

Supporting Information

High efficiency and low efficiency roll-off hole-transporting layer-free solution-processed fluorescent NIR-OLEDs based on oligothiophene-benzothiadiazole derivatives

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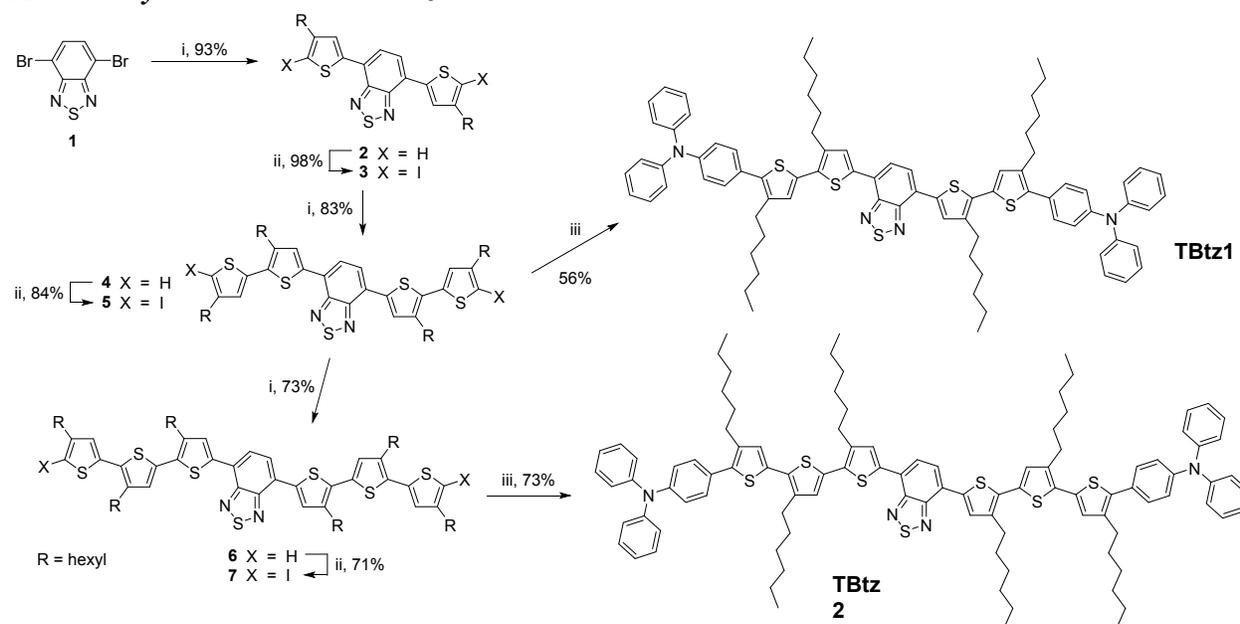
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Materials synthesis and characterizations



4,7-Dibromobenzo[c][1,2,5]thiadiazole (1)

A dry 250 mL round-bottomed flask with a magnetic stirring bar was placed with benzo[c][1,2,5]thiadiazole (4.26 g, 31.29 mmol) and HBr (50 mL). Then Br₂ (mixture between bromine in HBr) was added dropwise at reflux for 2 h. The reaction was cooled to room temperature and separated. The aqueous solution was extracted with CH₂Cl₂ (3 x 50 ml) and the combined organic layers with

aqueous sodium thiosulfate solution until red color of bromine disappeared. After that were added NaHCO₃ solution to be neutral and dried over anhydrous Na₂SO₃, filtered and the solvent was removed under reduced pressure. The finally was purified by column chromatography on silica gel eluting with a mixture of CH₂Cl₂/hexane to give white solids (8.36 g, 91 %); mp: 169-170 °C; ¹H-NMR (500 MHz, CDCl₃) 7.73 (s, 2H). ¹³C-NMR (125 MHz, CDCl₃) δ = 132.37, 113.92; (APCI): clacd. for C₆H₂Br₂N₂S 293.8285, found: 294.8294 (M+).

4,7-Bis(4-hexylthiophen-2-yl)benzo[c][1,2,5]thiadiazole (2)

A mixture of **1** (0.70 g, 2.38 mmol), 4-hexylthiophen-2-yl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (1.47g, 5.00 mmol), Pd(PPh₃)₄ (0.14 g, 0.11 mmol) and 2 M Na₂CO₃ (20 mL) in THF (30 mL) was degassed with N₂ for 10 min. The mixture was stirred at reflux under N₂ for 24 h. After cooling, water (50 mL) was added and the mixture was extracted with CH₂Cl₂ (3 x 50 mL). The combined organic phase was washed with water (50 mL), brine solution (50 mL), dried with anhydrous Na₂SO₄ and filtered. The solvent was removed to dryness and the crude product was purified by column chromatography on silica gel eluting with a mixture of CH₂Cl₂/hexane to give orange solids (1.04 g, 93%); m.p. 93-94 °C; ¹H-NMR (500 MHz, CDCl₃) δ = 7.97 (s, 2H), 7.82 (s, 2H), 7.038 (s, 2H), 2.69 (t, *J* = 7.5 Hz, 4H), 1.73-1.67 (m, 4H), 1.40-1.32 (m, 12H), 0.90 (t, *J* = 6.5 Hz, 6H); ¹³C-NMR (125 MHz, CDCl₃) δ = 152.65, 144.37, 139.01, 132.26, 129.62, 129.00, 126.03, 125.59, 125.54, 122.07, 121.53, 31.71, 30.67, 30.61, 30.49, 29.06, 22.64, 14.12; (MALDI-TOF): clacd. for C₂₆H₃₂N₂S₃ 468.1728, found : 468.1920 (M+).

4,7-Bis(4-hexyl-5-iodothiophen-2-yl)benzo[c][1,2,5]thiadiazole (3)

Compound **2** (1.00 g, 1.39 mmol) was dissolved in a mixture solvent between CH₃COOH/CHCl₃ (1:1) (25 mL). After that NIS (0.65 g, 2.91 mmol) was slowly added. When reaction completed, the reaction mixture was poured into water and extracted with CH₂Cl₂ (3 x 50 mL). The combined organic phase was washed with water (50mL), brine solution (50 mL), dried with anhydrous Na₂CO₃, filtered and the solvent was removed in vacuum. The crude product was purified by column chromatography on silica gel eluting with a mixture of CH₂Cl₂/hexane to give orange-red solids (1.51g, 98%); m.p. 98-99 °C; ¹H-NMR (500 MHz, CDCl₃) δ = 7.75 (s, 2H), 7.70 (s, 2H), 2.61 (t, *J* = 8 Hz, 4H), 1.67-1.64 (m, 4H), 1.55 (s, 6H), 1.42-1.33 (m, 14H), 0.90(t, *J* = 6.5 Hz, 6H); ¹³C-NMR (125 MHz, CDCl₃) δ = 152.25, 148.27, 143.61, 127.75, 125.44, 125.04, 32.25, 31.67, 30.06, 29.71, 28.96, 22.63, 14.12 ppm; (MALDI-TOF): clacd. for C₂₆H₃₀I₂N₂S₃ : 719.9660, found : 719.9730 (M+).

4,7-Bis(3,4'-dihexyl-[2,2'-bithiophen]-5-yl)benzo[c][1,2,5]thiadiazole (4)

A mixture of **3** (0.33 g, 0.45 mmol), 4-hexylthiophen-2-yl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (0.28 g, 0.95 mmol), Pd(PPh₃)₄ (0.02 g, 0.02 mmol) and 2 M Na₂CO₃ (15 mL) in THF (30 mL) was degassed with N₂ for 10 min. The mixture was stirred at reflux under N₂ for 24 h. After cooling, water (50 mL) was added, and the mixture was extracted with CH₂Cl₂ (3 x 50 mL). The combined organic phase was washed with water (50 mL), brine solution (50 mL), dried with anhydrous Na₂SO₄ and filtered. The solvent was removed to dryness and the crude product was purified by column chromatography on silica gel eluting with a mixture of CH₂Cl₂/hexane to give red solids (0.30g, 83%); m.p. 94-95 °C; ¹H-NMR (600 MHz, CDCl₃) δ = 7.95 (s, 2H), 7.78 (s, 2H), 7.07 (s, 2H), 6.93 (s, 2H), 2.83 (t, *J* = 7.8 Hz, 4H) 2.63 (t, *J* = 7.8 Hz, 4H), 1.76-1.71 (m, 4H), 1.69-1.64 (m, 4H), 1.44-1.41 (m, 4H), 1.39-1.33 (m, 20H); ¹³C-NMR (150 MHz, CDCl₃) δ = 152.57, 144.38, 143.75, 140.23, 136.61, 135.70, 132.89, 130.59, 129.01, 127.39, 125.50, 125.44, 125.14, 121.56, 120.27, 31.71, 30.61, 30.53, 30.43, 29.53, 29.33, 29.04, 28.06, 22.67, 22.64, 14.11 ppm; (MALDI-TOF): clacd. for C₄₆H₆₀N₂S₅ : 800.3360, found : 800.3821 (M+).

4,7-Bis(3,4'-dihexyl-5'-iodo-[2,2'-bithiophen]-5-yl)benzo[c][1,2,5]thiadiazole (5)

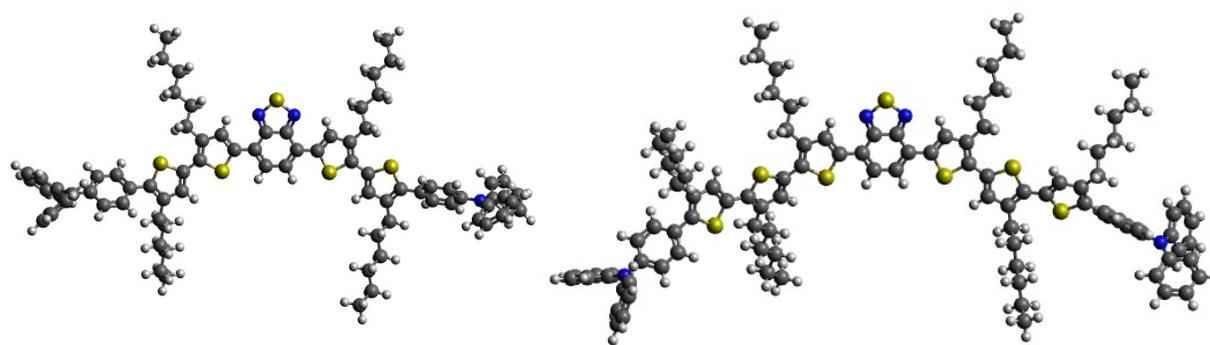
Compound **4** (0.23 g, 0.28 mmol) was dissolved in a mixture solvent between CH₃COOH/CHCl₃ (1:1) (15 mL). After that NIS (0.13 g, 0.59 mmol) was slowly added. When reaction completed, the reaction mixture was poured into water and extracted with CH₂Cl₂ (3 x 50 mL). The combined organic phase was washed with water (50mL), brine solution (50 mL), dried with anhydrous Na₂CO₃, filtered and the solvent was removed in vacuum. The crude product was purified by column chromatography on silica gel eluting with a mixture of CH₂Cl₂/hexane to yield red solids (0.25 g, 84%); m.p. 89-90 °C; ¹H-NMR (500 MHz, CDCl₃) δ = 7.94 (s, 2H), 7.81 (s, 2H), 6.88 (s, 2H), 2.79 (t, *J* = 7.5 Hz, 4H) 2.56 (t, *J* = 8.0 Hz, 4H), 1.73-1.70 (m, 4H), 1.63-1.60 (m, 12H), 1.44-1.32 (m, 26H), 0.92-89 (m, 14H); ¹³C-NMR (125 MHz, CDCl₃) δ = 152.54, 147.74, 140.78, 140.60, 137.04, 132.08, 130.51, 126.60, 125.45, 125.27, 32.38, 31.69, 31.67, 30.61, 29.99, 29.72, 29.53, 29.28, 28.95, 22.66, 22.63, 14.13 ppm; (MALDI-TOF): clacd. for C₄₆H₅₈I₂N₂S₅ : 1052.1293, found : 1051.9563 (M+).

4,7-Bis(3,4',4''-trihexyl-[2,2':5',2''-terthiophen]-5-yl)benzo[c][1,2,5]thiadiazole (6)

A mixture of **5** (0.18 g, 0.17 mmol), 4-hexylthiophen-2-yl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (0.11 g, 0.36 mmol), Pd(PPh₃)₄ (0.01 g, 0.01 mmol) and 2 M Na₂CO₃ (15 mL) in THF (30 mL) was degassed with N₂ for 10 min. The mixture was stirred at reflux under N₂ for 24 h. After cooling, water (50 mL) was added, and the mixture was extracted with CH₂Cl₂ (3 x 50 mL). The combined organic phase was washed with water (50 mL), brine solution (50 mL), dried with anhydrous Na₂SO₄ and filtered. The solvent was removed to dryness and the crude product was purified by column chromatography on silica gel eluting with a mixture of CH₂Cl₂/hexane to yield red-purple solids (0.14 g, 73%); m.p. 97-98 °C; ¹H-NMR (600 MHz, CDCl₃) δ = 7.98 (s, 2H), 7.83 (s, 2H), 7.07 (s, 2H), 6.99 (s, 2H), 6.91 (s, 2H), 2.87 (t, *J* = 7.8 Hz, 4H), 2.77 (t, *J* = 7.8 Hz, 4H), 2.62 (t, *J* = 7.8 Hz, 4H), 1.77-1.73 (m, 4H), 1.70-1.62 (m, 8H), 1.47-1.32 (m, 38H), 0.90 (s, 18H); ¹³C-NMR (150 MHz, CDCl₃) δ = 152.61, 143.71, 140.42, 139.72, 136.67, 135.50, 133.64, 132.57, 131.34, 130.75, 128.77, 127.24, 125.46, 125.20, 120.10, 31.69, 31.62, 30.58, 30.56, 30.41, 29.65, 29.31, 29.26, 29.01, 22.65, 22.63, 22.62, 14.11, 14.08 ppm; (MALDI-TOF): clacd. for C₆₆H₈₈N₂S₇ : 1132.4992, found : 1132.5853 (M+).

4,7-Bis(3,4',4''-trihexyl-5'-iodo-[2,2':5',2''-terthiophen]-5-yl)benzo[c][1,2,5]thiadiazole (7)

Compound **6** (0.14 g, 1.26 mmol) was dissolved in a mixture solvent between CH₃COOH/CHCl₃ (1:1) (15 mL). After that NIS (0.06 g, 0.26 mmol) was slowly added. When reaction completed, the reaction mixture was poured into water and extracted with CH₂Cl₂ (3 x 50 mL). The combined organic phase was washed with water (50mL), brine solution (50 mL), dried with anhydrous Na₂CO₃, filtered and the solvent was removed in vacuum. The crude product was purified by column chromatography on silica gel eluting with a mixture of CH₂Cl₂/hexane to give purple solids (0.12 g, 71%); m.p. 88-89 °C; ¹H-NMR (600 MHz, CDCl₃) δ = 7.97 (s, 2H), 7.82 (s, 2H), 7.06 (s, 2H), 6.80 (s, 2H), 2.86 (t, *J* = 7.8 Hz, 4H), 2.73 (t, *J* = 7.8 Hz, 4H), 2.55 (t, *J* = 7.8 Hz, 4H), 1.75-1.74 (m, 4H), 1.67-1.66 (m, 4H), 1.62-1.60 (m, 4H), 1.53 (s, 8H), 1.47-1.33 (m, 48H), 0.91 (m, 18H); ¹³C-NMR (150 MHz, CDCl₃) δ = 152.59, 143.70, 140.40, 139.70, 136.67, 135.51, 133.65, 132.56, 131.33, 130.74, 128.74, 127.23, 125.43, 125.17, 120.08, 31.69, 30.58, 30.55, 30.51, 30.40, 29.66, 29.31, 29.26, 29.02, 22.66, 22.63, 22.62, 14.11, 14.08 ppm; (MALDI-TOF): clacd. for C₆₆H₈₆I₂N₂S₇ : 1384.2925, found : 1384.4622 (M+).



TBtz1

TBtz2

Fig. S1 The optimized structures of **TBtz1-2** calculated by TD-DFT B3LYP/6-31G(d,p) in CH_2Cl_2 .

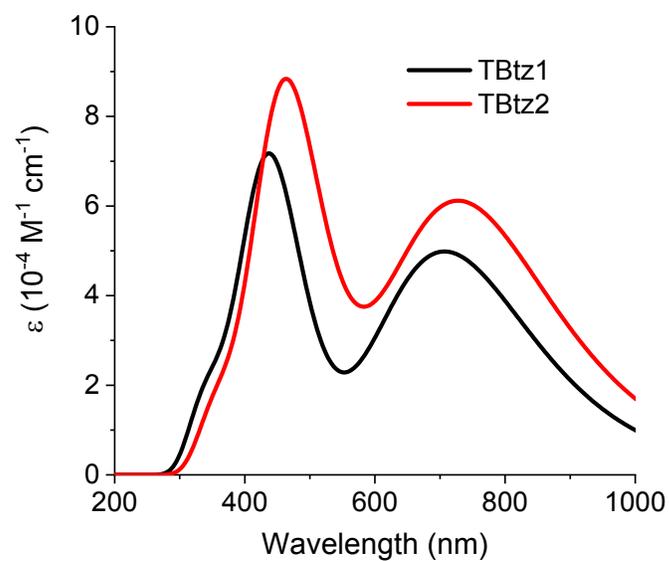


Fig. S2 Simulated UV-vis absorption of **TBtz1-2** obtained from TD-DFT calculation using B3LYP/6-31G(d,p) in CH_2Cl_2 .

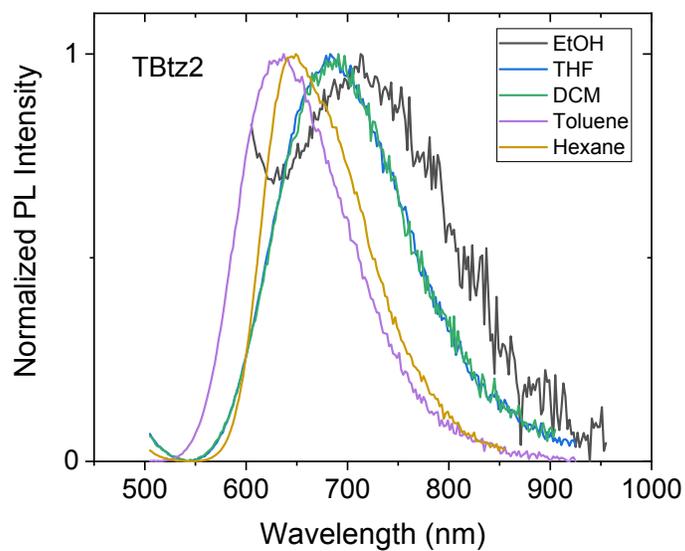
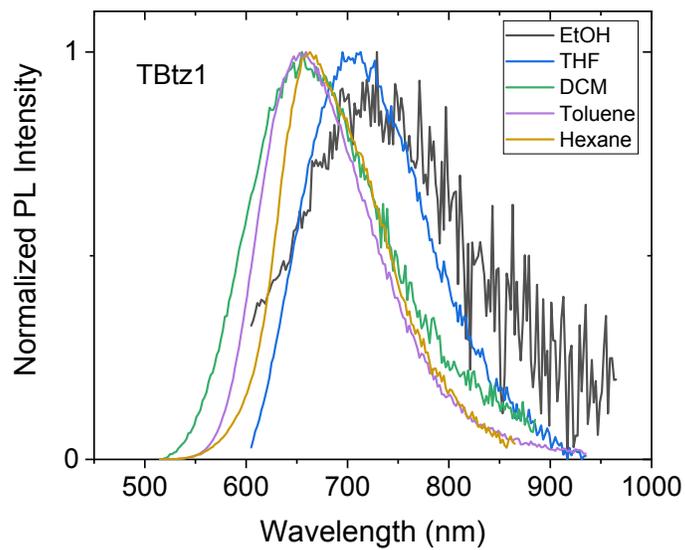


Fig. S3 PL spectra of **TBtz1-2** in different solvents (ethanol (EtOH), tetrahydrofuran (THF), dichloromethane (DCM), toluene and hexane).

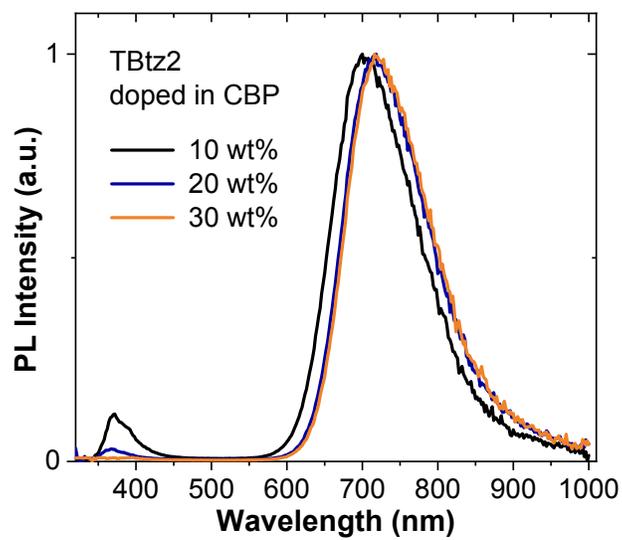
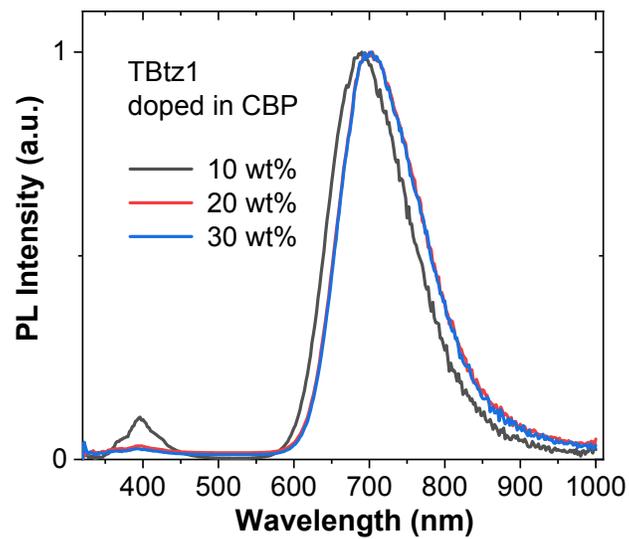


Fig. S4 Normalized PL spectra of thin films spin-coated on fused silica substrates of **TBtz1-2** doped (10, 20 and 30 wt%) in CBP.

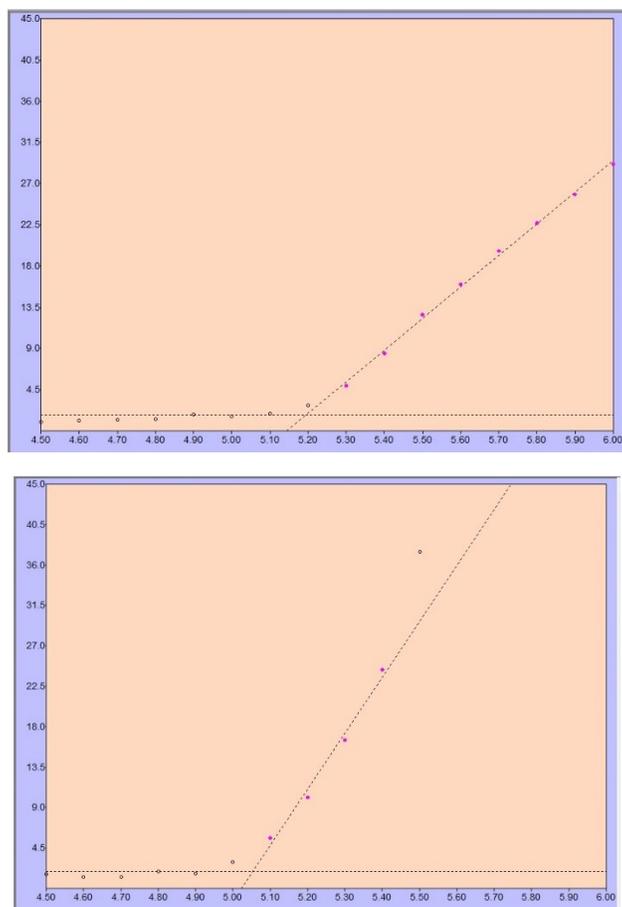


Fig. S5 Photoemission yield spectroscopy in air (PYS) spectra for **TBtz1** (top) and **TBtz2** (bottom).

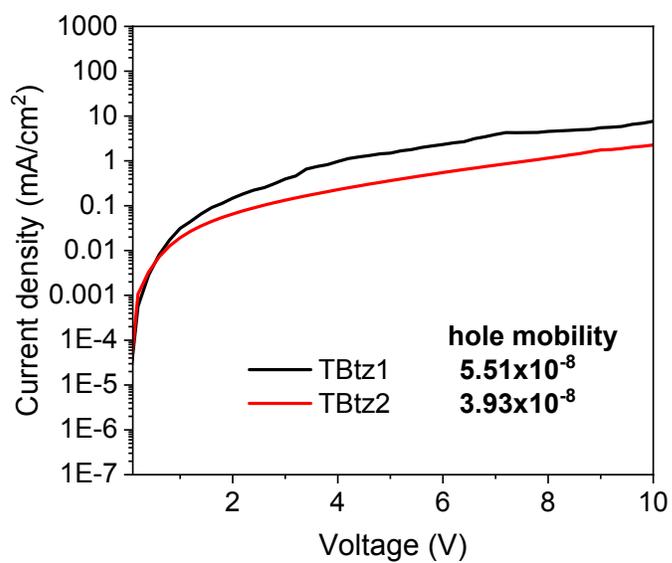
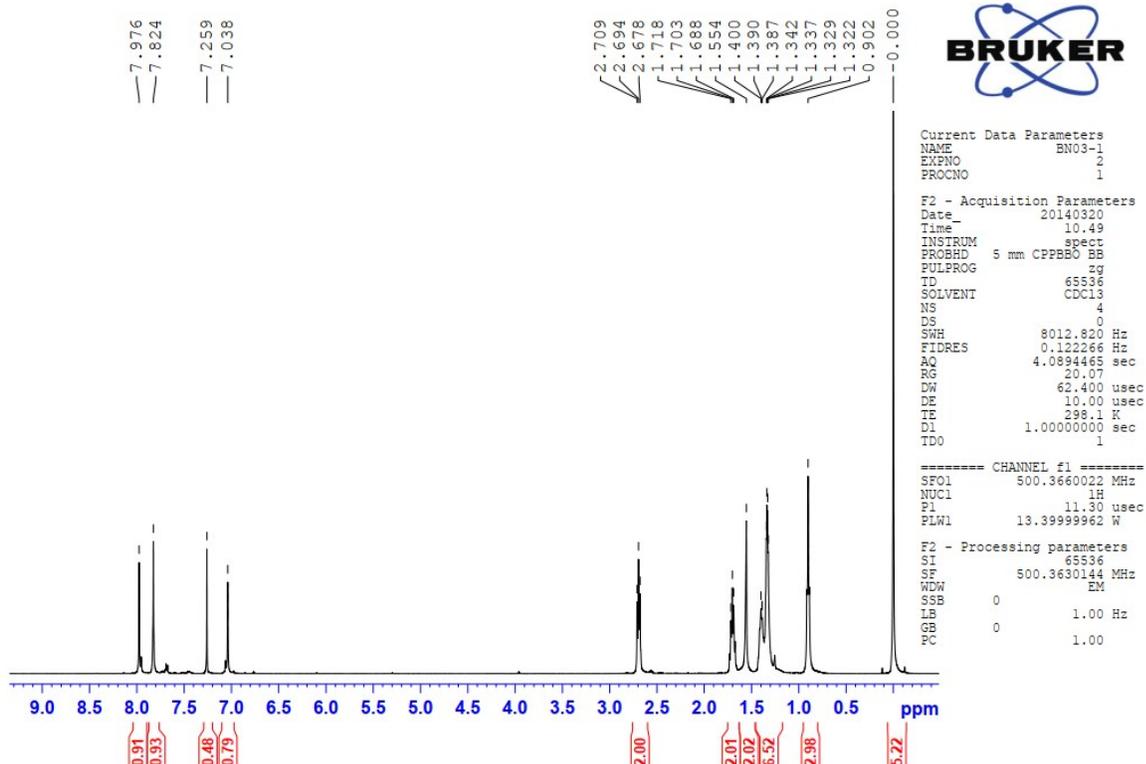


Fig. S6 Current density-voltage (J - V) characteristic of hole only device (ITO/PEDOT:PSS/**TBtz1-2** (170nm)/MoO₃/Al).

Compound 2



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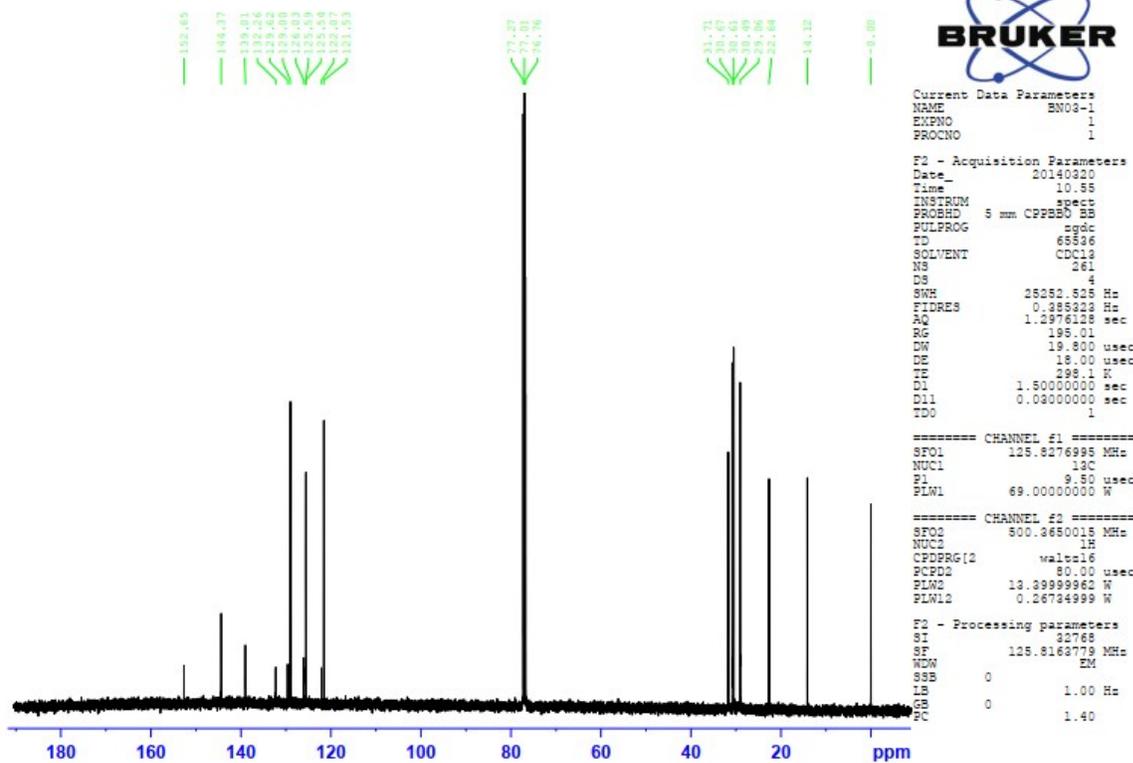
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TE        298.1 K
D1        1.00000000 sec
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BRUKER

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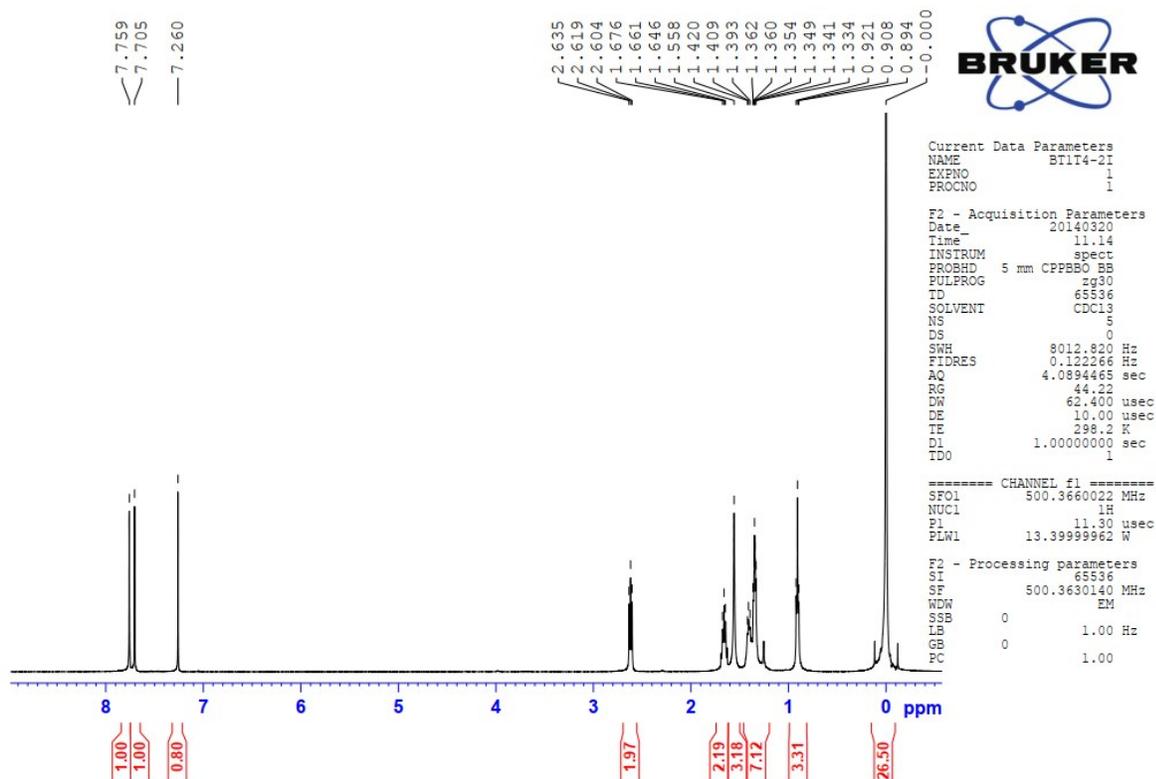
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Compound 3



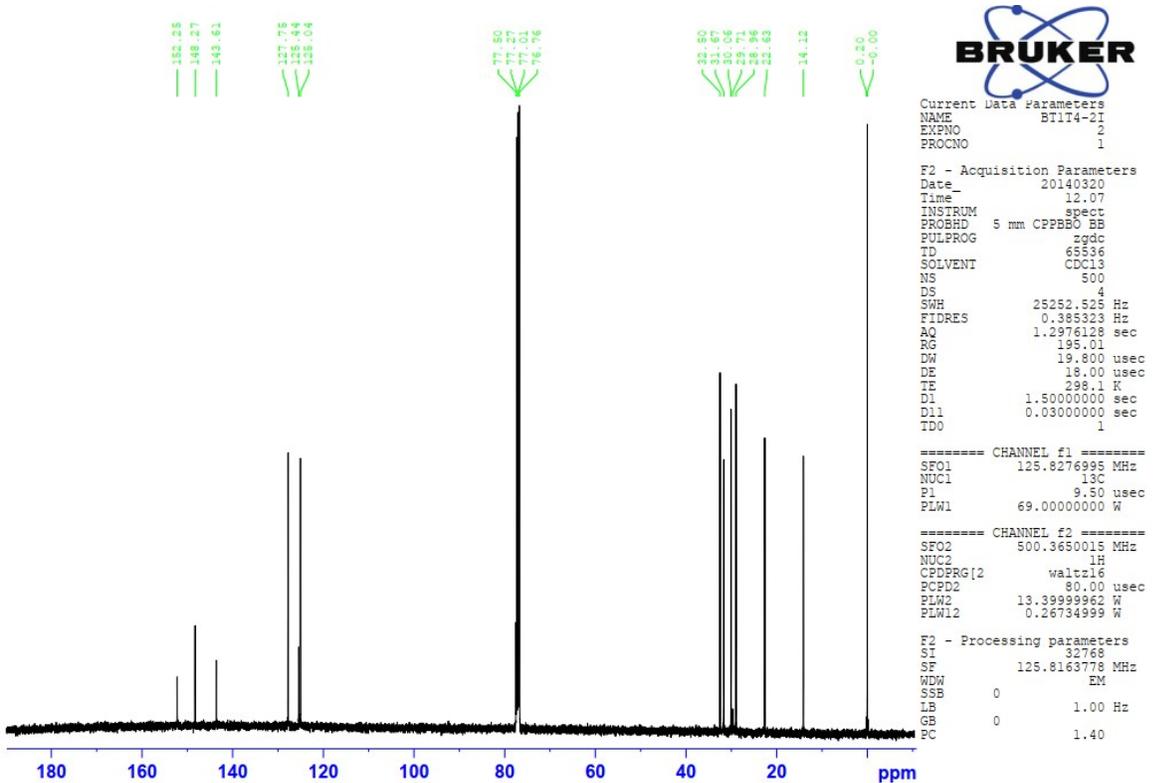
BRUKER

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 TE 298.2 K
 D1 1.0000000 sec
 TDO 1

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 P1 11.30 usec
 PLW1 13.39999962 W

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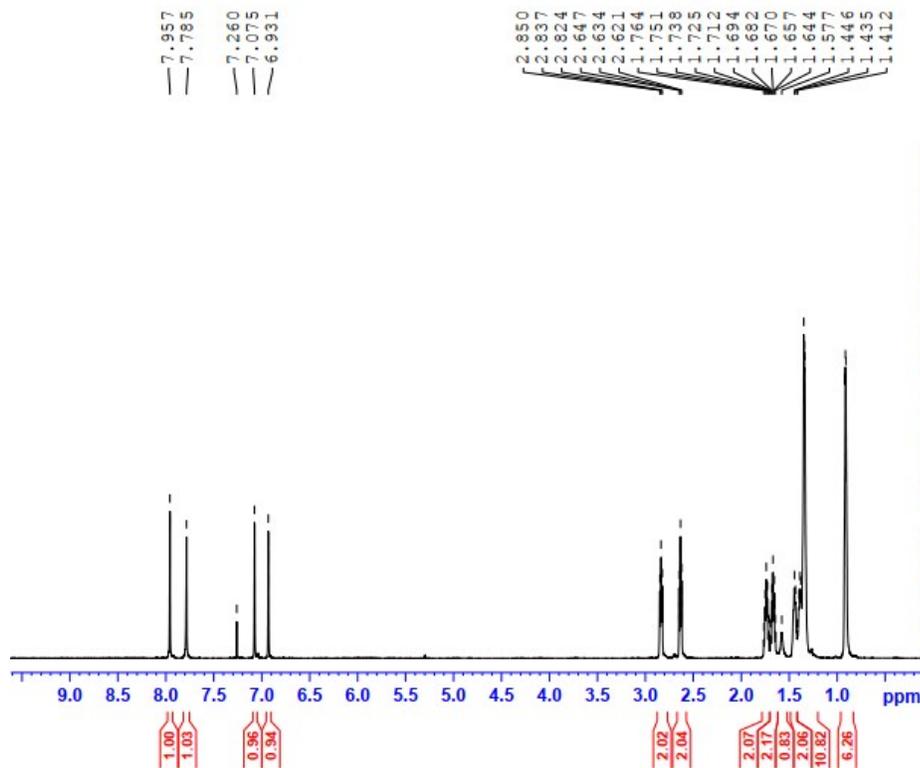
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 TDO 1

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Compound 4

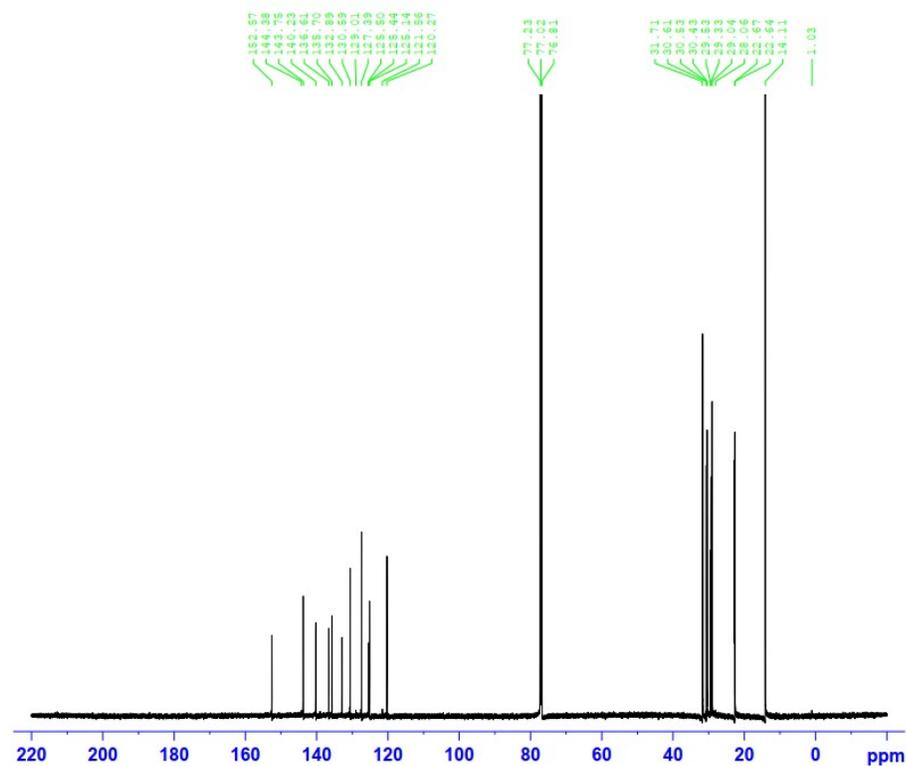


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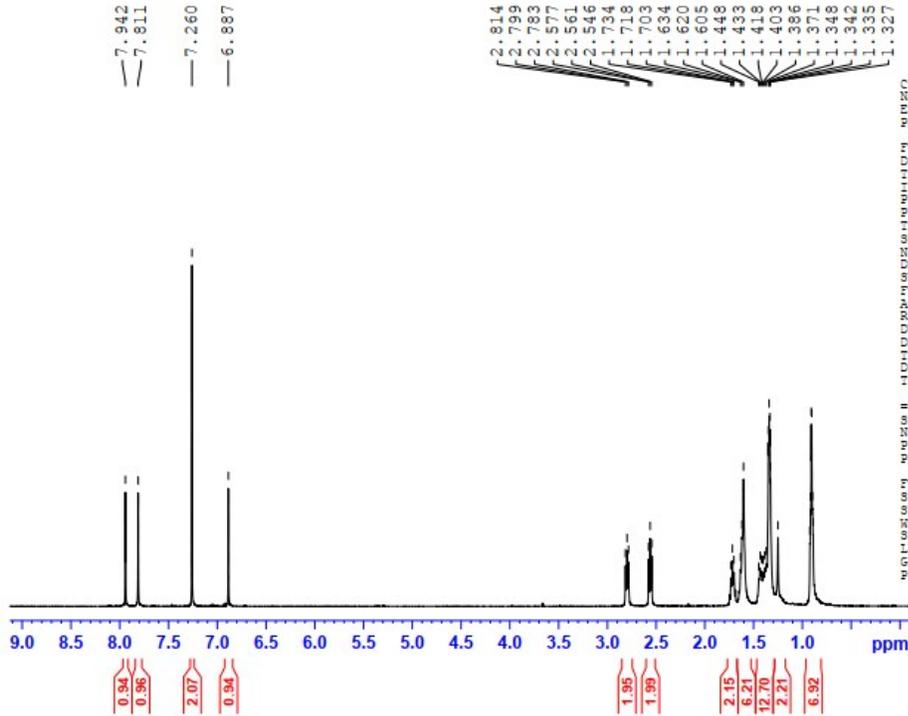
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Compound 5



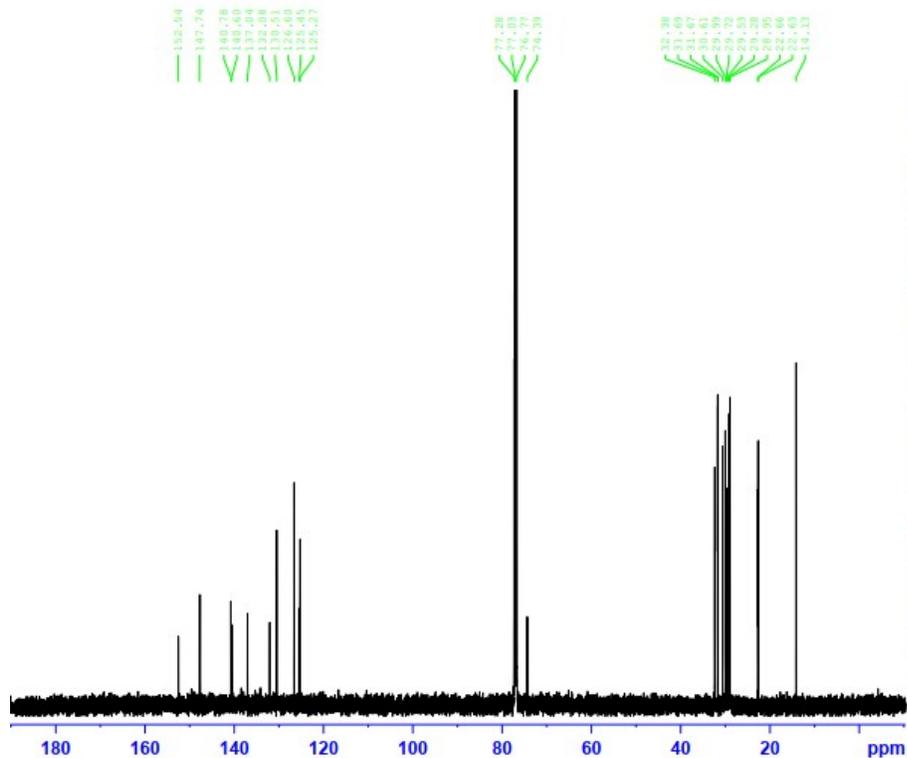
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TE        298.1 K
D1        1.00000000 sec
D11       1
TD0       1

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NUC1     1H
P1       11.30 usec
PLW1    13.39999962 W

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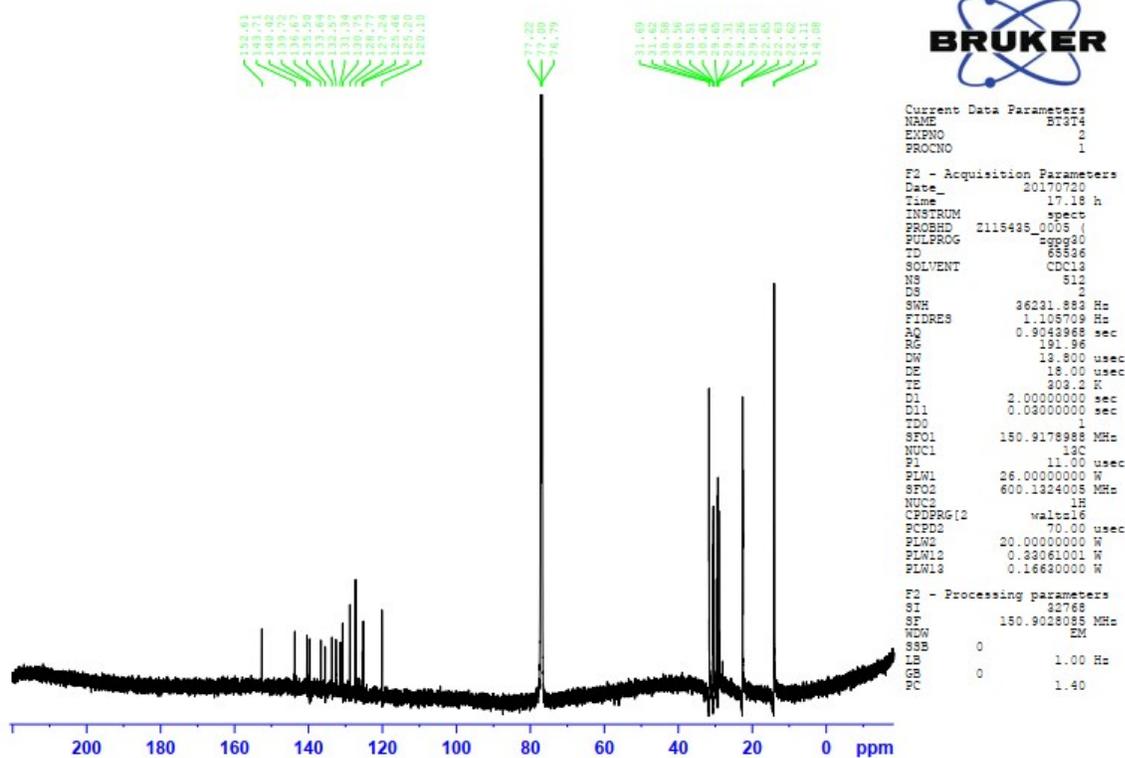
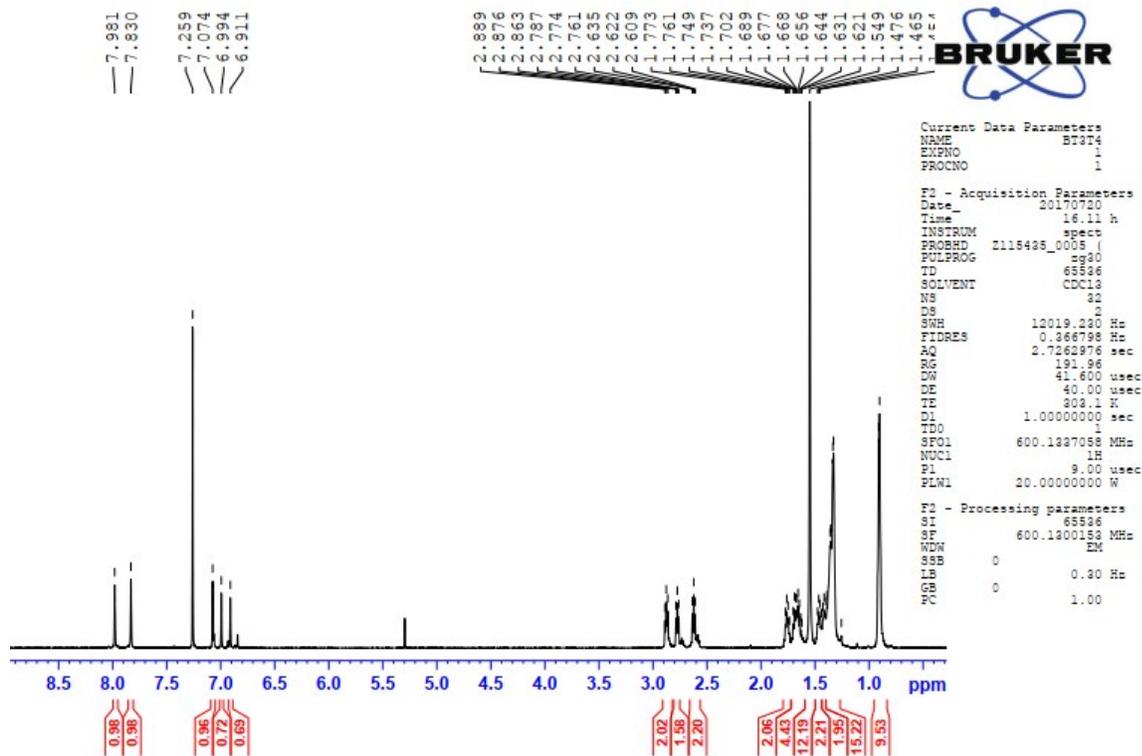
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PULPROG  zgdc
TD        65536
SOLVENT  CDCl3
NS        261
DS        4
SWH       25252.528 Hz
FIDRES    0.385223 Hz
AQ         1.2976128 sec
RG         195.01
CW         19.800 usec
TE        18.00 usec
TE        298.2 K
D1        1.50000000 sec
D11       0.03000000 sec
TD0       1

===== CHANNEL f1 =====
SF01     125.8276996 MHz
NUC1     13C
P1       9.50 usec
PLW1    69.00000000 W

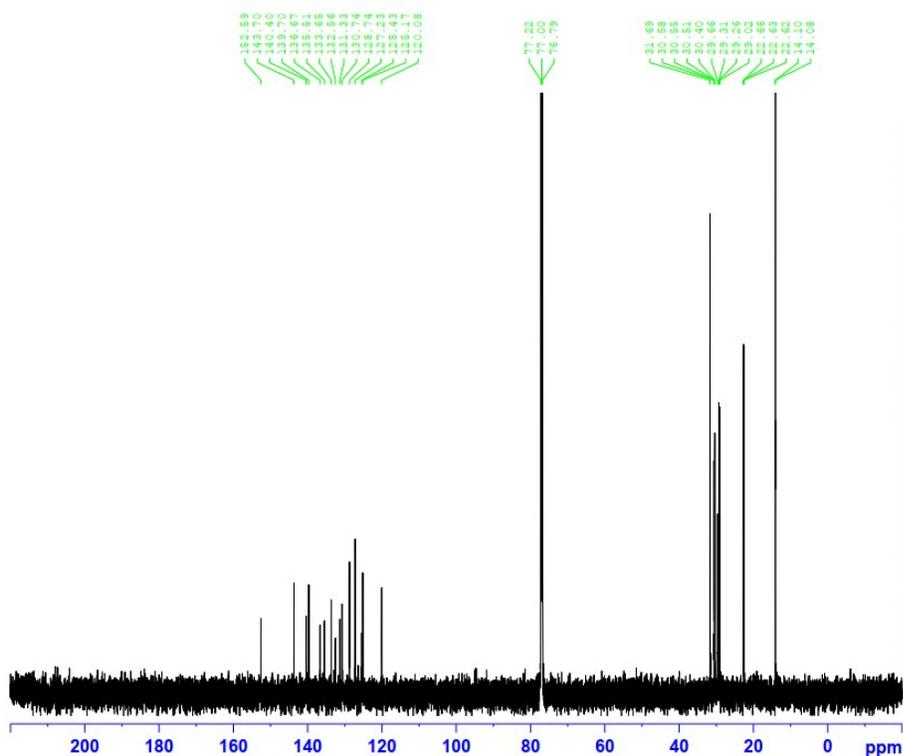
===== CHANNEL f2 =====
SF02     500.2650018 MHz
NUC2     1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2    13.39999962 W
PLWL2    0.26724999 W

F2 - Processing parameters
SI        32768
SF        125.8163760 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

Compound 6



Compound 7

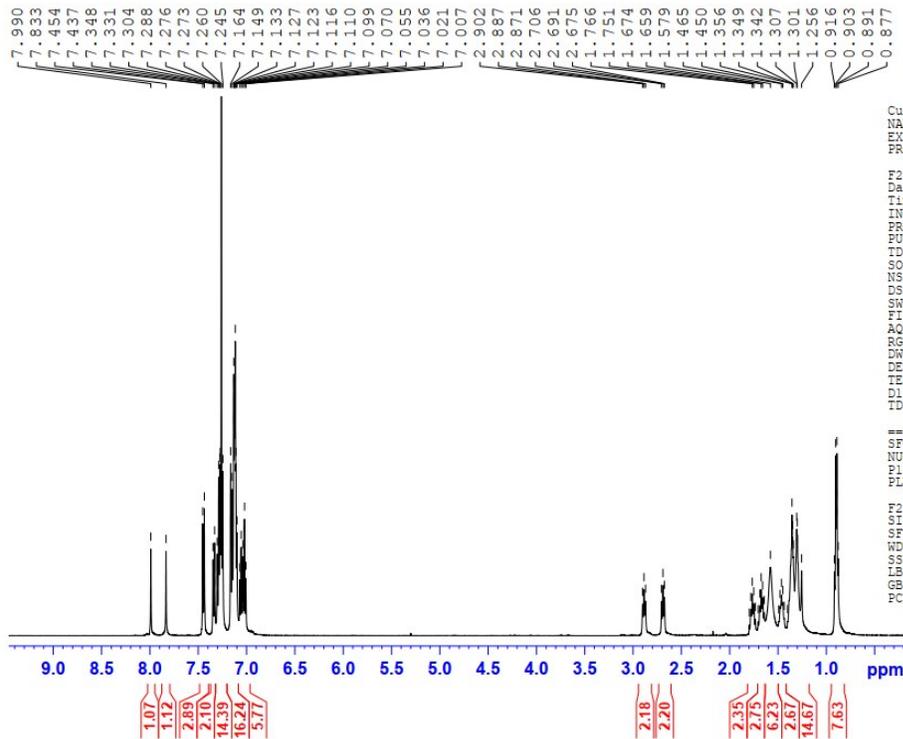


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Current Data Parameters
NAME      BT3T4-2I
EXPNO     3
PROCNO    1

F2 - Acquisition Parameters
Date_     20170726
Time      15.17 h
INSTRUM   spect
PROBHD    Z114607_0208 (
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         303.1 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
SFO1       150.9178993 MHz
NUC1       13C
P1         9.70 usec
PLW1       100.69000244 W
SFO2       600.1324005 MHz
NUC2       1H
CPDPRG2    waltz16
PCPD2      70.00 usec
PLW2       23.00000000 W
PLW12      0.44165000 W
PLW13      0.22215000 W

F2 - Processing parameters
SI         32768
SF         150.9028090 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

TBtz1



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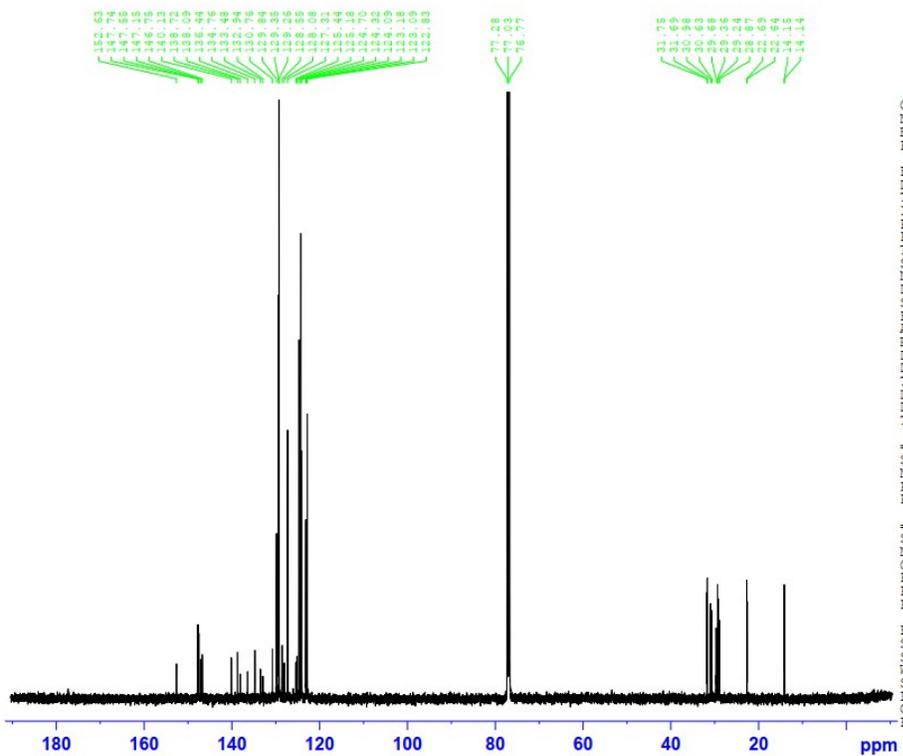
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Current Data Parameters
NAME      BT2T4-2TPA
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150716
Time     11.54
INSTRUM  spect
PROBHD   5 mm CPPBBO BB
PULPROG  zg30
ID       65536
SOLVENT  CDC13
NS       16
DS       0
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894465 sec
RG       48.32
DW       62.400 usec
DE       10.00 usec
TE       298.1 K
D1       1.00000000 sec
D10      1
TDO

===== CHANNEL f1 =====
SF01    500.3660022 MHz
NUC1    1H
P1      11.30 usec
PLW1    13.39999962 W

F2 - Processing parameters
SI      65536
SF      500.3630137 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.00
    
```



BRUKER

```

Current Data Parameters
NAME      BT2T4-2TPA
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20150716
Time     12.10
INSTRUM  spect
PROBHD   5 mm CPPBBO BB
PULPROG  zgdc
ID       65536
SOLVENT  CDC13
NS       512
DS       4
SWH      25252.525 Hz
FIDRES   0.385323 Hz
AQ       1.2976128 sec
RG       195.01
DW       19.800 usec
DE       18.00 usec
TE       298.1 K
D1       1.50000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
SF01    125.8276995 MHz
NUC1    13C
P1      9.00 usec
PLW1    69.00000000 W

===== CHANNEL f2 =====
SF02    500.3650015 MHz
NUC2    1H
CPDPRG2  waltz16
PCPD2    80.00 usec
PLW2    13.39999962 W
PLW12   0.26734999 W

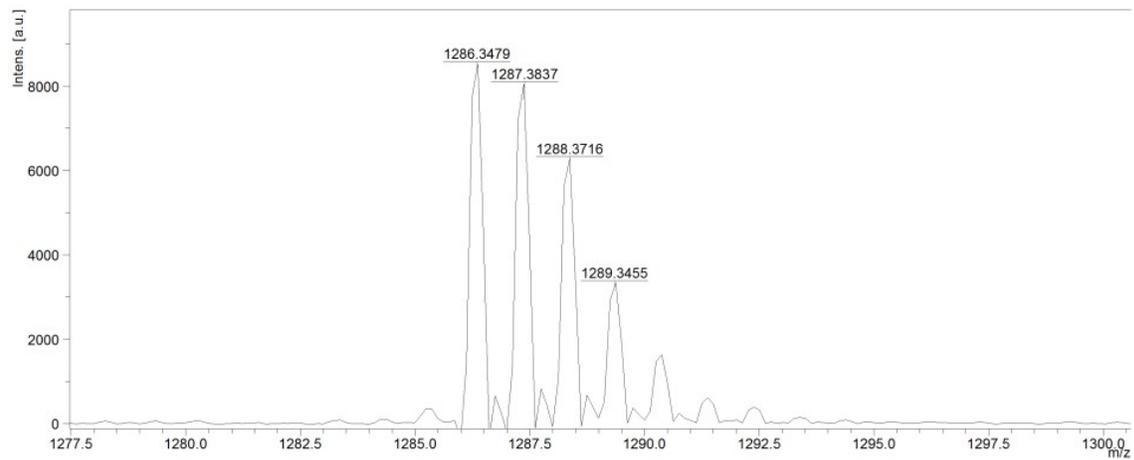
F2 - Processing parameters
SI      32768
SF      125.8163760 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
    
```

MALDI-TOF-MS Report

Frontier Research Center, Vidyasirimedhi Institute of Science and Technology

Comment 1 m/z = 1286.5456

Comment 2



TBtz2

CP_PROTON8 CDC13 {C:\VISTEC NMR Data\VP} vptk 2

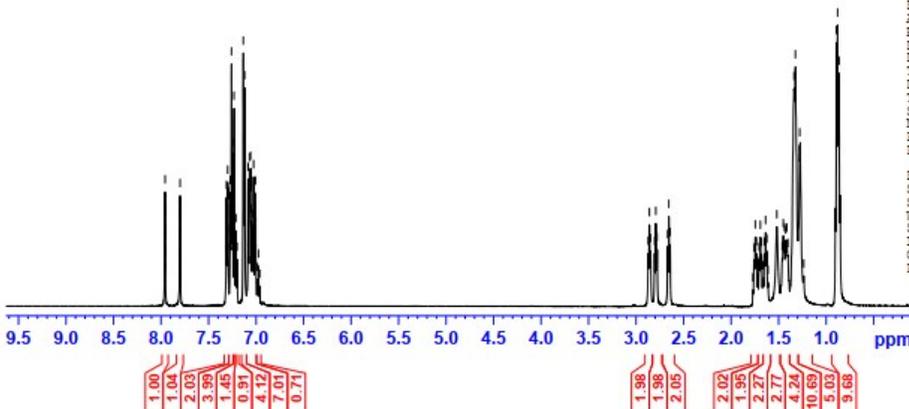
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Current Data Parameters
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 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180320
 Time 12.07 h
 INSTRUM spect
 PROBRD Z115435_0005 4
 PULPROG zgpg30
 ID 65536
 SOLVENT CDC13
 NS 32
 DS 2
 SWH 12019.220 Hz
 FIDRES 0.366798 Hz
 AQ 2.7262976 sec
 RG 107.65
 DW 41.600 usec
 DE 40.00 usec
 TE 303.1 K
 D1 1.00000000 sec
 TDO 1
 SFO1 600.1337055 MHz
 NUC1 1H
 P1 9.00 usec
 PLM1 20.00000000 W

F2 - Processing parameters
 SI 65536
 SF 600.1330319 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



CP_C13CPD32_DEI2 CDC13 {C:\VISTEC NMR Data\VP} vptk 2

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