Electronic Supporting Information

Rendering the Cross-conjugated Azophenine Derivatives Emissive to Probe the Silent Photophysical Properties of Emeraldine

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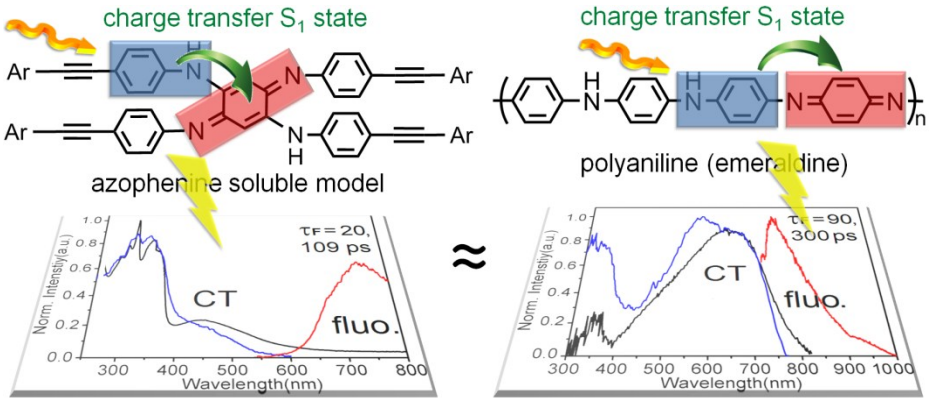

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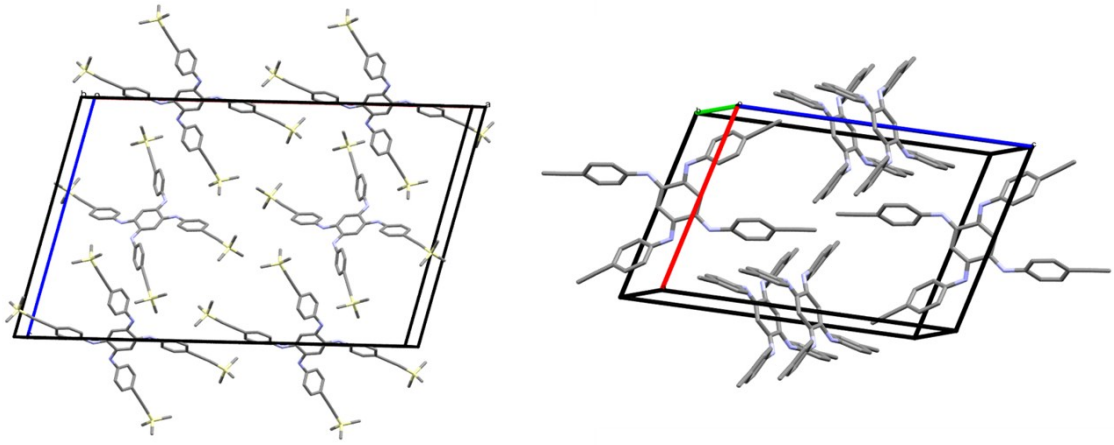


Figure S1. Stick representations of **1** (left) and **3** (right) inside their unit cells. The dichloromethane and methanol molecules and the hydrogen atoms are omitted for clarity.

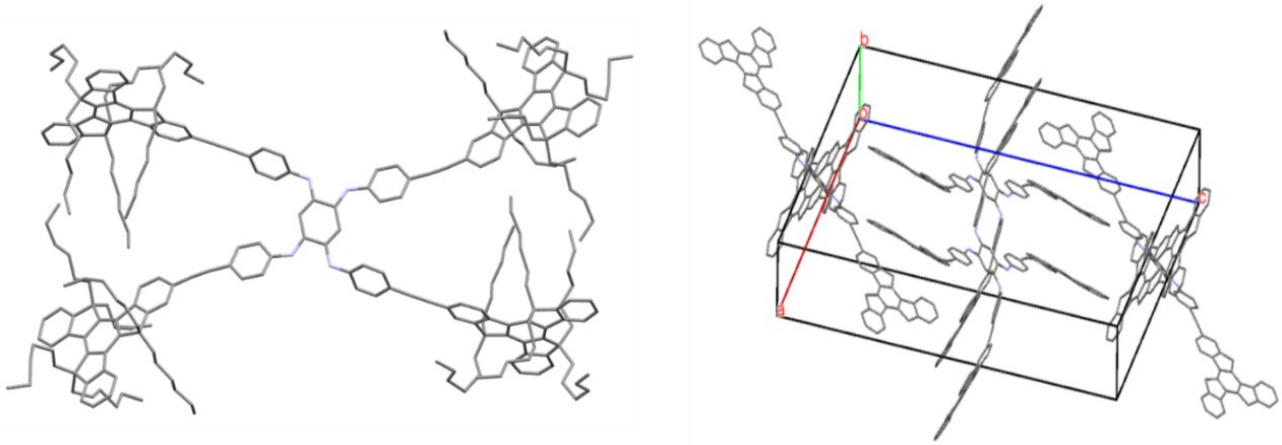


Figure S2. Stick representations of **4** (left; the hydrogen atoms are omitted for clarity) and inside the unit cell (the hydrogen atoms alkyl chains, dichloromethane and methanol molecules are omitted for clarity).

Table S1. Crystal data and structure refinement of compounds **1**, **3** and **4**.

Compound	**1**	**3**	**4**
Formula	$C_{52}H_{64}N_4O_2Si_4$	$C_{20}H_{14}Cl_2N_2$	$C_{290}H_{380}N_4O_4$
Formula weight	889.43	353.23	3985.98
Temp(K)	173(2)	173(2)	173(2)
Wavelength(Å)	1.54178	1.54178	0.71073
Crystal size(mm)	0.010 x 0.115 x 0.650	0.040 x 0.050 x 0.540	0.150 x 0.160 x 0.929
Crystal habit	Clear intense pink Needle	Clear intense purple Needle	Translucent dark purple Needle
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	C 1 2/c 1	P 1 21/n 1	P 1 21/c 1
a (Å)	38.446(2)	14.2044(5)	19.6056(17)
b (Å)	5.7728(3)	6.0526(3)	18.2484(16)
c (Å)	26.2153(14)	20.7810(8)	36.537(3) Å
α (deg)	90	90	90
β (deg)	102.956(4)	106.451(2)	104.497(2)
γ (deg)	90	90	90
Volume($Å^3$)	5670.1(5)	1713.48(12)	12655.7(19)
Z	4	4	2
Density (calculated)	1.042 g/cm^3	1.369 g/cm^3	1.046 g/cm3
Absorption coefficient	1.263 mm^{-1}	3.416 mm^{-1}	0.060 mm-1
F(000)	1904	728	4360
Reflections collected	33991	8918	101846
Independent reflections	5394 [R(int) = 0.2965]	3206 [R(int) = 0.0688]	21121 [R(int) = 0.1455]
Maximum θ angle	72.02°	70.72°	26.38°
Data/restraints/parameters	5394 / 4 / 285	3206 / 0 / 217	21121 / 12 / 1151
Goodness-of-fit on F^2	1.213	1.087	1.266
R indices（all data）	0.2822/0.4369	0.1402/0.3147	0.4318/0.5143
Largest diff. peak and hole	0.943 and -0.673 $eÅ^{-3}$	0.867 and -0.855 $eÅ^{-3}$	1.130 and -0.985 eÅ-3

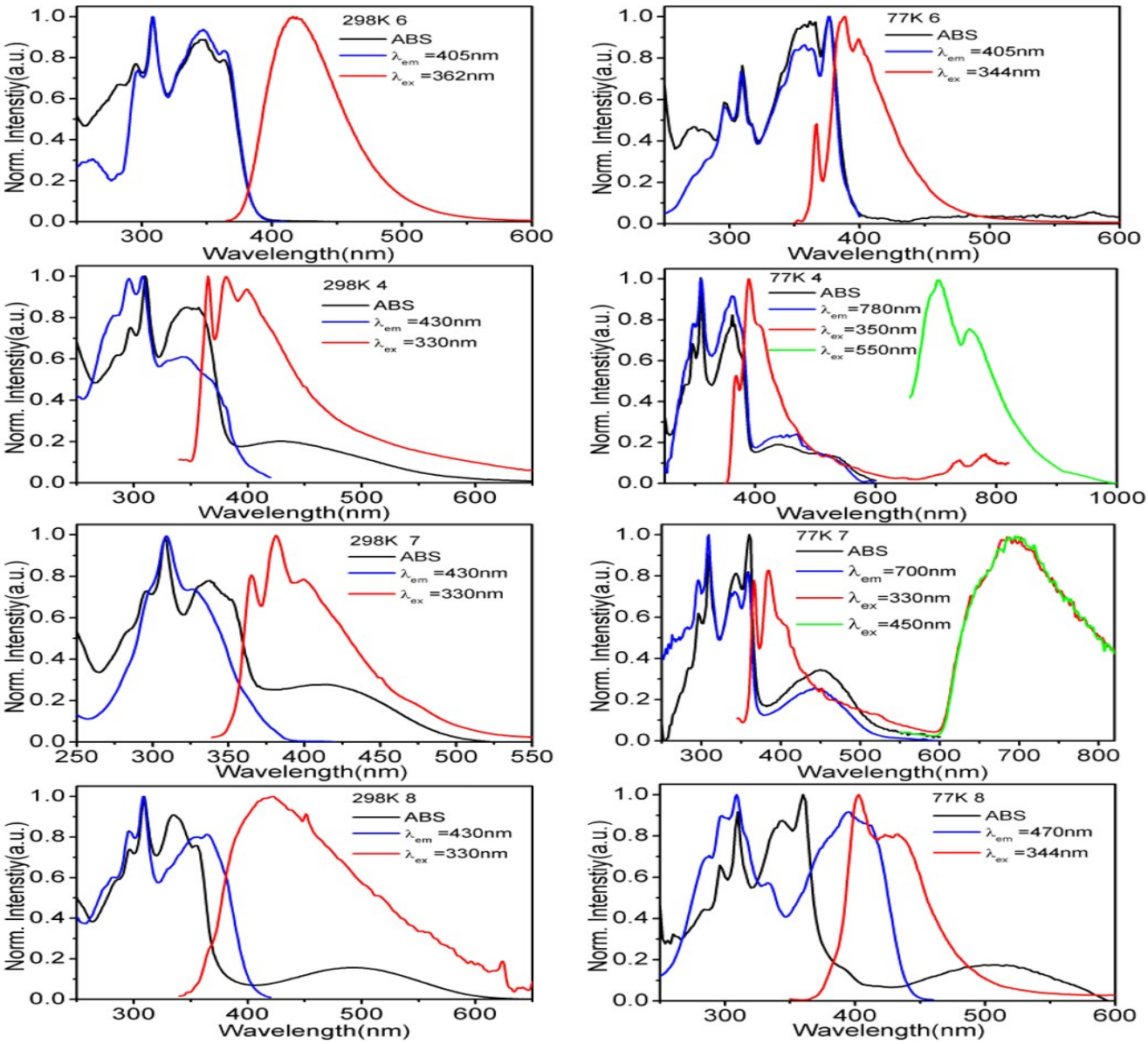


Figure S3. Comparison of the UV-vis absorption (black), excitation (blue) and emission (red) spectra of **4**, **6, 7, 8** in 2MeTHF at 298 K (left) and 77 K (right).

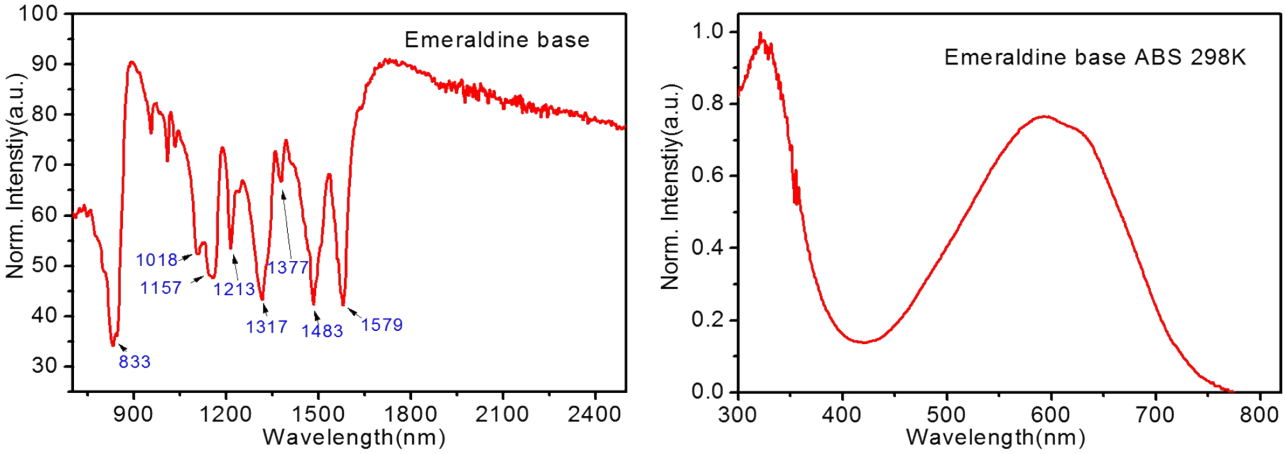


Figure S4. IR and UV-vis absorption spectra (in 2MeTHF at 298 K) of **emeraldine base**.

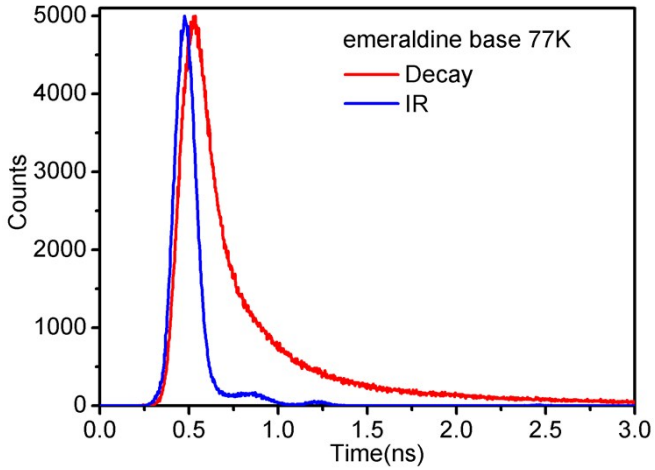


Figure S5. Room temperature emission decay trace for **emeraldine base** (bule) and IRF lamp profile (red) in 2MeTHF at 77K.

Table S2. Lifetime data for **emeraldine base** in 2MeTHF at 77K.

Peak number	f	τ (ns)	Std τ(ns)
1	92.7	0.092	0.025
2	5.7	0.297	0.028
3	1.5	1.009	0.090

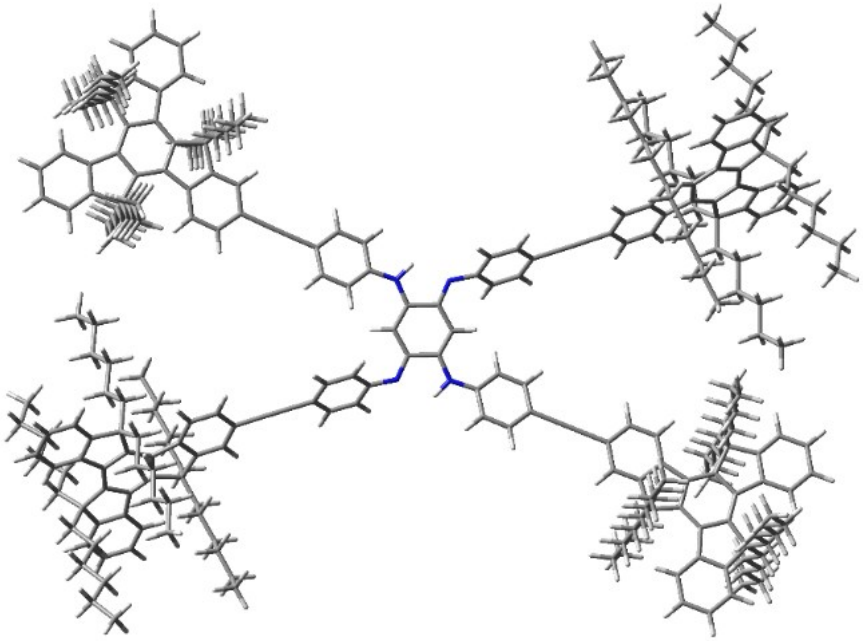


Figure S6. Optimized geometry for **4** using a THF solvent field (top view).

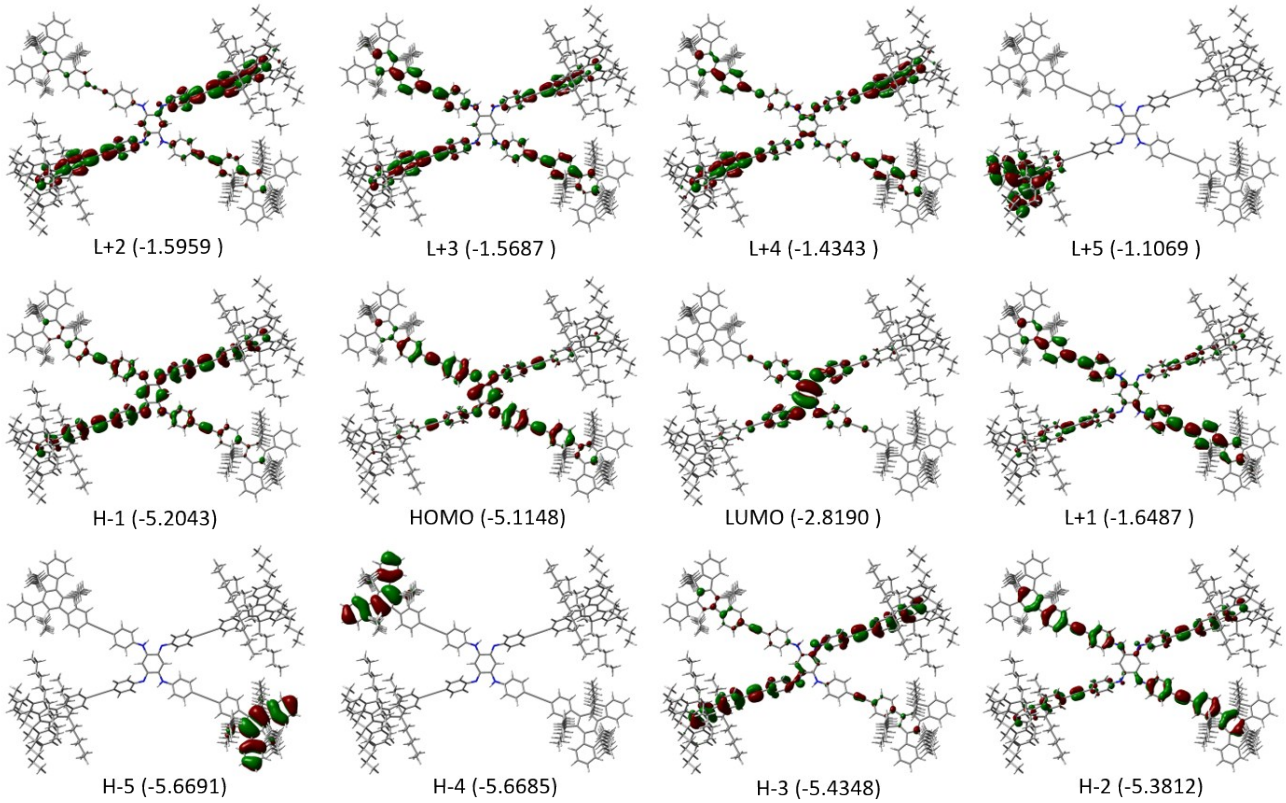


Figure S7. Representations of the frontier MOs of **4** using a THF solvent field (energies in eV).

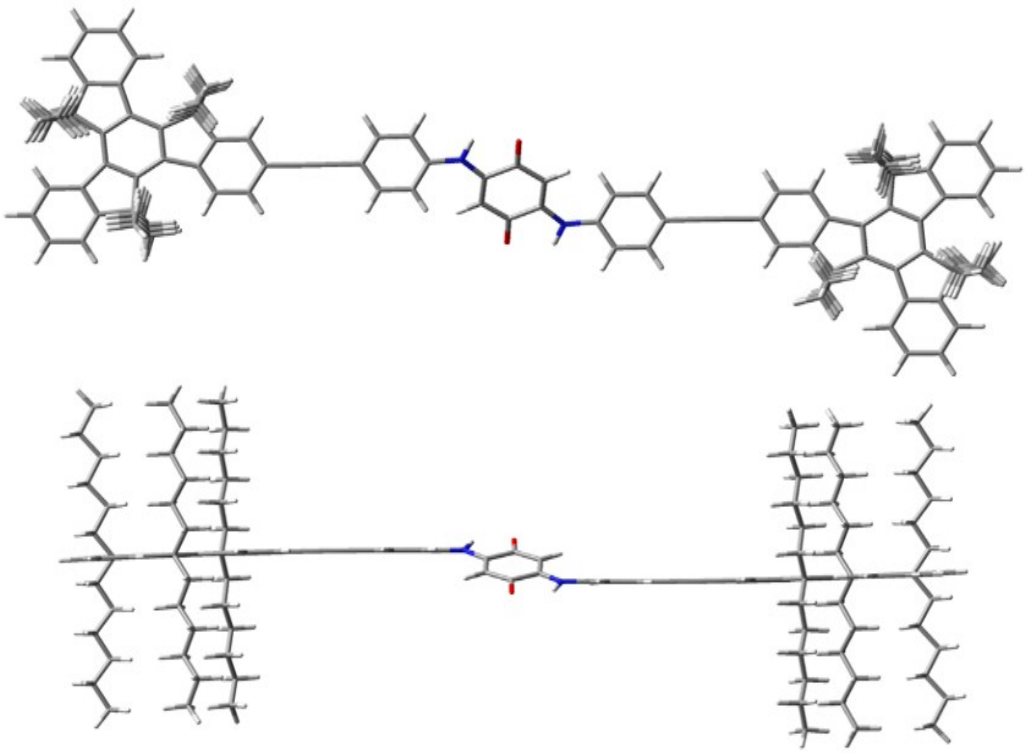


Figure S8. Optimized geometry of **7** using a THF solvent field (up: side view; down: top view).

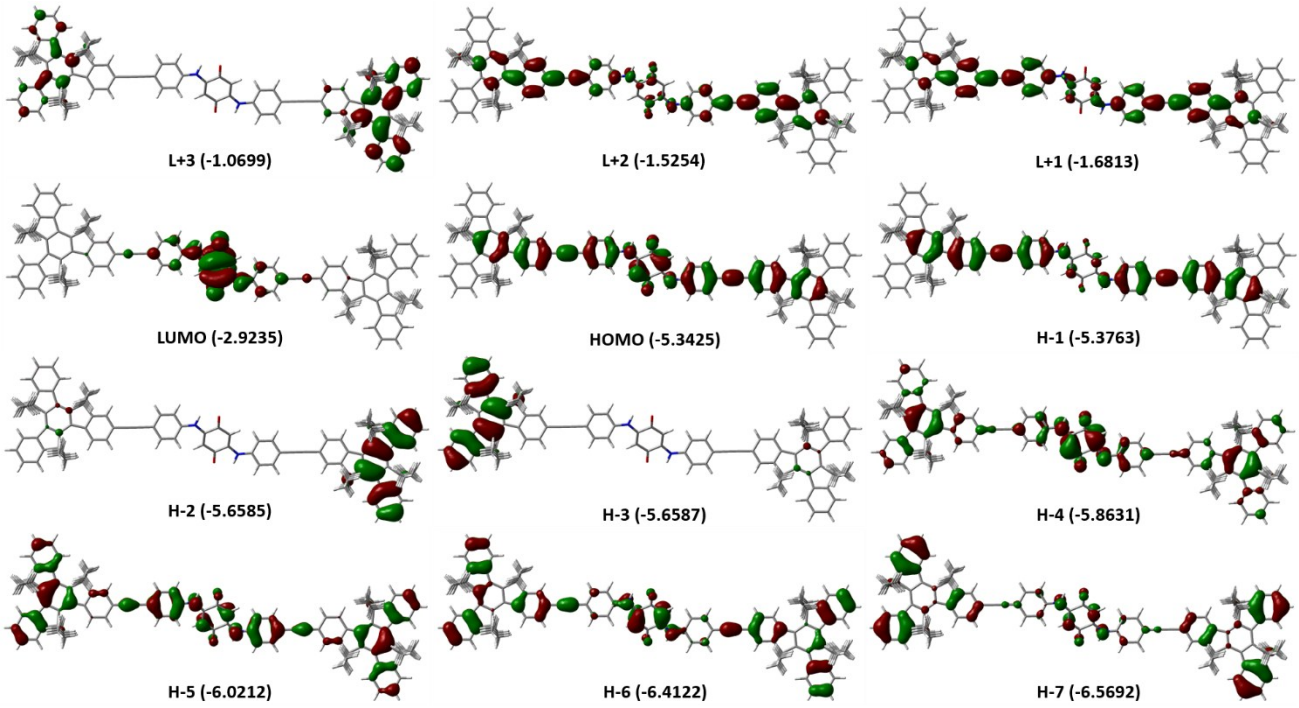


Figure S9. Representations of the frontier MOs of **7** using a THF solvent field (energies in eV).

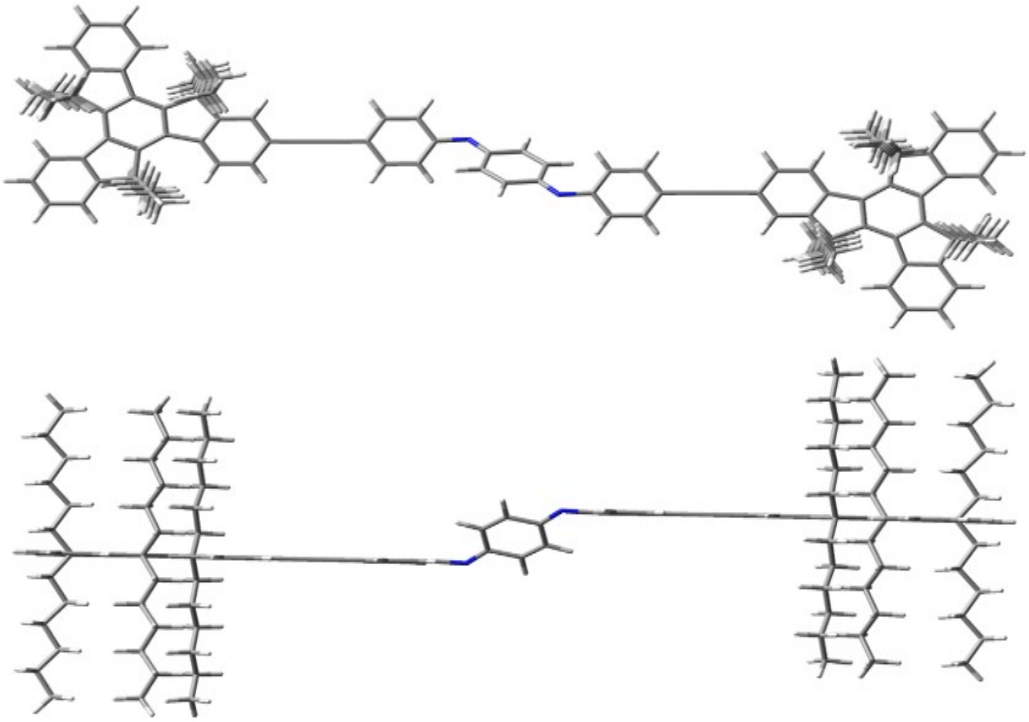


Figure S10. Optimized geometry of **8** using THF solvent field (up: side view; down: top view).

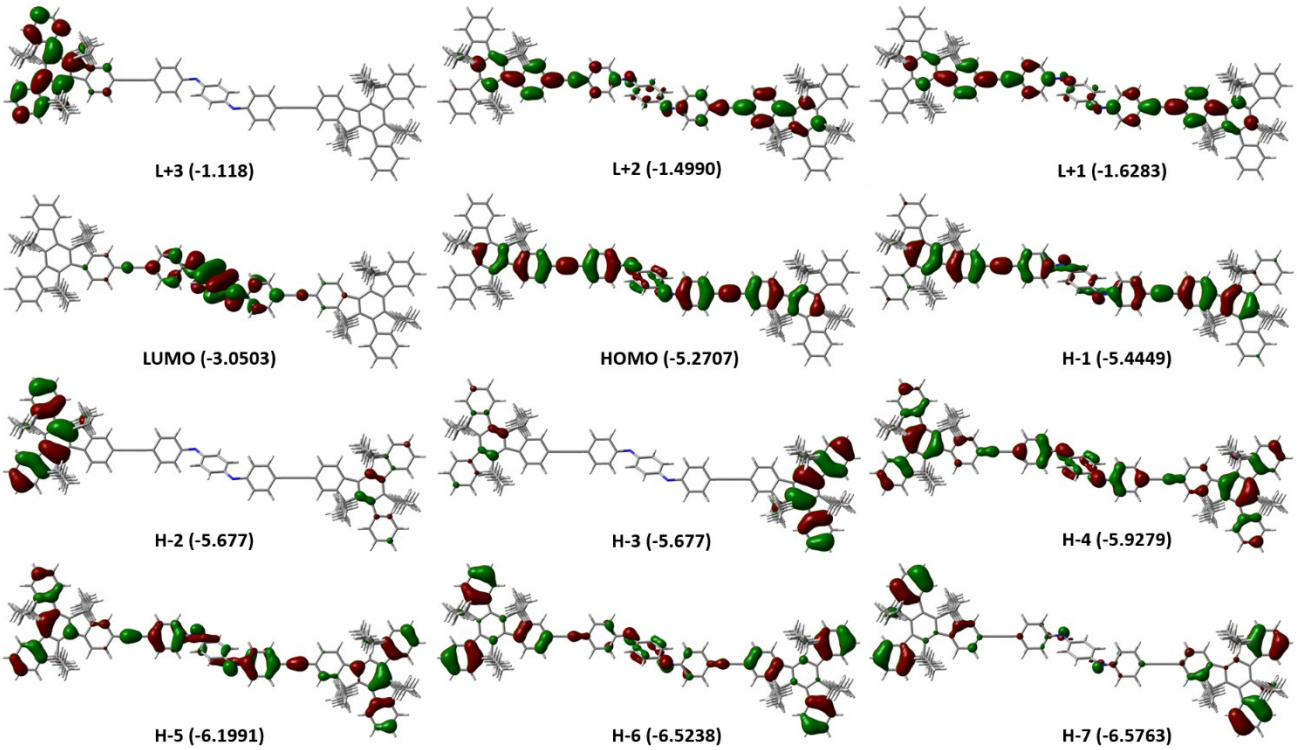
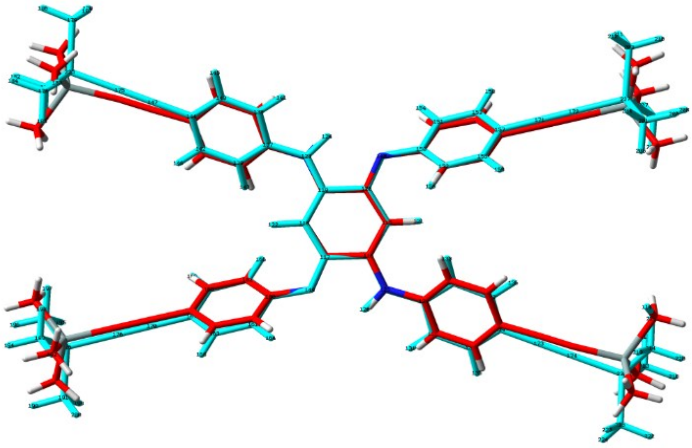
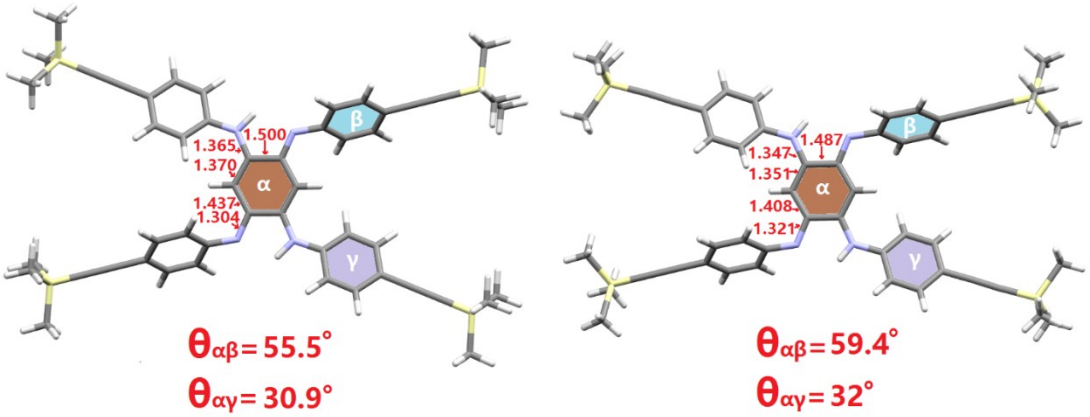


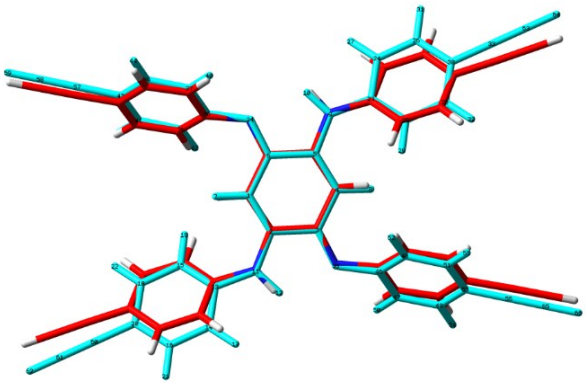
Figure S11. Representations of the frontier MOs of **8** using a THF solvent field (energies in eV).



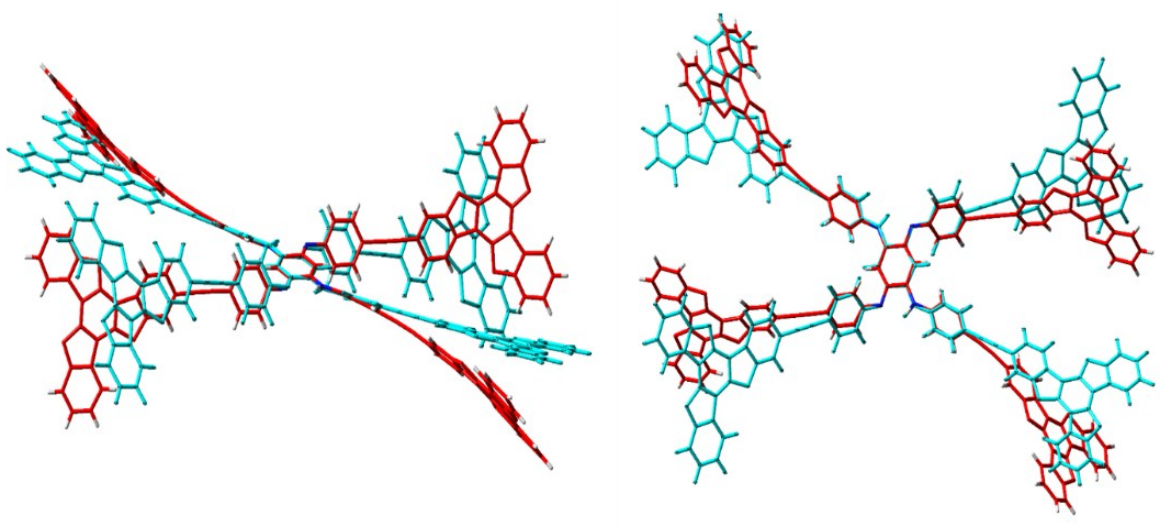
Fingure S12. Structure overlay of the optimized geometry of **1** using a THF solvent field (DFT; turquoise) with the X-ray molecular structure (red).



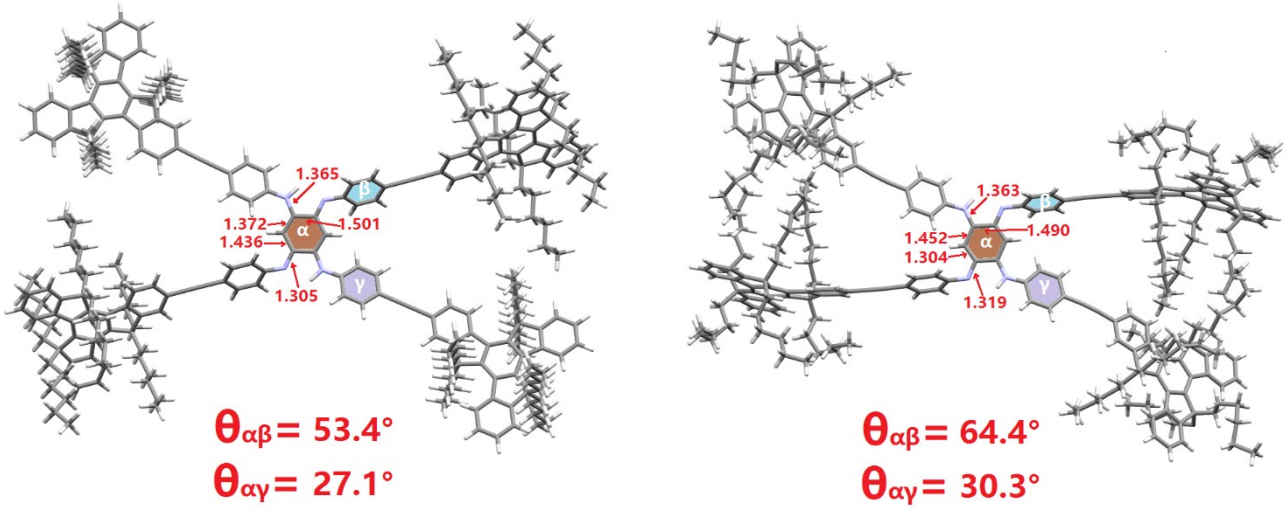
Fingure S13. Comparison of the CN bond lengths (upper) and dihedral angles between the quinone diimine plane and the NH-C_6H_4 (middle) and C=N-C_6H_4 groups (down) for the optimized geometry by DFT computations using a THF solvent field (left) with of those in the crystal (right) for **1**.



Fingure S14. Structure overlay of the optimized geometry of **3** using a THF solvent field (DFT; turquoise) with the X-ray molecular structure (red).



Fingure S15. Structure overlay of the optimized geometry of **4** using a THF solvent field (DFT; turquoise) with the X-ray molecular structure (red).



Fingure S16. Comparison of the CN bond lengths (upper) and dihedral angles between the quinone diimine plane and the NH-C_6H_4 (middle) and C=N-C_6H_4 groups (down) for the optimized geometry by DFT computations using a THF solvent field (left) with of those in the crystal (right) for **4**.

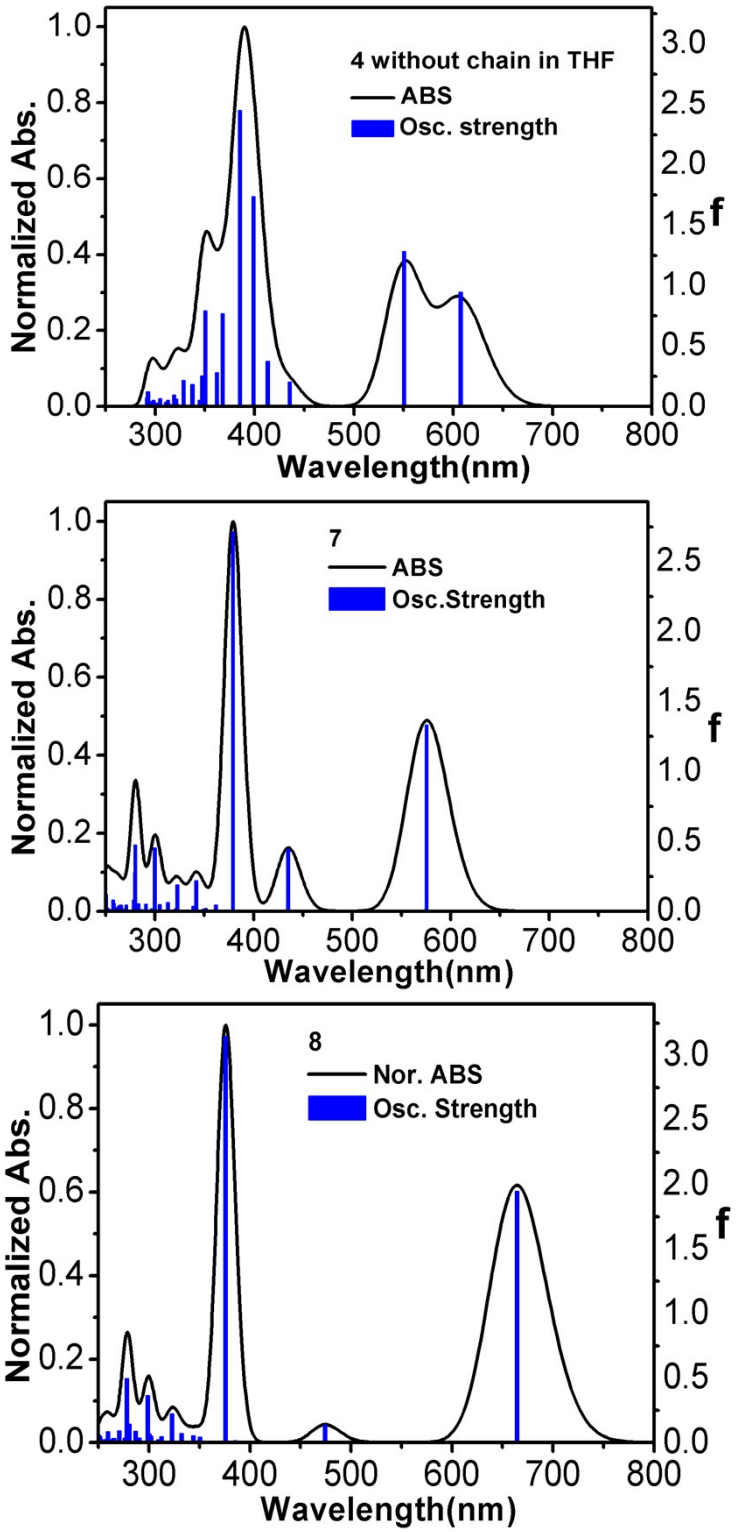


Figure S17. Computed positions and oscillator strengths (f) for the 100st electronic transitions for **4** (left), **7** (middle) and **8** (right) (THF solvent field applied). The black line is generated by applying a thickness of 1500 cm^{-1}. For **4**, TDDFT was calculated with the structure without alkyl chain for saving computation source, from the optimization of **4** with the structure with the alkyl chain and without alkyl chain, the geometry difference is very small (see **Figure S18** below).

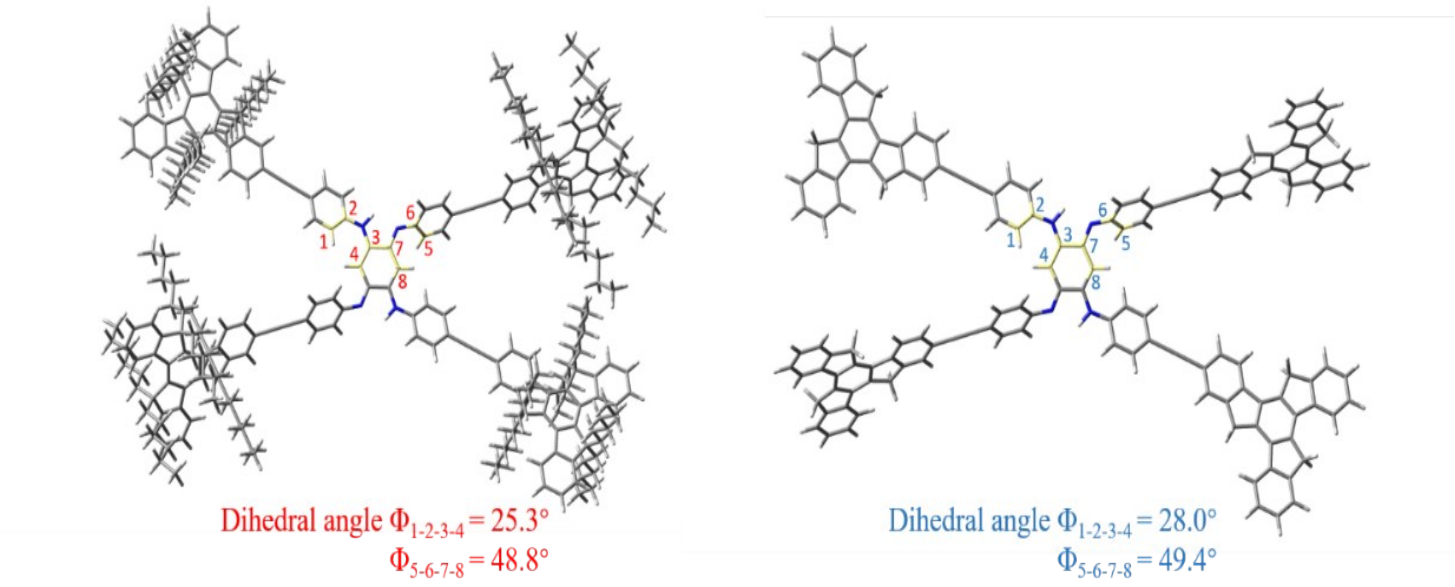


Figure S18. Comparison of the dihedral angles formed atoms 1-2-3-4 and 5-6-7-8 in **4** between the optimized geometries (DFT using a THF solvent field) with (left) and without (right) alkyl chains.

Table S3. Calculated positions, oscillator strengths (f), and major contributions of the pure electronic transitions for **4**, **7** and **8** using a THF solvent field.

No.	λ (nm)	Osc. Strength	Major contribs for 4 without chain
1	677	0.0115	HOMO→LUMO (97%)
2	619	1.1706	H-1→LUMO (97%)
3	556	1.3281	H-2→LUMO (97%)
4	522	0.0011	H-3→LUMO (96%)
5	470	0.0002	H-8→LUMO (93%)
6	457	0.0004	H-6→LUMO (100%)
7	457	0.0004	H-7→LUMO (100%)
8	456	0.0002	H-4→LUMO (100%)
9	456	0.0002	H-5→LUMO (100%)
10	440	0.1462	H-9→LUMO (95%)
11	417	0.3601	H-10→LUMO (88%)
12	411	0.0017	H-11→LUMO (87%)
13	403	1.5237	HOMO→L+1 (86%)
14	389	0.023	H-1→L+1 (73%)
15	388	2.5087	H-1→L+3 (10%), HOMO→L+2 (78%)
16	383	0.0008	H-12→LUMO (86%)
17	374	0.003	HOMO→L+3 (82%)
18	370	0.6806	H-13→LUMO (35%), H-1→L+3 (21%), HOMO→L+2 (14%)
19	369	0.0004	H-1→L+1 (11%), H-1→L+2 (79%)
20	363	0.3869	H-13→LUMO (23%), H-1→L+3 (61%)
21	360	0.1246	H-28→LUMO (15%), H-14→LUMO (27%), H-13→LUMO (27%)

22	359	0.0044	HOMO→L+4 (79%)
23	354	0.0086	H-2→L+1 (76%), HOMO→L+4 (10%)
24	351	0	H-23→LUMO (30%), H-19→LUMO (11%), H-15→LUMO (36%)
25	349	0.0021	H-2→L+2 (74%)
26	349	0.7002	H-14→LUMO (12%), H-3→L+1 (32%), H-1→L+4 (36%)
27	346	0.2516	H-14→LUMO (10%), H-3→L+2 (19%), H-2→L+3 (41%)
28	344	0.3744	H-3→L+1 (42%), H-3→L+2 (11%), H-1→L+4 (33%)
29	341	0.009	H-4→L+1 (31%), H-4→L+3 (19%), HOMO→L+8 (13%)
30	341	0.0075	H-5→L+1 (31%), H-5→L+3 (19%), HOMO→L+7 (12%)
31	339	0.0051	H-6→L+1 (11%), H-6→L+2 (24%), H-6→L+3 (10%), H-6→L+4 (11%), H-1→L+6 (10%)
32	339	0.0072	H-7→L+1 (11%), H-7→L+2 (24%), H-7→L+3 (11%), H-7→L+4 (11%), H-1→L+5 (10%)
33	335	0.1303	H-3→L+2 (49%), H-2→L+3 (34%)
34	333	0.0097	H-18→LUMO (15%), H-16→LUMO (39%), H-14→LUMO (22%)
35	333	0.0016	H-18→LUMO (20%), H-16→LUMO (52%), H-14→LUMO (12%)
36	332	0.0003	H-19→LUMO (28%), H-15→LUMO (41%)
37	332	0.0026	H-17→LUMO (72%), H-3→L+3 (11%)
38	332	0.0001	H-17→LUMO (16%), H-3→L+3 (65%), H-2→L+2 (10%)
39	331	0.0027	H-30→LUMO (85%)
40	331	0.0025	H-31→LUMO (73%), H-19→LUMO (11%)
41	330	0.0002	H-22→LUMO (23%), H-18→LUMO (48%)
42	329	0.0002	H-23→LUMO (17%), H-21→LUMO (13%), H-20→LUMO (50%), H-19→LUMO (10%)
43	329	0.0004	H-21→LUMO (67%)
44	329	0	H-23→LUMO (22%), H-20→LUMO (41%), H-19→LUMO (21%)
45	328	0.0557	H-22→LUMO (31%), H-2→L+4 (31%)
46	327	0.1467	H-22→LUMO (11%), H-2→L+4 (56%)
47	324	0.0056	H-24→LUMO (84%)
48	323	0.0053	H-26→LUMO (36%), H-25→LUMO (50%)
49	323	0.0092	H-27→LUMO (81%)
50	322	0.0357	H-4→L+1 (13%), HOMO→L+7 (13%), HOMO→L+8 (41%)
51	322	0.0755	H-5→L+1 (13%), HOMO→L+7 (42%), HOMO→L+8 (14%)
52	321	0.0093	H-32→LUMO (68%)
53	320	0.0023	H-33→LUMO (72%), H-3→L+4 (10%)
54	320	0.0047	H-33→LUMO (11%), H-3→L+4 (73%)
55	320	0.002	H-32→LUMO (14%), H-28→LUMO (11%), H-25→LUMO (16%), HOMO→L+6 (10%)
56	320	0.0412	HOMO→L+5 (22%), HOMO→L+6 (28%)
57	320	0.0672	H-26→LUMO (21%), HOMO→L+5 (20%), HOMO→L+6 (12%)
58	319	0.0175	H-8→L+1 (77%)
59	315	0.0003	H-29→LUMO (48%), H-6→L+1 (20%)
60	315	0	H-29→LUMO (18%), H-6→L+1 (53%), H-6→L+2 (11%)
61	314	0	H-7→L+1 (71%), H-7→L+2 (14%)

62	313	0.0073	H-4→L+1 (33%), H-4→L+2 (44%), H-4→L+3 (13%)
63	313	0.0627	H-8→L+2 (73%)
64	312	0.0044	H-5→L+1 (34%), H-5→L+2 (42%), H-5→L+3 (12%)
65	312	0.0183	H-9→L+1 (12%), H-8→L+3 (10%), H-1→L+5 (32%), HOMO→L+5 (23%)
66	312	0.016	H-9→L+1 (24%), H-8→L+3 (22%), H-1→L+5 (15%), HOMO→L+5 (11%)
67	312	0.0305	H-1→L+6 (47%), HOMO→L+6 (33%)
68	309	0.0008	H-9→L+1 (39%), H-9→L+2 (22%), H-8→L+3 (25%)
69	309	0.007	H-1→L+7 (76%), HOMO→L+7 (19%)
70	309	0.0052	H-1→L+8 (77%), HOMO→L+8 (19%)
71	306	0.0605	HOMO→L+9 (84%)
72	306	0.0001	H-4→L+2 (39%), H-4→L+3 (47%)
73	306	0.0004	H-5→L+2 (39%), H-5→L+3 (48%)
74	305	0	H-6→L+2 (29%), H-6→L+3 (70%)
75	305	0	H-7→L+2 (31%), H-7→L+3 (69%)
76	304	0	H-35→LUMO (69%), H-34→LUMO (13%)
77	304	0.0001	H-35→LUMO (16%), H-34→LUMO (72%)
78	303	0.0032	H-9→L+2 (43%), H-8→L+3 (16%), HOMO→L+10 (16%)
79	303	0.011	H-9→L+2 (14%), H-9→L+3 (12%), HOMO→L+10 (49%)
80	302	0.0404	H-4→L+3 (12%), H-3→L+8 (12%), H-2→L+8 (46%)
81	302	0.0331	H-5→L+3 (11%), H-3→L+7 (11%), H-2→L+7 (46%)
82	301	0.0121	H-6→L+4 (15%), H-3→L+6 (17%), H-2→L+6 (27%), H-1→L+6 (20%)
83	301	0.013	H-7→L+4 (15%), H-3→L+5 (17%), H-2→L+5 (27%), H-1→L+5 (20%)
84	300	0.0017	H-39→LUMO (21%), H-10→L+1 (12%), H-1→L+10 (21%), HOMO→L+11 (21%)
85	300	0.0056	H-1→L+9 (51%)
86	299	0.0221	H-38→LUMO (10%), H-9→L+3 (51%), HOMO→L+10 (12%)
87	299	0.0017	H-37→LUMO (68%), H-36→LUMO (15%)
88	299	0.0029	H-37→LUMO (13%), H-36→LUMO (73%)
89	297	0.0359	H-4→L+4 (77%), H-2→L+8 (10%)
90	297	0.0408	H-6→L+4 (60%), H-2→L+6 (21%)
91	297	0.0502	H-7→L+4 (61%), H-2→L+5 (21%)
92	297	0.0293	H-5→L+4 (79%), H-2→L+7 (11%)
93	296	0.0014	H-39→LUMO (10%), H-8→L+4 (58%)
94	296	0.0073	H-38→LUMO (51%), H-28→LUMO (11%), H-9→L+3 (10%)
95	295	0.0028	H-39→LUMO (18%), H-10→L+1 (38%), H-8→L+4 (20%)
96	293	0.0042	H-11→L+2 (15%), HOMO→L+13 (24%)
97	293	0.0024	H-10→L+1 (10%), HOMO→L+11 (29%), HOMO→L+14 (24%)
98	292	0.0011	H-10→L+2 (34%), H-1→L+9 (10%), H-1→L+10 (13%)
99	292	0.0905	HOMO→L+13 (40%)
100	291	0.0048	HOMO→L+11 (29%), HOMO→L+14 (33%)

No.	λ (nm)	Osc. Strength	Major contribs for 7
1	581	0	HOMO→LUMO (94%)
2	576	1.3323	H-1→LUMO (98%)
3	481	0	H-4→LUMO (84%)
4	481	0.0006	H-3→LUMO (53%), H-2→LUMO (47%)
5	481	0	H-3→LUMO (46%), H-2→LUMO (52%)
6	435	0.4431	H-5→LUMO (95%)
7	402	0	H-18→LUMO (12%), H-15→LUMO (34%), H-14→LUMO (16%), H-6→LUMO (30%)
8	388	0	H-15→LUMO (27%), H-6→LUMO (57%)
9	379	2.711	H-1→L+2 (15%), HOMO→L+1 (75%)
10	370	0	H-1→L+1 (73%), HOMO→L+2 (24%)
11	366	0.0035	H-21→LUMO (91%)
12	362	0.046	H-7→LUMO (86%)
13	353	0	H-8→LUMO (93%)
14	352	0.0204	H-3→L+1 (19%), H-3→L+2 (17%), H-2→L+1 (29%), H-2→L+2 (11%)
15	352	0	H-3→L+1 (29%), H-3→L+2 (11%), H-2→L+1 (19%), H-2→L+2 (17%)
16	349	0.015	H-11→LUMO (77%)
17	346	0	H-10→LUMO (100%)
18	346	0.0001	H-9→LUMO (96%)
19	346	0	H-1→L+1 (24%), HOMO→L+2 (73%)
20	342	0.2191	H-11→LUMO (10%), H-1→L+2 (69%), HOMO→L+1 (11%)
21	340	0	H-12→LUMO (95%)
22	339	0.0348	H-13→LUMO (90%)
23	323	0	H-18→LUMO (31%), H-15→LUMO (28%), H-14→LUMO (18%)
24	323	0.0064	H-17→LUMO (79%)
25	323	0.1875	H-3→L+1 (10%), H-2→L+1 (16%), H-1→L+4 (29%), HOMO→L+3 (31%)
26	323	0.0001	H-18→LUMO (16%), H-3→L+1 (14%), H-1→L+3 (24%), HOMO→L+4 (26%)
27	321	0	H-18→LUMO (28%), H-14→LUMO (58%)
28	321	0.0184	H-4→L+1 (87%)
29	313	0.0012	H-3→L+1 (11%), H-3→L+2 (18%), H-2→L+1 (12%), H-2→L+2 (49%)
30	313	0.0646	H-3→L+1 (12%), H-3→L+2 (50%), H-2→L+1 (11%), H-2→L+2 (18%)
31	312	0	H-5→L+1 (46%), H-4→L+2 (44%)
32	305	0.0027	H-20→LUMO (80%)
33	305	0	H-19→LUMO (88%)
34	305	0.0486	H-16→LUMO (72%)
35	301	0	H-5→L+1 (37%), H-4→L+2 (44%)

36	300	0.4522	H-3→L+3 (17%), H-3→L+4 (18%), H-2→L+3 (18%), H-2→L+4 (17%), HOMO→L+5 (15%)
37	299	0	H-3→L+3 (21%), H-2→L+4 (21%)
38	299	0.0095	H-1→L+4 (47%), HOMO→L+3 (49%)
39	299	0	H-1→L+3 (44%), HOMO→L+4 (43%)
40	297	0.0178	H-5→L+2 (21%), HOMO→L+5 (45%)
41	292	0	H-1→L+5 (55%), HOMO→L+6 (18%)
42	291	0.0507	H-5→L+2 (55%), HOMO→L+5 (18%)
43	286	0.0129	H-5→L+4 (11%), H-4→L+3 (15%), H-2→L+5 (25%), H-2→L+6 (12%)
44	286	0.0006	H-5→L+3 (11%), H-4→L+4 (15%), H-3→L+5 (25%), H-3→L+6 (13%)
45	283	0.0529	H-7→L+2 (10%), H-6→L+1 (50%)
46	283	0	H-1→L+7 (28%), HOMO→L+8 (47%)
47	283	0.0293	H-1→L+8 (27%), HOMO→L+7 (48%)
48	282	0	H-13→L+1 (11%), H-7→L+1 (21%)
49	280	0.4742	H-6→L+1 (18%), H-4→L+3 (10%)
50	280	0	H-5→L+3 (13%), H-4→L+4 (26%), HOMO→L+6 (17%)
51	280	0.2747	H-12→L+1 (10%), H-5→L+4 (11%), H-4→L+3 (25%)
52	280	0	H-1→L+5 (12%), HOMO→L+6 (44%)
53	278	0.0816	H-1→L+6 (67%), HOMO→L+5 (14%)
54	277	0	H-2→L+3 (59%), H-2→L+4 (39%)
55	277	0	H-3→L+3 (40%), H-3→L+4 (59%)
56	276	0	H-7→L+1 (22%), H-6→L+2 (35%)
57	271	0.0464	H-11→L+2 (12%), H-8→L+1 (54%), H-7→L+2 (12%)
58	270	0	H-11→L+1 (32%), H-8→L+2 (23%), H-7→L+1 (15%)
59	269	0	H-31→LUMO (10%), H-24→LUMO (71%)
60	269	0.006	H-23→LUMO (94%)
61	269	0	H-22→LUMO (94%)
62	268	0.0141	H-10→L+1 (60%), H-9→L+2 (26%)
63	268	0	H-10→L+2 (28%), H-9→L+1 (61%)
64	266	0.0385	H-25→LUMO (45%), H-1→L+8 (14%)
65	265	0.0439	H-25→LUMO (26%), H-4→L+5 (13%)
66	265	0	H-11→L+1 (13%), H-7→L+1 (13%), H-6→L+2 (20%), H-1→L+7 (21%), HOMO→L+8 (11%)
67	265	0	H-7→L+1 (12%), H-6→L+2 (17%), H-1→L+7 (27%), HOMO→L+8 (17%)
68	264	0.0179	H-1→L+8 (33%), HOMO→L+7 (20%)
69	264	0	H-5→L+3 (27%), H-4→L+4 (27%), H-1→L+7 (10%)
70	263	0.0374	H-5→L+4 (27%), H-4→L+3 (20%), H-4→L+5 (16%), HOMO→L+9 (10%)
71	262	0.0067	HOMO→L+9 (27%)
72	262	0	H-5→L+3 (20%), H-5→L+5 (10%), H-4→L+6 (10%)
73	260	0	H-11→L+1 (11%), H-1→L+9 (14%)

74	260	0.0131	H-3→L+5 (13%), H-3→L+6 (24%), H-2→L+5 (20%), H-2→L+6 (15%)
75	260	0	H-3→L+5 (19%), H-3→L+6 (16%), H-2→L+5 (12%), H-2→L+6 (25%)
76	260	0.0268	H-10→L+3 (12%), H-9→L+4 (10%)
77	259	0	H-26→LUMO (96%)
78	259	0.0029	H-27→LUMO (90%)
79	259	0	H-1→L+9 (26%)
80	258	0.0572	H-4→L+5 (27%)
81	258	0.0024	H-20→L+2 (32%), H-19→L+1 (49%)
82	258	0	H-20→L+1 (51%), H-19→L+2 (33%)
83	257	0.0794	H-7→L+2 (33%)
84	255	0	H-5→L+5 (22%), H-4→L+6 (34%)
85	253	0	H-11→L+1 (19%), H-8→L+2 (61%), H-7→L+1 (10%)
86	253	0.0156	H-11→L+2 (36%), H-8→L+1 (17%)
87	253	0	H-31→LUMO (73%), H-24→LUMO (13%)
88	252	0.0031	H-30→LUMO (51%), H-28→LUMO (19%)
89	252	0.0098	H-3→L+10 (18%), H-2→L+9 (14%), H-2→L+10 (13%)
90	252	0	H-3→L+9 (14%), H-3→L+10 (13%), H-2→L+10 (19%)
91	252	0	H-13→L+1 (11%), H-1→L+9 (12%), HOMO→L+10 (30%)
92	251	0.0245	H-1→L+10 (12%), HOMO→L+13 (17%)
93	251	0	H-10→L+2 (64%), H-9→L+1 (30%)
94	251	0.01	H-10→L+1 (30%), H-9→L+2 (58%)
95	250	0.1197	H-12→L+1 (25%), H-11→L+2 (13%), H-1→L+12 (12%), HOMO→L+11 (10%), HOMO→L+13 (12%)
96	250	0	H-13→L+1 (23%), H-1→L+13 (18%), HOMO→L+12 (22%)
97	250	0.0881	H-1→L+14 (29%), HOMO→L+15 (33%)
98	250	0	H-1→L+15 (31%), HOMO→L+14 (31%)
99	249	0	H-29→LUMO (92%)
100	249	0.007	H-30→LUMO (26%), H-28→LUMO (71%)

No.	**λ (nm)**	**Osc. Strength**	**Major contribs for 8**
1	664	1.9468	HOMO→LUMO (97%)
2	590	0	H-1→LUMO (95%)
3	508	0.0002	H-3→LUMO (21%), H-2→LUMO (79%)
4	508	0.0005	H-3→LUMO (79%), H-2→LUMO (21%)
5	474	0.1371	H-4→LUMO (93%)
6	464	0	H-5→LUMO (82%)
7	387	0	H-11→LUMO (37%), H-7→LUMO (34%), H-5→LUMO (13%)
8	385	0.0163	H-6→LUMO (77%)
9	376	3.1451	H-14→LUMO (19%), H-1→L+1 (25%), HOMO→L+2 (43%)
10	373	0	H-1→L+2 (10%), HOMO→L+1 (87%)
11	366	0	H-11→LUMO (27%), H-7→LUMO (60%)

12	365	0.0007	H-8→LUMO (77%), H-6→LUMO (13%)
13	360	0	H-9→LUMO (92%)
14	360	0.0001	H-10→LUMO (92%)
15	354	0.0013	H-12→LUMO (88%)
16	354	0	H-13→LUMO (78%), H-11→LUMO (17%)
17	352	0	H-15→LUMO (95%)
18	351	0.044	H-16→LUMO (53%), H-14→LUMO (35%)
19	349	0	H-3→L+2 (22%), H-2→L+1 (31%)
20	349	0.0156	H-3→L+1 (31%), H-2→L+2 (22%)
21	344	0.0535	H-1→L+1 (63%), HOMO→L+2 (34%)
22	335	0	H-1→L+2 (84%), HOMO→L+1 (10%)
23	332	0.0716	H-20→LUMO (29%), H-16→LUMO (11%), HOMO→L+2 (16%)
24	326	0	H-21→LUMO (62%), H-17→LUMO (29%)
25	323	0	H-2→L+1 (19%), H-1→L+4 (10%), HOMO→L+3 (28%), HOMO→L+4 (22%)
26	323	0.2233	H-3→L+1 (20%), H-1→L+3 (10%), HOMO→L+3 (22%), HOMO→L+4 (29%)
27	321	0	H-19→LUMO (76%)
28	321	0.0002	H-18→LUMO (89%)
29	320	0	H-21→LUMO (31%), H-17→LUMO (54%)
30	313	0.0473	H-20→LUMO (37%), H-16→LUMO (19%), H-14→LUMO (14%)
31	309	0	H-5→L+2 (10%), H-4→L+1 (69%)
32	309	0.0233	H-3→L+1 (26%), H-3→L+2 (13%), H-2→L+2 (50%)
33	309	0	H-3→L+2 (44%), H-2→L+1 (23%), H-2→L+2 (11%)
34	302	0.0486	H-5→L+1 (32%), H-4→L+2 (29%)
35	300	0	H-1→L+3 (19%), H-1→L+4 (25%), HOMO→L+3 (15%), HOMO→L+4 (11%)
36	300	0.069	H-1→L+3 (32%), H-1→L+4 (24%), HOMO→L+3 (13%), HOMO→L+4 (17%)
37	300	0	H-3→L+4 (25%), H-2→L+3 (25%), HOMO→L+5 (16%)
38	299	0.3644	H-3→L+4 (33%), H-2→L+3 (33%)
39	295	0	H-3→L+4 (11%), H-2→L+3 (11%), HOMO→L+5 (57%)
40	291	0.0348	H-5→L+1 (48%), H-4→L+2 (47%)
41	287	0.0896	H-1→L+5 (20%), HOMO→L+6 (40%)
42	286	0	H-5→L+2 (78%)
43	284	0	H-4→L+3 (10%), H-3→L+6 (15%), H-2→L+5 (21%)
44	284	0.0051	H-4→L+4 (10%), H-3→L+5 (22%), H-2→L+6 (15%)
45	283	0	HOMO→L+7 (78%)
46	280	0	H-12→L+1 (14%), H-6→L+1 (10%), H-1→L+10 (10%), HOMO→L+12 (11%)
47	280	0.145	H-13→L+1 (11%), HOMO→L+10 (15%)
48	279	0.0876	H-1→L+5 (51%), HOMO→L+6 (26%)
49	278	0	H-4→L+3 (20%), H-4→L+4 (15%)
50	278	0.4971	H-4→L+3 (14%), H-4→L+4 (18%)

51	277	0	H-3→L+3 (90%)
52	277	0	H-2→L+4 (90%)
53	277	0	H-22→LUMO (94%)
54	277	0.0378	H-23→LUMO (94%)
55	276	0.0316	H-1→L+7 (14%), HOMO→L+8 (60%)
56	276	0	H-26→LUMO (12%), H-1→L+6 (51%)
57	273	0	H-32→LUMO (10%), H-26→LUMO (37%), H-6→L+1 (10%), H-1→L+6 (16%)
58	272	0	H-7→L+2 (14%), H-6→L+1 (43%)
59	271	0	H-1→L+8 (14%), HOMO→L+11 (56%)
60	271	0.0939	H-7→L+1 (42%), H-6→L+2 (22%)
61	268	0.0026	H-27→LUMO (57%), H-25→LUMO (21%)
62	267	0	H-24→LUMO (93%)
63	267	0	H-11→L+2 (13%), H-8→L+1 (46%)
64	266	0.0057	H-25→LUMO (72%)
65	266	0.0326	H-10→L+1 (16%), H-10→L+2 (12%), H-9→L+1 (22%)
66	265	0	H-10→L+1 (34%), H-10→L+2 (13%), H-9→L+1 (25%), H-9→L+2 (18%)
67	265	0.0319	H-11→L+1 (23%), H-9→L+1 (12%), H-8→L+2 (14%)
68	264	0.002	H-1→L+7 (58%), HOMO→L+8 (11%)
69	262	0	
70	261	0.0215	
71	261	0	H-26→LUMO (14%), H-8→L+1 (10%), HOMO→L+9 (16%)
72	259	0.0869	H-10→L+4 (14%), H-9→L+3 (14%)
73	259	0	H-10→L+4 (15%), H-9→L+3 (15%)
74	259	0	H-5→L+3 (18%), H-5→L+4 (23%), H-4→L+3 (11%)
75	259	0.0305	H-5→L+3 (27%), H-5→L+4 (21%), H-4→L+4 (11%)
76	258	0	H-32→LUMO (22%), HOMO→L+9 (12%)
77	257	0.0226	H-3→L+5 (30%), H-3→L+6 (10%), H-2→L+6 (38%)
78	257	0	H-3→L+6 (36%), H-2→L+5 (29%)
79	257	0.0058	H-37→LUMO (15%), H-29→LUMO (25%)
80	256	0	H-28→LUMO (91%)
81	256	0.0006	H-29→LUMO (71%)
82	256	0.0209	H-7→L+1 (12%), H-6→L+2 (39%)
83	256	0	H-19→L+2 (15%), H-18→L+1 (48%), H-17→L+2 (18%)
84	255	0.0035	H-19→L+1 (19%), H-18→L+2 (25%), H-17→L+1 (20%), H-6→L+2 (14%)
85	255	0	H-1→L+8 (67%), HOMO→L+11 (20%)
86	254	0	H-7→L+2 (28%), H-4→L+5 (26%)
87	254	0	H-7→L+2 (16%), H-4→L+5 (32%)
88	253	0.0024	H-37→LUMO (19%), HOMO→L+13 (19%)
89	253	0	H-31→LUMO (13%), H-30→LUMO (78%)
90	253	0	H-31→LUMO (78%), H-30→LUMO (13%)
91	252	0.0007	H-1→L+11 (68%), HOMO→L+8 (13%)

92	252	0	H-3→L+10 (10%), HOMO→L+14 (24%), HOMO→L+16 (15%)
93	252	0.0479	H-1→L+16 (15%), HOMO→L+15 (40%)
94	251	0	H-1→L+15 (14%), HOMO→L+14 (22%), HOMO→L+16 (21%)
95	251	0	H-36→LUMO (23%), H-34→LUMO (57%), H-32→LUMO (16%)
96	251	0.0001	H-35→LUMO (23%), H-33→LUMO (73%)
97	251	0.0588	H-13→L+1 (16%), H-1→L+9 (19%), HOMO→L+10 (39%)
98	251	0	H-12→L+1 (25%), HOMO→L+12 (33%)
99	251	0.0154	H-35→LUMO (12%), H-3→L+9 (10%), H-2→L+10 (15%), HOMO→L+15 (10%)
100	251	0.0033	H-35→LUMO (47%), H-33→LUMO (18%)

H[1] NMR, C[13] NMR and MALDI-TOF spectra

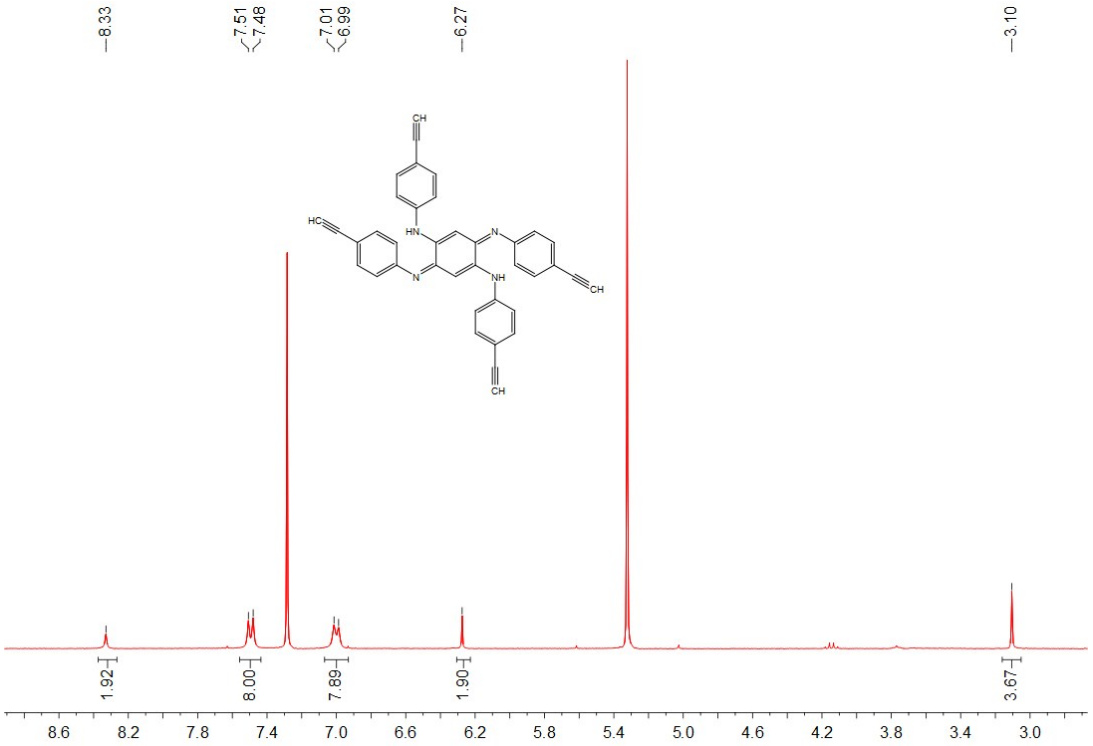


Figure S19. ^{1}H NMR spectrum of **3** ($CDCl_3$, 300 MHz, 298 K).

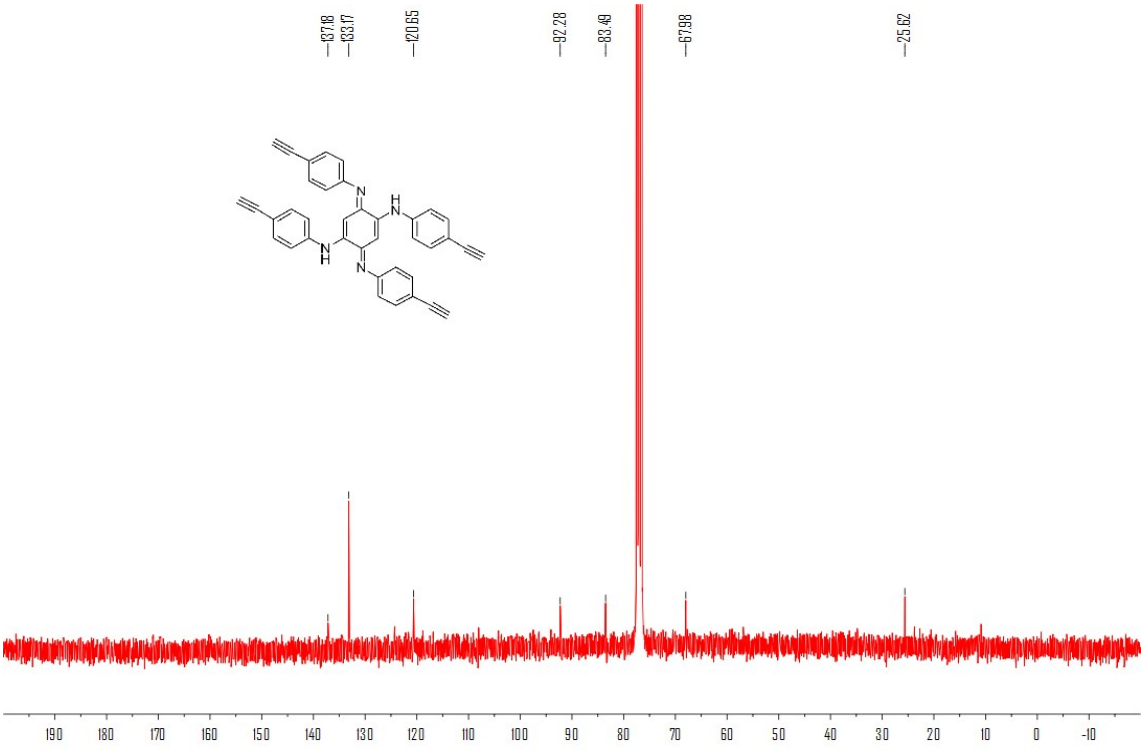


Figure S20. ^{13}C NMR spectrum of **3** ($CDCl_3$, 76 MHz, 298 K).

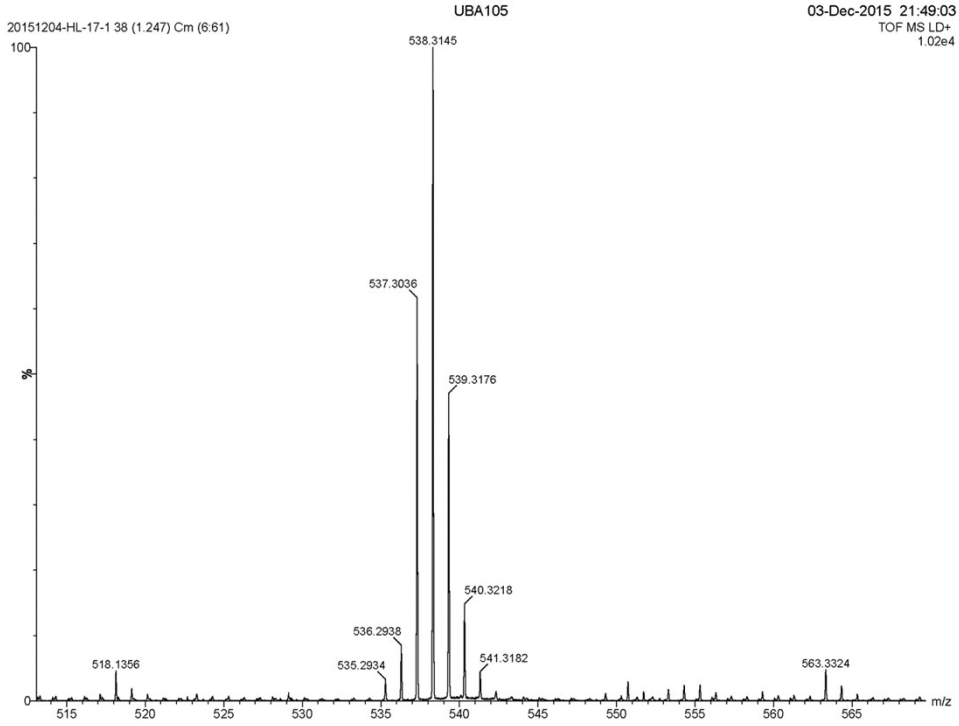


Figure S21. MALDI-TOF spectrum of **3**.

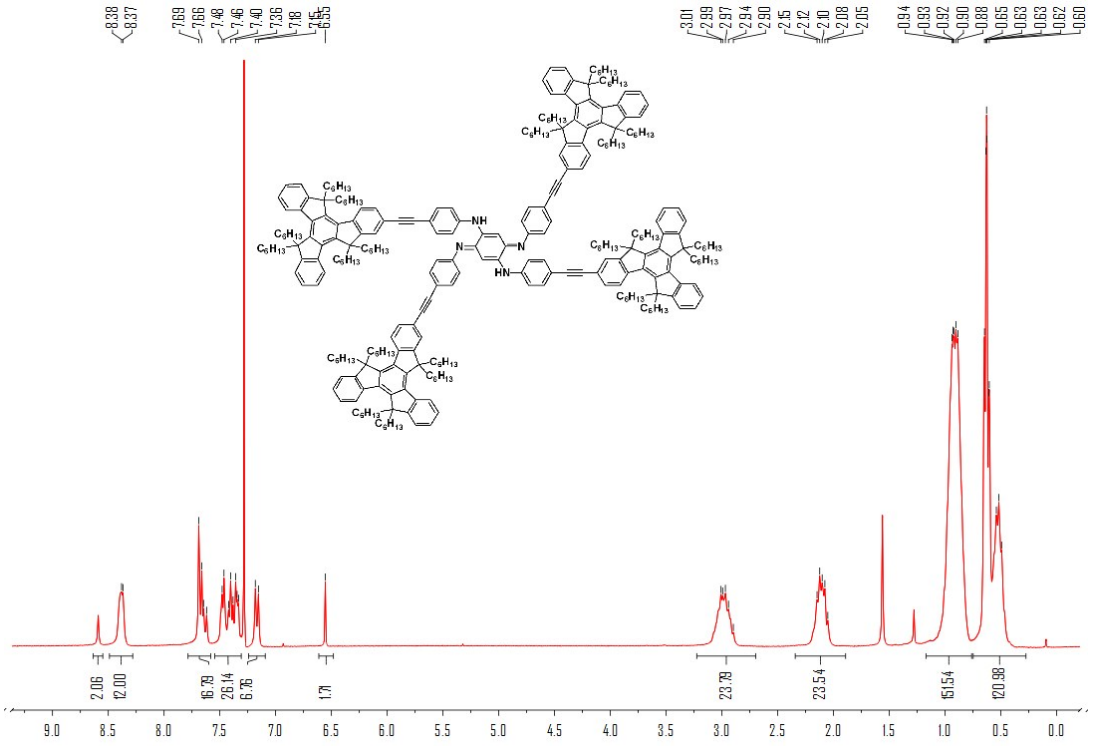


Figure S22. ^{1}H NMR spectrum of **4** ($CDCl_3$, 300 MHz, 298 K).

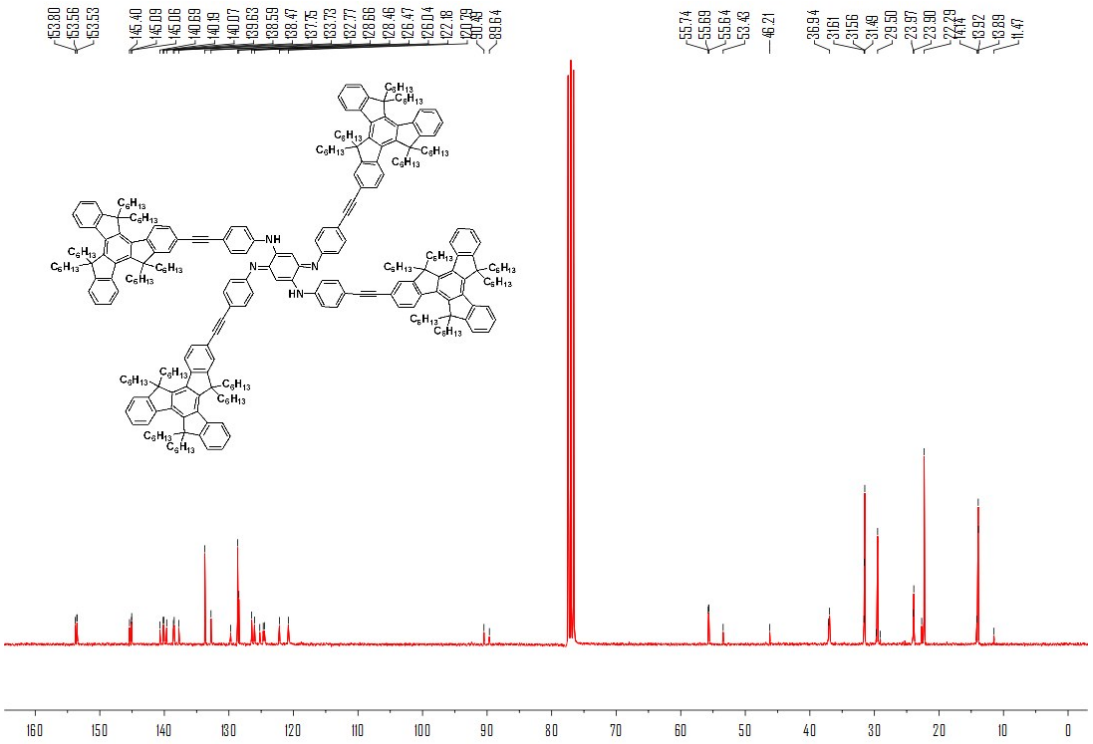


Figure S23. ^{13}C NMR spectrum of **4** ($CDCl_3$, 76 MHz, 298 K).

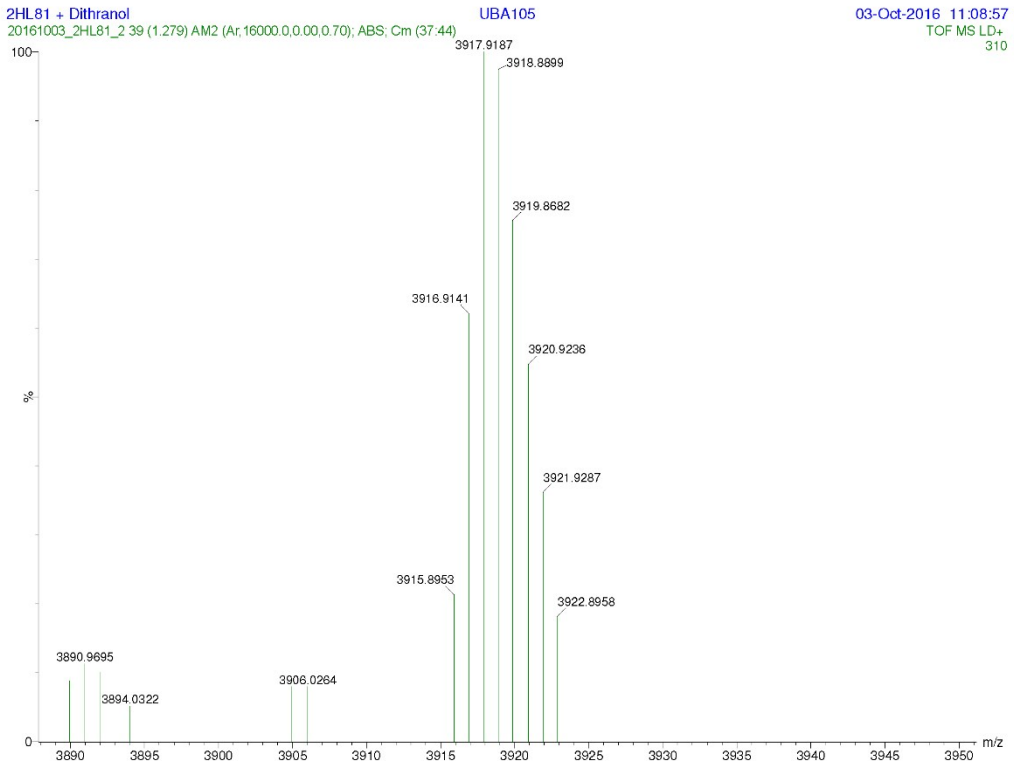


Figure S24. MALDI-TOF spectrum of **4**.

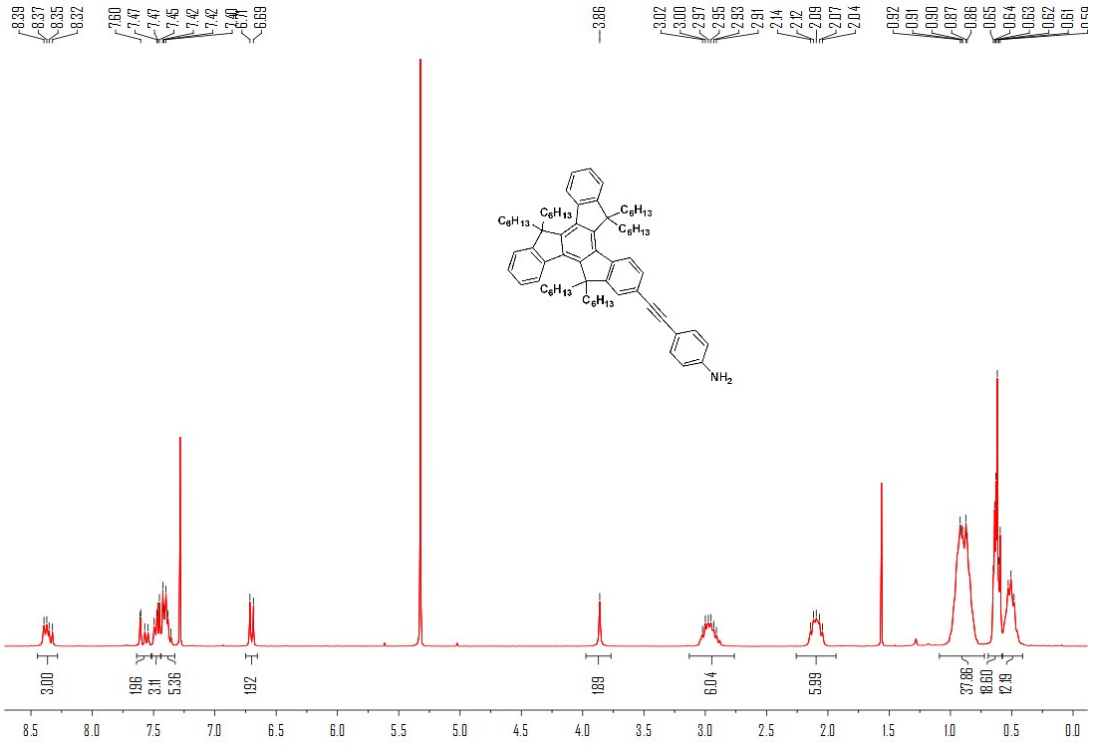


Figure S25. ^{1}H NMR spectrum of **6** ($CDCl_3$, 300 MHz, 298 K).

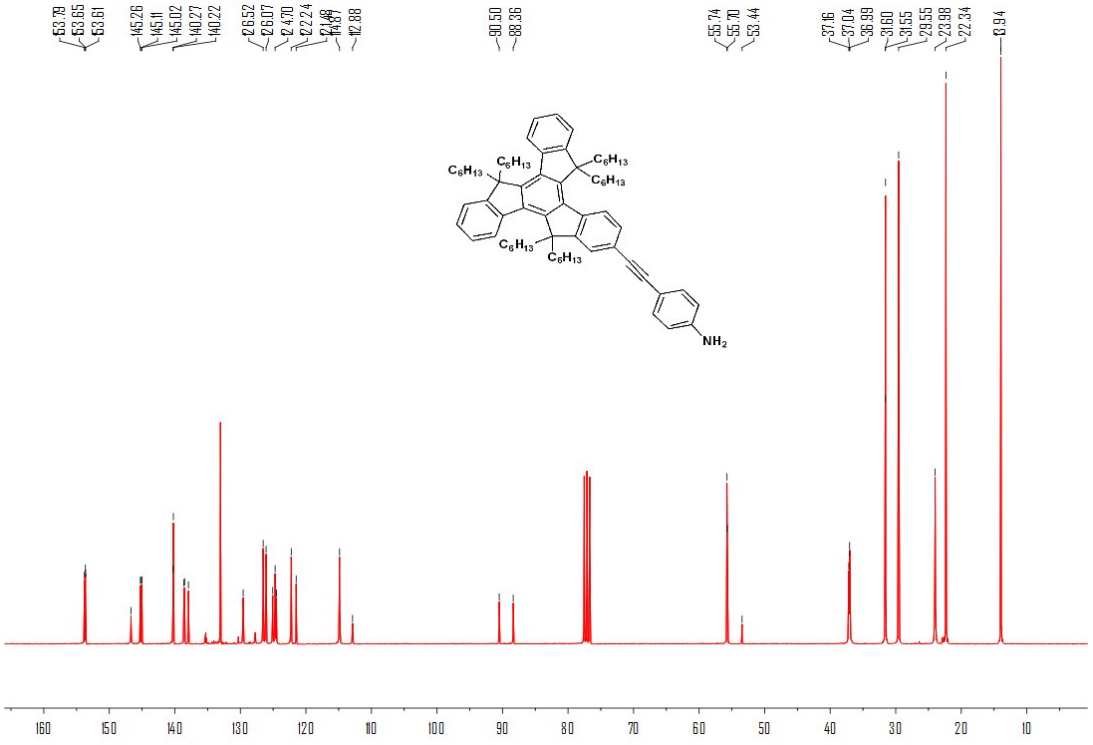


Figure S26. ^{13}C NMR spectrum of **6** ($CDCl_3$, 76 MHz, 298 K).

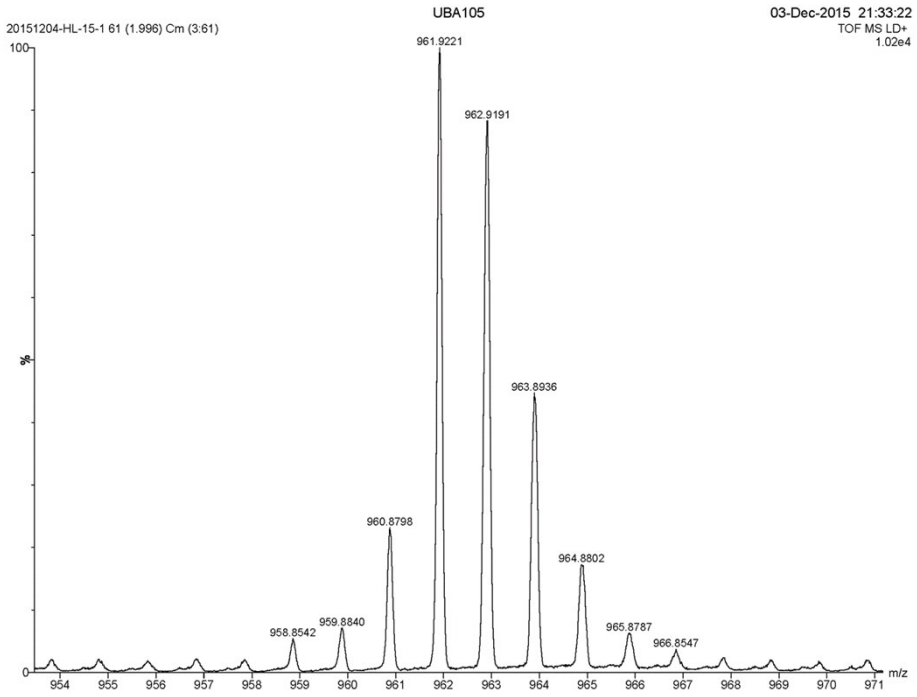


Figure S27. MALDI-TOF spectrum of **6**.

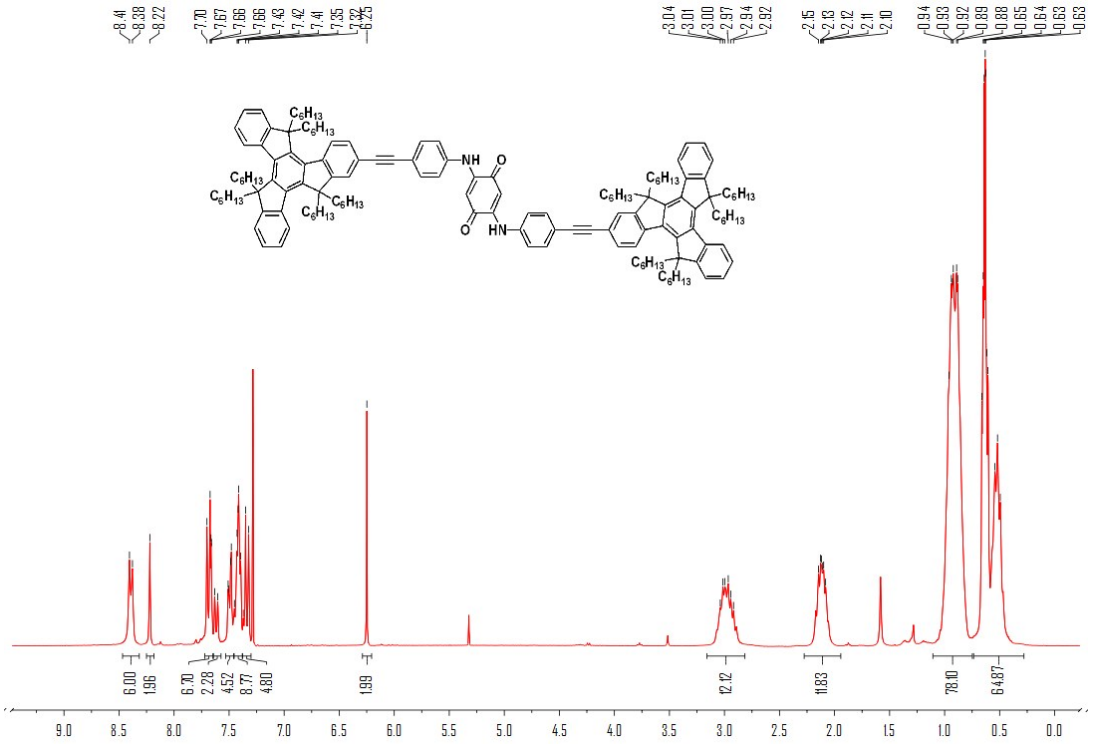


Figure S28. ^{1}H NMR spectrum of **7** ($CDCl_3$, 300 MHz, 298 K).

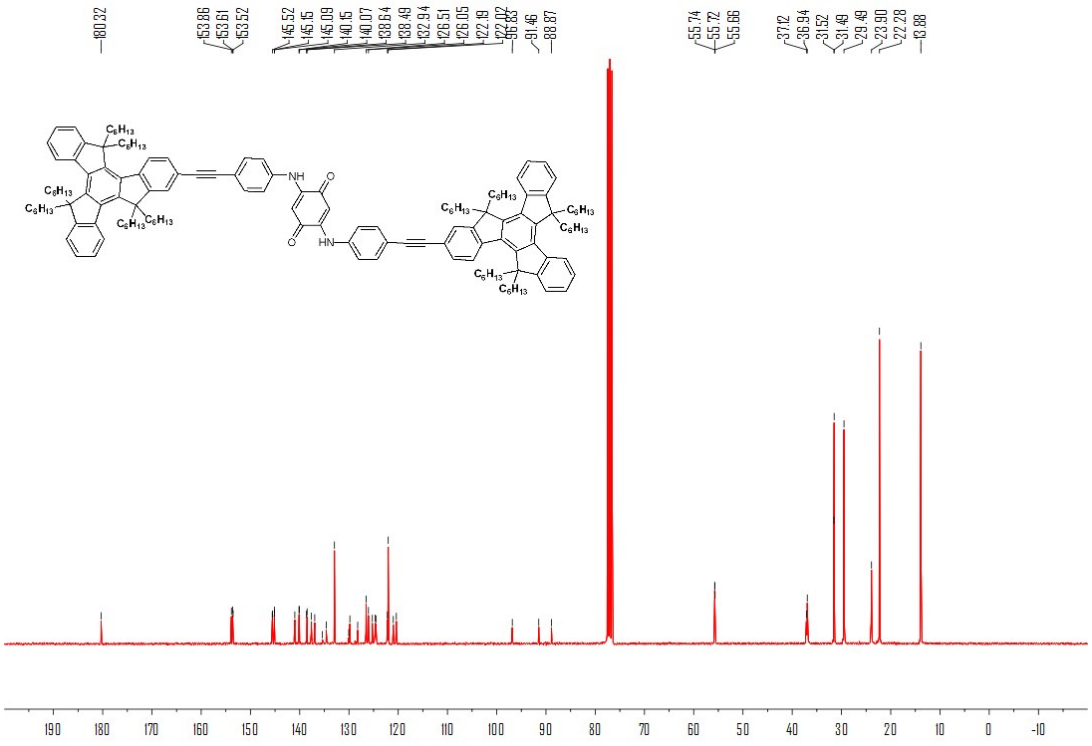


Figure S29. ^{13}C NMR spectrum of **7** ($CDCl_3$, 76 MHz, 298 K).

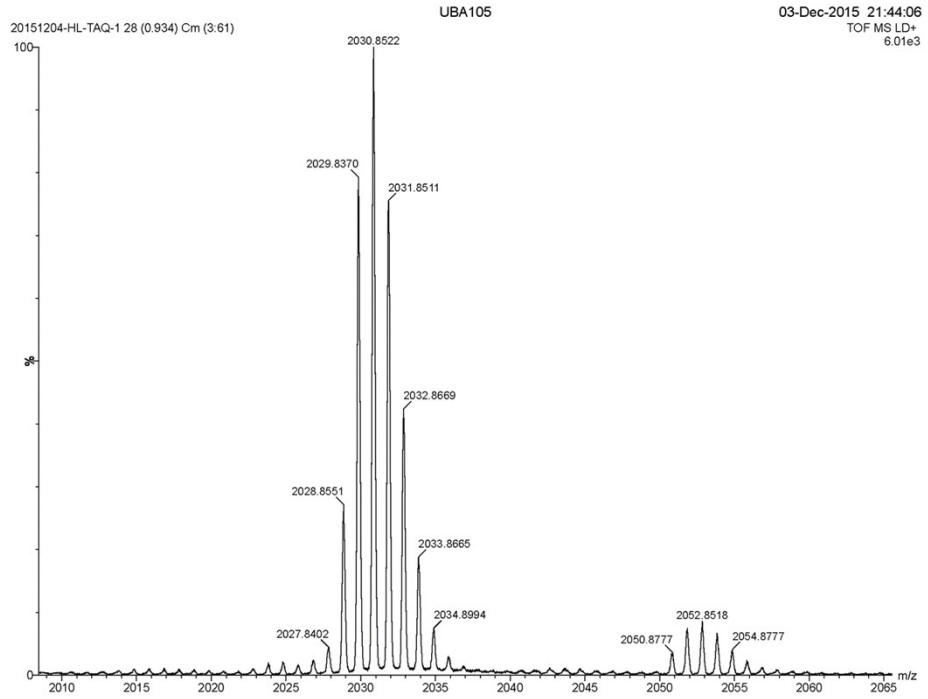


Figure S30. MALDI-TOF spectrum of **7**.

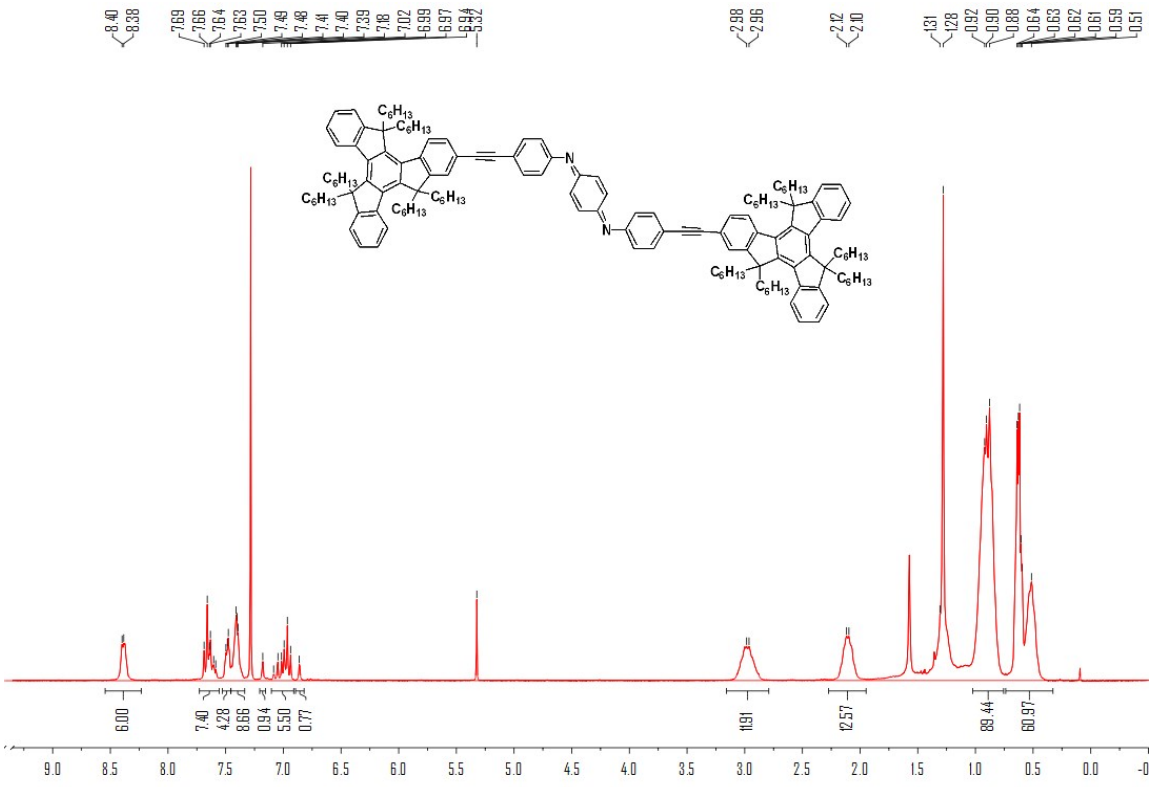


Figure S31. ^{1}H NMR spectrum of **8** ($CDCl_3$, 300 MHz, 298 K).

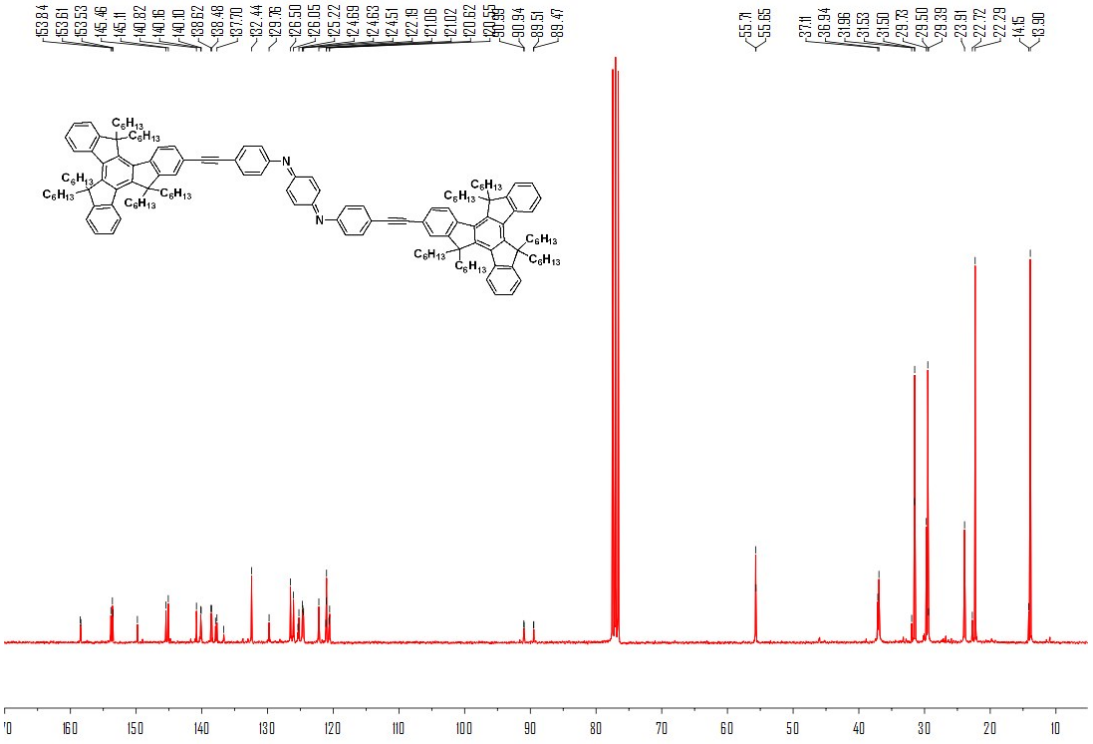


Figure S32. ^{13}C NMR spectrum of **8** ($CDCl_3$, 76 MHz, 298 K).

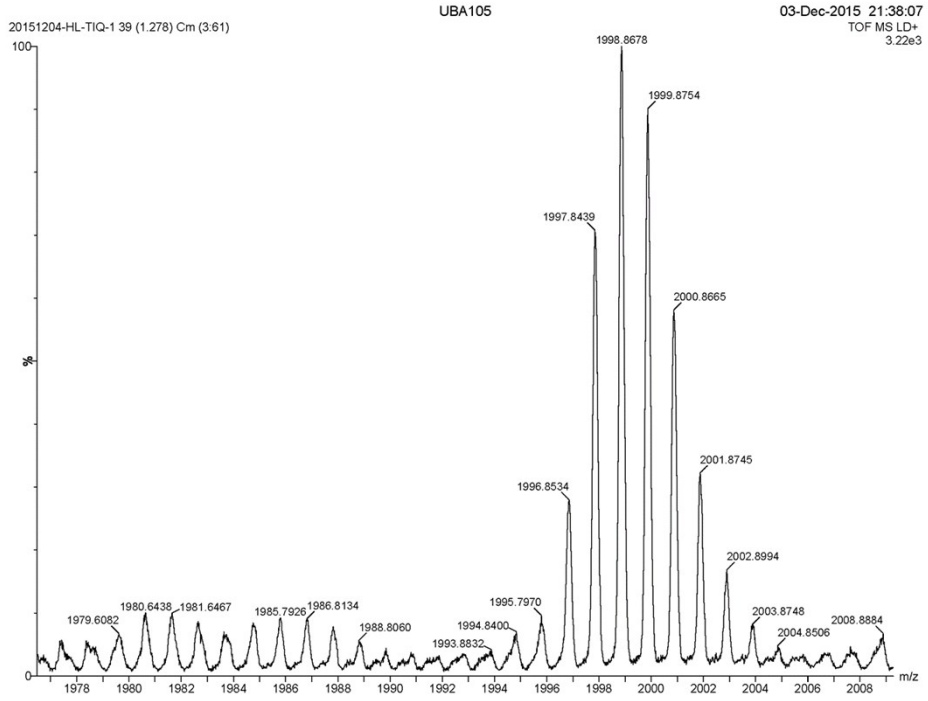


Figure S33. MALDI-TOF spectrum of **8**.