

Supporting Information

CF₃-Pyridyl-Substituted Hetero- and Homocyclic Conjugated Molecules: From Non-Emissive to Highly Emissive through Core Engineering

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Photophysical Properties

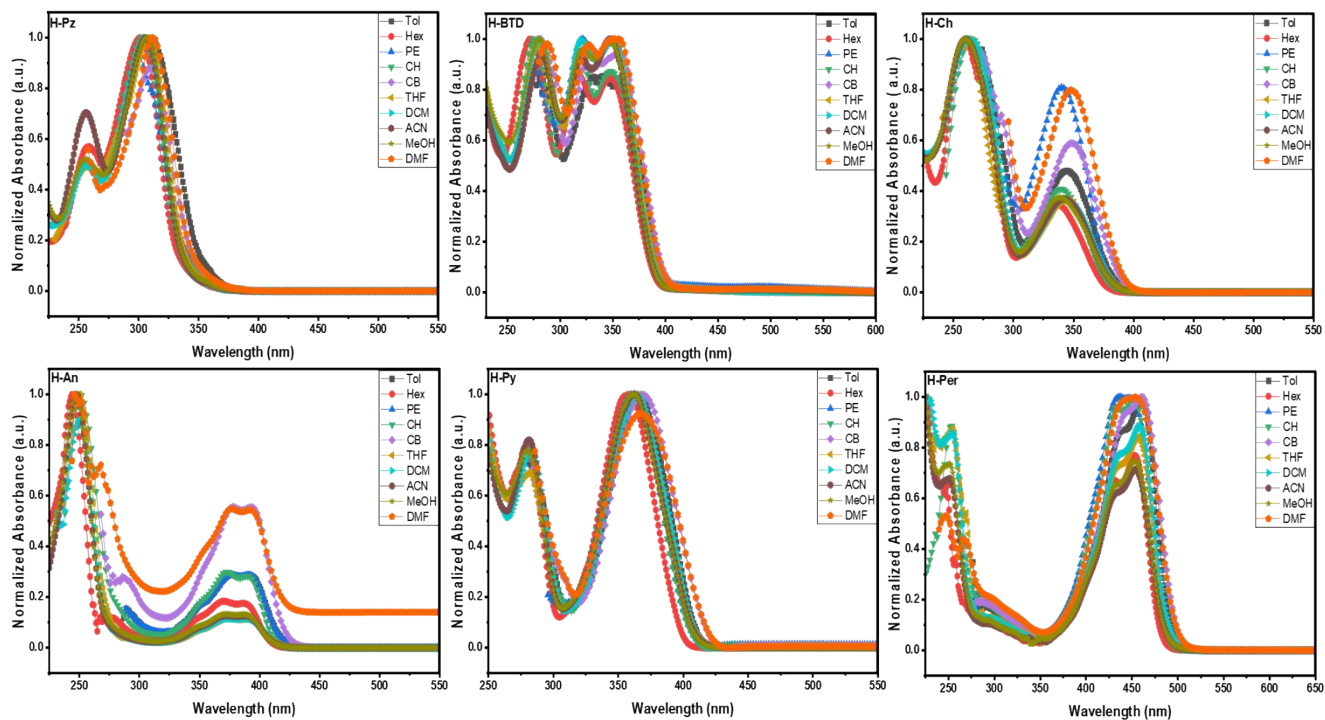


Figure S1. Absorbance spectra of all compounds in solution where Tol, Hex, PE, CH, CB, THF, DCM, ACN MeOH, DMF is (Toluene, Hexane, Petroleum Ether, Cyclohexane, Chlorobenzene, Tetrahydrofuran, Dichloromethane, Acetonitrile, Methanol, and Dimethyl formamide) respectively.

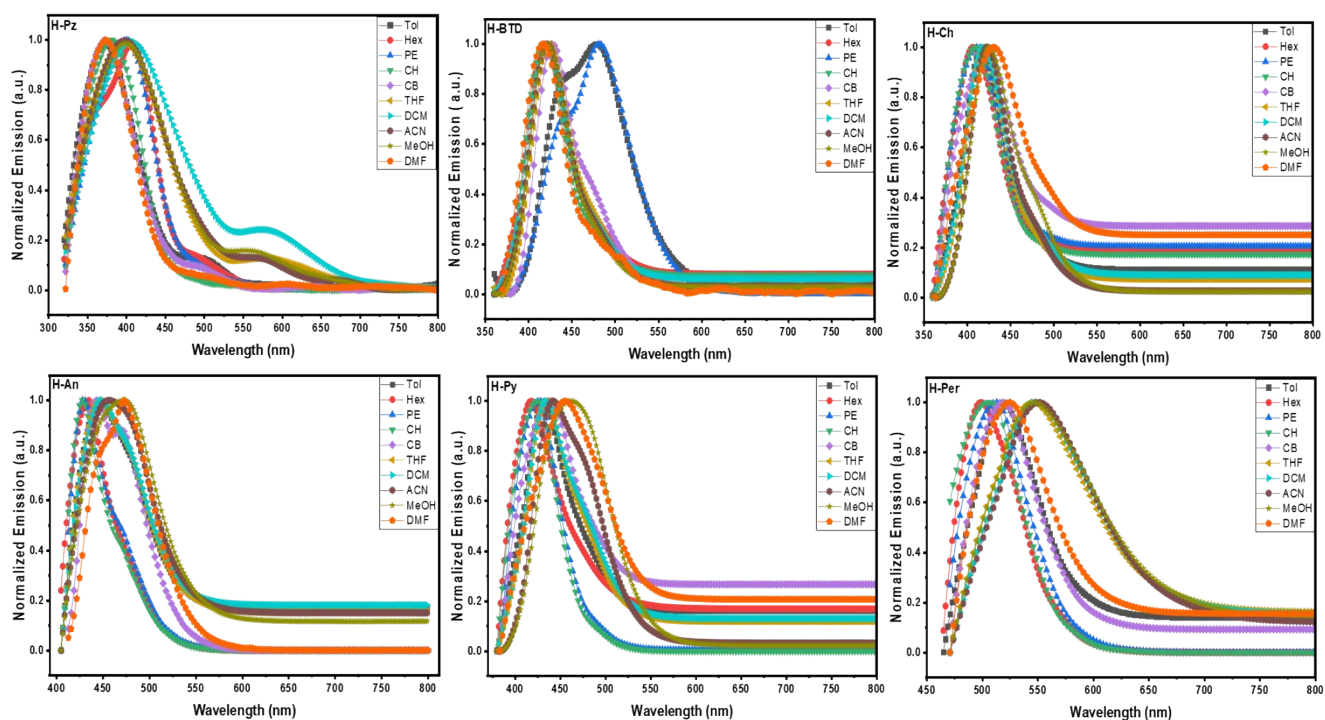


Figure S2. Emission spectra of all compounds in solution where Tol, Hex, PE, CH, CB, THF, DCM, ACN MeOH, DMF is (Toluene, Hexane, Petroleum Ether, Cyclohexane, Chlorobenzene, Tetrahydrofuran, Dichloromethane, Acetonitrile, Methanol, and Dimethyl formamide) respectively

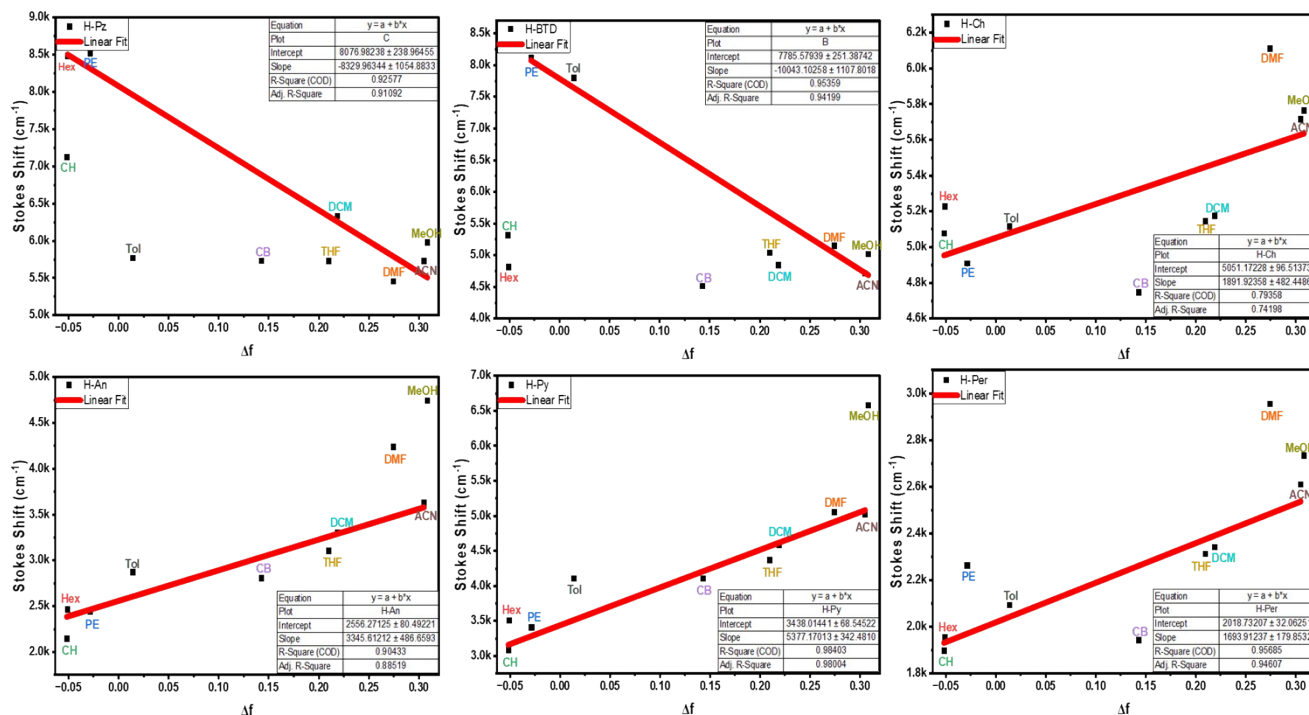


Figure S3. Lippert-Mataga slope linear fits for all compounds

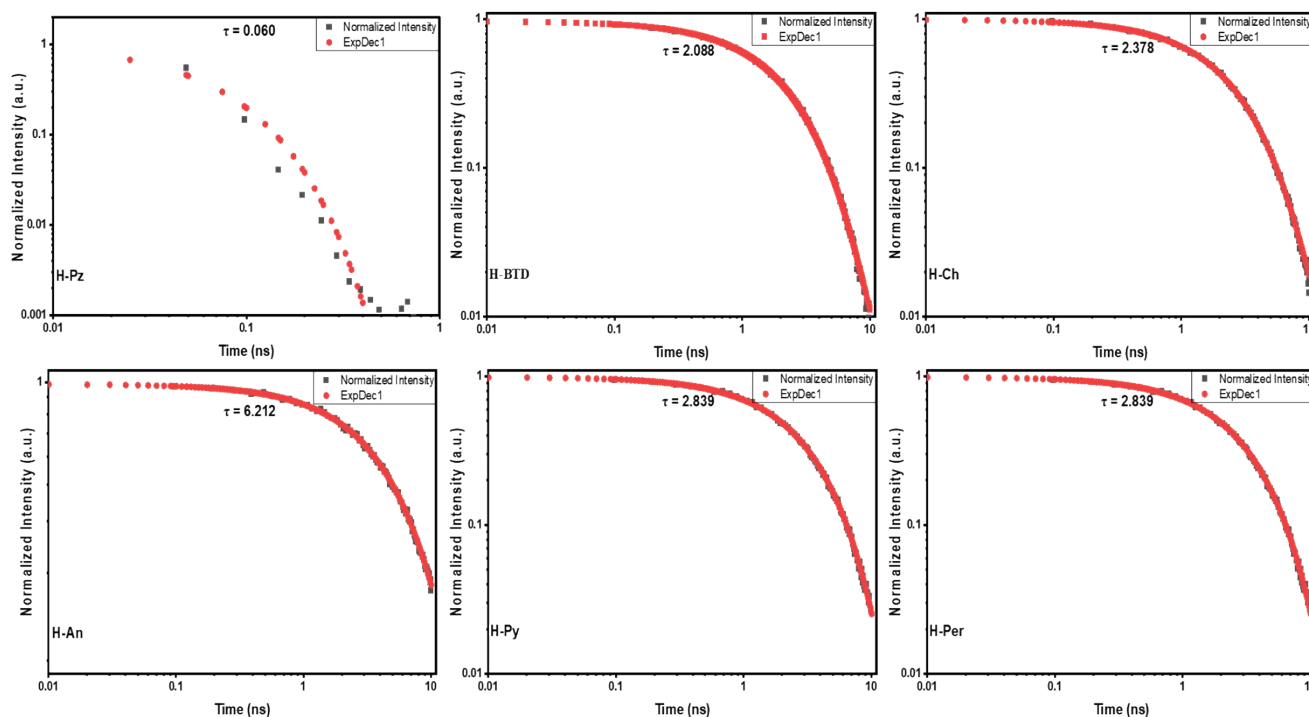
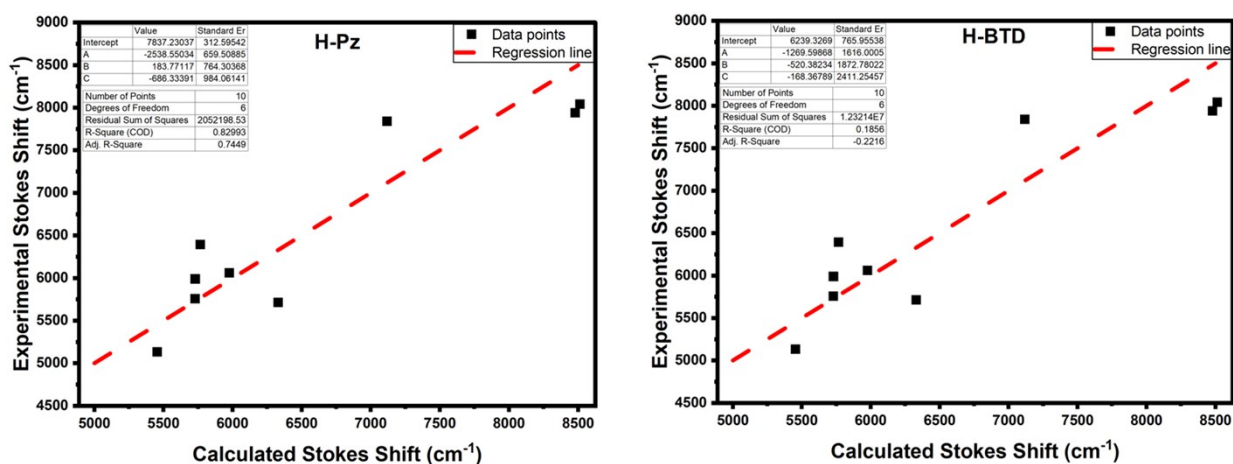


Figure S4. Normalized fluorescence lifetime decay plots for all compounds in CHCl_3 . Excitation wavelengths for H-Pz (374 nm), H-BTD (550 nm), H-Ch (566 nm), H-An (545 nm), H-Py (472 nm), H-Per (650 nm) and Bandwidth (10 nm)

Table S1. Photophysical data of all compounds in ten solvents: Tol, Hex, PE, CH, CB, THF, DCM, ACN MeOH, DMF is (Toluene, Hexane, Petroleum Ether, Cyclohexane, Chlorobenzene, Tetrahydrofuran, Dichloromethane, Acetonitrile, Methanol, and Dimethyl formamide) respectively. Also 1-6 numbers refer to H-Pz to H-Per compounds

Solvent	λ_{abs} (nm)						λ_{em} (nm)						$\Delta\nu$ (nm)					
	1	2	3	4	5	6	1	2	3	4	5	6	1	2	3	4	5	6
Tol	309	345	343	393	364	463	376	472	416	443	428	509	67	127	73	50	64	46
Hex	302	348	339	388	363	453	406	418	412	429	416	497	104	70	73	41	53	44
PE	300	346	342	390	362	443	403	481	411	431	413	501	103	135	69	41	51	58
CH	304	346	338	392	364	452	388	424	408	428	410	492	84	78	70	36	46	40
CB	310	358	346	394	364	460	377	427	414	443	428	510	67	69	68	49	64	50
THF	308	348	344	391	362	457	374	422	418	445	430	511	66	74	74	58	68	54
DCM	305	349	345	391	362	458	378	420	420	449	434	513	73	71	75	54	72	55
ACN	308	352	340	389	359	454	374	422	422	453	438	515	66	70	82	64	79	61
MeOH	307	351	342	389	359	455	376	426	426	477	470	517	69	75	84	88	111	62
DMF	312	346	344	394	362	451	376	421	426	473	443	519	64	75	82	79	81	68



Kamlet-Taft relationship: $\Delta\nu = \text{Intercept} + A\pi^* + B\alpha + C\beta$

A is coefficient for solvent acidity (α), B is coefficient for solvent basicity (β), and C is coefficient for solvent dipolarity (π^*)

H-Pz: $\Delta\nu = 7837 - 2539(\pi^*) + 184(\alpha) - 686(\beta)$

H-BTD: $\Delta\nu = 6239 - 1270(\pi^*) - 168(\alpha) - 520(\beta)$

Figure S5. Kamlet-Taft regression plot for heterocyclic compounds

Table S2. Kamlet-Taft solvatochromic parameters for solvents used for regression analysis

Parameters	Tol	Hex	PE	CH	CB	THF	DCM	ACN	MeOH	DMF
π^*	-0.04	-0.08	0.00	0.54	0.71	0.58	0.82	0.75	0.88	0.60
α	0.00	0.00	0.00	0.00	0.00	0.00	0.13	0.19	0.00	0.93
β	0.00	0.00	0.00	0.11	0.07	0.55	0.10	0.31	0.69	0.62

Table S3. Computed ground-state dipole moment (μ_g) for all compounds against four different functionals at 6-31G(d,p) basis set.

Compd	B3LYP	CAM-B3LYP	MPW1PW91	WB97XD
H-Pz	0.127100	0.091700	0.137600	0.129800
H-BTD	0.305301	0.364201	0.327300	0.459600
H-Ch	0.000361	0.000100	0.000141	0.000141
H-An	0.008305	0.002900	0.000000	0.000000
H-Py	0.000100	0.000000	0.000000	0.000100
H-Per	0.778600	0.674000	0.673600	0.511603

Table S4. Parameters for dipole moment change calculations (^avalues computed by B3LYP/6-31G(d,p))

Compd	Free Energy ^a (au)	Onsager radii ^a (Å)	μ_g^a (D)	Slope	$\Delta\mu$ (D)	μ_e (D)
H-Ch	-2535.52188	8.39195	0.0004	1891.9236	10.3098	10.3094
H-An	-2381.859958	7.1938	0.0083	3345.6121	10.8812	10.8729
H-Py	-2458.110717	8.62774	0.0001	5377.1701	18.1187	18.1185
H-Per	-2611.74707	9.56516	0.7786	1693.9124	11.8710	11.0923

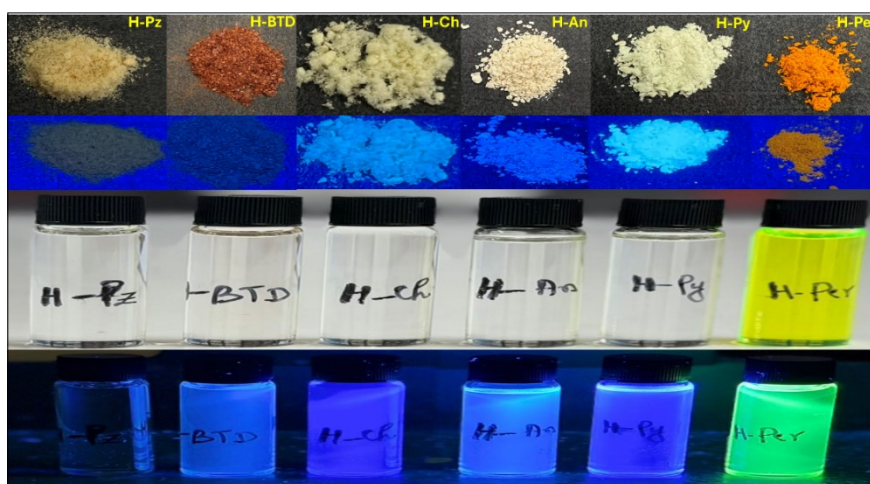


Figure S6. Images of all compounds in solid (1-2 rows) and solution state (3-4 rows); 1st and 3rd rows are under ambient light while 2nd and 4th rows are under 365 nm light.

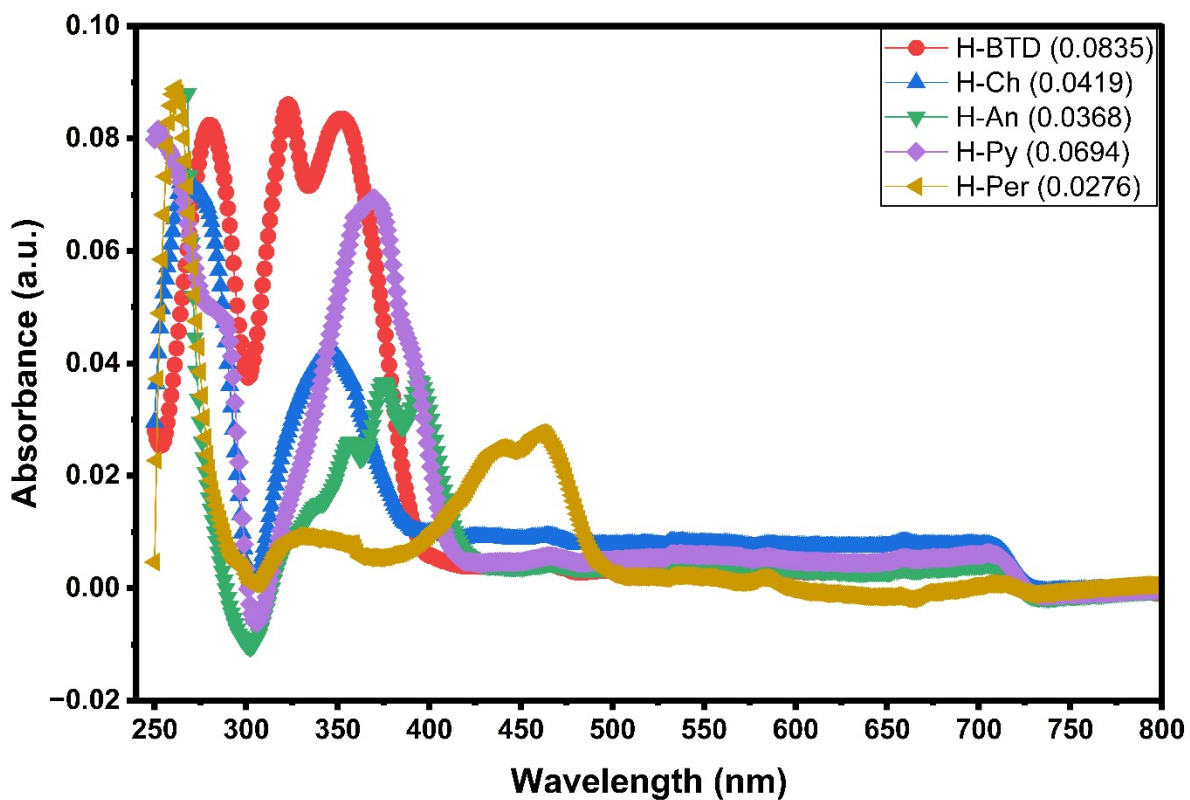


Figure S7. Absorbance profiles of all compounds in CHCl_3 used for PLQY (ϕ_{PL}) measurements

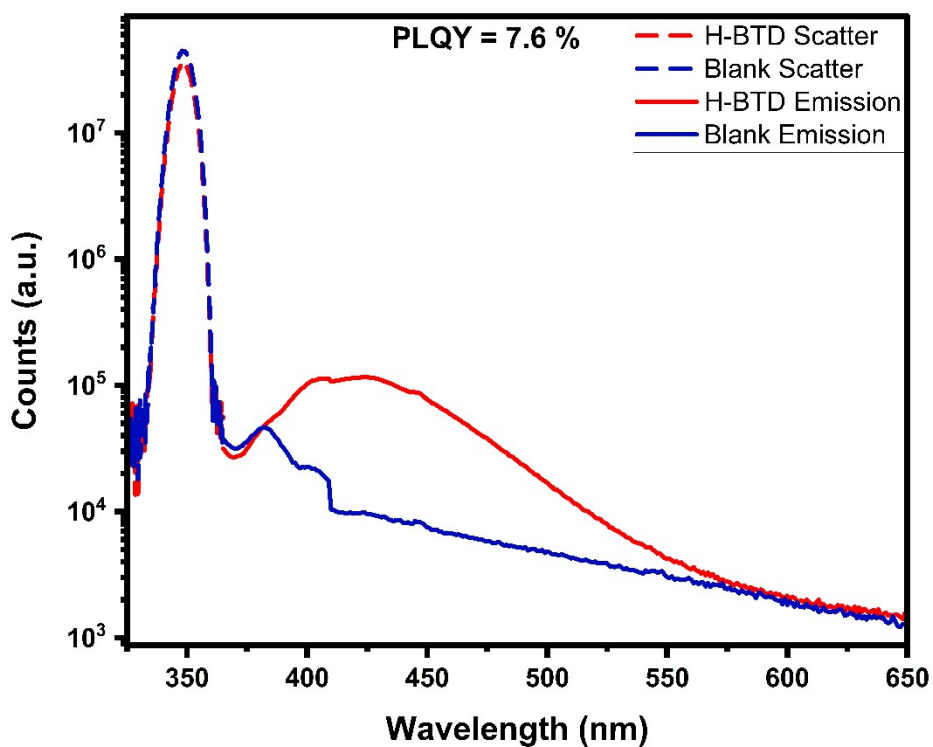


Figure S8. PLQY graph of H-BTD (Excitation at 345 nm)

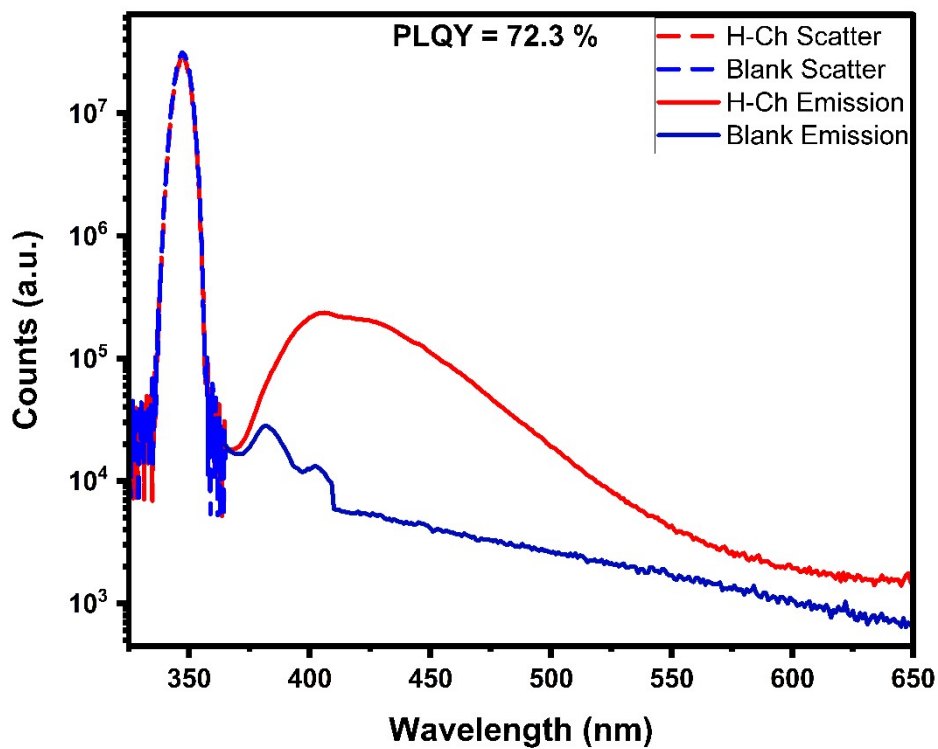


Figure S9. PLQY graph of H-Ch (Excitation at 345 nm)

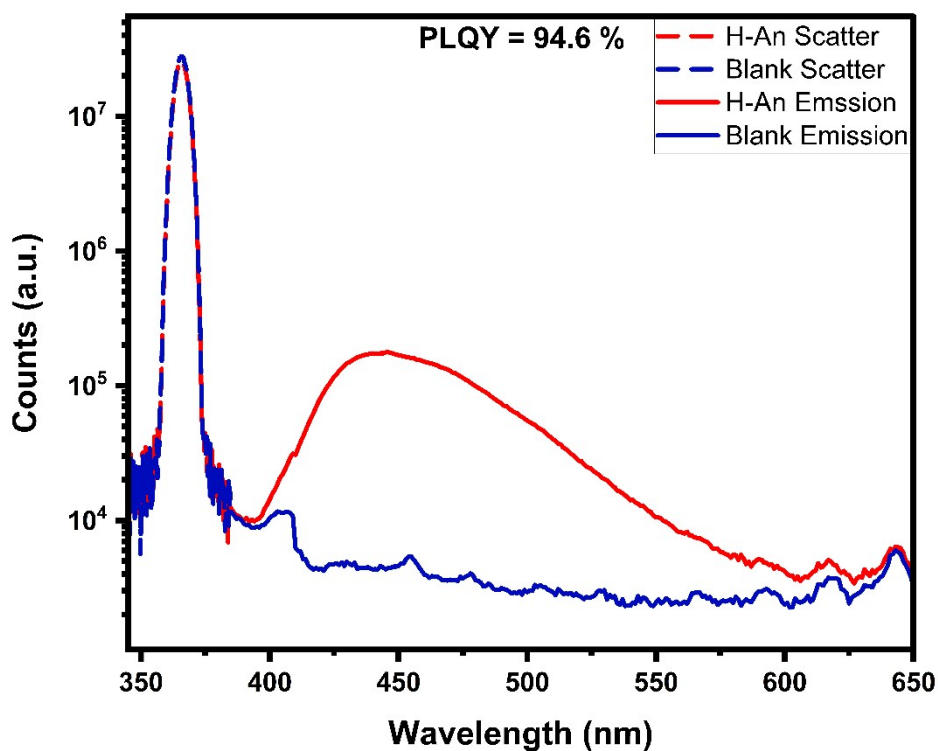


Figure S10. PLQY graph of H-An (Excitation at 365 nm)

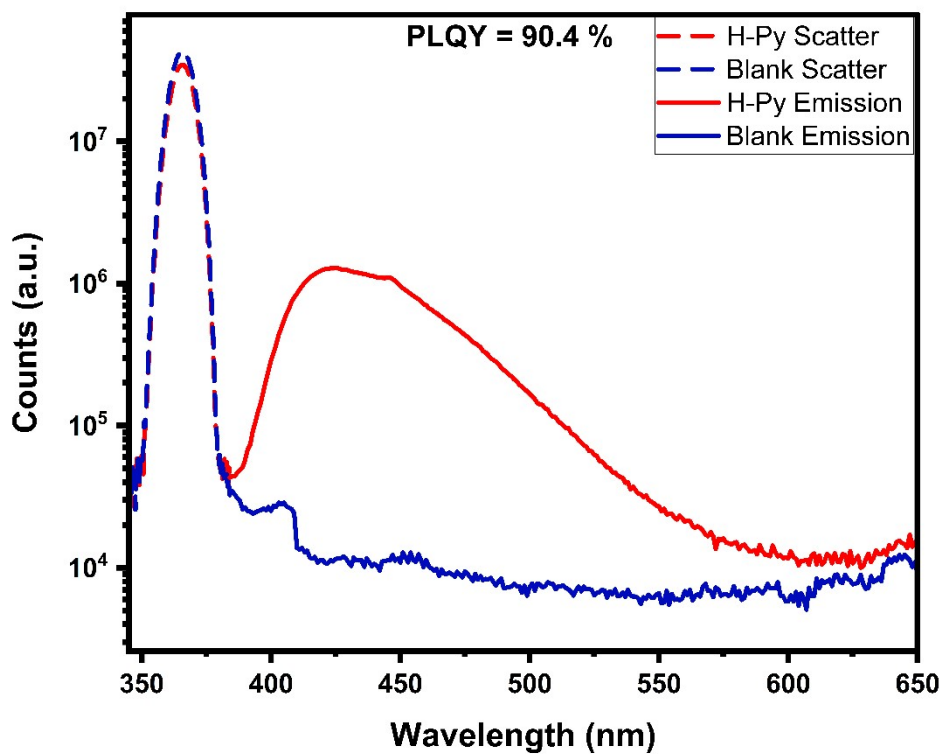


Figure S11. PLQY graph of H-Py (Excitation at 364 nm)

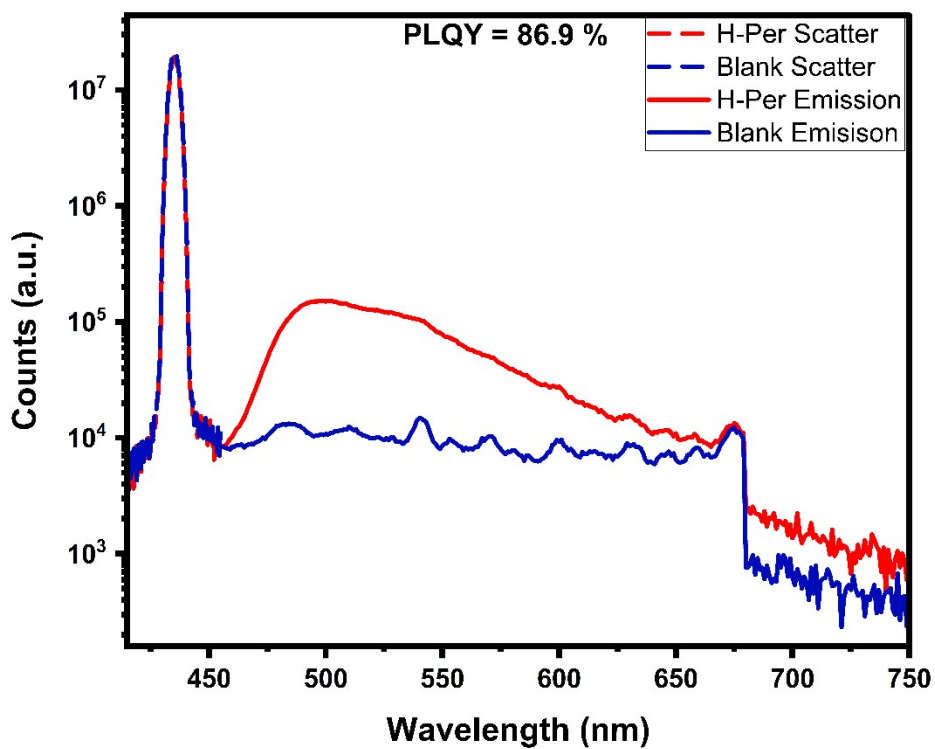


Figure S12. PLQY graph of H-Per (Excitation at 435 nm)

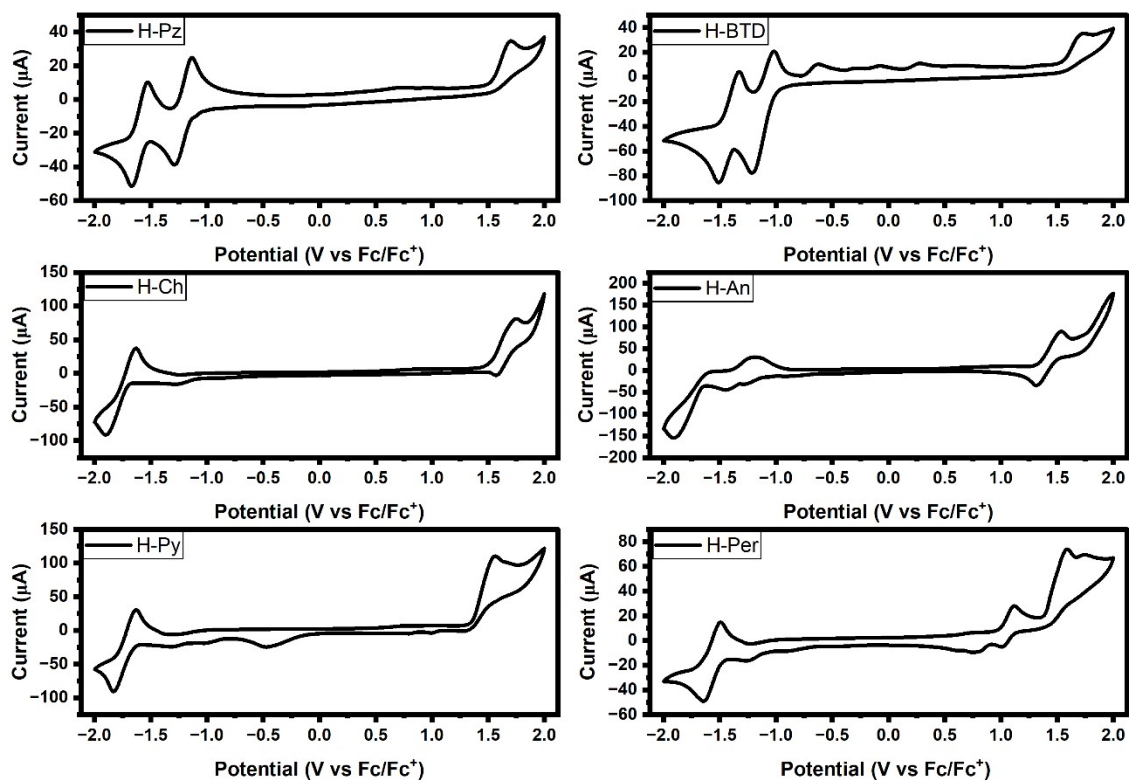


Figure S13. Cyclic voltametric curves for all compounds acquired in 0.1 M Bu_4NPF_6 as supporting electrolyte in anhydrous DCM solvent at 100 mV/s scan rate and potential window potential (-2 – 2 V)

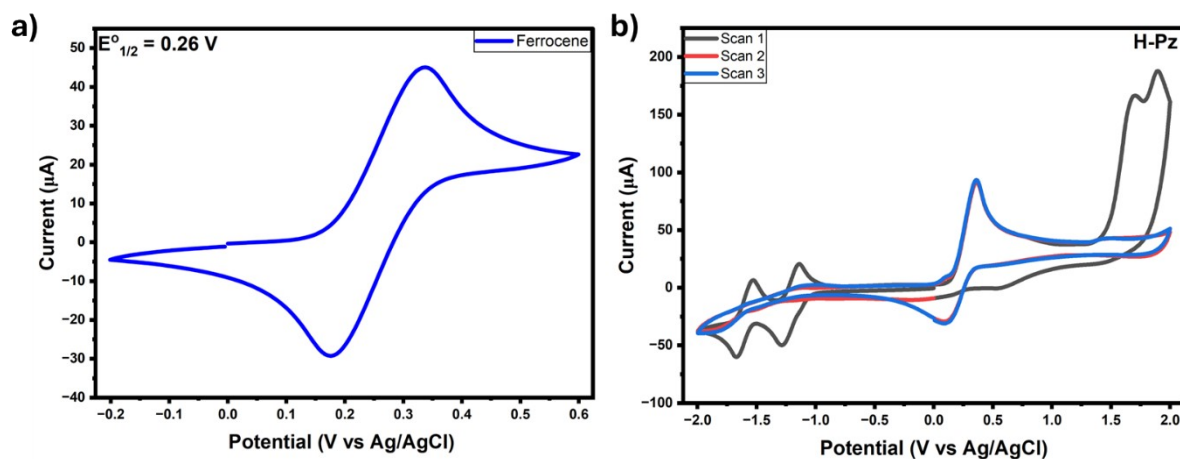


Figure S14. Cyclic voltametric curves acquired in 0.1 M Bu_4NPF_6 as supporting electrolyte in anhydrous DCM solvent at 100 mV/s scan rate and potential window potential (-2 – 2 V) **a)** Ferrocene **b)** H-Pz with ferrocene as an internal standard

Experimental Section

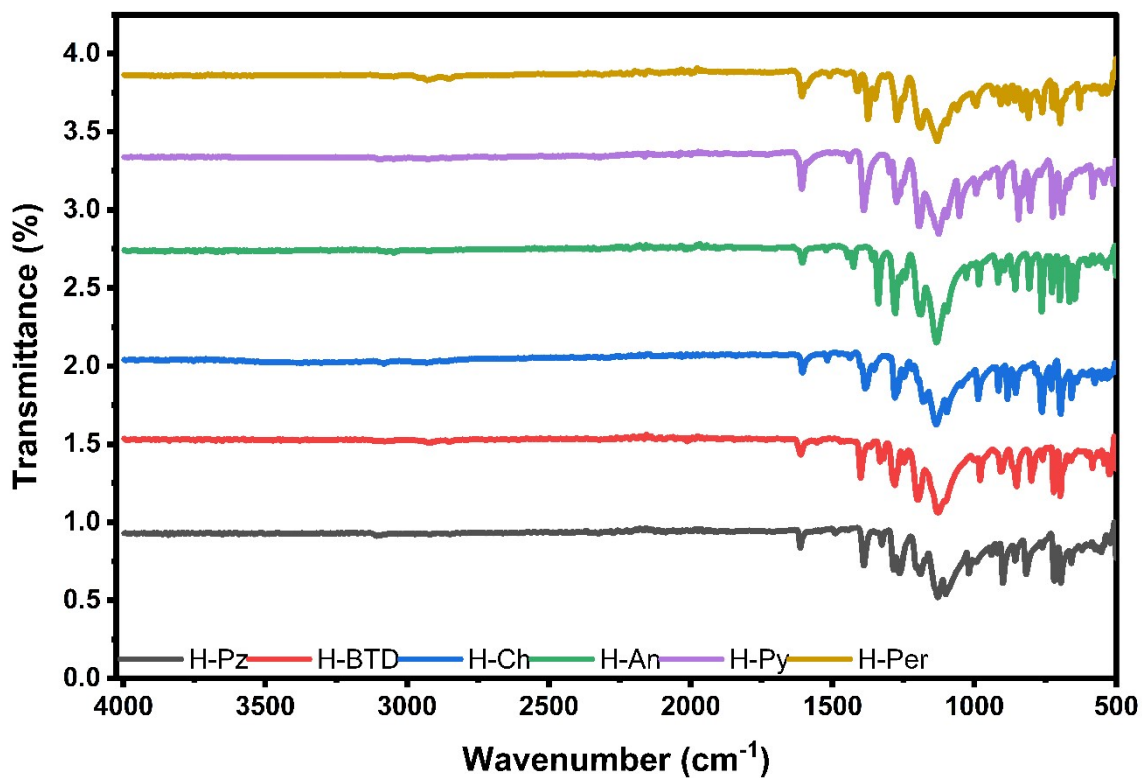


Figure S15. FTIR spectra of all synthesized compounds

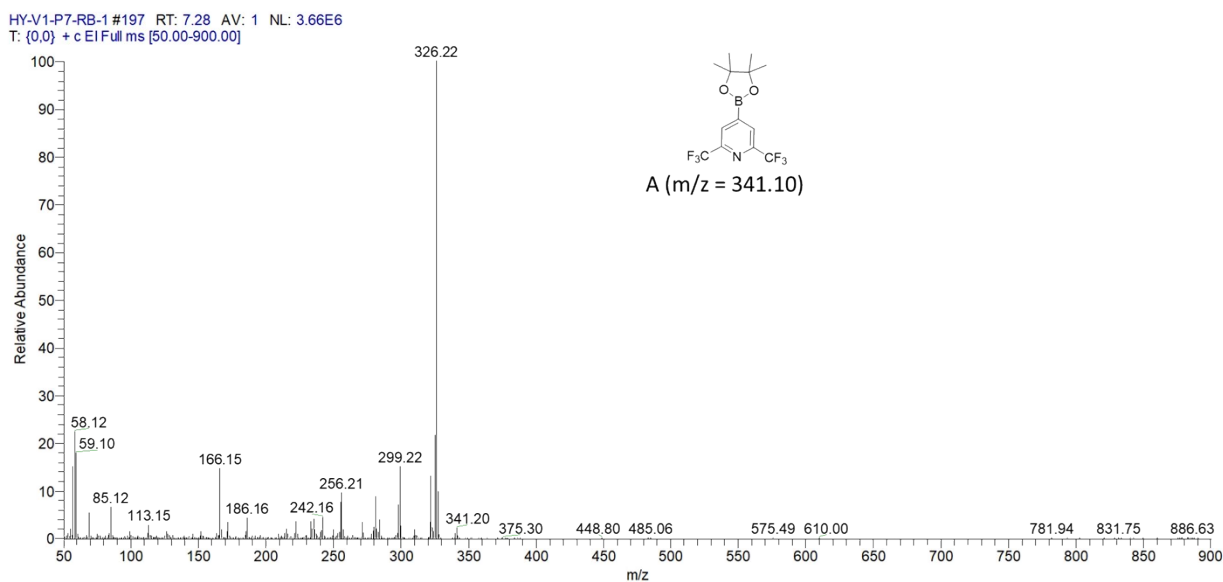


Figure S16. Mass spectrum of A

HY-V1-P26-YELLOW #465 RT: 11.77 AV: 1 NL: 4.65E6
T: {0.0} + c EI Full ms [50.00-900.00]

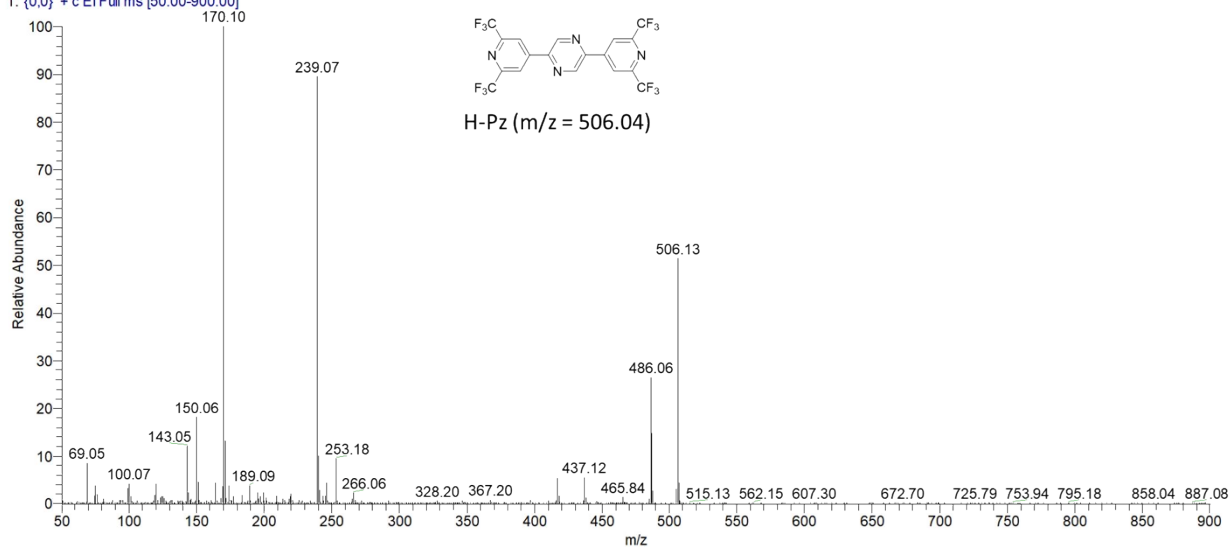


Figure S17. Mass spectrum of H-Pz

HY-V1-P19-RBF #592 RT: 13.89 AV: 1 NL: 9.05E5
T: {0.0} + c EI Full ms [50.00-900.00]

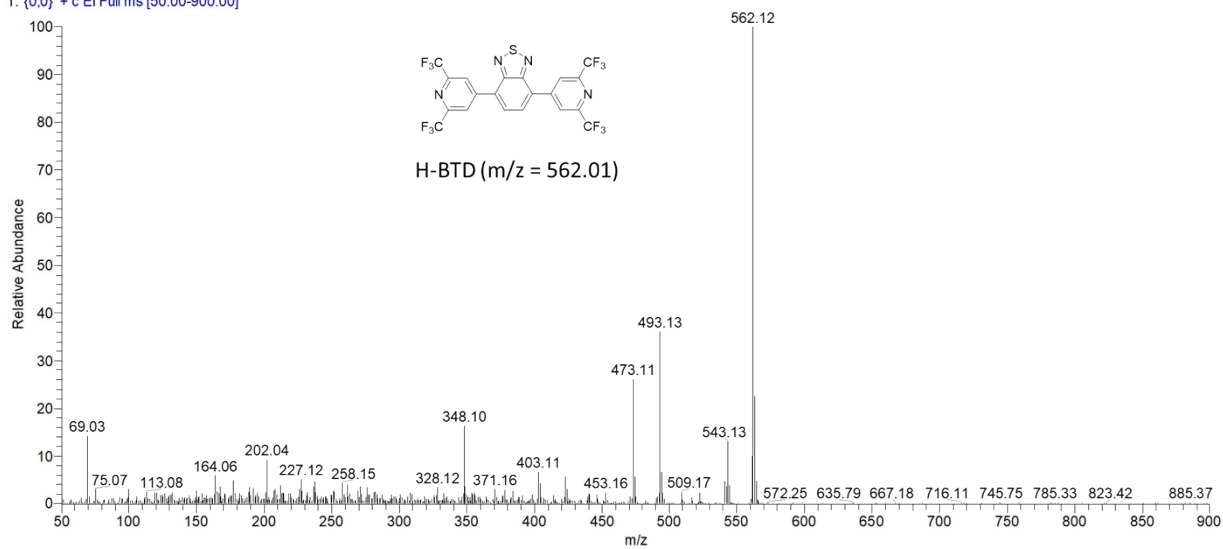


Figure S18. Mass spectrum of H-BTD

HY-V1-P6-RM-W#984 RT: 20.45 AV: 1 NL: 1.69E5
T: {0.0} + c EI Full ms [50.00-900.00]

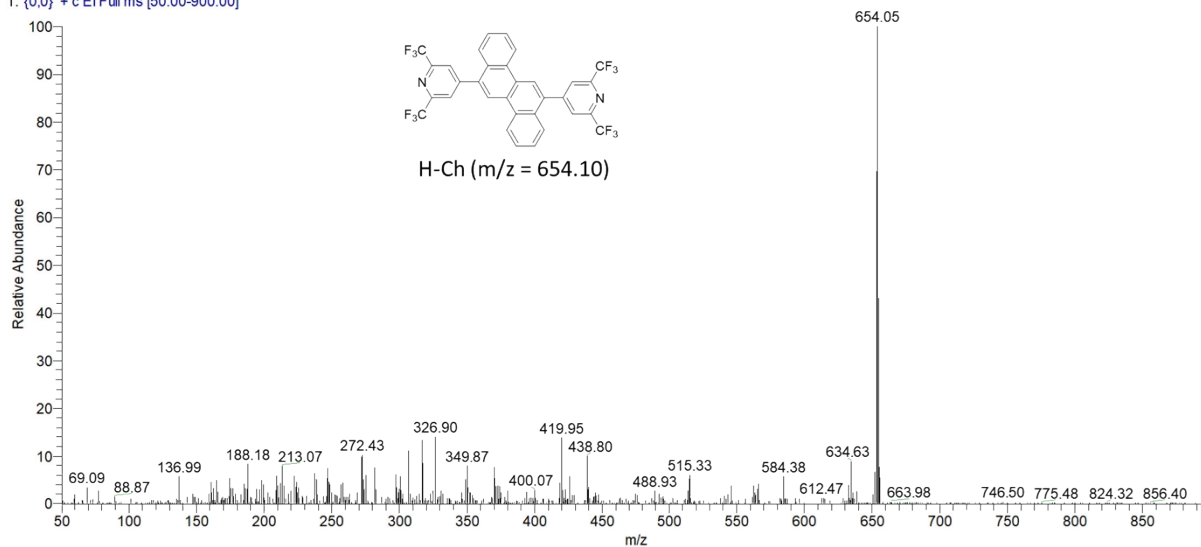


Figure S19. Mass spectrum of H-Ch

HY-V1-P20-YELLOW#573 RT: 13.57 AV: 1 NL: 1.51E6
T: {0.0} + c EI Full ms [50.00-900.00]

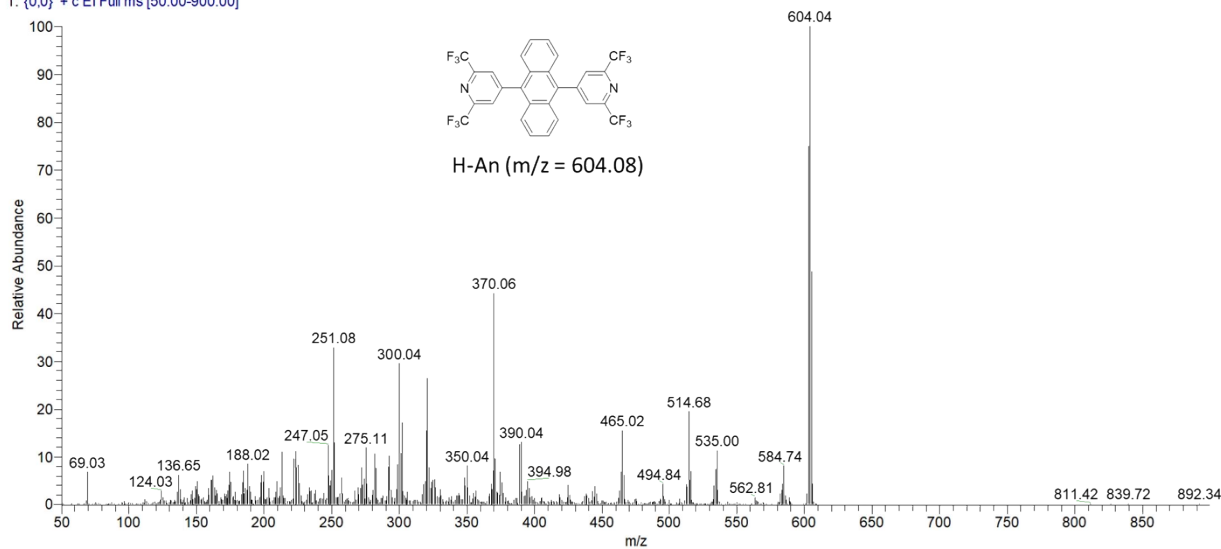


Figure S20. Mass spectrum of H-An

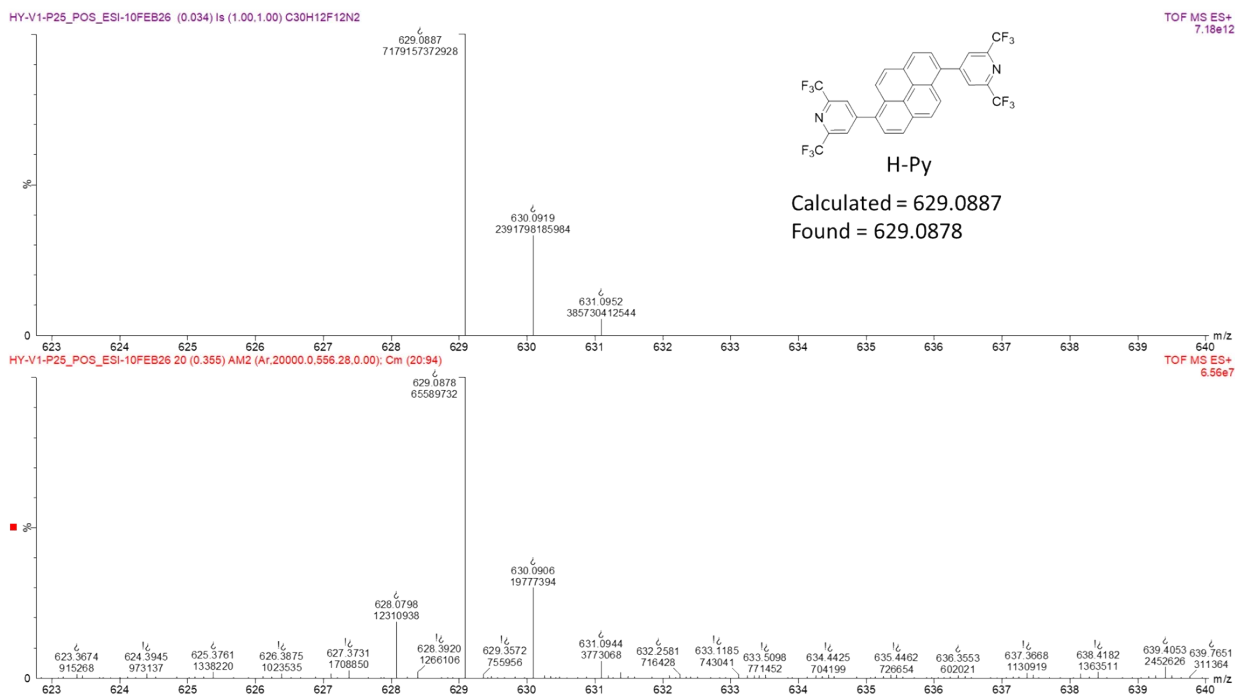


Figure S21. HRMS spectrum of H-Py

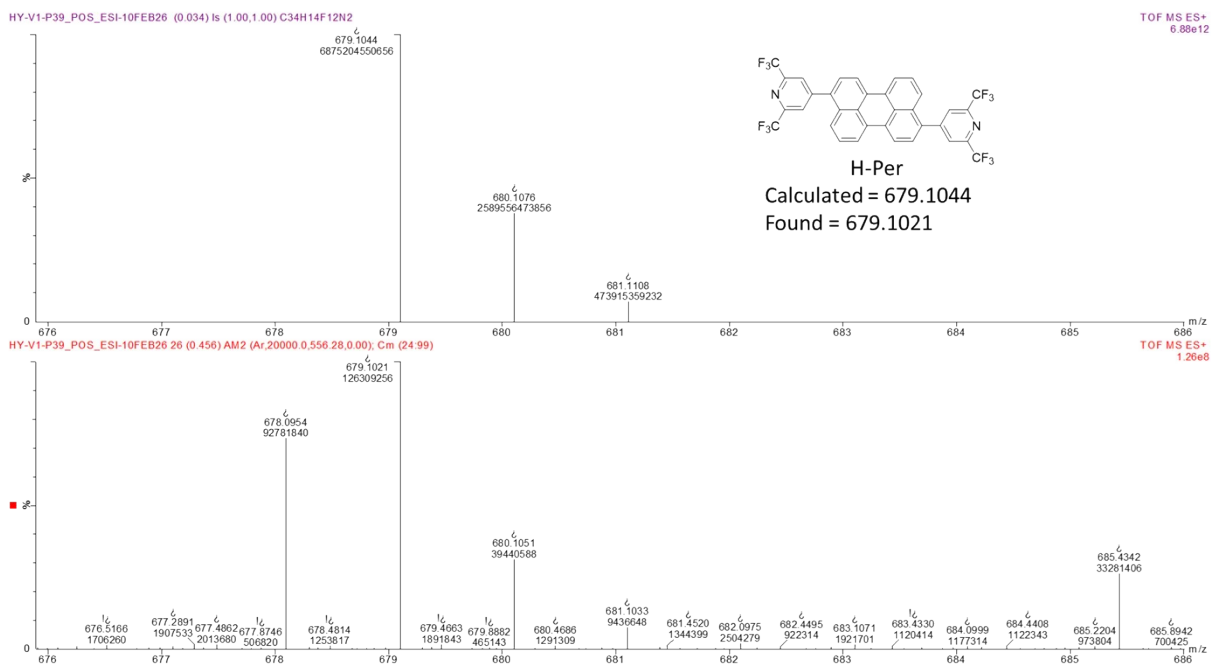


Figure S22. HRMS spectrum of H-Per

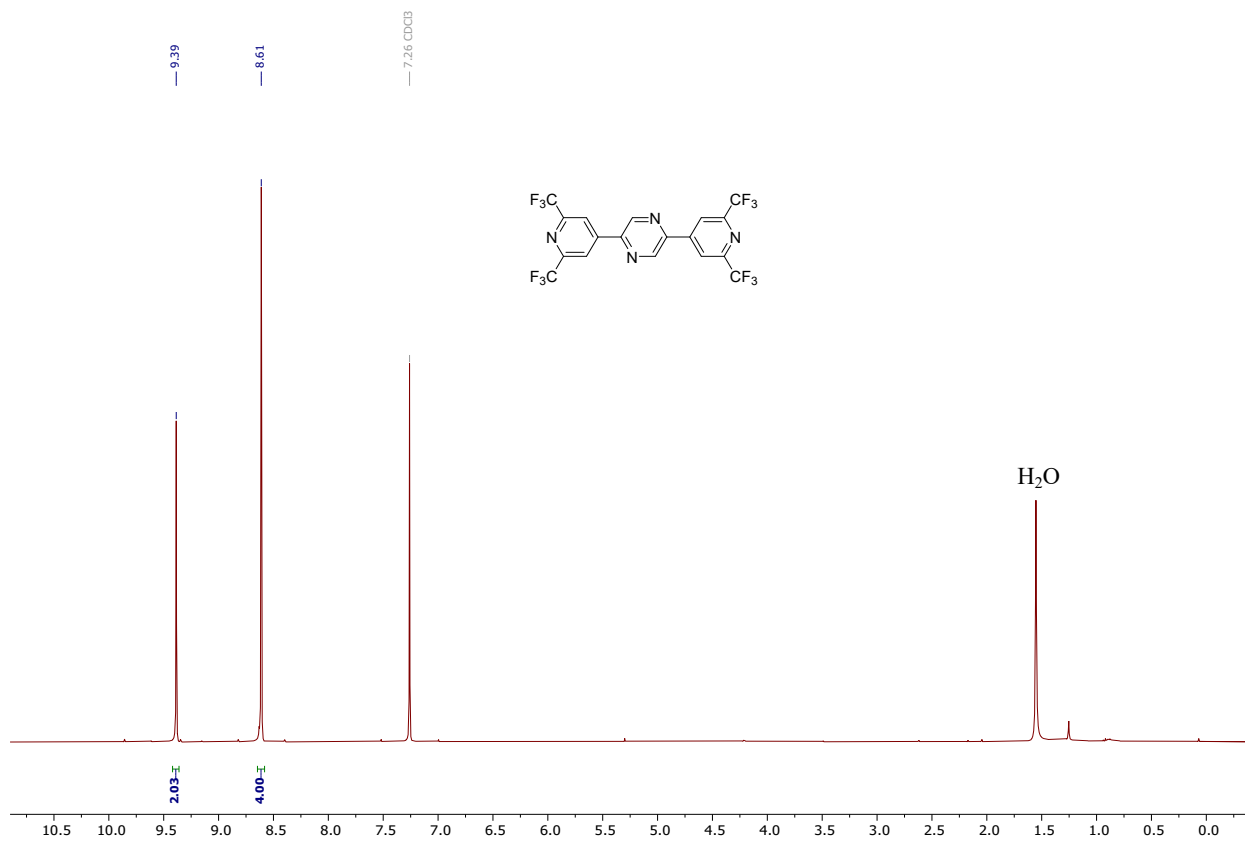


Figure S23. ¹H NMR spectrum of H-Pz

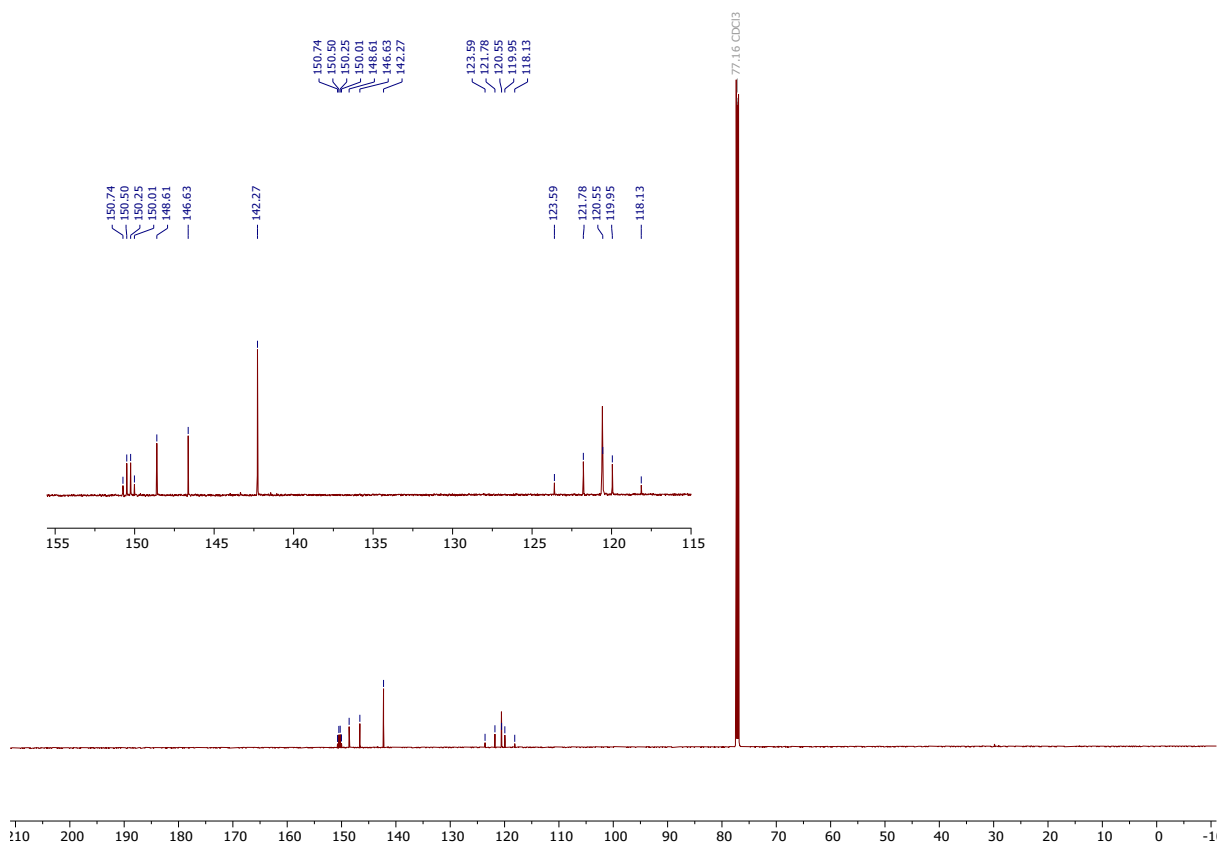


Figure S24. ^{13}C NMR spectrum of H-Pz

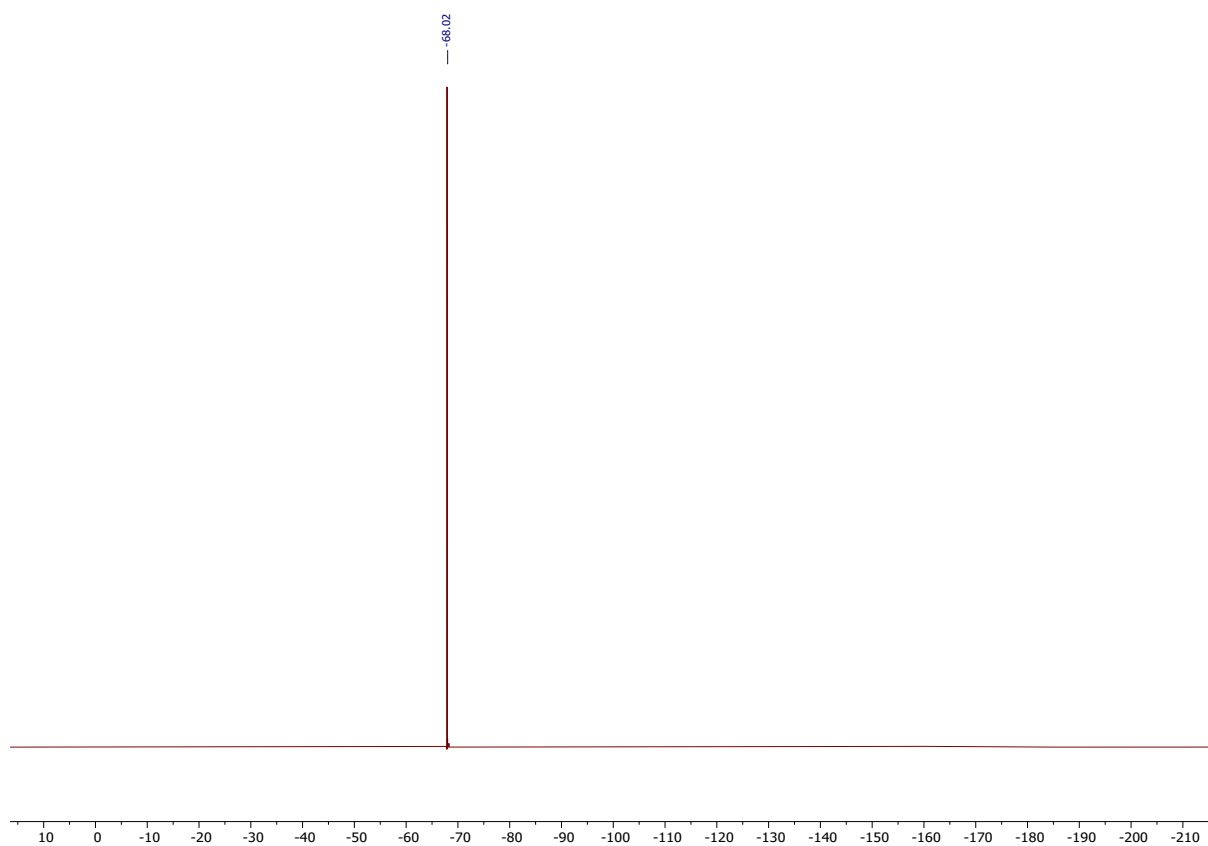


Figure S25. ^{19}F NMR spectrum of H-Pz

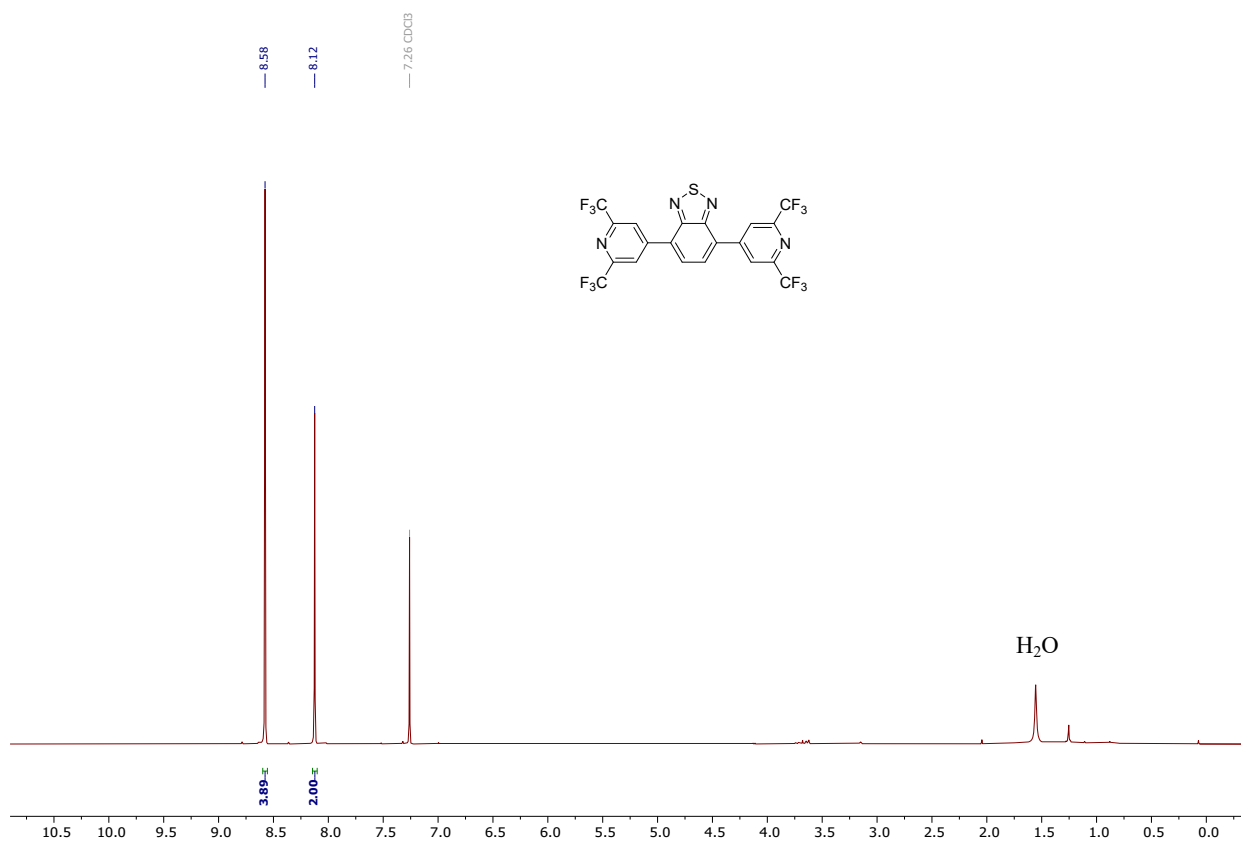


Figure S26. ¹H NMR spectrum of H-BTD

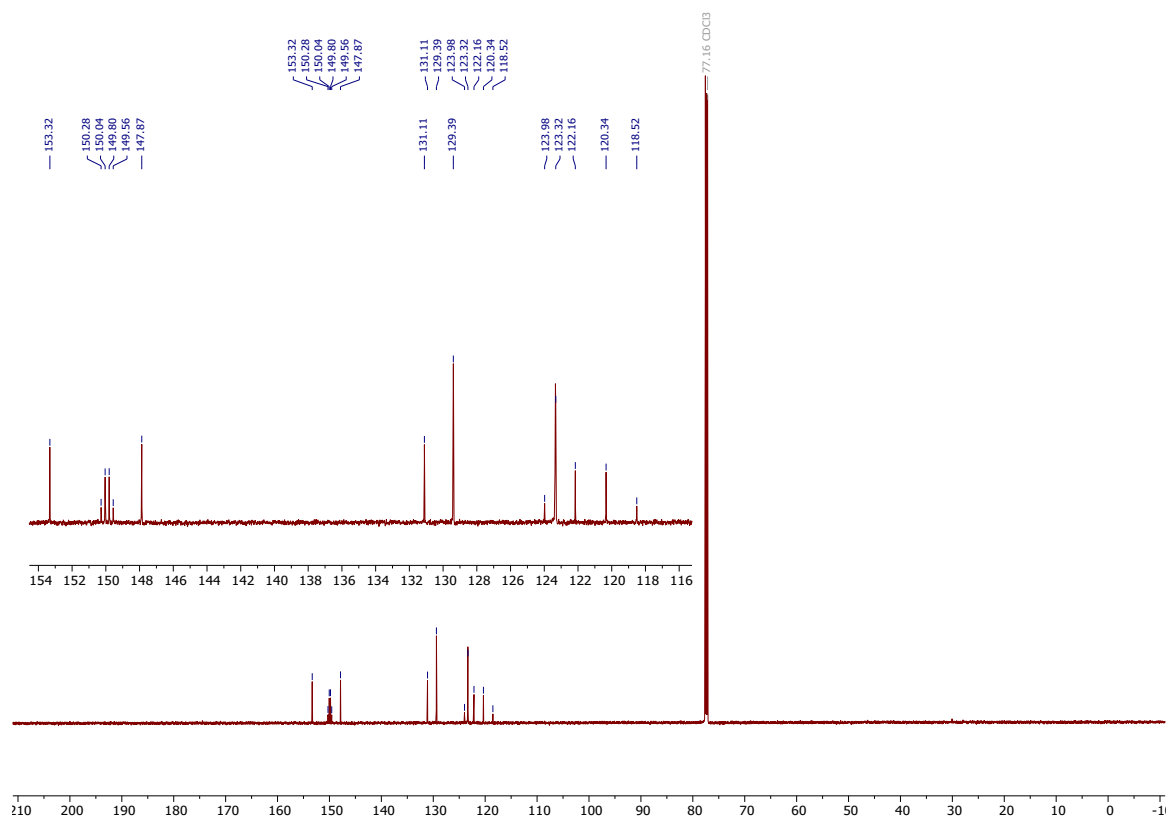


Figure S27. ¹³C NMR spectrum of H-BTD

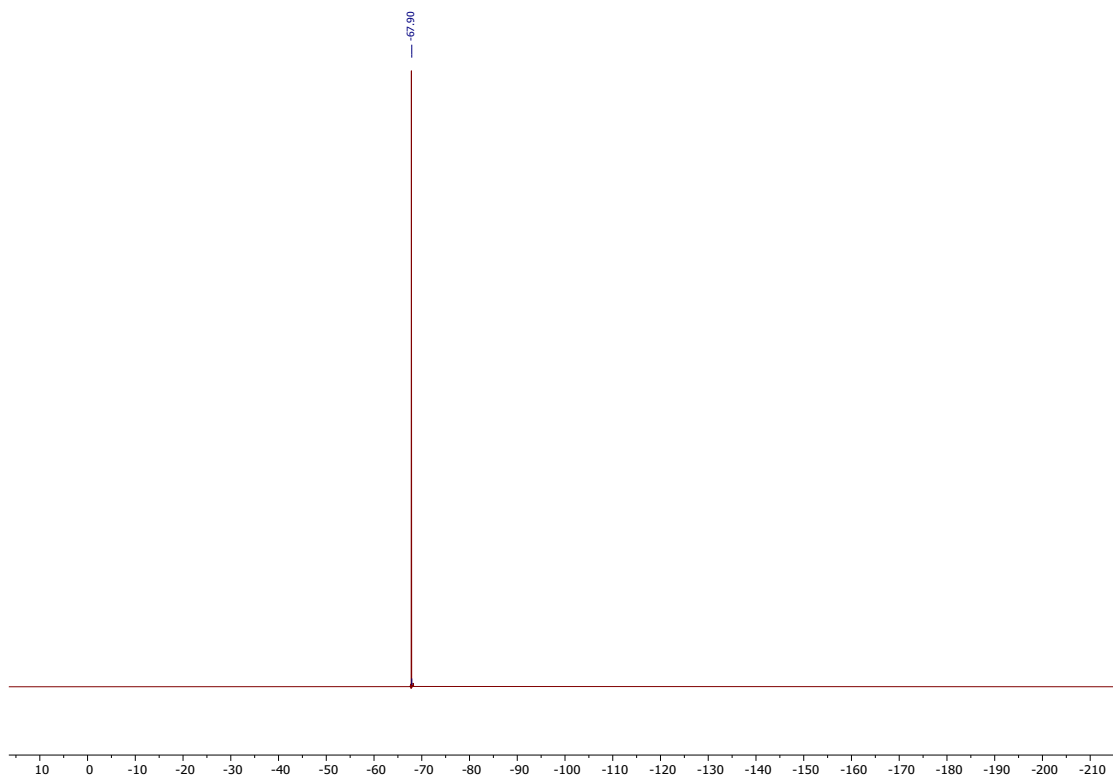


Figure S28. ^{19}F NMR spectrum of H-BTD

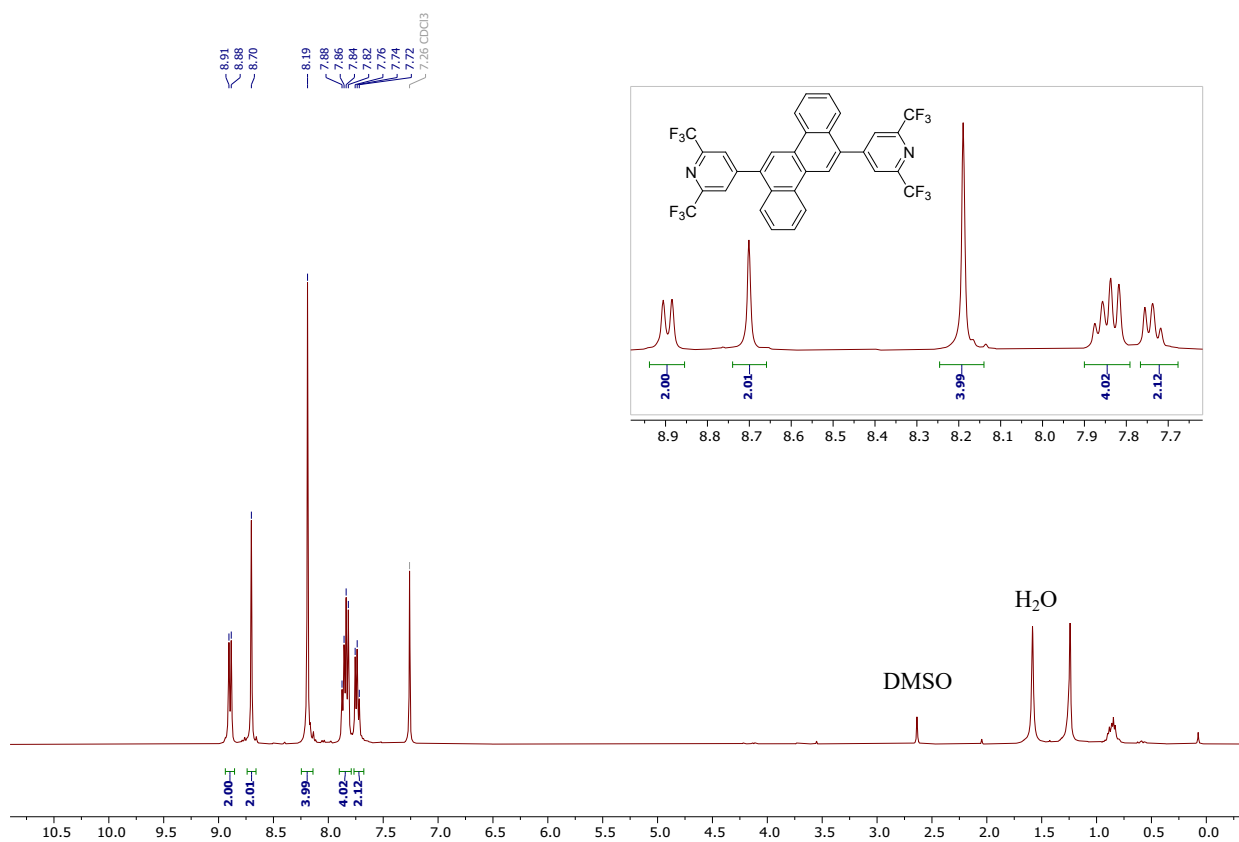


Figure S29. ^1H NMR spectrum of H-Ch

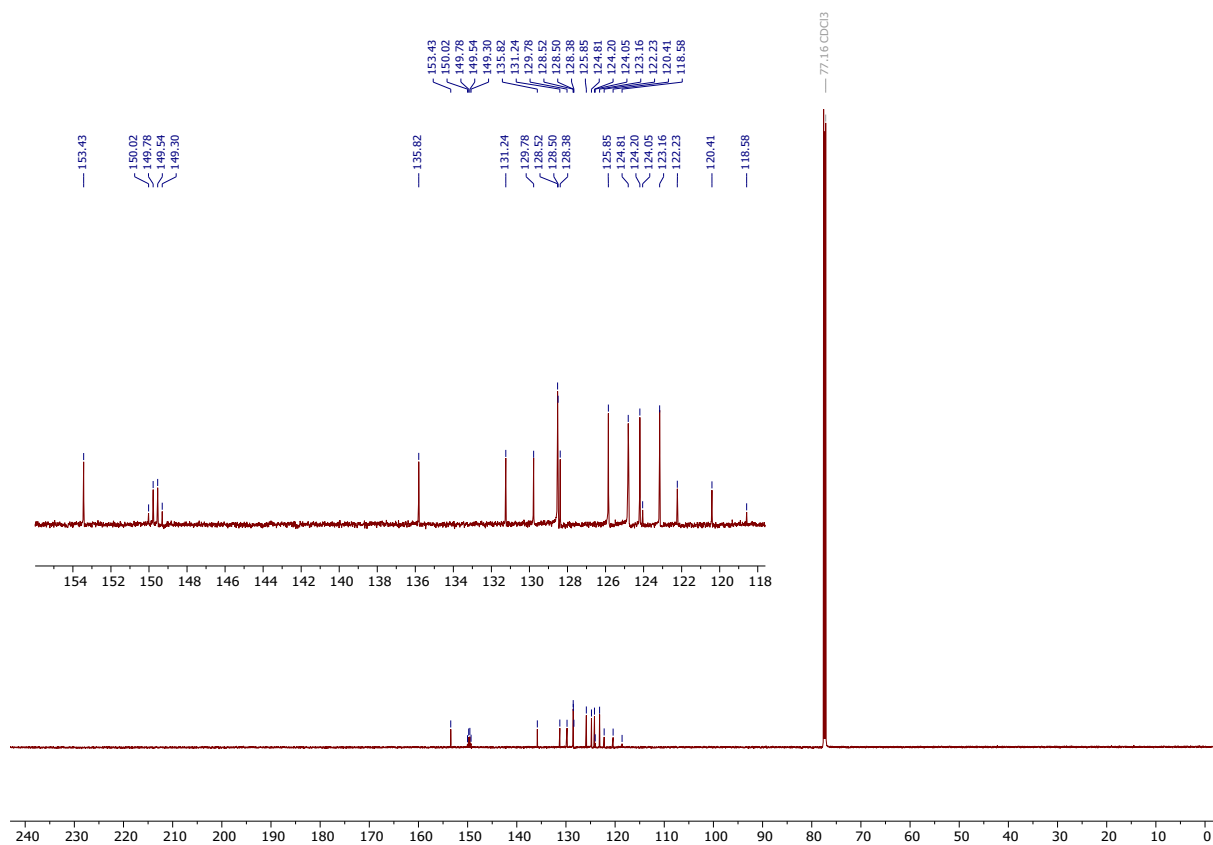


Figure S30. ¹³C NMR spectrum of H-Ch

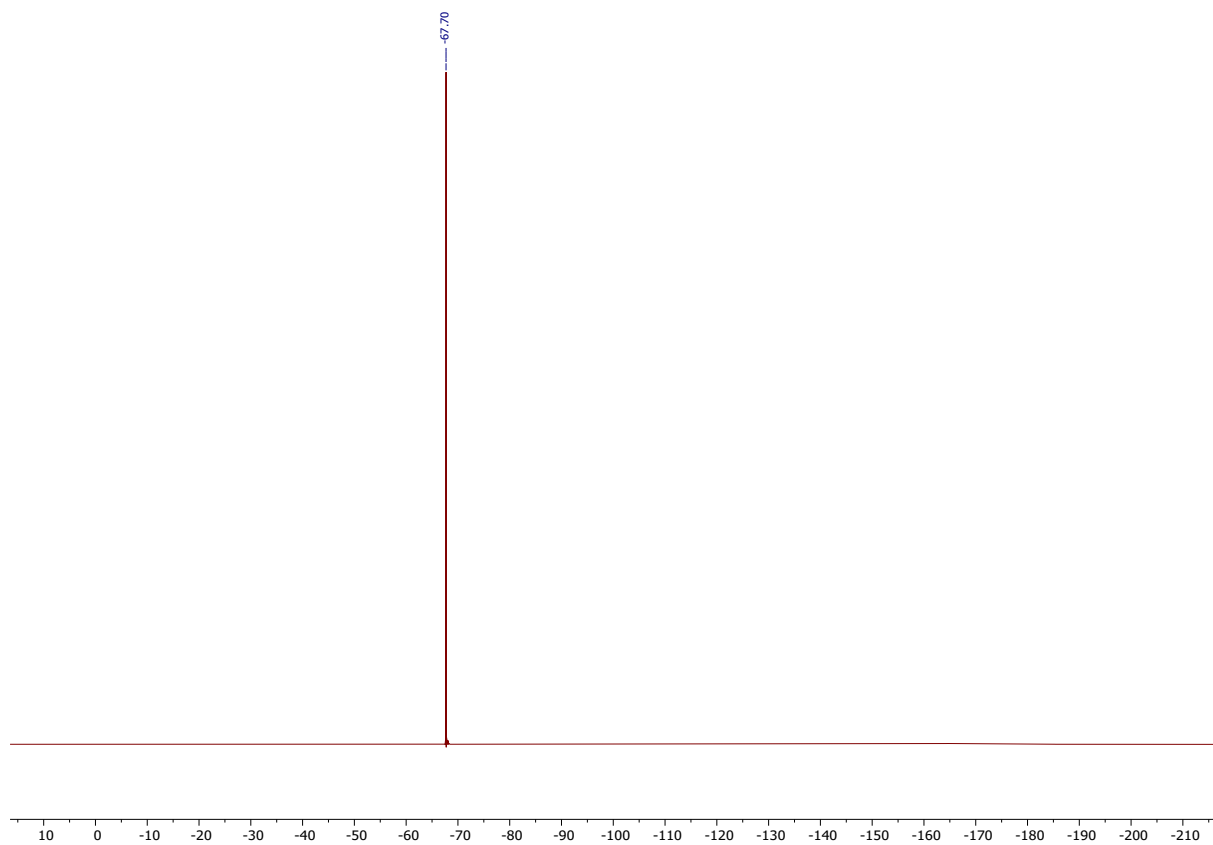


Figure S31. ^{19}F NMR spectrum of H-Ch

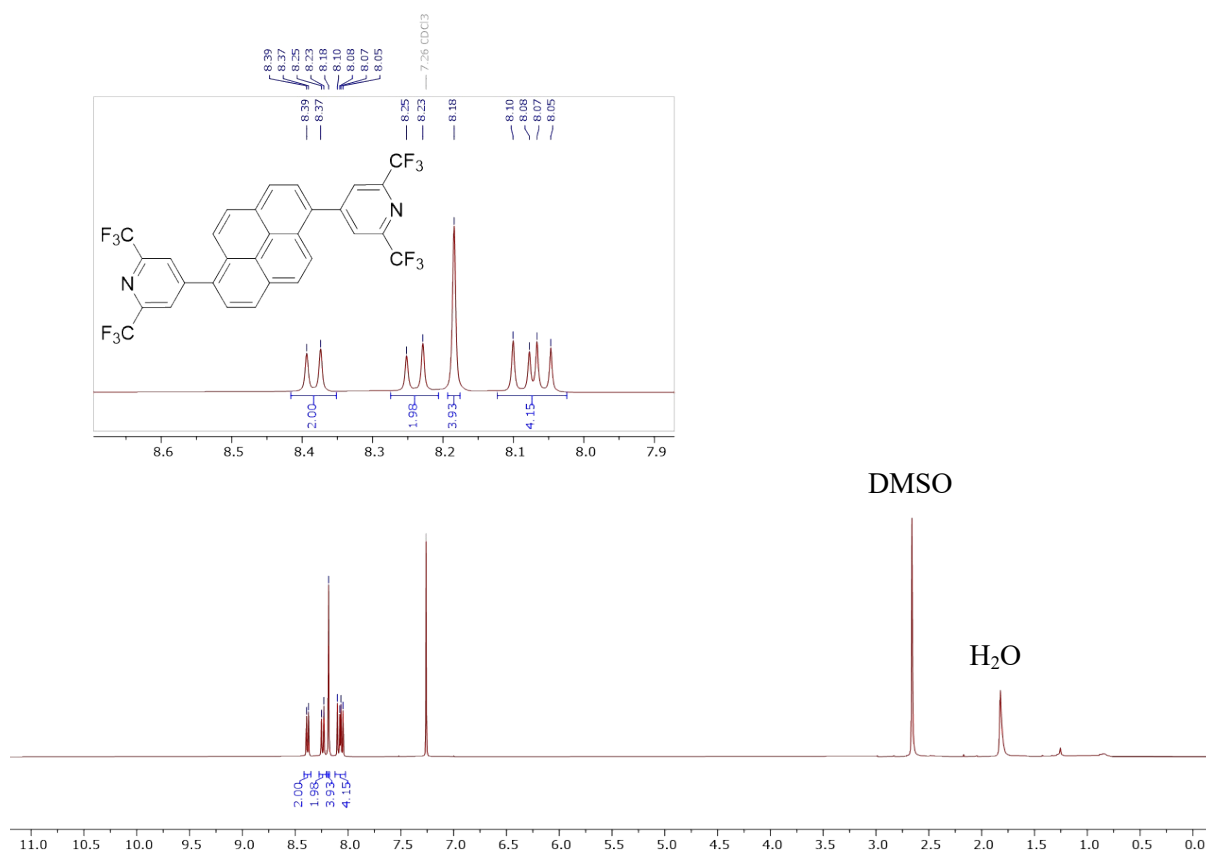


Figure S32. ^1H NMR spectrum of H-Py

DMSO

H₂O

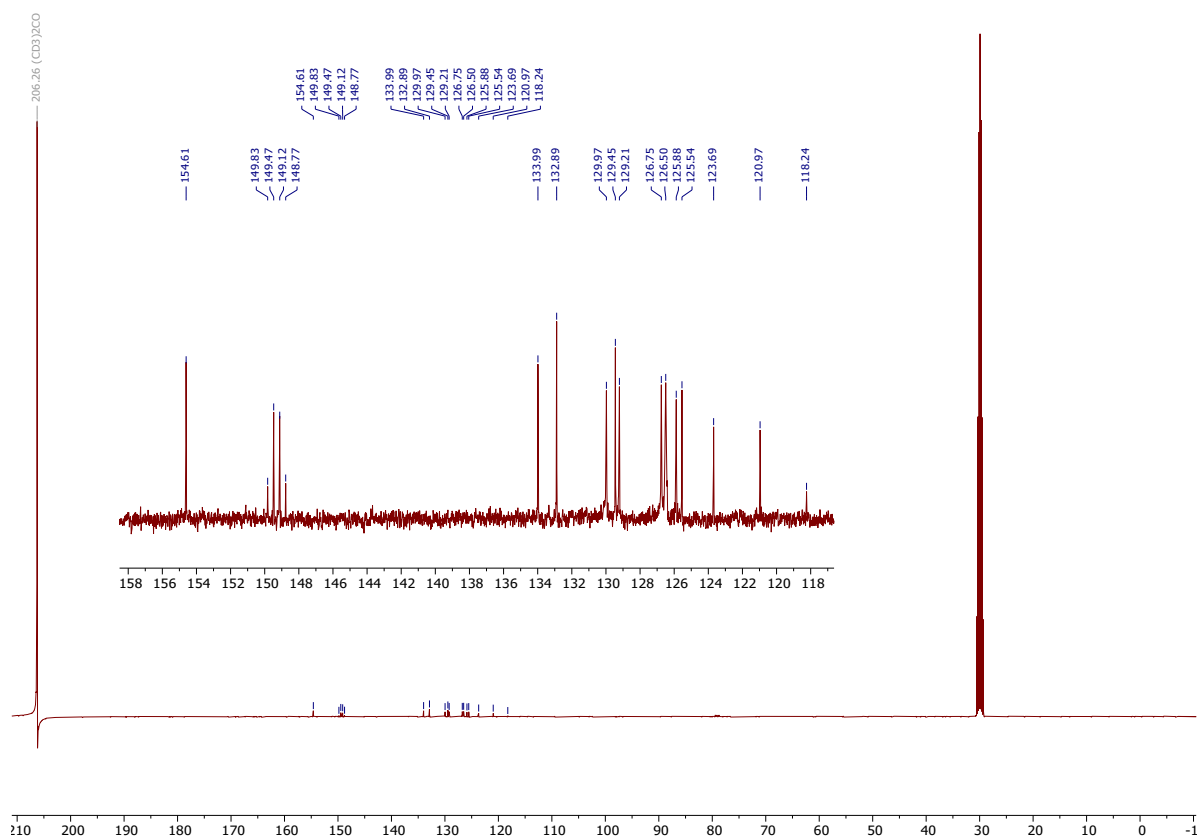


Figure S33. ¹³C NMR spectrum of H-Py

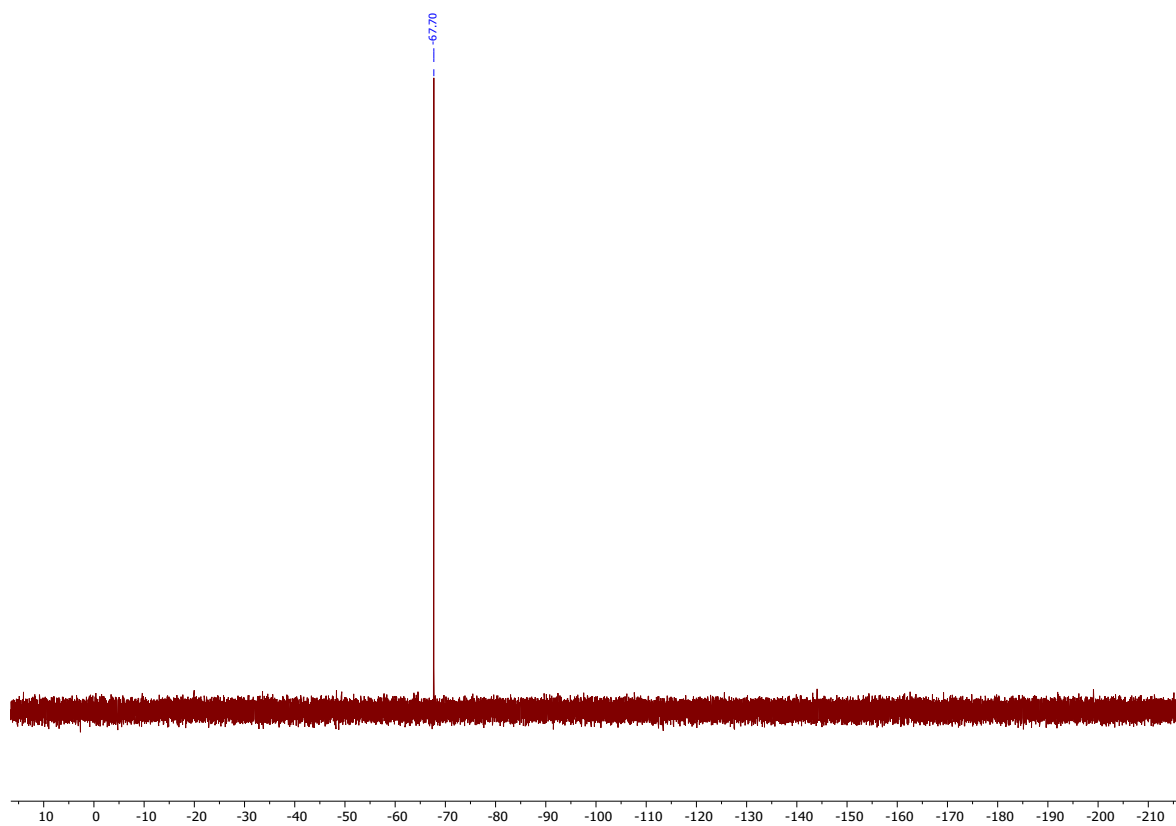


Figure S34. ¹⁹F NMR spectrum of H-Py

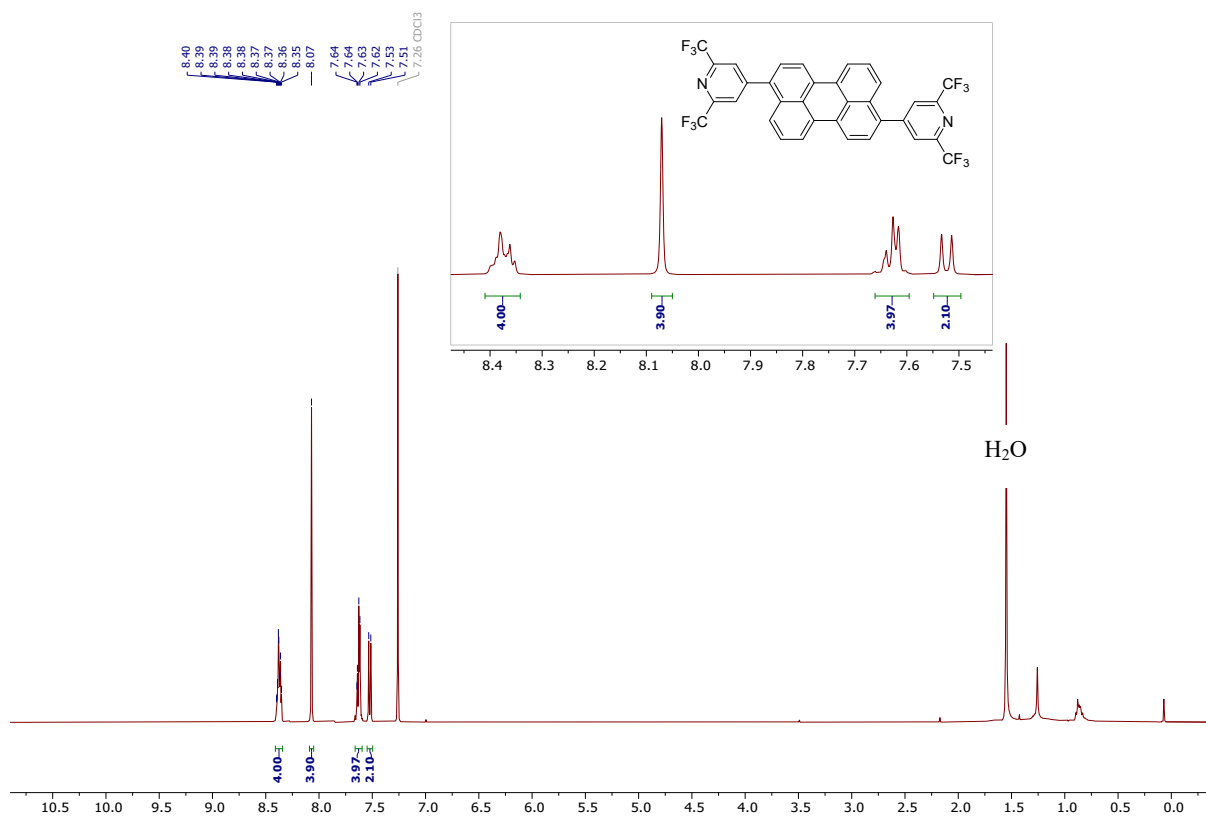


Figure S35. ¹H NMR spectrum of H-Per

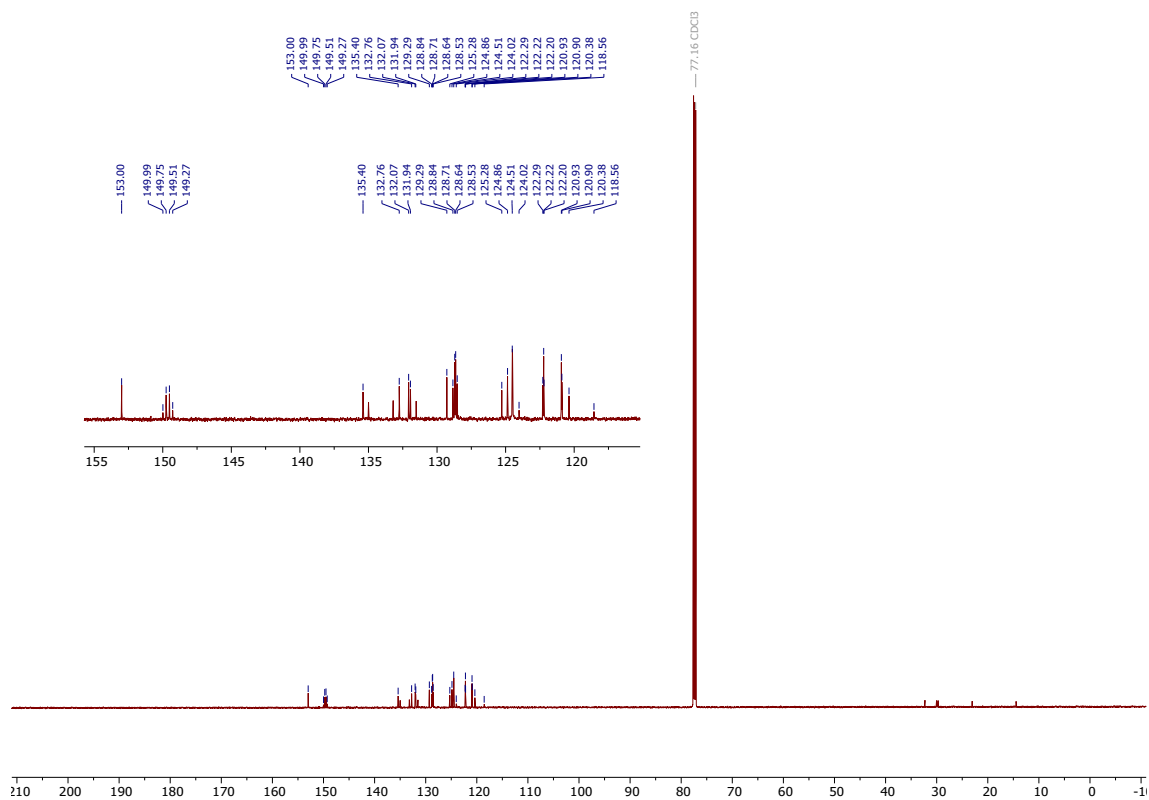


Figure S36. ¹³C NMR spectrum of H-Per

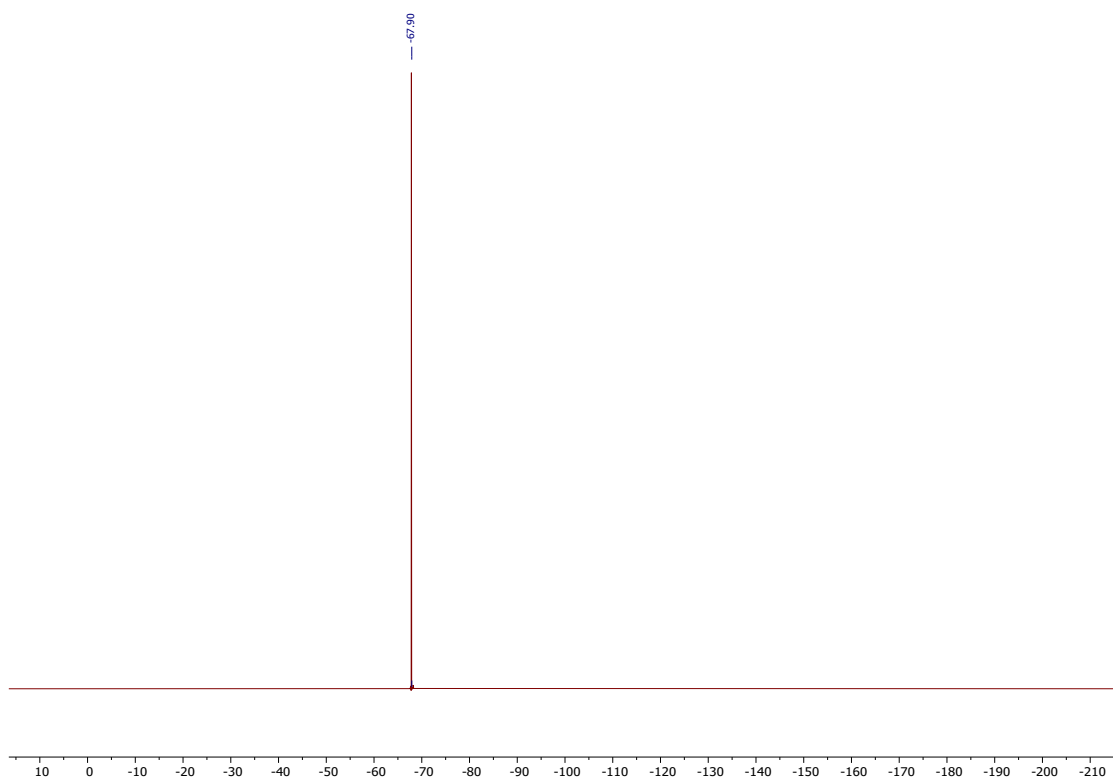


Figure S37. ^{19}F NMR spectrum of H-Per

Computational Studies

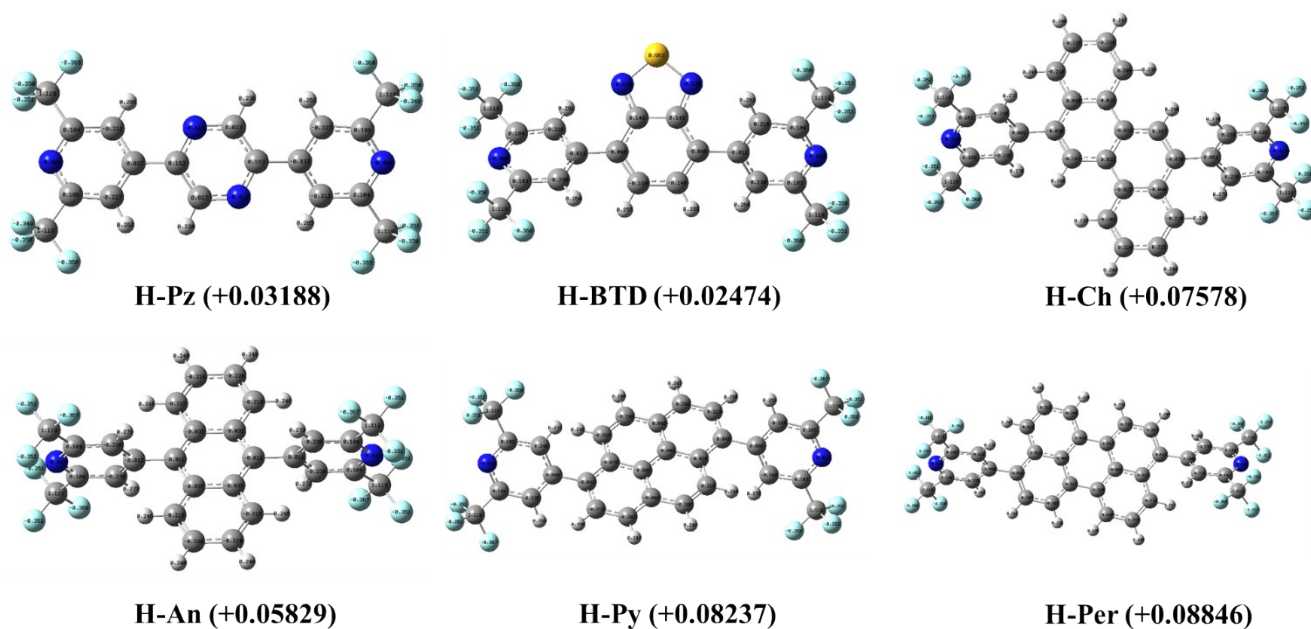


Figure S38. Natural Population Analysis (NPA) analysis of all compounds at B3LYP/6-31G(d,p). Values in parentheses represent the total NPA charges summed over the central core, illustrating the degree of ground-state electronic redistribution.

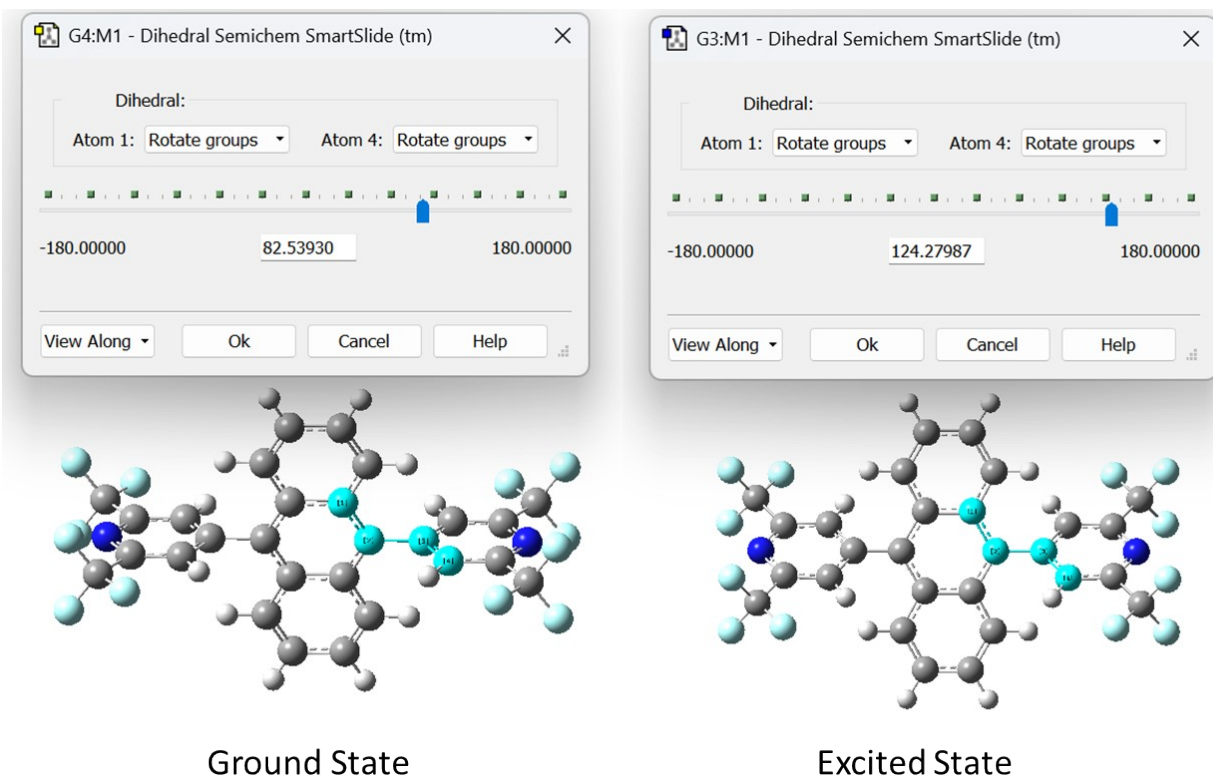


Figure S39. Comparison of Dihedral angles of ground and excited state geometries of H-An at B3LYP/6-31G(d,p)

Table S5. Optimized Coordinates of H-Pz (B3LYP/6-31G(d,p), ground state)

Atom	X	Y	Z
C	0.58457	1.19828	-0.09055
C	1.35458	0.0205	-0.05859
N	0.74524	-1.17663	-0.08416
C	-0.58457	-1.19828	-0.09057
C	-1.35458	-0.0205	-0.0586
N	-0.74524	1.17663	-0.08416
H	1.04693	2.18	-0.13857
H	-1.04693	-2.18	-0.13861
C	2.83801	0.02814	-0.02598
C	3.55299	-1.12449	-0.38434
C	3.5712	1.15819	0.36304
C	4.94469	-1.08047	-0.34762
H	3.02572	-2.02171	-0.68035
C	4.964	1.08027	0.36063
H	3.08831	2.07312	0.68092
N	5.64889	-0.00695	0.01302
C	-2.83801	-0.02814	-0.02601
C	-3.55299	1.1245	-0.38437
C	-3.57121	-1.15819	0.36298
C	-4.94468	1.08048	-0.34767
H	-3.02571	2.02172	-0.68036
C	-4.96401	-1.08028	0.36056
H	-3.08832	-2.07313	0.68086
N	-5.64889	0.00695	0.01295

C	5.78327	-2.29175	-0.72929
C	5.81935	2.26912	0.77369
C	-5.78326	2.29175	-0.72934
C	-5.81936	-2.26913	0.77359
F	5.00139	-3.34067	-1.08433
F	6.55967	-2.69543	0.29728
F	6.59289	-2.01965	-1.77373
F	6.63642	2.65893	-0.22534
F	6.58679	1.97784	1.84314
F	5.04864	3.33653	1.10672
F	-5.00137	3.34068	-1.08435
F	-6.55967	2.69543	0.29722
F	-6.59286	2.01968	-1.77379
F	-6.63642	-2.65893	-0.22546
F	-6.58682	-1.97786	1.84304
F	-5.04866	-3.33654	1.10662

Table S6. Optimized Coordinates of H-BTD (B3LYP/6-31G(d,p), ground state)

Atom	X	Y	Z
C	0.71103	1.33883	0.00236
C	-0.71103	1.33883	-0.00246
C	-1.46616	0.18139	-0.00204
C	-0.72721	-1.05098	0.00555
C	0.72721	-1.05098	-0.00559
C	1.46616	0.18139	0.00198
H	1.21362	2.30064	-0.01309
H	-1.21362	2.30064	0.01299
C	-2.94667	0.22309	-0.01558
C	-3.62426	1.22349	-0.73113
C	-3.72747	-0.70743	0.68903
C	-5.01713	1.25105	-0.69342
H	-3.08442	1.95042	-1.32482
C	-5.11487	-0.57574	0.65335
H	-3.26876	-1.51	1.24875
N	-5.76109	0.37703	-0.01781
C	2.94667	0.22309	0.01555
C	3.62425	1.2235	0.73109
C	3.72749	-0.70744	-0.68903
C	5.01711	1.25107	0.69342
H	3.08439	1.95045	1.32476
C	5.11489	-0.57574	-0.65333
H	3.2688	-1.51001	-1.24875
N	5.76109	0.37704	0.01784
N	-1.25298	-2.28308	0.00632
N	1.25298	-2.28309	-0.00629
S	0.	-3.33825	-0.00006
C	-5.80524	2.3091	-1.45059
C	-6.01608	-1.54578	1.4031
C	5.8052	2.30913	1.45059
C	6.01612	-1.54579	-1.40304
F	-5.29185	-2.47124	2.08028

F	-6.83301	-2.21127	0.56021
F	-6.79086	-0.90418	2.30247
F	-6.57169	3.04339	-0.61835
F	-6.61681	1.75592	-2.37474
F	4.97795	3.16794	2.10103
F	6.57168	3.04341	0.61835
F	5.2919	-2.47125	-2.08023
F	6.83303	-2.21127	-0.56013
F	6.79092	-0.90419	-2.3024
F	6.61674	1.75597	2.37477
F	-4.97801	3.16789	-2.10108

Table S7. Optimized Coordinates of H-Ch (B3LYP/6-31G(d,p), ground state)

Atom	X	Y	Z
C	-0.30515	0.56779	-0.28902
C	0.30517	-0.56721	0.2898
C	-0.51459	-1.59622	0.90691
C	-1.93873	-1.46267	0.91432
C	-2.53078	-0.30975	0.27991
C	-1.72778	0.65709	-0.27171
H	1.12096	-2.88273	1.531
C	0.04738	-2.74069	1.52629
C	-2.72029	-2.44352	1.57552
H	-2.21184	1.50092	-0.74667
C	-2.13726	-3.53964	2.17557
C	-0.73962	-3.69364	2.14008
H	-3.79588	-2.32079	1.62244
H	-2.75538	-4.27704	2.67805
H	-0.27549	-4.55745	2.60588
C	0.51461	1.59689	-0.90598
C	1.72779	-0.65663	0.27224
C	1.93873	1.46324	-0.9136
C	2.53079	0.31017	-0.27946
C	-0.04735	2.74161	-1.52491
C	2.72027	2.44416	-1.57474
C	0.73962	3.69464	-2.1386
C	2.13725	3.54048	-2.17443
C	-4.00488	-0.13393	0.17601
C	-4.82921	-1.10131	-0.41806
C	-4.6194	1.04552	0.61832
C	-6.19312	-0.843	-0.53451
H	-4.41635	-2.02703	-0.79796
C	-5.99481	1.19521	0.44804
H	-4.03957	1.82494	1.09654
N	-6.78129	0.27787	-0.11395
C	4.00489	0.1341	-0.17596
C	4.61909	-1.04541	-0.6186
C	4.82953	1.10123	0.41804
C	5.99451	-1.19537	-0.44868
H	4.039	-1.82463	-1.09683
C	6.19342	0.84265	0.53412

H	4.41694	2.02698	0.79818
N	6.78129	-0.27825	0.11325
H	2.21185	-1.50063	0.74691
H	3.79584	2.32134	-1.62189
H	2.75534	4.27794	-2.67684
H	0.27551	4.55864	-2.60405
H	-1.12091	2.88382	-1.52924
C	-7.12939	-1.8536	-1.17247
C	-6.70925	2.45284	0.90965
C	7.13005	1.85292	1.17208
C	6.70859	-2.45312	-0.91054
F	-7.3037	3.07916	-0.12151
F	-5.84362	3.32561	1.4752
F	-7.65665	2.16946	1.82001
F	-8.07158	-2.25814	-0.30189
F	-7.75474	-1.33223	-2.242
F	-6.45469	-2.9511	-1.58554
F	6.45578	2.95082	1.58479
F	8.07265	2.25682	0.30167
F	7.65653	-2.16983	-1.82032
F	5.84282	-3.32527	-1.47681
F	7.30228	-3.08014	0.12068
F	7.75487	1.33143	2.24188

Table S8. Optimized Coordinates of H-An (B3LYP/6-31G(d,p), ground state)

Atom	X	Y	Z
C	-9.0608	0.9173	-0.01282
C	-7.69618	0.9173	-0.01282
C	-6.96329	2.14852	-0.01282
C	-7.68729	3.38027	-0.01833
C	-9.11953	3.33878	-0.01963
C	-9.78331	2.14649	-0.01626
C	-5.56439	2.17141	-0.00792
C	-6.98691	4.59144	-0.02006
C	-5.58797	4.61432	-0.01443
C	-4.864	3.38262	-0.00701
C	-3.43182	3.42424	0.0001
H	-2.88595	2.46872	0.0067
C	-2.76808	4.6166	0.00114
C	-3.49056	5.84571	-0.00703
C	-4.85521	5.84557	-0.0144
H	-9.62668	-0.02597	-0.01041
H	-7.12685	-0.02443	-0.00971
H	-9.66534	4.29433	-0.02424
H	-10.88271	2.11032	-0.01769
H	-1.66867	4.6525	0.0073
H	-2.92448	6.78889	-0.00594
H	-5.42475	6.78719	-0.02067
C	-4.78428	0.84363	-0.00188
C	-4.42843	0.23397	1.20258
C	-4.41868	0.22826	-1.20038

C	-3.71498	-0.97774	1.15719
H	-4.69626	0.68423	2.16688
C	-3.70549	-0.98318	-1.1429
H	-4.67832	0.67367	-2.16917
N	-3.35417	-1.58528	0.01016
C	-7.76763	5.91886	-0.02603
C	-8.12354	6.52856	-1.23045
C	-8.13119	6.53536	1.17251
C	-8.83542	7.74119	-1.18499
H	-7.85741	6.07734	-2.19478
C	-8.84264	7.74783	1.1151
H	-7.87127	6.09006	2.14128
N	-9.19431	8.34979	-0.03793
C	-3.2759	-1.70711	-2.43247
C	-3.29612	-1.69517	2.4539
C	-9.25456	8.45852	-2.48166
C	-9.27021	8.47287	2.40471
F	-9.92294	9.59036	-2.17391
F	-8.15462	8.76693	-3.20104
F	-8.71423	9.70269	2.435
F	-10.61516	8.58625	2.43243
F	-8.85607	7.76526	3.47722
F	-10.05355	7.6471	-3.20672
F	-2.17919	-1.10668	-2.94158
F	-4.27866	-1.65229	-3.33467
F	-2.99328	-2.99697	-2.15162
F	-3.69934	-0.97079	3.51935
F	-1.95284	-1.82682	2.48159
F	-3.869	-2.91681	2.49748

Table S9. Optimized Coordinates of H-Py (B3LYP/6-31G(d,p), ground state)

Atom	X	Y	Z
C	2.68426	-1.70679	-1.51318
C	1.38019	-2.03858	-1.85064
C	0.29745	-1.3621	-1.2699
C	0.55022	-0.33879	-0.30785
C	1.89875	0.00473	0.03602
C	2.9675	-0.68325	-0.59626
C	-1.05856	-1.65867	-1.62483
C	-0.55022	0.33869	0.30794
C	-1.89875	-0.00482	-0.03594
C	-2.10415	-1.00923	-1.04483
C	-2.9675	0.68317	0.59632
C	-2.68426	1.70671	1.51324
C	-1.38019	2.03848	1.85073
C	-0.29745	1.362	1.27
C	1.05857	1.65856	1.62494
C	2.10415	1.00913	1.04493
H	3.11455	1.24184	1.35884
H	1.23965	2.41416	2.38417
H	-1.23965	-2.41428	-2.38405

H	3.50882	-2.22375	-1.99432
H	1.18991	-2.81924	-2.58134
H	-3.11455	-1.24195	-1.35874
H	-3.50883	2.22369	1.99436
H	-1.18992	2.81914	2.58143
C	-4.39511	0.35717	0.34145
C	-5.31114	1.36633	0.00977
C	-4.90187	-0.94423	0.47807
C	-6.65111	1.0302	-0.17152
H	-4.98318	2.39045	-0.11782
C	-6.26206	-1.16311	0.27086
H	-4.25628	-1.76618	0.75966
C	4.90178	0.94425	-0.47786
C	5.31124	-1.3664	-0.01007
C	6.26199	1.16316	-0.27074
H	4.25613	1.76622	-0.7592
C	6.65122	-1.03025	0.17101
H	4.98333	-2.39054	0.11744
N	-7.13383	-0.20642	-0.04973
N	7.13386	0.20642	0.04941
C	4.39512	-0.35722	-0.34148
C	-6.86201	-2.55089	0.4088
C	-7.68262	2.08348	-0.53426
C	6.86186	2.55099	-0.40857
F	-7.11329	3.3052	-0.6507
F	-8.64015	2.16814	0.40625
F	-8.27983	1.79801	-1.70425
F	-5.91596	-3.46245	0.73325
F	-7.43306	-2.94853	-0.74212
F	-7.80397	-2.58165	1.3671
F	7.43284	2.94858	0.74241
F	5.9158	3.46256	-0.73299
F	7.80388	2.58188	-1.36679
C	7.68275	-2.08347	0.53389
F	7.11369	-3.30542	0.64917
F	8.2789	-1.79851	1.70463
F	8.64107	-2.16728	-0.40579

Table S10. Optimized Coordinates of H-Per (B3LYP/6-31G(d,p), ground state)

Atom	X	Y	Z
C	-3.20051	0.59318	-0.00035
C	-1.82771	0.59318	-0.00035
C	-1.10577	1.8183	-0.00035
C	-1.82364	3.04216	0.00002
C	-3.24506	3.01279	0.00018
C	-3.91656	1.81482	-0.00011
H	-3.76124	-0.35317	-0.00043
C	0.31595	1.84784	-0.00061
C	-1.10089	4.26689	0.00014
H	-3.7923	3.96725	0.00026
H	-5.0162	1.78845	-0.00001

C	0.27197	4.26696	-0.00014
C	0.98798	3.04507	-0.0006
H	0.83266	5.21329	-0.00031
H	2.08761	3.07153	-0.00078
C	1.08203	0.5119	-0.00058
C	-1.03724	-0.72847	-0.00067
C	0.59193	-0.92142	-0.00028
C	1.22201	-2.13974	-0.00033
C	0.27902	-3.46447	-0.00033
C	-1.35084	-3.08098	-0.00033
C	-1.88022	-1.81045	-0.00033
C	2.59217	-2.19804	-0.00031
C	2.96413	-0.93533	0.00057
C	2.4042	0.31666	-0.01621
H	3.05021	1.16922	-0.0428
H	4.03154	-0.86356	0.0205
H	3.21466	-3.06833	-0.00088
H	-2.94069	-1.66799	-0.00007
H	-2.04305	-3.89691	-0.00033
C	0.8223	-4.90546	-0.00033
C	1.07145	-5.57099	-1.20201
C	1.07331	-5.57075	1.20097
C	1.56635	-6.88696	-1.1511
H	0.88786	-5.08436	-2.16836
C	1.56801	-6.88685	1.14901
H	0.8912	-5.08437	2.16774
N	1.81421	-7.54385	-0.00131
C	-1.89088	5.58883	0.0005
C	-2.25433	6.19983	-1.20101
C	-2.25548	6.19898	1.20197
C	-2.97453	7.40729	-1.14977
H	-1.98768	5.75354	-2.16749
C	-2.97554	7.40662	1.15034
H	-1.98981	5.75245	2.16861
N	-3.33455	8.00974	0.00019
C	1.86345	-7.66967	2.44188
C	1.85966	-7.66964	-2.44454
C	-3.40465	8.12457	2.44341
C	-3.40221	8.12578	-2.44301
F	0.80176	-7.58548	3.27148
F	2.09736	-8.96461	2.14036
F	0.86227	-7.46417	-3.33083
F	1.94737	-8.98709	-2.16323
F	-4.47768	7.49799	2.97114
F	-3.7249	9.40545	2.16188
F	-2.45617	7.9493	-3.38978
F	-4.57357	7.61321	-2.87627
F	2.9502	-7.14516	3.04715
F	-2.38753	8.09962	3.33073
F	-3.55181	9.44465	-2.19668
F	3.02645	-7.24377	-2.97343

Table S11. H-Pz (TD-DFT B3LYP/6-31G(d,p))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	28394.94	352.1754	0.0013	H-1->LUMO (97%)
2	32489.04	307.7961	0.9411	HOMO->LUMO (97%)
3	34061.84	293.5837	0.009	H-2->LUMO (89%)
4	34096.52	293.2851	0.0012	H-1->L+1 (90%)
5	34364.3	290.9997	0.0031	H-3->LUMO (86%)
6	36255.68	275.8189	0.0391	H-4->LUMO (70%), HOMO->L+1 (21%)
7	36581.53	273.362	0.0042	H-5->LUMO (86%)
8	38130.12	262.2598	0.0601	H-4->LUMO (20%), HOMO->L+1 (70%)
9	40097.32	249.3932	0.0098	H-7->LUMO (37%), H-1->L+2 (51%)
10	40924.05	244.3551	0.0001	H-6->LUMO (27%), HOMO->L+2 (68%)
11	40978.09	244.0329	0.0043	H-3->L+3 (27%), H-2->L+1 (46%), H-2->L+4 (16%)
12	41055.52	243.5726	0.0002	H-3->L+1 (43%), H-3->L+4 (16%), H-2->L+3 (32%)
13	41592.69	240.4269	0.0028	H-7->LUMO (51%), H-1->L+2 (43%)
14	42421.02	235.7322	0.0007	H-5->L+1 (20%), HOMO->L+3 (58%)
15	43033.2	232.3787	0.0166	H-4->L+1 (25%), HOMO->L+4 (45%)
16	43282.43	231.0406	0.0007	H-1->L+3 (92%)
17	43365.5	230.598	0.0025	H-6->LUMO (39%), H-5->L+1 (26%), HOMO->L+2 (10%), HOMO->L+3 (16%)
18	43787.34	228.3765	0	H-1->L+4 (89%)
19	43976.88	227.3922	0.0416	H-4->L+1 (39%), H-2->L+1 (14%), HOMO->L+4 (13%)
20	44167.23	226.4122	0.0007	H-3->L+1 (14%), H-3->L+4 (12%), H-2->L+2 (39%), H-2->L+3 (13%)

Table S12. H-BTD (TD-DFT B3LYP/6-31G(d,p))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	26482.59	377.6066	0.3763	HOMO->LUMO (98%)
2	32033.34	312.1748	0.0067	H-3->LUMO (23%), H-1->LUMO (69%)
3	32277.72	309.8112	0.0006	H-2->LUMO (94%)
4	33239.14	300.8501	0.0017	H-5->LUMO (44%), H-3->LUMO (39%)

5	33683.56	296.8807	0.0066	H-4->LUMO (96%)
6	34607.88	288.9516	0.1091	H-5->LUMO (42%), H-3->LUMO (28%), H-1->LUMO (13%)
7	34904.69	286.4944	0.3515	HOMO->L+1 (93%)
8	35615.27	280.7784	0.0161	H-8->LUMO (34%), H-6->LUMO (50%)
9	37839.76	264.2723	0.0046	H-8->LUMO (43%), H-6->LUMO (23%), HOMO->L+2 (29%)
10	39475.47	253.3219	0	H-6->LUMO (10%), HOMO->L+2 (21%), HOMO->L+3 (49%)
11	39719.05	251.7684	0.0017	HOMO->L+4 (76%)
12	39862.61	250.8616	0.0069	H-9->LUMO (11%), H-7->LUMO (22%), H-2->L+1 (34%), H-1->L+2 (10%)
13	39863.42	250.8565	0.0007	H-1->L+1 (13%), HOMO->L+2 (20%), HOMO->L+3 (33%)
14	40424.79	247.373	0.002	H-2->L+2 (18%), H-1->L+1 (33%), HOMO->L+2 (17%)
15	40521.57	246.7821	0.0684	H-7->LUMO (68%), H-2->L+1 (17%)
16	41681.41	239.9151	0.0027	H-9->LUMO (83%)
17	42028.23	237.9353	0.0003	H-2->L+3 (47%), H-1->L+4 (33%)
18	42029.84	237.9262	0.0009	H-2->L+4 (47%), H-1->L+3 (34%)
19	43145.31	231.7749	0.043	H-5->L+1 (23%), H-3->L+1 (41%), H-1->L+1 (29%)
20	43883.32	227.877	0.0205	H-5->L+1 (40%), H-3->L+1 (32%), HOMO->L+3 (10%)

Table S13. H-Ch (TD-DFT B3LYP/6-31G(d,p))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	26674.55	374.8891	0.4153	HOMO->LUMO (97%)
2	29029.71	344.4747	0.0251	H-1->LUMO (66%), HOMO->L+2 (23%)
3	31100.15	321.5419	0	HOMO->L+1 (98%)
4	32878.61	304.1491	0.0266	HOMO->L+2 (56%), HOMO->L+4 (15%), HOMO->L+5 (18%)
5	32976.21	303.249	0	H-2->LUMO (88%)
6	33143.16	301.7213	0	HOMO->L+3 (97%)
7	33784.38	295.9948	0.0093	HOMO->L+4 (59%), HOMO->L+5 (33%)
8	34336.07	291.239	0.1557	H-1->LUMO (21%), H-1->L+2 (12%), HOMO->L+4 (18%), HOMO->L+5 (27%)
9	35273.29	283.5006	0	H-1->L+1 (88%)

10	36476.68	274.1478	0	H-1->L+1 (10%), HOMO->L+6 (63%)
11	37559.08	266.2472	0.2583	H-1->L+2 (63%), H-1->L+4 (27%)
12	37676.03	265.4207	0	H-2->L+2 (21%), H-1->L+3 (39%), H-1->L+6 (17%), HOMO->L+6 (12%)
13	37934.13	263.6149	0	H-2->L+2 (11%), H-1->L+3 (57%), H-1->L+6 (16%)
14	38011.56	263.0779	0.0032	H-6->LUMO (25%), H-5->L+1 (18%), H-4->LUMO (18%), H-2->L+1 (25%)
15	38250.3	261.4358	0	H-6->L+1 (19%), H-5->LUMO (64%)
16	38731.01	258.191	0.0474	H-6->LUMO (19%), H-2->L+1 (43%), H-1->L+5 (18%)
17	39111.71	255.6779	0.6797	H-1->L+2 (17%), H-1->L+4 (61%)
18	39536.76	252.9291	0.1074	H-2->L+1 (29%), H-1->L+5 (52%)
19	39990.86	250.0572	0	H-3->LUMO (77%), H-1->L+6 (17%)
20	40445.76	247.2447	0.2865	H-6->LUMO (24%), H-4->LUMO (63%)

Table S14. H-An (TD-DFT B3LYP/6-31G(d,p))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	25239.68	396.2015	0.158	HOMO->LUMO (97%)
2	27343.19	365.7218	0	HOMO->L+1 (99%)
3	27721.47	360.7313	0.0009	HOMO->L+2 (98%)
4	29475.74	339.2621	0.0029	H-1->LUMO (16%), HOMO->L+3 (82%)
5	29984.67	333.5037	0	HOMO->L+4 (100%)
6	31943	313.0576	0.0162	H-1->LUMO (40%), HOMO->L+3 (14%), HOMO->L+5 (45%)
7	35634.63	280.6259	0	H-2->LUMO (90%)
8	37887.35	263.9403	0.0002	H-1->L+1 (99%)
9	38024.46	262.9886	0.0154	H-1->L+2 (94%)
10	39299.64	254.4553	0	H-4->L+1 (29%), H-3->LUMO (16%), H-3->L+2 (31%)
11	39391.58	253.8613	0	H-4->LUMO (10%), H-4->L+1 (12%), H-4->L+2 (29%), H-3->L+1 (37%)
12	40285.25	248.2298	0	H-2->L+2 (13%), HOMO->L+6 (76%)
13	40400.59	247.5211	0.0411	H-1->L+3 (93%)
14	40427.21	247.3582	0.0027	H-1->L+4 (92%)
15	40721.6	245.5699	0.0039	H-2->L+1 (96%)
16	41151.5	243.0045	0.1373	H-5->LUMO (17%), H-3-

				>LUMO (41%), H-2->L+2 (18%)
17	41173.27	242.876	0.0386	H-2->L+2 (66%)
18	41482.19	241.0673	0.2321	H-5->LUMO (43%), H-3->LUMO (28%)
19	41612.85	240.3104	0	H-4->L+3 (11%), H-4->L+4 (37%), H-3->L+3 (41%)
20	41621.72	240.2592	0	H-4->L+3 (36%), H-3->L+4 (42%)

Table S15. H- Py (TD-DFT B3LYP/6-31G(d,p))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	25613.12	390.4249	0.6241	HOMO->LUMO (94%)
2	29048.26	344.2547	0.0252	H-1->LUMO (56%), HOMO->L+2 (26%), HOMO->L+5 (14%)
3	29216.02	342.2779	0	HOMO->L+1 (98%)
4	32036.56	312.1433	0	HOMO->L+3 (98%)
5	32129.32	311.2422	0.0116	HOMO->L+2 (37%), HOMO->L+4 (54%)
6	33398.84	299.4116	0.0502	HOMO->L+2 (22%), HOMO->L+4 (38%), HOMO->L+5 (29%)
7	34276.38	291.7461	0	H-2->LUMO (94%)
8	35122.46	284.7181	0.222	H-1->LUMO (34%), HOMO->L+5 (44%)
9	36225.03	276.0522	0	HOMO->L+6 (90%)
10	36503.29	273.9479	0	H-1->L+1 (90%)
11	37709.1	265.188	0.0072	H-5->LUMO (67%), H-4->L+1 (22%)
12	37765.56	264.7915	0	H-5->L+1 (21%), H-4->LUMO (64%)
13	38543.08	259.4499	0	H-3->LUMO (84%), HOMO->L+7 (10%)
14	39320.61	254.3196	0.0427	H-1->L+2 (70%)
15	39618.23	252.4091	0	H-6->LUMO (10%), H-1->L+3 (82%)
16	40123.94	249.2278	0.0054	H-7->LUMO (13%), H-1->L+4 (61%)
17	40549	246.6152	0	H-6->LUMO (76%), H-1->L+3 (12%)
18	40648.2	246.0133	0.0312	H-7->LUMO (70%), H-1->L+4 (16%)
19	41783.03	239.3316	0.0471	H-5->L+2 (16%), H-5->L+4 (18%), H-4->L+3 (29%), H-2->L+1 (17%)
20	41804	239.2115	0	H-5->L+3 (41%), H-4->L+2 (19%), H-4->L+4 (24%)

Table S16. H-Per (TD-DFT B3LYP/6-31G(d,p))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	21229.47	471.0434	0.7294	HOMO->LUMO (99%)
2	25555.05	391.3121	0.0007	HOMO->L+1 (98%)
3	28500.6	350.8698	0.0039	HOMO->L+2 (97%)
4	29099.88	343.644	0.0001	H-1->LUMO (20%), HOMO->L+3 (57%), HOMO->L+5 (21%)
5	29620.11	337.6085	0.0042	HOMO->L+4 (97%)
6	29791.1	335.6707	0.0002	H-1->LUMO (23%), HOMO->L+3 (41%), HOMO->L+5 (31%)
7	31648.61	315.9697	0	H-4->LUMO (33%), H-2->LUMO (29%), H-1->LUMO (15%), HOMO->L+5 (22%)
8	31819.6	314.2717	0.0159	H-3->LUMO (65%), HOMO->L+7 (31%)
9	32777.79	305.0846	0.0003	H-4->LUMO (19%), H-2->LUMO (56%)
10	33263.34	300.6313	0.0002	H-4->LUMO (20%), H-1->LUMO (17%), HOMO->L+6 (47%)
11	36027.42	277.5663	0.0002	H-4->LUMO (25%), HOMO->L+5 (12%), HOMO->L+6 (43%)
12	36730.74	272.2515	0.0001	HOMO->L+8 (81%)
13	37192.9	268.8685	0.0121	H-6->L+1 (17%), H-5->LUMO (68%)
14	37354.21	267.7074	0.0007	H-6->LUMO (67%), H-5->L+1 (18%)
15	37960.75	263.43	0.2565	H-3->LUMO (19%), H-2->L+1 (18%), H-1->L+1 (17%), HOMO->L+7 (38%)
16	38387.42	260.502	0.0741	H-1->L+1 (72%)
17	39210.91	255.031	0.0001	H-7->LUMO (89%)
18	39242.37	254.8266	0.0121	H-8->LUMO (90%)
19	39364.16	254.0382	0.0001	H-3->L+1 (77%), H-1->L+2 (15%)
20	39525.47	253.0014	0.1664	H-2->L+1 (73%)

Table S17. H-Pz (TD-DFT B3LYP/6-31G(d,p)scrf=(smd,solvent=chloroform))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	28019.89	356.8893	0.0015	H-1->LUMO (97%)
2	31139.67	321.1338	1.1098	HOMO->LUMO (98%)
3	34570.77	289.2617	0.0024	H-1->L+1 (89%)
4	35882.24	278.6894	0.005	H-4->LUMO (80%)
5	36270.2	275.7085	0.0031	H-5->LUMO (86%), H-4->L+2 (10%)
6	36539.59	273.6758	0.0531	H-2->LUMO (51%), HOMO-

				>L+1 (34%)
7	36973.52	270.4639	0.0066	H-3->LUMO (81%), HOMO->L+3 (13%)
8	38326.12	260.9187	0.0392	H-2->LUMO (29%), HOMO->L+1 (58%)
9	39352.06	254.1163	0.013	H-7->LUMO (12%), H-1->L+2 (82%)
10	39966.66	250.2085	0.0002	H-6->LUMO (10%), HOMO->L+2 (88%)
11	41231.35	242.5339	0.0021	H-7->LUMO (69%), H-1->L+2 (16%)
12	41680.6	239.9198	0.0048	H-3->LUMO (14%), HOMO->L+3 (78%)
13	42038.71	237.876	0.0022	H-1->L+3 (91%)
14	42541.2	235.0662	0.0006	H-5->L+1 (12%), H-4->L+3 (11%), H-1->L+4 (62%)
15	42562.98	234.946	0.031	H-8->LUMO (14%), HOMO->L+4 (65%)
16	42908.19	233.0558	0.0013	H-5->L+3 (32%), H-4->L+1 (42%), H-4->L+4 (13%)
17	43090.47	232.0699	0	H-5->L+1 (30%), H-5->L+4 (12%), H-4->L+3 (28%), H-1->L+4 (25%)
18	43313.08	230.8771	0.0009	H-6->LUMO (77%)
19	45239.95	221.0436	0.1407	H-2->L+1 (83%)
20	45648.07	219.0673	0.0418	H-8->LUMO (55%), H-7->LUMO (11%), HOMO->L+4 (12%)

Table S18. H-BTD (TD-DFT B3LYP/6-31G(d,p)scrf=(smd,solvent=chloroform))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	25805.8872	387.5084752	0.4923	HOMO->LUMO (99%)
2	33052.02224	302.5533484	0.1826	H-1->LUMO (88%)
3	33121.3864	301.9197288	0.334	HOMO->L+1 (97%)
4	34078.77312	293.4377938	0	H-8->LUMO (10%), H-2->LUMO (72%)
5	35133.7536	284.6265763	0.0042	H-4->LUMO (12%), H-3->LUMO (77%)
6	35529.77456	281.4540797	0.0157	H-4->LUMO (78%), H-3->LUMO (11%)
7	35804.81152	279.2920721	0.0129	H-5->LUMO (74%)
8	36045.1664	277.4297083	0.0115	H-6->LUMO (28%), HOMO->L+2 (48%)
9	36916.2512	270.8834097	0.0001	H-8->LUMO (23%), H-6->LUMO (14%), HOMO->L+2 (34%)
10	37491.32848	266.7283451	0.0095	H-2->LUMO (12%), HOMO->L+3 (73%)
11	37617.15184	265.8361814	0.0058	H-3->LUMO (11%), HOMO->L+4 (85%)
12	39427.87904	253.6276423	0.005	H-8->LUMO (50%), H-6->LUMO (39%)

13	40617.55504	246.1989647	0.0467	H-7->LUMO (79%)
14	40783.7064	245.1959589	0.0533	H-1->L+1 (93%)
15	41408.7904	241.4946175	0.0252	H-9->LUMO (43%), H-7->LUMO (17%), H-4->L+1 (22%)
16	42433.92816	235.6604829	0.0237	H-5->L+1 (44%), H-4->L+2 (27%), H-2->L+1 (11%)
17	42798.49328	233.6530853	0.0022	H-9->LUMO (38%), H-4->L+1 (19%), H-1->L+2 (25%)
18	43227.5832	231.3337749	0.0006	H-5->L+3 (32%), H-4->L+4 (36%), H-1->L+2 (11%)
19	43250.97344	231.208669	0.0024	H-5->L+4 (36%), H-4->L+3 (43%)
20	43380.02304	230.520855	0.001	H-1->L+2 (61%)

Table S19. H-Ch (TD-DFT B3LYP/6-31G(d,p)scrf=(smd,solvent=chloroform))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	25917.19	385.8443	0.5381	HOMO->LUMO (98%)
2	28840.97	346.7289	0.0352	H-1->LUMO (71%), HOMO->L+2 (16%)
3	30150.83	331.6659	0	HOMO->L+1 (98%)
4	32209.17	310.4706	0.0542	HOMO->L+2 (75%), HOMO->L+5 (10%)
5	32453.55	308.1327	0	HOMO->L+3 (98%)
6	32632.61	306.4419	0	H-2->LUMO (92%)
7	33284.31	300.4418	0.0034	HOMO->L+4 (81%), HOMO->L+5 (11%)
8	33679.53	296.9163	0.2931	H-1->LUMO (19%), HOMO->L+5 (56%)
9	34530.45	289.5995	0	H-1->L+1 (95%)
10	36334.72	275.2188	0	HOMO->L+6 (71%)
11	36772.68	271.941	0.4464	H-1->L+2 (86%)
12	37167.9	269.0494	0	H-1->L+3 (92%)
13	37641.35	265.6653	0.0544	H-2->L+1 (73%), H-1->L+4 (14%)
14	37764.75	264.7972	0	H-2->L+2 (27%), H-2->L+5 (13%), H-1->L+6 (30%), HOMO->L+6 (11%)
15	38218.04	261.6565	0.7268	H-1->L+4 (71%)
16	38949.59	256.7421	0.1685	H-2->L+1 (12%), H-1->L+5 (75%)
17	39455.3	253.4514	0	H-8->L+1 (27%), H-7->LUMO (58%)
18	39515.79	253.0634	0.0484	H-8->LUMO (50%), H-7->L+1 (24%), H-4->LUMO (12%)
19	39807.77	251.2072	0	H-3->LUMO (78%), H-1->L+6 (11%)
20	40117.49	249.2679	0.2841	H-4->LUMO (78%)

Table S20. H-An (TD-DFT B3LYP/6-31G(d,p)scrf=(smd,solvent=chloroform))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	24833.17584	402.6871176	0.2008	HOMO->LUMO (96%)

2	26660.8408	375.0819442	0	HOMO->L+1 (99%)
3	27087.51104	369.1738228	0.004	HOMO->L+2 (97%)
4	29112.7832	343.4917208	0.0082	H-1->LUMO (10%), HOMO->L+3 (88%)
5	29486.22048	339.1414646	0	HOMO->L+4 (100%)
6	31767.17216	314.7903738	0.0285	H-1->LUMO (47%), HOMO->L+5 (43%)
7	35642.69296	280.5624146	0	H-2->LUMO (92%)
8	37296.94752	268.1184565	0.0017	H-1->L+1 (98%)
9	37399.38064	267.3841071	0.0557	H-1->L+2 (88%)
10	39698.8832	251.8962549	1.5669	H-1->LUMO (33%), HOMO->L+5 (46%)
11	39969.88736	250.1883458	0.0586	H-1->L+3 (99%)
12	39987.63168	250.0773259	0.0129	H-2->L+2 (27%), HOMO->L+6 (60%)
13	40030.37936	249.8102731	0.0001	H-1->L+4 (97%)
14	40080.38608	249.4985947	0.1077	H-2->L+1 (82%)
15	40370.74768	247.7041069	0.0076	H-6->L+2 (30%), H-4->L+1 (28%)
16	40478.82672	247.0427335	0.1034	H-6->L+1 (37%), H-4->L+2 (27%)
17	40689.33888	245.7646223	0.0001	H-2->L+2 (61%), HOMO->L+6 (18%)
18	42201.63888	236.9576222	0.0883	H-3->LUMO (85%)
19	42395.21328	235.8756856	0.0019	H-5->LUMO (91%)
20	42457.3184	235.5306547	0.0001	H-2->L+3 (86%)

Table S21. H-Py (TD-DFT B3LYP/6-31G(d,p)scrf=(smd,solvent=chloroform))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	24562.98	407.1168	0.7867	HOMO->LUMO (96%)
2	28168.3	355.009	0	HOMO->L+1 (99%)
3	28928.08	345.6849	0.0345	H-1->LUMO (59%), HOMO->L+2 (19%), HOMO->L+5 (18%)
4	31159.03	320.9343	0	HOMO->L+3 (99%)
5	31237.26	320.1305	0.0211	HOMO->L+2 (56%), HOMO->L+4 (34%)
6	32628.58	306.4798	0.102	HOMO->L+2 (18%), HOMO->L+4 (59%), HOMO->L+5 (12%)
7	34069.9	293.5142	0	H-2->LUMO (95%)
8	34398.98	290.7063	0.3011	H-1->LUMO (31%), HOMO->L+5 (58%)
9	35570.1	281.135	0	H-1->L+1 (96%)
10	36155.67	276.5818	0	HOMO->L+6 (95%)
11	38242.24	261.491	0	H-3->LUMO (87%)
12	38510.82	259.6673	0.069	H-1->L+2 (85%)
13	38832.64	257.5153	0	H-1->L+3 (89%)
14	39072.19	255.9365	0.0044	H-7->LUMO (48%), H-6->L+1 (19%), H-5->LUMO (11%)
15	39152.84	255.4093	0	H-7->L+1 (23%), H-6->LUMO

				(49%), H-4->LUMO (10%)
16	39410.94	253.7366	0.0075	H-2->L+1 (13%), H-1->L+4 (74%)
17	40895.01	244.5286	0.3555	H-2->L+1 (71%)
18	40924.05	244.3551	0	H-6->LUMO (12%), H-4->LUMO (68%)
19	41024.87	243.7546	0.0728	H-5->LUMO (65%)
20	42050.01	237.8121	0	H-2->L+2 (40%), H-2->L+5 (16%), H-1->L+6 (28%)

Table S22. H-Per (TD-DFT B3LYP/6-31G(d,p)scrf=(smd,solvent=chloroform))

No.	Excitation Energy (cm-1)	Wavelength (nm)	Oscillator Strength	Major contribs
1	20276.11	493.1912	0.8898	HOMO->LUMO (99%)
2	24633.15	405.957	0.0009	HOMO->L+1 (99%)
3	27573.87	362.6622	0.0047	HOMO->L+2 (98%)
4	28476.41	351.1679	0.0004	HOMO->L+3 (92%)
5	28743.38	347.9062	0.0055	HOMO->L+4 (98%)
6	29551.55	338.3917	0.0001	H-1->LUMO (41%), HOMO->L+5 (49%)
7	31617.15	316.284	0	H-4->LUMO (33%), H-2->LUMO (24%), H-1->LUMO (17%), HOMO->L+5 (24%)
8	31728.46	315.1745	0.0322	H-3->LUMO (70%), HOMO->L+7 (27%)
9	32586.64	306.8743	0.0005	H-2->LUMO (66%), H-1->LUMO (15%)
10	33010.89	302.9304	0.0001	H-4->LUMO (37%), H-1->LUMO (10%), HOMO->L+6 (46%)
11	35578.17	281.0712	0.0001	H-4->LUMO (22%), H-1->LUMO (11%), HOMO->L+5 (13%), HOMO->L+6 (49%)
12	36372.63	274.932	0.0001	HOMO->L+8 (86%)
13	37371.96	267.5803	0.3428	H-3->LUMO (16%), H-2->L+1 (19%), H-1->L+1 (25%), HOMO->L+7 (36%)
14	37499.39	266.671	0.1575	H-1->L+1 (65%), HOMO->L+7 (16%)
15	38416.45	260.3051	0	H-3->L+1 (68%), H-1->L+2 (14%)
16	38559.21	259.3414	0.1037	H-7->LUMO (19%), H-2->L+1 (46%)
17	38857.64	257.3496	0.2465	H-7->LUMO (23%), H-4->L+1 (13%), H-2->L+1 (28%)
18	38970.56	256.604	0.0006	H-8->LUMO (48%), H-7->L+1 (19%), H-3->L+1 (12%)
19	39374.65	253.9705	0.1649	H-7->LUMO (11%), H-4->L+1 (77%)
20	39843.26	250.9835	0.0044	H-7->LUMO (11%), H-5->LUMO (71%)