Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Self-assembbly of T-shape 2*H*-benzo[d][1,2,3]-triazoles. Optical wadeguide and photophysical properties.

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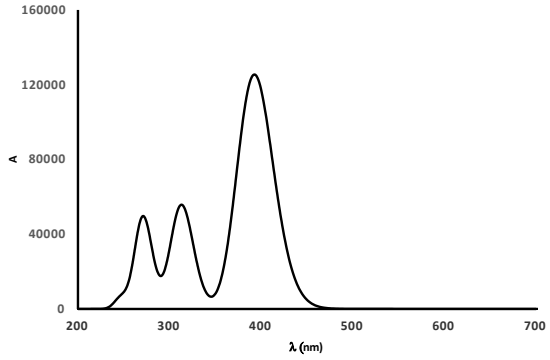
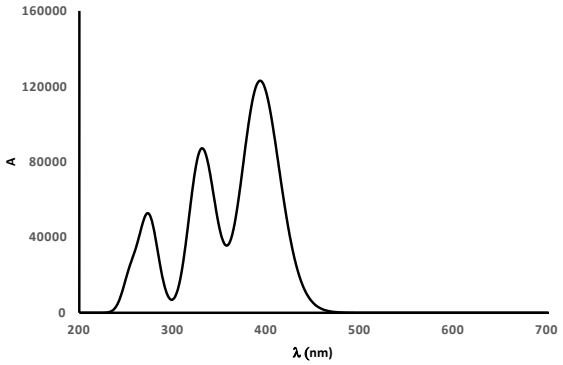
Figure S1. Theoretical UV-Vis absorption spectra, wavelength and oscillator strength values and orbitals contribution for the transition of compounds **1a** (a), **1b** (b), **1c** (c) and **1d** (d), calculated at CPCM-M06-2X/6-311+G(2d,p) in dichloromethane.

a)



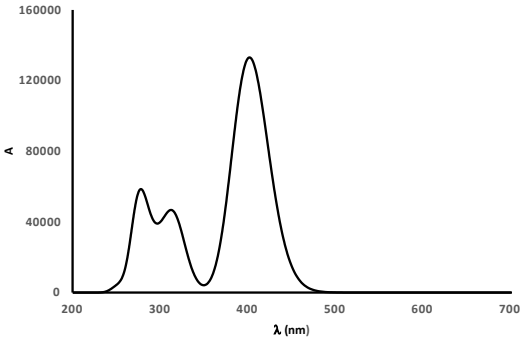
λ (nm)	Osc. Strength	Major contribs
392.3	1.7286	HOMO->LUMO (96%)
312.9	0.7674	H-1->LUMO (83%)
279.6	0.0617	H-2->LUMO (81%)
270.6	0.6414	HOMO->L+1 (85%)
262.4	0.0	H-7->LUMO (73%)
262.2	0.0	H-8->LUMO (75%)
250.1	0.0162	H-5->LUMO (58%), H-5->L+1 (15%), H-1->L+3 (13%)
249.6	0.0028	H-3->LUMO (36%), HOMO->L+5 (20%)
249.5	0.0	H-4->LUMO (37%), HOMO->L+6 (20%)
247.4	0.0731	HOMO->L+2 (70%)

b)



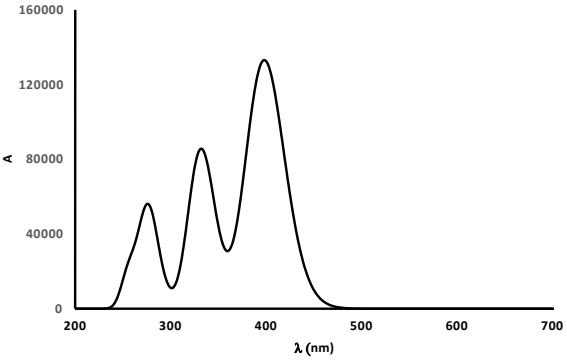
λ (nm)	Osc. Strength	Major contribs
393.3	1.7005	HOMO->LUMO (95%)
331.1	1.2047	H-1->LUMO (78%)
280.5	0.0522	H-2->LUMO (79%)
274.0	0.647	HOMO->L+1 (80%)
262.5	0.0	H-9->LUMO (71%)
262.3	0.0002	H-10->LUMO (73%)
256.2	0.277	H-6->LUMO (24%), H-1->L+1 (40%)
255.6	0.0036	H-7->LUMO (38%)
249.6	0.0165	H-4->LUMO (37%),
245.46	0.0174	HOMO->L+2 (62%)

c)



λ (nm)	Osc. Strength	Major contribs
402.0	1.8377	HOMO->LUMO (93%)
315.9	0.5637	H-4->LUMO (49%), H-1->LUMO (36%)
296.0	0.2599	H-4->LUMO (38%), H-1->LUMO (49%)
280.7	0.0017	H-3->LUMO (72%), H-2->L+2 (13%)
280.7	0.0954	H-3->L+2 (13%), H-2->LUMO (72%)
276.0	0.666	HOMO->L+1 (77%)
260.6	0.0001	H-9->LUMO (10%), H-8->LUMO (62%)
260.6	0.0002	H-9->LUMO (63%), H-8->LUMO (10%)
260.1	0.001	H-12->LUMO (30%), H-9->LUMO (27%)
252.8	0.0528	H-1->L+1 (11%), HOMO->L+2 (72%)

d)



λ (nm)	Osc. Strength	Major contribs
397.8	1.835	HOMO->LUMO(94%)
331.8	1.1802	H-1->LUMO (78%)
289.4	0.0717	H-2->LUMO (81%)
276.3	0.7009	HOMO->L+1 (77%)
264.9	0.0009	H-4->L+2(10%), H-3->LUMO (40%)
264.8	0.0294	H-4->LUMO (42%), H-3->L+2 (11%)
260.3	0.0001	H-11->LUMO(25%), H-10->LUMO(27%)
256.5	0.0018	H-5->LUMO (70%), HOMO->L+1 (10%)
256.7	0.2771	H-7->LUMO (22%), H-1->L+1 (37%)
255.9	0.0045	H-8->LUMO (34%), H-1->L+3 (29%)

Figure S2. Horizontal and vertical aggregates of compound **1b computed at B97D/**6-31G*

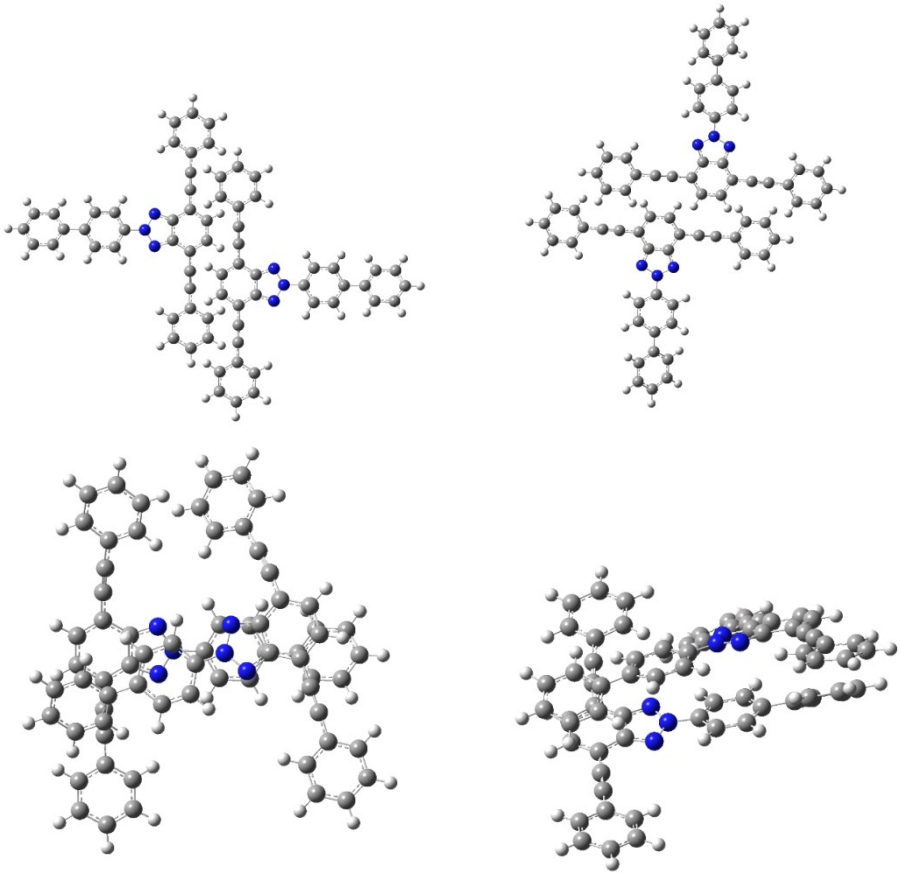
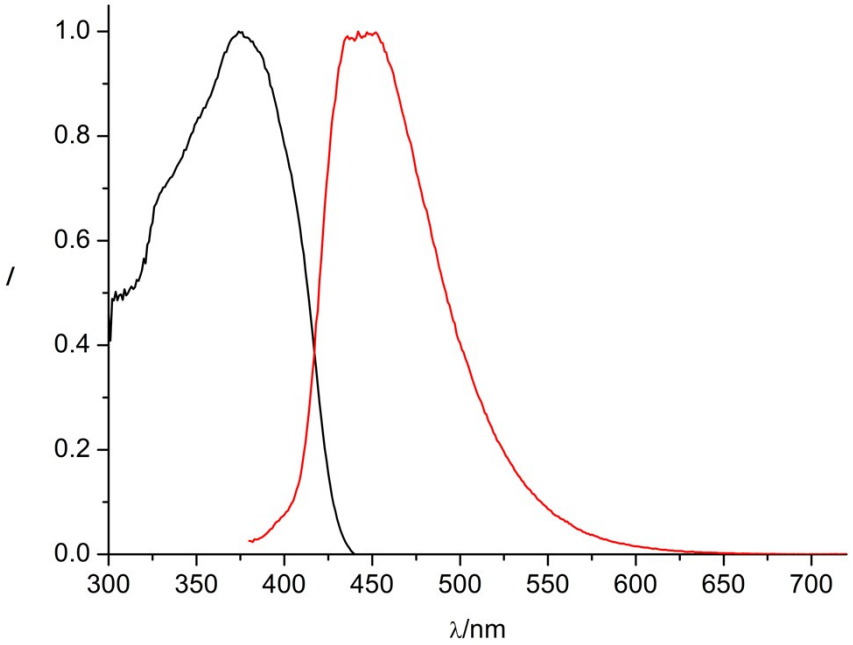
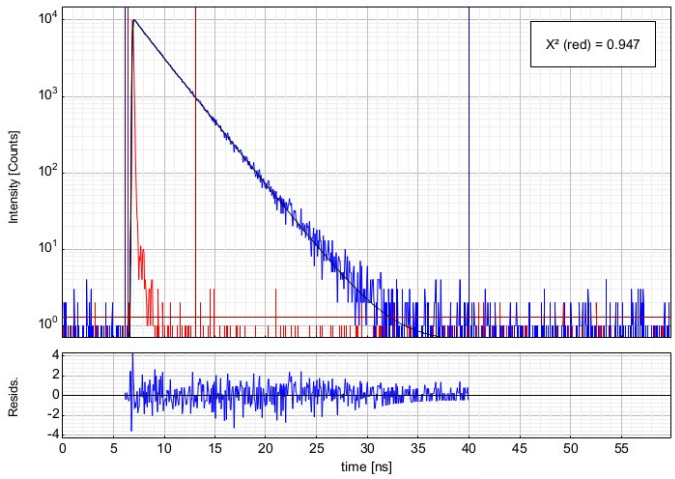


Figure S3. Photopysical dates

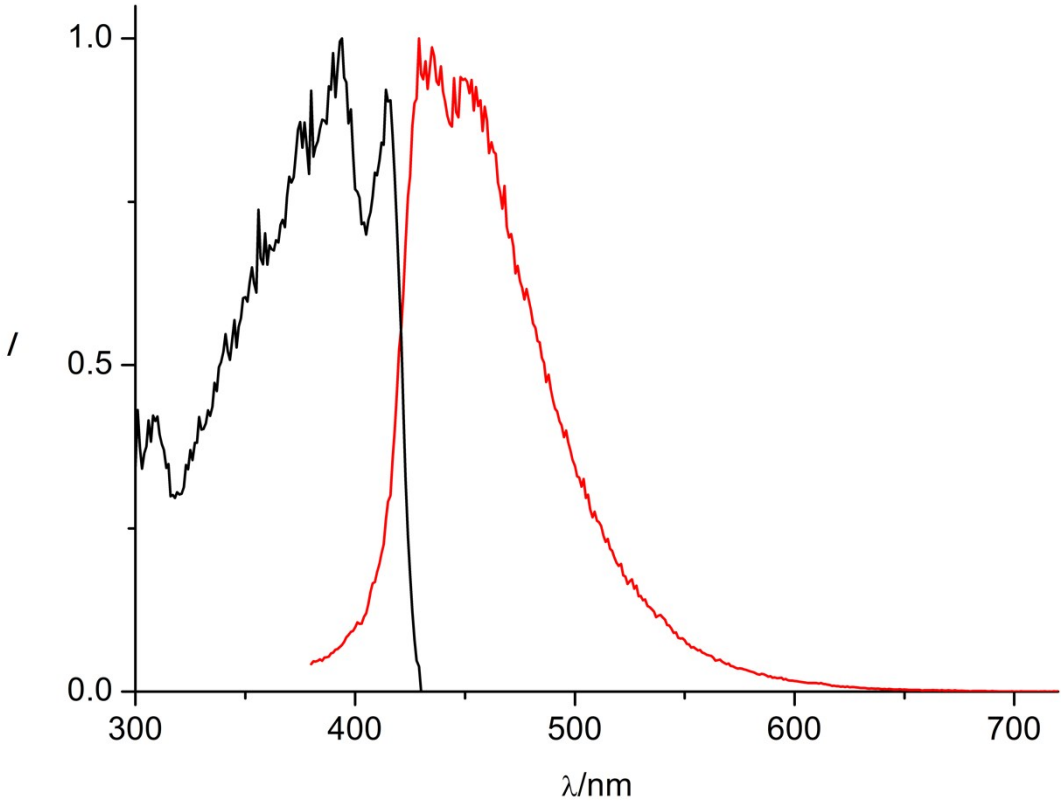


Excitation (black) and *emission* (red) spectra of **1a** in CH_2Cl_2 (λ_{exc} = 320 nm; λ_{em} = 460 nm).

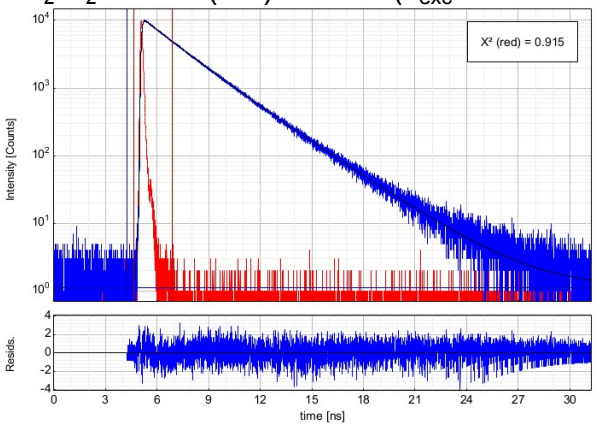


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	10438.5	-57.4	+57.4
τ_1 [ns]	2.6392	-0.0102	+0.0102
A_2 [Cnts]	1062	-147	+147
τ_2 [ns]	0.767	-0.121	+0.121
Bkgr. Dec [Cnts]	0.605	-0.377	+0.377
Bkgr. IRF [Cnts]	1.273	-0.796	+0.796
Shift IRF [ns]	0.08752	-0.00240	+0.00240

Left: Time-resolved luminescence decay of **1a** in CH_2Cl_2 including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

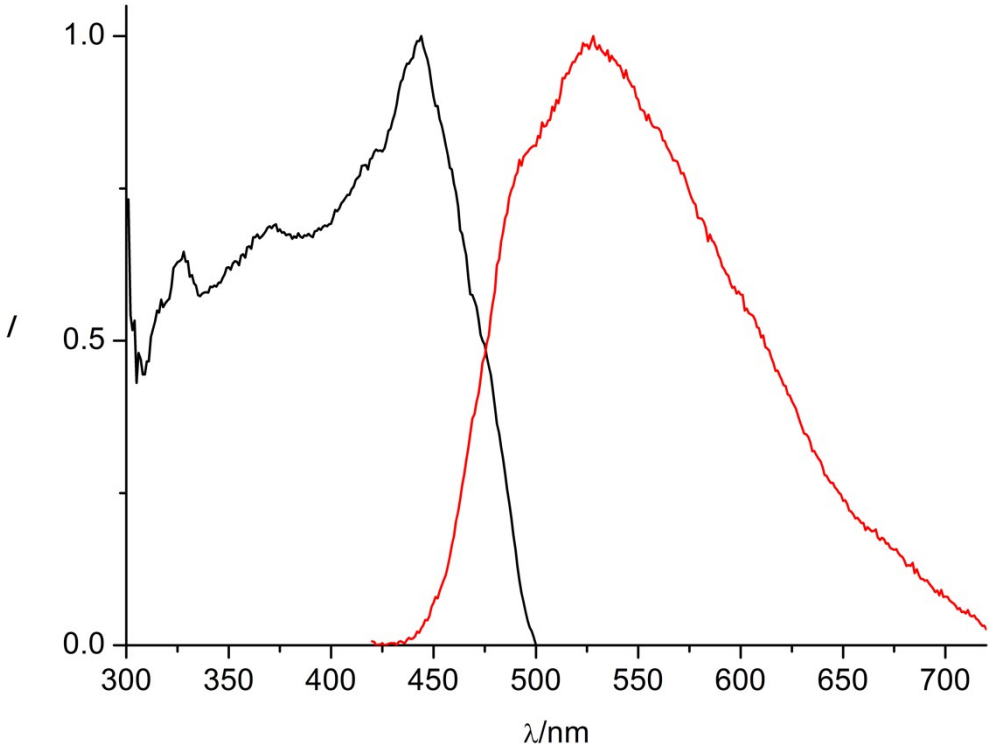


Excitation (black) and *emission* (red) spectra of **1a** in a frozen glassy matrix of *CH_2Cl_2:MeOH* (1:1) at 77 K (λ_{exc} = 320 nm; λ_{em} = 450 nm).

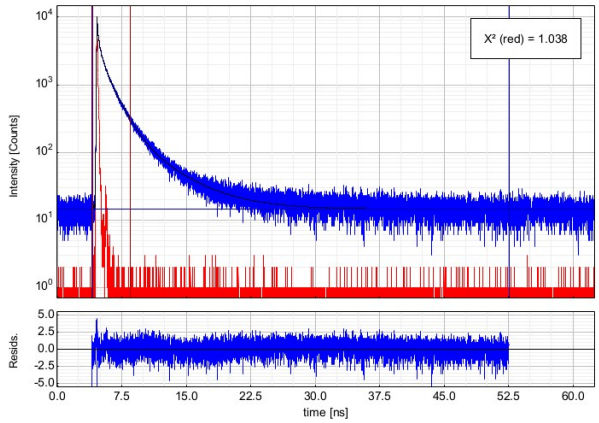


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	5921.6	-46.1	+46.1
τ_1 [ns]	2.6657	-0.0135	+0.0135
A_2 [Cnts]	5150.5	-69.0	+69.0
τ_2 [ns]	1.7417	-0.0204	+0.0204
Bkgr. $_{Dec}$ [Cnts]	1.112	-0.496	+0.496
Bkgr. $_{IRF}$ [Cnts]	-1.24	-1.97	+1.97
Shift $_{IRF}$ [ns]	0.01325	-0.00188	+0.00188

Left: Time-resolved luminescence decay of **1a** in a frozen glassy matrix *CH_2Cl_2:MeOH* (1:1) at 77K including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

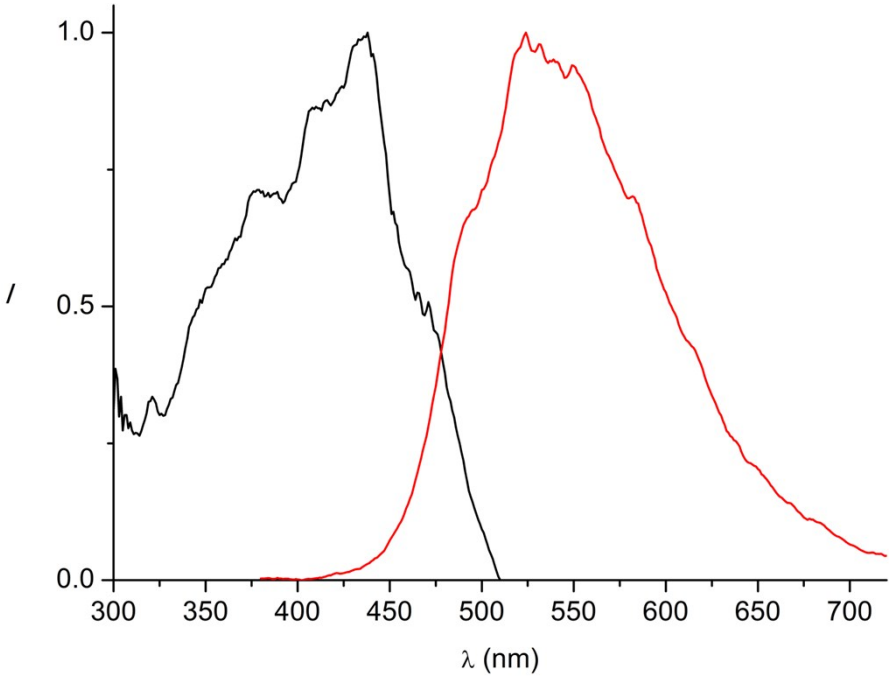


Excitation (black) and *emission* (red) spectra of **1a** in the solid state (λ_{exc} = 320 nm; λ_{em} = 530 nm).

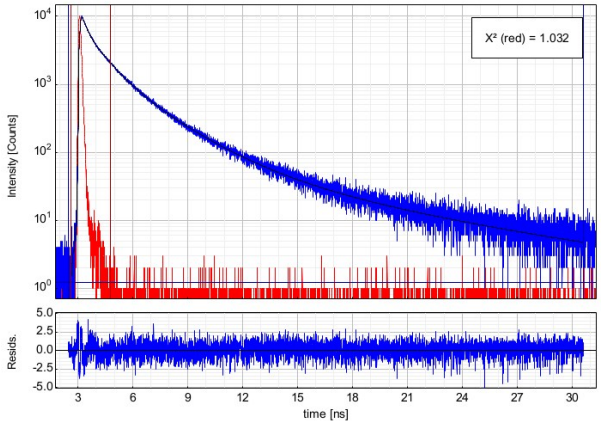


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	306.3	-16.2	+16.2
τ_1 [ns]	4.374	-0.150	+0.150
A_2 [Cnts]	2835.5	-64.2	+64.2
τ_2 [ns]	1.3601	-0.0242	+0.0242
A_3 [Cnts]	3541	-247	+247
τ_3 [ns]	0.2810	-0.0194	+0.0194
Bkgr. $_{Dec}$ [Cnts]	14.457	-0.771	+0.771
Bkgr. $_{IRF}$ [Cnts]	-0.0270	-2.75	+2.75
Shift $_{IRF}$ [ns]	-0.01671	-0.00192	+0.00192
A $_{Scat}$ [Cnts]	253800	-11400	+11400

Left: Time-resolved luminescence decay of **1a** in the solid state including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Excitation (black) and *emission* (red) spectra of **1a** in crystal (λ_{exc} = 320 nm; λ_{em} = 540 nm).



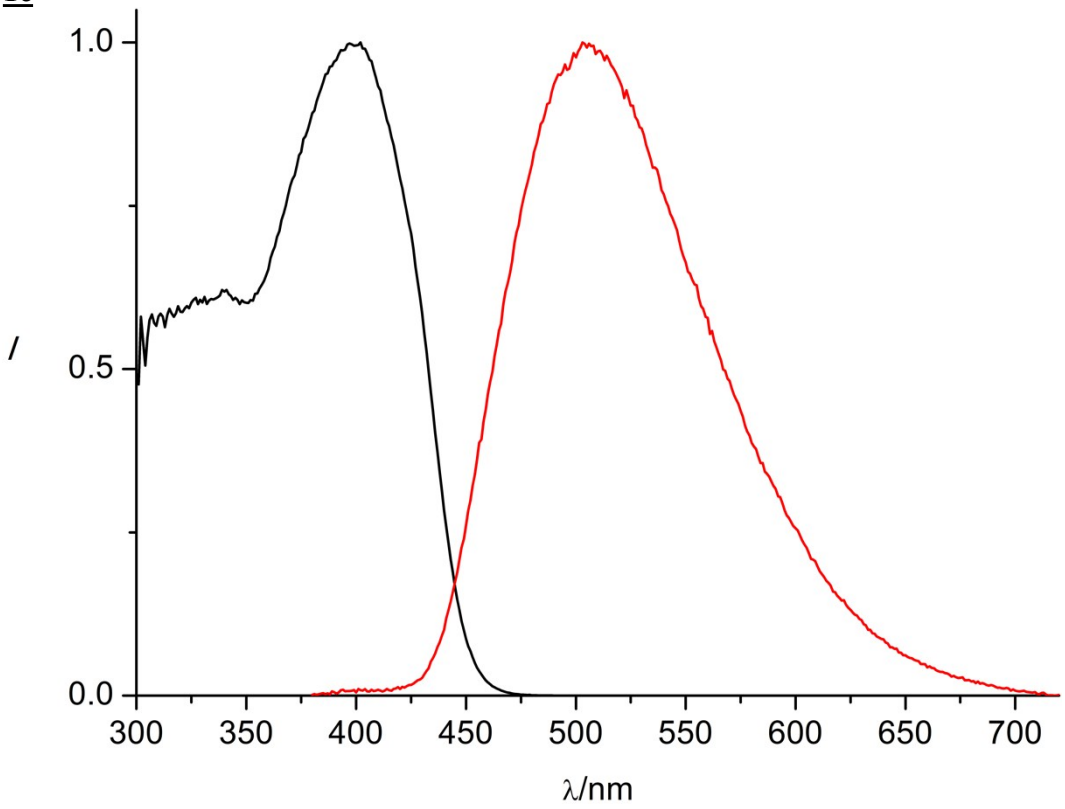
Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	115.32	-6.22	+6.22
τ_1 [ns]	7.881	-0.249	+0.249
A_2 [Cnts]	2173.4	-37.5	+37.5
τ_2 [ns]	2.3180	-0.0260	+0.0260
A_3 [Cnts]	5367.6	-93.7	+93.7
τ_3 [ns]	0.9366	-0.0144	+0.0144
A_4 [Cnts]	6564	-287	+287
τ_4 [ns]	0.2029	-0.0103	+0.0103
Bkgr. $_{Dec}$ [Cnts]	1.232	-0.704	+0.704
Bkgr. $_{IRF}$ [Cnts]	-1.60	-2.07	+2.07
Shift $_{IRF}$ [ns]	0.08974	-0.00182	+0.00182

Left: Time-resolved luminescence decay of **1a** in crystal including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

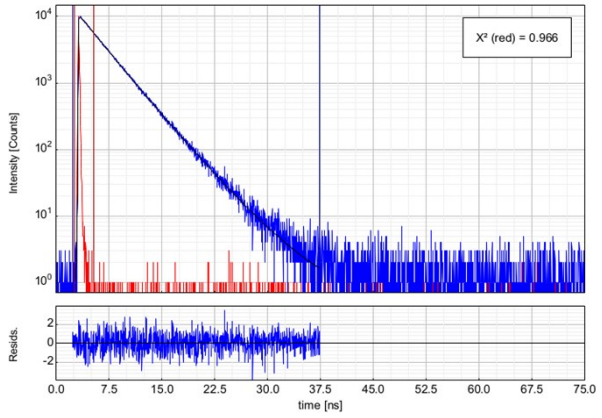
	λ_{Exc} (nm)	λ_{Em} (nm)	τ (ns)	Φ (λ_{exc}=320nm)
aerated	374	442	2,586	0,55
77K	394	429	2,331	
solid	444	528	1,839	0,05
crystal	438	524	1,936	0,10

Summary of photophysical data for **1a**. Intesity-weighted average lifetimes.

1c

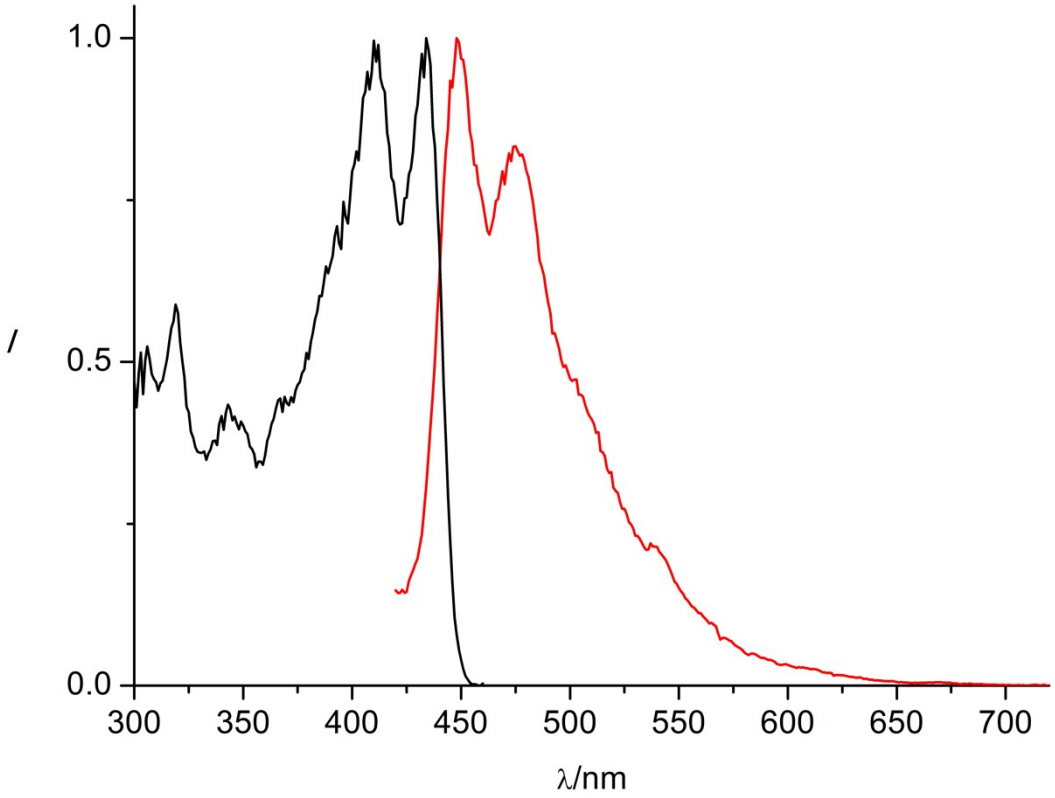


Excitation (black) and *emission* (red) spectra of **1c** in CH_2Cl_2 (λ_{exc} = 320 nm; λ_{em} = 510 nm).

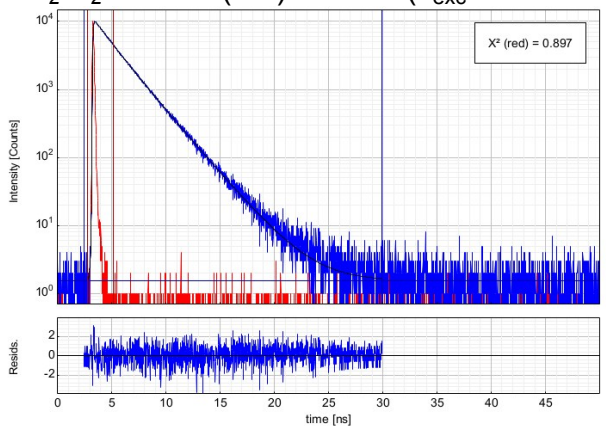


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	1072.0	-34.6	+34.6
τ_1 [ns]	4.7939	-0.0817	+0.0817
A_2 [Cnts]	9795.6	-55.0	+55.0
τ_2 [ns]	3.2113	-0.0136	+0.0136
Bkgr. $_{Dec}$ [Cnts]	0.550	-0.589	+0.589
Bkgr. $_{IRF}$ [Cnts]	-0.63	-1.43	+1.43
Shift $_{IRF}$ [ns]	0.15753	-0.00170	+0.00170

Left: Time-resolved luminescence decay of **1C** in CH_2Cl_2 including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

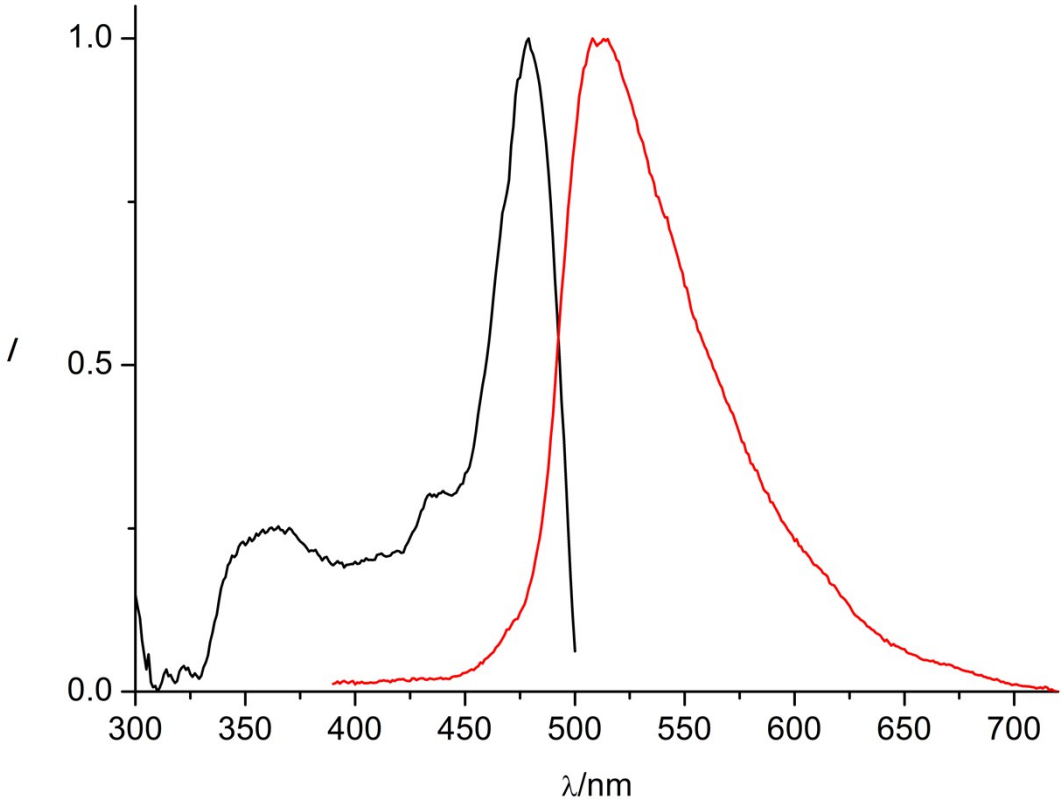


Excitation (black) and *emission* (red) spectra of **1C** in a frozen glassy matrix of CH_2Cl_2:*MeOH* (1:1) at 77 K (λ_{exc} = 320 nm; λ_{em} = 480 nm).

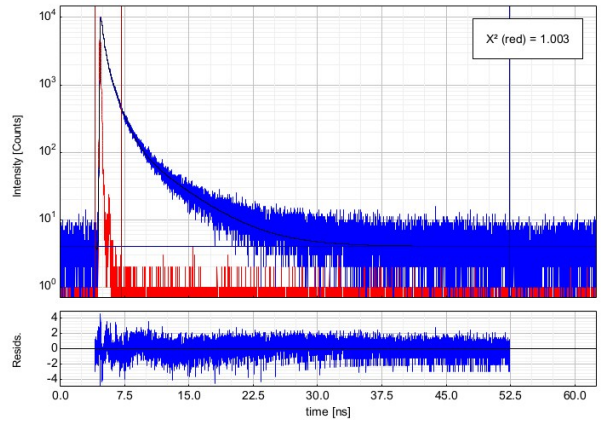


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	7838.3	-50.7	+50.7
τ_1 [ns]	2.3908	-0.0104	+0.0104
A_2 [Cnts]	3478.8	-79.3	+79.3
τ_2 [ns]	1.4512	-0.0308	+0.0308
Bkgr. $_{Dec}$ [Cnts]	1.542	-0.457	+0.457
Bkgr. $_{IRF}$ [Cnts]	-0.210	-1.54	+1.54
Shift $_{IRF}$ [ns]	0.06760	-0.00190	+0.00190

Left: Time-resolved luminescence decay of **1C** in a frozen glassy matrix CH_2Cl_2:*MeOH* (1:1) at 77K including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

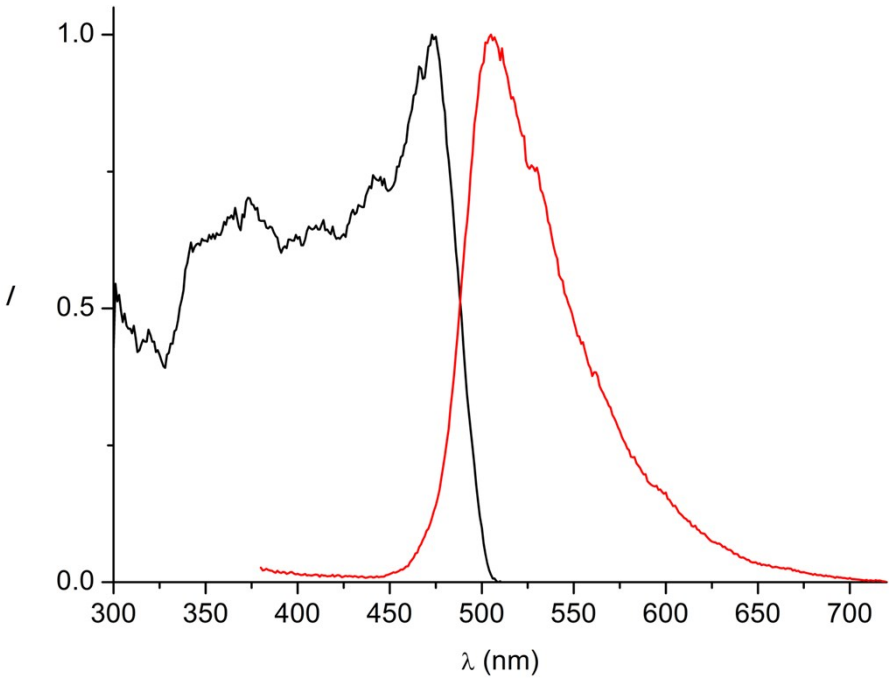


Excitation (black) and *emission* (red) spectra of **1C** in the solid state (λ_{exc} = 320 nm; λ_{em} = 530 nm).

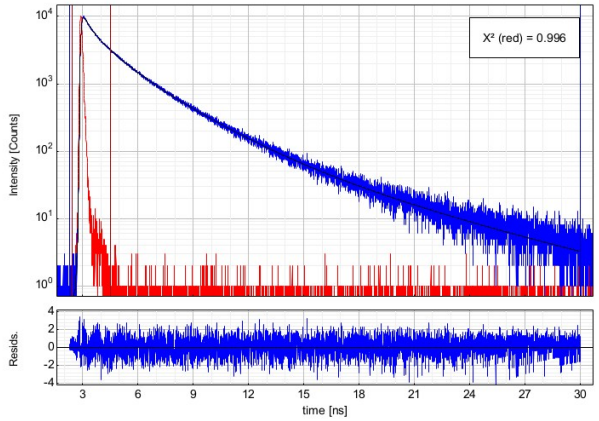


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	242.0	-12.9	+12.9
τ_1 [ns]	4.321	-0.138	+0.138
A_2 [Cnts]	3804.3	-89.7	+89.7
τ_2 [ns]	0.9950	-0.0169	+0.0169
A_3 [Cnts]	10801	-310	+310
τ_3 [ns]	0.25353	-0.00733	+0.00733
Bkgr. $_{Dec}$ [Cnts]	4.025	-0.464	+0.464
Bkgr. $_{IRF}$ [Cnts]	0.427	-2.37	+2.37
Shift $_{IRF}$ [ns]	0.02348	-0.00226	+0.00226
A $_{Scat}$ [Cnts]	7610	-8120	+8120

Left: Time-resolved luminescence decay of **1C** in the solid state including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Excitation (black) and *emission* (red) spectra of **1C** in crystal (λ_{exc} = 320 nm; λ_{em} = 540 nm).

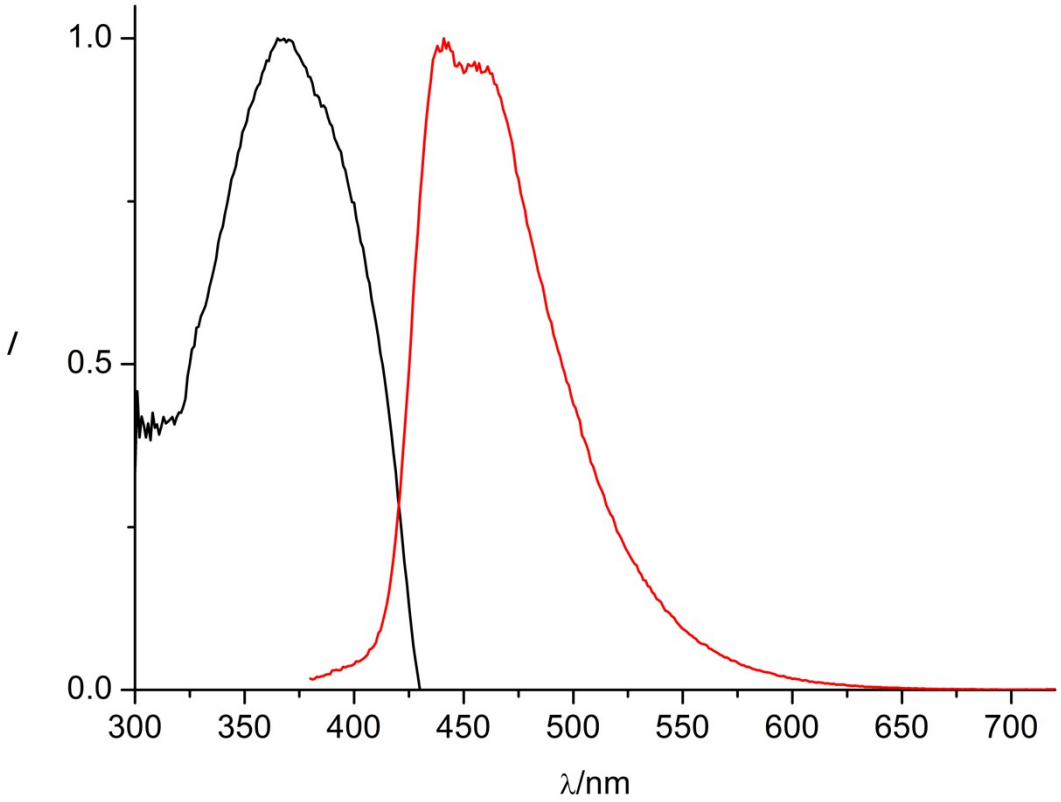


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	312.1	-12.6	+12.6
τ_1 [ns]	5.759	-0.118	+0.118
A_2 [Cnts]	3844.9	-43.3	+43.3
τ_2 [ns]	2.4108	-0.0188	+0.0188
A_3 [Cnts]	4519.5	-95.1	+95.1
τ_3 [ns]	1.0167	-0.0205	+0.0205
A_4 [Cnts]	4093	-234	+234
τ_4 [ns]	0.2716	-0.0186	+0.0186
Bkgr. Dec [Cnts]	0.391	-0.673	+0.673
Bkgr. IRF [Cnts]	-0.262	-1.58	+1.58
Shift IRF [ns]	-0.10763	-0.00185	+0.00185

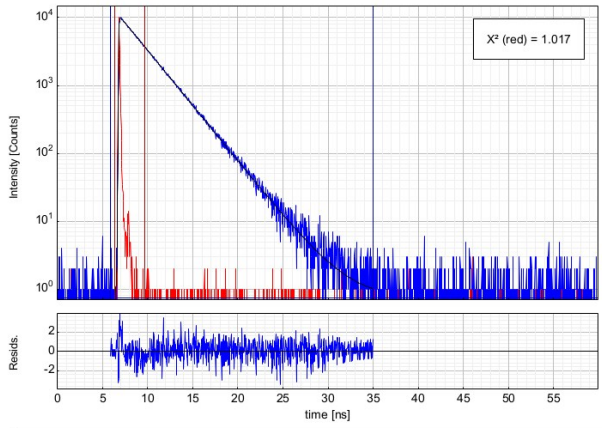
Left: Time-resolved luminescence decay of **1C** in crystal including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

	λ_{Exc} (nm)	λ_{Em} (nm)	τ (ns)	Φ (λ_{exc}=320nm)
aerated	402	503	3,434	0,65
77K	434	448	2,191	
solid	479	508	1,186	0,03
crystal	473	505	2,246	0,16

Summary of photophysical data for **1C**. Intensity-weighted average lifetimes.

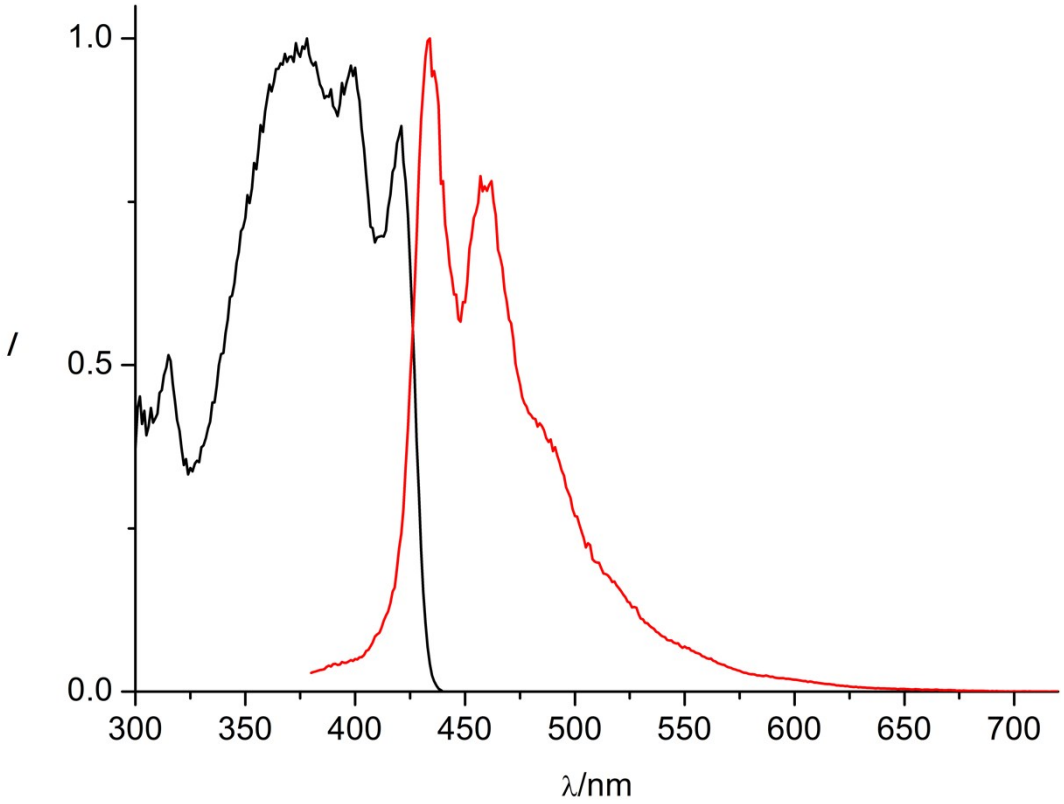


Excitation (black) and *emission* (red) spectra of **1E** in CH_2Cl_2 (λ_{exc} = 320 nm; λ_{em} = 460 nm).

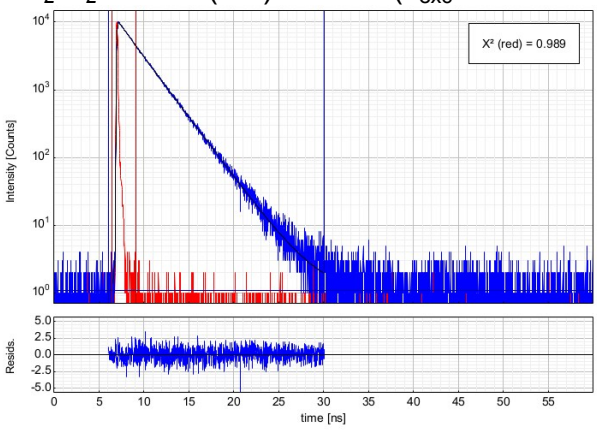


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	10897.6	-55.3	+55.3
τ_1 [ns]	2.66501	-0.00967	+0.00967
Bkgr. $_{Dec}$ [Cnts]	0.733	-0.495	+0.495
Bkgr. $_{IRF}$ [Cnts]	-0.097	-1.10	+1.10
Shift $_{IRF}$ [ns]	0.19817	-0.00225	+0.00225

Left: Time-resolved luminescence decay of **1E** in CH_2Cl_2 including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

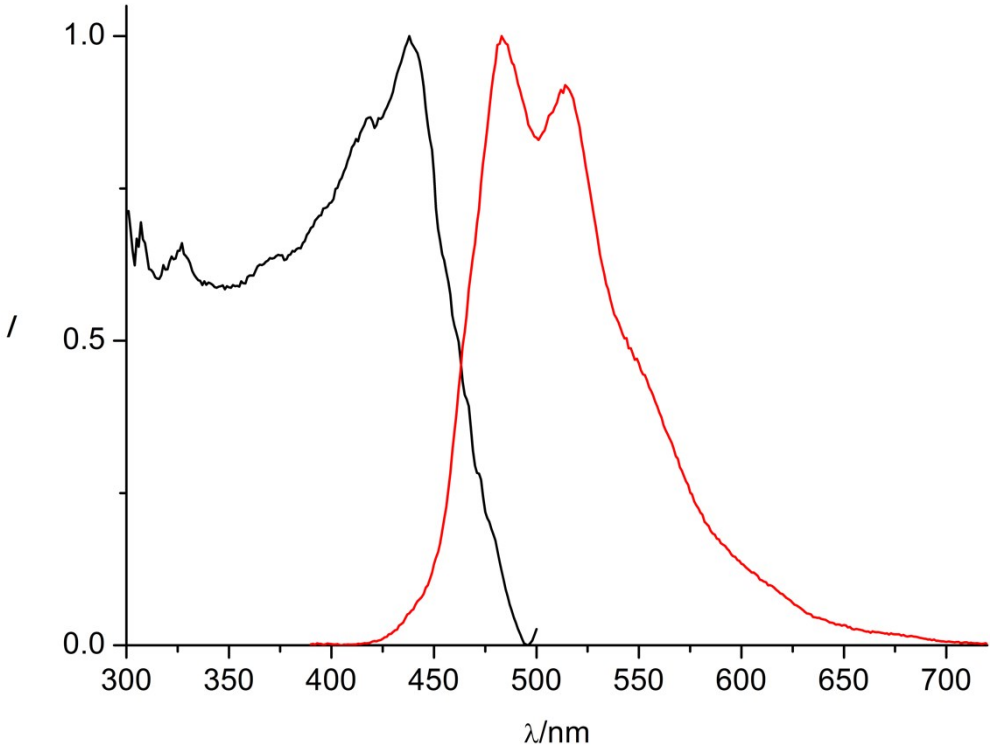


Excitation (black) and *emission* (red) spectra of **1E** in a frozen glassy matrix of *CH_2Cl_2:MeOH* (1:1) at 77 K (λ_{exc} = 320 nm; λ_{em} = 460 nm).

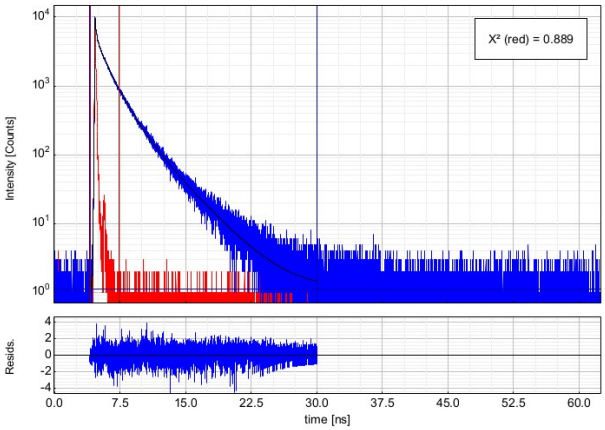


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	10195.9	-50.8	+50.8
τ_1 [ns]	2.45840	-0.00863	+0.00863
A_2 [Cnts]	1004	-104	+104
τ_2 [ns]	0.979	-0.112	+0.112
Bkgr. $_{Dec}$ [Cnts]	1.090	-0.602	+0.602
Bkgr. $_{IRF}$ [Cnts]	-0.316	-1.17	+1.17
Shift $_{IRF}$ [ns]	0.36416	-0.00169	+0.00169

Left: Time-resolved luminescence decay of **1E** in a frozen glassy matrix *CH_2Cl_2:MeOH* (1:1) at 77K including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

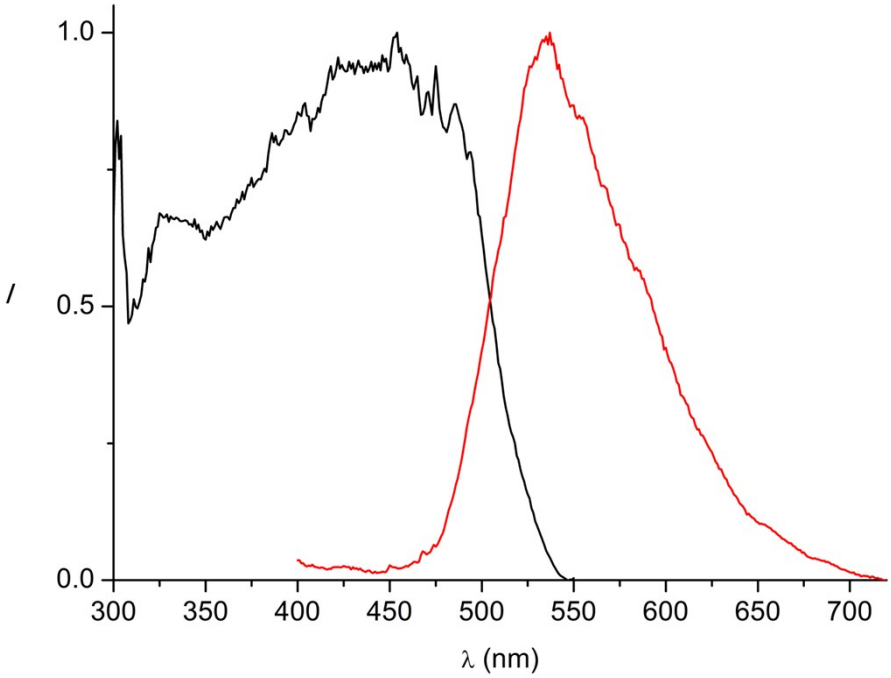


Excitation (black) and *emission* (red) spectra of **1E** in the solid state (λ_{exc} = 320 nm; λ_{em} = 520 nm).

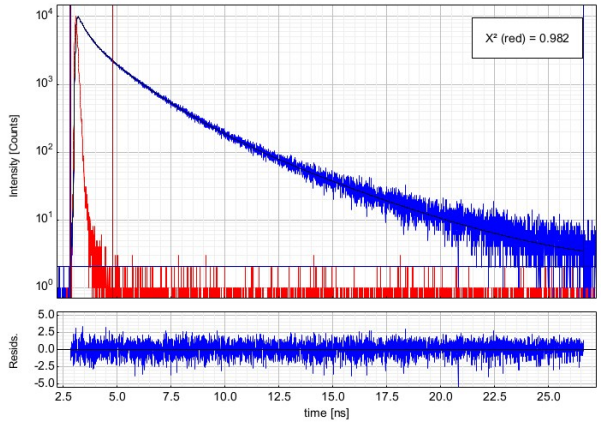


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	3646.6	-51.1	+51.1
τ_1 [ns]	1.3768	-0.0158	+0.0158
A_2 [Cnts]	2022	-158	+158
τ_2 [ns]	0.3327	-0.0272	+0.0272
A_3 [Cnts]	281500	-5590	+5590
τ_3 [ns]	0.007317	-0.000115	+0.000115
A_4 [Cnts]	921.1	-19.6	+19.6
τ_4 [ns]	3.1936	-0.0390	+0.0390
Bkgr. $_{Dec}$ [Cnts]	1.122	-0.446	+0.446
Bkgr. $_{IRF}$ [Cnts]	0.186	-1.22	+1.22
Shift $_{IRF}$ [ns]	-0.04343	-0.00140	+0.00140
A $_{Scat}$ [Cnts]	-145110	-7400	+7400

Left: Time-resolved luminescence decay of **1E** in the solid state including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Excitation (black) and *emission* (red) spectra of **1E** in crystal (λ_{exc} = 320 nm; λ_{em} = 540 nm).

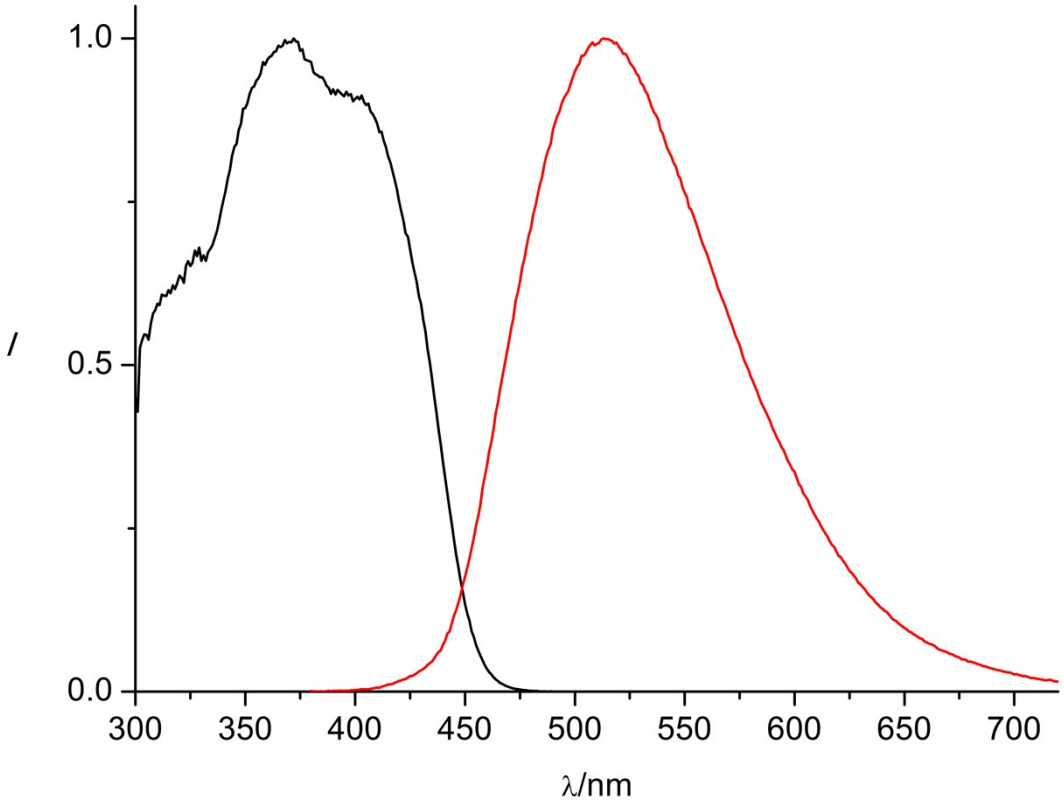


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	838.6	-19.0	+19.0
τ_1 [ns]	3.6709	-0.0457	+0.0457
A_2 [Cnts]	4489.2	-54.0	+54.0
τ_2 [ns]	1.5686	-0.0146	+0.0146
A_3 [Cnts]	5457	-150	+150
τ_3 [ns]	0.4530	-0.0130	+0.0130
A_4 [Cnts]	7740	-618	+618
τ_4 [ns]	0.06014	-0.00561	+0.00561
Bkgr. Dec [Cnts]	2.066	-0.679	+0.679
Bkgr. IRF [Cnts]	-2.46	-3.80	+3.80
Shift IRF [ns]	-0.00667	-0.00160	+0.00160

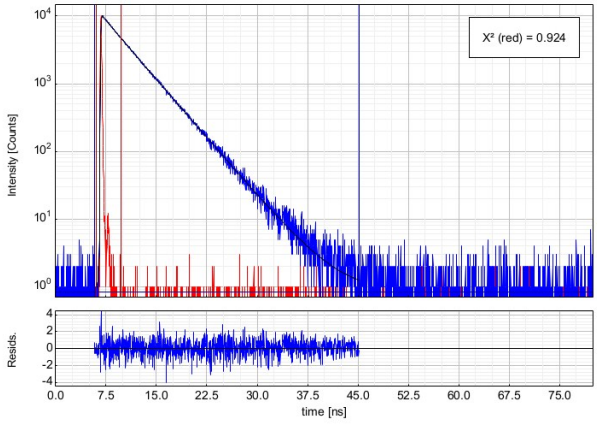
Left: Time-resolved luminescence decay of **1E** in crystal including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

	λ_{Exc} (nm)	λ_{Em} (nm)	τ (ns)	Φ (λ_{exc}=320nm)
aerated	365	441	2,665	0,54
77K	378	434	2,403	
solid	438	483	1,547	0,11
crystal	454	537	1,799	0,13

Summary of photophysical data for **1E**. Intensity-weighted average lifetimes.

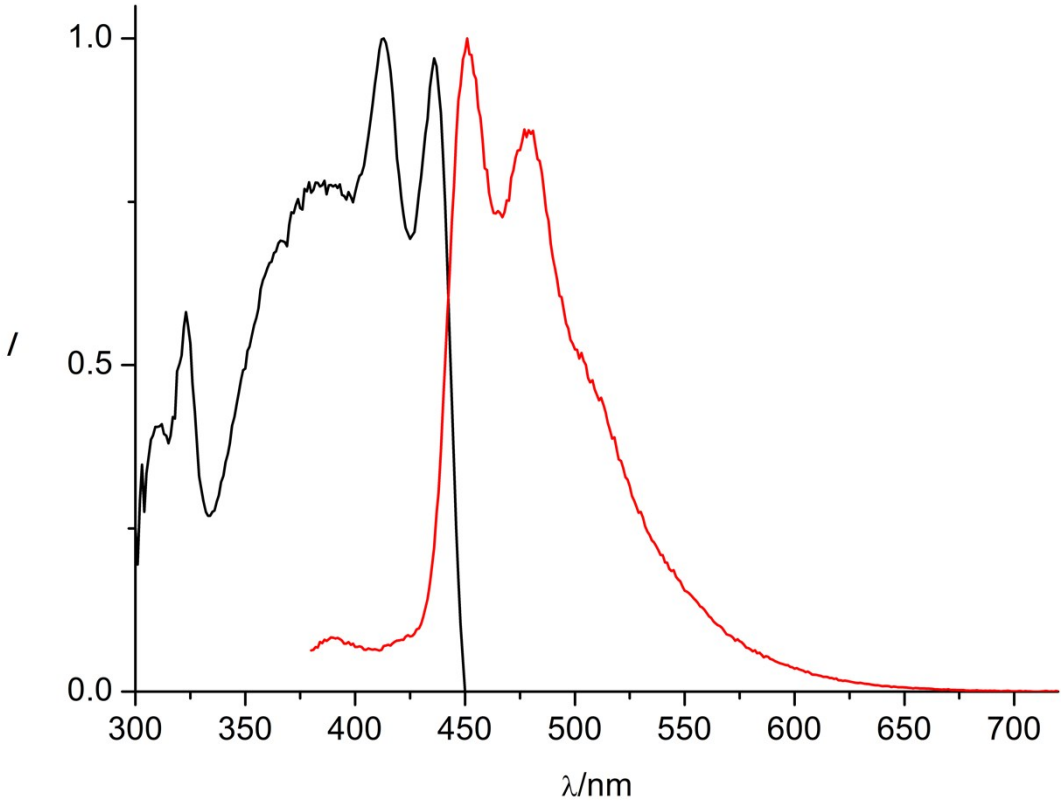


Excitation (black) and *emission* (red) spectra of **1F** in CH_2Cl_2 (λ_{exc} = 370 nm; λ_{em} = 510 nm).

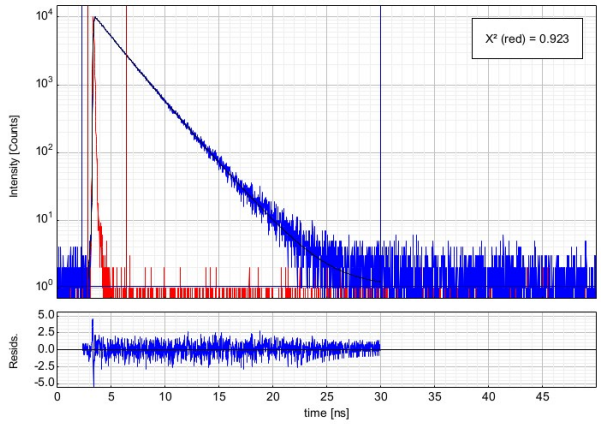


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	10249.6	-50.4	+50.4
τ_1 [ns]	3.7965	-0.0132	+0.0132
A_2 [Cnts]	718	-105	+105
τ_2 [ns]	1.471	-0.240	+0.240
Bkgr. $_{Dec}$ [Cnts]	0.833	-0.508	+0.508
Bkgr. $_{IRF}$ [Cnts]	-0.278	-0.968	+0.968
Shift $_{IRF}$ [ns]	0.16692	-0.00246	+0.00246

Left: Time-resolved luminescence decay of **1F** in CH_2Cl_2 including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

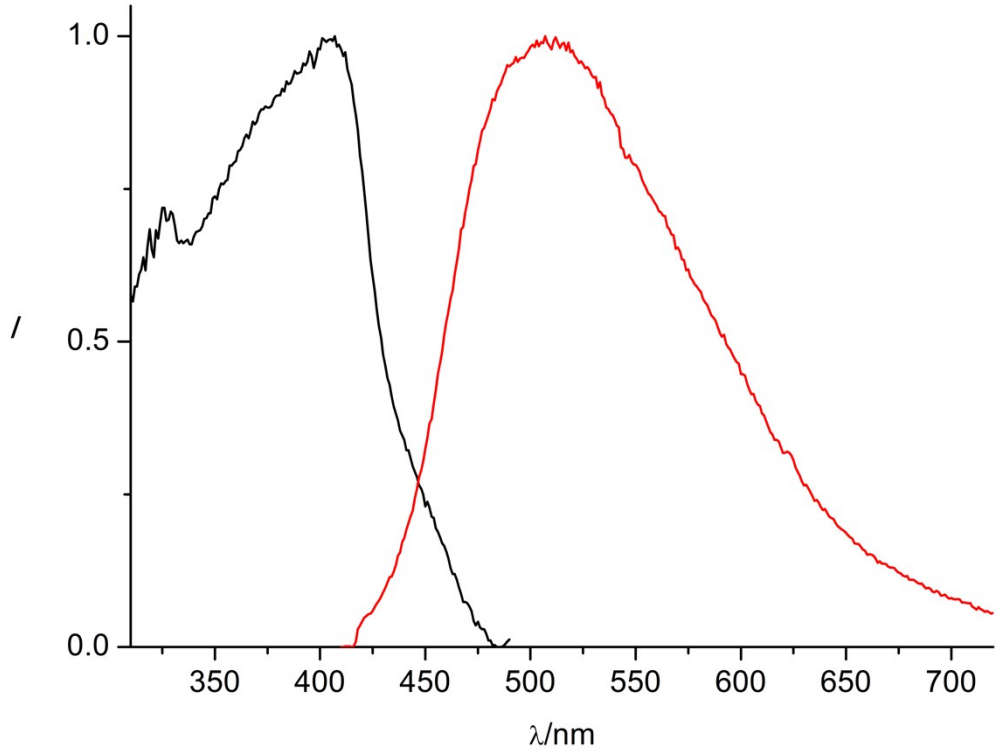


Excitation (black) and *emission* (red) spectra of **1F** in a frozen glassy matrix of *CH_2Cl_2:MeOH* (1:1) at 77 K (λ_{exc} = 320 nm; λ_{em} = 480 nm).

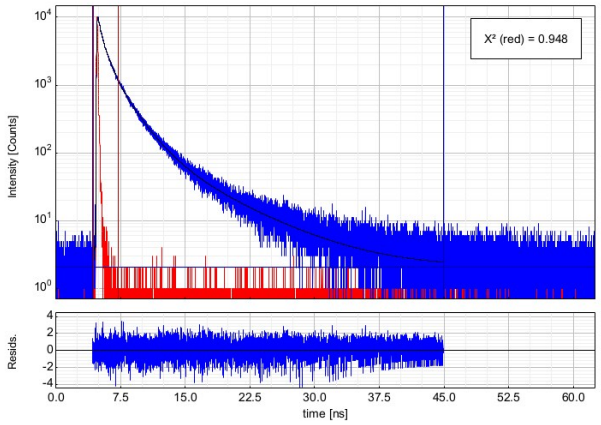


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	6408.4	-49.4	+49.4
τ_1 [ns]	2.5186	-0.0128	+0.0128
A_2 [Cnts]	4666.3	-68.6	+68.6
τ_2 [ns]	1.7852	-0.0224	+0.0224
Bkgr. $_{Dec}$ [Cnts]	1.063	-0.451	+0.451
Bkgr. $_{IRF}$ [Cnts]	-1.66	-1.25	+1.25
Shift $_{IRF}$ [ns]	0.11495	-0.00200	+0.00200

Left: Time-resolved luminescence decay of **1F** in a frozen glassy matrix *CH_2Cl_2:MeOH* (1:1) at 77K including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

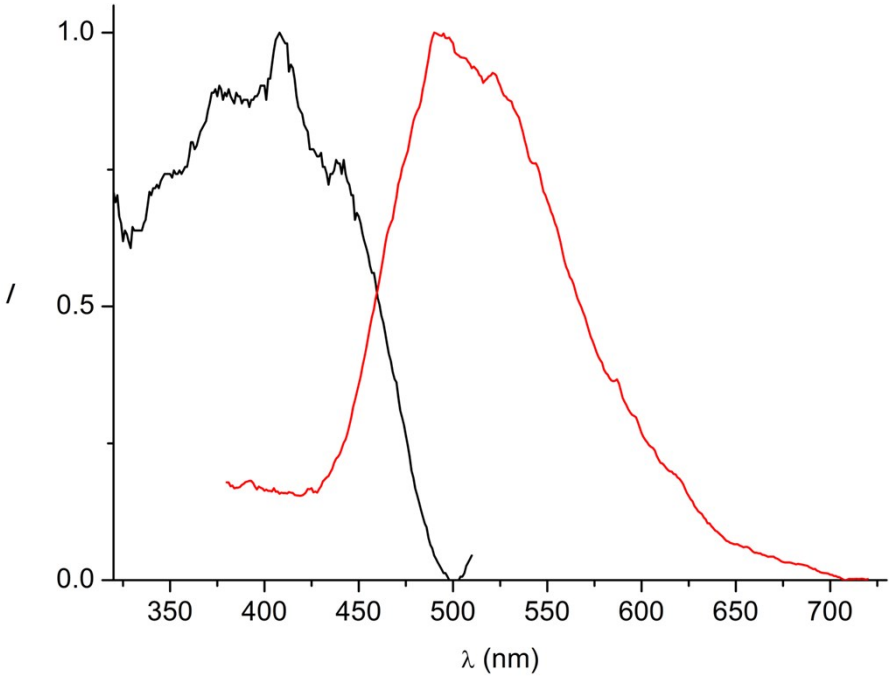


Excitation (black) and *emission* (red) spectra of **1F** in the solid state (λ_{exc} = 370 nm; λ_{em} = 510 nm).

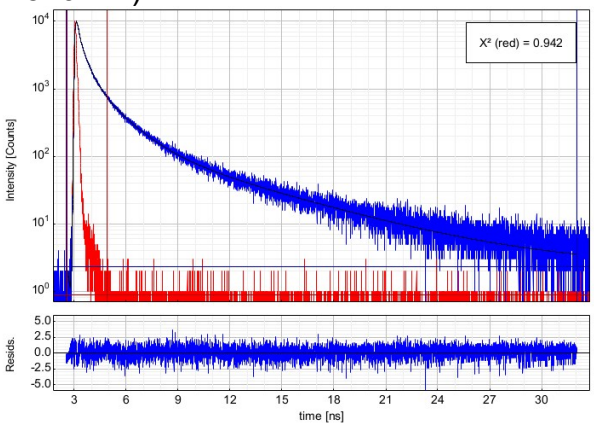


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	2648.3	-49.1	+49.1
τ_1 [ns]	2.0530	-0.0259	+0.0259
A_2 [Cnts]	5573	-130	+130
τ_2 [ns]	0.7464	-0.0160	+0.0160
A_3 [Cnts]	4891	-347	+347
τ_3 [ns]	0.1992	-0.0158	+0.0158
A_4 [Cnts]	208.9	-10.0	+10.0
τ_4 [ns]	6.408	-0.166	+0.166
Bkgr. $_{Dec}$ [Cnts]	2.038	-0.485	+0.485
Bkgr. $_{IRF}$ [Cnts]	-0.444	-2.34	+2.34
Shift $_{IRF}$ [ns]	0.00884	-0.00198	+0.00198
A $_{Scat}$ [Cnts]	75870	-8510	+8510

Left: Time-resolved luminescence decay of **1F** in the solid state including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Excitation (black) and *emission* (red) spectra of **1F** in crystal (λ_{exc} = 320 nm; λ_{em} = 540 nm).

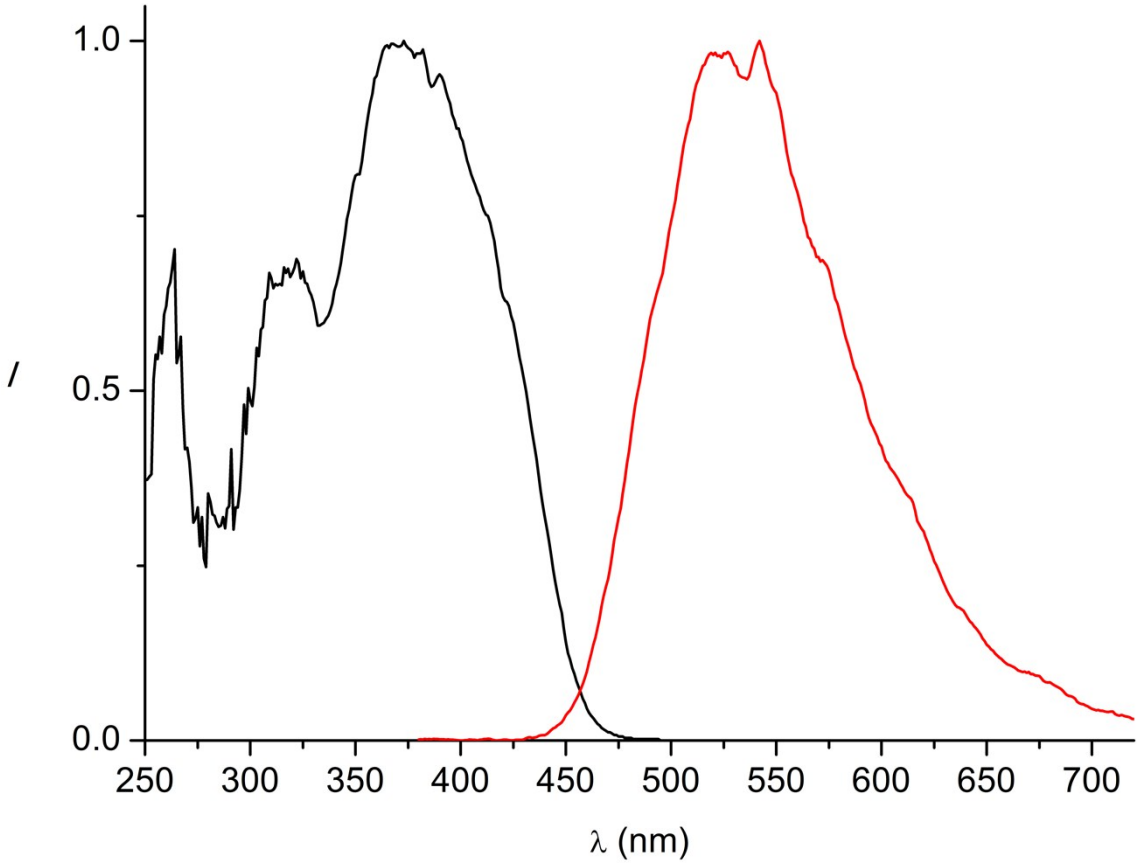


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	1891.7	-44.8	+44.8
τ_1 [ns]	1.4130	-0.0238	+0.0238
A_2 [Cnts]	6388	-152	+152
τ_2 [ns]	0.41177	-0.00877	+0.00877
A_3 [Cnts]	213.98	-7.66	+7.66
τ_3 [ns]	5.644	-0.123	+0.123
A_4 [Cnts]	12222	-552	+552
τ_4 [ns]	0.07898	-0.00397	+0.00397
Bkgr. Dec [Cnts]	2.291	-0.578	+0.578
Bkgr. IRF [Cnts]	0.87	-1.70	+1.70
Shift IRF [ns]	0.03433	-0.00160	+0.00160

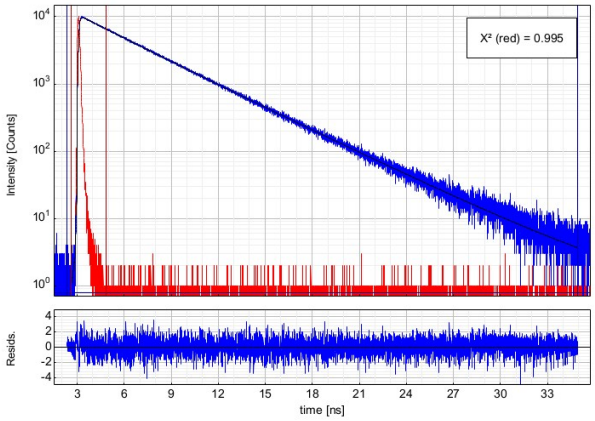
Left: Time-resolved luminescence decay of **1F** in crystal including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

	λ_{Exc} (nm)	λ_{Em} (nm)	τ (ns)	Φ (λ_{exc}=320nm)
aerated	372	513	3,735	0,57
77K	413	451	2,269	
solid	407	507	1,935	0,05
crystal	408	490	1,572	0,05

Summary of photophysical data for **1F**. Amplitude-weighted average lifetimes.

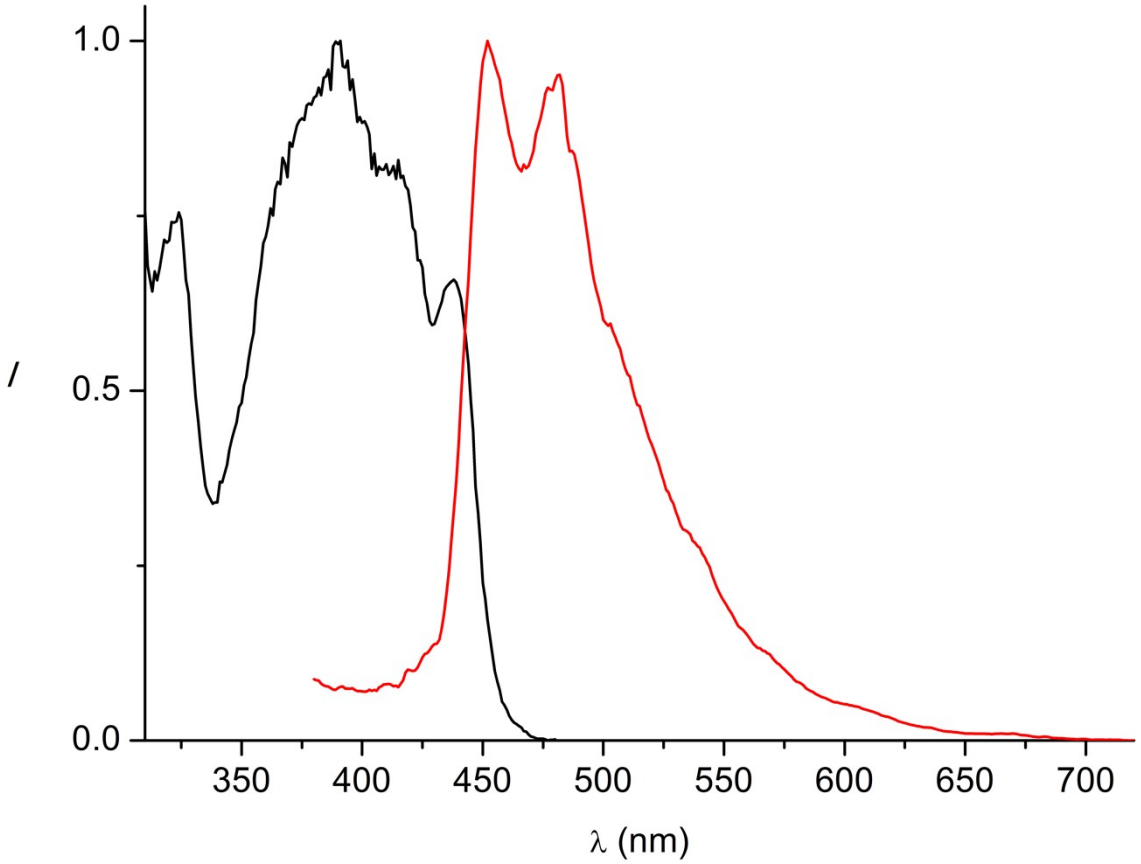


Excitation (black) and *emission* (red) spectra of **1g** in CH_2Cl_2 (λ_{exc} = 320 nm; λ_{em} = 540 nm).

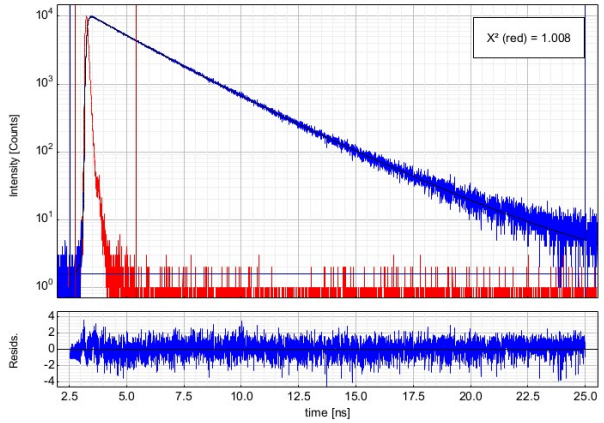


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	6141.1	-43.5	+43.5
τ_1 [ns]	4.1146	-0.0199	+0.0199
A_2 [Cnts]	4443.8	-55.4	+55.4
τ_2 [ns]	3.2004	-0.0325	+0.0325
Bkgr. $_{Dec}$ [Cnts]	0.796	-0.815	+0.815
Bkgr. $_{IRF}$ [Cnts]	-0.459	-1.69	+1.69
Shift $_{IRF}$ [ns]	-0.05648	-0.00208	+0.00208

Left: Time-resolved luminescence decay of **1g** in CH_2Cl_2 including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

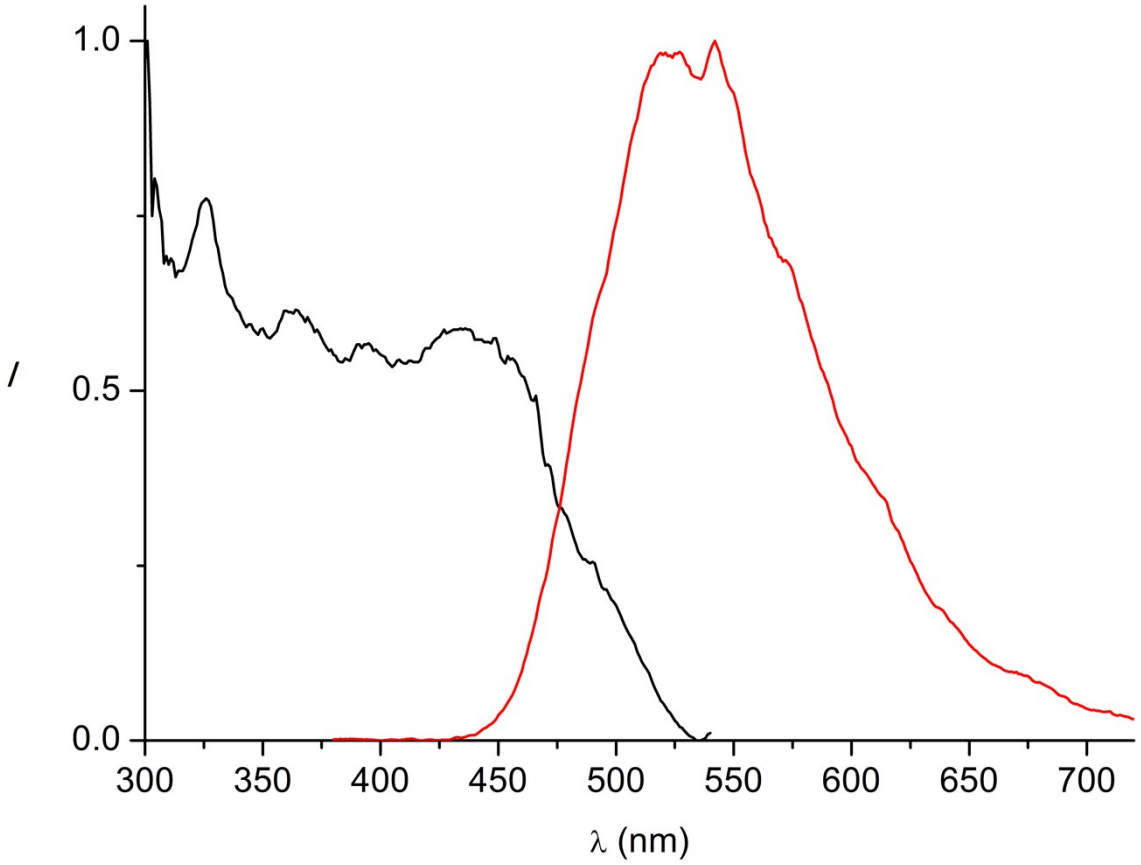


Excitation (black) and *emission* (red) spectra of **1g** in a frozen glassy matrix of *CH_2Cl_2:MeOH* (1:1) at 77 K (λ_{exc} = 320 nm; λ_{em} = 520 nm).

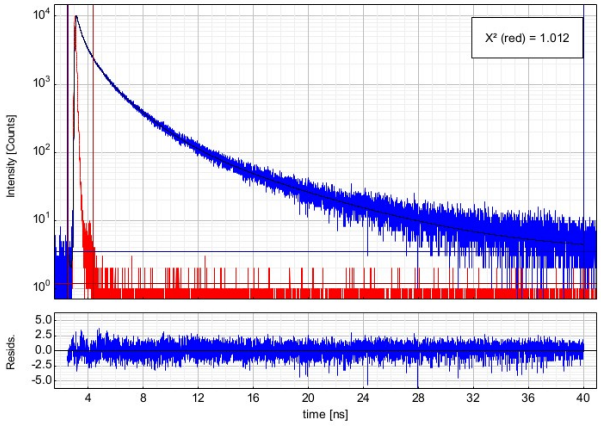


Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	2853.0	-37.0	+37.0
τ_1 [ns]	3.1976	-0.0242	+0.0242
A_2 [Cnts]	8228.7	-58.1	+58.1
τ_2 [ns]	2.0793	-0.0119	+0.0119
Bkgr. $_{Dec}$ [Cnts]	1.578	-0.843	+0.843
Bkgr. $_{IRF}$ [Cnts]	-0.195	-0.786	+0.786
Shift $_{IRF}$ [ns]	0.03155	-0.00170	+0.00170

Left: Time-resolved luminescence decay of **1g** in a frozen glassy matrix *CH_2Cl_2:MeOH* (1:1) at 77K including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.



Excitation (black) and *emission* (red) spectra of **1g** in the solid state (λ_{exc} = 320 nm; λ_{em} = 570 nm).



Parameter	Value	Conf. Lower	Conf. Upper
A_1 [Cnts]	304.2	-11.0	+11.0
τ_1 [ns]	6.455	-0.139	+0.139
A_2 [Cnts]	2670.9	-49.1	+49.1
τ_2 [ns]	2.0342	-0.0271	+0.0271
A_3 [Cnts]	5702	-142	+142
τ_3 [ns]	0.6434	-0.0152	+0.0152
A_4 [Cnts]	7740	-456	+456
τ_4 [ns]	0.12783	-0.00876	+0.00876
Bkgr. Dec [Cnts]	3.449	-0.642	+0.642
Bkgr. IRF [Cnts]	1.17	-1.85	+1.85
Shift IRF [ns]	0.03486	-0.00195	+0.00195

Left: Time-resolved luminescence decay of **1g** in the solid state including the instrument response function and the residuals (λ_{exc} = 376.7 nm). Right: Fitting parameters including pre-exponential factors and confidence limits.

	λ_{Exc} (nm)	λ_{Em} (nm)	τ (ns)	Φ (λ_{exc}=320nm)

aerated	373	542	3,785	0,82
77K	391	452	2,468	
solid	301	542	2,175	0,01

Summary of photophysical data for **1g**. Amplitude-weighted average lifetimes.

Figure S4. Expansion of a collection of ^{1}H NMR spectra for compound **1a** in $CDCl_3$ at 298K. There is not any chemical shift variation in any type of proton when concentration increases.

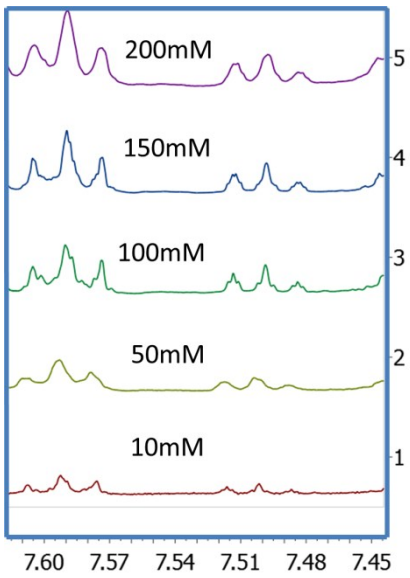


Figure S5. SEM Images

Figure S5a. SEM images of supramolecular structures formed by the self-assembly of benzotriazol **1a**. The samples were prepared by slow diffusion of hexane vapor into dilute chloroform solutions of **1a.**

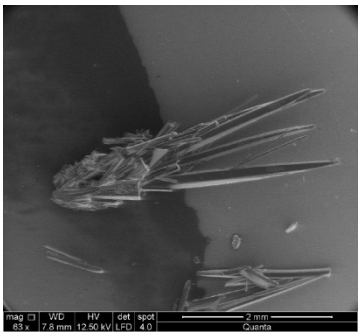


Figure S5b. SEM images of supramolecular structures formed by the self-assembly of benzotriazol **1e**. The samples were prepared by slow diffusion of hexane vapor into dilute tetrahydrofurane solutions of **1e.**

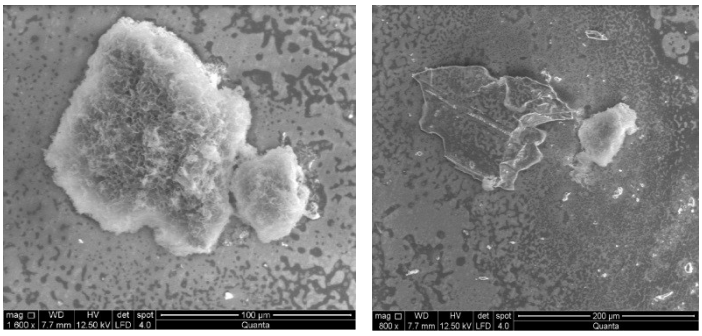
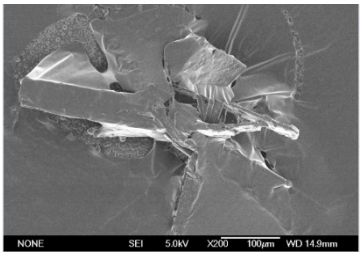


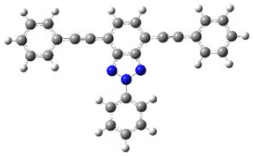
Figure S5c. SEM images of supramolecular structures formed by the self-assembly of benzotriazol **1g**. The samples were prepared by slow diffusion of methanol vapor into dilute chloroform solutions of **1g.**



Theoretical dates

Z-Matrix of the different compounds 1a, 1c, 1e, 1f and 1g.

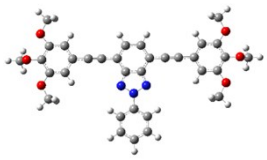
1a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.712430	-0.250136	-0.000037
2	6	0	0.712435	-0.250105	-0.000051
3	6	0	1.464184	-1.464713	-0.000068
4	6	0	0.705875	-2.636946	-0.000108
5	6	0	-0.705770	-2.636976	-0.000096
6	6	0	-1.464128	-1.464776	-0.000046
7	7	0	1.138403	1.025920	-0.000037
8	7	0	-1.138449	1.025871	-0.000028
9	7	0	-0.000038	1.721838	-0.000026
10	6	0	-0.000066	3.147356	-0.000009
11	6	0	-1.217851	3.833414	0.000129
12	6	0	1.217695	3.833461	-0.000141
13	6	0	-1.207740	5.226585	0.000131
14	1	0	-2.145109	3.273878	0.000223
15	6	0	1.207531	5.226631	-0.000128
16	1	0	2.144974	3.273960	-0.000249

17	6	0	-0.000118	5.928079	0.000007
18	1	0	-2.151442	5.764563	0.000234
19	1	0	2.151212	5.764646	-0.000231
20	6	0	-2.879045	-1.471733	-0.000029
21	6	0	-4.096348	-1.477294	-0.000015
22	6	0	2.879103	-1.471609	-0.000054
23	6	0	4.096406	-1.477143	-0.000039
24	6	0	-5.519139	-1.471663	0.000014
25	6	0	-6.227896	-0.252529	0.000023
26	6	0	-6.243690	-2.681191	0.000031
27	6	0	-7.619568	-0.249043	0.000049
28	1	0	-5.672029	0.679879	0.000010
29	6	0	-7.635402	-2.667045	0.000054
30	1	0	-5.701817	-3.621961	0.000022
31	6	0	-8.328207	-1.453531	0.000065
32	1	0	-8.154408	0.696900	0.000056
33	1	0	-8.182268	-3.606072	0.000064
34	6	0	5.519200	-1.471555	0.000010
35	6	0	6.227993	-0.252444	0.000054
36	6	0	6.243718	-2.681106	0.000026
37	6	0	7.619668	-0.248998	0.000100
38	1	0	5.672157	0.679983	0.000049
39	6	0	7.635428	-2.667001	0.000069
40	1	0	5.701815	-3.621860	-0.000001
41	6	0	8.328270	-1.453505	0.000106
42	1	0	8.154531	0.696931	0.000131
43	1	0	8.182270	-3.606042	0.000075
44	1	0	-1.226417	-3.589231	-0.000129
45	1	0	1.226561	-3.589180	-0.000144
46	1	0	9.414791	-1.446520	0.000143
47	1	0	-9.414727	-1.446510	0.000083
48	1	0	-0.000138	7.014328	0.000010

1c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.712618	0.216582	-0.077629
2	6	0	-0.712614	0.216582	-0.077629
3	6	0	-1.465421	-0.997820	-0.092637
4	6	0	-0.705717	-2.169365	-0.107409
5	6	0	0.705719	-2.169365	-0.107410
6	6	0	1.465424	-0.997820	-0.092638
7	7	0	-1.138542	1.492472	-0.061398
8	7	0	1.138546	1.492472	-0.061398
9	7	0	0.000002	2.188661	-0.052684
10	6	0	0.000002	3.613581	-0.034819
11	6	0	1.217511	4.300146	-0.026318
12	6	0	-1.217508	4.300146	-0.026339
13	6	0	1.207454	5.693215	-0.008839
14	1	0	2.144488	3.740224	-0.033668
15	6	0	-1.207450	5.693215	-0.008859
16	1	0	-2.144484	3.740224	-0.033705
17	6	0	0.000002	6.394892	-0.000023
18	1	0	2.151100	6.231340	-0.002330
19	1	0	-2.151097	6.231340	-0.002366
20	6	0	2.879820	-1.005195	-0.091755
21	6	0	4.097473	-1.012489	-0.090866

22	6	0	-2.879816	-1.005193	-0.091751
23	6	0	-4.097470	-1.012484	-0.090860
24	6	0	5.519796	-1.009574	-0.087072
25	6	0	6.214084	0.214653	-0.074344
26	6	0	6.225626	-2.227222	-0.093118
27	6	0	7.610771	0.217435	-0.069047
28	1	0	5.647317	1.136580	-0.065339
29	6	0	7.622391	-2.217248	-0.087556
30	1	0	5.669523	-3.155715	-0.098072
31	6	0	8.323451	-0.996513	-0.087489
32	6	0	-5.519792	-1.009563	-0.087061
33	6	0	-6.214078	0.214662	-0.074211
34	6	0	-6.225634	-2.227204	-0.093231
35	6	0	-7.610765	0.217456	-0.068906
36	1	0	-5.647307	1.136586	-0.065126
37	6	0	-7.622397	-2.217223	-0.087658
38	1	0	-5.669539	-3.155701	-0.098291
39	6	0	-8.323462	-0.996485	-0.087435
40	1	0	1.225979	-3.121820	-0.119569
41	1	0	-1.225977	-3.121819	-0.119566
42	1	0	0.000002	7.481048	0.013424
43	8	0	8.404571	-3.333367	-0.080373
44	8	0	9.690676	-0.990103	-0.157840
45	8	0	8.382365	1.340617	-0.045085
46	8	0	-8.404575	-3.333348	-0.080619
47	8	0	-9.690681	-0.990070	-0.157795
48	8	0	-8.382334	1.340656	-0.044864
49	6	0	10.353118	-0.987782	1.108097
50	1	0	10.103414	-1.886576	1.685311
51	1	0	11.423937	-0.982573	0.891220
52	1	0	10.094882	-0.092355	1.686661
53	6	0	7.762969	-4.598286	-0.116467
54	1	0	7.127758	-4.756025	0.765333
55	1	0	7.156127	-4.716411	-1.023602
56	1	0	8.565449	-5.338133	-0.120221
57	6	0	7.728011	2.599606	-0.062074
58	1	0	7.119650	2.724823	-0.967159
59	1	0	7.091498	2.737351	0.822056
60	1	0	8.523177	3.347311	-0.054913
61	6	0	-7.762970	-4.598260	-0.116873
62	1	0	-7.156128	-4.716268	-1.024022
63	1	0	-7.127759	-4.756110	0.764907
64	1	0	-8.565448	-5.338109	-0.120721
65	6	0	-10.353203	-0.987899	1.108105
66	1	0	-10.095026	-0.092522	1.686767
67	1	0	-11.424006	-0.982702	0.891151
68	1	0	-10.103504	-1.886745	1.685234
69	6	0	-7.727957	2.599633	-0.061776
70	1	0	-7.091437	2.737311	0.822359
71	1	0	-7.119599	2.724898	-0.966857
72	1	0	-8.523110	3.347352	-0.054563

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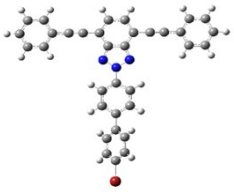

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.008449	0.712634	-0.002872
2	6	0	-3.008438	-0.712679	0.002874

3	6	0	-4.223138	-1.464478	0.006659
4	6	0	-5.395114	-0.705905	0.003336
5	6	0	-5.395125	0.705824	-0.003327
6	6	0	-4.223161	1.464415	-0.006654
7	7	0	-1.732761	-1.138996	0.004199
8	7	0	-1.732778	1.138970	-0.004200
9	7	0	-1.036671	-0.000007	-0.000001
10	6	0	0.385805	0.000003	-0.000002
11	6	0	1.077653	1.214199	0.006716
12	6	0	1.077671	-1.214183	-0.006719
13	6	0	2.467859	1.203800	0.006590
14	1	0	0.523319	2.144611	0.002014
15	6	0	2.467876	-1.203763	-0.006592
16	1	0	0.523351	-2.144602	-0.002016
17	6	0	3.193832	0.000024	-0.000001
18	1	0	2.999497	2.150411	-0.015898
19	1	0	2.999529	-2.150365	0.015896
20	6	0	-4.229945	2.879233	-0.014227
21	6	0	-4.235617	4.096525	-0.021731
22	6	0	-4.229901	-2.879296	0.014233
23	6	0	-4.235549	-4.096587	0.021736
24	6	0	-4.230800	5.519288	-0.031134
25	6	0	-5.440868	6.242938	-0.032549
26	6	0	-3.012142	6.228777	-0.039584
27	6	0	-5.427649	7.634611	-0.042173
28	1	0	-6.381259	5.700457	-0.026108
29	6	0	-3.009586	7.620409	-0.049191
30	1	0	-2.079335	5.673576	-0.038718
31	6	0	-4.214587	8.328166	-0.050505
32	1	0	-6.367012	8.180866	-0.043222
33	1	0	-2.064054	8.155911	-0.055810
34	6	0	-4.230676	-5.519351	0.031135
35	6	0	-5.440716	-6.243049	0.032553
36	6	0	-3.011990	-6.228792	0.039578
37	6	0	-5.427442	-7.634722	0.042173
38	1	0	-6.381128	-5.700605	0.026117
39	6	0	-3.009379	-7.620424	0.049180
40	1	0	-2.079204	-5.673554	0.038708
41	6	0	-4.214352	-8.328228	0.050498
42	1	0	-6.366783	-8.181013	0.043225
43	1	0	-2.063826	-8.155889	0.055794
44	1	0	-6.347445	1.226320	-0.005982
45	1	0	-6.347426	-1.226415	0.005994
46	1	0	-4.208038	-9.414714	0.058060
47	1	0	-4.208316	9.414652	-0.058071
48	6	0	4.676862	0.000035	-0.000001
49	6	0	5.401232	0.949381	0.740621
50	6	0	5.401246	-0.949301	-0.740622
51	6	0	6.794407	0.955572	0.745745
52	1	0	4.869717	1.678721	1.344940
53	6	0	6.794421	-0.955471	-0.745745
54	1	0	4.869743	-1.678648	-1.344941
55	6	0	7.481733	0.000055	0.000000
56	1	0	7.340648	1.688230	1.329860
57	1	0	7.340674	-1.688121	-1.329859
58	35	0	9.392771	0.000069	0.000001

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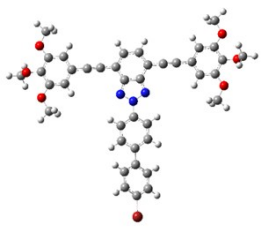

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	6	0	-0.712887	-1.925417	-0.013273
3	6	0	-1.465748	-3.139929	-0.026670
4	6	0	-0.705948	-4.311371	-0.012792
5	6	0	0.705332	-4.311471	0.012761
6	6	0	1.465293	-3.140134	0.026635
7	7	0	-1.138964	-0.649743	-0.021517
8	7	0	1.138857	-0.649906	0.021475
9	7	0	-0.000003	0.046583	-0.000031
10	6	0	0.000101	1.468565	-0.000035
11	6	0	1.213643	2.160851	0.033650
12	6	0	-1.213339	2.161033	-0.033719
13	6	0	1.203412	3.551059	0.033363
14	1	0	2.143598	1.606004	0.049815
15	6	0	-1.202899	3.551239	-0.033427
16	1	0	-2.143377	1.606324	-0.049883
17	6	0	0.000311	4.277340	-0.000029
18	1	0	2.150229	4.082872	0.032084
19	1	0	-2.149636	4.083194	-0.032147
20	6	0	2.879379	-3.147705	0.051407
21	6	0	4.096867	-3.156128	0.072530
22	6	0	-2.879836	-3.147321	-0.051425
23	6	0	-4.097325	-3.155625	-0.072518
24	6	0	5.518993	-3.156030	0.095135
25	6	0	6.216069	-1.933323	0.099149
26	6	0	6.221824	-4.375335	0.110838
27	6	0	7.612606	-1.933711	0.120642
28	1	0	5.651724	-1.010033	0.081880
29	6	0	7.618456	-4.368539	0.132283
30	1	0	5.663701	-5.302590	0.102425
31	6	0	8.322088	-3.149355	0.149464
32	6	0	-5.519451	-3.155386	-0.095126
33	6	0	-6.216407	-1.932608	-0.099126
34	6	0	-6.222400	-4.374620	-0.110842
35	6	0	-7.612941	-1.932857	-0.120610
36	1	0	-5.651967	-1.009376	-0.081851
37	6	0	-7.619036	-4.367687	-0.132280
38	1	0	-5.664369	-5.301929	-0.102438
39	6	0	-8.322544	-3.148436	-0.149440
40	1	0	1.225284	-5.264109	0.022114
41	1	0	-1.226036	-5.263936	-0.022135
42	8	0	8.398102	-5.486278	0.137138
43	8	0	9.687462	-3.146138	0.247156
44	8	0	8.387069	-0.812357	0.114867
45	8	0	-8.398790	-5.485350	-0.137130
46	8	0	-9.687917	-3.145096	-0.247120
47	8	0	-8.387296	-0.811429	-0.114833
48	6	0	10.375857	-3.143297	-1.005045
49	1	0	10.131607	-2.246314	-1.587214
50	1	0	11.441940	-3.140882	-0.766045
51	1	0	10.136064	-4.040595	-1.588682
52	6	0	7.753246	-6.749979	0.156291
53	1	0	7.128316	-6.869674	1.050840
54	1	0	7.135371	-6.903405	-0.738481
55	1	0	8.553956	-7.491524	0.173516
56	6	0	7.735673	0.448207	0.120985
57	1	0	7.117304	0.589094	-0.775448
58	1	0	7.109722	0.573383	1.014039
59	1	0	8.532670	1.193911	0.131000
60	6	0	-7.754063	-6.749118	-0.156329
61	1	0	-7.129160	-6.868852	-1.050891
62	1	0	-7.136192	-6.902632	0.738430

63	1	0	-8.554850	-7.490580	-0.173561
64	6	0	-10.376318	-3.142074	1.005080
65	1	0	-10.132079	-2.245000	1.587111
66	1	0	-11.442398	-3.139714	0.766072
67	1	0	-10.136516	-4.039278	1.588857
68	6	0	-7.735777	0.449071	-0.120833
69	1	0	-7.117383	0.589807	0.775605
70	1	0	-7.109824	0.574274	-1.013883
71	1	0	-8.532701	1.194855	-0.130766
72	6	0	0.000422	5.760312	-0.000023
73	6	0	-0.931722	6.484876	-0.762017
74	6	0	0.932672	6.484728	0.761981
75	6	0	-0.937750	7.878063	-0.767262
76	1	0	-1.647142	5.953489	-1.382920
77	6	0	0.938904	7.877915	0.767247
78	1	0	1.648014	5.953228	1.382878
79	6	0	0.000627	8.565349	-0.000002
80	1	0	-1.656907	8.424248	-1.367940
81	1	0	1.658141	8.423985	1.367934
82	35	0	0.000764	10.476360	0.000014

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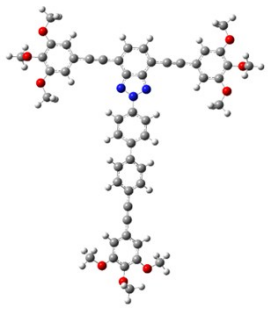

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.419449	0.723731	-0.002826
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3	6	0	5.642017	-1.449965	-0.016306
4	6	0	6.810869	-0.685857	-0.017035
5	6	0	6.805645	0.725491	-0.011219
6	6	0	5.631175	1.480911	-0.003985
7	7	0	3.150557	-1.132786	-0.007051
8	7	0	3.142054	1.145202	0.003898
9	7	0	2.449857	0.003589	0.000883
10	6	0	1.027759	-0.001917	0.006416
11	6	0	0.330213	1.209054	0.024123
12	6	0	0.339799	-1.218434	-0.005635
13	6	0	-1.059716	1.193172	0.029887
14	1	0	0.881083	2.141546	0.023300
15	6	0	-1.050159	-1.213641	0.000487
16	1	0	0.898065	-2.146503	-0.009343
17	6	0	-1.782771	-0.013161	0.018386
18	1	0	-1.594825	2.137917	0.015741
19	1	0	-1.577566	-2.162609	0.019472
20	6	0	5.633227	2.895293	0.001087
21	6	0	5.635858	4.112966	0.005150
22	6	0	5.654479	-2.864292	-0.020951
23	6	0	5.666142	-4.081915	-0.024351
24	6	0	5.627656	5.535262	0.007309
25	6	0	4.400830	6.225059	0.004629
26	6	0	6.842714	6.245575	0.009258
27	6	0	4.392878	7.621748	0.005261
28	1	0	3.480952	5.654934	-0.001724

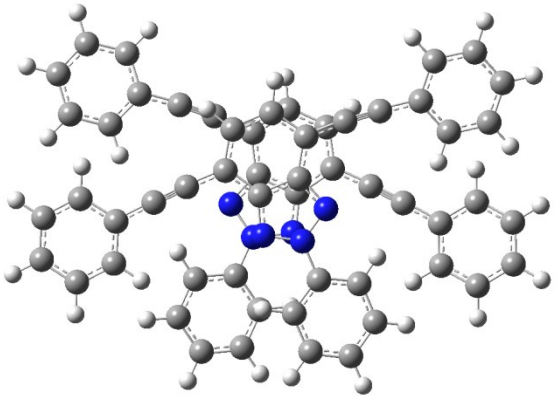
29	6	0	6.827568	7.642286	0.009935
30	1	0	7.773260	5.692905	0.006422
31	6	0	5.604278	8.338841	0.019964
32	6	0	5.668395	-5.504233	-0.025483
33	6	0	4.446708	-6.203014	-0.014730
34	6	0	6.888614	-6.205593	-0.034369
35	6	0	4.448997	-7.599703	-0.014302
36	1	0	3.522722	-5.639667	-0.003157
37	6	0	6.883710	-7.602403	-0.033808
38	1	0	7.815083	-5.646107	-0.037555
39	6	0	5.665517	-8.307905	-0.035873
40	1	0	7.756227	1.249298	-0.012322
41	1	0	7.765296	-1.202595	-0.022277
42	8	0	7.940720	8.428643	-0.000146
43	8	0	5.592935	9.705670	0.096472
44	8	0	3.266724	8.389223	-0.009063
45	8	0	8.002647	-8.380521	-0.029790
46	8	0	5.664195	-9.674834	-0.111231
47	8	0	3.328662	-8.375484	0.007464
48	6	0	5.586303	10.373974	-1.166422
49	1	0	4.691094	10.114852	-1.744939
50	1	0	5.577105	11.443732	-0.944521
51	1	0	6.485270	10.130539	-1.745982
52	6	0	9.208259	7.791656	0.025149
53	1	0	9.334217	7.181017	0.928674
54	1	0	9.362944	7.161217	-0.860600
55	1	0	9.945089	8.596904	0.028170
56	6	0	2.010329	7.730026	0.009737
57	1	0	1.871442	7.097294	-0.876912
58	1	0	1.891027	7.116804	0.912368
59	1	0	1.259591	8.522364	0.009423
60	6	0	9.265229	-7.734151	-0.062537
61	1	0	9.381659	-7.123230	-0.967154
62	1	0	9.420092	-7.101932	0.821911
63	1	0	10.008011	-8.533895	-0.069077
64	6	0	5.662154	-10.342115	1.152241
65	1	0	4.764801	-10.089411	1.730217
66	1	0	5.661319	-11.412099	0.931246
67	1	0	6.559049	-10.091260	1.731892
68	6	0	2.067232	-7.725738	-0.003770
69	1	0	1.929213	-7.093497	0.883356
70	1	0	1.937624	-7.114043	-0.906016
71	1	0	1.322489	-8.523688	0.001784
72	6	0	-3.264086	-0.019611	0.025638
73	6	0	-3.990270	-0.985435	-0.694611
74	6	0	-3.991833	0.939016	0.753860
75	6	0	-5.378967	-0.996535	-0.689686
76	1	0	-3.457157	-1.721062	-1.290073
77	6	0	-5.380579	0.935392	0.765468
78	1	0	-3.459519	1.680076	1.343274
79	6	0	-6.104292	-0.034669	0.042541
80	1	0	-5.919969	-1.744845	-1.260584
81	1	0	-5.922622	1.677600	1.343302
82	6	0	-7.526770	-0.043729	0.052368
83	6	0	-8.743762	-0.053584	0.062091
84	6	0	-10.168023	-0.066185	0.073296
85	6	0	-10.871714	0.913884	0.796966
86	6	0	-10.864914	-1.058588	-0.640201
87	6	0	-12.268786	0.897862	0.807071
88	1	0	-10.314131	1.670364	1.333679
89	6	0	-12.261836	-1.069810	-0.625652
90	1	0	-10.302211	-1.799575	-1.192948
91	6	0	-12.972186	-0.100207	0.106829
92	8	0	-13.047736	1.803314	1.463197
93	8	0	-14.337963	-0.157930	0.182791
94	8	0	-13.034896	-1.976370	-1.287759
95	6	0	-12.402500	2.816601	2.218084
96	1	0	-11.779110	2.390423	3.014913

97	1	0	-11.782909	3.463298	1.582530
98	1	0	-13.203063	3.409305	2.664328
99	6	0	-12.382984	-3.004904	-2.015976
100	1	0	-11.761366	-2.597862	-2.824593
101	1	0	-11.760207	-3.628878	-1.361788
102	1	0	-13.179580	-3.615137	-2.445350
103	6	0	-15.023927	0.552332	-0.849939
104	1	0	-14.779634	0.144615	-1.838435
105	1	0	-16.090507	0.416862	-0.655648
106	1	0	-14.781989	1.621937	-0.820160

Z-Matrix of aggregates of derivatives 1a, 1c and 1e.

1a

Vartical aggregate

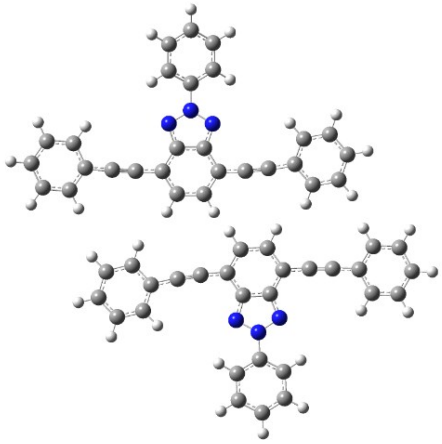


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.635200	0.121288	-1.612515
2	6	0	-0.674039	0.693462	-1.619351
3	6	0	-0.877695	2.110764	-1.657165
4	6	0	0.292157	2.890518	-1.719048
5	6	0	1.587850	2.325477	-1.710541
6	6	0	1.811868	0.937261	-1.643621
7	1	0	0.191550	3.974839	-1.738967
8	1	0	2.452038	2.987030	-1.717006
9	7	0	-1.583549	-0.302321	-1.550422
10	7	0	-0.812994	-1.397106	-1.497525
11	7	0	0.517840	-1.222466	-1.533251
12	6	0	-1.383726	-2.696071	-1.354839
13	6	0	-2.743146	-2.817553	-1.016636
14	6	0	-0.574018	-3.828671	-1.541072
15	6	0	-3.293274	-4.097357	-0.881099
16	1	0	-3.338179	-1.923133	-0.851935
17	6	0	-1.141289	-5.099950	-1.392511
18	1	0	0.478333	-3.701698	-1.780705
19	6	0	-2.499255	-5.241787	-1.067272
20	1	0	-4.348493	-4.193133	-0.624835
21	1	0	-0.513190	-5.980485	-1.528943
22	6	0	1.384025	-2.696605	1.354778

23	7	0	0.813176	-1.397711	1.497575
24	6	0	2.743326	-2.817948	1.016039
25	6	0	0.574530	-3.829288	1.541419
26	7	0	1.583625	-0.302852	1.550464
27	7	0	-0.517679	-1.223226	1.533366
28	6	0	3.293545	-4.097698	0.880345
29	1	0	3.338198	-1.923471	0.851054
30	6	0	1.141888	-5.100510	1.392714
31	1	0	-0.477737	-3.702409	1.781476
32	6	0	0.674014	0.692829	1.619456
33	6	0	-0.635167	0.120517	1.612647
34	6	0	2.499736	-5.242207	1.066917
35	1	0	4.348672	-4.193369	0.623653
36	1	0	0.513959	-5.981114	1.529485
37	6	0	0.877522	2.110151	1.657322
38	6	0	-1.811918	0.936372	1.643740
39	6	0	-0.292407	2.889780	1.719226
40	6	0	-1.588043	2.324607	1.710694
41	1	0	-0.191912	3.974110	1.739172
42	1	0	-2.452296	2.986075	1.717142
43	1	0	2.936490	-6.235500	0.957080
44	1	0	-2.935940	-6.235123	-0.957554
45	6	0	2.180902	2.644235	1.570429
46	6	0	3.347256	3.005357	1.443260
47	6	0	-3.100144	0.366092	1.561746
48	6	0	-4.198661	-0.174627	1.474278
49	6	0	-5.451400	-0.831465	1.351455
50	6	0	-6.663062	-0.093863	1.302061
51	6	0	-5.505227	-2.248417	1.268660
52	6	0	-7.886023	-0.758091	1.158926
53	1	0	-6.623658	0.992172	1.365887
54	6	0	-6.734669	-2.899580	1.125627
55	1	0	-4.575355	-2.813425	1.314151
56	6	0	-7.928793	-2.159981	1.066861
57	1	0	-8.811111	-0.180596	1.122539
58	1	0	-6.764029	-3.988664	1.064075
59	1	0	-8.885093	-2.672242	0.955077
60	6	0	4.714329	3.353803	1.282045
61	6	0	5.147624	4.703519	1.342735
62	6	0	5.674095	2.331270	1.054801
63	6	0	6.502227	5.016002	1.185509
64	1	0	4.412529	5.489400	1.515805
65	6	0	7.025514	2.657382	0.903766
66	1	0	5.339544	1.296704	0.994602
67	6	0	7.445806	3.997329	0.968319
68	1	0	6.824584	6.057010	1.234613
69	1	0	7.750432	1.860397	0.734642
70	1	0	8.501175	4.246463	0.850296
71	6	0	3.100145	0.367072	-1.561756
72	6	0	4.198679	-0.173641	-1.474462
73	6	0	-2.181119	2.644716	-1.570204
74	6	0	-3.347490	3.005752	-1.442940
75	6	0	5.451383	-0.830585	-1.351840
76	6	0	6.663127	-0.093114	-1.302557
77	6	0	5.505070	-2.247551	-1.269146
78	6	0	7.886037	-0.757486	-1.159640
79	1	0	6.623829	0.992931	-1.366279
80	6	0	6.734460	-2.898857	-1.126337
81	1	0	4.575130	-2.812455	-1.314546
82	6	0	7.928672	-2.159387	-1.067690
83	1	0	8.811188	-0.180090	-1.123331
84	1	0	6.763714	-3.987950	-1.064872
85	1	0	8.884933	-2.671758	-0.956080
86	6	0	-4.714561	3.354155	-1.281606
87	6	0	-5.147911	4.703847	-1.342478
88	6	0	-5.674259	2.331634	-1.054027
89	6	0	-6.502499	5.016317	-1.185095
90	1	0	-4.412869	5.489720	-1.515806

91	6	0	-7.025663	2.657734	-0.902830
92	1	0	-5.339680	1.297085	-0.993716
93	6	0	-7.446011	3.997655	-0.967561
94	1	0	-6.824896	6.057305	-1.234342
95	1	0	-7.750532	1.860754	-0.733472
96	1	0	-8.501369	4.246776	-0.849413

Horizontal aggregate



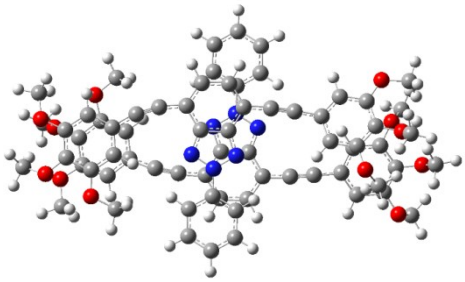
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.785638	-1.529862	-0.488980
2	6	0	-2.551940	-2.255637	-0.529275
3	6	0	-1.304954	-1.608305	-0.817245
4	6	0	-1.382183	-0.220311	-1.048256
5	6	0	-2.599871	0.495627	-1.009815
6	6	0	-3.838146	-0.118299	-0.735564
7	1	0	-0.462437	0.324232	-1.250704
8	1	0	-2.581027	1.569339	-1.183899
9	7	0	-2.805945	-3.554598	-0.257268
10	7	0	-4.135845	-3.560879	-0.069996
11	7	0	-4.783912	-2.390807	-0.192580
12	6	0	-4.834690	-4.765548	0.250886
13	6	0	-4.122183	-5.974565	0.345129
14	6	0	-6.223567	-4.721965	0.468368
15	6	0	-4.816155	-7.148582	0.661977
16	1	0	-3.049050	-5.978256	0.171348
17	6	0	-6.898941	-5.907083	0.783889
18	1	0	-6.748168	-3.773127	0.388508
19	6	0	-6.202672	-7.122499	0.882497
20	1	0	-4.267139	-8.087760	0.735735
21	1	0	-7.975653	-5.876961	0.953335
22	1	0	-6.735840	-8.041175	1.128724
23	6	0	-5.049279	0.607490	-0.693952
24	6	0	-6.095321	1.248706	-0.650943
25	6	0	-0.084663	-2.318803	-0.862216
26	6	0	0.976777	-2.934718	-0.906451
27	6	0	-7.293035	2.009529	-0.585645

28	6	0	-7.274073	3.404698	-0.851573
29	6	0	-8.524053	1.391349	-0.242893
30	6	0	-8.453423	4.152080	-0.771495
31	1	0	-6.328049	3.880478	-1.104800
32	6	0	-9.696428	2.150354	-0.167543
33	1	0	-8.538367	0.320818	-0.039459
34	6	0	-9.667212	3.530864	-0.429955
35	1	0	-8.427373	5.223066	-0.977994
36	1	0	-10.636824	1.665026	0.097101
37	1	0	-10.584203	4.118254	-0.369356
38	6	0	2.210697	-3.637331	-0.958773
39	6	0	3.412307	-2.957104	-1.288367
40	6	0	2.261652	-5.028089	-0.675699
41	6	0	4.624807	-3.651405	-1.331942
42	1	0	3.380114	-1.887803	-1.488544
43	6	0	3.481130	-5.711095	-0.722952
44	1	0	1.339103	-5.549634	-0.421567
45	6	0	4.665283	-5.027367	-1.050630
46	1	0	5.542761	-3.114844	-1.566741
47	1	0	3.509488	-6.779270	-0.503053
48	1	0	5.616709	-5.559708	-1.081501
49	1	0	0.462746	-0.324884	1.251481
50	6	0	1.382413	0.219710	1.048797
51	6	0	1.304922	1.607702	0.817844
52	6	0	2.600191	-0.496059	1.010016
53	6	0	2.551720	2.255228	0.529514
54	6	0	0.084533	2.318014	0.863186
55	6	0	3.838295	0.118070	0.735436
56	1	0	2.581557	-1.569779	1.184084
57	6	0	3.785505	1.529629	0.488878
58	7	0	2.805463	3.554230	0.257432
59	6	0	-0.977002	2.933743	0.907737
60	6	0	5.049585	-0.607443	0.693470
61	7	0	4.783582	2.390716	0.192217
62	7	0	4.135313	3.560694	0.069808
63	6	0	-2.210990	3.636214	0.960385
64	6	0	6.095899	-1.248187	0.650052
65	6	0	4.833919	4.765451	-0.251249
66	6	0	-3.412489	2.955819	1.290035
67	6	0	-2.262108	5.027021	0.677587
68	6	0	7.294018	-2.008340	0.584353
69	6	0	4.121225	5.974362	-0.345391
70	6	0	6.222758	4.722043	-0.468997
71	6	0	-4.625045	3.650001	1.333928
72	1	0	-3.380169	1.886482	1.489995
73	6	0	-3.481637	5.709915	0.725178
74	1	0	-1.339642	5.548693	0.423411
75	6	0	7.276111	-3.403389	0.850970
76	6	0	8.524426	-1.389556	0.240498
77	6	0	4.814976	7.148463	-0.662416
78	1	0	3.048125	5.977906	-0.171399
79	6	0	6.897914	5.907243	-0.784677
80	1	0	6.747490	3.773271	-0.389209
81	6	0	-4.665678	5.026021	1.052911
82	1	0	-5.542932	3.113309	1.568702
83	1	0	-3.510123	6.778132	0.505500
84	6	0	8.455885	-4.150062	0.770510
85	1	0	6.330560	-3.879640	1.105079
86	6	0	9.697232	-2.147855	0.164763
87	1	0	8.537932	-0.319117	0.036530
88	6	0	6.201456	7.122559	-0.883192
89	1	0	4.265821	8.087567	-0.736102
90	1	0	7.974599	5.877267	-0.954323
91	1	0	-5.617150	5.558262	1.084008
92	6	0	9.669062	-3.528250	0.427881
93	1	0	8.430647	-5.220962	0.977557
94	1	0	10.637146	-1.662060	-0.100738
95	1	0	6.734453	8.041300	-1.129548

96	1	0	10.586384	-4.115092	0.366988

1c

Vartical aggregate

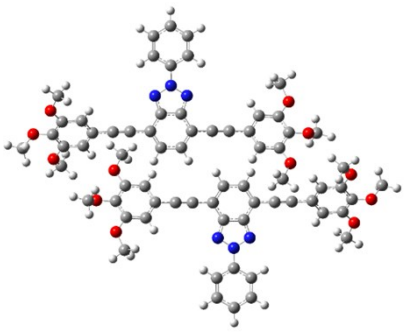


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.043057	-0.405743	-1.432906
2	6	0	-0.384511	-0.370635	-1.488115
3	6	0	-1.169707	-1.571540	-1.485124
4	6	0	-0.439958	-2.772322	-1.427061
5	6	0	0.973254	-2.805623	-1.372002
6	6	0	1.765357	-1.642345	-1.372360
7	1	0	-0.987974	-3.712203	-1.395952
8	1	0	1.471389	-3.772182	-1.314770
9	7	0	-0.784294	0.918786	-1.533926
10	7	0	0.382288	1.585552	-1.510989
11	7	0	1.508952	0.859548	-1.455087
12	6	0	0.423907	3.010411	-1.503151
13	6	0	-0.765300	3.737670	-1.680426
14	6	0	1.649331	3.661002	-1.278348
15	6	0	-0.721118	5.135305	-1.622303
16	1	0	-1.698384	3.203432	-1.839336
17	6	0	1.673254	5.059647	-1.225111
18	1	0	2.546343	3.069523	-1.116860
19	6	0	0.493291	5.802873	-1.393626
20	1	0	-1.642309	5.704038	-1.754703
21	1	0	2.620128	5.568506	-1.041602
22	1	0	0.519728	6.892016	-1.346262
23	6	0	3.177209	-1.652607	-1.342809
24	6	0	4.402452	-1.576563	-1.366524
25	6	0	-2.577058	-1.479737	-1.532384
26	6	0	-3.776429	-1.222157	-1.595381
27	6	0	5.814195	-1.458869	-1.459246

28	6	0	6.613855	-2.584614	-1.780798
29	6	0	6.432268	-0.195758	-1.276828
30	6	0	8.003175	-2.457376	-1.901085
31	1	0	6.161121	-3.564123	-1.922896
32	6	0	7.815547	-0.069894	-1.424517
33	1	0	5.842197	0.677967	-1.009175
34	6	0	8.617608	-1.193701	-1.734778
35	6	0	-5.108690	-0.737230	-1.663666
36	6	0	-6.221483	-1.600773	-1.788350
37	6	0	-5.288296	0.664967	-1.588166
38	6	0	-7.513921	-1.054654	-1.829619
39	1	0	-6.063657	-2.673993	-1.844900
40	6	0	-6.581753	1.201774	-1.623851
41	1	0	-4.413850	1.294390	-1.456611
42	6	0	-7.700146	0.344588	-1.739158
43	1	0	0.586691	4.051404	1.595598
44	6	0	0.039923	3.111991	1.652469
45	6	0	0.776933	1.913384	1.692161
46	6	0	-1.375082	3.147709	1.646841
47	6	0	-0.003195	0.710561	1.733001
48	6	0	2.186677	1.851193	1.671597
49	6	0	-2.161371	1.983279	1.678134
50	1	0	-1.873840	4.114916	1.603236
51	6	0	-1.430716	0.747185	1.717972
52	7	0	0.396663	-0.579834	1.760423
53	6	0	3.403764	1.693377	1.649691
54	6	0	-3.570300	1.911532	1.669787
55	7	0	-1.897563	-0.518125	1.739565
56	7	0	-0.770162	-1.246208	1.761976
57	6	0	4.800717	1.442215	1.693049
58	6	0	-4.747018	1.552535	1.683909
59	6	0	-0.813638	-2.670074	1.742852
60	6	0	5.736957	2.445777	1.367887
61	6	0	5.261961	0.161735	2.090143
62	6	0	-5.988528	0.869343	1.658220
63	6	0	0.374716	-3.401090	1.907996
64	6	0	-2.040845	-3.317957	1.519631
65	6	0	7.122934	2.214417	1.466516
66	1	0	5.401755	3.433664	1.057358
67	6	0	6.631848	-0.073733	2.190297
68	1	0	4.561101	-0.635917	2.324412
69	6	0	-7.243711	1.506792	1.615080
70	6	0	-5.913293	-0.545562	1.631756
71	6	0	0.326007	-4.798629	1.842347
72	1	0	1.310619	-2.870305	2.062370
73	6	0	-2.070071	-4.715863	1.459523
74	1	0	-2.937343	-2.724874	1.366716
75	6	0	7.580956	0.941238	1.895066
76	6	0	-8.418473	0.741608	1.536097
77	1	0	-7.295578	2.591320	1.635378
78	6	0	-7.078626	-1.305093	1.534274
79	1	0	-4.929895	-1.005192	1.635029
80	6	0	-0.891049	-5.462891	1.618124
81	1	0	1.246886	-5.369407	1.966045
82	1	0	-3.019477	-5.221670	1.279029
83	6	0	-8.356967	-0.678231	1.480025
84	1	0	-0.920248	-6.551735	1.566687
85	8	0	-9.427316	-1.519643	1.416721
86	8	0	-9.669907	1.304721	1.516903
87	8	0	7.046656	-1.305413	2.659965
88	8	0	8.934695	0.663800	2.008184
89	8	0	7.883146	3.305597	1.153197
90	8	0	8.751904	-3.596049	-2.112432
91	8	0	9.984725	-1.059568	-1.872776
92	8	0	8.401793	1.160962	-1.204531
93	8	0	-6.871593	2.536201	-1.532880
94	8	0	-8.971884	0.877453	-1.700150
95	8	0	-8.663637	-1.786523	-1.956118

96	8	0	-7.086420	-2.676340	1.440132
97	6	0	-10.578521	-1.167300	0.613743
98	1	0	-10.268433	-0.678118	-0.317046
99	1	0	-11.066239	-2.126921	0.392911
100	1	0	-11.262729	-0.517480	1.175377
101	6	0	-9.533407	1.093294	-3.008362
102	1	0	-9.623940	0.140726	-3.554582
103	1	0	-10.530234	1.524544	-2.846310
104	1	0	-8.912588	1.799085	-3.584782
105	6	0	-5.768673	3.421928	-1.295264
106	1	0	-5.241932	3.156590	-0.364935
107	1	0	-5.054439	3.398370	-2.136643
108	1	0	-6.208848	4.422980	-1.212764
109	6	0	-8.583823	-3.188160	-1.657164
110	1	0	-7.960365	-3.720161	-2.396271
111	1	0	-8.187904	-3.337286	-0.642115
112	1	0	-9.614199	-3.558029	-1.719269
113	6	0	-9.763203	2.645332	1.014443
114	1	0	-9.383519	3.375154	1.750734
115	1	0	-9.207387	2.738609	0.069321
116	1	0	-10.833131	2.825886	0.850162
117	6	0	-5.810595	-3.320898	1.386059
118	1	0	-5.220796	-2.961860	0.525840
119	1	0	-5.236139	-3.151018	2.312383
120	1	0	-6.025016	-4.391154	1.276140
121	6	0	7.733181	-2.122017	1.685549
122	1	0	7.086142	-2.311009	0.817197
123	1	0	8.662964	-1.643150	1.350639
124	1	0	7.959288	-3.067569	2.195569
125	6	0	9.389728	0.555861	3.372156
126	1	0	10.455511	0.296534	3.316986
127	1	0	9.269775	1.520961	3.894484
128	1	0	8.836976	-0.229017	3.908115
129	6	0	9.317934	3.252028	1.117185
130	1	0	9.741793	3.092481	2.120759
131	1	0	9.668339	2.464220	0.441000
132	1	0	9.619536	4.241811	0.748011
133	6	0	9.422483	-3.647017	-3.388076
134	1	0	8.688316	-3.603050	-4.211225
135	1	0	10.145762	-2.825266	-3.491055
136	1	0	9.944326	-4.612438	-3.414046
137	6	0	10.671942	-1.039876	-0.600891
138	1	0	11.727017	-0.837728	-0.828303
139	1	0	10.262657	-0.254493	0.051301
140	1	0	10.580631	-2.021946	-0.107903
141	6	0	8.916020	1.788032	-2.395161
142	1	0	9.700222	1.171121	-2.858934
143	1	0	8.102082	1.965893	-3.118261
144	1	0	9.334816	2.749234	-2.070541

Horizontal aggregate



Center	Atomic	Atomic	Coordinates (Angstroms)

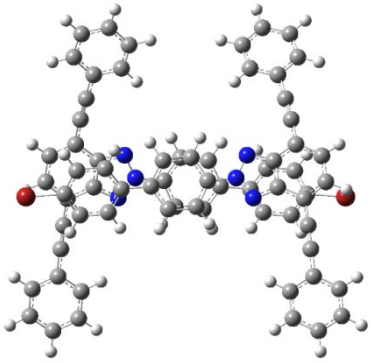
Number	Number	Type	X	Y	Z
1	6	0	-3.570881	2.748074	0.392943
2	6	0	-2.243501	3.170992	0.212862
3	6	0	-1.147595	2.259491	0.323410
4	6	0	-1.474971	0.966942	0.598995
5	6	0	-2.826105	0.535626	0.779659
6	6	0	-3.886660	1.386118	0.693843
7	1	0	-0.695203	0.234258	0.690678
8	1	0	-3.000395	-0.501701	0.996532
9	7	0	-2.263042	4.466086	-0.047474
10	7	0	-3.527897	4.770659	-0.018778
11	7	0	-4.355702	3.799579	0.236769
12	6	0	-3.982160	6.099552	-0.254461
13	6	0	-3.055299	7.117289	-0.412232
14	6	0	-5.342778	6.352107	-0.321542
15	6	0	-3.505438	8.405223	-0.641687
16	1	0	-2.007555	6.899429	-0.354052
17	6	0	-5.774848	7.646259	-0.550663
18	1	0	-6.041693	5.549409	-0.196149
19	6	0	-4.862099	8.675530	-0.711775
20	1	0	-2.790022	9.198555	-0.763509
21	1	0	-6.829759	7.847189	-0.604204
22	1	0	-5.204849	9.678952	-0.889766
23	6	0	-5.239980	0.965423	0.906325
24	6	0	-6.367877	0.634943	1.101241
25	6	0	0.207313	2.703757	0.167675
26	6	0	1.325723	3.097701	0.054453
27	6	0	-7.734038	0.262287	1.362141
28	6	0	-8.050783	-1.062546	1.635812
29	6	0	-8.716813	1.244741	1.355719
30	6	0	-9.367776	-1.404065	1.912024
31	1	0	-7.272013	-1.797823	1.638052
32	6	0	-10.031616	0.895296	1.628373
33	1	0	-8.439662	2.257710	1.146327
34	6	0	-10.362784	-0.429963	1.899929
35	6	0	2.673173	3.594485	-0.067773
36	6	0	2.956588	4.574760	-1.010910
37	6	0	3.666330	3.098624	0.768092
38	6	0	4.250661	5.065174	-1.115024
39	1	0	2.169044	4.939268	-1.638298
40	6	0	4.958098	3.597937	0.662784
41	1	0	3.417703	2.346305	1.488370
42	6	0	5.254450	4.576710	-0.282223
43	1	0	1.187424	-0.214985	-1.564117
44	6	0	1.813702	-1.004086	-1.191647
45	6	0	1.289056	-2.250034	-1.024679
46	6	0	3.177598	-0.695458	-0.897498
47	6	0	2.189149	-3.243107	-0.525961
48	6	0	-0.072434	-2.566059	-1.340229
49	6	0	4.056786	-1.624133	-0.429109
50	1	0	3.514169	0.311512	-1.058609
51	6	0	3.530628	-2.939847	-0.237828
52	7	0	1.995782	-4.521477	-0.254782
53	6	0	-1.197198	-2.842621	-1.619140
54	6	0	5.427473	-1.314133	-0.150844
55	7	0	4.110052	-4.043480	0.199521
56	7	0	3.158014	-4.930190	0.165181
57	6	0	-2.545816	-3.200488	-1.974944
58	6	0	6.569636	-1.053699	0.066976
59	6	0	3.376774	-6.278343	0.567124
60	6	0	-3.442729	-2.214116	-2.366847
61	6	0	-2.926201	-4.536296	-1.931195
62	6	0	7.950130	-0.733508	0.322910
63	6	0	2.324943	-7.179476	0.529331
64	6	0	4.637956	-6.666720	0.989543
65	6	0	-4.733922	-2.573484	-2.729377
66	1	0	-3.123546	-1.192059	-2.385666

67	6	0	-4.219132	-4.888012	-2.292338
68	1	0	-2.211965	-5.271986	-1.622291
69	6	0	8.400148	0.563785	0.112165
70	6	0	8.811639	-1.726322	0.774011
71	6	0	2.546715	-8.487421	0.921840
72	1	0	1.357742	-6.857222	0.199041
73	6	0	4.841384	-7.978668	1.378624
74	1	0	5.437150	-5.953083	1.010359
75	6	0	-5.122260	-3.911062	-2.702523
76	6	0	9.731722	0.872001	0.359251
77	1	0	7.713829	1.309884	-0.232549
78	6	0	10.140853	-1.411550	1.018695
79	1	0	8.434939	-2.717866	0.921575
80	6	0	3.801098	-8.892563	1.347011
81	1	0	1.733360	-9.190150	0.894111
82	1	0	5.818529	-8.284458	1.706917
83	6	0	10.602424	-0.112370	0.822012
84	1	0	3.966401	-9.910674	1.650607
85	8	0	-9.777726	-2.648232	2.214864
86	8	0	-11.653284	-0.776212	2.111920
87	8	0	-11.053761	1.767866	1.659067
88	8	0	5.985349	3.198929	1.431111
89	8	0	6.525192	5.030529	-0.411236
90	8	0	4.628932	6.018869	-1.983105
91	8	0	11.885844	0.200503	1.117807
92	8	0	11.059746	-2.297040	1.444682
93	8	0	10.267740	2.087911	0.177923
94	8	0	-4.691529	-6.147011	-2.273462
95	8	0	-6.361237	-4.266283	-3.115144
96	8	0	-5.678959	-1.704363	-3.121031
97	6	0	-8.887764	-3.723039	2.100033
98	1	0	-8.518498	-3.818088	1.084062
99	1	0	-8.050038	-3.626644	2.783251
100	1	0	-9.451821	-4.607697	2.356348
101	6	0	-12.082866	-0.735443	3.451720
102	1	0	-13.121922	-1.034205	3.453309
103	1	0	-11.510674	-1.424896	4.062981
104	1	0	-11.997865	0.267763	3.855302
105	6	0	-10.832028	3.111028	1.332482
106	1	0	-11.794396	3.597291	1.394351
107	1	0	-10.148660	3.584010	2.031009
108	1	0	-10.444329	3.215078	0.324056
109	6	0	5.781202	2.224858	2.423403
110	1	0	5.065268	2.564933	3.164718
111	1	0	5.446888	1.287836	1.993894
112	1	0	6.740563	2.074539	2.894331
113	6	0	6.831448	6.184011	0.338127
114	1	0	6.202313	7.015330	0.041481
115	1	0	6.714367	5.996410	1.399997
116	1	0	7.864319	6.426229	0.129395
117	6	0	3.706413	6.524631	-2.908267
118	1	0	2.880789	7.026701	-2.413773
119	1	0	4.247258	7.240044	-3.509806
120	1	0	3.318214	5.740224	-3.549754
121	6	0	9.454523	3.145671	-0.266545
122	1	0	10.095672	4.014035	-0.306403
123	1	0	9.059079	2.950603	-1.257769
124	1	0	8.632637	3.332436	0.411820
125	6	0	12.798212	0.092676	0.052096
126	1	0	13.766743	0.372839	0.442888
127	1	0	12.842736	-0.926249	-0.317975
128	1	0	12.530471	0.763579	-0.756732
129	6	0	10.678215	-3.614189	1.723067
130	1	0	10.306173	-4.118286	0.836304
131	1	0	11.568895	-4.117903	2.069026
132	1	0	9.922389	-3.652979	2.501257
133	6	0	-3.827837	-7.208856	-1.980237
134	1	0	-2.997556	-7.249264	-2.677952

135	1	0	-3.442492	-7.142366	-0.967256
136	1	0	-4.416329	-8.109456	-2.076185
137	6	0	-7.361010	-4.247474	-2.126324
138	1	0	-7.132780	-4.953964	-1.334280
139	1	0	-7.476714	-3.252732	-1.709903
140	1	0	-8.282542	-4.540639	-2.609757
141	6	0	-5.381248	-0.336620	-3.201759
142	1	0	-6.283903	0.144696	-3.547488
143	1	0	-5.110618	0.068582	-2.233124
144	1	0	-4.582458	-0.147827	-3.911932

1e

Vertical aggregate



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.344671	1.032428	-0.967382
2	6	0	-4.540469	-0.278086	-1.501199
3	6	0	-5.849305	-0.847121	-1.627795
4	6	0	-6.914418	-0.019125	-1.225404
5	6	0	-6.717910	1.269289	-0.679268
6	6	0	-5.440287	1.831953	-0.507473
7	1	0	-7.926957	-0.413076	-1.286126
8	1	0	-7.584814	1.829461	-0.333272
9	7	0	-3.333714	-0.809537	-1.797542
10	7	0	-2.487738	0.175989	-1.451975
11	7	0	-3.021070	1.300466	-0.949408
12	6	0	-1.079927	0.038276	-1.617535
13	6	0	-0.520956	-1.237871	-1.796731
14	6	0	-0.262177	1.180478	-1.582979
15	6	0	0.863406	-1.361779	-1.923654
16	1	0	-1.173003	-2.107038	-1.833909
17	6	0	1.119484	1.036887	-1.704656
18	1	0	-0.716340	2.156329	-1.432123
19	6	0	1.713412	-0.234319	-1.867441
20	1	0	1.296109	-2.349973	-2.077104
21	1	0	1.756978	1.913869	-1.610837
22	6	0	3.184212	-0.378279	-1.947385
23	6	0	3.985022	0.640531	-2.509060
24	6	0	3.828561	-1.523643	-1.431144

25	6	0	5.377665	0.530021	-2.548598
26	1	0	3.514681	1.531970	-2.921988
27	6	0	5.221633	-1.651508	-1.462195
28	1	0	3.239830	-2.299830	-0.944083
29	6	0	5.982652	-0.618093	-2.021670
30	1	0	5.984297	1.330011	-2.967924
31	1	0	5.708039	-2.519396	-1.022051
32	6	0	1.080169	0.038006	1.617769
33	7	0	2.487952	0.176042	1.452239
34	6	0	0.521468	-1.238256	1.797003
35	6	0	0.262171	1.180027	1.583114
36	7	0	3.334160	-0.809323	1.797711
37	7	0	3.021024	1.300676	0.949747
38	6	0	-0.862877	-1.362460	1.923845
39	1	0	1.173703	-2.107280	1.834264
40	6	0	-1.119463	1.036142	1.704714
41	1	0	0.716128	2.155966	1.432230
42	6	0	4.540790	-0.277576	1.501379
43	6	0	4.344680	1.032931	0.967663
44	6	0	-1.713123	-0.235185	1.867520
45	1	0	-1.295379	-2.350739	2.077318
46	1	0	-1.757154	1.912967	1.610780
47	6	0	5.849767	-0.846314	1.627867
48	6	0	5.440084	1.832729	0.507719
49	6	0	-3.183899	-0.379445	1.947358
50	6	0	6.914669	-0.018050	1.225454
51	6	0	6.717845	1.270347	0.679386
52	6	0	-3.984950	0.639197	2.508995
53	6	0	-3.827981	-1.524929	1.431053
54	1	0	7.927301	-0.411776	1.286102
55	1	0	7.584601	1.830718	0.333345
56	6	0	-5.377574	0.528406	2.548444
57	1	0	-3.514813	1.530722	2.921968
58	6	0	-5.221030	-1.653077	1.462018
59	1	0	-3.239057	-2.300995	0.944030
60	6	0	-5.982294	-0.619827	2.021466
61	1	0	-5.984394	1.328263	2.967750
62	1	0	-5.707232	-2.521061	1.021836
63	35	0	-7.893954	-0.756251	2.023110
64	35	0	7.894340	-0.754113	-2.023385
65	6	0	-5.206195	3.066307	0.136984
66	6	0	-4.918264	4.096735	0.739646
67	6	0	-6.038283	-2.171231	-2.081404
68	6	0	-6.171050	-3.336783	-2.444426
69	6	0	6.039085	-2.170402	2.081388
70	6	0	6.172161	-3.335943	2.444332
71	6	0	5.205578	3.067024	-0.136700
72	6	0	4.917071	4.097290	-0.739366
73	6	0	6.307215	-4.685470	2.867661
74	6	0	5.161662	-5.432679	3.249482
75	6	0	7.581032	-5.310184	2.911333
76	6	0	5.293038	-6.762973	3.660120
77	1	0	4.184126	-4.951827	3.218031
78	6	0	7.699072	-6.641300	3.324023
79	1	0	8.461446	-4.738504	2.618569
80	6	0	6.558933	-7.372494	3.698924
81	1	0	4.406292	-7.327243	3.951991
82	1	0	8.683038	-7.111228	3.353649
83	1	0	6.656389	-8.410281	4.019934
84	6	0	4.547787	5.274805	-1.442859
85	6	0	3.174778	5.592777	-1.620324
86	6	0	5.529322	6.143176	-1.987487
87	6	0	2.802250	6.743047	-2.322648
88	1	0	2.420955	4.927898	-1.198252
89	6	0	5.143931	7.291616	-2.686774
90	1	0	6.583472	5.901756	-1.852590
91	6	0	3.782676	7.596138	-2.858193
92	1	0	1.744739	6.976386	-2.453652

93	1	0	5.907132	7.951943	-3.100655
94	1	0	3.487588	8.492139	-3.405419
95	6	0	-6.305747	-4.686320	-2.867844
96	6	0	-7.579366	-5.311454	-2.911304
97	6	0	-5.160027	-5.433114	-3.249973
98	6	0	-7.697051	-6.642573	-3.324083
99	1	0	-8.459908	-4.740091	-2.618306
100	6	0	-5.291048	-6.763416	-3.660698
101	1	0	-4.182644	-4.951939	-3.218688
102	6	0	-6.556748	-7.373356	-3.699287
103	1	0	-8.680867	-7.112825	-3.353543
104	1	0	-4.404175	-7.327365	-3.952807
105	1	0	-6.653924	-8.411148	-4.020366
106	6	0	-4.549828	5.274543	1.443099
107	6	0	-3.177058	5.592942	1.621613
108	6	0	-5.532058	6.142845	1.986587
109	6	0	-2.805431	6.743572	2.323829
110	1	0	-2.422698	4.928106	1.200438
111	6	0	-5.147567	7.291650	2.685769
112	1	0	-6.586028	5.901094	1.850879
113	6	0	-3.786539	7.596602	2.858219
114	1	0	-1.748095	6.977240	2.455648
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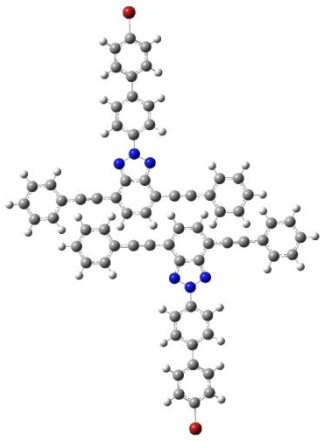
Horizontal aggregate



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.641368	1.755677	0.790854
2	6	0	3.328052	0.359893	0.865143
3	6	0	1.980601	-0.102822	1.030924
4	6	0	0.999607	0.905747	1.109844
5	6	0	1.308995	2.282683	1.037756
6	6	0	2.624535	2.762625	0.880646
7	1	0	-0.041760	0.609910	1.217243
8	1	0	0.496656	3.004366	1.090333
9	7	0	4.473687	-0.347116	0.749865
10	7	0	5.400521	0.616441	0.615708
11	7	0	4.975929	1.891394	0.631317
12	6	0	6.781589	0.299217	0.460914
13	6	0	7.200260	-1.042277	0.520106
14	6	0	7.713549	1.331356	0.250049
15	6	0	8.555425	-1.341109	0.367147
16	1	0	6.466496	-1.825058	0.695343
17	6	0	9.063541	1.010852	0.097663
18	1	0	7.368934	2.361053	0.197292
19	6	0	9.516728	-0.327081	0.152405

20	1	0	8.880495	-2.378543	0.443439
21	1	0	9.778063	1.810414	-0.096591
22	6	0	2.921613	4.141597	0.805460
23	6	0	3.162293	5.343331	0.733176
24	6	0	1.664487	-1.477605	1.106213
25	6	0	1.389430	-2.672411	1.175127
26	6	0	3.410033	6.738395	0.632419
27	6	0	2.343990	7.666787	0.771640
28	6	0	4.718588	7.226732	0.379155
29	6	0	2.586364	9.039066	0.655018
30	1	0	1.338725	7.291828	0.956542
31	6	0	4.947378	8.601972	0.265902
32	1	0	5.536783	6.514695	0.273412
33	6	0	3.885487	9.512608	0.402093
34	1	0	1.760083	9.743153	0.763679
35	1	0	5.956809	8.966207	0.070305
36	1	0	4.069337	10.583905	0.312245
37	6	0	1.058517	-4.051967	1.253485
38	6	0	-0.285587	-4.458585	1.461397
39	6	0	2.065387	-5.044165	1.117064
40	6	0	-0.607118	-5.817211	1.529692
41	1	0	-1.062165	-3.701308	1.550114
42	6	0	1.730274	-6.400176	1.186624
43	1	0	3.096905	-4.731389	0.956196
44	6	0	0.395591	-6.791719	1.392367
45	1	0	-1.644266	-6.117107	1.670951
46	1	0	2.511021	-7.154536	1.079509
47	1	0	0.134095	-7.849451	1.440050
48	1	0	0.041636	-0.609320	-1.217681
49	6	0	-0.999662	-0.905334	-1.110115
50	6	0	-1.980724	0.103170	-1.031096
51	6	0	-1.308936	-2.282287	-1.038040
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53	6	0	-1.664646	1.477956	-1.106509
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55	1	0	-0.496561	-3.003916	-1.090774
56	6	0	-3.641323	-1.755440	-0.790869
57	7	0	-4.473799	0.347291	-0.749731
58	6	0	-1.389478	2.672726	-1.175564
59	6	0	-2.921432	-4.141309	-0.805781
60	7	0	-4.975859	-1.891263	-0.631203
61	7	0	-5.400546	-0.616343	-0.615510
62	6	0	-1.058519	4.052258	-1.254142
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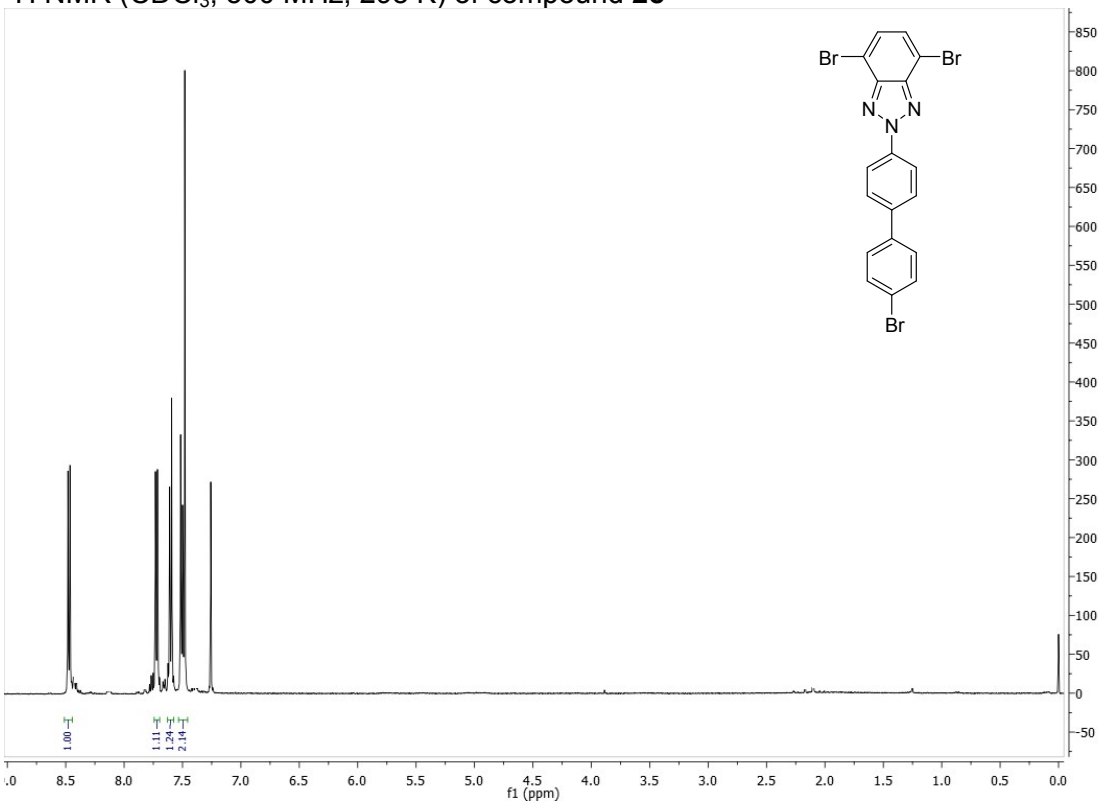
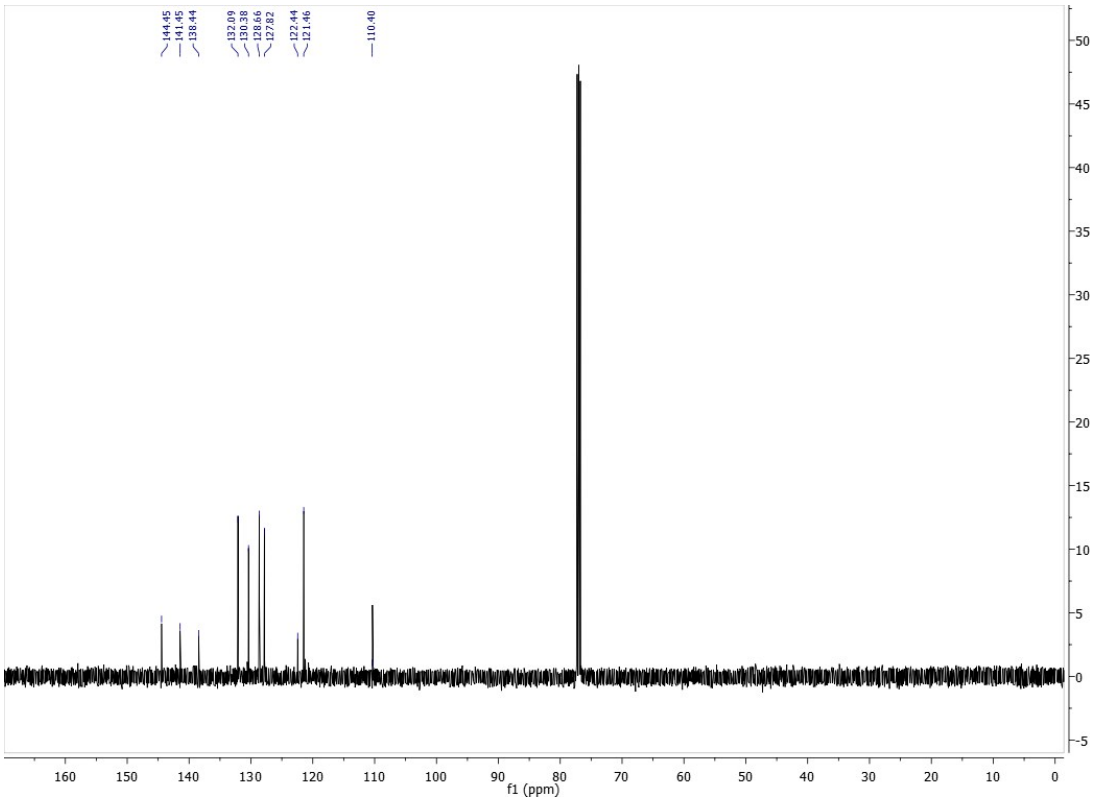
65	6	0	0.285638	4.458823	-1.461827
66	6	0	-2.065420	5.044489	-1.118196
67	6	0	-3.409826	-6.738123	-0.632973
68	6	0	-7.200413	1.042226	-0.519688
69	6	0	-7.713488	-1.331460	-0.249706
70	6	0	0.607186	5.817435	-1.530371
71	1	0	1.062238	3.701523	-1.550163
72	6	0	-1.730292	6.400481	-1.188020
73	1	0	-3.096976	4.731753	-0.957504
74	6	0	-2.343795	-7.666502	-0.772382
75	6	0	-4.718363	-7.226487	-0.379667
76	6	0	-8.555591	1.340939	-0.366613
77	1	0	-6.466730	1.825076	-0.694948
78	6	0	-9.063496	-1.011074	-0.097211
79	1	0	-7.368786	-2.361132	-0.197024
80	6	0	-0.395562	6.791973	-1.393542
81	1	0	1.644373	6.117306	-1.671405
82	1	0	-2.511064	7.154868	-1.081282
83	6	0	-2.586163	-9.038795	-0.655904
84	1	0	-1.338549	-7.291528	-0.957364
85	6	0	-4.947148	-8.601740	-0.266558
86	1	0	-5.536548	-6.514460	-0.273779
87	6	0	-9.516799	0.326823	-0.151862

88	1	0	-8.880746	2.378352	-0.442829
89	1	0	-9.777936	-1.810707	0.097054
90	1	0	-0.134060	7.849695	-1.441423
91	6	0	-3.885269	-9.512364	-0.402934
92	1	0	-1.759894	-9.742873	-0.764711
93	1	0	-5.956566	-8.965995	-0.070927
94	1	0	-4.069115	-10.583670	-0.313195
95	6	0	10.952491	-0.654544	-0.012082
96	6	0	11.358946	-1.857945	-0.631414
97	6	0	11.956870	0.228758	0.443696
98	6	0	12.712936	-2.172699	-0.794711
99	1	0	10.604812	-2.544488	-1.016652
100	6	0	13.315251	-0.069412	0.288060
101	1	0	11.671058	1.150144	0.951369
102	6	0	13.682677	-1.271545	-0.332810
103	1	0	13.012681	-3.098472	-1.283189
104	1	0	14.078934	0.615794	0.652034
105	6	0	-10.952575	0.654175	0.012736
106	6	0	-11.956933	-0.229190	-0.442967
107	6	0	-11.359062	1.857559	0.632077
108	6	0	-13.315321	0.068903	-0.287249
109	1	0	-11.671101	-1.150563	-0.950654
110	6	0	-12.713059	2.172240	0.795455
111	1	0	-10.604943	2.544151	1.017257
112	6	0	-13.682778	1.271026	0.333625
113	1	0	-14.078988	-0.616351	-0.651167
114	1	0	-13.012824	3.098003	1.283938
115	35	0	15.542013	-1.687379	-0.555643
116	35	0	-15.542121	1.686764	0.556559

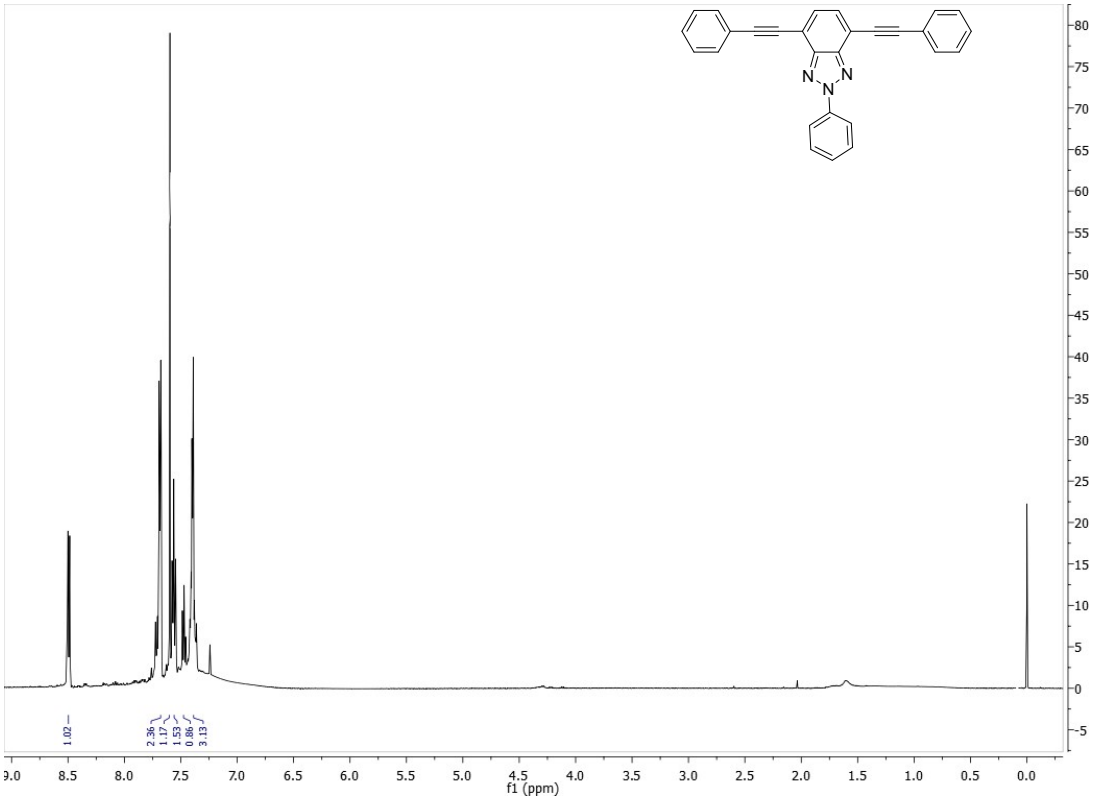
Collection of spectra

^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) of compound **2c**

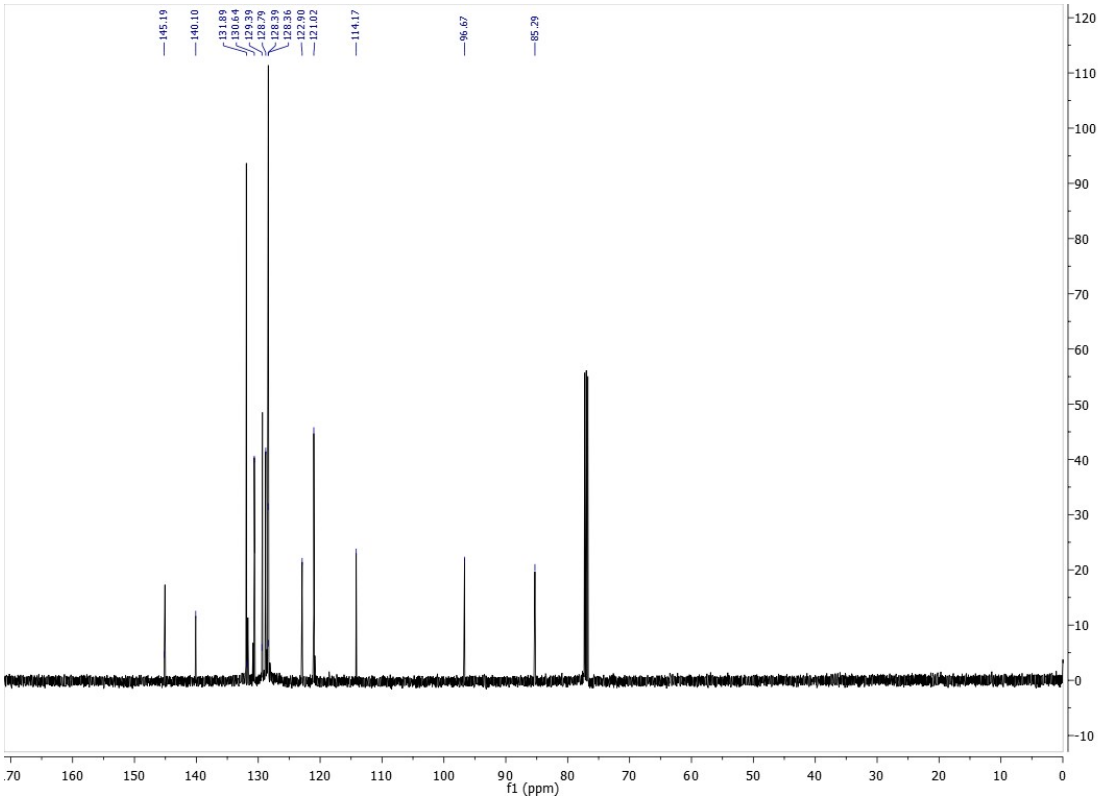




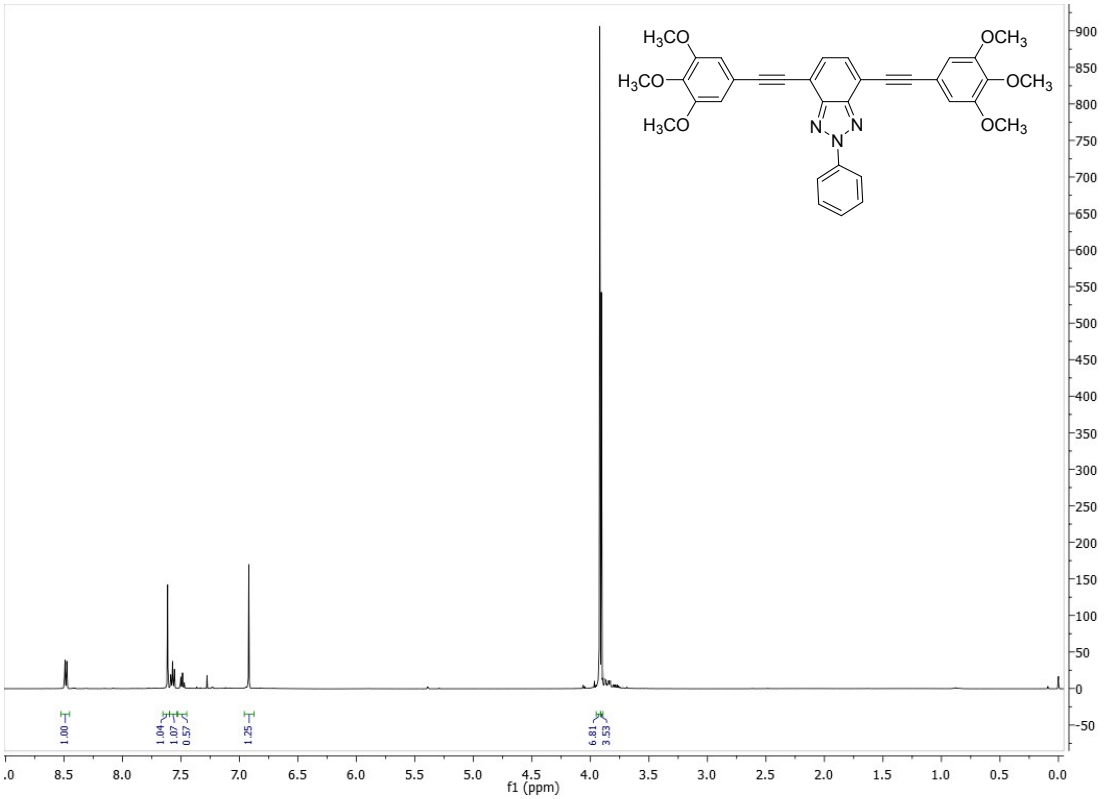
^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) of compound **1a**



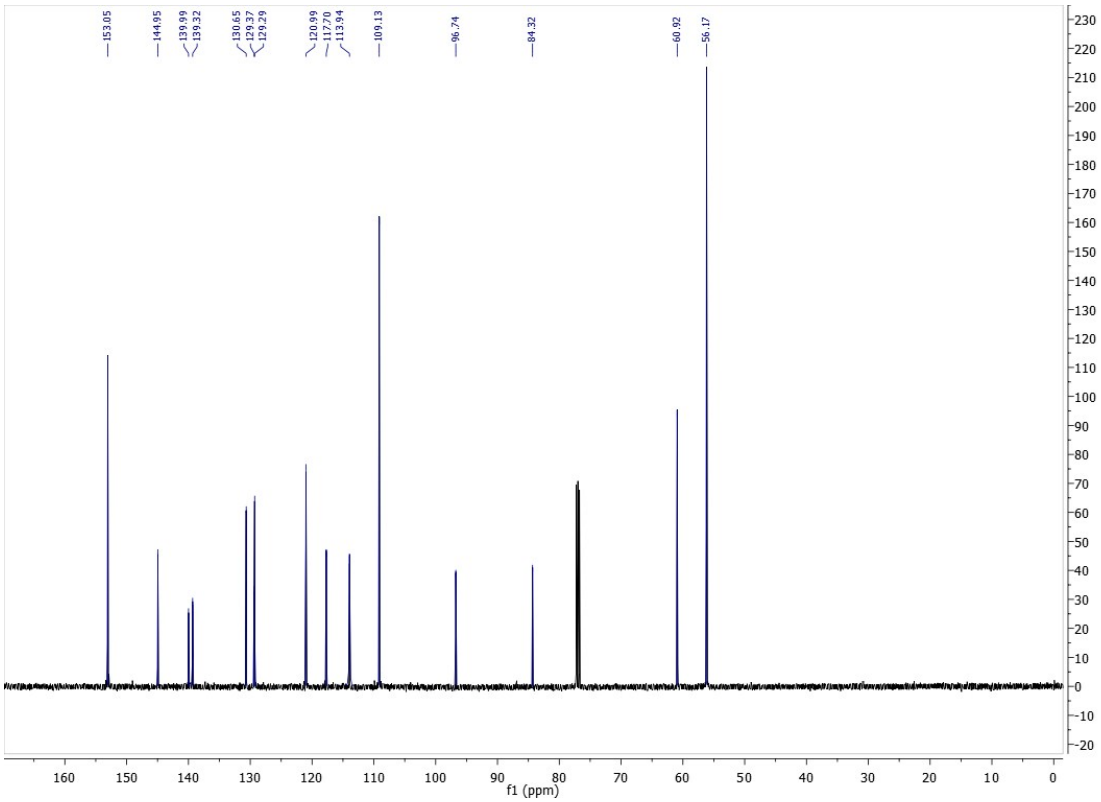
^{13}C NMR ($CDCl_3$, 125 MHz, 298 K) of compound **1a**



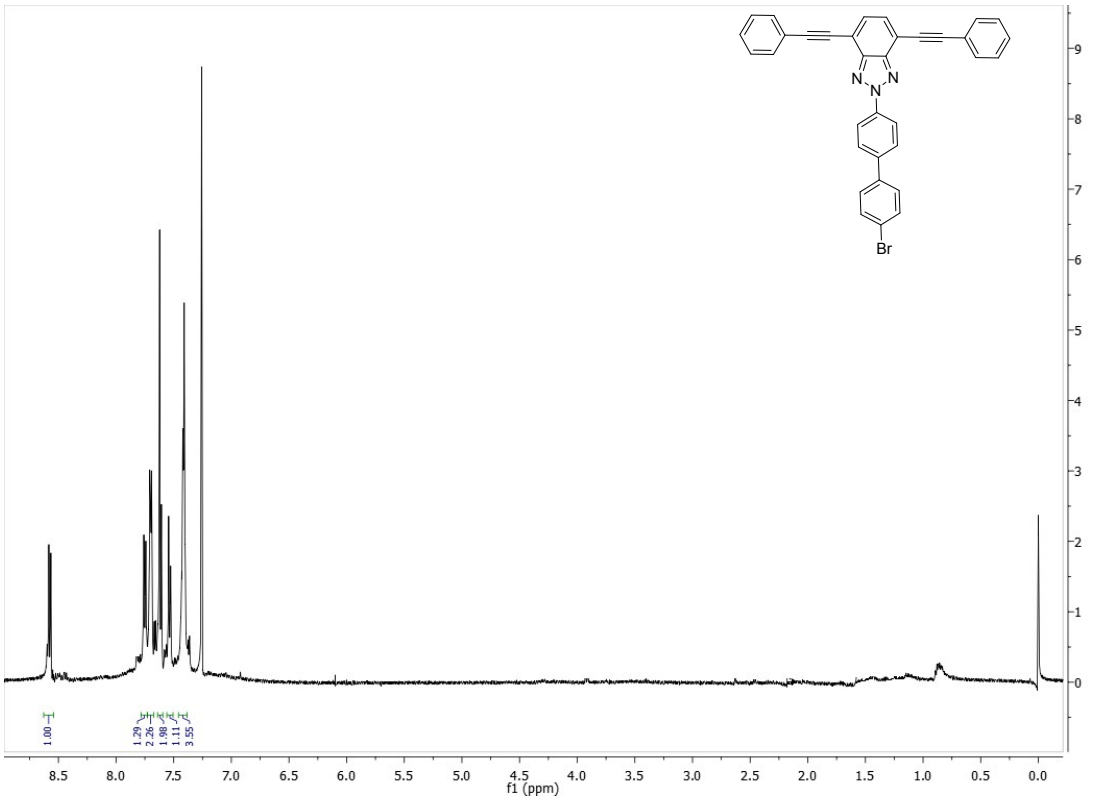
^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) of compound **1c**



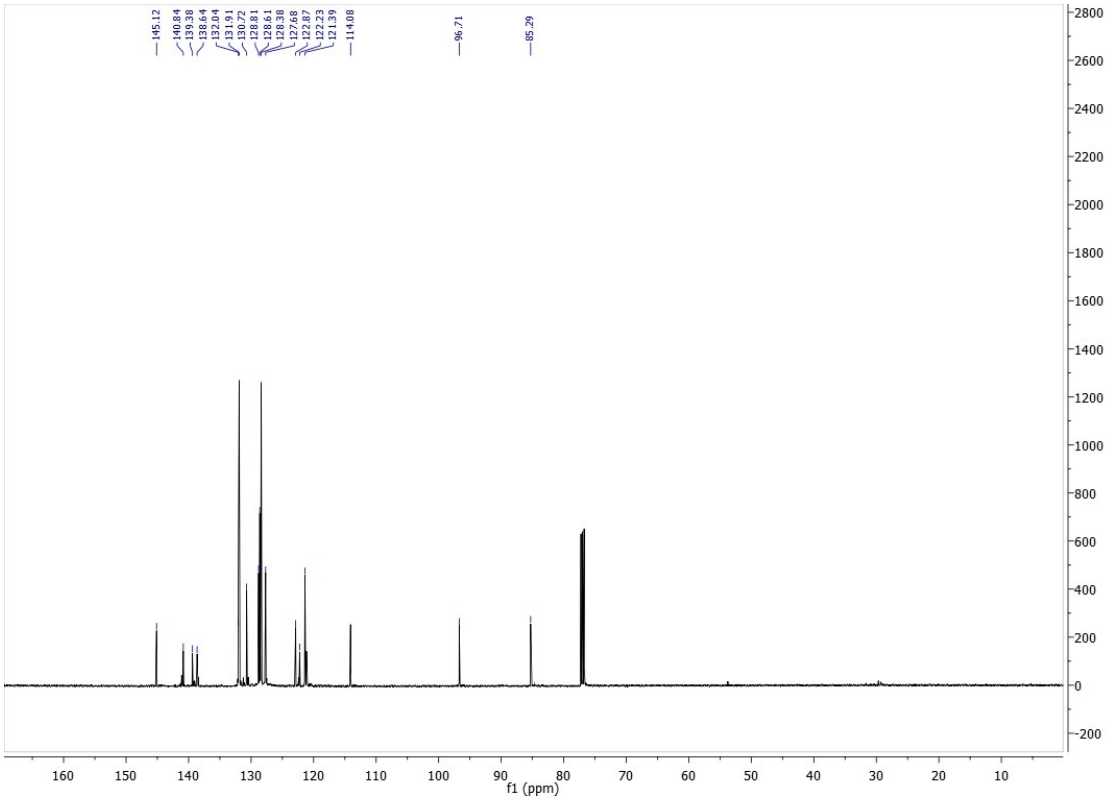
^{13}C NMR ($CDCl_3$, 125 MHz, 298 K) of compound **1c**



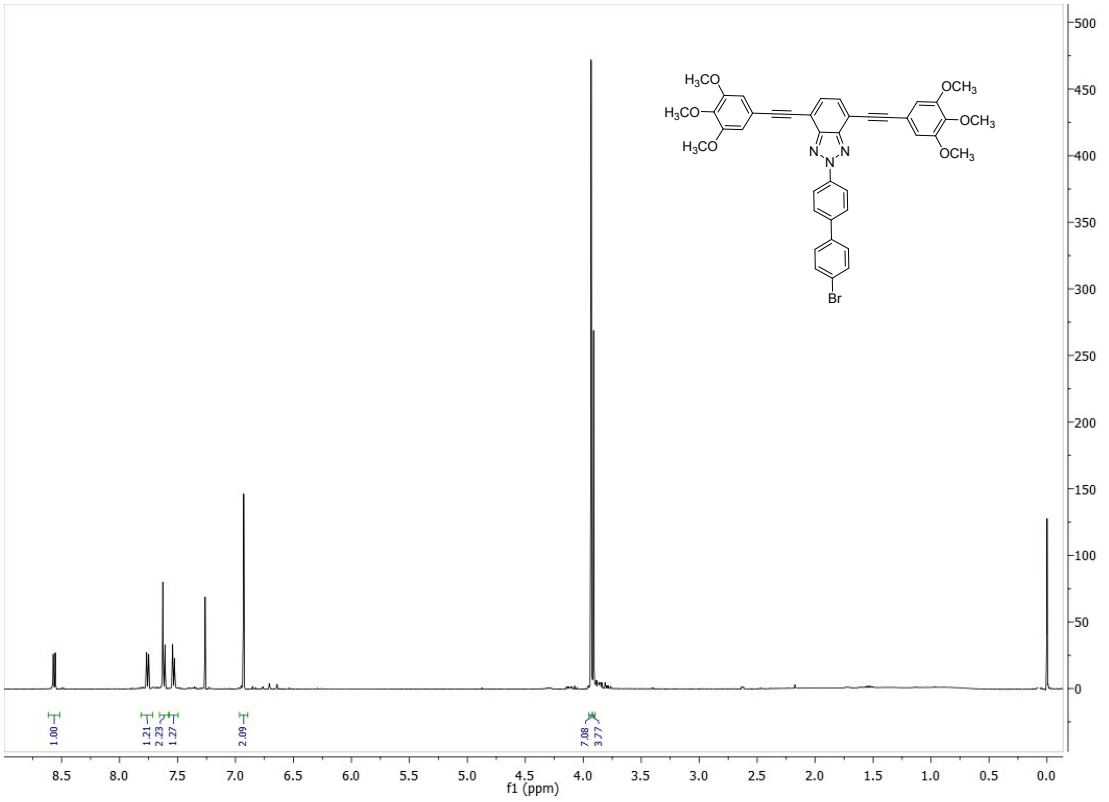
^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) of compound **1e**



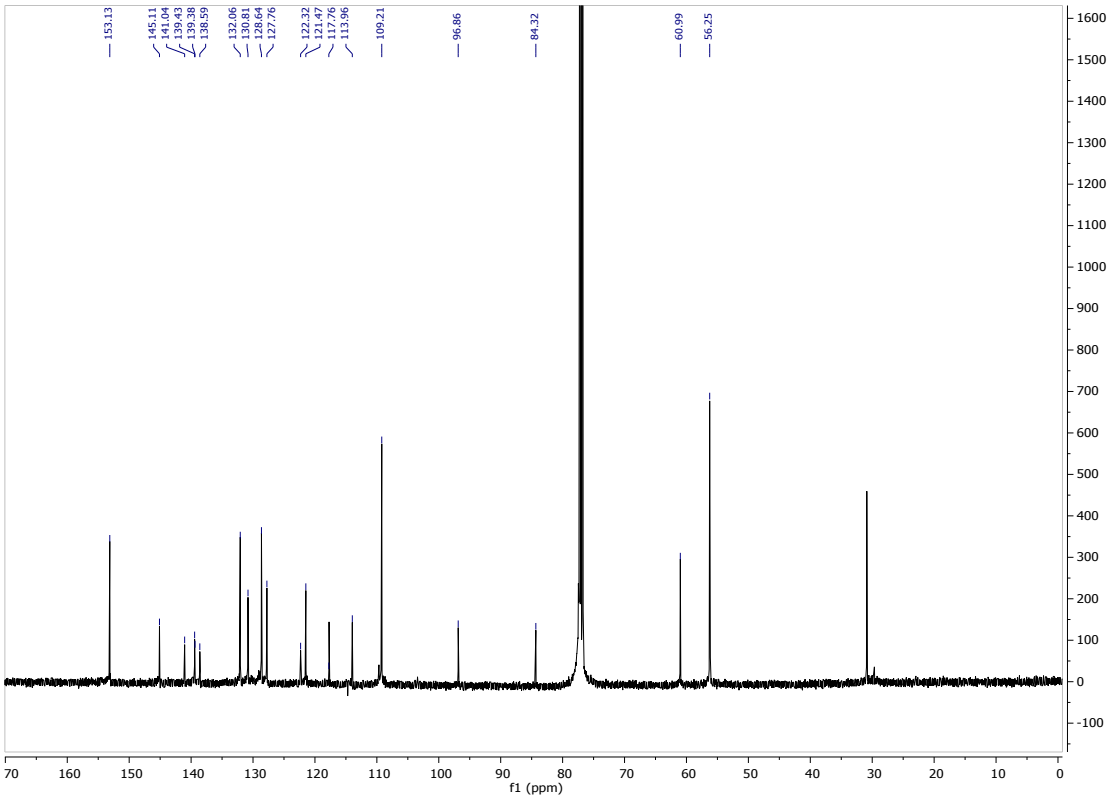
^{13}C NMR ($CDCl_3$, 125 MHz, 298 K) of compound **1e**



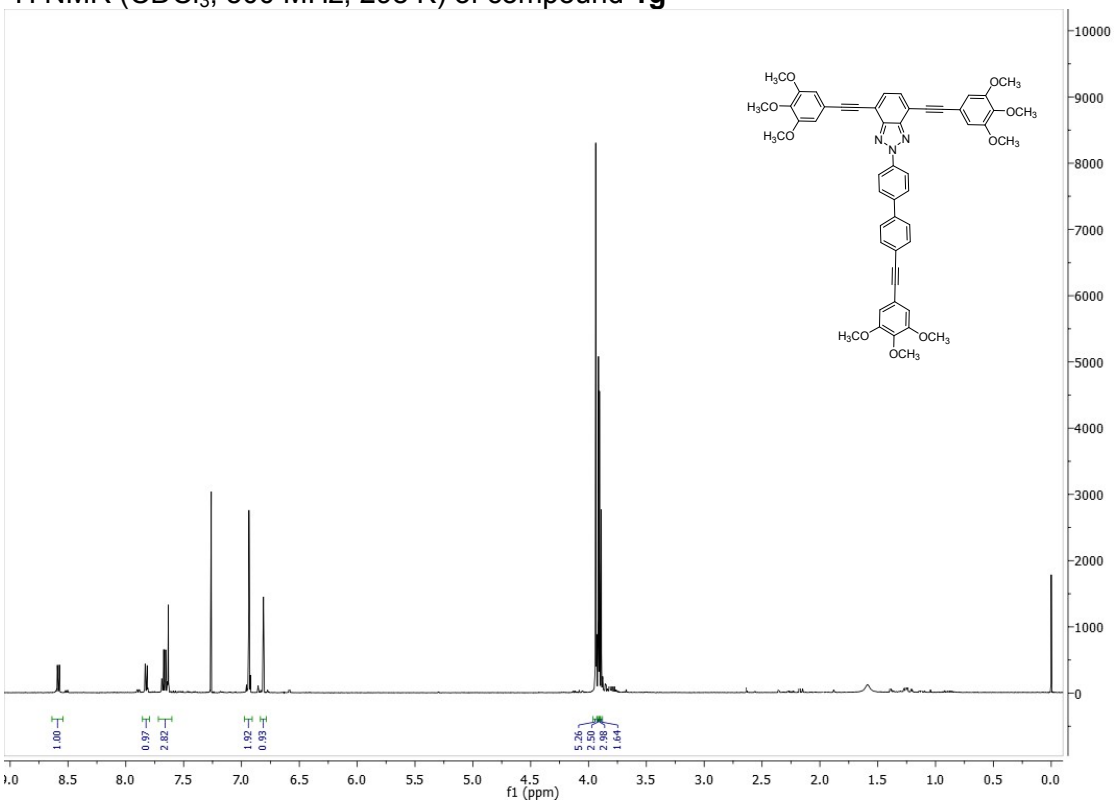
^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) of compound **1f**



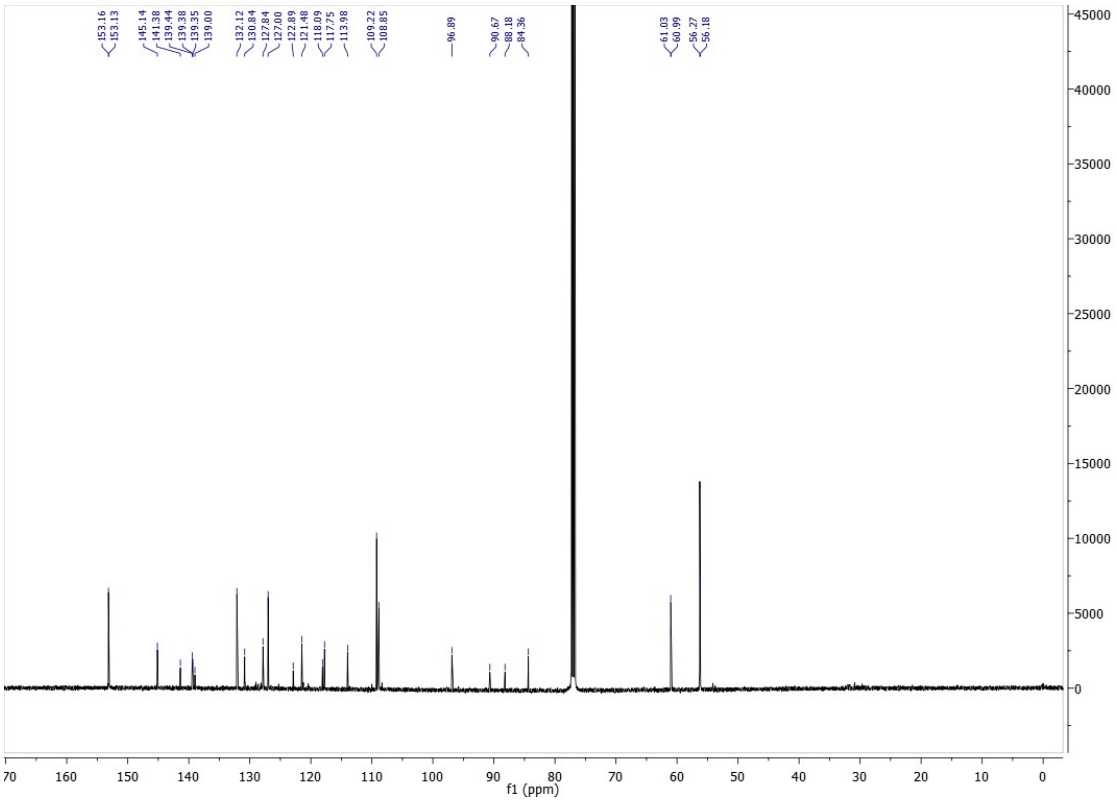
^{13}C NMR ($CDCl_3$, 125 MHz, 298 K) of compound **1f**



^{1}H NMR ($CDCl_3$, 500 MHz, 298 K) of compound **1g**



^{13}C NMR ($CDCl_3$, 125 MHz, 298 K) of compound **1g**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130.84
127.84
127.00
122.89
121.48
118.09
117.75
113.98
109.22
108.85
96.89
90.67
88.18
84.36
61.03
60.99
56.27
56.18
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
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160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)