Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis of coumarin derivative of resorcin[4]arene with solvent-controlled chirality

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Supporting Information

Table of contents

1. Spectral data for compound (**1).**

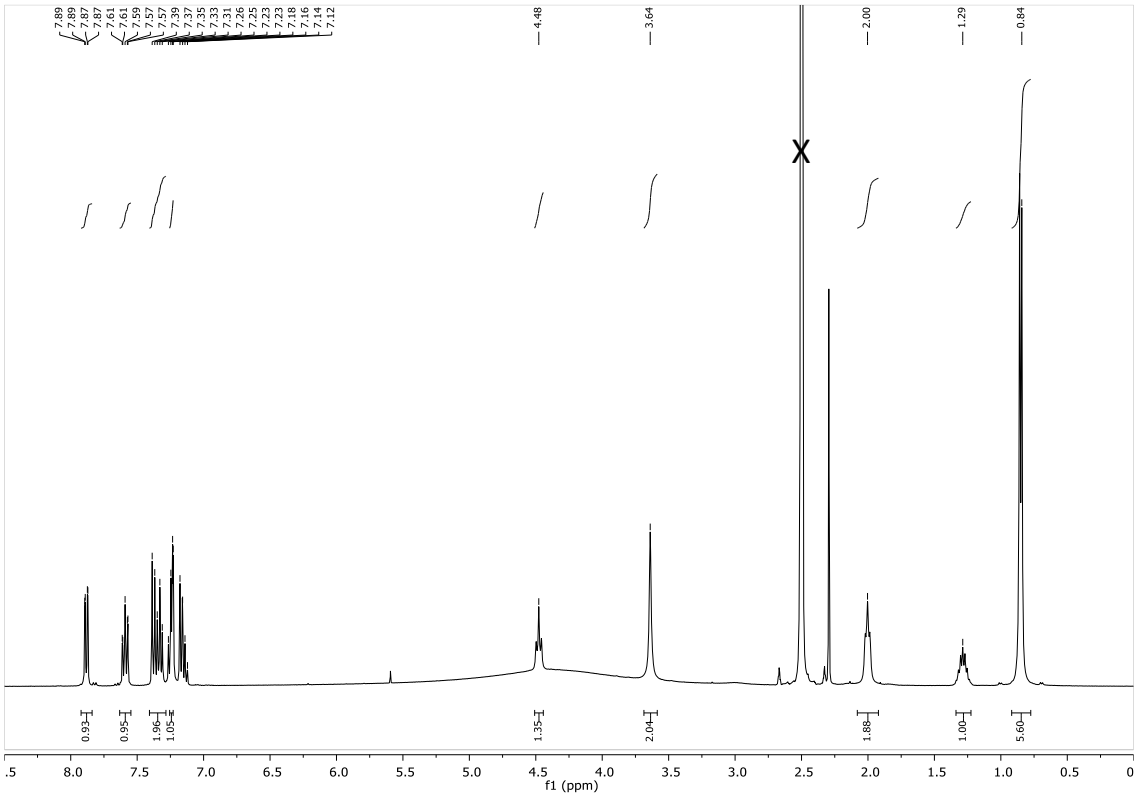

Figure S1. ^{1}H NMR spectrum of compound (**1)** (400 MHz, DMSO-d_6). The signals of DMSO-d_6 have been crossed out.

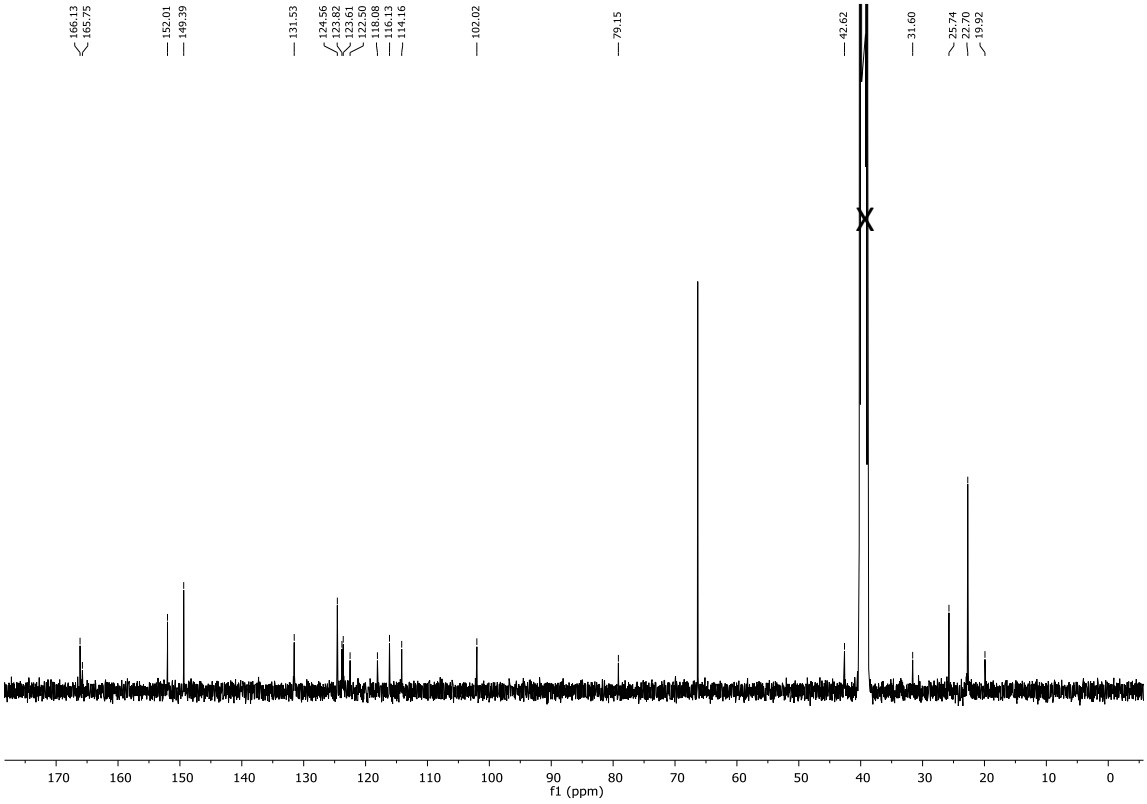

Figure S2. ^{13}C NMR spectrum of compound (**1)** (400 MHz, DMSO-d_6. The signals of DMSO-d_6 have been crossed out.

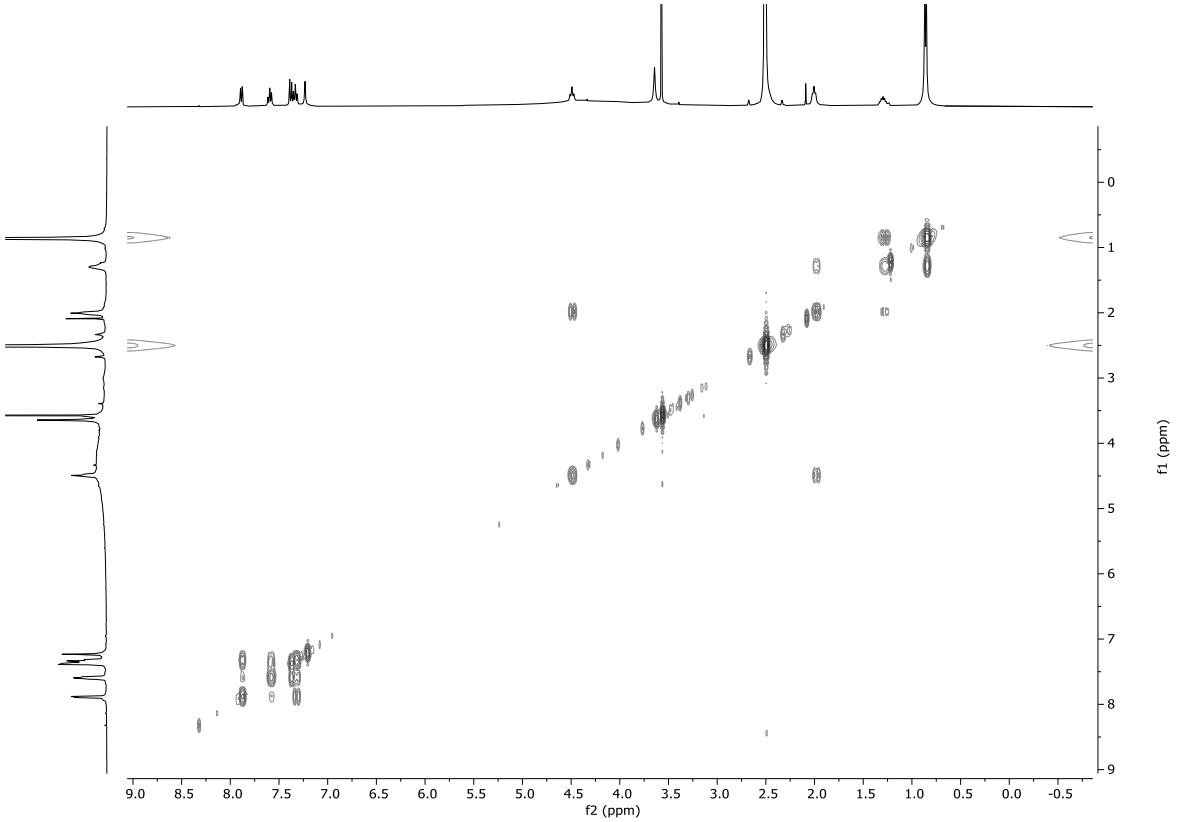

Figure S3. COSY (^{1}H-^{1}H) spectrum of compound (**1)** (400 MHz, DMSO-d_6).

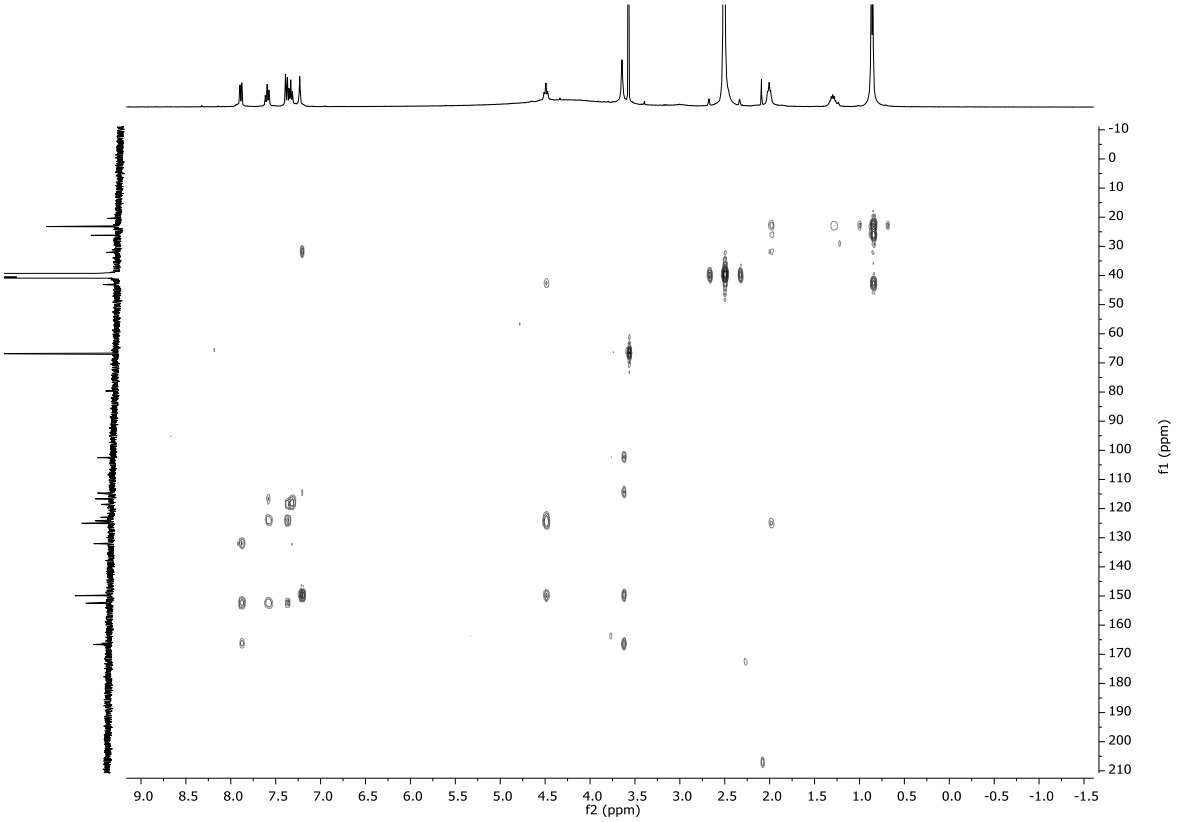

Figure S4. COSY (^{1}H-^{13}C) spectrum of compound (**1)** (400 MHz, DMSO-d_6).

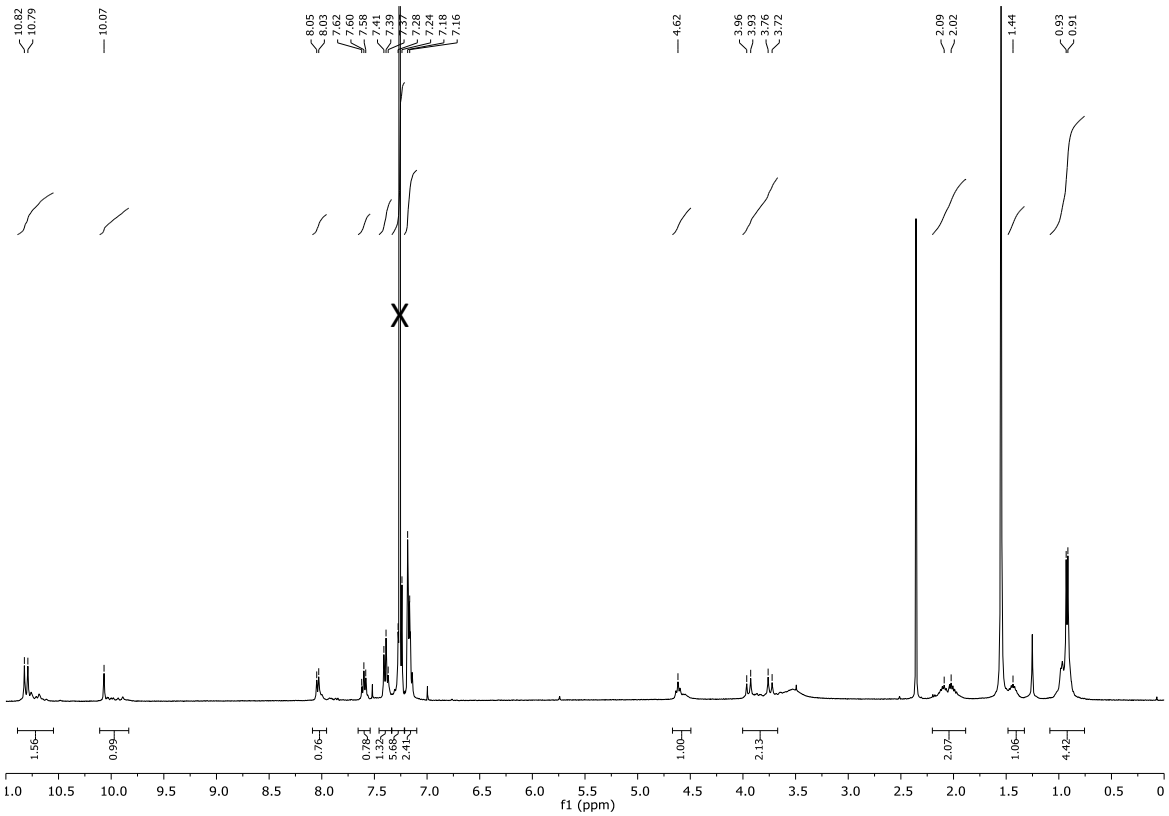

Figure S5. ^{1}H NMR spectrum of compound (**1)** (400 MHz, $CDCl_3$). The signals of $CDCl_3$ have been crossed out.

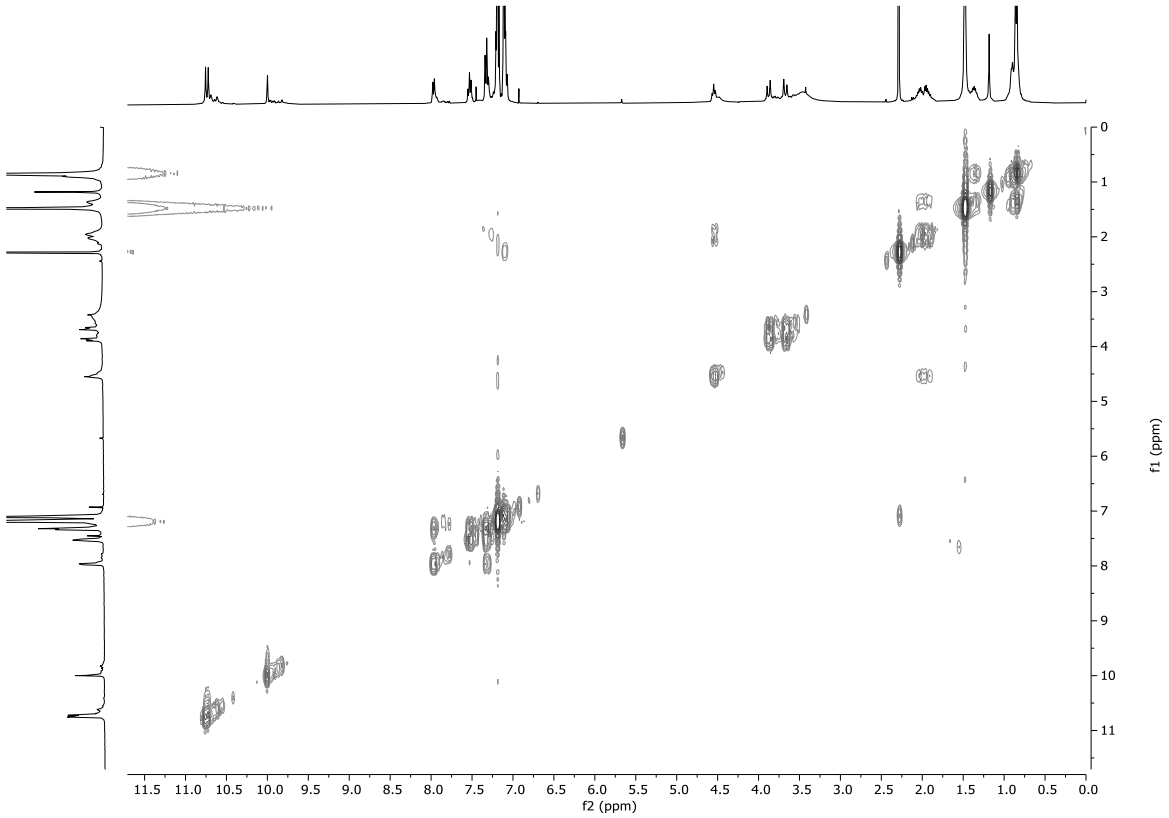

Figure S6. COSY (^{1}H-^{1}H) spectrum of compound (**1)** (400 MHz, $CDCl_3$).

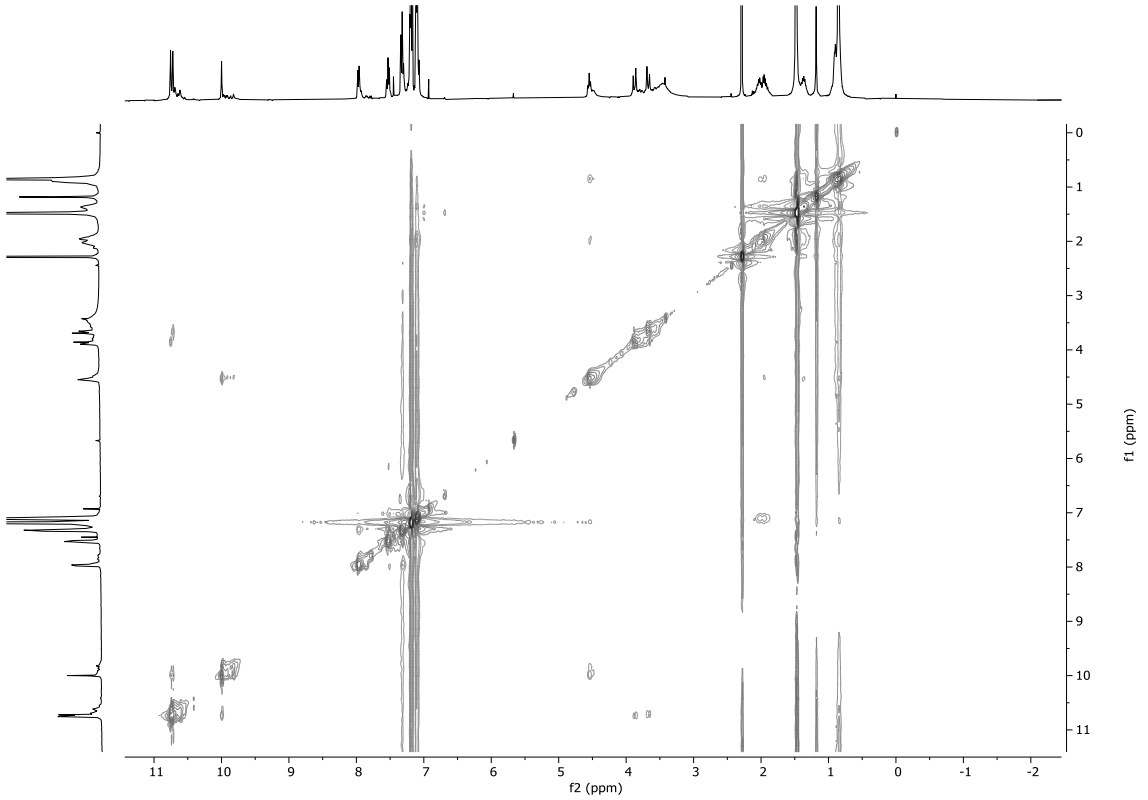

Figure S7. ROESY (^{1}H-^{1}H) spectrum of compound (**1)** (400 MHz, $CDCl_3$).

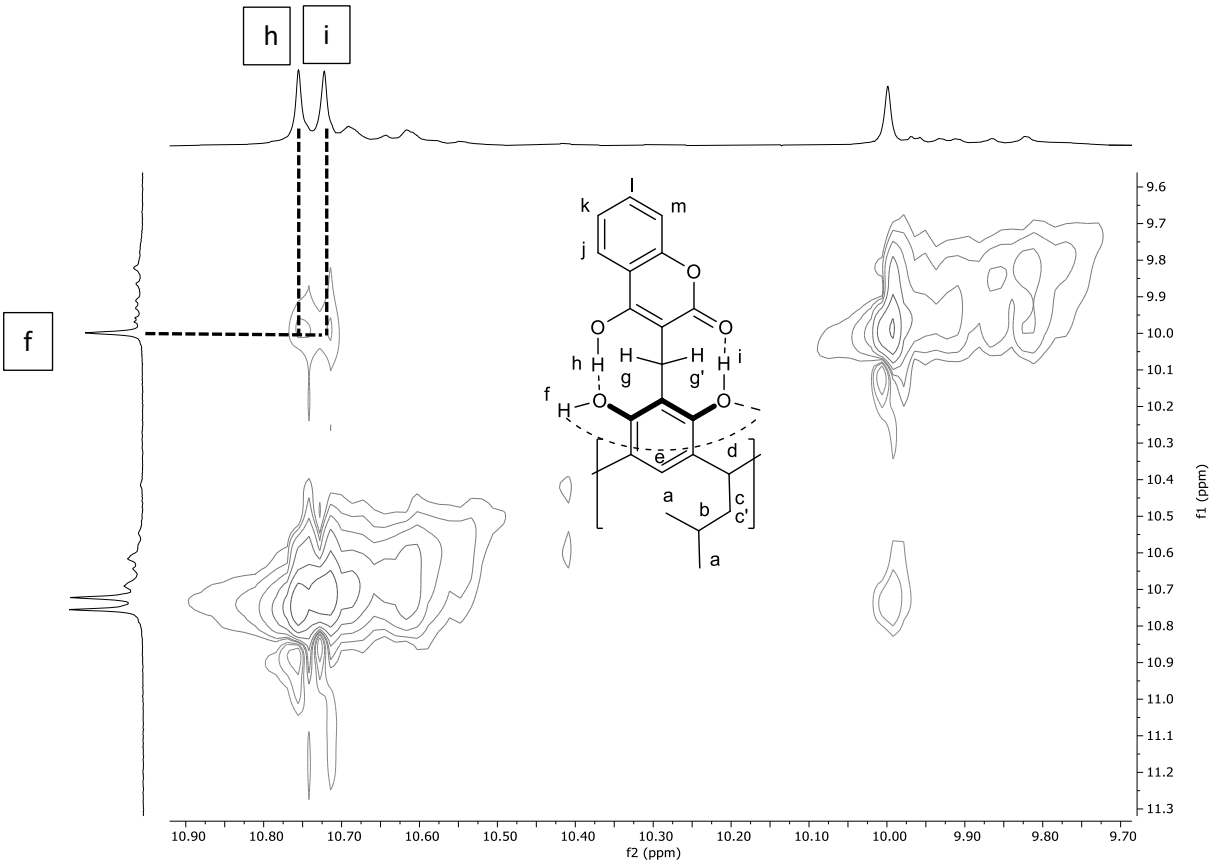

Figure S8. Fragment of ROESY (^{1}H-^{1}H) spectrum of compound (**1)** (400 MHz, $CDCl_3$) at 298 °C. Interaction of hydroxyl group OH(**f**) with hydroxyl groups OH (**h,i**).

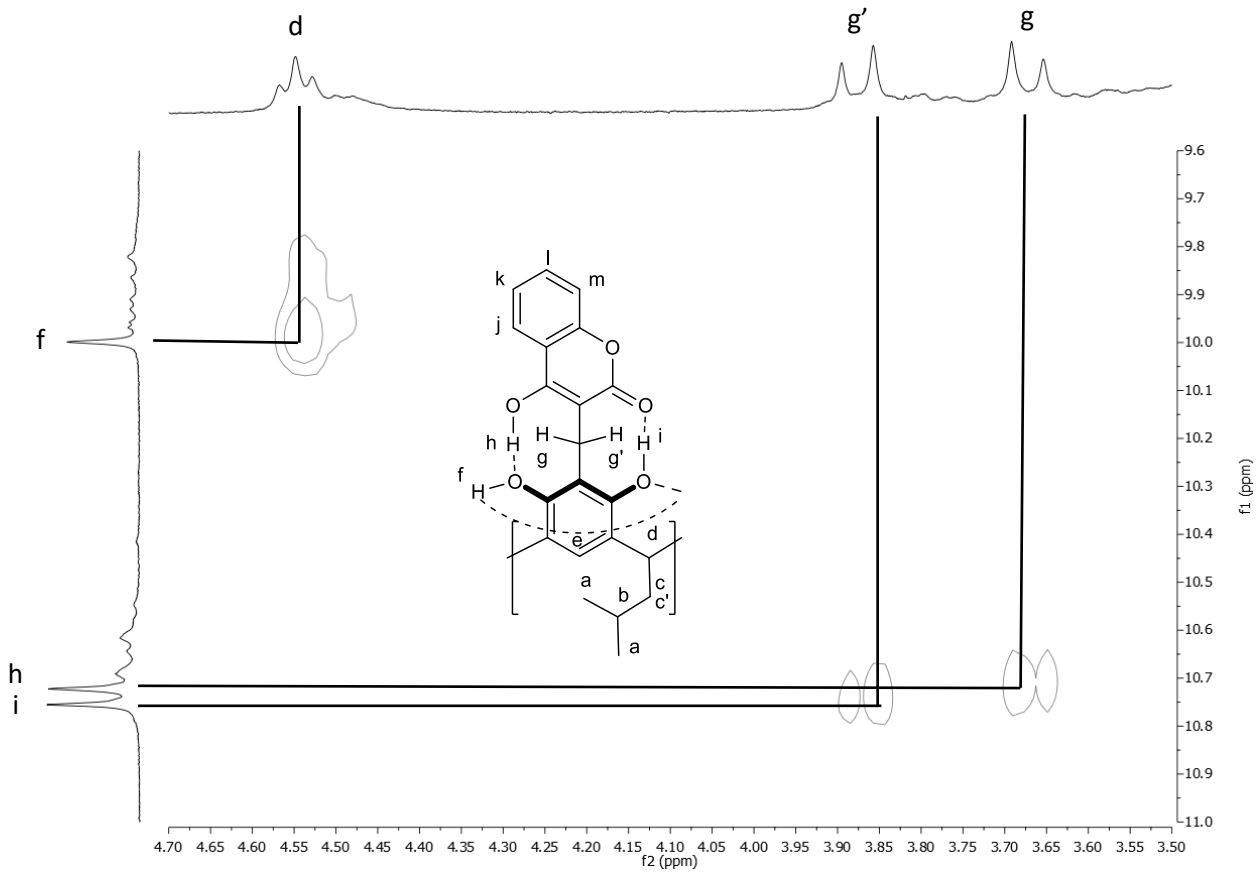

Figure S9. Fragment of the ROESY spectrum of compound (**1**) in $CDCl_3$ at 298 ºC.

The proton of the hydroxyl group OH (**f**) of the resorcin[4]arene was in close proximity to the proton of the methine group (**d**) of the lower rim of the resorcin[4]arene. The OH proton (**i**) of resorcin[4]arene interacted with the carbonyl group from the coumarin part of the resorcin[4]arene and was adjacent to the proton of the methylene group (**g'**). The proton from the hydroxyl group OH (**h**) of the coumarin portion stayed in contact with the second proton of the rigid methylene group (**g**).

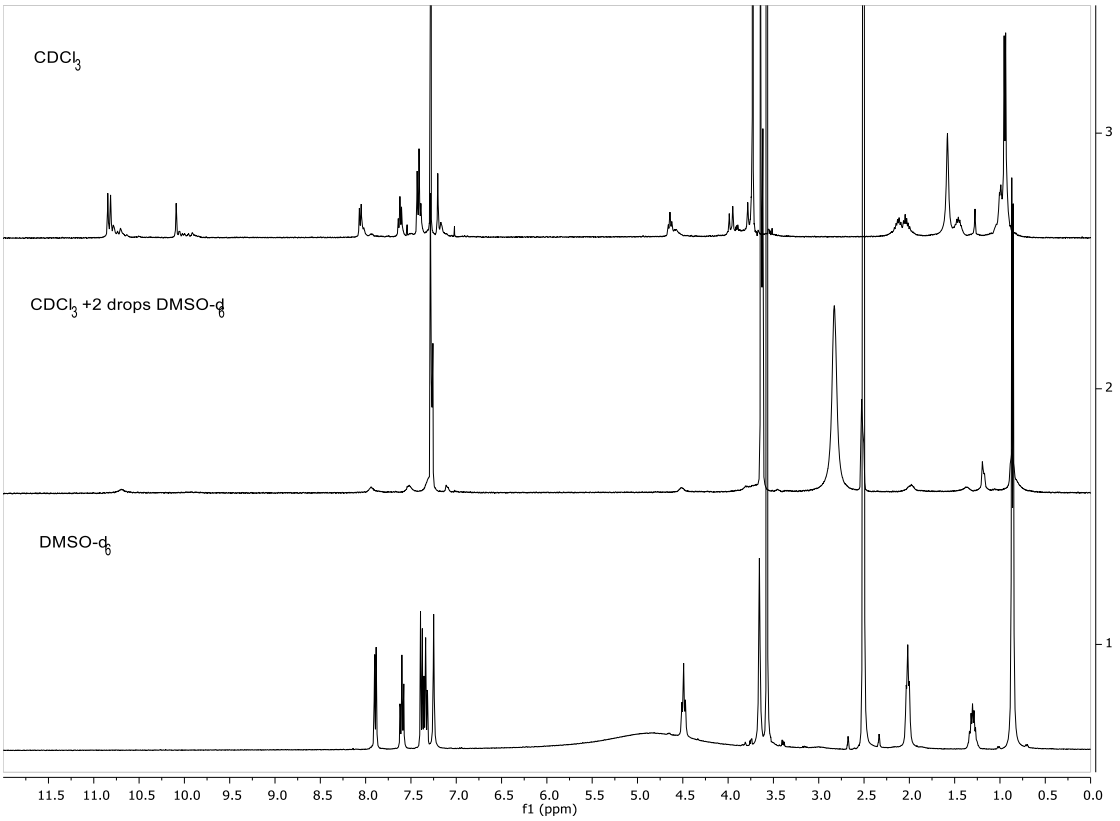

Figure S10. ^{1}H NMR spectrum of compound (**1)** (400 MHz): above, ^{1}H NMR spectrum in $CDCl_3$; inside ^{1}H NMR spectrum in $CDCl_3$ + 2 drops of DMSO-d_6; bottom ^{1}H-NMR spectrum in DMSO-d_6

2. Spectral data for compound (**1)** with chiral auxialiers

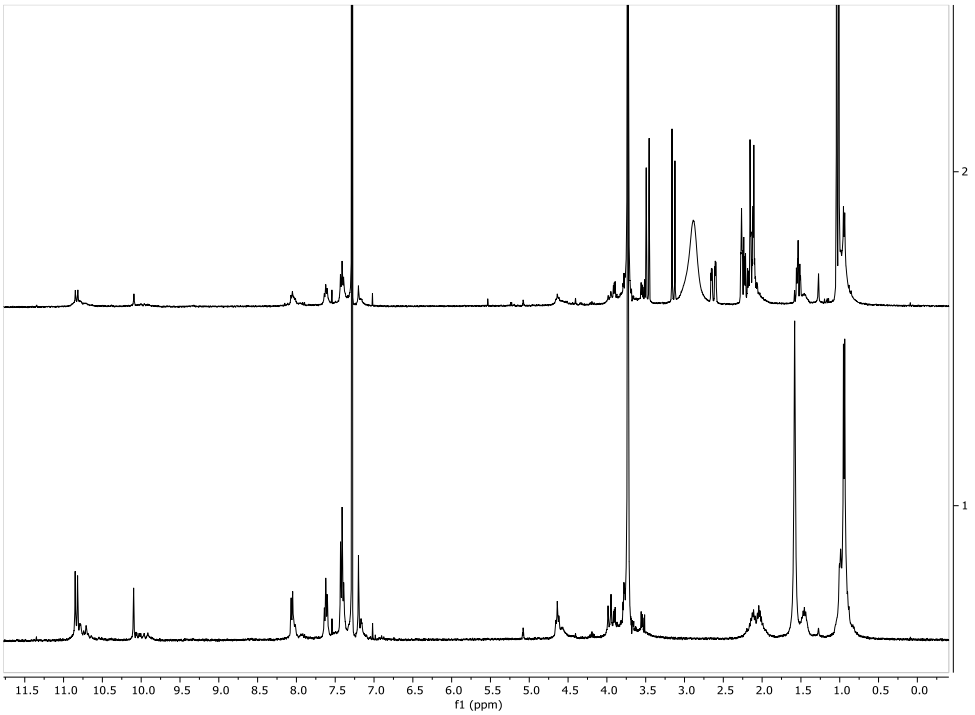

Figure S11. ^{1}H NMR spectrum of compound (**1)** (400 MHz, $CDCl_3$): at the top ^{1}H NMR spectrum after adding 4 equivalents of *D*(+)-camphorsulfonic acid; bottom ^{1}H-NMR spectrum in chloroform .

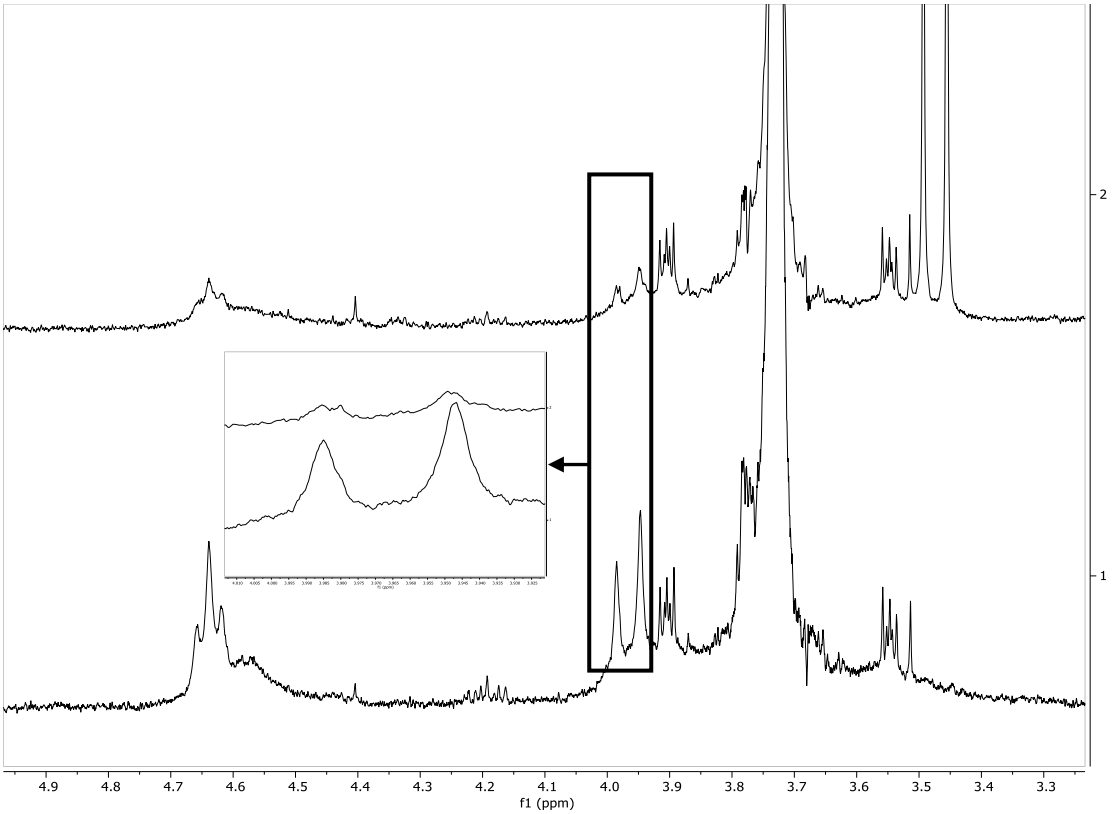

Figure S12. Enlarged fragment of ^{1}H NMR spectrum of compound (**1)** (400 MHz, $CDCl_3$) with *D*(+)-camphorsulfonic acid. The area of one of the diastereotopic protons (g') is marked in frame: at the top with *D*(+)-camphorsulfonic acid; bottom without *D*(+)-camphorsulfonic acid.

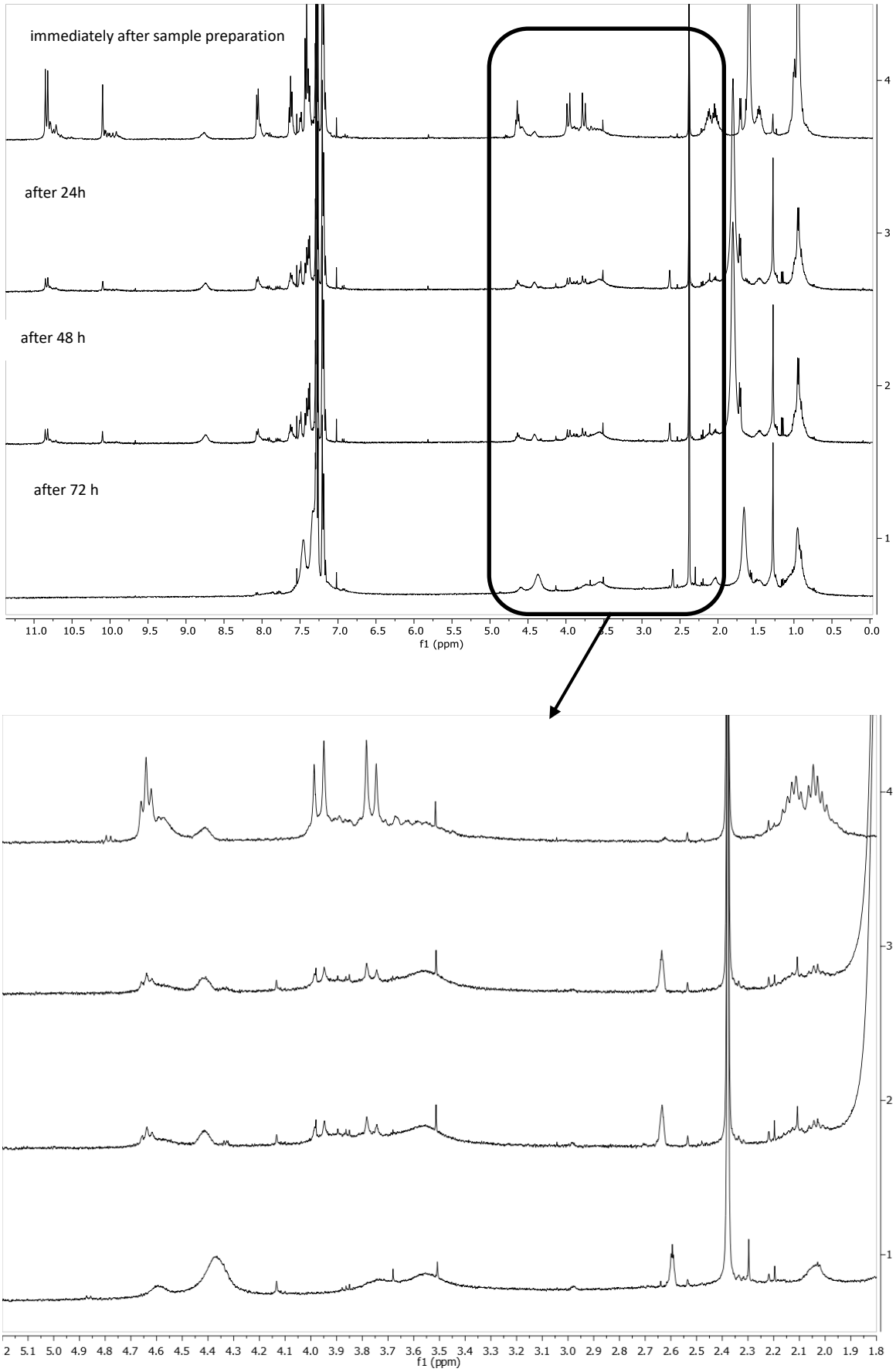

Figure S13. ^{1}H NMR spectrum of compound (**1)** (400 MHz, $CDCl_3$) in the presence of 4 equivalents of *S*(-)-phenylethylamine: at the top the spectrum after adding 4 equivalents of *S*(-)-Phenylethylamine and its change over time 24, 48 and 72 hours; bottom an enlarged fragment marked with a frame.

3. HRMS-ESI spectra for compound (**1)**

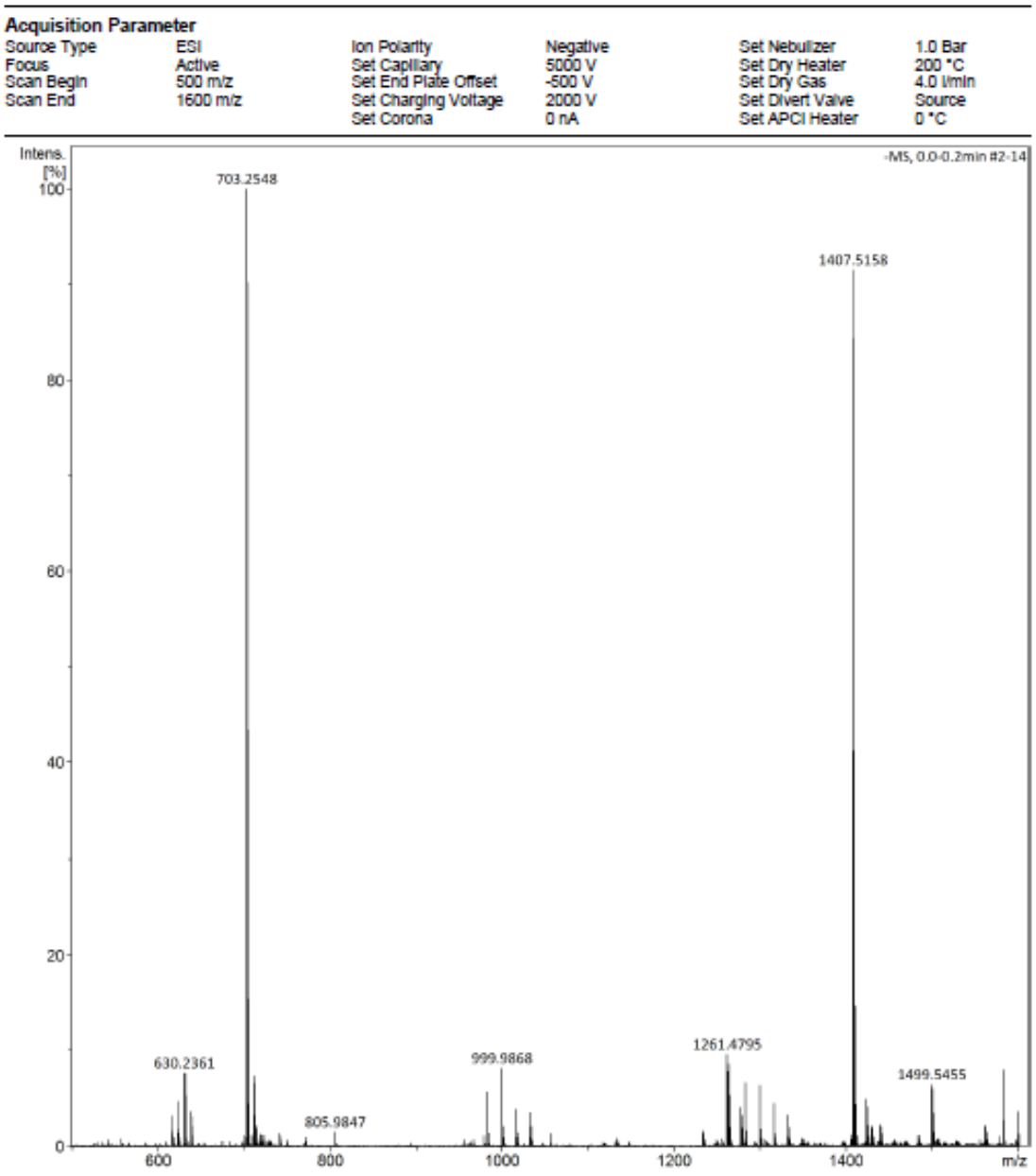

Figure S14. HRMS-ESI spectrum of compound (**1)**.

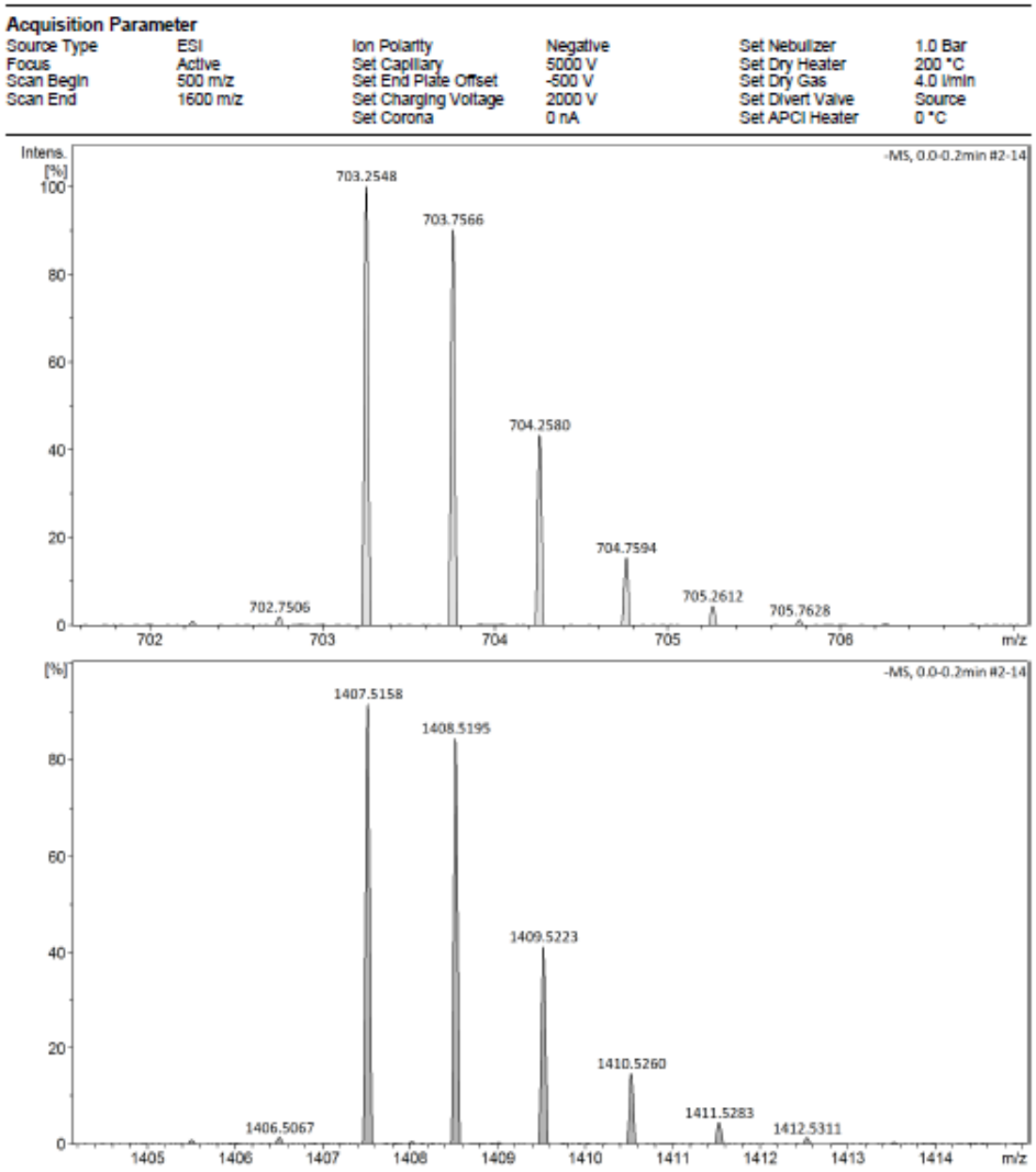

Figure S15. Isotope profiles of compound (**1)**.

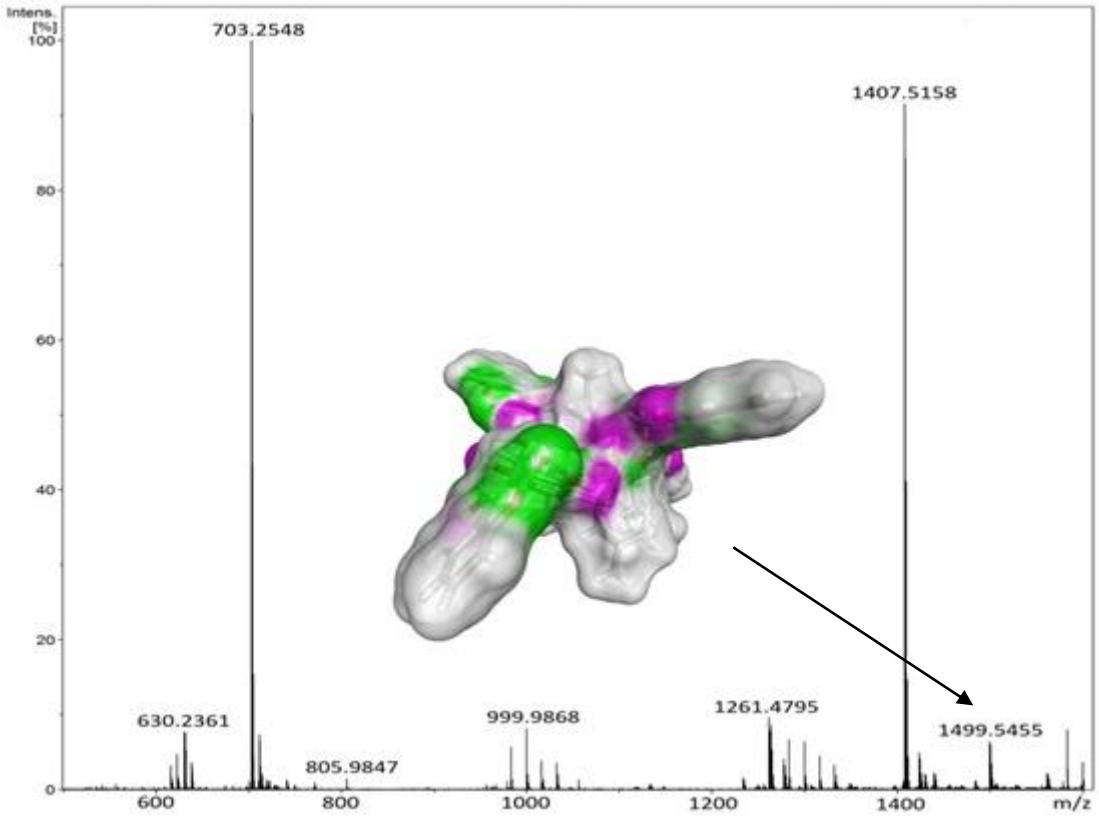

Figure S16. HRMS spectrum of compound (**1**) performed in negative ionization mode with a peak corresponding to the formation of the compound (**1**) complex with toluene.

The calculated model of the coumarin[4]arene-toluene complex by the PM7 method using the MOPAC program[1] with marked areas of hydrogen bonds and van der Waals clouds.

[1] *MOPAC2016*, J.J.P. Stewart, Stewart Computational Chemistry, Colorado Springs, CO, USA

4. IR spectrum for compound (**1)**

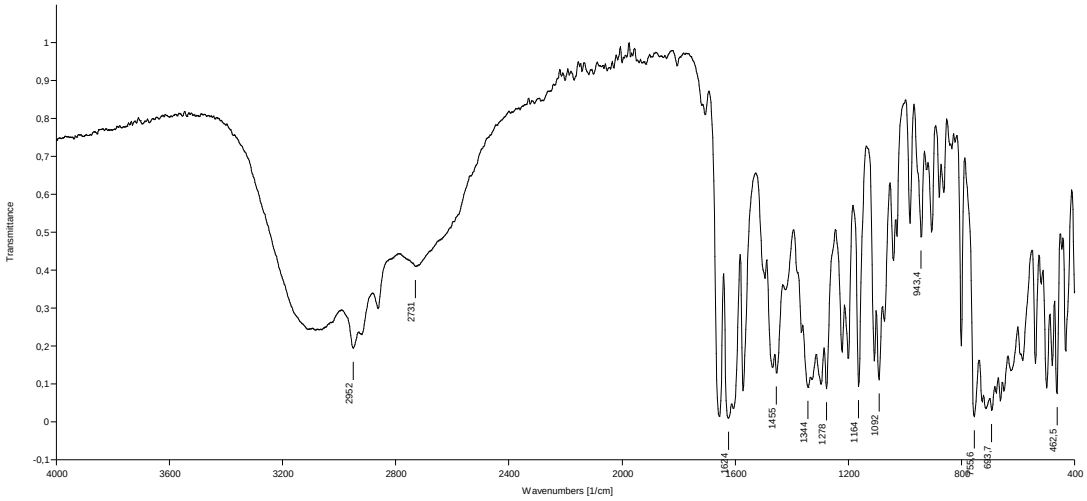

Figure S17. IR spectrum (ATR) of compounds (**1)**.

5. UV-VIS and fluorescence spectra for compound (**1)** and 4-hydroxycoumarin

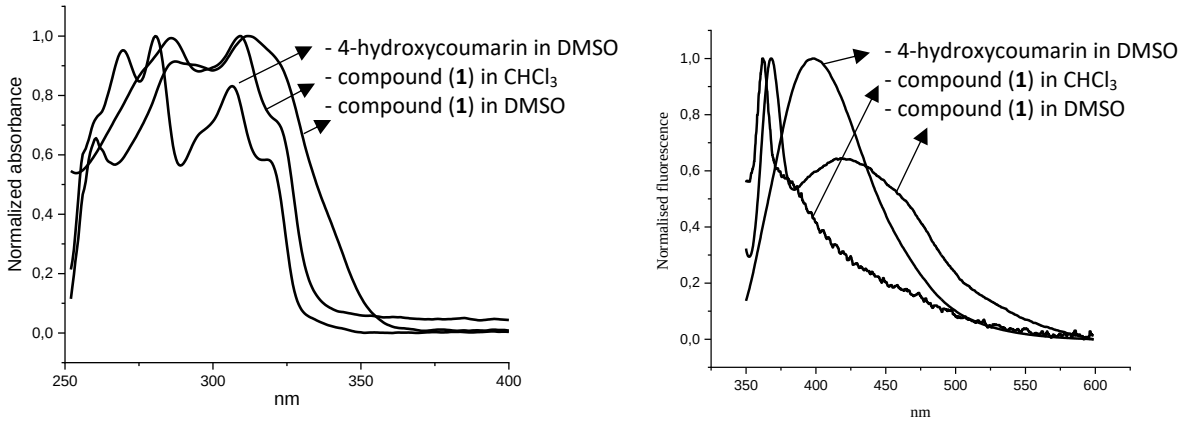

Figure S18. Normalized UV-VIS and fluorescence spectra of compound (**1**) and 4-hydroxycoumarin: on the left the absorption spectra of coumarin[4]arene ($2.64x10^{-6}$M) in DMSO and chloroform and 4-hydrozycoumarin ($7.03x10^{-7}$M) in DMSO; on the right side fluorescence spectra of coumarin[4]arene **1** (λ_{exc} = 320 nm) in DMSO and chloroform and 4-hydroxycoumarin (λ_{exc} = 320 nm) in DMSO.

6. Atomic coordinates for DFT calculated geometries and energies of compound (**1)**

All calculations were performed within the density functional theory (DFT) using Gaussian 09 program suite. Geometries of compound (**1)** were calculated using method: DFT B3LYP/6-311(d,p) [2].

Atomic coordinates for calculated geometries of compound 1 in gas phase:

E(RB3LYP) = -4753.82593905 A.U.

Cartesian coordinates

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
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34	6	-0.000006042	0.000004020	0.000003570
35	6	-0.000002461	0.000002472	-0.000005178

(1) [2] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision D.01*, Gaussian, Inc., Wallingford CT, **2009**.

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165	1	0.000000568	0.000000531	-0.000000056
166	1	-0.000000072	0.000001003	-0.000000123
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169	1	0.000000030	0.000000118	0.000000123
170	1	0.000000790	-0.000000290	0.000000426
171	1	-0.000001751	-0.000000697	-0.000000265
172	1	-0.000000157	-0.000000307	0.000000588
173	1	-0.000000093	0.000001378	0.000001764

174	1	-0.000000629	-0.000000787	0.000000673
175	1	-0.000000303	0.000000355	-0.000000297
176	1	-0.000000316	-0.000000116	-0.000000212
177	1	-0.000000665	-0.000000158	0.000000129
178	1	-0.000000460	-0.000000578	-0.000000002
179	1	-0.000000250	0.000000691	0.000000367
180	1	-0.000000048	0.000000180	-0.000000083
181	1	-0.000000659	0.000000373	-0.000000312
182	1	-0.000000468	0.000000735	0.000000238
183	1	-0.000000558	0.000000029	-0.000000306
184	1	-0.000000341	0.000000417	0.000000028

Atomic coordinates for calculated geometries of compound **1** in $CHCl_3$:

E(RB3LYP) = -4753.87529866 A.U

Cartesian coordinates

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000005857	-0.000001487	-0.000003728
2	6	-0.000002523	0.000000560	0.000003851
3	6	-0.000002057	0.000002297	-0.000002832
4	6	-0.000000238	0.000001290	0.000000947
5	6	0.000000108	-0.000000002	-0.000004373
6	6	-0.000002941	0.000003239	0.000001997
7	8	0.000002499	-0.000002083	0.000002441
8	8	0.000000147	-0.000002113	0.000005079
9	1	0.000000815	-0.000001362	-0.000001058
10	6	0.000004696	-0.000002826	0.000003066
11	6	-0.000008587	0.000003226	-0.000001540
12	6	0.000004597	-0.000000103	0.000006657
13	6	-0.000002596	-0.000000157	0.000002621
14	6	-0.000002210	0.000003422	-0.000004934
15	6	0.000003143	0.000000318	-0.000001275
16	6	0.000001341	0.000000094	0.000004583
17	8	-0.000003499	0.000001082	-0.000003416
18	1	0.000000086	0.000000001	-0.000001514
19	6	0.000003372	-0.000003613	-0.000000425
20	6	-0.000002346	0.000000715	0.000006351
21	6	-0.000002544	0.000000561	-0.000002632
22	6	0.000005220	-0.000001098	-0.000001332
23	6	-0.000002345	-0.000001695	0.000010886
24	6	0.000001583	-0.000005795	-0.000001737
25	6	-0.000002836	0.000003059	-0.000000839
26	8	-0.000000285	0.000001831	-0.000002475
27	8	-0.000004969	0.000003455	-0.000003120
28	1	-0.000000742	0.000001261	0.000000348
29	6	-0.000006175	0.000001193	0.000002597
30	6	0.000008724	-0.000003072	-0.000003663
31	6	-0.000001143	0.000002872	-0.000004241
32	6	0.000004537	-0.000009476	-0.000004887
33	6	-0.000012509	-0.000001076	0.000005120
34	6	0.000003301	-0.000001794	-0.000002375
35	6	-0.000002787	-0.000001320	0.000003025
36	8	0.000002550	-0.000000468	-0.000000027
37	8	0.000004828	0.000001609	-0.000005758
38	1	0.000000783	-0.000000100	-0.000001177
39	6	-0.000002675	0.000002670	-0.000000723
40	6	-0.000002617	0.000000913	-0.000001685
41	6	-0.000001375	-0.000001323	0.000005641
42	1	0.000001185	0.000002612	-0.000000668
43	6	-0.000000354	-0.000001287	-0.000002664
44	1	0.000000556	0.000001619	-0.000002356

45	6	0.000002171	0.000001121	-0.000002264
46	1	0.000000316	-0.000002046	-0.000001735
47	1	0.000000850	0.000001106	0.000001036
48	1	0.000000570	0.000001192	0.000000915
49	6	0.000001755	-0.000005043	0.000001885
50	1	0.000000676	0.000000231	0.000000260
51	1	0.000002364	0.000000199	-0.000001162
52	6	0.000004541	0.000000360	-0.000003119
53	6	0.000000126	0.000001241	0.000002202
54	1	0.000000773	-0.000000021	0.000001016
55	1	0.000000021	-0.000000329	-0.000000106
56	1	0.000000270	0.000000370	0.000000976
57	1	0.000001400	0.000000822	0.000000602
58	6	-0.000001670	-0.000001109	0.000001622
59	1	-0.000000130	0.000000830	-0.000000182
60	6	-0.000004423	0.000003539	0.000002562
61	1	0.000000593	0.000001627	0.000000996
62	1	-0.000002257	0.000000589	0.000005999
63	1	-0.000001657	-0.000002509	-0.000010482
64	1	0.000001942	-0.000002505	-0.000002617
65	1	0.000000846	-0.000001607	0.000001849
66	1	0.000000699	0.000002851	0.000000877
67	8	-0.000007764	-0.000004352	0.000003606
68	6	-0.000001875	-0.000004103	0.000001161
69	1	0.000000496	0.000002782	-0.000001143
70	6	0.000000935	-0.000003984	-0.000001008
71	1	0.000007696	0.000011322	0.000004076
72	6	-0.000003021	0.000004325	-0.000001102
73	6	0.000000209	-0.000000803	-0.000001826
74	6	0.000001060	0.000002606	0.000001461
75	6	-0.000004616	-0.000000927	0.000002077
76	8	0.000002542	0.000001708	-0.000002690
77	6	0.000002922	0.000000893	0.000005610
78	8	-0.000002033	-0.000001007	-0.000001429
79	8	-0.000000668	0.000000587	-0.000003167
80	6	-0.000002389	-0.000000660	-0.000001277
81	6	0.000000964	-0.000001113	0.000000032
82	6	-0.000002178	0.000001568	0.000000576
83	6	0.000000367	0.000000295	-0.000000918
84	6	-0.000005462	0.000003421	-0.000003180
85	6	-0.000002684	0.000000002	0.000002348
86	6	0.000000026	0.000001501	0.000002281
87	6	0.000001214	-0.000001526	0.000003275
88	8	-0.000005405	0.000004270	-0.000000229
89	6	0.000023202	0.000002959	0.000012015
90	8	-0.000009111	-0.000004641	-0.000008608
91	6	0.000000903	0.000001077	0.000001643
92	6	0.000001201	0.000002292	0.000000949
93	6	0.000001203	0.000000796	0.000002868
94	6	0.000000187	0.000002613	0.000000466
95	8	0.000005591	0.000001712	0.000000708
96	6	0.000000776	0.000000580	0.000000175
97	6	-0.000005946	0.000002899	0.000001904
98	6	0.000000560	0.000000865	-0.000001192
99	8	-0.000002748	-0.000001359	-0.000001778
100	6	0.000003071	-0.000001382	0.000001853
101	8	-0.000002725	-0.000001203	0.000001869
102	6	0.000001975	0.000002783	0.000004972
103	6	-0.000000604	0.000000086	-0.000000670
104	8	-0.000000355	-0.000005038	-0.000009102
105	6	-0.000001582	-0.000000959	0.000000279
106	6	-0.000001698	0.000001371	-0.000000311
107	6	-0.000000693	0.000000779	0.000000014
108	6	-0.000002770	-0.000000389	-0.000000313
109	6	0.000001395	-0.000003185	-0.000003324
110	6	-0.000000843	-0.000003083	-0.000003109
111	8	0.000004453	0.000001557	0.000001981
112	6	-0.000009353	-0.000004895	0.000004051
113	8	-0.000001104	0.000000495	-0.000006787

114	6	-0.000002025	-0.000010848	0.000005145
115	6	-0.000000181	-0.000000451	-0.000003070
116	8	0.000002980	0.000010318	-0.000007380
117	6	0.000000436	-0.000002010	-0.000000948
118	6	-0.000001496	-0.000003260	-0.000000490
119	6	-0.000000348	-0.000001030	-0.000003148
120	6	0.000001731	-0.000000894	-0.000002071
121	1	0.000001562	0.000005374	-0.000000204
122	1	-0.000001271	-0.000002395	0.000002472
123	1	-0.000000227	-0.000000227	0.000000032
124	1	-0.000002505	0.000000148	-0.000000590
125	1	-0.000001128	0.000000926	-0.000001497
126	1	0.000000319	0.000001820	0.000002356
127	1	-0.000000246	-0.000001124	0.000000156
128	1	-0.000000362	0.000000532	-0.000000392
129	1	-0.000001004	0.000000449	-0.000000044
130	1	-0.000000888	-0.000000002	-0.000000276
131	1	-0.000000570	0.000000707	0.000000494
132	1	0.000000209	0.000001057	0.000001507
133	1	0.000000972	0.000001567	0.000002051
134	1	0.000001252	0.000001558	0.000001850
135	1	0.000001179	0.000001038	0.000001745
136	1	0.000000130	0.000001271	0.000001940
137	1	-0.000000132	-0.000000194	0.000000164
138	1	-0.000000175	-0.000000365	-0.000002965
139	1	-0.000000140	0.000002535	0.000002873
140	1	-0.000001740	0.000000573	-0.000000617
141	1	-0.000001237	0.000000493	0.000000201
142	1	-0.000001429	0.000000253	-0.000000720
143	1	-0.000001199	0.000000061	-0.000000435
144	1	-0.000000671	-0.000003325	-0.000000280
145	1	0.000000923	-0.000000515	-0.000001294
146	1	-0.000000079	-0.000002151	-0.000001718
147	1	0.000000118	-0.000001982	-0.000001904
148	1	-0.000000285	-0.000001764	-0.000001339
149	6	0.000000140	-0.000002569	-0.000001841
150	6	0.000001711	-0.000002928	-0.000001636
151	6	0.000000626	-0.000000725	0.000000760
152	6	-0.000000255	0.000000530	-0.000000510
153	6	-0.000000641	-0.000000058	0.000000583
154	6	0.000000937	0.000005137	0.000000983
155	6	-0.000000964	-0.000000226	-0.000001729
156	6	0.000002449	-0.000002130	0.000000204
157	1	0.000000764	0.000000070	0.000000334
158	1	-0.000000062	0.000000108	0.000000252
159	1	0.000000208	-0.000000435	-0.000000822
160	1	0.000001061	-0.000001138	0.000000029
161	1	0.000000608	-0.000000579	-0.000000220
162	1	0.000000925	-0.000000246	-0.000000485
163	1	0.000000551	-0.000000826	-0.000000664
164	1	-0.000001310	-0.000000466	0.000000078
165	1	0.000000100	-0.000001518	-0.000000898
166	1	0.000000334	-0.000000384	0.000000268
167	1	0.000000674	0.000000021	0.000000348
168	1	0.000000890	0.000000390	0.000000106
169	1	0.000000962	0.000000304	0.000000502
170	1	-0.000000077	-0.000000075	-0.000000651
171	1	0.000001286	-0.000000490	0.000000096
172	1	0.000000478	0.000000298	0.000000191
173	1	0.000000468	0.000001525	0.000002336
174	1	0.000001413	0.000000377	0.000000841
175	1	0.000001373	0.000001279	0.000000095
176	1	0.000001387	-0.000001218	0.000001093
177	1	0.000000840	0.000000254	0.000001024
178	1	0.000002074	0.000000317	0.000000566
179	1	-0.000000341	-0.000001161	-0.000000153
180	1	-0.000000003	0.000000205	-0.000000230
181	1	0.000001011	-0.000000710	0.000000697
182	1	0.000001220	-0.000001002	-0.000000753

183	1	0.000000963	-0.000001218	0.000000057
184	1	0.000001058	-0.000000954	-0.000000424

Atomic coordinates for calculated geometries of compound **1** in DMSO:

E(RB3LYP) = -4753.89949933 A.U.

Cartesian coordinates

Center Number	Atomic Number	X	Y	Z
1	6	0.000001893	0.000001804	-0.000000673
2	6	-0.000000148	-0.000000408	0.000000788
3	6	0.000002231	0.000000463	-0.000000380
4	6	-0.000000013	0.000001236	-0.000001786
5	6	0.000000928	0.000001900	0.000002052
6	6	-0.000000753	-0.000001668	0.000001917
7	8	-0.000003261	0.000001492	-0.000002150
8	8	0.000000976	0.000001539	-0.000004833
9	1	-0.000000082	0.000000634	0.000000919
10	6	-0.000000788	0.000001438	-0.000000177
11	6	0.000000583	0.000000930	0.000000326
12	6	-0.000000568	0.000001259	-0.000002178
13	6	0.000000191	0.000003031	-0.000000773
14	6	-0.000002743	-0.000001171	0.000000016
15	6	0.000005115	0.000000335	-0.000000319
16	6	-0.000000730	-0.000000879	0.000001538
17	8	0.000002160	-0.000000879	0.000001725
18	1	-0.000000217	-0.000000356	0.000000182
19	6	-0.000002597	-0.000000396	-0.000000374
20	6	-0.000000527	0.000001610	0.000000521
21	6	-0.000000179	0.000000702	-0.000001519
22	6	0.000000957	-0.000000771	0.000000384
23	6	-0.000000654	-0.000002604	-0.000003029
24	6	-0.000002342	0.000000852	-0.000001587
25	6	-0.000000028	-0.000000401	0.000000244
26	8	-0.000001369	-0.000000632	-0.000001215
27	8	-0.000003054	0.000000940	0.000002498
28	1	-0.000000598	-0.000000607	-0.000000449
29	6	0.000001949	0.000000408	0.000000985
30	6	-0.000000985	-0.000002341	-0.000000919
31	6	-0.000001057	-0.000001855	-0.000002366
32	6	0.000000507	0.000003252	0.000003312
33	6	0.000002586	0.000001576	-0.000004516
34	6	0.000000656	-0.000001151	-0.000000045
35	6	-0.000001435	0.000001387	0.000000007
36	8	-0.000000577	-0.000001437	-0.000000840
37	8	-0.000001623	-0.000004940	0.000003790
38	1	0.000000257	-0.000000623	-0.000000332
39	6	-0.000000696	0.000000277	-0.000000073
40	6	0.000000086	0.000000244	0.000000469
41	6	-0.000000182	-0.000001902	0.000000705
42	1	0.000000215	-0.000000636	-0.000000386
43	6	0.000000852	-0.000000767	0.000000327
44	1	0.000000478	0.000000595	0.000000065
45	6	0.000001187	0.000000961	0.000000836
46	1	-0.000001047	-0.000000574	0.000000189
47	1	0.000000690	0.000000219	0.000000514
48	1	0.000001066	0.000000071	0.000001170
49	6	0.000001937	-0.000000668	0.000001252
50	1	0.000000086	0.000000149	-0.000000361
51	1	0.000001334	-0.000000305	-0.000000610

52	6	0.000000401	-0.000000087	0.000000412
53	6	0.000000119	0.000000005	-0.000000560
54	1	0.000001415	-0.000000805	-0.000000376
55	1	-0.000000152	-0.000000573	0.000000284
56	1	0.000000405	-0.000000278	0.000000217
57	1	-0.000000170	-0.000000609	0.000000102
58	6	0.000000096	-0.000000296	0.000000685
59	1	0.000000654	-0.000000124	0.000001313
60	6	0.000001438	-0.000002097	-0.000001492
61	1	-0.000000096	0.000000850	0.000002012
62	1	0.000000626	-0.000000310	0.000000666
63	1	-0.000001018	-0.000001044	-0.000003693
64	1	0.000000188	0.000000306	-0.000001421
65	1	0.000000068	0.000002084	-0.000000421
66	1	-0.000001494	-0.000000624	-0.000001044
67	8	0.000002746	0.000003171	0.000002454
68	6	-0.000001803	0.000001042	-0.000001287
69	1	0.000000024	-0.000001094	0.000001292
70	6	-0.000000700	0.000000378	0.000001376
71	1	-0.000001313	-0.000002895	0.000001873
72	6	0.000001097	0.000000083	0.000001764
73	6	-0.000000834	-0.000000691	-0.000001279
74	6	-0.000000050	0.000000772	0.000000275
75	6	0.000001346	0.000000745	-0.000000676
76	8	-0.000000544	-0.000000076	-0.000000005
77	6	-0.000000249	0.000006840	0.000003862
78	8	-0.000001940	-0.000002301	0.000002305
79	8	0.000001561	0.000001642	0.000001116
80	6	-0.000000066	0.000000779	0.000000039
81	6	-0.000000261	0.000000845	0.000000300
82	6	0.000000469	0.000001303	0.000000565
83	6	-0.000001011	0.000001089	0.000001026
84	6	0.000000381	0.000000087	0.000000418
85	6	-0.000000447	0.000000354	0.000002077
86	6	0.000000934	0.000000675	-0.000000016
87	6	-0.000000055	0.000001821	0.000000035
88	8	0.000001231	-0.000000449	0.000000425
89	6	-0.000002064	0.000002607	0.000001571
90	8	0.000001599	-0.000001125	-0.000000358
91	6	0.000000372	0.000000682	0.000001350
92	6	0.000000543	0.000000679	0.000001296
93	6	0.000000409	0.000001129	0.000001226
94	6	0.000000878	-0.000000325	0.000001342
95	8	-0.000001140	0.000003042	0.000000118
96	6	0.000000137	-0.000000447	-0.000000239
97	6	0.000002097	0.000000497	-0.000000412
98	6	-0.000003192	-0.000000417	-0.000000521
99	8	0.000000460	0.000001162	-0.000002230
100	6	-0.000003481	-0.000002138	-0.000000839
101	8	0.000002179	0.000001658	-0.000000313
102	6	-0.000001884	0.000000718	-0.000003130
103	6	-0.000001140	0.000001114	-0.000000812
104	8	-0.000001349	-0.000000058	0.000004167
105	6	-0.000000571	0.000000571	-0.000000956
106	6	-0.000000440	0.000000431	-0.000001200
107	6	-0.000001476	-0.000000163	-0.000001081
108	6	0.000000039	-0.000000018	-0.000001054
109	6	-0.000001364	0.000002274	0.000000625
110	6	0.000001473	-0.000000130	0.000002385
111	8	-0.000003411	-0.000001647	-0.000002672
112	6	0.000005716	-0.000001455	-0.000004797
113	8	-0.000001122	0.000000270	0.000002325
114	6	0.000000225	0.000002452	-0.000006306
115	6	0.000000023	-0.000002121	0.000000594
116	8	-0.000001302	-0.000004661	0.000003692
117	6	0.000000893	-0.000000505	0.000000054
118	6	0.000000174	-0.000000618	-0.000001515
119	6	0.000000117	-0.000001475	0.000000373
120	6	-0.000000907	-0.000001031	-0.000001231

121	1	-0.000001258	-0.000001904	-0.000000640
122	1	-0.000000600	-0.000000628	-0.000001416
123	1	-0.000000407	0.000001151	0.000000441
124	1	-0.000000132	0.000000023	0.000000117
125	1	0.000000105	0.000000534	-0.000000015
126	1	-0.000000032	0.000000683	0.000000363
127	1	-0.000000548	0.000000318	-0.000000541
128	1	-0.000000019	0.000000762	0.000000203
129	1	-0.000000230	0.000001128	0.000000305
130	1	-0.000000205	0.000001347	0.000000442
131	1	0.000000045	0.000001355	0.000000494
132	1	0.000000754	0.000000785	0.000001199
133	1	0.000000627	0.000000999	0.000001299
134	1	0.000000633	0.000000768	0.000001341
135	1	0.000000588	0.000000529	0.000000918
136	1	-0.000000433	0.000001701	0.000000064
137	1	0.000000444	0.000000443	-0.000000147
138	1	-0.000000026	0.000000009	-0.000000673
139	1	-0.000001473	-0.000000964	-0.000003476
140	1	-0.000000568	0.000000945	-0.000000368
141	1	-0.000001033	0.000000390	-0.000001068
142	1	-0.000001051	0.000000036	-0.000001341
143	1	-0.000000979	-0.000000051	-0.000001392
144	1	0.000000885	-0.000000136	-0.000000823
145	1	-0.000001056	-0.000001898	-0.000001252
146	1	0.000000186	-0.000001415	-0.000000708
147	1	0.000000064	-0.000001368	-0.000000611
148	1	-0.000000024	-0.000000733	-0.000000622
149	6	-0.000000011	-0.000000959	0.000000075
150	6	-0.000000284	-0.000000763	-0.000000637
151	6	0.000000037	-0.000000558	-0.000000135
152	6	-0.000000419	-0.000001735	-0.000000489
153	6	0.000000002	-0.000000108	0.000000502
154	6	0.000000492	0.000000502	0.000000670
155	6	0.000000647	-0.000001061	0.000000365
156	6	0.000000533	-0.000000754	0.000000768
157	1	-0.000000343	0.000000227	0.000000065
158	1	-0.000000048	0.000000154	0.000000050
159	1	-0.000000240	-0.000000883	-0.000000230
160	1	0.000000767	-0.000000648	0.000000117
161	1	0.000000152	-0.000001127	-0.000000266
162	1	0.000000295	-0.000001060	-0.000000336
163	1	0.000000271	-0.000001273	-0.000000451
164	1	-0.000000234	-0.000000808	-0.000000294
165	1	0.000000060	-0.000001205	-0.000000477
166	1	0.000000268	-0.000001229	-0.000000769
167	1	0.000000206	-0.000000582	-0.000000084
168	1	0.000000321	-0.000000408	0.000000240
169	1	0.000000420	-0.000000637	0.000000128
170	1	0.000000195	-0.000000524	0.000000315
171	1	0.000000458	-0.000000408	-0.000000137
172	1	0.000000249	-0.000000464	-0.000000331
173	1	0.000000401	0.000000034	0.000000561
174	1	0.000000564	-0.000000059	0.000000962
175	1	0.000000766	0.000000078	0.000000794
176	1	0.000000681	-0.000000089	0.000000893
177	1	0.000000634	0.000000171	0.000001002
178	1	0.000000812	-0.000000034	0.000001103
179	1	0.000000222	-0.000000189	0.000000537
180	1	0.000000095	0.000000108	0.000000582
181	1	0.000000319	0.000000033	0.000000704
182	1	0.000000628	-0.000000389	0.000000597
183	1	0.000000443	-0.000000562	0.000000320
184	1	0.000000232	-0.000000401	0.000000277