Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

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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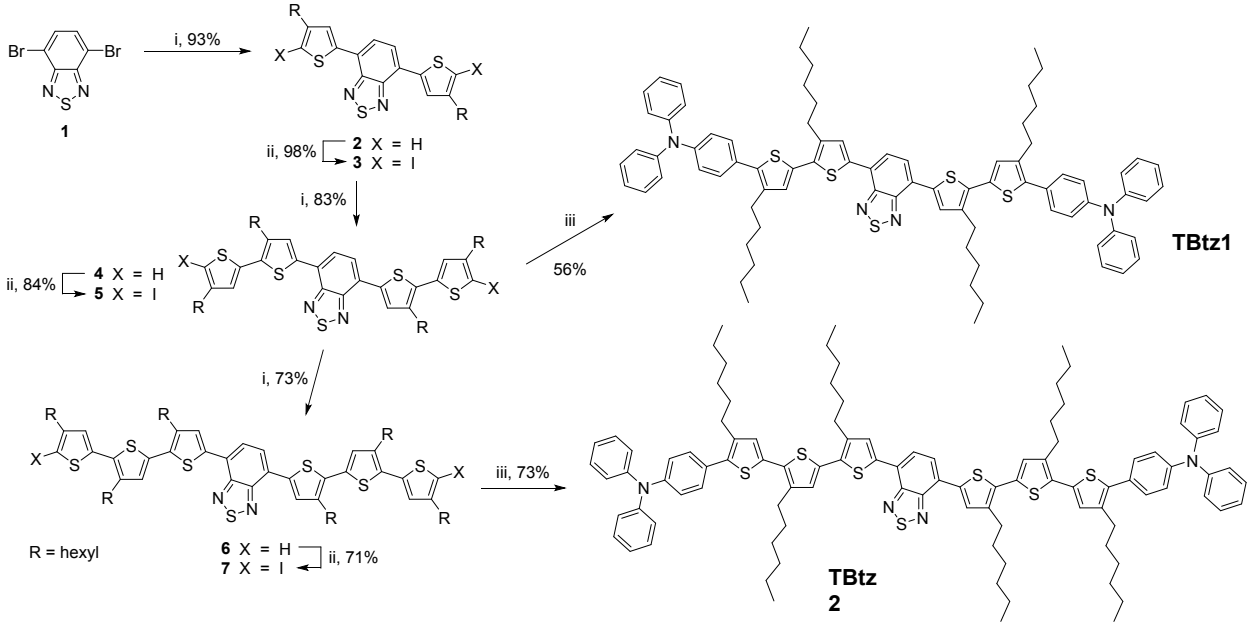
Materials synthesis and characterizations



Scheme S1 Synthesis of **TBtz1-2**. *Reagents and Conditions:* i) 4-hexylthiophen-2-yl-4,4,5,5-tetramethyl-1,3,2-dioxaborolane $Pd(PPh_3)_4$, 2M Na_2CO_3, THF, reflux. ii) NIS, THF. iii) (4-(diphenylamino)phenyl)boronic acid, $Pd(PPh_3)_4$, 2M Na_2CO_3, THF, reflux.

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 Br_2 (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 CH_2Cl_2 (3 x 50 ml) and the combined organic layers with

aqueous sodium thiosulfate solution until red color of bromine disappeared. After that were added $NaHCO_3$ solution to be neutral and dried over anhydrous Na_2SO_3, filtered and the solvent was removed under reduced pressure. The finally was purified by column chromatography on silica gel eluting with a mixture of CH_2Cl_2/hexane to give white solids (8.36 g, 91 %); mp: 169-170 ^oC; ^1H-NMR (500 MHz, $CDCl_3$) 7.73 (s, 2H). ^{13}C-NMR (125 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 132.37, 113.92; (APCI): clacd. for $C_6H_2Br_2N_2S$ 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), $Pd(PPh_3)_4$ (0.14 g, 0.11 mmol) and 2 M Na_2CO_3 (20 mL) in THF (30 mL) was degassed with N_2 for 10 min. The mixture was stirred at reflux under N_2 for 24 h. After cooling, water (50 m) was added and the mixture was extracted with CH_2Cl_2 (3 x 50 mL). The combined organic phase was washed with water (50 mL), brine solution (50 mL), dried with anhydrous Na_2SO_4 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 CH_2Cl_2/hexane to give orange solids (1.04 g, 93%); m.p. 93-94 ^oC; ^1H-NMR (500 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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); ^{13}C-NMR (125 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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 $C_{26}H_{32}N_2S_3$ 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 CH_3COOH/ $CHCl_3$ (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 CH_2Cl_2 (3 x 50 ml). The combined organic phase was washed with water (50mL), brine solution (50 mL), dried with anhydrous Na_2CO_3, filtered and the solvent was removed in vacuum. The crude product was purified by column chromatography on silica gel eluting with a mixture of CH_2Cl_2/hexane to give orange-red solids (1.51g, 98%); m.p. 98-99 ^oC; ^1H-NMR (500 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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); ^{13}C-NMR (125 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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 $C_{26}H_{30}I_2N_2S_3$: 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), $Pd(PPh_3)_4$ (0.02 g, 0.02 mmol) and 2 M Na_2CO_3 (15 mL) in THF (30 mL) was degassed with N_2 for 10 min. The mixture was stirred at reflux under N_2 for 24 h. After cooling, water (50 mL) was added, and the mixture was extracted with CH_2Cl_2 (3 x 50 mL). The combined organic phase was washed with water (50 mL), brine solution (50 mL), dried with anhydrous Na_2SO_4 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 CH_2Cl_2/hexane to give red solids (0.30g, 83%); m.p. 94-95 ^oC; ^1H-NMR (600 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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); ^{13}C-NMR (150 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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 $C_{46}H_{60}N_2S_5$: 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)

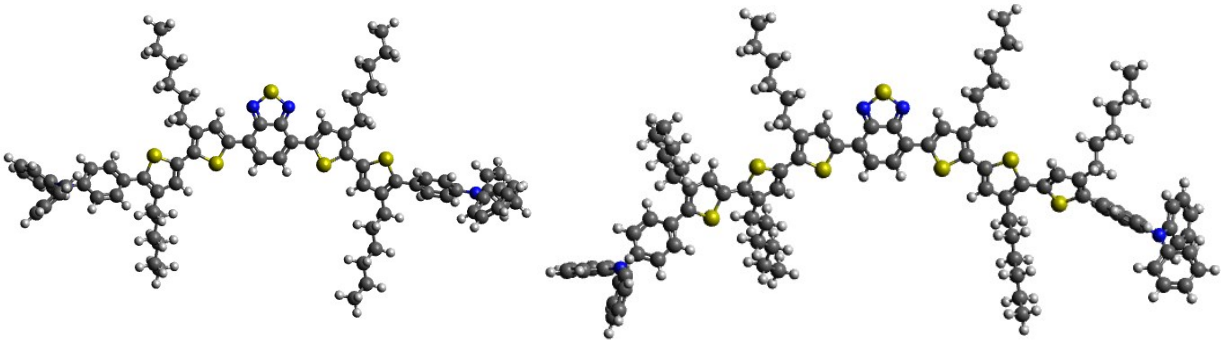
Compound **4** (0.23 g, 0.28 mmol) was dissolved in a mixture solvent between CH_3COOH/ $CHCl_3$ (1:1) (15 mL). After that NIS (0.13 g, 0.59 mmol) was slowly added. When reaction completed, the reaction mixture was poured into water and extracted with CH_2Cl_2 (3 x 50 mL). The combined organic phase was washed with water (50mL), brine solution (50 mL), dried with anhydrous Na_2CO_3, filtered and the solvent was removed in vacuum. The crude product was purified by column chromatography on silica gel eluting with a mixture of CH_2Cl_2/hexane to yield red solids (0.25 g, 84%); m.p. 89-90 ^oC; ^1H-NMR (500 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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); ^{13}C-NMR (125 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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 $C_{46}H_{58}I_2N_2S_5$: 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), $Pd(PPh_3)_4$ (0.01 g, 0.01 mmol) and 2 M Na_2CO_3 (15 mL) in THF (30 mL) was degassed with N_2 for 10 min. The mixture was stirred at reflux under N_2 for 24 h. After cooling, water (50 mL) was added, and the mixture was extracted with CH_2Cl_2 (3 x 50 mL). The combined organic phase was washed with water (50 mL), brine solution (50 mL), dried with anhydrous Na_2SO_4 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 CH_2Cl_2/hexane to yield red-purple solids (0.14 g, 73%); m.p. 97-98 ^oC; ^1H-NMR (600 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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); ^{13}C-NMR (150 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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 $C_{66}H_{88}N_2S_7$: 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 CH_3COOH/ $CHCl_3$ (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 CH_2Cl_2 (3 x 50 mL). The combined organic phase was washed with water (50mL), brine solution (50 mL), dried with anhydrous Na_2CO_3, filtered and the solvent was removed in vacuum. The crude product was purified by column chromatography on silica gel eluting with a mixture of CH_2Cl_2/hexane to give purple solids (0.12 g, 71%); m.p. 88-89 ^oC; ^1H-NMR (600 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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); ^{13}C-NMR (150 MHz, $CDCl_3$) $\boldsymbol{\delta}$ = 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 $C_{66}H_{86}I_2N_2S_7$: 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.

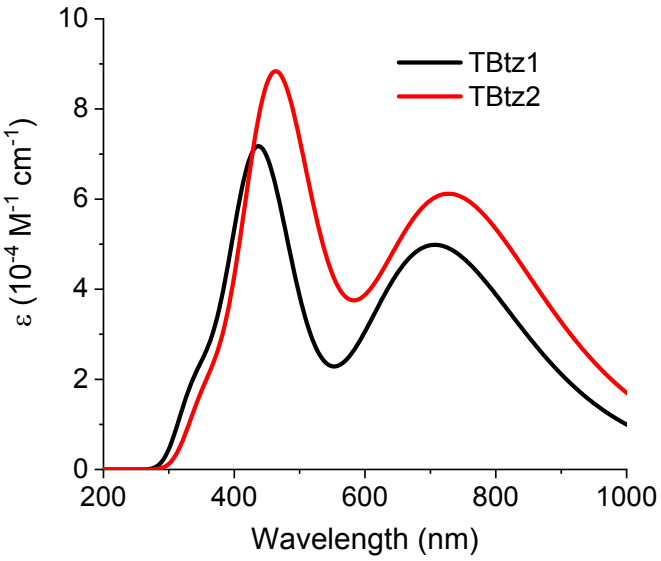


Fig. S2 Simulated UV-vis absorption of **TBtz1-2** obtained from TD-DFT calculation using B3LYP/6-31G(d,p) in CH_2Cl_2.

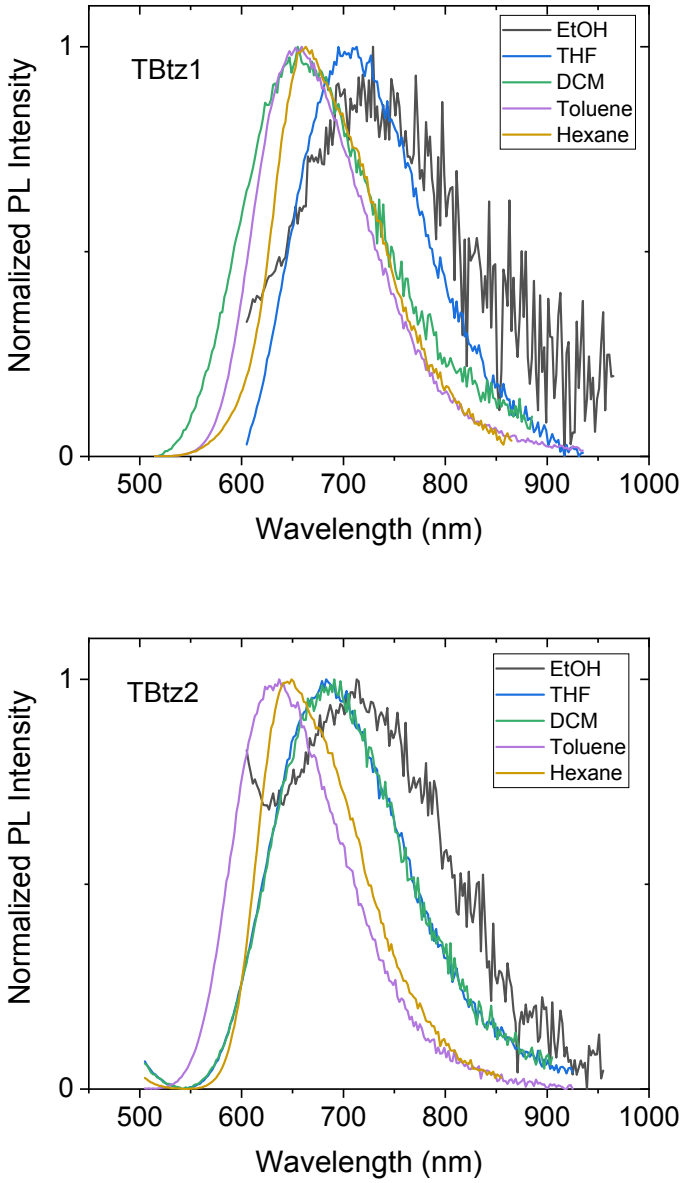


Fig. S3 PL spectra of **TBtz1-2** in different solvents (ethanol (EtOH), tetrahydrofuran (THF), dichloromethane (DCM), toluene and hexane).

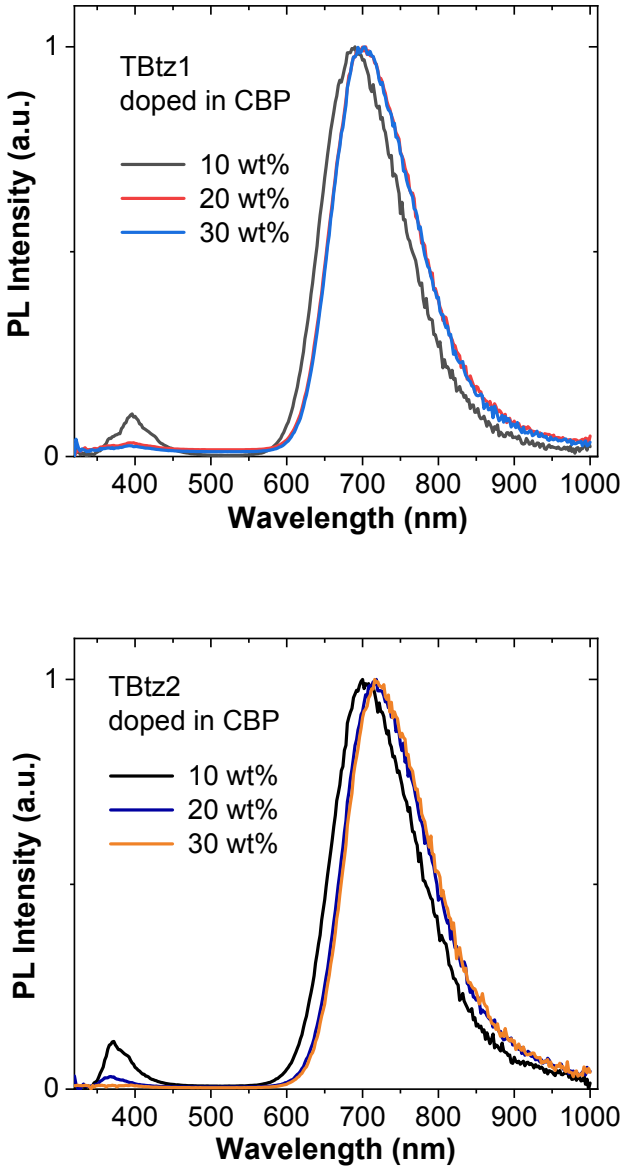


Fig. S4 Normalized PL spectra of thin films spin-coated on fused silica substrates of **TBtz1-2** doped (10, 20 and 30 wt%) in CBP.

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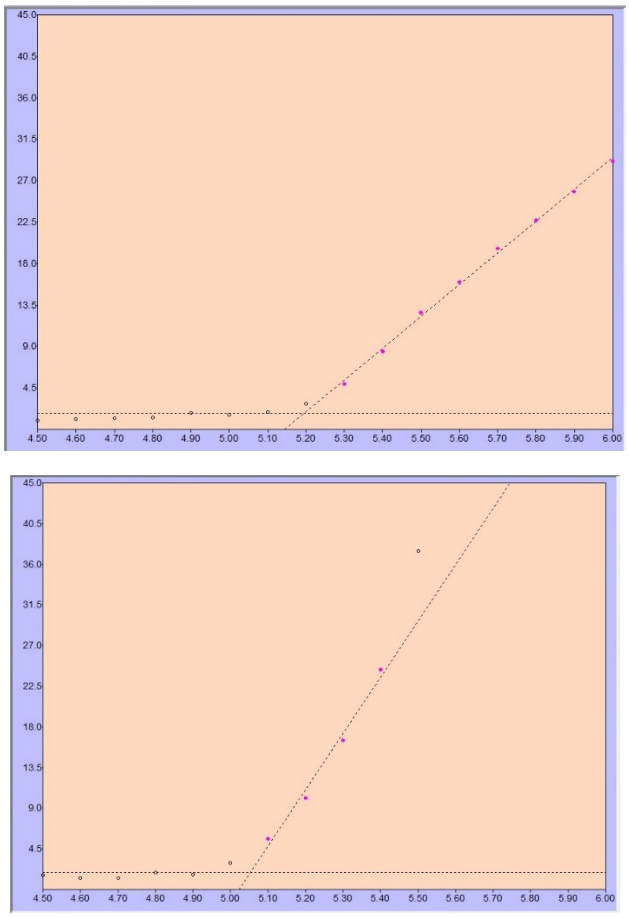


Fig. S5 Photoemission yield spectroscopy in air (PYSA) spectra for **TBtz1** (top) and **TBtz2** (bottom).

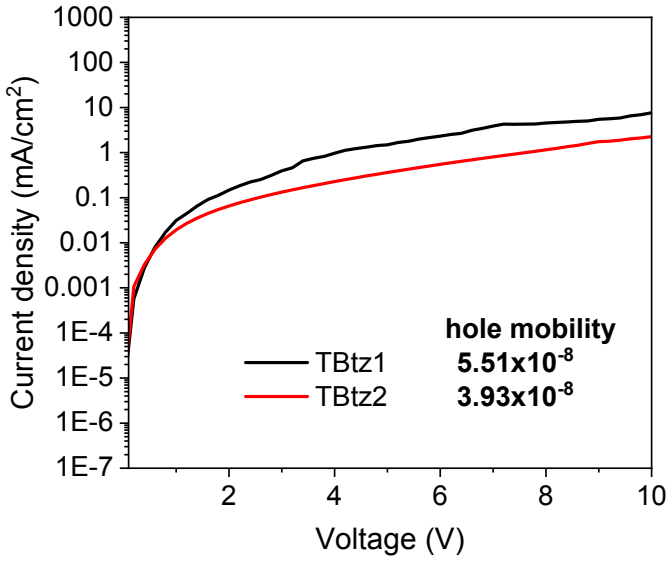
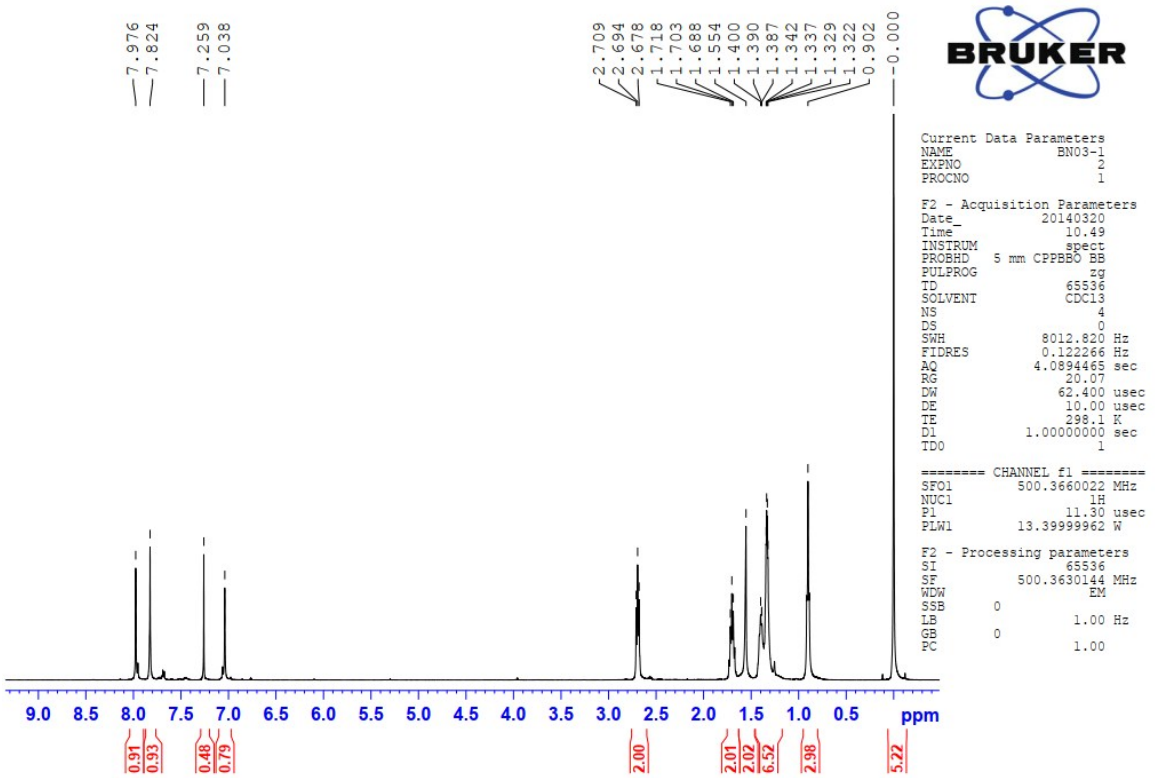
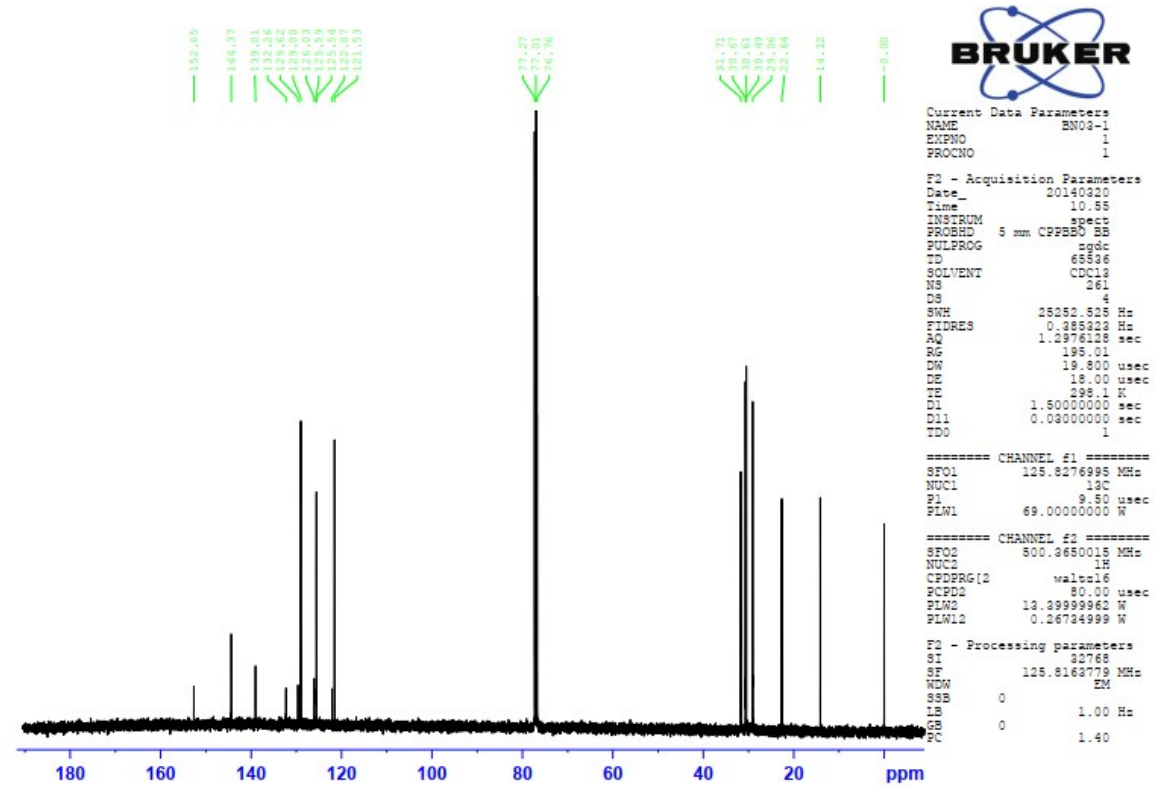


Fig. S6 Current density-voltage (*J-V*) characteristic of hole only device (ITO/PEDOT:PSS/**TBtz1-2** (170nm)/MoO_3/Al).

Compound 2



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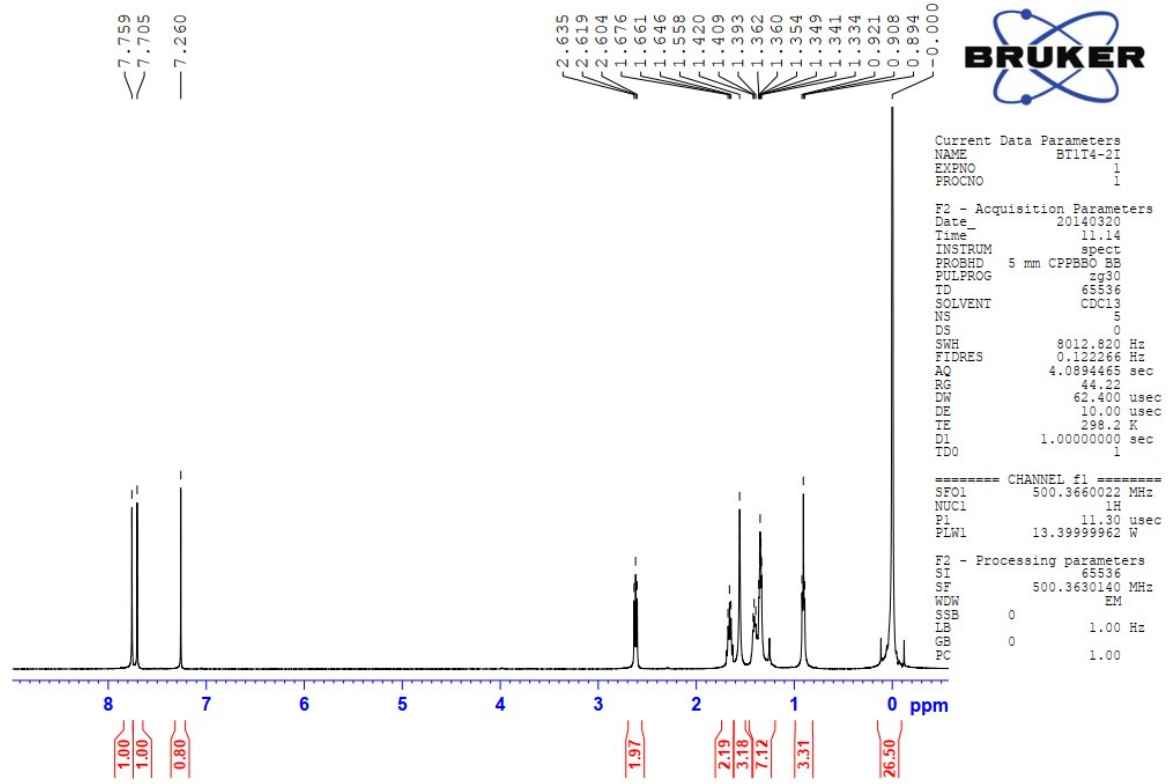
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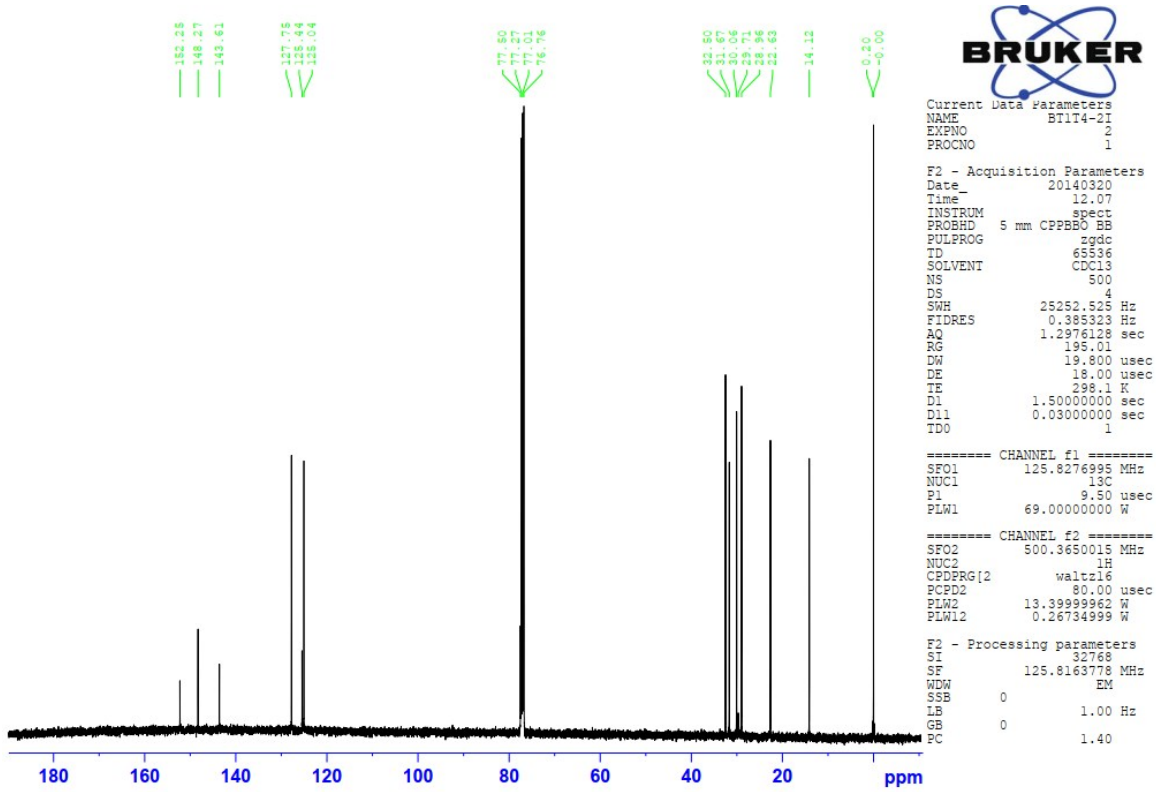
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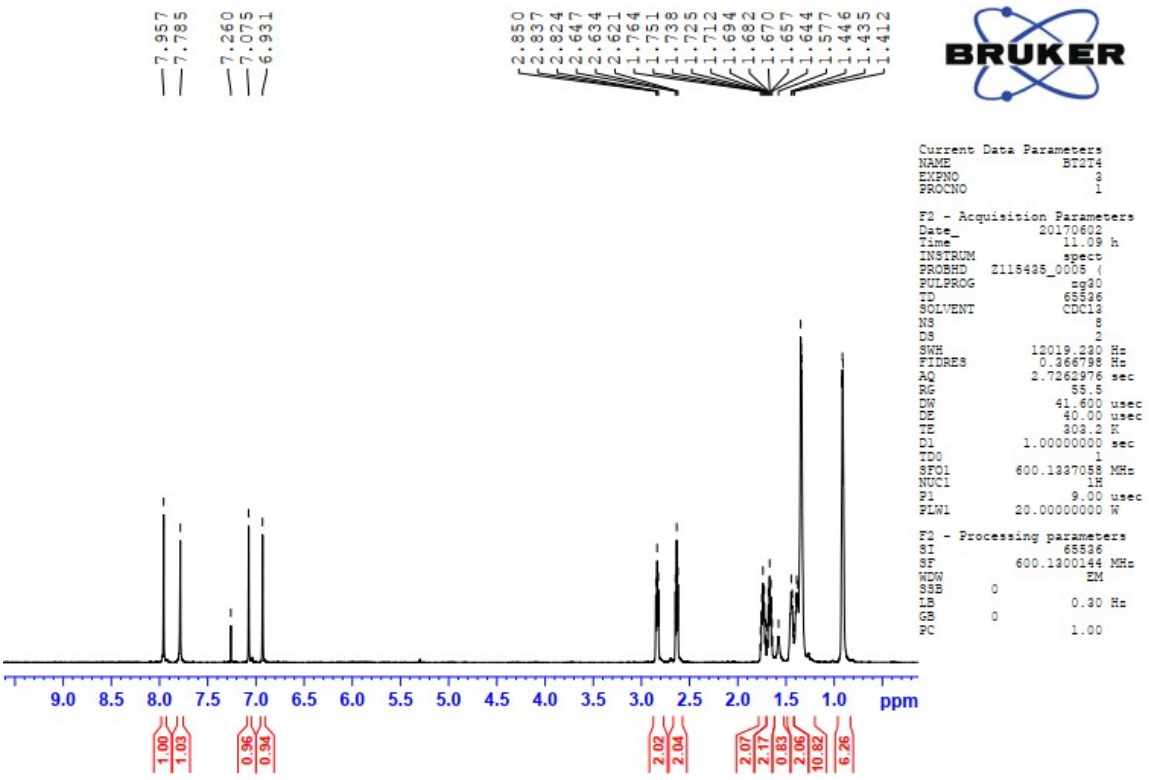
Compound 4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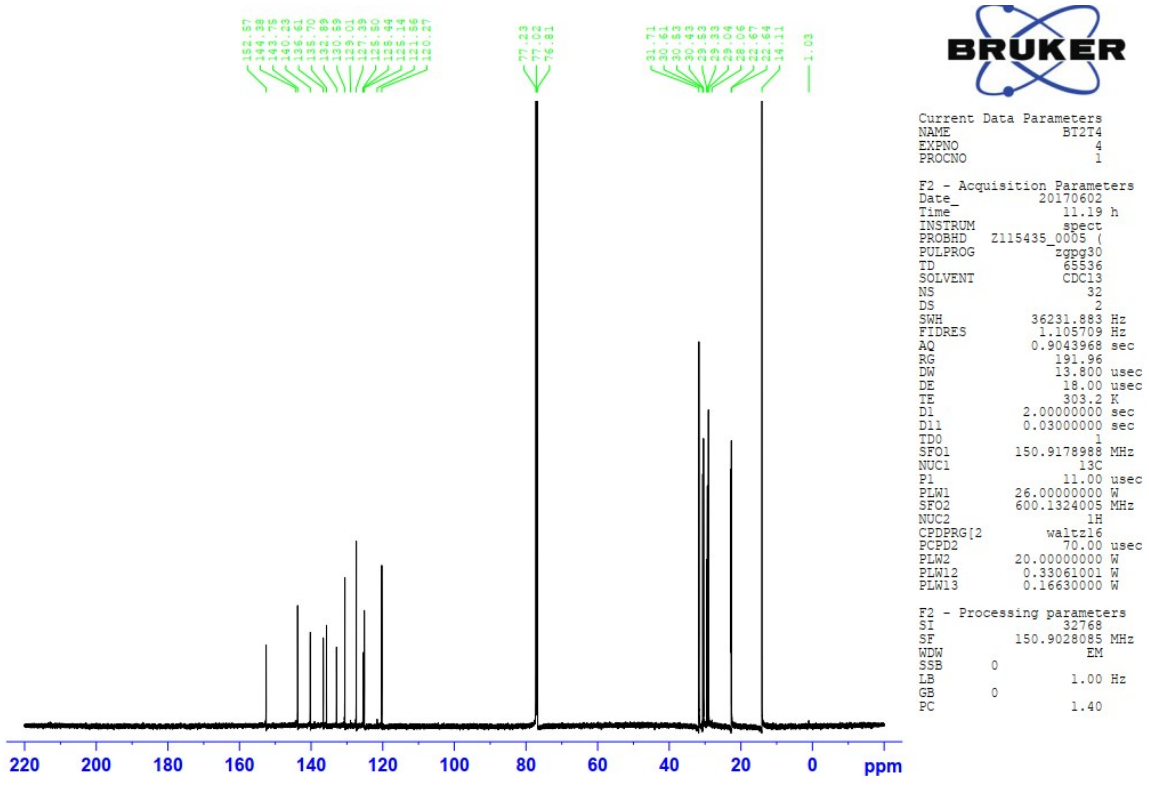
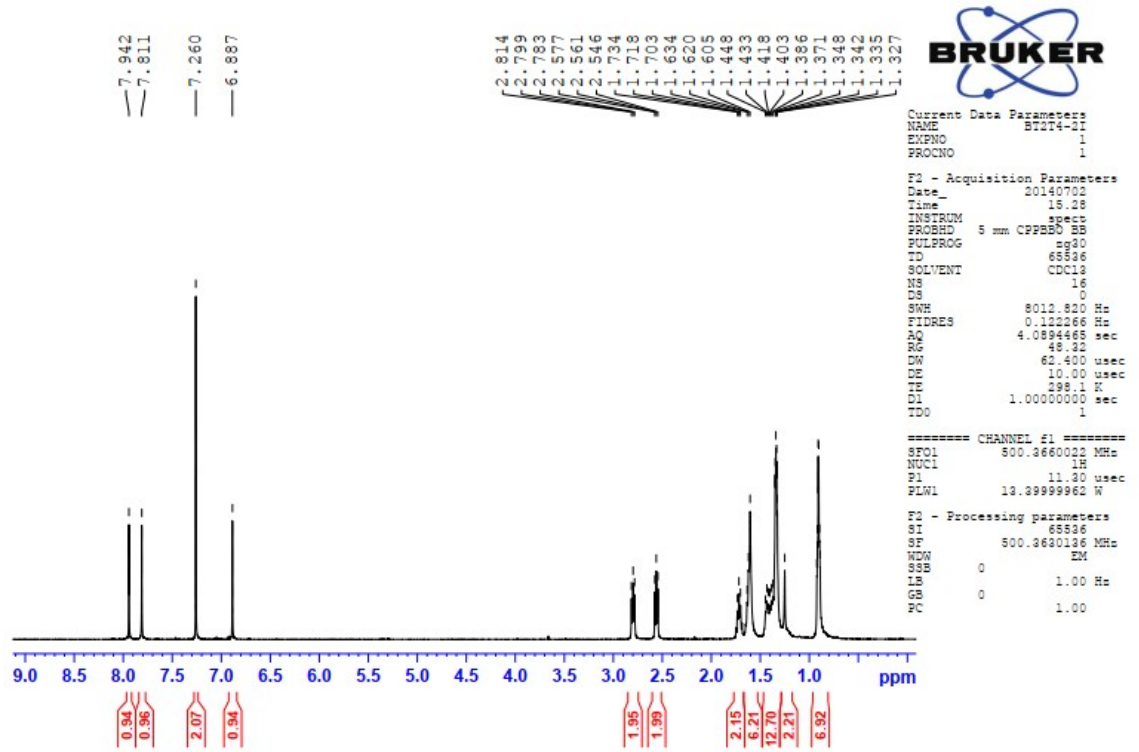
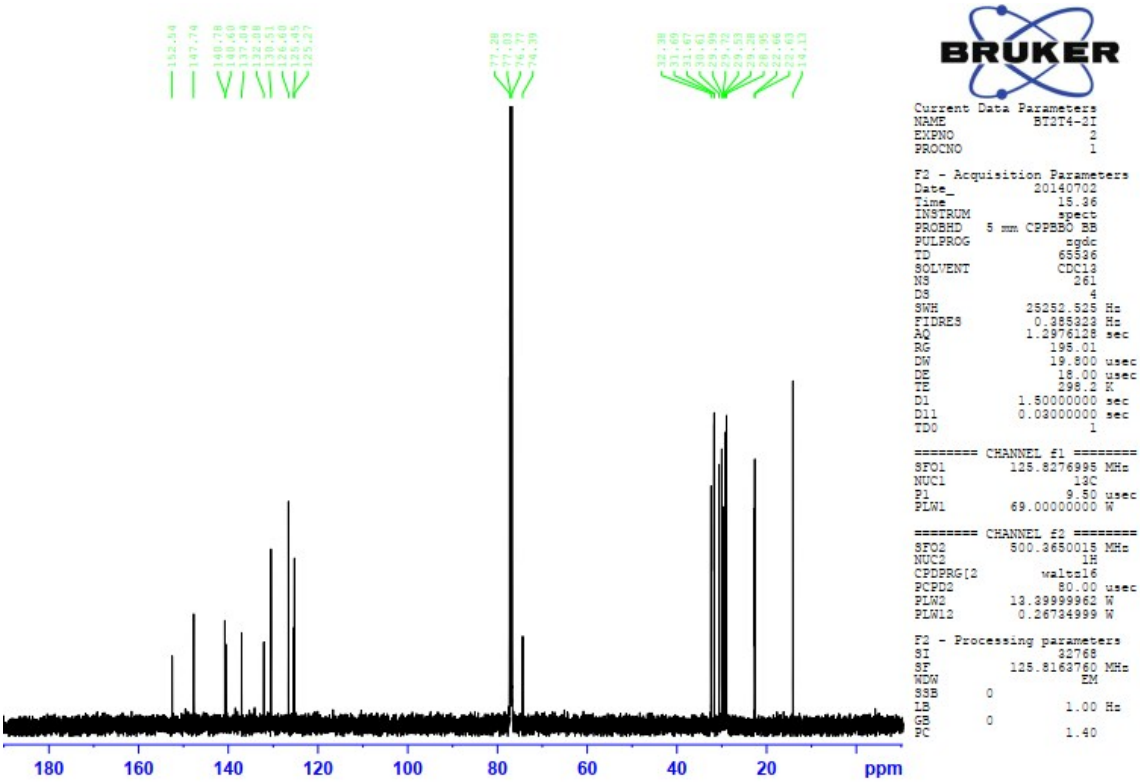
10.82
6.26


152.57
144.98
140.75
140.23
136.63
135.70
132.89
130.59
129.01
127.39
126.50
126.44
125.14
121.56
120.27
77.23
77.02
76.81
31.71
30.61
30.53
30.43
29.53
29.33
29.04
28.06
22.67
22.64
14.11
1.03
BRUKER
Current Data Parameters
NAME BT2T4
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170602
Time 11.19 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
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 150.9178988 MHz
NUC1 13C
P1 11.00 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.33061001 W
PLW13 0.16630000 W
F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
220 200 180 160 140 120 100 80 60 40 20 0 ppm

Compound 5

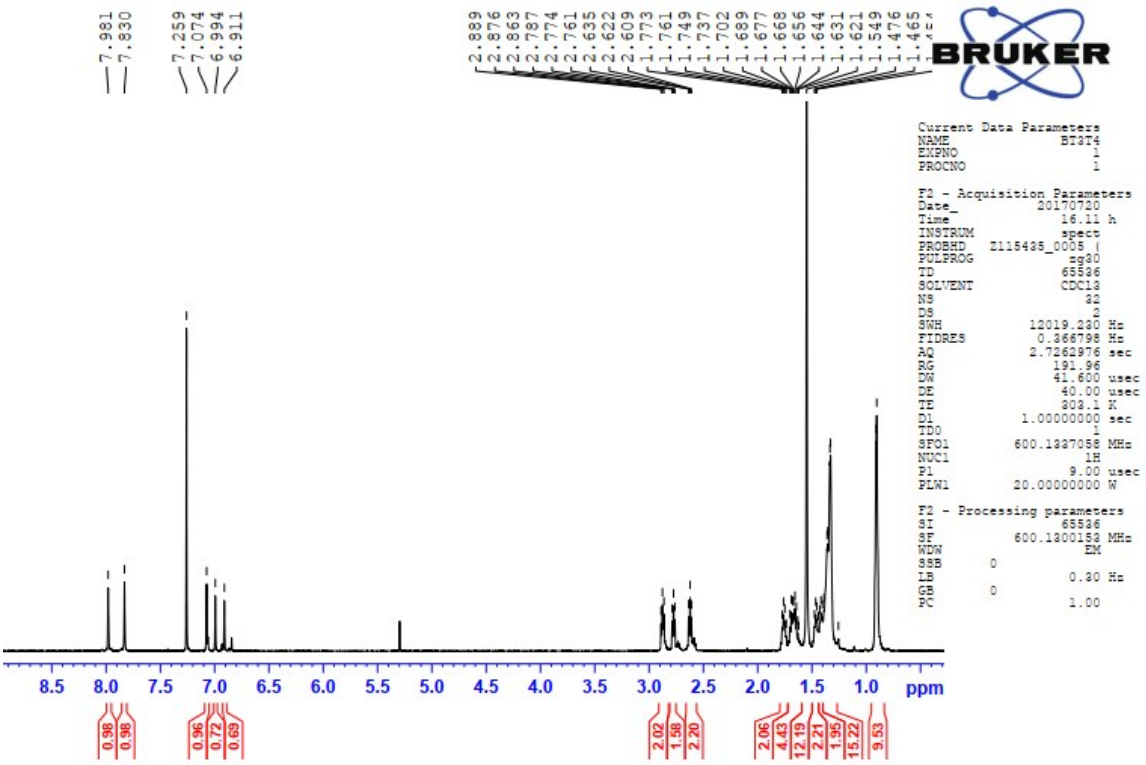


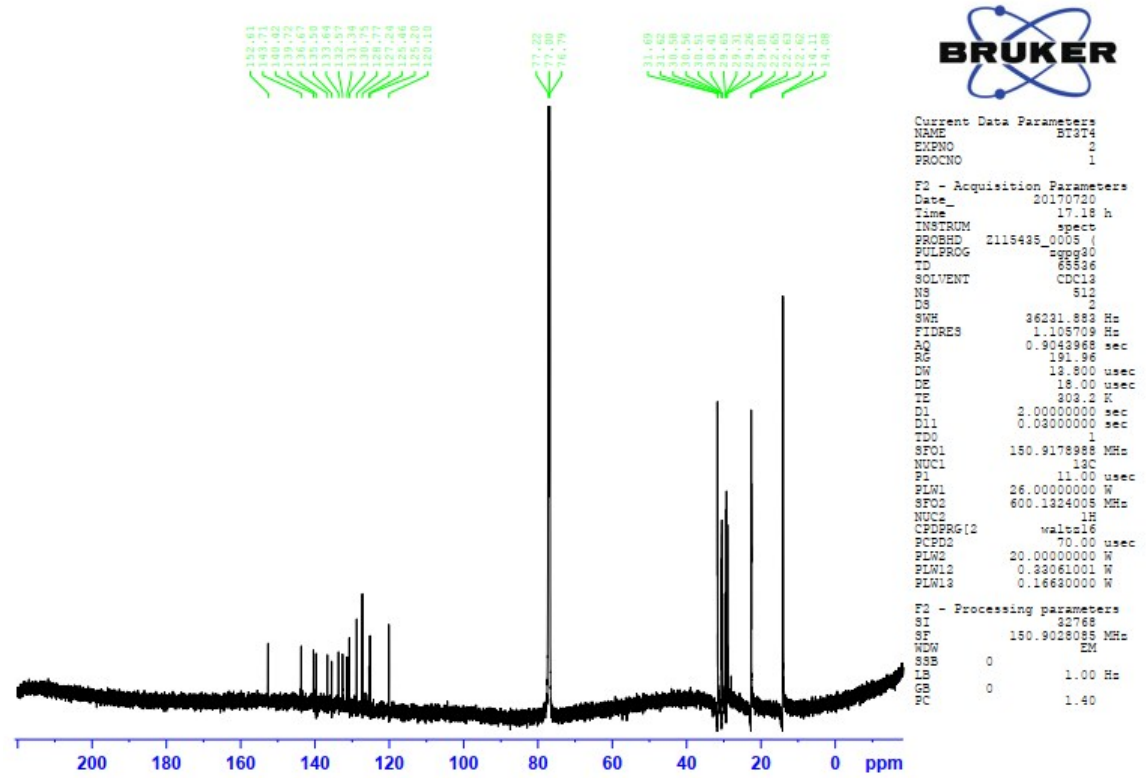

```
Current Data Parameters
NAME                  BT2T4-2I
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140702
Time                   15.28
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
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
TD0                          1

======== CHANNEL f1 ========
SFO1               500.3660022 MHz
NUC1                       1H
P1                      11.30 usec
PLW1               13.39999962 W

F2 - Processing parameters
SI                       65536
SF                 500.3630136 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.00
```



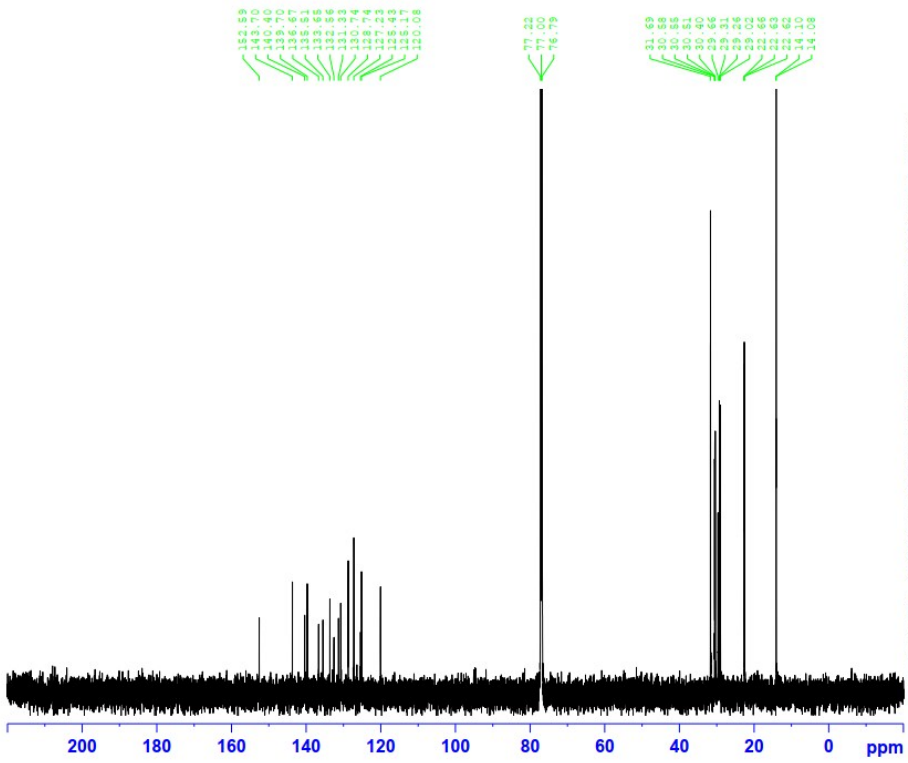

```
Current Data Parameters
NAME                  BT2T4-3I
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20140702
Time                   15.36
INSTRUM                spect
PROBHD    5 mm CPPBBO BB
PULPROG                zgdc
TD                    65536
SOLVENT               CDCl3
NS                      261
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                    298.2 K
D1                 1.50000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1               125.8276995 MHz
NUC1                       13C
P1                       9.50 usec
PLW1               69.00000000 W

======== CHANNEL f2 ========
SFO2               500.3650015 MHz
NUC2                       1H
CPDPRG[2                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
```

Compound 6


7.981
7.830
7.259
7.074
6.994
6.911
2.889
2.876
2.863
2.787
2.774
2.761
2.635
2.622
2.609
1.773
1.761
1.749
1.737
1.702
1.689
1.677
1.668
1.656
1.644
1.631
1.621
1.549
1.476
1.465
BRUKER
Current Data Parameters
NAME BT3T4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170720
Time 16.11 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 191.96
DW 41.600 usec
DE 40.00 usec
TE 303.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 9.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300153 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.98 0.98 0.96 0.72 0.69 2.02 1.58 2.20 2.06 4.43 12.19 2.21 1.95 15.22 9.53

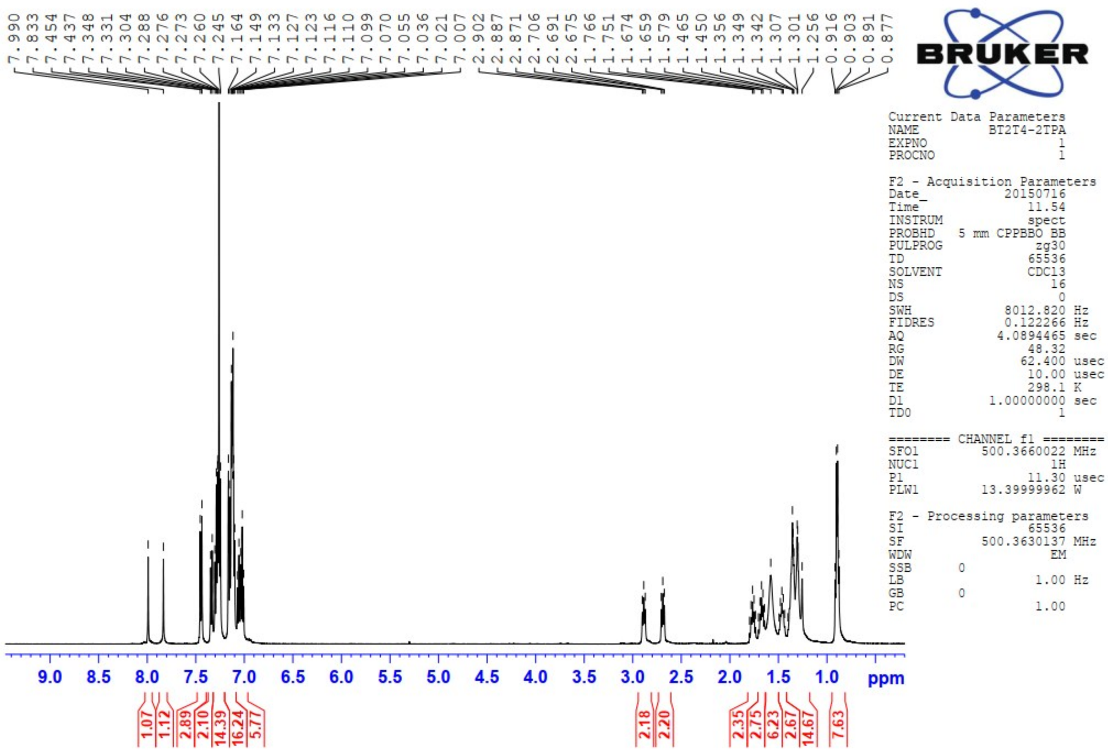

77.22
77.00
76.79
BRUKER
Current Data Parameters
NAME BT3T4
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170720
Time 17.18 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 18.00 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 11.00 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.33061001 W
PLW13 0.16630000 W
F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

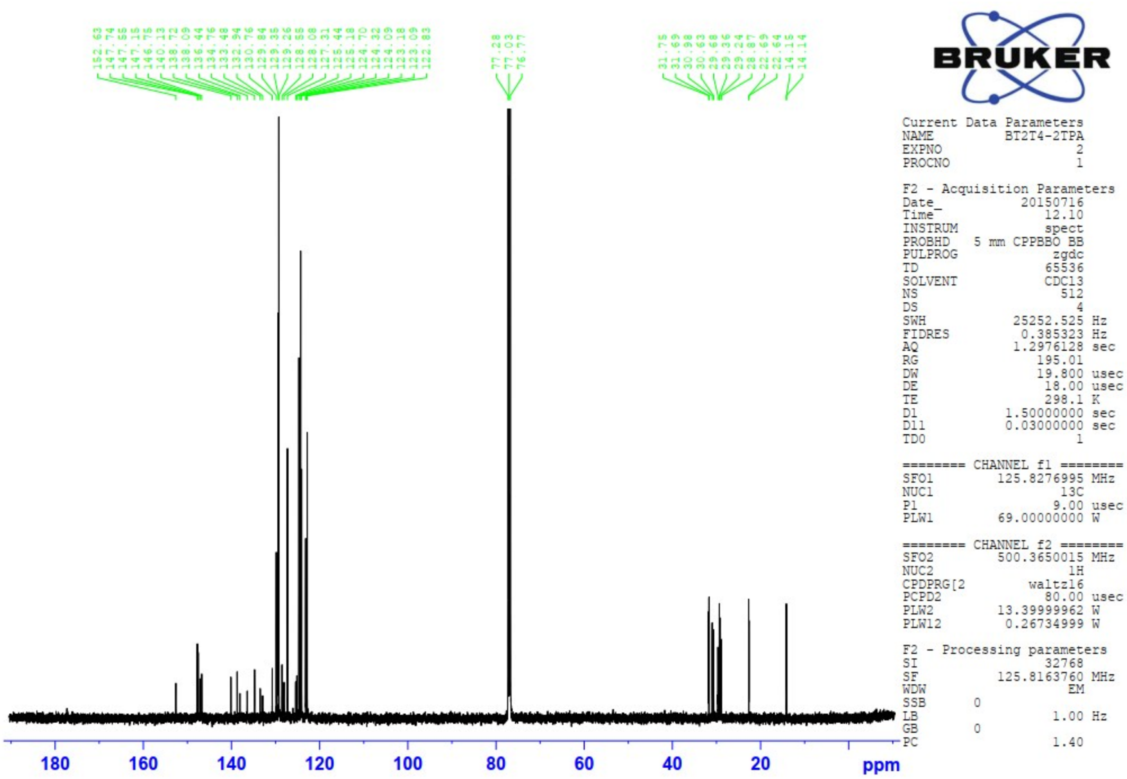
Compound 7




```
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
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          150.9028090 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

TBtz1


7.990 7.833 7.454 7.437 7.348 7.331 7.304 7.288 7.276 7.273 7.260 7.245 7.164 7.149 7.133 7.127 7.123 7.116 7.110 7.099 7.070 7.055 7.036 7.021 7.007 2.902 2.887 2.871 2.706 2.691 2.675 1.766 1.751 1.674 1.659 1.579 1.465 1.450 1.356 1.349 1.342 1.307 1.301 1.256 0.916 0.903 0.891 0.877
BRUKER
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
TD 65536
SOLVENT CDCl3
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
TD0 1
======== CHANNEL f1 ========
SFO1 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
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.07 1.12 2.89 2.10 14.39 16.24 5.77 2.18 2.20 2.35 2.75 6.23 2.67 14.67 7.63


152.63 147.74 147.55 147.15 146.75 140.13 138.72 138.09 136.44 134.76 133.48 132.94 130.76 129.84 129.35 129.26 128.55 128.08 127.31 125.44 125.18 124.70 124.32 124.09 123.18 123.09 122.83
77.28 77.03 76.77
31.75 31.69 30.98 30.63 29.68 29.36 29.24 28.87 22.69 22.64 14.15 14.14
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
TD 65536
SOLVENT CDCl3
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
TD0 1
======== CHANNEL f1 ========
SFO1 125.8276995 MHz
NUC1 13C
P1 9.00 usec
PLW1 69.00000000 W
======== CHANNEL f2 ========
SFO2 500.3650015 MHz
NUC2 1H
CPDPRG[2 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
180 160 140 120 100 80 60 40 20 ppm

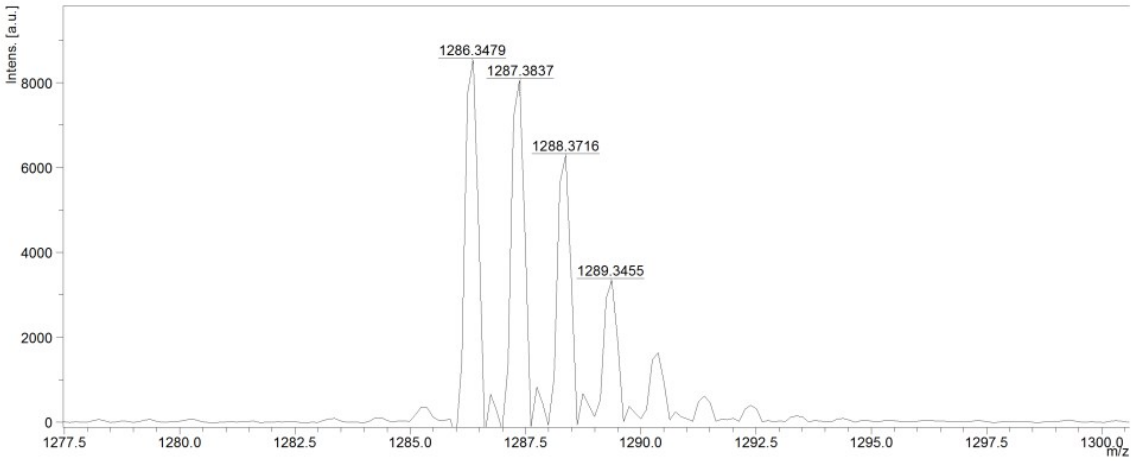
D:\Data\MSE\POSD\Ball\BT2T4-2TPA\0_M13\1\1SRef

MALDI-TOF-MS Report

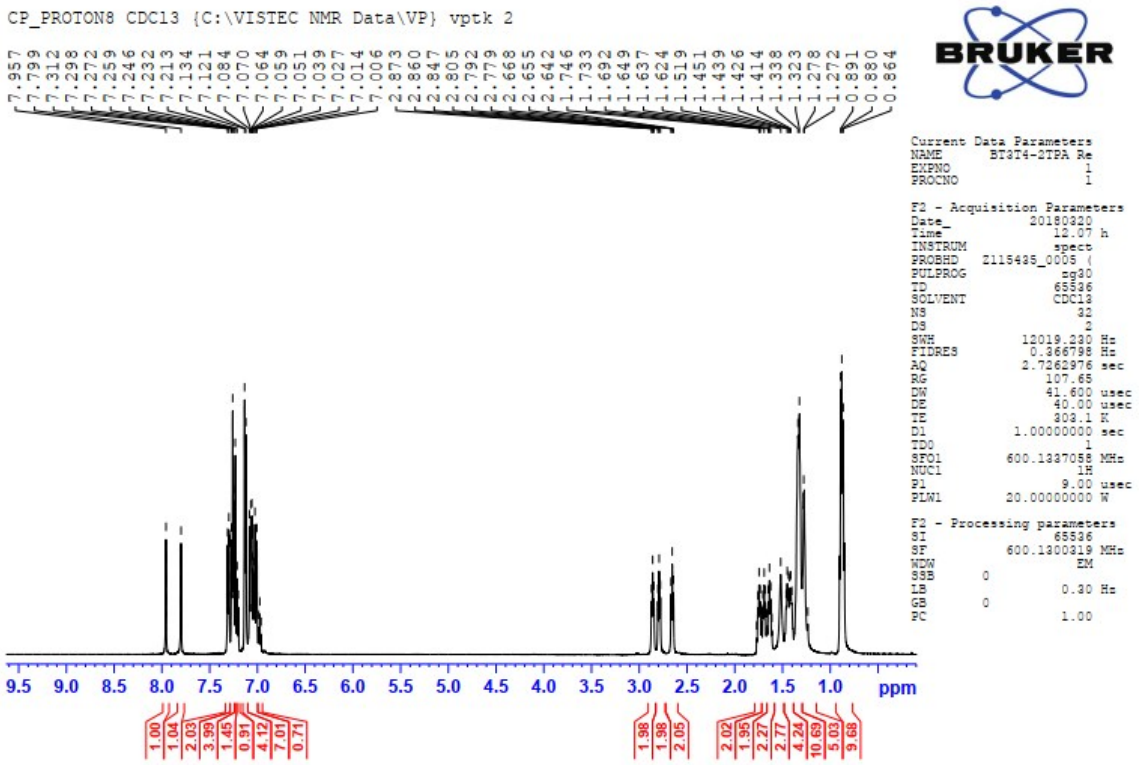
Frontier Research Center, Vidyasirimedhi Institute of Science and Technology

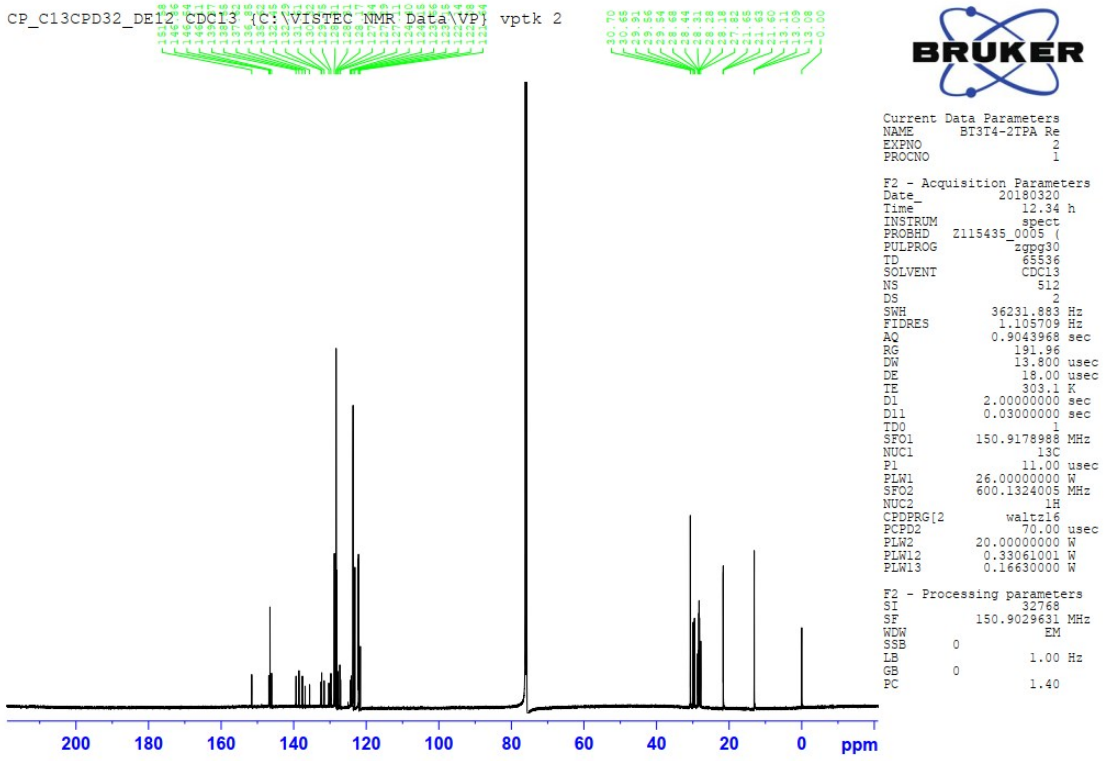
Comment 1 m/z = 1286.5456

Comment 2



TBtz2


CP_PROTON8 CDCl3 {C:\VISTEC NMR Data\VP} vptk 2
BRUKER
Current Data Parameters
NAME BT3T4-2TPA Re
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180320
Time 12.07 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 12019.230 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
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 9.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300319 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
ppm


CP_C13CPD32_DE12 CDCl3 {C:\VISTEC NMR Data\VP} vptk 2
BRUKER
Current Data Parameters
NAME BT3T4-2TPA Re
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20180320
Time 12.34 h
INSTRUM spect
PROBHD Z115435_0005 (
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 18.00 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 11.00 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.33061001 W
PLW13 0.16630000 W
F2 - Processing parameters
SI 32768
SF 150.9029631 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
ppm

D:\Data\MSE\POSD\Ball\BT3T4-2TPA\0_K9\1\1SRef

MALDI-TOF-MS Report

Frontier Research Center, Vidyasirimedhi Institute of Science and Technology

Comment 1 m/z = 1619.7122

Comment 2