3-(4-Formylphenyl)-triazole functionalized coumarins as violet-blue luminophores and n-type semiconductors: synthesis, photophysical, electrochemical and thermal properties

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Table S1. Yields compounds **1a-g**

Substituent	Compound	Yield (%)
H	**1a**	87
6-OCH_3	**1b**	97
7-NEt_2	**1c**	75
6-Br	**1d**	93
6-Cl	**1e**	87
8-OEt	**1f**	84
7-OH	**1g**	77

Table S2. Calculated torsion angles **1a-g**

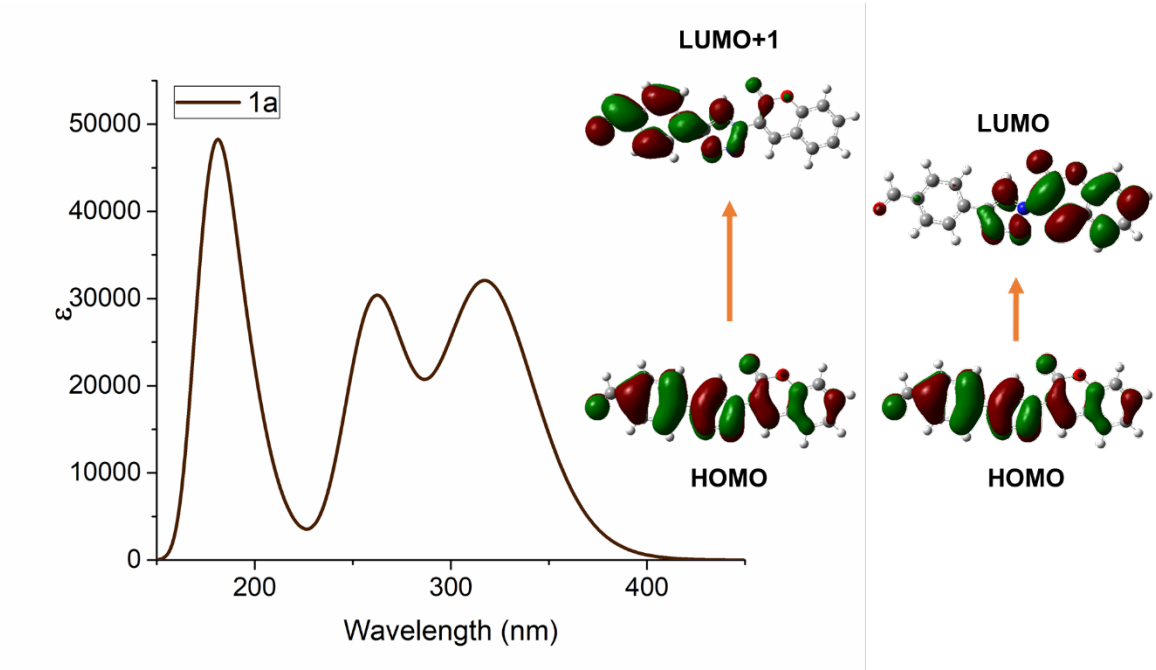
	Ángulo de torsión C2-C3-N-C9	Ángulo de torsión N-C10-C11-C12
1a	0.014	0.017
1b	0.025	0.0059
1c	0.25	0.17
1d	0.024	0.0049
1e	0.012	0.039
1f	0.0032	0.026
1g	0.031	0.04

Tables S3. Table S3. Computed electronic transitions of PhTCs 1a-g: wavelength of excitation (λ_{DFT}) in nm, energy (E) in eV, oscillation strength (f) and MO configuration (% probability), in bold the most probable transition in both the gas phase and CH_2Cl_2 solutions.

Table S3.1. First thirty electronic transitions of **1a**, obtained by BhandHLYP/6-31G (d, p), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1a	318.16	3.8969	**0.7810**	H-1→L (11%), **H→L (84%)**
	312.67	3.9653	0.0002	H-4→L (3%), H-4→L+1 (75%), H-4→L+6 (17%)
	272.04	4.5576	0.0177	H-3→L (21%), H-1→L (61%), H→L (7%)
	262.07	4.7310	**0.6731**	H-1→L+1 (6%), H→L (2%), **H→L+1 (83%)**
	257.46	4.8156	0.0416	H-3→L (62%), H-1→L (19%), H-1→L+2 (5%), H→L+1 (4%), H→L+2 (2%)
	248.66	4.9862	0.0180	H-2→L (10%), H-2→L+1 (63%), H-1→L+5 (2%), H→L+3 (3%), H→L+4 (6%), H→L+5 (9%).
	235.67	5.2609	0.0007	H-8→L (60%), H-8→L+1 (2%), H-8→L+2 (6%), H-8→L+3 (12%), H-6→L (7%)
	229.41	5.4045	0.0046	H-8→L (8%), H-6→L (46%), H-6→L+1 (3%), H-6→L+2 (6%), H-6→L+3 (5%), H-6→L+4 (8%), H-6→L+5 (7%), H-5→L (3%), H-2→L (3%)
	219.27	5.6545	0.0096	H-6→L (2%), H-2→L (83%), H-2→L+1 (7%)
	215.76	5.7463	0.0475	H-7→L (2%), H-3→L (2%), H-2→L+1 (3%), H-1→L+1 (8%), H-1→L+2 (2%), H→L+2 (38%), H→L+3 (18%), H→L+4 (7%), H→L+5 (7%)
	207.51	5.9748	0.0271	H-3→L (8%), H-3→L+2 (4%), H-3→L+4 (7%), H-1→L+2 (15%), H-1→L+3 (14%), H-1→L+4 (2%), H→L+2 (10%), H→L+3 (27%)
	206.18	6.0134	0.0158	H-7→L (5%), H-5→L (24%), H-5→L+1 (5%), H-1→L+1 (41%), H→L+1 (5%), H→L+2 (3%),
	202.02	6.1371	0.0564	H-7→L (9%), H-5→L (14%), H-1→L+1 (8%), H-1→L+2 (10%), H-1→L+3 (6%), H-1→L+4 (3%), H→L+4 (34%)
	199.27	6.2218	**0.1130**	H-7→L (11%), **H-5→L (16%), H-3→L+2 (16%),** H-3→L+3 (2%), H-1→L+1 (12%), H-1→L+2 (3%), H-1→L+4 (8%), H→L+2 (6%), H→L+3 (8%), H→L+4 (5%), H→L+5 (3%)
	195.90	6.3290	**0.1108**	**H-7→L (32%),** H-5→L (25%), H-3→L+2 (7%), H-2→L+1 (5%), H-1→L+1 (8%), H-1→L+3 (4%), H→L+4 (4%), H→L+5 (3%)
	192.78	6.4315	**0.1391**	H-7→L (12%), H-4→L (2%), H-2→L+1 (15%), H-1→L+4 (3%), H→L+4 (4%), **H→L+5 (50%)**
	192.16	6.4520	0.0046	H-4→L (98%)
	190.37	6.5126	0.0016	H-6→L (14%), H-6→L+1 (18%), H-6→L+6 (5%), H-5→L+1 (26%), H-4→L (4%), H-1→L+2 (5%), H-1→L+3 (4%), H→L+2 (2%), H→L+6 (2%)

	188.10	6.5914	0.0612	H-6→L (7%), H-6→L+1 (20%), H-6→L+6 (4%), H-5→L+1 (8%), H-1→L+2 (14%), H-1→L+3 (5%), H-1→L+5 (4%), H→L+2 (5%), H→L+4 (4%), H→L+6 (4%)
	184.85	6.7071	0.3838	H-7→L (6%), H-5→L+1 (20%), H-3→L+2 (6%), H-2→L+4 (3%), H-2→L+5 (6%), H-1→L+1 (3%), H-1→L+2 (10%), H-1→L+3 (12%), H-1→L+4 (7%), H-1→L+5 (5%), H→L+2 (2%), H→L+3 (4%)
	181.51	6.8308	0.2159	H-9→L (4%), H-7→L (8%), H-5→L+1 (7%), H-3→L+2 (21%), H-3→L+3 (6%), H-1→L+2 (7%), H-1→L+3 (3%), H-1→L+5 (2%), H→L+2 (6%), H→L+4 (12%), H→L+5 (9%)
	181.09	6.8464	0.0749	H-5→L+1 (3%), H-3→L+1 (4%), H-3→L+2 (4%), H-3→L+3 (14%), H-3→L+4 (17%), H-1→L+3 (6%), H→L+2 (15%), H→L+3 (21%), H→L+4 (3%)
	177.76	6.9748	0.2642	H-5→L+1 (4%), H-3→L+1 (7%), H-2→L+2 (3%), H-2→L+3 (9%), H-2→L+4 (14%), H-2→L+5 (13%), H-1→L+2 (2%), H-1→L+6 (4%), H→L+6 (28%)
	176.92	7.0081	0.0034	H-13→L (11%), H-12→L (4%), H-10→L (3%), H-10→L+1 (3%), H-8→L (5%), H-8→L+2 (6%), H-8→L+3 (3%). H-6→L (2%), H-6→L+1 (22%), H-6→L+2 (4%), H-6→L+3 (7%), H-6→L+4 (3%), H-6→L+5 (4%), H-3→L+1 (3%)
	176.20	7.0364	0.0245	H-3→L+1 (73%), H→L+3 (3%)
	174.57	7.1023	0.0020	H-15→L (2%), H-12→L (14%), H-12→L+2 (3%), H-12→L+3 (3%), H-12→L+4 (4%), H-12→L+5 (4%), H-11→L (9%), H-11→L+4 (2%), H-10→L (4%), H-6→L (7%), H-6→L+1 (2%), H-6→L+2 (3%), H-6→L+3 (4%), H-6→L+4 (3%)
	172.94	7.1690	0.1945	H-5→L+1 (15%), H-2→L+3 (5%), H-2→L+4 (9%), H-2→L+5 (10%). H→L+6 (42%)
	171.71	7.2204	0.1002	H-11→L (3%), H-9→L (27%) H-3→L+1 (3%), H-3→L+3 (19%), H-3→L+4 (5%), H-3→L+4 (5%), H-1→L+2 (10%), H-1→L+4 (12%), H-1→L+5 (3%), H→L+2 (2%)
	170.19	7.2850	0.0038	H-13→L (21%), H-12→L (3%), H-10→L+1 (2%), H-8→L (12%), H-8→L+2 (14%), H-8→L+3 (6%), H-8→L+4 (2%). H-8→L+8 (2%), H-6→L (3%), H-6→L+1 (5%), H-6→L+2 (3%), H-6→L+3 (3%)
	169.24	7.3259	0.1286	H-9→L (5%), H-3→L+2 (5%) H-3→L+3 (9%), H-3→L+4 (7%), H-1→L+2 (4%), H-1→L+3 (19%), H-1→L+4 (9%), H→L+3 (9%), H→L+4 (6%)



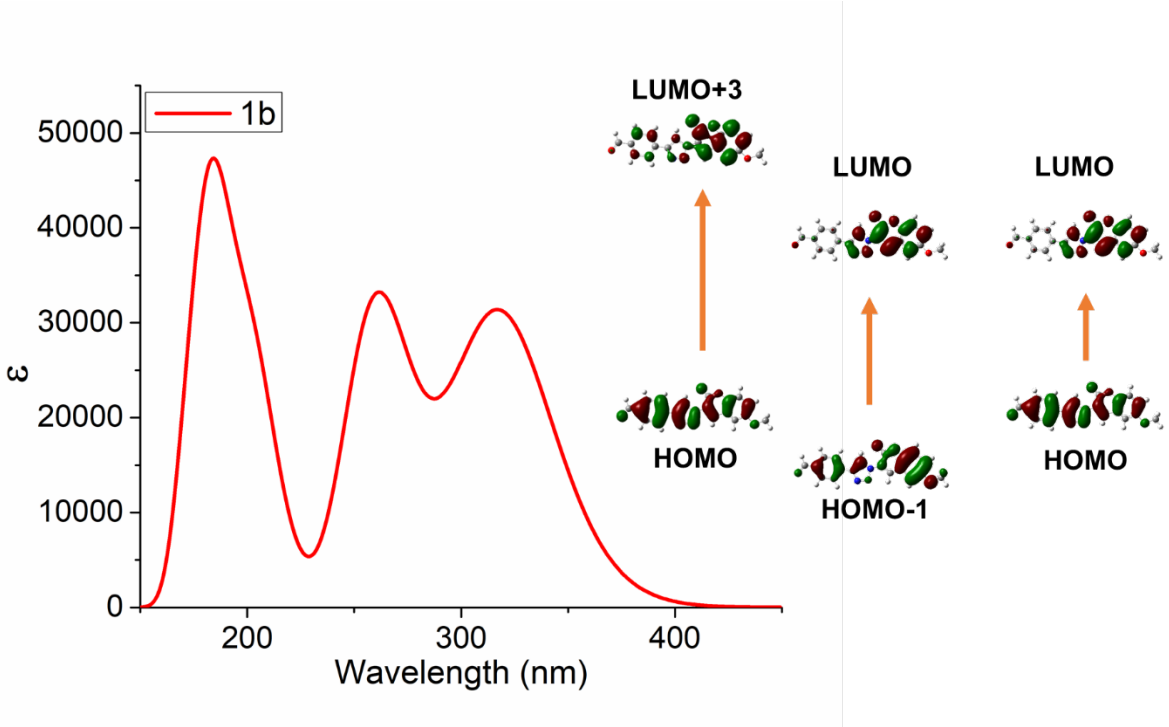
Molecular orbitals of the main electronic transitions calculated by TDDFT BandHLYP/6-31G (d, p).

Table S3.2. First thirty electronic transitions of **1b**, obtained by BhandHLYP/6-31G (d, p), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1b	319.21	3.8841	**0.7302**	H-1→L (16%), **H→L (78%)**
	306.16	4.0496	0.0001	H-4→L (3%), H-4→L+1 (74%), H-4→L+6 (18%)
	292.8	4.2345	0.0737	H-3→L (2%), H-2→L (6%), H-1→L (72%), H→L (12%)
	261.48	4.7417	**0.7004**	H-2→L+1 (2%), H-1→L+1 (7%), H→L (2%), **H→L+1 (80%)**
	257.19	4.8207	0.0899	H-5→L (2%), H-3→L (23%), H-2→L (56%), H-1→L (5%), H-1→L+2 (3%), H→L (3%), H→L+1 (3%)
	247.56	5.0083	0.0172	H-3→L (6%), H-3→L+1 (40%), H-2→L (4%), H-2→L+1 (23%), H→L+2 (2%), H→L+3 (2%), H→L+4 (10%), H→L+5 (4%),
	232.18	5.3401	0.0021	H-8→L (46%), H-8→L+2 (3%), H-8→L+3 (10%), H-6→L (24%), H-6→L+2 (4%), H-6→L+5 (3%)
	227.85	5.4415	0.0031	H-8→L (23%), H-8→L+3 (6%), H-6→L (38%), H-6→L+1 (3%), H-6→L+2 (9%), H-6→L+5 (8%)
	217.95	5.6885	0.0251	H-3→L (60%), H-3→L+1 (4%), H-2→L (27%), H-2→L+1 (3%)
	213.26	5.8139	0.0337	H-3→L+1 (6%), H-2→L+2 (4%), H-1→L (3%), H-1→L+1 (5%), H-1→L+2 (4%), H-1→L+3 (15%), H→L+2 (44%), H→L+5 (3%)
	210.83	5.8807	0.0345	H-7→L (5%), H-3→L+1 (5%), H-1→L+1 (7%), H-1→L+2 (12%), H-1→L+3 (19%), H→L+3 (28%), H→L+5 (7%)
	206.81	5.9950	0.1512	H-7→L (6%), H-5→L (6%), H-2→L+1 (8%), H-2→L+2 (2%), H-1→L+1 (34%), H-1→L+2 (10%), H-1→L+4 (3%), H→L+1 (6%), H→L+2 (5%), H→L+4 (8%)

	203.15	6.1031	**0.2440**	H-5→L (6%), H-3→L+3 (2%), H-2→L+1 (6%), H-2→L+2 (5%), H-2→L+2 (3%), H-1→L+1 (4%), H-1→L+2 (19%), H-1→L+4 (14%), H-1→L+5 (3%), H→L+2 (6%), H→L+3 (15%),
	199.44	6.2165	0.0722	H-7→L (19%), H-5→L (45%), H-1→L+1 (9%), H→L+4 (6%)
	195.24	6.3502	**0.1685**	H-7→L (13%), H-5→L (13%), H-2→L+1 (11%), H-2→L+3 (4%), H-1→L+1 (16%), H→L+4 (26%), H→L+5 (2%)
	191.11	6.4874	0.0309	H-7→L (28%), H-5→L (15%), H-2→L+1 (19%), H-1→L+1 (6%), H→L+4 (3%), H→L+5 (16%)
	190.71	6.5012	0.0005	H-6→L+1 (10%), H-4→L (80%)
	190.09	6.5224	0.1620	H-7→L (3%), H-5→L+1 (12%), H-3→L+1 (22%), H-3→L+2 (3%), H-3→L+4 (4%), H-2→L+1 (7%), H-2→L+3 (2%), H-1→L+1 (5%), H-1→L+3 (8%), H→L+2 (3%), H→L+3 (3%), H→L+4 (5%), H→L+5 (13%),
	189.3	6.5495	0.0021	H-6→L (17%), H-6→L+1 (44%), H-6→L+6 (9%), H-4→L (15%),
	185.61	6.6799	0.0996	H-5→L+1 (13%), H-3→L+1 (10%), H-3→L+2 (2%), H-2→L+1 (11%), H-2→L+2 (3%), H-2→L+5 (3%), H-1→L+1 (3%), H-1→L+2 (9%), H-1→L+3 (10%), H-1→L+4 (2%), H→L+3 (10%), H→L+4 (7%), H→L+6 (6%)
	185.07	6.6995	0.1143	H-7→L (5%), H-5→L+1 (19%), H-3→L+3 (4%), H-3→L+4 (3%), H-2→L+2 (12%), H-2→L+3 (3%), H-1→L+3 (17%), H→L+2 (10%), H→L+5 (9%)
	183.23	6.7664	**0.4857**	H-7→L (12%), H-3→L+2 (3%), H-3→L+3 (3%), H-2→L+2 (12%), H-2→L+3 (11%), H-1→L+4 (10%), H-1→L+5 (11%), H→L+2 (7%), **H→L+3 (17%)**
	181.13	6.8452	0.0010	H-5→L+1 (18%), H-3→L+1 (4%), H-3→L+2 (2%), H-3→L+5 (4%), H-2→L+3 (2%), H-2→L+4 (10%), H-1→L+2 (15%), H→L+4 (12%), H→L+5 (19%)
	177.20	6.9969	0.2413	H-9→L (18%), H-5→L+1 (3%), H-3→L+2 (5%), H-3→L+4 (11%), H-2→L+3 (4%), H-2→L+4 (2%), H-1→L+2 (8%), H-1→L+5 (2%), H-1→L+6 (3%), H→L+4 (2%), H→L+6 (21%),
	176.07	7.0417	0.0002	H-16→L (7%), H-13→L (12%), H-13→L+2 (3%), H-12→L (7%), H-10→L (8%), H-8→L (7%), H-8→L+2 (6%), H-8→L+3 (5%), H-6→L+1 (12%), H-6→L+2 (4%), H-6→L+3 (2%), H-6→L+5 (4%)
	175.95	7.0467	0.0094	H-9→L (63%), H-3→L+2 (3%), H-3→L+3 (2%), H-3→L+4 (3%), H-2→L+4 (4%), H→L+6 (9%)
	173.29	7.1546	0.0020	H-15→L (7%), H-13→L (21%), H-13→L+2 (6%), H-10→L (3%), H-10→L+2 (2%), H-10→L+5 (2%), H-6→L (9%), H-6→L+1 (4%), H-6→L+2 (10%), H-6→L+3 (4%), H-6→L+5 (8%)
	172.15	7.2023	0.1634	H-5→L+1 (23%), H-3→L+2 (5%), H-3→L+3 (8%), H-3→L+4 (7%), H-2→L+4 (7%), H-2→L+5 (3%), H-1→L+2 (3%), H-1→L+6 (2%), H→L+6 (31%)
	170.28	7.2814	0.1162	H-9→L (2%), H-3→L+3 (11%), H-2→L+3 (32%), H-1→L+2 (7%), H-1→L+4 (3%), H→L+3 (14%), H→L+6 (11%),

	168.84	7.3434	0.0004	H-15→L (9%), H-13→L (5%), H-12→L (10%), H-10→L+1 (3%), H-8→L (10%), H-8→L+2 (7%), H-8→L+3 (7%), H-8→L+4 (3%), H-6→L (5%), H-6→L+1 (5%), H-6→L+2 (8%), H-6→L+3 (4%), H-6→L+5 (4%)



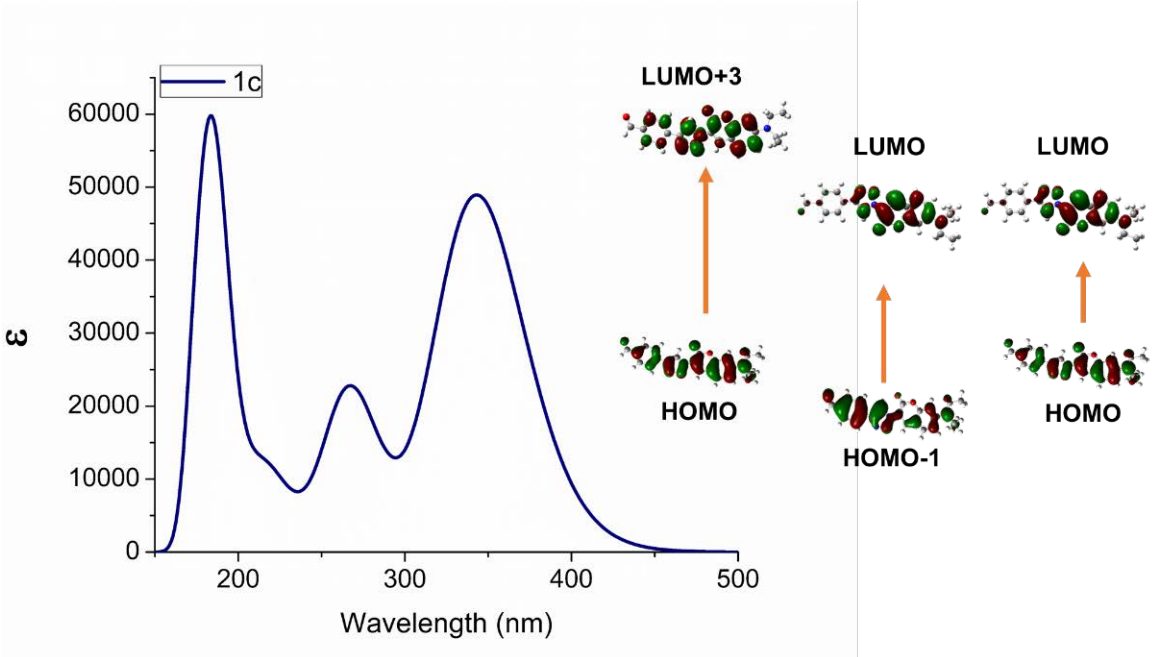
Molecular orbitals of the main electronic transitions calculated by TDDFT BandHLYP/6-31G (d, p).

Table S3.3. First thirty electronic transitions of **1c**, obtained by BhandHLYP/6-31G (d, p), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1c	343.16	3.6130	**1.2071**	**H→L (94%)**
	311.42	3.9813	0.0001	H-5→L+1 (6%), H-4→L (3%), H-4→L+1 (70%), H-4→L+6 (16%)
	272.59	4.5484	**0.1547**	**H-1→L (56%)**, H-1→L+1 (11%), H→L+1 (24%), H→L+2 (2%)
	266.06	4.6600	0.3924	H-1→L (34%), H-1→L+1 (28%), H→L+2 (31%)
	262.21	4.7284	0.0116	H-5→L (3%), H-3→L (49%), H-1→L+2 (3%), H→L+2 (31%), H→L+3 (3%)
	248.22	4.9950	0.0158	H-2→L (8%), H-2→L+1 (64%), H-1→L+3 (9%), H-1→L+4 (6%), H→L+3 (4%), H→L+4 (2%)
	234.05	5.2973	0.0521	H-3→L (38%), H-1→L+1 (9%), H→L+1 (7%), H→L+2 (35%)
	231.66	5.3519	0.0300	H-5→L+1 (3%), H-3→L (7%), H-1→L+1 (35%), H→L+1 (29%), H→L+2 (5%), H→L+3 (6%), H→L+4 (3%)
	230.99	5.3676	0.0007	H-8→L (61%), H-8→L+1 (3%), H-8→L+2 (2%), H-8→L+3 (5%), H-8→L+4 (11%). H-7→L (3%)

	223.54	5.5463	0.0064	H-8→L (3%), H-7→L (44%), H-7→L+1 (6%), H-7→L+2 (7%), H-7→L+3 (9%), H-7→L+4 (3%), H-7→L+5 (13%), H-7→L+6 (2%), H-6→L (3%)
	219.19	5.6564	**0.1094**	H-5→L (8%), H-1→L+1 (3%), H-1→L+2 (3%), H→L+1 (3%), H→L+2 (4%), **H→L+3 (39%)**, H→L+4 (23%)
	213.56	5.8057	0.0891	H-6→L (4%), H-5→L (66%), H-4→L (6%), H-2→L (3%), H→L+2 (9%), H→L+3 (3%)
	210.27	5.8965	0.0549	H-3→L+2 (4%), H-2→L (15%), H-1→L+2 (3%), H-1→L+3 (5%), H→L+3 (3%), H→L+4 (18%), H→L+5 (41%)
	208.62	5.9430	0.0053	H-5→L (3%), H-2→L (70%), H-2→L+1 (6%), H→L+5 (12%)
	199.58	6.2124	0.0770	H-6→L (2%), H-6→L+1 (8%), H-2→L+1 (17%), H-1→L+2 (3%), H-1→L+3 (25%), H-1→L+4 (3%), H→L+4 (9%), H→L+5 (16%)
	195.53	6.3410	0.0294	H-9→L (3%), H-7→L+1 (3%), H-6→L (55%), H-6→L+1 (11%), H-5→L (2%), H-5→L (2%), H-1→L+3 (4%), H→L+4 (3%)
	193.95	6.3926	0.1099	H-2→L+1 (4%), H-1→L+2 (31%), H-1→L+3 (4%), H-1→L+4 (16%), H-1→L+5 (11%), H→L+3 (16%), H→L+4 (5%)
	190.37	6.5128	0.0689	H-9→L (4%), H-7→L (25%), H-7→L+1 (25%), H-7→L+6 (6%), H-6→L (10%), H-6→L+1 (15%)
	187.74	6.6041	0.4660	H-9→L (3%), H-7→L (4%), H-7→L+1 (21%), H-7→L+6 (3%), H-6→L (4%), H-6→L+1 (21%), H-5→L+1 (3%), H-3→L+2 (11%), H-2→L+3 (5%), H-2→L+4 (3%), H→L+4 (3%)
	184.88	6.7062	0.3712	H-9→L (2%), H-6→L (3%), H-6→L+1 (6%), H-3→L+1 (7%), H-3→L+2 (44%), H-1→L+2 (6%), H-1→L+3 (7%), H-1→L+5 (3%), H-2→L+2 (3%), H-2→L+5 (3%)
	183.22	6.7669	0.0332	H-9→L (2%), H-5→L (5%), H-5→L+2 (4%), H-4→L (63%), H-1→L+2 (6%), H-1→L+3 (4%)
	183.14	6.7697	0.1433	H-9→L (4%), H-5→L+2 (12%), H-4→L (23%), H-3→L+1 (2%), H-3→L+2 (5%), H-1→L+2 (17%), H-1→L+3 (10%), H-1→L+4 (4%), H-1→L+5 (2%), H→L+2 (2%), H→L+5 (3%)
	179.86	6.8934	0.0003	H-9→L (27%), H-3→L+1 (12%), H-2→L+3 (5%), H-1→L+1 (2%), H-1→L+5 (4%), H-1→L+6 (17%), H→L+6 (12%)
	179.32	6.9141	0.0083	H-6→L+1 (5%), H-5→L+1 (5%), H-3→L+1 (47%), H-3→L+2 (2%), H-3→L+3 (2%), H-2→L+3 (4%), H-1→L+6 (7%), H→L+6 (11%)
	177.22	6.9961	0.3311	H-9→L (30%), H-7→L+1 (2%), H-3→L+1 (10%), H-3→L+2 (6%), H-2→L+3 (13%), H-2→L+4 (5%), H-1→L+6 (5%), H→L+5 (4%), H→L+6 (3%)
	176.87	7.0099	0.0020	H-5→L+1 (21%), H-3→L+1 (11%), H-1→L+3 (7%), H-1→L+4 (8%), H-1→L+5 (3%), H→L+3 (8%), H→L+4 (13%), H→L+5 (4%), H→L+6 (2%)
	175.69	7.0570	0.1114	H-7→L+1 (6%), H-6→L+1 (8%), H-5→L+1 (15%), H-5→L+2 (3%). H-3→L+1 (2%), H-2→L+3 (4%), H-1→L+3 (4%), H-1→L+4 (14%), H-1→L+5 (3%), H→L+3 (7%), H→L+4 (5%), H→L+5 (3%)
	175.08	7.0815	0.0901	H-17→L (3%), H-13→L (3%) H-12→L (4%), H-11→L (4%), H-8→L (4%), H-8→L+2 (5%), H-8→L+4 (2%), H-7→L (4%), H-

				7→L+1 (7%), H-7→L+2 (4%), H-7→L+3 (8%), H-7→L+4 (2%), H-7→L+5 (3%), H-6→L+1 (6%), H-2→L+3 (8%), H-2→L+4 (5%), H-2→L+6 (2%)
	174.37	7.1105	0.0590	H-9→L (3%), H-7→L+1 (3%), H-5→L+1 (9%), H-5→L+2 (4%), H-3→L+3 (3%), H-3→L+4 (14%), H-3→L+5 (12%), H-2→L+3 (9%), H-2→L+4 (4%), H-1→L+4 (9%), H-1→L+5 (3%), H→L+6 (4%)
	172.75	7.1771	0.1098	H-9→L (4%), H-5→L+1 (15%), H-5→L+2 (3%), H-3→L+1 (2%), H-3→L+3 (5%), H-3→L+4 (19%), H-3→L+5 (14%), H-2→L+3 (4%), H-1→L+6 (6%), H→L+6 (7%)



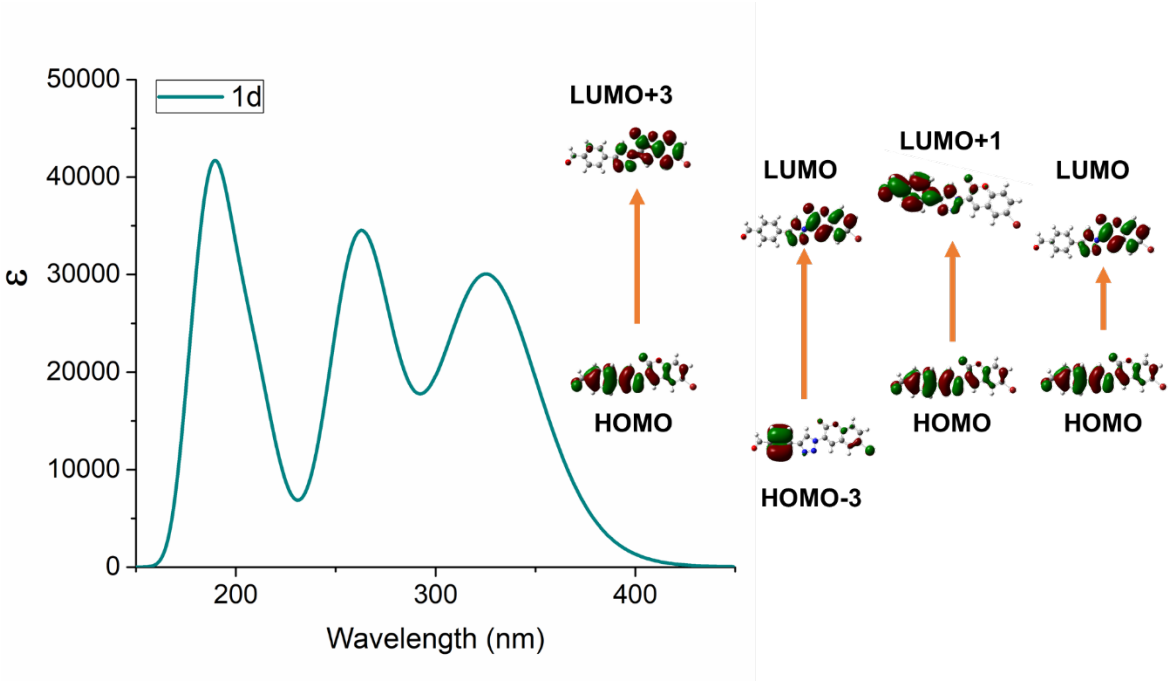
Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p).

Table S3.4. First thirty electronic transitions of **1d**, obtained by BhandHLYP/6-31G (d, p), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1d	325.84	3.8051	**0.7358**	H-1→L (10%), **H→L (84%)**
	313.15	3.9593	0.0001	H-4→L (2%), H-4→L+1 (75%), H-4→L+7 (17%)
	283.13	4.3791	0.0134	H-3→L (10%), H-1→L (73%), H→L (7%)
	262.94	4.7154	**0.8143**	H-3→L (18%), H-1→L (2%), H-1→L+1 (3%), H→L (3%), **H→L+1 (65%)**
	259.08	4.7856	**0.1049**	**H-3→L (54%)**, H-1→L (7%), H-1→L+2 (4%), H→L+1 (23%), H→L+2 (2%)
	249.15	4.9764	0.0187	H-2→L (13%), H-2→L+1 (61%), H→L+4 (6%), H→L+6 (11%)
	237.24	5.2261	0.0013	H-10→L (45%), H-10→L+2 (3%), H-10→L+3 (10%), H-9→L (9%), H-9→L+3 (2%), H-6→L (15%), H-6→L+4 (3%)

	232.97	5.3220	0.0030	H-10→L (12%), H-10→L+3 (3%), H-9→L (2%), H-6→L (39%), H-6→L+2 (3%), H-6→L+4 (14%), H-6→L+6 (4%), H-5→L (6%), H-2→L (4%)
	225.45	5.4994	0.0104	H-6→L (3%), H-2→L (79%), H-2→L+1 (9%)
	217.09	5.7111	0.0867	H-3→L (4%), H-3→L+1 (2%), H-3→L+2 (4%), H-1→L+1 (3%), H-1→L+2 (5%), H→L+2 (44%), H→L+4 (20%), H→L+6 (3%)
	212.46	5.8355	0.0896	H-8→L (5%), H-3→L (6%), H-1→L+2 (20%), H-1→L+3 (12%), H→L+2 (4%), H→L+3 (12%), H→L+4 (24%), H→L+6 (2%)
	209.90	5.9068	0.0008	H-8→L+5 (5%), H-3→L+5 (26%), H-1→L+5 (55%), H→L+5 (6%)
	207.57	5.9732	**0.2064**	H-8→L (3%), H-3→L+2 (18%), H-1→L+1 (5%), H-1→L+2 (15%), H-1→L+3 (19%), H-1→L+4 (2%), **H→L+3 (22%**), H→L+4 (5%)
	207.09	5.9870	0.0108	H-5→L (4%), H-2→L (4%), H-6→L (3%), H-5→L (51%), H-5→L+1 (3%), H-3→L+1 (3%), H-1→L+1 (12%), H→L+1 (2%), H→L+2 (3%)
	201.41	6.1559	0.1466	H-10→L (3%), H-9→L (21%), H-5→L (3%), H-5→L+1 (3%), H-3→L+1 (5%), H-3→L+2 (8%), H-2→L+1 (4%), H-1→L+1 (23%), H-1→L+4 (2%), H→L+4 (17%), H→L+6 (2%),
	198.92	6.2330	0.0209	H-8→L (26%), H-6→L (2%), H-5→L (24%), H-3→L+1 (3%), H-1→L+1 (18%), H-1→L+3 (2%), H→L+2 (4%), H→L+3 (5%), H→L+4 (4%)
	197.18	6.2787	0.0006	H-4→L (96%)
	194.18	6.3850	0.0003	H-7→L (94%), H-7→L+3 (3%)
	193.3	6.4142	0.2142	H-9→L (18%), H-3→L+2 (2%), H-2→L+1 (13%), H-1→L+1 (4%), H-1→L+2 (7%), H→L+2 (6%), H→L+4 (5%), H→L+6 (32%)
	191.37	6.4788	0.1703	H-8→L (2%), H-6→L (3%), H-6→L+1 (3%), H-5→L+1 (19%), H-3→L+4 (3%), H-1→L+1 (3%), H-1→L+2 (14%), H-1→L+4 (3%), H→L+2 (8%), H→L+3 (5%), H→L+6 (16%), H→L+7 (3%)
	189.94	6.5275	0.0732	H-10→L (4%), H-9→L (15%), H-8→L (12%), H-6→L (3%), H-6→L+1 (3%), H-5→L+1 (4%), H-3→L+2 (14%), H-3→L+3 (2%), H-2→L+1 (2%), H-1→L+3 (9%), H-1→L+6 (3%), H→L+6 (13%)
	188.75	6.5687	0.0214	H-13→L (2%), H-10→L (2%), H-9→L (6%), H-6→L (12%), H-6→L+1 (31%), H-6→L+4 (6%), H-6→L+7 (8%), H-1→L+2 (4%), H→L+3 (2%)
	187.11	6.6264	0.3398	H-8→L (3%), H-3→L+2 (10%), H-3→L+3 (19%), H-1→L+1 (3%), H-1→L+2 (3%), H-1→L+3 (4%), H-1→L+4 (5%), H→L+2 (16%), H→L+3 (22%)
	185.37	6.6886	0.0151	H-10→L (4%), H-9→L (26%), H-6→L+1 (3%), H-5→L+1 (24%), H-3→L+2 (3%), H-2→L+4 (2%), H-2→L+6 (3%), H-1→L+1 (7%), H-1→L+2 (2%), H→L (4%)
	182.82	6.7818	0.0446	H-10→L (3%), H-9→L (18%), H-5→L+1 (13%), H-3→L+3 (3%), H-3→L+1 (4%), H-2→L+4 (3%), H-2→L+6 (3%), H-1→L+1 (2%), H-1→L+2 (5%), H-1→L+3 (12%), H-1→L+4 (13%) H→L+3 (4%)

	180.68	6.8622	0.0003	H-8→L+5 (2%), H-3→L+5 (42%), H-1→L+5 (5%), H→L+5 (44%)
	179.05	6.9246	0.0162	H-5→L+1 (6%), H-3→L+1 (64%), H-1→L+1 (10%), H→L+7 (3%)
	178.05	6.9633	0.2801	H-3→L+1 (9%), H-3→L+2 (4%) H-3→L+3 (2%), H-2→L+4 (19%), H-2→L+6 (18%), H-1→L+2 (2%), H-1→L+3 (2%), H-1→L+7 (2%), H→L+7 (22%)
	177.55	6.9832	0.0106	H-18→L (3%), H-15→L (5%), H-14→L (2%), H-13→L (8%), H-13→L+4 (2%), H-11→L (3%), H-11→L+1 (2%), H-10→L (4%), H-10→L+2 (3%), H-10→L+3 (3%), H-6→L+1 (25%), H-6→L+4 (9%), H-6→L+6 (2%), H→L+7 (3%)
	176.90	7.0088	0.0034	H-7→L+5 (12%), L→L+6 (9%), L→L+7 (4%), L+1→L+7 (5%), L+1→L+8 (3%), L+2→L+9 (4%)



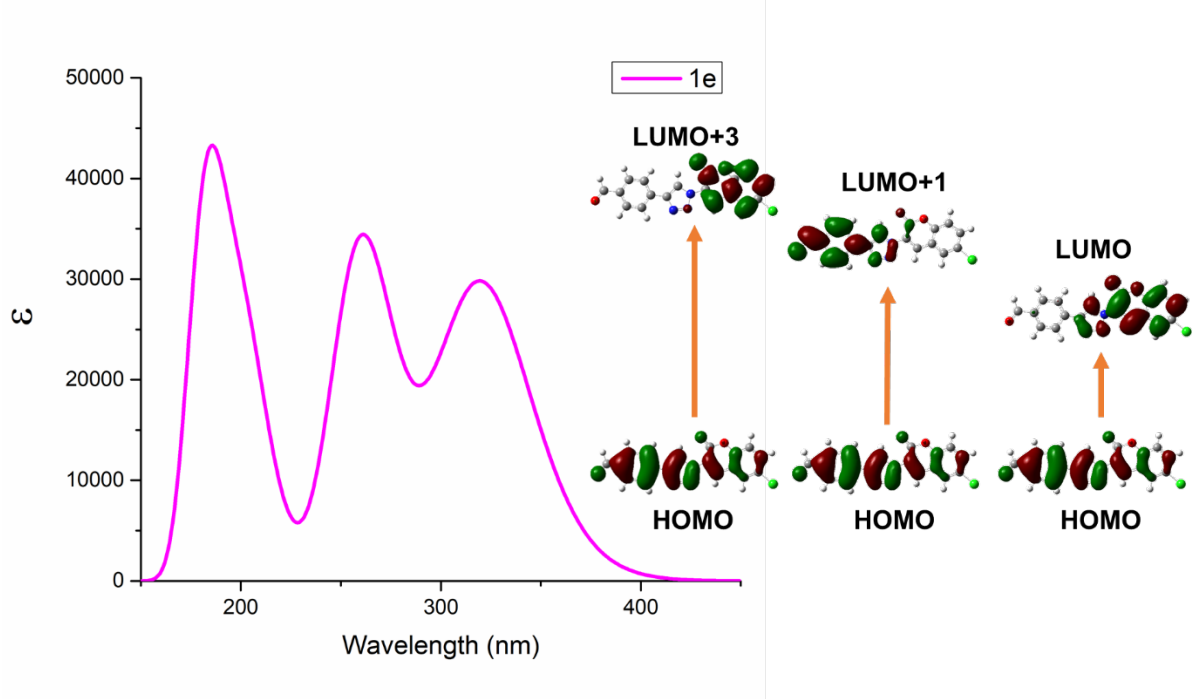
Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p).

Table S3.5. First thirty electronic transitions of 1e, obtained by BhandHLYP/6-31G (d, p), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1e	320.42	3.8694	**0.7260**	H-1→L (10%), **H→L (85%)**
	306.79	4.0413	0.0001	H-4→L (2%), H-4→L+1 (74%), H-4→L+7 (18%), H-4→L+12 (2%)
	277.68	4.4650	0.0328	H-3→L (11%), H-4→L+1 (74%), H-4→L+7 (18%), H-4→L+12 (2%)
	260.95	4.7512	**0.7823**	H-3→L (7%), H-1→L+1 (4%), H→L (2%), **H→L+1 (80%)**
	255.37	4.8551	0.0306	H-3→L (64%), H-1→L (11%), H-1→L+2 (6%), H→L+1 (8%), H→L+2 (3%)

	247.97	4.9999	0.0189	H-2→L (13%), H-2→L+1 (59%), H→L+4 (10%), H→L+5 (10%)
	233.39	5.3124	0.0033	H-8→L (26%), H-8→L+3 (5%), H-6→L (43%), H-6→L+4 (9%), H-6→L+5 (4%)
	229.17	5.4101	0.0015	H-8→L (41%), H-8→L+2 (3%), H-8→L+3 (10%), H-6→L (22%), H-6→L+4 (7%), H-6→L+5 (3%)
	223.86	5.5386	0.0154	H-2→L (83%), H-2→L+1 (9%)
	214.25	5.7868	0.0705	H-3→L (6%), H-3→L+2 (4%), H-3→L+3 (2%), H-2→L+1 (3%), H-1→L+2 (6%), H-1→L+3 (2%), H→L+2 (46%), H→L+4 (16%), H→L+5 (3%)
	209.33	5.9320	0.0641	H-7→L (6%), H-5→L (3%), H-3→L (5%), H-3→L+3 (3%), H-2→L+1 (2%), H-1→L+2 (16%), H-1→L+3 (12%), H→L+3 (9%), H→L+4 (30%), H→L+5 (3%)
	204.96	6.0491	**0.2086**	H-3→L+2 (18%), H-1→L+1 (5%), H-1→L+2 (14%), H-1→L+3 (20%), **H→L+3 (26%)**, H→L+4 (4%)
	204.22	6.0710	0.0105	H-3→L (7%), H-5→L (56%), H-3→L+1 (2%), H-1→L+1 (13%), H→L+2 (2%)
	199.10	6.2273	0.2163	H-7→L (18%), H-5→L (3%), H-3→L+1 (4%), H-3→L+2 (11%), H-2→L+1 (4%), H-1→L+1 (27%), H-1→L+4 (3%), H→L+4 (17%), H→L+5 (4%),
	195.88	6.3297	0.0000	H-4→L (96%)
	195.44	6.3437	0.0758	H-7→L (19%), H-5→L (24%), H-3→L+2 (5%), H-2→L+1 (3%), H-1→L+1 (22%), H-1→L+3 (3%), H→L+2 (5%), H→L+3 (7%), H→L+4 (3%)
	190.80	6.4980	0.0948	H-7→L (19%), H-2→L+1 (11%), H-1→L+2 (10%), H→L+2 (9%), H→L+4 (4%), H→L+5 (34%)
	188.98	6.5609	0.0031	H-6→L (17%), H-6→L+1 (50%), H-6→L+4 (6%), H-6→L+7 (11%)
	188.72	6.5699	0.1966	H-5→L+1 (19%), H-3→L+4 (3%), H-2→L+1 (4%), H-2→L+4 (3%), H-2→L+5 (2%), H-1→L+2 (15%), H-1→L+4 (4%), H→L+2 (8%), H→L+3 (5%), H→L+5 (19%), H→L+7 (4%)
	185.63	6.6792	0.1722	H-5→L+1 (4%), H-3→L+3 (20%), H-1→L+1 (3%), H-1→L+3 (10%), H→L+2 (15%), H→L+3 (23%), H→L+4 (4%), H→L+5 (4%)
	183.77	6.7468	0.0007	H-10→L+6 (4%), H-7→L+6 (3%), H-3→L+6 (29%), H-2→L+6 (3%), H-1→L+6 (52%), H→L+6 (7%)
	183.67	6.7505	0.2356	H-7→L (19%), H-5→L+1 (9%), H-3→L+2 (23%), H-1→L+3 (2%), H-1→L+4 (15%), H-1→L+5 (6%), H→L+3 (5%), H→L+5 (7%)
	181.86	6.8177	0.1616	H-10→L (3%), H-5→L+1 (26%), H-3→L+3 (3%), H-2→L+4 (9%), H-2→L+5 (9%), H-1→L+1 (7%), H-1→L+2 (7%), H-1→L+3 (6%), H-1→L+4 (11%), H→L+3 (7%)
	177.24	6.9953	0.2177	H-5→L+1 (7%), H-3→L+1 (3%), H-3→L+2 (3%), H-3→L+3 (6%), H-2→L+2 (2%), H-2→L+4 (21%), H-2→L+5 (8%), H-1→L+2 (3%), H-1→L+7 (3%), H→L+7 (29%)
	176.55	7.0228	0.0001	H-16→L (2%), H-15→L (6%), H-13→L (20%), H-13→L+4 (5%), H-13→L+5 (3%), H-11→L (7%), H-8→L (7%), H-8→L+2

				(5%), H-8→L+3 (3%), H-8→L+4 (2%), H-6→L+1 (14%), H-6→L+4 (6%), H-6→L+5 (2%)
	176.07	7.0418	0.0001	H-10→L (10%), H-3→L+1 (62%), H-2→L+4 (3%), H-1→L+1 (6%), H-1→L+3 (3%), H→L+7 (2%)
	174.3	7.1132	0.0168	H-10→L (71%), H-3→L+1 (11%), H-1→L+3 (3%)
	174.09	7.1218	0.0022	H-16→L (7%), H-13→L (16%) H-13→L+4 (7%), H-13→L+5 (3%), H-6→L (11%), H-6→L+1 (7%), H-6→L+2 (4%), H-6→L+4 (19%), H-6→L+5 (6%)
	172.68	7.1799	0.0966	H-5→L+1 (9%), H-3→L+2 (8%), H-3→L+3 (21%), H-3→L+4 (5%), H-2→L+4 (10%), H-2→L+5 (2%), H-1→L+2 (7%), H-1→L+4 (15%), H-1→L+5 (5%), H→L+2 (3%)
	171.69	7.2212	0.0003	H-9→L (86%), H-9→L+3 (4%)



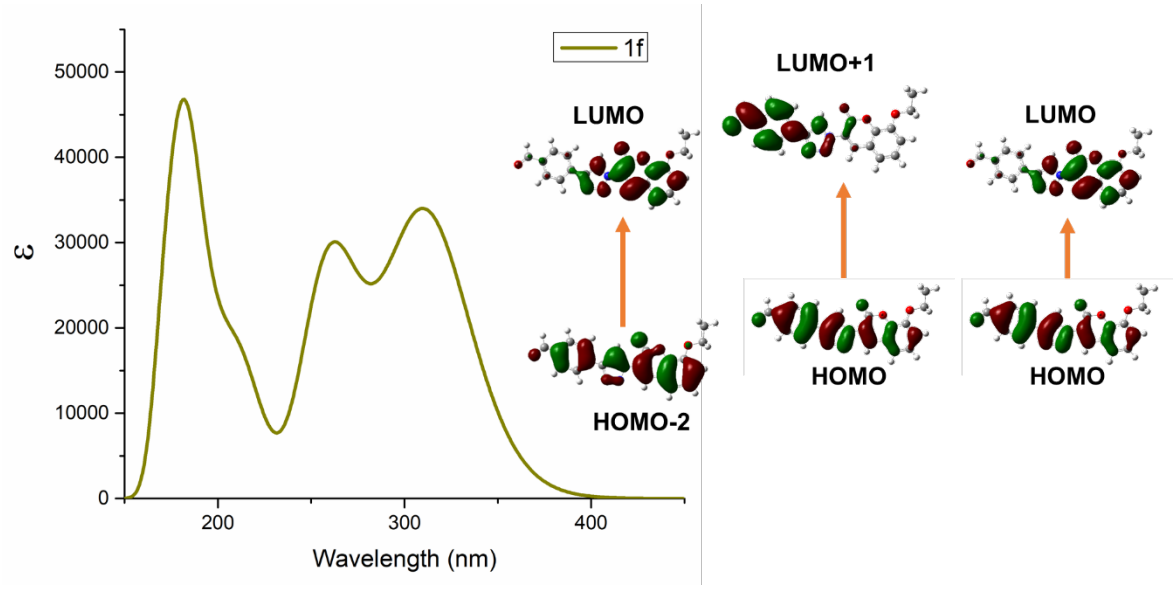
Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p).

Table S3.6. First thirty electronic transitions of **1f**, obtained by BhandHLYP/6-31G (d, p), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1f	312	3.9733	**0.7959**	H-1→L (10%), **H→L (83%)**
	306.03	4.0514	0.0001	H-4→L (3%), H-4→L+1 (74%), H-4→L+6 (18%)
	290.08	4.2741	0.0420	H-2→L+2 (3%), H-1→L (88%), H→L (3%)
	261.49	4.7414	**0.3278**	H-2→L (14%), H-2→L+1 (4%), **H→L+1 (76%)**
	260.73	4.7552	**0.3717**	H-5→L (3%), **H-2→L (66%)**. H-2→L+1 (3%), H→L (9%), H→L+1 (11%)

	247.40	5.0115	0.0172	H-3→L (10%), H-3→L+1 (61%), H-2→L+3 (2%), H→L+3 (12%), H→L+5 (6%)
	230.90	5.3695	0.0021	H-8→L (44%), H-8→L+1 (2%), H-8→L+2 (9%), H-8→L+4 (6%), H-6→L (24%), H-6→L+3 (3%), H-6→L+5 (4%)
	226.61	5.4713	0.0032	H-8→L (22%), H-8→L+2 (5%), H-8→L+4 (3%), H-6→L (38%), H-6→L+1 (3%), H-6→L+2 (3%), H-8→L (44%), H-8→L+1 (2%), H-8→L+2 (9%), H-6→L+3 (9%), H-6→L+5 (9%)
	216.28	5.7326	0.2071	H-7→L (8%), H-3→L (14%), H-3→L+1 (4%), H-2→L+2 (7%), H-2→L+4 (2%), H-1→L (2%), H-1→L+2 (27%), H-1→L+3 (3%), H→L+2 (18%), H→L+5 (3%)
	214.93	5.7685	0.0054	H-3→L (72%), H-3→L+1 (3%), H-1→L+2 (4%), H→L+2 (7%), H→L+3 (5%)
	209.75	5.9112	0.1029	H-3→L+1 (5%), H-2→L+1 (13%), H-2→L+4 (6%), H-1→L+2 (24%), H→L+2 (12%), H→L+3 (16%), H→L+4 (9%), H→L+5 (3%)
	204.23	6.0707	0.0063	H-7→L (7%), H-7→L+1 (3%), H-5→L (17%), H-5→L+1 (3%), H-2→L+1 (44%), H→L+1 (4%), H→L+2 (3%), H→L+3 (8%)
	203.47	6.0934	0.0857	H-3→L+1 (2%), H-2→L+2 (22%), H-1→L+2 (11%), H-1→L+4 (10%), H→L+2 (11%), H→L+3 (25%), H→L+5 (5%)
	199.75	6.2071	0.1253	H-7→L (38%), H-5→L (12%), H-3→L+1 (3%), H-2→L+1 (9%), H-2→L+3 (3%), H-2→L+4 (2%), H-1→L+4 (10%), H→L+2 (8%), H→L+3 (8%)
	195.19	6.3519	0.0015	H-1→L+1 (91%)
	193.33	6.4129	0.0400	H-7→L (12%), H-5→L (54%), H-3→L+1 (2%), H-2→L+1 (10%), H-1→L+4 (6%)
	190.97	6.4924	0.1770	H-7→L (8%), H-5→L+1 (4%), H-3→L+1 (15%), H-2→L+3 (5%), H→L+2 (2%), H→L+3 (5%), H→L+4 (6%), H→L+5 (45%)
	189.55	6.5408	0.0022	H-6→L (14%), H-6→L+1 (50%), H-6→L+3 (2%), H-6→L+6 (10%), H-4→L (12%)
	187.81	6.6016	0.0002	H-6→L (5%), H-6→L+1 (6%), H-4→L (83%), H-4→L+1 (3%)
	186.73	6.6396	0.1405	H-5→L (3%), H-5→L+1 (32%), H-3→L+3 (5%), H-2→L+2 (12%), H-2→L+5 (3%), H-1→L+4 (3%), H→L+2 (12%), H→L+4 (5%), H→L+6 (8%)
	183.36	6.7619	0.1772	H-7→L (2%), H-5→L+1 (10%), H-3→L+3 (3%), H-2→L+1 (2%), H-2→L+4 (3%), H-1→L+4 (35%), H-1→L+5 (3%), H→L+2 (14%), H→L+3 (4%), H→L+4 (9%), H→L+5 (3%)
	182.74	6.7849	**0.3779**	H-7→L (14%), H-2→L+2 (13%), **H-2→L+3 (18%)**, H-2→L+4 (12%), H-2→L+5 (7%), H-1→L+2 (5%), H-1→L+4 (6%), H→L+4 (6%), H→L+5 (6%)
	180.99	6.8504	0.0553	H-5→L+1 (16%), H-3→L+3 (5%), H-3→L+5 (3%), H-2→L+2 (8%), H-2→L+3 (3%), H-2→L+4 (6%), H-2→L+5 (2%), H-1→L+2 (11%), H-1→L+4 (3%), H→L+4 (22%), H→L+5 (10%)
	176.96	7.0062	0.2009	H-5→L+1 (4%), H-3→L+2 (3%), H-3→L+3 (23%), H-3→L+5 (6%), H-2→L+2 (6%), H-2→L+6 (4%), H→L+2 (2%), H→L+3 (2%), H→L+6 (34%)
	175.67	7.0578	0.0002	H-17→L (2%), H-15→L (5%), H-13→L (15%), H-13→L+1 (2%), H-13→L+3 (3%), H-13→L+5 (4%), H-10→L (8%), H-

				8→L (11%), H-8→L+2 (14%), H-8→L+4 (4%), H-6→L+1 (8%), H-6→L+3 (4%), H-6→L+5 (2%)
	172.47	7.1888	0.1751	H-9→L (3%), H-5→L+1 (18%), H-3→L+3 (22%), H-3→L+5 (5%), H-2→L+2 (4%), H-2→L+3 (3%), H-2→L+5 (3%), H-1→L+3 (4%), H-1→L+4 (3%), H→L+4 (2%), H→L+6 (16%)
	172.42	7.1910	0.0024	H-15→L (8%), H-13→L (17%), H-13→L+3 (5%), H-13→L+5 (5%), H→L (3%), H→L+5 (2%), H-6→L (9%), H-6→L+1 (3%), H-6→L+2 (5%), H-6→L+3 (10%), H-6→L+5 (7%)
	171.4	7.2337	0.1824	H-9→L (6%), H-5→L+1 (5%), H-2→L+2 (6%), H-2→L+3 (19%), H-2→L+5 (6%), H-1→L+4 (7%), H→L+2 (3%), H→L+4 (6%), H→L+6 (24%)
	170.01	7.2928	0.0574	H-2→L+2 (6%), H-2→L+3 (4%), H-1→L+2 (7%), H-1→L+3 (50%), H-1→L+5 (21%), H→L+4 (2%)
	169.01	7.3357	0.0003	H-15→L (3%), H-13→L (4%), H-13→L+1 (2%), H→L (3%), H→L+1 (4%), H-8→L (14%), H-8→L+2 (19%), H-8→L+4 (5%), H-8→L+11 (2%), H-6→L (5%), H-6→L+1 (6%), H-6→L+2 (7%), H-6→L+3 (8%), H-6→L+5 (5%), H-4→L+3 (2%)



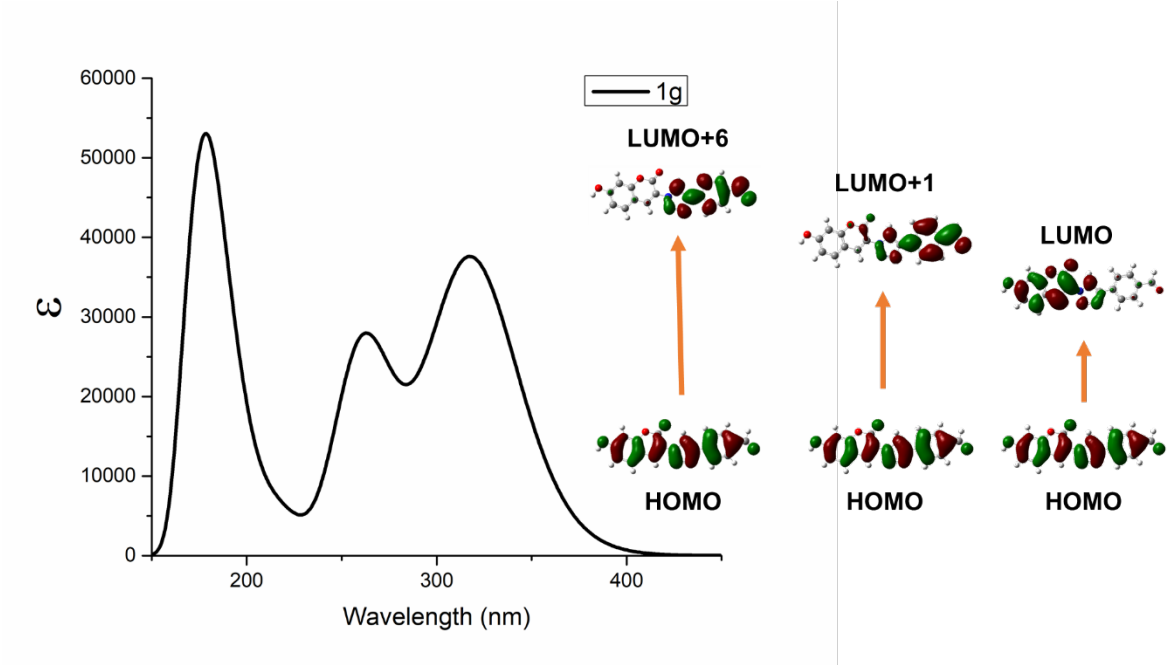
Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p).

Table S3.7. First thirty electronic transitions of **1g**, obtained by BhandHLYP/6-31G (d, p), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1g	318.24	3.8959	**0.9188**	H-1→L (8%), **H→L (86%)**
	306.00	4.0518	0.0001	H-4→L (3%), H-4→L+1 (74%), H-4→L+6 (18%)
	266.77	4.6476	0.0114	H-5→L (2%), H-3→L (4%), H-1→L (76%), H→L (6%), H→L+1 (7%)
	262.38	4.7254	**0.6522**	H-1→L (4%), H-1→L+1 (12%), H→L (3%), **H→L+1 (75%)**
	252.46	4.9111	0.0050	H-3→L (64%), H-1→L (4%), H-1→L+2 (12%), H→L+2 (13%)

	247.31	5.0133	0.0168	H-2→L (8%), H-2→L+1 (63%), H-1→L+3 (3%), H-1→L+5 (2%), H→L+3 (8%), H→L+4 (4%), H→L+5 (4%)
	228.91	5.4162	0.0021	H-8→L (46%), H-8→L+1 (2%), H-8→L+2 (3%), H-8→L+3 (7%), H-8→L+4 (6%), H-6→L+3 (3%), H-6→L+8 (4%)
	225.06	5.5089	0.0034	H-8→L (21%), H-8→L+3 (3%), H-8→L+4 (3%), H-6→L (37%), H-6→L+1 (3%), H-6→L+2 (4%), H-6→L+3 (8%), H-6→L+5 (9%)
	219.48	5.6490	0.0878	H-7→L (3%), H-3→L (23%), H-1→L+1 (6%), H-1→L+2 (10%), H→L+2 (44%), H→L+3 (2%), H→L+5 (2%)
	214.65	5.7761	0.0212	H-2→L (88%), H-2→L+1 (6%)
	213.38	5.8106	0.0027	H-7→L+1 (2%), H-3→L (5%), H-1→L+1 (29%), H-1→L+2 (9%), H-1→L+3 (2%), H→L+1 (5%), H→L+3 (27%), H→L+4 (2%), H→L+5 (5%)
	208.10	5.9580	0.0240	H-7→L (5%), H-5→L (5%), H-5→L+1 (2%), H-2→L+1 (2%), H-1→L+1 (35%), H-1→L+2 (2%), H→L+1 (6%), H→L+2 (3%), H→L+3 (30%)
	201.42	6.1555	0.0569	H-7→L (21%), H-5→L (7%), H-3→L+2 (3%), H-2→L+1 (4%), H-1→L+2 (4%), H-1→L+3 (8%), H-1→L+4 (7%), H→L+4 (32%), H→L+5 (4%)
	198.78	6.2371	0.1059	H-7→L (37%), H-5→L (9%), H-3→L+2 (20%), H-1→L+1 (2%), H-1→L+4 (6%), H→L+2 (6%), H→L+3 (2%), H→L+4 (10%), H→L+5 (4%)
	193.83	6.3964	0.0702	H-7→L (8%), H-5→L (52%), H-3→L+2 (3%), H-2→L+1 (6%), H-1→L+1 (5%), H-1→L+3 (3%), H→L+4 (4%), H→L+5 (8%)
	192.03	6.4563	0.1548	H-7→L (12%), H-5→L (11%), H-5→L+1 (3%), H-2→L+1 (12%), H-1→L+3 (3%), H-1→L+4 (5%), H→L+2 (3%), H→L+3 (4%), H→L+4 (6%), H→L+5 (34%)
	189.45	6.5443	0.0022	H-6→L (15%), H-6→L+1 (51%), H-6→L+3 (2%), H-6→L+6 (10%), H-4→L (10%)
	189.02	6.5592	0.0092	H-7→L (3%), H-7→L+3 (2%), H-5→L+1 (9%), H-1→L+2 (32%), H-1→L+3 (16%), H-1→L+5 (8%), H→L+2 (11%), H→L+3 (4%), H→L+4 (3%), H→L+6 (3%)
	187.50	6.6125	0.0002	H-6→L (2%), H-6→L+1 (10%), H-4→L (3%), H-4→L+1 (2%)
	185.25	6.6929	0.4117	H-7→L (4%), H-5→L (4%), H-5→L+1 (44%), H-5→L+2 (5%), H-2→L+3 (7%), H-2→L+4 (4%), H-2→L+5 (5%), H-1→L+1 (2%), H-1→L+2 (4%), H-1→L+3 (2%), H→L+3 (4%), H→L+6 (3%)
	181.80	6.8199	0.0918	H-7→L+2 (6%), H-3→L+4 (5%), H-1→L+2 (8%), H-1→L+3 (24%), H-1→L+5 (9%), H→L+2 (15%), H→L+3 (5%), H→L+4 (3%), H→L+5 (7%), H→L+6 (3%)
	178.94	6.9289	**0.2307**	H-9→L (2%), H-7→L (2%), H-5→L+1 (6%), H-3→L+1 (2%), H-3→L+2 (36%), H-2→L+3 (3%), H→L+4 (13%), H→L+5 (10%), H→L+6 (8%)
	176.70	7.0167	**0.4490**	H-5→L+1 (7%), H-3→L+1 (3%), H-3→L+2 (4%), H-3→L+4 (4%), H-2→L+2 (3%), H-2→L+3 (21%), H-2→L+4 (8%), H-2→L+5 (5%), H-1→L+3 (2%), H-1→L+5 (2%), H→L+4 (4%), H→L+6 (22%)

	174.70	7.0971	0.0005	H-13→L (5%), H-11→L (15%), H-11→L+1 (3%), H-11→L+3 (4%), H-11→L+5 (4%), H-10→L (8%), H-8→L (6%), H-8→L+2 (5%), H-8→L+3 (4%), H-6→L+1 (12%), H-6→L+2 (2%), H-6→L+3 (9%), H-6→L+5 (5%)
	172.47	7.1887	0.0324	H-5→L+1 (12%), H-3→L+1 (34%), H-3→L+3 (4%), H-3→L+4 (6%), H-2→L+3 (10%), H-2→L+4 (4%), H-2→L+5 (3%), H-1→L+4 (4%), H→L+6 (12%)
	172.28	7.1966	0.0023	H-13→L (3%), H-11→L (15%), H-11→L+2 (2%), H-11→L+3 (5%), H-11→L+5 (6%), H-10→L (3%), H-10→L+3 (2%), H-10→L+5 (2%), H-6→L (13%), H-6→L+1 (2%), H-6→L+2 (5%), H-6→L+3 (15%), H-6→L+5 (15%)
	171.99	7.2089	0.1052	H-9→L (4%), H-5→L+1 (8%), H-3→L+1 (30%), H-3→L+2 (3%), H-3→L+3 (2%), H-2→L+3 (5%), H-2→L+4 (2%), H-1→L+6 (3%), H→L+4 (4%), H→L+6 (26%)
	168.57	7.3552	0.2163	H-9→L (6%), H-3→L+1 (25%), H-3→L+2 (4%), H-3→L+3 (7%), H-3→L+4 (28%), H-3→L+5 (3%), H-1→L+2 (4%), H-1→L+3 (3%), H-1→L+4 (10%)
	168.15	7.3732	0.1895	H-9→L (24%), H-7→L+1 (2%), H-3→L+2 (8%), H-3→L+3 (6%), H-3→L+4 (12%), H-1→L+2 (5%), H-6→L+3 (6%), H-6→L+4 (19%), H-6→L+5 (3%)
	167.57	7.3988	0.0045	H-12→L (3%), H-9→L (45%), H-1→L+5 (3%), H→L+4 (6%), H→L+5 (4%)

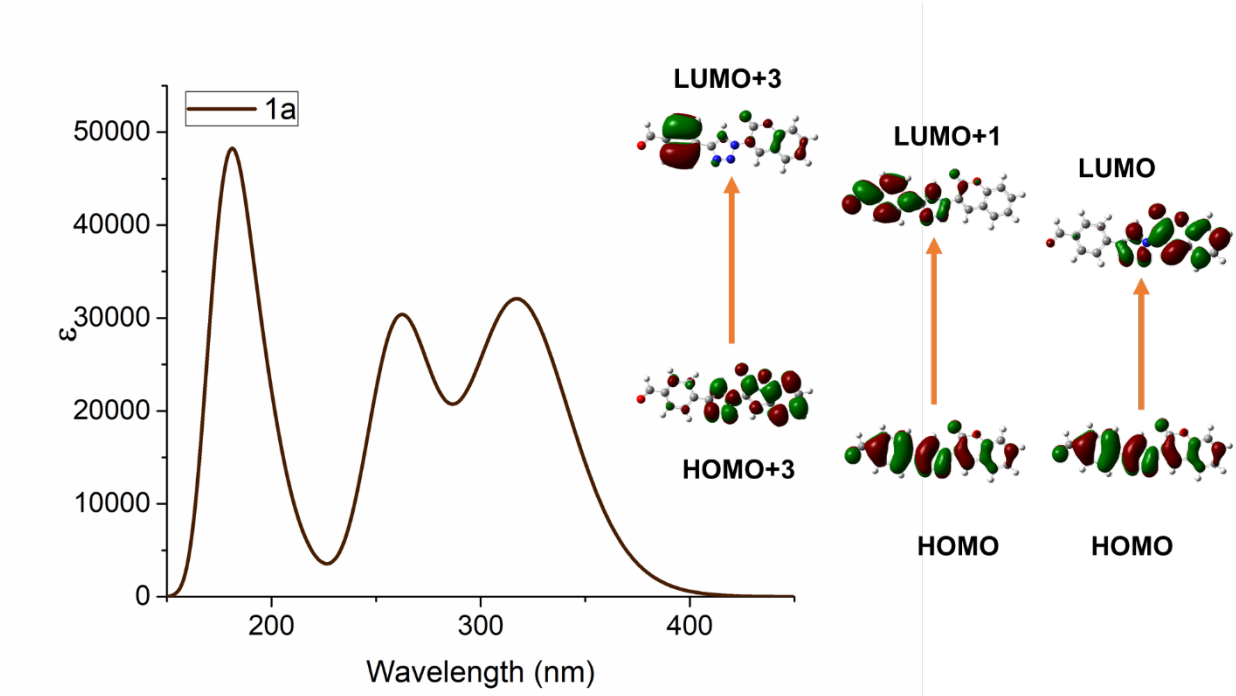


Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p).

TDDFT (dichloromethane)

Table S3.8. First thirty electronic transitions of **1a**, obtained by BhandHLYP/6-31G (d, p), CPCM solvent model (dichloromethane), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1a	318.4798	3.8935	**1.0616**	H-1->LUMO (12%), HOMO->LUMO (83%)
	303.4069	4.0869	0.0001	H-4->L+1 (75%), H-4->L+6 (16%)
	274.3802	4.5193	**0.251**	H-2->LUMO (20%), H-1->LUMO (30%), HOMO->L+1 (38%)
	268.7655	4.6137	**0.2251**	H-2->LUMO (37%), HOMO->L+1 (39%)
	256.9567	4.8257	**0.206**	H-2->LUMO (31%), H-1->LUMO (44%)
	250.5693	4.9487	0.0312	H-3->L+1 (68%)
	227.5148	5.4502	0.0016	H-8->LUMO (53%), H-8->L+2 (12%)
	221.5824	5.5961	0.0065	H-8->LUMO (10%), H-6->LUMO (30%), H-6->L+2 (13%)
	219.5226	5.6486	0.0523	H-1->L+1 (27%), HOMO->L+2 (40%)
	212.5237	5.8346	0.0316	H-1->L+1 (39%), HOMO->L+2 (29%)
	209.8581	5.9088	0.0234	H-3->LUMO (85%)
	205.8922	6.0226	0.0482	H-1->L+4 (14%), HOMO->L+3 (24%), HOMO->L+4 (17%)
	201.1914	6.1633	0.1398	H-1->L+2 (19%), HOMO->L+3 (18%), HOMO->L+4 (16%)
	198.7627	6.2386	0.2707	H-7->LUMO (20%), H-2->L+2 (15%), H-1->L+3 (12%), HOMO->L+5 (14%)
	196.2924	6.3171	0.1494	H-7->LUMO (13%), H-5->LUMO (19%), HOMO->L+4 (11%), HOMO->L+5 (14%)
	193.5741	6.4058	0.0663	H-5->LUMO (19%), H-5->L+1 (32%), HOMO->L+5 (10%)
	189.5261	6.5426	0.0014	H-5->LUMO (18%), H-2->L+1 (10%), H-1->L+2 (29%)
	188.0030	6.5956	0.0978	H-2->L+1 (60%)
	187.1883	6.6243	0.1477	H-7->LUMO (18%), H-5->LUMO (22%), H-5->L+1 (22%)
	186.5265	6.6478	0.1075	H-6->LUMO (13%), H-6->L+1 (28%), H-2->L+1 (15%)
	182.2118	6.8053	0.1317	H-2->L+2 (16%), HOMO->L+5 (17%)
	180.7350	6.8609	**0.6853**	H-3->L+3 (26%), HOMO->L+6 (13%)
	179.1446	6.9218	0.0068	H-4->LUMO (88%)
	178.7211	6.9382	0.1446	H-2->L+4 (37%), H-2->L+5 (16%)
	175.2352	7.0762	0.0761	H-12->LUMO (10%), HOMO->L+6 (27%)
	174.8177	7.0931	0.06	H-12->LUMO (17%), H-6->L+1 (10%), HOMO->L+6 (18%)
	170.9702	7.2527	0.0087	H-13->LUMO (19%)
	169.0655	7.3344	0.043	H-9->LUMO (39%)
	168.8307	7.3446	0.0006	H-12->LUMO (10%), H-10->L+1 (50%)
	167.6028	7.3984	0.146	H-9->LUMO (18%), H-2->L+2 (10%), H-1->L+3 (32%), H-1->L+5 (12%)

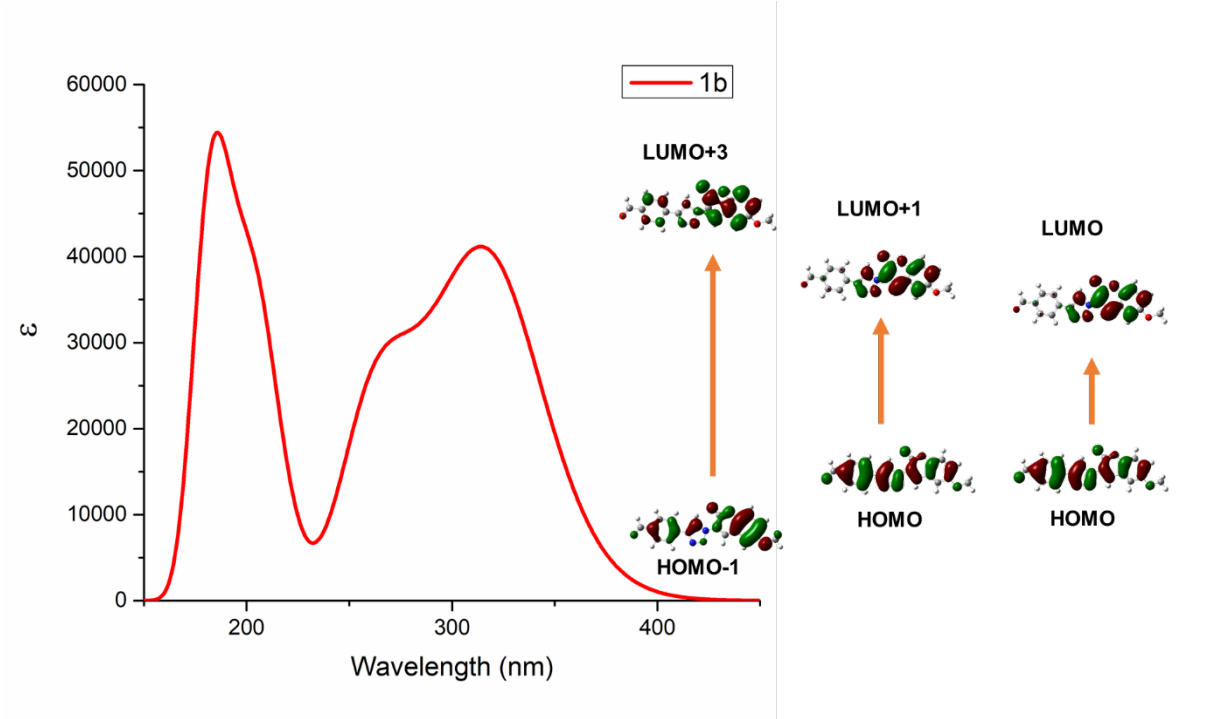


Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p) and CPCM in dichloromethane.

Table S3.9. First thirty electronic transitions of **1b**, obtained by BhandHLYP/6-31G (d, p), CPCM solvent model (dichloromethane), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1b	322.64	3.8433	**0.8154**	HOMO->LUMO (85%)
	297.95	4.1618	0.0001	H-4->L+1 (74%), H-4->L+6 (17%)
	294.74	4.2070	**0.3513**	H-2->LUMO (11%), H-1->LUMO (74%)
	269.77	4.5965	**0.4187**	H-1->L+1 (25%), HOMO->L+1 (59%)
	255.27	4.8576	**0.2298**	H-2->LUMO (68%)
	249.16	4.9767	0.0307	H-3->L+1 (65%)
	224.88	5.5141	0.0032	H-8->LUMO (40%), H-7->LUMO (25%)
	220.34	5.6277	0.0044	H-8->LUMO (25%), H-7->LUMO (28%), H-7->L+2 (15%)
	219.36	5.6528	0.0502	H-2->L+1 (15%), H-1->L+1 (34%), HOMO->L+1 (27%), HOMO->L+2 (11%)
	212.69	5.8300	0.0119	H-1->L+4 (18%), HOMO->L+2 (39%), HOMO->L+4 (11%)
	210.66	5.8863	0.1423	H-1->L+2 (15%), H-1->L+4 (10%), HOMO->L+2 (11%), HOMO->L+4 (19%)
	209.43	5.9210	0.027	H-3->LUMO (81%)
	206.20	6.0135	**0.3987**	H-1->L+2 (13%), H-1->L+3 (14%), H-1->L+5 (10%), HOMO->L+2 (11%), HOMO->L+4 (12%)
	202.19	6.1329	0.0399	H-2->L+1 (47%), H-1->L+1 (24%)
	198.91	6.2341	0.2319	H-6->LUMO (29%), H-3->L+1 (12%), H-2->L+2 (12%), HOMO->L+3 (18%)

	193.53	6.4074	0.2032	H-6->LUMO (27%), H-1->L+3 (10%), HOMO->L+3 (10%), HOMO->L+5 (15%)
	190.75	6.5005	0.0084	H-5->LUMO (40%), H-5->L+1 (22%)
	187.56	6.6112	0.0136	H-2->L+2 (23%), H-1->L+2 (17%), H-1->L+4 (20%)
	187.45	6.6149	0.002	H-7->LUMO (23%), H-7->L+1 (52%)
	186.71	6.6414	**0.4609**	H-6->LUMO (12%), H-5->LUMO (22%), H-5->L+1 (26%)
	183.79	6.7470	**0.2979**	H-2->L+4 (30%), H-1->L+4 (16%), HOMO->L+4 (11%)
	182.26	6.8035	0.0718	H-2->L+3 (10%), H-1->L+2 (10%), HOMO->L+5 (27%)
	180.32	6.8768	0.2312	H-3->L+2 (13%), H-3->L+3 (19%), H-1->L+2 (11%), HOMO->L+6 (15%)
	178.68	6.9397	0	H-4->LUMO (92%)
	176.06	7.0431	0.1348	H-9->LUMO (40%), H-5->L+1 (10%)
	174.30	7.1140	0.1244	H-9->LUMO (41%)
	174.23	7.1169	0.0005	H-15->LUMO (16%), H-10->LUMO (15%), H-8->L+2 (10%)
	173.12	7.1625	0.0245	H-2->L+2 (14%), H-2->L+5 (10%), H-1->L+6 (11%), HOMO->L+6 (26%)
	170.43	7.2756	0.0007	H-13->LUMO (25%), H-13->L+2 (14%)
	167.70	7.3939	0.0007	H-11->L+1 (53%)

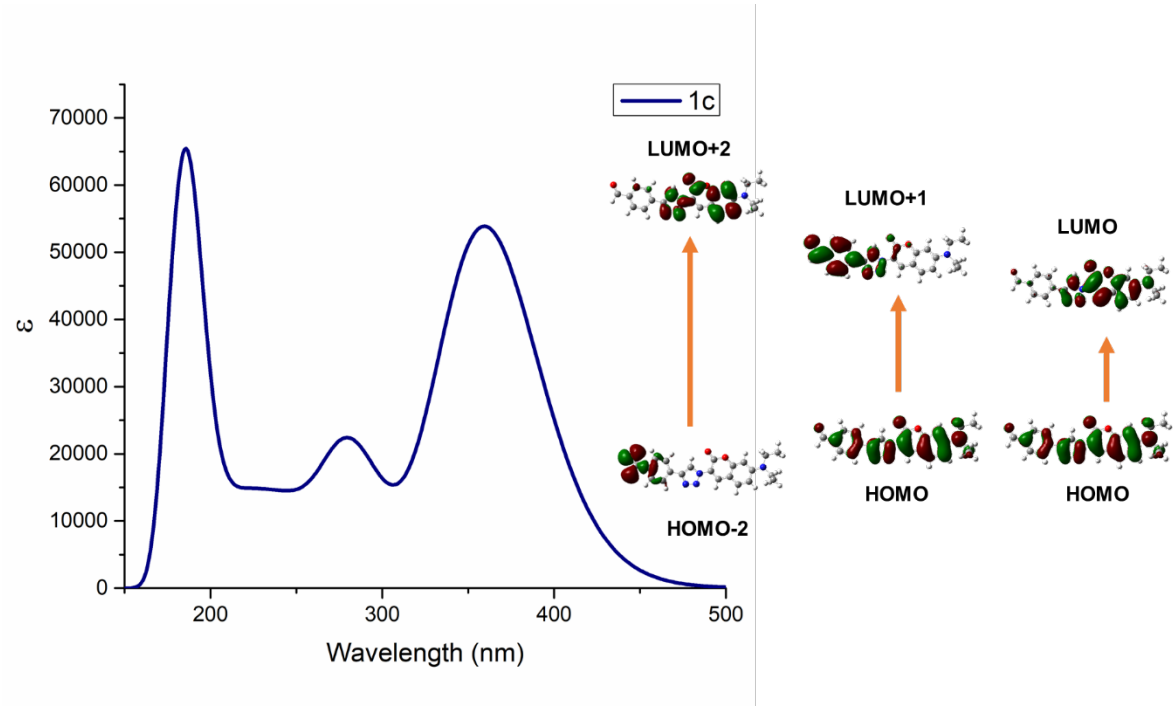


Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p) and CPCM in dichloromethane.

Table S3.10. First thirty electronic transitions of **1c**, obtained by BhandHLYP/6-31G (d, p), CPCM solvent model (dichloromethane), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***

1c	360.19	3.4426	**1.3311**	HOMO->LUMO (93%)
	302.98	4.0927	0.0001	H-5->L+1 (72%), H-5->L+6 (15%)
	282.47	4.3899	**0.5041**	H-1->LUMO (13%), H-1->L+1 (33%), HOMO->L+1 (49%)
	265.57	4.6692	0.0128	H-2->LUMO (55%), HOMO->L+2 (17%), HOMO->L+3 (10%)
	260.38	4.7622	0.0294	H-1->LUMO (74%)
	250.45	4.9511	0.0409	H-3->LUMO (11%), H-3->L+1 (61%)
	248.30	4.9940	0.1298	H-1->L+1 (43%), HOMO->L+1 (37%)
	237.91	5.2120	0.1084	H-2->LUMO (32%), HOMO->L+2 (37%), HOMO->L+3 (13%)
	226.65	5.4709	0.11	HOMO->L+2 (25%), HOMO->L+3 (11%), HOMO->L+4 (43%)
	222.22	5.5801	0.0045	H-9->LUMO (49%), H-9->L+2 (13%)
	219.00	5.6622	0.1228	H-4->LUMO (76%)
	216.75	5.7208	0.015	H-7->LUMO (25%), H-7->L+1 (13%), H-7->L+2 (18%), H-7->L+4 (10%)
	211.84	5.8535	0.0524	HOMO->L+5 (69%)
	203.73	6.0866	0.1054	H-3->LUMO (12%), H-1->L+2 (19%), H-1->L+3 (21%), HOMO->L+4 (12%)
	200.86	6.1735	0.0315	H-3->LUMO (70%), H-3->L+1 (19%)
	197.01	6.2940	0.0995	H-1->L+2 (35%), H-1->L+4 (21%), HOMO->L+3 (17%)
	195.66	6.3374	0.0499	H-6->LUMO (22%), H-6->L+1 (34%), H-4->L+1 (10%)
	190.95	6.4937	0.2859	H-2->L+1 (68%), H-2->L+2 (13%)
	187.74	6.6050	**0.7133**	H-8->LUMO (10%), H-6->LUMO (13%), H-2->L+1 (12%), H-2->L+2 (20%), H-2->L+3 (12%)
	186.97	6.6321	0.0151	H-7->LUMO (32%), H-7->L+1 (30%)
	185.66	6.6789	0.0233	H-6->L+1 (12%), H-4->L+1 (14%), HOMO->L+3 (18%), HOMO->L+4 (11%)
	184.38	6.7253	0.054	H-6->LUMO (27%), H-4->L+1 (22%), H-2->L+2 (11%)
	182.77	6.7847	0.0937	H-6->L+1 (11%), H-4->L+1 (17%), H-1->L+3 (16%)
	182.21	6.8054	0.1034	H-3->L+3 (14%), H-1->L+6 (27%), HOMO->L+6 (17%)
	179.07	6.9248	0.0211	H-8->LUMO (19%), H-6->LUMO (10%), H-4->L+2 (18%), H-1->L+4 (16%)
	178.15	6.9603	**0.449**	H-8->LUMO (12%), H-3->L+3 (19%)
	177.11	7.0012	0.0466	H-8->LUMO (16%), H-2->L+5 (18%)
	174.12	7.1217	0.1032	H-8->LUMO (12%), H-2->L+4 (19%), H-2->L+5 (32%)
	172.91	7.1712	0.0049	H-5->LUMO (30%)
	172.61	7.1839	0.0034	H-5->LUMO (58%)

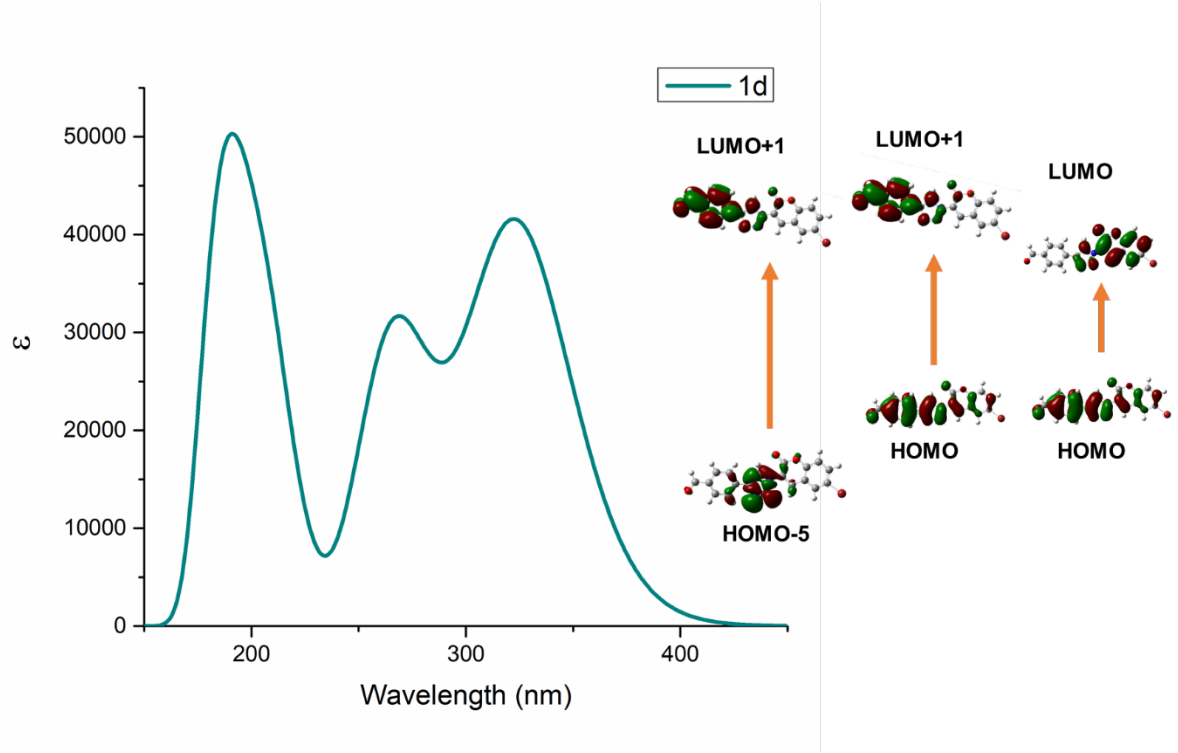


Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p) and CPCM in dichloromethane.

Table S3.11. First thirty electronic transitions of **1d**, obtained by BhandHLYP/6-31G (d, p), CPCM solvent model (dichloromethane), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1d	323.82	3.8293	**1.0112**	H-1->LUMO (11%), HOMO->LUMO (82%)
	303.51	4.0855	0.0001	H-4->L+1 (76%), H-4->L+7 (16%)
	281.21	4.4095	0.0701	H-2->LUMO (15%), H-1->LUMO (64%)
	270.35	4.5867	**0.5029**	H-1->L+1 (10%), HOMO->L+1 (74%)
	258.94	4.7887	**0.2246**	H-2->LUMO (60%), H-1->LUMO (15%)
	250.87	4.9428	0.0323	H-3->L+1 (64%)
	229.38	5.4059	0.0021	H-10->LUMO (48%), H-8->LUMO (16%)
	224.67	5.5192	0.0042	H-10->LUMO (15%), H-8->LUMO (33%), H-8->L+3 (10%)
	218.98	5.6627	0.1022	H-1->L+1 (12%), HOMO->L+2 (42%), HOMO->L+3 (14%)
	215.31	5.7592	0.0209	H-3->LUMO (79%)
	211.53	5.8619	0.0426	H-1->L+1 (27%), HOMO->L+2 (19%)
	210.67	5.8861	0.1959	H-1->L+1 (13%), H-1->L+2 (18%), HOMO->L+3 (33%)
	209.17	5.9282	0.0004	H-2->L+6 (20%), H-1->L+6 (58%), HOMO->L+6 (10%)
	207.12	5.9869	**0.2264**	H-2->L+2 (18%), H-1->L+2 (15%), H-1->L+4 (18%), HOMO->L+4 (20%)
	201.56	6.1519	0.1905	H-7->LUMO (40%), HOMO->L+3 (11%), HOMO->L+4 (11%)
	197.07	6.2922	0.1918	H-5->LUMO (20%), H-1->L+1 (12%), HOMO->L+5 (27%)
	195.44	6.3447	0.0506	H-7->LUMO (17%), H-5->LUMO (34%), HOMO->L+5 (18%)
	192.03	6.4573	0.001	H-6->LUMO (93%)

	191.80	6.4650	0.3482	H-7->LUMO (10%), H-5->LUMO (13%), H-5->L+1 (19%)
	190.15	6.5212	0.1647	H-7->LUMO (11%), H-2->L+2 (21%), H-1->L+3 (16%)
	188.13	6.5911	0.0069	H-2->L+1 (42%), H-1->L+1 (10%), H-1->L+2 (12%)
	187.45	6.6150	0.0113	H-8->LUMO (13%), H-8->L+1 (21%), H-5->L+1 (14%)
	186.16	6.6609	0.0142	H-8->L+1 (24%), H-5->L+1 (17%)
	184.62	6.7164	0.2137	H-9->LUMO (24%), H-2->L+4 (25%), H-1->L+4 (10%), HOMO->L+4 (13%)
	183.21	6.7684	0.0004	H-4->LUMO (91%)
	181.66	6.8259	0.0745	H-9->LUMO (42%), H-2->L+4 (13%)
	180.97	6.8520	**0.3193**	H-3->L+3 (23%), H-3->L+5 (20%), HOMO->L+7 (19%)
	179.51	6.9078	0.0009	H-2->L+6 (44%), HOMO->L+6 (44%)
	175.61	7.0610	0.1083	HOMO->L+7 (24%)
	175.52	7.0648	0.0076	H-6->L+6 (88%)

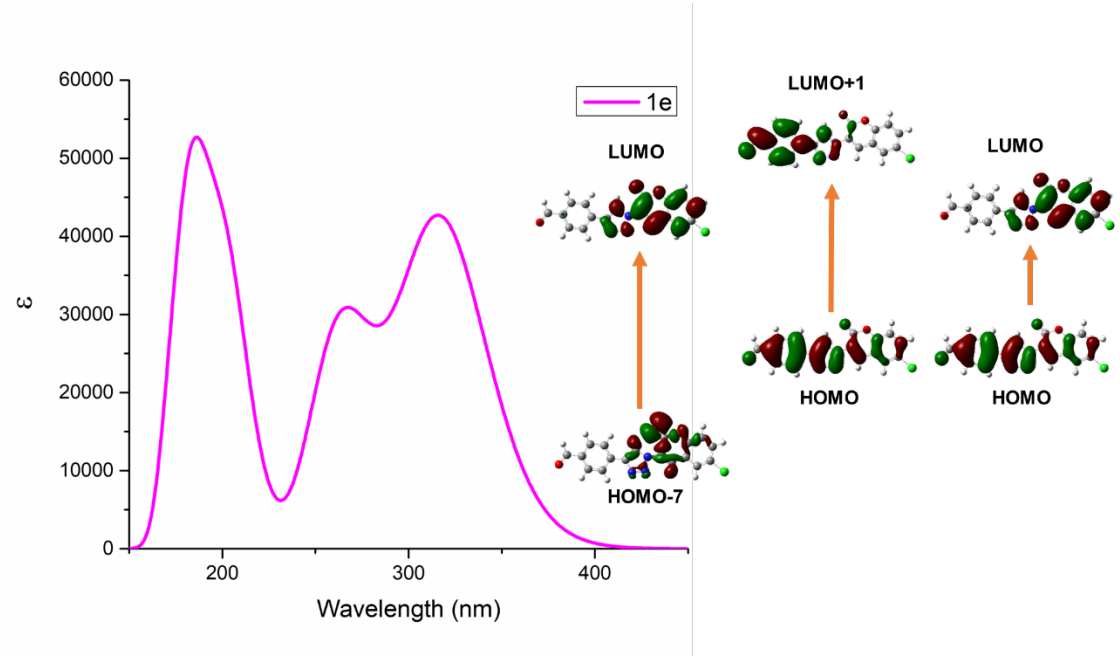


Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p) and CPCM in dichloromethane.

Table S3.12. First thirty electronic transitions of **1e**, obtained by BhandHLYP/6-31G (d, p), CPCM solvent model (dichloromethane), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1e	317.59	3.9044	**1.0324**	H-1->LUMO (13%), HOMO->LUMO (81%)
	298.07	4.1601	0.0001	H-4->L+1 (75%), H-4->L+6 (17%)
	276.02	4.4925	0.0937	H-2->LUMO (11%), H-1->LUMO (57%), HOMO->L+1 (14%)
	268.02	4.6266	**0.4613**	HOMO->L+1 (69%)

	255.54	4.8525	0.2191	H-3->LUMO (26%), H-2->LUMO (38%), H-1->LUMO (17%)
	249.36	4.9727	0.0317	H-3->L+1 (41%), H-2->L+1 (27%)
	225.73	5.4933	0.0042	H-8->LUMO (31%), H-6->LUMO (34%)
	221.35	5.6021	0.0031	H-8->LUMO (35%), H-6->LUMO (22%)
	215.55	5.7528	0.086	H-1->L+1 (14%), HOMO->L+2 (41%), HOMO->L+3 (11%)
	213.29	5.8136	0.0285	H-3->LUMO (56%), H-2->LUMO (32%)
	208.99	5.9333	0.0165	H-1->L+1 (35%), HOMO->L+2 (15%)
	207.76	5.9684	0.1667	H-1->L+1 (10%), H-1->L+2 (19%), HOMO->L+3 (37%)
	204.56	6.0618	**0.2561**	H-2->L+2 (15%), H-1->L+2 (15%), H-1->L+4 (16%), HOMO->L+4 (21%)
	199.45	6.2171	**0.3052**	H-7->LUMO (35%), HOMO->L+3 (15%)
	194.45	6.3771	0.1739	H-5->LUMO (26%), H-1->L+1 (10%), HOMO->L+5 (28%)
	191.64	6.4704	0.0781	H-7->LUMO (12%), H-5->LUMO (23%), H-5->L+1 (17%), HOMO->L+5 (21%)
	188.27	6.5861	0.1395	H-5->LUMO (26%), H-5->L+1 (12%), H-1->L+2 (11%)
	187.31	6.6200	0.0024	H-6->LUMO (20%), H-6->L+1 (53%), H-6->L+6 (10%)
	185.69	6.6779	**0.4569**	H-7->LUMO (24%), H-2->L+2 (16%), H-1->L+3 (16%), H-1->L+5 (10%)
	185.37	6.6894	0.0103	H-3->L+1 (21%), H-2->L+1 (36%)
	184.40	6.7244	0.0035	H-5->L+1 (28%)
	183.79	6.7468	0.0009	H-2->L+7 (18%), H-1->L+7 (54%), HOMO->L+7 (10%)
	181.70	6.8243	0	H-4->LUMO (93%)
	181.54	6.8304	0.0985	H-3->L+4 (14%), H-2->L+4 (28%), H-1->L+4 (13%), HOMO->L+2 (10%), HOMO->L+4 (15%)
	180.10	6.8850	**0.3519**	H-3->L+3 (20%), H-2->L+3 (10%), HOMO->L+6 (23%)
	174.01	7.1260	0.112	H-5->L+1 (23%), HOMO->L+6 (40%)
	174.00	7.1263	0.0017	H-15->LUMO (14%), H-8->L+2 (11%)
	172.50	7.1882	0.0834	H-10->LUMO (65%)
	171.47	7.2317	0.1671	H-10->LUMO (12%), H-1->L+3 (17%)
	170.78	7.2607	0.0007	H-13->LUMO (19%), H-9->LUMO (20%)

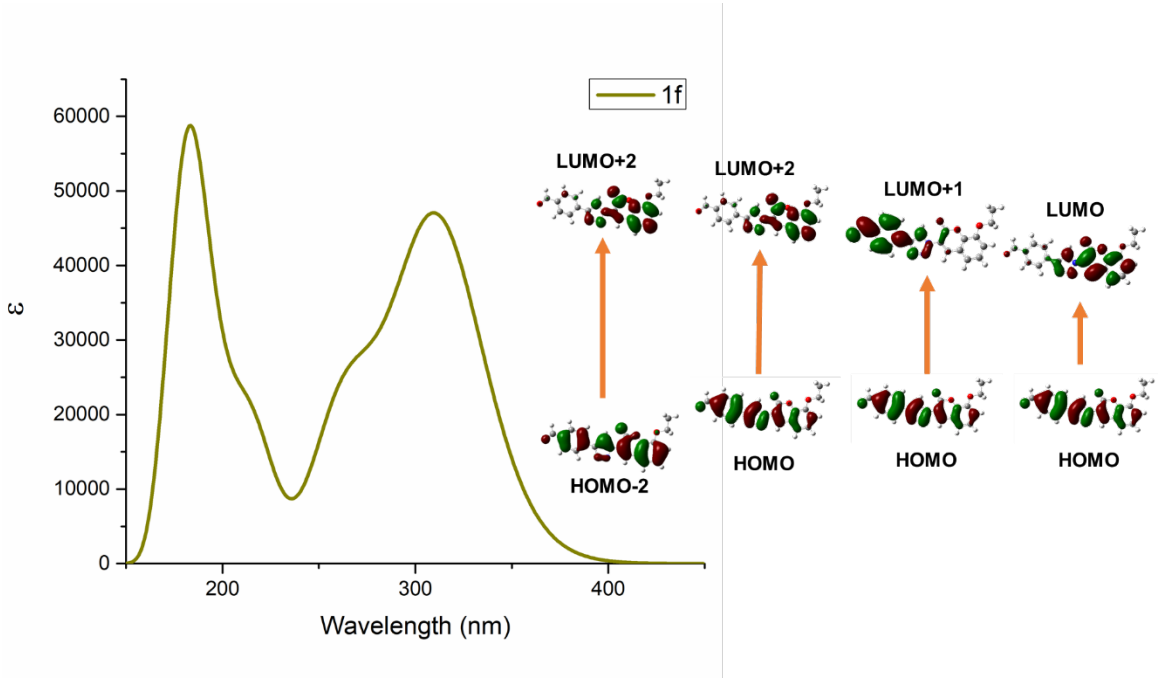


Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p) and CPCM in dichloromethane.

Table S3.13. First thirty electronic transitions of **1f**, obtained by BhandHLYP/6-31G (d, p), CPCM solvent model (dichloromethane), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1f	312.43	3.9689	**1.0845**	H-2->LUMO (11%), HOMO->LUMO (81%)
	297.96	4.1616	0.0001	H-4->L+1 (73%), H-4->L+6 (17%)
	297.51	4.1679	0.0473	H-1->LUMO (88%)
	270.69	4.5809	**0.4209**	H-2->LUMO (10%), HOMO->L+1 (75%)
	256.76	4.8294	0.199	H-2->LUMO (66%), HOMO->LUMO (10%)
	249.08	4.9782	0.0314	H-3->L+1 (65%)
	223.58	5.5462	0.004	H-8->LUMO (33%), H-8->L+2 (10%), H-7->LUMO (29%)
	219.33	5.6536	0.0039	H-8->LUMO (30%), H-7->LUMO (23%)
	218.50	5.6751	0.2132	H-1->L+2 (16%), H-1->L+3 (12%), HOMO->L+2 (30%)
	214.19	5.7892	0.178	H-2->L+1 (38%), H-1->L+2 (19%)
	209.71	5.9129	0.0114	H-2->L+1 (15%), H-1->L+1 (25%), HOMO->L+2 (26%)
	208.03	5.9606	0.0258	H-3->LUMO (76%)
	207.02	5.9898	0.0029	H-1->L+1 (54%)
	202.77	6.1154	0.095	H-2->L+2 (20%), H-1->L+5 (11%), HOMO->L+3 (31%)
	199.64	6.2112	0.1172	H-6->LUMO (48%), H-1->L+5 (19%)
	194.34	6.3804	**0.2877**	H-6->LUMO (13%), H-3->L+1 (11%), HOMO->L+4 (43%)
	190.92	6.4947	0.015	H-5->LUMO (39%), H-5->L+1 (28%)
	187.21	6.6235	0.0019	H-7->LUMO (24%), H-7->L+1 (52%)
	186.31	6.6555	0.163	H-5->LUMO (26%), H-5->L+1 (16%), H-2->L+2 (19%)
	185.63	6.6800	**0.3566**	H-2->L+2 (26%), H-2->L+4 (15%)

	184.18	6.7326	**0.3027**	H-1->L+5 (39%)
	181.92	6.8162	0.0093	H-3->L+3 (11%), H-1->L+2 (13%), HOMO->L+5 (28%)
	179.55	6.9063	0.3143	H-3->L+3 (22%), HOMO->L+6 (17%)
	177.36	6.9913	0	H-4->LUMO (92%)
	176.16	7.0392	0.2433	H-1->L+2 (16%), H-1->L+3 (28%), H-1->L+4 (25%), HOMO->L+5 (14%)
	173.91	7.1303	0.12	H-5->L+1 (19%), HOMO->L+6 (42%)
	173.13	7.1622	0.0006	H-8->LUMO (13%), H-8->L+2 (19%)
	169.54	7.3137	0.0019	H-13->LUMO (21%)
	169.23	7.3272	0.1744	H-2->L+3 (40%), H-2->L+4 (10%)
	167.44	7.4055	0.0162	H-10->LUMO (14%), H-9->LUMO (63%)

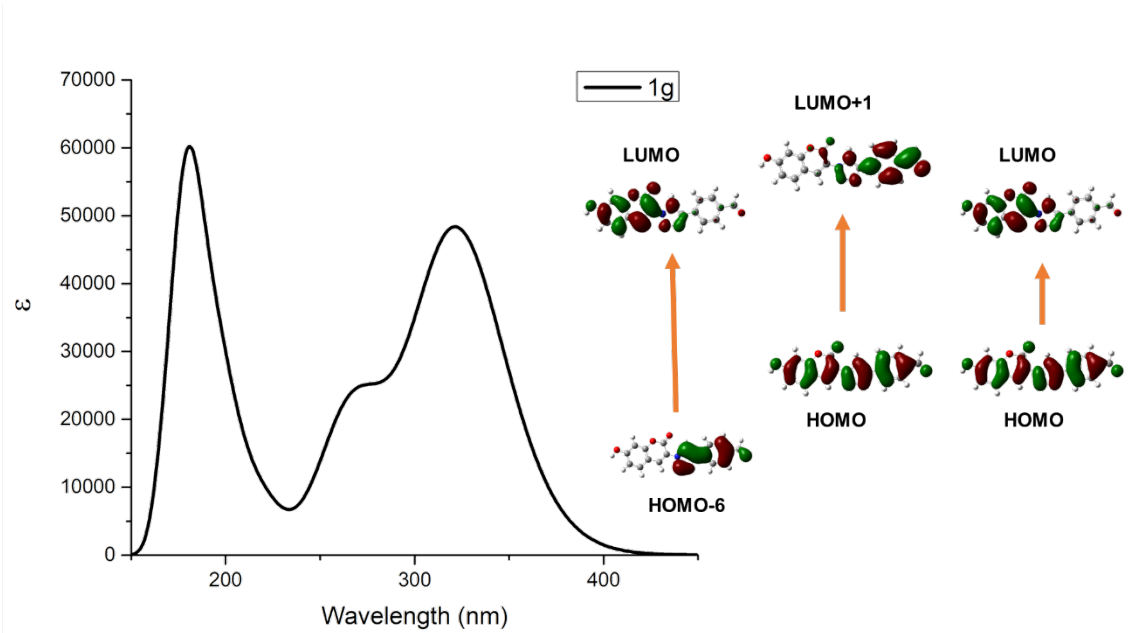


Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p) and CPCM in dichloromethane.

Table S3.14. First thirty electronic transitions of **1g**, obtained by BhandHLYP/6-31G (d, p), CPCM solvent model (dichloromethane), oscillator strength and probable character of molecular orbital.

Molecule	**λ_{ab} (nm)**	**E(tr) (eV)**	***OS(f)***	***MO/Character***
1g	322.90	3.8402	**1.176**	HOMO->LUMO (90%)
	297.80	4.1638	0.0001	H-4->L+1 (73%), H-4->L+6 (17%)
	273.76	4.5295	**0.4499**	H-1->LUMO (13%), H-1->L+1 (20%), HOMO->L+1 (61%)
	259.35	4.7811	0.0913	H-2->LUMO (30%), H-1->LUMO (34%)
	254.31	4.8760	0.0819	H-2->LUMO (34%), H-1->LUMO (34%)
	248.90	4.9818	0.03	H-3->L+1 (56%)
	225.08	5.5092	0.0461	H-1->L+1 (43%), HOMO->L+1 (21%), HOMO->L+2 (15%)
	221.18	5.6062	0.0037	H-8->LUMO (35%), H-7->LUMO (25%)

	219.08	5.6600	0.1129	H-2->LUMO (11%), H-1->L+1 (13%), HOMO->L+2 (46%)
	217.35	5.7051	0.0045	H-8->LUMO (26%), H-7->LUMO (22%), H-7->L+2 (10%)
	211.83	5.8537	0.0297	HOMO->L+3 (38%), HOMO->L+4 (25%)
	205.29	6.0403	0.0766	H-3->LUMO (68%), H-2->LUMO (10%)
	201.32	6.1593	0.1148	H-3->L+1 (11%), HOMO->L+4 (22%), HOMO->L+5 (13%)
	198.96	6.2323	0.13	H-6->LUMO (12%), H-5->LUMO (34%), H-2->L+2 (12%), HOMO->L+5 (12%)
	195.66	6.3375	0.2391	H-6->LUMO (12%), H-5->LUMO (12%), H-1->L+3 (11%), HOMO->L+4 (12%), HOMO->L+5 (24%)
	191.34	6.4805	0.0294	H-6->LUMO (12%), H-6->L+1 (27%), H-5->LUMO (14%)
	189.26	6.5517	0.1384	H-1->L+2 (32%), H-1->L+4 (14%), HOMO->L+3 (11%)
	187.17	6.6250	0.0016	H-7->LUMO (27%), H-7->L+1 (51%)
	184.57	6.7184	**0.3904**	H-6->LUMO (29%), H-5->LUMO (18%), H-2->L+1 (13%)
	183.67	6.7511	0.0055	H-2->L+1 (55%)
	181.05	6.8491	0.0002	H-3->L+2 (12%), H-3->L+3 (14%), H-2->L+3 (13%), H-1->L+6 (10%), HOMO->L+6 (14%)
	179.48	6.9088	**0.7949**	H-3->L+3 (15%), H-2->L+2 (27%), HOMO->L+5 (13%)
	175.68	7.0582	0.0595	H-2->L+4 (15%), H-2->L+5 (16%), H-1->L+3 (10%)
	175.19	7.0782	0	H-4->LUMO (91%)
	174.78	7.0945	0.1174	H-6->L+1 (24%), H-3->L+3 (11%), HOMO->L+6 (32%)
	172.00	7.2091	0.0008	H-11->LUMO (10%), H-8->L+2 (12%)
	170.58	7.2692	0.055	H-2->L+4 (11%), H-1->L+3 (40%)
	168.68	7.3510	0.0019	H-13->LUMO (10%), H-11->LUMO (14%), H-7->LUMO (11%)
	168.61	7.3543	0.2531	H-2->L+4 (13%), H-1->L+4 (25%), H-1->L+5 (10%), HOMO->L+3 (10%)
	168.21	7.3719	0.0237	H-9->LUMO (38%), H-5->L+1 (30%)



Molecular orbitals of the main electronic transitions calculated by TDDFT BhandHLYP/6-31G (d, p) and CPCM in dichloromethane.

Table S4. Resistivity values of TCs **1a-g**.

FPhTC	**Resistivity**/10^4 (Ωcm)
1a	9.91(±0.05)
1b	0.553(±0.080)
1c	1.82(±0.003)
1d	9.41(±0.10)
1e	10.6(±0.10)
1f	9.11(±0.08)
1g	2.07(±0.03)

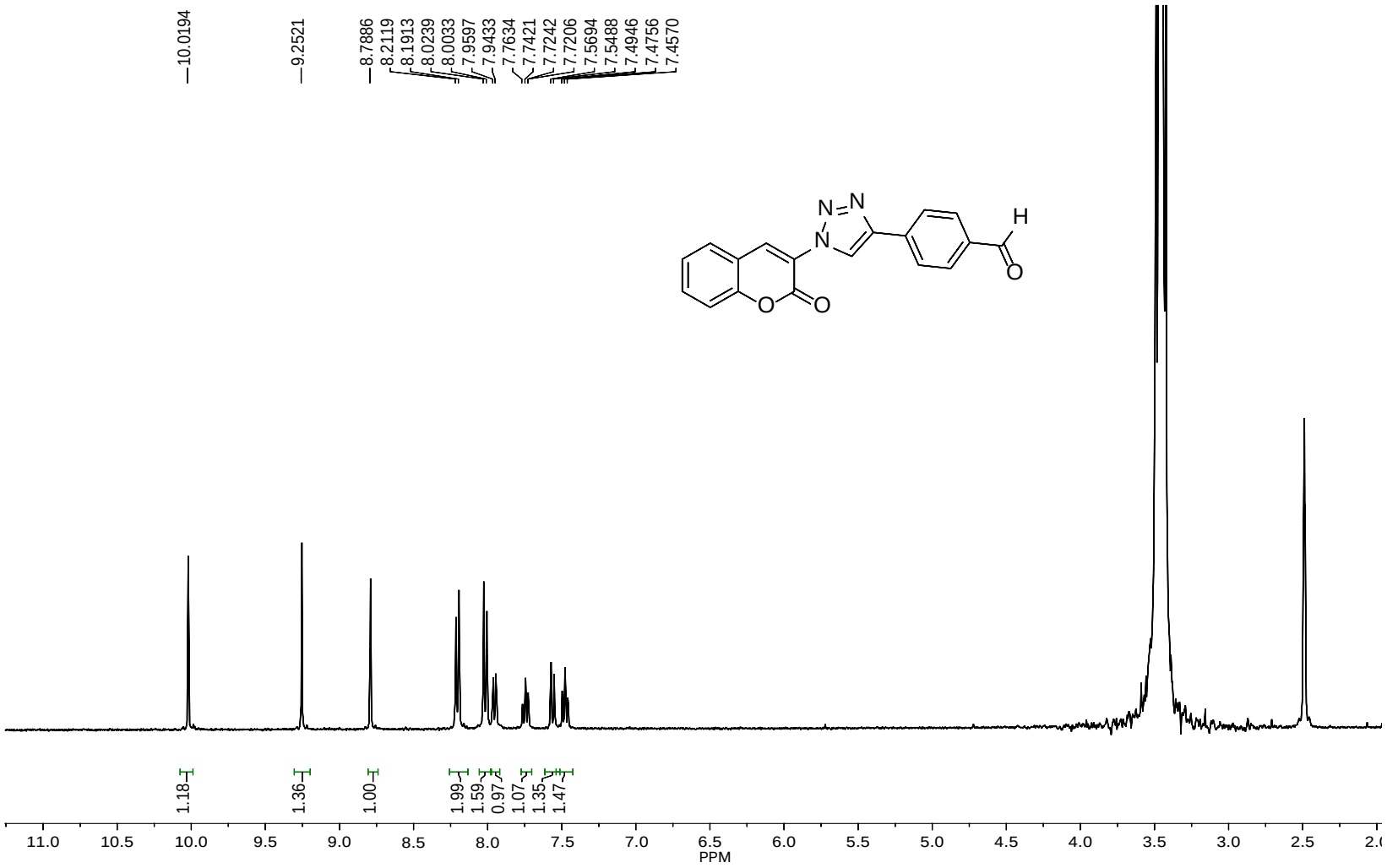


Figure S1. ^{1}H NMR (DMSO-d_6, 400 MHz) spectrum of **1a**

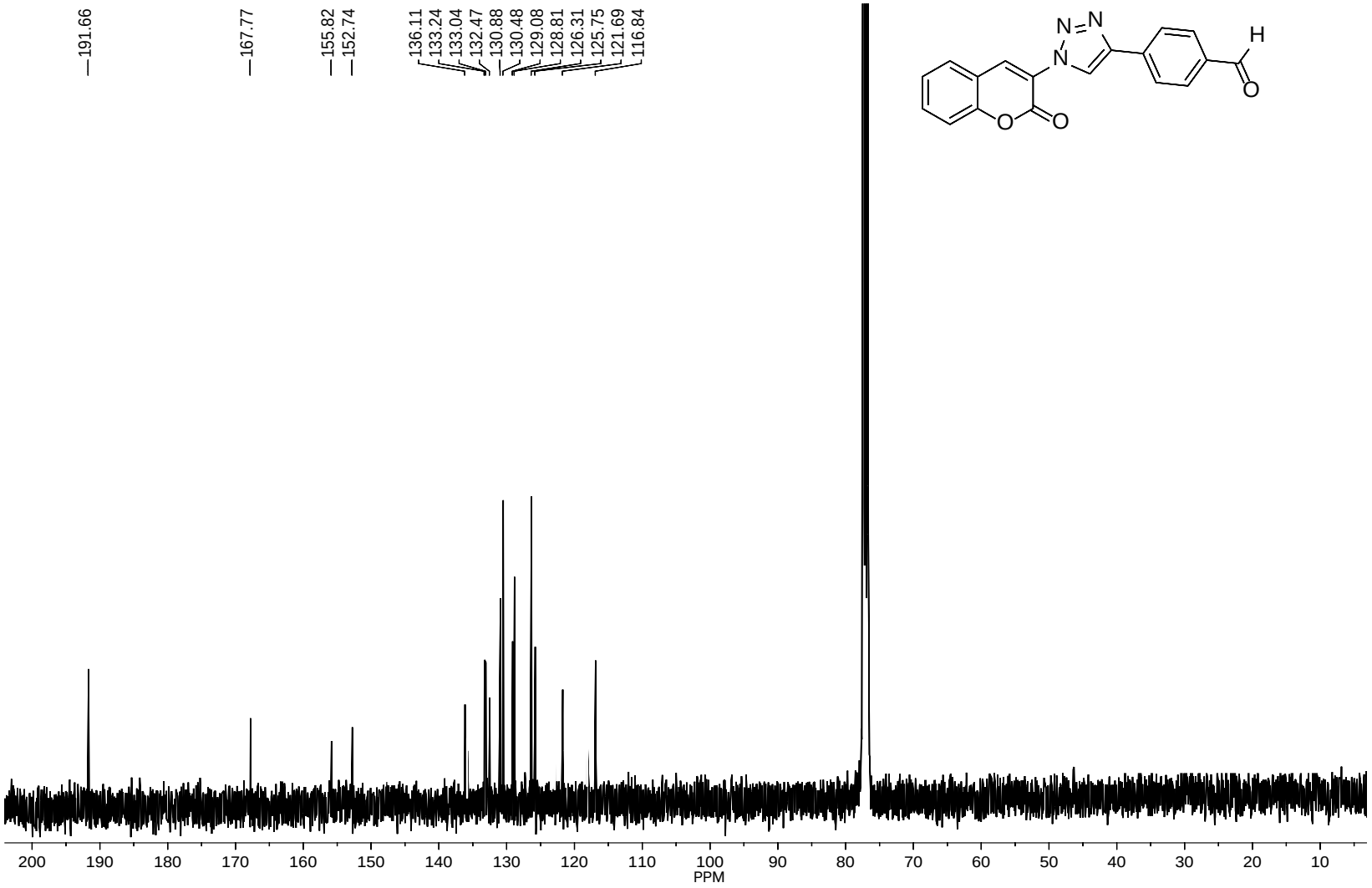


Figure S2. ^{13}C NMR ($CDCl_3$, 100.6 MHz) spectrum of **1a**.

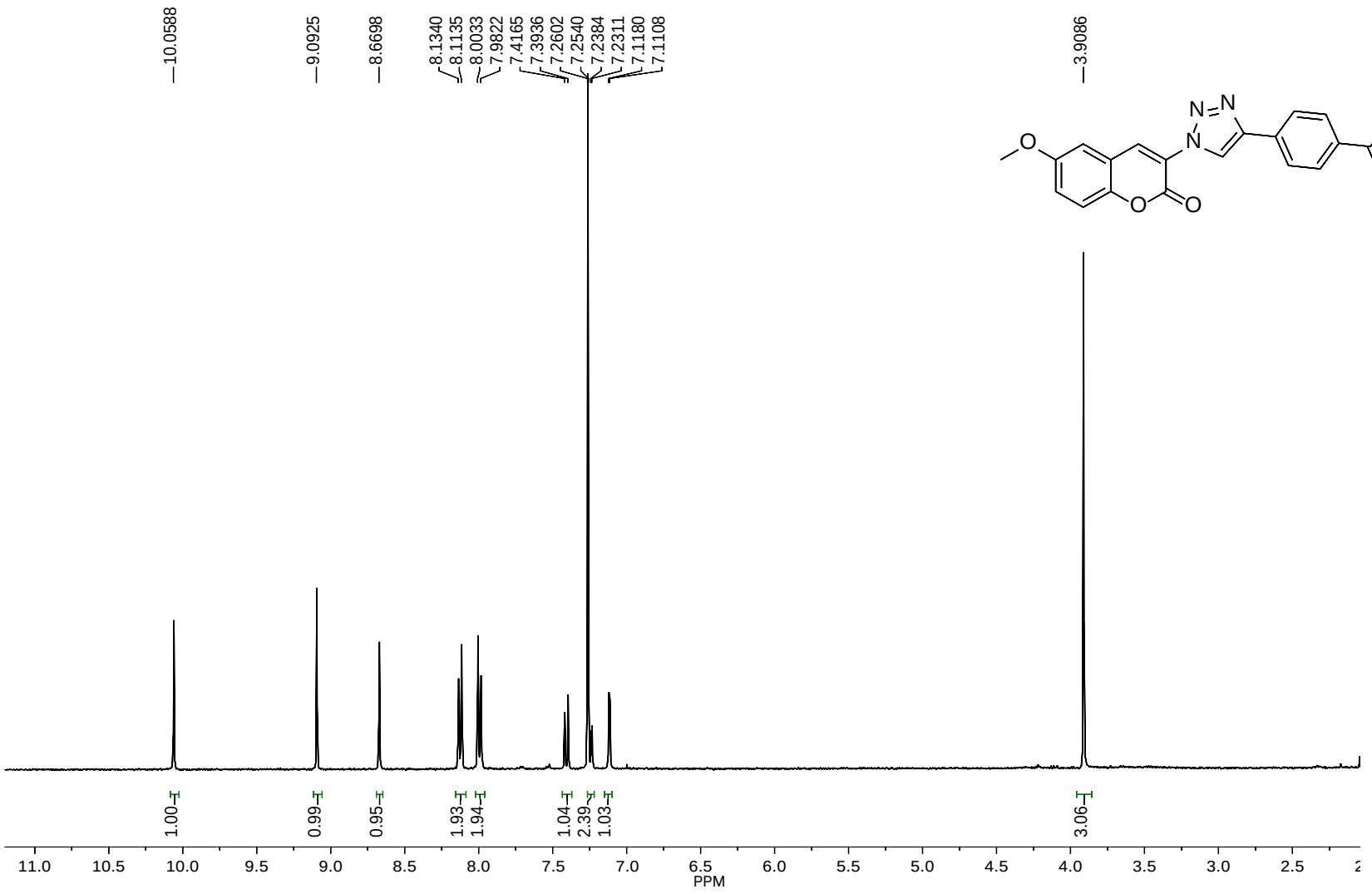


Figure S3. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **1b**.

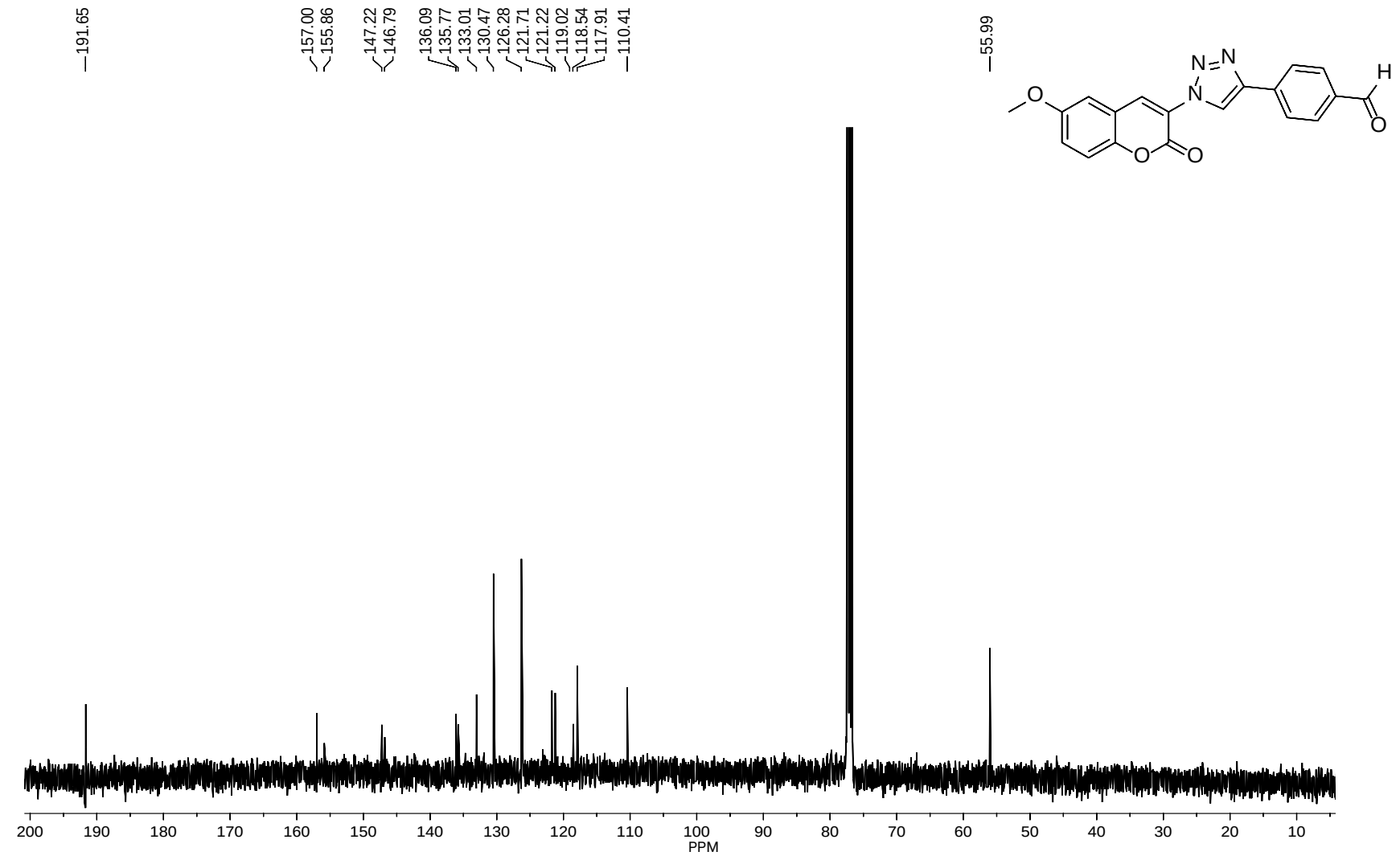


Figure S4. ^{13}C NMR ($CDCl_3$, 100.6 MHz) spectrum of **1b**.

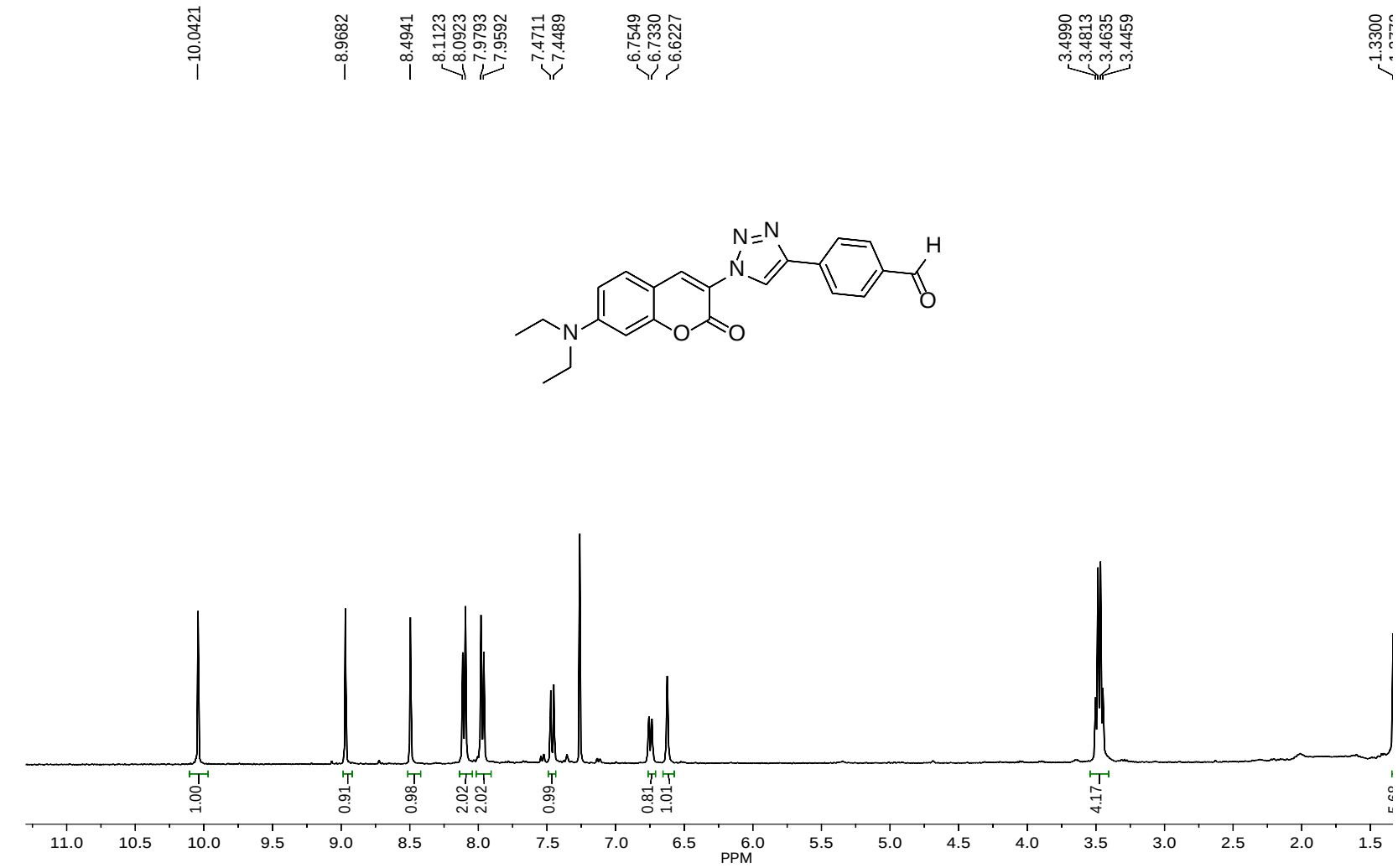


Figure S5. ^{1}H NMR ($CDCl_3$, 400 MHz) spectrum of **1c**.

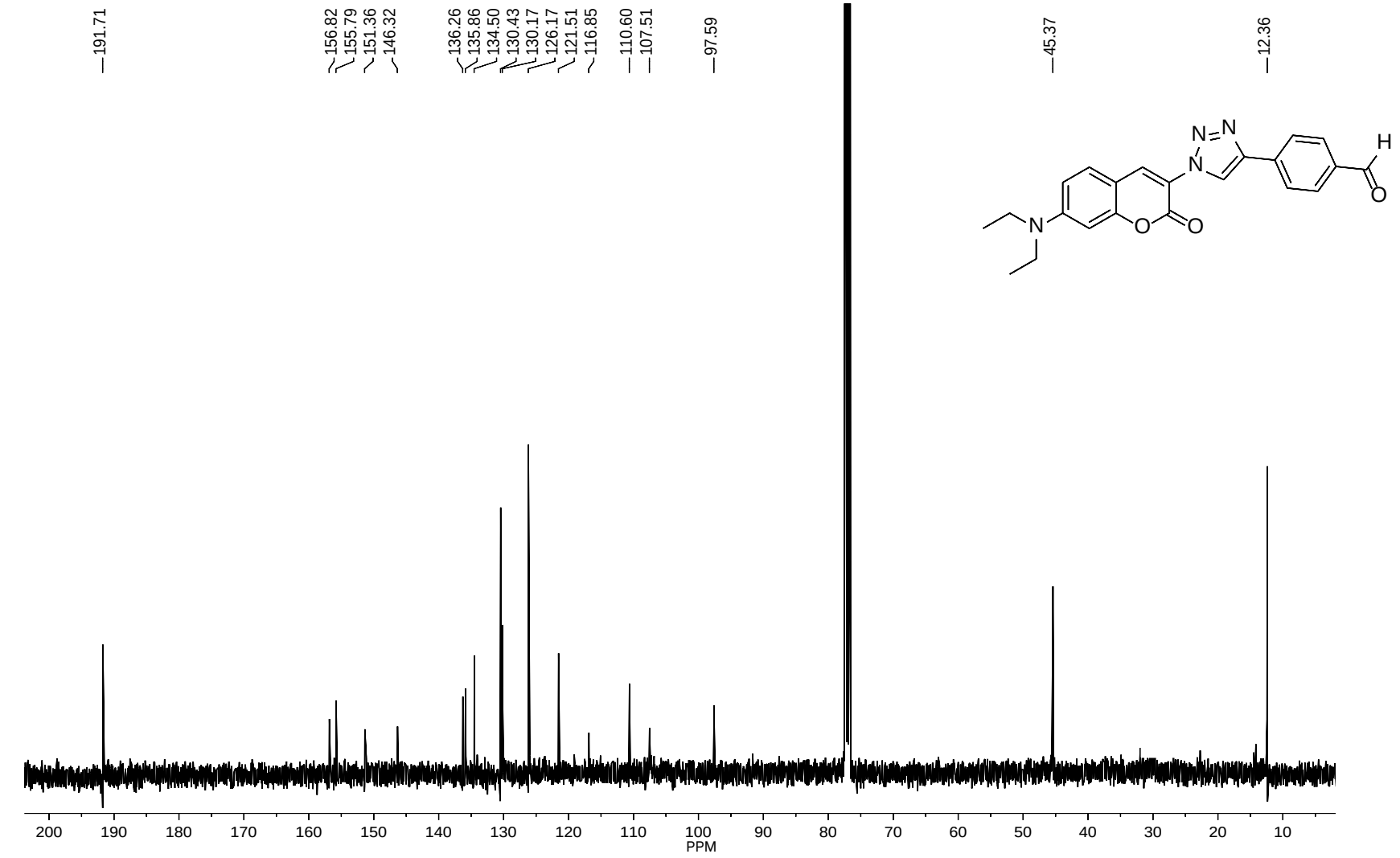


Figure S6. ^{13}C NMR ($CDCl_3$, 100.6 MHz) spectrum of **1c**.

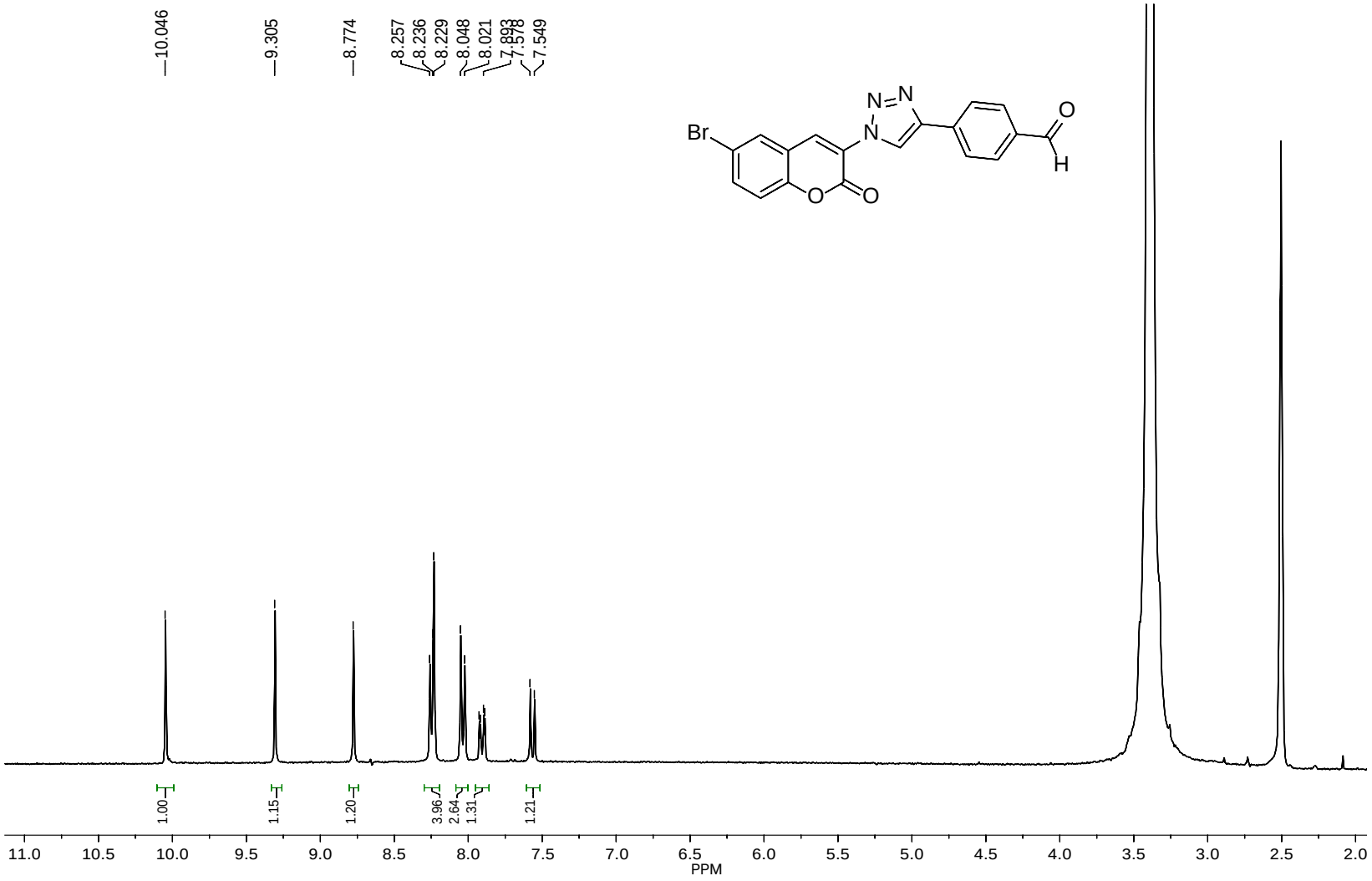


Figure S7. ^{1}H NMR (DMSO-d_6, 300 MHz) spectrum of **1d**.

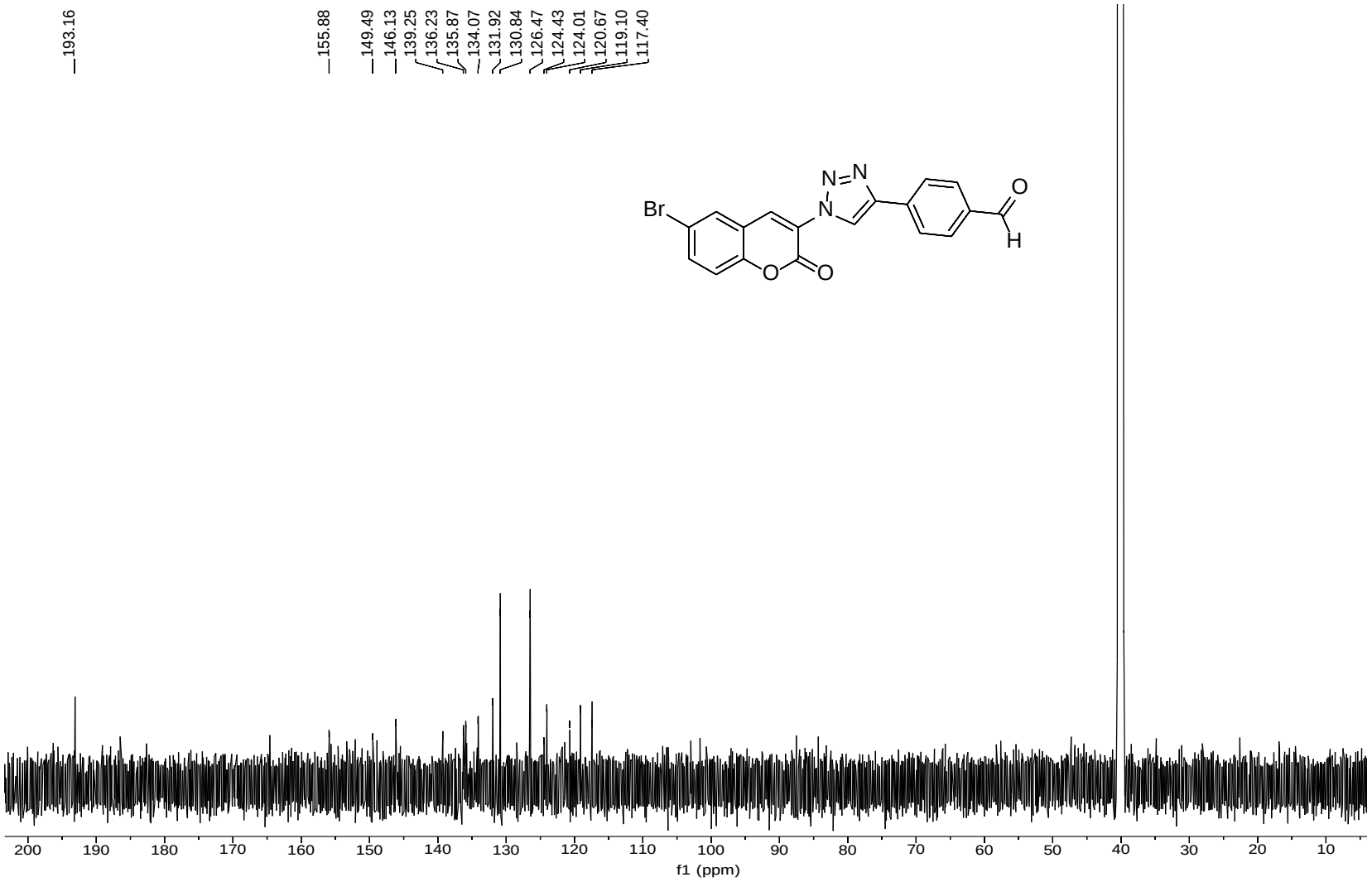


Figure S8. ^{13}C NMR (DMSO-d_6, 75.4 MHz) spectrum of **1d**.

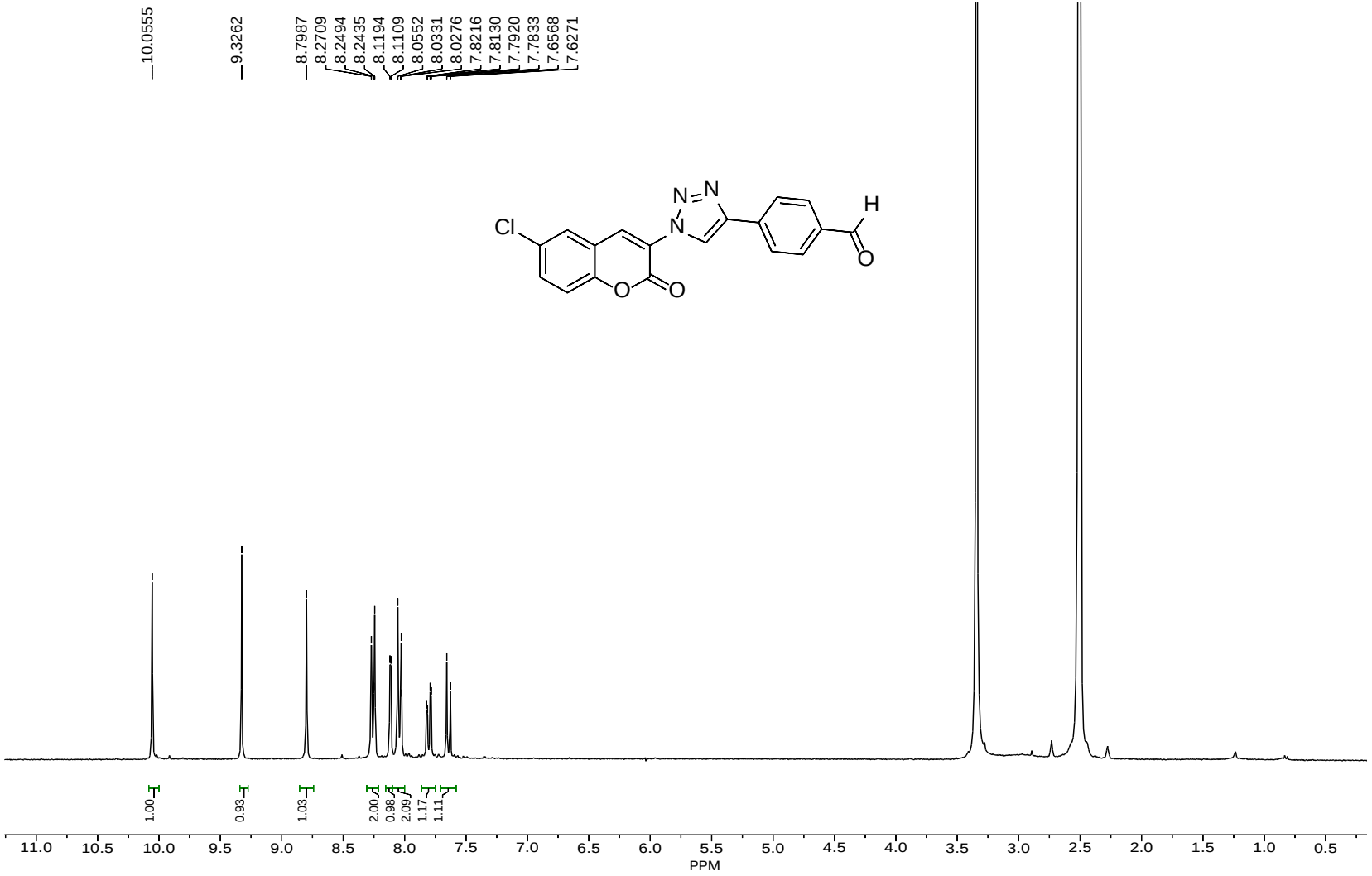


Figure S9. ^{1}H NMR (DMSO-d_6, 300 MHz) spectrum of **1e**.

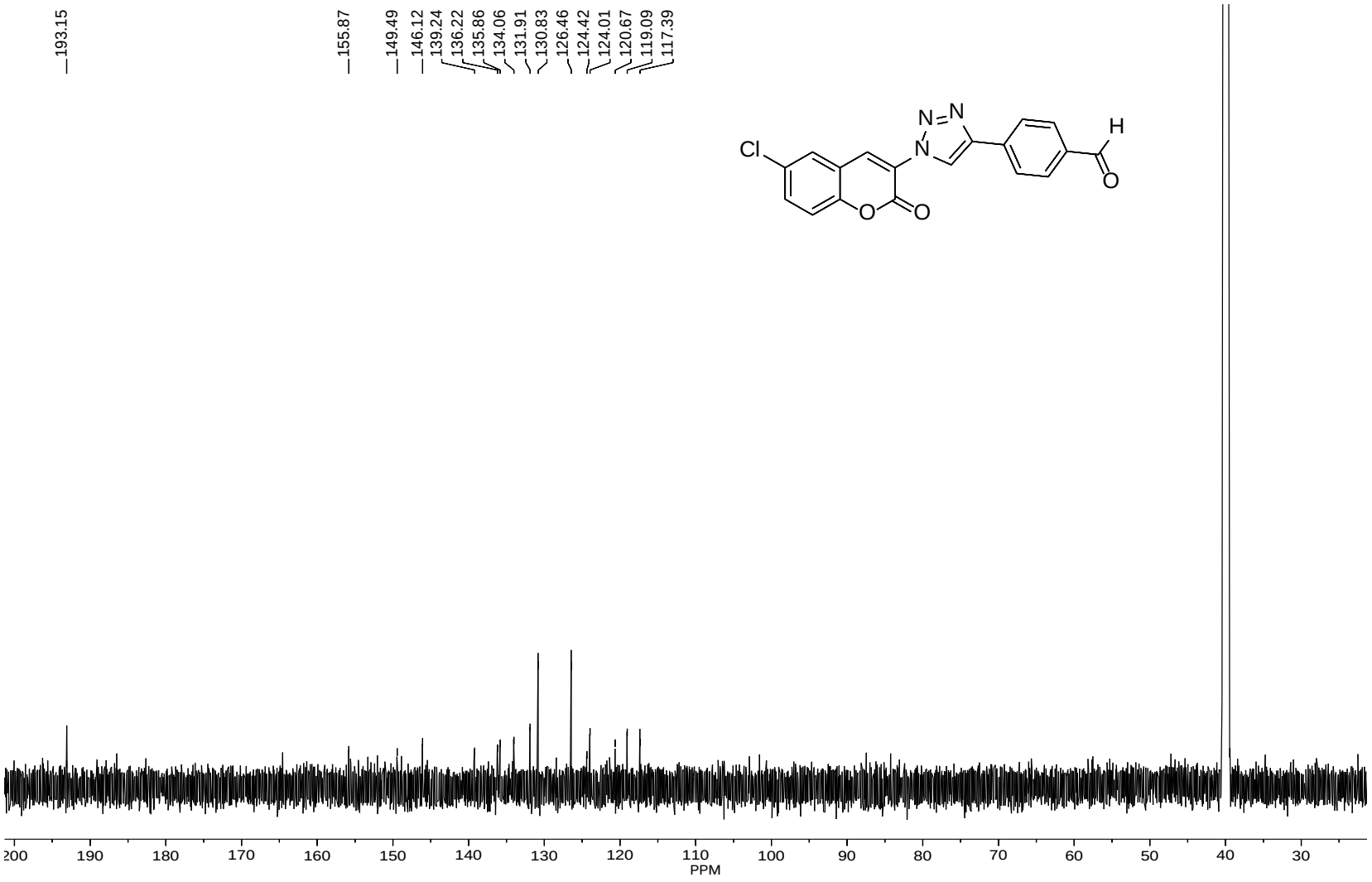


Figure S10. ^{13}C NMR (DMSO-d_6, 75.4 MHz) spectrum of **1e**.

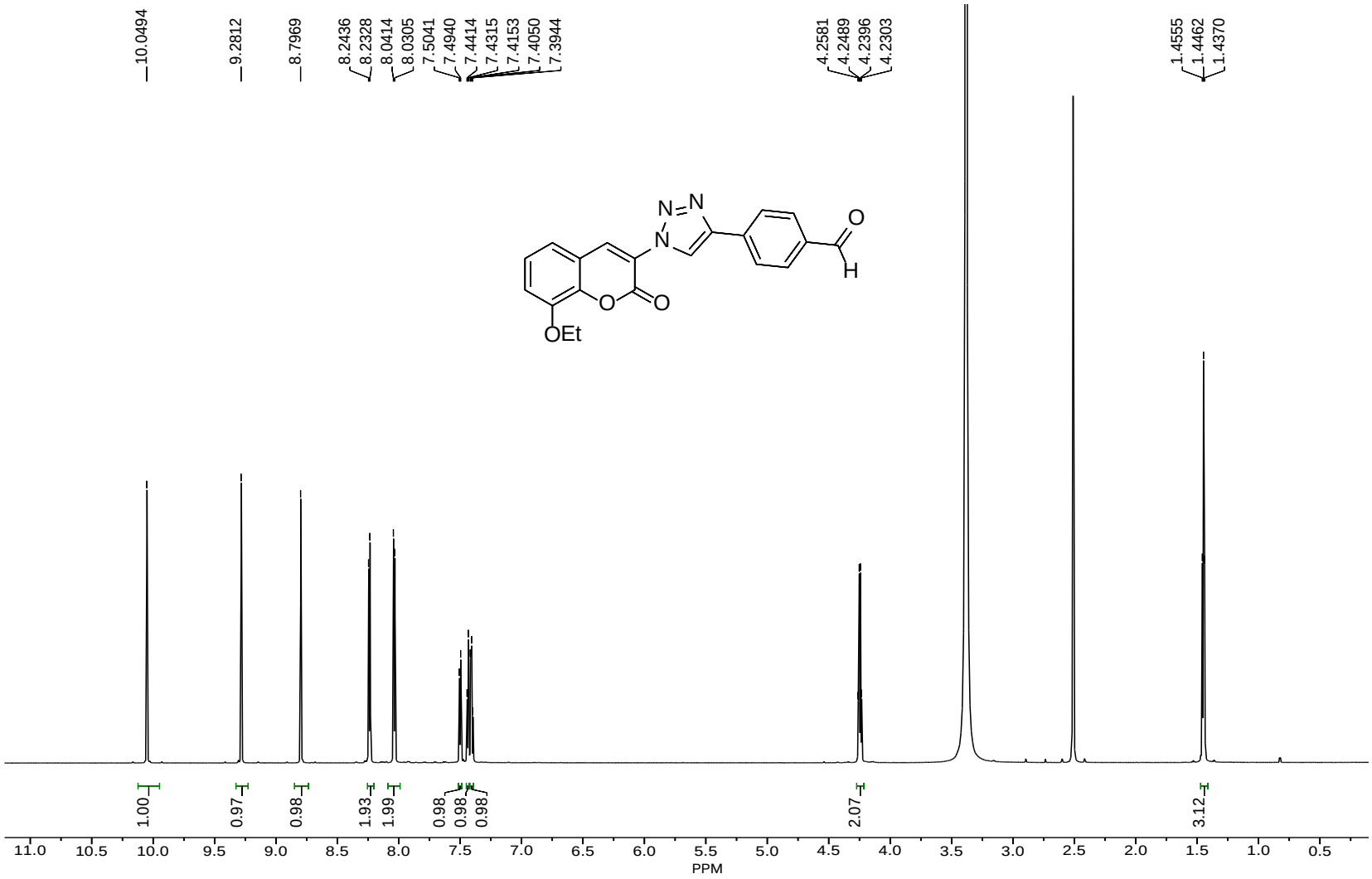


Figure S11. ^{1}H NMR (DMSO-d_6, 750 MHz) spectrum of **1f**.

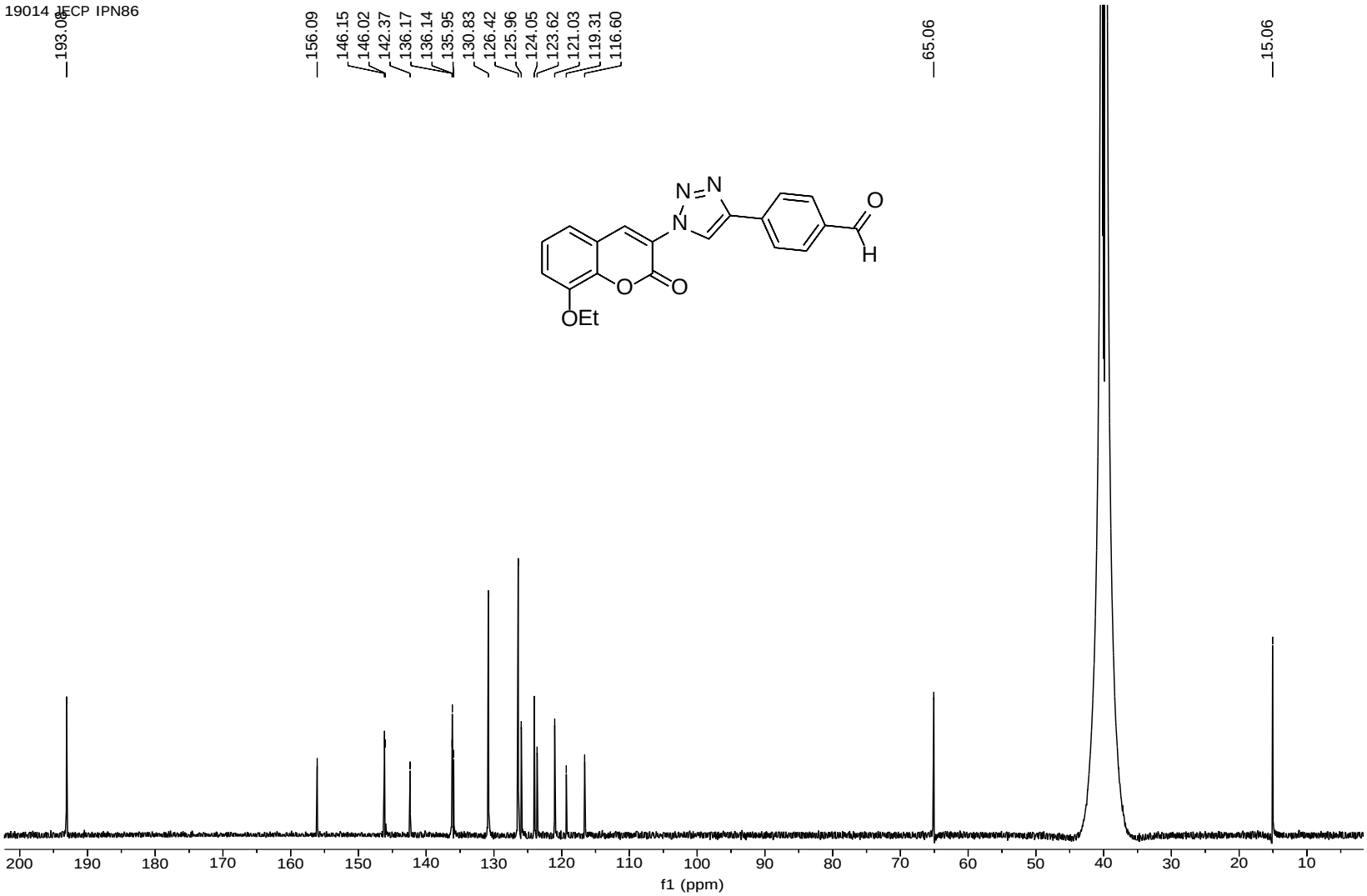


Figure S12. ^{13}C NMR (DMSO-d_6, 188.6 MHz) spectrum of **1f.**

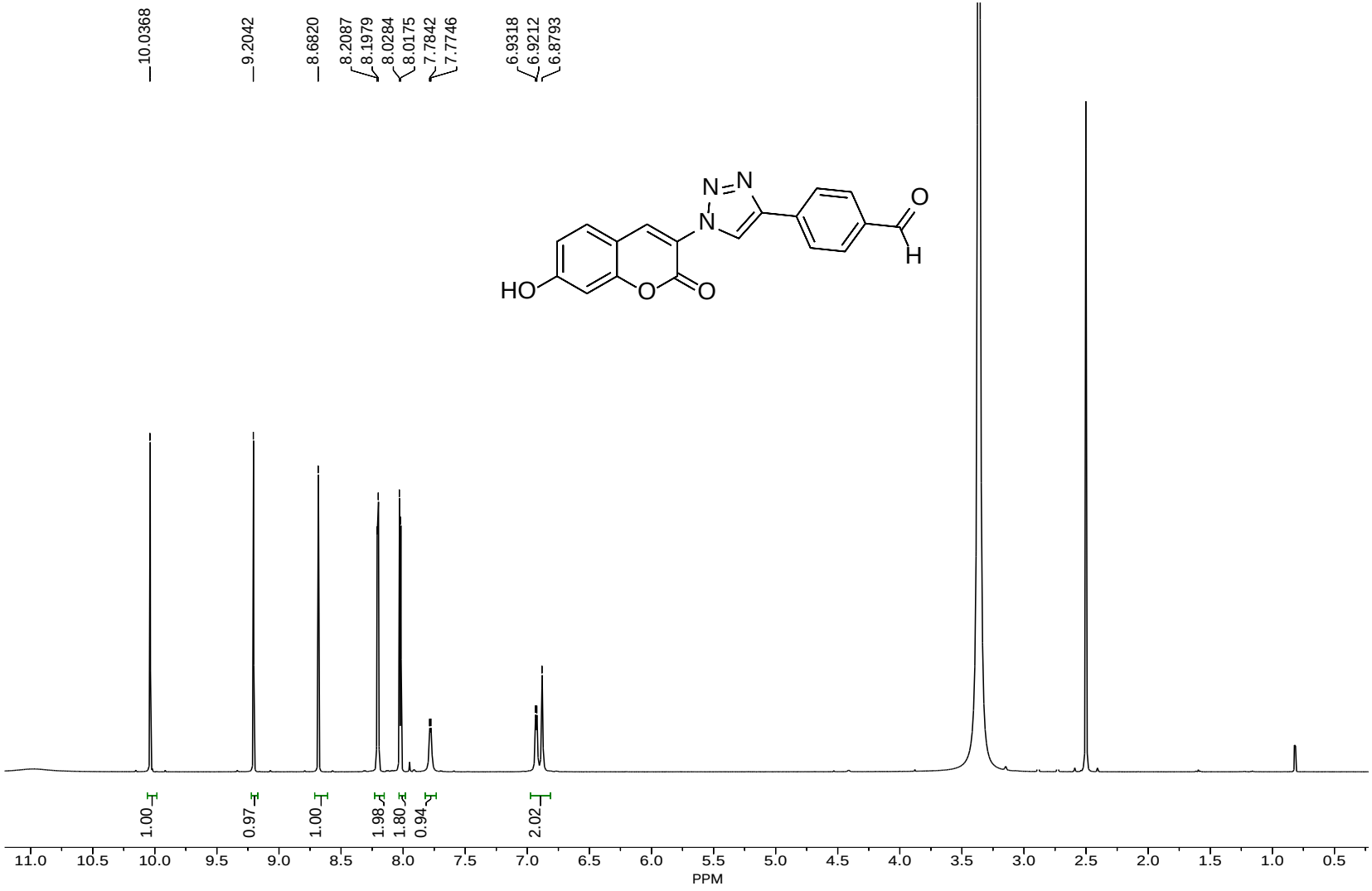


Figure S13. [1] H NMR (DMSO-d_6, 750 MHz) spectrum of **1g**.

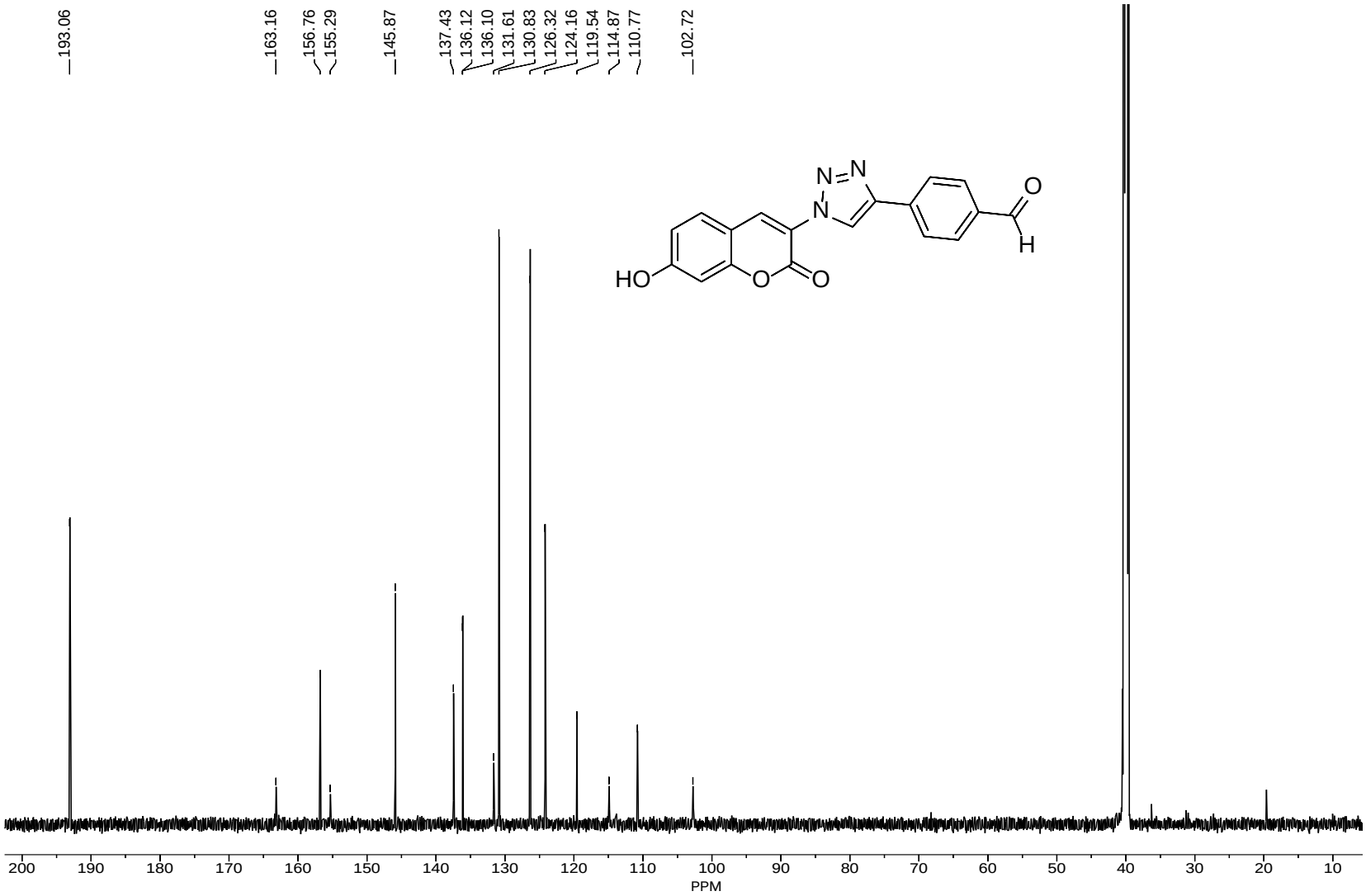


Figure S14. ^{13}C NMR (DMSO-d_6, 188.6 MHz) spectrum of **1g**.

Sample Name	1118-8-7	**Position**	P1-E8	**Instrument Name**	QTOF_MEDICINA_IPN
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	1118-8-7_SU22011_1.d
ACQ Method	MS_ESID.m	**Comment**	JECP-IPN38	**Acquired Time**	1/22/2019 12:02:20 PM

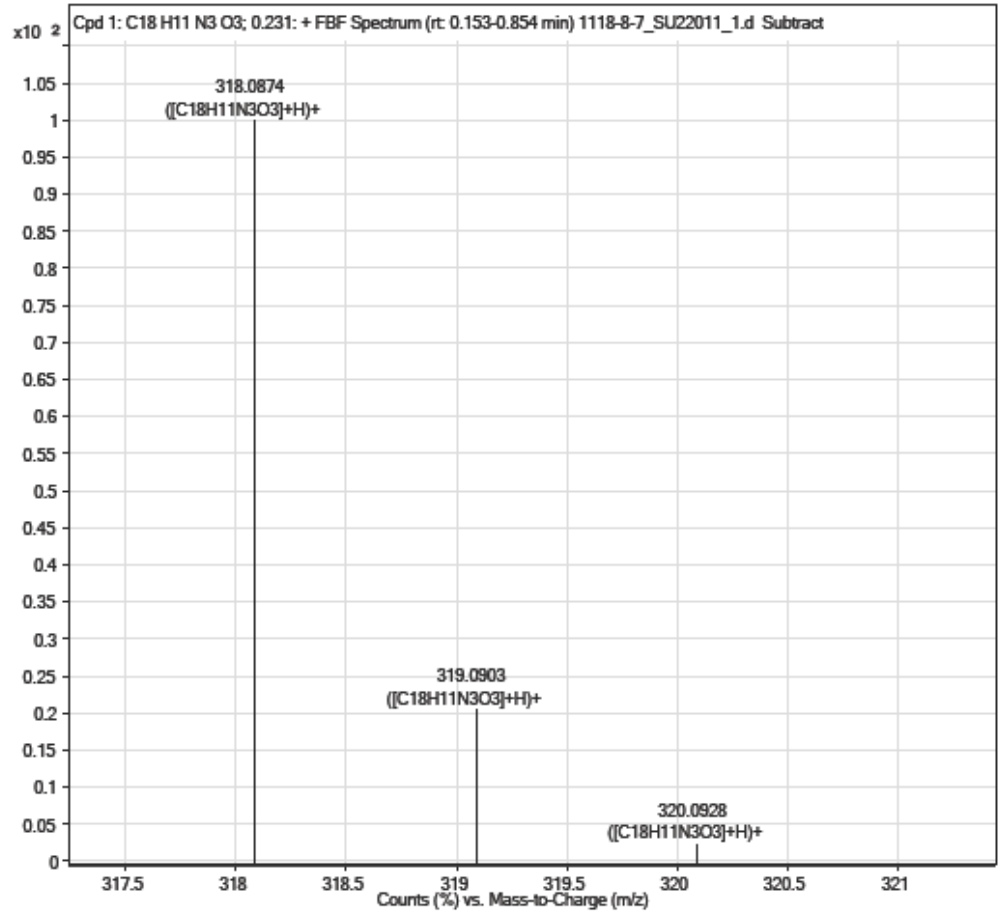


Figure S15. The HRMS mass spectrum of compound **1a**

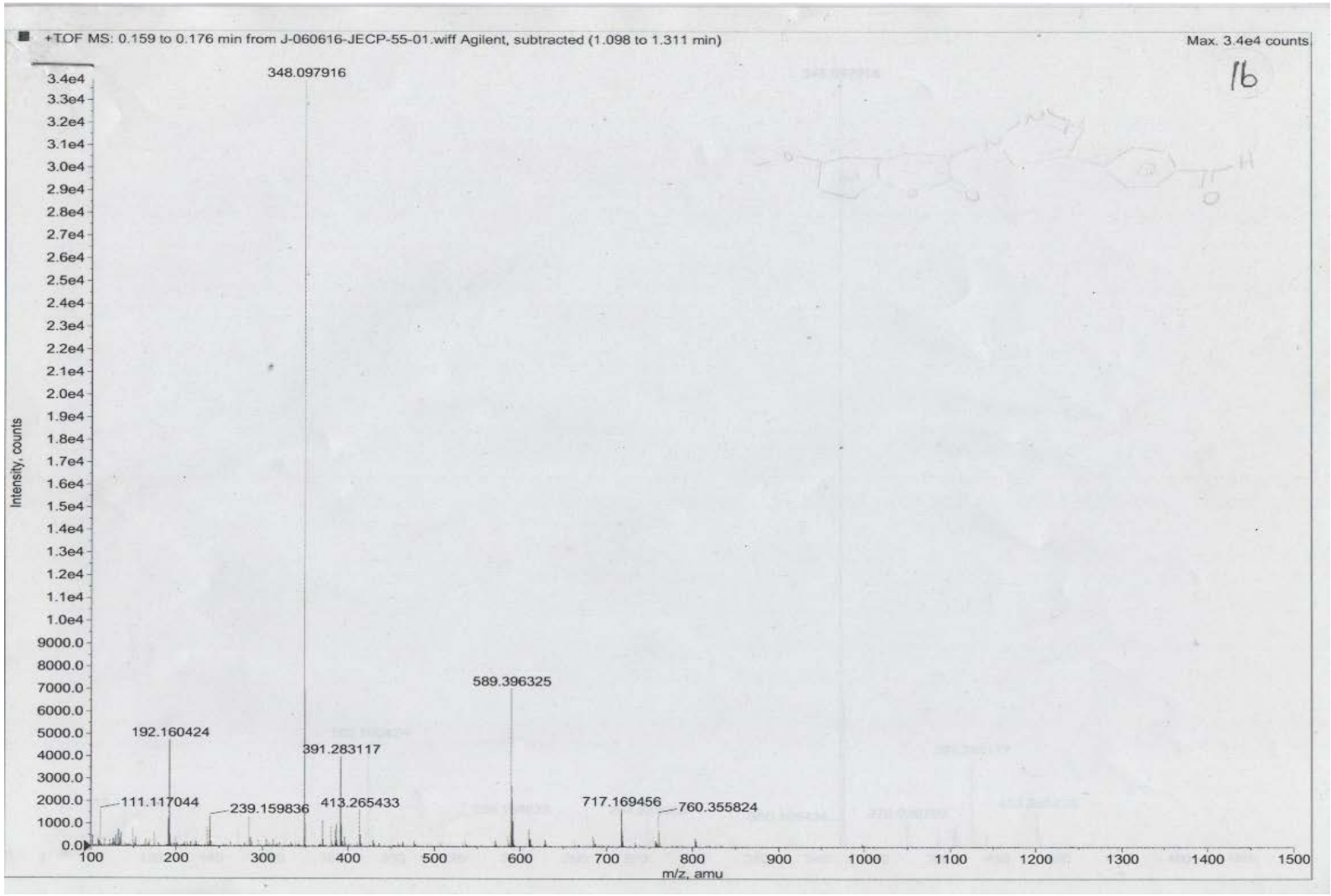


Figure S16. The HRMS mass spectrum of compound **1b**.

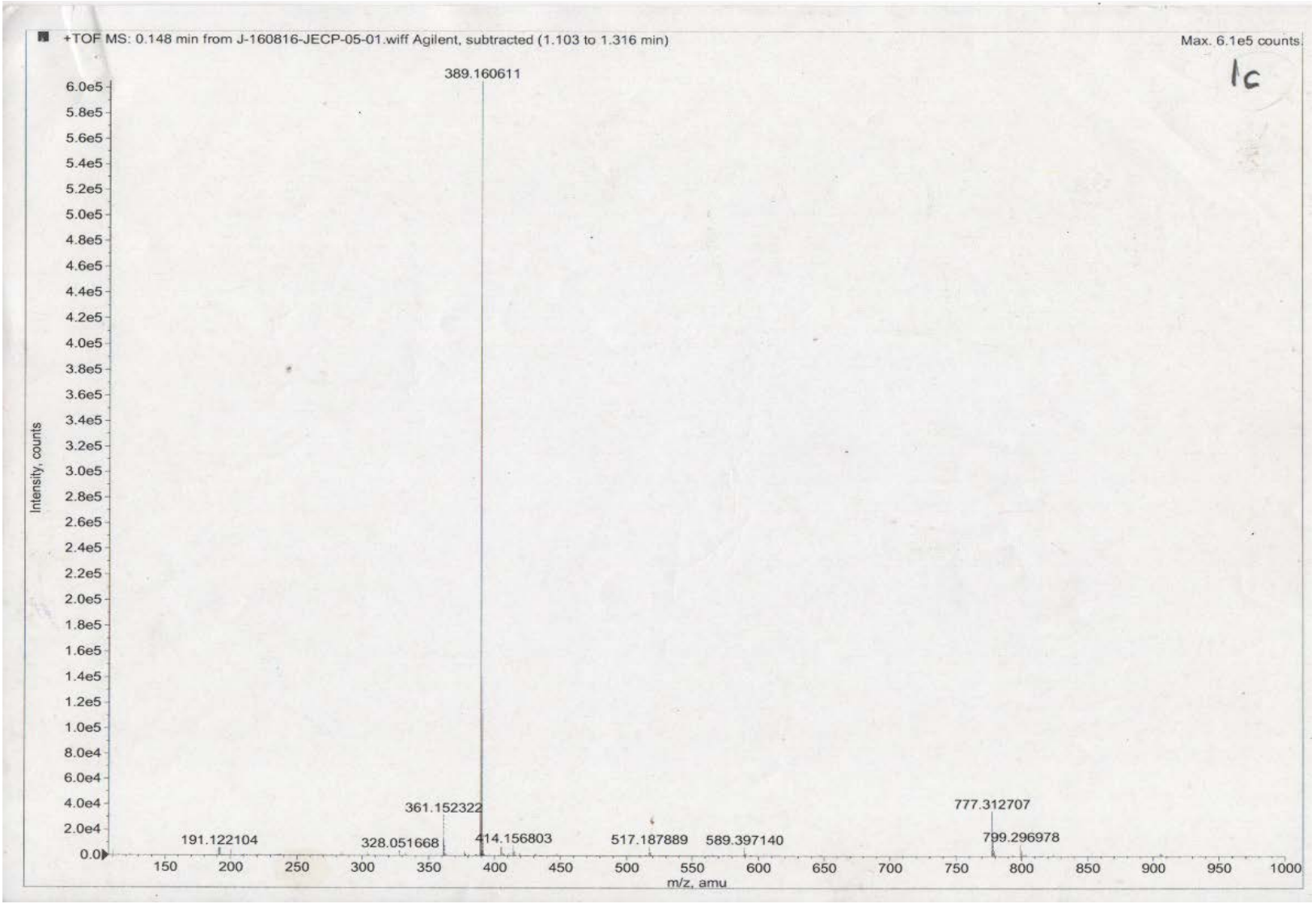


Figure S17. The HRMS mass spectrum of compound **1c**.

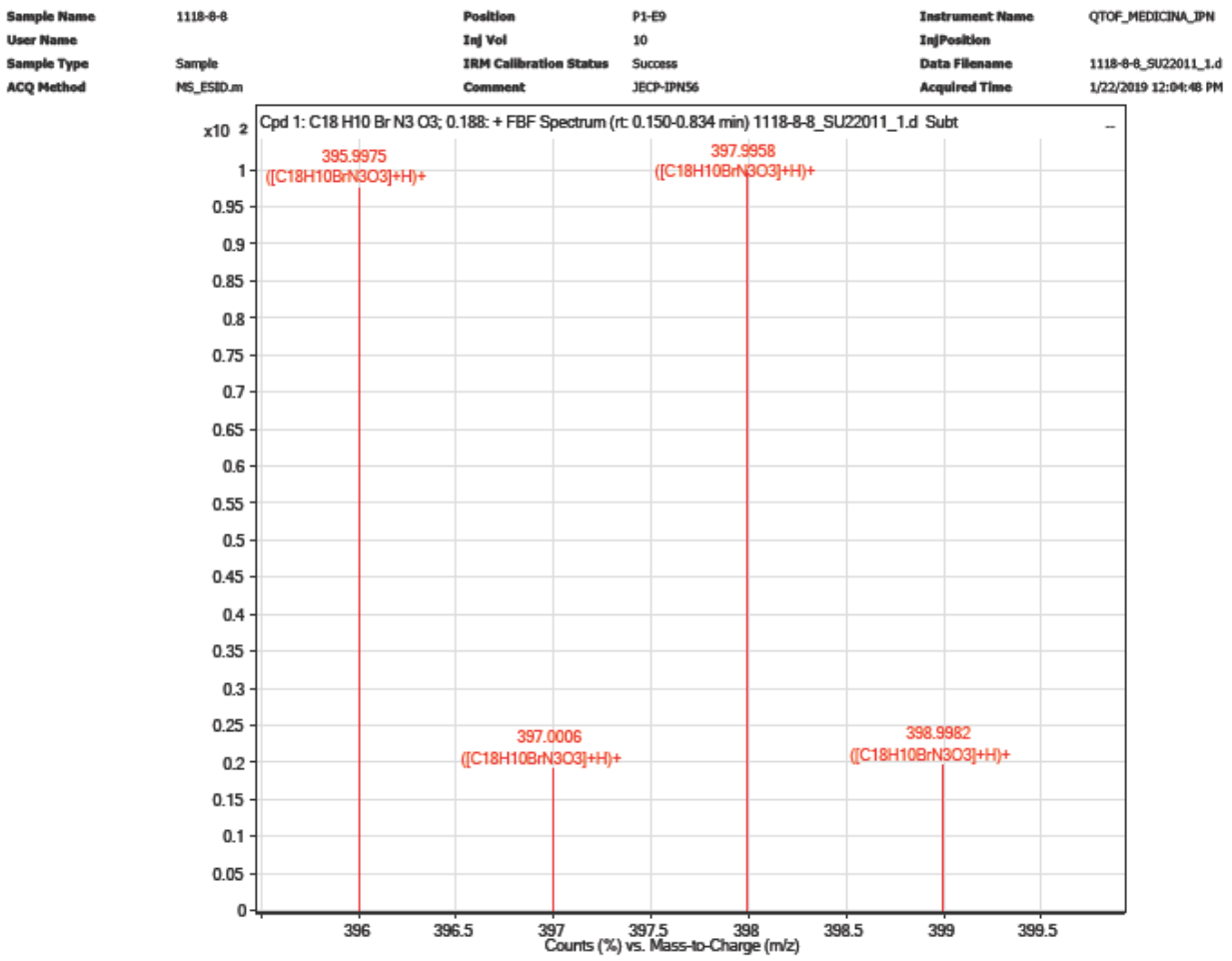


Figure S18. The HRMS mass spectrum of compound **1d**.

Sample Name	1118-8-10	**Position**	P1-E11	**Instrument Name**	QTOF_MEDICINA_IPN
User Name		**Inj Vol**	10	**InjPosition**	
Sample Type	Sample	**IRM Calibration Status**	Success	**Data Filename**	1118-8-10_SU22011_1.d
ACQ Method	MS_ESID.m	**Comment**	JECP-IPN65	**Acquired Time**	1/22/2019 12:09:42 PM

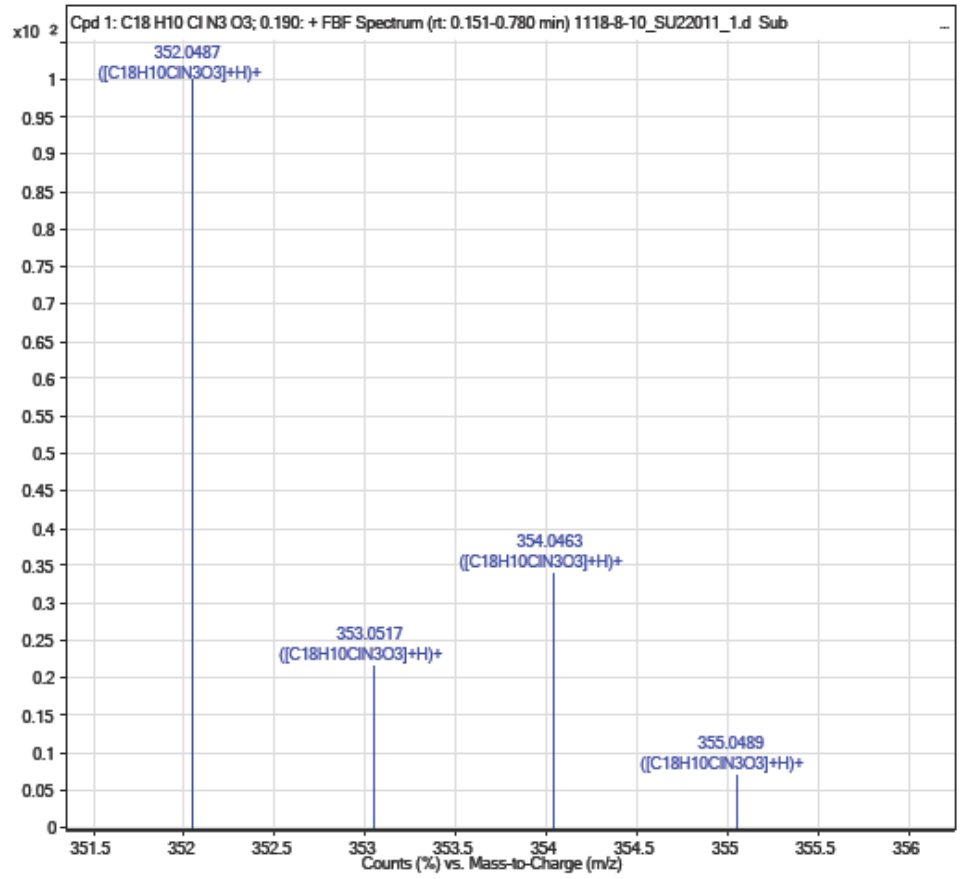


Figure S19. The HRMS mass spectrum of compound **1e**.

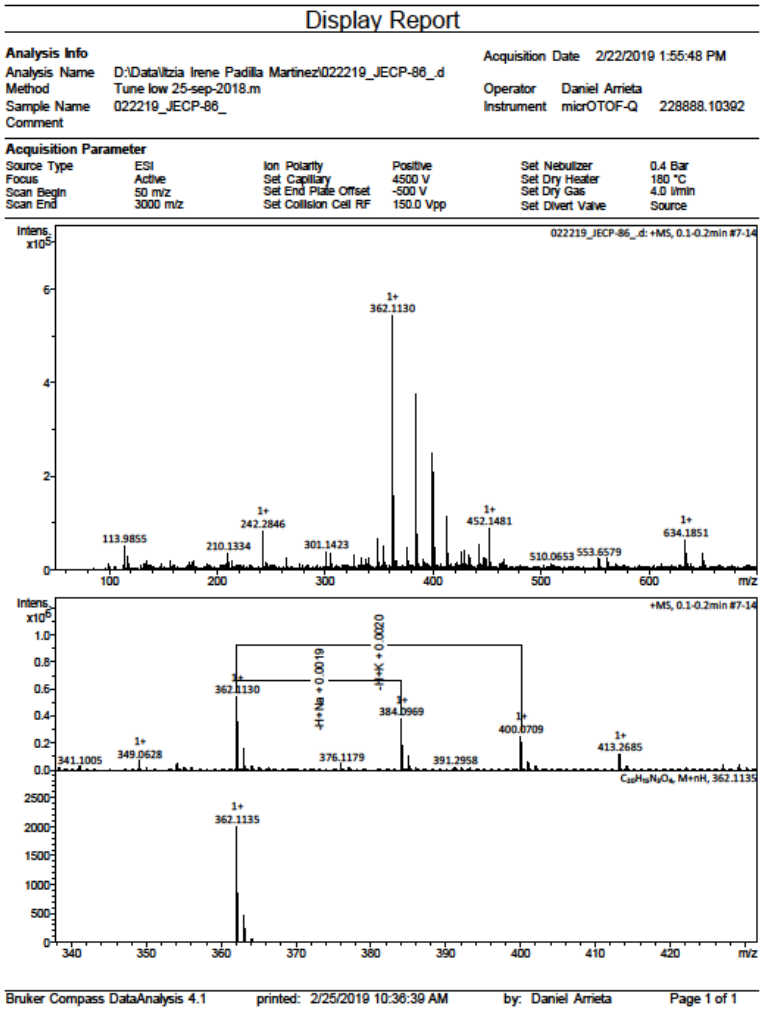


Figure S20. The HRMS mass spectrum of compound **1f**.

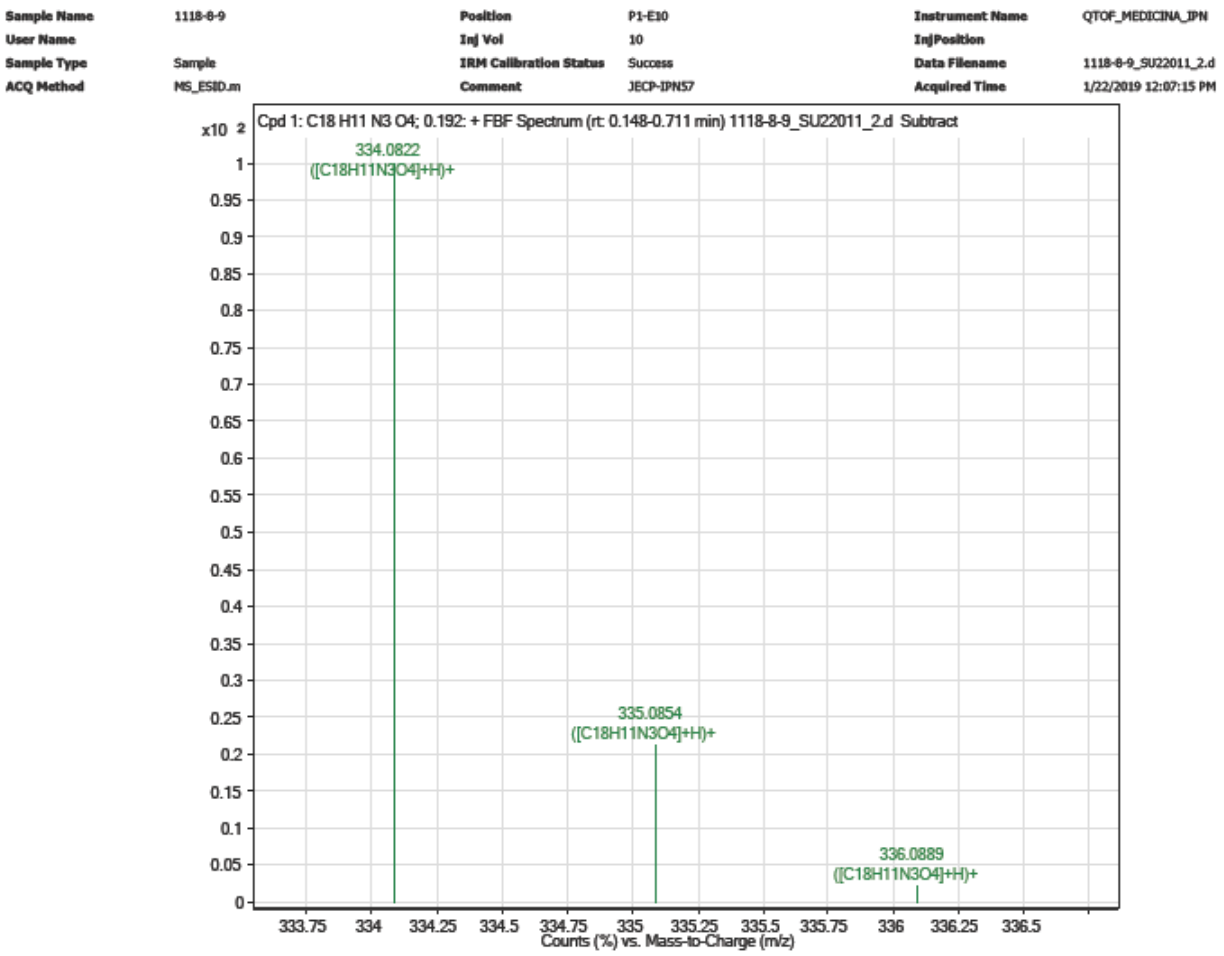


Figure S21. The HRMS mass spectrum of compound **1g**.

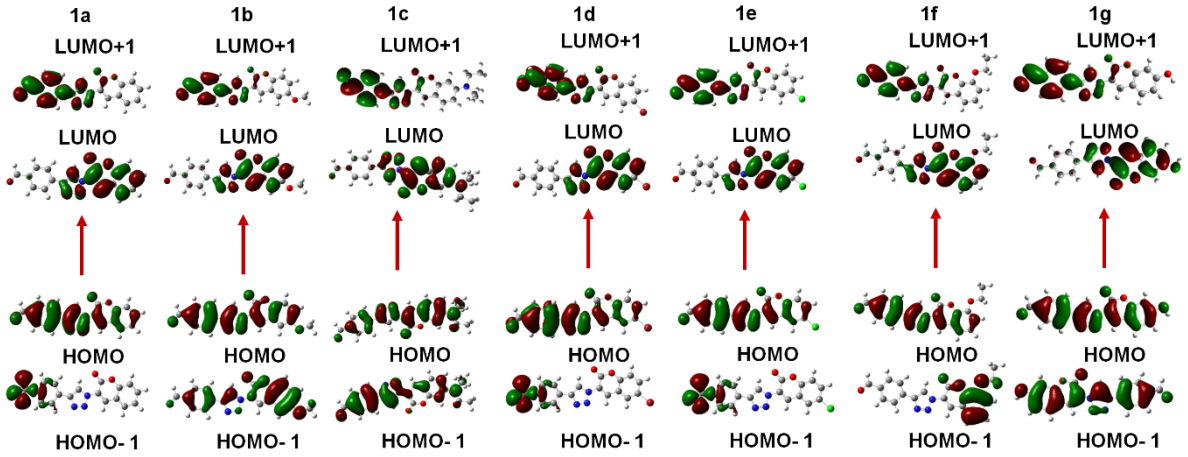
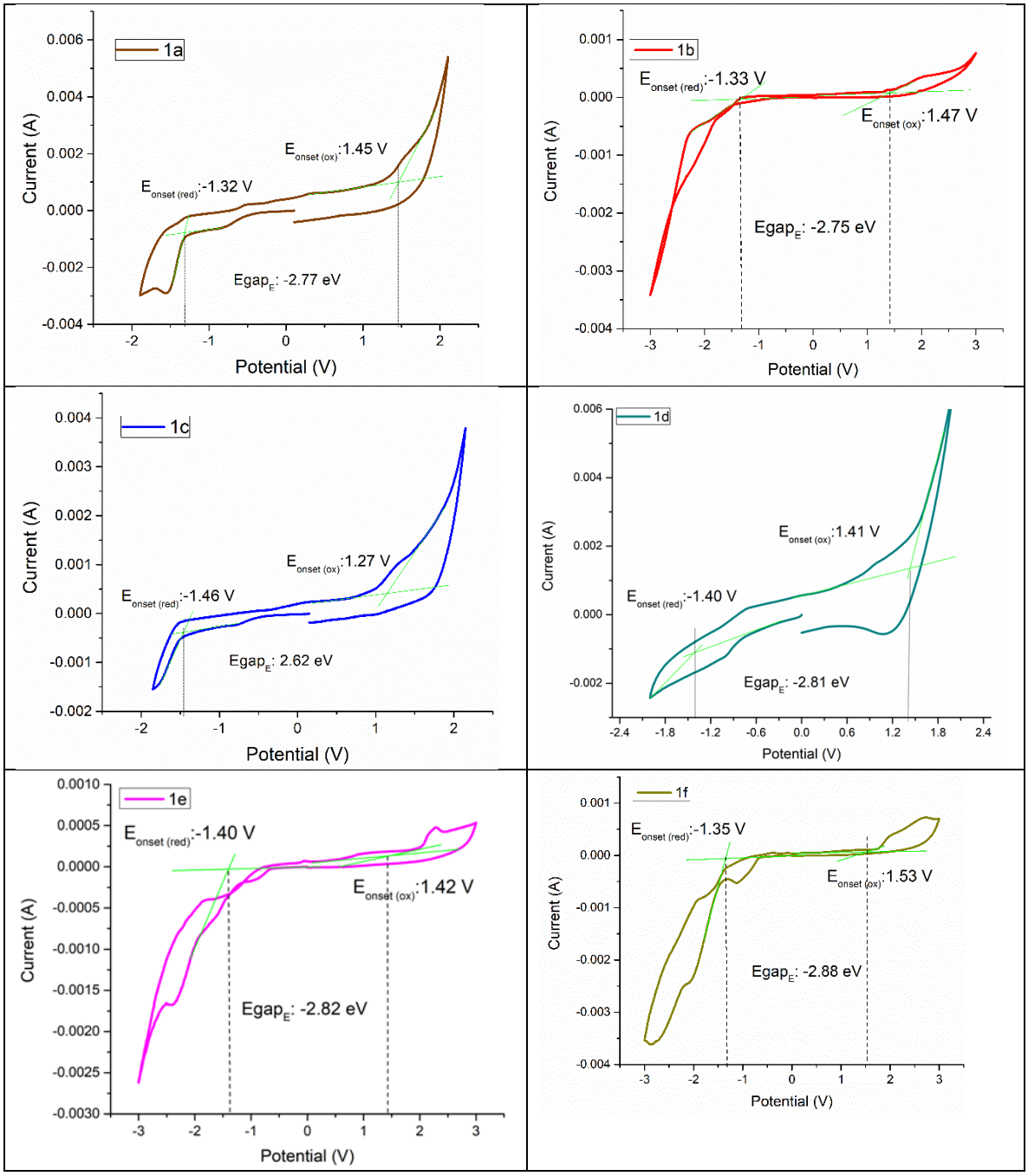


Figure S22. Isosurfaces of the HOMO, LUMO, HOMO-1 and LUMO+1 orbitals of **1a-g**.


1a
$E_{onset\ (red)}$:-1.32 V
$E_{onset\ (ox)}$:1.45 V
$Egap_E$: -2.77 eV
1b
$E_{onset\ (red)}$:-1.33 V
$E_{onset\ (ox)}$:1.47 V
$Egap_E$: -2.75 eV
1c
$E_{onset\ (red)}$:-1.46 V
$E_{onset\ (ox)}$:1.27 V
$Egap_E$: 2.62 eV
1d
$E_{onset\ (red)}$:-1.40 V
$E_{onset\ (ox)}$:1.41 V
$Egap_E$: -2.81 eV
1e
$E_{onset\ (red)}$:-1.40 V
$E_{onset\ (ox)}$:1.42 V
$Egap_E$: -2.82 eV
1f
$E_{onset\ (red)}$:-1.35 V
$E_{onset\ (ox)}$:1.53 V
$Egap_E$: -2.88 eV
Current (A)
Potential (V)

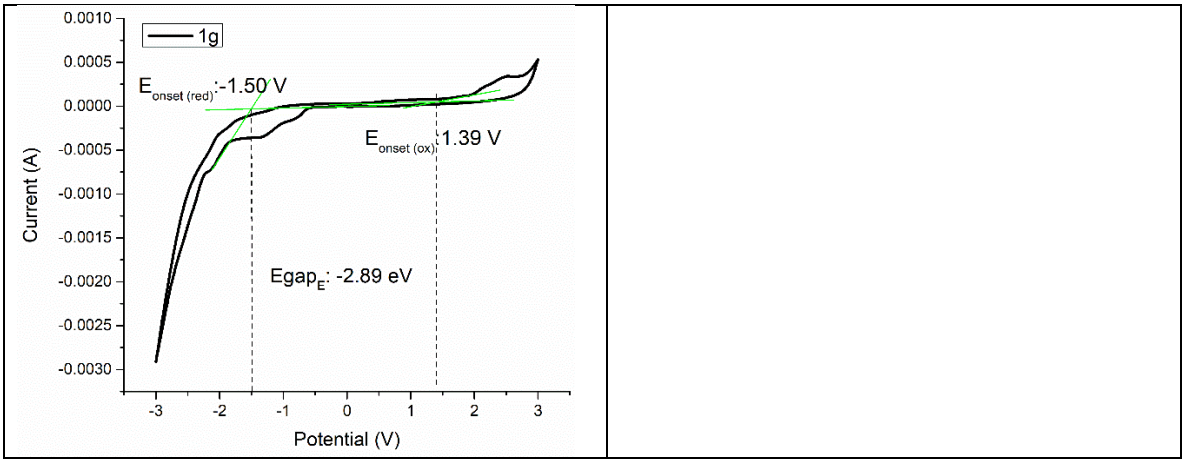


Figure S23. Individual cyclic voltammograms of compounds **1a-g.**

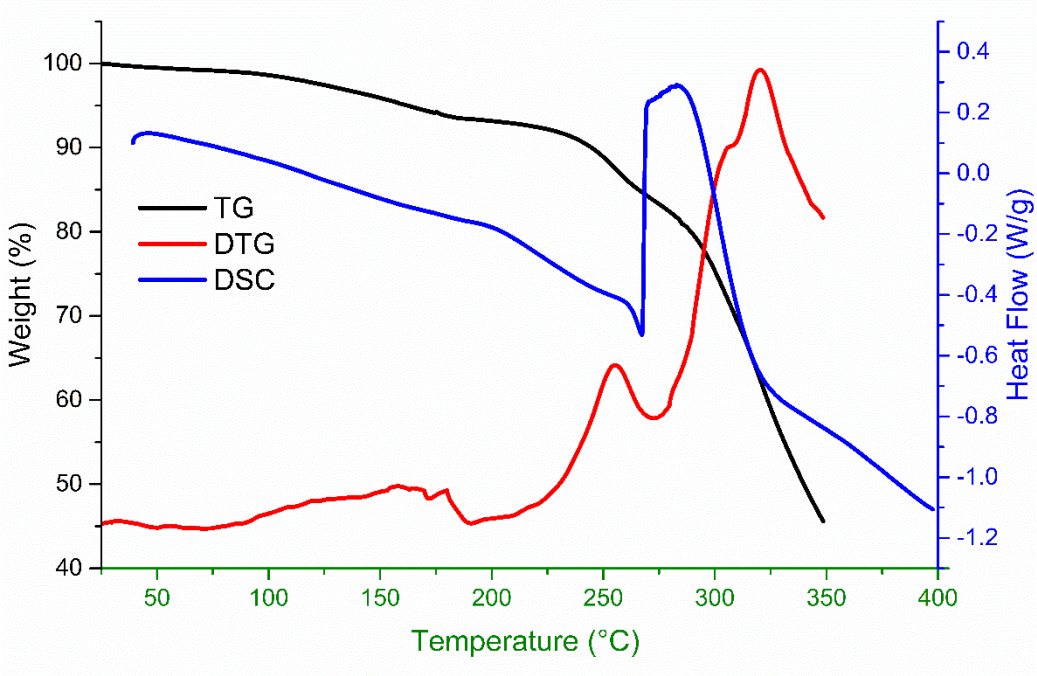


Figure S24. Thermal characterization of compound **1a**.

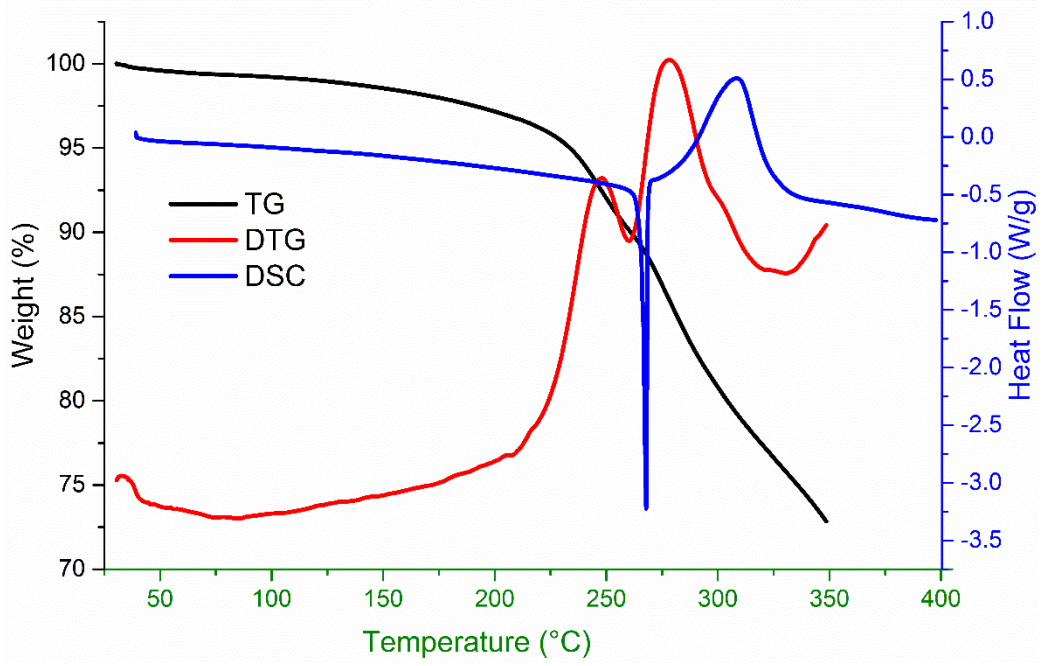


Figure S25. Thermal characterization of compound **1b**.

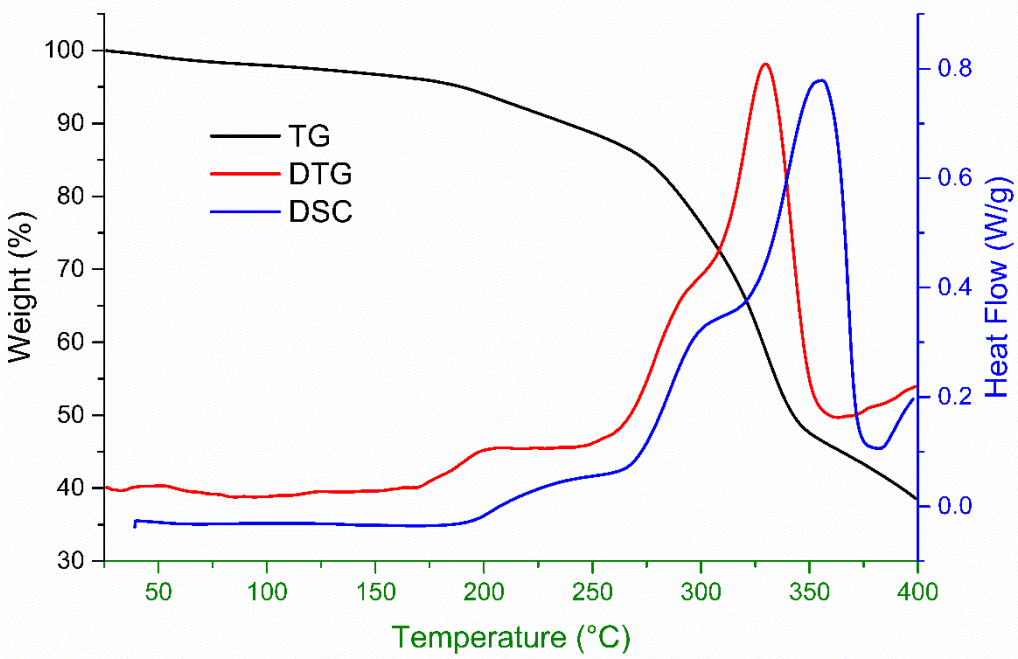


Figure S26. Thermal characterization of compound **1c**.

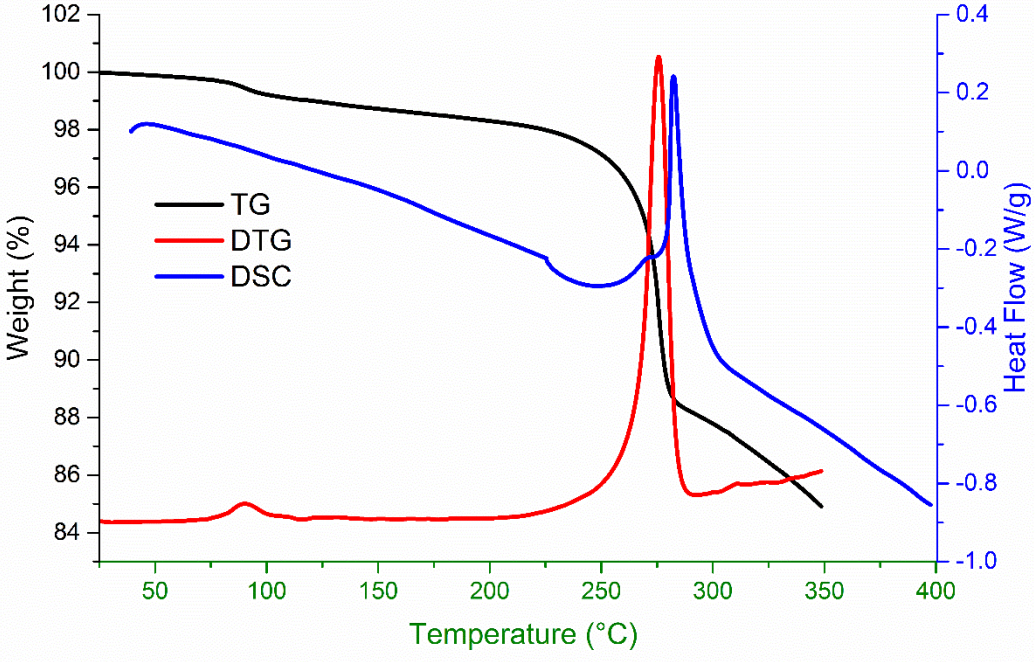


Figure S27. Thermal characterization of compound **1d**.

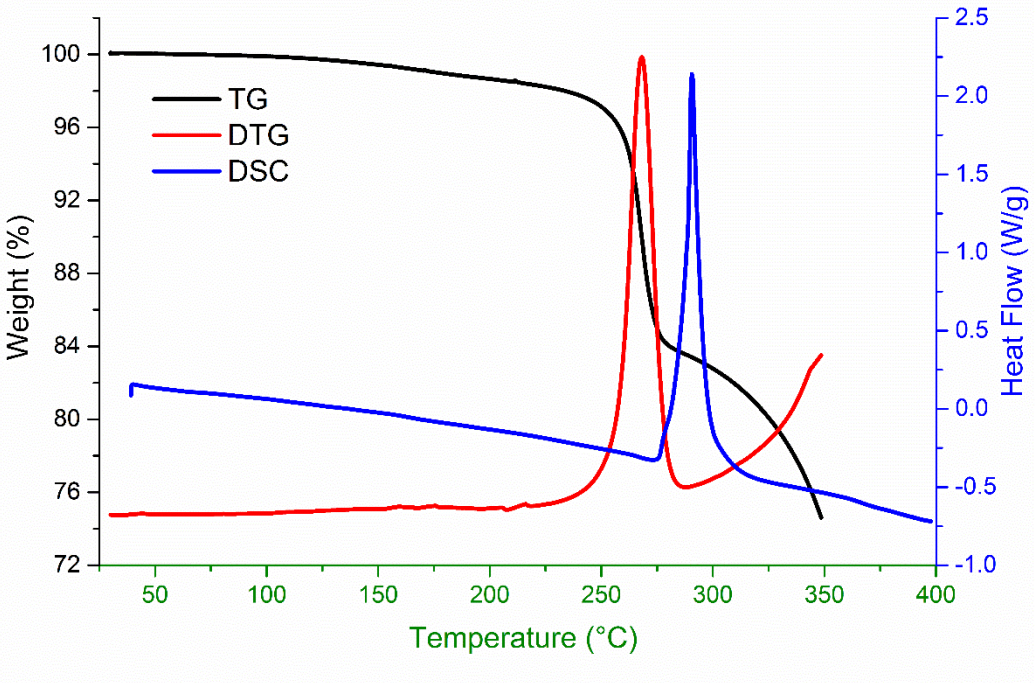


Figure S28. Thermal characterization of compound **1e**.

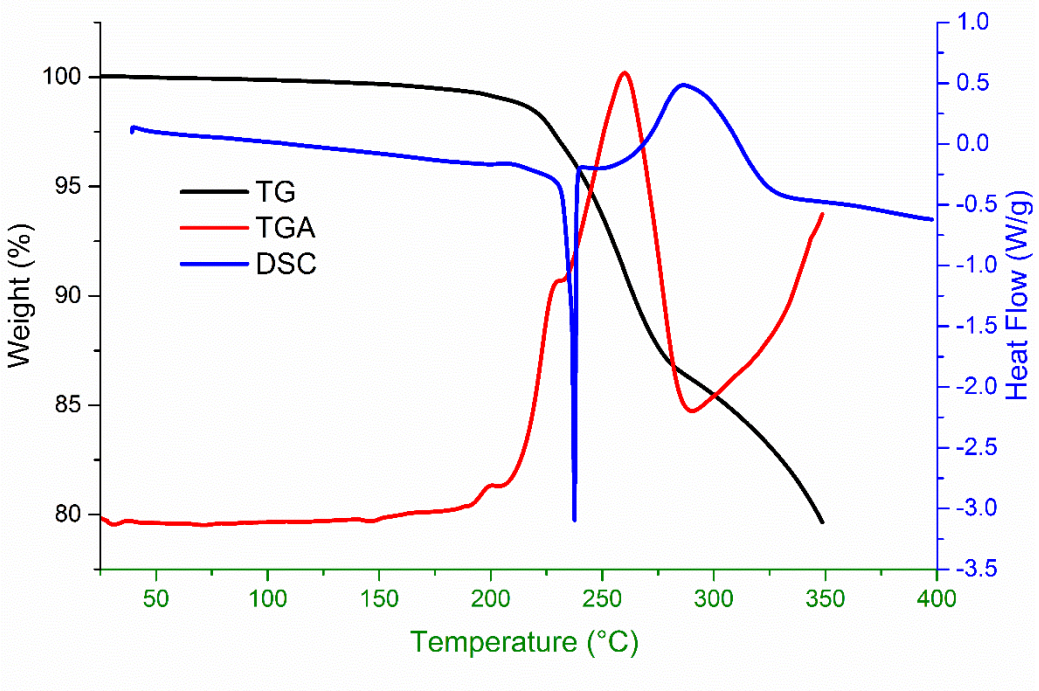


Figure S29. Thermal characterization of compound **1f**.

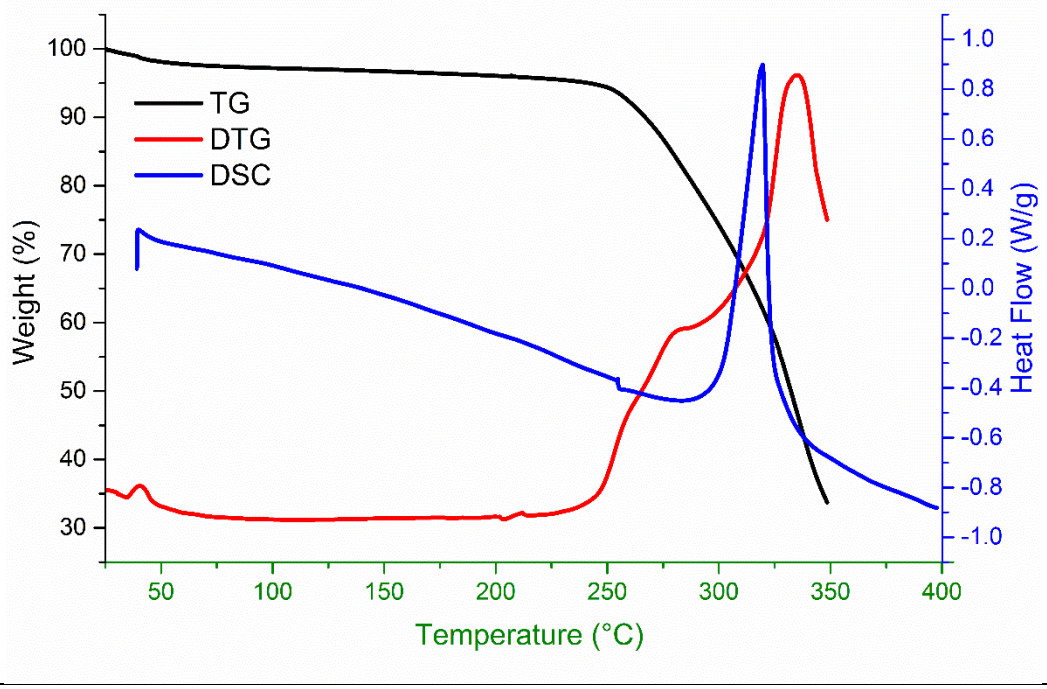


Figure S30. Thermal characterization of compound **1g**.