

Understanding the Influence of Geometric and Electronic Structure on the Excited State Dynamical and Photoredox Properties of Perinone Chromophores

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1. Structural Characterization Data

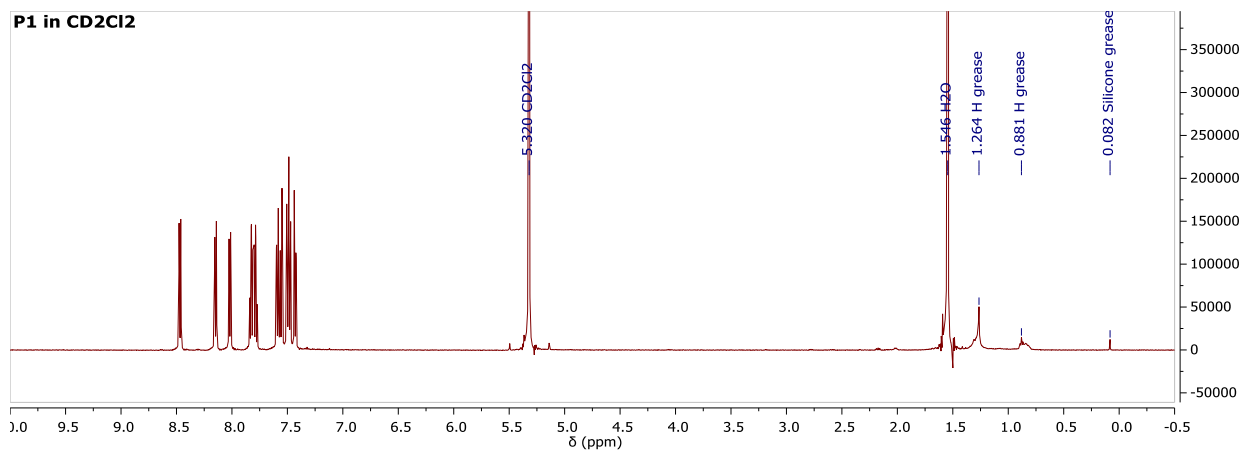


Figure S1. ¹H NMR spectrum of **1** in CD₂Cl₂ (500 MHz).

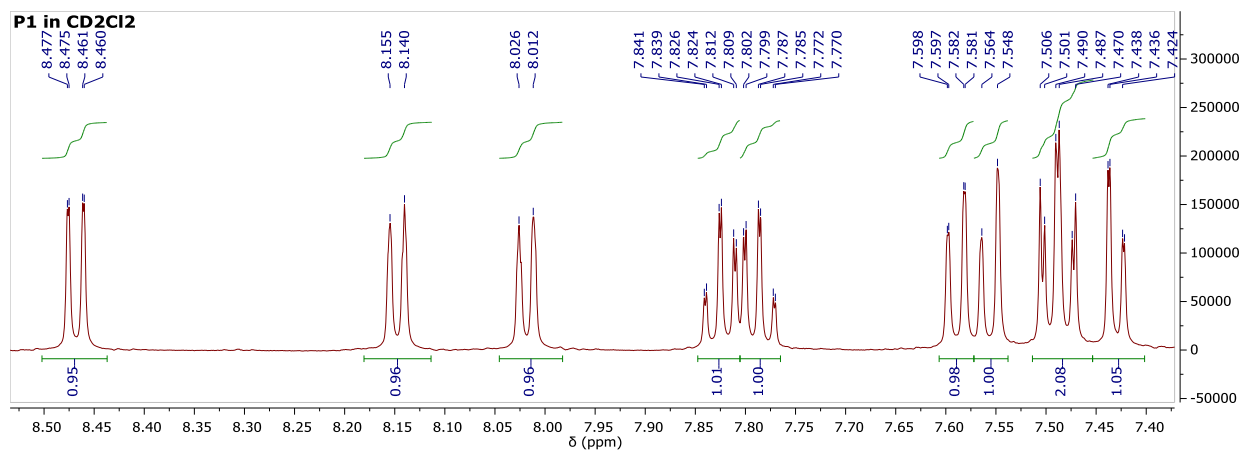


Figure S2. ¹H NMR spectrum of **1** (zoomed into aromatic region) in CD₂Cl₂ (500 MHz).

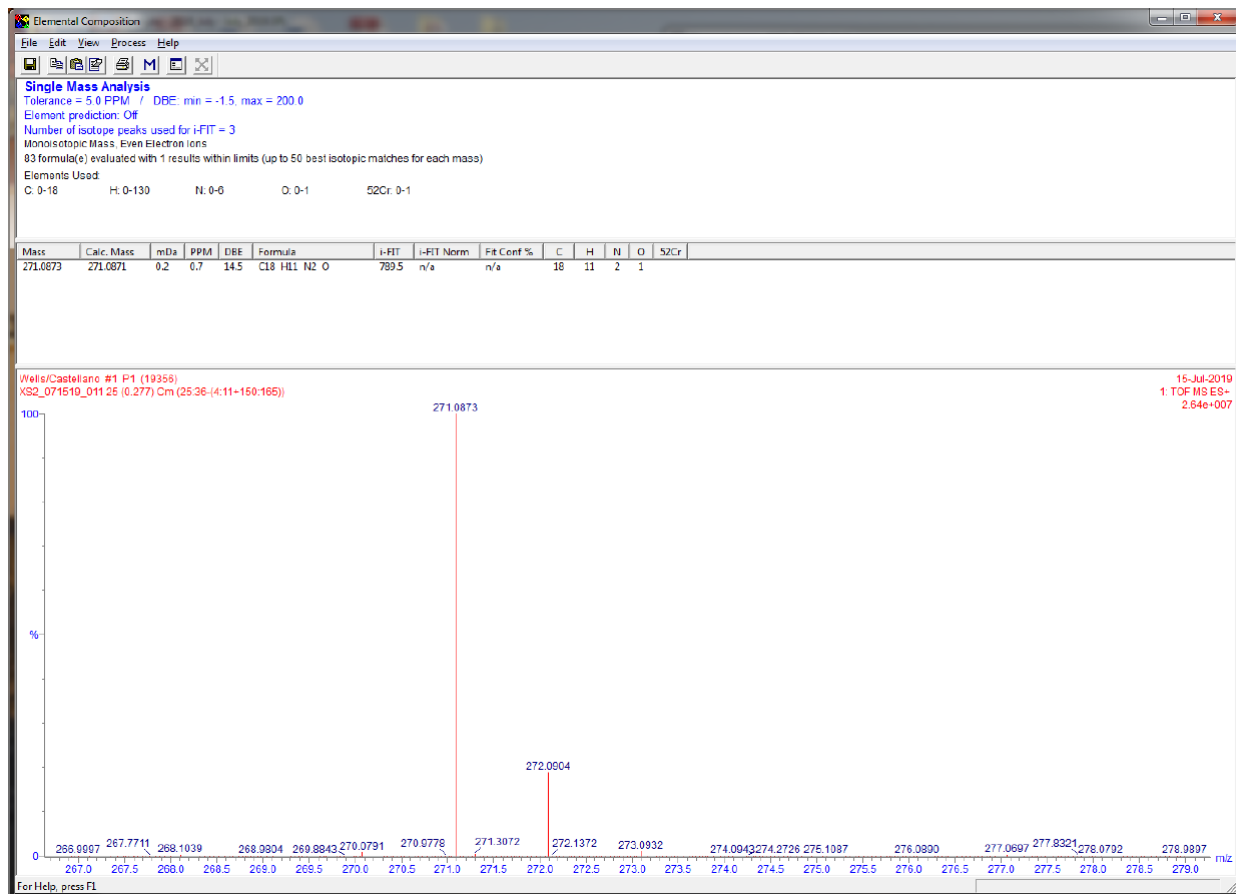


Figure S3. High resolution mass spectrum of **1**.

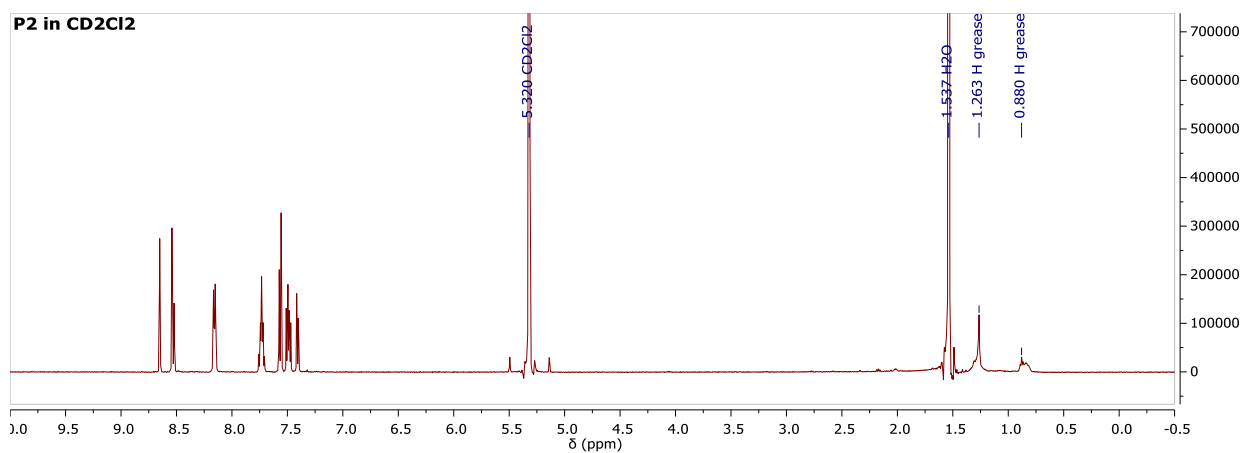


Figure S4. ¹H NMR spectrum of **2** in CD₂Cl₂ (500 MHz).

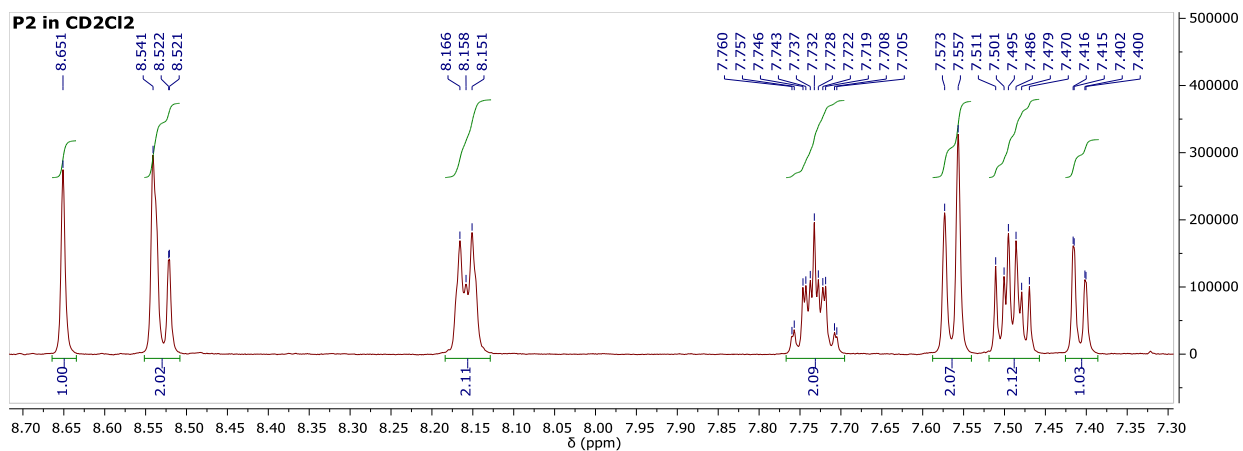


Figure S5. ^1H NMR spectrum of **2** (zoomed into aromatic region) in CD_2Cl_2 (500 MHz).

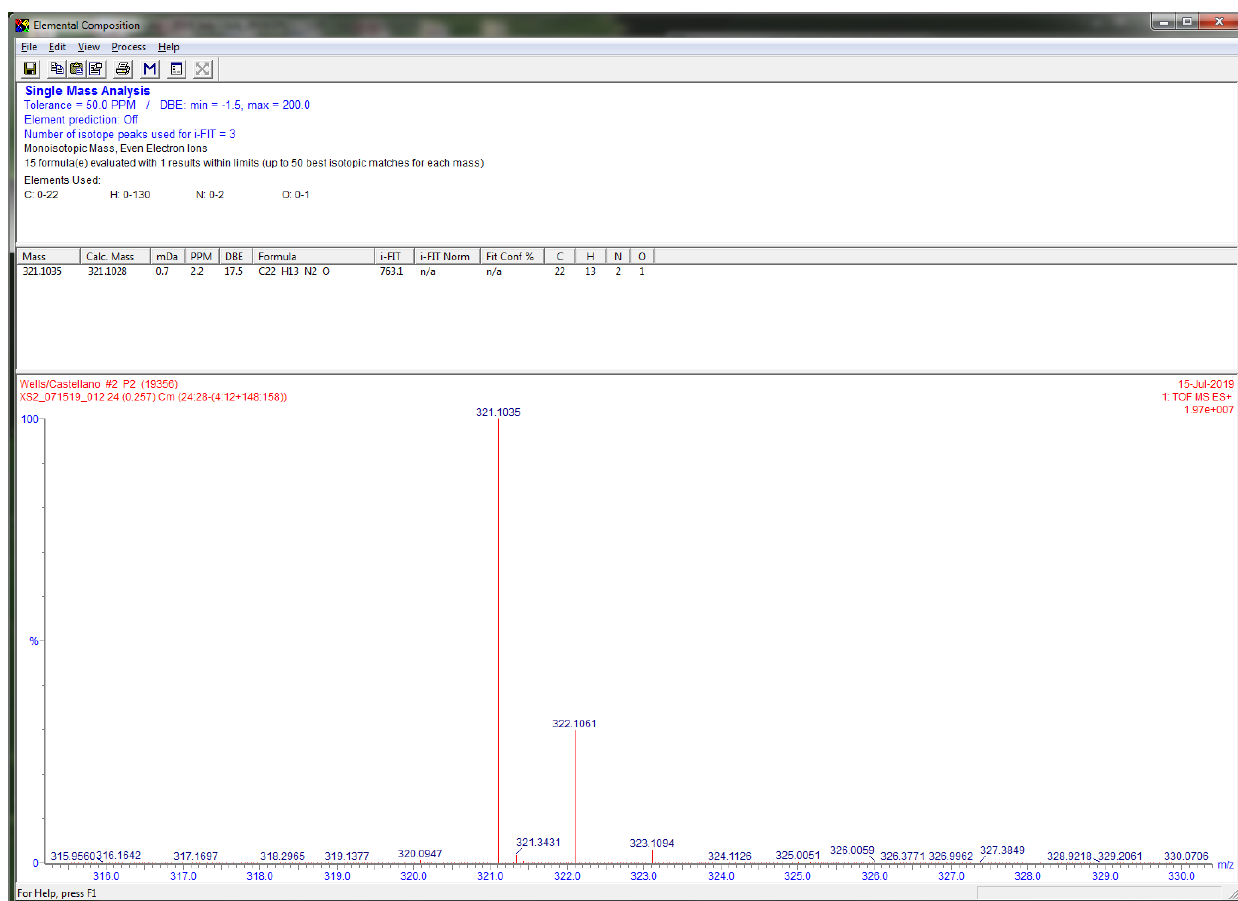


Figure S6. High resolution mass spectrum of **2**.

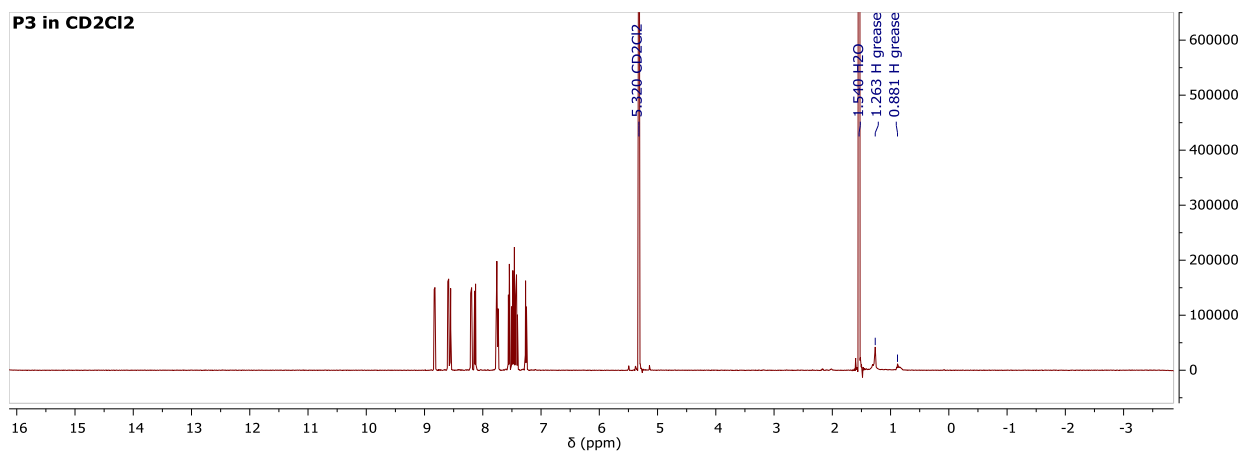


Figure S7. ^1H NMR spectrum of **3** in CD_2Cl_2 (500 MHz).

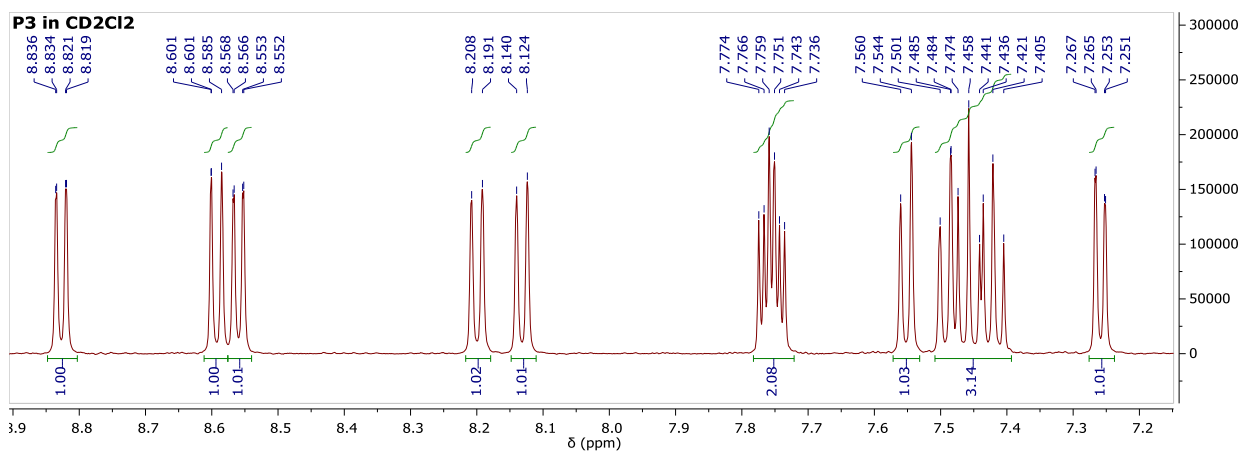


Figure S8. ^1H NMR spectrum of **3** (zoomed into aromatic region) in CD_2Cl_2 (500 MHz).

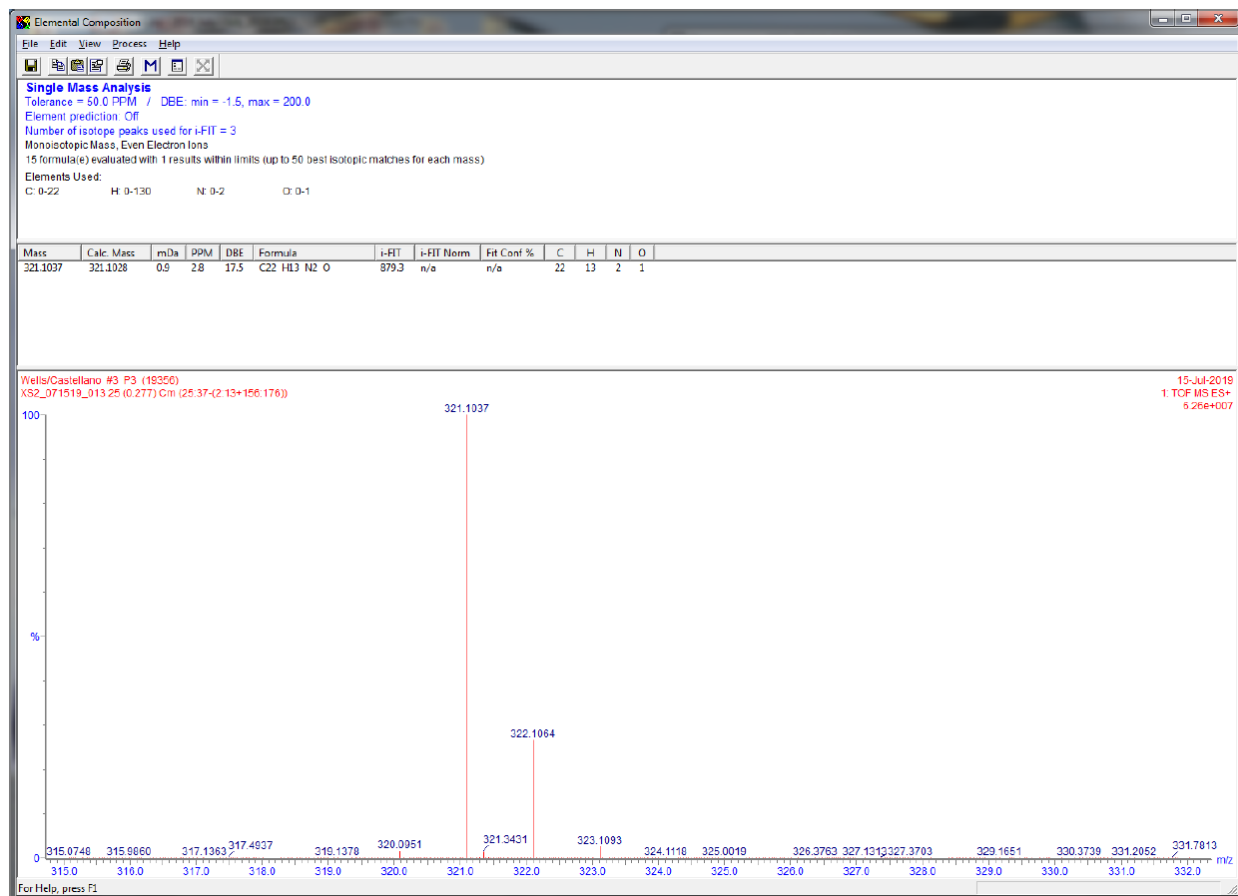


Figure S9. High resolution mass spectrum of **3**.

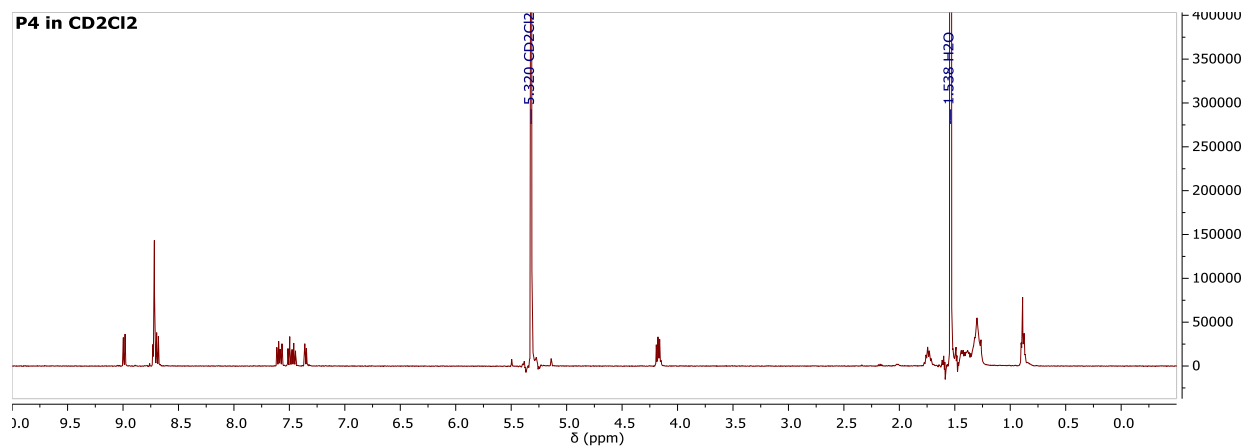


Figure S10. ^1H NMR spectrum of **4** in CD_2Cl_2 (500 MHz).

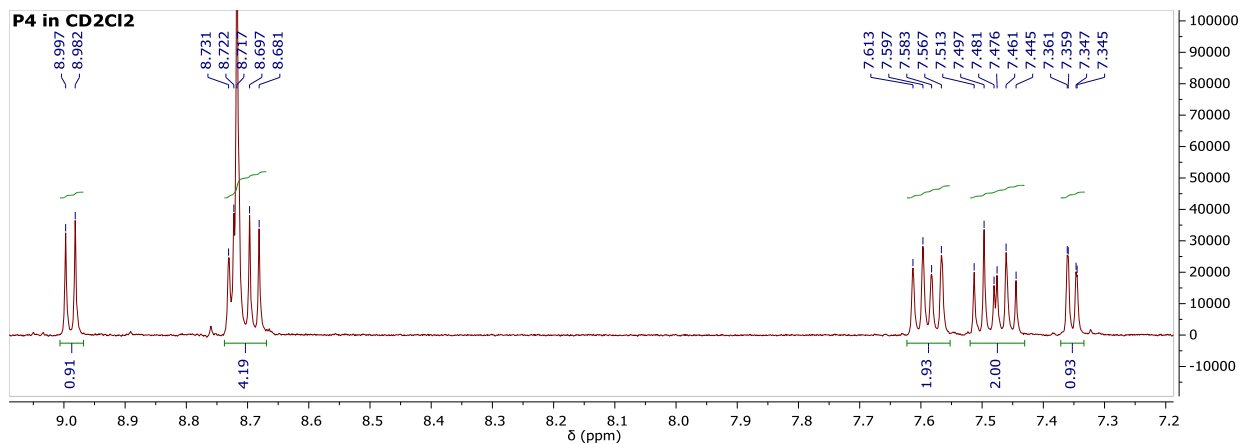


Figure S11. ¹H NMR spectrum of **4** (zoomed into aromatic region) in CD₂Cl₂ (500 MHz).

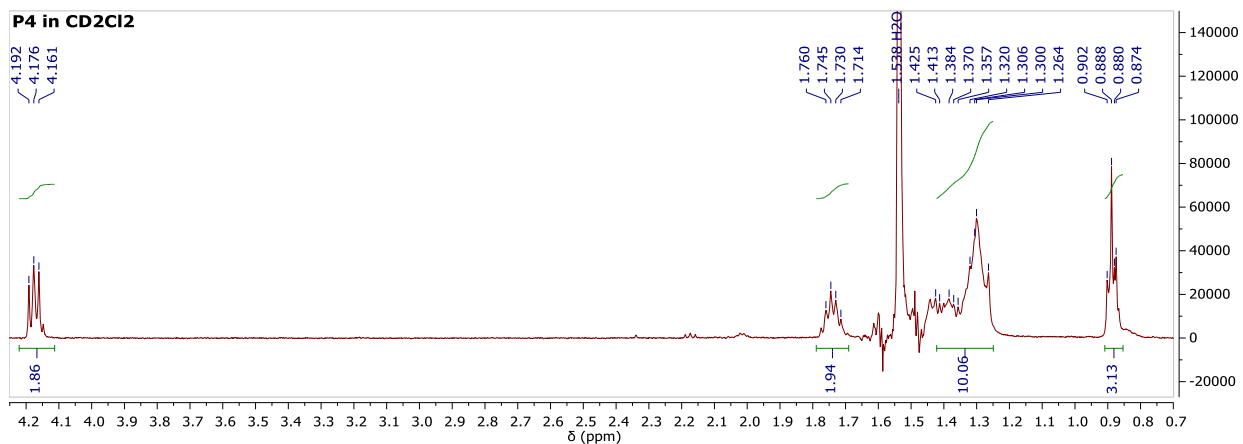


Figure S12. ¹H NMR spectrum of **4** (zoomed into aliphatic region) in CD₂Cl₂ (500 MHz).

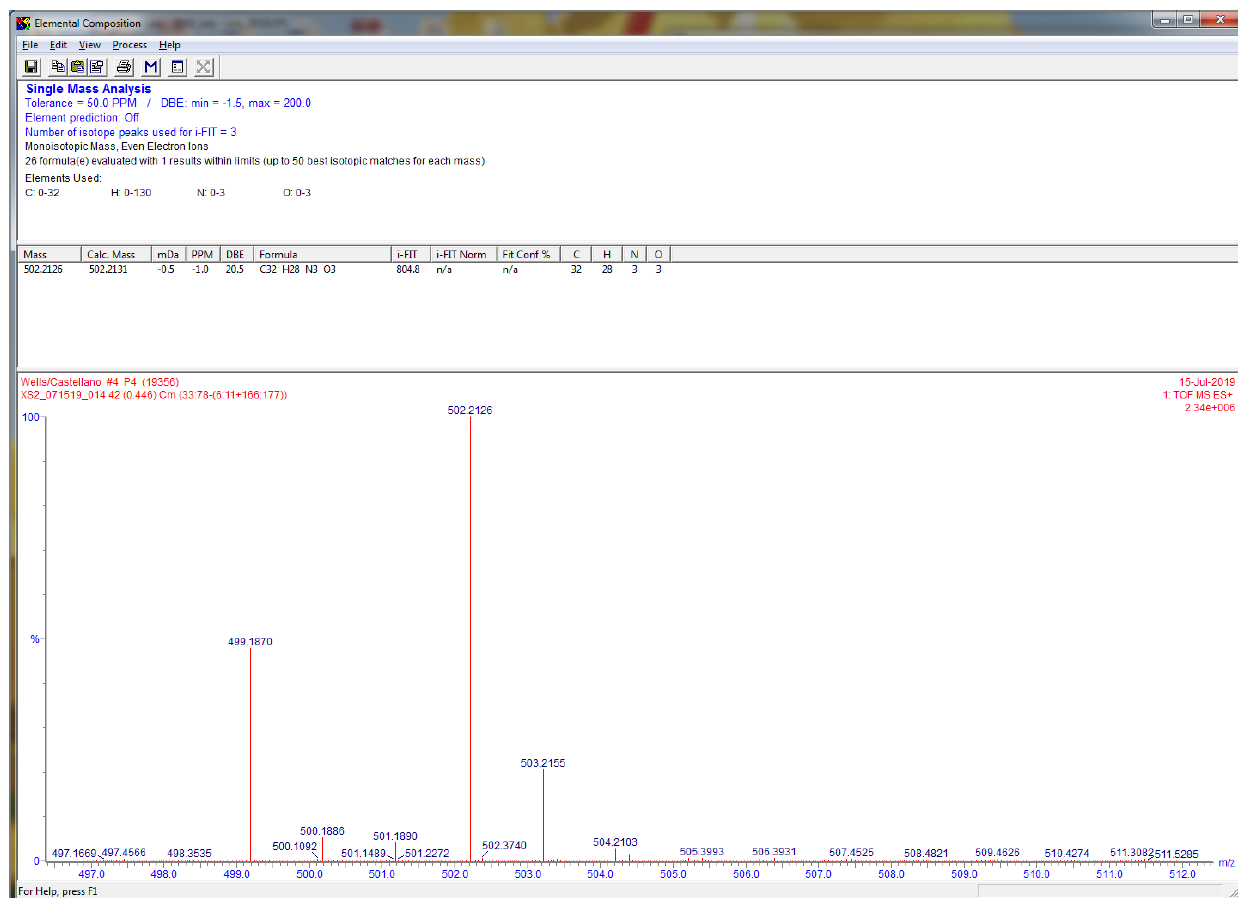


Figure S13. High resolution mass spectrum of **4**.

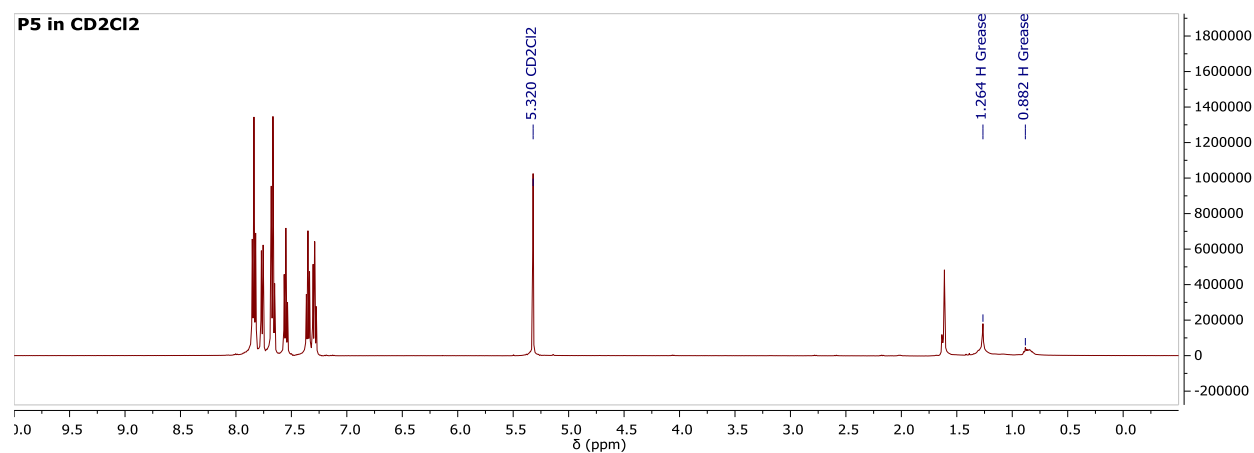


Figure S14. ¹H NMR spectrum of **5** in CD₂Cl₂ (500 MHz).

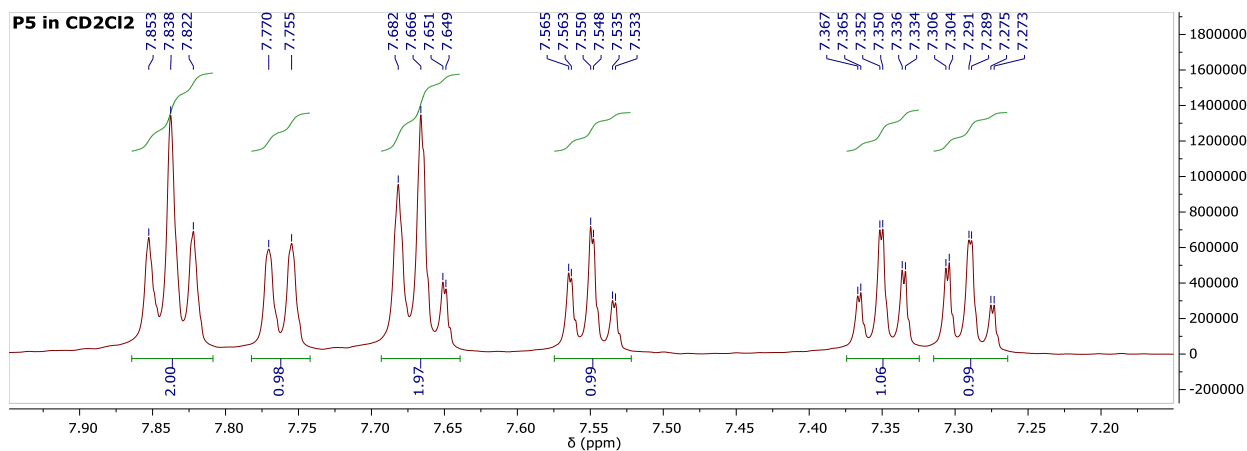


Figure S15. ^1H NMR spectrum of **5** (zoomed into aromatic region) in CD_2Cl_2 (500 MHz).

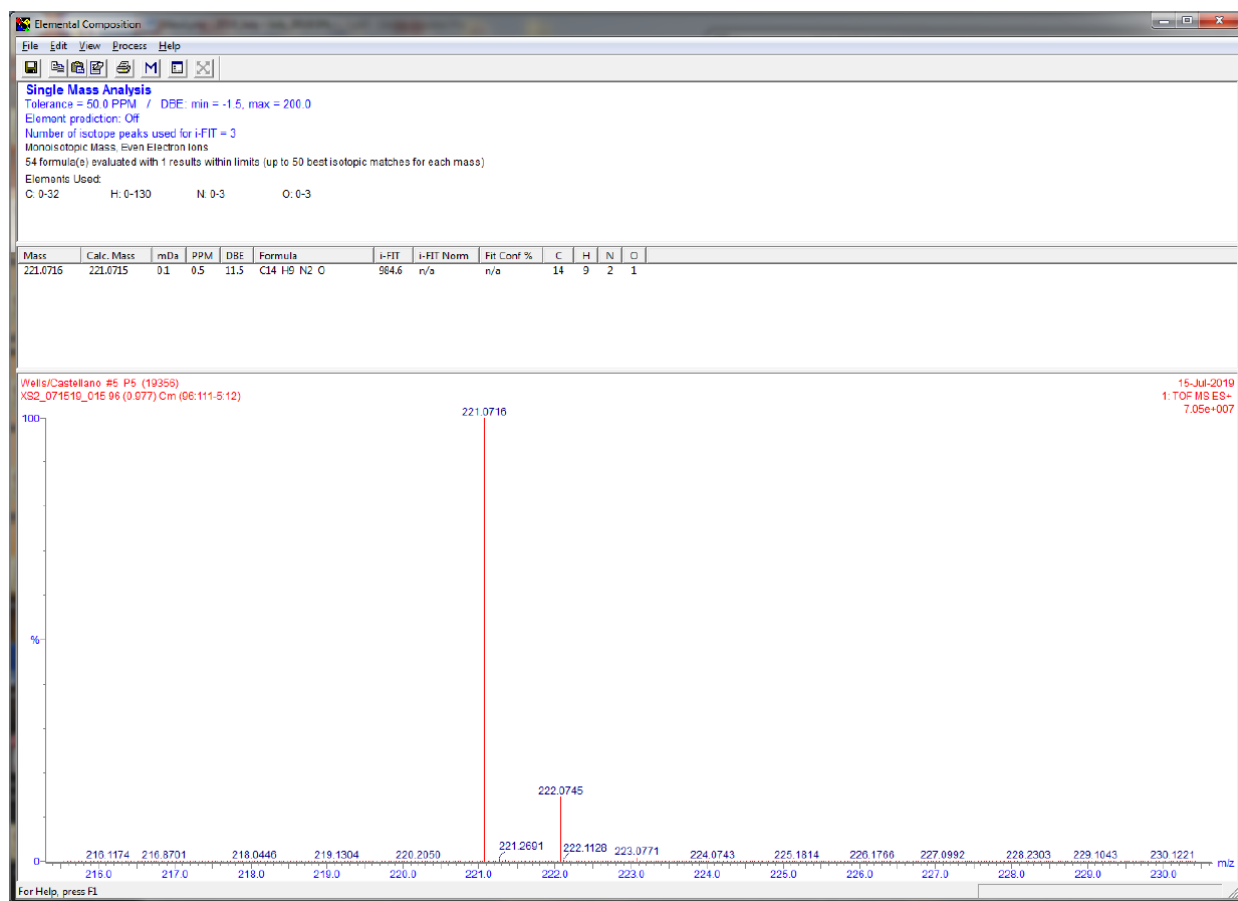


Figure S16. High resolution mass spectrum of **5**.

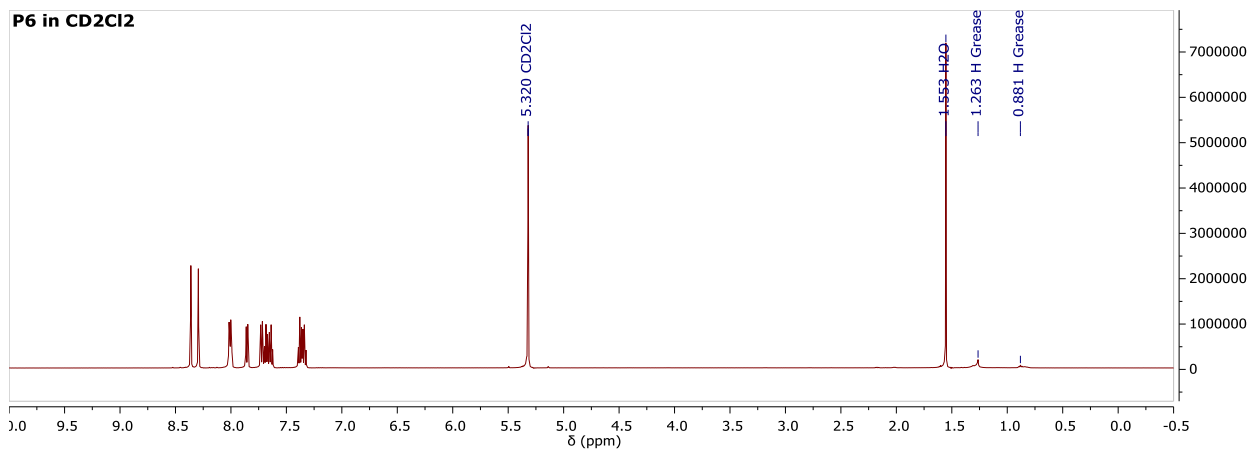


Figure S17. ¹H NMR spectrum of **6** in CD₂Cl₂ (500 MHz).

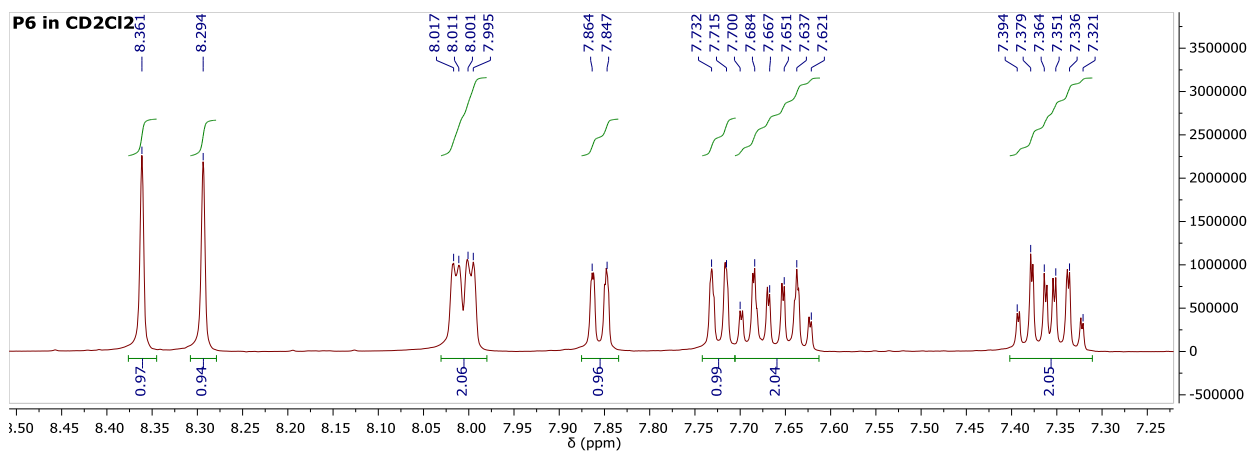


Figure S18. ¹H NMR spectrum of **6** (zoomed into aromatic region) in CD₂Cl₂ (500 MHz).

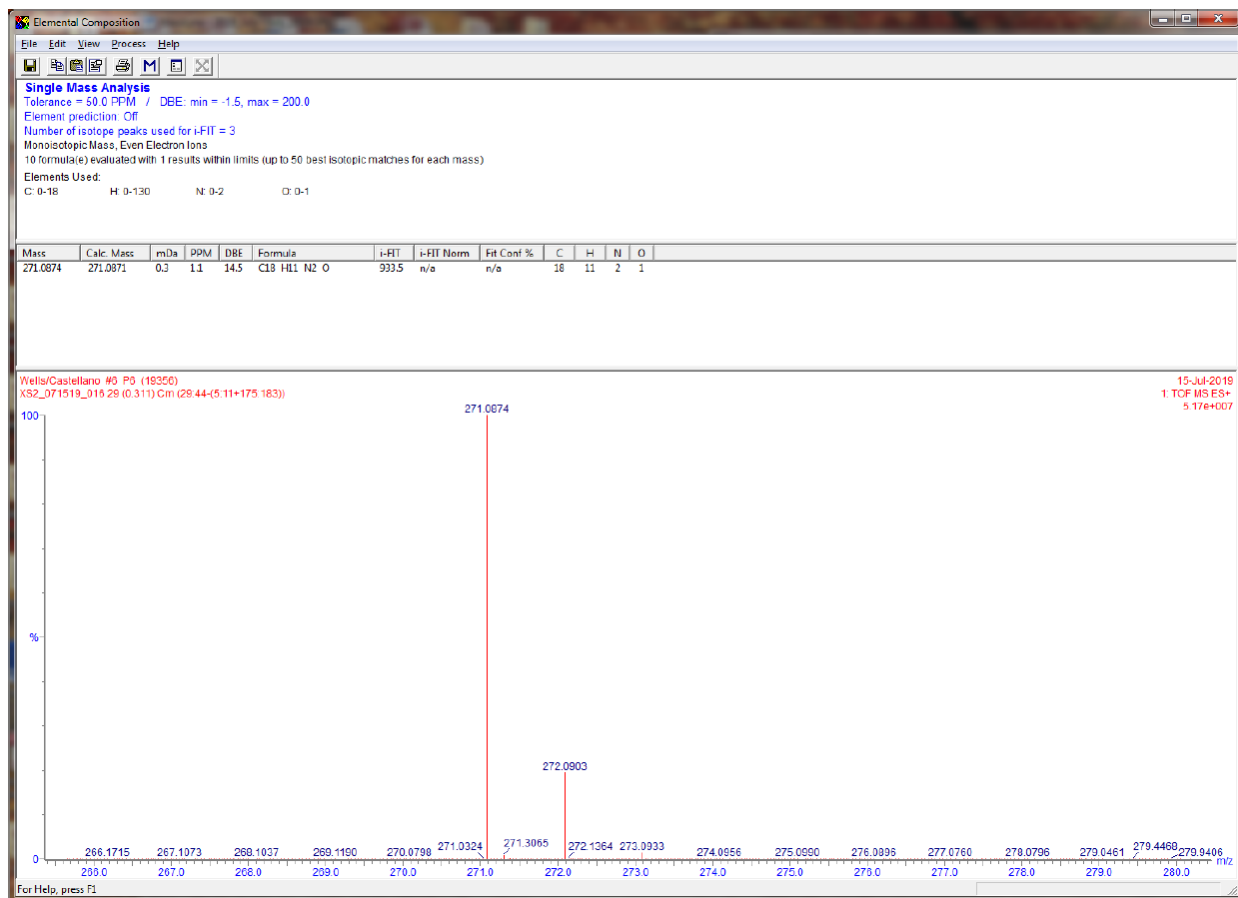


Figure S19. High resolution mass spectrum of 6.

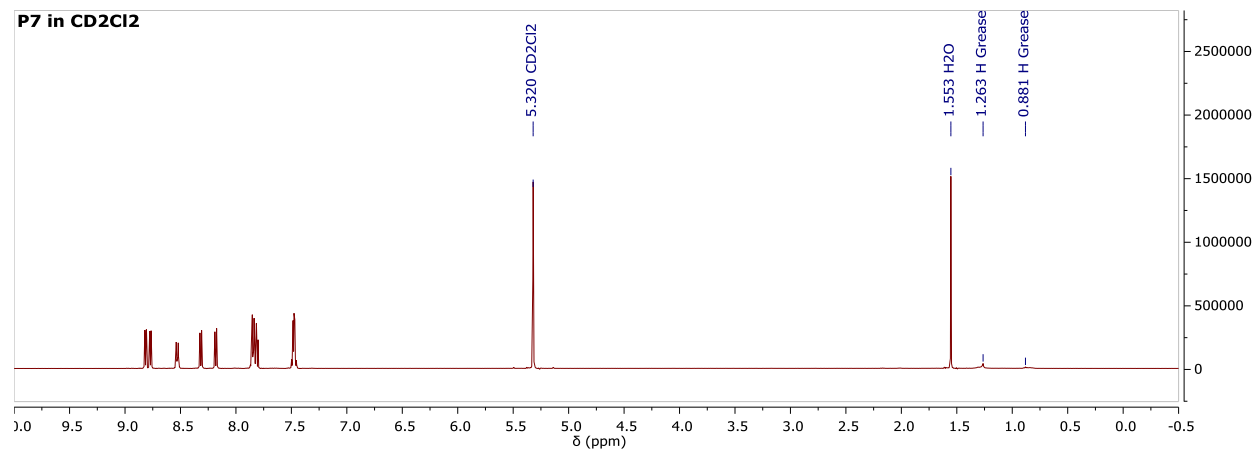


Figure S20. ¹H NMR spectrum of 7 in CD₂Cl₂ (500 MHz).

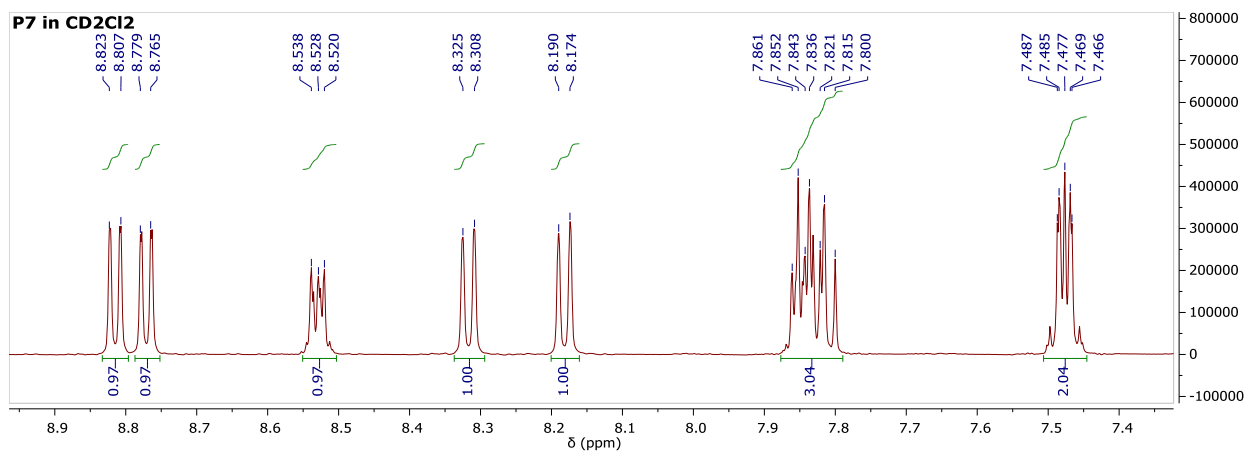


Figure S21. ¹H NMR spectrum of **7** (zoomed into aromatic region) in CD₂Cl₂ (500 MHz).

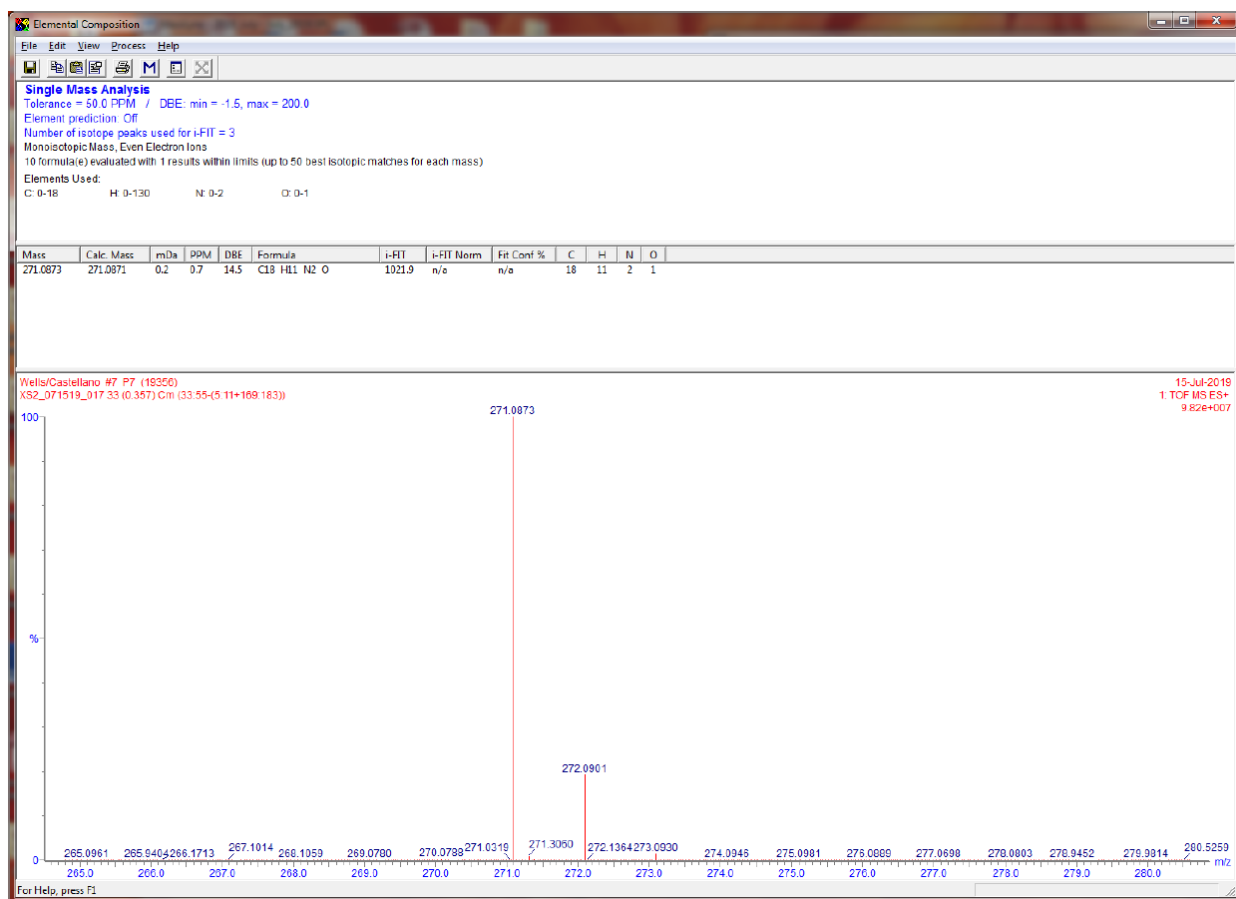


Figure S22. High resolution mass spectrum of **7**.

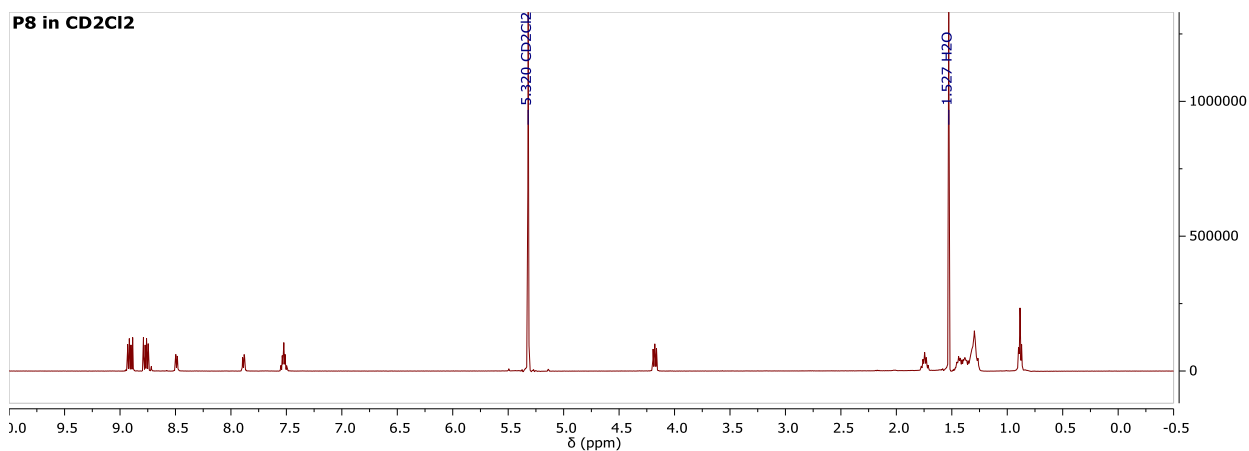


Figure S23. ¹H NMR spectrum of **8** in CD₂Cl₂ (500 MHz).

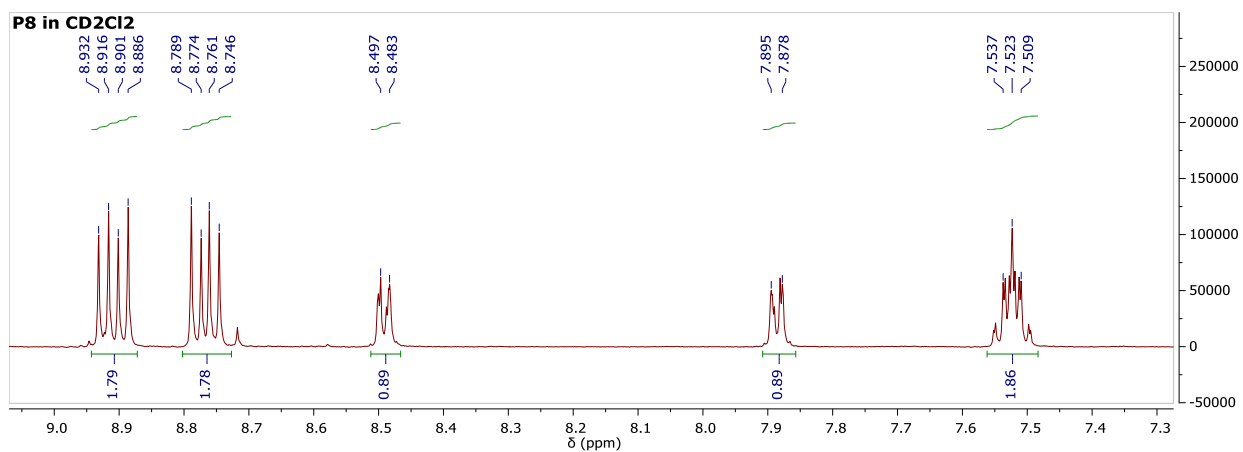


Figure S24. ¹H NMR spectrum of **8** (zoomed into aromatic region) in CD₂Cl₂ (500 MHz).

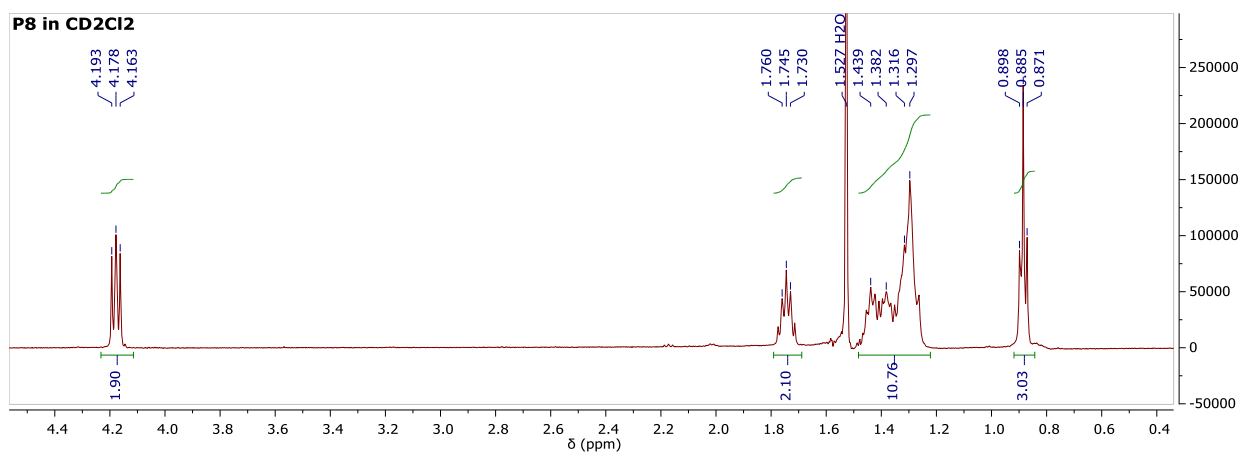


Figure S25. ¹H NMR spectrum of **8** (zoomed into aliphatic region) in CD₂Cl₂ (500 MHz).

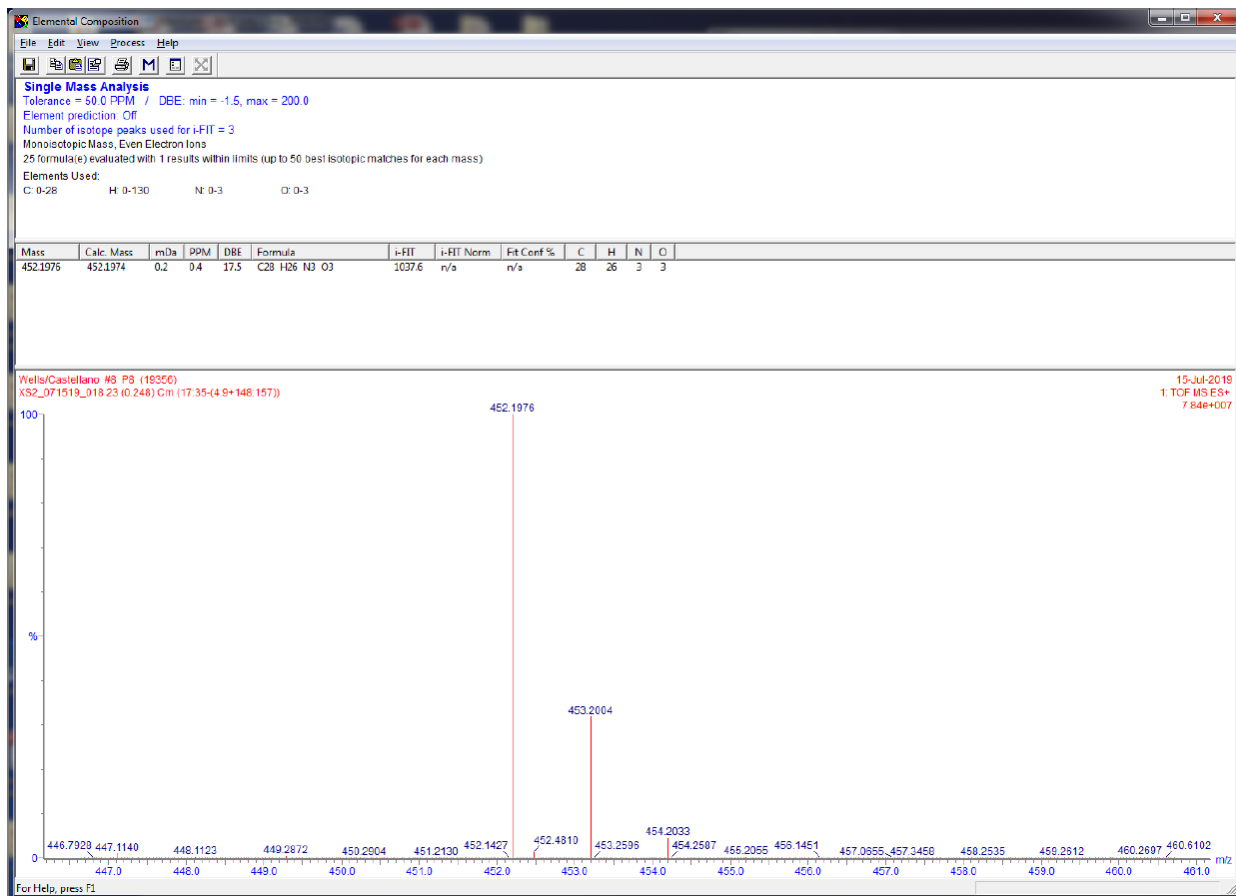


Figure S26. High resolution mass spectrum of 8.

2. Additional DFT Results

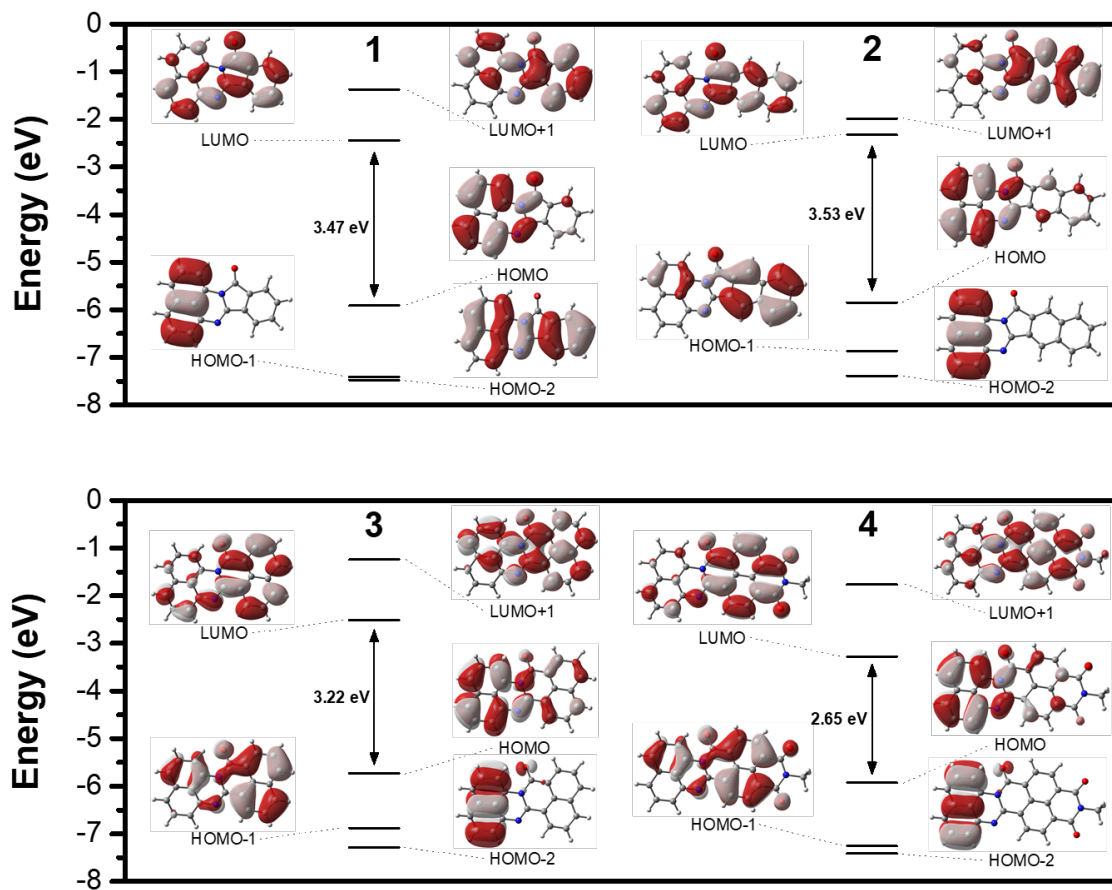


Figure S27. Frontier orbital diagram of 1-4 using M06-D3/Def2-TZVP level of theory.

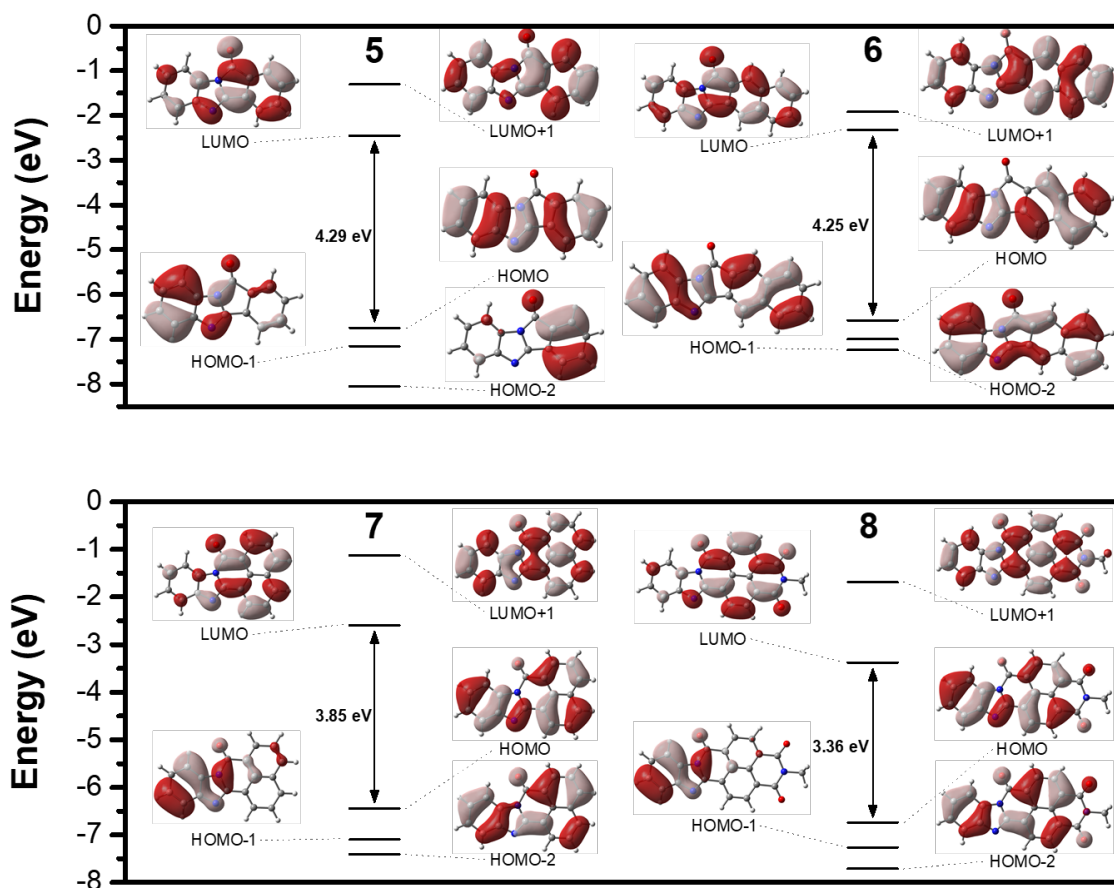


Figure S28. Frontier orbital diagram of **5-8** using M06-D3/Def2-TZVP level of theory.

Table S1. Select frontier molecular orbital energies (eV) as determined at the M06-D3/Def2-TZVP level of theory.

	1	2	3	4	5	6	7	8
LUMO+1	-1.372	-1.988	-1.242	-1.766	-1.304	-1.920	-1.122	-1.686
LUMO	-2.444	-2.322	-2.514	-3.277	-2.452	-2.321	-2.592	-3.378
HOMO	-5.911	-5.848	-5.733	-5.922	-6.744	-6.573	-6.443	-6.742
HOMO-1	-7.406	-6.866	-6.878	-7.251	-7.148	-6.999	-7.100	-7.264
HOMO-2	-7.477	-7.385	-7.283	-7.415	-8.049	-7.235	-7.408	-7.710

Table S2. Selected electronic excitation wavelengths (nm) and corresponding oscillator strengths (f), compositions, and contributions.

molecule	electronic transitions	λ_{calc} (nm)	f	composition ^[a]
1	$S_0 \rightarrow S_1$	459.8	0.2795	H \rightarrow L (96%)
	$S_0 \rightarrow S_2$	341.1	0.0710	H \rightarrow L +1 (87%)
2	$S_0 \rightarrow S_1$	451.2	0.3724	H \rightarrow L (92%)
	$S_0 \rightarrow S_2$	396.5	0.1171	H \rightarrow L +1 (85%)
3	$S_0 \rightarrow S_1$	493.7	0.3415	H \rightarrow L (98%)
	$S_0 \rightarrow S_2$	356.3	0.0469	H \rightarrow L +1 (89%)
4	$S_0 \rightarrow S_1$	608.6	0.3636	H \rightarrow L (99%)
	$S_0 \rightarrow S_2$	384.3	0.3868	H -1 \rightarrow L (94%)
5	$S_0 \rightarrow S_1$	385.4	0.0659	H \rightarrow L (94%)
	$S_0 \rightarrow S_2$	326.1	0.1638	H -1 \rightarrow L (87%)
6	$S_0 \rightarrow S_1$	379.5	0.1507	H \rightarrow L (92%)
	$S_0 \rightarrow S_2$	344.6	0.0113	H -1 \rightarrow L (63%) H \rightarrow L +1 (30%)
7	$S_0 \rightarrow S_1$	400.7	0.3584	H \rightarrow L (98%)
	$S_0 \rightarrow S_2$	340.7	0.0430	H -2 \rightarrow L (90%)
8	$S_0 \rightarrow S_1$	465.1	0.4268	H \rightarrow L (97%)
	$S_0 \rightarrow S_2$	396.8	0.0658	H -1 \rightarrow L (97%)

[a] Only contributions >10% are included.

3. Additional Optical Spectra

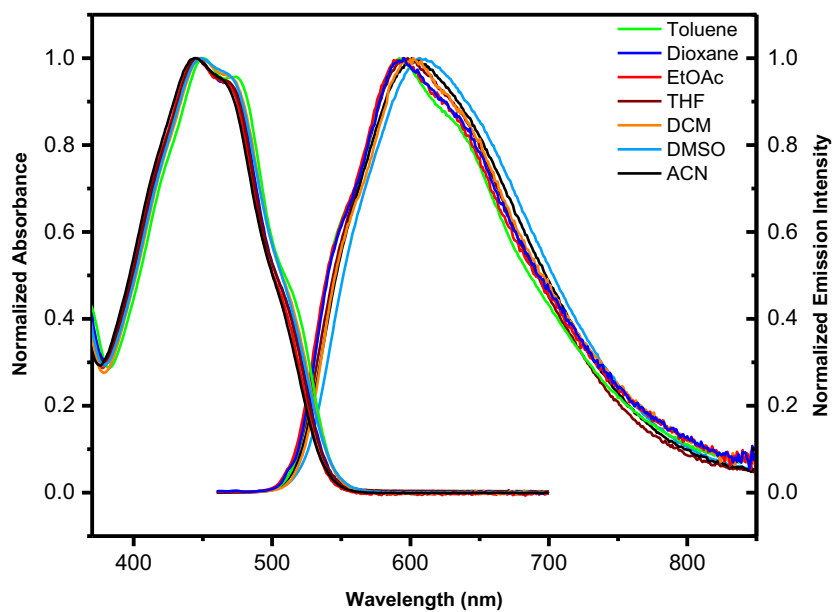


Figure S29. Solvent-Dependent Absorbance and Emission of Chromophore 1.

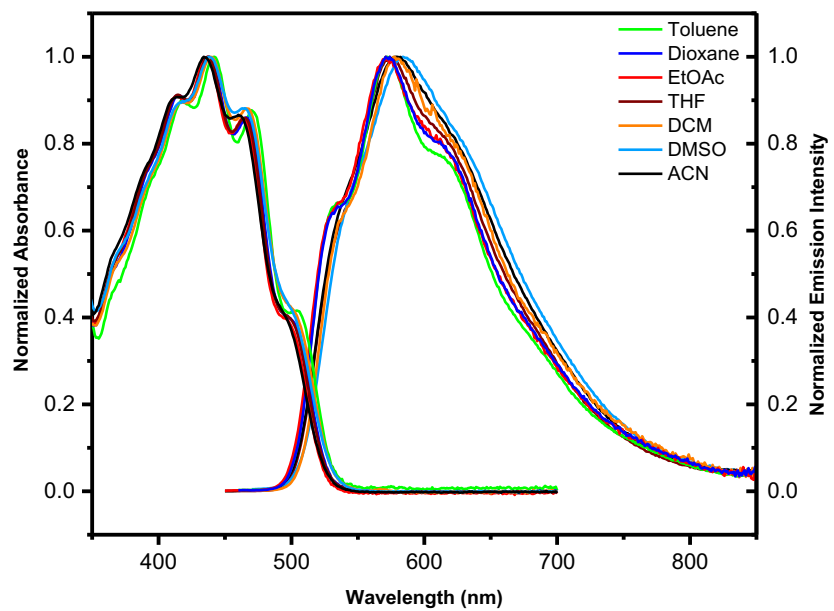


Figure S30. Solvent-Dependent Absorbance and Emission of Chromophore 2.

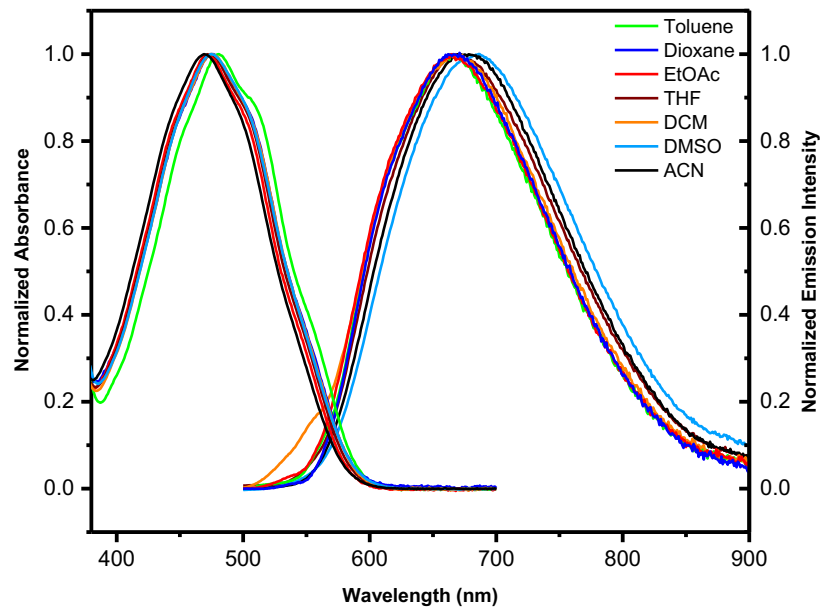


Figure S31. Solvent-Dependent Absorbance and Emission of Chromophore 3.

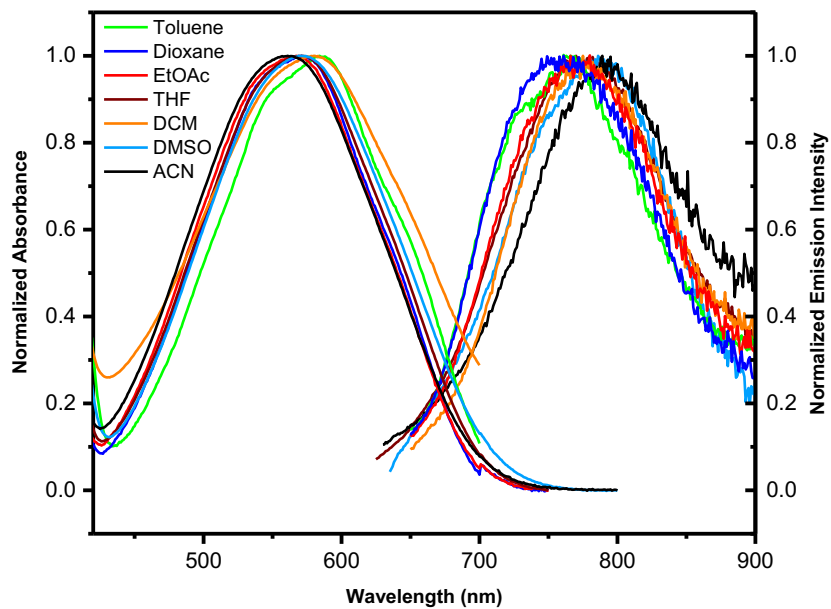


Figure S32. Solvent-Dependent Absorbance and Emission of Chromophore 4.

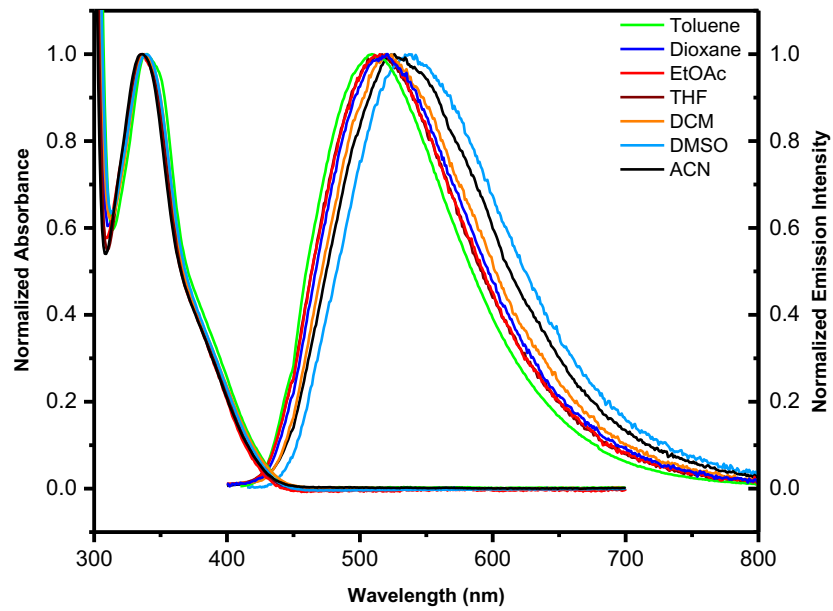


Figure S33. Solvent-Dependent Absorbance and Emission of Chromophore **5**.

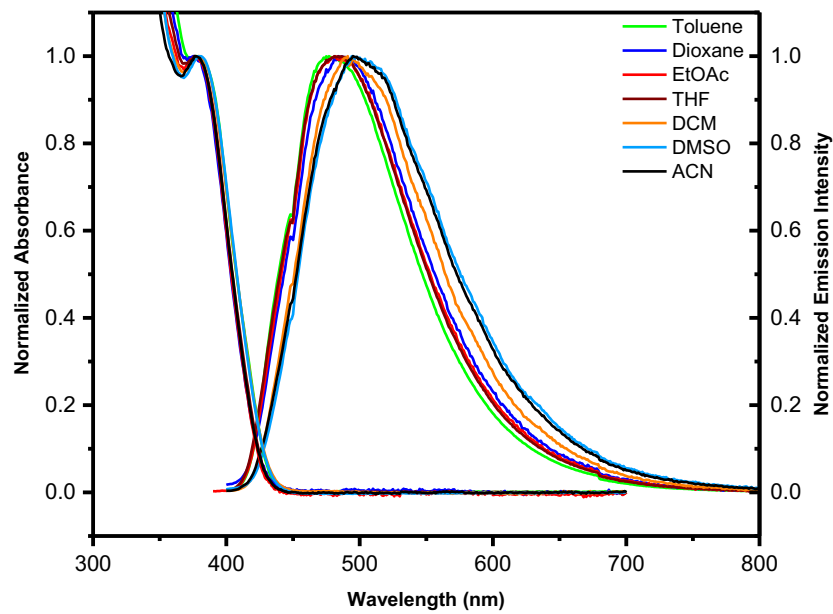


Figure S34. Solvent-Dependent Absorbance and Emission of Chromophore **6**.

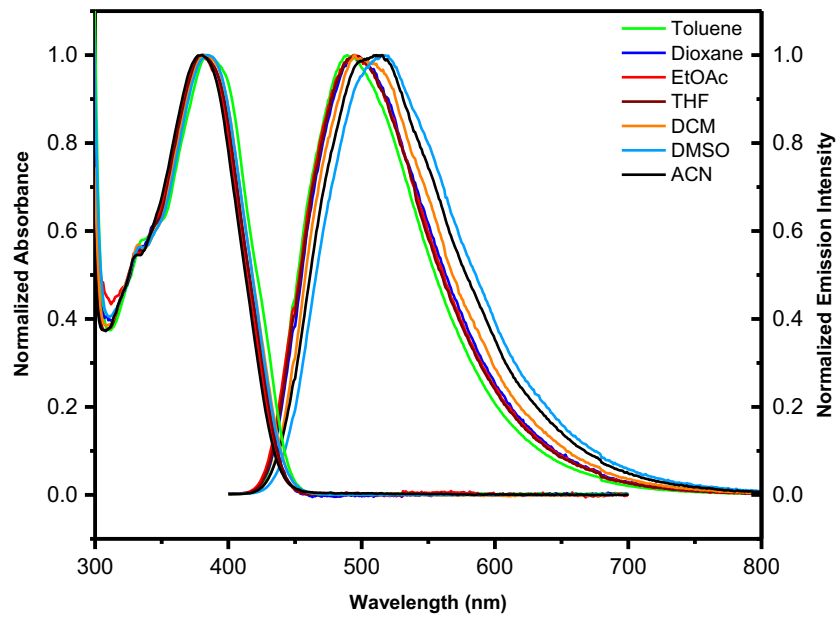


Figure S35. Solvent-Dependent Absorbance and Emission of Chromophore **7**.

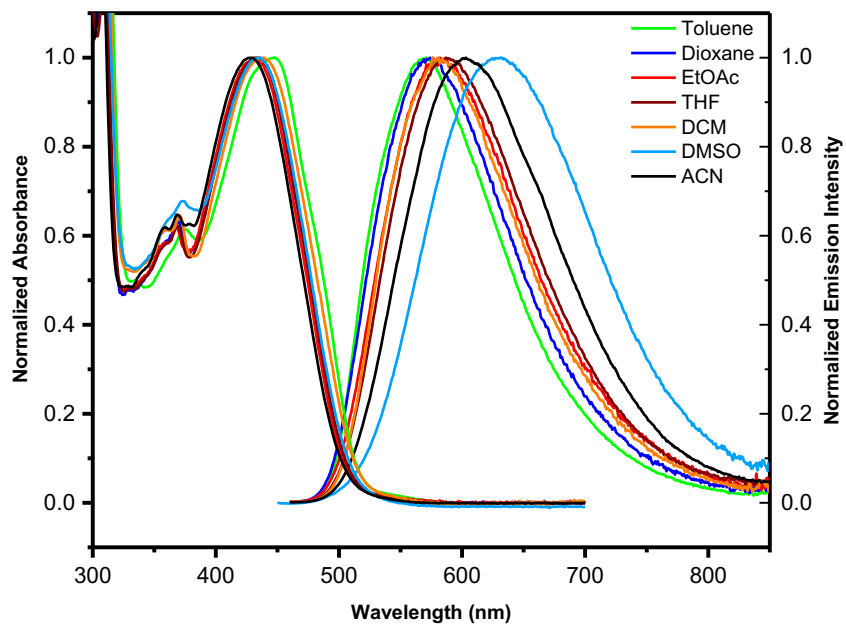


Figure S36. Solvent-Dependent Absorbance and Emission of Chromophore **8**.

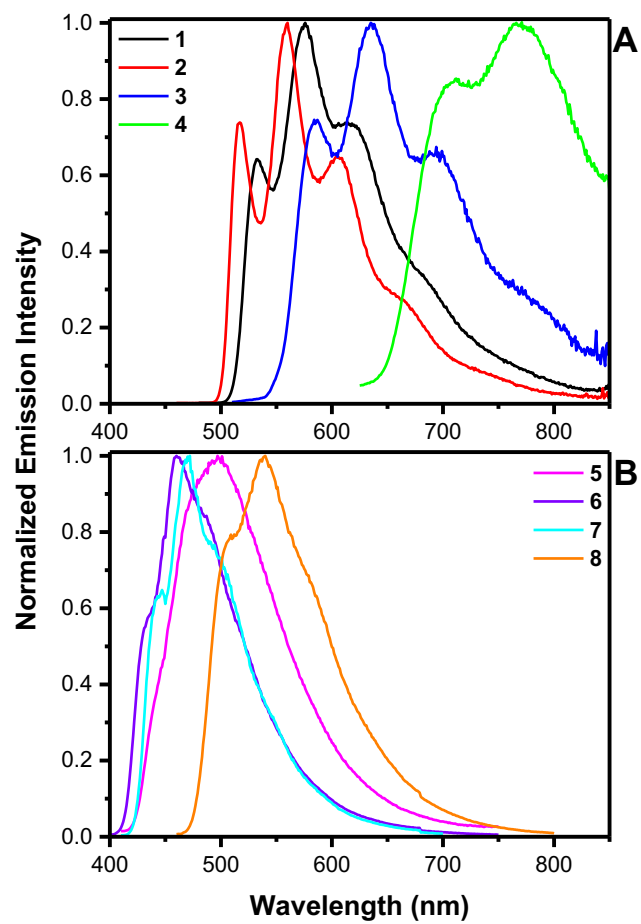


Figure S37. Static 77 K photoluminescence emission spectra of **1-4** (A) and **5-8** (B) in 2-methyl-THF.

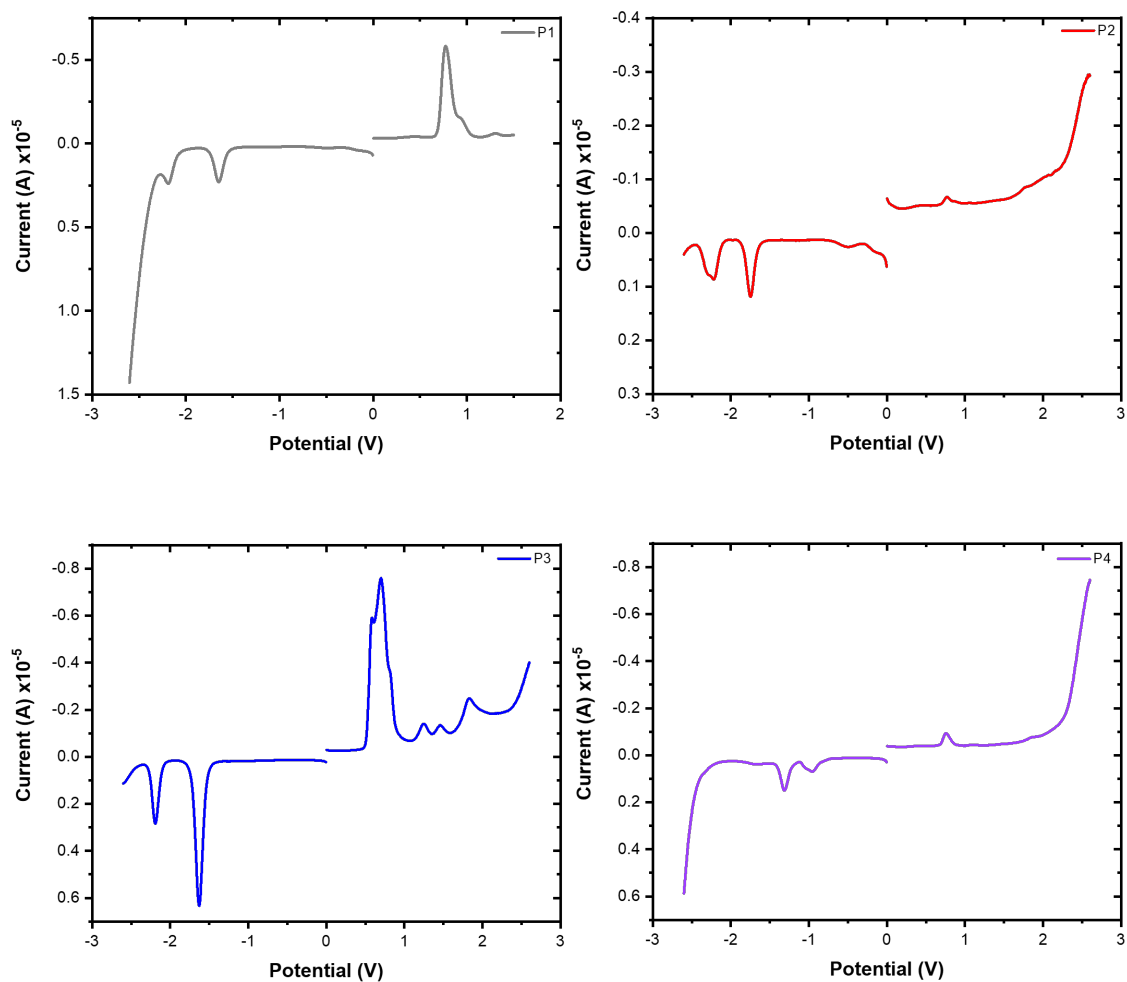


Figure S38. Normalized differential voltametric measurement for 1-4 (1 grey, 2 red, 3 blue, 4 purple) in ACN vs Ag/AgNO₃. Fc/Fc⁺ = 0.032.

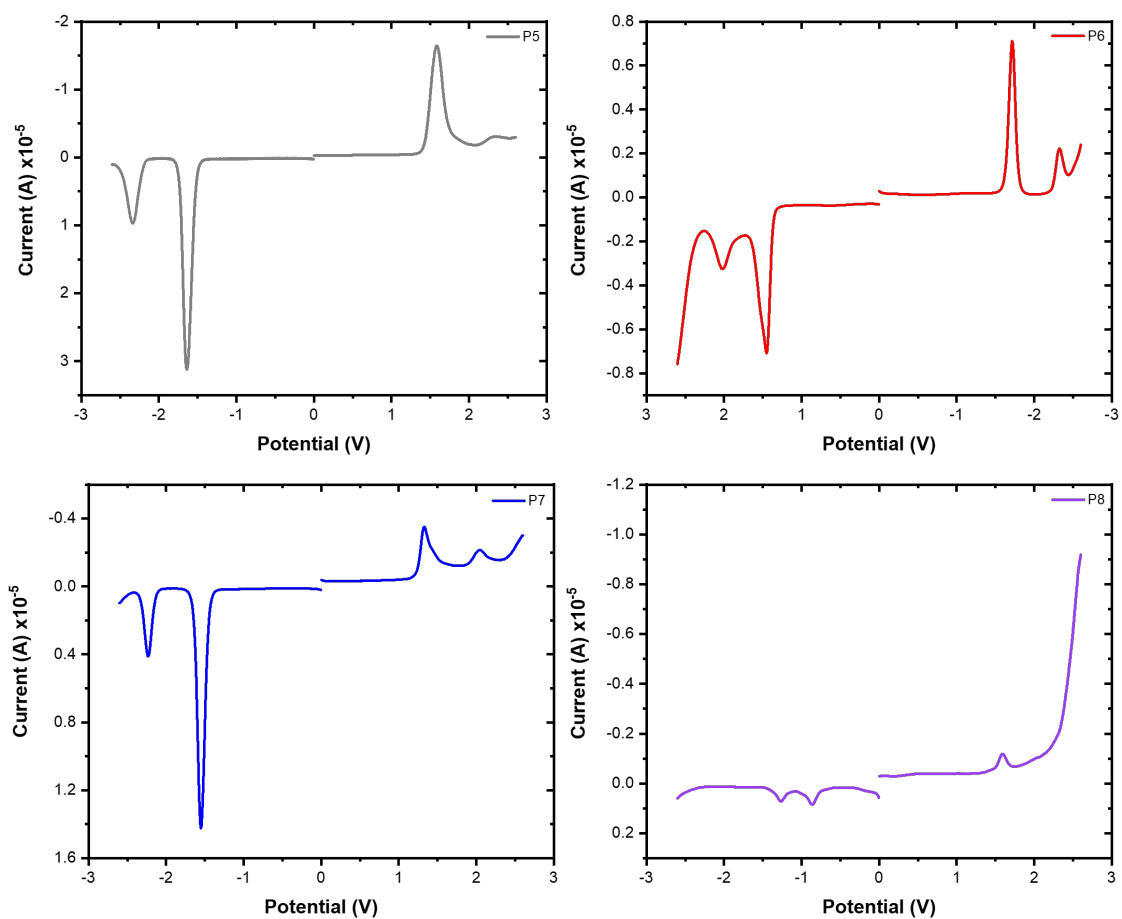


Figure S39. Normalized differential voltametric measurement for 5-8 (5 grey, 6 red, 7 blue, 8 purple) in ACN vs Ag/AgNO₃. Fc/Fc⁺ = 0.032.

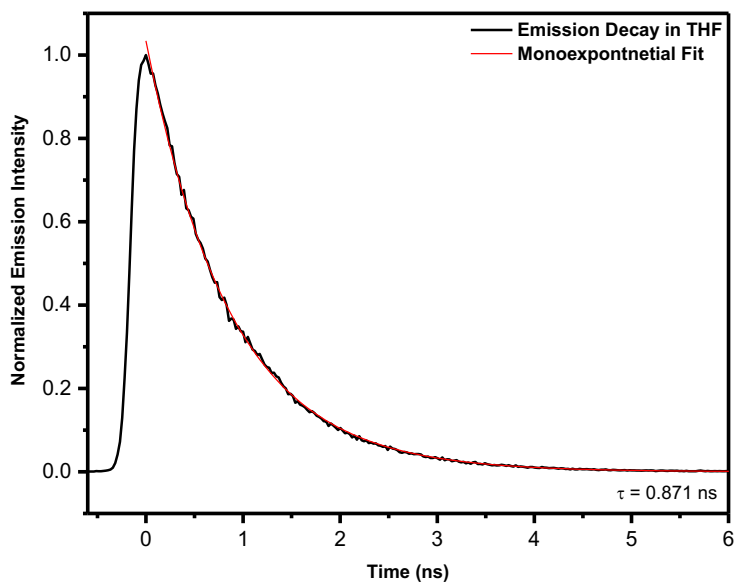


Figure S40. Photoluminescence decay of chromophore **1** in THF.

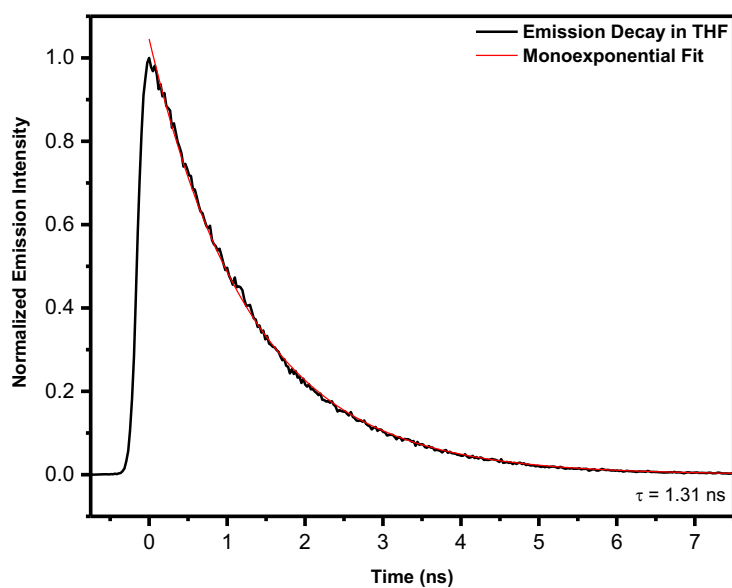


Figure S41. Photoluminescence decay of chromophore **2** in THF.

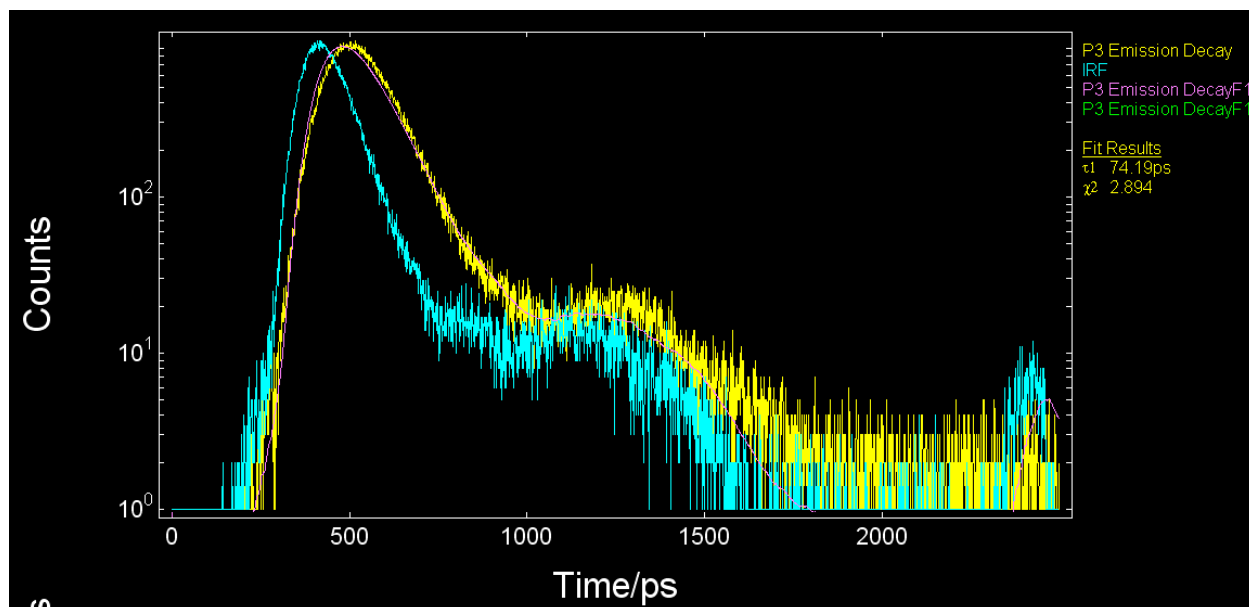


Figure S42. Photoluminescence decay of chromophore **3** in THF. Due to the short lifetime of this molecule, the instrument response function (IRF) was used in a deconvolution procedure to obtain the lifetime.

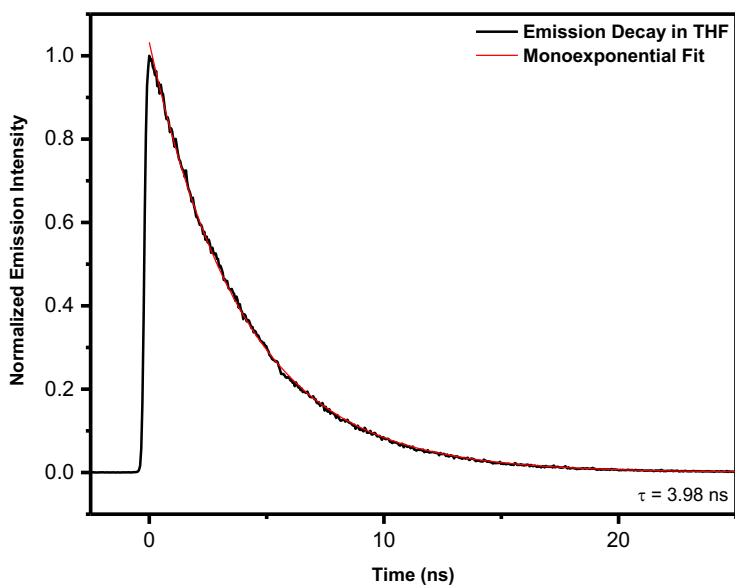


Figure S43. Photoluminescence decay of chromophore **5** in THF.

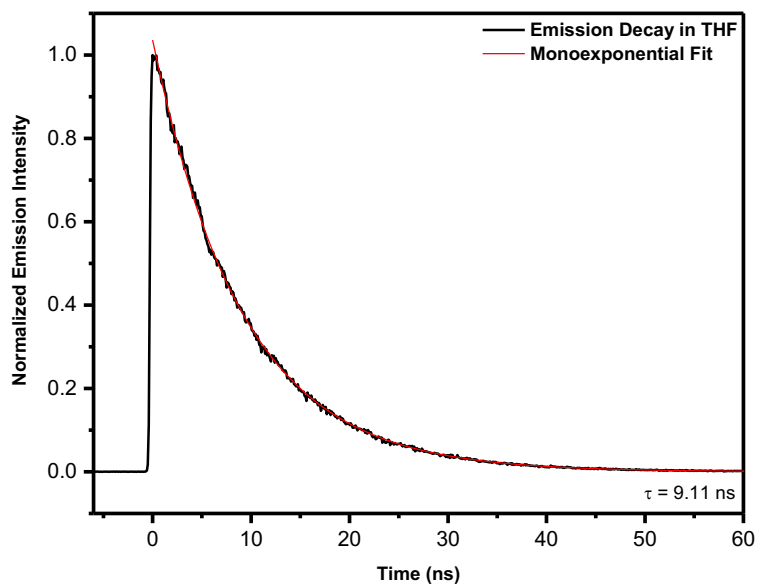


Figure S44. Photoluminescence decay of chromophore **6** in THF.

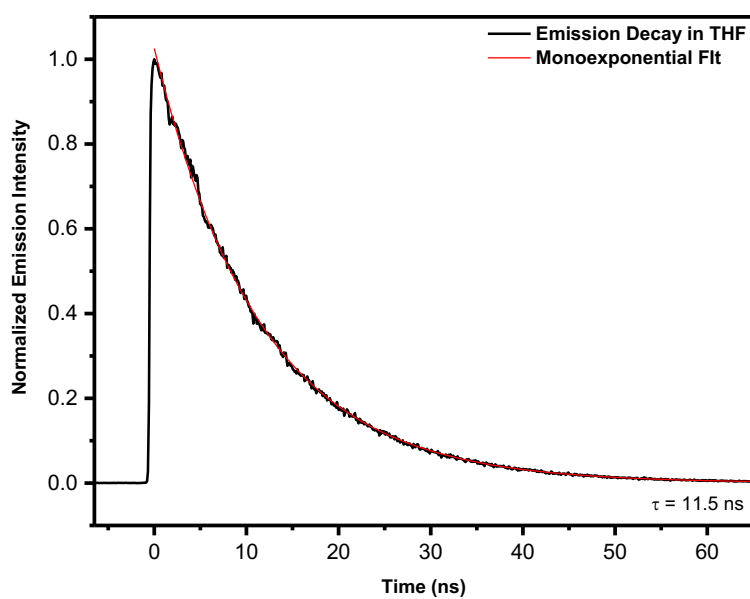


Figure S45. Photoluminescence decay of chromophore **7** in THF.

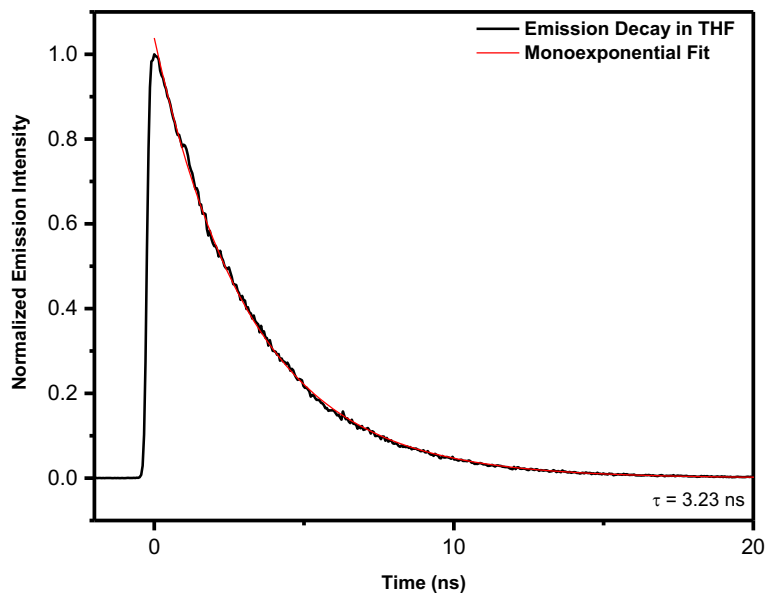


Figure S46. Photoluminescence decay of chromophore **8** in THF.

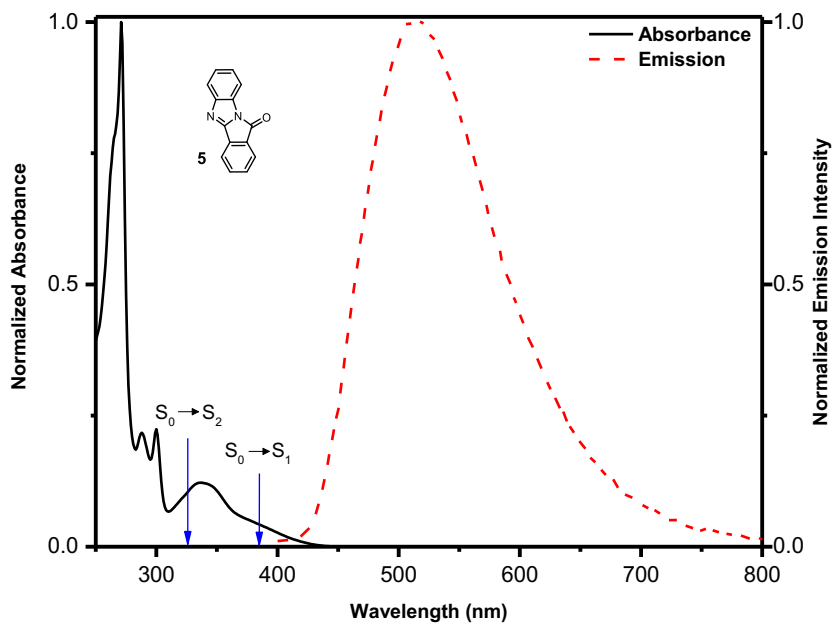


Figure S47. Normalized absorption (black) and emission (red) spectra of chromophore **5** overlaid with the two lowest energy vertical transitions (blue) calculated at the M06-D3/Def2-TZVP level of theory.

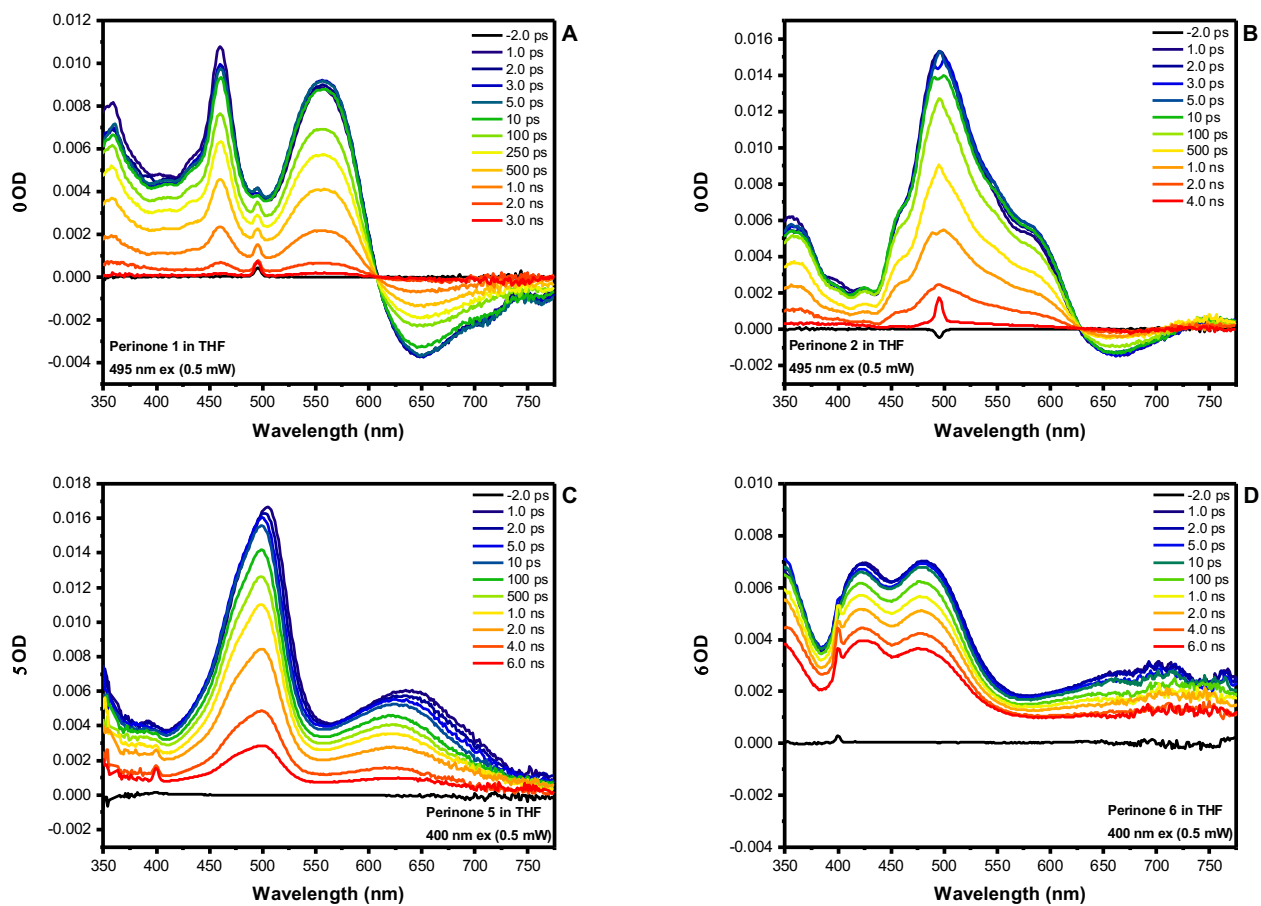


Figure S48. Excited-state difference spectra of **1** (A) and **2** (B) in THF following 495 nm pulsed excitation and **5** (C) and **6** (D) in THF following 400 nm pulsed excitation (105 fs fwhm).

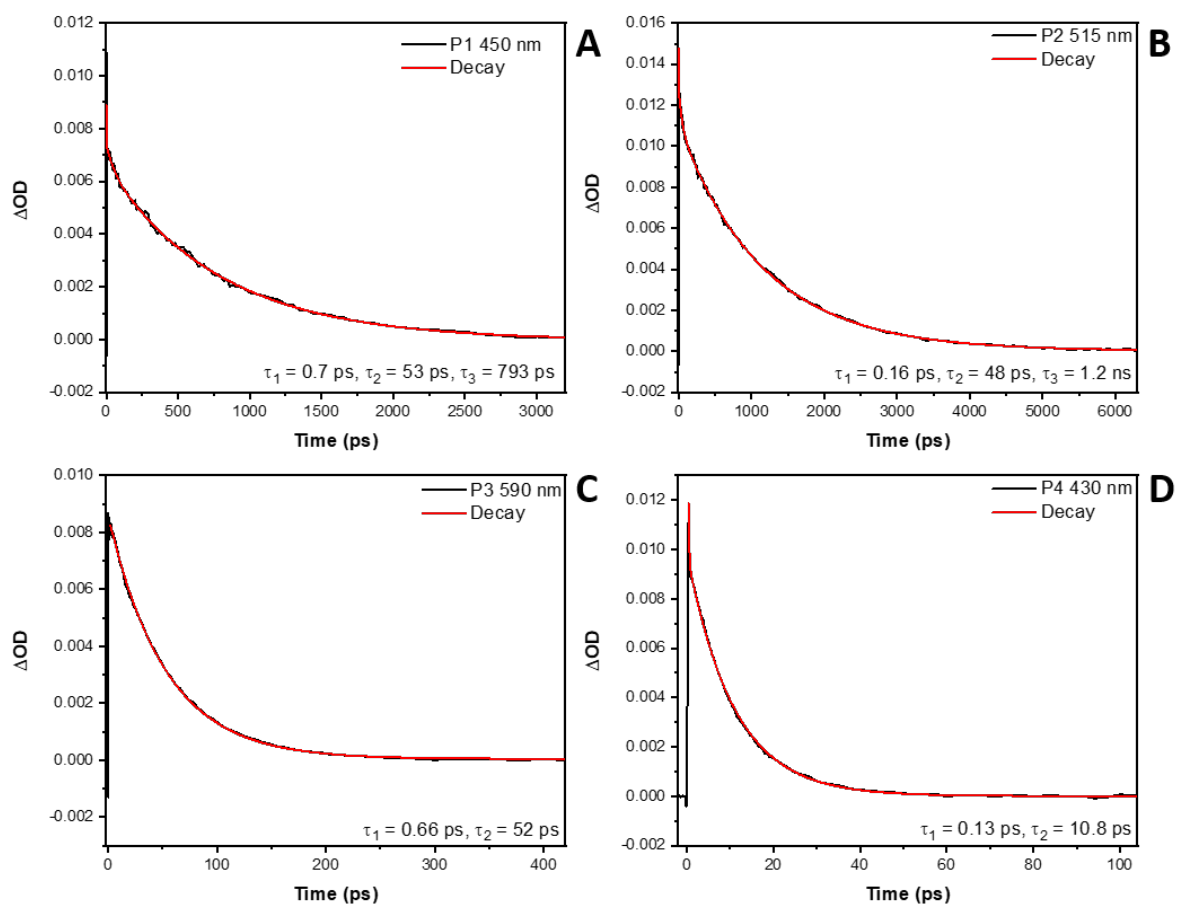


Figure S49. Ultrafast transient absorption kinetic data of **1-4** in THF (**1** (A), **2** (B), and **3** (C) following 495 nm excitation and **4** (D) following 650 nm excitation). Single wavelength kinetic analysis at specified wavelength.

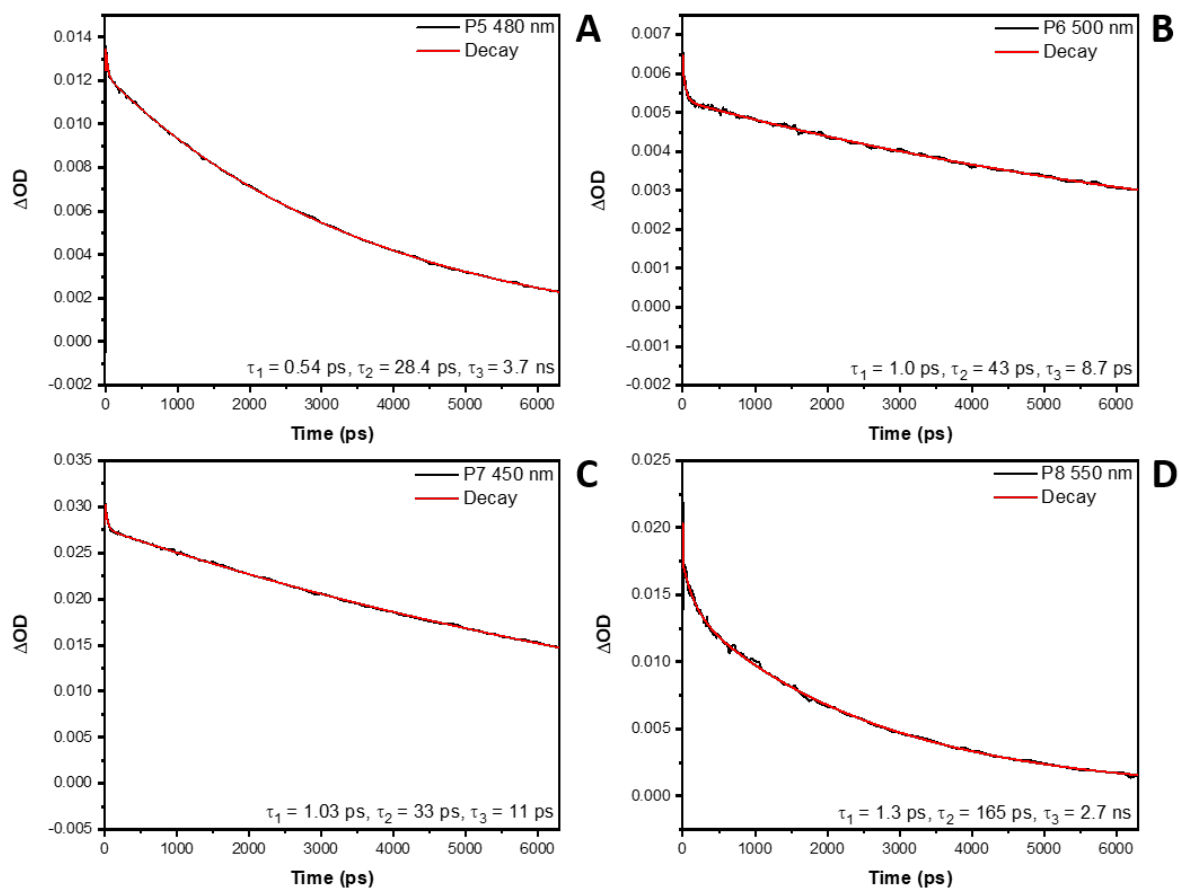


Figure S50. Ultrafast transient absorption kinetic data of **5-8** in THF (**5** (A), **6** (B), and **7** (C) following 400 nm excitation and **8** (D) following 495 nm excitation). Single wavelength kinetic analysis at specified wavelength.

Table S3. Absorbance and Emission Solvent Dependence Data for Chromophores **1-8**.

molecule	solvents	Δf	ν_A (cm^{-1})	ν_F (cm^{-1})	$\nu_A - \nu_F$ (cm^{-1})	fitted slope ^[a] (cm^{-1})	cavity volume ^[b] ($\times 10^{-22} \text{ cm}^3$)	$\mu_e - \mu_g$ ^[c] (D)
1	toluene	0.0132	22272	16892	5380	1270	3.46	6.6
	dioxane	0.0246	22422	16807	5615			
	EtOAc	0.1998	22523	16807	5716			
	THF	0.2096	22422	16722	5700			
	DCM	0.2172	22321	16611	5710			
	DMSO	0.2635	22272	16475	5797			
	ACN	0.3055	22523	16639	5884			
2	toluene	0.0132	22624	17483	5141	1694	4.09	8.3
	dioxane	0.0246	22831	17513	5318			
	EtOAc	0.1998	22883	17513	5370			
	THF	0.2096	22831	17422	5409			
	DCM	0.2172	22779	17331	5448			
	DMSO	0.2635	22831	17123	5708			
	ACN	0.3055	23042	17271	5771			
3	toluene	0.0132	20790	15015	5775	2030	4.05	9.0
	dioxane	0.0246	21053	15106	5947			
	EtOAc	0.1998	21186	15038	6148			
	THF	0.2096	21097	15015	6082			
	DCM	0.2172	21053	15083	5970			
	DMSO	0.2635	21053	14577	6476			
	ACN	0.3055	21322	14815	6507			
4	toluene	0.0132	17123	13055	4068	2612	4.82	11.2
	dioxane	0.0246	17513	13141	4372			
	EtOAc	0.1998	17637	13055	4582			
	THF	0.2096	17544	12987	4557			
	DCM	0.2172	17241	12903	4338			
	DMSO	0.2635	17575	12723	4852			
	ACN	0.3055	17825	12674	5151			
5	toluene	0.0132	29412	19646	9766	2214	2.86	7.9
	dioxane	0.0246	29762	19231	10531			
	EtOAc	0.1998	29851	19417	10434			
	THF	0.2096	29762	19268	10494			
	DCM	0.2172	29586	19268	10318			
	DMSO	0.2635	29499	18622	10877			
	ACN	0.3055	29762	19011	10751			
6	toluene	0.0132	26525	20964	5561	1569	3.52	7.4
	dioxane	0.0246	26667	20661	6006			
	EtOAc	0.1998	26596	20747	5849			
	THF	0.2096	26525	20576	5949			
	DCM	0.2172	26316	20367	5949			
	DMSO	0.2635	26385	20202	6183			
	ACN	0.3055	26525	20202	6323			
7	toluene	0.0132	25974	20450	5524	3134	3.44	10.3
	dioxane	0.0246	26316	20202	6114			
	EtOAc	0.1998	26385	20202	6183			
	THF	0.2096	26316	20243	6073			
	DCM	0.2172	26110	20202	5908			
	DMSO	0.2635	26042	19380	6662			
	ACN	0.3055	26318	19380	6938			
8	toluene	0.0132	22371	17513	4858	5793	4.25	15.6
	dioxane	0.0246	22936	17422	5514			
	EtOAc	0.1998	23202	17182	6020			
	THF	0.2096	23148	17036	6112			
	DCM	0.2172	22831	17241	5590			
	DMSO	0.2635	23042	15823	7219			
	ACN	0.3055	23310	16584	6726			

[a] Fitted slopes obtained from linear regressions on plots in Figure 8. [b] Solvent cavity volumes were obtained from the ground state geometry optimization (M06-D3/Def2-TZVP) using the PCM solvation model.

Cartesian coordinates of all ground state optimized structures:

P1 Optimized Structure

C	2.27000700	-2.51136300	0.00000200
C	1.38811000	-1.45683000	0.00000100
C	1.87983500	-0.12575600	0.00000000
C	3.27410900	0.11007400	0.00000100
C	4.14431800	-1.00137900	0.00000200
C	3.65079100	-2.27711700	0.00000200
H	1.87216200	-3.51922000	0.00000200
C	0.98904500	0.97333100	-0.00000100
C	3.73671700	1.44269300	0.00000000
H	5.21397000	-0.82204900	0.00000200
H	4.33207800	-3.11980700	0.00000300
C	2.84931300	2.48063500	-0.00000100
C	1.46285800	2.26197900	-0.00000100
H	4.80571200	1.62496600	0.00000100
H	3.21279200	3.50155100	-0.00000100
H	0.77310900	3.09219300	-0.00000200
N	-0.37190800	0.63782200	-0.00000200
N	0.01894400	-1.70999800	0.00000000
C	-0.76324400	-0.70888500	-0.00000100
C	-1.48926800	1.48885400	-0.00000400
C	-4.00319800	0.90346000	0.00000000
C	-4.90433800	-0.15064300	0.00000200
C	-4.46304400	-1.47110300	0.00000200
C	-3.11031900	-1.77775800	0.00000000
C	-2.21966800	-0.72387400	-0.00000100
C	-2.65946100	0.59208000	-0.00000100
H	-4.33492500	1.93500500	0.00000000
H	-5.96832700	0.05278900	0.00000200
H	-5.19224900	-2.27233700	0.00000300
H	-2.76022400	-2.80286100	0.00000100
O	-1.45984300	2.69307600	-0.00000200

P2 Optimized Structure

C	3.01707200	-2.65546500	0.00000100
C	2.26027900	-1.50775800	-0.00000100
C	2.90050000	-0.24147600	0.00000000
C	4.31271600	-0.16621800	0.00000300
C	5.05148900	-1.36909200	0.00000500
C	4.41553900	-2.58003300	0.00000400
H	2.50716100	-3.61147100	0.00000000
C	2.14048900	0.95236800	-0.00000200
C	4.92402500	1.10516500	0.00000400
H	6.13459700	-1.31229700	0.00000700
H	4.99624800	-3.49500000	0.00000500
C	4.16094600	2.23748900	0.00000200
C	2.75867800	2.17853300	-0.00000100
H	6.00684100	1.16438500	0.00000600
H	4.63842100	3.21034900	0.00000200
H	2.16936900	3.08238900	-0.00000300
N	0.74919900	0.77509700	-0.00000500
N	0.87165200	-1.60304400	-0.00000400
C	0.20714900	-0.51947800	-0.00000500
C	-0.25896100	1.75549600	-0.00000900
C	-2.80372000	1.47484600	0.00000000
C	-3.86292300	0.54047100	0.00000100
C	-3.57401200	-0.85791000	0.00000000
C	-2.23229700	-1.30143200	-0.00000300
C	-1.24059700	-0.36990400	-0.00000500
C	-1.52650400	1.00793600	-0.00000400
H	-3.01484000	2.53909100	0.00000100
H	-2.01068300	-2.36330400	-0.00000400
O	-0.08322100	2.94732900	-0.00000300
C	-5.20982000	0.95713800	0.00000500
C	-4.64799500	-1.77147100	0.00000200
C	-6.22546400	0.04429500	0.00000700
C	-5.94140100	-1.33293500	0.00000500
H	-5.42216800	2.02091400	0.00000600
H	-7.25593400	0.37882700	0.00000900
H	-6.75590800	-2.04743500	0.00000600
H	-4.42442100	-2.83285300	0.00000100

P3 Optimized Structure

C	-3.01168100	2.41457000	0.42945400
C	-2.09812600	1.40945800	0.21158600
C	-2.53731000	0.08247500	0.00742500
C	-3.92409400	-0.19432300	-0.05404000
C	-4.83224200	0.86131700	0.18007600
C	-4.38255800	2.12901700	0.42970400
H	-2.64758100	3.42424500	0.57816700
C	-1.59168000	-0.94861900	-0.17936900
C	-4.33696000	-1.50380100	-0.36434400
H	-5.89486300	0.64690900	0.14541300
H	-5.09234800	2.92897200	0.60542800
C	-3.40386700	-2.46642700	-0.62152600
C	-2.02889300	-2.20467900	-0.53016500
H	-5.39748700	-1.72565500	-0.41096300
H	-3.71897000	-3.46825300	-0.88913000
H	-1.32981900	-3.00220700	-0.71586600
N	-0.21476500	-0.60029300	-0.01953700
N	-0.75430200	1.70484800	0.12540500
C	0.11196000	0.77386600	0.00320700
C	0.74373200	-1.59405200	0.27487300
O	0.41917300	-2.72452400	0.55288200
C	3.24278000	2.80681100	-0.41577600
C	4.22066900	1.85453900	-0.31365100
C	3.88275500	0.50425900	-0.10487300
C	2.51449700	0.15080400	-0.01501300
C	1.52323000	1.14294900	-0.11475200
C	1.89356000	2.45403400	-0.31105000
H	5.90015500	-0.23829500	-0.04225300
H	3.50907000	3.84416400	-0.57736700
H	5.26835000	2.12527600	-0.38828100
C	4.85226500	-0.50973100	0.02933800
C	2.15642500	-1.19037500	0.20665500
H	1.12109300	3.20857700	-0.38583300
C	3.12946800	-2.15103900	0.34254300
C	4.48351900	-1.80828800	0.25108000
H	2.83002700	-3.17756700	0.51326400
H	5.23775100	-2.57843600	0.35500500

P4 Optimized Structure

C	-4.12873400	-2.60602200	-0.44403000
C	-3.32856300	-1.50799900	-0.22842000
C	-3.90315700	-0.23924100	0.00578600
C	-5.31013800	-0.11809400	0.09357600
C	-6.10053500	-1.26457700	-0.14051100
C	-5.52181800	-2.47335700	-0.41590200
H	-3.65769300	-3.56657800	-0.61506200
C	-3.07387100	0.88692000	0.19561000
C	-5.86063800	1.13309500	0.42842900
H	-7.17937800	-1.16786100	-0.08534800
H	-6.14358000	-3.34338900	-0.59048900
C	-5.03583600	2.19022500	0.68304200
C	-3.64200600	2.08306800	0.56772400
H	-6.93811400	1.23505700	0.49461600
H	-5.45471500	3.14812100	0.96782000
H	-3.03320700	2.95111100	0.75363100
N	-1.66695900	0.69288700	0.01435500
N	-1.96008900	-1.65515500	-0.17498500
C	-1.19851200	-0.63941900	-0.04864600
C	-0.82307000	1.78826700	-0.24743100
O	-1.25560800	2.89356400	-0.46887400
C	2.13418800	-2.34801600	0.22108000
C	3.01158400	-1.29145000	0.13774400
C	2.51679200	0.01334200	-0.00830800
C	1.12357000	0.22620300	-0.05695600
C	0.24566900	-0.86686800	0.02469000
C	0.75779500	-2.13975300	0.16017400
H	2.53143800	-3.34911500	0.33396300
C	3.38505400	1.11261300	-0.11606600
C	0.62946400	1.52945300	-0.21765600
H	0.07356300	-2.97544000	0.22137800
C	1.49923500	2.58884500	-0.33156700
C	2.87836500	2.37923000	-0.27772300
H	1.09771500	3.58617600	-0.45604000
H	3.56587300	3.21165800	-0.36161300
C	4.84350700	0.90227000	-0.06059700
C	4.46425200	-1.53343200	0.19709500
N	5.28498600	-0.40831100	0.09228900
O	5.63951100	1.81048200	-0.14146700
O	4.93171600	-2.64139000	0.32906300
C	6.72820600	-0.59262000	0.14447400
H	7.18559800	-0.21707600	-0.77008700
H	6.93171700	-1.65220400	0.25410200
H	7.14543700	-0.04375500	0.98806700

P5 Optimized Structure

N	-0.32865500	0.48137900	-0.00000100
N	-0.73219300	-1.72866800	0.00000000
C	0.17326100	-0.81149100	-0.00000100
C	0.68576300	1.45054700	0.00000300
O	0.52862700	2.63836200	0.00000200
C	-3.23508600	-1.50313600	-0.00000100
C	-4.26871100	-0.58145500	-0.00000100
C	-1.93701700	-1.02065300	-0.00000100
C	-4.02071000	0.79057000	-0.00000100
C	-1.70700400	0.36964500	-0.00000100
C	-2.72938300	1.29535600	-0.00000100
C	2.61925400	-1.66962700	0.00000000
C	3.93841200	-1.22790700	0.00000000
C	1.62525500	-0.71659800	0.00000000
C	4.24763800	0.12482800	0.00000000
C	1.93814300	0.64664400	0.00000100
C	3.24143600	1.08472100	0.00000100
H	3.46900900	2.14430100	0.00000200
H	2.38112900	-2.72621100	-0.00000100
H	4.74159500	-1.95498400	0.00000000
H	5.28542300	0.43459300	0.00000100
H	-3.42560900	-2.56953500	0.00000000
H	-5.29395400	-0.93172400	-0.00000100
H	-4.85678300	1.47960500	-0.00000100
H	-2.53140300	2.35941100	-0.00000200

P6 Optimized Structure

N	1.49635300	0.53295300	0.00000100
N	1.71308400	-1.70465200	0.00000000
C	0.88597000	-0.71468700	0.00000000
C	0.57436600	1.59121000	0.00000400
O	0.84296800	2.75987600	0.00000200
C	4.22448900	-1.69038600	-0.00000100
C	5.33163700	-0.85960300	-0.00000100
C	2.97088100	-1.10029800	0.00000000
C	5.20106400	0.52914700	-0.00000100
C	2.85953200	0.30479700	0.00000000
C	3.95756700	1.14094000	-0.00000100
C	-1.60506000	-1.35496800	0.00000000
C	-2.91652800	-0.81842200	0.00000000
C	-0.54918500	-0.50089600	0.00000100
C	-4.04847600	-1.65518200	-0.00000100
C	-3.10902200	0.59405800	0.00000000
C	-0.74293700	0.90646000	0.00000100
C	-5.31040100	-1.12793200	-0.00000100
H	-3.89920100	-2.72953900	-0.00000100
C	-4.42091600	1.10390000	-0.00000100
C	-1.98378900	1.45390200	0.00000000
C	-5.49934100	0.26317700	-0.00000100
H	-6.17156200	-1.78548800	-0.00000100
H	-4.55871400	2.17984700	-0.00000100
H	-2.12270300	2.53018400	0.00000000
H	-6.50397800	0.66853600	-0.00000100
H	-1.46396700	-2.43031800	0.00000000
H	3.85063100	2.21790400	-0.00000100
H	6.09255200	1.14476900	-0.00000200
H	6.32368600	-1.29522200	-0.00000100
H	4.32435200	-2.76908900	0.00000000

P7 Optimized Structure

N	0.90166800	-0.40641000	0.00000000
N	1.43542800	1.77494800	0.00000000
C	0.46218400	0.91722500	0.00000000
C	0.08684100	-1.54039800	0.00000100
O	0.56703500	-2.64858600	-0.00000100
C	-2.83155200	2.69422800	0.00000100
C	-3.70455700	1.64044500	0.00000000
C	-3.23220200	0.31239400	0.00000000
C	-1.83607800	0.08000300	0.00000000
C	-0.95477100	1.18501700	0.00000100
C	-1.45127300	2.46740000	0.00000100
H	-3.20534800	3.71059100	0.00000100
C	-4.10571000	-0.79352100	0.00000000
C	-1.35711400	-1.25098600	0.00000000
H	-0.75571600	3.29803000	0.00000100
C	-2.24279000	-2.30204100	0.00000000
C	-3.62277000	-2.07361000	0.00000000
H	-1.85042600	-3.31194300	0.00000000
H	-4.30514000	-2.91432200	-0.00000100
C	3.91436000	1.44427500	0.00000000
C	2.59283800	1.01932300	0.00000000
C	2.29310700	-0.35042000	0.00000000
C	3.27577200	-1.32472200	0.00000000
C	4.58782000	-0.88148400	-0.00000100
C	4.90254400	0.47859000	-0.00000100
H	4.15036100	2.50162800	0.00000000
H	3.02778100	-2.37640200	0.00000000
H	5.38955200	-1.61033500	-0.00000100
H	5.94352900	0.77965000	-0.00000100
H	-5.17462900	-0.60849200	0.00000000
H	-4.77580800	1.81018900	0.00000000

P8 Optimized Structure

N	-2.37171500	0.41423700	0.00000600
N	-2.73660000	-1.80118100	-0.00000500
C	-1.83294000	-0.87251300	0.00000000
C	-1.64744500	1.60543700	0.00001900
O	-2.20009800	2.67642200	0.00003600
C	1.58620800	-2.38970000	0.00000700
C	2.38264800	-1.26889600	0.00000500
C	1.79727900	0.00963400	0.00000200
C	0.39319600	0.13488000	0.00000500
C	-0.39990900	-1.03454700	0.00000200
C	0.19667600	-2.27532600	0.00000300
H	2.05705600	-3.36473600	0.00001200
C	2.59538300	1.16684900	-0.00000200
C	-0.18004800	1.42502400	0.00001400
H	-0.42807700	-3.15980400	0.00000200
C	0.62462600	2.53918600	0.00001700
C	2.01452100	2.41100900	0.00000600
H	0.16144800	3.51800300	0.00002600
H	2.65050200	3.28725200	0.00000400
C	4.06738900	1.04702600	-0.00002200
C	3.84997300	-1.41846000	0.00001300
N	4.59577600	-0.23806800	-0.00001300
O	4.79885500	2.01068200	-0.00004200
O	4.38921900	-2.50088300	0.00004100
C	6.04886100	-0.33154300	-0.00002200
H	6.45457700	0.15962900	-0.88369200
H	6.32166700	-1.38113100	-0.00002400
C	-5.23382400	-1.66314100	-0.00001700
C	-3.94877300	-1.13737300	-0.00000700
C	-3.75428100	0.25137700	-0.00000100
C	-4.80706300	1.14867000	-0.00000500
C	-6.08039300	0.60545700	-0.00001400
C	-6.29141100	-0.77502900	-0.00002100
H	-5.38844500	-2.73521800	-0.00002200
H	-4.64114000	2.21606900	0.00000100
H	-6.93552700	1.27071100	-0.00001700
H	-7.30671900	-1.15320300	-0.00002800
H	6.45459100	0.15962900	0.88364200