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Supporting Information

Oligoarylenes End-Capped with Carbazol-*N*-yl-Carbazole as Color Tunable Light-Emitting and Hole-Transporting Materials for Solution-Processed OLEDs

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Synthesis and characterization of 1-5

6-Bromo-3-(3',6'-di-*tert*-butylcarbazol-*N'*-yl)-*N*-dodecylcarbazole (1)

A mixture of dodecylcarbazole (31.44 g, 63.48 mmol), 3,6-di-*tert*-butylcarbazole (4.43 g, 15.87 mmol), CuI (1.51 g, 7.94 mmol), K_3PO_4 (8.42 g, 39.68 mmol) and ±*trans*-1,2-diaminocyclohexane (0.90 g, 7.94 mmol) in toluene (200 ml) was stirred at refluxed under N_2 atmosphere for 48 h. Water (50 ml) was added and the mixture was extracted with CH_2Cl_2 (50 ml x 2). The combined organic phase was washed with water (50 ml x 2) and brine solution (100 ml), dried over anh. Na_2SO_4, filtered and the solvents were removed to dryness. Purification by column chromatography over silica gel eluting with a mixture of CH_2Cl_2 and hexane (1:5) followed by recrystallization with a mixture of CH_2Cl_2 and methanol afforded the product (8.43 g, 77%) as a white solid (mp 176 ^oC). ^1H NMR (300 MHz, $CDCl_3$): δ = 8.18-8.15 (m, 4H), 7.57-7.45 (m, 3H), 7.44 (d, 2H, *J* = 1.13 Hz), 7.32-7.27 (m, 3H), 4.38 (t, 2H, *J* = 7.20 Hz), 1.96 (t, 2H, *J* = 6.90 Hz), 1.65-1.25 (m, 36H), 0.93 (t, 3H, *J* = 6.30 Hz) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 139.29, 129.54, 128.42, 123.45, 123.42, 123.24, 111.95, 111.89, 111.31, 111.19, 111.10, 110.60, 109.54, 43.36, 31.93, 30.70, 29.95, 29.58, 29.35, 28.84, 28.28, 28.01, 12.74, 27.22, 22.71, 14.82 ppm. HRMS: *m/z* calcd. for $C_{44}H_{55}BrN_2$, 690.3549; found, 692.3601 [MH_2^+].

6-(Thiophen-2-yl)-3-(3',6'-di-*tert*-butylcarbazol-*N'*-yl)-*N*-dodecylcarbazole (2)

A mixture of **1** (1.00 g, 1.44 mmol), 2-thiophene boronic acid (0.09 g, 1.21 mmol), $Pd(PPh_3)_4$ (0.02 g, 0.02 mmol) and 2 M Na_2CO_3 solution (15 ml) in THF (20 ml) was degassed with N_2 for 3 min. The mixture was heated at reflux under N_2 atmosphere for 48 h. After cooling, water (50 ml) was added and the mixture was extracted with CH_2Cl_2 (50 ml x 2). The combined organic phase was washed with water (50 ml x 2) and brine solution (50 ml), dried over anh. Na_2SO_4, filtered and the solvents were removed to dryness. Purification by column chromatography over silica gel eluting with a mixture of CH_2Cl_2 and hexane (1:6) gave the product (0.85 g, 86%) as a white pearl solid (mp. 132 ^oC). ^1H NMR (300 MHz, $CDCl_3$): δ = 8.28 (d, 2H, *J* = 4.80 Hz), 8.20 (s, 2H), 7.79 (d, 1H, *J* = 8.40 Hz), 7.59 (q, 2H), 7.48 (m, 3H), 7.35 (m, 3H), 7.24 (s, 2H), 7.10 (t, 1H, *J* = 4.50 Hz), 4.39 (t, 2H, *J* = 7.20 Hz), 1.97 (t, 2H, *J* = 6.90 Hz), 1.56-1.27 (m, 36H), 0.87 (t, 3H, *J* = 6.90 Hz) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 145.51, 142.44, 140.61, 140.31, 139.81, 129.64, 128.01, 126.09, 125.35, 124.88, 123.80, 123.68, 123.50, 123.07, 122.97, 122.14, 119.37, 118.05, 116.20, 109.77, 109.34, 109.19, 43.53, 34.76, 32.09, 31.93, 29.64, 29.55, 29.45, 29.36, 29.13, 27.37, 22.70, 14.13 ppm. HRMS: *m/z* calcd. for $C_{48}H_{58}N_2S$, 694.4321; found, 695.4405 [MH^+].

6-(5-Bromothiophen-2-yl)-3-(3',6'-di-*tert*-butylcarbazol-*N'*-yl)-*N*-dodecylcarbazole (3)

To a stirred solution of **2** (3.30 g, 4.75 mmol) in THF (70 ml) NBS (0.87 g, 4.98 mmol) was added in small portions. The mixture was stirred at room temperature for 3 h. Water (20 ml) was added and the mixture was extracted with CH_2Cl_2 (50 ml x 3). The combined organic phase was washed with water (50 ml), and brine solution (50 ml), dried over anh. Na_2SO_4, filtered and the solvents were removed to dryness. The. Purification by column chromatography over silica gel eluting with a mixture of CH_2Cl_2 and hexane (1:3) followed by recrystallization with a mixture of CH_2Cl_2 and methanol afforded the product (3.33 g, 91%) as a green solid (mp. 174 ^oC). ^1H NMR (300 MHz, $CDCl_3$): δ = 8.26 (s, 2H), 8.21 (s, 2H), 7.69 (d, 3H, *J* = 8.40 Hz), 7.61 (d, 3H, *J* = 6.90 Hz), 7.50-7.46 (m, 3H), 7.35 (d, 2H, *J* = 8.70 Hz), 7.08-7.04 (q, 2H), 4.40 (t, 2H, *J* = 7.20 Hz), 1.98 (t, 2H, *J* = 6.90 Hz), 1.57-1.27 (m, 36H), 0.89 (t, 3H, *J* = 6.90 Hz) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 147.02, 142.48, 140.76, 140.26, 139.81, 130.82, 129.79, 125.50, 125.30, 124.49, 123.54, 123.50, 123.08, 123.00, 122.23, 119.34, 117.80, 116.21, 110.03, 109.85, 109.47, 109.15, 43.55, 34.75, 32.08, 31.92, 29.63, 29.60, 29.53, 29.43, 29.35, 29.10, 27.35, 22.69, 14.12 ppm. HRMS: *m/z* calcd. for $C_{48}H_{57}BrN_2S$, 772.3426; found, 773.3482 [MH^+].

6-(2,2'-Bithiophen-5-yl)-3-(3',6'-di-*tert*-butylcarbazol-*N'*-yl)-*N*-dodecylcarbazole (4)

Compound **4** (1.35 g, 80%) was synthesized in similar manner to **2** from **3** and obtained as a pale yellow solid (mp. 142 °C). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.27 (s, 2H), 8.20 (s, 2H), 7.78 (d, 1H, *J* = 8.40 Hz), 7.60 (q, 2H), 7.49-7.46 (m, 3H), 7.36 (d, 2H, *J* = 8.4 Hz), 7.27-7.16 (m, 3H), 7.03 (t, 1H, *J* = 3.9 Hz), 4.39 (t, 2H, *J* = 7.20 Hz), 1.97 (t, 2H, *J* = 6.90 Hz), 1.50-1.27 (m, 36H), 0.89 (t, 3H, *J* = 6.90 Hz) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 144.35, 142.46, 140.68, 140.28, 139.81, 137.73, 135.62, 129.74, 127.81, 125,71, 125.39, 124.68, 124.50, 124.02, 123.64, 123.50, 123.29, 123.08, 123.03, 122.66, 119.34, 117.73, 116.19, 109.81, 109.41, 109.19, 43.55, 34.75, 32.08, 31.92, 29.63, 29.60, 29.54, 29.43, 29.35, 29.12, 27.36, 22.69, 14.12 ppm. HRMS: *m/z* calcd. for $C_{52}H_{60}N_2S_2$, 776.4198; found, 777.4290 [MH^+].

6-(5'-Bromo-2,2'-bithiophen-5-yl)-3-(3',6'-di-*tert*-butylcarbazol-*N'*-yl)-*N*-dodecylcarbazole (5)

Compound **5** (93%) was synthesized in similar manner to **3** from **4** and obtained as a green solid (mp. 234 °C). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 8.24 (s, 2H), 8.17 (s, 2H), 7.74 (d, 1H, *J* = 5.58 Hz), 7.59-7.57 (m, 2H), 7.47 (d, 3H, *J* = 8.60 Hz), 7.33 (d, 3H, *J* = 8.60 Hz), 7.21 (d, 1H, *J* = 3.72 Hz), 7.10 (d, 1H, *J* = 3.72 Hz), 6.97-6.90 (q, 2H), 4.37 (t, 2H, *J* = 7.20 Hz), 1.98 (t, 2H, *J* = 6.90 Hz), 1.57-1.27 (m, 36H), 0.85 (t, 3H, *J* = 6.90 Hz) ppm. ^{13}C NMR (75 MHz, $CDCl_3$): δ = 144.90, 142.48, 140.75, 140.26, 139.81, 139.22, 134.50, 130.64, 129.78, 125.45, 124.95, 124.50, 123.59, 123.50, 123.30, 123.08, 122.69, 119.34, 117.79, 116.21, 110.48, 109.85, 109.45, 109.17, 43.55, 34.75, 32.08, 31.92, 30.92, 29.63, 29.60, 29.54, 29.43, 29.35, 29.11, 27.36, 22.70, 14.12 ppm. HRMS: *m/z* calcd. for $C_{52}H_{59}BrN_2S_2$, 854.3303; found, 855.3364 [MH^+].

Quantum chemical calculation

- All calculations were performed by Gaussian 09 code
- Geometry optimizations were done by B3LYP/6-31G(d,p) method
- Ground to excited state excitation energies were calculated by TD-B3LYP/6-31G(d,p) in CH_2Cl_2 solvent

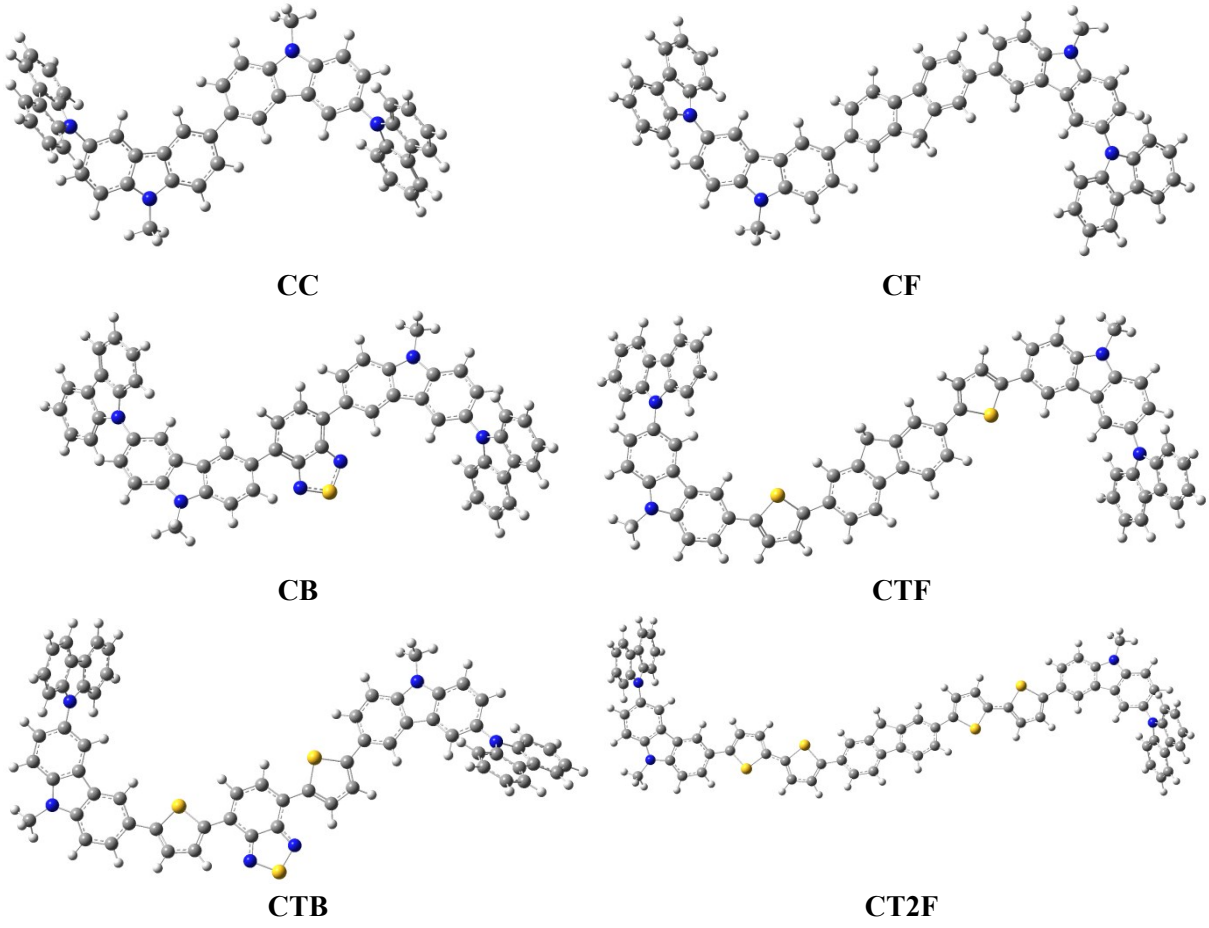
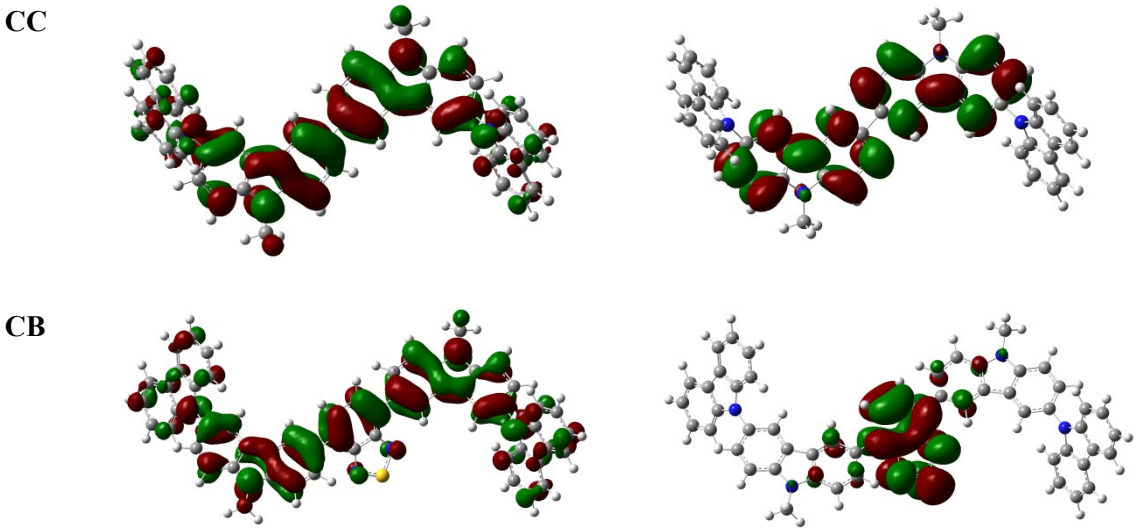


Figure S1. The optimized structure of the compounds calculated by B3LYP/6-31G(d,p) in CH_2Cl_2.



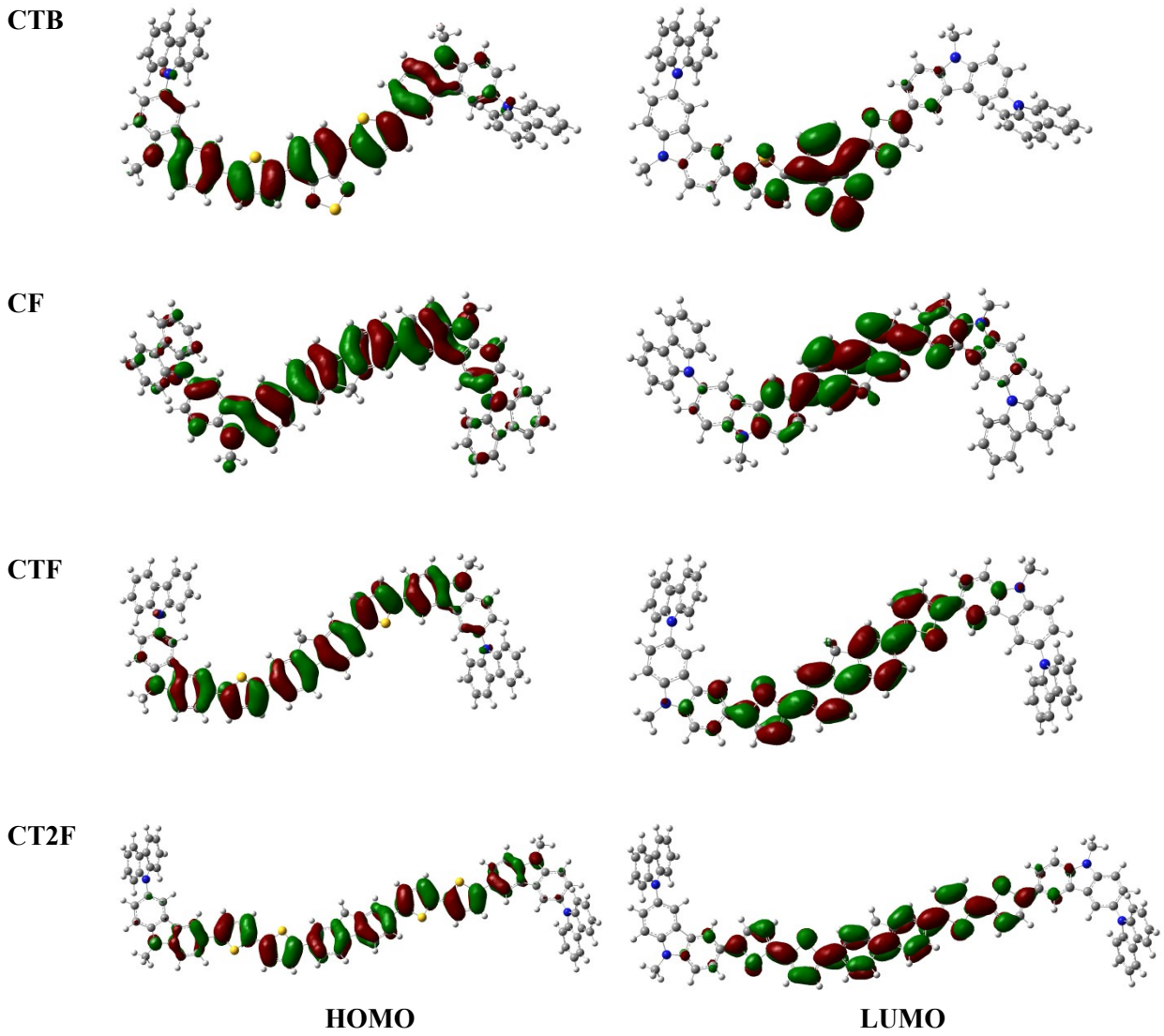


Figure S2. HOMO and LUMO of the compounds calculated by B3LYP/6-31G(d,p) in CH_2Cl_2.

Table S1. The calculated HOMO, LUMO and HOMO-LUMO energy gap (Δ_{H-L}) of the compounds by B3LYP/6-31G(d,p).

Compounds	HOMO (eV)	LUMO (eV)	Δ_{H-L} (eV)	E_{ex}[a] (eV/nm)
CC	-5.16	-1.05	4.11	3.47 (357)
CB	-5.21	-2.39	2.83	2.37 (522)
CTB	-4.98	-2.67	2.30	1.91 (647)
CF	-5.15	-1.23	3.92	3.35 (370)
CTF	-4.98	-1.74	3.24	2.81 (441)
CT2F	-4.90	-1.99	2.91	2.50 (496)

[a] exciation energies from ground to excited states are calculated by TD-B3LYP/6-31G(d,p) in CH_2Cl_2 solvent

Table S2. The three lowest excitations of from ground to excited states are calculated by TD-B3LYP/6-31G(d,p) in CH_2Cl_2 solvent

Compounds		E_{ex}[a] (eV/nm)	Oscillator strength (f)	Transition
CC	$S_0 \rightarrow S_1$	3.57 (347)	0.0038	H→L (67%)
	$S_0 \rightarrow S_2$	3.62 (342)	0.0409	H→L+1 (67%)
	$S_0 \rightarrow S_3$	3.86 (321)	0.1714	H-1→L (54%) + H-2→L (35%)
CB	$S_0 \rightarrow S_1$	2.37 (522)	0.3894	H→L (69%)
	$S_0 \rightarrow S_2$	2.63 (471)	0.0023	H-1→L (70%)
	$S_0 \rightarrow S_3$	2.77 (447)	0.0575	H-2→L (68%)
CTB	$S_0 \rightarrow S_1$	1.91 (647)	0.9203	H→L (70%)
	$S_0 \rightarrow S_2$	2.38 (521)	0.0363	H-1→L (69%)
	$S_0 \rightarrow S_3$	2.50 (496)	0.0131	H-2→L (70%)
CF	$S_0 \rightarrow S_1$	3.45 (359)	1.8677	H→L (69%)
	$S_0 \rightarrow S_2$	3.60 (344)	0.0031	H→L+1 (59%)
	$S_0 \rightarrow S_3$	3.61 (344)	0.1441	H→L+2 (59%)
CTF	$S_0 \rightarrow S_1$	2.81 (441)	2.4444	H→L (69%)
	$S_0 \rightarrow S_2$	3.20 (387)	0.0286	H-1→L (69%)
	$S_0 \rightarrow S_3$	3.41 (364)	0.0705	H-2→L (68%)
CT2F	$S_0 \rightarrow S_1$	2.50 (496)	3.3319	H→L (69%)
	$S_0 \rightarrow S_2$	2.49 (439)	0.0684	H-1→L+1 (67%)
	$S_0 \rightarrow S_3$	2.97 (417)	0.0276	H→L+1 (67%)

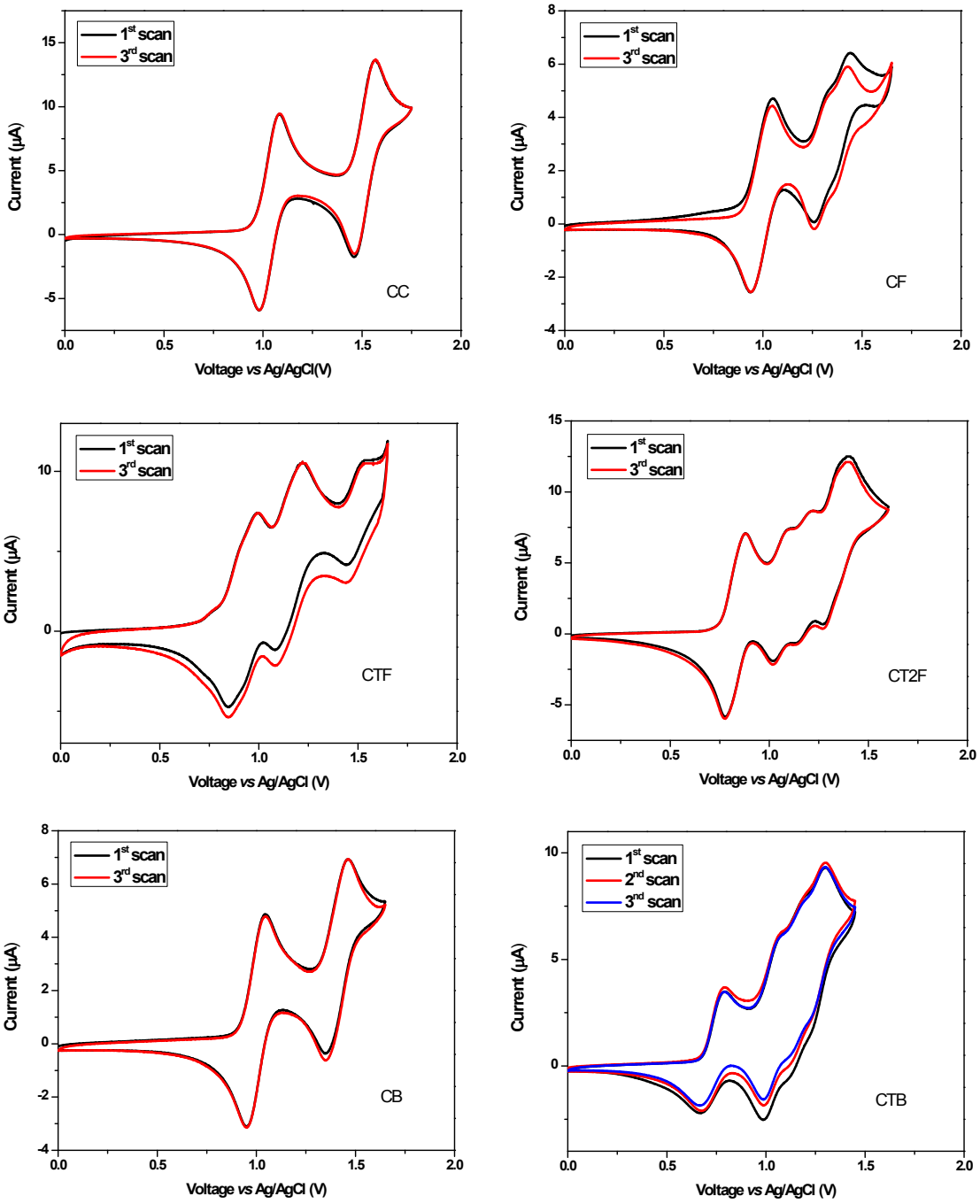


Figure S3. Multiple scan CV traces.

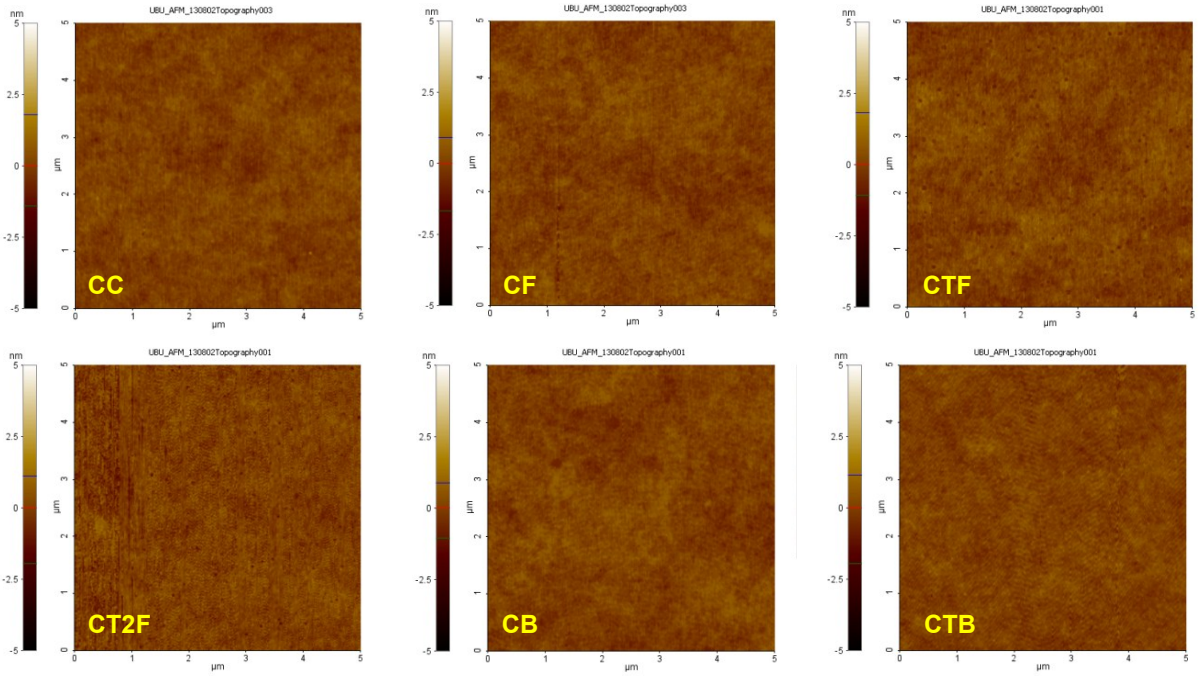
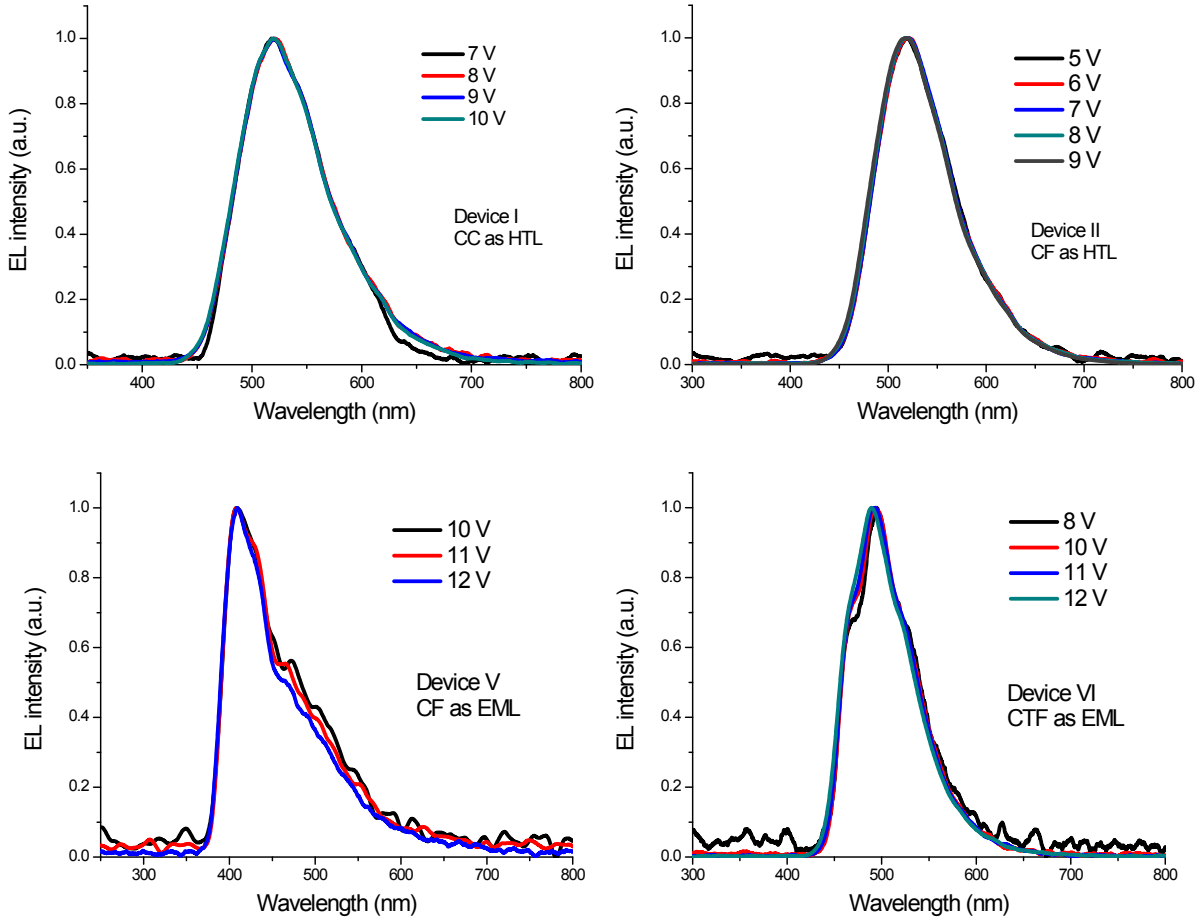


Figure S4. Tapping mode AFM images of the spin-coated thin films.



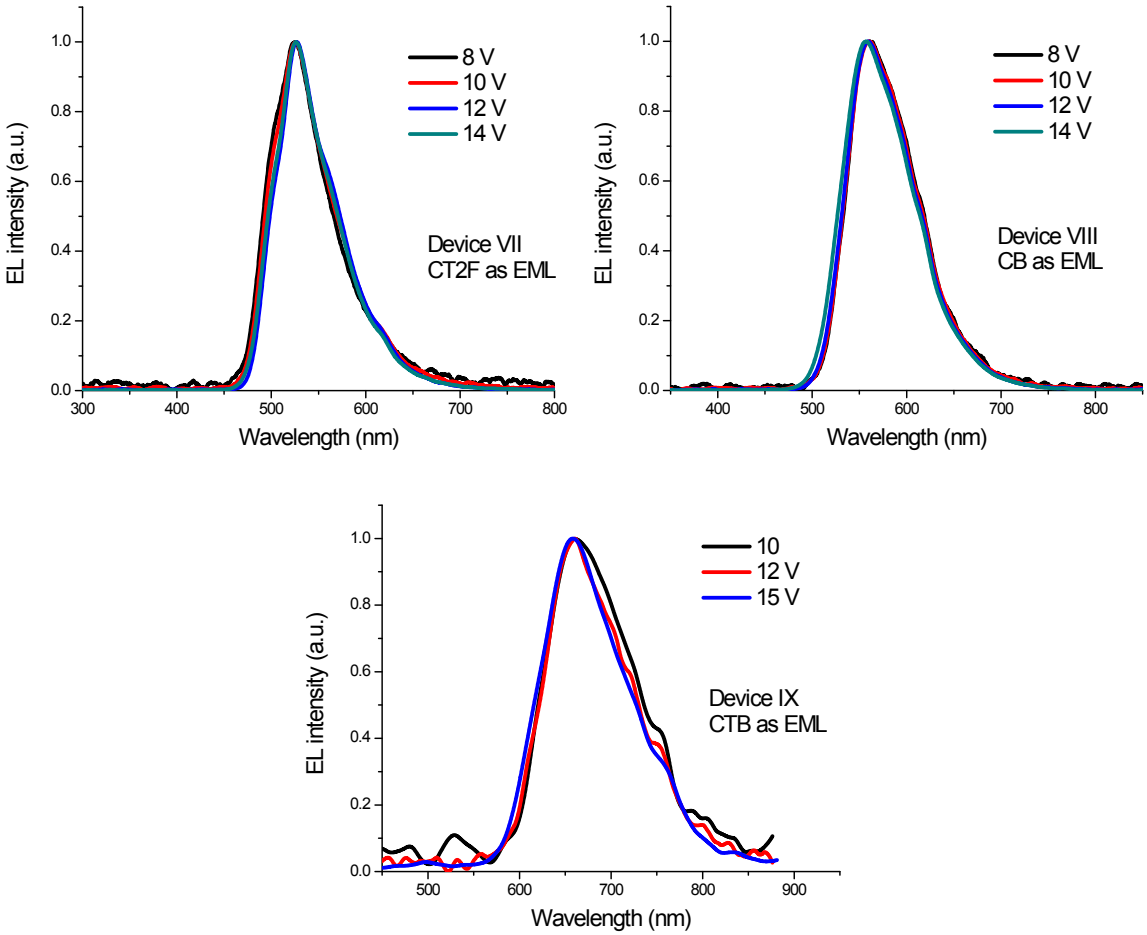


Figure S5. EL spectra of the OELDs at different applied voltages.

^{1}H-NMR and ^{13}C NMR spectra
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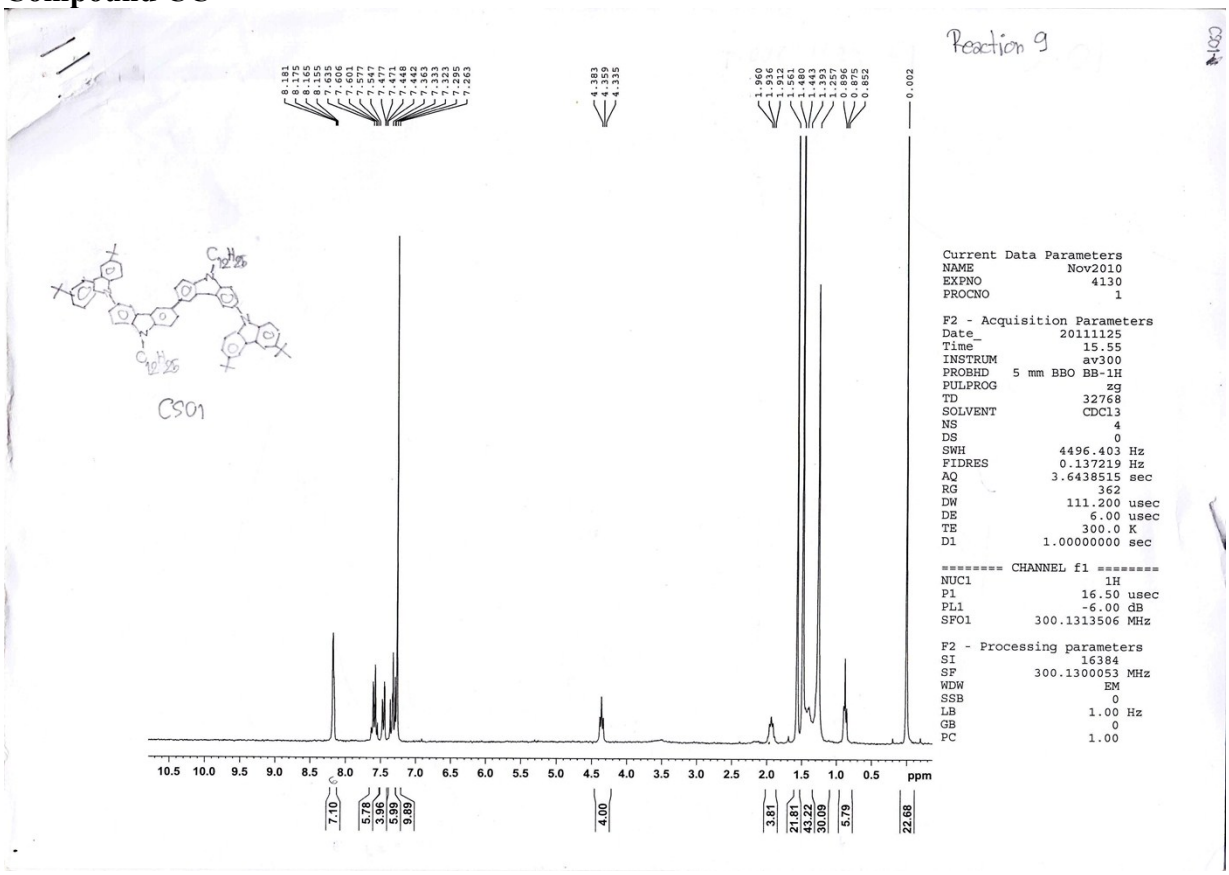

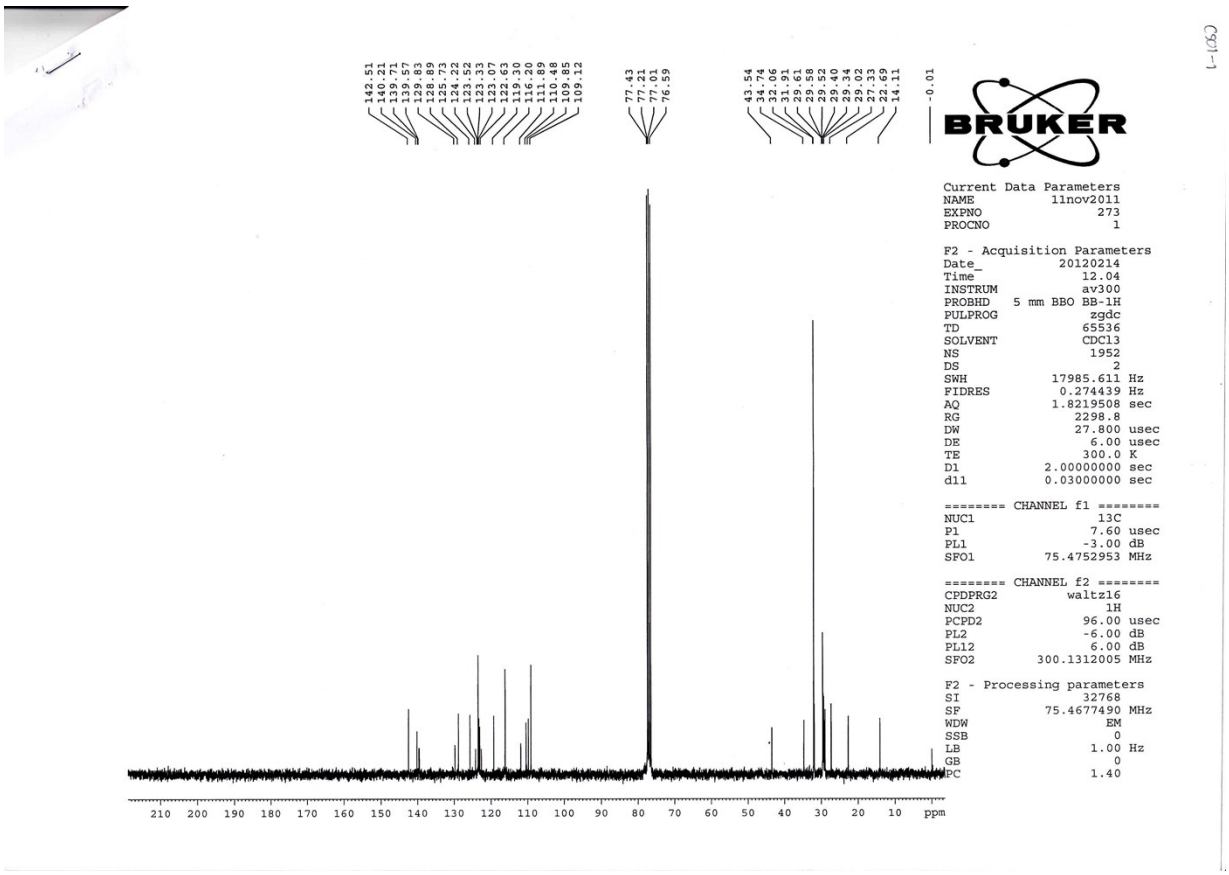

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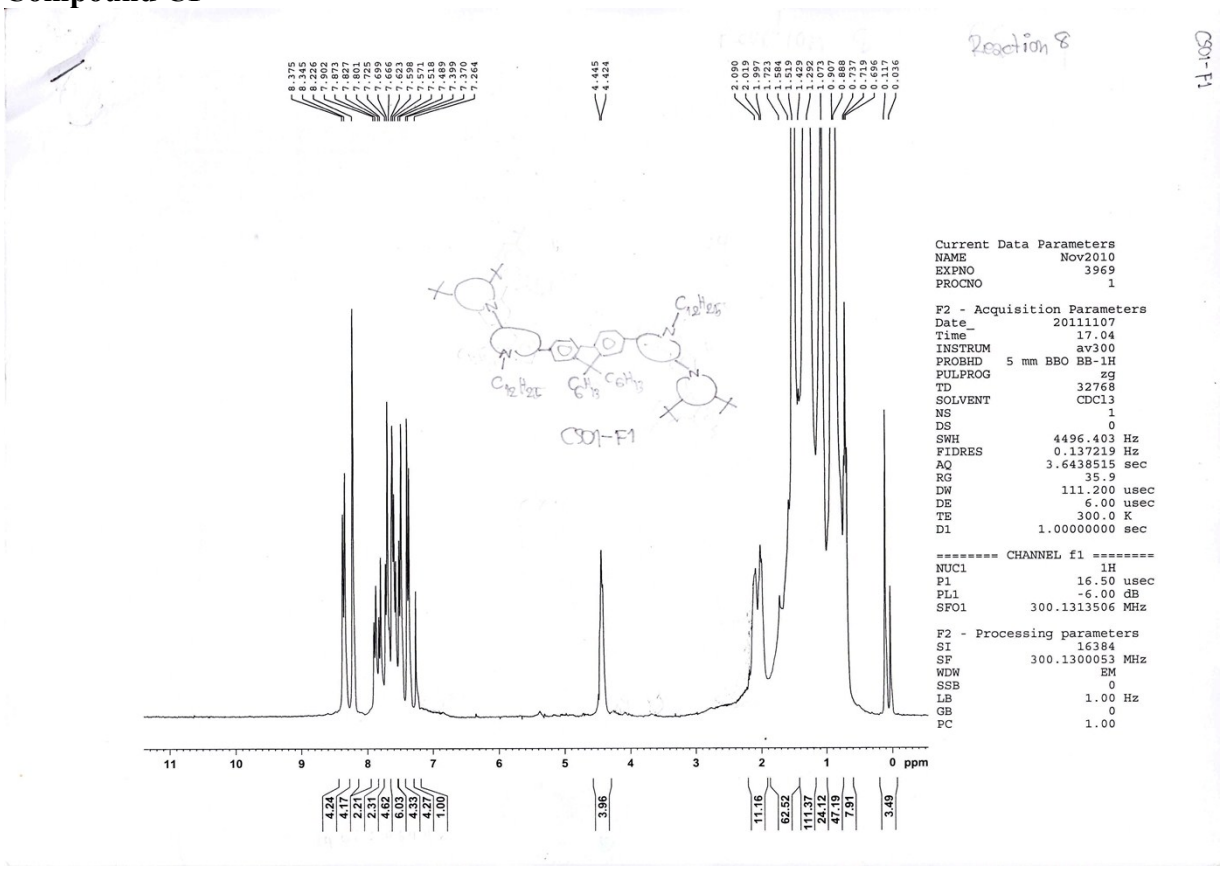
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SSB 0
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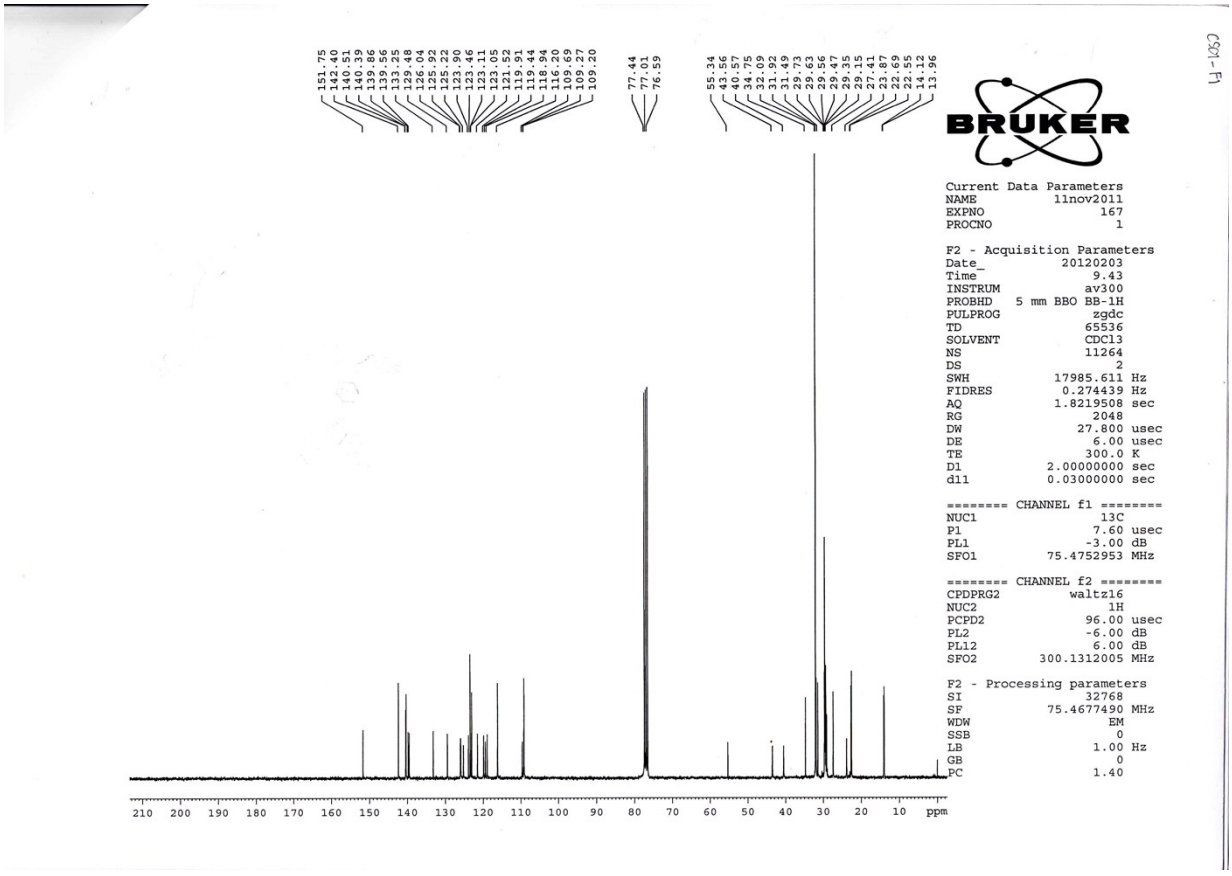
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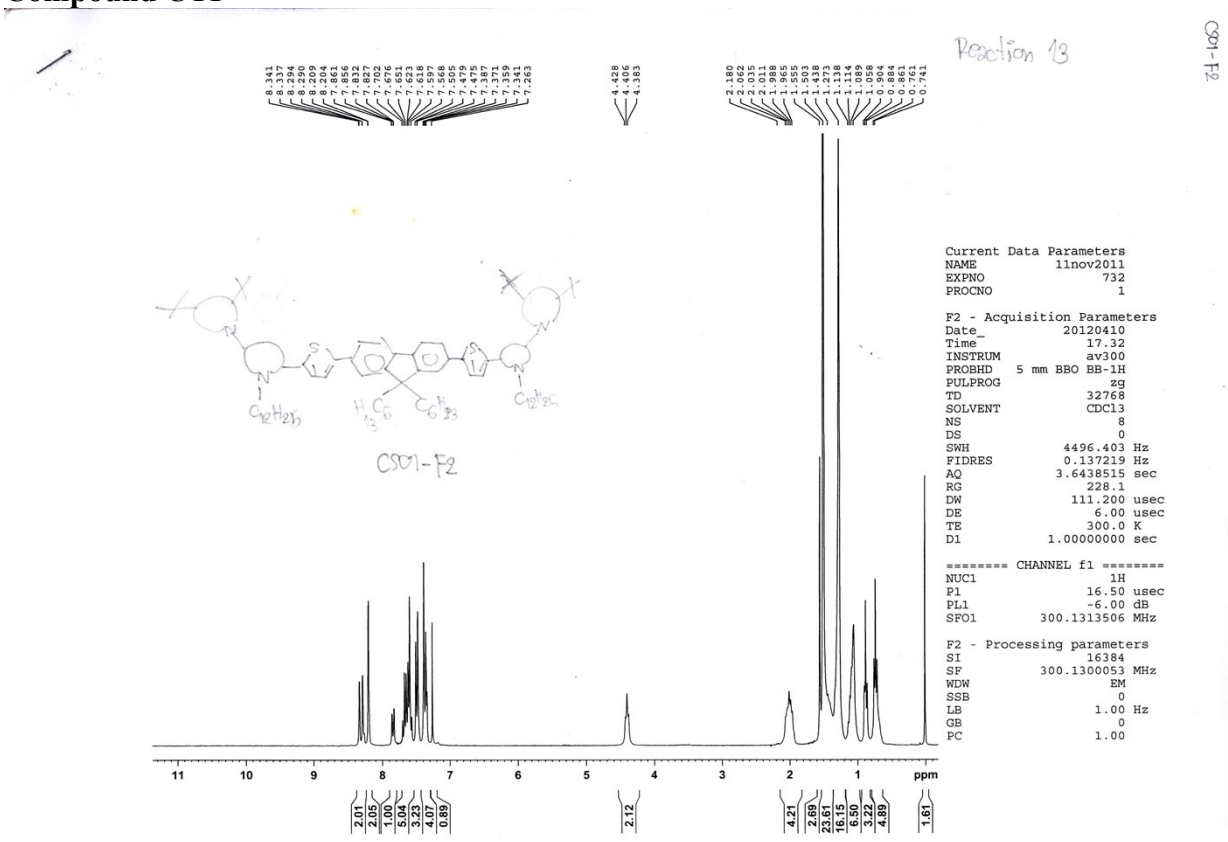
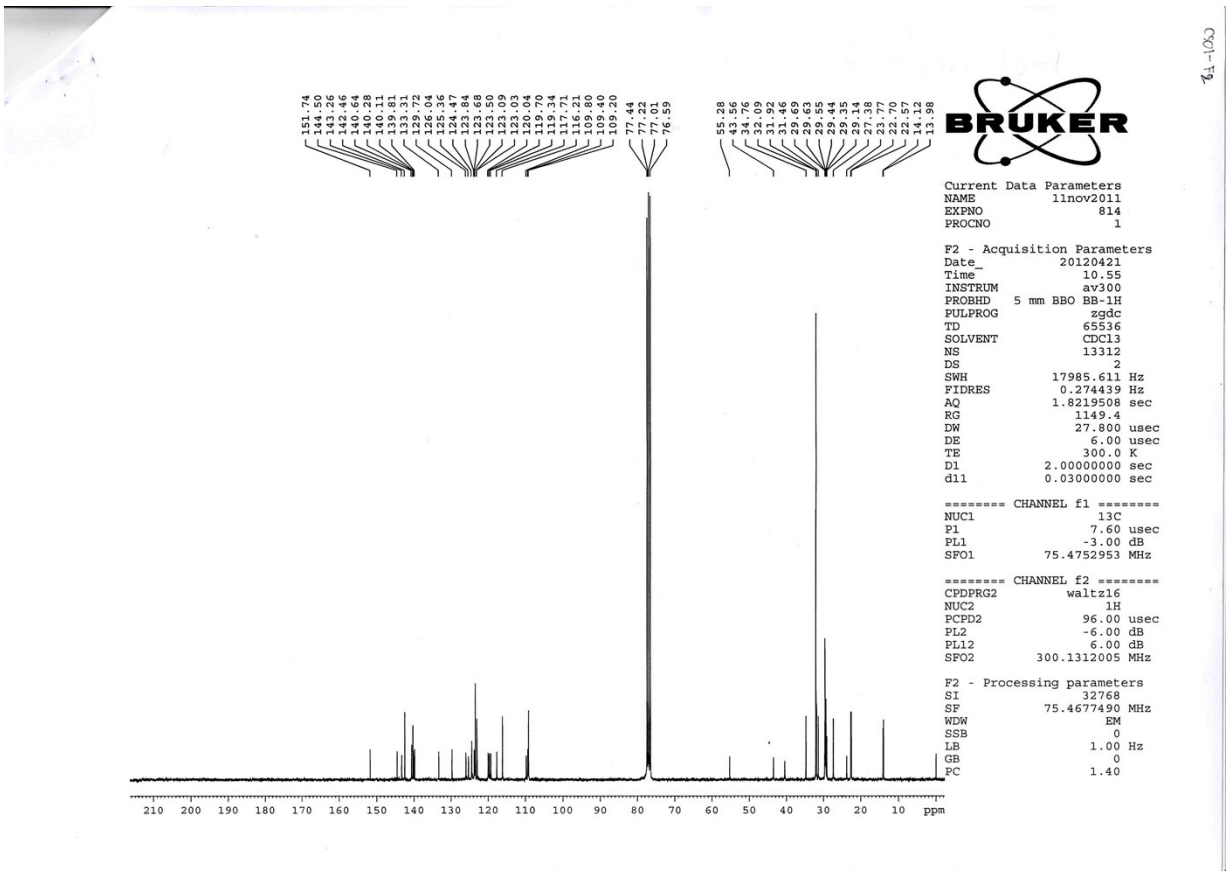
Compound CTF





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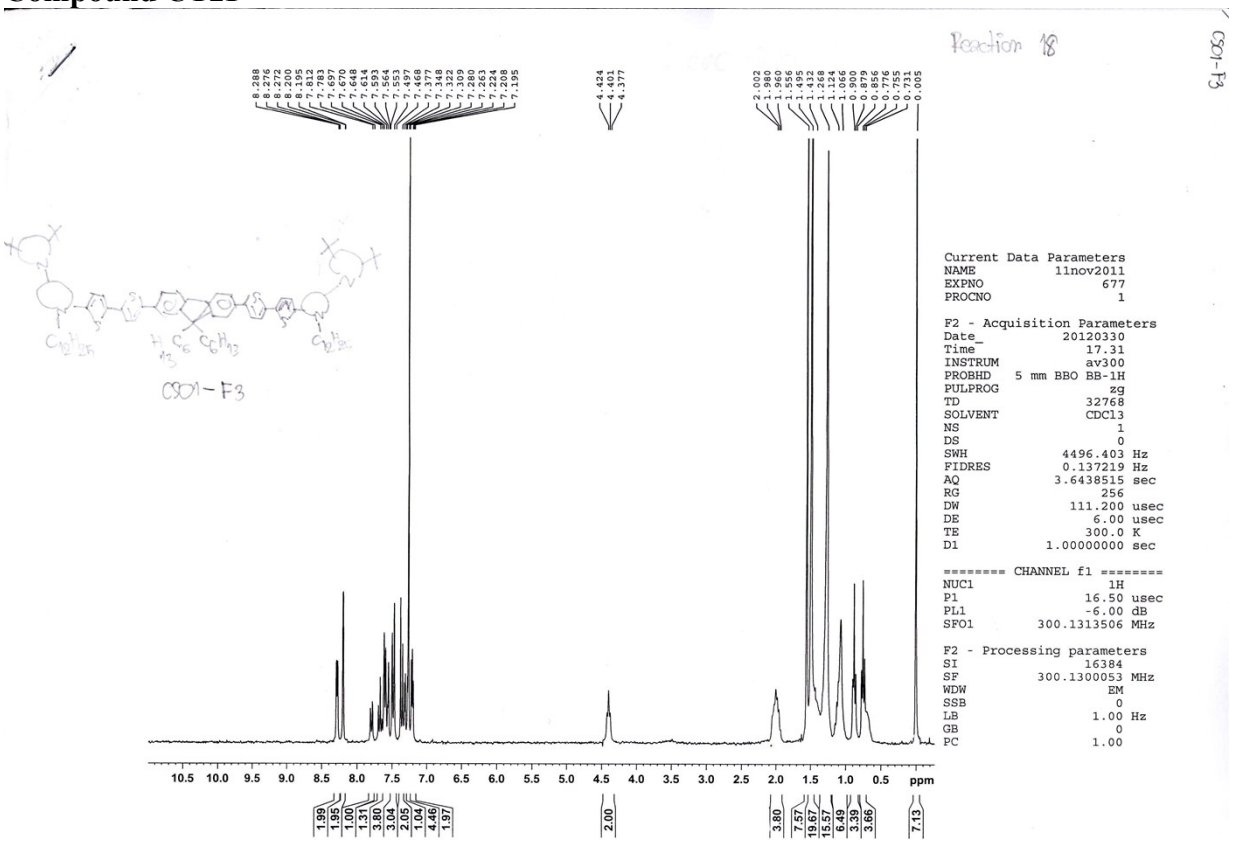

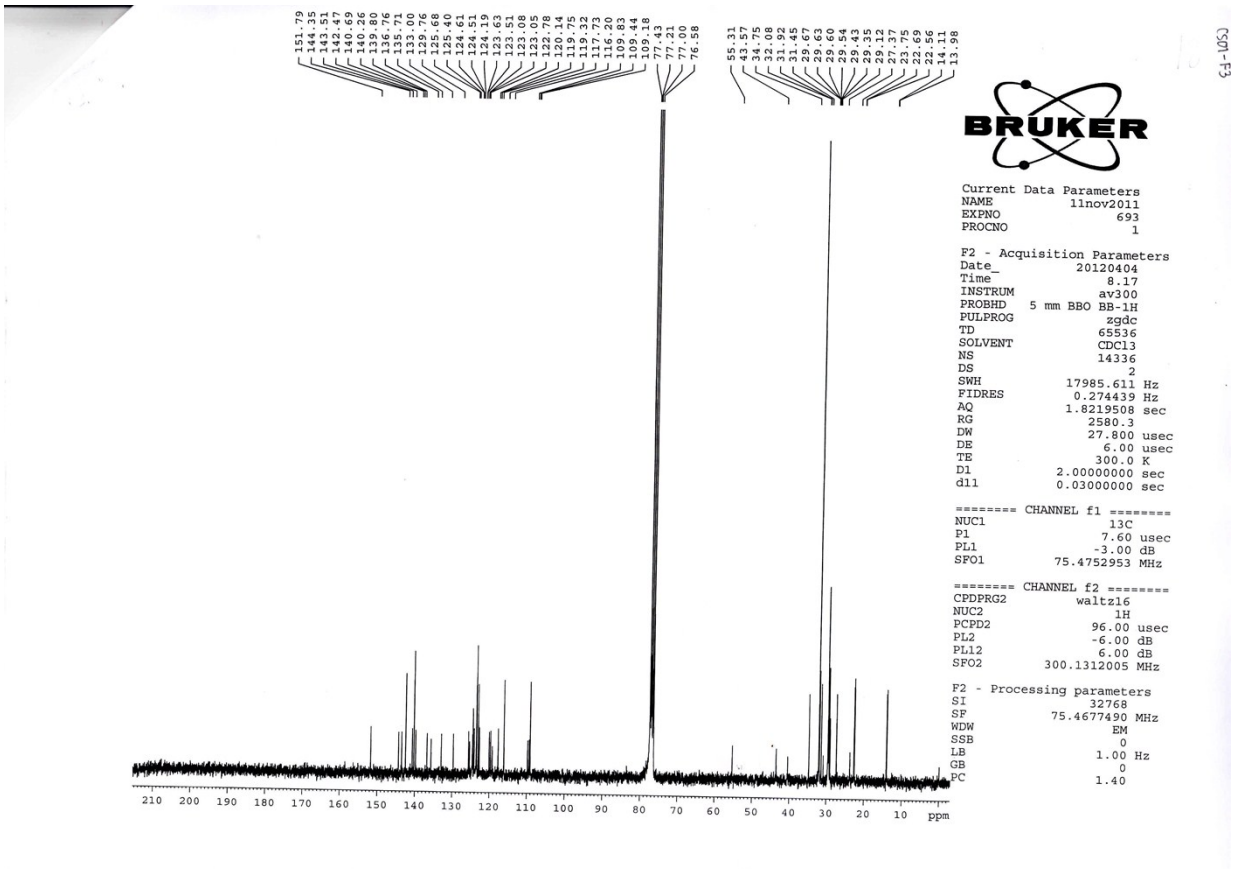

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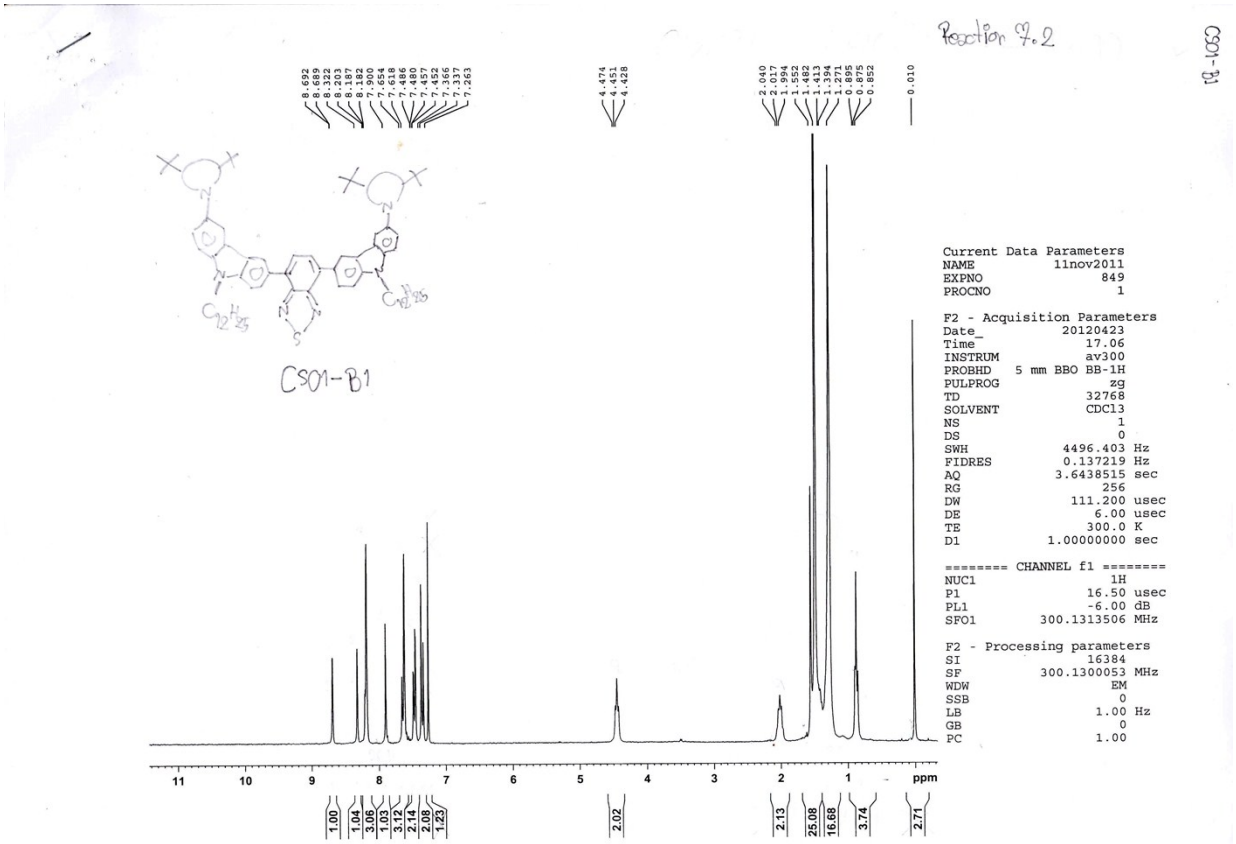
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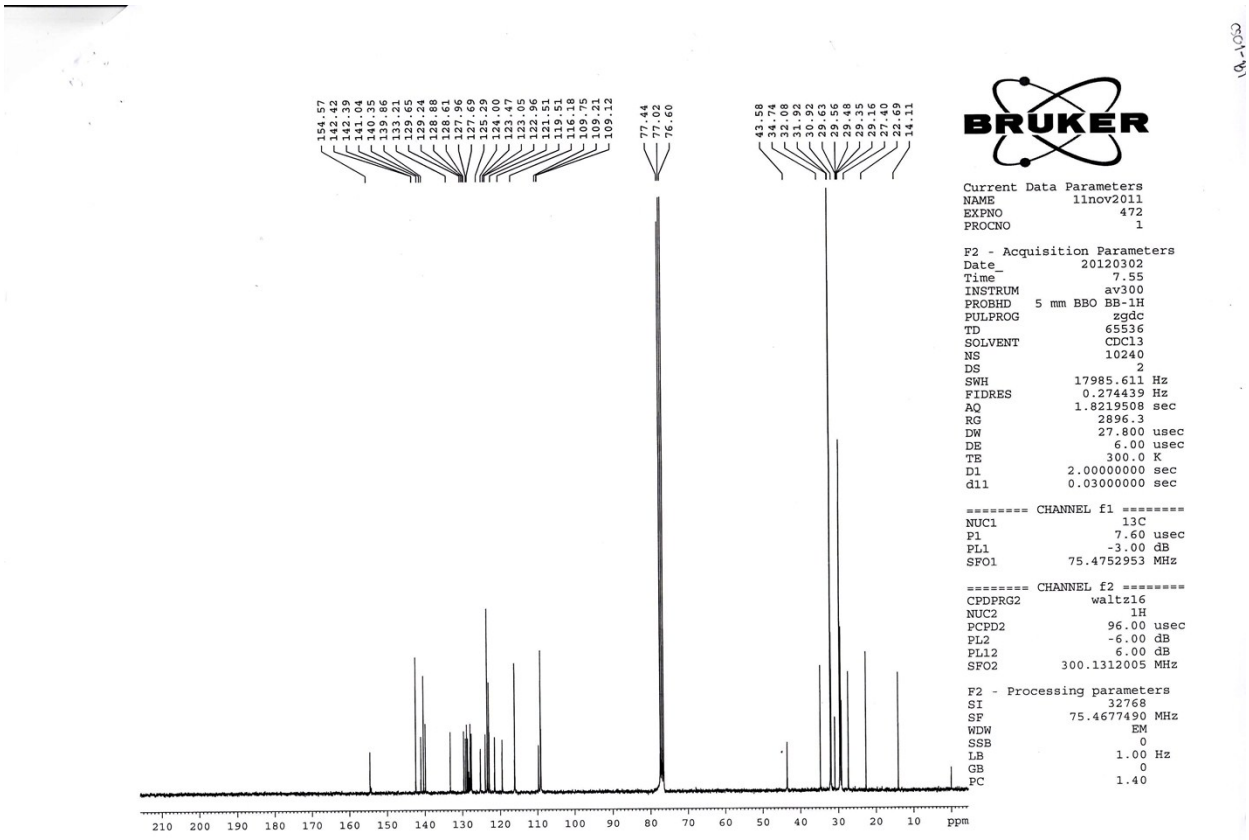
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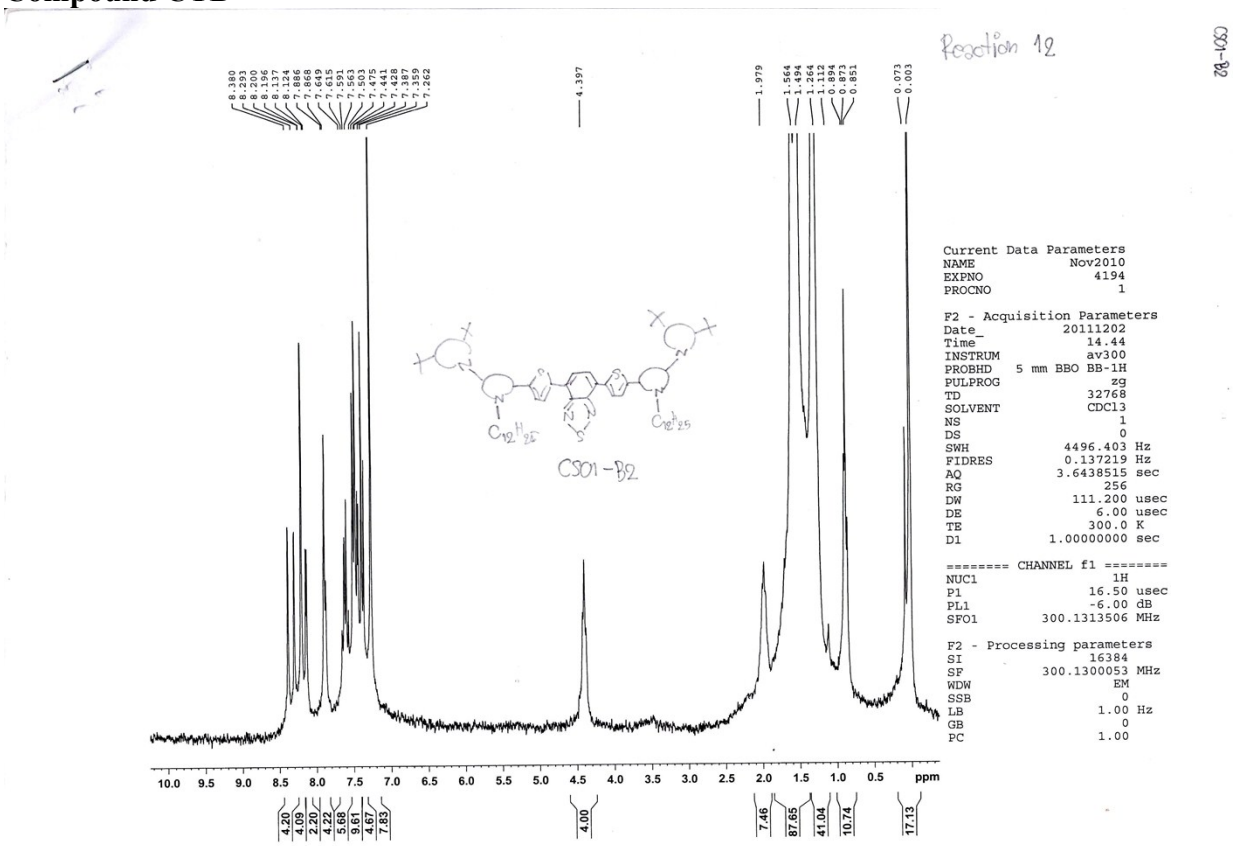
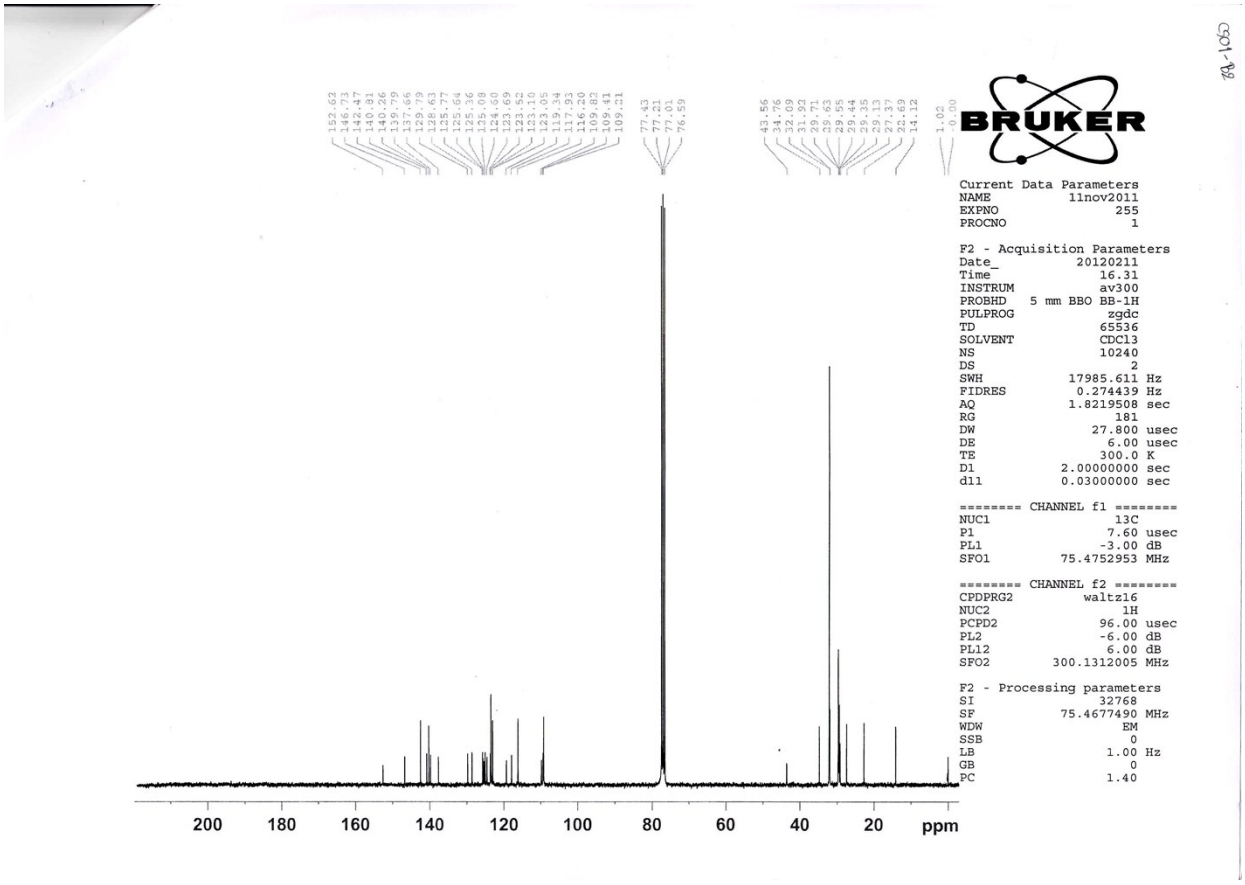
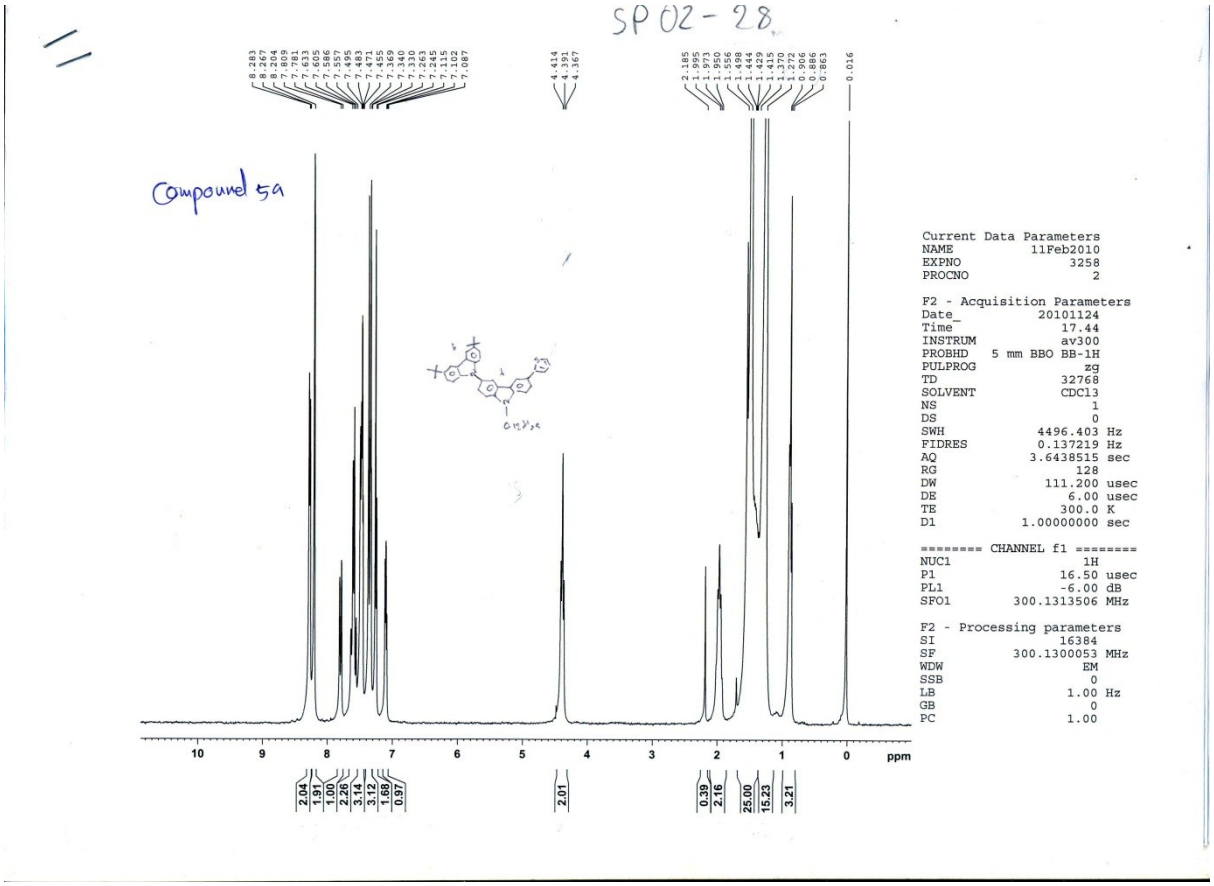
27.40
22.69
14.11
BRUKER
Current Data Parameters
NAME 11nov2011
EXPNO 472
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120302
Time 7.55
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 10240
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2896.3
DW 27.800 usec
DE 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
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

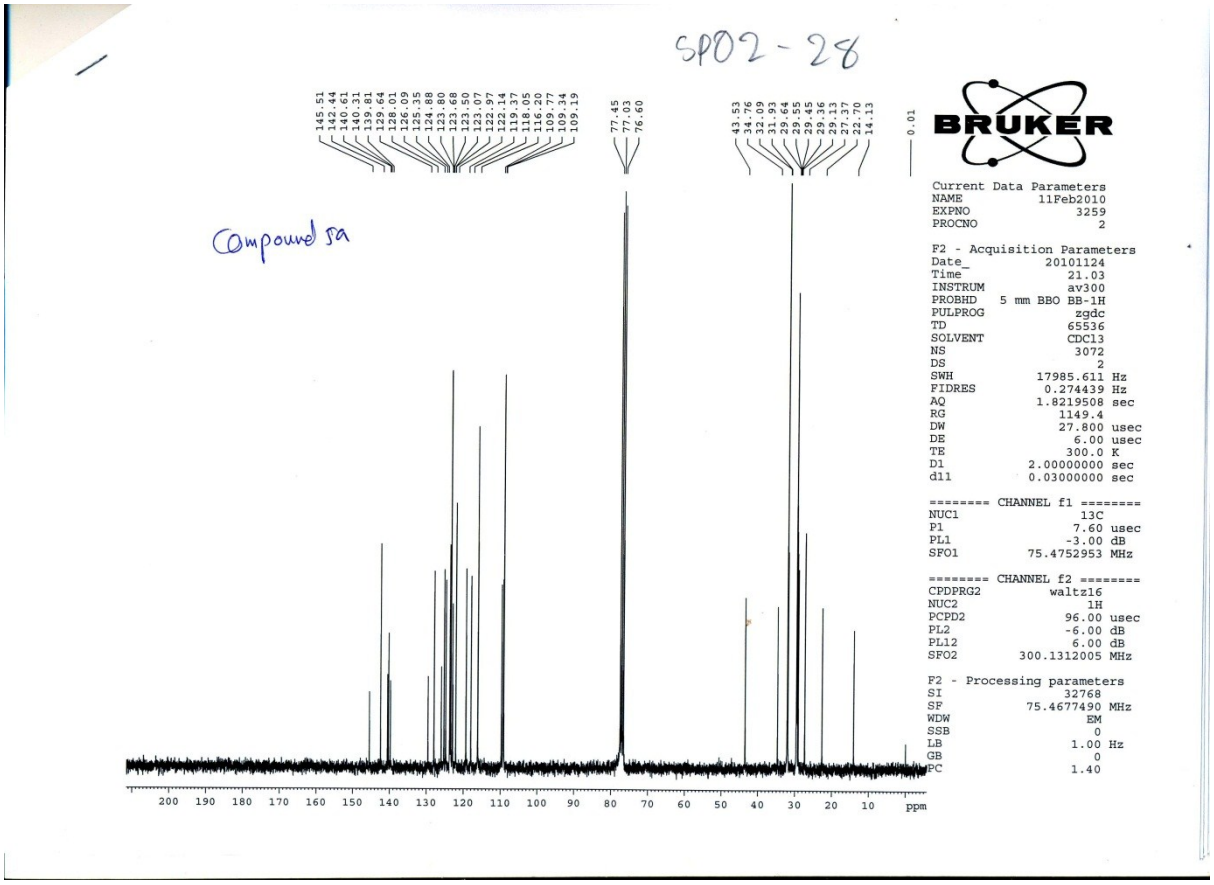
Compound CTB



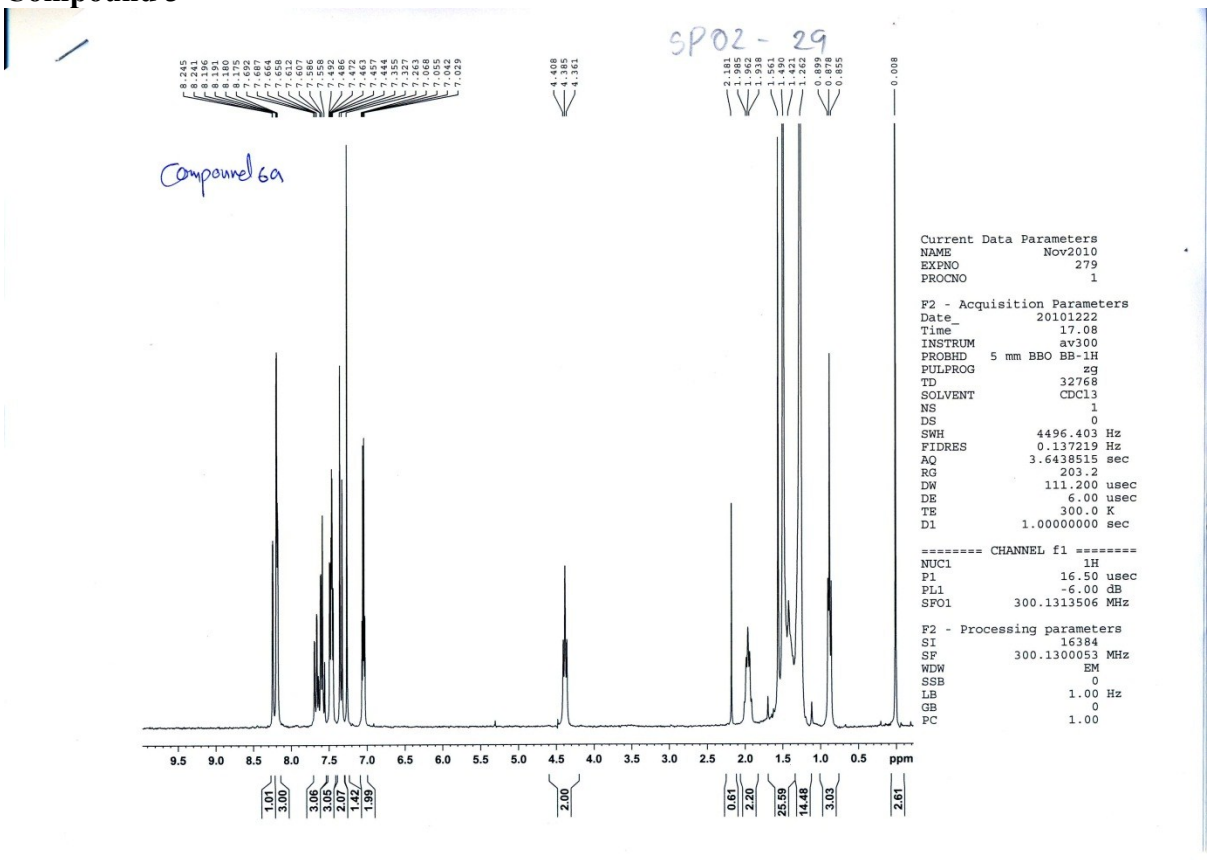


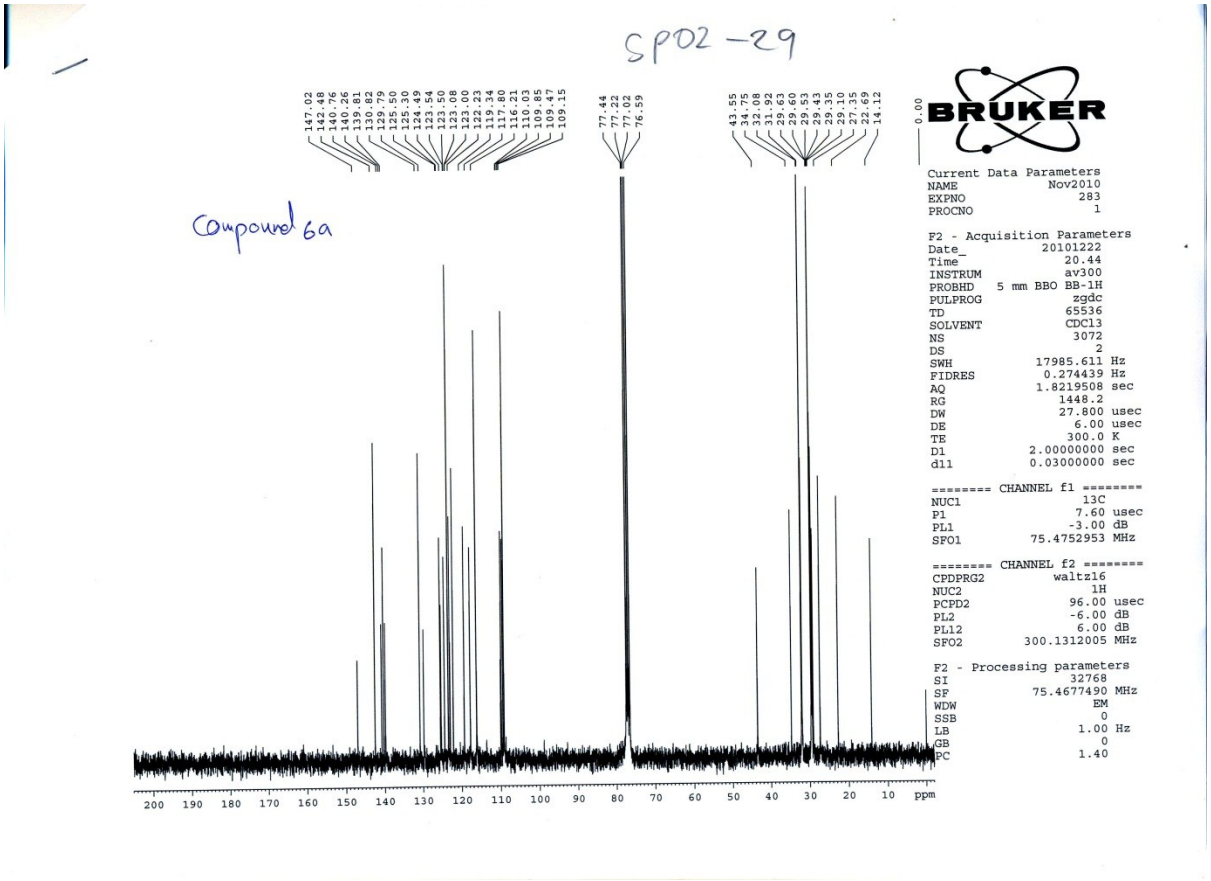
Compound 2


SP02-28
Compound 5a
Current Data Parameters
NAME 11Feb2010
EXPNO 3258
PROCNO 2
F2 - Acquisition Parameters
Date_ 20101124
Time 17.44
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 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 1.00
ppm

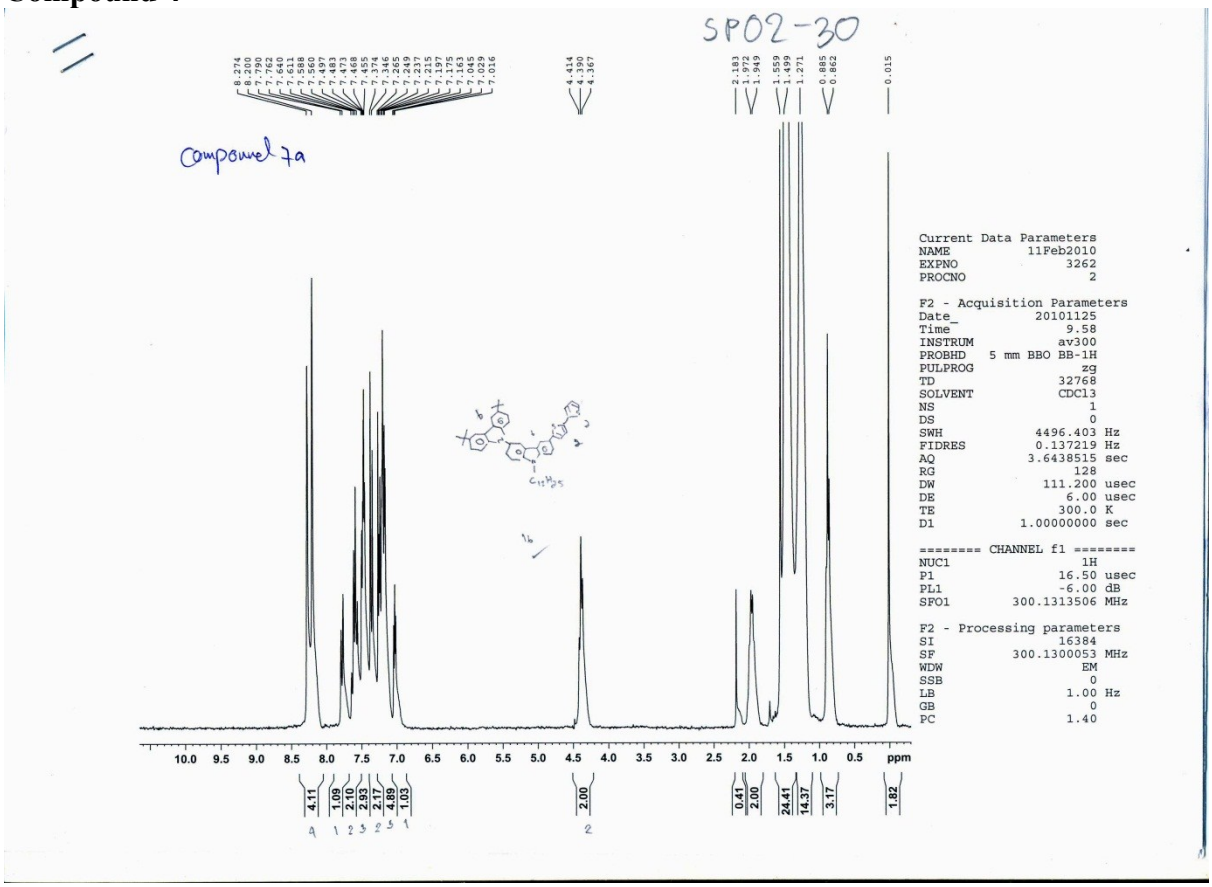

SP02-28
Compound 5a
BRUKER
Current Data Parameters
NAME 11Feb2010
EXPNO 3259
PROCNO 2
F2 - Acquisition Parameters
Date_ 20101124
Time 21.03
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 3072
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1149.4
DW 27.800 usec
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
ppm

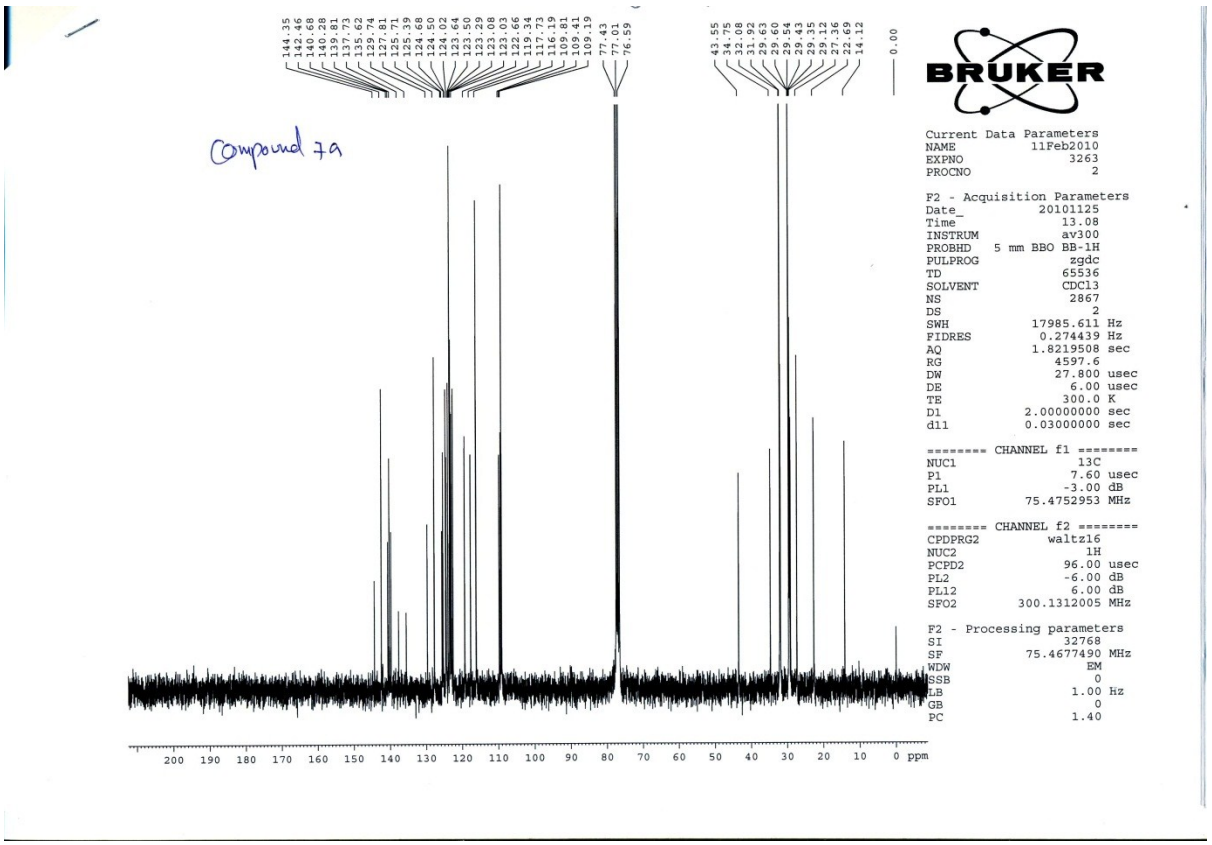
Compound 3


SP02 - 29
Compound 6a
Current Data Parameters
NAME Nov2010
EXPNO 279
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101222
Time 17.08
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 203.2
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 1.00
ppm

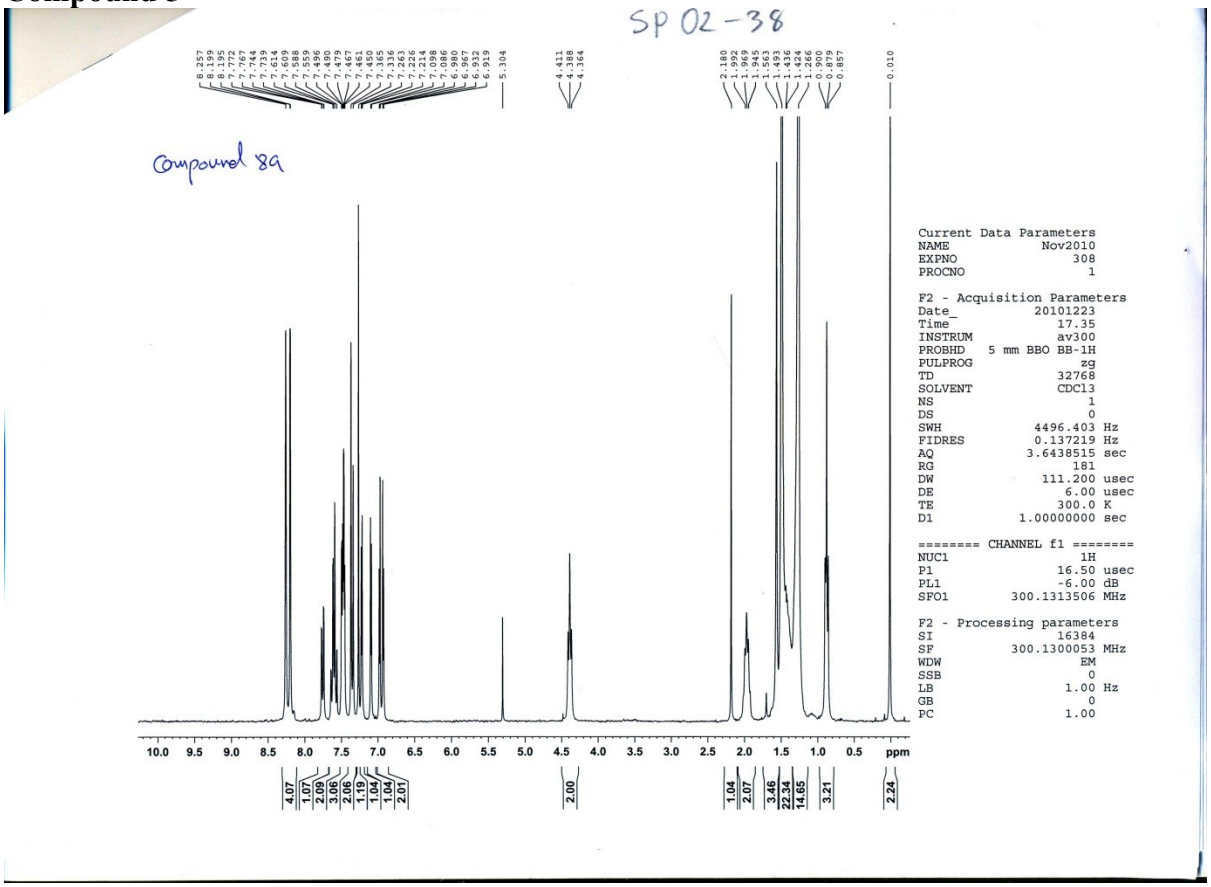

SP02 -29
Compound 6a
BRUKER
Current Data Parameters
NAME Nov2010
EXPNO 283
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101222
Time 20.44
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 3072
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1448.2
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 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
ppm

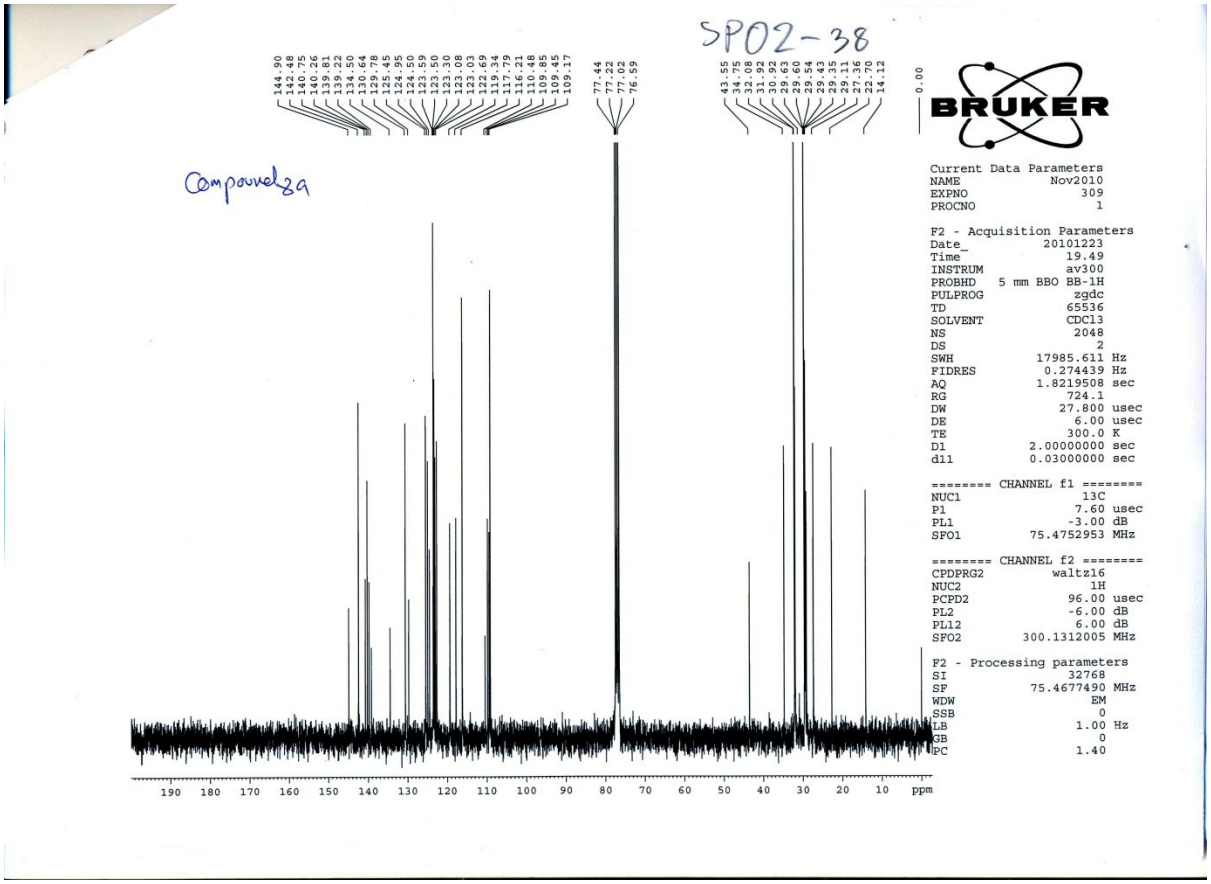
Compound 4


SP02-30
Compound 7a
Current Data Parameters
NAME 11Feb2010
EXPNO 3262
PROCNO 2
F2 - Acquisition Parameters
Date_ 20101125
Time 9.58
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 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


Compound 7a
BRUKER
Current Data Parameters
NAME 11Feb2010
EXPNO 3263
PROCNO 2
F2 - Acquisition Parameters
Date_ 20101125
Time 13.08
INSTRUM av300
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 2867
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 4597.6
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

Compound 5


SP 02-38
Compound 8a
Current Data Parameters
NAME Nov2010
EXPNO 308
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101223
Time 17.35
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 1.00
ppm


SP02-38
Compound 8a
BRUKER
Current Data Parameters
NAME Nov2010
EXPNO 309
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101223
Time 19.49
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 724.1
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 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
ppm