Supplementary Information

Turn-on Fluorogenic Sensors Based on An Anthraquinone Signaling Unit for The Detection of Zn(II) and Cd(II) ions

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To investigate the stability of **1**-Zn(II) and **1**-Cd(II) complexes, the distances between each metal and linkers from the chemosensor were evaluated and shown in **Table S1**, where the notations are depicted in **Fig. 10a** and **10b** for **1**-Zn(II) and **1**-Cd(II) complexes, respectively. After the optimization, we found that the distance in the **1**-Zn(II) complex is less than the **1**-Cd(II) complex, indicating that the Zn(II) favorably interact with the chemosensor **1**. This finding is also consistent with our experiment as already described in sections of fluorescence titration of Zn(II) and Cd(II) ions with chemosensor **1** with the most stable metal complexes for the chemosensor **1** and their corresponding fluorescent spectra *via* computational approach. Moreover, the distance values from calculations are in the range of bond lengths reported in the previous literature.[1]

Table S1 Selected distances between the metal (**M** = Zn(II) or Cd(II)) atom and the chelating atoms of the chemosensor **1** in angstrom (Å).

Atom pair	**M** and chelating atom distance (Å)	
	1-Zn(II)	**1**-Cd(II)
M1···N1	2.16	2.41
M1···N2	2.25	2.47
M1···N3	2.15	2.40
M1···O1	2.11	2.37
M2···N4	2.13	2.40
M2···N5	2.25	2.50
M2···N6	2.11	2.37
M2···O2	2.17	2.52

Table S2 Atomic coordinates for structures at a stationary point

Chemosensor **1**

C	3.4403760	3.9366000	-1.3042720
C	2.2971510	4.6047270	-0.8785470
C	3.4990200	2.5545190	-1.2499520
C	1.1970860	3.8740500	-0.4446510
C	2.4291130	1.7915840	-0.7468910
C	-2.2971120	4.6047030	0.8787580
C	0.0000160	4.6386530	0.0000960
C	1.2208840	2.4611540	-0.3928640
C	-3.4403310	3.9365650	1.3044840
C	-1.1970470	3.8740360	0.4448400
C	0.0000260	1.7130090	0.0000810
C	-3.4989700	2.5544850	1.2501380
C	-1.2208400	2.4611400	0.3930320
C	-2.4290680	1.7915660	0.7470520
C	-3.6106960	-0.4404590	0.3924440
C	-4.8077770	0.1234530	-0.3785870
C	-6.1809530	-2.3640800	-4.7283790
C	-6.1132390	-0.9759690	-4.7232970
C	-6.5412720	-3.0093030	-3.5457090
C	-6.4002830	-0.2980010	-3.5407740
C	-6.7443640	-1.0300170	-2.4016780
C	-7.0756900	-0.3434470	-1.0923100
C	-6.5400730	-0.1948920	1.2802420
C	-7.5804900	-1.1583840	1.8142420
C	-8.0134740	-3.2372030	2.6838590
C	-9.3762650	-2.9708210	2.8120990
C	-9.8395250	-1.7200530	2.4212920
C	-8.9262540	-0.7980710	1.9155000
C	3.6108070	-0.4404120	-0.3923420
C	4.8078360	0.1235300	0.3787560
C	6.1810590	-2.3647360	4.7281240
C	6.1133950	-0.9766220	4.7233410
C	6.5413150	-3.0097190	3.5453040
C	6.4004340	-0.2984080	3.5409560
C	6.7444610	-1.0301930	2.4016950
C	7.0757690	-0.3433600	1.0924560
C	6.5401810	-0.1945610	-1.2801100
C	7.5804010	-1.1581530	-1.8143260
C	8.0129080	-3.2367960	-2.6846110
C	9.3757890	-2.9707530	-2.8125960

C	9.8393510	-1.7202480	-2.4213090
C	8.9262780	-0.7981820	-1.9153120
H	4.2838270	4.4922460	-1.6963540
H	2.2301830	5.6839030	-0.8958320
H	4.3706590	2.0438000	-1.6336520
H	-2.2301480	5.6838790	0.8960570
H	-4.2837780	4.4922020	1.6965890
H	-4.3706000	2.0437530	1.6338450
H	-1.6481950	-0.0874400	0.7027850
H	-4.5580830	-0.0894450	-1.4239060
H	-4.8785740	1.2172510	-0.3011620
H	-5.9663680	-2.9379420	-5.6216380
H	-5.8420530	-0.4296170	-5.6194950
H	-6.6133810	-4.0930360	-3.5140490
H	-6.3595740	0.7844660	-3.4991600
H	-8.0068860	-0.7766420	-0.7235580
H	-7.2592180	0.7312030	-1.2745630
H	-6.9409130	0.8345410	1.3078160
H	-5.6878160	-0.2391670	1.9620730
H	-7.6128620	-4.2002670	2.9883580
H	-10.0459510	-3.7226940	3.2115490
H	-10.8896180	-1.4648090	2.5070870
H	-9.2506600	0.1878960	1.6029730
H	1.6482720	-0.0874430	-0.7026190
H	4.5581500	-0.0894730	1.4240580
H	4.8785530	1.2173380	0.3014260
H	5.9664740	-2.9387840	5.6212640
H	5.8422480	-0.4304540	5.6196630
H	6.6133700	-4.0934490	3.5134050
H	6.3597360	0.7840690	3.4995710
H	8.0070000	-0.7764310	0.7236290
H	7.2592320	0.7312670	1.2749060
H	6.9411840	0.8348120	-1.3075460
H	5.6878860	-0.2385990	-1.9619080
H	7.6120610	-4.1996420	-2.9894910
H	10.0453110	-3.7226760	-3.2122260
H	10.8895240	-1.4652660	-2.5069010
H	9.2509220	0.1875930	-1.6024310
N	-7.1297090	-2.3605740	2.2026570
N	-6.8208930	-2.3696960	-2.4081780
N	-2.5370340	0.4044230	0.6757770
N	-6.0547310	-0.5520750	-0.0589410
N	7.1293320	-2.3600850	-2.2032100

N	6.8209290	-2.3698780	2.4079040
N	2.5370970	0.4044400	-0.6756070
N	6.0548370	-0.5518740	0.0590470
O	0.0000040	5.8606000	0.0000870
O	0.0000370	0.4743470	0.0000760
O	-3.4996200	-1.6265800	0.6211580
O	3.4997940	-1.6265280	-0.6211160

Chemosensor **1**-Cd(II) complex

C	-3.3974120	4.8133150	1.5895240
C	-2.3305900	5.4554620	0.9929350
C	-3.4513160	3.4123490	1.6010230
C	-1.2620550	4.7201590	0.4582140
C	-2.4528350	2.6540990	1.0108260
C	2.0571140	5.3788490	-1.2713990
C	-0.1633650	5.4577310	-0.1511490
C	-1.2678560	3.2895090	0.4949940
C	3.1661120	4.7141760	-1.7655320
C	0.9980950	4.6669110	-0.6324730
C	-0.1124720	2.5362430	0.0742790
C	3.2893340	3.3442400	-1.5609270
C	1.0504100	3.2881570	-0.4753370
C	2.2980880	2.6321900	-0.8581000
C	3.5244230	0.4828440	-0.2959250
C	4.8944140	1.0499490	0.0586000
C	6.7056110	-1.0859910	4.6589660
C	7.4101660	0.0932580	4.4388820
C	6.1447740	-1.7335530	3.5669920
C	7.5295870	0.5764890	3.1396000
C	6.9499410	-0.1335900	2.0915260
C	7.1404450	0.3253970	0.6570240
C	6.3171910	0.0425250	-1.6393450
C	7.0147860	-1.2327850	-2.0735960
C	7.1149220	-3.5503710	-2.0022560
C	8.1019690	-3.5918660	-2.9764000
C	8.5645160	-2.3891180	-3.5002270
C	8.0161430	-1.1956490	-3.0400060
C	-3.5561600	0.4286240	0.5753130
C	-4.8697510	0.9920160	0.0270210
C	-6.0439580	-1.3500000	-4.6771570
C	-6.8177330	-0.1951280	-4.6088760
C	-5.5957050	-1.9136590	-3.4914500

C	-7.1139100	0.3473760	-3.3628710
C	-6.6411490	-0.2826560	-2.2140180
C	-7.0261180	0.2357710	-0.8397680
C	-6.5293460	0.0525630	1.5500930
C	-7.2676880	-1.2178210	1.9348470
C	-7.3720040	-3.5349120	1.9020890
C	-8.4635760	-3.5524570	2.7587800
C	-8.9743870	-2.3372500	3.2036600
C	-8.3716580	-1.1565270	2.7821500
Cd	5.2209400	-2.2361260	0.3748230
Cd	-5.0802530	-2.2326150	-0.1913290
H	-4.1961660	5.3827040	2.0496380
H	-2.2817710	6.5359280	0.9438770
H	-4.2748890	2.9225510	2.1033590
H	1.9428140	6.4493890	-1.3801110
H	3.9352540	5.2507390	-2.3065430
H	4.1370110	2.8206520	-1.9765990
H	1.5123390	0.8882690	-0.2578440
H	4.8412160	1.2411650	1.1364010
H	5.0987550	2.0148970	-0.4053460
H	6.5854750	-1.4975900	5.6530870
H	7.8571950	0.6327990	5.2656100
H	5.5831260	-2.6514840	3.6926840
H	8.0695340	1.4937030	2.9364230
H	7.9778990	-0.2322300	0.2289070
H	7.4258410	1.3823720	0.6397140
H	6.9270150	0.9106850	-1.9108860
H	5.3889130	0.1157400	-2.2147320
H	6.7343390	-4.4610130	-1.5550830
H	8.5004040	-4.5439240	-3.3032820
H	9.3441760	-2.3775730	-4.2528770
H	8.3582250	-0.2445000	-3.4295220
H	-1.6359010	0.7796330	0.9439740
H	-4.6871590	1.1451770	-1.0414620
H	-5.1230140	1.9689370	0.4357040
H	-5.7861350	-1.8044600	-5.6254390
H	-7.1816580	0.2802060	-5.5123520
H	-4.9829380	-2.8078430	-3.4929670
H	-7.7085740	1.2489540	-3.2777950
H	-7.9135360	-0.3106780	-0.5074900
H	-7.3163230	1.2899970	-0.9088880
H	-7.1852660	0.9176450	1.6993670
H	-5.6929710	0.1698390	2.2455910

H	-6.9498580	-4.4567190	1.5195280
H	-8.9021100	-4.4958920	3.0583870
H	-9.8334290	-2.3069590	3.8638850
H	-8.7517370	-0.1953620	3.1070840
N	6.5797900	-2.3995410	-1.5628070
N	6.2662390	-1.2719380	2.3120710
N	2.4340870	1.3125050	-0.5071180
N	5.9606680	0.0761240	-0.2020200
N	-6.7837920	-2.3965070	1.5016000
N	-5.8903820	-1.3963160	-2.2874520
N	-2.5476490	1.2412090	0.9556400
N	-5.9764280	0.0336090	0.1799570
O	-0.1622670	6.6864070	-0.2902780
O	-0.0500180	1.2656920	0.1587620
O	3.3059610	-0.7232670	-0.2537760
O	-3.3572720	-0.8002600	0.5747990

Chemosensor **1**-Zn(II) complex

C	-3.4712920	4.9019850	1.2478830
C	-2.4145340	5.5111480	0.6001050
C	-3.4832190	3.5082580	1.4040290
C	-1.3187270	4.7578650	0.1524940
C	-2.4520030	2.7278550	0.9102630
C	1.9719490	5.3079550	-1.6725480
C	-0.2343680	5.4577830	-0.5247790
C	-1.2828760	3.3401090	0.3389360
C	3.0844060	4.6160890	-2.1255390
C	0.9412440	4.6461330	-0.9379380
C	-0.1044830	2.5805920	0.0097610
C	3.2424560	3.2780310	-1.7864260
C	1.0304610	3.2945200	-0.6384950
C	2.2853610	2.6279080	-0.9821040
C	3.5198650	0.5461900	-0.2225950
C	4.9677140	1.0244520	-0.1617890
C	7.1245930	-1.1097730	4.4482250
C	8.0145760	-0.1173700	4.0463690
C	6.2617810	-1.6457850	3.5056470
C	8.0158230	0.2965620	2.7183670
C	7.1331800	-0.2954210	1.8215980
C	7.1726070	0.0532270	0.3450590
C	6.0041200	-0.5305840	-1.7480070
C	6.1968420	-2.0255520	-1.9271380

C	5.7019870	-4.1783550	-1.1909240
C	6.3383750	-4.7497490	-2.2807370
C	6.9364980	-3.9097100	-3.2161160
C	6.8673330	-2.5322060	-3.0353460
C	-3.4855500	0.4569560	0.6680460
C	-4.7689290	0.9335910	-0.0140350
C	-4.6301990	-2.5520790	-4.1128760
C	-5.4748350	-1.5321170	-4.5429120
C	-4.4520460	-2.7315710	-2.7500850
C	-6.1097350	-0.7318970	-3.5985790
C	-5.8928050	-0.9753320	-2.2465550
C	-6.6195290	-0.1831850	-1.1754550
C	-6.6814570	0.0808740	1.2720590
C	-7.3031210	-1.2270060	1.7287110
C	-7.0703290	-3.5297720	1.9819040
C	-8.2768050	-3.6269570	2.6573050
C	-9.0190760	-2.4667630	2.8597910
C	-8.5286670	-1.2540030	2.3858930
H	-4.2926100	5.4912200	1.6375210
H	-2.3970420	6.5820470	0.4414230
H	-4.2977880	3.0421780	1.9437520
H	1.8314840	6.3584490	-1.8908700
H	3.8262870	5.1091440	-2.7404380
H	4.0871620	2.7288460	-2.1749390
H	1.5320490	0.9771730	-0.1349090
H	5.0952280	1.4407490	0.8437500
H	5.2033720	1.8271340	-0.8567840
H	7.0908890	-1.4591230	5.4721020
H	8.6968280	0.3320330	4.7581680
H	5.5432970	-2.4107430	3.7721210
H	8.6953370	1.0679650	2.3768280
H	7.8840280	-0.6215650	-0.1380040
H	7.5558730	1.0674490	0.2031820
H	6.8140380	0.0208340	-2.2327210
H	5.0853540	-0.2533750	-2.2725080
H	5.2362090	-4.7874760	-0.4264460
H	6.3732280	-5.8265860	-2.3833900
H	7.4553530	-4.3213390	-4.0737790
H	7.3266390	-1.8563240	-3.7462950
H	-1.5935680	0.8714050	1.1051880
H	-4.4937210	1.0704380	-1.0640300
H	-5.1149650	1.9025480	0.3370370
H	-4.1159410	-3.1951000	-4.8155120

H	-5.6348480	-1.3583430	-5.6005040
H	-3.8019240	-3.5068000	-2.3625480
H	-6.7695980	0.0709420	-3.9038550
H	-7.5519150	-0.7031820	-0.9400310
H	-6.8976030	0.8056330	-1.5535270
H	-7.4567020	0.8359030	1.1103120
H	-6.0476060	0.4476260	2.0839990
H	-6.4614950	-4.4043540	1.7880800
H	-8.6257040	-4.5903190	3.0064430
H	-9.9720390	-2.5054190	3.3743650
H	-9.0888850	-0.3373980	2.5250250
N	5.6309810	-2.8452490	-1.0193730
N	6.2679790	-1.2481280	2.2204290
N	2.4474980	1.3602760	-0.4807870
N	5.8643830	-0.1310300	-0.3255260
N	-6.5949610	-2.3557060	1.5313950
N	-5.0700870	-1.9607340	-1.8379180
N	-2.5098170	1.3117540	1.0082380
N	-5.8300980	-0.0861170	0.0731350
O	-0.2565940	6.6662570	-0.7797880
O	-0.0017830	1.3326120	0.2547610
O	3.2552900	-0.6210850	0.0918080
O	-3.2845070	-0.7701380	0.8086250
Zn	4.9060920	-1.8841570	0.7106930
Zn	-4.8487130	-2.0940520	0.2917270

Table S3 Data of Zn(II) and Cd(II) ions solutions and their corresponding mole ratios in titration experiments with chemosensor **1**

Chemical formula	Weight (g)	Mole	Stock volume (mL)	Concentration (M)	Mole equivalence per 10 μL
$Zn(ClO_4)_2 \cdot 6H_2O$	0.047544	1.2767×10^{-4}	50	2.5534×10^{-3}	0.2
$Cd(ClO_4)_2 \cdot xH_2O$	0.020690	6.6461×10^{-5}	25	2.6580×10^{-3}	0.2

Table S4 Data regarding ligand-to-metal ratios and their relevant amounts of metal ion solution (Zn(II) and Cd(II)) used in titration experiments for both UV-vis and fluorescence spectroscopic techniques

Ligand : Metal ratio	Amount of ligand (mL)	Amount of metal ion solution (μL)
1 : 0.0	2.5	0
1 : 0.2		10
1 : 0.4		20
1 : 0.6		30
1 : 0.8		40
1 : 1.0		50
1 : 1.1		55
1 : 1.2		60
1 : 1.3		65
1 : 1.4		70
1 : 1.5		75
1 : 1.6		80
1 : 1.7		85
1 : 1.8		90
1 : 1.9		95
1 : 2.0		100
1 : 3.0		150
1 : 4.0		200
1 : 5.0		250

The calculation of the binding constants of both **1**-Zn(II) and **1**-Cd(II) complexes utilized the data of fluorescence titration experiments, then used the Benesi–Hildebrand method model for a ligand-to-metal ratio of 1:2. The results used for the plots were described in **Table S4** and **S5** for Zn(II) and Cd(II) ion, respectively.

Table S5. Fluorescence titration data of **1**-Zn(II) used for the Benesi–Hildebrand plot

Ratio of metal ions	$[Zn(II)]_f$ ($\times 10^{-5}$ M)	$[Zn(II)]_f^2$ ($\times 10^{-10}$ M^2)	$1/[Zn(II)]_f^2$ ($\times 10^{8}$ M^{-2})	F-F_0	$1/(F$-$F_0)$
0.2	1.017	1.035	96.63	31.75	0.03150
0.4	2.027	4.107	24.35	80.40	0.01244
0.6	3.028	9.167	10.91	134.5	0.007435
0.8	4.021	16.17	6.185	175.1	0.005711
1.0	5.007	25.07	3.989	219.1	0.004564
1.1	5.486	30.09	3.323	268.2	0.003728
1.2	5.961	35.54	2.814	345.3	0.002896
1.3	6.433	41.38	2.416	404.8	0.002470
1.4	6.901	47.62	2.100	444.1	0.002252
1.5	7.366	54.25	1.843	424.3	0.002357

Table S6. Fluorescence titration data of **1**-Cd(II) used for the Benesi–Hildebrand plot

Ratio of metal ions	$[Cd(II)]_f$ ($\times 10^{-5}$ M)	$[Cd(II)]_f^2$ ($\times 10^{-10}$ M^2)	$1/[Cd(II)]_f^2$ ($\times 10^{8}$ M^{-2})	F-F_0	$1/(F$-$F_0)$
0.2	1.059	1.121	89.17	30.98	0.03228
0.4	2.110	4.450	22.47	94.76	0.01055
0.6	3.152	9.934	10.07	170.8	0.005854
0.8	4.186	17.52	5.707	253.1	0.003951
1.0	5.212	27.16	3.682	339.1	0.002949
1.1	5.711	32.61	3.067	379.2	0.002637
1.2	6.206	38.51	2.597	422.4	0.002367
1.3	6.697	44.84	2.230	467.0	0.002128
1.4	7.184	51.61	1.938	518.4	0.001929
1.5	7.667	58.79	1.701	562.1	0.001779

* $[M(II)]_f$ is the final concentration of metal ion M at the total volume of solution in a cuvette containing both chemosensor **1** at fixed concentrations and added metal ion solution, F is the fluorescence intensity at 520 nm as a function related to the metal ion concentration and F_0 the fluorescence intensity of pure chemosensor **1** at 520 nm.

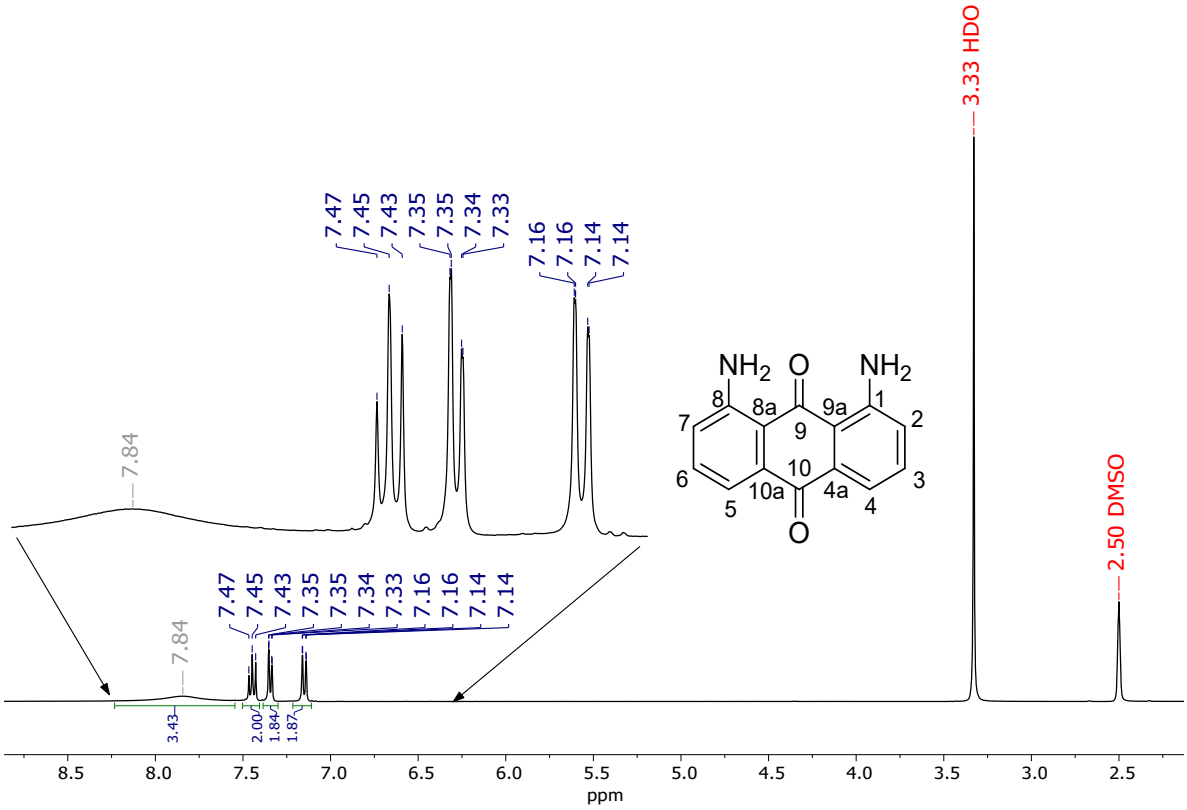
SI 1 Determination of the overall binding constants (β_{12})

The overall binding constant (β_{12}) was determined by linear fitting of the fluorescence titration curve (**Fig. 9a** and **9b**) using **Equation 1**. Due to the binding model of chemosensor **1** might bind with metal ions in the ratio of 1:2 (ligand : metal), so the binding constant might be K_{12} or β_{12} which is related to the binding of first metal ion and second metal ions.

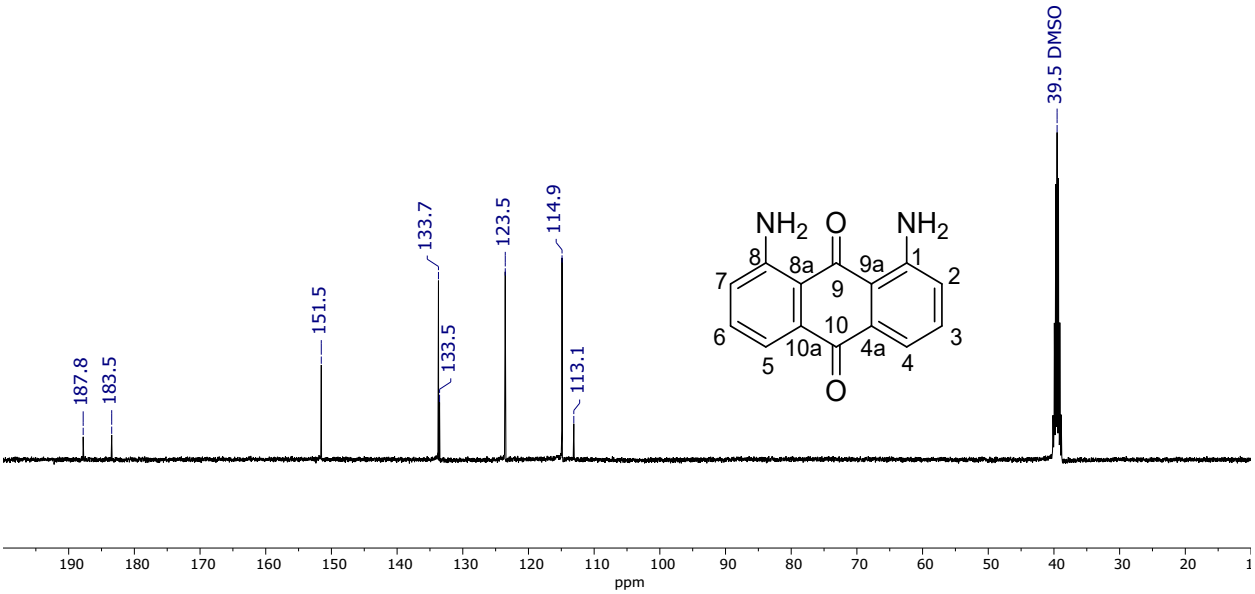
Equation 1: β_{12} = intercept / slope

For the **1**-Zn(II) binding constant, the intercept value is $0.00284 \pm (4.55229 \times 10^{-4})$, while its slope is $3.03643 \times 10^{-12} \pm (1.42987 \times 10^{-13})$. These results can be calculated into the overall binding constant (β_{12}) of 9.3531×10^{8}.

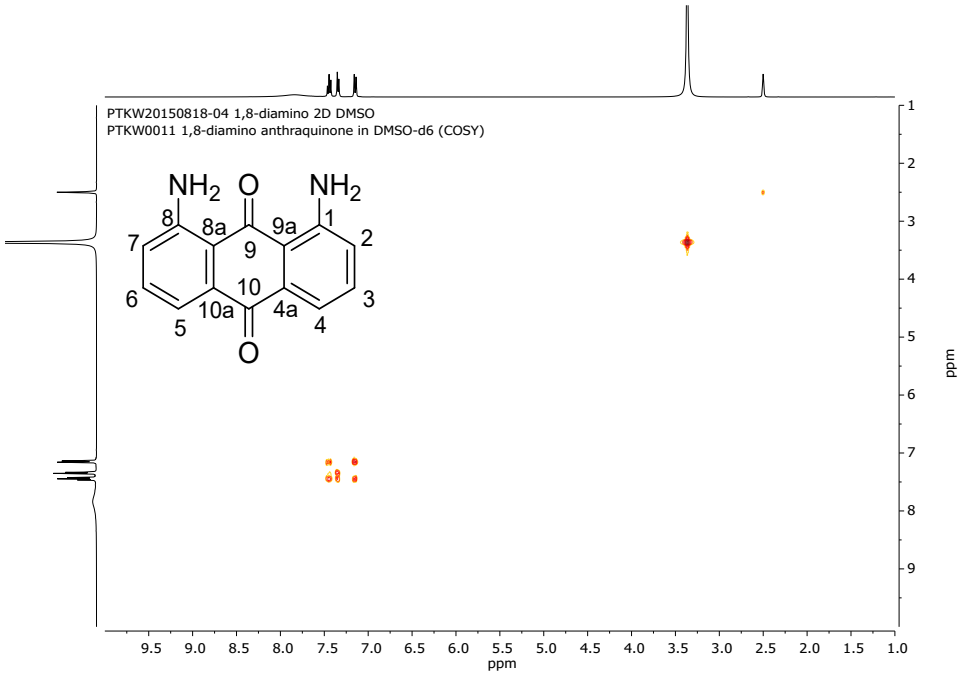
For the **1**-Cd(II) binding constant, the intercept value is $0.0017 \pm (1.98115 \times 10^{-4})$, while its slope is $3.46472 \times 10^{-12} \pm (6.74307 \times 10^{-14})$. These results can be calculated into the overall binding constant (β_{12}) of 4.9066×10^{8}.



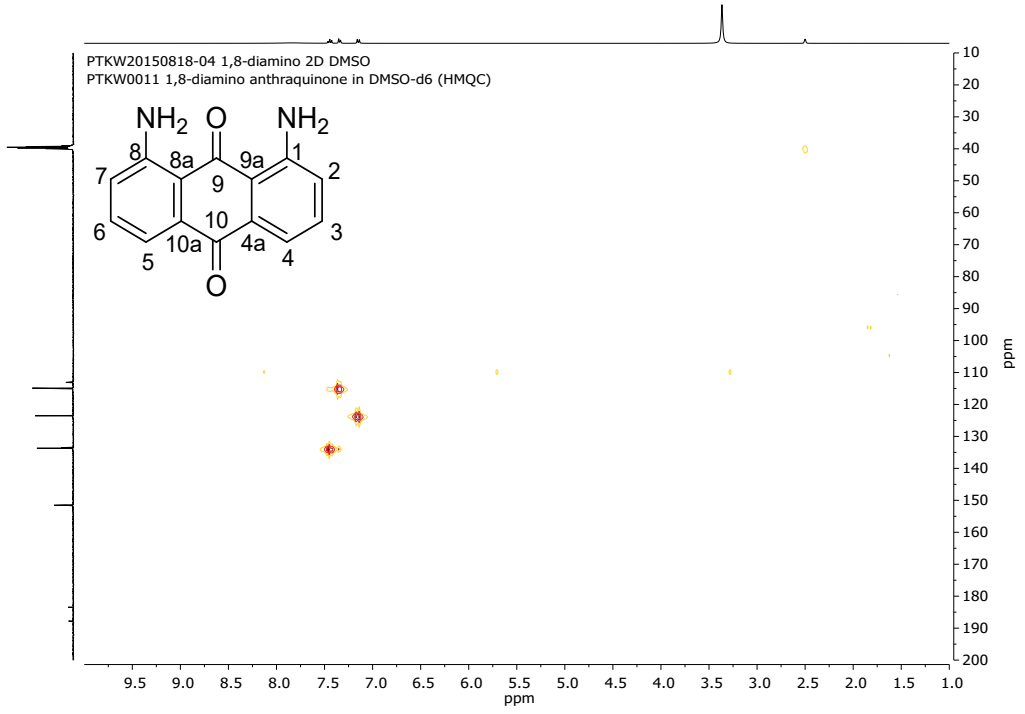
SI 2 Full and partial ^{1}H NMR spectrum of 1,8-diaminoanthraquinone (**4**) in DMSO-d_6 (400 MHz)



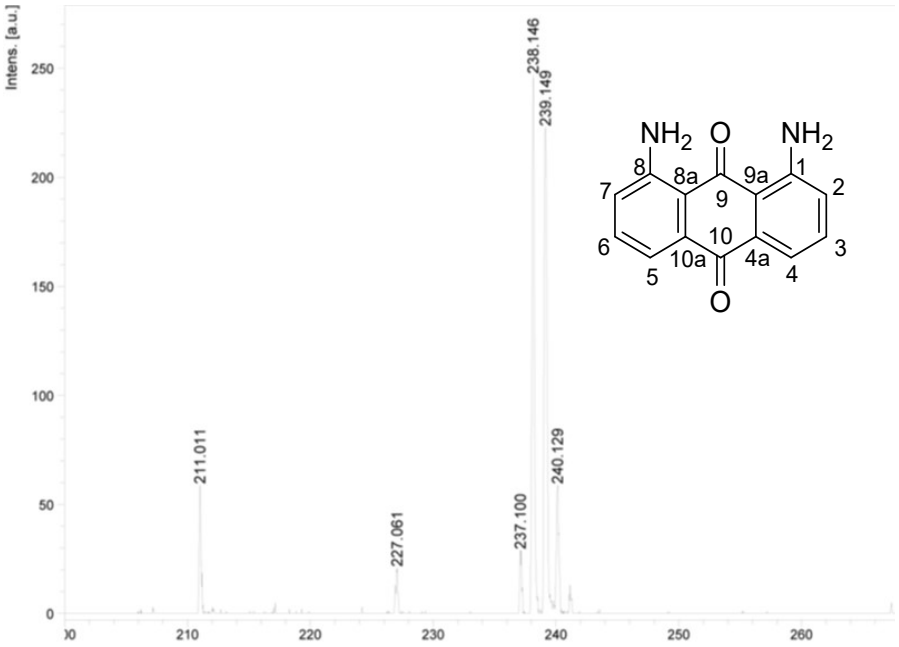
SI 3 ^{13}C NMR spectrum of 1,8-diaminoanthraquinone (**4**) in DMSO-d_6 (100 MHz)



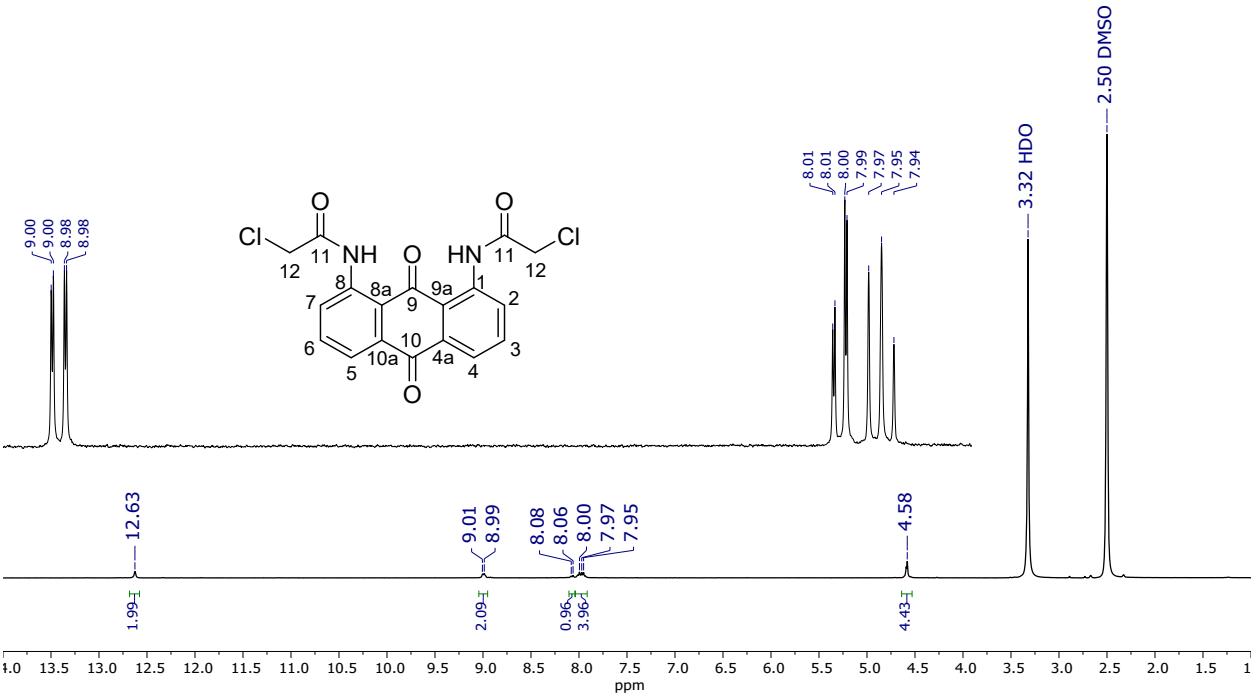
SI 4 COSY ^{1}H–^{1}H spectrum of 1,8-diaminoanthraquinone (**4**) in DMSO-d_6 (400 MHz)



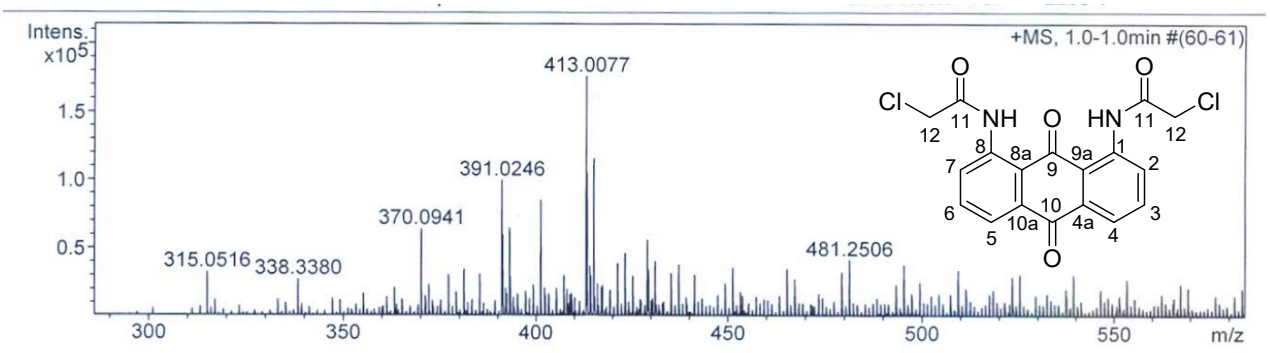
SI 5 HMQC ^{1}H–^{13}C spectrum of 1,8-diaminoanthraquinone (**4**) in DMSO-d_6 (400 MHz and 100 MHz for ^{1}H and ^{13}C NMR, respectively)



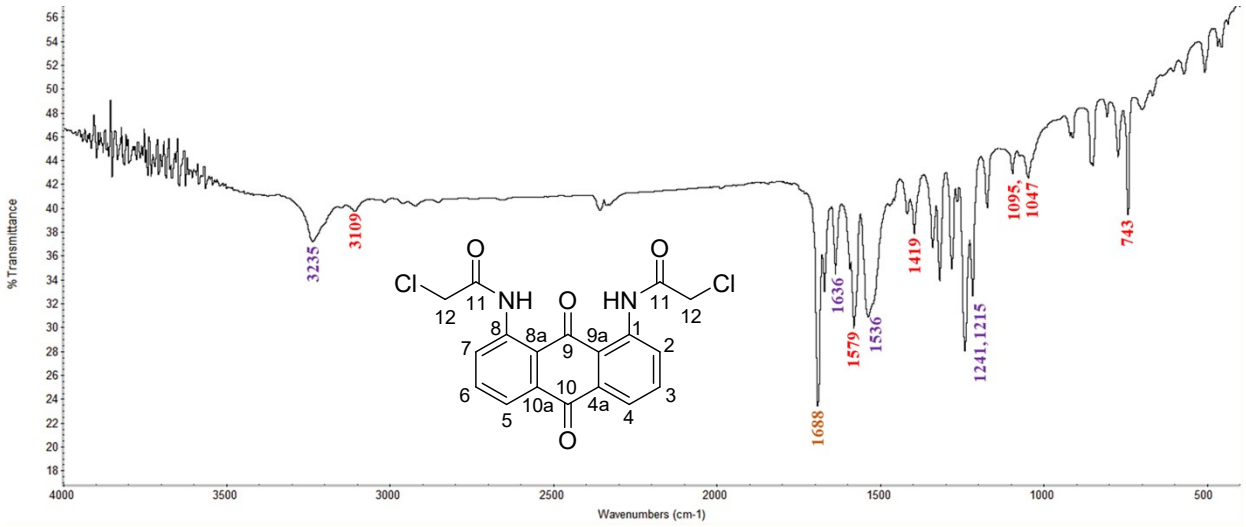
SI 6 MALDI-TOF mass spectrum of 1,8-diaminoanthraquinone (**4**) (Found = 238.146 m/z $[M]^+$)



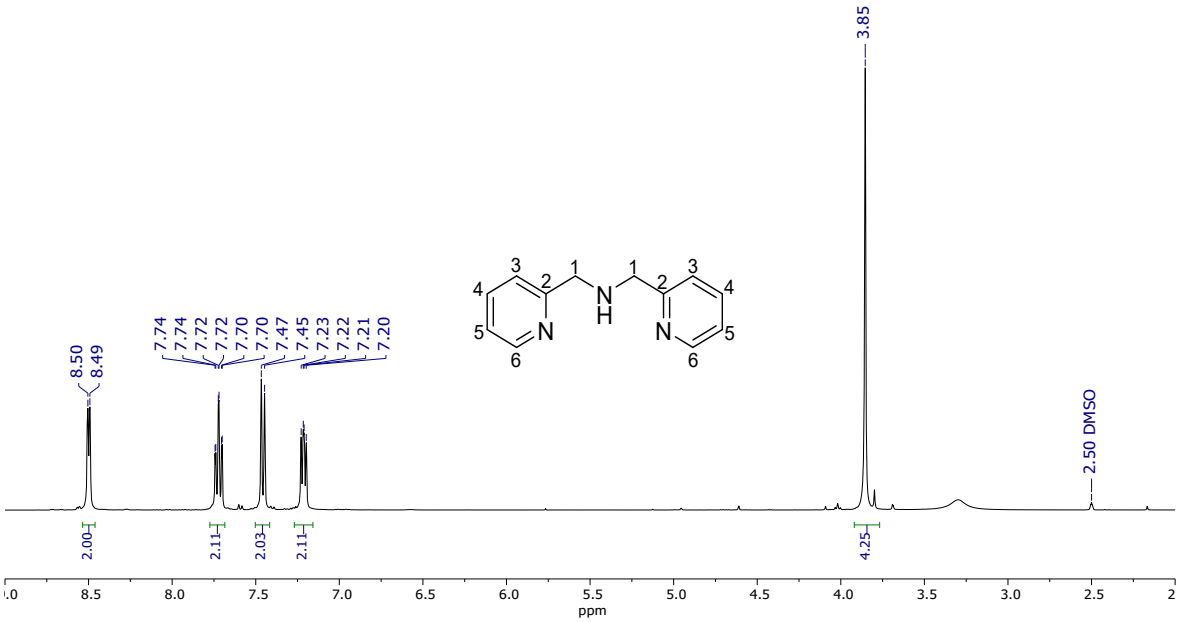
SI 7 Full and partial ^{1}H NMR spectra of *N,N'*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-chloroacetamide) (**6**) in DMSO-d_6 (500 MHz)



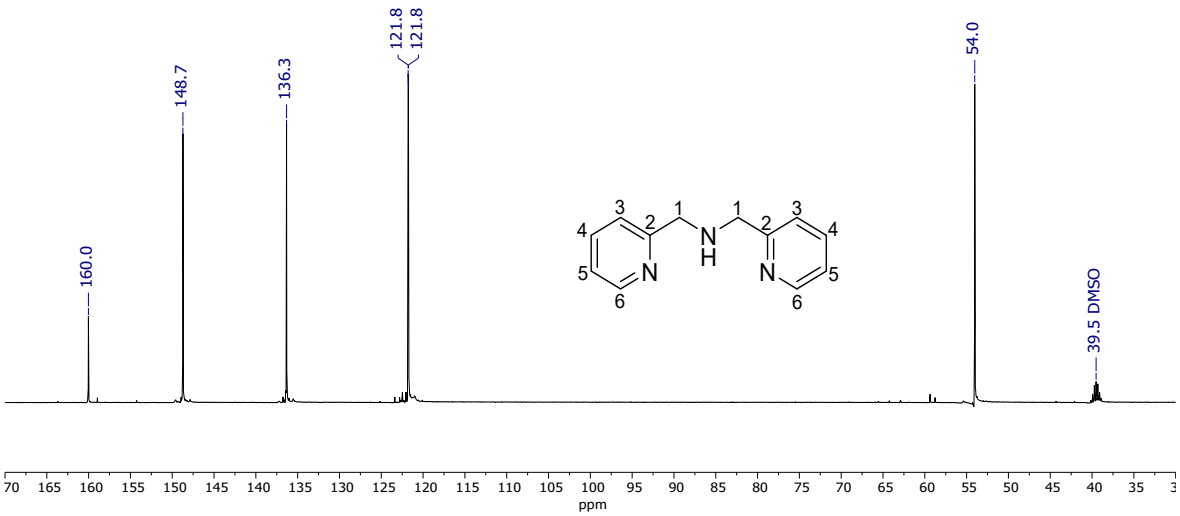
SI 8 ESI high resolution mass spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-chloroacetamide) (**6**) (Found = 413.0077 m/z [M + Na^+])



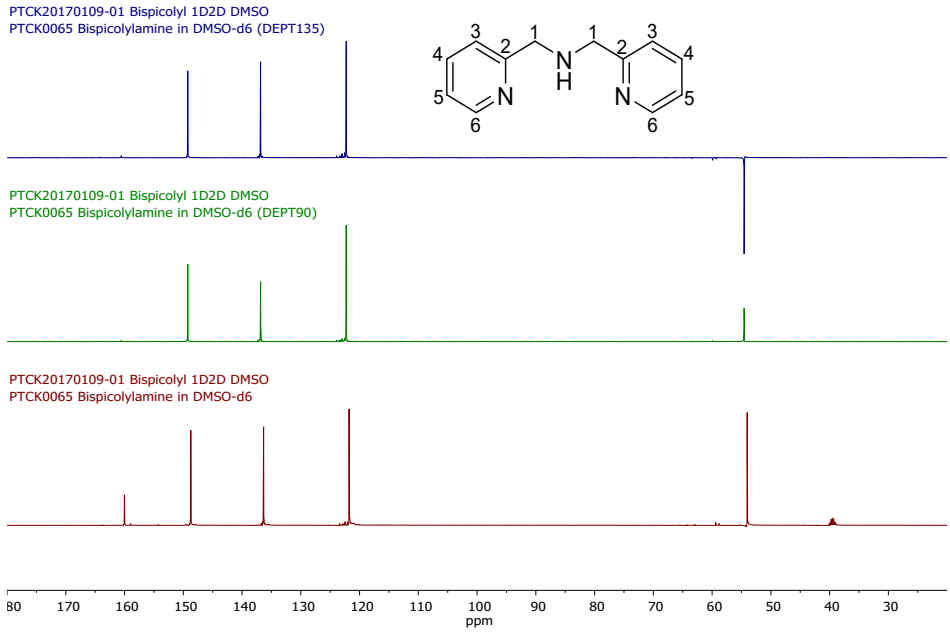
SI 9 FTIR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-chloroacetamide) (**6**)



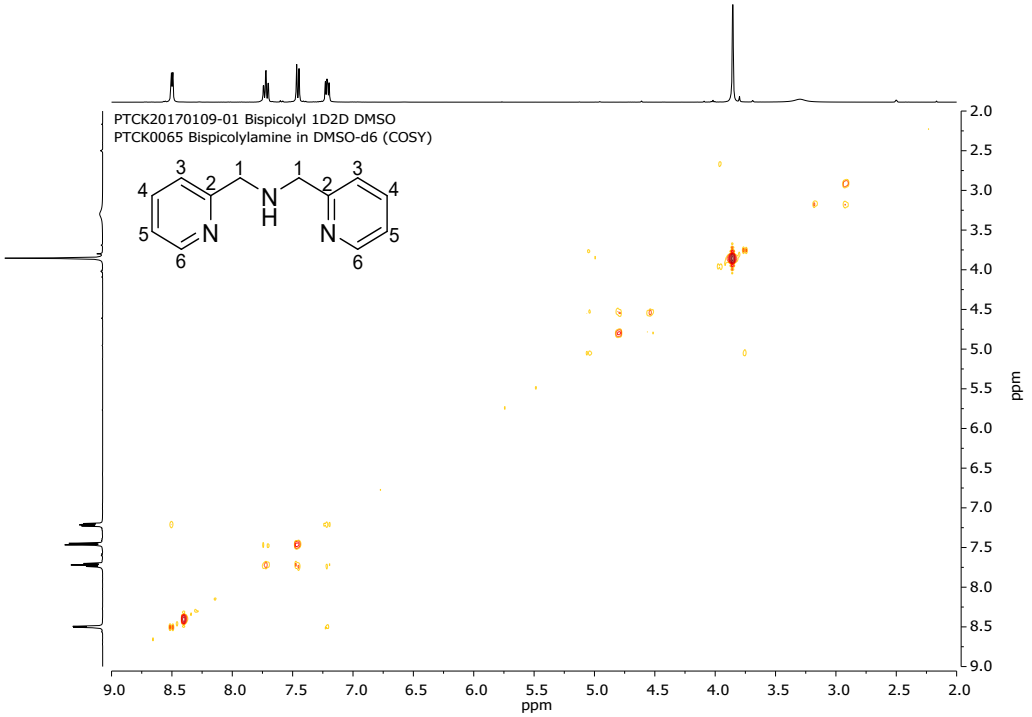
SI 10 ^{1}H NMR spectrum of *bis*(pyridin-2-ylmethyl)amine (**9**) in DMSO-d_6 (400 MHz)



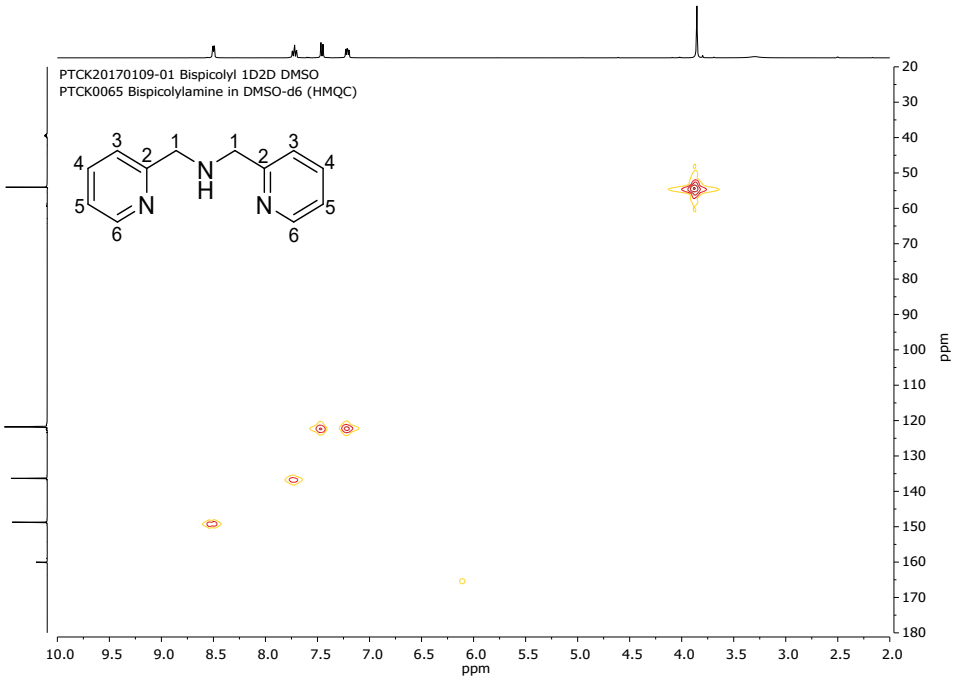
SI 11 ^{13}C NMR spectrum of *bis*(pyridin-2-ylmethyl)amine (**9**) in DMSO-d_6 (100 MHz)



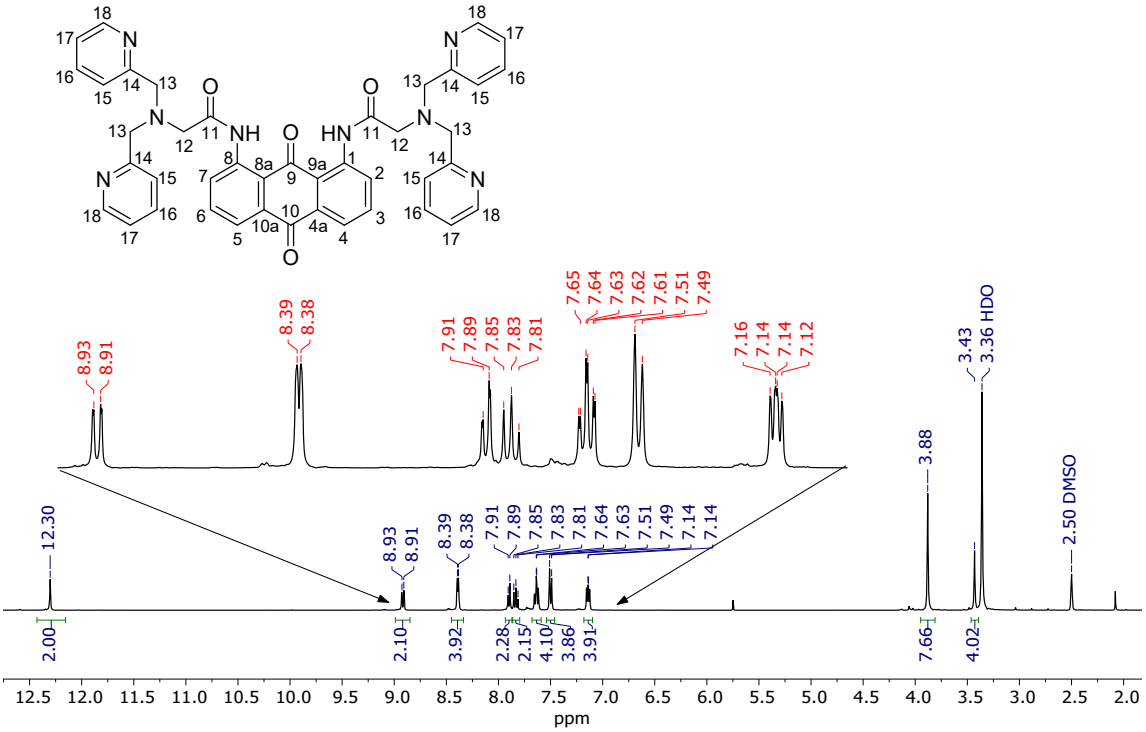
SI 12 DEPT-90 and 135 spectra comparing to ^{13}C-NMR spectrum of *bis*(pyridin-2-ylmethyl)amine (**9**) in DMSO-d_6 (100 MHz)



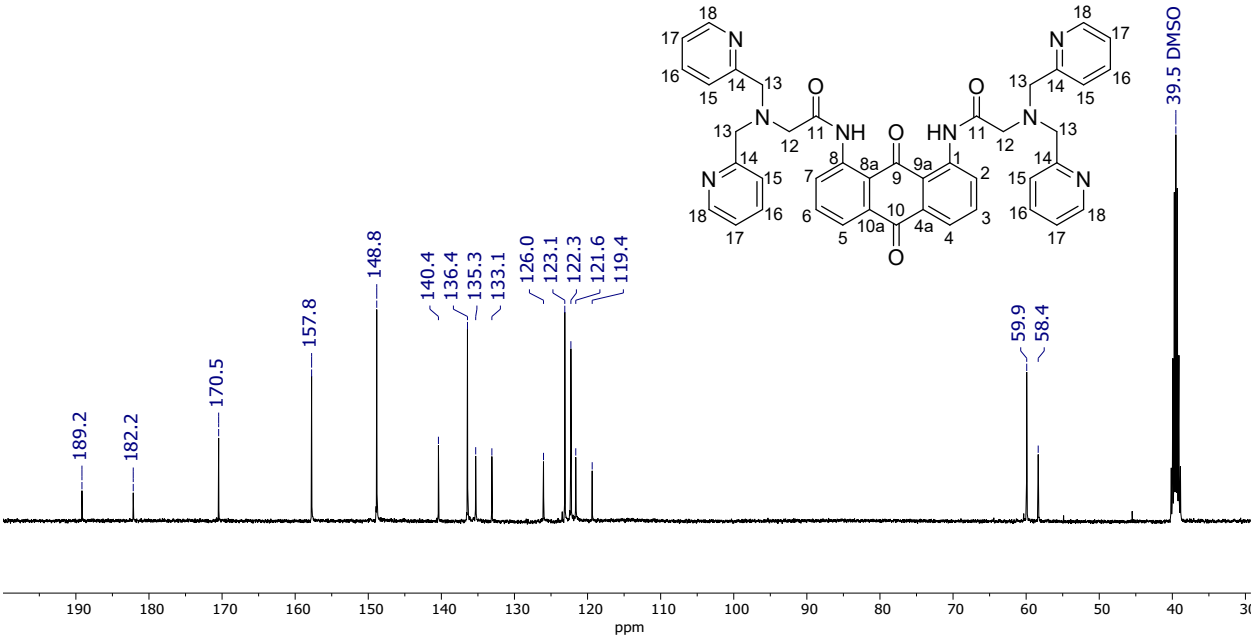
SI 13 COSY ^{1}H–^{1}H spectrum of *bis*(pyridin-2-ylmethyl)amine (**9**) in DMSO-d_6 (400 MHz)



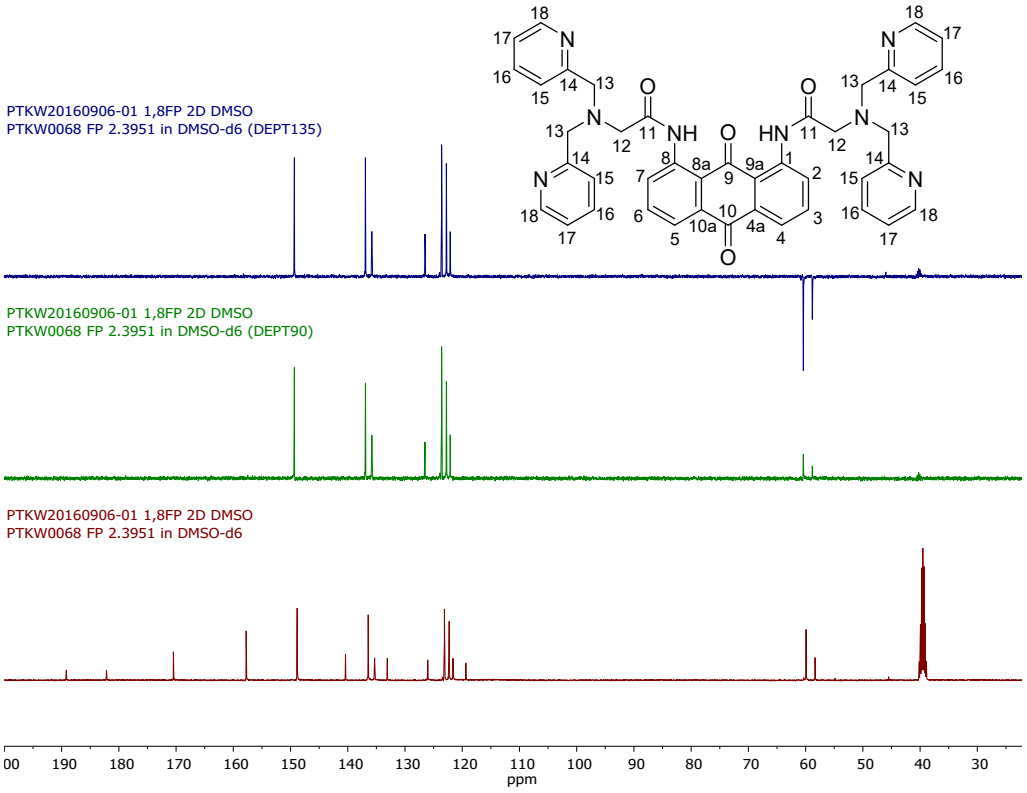
SI 14 HMQC ^{1}H–^{13}C spectrum of *bis*(pyridin-2-ylmethyl)amine (**9**) in DMSO-d_6 (400 MHz and 100 MHz for ^{1}H and ^{13}C NMR, respectively)



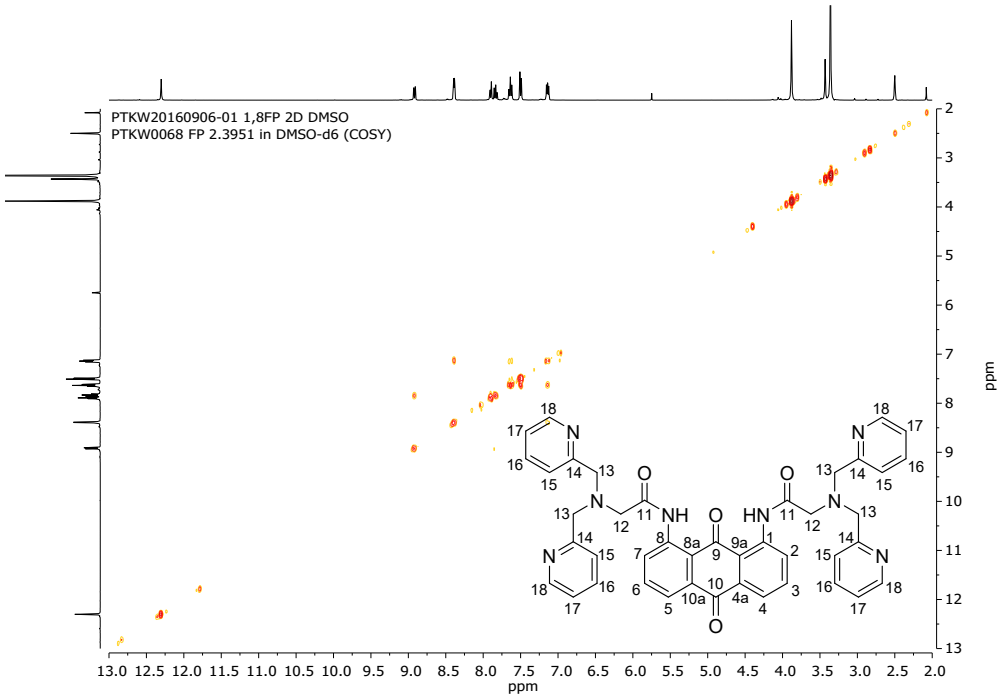
SI 15 Full and partial ^{1}H NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**1**) in DMSO-d_6 (400 MHz)



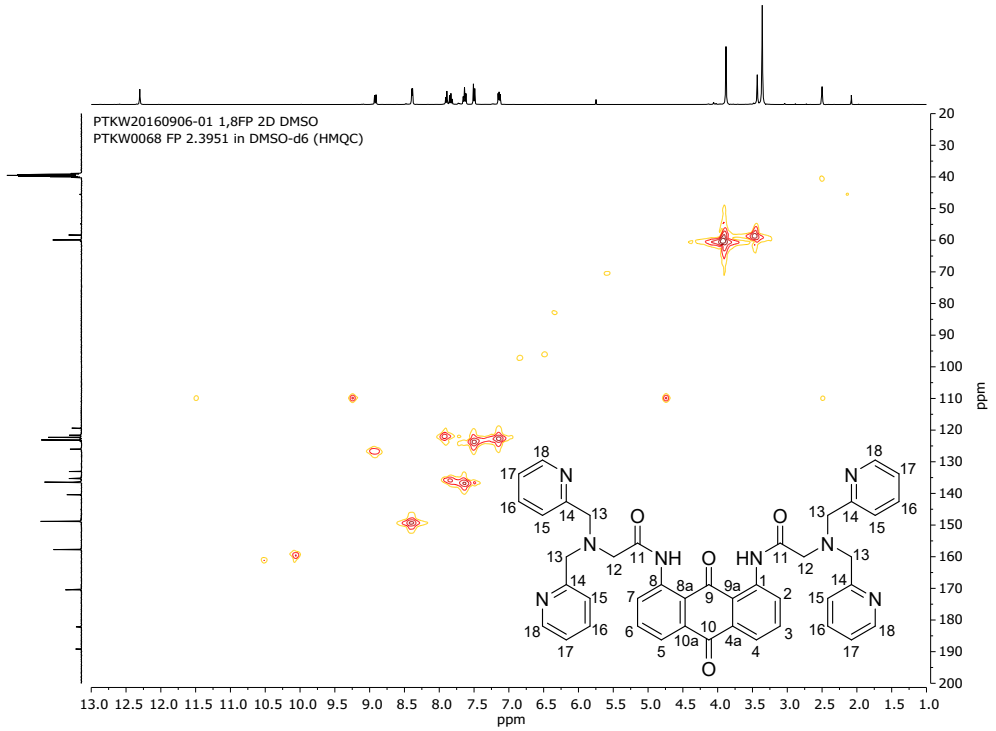
SI 16 ^{13}C NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**1**) in DMSO-d_6 (100 MHz)



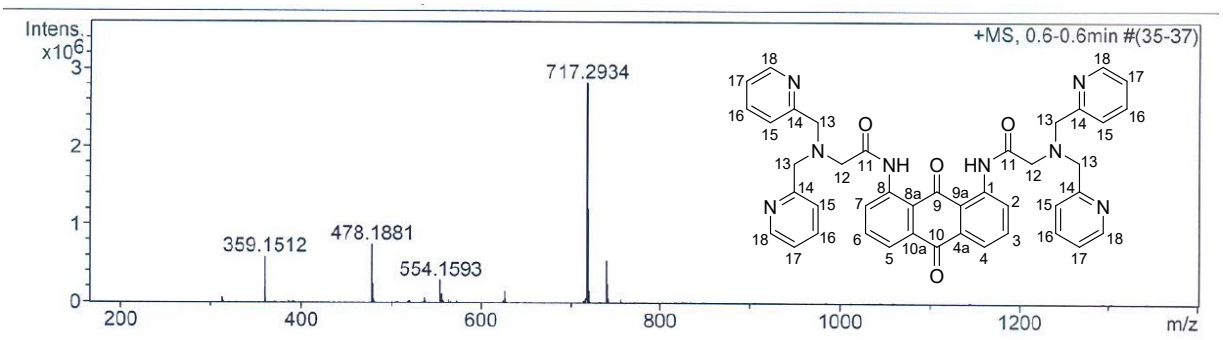
SI 17 DEPT-90 and 135 spectra comparing to ^{13}C NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**1**) in DMSO-d_6 (100 MHz)



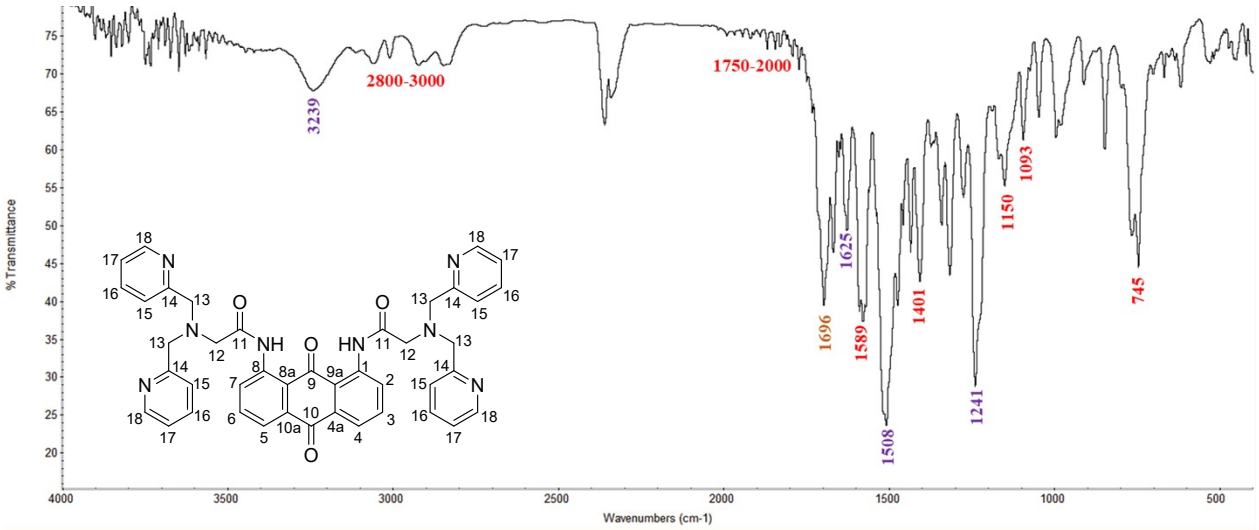
SI 18 COSY ^{1}H–^{1}H spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**1**) in DMSO-d_6 (400 MHz)



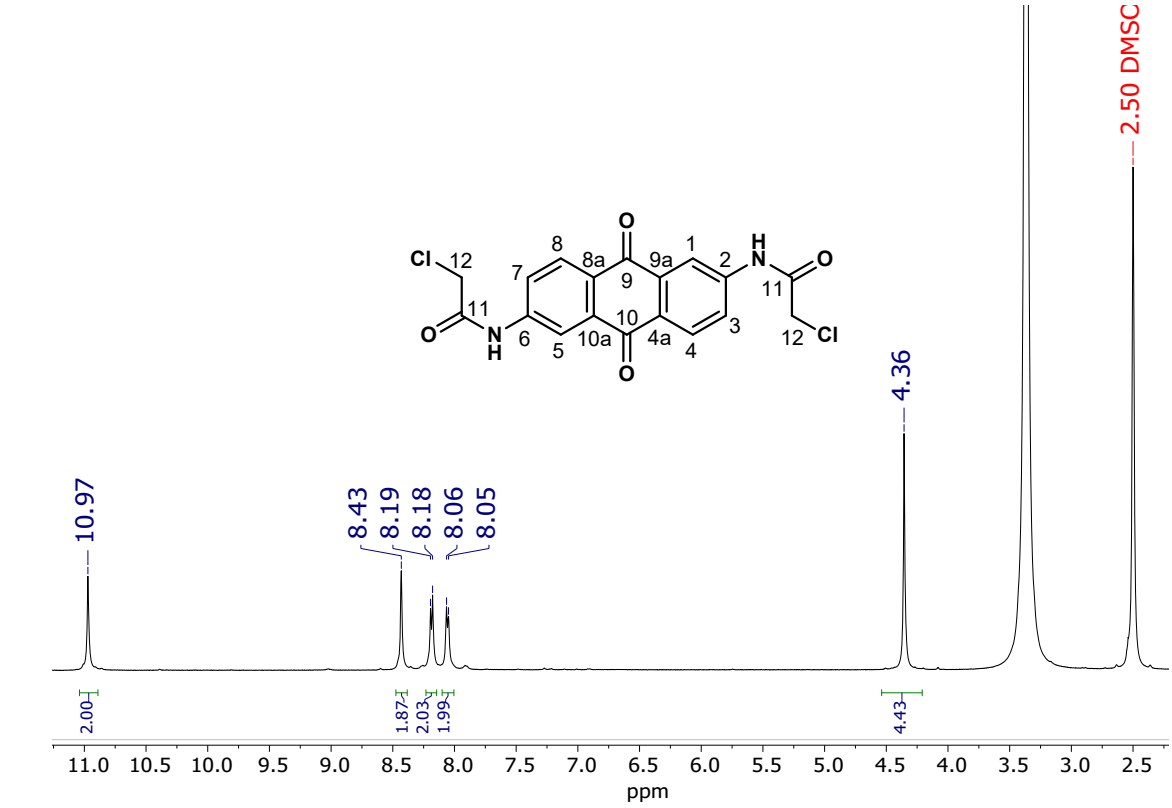
SI 19 HMQC ^{1}H–^{13}C spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**1**) in DMSO-d_6
(400 MHz and 100 MHz for ^{1}H and ^{13}C NMR, respectively)



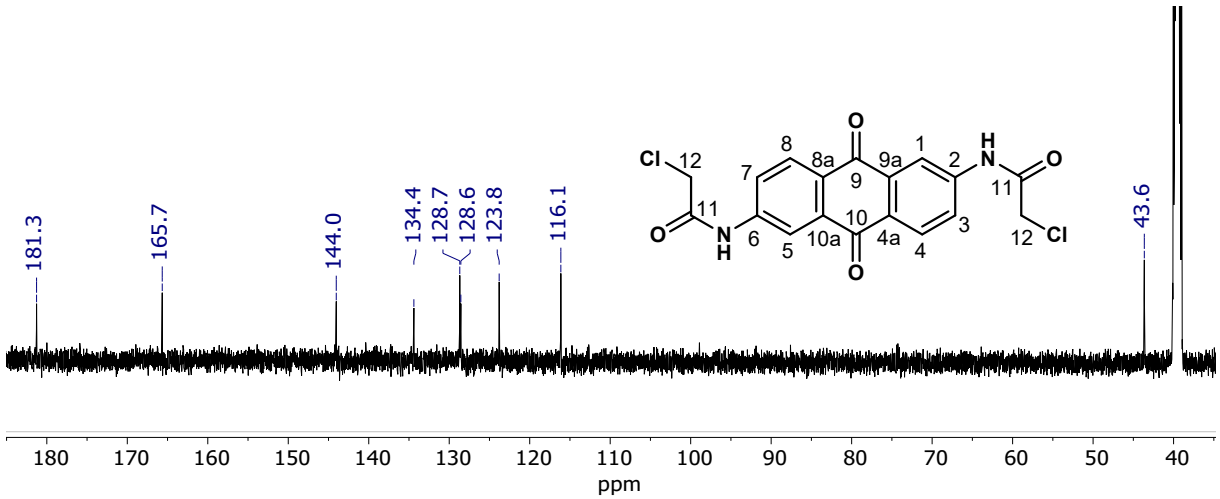
SI 20 ESI high resolution mass spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-(bis(pyridin-2-ylmethyl)amino)acetamide) (**1**) (Found = 717.2934 m/z $[M + H]^+$)



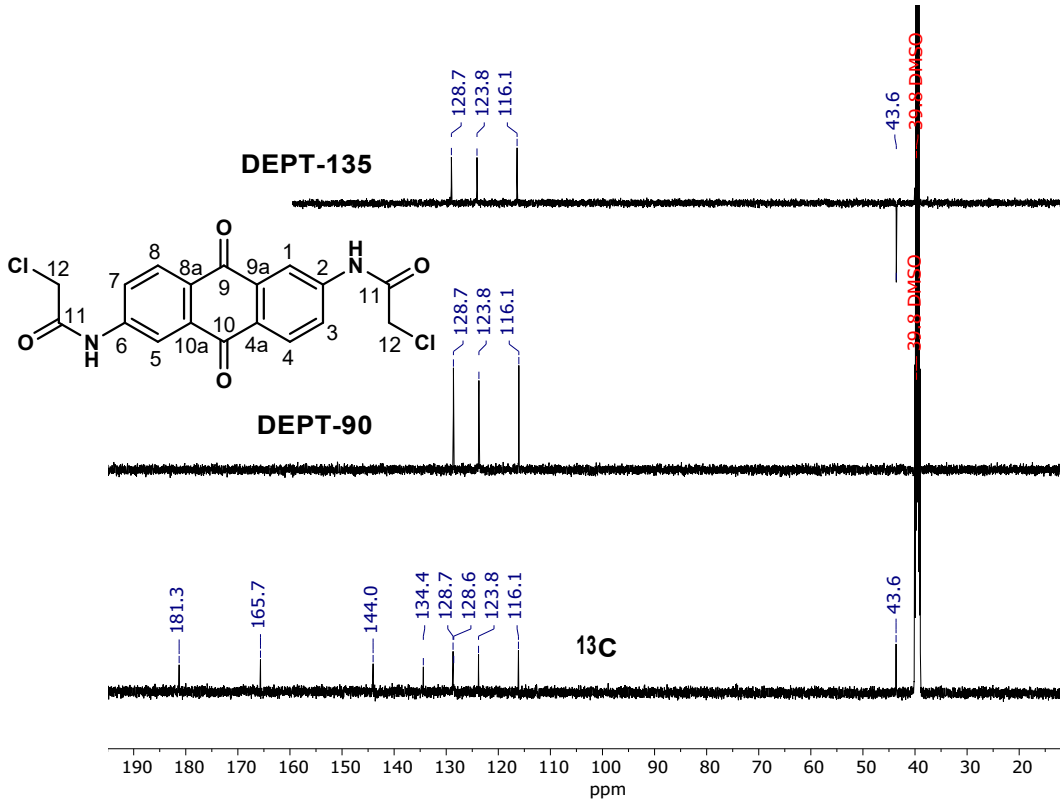
SI 21 FTIR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-1,8-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**1**)



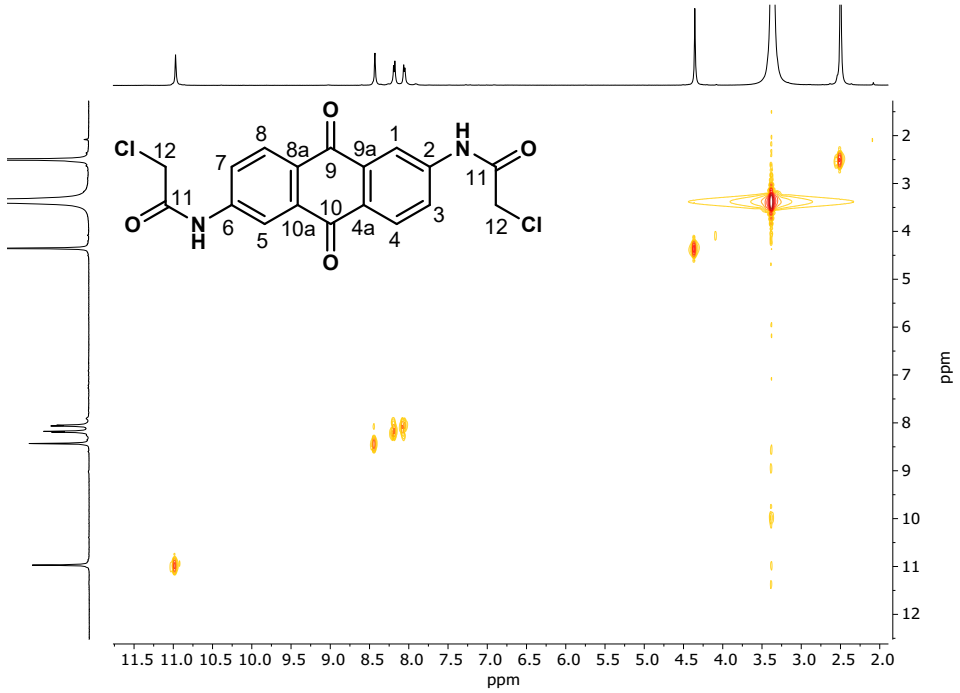
SI 22 ^{1}H NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-chloro acetamide) (**11**) in DMSO-d_6 (500 MHz)



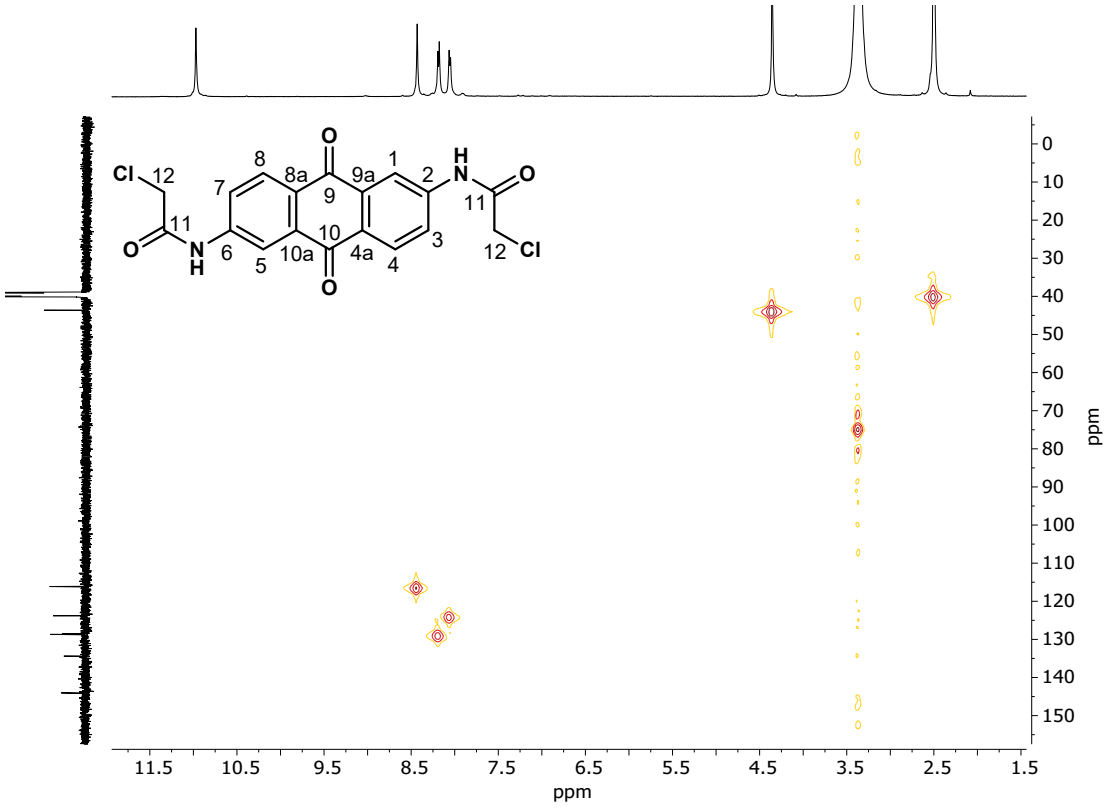
SI 23 ^{13}C NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-chloro acetamide) (**11**) in DMSO-d_6 (125 MHz)



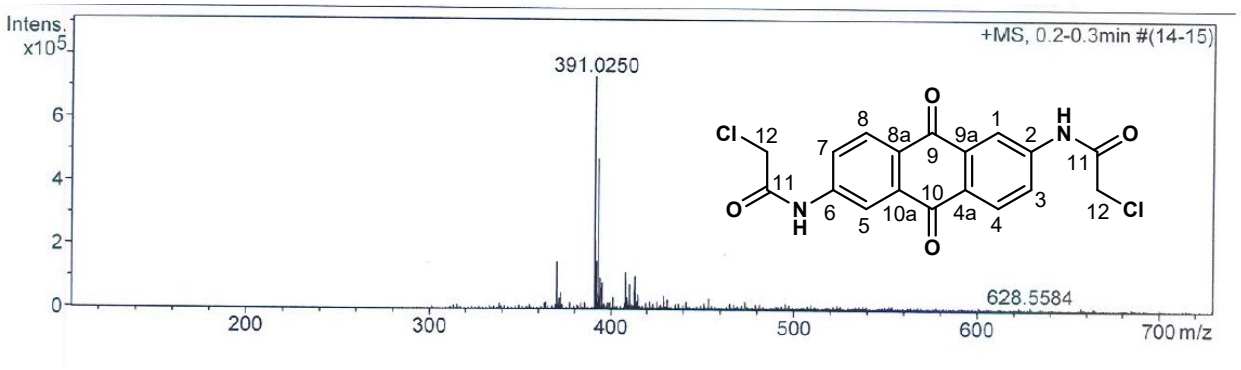
SI 24 DEPT-90 and 135 spectra comparing to ^{13}C-NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-chloroacetamide) (**11**) in DMSO-d_6 (125 MHz)



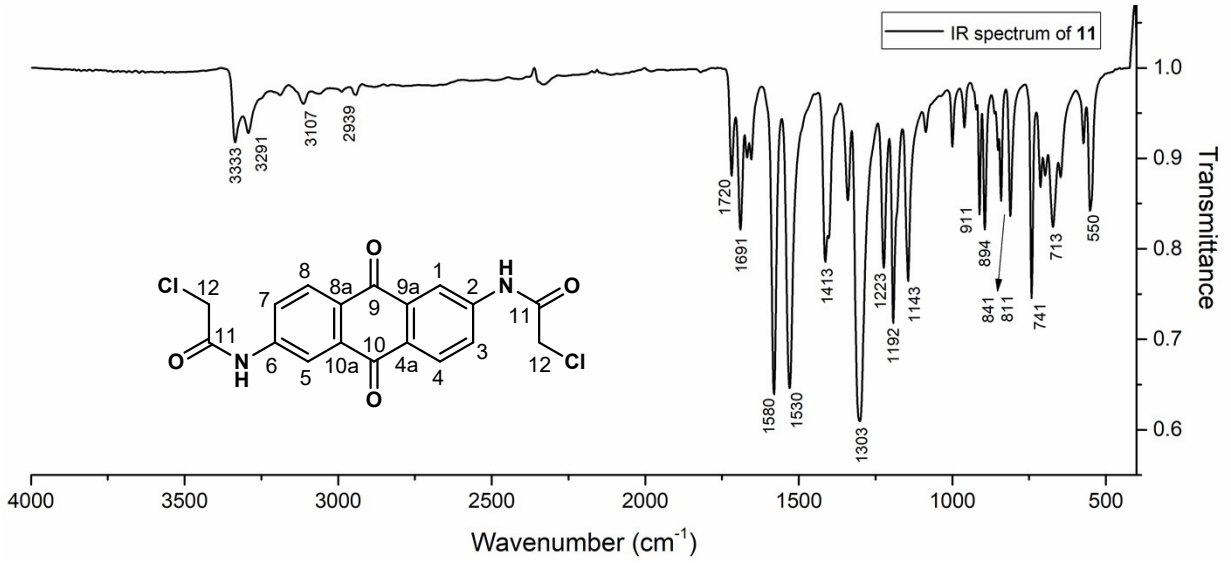
SI 25 COSY ^{1}H–^{1}H spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-chloro acetamide) (**11**) in DMSO-d_6 (500 MHz)



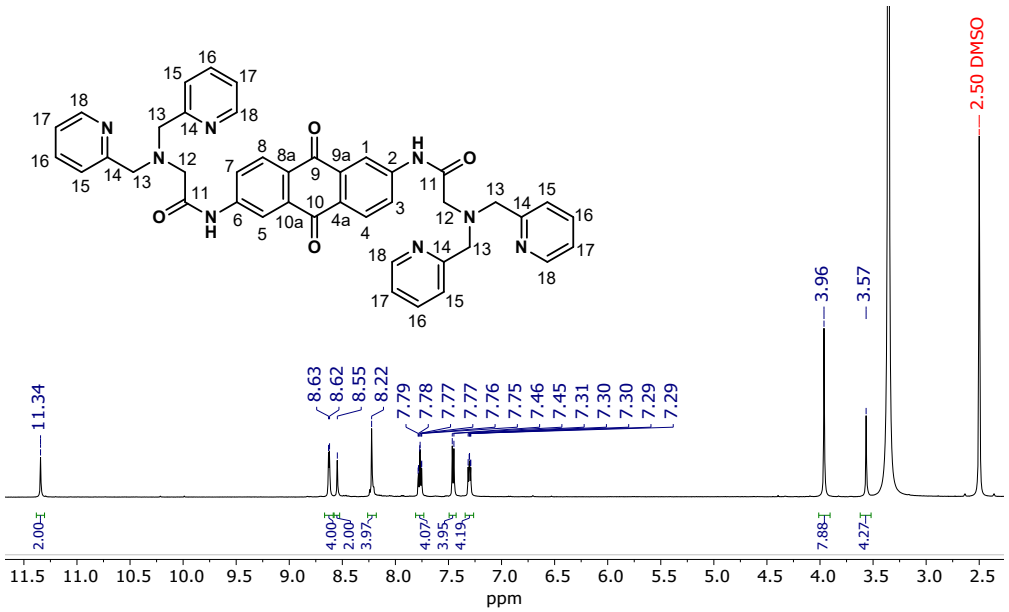
SI 26 HMQC ^{1}H–^{13}C spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-chloroacetamide) (**11**) in DMSO-d_6 (500 MHz and 125 MHz for ^{1}H and ^{13}C NMR, respectively)



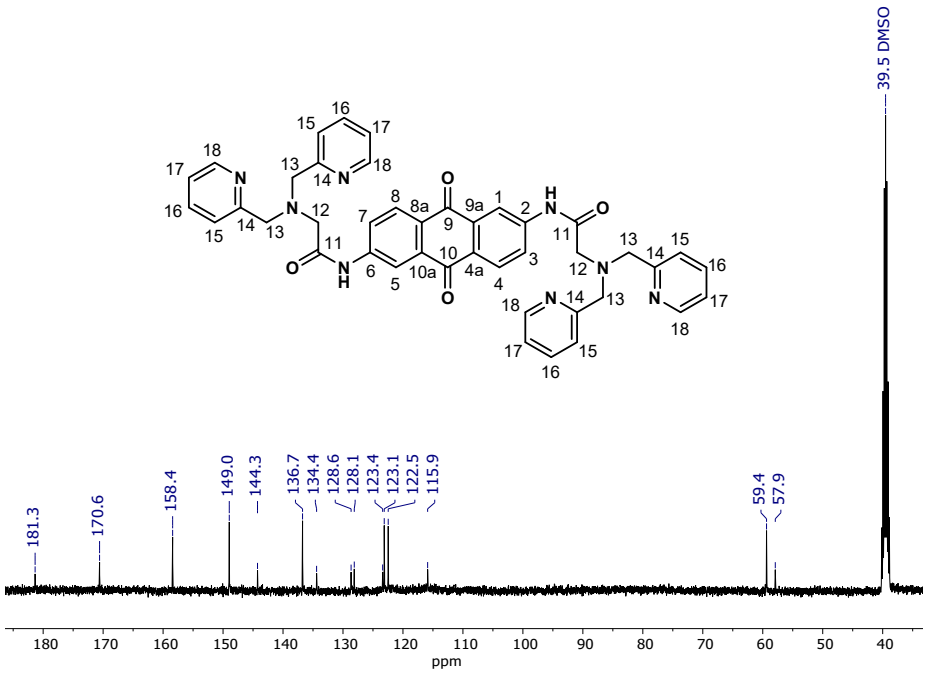
SI 27 ESI high resolution mass spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-chloroacetamide) (**11**) (Found = 391.0250 m/z ($[M+H]^{+}$))



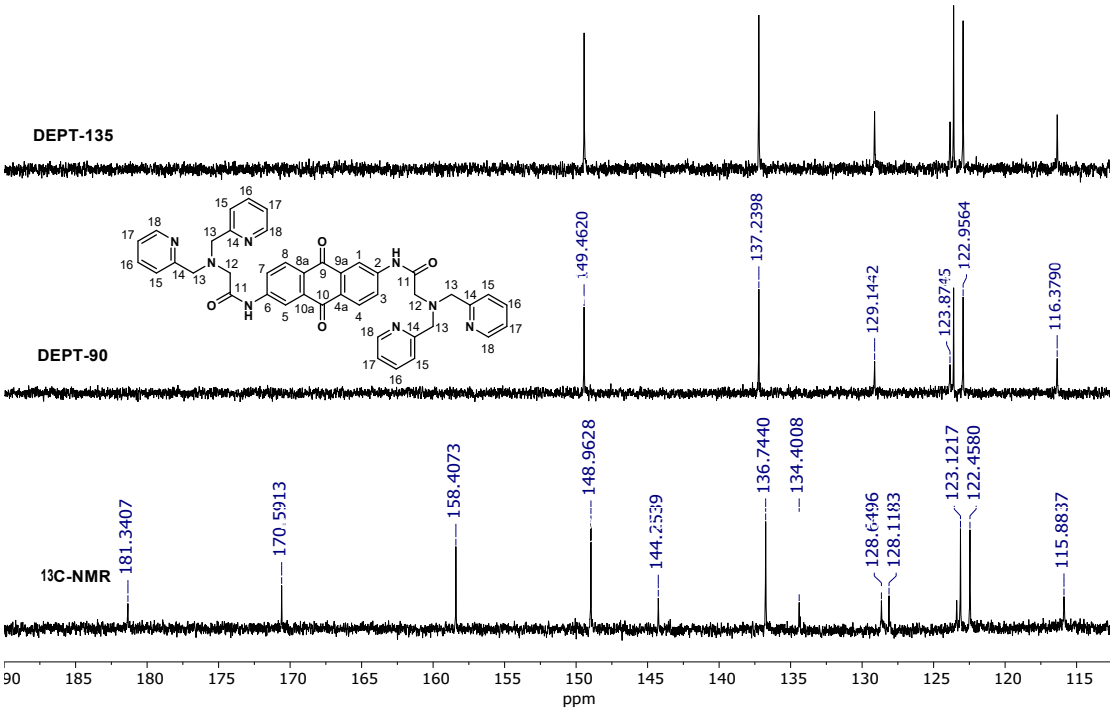
SI 28 ATR-FTIR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-chloroacetamide) (**11**)



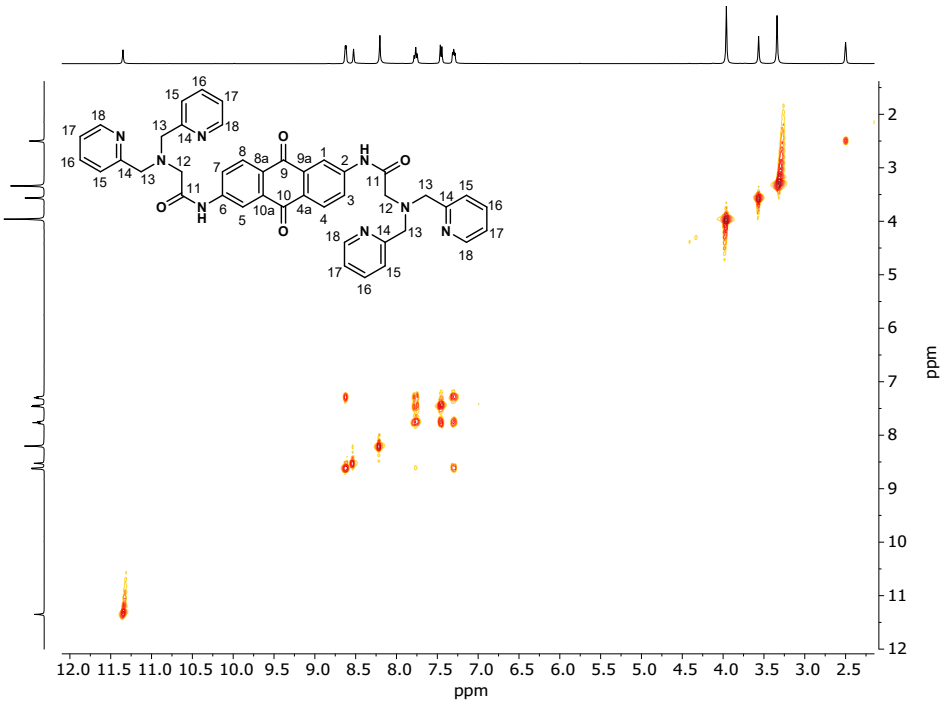
SI 29 ^{1}H NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**2**) in DMSO-d_6 (500 MHz)



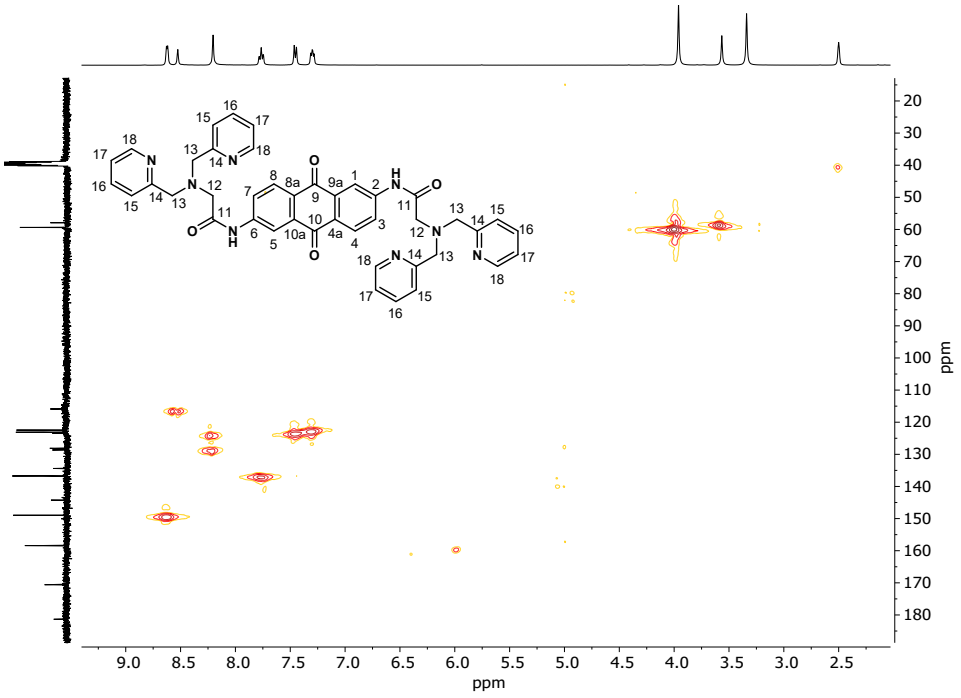
SI 30 ^{13}C NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**2**) in DMSO-d_6 (125 MHz)



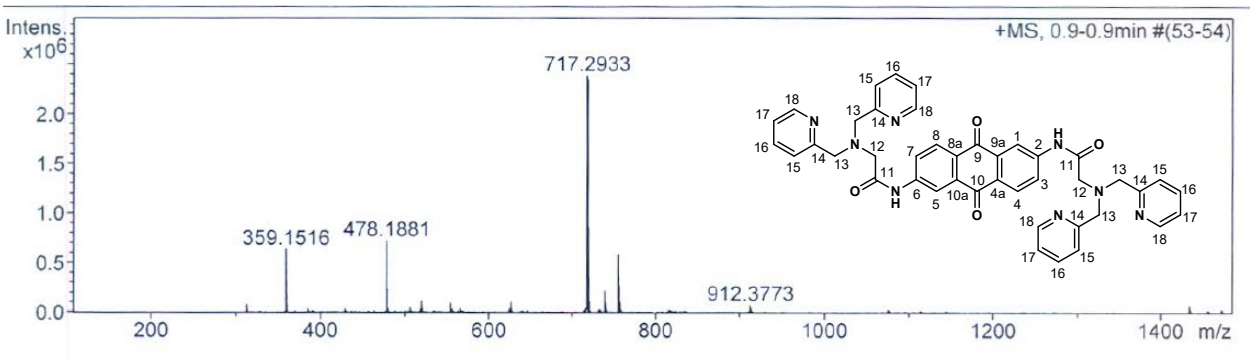
SI 31 DEPT-90 and 135 spectra comparing to ^{13}C-NMR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**2**) in DMSO-d_6 (125 MHz)



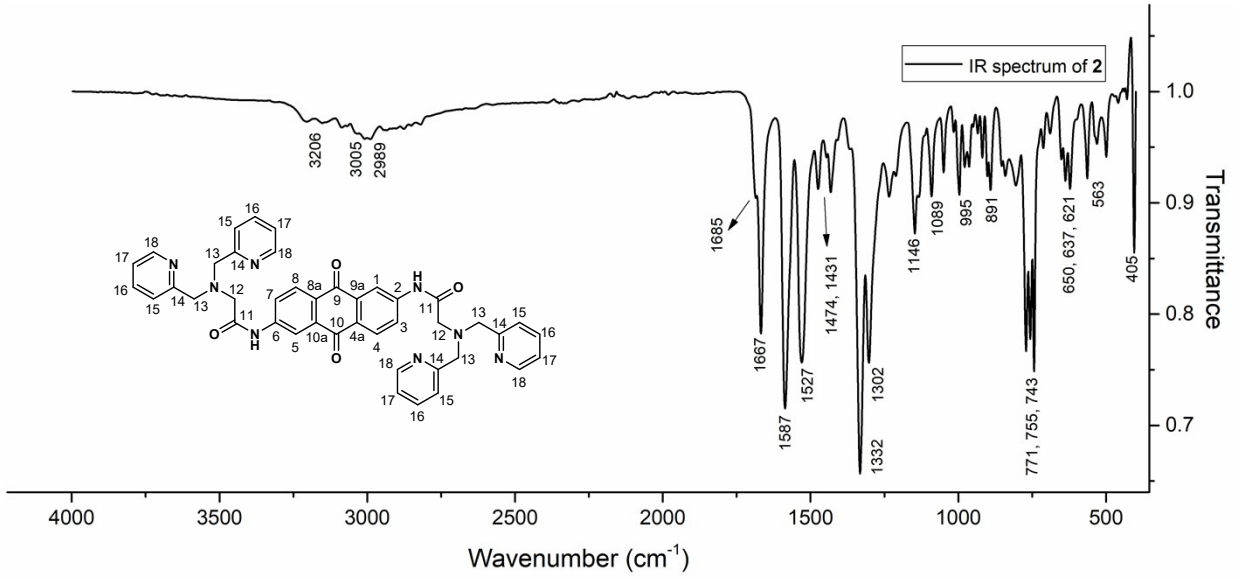
SI 32 COSY ^{1}H–^{1}H spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**2**) in DMSO-d_6 (500 MHz)



SI 33 HMQC ^{1}H–^{13}C spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**2**) in DMSO-d_6
(500 MHz and 125 MHz for ^{1}H and ^{13}C NMR, respectively)



SI 34 ESI high resolution mass of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**2**) (Found = 717.2933 m/z $[M + H]^+$)



SI 35 ATR-FTIR spectrum of *N,N′*-(9,10-dioxo-9,10-dihydroanthracene-2,6-diyl)*bis*(2-(*bis*(pyridin-2-ylmethyl)amino)acetamide) (**2**)

References

1 (**a**) R. Shannon, *Acta Crystallogr. A*, 1976, **32**, 751-767; (**b**) S. Gomes, J.-M. Nedelec, E. Jallot, D. Sheptyakov and G. Renaudin, *Chem. Mater.*, 2011, **23**, 3072-3085; (**c**) N. Jagannatha and P. Mohan Rao, *Bull. Mater. Sci.*, 1993, **16**, 365-369; (**d**) S. Marbumrung, K. Wongravee, V. Ruangpornvisuti, G. Tumcharern, T. Tuntulani and B. Tomapatanaget, *Sens. Actuators B Chem.*, 2012, **171-172**, 969-975.