SUPPORTING INFORMATION

Carbazole-terpyridine donor-acceptor luminophores

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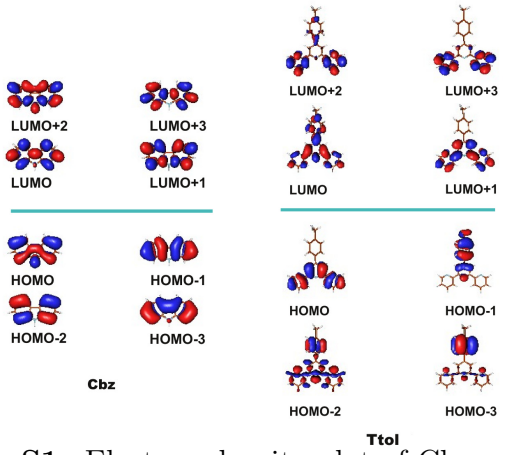

Figure S1: Electron density plot of Cbz and Ttol.

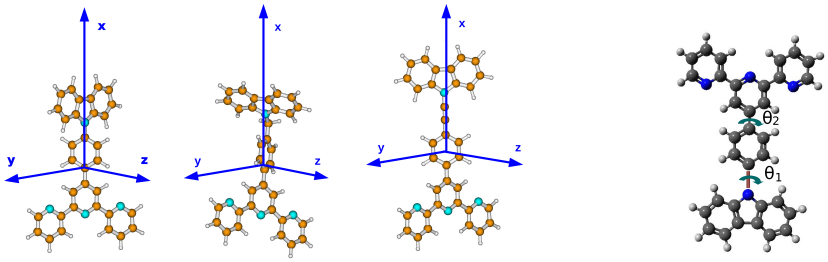

Figure S2: Reference axes of the transition dipole moment components (μ_α, α = x, y , and z)(left) of **1-3**; significant dihedral angles (right).

Table S1: Comparison among *a)* the calculated dihedral angles (*degrees*) between the central phenyl unit, and Cbz (θ_1) and the pyridine units of Ttol (θ_2), *b)* the NBO charge distribution on the fragments ρ_{Cbz}, ρ_{Ttol} and ρ_{linker} (linker = -C -CH_2- in **2** and -C≡C- in **3**), and *c)* the VIP/IP and EA/VEA calculated by PBE0/6-311+G(2d,p) in DMF.

		1			**2**			**3**		
		neutral	cation	anion	neutral	cation	anion	neutral	cation	anion
a)	θ_1	55.6	49.7	64.2	88.5	92.0	89.3	1.4	0.5	90.0
	θ_2	35.9	35.1	6.0	35.4	36.7	7.3	34.1	33.5	0.5
b)	ρ_{cbz}	-0.2093	0.6245	-0.2448	-0.2375	0.6887	-0.2465	-0.1164	0.4421	-0.1722
	ρ_{Ttol}	0.2093	0.3756	-0.7552	-0.0146	0.0293	-0.9925	-0.0415	0.2157	-0.9351
	ρ_{linker}	-	-	-	0.2522	0.2820	0.2390	0.1580	0.3422	0.1072
c)	VIP/IP	5.75/5.69			5.79/5.71			5.69/5.63		
	VEA/EA	2.21/2.40			2.16/2.32			2.28/2.53		

Table S2: $S_0 \rightarrow S_n$ transitions of **1** calculated by PBE0/6-311+G(2d,p) in toluene. ΔE (eV), λ (nm), $f_{osc.}$, and the transition electric dipole moment components μ_α (a.u.) with α = x, y, and z are reported, along with the two most significant excitations.

n.	ΔE/λ	μ_x	μ_y	μ_z	$f_{osc.}$	*excitations*
1	3.51/353	-2.0397	0.0000	-0.0001	0.3581	0.69 $h \rightarrow l$ -0.11 $h \rightarrow l_4$
2	3.74/331	-0.0002	-0.0902	0.0165	0.0008	0.69 $h \rightarrow l_1$ -0.11 $h_2 \rightarrow l$
3	3.99/310	-0.8187	-0.0002	0.0000	0.0655	0.69 $h \rightarrow l_2$ -0.14 $h_1 \rightarrow l_7$
4	4.04/306	0.0003	-0.0023	0.0026	0.0000	0.69 $h_1 \rightarrow l$
5	4.08/303	0.0001	1.6250	-0.1293	0.2659	0.67 $h_2 \rightarrow l$ -0.15 $h_3 \rightarrow l_1$
6	4.27/290	-0.0153	0.0000	0.0000	0.0000	0.71 $h_1 \rightarrow l_1$
7	4.30/288	0.0000	0.0593	0.1300	0.0022	0.63 $h_4 \rightarrow l$ +0.20 $h_7 \rightarrow l_1$
8	4.35/284	1.8846	0.0000	0.0000	0.3787	0.53 $h_2 \rightarrow l_1$ +0.28 $h \rightarrow l_3$
9	4.37/283	0.8041	0.0000	0.0000	0.0692	0.58 $h_4 \rightarrow l_1$ +0.22 $h_2 \rightarrow l_1$
10	4.38/283	0.0000	0.0098	0.2195	0.0052	0.61 $h \rightarrow l_6$ -0.30 $h \rightarrow l_5$
11	4.43/279	-0.2473	0.0003	0.0001	0.0066	0.52 $h \rightarrow l_3$ -0.37 $h_2 \rightarrow l_1$
12	4.50/275	-0.0005	1.3227	0.3761	0.2084	0.63 $h_1 \rightarrow l_2$ +0.27 $h \rightarrow l_7$
13	4.63/267	-0.0001	-0.1105	0.1028	0.0026	0.56 $h_7 \rightarrow l_1$ +0.26 $h_9 \rightarrow l$
14	4.73/262	-0.5183	-0.0057	0.0005	0.0311	0.56 $h \rightarrow l_4$ -0.33 $h \rightarrow l_3$
15	4.73/262	-0.0008	2.1522	-0.1678	0.5396	0.56 $h_3 \rightarrow l_1$ +0.26 $h_2 \rightarrow l_3$
16	4.75/260	-1.6695	0.0007	0.0000	0.3245	0.59 $h_3 \rightarrow l$ -0.22 $h \rightarrow l_4$
17	4.79/258	-0.7584	0.0000	0.0000	0.0675	0.52 $h_7 \rightarrow l$ +0.30 $h_9 \rightarrow l_1$
18	4.87/254	0.0000	0.1736	-0.0190	0.0036	0.63 $h \rightarrow l_5$ +0.30 $h \rightarrow l_6$
19	4.91/252	-0.0003	0.2870	0.1009	0.0111	0.57 $h_1 \rightarrow l_3$ +0.31 $h_1 \rightarrow l_4$
20	4.94/250	0.0000	0.4344	-0.0122	0.0229	0.48 $h_2 \rightarrow l_3$ -0.34 $h_3 \rightarrow l_1$
21	5.00/248	0.0470	0.0009	0.0004	0.0003	0.62 $h_1 \rightarrow l_6$ -0.32 $h_1 \rightarrow l_5$
22	5.02/247	-0.5526	0.0001	0.0002	0.0375	0.39 $h_6 \rightarrow l$ +0.37 $h_9 \rightarrow l_1$
23	5.03/246	0.0173	-0.1390	-0.3397	0.0166	0.47 $h_8 \rightarrow l$ -0.37 $h_5 \rightarrow l$
24	5.03/246	-0.9377	-0.0026	-0.0063	0.1083	0.55 $h_6 \rightarrow l$ +0.22 $h_7 \rightarrow l$

Table S3: $S_0 \rightarrow S_n$ transitions of **2** calculated by PBE0/6-311+G(2d,p) in toluene. ΔE (eV), λ (nm), $f_{osc.}$, and the transition electric dipole moment components μ_α (a.u.) with α = x, y, and z are reported, along with the two most significant excitations.

n.	$\Delta E/\lambda$	μ_x	μ_y	μ_z	$f_{osc.}$	*excitations*
1	3.77/329	0.0832	-0.0436	-0.0211	0.0009	0.70 $h \rightarrow l$
2	3.92/316	0.1150	-0.0265	0.0050	0.0013	0.70 $h \rightarrow l_1$
3	4.02/308	0.6662	0.2762	0.3943	0.0665	0.68 $h \rightarrow l_2$ -0.15 $h_1 \rightarrow l_6$
4	4.08/304	-0.3577	-1.4349	-0.1440	0.2205	0.64 $h_2 \rightarrow l$ -0.26 $h_3 \rightarrow l_1$
5	4.15/298	-0.4501	0.0445	0.0266	0.0209	0.70 $h_1 \rightarrow l$
6	4.28/289	-0.0189	-0.2620	-0.0381	0.0074	0.70 $h_1 \rightarrow l_1$
7	4.31/287	0.0603	-0.0017	0.1480	0.0027	0.59 $h_4 \rightarrow l$ +0.27 $h_5 \rightarrow l$
8	4.37/283	-1.0457	0.2151	0.1674	0.1249	0.49 $h_4 \rightarrow l_1$ -0.37 $h_2 \rightarrow l_1$
9	4.38/283	1.8911	-0.3148	-0.2906	0.4031	0.57 $h_2 \rightarrow l_1$ +0.31 $h_4 \rightarrow l_1$
10	4.48/277	0.1562	0.9705	-0.9959	0.2147	0.64 $h_1 \rightarrow l_2$ +0.24 $h \rightarrow l_6$
11	4.50/275	-1.8281	0.4907	0.1842	0.3984	0.68 $h_3 \rightarrow l$ +0.11 $h_2 \rightarrow l_1$
12	4.54/273	-0.5972	-1.6918	-0.1029	0.3591	0.63 $h_3 \rightarrow l_1$ +0.25 $h_2 \rightarrow l$
13	4.63/267	0.0821	0.1534	-0.1452	0.0058	0.55 $h \rightarrow l_3$ +0.35 $h \rightarrow l_5$
14	4.64/267	0.0546	0.2900	-0.1090	0.0112	0.53 $h_8 \rightarrow l_1$ -0.26 $h_9 \rightarrow l$
15	4.74/261	0.0222	0.1156	-0.1330	0.0037	0.57 $h \rightarrow l_6$ -0.29 $h \rightarrow l_3$
16	4.80/258	0.1274	-0.0138	-0.0107	0.0019	0.54 $h_8 \rightarrow l$ -0.35 $h_9 \rightarrow l_1$
17	4.86/255	0.3121	1.3341	0.1288	0.2254	0.46 $h_2 \rightarrow l_3$ +0.38 $h_6 \rightarrow l_1$
18	4.90/253	0.0241	0.3880	0.1390	0.0204	0.42 $h_7 \rightarrow l$ +0.28 $h_3 \rightarrow l_6$
19	4.90/252	0.0510	0.0873	0.0317	0.0013	0.53 $h \rightarrow l_5$ -0.35 $h \rightarrow l_6$
20	5.00/248	-0.0530	0.0161	0.0077	0.0004	0.68 $h \rightarrow l_4$
21	5.02/246	-0.0509	0.0131	0.0116	0.0004	0.39 $h_9 \rightarrow l_1$ +0.32 $h_8 \rightarrow l_3$
22	5.03/246	-0.2393	-0.0641	-0.0146	0.0076	0.64 $h_1 \rightarrow l_3$ +0.27 $h_1 \rightarrow l_5$
23	5.05/245	-0.7176	0.0791	0.1013	0.0658	0.62 $h_6 \rightarrow l$ -0.27 $h_5 \rightarrow l$
24	5.10/243	0.0238	0.1712	-0.0326	0.0039	0.44 $h_9 \rightarrow l$ +0.28 $h_8 \rightarrow l_4$

Table S4: $S_0 \rightarrow S_n$ transitions of **3** calculated by PBE0/6-311+G(2d,p) in toluene. ΔE (eV), λ (nm), $f_{osc.}$, and the transition electric dipole moment components μ_α (a.u.) with α = x, y, and z are reported, along with the two most significant excitations.

n.	ΔE/λ	μ_x	μ_y	μ_z	$f_{osc.}$	*excitations*
1	3.42/362	-3.8201	0.0000	-0.0001	1.2216	0.69 $h \rightarrow l$ +0.11 $h \rightarrow l_3$
2	3.70/335	0.0001	0.1187	0.0082	0.0013	0.68 $h \rightarrow l_1$ -0.15 $h_2 \rightarrow l$
3	3.86/321	-0.5395	-0.0001	-0.0001	0.0275	0.69 $h \rightarrow l_2$ +0.10 $h_1 \rightarrow l_7$
4	4.06/305	0.0001	-1.6114	-0.2651	0.2651	0.66 $h_2 \rightarrow l$ +0.17 $h \rightarrow l_1$
5	4.23/293	-2.1015	0.0000	-0.0001	0.4577	0.63 $h \rightarrow l_3$ -0.22 $h_2 \rightarrow l_1$
6	4.25/291	0.0001	-0.0836	0.0335	0.0008	0.69 $h_1 \rightarrow l$ +0.13 $h_1 \rightarrow l_3$
7	4.28/289	-0.0004	-0.0317	-0.1529	0.0026	0.63 $h_4 \rightarrow l$ -0.18 $h_4 \rightarrow l_3$
8	4.37/283	-0.0083	-0.0004	0.0000	0.0000	0.63 $h_4 \rightarrow l_1$ +0.20 $h_6 \rightarrow l$
9	4.40/281	1.0295	-0.0002	-0.0001	0.1142	0.64 $h_2 \rightarrow l_1$ +0.23 $h \rightarrow l_3$
10	4.48/276	0.0001	0.1113	-0.0796	0.0021	0.59 $h \rightarrow l_6$ -0.29 $h_8 \rightarrow l$
11	4.54/273	0.0001	-1.1533	0.4723	0.1726	0.60 $h_1 \rightarrow l_2$ -0.33 $h \rightarrow l_7$
12	4.59/270	0.0018	0.0001	0.0000	0.0000	0.71 $h_1 \rightarrow l_1$
13	4.62/268	0.0005	0.0903	-0.0919	0.0019	0.57 $h_6 \rightarrow l_1$ +0.24 $h_9 \rightarrow l$
14	4.66/266	0.0896	-0.0001	-0.0001	0.0009	0.67 $h \rightarrow l_4$ -0.14 $h \rightarrow l_3$
15	4.68/264	-1.3443	-0.0002	0.0000	0.2072	0.67 $h_3 \rightarrow l$ +0.13 $h \rightarrow l_4$
16	4.75/261	0.0004	-2.0789	-0.3597	0.5180	0.45 $h_3 \rightarrow l_1$ +0.35 $h_5 \rightarrow l_1$
17	4.77/259	-0.2087	-0.0028	-0.0005	0.0051	0.56 $h_6 \rightarrow l$ +0.30 $h_9 \rightarrow l_1$
18	4.84/256	0.0000	-0.4415	-0.0546	0.0234	0.67 $h \rightarrow l_5$ +0.14 $h \rightarrow l_6$
19	4.90/252	0.0000	0.5118	0.0544	0.0318	0.50 $h_2 \rightarrow l_3$ +0.41 $h_3 \rightarrow l_1$
20	4.92/252	0.0001	-1.5421	0.6126	0.3317	0.52 $h \rightarrow l_7$ -0.32 $h_1 \rightarrow l_3$
21	4.97/249	0.7661	0.0001	-0.0001	0.0714	0.69 $h_5 \rightarrow l$
22	5.01/247	0.0372	-0.0005	-0.0001	0.0002	0.44 $h_9 \rightarrow l_1$ +0.32 $h_6 \rightarrow l_4$
23	5.03/246	0.0000	-0.0635	0.0060	0.0005	0.38 $h_5 \rightarrow l_1$ +0.34 $h_2 \rightarrow l_3$
24	5.04/245	0.0002	-1.0069	0.3712	0.1423	0.46 $h_1 \rightarrow l_3$ +0.24 $h \rightarrow l_7$

Table S5: Comparison among the $S_0 \rightarrow S_n$ transitions of **1**, **2**, and **3** in ACN calculated by PBE0/6-311+G(2d,p). ΔE (eV), λ (nm), and $f_{osc.}$ are reported. The assignment of these transitions are similar to those reported in Tables S2-S4.

	1		**2**		**3**	
n.	$\Delta E/\lambda$	$f_{osc.}$	$\Delta E/\lambda$	$f_{osc.}$	$\Delta E/\lambda$	$f_{osc.}$
1	3.52/353	0.9988	3.74/331	0.0052	3.41/363	1.1687
2	3.69/336	0.0037	3.90/317	0.0025	3.69/336	0.0011
3	3.99/311	0.0130	4.01/309	0.0605	3.88/319	0.0287
4	4.07/305	0.2465	4.08/303	0.1949	4.06/305	0.2364
5	4.09/303	0.0009	4.16/298	0.0188	4.21/294	0.0009
6	4.28/290	0.0017	4.29/289	0.0067	4.24/292	0.4713
7	4.35/285	0.4190	4.33/286	0.0029	4.29/289	0.0023
8	4.38/283	0.0000	4.39/282	0.0296	4.39/282	0.0002
9	4.39/282	0.0009	4.39/282	0.5140	4.42/280	0.1034
10	4.52/274	0.1528	4.48/276	0.3620	4.49/276	0.0011
11	4.52/274	0.0712	4.49/276	0.1725	4.56/272	0.1479
12	4.56/272	0.0212	4.53/273	0.3113	4.56/271	0.0000
13	4.64/267	0.0016	4.66/266	0.0078	4.64/267	0.0025
14	4.77/260	0.4992	4.66/265	0.0053	4.67/265	0.1919
15	4.77/260	0.0000	4.76/260	0.0039	4.68/264	0.0180
16	4.80/258	0.0452	4.82/257	0.0051	4.76/260	0.4822
17	4.81/258	0.0748	4.86/255	0.1533	4.78/259	0.0051
18	4.92/252	0.0087	4.88/254	0.1266	4.86/254	0.0135
19	4.96/250	0.1354	4.92/251	0.0022	4.92/252	0.0576
20	4.97/249	0.0885	5.02/247	0.0556	4.93/251	0.0698
21	4.99/249	0.0468	5.02/247	0.0049	4.93/251	0.1811
22	5.03/246	0.0111	5.05/245	0.0005	5.03/246	0.0003
23	5.04/246	0.0000	5.07/244	0.0115	5.04/246	0.0000
24	5.09/244	0.3613	5.11/242	0.0277	5.04/245	0.0426

Table S6: $S_0 \rightarrow S_n$ excitations of $\mathbf{3}^{\perp}$ calculated by TD-PBE0/6-311+G* at the S_1 geometry in acetonitrile (ACN). The assignements are based on the two most significant excitations. Cbz^a = Cbz + acetylenic group and DPh = diphenyl. $\Delta E/\lambda$ (eV/nm).

n.	$\Delta E/\lambda$	$f_{osc.}$	*excitations*	*assignments*
1	2.89/430	0.0000	$0.68h \rightarrow l + 0.14h \rightarrow l_2$	Cbz^a →DPh
2	3.62/342	0.1982	$0.68h_3 \rightarrow l$ - $0.17h \rightarrow l_1$	Tpy→DPh + Cbz^a →Tpy
3	3.78/328	0.0000	$0.70h_2 \rightarrow l$	Cbz^a →DPh

Table S7: $S_0 \rightarrow S_n$ excitations of **1-3** calculated by TD-CAM-B3LYP in acetonitrile (ACN) and toluene (TOL) at the geometries optimized by PBE0 (S_0) and TD-PBE0 (S_1). The assignements are based on the two most significant excitations and always refer to the those of the right column. [a] indicates Cbz+Ph, [b] Cbz+Dph, and [c] Cbz + acetylenic group (Ph = phenyl and DPh = diphenyl). ΔE (eV).

1		S_0/ACN		S_1/ACN	
n	ΔE	*excitations*	ΔE	*excitations*	*assignments*
1	4.25	$0.56h \rightarrow l_2$ -0.29$h \rightarrow l$	4.22	$0.44h \rightarrow l$ -0.41$h \rightarrow l_2$	Cbz[a] →Ttol+Cbz[a] →Cbz
2	4.29	$0.49h \rightarrow l$+0.35$h \rightarrow l_2$	4.29	$0.52h \rightarrow l_2$+0.35$h \rightarrow l$	Cbz[a] →Cbz+Cbz[a] →Ttol
3	4.37	$0.64h_2 \rightarrow l$ +0.15$h_3 \rightarrow l_1$	4.33	$0.65h_2 \rightarrow l$ -0.10$h_2 \rightarrow l_3$	Tpy→Ttol
2		S_0/ACN		S_0/TOL	
n	ΔE	*excitations*	ΔE	*excitations*	*assignments*
1	4.25	$0.67h \rightarrow l_2$ +0.19$h_1 \rightarrow l_9$	4.25	$0.67h \rightarrow l_2$ +0.19$h \rightarrow l_9$	Cbz→Cbz
2	4.39	$0.64h_2 \rightarrow l$ +0.18$h_3 \rightarrow l_1$	4.38	$0.65h_2 \rightarrow l$ +0.17$h_3 \rightarrow l_1$	Tpy→Ttol+DPh→Tpy
3	4.66	$0.64h_1 \rightarrow l_2$ -0.20$h \rightarrow l_8$	4.64	$0.65h_1 \rightarrow l_2$ -0.18$h \rightarrow l_8$	Cbz→Cbz
3‖		S_0/ACN		S_1/ACN	
n	ΔE	*excitations*	ΔE	*excitations*	*assignments*
1	3.94	$0.59h \rightarrow l$ +0.26$h \rightarrow l_3$	3.36	$0.65h \rightarrow l$ +0.16$h \rightarrow l_3$	Cbz[a] →Ttol
2	4.29	$0.63h \rightarrow l_2$ +0.19$h \rightarrow l_3$	4.04	$0.54h_2 \rightarrow l$ +0.32$h \rightarrow l_1$	Tpy→Ttol+Cbz[a] →Ttol
3	4.34	$0.60h \rightarrow l_2$ +0.20$h \rightarrow l_1$	4.23	$0.63h \rightarrow l_2$ -0.23$h_3 \rightarrow l_2$	Cbz[a] →Cbz+Cbz[b] →Cbz
3 ‖ *and* ⊥		$S_1^{\parallel}$/ACN		$S_1^{\perp}$/ACN	
n	ΔE	*excitations*	ΔE	*excitations*	*assignments*
1	3.36	$0.65h \rightarrow l$ +0.16$h \rightarrow l_3$	3.57	$0.59h \rightarrow l$ +0.22$h \rightarrow l_3$	Cbz[c] →Ttol, Cbz
2	4.04	$0.54h_2 \rightarrow l$ +0.32$h \rightarrow l_1$	3.85	$0.68h_1 \rightarrow l$ +0.10$h_1 \rightarrow l_3$	Ttol→Ttol + Ttol→Cbz
3	4.23	$0.63h \rightarrow l_2$ -0.23$h_3 \rightarrow l_2$	4.03	$0.62h_3 \rightarrow l$ -0.20$h_1 \rightarrow l_1$	Tpy→Ttol +DPh→Tpy

References

The DFT and TD-DFT calculations were performed with:

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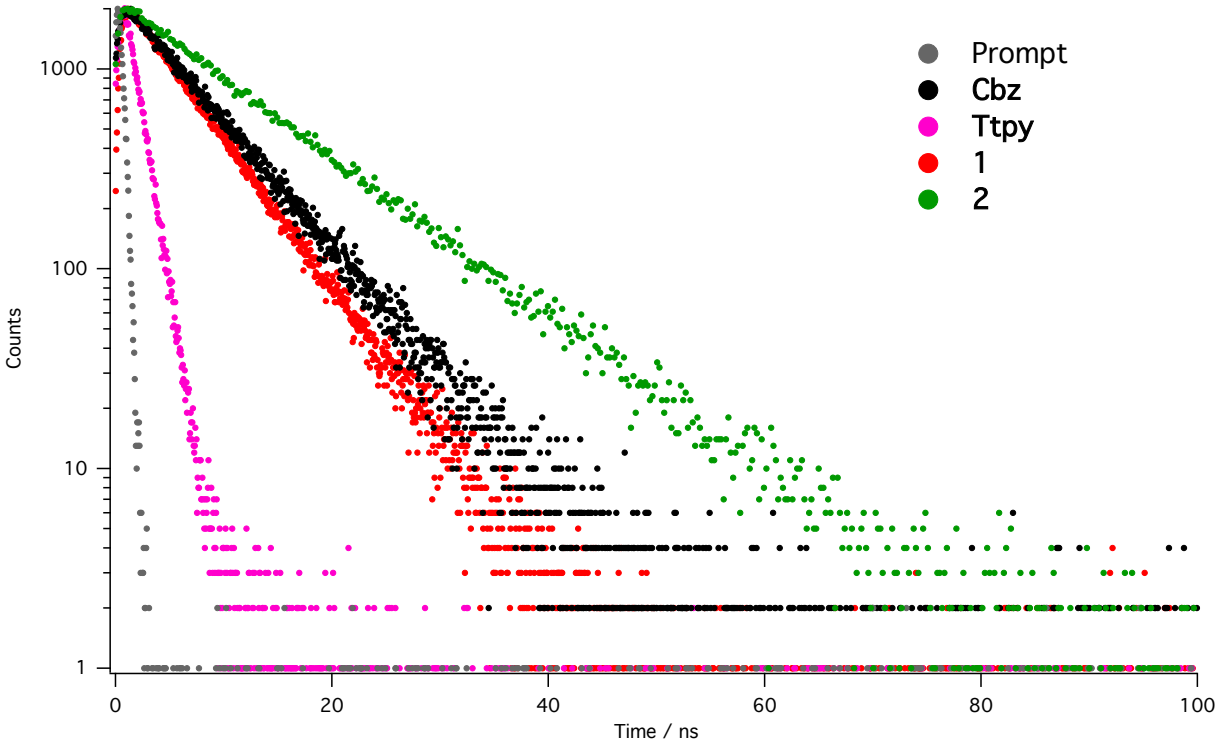

Figure S3: Emission lifetimes of **Cbz**, **Ttpy**, **1** and **2** in RT ACN at emission maximum: all reported decays are monoexponential.

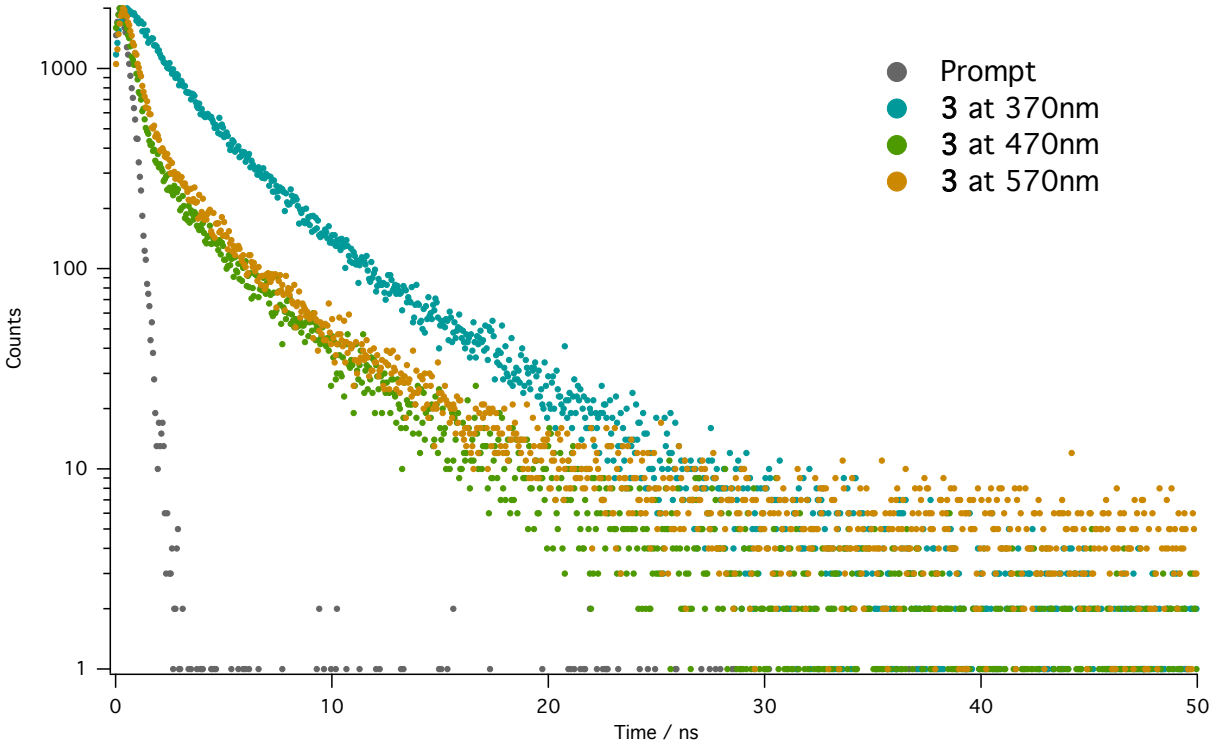

Figure S4: Emission lifetimes of compound **3** in RT ACN at room temperature at different wavelengths: all reported decays are multiexponential.

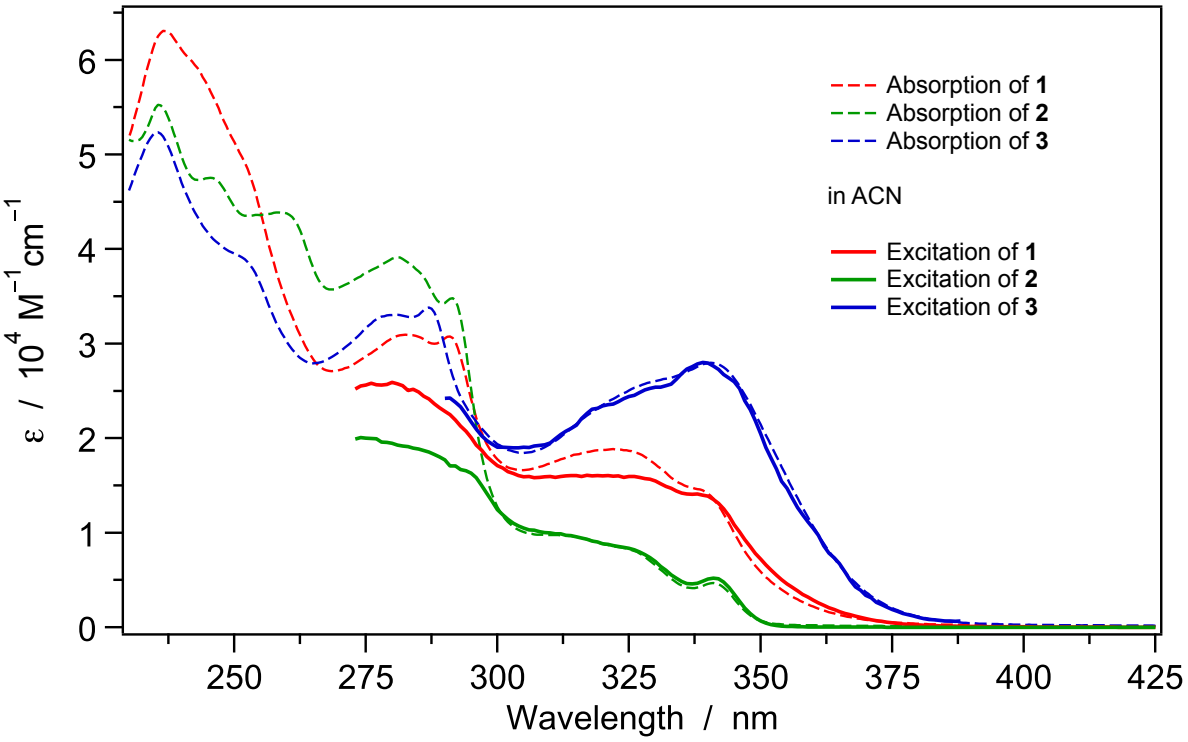

Figure S5: Excitation spectra of **1**, **2** and **3** in ACN at emission maximum (absorption spectra are reported for comparison).