Supporting Information

Deep-blue high-efficiency triplet-triplet annihilation organic light-emitting diodes using hydroxyl-substituted tetraphenylimidazole-functionalized anthracene fluorescent emitter

Wan Li,[a] Pongsakorn Chasing,[a] Phattananawee Nalaoh,[a] Thanyarat Chawanpunyawat,[a] Nuttapong Chantanop,[a] Chattarika Sukpattanacharoen,[b] Nawee Kungwan,[b] Praweena Wongkaew,[c] Taweesak Sudyoadsuk[a] and Vinich Promarak*[ac]

[a]*Department of Materials Science and Engineering, School of Molecular Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Wangchan, Rayong 21210, Thailand.*
E-mail: vinich.p@vistec.ac.th
[b]*Department of Chemistry, Faculty of Science, Chiang Mai University, Amphur Muang, Chiang Mai 50200, Thailand.*
[c]*Research Network of NANOTEC-VISTEC on Nanotechnology for Energy, Vidyasirimedhi Institute of Science and Technology, Wangchan, Rayong 21210, Thailand.*

Synthesis and characterization

9,10-Bis(4-bromophenyl)anthracene (2): A mixture of **1** (1.00 g, 2.32 mmol), 1-bromo-4-iodobenzene (1.51 g, 5.34 mmol), $Pd(PPh_3)_4$ (135 mg, 0.12 mmol), 2M sodium carbonate (4.90 g, 46.27 mmol) aqueous solution and anhydrous THF (40 mL)was degassed with nitrogen for 15 min while stirring. Then the stirring reaction was heated and refluxed under nitrogen atmosphere for 36 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 with brine (20 mL) and extracted with a certain amount of dichloromethane, then dried over anhydrous sodium sulfate and filtered. The extract was concentrated under reduced pressure and finally purified by silica gel column chromatography eluting with 10% v/v dichloromethane-hexane to get white solids (795 mg, 70%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.75 (d, J = 8.2 Hz, 4H), 7.67 (dd, J = 6.8, 3.3 Hz, 4H), 7.39-7.33 (m, 8H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 137.88, 136.00, 133.00, 131.74, 129.74, 126.69, 125.39, 121.86. HSMS (APCI): m/z calcd for $C_{26}H_{16}Br_2$ (M+): 487.9598, found: 489.0103 (MH+).

3-(4-(10-(4-Bromophenyl)anthracen-9-yl)phenyl)-9-phenyl-9H-carbazole (3): A mixture of **2** (2.50 g, 5.12 mmol), (9-phenyl-9H-carbazol-3-yl)boronic acid (490 mg, 1.71 mmol), $Pd(PPh_3)_4$ (39 mg, 0.03 mmol), 2M aqueous solution of sodium carbonate (10 mL) and anhydrous THF (40 mL) was degassed with nitrogen for 15 min while stirring. Then the stirring reaction was heated and refluxed under nitrogen atmosphere for 12 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 with brine (20 mL) and extracted with a certain amount of dichloromethane, then dried over anhydrous sodium sulfate and filtered. The extract was concentrated under reduced pressure and finally purified by silica gel column chromatography eluting with 10% v/v dichloromethane-hexane to get white solids (800 mg, 72%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.25 (d, J = 7.2 Hz, 1H), 7.97 (d, J = 8.4 Hz, 2H), 7.88-7.82 (m, 3H), 7.76 (d, J = 7.8 Hz, 2H), 7.70-7.67 (m, 2H), 7.67-7.63 (m, 4H), 7.59 (d, J = 7.8 Hz, 2H), 7.56 (d, J = 8.4 Hz, 1H), 7.53-7.50 (m, 1H), 7.48-

7.44 (m, 2H), 7.41-7.37 (m, 6H), 7.38 - 7.33 (m, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 139.55, 139.28, 138.67, 136.21, 135.81, 135.58, 135.19, 133.62, 131.19, 129.86, 129.81, 128.09, 128.07, 127.92, 125.69, 125.37, 125.33, 125.24, 124.69, 124.32, 123.59, 123.45, 123.22, 122.14, 121.65, 119.86, 118.49, 118.27, 117.00, 108.28, 108.11. HSMS (APCI): m/z calcd for $C_{44}H_{28}BrN$ (M+): 649.1405, found: 650.1385 (MH+).

9-Phenyl-3-(4-(10-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)anthracen-9-yl)phenyl)-9H-carbazole (4): A mixture of **3** (500 mg, 0.77 mmol), bis(pinacolato)diboron (587 mg, 2.31 mmol), KOAc (906 mg, 9.25 mmol), and $Pd(dppf)_2Cl_2{\cdot}CH_2Cl_2$ (31 mg, 0.32 mmol) were mixed followed by adding 30 mL 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 with brine (20 mL) and extracted with a certain amount of dichloromethane, then dried over anhydrous sodium sulfate and filtered. The extract was concentrated under reduced pressure and finally purified by silica gel column chromatography eluting with 30% v/v dichloromethane-hexane to get white solids (419 mg, 78%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.25 (d, J = 7.2 Hz, 1H), 8.07 (d, J = 7.2 Hz, 2H), 7.97 (d, J = 7.2 Hz, 2H), 7.88-7.82 (m, 3H), 7.71 (d, J = 8.4 Hz, 2H), 7.68-7.63 (m, 4H), 7.60 (d, J = 7.2 Hz, 2H), 7.57-7.49 (m, 4H), 7.48-7.43 (m, 2H), 7.35 (dt, J = 20.4, 6.6 Hz, 5H), 1.44 (s, 12H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.28, 141.46, 141.09, 140.56, 137.74, 137.28, 137.07, 137.01, 134.81, 133.16, 131.82, 130.84, 129.99, 129.96, 129.76, 127.57, 127.25, 127.14, 127.09, 126.97, 126.19, 125.51, 125.07, 125.04, 124.04, 123.57, 120.40, 120.16, 118.90, 110.17, 109.99, 83.97, 24.99. HSMS (APCI): m/z calcd for $C_{50}H_{40}BNO_2$ (M+): 697.3125, found: 698.2077 (MH+).

4-Bromo-2-(1,4,5-triphenyl-1H-imidazol-2-yl)phenol (6) & 2-(3-Bromophenyl)-1,4,5-triphenyl-1H-imidazole (7): A mixture of **5** (500 mg, 2.38 mmol) and 5-bromosalicylaldehyde (478 mg, 2.38 mmol) or 3-bromobenzaldehyde (440 mg, 2.38 mmol) were mixed at room temperature followed by adding 30 mL of acetic acid. Aniline of 1.022 g/mL (0.33 mL, 3.57 mmol or 0.33 mL, 3.60 mmol) was then added to this solution drop by drop, and ammonium acetate (917 mg, 11.9 mmol or 925 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 the reaction, the dark solution was poured into a copious amount of water in a 1000 mL beaker. Then a certain amount of sodium hydrogen carbonate was added to the mixture until neutralizing. The crude product was purified by recrystallization in dichloromethane.

6 as white solids (678 mg, 61%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.57-7.53 (m, 2H), 7.47-7.40 (m, 3H), 7.32-7.22 (m, 7H), 7.22-7.14 (m, 5H), 6.98 (d, J = 8.4 Hz, 1H), 6.62 (s, 1H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 157.39, 143.44, 136.23, 134.83, 132.91, 132.05, 131.27, 130.80, 129.80, 129.67, 129.12, 129.01, 128.78, 128.60, 128.43, 128.42, 127.48, 127.10, 119.57, 114.22, 109.76. HSMS (APCI): m/z calcd for $C_{27}H_{19}BrN_2O$ (M+): 466.0681, found: 467.0786 (MH+).

7 as white solids (848 mg, 79%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.72 (s, 1H), 7.59 (d, J = 7.2 Hz, 2H), 7.39 (d, J = 7.8 Hz, 1H), 7.35-7.18 (m, 10H), 7.13 (d, J = 7.2 Hz, 2H), 7.08-7.02 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 145.27, 138.58, 136.81, 134.23, 132.49, 131.92, 131.33, 131.21, 131.10, 130.39, 129.47, 129.25, 128.58, 128.40, 128.38, 128.22, 128.12, 127.38, 127.17, 126.76, 122.29. HSMS (APCI): m/z calcd for $C_{27}H_{19}BrN_2$ (M+): 450.0732, found: 451.0560 (MH+).

All crystallographic information (CIF) data including CCDC numbers of 2017513 and 2051106 for HO-PIAC and PIAC, respectively, were deposited on and can be obtained with no cost at https://www.ccdc.cam.ac.uk/.

Table S1. Crystallographic data

Compound name	**HO-PIAC**	**PIAC**
CCDC number	2017513	2051106
Empirical formula	$C_{72}H_{48}Cl_3N_3O$	$C_{71}H_{47}N_3$
Formula weight	1077.48	942.11
Temperature/K	100	100
Crystal system	triclinic	monoclinic
Space group	*P-1*	*C2/c*
a/Å b/Å c/Å	9.8323(5) 15.2021(8) 19.9693(11)	41.3796(13) 8.3576(3) 30.6626(9)
α/° β/° γ/°	71.560(2) 88.608(2) 74.215(2)	90 100.697(2) 90
Volume/Å^3	2718.6(3)	10419.9(6)
Z	2	8
ρ_{calc}/g/cm^3	1.316	1.201
μ/mm^{-1}	0.219	0.532
F(000)	1120.0	3952.0
Crystal size/mm^3	0.42 × 0.05 × 0.02	0.57 × 0.23 × 0.09
Radiation	MoKα (λ = 0.71073)	CuKα (λ = 1.54178)
2Θ range for data collection/°	4.168 to 52.21	4.346 to 136.472
Index ranges	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -24 ≤ l ≤ 24	-49 ≤ h ≤ 49, -9 ≤ k ≤ 10, -32 ≤ l ≤ 36
Reflections collected	83699	61803
Independent reflections	10787 [R_{int} = 0.1341, R_{sigma} = 0.0750]	9533 [R_{int} = 0.0856, R_{sigma} = 0.0432]
Data/restraints/parameters	10787/0/717	9533/0/667
Goodness-of-fit on F^2	1.040	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0690, wR_2 = 0.1461	R_1 = 0.0531, wR_2 = 0.1340
Final R indexes [all data]	R_1 = 0.1352, wR_2 = 0.1719	R_1 = 0.0687, wR_2 = 0.1432
Largest diff. peak/hole / e Å^{-3}	0.64/-0.60	0.66/-0.35

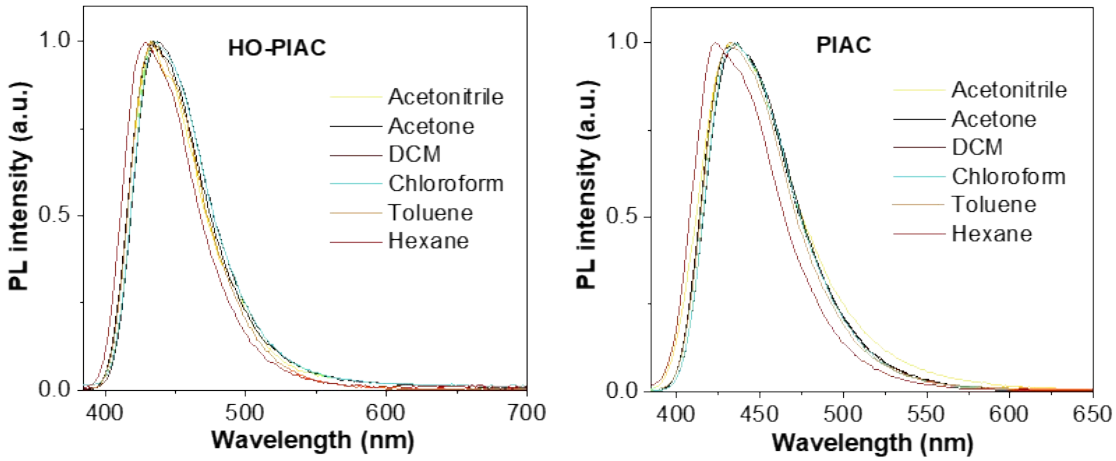

Fig .S1 Normalized PL spectra in varying solvents.

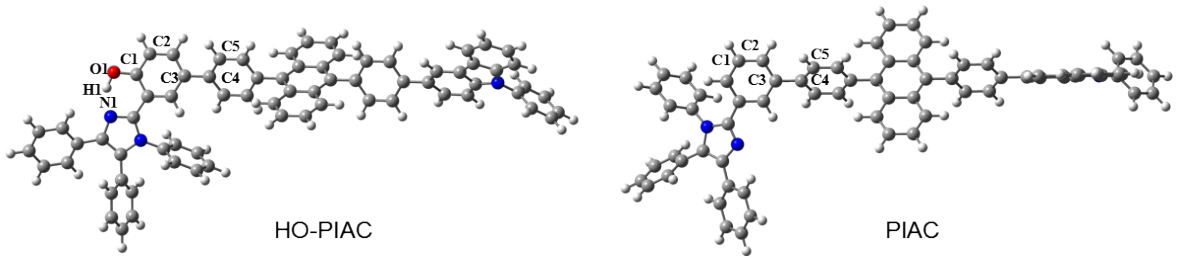

Fig. S2 S_0 optimized geometries of enol forms computed at B3LYP/6-31G(d,p) level.

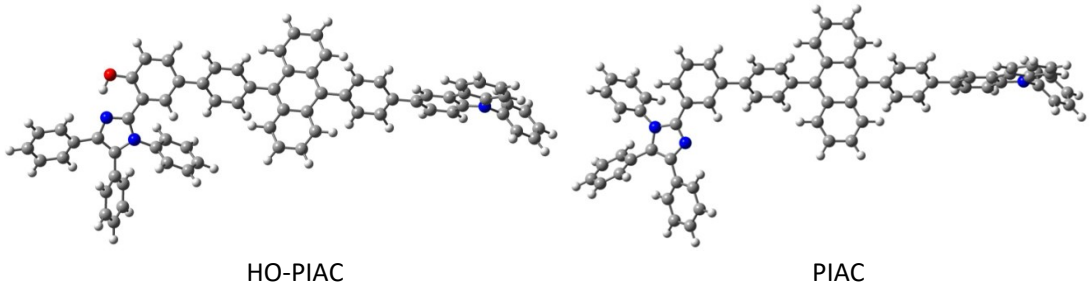

Fig. S3 S_1 optimized geometries of enol forms computed at B3LYP/6-31G(d,p) level.

Table S2 Summary of relative proton transfer barriers and computed energy differences between the enol and keto forms ($\Delta E=E_{keto} - E_{enol}$) between S_0 and S_1 computed at B3LYP/ 6-31G(d,p) level.

Molecule	PT barrier (kcal/mol)		ΔE (kcal/mol)	
	S_0	S_1	S_0	S_1
HO-PIAC	11.75	5.93	10.62	4.04

Table S3 Selected bond lengths (Å) and torsional angles (°) at S_0 and S_1 optimized geometries computed at B3LYP/6-31G(d,p) and TD-B3LYP/6-31G(d,p) levels, respectively.

Molecule	State	Enol form				Keto form			
		Distance (Å)			Torsional angle (°)	Distance (Å)			Torsional angle (°)
		O1-H1	N1···H1	C3-C4	C2C3C4C5	O1···H1	N1-H1	C3-C4	C2C3C4C5
HO-PIAC	S_0	0.996	1.697	1.483	36.06	1.552	1.035	1.480	33.46
	S_1	0.999	1.681	1.473	28.92	1.695	1.035	1.467	29.02
PIAC	S_0	-	-	1.485	36.48	-	-	-	-
	S_1	-	-	1.479	30.96	-	-	-	-

Table S4 Simulated enol absorption maximum wavelengths (λ_{abs}), enol and keto emission maximum wavelengths (λ_{em}), oscillator strength (f), molecular orbitals (MOs) contribution, and Stokes shift calculated by TD-B3LYP/6-31G(d,p) level.

	Absorption			Emission		Stokes shift (nm)
	Enol			Enol	Keto	
	λ_{abs} (nm)	f	MOs Contribution	λ_{em} (nm)	λ_{em} (nm)	
HO-PIAC	399	0.3927	HOMO → LUMO (97%)	499	549	150
PIAC	396	0.3582	HOMO → LUMO (97%)	494	-	98

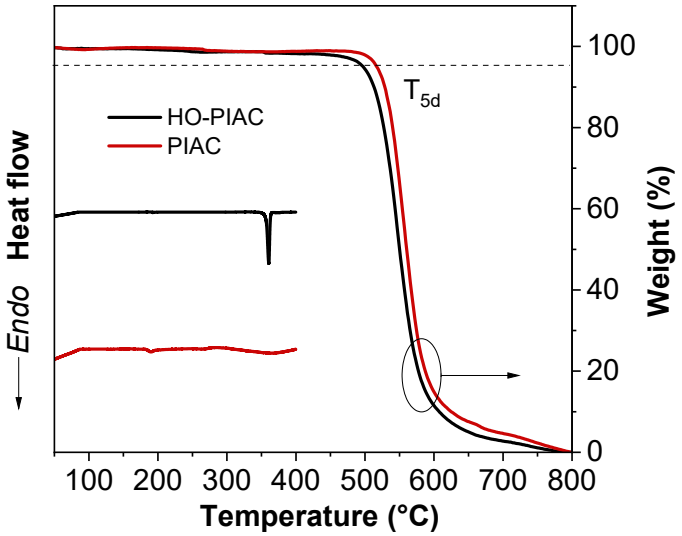

Fig. S4 DSC and TGA thermograms analyzed at a heating rate of 10°C min^{-1} under N_2 flow.

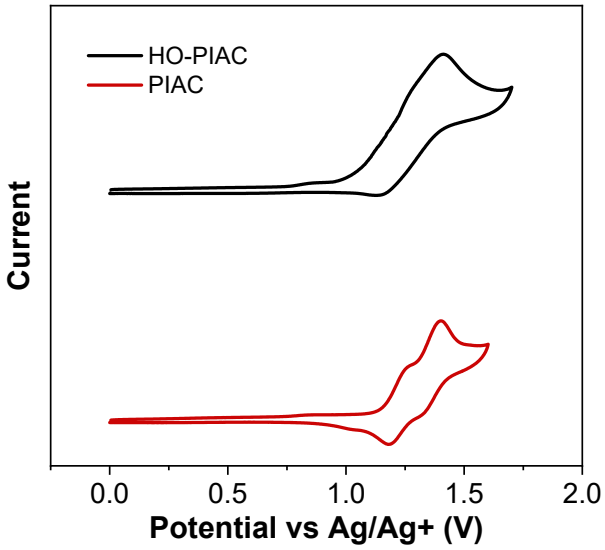

Fig. S5 Cyclic voltammograms recorded in dry dichloromethane containing *n*-Bu_4NPF_6 at a scan rate of 50 mV s^{-1} under argon atmosphere.

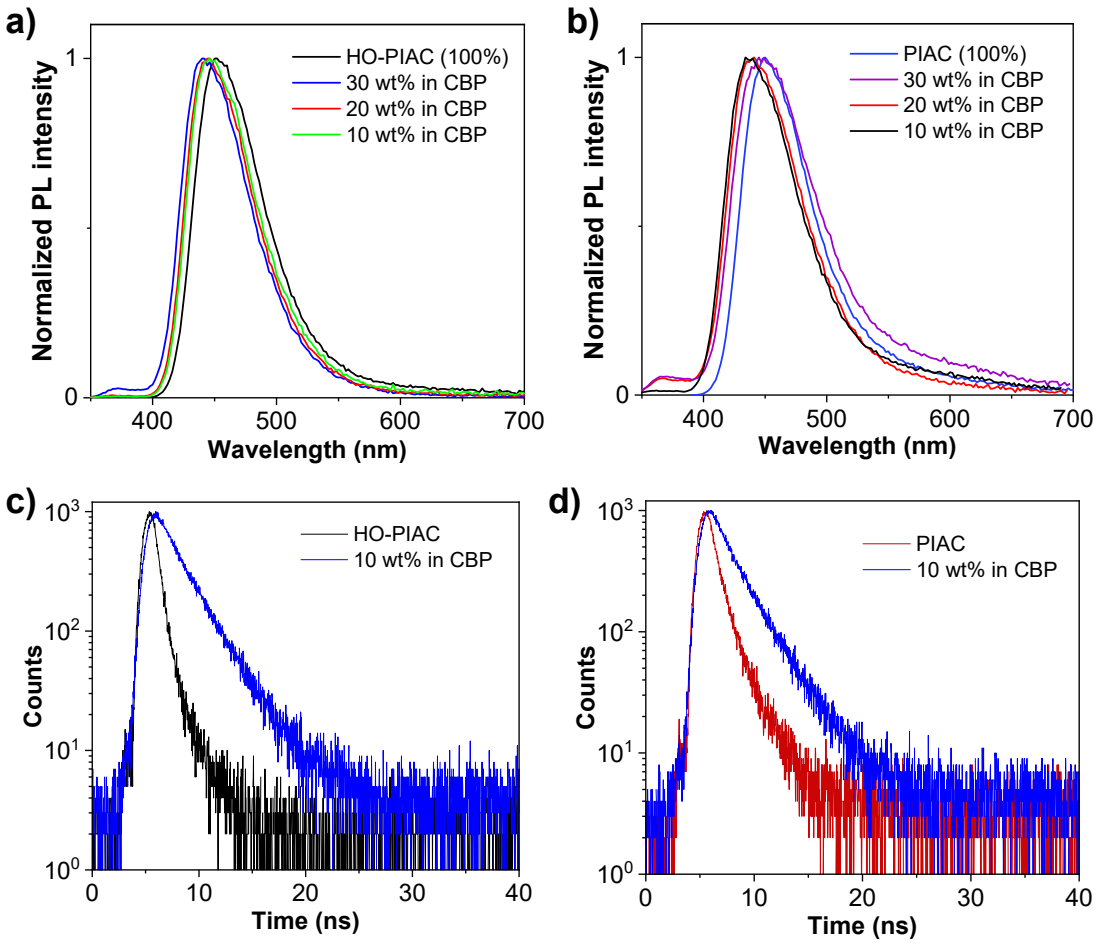

Fig. S6 a) and b) PL spectra and c) and d) transient PL decay spectra in neat films and doped (10, 20, 30 wt% doped CBP thin films.

Table S5 Photoluminescent properties of doped films in various conditions.

	HO-PIAC (doped in CBP)		PIAC (doped in CBP)	
	neat	10%	neat	10%
λ_{em} (nm)	451	441	450	437
τ (ns)	0.70	2.62	1.21	2.54
Φ_{PL} (%)	19	56	40	57

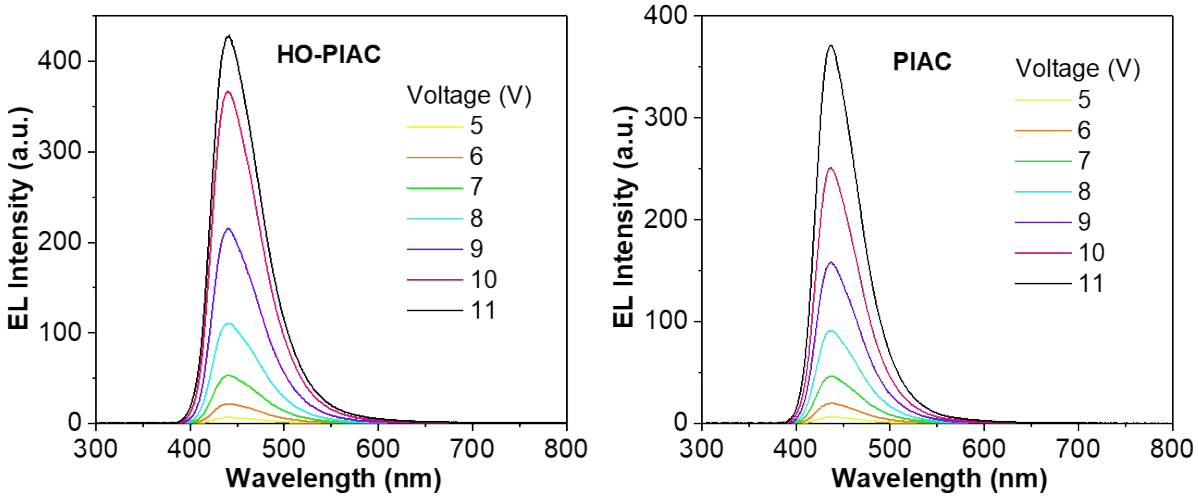

Fig. S7 EL spectra of OLEDs at different applied voltages.

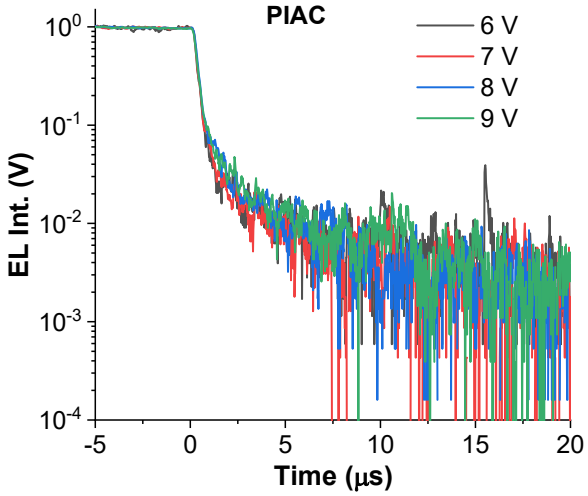

Fig. S8 Transient EL decay of OLED device based on PIAC at different voltages.

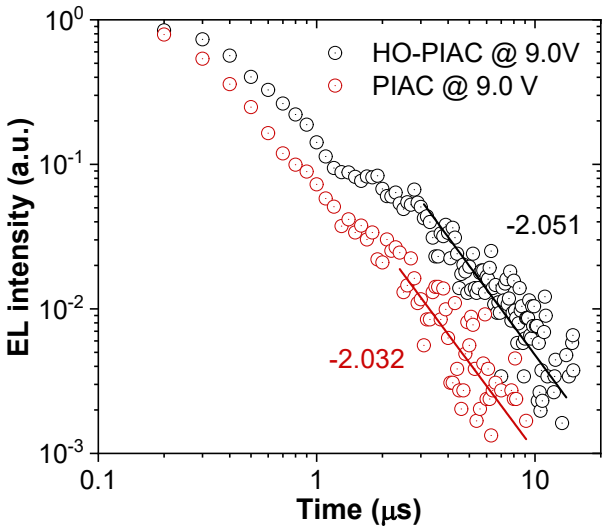

Fig. S9 Amplified transient EL decay plots of the delayed component at a driving voltage of 10 V.

Fig. S10 Photocopies of Mass spectra, ^{1}H-NMR, and ^{13}C-NMR spectra.

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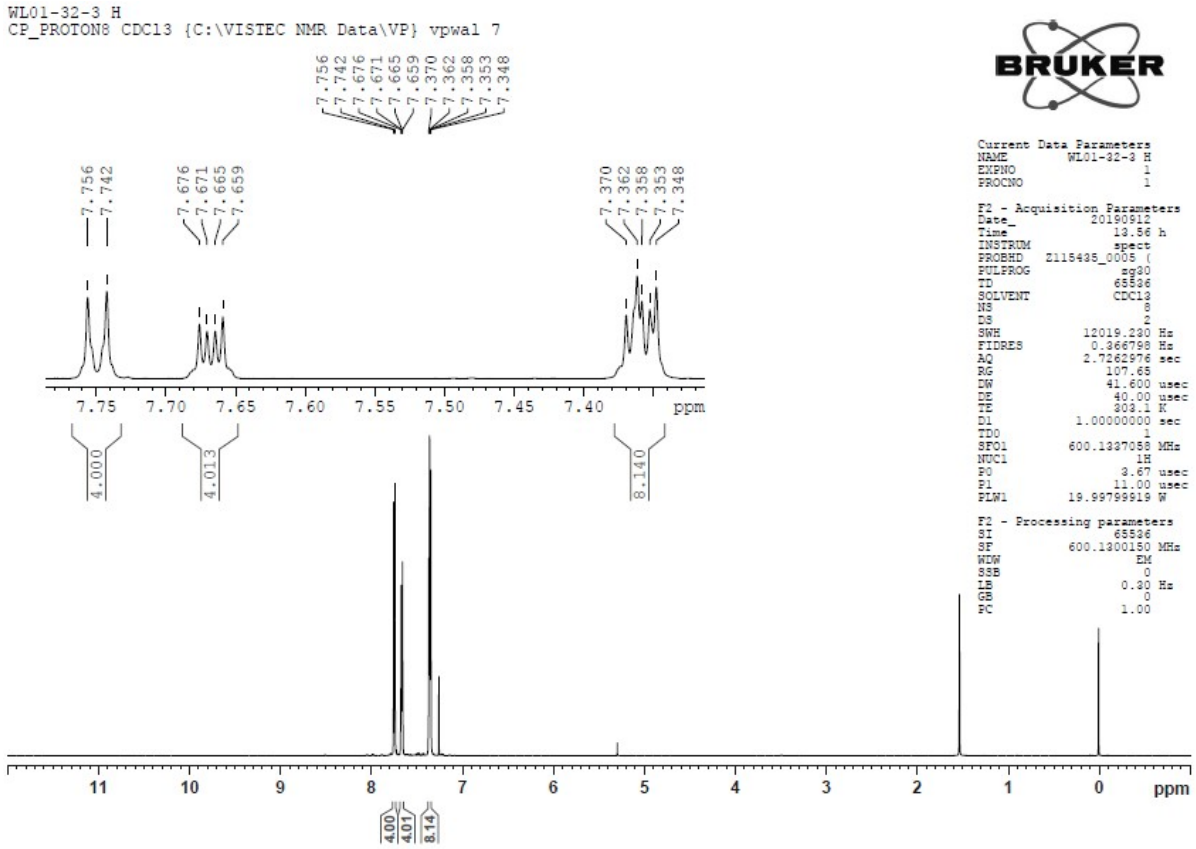

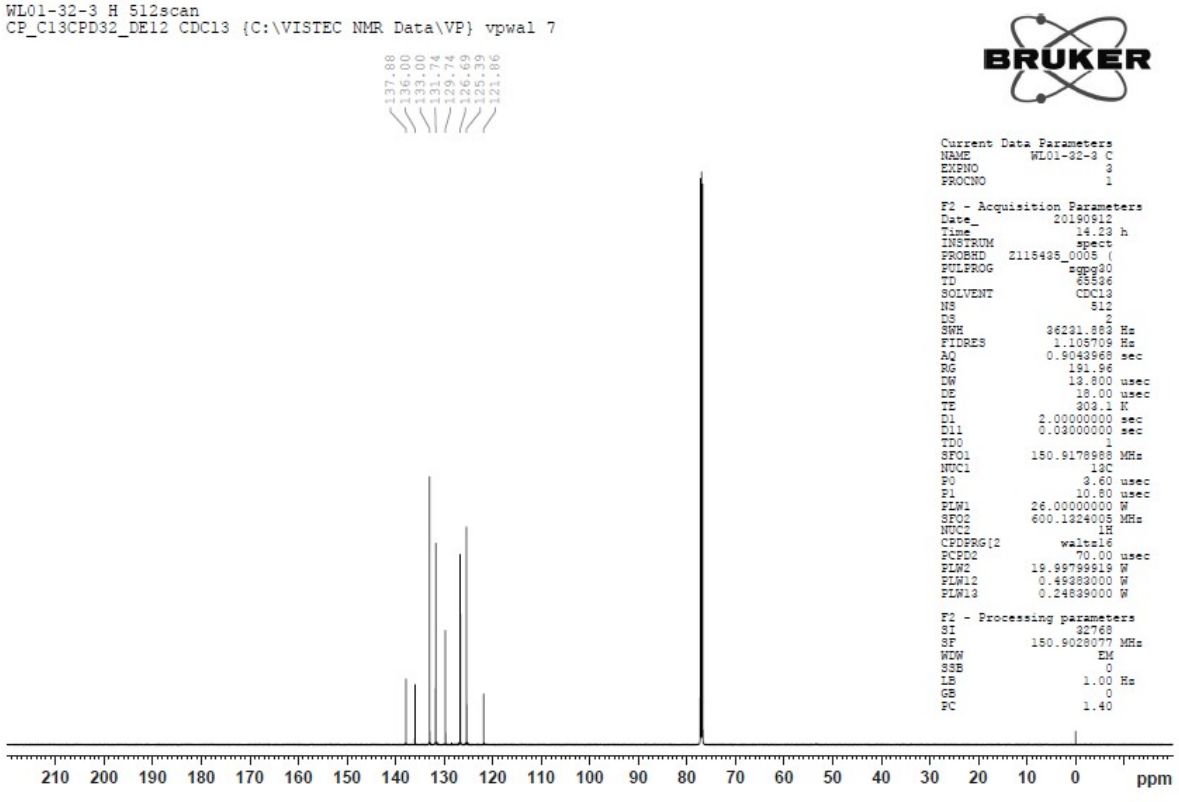

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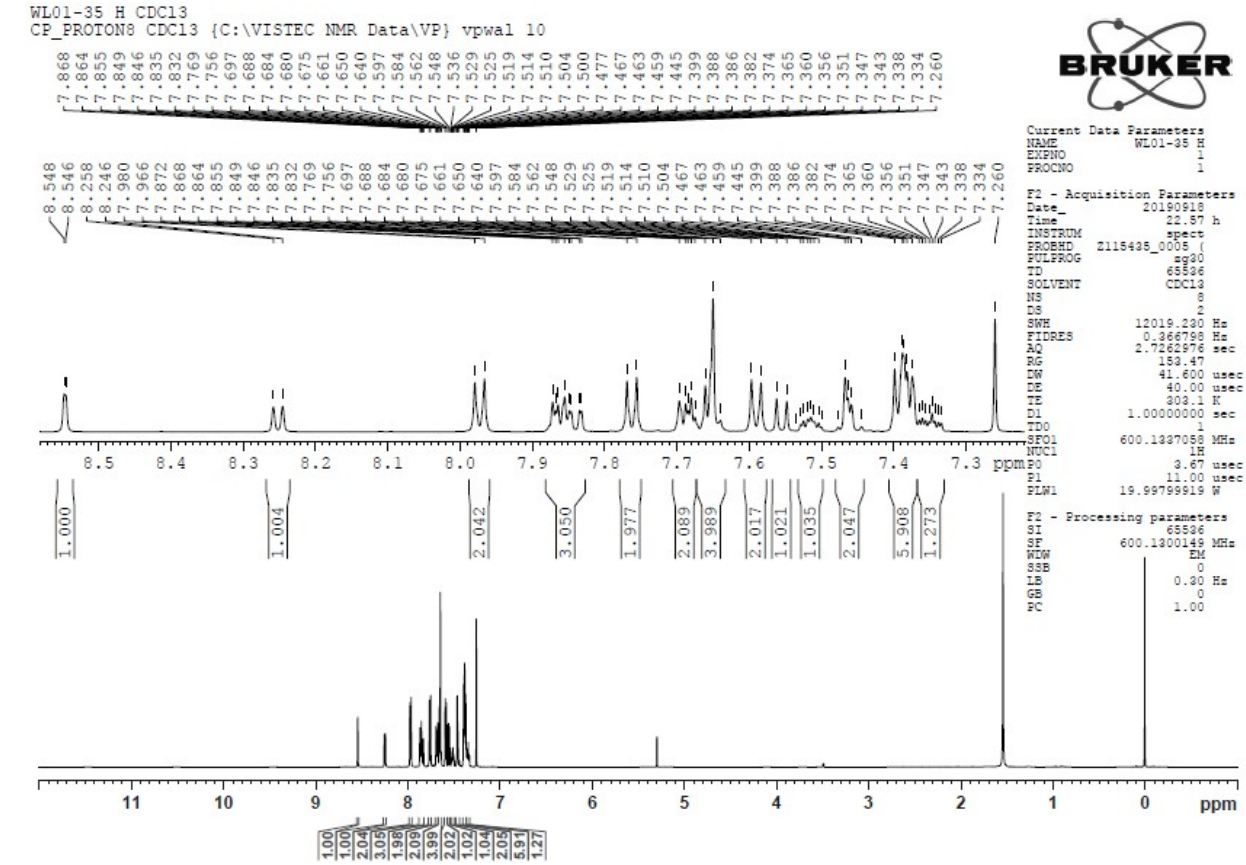
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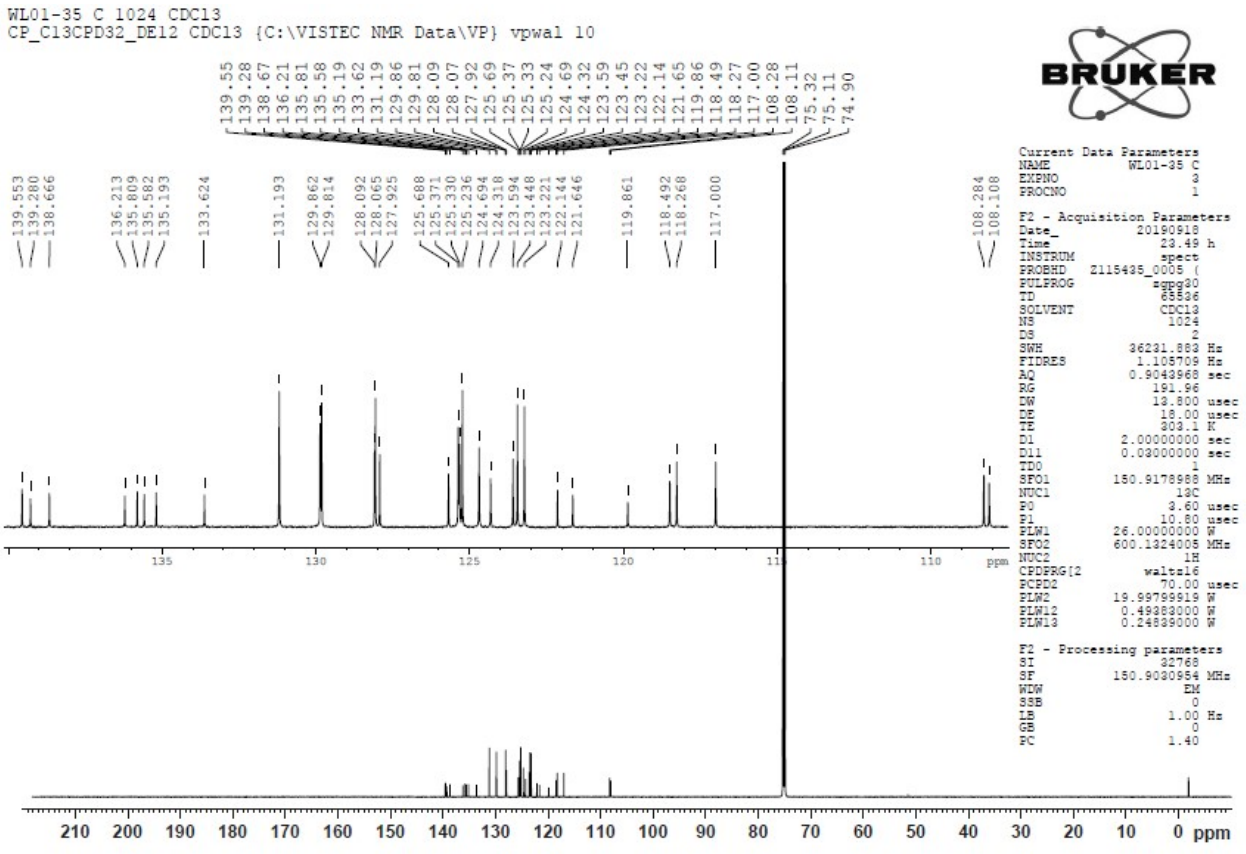
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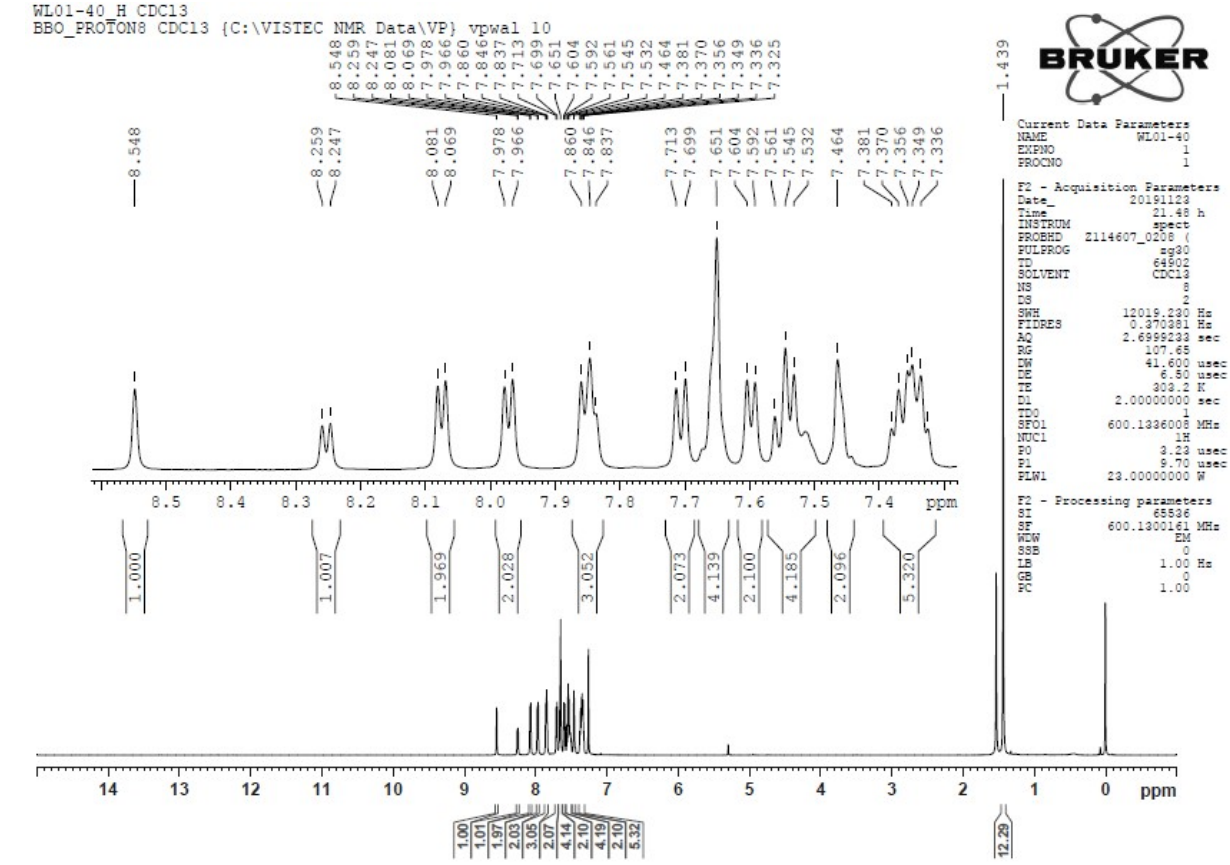
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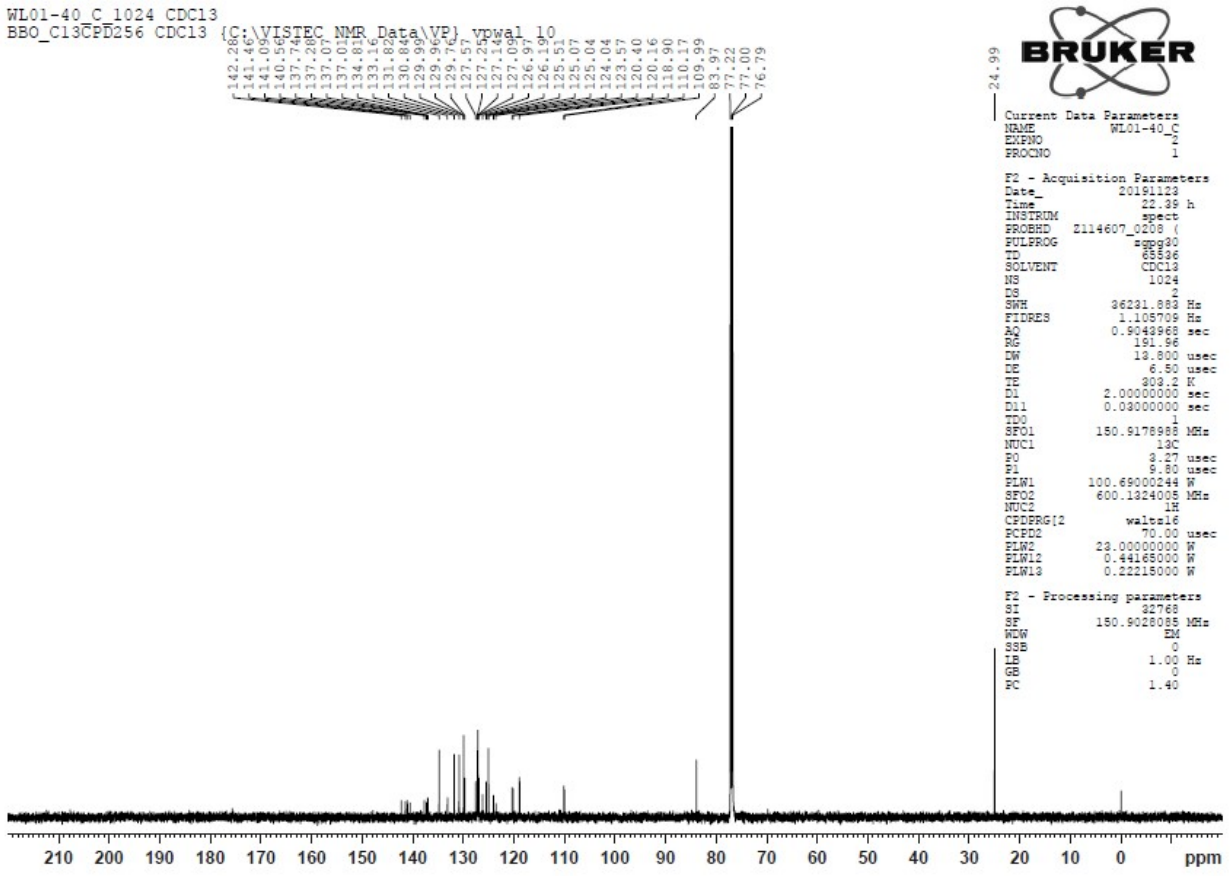
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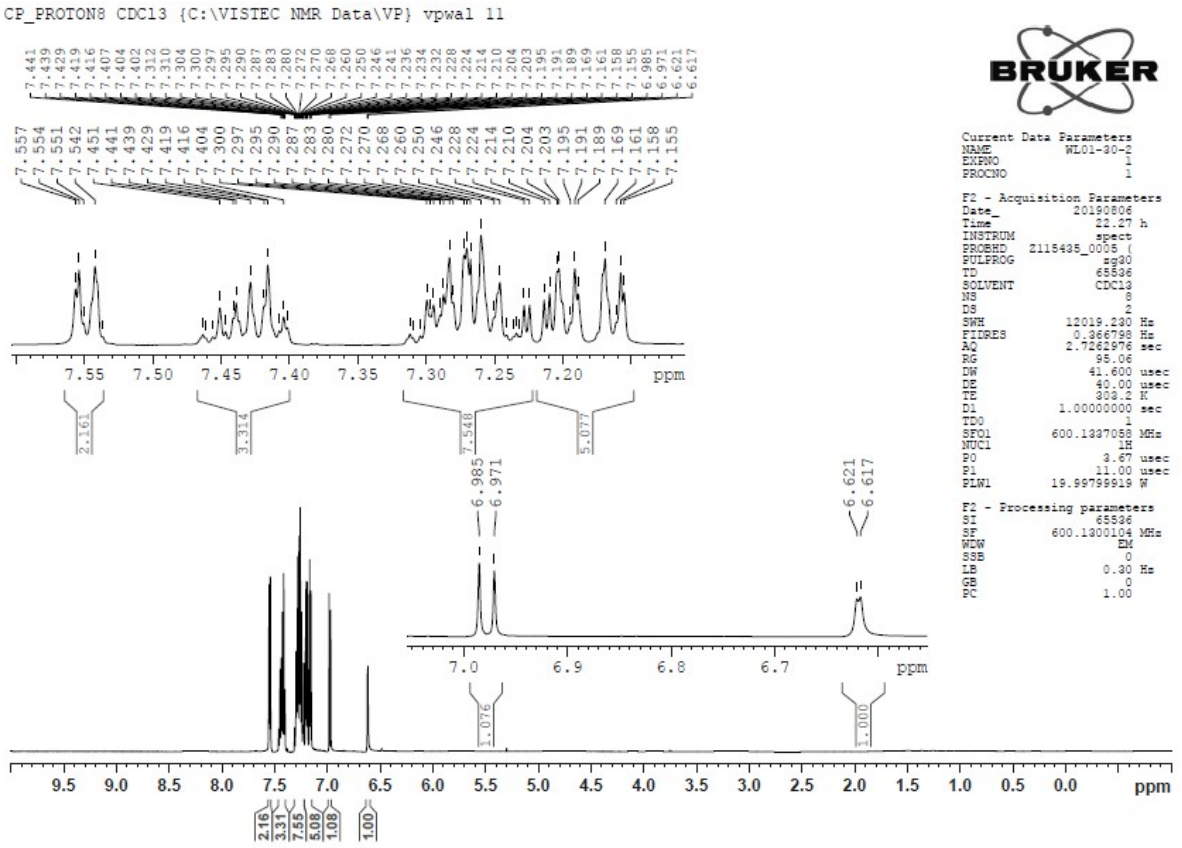
Compound 6: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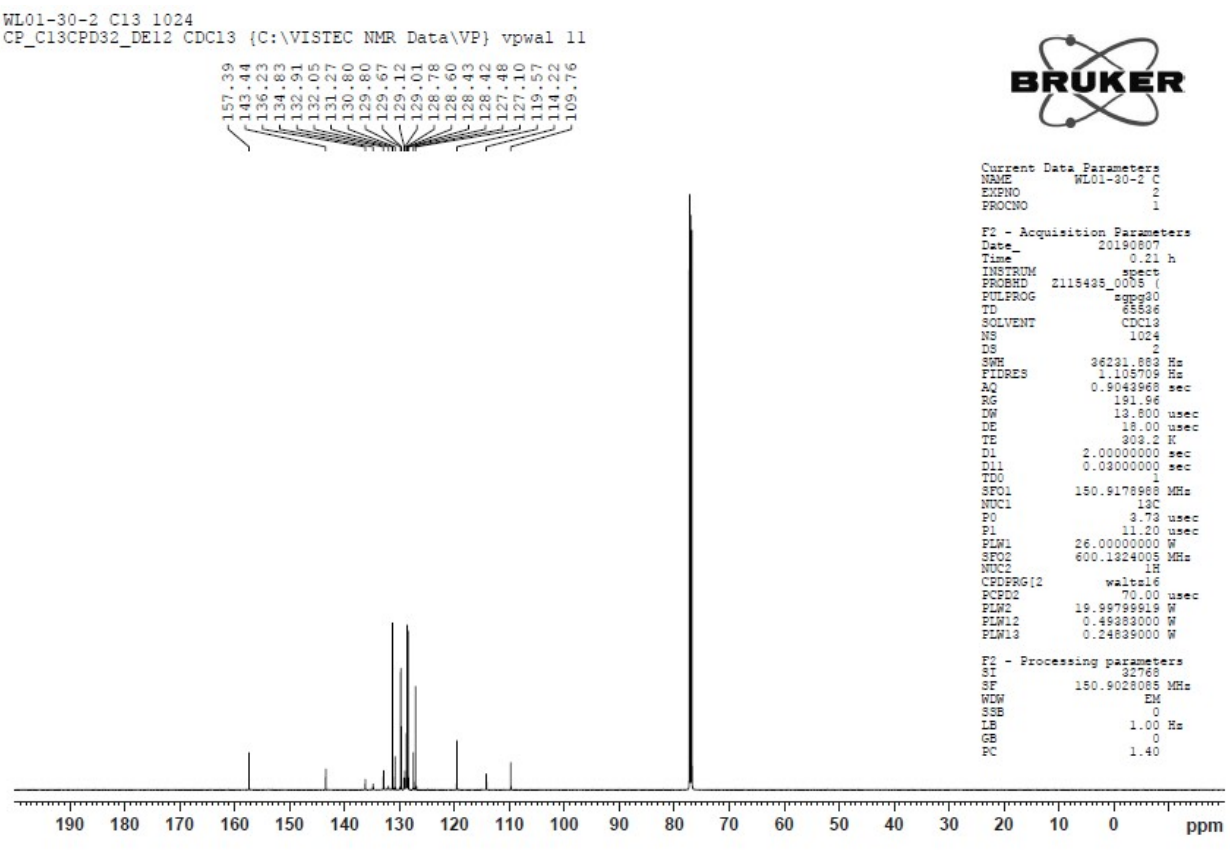
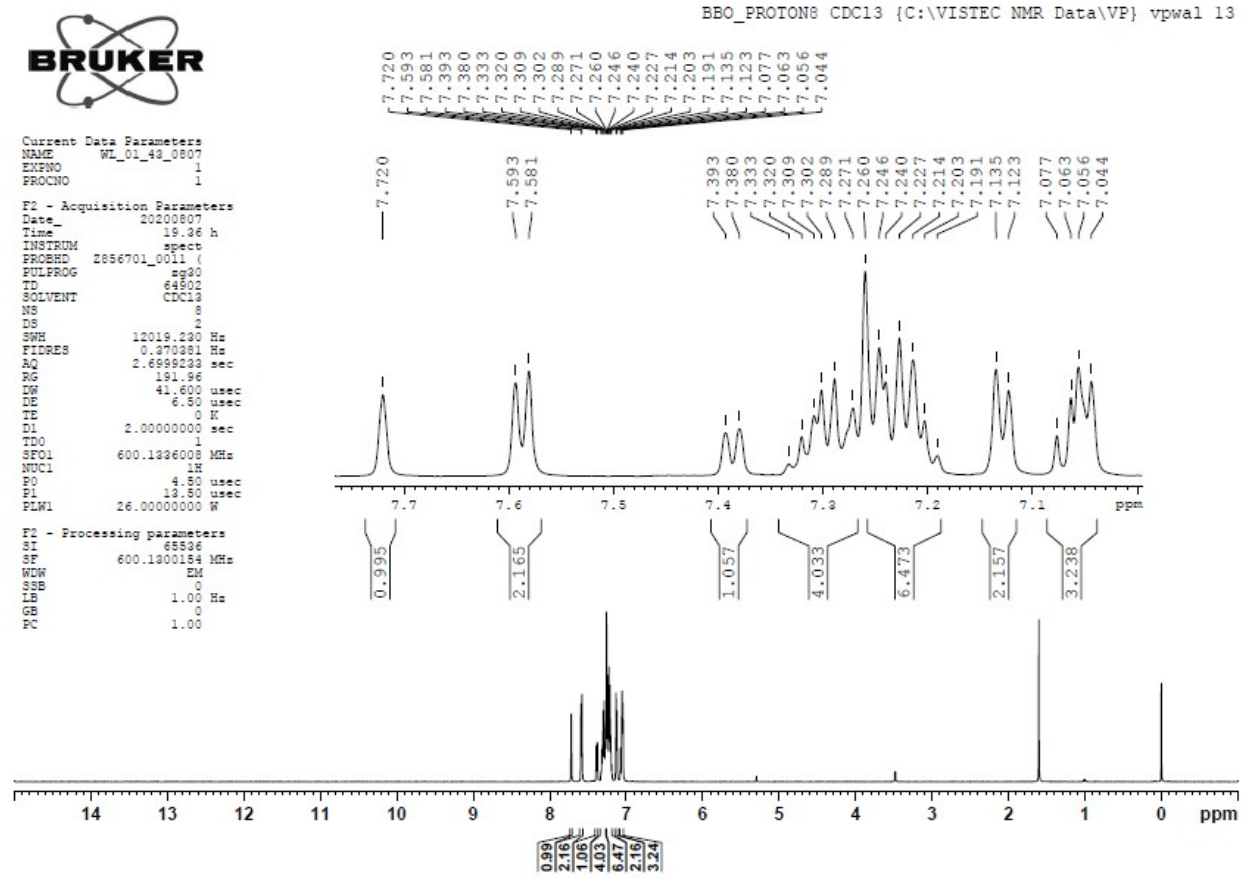
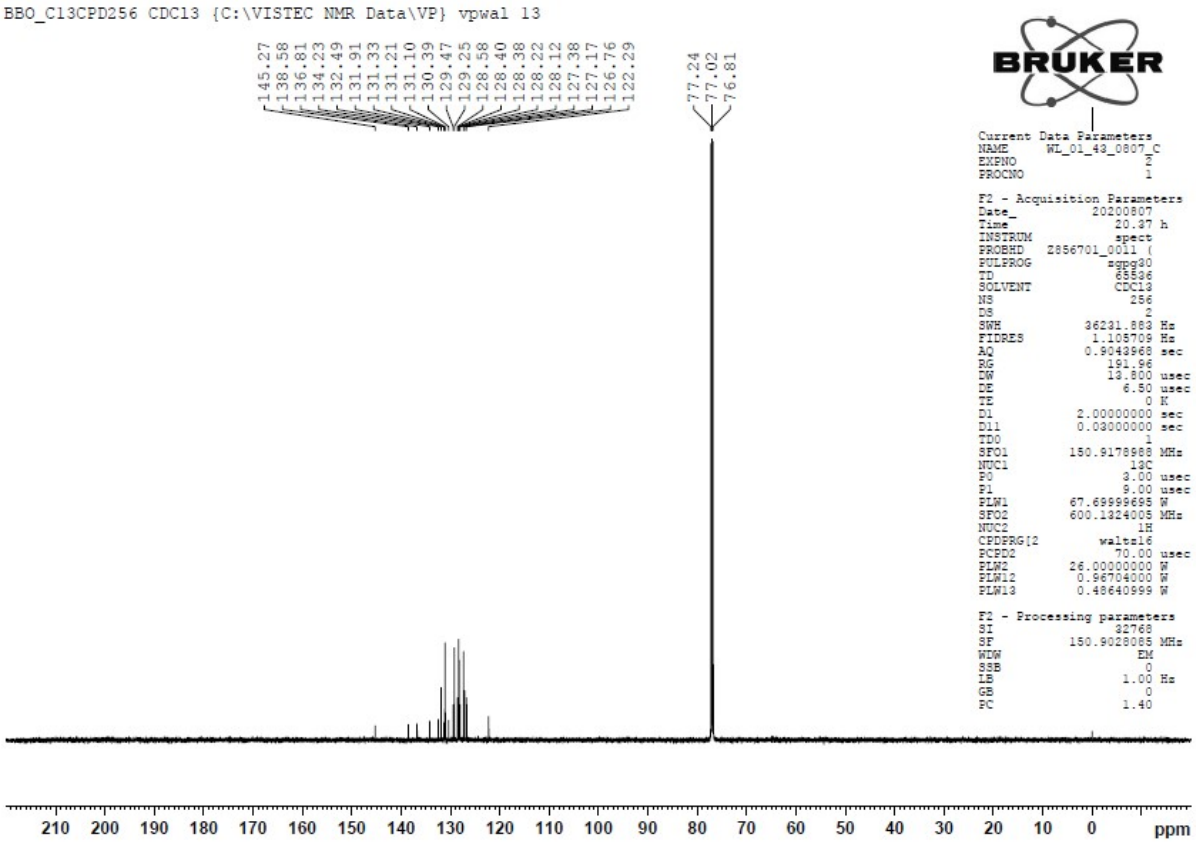
DW 41.600 usec
DE 40.00 usec
TE 303.2 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.67 usec
P1 11.00 usec
PLW1 19.99799919 W
F2 - Processing parameters
SI 65536
SF 600.1300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm


WL01-30-2 C13 1024
CP_C13CPD32_DE12 CDCl3 {C:\VISTEC NMR Data\VP} vpwal 11
BRUKER
Current Data Parameters
NAME WL01-30-2 C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190807
Time 0.21 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 18.00 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178968 MHz
NUC1 13C
P0 9.73 usec
P1 11.20 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 19.99799919 W
PLW12 0.49383000 W
PLW13 0.24839000 W
F2 - Processing parameters
SI 32768
SF 150.9028065 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

Compound 7:


BBO_PROTON8 CDC13 {C:\VISTEC NMR Data\VP} vpwal 13
Current Data Parameters
NAME WL_01_43_0807
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200807
Time 19.36 h
INSTRUM spect
PROBHD Z856701_0011 (
PULPROG zg30
TD 64902
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.370381 Hz
AQ 2.6999233 sec
RG 191.96
DW 41.600 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
TD0 1
SFO1 600.1336008 MHz
NUC1 1H
P0 4.50 usec
P1 13.50 usec
PLW1 26.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300154 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
7.720
7.593
7.581
7.393
7.380
7.333
7.320
7.309
7.302
7.289
7.271
7.260
7.246
7.240
7.227
7.214
7.203
7.191
7.135
7.123
7.077
7.063
7.056
7.044
0.99
2.16
1.06
4.03
6.47
2.16
3.24
ppm


BBO_C13CPD256 CDC13 {C:\VISTEC NMR Data\VP} vpwal 13
145.27
138.58
136.81
134.23
132.49
131.91
131.33
131.21
131.10
130.39
129.47
129.25
128.58
128.40
128.38
128.22
128.12
127.38
127.17
126.76
122.29
77.24
77.02
76.81
Current Data Parameters
NAME WL_01_43_0807_C
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200807
Time 20.97 h
INSTRUM spect
PROBHD Z856701_0011 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 6.50 usec
TE 0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P0 3.00 usec
P1 9.00 usec
PLW1 67.69999695 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 26.00000000 W
PLW12 0.96704000 W
PLW13 0.48640999 W
F2 - Processing parameters
SI 32768
SF 150.9028086 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

HO-PIAC:

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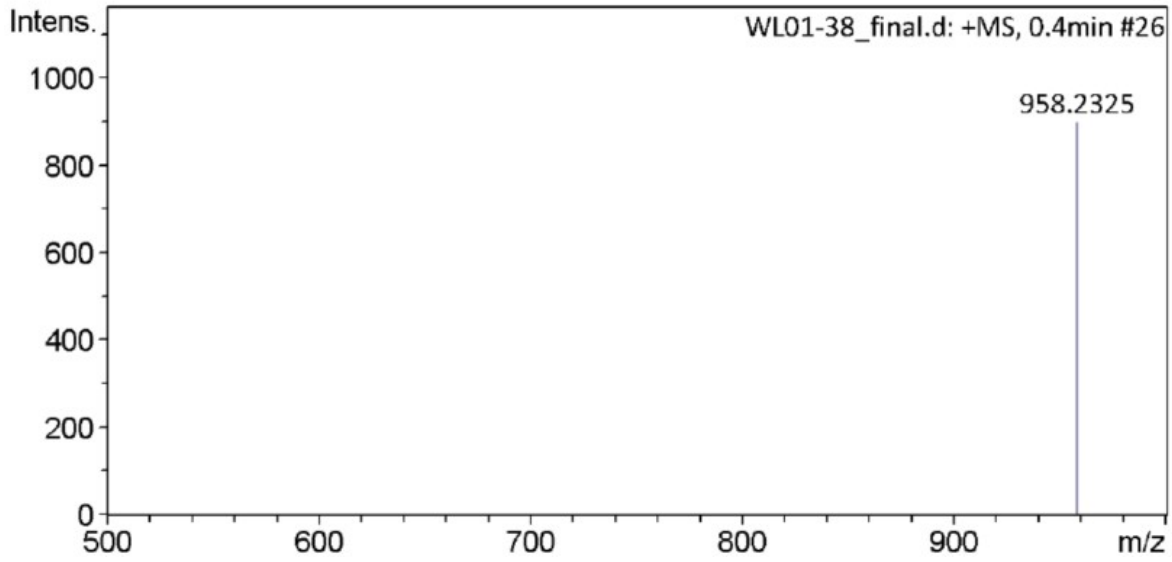
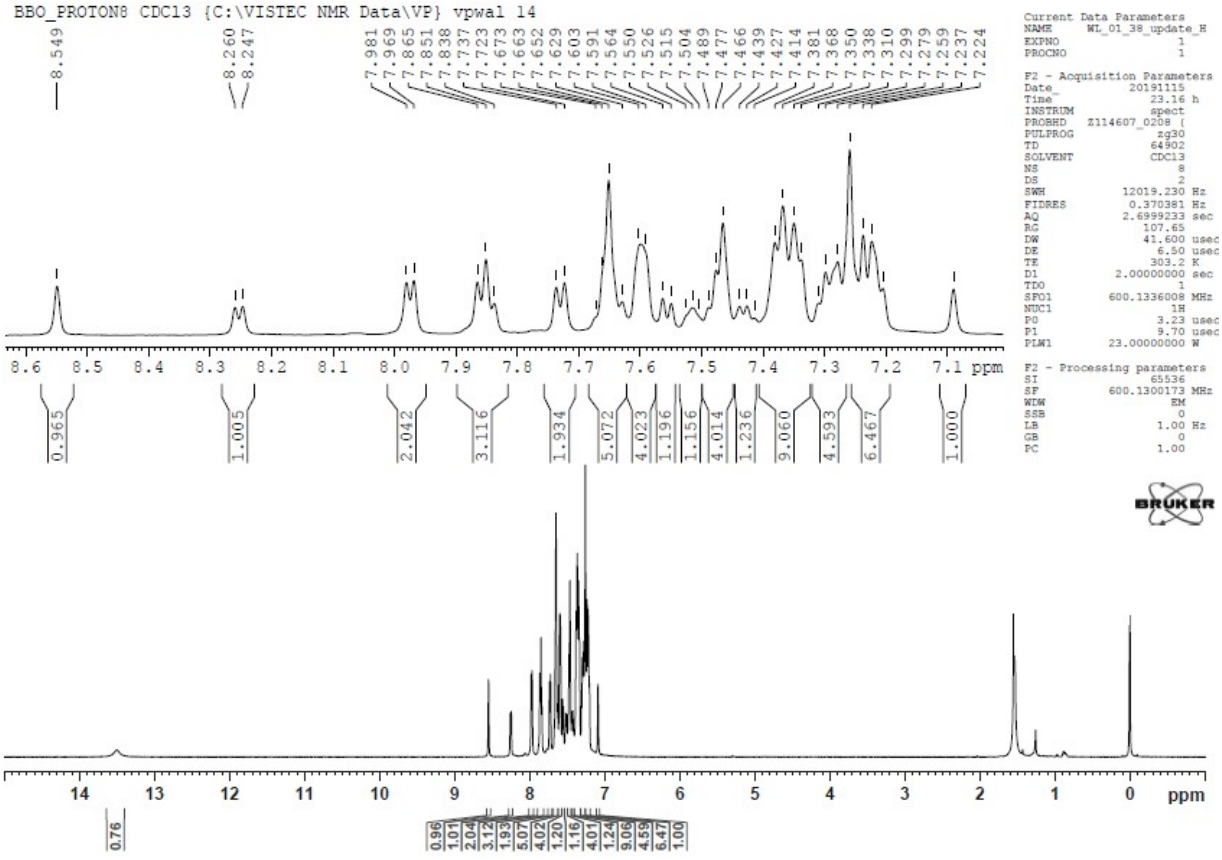
Analysis Info

Analysis Name	D:\Data\VISTEC Data QTOF\Vinich\Li Wan\WL01-38_final.d	Acquisition Date	11/19/2019 7:26:07 PM
Method	APCI_DirectProbe.m	Operator	VISTEC
Sample Name	WL01-38_final	Instrument	compact 8255754.20068
Comment	m/z957.37		



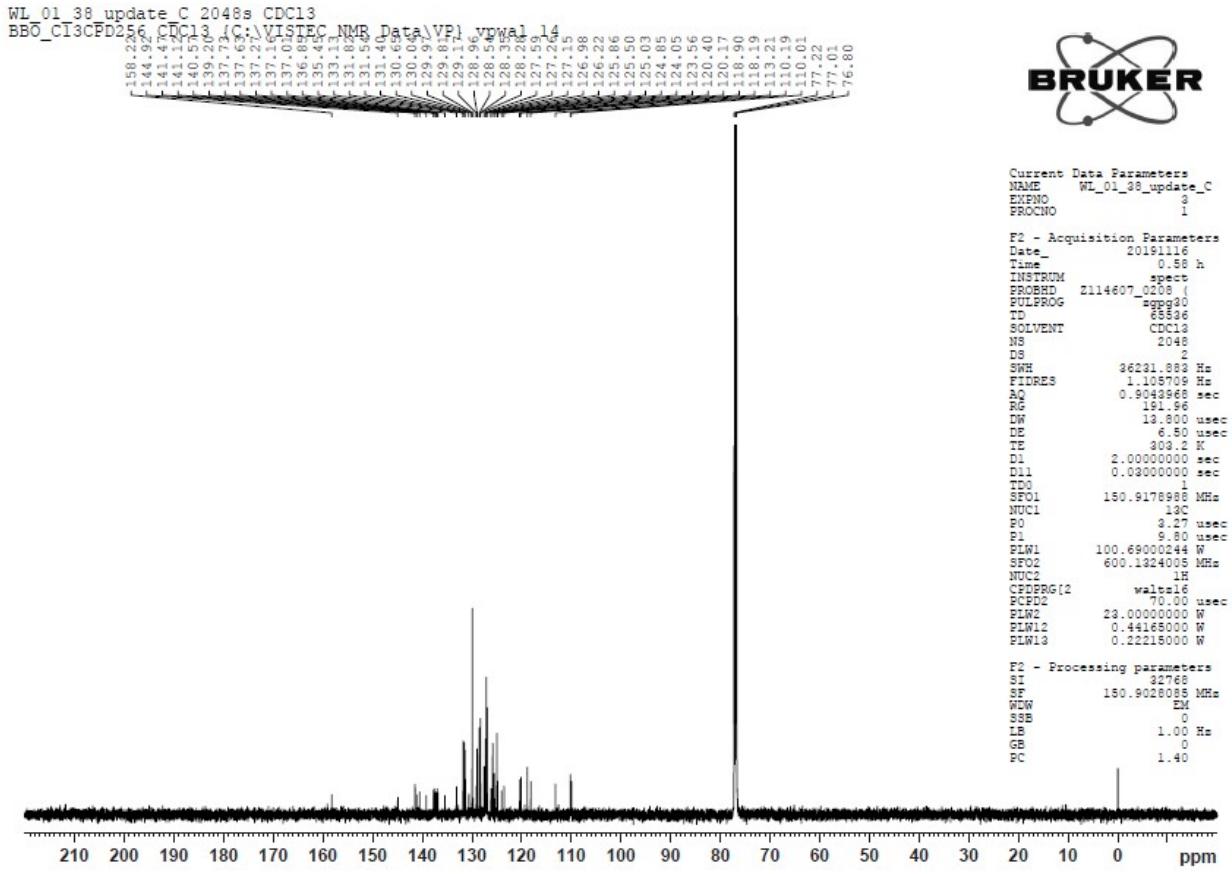


Current Data Parameters
NAME WL_01_38_update_H
EXPNO 1
PROCNO 1

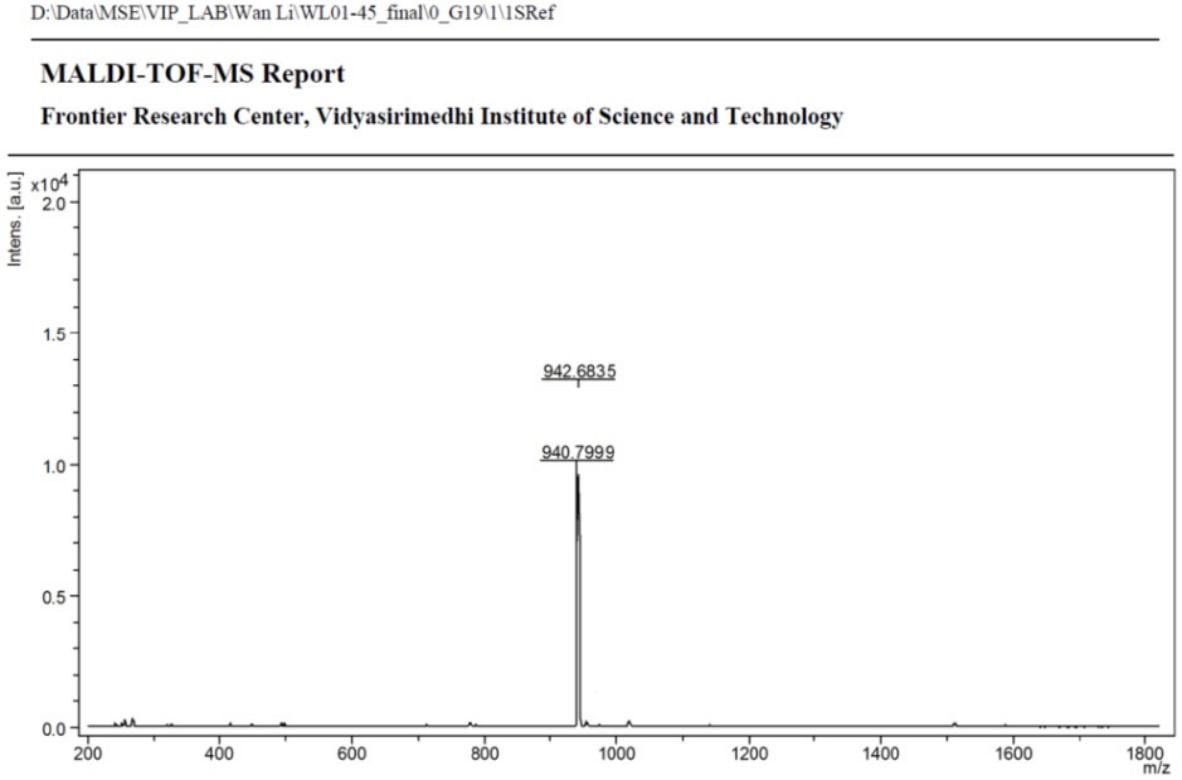
F2 - Acquisition Parameters
Date_ 20191115
Time 23.16 h
INSTRUM spect
PROBHD Z114607_0208 (
PULPROG zg30
TD 64902
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.370381 Hz
AQ 2.6999233 sec
RG 107.65
DW 41.600 usec
DE 6.50 usec
TE 303.2 K
D1 2.00000000 sec
TD0 1
SFO1 600.1336008 MHz
NUC1 1H
P0 3.23 usec
P1 9.70 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 600.1300173 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

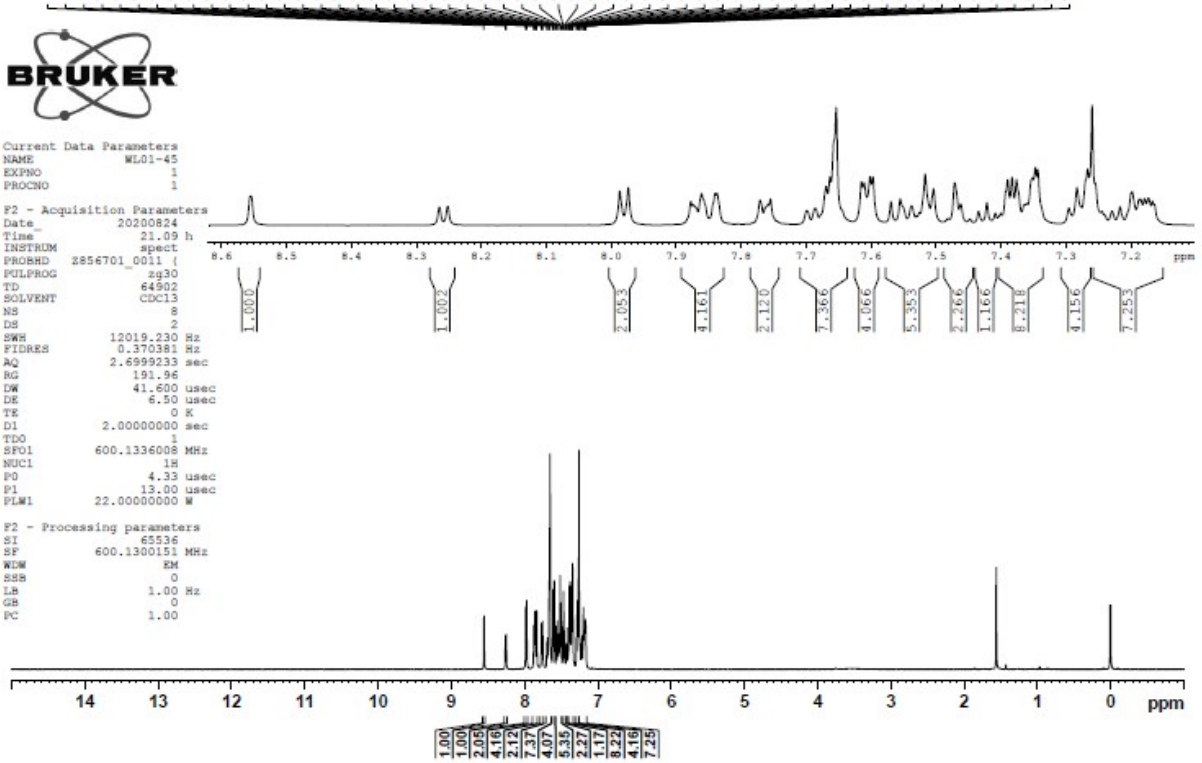
BRUKER


WL_01_38_update_C 2048s CDCl3
BBO_CI3CPD256_CDCl3 (C:\VISTEC_NMR_Data\VP) vpwal_14
BRUKER
Current Data Parameters
NAME WL_01_38_update_C
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191116
Time 0.58 h
INSTRUM spect
PROBHD Z114607_0208 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 6.50 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9176988 MHz
NUC1 13C
P0 3.27 usec
P1 9.80 usec
PLW1 100.69000244 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 23.00000000 W
PLW12 0.44165000 W
PLW13 0.22215000 W
F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

PIAC:


D:\Data\MSE\VIP_LAB\Wan Li\WL01-45_final\0_G19\1\1SRef
MALDI-TOF-MS Report
Frontier Research Center, Vidyasirimedhi Institute of Science and Technology
Intens. [a.u.]
x10^4
942.6835
940.7999
m/z

BBO_PROTON8 CDCl3 {C:\VISTEC NMR Data\VP} vpwal 12



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Current Data Parameters
NAME                  WL01-45
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20200824
Time                   21.09 h
INSTRUM                spect
PROBHD    Z856701_0011 (
PULPROG                 zg30
TD                     64902
SOLVENT                CDCl3
NS                         8
DS                         2
SWH               12019.230 Hz
FIDRES                0.370381 Hz
AQ                 2.6999233 sec
RG                    191.96
DW                   41.600 usec
DE                    6.50 usec
TE                       0 K
D1                2.00000000 sec
TD0                        1
SFO1              600.1336008 MHz
NUC1                      1H
P0                    4.33 usec
P1                   13.00 usec
PLW1             22.00000000 W

F2 - Processing parameters
SI                     65536
SF                600.1300151 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      1.00
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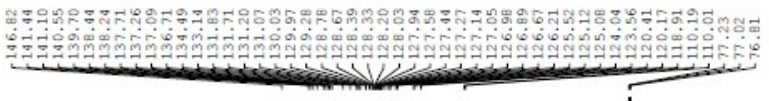
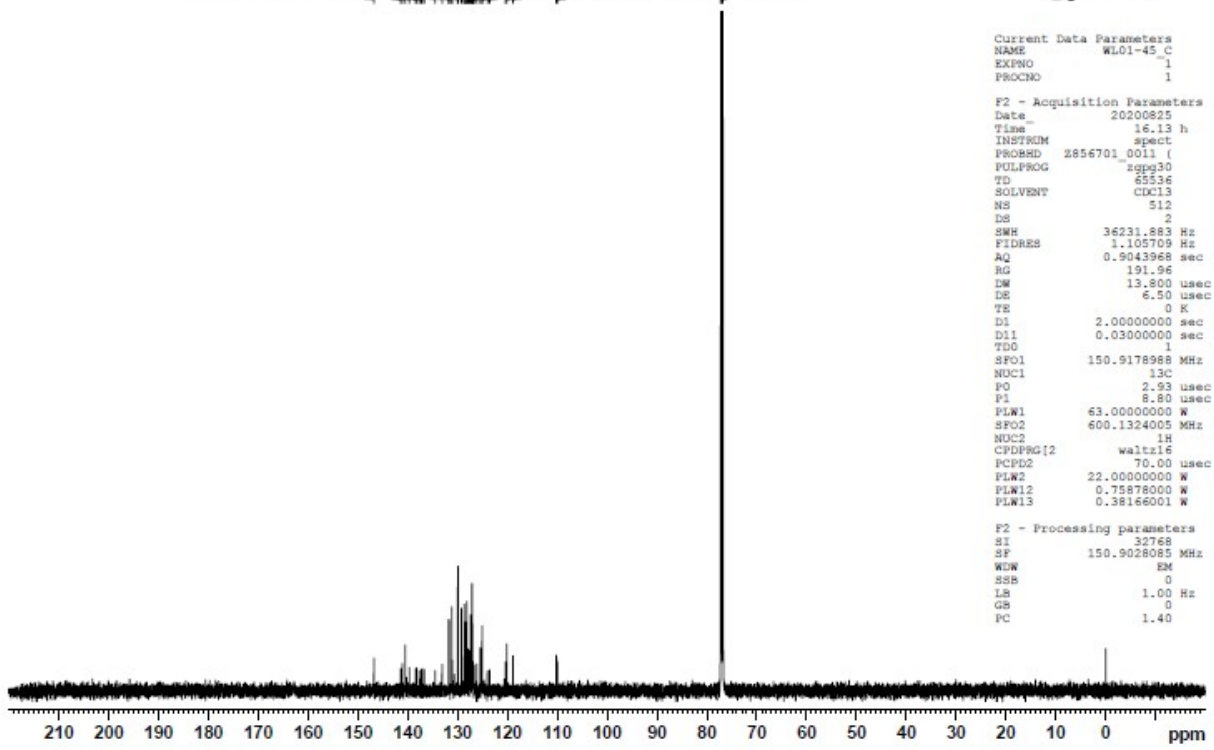
BBO_C13CPD256 CDCl3 {C:\VISTEC NMR Data\VP} vpwal 16





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Current Data Parameters
NAME                  WL01-45_C
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20200825
Time                   16.13 h
INSTRUM                spect
PROBHD    Z856701_0011 (
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       512
DS                         2
SWH               36231.883 Hz
FIDRES                1.105709 Hz
AQ                 0.9043968 sec
RG                    191.96
DW                   13.800 usec
DE                    6.50 usec
TE                       0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1              150.9178988 MHz
NUC1                      13C
P0                    2.93 usec
P1                    8.80 usec
PLW1             63.00000000 W
SFO2              600.1324005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                70.00 usec
PLW2             22.00000000 W
PLW12             0.75878000 W
PLW13             0.38166001 W

F2 - Processing parameters
SI                     32768
SF                150.9028085 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      1.40
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