5.319275	-3.376923	-0.740981
H	-2.850965	-3.452838	-0.788303
H	-6.485752	-1.350107	0.097843
C	-0.395168	0.825112	-0.012209

C	-0.502487	2.190467	-0.062404
C	-0.555516	2.966549	1.134043
C	-0.697162	4.338573	1.068127
C	-0.790266	4.990495	-0.165644
C	-0.737537	4.244588	-1.347867
C	-0.598082	2.871607	-1.312546
H	-0.474036	2.462068	2.089513
H	-0.732911	4.913935	1.987194
H	-0.901825	6.068012	-0.205681
H	-0.807015	4.747141	-2.306790
H	-0.557807	2.293461	-2.227810

4 – singlet C^1-C^5 diradical product – **4-Lin**

N	5.276279	-1.516162	-0.016671
C	3.942745	-1.253983	-0.029271
C	3.032103	-2.338772	-0.060856
H	3.447228	-3.339570	-0.073599
C	1.673330	-2.116411	-0.075847
H	0.976575	-2.947278	-0.100312
C	1.194992	-0.797067	-0.061477
C	2.068130	0.298086	-0.027294
C	3.465304	0.093565	-0.010672
N	4.317261	1.148542	0.021975
C	5.595952	0.856877	0.033420
H	6.297703	1.687217	0.059260
C	6.075283	-0.476760	0.013500
H	7.145579	-0.669506	0.023473
C	1.254958	1.478774	-0.016656
C	-0.069900	1.242371	-0.055836
C	-0.187244	-0.272280	-0.064763
C	-1.283295	-0.986355	-0.021362
C	-2.479068	-1.663642	0.045522
C	-3.074514	-1.970949	1.303781
C	-4.269092	-2.662118	1.357789
C	-4.913201	-3.069801	0.185538
C	-4.342942	-2.776937	-1.056774
C	-3.147623	-2.089193	-1.139716
H	-2.576759	-1.649731	2.210870
H	-4.710663	-2.886571	2.322752
H	-4.840001	-3.092546	-1.967755
H	-2.701755	-1.866499	-2.102173
C	-1.164793	2.208526	-0.059824
C	-0.948374	3.487866	0.476396
C	-1.956584	4.440390	0.472334
C	-3.207174	4.136213	-0.061867
C	-3.433626	2.872773	-0.598166
C	-2.423263	1.917849	-0.601296
H	0.021125	3.717769	0.905556
H	-1.769128	5.422006	0.894561
H	-4.400781	2.628404	-1.024592
H	-2.608076	0.946896	-1.044091
H	-3.997391	4.879227	-0.060636
H	-5.851046	-3.610612	0.239942

4 – triplet C^1-C^5 diradical product – **4-Lin**

N	4.975080	1.658417	0.021481
C	3.664761	1.298345	0.022600
C	2.675463	2.313265	0.033098
H	3.015558	3.342033	0.039870
C	1.336631	1.991101	0.035058
H	0.578652	2.767410	0.042946
C	0.960460	0.639877	0.027950
C	1.909959	-0.383762	0.015903
C	3.289502	-0.081158	0.013064
N	4.216653	-1.070287	0.001441
C	5.470735	-0.684826	0.000549
H	6.232261	-1.461041	-0.008594
C	5.849278	0.680637	0.010904
H	6.902375	0.952331	0.010066
C	1.176114	-1.617463	0.008562
C	-0.169163	-1.465197	0.021857
C	-0.387828	0.012035	0.024106
C	-1.519933	0.686141	-0.005427
C	-2.387334	1.761343	-0.030242
C	-2.854864	2.294014	-1.266616
C	-3.757950	3.339433	-1.277757
C	-4.233065	3.885263	-0.081381
C	-3.790113	3.370161	1.140544
C	-2.886846	2.325386	1.179607
H	-2.488088	1.866953	-2.192502
H	-4.099474	3.738308	-2.226888
H	-4.156046	3.793210	2.069921
H	-2.542767	1.924324	2.125799
C	-1.181622	-2.516749	0.021035
C	-0.798984	-3.836765	-0.268608
C	-1.729386	-4.864487	-0.266227
C	-3.067734	-4.599511	0.019655
C	-3.460681	-3.296499	0.306968
C	-2.528659	-2.265062	0.310901
H	0.240369	-4.042872	-0.503336
H	-1.411729	-5.876488	-0.494058
H	-4.499015	-3.079265	0.534343
H	-2.846732	-1.256208	0.548870
H	-3.796645	-5.402720	0.017646
H	-4.943301	4.703967	-0.101170

4 – singlet C^1-C^6 diradical product – **4-BC**

N	-5.554214	-0.534735	0.002127
C	-4.236075	-0.830791	0.010904
C	-3.838918	-2.204576	0.044534
H	-4.626276	-2.948982	0.059571
C	-2.524358	-2.548532	0.056639
H	-2.223645	-3.589762	0.079796
C	-1.498046	-1.549572	0.037772
C	-1.860422	-0.161463	-0.000989
C	-3.255407	0.193657	-0.013578
N	-3.601118	1.495744	-0.048345
C	-4.892665	1.759229	-0.056399
H	-5.186617	2.805367	-0.084605
C	-5.868382	0.744711	-0.030411
H	-6.925471	0.998081	-0.037380

C	-0.812767	0.745099	-0.011976
C	0.529416	0.482199	0.017477
C	-0.134396	-1.810872	0.041333
C	0.900551	-0.918376	0.001447
C	2.295444	-1.411756	-0.101671
C	3.195840	-0.870994	-1.026838
C	4.479774	-1.388844	-1.144606
C	4.886359	-2.451220	-0.341180
C	3.997003	-2.998549	0.578549
C	2.710397	-2.485025	0.695321
H	2.883352	-0.048391	-1.659649
H	5.164444	-0.962724	-1.870078
H	5.890360	-2.851244	-0.433665
H	4.304638	-3.826861	1.207928
H	2.015235	-2.907719	1.413026
C	1.496095	1.602815	0.107473
C	1.290503	2.752046	-0.665395
C	2.150243	3.839149	-0.560977
C	3.225468	3.797481	0.321593
C	3.432351	2.662850	1.101909
C	2.576345	1.573409	0.997335
H	0.450117	2.782227	-1.350714
H	1.978861	4.720196	-1.170238
H	3.896834	4.645486	0.404056
H	4.261526	2.626848	1.800388
H	2.737873	0.697966	1.615488

4 – triplet C^1-C^6 diradical product – **4-BC**

N	-5.546846	-0.550645	0.000062
C	-4.228129	-0.842388	0.013416
C	-3.826445	-2.216008	0.057721
H	-4.612603	-2.961645	0.077075
C	-2.511272	-2.557104	0.073800
H	-2.205999	-3.597074	0.104549
C	-1.492500	-1.550279	0.048107
C	-1.856848	-0.171066	0.001779
C	-3.251466	0.185841	-0.016435
N	-3.599938	1.485992	-0.060885
C	-4.892686	1.745450	-0.073319
H	-5.190141	2.790339	-0.109351
C	-5.864776	0.728019	-0.042116
H	-6.922644	0.977930	-0.052889
C	-0.804833	0.734143	-0.010027
C	0.542454	0.484151	0.020673
C	-0.123981	-1.798797	0.050401
C	0.916096	-0.908444	0.005816
C	2.305812	-1.413611	-0.100285
C	3.214557	-0.868306	-1.014801
C	4.493373	-1.397597	-1.136605
C	4.886406	-2.476233	-0.348087
C	3.988869	-3.027928	0.561025
C	2.707502	-2.502450	0.682195
H	2.912238	-0.033506	-1.636508
H	5.184658	-0.967996	-1.853716
H	5.886553	-2.885120	-0.443596
H	4.286468	-3.868209	1.179269
H	2.006262	-2.927381	1.392769

C	1.491940	1.618631	0.109210
C	1.256363	2.771973	-0.648822
C	2.099129	3.872317	-0.545310
C	3.187859	3.839321	0.320930
C	3.425126	2.700259	1.086153
C	2.585720	1.597894	0.982872
H	0.406223	2.794506	-1.322464
H	1.904768	4.756409	-1.143155
H	3.846509	4.697354	0.402298
H	4.265088	2.671084	1.771967
H	2.770495	0.719159	1.589774

3 – C^1-C^5 NMR product – isomer – **24-*E***

N	4.343859	0.089180	-0.132692
C	3.158368	-0.578852	-0.055539
C	1.948465	0.170939	-0.050592
H	2.032670	1.248608	-0.117737
C	0.743045	-0.485822	0.039426
C	0.714679	-1.930468	0.082257
C	1.871979	-2.678108	0.085718
H	1.860273	-3.765440	0.117245
C	3.122074	-2.011662	0.025212
N	4.275555	-2.741882	0.031022
C	5.404516	-2.062291	-0.042846
H	6.335054	-2.631212	-0.038799
C	5.440014	-0.646948	-0.126304
H	6.396629	-0.127260	-0.188356
C	-0.673418	-2.350739	0.092428
C	-1.493577	-1.261923	0.042386
C	-0.668102	-0.024784	0.007371
C	-1.203423	1.214670	-0.152287
C	-2.968362	-1.320265	0.050129
C	-3.636913	-2.239647	-0.779401
C	-5.027221	-2.344081	-0.757350
H	-3.056587	-2.862833	-1.456433
C	-5.779986	-1.531881	0.095031
H	-5.524010	-3.057807	-1.411847
C	-3.739114	-0.510639	0.905841
C	-5.130171	-0.617708	0.927472
H	-3.244156	0.184257	1.579657
H	-5.706561	0.011241	1.603273
H	-6.865125	-1.611910	0.110984
C	-0.582713	2.543312	-0.099698
C	-1.049625	3.543451	-0.975728
C	-0.520556	4.831713	-0.938240
H	-1.825921	3.296470	-1.698320
C	0.463822	5.157948	-0.000855
H	-0.882881	5.585032	-1.634984
C	0.909135	4.187433	0.901004
H	0.870818	6.166404	0.036487
H	1.656138	4.440664	1.650727
C	0.392238	2.893461	0.853694
H	0.719213	2.155564	1.581404
H	-0.999805	-3.384032	0.162548
H	-2.272578	1.238518	-0.358954

3 – C^1-C^5 NMR product – isomer 2 – **24-*Z***

N	4.827243	1.689677	0.196778
C	3.860269	0.735492	0.085663
C	2.494082	1.126995	0.154336
H	2.278653	2.185183	0.287961
C	1.517288	0.166452	0.058825
C	1.865700	-1.217774	-0.127019
C	3.179986	-1.623415	-0.208298
H	3.462944	-2.663795	-0.352955
C	4.205320	-0.647916	-0.099281
N	5.511065	-1.038093	-0.172019
C	6.420145	-0.087497	-0.061785
H	7.468042	-0.384586	-0.117799
C	6.079263	1.276345	0.123231
H	6.863988	2.028537	0.210024
C	0.626304	-1.970374	-0.166300
C	-0.451034	-1.138010	-0.031212
C	0.036317	0.261901	0.067611
C	-0.599785	1.464280	0.105812
C	-1.831038	-1.641314	0.133242
C	-2.327775	-2.636515	-0.726420
C	-3.600657	-3.175169	-0.534975
H	-1.713797	-2.977308	-1.557698
C	-4.397388	-2.733872	0.523866
H	-3.969952	-3.939820	-1.215885
C	-2.642792	-1.205785	1.195137
C	-3.911647	-1.749339	1.388792
H	-2.269836	-0.447515	1.878740
H	-4.522689	-1.404207	2.220662
H	-5.389958	-3.153812	0.674619
C	-1.996747	1.849385	-0.106284
C	-2.851656	1.194677	-1.013849
C	-4.153533	1.647305	-1.215904
H	-2.484145	0.345642	-1.579602
C	-4.631392	2.760717	-0.518920
H	-4.796290	1.132169	-1.926938
C	-3.789179	3.434559	0.370308
H	-5.649264	3.110602	-0.679589
H	-4.147825	4.310887	0.906662
C	-2.482333	2.992663	0.561304
H	-1.823754	3.528042	1.243758
H	0.048415	2.319995	0.303954
H	0.570997	-3.053848	-0.216507

3 – C^1-C^6 NMR product

N	-5.255949	-1.426871	-0.001295
C	-6.357523	-0.717601	-0.001274
C	-6.357742	0.715541	-0.000921
N	-5.256394	1.425155	0.000017
C	-4.073864	0.720523	0.000499
C	-4.073652	-0.721877	-0.000702
C	-2.858953	-1.413954	-0.001928
C	-1.640342	-0.721656	-0.002775
C	-1.640516	0.721063	0.004113
C	-2.859394	1.412974	0.002465
C	-0.383928	1.394942	-0.006575
C	0.821118	0.726106	-0.013327

C	0.821095	-0.725496	0.014109
C	-0.383414	-1.394993	0.007737
C	2.074157	-1.530198	0.097738
C	2.073998	1.530869	-0.097096
C	2.285585	-2.600273	-0.787604
C	3.424806	-3.400484	-0.684398
C	4.370707	-3.148277	0.311165
C	4.169805	-2.088982	1.200503
C	3.035246	-1.285446	1.093440
C	2.277874	2.611242	0.777701
C	3.416677	3.411819	0.673748
C	4.370307	3.149666	-0.311821
C	4.177316	2.080099	-1.190539
C	3.043253	1.276053	-1.082354
H	1.543302	2.814342	1.554460
H	3.558632	4.239368	1.366313
H	5.258200	3.773344	-0.395259
H	4.911457	1.871873	-1.966585
H	2.899520	0.452735	-1.776613
H	2.885479	-0.469693	1.795510
H	4.897987	-1.888694	1.984221
H	5.258838	-3.771681	0.394103
H	3.572883	-4.220113	-1.385055
H	1.556378	-2.795976	-1.571307
H	-2.879897	2.501043	0.002365
H	-2.879111	-2.502031	-0.002030
H	-7.307334	1.252739	-0.001411
H	-7.306946	-1.255098	-0.001631
H	-0.390066	2.482162	-0.050731
H	-0.388618	-2.482268	0.051156

4 – C^1-C^5 NMR product – isomer 1

N	5.402364	0.200070	0.006007
C	4.209111	-0.455403	-0.065029
C	4.221402	-1.862498	-0.268757
H	5.188051	-2.351172	-0.363789
C	3.040969	-2.566916	-0.338609
H	3.046593	-3.643860	-0.496733
C	1.813259	-1.878025	-0.202883
C	1.754872	-0.489384	-0.000432
C	2.962466	0.256104	0.066270
N	2.963692	1.607544	0.265517
C	4.135502	2.207184	0.329918
H	4.139427	3.286615	0.487104
C	5.359431	1.504054	0.200472
H	6.307861	2.038945	0.258278
C	0.325313	-0.101869	0.043848
C	-0.437996	-1.375744	-0.047177
C	0.457577	-2.395239	-0.212759
C	-1.881916	-1.602091	0.170390
C	-2.561753	-1.002058	1.245227
C	-3.904712	-1.286619	1.486441
C	-4.597936	-2.175240	0.659831
C	-3.934069	-2.780516	-0.409632
C	-2.588984	-2.498203	-0.650576
H	-2.027640	-0.319086	1.900588
H	-4.411180	-0.815493	2.326791

H	-4.464366	-3.472360	-1.061557
H	-2.079508	-2.962784	-1.492401
H	-5.647171	-2.393979	0.848379
C	-0.085665	1.198802	0.076027
C	-1.395120	1.809791	-0.157671
H	0.710650	1.914466	0.268919
C	-1.692779	3.020060	0.502257
C	-2.903090	3.674730	0.287521
C	-3.827383	3.152821	-0.622207
C	-3.530118	1.975002	-1.314189
C	-2.328908	1.308578	-1.085355
H	-0.966344	3.437285	1.198060
H	-3.120662	4.598884	0.819344
H	-4.767847	3.669834	-0.802757
H	-4.235318	1.577043	-2.041081
H	-2.097238	0.408865	-1.644763
H	0.205457	-3.450406	-0.262605

4 – C^1-C^5 NMR product – isomer 2

N	-4.145014	-2.230158	0.302106
C	-2.805724	-2.252566	0.047266
C	-2.224503	-3.464431	-0.416313
H	-2.883244	-4.315664	-0.570830
C	-0.864953	-3.553131	-0.611506
H	-0.409021	-4.492741	-0.917946
C	-0.055678	-2.412476	-0.398579
C	-0.603582	-1.166611	-0.035564
C	-1.987218	-1.089994	0.278271
N	-2.527730	0.027556	0.841841
C	-3.820200	0.006742	1.095431
H	-4.255298	0.896279	1.553104
C	-4.638269	-1.114860	0.805144
H	-5.709059	-1.081949	1.008666
C	0.518251	-0.212666	0.079422
C	1.757758	-1.033898	-0.074194
C	1.391269	-2.298682	-0.430539
C	3.147116	-0.556627	0.057163
C	3.556558	0.207052	1.166838
C	4.884985	0.610324	1.305665
C	5.832018	0.258659	0.340917
C	5.441024	-0.503005	-0.763649
C	4.113230	-0.904947	-0.904660
H	2.833345	0.460230	1.938839
H	5.181911	1.193744	2.175109
H	6.170959	-0.779240	-1.522234
H	3.810055	-1.482228	-1.775363
H	6.867595	0.574726	0.449315
C	0.585496	1.149073	0.076820
C	-0.408970	2.192740	-0.174087
H	1.587993	1.551290	0.215198
C	-1.482693	2.029212	-1.069778
C	-2.338766	3.089791	-1.352341
C	-2.150539	4.332705	-0.738943
C	-1.082229	4.515378	0.142861
C	-0.209544	3.461259	0.405254
H	-1.619256	1.076480	-1.570983
H	-3.154536	2.949141	-2.058718

H	-2.823947	5.158480	-0.960231
H	-0.919901	5.482747	0.613911
H	0.634894	3.612690	1.075968
H	2.067685	-3.119999	-0.646830

4 – C^1-C^5 NMR product – isomer 3

N	5.005843	0.884204	-0.079075
C	3.648471	0.730599	-0.064663
C	2.815236	1.875512	-0.157771
H	3.293918	2.847469	-0.249569
C	1.438971	1.754602	-0.135781
H	0.828789	2.645850	-0.221984
C	0.842103	0.479579	-0.005620
C	1.646028	-0.672463	0.042661
C	3.060447	-0.574520	0.027641
N	3.833506	-1.696536	0.089325
C	5.138930	-1.510994	0.070832
H	5.775486	-2.395193	0.121265
C	5.724572	-0.219197	-0.010905
H	6.810285	-0.114597	-0.020299
C	0.798903	-1.848881	0.071516
C	-0.510398	-1.466065	0.022349
C	-0.567686	0.021115	-0.024380
C	-1.729050	0.711310	-0.180228
C	-1.999368	2.151159	-0.110155
C	-2.952691	2.708495	-0.985362
C	-3.266455	4.064590	-0.928673
C	-2.660965	4.884492	0.028430
C	-1.743809	4.337311	0.930233
C	-1.414614	2.984239	0.863030
H	-3.436023	2.069292	-1.722755
H	-3.991889	4.481065	-1.624791
H	-1.289933	4.964054	1.695458
H	-0.726993	2.557708	1.588848
C	-1.665113	-2.382797	0.051095
C	-1.658960	-3.541218	-0.749262
C	-2.719535	-4.445309	-0.710174
C	-3.813770	-4.211080	0.127345
C	-3.833736	-3.068045	0.929645
C	-2.771532	-2.163525	0.894175
H	-0.818553	-3.718778	-1.416895
H	-2.694657	-5.331881	-1.341244
H	-4.675045	-2.882266	1.594859
H	-2.784204	-1.296806	1.550221
H	-4.643157	-4.915111	0.155441
H	-2.914876	5.941363	0.081721
H	1.166679	-2.865903	0.151384
H	-2.611133	0.106614	-0.389273

4 – C^1-C^5 NMR product – isomer 4

N	-5.591582	-0.991236	0.009320
C	-4.227262	-0.964726	0.059673
C	-3.514341	-2.181295	0.234096
H	-4.090461	-3.098637	0.326674
C	-2.133411	-2.190050	0.282179
H	-1.608397	-3.134752	0.410248
C	-1.423942	-0.975610	0.176195

C	-2.099030	0.238872	-0.000129
C	-3.514338	0.275734	-0.064732
N	-4.174086	1.456367	-0.240101
C	-5.490698	1.391607	-0.284414
H	-6.037256	2.325148	-0.423232
C	-6.199194	0.167233	-0.158923
H	-7.289041	0.163001	-0.200840
C	-1.117608	1.303569	-0.068529
C	0.146095	0.787276	0.038977
C	0.030428	-0.689561	0.153614
C	0.948386	-1.696013	0.164514
C	2.385905	-1.722460	-0.106703
C	3.015947	-0.858781	-1.023812
C	4.379111	-0.974197	-1.283973
C	5.142336	-1.949703	-0.635546
C	4.528589	-2.827586	0.262705
C	3.162141	-2.725225	0.510456
H	2.428328	-0.114493	-1.549082
H	4.847324	-0.303785	-2.001754
H	5.113014	-3.598771	0.760496
H	2.682315	-3.419444	1.198856
C	1.350895	1.631811	0.174016
C	1.543358	2.729030	-0.684144
C	2.638461	3.578878	-0.524670
C	3.561722	3.350355	0.498150
C	3.378784	2.266250	1.361109
C	2.286172	1.415404	1.201635
H	0.833109	2.904812	-1.489516
H	2.771266	4.419260	-1.203607
H	4.088052	2.084481	2.166454
H	2.145004	0.583003	1.886077
H	4.416802	4.011792	0.623020
H	6.207547	-2.035375	-0.841237
H	-1.363369	2.358581	-0.123412
H	0.544414	-2.685590	0.385865

4 – C^1-C^6 NMR product – **22**

N	5.581578	-0.504944	-0.001465
C	4.257632	-0.807942	0.001171
C	3.862225	-2.186395	0.009120
H	4.648623	-2.937374	0.012978
C	2.542225	-2.525166	0.012056
H	2.243269	-3.572131	0.019410
C	1.511737	-1.522917	0.005029
C	1.863484	-0.146204	0.000648
C	3.266895	0.216357	-0.002356
N	3.620690	1.523415	-0.007233
C	4.917144	1.795754	-0.009795
H	5.209939	2.845919	-0.013991
C	5.897470	0.781389	-0.007146
H	6.956828	1.039004	-0.009787
C	0.837975	0.817784	-0.014194
C	-0.509904	0.471341	-0.016157
C	0.144252	-1.868070	0.016024
C	-0.868601	-0.915048	0.016385
C	-2.280285	-1.391576	0.096054
C	-3.152089	-0.926786	1.095157

C	-4.450005	-1.426398	1.196543
C	-4.904841	-2.396047	0.298697
C	-4.048602	-2.866184	-0.698877
C	-2.747004	-2.370721	-0.796390
H	-2.806586	-0.178478	1.803416
H	-5.107329	-1.059137	1.982457
H	-5.919276	-2.782118	0.377187
H	-4.392925	-3.618841	-1.405737
H	-2.087344	-2.735171	-1.581581
C	-1.515227	1.570819	-0.096401
C	-1.438971	2.662496	0.784392
C	-2.338573	3.725478	0.686671
C	-3.327701	3.718729	-0.298828
C	-3.410119	2.641165	-1.184913
C	-2.514898	1.576814	-1.083781
H	-0.675123	2.670271	1.559396
H	-2.266186	4.558206	1.383795
H	-4.028887	4.547271	-0.377397
H	-4.172191	2.630497	-1.961919
H	-2.582494	0.748606	-1.783933
H	1.120742	1.864485	-0.058036
H	-0.122260	-2.922340	0.059960