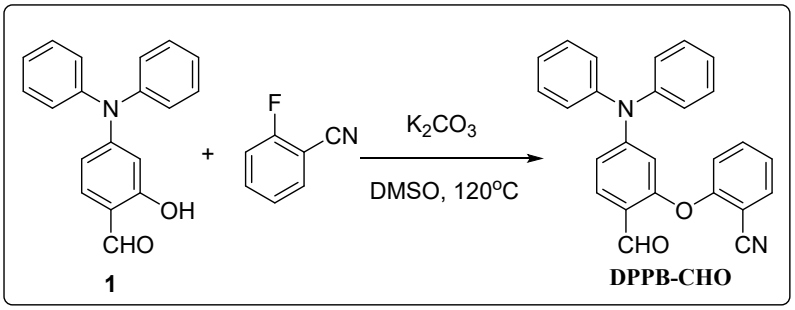
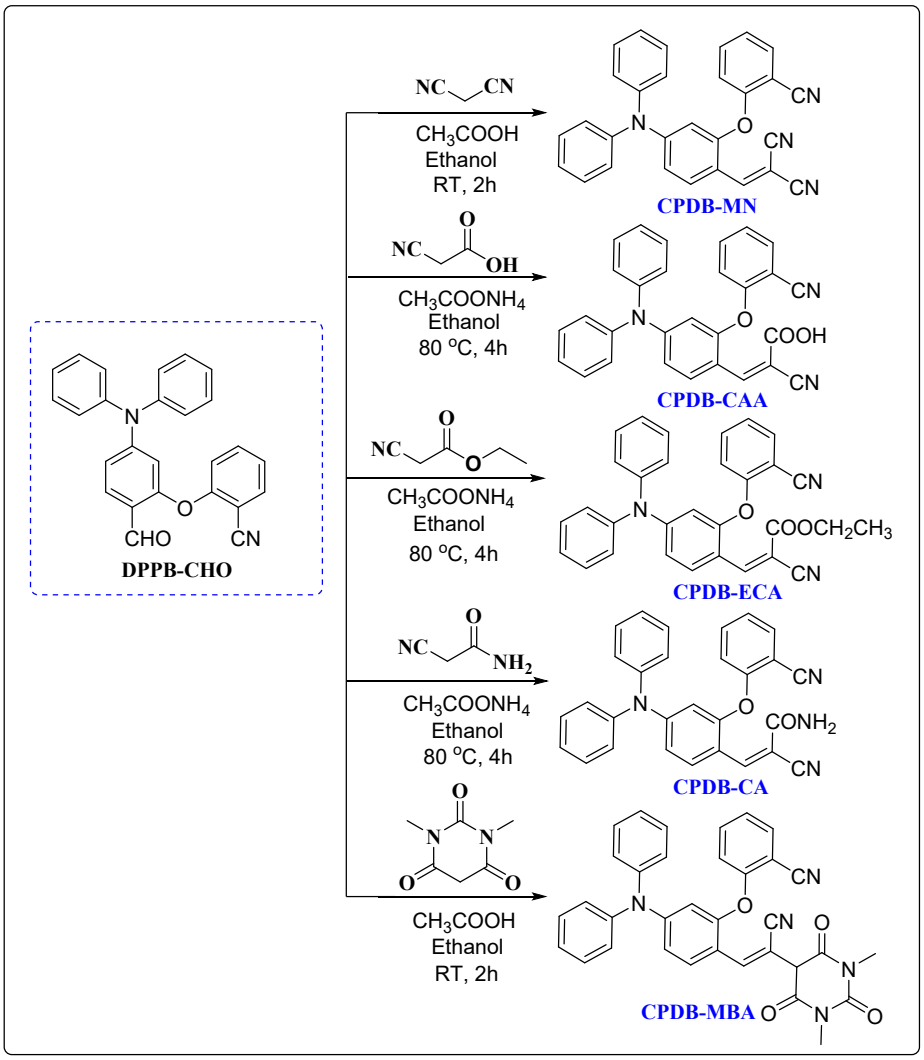
Electronic Supplementary Information (ESI)

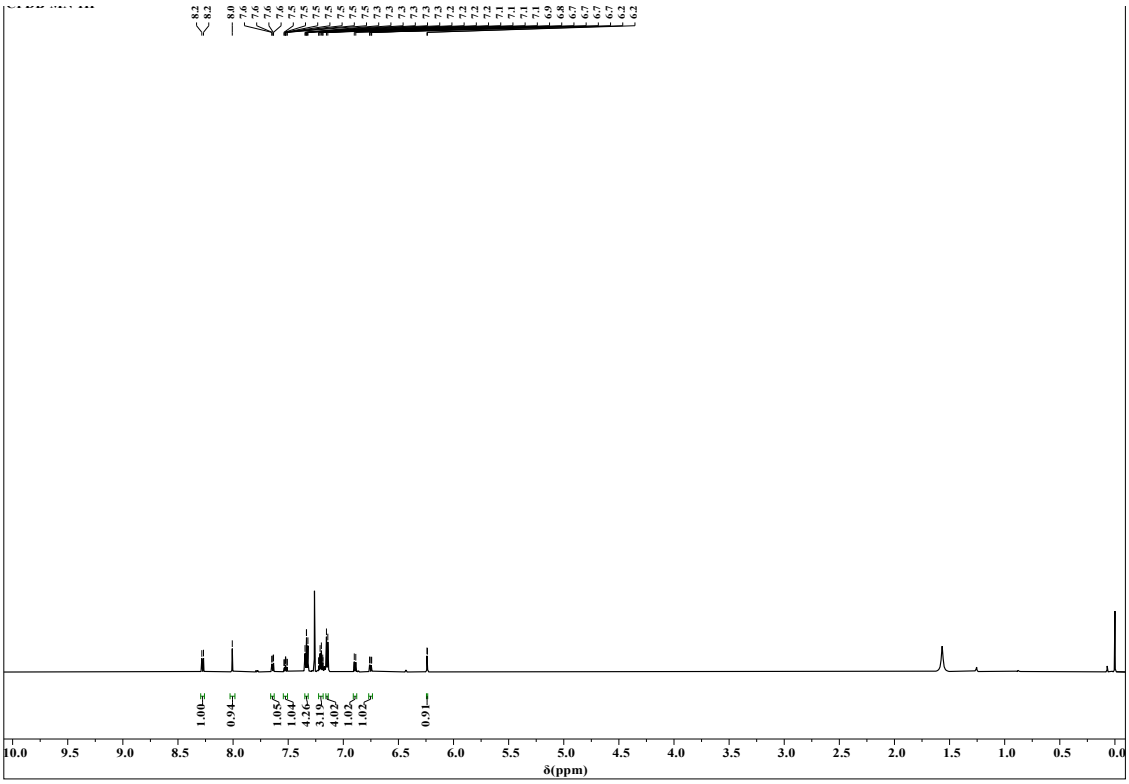
Synthesis of dual state emissive twisted donor-acceptor fluorophores: tunable fluorescence and self-reversible mechanofluorochromism



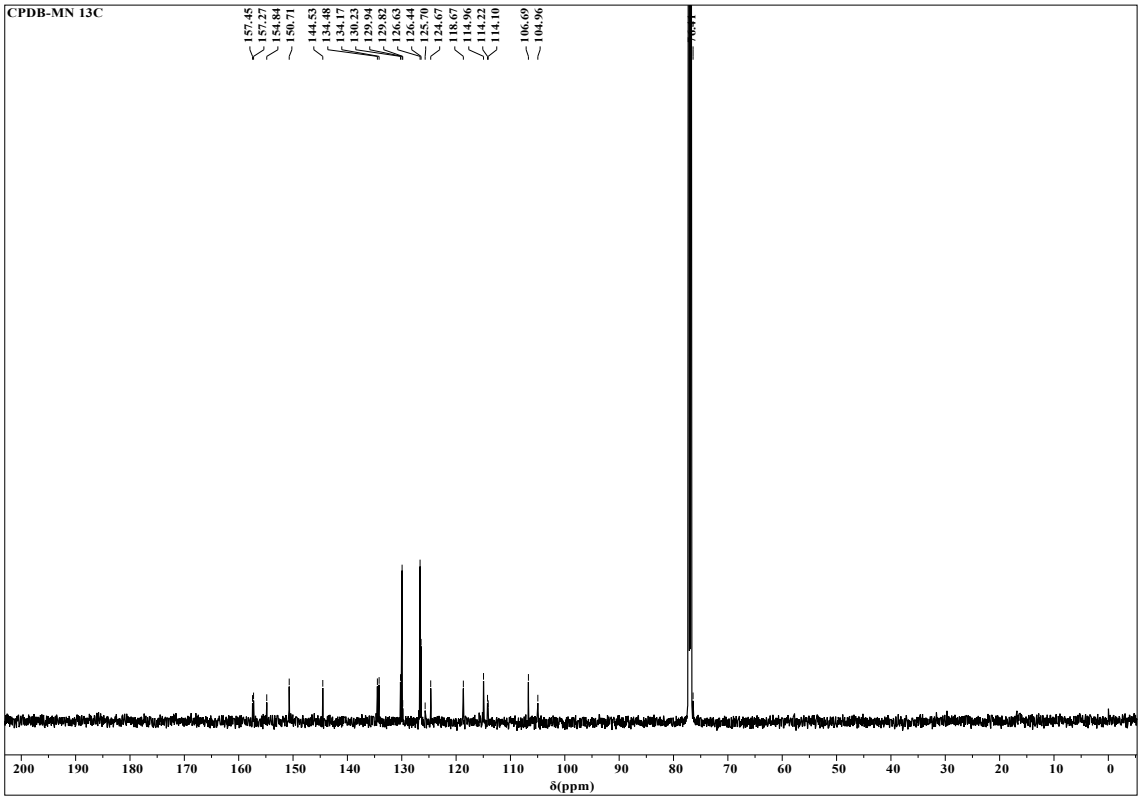
Scheme S1. Synthesis of **DPPB-CHO**.



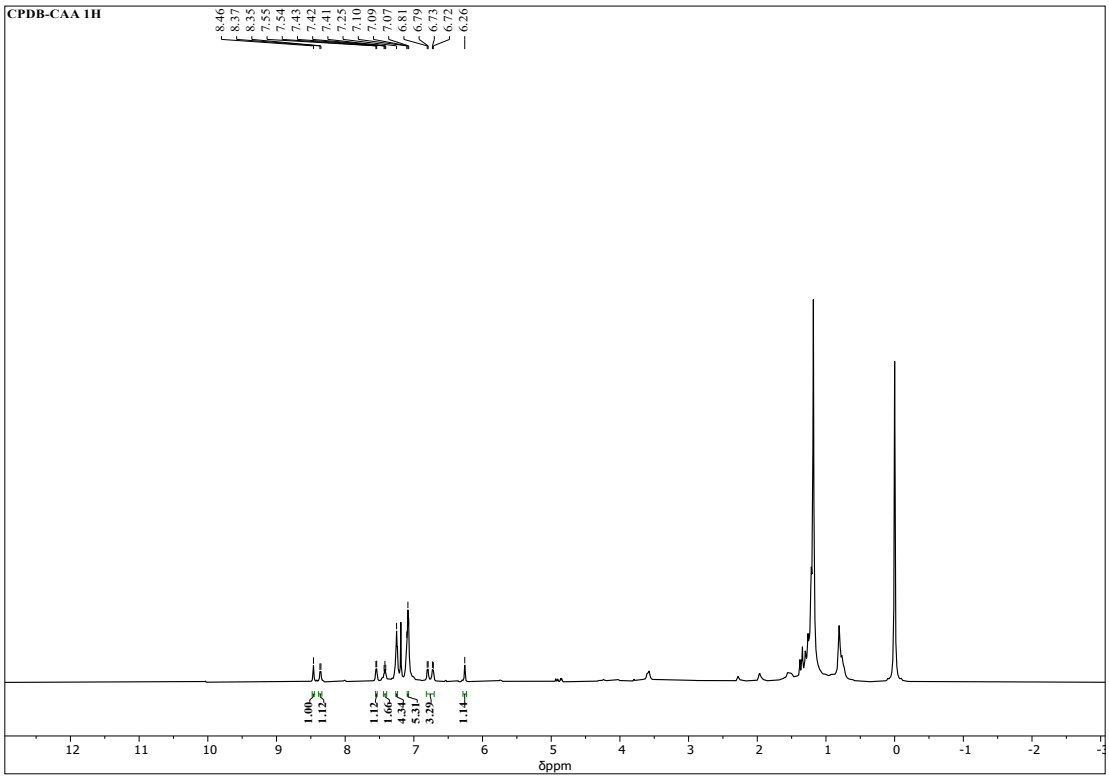
Scheme S2. Synthesis of **CPDP-acceptor derivatives**.



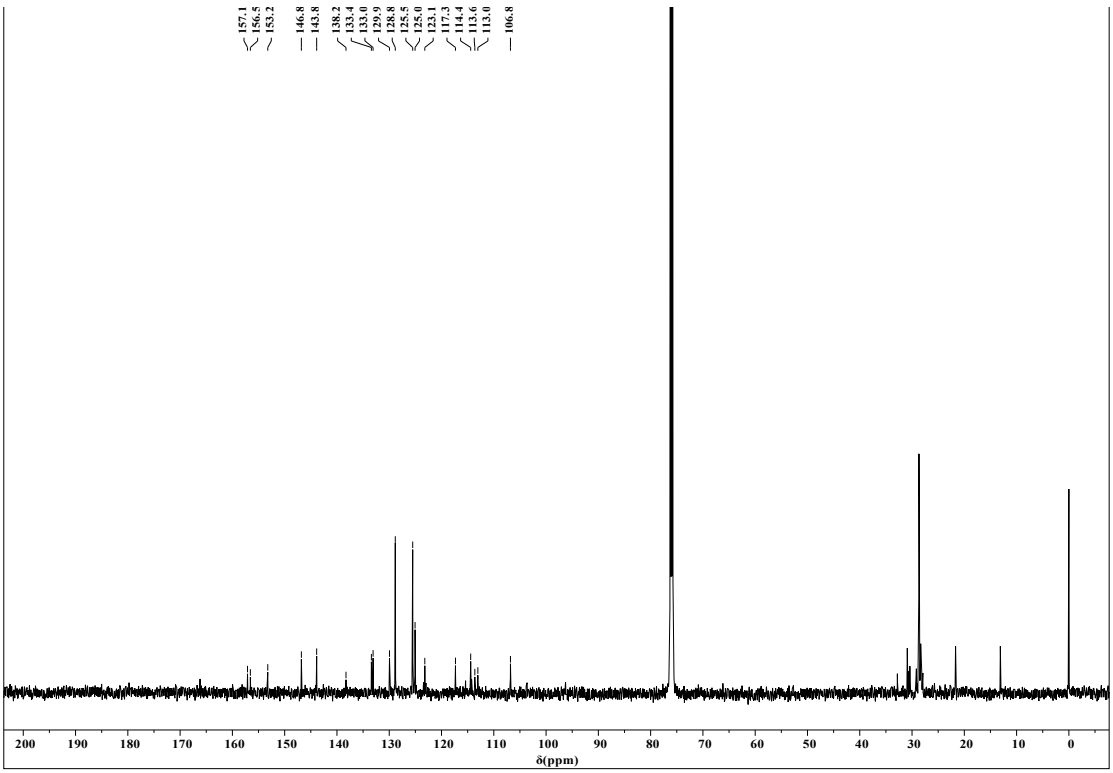
[1]H NMR spectra of CPDB-MN



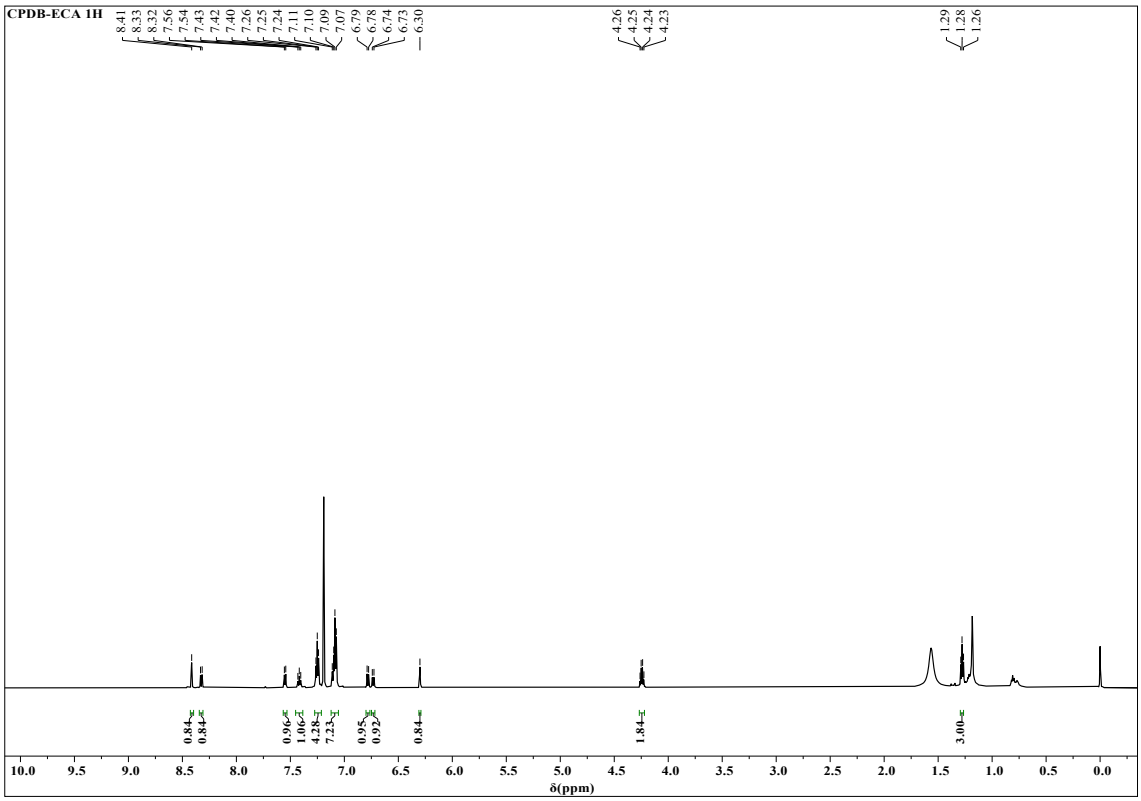
[13]C NMR spectra of CPDB-MN



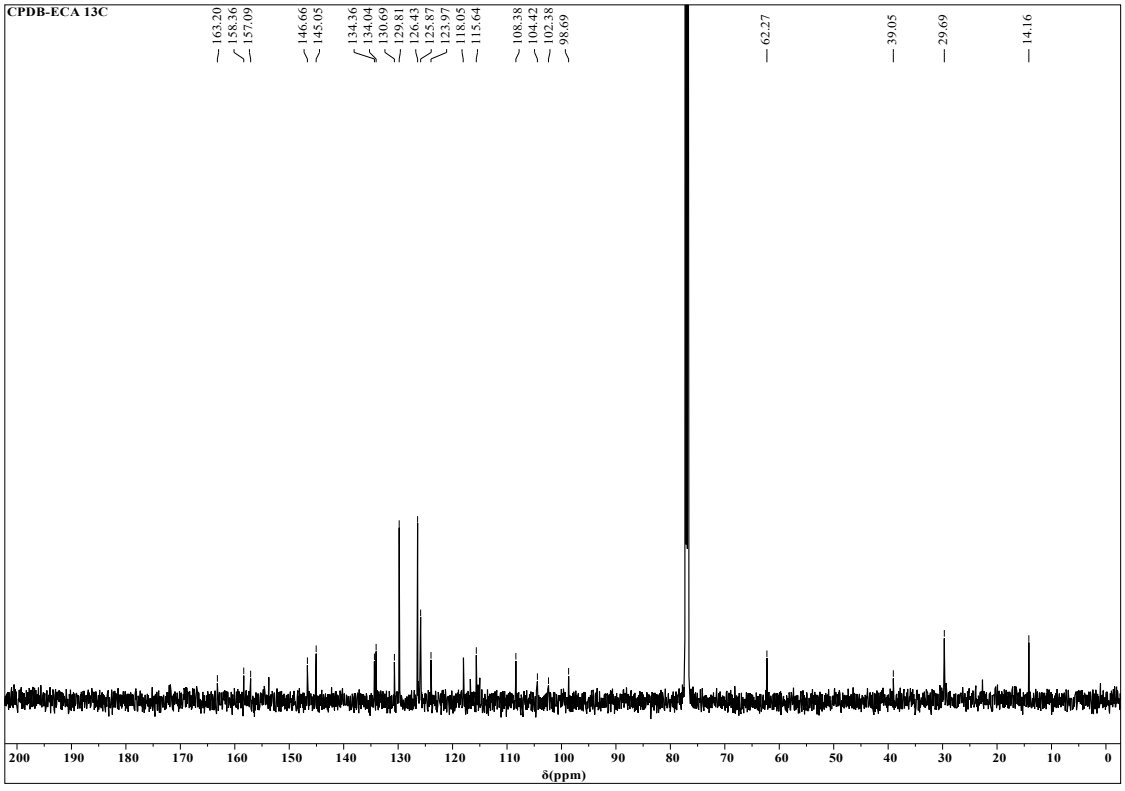
[1]H NMR spectra of CPDB-CAA



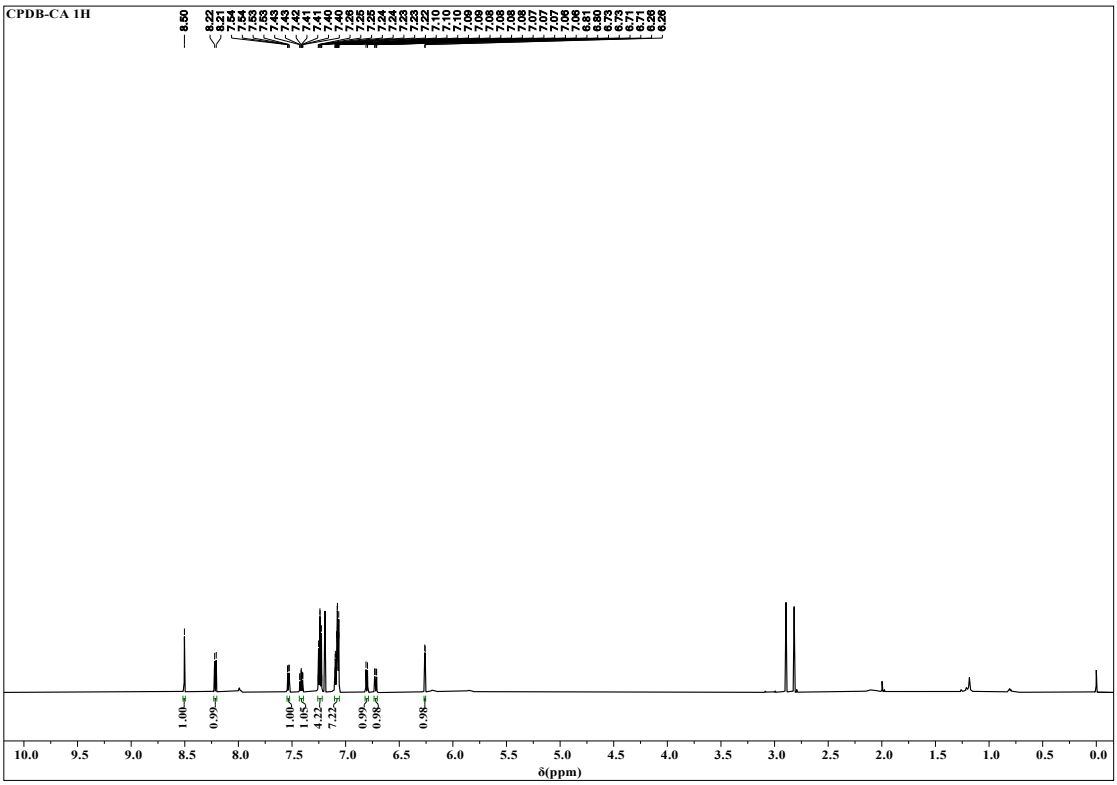
[13]C NMR spectra of CPDB-CAA



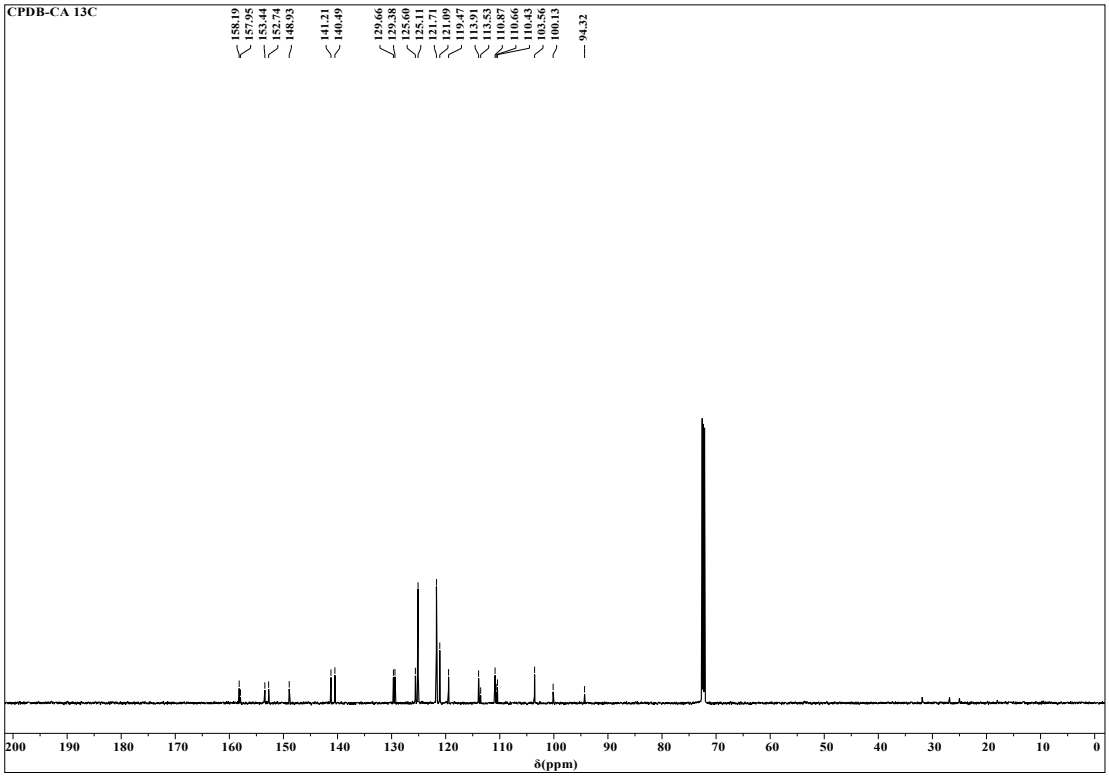
[1]H NMR spectra of CPDB-ECA



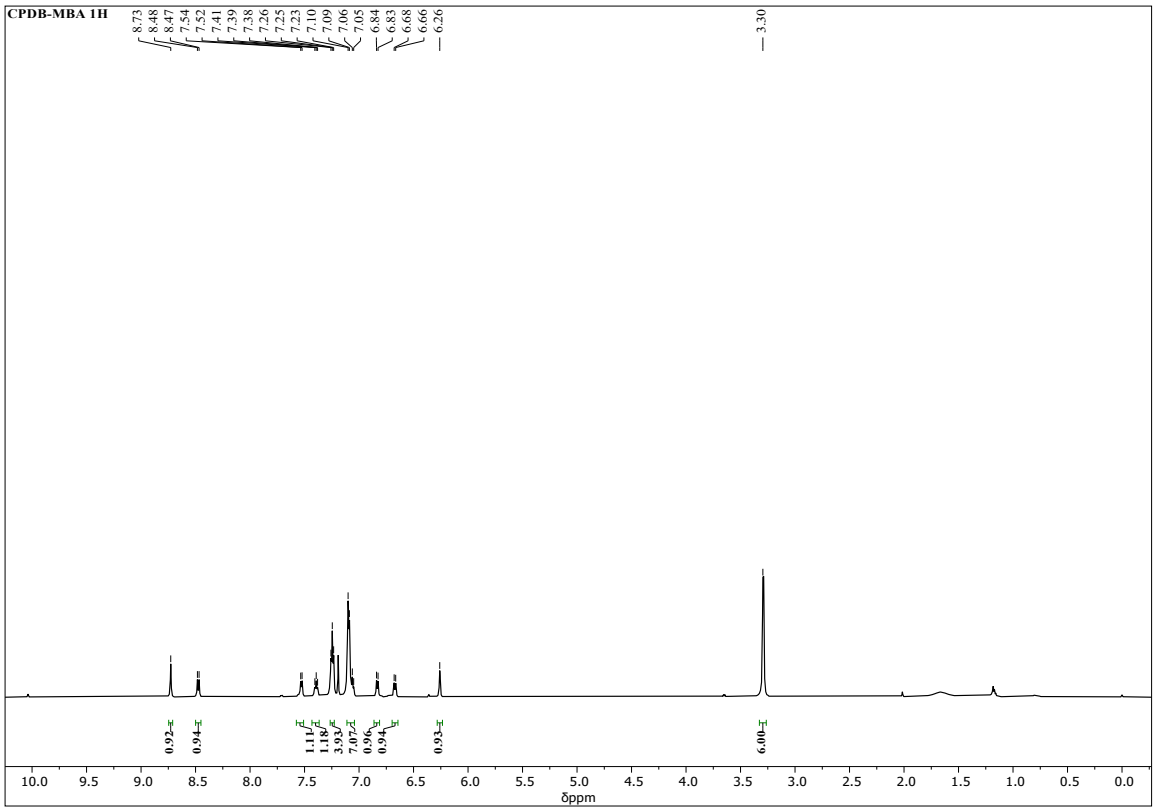
[13]C NMR spectra of CPDB-ECA



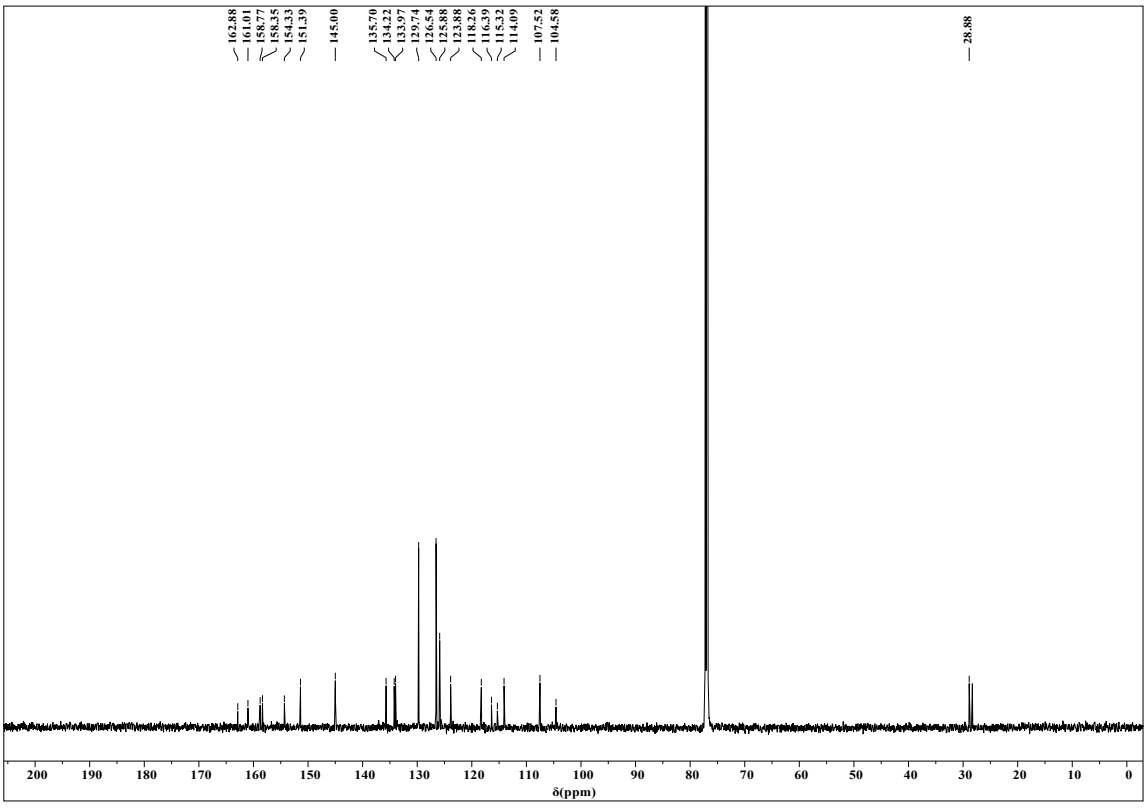
[1]H NMR spectra of CPDB-CA



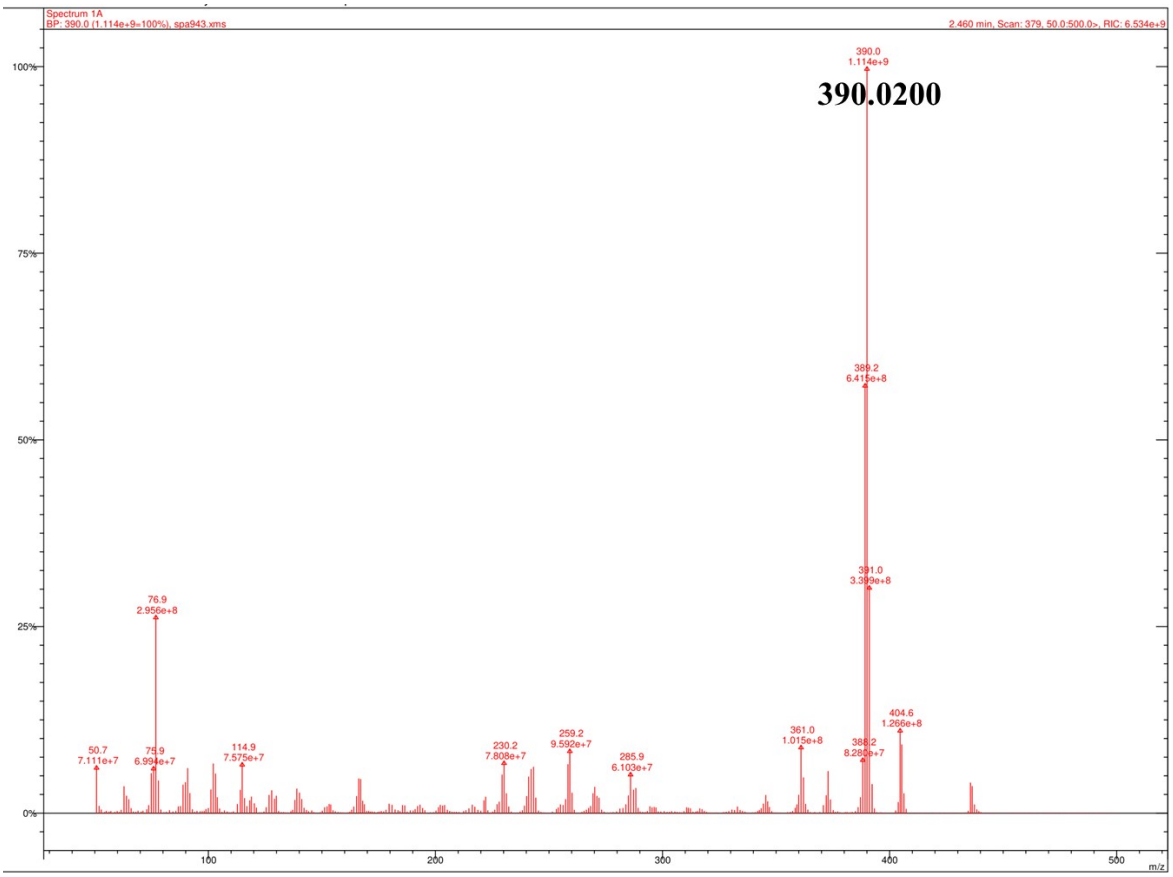
[13]C NMR spectra of CPDB-CA



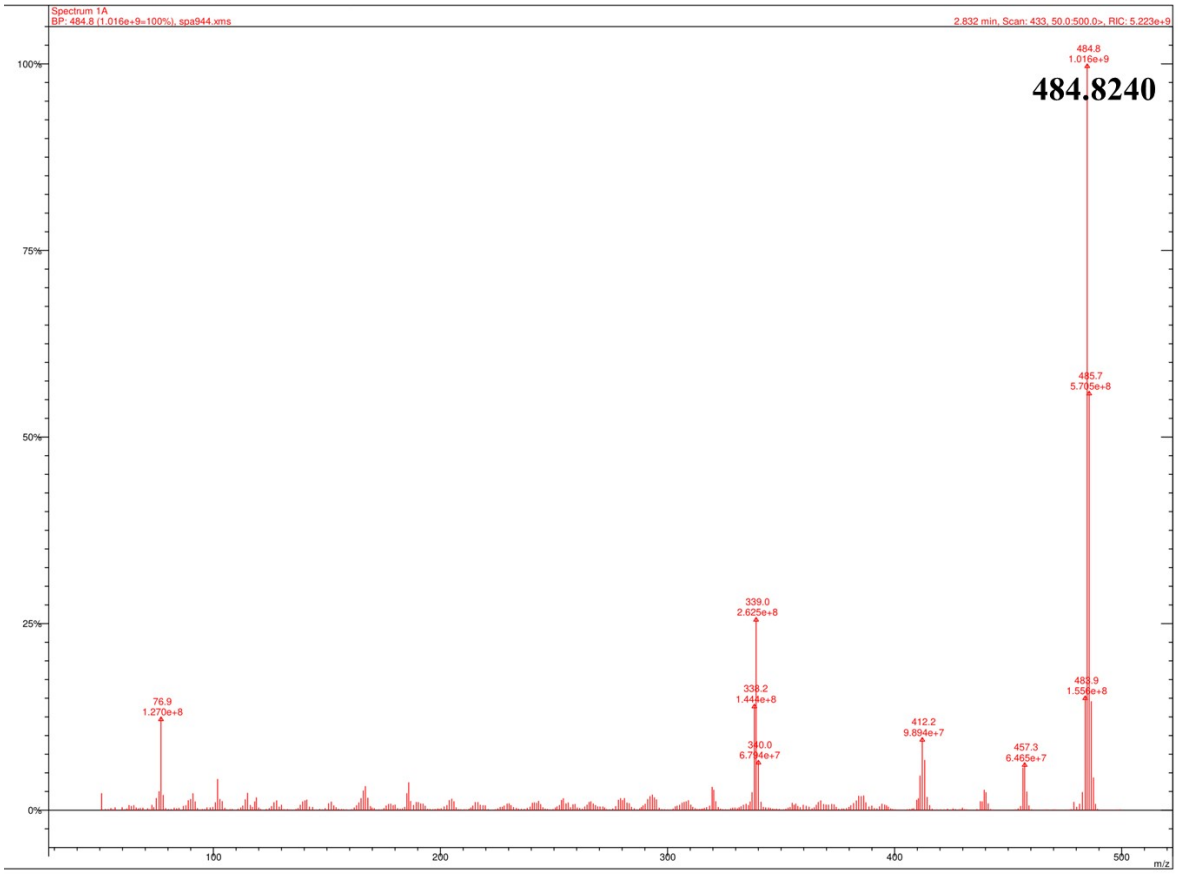
[1]HNMR spectra of CPDB-MBA



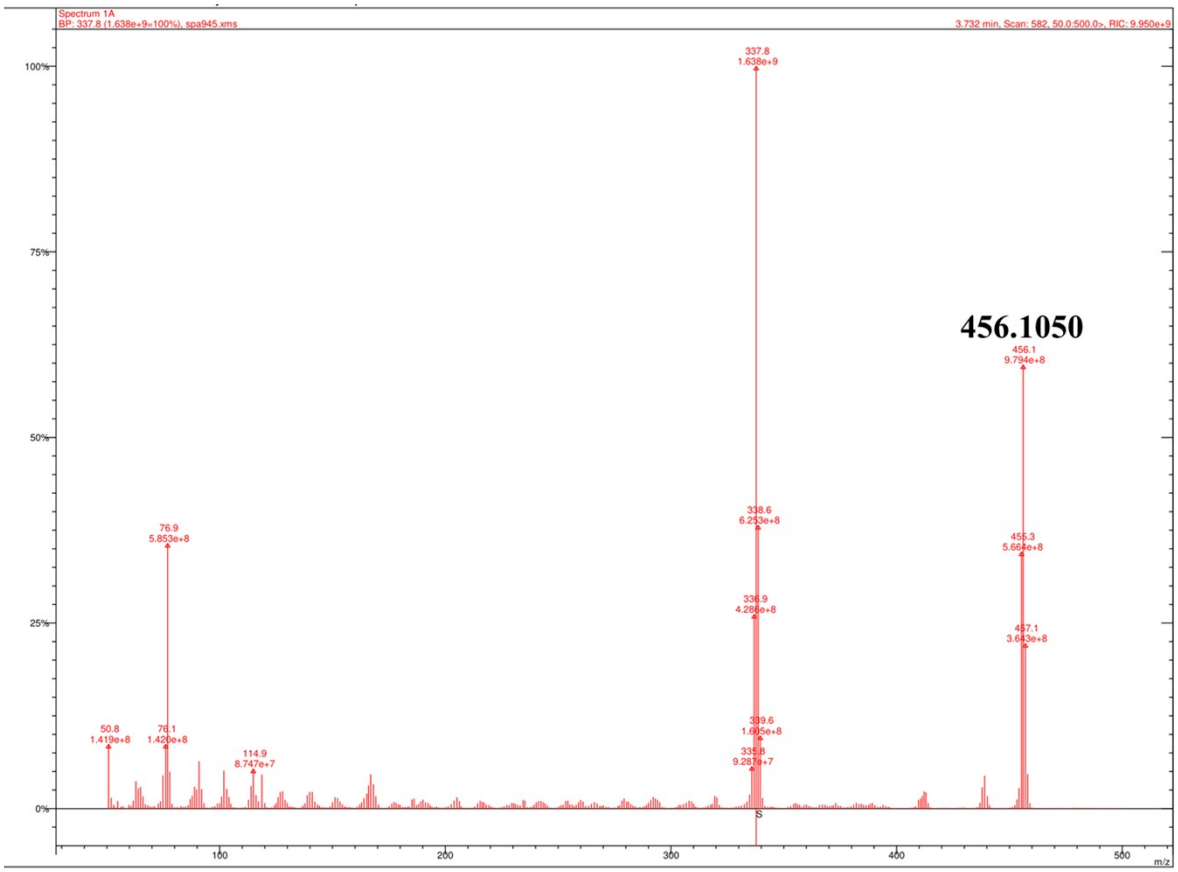
[13]C NMR spectra of CPDB-MBA



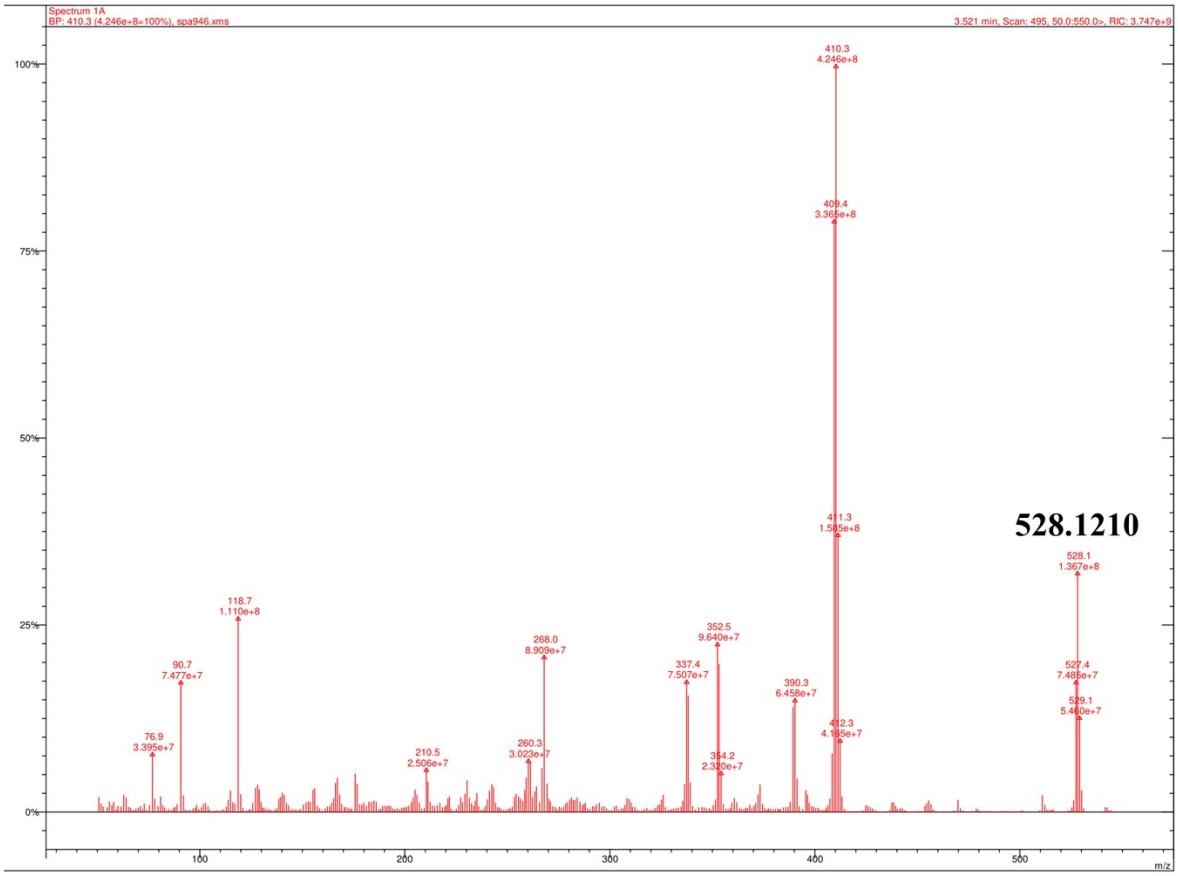
HRMS spectra of ***CPDP-CHO***. Calculated: 390.1368; found: 390.0200.



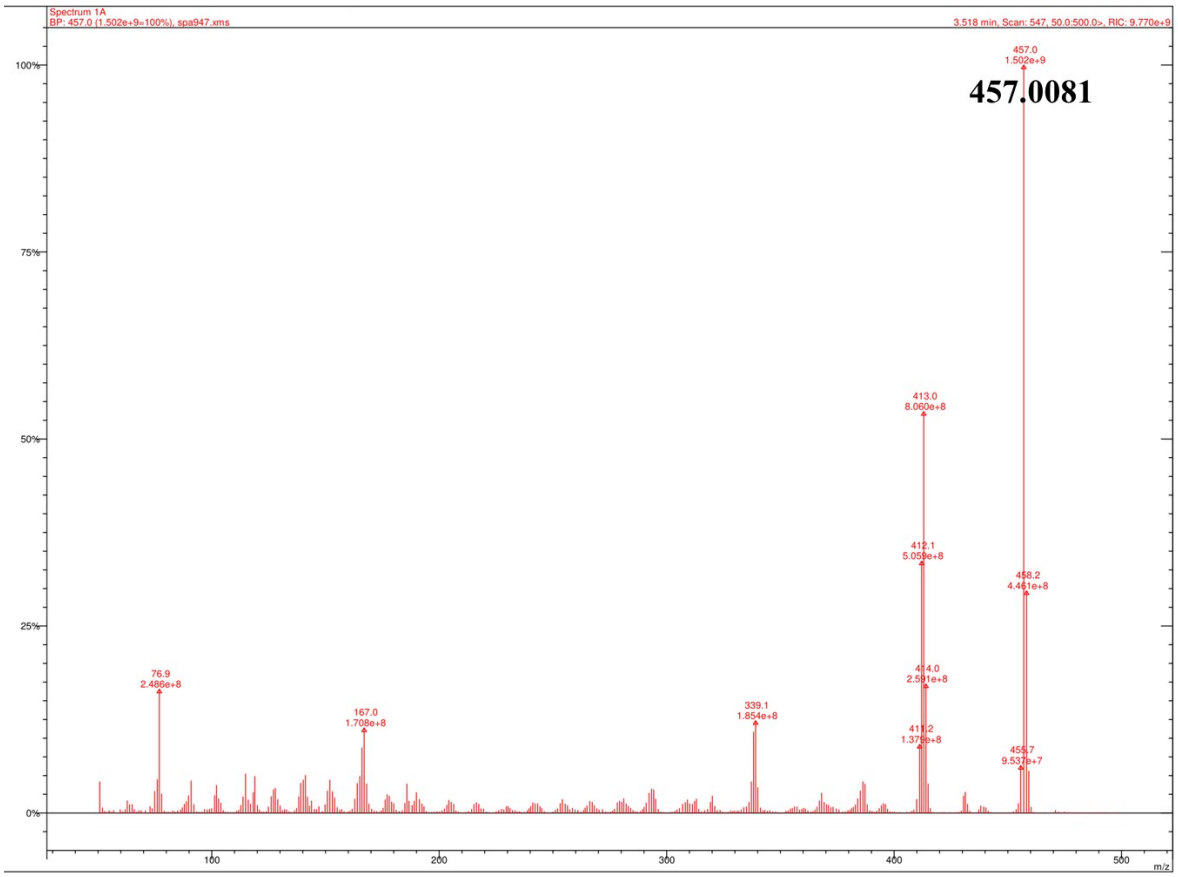
HRMS spectra of ***CPDP-ECA***. Calculated: 485.1739; found: 484.8240.



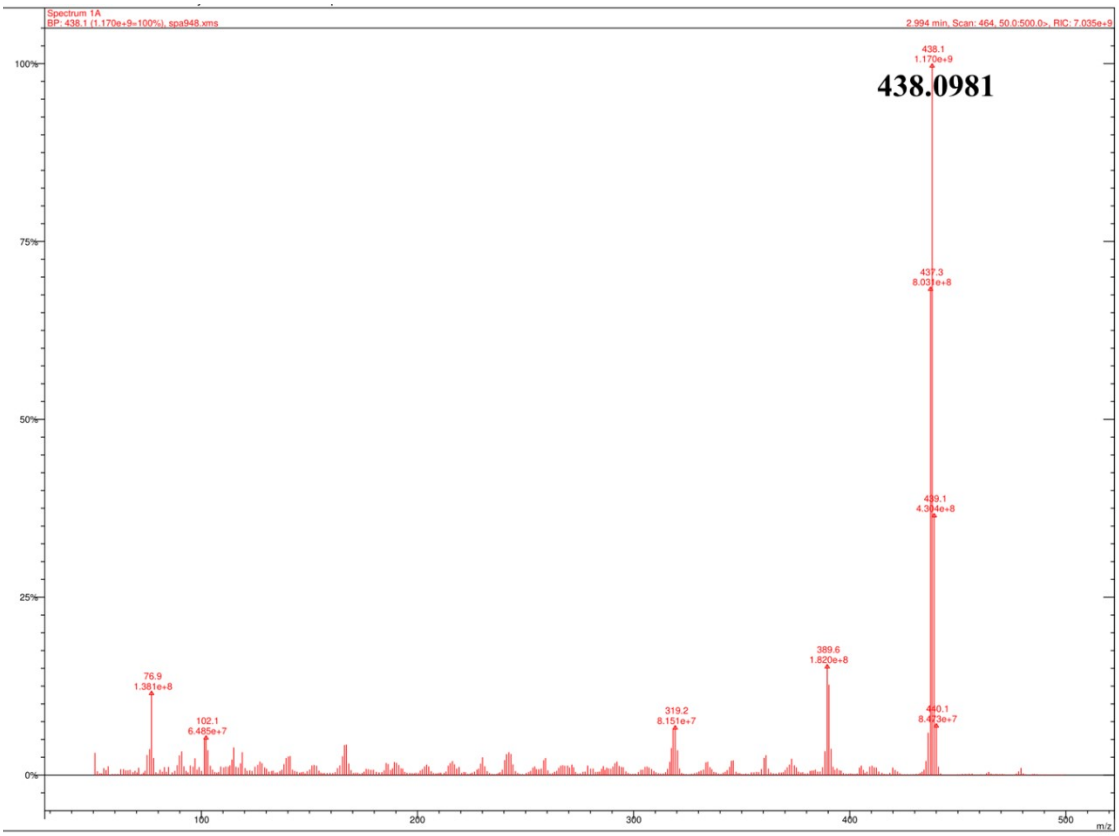
HRMS spectra of ***CPDP-CA***. Calculated: 456.1586; found: 456.1050.



HRMS spectra of ***CPDP-MBA***. Calculated: 528.1798; found: 528.1210.



HRMS spectra of ***CPDP-CAA***. Calculated: 457.1426; found: 457.0081.



HRMS spectra of ***CPDP-MN***. Calculated: 438.1481; found: 438.0981.

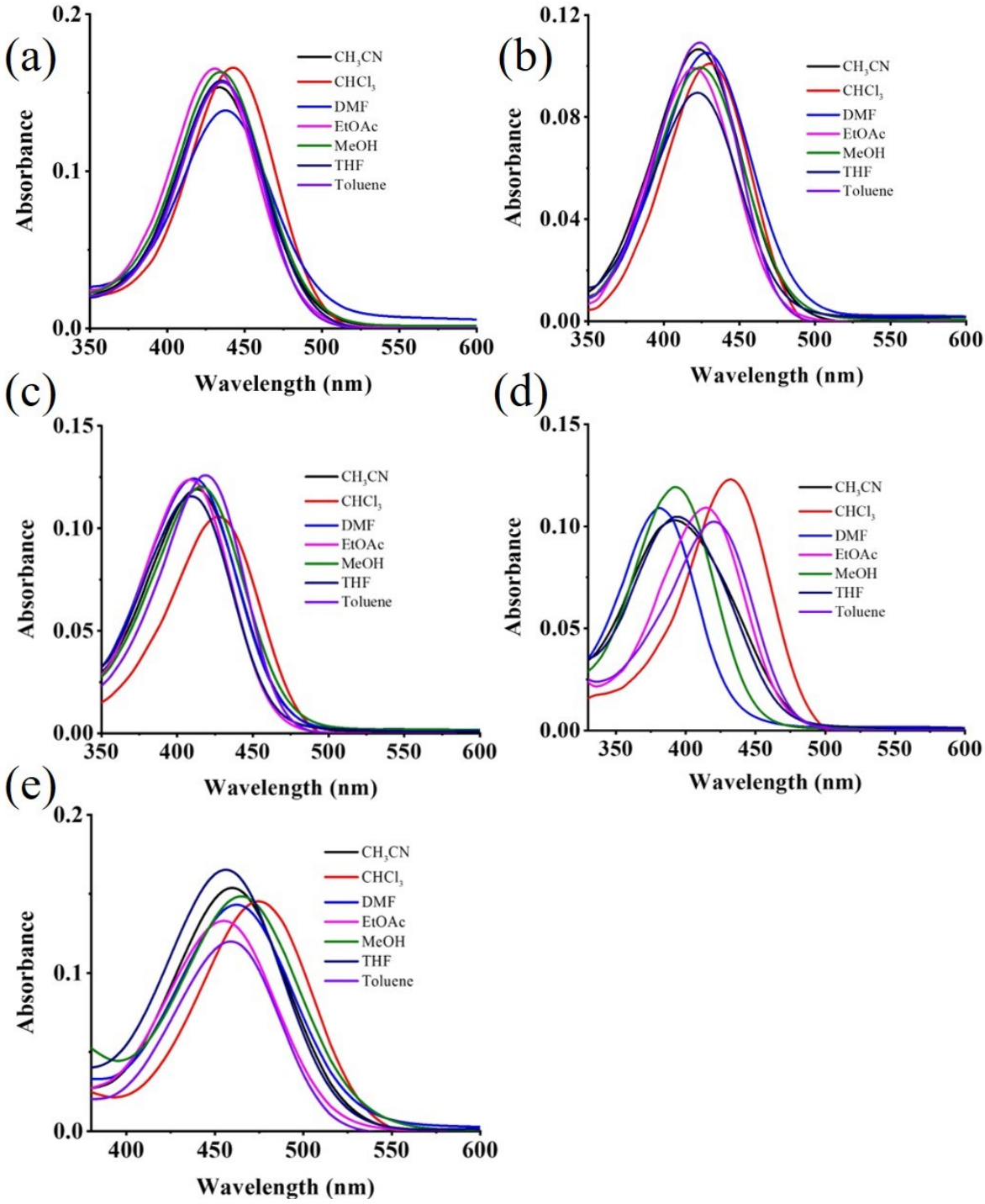


Figure S1. Absorption spectra (a) CPDB-MN, (b) CPDB-ECA, (c) CPDB-CA, (d) CPDB-CAA, and (e) CPDB-MBA in different solvents.

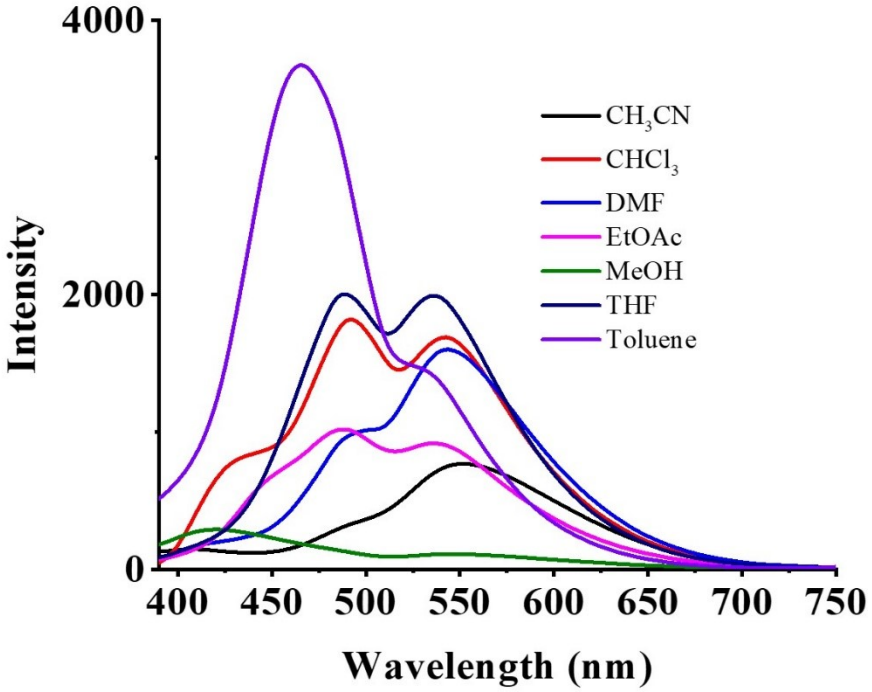


Figure S2. Fluorescencce spectra of CPDB-CAA in different solvents.

Table S1. Fluorescence λ_{max} and quantum yield (compared to quinine sulphate standard) of CPDB fluorophores in different solvents.

	CPDB-MN		CPDB-ECA		CPDB-CA		CPDB-CAA		CPDB-MBA	
	λ_{max}	ϕ_f	λ_{max}	ϕ_f	λ_{max}	ϕ_f	λ_{max}	ϕ_f	λ_{max}	ϕ_f
CH_3CN	407, 461, 542	0.04	422, 545	0.01	480, 580	0.01	485, 552	0.03	470	0.03
$CHCl_3$	489, 537	0.2	446, 548	0.06	563	0.2	426, 490, 542	0.02	489, 536	0.14
DMF	425, 537	0.17	429, 542	0.05	479, 571	0.03	488, 543	0.04	464, 551	0.13
EtOAc	484, 535	0.19	460, 555	0.09	487, 561	0.18	446, 487	0.01	473, 539	0.14
MeOH	436, 481	0.03	432	0.03	481, 554	0.01	418, 546	0.02	419	0.01
THF	477, 534	0.16	458, 524	0.11	485, 560	0.05	439, 535	0.02	481, 536	0.07
Toluene	467, 537	0.19	482	0.14	496, 539	0.04	465, 534	0.01	470	0.16

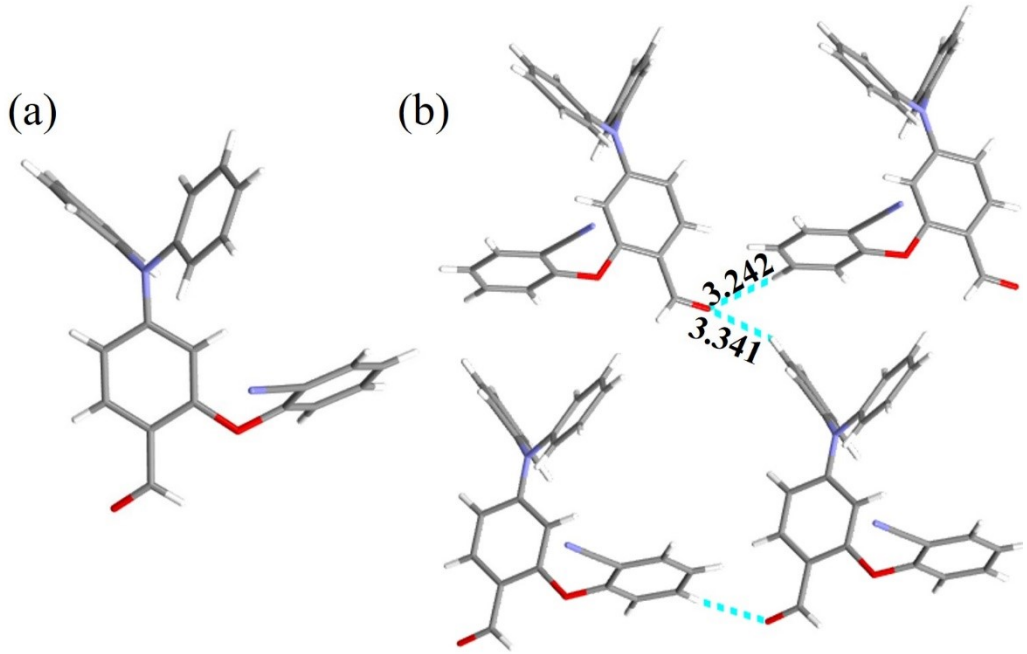


Figure S3. (a) Molecular structure and (b) intermolecular interactions in the crystal lattice of DPPB-CHO**.** C (grey), H (white), N (blue) and O (red). Dotted lines indicate the hydrogen bonding interactions in Å.

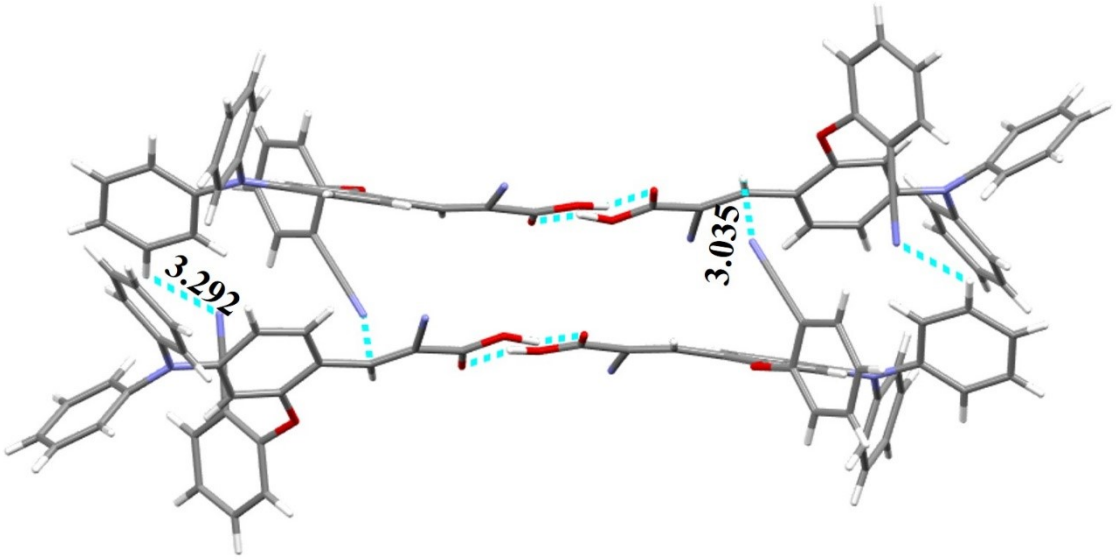


Figure S4. Intermolecular interactions in the crystal lattice of CPDB-CAA**.** C (grey), H (white), N (blue) and O (red). Dotted lines indicate the hydrogen bonding interactions in Å.

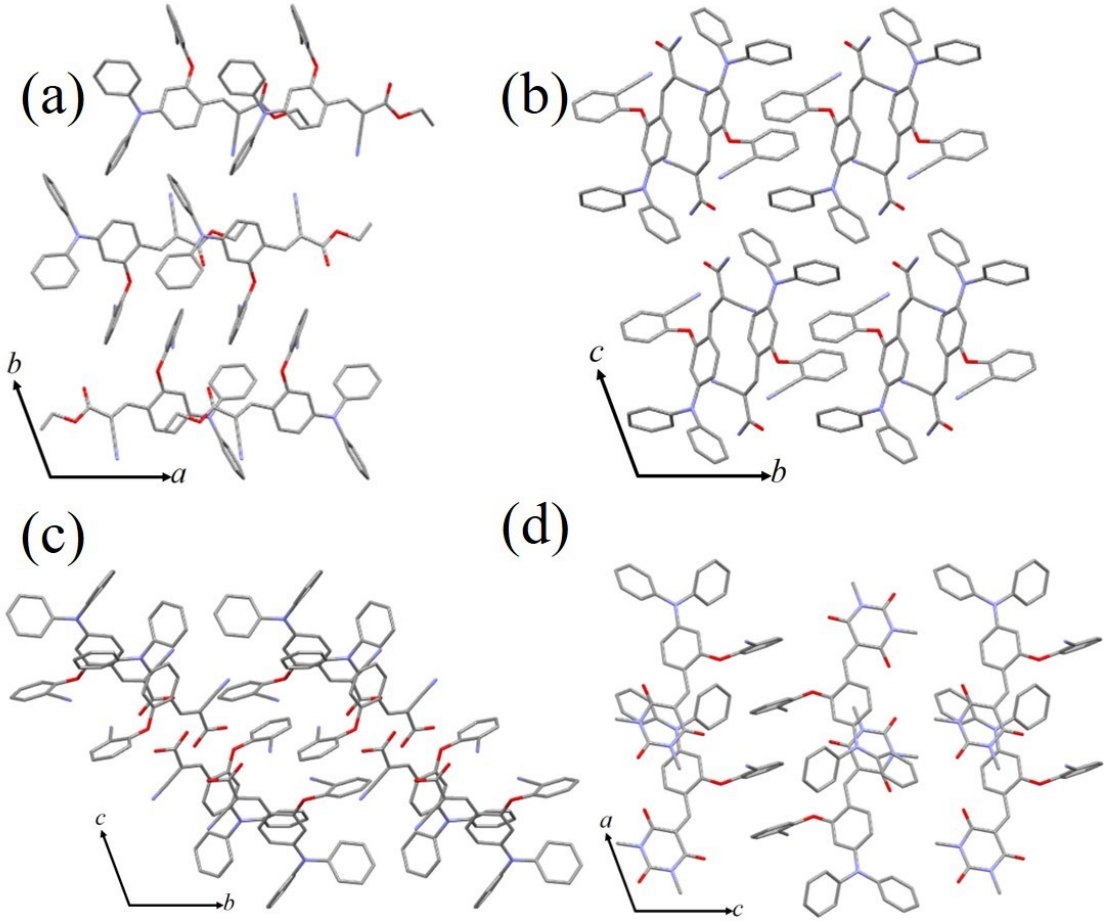


Figure S5. Molecular packing in the crystal lattice of (a) CPDB-ECA, (b) CPDB-CA, (c) CPDB-CAA and (d) CPDB-MBA**.** C (grey), H (white), N (blue) and O (red). H-atoms are omitted for clarity.

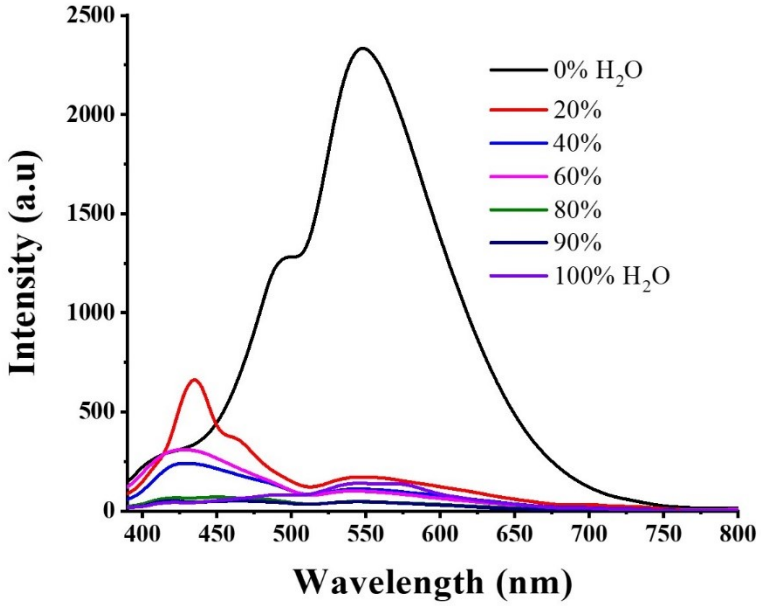
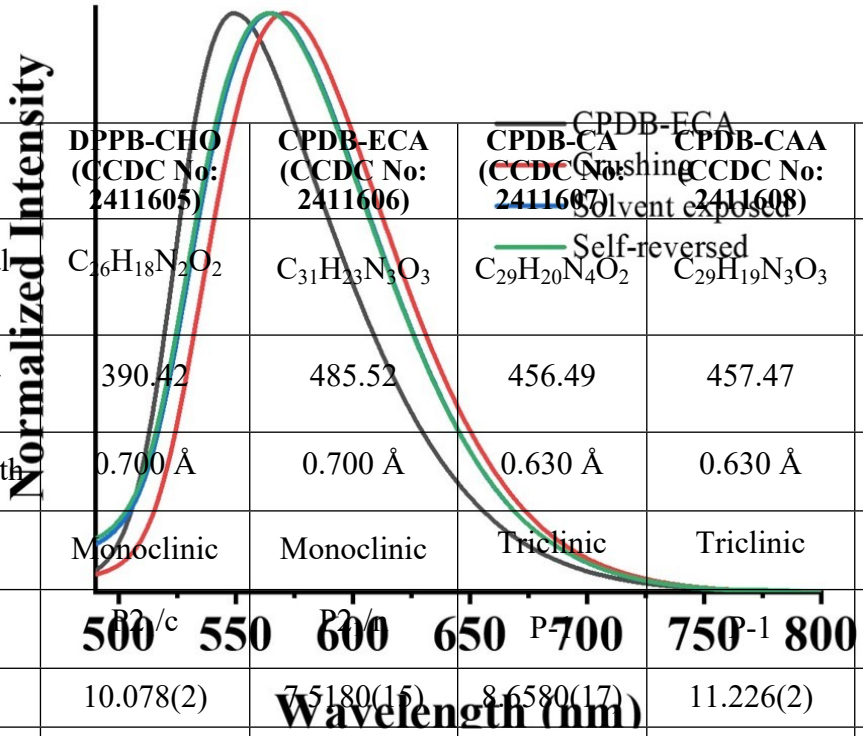


Figure S6. AIE of CPDB-CAA in different H_2O:CH_3CN mixture.

Table S2. Crystallographic details of DPPB-CHO and CPDB derivatives.



	DPPB-CHO (CCDC No: 2411605)	CPDB-ECA (CCDC No: 2411606)	CPDB-CA (CCDC No: 2411607)	CPDB-CAA (CCDC No: 2411608)	CPDB-MBA (CCDC No: 2411609)
Empirical formula	$C_{16}H_{18}N_2O_2$	$C_{31}H_{23}N_3O_3$	$C_{29}H_{20}N_4O_2$	$C_{29}H_{19}N_3O_3$	$C_{32}H_{24}N_4O_4$
Formula weight	390.42	485.52	456.49	457.47	528.55
Wavelength	0.700 Å	0.700 Å	0.630 Å	0.630 Å	0.630 Å
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	P2$_1$/c	P2$_1$/n	P-1	P-1	P-1
a (Å)	10.078(2)	7.5180(15)	8.6580(17)	11.226(2)	7.6840(15)
b (Å)	9.888(2)	36.519(7)	10.746(2)	13.215(3)	8.6090(17)
c (Å)	20.434(4)	9.0830(18)	13.271(3)	16.773(3)	19.253(4)
α	90°	90°	76.39(3)°	81.42(3)°	87.90(3)°
β	101.85(3)°	97.19(3)°	74.05(3)°	87.99(3)°	89.11(3)°
γ	90°	90°	83.35(3)°	69.34(3)°	78.07(3)°
Volume Å^3	1992.9(7)	2474.1(9)	1152.1(5)	2301.8(9)	1245.2(4)
Z	4	4	2	4	2
Density (calculated) Mg/m^3	1.301	1.303	1.316	1.320	1.410
F(000)	816	1016	476	952	552
Independent reflections	4931 [R(int) = 0.0719]	5903 [R(int) = 0.0712]	6477 [R(int) = 0.0266]	13005 [R(int) = 0.0318]	6899 [R(int) = 0.0309]
Goodness-of-fit on F^2	1.034	1.018	1.045	1.069	1.104
R indices (all data)	R1 = 0.0949, wR2 = 0.1660	R1 = 0.1111, wR2 = 0.1413	R1 = 0.0546, wR2 = 0.1240	R1 = 0.1026, wR2 = 0.2387	R1 = 0.1113, wR2 = 0.3147

Figure S7. Mechanofluorochromism of CPDB-ECA.

Table S3. HOMO-LUMO of CPDP derivatives.

	HOMO	**LUMO**	**band gap (eV)**
CPDP-ECA	-5.78	-2.41	3.37
CPDP-CA	-6.02	-2.32	3.70
CPDP-CAA	-5.74	-2.43	3.31
CPDP-MBA	-5.65	-2.75	2.90