Supporting Information

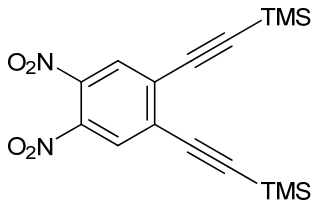
Syntheses, Thermal Reactivity and Computational Studies of Aryl–Fused Quinoxalenediynes: Effect of Extended Benzannelation on Bergman Cyclization Energetics

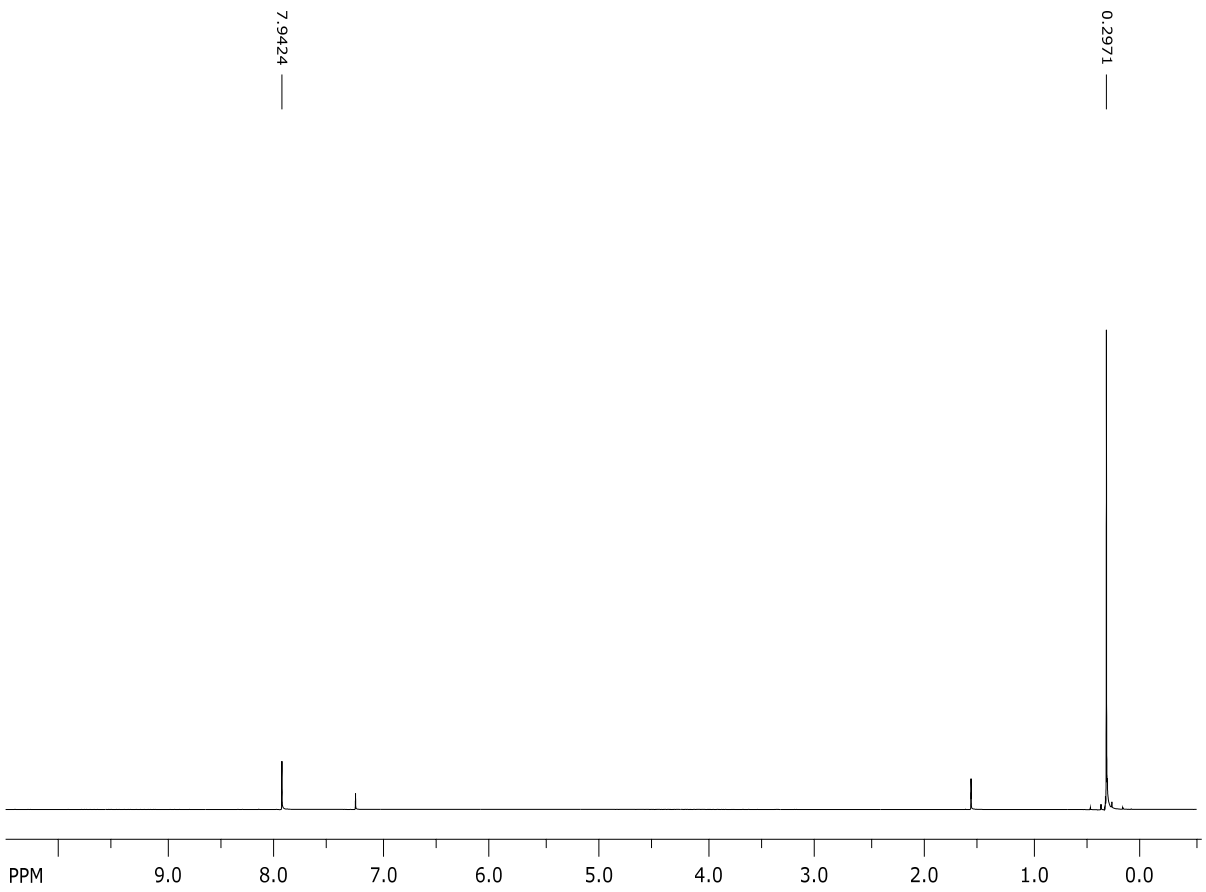
John D. Spence,* Andro C. Rios, Megan A. Frost, Claire M. McCutcheon, Christopher D. Cox, Sonia Chavez, Ramiro Fernandez and Benjamin F. Gherman*

Department of Chemistry, California State University, Sacramento, Sacramento CA, 95819
jspence@csus.edu; ghermanb@csus.edu

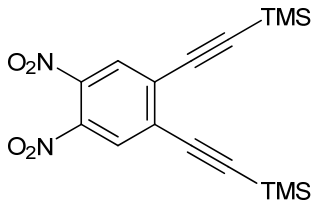
Table of Contents:

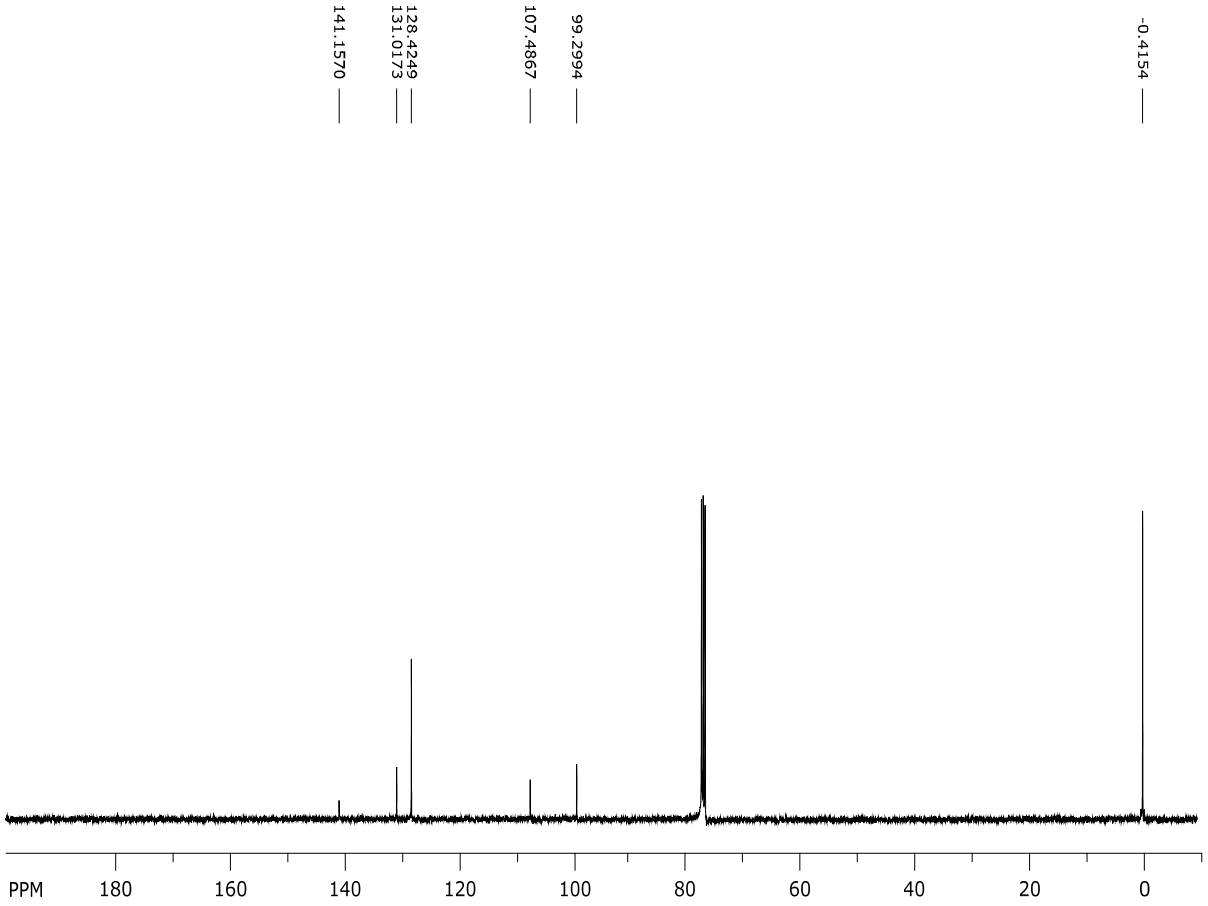
^{1}H NMR spectrum of **4** (300 MHz, $CDCl_3$)





^{13}C NMR spectrum of **4** (75 MHz, $CDCl_3$)





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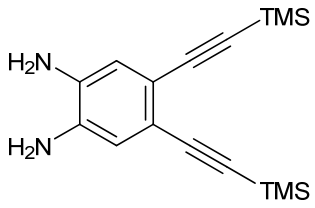
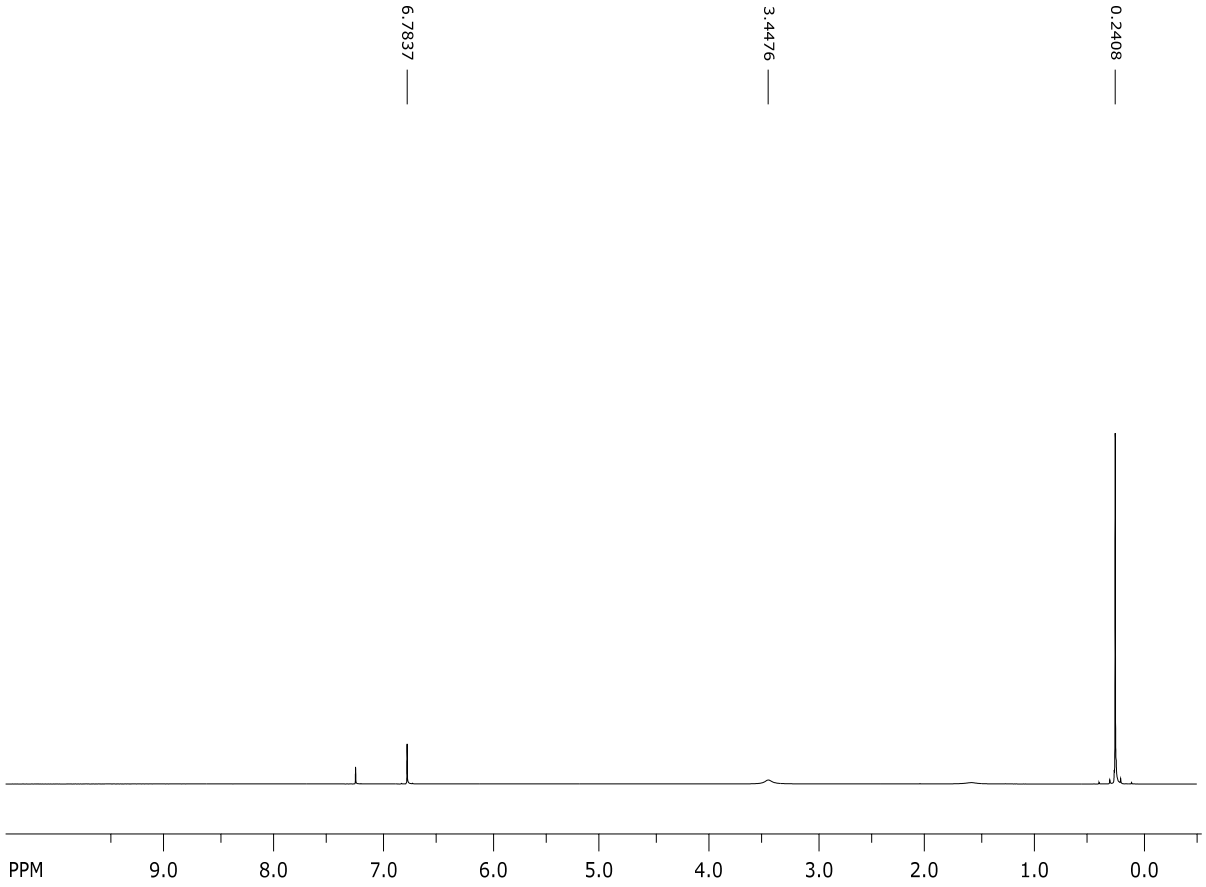
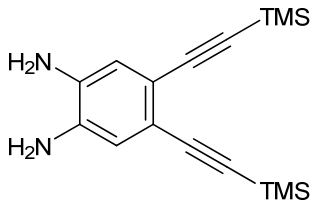
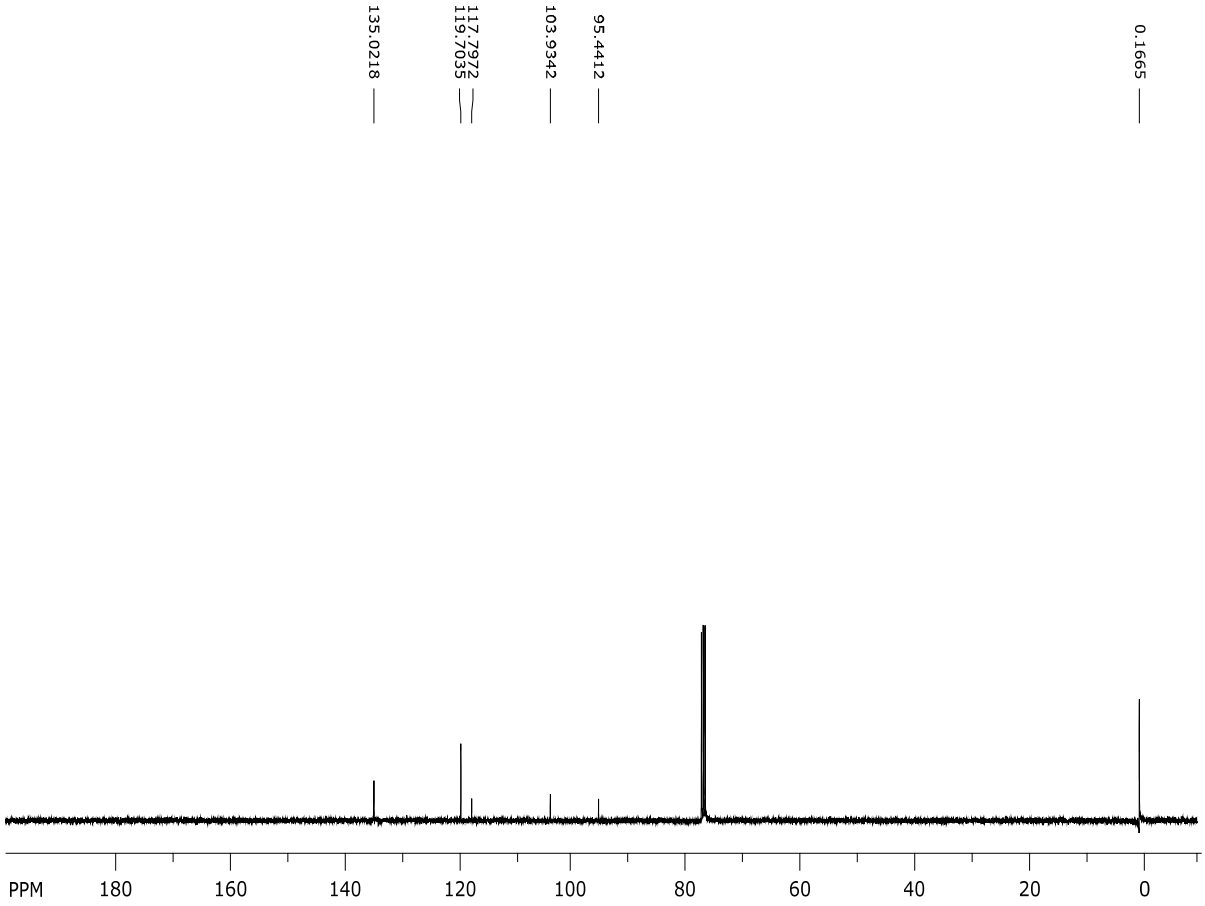




^{13}C NMR spectrum of **5** (75 MHz, $CDCl_3$)





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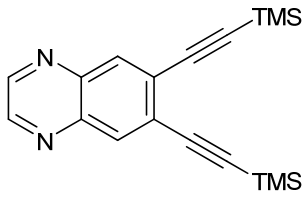
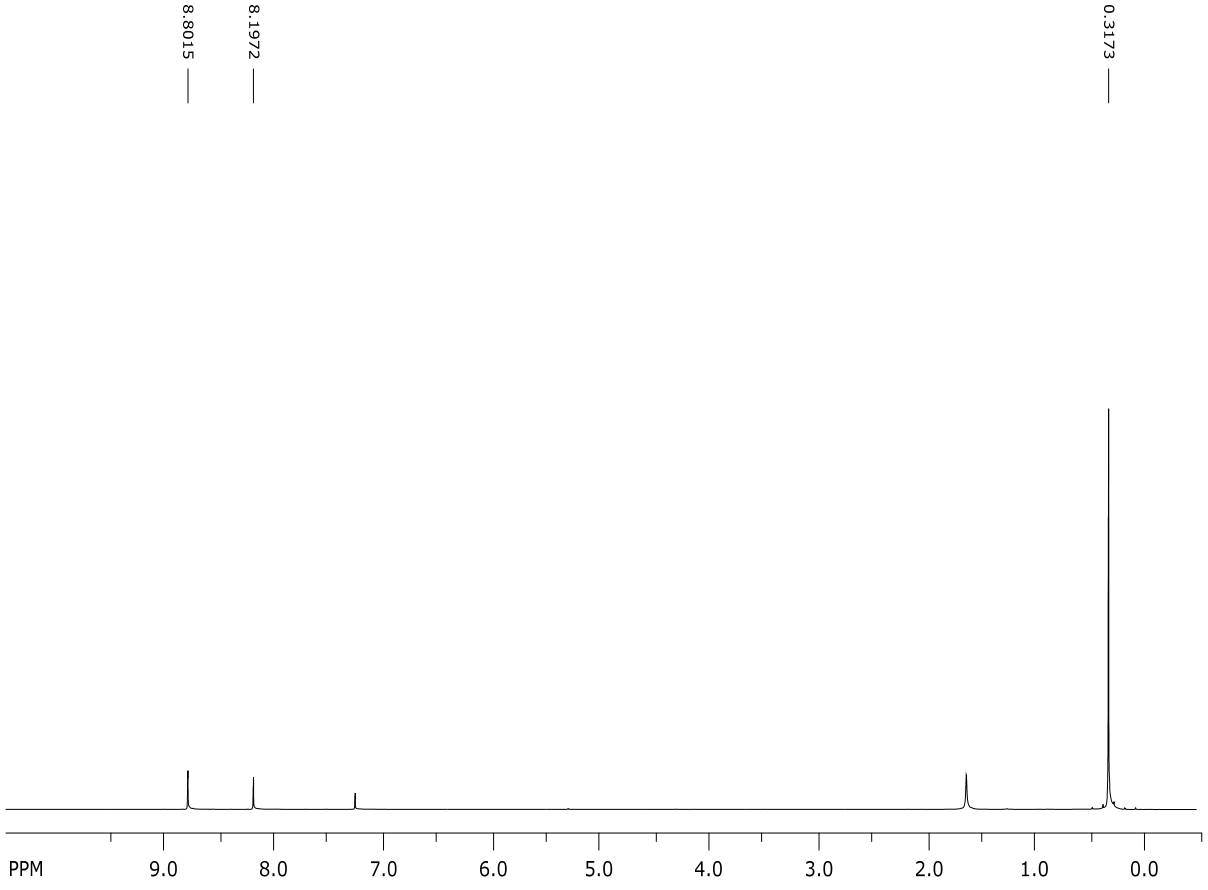
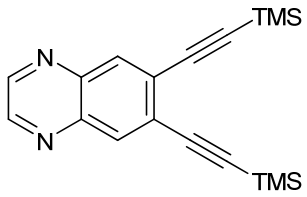
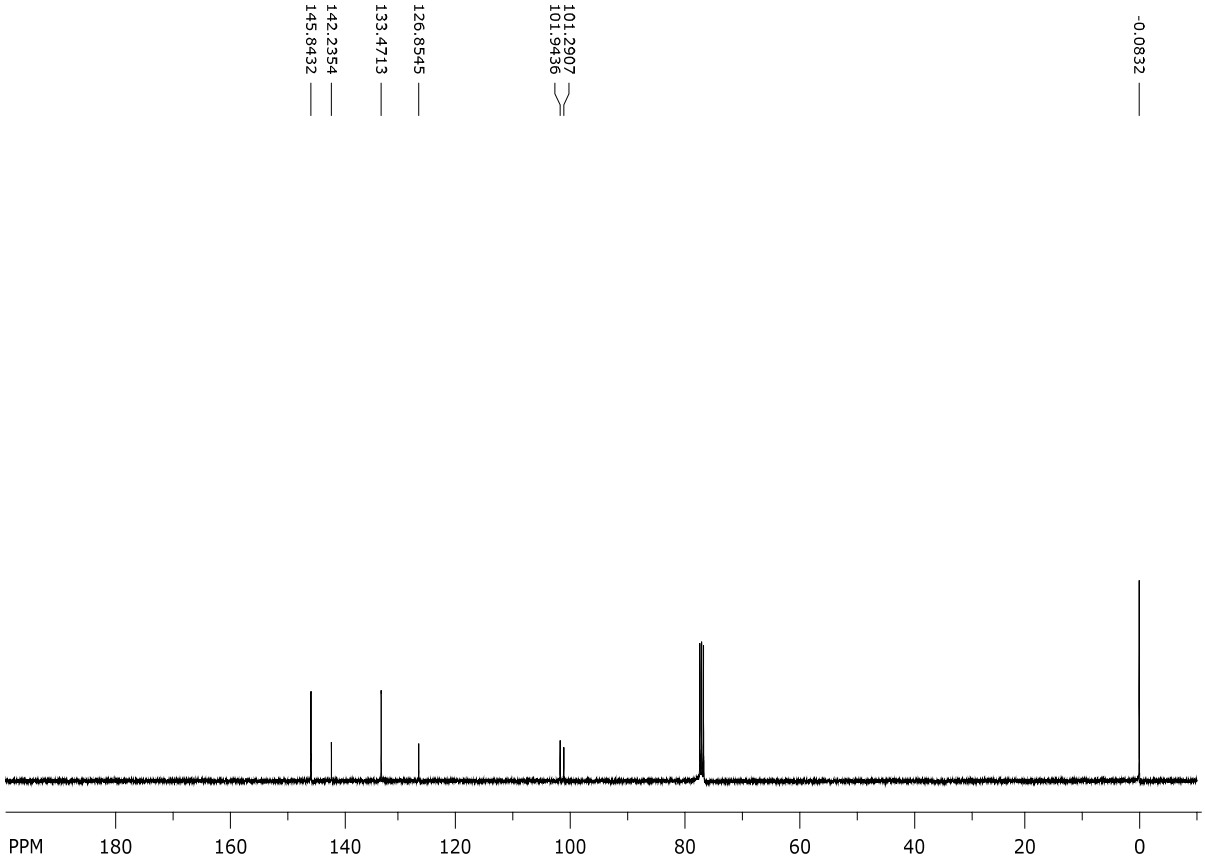




^{13}C NMR spectrum of **7a** (75 MHz, $CDCl_3$)





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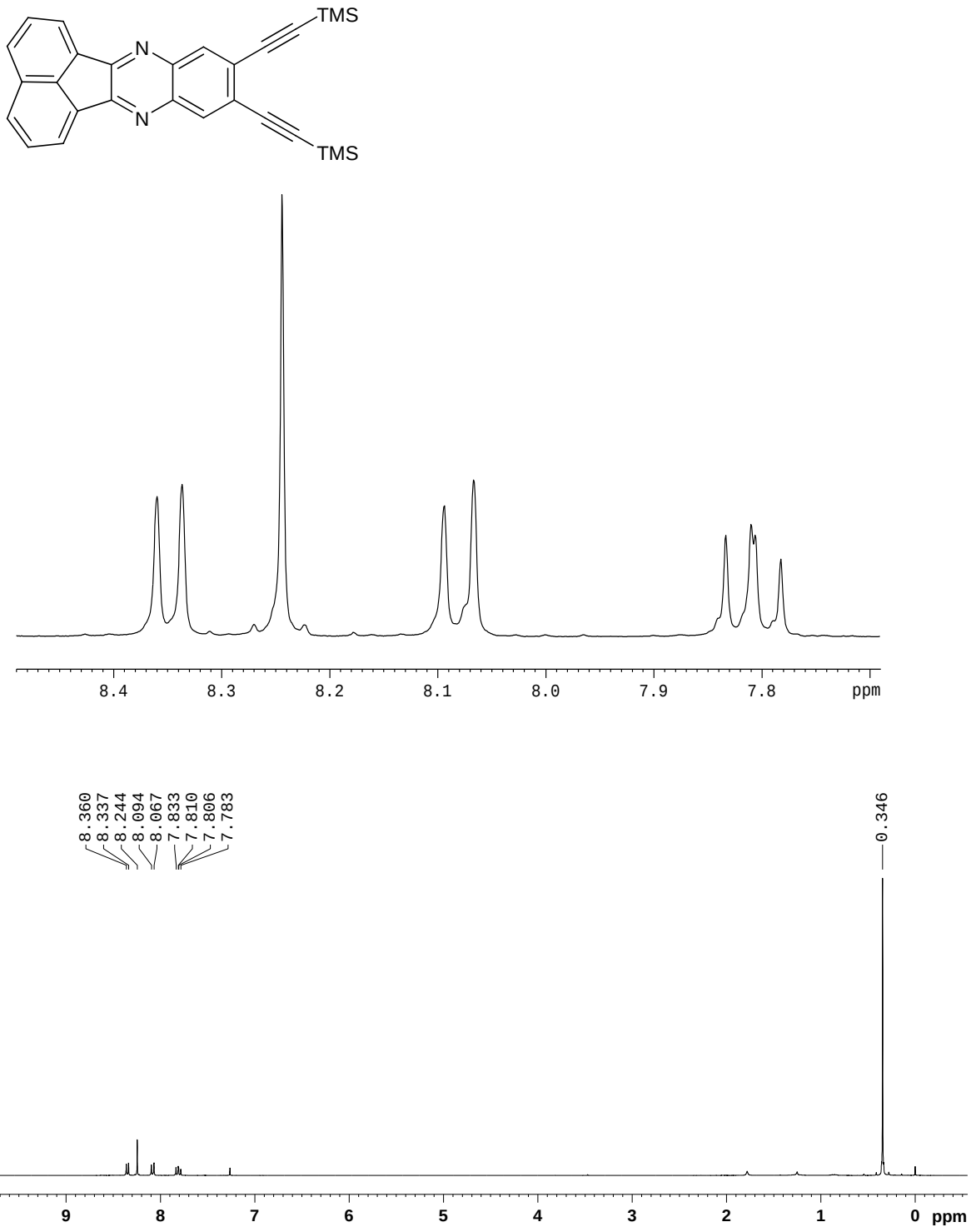
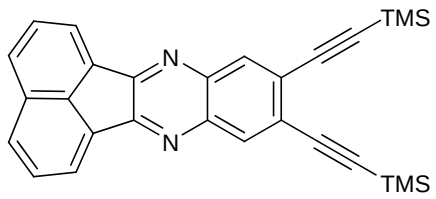
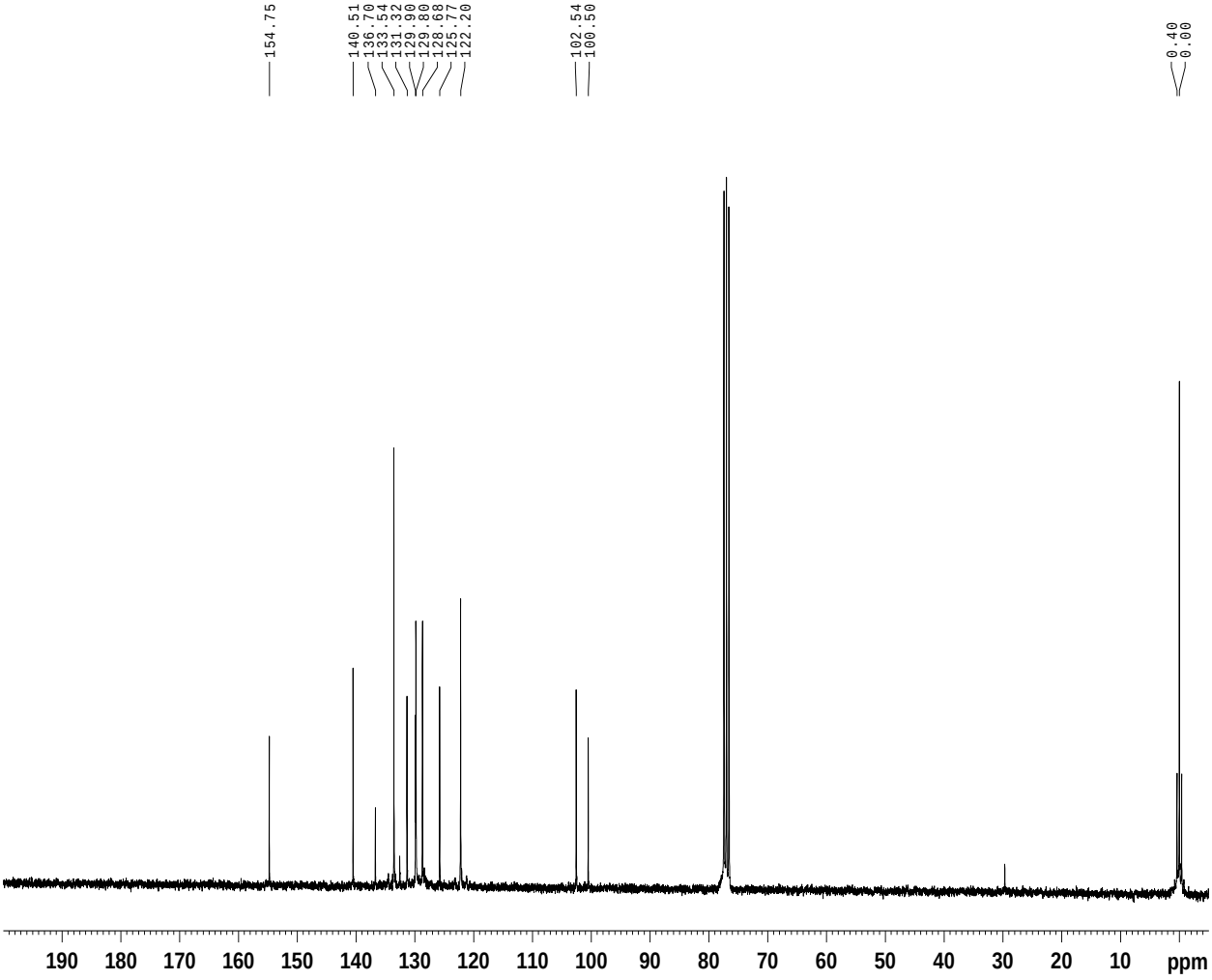


^{13}C NMR spectrum of **7b** (75 MHz, $CDCl_3$)





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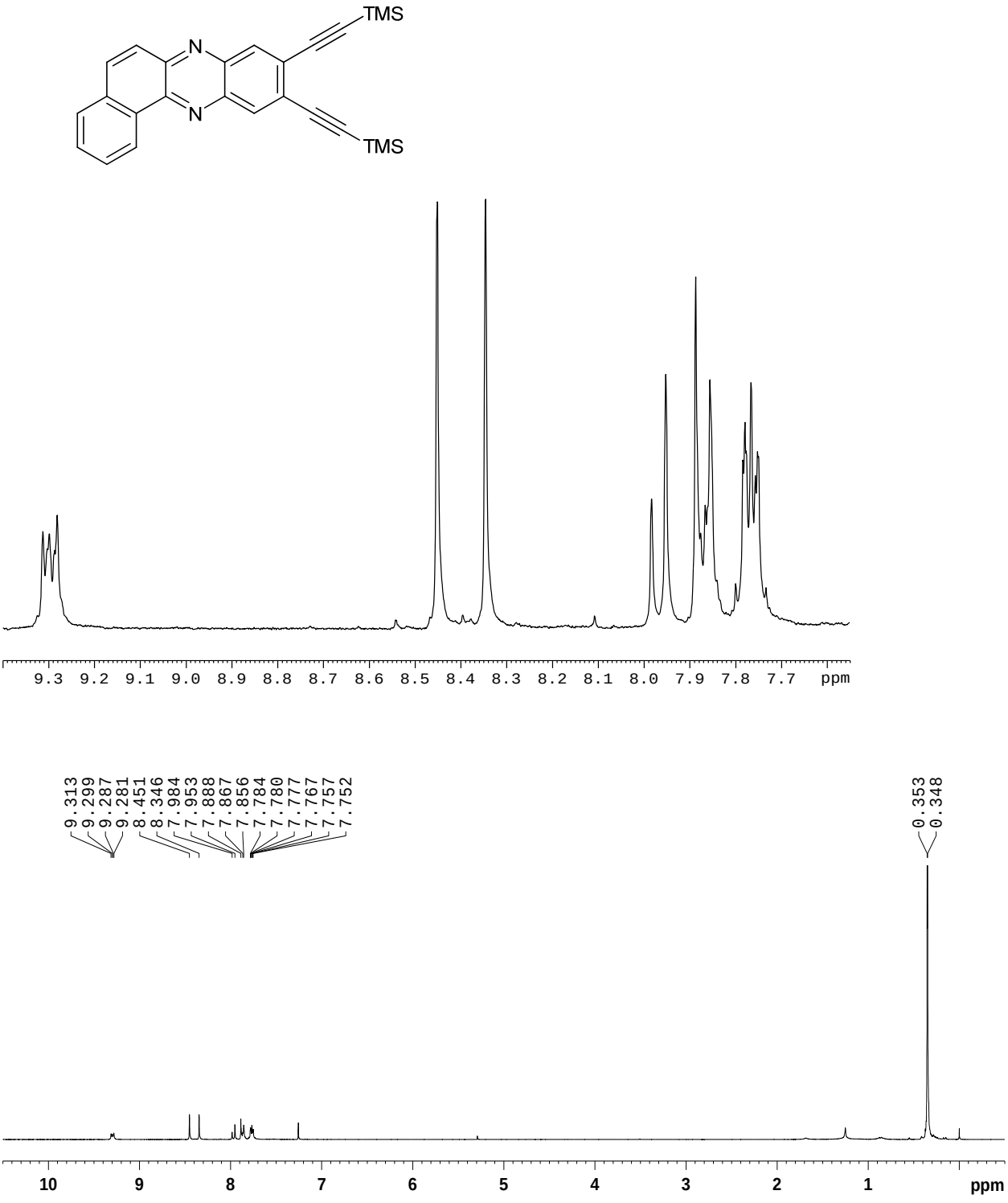
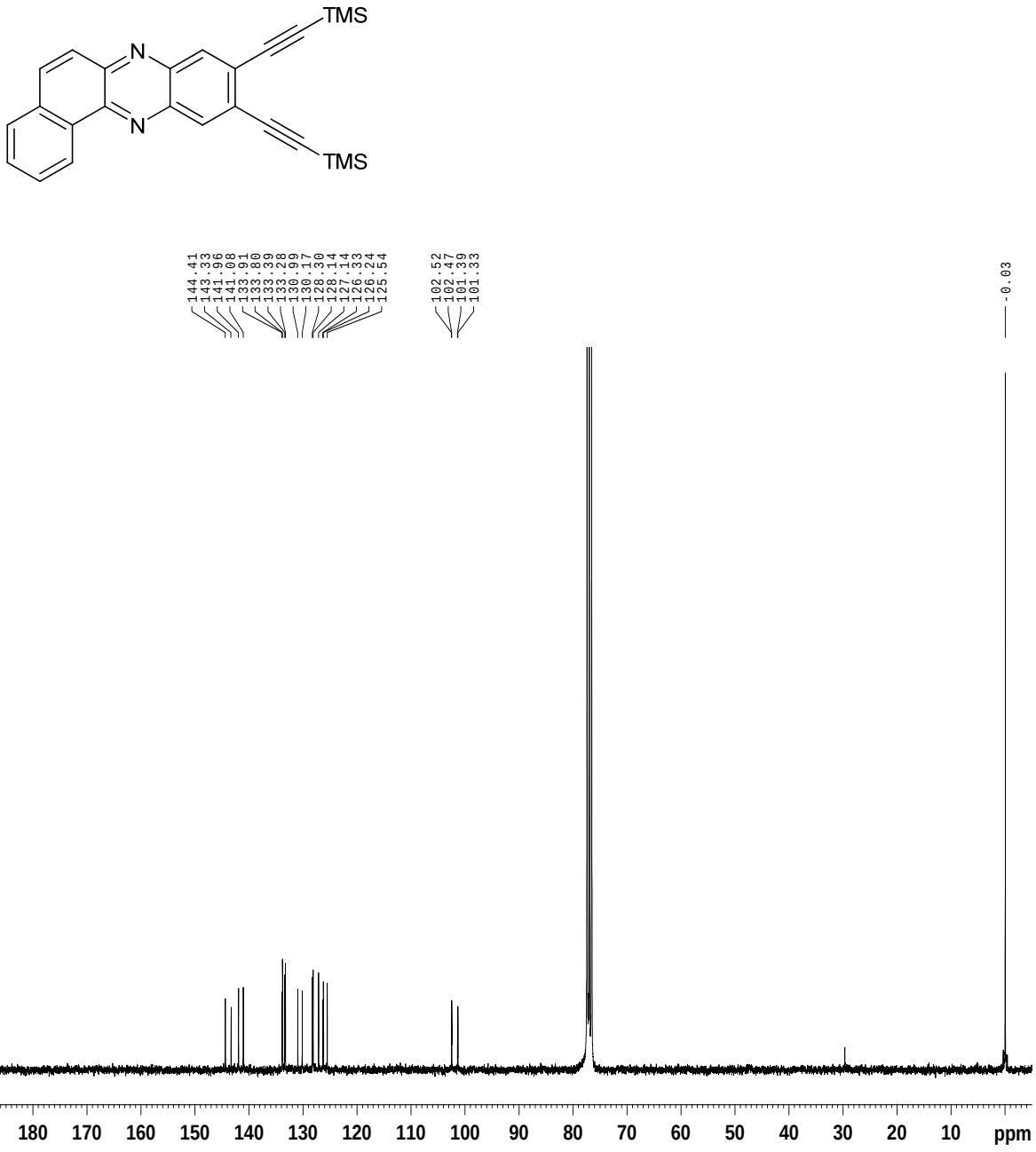


^{13}C NMR spectrum of **7c** (75 MHz, $CDCl_3$)



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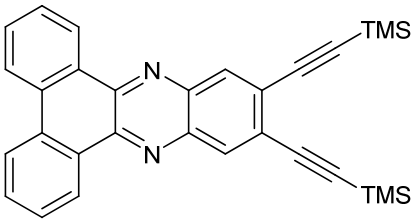
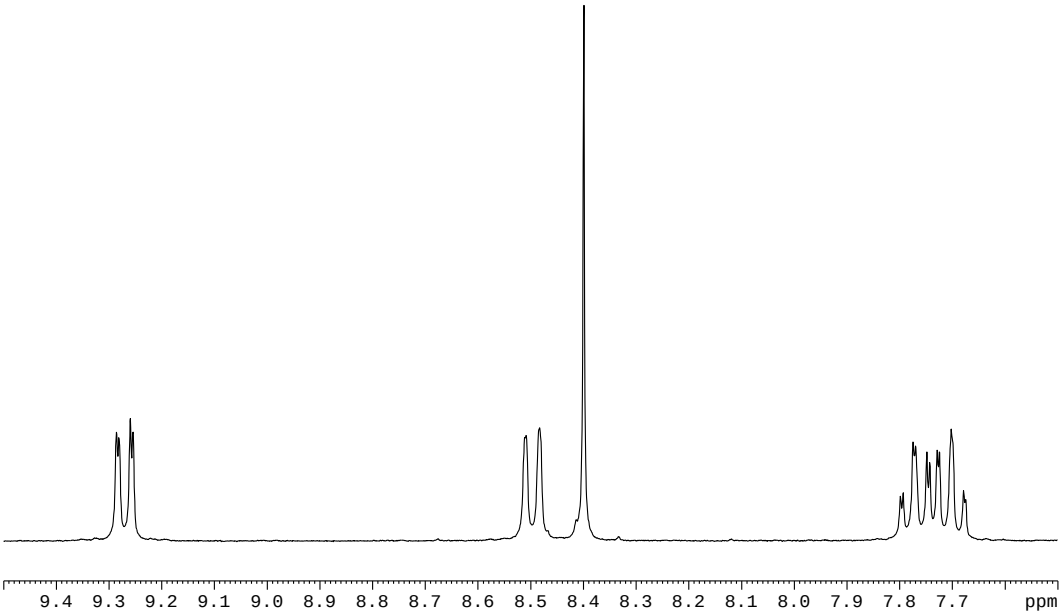
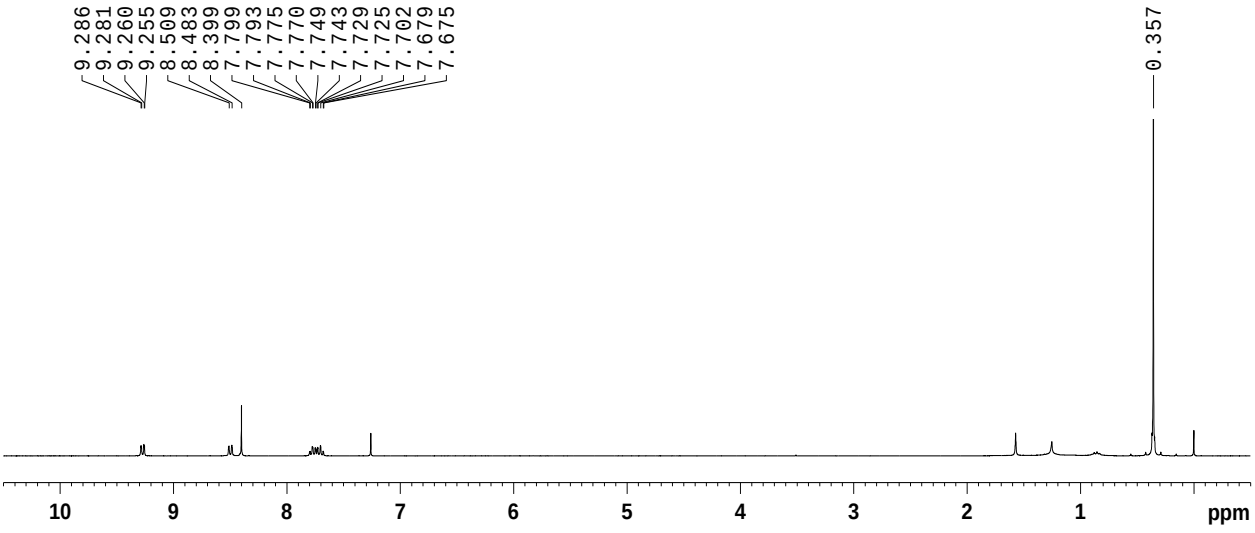
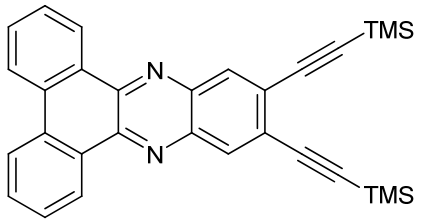
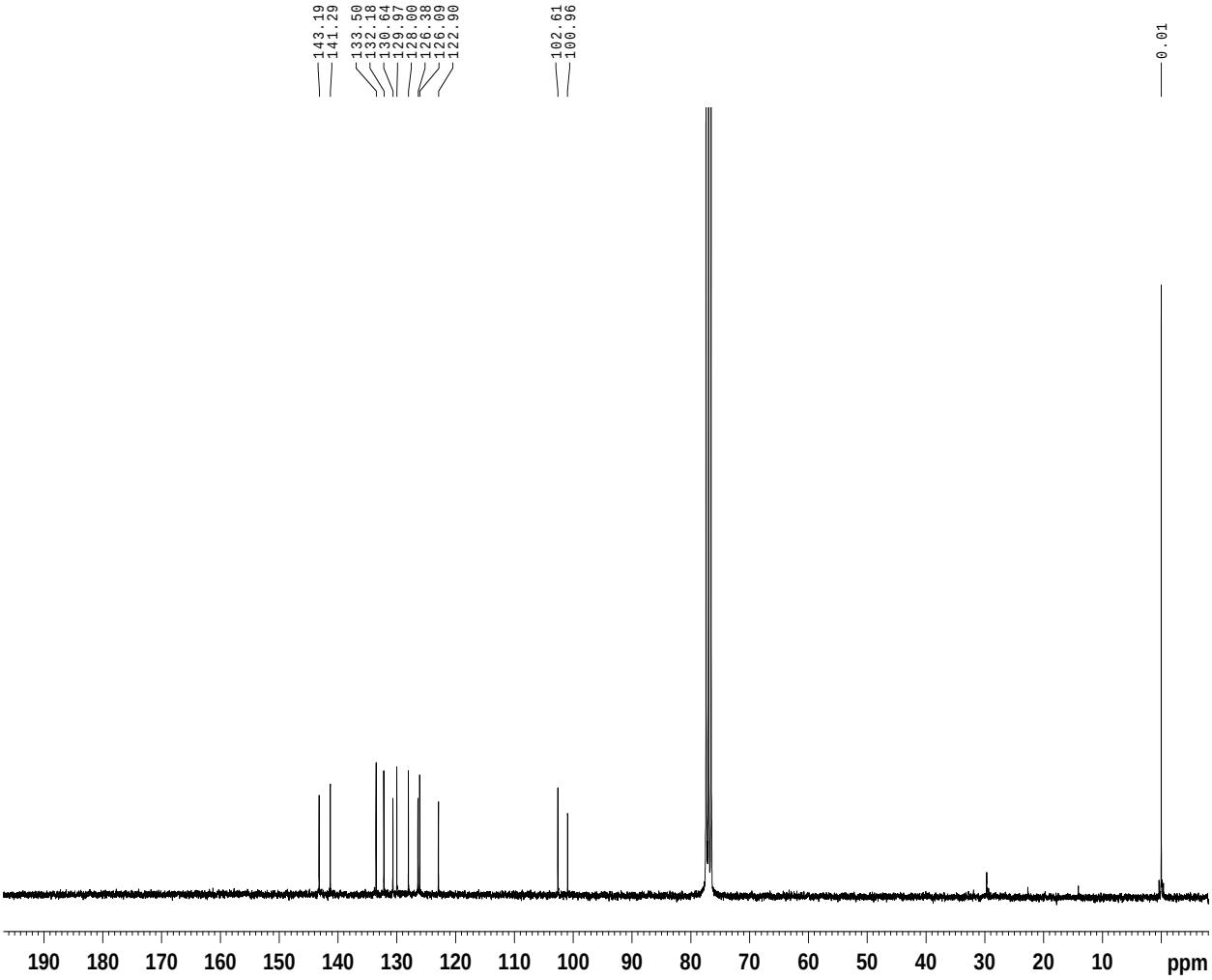




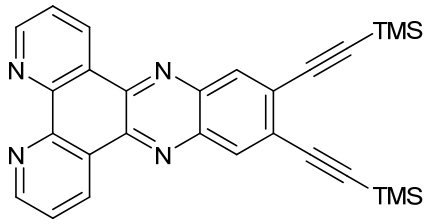


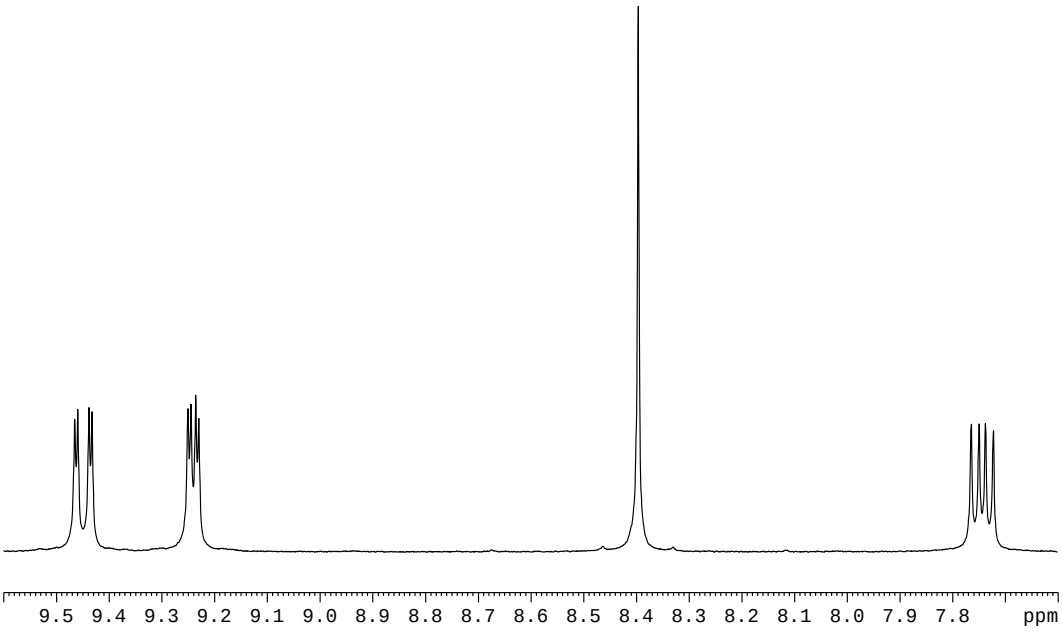
^{13}C NMR spectrum of **7d** (75 MHz, $CDCl_3$)

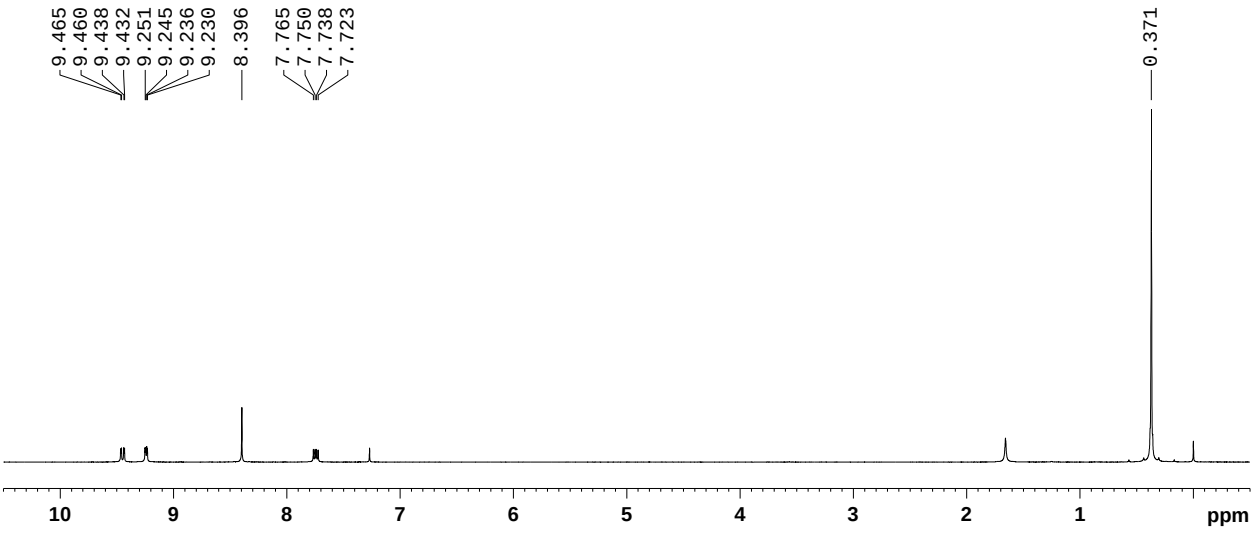




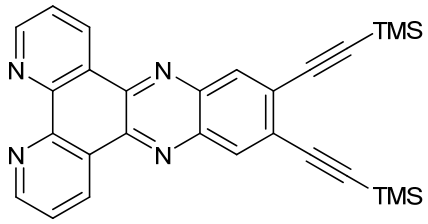
^{1}H NMR spectrum of **7e** (300 MHz, $CDCl_3$)

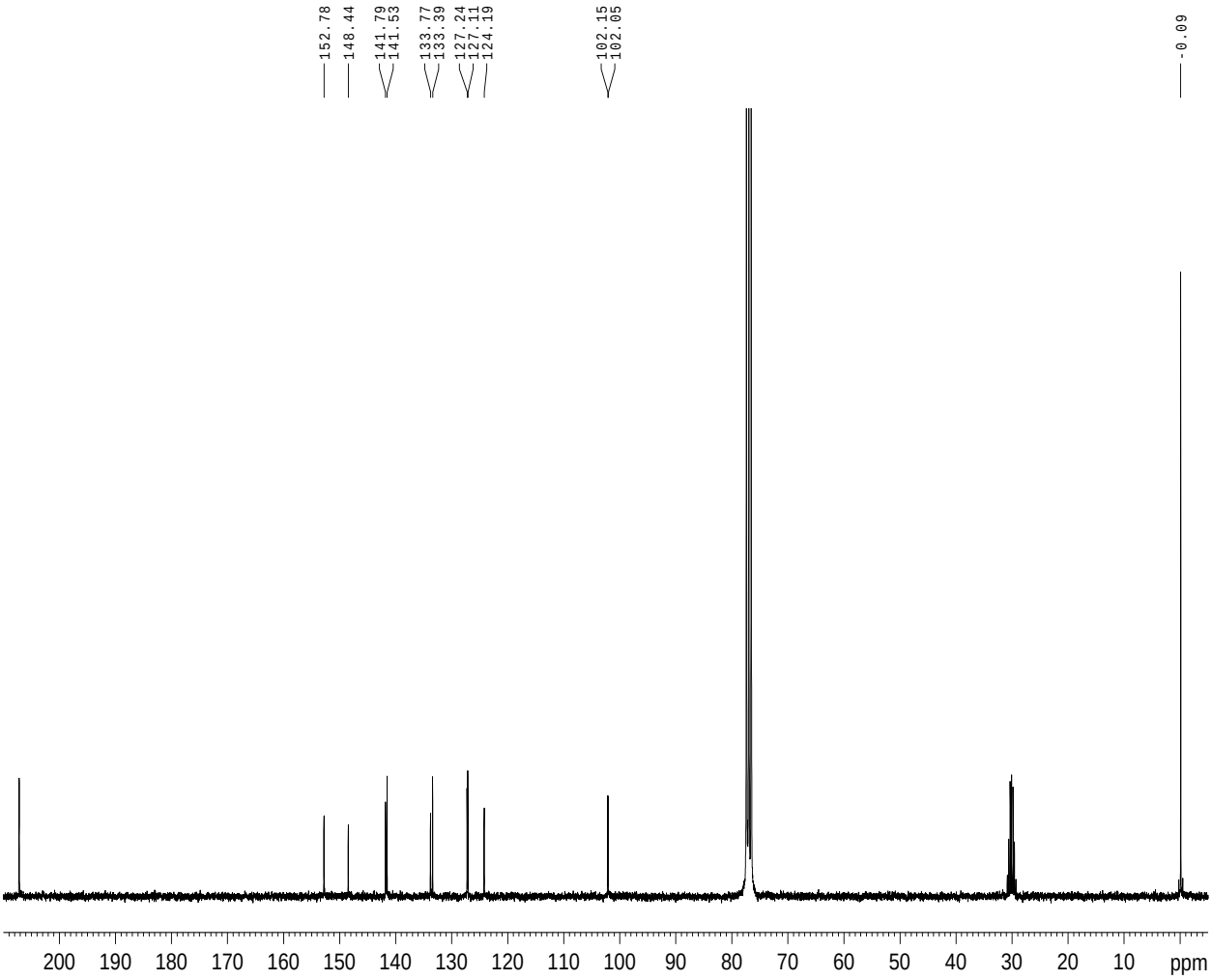




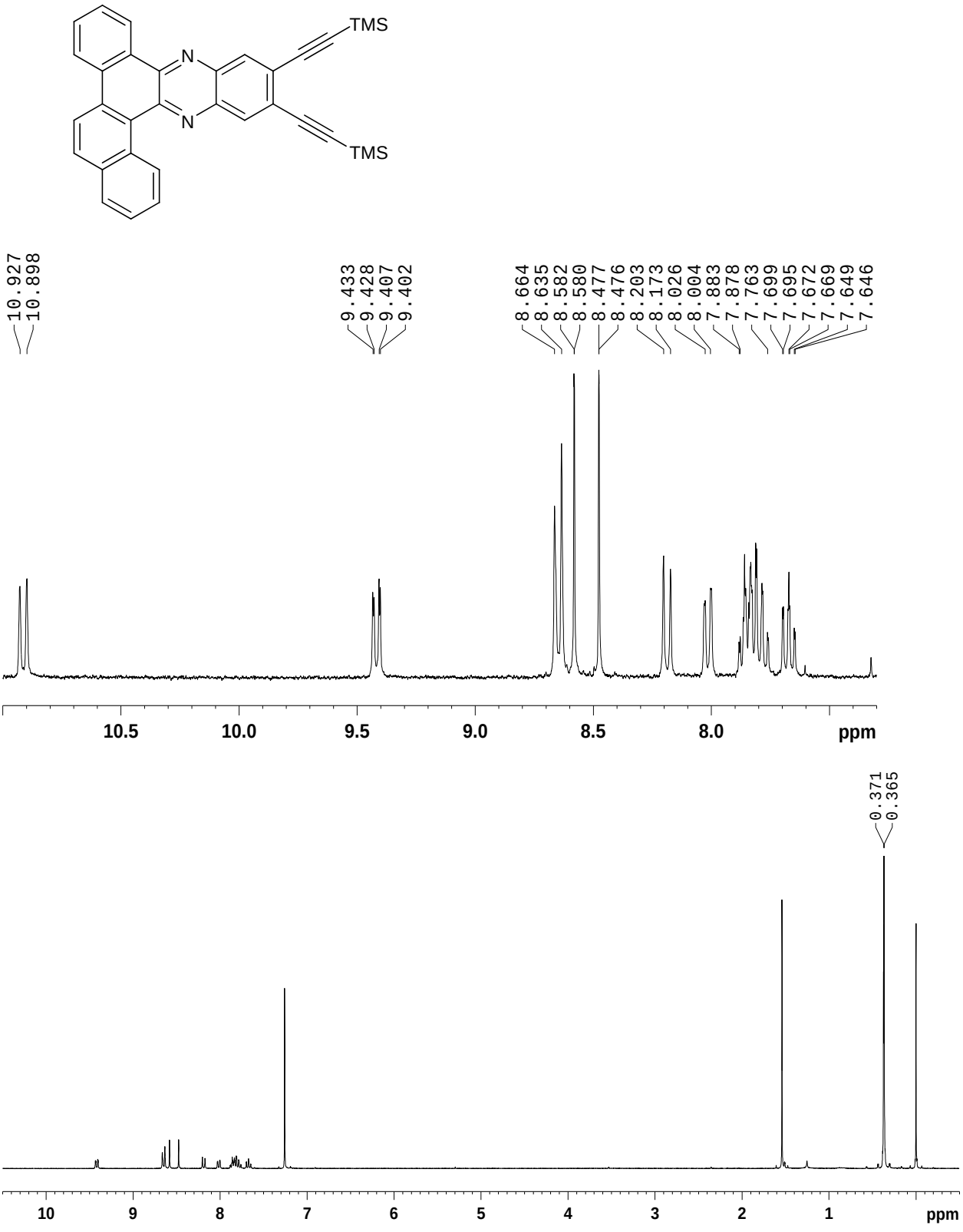


^{13}C NMR spectrum of **7e** (75 MHz, $CDCl_3$/d_6-acetone)

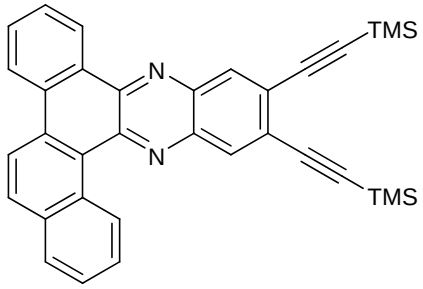


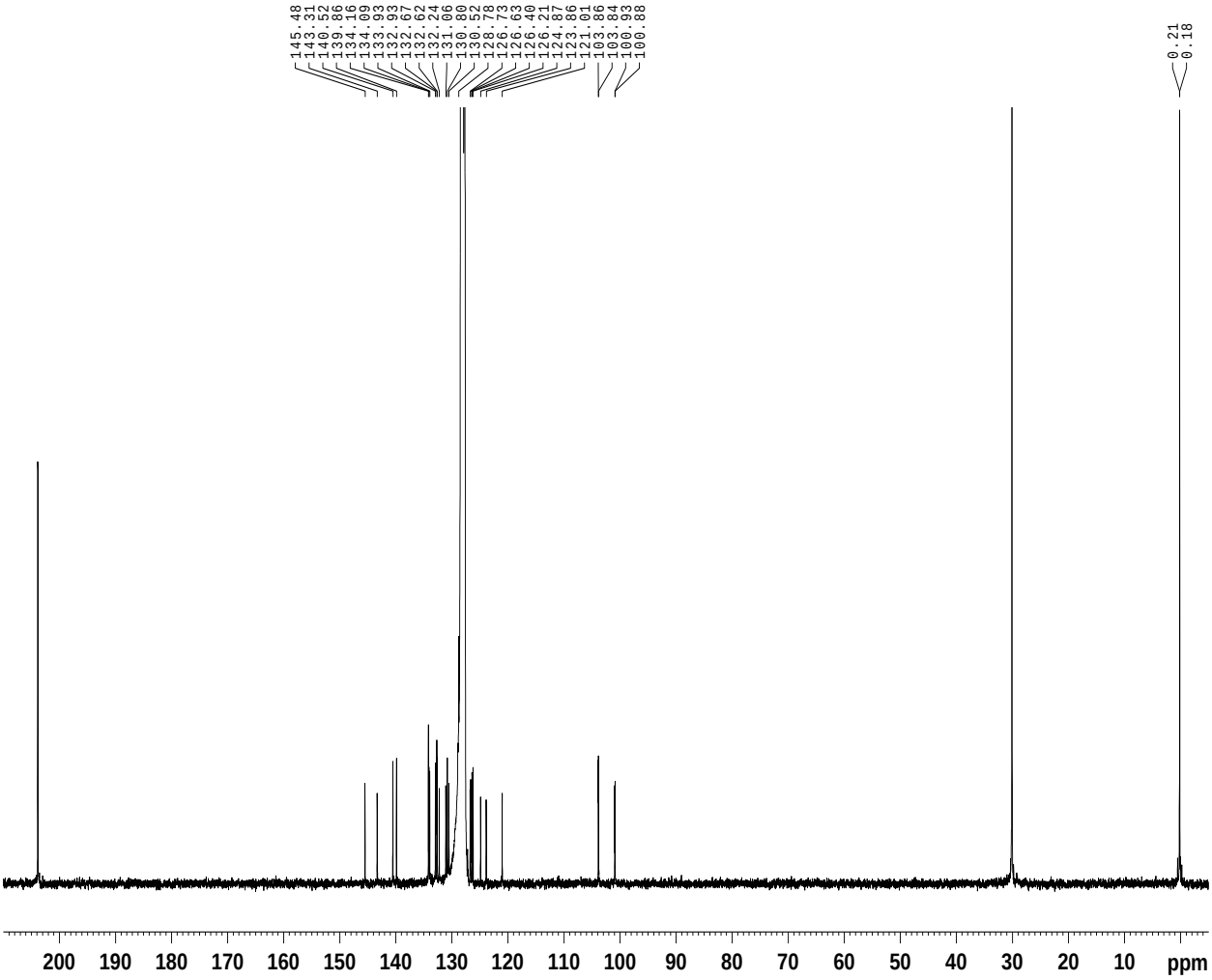


^{1}H NMR spectrum of **7f** (300 MHz, $CDCl_3$)

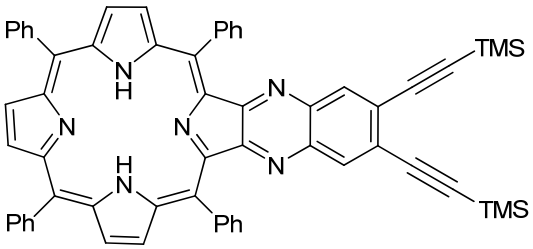


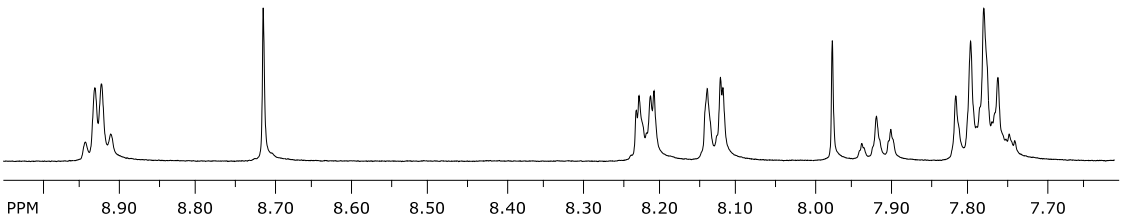
^{13}C NMR spectrum of **7f** (75 MHz, C_6D_6/acetone)

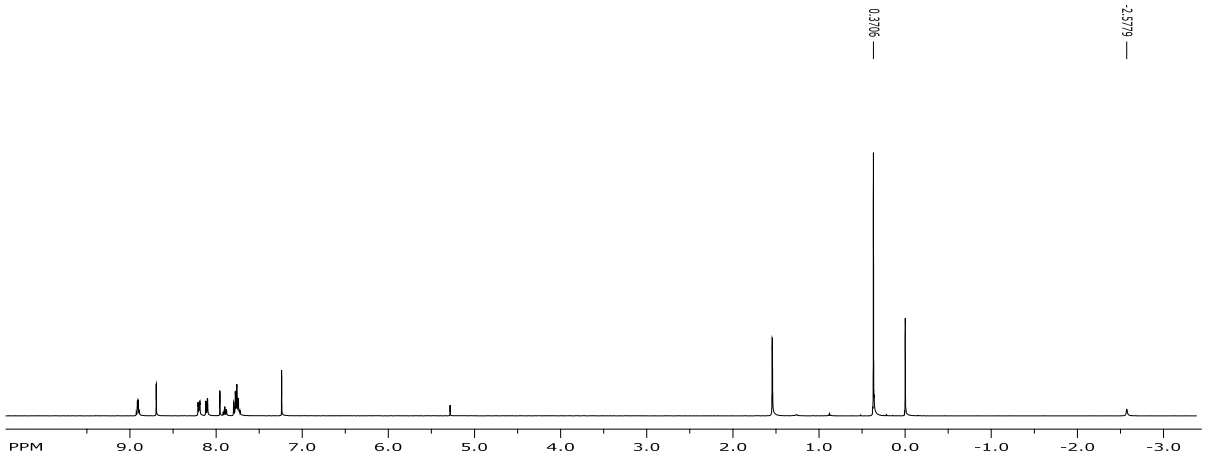




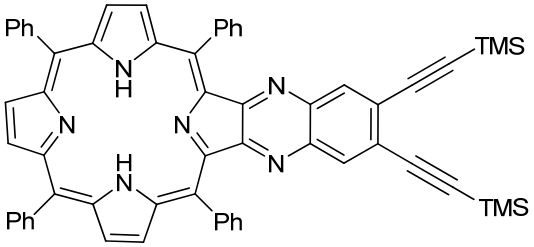
^{1}H NMR spectrum of **7g** (300 MHz, $CDCl_3$)

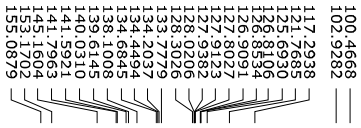


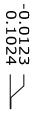


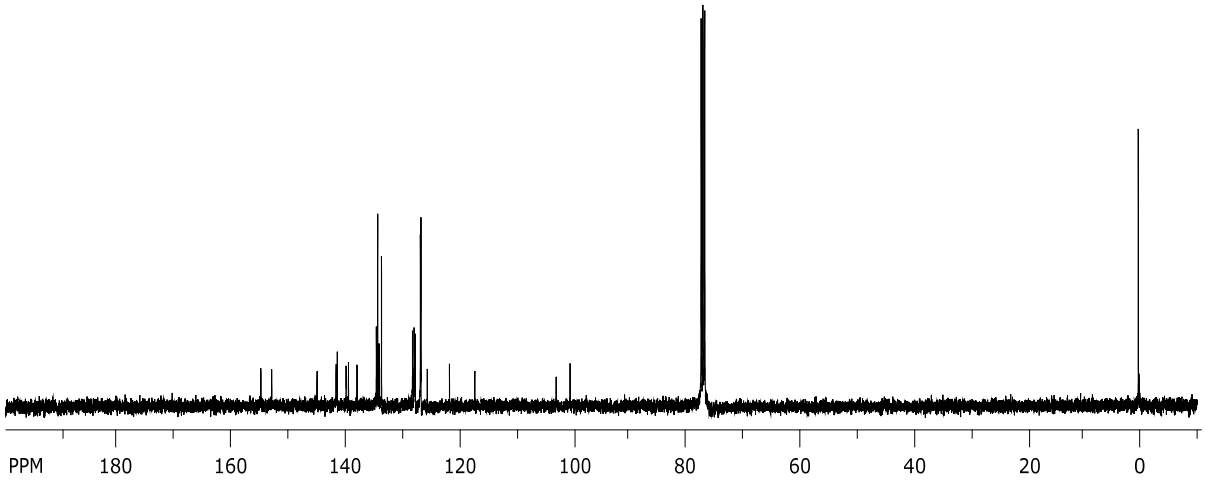


^{13}C NMR spectrum of **7g** (75 MHz, $CDCl_3$)

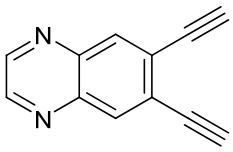


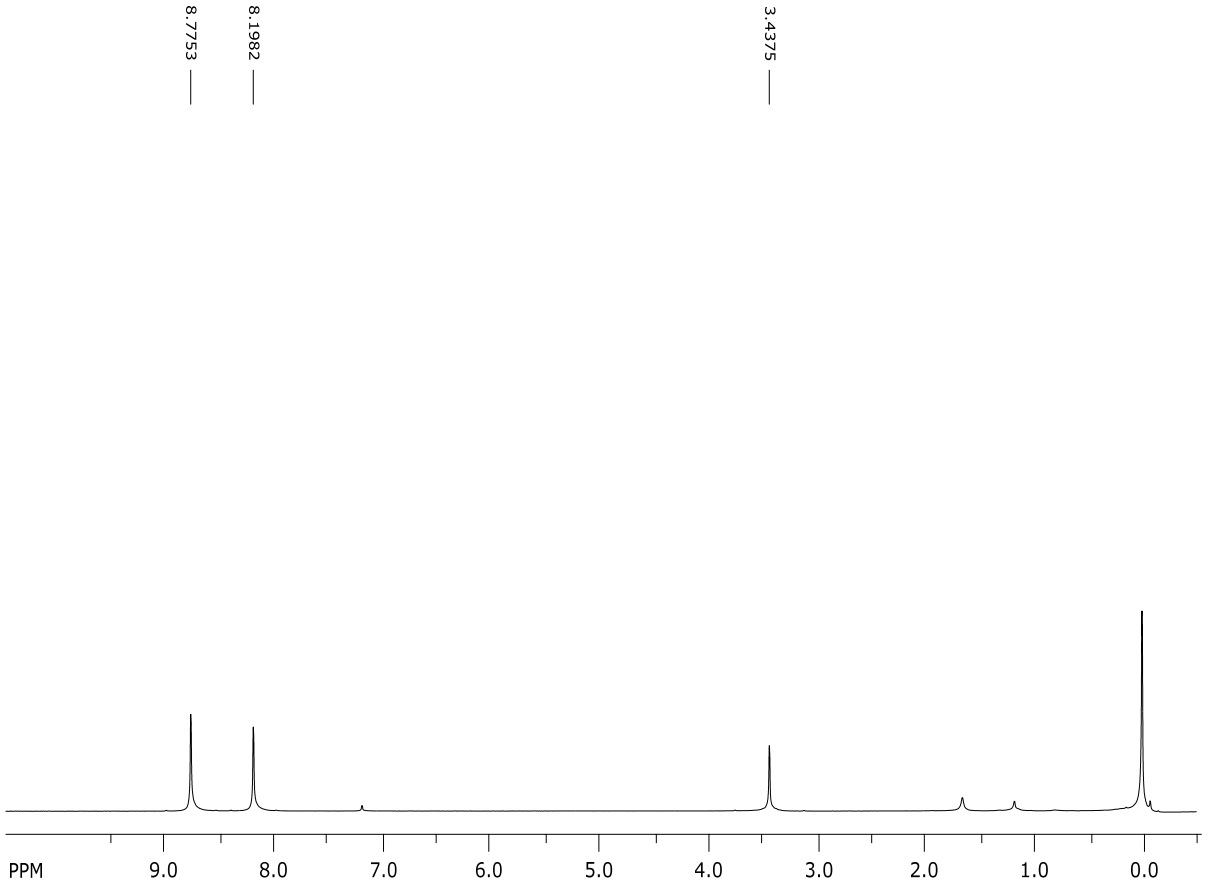




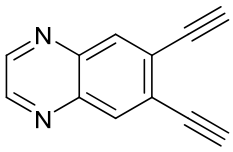


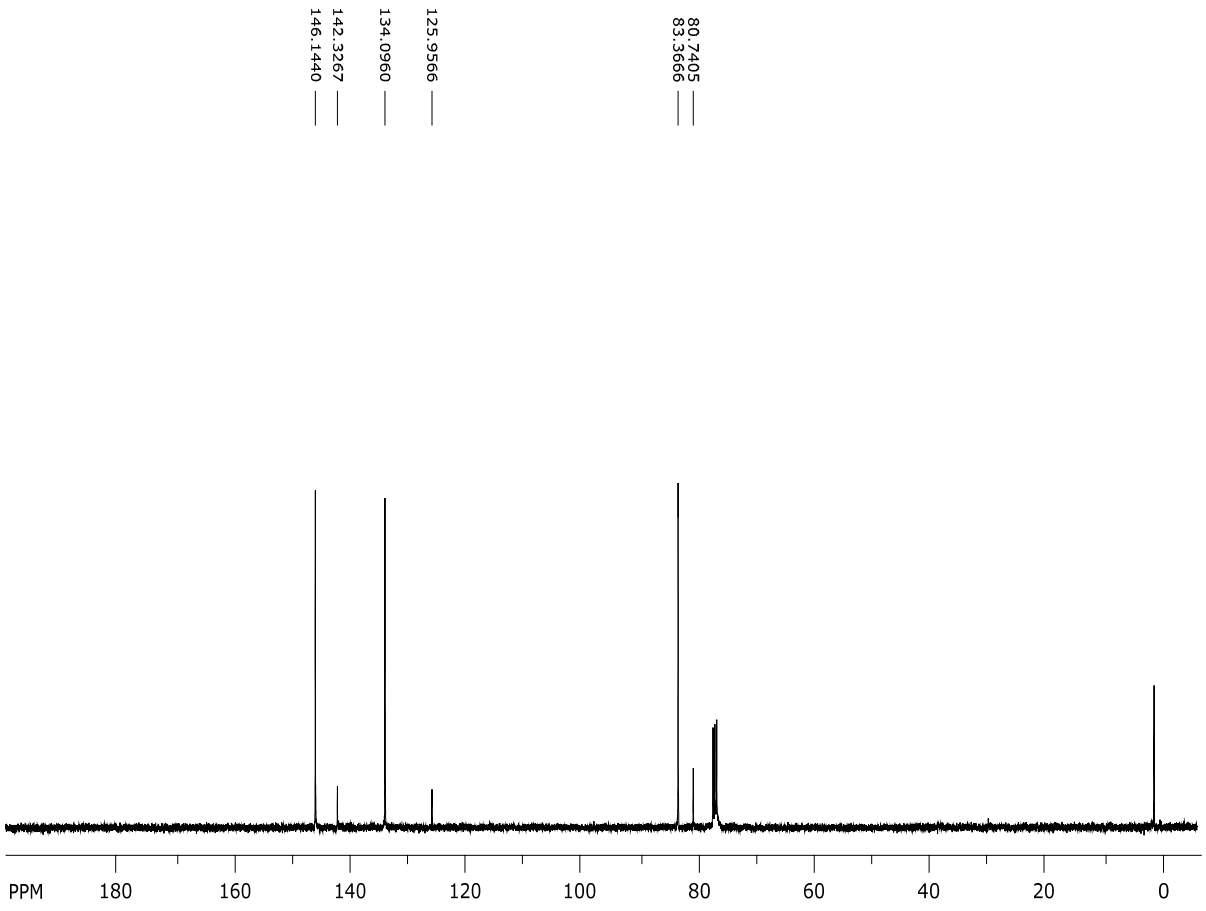
^{1}H NMR spectrum of **8a** (300 MHz, $CDCl_3$)



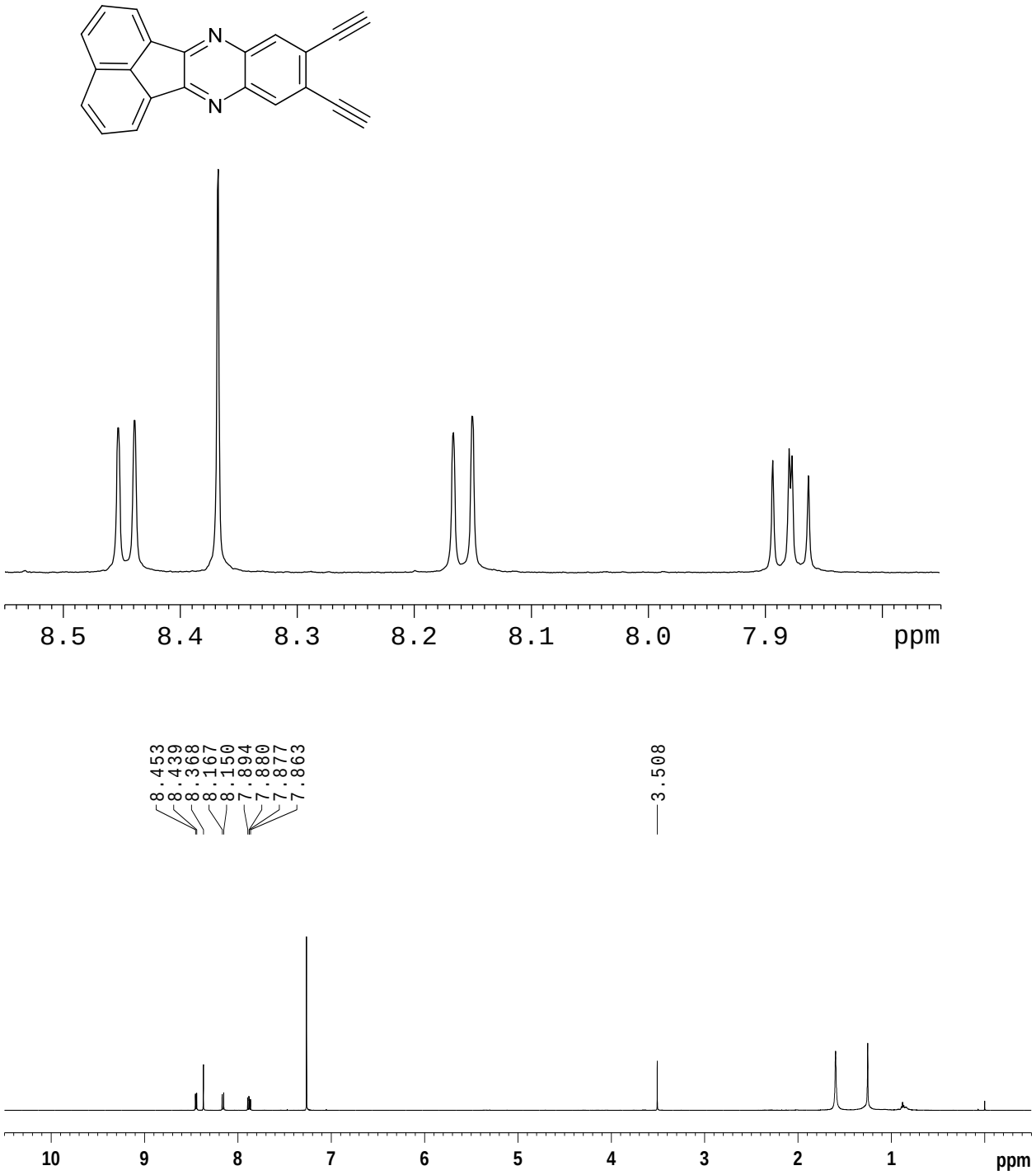


^{13}C NMR spectrum of **8a** (75 MHz, $CDCl_3$)

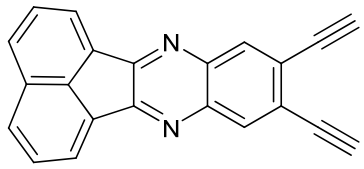


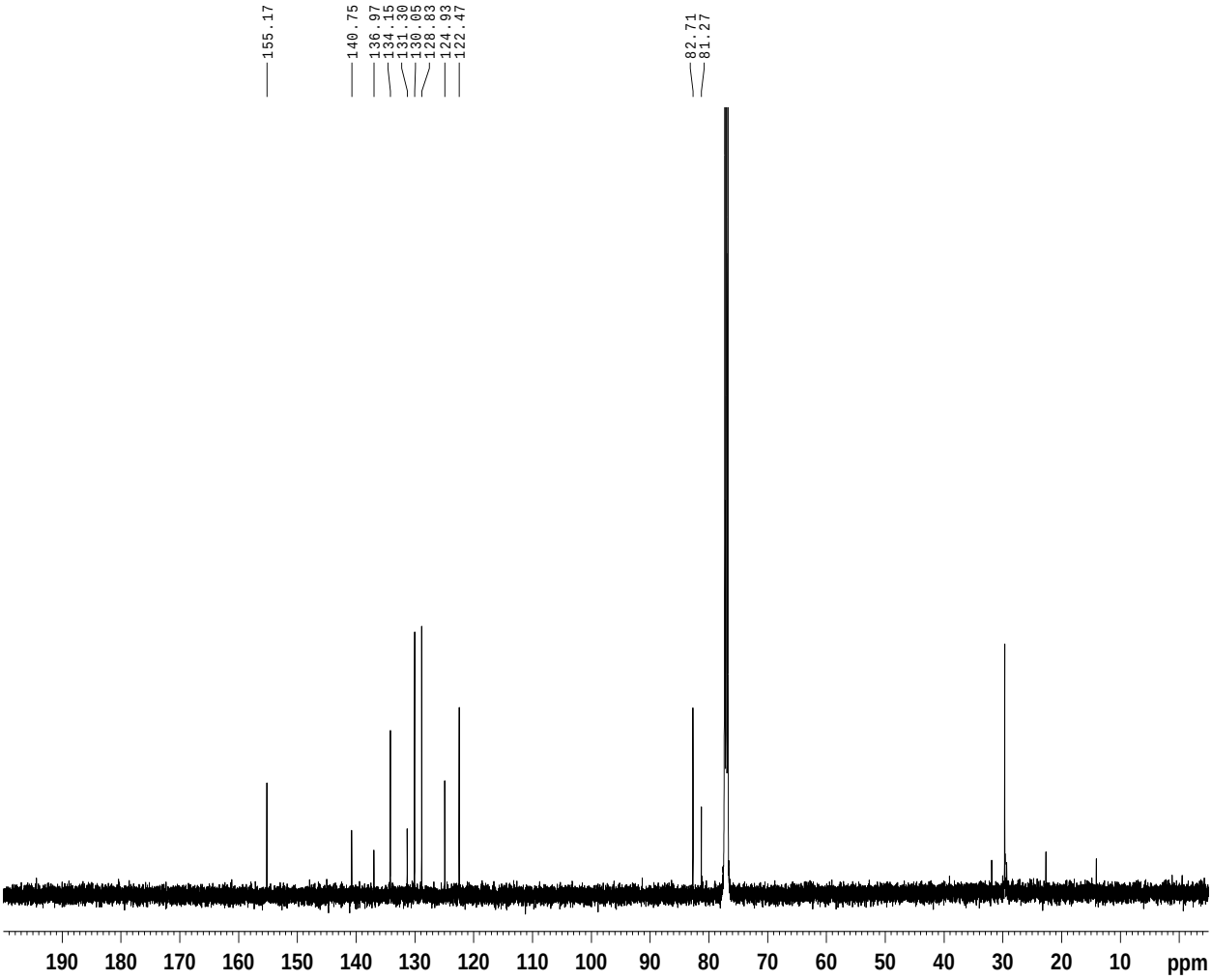


^{1}H NMR spectrum of **8b** (500 MHz, $CDCl_3$)

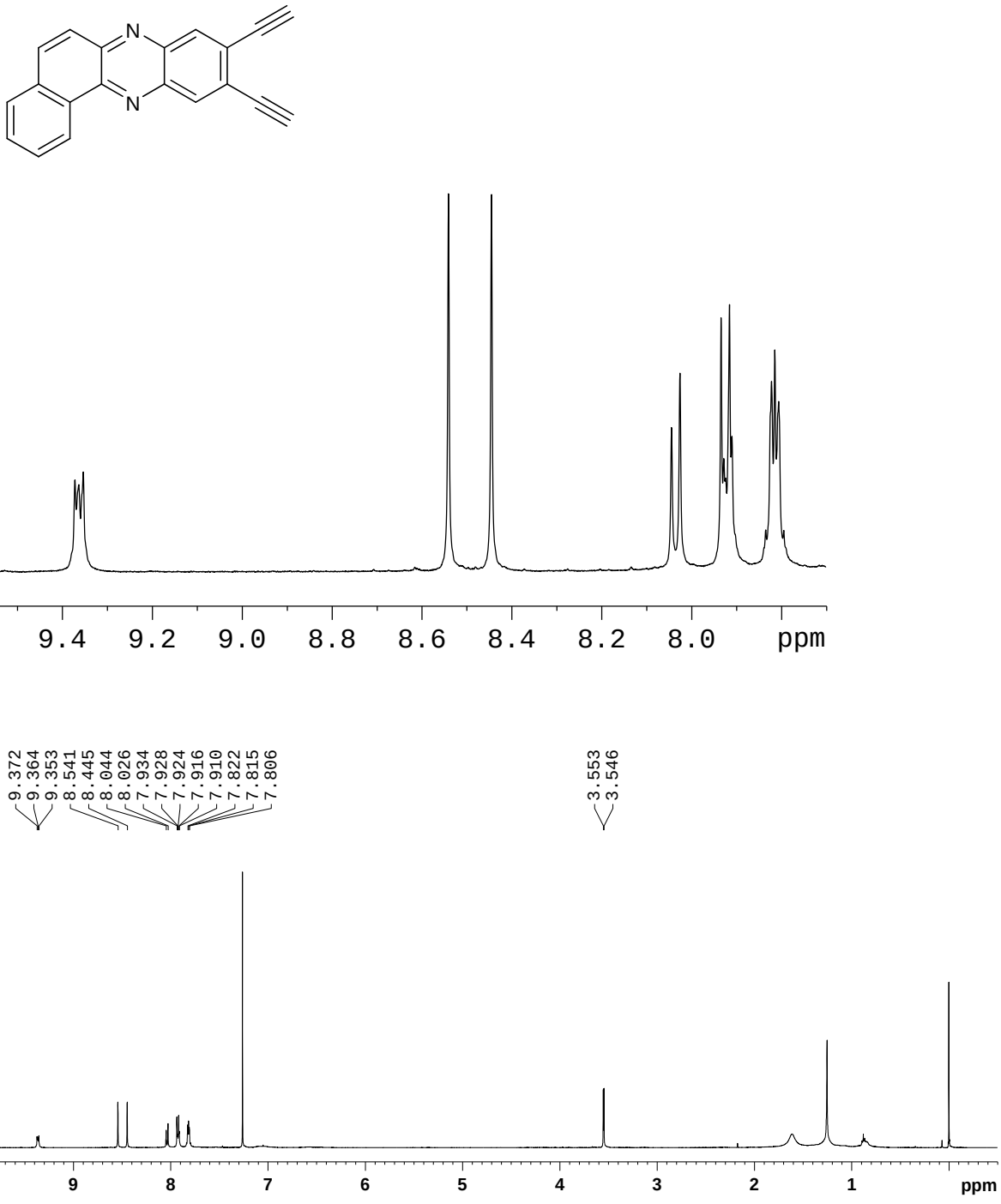


^{13}C NMR spectrum of **8b** (125 MHz, $CDCl_3$)

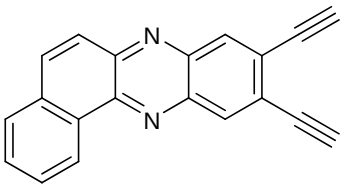


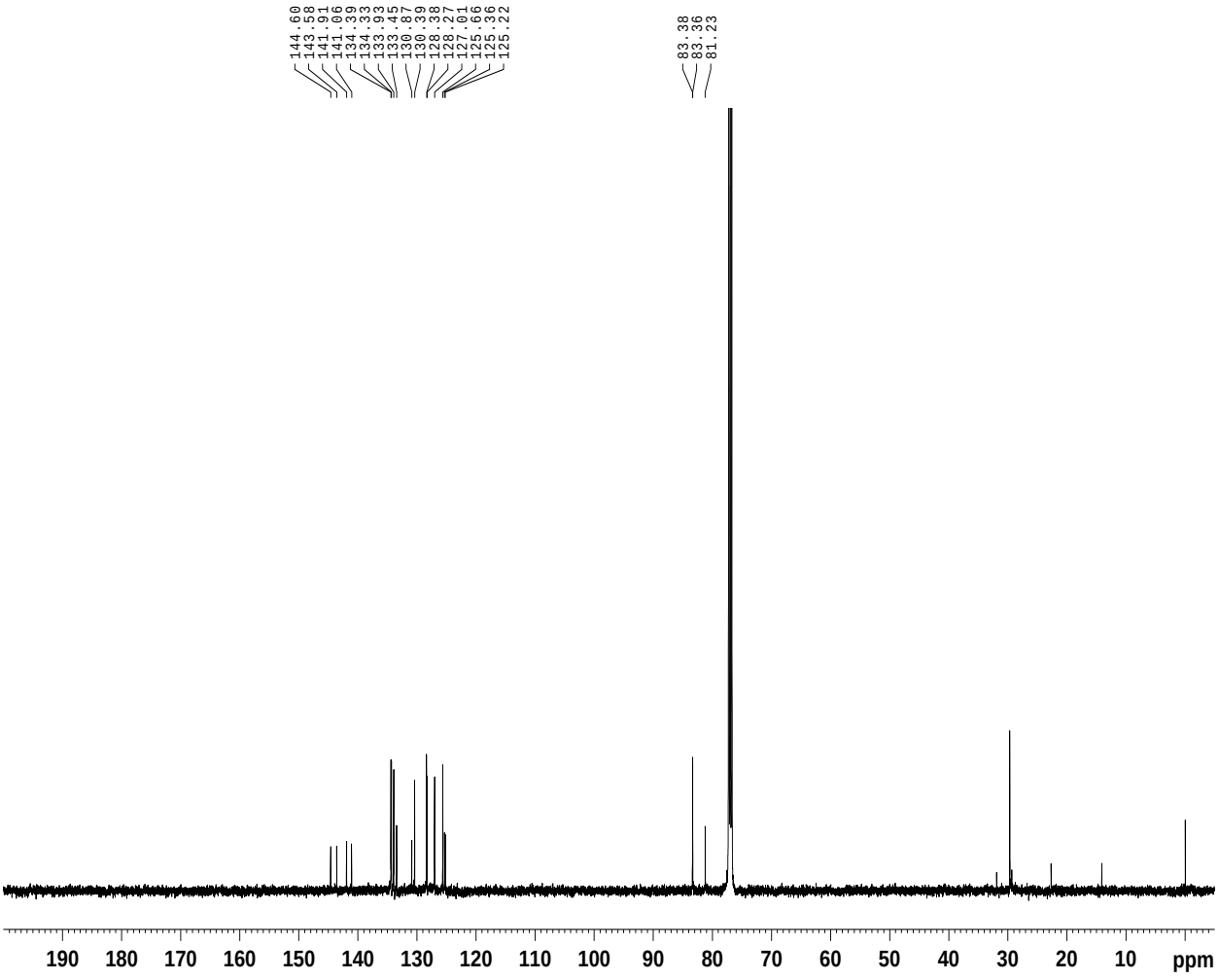


^{1}H NMR spectrum of **8c** (500 MHz, $CDCl_3$)

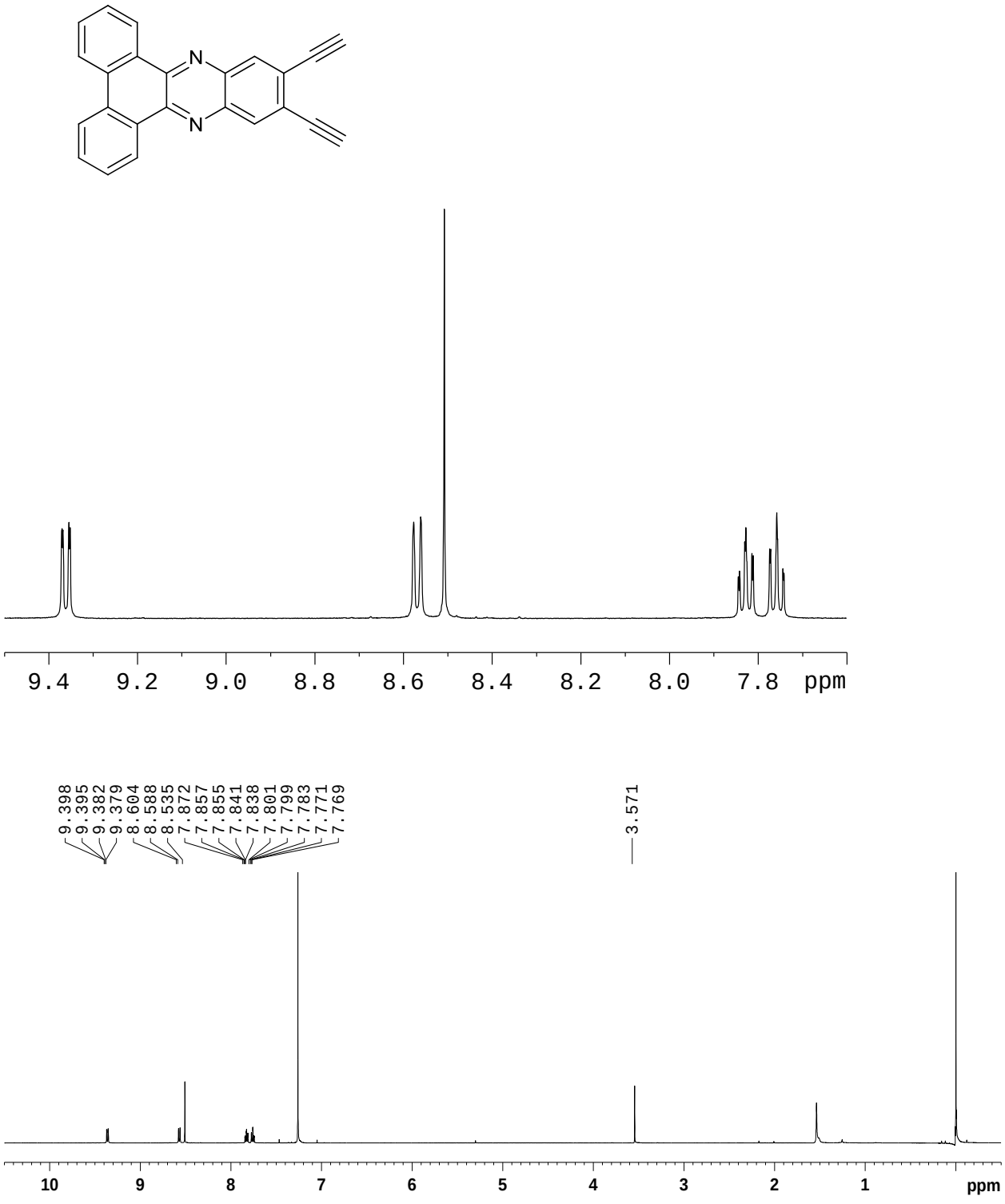


^{13}C NMR spectrum of **8c** (125 MHz, $CDCl_3$)

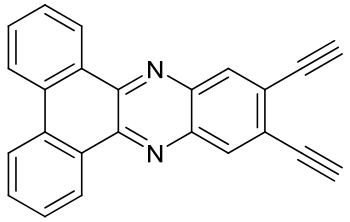


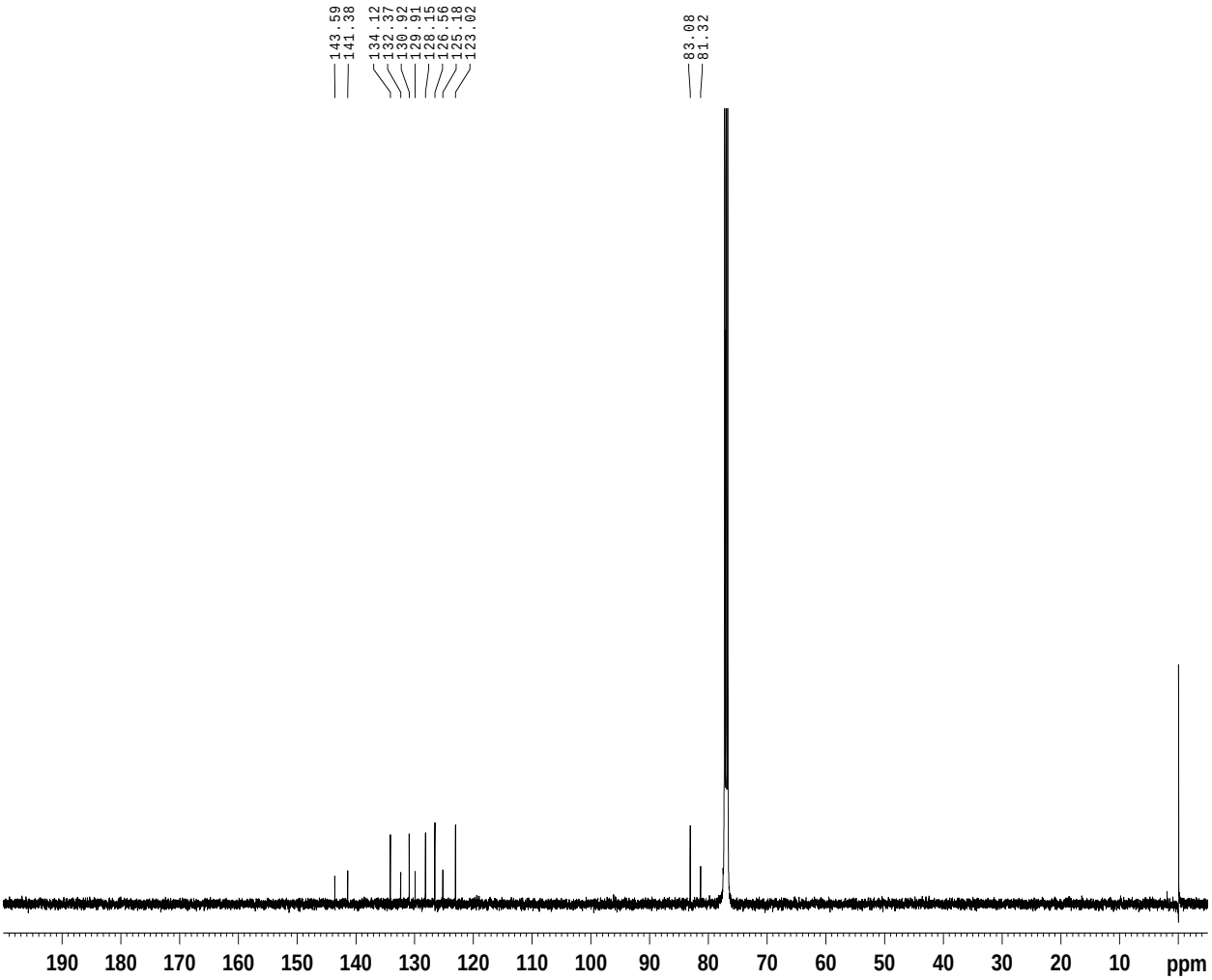


^{1}H NMR spectrum of **8d** (500 MHz, $CDCl_3$)

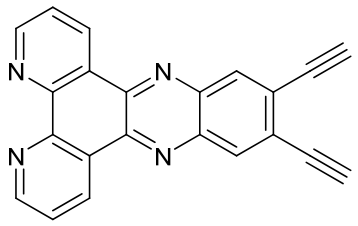


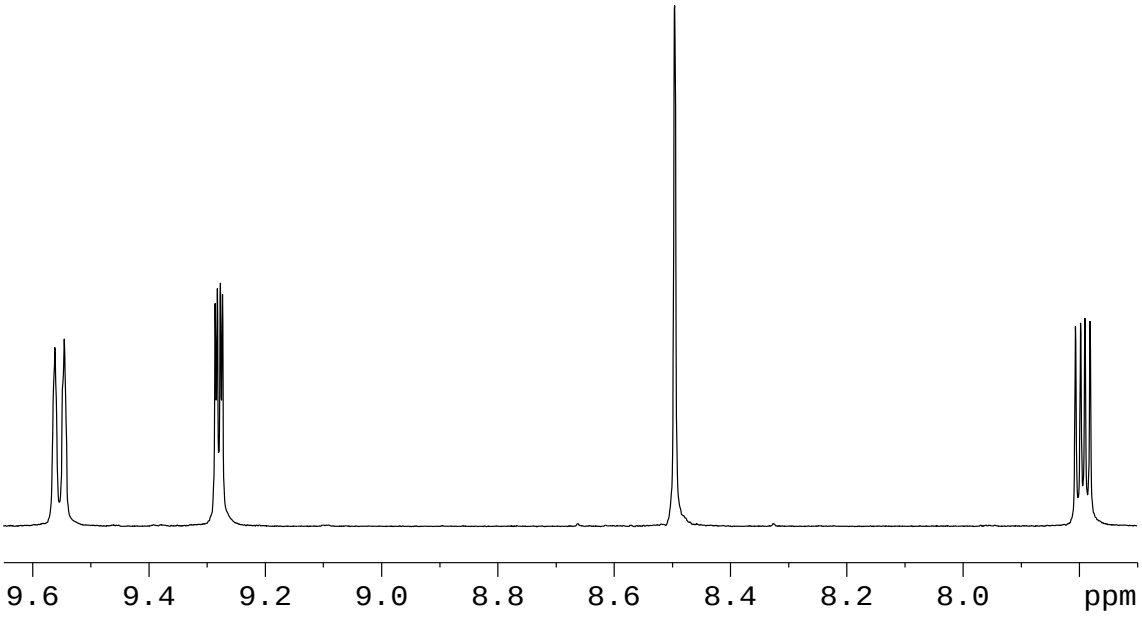
^{13}C NMR spectrum of **8d** (125 MHz, $CDCl_3$)

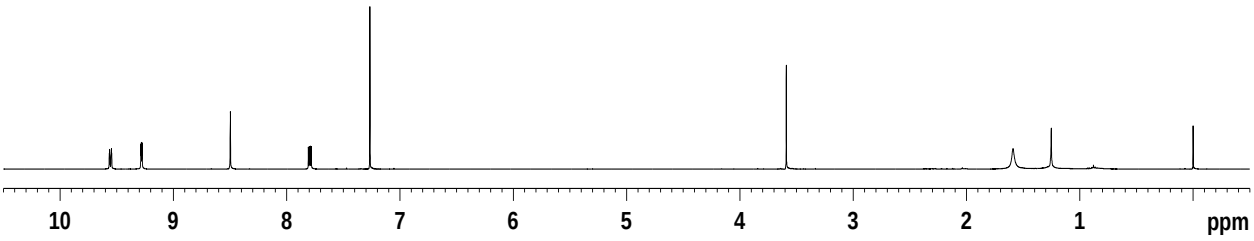




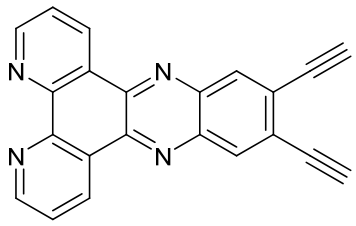
^{1}H NMR spectrum of **8e** (500 MHz, $CDCl_3$)

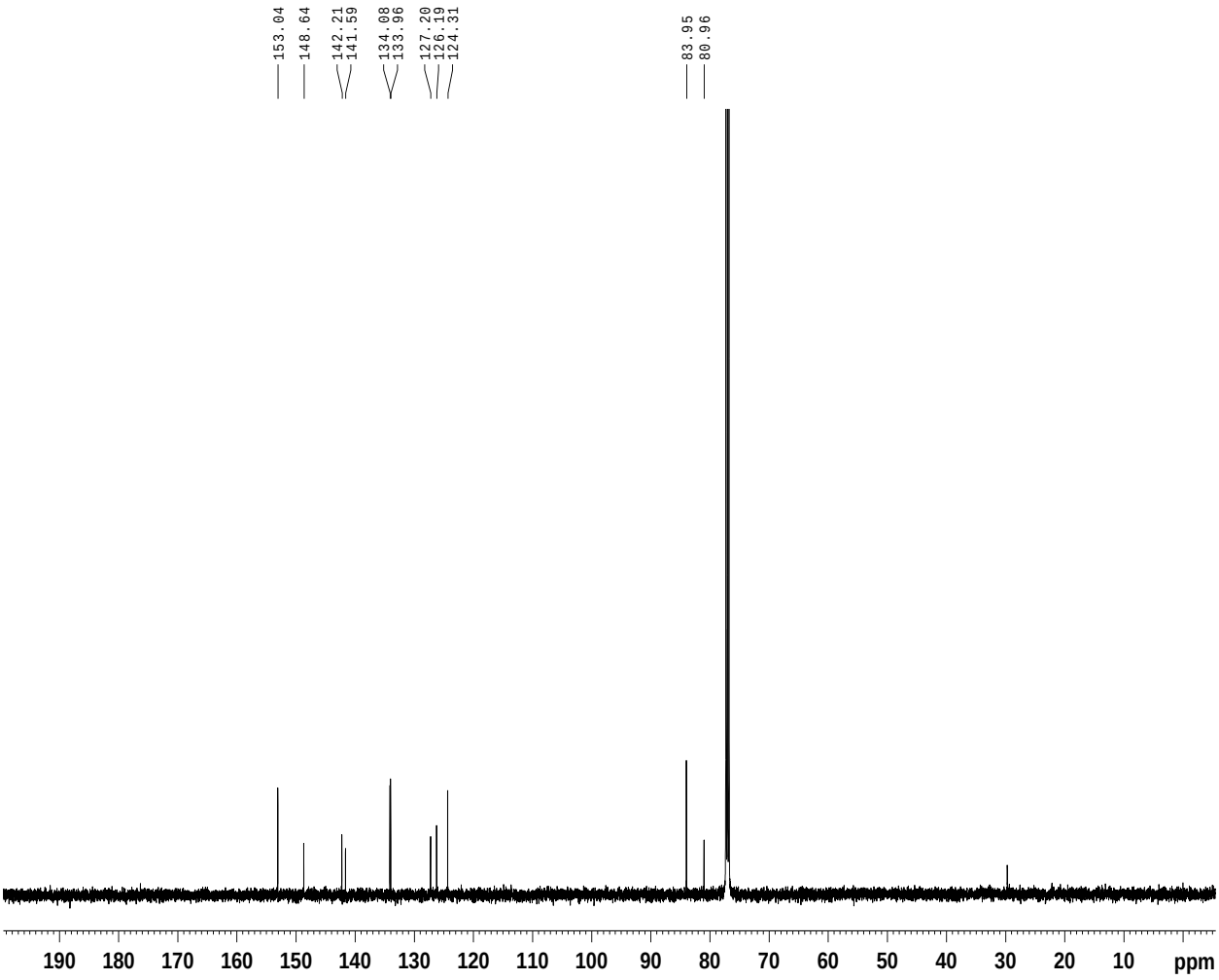




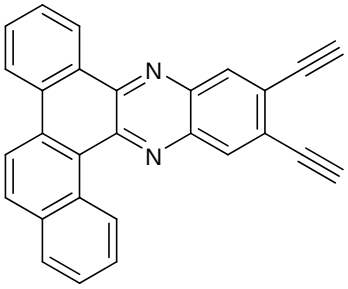


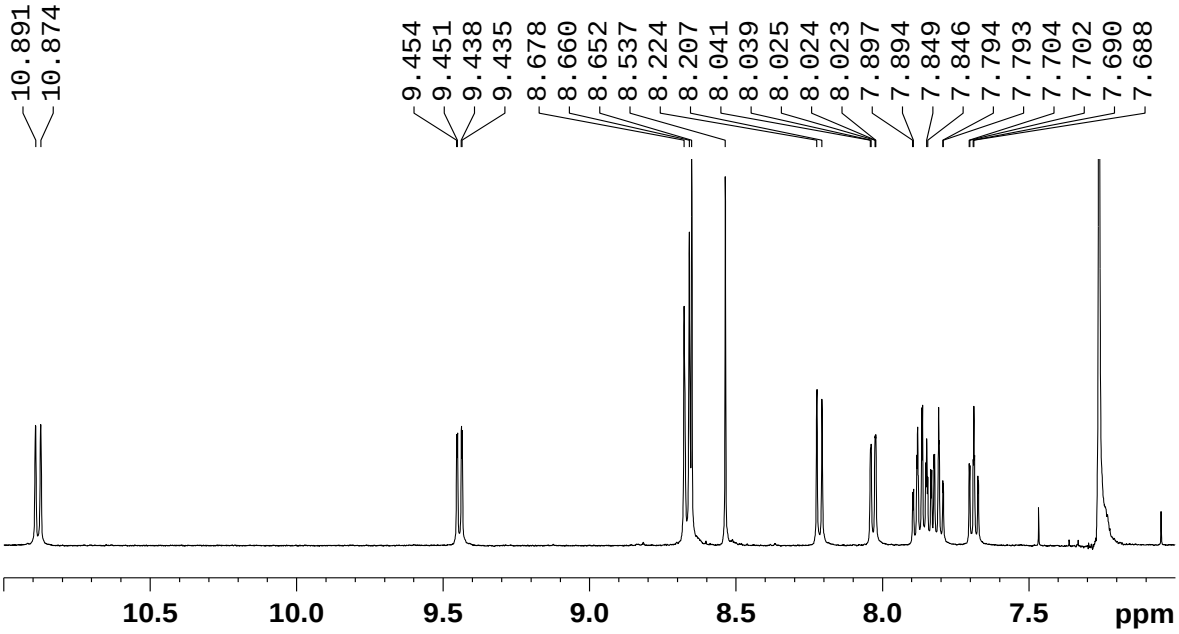
^{13}C NMR spectrum of **8e** (125 MHz, $CDCl_3$)

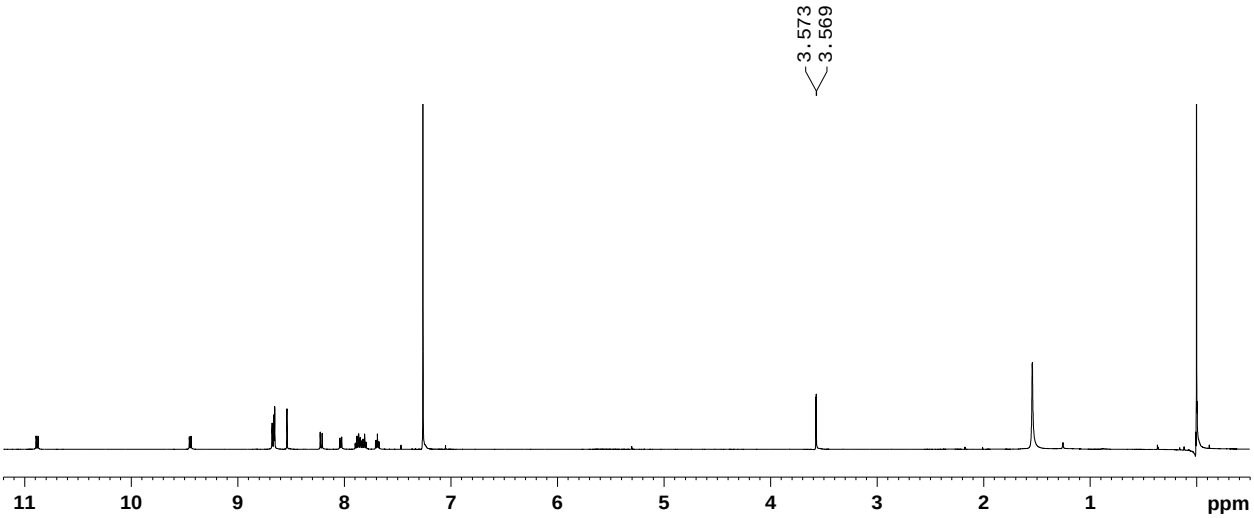




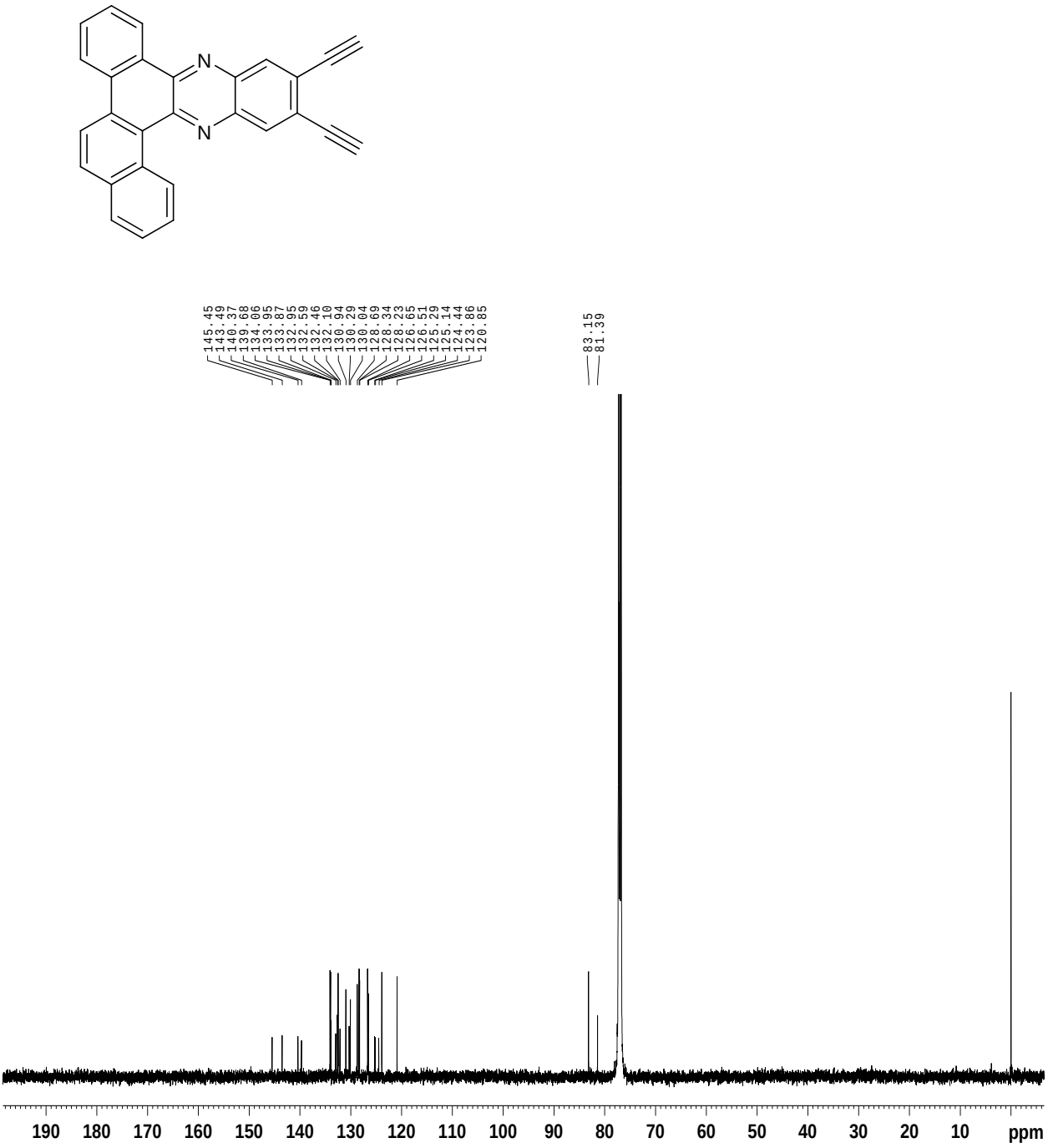
^{1}H NMR spectrum of **8f** (500 MHz, $CDCl_3$)



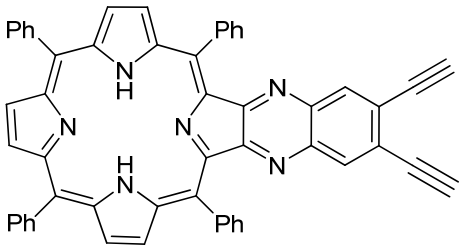


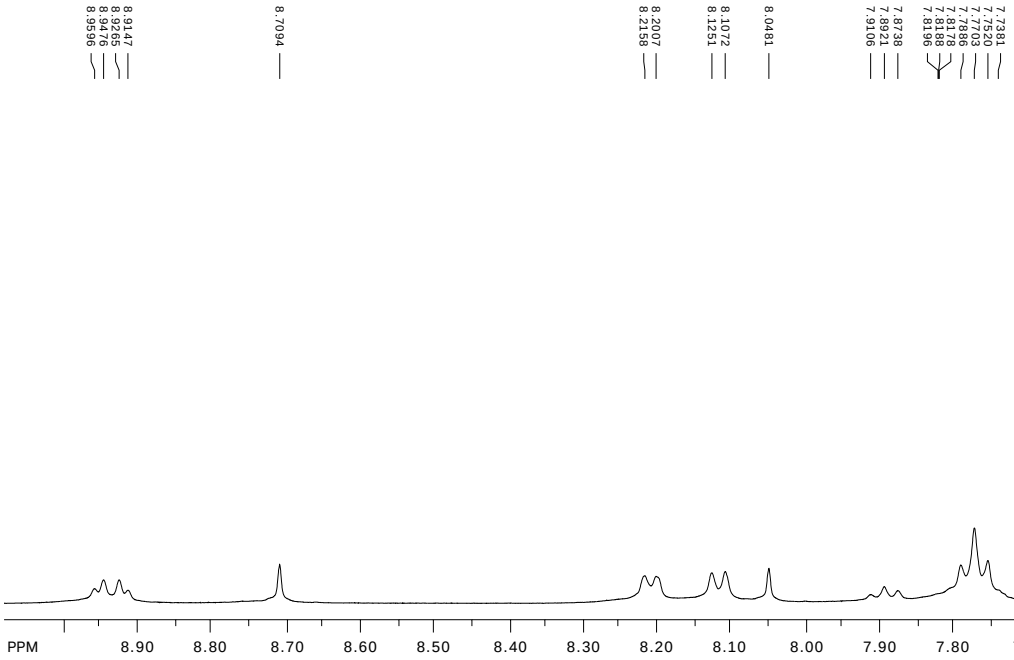


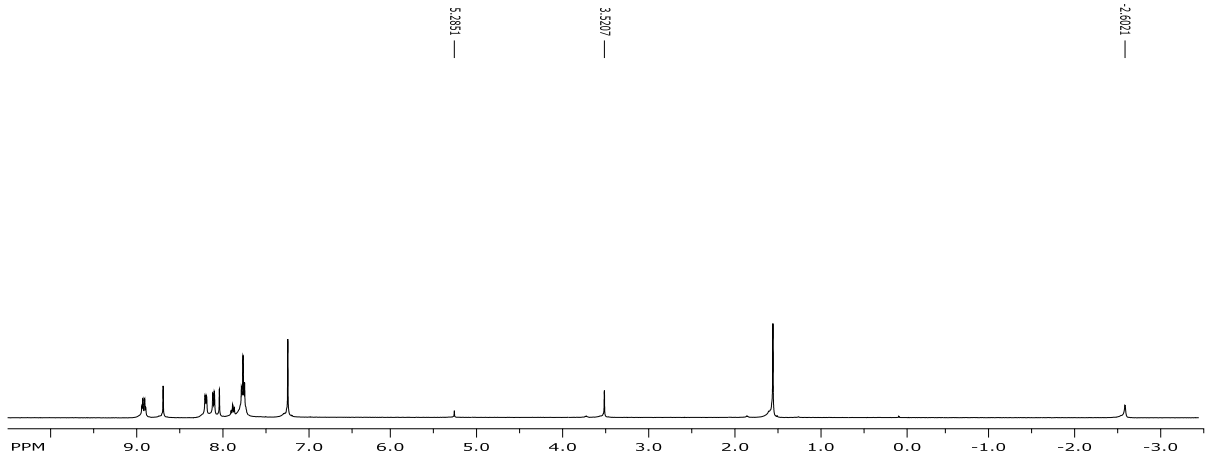
^{13}C NMR spectrum of **8f** (125 MHz, $CDCl_3$)



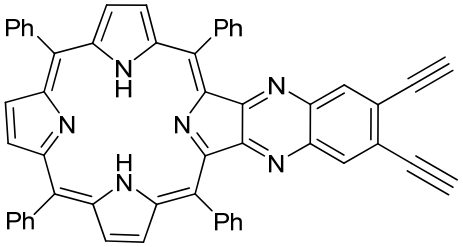
^{1}H NMR spectrum of **8g** (300 MHz, $CDCl_3$)

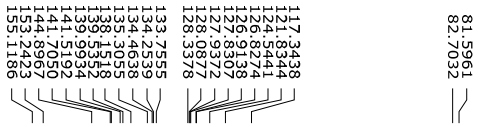


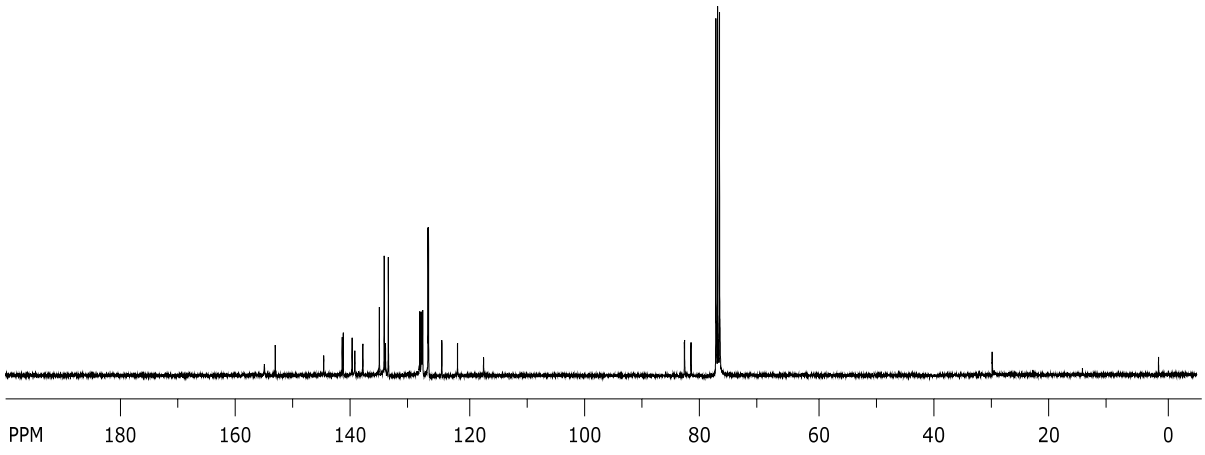




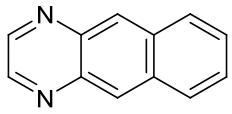
^{13}C NMR spectrum of **8g** (75 MHz, $CDCl_3$)

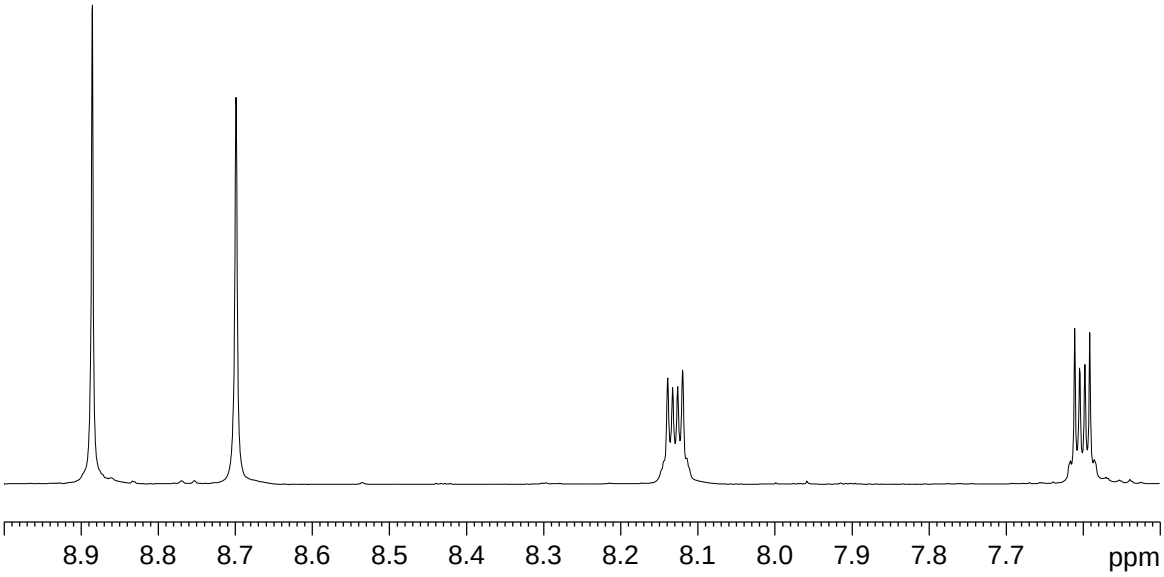


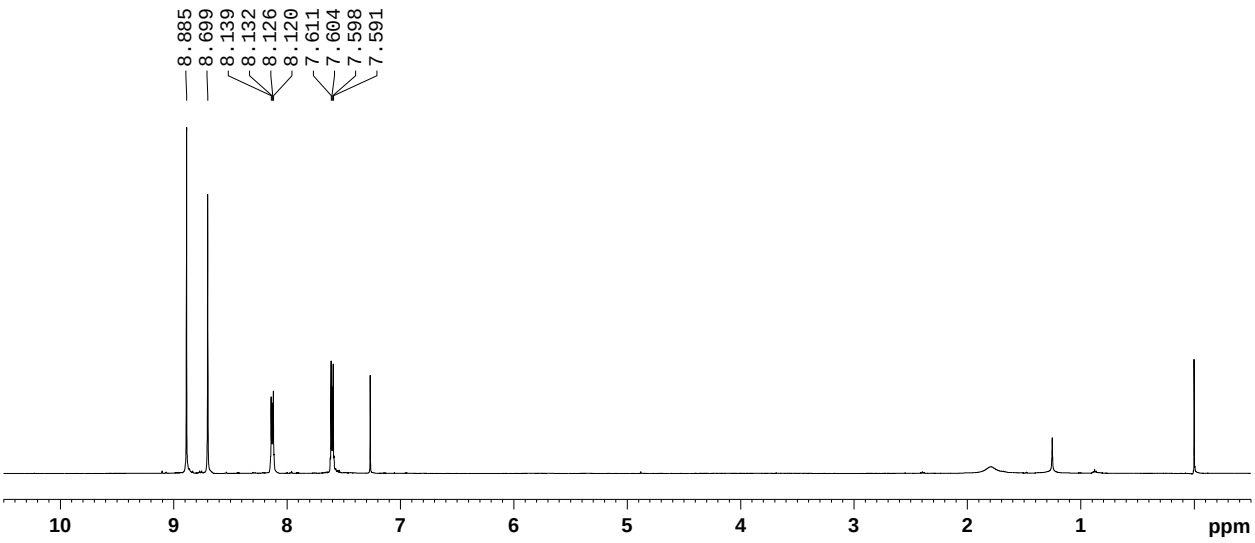




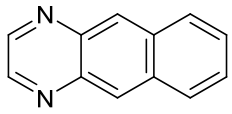
^{1}H NMR spectrum of **9** (500 MHz, $CDCl_3$)

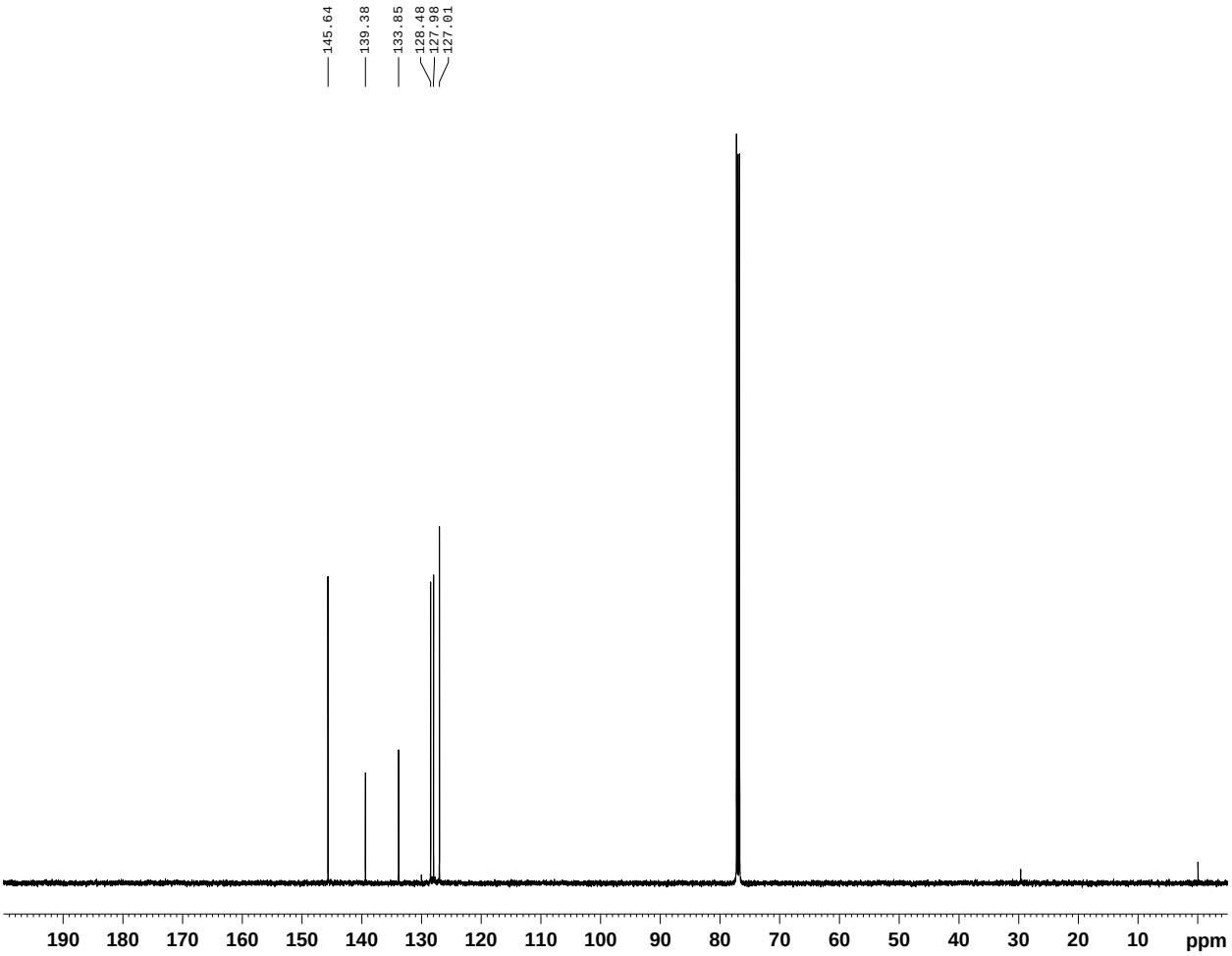




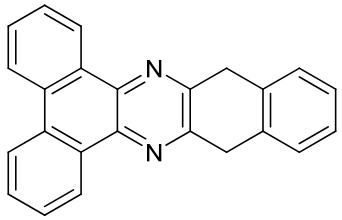


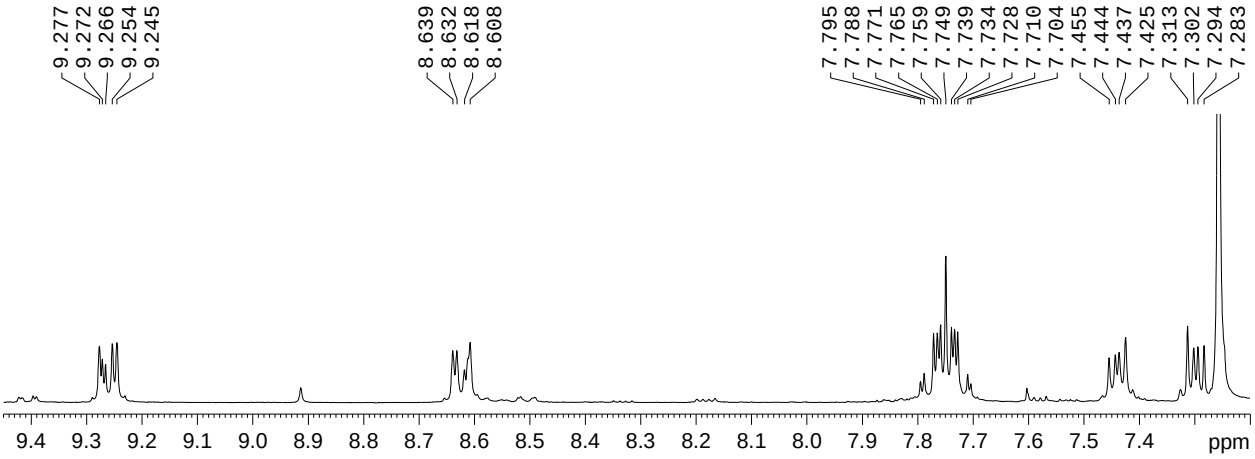
^{13}C NMR spectrum of **9** (125 MHz, $CDCl_3$)

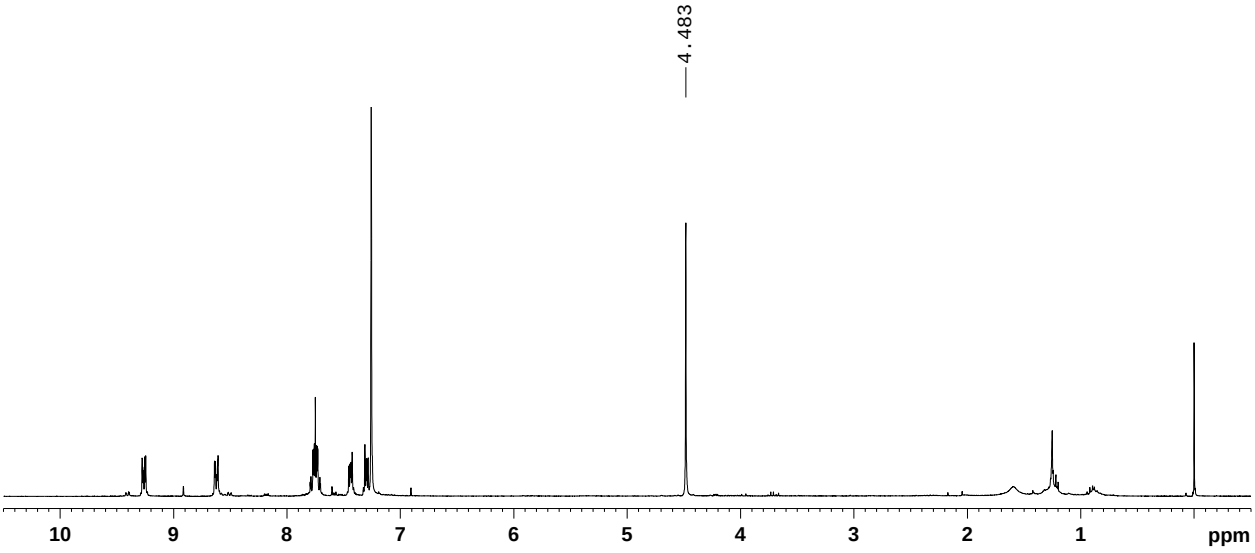




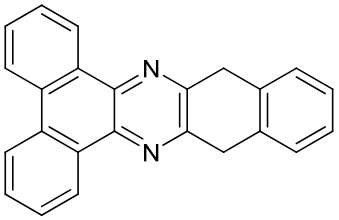
^{1}H NMR spectrum of **12** (300 MHz, $CDCl_3$)

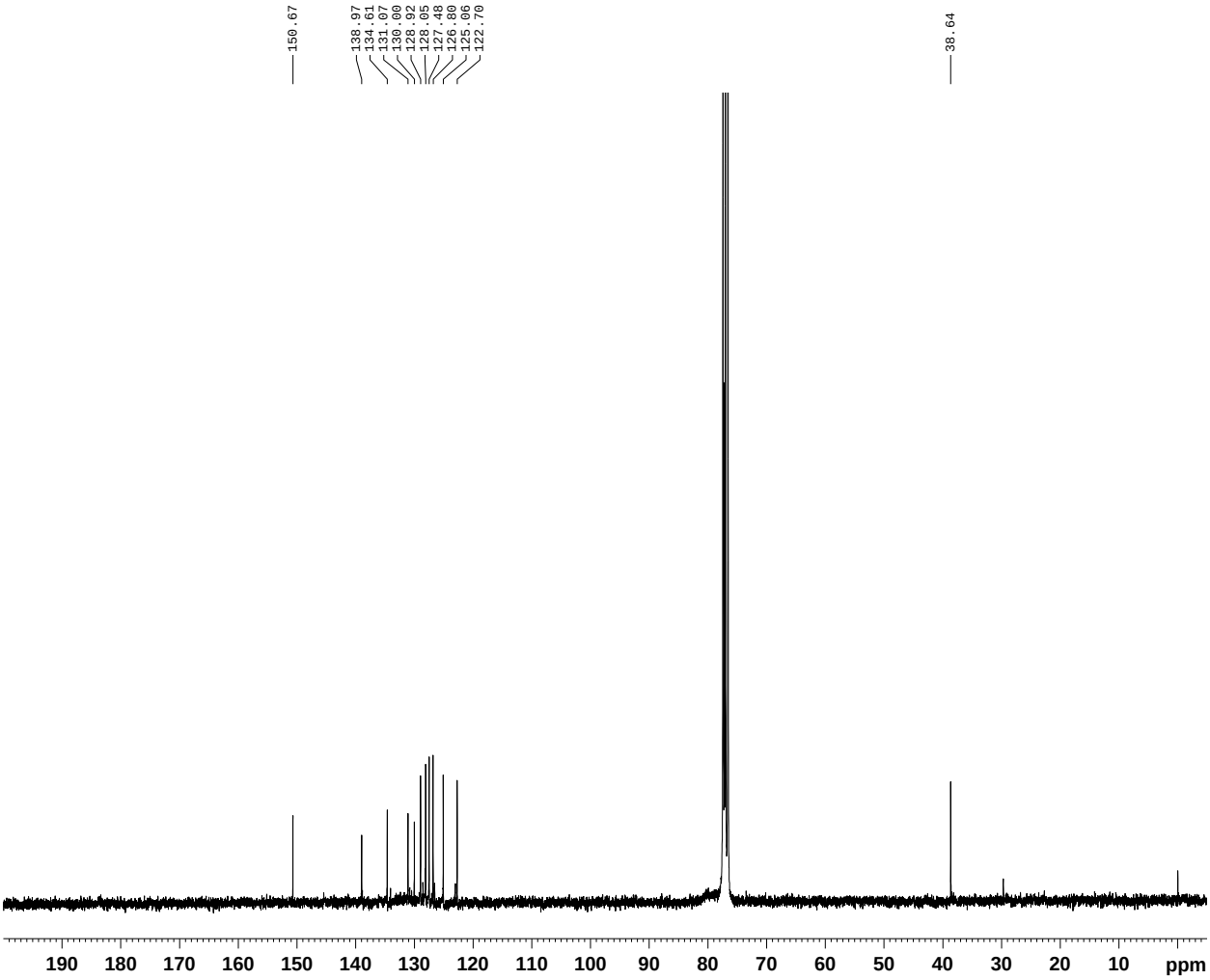




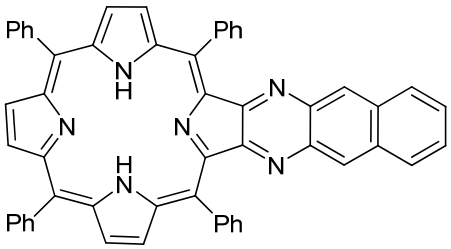


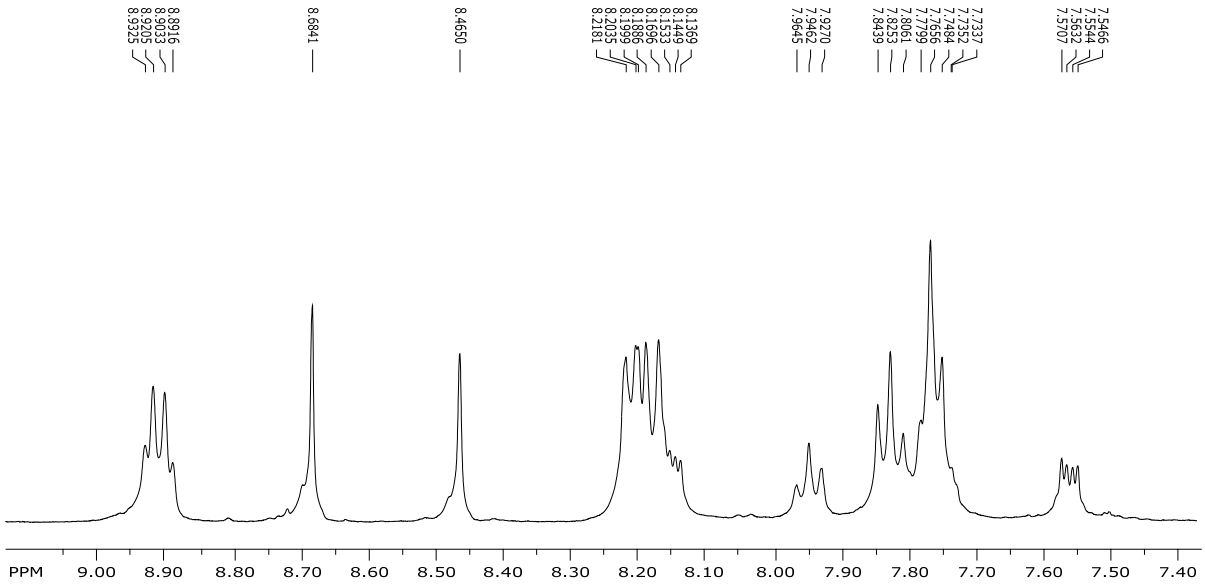
^{13}C NMR spectrum of **12** (75 MHz, $CDCl_3$)

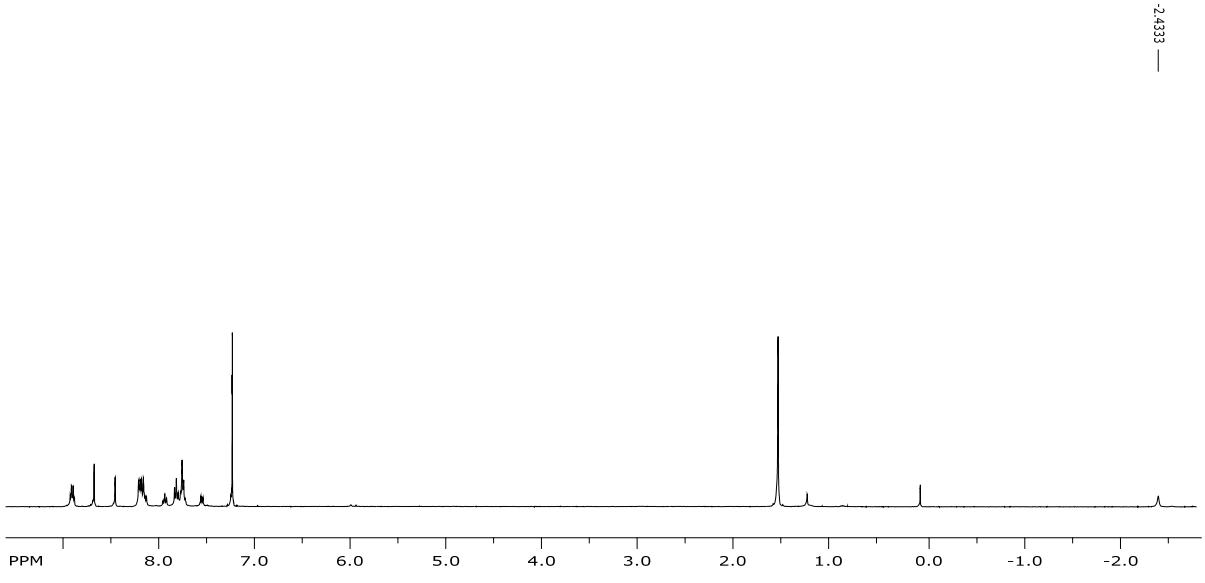




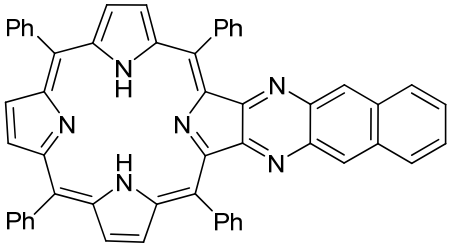
^{1}H NMR spectrum of **13** (300 MHz, $CDCl_3$)

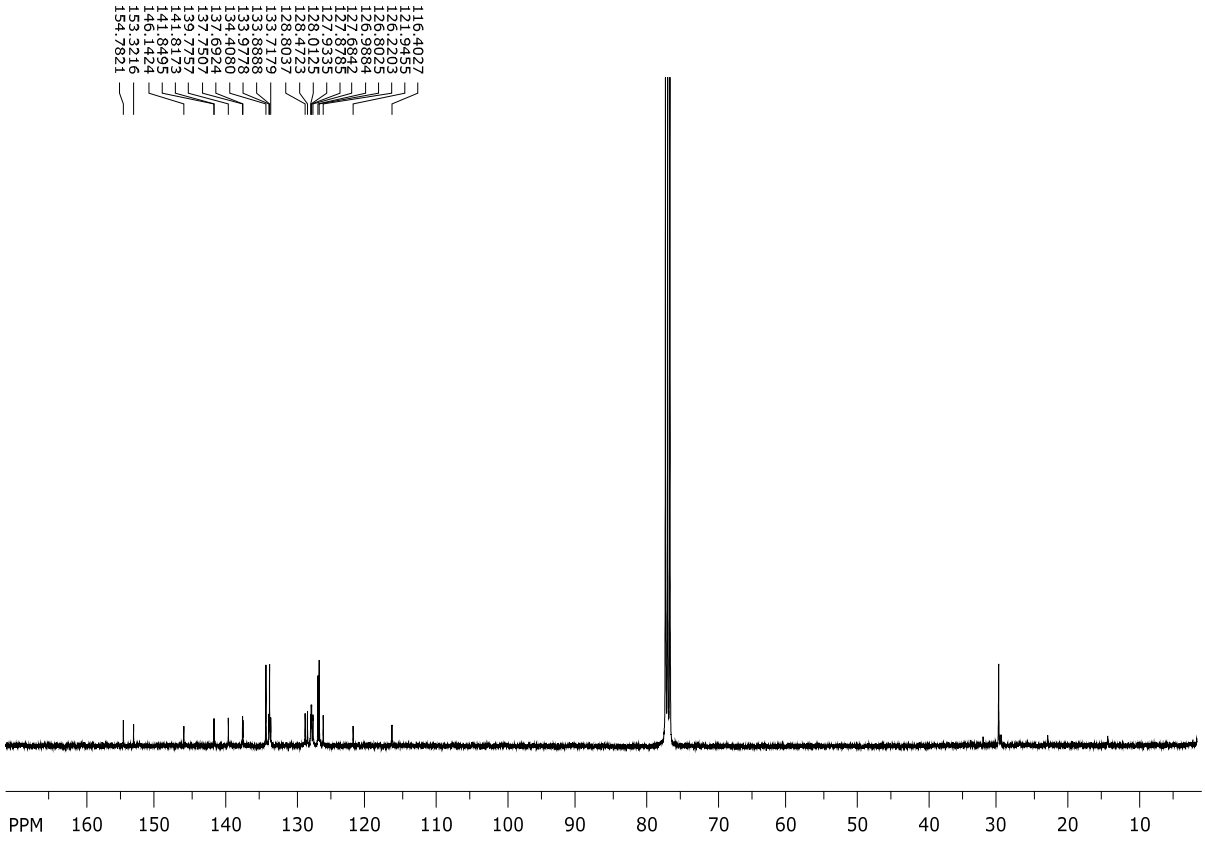




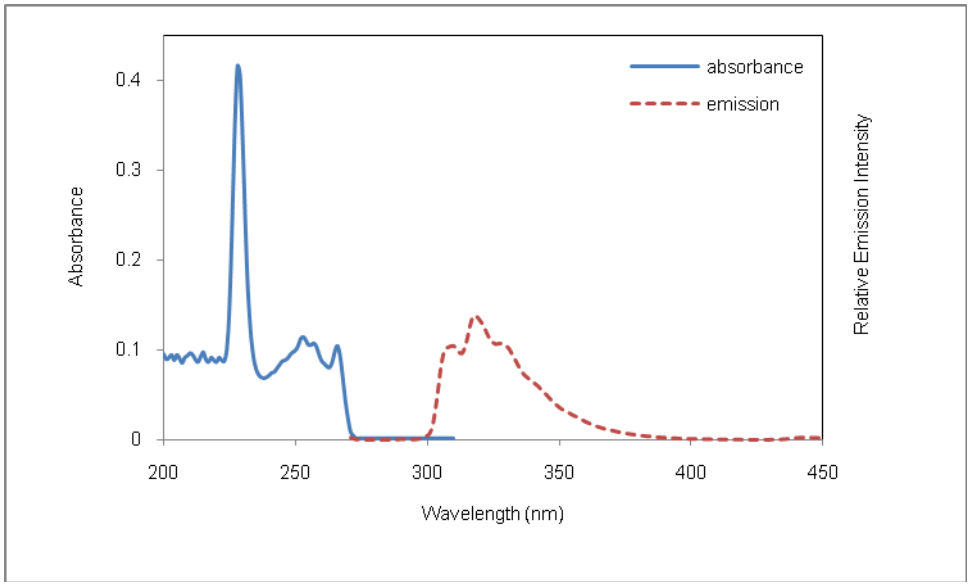


^{13}C NMR spectrum of **13** (75 MHz, $CDCl_3$)

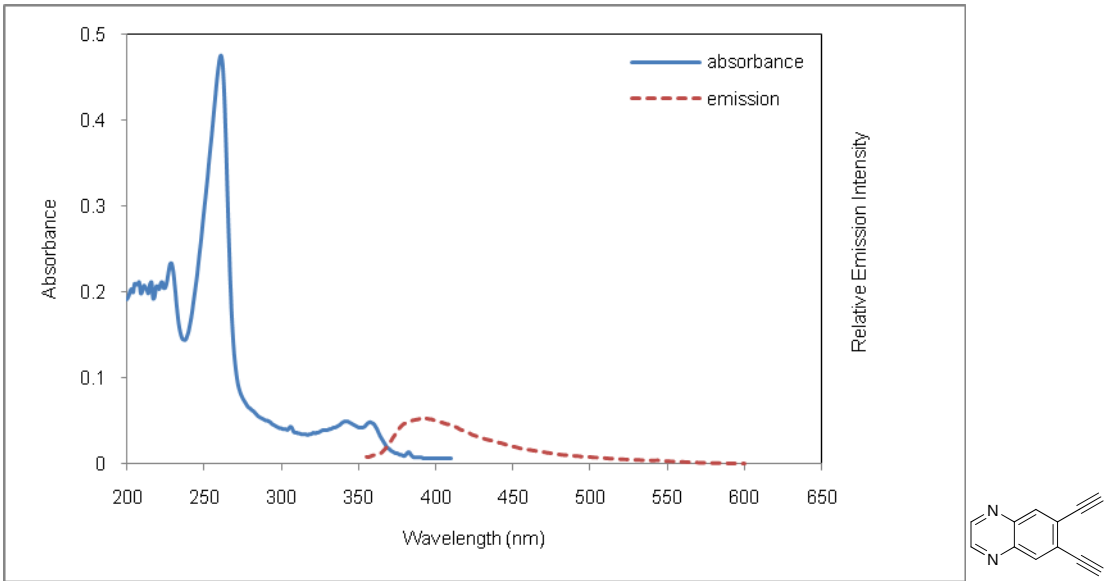




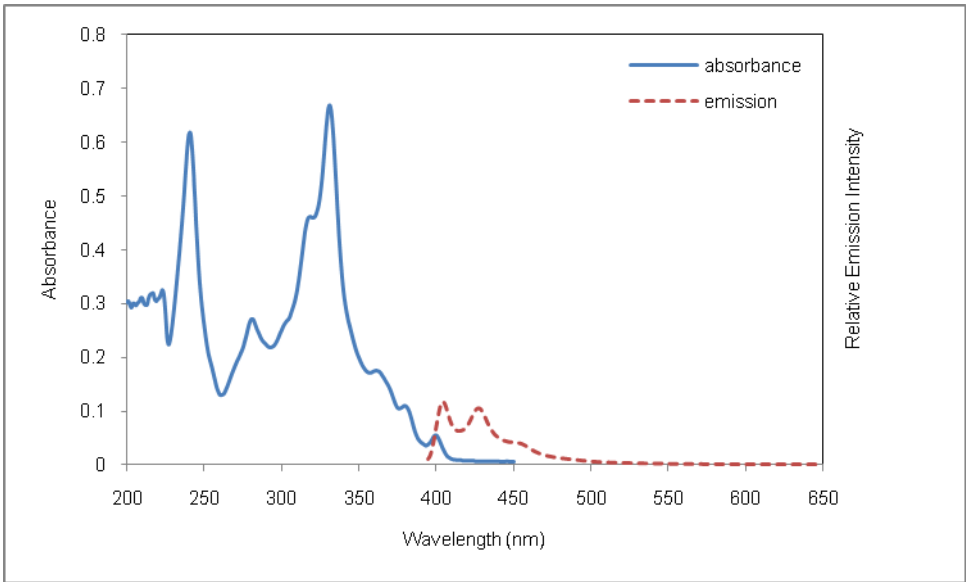
Absorbance and emission spectra of **2**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 266 nm). Absorbance and emission spectra 1.00×10^{-5} M in CH_2Cl_2.

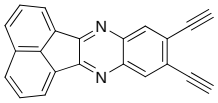


Absorbance and emission spectra of **8a**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 350 nm). Absorbance spectra 1.08×10^{-5} M in CH_2Cl_2. Emission spectra 1.08×10^{-4} M in CH_2Cl_2.

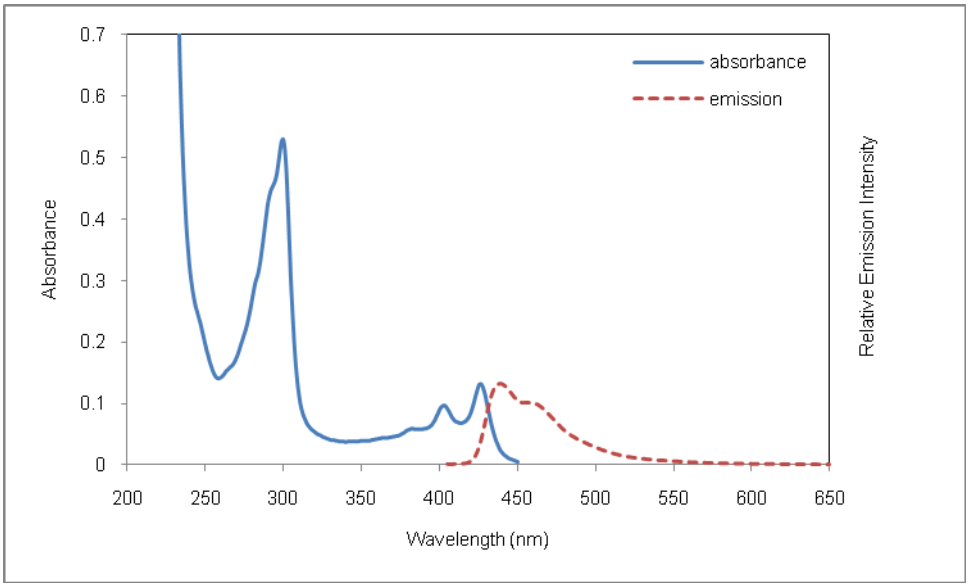


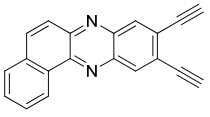
Absorbance and emission spectra of **8b**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 350 nm). Absorbance and emission spectra 1.05×10^{-5} M in CH_2Cl_2.



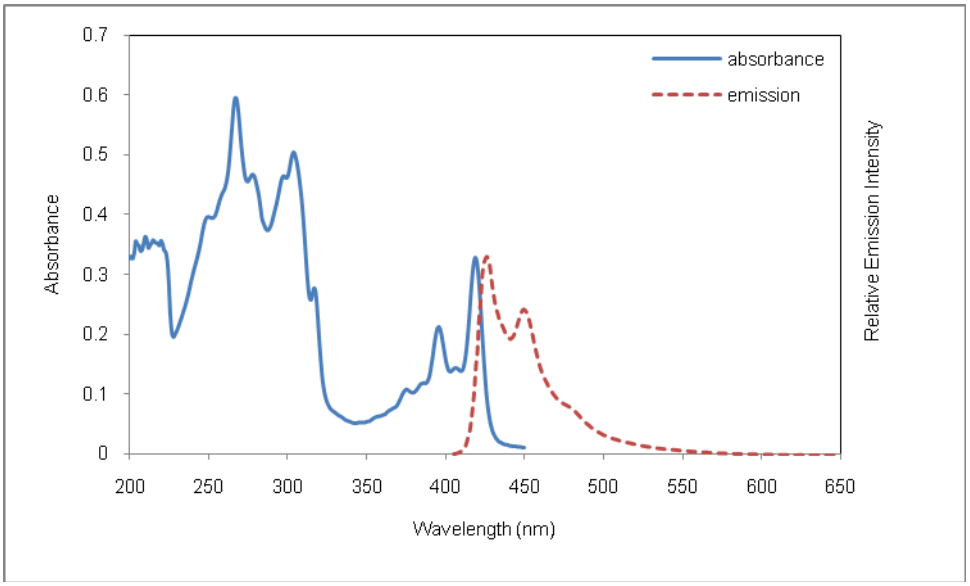


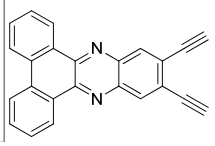
Absorbance and emission spectra of **8c**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 400 nm). Absorbance and emission spectra 1.10×10^{-5} M in CH_2Cl_2.



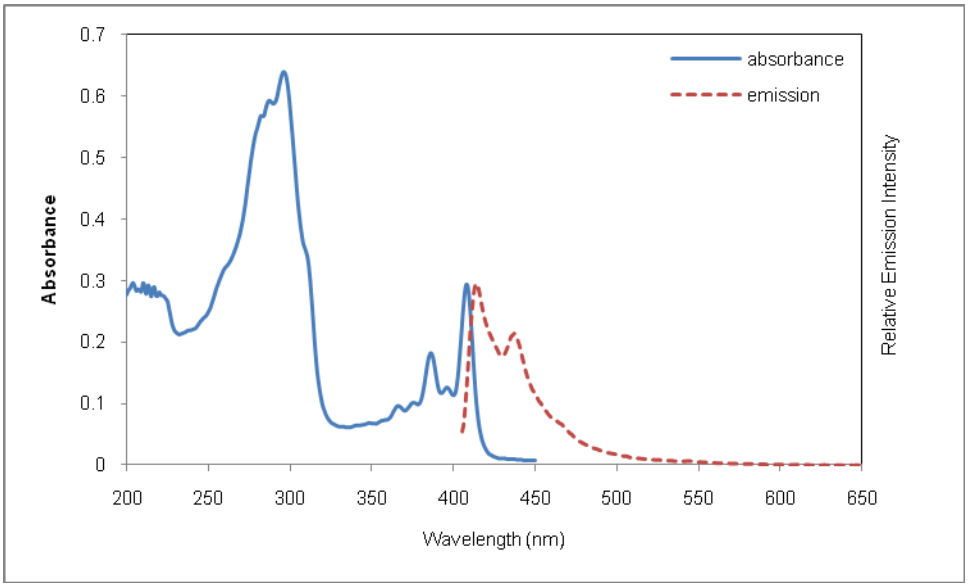


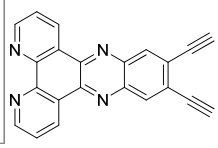
Absorbance and emission spectra of **8d**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 400 nm). Absorbance and emission spectra 1.00×10^{-5} M in CH_2Cl_2.



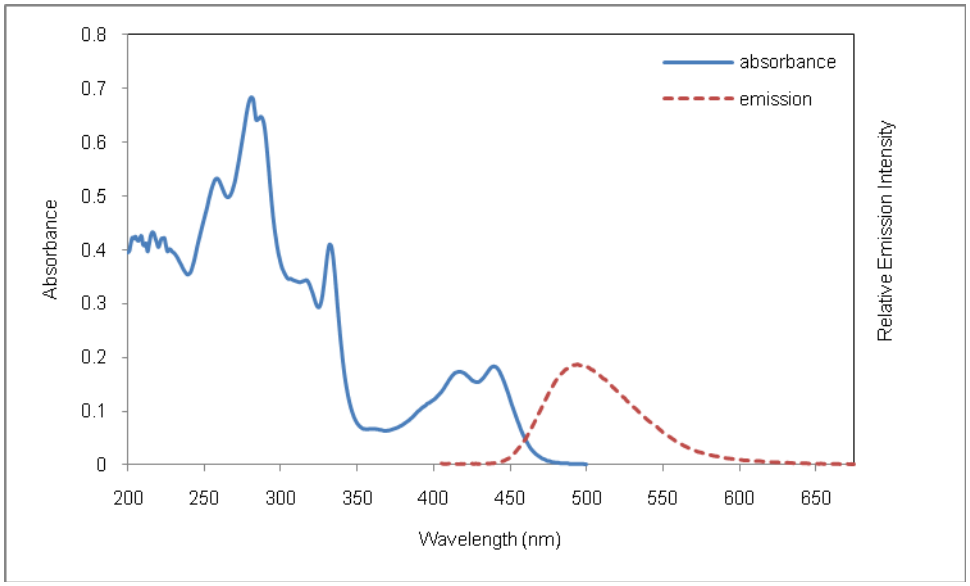


Absorbance and emission spectra of **8e**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 400 nm). Absorbance and emission spectra 1.02×10^{-5} M in CH_2Cl_2.

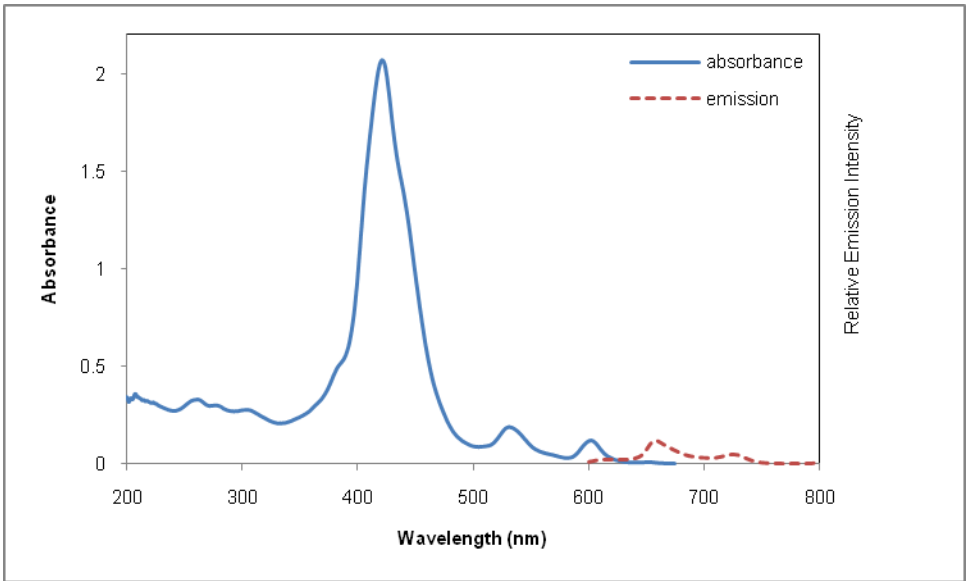




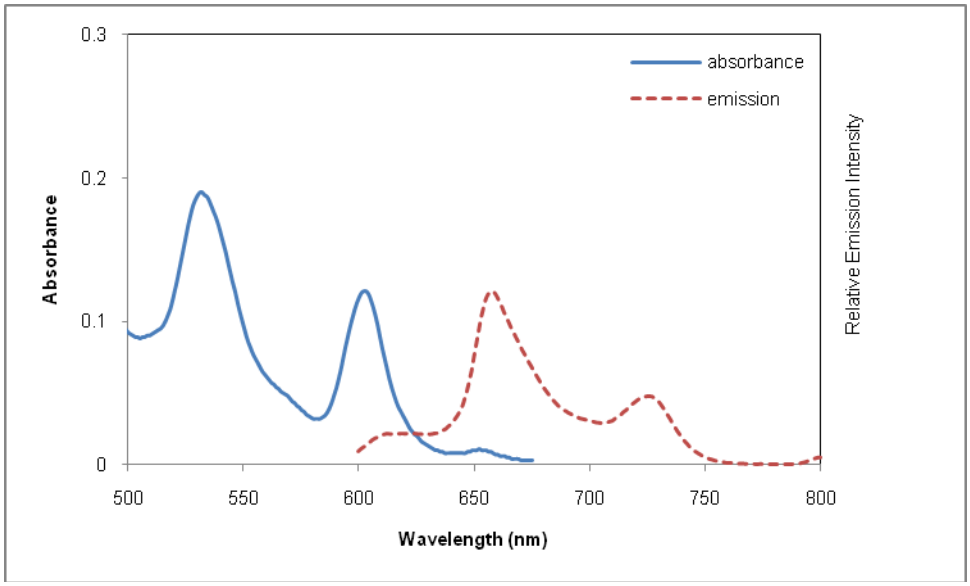
Absorbance and emission spectra of **8f**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 400 nm). Absorbance and emission spectra 1.02×10^{-5} M in CH_2Cl_2.



Absorbance and emission spectra of **8g**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 400 nm). Absorbance and emission spectra 1.01×10^{-5} M in CH_2Cl_2.



Absorbance and emission spectra of **8g**. Fluorescence spectra normalized to facilitate comparison (excitation λ = 400 nm). Absorbance and emission spectra 1.01×10^{-5} M in CH_2Cl_2.



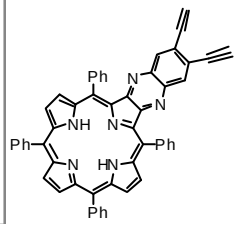


Table S1. Computed free energy (25 °C, gas phase, kcal/mol) difference between the singlet and triplet states for the cyclization transition states and diradical products. All values tabulated as singlet minus triplet.

Structure	Compound	transition state	diradical product
enediynes	**1**	-65.86	-1.69[a]
	2	n/a[b]	-1.83
	14	-50.38	-2.18
quinoxalenediynes	**8a**	-49.92	-2.17
	15	-52.14	-1.83
	16	-43.27	-1.39
[b]fused	**8c**	-41.11	-2.31
quinoxalenediynes	**8d**	-43.94	-2.21
	17	-36.01	-2.50

[a] If the sum correction[1,2] is applied here to account for triplet contamination in the broken-symmetry unrestricted wave function for the singlet diradical product, the singlet-triplet splitting becomes -3.86 kcal/mol, in excellent agreement with the experimental value of -3.8 ± 0.4 kcal/mol[3] and consistent with other DFT calculations for this quantity.[1] [b] A triplet geometry that was stable under optimization could not be obtained for this case.

Table S2. Computed free energies (25 °C, gas phase, kcal/mol) pertinent to the thermal reactivity of enediynes.

Structure	Compound	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}_{retro}$
enediynes	**1**	31.83	3.42	28.41
	2	32.62	11.57	21.05
	14	33.20	15.23	17.97
quinoxalenediynes	**8a**	32.94	14.62	18.32
	15	32.20	13.19	19.01
	16	31.95	7.74	24.21
[b]fused	**8c**	32.85	15.48	17.37
quinoxalenediynes	**8d**	32.87	15.23	17.64
	17	32.95	16.14	16.81

Table S3. Computed enthalpies (25 °C, kcal/mol) pertinent to the thermal reactivity of enediynes in solvent.

a) benzene

Structure	Compound	$\Delta H^{\ddagger}$	ΔH_{rxn}	$\Delta H^{\ddagger}_{retro}$
enediynes	**1**	29.97	1.92	28.05
	2	30.86	10.18	20.68
	14	31.68	13.90	17.78
quinoxalenediynes	**8a**	31.15	13.12	18.03
	15	30.59	11.72	18.87
	16	30.22	6.25	23.97
[b]fused	**8c**	31.48	14.04	17.44
quinoxalenediynes	**8d**	31.46	13.84	17.62
	17	31.54	14.68	16.86

b) isopropanol

Structure	Compound	$\Delta H^{\ddagger}$	ΔH_{rxn}	$\Delta H^{\ddagger}_{retro}$
enediynes	**1**	29.84	3.29	26.55
	2	30.82	11.48	19.34
	14	31.83	15.19	16.64
quinoxalenediynes	**8a**	31.07	14.21	16.86
	15	30.57	12.89	17.68
	16	30.19	7.49	22.70
[b]fused	**8c**	31.53	15.07	16.46
quinoxalenediynes	**8d**	31.48	15.16	16.32
	17	31.62	15.76	15.86

c) acetonitrile

Structure	Compound	$\Delta H^{\ddagger}$	ΔH_{rxn}	$\Delta H^{\ddagger}_{retro}$
enediynes	**1**	29.83	3.41	26.42
	2	30.82	11.59	19.23
	14	31.86	15.30	16.56
quinoxalenediynes	**8a**	31.07	14.31	16.76
	15	30.57	12.99	17.58
	16	30.22	7.64	22.58
[b]fused	**8c**	31.55	15.18	16.37
quinoxalenediynes	**8d**	31.48	15.03	16.45
	17	31.63	15.85	15.78

Table S4. Computed free energies (25 °C, kcal/mol) pertinent to the thermal reactivity of enediynes in solvent.

a) benzene

Structure	Compound	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}_{retro}$
enediynes	**1**	31.77	4.45	27.32
	2	32.65	12.56	20.09
	14	33.38	16.24	17.14
quinoxalenediynes	**8a**	32.94	15.47	17.47
	15	32.29	14.09	18.20
	16	31.93	8.61	23.32
[b]fused	**8c**	33.04	16.37	16.67
quinoxalenediynes	**8d**	33.06	16.18	16.88
	17	33.12	17.02	16.10

b) isopropanol

Structure	Compound	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}_{retro}$
enediynes	**1**	31.64	5.82	25.82
	2	32.60	13.86	18.74
	14	33.53	17.53	16.00
quinoxalenediynes	**8a**	32.86	16.56	16.30
	15	32.28	15.26	17.02
	16	31.90	9.84	22.06
[b]fused	**8c**	33.09	17.41	15.68
quinoxalenediynes	**8d**	33.07	17.50	15.57
	17	33.21	18.10	15.11

c) acetonitrile

Structure	Compound	$\Delta G^{\ddagger}$	ΔG_{rxn}	$\Delta G^{\ddagger}_{retro}$
enediynes	**1**	31.63	5.95	25.68
	2	32.61	13.98	18.63
	14	33.56	17.65	15.91
quinoxalenediynes	**8a**	32.86	16.66	16.20
	15	32.28	15.36	16.92
	16	31.94	9.99	21.95
[b]fused	**8c**	33.11	17.52	15.59
quinoxalenediynes	**8d**	33.08	17.37	15.71
	17	33.21	18.19	15.02

Table S5. Raw computational data used to calculate the thermodynamics of the cyclization reactions.

a) Compound **1**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-230.89560	-230.81856	-230.82266	-230.82805	-230.82851
singlet transition state	-230.84504	-230.77128	-230.77547	-230.78107	-230.78155
triplet transition state	-230.73637	-230.66393	-230.66774	-230.67272	-230.67313
singlet diradical product	-230.89591	-230.82736	-230.82981	-230.83302	-230.83328
triplet diradical product	-230.89246	-230.82390	-230.82620	-230.82921	-230.82945

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	44.847	4.454	77.023
singlet transition state	43.865	3.742	71.000
triplet transition state	42.337	3.712	73.584
singlet diradical product	47.073	3.308	68.533
triplet diradical product	47.270	3.320	70.807

b) Compound **2**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-384.56521	-384.44594	-384.45076	-384.45710	-384.45765
singlet transition state	-384.51363	-384.39818	-384.40295	-384.40936	-384.40990
triplet transition state[b]	-	-	-	-	-
singlet diradical product	-384.55215	-384.44127	-384.44450	-384.44877	-384.44914
triplet diradical product	-384.54848	-384.43744	-384.44056	-384.44471	-384.44505

[a] 6-31G(d,p) basis.
[b] A triplet geometry that was stable under optimization could not be obtained for this case.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	74.960	5.916	89.652
singlet transition state	74.171	5.175	83.660
triplet transition state[b]	-	-	-
singlet diradical product	77.043	4.820	81.650
triplet diradical product	77.245	4.829	83.940

c) Compound **14**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-538.22183	-538.06006	-538.06585	-538.07358	-538.07427
singlet transition state	-538.16938	-538.01209	-538.01758	-538.02507	-538.02571
triplet transition state	-538.08048	-537.92212	-537.92783	-537.93561	-537.93627
singlet diradical product	-538.20263	-538.04947	-538.05366	-538.05933	-538.05983
triplet diradical product	-538.19846	-538.04513	-538.04922	-538.05476	-538.05524

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	104.585	7.541	102.535
singlet transition state	103.899	6.800	96.808
triplet transition state	99.803	7.516	103.598
singlet diradical product	106.497	6.469	94.672
triplet diradical product	106.735	6.475	96.954

d) Compound **8a**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-570.29182	-570.11766	-570.12414	-570.13232	-570.13300
singlet transition state	-570.23974	-570.06955	-570.07604	-570.08434	-570.08503
triplet transition state	-570.15223	-569.98124	-569.98828	-569.99720	-569.99793
singlet diradical product	-570.27362	-570.10796	-570.11308	-570.11953	-570.12004
triplet diradical product	-570.26948	-570.10362	-570.10866	-570.11501	-570.11550

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	89.555	7.361	101.648
singlet transition state	88.766	6.624	95.667
triplet transition state	85.118	7.280	102.380
singlet diradical product	91.475	6.289	93.766
triplet diradical product	91.717	6.298	96.063

e) Compound **15**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-570.28897	-570.11508	-570.12168	-570.13009	-570.13080
singlet transition state	-570.23761	-570.06771	-570.07415	-570.08259	-570.08329
triplet transition state	-570.14642	-569.97562	-569.98341	-569.99371	-569.99457
singlet diradical product	-570.27297	-570.10728	-570.11244	-570.11898	-570.11953
triplet diradical product	-570.26945	-570.10350	-570.10860	-570.11504	-570.11558

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	89.477	7.345	101.635
singlet transition state	88.449	6.640	95.916
triplet transition state	84.605	7.299	102.292
singlet diradical product	91.319	6.280	93.675
triplet diradical product	91.615	6.284	95.936

f) Compound **16**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-570.29013	-570.11645	-570.12301	-570.13167	-570.13247
singlet transition state	-570.23964	-570.07009	-570.07668	-570.08539	-570.08614
triplet transition state	-570.16520	-569.99452	-570.00060	-570.00904	-570.00973
singlet diradical product	-570.28332	-570.11809	-570.12328	-570.12997	-570.13053
triplet diradical product	-570.28034	-570.11495	-570.12004	-570.12661	-570.12716

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	89.584	7.372	101.592
singlet transition state	88.875	6.631	95.842
triplet transition state	86.456	7.045	100.664
singlet diradical product	91.803	6.267	93.694
triplet diradical product	91.993	6.274	95.966

g) Compound **8c**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-877.61178	-877.35348	-877.36089	-877.37050	-877.37139
singlet transition state	-877.55963	-877.30580	-877.31291	-877.32244	-877.32330
triplet transition state	-877.48800	-877.23318	-877.24102	-877.25162	-877.25254
singlet diradical product	-877.59208	-877.34231	-877.34830	-877.35626	-877.35699
triplet diradical product	-877.58776	-877.33778	-877.34368	-877.35153	-877.35224

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	148.826	10.695	127.283
singlet transition state	148.122	9.961	122.041
triplet transition state	145.059	10.326	125.862
singlet diradical product	150.679	9.628	119.445
triplet diradical product	150.960	9.636	121.766

h) Compound **8d**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-1031.27419	-1030.97422	-1030.98204	-1030.99217	-1030.99322
singlet transition state	-1031.22208	-1030.92660	-1030.93412	-1030.94422	-1030.94526
triplet transition state	-1031.14520	-1030.84859	-1030.85688	-1030.86805	-1030.86921
singlet diradical product	-1031.25496	-1030.96361	-1030.96992	-1030.97794	-1030.97920
triplet diradical product	-1031.25077	-1030.95918	-1030.96540	-1030.97371	-1030.97433

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	178.612	12.426	140.543
singlet transition state	177.920	11.685	135.182
triplet transition state	174.460	12.164	139.628
singlet diradical product	180.504	11.353	132.703
triplet diradical product	180.766	11.361	135.018

i) Compound **17**

	E (gas phase, ccpvtz basis, a.u.)	E (gas phase, a.u.)[a]	E (benzene, a.u.)[a]	E (isopropanol, a.u.)[a]	E (acetonitrile, a.u.)[a]
enediyne	-723.94652	-723.73001	-723.73708	-723.74590	-723.74662
singlet transition state	-723.89426	-723.68228	-723.68907	-723.69774	-723.69847
triplet transition state	-723.83134	-723.61817	-723.62580	-723.63554	-723.63636
singlet diradical product	-723.92560	-723.71764	-723.72330	-723.73040	-723.73099
triplet diradical product	-723.92108	-723.71284	-723.71842	-723.72542	-723.72600

[a] 6-31G(d,p) basis.

	zero-point energy (kcal/mol)	H (thermal, 25°C, kcal/mol)	S (thermal, 25°C, cal/mol*K)
enediyne	119.015	9.027	114.467
singlet transition state	118.320	8.293	109.144
triplet transition state	115.546	8.579	112.471
singlet diradical product	120.751	7.965	106.604
triplet diradical product	121.105	7.974	108.944

Table S6. Number of imaginary frequencies for all stationary points identified through DFT computations. Imaginary frequencies (cm^{-1}) for the transition states are given in parentheses.

Structure	Compound	enediyne reactant	singlet transition state	triplet transition state	singlet diradical product	triplet diradical product
enediynes	**1**	0	1 (-1048.26)	1 (-591.35)	0	0
	2	0	1 (-989.84)	n/a[a]	0	0
	14	0	1 (-942.70)	1 (-637.62)	0	0
quinoxalenediynes	**8a**	0	1 (-978.33)	1 (-705.74)	0	0
	15	0	1 (-966.89)	1 (-812.44)	0	0
	16	0	1 (-980.56)	1 (-956.94)	0	0
[b]fused	**8c**	0	1 (-934.59)	1 (-769.18)	0	0
quinoxalenediynes	**8d**	0	1 (-938.04)	1 (-775.98)	0	0
	17	0	1 (-924.31)	1 (-965.79)	0	0

[a] A triplet geometry that was stable under optimization could not be obtained for this case.

References

(1) Graefenstein, J.; Hjerpe, A. M.; Kraka, E.; Cremer, D. *J. Phys. Chem. A* **2000**, *104*, 1748-1761.
(2) Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*; 2nd ed.; John Wiley & Sons, Ltd.: West Sussex, England, 2004.
(3) Wenthold, P. G.; Squires, R. R.; Lineberger, W. C. *J. Am. Chem. Soc.* **1998**, *120*, 5279-5290.

Cartesian coordinates of optimized geometries from DFT calculations

1 – enediyne

C	-3.686386	-0.429193	-0.018365
C	-3.431873	0.896951	-0.019014
C	-4.975451	-1.010981	-0.007388
C	-4.413944	1.914585	-0.009136
C	-6.058978	-1.548729	0.001134
C	-5.218901	2.817529	-0.000498
H	-7.020688	-2.005909	0.009411
H	-5.943062	3.598248	0.005828
H	-2.394809	1.220272	-0.028032
H	-2.842909	-1.113772	-0.026940

1 – singlet transition state

C	-0.364273	1.283225	0.000000
C	-0.583285	-1.433428	0.000000
C	-1.748747	-0.672767	0.000000
C	0.647432	-1.166893	0.000000
H	1.865012	0.996666	0.000000
H	1.663703	-1.508158	0.000000
H	-2.548007	1.304146	0.000000
H	-2.742620	-1.103765	0.000000
C	-1.636560	0.718592	0.000000
C	0.807345	0.821382	0.000000

1 – triplet transition state

H	1.686315	-2.241671	0.000000
C	1.185832	1.005134	0.000000
H	-2.441848	-1.084041	0.000000
H	-2.185501	1.286659	0.000000
H	2.244865	1.146733	0.000000
C	0.962557	-1.416760	0.000000
C	-0.378980	-1.651523	0.000000
C	-0.020697	1.292447	0.000000
C	-1.415960	-0.714329	0.000000
C	-1.280584	0.681350	0.000000

1 – singlet diradical product

H	-5.604871	1.250308	0.000000
H	-5.604391	-1.251135	0.000000
C	-2.224472	0.707051	0.000000
C	-4.666195	0.706595	0.000000
C	-4.665927	-0.707056	0.000000
C	-3.444944	-1.334518	0.000000
C	-2.224204	-0.706589	0.000000
C	-3.445457	1.334518	0.000000
H	-1.285530	-1.250299	0.000000
H	-1.286009	1.251125	0.000000

1 – triplet diradical product

H	-5.604983	1.264736	0.000000
H	-5.604500	-1.265563	0.000000
C	-2.213767	0.702179	0.000000
C	-4.676897	0.701714	0.000000
C	-4.676630	-0.702184	0.000000
C	-3.444946	-1.318604	0.000000
C	-2.213500	-0.701709	0.000000
C	-3.445454	1.318604	0.000000
H	-1.285419	-1.264732	0.000000
H	-1.285903	1.265558	0.000000

2– enediyne

C	-4.942331	-0.984078	0.000507
H	-7.066906	-1.791818	0.001821
C	-2.535903	-1.410726	0.003061
C	-4.376939	1.846513	-0.002854
C	-5.249820	2.681818	-0.006106
C	-1.221823	-0.965927	0.003755
C	-3.324919	0.886432	-0.000531
H	-6.028197	3.408431	-0.008011
C	-0.948889	0.400497	0.002351
C	-1.991262	1.315978	0.000245
C	-6.069119	-1.419983	0.001810
C	-3.602211	-0.501806	0.001029
H	-2.758569	-2.471246	0.004141
H	-1.789433	2.380660	-0.000884
H	0.076761	0.752348	0.002889
H	-0.410041	-1.684791	0.005376

2– singlet transition state

H	0.120710	2.575146	0.000094
C	0.031964	1.495705	0.000051
C	-0.197114	-1.284633	-0.000061
C	-1.332584	-0.491239	-0.000174
C	-1.218052	0.898855	-0.000120
H	4.522068	-1.536180	0.000488
C	2.510037	1.265128	0.000340
H	4.728678	0.971452	0.000581
C	1.208771	0.736357	0.000162
C	3.672488	0.784578	0.000459
C	2.285279	-1.462762	0.000228
C	3.510708	-1.178956	0.000381
C	1.088107	-0.728139	0.000102
H	-0.286241	-2.364043	-0.000108
H	-2.107996	1.518366	-0.000215
H	-2.311924	-0.956736	-0.000307

2– triplet transition state
(not stable under optimization)

2– singlet diradical product

C	-1.270418	0.726361	0.000018
C	-0.028257	-1.405328	-0.000054
C	-0.028257	1.405328	-0.000001
C	-2.524780	-1.342296	0.000007
C	-1.270418	-0.726361	-0.000007
C	1.153289	-0.705398	-0.000064
C	-2.524780	1.342296	0.000039
C	-3.725030	-0.719659	0.000054
C	-3.725030	0.719659	0.000059
C	1.153289	0.705398	-0.000035
H	-4.669445	-1.253219	0.000049
H	-4.669445	1.253219	0.000057
H	-0.031349	-2.489278	-0.000080
H	-0.031349	2.489278	0.000009
H	2.096289	1.241200	-0.000047
H	2.096289	-1.241200	-0.000102

2– triplet diradical product

C	-0.858784	-0.719217	0.001141
C	-2.095729	1.408162	-0.003545
C	-2.095866	-1.408289	0.012468
C	0.404848	1.327249	-0.018083
C	-0.858714	0.718883	-0.007036

C	-3.275730	0.706612	0.007516
C	0.404717	-1.327796	-0.002957
C	1.615353	0.713540	-0.021851
C	1.615282	-0.714287	-0.013681
C	-3.275802	-0.706546	0.015546
H	2.548320	1.268435	-0.030644
H	2.548195	-1.269338	-0.016101
H	-2.090248	2.492489	-0.009748
H	-2.090494	-2.492618	0.018603
H	-4.220112	1.240086	0.010137
H	-4.220234	-1.239864	0.024234

14– enediyne

C	-4.942394	-0.983169	-0.000003
H	-7.079089	-1.758300	0.002442
C	-2.550268	-1.412764	0.002721
C	-4.377190	1.845927	-0.002618
H	0.634514	1.908574	0.001887
H	2.481687	0.270838	0.007719
C	-5.264261	2.666180	-0.006507
C	-1.203555	-0.986223	0.003710
H	1.995575	-2.165423	0.009780
C	-0.122762	-1.903145	0.006359
C	-3.315995	0.896235	-0.000703
H	-6.052604	3.381921	-0.008492
C	-0.924134	0.412196	0.002471
C	0.425889	0.843549	0.003830
C	-2.003605	1.323443	0.000454
C	-6.076401	-1.399996	0.002539
H	-0.339424	-2.966587	0.006539
C	1.174716	-1.454912	0.008016
C	-3.597763	-0.514078	0.000676
C	1.451229	-0.069207	0.006784
H	-2.768412	-2.475168	0.003619
H	-1.796754	2.388108	-0.000222

14– singlet transition state

C	-2.367763	1.698541	-0.000092
C	-2.597670	-1.092000	-0.000184
H	0.177669	2.576439	0.000139
H	-4.500122	1.716228	-0.000265
C	0.095208	1.495767	0.000106
C	-0.134724	-1.295064	0.000013
C	-1.304912	-0.509613	-0.000062
C	-1.187752	0.912426	-0.000017
H	4.562841	-1.517619	0.000406
C	2.560878	1.265082	0.000308
H	4.765855	0.946491	0.000480
C	1.257414	0.750346	0.000181
H	-4.704172	-0.760453	-0.000345
C	3.710936	0.746754	0.000411
C	-3.604023	1.105247	-0.000207
C	2.335454	-1.471035	0.000210
C	3.554837	-1.147921	0.000347
C	1.133811	-0.749907	0.000129
H	-0.230242	-2.374660	-0.000030
C	-3.720160	-0.304371	-0.000254
H	-2.274903	2.780004	-0.000057
H	-2.683062	-2.174079	-0.000219

14– triplet transition state

C	-2.332081	1.877760	-0.007303
C	-2.688780	-0.886234	0.005094
H	0.264465	2.631581	-0.004409
H	-4.498503	2.004652	-0.025059
C	0.110654	1.560010	0.023944
C	-0.247648	-1.219168	0.028085
C	-1.393768	-0.378333	0.018625
C	-1.203113	1.048750	0.013275
H	4.470597	-1.719906	-0.030739
C	2.589826	1.178652	0.020039
H	4.806276	0.793035	0.014422
C	1.284181	0.712407	0.056140
H	-4.820504	-0.449915	-0.013518
C	3.743392	0.672938	-0.057834
C	-3.646341	1.334368	-0.013308
C	2.232624	-1.512804	0.009827
C	3.474169	-1.326590	-0.067391
C	1.088493	-0.714805	0.054823
H	-0.384345	-2.293218	0.000405
C	-3.825010	-0.020955	-0.007006
H	-2.195241	2.954089	-0.018470
H	-2.835143	-1.961511	0.003159

14– singlet diradical product

C	-0.855709	-0.733312	0.001072
C	-5.721903	-0.710416	0.029940
C	-2.076688	1.406438	-0.003756
C	-5.721829	0.710905	0.022021
C	-2.076829	-1.406570	0.012143
C	0.408731	1.347306	-0.018312
C	-0.855637	0.732981	-0.007242
C	-3.293681	0.719240	0.007415
C	0.408603	-1.347855	-0.002787
C	-4.544321	-1.402711	0.026826
C	-4.544174	1.402997	0.011063
C	1.602100	0.724685	-0.021831
C	1.602033	-0.725431	-0.013431
C	-3.293755	-0.719165	0.015481
H	2.548161	1.255299	-0.030617

H	2.548044	-1.256202	-0.015647
H	-2.076172	2.491390	-0.009779
H	-2.076423	-2.491520	0.018349
H	-4.541076	2.488526	0.004910
H	-4.541330	-2.488238	0.032838
H	-6.666509	1.243900	0.024556
H	-6.666638	-1.243244	0.038790

14– triplet diradical product

C	-0.862693	-0.725107	0.001337
C	-5.723189	-0.710527	0.029816
C	-2.078631	1.409325	-0.003860
C	-5.723115	0.711017	0.021887
C	-2.078771	-1.409465	0.012607
C	0.411105	1.332462	-0.018071
C	-0.862629	0.724769	-0.007133
C	-3.294075	0.720708	0.007450
C	0.410982	-1.333010	-0.002990
C	-4.546002	-1.402981	0.027017
C	-4.545857	1.403270	0.011028
C	1.614439	0.718346	-0.021718
C	1.614373	-0.719089	-0.013998
C	-3.294148	-0.720635	0.015860
H	2.548438	1.271868	-0.029589
H	2.548309	-1.272763	-0.017035
H	-2.074878	2.494648	-0.010185
H	-2.075128	-2.494788	0.018824
H	-4.544034	2.488792	0.004887
H	-4.544298	-2.488498	0.033202
H	-6.667531	1.244666	0.024535
H	-6.667664	-1.244008	0.038130

8a– enediyne

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

8a– singlet 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

8a – triplet transition state

N	-2.295247	1.906456	0.000940
N	-2.645175	-0.917681	0.001097
H	0.188665	2.646996	-0.001207
H	-4.371975	1.992500	0.001833
C	0.059577	1.572489	-0.000307
C	-0.282064	-1.214207	0.002466
C	-1.443199	-0.365098	0.001366
C	-1.255972	1.059237	0.000840
H	4.431923	-1.725645	0.001318
C	2.540560	1.186057	-0.002634
H	4.762803	0.797432	-0.004050
C	1.242277	0.716804	-0.000371
H	-4.686215	-0.477990	0.000232
C	3.698052	0.672081	-0.004398
C	-3.518475	1.321540	0.001334
C	2.192387	-1.509495	-0.000349
C	3.435349	-1.331619	-0.002765
C	1.042936	-0.713360	0.001001
H	-0.452203	-2.283177	0.004106
C	-3.694003	-0.039323	0.000549

8a – singlet diradical product

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

8a – triplet diradical product

C	3.756599	0.714687	0.002235
C	1.279525	0.723828	0.000608
C	1.278372	-0.728730	0.003562
C	2.551934	-1.336091	0.005607
C	2.553961	1.329321	0.000206
C	3.755431	-0.723211	0.004888
H	4.688923	-1.277118	0.006553
H	4.690830	1.267311	0.002143
C	-3.409577	-0.713271	0.000429
C	-3.408439	0.715931	-0.002696
C	-1.138806	0.718238	-0.001164
C	-1.139949	-0.719196	0.002030
C	0.065660	-1.419195	0.004295
C	0.067939	1.416286	-0.001832
H	-4.355122	-1.251116	0.001012
H	-4.353123	1.255279	-0.004483
H	0.039933	-2.502557	0.006588
H	0.043992	2.499687	-0.004229
N	-2.312907	1.422026	-0.003504

N	-2.315176	-1.421111	0.002752

15 – enediyne

C	1.538497	-2.715738	0.515294
C	1.538410	-4.074895	0.908845
C	2.709836	-4.788356	0.966335
C	3.931601	-4.161128	0.629233
C	3.931691	-2.792520	0.232980
C	2.710013	-2.082072	0.182746
N	5.081961	-2.158931	-0.096753
N	5.081763	-4.873058	0.688917
C	6.195044	-2.860051	-0.035348
C	6.194908	-4.247781	0.366072
C	7.420891	-2.213663	-0.378087
C	7.420555	-4.977692	0.420927
C	8.460194	-1.671055	-0.665220
C	8.459087	-5.591485	0.462534
H	0.600519	-2.172732	0.477424
H	0.600370	-4.554010	1.166959
H	9.376873	-1.191524	-0.919102
H	9.375142	-6.133774	0.500888
H	2.739265	-5.829974	1.264169
H	2.739579	-1.042463	-0.122013

15 – singlet transition state

C	-2.290696	1.700855	-0.000142
C	-2.522020	-1.106900	-0.000146
H	-4.422573	1.706445	-0.000694
N	0.088719	1.503953	0.000590
N	-0.142464	-1.302080	0.000420
C	-1.238120	-0.512581	0.000164
C	-1.121376	0.904420	0.000178
H	4.481435	-1.512196	-0.000366
C	2.484469	1.291296	0.000993
H	4.684659	0.954465	-0.000331
C	1.174128	0.768726	0.000779
H	-4.626068	-0.763498	-0.000662
C	3.627729	0.766045	0.000386
C	-3.524005	1.099314	-0.000435
C	2.255785	-1.484391	0.000520
C	3.469595	-1.153335	0.000129
C	1.048640	-0.754411	0.000607
C	-3.640250	-0.311618	-0.000441
H	-2.172232	2.778067	-0.000117
H	-2.581455	-2.188976	-0.000131

15 – triplet transition state

C	-2.257323	1.873849	-0.000661
C	-2.594301	-0.899291	0.002847
H	-4.424113	1.998830	0.000528
N	0.096969	1.587009	-0.002490
N	-0.248021	-1.250653	0.001469
C	-1.297443	-0.394553	0.001176
C	-1.104875	1.032460	-0.000686
H	4.386256	-1.708428	0.000604
C	2.494420	1.202002	-0.002107
H	4.710765	0.809512	-0.003983
C	1.188241	0.725996	-0.002066
H	-4.737403	-0.458742	0.002891
C	3.646491	0.681186	-0.001570
C	-3.571870	1.329322	0.000822
C	2.149217	-1.518504	-0.000803
C	3.387935	-1.318781	-0.000493

C	0.989003	-0.716356	-0.000795
C	-3.745451	-0.022696	0.002283
H	-2.090331	2.944718	-0.001972
H	-2.720466	-1.975882	0.004906

15 – singlet diradical product

C	3.698832	0.720315	0.002039
C	1.248346	0.734650	0.000560
C	1.247186	-0.739307	0.003582
C	2.511062	-1.364017	0.005798
C	2.513201	1.357375	-0.000055
C	3.697692	-0.728822	0.005245
H	4.645031	-1.257384	0.006955
H	4.646991	1.247405	0.001517
C	-3.451303	-0.710419	0.000335
C	-3.450184	0.713135	-0.002671
C	-1.033472	0.718590	-0.001035
C	-1.034603	-0.719667	0.002019
N	0.104259	-1.421719	0.004271
N	0.106491	1.418855	-0.001711
H	-4.398841	-1.237989	0.000802
H	-4.396891	1.242193	-0.004442
C	-2.276032	1.412411	-0.003345
C	-2.278251	-1.411537	0.002622
H	-2.248196	2.495748	-0.005614
H	-2.252119	-2.494915	0.004928

15 – triplet diradical product

C	3.708741	0.715040	0.002116
C	1.240934	0.725251	0.000491
C	1.239797	-0.729901	0.003558
C	2.510261	-1.347697	0.005696
C	2.512362	1.341069	0.000013
C	3.707615	-0.723534	0.005147
H	4.644324	-1.272424	0.006943
H	4.646306	1.262467	0.001607
C	-3.451711	-0.710934	0.000371
C	-3.450596	0.713614	-0.002654
C	-1.032690	0.720448	-0.001058
C	-1.033817	-0.721543	0.002009
N	0.102293	-1.426462	0.004273
N	0.104524	1.423590	-0.001773
H	-4.399444	-1.238179	0.000863
H	-4.397503	1.242340	-0.004412
C	-2.277360	1.412719	-0.003355
C	-2.279571	-1.411870	0.002645
H	-2.249831	2.496069	-0.005639
H	-2.253733	-2.495262	0.004959

16 – enediyne

N	2.622929	-4.724889	1.022908
C	3.808896	-4.156385	0.687900
C	3.830011	-2.804051	0.273380
C	5.015259	-2.213151	-0.067354
C	5.023634	-4.896203	0.746855
C	6.241982	-2.930999	-0.016721
C	6.257088	-4.269631	0.386884
C	7.442228	-2.260623	-0.382749
C	7.469330	-5.006336	0.446496
C	8.441374	-1.659107	-0.698529
C	8.508560	-5.620181	0.488483
H	5.044624	-1.177821	-0.385133
N	5.032438	-6.192688	1.140115

H	9.329470	-1.141011	-0.976234
H	9.424173	-6.162366	0.527430
C	2.663718	-5.980977	1.399371
C	3.872648	-6.716127	1.457837
H	1.722915	-6.452756	1.671621
H	3.864823	-7.755889	1.775313
H	2.889600	-2.267011	0.238827

16 – singlet transition state

N	-2.605757	-1.084366	-0.000194
H	0.091918	2.536749	-0.000112
C	-0.003064	1.458208	0.000183
C	-0.199138	-1.346841	0.000514
C	-1.365093	-0.534538	0.000092
C	-1.238670	0.875551	-0.000116
H	4.527659	-1.534427	0.000036
C	2.482961	1.251648	0.000687
H	4.696829	0.937952	-0.000539
C	1.197048	0.695474	0.000707
C	3.640246	0.747724	0.000214
C	2.291328	-1.474975	0.001091
C	3.514802	-1.181322	0.000458
C	1.097999	-0.753946	0.000964
N	-0.290955	-2.700678	0.000540
C	-2.663509	-2.394973	-0.000142
C	-1.502324	-3.204137	0.000179
H	-3.649879	-2.852606	-0.000321
H	-1.590535	-4.287927	0.000121
H	-2.147567	1.465330	-0.000562

16 – triplet transition state

N	-2.653554	-0.884339	0.024471
H	0.209475	2.603125	0.271132
C	0.079901	1.527332	0.232537
C	-0.289389	-1.322931	-0.042400
C	-1.394419	-0.434501	0.075007
C	-1.175343	0.981786	0.264560
H	4.357930	-1.584568	0.900566
C	2.490805	1.133940	-0.305891
H	4.592769	0.751370	-0.994295
C	1.219401	0.717055	0.035066
C	3.659859	0.685846	-0.468400
C	2.192431	-1.484322	0.327525
C	3.448676	-1.312866	0.397669
C	1.046099	-0.785460	0.083435
N	-0.464853	-2.641396	-0.190598
C	-2.809290	-2.196204	-0.146219
C	-1.724475	-3.065674	-0.249811
H	-3.828264	-2.569884	-0.191891
H	-1.878161	-4.133812	-0.375295
H	-2.058997	1.599205	0.373233

16 – singlet diradical product

C	3.737121	0.704718	0.002253
C	1.284325	0.681419	0.000623
C	1.307339	-0.758093	0.003539
C	2.555834	-1.365519	0.005574
C	2.522689	1.314699	0.000207
C	3.754265	-0.723588	0.005095
H	4.702277	-1.250797	0.006806
H	4.671753	1.255363	0.001777
C	-1.149418	0.682129	-0.001013
C	-1.164168	-0.747290	0.001843

C	0.055799	-1.470570	0.004124
C	0.024503	1.365122	-0.001596
N	0.071497	-2.818966	0.006844
H	0.035304	2.448944	-0.003761
N	-2.355293	-1.386103	0.002327
C	-2.314355	-2.702776	0.005012
C	-1.101819	-3.418768	0.007263
H	-1.105679	-4.505942	0.009440
H	-3.264248	-3.231788	0.005422
H	-2.107327	1.188906	-0.002675

16 – triplet diradical product

C	3.748763	0.700469	0.002291
C	1.278173	0.677206	0.000583
C	1.301311	-0.750623	0.003426
C	2.557262	-1.351568	0.005519
C	2.525057	1.301990	0.000225
C	3.765444	-0.718137	0.005136
H	4.703470	-1.264308	0.006884
H	4.673036	1.269659	0.001806
C	-1.150341	0.685428	-0.001164
C	-1.165107	-0.745918	0.001660
C	0.053958	-1.470846	0.003966
C	0.022782	1.369610	-0.001683
N	0.070992	-2.817954	0.006651
H	0.035796	2.453791	-0.003823
N	-2.355929	-1.384362	0.002081
C	-2.314681	-2.701580	0.004729
C	-1.102808	-3.418013	0.007012
H	-3.264651	-3.230428	0.005095
H	-1.107185	-4.505159	0.009158
H	-2.109242	1.190443	-0.002852

8c – enediyne

C	5.050431	-2.106746	0.615166
C	2.690286	-1.624129	0.877876
C	3.927279	-1.219488	0.505343
C	2.446452	-2.945760	1.394831
C	3.520144	-3.859227	1.523202
C	4.853605	-3.439061	1.127460
C	7.079423	-3.855875	0.866392
C	7.273031	-2.532596	0.357857
C	8.572456	-2.124361	-0.027512
C	8.191058	-4.724819	0.972164
C	9.646839	-2.978881	0.080070
C	9.450738	-4.316093	0.593804
C	1.156417	-3.352922	1.777942
C	3.279487	-5.146421	2.027201
C	0.936253	-4.623856	2.272370
C	10.944964	-2.546742	-0.313129
C	10.555158	-5.206717	0.708202
C	12.039667	-2.161311	-0.648199
C	11.480935	-5.976247	0.808467
C	2.003095	-5.524379	2.397358
H	1.845874	-0.947345	0.791839
H	4.118304	-0.226650	0.115476
H	8.699727	-1.119259	-0.410148
H	8.026438	-5.722819	1.359120
H	0.332814	-2.652777	1.679724
H	4.117647	-5.827120	2.115875
H	-0.063779	-4.925687	2.564441
H	13.006915	-1.828520	-0.944450
H	12.302405	-6.648185	0.896497
H	1.825693	-6.521233	2.785990

N	5.863966	-4.288047	1.244717
N	6.248278	-1.671726	0.239051

8c – singlet transition state

N	0.143142	1.913136	0.000435
N	-0.385775	-0.865775	0.000472
H	2.646606	2.535046	0.000756
C	-2.192370	2.366469	0.000096
C	2.479061	1.465705	0.000788
C	1.952071	-1.306805	0.000843
C	0.875057	-0.393874	0.000647
C	1.141703	1.011294	0.000626
H	6.595339	-2.009744	0.001042
C	4.899900	0.968195	0.000991
H	7.056949	0.419517	0.000950
C	3.548807	0.598367	0.000985
C	-2.745893	-0.438624	0.000089
C	5.986917	0.327920	0.001162
C	-1.096264	1.438727	0.000269
C	4.386980	-1.731690	0.001079
C	5.632991	-1.532996	0.001249
C	3.265707	-0.891996	0.001020
H	1.717431	-2.363471	0.000856
C	-1.367065	0.022026	0.000281
C	-3.789097	0.517923	-0.000087
C	-3.471035	1.922868	-0.000074
C	-5.122131	0.071853	-0.000271
C	-5.413634	-1.278718	-0.000281
C	-4.376813	-2.221512	-0.000107
C	-3.058736	-1.806120	0.000077
H	-1.946311	3.421786	0.000106
H	-4.294066	2.630780	-0.000207
H	-5.922346	0.805224	-0.000404
H	-6.446483	-1.609888	-0.000424
H	-4.609703	-3.280753	-0.000118
H	-2.242707	-2.518748	0.000212

8c – triplet transition state

N	-0.164145	1.925812	-0.000004
N	0.398691	-0.888996	0.000234
H	-2.656038	2.526673	-0.000353
C	2.186357	2.336472	0.000018
C	-2.482232	1.457976	0.000057
C	-1.937138	-1.286874	0.000356
C	-0.869698	-0.402004	0.000288
C	-1.136917	1.017946	0.000166
H	-6.624953	-2.038279	0.000104
C	-4.921957	0.960901	0.000118
H	-7.110149	0.452565	-0.000006
C	-3.577865	0.571610	0.000538
C	2.752827	-0.427883	0.000232
C	-6.040206	0.388153	-0.000244
C	1.125910	1.422611	0.000082
C	-4.399601	-1.714061	0.000394
C	-5.655685	-1.579442	-0.000814
C	-3.306440	-0.856787	0.000588
H	-1.721619	-2.347930	0.000224
C	1.389435	0.027995	0.000194
C	3.504128	1.905393	0.000076
C	3.815097	0.529956	0.000181
C	5.156158	0.066685	0.000231
C	5.433470	-1.276257	0.000322
C	4.379382	-2.217685	0.000368
C	3.068172	-1.802398	0.000326
H	1.939100	3.392074	-0.000080
H	4.312424	2.629252	0.000033
H	5.959113	0.797041	0.000194

H	6.461976	-1.620420	0.000359
H	4.609725	-3.277724	0.000439
H	2.249415	-2.511439	0.000363

8c – singlet diradical product

C	0.794806	1.317371	-0.007951
C	0.869202	-0.118631	-0.002177
C	2.118449	-0.751822	-0.005719
C	3.295753	-0.011056	-0.015436
C	3.219908	1.460776	-0.021527
C	1.972683	2.076000	-0.017443
N	-0.399809	1.954458	-0.003670
C	-1.484028	1.201230	0.004499
C	-1.411182	-0.246077	0.009421
N	-0.254305	-0.875034	0.006515
C	-2.772847	1.840495	0.008775
C	-3.907948	1.105983	0.017340
C	-3.884144	-0.336711	0.021991
C	-2.645345	-1.019071	0.017666
C	-5.073467	-1.083569	0.030079
C	-5.038530	-2.465959	0.033956
C	-3.809501	-3.136686	0.029838
C	-2.626288	-2.420691	0.021656
C	4.591962	-0.557371	-0.020699
C	5.750257	0.125942	-0.029919
C	5.675502	1.577152	-0.035538
C	4.453083	2.137651	-0.031337
H	6.594150	2.153665	-0.042509
H	6.723403	-0.352864	-0.033528
H	-2.784849	2.924065	0.004636
H	-4.875876	1.597666	0.020556
H	-6.024291	-0.559962	0.033100
H	-5.964350	-3.031040	0.040352
H	-3.784963	-4.220964	0.032685
H	-1.664916	-2.920300	0.018284
H	1.889204	3.156100	-0.021603
H	2.148277	-1.834745	-0.001293

8c – triplet diradical product

C	0.795185	1.318494	-0.007777
C	0.869766	-0.119782	-0.001867
C	2.117107	-0.754088	-0.005512
C	3.288265	-0.002428	-0.015420
C	3.213238	1.451627	-0.021322
C	1.970907	2.078167	-0.017307
N	-0.401542	1.954587	-0.003642
C	-1.484349	1.201709	0.004428
C	-1.411562	-0.246827	0.009501
N	-0.255769	-0.875679	0.007110
C	-2.774027	1.840611	0.008602
C	-3.908616	1.106053	0.017032
C	-3.884873	-0.337172	0.021825
C	-2.646421	-1.019644	0.017674
C	-5.074172	-1.083575	0.030100
C	-5.039536	-2.466148	0.034093
C	-3.810850	-3.137013	0.029835
C	-2.627444	-2.421026	0.021606
C	4.594004	-0.541709	-0.021042
C	5.762386	0.133066	-0.030343
C	5.688153	1.571968	-0.035437
C	4.456480	2.122734	-0.031050
H	6.593551	2.170718	-0.042164
H	6.724716	-0.369087	-0.034390
H	-2.785881	2.924199	0.004532

H	-4.876761	1.597339	0.019988
H	-6.024930	-0.559834	0.033150
H	-5.965507	-3.030989	0.040721
H	-3.786489	-4.221299	0.032584
H	-1.666028	-2.920568	0.018205
H	1.890629	3.158851	-0.021587
H	2.150371	-1.837256	-0.001129

8d – enediyne

C	5.045650	-2.054909	0.597591
C	2.623164	-1.553102	0.864529
C	3.917314	-1.138534	0.478074
C	2.409995	-2.907757	1.387713
C	3.497974	-3.800717	1.506294
C	4.836882	-3.380046	1.109398
C	7.062450	-3.822646	0.857530
C	7.269801	-2.506212	0.349101
C	8.570691	-2.108267	-0.032656
C	8.162047	-4.702901	0.969384
C	9.638219	-2.973766	0.079973
C	9.428315	-4.306308	0.594360
C	1.141991	-3.365044	1.784631
C	3.298716	-5.096383	2.005837
C	0.957680	-4.644735	2.275713
C	10.941268	-2.553779	-0.309830
C	10.523155	-5.208068	0.714549
C	12.040611	-2.180061	-0.643111
C	11.440495	-5.986806	0.821075
C	2.041531	-5.519702	2.388627
H	8.709702	-1.105198	-0.416532
H	7.986262	-5.698584	1.357389
H	0.281375	-2.712520	1.710056
H	4.160395	-5.748398	2.080032
H	-0.034787	-4.965832	2.573228
H	13.012596	-1.858485	-0.936266
H	12.254596	-6.667088	0.913604
H	1.897286	-6.523085	2.773630
N	5.836965	-4.236420	1.231081
N	6.245753	-1.640530	0.228501
C	1.572446	-0.629733	0.728262
C	4.125714	0.155016	-0.022433
C	1.790699	0.643460	0.234039
H	0.565461	-0.906678	1.013430
H	5.133680	0.431316	-0.306705
C	3.075249	1.042146	-0.144924
H	0.957557	1.331963	0.142181
H	3.246501	2.040393	-0.532257

8d – singlet transition state

N	0.142173	1.946080	0.000483
N	-0.410809	-0.811214	0.000221
H	2.658102	2.549517	0.001002
C	-2.198248	2.452654	0.000062
C	2.478158	1.482187	0.000884
C	1.923405	-1.283940	0.000569
C	0.859234	-0.359036	0.000453
C	1.139642	1.039147	0.000602
H	6.560505	-2.035788	0.001379
C	4.894712	0.959830	0.001299
H	7.046571	0.387849	0.001660
C	3.540250	0.602553	0.001013
C	-2.765574	-0.376157	-0.000046
C	5.975569	0.309282	0.001454
C	-1.098750	1.493786	0.000242

C	4.354500	-1.733790	0.000981
C	5.602621	-1.550324	0.001236
C	3.242546	-0.881868	0.000839
H	1.677875	-2.338117	0.000449
C	-1.381366	0.084597	0.000125
C	-3.824366	0.558777	-0.000063
C	-3.535671	1.998287	-0.000085
C	-5.137873	0.059322	-0.000029
C	-5.393179	-1.299991	-0.000133
C	-4.337608	-2.215616	-0.000230
C	-3.036903	-1.752391	-0.000154
H	-5.978321	0.741571	0.000164
H	-6.419282	-1.651752	-0.000124
H	-4.537349	-3.281427	-0.000312
H	-2.195292	-2.434168	-0.000158
C	-4.554993	2.965573	-0.000340
C	-1.917920	3.827112	0.000032
C	-4.266439	4.318239	-0.000301
H	-5.593516	2.660151	-0.000623
H	-0.878497	4.131625	0.000121
C	-2.939413	4.756059	-0.000146
H	-5.077585	5.038422	-0.000443
H	-2.712708	5.816462	-0.000186

8d – triplet transition state

N	-0.156408	1.952374	0.000011
N	0.415670	-0.834703	0.000361
H	-2.664712	2.537421	-0.000157
C	2.203200	2.429066	0.000003
C	-2.476461	1.471267	-0.000058
C	-1.913677	-1.271804	0.000265
C	-0.843901	-0.369970	0.000221
C	-1.125611	1.044375	0.000047
H	-6.600030	-2.060969	0.000100
C	-4.915575	0.948804	-0.000116
H	-7.101015	0.419459	-0.000226
C	-3.572354	0.567933	-0.000049
C	2.774732	-0.366532	0.000346
C	-6.030419	0.367569	-0.000065
C	1.134377	1.471500	0.000096
C	-4.375580	-1.718119	0.000170
C	-5.632667	-1.598485	0.000150
C	-3.291538	-0.851163	0.000112
H	-1.687939	-2.330584	0.000419
C	1.408596	0.099718	0.000291
C	3.557500	1.988439	0.000114
C	3.846465	0.565972	0.000135
C	5.162085	0.058499	-0.000071
C	5.409022	-1.297489	0.000104
C	4.343186	-2.210973	0.000453
C	3.046769	-1.749125	0.000530
H	6.004010	0.739288	-0.000480
H	6.432323	-1.657287	-0.000060
H	4.541654	-3.277301	0.000608
H	2.203674	-2.428469	0.000708
C	4.568310	2.969889	0.000287
C	1.913890	3.811724	-0.000185
C	4.265187	4.315027	0.000049
H	5.609520	2.673047	0.000519
C	2.926401	4.741376	-0.000152
H	0.872522	4.107471	-0.000106
H	5.066822	5.045773	0.000148
H	2.694071	5.800783	-0.000323

8d – singlet diradical product

C	0.785893	1.344425	-0.008373
C	0.845268	-0.089878	-0.003576
C	2.085027	-0.737222	-0.007611
C	3.271204	-0.007504	-0.016292
C	3.210327	1.462813	-0.021239
C	1.967873	2.092010	-0.017113
N	-0.407882	1.986512	-0.004535
C	-1.499888	1.254292	0.003659
C	-1.440180	-0.189045	0.008452
N	-0.291285	-0.828468	0.004856
C	-2.798625	1.922778	0.008030
C	-3.989144	1.163761	0.016855
C	-3.928398	-0.304582	0.021652
C	-2.679133	-0.962642	0.017515
C	-5.086320	-1.099613	0.030377
C	-5.013702	-2.481331	0.034801
C	-3.772248	-3.121564	0.030629
C	-2.617705	-2.363500	0.022059
C	4.561318	-0.567385	-0.020876
C	5.727080	0.104361	-0.029255
C	5.667047	1.554258	-0.034151
C	4.449742	2.127379	-0.029968
H	6.590718	2.122739	-0.040914
H	6.694585	-0.385851	-0.032445
H	-6.064226	-0.635293	0.033794
H	-5.927942	-3.065071	0.041533
H	-3.714270	-4.204368	0.034080
H	-1.638545	-2.826580	0.018629
H	1.896931	3.172985	-0.020605
H	2.103710	-1.820361	-0.003833
C	-5.209187	1.860529	0.020811
C	-2.853108	3.323937	0.003416
C	-5.250768	3.243680	0.016464
H	-6.145315	1.316901	0.027507
H	-1.915431	3.866092	-0.004058
C	-4.066282	3.984035	0.007724
H	-6.209893	3.750332	0.019813
H	-4.098045	5.067939	0.004390

8d – triplet diradical product

C	0.786158	1.345570	-0.008446
C	0.845711	-0.091009	-0.003632
C	2.083538	-0.739501	-0.007635
C	3.264051	0.000872	-0.016301
C	3.203808	1.454088	-0.021174
C	1.966065	2.094253	-0.017138
N	-0.409553	1.986650	-0.004622
C	-1.500566	1.254847	0.003542
C	-1.440691	-0.189766	0.008370
N	-0.292852	-0.828804	0.004800
C	-2.799820	1.922923	0.007823
C	-3.990088	1.163762	0.016629
C	-3.929334	-0.304867	0.021522
C	-2.680174	-0.963080	0.017456
C	-5.087252	-1.099975	0.030269
C	-5.014690	-2.481740	0.034793
C	-3.773360	-3.121958	0.030706
C	-2.618799	-2.363845	0.022106
C	4.563479	-0.551988	-0.020967
C	5.739368	0.111087	-0.029332
C	5.679758	1.549042	-0.034147
C	4.453021	2.112558	-0.029894
H	6.590787	2.139194	-0.040886

H	6.696118	-0.401668	-0.032391
H	-6.065106	-0.635689	0.033626
H	-5.928926	-3.065483	0.041544
H	-3.715364	-4.204767	0.034245
H	-1.639646	-2.826934	0.018734
H	1.898422	3.175781	-0.020646
H	2.105647	-1.822917	-0.003887
C	-5.209933	1.860412	0.020437
C	-2.854417	3.323983	0.003165
C	-5.251880	3.243536	0.015746
H	-6.146002	1.316807	0.027013
H	-1.916861	3.866325	-0.002861
C	-4.067636	3.984143	0.007343
H	-6.211197	3.749829	0.019132
H	-4.099384	5.068025	0.003658

17 – enediyne

C	1.066591	-1.457592	-0.001328
C	3.437938	-1.930014	-0.002361
C	2.149564	-2.382658	-0.001638
C	3.720900	-0.533593	-0.002195
C	2.711436	0.385705	-0.002053
C	1.353385	-0.043471	-0.001774
C	-0.876852	0.405836	-0.001155
C	-1.162519	-1.003388	-0.000616
C	-2.515796	-1.432338	-0.000067
C	-1.956479	1.327704	-0.001023
C	-3.548774	-0.526231	0.000178
C	-3.260705	0.895197	-0.000534
C	-4.897942	-0.979607	0.001022
C	-4.326964	1.837990	-0.000635
C	-6.037289	-1.381021	0.004762
C	-5.220405	2.651013	-0.002952
H	4.260950	-2.636165	-0.003127
H	1.906372	-3.438837	-0.001588
H	-2.711878	-2.497338	0.000235
H	-1.722506	2.385038	-0.001389
H	-7.044242	-1.727800	0.005914
H	-6.013143	3.362183	-0.003585
N	0.377281	0.869100	-0.001777
N	-0.187623	-1.918200	-0.000766
H	4.754627	-0.204876	-0.002948
H	2.899072	1.453362	-0.002602

17 – singlet transition state

N	0.146909	1.925565	0.000402
N	-0.390300	-0.865995	0.000431
H	2.646722	2.537931	0.000677
C	-2.194860	2.367441	0.000115
C	2.476775	1.468998	0.000693
C	1.942613	-1.306733	0.000722
C	0.860862	-0.391235	0.000563
C	1.132508	1.020363	0.000547
H	6.580753	-2.017964	0.001319
C	4.894306	0.965035	0.001006
H	7.047616	0.408053	0.001294
C	3.541570	0.601044	0.000851
C	-2.728873	-0.407205	0.000145
C	5.977339	0.317137	0.001162
C	-1.101915	1.453179	0.000272
C	4.374520	-1.735995	0.001034
C	5.620659	-1.536323	0.001182
C	3.253489	-0.895952	0.000867
H	1.703703	-2.362395	0.000730

C	-1.374601	0.036133	0.000287
C	-3.747242	0.501846	-0.000002
C	-3.477875	1.901346	-0.000017
H	-4.777327	0.162427	-0.000110
H	-2.906854	-1.476272	0.000160
H	-1.963319	3.426198	0.000106
H	-4.308378	2.598874	-0.000137

17 – triplet transition state

N	-0.153479	1.945180	0.000003
N	0.392519	-0.890529	0.000252
H	-2.647077	2.524381	-0.000052
C	2.193664	2.344118	0.000027
C	-2.466373	1.456793	-0.000006
C	-1.938276	-1.287387	0.000195
C	-0.866011	-0.395554	0.000167
C	-1.136743	1.022888	0.000049
H	-6.617232	-2.039810	0.000030
C	-4.908370	0.955854	-0.000022
H	-7.091410	0.432322	-0.000009
C	-3.568215	0.565232	0.000005
C	2.720870	-0.394899	0.000276
C	-6.021109	0.367331	0.000042
C	1.123447	1.448567	0.000074
C	-4.394362	-1.722040	0.000138
C	-5.646975	-1.583075	0.000161
C	-3.295498	-0.864188	0.000105
H	-1.713912	-2.346650	0.000292
C	1.392667	0.041826	0.000200
C	3.519063	1.883475	0.000100
C	3.780642	0.523123	0.000224
H	4.803201	0.162831	0.000284
H	2.899950	-1.464213	0.000370
H	1.965457	3.404054	-0.000067
H	4.334962	2.597470	0.000063

17 – singlet diradical product

H	3.914497	-1.049290	0.016289
H	1.809550	-2.369655	-0.044899
H	-7.642725	1.097859	0.007720
H	-7.565632	-1.414722	-0.079573
C	-5.426572	-1.443011	-0.065069
C	2.950832	-0.551742	0.026787
C	2.907057	0.875145	0.076254
N	-0.576491	-1.367816	-0.027353
H	-3.040287	2.480357	0.089423
C	0.532278	-0.635068	0.006244
C	-5.509381	1.256003	0.028704
C	1.803274	-1.286619	-0.007332
C	1.716586	1.538966	0.090923
C	0.487897	0.811446	0.056528
C	-1.746295	-0.702879	-0.012517
C	-6.680677	0.596978	-0.002796
C	-6.636085	-0.856349	-0.053282
H	-2.887016	-2.515132	-0.084114
H	3.838425	1.430287	0.102388
N	-0.663723	1.475497	0.071428
C	-1.790586	0.740759	0.037646
H	1.656463	2.620363	0.128096
C	-3.034755	1.397948	0.051631
C	-4.222531	0.682967	0.017953
C	-4.177250	-0.792886	-0.033332
C	-2.947854	-1.434405	-0.046748

17 – triplet diradical product

H	3.914708	-1.049255	0.015773
H	1.810911	-2.370200	-0.044661
H	-7.643161	1.113132	0.008069
H	-7.565033	-1.430065	-0.079925
C	-5.429511	-1.427350	-0.064079
C	2.950846	-0.552157	0.026431
C	2.907053	0.875460	0.077069
N	-0.574288	-1.368169	-0.027762
H	-3.042098	2.482947	0.089000
C	0.532436	-0.635881	0.005359
C	-5.511367	1.240049	0.028220
C	1.804405	-1.287224	-0.006988
C	1.717713	1.539557	0.091486
C	0.488019	0.812319	0.055425
C	-1.746524	-0.703944	-0.012127
C	-6.691729	0.590900	-0.003165
C	-6.647363	-0.850979	-0.052917
H	-2.888758	-2.517700	-0.084131
H	3.838657	1.430170	0.102752
N	-0.661511	1.476036	0.070719
C	-1.790860	0.741838	0.037813
H	1.657867	2.620902	0.129043
C	-3.032538	1.400195	0.051420
C	-4.214000	0.674109	0.017785
C	-4.169325	-0.783312	-0.032778
C	-2.945549	-1.436379	-0.046832