Supporting Information

CuCl-catalyzed green oxidative alkyne homocoupling without palladium, ligands and bases

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1. General experimental details

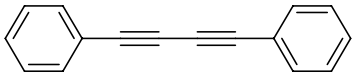
All chemicals were purchased from commercial vendors and used without further purification, unless indicated otherwise.The ^{1}H NMR spectra were recorded on Brucker AC – 500 (500 MHz) spectrometer and ^{13}C NMR spectra were measured with Brucker AC – 125 spectrometer. EI-MS were determined with a Agilent 5975N mass spectrometer. Melting points were obtained on a Fisher-Johns apparatus without correction. Chemical yields referred to pure isolated product.

1.1 General procedure:

To a stirred solution of alkyne (1.0 mmol) in DMSO (1.0 mL), CuCl (5 mol %, see Table 3) were added successively in the open air. The resulting mixture was then allowed to react at 90 ^{o}C in air. Progress of this reaction was monitored by TLC and the reaction phenomena (The reactions passed through cyan, yellowness to black from starting to end). After completion of the reaction, 10 mL of ethyl acetate was added. The mixture was filtered through a pad of diatomite under reduced pressure, and the filtration residue was washed with ethyl acetate. Ethyl acetate was removed under reduced pressure. The residue was then purified by column chromatography on silica gel using petroleum ether as eluent to afford the corresponding 1,3-diynes. All of the products are known and were characterized by comparison of their spectral data with those of authentic samples.

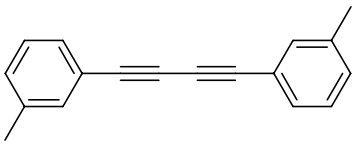
2. Experimental characterization data for compounds

1,4-Diphenyl buta-1,3-diyne (2a):



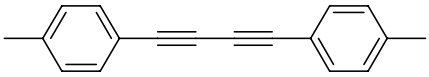
m.p. 86-87 °C (lit.[1] 86-88 °C). ^{1}H NMR ($CDCl_3$, 500 MHz): δ (ppm) = 7.55-7.53 (m, 4H), 7.39-7.33 (m, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ (ppm) = 132.6, 129.3, 128.6, 121.9, 81.7, 74.1. MS: m/z: 202 [M^{+}].

1,4-Bis(3-methylphenyl) buta-1,3-diyne (2b):



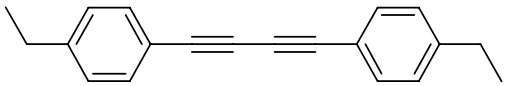
m.p. 74-75 °C (lit.[2] 68-70 °C).^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.40-7.38 (m, 4H), 7.29-7.22 (m, 4H), 2.39 (s, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 138.2, 133.1, 130.2, 129.7, 128.4, 121.7, 81.7, 73.7, 21.3. MS: m/z: 230 [M^{+}].

1,4-Bis(4-methylphenyl) buta-1,3-diyne (2c):



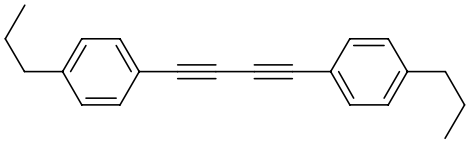
m.p. 183-184 °C (lit.[3] 183 °C). ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.43 (d, 4H, *J* = 8.0 Hz), 7.15 (d, 4H, *J* = 7.5 Hz), 2.37 (s, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 139.6, 132.5, 129.3, 118.9, 81.6, 73.5, 21.7. MS: m/z: 230 [M^{+}].

1,4-Bis(4-ethylphenyl) buta-1,3-diyne (2d):



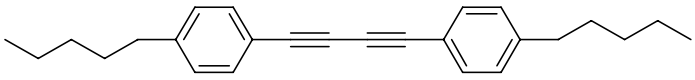
m.p. 96-97 °C (lit.[4] 98-99 °C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.45 (d, 4H, *J* = 8.5 Hz), 7.17 (d, 4H, *J* = 8.5 Hz), 2.67 (q, 4H, *J* = 8.0 Hz), 1.24 (t, 6H, *J*=8.0 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 145.8, 132.6, 128.1, 119.1, 81.9, 73.5, 29.0, 15.3.

1,4-Bis(4-n-propylphenyl) buta-1,3-diyne (2e):



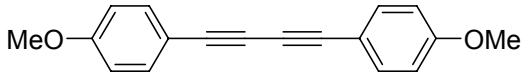
m.p. 107-108 °C (lit.[5] 107.6 °C). ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.44 (d, 4H, *J* = 8.0 Hz), 7.15 (d, 4H, *J* = 8.0 Hz), 2.59 (t, 4H, *J* = 8.0 Hz), 1.66-1.62 (m, 4H), 0.94 (t, 6H, *J* = 7.5 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 144.3, 132.5, 128.7, 119.1, 81.7, 73.6, 38.1, 24.4, 13.9. MS: m/z: 286 [M^{+}].

1,4-Bis(4-n-pentylphenyl) buta-1,3-diyne (2f):



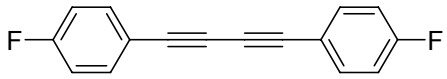
m.p. 84 °C (lit.[6] 85-86 °C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.44 (d, 4H, *J* = 8.5 Hz), 7.15 (d, 4H, *J* = 8.5 Hz), 2.61 (t, 4H, *J* = 8.0 Hz), 1.63-1.56 (m, 4H), 1.33-1.30 (m, 8H), 0.89 (t, 6H, *J* = 7.0 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 144.6, 132.5, 128.7, 119.1, 81.7, 73.6, 36.1, 31.5, 31.0, 22.6, 14.1.

1,4-Bis(4-methoxylphenyl) buta-1,3-diyne (2g):



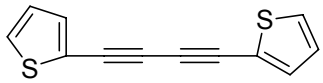
m.p. 139-140 °C (lit.[1] 138-140 °C); ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.46 (d, 4H, *J* = 9.0 Hz), 6.85 (d, 4H, *J* = 9.0 Hz), 3.81 (s, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 160.3, 134.1, 114.2, 114.0, 81.3, 73.0, 55.4. MS: m/z: 262 [M^+].

1,4-Bis(4-fluorophenyl) buta-1,3-diyne (2h):



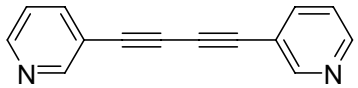
m.p. 192-193 °C (lit.[7] 190-191 °C). ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.53-7.49 (m, 4H), 7.04 (t, 4H, *J* = 8.5 Hz); ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 164.2, 162.2, 134.7, 134.6, 118.0, 117.9, 116.1, 116, 80.5, 73.6. MS: m/z: 238 [M^+].

1,4-Bis(2-thienyl) buta-1,3-diyne (2i):



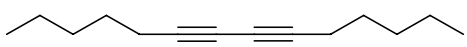
m.p. 89-90 °C (lit.[8] 92-93 °C). ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.35-7.32 (m, 4H), 7.0 (dd, 2H, *J* = 4.0 Hz, *J* = 9.0 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 134.5, 129.0, 127.3, 112.0, 77.8, 76.7. MS: m/z: 214 [M^+].

1,4-Bis(3-pyridyl) buta-1,3-diyne (2j):



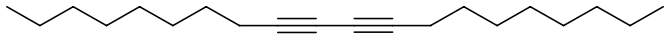
m.p. 144-145 °C (lit.[9] 145-146 °C). ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 8.79 (d, 2H, *J* = 1.0 Hz), 8.62 (dd, 2H, *J* = 1.5 Hz, *J* = 6.5 Hz), 7.85-7.83 (m, 2H), 7.33-7.28 (m, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 153.2, 149.6, 139.5, 123.2, 118.9, 79.2, 76.7. MS: m/z: 204 [M^+].

Ttetradeca-6,8-diyne (2k):



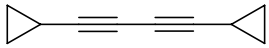
Colorless oil.[1] ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 2.22 (t, 4H, *J* = 7.0 Hz), 1.54-1.47 (m, 4H), 1.37-1.26 (m, 8H), 0.87 (t, 6H, *J* = 7.0 Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 77.5, 65.3, 31.1, 28.1, 22.2, 19.2, 14.0. MS: m/z: 190 [M^+].

Eicosa-9,11-diyne (2l):



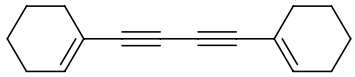
Colorless oil.[1] ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 2.22 (t, 4H, *J* = 7.0Hz), 1.51-1.25 (m, 24H), 0.86 (t, 6H, *J* = 7.5Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 77.4, 65.4, 31.9, 29.3, 29.2, 28.9, 28.5, 22.7, 19.3, 14.1. MS: m/z: 274 [M^+].

1,4-Dicyclopropyl buta-1,3-diyne (2m):



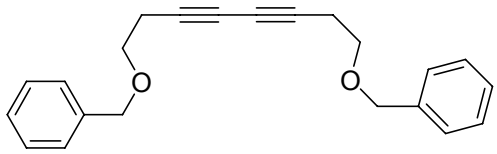
Colorless oil.[10] ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 1.28-1.22 (m, 2H), 0.78-0.72 (m, 8H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 80.0, 60.9, 8.8, 1.1.

1,4-Bis(cyclohex-1-enyl) buta-1,3-diyne (2n):



m.p. 65-66 ^{o}C (lit.[1] 63-65 ^{o}C). ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 6.24-6.22 (m, 2H), 2.12-2.08 (m, 8H), 1.63-1.55 (m, 8H). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 138.2, 120.0, 82.8, 71.6, 28.8, 25.9, 22.2, 21.4. MS: m/z: 210 [M^+].

1,8-Bis(benzyloxy) octa-3,5-diyne (2o):



m.p. 38-39 ^{o}C (lit.[11] 39 ^{o}C). ^{1}H NMR ($CDCl_3$, 500 MHz) δ (ppm) = 7.35-7.26 (m, 10H), 4.54 (s, 4H), 3.59 (t, 4H, *J* = 7.0Hz), 2.56 (t, 4H, *J* = 7.0Hz). ^{13}C NMR ($CDCl_3$, 125 MHz) δ (ppm) = 138.0, 128.5, 127.9, 127.8, 74.8, 73.1, 68.0, 66.3, 20.8. MS: m/z: 317 [M^+–1].

References

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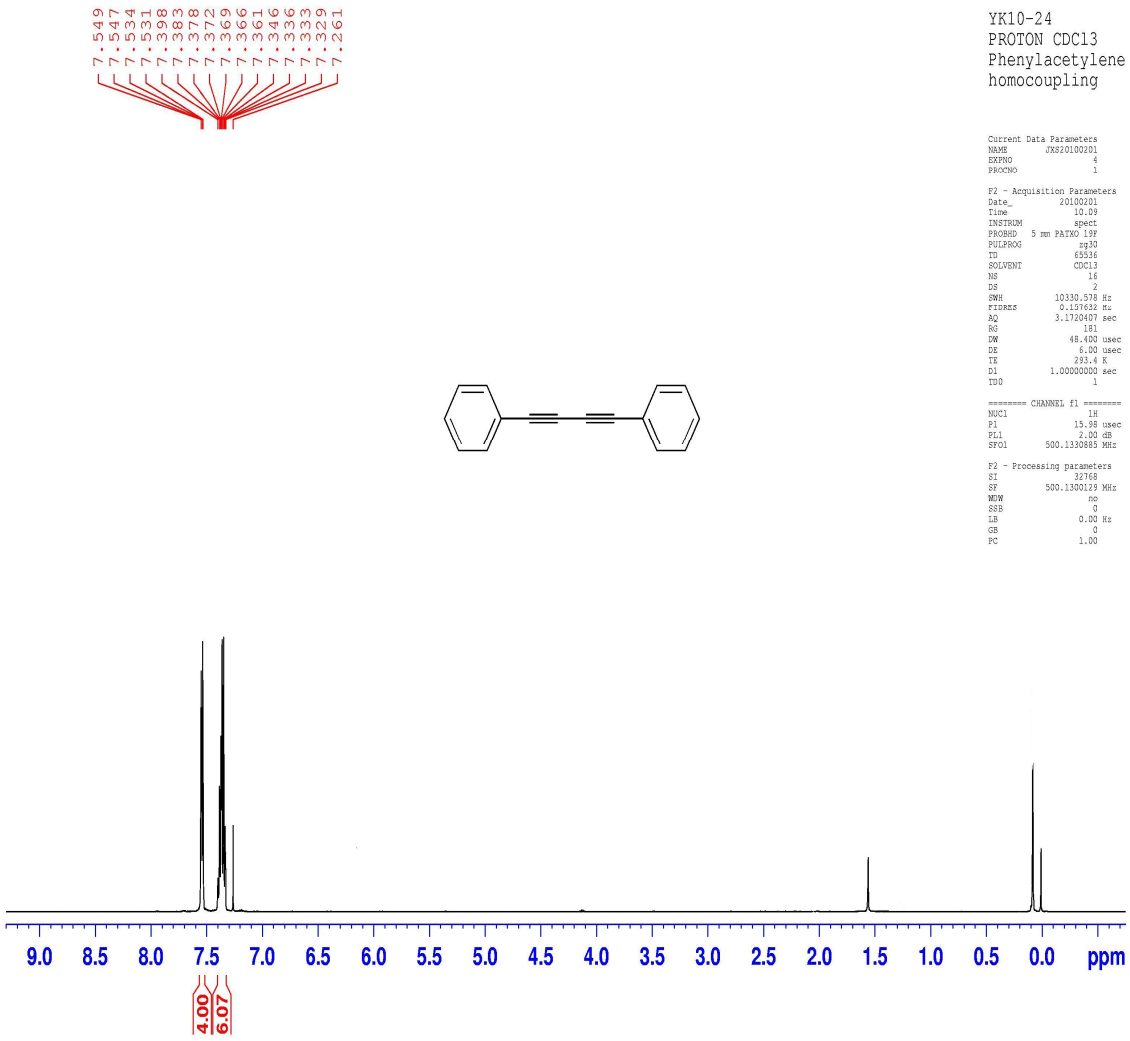
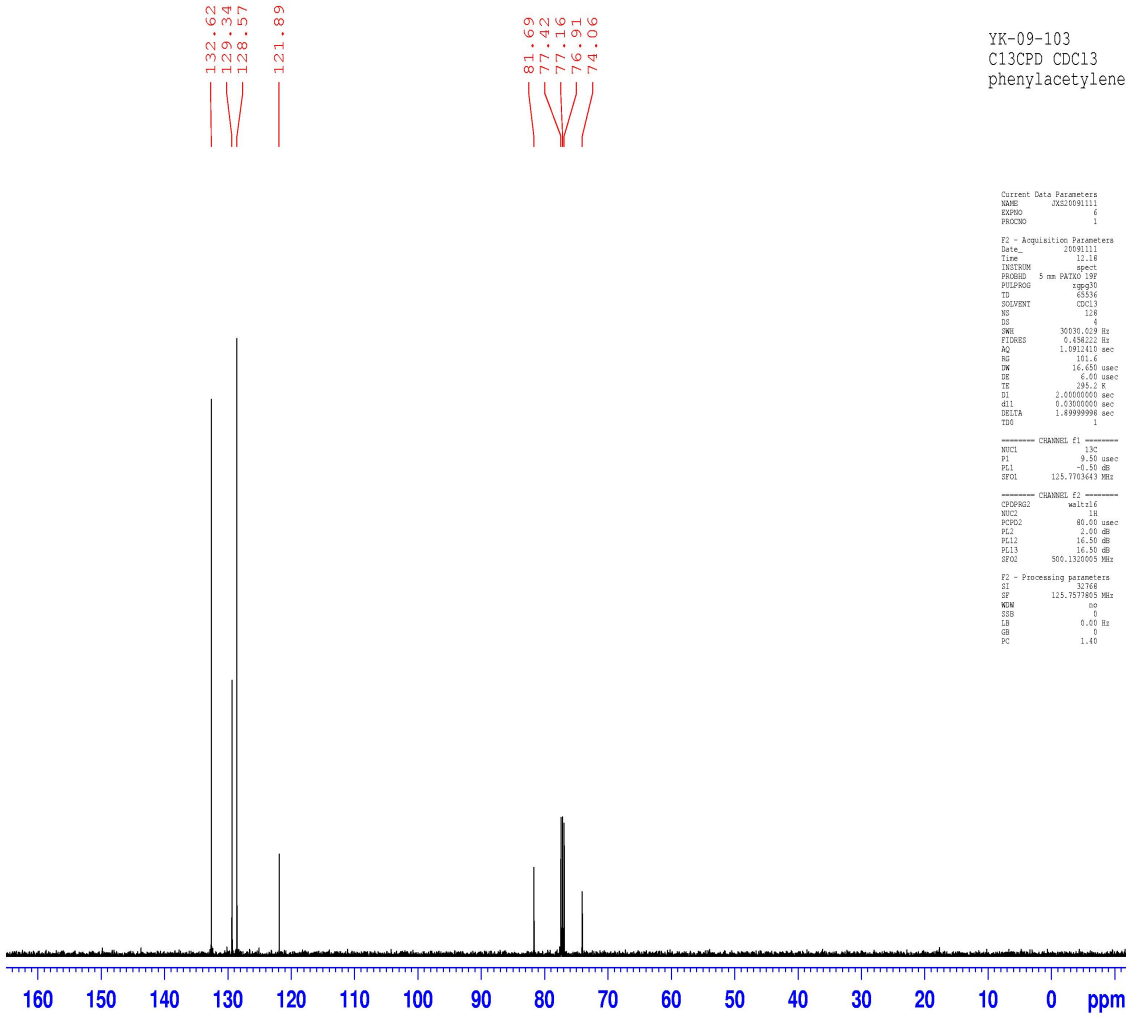
3. Copies of product ^{1}H NMR and ^{13}C NMR 2a-o:

2a:

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128.57
121.89
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77.42
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76.91
74.06
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150
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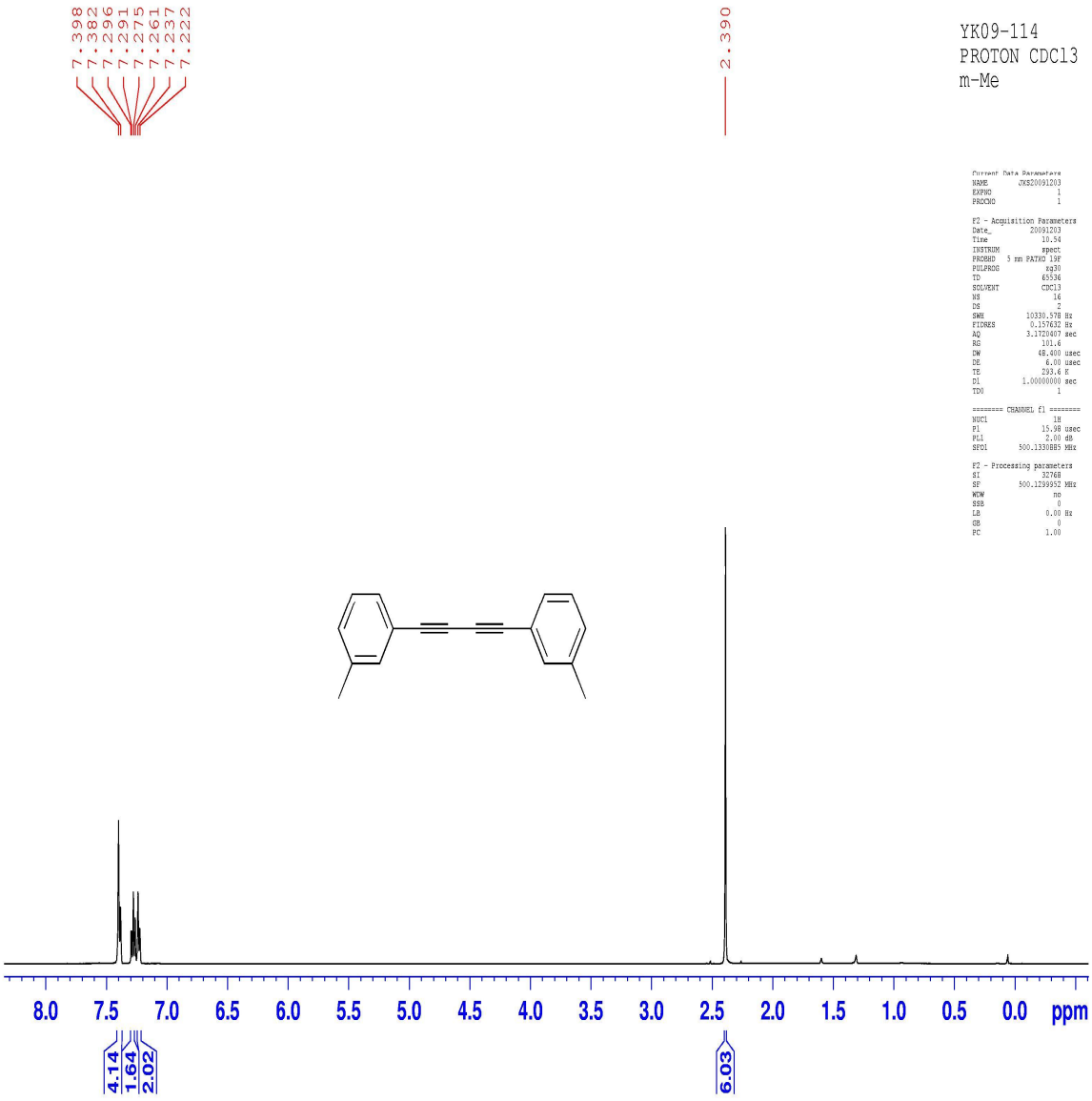
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

2b: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7.296
7.291
7.275
7.261
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7.222
2.390
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m-Me
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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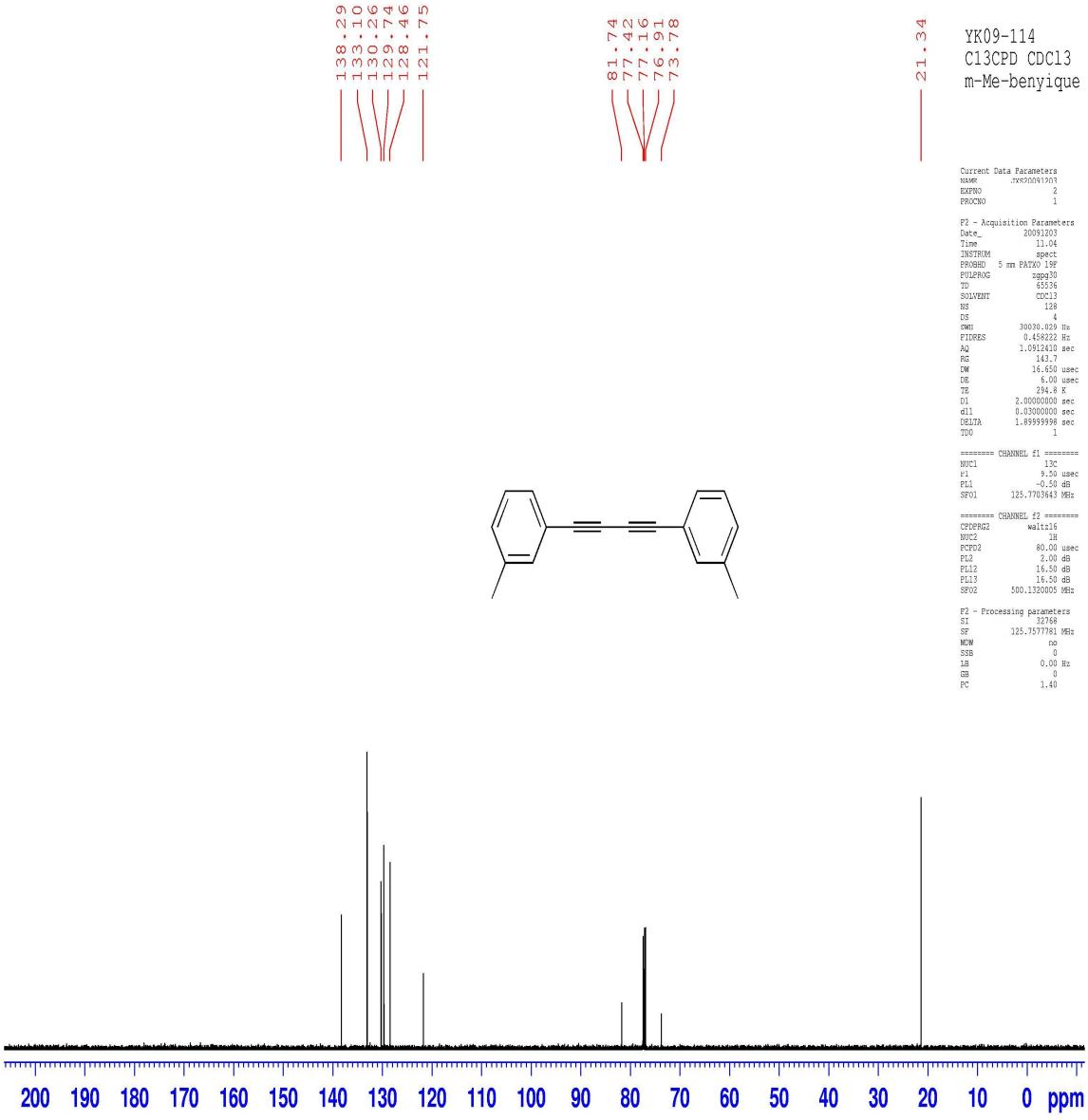
2.02
6.03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76.91
73.78
21.34
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NAME YK09091203
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PROCNO 1
F2 - Acquisition Parameters
Date_ 20091203
Time 11.04
INSTRUM spect
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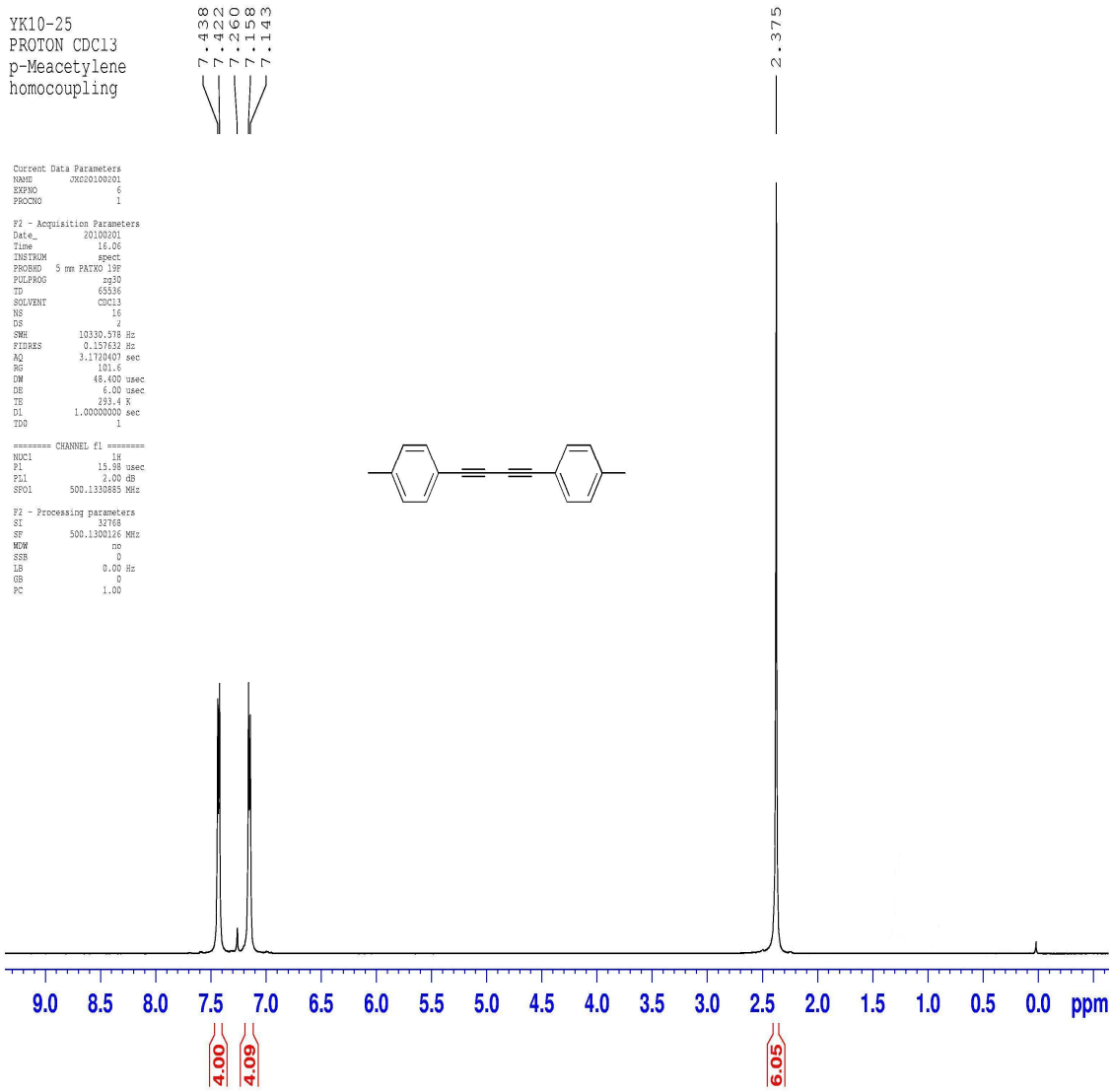
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577781 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2c: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homocoupling
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7.422
7.260
7.158
7.143
2.375
Current Data Parameters
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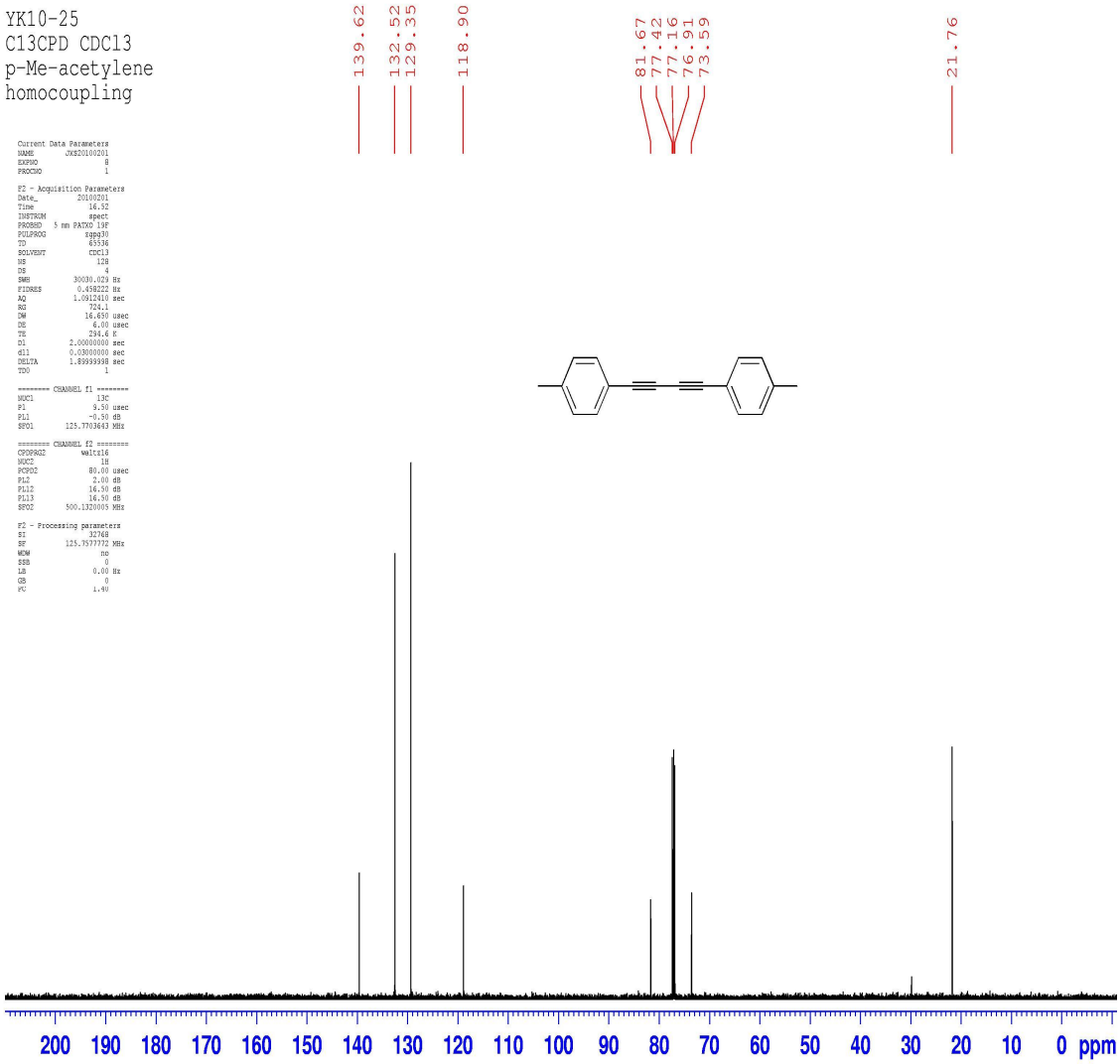
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100201
Time 16.06
INSTRUM spect
PROBHD 5 mm PATXO 13F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 101.6
DW 48.400 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.98 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300126 MHz
WDW no
SSB 0
LB 0.00 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 0.5 0.0 ppm
4.00
4.09
6.05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118.90
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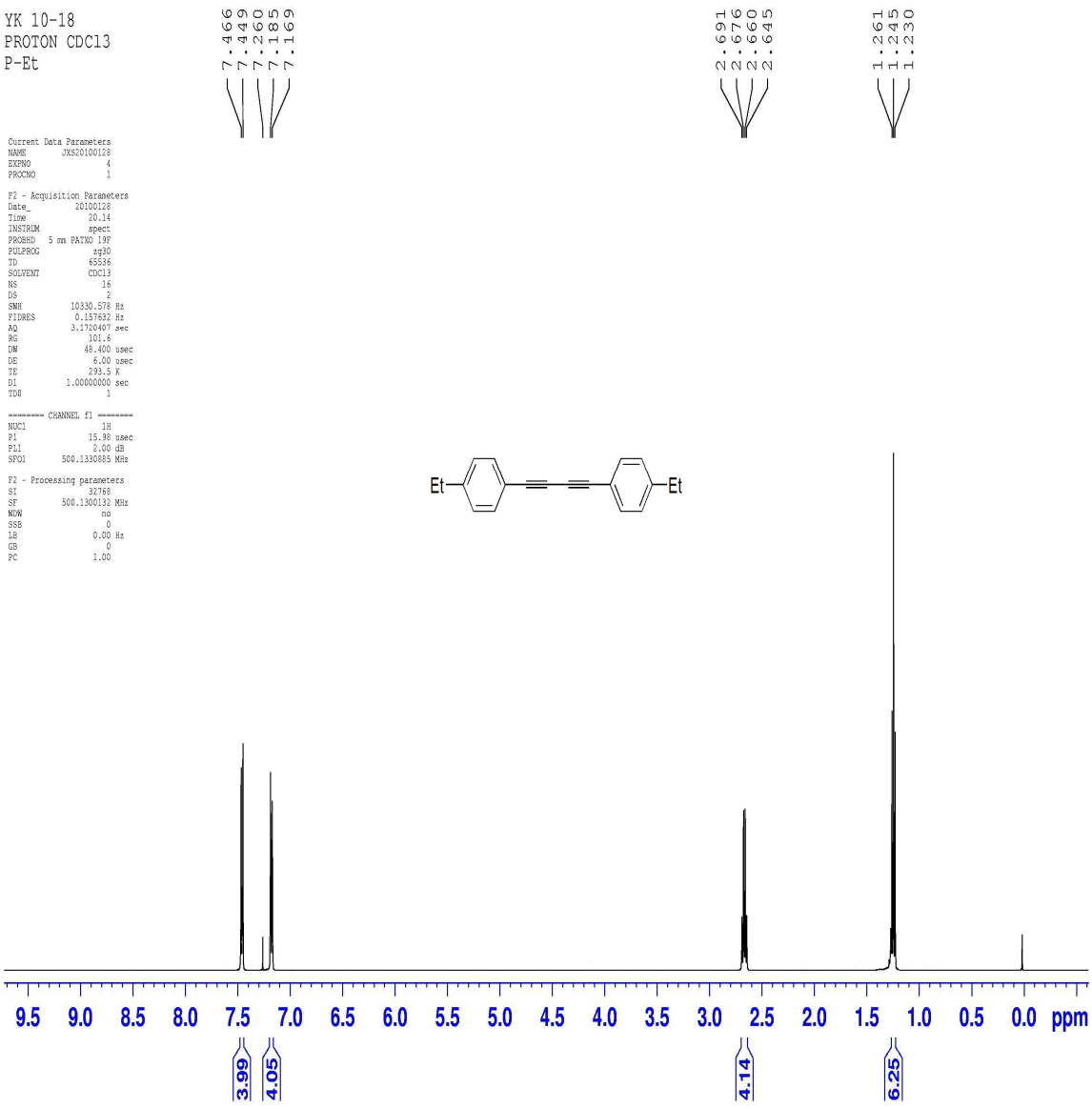
76.91
73.59
21.76
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2d: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7.260
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2.691
2.676
2.660
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1.245
1.230
Et
Et
9.5 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 0.5 0.0 ppm
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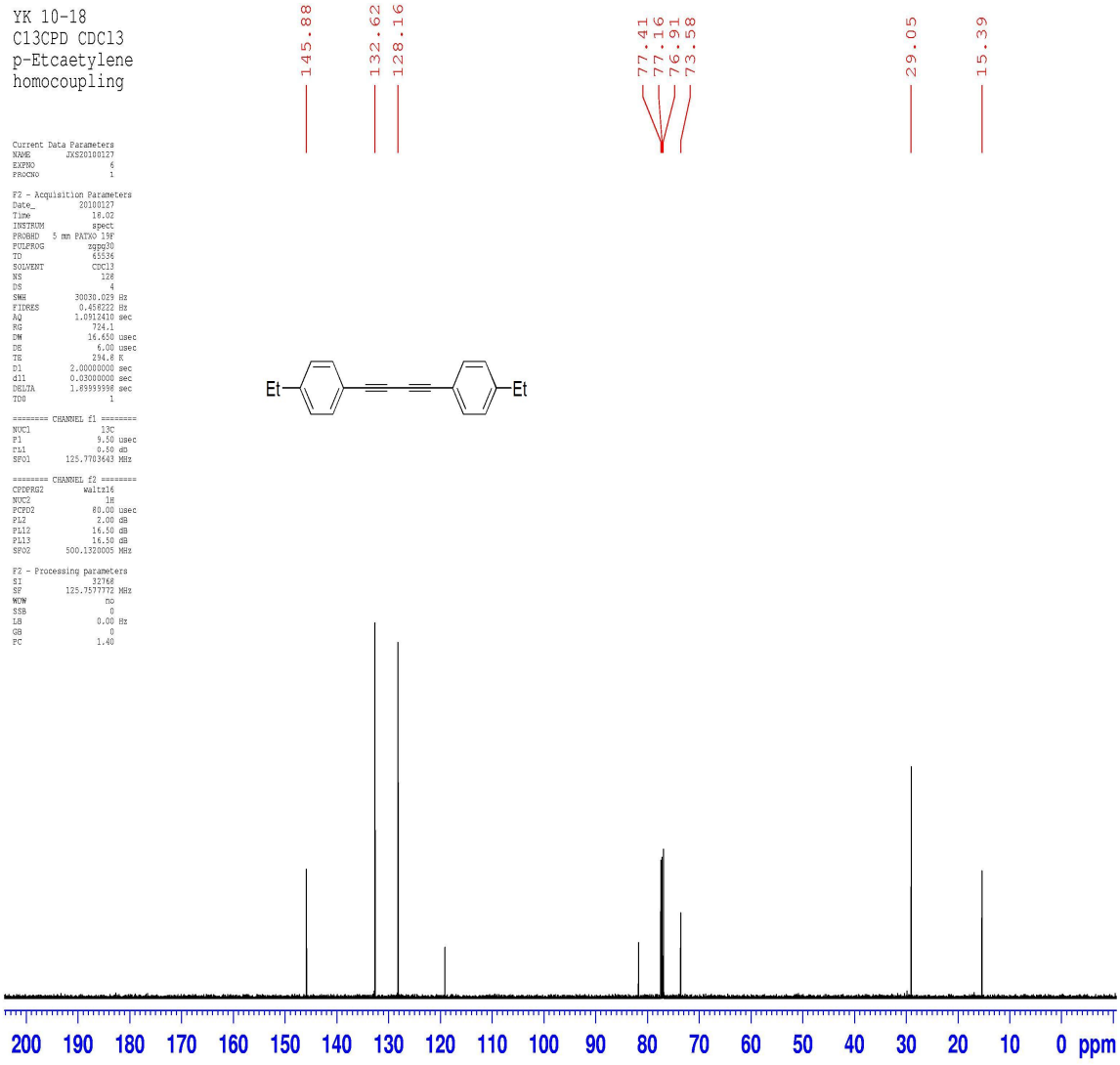
4.05
4.14
6.25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C13CPD CDCl3
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homocoupling
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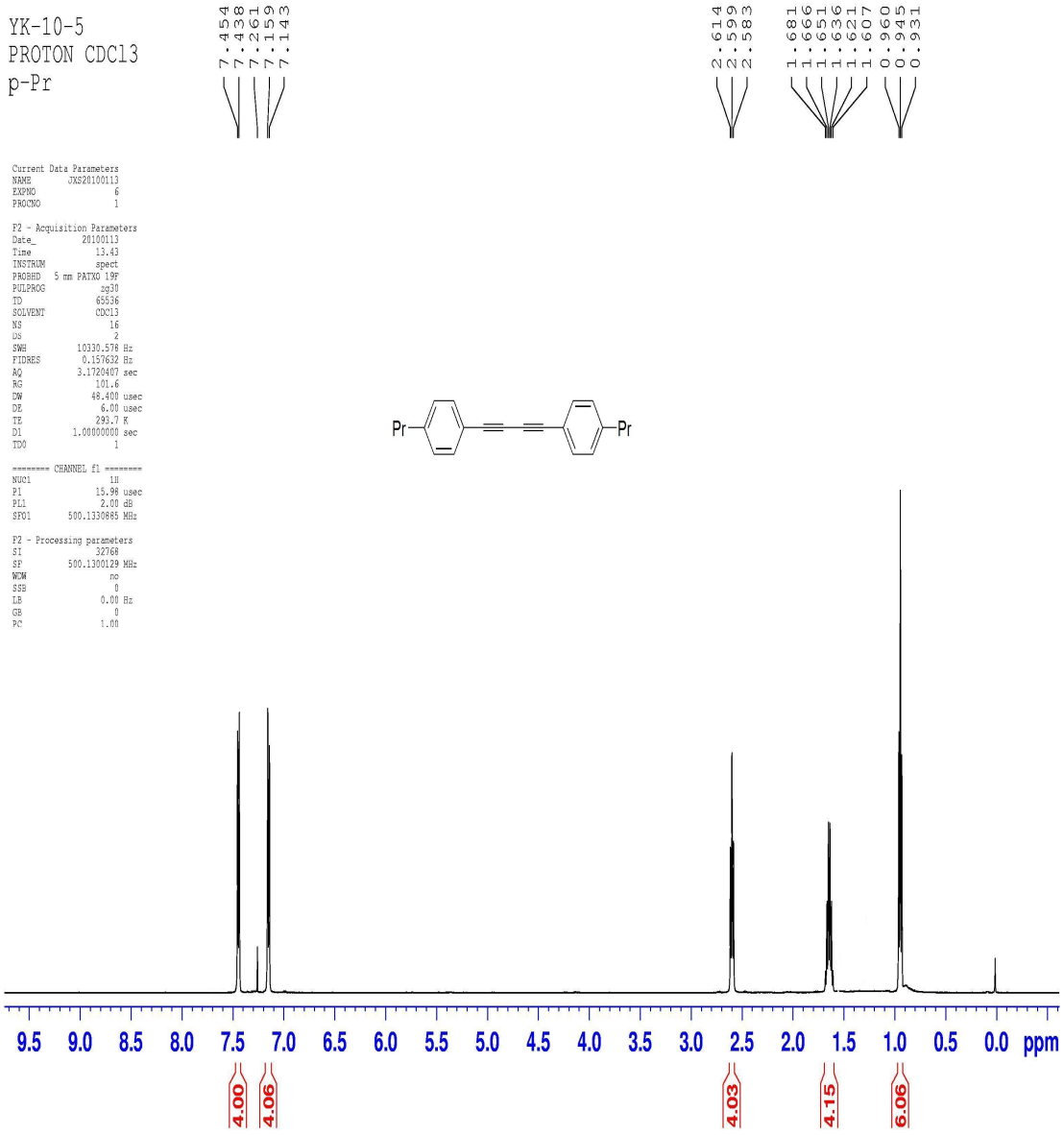
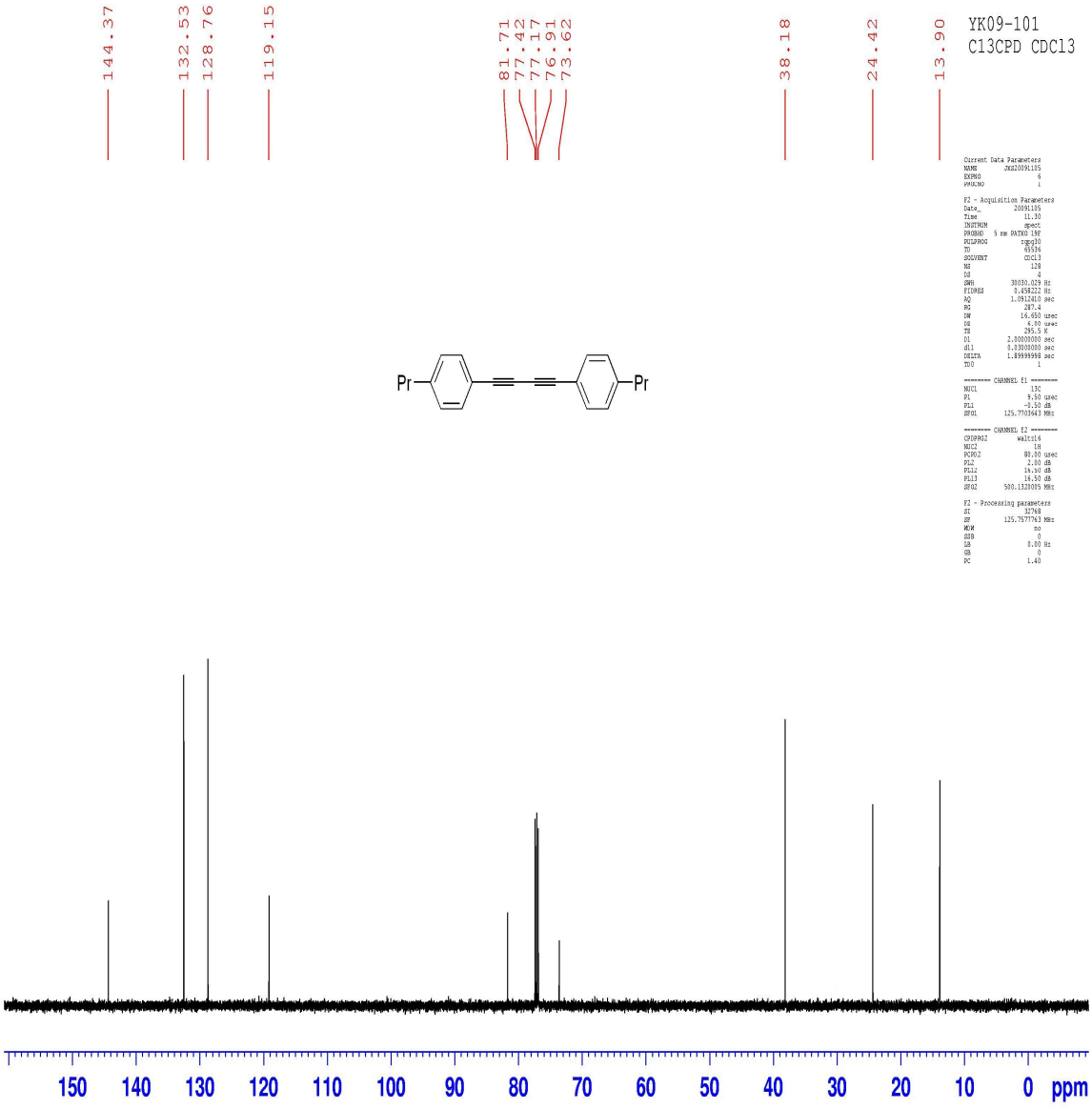
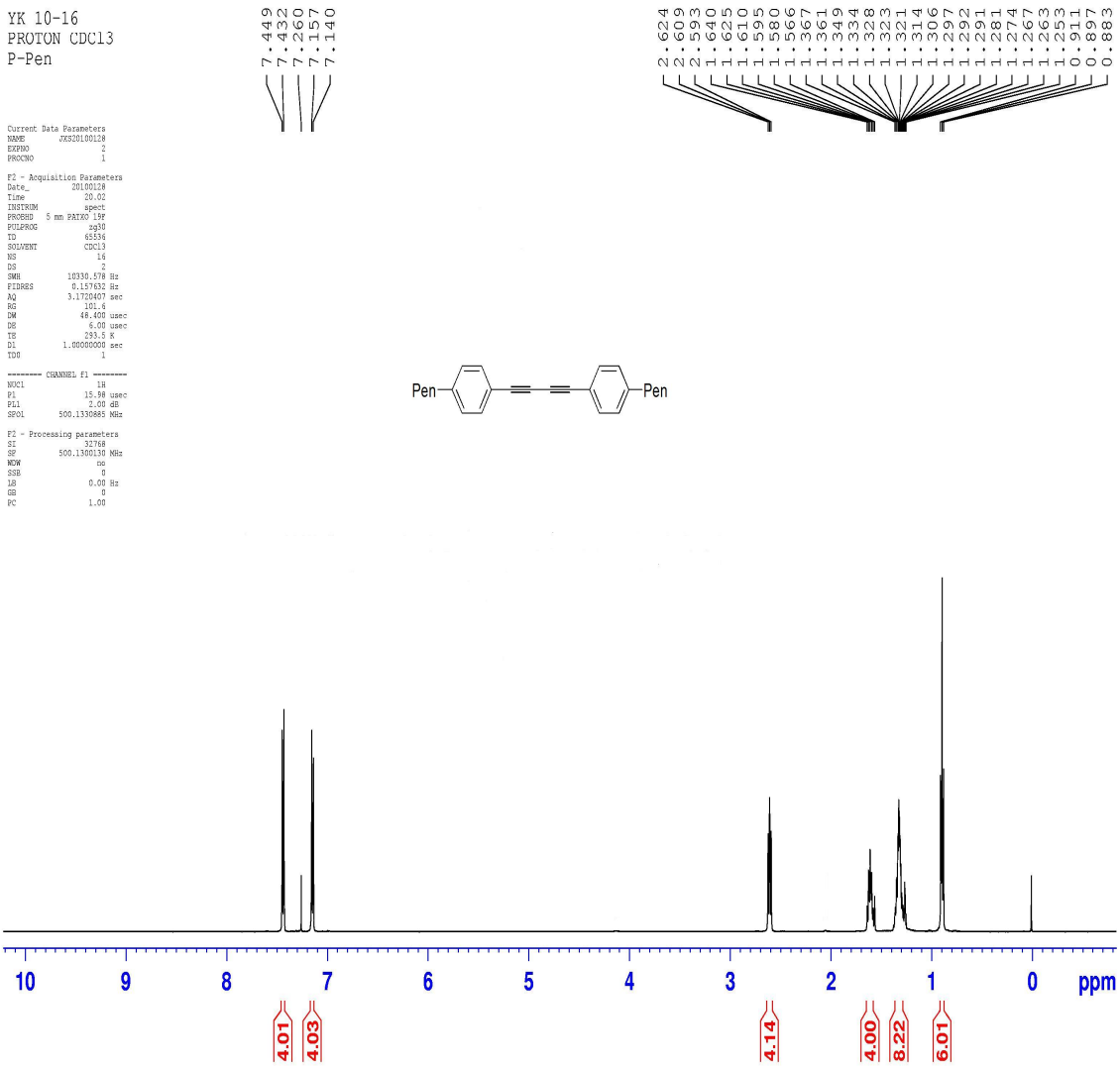
132.62
128.16
77.41
77.16
76.91
73.58
29.05
15.39
Et
Et
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

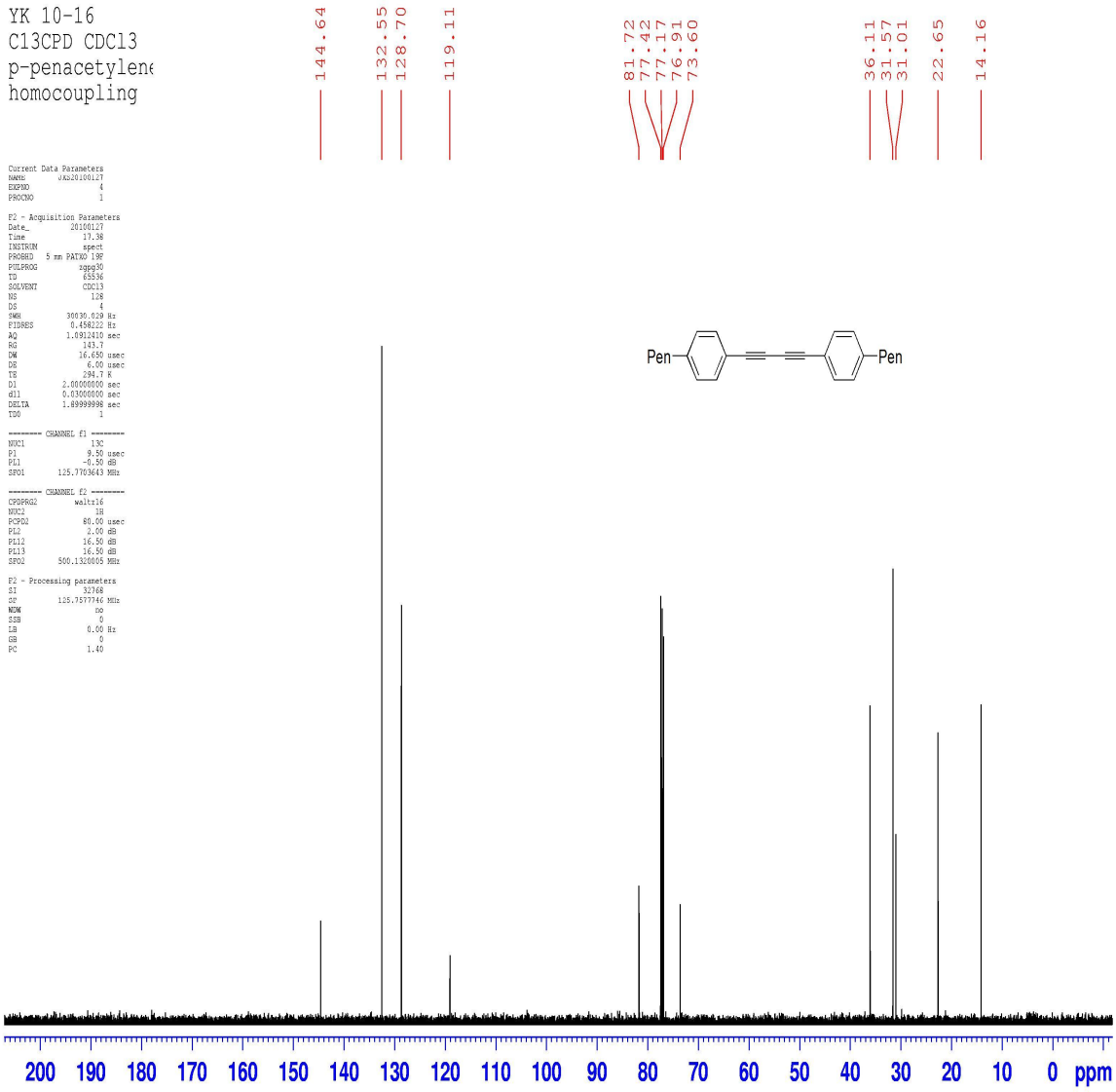
2e:


YK-10-5
PROTON CDCl3
p-Pr
7.454
7.438
7.261
7.159
7.143
2.614
2.599
2.583
1.681
1.666
1.651
1.636
1.621
1.607
0.960
0.945
0.931
Pr
Pr
9.5 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 0.5 0.0 ppm
4.00
4.06
4.03
4.15
6.06

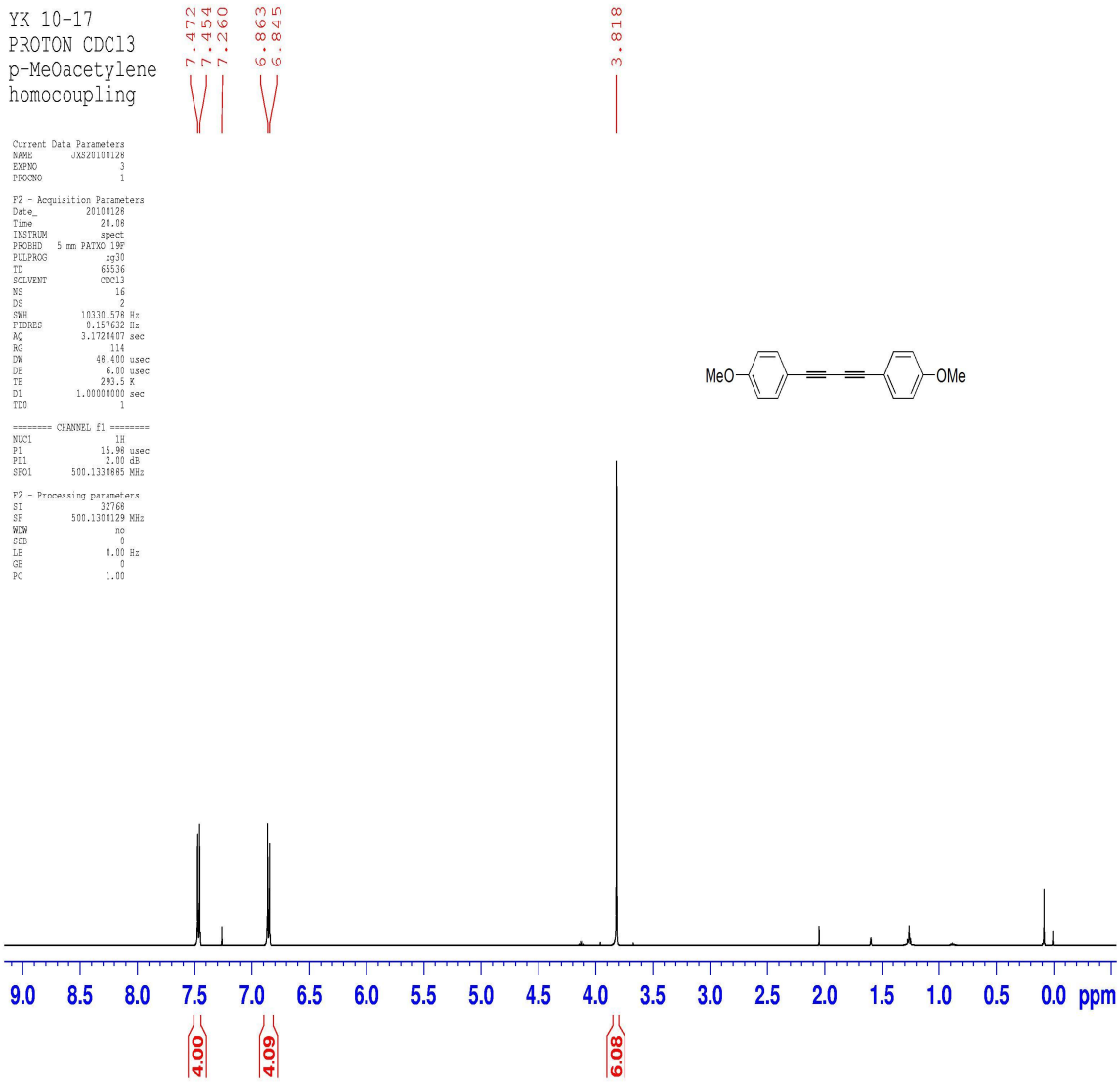

144.37
132.53
128.76
119.15
81.71
77.42
77.17
76.91
73.62
38.18
24.42
13.90
YK09-101
C13CPD CDCl3
Pr
Pr
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

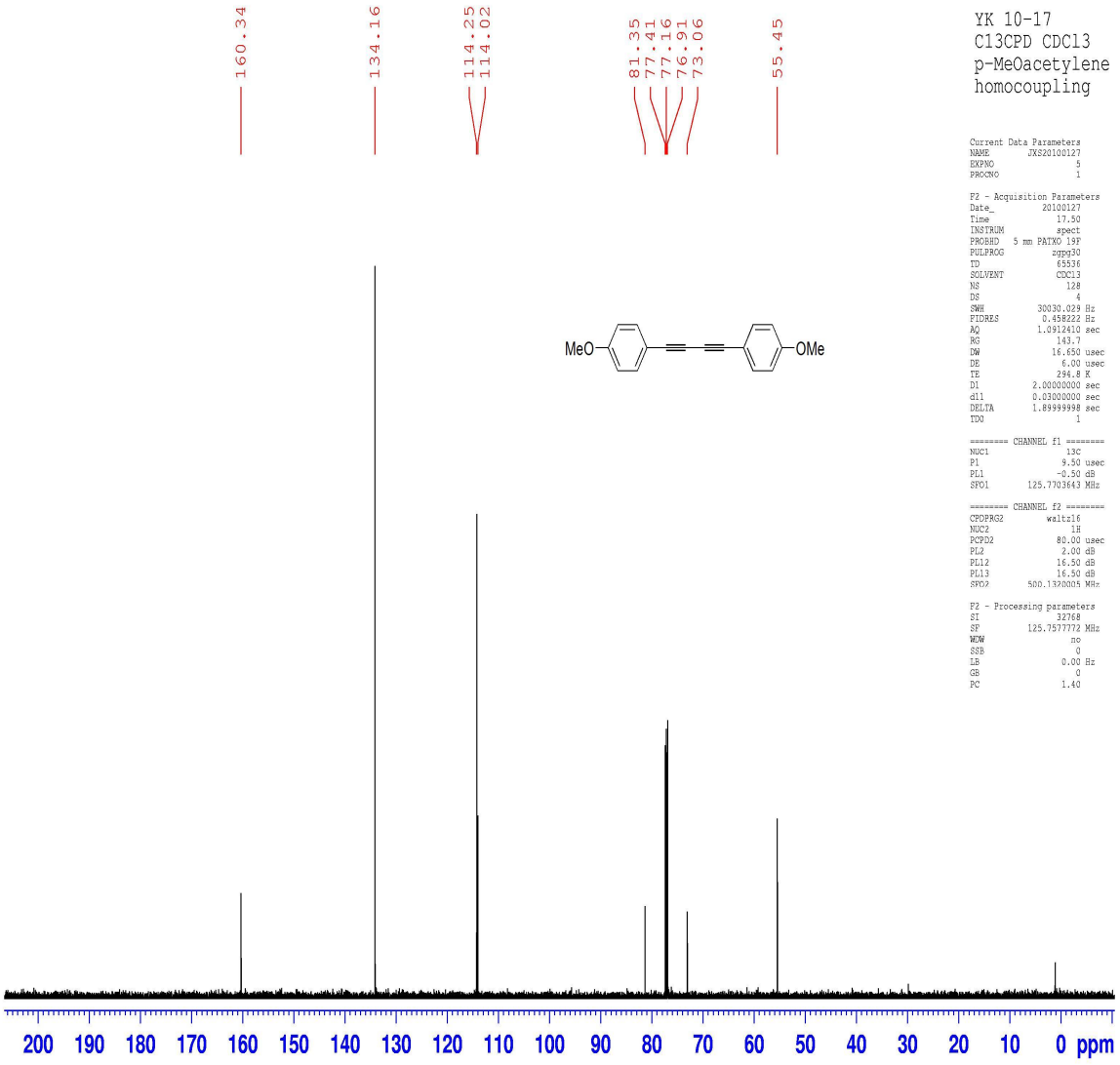
2f:


YK 10-16
PROTON CDCl3
P-Pen
7.449
7.432
7.260
7.157
7.140
2.624
2.609
2.593
1.640
1.625
1.610
1.595
1.580
1.566
1.367
1.361
1.349
1.334
1.328
1.323
1.321
1.314
1.306
1.297
1.292
1.291
1.281
1.274
1.267
1.263
1.253
0.911
0.897
0.883
Pen
Pen
10
9
8
7
6
5
4
3
2
1
0
ppm
4.01
4.03
4.14
4.00
8.22
6.01

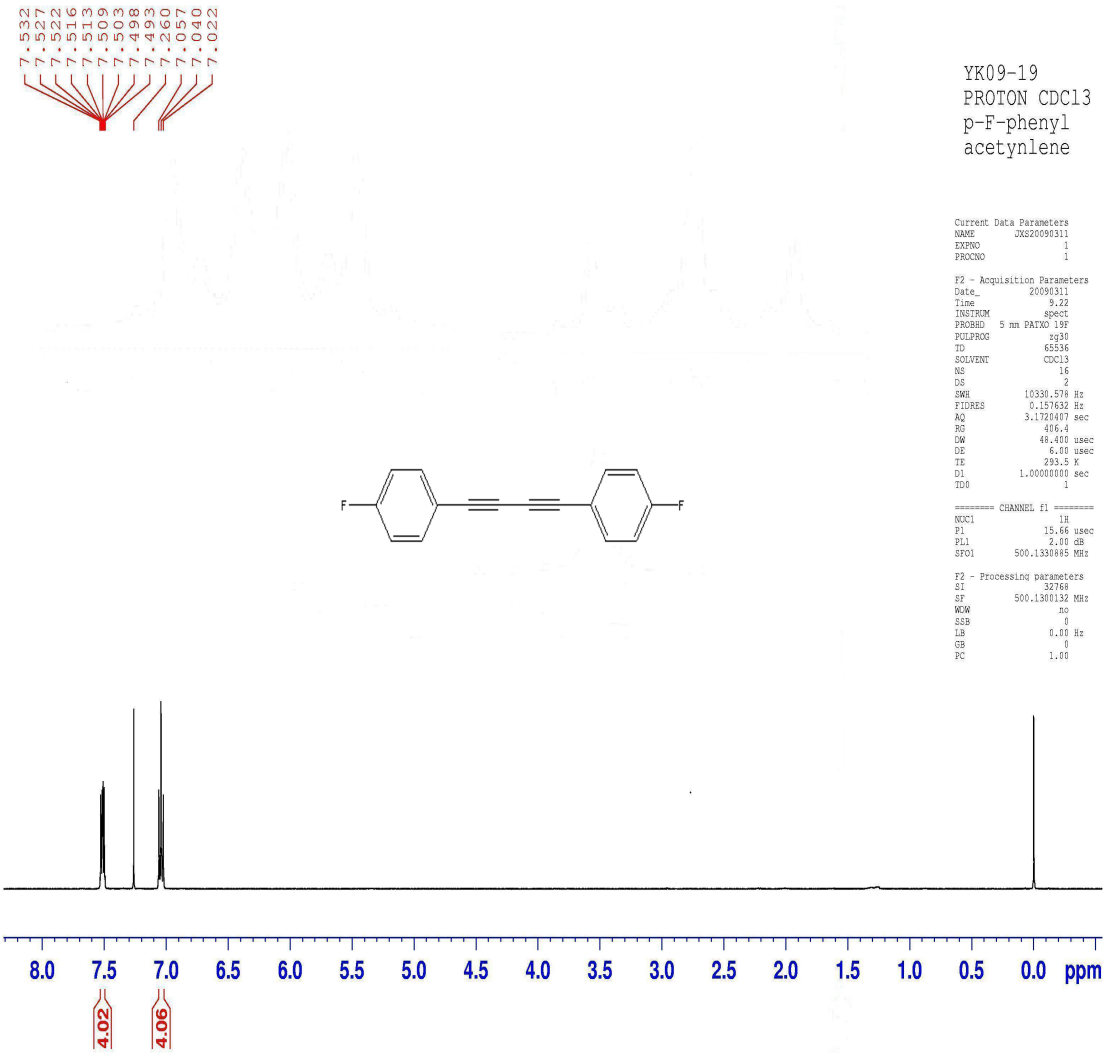

YK 10-16
C13CPD CDCl3
p-penacetylene
homocoupling
144.64
132.55
128.70
119.11
81.72
77.42
77.17
76.91
73.60
36.11
31.57
31.01
22.65
14.16
Pen
Pen
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

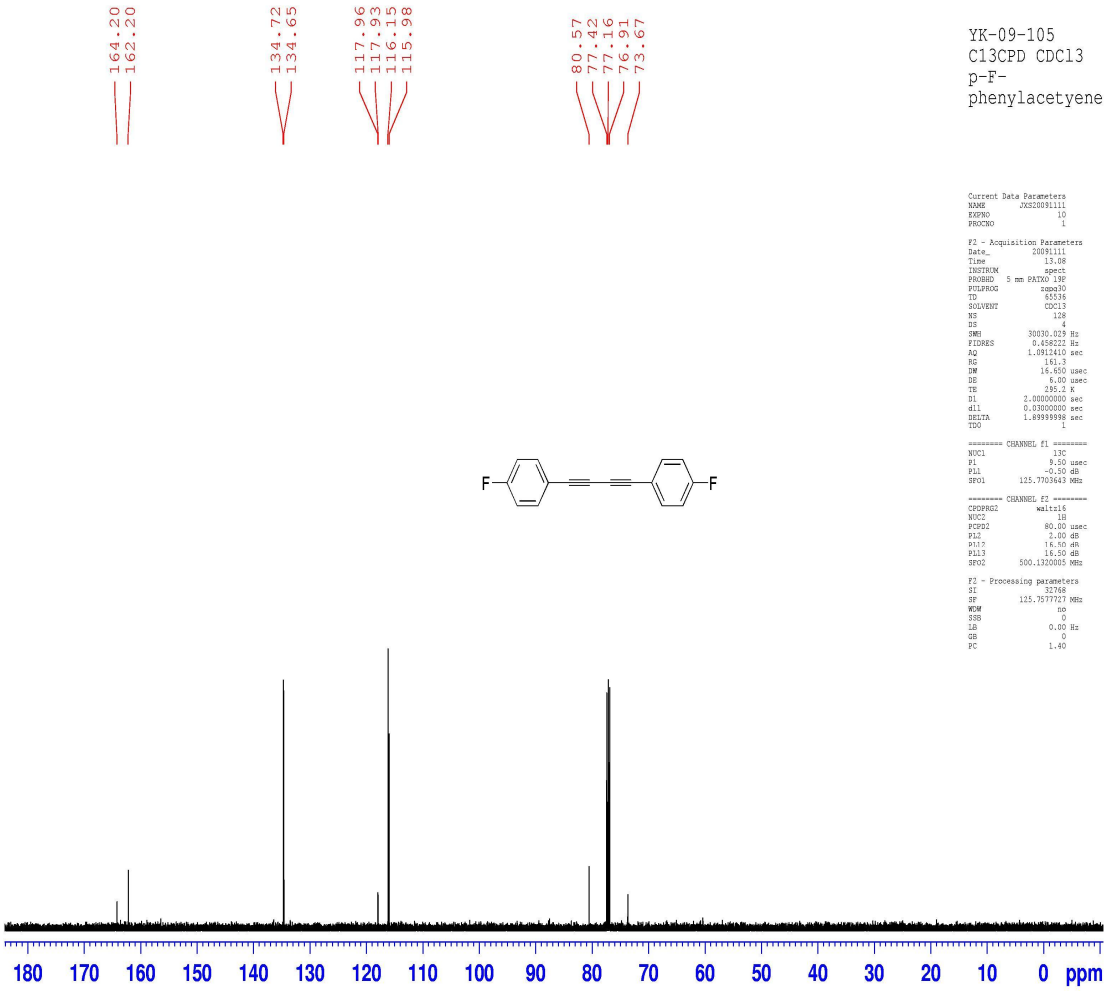
2g:


YK 10-17
PROTON CDCl3
p-MeOacetylene
homocoupling
7.472
7.454
7.260
6.863
6.845
3.818
MeO
OMe
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 0.5 0.0 ppm
4.00
4.09
6.08

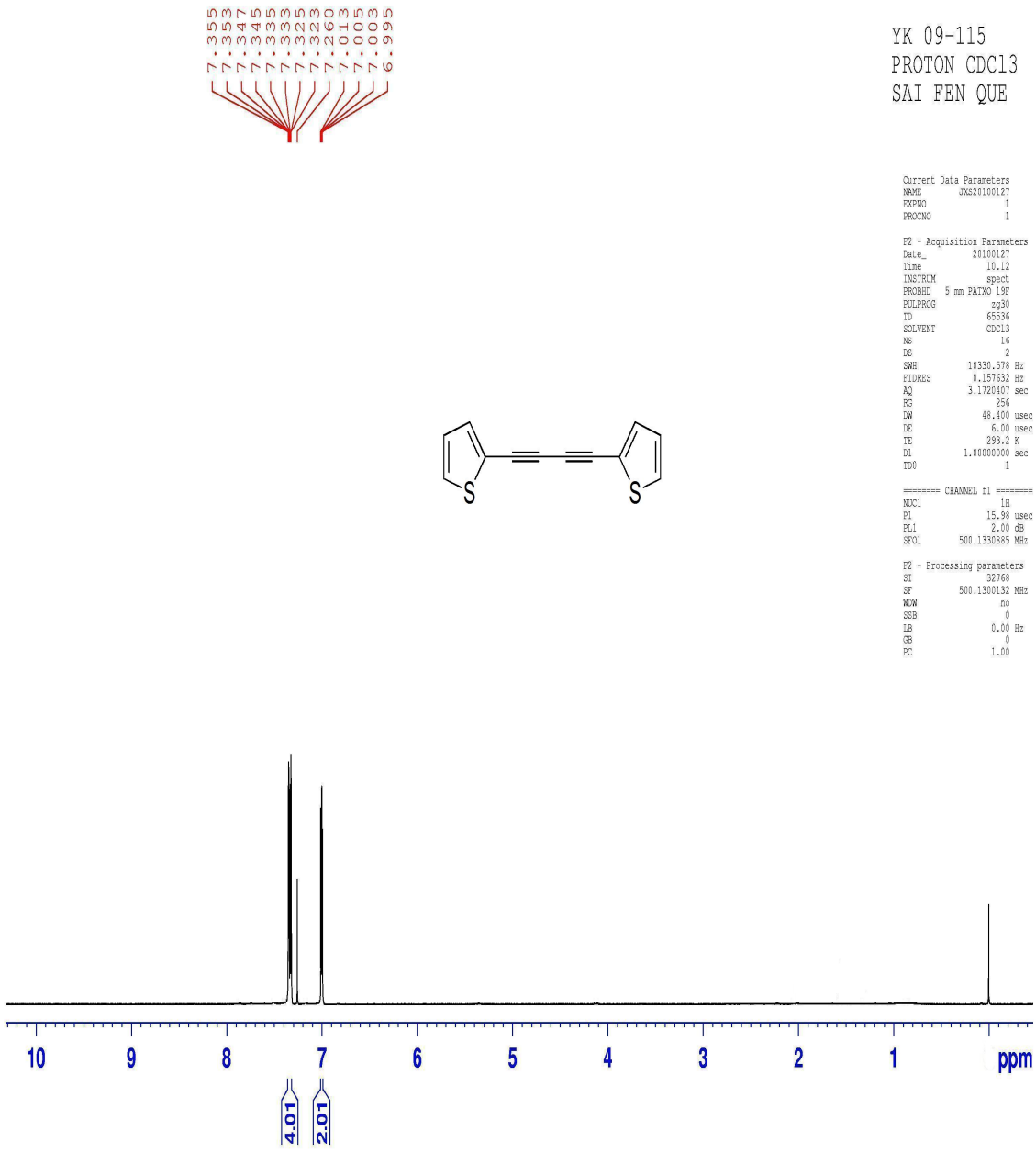

160.34
134.16
114.25
114.02
81.35
77.41
77.16
76.91
73.06
55.45
YK 10-17
C13CPD CDCl3
p-MeOacetylene
homocoupling
MeO
OMe
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

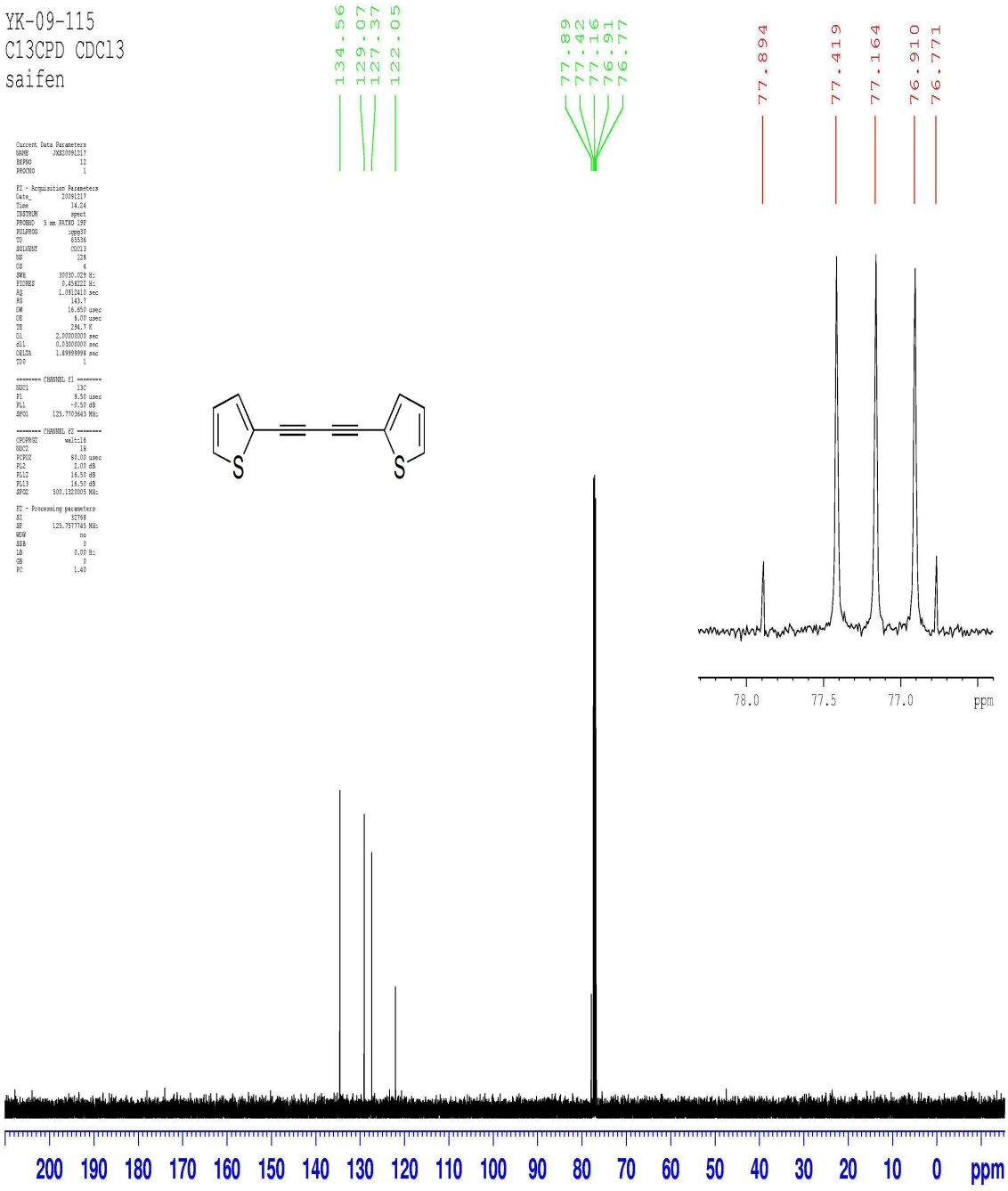
2h:


7.532
7.527
7.522
7.516
7.513
7.509
7.503
7.498
7.493
7.260
7.057
7.040
7.022
YK09-19
PROTON CDCl3
p-F-phenyl
acetynlene
F
F
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
0.5
0.0
ppm
4.02
4.06

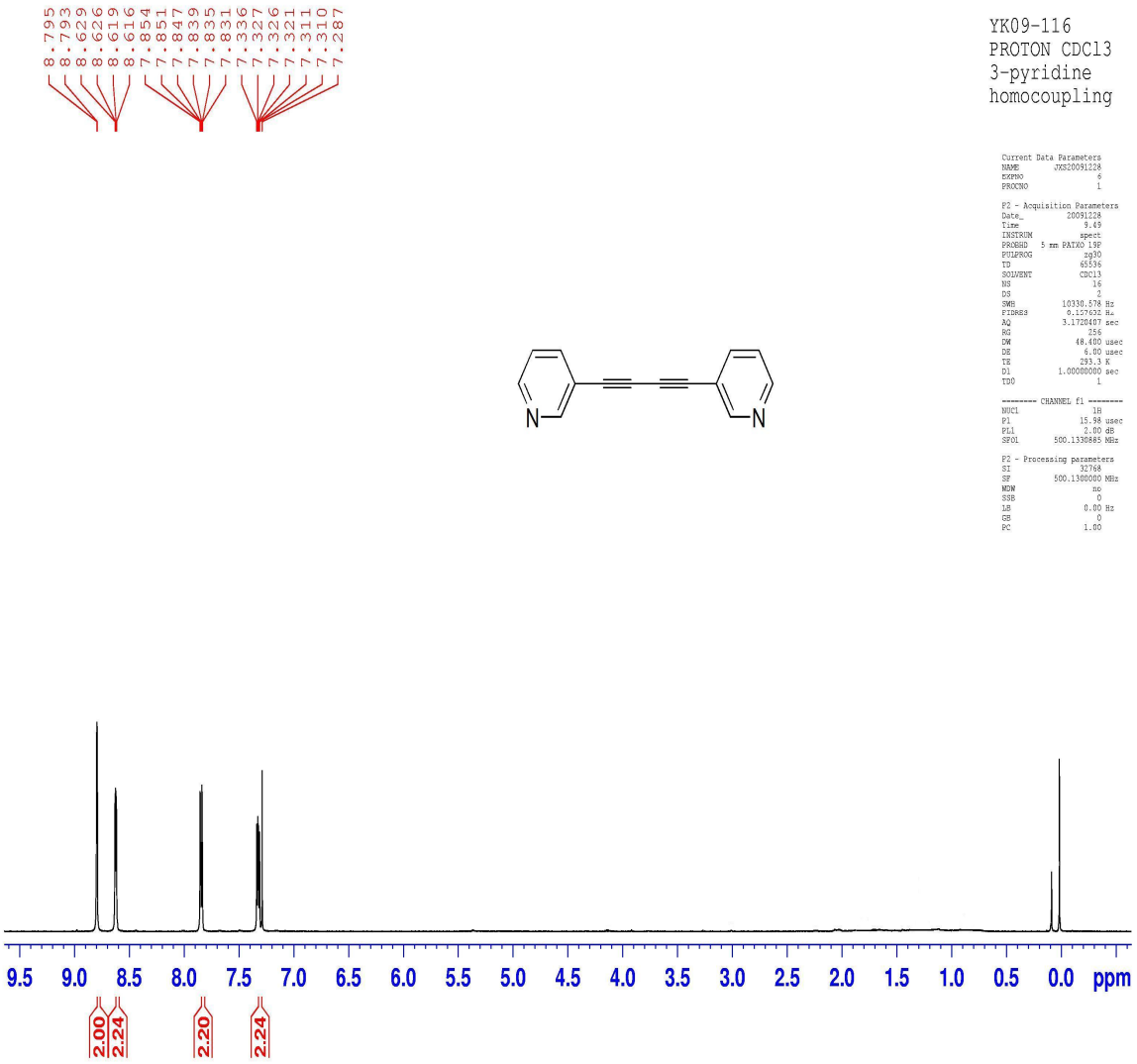

164.20
162.20
134.72
134.65
117.96
117.93
116.15
115.98
80.57
77.42
77.16
76.91
73.67
YK-09-105
C13CPD CDCl3
p-F-
phenylacetyene
F
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

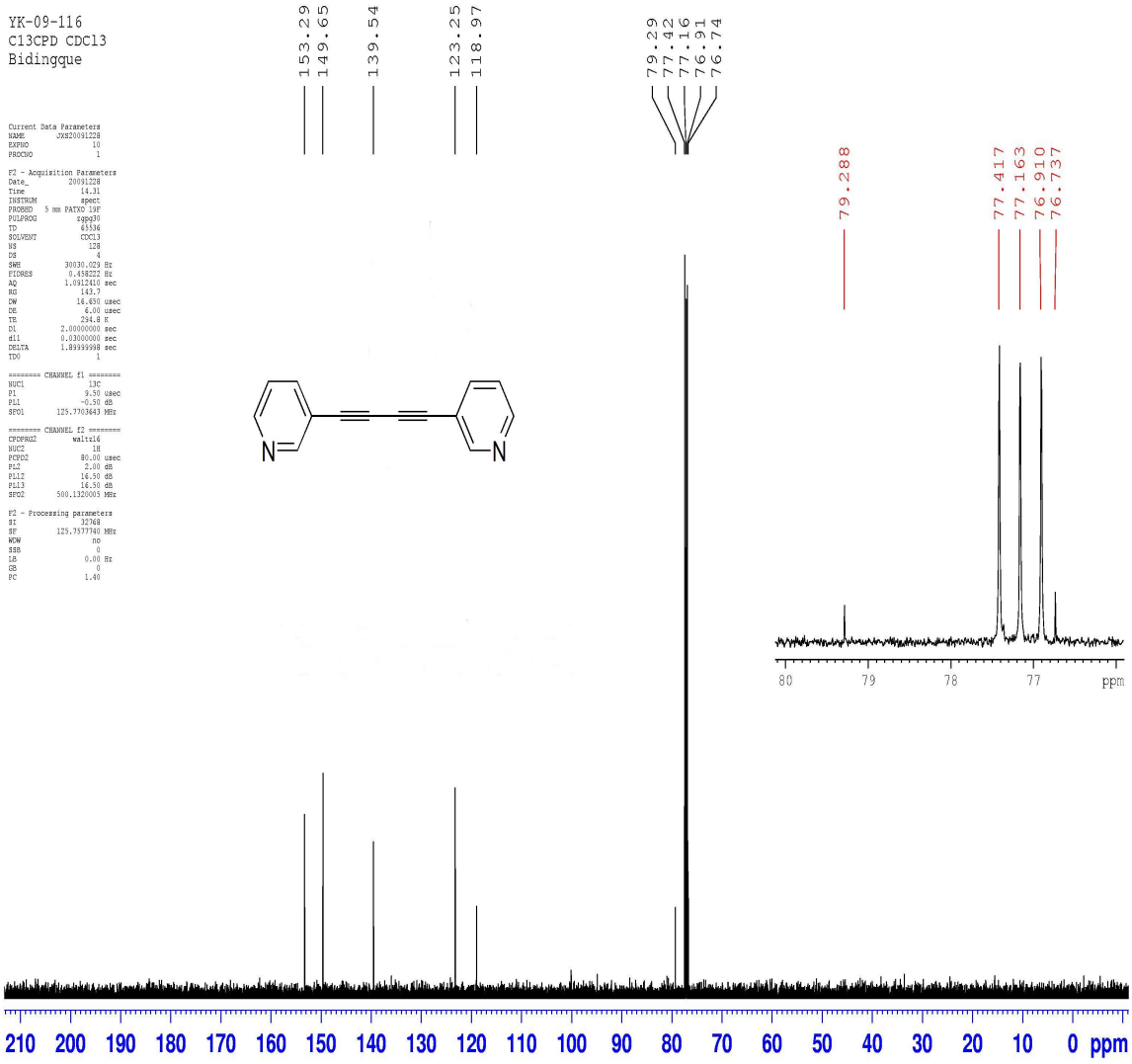
2i:


7.355
7.353
7.347
7.345
7.335
7.333
7.325
7.323
7.260
7.013
7.005
7.003
6.995
YK 09-115
PROTON CDCl3
SAI FEN QUE
Current Data Parameters
NAME JXS20100127
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100127
Time 10.12
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 256
DW 48.400 usec
DE 6.00 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.98 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
S
S
10
9
8
7
6
5
4
3
2
1
ppm
4.01
2.01

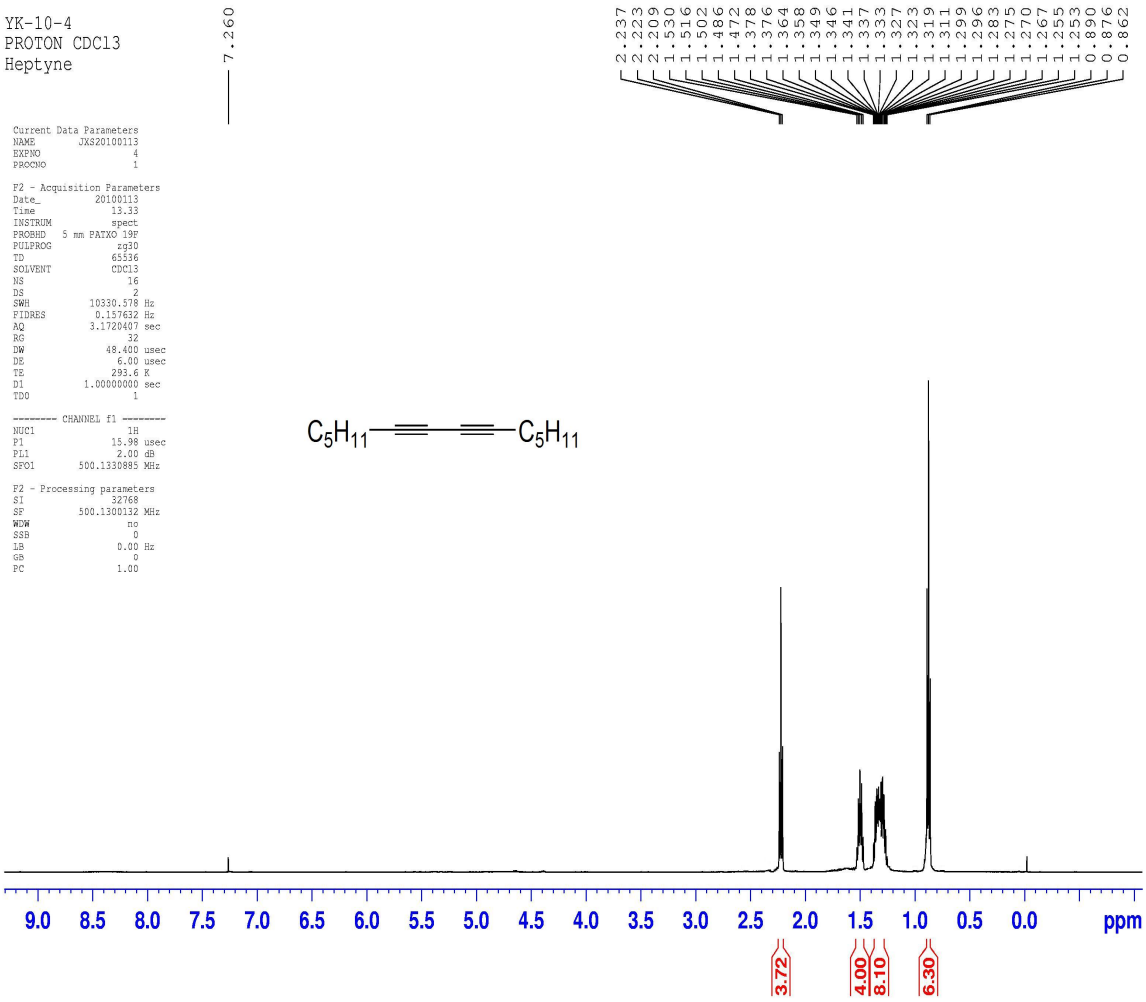

YK-09-115
C13CPD CDCl3
saifen
134.56
129.07
127.37
122.05
77.89
77.42
77.16
76.91
76.77
77.894
77.419
77.164
76.910
76.771
78.0
77.5
77.0
ppm
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

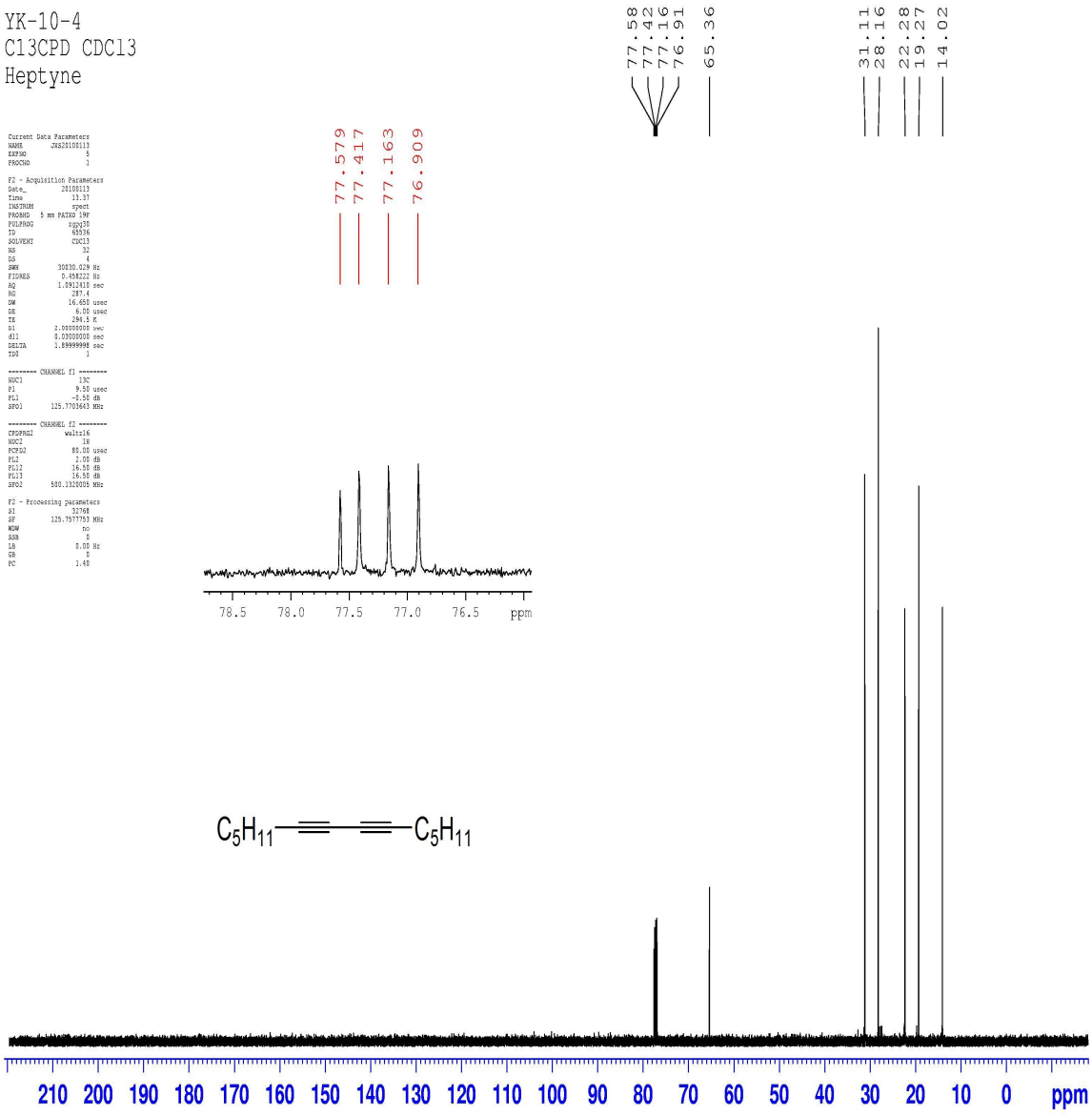
2j:


8.795
8.793
8.629
8.626
8.619
8.616
7.854
7.851
7.847
7.839
7.835
7.831
7.336
7.327
7.326
7.321
7.311
7.310
7.287
YK09-116
PROTON CDCl3
3-pyridine
homocoupling
N
N
9.5 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 0.5 0.0 ppm
2.00
2.24
2.20
2.24

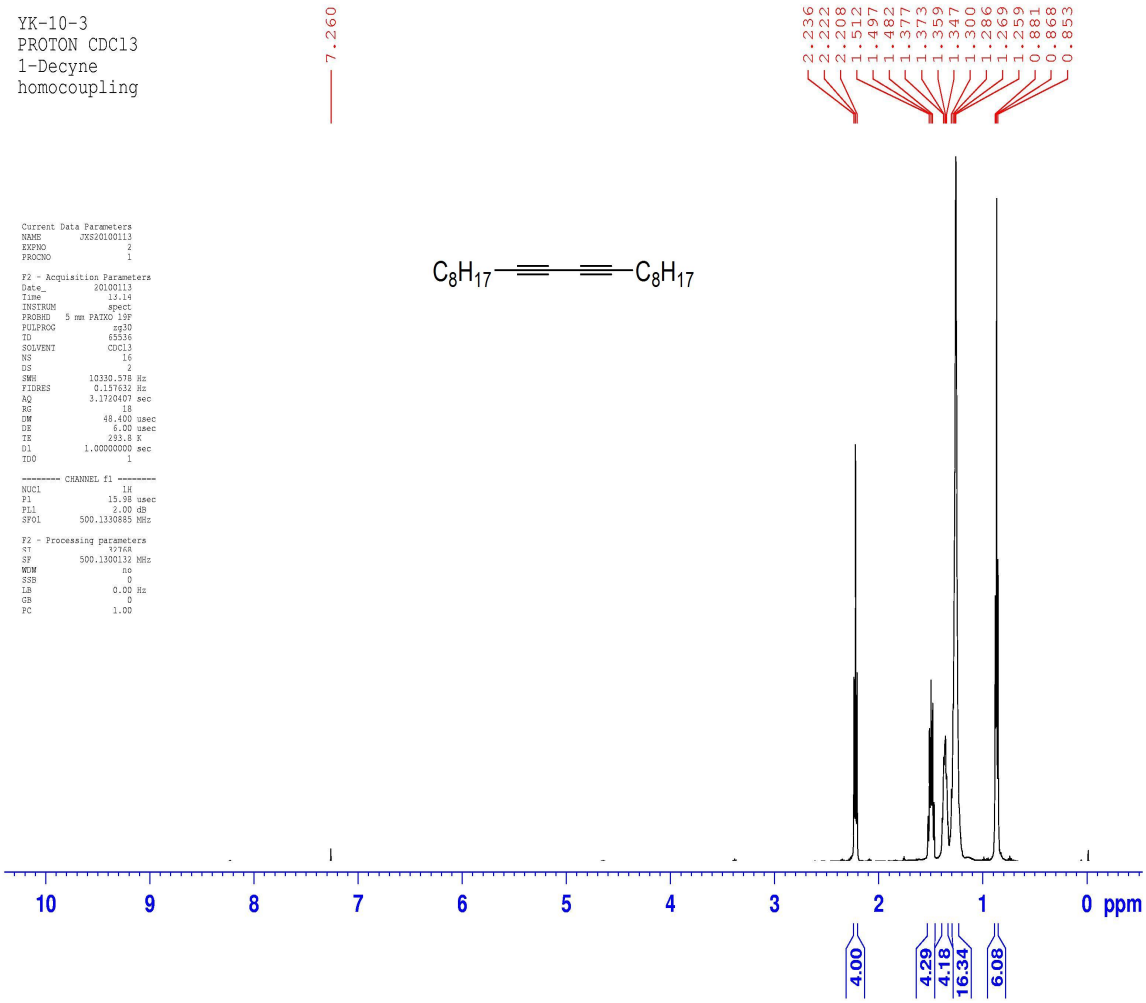

YK-09-116
C13CPD CDCl3
Bidingque
153.29
149.65
139.54
123.25
118.97
79.29
77.42
77.16
76.91
76.74
79.288
77.417
77.163
76.910
76.737
N
N
80
79
78
77
ppm
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

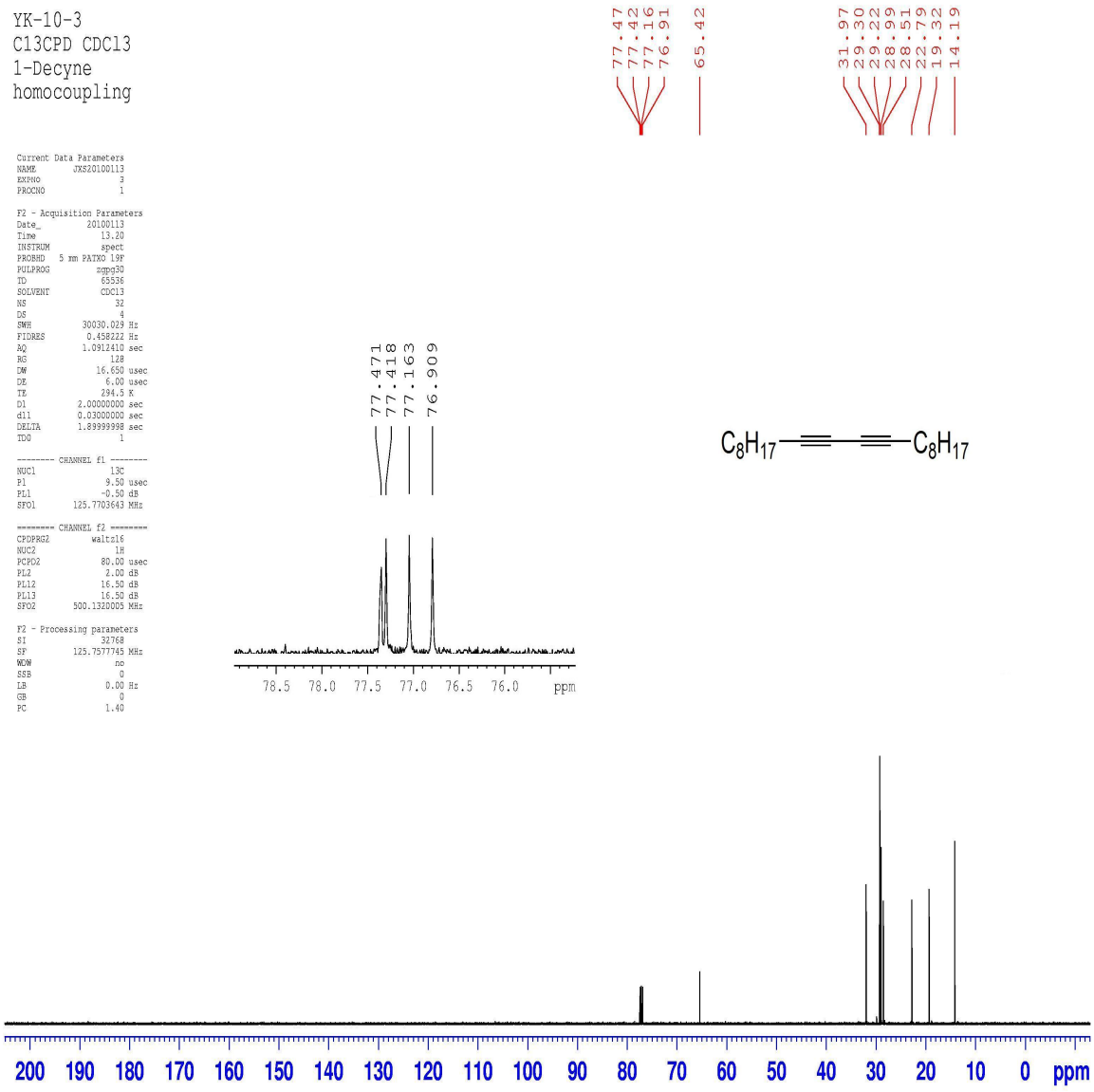
2k:


YK-10-4
PROTON CDCl3
Heptyne
7.260
2.237
2.223
2.209
1.530
1.516
1.502
1.486
1.472
1.378
1.376
1.364
1.358
1.349
1.346
1.341
1.337
1.333
1.327
1.323
1.319
1.311
1.299
1.296
1.283
1.275
1.270
1.267
1.255
1.253
0.890
0.876
0.862
Current Data Parameters
NAME JXS20100113
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100113
Time 13.33
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 32
DW 48.400 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 15.98 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
C5H11
C5H11
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
0.5
0.0
ppm
3.72
4.00
8.10
6.30


YK-10-4
C13CPD CDCl3
Heptyne
77.58
77.42
77.16
76.91
65.36
31.11
28.16
22.28
19.27
14.02
77.579
77.417
77.163
76.909
78.5
78.0
77.5
77.0
76.5
ppm
C5H11
C5H11
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2l:


YK-10-3
PROTON CDCl3
1-Decyne
homocoupling
7.260
2.236
2.222
2.208
1.512
1.497
1.482
1.377
1.373
1.359
1.347
1.300
1.286
1.269
1.259
0.881
0.868
0.853
Current Data Parameters
NAME JXS20100113
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100113
Time 13.14
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 18
DW 48.400 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 15.98 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
C8H17
C8H17
10
9
8
7
6
5
4
3
2
1
0 ppm
4.00
4.29
4.18
16.34
6.08



Current Data Parameters
NAME JXS20100113
EXPNO 3
PROCNO 1

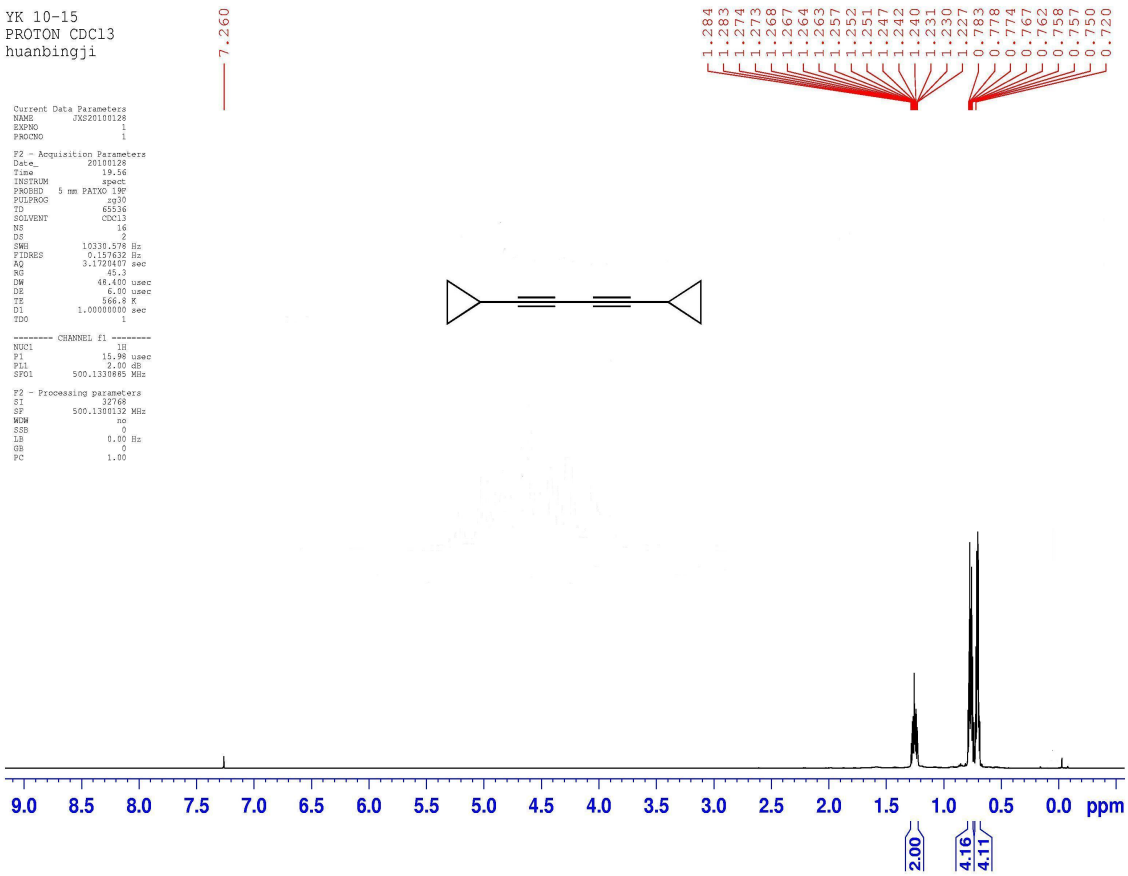
F2 - Acquisition Parameters
Date_ 20100113
Time 13.20
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 128
DW 16.650 usec
DE 6.00 usec
TE 294.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

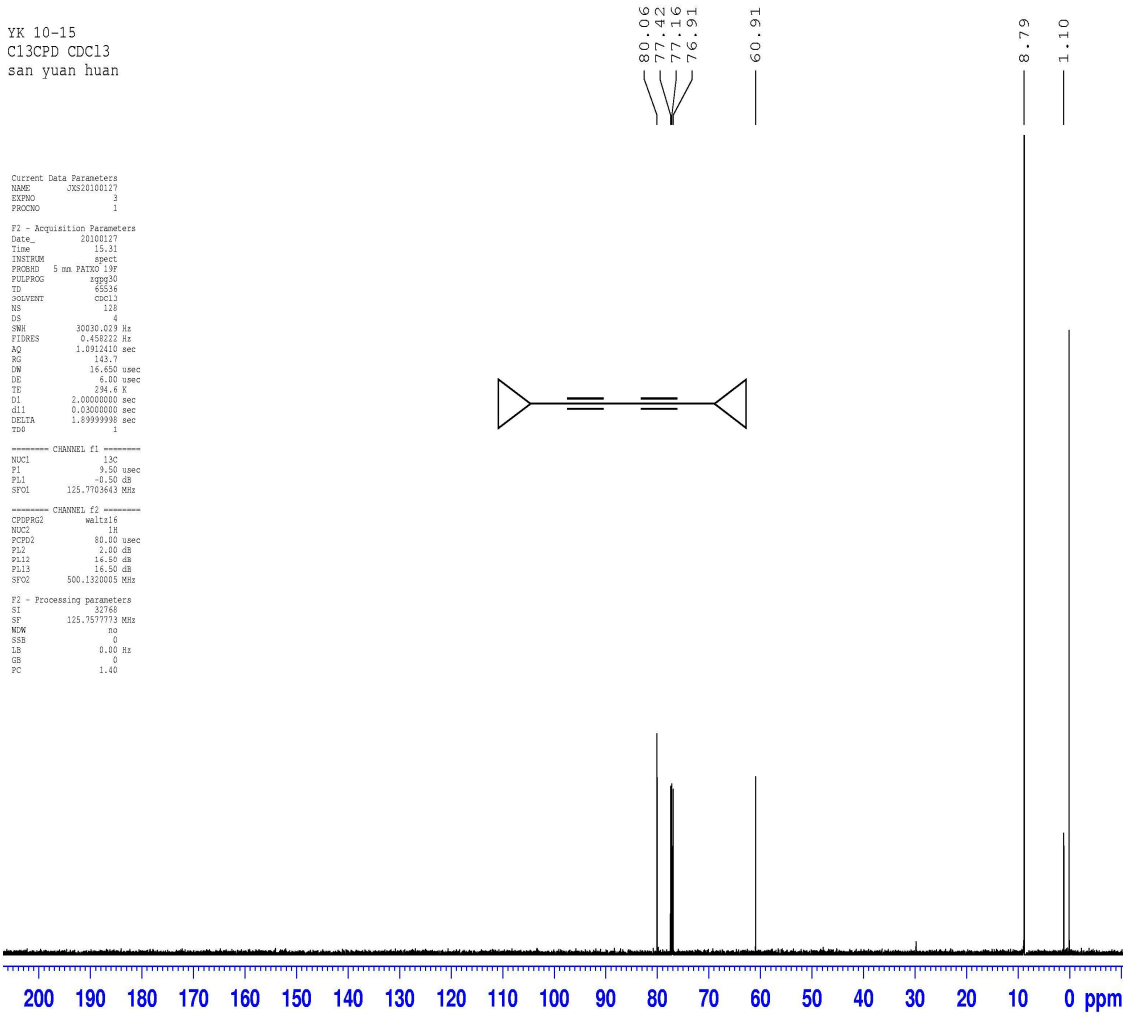
-------- CHANNEL f1 --------
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577745 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

2m:


YK 10-15
PROTON CDCl3
huanbingji
7.260
1.284
1.283
1.274
1.273
1.268
1.267
1.264
1.263
1.257
1.252
1.251
1.247
1.242
1.240
1.231
1.230
1.227
0.783
0.778
0.774
0.767
0.762
0.758
0.757
0.750
0.720
Current Data Parameters
NAME JXS20100128
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100128
Time 19.56
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 45.3
DW 48.400 usec
DE 6.00 usec
TE 566.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.98 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW no
SSB 0
LB 0.00 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 0.5 0.0 ppm
2.00
4.16
4.11



Current Data Parameters
NAME XKS20100127
EXPNO 3
PROCNO 1

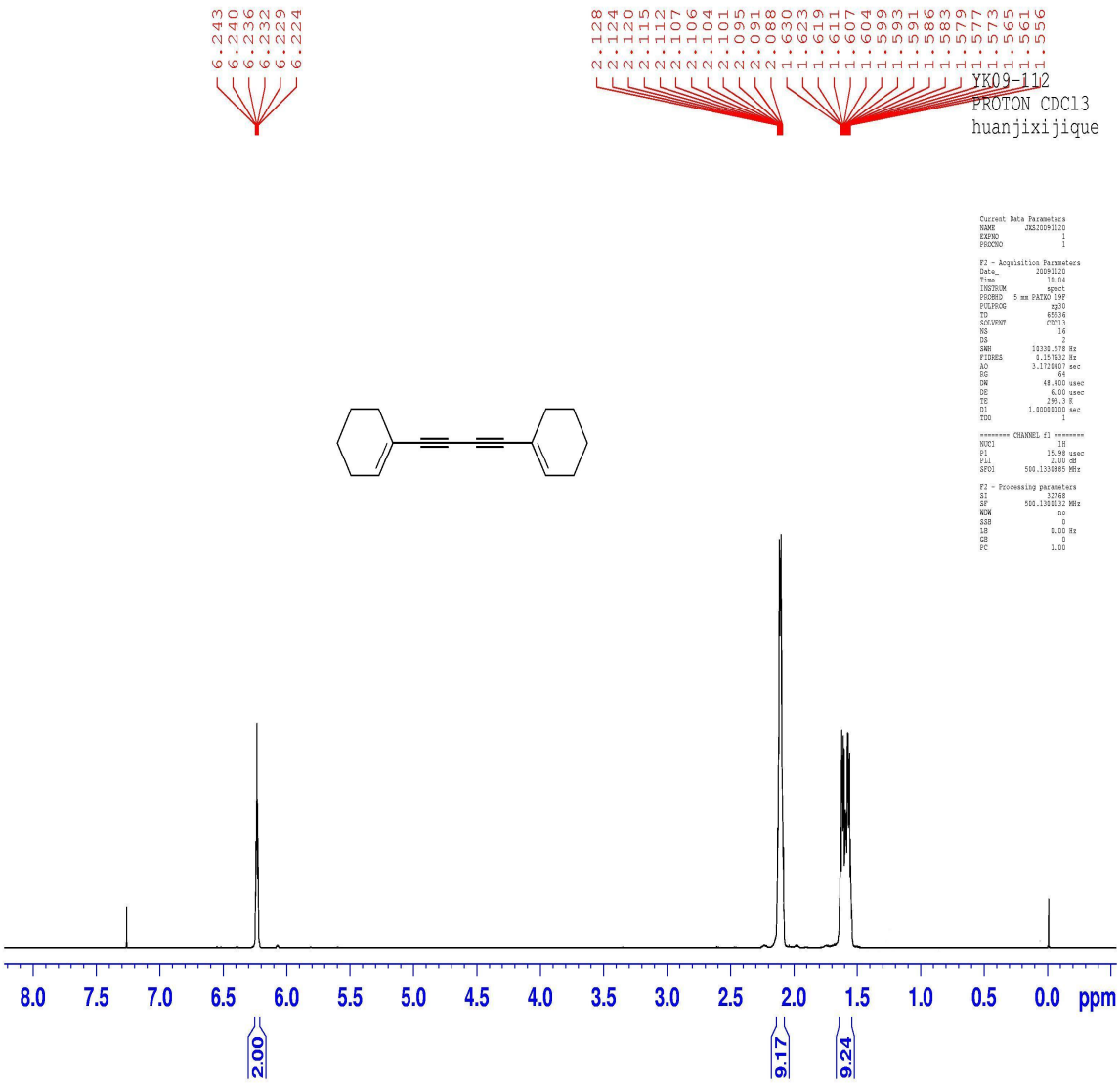
F2 - Acquisition Parameters
Date_ 20100127
Time 15.31
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT cdcl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 294.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

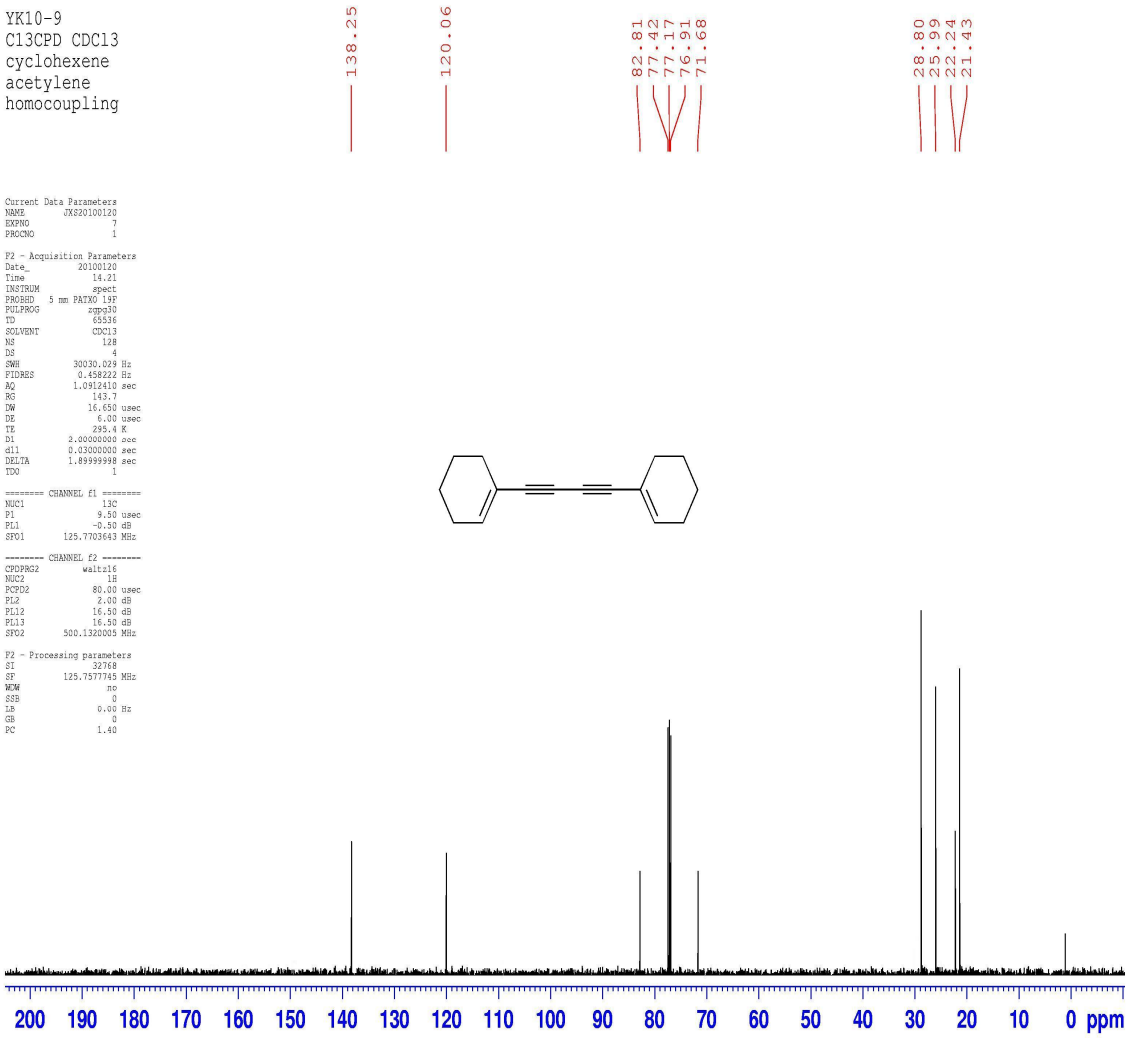
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz

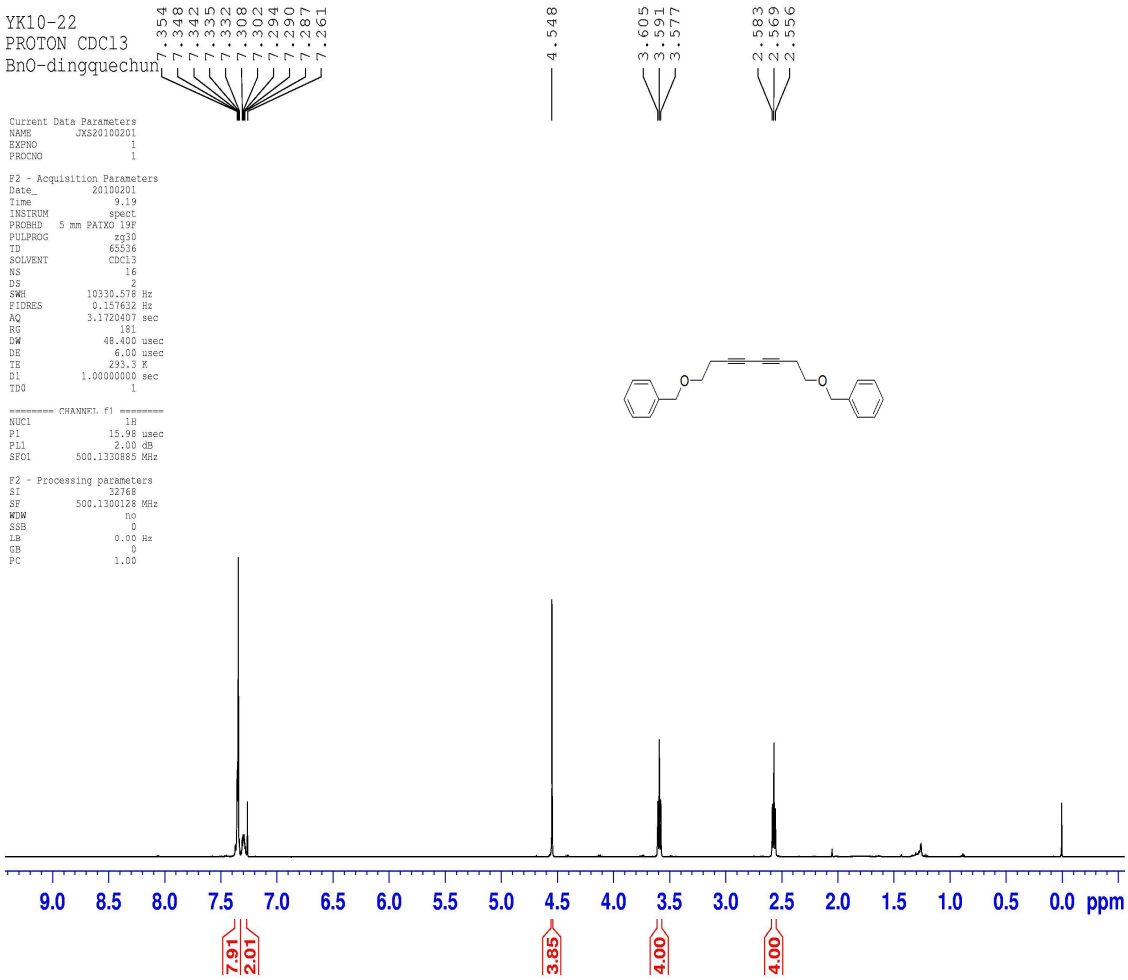
F2 - Processing parameters
SI 32768
SF 125.7577773 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

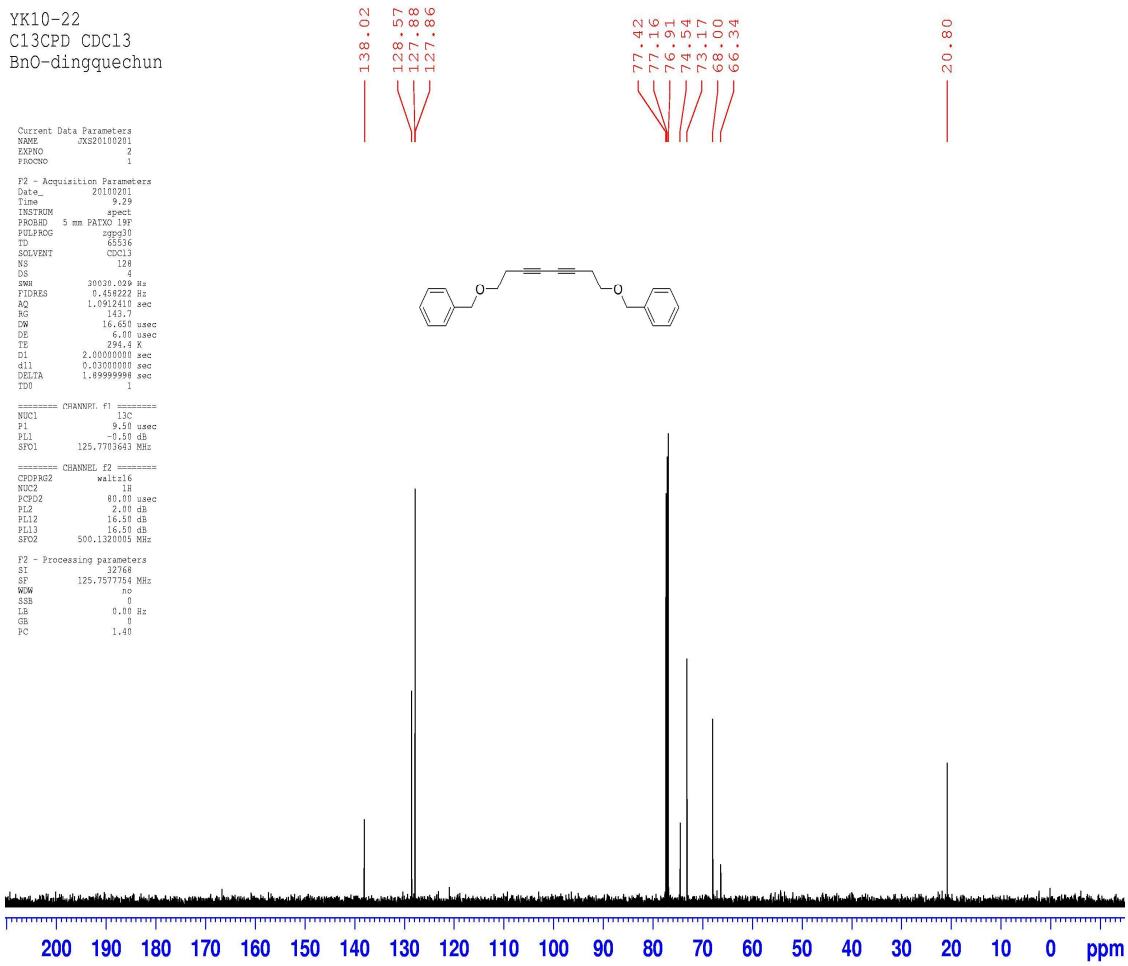
2n:


6.243
6.240
6.236
6.232
6.229
6.224
2.128
2.124
2.120
2.115
2.112
2.107
2.106
2.104
2.101
2.095
2.091
2.088
1.630
1.623
1.619
1.611
1.607
1.604
1.599
1.593
1.591
1.586
1.583
1.579
1.577
1.573
1.565
1.561
1.556
YK09-112
PROTON CDC13
huanjixijique
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
0.5
0.0
ppm
2.00
9.17
9.24


YK10-9
C13CPD CDCl3
cyclohexene
acetylene
homocoupling
138.25
120.06
82.81
77.42
77.17
76.91
71.68
28.80
25.99
22.24
21.43
Current Data Parameters
NAME JXS20100120
EXPNO 7
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100120
Time 14.21
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577745 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

2o:


YK10-22
PROTON CDCl3
BnO-dingquechun
7.354
7.348
7.342
7.335
7.332
7.308
7.302
7.294
7.290
7.287
7.261
4.548
3.605
3.591
3.577
2.583
2.569
2.556
Current Data Parameters
NAME JXS20100201
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100201
Time 9.19
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 181
DW 48.400 usec
DE 6.00 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.98 usec
PL1 2.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300128 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O
O
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 0.5 0.0 ppm
7.91
2.01
3.85
4.00
4.00



Current Data Parameters
NAME JXS20100201
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20100201
Time 9.29
INSTRUM spect
PROBHD 5 mm PATXO 19F
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 143.7
DW 16.650 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======= CHANNEL f1 =======
NUC1 13C
P1 9.50 usec
PL1 -0.50 dB
SFO1 125.7703643 MHz

======= CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.00 dB
PL12 16.50 dB
PL13 16.50 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577754 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40