Supplementary Data

Theoretical and experimental study of new photochromic bis-spiropyrans with hydroxyethyl and carboxyethyl substituents

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Geometries of the compounds (2a,b) calculated by the CPCM-PBE0/6-311G method**

Table 1 - Optimized structure (Cartesian coordinates, Å) of (2a) –TTC-Sp

Атом	X	Y	Z	Атом	X	Y	Z
1 C	5.518462	-3.859415	-0.296475	49 C	-4.678958	-1.817690	0.216744
2 C	6.531226	-2.917638	-0.150480	50 H	-5.153344	1.173923	-0.709707
3 C	6.244773	-1.556629	-0.063727	51 H	-4.471792	3.553582	-0.551582
4 C	4.910888	-1.182104	-0.131378	52 O	-3.112729	-0.148953	0.888779
5 C	3.886746	-2.111334	-0.276996	53 N	-3.313076	-0.689220	-1.407114
6 C	4.183163	-3.458109	-0.361711	54 C	-4.448247	-1.184766	2.539351
7 C	2.561157	-1.387305	-0.327757	55 C	-5.657196	-2.746441	0.567300
8 C	3.001774	0.071451	-0.165639	56 C	-5.422029	-2.114188	2.872406
9 N	4.358280	0.104912	-0.078311	57 C	-6.035580	-2.893604	1.890786
10 C	1.661177	-1.848427	0.829303	58 O	-4.581812	-2.464568	-2.058049
11 C	1.891487	-1.628594	-1.691273	59 H	-3.966126	-0.567385	3.288741
12 C	5.181921	1.297077	0.031015	60 H	-5.712083	-2.227874	3.912015
13 C	2.225400	1.216023	-0.115914	61 H	-6.798416	-3.613635	2.164725
14 O	1.656371	3.995066	0.033142	62 H	-6.093400	-3.346610	-0.223641
15 C	0.836573	1.216222	-0.255111	63 C	-2.915693	-0.402134	-2.775215
16 C	-0.017113	2.316835	-0.238537	64 H	-3.328587	0.557032	-3.105010
17 C	0.458097	3.707833	-0.066685	65 H	-1.829098	-0.365268	-2.859480
18 C	-0.568329	4.734456	-0.013892	66 H	-3.311507	-1.200755	-3.399097
19 C	-1.884625	4.438843	-0.131516				
20 C	-2.353256	3.101764	-0.317570				
21 C	-1.421040	2.093225	-0.375972				
22 H	5.768088	-4.912821	-0.359290				
23 H	7.564604	-3.243679	-0.099946				
24 H	7.042323	-0.832288	0.054466				
25 H	3.395321	-4.196283	-0.477690				
26 H	2.139143	-1.663798	1.794618				
27 H	0.694214	-1.342424	0.823302				
28 H	1.481142	-2.923327	0.741686				
29 H	1.719488	-2.699931	-1.825782				
30 H	0.929818	-1.118388	-1.765836				
31 H	2.530051	-1.281031	-2.506831				
32 H	4.643447	2.134655	-0.414965				
33 H	6.085743	1.132722	-0.564401				
34 H	2.695750	2.175479	0.055565				
35 H	0.335663	0.264682	-0.384337				
36 H	-2.626789	5.232560	-0.090764				
37 H	-0.221472	5.752847	0.121555				
38 C	-3.737766	2.754544	-0.488636				
39 C	5.561977	1.625762	1.469991				
40 H	6.251785	2.473927	1.449472				
41 H	6.095442	0.774934	1.917707				
42 O	4.465902	2.020258	2.255954				
43 H	3.885181	1.265198	2.378136				
44 C	-4.120329	1.473516	-0.575979				
45 C	-3.112936	0.377731	-0.439588				
46 O	-1.796609	0.807532	-0.626933				
47 C	-4.085821	-1.037585	1.204955				
48 C	-4.214234	-1.702749	-1.179933				

Table 2 - Optimized structure (Cartesian coordinates, Å) of (2a) –TTC-Sp-ox

Атом	X	Y	Z	Атом	X	Y	Z
1 C	-7.077267	-2.165374	0.576332	49 C	4.668980	-1.961314	0.159842
2 C	-7.047412	-2.139212	-0.813346	50 H	5.132998	1.044824	0.911356
3 C	-6.020984	-1.491365	-1.499217	51 H	4.587740	3.420476	0.455297
4 C	-5.022300	-0.874395	-0.757720	52 O	3.222510	-0.324296	-0.800019
5 C	-5.044710	-0.894531	0.637286	53 N	3.163163	-0.694301	1.537340
6 C	-6.070121	-1.534541	1.308839	54 C	4.697192	-1.509486	-2.215891
7 C	-3.878541	-0.091835	1.167878	55 C	5.656051	-2.929862	-0.012989
8 C	-2.984422	-0.024358	-0.111755	56 C	5.678409	-2.477249	-2.371563
9 N	-3.919397	-0.141074	-1.237668	57 C	6.167356	-3.186216	-1.273677
10 C	-3.151801	-0.736514	2.340943	58 O	4.310390	-2.435870	2.451181
11 C	-4.379144	1.303324	1.566599	59 H	4.309957	-0.946783	-3.057659
12 C	-3.119003	-0.734105	-2.300974	60 H	6.072068	-2.677477	-3.362894
13 C	-2.143015	1.215062	-0.239163	61 H	6.936794	-3.937854	-1.409289
14 O	-1.457066	3.890211	-0.904557	62 H	5.991638	-3.473781	0.863129
15 C	-0.809463	1.186518	-0.132121	63 C	2.594337	-0.318005	2.820576
16 C	0.142676	2.290238	-0.220518	64 H	2.978621	0.654515	3.146336
17 C	-0.171596	3.610081	-0.603539	65 H	1.507415	-0.266996	2.754786
18 C	0.807555	4.601509	-0.678855	66 H	2.890765	-1.080954	3.537302
19 C	2.120967	4.309455	-0.369520				
20 C	2.487766	3.020077	0.013312				
21 C	1.492667	2.040804	0.075300				
22 H	-7.883617	-2.676674	1.091313				
23 H	-7.833787	-2.630764	-1.377489				
24 H	-6.010942	-1.470804	-2.584222				
25 H	-6.090040	-1.555707	2.394778				
26 H	-2.811086	-1.740459	2.088881				
27 H	-2.282910	-0.136892	2.630288				
28 H	-3.819049	-0.794596	3.206360				
29 H	-5.104286	1.210044	2.379795				
30 H	-3.553902	1.932326	1.913276				
31 H	-4.874202	1.806117	0.731246				
32 H	-2.593761	0.057206	-2.841037				
33 H	-3.744975	-1.280042	-3.007203				
34 H	-2.683334	2.134200	-0.418896				
35 H	-0.358136	0.217092	0.052059				
36 H	2.878631	5.084918	-0.420581				
37 H	0.522280	5.606176	-0.978742				
38 C	3.832042	2.643343	0.382223				
39 C	-2.134554	-1.641275	-1.538854				
40 H	-1.114875	-1.557369	-1.928933				
41 H	-2.440368	-2.691516	-1.565259				
42 O	-2.183120	-1.203427	-0.186038				
43 H	-1.526804	4.809220	-1.183939				
44 C	4.136332	1.367428	0.632051				
45 C	3.098904	0.295980	0.477516				
46 O	1.792710	0.782032	0.503036				
47 C	4.201585	-1.252288	-0.942722				
48 C	4.059419	-1.735233	1.485964				

Table 3 - Optimized structure (Cartesian coordinates, Å) of (2a) –TTC-TTC

Атом	X	Y	Z	Атом	X	Y	Z
1 C	7.595105	-3.271677	-0.109876	49 C	7.448192	-1.041912	0.076541
2 C	8.385058	-2.131870	-0.208265	50 H	2.634565	-0.813114	0.110010
3 C	7.816265	-0.860089	-0.257402	51 H	3.795796	2.024177	-0.133316
4 C	6.432040	-0.777273	-0.207622	52 O	5.657369	0.536303	-0.032395
5 C	5.628493	-1.908712	-0.107305	53 N	5.140075	-1.736109	0.166158
6 C	6.203897	-3.163307	-0.058888	54 C	7.866997	1.334534	-0.132149
7 C	4.176284	-1.488848	-0.080730	55 C	8.821535	-1.287514	0.077444
8 C	4.295074	0.037883	-0.161645	56 C	9.227884	1.073407	-0.129398
9 N	5.620158	0.361033	-0.251408	57 C	9.710218	-0.233208	-0.025082
10 C	3.520039	-1.944778	1.231349	58 O	6.793965	-3.302786	0.280482
11 C	3.443822	-2.067746	-1.302273	59 H	7.475596	2.341946	-0.212524
12 C	6.163518	1.697797	-0.410357	60 H	9.924793	1.900824	-0.210003
13 C	3.296645	0.986482	-0.161214	61 H	10.778119	-0.418610	-0.024661
14 O	2.061779	3.563741	-0.388686	62 H	9.156879	-2.315100	0.159817
15 C	1.927205	0.675377	-0.128199	63 C	4.124558	-2.777925	0.270064
16 C	0.844030	1.528437	-0.180430	64 H	3.508354	-2.615217	1.156509
17 C	0.974959	2.986521	-0.317193	65 H	3.490911	-2.775942	-0.619052
18 C	-0.266246	3.754815	-0.371746	66 H	4.648104	-3.726655	0.350435
19 C	-1.476081	3.166384	-0.305669				
20 C	-1.673046	1.744477	-0.178572				
21 C	-0.477955	0.873239	-0.113218				
22 H	8.062019	-4.249678	-0.071267				
23 H	9.465064	-2.228193	-0.244822				
24 H	8.443703	0.020950	-0.328012				
25 H	5.588572	-4.054971	0.015978				
26 H	4.041727	-1.525286	2.095322				
27 H	2.471076	-1.648892	1.285045				
28 H	3.569956	-3.034972	1.303240				
29 H	3.509185	-3.159286	-1.280185				
30 H	2.388605	-1.789692	-1.310165				
31 H	3.899849	-1.718680	-2.231835				
32 H	5.421871	2.317229	-0.918310				
33 H	7.036033	1.627083	-1.067856				
34 H	3.558876	2.036300	-0.182428				
35 H	1.629103	-0.366001	-0.055351				
36 H	-2.372054	3.782537	-0.350429				
37 H	-0.157796	4.829650	-0.469715				
38 C	-2.960952	1.269709	-0.126513				
39 C	6.566588	2.339490	0.911311				
40 H	7.063118	3.288556	0.690640				
41 H	7.294665	1.695817	1.426560				
42 O	5.472339	2.646371	1.739191				
43 H	5.030814	1.828387	1.981504				
44 C	-3.390687	-0.073796	-0.009941				
45 C	-4.711941	-0.415389	0.029541				
46 O	-0.578432	-0.352182	-0.006209				
47 C	-6.963539	0.324928	-0.011658				
48 C	-6.500554	-2.087608	0.179846				

Table 4 - Optimized structure (Cartesian coordinates, Å) of (2a) –TTC-TTC-ox

Атом	X	Y	Z	Атом	X	Y	Z
1 C	-7.077267	-2.165374	0.576332	49 C	4.668980	-1.961314	0.159842
2 C	-7.047412	-2.139212	-0.813346	50 H	5.132998	1.044824	0.911356
3 C	-6.020984	-1.491365	-1.499217	51 H	4.587740	3.420476	0.455297
4 C	-5.022300	-0.874395	-0.757720	52 O	3.222510	-0.324296	-0.800019
5 C	-5.044710	-0.894531	0.637286	53 N	3.163163	-0.694301	1.537340
6 C	-6.070121	-1.534541	1.308839	54 C	4.697192	-1.509486	-2.215891
7 C	-3.878541	-0.091835	1.167878	55 C	5.656051	-2.929862	-0.012989
8 C	-2.984422	-0.024358	-0.111755	56 C	5.678409	-2.477249	-2.371563
9 N	-3.919397	-0.141074	-1.237668	57 C	6.167356	-3.186216	-1.273677
10 C	-3.151801	-0.736514	2.340943	58 O	4.310390	-2.435870	2.451181
11 C	-4.379144	1.303324	1.566599	59 H	4.309957	-0.946783	-3.057659
12 C	-3.119003	-0.734105	-2.300974	60 H	6.072068	-2.677477	-3.362894
13 C	-2.143015	1.215062	-0.239163	61 H	6.936794	-3.937854	-1.409289
14 O	-1.457066	3.890211	-0.904557	62 H	5.991638	-3.473781	0.863129
15 C	-0.809463	1.186518	-0.132121	63 C	2.594337	-0.318005	2.820576
16 C	0.142676	2.290238	-0.220518	64 H	2.978621	0.654515	3.146336
17 C	-0.171596	3.610081	-0.603539	65 H	1.507415	-0.266996	2.754786
18 C	0.807555	4.601509	-0.678855	66 H	2.890765	-1.080954	3.537302
19 C	2.120967	4.309455	-0.369520				
20 C	2.487766	3.020077	0.013312				
21 C	1.492667	2.040804	0.075300				
22 H	-7.883617	-2.676674	1.091313				
23 H	-7.833787	-2.630764	-1.377489				
24 H	-6.010942	-1.470804	-2.584222				
25 H	-6.090040	-1.555707	2.394778				
26 H	-2.811086	-1.740459	2.088881				
27 H	-2.282910	-0.136892	2.630288				
28 H	-3.819049	-0.794596	3.206360				
29 H	-5.104286	1.210044	2.379795				
30 H	-3.553902	1.932326	1.913276				
31 H	-4.874202	1.806117	0.731246				
32 H	-2.593761	0.057206	-2.841037				
33 H	-3.744975	-1.280042	-3.007203				
34 H	-2.683334	2.134200	-0.418896				
35 H	-0.358136	0.217092	0.052059				
36 H	2.878631	5.084918	-0.420581				
37 H	0.522280	5.606176	-0.978742				
38 C	3.832042	2.643343	0.382223				
39 C	-2.134554	-1.641275	-1.538854				
40 H	-1.114875	-1.557369	-1.928933				
41 H	-2.440368	-2.691516	-1.565259				
42 O	-2.183120	-1.203427	-0.186038				
43 H	-1.526804	4.809220	-1.183939				
44 C	4.136332	1.367428	0.632051				
45 C	3.098904	0.295980	0.477516				
46 O	1.792710	0.782032	0.503036				
47 C	4.201585	-1.252288	-0.942722				
48 C	4.059419	-1.735233	1.485964				

Table 5 - Optimized structure (Cartesian coordinates, Å) of (2b)

Атом	X	Y	Z	Атом	X	Y	Z
1 C	6.640008	-2.781086	0.521440	49 H	-2.996278	1.206715	3.565697
2 C	7.186364	-1.620772	-0.009827	50 O	-3.857263	-0.913402	0.021140
3 C	6.378271	-0.616508	-0.548688	51 N	-4.294404	1.296716	-0.706024
4 C	5.003401	-0.814599	-0.536559	52 C	-5.563828	-2.541268	0.165176
5 C	4.446448	-1.990904	-0.029809	53 C	-7.408615	-0.681314	-0.799309
6 C	5.254322	-2.973438	0.502994	54 C	-6.892566	-2.893839	-0.019764
7 C	2.961117	-1.978253	-0.307070	55 C	-7.821349	-1.967184	-0.495187
8 C	2.716003	-0.447885	-0.585922	56 O	-6.318012	1.829852	-1.601997
9 N	3.997805	0.019180	-1.011548	57 H	-4.831168	-3.248232	0.538174
10 C	2.106079	-2.543451	0.818972	58 H	-7.209540	-3.904757	0.215755
11 C	2.713480	-2.783196	-1.593180	59 H	-8.857837	-2.255077	-0.630394
12 C	4.267875	1.308491	-1.602265	60 H	-8.095862	0.060929	-1.190186
13 C	1.618579	-0.151498	-1.561353	61 C	-3.767841	2.630922	-0.944337
14 O	2.431566	0.239055	0.699576	62 H	-3.543040	3.133190	0.002273
15 C	0.387557	0.185486	-1.168296	63 H	-2.861225	2.583428	-1.548187
16 C	0.084158	0.353930	0.238873	64 H	-4.536254	3.190114	-1.473709
17 C	1.148767	0.371656	1.145281	65 C	3.941751	3.403880	-0.121043
18 C	0.952888	0.595775	2.502335	66 O	4.051289	4.585502	-0.327072
19 C	-0.336687	0.781324	2.970872	67 O	2.941960	2.946117	0.637753
20 C	-1.433740	0.751246	2.106539	68 H	2.956782	1.972816	0.697019
21 C	-1.201988	0.541360	0.745336				
22 H	7.287590	-3.541839	0.943750				
23 H	8.262830	-1.481585	-0.003019				
24 H	6.823553	0.282751	-0.959420				
25 H	4.824768	-3.891546	0.893674				
26 H	2.304259	-2.046829	1.769609				
27 H	1.040347	-2.456891	0.588642				
28 H	2.328369	-3.607665	0.938791				
29 H	3.019579	-3.819392	-1.428964				
30 H	1.653817	-2.777667	-1.864894				
31 H	3.293794	-2.387689	-2.431270				
32 H	3.336645	1.680203	-2.039071				
33 H	4.957419	1.156523	-2.440024				
34 H	1.856550	-0.276885	-2.611918				
35 H	-0.402817	0.341948	-1.893694				
36 H	-0.507533	0.948152	4.029931				
37 H	1.806956	0.613197	3.169617				
38 C	-2.800668	0.957099	2.526517				
39 C	4.897421	2.370438	-0.665316				
40 H	5.670421	2.919562	-1.204623				
41 H	5.381741	1.867899	0.179212				
42 C	-3.802626	0.842095	1.651209				
43 C	-3.550752	0.461932	0.223212				
44 O	-2.213003	0.571406	-0.164296				
45 C	-5.165374	-1.243333	-0.132516				
46 C	-5.605459	1.030008	-1.017218				
47 C	-6.076187	-0.311611	-0.621283				
48 H	-4.840822	0.986101	1.930504				

Table 6 - Optimized structure (Cartesian coordinates, Å) of (2b)–TTC-SP

Атом	X	Y	Z	Атом	X	Y	Z
1 C	5.102407	-4.072412	-0.682570	49 H	-4.708103	3.519531	-0.851382
2 C	6.149822	-3.158066	-0.643282	50 O	-3.321436	-0.009259	0.917495
3 C	5.910026	-1.788051	-0.554486	51 N	-3.641084	-0.820332	-1.285459
4 C	4.585648	-1.376440	-0.503278	52 C	-4.584797	-0.818175	2.743460
5 C	3.529205	-2.276661	-0.564081	53 C	-5.890138	-2.599556	1.037314
6 C	3.778227	-3.633207	-0.649253	54 C	-5.545663	-1.690234	3.233242
7 C	2.226664	-1.513847	-0.557128	55 C	-6.207251	-2.579117	2.384682
8 C	2.718402	-0.064574	-0.483311	56 O	-4.936221	-2.656708	-1.648641
9 N	4.071574	-0.072038	-0.418163	57 H	-4.066297	-0.118617	3.389619
10 C	1.400079	-1.887693	0.684868	58 H	-5.787257	-1.671940	4.291227
11 C	1.459936	-1.804906	-1.857288	59 H	-6.959493	-3.252343	2.780259
12 C	4.951110	1.082468	-0.330482	60 H	-6.367418	-3.288632	0.349184
13 C	1.966573	1.102294	-0.495839	61 C	-3.307692	-0.705577	-2.695661
14 O	1.449562	3.910323	-0.560161	62 H	-3.731734	0.210774	-3.119301
15 C	0.580165	1.122698	-0.566841	63 H	-2.226331	-0.690688	-2.834216
16 C	-0.259072	2.243527	-0.603054	64 H	-3.735002	-1.569358	-3.200187
17 C	0.240231	3.631458	-0.576682	65 C	4.821250	1.463905	2.183731
18 C	-0.768379	4.673845	-0.567452	66 O	3.646395	1.699711	2.121483
19 C	-2.095672	4.394282	-0.602231	67 O	5.441767	1.456110	3.372894
20 C	-2.588528	3.057588	-0.646055	68 H	6.383712	1.254881	3.281204
21 C	-1.667797	2.032599	-0.652081				
22 H	5.316453	-5.133584	-0.748537				
23 H	7.174495	-3.511946	-0.684154				
24 H	6.736983	-1.087425	-0.541684				
25 H	2.962539	-4.348502	-0.696400				
26 H	1.953238	-1.667626	1.601060				
27 H	0.451186	-1.349458	0.719855				
28 H	1.183242	-2.959201	0.664110				
29 H	1.241486	-2.874632	-1.914797				
30 H	0.514200	-1.263523	-1.903752				
31 H	2.056014	-1.531487	-2.731262				
32 H	4.364333	1.984388	-0.489007				
33 H	5.674403	1.014912	-1.150431				
34 H	2.460014	2.060306	-0.423541				
35 H	0.054625	0.176413	-0.583134				
36 H	-2.823040	5.202742	-0.601887				
37 H	-0.404527	5.695461	-0.538531				
38 C	-3.982699	2.718414	-0.734269				
39 C	5.701856	1.174759	0.991392				
40 H	6.439092	1.984212	0.913655				
41 H	6.277924	0.265317	1.192229				
42 C	-4.383943	1.440639	-0.684329				
43 C	-3.382931	0.353093	-0.464914				
44 O	-2.073809	0.735695	-0.766519				
45 C	-4.283781	-0.840265	1.385966				
46 C	-4.526678	-1.791633	-0.889889				
47 C	-4.925573	-1.730368	0.529639				
48 H	-5.424291	1.144912	-0.756276				

Table 7 - Optimized structure (Cartesian coordinates, Å) of (2b)–TTC-TTC

Атом		X	Y	Z	Атом		X	Y	Z
1	C	-7.153113	3.625011	-0.313172	49	H	4.017971	-1.908319	-0.542994
2	C	-7.987509	2.519239	-0.433809	50	O	5.909451	-0.573024	-0.121196
3	C	-7.470212	1.225381	-0.484063	51	N	5.505066	1.679320	0.380815
4	C	-6.091390	1.086233	-0.404281	52	C	8.072868	-1.489309	-0.190424
5	C	-5.244835	2.182924	-0.291874	53	C	9.150007	1.006396	0.471441
6	C	-5.768365	3.460324	-0.242900	54	C	9.441961	-1.320805	-0.057628
7	C	-3.812378	1.704515	-0.263452	55	C	9.985696	-0.077259	0.272837
8	C	-3.988771	0.184734	-0.388936	56	O	7.228570	3.102307	0.829008
9	N	-5.326084	-0.086217	-0.437287	57	H	7.634854	-2.447540	-0.445879
10	C	-3.158325	2.094038	1.072033	58	H	10.096540	-2.171835	-0.213840
11	C	-3.047906	2.299556	-1.457073	59	H	11.059106	0.036430	0.372725
12	C	-5.956000	-1.388792	-0.562225	60	H	9.535800	1.986354	0.728712
13	C	-3.013637	-0.786989	-0.474166	61	C	4.543177	2.756984	0.569696
14	O	-1.792603	-3.332536	-1.087688	62	H	3.970863	2.916177	-0.346792
15	C	-1.641920	-0.504081	-0.429010	63	H	3.861822	2.515547	1.388504
16	C	-0.561852	-1.357073	-0.581228	64	H	5.107923	3.652865	0.812564
17	C	-0.701293	-2.779204	-0.914887	65	C	-5.734458	-2.351018	1.772991
18	C	0.532863	-3.547169	-1.052014	66	O	-4.651786	-2.814691	1.541350
19	C	1.747418	-2.986753	-0.886777	67	O	-6.194593	-2.314515	3.031387
20	C	1.951303	-1.597946	-0.565975	68	H	-7.072718	-1.909976	3.071851
21	C	0.763010	-0.729677	-0.416467					
22	H	-7.580309	4.621207	-0.275772					
23	H	-9.061665	2.659870	-0.493621					
24	H	-8.132896	0.373704	-0.588708					
25	H	-5.118243	4.326066	-0.157313					
26	H	-3.701300	1.657918	1.914272					
27	H	-2.117936	1.768827	1.127026					
28	H	-3.181228	3.182098	1.180575					
29	H	-3.074808	3.391082	-1.395634					
30	H	-2.003140	1.985286	-1.467296					
31	H	-3.507503	2.000437	-2.402270					
32	H	-5.199565	-2.126291	-0.824465					
33	H	-6.670219	-1.338736	-1.390309					
34	H	-3.302113	-1.824824	-0.563344					
35	H	-1.329612	0.517863	-0.240248					
36	H	2.639224	-3.600642	-0.998324					
37	H	0.419113	-4.597807	-1.298053					
38	C	3.243960	-1.155579	-0.406715					
39	C	-6.673459	-1.826780	0.707631					
40	H	-7.351106	-2.654512	0.459404					
41	H	-7.302780	-1.025653	1.107131					
42	C	3.695439	0.144281	-0.082519					
43	C	5.026110	0.428255	0.061068					
44	O	0.874962	0.474929	-0.159474					
45	C	7.249842	-0.389844	0.013060					
46	C	6.858804	1.982883	0.543203					
47	C	7.769045	0.854322	0.341313					
48	H	2.962545	0.922114	0.056227					

Table 8 - Optimized structure (Cartesian coordinates, Å) of (2b)–TTC-Sp-Zn^{++}

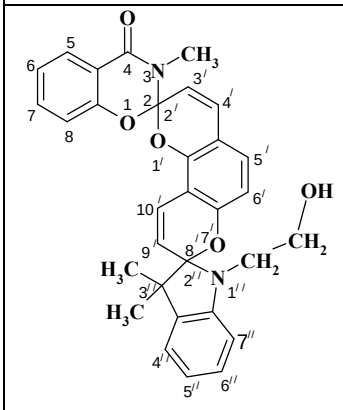
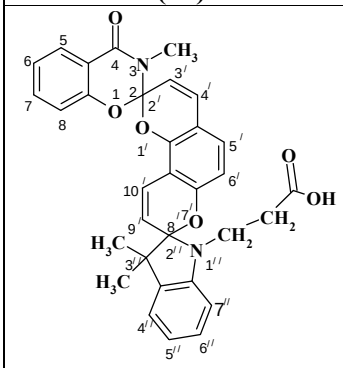
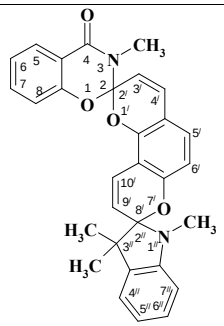
Атом	X	Y	Z	Атом	X	Y	Z
1 C	-3.869992	4.933674	0.027749	49 H	4.670465	-3.761698	-0.684620
2 C	-4.985618	4.334467	-0.552107	50 O	3.613833	-0.006982	0.825959
3 C	-4.987516	2.982149	-0.880457	51 N	3.885825	0.592296	-1.446614
4 C	-3.834987	2.269800	-0.589005	52 C	4.972040	0.900777	2.534561
5 C	-2.708229	2.853463	-0.035246	53 C	6.280202	2.483164	0.640792
6 C	-2.713970	4.199357	0.282392	54 C	5.980768	1.773371	2.916664
7 C	-1.610529	1.826621	0.059683	55 C	6.641957	2.562198	1.974546
8 C	-2.319276	0.580145	-0.467381	56 O	5.247337	2.323913	-2.016504
9 N	-3.565074	0.891927	-0.803083	57 H	4.451811	0.277811	3.253469
10 C	-1.141538	1.660344	1.514936	58 H	6.259416	1.834108	3.963685
11 C	-0.463288	2.263321	-0.878244	59 H	7.431070	3.236640	2.287251
12 C	-4.608640	0.001782	-1.309765	60 H	6.759499	3.092297	-0.117550
13 C	-1.763906	-0.732838	-0.593637	61 C	3.520719	0.350575	-2.835031
14 O	-1.486247	-3.630789	0.063460	62 H	3.901693	-0.618230	-3.174278
15 C	-0.396863	-0.952963	-0.349665	63 H	2.437246	0.369562	-2.956752
16 C	0.340389	-2.140171	-0.387032	64 H	3.972284	1.142543	-3.428206
17 C	-0.224223	-3.450133	-0.150905	65 C	-5.360339	-0.907806	0.943336
18 C	0.646351	-4.555409	-0.093573	66 O	-4.383109	-1.653500	1.005779
19 C	2.000058	-4.389063	-0.242726	67 O	-6.096864	-0.802984	2.002213
20 C	2.594853	-3.121774	-0.425263	68 H	-6.863925	-0.213691	1.881693
21 C	1.761430	-2.026451	-0.481707	69 Zn	-2.687368	-2.338974	0.618842
22 H	-3.898123	5.989437	0.273804				
23 H	-5.868641	4.928273	-0.760095				
24 H	-5.852991	2.535235	-1.356713				
25 H	-1.842359	4.679554	0.715803				
26 H	-1.966248	1.364245	2.168479				
27 H	-0.339114	0.927075	1.615691				
28 H	-0.760313	2.620251	1.871221				
29 H	-0.140918	3.262722	-0.577774				
30 H	0.409503	1.611351	-0.828015				
31 H	-0.801882	2.314065	-1.915750				
32 H	-4.173188	-0.955473	-1.596862				
33 H	-5.009604	0.445568	-2.226480				
34 H	-2.229408	-1.386755	-1.348345				
35 H	0.202310	-0.088913	-0.094355				
36 H	2.649299	-5.259877	-0.212768				
37 H	0.211360	-5.532296	0.079841				
38 C	4.011615	-2.901972	-0.604003				
39 C	-5.743385	-0.183530	-0.308283				
40 H	-6.521632	-0.796668	-0.787696				
41 H	-6.226985	0.761894	-0.047727				
42 C	4.493306	-1.658180	-0.675579				
43 C	3.593320	-0.470387	-0.510737				
44 O	2.229921	-0.785525	-0.723711				
45 C	4.628133	0.825503	1.191595				
46 C	4.827759	1.559998	-1.165866				
47 C	5.267438	1.612451	0.240544				
48 H	5.547974	-1.447336	-0.815427				

Table 9 - Optimized structure (Cartesian coordinates, Å) of (2b) –TTC-TTC-Zn^{++}

Атом	X	Y	Z	Атом	X	Y	Z
1 C	-6.517043	4.075577	0.561382	49 H	4.334983	-1.887216	0.014006
2 C	-7.322184	3.295937	-0.263188	50 O	6.285850	-0.570473	0.003402
3 C	-6.851405	2.105439	-0.812481	51 N	5.974685	1.730706	-0.027704
4 C	-5.555522	1.736849	-0.491667	52 C	8.409141	-1.585123	0.023599
5 C	-4.728904	2.517777	0.299577	53 C	9.612044	0.946342	-0.001833
6 C	-5.204838	3.697463	0.840746	54 C	9.788614	-1.453856	0.026646
7 C	-3.352745	1.902971	0.339723	55 C	10.392855	-0.193890	0.014048
8 C	-3.569057	0.622195	-0.464380	56 O	7.762111	3.151595	-0.033283
9 N	-4.830061	0.587140	-0.901699	57 H	7.923287	-2.554181	0.033052
10 C	-2.900280	1.606720	1.775986	58 H	10.404131	-2.347025	0.038838
11 C	-2.382048	2.865736	-0.380725	59 H	11.473770	-0.112439	0.016583
12 C	-5.464474	-0.486969	-1.656358	60 H	10.049023	1.938338	-0.012066
13 C	-2.629715	-0.420355	-0.668000	61 C	5.060170	2.871092	-0.046963
14 O	-1.573200	-3.132565	0.019754	62 H	4.441441	2.840604	-0.945628
15 C	-1.234168	-0.237045	-0.331277	63 H	4.429916	2.861285	0.844101
16 C	-0.228652	-1.149857	-0.199398	64 H	5.672263	3.768622	-0.053503
17 C	-0.413059	-2.591001	-0.070872	65 C	-6.187038	-1.886281	0.377871
18 C	0.724545	-3.415189	-0.000405	66 O	-5.030852	-2.167839	0.693635
19 C	1.985439	-2.871818	-0.000760	67 O	-7.119876	-2.250155	1.203750
20 C	2.267487	-1.488242	-0.034301	68 H	-8.014020	-2.006096	0.904858
21 C	1.145220	-0.550697	-0.092644	69 Zn	-3.186141	-2.212014	0.255617
22 H	-6.910479	4.995299	0.980038				
23 H	-8.332769	3.617054	-0.489958				
24 H	-7.480215	1.523528	-1.477092				
25 H	-4.573668	4.324050	1.463380				
26 H	-3.603432	0.942914	2.286303				
27 H	-1.906164	1.155247	1.804642				
28 H	-2.856830	2.544117	2.335729				
29 H	-2.458344	3.845428	0.096105				
30 H	-1.339609	2.554324	-0.314380				
31 H	-2.649407	2.980707	-1.433780				
32 H	-4.707700	-1.198623	-1.988168				
33 H	-5.892039	-0.057133	-2.568446				
34 H	-2.781206	-1.023990	-1.582364				
35 H	-0.877256	0.777765	-0.189038				
36 H	2.833776	-3.551003	0.049921				
37 H	0.572334	-4.484711	0.079147				
38 C	3.604774	-1.080972	-0.010949				
39 C	-6.580347	-1.186191	-0.885962				
40 H	-7.013510	-1.955912	-1.542133				
41 H	-7.404012	-0.504449	-0.654717				
42 C	4.096432	0.216272	-0.022780				
43 C	5.463451	0.474293	-0.015480				
44 O	1.287651	0.667625	-0.080177				
45 C	7.644912	-0.429098	0.007376				
46 C	7.362631	2.012741	-0.023418				
47 C	8.220430	0.832763	-0.005541				
48 H	3.404135	1.042004	-0.040182				

Data of NMR ^{1}H and IR-spectroscopy for compounds (2a,b, c)

NMR ^{1}H data for (**2a-c**)

Structure	NMR ^{1}H data ($CDCl_3$), δ, ppm, *J*(Hz)
 **(2a)**	1,07 and 1,24 (6H, 2s., hem. ($C\underline{H}_3$)$_2$); 3,16 (3H, d., J = 1,9; -N-$C\underline{H}_3$); 3,36 (2H, m., N-CH_2-$C\underline{H}_2$-OH); 3,7 (2H, m., N-$C\underline{H}_2$-CH_2-OH); 5,50(1H, dd., J =7,9; 10,4; 9'-<u>H</u>); 5,88 (1H, d., J = 9,8; 3'-<u>H</u>); 6,39 (1H, d., J = 8,5; 6'-<u>H</u>); 6,55 – 6,76 (2H, m., 7"-<u>H,</u> 10'-<u>H</u>); 6,78 – 6,94 (3H, m., 8-<u>H</u>, 4'-<u>H</u>, 5"-<u>H</u>); 6,98 (1H, d., J = 8,2; 5'-<u>H</u>); 7,05 (1H, d., J = 7,3; 4"-<u>H</u>); 7,09 – 7,23 (2H, m., 6-<u>H,</u> 6"-<u>H</u>); 7,49 (1H, m., 7-<u>H</u>); 8,08 (1H, d., J = 7,9; 5-<u>H</u>). (Figure 1 and 2)
 **(2b)**	1,06 и 1,22 (6H, 2s., hem. ($C\underline{H}_3$)$_2$); 2,6 (2H, m., N-$C\underline{H}_2$-CH_2-); 3,19 (3H, d., J = 4,4; -N-$C\underline{H}_3$); 3,55 (2H, m., N-CH_2-$C\underline{H}_2$-); 5,50 (1H, dd., J =7,9; 10,4; 9'-<u>H</u>); 5,85 (1H, dd., J = 4,1; 9,8; 3'-<u>H</u>); 6,38 (1H, dd., J = 3,5; 8,2; 6'-<u>H</u>); 6,55 (1H, d., J = 7,9; 7"-<u>H</u>); 6,7 (1H, m., 10'-<u>H</u>); 6,81 – 7,00 (4H, m., 8-<u>H</u>, 4'-<u>H</u>, 5'-<u>H</u>, 5"-<u>H</u>); 7,06 (1H, d., J = 7,3; 4"-<u>H</u>); 7,10 – 7,26 (2H, m., 6-<u>H,</u> 6"-<u>H</u>); 7,5 (1H, t., J = 7,6; 7-<u>H</u>); 8,11 (1H, m., 5-<u>H</u>). (Figure 3 and 4)
 **(2c)**	1.25 (6H, c, 3"- ($C\underline{H}_3$)$_2$); 2.65 (3H, s., 1"- $C\underline{H}_3$); 3.17 (3H, s., 3-$C\underline{H}_3$); 5.50 (1H, dd., J = 8.8, 19.2, 9′-<u>H</u>); 5.87 (1H, d., J = 9.8, 3′-<u>H</u>); 6.40 (1H, d., J = 8.1, 6′-<u>H</u>);6.5 (1H, d., J = 7.7, 7"-<u>H</u>); 6.6 – 7.3 (8H, m., 7-H, 8-<u>H</u>, 4'-<u>H</u>, 5'-<u>H</u>, 10'-<u>H</u>, 4"-<u>H</u>, 5"-<u>H</u>, 6"-<u>H</u>); 7.48 (1H, t., J = 7.4, 6-<u>H</u>); 8.08 (1H, d., J = 7.8, 5-<u>H</u>). (Figure 5 and 6)

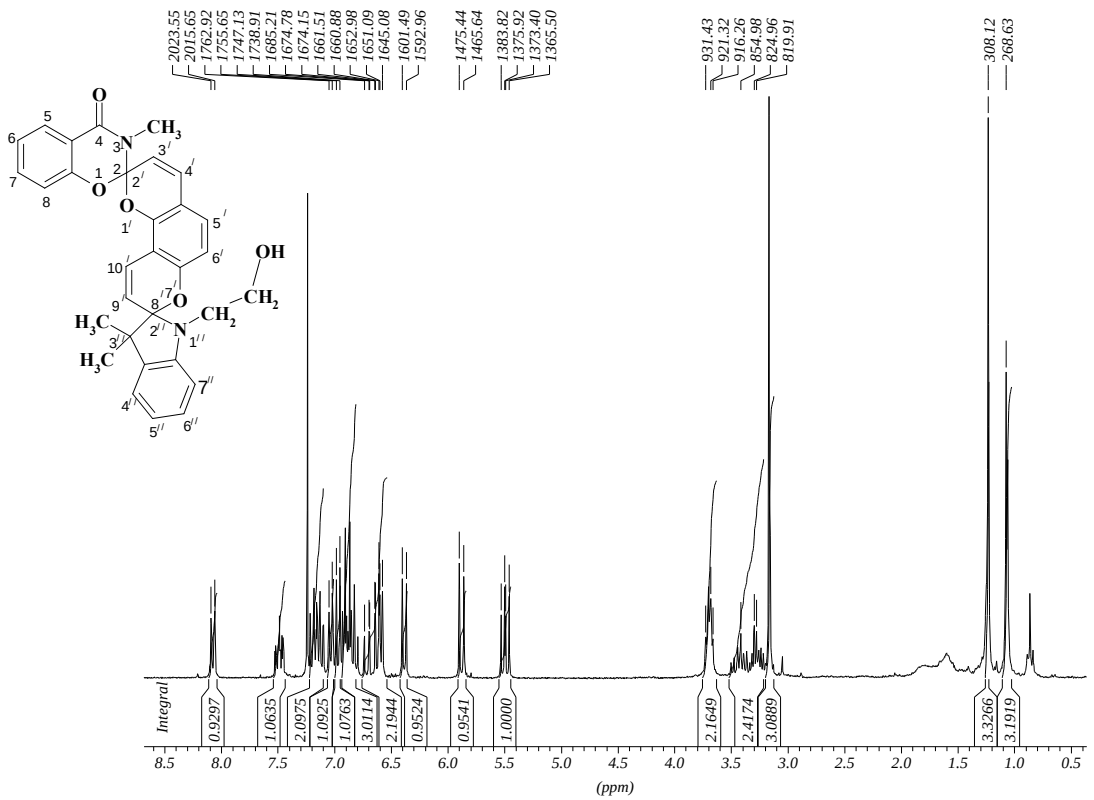


Figure 1. General NMR ^{1}H spectrum of (**2a**)

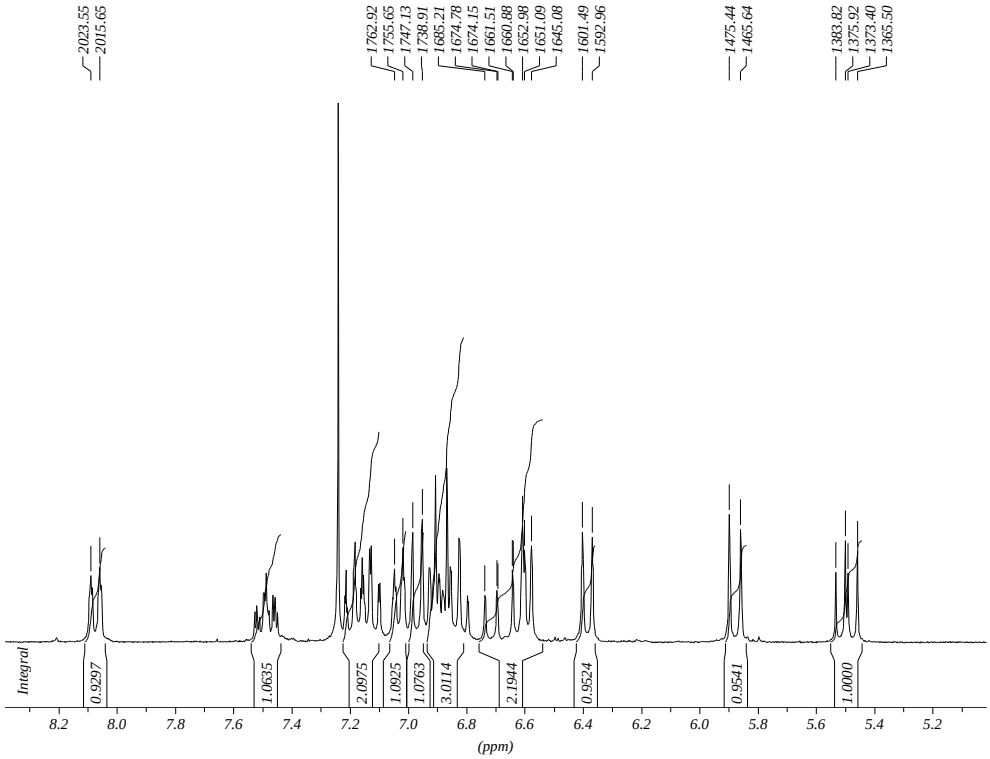


Figure 2. 5,2 - 8,2 ppm. area of NMR ^{1}H spectrum of (**2a**)

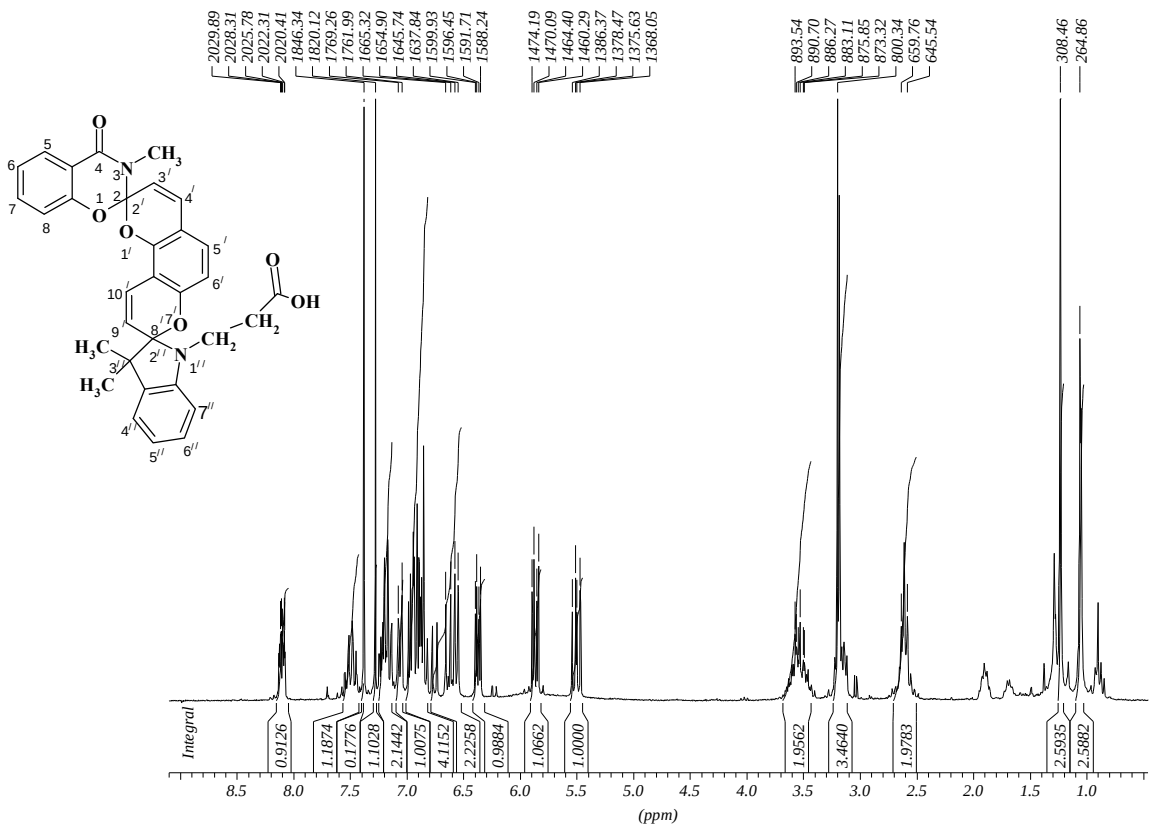


Figure 3. General NMR ^{1}H spectrum of (**2b**)

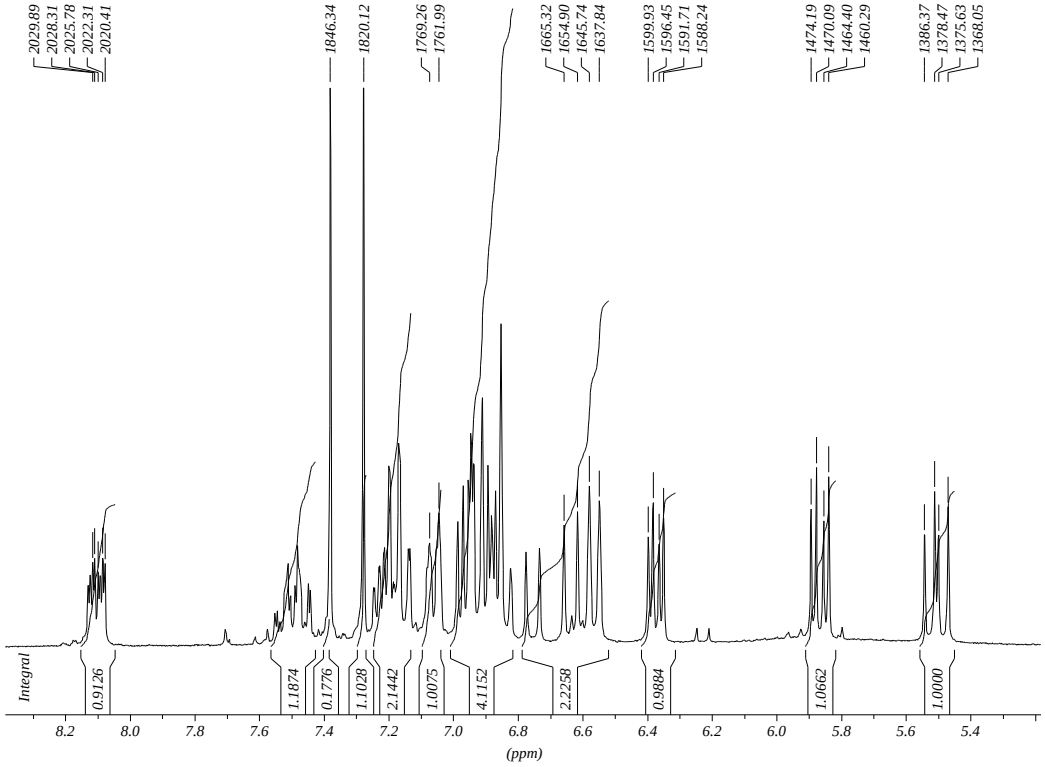


Figure 4. 5,4 - 8,3 ppm. area of NMR ^{1}H spectrum of (**2b**)

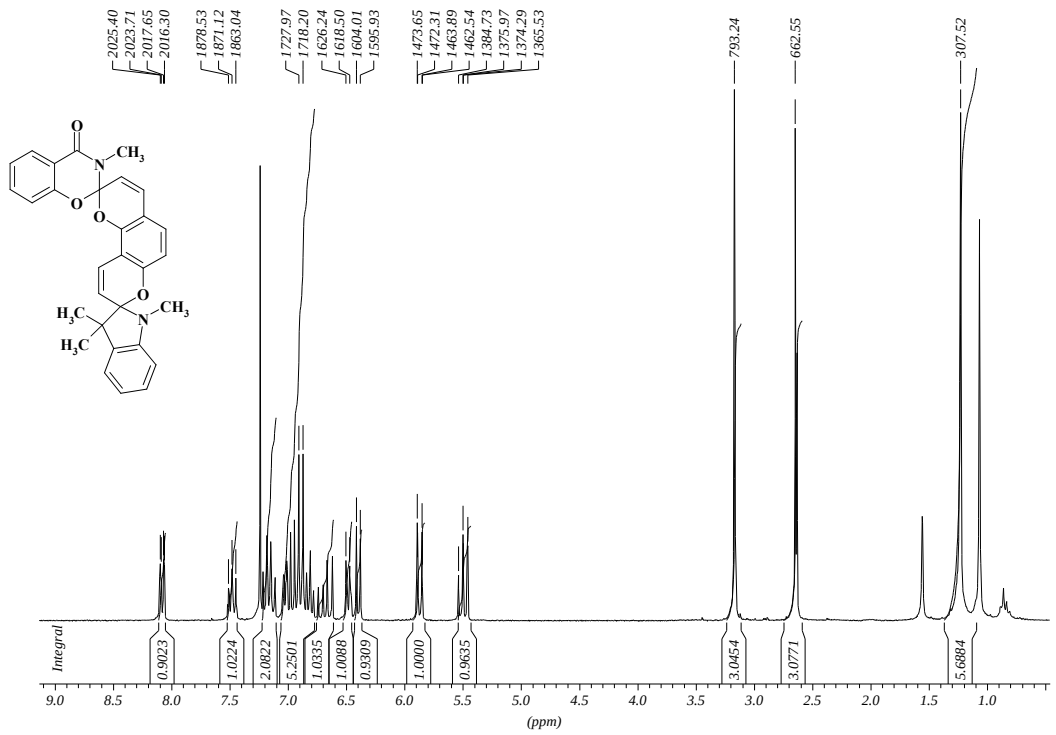


Figure 5. General NMR ^{1}H spectrum of (**2c**)

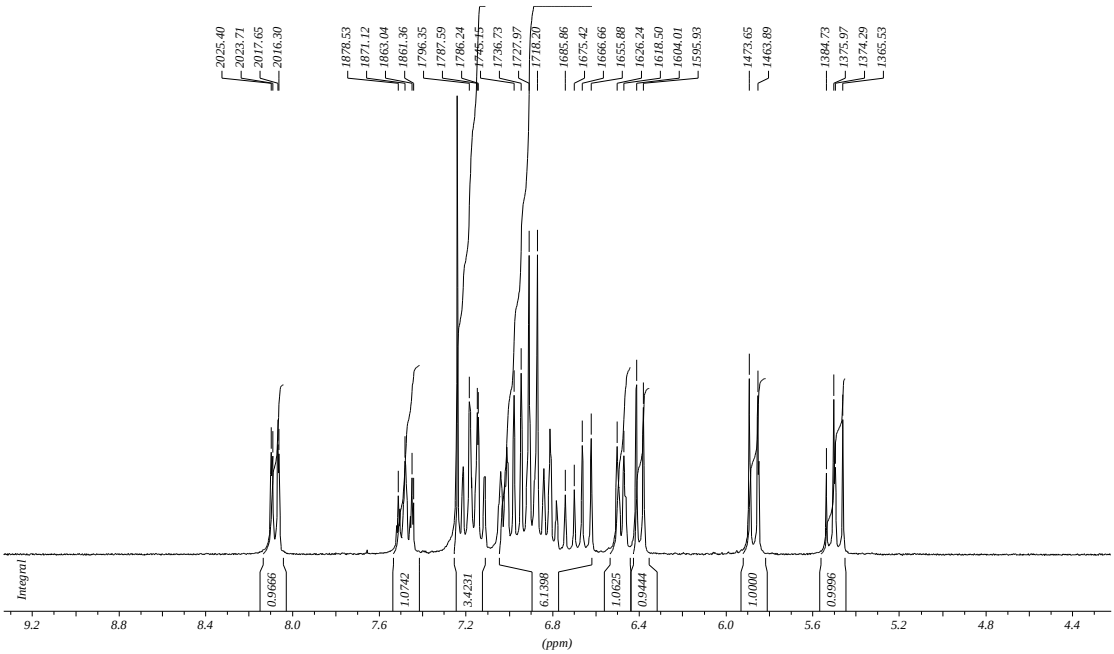


Figure 6. 4.4 – 9.2 ppm. area of NMR ^{1}H spectrum of (**2c**)

Data of IR-spectra for (2a-c)

№	ν_{O-H}	$\nu_{C=O}$, sm^{-1}	$\nu_{C=C}$, sm^{-1}	$\nu C_{spiro-O}$, sm^{-1}
(2a)	3415	1654	1605	936, 954
(2b)	3380, 3424	1683, 1744	1606, 1643	1007, 1023
(2c)	-	1683	1606, 1643	951, 1007

^{1}H NMR spectra were recorded on a FT-NMR AVANCE 600 МГц in $CDCl_3$. The chemical shifts were recorded in ppm (δ units). IR spectra were recorded on a Varian Excalibur 3100 FT-IR spectrometer.