Supplementary information

Towards asymmetrical Methylene Blue analogues: synthesis and reactivity of 3-*N*'-arylaminophenothiazines

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Content

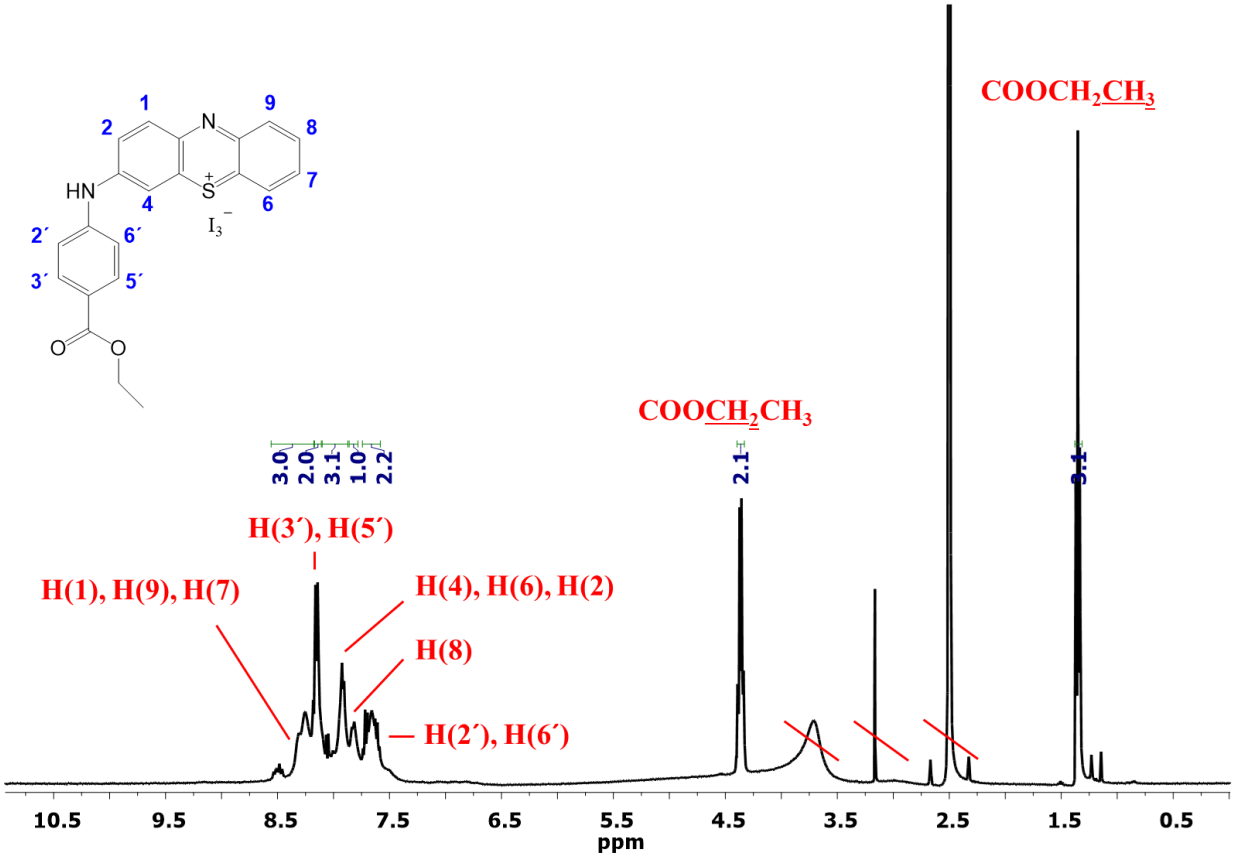

Figure S1. ^{1}H NMR spectrum of the compound **10**, DMSO-d_6, 300 K, 400 MHz.

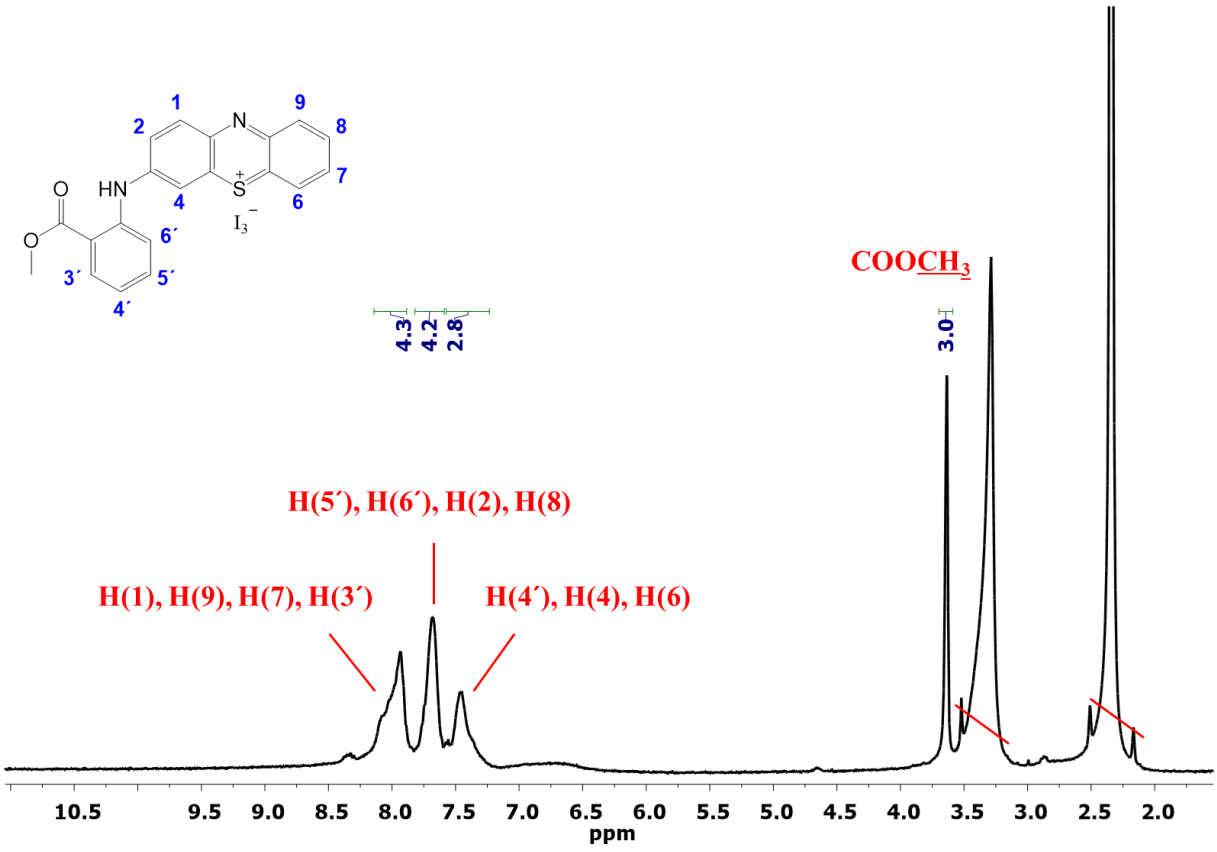

Figure S2. ^{1}H NMR spectrum of the compound **11**, DMSO-d_6, 300 K, 400 MHz.

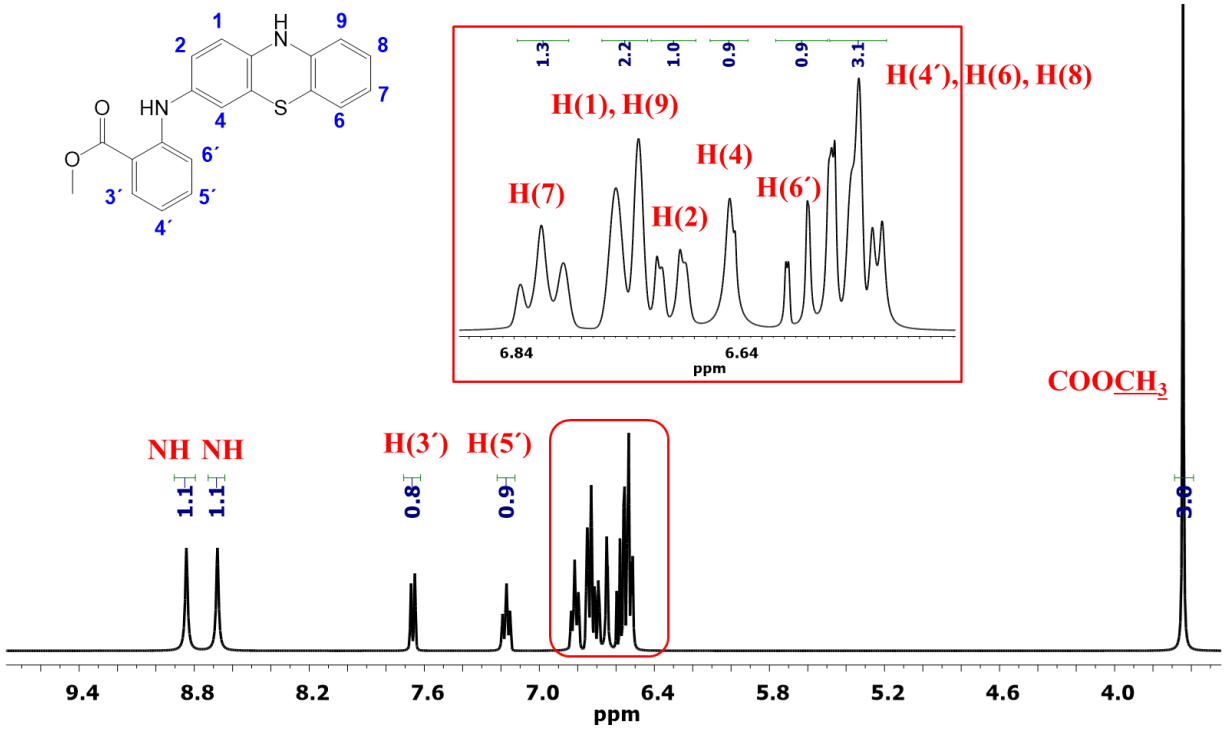

Figure S3. ^{1}H NMR spectrum of leuco form of the compound **11**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

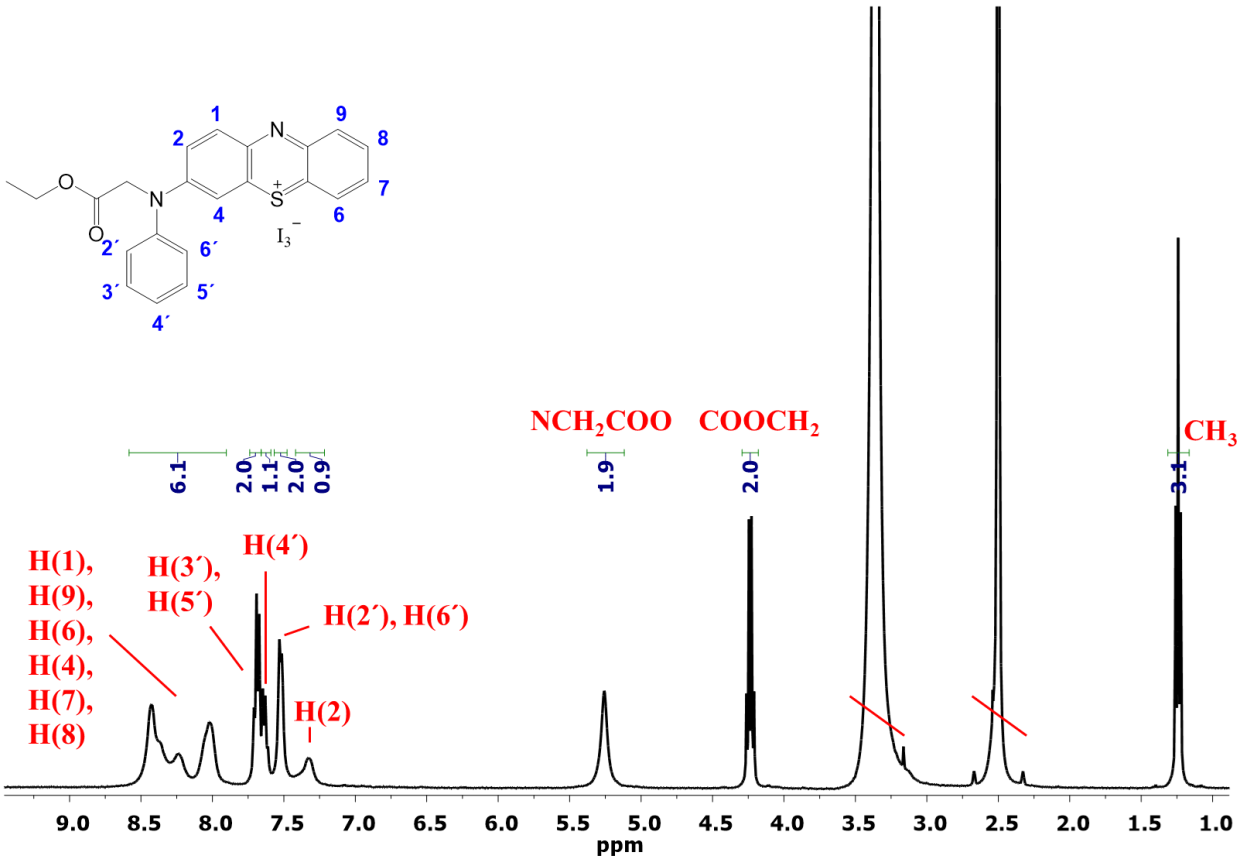

Figure S4. ^{1}H NMR spectrum of the compound **12**, DMSO-d_6, 300 K, 400 MHz.

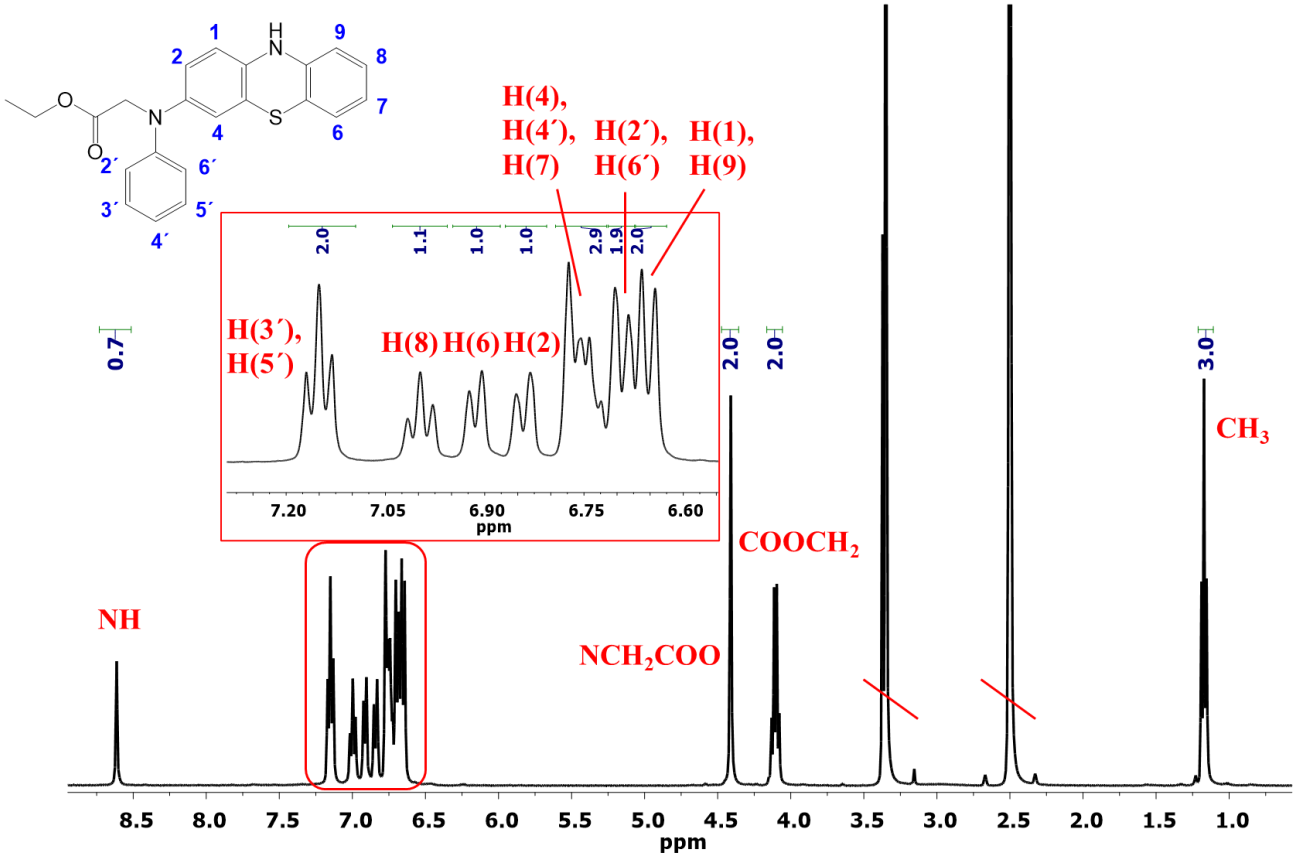

Figure S5. ^{1}H NMR spectrum of leuco form of the compound **12**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

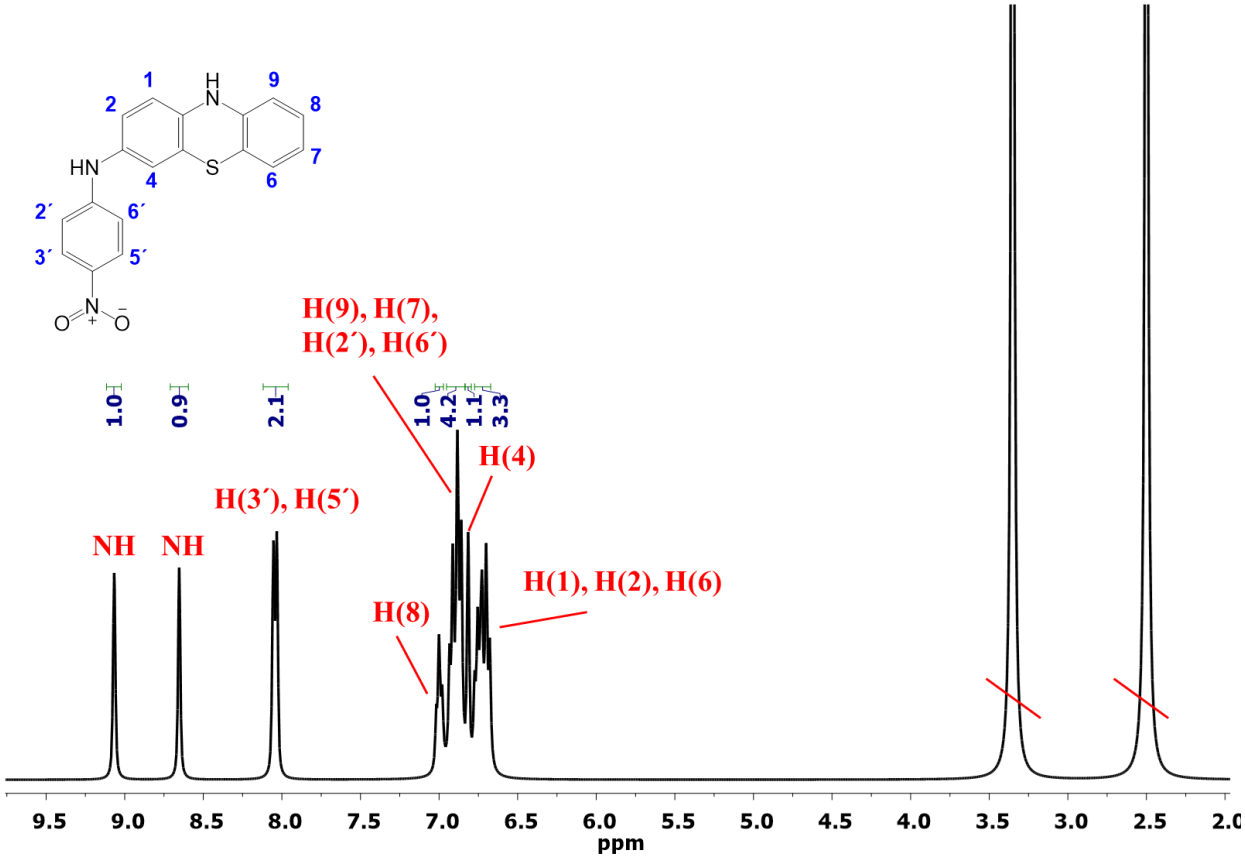

Figure S6. ^{1}H NMR spectrum of the compound **13**, DMSO-d_6, 300 K, 400 MHz.

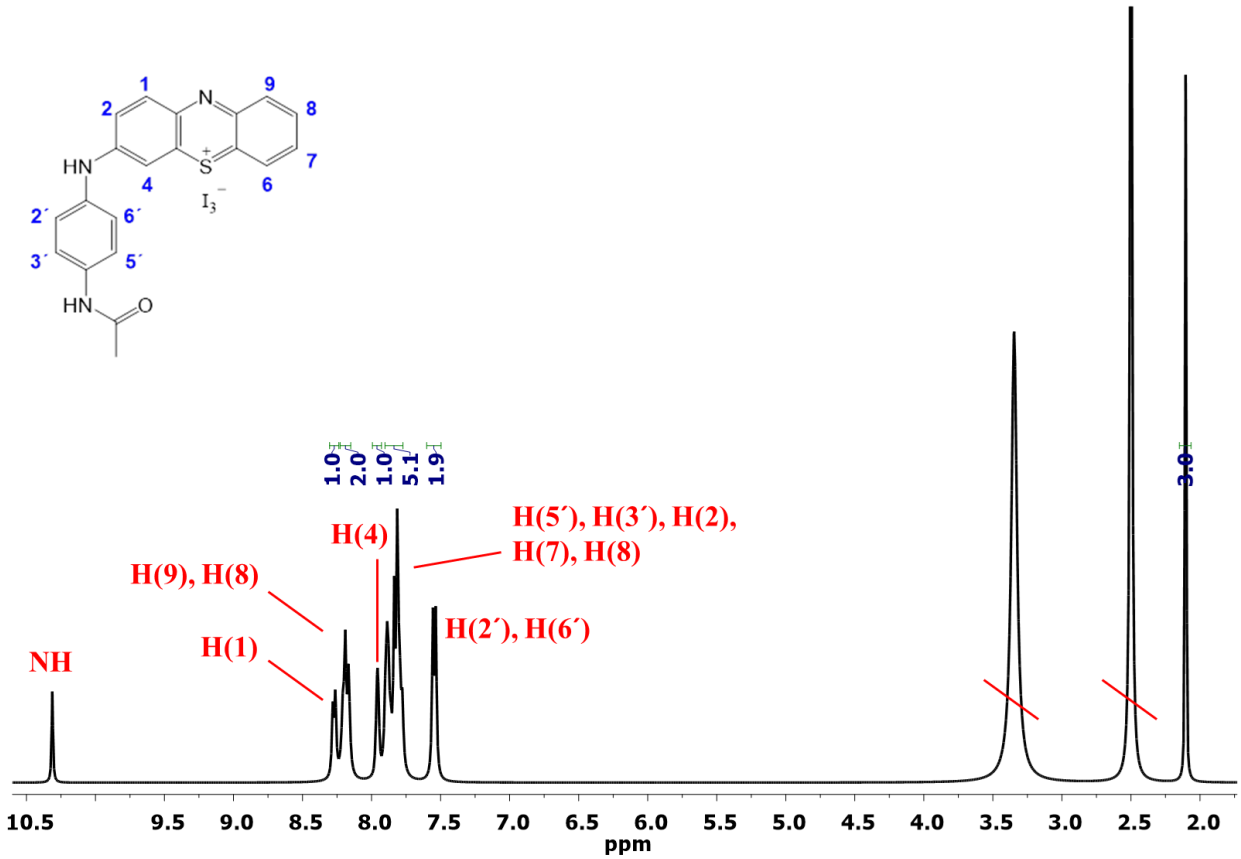

Figure S7. ^{1}H NMR spectrum of the compound **14**, DMSO-*d*$_6$, 300 K, 400 MHz.

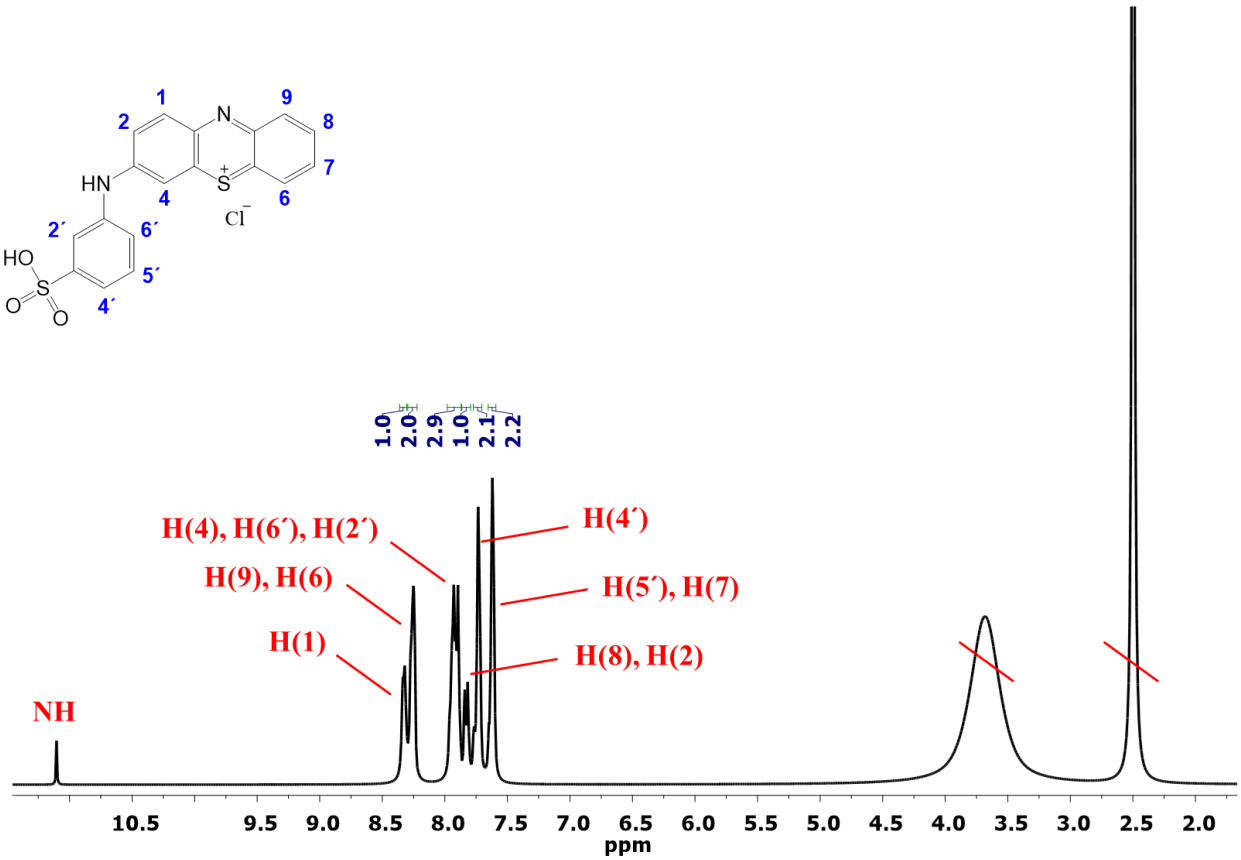

Figure S8. ^{1}H NMR spectrum of the compound **15**, DMSO-*d*$_6$, 300 K, 400 MHz.

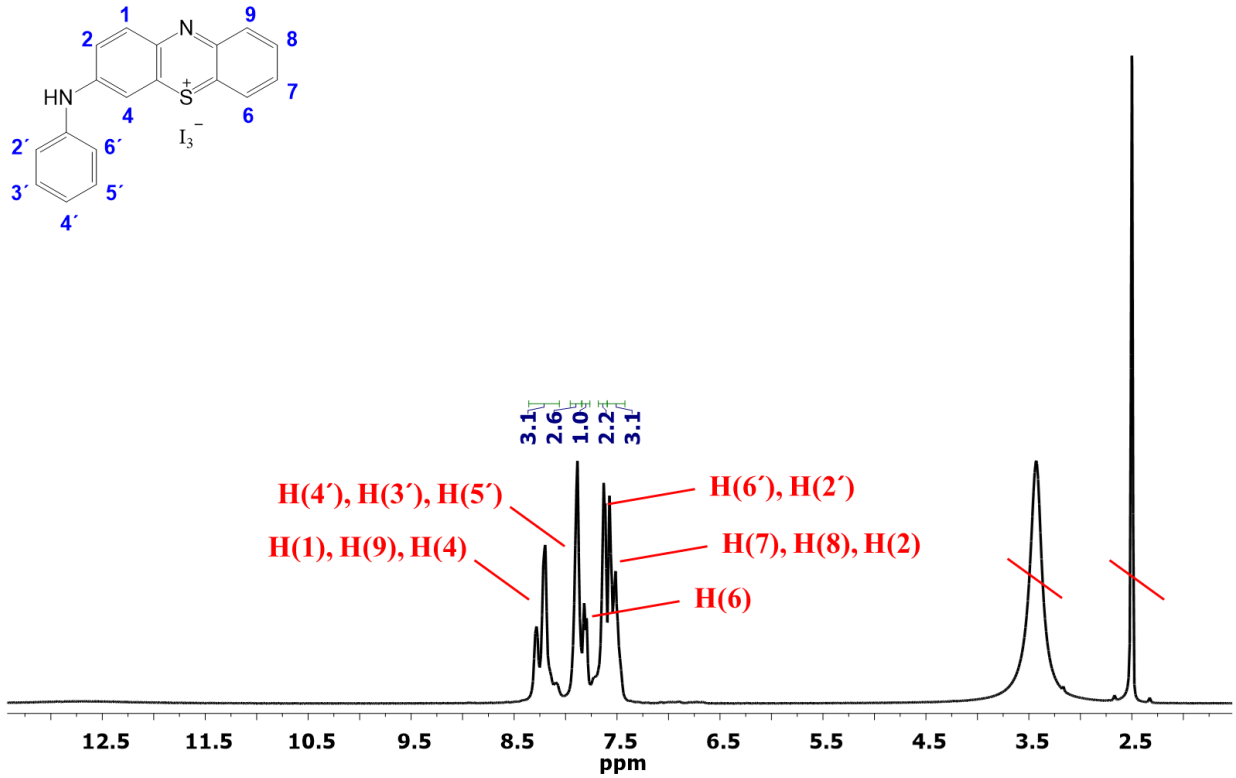

Figure S9. ^{1}H NMR spectrum of the compound **16**, DMSO-d_6, 300 K, 400 MHz.

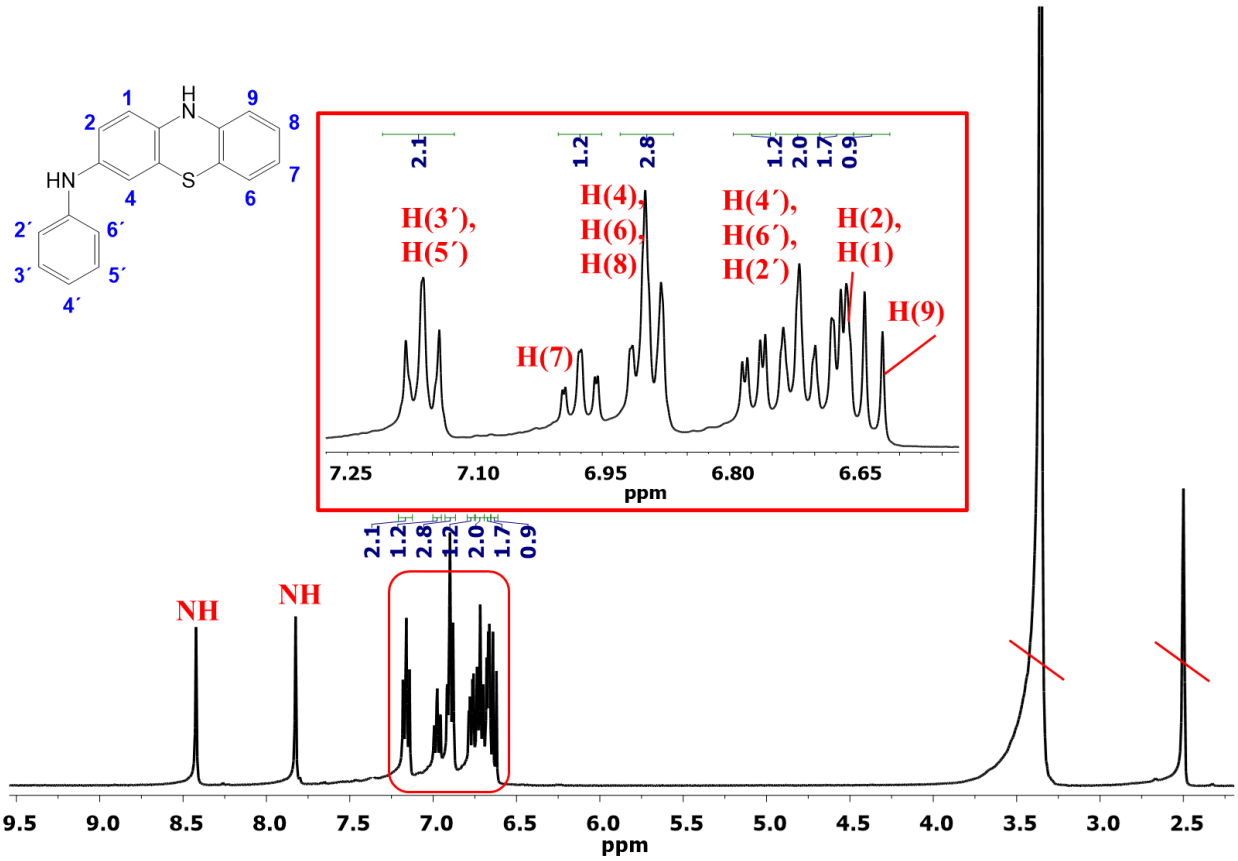

Figure S10. ^{1}H NMR spectrum of leuco form of the compound **16**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

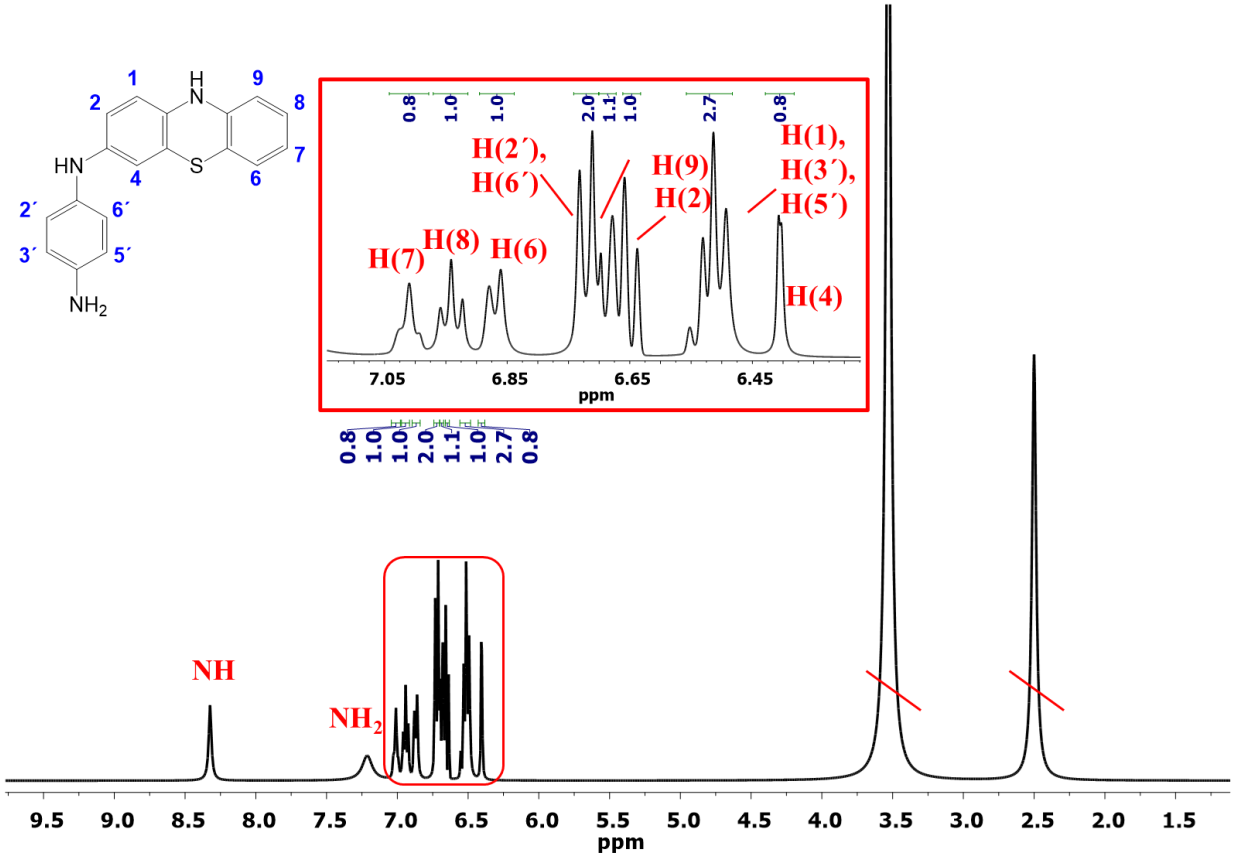

Figure S11. ^{1}H NMR spectrum of leuco form of the compound **17**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

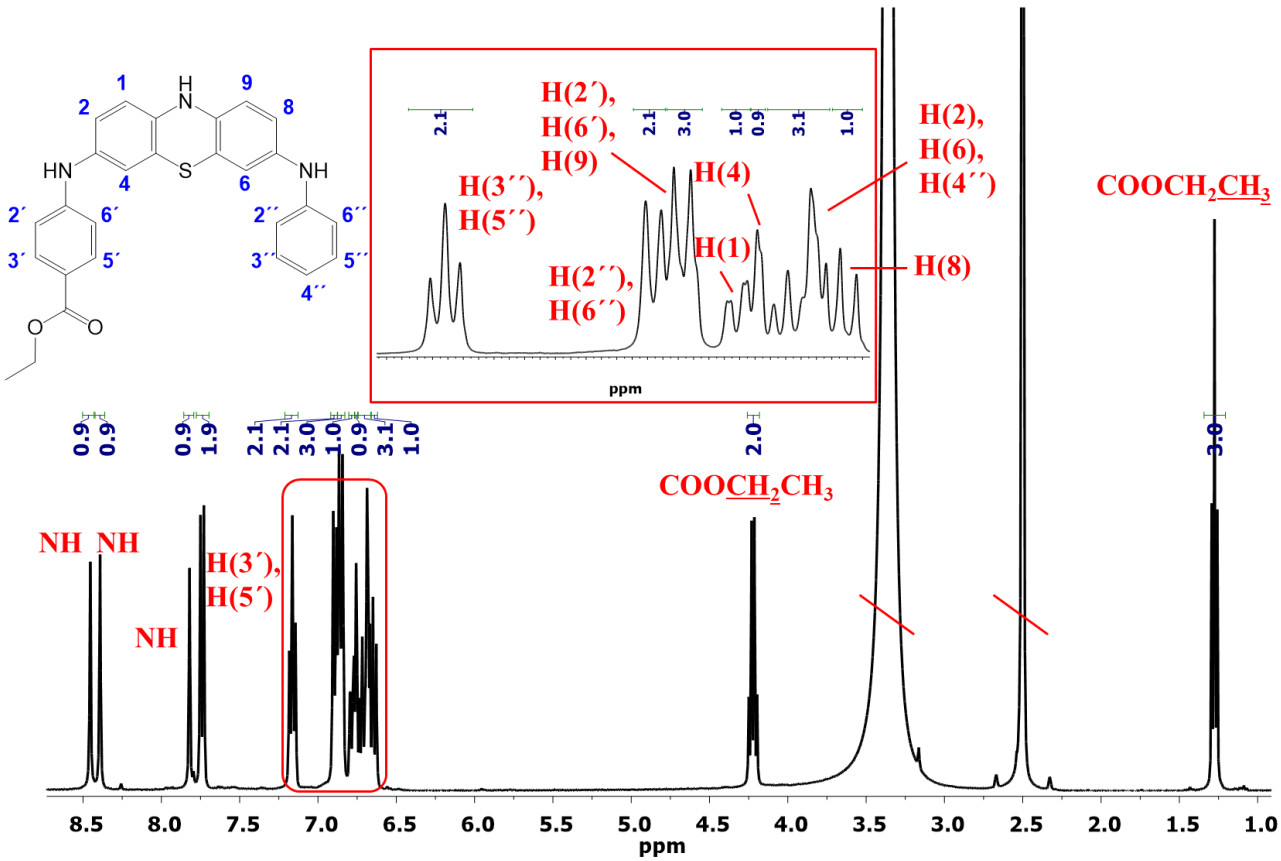

Figure S12. ^{1}H NMR spectrum of leuco form of the compound **18**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

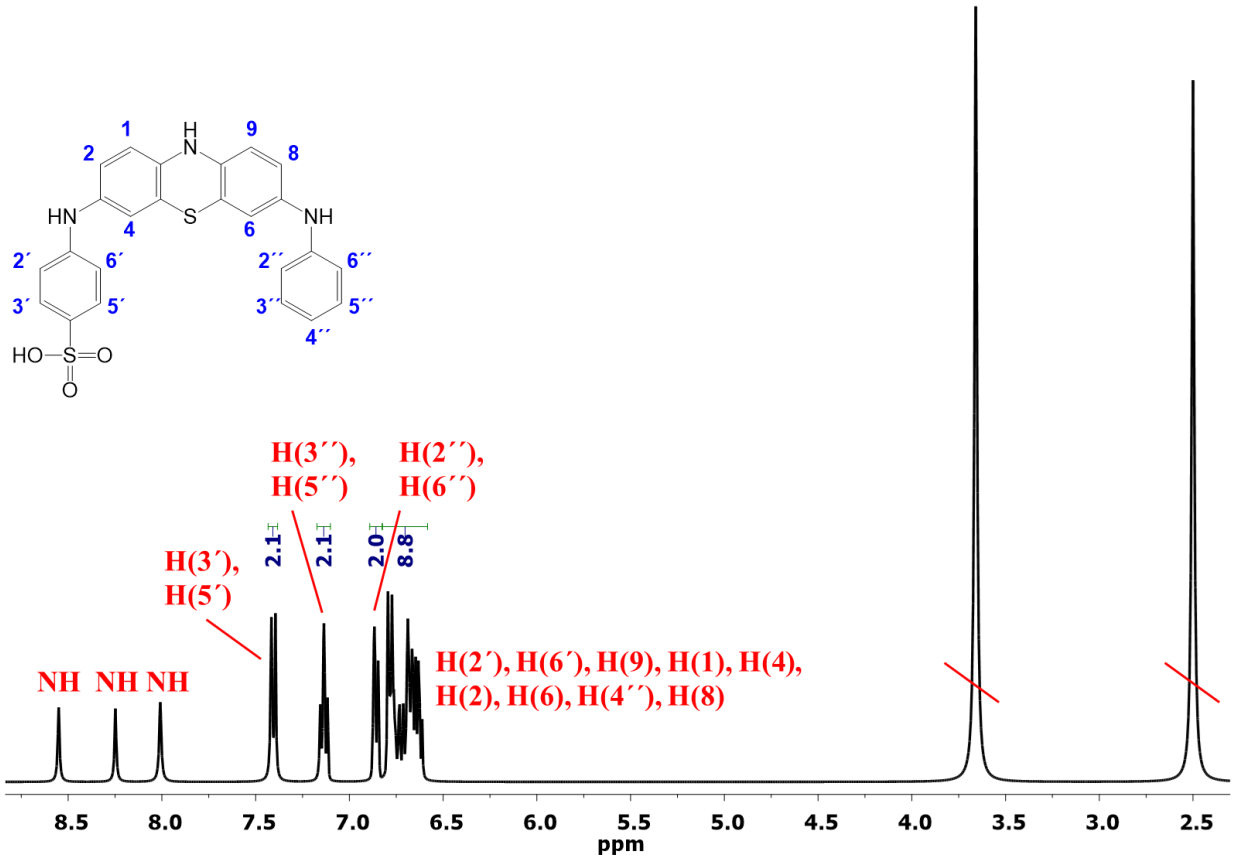

Figure S13. ^{1}H NMR spectrum of leuco form of the compound **19**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

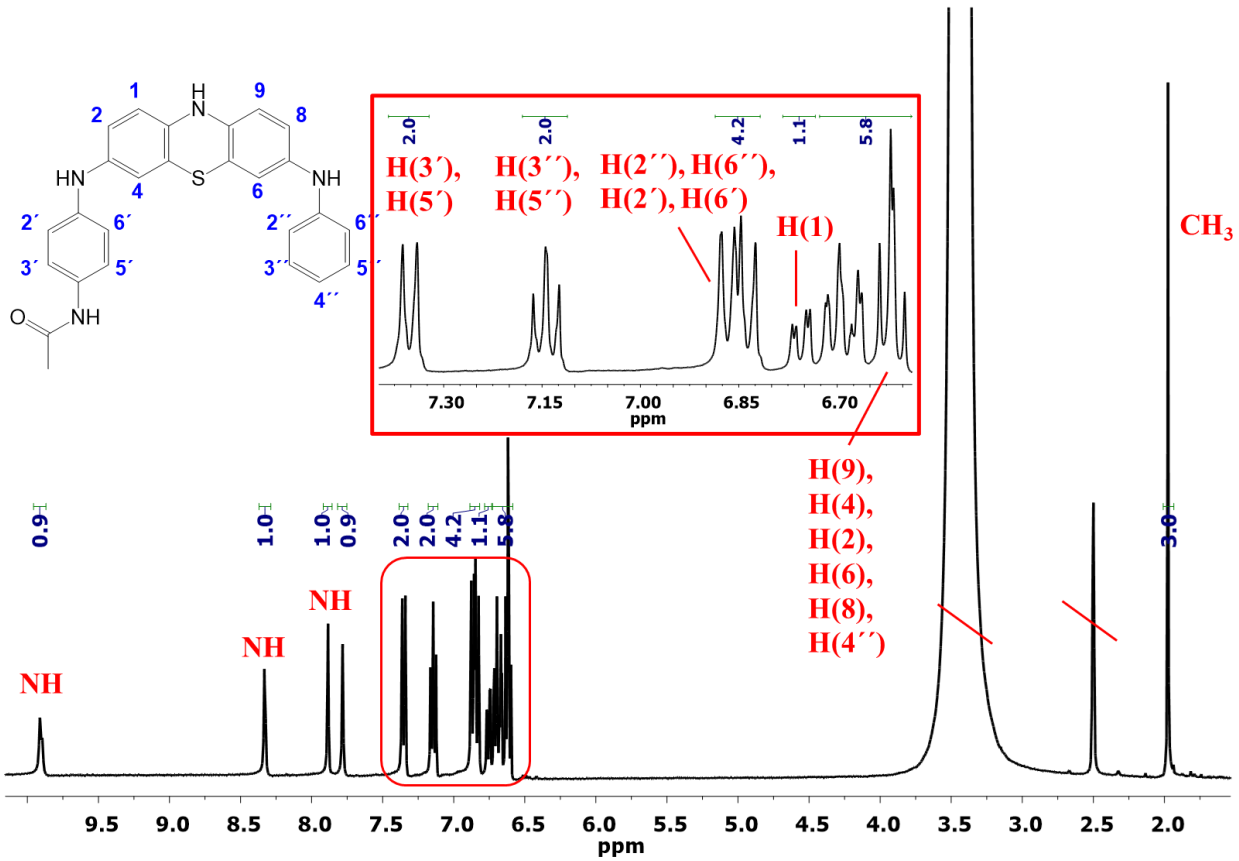

Figure S14. ^{1}H NMR spectrum of leuco form of the compound **20**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

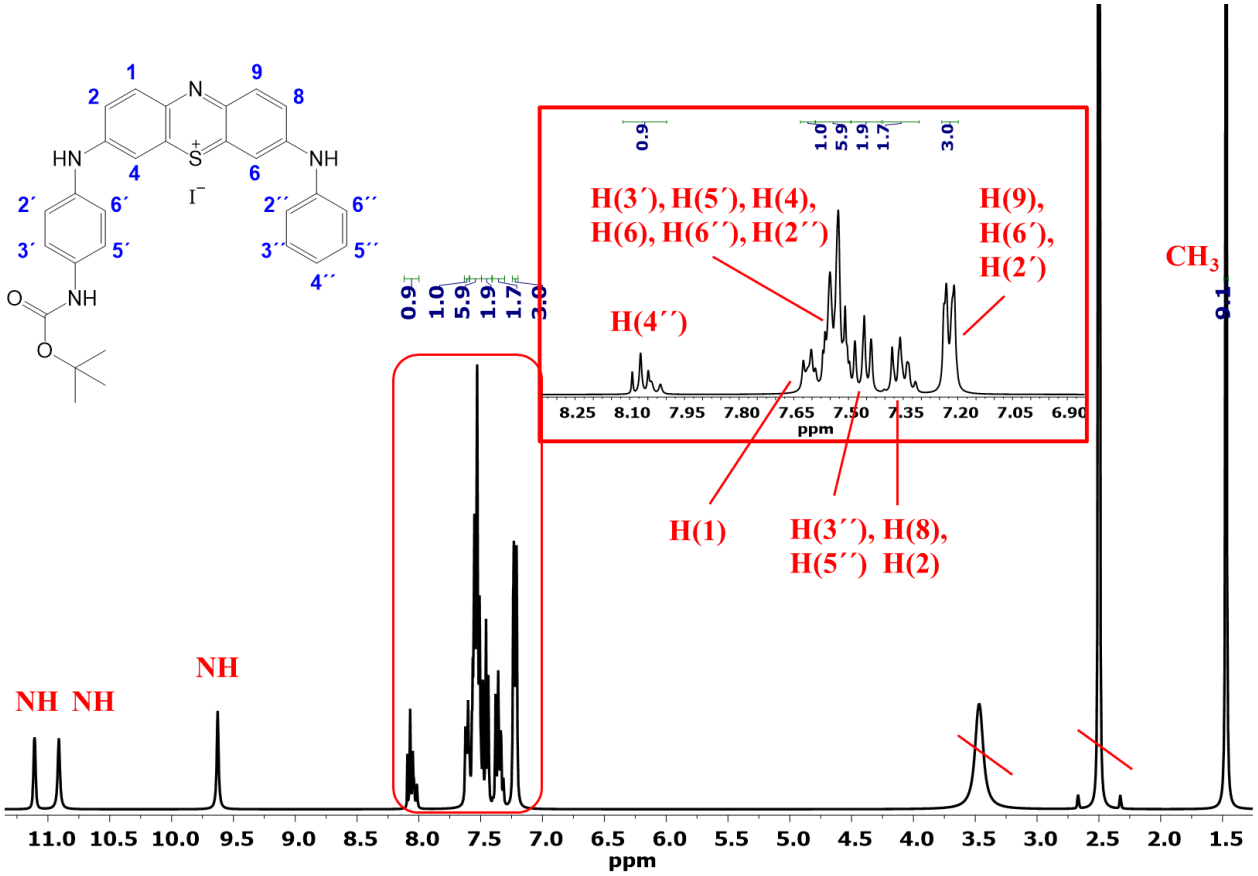

Figure S15. ^{1}H NMR spectrum of the compound **21**, DMSO-d_6, 300 K, 400 MHz.

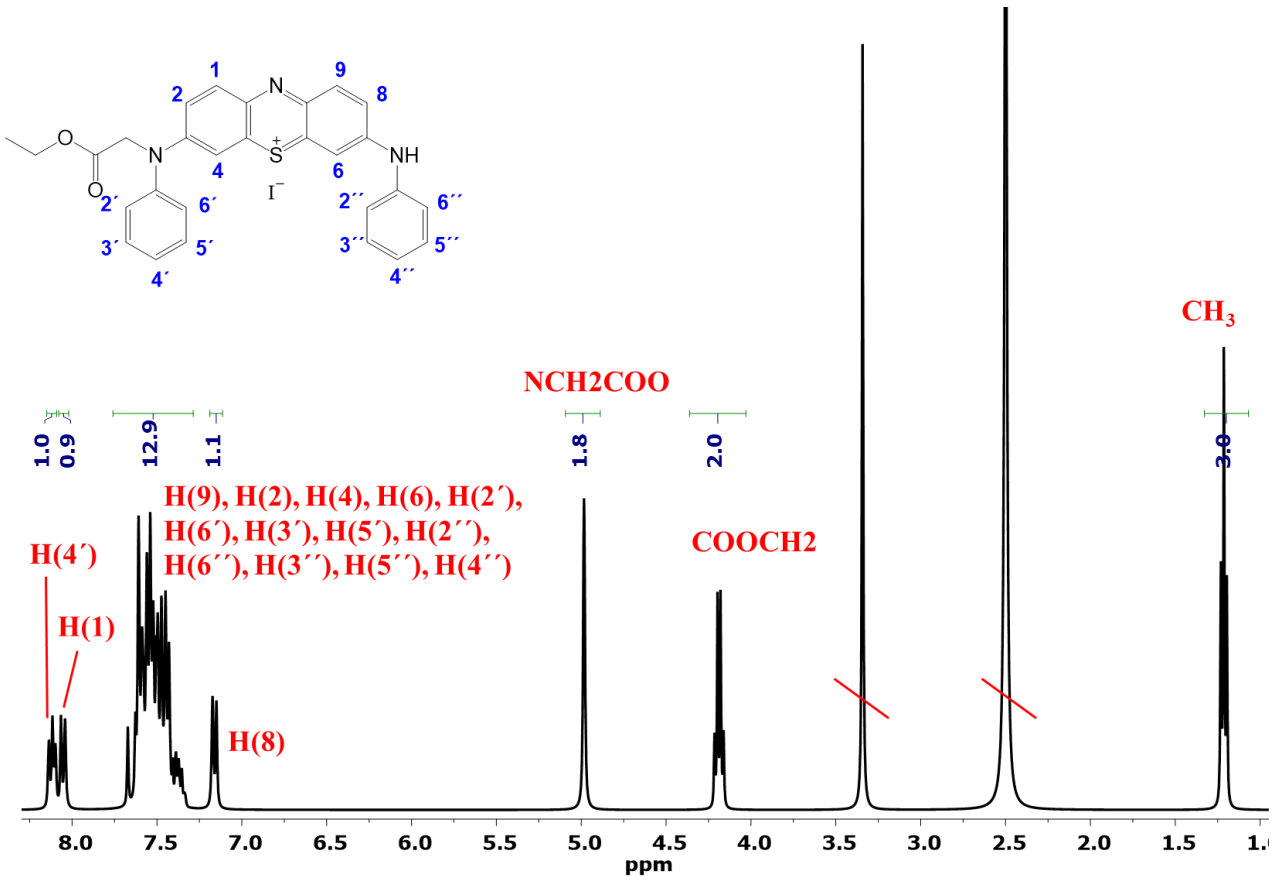

Figure S16. ^{1}H NMR spectrum of the compound **22**, DMSO-d_6, 300 K, 400 MHz.

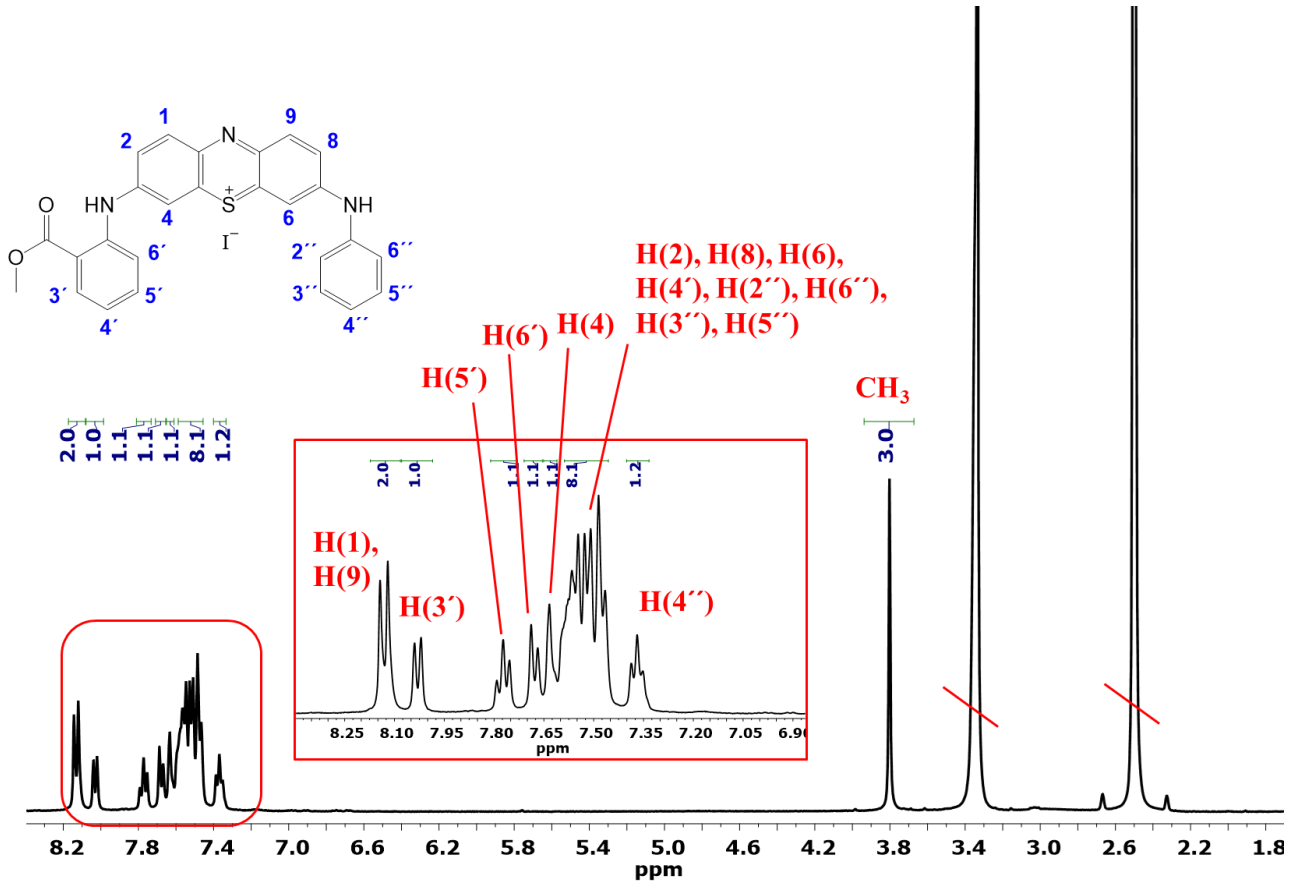

Figure S17. ^{1}H NMR spectrum of the compound **23**, DMSO-d_6, 300 K, 400 MHz.

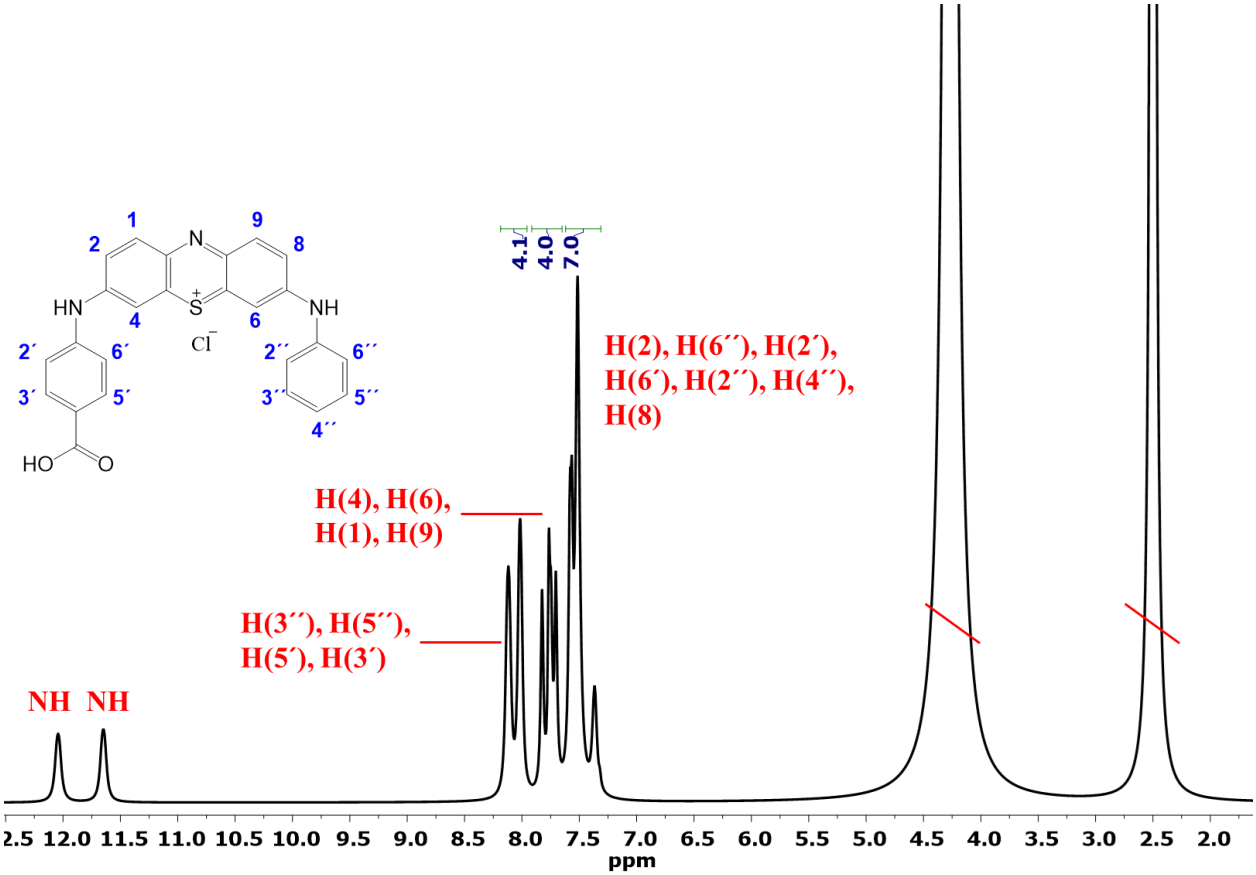

Figure S18. ^{1}H NMR spectrum of the compound **24**, DMSO-d_6, 300 K, 400 MHz.

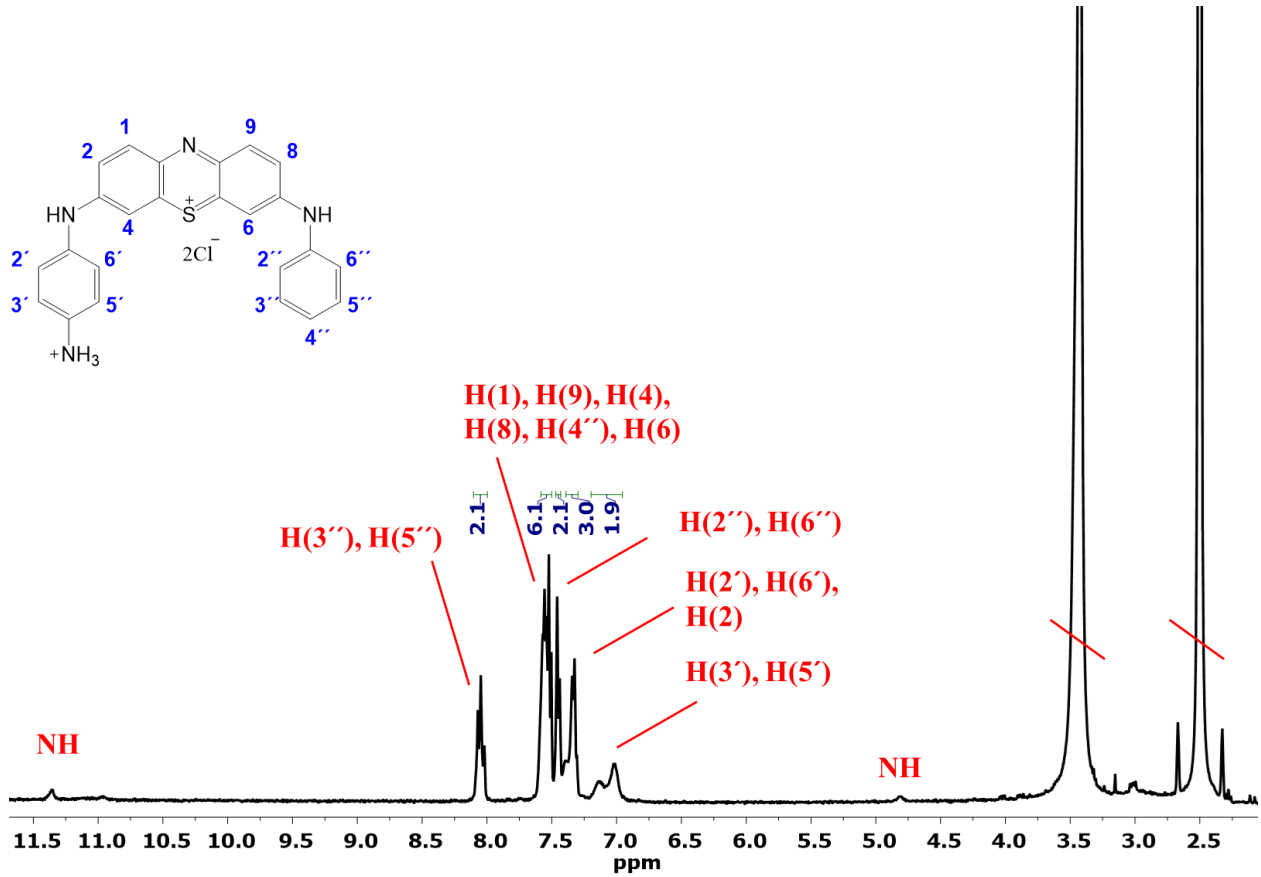

Figure S19. ^{1}H NMR spectrum of the compound **25**, DMSO-d_6, 300 K, 400 MHz.

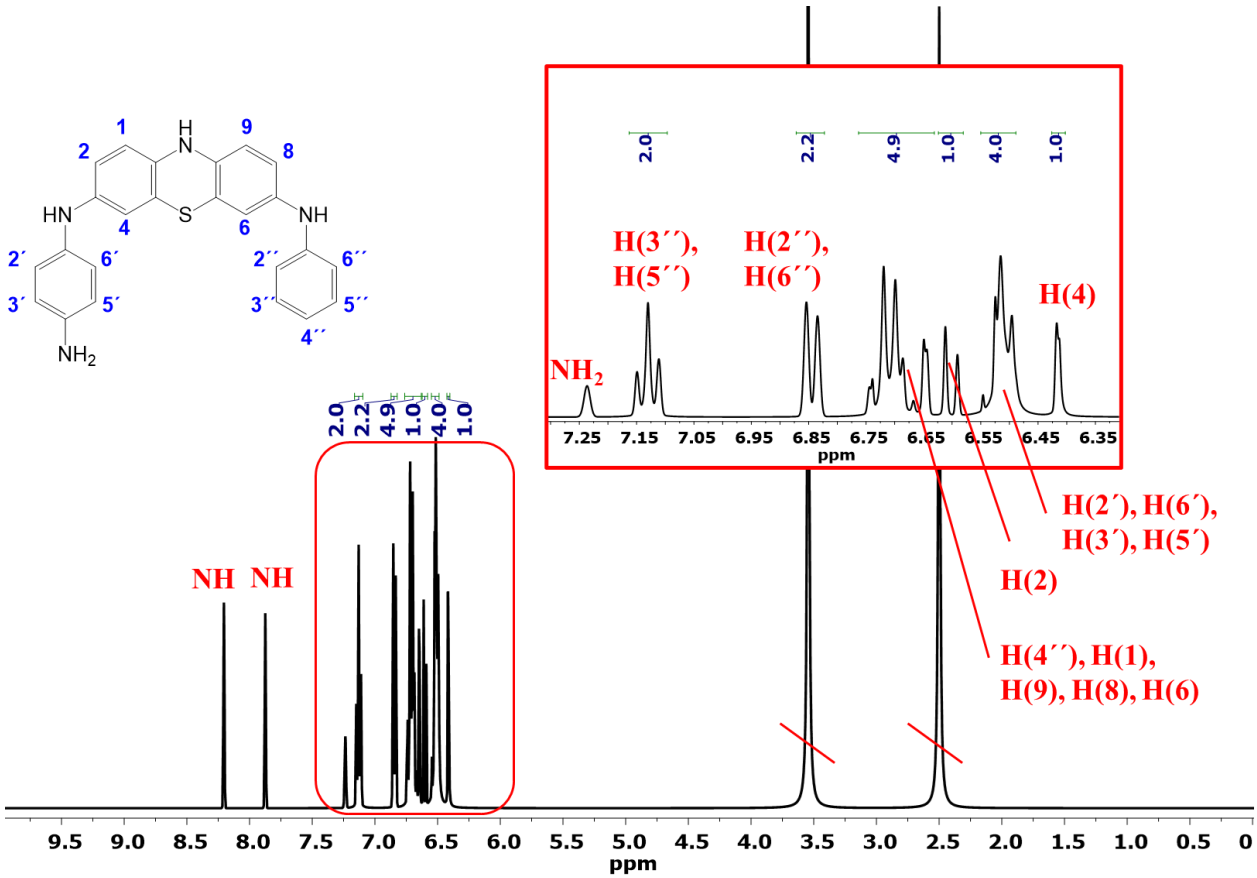

Figure S20. ^{1}H NMR spectrum of leuco form of the compound **25**, DMSO-d_6 + 2 % $N_2H_4 \cdot H_2O$, 300 K, 400 MHz.

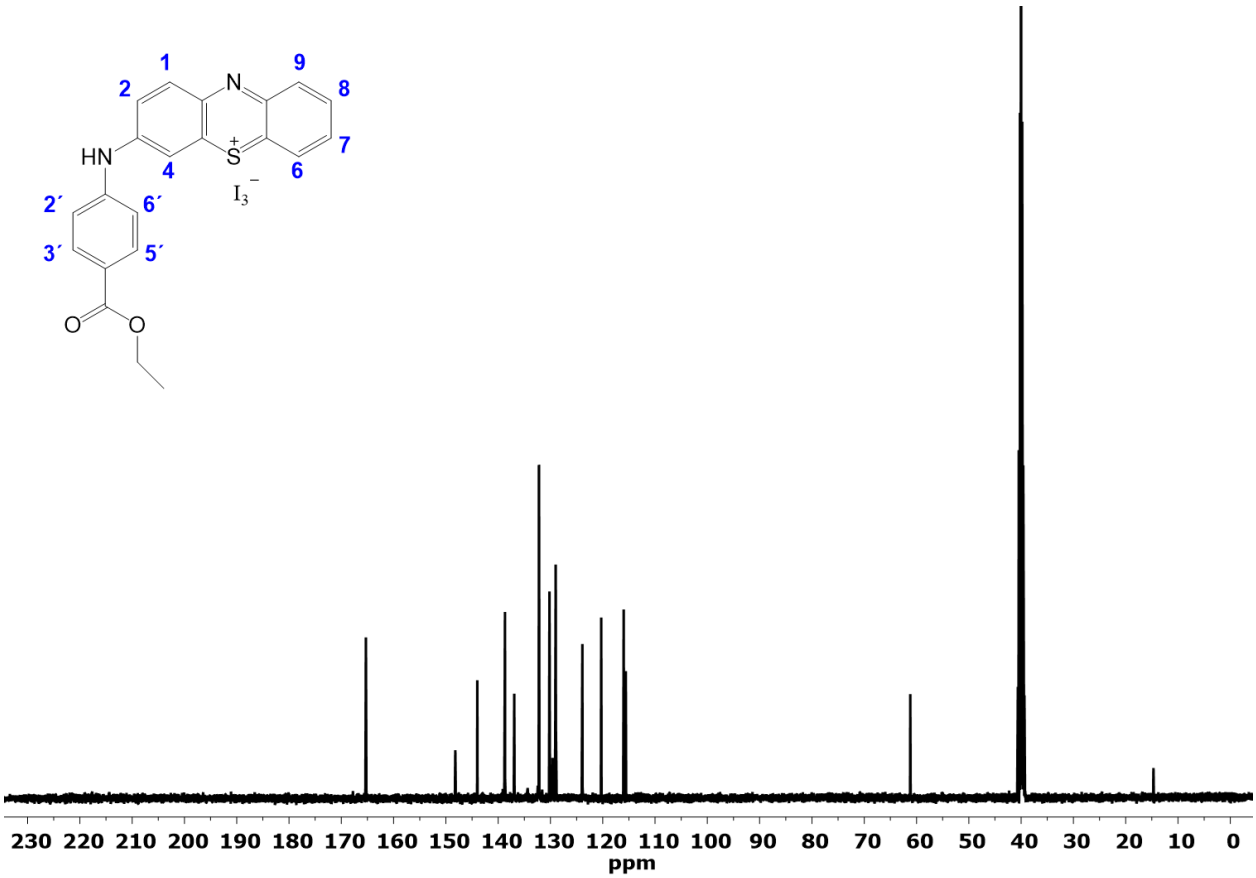

Figure S21. ^{13}C NMR spectrum of the compound **10**, DMSO-*d*$_6$, 300 K, 100 MHz.

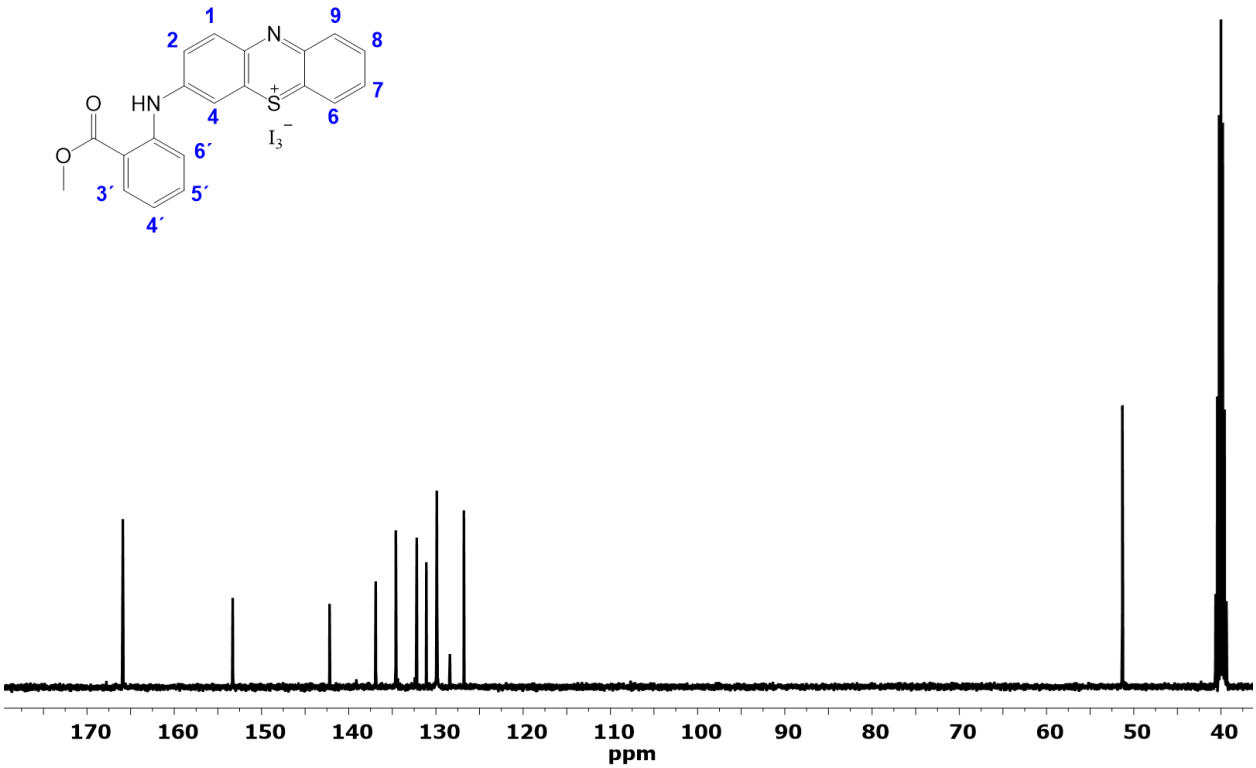

Figure S22. ^{13}C NMR spectrum of the compound **11**, DMSO-*d*$_6$, 300 K, 100 MHz.

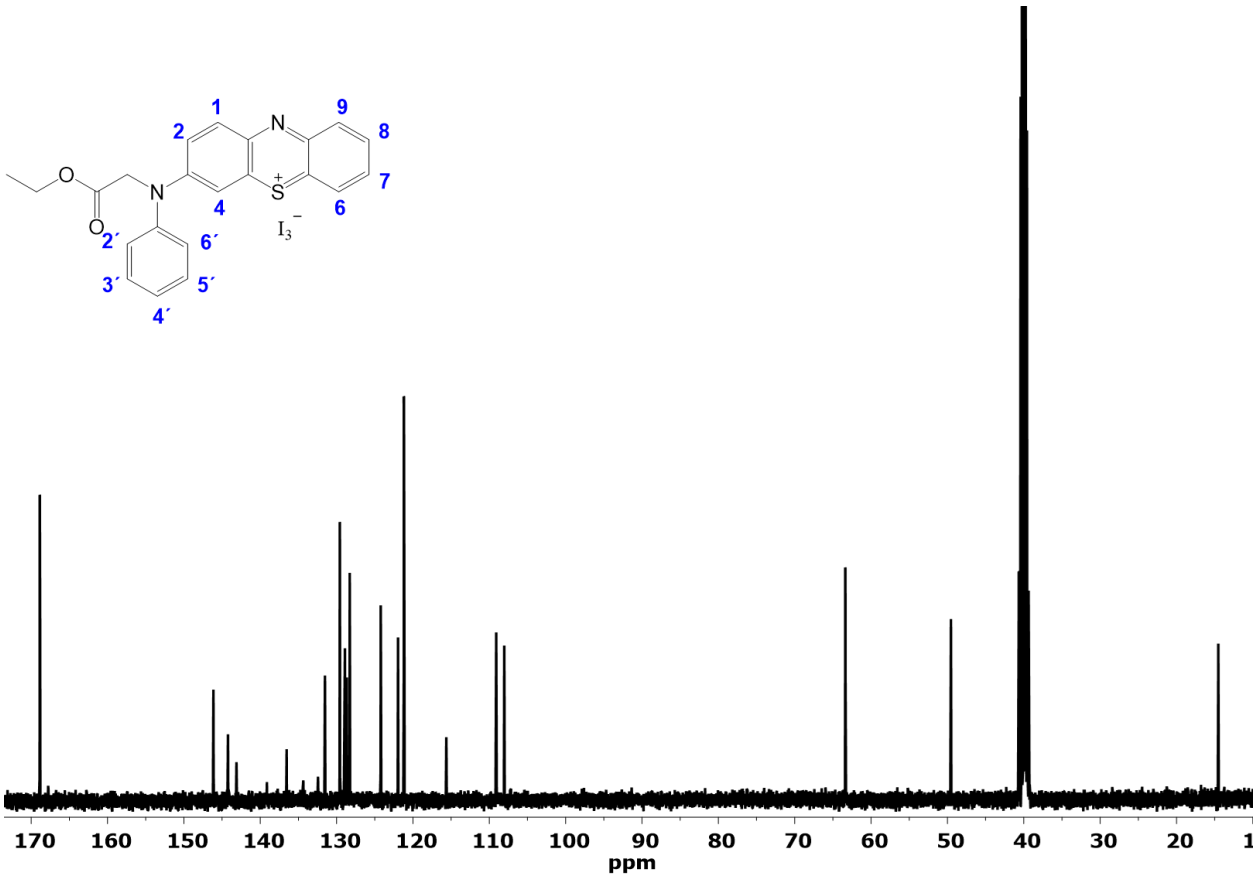

Figure S23. ^{13}C NMR spectrum of the compound **12**, DMSO-*d*$_6$, 300 K, 100 MHz.

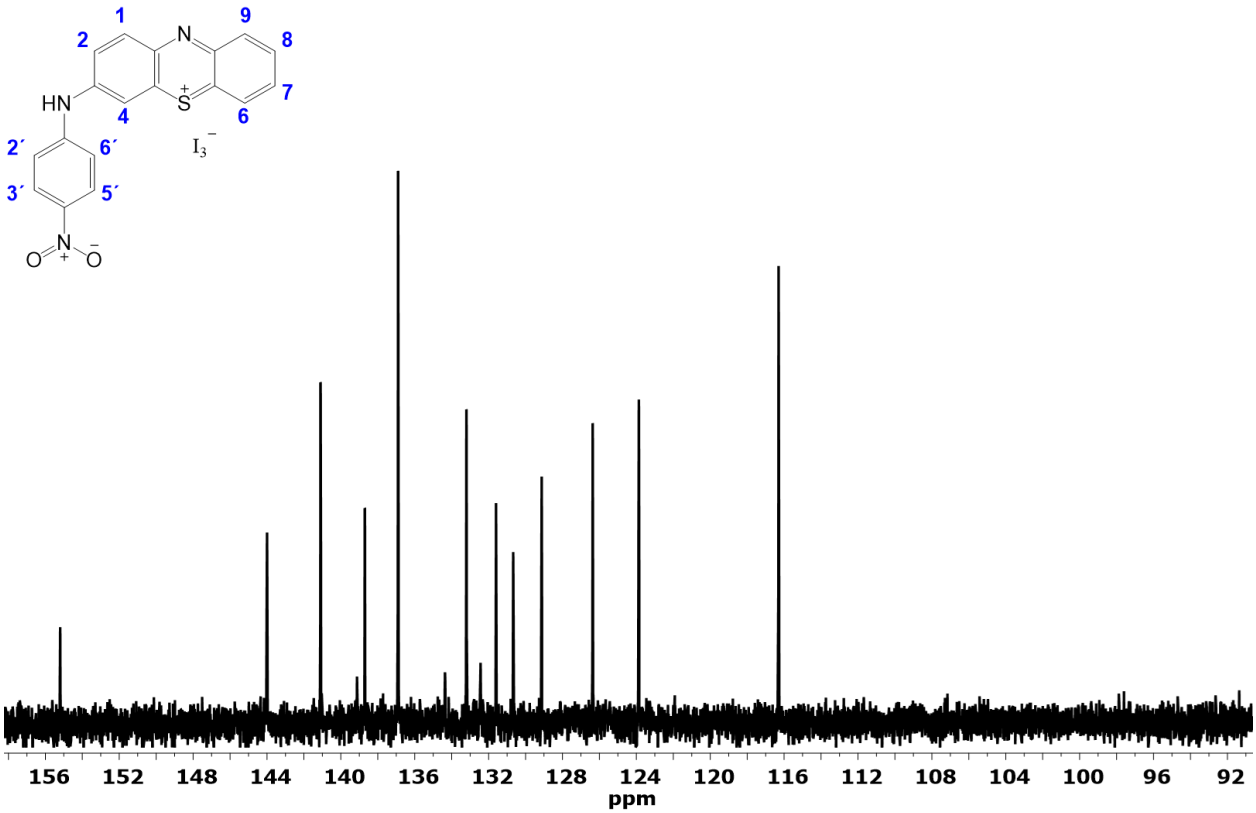

Figure S24. ^{13}C NMR spectrum of the compound **13**, DMSO-*d*$_6$, 300 K, 100 MHz.

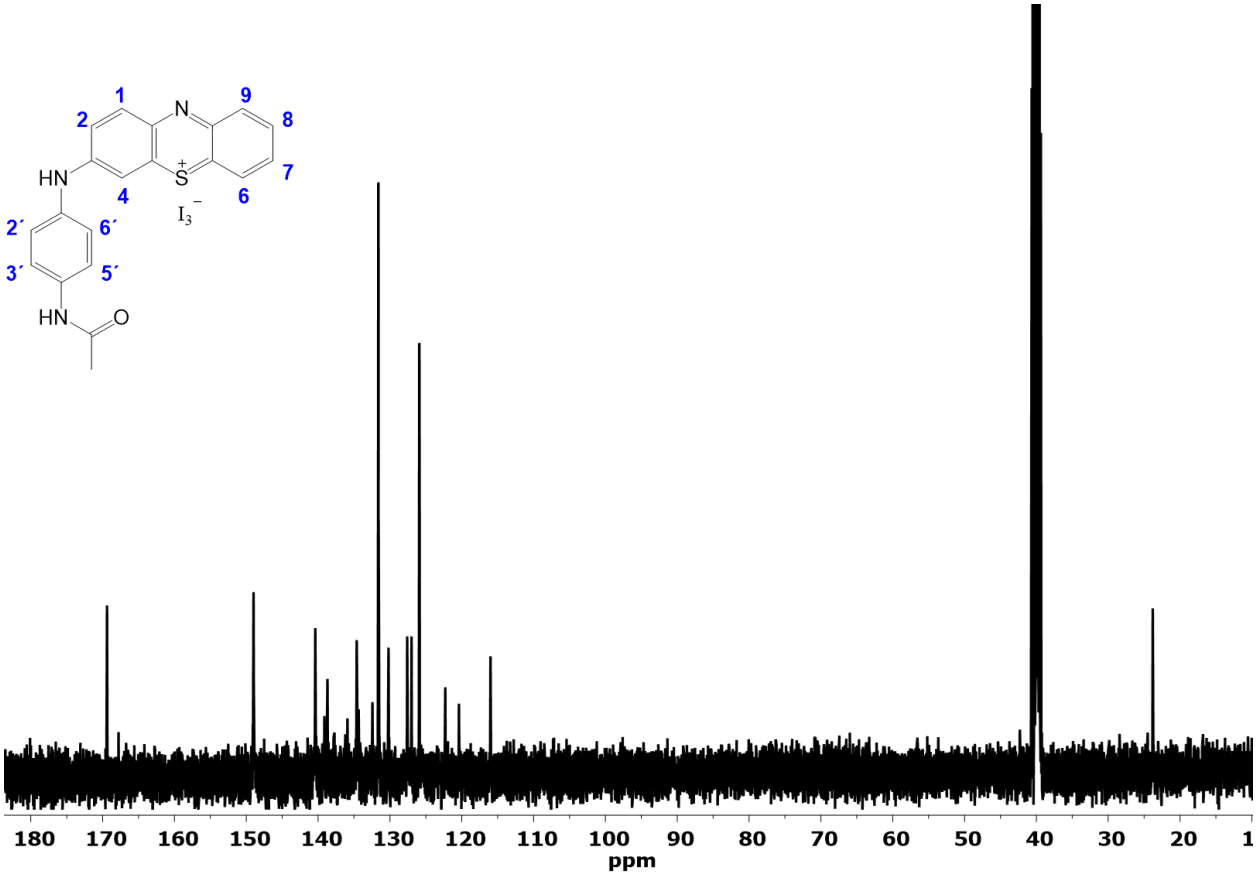

Figure S25. ^{13}C NMR spectrum of the compound **14**, DMSO-*d*$_6$, 300 K, 100 MHz.

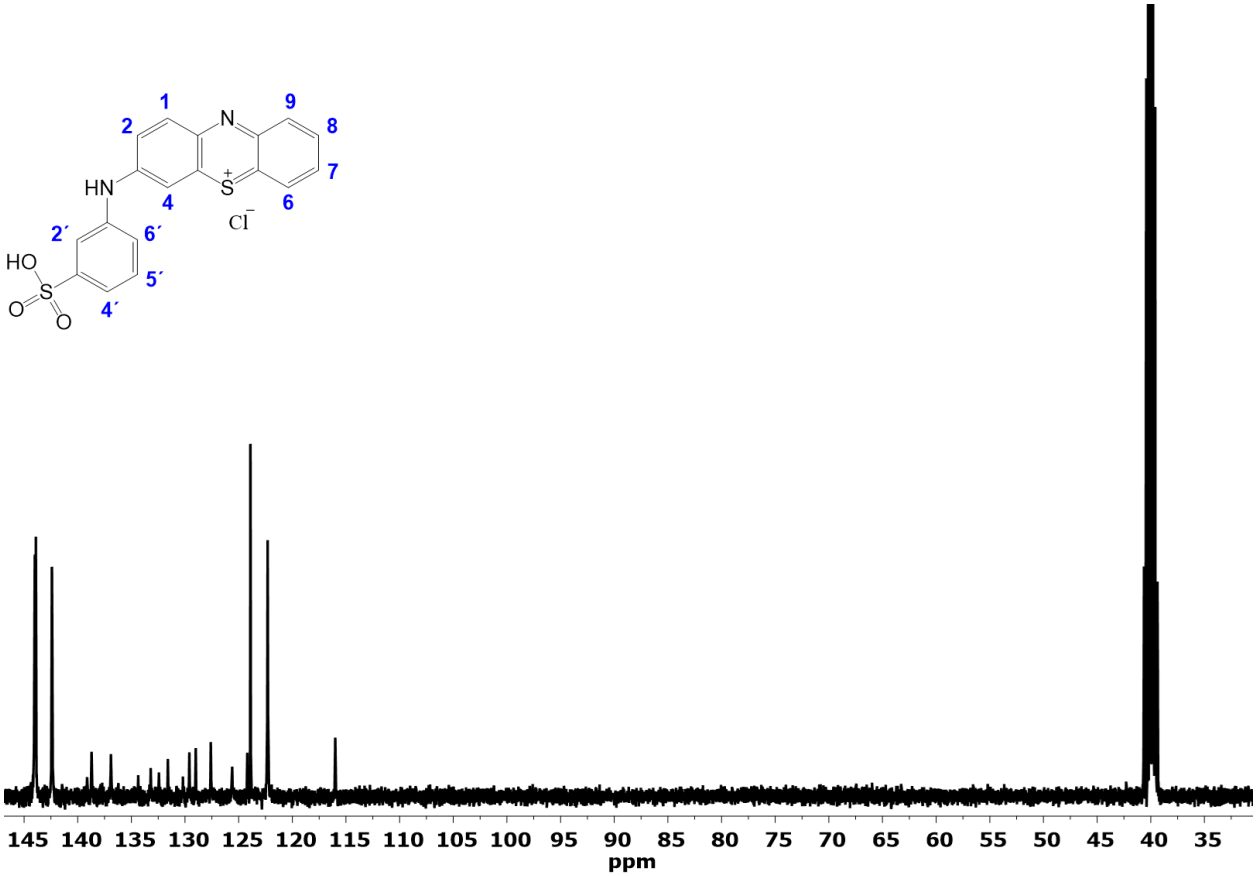

Figure S26. ^{13}C NMR spectrum of the compound **15**, DMSO-*d*$_6$, 300 K, 100 MHz.

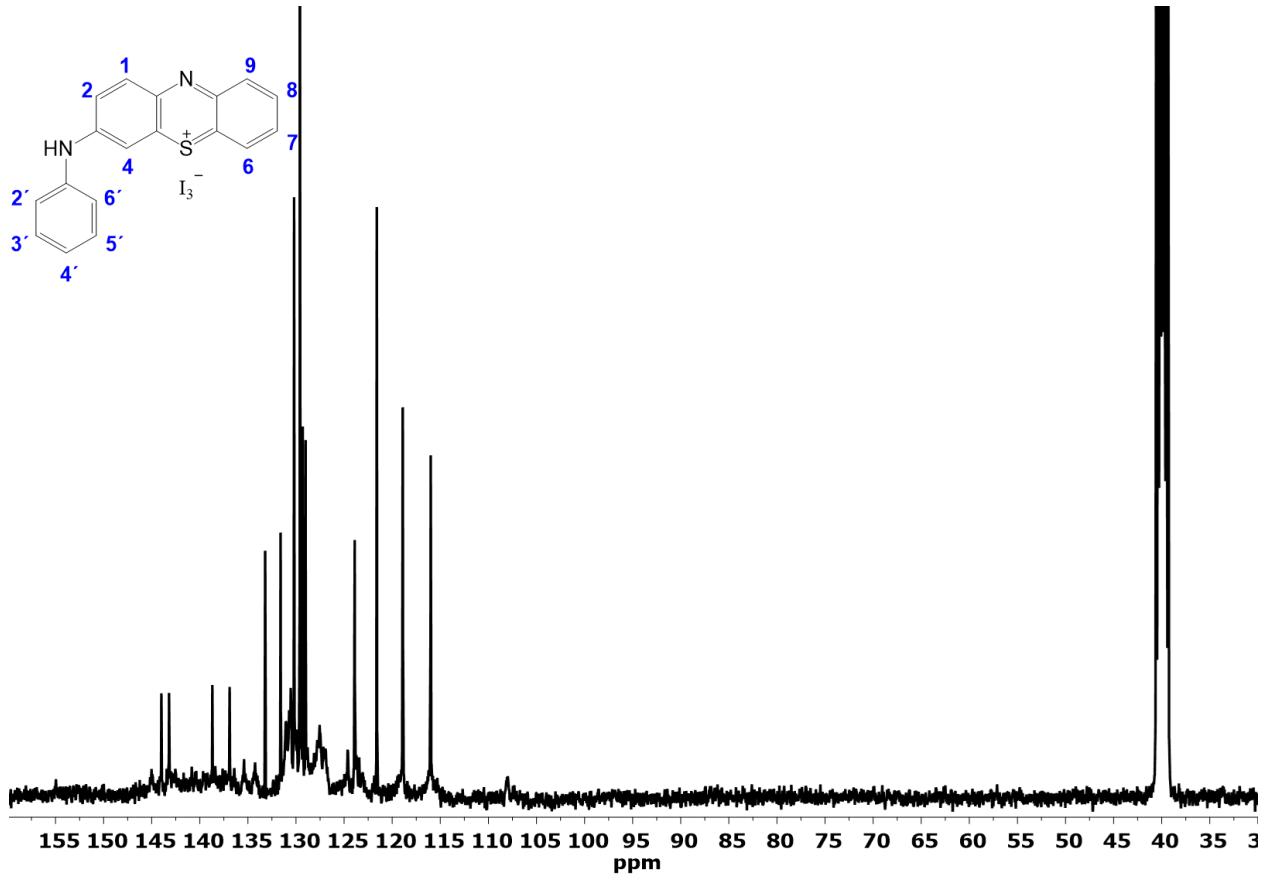

Figure S27. ^{13}C NMR spectrum of the compound **16**, DMSO-*d*$_6$, 300 K, 100 MHz.

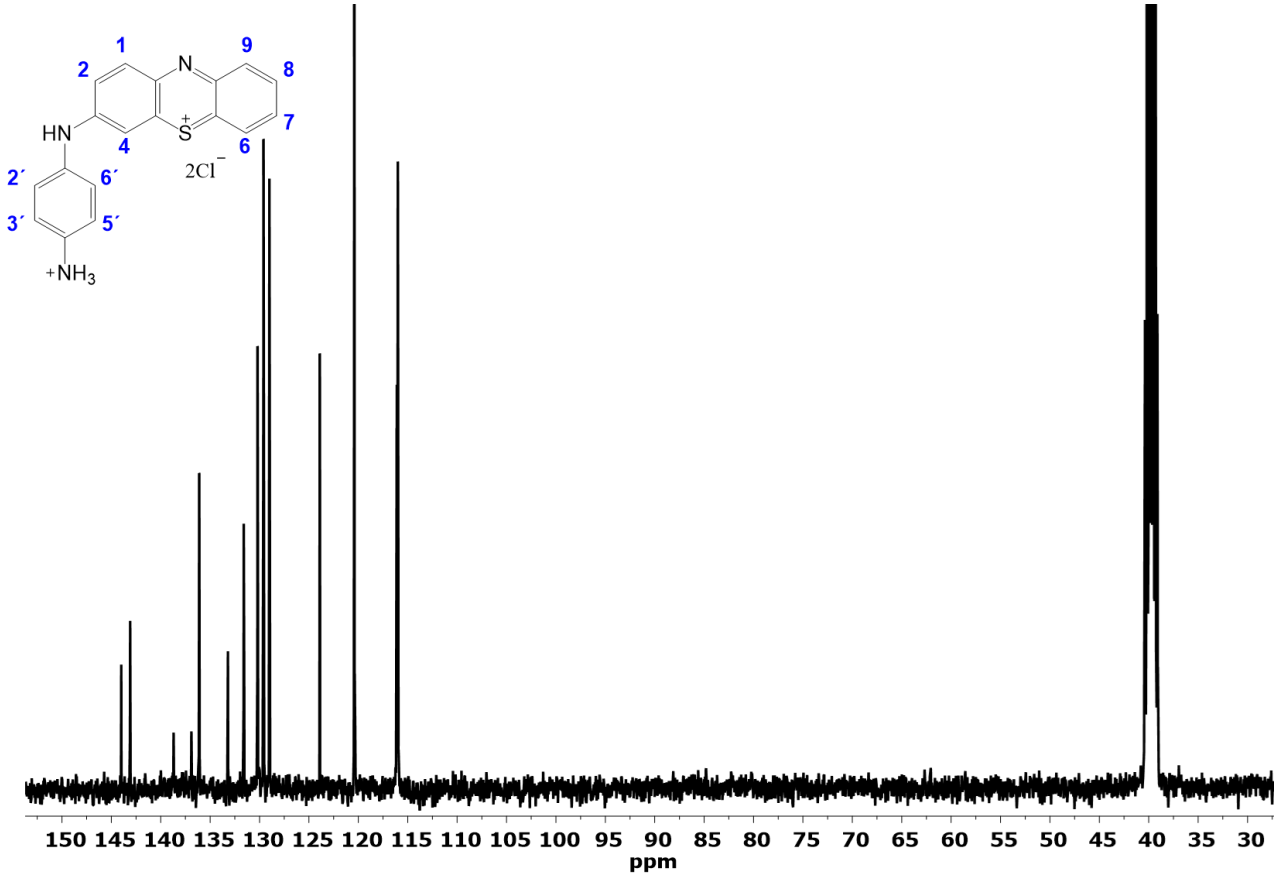

Figure S28. ^{13}C NMR spectrum of the compound **17**, DMSO-*d*$_6$, 300 K, 100 MHz.

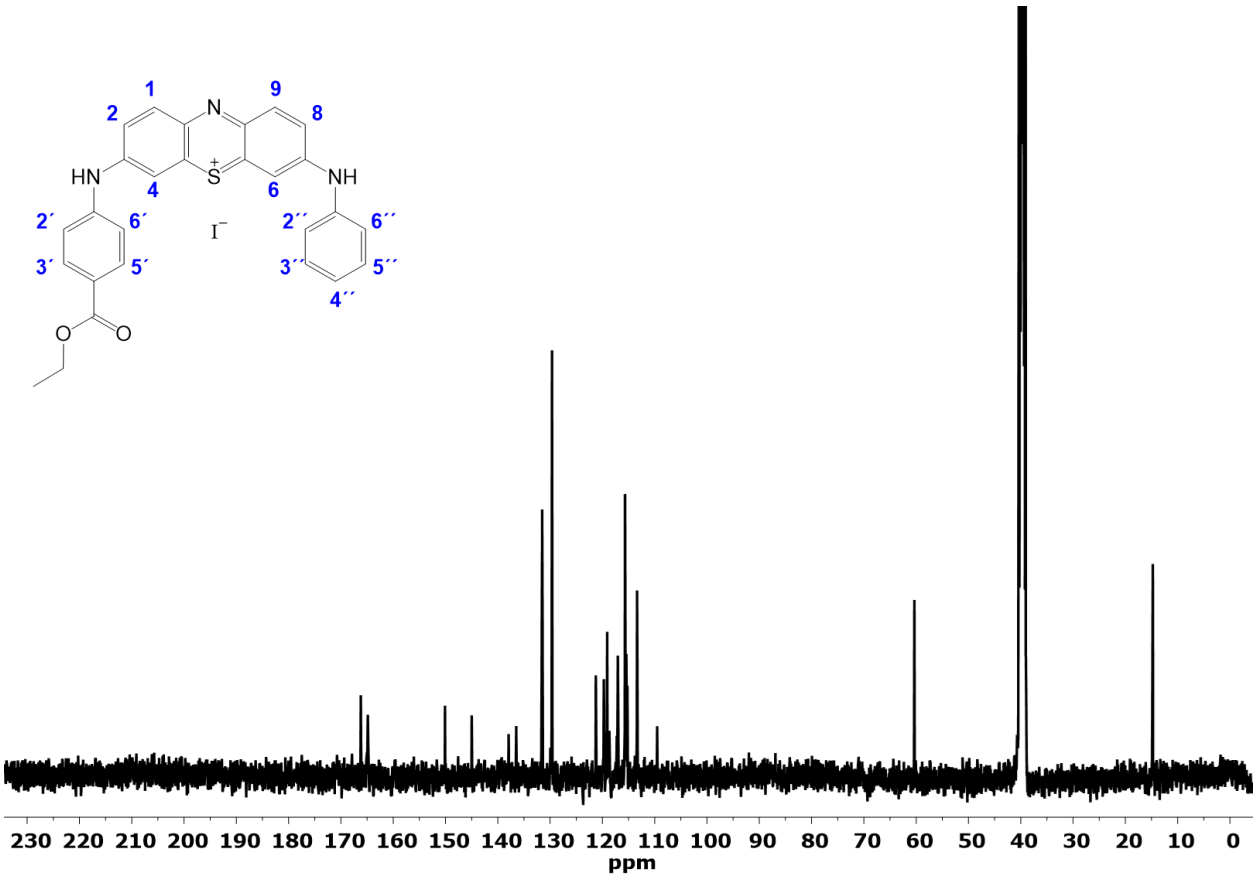

Figure S29. ^{13}C NMR spectrum of the compound **18**, DMSO-d_6, 300 K, 100 MHz.

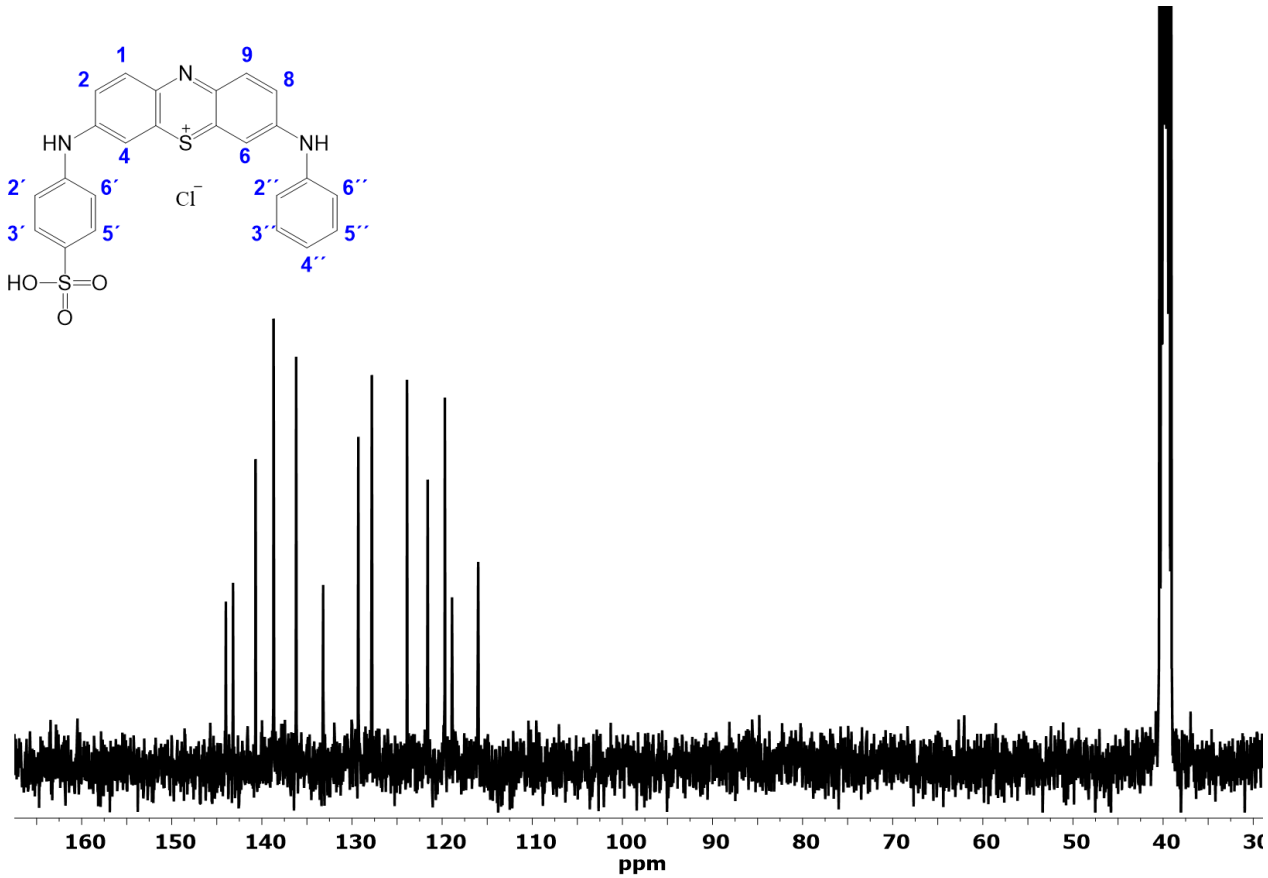

Figure S30. ^{13}C NMR spectrum of the compound **19**, DMSO-d_6, 300 K, 100 MHz.

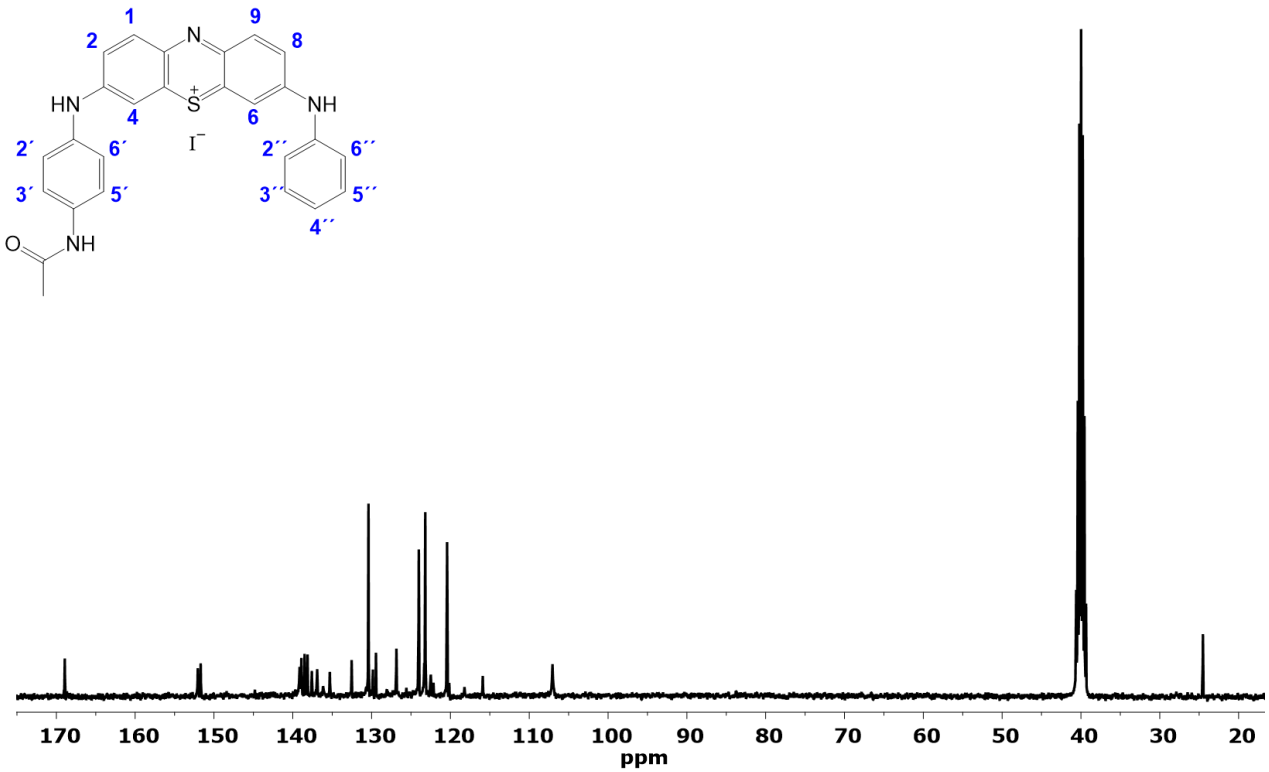

Figure S31. ^{13}C NMR spectrum of the compound **20**, DMSO-d_6, 300 K, 100 MHz.

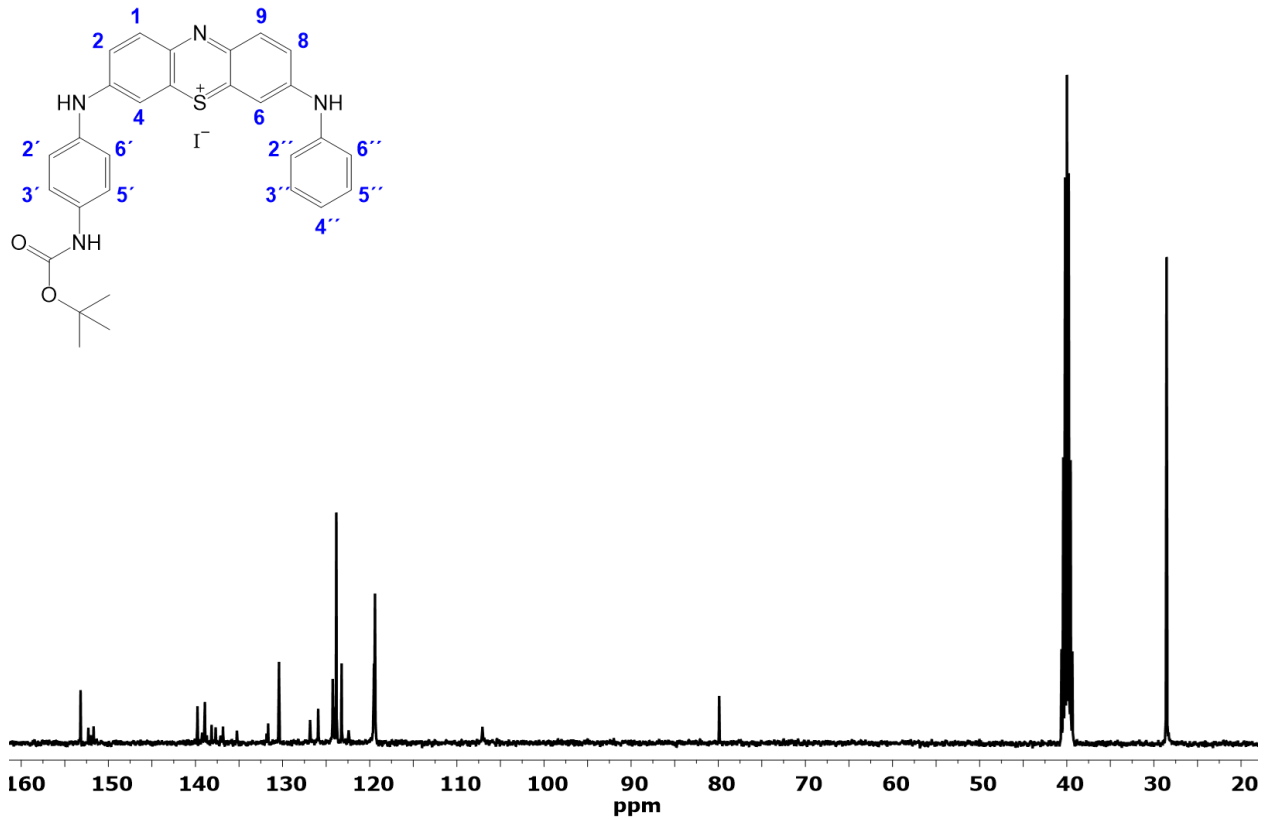

Figure S32. ^{13}C NMR spectrum of the compound **21**, DMSO-d_6, 300 K, 100 MHz.

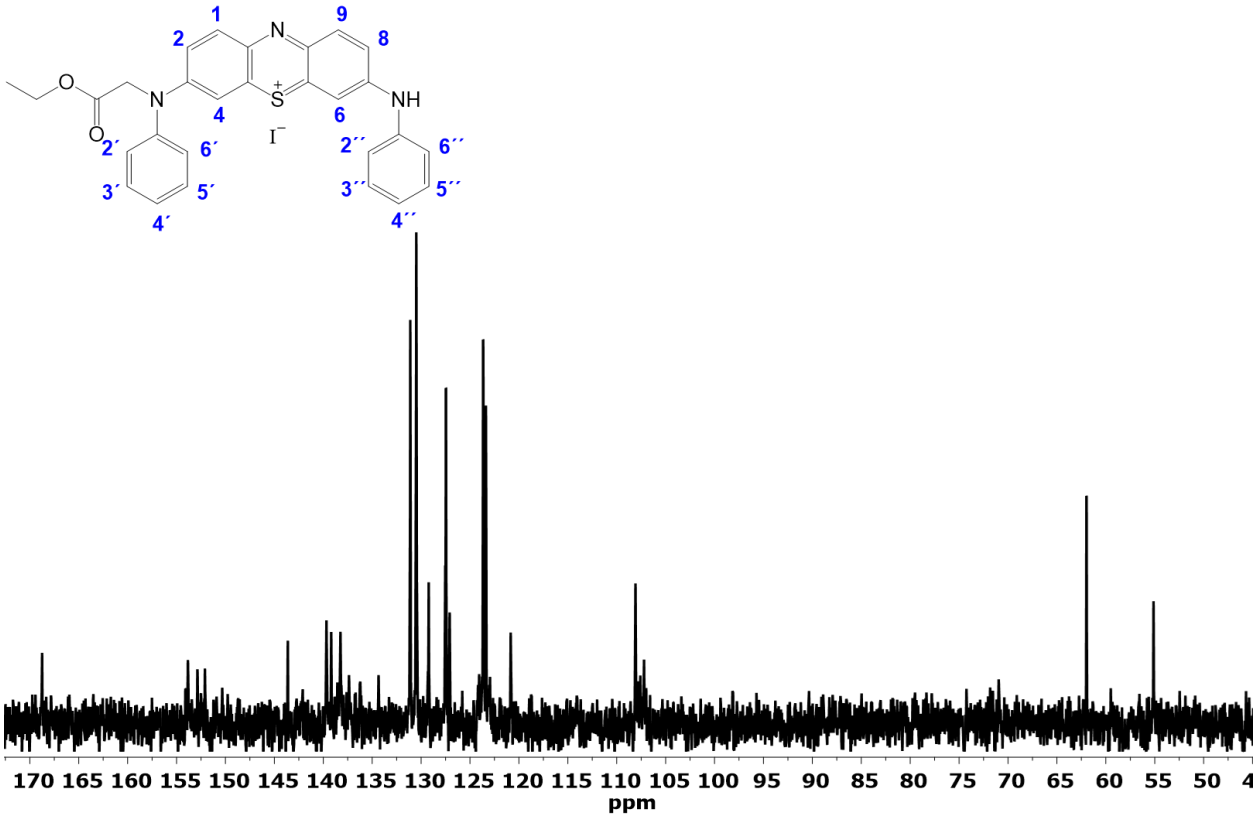

Figure S33. ^{13}C NMR spectrum of the compound **22**, DMSO-*d*$_6$, 300 K, 100 MHz.

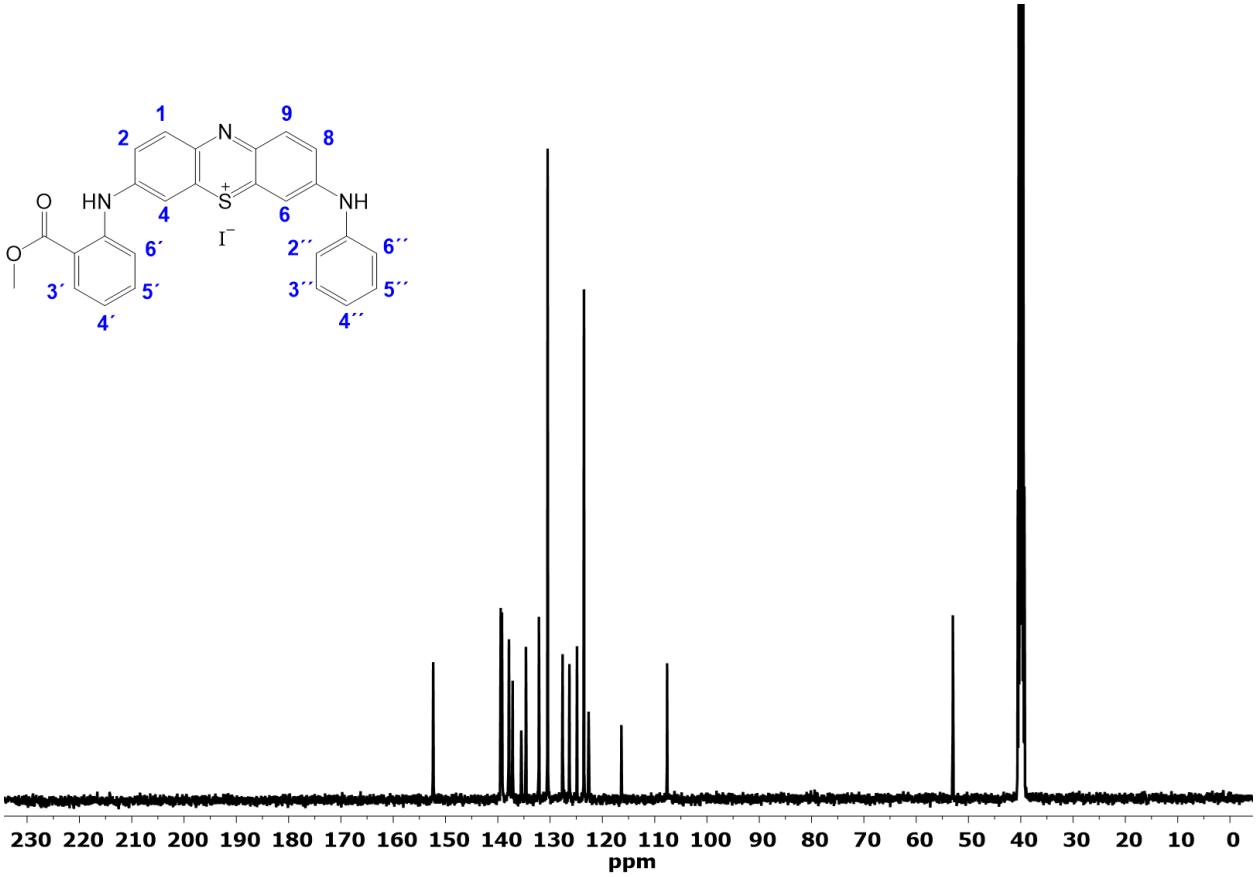

Figure S34. ^{13}C NMR spectrum of the compound **23**, DMSO-*d*$_6$, 300 K, 100 MHz.

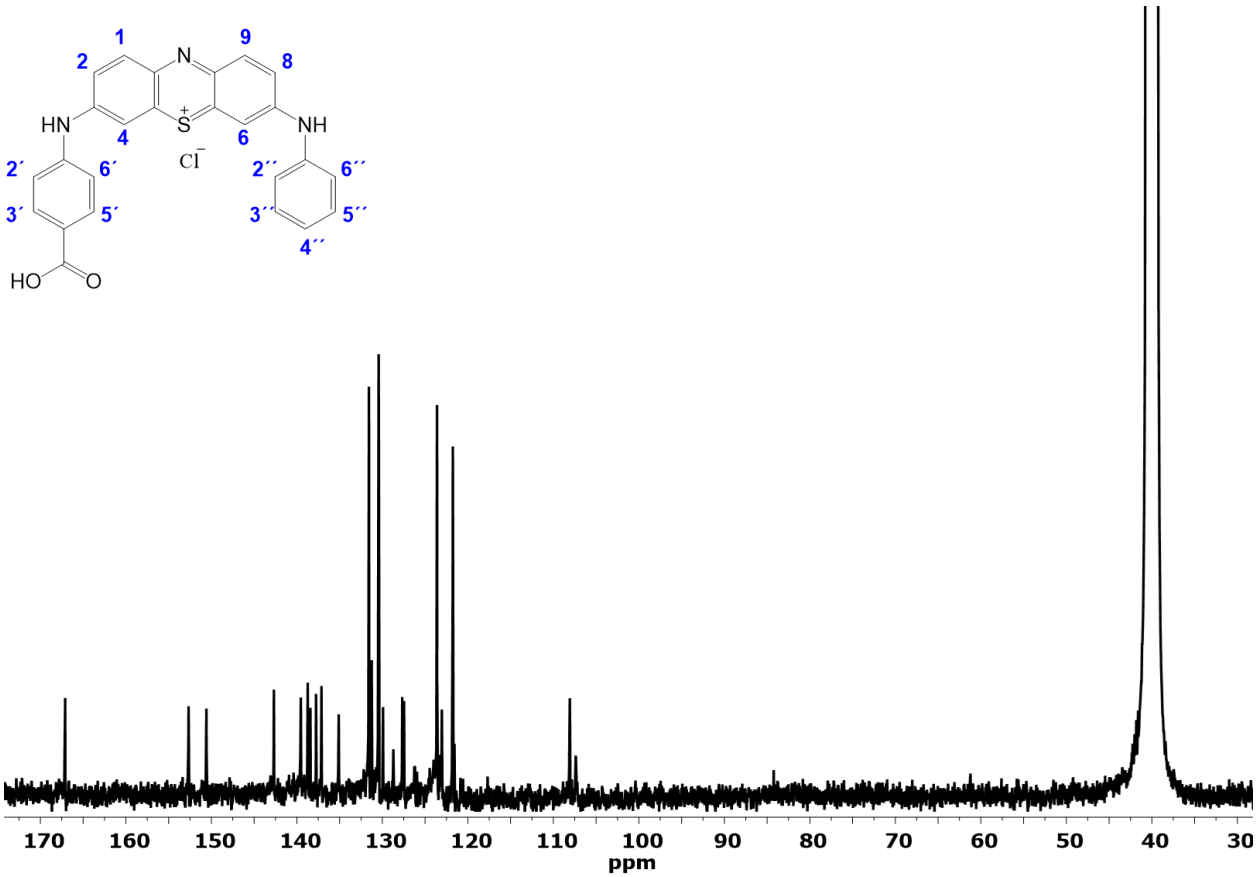

Figure S35. ^{13}C NMR spectrum of the compound **24**, DMSO-d_6, 300 K, 100 MHz.

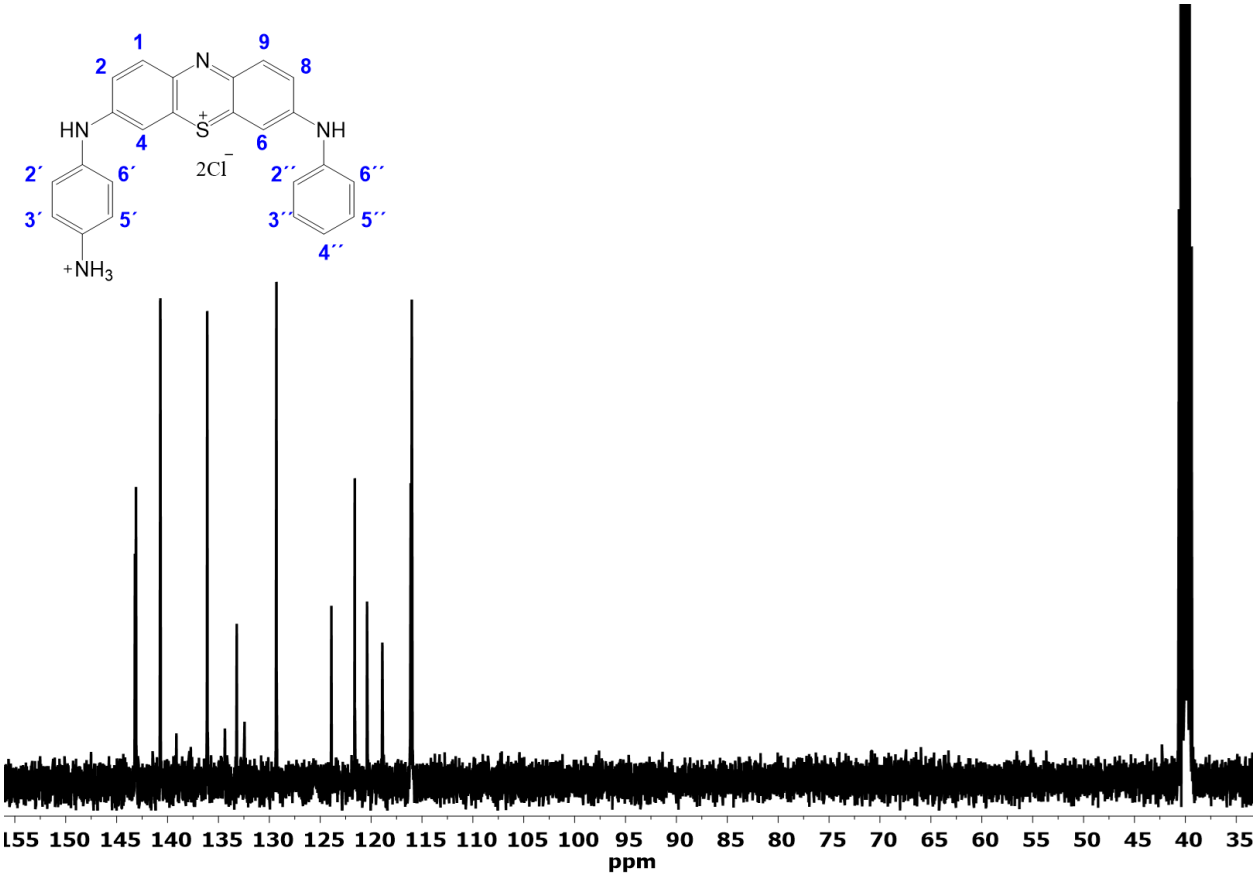

Figure S36. ^{13}C NMR spectrum of the compound **25**, DMSO-d_6, 300 K, 100 MHz.

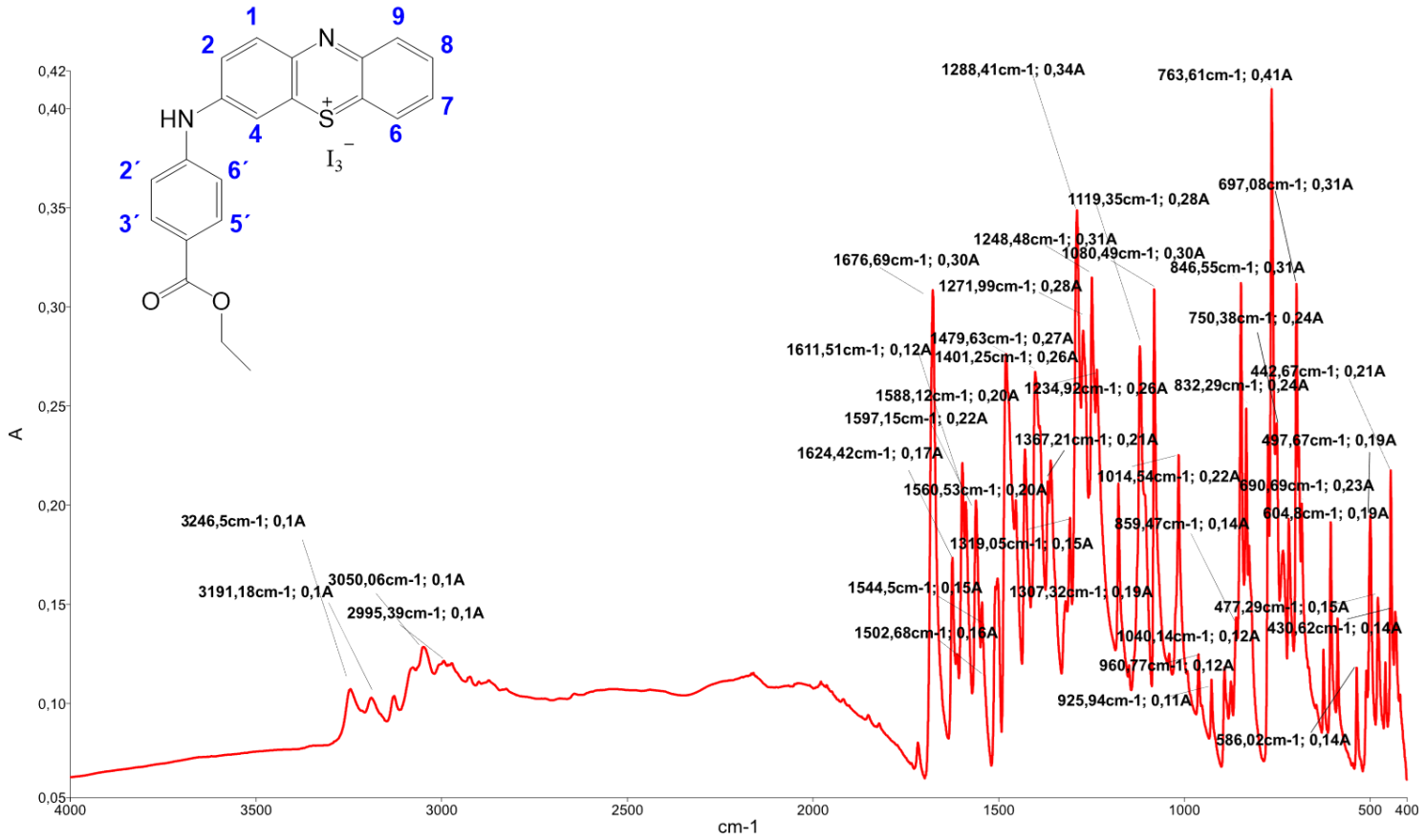

Figure S37. FT-IR spectrum of the compound **10**.

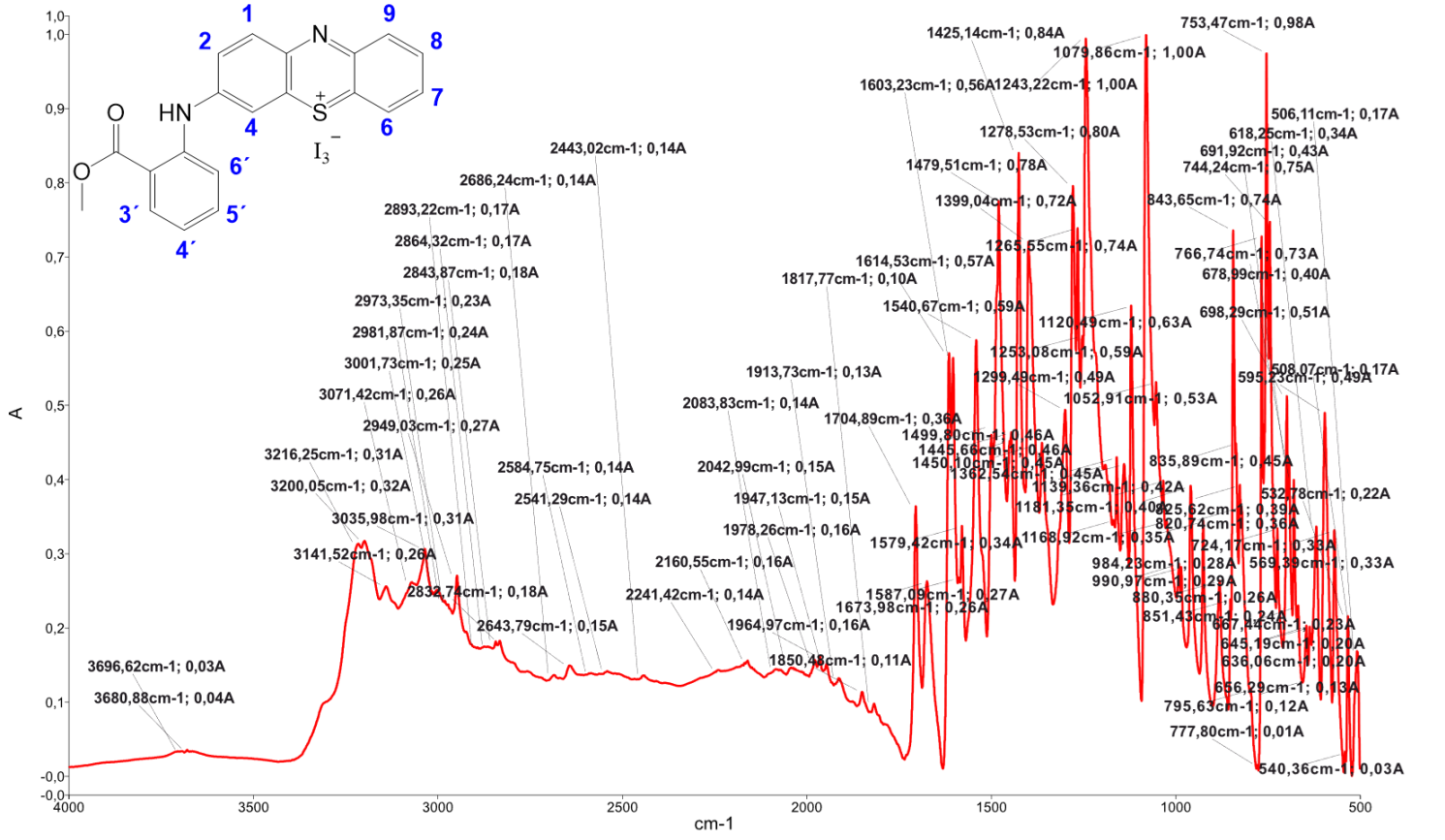

Figure S38. FT-IR spectrum of the compound **11**.

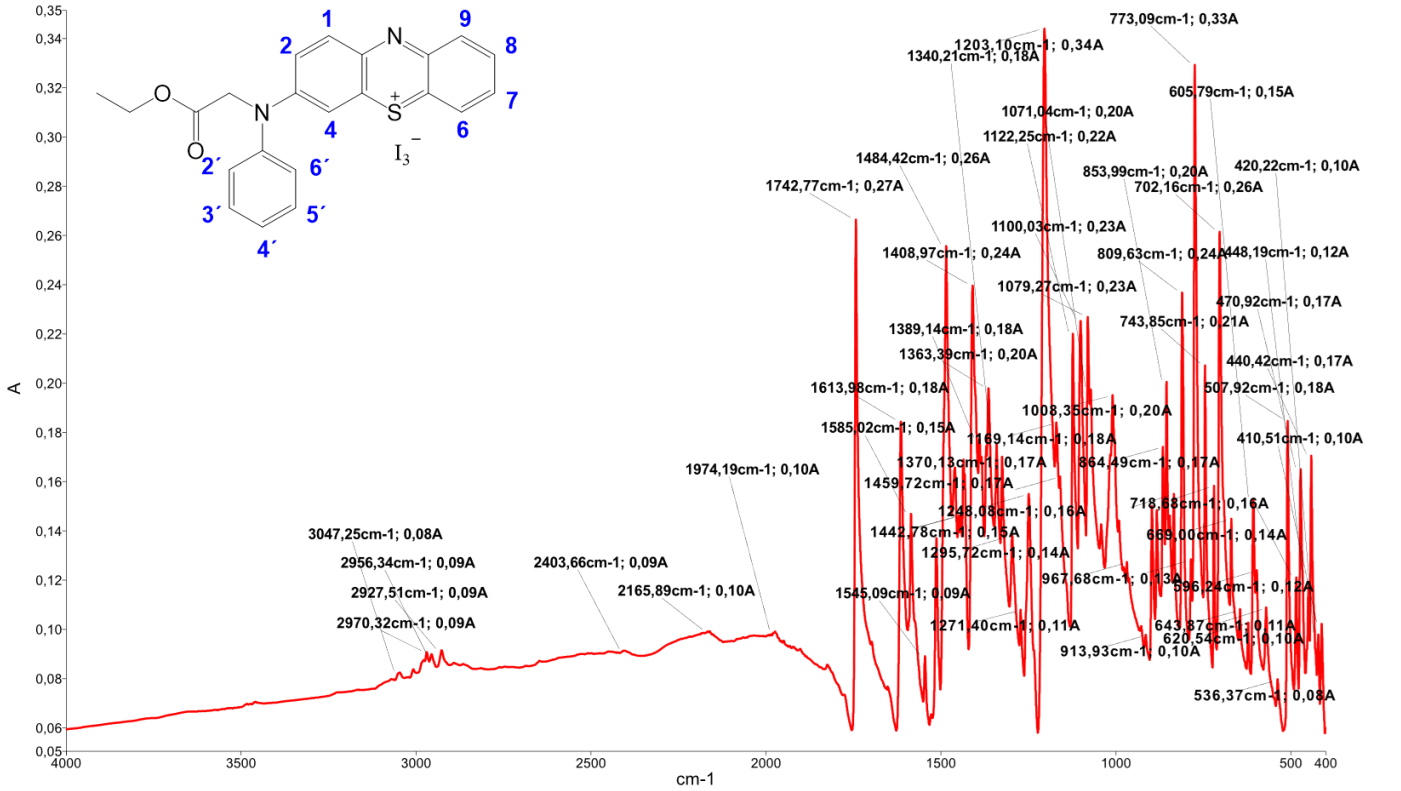

Figure S39. FT-IR spectrum of the compound **12**.

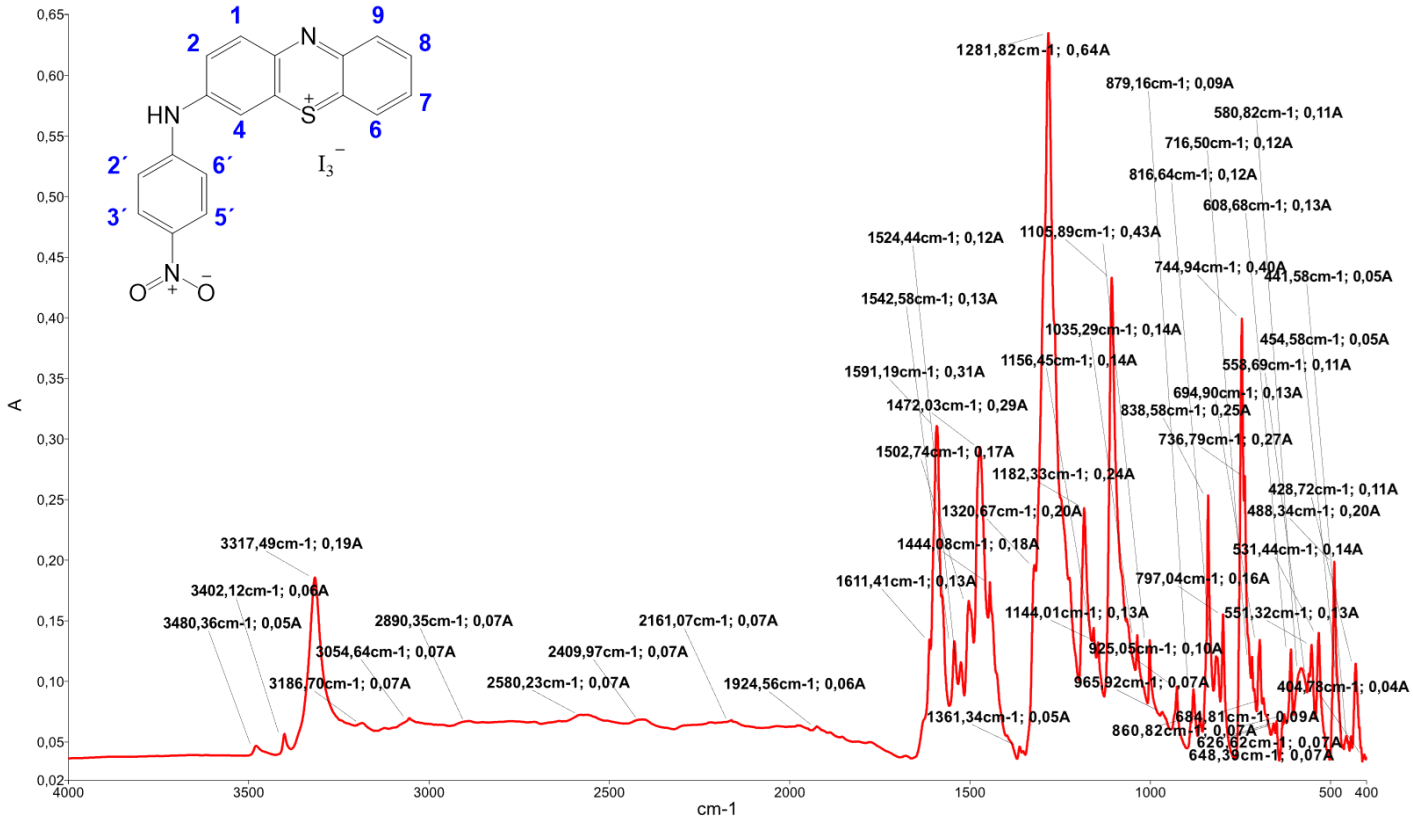

Figure S40. FT-IR spectrum of the compound **13**.

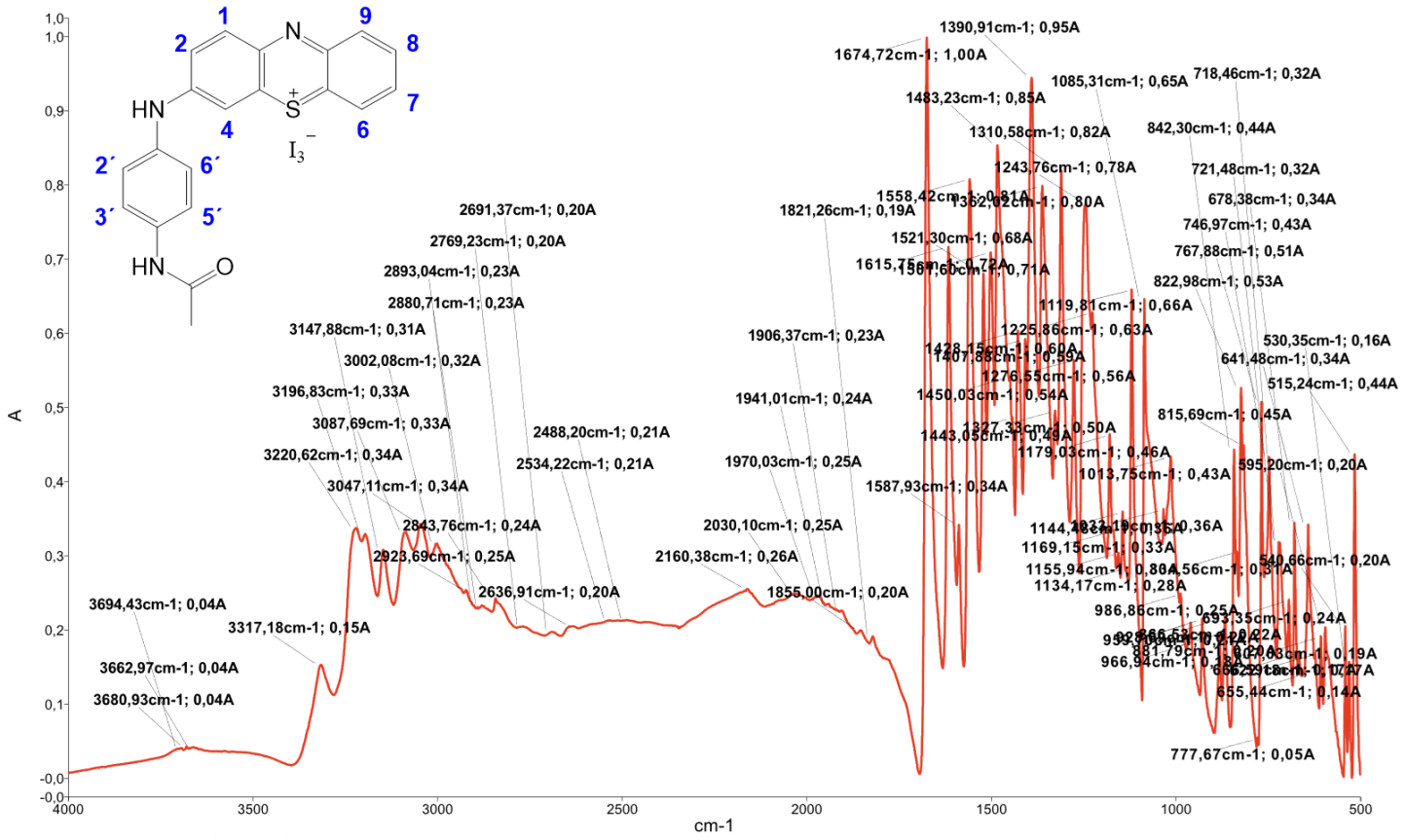

Figure S41. FT-IR spectrum of the compound **14**.

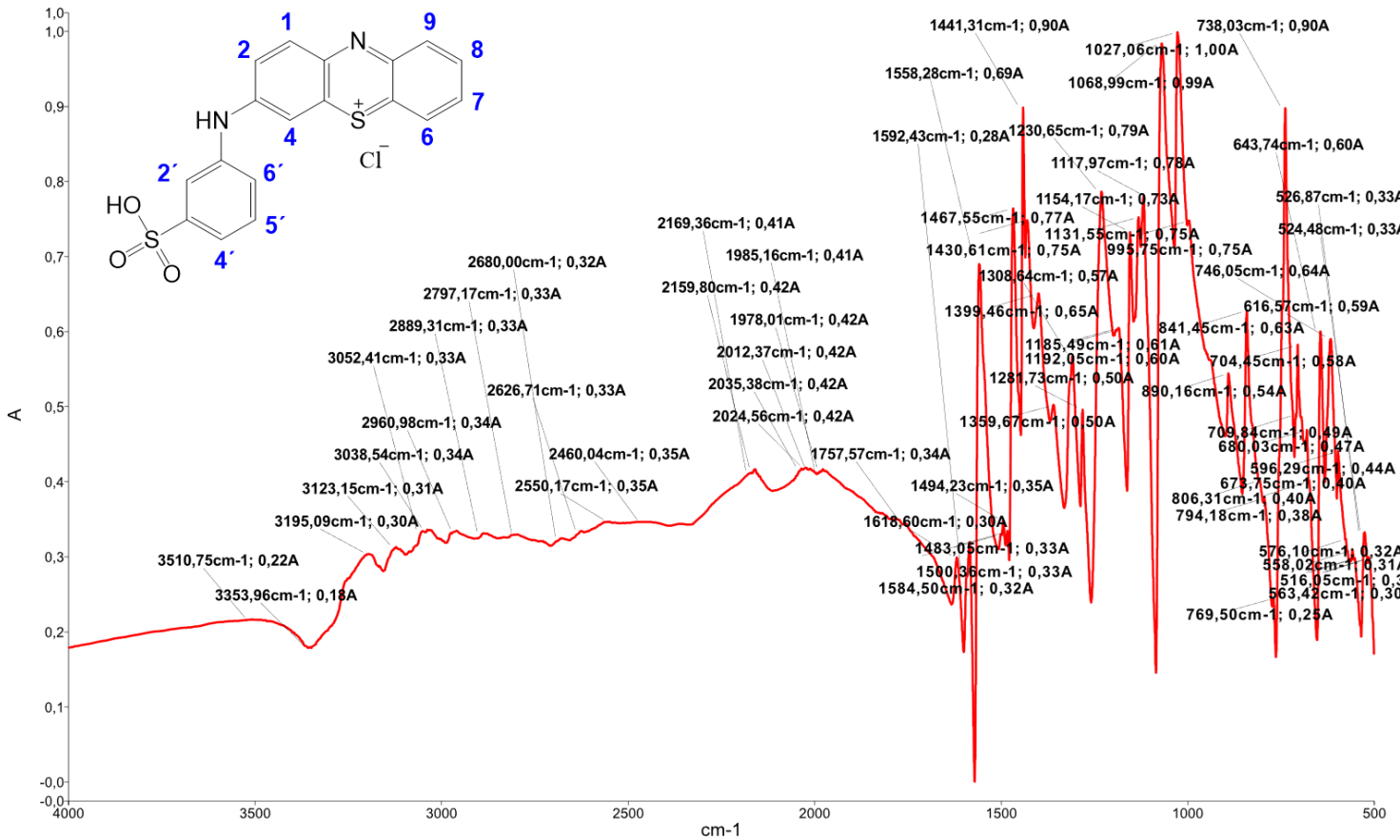

Figure S42. FT-IR spectrum of the compound **15**.

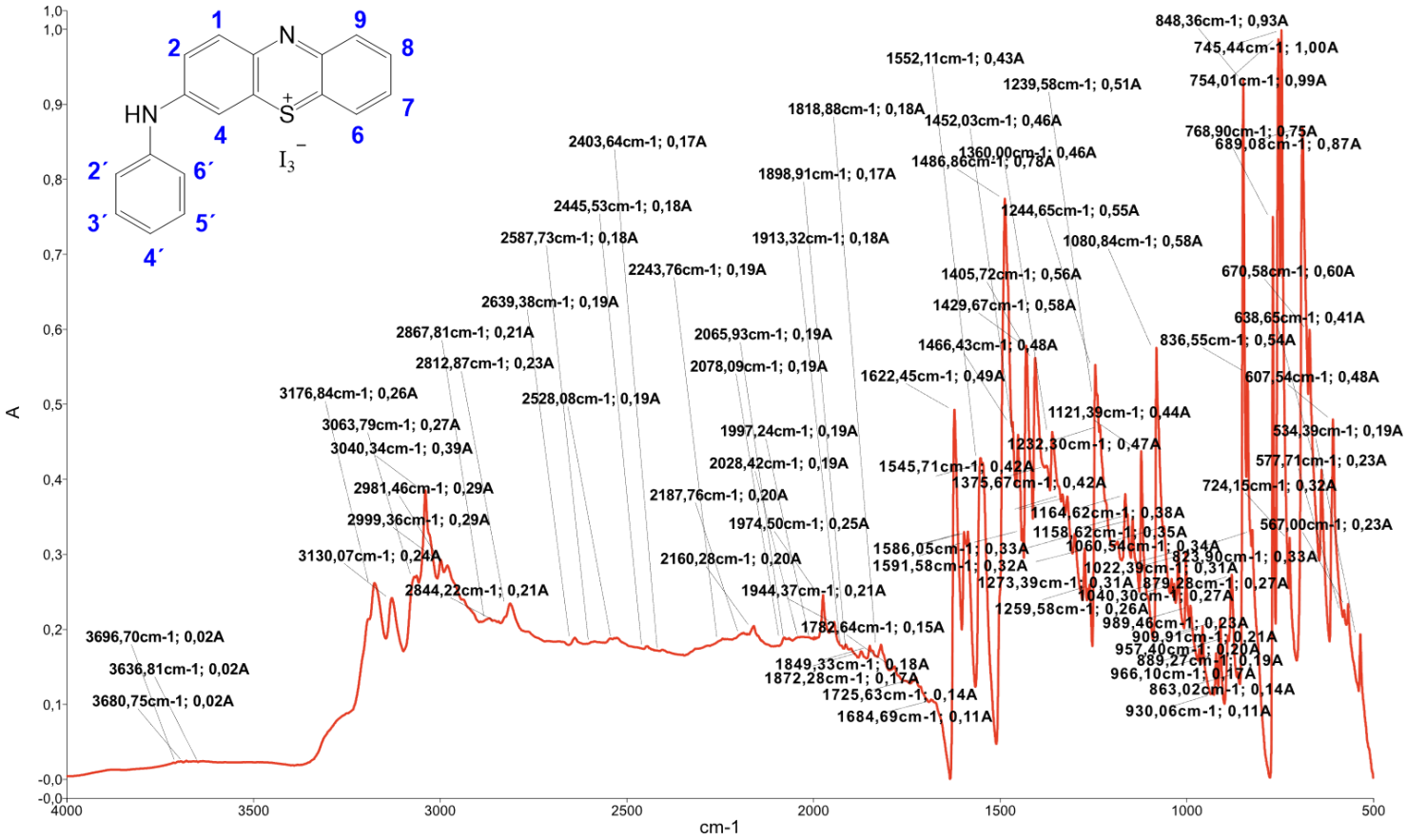

Figure S43. FT-IR spectrum of the compound **16**.

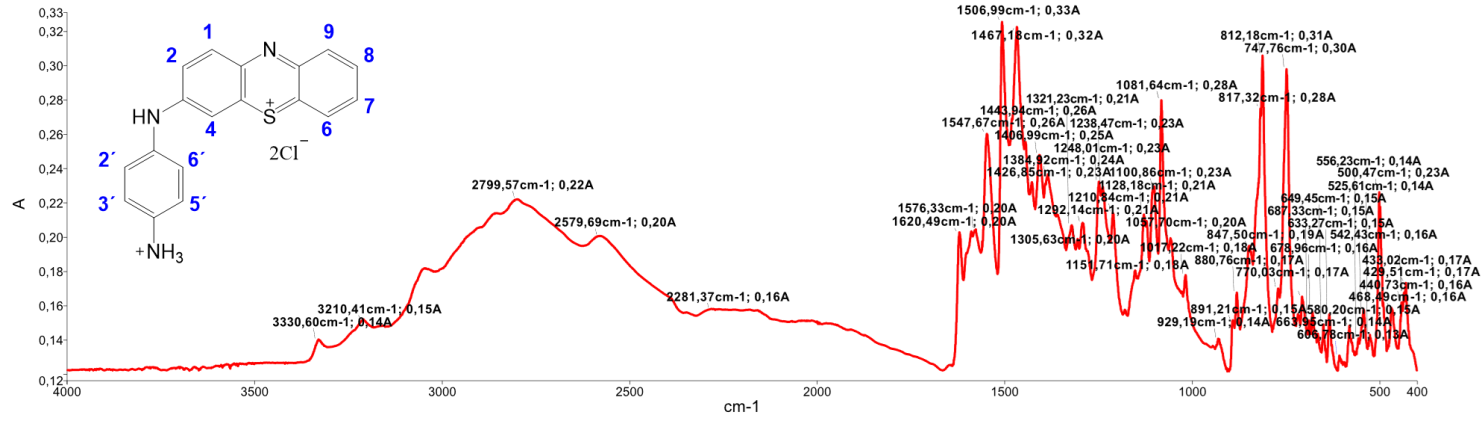

Figure S44. FT-IR spectrum of the compound **17**.

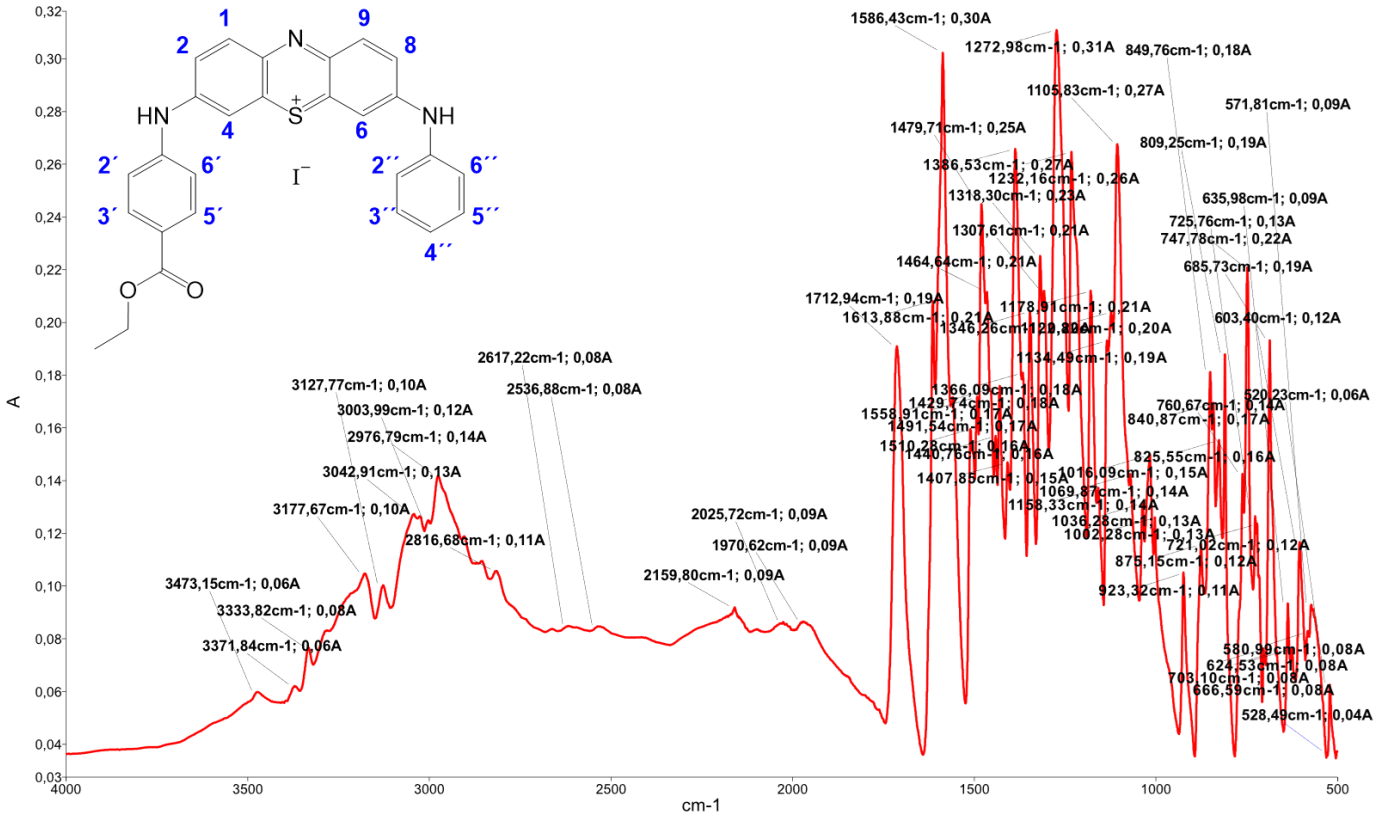

Figure S45. FT-IR spectrum of the compound **18**.

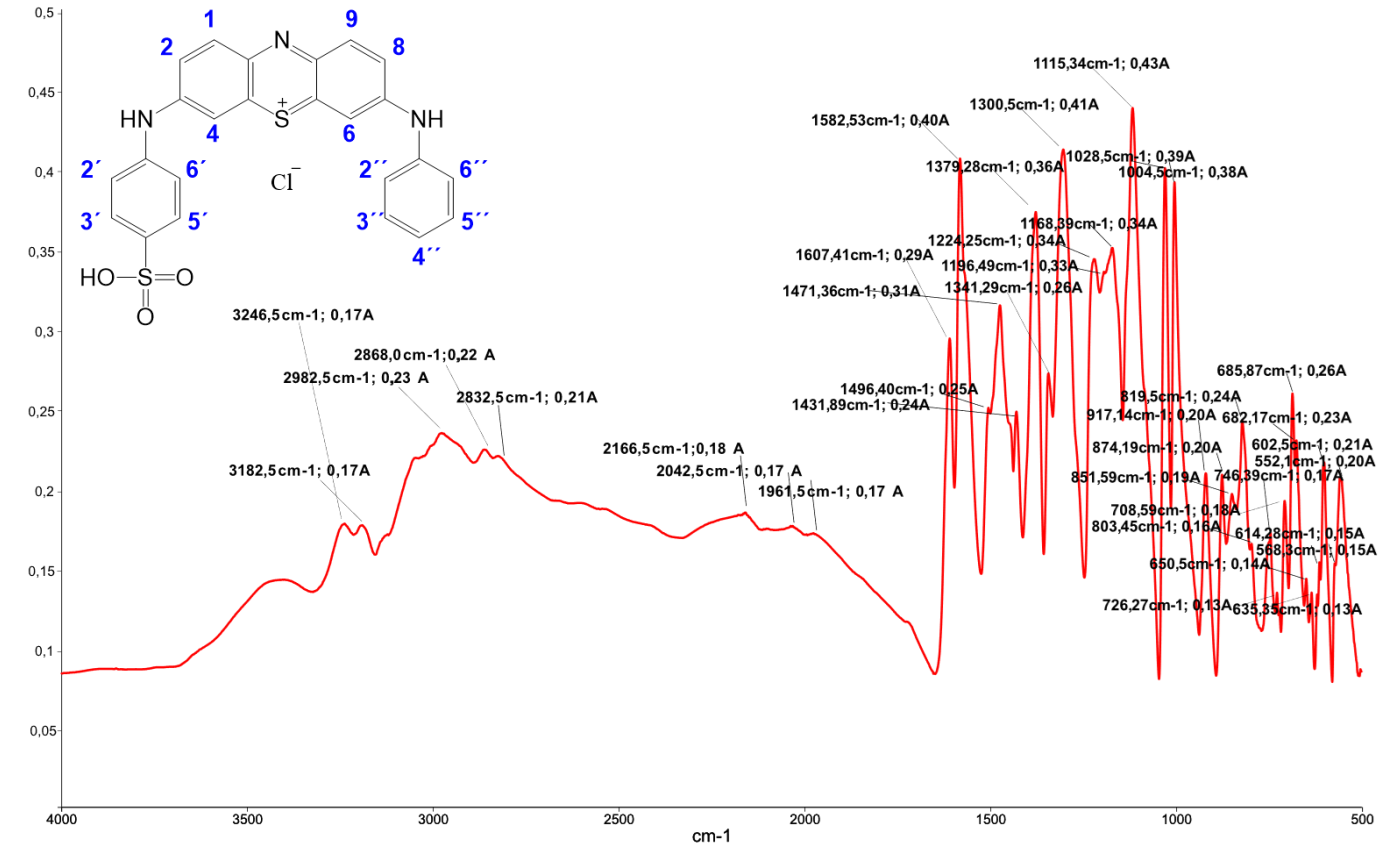

Figure S46. FT-IR spectrum of the compound **19**.

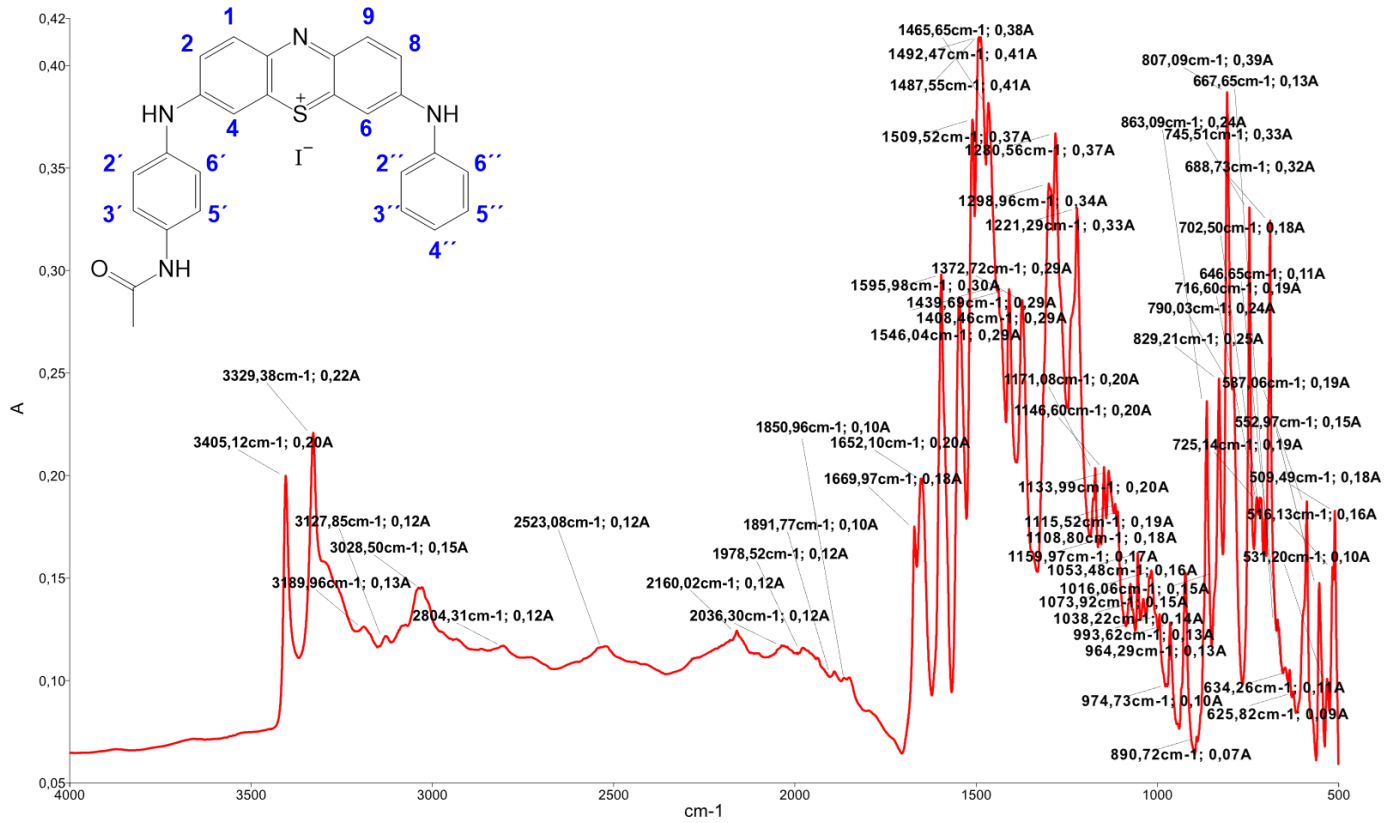

Figure S47. FT-IR spectrum of the compound **20**.

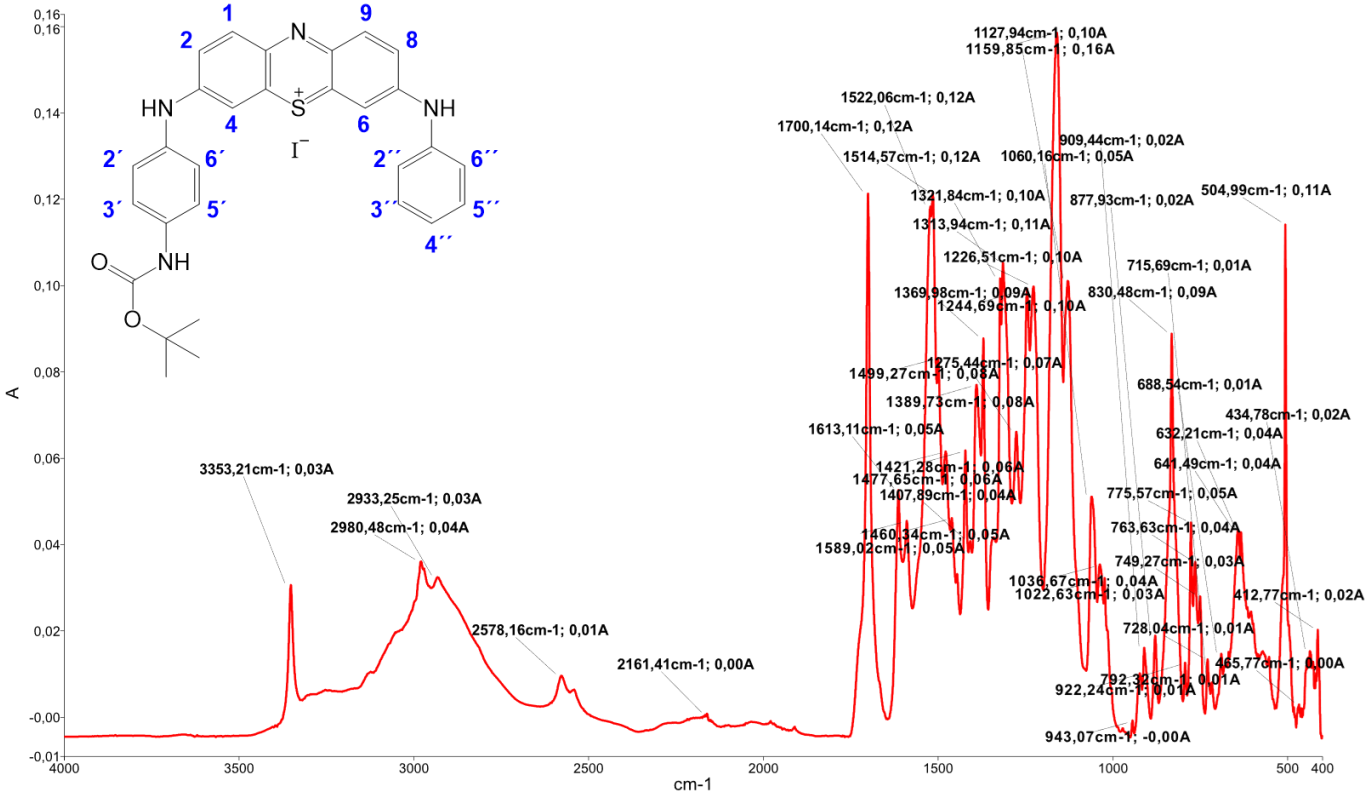

Figure S48. FT-IR spectrum of the compound **21**.

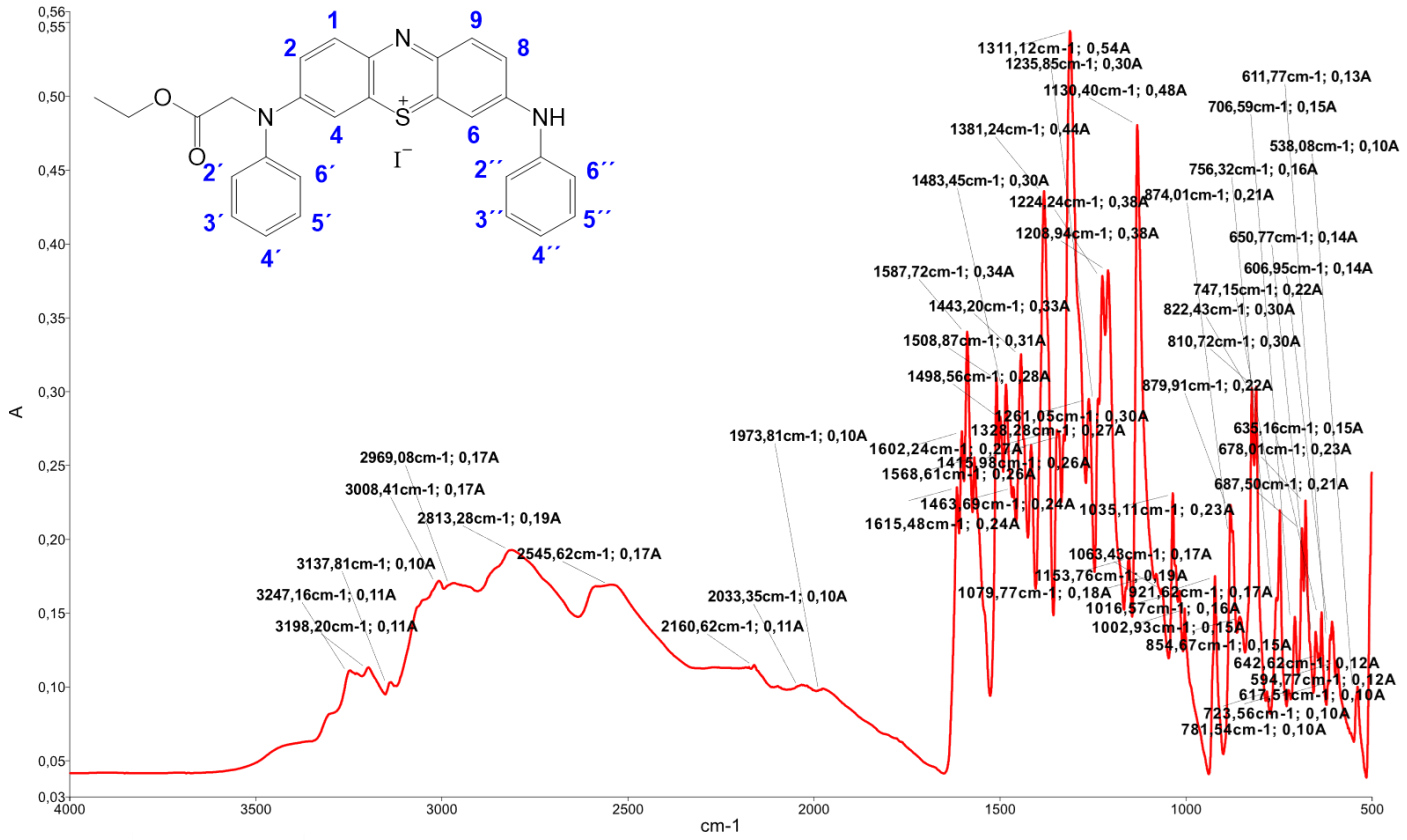

Figure S49. FT-IR spectrum of the compound **22**.

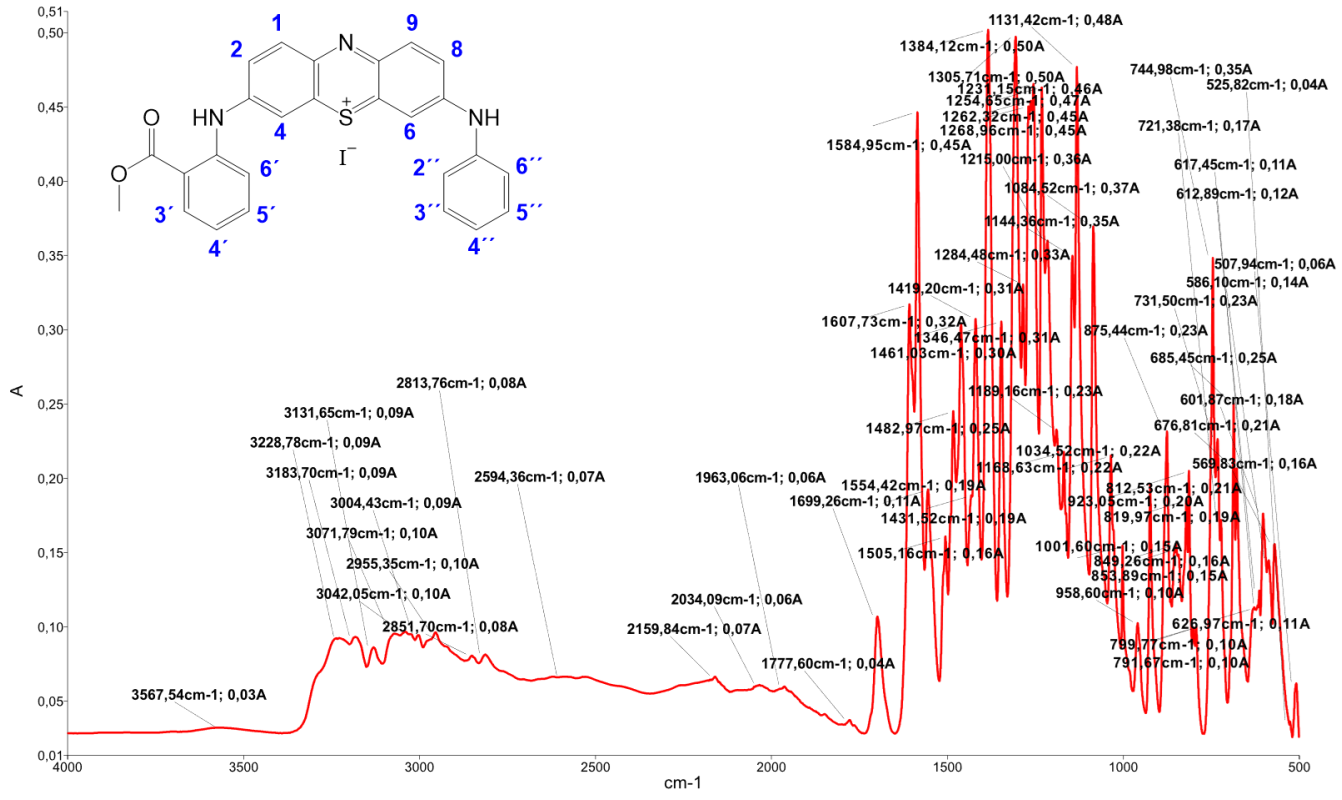

Figure S50. FT-IR spectrum of the compound **23**.

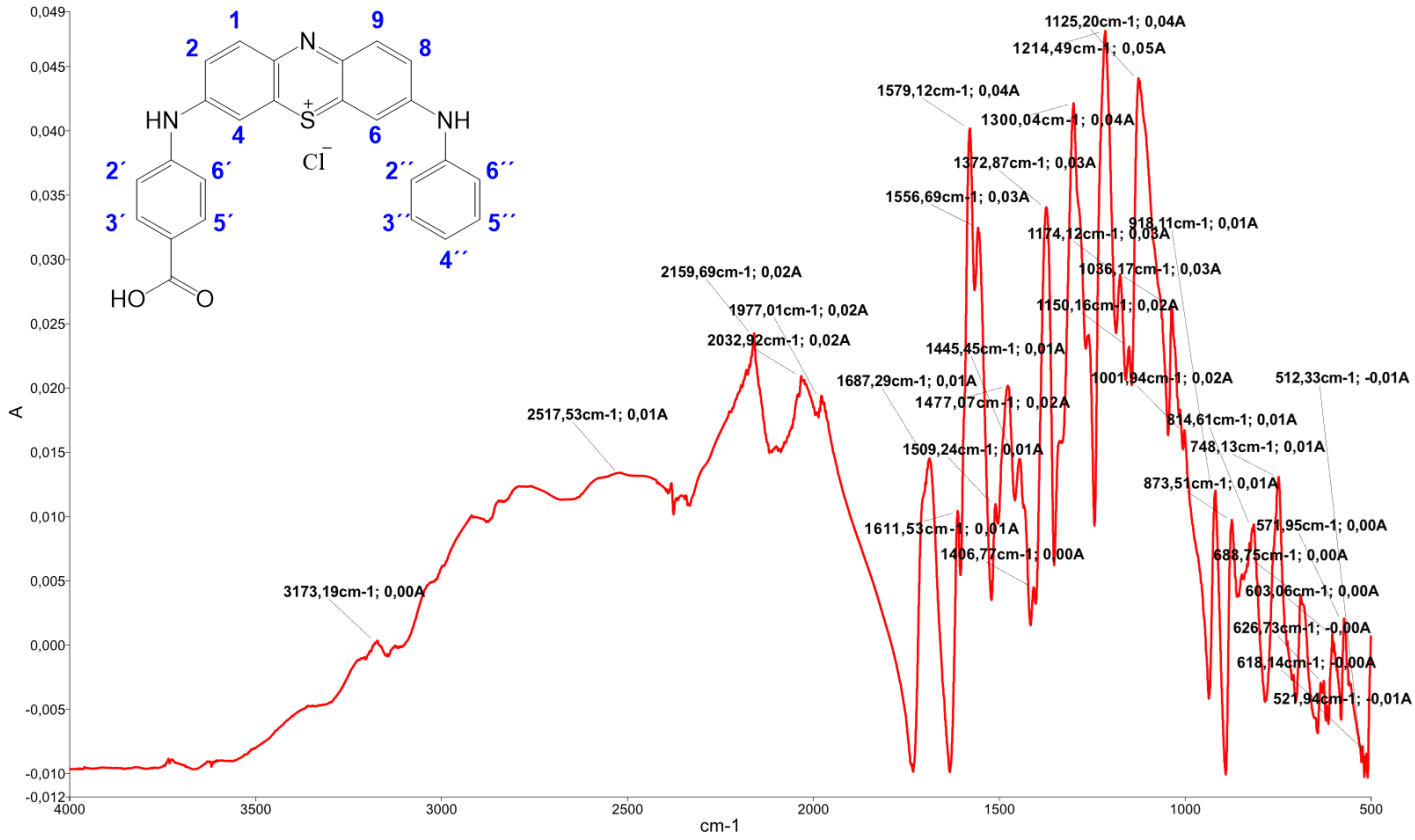

Figure S51. FT-IR spectrum of the compound **24**.

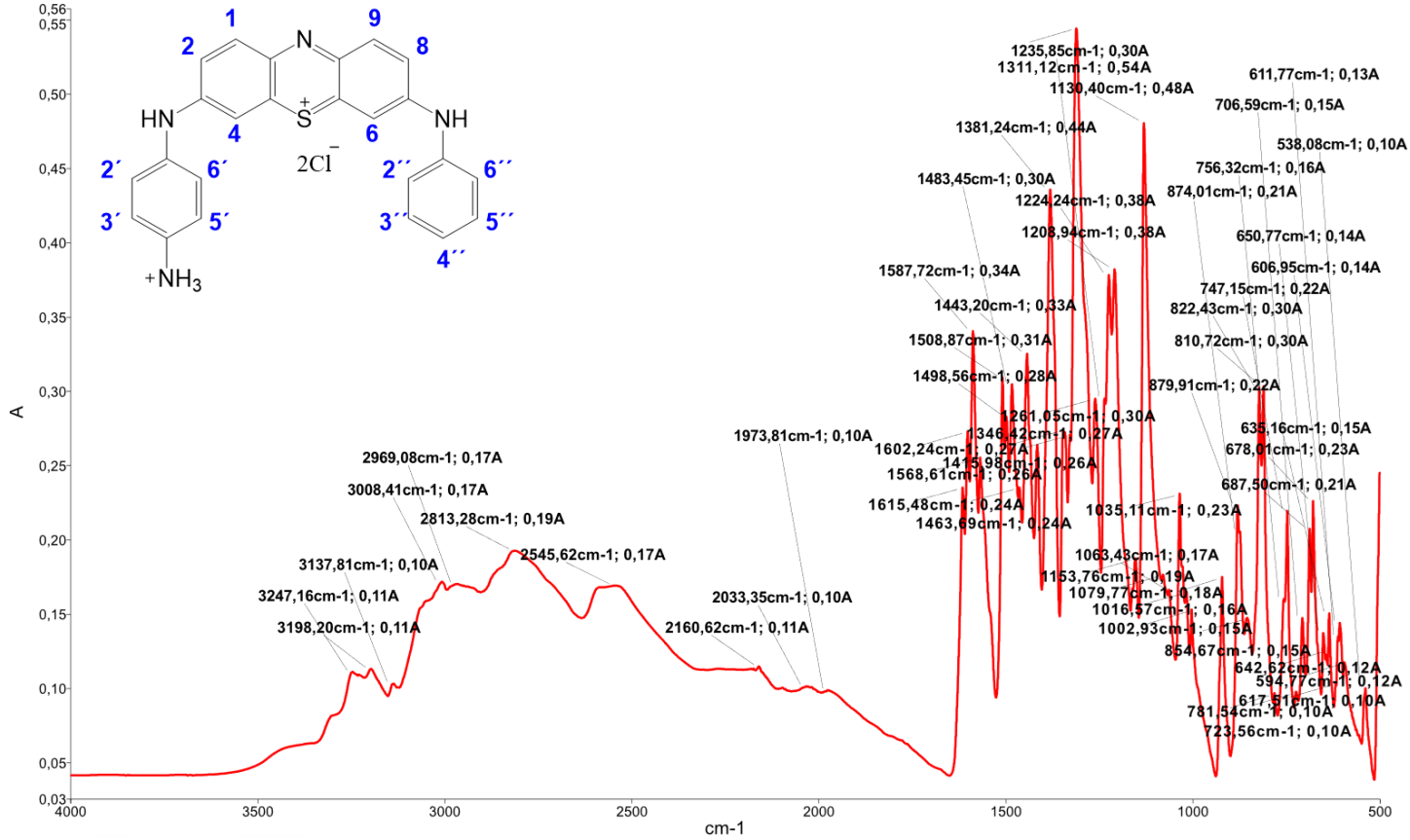

Figure S52. FT-IR spectrum of the compound **25**.

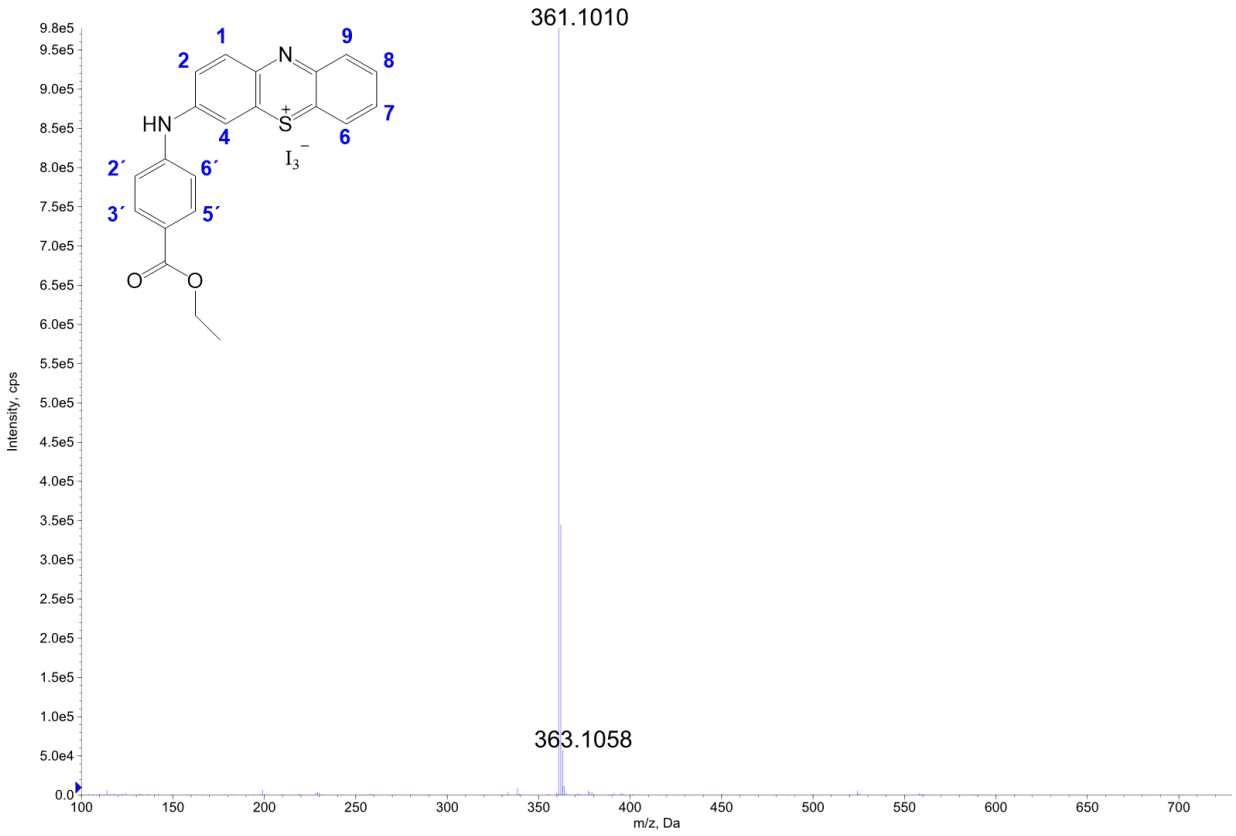

Figure S53. HRMS spectrum of the compound **10**.

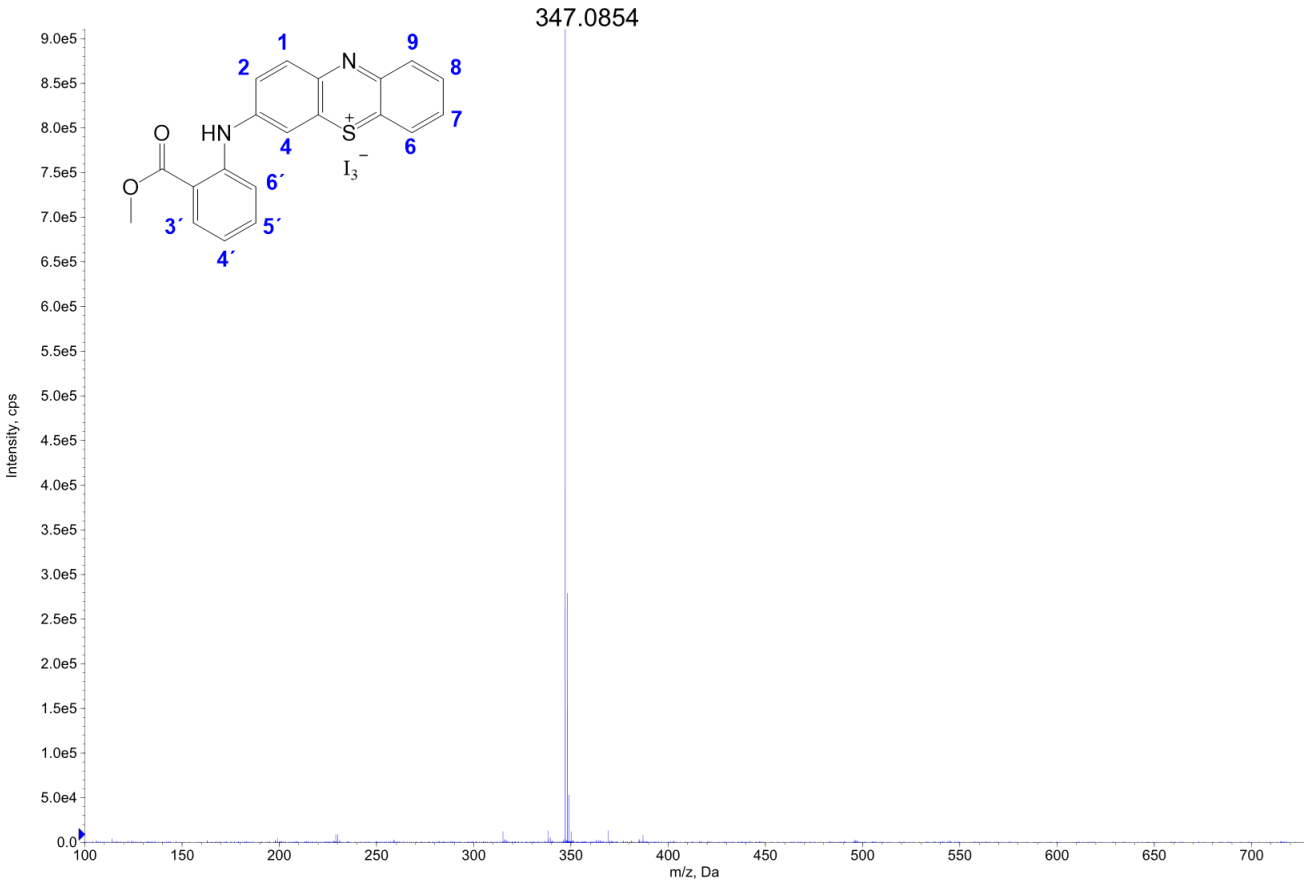

Figure S54. HRMS spectrum of the compound **11**.

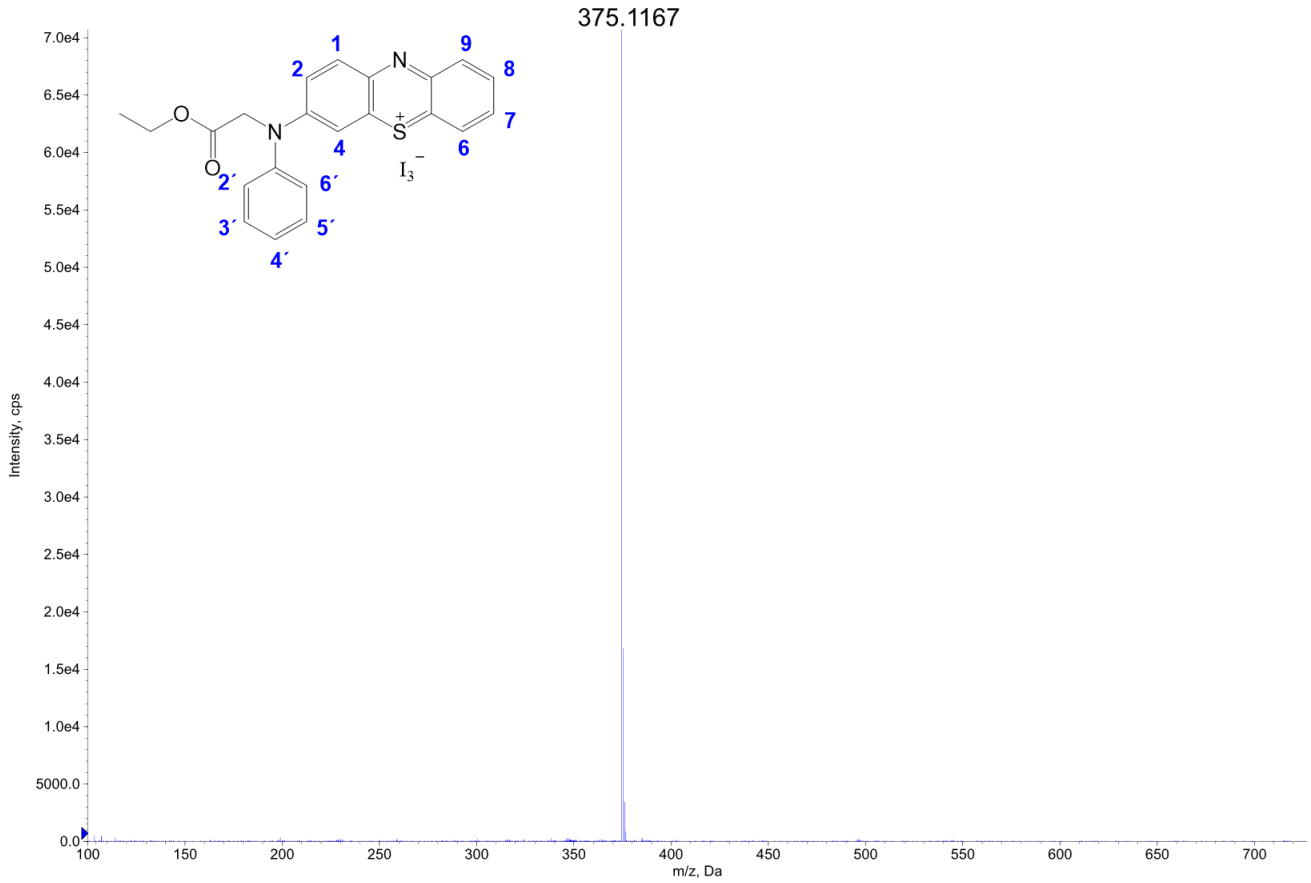

Figure S55. HRMS spectrum of the compound **12**.

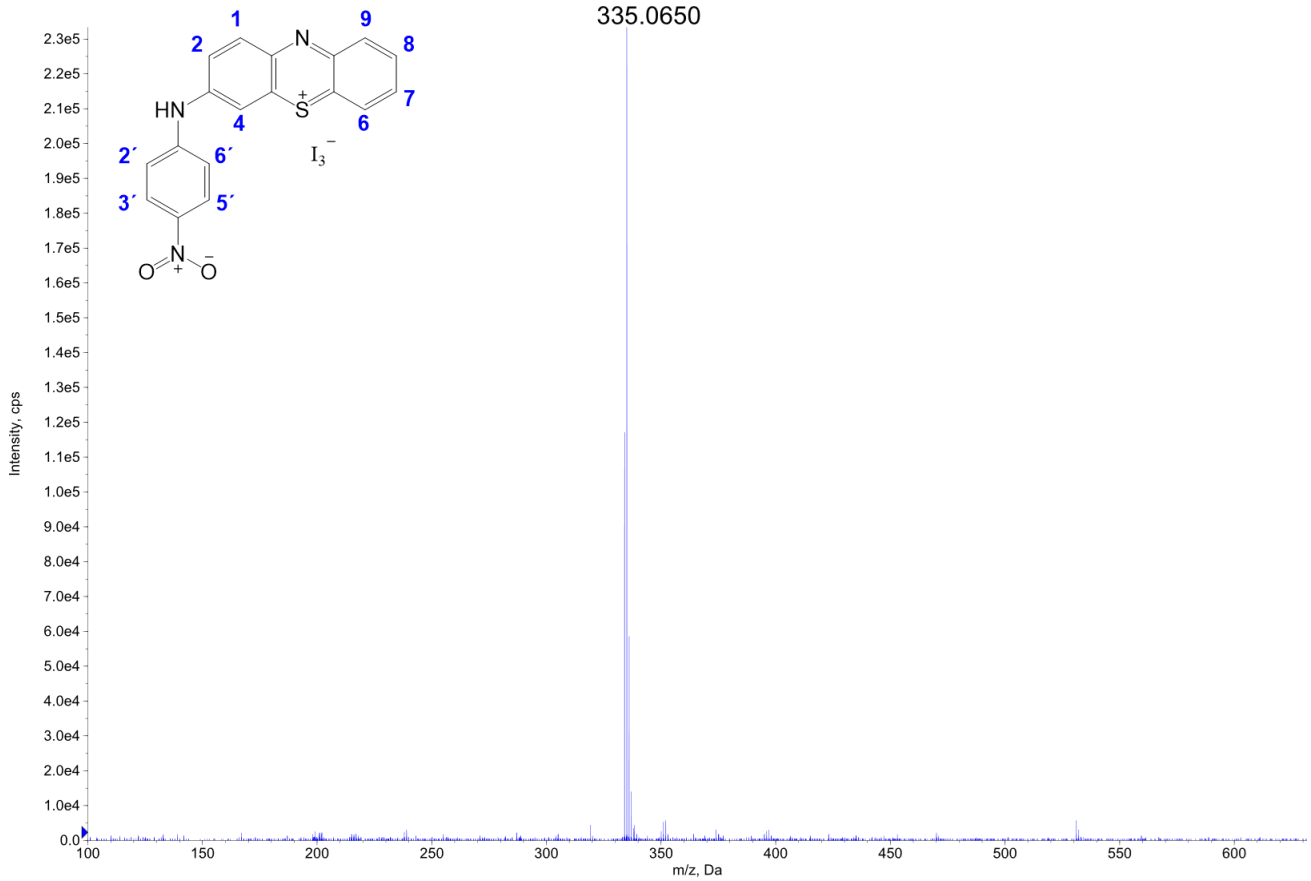

Figure S56. HRMS spectrum of the compound **13**.

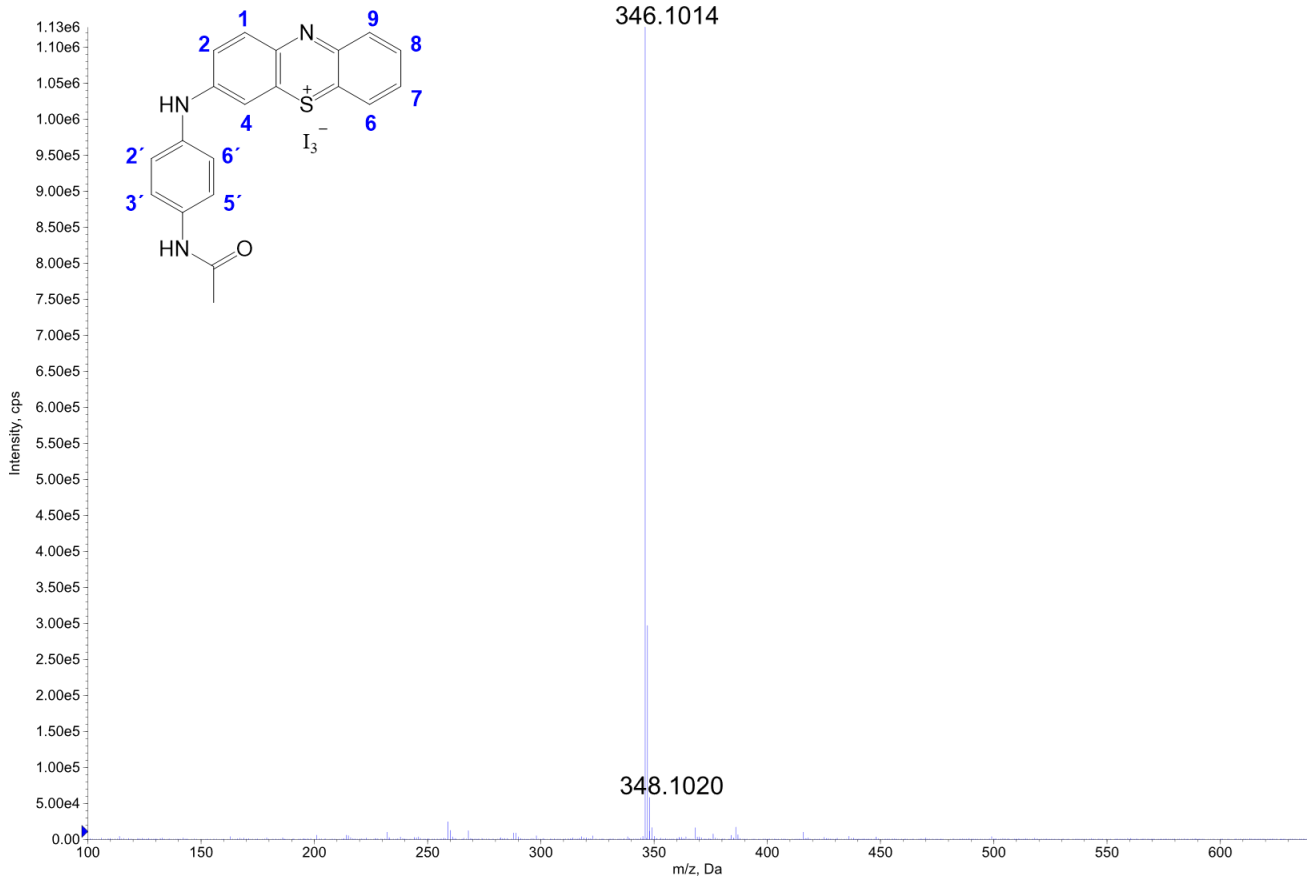

Figure S57. HRMS spectrum of the compound **14**.

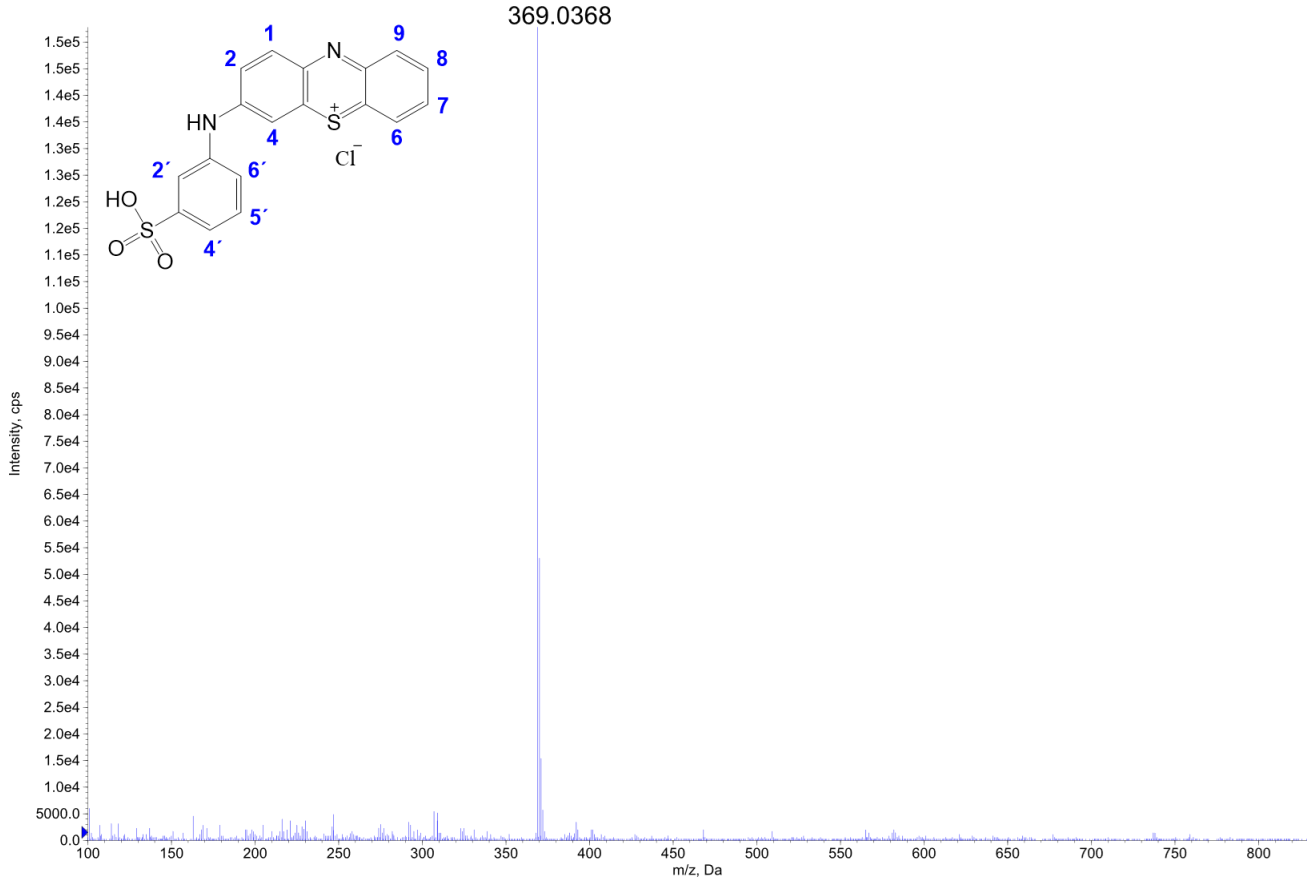

Figure S58. HRMS spectrum of the compound **15**.

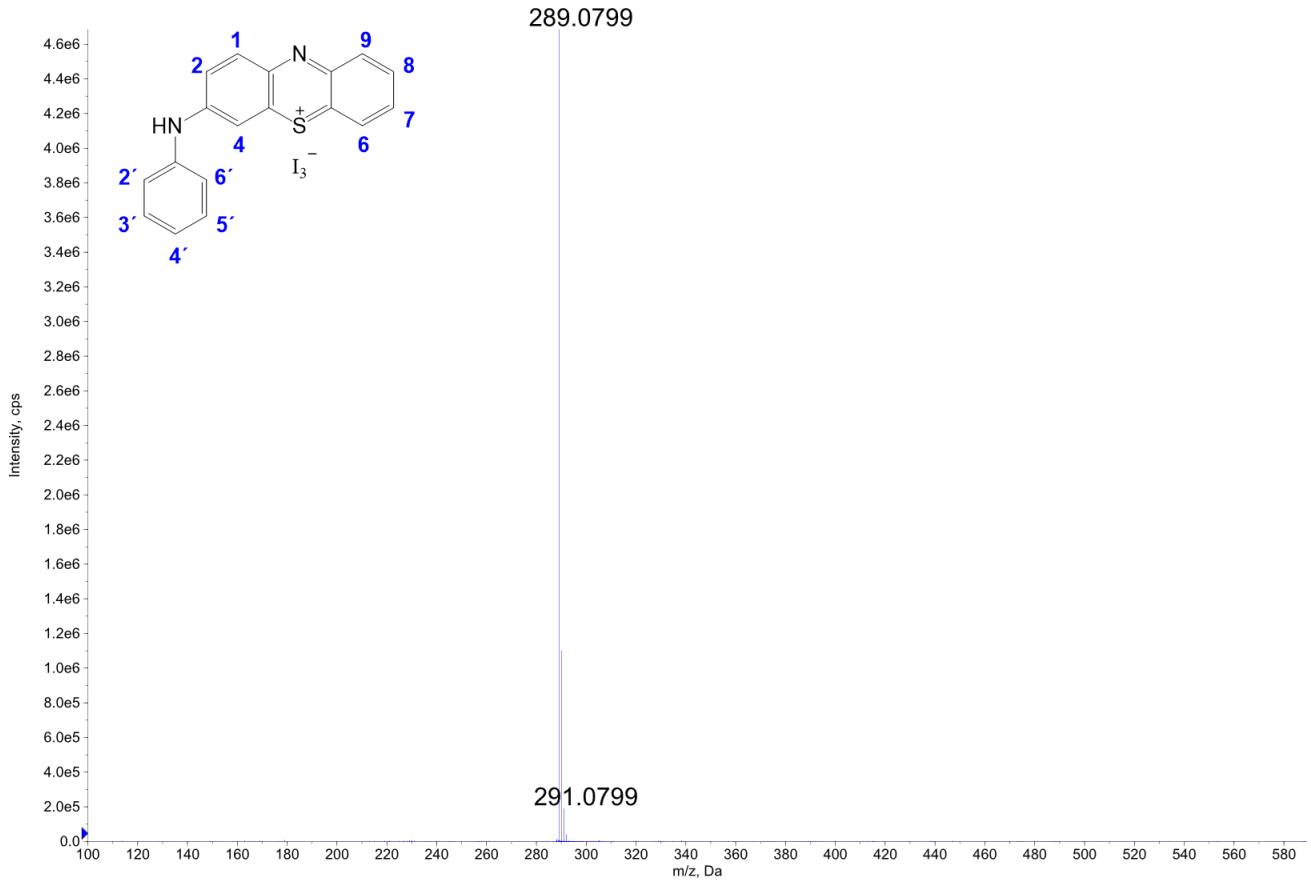

Figure S59. HRMS spectrum of the compound **16**.

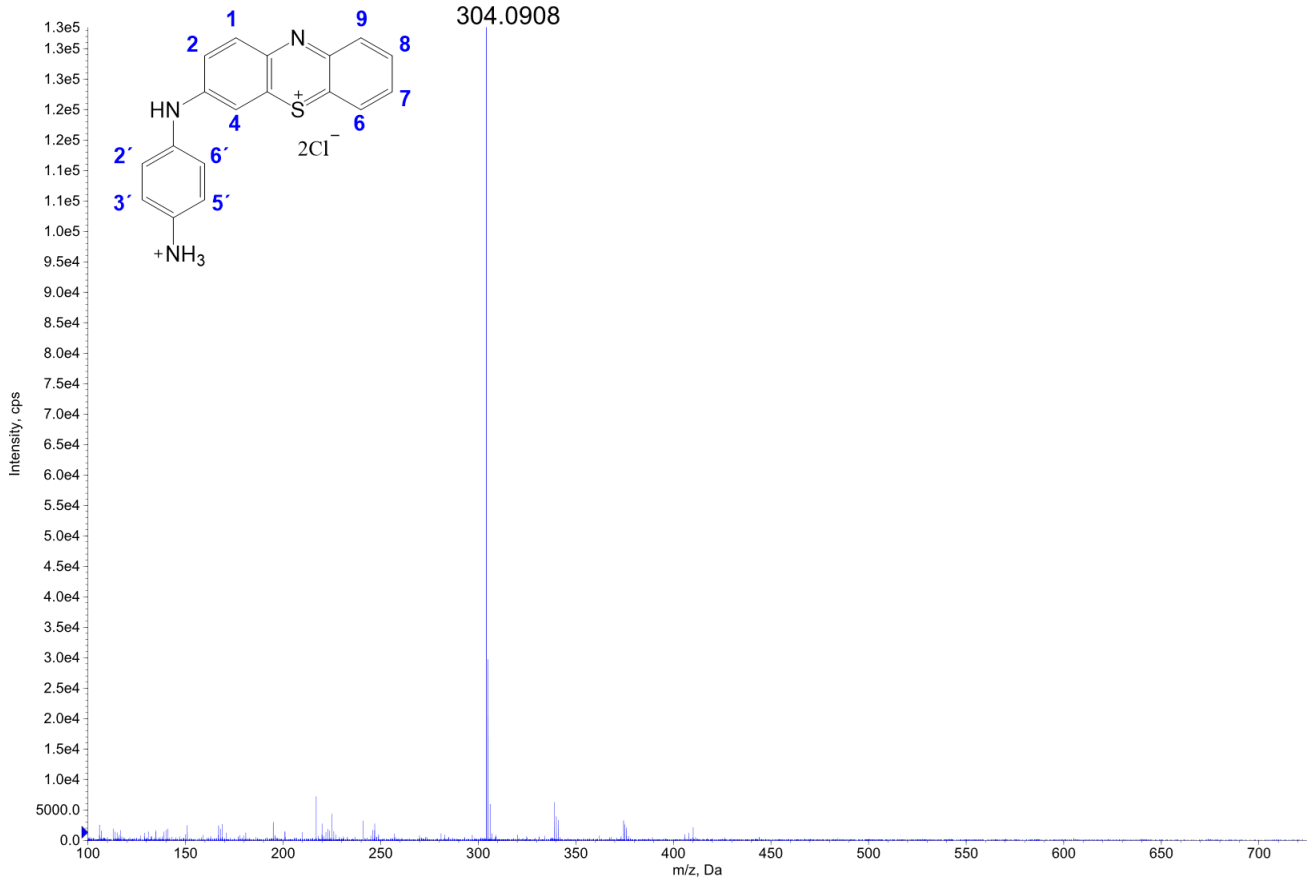

Figure S60. HRMS spectrum of the compound **17**.

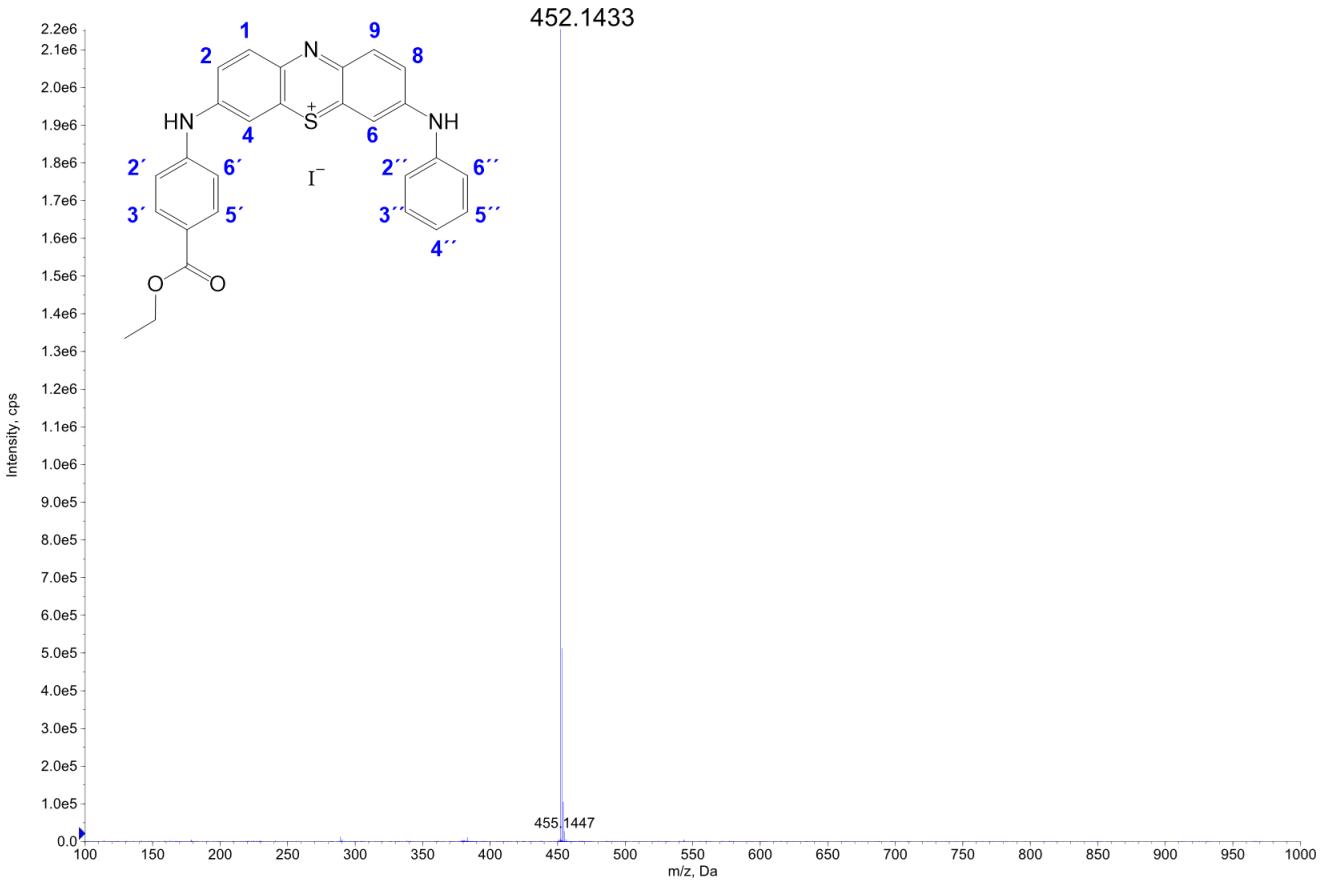

Figure S61. HRMS spectrum of the compound **18**.

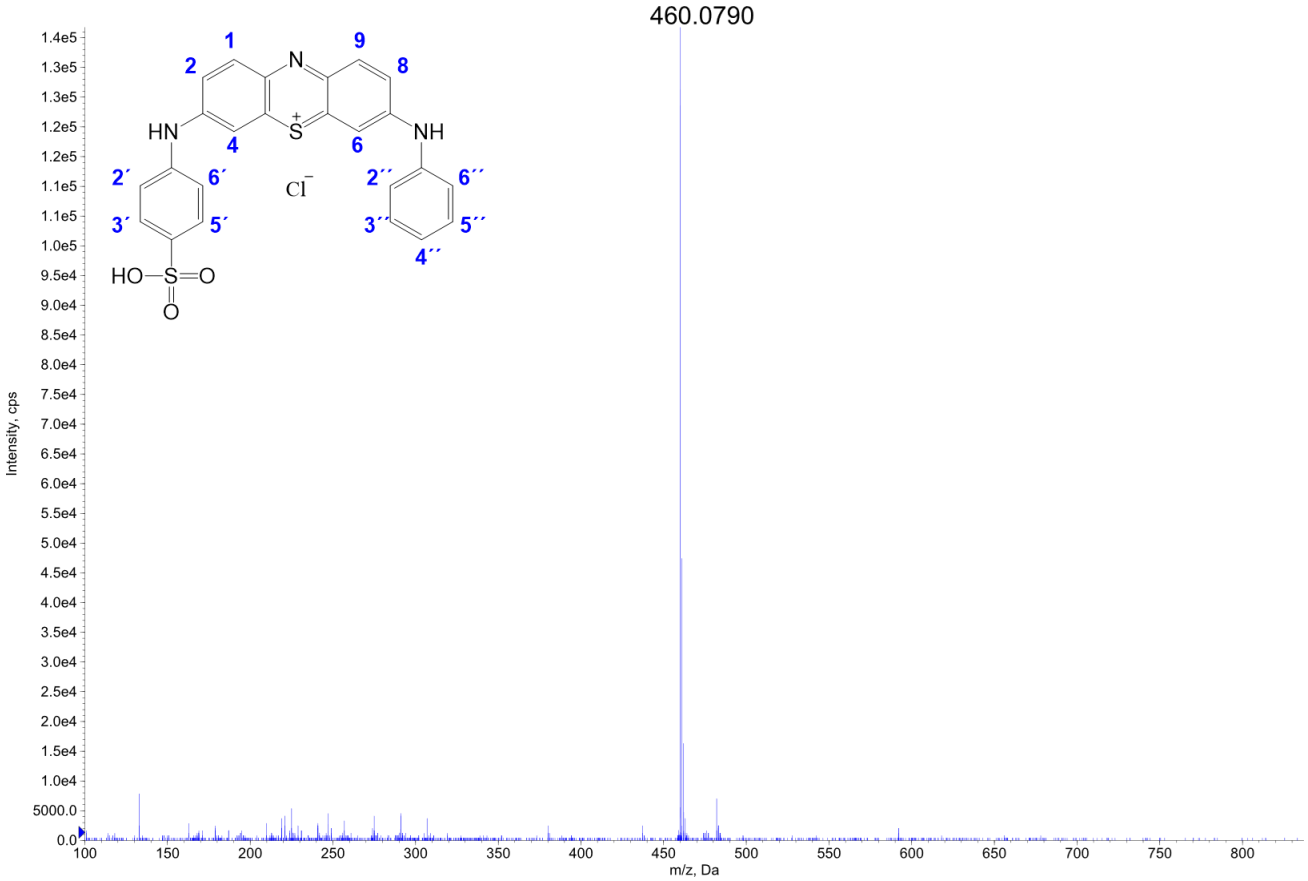

Figure S62. HRMS spectrum of the compound **19**.

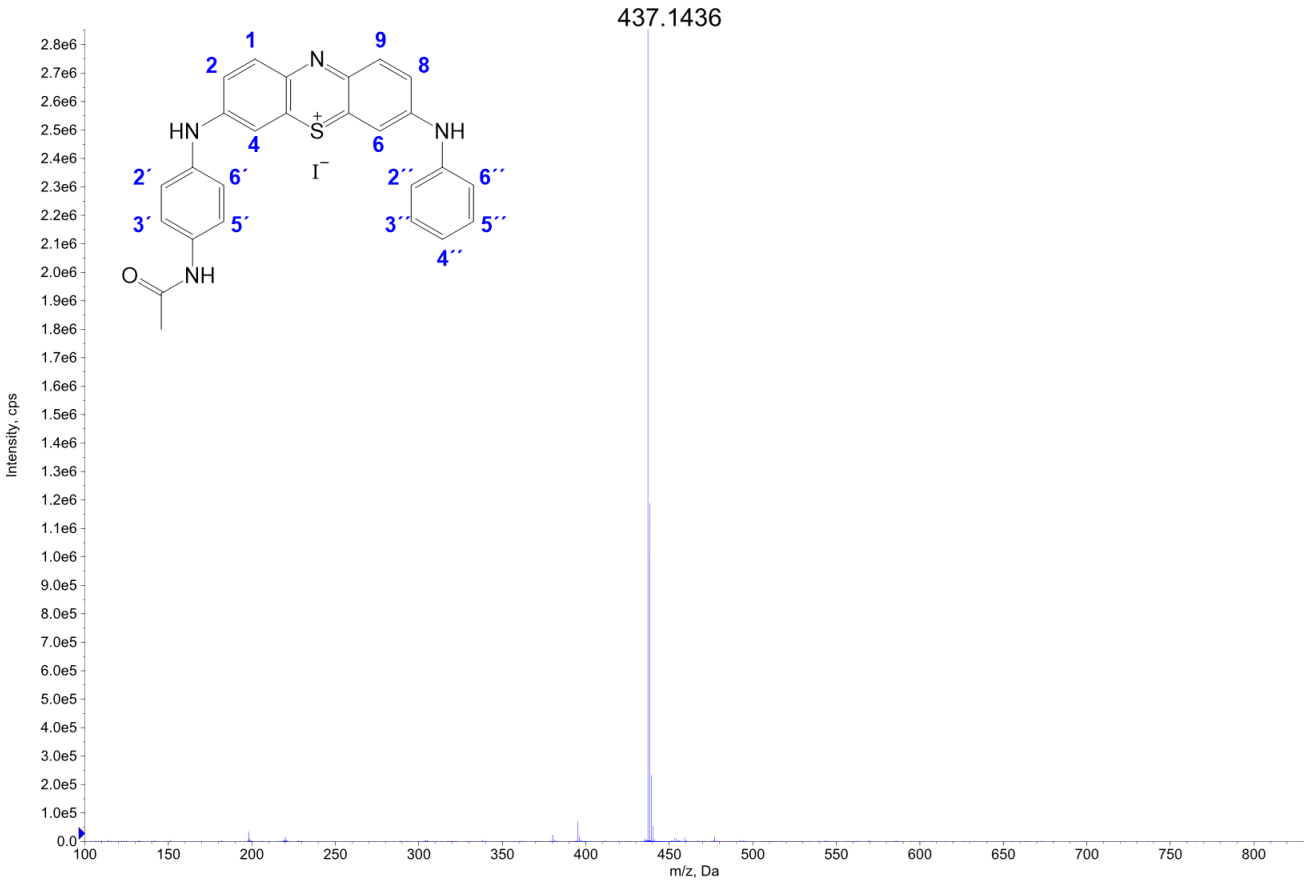

Figure S63. HRMS spectrum of the compound **20**.

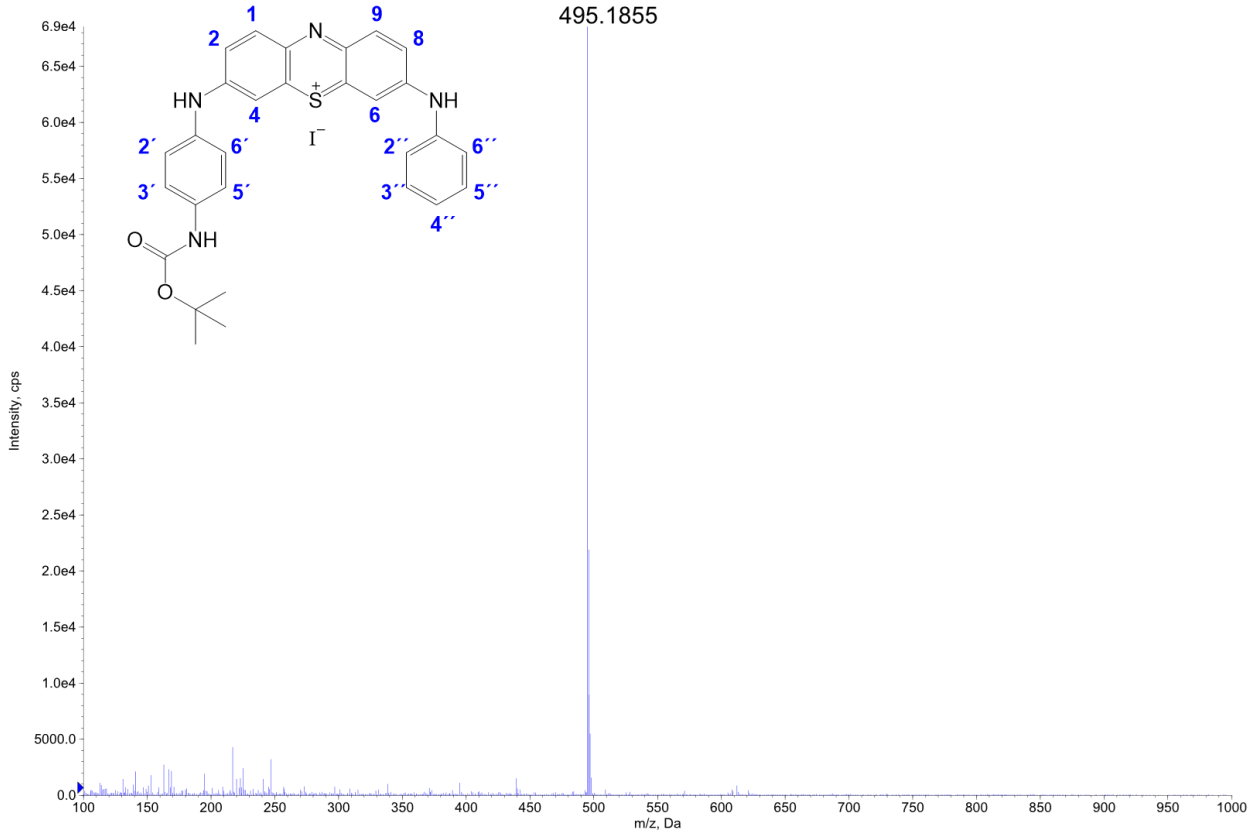

Figure S64. HRMS spectrum of the compound **21**.

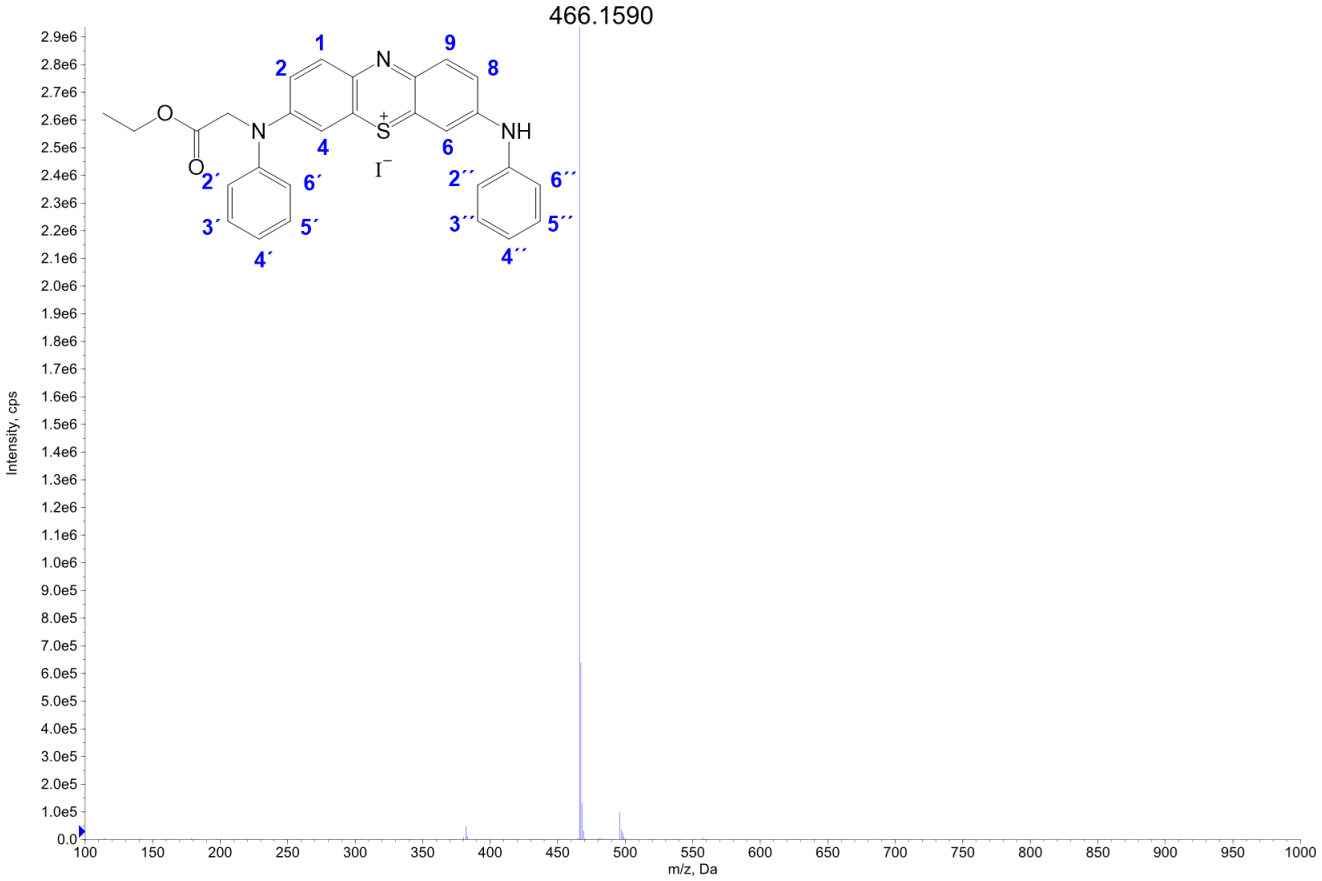

Figure S65. HRMS spectrum of the compound **22**.

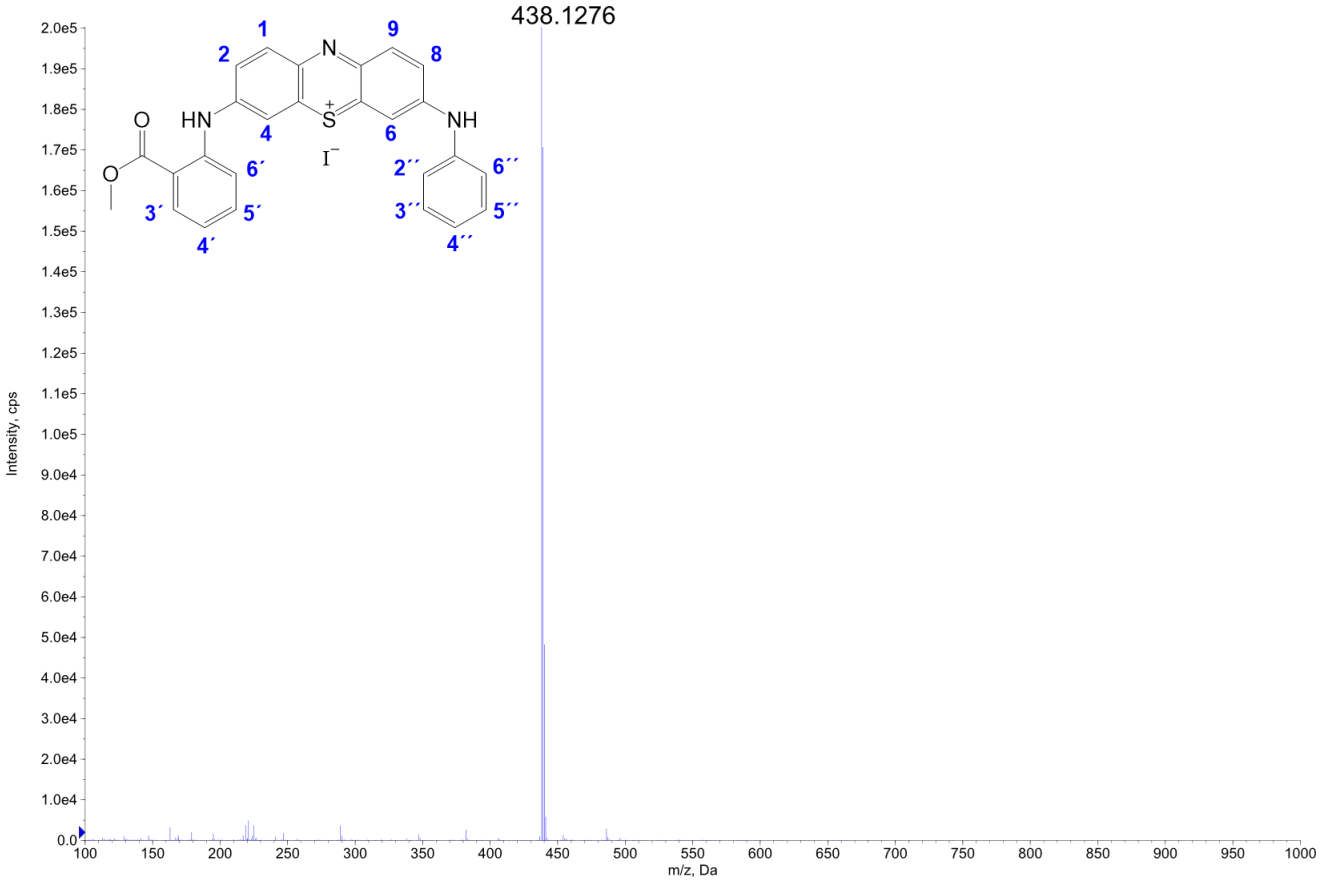

Figure S66. HRMS spectrum of the compound **23**.

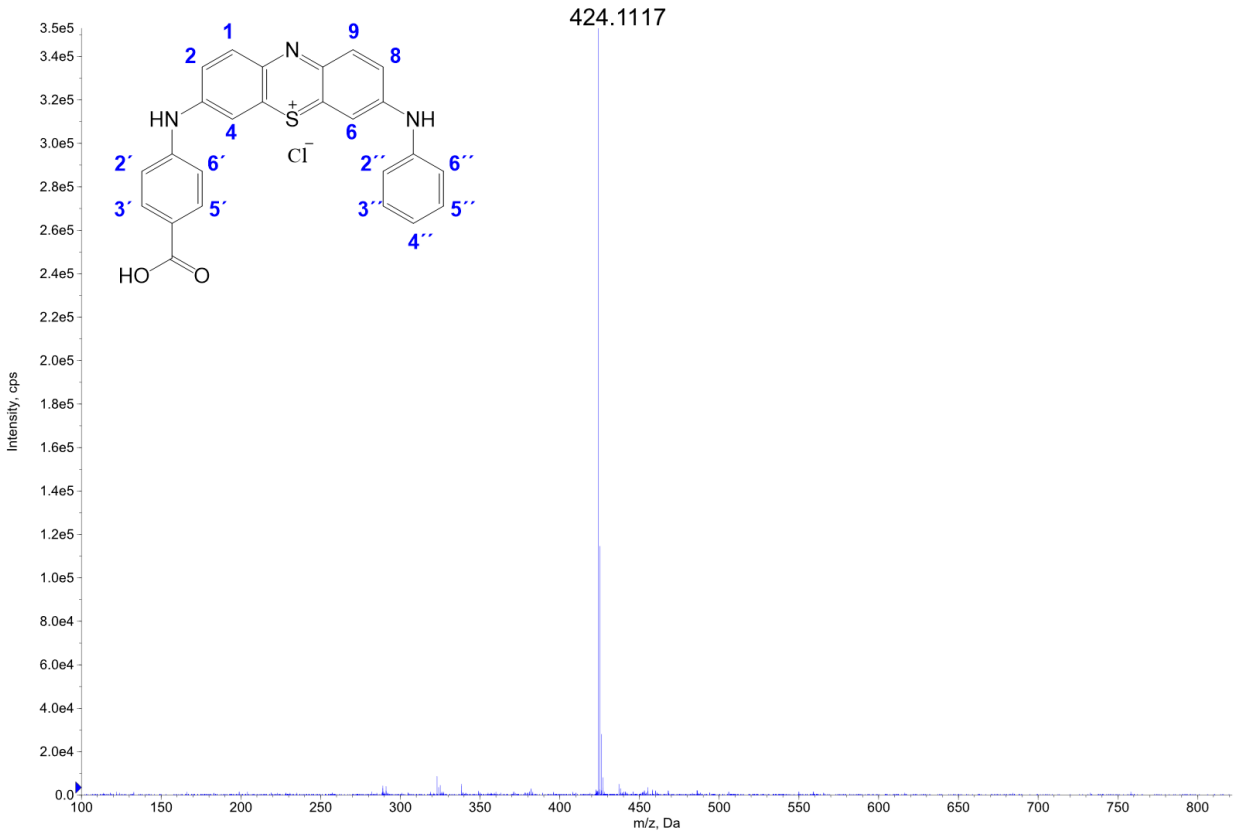

Figure S67. HRMS spectrum of the compound **24**.

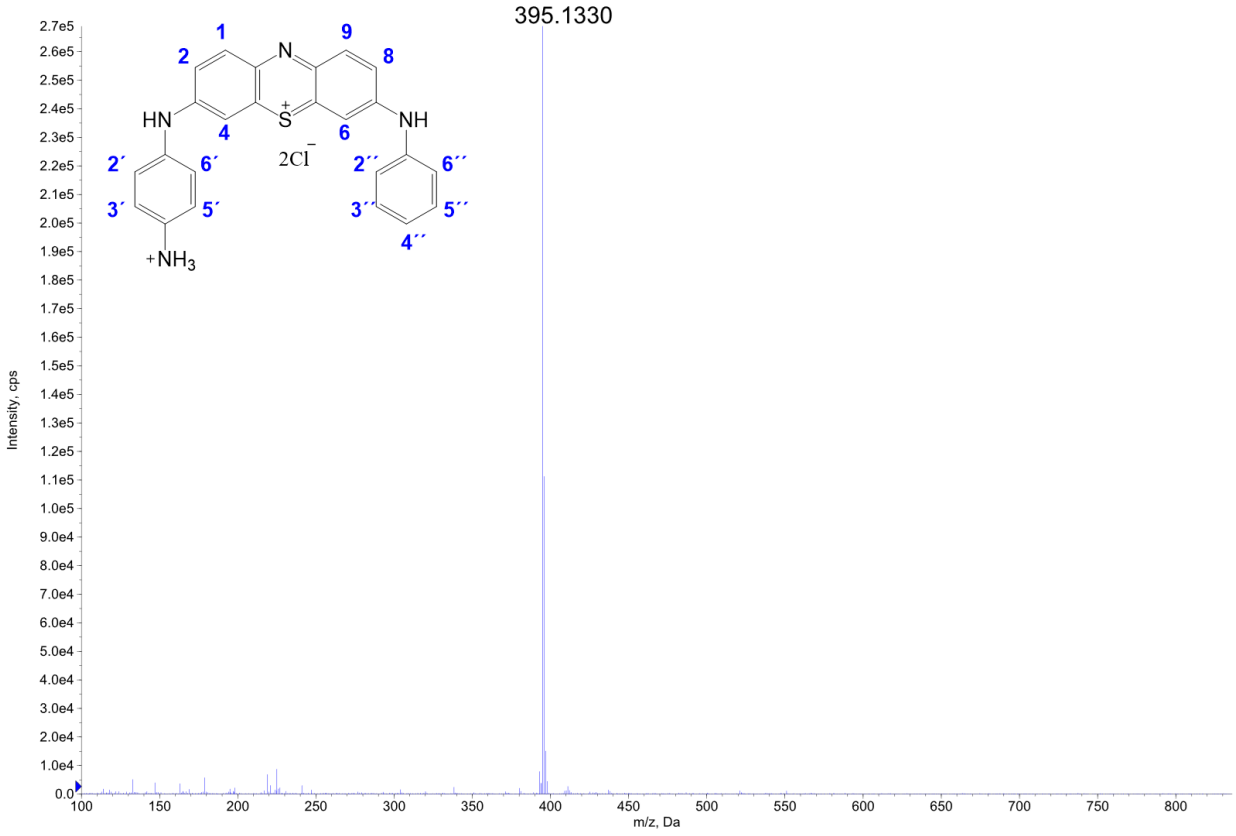

Figure S68. HRMS spectrum of the compound **25**.

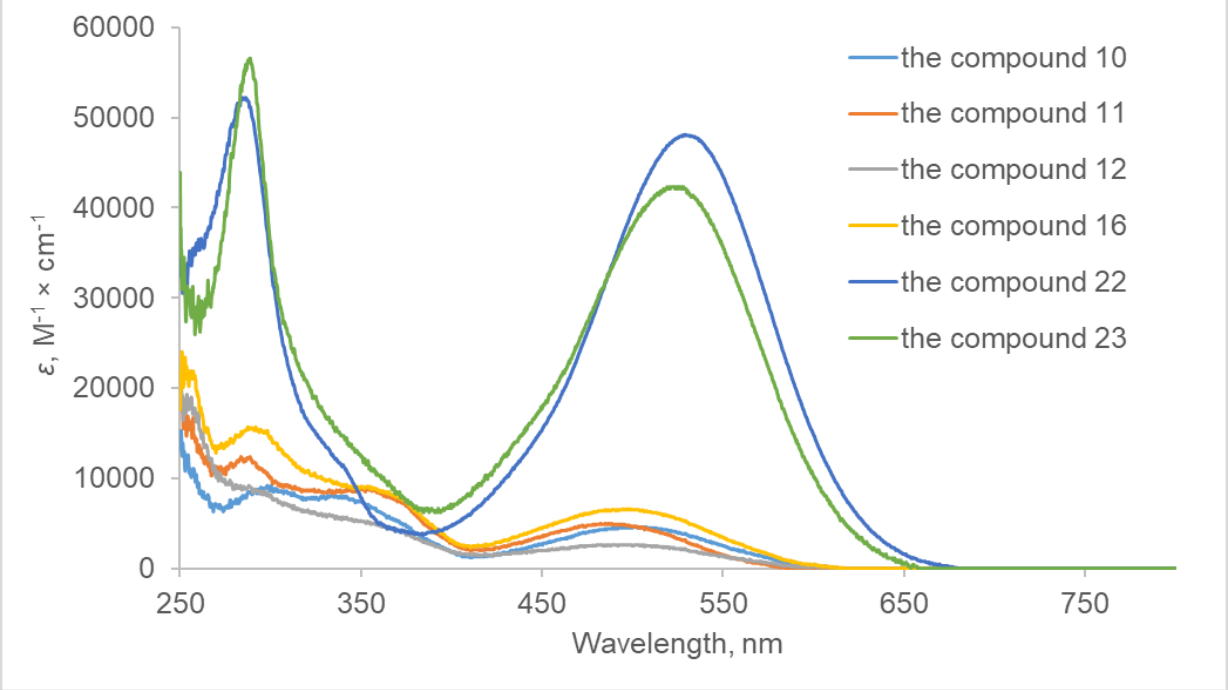

Figure S69. UV-Vis spectra of the compounds **10**, **11**, **12**, **16**, **22**, and **23** (THF, 1×10^{-5} M).

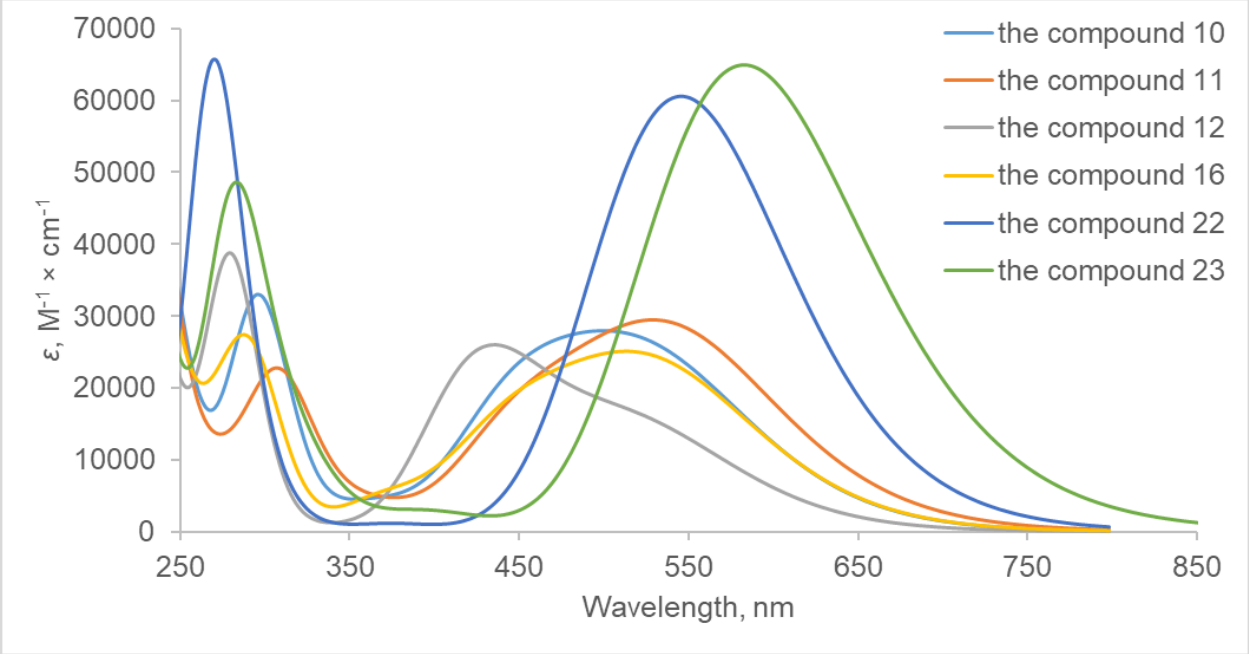

Figure S70. Calculated (TD-DFT M06-HF/6-311++G(d,p)/IEFPCM) UV-Vis absorption spectra of the compounds **10**, **11**, **12**, **16**, **22**, and **23** in THF.

Table S1. Absolute energies, minimum frequencies and calculated atomic coordinates for cations **1, 10-16** (DFT B3LYP/6-311++G(d,p)).

1: E = -914.9304313 a.u., ω1=78.6 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.740514	-0.362518	0.000318
2	6	0	-3.596718	1.046692	0.000097
3	6	0	-2.349490	1.609784	-0.000143
4	6	0	-1.179339	0.788075	-0.000150
5	6	0	-1.354194	-0.643894	0.000027
6	6	0	-2.642132	-1.200122	0.000288
7	16	0	0.000050	-1.707209	-0.000074
8	6	0	1.353892	-0.644081	-0.000410
9	6	0	1.179398	0.788017	-0.000666
10	7	0	0.000089	1.413530	-0.000351
11	6	0	2.642269	-1.200256	-0.000117
12	6	0	3.740371	-0.362479	-0.000073
13	6	0	3.596781	1.046778	0.000532
14	6	0	2.349538	1.609853	0.000337
15	1	0	-4.733817	-0.796000	0.000525
16	1	0	-4.480069	1.672955	0.000141
17	1	0	-2.197905	2.681793	-0.000278
18	1	0	-2.772821	-2.275977	0.000480
19	1	0	2.772738	-2.276095	0.000147
20	1	0	4.480114	1.673012	0.000848
21	1	0	2.197401	2.681766	0.000551
22	1	0	4.733766	-0.795919	0.000984

10A: E = -1468.710065 a.u., ω1=21.5 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.891726	0.760002	-0.223656
2	6	0	-7.478576	1.927103	0.446906
3	6	0	-6.147471	2.117606	0.735951
4	6	0	-5.178646	1.147428	0.367492
5	6	0	-5.620455	-0.027781	-0.308948
6	6	0	-6.976795	-0.209882	-0.600624
7	16	0	-4.503813	-1.273277	-0.796726
8	6	0	-2.968104	-0.669988	-0.258728

9	6	0	-2.882318	0.618349	0.410923
10	7	0	-3.888607	1.418566	0.683778
11	6	0	-1.840369	-1.432916	-0.492129
12	6	0	-0.572189	-0.967164	-0.086101
13	6	0	-0.465198	0.316721	0.559187
14	6	0	-1.566804	1.064832	0.798608
15	7	0	0.565353	-1.662566	-0.290269
16	6	0	0.723549	-2.983375	-0.805611
17	6	0	1.687173	-3.199718	-1.794830
18	6	0	1.894485	-4.483208	-2.281030
19	6	0	1.145912	-5.555869	-1.787362
20	6	0	0.193407	-5.333161	-0.788335
21	6	0	-0.015874	-4.052099	-0.290388
22	6	0	1.417685	-6.918598	-2.353397
23	8	0	0.641467	-7.861171	-1.801995
24	8	0	2.245090	-7.125619	-3.208759
25	6	0	0.835271	-9.226378	-2.279930
26	6	0	-0.139866	-10.114909	-1.539270
27	1	0	-8.941027	0.613511	-0.450880
28	1	0	-8.211038	2.672028	0.731504
29	1	0	-5.791773	3.002973	1.247879
30	1	0	-7.309263	-1.103296	-1.116537
31	1	0	-1.920709	-2.379228	-1.010042
32	1	0	0.514515	0.670094	0.861865
33	1	0	-1.506008	2.027580	1.290315
34	1	0	1.427431	-1.171484	-0.088726
35	1	0	2.259956	-2.367075	-2.187758
36	1	0	2.632457	-4.672610	-3.050495
37	1	0	-0.366608	-6.168193	-0.389087
38	1	0	-0.720497	-3.891681	0.516511
39	1	0	0.669225	-9.234745	-3.358698
40	1	0	1.874230	-9.505355	-2.095091
41	1	0	-0.017168	-11.146880	-1.877156
42	1	0	0.039197	-10.086695	-0.462281
43	1	0	-1.172262	-9.814832	-1.731707

10B: E = -1468.7093167 a.u., ω1=20.1 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.612672	-2.507051	-0.332884
2	6	0	-7.766388	-1.249816	0.281732
3	6	0	-6.658844	-0.485001	0.565067
4	6	0	-5.355428	-0.947990	0.245042

5	6	0	-5.223956	-2.224735	-0.376823
6	6	0	-6.357459	-2.993943	-0.661215
7	16	0	-3.664999	-2.876102	-0.805023
8	6	0	-2.560625	-1.638031	-0.292311
9	6	0	-3.060126	-0.418927	0.324824
10	7	0	-4.320759	-0.129762	0.558374
11	6	0	-1.208444	-1.826644	-0.483815
12	6	0	-0.276533	-0.838211	-0.090539
13	6	0	-0.750842	0.366144	0.537876
14	6	0	-2.078575	0.554886	0.732780
15	7	0	1.039035	-1.062689	-0.285225
16	6	0	2.132373	-0.164296	-0.094597
17	6	0	3.252747	-0.619064	0.606416
18	6	0	4.346240	0.220361	0.768447
19	6	0	4.330327	1.513386	0.236457
20	6	0	3.210874	1.955839	-0.474517
21	6	0	2.114752	1.118312	-0.649620
22	6	0	5.542030	2.372377	0.449911
23	8	0	5.408891	3.584506	-0.104377
24	8	0	6.517921	1.998568	1.055920
25	6	0	6.538236	4.496625	0.045698
26	6	0	6.178173	5.792054	-0.647809
27	1	0	-8.486889	-3.107621	-0.554692
28	1	0	-8.756856	-0.889122	0.529242
29	1	0	-6.737106	0.486602	1.036595
30	1	0	-6.254660	-3.963788	-1.134232
31	1	0	-0.846272	-2.736446	-0.951247
32	1	0	-0.036249	1.102730	0.877165
33	1	0	-2.456753	1.445022	1.220030
34	1	0	1.294443	-1.993216	-0.592352
35	1	0	3.260368	-1.616015	1.032663
36	1	0	5.222340	-0.108470	1.313286
37	1	0	3.209449	2.948238	-0.905164
38	1	0	1.267960	1.447576	-1.239685
39	1	0	6.723353	4.633530	1.112697
40	1	0	7.417801	4.021216	-0.392231
41	1	0	7.008588	6.496028	-0.552429
42	1	0	5.989410	5.631744	-1.711501
43	1	0	5.293121	6.248197	-0.198934

11A: E = - 1429.38786070 a.u., ω1=20.6 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-6.980957	0.664434	-0.126641
2	6	0	-6.953582	-0.545219	0.592467
3	6	0	-5.751410	-1.160268	0.856098
4	6	0	-4.530455	-0.587835	0.414062
5	6	0	-4.582297	0.638435	-0.310148
6	6	0	-5.810445	1.253672	-0.576821
7	16	0	-3.133596	1.416161	-0.889702
8	6	0	-1.865842	0.357375	-0.354251
9	6	0	-2.189048	-0.860962	0.372490
10	7	0	-3.392605	-1.266111	0.708850
11	6	0	-0.558388	0.693118	-0.647545
12	6	0	0.501246	-0.151326	-0.249306
13	6	0	0.193931	-1.381831	0.438727
14	6	0	-1.082869	-1.710692	0.739741
15	7	0	1.806484	0.087290	-0.489559
16	6	0	2.452829	1.210881	-1.041887
17	6	0	3.637975	1.012981	-1.796883
18	6	0	4.288948	2.127806	-2.336271
19	6	0	3.808016	3.414465	-2.125326
20	6	0	2.671531	3.603263	-1.342078
21	6	0	2.000582	2.512854	-0.800428
22	1	0	-7.929254	1.145936	-0.333895
23	1	0	-7.880064	-0.989147	0.934564
24	1	0	-5.691466	-2.092732	1.403269
25	1	0	-5.845505	2.185262	-1.129854
26	1	0	-0.350665	1.584859	-1.221629
27	1	0	1.013005	-2.032179	0.724045
28	1	0	-1.326575	-2.623500	1.268610
29	1	0	2.437292	-0.721166	-0.432094
30	6	0	4.219578	-0.349488	-1.970670
31	1	0	5.187036	1.970384	-2.917607
32	1	0	2.312933	4.604430	-1.134211
33	1	0	1.155562	2.678518	-0.146332
34	8	0	3.841054	-1.338108	-1.357239
35	8	0	5.215148	-0.383967	-2.848894
36	6	0	5.871023	-1.661925	-3.046914
37	1	0	4.329120	4.263863	-2.548858
38	1	0	5.152987	-2.396598	-3.409712
39	1	0	6.309226	-2.004196	-2.109972
40	1	0	6.640636	-1.471159	-3.789461

11B: E = -1429.3872594 a.u., ω1=22.6 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-7.583332	-2.730344	0.221758
2	6	0	-7.815382	-1.424646	-0.249897
3	6	0	-6.755827	-0.571223	-0.453990
4	6	0	-5.424723	-0.990324	-0.195263
5	6	0	-5.213163	-2.317453	0.280654
6	6	0	-6.298287	-3.176672	0.485879
7	16	0	-3.614326	-2.924218	0.620573
8	6	0	-2.588699	-1.571319	0.247595
9	6	0	-3.165047	-0.322650	-0.227308
10	7	0	-4.441948	-0.082457	-0.422716
11	6	0	-1.227958	-1.698873	0.416360
12	6	0	-0.354718	-0.617282	0.145842
13	6	0	-0.905556	0.613111	-0.358731
14	6	0	-2.243599	0.742544	-0.533996
15	7	0	0.966058	-0.817616	0.333623
16	6	0	2.046713	0.085182	0.284735
17	6	0	3.311780	-0.387354	-0.150377
18	6	0	4.388512	0.505252	-0.189744
19	6	0	4.241249	1.828886	0.207218
20	6	0	3.007389	2.271869	0.678954
21	6	0	1.919941	1.407167	0.725481
22	1	0	-8.419151	-3.401060	0.381964
23	1	0	-8.827510	-1.096153	-0.450123
24	1	0	-6.894761	0.440273	-0.814632
25	1	0	-6.134439	-4.185082	0.848119
26	1	0	-0.806562	-2.629791	0.780035
27	1	0	-0.243223	1.418301	-0.640909
28	1	0	-2.674971	1.651500	-0.934654
29	1	0	1.287455	-1.792155	0.364937
30	6	0	3.514071	-1.820830	-0.507462
31	1	0	5.348573	0.141922	-0.529629
32	1	0	2.891915	3.289735	1.032074
33	1	0	0.984662	1.747603	1.148946
34	8	0	2.694820	-2.702980	-0.287819
35	8	0	4.692540	-2.056701	-1.073067
36	6	0	4.993785	-3.433111	-1.413379
37	1	0	5.088079	2.502677	0.171442
38	1	0	4.259480	-3.810303	-2.124385
39	1	0	4.988561	-4.048606	-0.514326
40	1	0	5.984600	-3.402815	-1.857781

12A: E = -1508.0227938 a.u., ω1=15.8 cm^{-1}

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	-6.484988	0.504154	-0.117987
2	6	0	-6.319132	-0.040377	1.169348
3	6	0	-5.068799	-0.425285	1.594859
4	6	0	-3.937430	-0.279883	0.750454
5	6	0	-4.128288	0.274817	-0.548402
6	6	0	-5.404971	0.662148	-0.971368
7	16	0	-2.798419	0.494793	-1.653657
8	6	0	-1.432017	-0.099524	-0.758629
9	6	0	-1.611100	-0.614777	0.589974
10	7	0	-2.743199	-0.687168	1.250904
11	6	0	-0.189919	-0.071099	-1.351944
12	6	0	0.957497	-0.546105	-0.666474
13	6	0	0.793028	-1.055622	0.675119
14	6	0	-0.426877	-1.087257	1.260981
15	7	0	2.167356	-0.537163	-1.263675
16	6	0	2.359699	0.081575	-2.562229
17	6	0	2.376535	-0.718060	-3.704297
18	6	0	2.599829	-0.126519	-4.946398
19	6	0	2.805819	1.249448	-5.038933
20	6	0	2.789518	2.038719	-3.889756
21	6	0	2.566674	1.458575	-2.641799
22	1	0	-7.470726	0.806438	-0.451265
23	1	0	-7.176724	-0.154556	1.820447
24	1	0	-4.901925	-0.848640	2.577416
25	1	0	-5.547169	1.083595	-1.959841
26	1	0	-0.078308	0.315953	-2.355486
27	1	0	1.650622	-1.402914	1.231644
28	1	0	-0.559382	-1.462067	2.268234
29	1	0	2.613870	-0.741109	-5.838575
30	1	0	2.955279	3.107153	-3.960901
31	1	0	2.562607	2.054921	-1.737310
32	1	0	2.982711	1.705381	-6.005840
33	1	0	2.215553	-1.786981	-3.621330
34	6	0	3.383080	-0.997641	-0.594580
35	1	0	3.216696	-1.941411	-0.072002
36	1	0	4.135277	-1.193736	-1.358030
37	6	0	3.944737	0.039808	0.389926
38	8	0	3.402017	1.082211	0.656887
39	8	0	5.095279	-0.398592	0.888729
40	6	0	5.786735	0.470787	1.847804
41	1	0	5.115794	0.635868	2.692512
42	1	0	5.966283	1.429226	1.358361
43	6	0	7.067742	-0.223017	2.251458
44	1	0	7.604747	0.403310	2.968036

45	1	0	6.864553	-1.185296	2.725572
46	1	0	7.716615	-0.386766	1.388934

12B: E = -1508.0226831 a.u., ω1=16.2 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.235759	1.285540	-0.673412
2	6	0	-6.434473	-0.084350	-0.418645
3	6	0	-5.356826	-0.894192	-0.143211
4	6	0	-4.040488	-0.365196	-0.110351
5	6	0	-3.863346	1.024659	-0.368676
6	6	0	-4.965899	1.839269	-0.650317
7	16	0	-2.284342	1.762933	-0.345202
8	6	0	-1.226877	0.439742	0.039146
9	6	0	-1.769676	-0.896297	0.231333
10	7	0	-3.035951	-1.236366	0.163094
11	6	0	0.126541	0.682042	0.139644
12	6	0	1.034504	-0.367930	0.428086
13	6	0	0.506913	-1.700060	0.617221
14	6	0	-0.821356	-1.940623	0.526755
15	7	0	2.360342	-0.150764	0.552677
16	6	0	3.302642	-1.248949	0.668702
17	6	0	3.847018	-1.554635	1.915539
18	6	0	4.778008	-2.586444	2.017512
19	6	0	5.158739	-3.300039	0.881521
20	6	0	4.611580	-2.982351	-0.360627
21	6	0	3.680485	-1.951236	-0.475342
22	1	0	-7.085870	1.921112	-0.891295
23	1	0	-7.435366	-0.496799	-0.441773
24	1	0	-5.469962	-1.952632	0.055330
25	1	0	-4.827224	2.896001	-0.847810
26	1	0	0.491393	1.683237	-0.038947
27	1	0	1.191292	-2.504762	0.844317
28	1	0	-1.226674	-2.933483	0.677058
29	1	0	5.201820	-2.832878	2.983672
30	1	0	4.911681	-3.532511	-1.244507
31	1	0	3.258626	-1.680418	-1.435634
32	1	0	5.883453	-4.101204	0.964556
33	1	0	3.540592	-0.998116	2.794127
34	6	0	2.950291	1.178715	0.419538
35	1	0	2.354151	1.927854	0.945086
36	1	0	3.929390	1.166435	0.897499
37	6	0	3.129072	1.603568	-1.046514

38	8	0	2.731551	0.968032	-1.989872
39	8	0	3.774268	2.764584	-1.096043
40	6	0	4.053267	3.322349	-2.424131
41	1	0	3.099790	3.457781	-2.937516
42	1	0	4.639937	2.587021	-2.976890
43	6	0	4.795188	4.624521	-2.225440
44	1	0	5.016678	5.064191	-3.201020
45	1	0	4.195728	5.339003	-1.657750
46	1	0	5.739524	4.464805	-1.701570

13A: E = -1405.9881632 a.u., ω1=20.0 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.167848	0.171851	0.174868
2	6	0	-6.871248	1.487810	-0.231679
3	6	0	-5.564219	1.869963	-0.419282
4	6	0	-4.502008	0.949847	-0.209949
5	6	0	-4.827118	-0.379012	0.199648
6	6	0	-6.161304	-0.755303	0.390566
7	16	0	-3.591816	-1.573724	0.475446
8	6	0	-2.122156	-0.719917	0.134252
9	6	0	-2.161773	0.677503	-0.260380
10	7	0	-3.245305	1.409421	-0.410504
11	6	0	-0.921281	-1.396297	0.257514
12	6	0	0.294230	-0.732190	0.003146
13	6	0	0.275348	0.658111	-0.369800
14	6	0	-0.896221	1.324304	-0.498487
15	7	0	1.500771	-1.334952	0.113069
16	6	0	1.787727	-2.707047	0.364886
17	6	0	2.746509	-3.019822	1.333515
18	6	0	3.080069	-4.346736	1.574159
19	6	0	2.440976	-5.339978	0.841971
20	6	0	1.496991	-5.047563	-0.135228
21	6	0	1.174617	-3.719007	-0.381761
22	1	0	-8.199509	-0.124788	0.322648
23	1	0	-7.675466	2.194501	-0.393538
24	1	0	-5.297000	2.872460	-0.729179
25	1	0	-6.405508	-1.763947	0.703344
26	1	0	-0.912491	-2.430525	0.574465
27	1	0	1.216331	1.163427	-0.557812
28	1	0	-0.929253	2.367543	-0.786492
29	1	0	2.307937	-0.727030	0.054604
30	1	0	1.044844	-5.851832	-0.699512

31	1	0	0.477263	-3.471625	-1.172170
32	7	0	2.783943	-6.761700	1.104790
33	1	0	3.220408	-2.230632	1.905694
34	8	0	2.165573	-7.608488	0.478091
35	8	0	3.655926	-6.981371	1.930346
36	1	0	3.814908	-4.618114	2.319855

13B: E = -1405.987215 a.u., ω1=19.8 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.724859	-2.683241	0.200706
2	6	0	-7.953766	-1.338042	-0.149349
3	6	0	-6.890739	-0.482728	-0.317225
4	6	0	-5.556780	-0.939712	-0.142251
5	6	0	-5.349401	-2.307743	0.211395
6	6	0	-6.439481	-3.168310	0.380443
7	16	0	-3.750740	-2.957311	0.442978
8	6	0	-2.718619	-1.594809	0.146963
9	6	0	-3.288588	-0.303504	-0.198059
10	7	0	-4.570174	-0.031849	-0.324902
11	6	0	-1.351340	-1.755914	0.252099
12	6	0	-0.477621	-0.669177	0.031978
13	6	0	-1.022536	0.610746	-0.330447
14	6	0	-2.364459	0.774489	-0.438676
15	7	0	0.856782	-0.871219	0.134968
16	6	0	1.907869	0.089382	0.104912
17	6	0	3.040163	-0.190604	-0.666946
18	6	0	4.103826	0.702197	-0.684360
19	6	0	4.011899	1.866775	0.068570
20	6	0	2.900772	2.155774	0.851498
21	6	0	1.844339	1.253822	0.877760
22	1	0	-8.565463	-3.354255	0.332263
23	1	0	-8.967538	-0.982587	-0.284553
24	1	0	-7.026360	0.557593	-0.585159
25	1	0	-6.280164	-4.206190	0.649205
26	1	0	-0.936862	-2.722177	0.520003
27	1	0	-0.353873	1.432406	-0.544905
28	1	0	-2.795387	1.725057	-0.727610
29	1	0	1.157074	-1.833339	0.230129
30	1	0	2.882736	3.062272	1.441160
31	1	0	0.993134	1.440901	1.520169
32	7	0	5.143451	2.829633	0.044916
33	1	0	3.083958	-1.095552	-1.261937

34	8	0	5.013332	3.857944	0.690906
35	8	0	6.120680	2.524588	-0.620310
36	1	0	4.989733	0.513683	-1.275334

14A: E = -1409.5088322 a.u., ω1=17.1 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.649332	0.123599	0.141191
2	6	0	-7.367306	1.442493	-0.260976
3	6	0	-6.062576	1.842008	-0.437459
4	6	0	-4.990606	0.937459	-0.221640
5	6	0	-5.300068	-0.393759	0.182734
6	6	0	-6.629964	-0.788742	0.363146
7	16	0	-4.049156	-1.575304	0.467172
8	6	0	-2.586474	-0.698731	0.137585
9	6	0	-2.645505	0.700705	-0.255352
10	7	0	-3.735645	1.417227	-0.411862
11	6	0	-1.378816	-1.355554	0.268627
12	6	0	-0.167767	-0.672647	0.025874
13	6	0	-0.205818	0.719649	-0.341643
14	6	0	-1.385767	1.367290	-0.478895
15	7	0	1.041432	-1.259802	0.137800
16	6	0	1.349364	-2.631223	0.362888
17	6	0	2.320106	-2.960058	1.311761
18	6	0	2.677094	-4.282743	1.532359
19	6	0	2.083427	-5.315603	0.787383
20	6	0	1.110787	-4.969429	-0.170687
21	6	0	0.749505	-3.650427	-0.385184
22	1	0	-8.677615	-0.188164	0.280854
23	1	0	-8.178842	2.139453	-0.428580
24	1	0	-5.806944	2.848674	-0.743693
25	1	0	-6.861481	-1.801335	0.672972
26	1	0	-1.353843	-2.390163	0.583640
27	1	0	0.729108	1.240248	-0.518630
28	1	0	-1.432865	2.411258	-0.762200
29	1	0	1.839609	-0.640420	0.072683
30	1	0	0.659738	-5.748598	-0.774813
31	1	0	0.035070	-3.412484	-1.163842
32	7	0	2.365437	-6.669246	0.965843
33	1	0	2.779469	-2.179791	1.908638
34	1	0	3.393441	-4.504291	2.308604
35	6	0	3.489876	-7.377127	1.418828
36	8	0	3.408679	-8.584642	1.478582
37	6	0	4.752141	-6.629932	1.777006

38	1	0	1.657310	-7.314448	0.635842
39	1	0	4.694776	-6.260331	2.804928
40	1	0	4.948731	-5.787514	1.112181
41	1	0	5.574209	-7.341409	1.724442

14B: E = -1409.5080404 a.u., ω1=16.8 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.799330	-2.619278	0.209148
2	6	0	-8.002401	-1.276577	-0.159932
3	6	0	-6.922081	-0.442770	-0.336012
4	6	0	-5.598405	-0.919737	-0.150432
5	6	0	-5.416848	-2.283461	0.222344
6	6	0	-6.521938	-3.122480	0.399618
7	16	0	-3.828229	-2.960472	0.470087
8	6	0	-2.770131	-1.618290	0.155498
9	6	0	-3.319265	-0.321304	-0.209759
10	7	0	-4.593197	-0.028648	-0.343728
11	6	0	-1.408448	-1.800202	0.264488
12	6	0	-0.512444	-0.730658	0.030222
13	6	0	-1.035998	0.552783	-0.354321
14	6	0	-2.373955	0.736627	-0.467378
15	7	0	0.814081	-0.948490	0.145304
16	6	0	1.875848	-0.000041	0.127864
17	6	0	3.017638	-0.275250	-0.628042
18	6	0	4.089093	0.606269	-0.640534
19	6	0	4.052936	1.784623	0.124486
20	6	0	2.897281	2.047199	0.885838
21	6	0	1.826902	1.169616	0.894404
22	1	0	-8.651452	-3.274163	0.347376
23	1	0	-9.008761	-0.903828	-0.303855
24	1	0	-7.038770	0.595867	-0.619063
25	1	0	-6.380440	-4.158998	0.683393
26	1	0	-1.010030	-2.768950	0.547929
27	1	0	-0.350726	1.357285	-0.581600
28	1	0	-2.788990	1.688371	-0.775085
29	1	0	1.096979	-1.912859	0.269702
30	1	0	2.858069	2.938105	1.502392
31	1	0	0.972628	1.375365	1.528025
32	7	0	5.073719	2.733415	0.148200
33	1	0	3.059198	-1.169670	-1.239870
34	1	0	4.934164	0.386149	-1.274361
35	6	0	6.459877	2.679309	-0.068121

36	8	0	7.082962	3.715329	0.012864
37	6	0	7.123642	1.354171	-0.357178
38	1	0	4.805977	3.660399	0.457738
39	1	0	7.034919	1.110014	-1.419715
40	1	0	6.703220	0.534051	0.226821
41	1	0	8.181707	1.466179	-0.127756

15A: E = -1825.3175971 a.u., ω1=1.1 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	7.651961	-0.422330	0.198996
2	6	0	7.476098	0.817809	0.843475
3	6	0	6.213468	1.341474	0.990877
4	6	0	5.077090	0.644147	0.500895
5	6	0	5.279534	-0.611215	-0.147362
6	6	0	6.569663	-1.133211	-0.293573
7	16	0	3.945511	-1.536453	-0.776140
8	6	0	2.563679	-0.560724	-0.396594
9	6	0	2.730974	0.710921	0.287977
10	7	0	3.871489	1.232632	0.683821
11	6	0	1.311429	-1.014232	-0.767695
12	6	0	0.167296	-0.239503	-0.489758
13	6	0	0.313626	1.027653	0.179085
14	6	0	1.536032	1.474404	0.549971
15	7	0	-1.074509	-0.633892	-0.839275
16	6	0	-1.436695	-1.873394	-1.462769
17	6	0	-1.958353	-1.851228	-2.754286
18	6	0	-2.335151	-3.057073	-3.336574
19	6	0	-2.193157	-4.271273	-2.672028
20	6	0	-1.671909	-4.273175	-1.379314
21	6	0	-1.300770	-3.078179	-0.768438
22	1	0	8.648838	-0.831203	0.084010
23	1	0	8.337518	1.355229	1.219651
24	1	0	6.038706	2.292273	1.478598
25	1	0	6.720987	-2.085962	-0.787717
26	1	0	1.204023	-1.955577	-1.290903
27	1	0	-0.573088	1.616848	0.385508
28	1	0	1.666529	2.422317	1.056769
29	1	0	-1.823987	0.030108	-0.690692
30	16	0	-2.993134	-3.025807	-5.012490
31	1	0	-1.564073	-5.208002	-0.843036
32	1	0	-0.919672	-3.076486	0.246055
33	1	0	-2.473943	-5.195448	-3.161625

34	1	0	-2.050868	-0.924630	-3.307678
35	8	0	-2.544551	-1.796540	-5.629486
36	8	0	-2.796490	-4.332148	-5.618345
37	8	0	-4.595910	-2.854164	-4.711397
38	1	0	-5.065477	-3.638716	-5.036563

15B: E = -1825.3168073 a.u., ω1=9.8 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.667316	-2.629379	0.047766
2	6	0	-7.829271	-1.353240	-0.525874
3	6	0	-6.736830	-0.537471	-0.702793
4	6	0	-5.439875	-0.966455	-0.313213
5	6	0	-5.300044	-2.263679	0.265675
6	6	0	-6.419254	-3.084723	0.441381
7	16	0	-3.749584	-2.874441	0.771683
8	6	0	-2.662736	-1.578900	0.382564
9	6	0	-3.166360	-0.353981	-0.217851
10	7	0	-4.420373	-0.100476	-0.523010
11	6	0	-1.318605	-1.728942	0.655745
12	6	0	-0.402716	-0.695437	0.357930
13	6	0	-0.880458	0.518570	-0.247409
14	6	0	-2.199791	0.671286	-0.518710
15	7	0	0.908236	-0.877594	0.624406
16	6	0	1.966859	0.075541	0.481152
17	6	0	3.046141	-0.243842	-0.340925
18	6	0	4.088995	0.669256	-0.449552
19	6	0	4.074895	1.887201	0.223415
20	6	0	2.989982	2.187266	1.044968
21	6	0	1.941456	1.282162	1.185865
22	1	0	-8.530460	-3.269890	0.185280
23	1	0	-8.814689	-1.019379	-0.825578
24	1	0	-6.821141	0.449551	-1.139965
25	1	0	-6.310941	-4.069490	0.881065
26	1	0	-0.953251	-2.644874	1.108158
27	1	0	-0.174304	1.295299	-0.506188
28	1	0	-2.579761	1.569866	-0.988727
29	1	0	1.186783	-1.801857	0.929730
30	16	0	5.472404	0.259825	-1.527264
31	1	0	2.966627	3.125139	1.586159
32	1	0	1.114753	1.503791	1.850387
33	1	0	4.890242	2.588451	0.097199
34	1	0	3.069315	-1.167068	-0.907175

35	8	0	5.009934	-0.741420	-2.463577
36	8	0	6.124410	1.490433	-1.942205
37	8	0	6.471402	-0.498086	-0.469496
38	1	0	7.292328	0.012987	-0.388018

16A: E = -1201.4362853 a.u., ω1=26.7 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.404214	-1.621204	-0.141055
2	6	0	5.822960	-0.283365	-0.011655
3	6	0	4.888824	0.722950	0.071236
4	6	0	3.500559	0.429841	0.029641
5	6	0	3.099617	-0.932138	-0.100408
6	6	0	4.058346	-1.947755	-0.186172
7	16	0	1.418168	-1.386496	-0.159946
8	6	0	0.586486	0.131529	-0.029097
9	6	0	1.340280	1.370876	0.085042
10	7	0	2.649059	1.482396	0.110437
11	6	0	-0.794153	0.131791	-0.046033
12	6	0	-1.505311	1.347832	0.042657
13	6	0	-0.775328	2.586855	0.141159
14	6	0	0.577140	2.592697	0.164805
15	7	0	-2.850682	1.408916	0.024428
16	6	0	-3.783923	0.324444	0.025040
17	6	0	-4.787676	0.303447	-0.945711
18	6	0	-5.732365	-0.718812	-0.932564
19	6	0	-5.674168	-1.715393	0.040817
20	6	0	-4.674734	-1.682921	1.012628
21	6	0	-3.730320	-0.660124	1.015091
22	1	0	6.142374	-2.411702	-0.207061
23	1	0	6.880027	-0.051057	0.021028
24	1	0	5.172606	1.763277	0.169519
25	1	0	3.750394	-2.982146	-0.286790
26	1	0	-1.339233	-0.796984	-0.149947
27	1	0	-1.329835	3.516752	0.205498
28	1	0	1.141807	3.513080	0.245166
29	1	0	-3.255454	2.335301	-0.028110
30	1	0	-6.510551	-0.737387	-1.685921
31	1	0	-4.640894	-2.443389	1.783572
32	1	0	-2.980270	-0.609046	1.795371
33	1	0	-6.411274	-2.509177	0.048102
34	1	0	-4.821726	1.073928	-1.707874

16B: E = -1201.4354139 a.u., ω1=25.8 cm^{-1}

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-7.617478	-2.676487	0.165200
2	6	0	-7.835807	-1.335255	-0.202009
3	6	0	-6.765850	-0.486256	-0.365611
4	6	0	-5.437340	-0.945965	-0.168758
5	6	0	-5.240218	-2.308458	0.202173
6	6	0	-6.335588	-3.163105	0.366527
7	16	0	-3.645684	-2.962998	0.464022
8	6	0	-2.603373	-1.606302	0.165167
9	6	0	-3.166509	-0.315790	-0.203283
10	7	0	-4.442991	-0.041323	-0.349358
11	6	0	-1.240515	-1.770015	0.287905
12	6	0	-0.357462	-0.687294	0.063648
13	6	0	-0.895346	0.591917	-0.318861
14	6	0	-2.234126	0.757377	-0.444821
15	7	0	0.969455	-0.883813	0.186040
16	6	0	2.015651	0.091637	0.131807
17	6	0	3.100225	-0.137032	-0.717669
18	6	0	4.147474	0.779000	-0.752504
19	6	0	4.111173	1.917152	0.052347
20	6	0	3.029780	2.133949	0.905209
21	6	0	1.982021	1.218677	0.956915
22	1	0	-8.461919	-3.343290	0.293372
23	1	0	-8.845924	-0.976202	-0.354119
24	1	0	-6.893946	0.551586	-0.646625
25	1	0	-6.182876	-4.198424	0.648792
26	1	0	-0.830797	-2.734181	0.570547
27	1	0	-0.218307	1.408353	-0.527726
28	1	0	-2.659911	1.705973	-0.747561
29	1	0	1.272301	-1.839626	0.327815
30	1	0	4.988186	0.605488	-1.413223
31	1	0	3.008999	3.006607	1.546865
32	1	0	1.162084	1.362623	1.650492
33	1	0	4.927723	2.628332	0.021814
34	1	0	3.116895	-1.015854	-1.352529