Supplementary Data

Figure S1. The ^{1}H-NMR spectrum of the compound **4** (dimethylsulfoxide-d_6, 400 MHz).

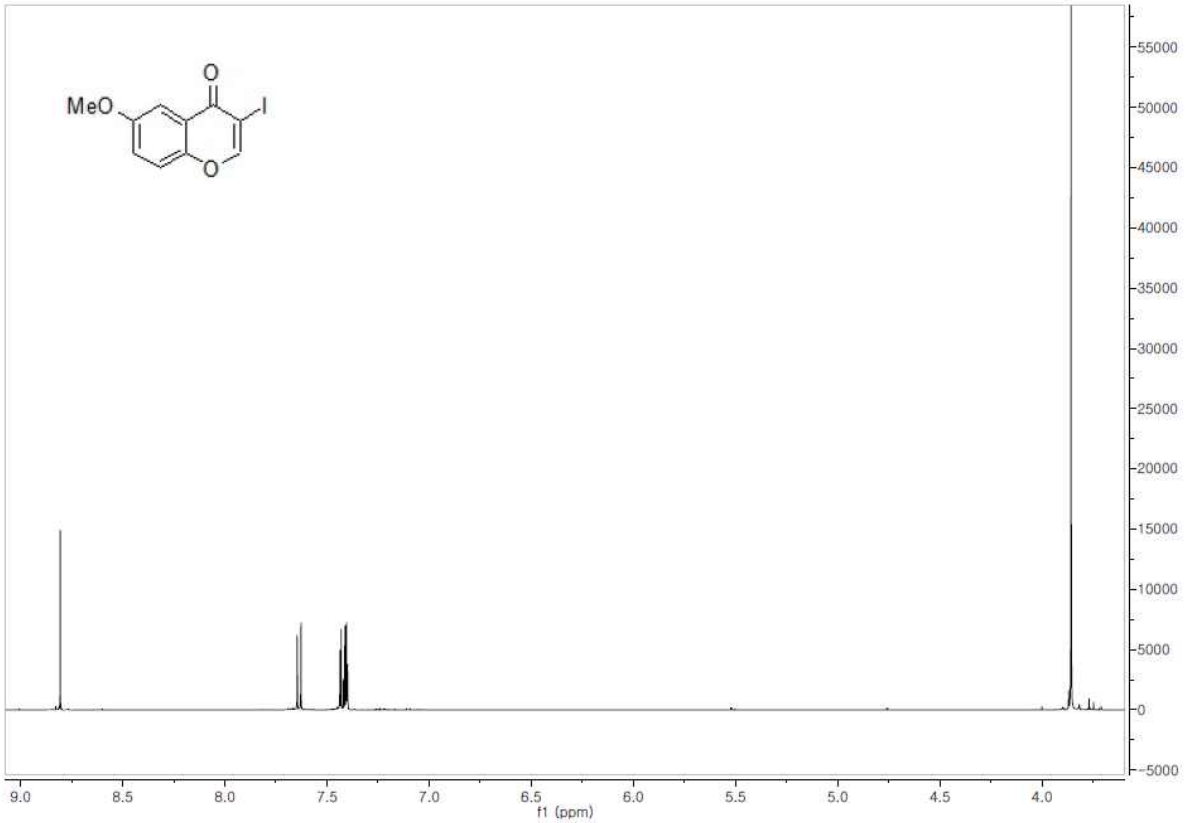

Figure S2. The ^{13}C-NMR spectrum of the compound **4** (dimethylsulfoxide-d_6, 100 MHz).

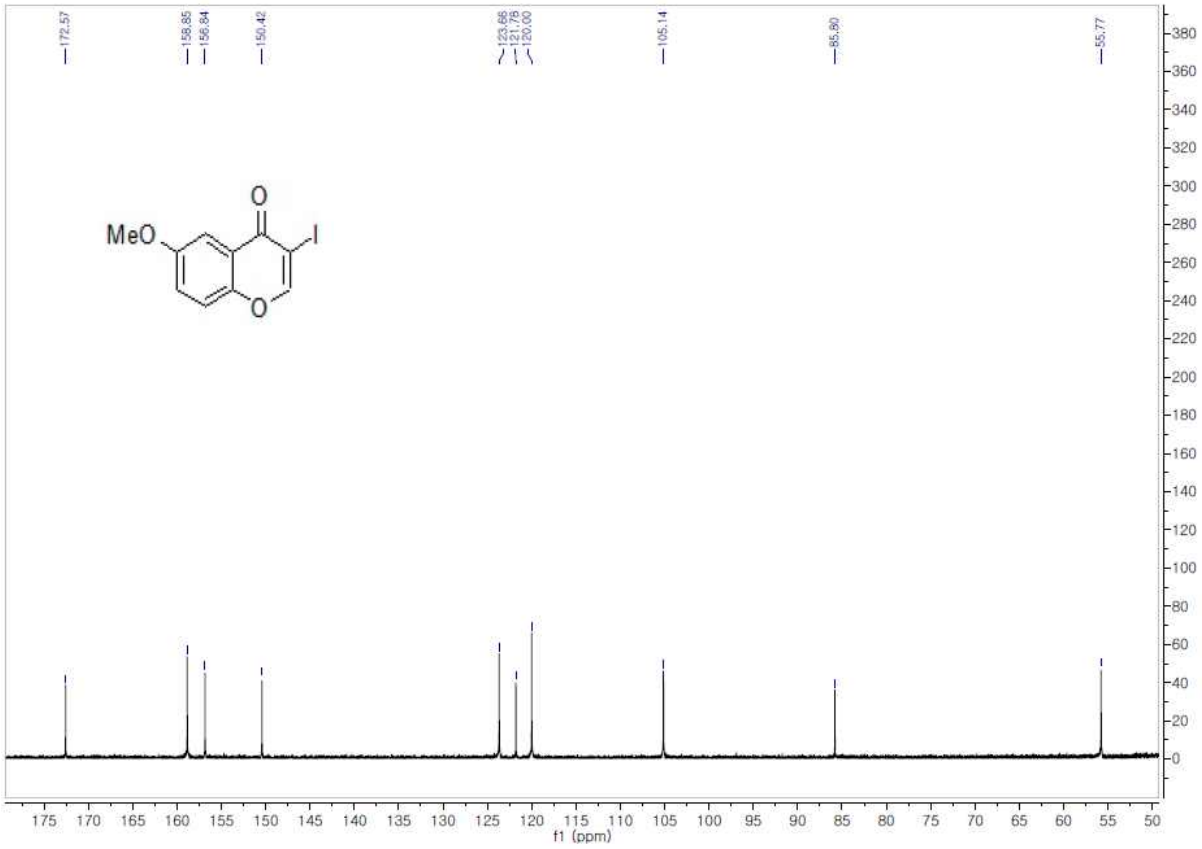

Figure S3. The ^{1}H-NMR spectrum of the compound **6** (dimethylsulfoxide-d_6, 400 MHz).

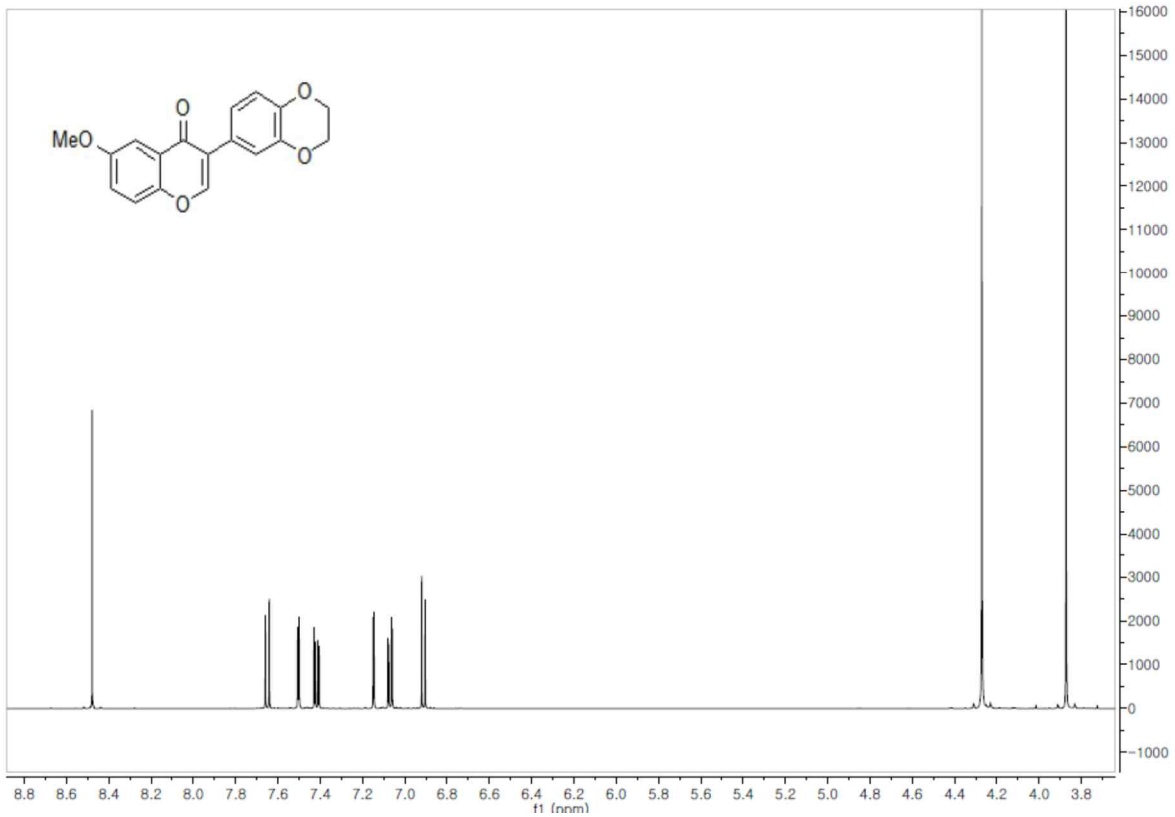

Figure S4. The ^{13}C-NMR spectrum of the compound **6** (dimethylsulfoxide-d_6, 100 MHz).

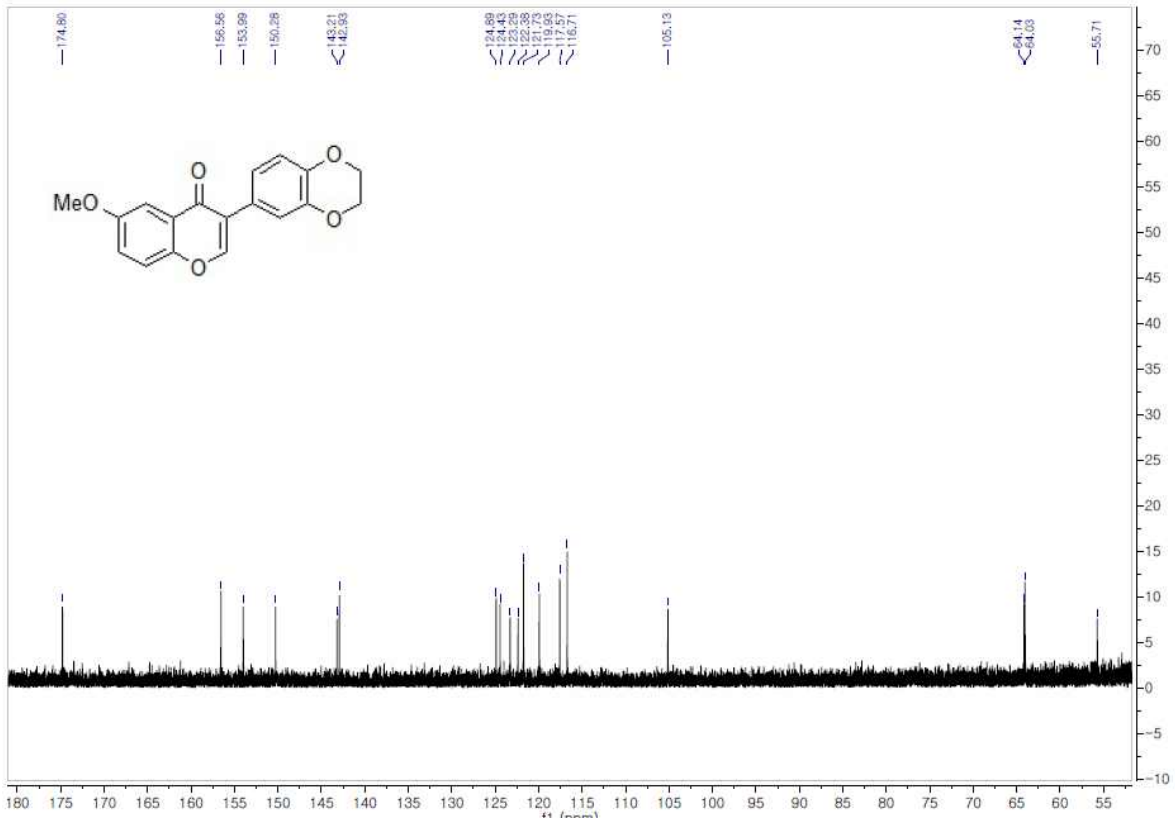

Figure S5. High resolution Mass Spectrum of compound **6**.

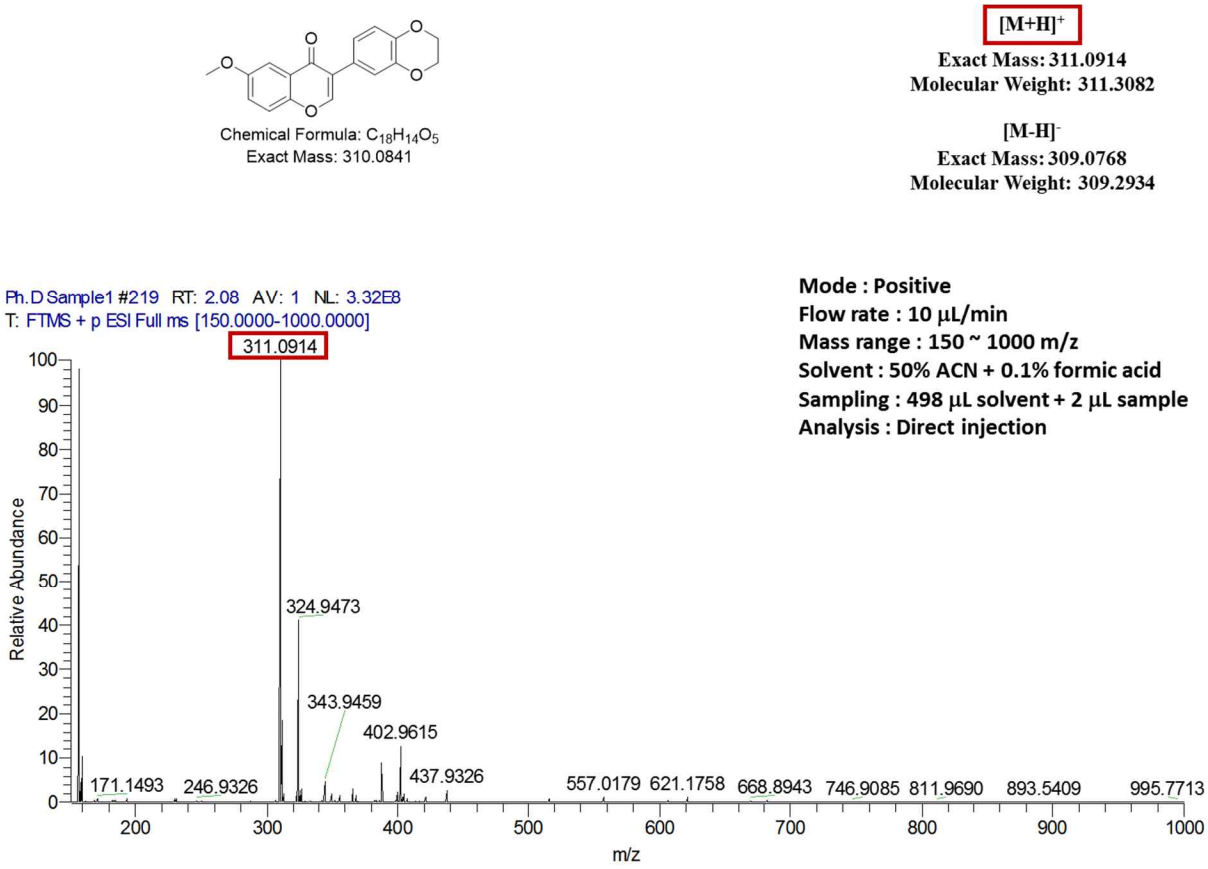

Figure S6. Optimized molecular structure with atom numbering of compound **6**.

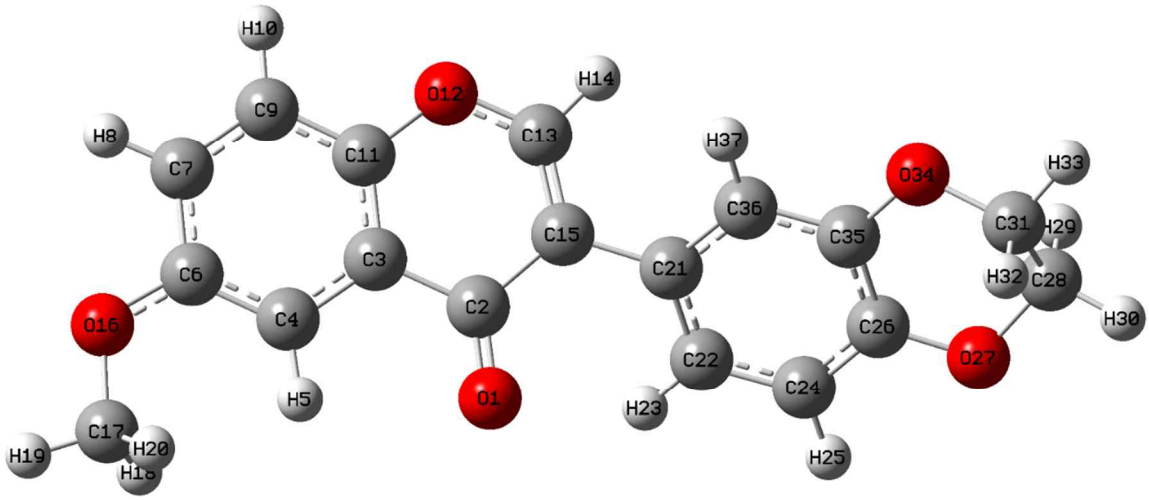

Table S1. Bond lengths (Å) of compound **6**.

Geometric parameters	X-ray	Calculation		Geometric parameters	X-ray	Calculation	
		vacuum	DMSO			vacuum	DMSO
R(1,2)	1.2292	1.2263	1.2344	R(15,21)	1.4893	1.4825	1.4846
R(2,3)	1.4770	1.4806	1.4762	R(16,17)	1.4250	1.424	1.4307
R(2,15)	1.4630	1.4754	1.4683	R(21,22)	1.4005	1.4043	1.4039
R(3,4)	1.4049	1.4070	1.4087	R(21,36)	1.3863	1.3995	1.3989
R(3,11)	1.3859	1.3931	1.3950	R(22,24)	1.3861	1.388	1.3891
R(4,6)	1.3775	1.3858	1.3862	R(24,26)	1.3877	1.3934	1.3948
R(6,7)	1.4046	1.4114	1.4126	R(26,27)	1.3759	1.3731	1.3708
R(6,16)	1.3661	1.3620	1.3607	R(26,35)	1.3961	1.4009	1.4025
R(7,9)	1.3667	1.3787	1.3784	R(27,28)	1.4400	1.4294	1.4381
R(9,11)	1.3947	1.3993	1.3994	R(28,31)	1.4899	1.5174	1.5143
R(11,12)	1.3755	1.3701	1.3694	R(31,34)	1.4367	1.4294	1.4377
R(12,13)	1.3494	1.3482	1.3440	R(34,35)	1.3721	1.3759	1.3726
R(13,15)	1.3493	1.3561	1.3574	R(35,36)	1.3875	1.3913	1.3933

Table S2. Bond angles (°) of compound **6**

Geometric Parameters	X-ray	Calculation		Geometric Parameters	X-ray	Calculation	
		vacuum	DMSO			vacuum	DMSO
A(1,2,3)	121.8648	121.7015	121.7607	A(13,15,21)	118.8496	119.6280	119.4680
A(1,2,15)	123.8063	123.8876	123.5074	A(6,16,17)	117.1009	118.1838	118.3373
A(3,2,15)	114.3289	114.4103	114.7284	A(15,21,22)	120.7945	121.3677	121.1824
A(2,3,4)	120.7133	120.2757	120.7552	A(15,21,36)	120.3565	120.1609	120.2580
A(2,3,11)	120.3787	120.5781	120.2251	A(22,21,36)	118.7523	118.4673	118.5522
A(4,3,11)	118.8985	119.1459	119.0182	A(21,22,24)	120.2779	120.5053	120.5250
A(3,4,6)	119.7066	120.0296	120.0343	A(22,24,26)	120.5706	120.6884	120.6644
A(4,6,7)	120.1745	119.8527	119.861	A(24,26,27)	118.6301	118.6835	118.6757
A(4,6,16)	124.9622	124.9269	124.8516	A(24,26,35)	119.3364	119.3260	119.3059
A(7,6,16)	114.8629	115.2204	115.2874	A(27,26,35)	122.0335	121.9786	122.0126
A(6,7,9)	120.7909	120.6298	120.6792	A(26,27,28)	113.2887	114.0182	114.1073
A(7,9,11)	118.7844	119.1336	119.0796	A(27,28,31)	110.6314	110.2612	110.1692
A(3,11,9)	121.6300	121.2082	121.3277	A(28,31,34)	110.2419	110.1749	110.1490
A(3,11,12)	122.0288	121.5628	121.5737	A(31,34,35)	112.8593	113.6936	113.9220
A(9,11,12)	116.3403	117.2283	117.0985	A(26,35,34)	122.2627	121.8329	121.8617
A(11,12,13)	117.8290	118.6579	118.9153	A(26,35,36)	119.8240	119.8710	119.8288
A(12,13,15)	125.8353	125.9324	125.4834	A(34,35,36)	117.8992	118.2958	118.3095
A(2,15,13)	119.4507	118.7982	119.0678	A(21,36,35)	121.0950	121.1054	121.1011
A(2,15,21)	121.6959	121.5738	121.4616				

Table S3. Dihedral angles (°) of compound **6**

Geometric Parameters	X-ray	Calculation		Geometric Parameters	X-ray	Calculation	
		vacuum	DMSO			vacuum	DMSO
D(1,2,3,4)	-4.2771	1.4182	-0.3955	D(12,13,15,2)	-0.3771	2.4396	0.9534
D(1,2,3,11)	176.8544	-178.7862	179.1459	D(12,13,15,21)	178.9230	-177.6270	-178.4775
D(15,2,3,4)	175.7952	-178.2956	-179.7417	D(2,15,21,22)	49.3755	42.4779	49.5214
D(15,2,3,11)	-3.0732	1.5000	-0.2003	D(2,15,21,36)	-134.2450	-138.2763	-131.4760
D(1,2,15,13)	-176.6634	177.5041	-179.7730	D(13,15,21,22)	-129.9082	-137.4535	-131.0618
D(1,2,15,21)	4.0571	-2.4279	-0.3538	D(13,15,21,36)	46.4713	41.7922	47.9409
D(3,2,15,13)	3.2627	-2.7892	-0.4396	D(15,21,22,24)	173.2024	177.3507	177.5833
D(3,2,15,21)	-176.0168	177.2788	178.9795	D(36,21,22,24)	-3.2343	-1.9075	-1.4360
D(2,3,4,6)	-178.4703	179.8215	179.6802	D(15,21,36,35)	-175.2673	-177.7442	-178.0390
D(11,3,4,6)	0.4146	0.0230	0.1334	D(22,21,36,35)	1.1854	1.5232	0.9896
D(2,3,11,9)	179.6292	-179.9404	-179.6731	D(21,22,24,26)	1.7727	0.6215	0.5207
D(2,3,11,12)	0.0002	0.3739	0.4242	D(22,24,26,27)	-178.2569	179.8507	-179.9988
D(4,3,11,9)	0.7404	-0.1425	-0.1238	D(22,24,26,35)	1.7616	1.0822	0.8614
D(4,3,11,12)	-178.8886	-179.8282	179.9735	D(24,26,27,28)	167.2632	166.0754	165.5555
D(3,4,6,7)	-1.0104	0.0811	-0.0865	D(35,26,27,28)	-12.7558	-15.1905	-15.3291
D(3,4,6,16)	179.2042	-179.9772	179.8993	D(24,26,35,34)	177.5991	178.3477	178.7352
D(4,6,7,9)	0.4672	-0.0690	0.0278	D(24,26,35,36)	-3.7940	-1.4640	-1.3023
D(16,6,7,9)	-179.7267	179.9838	-179.9594	D(27,26,35,34)	-2.3818	-0.3786	-0.3748
D(4,6,16,17)	-5.7978	-0.0149	0.0138	D(27,26,35,36)	176.2252	179.8097	179.5877
D(7,6,16,17)	174.4067	179.9293	-179.9998	D(26,27,28,31)	43.8989	44.5697	44.6684
D(6,7,9,11)	0.6666	-0.0478	-0.0165	D(27,28,31,34)	-62.4032	-61.2522	-60.8167
D(7,9,11,3)	-1.2793	0.1548	0.0658	D(28,31,34,35)	46.8129	45.8782	45.5193
D(7,9,11,12)	178.3698	179.8536	179.9727	D(31,34,35,26)	-15.8245	-16.5440	-16.1855
D(3,11,12,13)	3.0264	-1.0184	0.0145	D(31,34,35,36)	165.5430	163.2706	163.8514
D(9,11,12,13)	-176.6211	179.2839	-179.8921	D(26,35,36,21)	2.3277	0.1522	0.3738
D(11,12,13,15)	-2.9046	-0.4474	-0.7407	D(34,35,36,21)	-179.0052	-179.6661	-179.6624

Table S4. NPA charge on the atoms of compound **6**.

Atom	Charge	Atom	Charge
O1	-0.59255	H20	0.17345
C2	0.50307	C21	-0.04958
C3	-0.15992	C22	-0.18082
C4	-0.23688	H23	0.22507
H5	0.23862	C24	-0.22232
C6	0.31451	H25	0.21851
C7	-0.19783	C26	0.25378
H8	0.22206	O27	-0.54652
C9	-0.21801	C28	-0.05046
H10	0.22333	H29	0.17590
C11	0.30994	H30	0.19623
O12	-0.47240	C31	-0.05082
C13	0.23360	H32	0.17692
H14	0.19585	H33	0.19595
C15	-0.18767	O34	-0.55010
O16	-0.54062	C35	0.25023
C17	-0.20603	C36	-0.22493
H18	0.17326	H37	0.21507
H19	0.19209		

Figure S7. Molecular orbital surfaces of selected MOs of compound **6** in vacuum (A) and in DMSO (B).