Supporting Information

Intramolecular hydrogen bond-enhanced electroluminescent performance of hybridized local and charge transfer (HLCT) excited state blue emissive materials

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Material Synthesis and Characterizations:

9,10-Dibromoanthracene (1): A solution of Br_2 (2.90 mL, 56.60 mmol) in $CHCl_3$ (50 mL) was added dropwise into the solution of anthracene (5.0 g, 28.05 mmol) in $CHCl_3$ (100 mL) at room temperature. The mixture was stirred for 4 h, then the solvent was removed, and the crude product was purified by recrystallization in dichloromethane to obtain yellow needle-like crystal of 9.4 g (74 %). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.62 – 8.57 (m, 1H), 7.66 – 7.61 (m, 4H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 131.10, 128.30, 127.47, 123.54. Formula: $C_{14}H_8Br_2$, Mol. Wt: 336.03 Da, MS (APCI): m/z: 335.96 [M+].

4-(10-Bromoanthracene-9-yl)-N,N-diphenylaniline (2): A mixture of **1** (3.85 g, 11.53 mmol), 4-(diphenylamino)phenylboronic acid (667 mg, 2.31 mmol), $Pd(PPh_3)_4$ (57.78 mg, 0.05 mmol), 2M sodium carbonate (2.45 g, 23.10 mmol) aqueous solution and anhydrous THF was degassed with nitrogen for 15 min while stirring. Then the stirring reaction was heated and refluxed under nitrogen atmosphere for 48 h. The mixture was cooled to room temperature after confirming consumption of the starting materials by TLC in 10% v/v dichloromethane-hexane. Then the mixture was added to brine (20 ml) and extracted with a certain amount of dichloromethane. The extract was concentrated under reduce pressure and finally purified by silica gel column chromatography of 896 mg (78%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.61 (d, J = 8.4 Hz, 1H), 7.81 (d, J = 9 Hz, 1H), 7.60 (t, J=7.8, 1H), 7.43 (t, J=7.8, 1H), 7.34 (t, J = 7.8 Hz, 2H), 7.28-7.24 (m, 4H), 7.09 (t, J = 7.2 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 147.72, 147.44, 137.74, 131.95, 131.76, 131.27, 130.32, 129.42, 127.87, 127.50, 126.93, 125.48, 124.80, 123.24, 122.85, 122.56. Formula: $C_{32}H_{22}BrN$, Mol. Wt: 500.44 Da, MS (APCI): m/z: 501.99 [M+].

N,N-diphenyl-4-(10-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)anthracen-9-yl)aniline (3): **2** (500 mg, 1.00 mmol), bis(pinacolato)diboron (761.82 mg, 3.00 mmol), KOAc (1.18 g, 12.00 mmol), and $Pd(dppf)_2Cl_2{\cdot}CH_2Cl_2$ (40.83 mg, 0.05 mmol) were mixed followed by adding 30ml anhydrous Toluene. The mixture was degassed with nitrogen for 15 min while stirring. Then the stirring reaction was heated and refluxed under nitrogen atmosphere for 15 h. The mixture was cooled to room temperature after confirming consumption of the starting materials by TLC in 30% v/v dichloromethane-hexane. Then the mixture was added to brine (20 ml) and extracted with a certain amount of dichloromethane. The extract was concentrated under reduce pressure and finally purified

by silica gel column chromatography of 585 mg (65%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.43 (d, J = 9.0 Hz, 1H), 7.79 (d, J = 8.4 Hz, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.37 (t, J = 7.8 Hz, 1H), 7.33 (t, J = 7.8 Hz, 2H), 7.07 (t, J = 7.2 Hz, 1H), 1.60 (s, 6H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 147.83, 147.11, 139.46, 135.47, 132.80, 131.95, 129.93, 129.36, 128.44, 127.48, 125.40, 124.78, 124.62, 123.14, 123.03, 84.46, 25.23. Formula: $C_{38}H_{34}BNO_2$, Mol. Wt: 547.51 Da, MS (APCI): m/z: 548.26 [M+].

4-Bromo-2-(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)phenol (5): 9,10-phenanthrenequinone (500 mg, 2.40 mmol) and 5-bromosalicylaldehyde (482.4 mg, 2.40mmol) were mixed at room temperature followed by adding 30 ml of acetic acid. Aniline (335 mg, 3.60 mmol) was then added to this solution little by little, and ammonium acetate (924.96 mg, 12 mmol) was added subsequently. The mixture was heated at 110 °C for 12 h under nitrogen atmosphere and reflux device. After termination of reaction, the dark solution was poured into a copious amount of water in a 1000ml beaker. Then a certain amount of sodium hydrogen carbonate was added into the mixture until neutralizing. The crude product was purified by recrystallization in dichloromethane to obtain white solid power of 510 mg (45%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 13.92 (s, 1H), 8.78 (d, J = 7.8 Hz, 1H), 8.70 (dd, J = 14.4, 8.4 Hz, 2H), 7.86 – 7.81 (m, 1H), 7.81 – 7.75 (m, 3H), 7.69 (t, J = 7.8 Hz, 1H), 7.63 (d, J = 7.8 Hz, 2H), 7.54 (t, J = 7.8 Hz, 1H), 7.28 (d, J = 8.4 Hz, 2H), 7.14 (d, J = 8.4 Hz, 1H), 7.01 (d, J = 8.4 Hz, 1H), 6.74 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 158.28, 147.08, 138.62, 134.38, 133.22, 131.08, 130.94, 129.68, 128.88, 128.68, 128.56, 127.60, 127.16, 126.64, 126.25, 125.69, 125.55, 124.23, 123.27, 122.57, 122.50, 120.97, 119.71, 114.57, 109.73. Formula: $C_{27}H_{17}BrN_2O$, Mol. Wt: 465.35 Da, MS (APCI): m/z: 466.03 [M+].

5-Bromo-2-(1-phenyl-1H-phenanthro[9,10-d]imidazol-2-yl)phenol (6): The synthesis of **6** used the same conditions as **5** among which the 5-bromosalicylaldehyde was replaced by 4-bromosalicylaldehyde (482 mg, 2.40 mmol): **6** of 520 mg was obtained (51%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 14.12 (s, 1H), 8.77 (d, J = 8.4 Hz, 1H), 8.69 (dd, J = 13.2, 8.4 Hz, 2H), 7.83 – 7.72 (m, 4H), 7.69 (t, J = 7.8 Hz, 1H), 7.62 (d, J = 7.2 Hz, 2H), 7.53 (t, J = 7.8 Hz, 1H), 7.31 (s, 1H), 7.28 – 7.24(m, 1H), 7.05 (d, J = 8.4 Hz, 1H), 6.64 (d, J = 8.4 Hz, 1H), 6.54 (d, J = 9.0 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 160.10, 147.76, 138.80, 134.38, 131.03, 130.83, 129.62, 129.00, 128.54, 127.58, 127.14, 126.80, 126.61, 126.22, 125.66, 125.45, 124.23, 123.26, 122.57, 122.51, 121.31, 121.15, 120.89, 112.12. Formula: $C_{27}H_{17}BrN_2O$, Mol. Wt: 465.35 Da, MS (APCI): m/z: 466.13 [M+].

Fig. S1 ^{1}H-NMR and ^{13}C-NMR spectra

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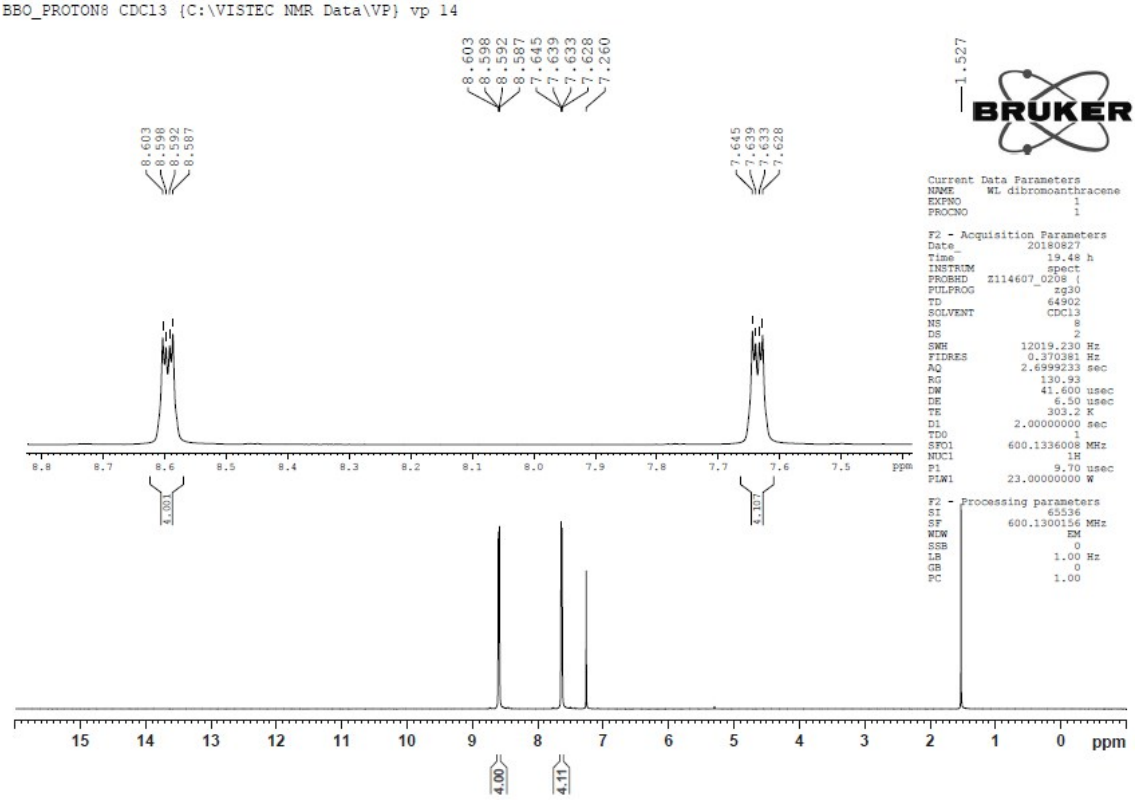

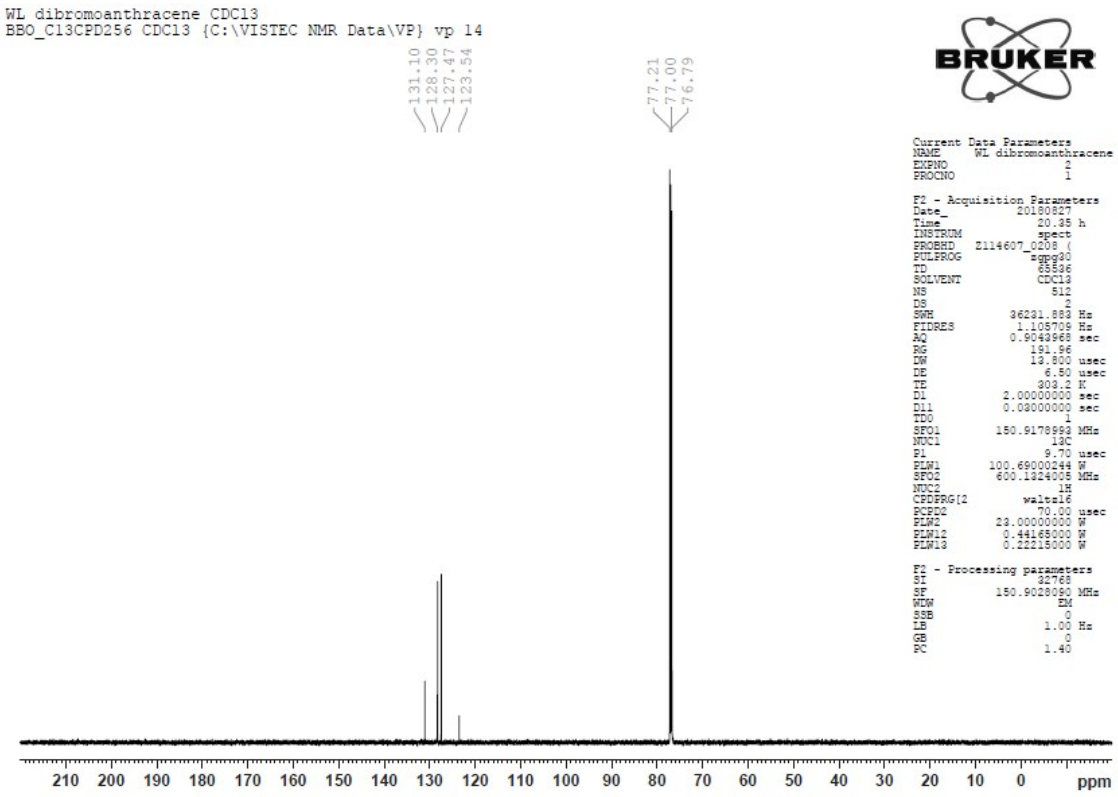

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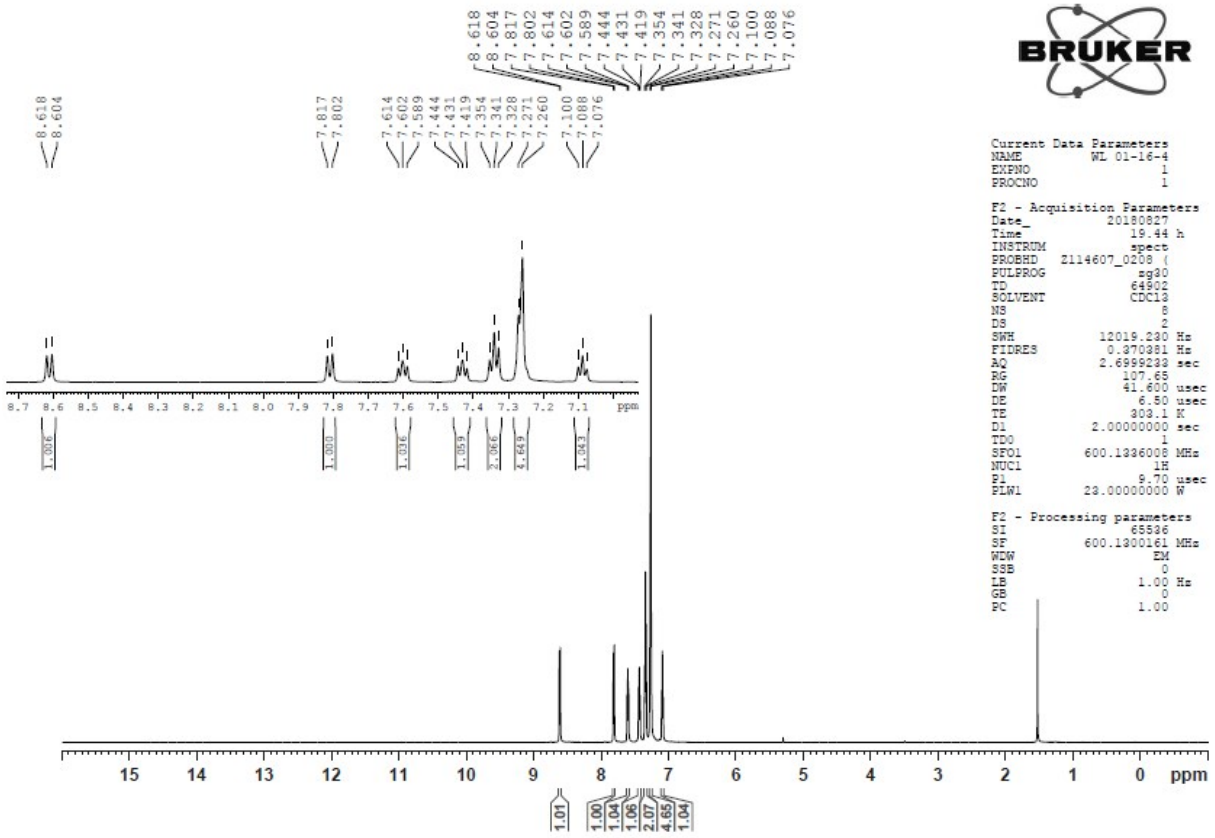

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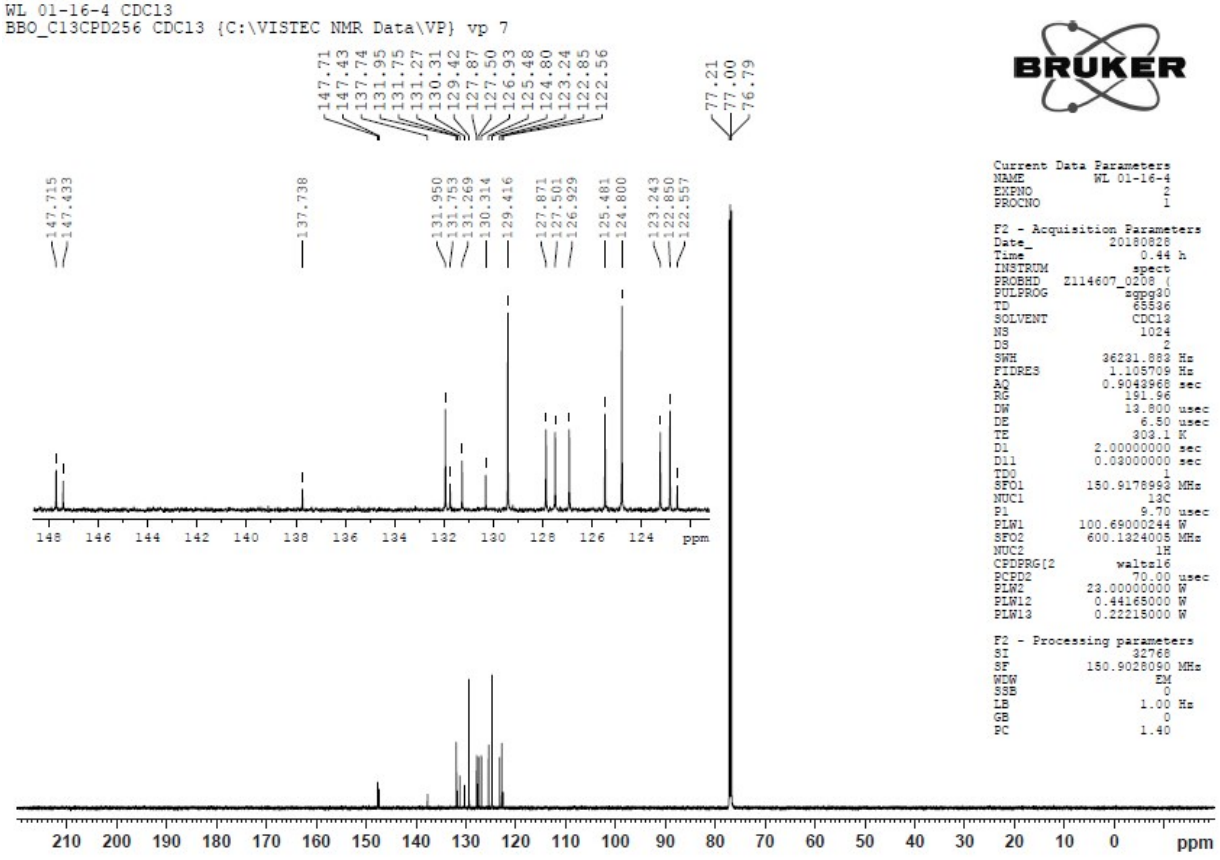

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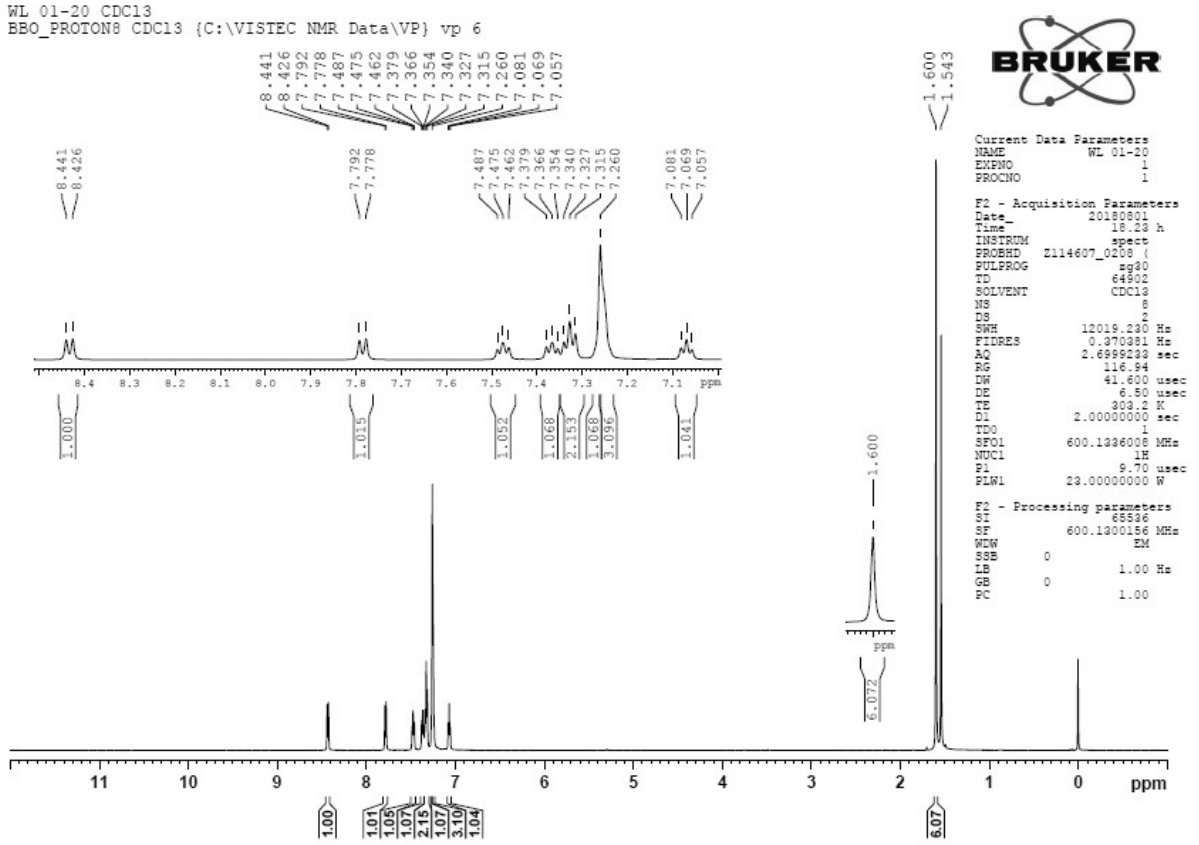
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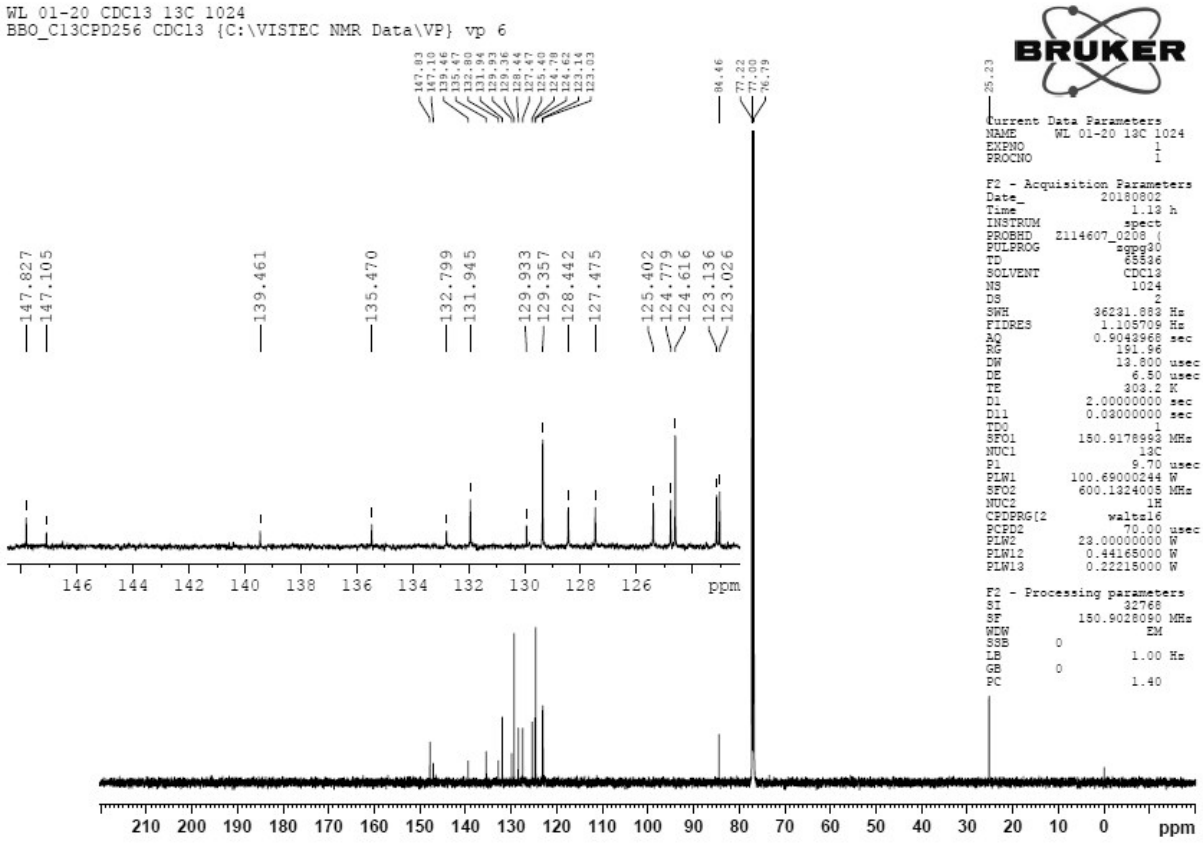
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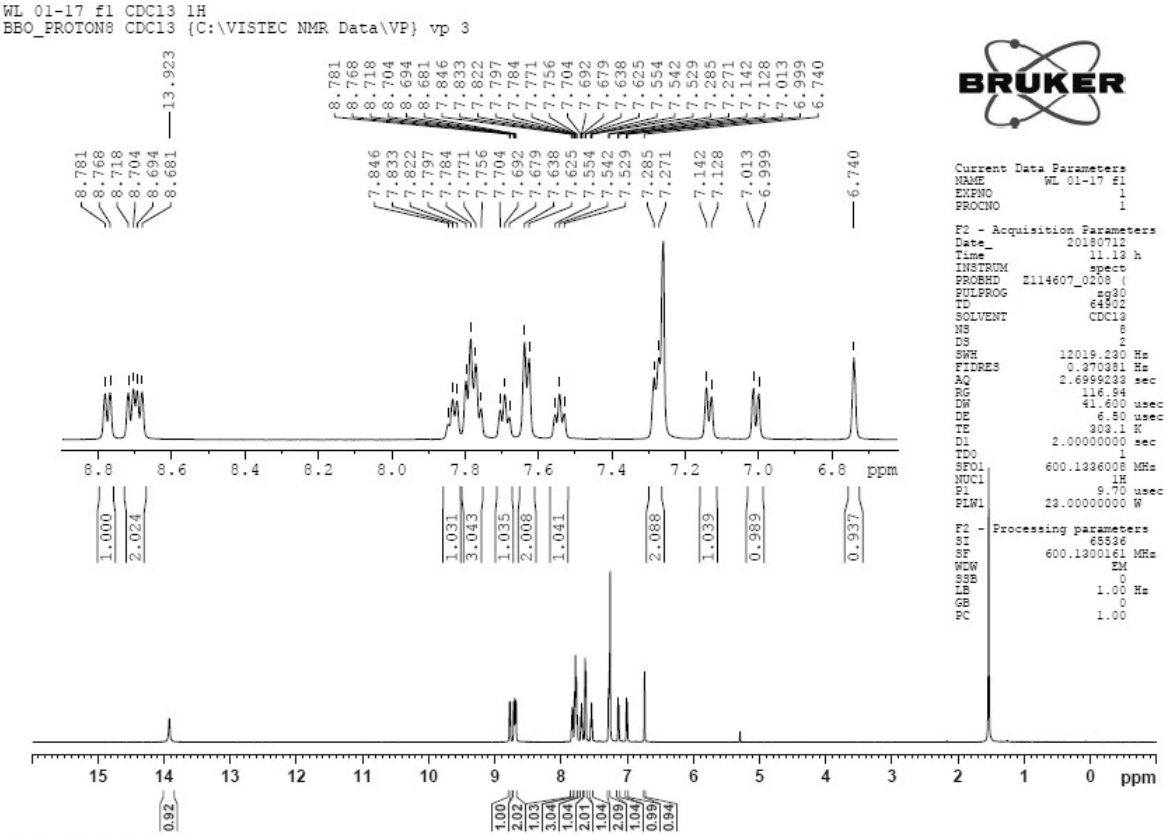
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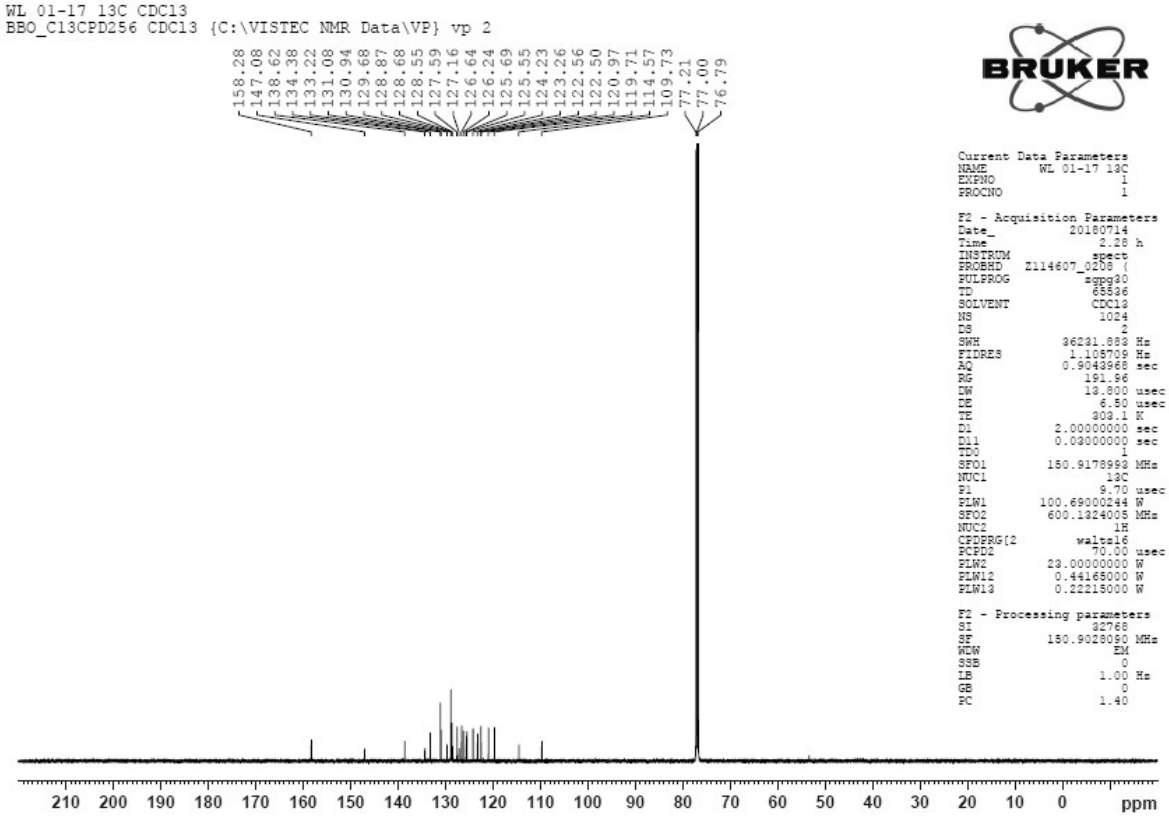
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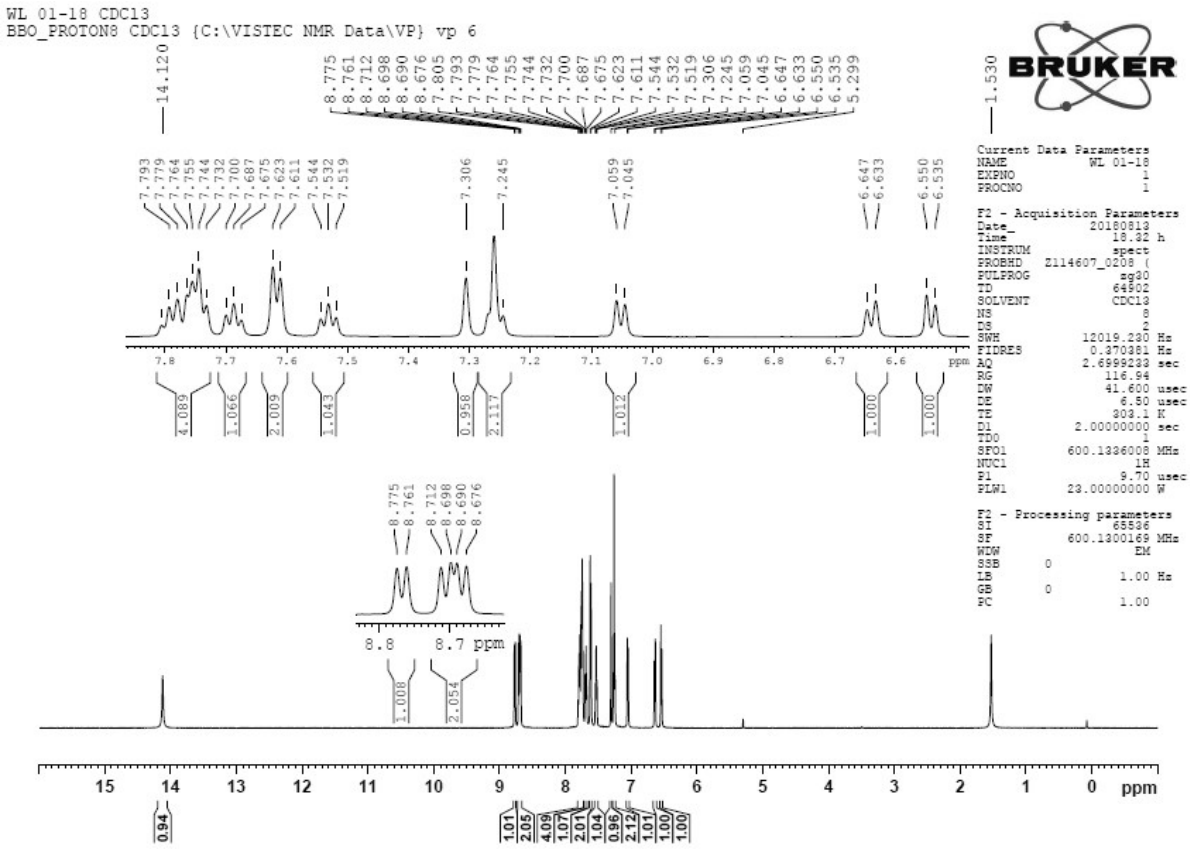
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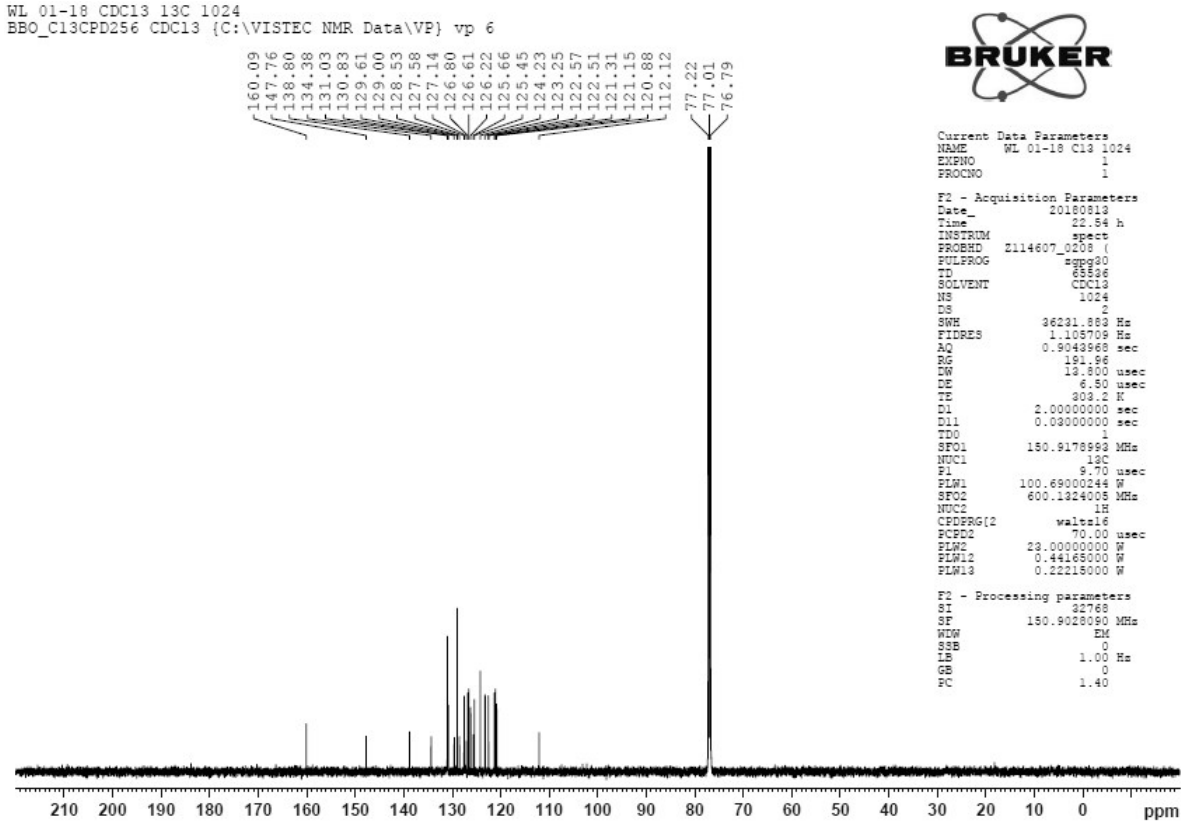
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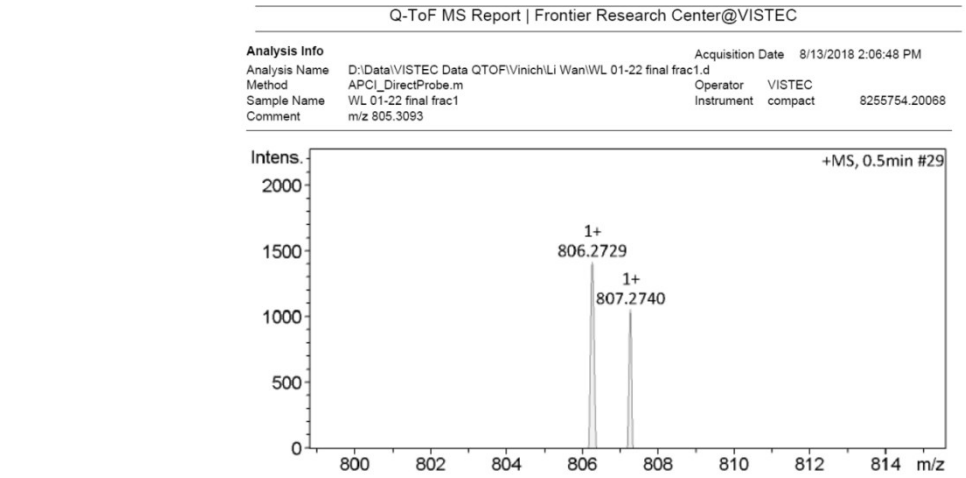
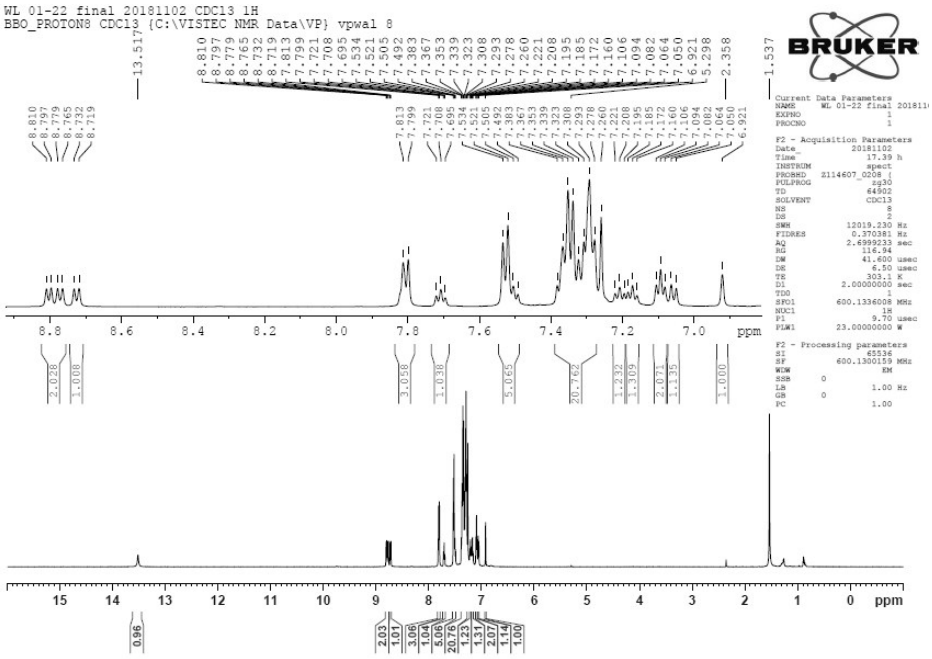
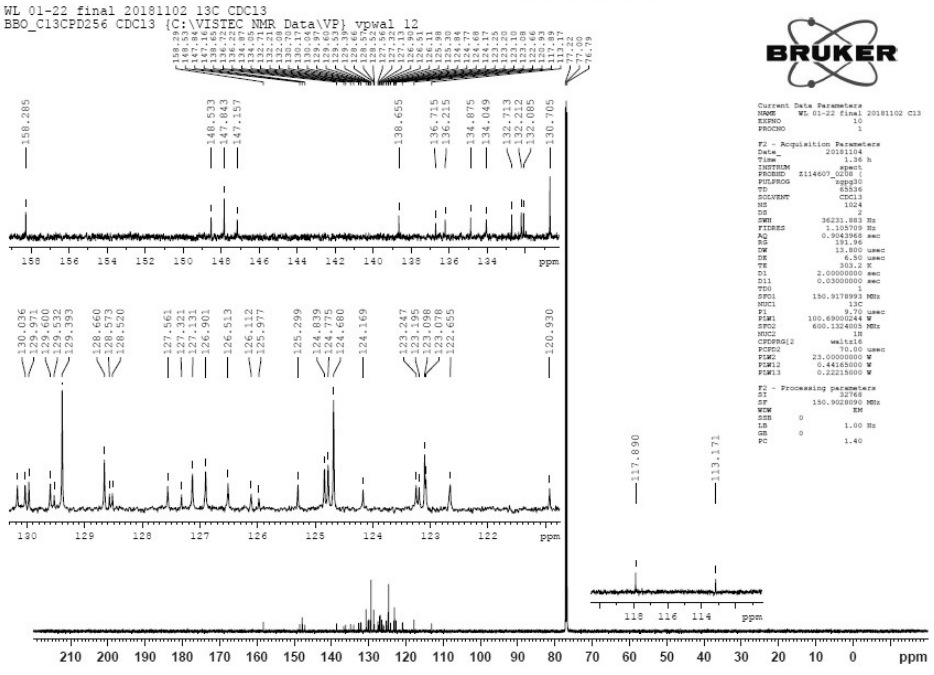
Compound mTAHPI:







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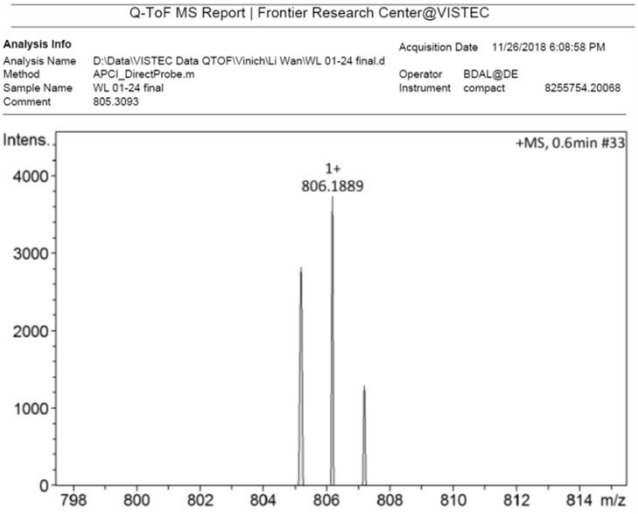

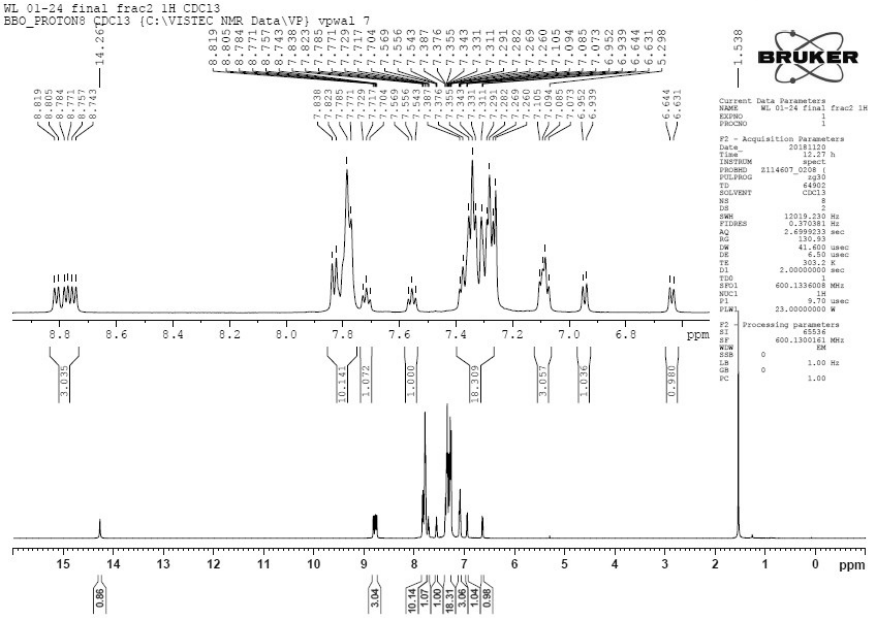

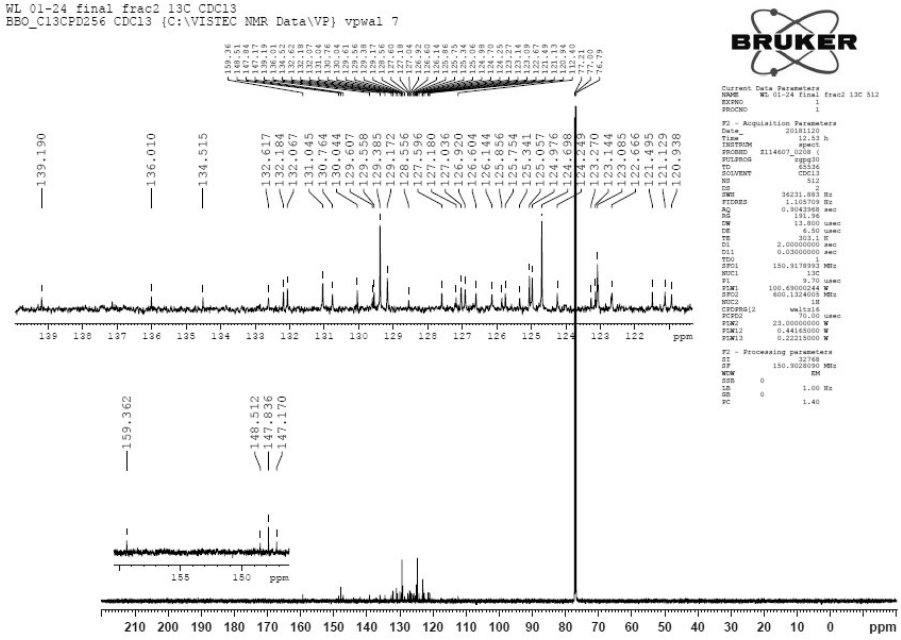

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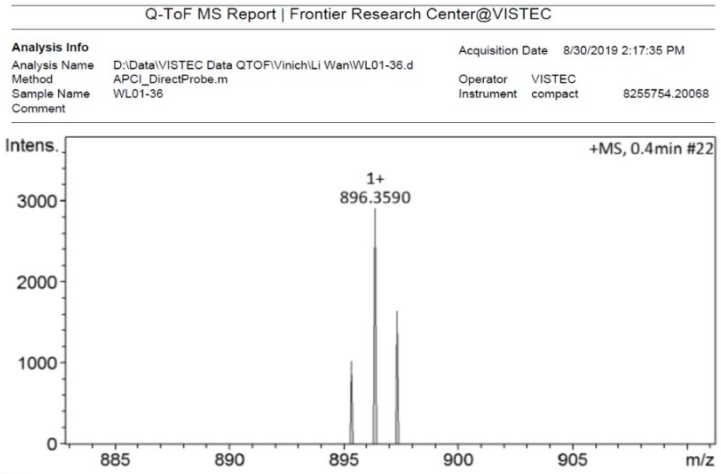
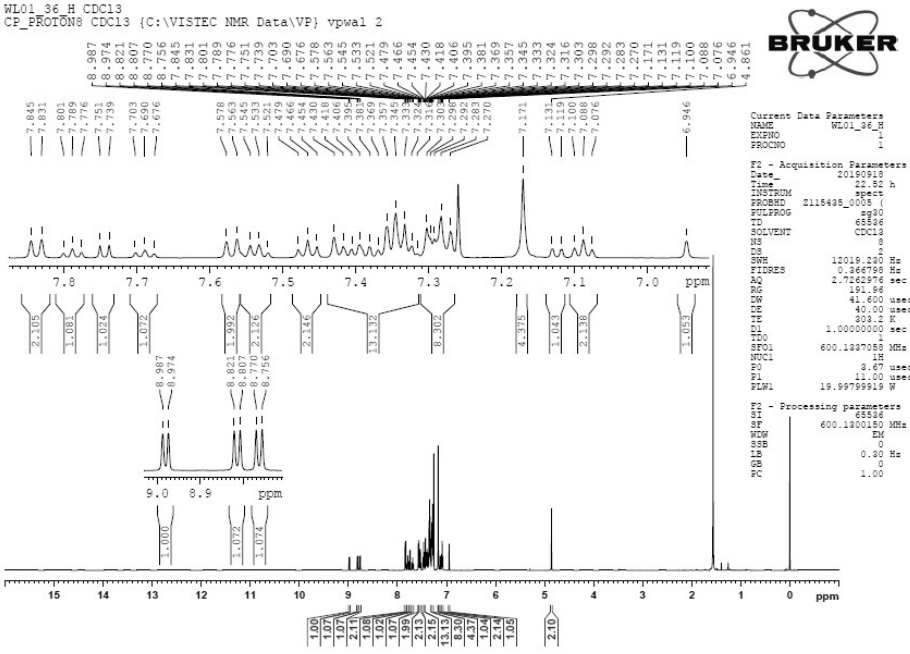
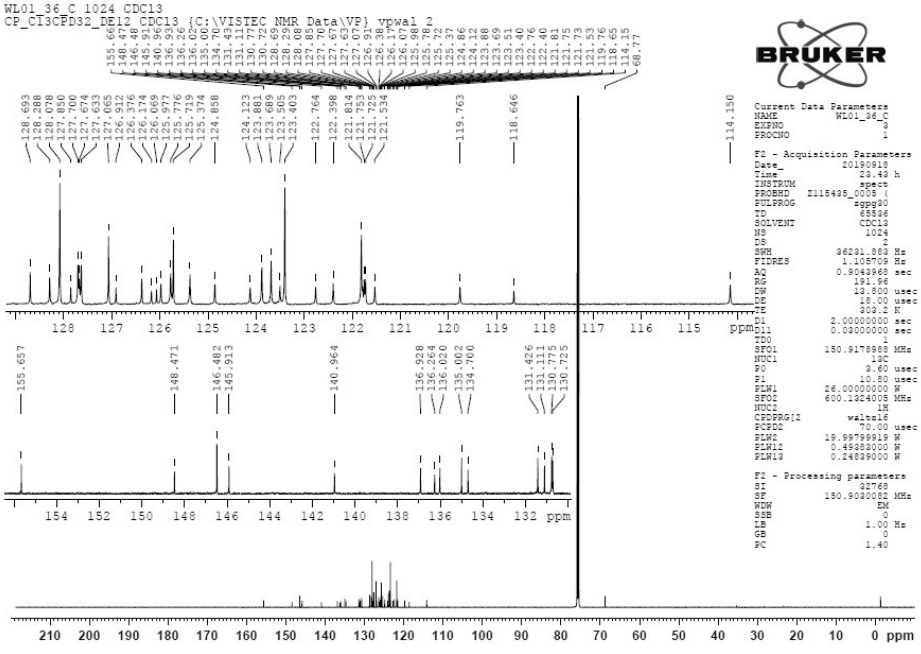


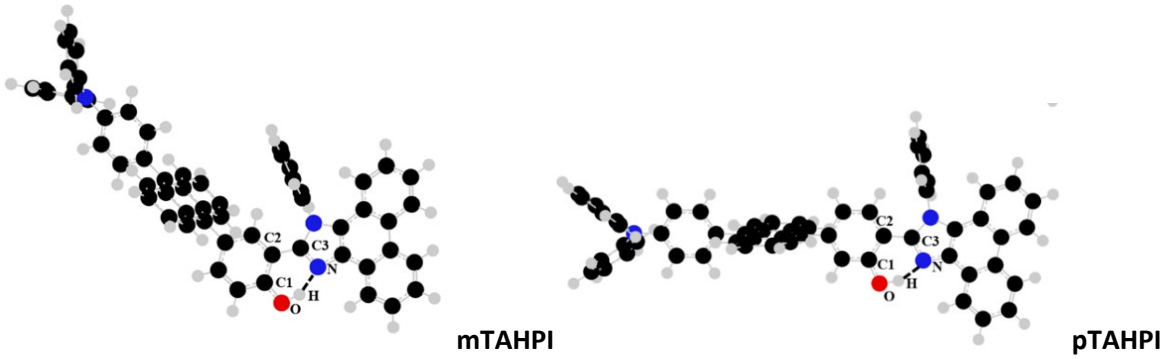




Characterization data

Table S1 Selected bond lengths (Å) and dihedral angles (°) for S_0 and S_1 optimized geometries of enol form computed at CAM-B3LYP/6-31 G(d,p) level.

Compound	State	Distance (Å)			Torsion
		O□H	N---H	O---N	OC1C2C3N
mTAHPI	S_0	0.999	1.656	2.609	10
	S_1	0.999	1.638	2.823	2
pTAHPI	S_0	0.999	1.652	2.556	6
	S_1	0.995	1.653	2.553	7



mTAHPI **pTAHPI**

Optimized geometries of target compounds in gas phase computed at CAM-B3LYP/6-31G(d,p) level.

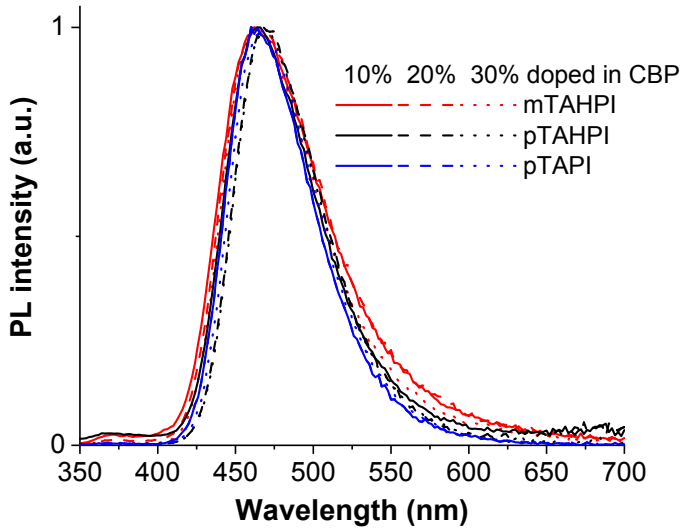


Fig. S2 PL spectra of **mTAHPI**, **pTAHPI** and **pTAPI** 10-30 wt% doped in CBP films.

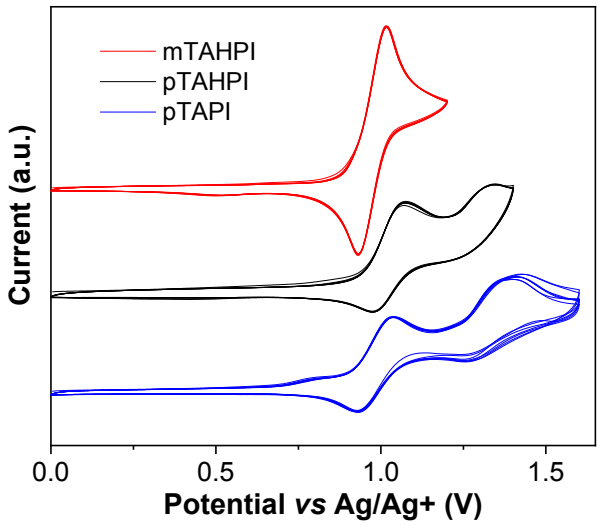


Fig. S3 Repeated cyclic voltammograms (7 scans) of **mTAHPI**, **pTAHPI** and **pTAPI** measured in CH_2Cl_2 containing n-Bu_4NPF_6 as a supporting electrolyte at a scan rate of 50 mV s^{-1} under Ar flow.

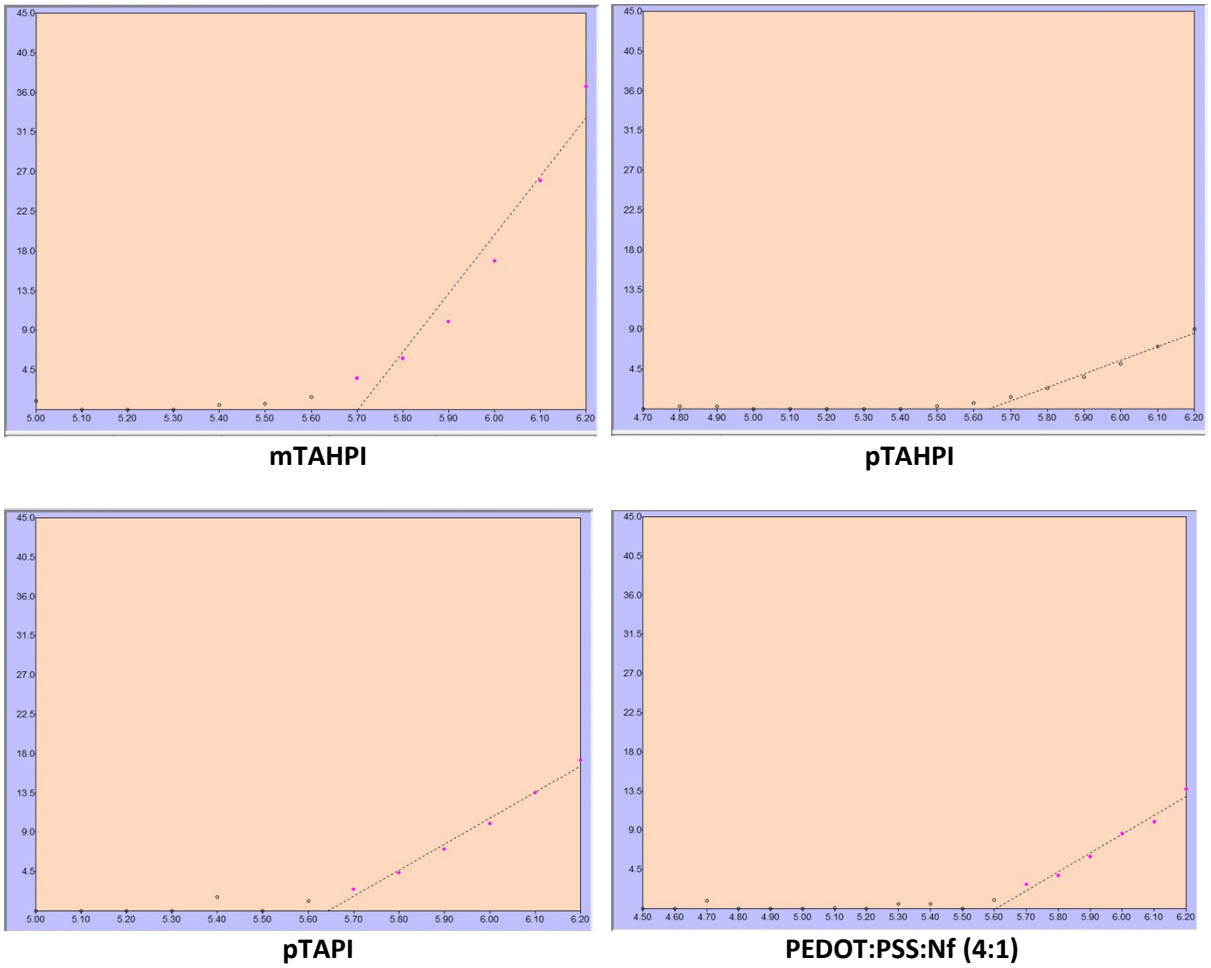


Fig. S4 Photoemission yield spectroscopy in air spectra (AC-2 plots) of **mTAHPI**, **pTAHPI**, **pTAPI** and **PEDOT:PSS:Nf (4:1)** thin films.

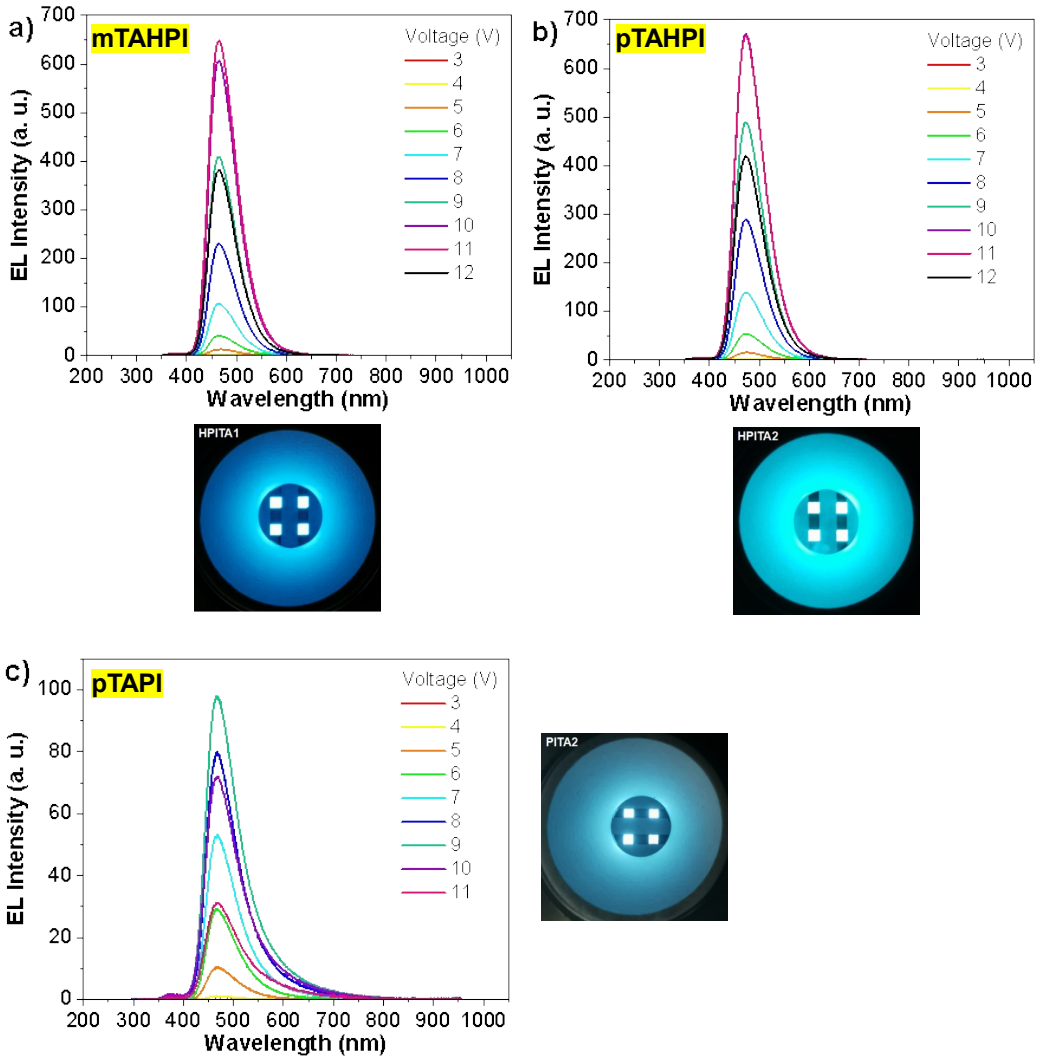


Fig. S4 EL spectra of the devices under different applied voltages (insert: images of blue OLEDs).

Table S2 Detailed data of **mTAHPI**, **pTAHPI** and **pTAPI** for fitting photophysical results in different solvents based on Lippert-Mataga equation.

For **mTAHPI**:

Solvent	ε	n	f(ε,n)	λ_{abs} (nm)	λ_{pl} (nm)	υ_a (cm^{-1})	υ_f (cm^{-1})	υ_a-υ_f (cm^{-1})
Hexane	1.9	1.3749	0.00126	366	439	27322.40437	22779.04328	4543.36109
Toluene	2.38	1.497	0.01321	368	452	27173.91304	22123.89381	5050.01924
1,4 Dioxane	2.25	1.422	0.02465	366	456	27322.40437	21929.82456	5392.57981
Chlorobenzene	5.62	1.5248	0.14294	368	465	27173.91304	21505.37634	5668.5367
Chloroform	4.81	1.4458	0.14829	366	470	27322.40437	21276.59574	6045.80863
Ethyl Ether	4.33	1.3524	0.16675	365	452	27397.26027	22123.89381	5273.36647
Ethyl Acetate	6.02	1.372	0.19978	366	468	27322.40437	21367.52137	5954.883
THF	7.58	1.407	0.20964	366	470	27322.40437	21276.59574	6045.80863
DCM	8.93	1.424	0.21717	366	490	27322.40437	20408.16327	6914.24111
DMF	36.7	1.4305	0.27438	366	521	27322.40437	19193.85797	8128.54641
Acetone	20.7	1.3587	0.28431	365	498	27397.26027	20080.32129	7316.93899
Acetonitrile	37.5	1.3441	0.30542	365	528	27397.26027	18939.39394	8457.86633

For **pTAHPI**:

Solvent	ε	n	f(ε,n)	λ_{abs} (nm)	λ_{pl} (nm)	υ_a (cm^{-1})	υ_f (cm^{-1})	υ_a-υ_f (cm^{-1})
Hexane	1.9	1.3749	0.00126	374	446	26737.96791	22421.52466	4316.44325
Toluene	2.38	1.497	0.01321	377	460	26525.19894	21739.13043	4786.0685
1,4 Dioxane	2.25	1.422	0.02465	376	462	26595.74468	21645.02165	4950.72304
Chlorobenzene	5.62	1.5248	0.14294	376	476	26595.74468	21008.40336	5587.34132
Chloroform	4.81	1.4458	0.14829	376	477	26595.74468	20964.36059	5631.38409
Ethyl Ether	4.33	1.3524	0.16675	373	459	26809.65147	21786.49237	5023.1591
Ethyl Acetate	6.02	1.3724	0.19964	374	476	26737.96791	21008.40336	5729.56455
THF	7.58	1.4072	0.20957	376	478	26595.74468	20920.50209	5675.24259
DCM	8.93	1.424	0.21717	375	496	26666.66667	20161.29032	6505.37634
DMF	36.7	1.4305	0.27438	376	536	26595.74468	18656.71642	7939.02826
Acetone	20.7	1.3587	0.28431	374	515	26737.96791	19417.47573	7320.49219
Acetone	37.5	1.3441	0.30542	374	541	26737.96791	18484.28835	8253.67956

For **pTAPI**:

Solvent	ε	n	f(ε,n)	λ_{abs} (nm)	λ_{pl} (nm)	υ_a (cm^{-1})	υ_f (cm^{-1})	υ_a-υ_f (cm^{-1})
Hexane	1.9	1.3749	0.00126	374	441	26737.96791	22675.73696	4062.23095
Toluene	2.38	1.497	0.01321	378	458	26455.02646	21834.06114	4620.96532
1,4 Dioxane	2.25	1.422	0.02465	376	464	26595.74468	21551.72414	5044.02054
Chlorobenzene	5.62	1.5248	0.14294	378	474	26455.02646	21097.04641	5357.98004
Chloroform	4.81	1.4458	0.14829	378	478	26455.02646	20920.50209	5534.52436
Ethyl Ether	4.33	1.3524	0.16675	374	457	26737.96791	21881.83807	4856.12984
Ethyl Acetate	6.02	1.372	0.19978	374	478	26737.96791	20920.50209	5817.46582
THF	7.58	1.407	0.20964	376	480	26595.74468	20833.33333	5762.41135
DCM	8.93	1.424	0.21717	377	500	26525.19894	20000	6525.19894
DMF	36.7	1.4305	0.27438	377	534	26525.19894	18726.59176	7798.60718
Acetone	20.7	1.3587	0.28431	375	513	26666.66667	19493.17739	7173.48928
Acetone	37.5	1.3441	0.30542	374	545	26737.96791	18348.62385	8389.34406

The dipole moment of ground state μ_g can be estimated by DFT calculation, and the the dipole moment of excited state are determined from the slope of linear fitted Stokes' shift (ν_a-ν_f) against orientation polarizability f(ε,n) in different solvents according to Lippert-Mataga equation.[1]

$$hc(\upsilon_a - \upsilon_f) = hc(\upsilon_a^0 - \upsilon_f^0) + \frac{2(\mu_e - \mu_g)^2}{a_0^3} f(\varepsilon, n),$$

$$f(\varepsilon, n) = \frac{\varepsilon - 1}{2\varepsilon + 1} + \frac{n^2 - 1}{2n^2 + 1},$$

Among which ε and n are dielectric constant and refractive index of solvent respectively, and a_0 is the solvent cavity radius

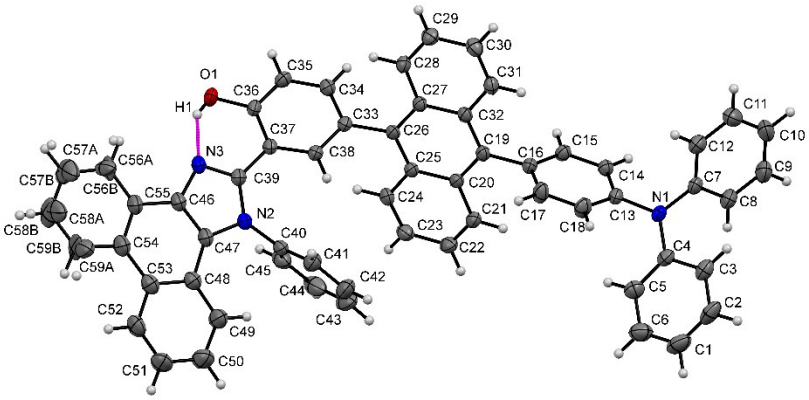
$$a_0 = \left(\frac{3M}{4N\pi d}\right)^{1/3},$$

where N is Avogadro number, M is molecular weight, and d is density. Two-region trends found in **mTAHPI**, **pTAHPI** and **pTAPI** are steady slopes of 4774, 5099, and 4854 for low-polar solvents and sharp slopes of 21838, 23295, and 23477 for high-polar solvents.

[1]C. Feng, J. Li, X. Han, X. He, L. Liu, X. Li, X. Sun, P. Lu and Y. Ma, *Faraday Discuss.* 2017, **196**, 163-176.

Table S3 Crystallographic data for **mTAHPI**.

Parameters	**mTAHPI**
Formula	$C_{59}H_{39}N_3O$
Formula Weight	805.93
Crystal System	triclinic
Space group	P-1
a [Å] b [Å] c [Å]	9.3925(5) 13.4585(7) 18.2373(9)
α [°] β [°] γ [°]	93.538(2) 95.122(2) 93.595(2)
V [Å^3]	2286.4(2)
Z	2
D(calc) [g/cm^3]	1.171
μ [mm^{-1}]	0.069
F (000)	844.0
Crystal Size [mm^3]	0.25 × 0.22 × 0.03
Temperature [K]	195
Radiation [Å]	MoKα (λ = 0.71073)
θ range [°]	4.364 to 52.04
Total no. of reflections	69877
Uniq. Data	9028
R_{int}	0.0624
Parameters	597
R	0.0448 [I>=2σ (I)], 0.0652 [all data]
wR2	0.1053 [I>=2σ (I)], 0.1142 [all data]
Goodness to fit	1.024
CCDC deposition number	2007054



Molecular structure of **mTAHPI** with 50% probability at 195 K. Intramolecular hydrogen bonding of O1—H1···N3 is highlighted.