Vertically π-Expanded Coumarins – the Synthesis and Optical Properties

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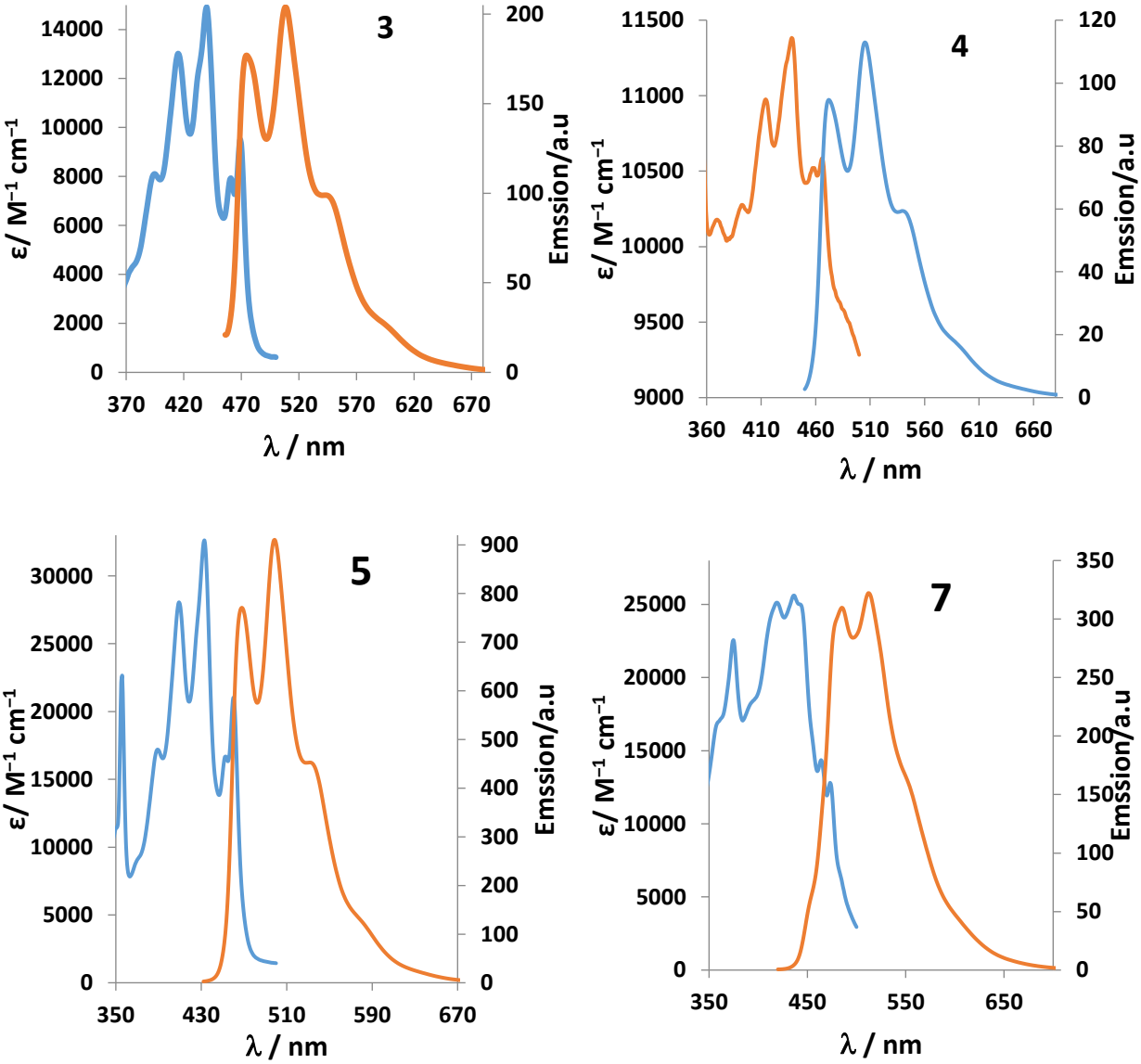
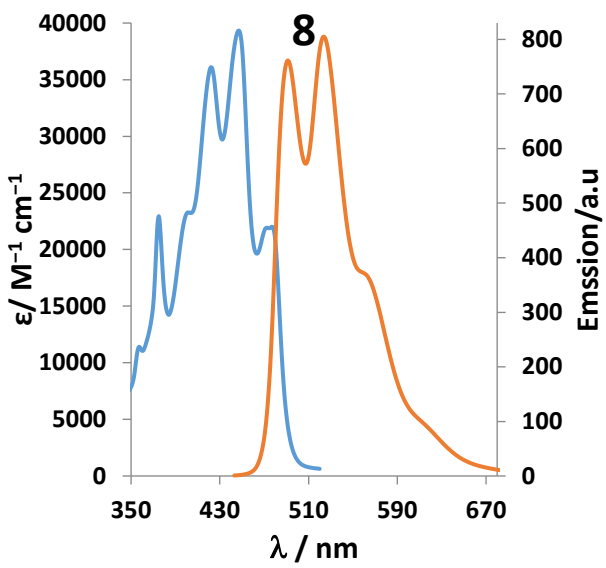
1. Absorption and normalized emission spectra for synthesized compounds.

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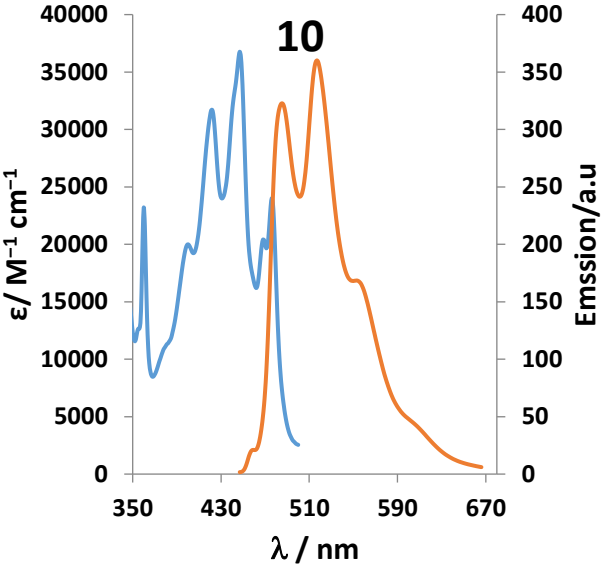
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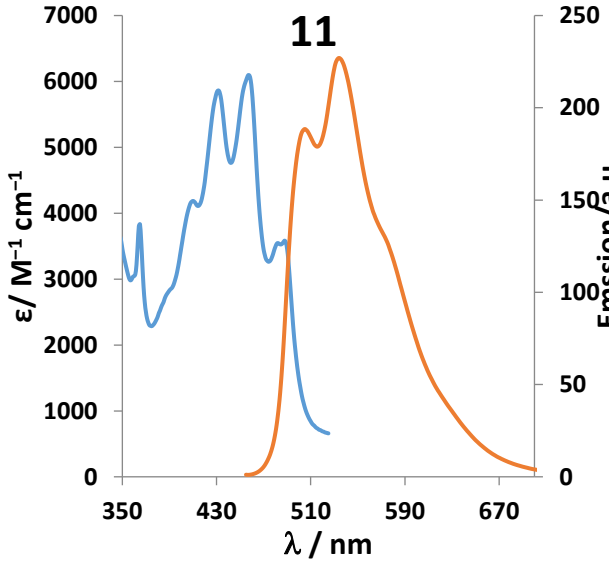
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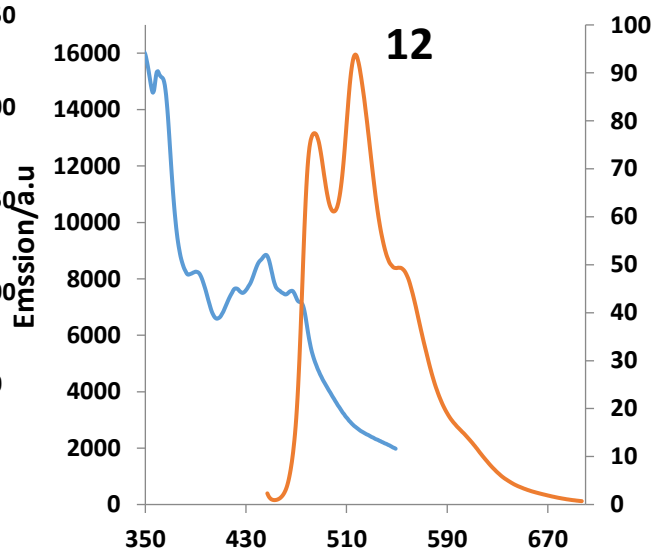
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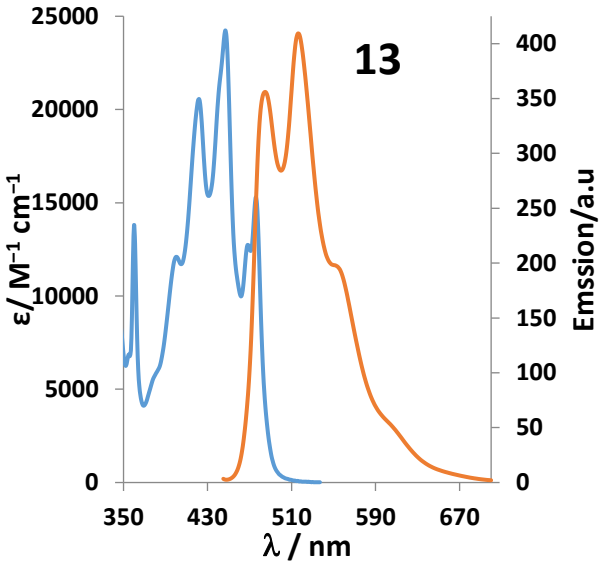
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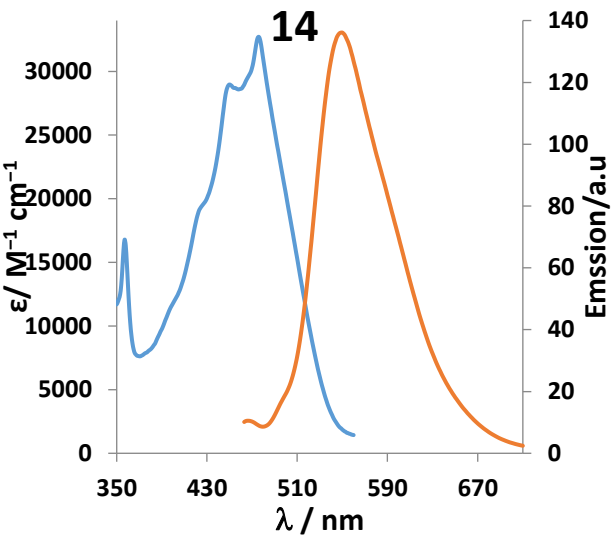
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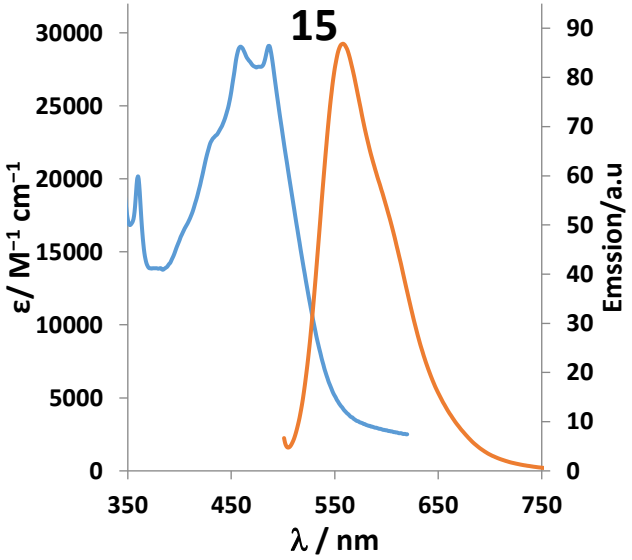
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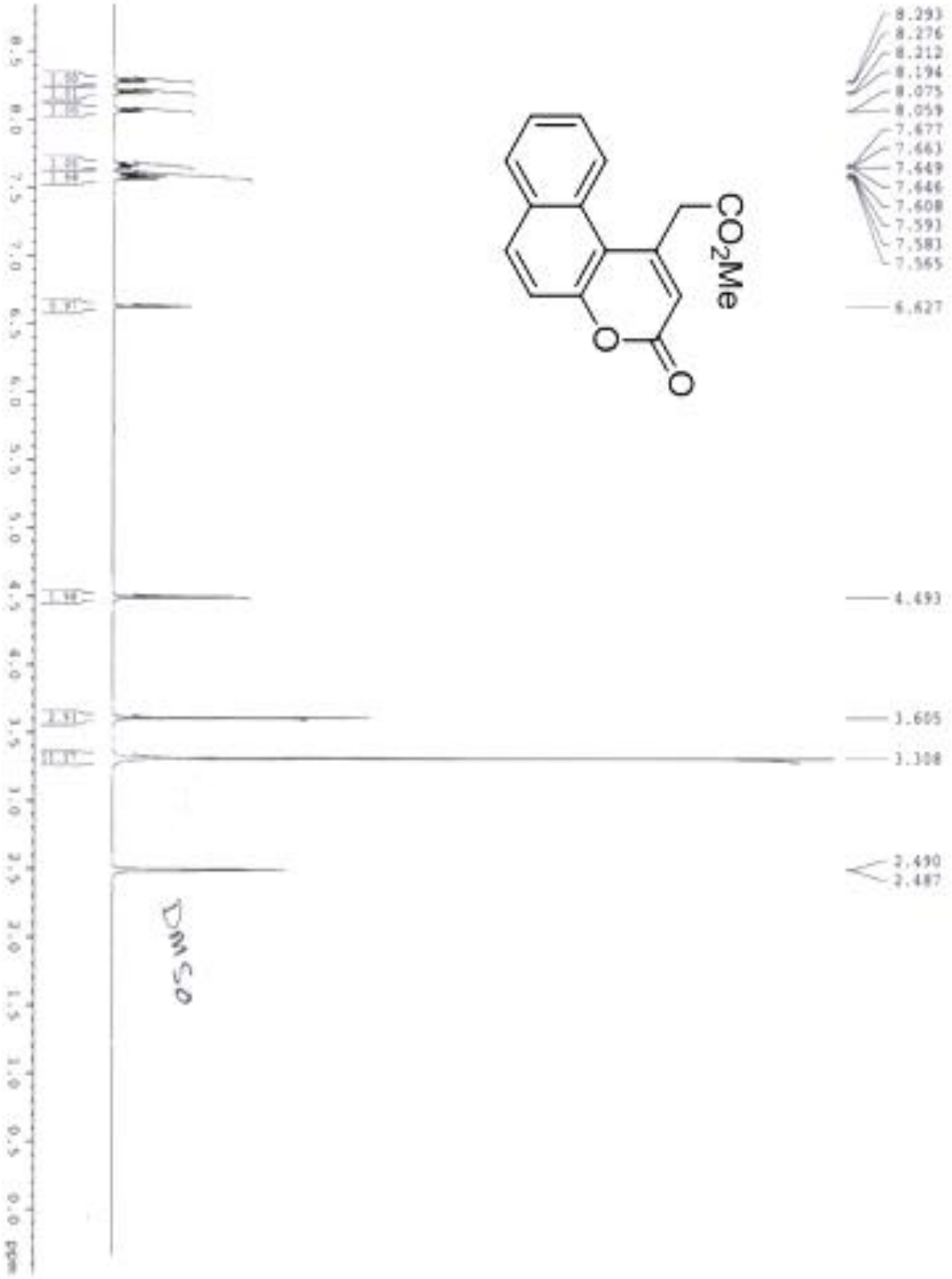
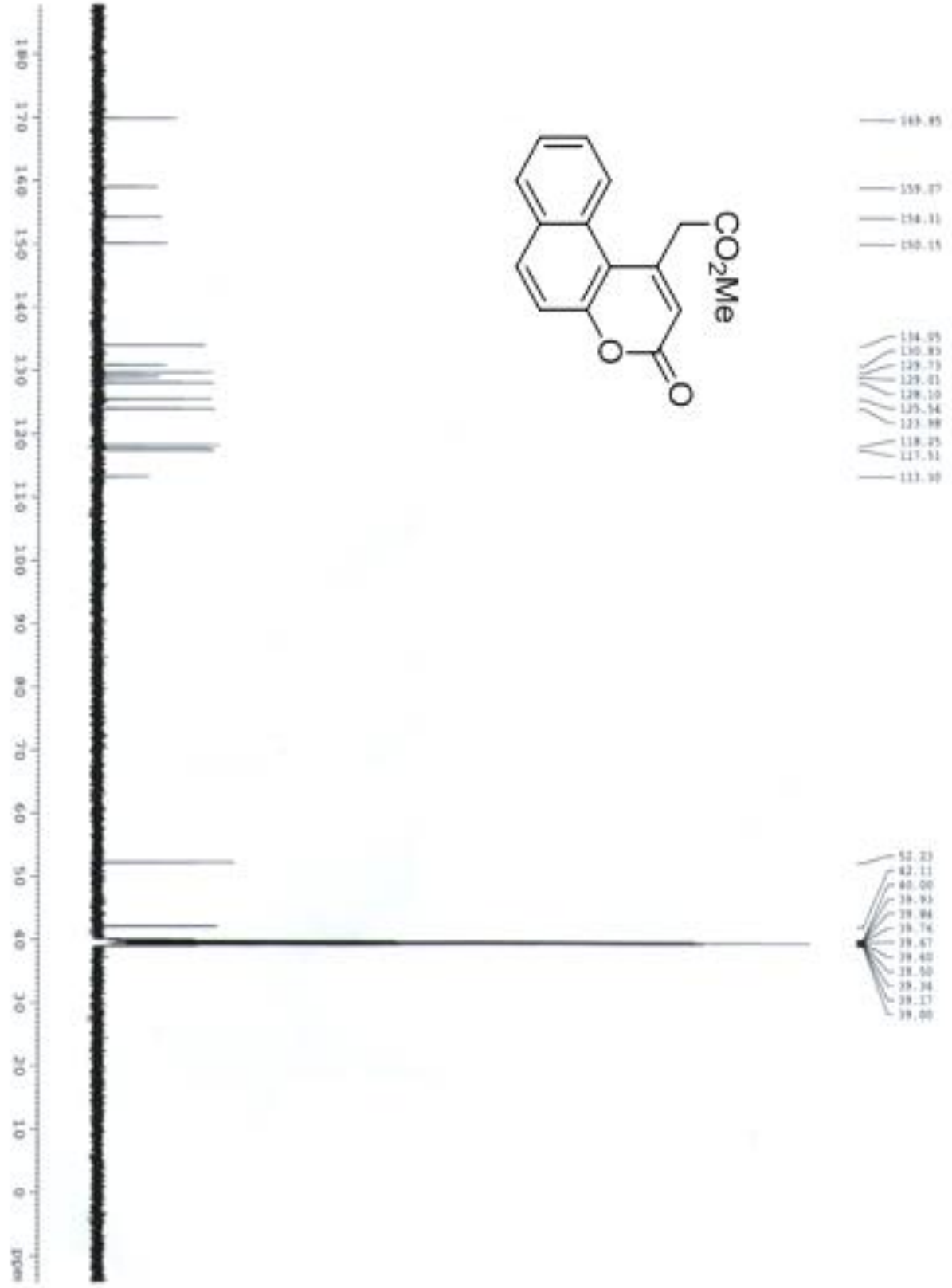
750

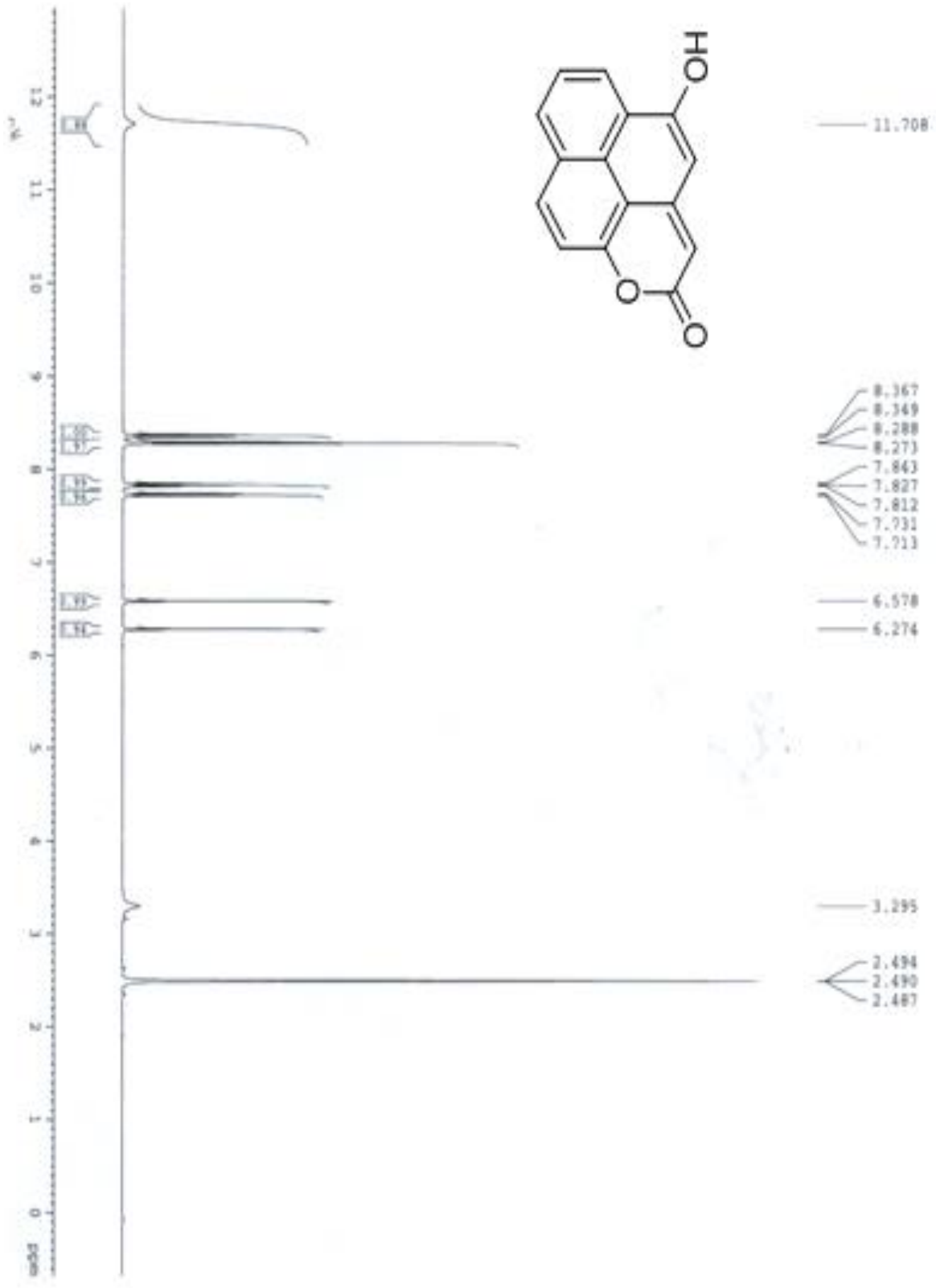
2. ^{1}H and ^{13}C NMR spectra of synthesized compounds:



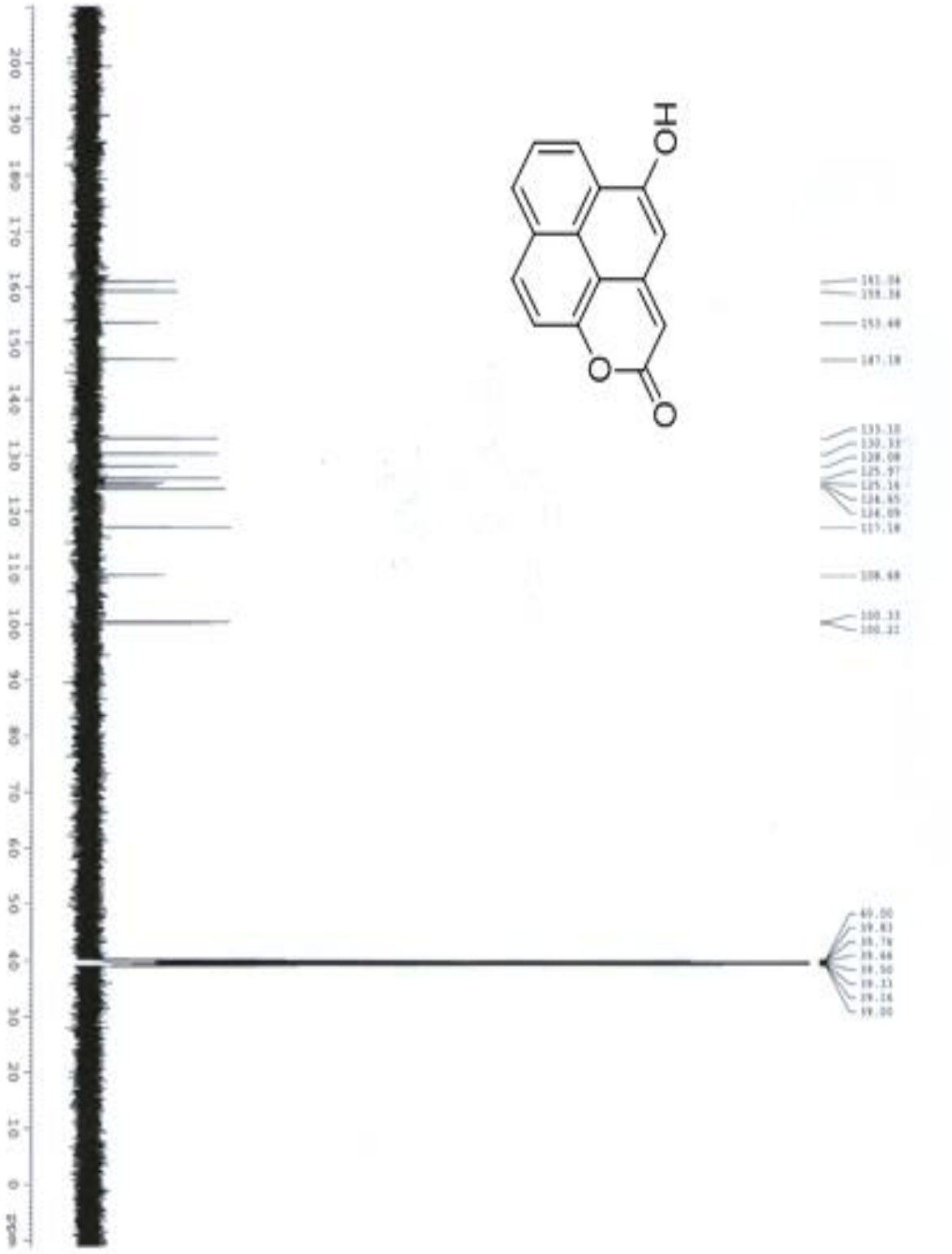
^{1}H NMR spectrum of **2** in DMSO.



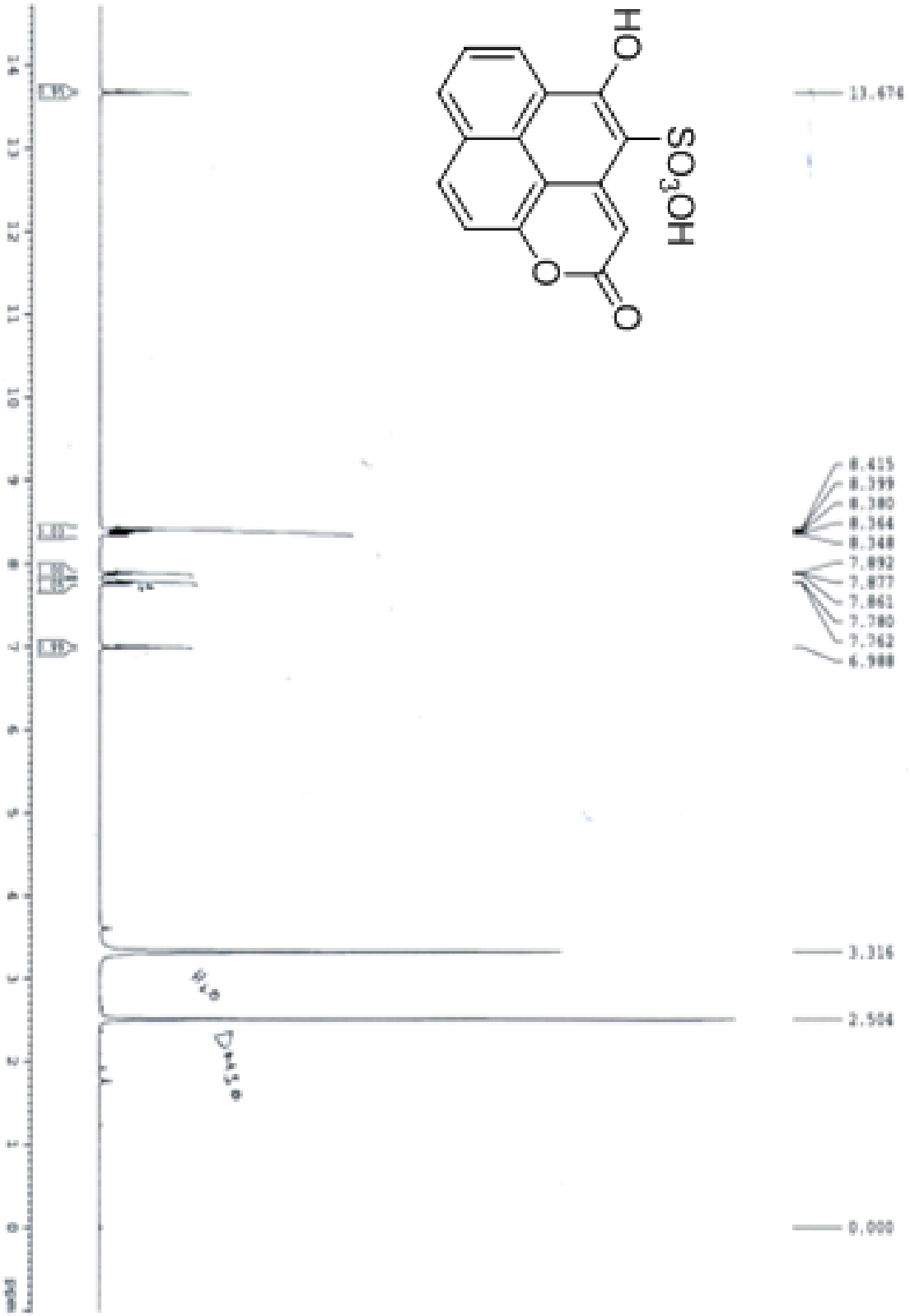
^{13}C NMR spectrum of **2** in DMSO.



^{1}H NMR spectrum of **3** in DMSO (prepared *via* method A).

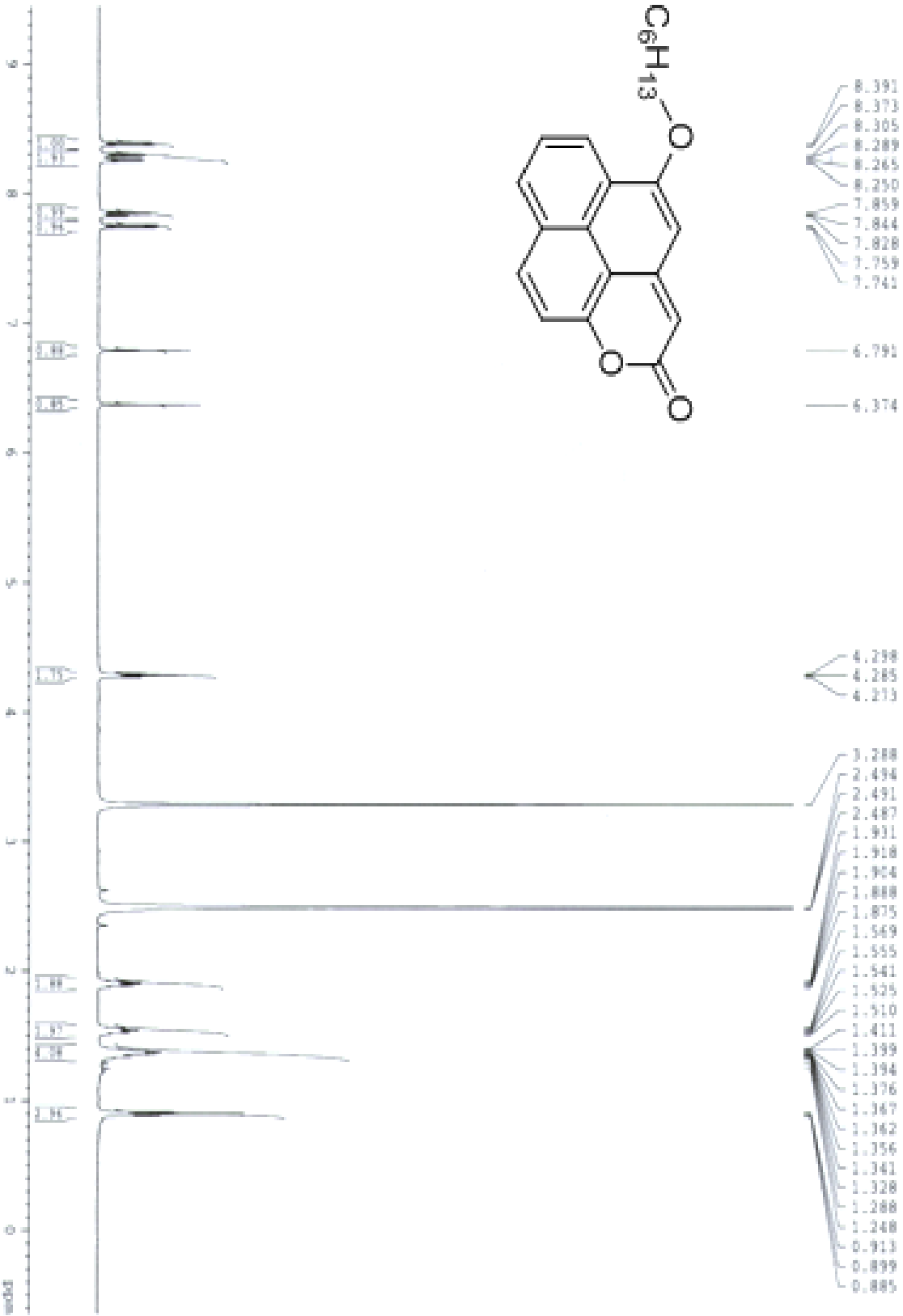


^{13}C NMR spectrum of **3** in DMSO (prepared *via* method A).

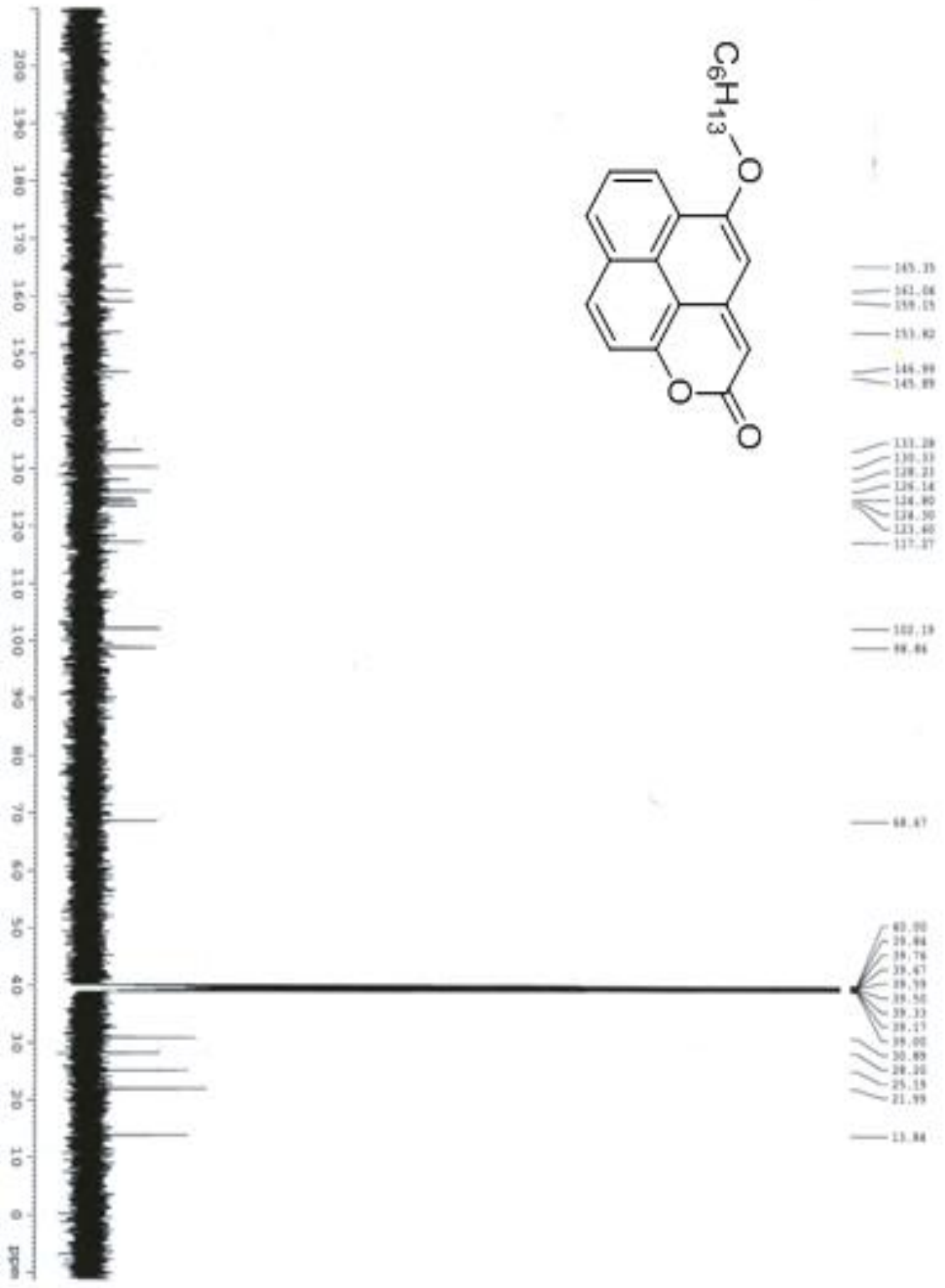


^{1}H NMR spectrum of **4** in DMSO.

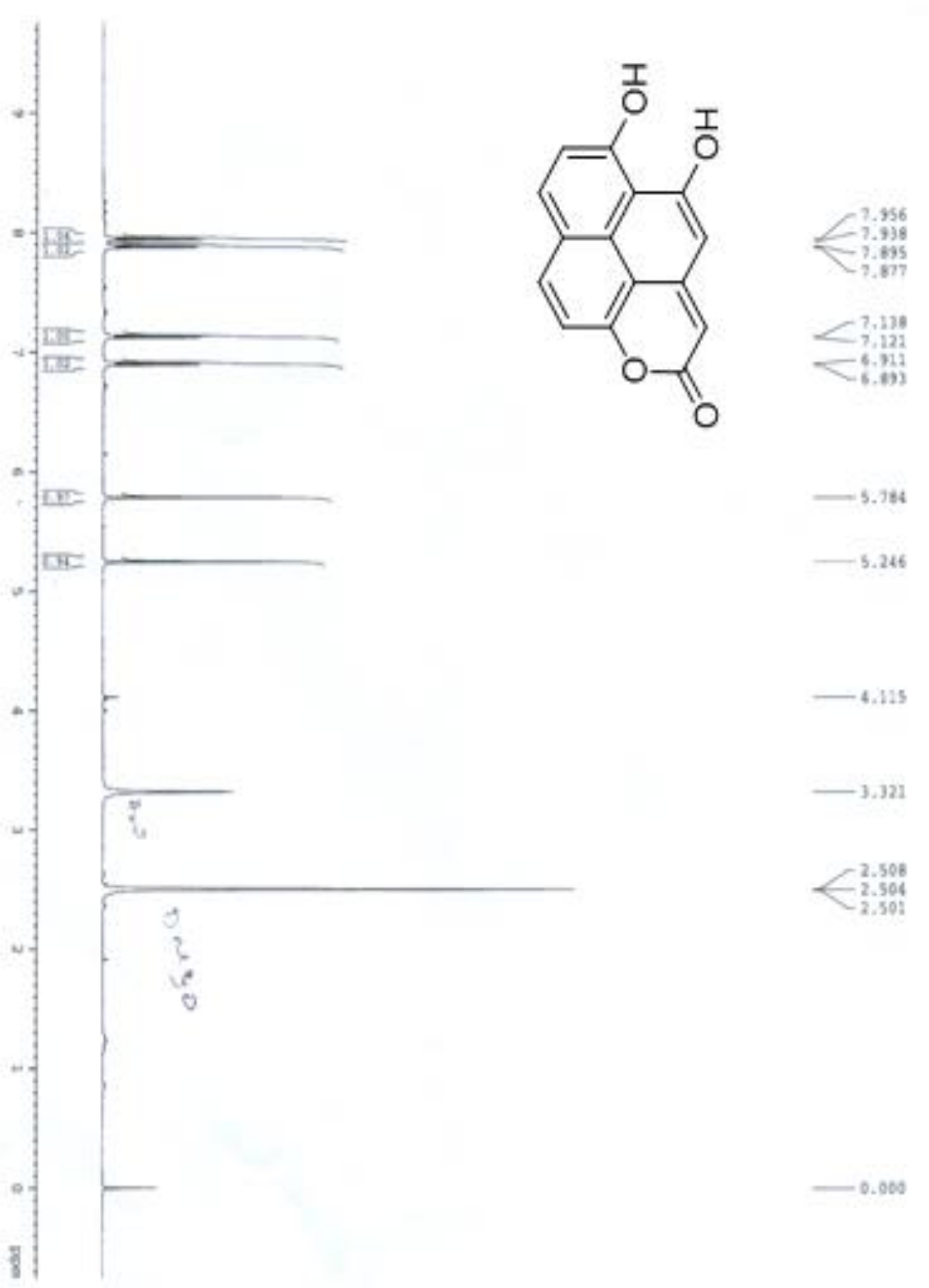
^{13}C NMR spectrum of **4** in DMSO.



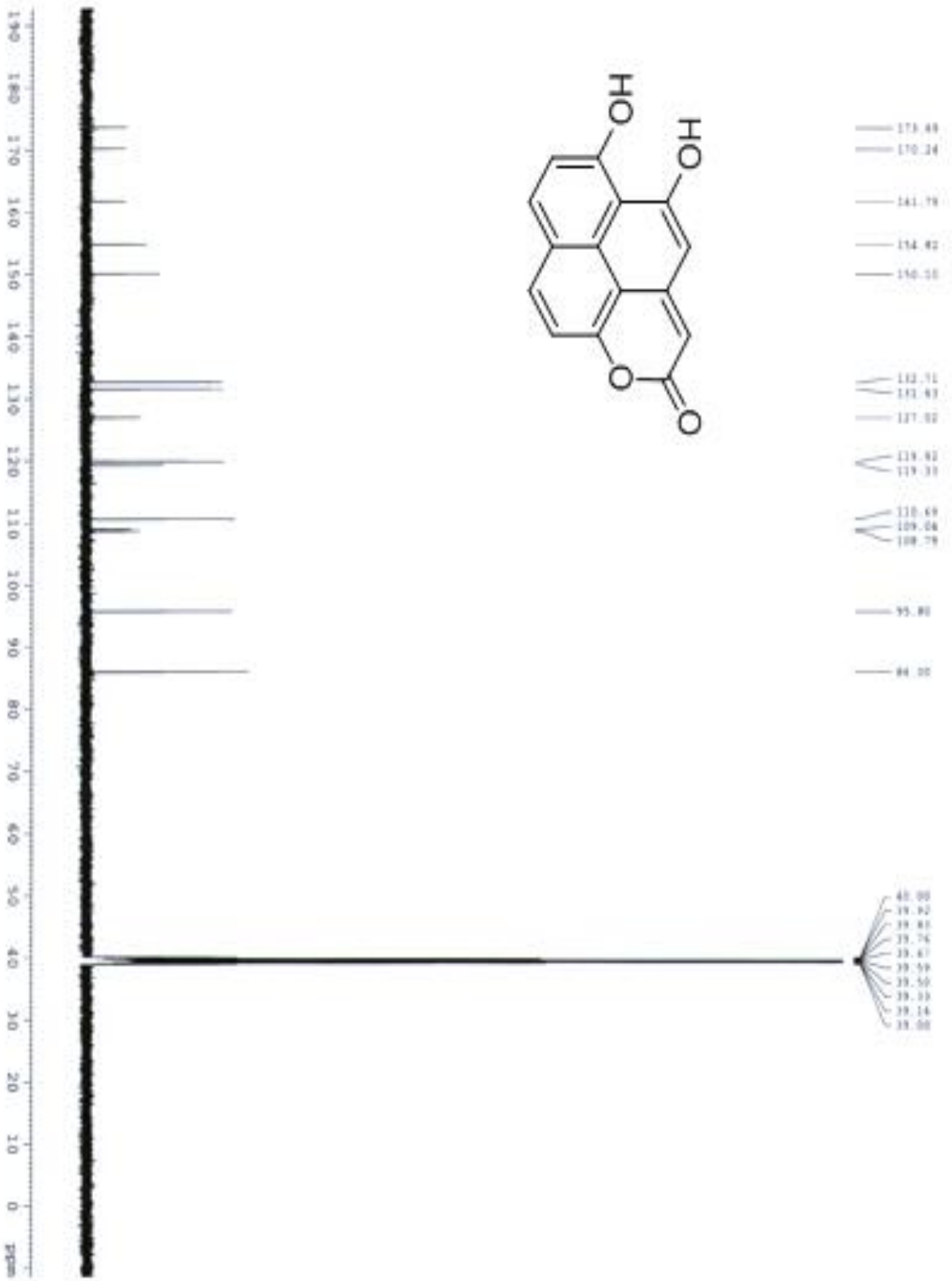
^{1}H NMR spectrum of **5** in DMSO.



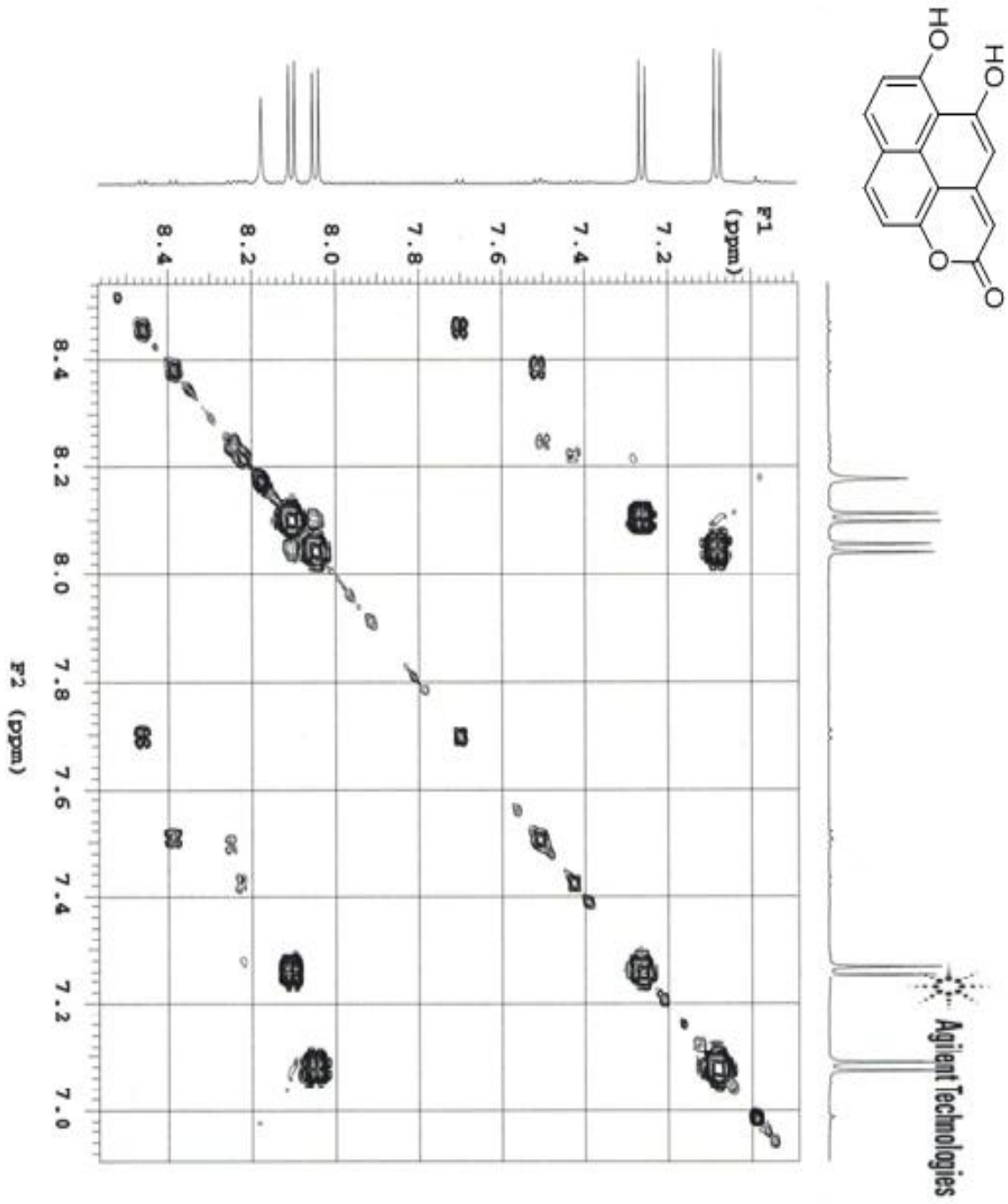
^{13}C NMR spectrum of **5** in DMSO.



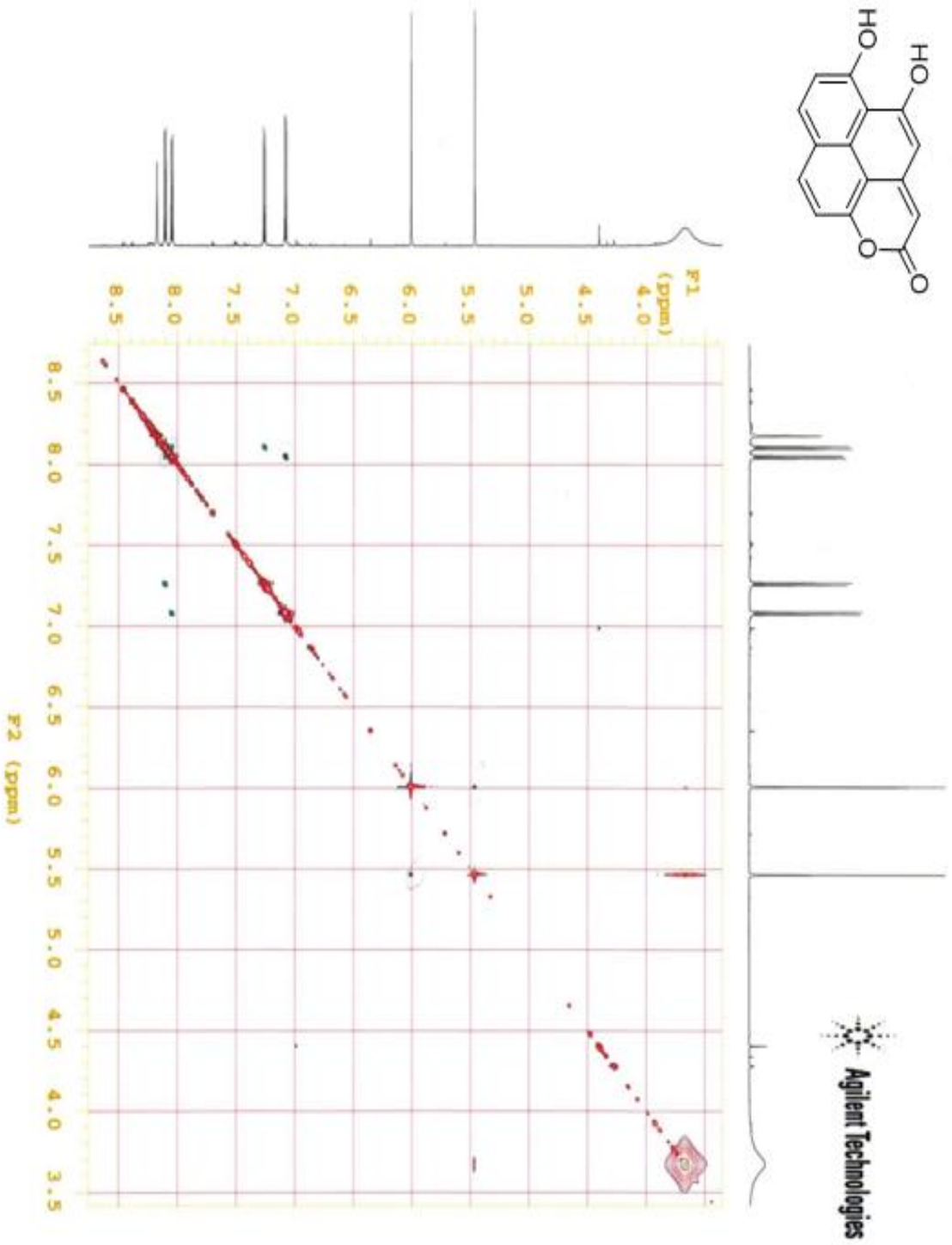
^{1}H NMR spectrum of **7** in DMSO.



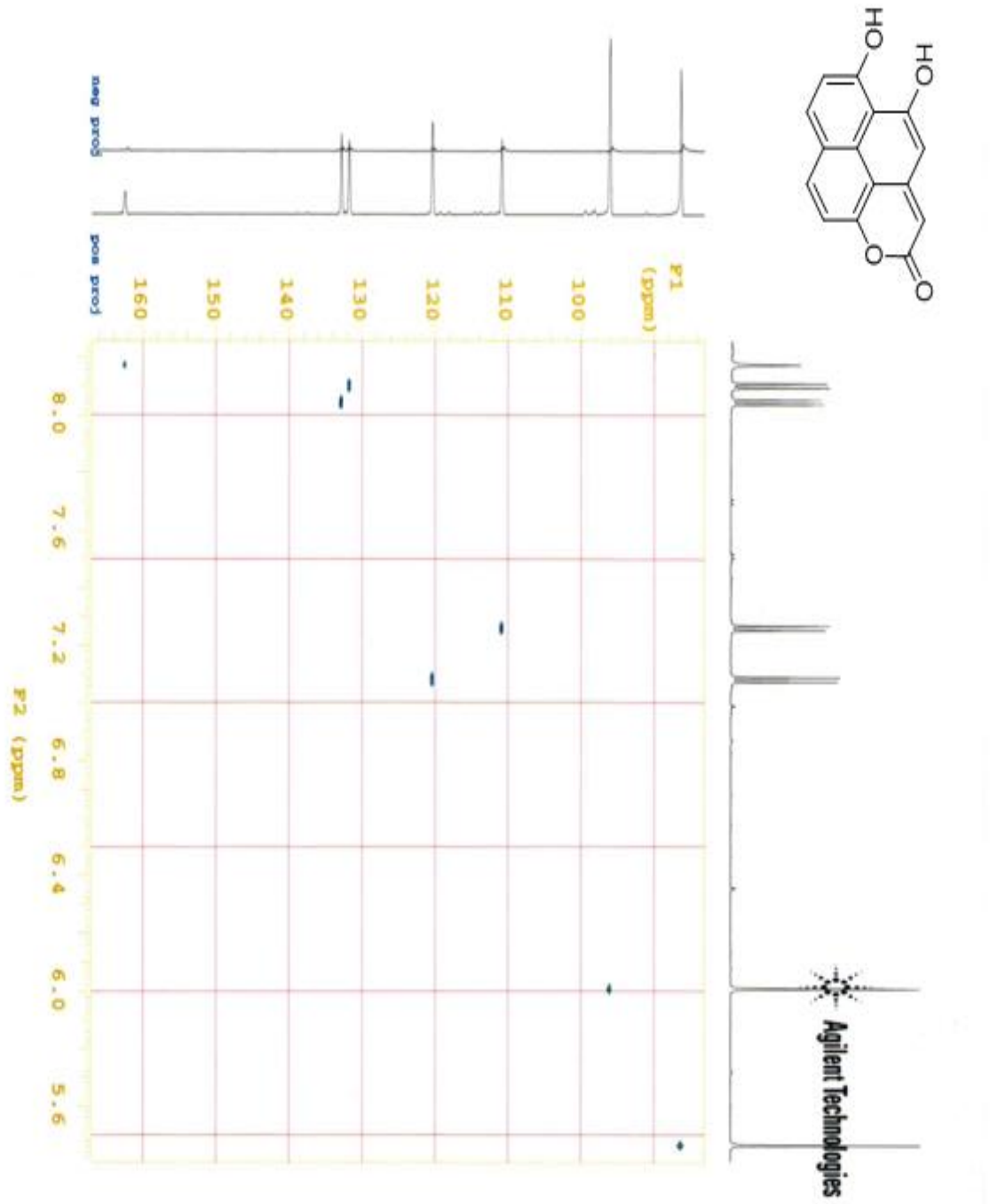
^{13}C NMR spectrum of **7** in DMSO.



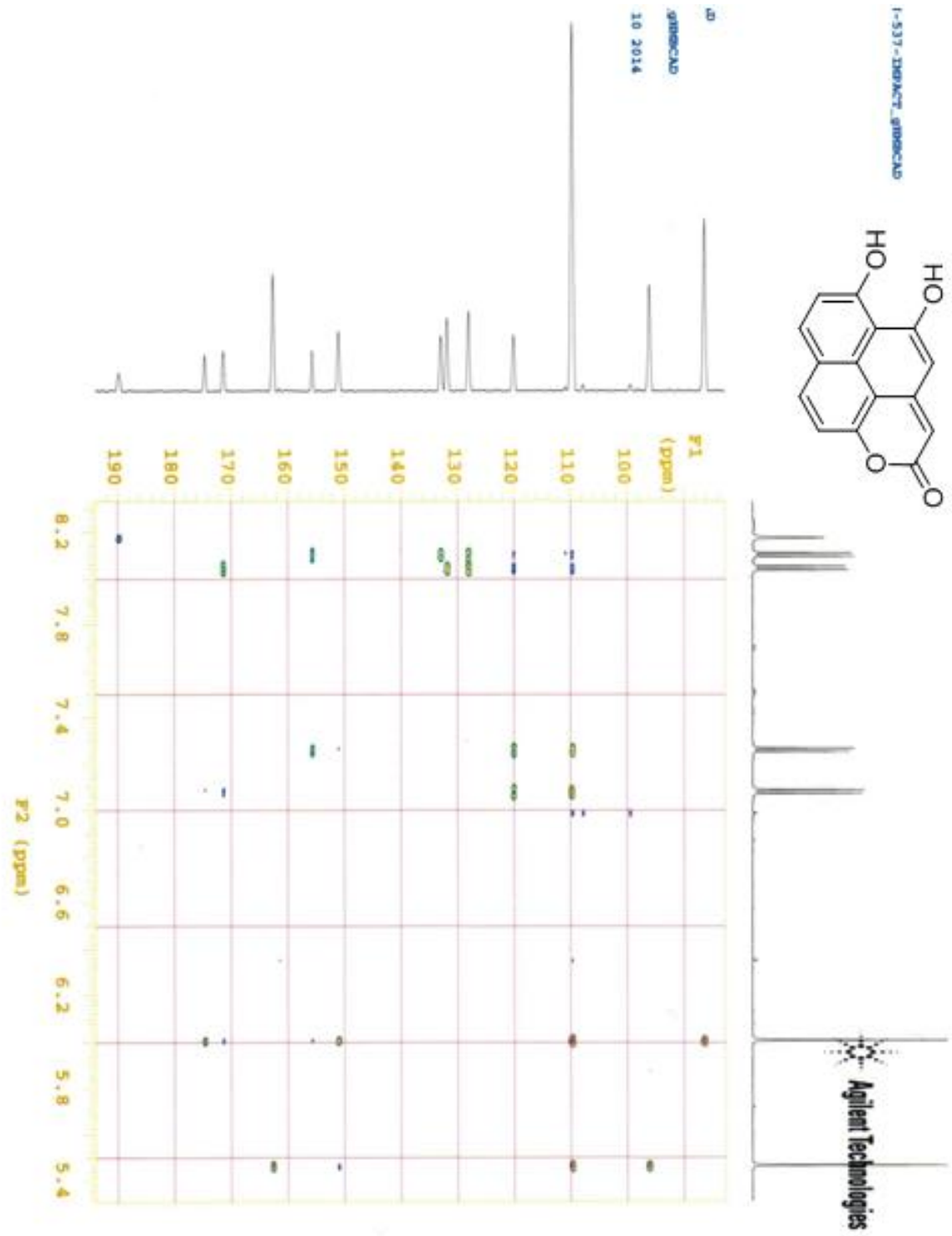
COSY NMR spectrum of **7** in DMSO.



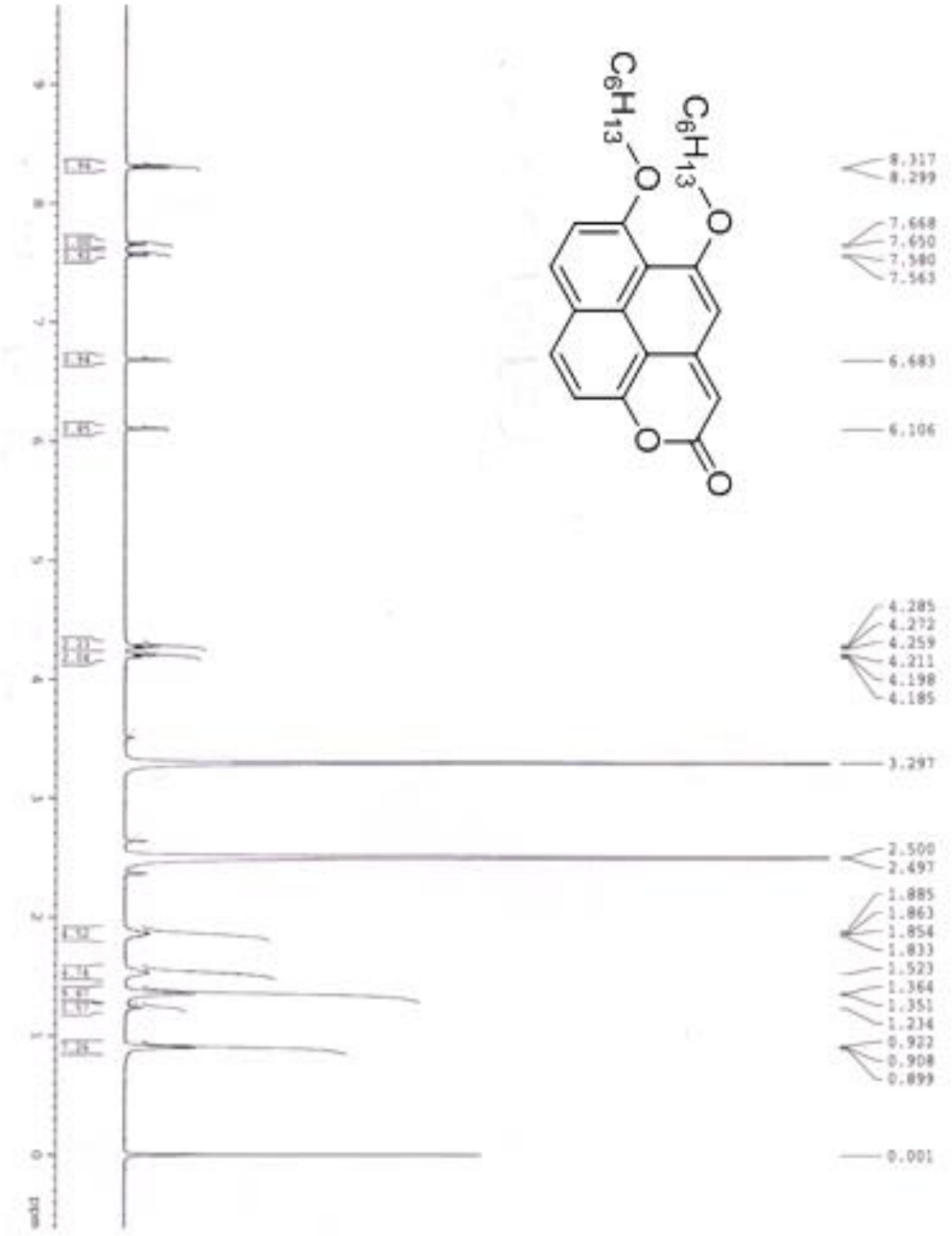
NOESY NMR spectrum of **7** in DMSO.



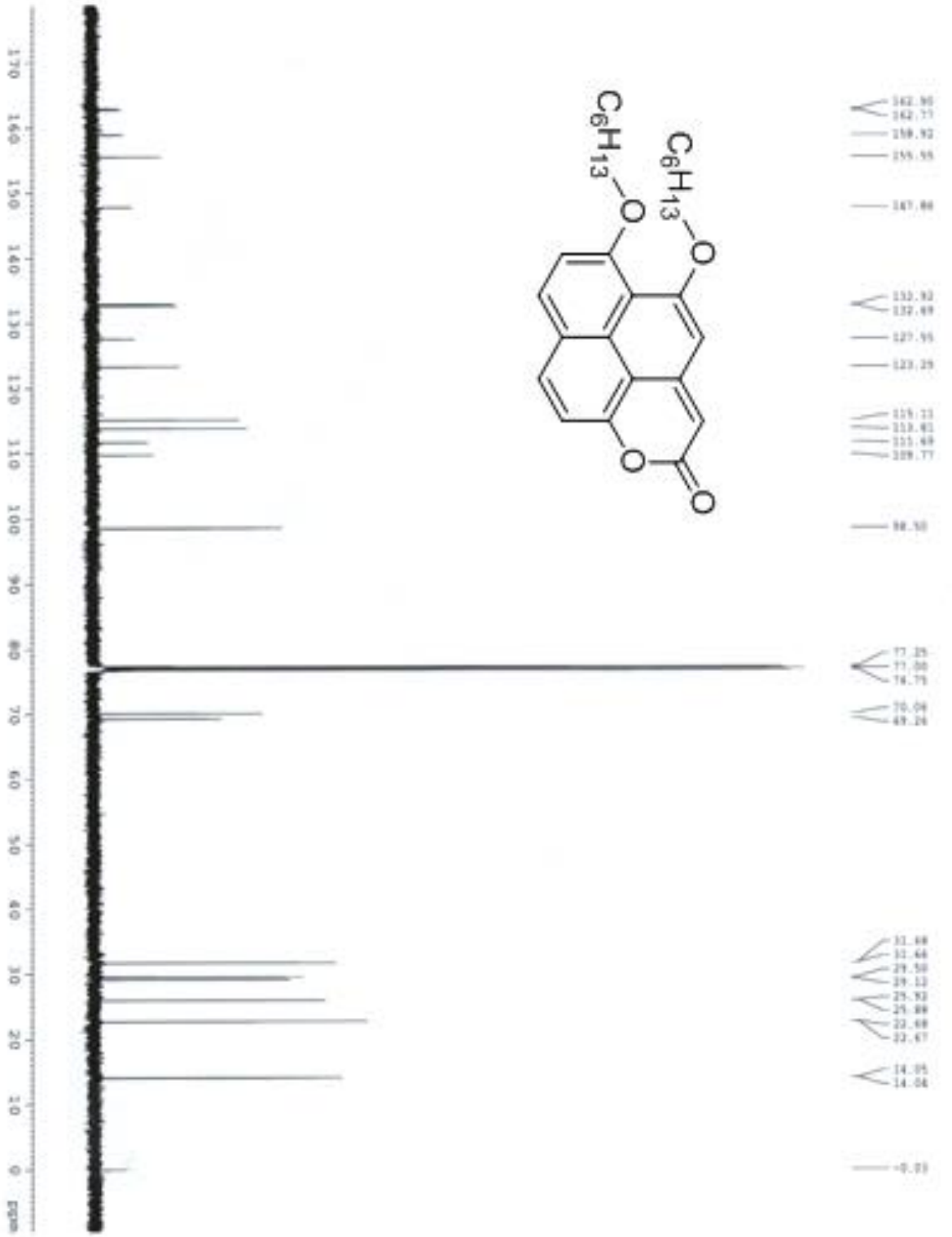
HSQCAD NMR spectrum of **7** in DMSO.



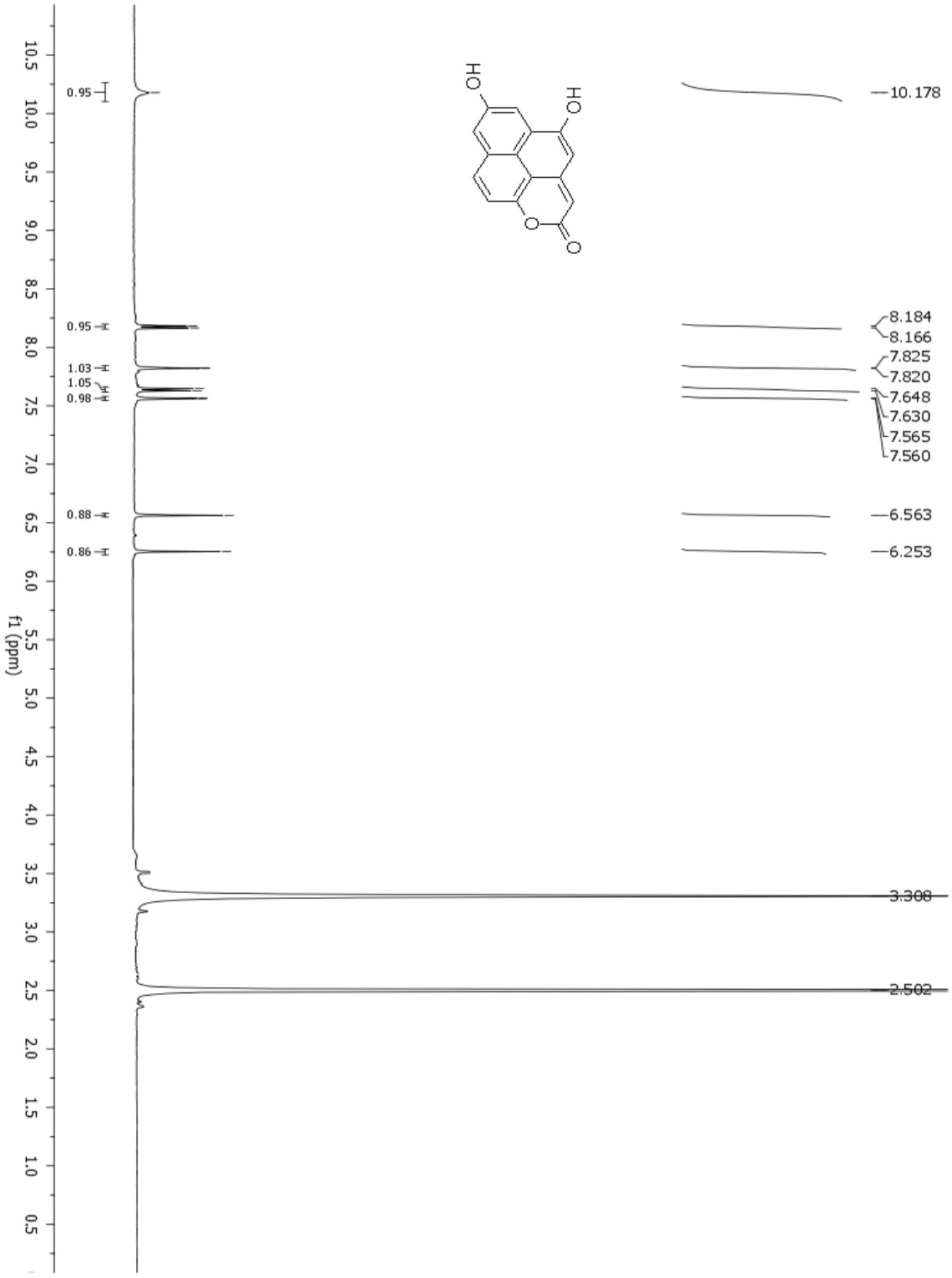
HMBCAD HMR spectrum of **7** in DMSO.



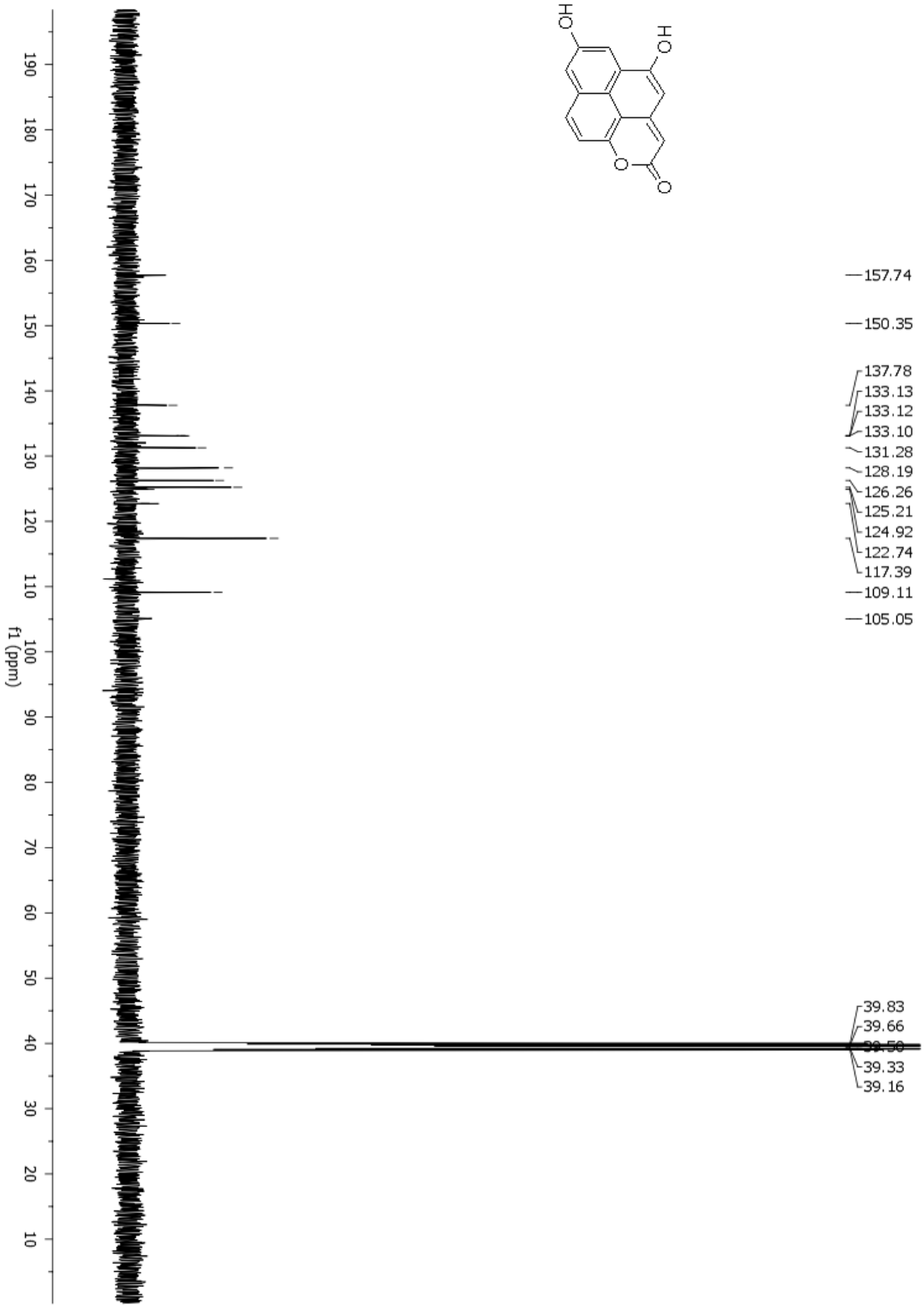
^{1}H NMR spectrum of **8** in DMSO.



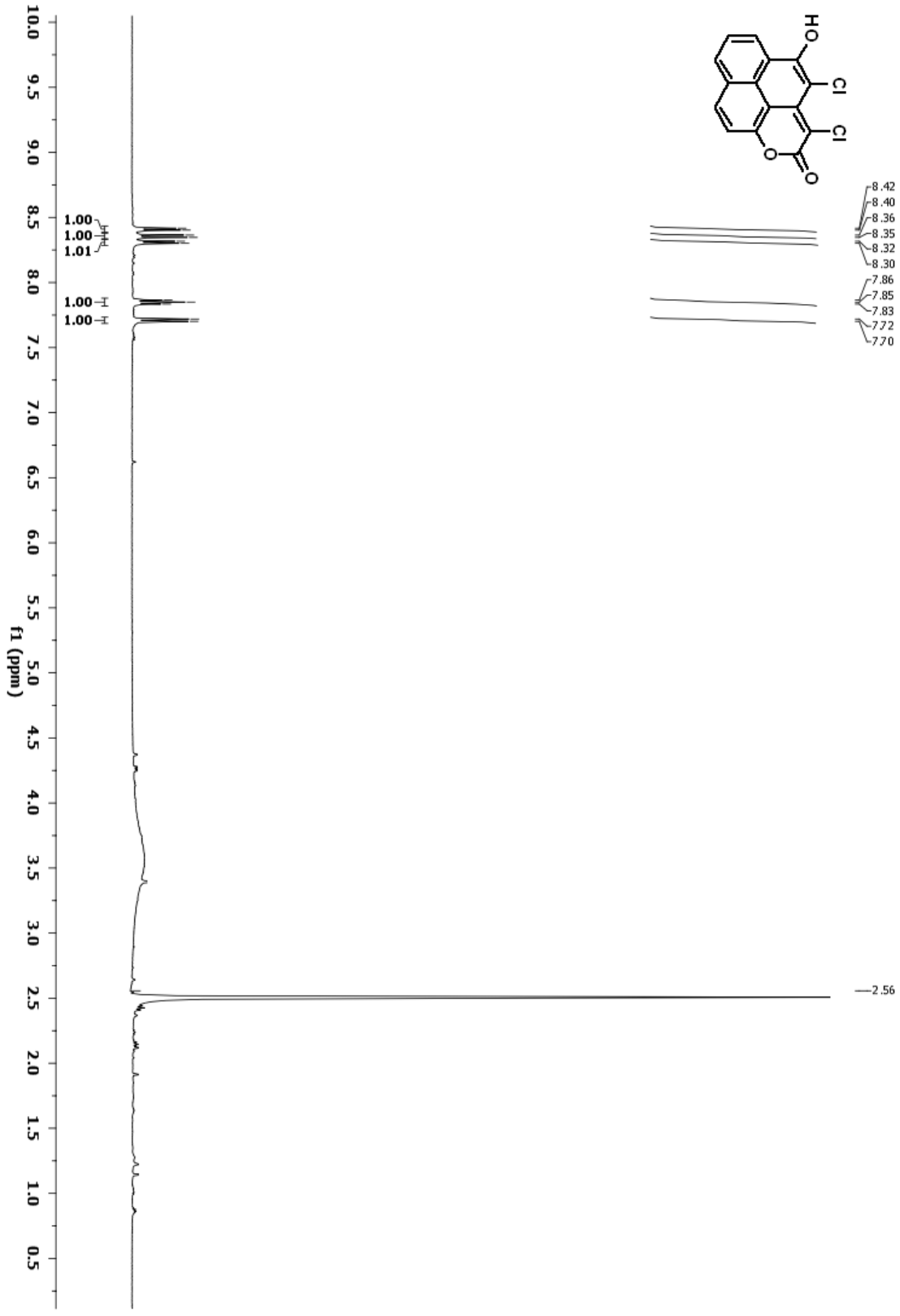
^{13}C NMR spectrum of **8** in DMSO.



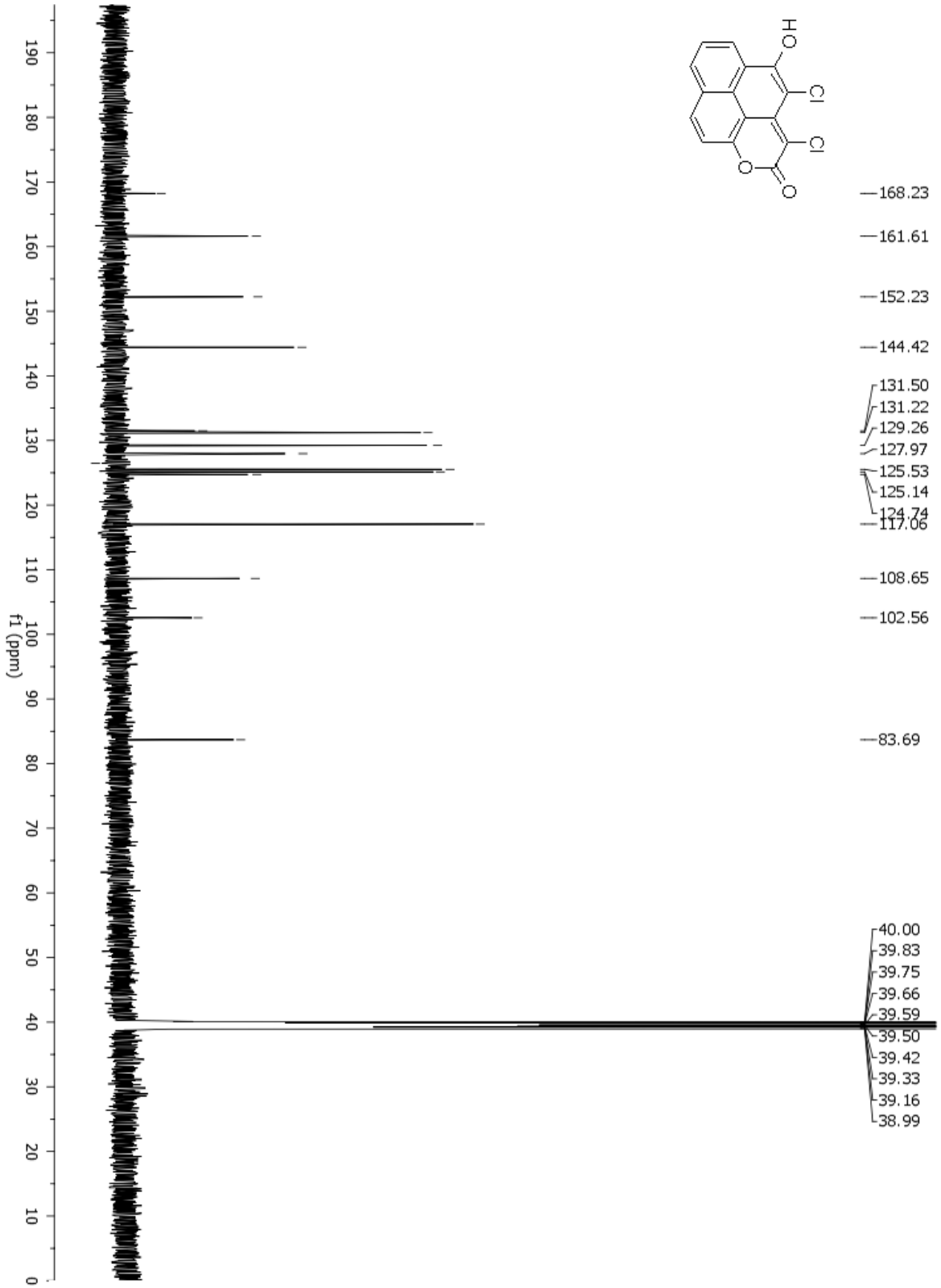
^{1}H NMR spectrum of **10** in DMSO.



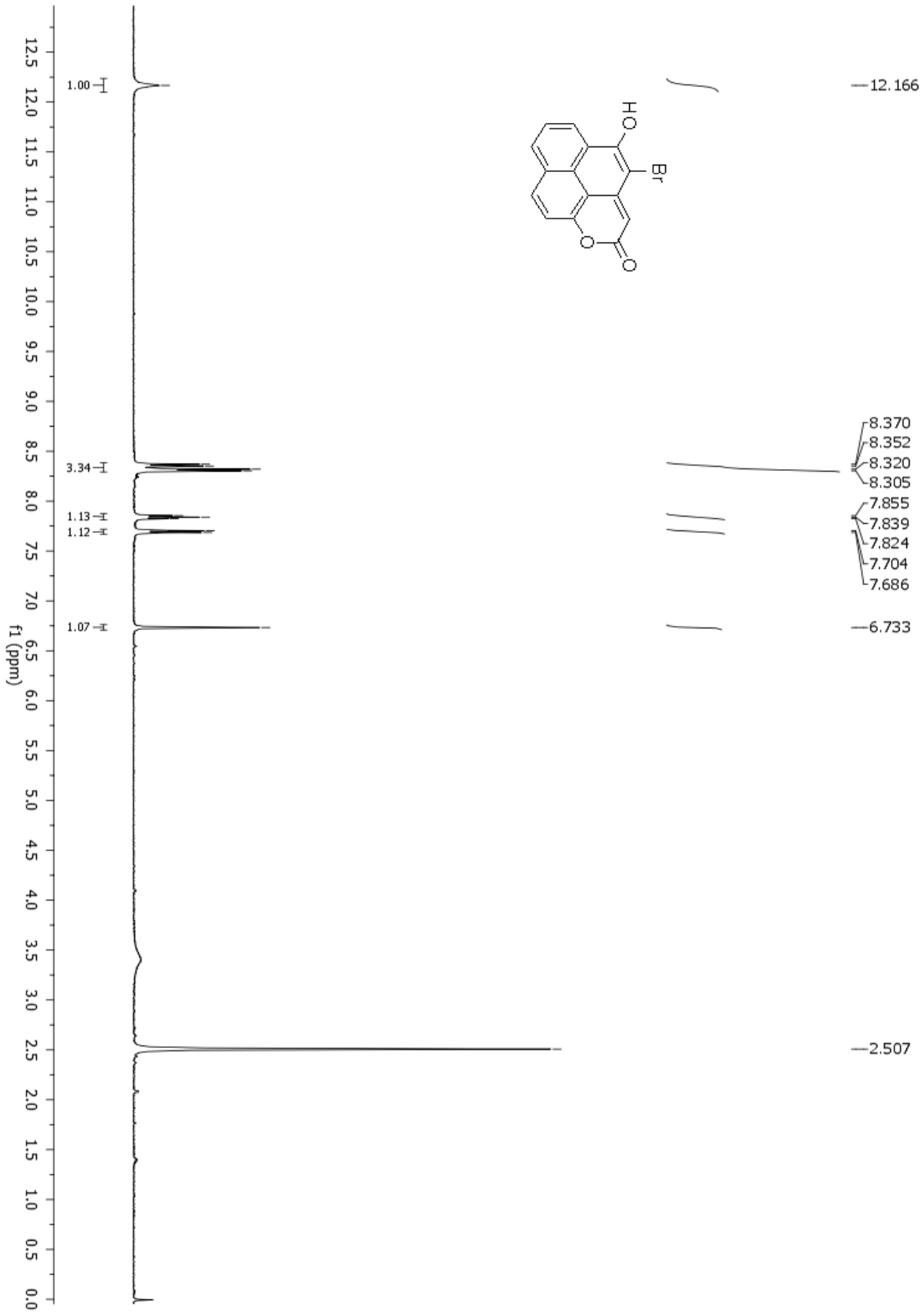
^{13}C NMR spectrum of **10** in DMSO.



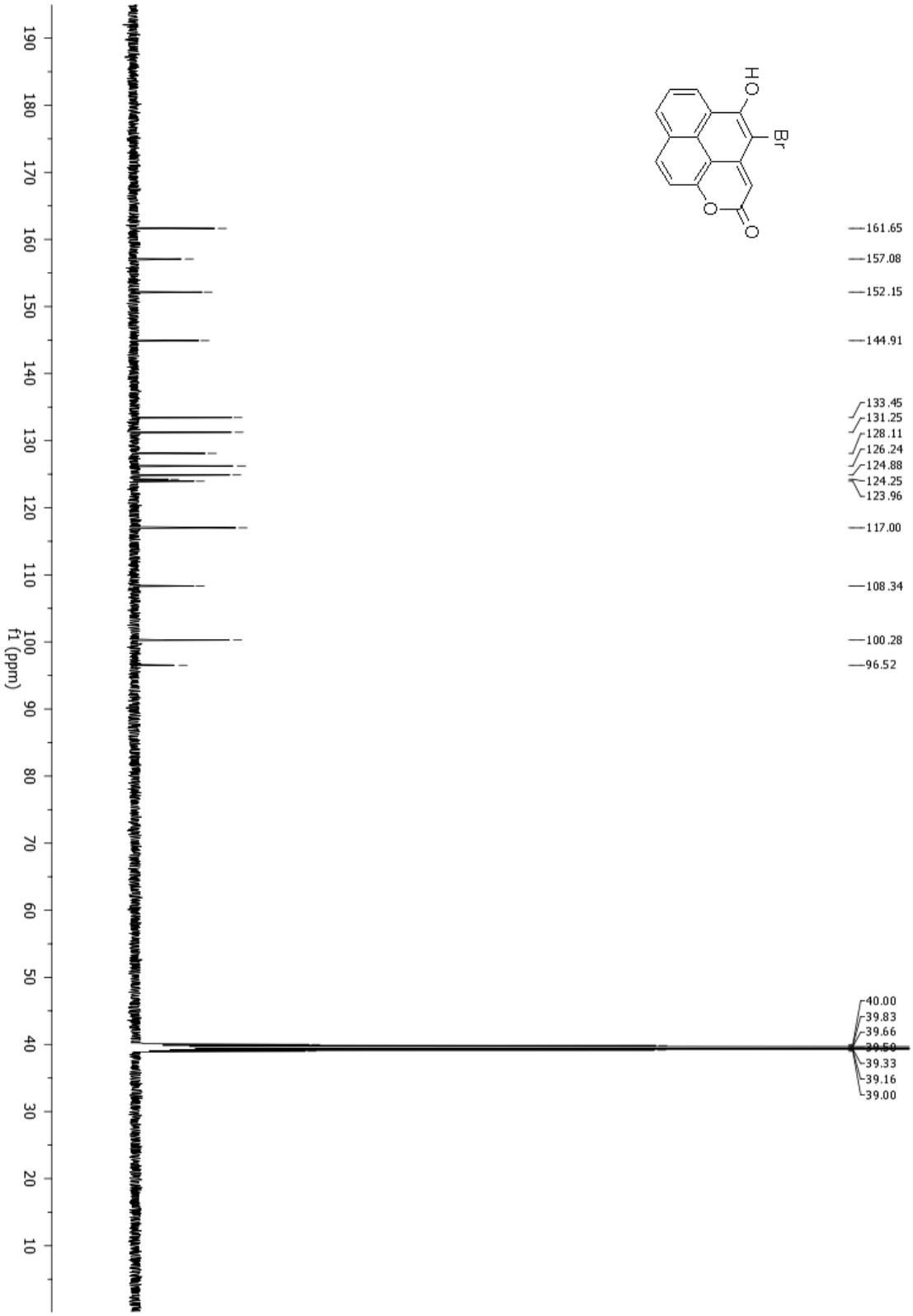
^{1}H NMR spectrum of **11** in DMSO.



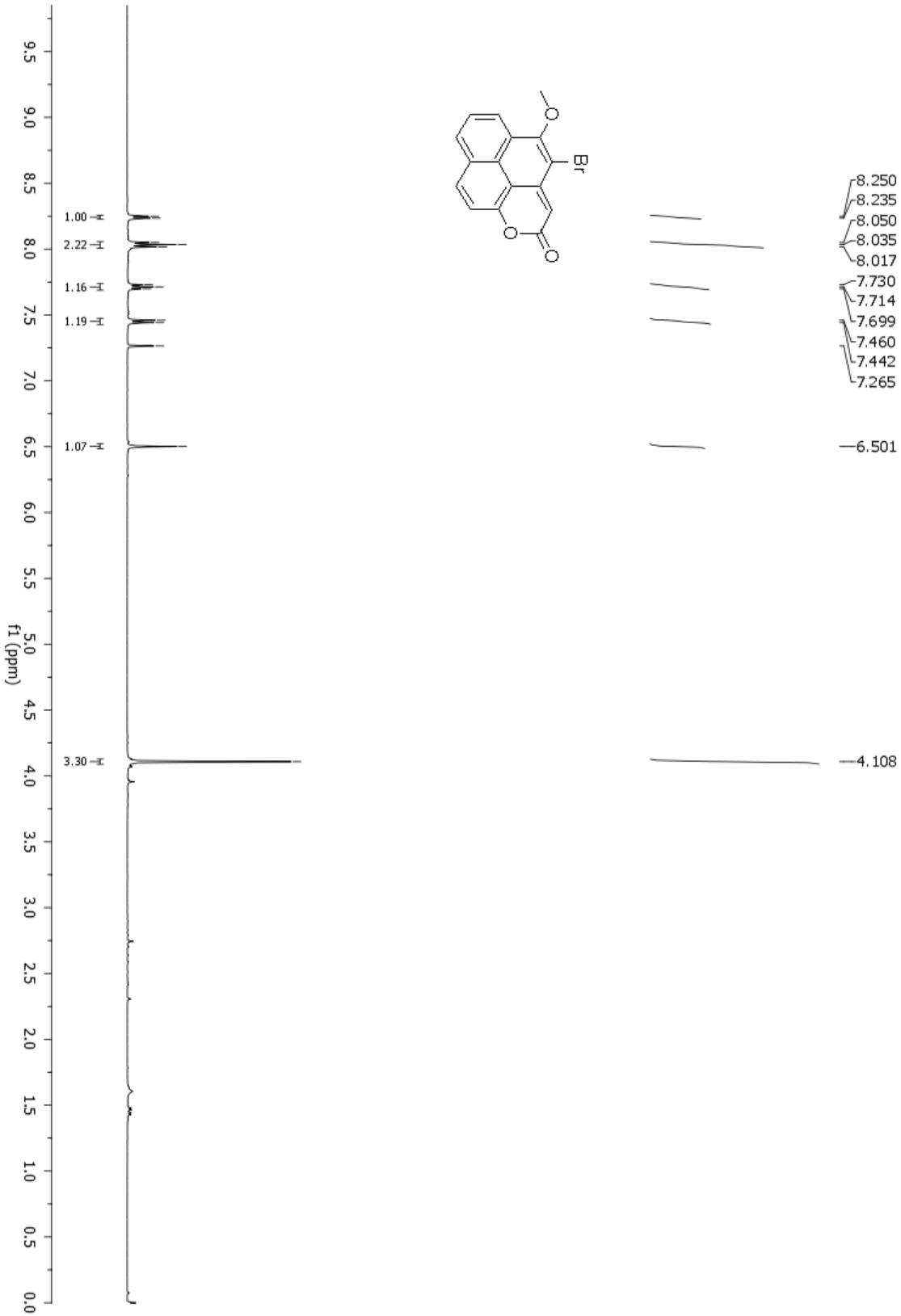
^{13}C NMR spectrum of **11** in DMSO.



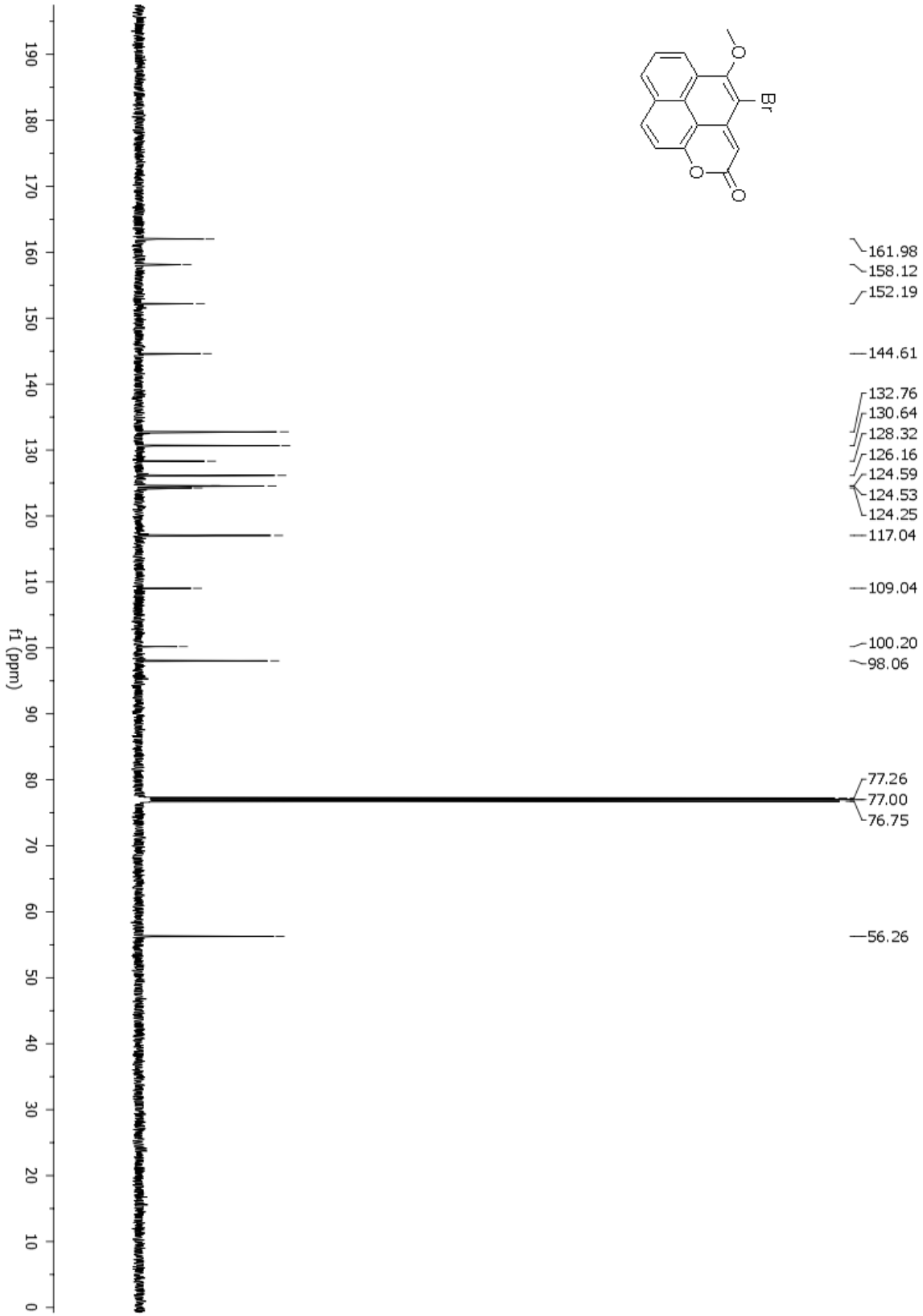
^{1}H NMR spectrum of **12** in DMSO.



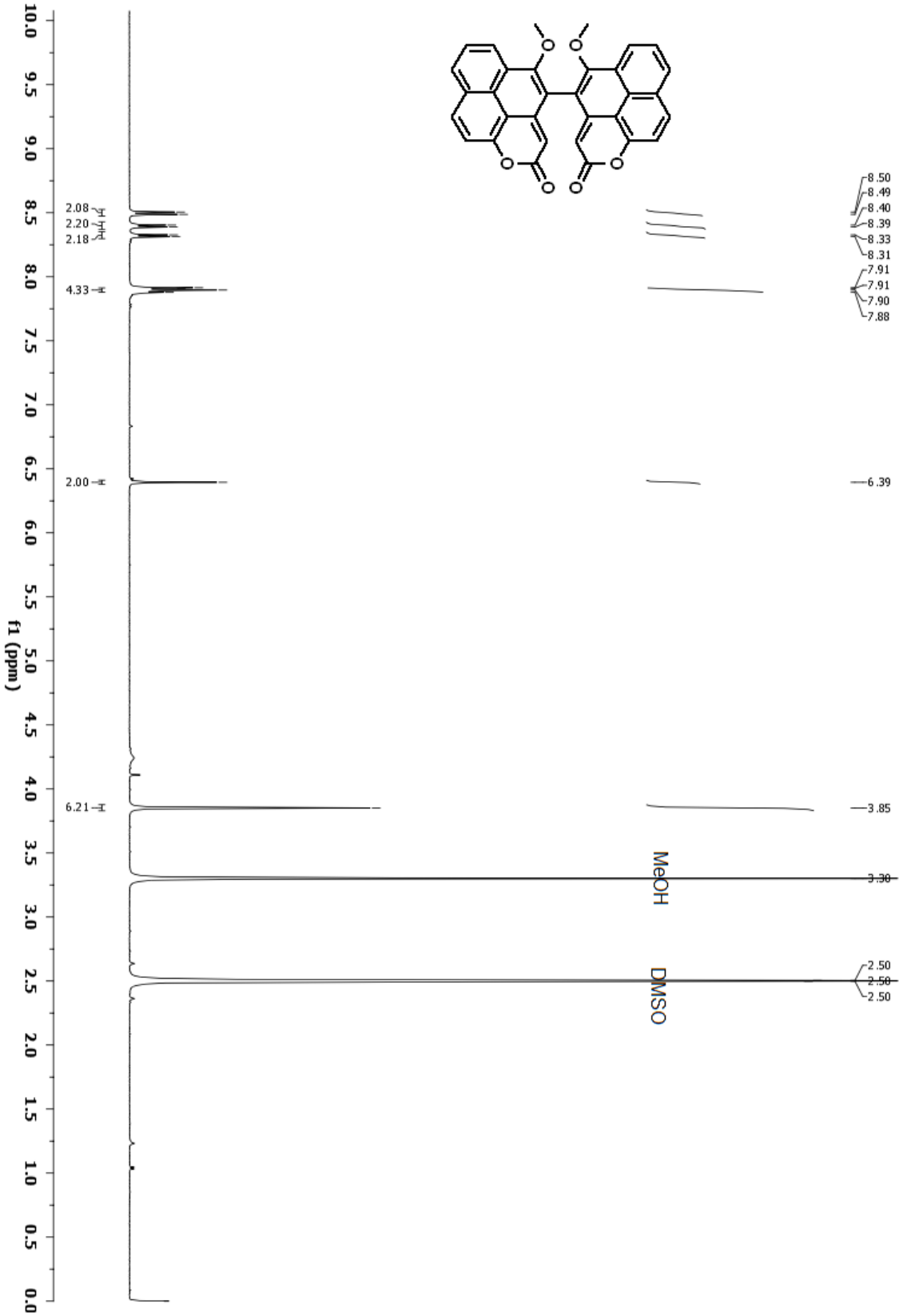
^{13}C NMR spectrum of **12** in DMSO.



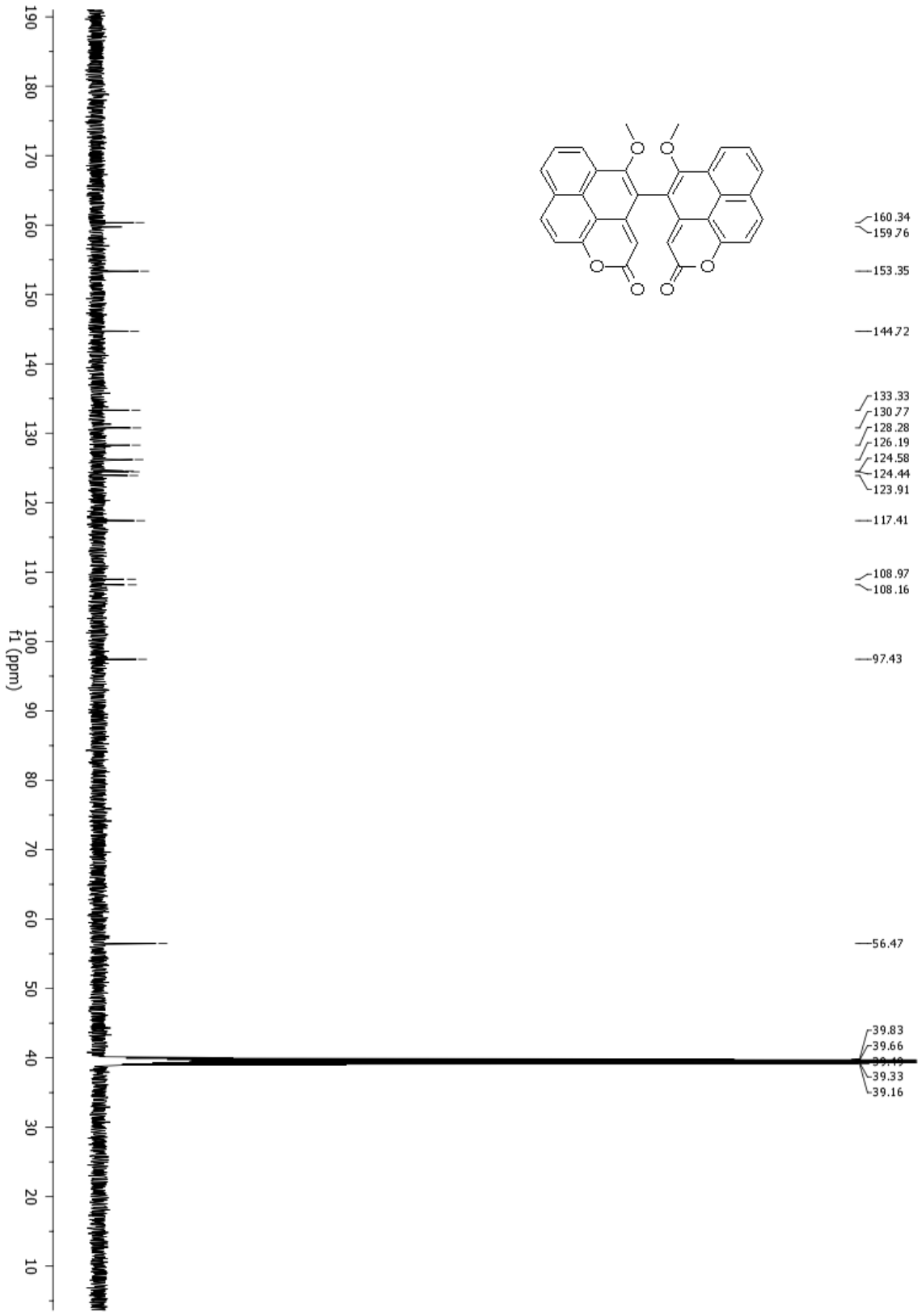
^{1}H NMR spectrum of **13** in DMSO.



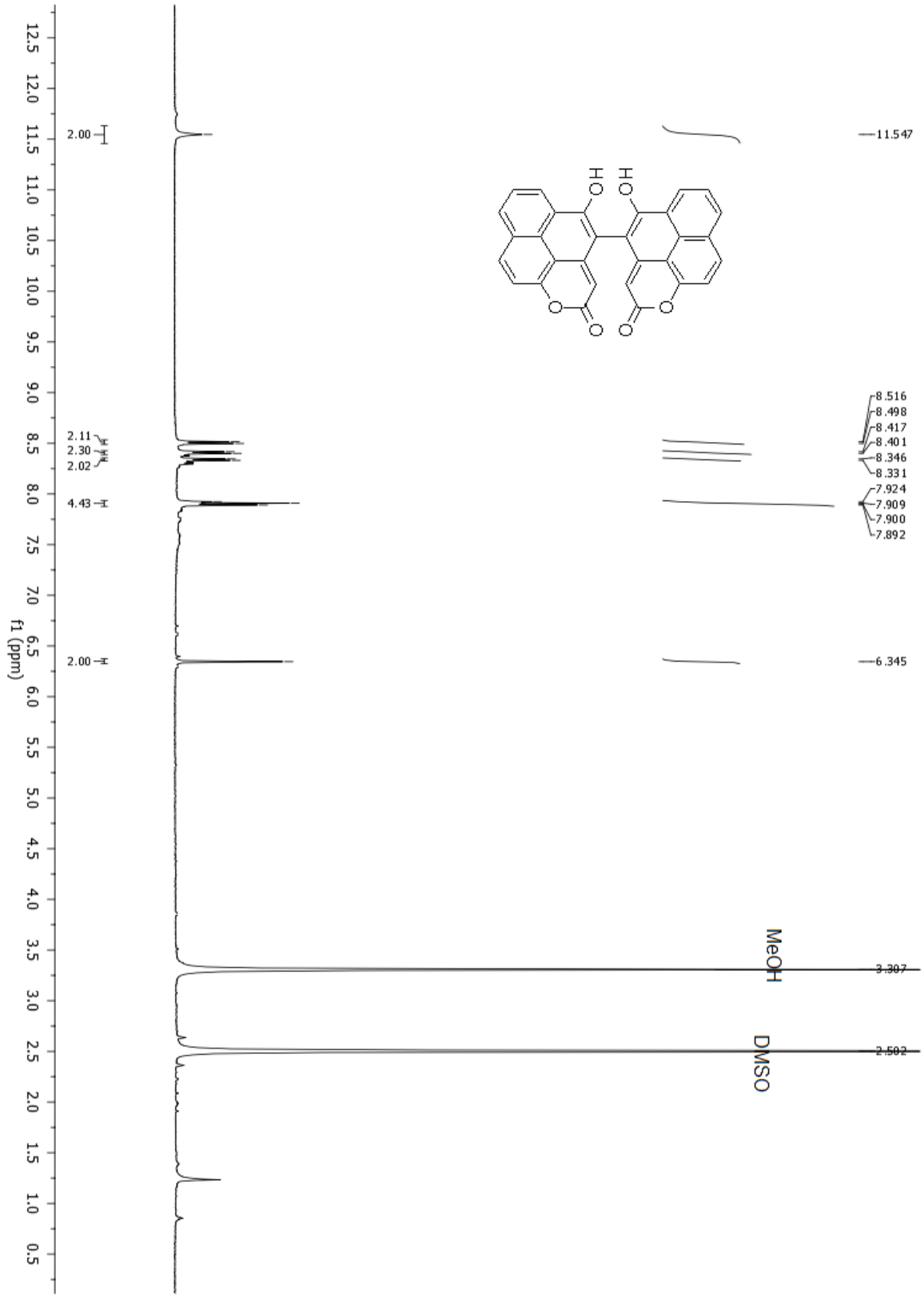
^{13}C NMR spectrum of **13** in DMSO.



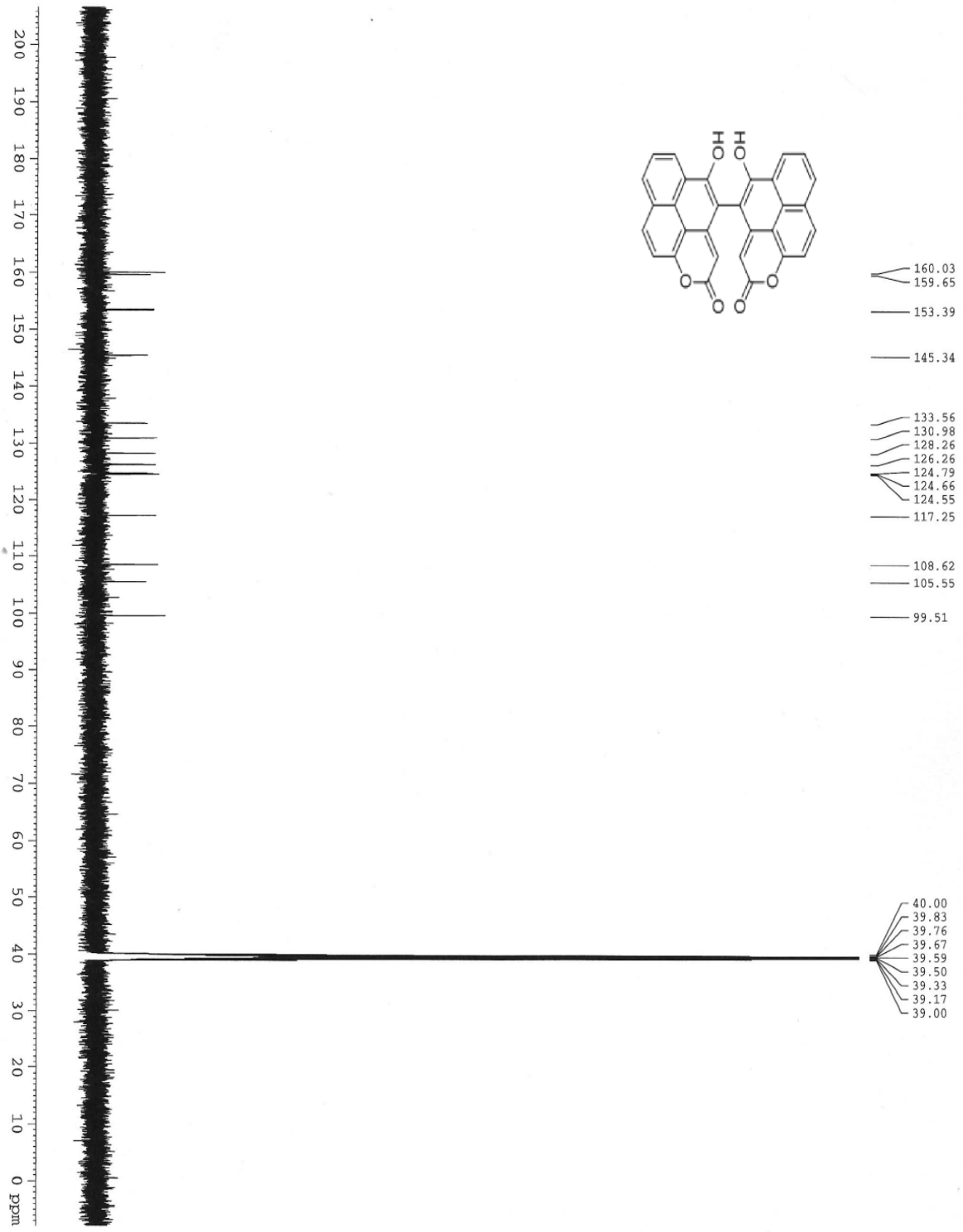
^{1}H NMR spectrum of **14** in DMSO.



^{13}C NMR spectrum of **14** in DMSO.



^{1}H NMR spectrum of **15** in DMSO (prepared *via* method C).



^{13}C NMR spectrum of **15** in DMSO (prepared *via* method C).

3. X-ray crystallography

Experimental

The X-ray measurement of **5** was performed at 100(2) K on a diffractometer equipped with a mirror monochromator and a CuKα IμS micro-focus source (λ=1.54178 Å). A total of 1385 frames were collected with APEX2 program.[1] The total exposure time was 46.17 hours. The frames were integrated with the SAINT software package [2] using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 20976 reflections to a maximum θ angle of 66.59° (0.84 Å resolution), of which 2927 were independent (average redundancy 7.166, completeness = 99.6%, R_{int} = 9.62%, R_{sig} = 3.99%) and 1793 (61.26%) were greater than $2\sigma(F^2)$. The final cell constants of a = 11.8416(3) Å, b = 16.6527(4) Å, c = 8.8363(2) Å, β = 107.638(2)°, volume = 1660.56(7) $Å^3$, are based upon the refinement of the XYZ-centroids of 6730 reflections above 20 σ(I) with 5.306° < 2θ < 134.1°. Data were corrected for absorption effects using the multi-scan method (SADABS).[3] The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7550 and 0.9110.

The structure was solved and refined using the SHELXTL Software Package[4], using the space group P 1 21/c 1, with Z = 4 for the formula unit, $C_{21}H_{20}O_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 219 variables converged at R1 = 4.73%, for the observed data and wR2 = 15.00% for all data. The goodness-of-fit was 1.055. The largest peak in the final difference electron density synthesis was 0.256 $e^-/Å^3$ and the largest hole was -0.154 $e^-/Å^3$ with an RMS deviation of 0.035 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.281 g/cm^3 and F(000), 680 e^-. The atomic scattering factors were taken from the International Tables [5].

Table 1. Sample and crystal data for 5.		
Identification code	**5**	
Chemical formula	$C_{21}H_{20}O_3$	
Formula weight	320.37 g/mol	
Temperature	296(2) K	
Wavelength	1.54178 Å	
Crystal size	0.140 x 0.402 x 0.439 mm	
Crystal habit	yellow plate	
Crystal system	monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 11.8416(3) Å	α = 90°
	b = 16.6527(4) Å	β = 107.638(2)°
	c = 8.8363(2) Å	γ = 90°
Volume	1660.56(7) $Å^3$	
Z	4	
Density (calculated)	1.281 g/cm^3	
Absorption coefficient	0.678 mm^{-1}	
F(000)	680	

Table 2. Data collection and structure refinement for 5.	
Theta range for data collection	3.92 to 66.59°
Index ranges	-13<=h<=11, -19<=k<=19, -10<=l<=10
Reflections collected	20976
Independent reflections	2927 [R(int) = 0.0962]
Coverage of independent reflections	99.6%
Absorption correction	multi-scan
Max. and min. transmission	0.9110 and 0.7550
Structure solution technique	direct methods
Structure solution program	SHELXL-2014 (Sheldrick, 2014)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	2927 / 0 / 219
Goodness-of-fit on F^2	1.055

Final R indices	1793 data; I>2σ(I)	R1 = 0.0473, wR2 = 0.1316
	all data	R1 = 0.0801, wR2 = 0.1500
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0803P)^2+0.0225P]$ where $P=(F_o^2+2F_c^2)/3$	
Extinction coefficient	0.0006(3)	
Largest diff. peak and hole	0.256 and -0.154 eÅ^{-3}	
R.M.S. deviation from mean	0.035 eÅ^{-3}	

References

[1] APEX2,. Bruker AXS Inc., Madison, Wisconsin, USA, **2013**.

[2] SAINT,. Bruker AXS Inc., Madison, Wisconsin, USA, **2013**.

[3] SADABS,. Bruker AXS Inc., Madison, Wisconsin, USA, **2012**.

[4] G. M. Sheldrick, *Acta Crystallogr*. **1990**, A46, 467-473; Sheldrick, G. M. *Acta Cryst*., **2008**, A64, 112–122.

[5] *International Tables for Crystallography*, Ed. A. J. C. Wilson, Kluwer: Dordrecht, **1992**, Vol.C.

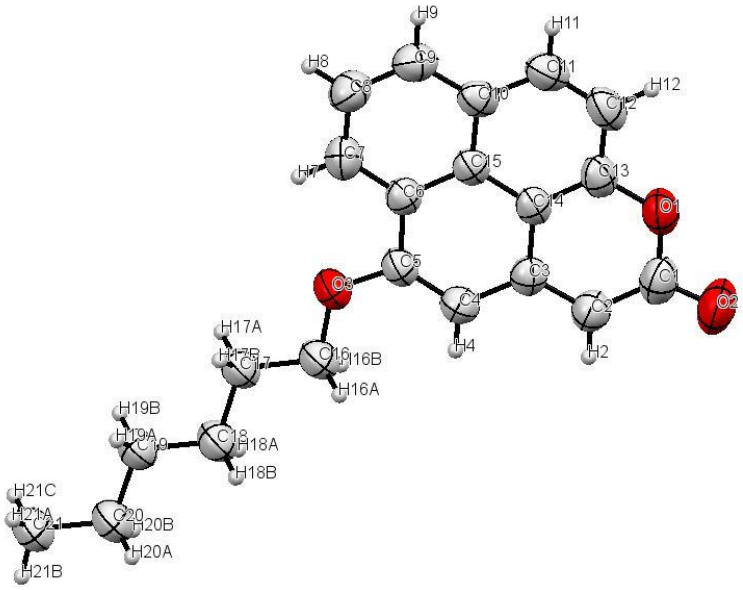
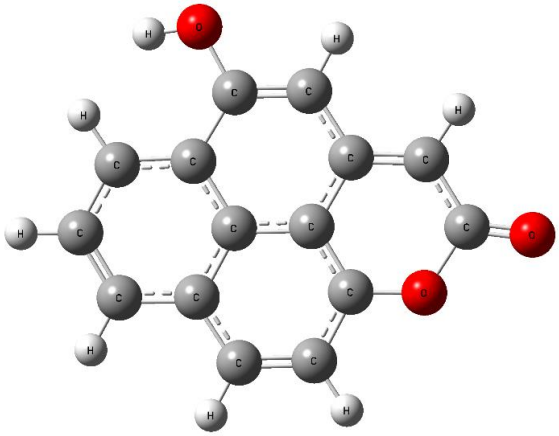


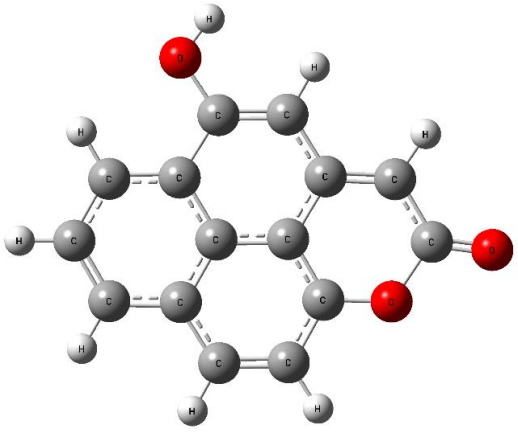
Figure S1. ORTEP structure of compound **5** (drawn at 50% of probability level)

4. Figure S2. Geometrical structures of compounds 3 and 7.

5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one (**3**). B3LYP/6-311+g(d,p)

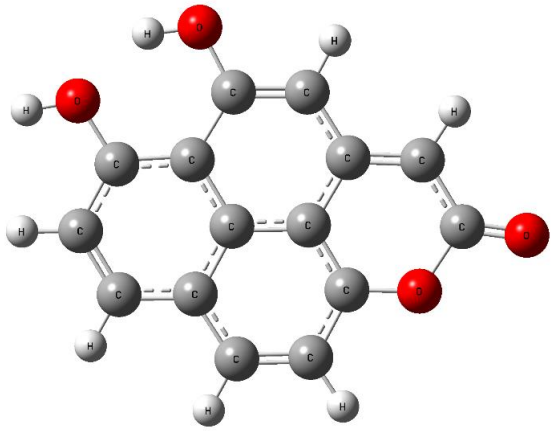


5HydNC-anti conformer.
E = -802.32245449

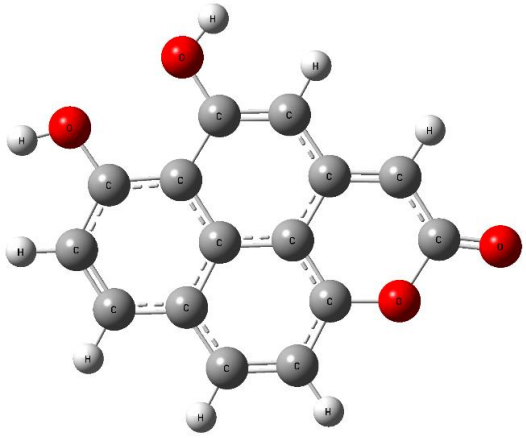


5HydNC-sin conformer.
E = -802.32615396

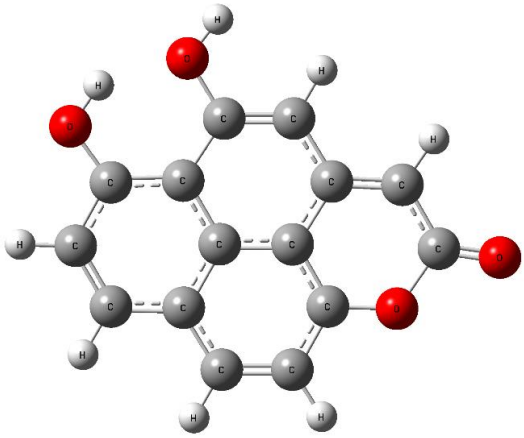
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one (**7**). B3LYP/6-311+g(d,p)



56DiHyd-anti-anti conformer.
E = -877.57526791



56DiHyd-anti-sin conformer.
E = -877.56665929



56DiHyd-sin-sin conformer.
E = -877.57822232

5. Table S1. 5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one (3) main visible transitions obtained with the IEFPCM-TD-X/6-311++g(d,p)//IEFPCM-X/6-311++g(d,p) approach.

Calculates photophysical properties (absorption λ^{calc}_{abs}, and emission λ^{calc}_{fl}, maxima and oscillator strength f corresponding to the indicated transitions) and experimentally measured absorption λ^{exp}_{abs} and emission λ^{exp}_{fl} maxima in various solvents and statistical analysis (sign error (SE) and mean absolute error (MAE)) for 5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one (**3**) compound.

Solvent	λ^{calc}_{abs} (nm)	f	λ^{calc}_{fl} (nm)	f	SE, (nm)		MAE, (nm)		Solvent: λ^{exp}_{abs} / λ^{exp}_{fl} (nm)
					λ_{abs}	λ_{fl}	λ_{abs}	λ_{fl}	
	B3LYP						51	19	Toluene: 465/471 DCM: 469 /473 MeOH: 461/473 DMSO: 470/480
Toluene	418.8	0.3280	483.3	0.3006	-46	12			
DCM	415.7	0.3316	493.8	0.4333	-53	21			
MeOH	413.3	0.3176	498.1	0.4849	-48	25			
DMSO	415.1	0.3362	498.7	0.4914	-55	19			
	PBE0						63	3	
Toluene	406.0	0.3476	467.6	0.3202	-59	-3			
DCM	402.9	0.3505	478.0	0.4574	-66	5			
MeOH	400.6	0.3355	482.3	0.5104	-60	9			
DMSO	402.3	0.3550	482.8	0.5171	-68	3			
	M06						59	11	
Toluene	410.1	0.3467	473.8	0.3213	-55	3			
DCM	407.2	0.3478	485.2	0.4573	-62	12			
MeOH	404.8	0.3323	489.8	0.5099	-56	17			
DMSO	406.6	0.3514	490.4	0.5165	-63	10			

6. Cartesian coordinate for studied molecules.

a) Cartesian coordinates for 5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one (**3**) in various IEFPCM solvents obtained with B3LYP, PBE1PBE and M06 functionals for ground and excited states.

Ground state. Toluene.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6155720	-0.9035720	0.0000360
6	-3.1539940	0.4225490	0.0000540
6	-1.7898370	0.6943320	0.0000390
6	-0.8611400	-0.3846620	0.0000050
6	-1.3305320	-1.7277560	-0.0000120
6	-2.7247730	-1.9603810	0.0000040
6	-1.2539100	2.0465090	0.0000570
6	0.5320750	-0.1241910	-0.0000110
6	1.0407400	1.2260570	0.0000060
6	0.0861310	2.2973480	0.0000400
6	2.4047210	1.4131980	-0.0000100
1	2.8414640	2.4031190	0.0000020
6	3.3314310	0.3205250	-0.0000450
6	1.4282420	-1.1859280	-0.0000430
6	0.9762510	-2.5253490	-0.0000600
6	-0.3711570	-2.7821390	-0.0000450
1	-0.7235630	-3.8077460	-0.0000580
1	1.7086140	-3.3227790	-0.0000850
1	-4.6820690	-1.0950210	0.0000480
1	-3.8607140	1.2421420	0.0000800
1	-3.0886250	-2.9821160	-0.0000100
1	0.4478540	3.3206150	0.0000520
8	2.7631650	-0.9774160	-0.0000590
8	4.5414630	0.3717770	-0.0000590
8	-2.1886580	3.0290770	0.0000900
1	-1.7627840	3.8950350	0.0001040

Excited state. Toluene.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6305880	-0.8870330	0.0000380
6	-3.2000630	0.4209800	0.0000550
6	-1.8001170	0.7139210	0.0000380
6	-0.8569970	-0.3724170	0.0000020
6	-1.3283540	-1.7238490	-0.0000130
6	-2.7118540	-1.9587020	0.0000040
6	-1.2906290	2.0285730	0.0000570
6	0.5260830	-0.1129670	-0.0000150
6	1.0174250	1.2282690	0.0000030
6	0.0921730	2.2843290	0.0000400
6	2.4216180	1.4083550	-0.0000140
1	2.8637780	2.3957400	0.0000080
6	3.3268240	0.3172150	-0.0000630
6	1.4478480	-1.1961940	-0.0000440
6	0.9945730	-2.5191150	-0.0000570
6	-0.3636660	-2.7764370	-0.0000440
1	-0.7141190	-3.8024020	-0.0000550
1	1.7213050	-3.3217350	-0.0000800
1	-4.6928840	-1.1023760	0.0000510
1	-3.9090410	1.2380320	0.0000810
1	-3.0764040	-2.9797970	-0.0000080
1	0.4471320	3.3097340	0.0000550
8	2.7909420	-0.9937620	-0.0000630
8	4.5465000	0.3689300	-0.0000390
8	-2.1898200	3.0429820	0.0000930
1	-1.7362920	3.8944080	0.0001090

Ground state. DCM.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6154150	-0.9037830	0.0000360
6	-3.1540880	0.4223350	0.0000540
6	-1.7895110	0.6952990	0.0000390
6	-0.8617250	-0.3841130	0.0000040
6	-1.3303580	-1.7273650	-0.0000120
6	-2.7244650	-1.9610820	0.0000040
6	-1.2536280	2.0475940	0.0000570
6	0.5314720	-0.1234830	-0.0000120
6	1.0390230	1.2262690	0.0000050
6	0.0882820	2.2977790	0.0000400
6	2.4062480	1.4124460	-0.0000110
1	2.8409290	2.4032080	0.0000050
6	3.3257780	0.3202350	-0.0000510
6	1.4262160	-1.1860350	-0.0000430
6	0.9766120	-2.5254950	-0.0000590
6	-0.3712110	-2.7822650	-0.0000450

Excited state. DCM.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6306560	-0.8871530	0.0000350
6	-3.1988900	0.4213870	0.0000530
6	-1.7978430	0.7129070	0.0000320
6	-0.8567760	-0.3737410	-0.0000100
6	-1.3277910	-1.7252330	-0.0000180
6	-2.7141630	-1.9583590	0.0000010
6	-1.2901390	2.0292760	0.0000580
6	0.5276550	-0.1148500	-0.0000350
6	1.0165310	1.2258080	-0.0000160
6	0.0939180	2.2830180	0.0000400
6	2.4224110	1.4092990	-0.0000370
1	2.8603560	2.3986960	0.0000230
6	3.3267090	0.3174670	-0.0001440
6	1.4455850	-1.1974770	-0.0000480
6	0.9948560	-2.5178190	-0.0000460
6	-0.3662620	-2.7774530	-0.0000390

1	-0.7235070	-3.8077010	-0.0000570	1	-0.7155520	-3.8035910	-0.0000410
1	1.7074660	-3.3242830	-0.0000840	1	1.7195210	-3.3224290	-0.0000590
1	-4.6817820	-1.0952630	0.0000490	1	-4.6930810	-1.1016460	0.0000520
1	-3.8625010	1.2404600	0.0000800	1	-3.9080150	1.2381960	0.0000860
1	-3.0879480	-2.9827160	-0.0000090	1	-3.0796340	-2.9791040	-0.0000070
1	0.4499830	3.3205800	0.0000540	1	0.4497820	3.3077280	0.0000630
8	2.7632820	-0.9745030	-0.0000600	8	2.7957390	-0.9904630	-0.0000770
8	4.5423040	0.3674520	-0.0000520	8	4.5499840	0.3725470	0.0000380
8	-2.1856370	3.0293610	0.0000910	8	-2.1890220	3.0414820	0.0001060
1	-1.7616180	3.8972110	0.0001050	1	-1.7398490	3.8961890	0.0001270

Ground state. MeOH.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6152650	-0.9039760	0.0000370
6	-3.1540740	0.4221480	0.0000540
6	-1.7893460	0.6956080	0.0000380
6	-0.8618710	-0.3839380	0.0000040
6	-1.3302030	-1.7272860	-0.0000120
6	-2.7242460	-1.9614360	0.0000040
6	-1.2536200	2.0480430	0.0000570
6	0.5312820	-0.1231790	-0.0000130
6	1.0383530	1.2264210	0.0000050
6	0.0890210	2.2980190	0.0000410
6	2.4068060	1.4123060	-0.0000120
1	2.8407410	2.4033970	0.0000070
6	3.3238610	0.3203650	-0.0000560
6	1.4255750	-1.1859950	-0.0000440
6	0.9768500	-2.5254680	-0.0000590
6	-0.3711050	-2.7823280	-0.0000440
1	-0.7232360	-3.8077370	-0.0000560
1	1.7072300	-3.3246920	-0.0000830
1	-4.6815710	-1.0955120	0.0000500
1	-3.8631080	1.2397280	0.0000800
1	-3.0875820	-2.9830400	-0.0000080
1	0.4512710	3.3204500	0.0000560
8	2.7633290	-0.9734080	-0.0000620
8	4.5427020	0.3660210	-0.0000470
8	-2.1851680	3.0290810	0.0000910
1	-1.7627650	3.8980430	0.0001030

Excited state. MeOH.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6306020	-0.8872750	0.0000350
6	-3.1982640	0.4215050	0.0000510
6	-1.7969030	0.7126690	0.0000260
6	-0.8566670	-0.3742210	-0.0000190
6	-1.3275620	-1.7256580	-0.0000220
6	-2.7150780	-1.9583540	0.0000010
6	-1.2898560	2.0297110	0.0000580
6	0.5282730	-0.1154480	-0.0000490
6	1.0163020	1.2250760	-0.0000270
6	0.0945930	2.2827980	0.0000410
6	2.4227330	1.4095980	-0.0000500
1	2.8593450	2.3996720	0.0000360
6	3.3266740	0.3174900	-0.0001940
6	1.4447140	-1.1978630	-0.0000530
6	0.9949180	-2.5173820	-0.0000420
6	-0.3671820	-2.7777590	-0.0000370
1	-0.7159840	-3.8039850	-0.0000330
1	1.7188600	-3.3227070	-0.0000500
1	-4.6930950	-1.1013470	0.0000570
1	-3.9074710	1.2382090	0.0000870
1	-3.0808530	-2.9789770	-0.0000020
1	0.4512440	3.3070730	0.0000710
8	2.7973140	-0.9892990	-0.0000860
8	4.5513110	0.3733260	0.0000900
8	-2.1891830	3.0408200	0.0001110
1	-1.7422100	3.8970110	0.0001340

Ground state. DMSO.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6152400	-0.9040080	0.0000370
6	-3.1540690	0.4221180	0.0000540
6	-1.7893230	0.6956440	0.0000380
6	-0.8618850	-0.3839170	0.0000040
6	-1.3301780	-1.7272800	-0.0000120
6	-2.7242120	-1.9614870	0.0000040
6	-1.2536250	2.0481030	0.0000570
6	0.5312610	-0.1231390	-0.0000130
6	1.0382660	1.2264440	0.0000050
6	0.0891100	2.2980530	0.0000410

Excited state. DMSO.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-B3LYP/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6305910	-0.8872910	0.0000350
6	-3.1981770	0.4215200	0.0000500
6	-1.7967790	0.7126450	0.0000240
6	-0.8566510	-0.3742800	-0.0000220
6	-1.3275320	-1.7257080	-0.0000230
6	-2.7151930	-1.9583570	0.0000020
6	-1.2898150	2.0297740	0.0000570
6	0.5283520	-0.1155200	-0.0000530
6	1.0162790	1.2249910	-0.0000290
6	0.0946810	2.2827810	0.0000420

6	2.4068750	1.4122960	-0.0000120
1	2.8407170	2.4034290	0.0000070
6	3.3236270	0.3203930	-0.0000570
6	1.4255000	-1.1859860	-0.0000440
6	0.9768870	-2.5254610	-0.0000590
6	-0.3710830	-2.7823370	-0.0000440
1	-0.7231870	-3.8077440	-0.0000560
1	1.7072110	-3.3247370	-0.0000830
1	-4.6815390	-1.0955540	0.0000500
1	-3.8631830	1.2396280	0.0000800
1	-3.0875290	-2.9830870	-0.0000080
1	0.4514590	3.3204270	0.0000560
8	2.7633360	-0.9732670	-0.0000620
8	4.5427560	0.3658520	-0.0000460
8	-2.1851440	3.0290240	0.0000910
1	-1.7629990	3.8981520	0.0001030

6	2.4227750	1.4096340	-0.0000510
1	2.8592320	2.3997900	0.0000410
6	3.3266700	0.3174890	-0.0002030
6	1.4446040	-1.1979090	-0.0000550
6	0.9949240	-2.5173310	-0.0000420
6	-0.3672960	-2.7777960	-0.0000370
1	-0.7160330	-3.8040350	-0.0000310
1	1.7187760	-3.3227450	-0.0000480
1	-4.6930940	-1.1013070	0.0000590
1	-3.9073940	1.2382100	0.0000880
1	-3.0810060	-2.9789640	0.0000010
1	0.4514560	3.3069920	0.0000730
8	2.7975030	-0.9891570	-0.0000890
8	4.5514780	0.3734000	0.0000990
8	-2.1892270	3.0407300	0.0001110
1	-1.7425700	3.8971260	0.0001350

Ground state. Toluene.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Atom	X	Y	Z
6	-3.5996570	-0.9017400	0.0000360
6	-3.1394620	0.4199700	0.0000540
6	-1.7820840	0.6902880	0.0000390
6	-0.8570720	-0.3833940	0.0000050
6	-1.3227260	-1.7188490	-0.0000120
6	-2.7112020	-1.9526000	0.0000040
6	-1.2508210	2.0387920	0.0000560
6	0.5302800	-0.1231200	-0.0000100
6	1.0355110	1.2218630	0.0000060
6	0.0838570	2.2892970	0.0000390
6	2.3922300	1.4068950	-0.0000100
1	2.8307610	2.3986640	0.0000020
6	3.3164060	0.3163360	-0.0000440
6	1.4247730	-1.1777550	-0.0000420
6	0.9748530	-2.5130440	-0.0000590
6	-0.3666480	-2.7692570	-0.0000450
1	-0.7232460	-3.7957110	-0.0000580
1	1.7118520	-3.3087200	-0.0000840
1	-4.6674710	-1.0940780	0.0000480
1	-3.8461300	1.2426440	0.0000790
1	-3.0709080	-2.9780800	-0.0000100
1	0.4466740	3.3147330	0.0000520
8	2.7505720	-0.9682560	-0.0000580
8	4.5193310	0.3700510	-0.0000610
8	-2.1812370	3.0085940	0.0000890
1	-1.7603030	3.8753390	0.0001040

Excited state. Toluene.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6139450	-0.8829090	0.0000360
6	-3.1843620	0.4198190	0.0000540
6	-1.7897360	0.7092750	0.0000390
6	-0.8514380	-0.3716950	0.0000060
6	-1.3205800	-1.7165620	-0.0000110
6	-2.6983390	-1.9508820	0.0000030
6	-1.2866780	2.0212210	0.0000570
6	0.5248230	-0.1137450	-0.0000100
6	1.0115340	1.2235620	0.0000080
6	0.0892170	2.2760700	0.0000410
6	2.4064800	1.4019260	-0.0000110
1	2.8513690	2.3908740	0.0000020
6	3.3144590	0.3105870	-0.0000470
6	1.4450410	-1.1901010	-0.0000420
6	0.9933770	-2.5071820	-0.0000580
6	-0.3602180	-2.7644090	-0.0000430
1	-0.7144170	-3.7914260	-0.0000560
1	1.7246640	-3.3082000	-0.0000820
1	-4.6777590	-1.0983020	0.0000470
1	-3.8921420	1.2409330	0.0000790
1	-3.0594780	-2.9756110	-0.0000100
1	0.4469750	3.3032100	0.0000540
8	2.7802510	-0.9861130	-0.0000600
8	4.5237910	0.3716680	-0.0000630
8	-2.1846840	3.0219990	0.0000900
1	-1.7386690	3.8756120	0.0001050

Ground state. DCM.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Atom	X	Y	Z
6	-3.5994490	-0.9019190	0.0000360
6	-3.1394360	0.4197580	0.0000540
6	-1.7816440	0.6911810	0.0000390
6	-0.8575300	-0.3828880	0.0000060
6	-1.3224950	-1.7185090	-0.0000120

Excited state. DCM.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6137780	-0.8831830	0.0000370
6	-3.1829340	0.4201020	0.0000560
6	-1.7872280	0.7084450	0.0000420
6	-0.8511310	-0.3730310	0.0000110
6	-1.3197670	-1.7178230	-0.0000100

6	-2.7108710	-1.9532890	0.0000040
6	-1.2506130	2.0398780	0.0000560
6	0.5298310	-0.1224500	-0.0000100
6	1.0338120	1.2221630	0.0000070
6	0.0859040	2.2898190	0.0000400
6	2.3937080	1.4063510	-0.0000090
1	2.8303330	2.3989280	0.0000010
6	3.3109590	0.3162500	-0.0000410
6	1.4228920	-1.1779670	-0.0000420
6	0.9752580	-2.5132720	-0.0000600
6	-0.3666570	-2.7694400	-0.0000450
1	-0.7231360	-3.7957250	-0.0000580
1	1.7107260	-3.3103360	-0.0000850
1	-4.6671420	-1.0942270	0.0000480
1	-3.8476760	1.2410810	0.0000790
1	-3.0702740	-2.9786480	-0.0000100
1	0.4485840	3.3148350	0.0000520
8	2.7507790	-0.9656650	-0.0000580
8	4.5198920	0.3661600	-0.0000640
8	-2.1785870	3.0085620	0.0000880
1	-1.7601120	3.8776400	0.0001030

6	-2.7006720	-1.9507590	0.0000040
6	-1.2860660	2.0220970	0.0000570
6	0.5265650	-0.1153860	-0.0000030
6	1.0107790	1.2214740	0.0000130
6	0.0908340	2.2750760	0.0000390
6	2.4074400	1.4028550	-0.0000030
1	2.8486570	2.3935490	-0.0000050
6	3.3138870	0.3104510	-0.0000150
6	1.4427310	-1.1913030	-0.0000400
6	0.9937600	-2.5058400	-0.0000620
6	-0.3626880	-2.7653440	-0.0000460
1	-0.7157810	-3.7925280	-0.0000630
1	1.7230460	-3.3088330	-0.0000900
1	-4.6777540	-1.0975960	0.0000470
1	-3.8909270	1.2409230	0.0000790
1	-3.0627860	-2.9751360	-0.0000120
1	0.4493070	3.3015580	0.0000500
8	2.7845210	-0.9826200	-0.0000530
8	4.5268770	0.3741120	-0.0000890
8	-2.1843700	3.0206310	0.0000860
1	-1.7429850	3.8777300	0.0000970

Ground state. MeOH.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Atom	X	Y	Z
6	-3.5993010	-0.9020900	0.0000360
6	-3.1394010	0.4195840	0.0000540
6	-1.7814610	0.6914790	0.0000390
6	-0.8576500	-0.3827240	0.0000060
6	-1.3223400	-1.7184450	-0.0000120
6	-2.7106680	-1.9536310	0.0000040
6	-1.2506260	2.0403270	0.0000560
6	0.5296840	-0.1221730	-0.0000100
6	1.0331540	1.2223230	0.0000080
6	0.0866090	2.2900490	0.0000400
6	2.3942510	1.4062610	-0.0000090
1	2.8301890	2.3991540	0.0000020
6	3.3091170	0.3164200	-0.0000400
6	1.4222920	-1.1779770	-0.0000420
6	0.9754940	-2.5132830	-0.0000600
6	-0.3665540	-2.7695210	-0.0000450
1	-0.7228570	-3.7957810	-0.0000590
1	1.7104770	-3.3107970	-0.0000860
1	-4.6669360	-1.0944370	0.0000480
1	-3.8482370	1.2403920	0.0000790
1	-3.0699710	-2.9789450	-0.0000100
1	0.4497690	3.3147050	0.0000540
8	2.7508480	-0.9647010	-0.0000580
8	4.5201780	0.3648560	-0.0000640
8	-2.1781180	3.0082920	0.0000870
1	-1.7612880	3.8785490	0.0001000

Excited state. MeOH.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6136550	-0.8833590	0.0000380
6	-3.1822400	0.4201740	0.0000560
6	-1.7862260	0.7082730	0.0000420
6	-0.8509910	-0.3735140	0.0000110
6	-1.3194600	-1.7182280	-0.0000090
6	-2.7015930	-1.9508370	0.0000050
6	-1.2857440	2.0226000	0.0000570
6	0.5272330	-0.1159100	-0.0000010
6	1.0106130	1.2208570	0.0000150
6	0.0914440	2.2749480	0.0000410
6	2.4077900	1.4031660	-0.0000010
1	2.8478470	2.3944520	-0.0000050
6	3.3137120	0.3103650	-0.0000100
6	1.4418630	-1.1916670	-0.0000400
6	0.9938640	-2.5053960	-0.0000640
6	-0.3635580	-2.7656390	-0.0000470
1	-0.7161460	-3.7929200	-0.0000630
1	1.7224520	-3.3090950	-0.0000920
1	-4.6777070	-1.0973280	0.0000480
1	-3.8903430	1.2408670	0.0000800
1	-3.0640770	-2.9750740	-0.0000120
1	0.4506530	3.3009850	0.0000510
8	2.7859030	-0.9814080	-0.0000530
8	4.5280390	0.3745380	-0.0000950
8	-2.1846520	3.0200820	0.0000830
1	-1.7454830	3.8786910	0.0000930

Ground state. DMSO.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Excited state. DMSO.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-M06/6-311++g(d,p)

Atom	X	Y	Z	Atom	X	Y	Z
6	-3.5992780	-0.9021180	0.0000370	6	-3.6136360	-0.8833820	0.0000380
6	-3.1393960	0.4195560	0.0000540	6	-3.1821460	0.4201830	0.0000560
6	-1.7814370	0.6915150	0.0000390	6	-1.7860970	0.7082570	0.0000430
6	-0.8576630	-0.3827050	0.0000060	6	-0.8509710	-0.3735730	0.0000120
6	-1.3223160	-1.7184400	-0.0000120	6	-1.3194210	-1.7182770	-0.0000090
6	-2.7106380	-1.9536800	0.0000040	6	-2.7017090	-1.9508510	0.0000040
6	-1.2506330	2.0403860	0.0000560	6	-1.2856990	2.0226720	0.0000570
6	0.5296660	-0.1221370	-0.0000100	6	0.5273180	-0.1159730	0.0000000
6	1.0330690	1.2223450	0.0000080	6	1.0105980	1.2207840	0.0000170
6	0.0866940	2.2900790	0.0000410	6	0.0915220	2.2749400	0.0000420
6	2.3943170	1.4062560	-0.0000090	6	2.4078340	1.4032040	0.0000000
1	2.8301700	2.3991890	0.0000020	1	2.8477550	2.3945620	-0.0000060
6	3.3088910	0.3164510	-0.0000400	6	3.3136910	0.3103520	-0.0000090
6	1.4222210	-1.1779750	-0.0000420	6	1.4417540	-1.1917110	-0.0000400
6	0.9755300	-2.5132820	-0.0000600	6	0.9938760	-2.5053440	-0.0000640
6	-0.3665340	-2.7695320	-0.0000450	6	-0.3636640	-2.7656750	-0.0000460
1	-0.7228090	-3.7957910	-0.0000590	1	-0.7161850	-3.7929710	-0.0000630
1	1.7104540	-3.3108500	-0.0000860	1	1.7223760	-3.3091320	-0.0000930
1	-4.6669050	-1.0944720	0.0000490	1	-4.6776980	-1.0972930	0.0000460
1	-3.8483070	1.2402980	0.0000790	1	-3.8902630	1.2408590	0.0000790
1	-3.0699290	-2.9789870	-0.0000100	1	-3.0642410	-2.9750690	-0.0000120
1	0.4499430	3.3146800	0.0000540	1	0.4508500	3.3009100	0.0000510
8	2.7508580	-0.9645780	-0.0000580	8	2.7860690	-0.9812590	-0.0000530
8	4.5202170	0.3647010	-0.0000640	8	4.5281840	0.3745710	-0.0000980
8	-2.1780850	3.0082450	0.0000870	8	-2.1847070	3.0200110	0.0000820
1	-1.7615050	3.8786700	0.0001000	1	-1.7458510	3.8788250	0.0000920

Ground state. Toluene.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6023470	-0.9057610	0.0000360
6	-3.1436230	0.4177800	0.0000540
6	-1.7838140	0.6894730	0.0000390
6	-0.8570000	-0.3839700	0.0000050
6	-1.3218610	-1.7226750	-0.0000120
6	-2.7116080	-1.9581250	0.0000040
6	-1.2547090	2.0401090	0.0000560
6	0.5306570	-0.1203150	-0.0000110
6	1.0349510	1.2263460	0.0000060
6	0.0821690	2.2935670	0.0000400
6	2.3950240	1.4108380	-0.0000100
1	2.8357840	2.4000170	0.0000020
6	3.3157500	0.3161000	-0.0000440
6	1.4276340	-1.1756840	-0.0000420
6	0.9799750	-2.5130030	-0.0000600
6	-0.3634750	-2.7722350	-0.0000450
1	-0.7146110	-3.7994740	-0.0000580
1	1.7155370	-3.3089850	-0.0000840
1	-4.6694380	-1.0994630	0.0000480
1	-3.8505260	1.2391350	0.0000790
1	-3.0727530	-2.9820140	-0.0000100
1	0.4425750	3.3184460	0.0000520
8	2.7537580	-0.9673350	-0.0000580
8	4.5222540	0.3702060	-0.0000600

Excited state. Toluene.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.6166920	-0.8894100	0.0000370
6	-3.1888370	0.4164340	0.0000540
6	-1.7937960	0.7084680	0.0000390
6	-0.8526330	-0.3715900	0.0000050
6	-1.3194700	-1.7190530	-0.0000120
6	-2.6988030	-1.9563630	0.0000040
6	-1.2911740	2.0224590	0.0000570
6	0.5253380	-0.1101230	-0.0000120
6	1.0114290	1.2283100	0.0000060
6	0.0872550	2.2801120	0.0000400
6	2.4105190	1.4058110	-0.0000120
1	2.8579280	2.3920040	0.0000040
6	3.3114400	0.3121100	-0.0000520
6	1.4477000	-1.1863060	-0.0000440
6	0.9982050	-2.5067580	-0.0000590
6	-0.3562460	-2.7663720	-0.0000440
1	-0.7056470	-3.7939170	-0.0000560
1	1.7280430	-3.3080240	-0.0000830
1	-4.6797290	-1.1062190	0.0000480
1	-3.8983280	1.2348310	0.0000800
1	-3.0605110	-2.9796920	-0.0000100
1	0.4420470	3.3069140	0.0000540
8	2.7825420	-0.9846310	-0.0000610
8	4.5263560	0.3695010	-0.0000520

8	-2.1872230	3.0101030	0.0000890
1	-1.7632190	3.8738670	0.0001030

8	-2.1884560	3.0249720	0.0000900
1	-1.7365180	3.8740680	0.0001030

Ground state. DCM.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6022220	-0.9059030	0.0000360
6	-3.1437160	0.4176570	0.0000540
6	-1.7834520	0.6904790	0.0000390
6	-0.8575490	-0.3834270	0.0000050
6	-1.3217170	-1.7223240	-0.0000120
6	-2.7113610	-1.9588340	0.0000040
6	-1.2543850	2.0413260	0.0000560
6	0.5301570	-0.1196740	-0.0000110
6	1.0333740	1.2265800	0.0000060
6	0.0843820	2.2941510	0.0000400
6	2.3965590	1.4103560	-0.0000100
1	2.8349300	2.4005660	0.0000030
6	3.3105370	0.3161530	-0.0000460
6	1.4257730	-1.1759390	-0.0000430
6	0.9803190	-2.5133670	-0.0000590
6	-0.3635460	-2.7724860	-0.0000450
1	-0.7146420	-3.7995760	-0.0000570
1	1.7142940	-3.3108100	-0.0000840
1	-4.6692200	-1.0995870	0.0000480
1	-3.8523430	1.2375470	0.0000790
1	-3.0722050	-2.9826360	-0.0000100
1	0.4447580	3.3186240	0.0000530
8	2.7536820	-0.9647100	-0.0000590
8	4.5230560	0.3659340	-0.0000570
8	-2.1844180	3.0101690	0.0000890
1	-1.7630350	3.8762370	0.0001020

Excited state. DCM.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.6167450	-0.8894900	0.0000380
6	-3.1875140	0.4169130	0.0000540
6	-1.7913650	0.7075630	0.0000360
6	-0.8522710	-0.3730160	0.0000000
6	-1.3188560	-1.7204500	-0.0000150
6	-2.7011920	-1.9561040	0.0000030
6	-1.2906230	2.0233160	0.0000550
6	0.5271110	-0.1120750	-0.0000190
6	1.0106790	1.2259100	-0.0000010
6	0.0891160	2.2790140	0.0000390
6	2.4114500	1.4069130	-0.0000170
1	2.8543590	2.3953380	0.0000110
6	3.3116670	0.3125550	-0.0000740
6	1.4457670	-1.1877110	-0.0000460
6	0.9984620	-2.5056690	-0.0000570
6	-0.3587910	-2.7674770	-0.0000440
1	-0.7070920	-3.7952160	-0.0000540
1	1.7261430	-3.3090490	-0.0000780
1	-4.6799550	-1.1053810	0.0000530
1	-3.8971540	1.2351120	0.0000820
1	-3.0639190	-2.9790890	-0.0000080
1	0.4448320	3.3051780	0.0000560
8	2.7869890	-0.9816010	-0.0000650
8	4.5298540	0.3726860	-0.0000270
8	-2.1879270	3.0232920	0.0000920
1	-1.7410670	3.8760740	0.0001060

Ground state. MeOH.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6021020	-0.9060660	0.0000360
6	-3.1437270	0.4175150	0.0000540
6	-1.7833010	0.6908160	0.0000390
6	-0.8577000	-0.3832530	0.0000050
6	-1.3215900	-1.7222600	-0.0000120
6	-2.7111870	-1.9591860	0.0000040
6	-1.2543610	2.0418240	0.0000560
6	0.5299960	-0.1194140	-0.0000110
6	1.0327590	1.2267130	0.0000060
6	0.0851370	2.2943980	0.0000410
6	2.3971090	1.4102880	-0.0000100
1	2.8346210	2.4008910	0.0000040
6	3.3087720	0.3163650	-0.0000470
6	1.4251860	-1.1759680	-0.0000430
6	0.9805390	-2.5134280	-0.0000600
6	-0.3634600	-2.7725960	-0.0000450
1	-0.7144080	-3.7996680	-0.0000580
1	1.7140120	-3.3113410	-0.0000840

Excited state. MeOH.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.6167020	-0.8896130	0.0000380
6	-3.1868690	0.4170420	0.0000540
6	-1.7904070	0.7073650	0.0000350
6	-0.8521270	-0.3735240	-0.0000010
6	-1.3186220	-1.7208920	-0.0000150
6	-2.7021310	-1.9561430	0.0000040
6	-1.2903380	2.0238020	0.0000560
6	0.5277780	-0.1126940	-0.0000210
6	1.0104950	1.2251930	-0.0000030
6	0.0898080	2.2788390	0.0000390
6	2.4118030	1.4072810	-0.0000200
1	2.8532580	2.3964670	0.0000120
6	3.3117440	0.3126520	-0.0000840
6	1.4450170	-1.1881350	-0.0000470
6	0.9985280	-2.5053010	-0.0000560
6	-0.3596790	-2.7678220	-0.0000440
1	-0.7074910	-3.7956640	-0.0000530
1	1.7254680	-3.3094240	-0.0000770

1	-4.6690510	-1.0997930	0.0000490	1	-4.6799920	-1.1050820	0.0000530
1	-3.8529920	1.2368570	0.0000800	1	-3.8966050	1.2351430	0.0000830
1	-3.0719220	-2.9829590	-0.0000090	1	-3.0652100	-2.9790010	-0.0000070
1	0.4459990	3.3185220	0.0000540	1	0.4462510	3.3045950	0.0000570
8	2.7536630	-0.9637340	-0.0000590	8	2.7884290	-0.9805200	-0.0000670
8	4.5234180	0.3645200	-0.0000560	8	4.5311610	0.3733270	-0.0000150
8	-2.1838910	3.0099410	0.0000890	8	-2.1880850	3.0226560	0.0000930
1	-1.7642000	3.8771820	0.0001010	1	-1.7435200	3.8769880	0.0001070

Ground state. Acetonitrile.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6020970	-0.9060720	0.0000360
6	-3.1437230	0.4175090	0.0000540
6	-1.7832920	0.6908300	0.0000390
6	-0.8577060	-0.3832500	0.0000060
6	-1.3215880	-1.7222590	-0.0000120
6	-2.7111840	-1.9592010	0.0000040
6	-1.2543630	2.0418470	0.0000560
6	0.5299910	-0.1194070	-0.0000100
6	1.0327300	1.2267110	0.0000070
6	0.0851660	2.2944020	0.0000400
6	2.3971290	1.4102830	-0.0000090
1	2.8345820	2.4009130	0.0000010
6	3.3087130	0.3163810	-0.0000410
6	1.4251680	-1.1759740	-0.0000420
6	0.9805450	-2.5134320	-0.0000600
6	-0.3634600	-2.7725990	-0.0000450
1	-0.7144060	-3.7996700	-0.0000590
1	1.7139950	-3.3113660	-0.0000860
1	-4.6690460	-1.0997930	0.0000480
1	-3.8530140	1.2368300	0.0000790
1	-3.0719150	-2.9829720	-0.0000100
1	0.4460500	3.3185130	0.0000540
8	2.7536610	-0.9637080	-0.0000580
8	4.5234340	0.3644730	-0.0000620
8	-2.1838660	3.0099460	0.0000870
1	-1.7642450	3.8772330	0.0000990

Excited state. Acetonitrile.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.6171120	-0.8886560	0.0000400
6	-3.1868560	0.4178760	0.0000580
6	-1.7902940	0.7077610	0.0000410
6	-0.8523750	-0.3734290	0.0000080
6	-1.3192820	-1.7206510	-0.0000120
6	-2.7029040	-1.9554640	0.0000040
6	-1.2898450	2.0240690	0.0000540
6	0.5276280	-0.1130270	-0.0000050
6	1.0107260	1.2247100	0.0000110
6	0.0903940	2.2786580	0.0000370
6	2.4121090	1.4064040	-0.0000030
1	2.8538190	2.3954800	-0.0000010
6	3.3117040	0.3114890	-0.0000170
6	1.4444870	-1.1887420	-0.0000410
6	0.9976220	-2.5057440	-0.0000640
6	-0.3606990	-2.7678720	-0.0000490
1	-0.7088080	-3.7956120	-0.0000660
1	1.7242890	-3.3101160	-0.0000910
1	-4.6804710	-1.1037830	0.0000520
1	-3.8963440	1.2361910	0.0000840
1	-3.0663100	-2.9782070	-0.0000130
1	0.4471830	3.3042880	0.0000480
8	2.7880370	-0.9814870	-0.0000530
8	4.5311830	0.3718030	-0.0000790
8	-2.1873060	3.0231560	0.0000830
1	-1.7425670	3.8774100	0.0000910

Ground state. DMSO.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.6020820	-0.9060930	0.0000370
6	-3.1437270	0.4174910	0.0000540
6	-1.7832810	0.6908570	0.0000390
6	-0.8577170	-0.3832330	0.0000050
6	-1.3215700	-1.7222550	-0.0000120
6	-2.7111610	-1.9592360	0.0000040
6	-1.2543640	2.0418900	0.0000560
6	0.5299770	-0.1193810	-0.0000110
6	1.0326790	1.2267320	0.0000060
6	0.0852280	2.2944300	0.0000410
6	2.3971760	1.4102850	-0.0000100
1	2.8345820	2.4009380	0.0000040
6	3.3085560	0.3164010	-0.0000470

Excited state. DMSO.
5-hydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.6166940	-0.8896310	0.0000380
6	-3.1867820	0.4170580	0.0000550
6	-1.7902830	0.7073460	0.0000360
6	-0.8521070	-0.3735870	-0.0000020
6	-1.3185920	-1.7209450	-0.0000150
6	-2.7022490	-1.9561520	0.0000030
6	-1.2902990	2.0238720	0.0000560
6	0.5278620	-0.1127690	-0.0000220
6	1.0104760	1.2251090	-0.0000040
6	0.0898960	2.2788250	0.0000390
6	2.4118480	1.4073260	-0.0000220
1	2.8531310	2.3966040	0.0000110
6	3.3117540	0.3126610	-0.0000880

6	1.4251180	-1.1759680	-0.0000430	6	1.4449220	-1.1881860	-0.0000460
6	0.9805730	-2.5134330	-0.0000600	6	0.9985360	-2.5052570	-0.0000550
6	-0.3634430	-2.7726110	-0.0000450	6	-0.3597880	-2.7678640	-0.0000440
1	-0.7143650	-3.7996820	-0.0000580	1	-0.7075340	-3.7957210	-0.0000530
1	1.7139860	-3.3114020	-0.0000840	1	1.7253840	-3.3094720	-0.0000750
1	-4.6690250	-1.0998280	0.0000490	1	-4.6799940	-1.1050440	0.0000530
1	-3.8530730	1.2367640	0.0000800	1	-3.8965310	1.2351450	0.0000840
1	-3.0718810	-2.9830050	-0.0000090	1	-3.0653730	-2.9789940	-0.0000080
1	0.4461770	3.3184990	0.0000550	1	0.4464500	3.3045210	0.0000570
8	2.7536620	-0.9636080	-0.0000590	8	2.7886010	-0.9803860	-0.0000670
8	4.5234660	0.3643520	-0.0000560	8	4.5313250	0.3733850	-0.0000110
8	-2.1838510	3.0099000	0.0000890	8	-2.1881220	3.0225750	0.0000940
1	-1.7644130	3.8773070	0.0001000	1	-1.7438740	3.8771160	0.0001080

b) Cartesian coordinates for 5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one (**5**) in various IEFPCM solvents obtained with PBE1PBE functional for ground and excited states.

Ground state. Toluene.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	2.9738940	2.1769920	0.0000300
6	2.9321710	0.7764760	0.0000490
6	1.7176060	0.1081970	0.0000330
6	0.5135340	0.8561510	-0.0000020
6	0.5552020	2.2731460	-0.0000200
6	1.8098680	2.9151950	-0.0000030
6	1.6228110	-1.3446630	0.0000520
6	-0.7317380	0.1896240	-0.0000180
6	-0.8064910	-1.2455310	0.0000010
6	0.4196260	-1.9857780	0.0000360
6	-2.0487900	-1.8292840	-0.0000170
1	-2.1724050	-2.9051480	-0.0000050
6	-3.2561670	-1.0620660	-0.0000510
6	-1.9037710	0.9271060	-0.0000520
6	-1.8780120	2.3370370	-0.0000710
6	-0.6738720	2.9867910	-0.0000550
1	-0.6470310	4.0720390	-0.0000700
1	-2.8183950	2.8758890	-0.0000980
1	3.9344150	2.6807470	0.0000430
1	3.8523650	0.2045860	0.0000750
1	1.8477120	4.0002660	-0.0000170
1	0.3613710	-3.0667390	0.0000500
8	-3.1067900	0.3302010	-0.0000680
8	-4.3905810	-1.4773670	-0.0000710
8	2.8122370	-1.9603160	0.0000850
6	2.8406090	-3.3777200	0.0001070
1	2.3554030	-3.7786970	0.8955100
1	2.3554420	-3.7787250	-0.8953050
1	3.8933080	-3.6543980	0.0001340

Excited state. Toluene.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.5930050	-0.8541120	0.0000390
6	-3.1435180	0.4451270	0.0000570
6	-1.7451640	0.7162140	0.0000410
6	-0.8240590	-0.3781290	0.0000060
6	-1.3105710	-1.7194900	-0.0000130
6	-2.6933520	-1.9356300	0.0000040
6	-1.2262710	2.0318690	0.0000590
6	0.5582340	-0.1383720	-0.0000090
6	1.0608530	1.1911640	0.0000090
6	0.1569420	2.2641300	0.0000430
6	2.4626770	1.3502060	-0.0000090
1	2.9230740	2.3303570	0.0000010
6	3.3490860	0.2445950	-0.0000400
6	1.4647660	-1.2288960	-0.0000440
6	0.9959630	-2.5415030	-0.0000630
6	-0.3633640	-2.7808860	-0.0000480
1	-0.7276640	-3.8031360	-0.0000630
1	1.7135640	-3.3538330	-0.0000900
1	-4.6595540	-1.0533120	0.0000510
1	-3.8394470	1.2746720	0.0000840
1	-3.0712810	-2.9531280	-0.0000110
1	0.5474640	3.2737020	0.0000570
8	2.8031770	-1.0449900	-0.0000600
8	4.5649880	0.2856020	-0.0000670
8	-2.1355520	3.0166180	0.0000920
6	-1.6969790	4.3654490	0.0001150
1	-1.1101320	4.5893590	0.8962170
1	-1.1101600	4.5893970	-0.8959970
1	-2.6026220	4.9692800	0.0001420

Ground state. DCM.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	2.9731460	2.1786380	0.0000300

Excited state. DCM.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.5933490	-0.8549070	0.0000380

6	2.9322830	0.7781430	0.0000490	6	-3.1427630	0.4449790	0.0000570
6	1.7178170	0.1083650	0.0000330	6	-1.7434510	0.7149590	0.0000420
6	0.5139830	0.8561940	-0.0000020	6	-0.8239680	-0.3795370	0.0000070
6	0.5543930	2.2731710	-0.0000200	6	-1.3100180	-1.7207550	-0.0000130
6	1.8084050	2.9166980	-0.0000040	6	-2.6957140	-1.9357730	0.0000040
6	1.6236910	-1.3445500	0.0000520	6	-1.2265460	2.0321140	0.0000600
6	-0.7310310	0.1889270	-0.0000180	6	0.5597970	-0.1398840	-0.0000090
6	-0.8044420	-1.2456420	0.0000010	6	1.0597930	1.1894100	0.0000090
6	0.4188300	-1.9862060	0.0000360	6	0.1578960	2.2628270	0.0000430
6	-2.0496410	-1.8300860	-0.0000170	6	2.4635930	1.3513990	-0.0000090
1	-2.1707590	-2.9062190	-0.0000050	1	2.9203310	2.3334990	0.0000010
6	-3.2507070	-1.0616730	-0.0000510	6	3.3491220	0.2451960	-0.0000420
6	-1.9023410	0.9272540	-0.0000520	6	1.4627310	-1.2298290	-0.0000440
6	-1.8792130	2.3366740	-0.0000710	6	0.9961420	-2.5401350	-0.0000630
6	-0.6749380	2.9869400	-0.0000560	6	-0.3658720	-2.7817490	-0.0000480
1	-0.6485290	4.0720420	-0.0000700	1	-0.7291000	-3.8042060	-0.0000630
1	-2.8186560	2.8771520	-0.0000980	1	1.7116070	-3.3544980	-0.0000900
1	3.9333740	2.6827590	0.0000430	1	-4.6600270	-1.0532920	0.0000500
1	3.8538200	0.2083460	0.0000760	1	-3.8389910	1.2742320	0.0000840
1	1.8454470	4.0016330	-0.0000170	1	-3.0742200	-2.9530760	-0.0000110
1	0.3611470	-3.0671150	0.0000500	1	0.5484610	3.2724310	0.0000570
8	-3.1059990	0.3267100	-0.0000680	8	2.8074040	-1.0420300	-0.0000600
8	-4.3918960	-1.4751620	-0.0000710	8	4.5683360	0.2886450	-0.0000650
8	2.8102990	-1.9600530	0.0000850	8	-2.1346370	3.0154060	0.0000930
6	2.8400500	-3.3804690	0.0001070	6	-1.6961010	4.3675100	0.0001150
1	2.3550870	-3.7799520	0.8955950	1	-1.1099220	4.5898540	0.8963580
1	2.3551260	-3.7799790	-0.8953910	1	-1.1099510	4.5898920	-0.8961390
1	3.8930080	-3.6549030	0.0001340	1	-2.6024850	4.9696400	0.0001420

Ground state. MeOH.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	2.9730370	2.1790920	0.0000300
6	2.9324090	0.7786060	0.0000490
6	1.7179370	0.1083390	0.0000330
6	0.5141920	0.8561520	-0.0000020
6	0.5542620	2.2731230	-0.0000200
6	1.8080600	2.9171270	-0.0000040
6	1.6239270	-1.3445550	0.0000520
6	-0.7307630	0.1886960	-0.0000180
6	-0.8037780	-1.2456680	0.0000000
6	0.4184460	-1.9863680	0.0000360
6	-2.0500580	-1.8303110	-0.0000170
1	-2.1703740	-2.9065660	-0.0000050
6	-3.2488660	-1.0614330	-0.0000510
6	-1.9017950	0.9274200	-0.0000520
6	-1.8794420	2.3366540	-0.0000710
6	-0.6750790	2.9870290	-0.0000550
1	-0.6486580	4.0720700	-0.0000700
1	-2.8184990	2.8778140	-0.0000970
1	3.9331910	2.6832820	0.0000430
1	3.8544120	0.2095230	0.0000750
1	1.8447540	4.0020150	-0.0000180
1	0.3609220	-3.0672530	0.0000500
8	-3.1057000	0.3257480	-0.0000680

Excited state. MeOH.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.5934930	-0.8553760	0.0000370
6	-3.1424450	0.4448000	0.0000560
6	-1.7428530	0.7145870	0.0000410
6	-0.8239190	-0.3800020	0.0000060
6	-1.3097920	-1.7210990	-0.0000130
6	-2.6966110	-1.9359720	0.0000030
6	-1.2265980	2.0322310	0.0000600
6	0.5603780	-0.1402940	-0.0000090
6	1.0594760	1.1890130	0.0000080
6	0.1581340	2.2625730	0.0000430
6	2.4638830	1.3519230	-0.0000110
1	2.9194840	2.3346910	-0.0000020
6	3.3490830	0.2454310	-0.0000440
6	1.4619690	-1.2300630	-0.0000430
6	0.9961700	-2.5396450	-0.0000620
6	-0.3667630	-2.7819560	-0.0000470
1	-0.7297370	-3.8044440	-0.0000620
1	1.7108370	-3.3547720	-0.0000880
1	-4.6602330	-1.0533990	0.0000490
1	-3.8388580	1.2738950	0.0000820
1	-3.0751210	-2.9532740	-0.0000110
1	0.5486640	3.2721860	0.0000570
8	2.8087710	-1.0409360	-0.0000600

8	-4.3924730	-1.4741470	-0.0000710	8	4.5695100	0.2893810	-0.0000660
8	2.8095190	-1.9601590	0.0000850	8	-2.1344720	3.0150560	0.0000940
6	2.8395030	-3.3815680	0.0001070	6	-1.6957500	4.3681330	0.0001160
1	2.3544960	-3.7804960	0.8955820	1	-1.1096520	4.5898720	0.8963420
1	2.3545360	-3.7805230	-0.8953760	1	-1.1096810	4.5899110	-0.8961190
1	3.8925110	-3.6554150	0.0001350	1	-2.6022860	4.9698720	0.0001440

Ground state. Acetonitrile.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	2.9730180	2.1791230	0.0000300
6	2.9324060	0.7786330	0.0000480
6	1.7179410	0.1083450	0.0000320
6	0.5141920	0.8561520	-0.0000020
6	0.5542420	2.2731220	-0.0000200
6	1.8080330	2.9171510	-0.0000030
6	1.6239400	-1.3445510	0.0000510
6	-0.7307580	0.1886830	-0.0000190
6	-0.8037550	-1.2456750	-0.0000010
6	0.4184430	-1.9863750	0.0000350
6	-2.0500650	-1.8303290	-0.0000190
1	-2.1703590	-2.9065870	-0.0000030
6	-3.2488020	-1.0614310	-0.0000590
6	-1.9017800	0.9274180	-0.0000520
6	-1.8794640	2.3366440	-0.0000690
6	-0.6750990	2.9870280	-0.0000540
1	-0.6486800	4.0720670	-0.0000680
1	-2.8185090	2.8778230	-0.0000950
1	3.9331690	2.6833170	0.0000430
1	3.8544310	0.2095850	0.0000750
1	1.8447080	4.0020370	-0.0000160
1	0.3609150	-3.0672580	0.0000500
8	-3.1056980	0.3256990	-0.0000690
8	-4.3924850	-1.4741360	-0.0000630
8	2.8095020	-1.9601480	0.0000860
6	2.8395300	-3.3815830	0.0001090
1	2.3545310	-3.7805060	0.8955820
1	2.3545720	-3.7805340	-0.8953740
1	3.8925470	-3.6553910	0.0001370

Excited state. Acetonitrile.
5-methoxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	2.9920550	2.1684170	0.0000300
6	2.9727210	0.7923470	0.0000470
6	1.7289510	0.0961390	0.0000290
6	0.5124520	0.8462490	-0.0000070
6	0.5519590	2.2720940	-0.0000220
6	1.8008990	2.9121680	-0.0000040
6	1.6532500	-1.3170120	0.0000500
6	-0.7262630	0.1833940	-0.0000250
6	-0.7820080	-1.2354160	-0.0000070
6	0.4111810	-1.9710960	0.0000330
6	-2.0639550	-1.8317190	-0.0000260
1	-2.1873650	-2.9079090	-0.0000020
6	-3.2521840	-1.0596960	-0.0000780
6	-1.9247540	0.9343830	-0.0000540
6	-1.8944070	2.3239730	-0.0000660
6	-0.6767850	2.9826050	-0.0000530
1	-0.6537570	4.0673610	-0.0000630
1	-2.8291220	2.8730560	-0.0000890
1	3.9424200	2.6918250	0.0000440
1	3.8945240	0.2243070	0.0000750
1	1.8403120	3.9968890	-0.0000150
1	0.3579420	-3.0522980	0.0000490
8	-3.1438200	0.3312750	-0.0000730
8	-4.3969180	-1.4852130	-0.0000430
8	2.8241130	-1.9644830	0.0000860
6	2.8331270	-3.3869130	0.0001110
1	2.3464800	-3.7816810	0.8963360
1	2.3465230	-3.7817130	-0.8961220
1	3.8828960	-3.6730520	0.0001410

c) Cartesian coordinates for 5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one (**7**) in various IEFPCM solvents obtained with PBE1PBE functional for ground and excited states.

Ground state. Toluene.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.2263680	1.3652670	0.0000610
6	-2.9308630	-0.0127780	0.0001170
6	-1.5971370	-0.4473150	0.0000780
6	-0.5610060	0.5307710	-0.0000090
6	-0.8682640	1.9131800	-0.0000630
6	-2.2265940	2.2998610	-0.0000270
6	-1.1906610	-1.8330830	0.0001270

Excited state. Toluene.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.2524680	1.3499320	0.0001010
6	-2.9756670	-0.0008500	0.0001580
6	-1.6041850	-0.4635360	0.0001190
6	-0.5564540	0.5231780	0.0000320
6	-0.8751380	1.9105250	-0.0000240
6	-2.2237120	2.2960350	0.0000090
6	-1.2271500	-1.8122780	0.0001660

6	0.7936370	0.1255030	-0.0000410
6	1.1656610	-1.2623310	0.0000150
6	0.1102110	-2.2248540	0.0000970
6	2.4997010	-1.5894830	-0.0000160
1	2.8336320	-2.6195110	0.0000230
6	3.5265120	-0.5974400	-0.0001010
6	1.7999490	1.0845110	-0.0001230
6	1.5016380	2.4582470	-0.0001780
6	0.1896900	2.8535880	-0.0001480
1	-0.0541350	3.9114600	-0.0001890
1	2.3168610	3.1719360	-0.0002410
1	-4.2711170	1.6543740	0.0000910
1	-2.4746230	3.3568680	-0.0000690
1	0.3588320	-3.2821670	0.0001360
8	3.0969880	0.7364740	-0.0001520
8	4.7221570	-0.7712730	-0.0001330
8	-2.2088800	-2.7336420	0.0002030
1	-1.8762520	-3.6366690	0.0002830
8	-3.9926830	-0.8299580	0.0002040
1	-3.6904960	-1.7509360	0.0002420

Ground state. DCM.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.2258720	1.3654090	0.0000610
6	-2.9303020	-0.0127700	0.0001170
6	-1.5959900	-0.4478270	0.0000750
6	-0.5612950	0.5305980	-0.0000110
6	-0.8678930	1.9131710	-0.0000640
6	-2.2262840	2.3007030	-0.0000270
6	-1.1915000	-1.8340620	0.0001240
6	0.7932700	0.1246320	-0.0000420
6	1.1631910	-1.2629430	0.0000140
6	0.1115340	-2.2256970	0.0000940
6	2.5009600	-1.5896940	-0.0000150
1	2.8323800	-2.6205440	0.0000250
6	3.5210350	-0.5980570	-0.0000990
6	1.7984920	1.0845860	-0.0001220
6	1.5023610	2.4580140	-0.0001760
6	0.1898030	2.8537640	-0.0001480
1	-0.0536010	3.9115590	-0.0001880
1	2.3160450	3.1735080	-0.0002380
1	-4.2701050	1.6566920	0.0000930
1	-2.4743940	3.3575290	-0.0000680
1	0.3588330	-3.2827700	0.0001340
8	3.0972010	0.7333700	-0.0001500
8	4.7233590	-0.7683370	-0.0001300
8	-2.2084340	-2.7293070	0.0001980
1	-1.8847330	-3.6366500	0.0002950
8	-3.9904470	-0.8313560	0.0002080
1	-3.6869110	-1.7532390	0.0002480

Ground state. MeOH.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

6	0.7890920	0.1205570	0.0000020
6	1.1387130	-1.2597310	0.0000560
6	0.1160550	-2.2108840	0.0001370
6	2.5135910	-1.5782240	0.0000220
1	2.8572640	-2.6053330	0.0000610
6	3.5240350	-0.5828630	-0.0000650
6	1.8212910	1.0940890	-0.0000820
6	1.5123810	2.4491810	-0.0001360
6	0.1892410	2.8466890	-0.0001080
1	-0.0500750	3.9053380	-0.0001500
1	2.3197690	3.1721960	-0.0002000
1	-4.2916520	1.6582350	0.0001300
1	-2.4712720	3.3526840	-0.0000350
1	0.3604490	-3.2691260	0.0001760
8	3.1343150	0.7550000	-0.0001130
8	4.7252130	-0.7755360	-0.0000910
8	-2.2144680	-2.7480930	0.0002380
1	-1.8540910	-3.6397900	0.0003150
8	-4.0102870	-0.8514860	0.0002520
1	-3.6857380	-1.7648700	0.0002910

Excited state. DCM.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.2519570	1.3500400	0.0001020
6	-2.9727740	-0.0020460	0.0001570
6	-1.5999210	-0.4621480	0.0001170
6	-0.5558710	0.5250820	0.0000310
6	-0.8745330	1.9125030	-0.0000240
6	-2.2272880	2.2961050	0.0000100
6	-1.2260050	-1.8144170	0.0001620
6	0.7914060	0.1224630	0.0000000
6	1.1384410	-1.2574180	0.0000580
6	0.1175170	-2.2102270	0.0001360
6	2.5143730	-1.5800430	0.0000280
1	2.8533400	-2.6089340	0.0000690
6	3.5245030	-0.5844740	-0.0000620
6	1.8188840	1.0956940	-0.0000840
6	1.5119200	2.4487180	-0.0001380
6	0.1863820	2.8493710	-0.0001080
1	-0.0516710	3.9080370	-0.0001490
1	2.3174240	3.1741020	-0.0002010
1	-4.2913650	1.6583400	0.0001330
1	-2.4765020	3.3524110	-0.0000320
1	0.3620090	-3.2679710	0.0001760
8	3.1380080	0.7509780	-0.0001170
8	4.7290610	-0.7785790	-0.0000960
8	-2.2153130	-2.7432420	0.0002270
1	-1.8666530	-3.6406690	0.0003220
8	-4.0054830	-0.8541380	0.0002520
1	-3.6788790	-1.7684990	0.0002930

Excited state. MeOH.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.2258150	1.3653090	0.0000610
6	-2.9301670	-0.0129210	0.0001170
6	-1.5955890	-0.4480520	0.0000740
6	-0.5614110	0.5305290	-0.0000120
6	-0.8678840	1.9131280	-0.0000650
6	-2.2263200	2.3008650	-0.0000280
6	-1.1917310	-1.8343730	0.0001230
6	0.7931460	0.1244250	-0.0000430
6	1.1623210	-1.2630650	0.0000130
6	0.1121290	-2.2258880	0.0000920
6	2.5014590	-1.5896690	-0.0000150
1	2.8318760	-2.6208620	0.0000250
6	3.5191650	-0.5982880	-0.0000980
6	1.7979860	1.0847780	-0.0001210
6	1.5024330	2.4580670	-0.0001750
6	0.1896040	2.8538720	-0.0001470
1	-0.0538540	3.9116000	-0.0001860
1	2.3154710	3.1743330	-0.0002360
1	-4.2698730	1.6573260	0.0000940
1	-2.4744120	3.3576300	-0.0000680
1	0.3589980	-3.2828760	0.0001310
8	3.0973170	0.7325540	-0.0001480
8	4.7238330	-0.7673930	-0.0001280
8	-2.2079870	-2.7279880	0.0001950
1	-1.8868240	-3.6366000	0.0003040
8	-3.9896220	-0.8320020	0.0002100
1	-3.6856820	-1.7542160	0.0002520

Atom	X	Y	Z
6	-3.2516340	1.3502220	0.0001020
6	-2.9715830	-0.0024970	0.0001580
6	-1.5984360	-0.4617350	0.0001140
6	-0.5557160	0.5257460	0.0000290
6	-0.8742960	1.9131330	-0.0000260
6	-2.2285840	2.2963020	0.0000080
6	-1.2255190	-1.8152450	0.0001580
6	0.7922520	0.1230600	0.0000000
6	1.1383350	-1.2567290	0.0000570
6	0.1179590	-2.2101730	0.0001320
6	2.5145360	-1.5806580	0.0000290
1	2.8518340	-2.6101680	0.0000690
6	3.5245160	-0.5851340	-0.0000600
6	1.8179550	1.0961600	-0.0000830
6	1.5116610	2.4486830	-0.0001370
6	0.1853820	2.8503180	-0.0001090
1	-0.0524420	3.9089550	-0.0001490
1	2.3165400	3.1748830	-0.0001990
1	-4.2911700	1.6583670	0.0001340
1	-2.4782230	3.3525110	-0.0000340
1	0.3625360	-3.2677430	0.0001710
8	3.1391740	0.7495730	-0.0001150
8	4.7303780	-0.7796500	-0.0000950
8	-2.2155530	-2.7416830	0.0002190
1	-1.8705100	-3.6408680	0.0003320
8	-4.0036990	-0.8548740	0.0002560
1	-3.6766410	-1.7697170	0.0003000

Ground state. Acetonitrile.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM-PBE1PBE/6-311++g(d,p)

Atom	X	Y	Z
6	-3.2258160	1.3653010	0.0000590
6	-2.9301640	-0.0129280	0.0001150
6	-1.5955750	-0.4480600	0.0000770
6	-0.5614150	0.5305260	-0.0000090
6	-0.8678870	1.9131260	-0.0000630
6	-2.2263230	2.3008670	-0.0000280
6	-1.1917370	-1.8343810	0.0001290
6	0.7931410	0.1244200	-0.0000400
6	1.1622900	-1.2630660	0.0000150
6	0.1121520	-2.2258920	0.0000970
6	2.5014770	-1.5896670	-0.0000170
1	2.8318530	-2.6208740	0.0000200
6	3.5191010	-0.5983020	-0.0000980
6	1.7979690	1.0847870	-0.0001220
6	1.5024330	2.4580710	-0.0001760
6	0.1895940	2.8538760	-0.0001470
1	-0.0538670	3.9116020	-0.0001870
1	2.3154460	3.1743670	-0.0002380
1	-4.2698670	1.6573460	0.0000880
1	-2.4744150	3.3576300	-0.0000690
1	0.3590050	-3.2828770	0.0001380
8	3.0973200	0.7325290	-0.0001500
8	4.7238520	-0.7673600	-0.0001390

Excited state. Acetonitrile.
5,6-dihydroxy-2H-naphtho[2,1,8-def]chromen-2-one
IEFPCM- PBE1PBE /6-311++g(d,p)

Atom	X	Y	Z
6	-3.2486380	1.3546460	0.0000620
6	-2.9705500	0.0014930	0.0001180
6	-1.5980720	-0.4597390	0.0000770
6	-0.5539450	0.5262140	-0.0000100
6	-0.8704760	1.9140680	-0.0000640
6	-2.2242530	2.2992180	-0.0000290
6	-1.2271840	-1.8138400	0.0001250
6	0.7934530	0.1215390	-0.0000420
6	1.1374690	-1.2587550	0.0000160
6	0.1157070	-2.2107180	0.0000980
6	2.5131990	-1.5847560	-0.0000150
1	2.8489210	-2.6147830	0.0000330
6	3.5246390	-0.5907250	-0.0001150
6	1.8205270	1.0931220	-0.0001240
6	1.5162490	2.4460790	-0.0001740
6	0.1905380	2.8497010	-0.0001450
1	-0.0457200	3.9086860	-0.0001850
1	2.3221750	3.1711220	-0.0002350
1	-4.2877240	1.6643170	0.0000940
1	-2.4723490	3.3557900	-0.0000700
1	0.3587300	-3.2686410	0.0001400
8	3.1413060	0.7445240	-0.0001580
8	4.7302600	-0.7870330	-0.0001230

8	-2.2079680	-2.7279410	0.0002070	8	-2.2186080	-2.7387350	0.0001960
1	-1.8868880	-3.6365950	0.0002880	1	-1.8750120	-3.6384860	0.0002840
8	-3.9895900	-0.8320310	0.0002030	8	-4.0039000	-0.8493720	0.0002130
1	-3.6856300	-1.7542550	0.0002440	1	-3.6781740	-1.7647130	0.0002540