Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supplementary information for:

Unexpected formation of dibenzo[*de*,*h*]isoquinolin-7-on from 1,5,9,10-tetramethoxyanthracene *via* the Duff reaction

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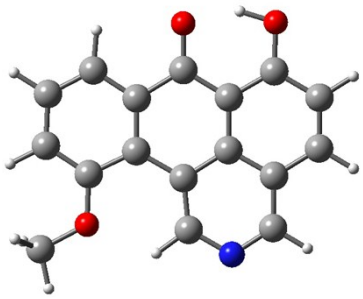
Table S1. Energy and oscillator strengths of the electronic transitions. The structure of **3** was optimized in the ground state (for the $S_0 \rightarrow S_i$ absorption transitions) and in the excited S_1 state (for the $S_1 \rightarrow S_0$ fluorescence).

hν [cm^{-1}]	λ [nm]	f
	$S_0 \rightarrow S_k$	
24599	406.52	0.1577
28446	351.55	0.0001
29265	341.70	0.0000
30100	332.23	0.0680
30707	325.65	0.0517
32564	307.09	0.0431
35861	278.85	0.2145
36853	271.35	0.0399
38292	261.15	0.0287
39858	250.89	0.0018
40794	245.13	0.0023
41410	241.49	0.1358
41838	239.02	0.0005
42061	237.75	0.0006
42479	235.41	0.0631
42530	235.13	0.0000
43438	230.21	0.0200
44402	225.22	0.0299
44588	224.27	0.0000
44847	222.98	0.0757
44945	222.50	0.0004
45271	220.89	0.0002
45694	218.85	0.0507

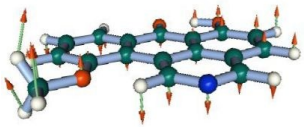
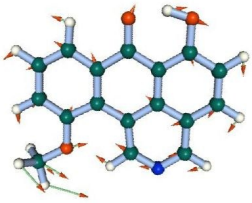
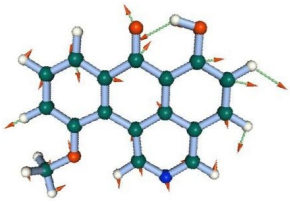
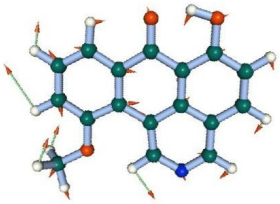
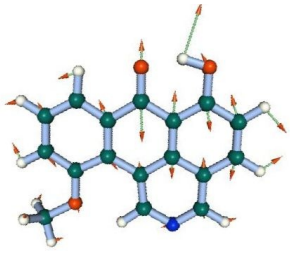
45929	217.73	0.4488
46040	217.20	0.0001
46142	216.72	0.0055
46865	213.38	0.0000
47178	211.96	0.0017
47331	211.28	0.0368
47960	208.51	0.0076
48336	206.88	0.0159
48478	206.28	0.0976
48941	204.33	0.0016
49568	201.74	0.0002
49728	201.09	0.4363
	$S_0 \rightarrow T_k$	
17895	558.81	0.0000
22915	436.39	0.0000
24227	412.77	0.0000
26242	381.07	0.0000
26612	375.76	0.0000
	$S_1 \rightarrow S_0$	
21384	467.64	0.1262

Table S2. Calculated bond lengths characterizing intramolecular hydrogen bonding in **3** molecule.



	R(O'O'')	<(O'HO'')	R(O'H)	R(HO'')
S_0(N)	2.512	151.2	1.013	1.577
S_0(TS)	2.378	158.2	1.259	1.162
S_0(PT)	2.463	154.2	1.487	1.038
S_1(N)	2.543	152.7	1.010	1.602

Table S3. Graphical presentation of main vibrations contributing to the fluorescence spectrum of **3**.

No.	hν [cm^{-1}]	
|1>	33	
|6>	181	
|21>	523	
|58>	1300	
|79>	1683	

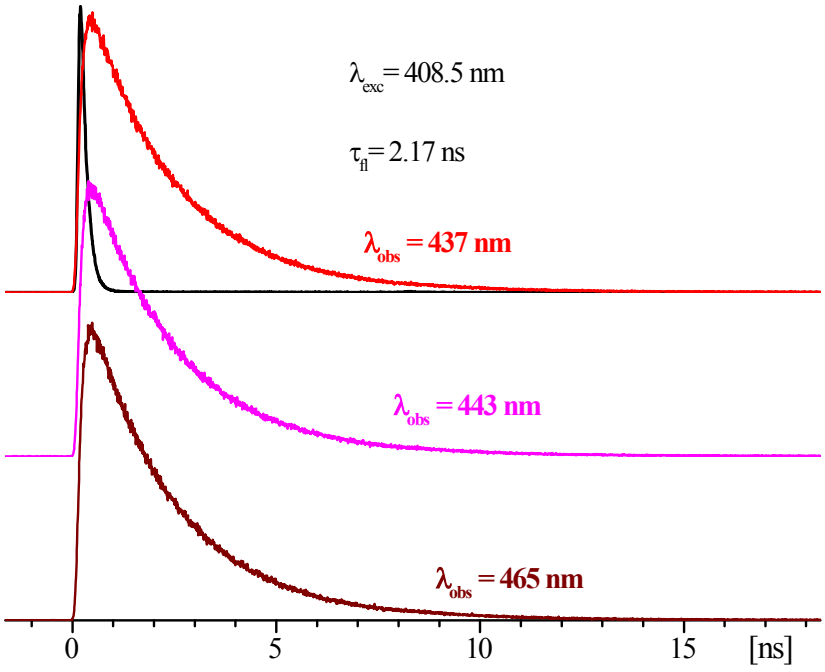


Figure S1. Fluorescence decay curves at room temperature, obtained with 408.5 nm excitation and 3 different observation wavelengths. Fluorescence decay is mono-exponential with the decay time 2.15 ns (independent on the observation wavelength).

NMR:

All spectra have been recorded at **Bruker Avance III 400 MHz** spectrometer equipped with 5 mm PABBO BB/19F-1H/D probe. Temperature of measurements was set at 303K. Solvent (**$CDCl_3$**) a priori to measurements was deacidified by passing through a short column packed with **Al_2O_3** (*SIGMA-ALDRICH; activated, basic, Brockmann I*).

All experiments have been carried out by standard pulse sequences available in *Bruker TopSpin3.2* library:

^{1}H – zg30

^{13}C – zgpg

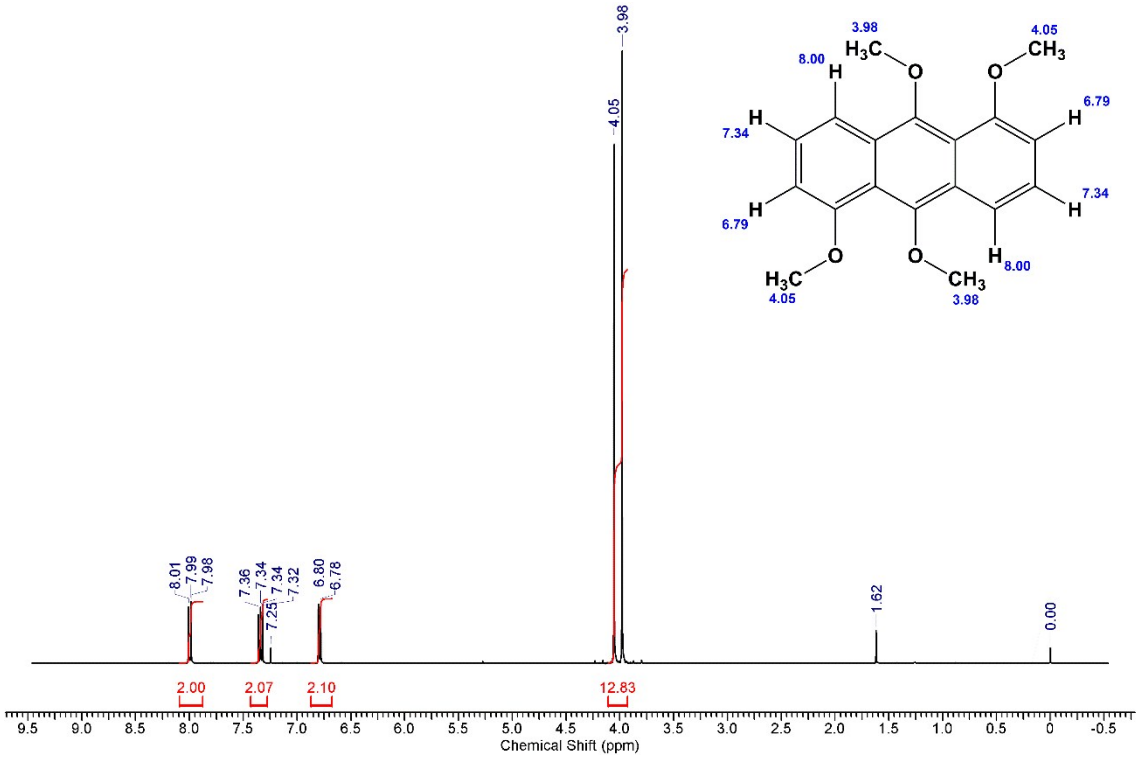
^{1}H - ^{1}H DQF-COSY – **cosygpmfphpp**

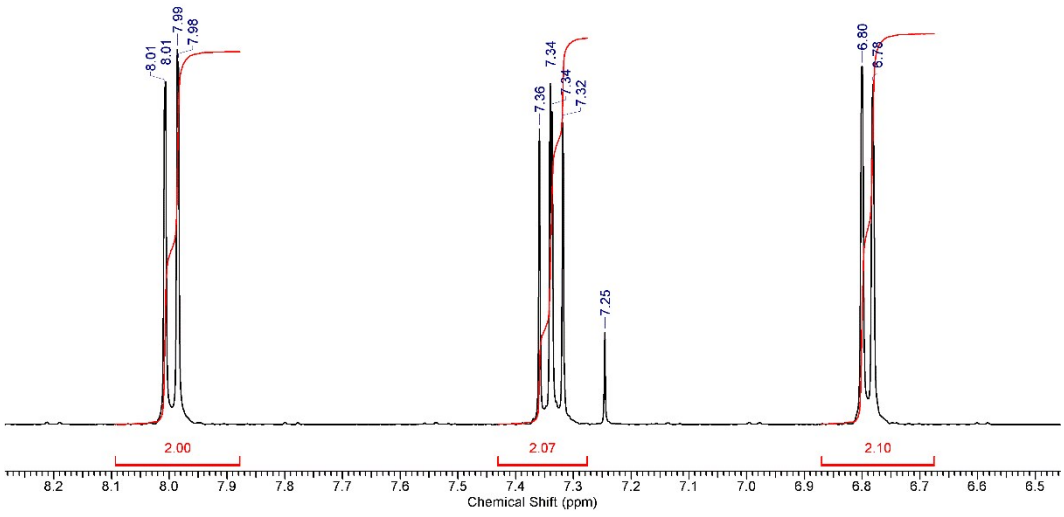
^{1}H - ^{1}H NOESY – **noesygpphpp**

^{1}H - ^{13}C HSQC – **hsqcedetgp**

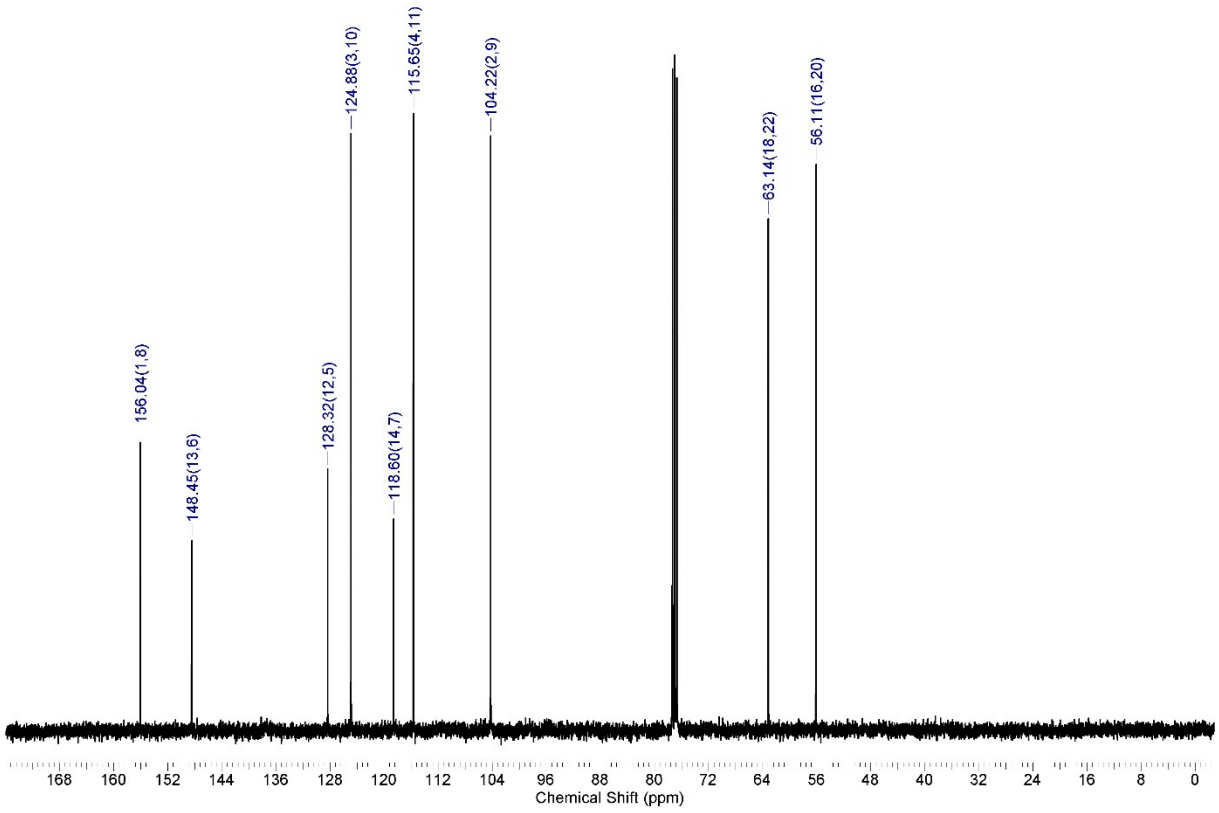
^{1}H - ^{13}C HMBC – **hmbcgpndqf**

(2) 1,5,9,10-tetramethoxyanthracene

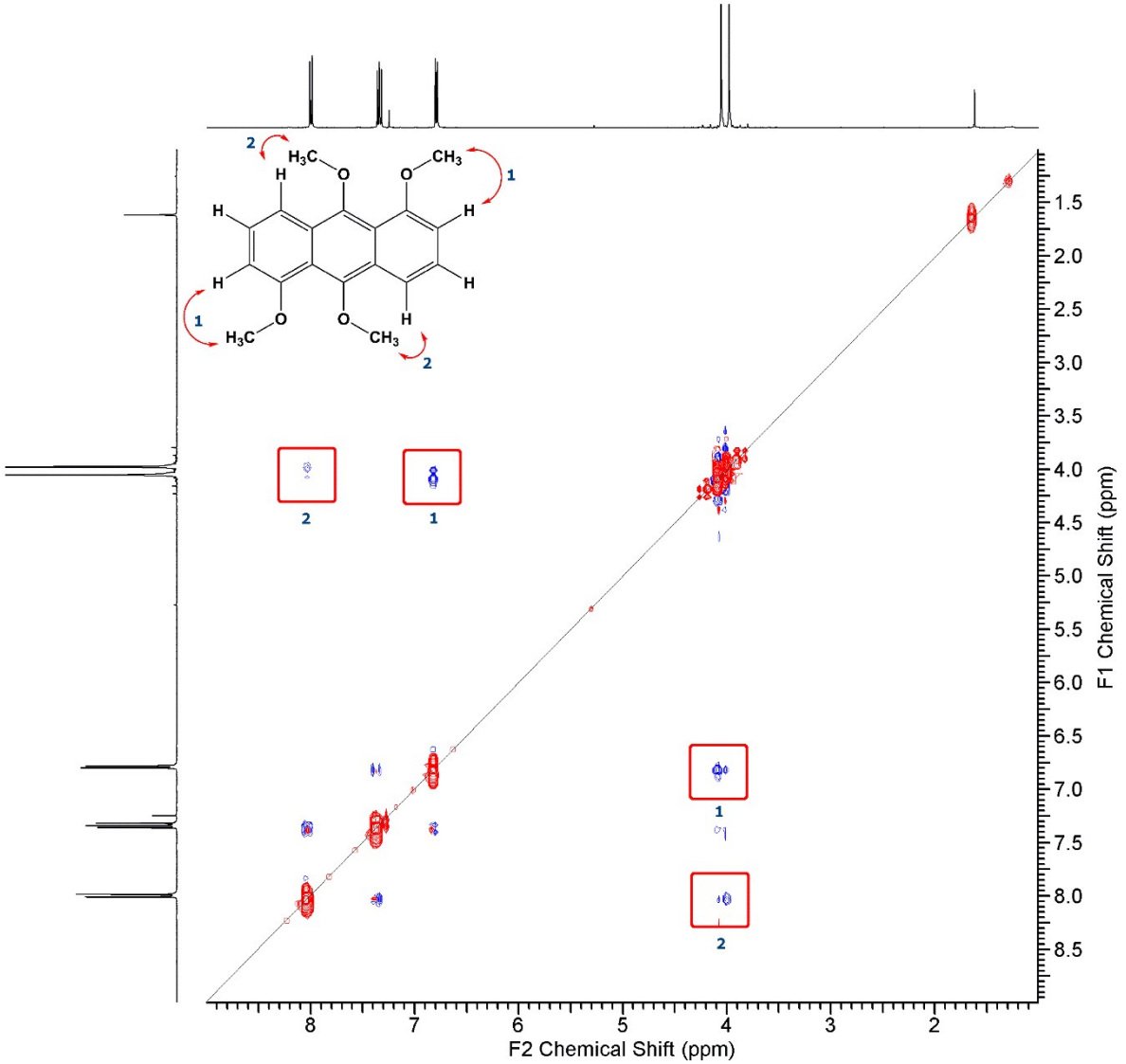




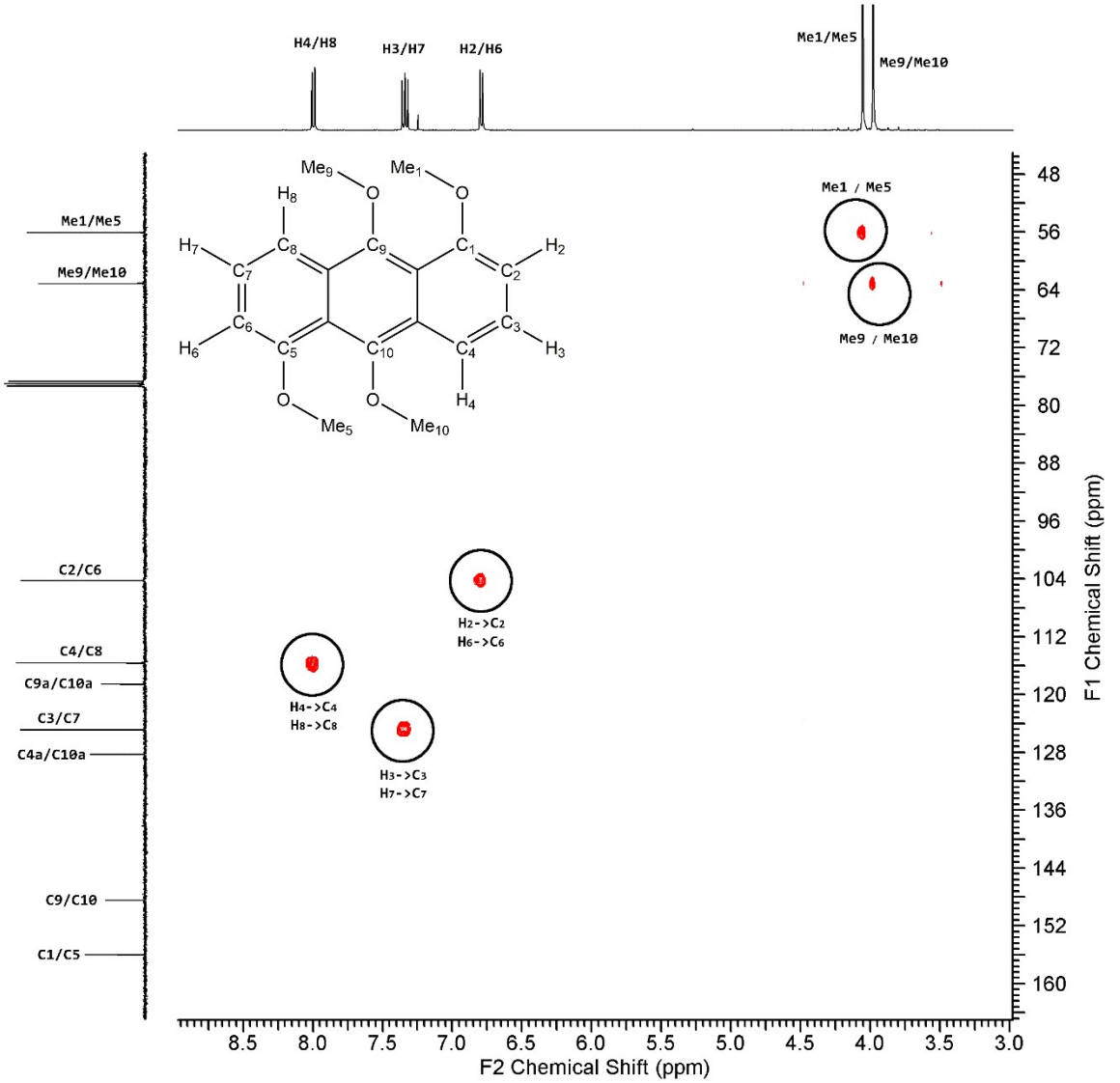
^{1}H NMR (400 MHz) spectrum of compound **(2)**. Whole spectrum is present at the top of the page, zoomed region at the bottom.



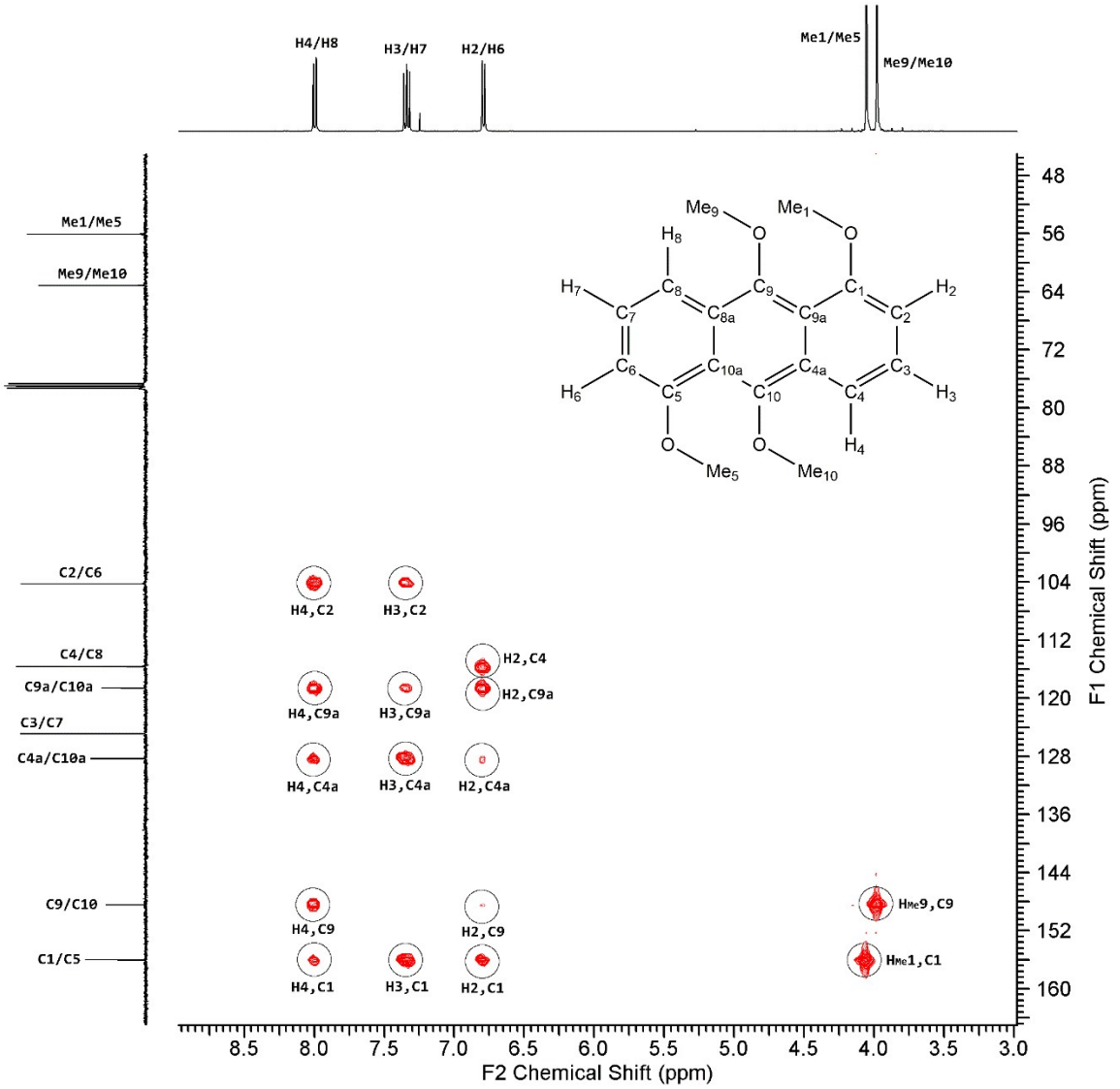
^{13}C NMR (100 MHz) spectrum of compound **(2)**.



^{1}H-^{1}H 2D gNOESY (400 MHz) spectrum of compound **(2)**.

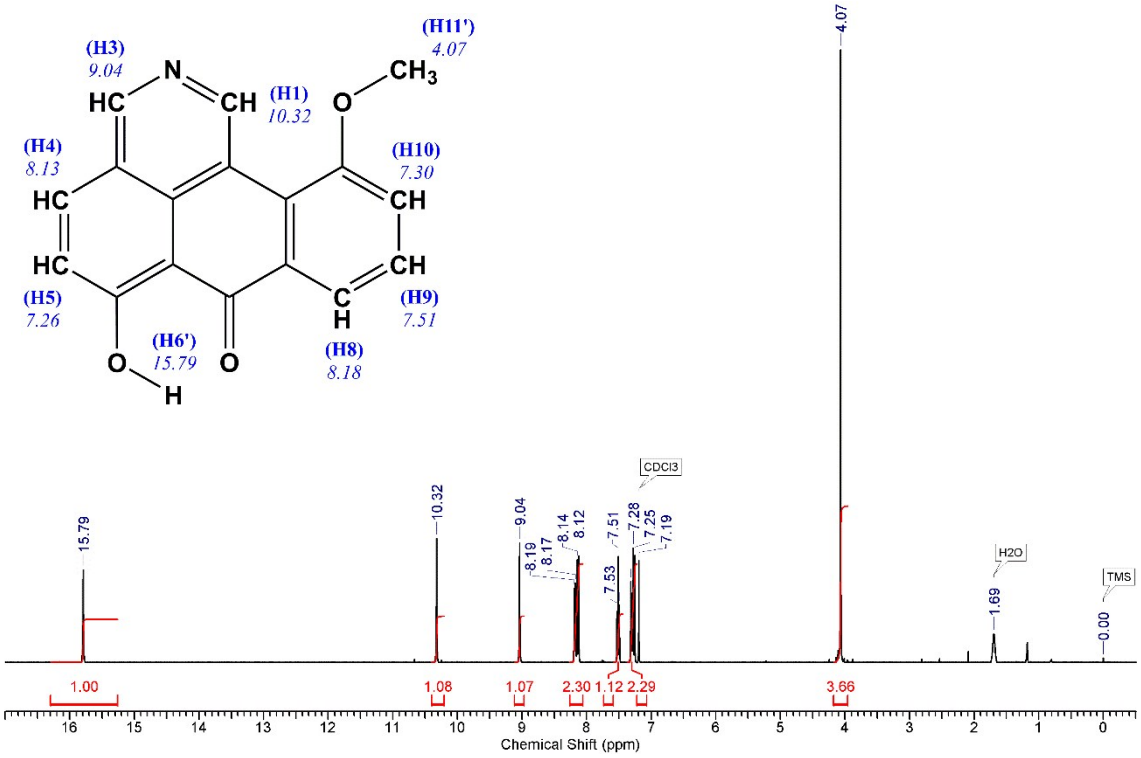


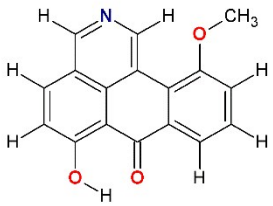
^{1}H-^{13}C 2D gHSQC NMR (400 MHz) spectrum of compound **(2)**.

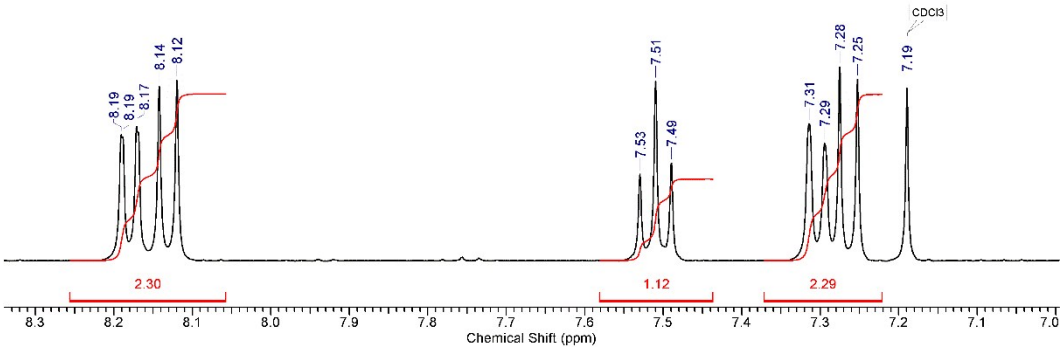


^{1}H-^{13}C 2D gHMBC NMR (400 MHz) spectrum of compound **(2)**.

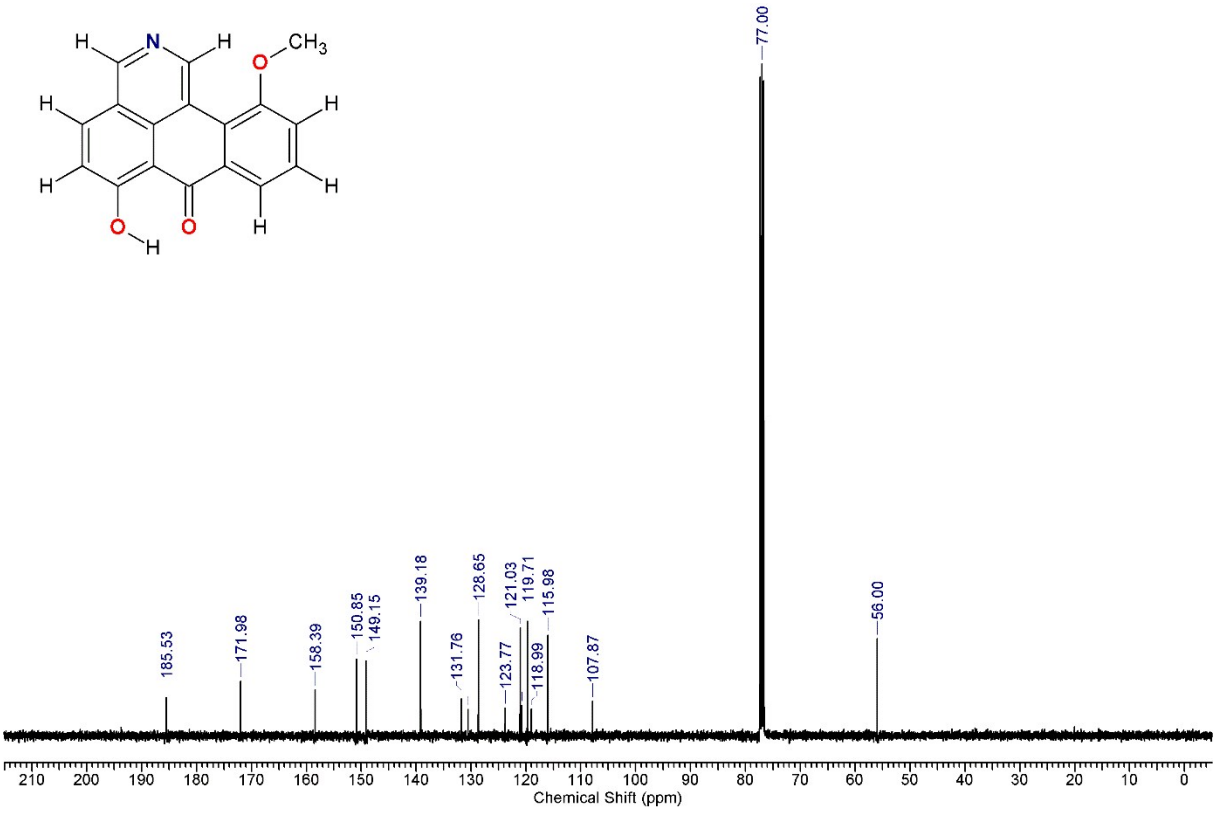
(3) 6-hydroxy-11-methoxy-2-azabenzanthrone

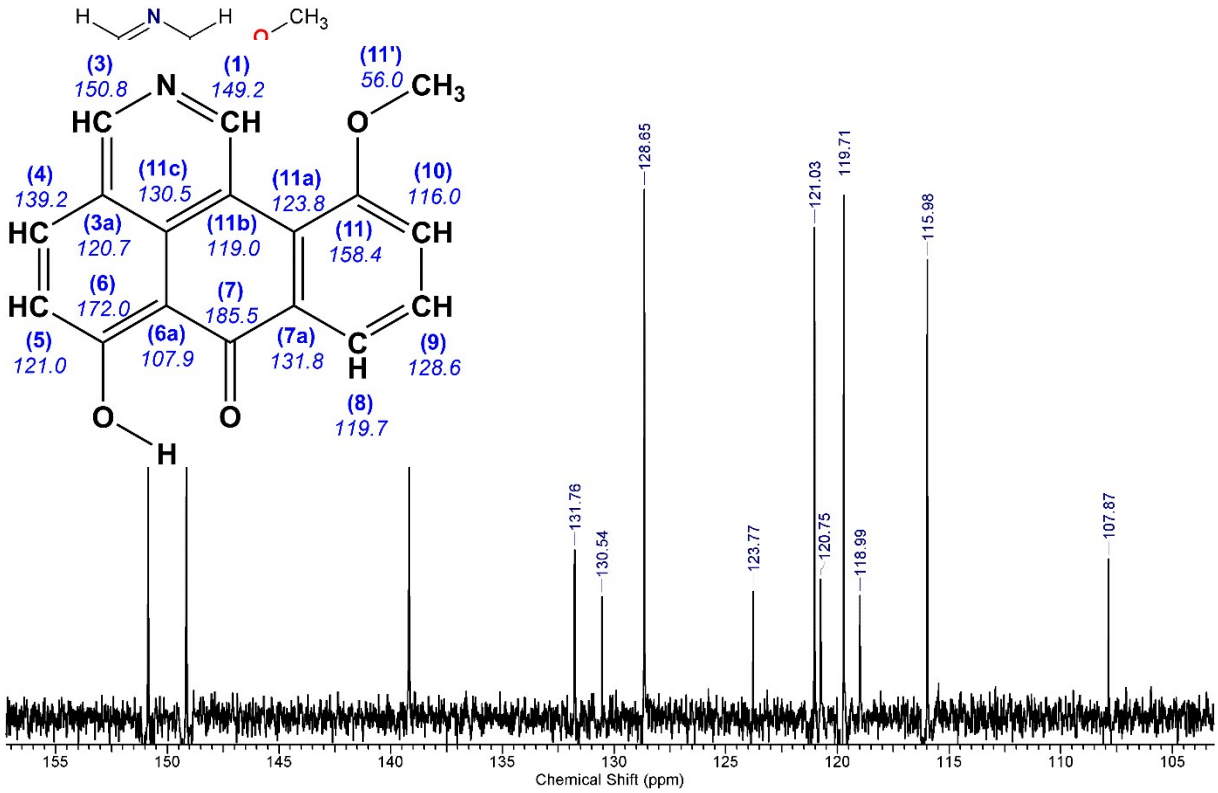




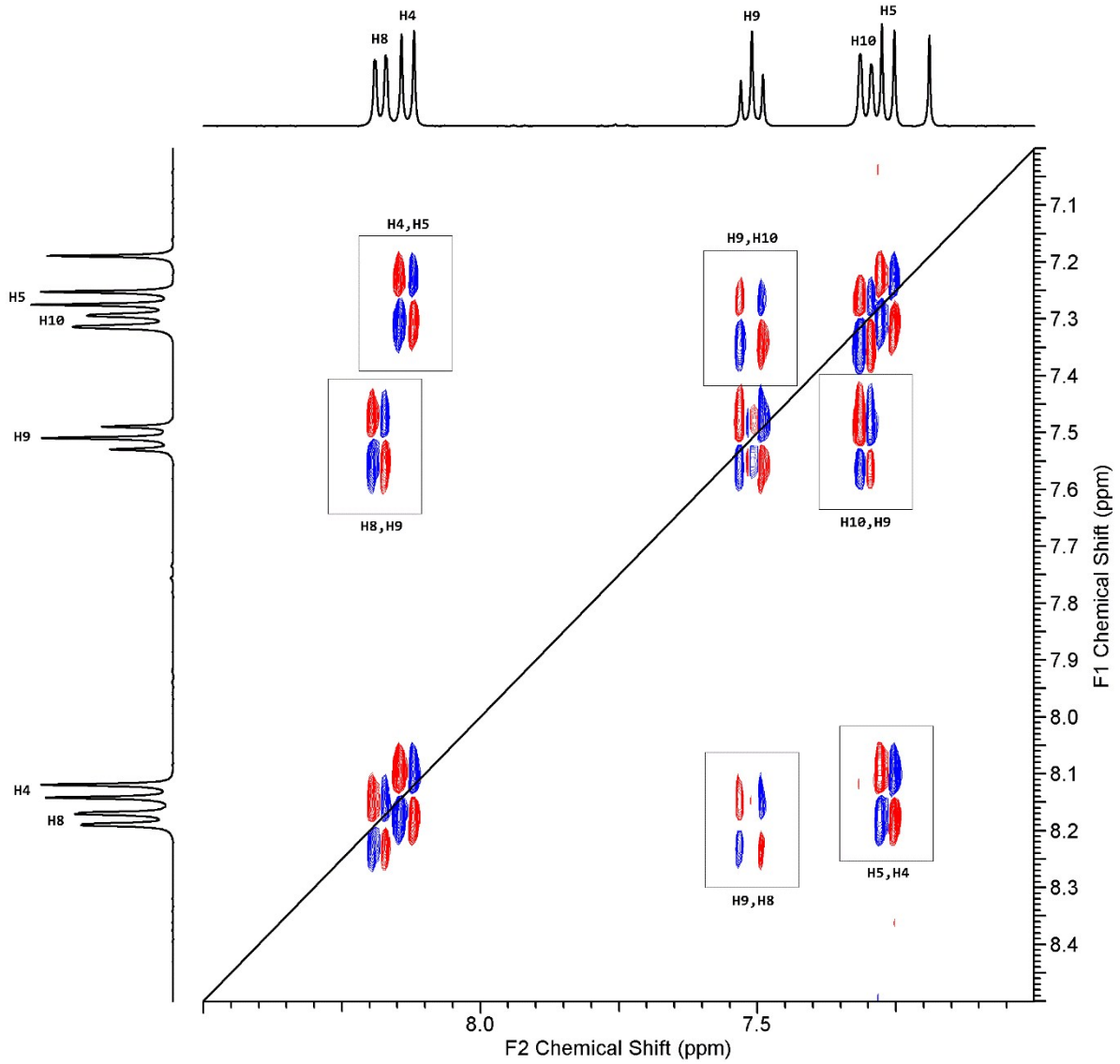


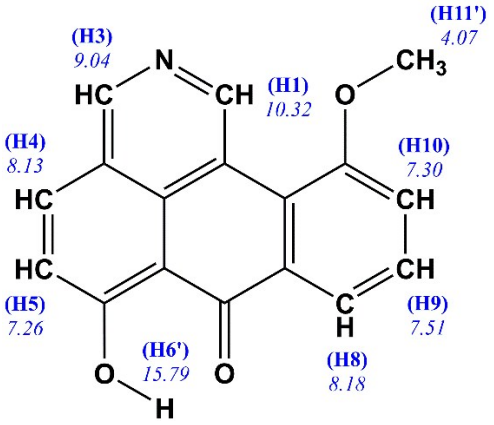
^{1}H NMR (400 MHz) spectrum of compound **(3)**. Whole spectrum is present at the top of the page, zoomed region at the bottom.



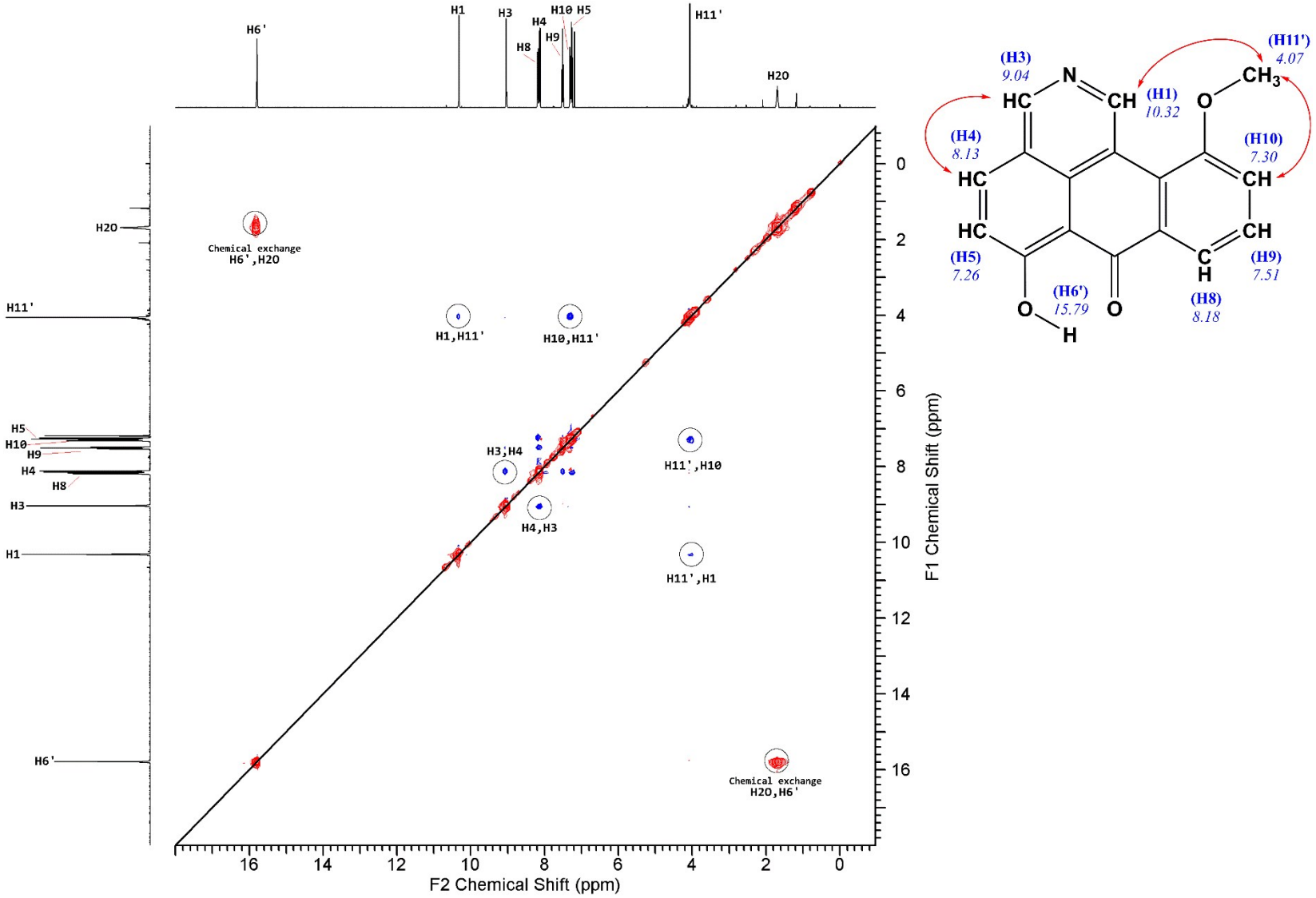


^{13}C NMR (100 MHz) spectrum of compound **(3)**. Whole spectrum is present at the top of the page, zoomed region at the bottom.

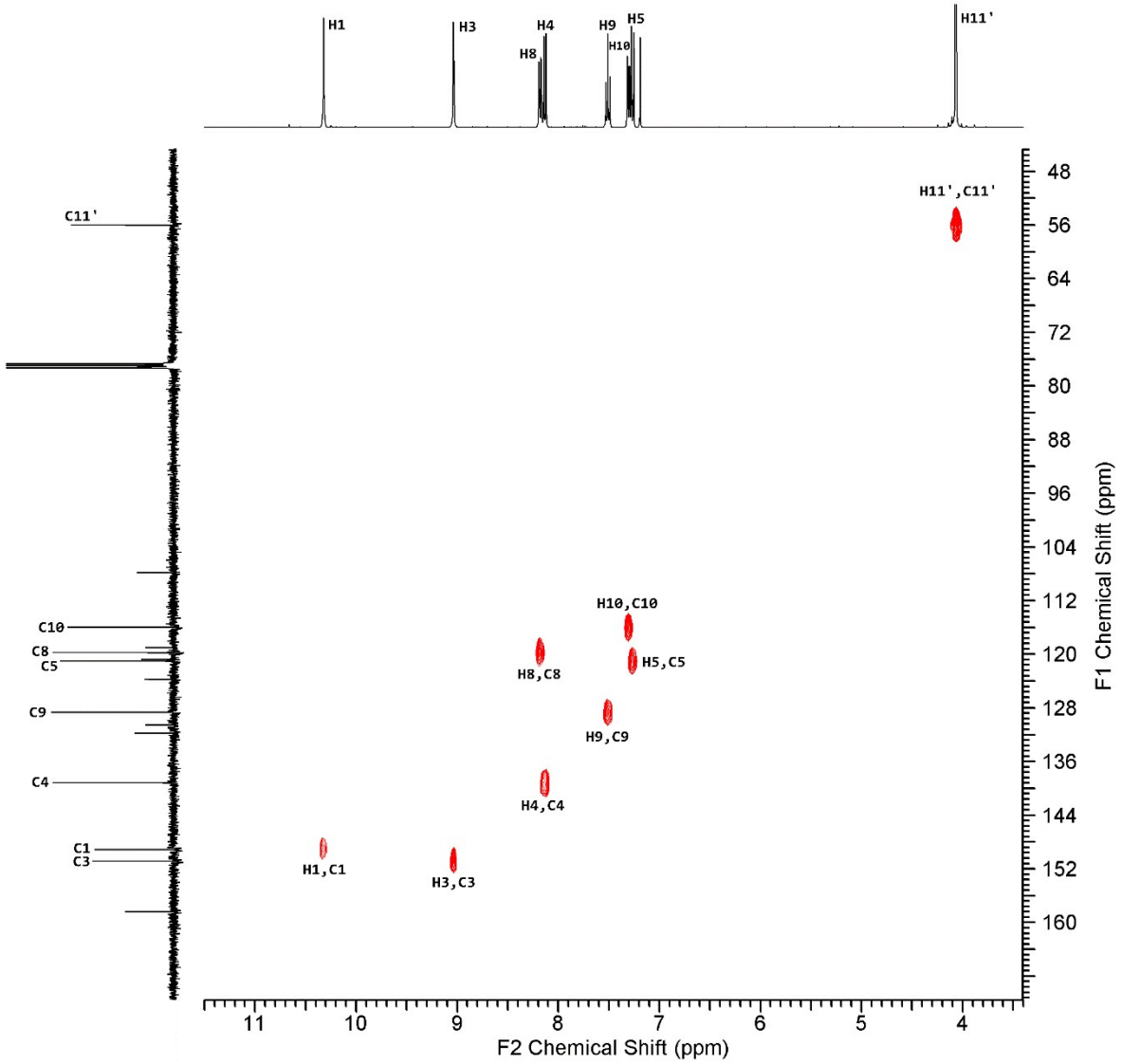


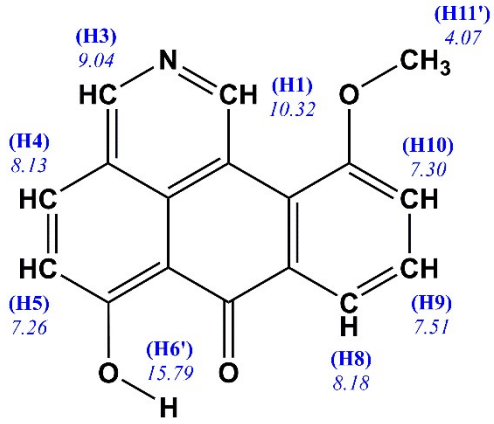


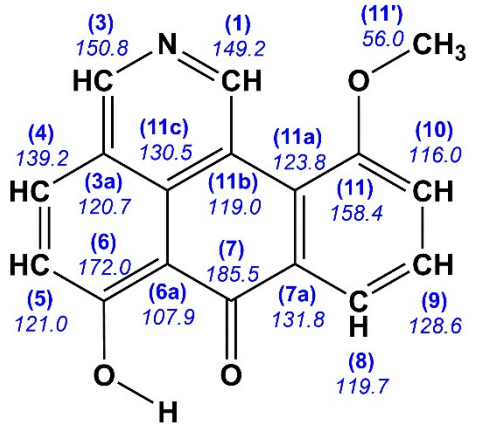
^{1}H-^{1}H DQF-gCOSY NMR (400 MHz) spectrum of compound **(3)**.



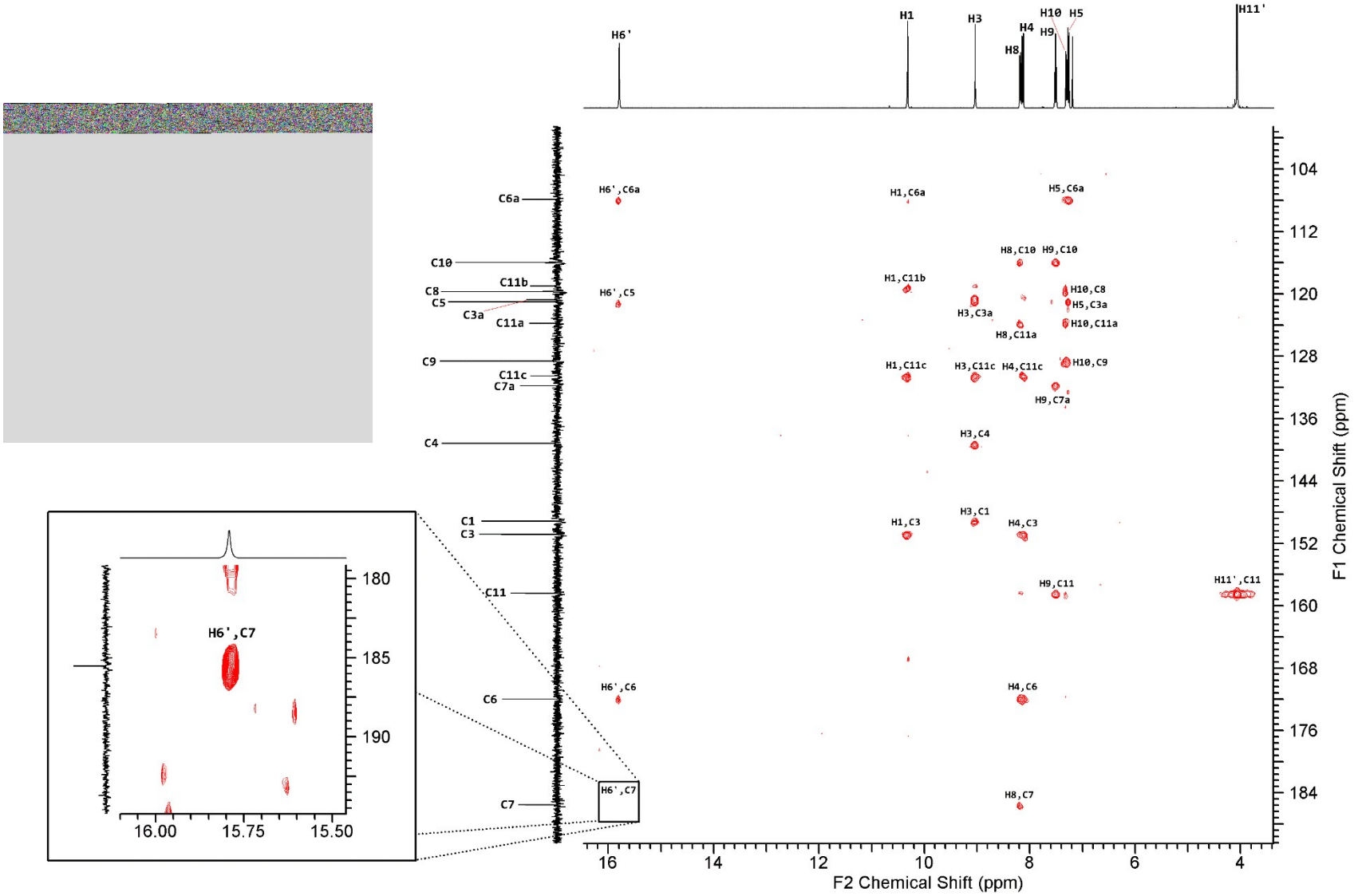
^{1}H-^{1}H 2D gNOESY (400 MHz) spectrum of compound **(3)**.







^{1}H-^{13}C 2D gHSQC NMR (400 MHz) spectrum of compound **(3)**.



^{1}H-^{13}C 2D gHMBC NMR (400 MHz) spectrum of compound **(3)**.