Electronic Supplementary Material (ESI) for Journal of Materials Chemistry
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Supporting Information

Synthesis and Properties of Fluorene-olithiophenes Perylenediimide Triads and Their Electropolymerizations

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1. Synthesis

2-Nitro-7-(5-bromothiophen-2-yl)-9,9-didodecylfluorene (7)

To a solution of **2** (0.83 g, 1.39 mmol) in THF (26 ml) under N_2 atmosphere, NBS (0.35 g, 1.98 mmol) was added in small portions. Water (100 ml) was added, the mixture was extracted with CH_2Cl_2 (2 x 50 ml). The combined organic layer was washed with water (100 ml), brine solution (100 ml), dried over anhydrous sodium sulfate, filtered and evaporated to dryness. Purification with column chromatography over silica gel eluting with CH_2Cl_2:hexane gave a light yellow viscous oil (0.86 g, 92%). IR (KBr): ν 727 cm^{-1}, 738, 797, 822, 886, 900, 990, 1006, 1079, 1127, 1208, 1339, 1443, 1460, 1521, 1588, 1611, 2851 and 2924; ^{1}H-NMR (300 MHz): δ 0.59 ppm (d, 4 H, *J* = 4.20 Hz), 0.86 (t, 7 H, *J* = 6.90 Hz), 1.20 (m, 35 H), 2.04 (t, 4 H, *J* = 7.50Hz), 7.07 (d, 1 H, *J* = 3.90 Hz), 7.17 (d, 1 H, *J* = 3.60 Hz), 7.51 (s, 1H), 7.55 (d, 1 H, *J* = 6.60 Hz), 7.77 (d, 1 H, *J* = 5.10 Hz), 8.19 (s, 1 H) and 8.25 (d, 1 H, *J* = 6.30 Hz); ^{13}C-NMR (75 MHz): δ 14.10 ppm, 22.67, 23.74, 29.16, 29.30, 29.47, 29.52, 29.58, 29.80, 31.89, 40.02, 55.84, 112.08, 118.26, 119.84, 119.92, 121.78, 123.42, 123.81, 125.05, 131.03, 134.55, 138.50, 145.74, 146.89, 147.20, 152.09 and 153.34; HRMS-ESI calcd for $C_{41}H_{58}BrNO_2S$: *m/z* 707.3372; found: *m/z* 707.7010 [M^+].

2-Nitro-7-(5′-bromo-2,2′-bithiophen-5-yl)-9,9-didodecylfluorene (8)

Compound **8** was synthesized from **3** in similar manner to **7** and obtained as a yellow solid (1.65 g, 97%). m.p. 48 °C; IR (KBr): ν 738 cm^{-1}, 788, 822, 881, 970, 1076, 1141, 1272, 1334, 1465, 1518, 1611, 2851 and 2929; ^{1}H-NMR (300 MHz): δ 0.62 ppm (s, 4 H), 0.85 (t, 6 H, *J* = 6.90 Hz), 1.15 (m, 36 H), 2.05 (t, 4 H, *J* = 7.89 Hz), 6.97 (dd, 2 H, *J* = 4.98 Hz), 7.11 (d, 1 H, *J* = 3.7 Hz), 7.20 (m, 1 H), 7.32 (d, 1 H, *J* = 3.80 Hz), 7.44 (m, 1 H), 7.57 (s, 1 H), 7.62 (dd, 1 H, *J* = 6.8 Hz), 7.76 (d, 2 H, *J* = 8.8 Hz), 8.20 (s, 1 H) and 8.30 (d, 1 H, *J* = 8.10 Hz); ^{13}C-NMR (75 MHz): δ 14.09 ppm, 22.66, 23.74, 29.17, 29.30, 29.47, 29.52, 29.58, 29.80,31.88, 40.04, 55.83, 111.27, 118.26, 119.79, 119.93, 121.74, 123.43, 123.85, 124.39, 124.95, 125.09, 130.76, 134.80, 136.21, 138.39, 138.71, 143.43, 146.98, 147.15, 152.08 and 153.31; HRMS-ESI calcd for $C_{45}H_{60}BrNO_2S_2$: *m/z* 789.3249; found: *m/z* 789.4159 [M^+].

2-Nitro-7-(5″-bromo-2,2′:5′,2″-terthiophen-5-yl)-9,9-didodecylfluorene (9)

Compound **9** was synthesized from **4** in similar manner to **7** and obtained as an orange solid (1.20 g, 91%). m.p. 80 °C; IR (KBr): ν 668 cm^{-1}, 738, 783, 794, 819, 967, 1074, 1138, 1219, 1328, 1462, 1518, 1588, 1608, 2341, 2364, 2851 and 2924; ^{1}H-NMR (300 MHz): δ 0.62 ppm (s, 4H), 0.84 (d, 12H, *J*=6.30 Hz), 1.17 (m, 30H), 2.08 (t, 4H, *J* = 7.50 Hz), 7.01 (t, 3H, *J* = 16.02 Hz), 7.14 (d, 2H, *J* = 19.21 Hz), 7.37 (s, 1H), 7.60 (t, 2H, *J* = 14.41 Hz), 7.79 (d, 2H, *J* = 8.1 Hz), 8.22 (s, 1H) and 8.28 (d, 1H, *J* = 8.10 Hz); ^{13}C-NMR (75 MHz): δ 14.11 ppm, 22.67, 23.74, 29.19, 29.32, 29.49; 29.54, 29.60, 29.82, 31.89, 40.07, 55.83, 118.25, 119.79, 119.87, 121.76, 123.45, 123.84, 124.38, 124.50, 124.70, 125.04, 130.76, 134.87, 138.20, 147.01, 147.10, 152.07, 153.31 and 155.12; HRMS-ESI calcd for $C_{49}H_{62}BrNO_2S_3$: *m/z* 871.3126; found: *m/z* 872.0018 [M^+].

2. Computer quantum calculation results

The ground state geometry of **PTF** was fully optimized using density functional theory (DFT) at the B3LYP/6-31G (d,p) level, as implemented in Gaussian 03. TDDFT/B3LYP calculation of lowest excitation energy was performed at the optimized geometry of the ground state.

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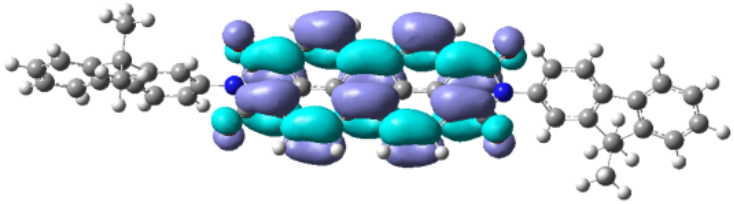

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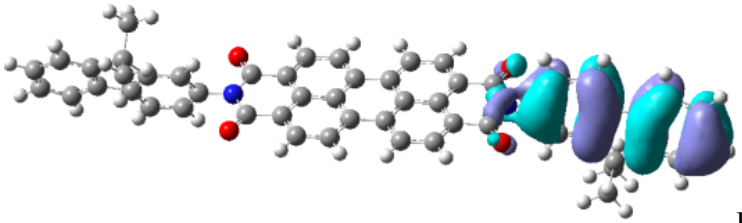

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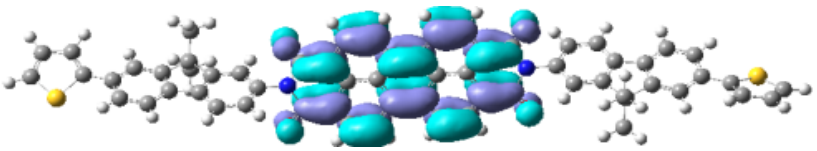

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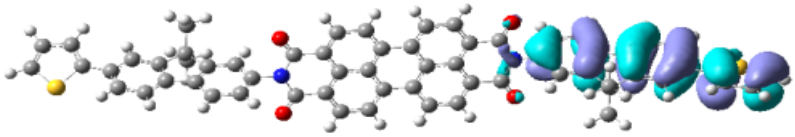

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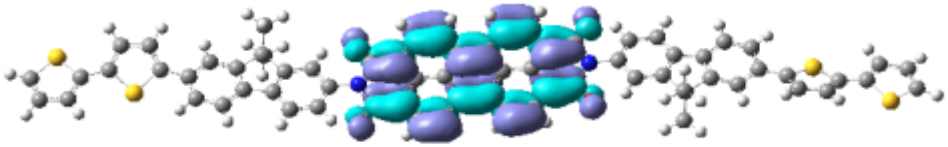

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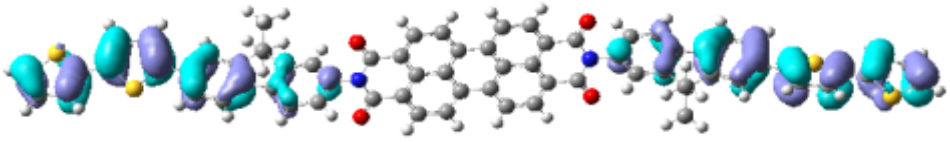

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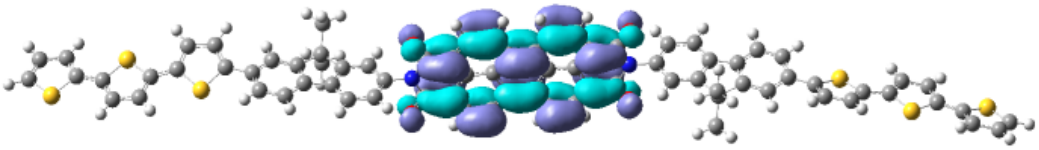

LUMO

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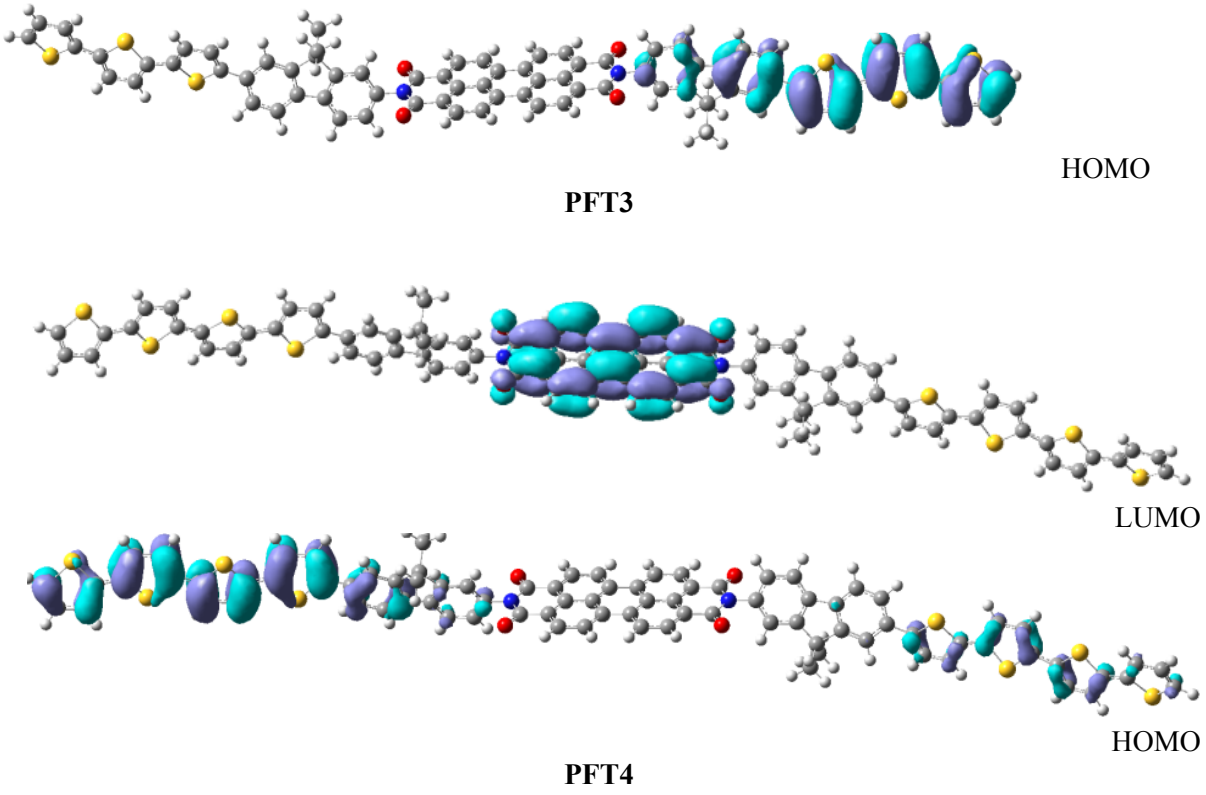

Fig. S1 The optimized geometries and HOMO-LUMO orbitals of **PFTn** by TDDFT/B3LYP(3,6)d.

Table S1. The calculated HOMO and LUMO energy levels and E_g of PFTn.

Compd	HOMO (eV)	LUMO (eV)	E_g (eV) Δ_{H-L}	E_g (eV) TDDFT
PF	-5.8164	-3.4226	2.3938	2.4182
PFT1	-5.4395	-3.4797	1.9598	2.4120
PFT2	-5.1715	-3.4648	1.7067	2.4074
PFT3	-4.9859	-3.4528	1.5331	2.4064
PFT4	-4.8948	-3.4716	1.4232	2.3913

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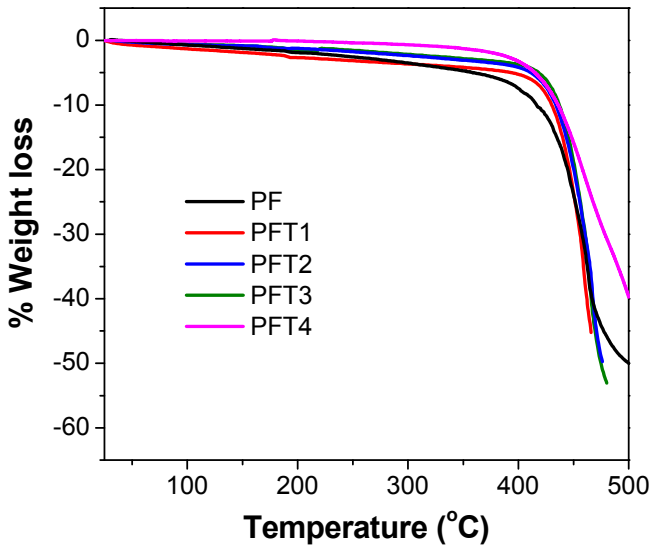

Fig. S2 TGA thermograms of **PFTn** measured at 10 °C/min under N_2.

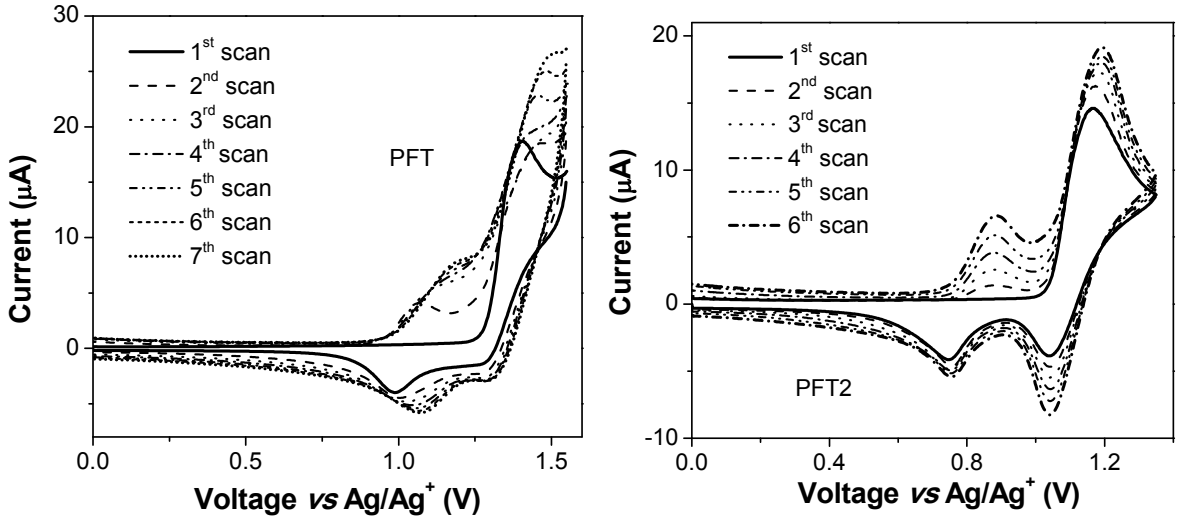

Figure S3 Repeated CV scans of **PFT1-2** in DCM/$TBAPF_6$ (0.1 M), scan rate of 100 mV/s, glassy carbon disk working electrode.

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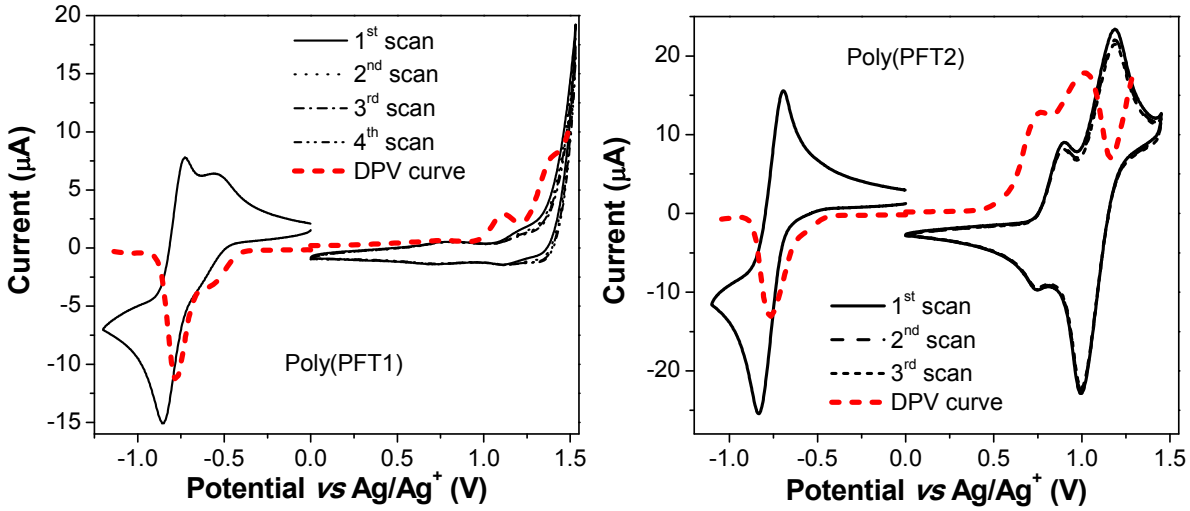

Figure S4 CV and DPV curves of polymer films, **poly(PFT1) and poly(PFT2)**, in DCM/$TBAPF_6$ (0.1 M), scan rate of 100 mV/s, glassy carbon disk working electrode.

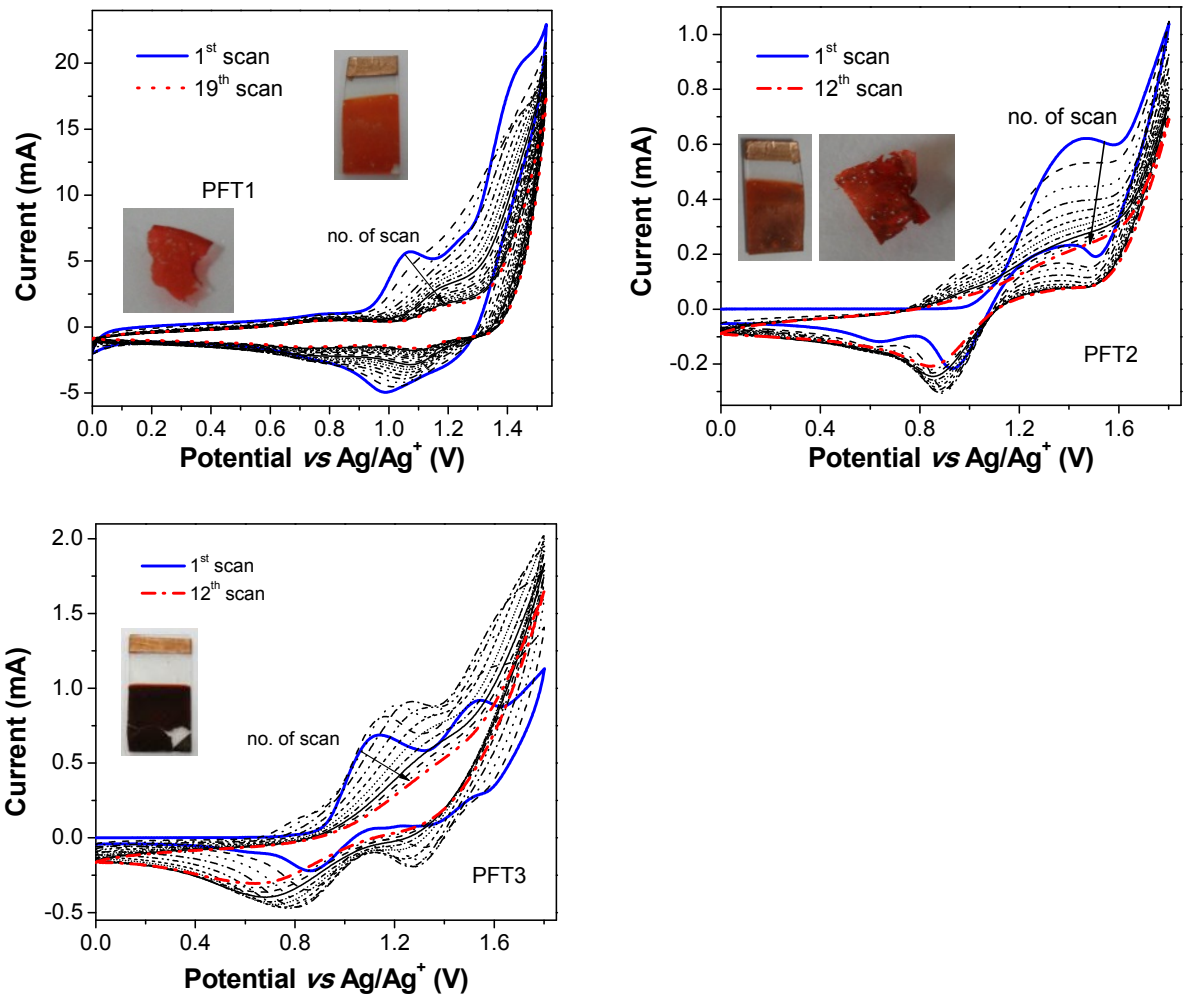

Figure S5 Repeated scan electropolymerization of **PFT1-3** in DCM/$TBAPF_6$ (0.1 M), scan rate of 100 mV/s, ITO/glass working electrode.

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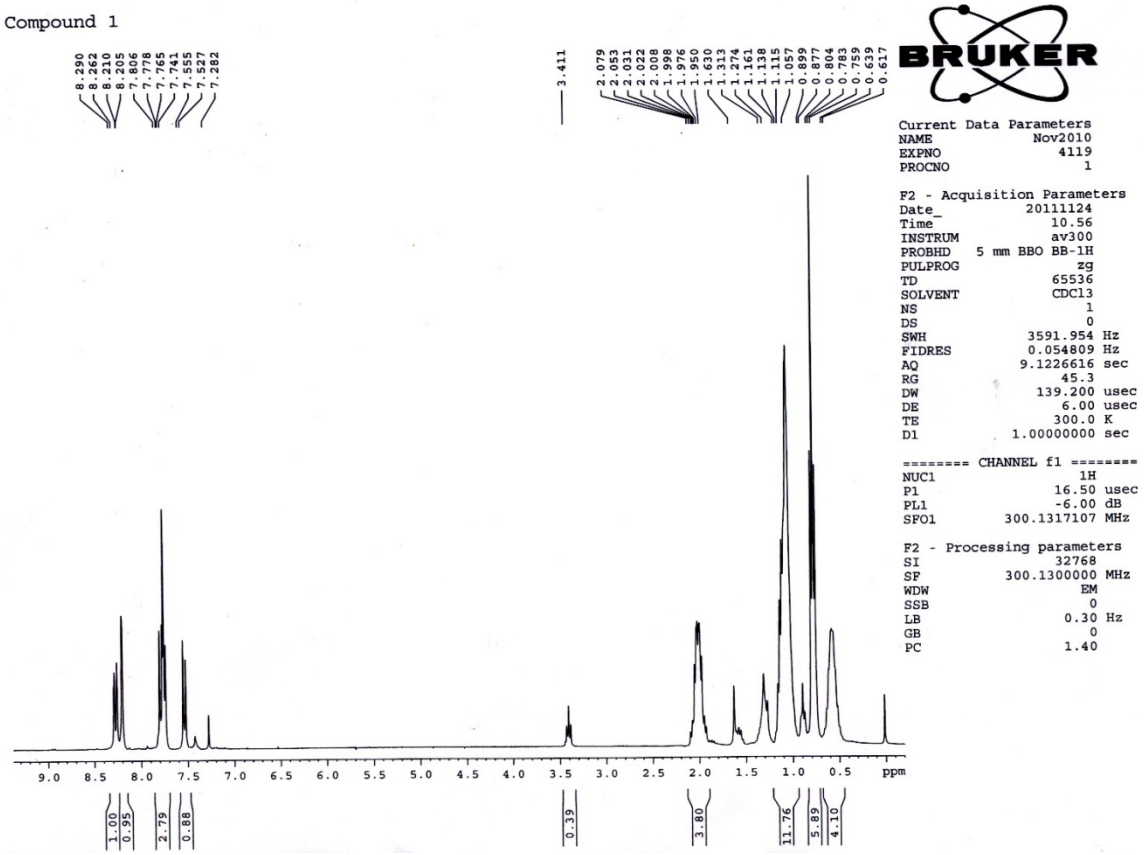
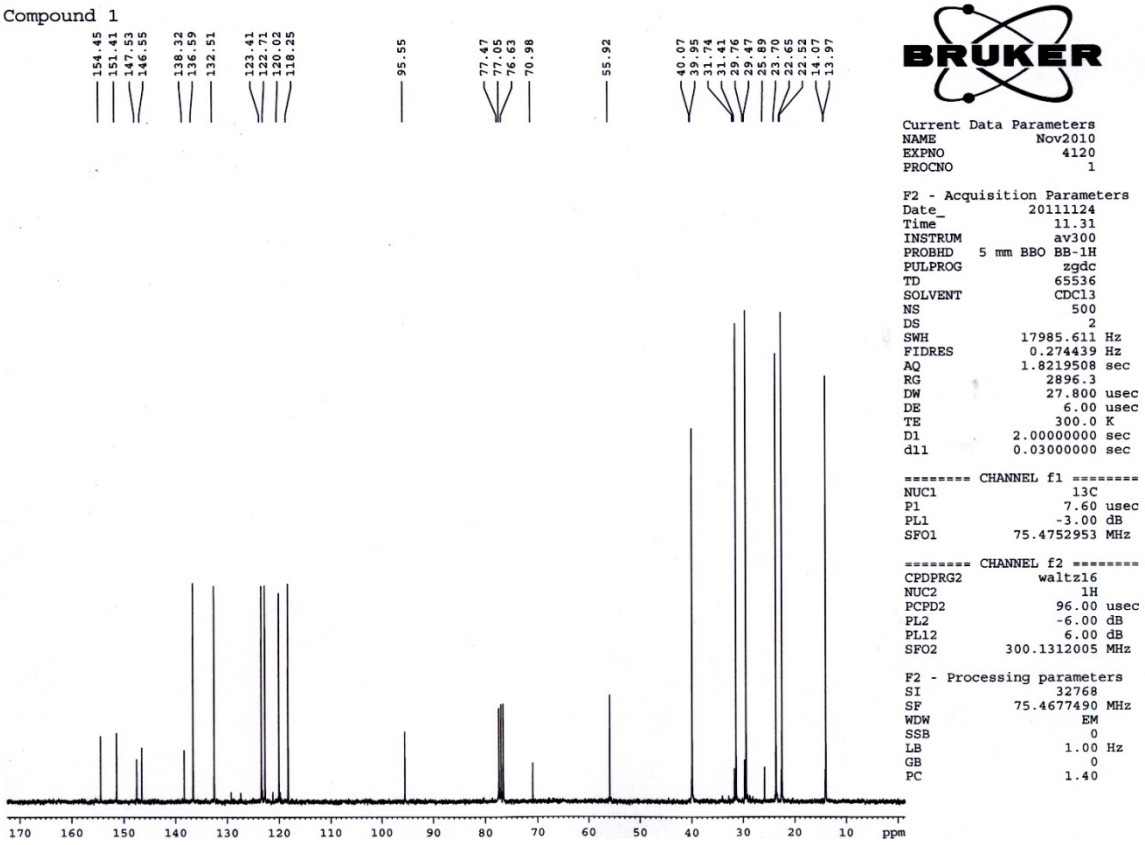
Figure S6. ^{1}H- and ^{13}C-NMR spectra





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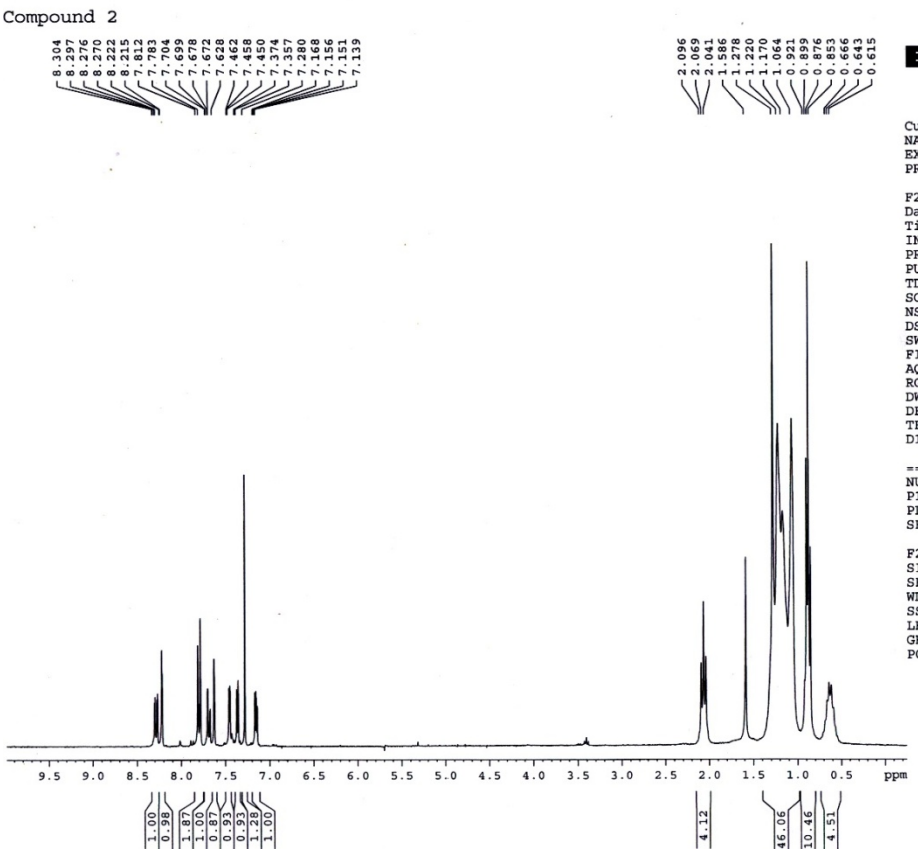

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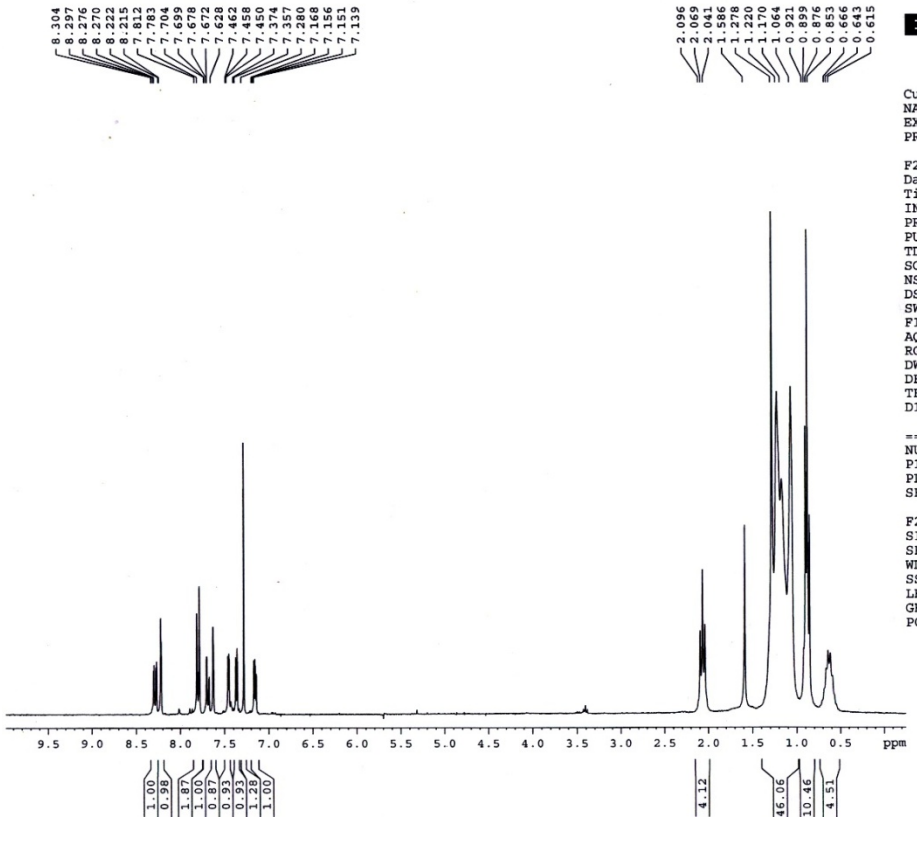

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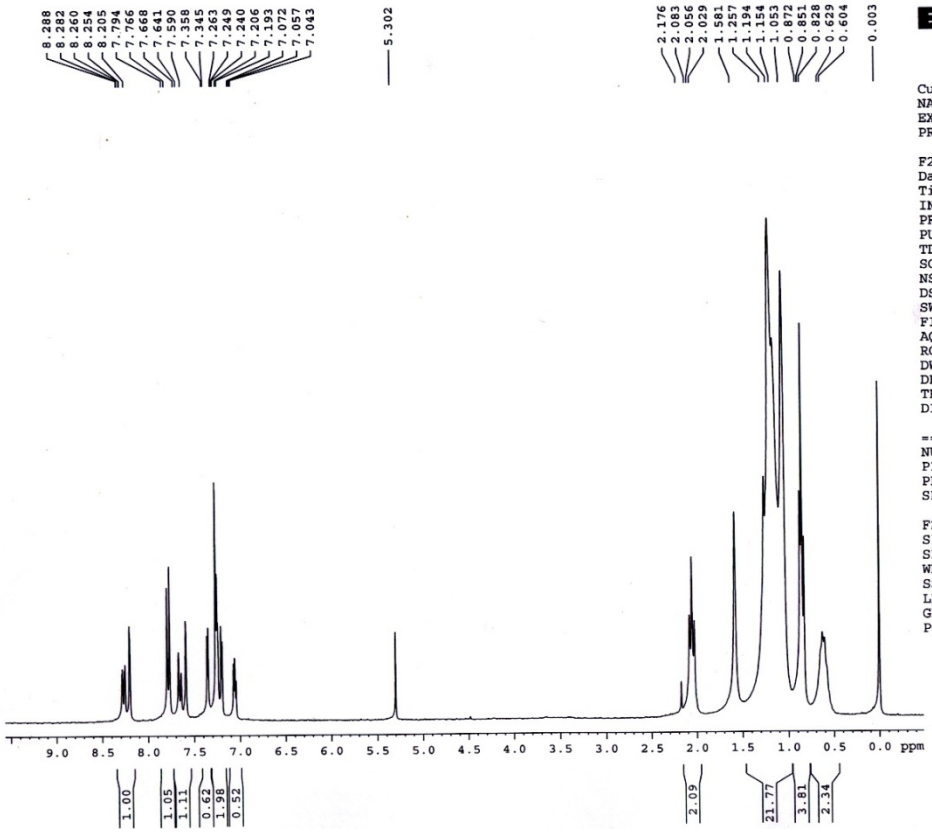
Compound 3



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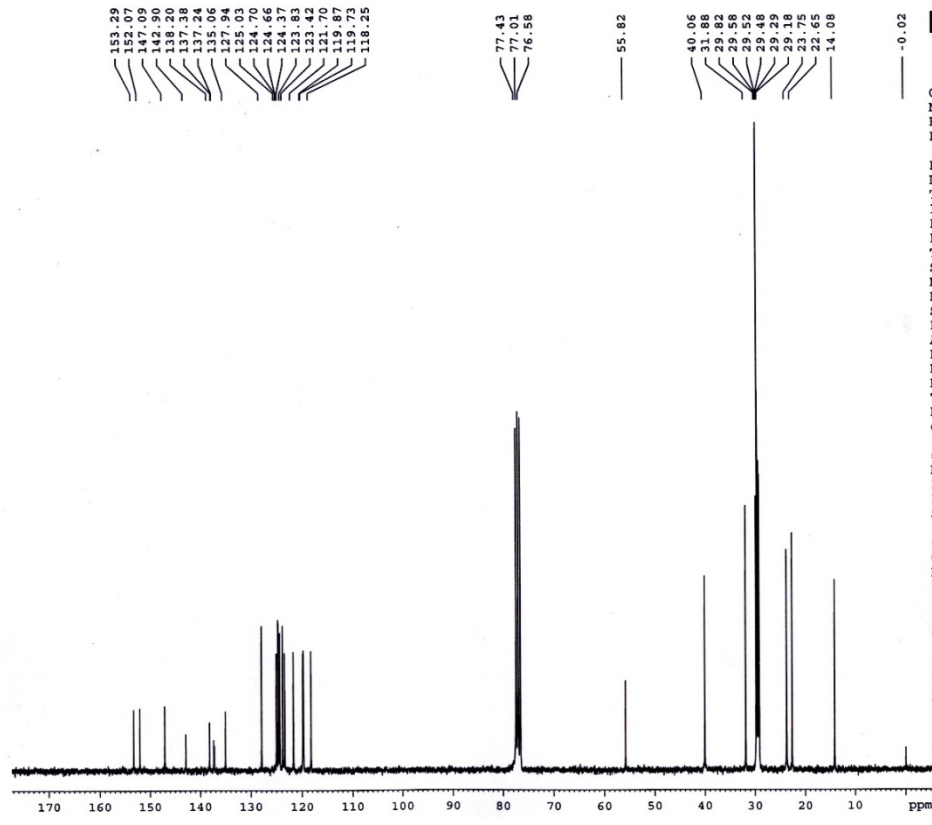

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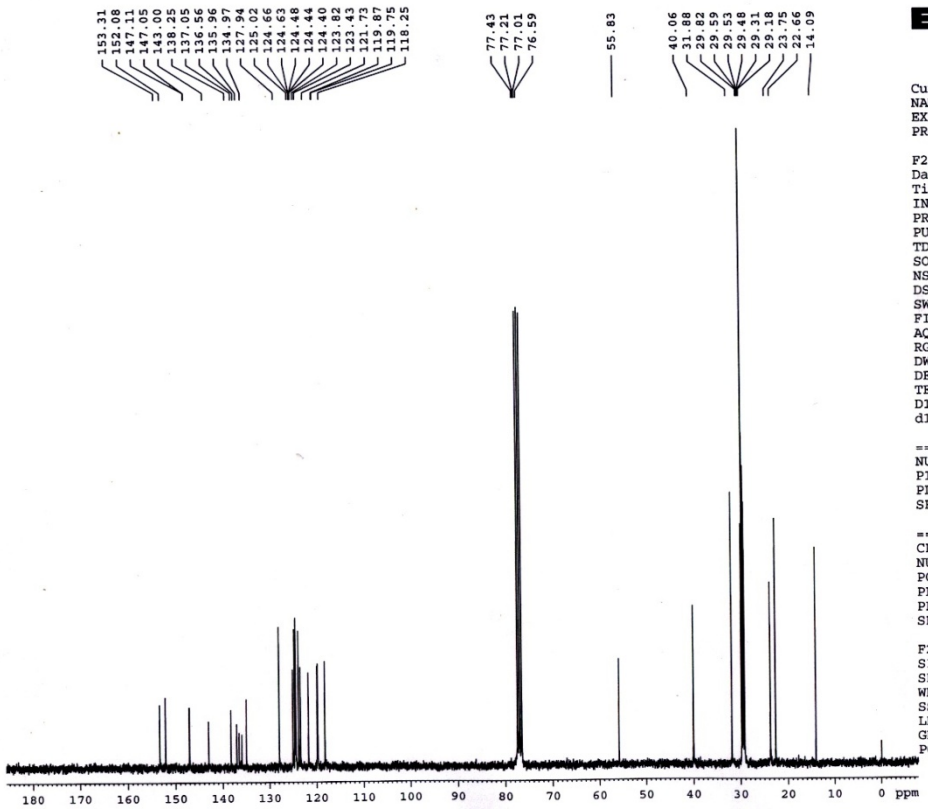

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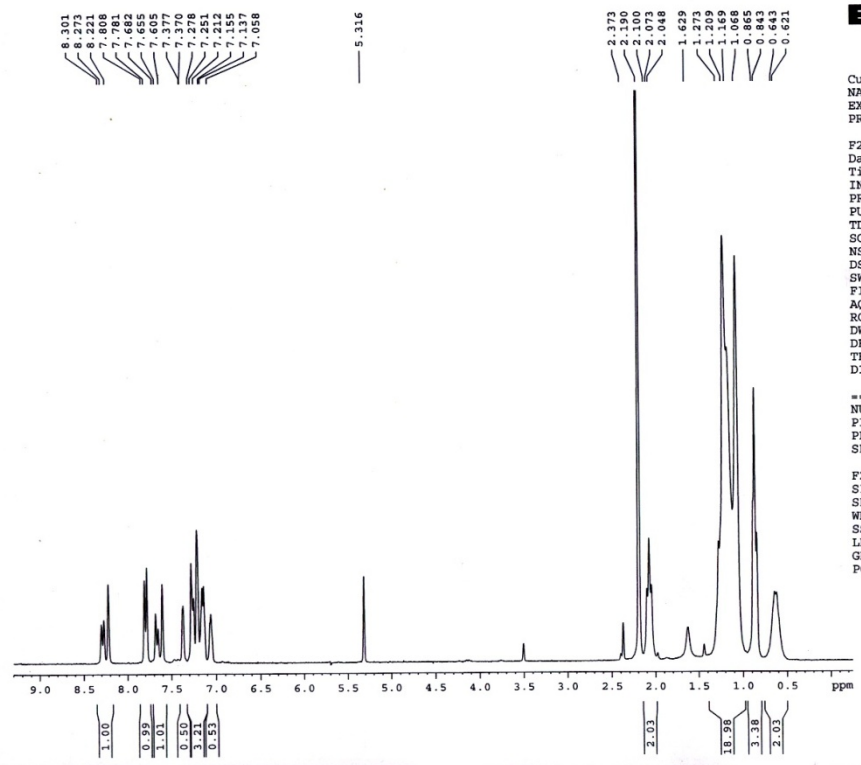

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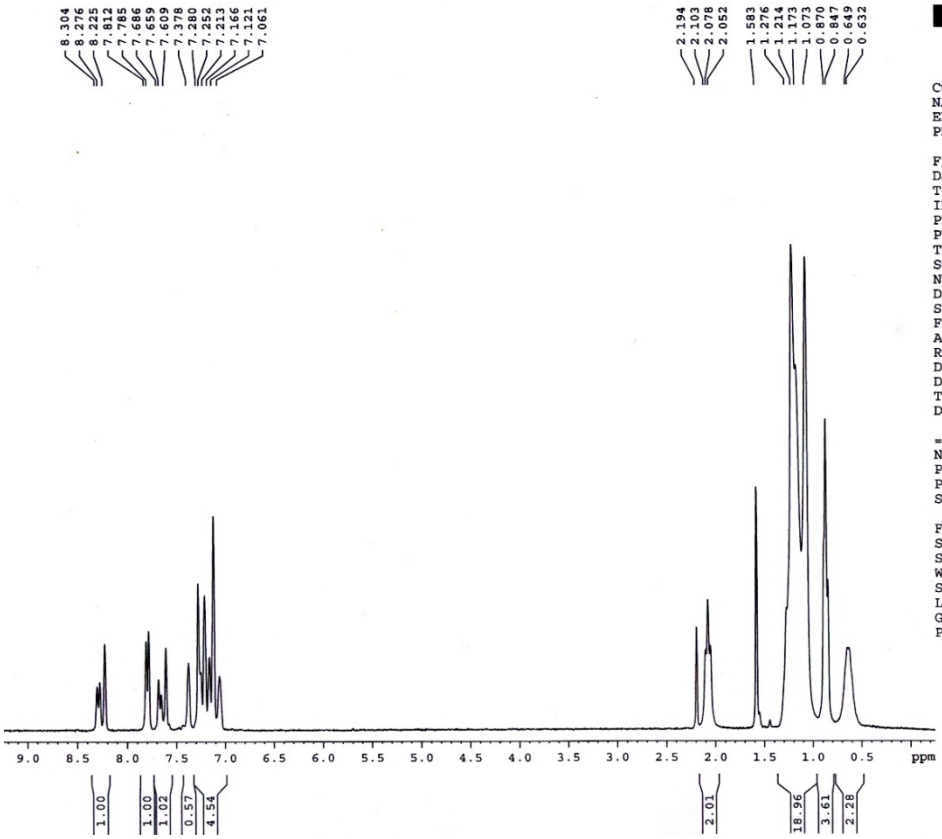

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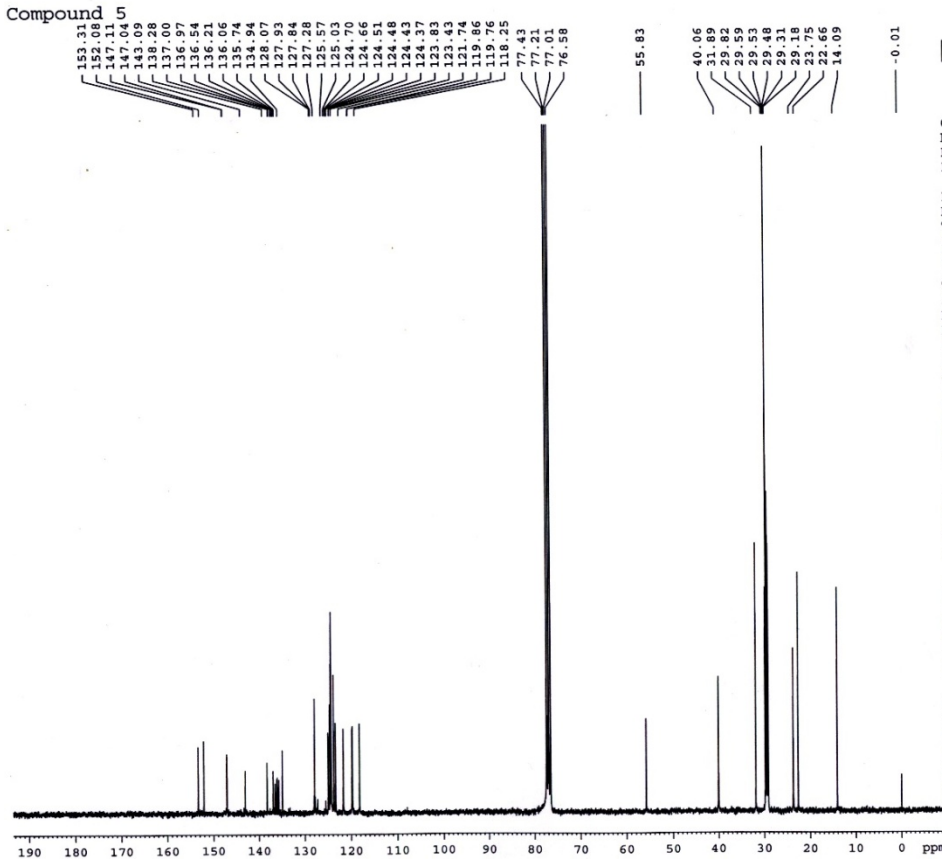

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SFO1 75.4752953 MHz

======== CHANNEL f2 ========
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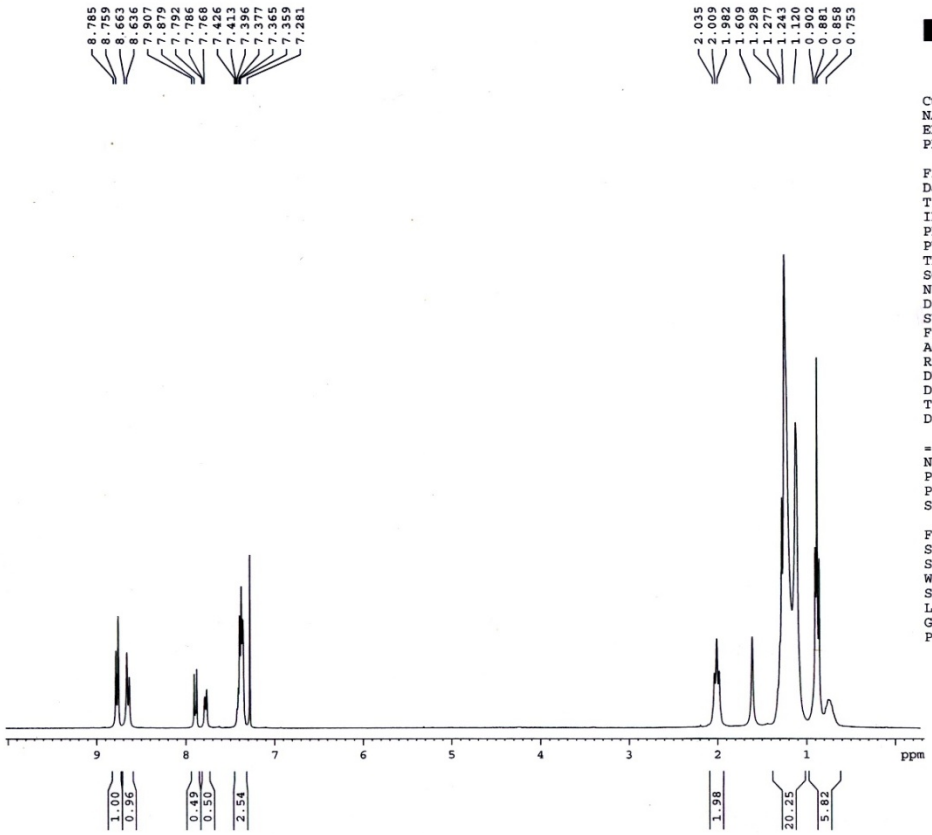
PF



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FIDRES                  0.054809 Hz
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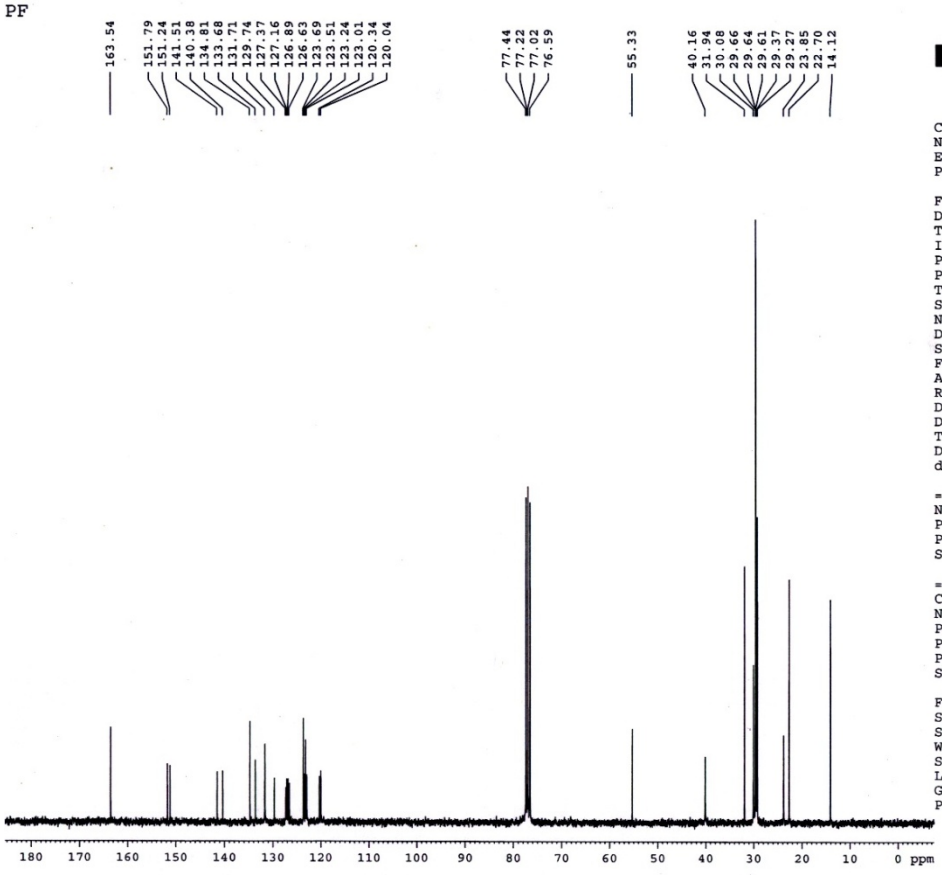
RG                           114
DW                       139.200 usec
DE                         6.00 usec
TE                        300.0 K
D1                    1.00000000 sec

======== CHANNEL f1 ========
NUC1                          1H
P1                         8.40 usec
PL1                       -1.00 dB
SFO1                300.1317107 MHz

F2 - Processing parameters
SI                         32768
SF                  300.1300000 MHz
WDW                           EM
SSB                            0
LB                          0.30 Hz
GB                             0
PC                          1.00
```

PF



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```
Current Data Parameters
NAME                  vp09-07-06
EXPNO                        439
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20070312
Time                       12.11
INSTRUM                    av300
PROBHD    5 mm BBO BB-1H
PULPROG                     zgdc
TD                         65536
SOLVENT                    CDCl3
NS                          2048
DS                             2
SWH                    17985.611 Hz
FIDRES                  0.274439 Hz
AQ                      1.8219508 sec
RG                          1024
DW                       27.800 usec
DE                         6.00 usec
TE                        300.0 K
D1                    2.00000000 sec
d11                   0.03000000 sec

======== CHANNEL f1 ========
NUC1                         13C
P1                         5.50 usec
PL1                       -6.00 dB
SFO1                75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                          1H
PCPD2                    100.00 usec
PL2                       -1.00 dB
PL12                      20.20 dB
SFO2                300.1312005 MHz

F2 - Processing parameters
SI                         32768
SF                  75.4677490 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40
```

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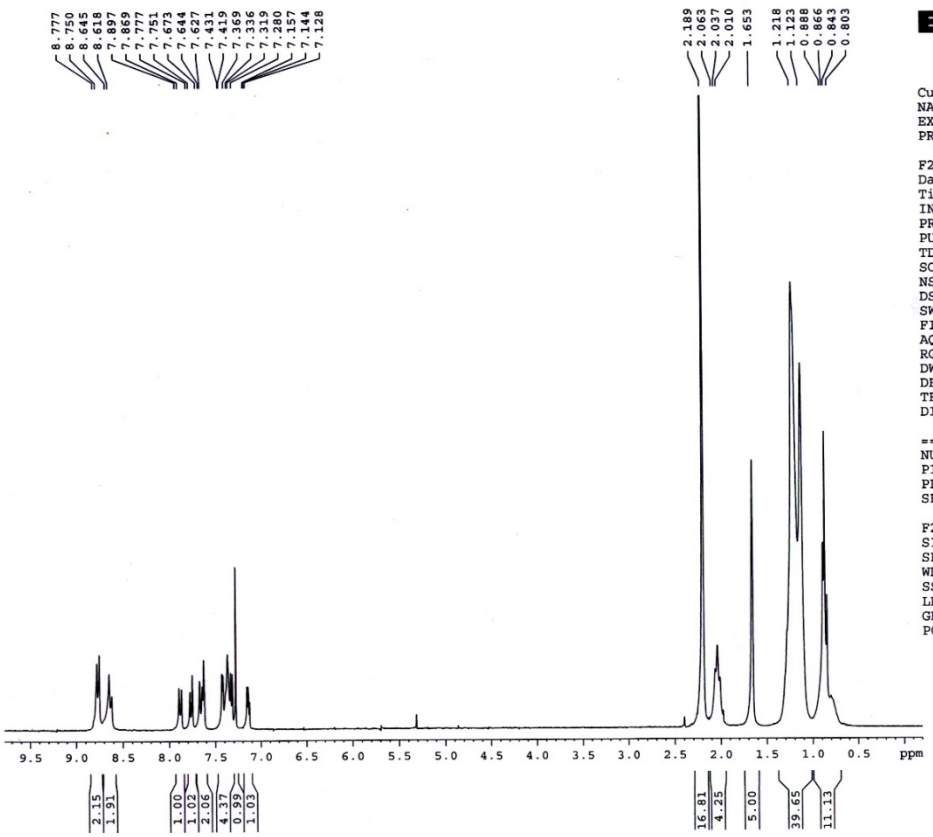
PFT1



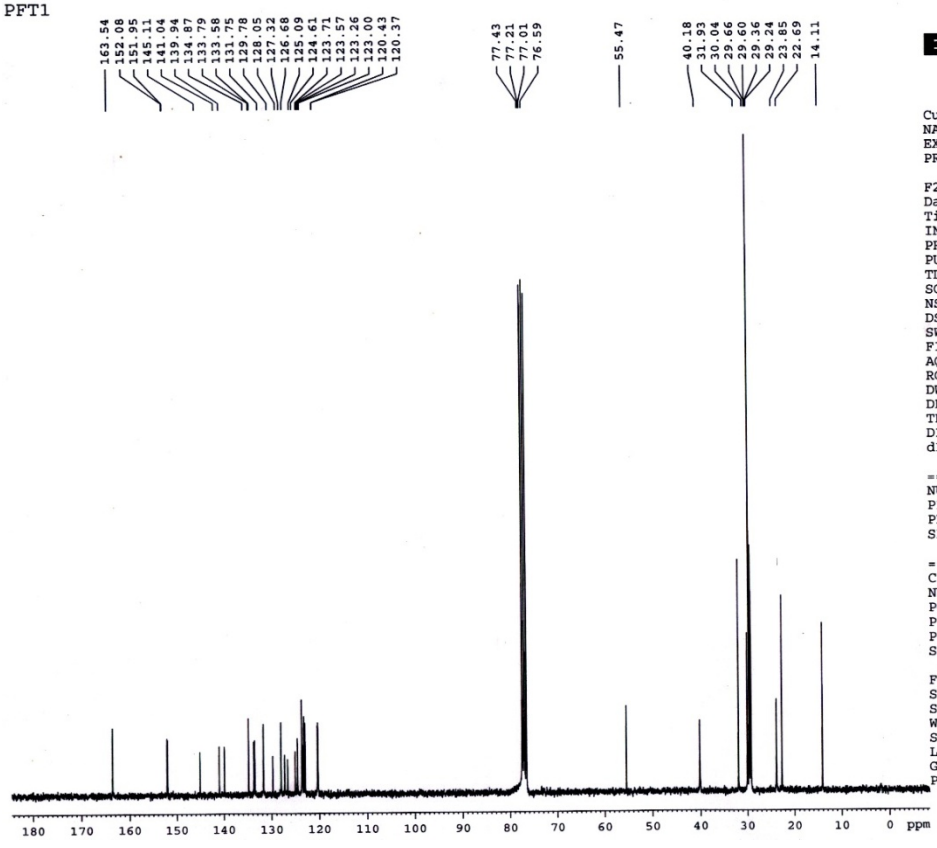
Current Data Parameters
NAME chem-04-07
EXPNO 335
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071101
Time 14.10
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 1
DS 0
SWH 3591.954 Hz
FIDRES 0.054809 Hz
AQ 9.1226616 sec
RG 90.5
DW 139.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
PL1 -1.00 dB
SFO1 300.1317107 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

PFT1



Current Data Parameters
NAME chem-04-07
EXPNO 573
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080123
Time 7.46
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 10240
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 645.1
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 5.60 usec
PL1 -6.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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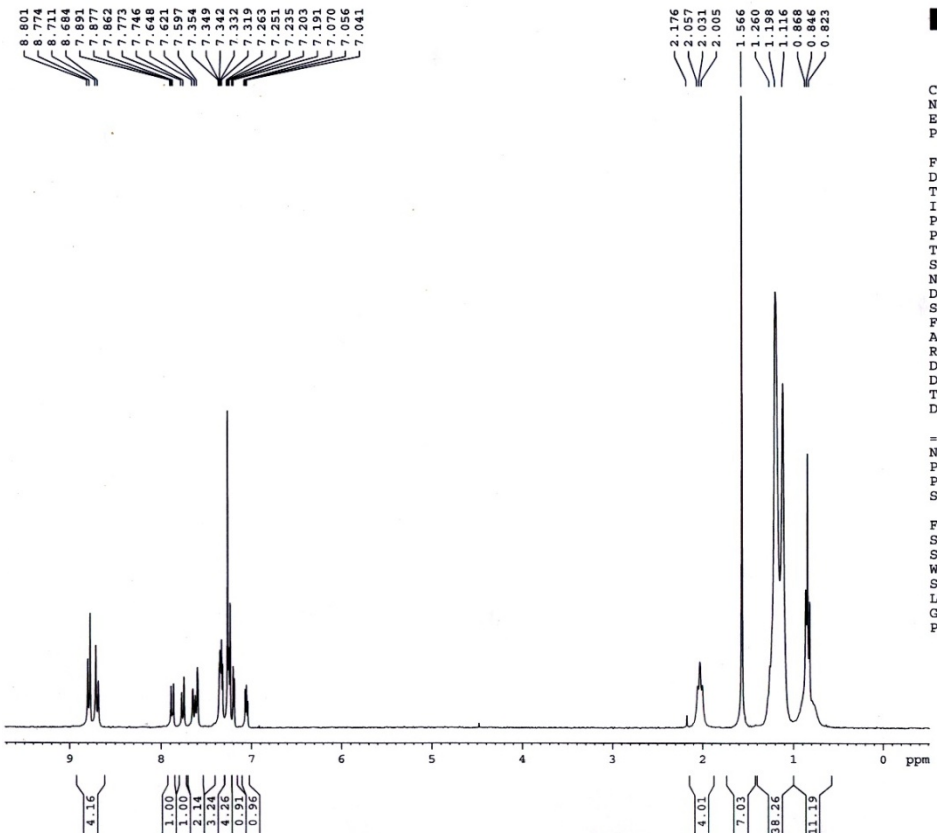
PFT2



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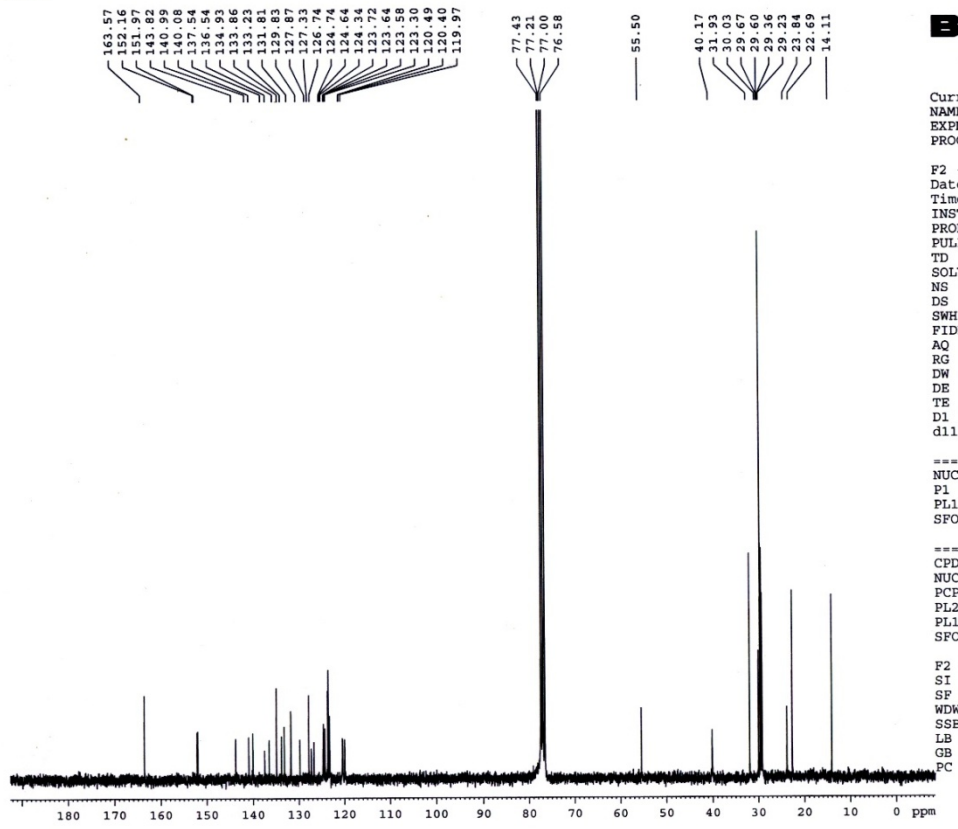
```
Current Data Parameters
NAME          chem-04-07
EXPNO                548
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080118
Time               19.10
INSTRUM            av300
PROBHD   5 mm BBO BB-1H
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                     1
DS                     0
SWH           4496.403 Hz
FIDRES        0.137219 Hz
AQ          3.6438515 sec
RG                   256
DW             111.200 usec
DE               6.00 usec
TE               300.0 K
D1          1.00000000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 8.60 usec
PL1               -1.00 dB
SFO1        300.1313506 MHz

F2 - Processing parameters
SI                 16384
SF          300.1300053 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

PFT2



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```
Current Data Parameters
NAME          chem-04-07
EXPNO                550
PROCNO                 1

F2 - Acquisition Parameters
Date_           20080119
Time               6.08
INSTRUM            av300
PROBHD   5 mm BBO BB-1H
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                  6144
DS                     2
SWH          17985.611 Hz
FIDRES        0.274439 Hz
AQ          1.8219508 sec
RG                1448.2
DW             27.800 usec
DE               6.00 usec
TE               300.0 K
D1          2.00000000 sec
d11         0.03000000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 5.60 usec
PL1               -6.00 dB
SFO1        75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2               -1.00 dB
PL12              20.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

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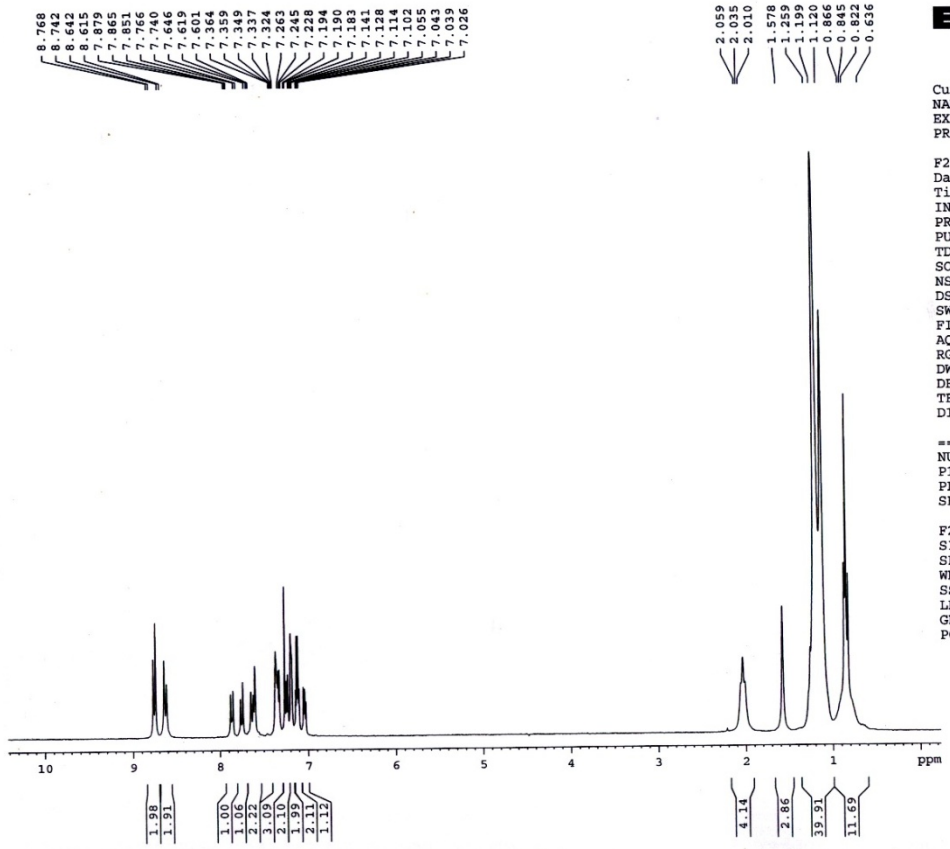
PFT3



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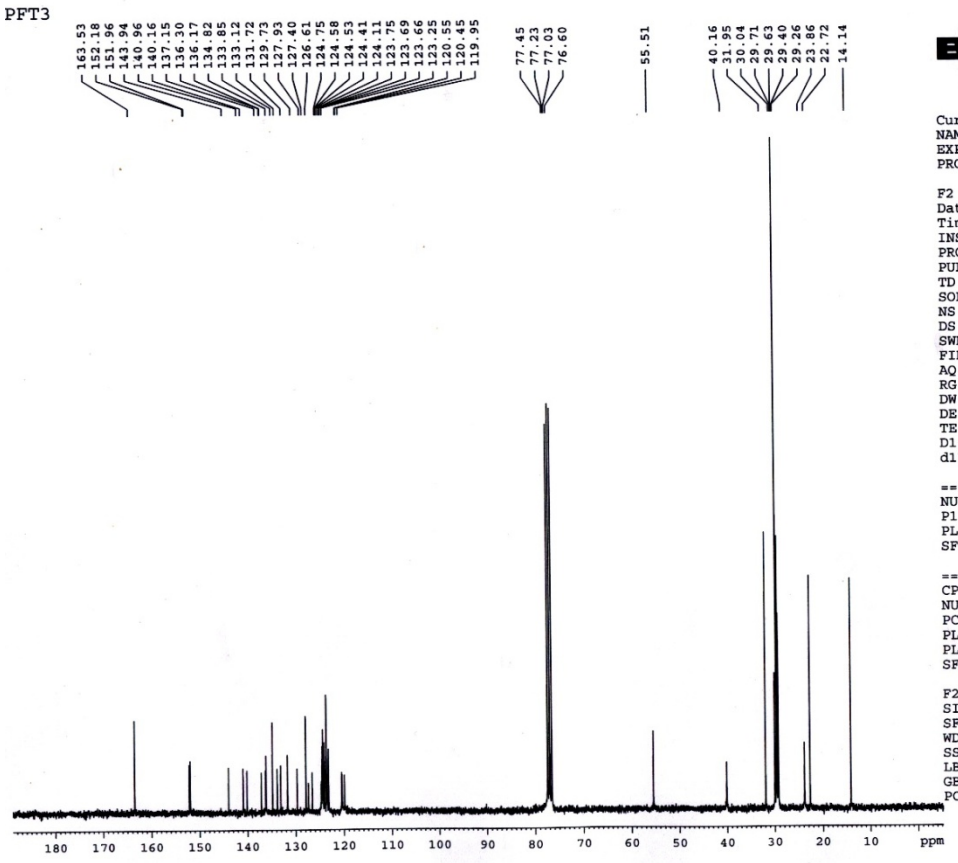
Current Data Parameters
NAME chem-04-07
EXPNO 511
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080115
Time 16.12
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 128
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 8.60 usec
PL1 -1.00 dB
SFO1 300.1313506 MHz

F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

PFT3



BRUKER

Current Data Parameters
NAME chem-04-07
EXPNO 514
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080115
Time 20.51
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 4096
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1448.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 5.60 usec
PL1 -6.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -1.00 dB
PL12 20.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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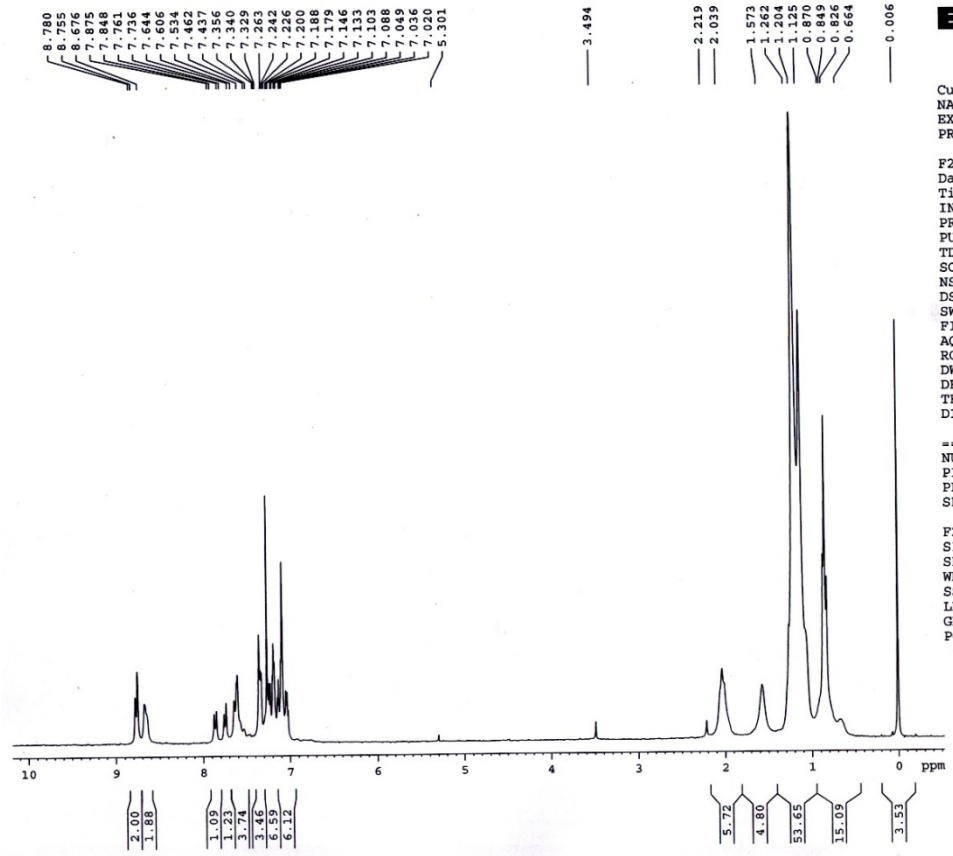
PFT4



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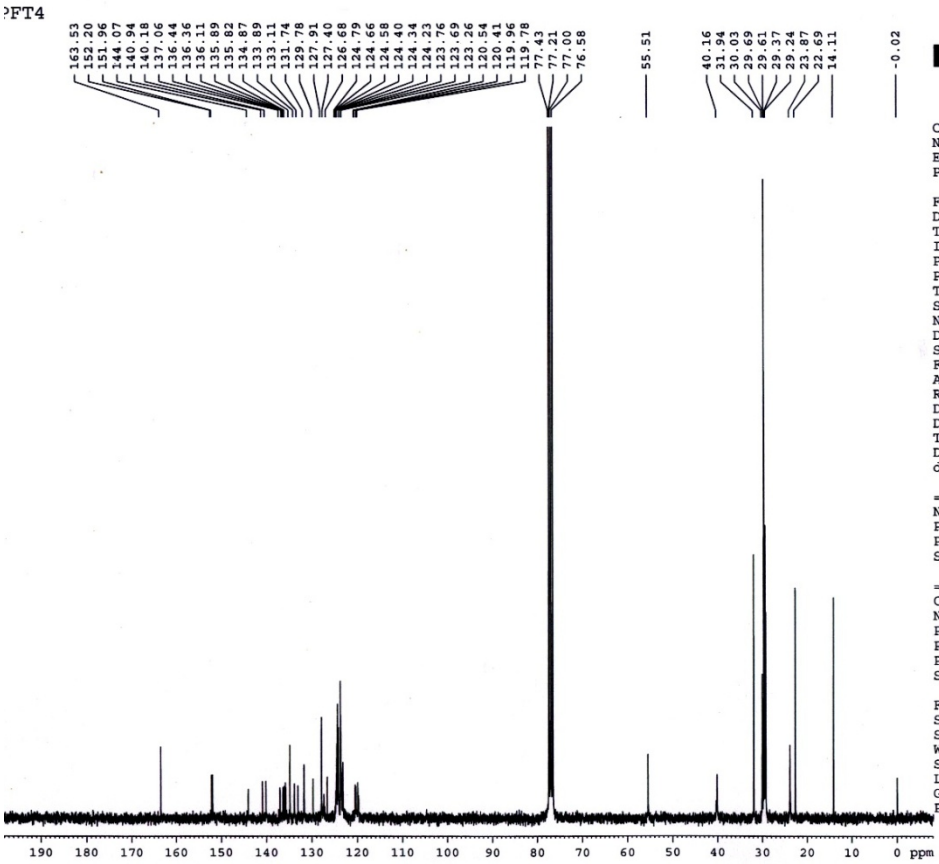
Current Data Parameters
NAME Nov2010
EXPNO 3352
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110902
Time 10.32
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 4496.403 Hz
FIDRES 0.137219 Hz
AQ 3.6438515 sec
RG 181
DW 111.200 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 16.50 usec
PL1 -6.00 dB
SFO1 300.1313506 MHz

F2 - Processing parameters
SI 16384
SF 300.1300053 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

PFT4



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Current Data Parameters
NAME Nov2010
EXPNO 3362
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110902
Time 22.32
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 5120
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4096
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -3.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.00 usec
PL2 -6.00 dB
PL12 6.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40