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Supporting Information

Quaternary Ammonium Salt as Alkylation Agent in the Three-Component Reactions for the Synthesis of Benzothiazoles in Water

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1. General experimental procedures

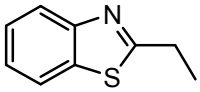
Unless otherwise noted, all reagents were purchased from commercial suppliers and used without further purification. Analytical thin layer chromatography (TLC) was performed using Merck silica gel GF254 plates. Column chromatography was performed using silica gel (200-300mesh) eluting with petroleum ether and ethyl acetate. All products were characterized by their NMR spectra. ^{1}H NMR spectra were recorded at 400 MHz and ^{13}C NMR spectra at 100 MHz (Bruker DPX) with $CDCl_3$ as solvent. Chemical shifts were reported in ppm using TMS as internal standard.

2. General procedure for the synthesis of benzothiazoles in water：

2-iodoaniline (1.0 mmol), tetrabutylammonium bromide (TBAB) (1.0 mml), sulfur (1.2 mmol), KOH (2.0 mmol) and water (10 mL) were added to a sealed tube. The reaction mixture was stirred at 140 °C for 14 h and then cooled to room temperature and extracted with ethyl acetate. The organic layer was then dried with anhydrous Na_2SO_4, and the solvent was removed under reduced pressure. The product was finally obtained by column chromatography on silica gel.

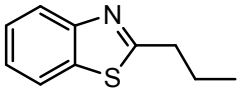
3. Experimental procedures and characterization data

(1) 2-ethylbenzothiazole[1]



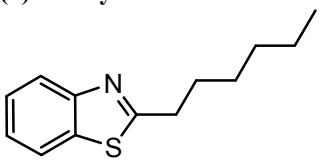
Purification by flash chromatography (petroleum ether/ethyl acetate 100:1). ^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.99 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 3.20-3.15 (m, 2H), 1.49 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:173.7, 153.1, 135.0, 126.0, 124.7, 122.5, 121.5, 27.7, 13.8; MS (EI, *m/z*): 163 [M^+].

(2) 2-propylbenzothiazole[2]



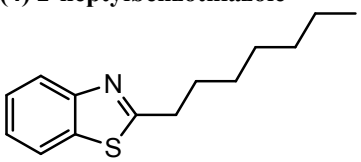
Purification by flash chromatography (petroleum ether/ethyl acetate 100:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.99 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.37 (t, J = 7.6 Hz, 1H), 3.13 (t, J = 7.6 Hz, 2H), 1.95-1.86 (m, 2H), 0.97 (t, J = 8.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:172.5, 153.4, 135.1, 125.9, 124.7, 122.5, 121.5, 35.7, 22.7, 13.9; MS (EI, *m/z*): 177 [M^+].

(3) 2-hexylbenzothiazole[3]



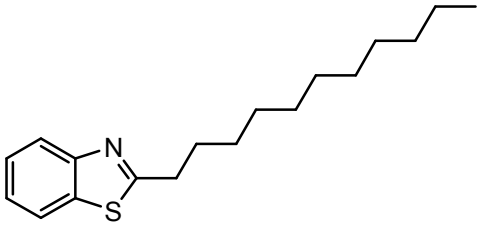
Purification by flash chromatography (petroleum ether/ethyl acetate 100:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.99 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 3.13 (t, J = 7.6 Hz, 2H), 1.93-1.86 (m, 2H), 1.39-1.27 (m, 6H), 0.91 (t, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:172.6, 153.1, 135.1, 125.9, 124.7, 122.5, 121.5, 34.3, 31.5, 29.7, 28.8, 22.5, 14.0; MS (EI, *m/z*): 219 [M^+].

(4) 2-heptylbenzothiazole[4]



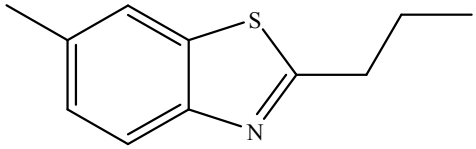
Purification by flash chromatography (petroleum ether/ethyl acetate 100:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.99 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.46 (t, J = 7.6 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 3.13 (t, J = 7.6 Hz, 2H), 1.93-1.86 (m, 2H), 1.42-1.31 (m, 8H), 0.90 (t, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:172.5, 153.2, 135.1, 125.9, 124.6, 122.5, 121.5, 34.3, 31.7, 29.7, 29.1, 29.0, 22.6, 14.1; MS (EI, *m/z*): 233 [M^+].

(5) 2-undecylbenzothiazole[5]



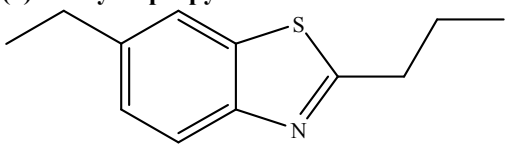
Purification by flash chromatography (petroleum ether/ethyl acetate 100:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 8.00 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 7.2 Hz, 1H), 7.37(t, J = 7.2 Hz, 1H), 3.14 (t, J = 8.0 Hz, 2H), 1.93-1.86 (m, 2H), 1.27 (m, 16H), 0.90 (t, J = 6.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:172.7, 153.0, 135.0, 125.9, 124.7, 122.4, 121.5, 34.3, 31.9, 30.9, 29.7, 29.6, 29.5,29.3, 29.3, 29.2, 22.7, 14.1; MS (EI, *m/z*): 289 [M^+].

(6) 6-methyl-2-propylbenzothiazole



Purification by flash chromatography (petroleum ether/ethyl acetate 100:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.86 (d, J = 8.4 Hz, 1H), 7.63(s, 1H), 7.26 (d, J = 8.4Hz, 1H), 3.08 (t, J = 7.6 Hz, 2H), 2.48 (s, 3H), 1.96-1.87 (m, 2H), 1.06 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:171.2, 151.1, 135.2, 134.7, 127.4, 121.9, 121.3, 36.1, 23.1, 21.4, 13.7; HRMS (ESI) calcd for $C_{11}H_{13}NS$ $[M+H]^+$ 192.0848, Found 192.0847.

(7) 6-ethyl-2-propylbenzothiazole



Purification by flash chromatography (petroleum ether/ethyl acetate 100:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.90 (d, J = 8.4 Hz, 1H), 7.68(s, 1H), 7.32 (d, J = 8.4Hz, 1H), 3.11 (t, J = 7.6 Hz, 2H), 2.82-2.77 (m, 2H), 1.98-1.88 (m, 2H), 1.32(t, J = 7.6 Hz, 3H), 1.08 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:171.4, 164.9, 141.2, 135.2, 126.4, 122.0, 120.1, 36.1, 28.9, 23.1, 15.9, 13.7; HRMS (ESI) calcd for $C_{12}H_{15}NS$ $[M + H]^+$ 206.1004, Found 206.1002.

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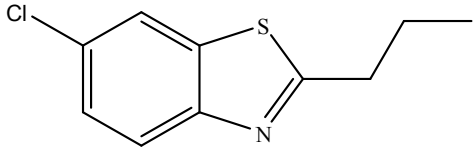
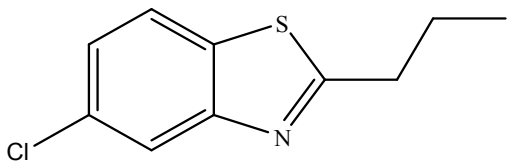
(8)6-chloro-2-propylbenzothiazole[6]



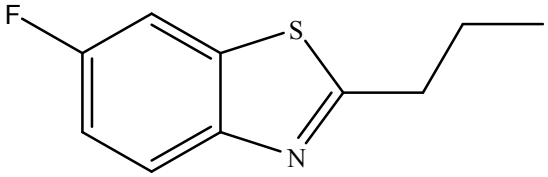
Purification by flash chromatography (petroleum ether/ethyl acetate 50:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.87 (d, J = 8.8 Hz, 1H), 7.82(s, 1H), 7.41 (d, J = 8.8Hz, 1H), 3.09 (t, J = 7.6 Hz, 2H), 1.94-1.89 (m, 2H), 1.07(t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:172.8, 151.7, 136.3, 130.6, 126.7, 123.2, 121.1, 36.2, 23.0, 13.7; MS (EI, *m/z*): 211.5 [M^+].

(9)5-chloro-2-propylbenzothiazole[7]



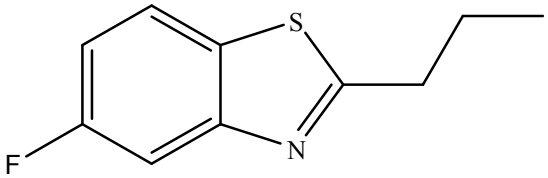
Purification by flash chromatography (petroleum ether/ethyl acetate 50:1).^{1}H NMR (400 MHz, $CDCl_3$): δ: 7.97 (s, 1H), 7.76 (d, J = 8.4 Hz, 1H), 7.34 (d, J = 8.4Hz, 1H), 3.10 (t, J = 7.2 Hz, 2H), 1.95-1.89 (m, 2H), 1.07(t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ:174.3, 154.1, 133.4, 131.9, 125.1, 122.4, 122.2, 36.3, 23.0, 13.7; MS (EI, *m/z*): 211.5 [M^+].

(10)6-fluoro-2-propylbenzothiazole



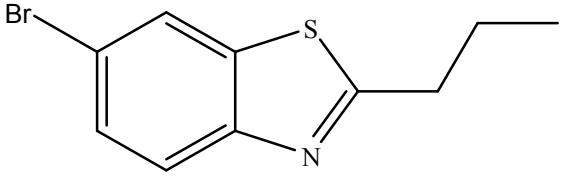
Purification by flash chromatography (petroleum ether/ethyl acetate 50:1).^{1}H NMR (400 MHz, $CDCl_3$): *δ*: 7.91-7.88 (m, 1H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.20-7.15 (m, 1H), 3.06 (t, *J* = 7.4 Hz, 2H), 1.94-1.85 (m, 2H), 1.05(t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ:*171.9, 160.2(d, *J* =243), 149.8, 136.1(d, *J* =10), 123.3, (d, *J* =10), 114.4(d, *J* =24), 107.7(d, *J* =27), 36.2, 23.0, 13.7; HRMS (ESI) calcd for $C_{10}H_{10}FNS$ $[M + H]^+$ 196.0597, Found 196.0594.

(11)5-fluoro-2-propylbenzothiazole



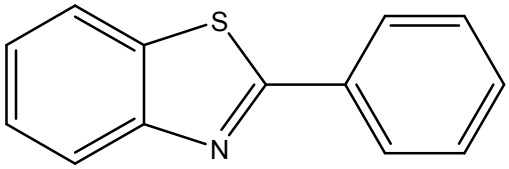
Purification by flash chromatography (petroleum ether/ethyl acetate 50:1).^{1}H NMR (400 MHz, $CDCl_3$): *δ*: 7.74-7.72 (m, 1H), 7.64 (d, *J* = 9.6 Hz, 1H), 7.12-7.08 (m, 1H), 3.09-3.05 (m, 2H), 1.92-1.85 (m, 2H), 1.05(t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ:*174.8, 161.7(d, *J* =242), 154.2(d, *J* =12), 130.5, 122.1(d, *J* =9), 113.2(d, *J* =25), 108.8(d, *J* =23), 36.3, 23.0, 13.7; HRMS (ESI) calcd for $C_{10}H_{10}FNS$ $[M + H]^+$ 196.0597, Found 196.0597.

(12)6-bromo-2-propylbenzothiazole[8]



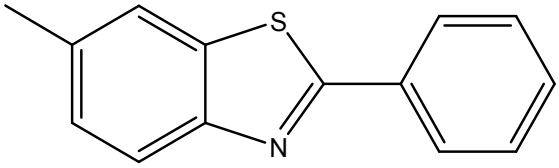
Purification by flash chromatography (petroleum ether/ethyl acetate50:1).^{1}H NMR (400 MHz, $CDCl_3$): *δ*: 7.98 (s, 1H), 7.83 (d, *J* = 8.8 Hz, 1H), 7.56 (d, *J* = 8.8 Hz, 1H), 3.09 (t, *J* = 7.6 Hz, 2H), 1.97-1.87 (m, 2H), 1.07(t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): *δ:*172.9, 152.1, 136.8, 129.4, 124.0, 123.6, 118.2, 36.2, 23.0, 13.7; MS (EI, *m/z*): 256 $[M^+]$.

(13)2-phenylbenzo[d]thiazole[9]



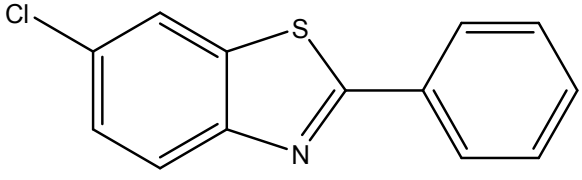
Purified by flash chromatography (petroleum ether/ethyl acetate 100:1), ^{1}H NMR (400MHz, $CDCl_3$): δ 8.15-8.11 (m, 3H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.55-7.51 (m, 4H), 7.43 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100MHz, $CDCl_3$): δ 168.2, 153.9, 135.0, 133.5, 131.1, 129.1, 127.6, 126.4, 125.3, 123.2, 121.7; MS (EI, m/z): 211$[M^+]$.

(14)6-methyl-2-phenylbenzothiazole[10]



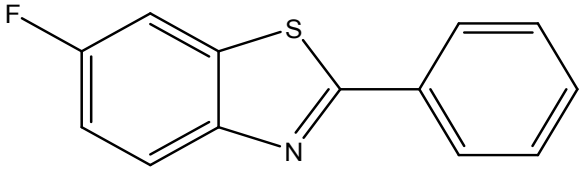
Purified by flash chromatography (petroleum ether/ethyl acetate 100:1),^{1}H NMR (400 MHz, CDCl3) δ = 8.10 (dd, J=6.5, 2.9, 2H), 7.98 (d, J=8.3, 1H), 7.72 (s, 1H), 7.51 (dd, J=4.8, 1.5, 3H), 7.36 – 7.26 (m, 1H), 2.52 (s, 3H);^{13}C NMR (100 MHz, CDCl3) δ = 167.04, 152.20, 135.39, 135.19, 133.71, 130.79, 129.00, 127.95, 127.44, 122.70, 121.45, 21.58.

(15)6-Chloro-2-phenylbenzothiazole[11]



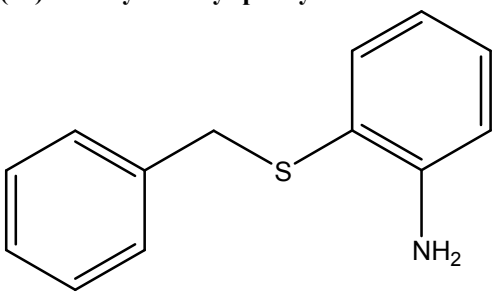
Purified by flash chromatography (petroleum ether/ethyl acetate 100:1),^{1}H NMR (400 MHz, CDCl3) δ = 8.08 (dd, J=6.5, 3.1, 2H), 7.99 (d, J=8.7, 1H), 7.88 (d, J=2.0, 1H), 7.52 (dd, J=5.0, 1.7, 3H), 7.47 (dd, J=8.7, 2.1, 1H);^{13}C NMR (100 MHz, CDCl3) δ = 168.53, 152.68, 136.21, 133.22, 131.25, 131.08, 129.10, 127.55, 127.14, 123.93 , 121.23.

(16)6-Fluoro-2-phenylbenzothiazole[12]



Purified by flash chromatography (petroleum ether/ethyl acetate 100:1),^{1}H NMR (400 MHz, CDCl3) δ = 8.10 – 8.00 (m, 3H), 7.59 (dd, J=8.1, 2.6, 1H), 7.52 (dd, J=6.7, 3.6, 3H), 7.29 – 7.21 (m, 1H);^{13}C NMR (100 MHz, CDCl3) δ = 163.03, 157.02, 154.47, 145.95, 131.41, 128.59, 126.31, 124.49, 122.91 , 110.26, 103.23.

(17)2-Benzylsulfanyl-phenylamine[13]



Purified by flash chromatography (petroleum ether/ethyl acetate 100:1),^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.35 – 7.25 (m, 4H), 7.24 – 7.18 (m, 2H), 7.16 (ddd, *J*=4.1, 2.0, 1.1, 1H), 6.78 – 6.72 (m, 1H), 6.69 (tdd, *J*=7.5, 2.8, 1.3, 1H), 4.18 (s, 2H), 3.96 (d, *J*=2.6, 2H).

References

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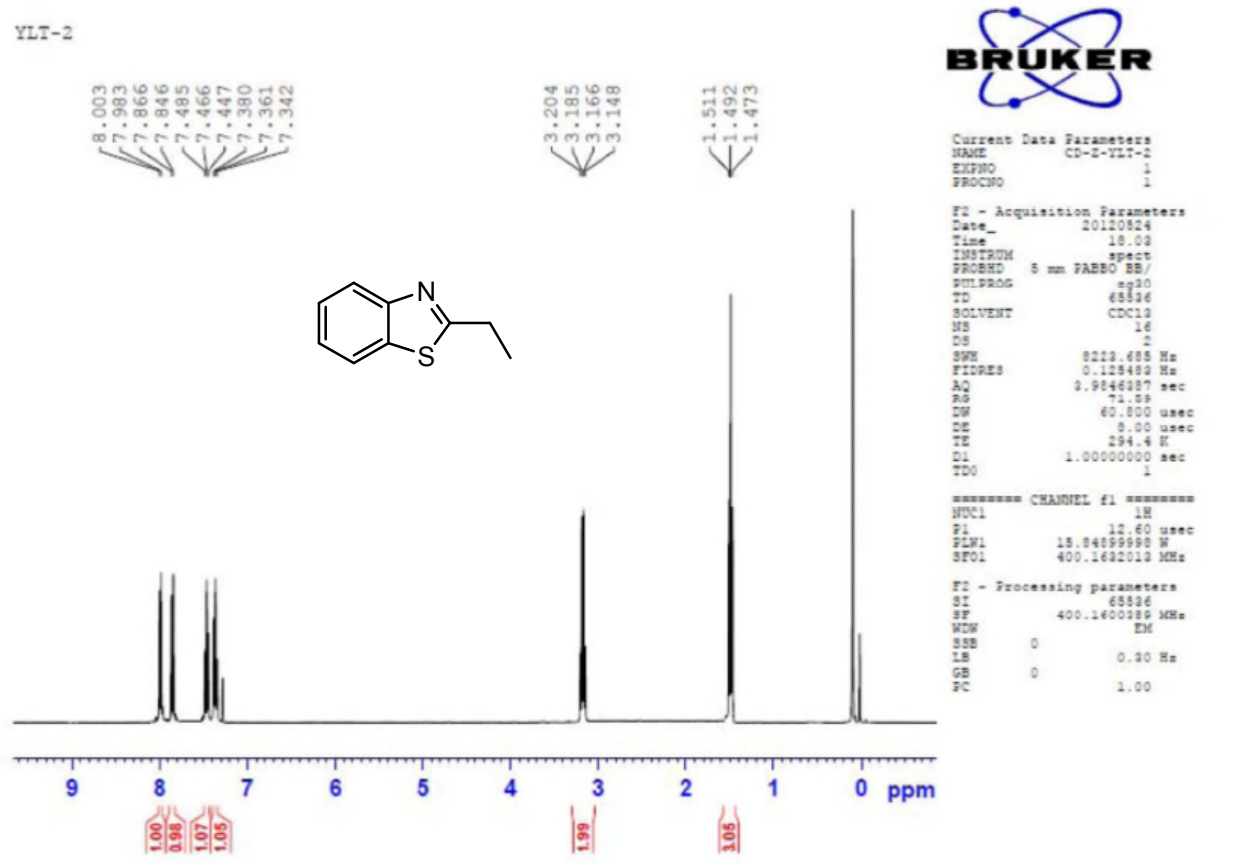
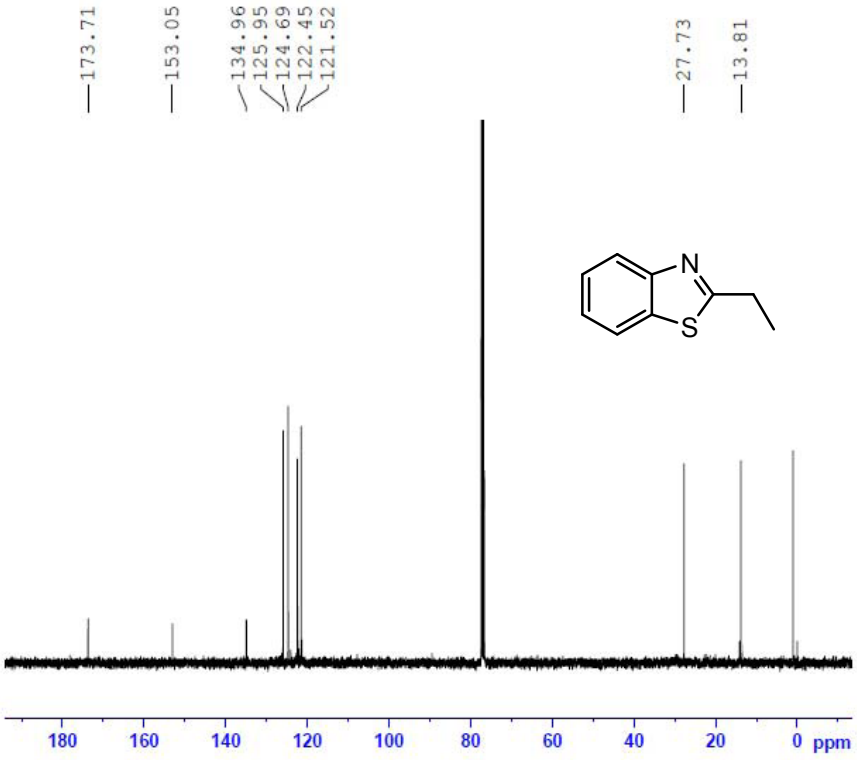
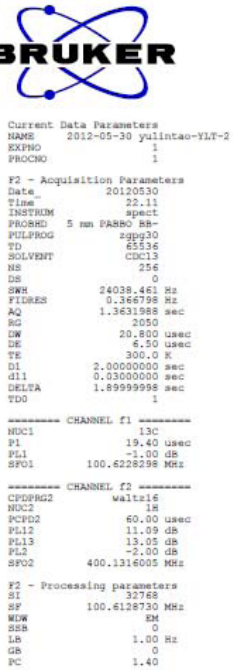
^{1}H NMR and ^{13}C NMR spectral for the products

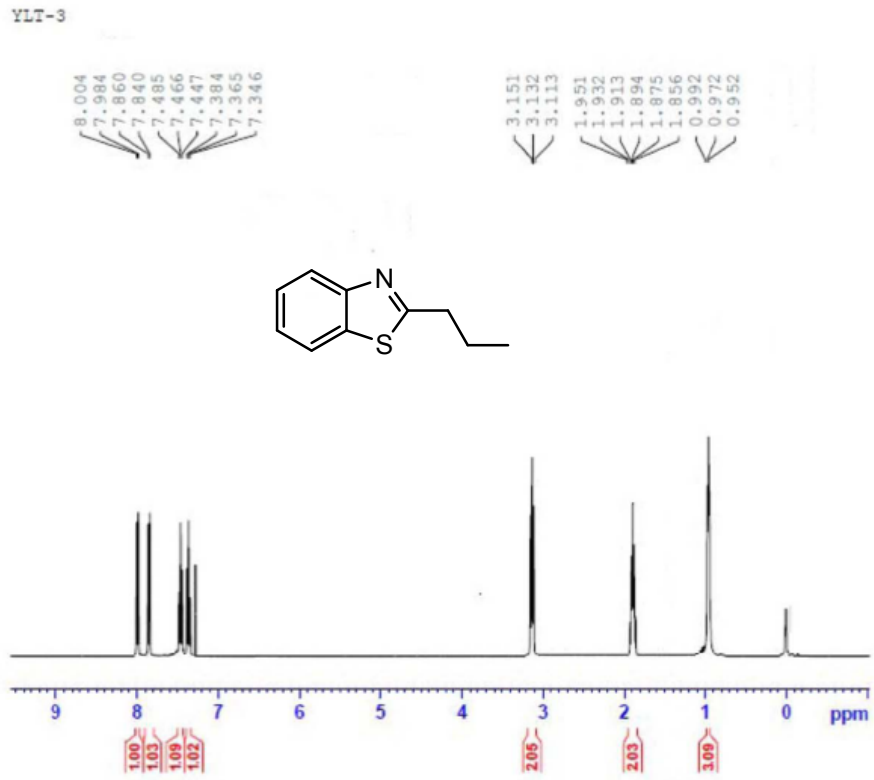
(1) 2-ethylbenzothiazole

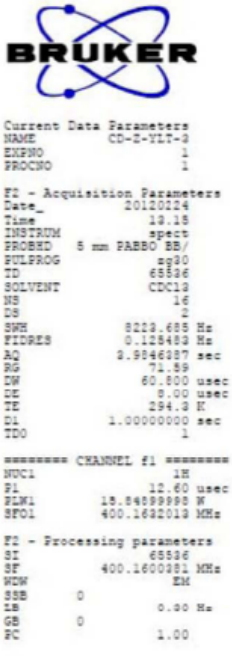


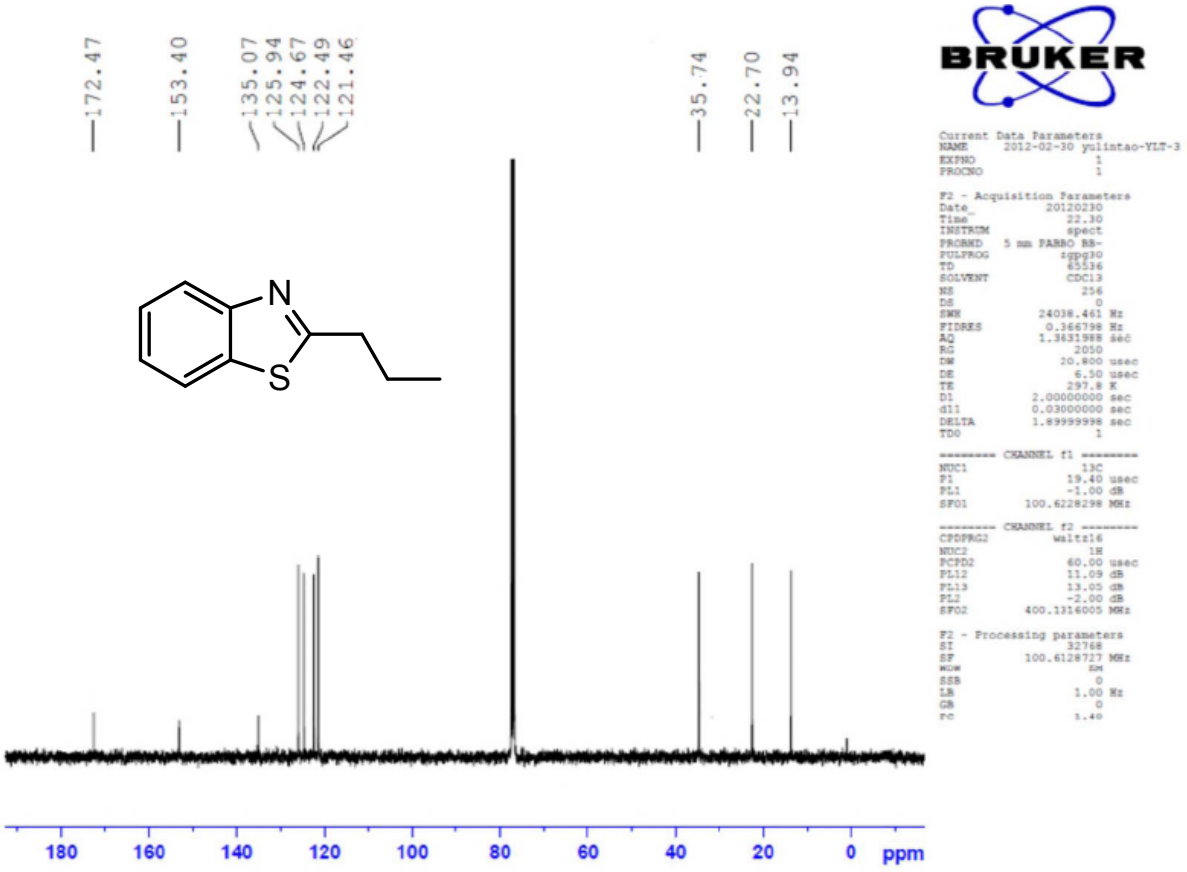




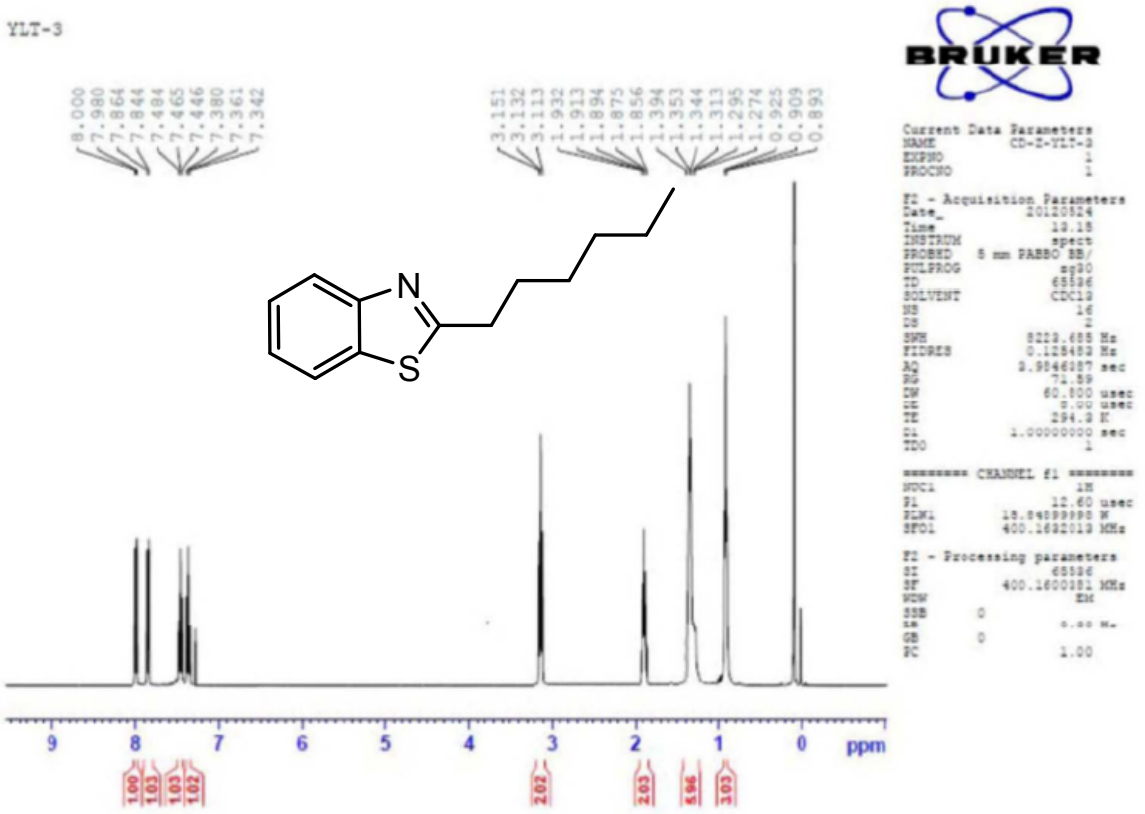
(2) 2-propylbenzothiazole

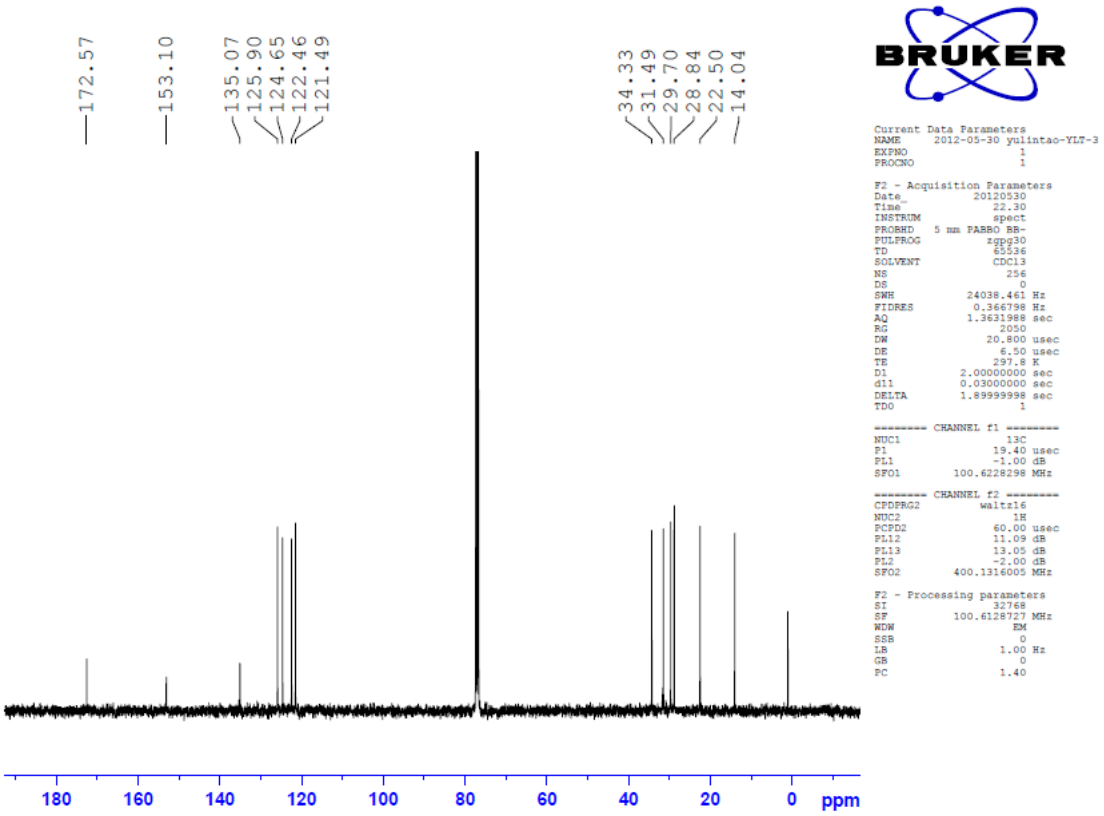






(3) 2-hexylbenzothiazole[3]





Current Data Parameters
NAME 2012-05-30 yulintao-YLT-3
EXPNO 1
PROCNO 1

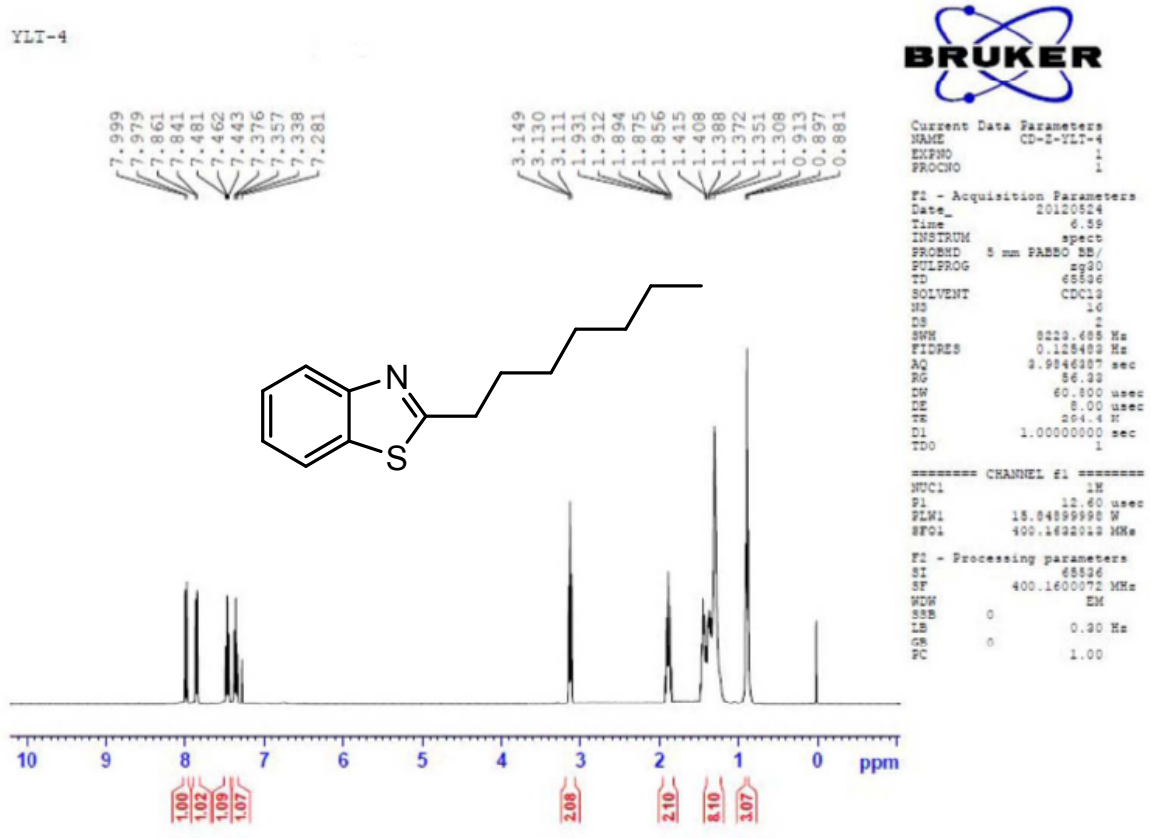
F2 - Acquisition Parameters
Date_ 20120530
Time 22.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 19.40 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 11.09 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128727 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(4) 2-heptylbenzothiazole

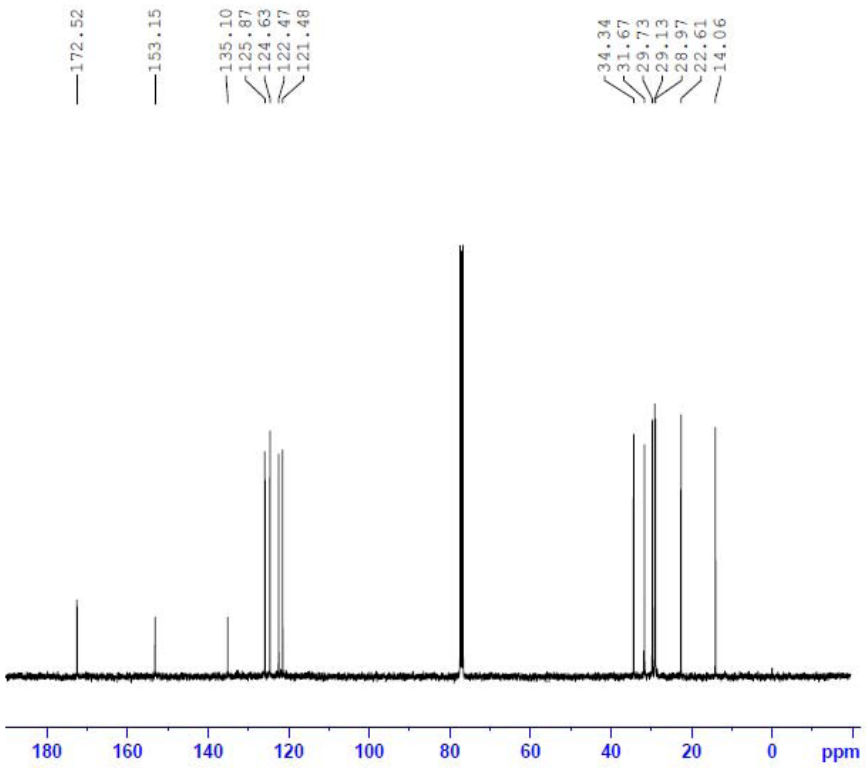


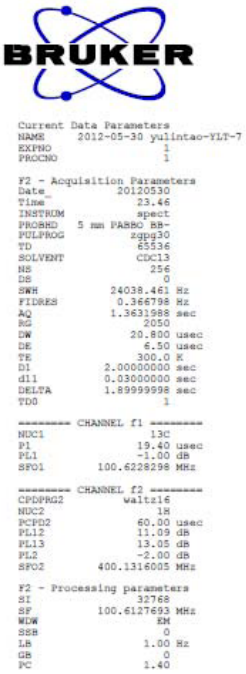
Current Data Parameters
NAME CD-2-YLT-4
EXPNO 1
PROCNO 1

F1 - Acquisition Parameters
Date_ 20120524
Time 6.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125403 Hz
AQ 3.9846307 sec
RG 56.33
DW 60.800 usec
DE 8.00 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

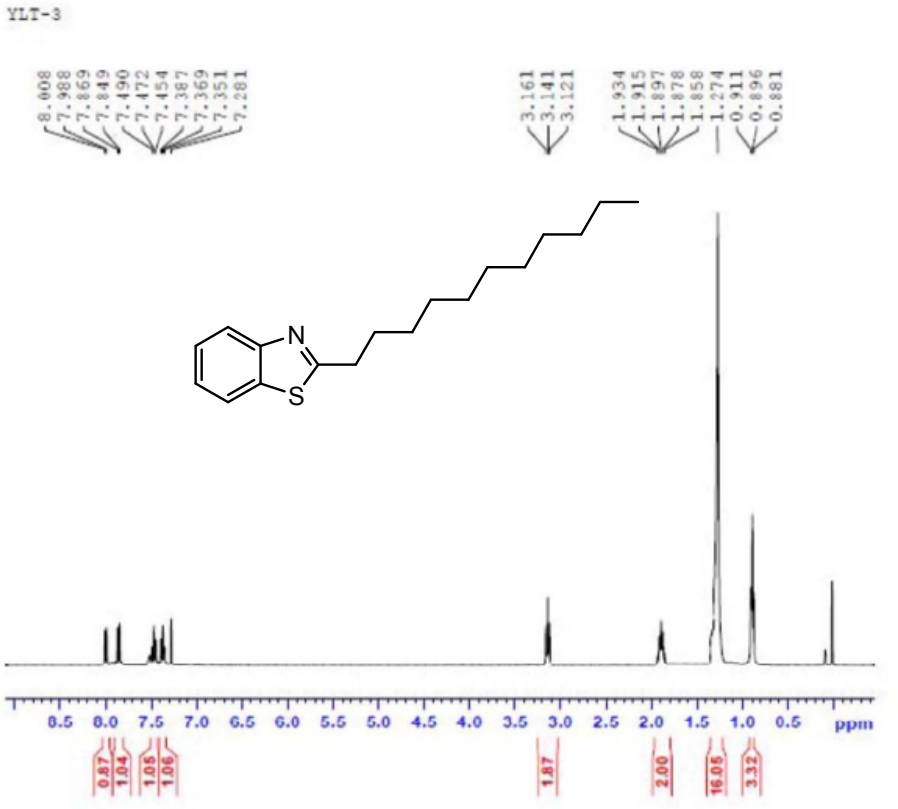
======== CHANNEL f1 ========
NUC1 1H
P1 12.60 usec
PLW1 15.04899998 W
SFO1 400.1622013 MHz

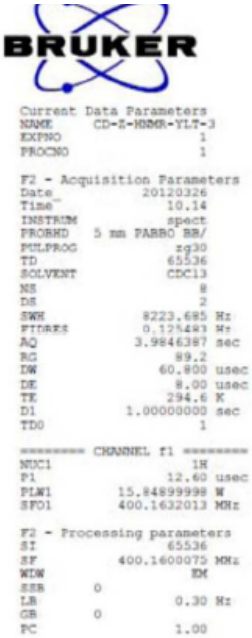
F1 - Processing parameters
SI 65536
SF 400.1600072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

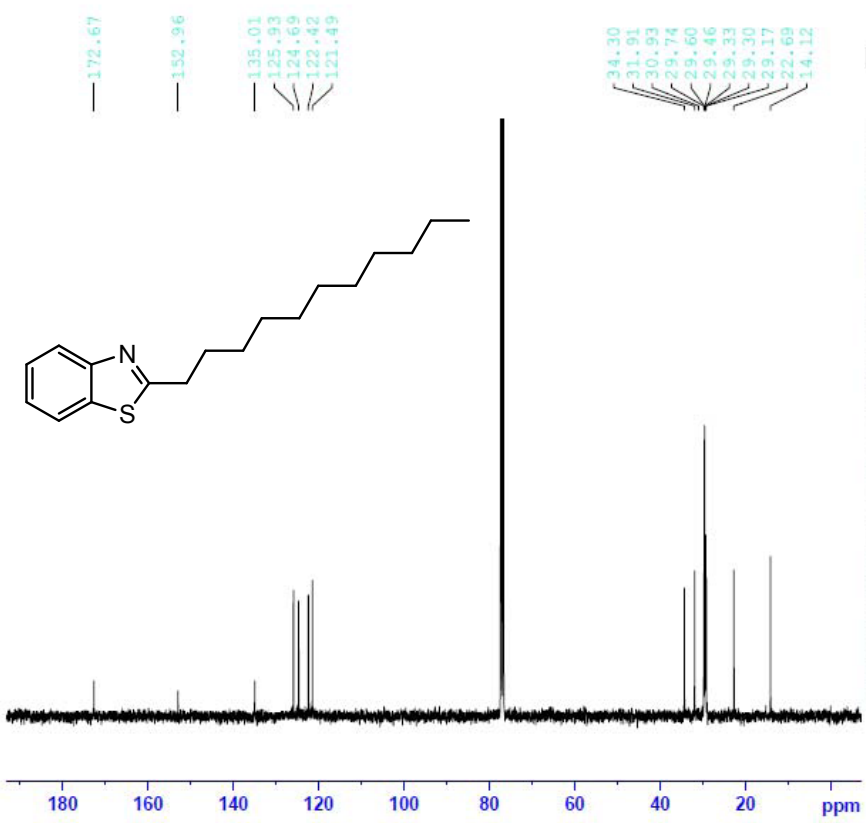


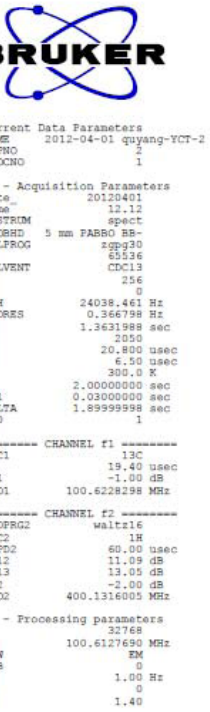


(5) 2-undecylbenzothiazole

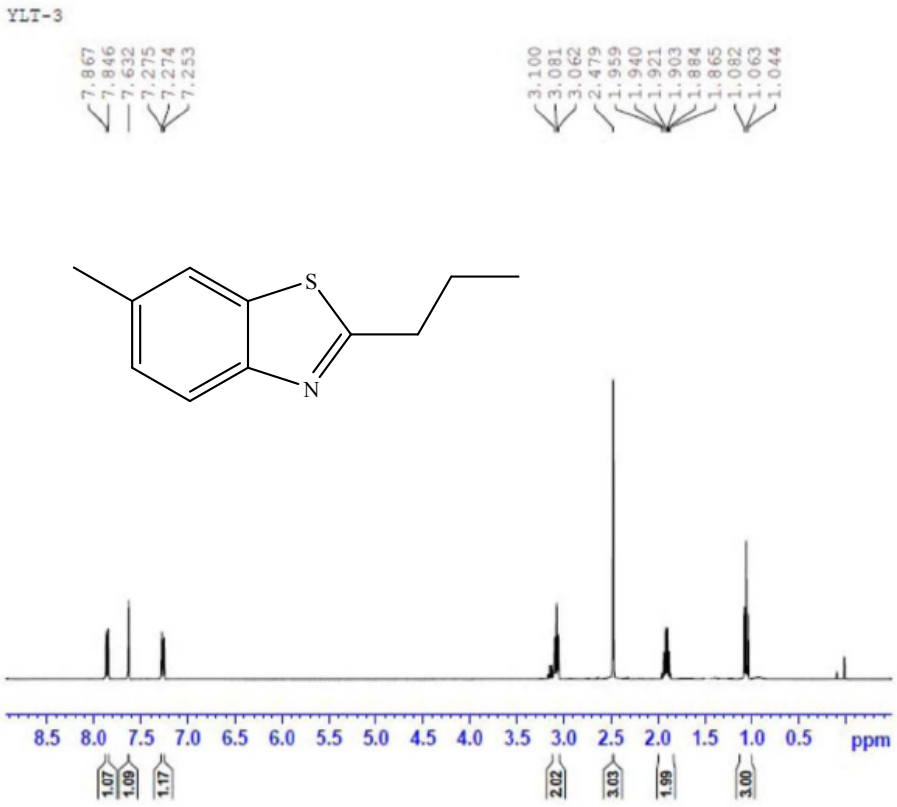


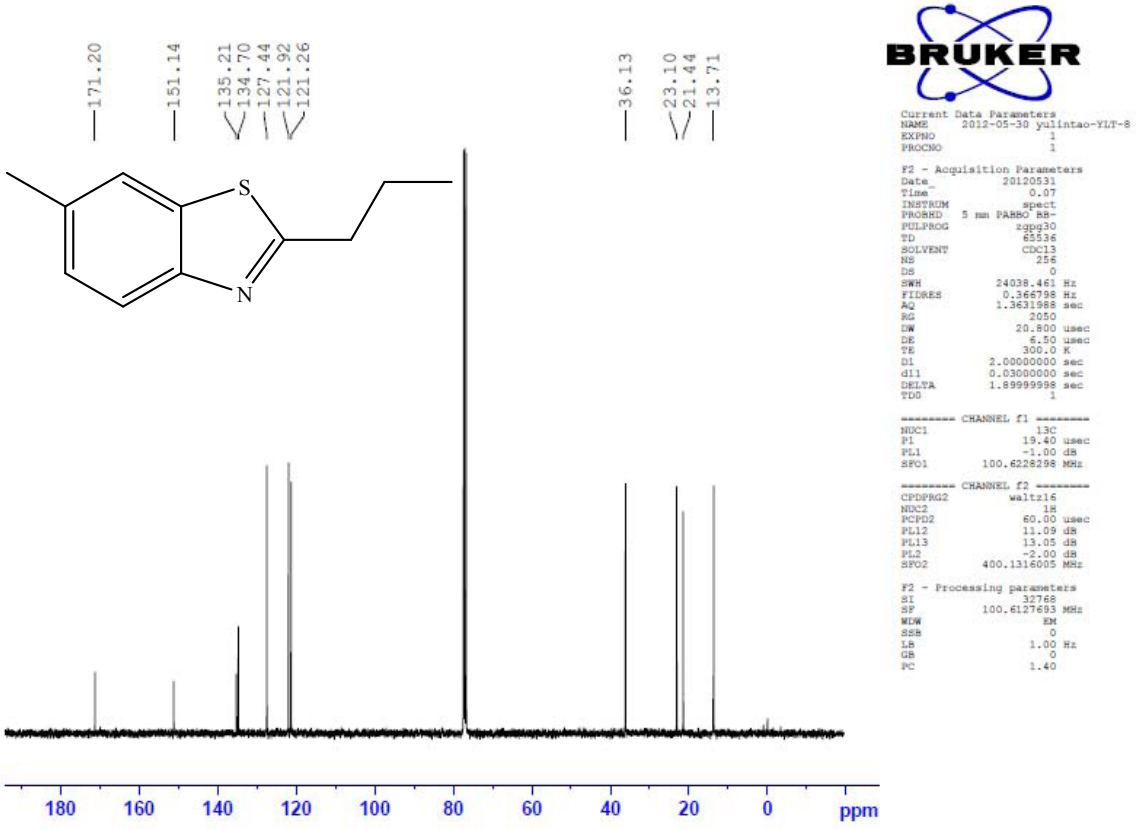






(6) 6-methyl-2-propylbenzothiazole





Current Data Parameters
NAME 2012-05-30 yulintao-YLT-8
EXPNO 1
PROCNO 1

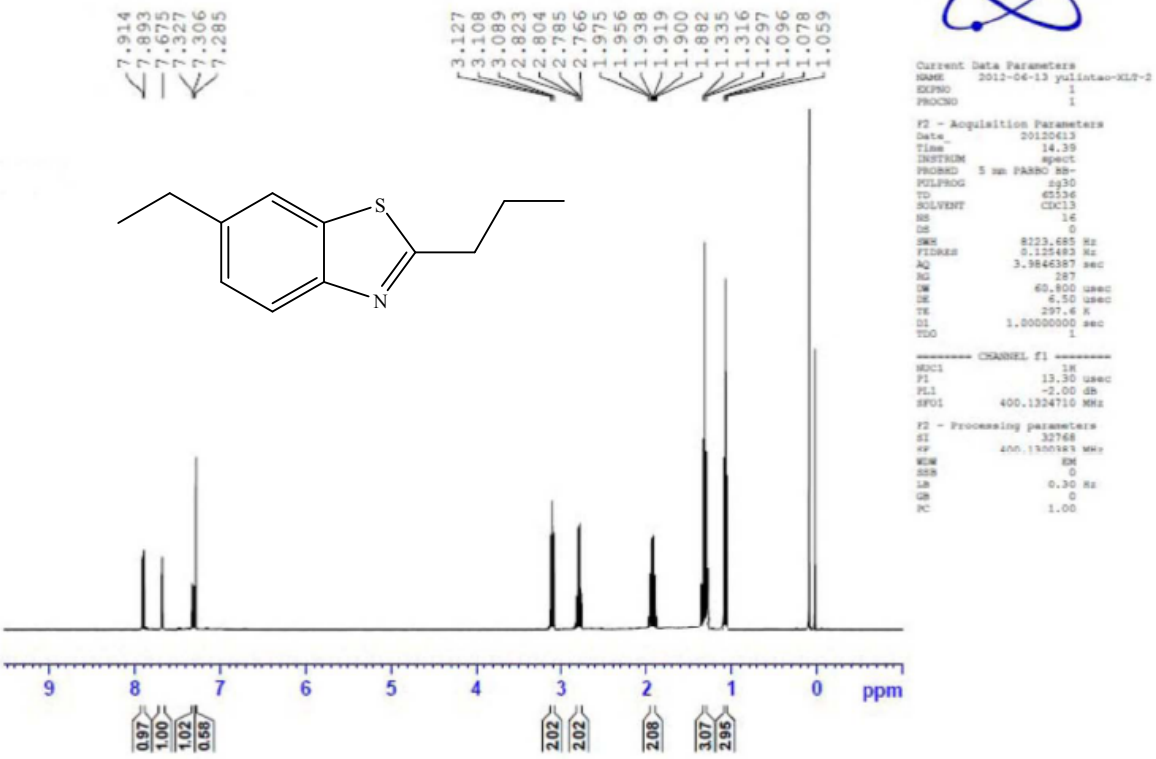
F2 - Acquisition Parameters
Date_ 20120531
Time 0.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 19.40 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 60.00 usec
PL12 11.09 dB
PL13 13.05 dB
PL2 -2.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127693 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

(7) 6-ethyl-2-propylbenzothiazole

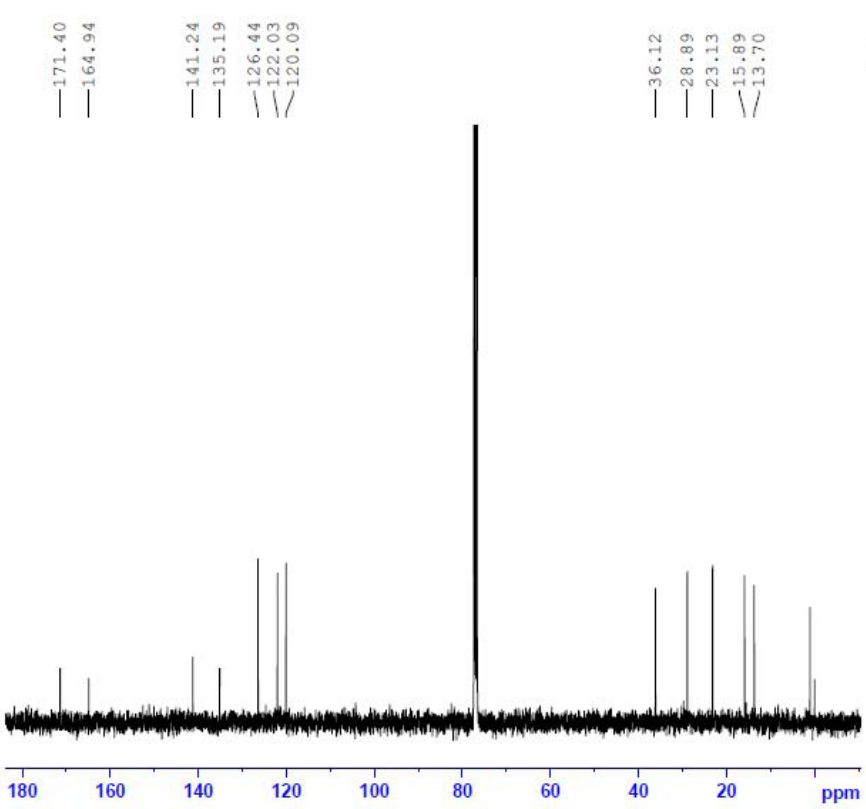


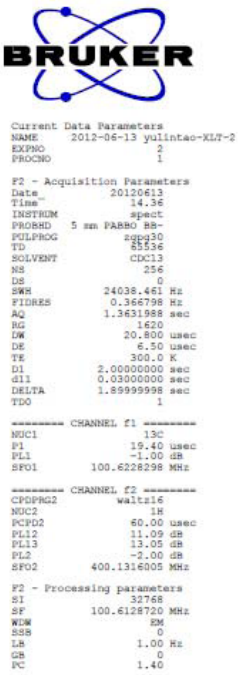
Current Data Parameters
NAME 2012-04-13 yulintao-XLT-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120613
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

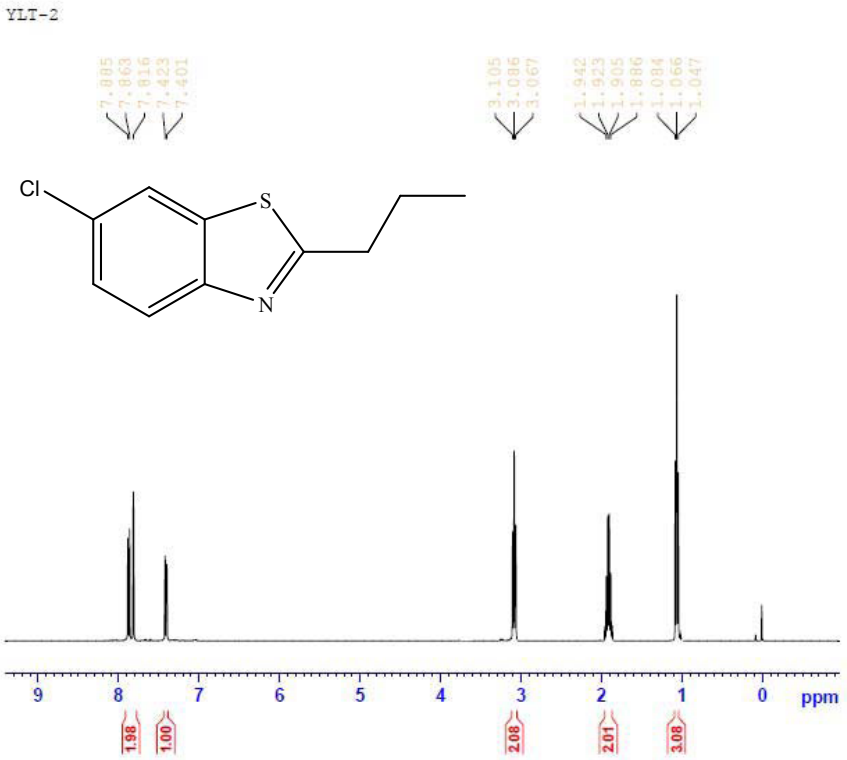
======== CHANNEL f1 ========
NUC1 1H
P1 13.30 usec
PL1 -2.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300183 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

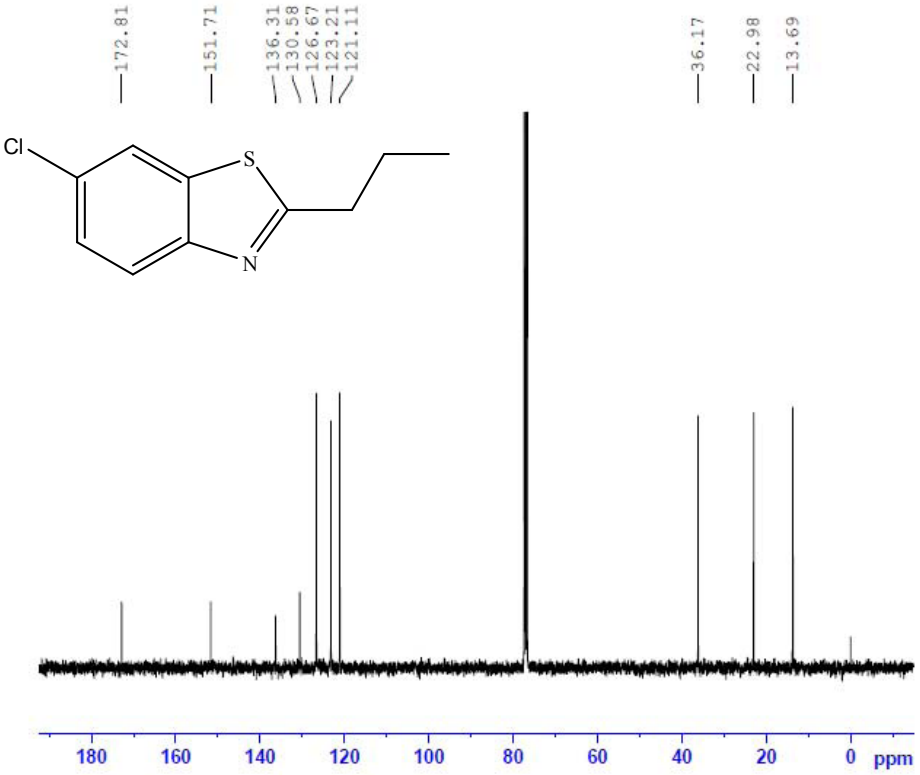




(8)6-chloro-2-propylbenzothiazole[6]

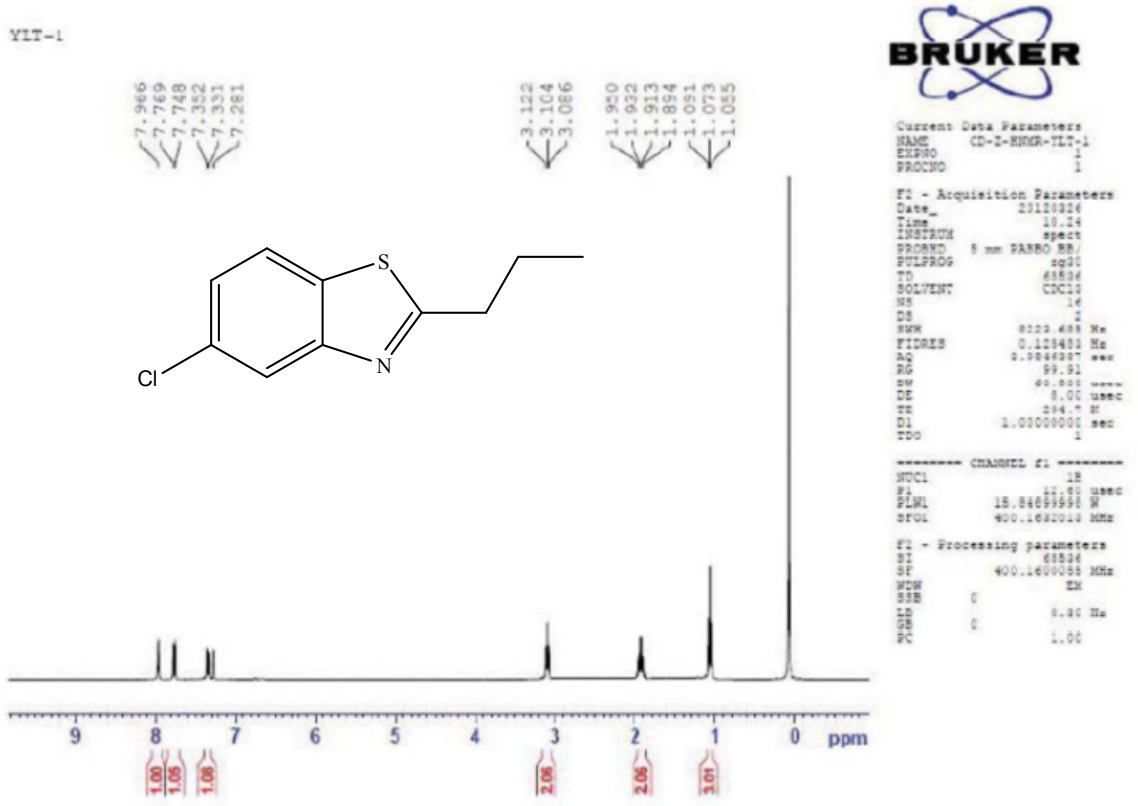



```
Current Data Parameters
NAME      CD-2-HNMR-YLT-2
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120419
Time              16.22
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                89.2
DW               60.800 usec
DE                6.00 usec
TE               294.6 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                12.60 usec
PLW1         15.84899998 W
SFO1         400.1632013 MHz

F2 - Processing parameters
SI               65536
SF           400.1600041 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

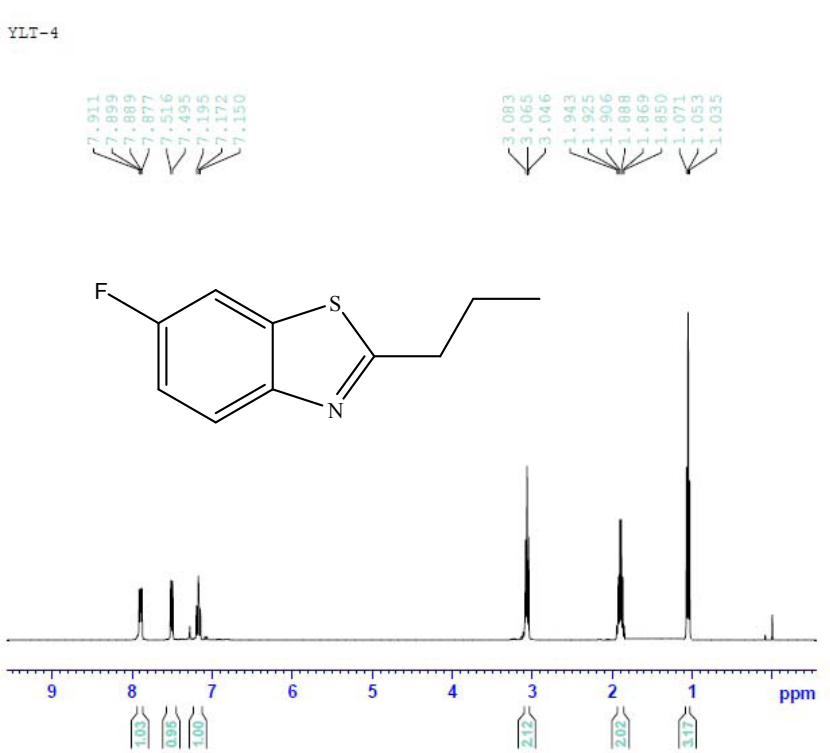



```
Current Data Parameters
NAME      2012-05-30 yulintao-YLT-4
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120530
Time              22.49
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD               65536
SOLVENT           CDCl3
NS                  256
DS                    0
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                2050
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                19.40 usec
PL1               -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6127687 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

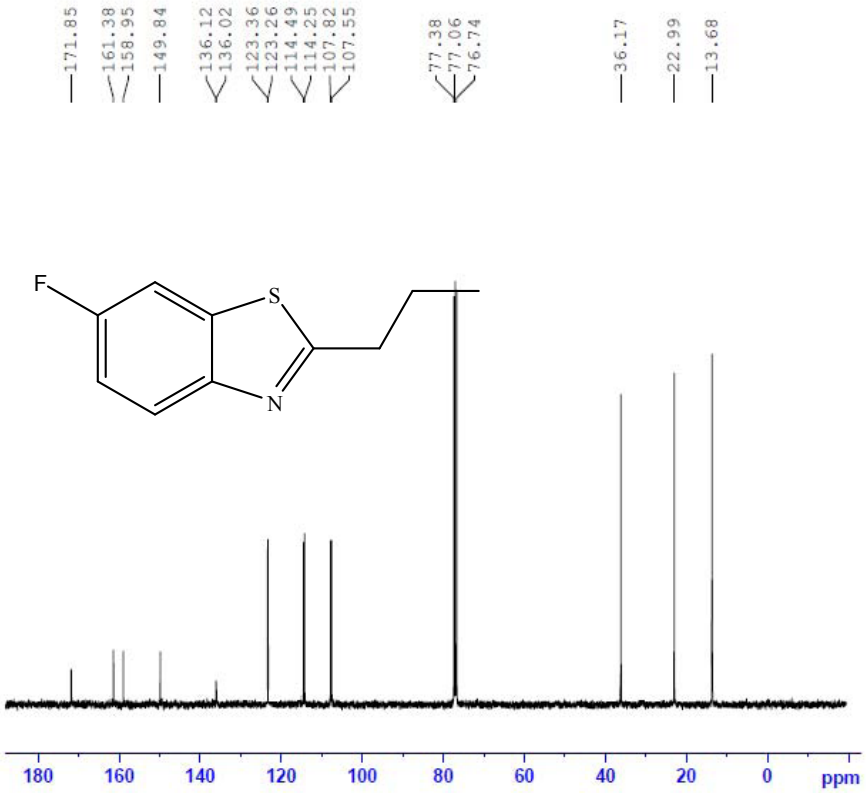
(9)5-chloro-2-propylbenzothiazole[7]



(10)6-fluoro-2-propylbenzothiazole

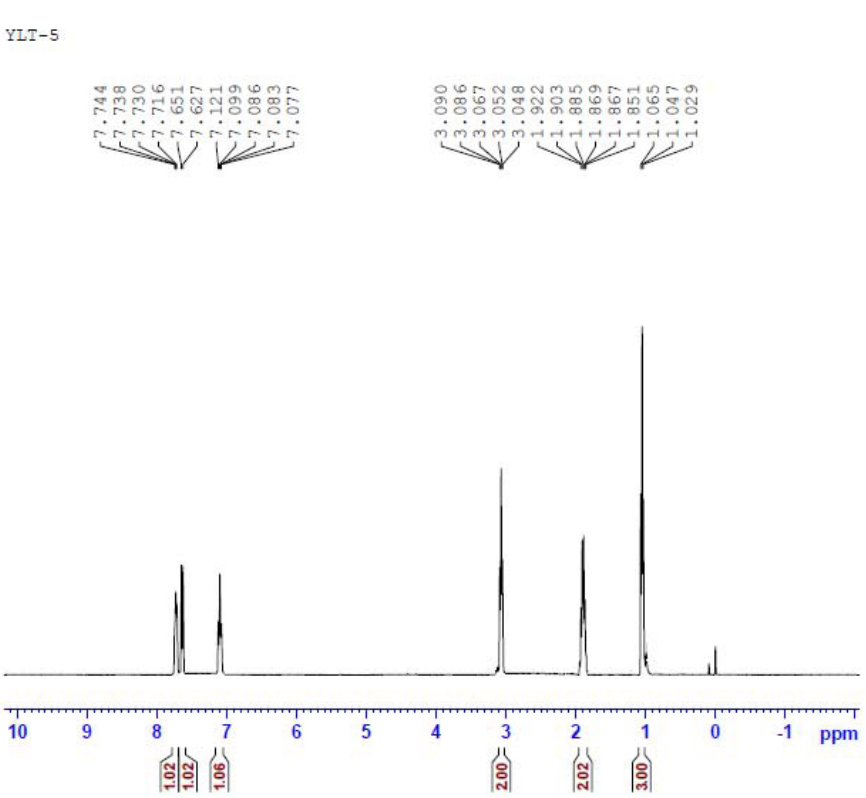



```
Current Data Parameters
NAME            CD-2-YLT-4
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120419
Time                 16.52
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             CDCl3
NS                      16
DS                       2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.98646387 sec
RG                    52.62
DW                  60.800 usec
DE                   6.00 usec
TE                  294.5 K
D1               1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   12.60 usec
PLW1          15.84899998 W
SFO1          400.1632013 MHz

F2 - Processing parameters
SI                   65536
SF            400.1600004 MHz
WDW                    EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```



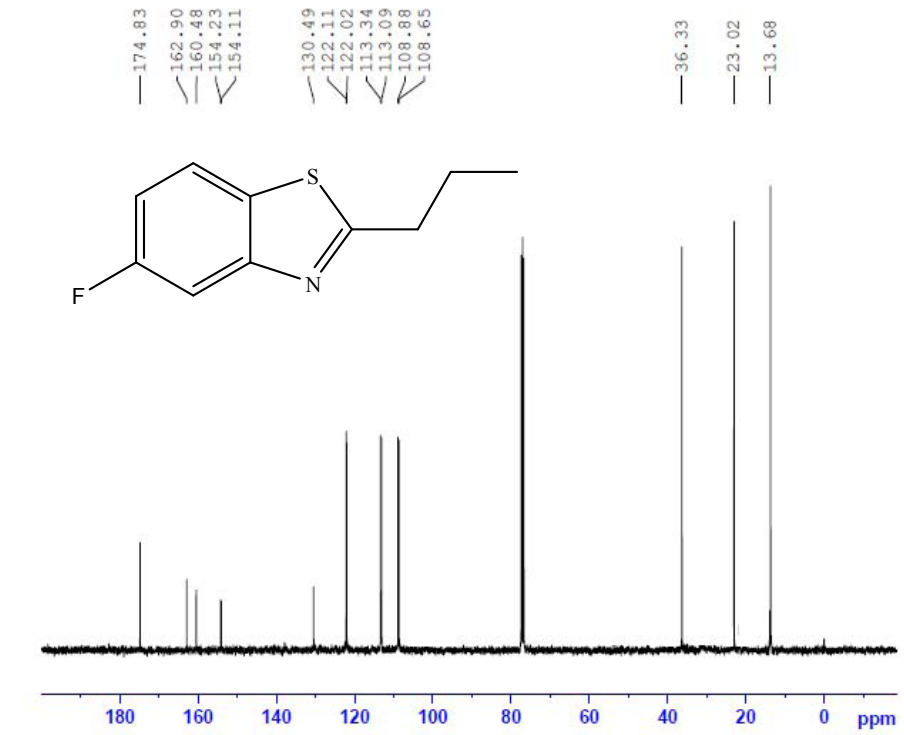

```
Current Data Parameters
NAME      2012-05-30 yulintao-YLT-9
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120531
Time                 0.26
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                 65536
SOLVENT             CDCl3
NS                     256
DS                       0
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                    2050
DW                  20.800 usec
DE                   6.50 usec
TE                  300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   19.40 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                60.00 usec
PL12                 11.09 dB
PL13                 13.05 dB
PL2                  -2.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127690 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                    1.40
```

(11)5-fluoro-2- propylbenzothiazole



BRUKER

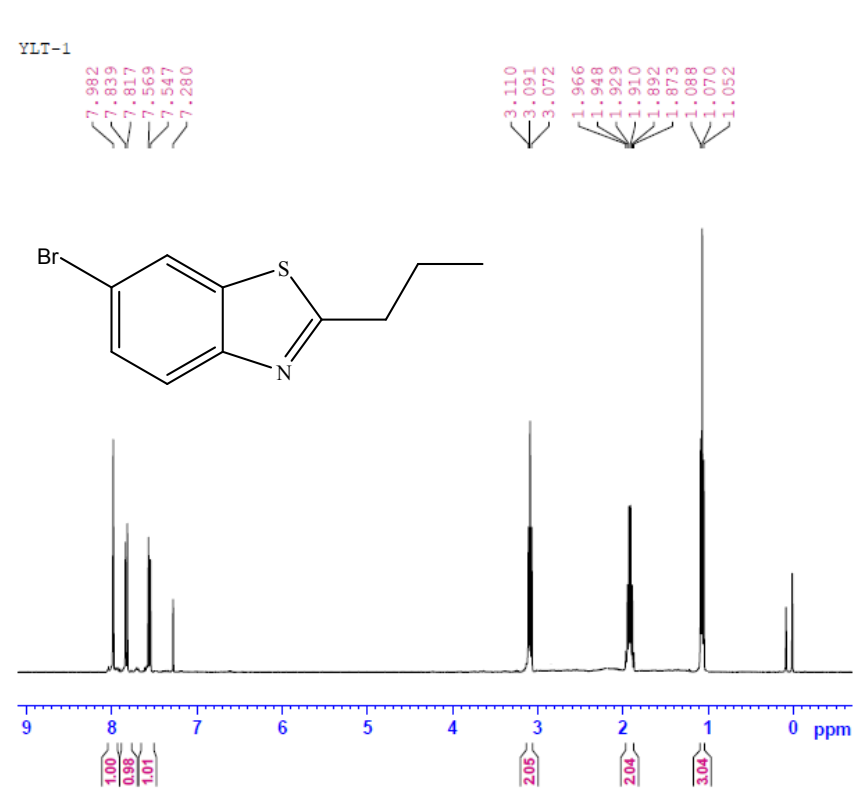
```
Current Data Parameters
NAME                  CD-Z-YLT-5
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20120524
Time                    6.44
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125489 Hz
AQ                  3.9846387 sec
RG                      31.68
DW                     60.800 usec
DE                      8.00 usec
TE                     294.7 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.60 usec
PLW1              15.84899998 W
SFO1              400.1632013 MHz

F2 - Processing parameters
SI                         65536
SF                400.1599992 MHz
WDW                           EM
SSB          0
LB                      0.30 Hz
GB           0
PC                      1.00
```



BRUKER

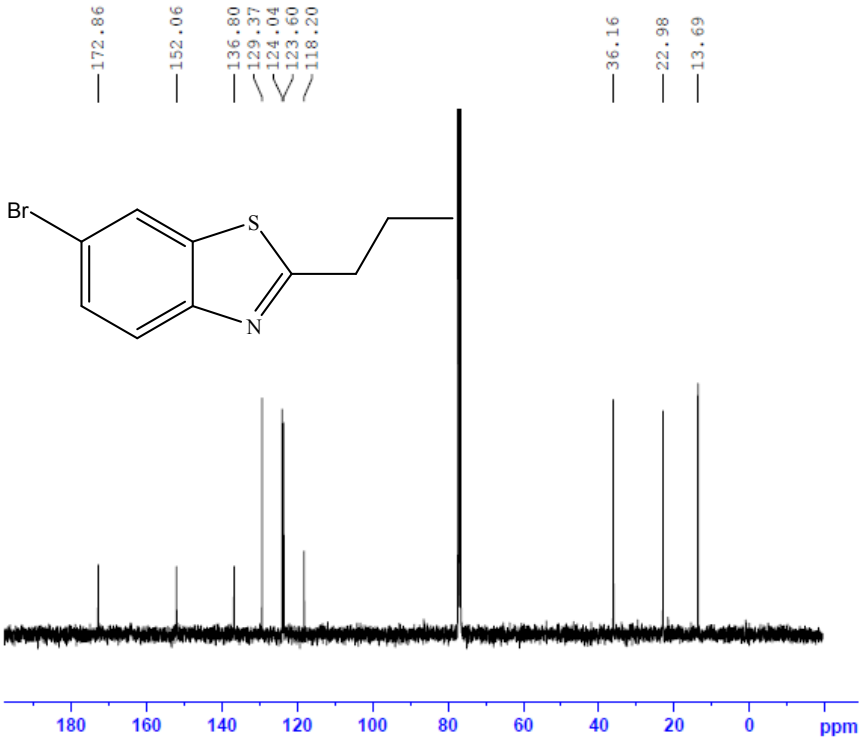
```
Current Data Parameters
NAME      2012-05-30 yulintao-YLT-5
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20120530
Time                   23.07
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       256
DS                         0
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631988 sec
RG                      2050
DW                     20.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      19.40 usec
PL1                     -1.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   60.00 usec
PL12                    11.09 dB
PL13                    13.05 dB
PL2                     -2.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                100.6127675 MHz
WDW                           EM
SSB                            0
LB                      1.00 Hz
GB                             0
PC                      1.40
```

(12)6-bromo-2-propylbenzothiazole[8]



BRUKER

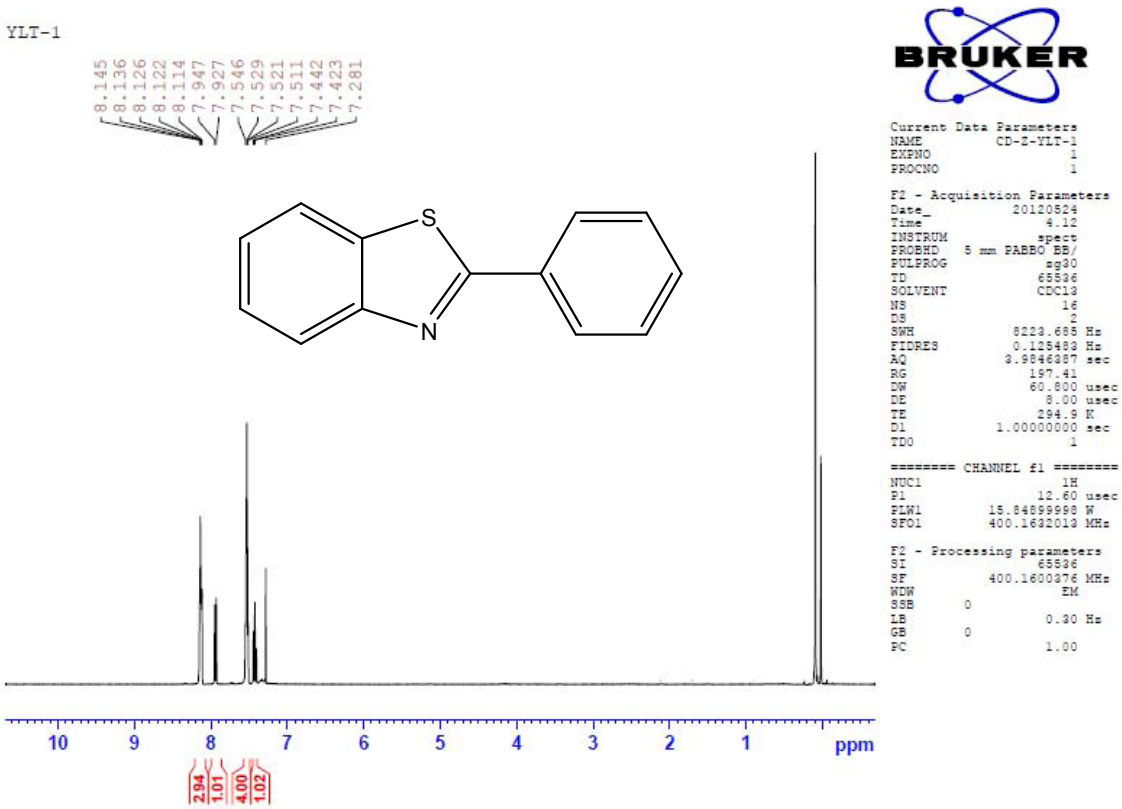
```
Current Data Parameters
NAME      CD-Z-HNMR-YLT-1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120419
Time              16.27
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zg30
TD              65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG                129.89
DW                60.800 usec
DE                 8.00 usec
TE               294.3 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                12.60 usec
PLW1        15.84899998 W
SFO1       400.1632013 MHz

F2 - Processing parameters
SI              65536
SF         400.1600053 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



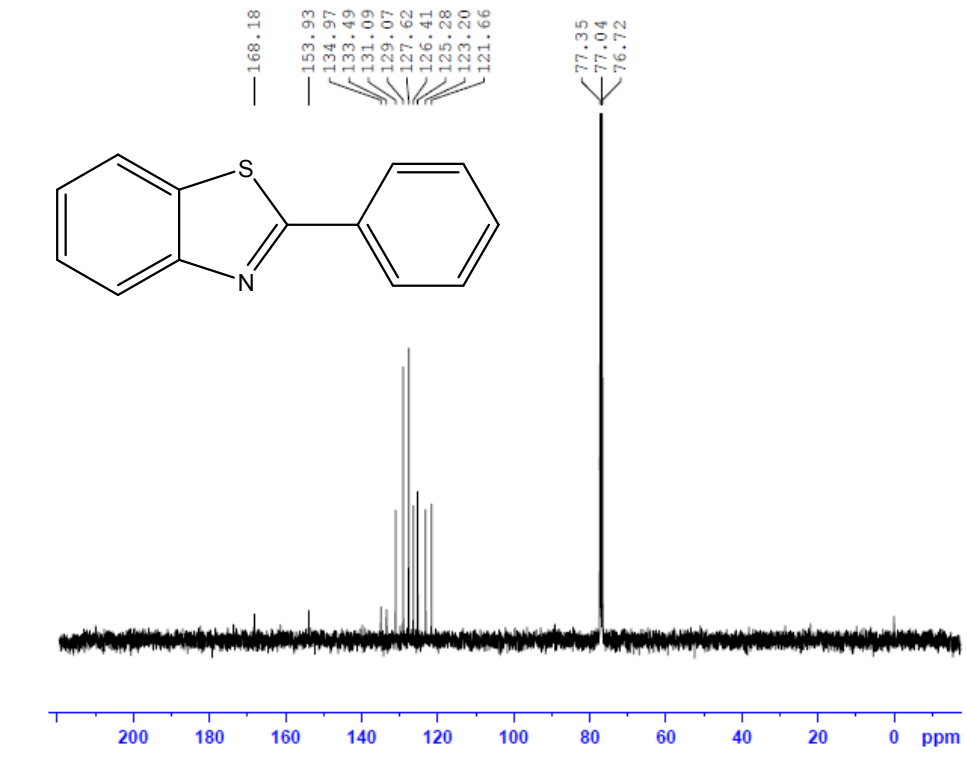
BRUKER

```
Current Data Parameters
NAME      2012-05-30 yulintao-YLT-6
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20120530
Time              23.27
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD              65536
SOLVENT          CDCl3
NS                 256
DS                   0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                2050
DW                20.800 usec
DE                 6.50 usec
TE               300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               13C
P1                19.40 usec
PL1               -1.00 dB
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2       400.1316005 MHz

F2 - Processing parameters
SI              32768
SF         100.6127690 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

(13)2-phenylbenzothiazole

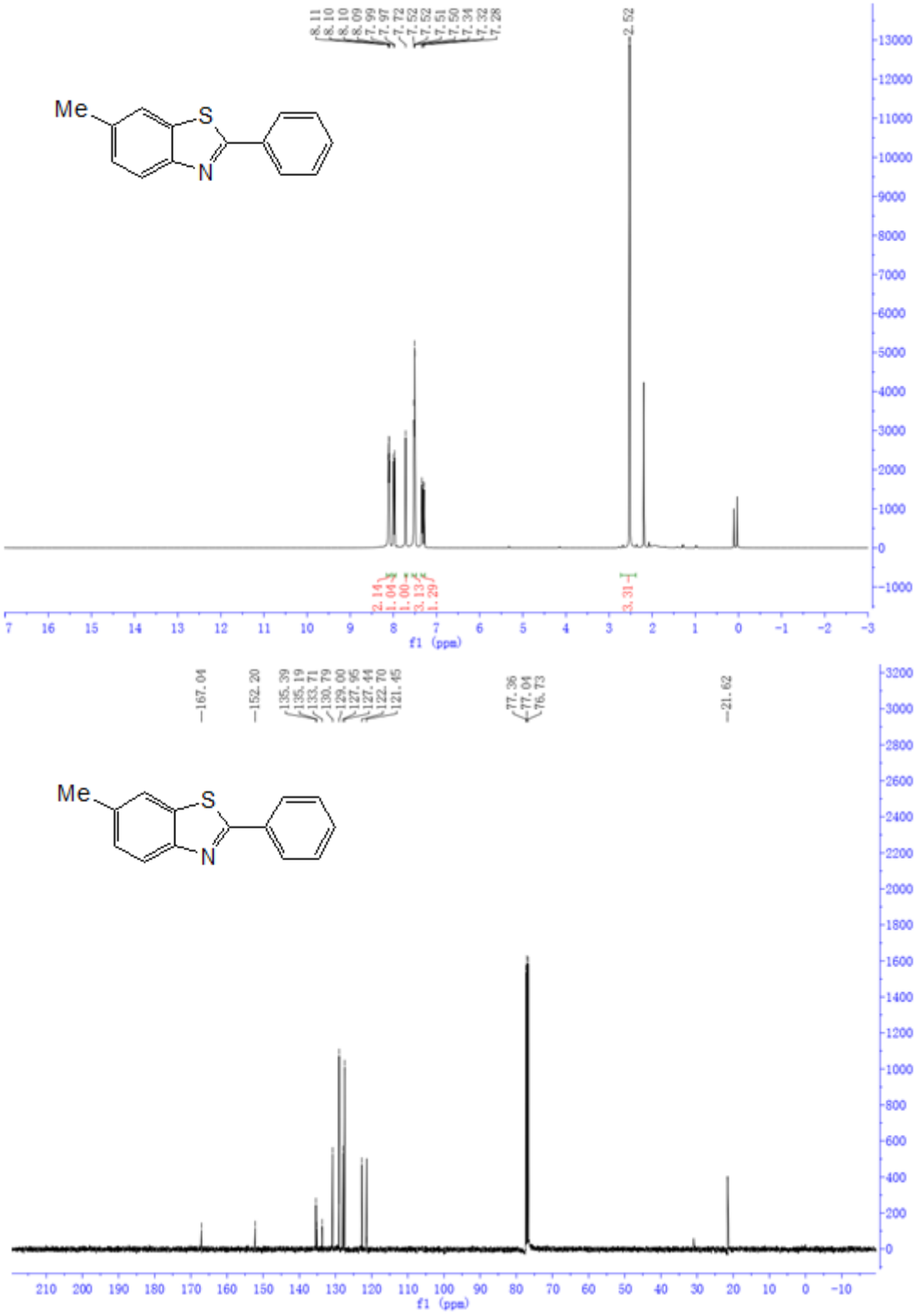



```
Current Data Parameters
NAME          CD-Z-YLT-1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20120524
Time               4.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8223.685 Hz
FIDRES        0.125483 Hz
AQ            3.9846387 sec
RG               197.41
DW              60.800 usec
DE               8.00 usec
TE              294.9 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                12.60 usec
PLW1        15.84899998 W
SFO1        400.1632013 MHz

F2 - Processing parameters
SI                 65536
SF          400.1600376 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

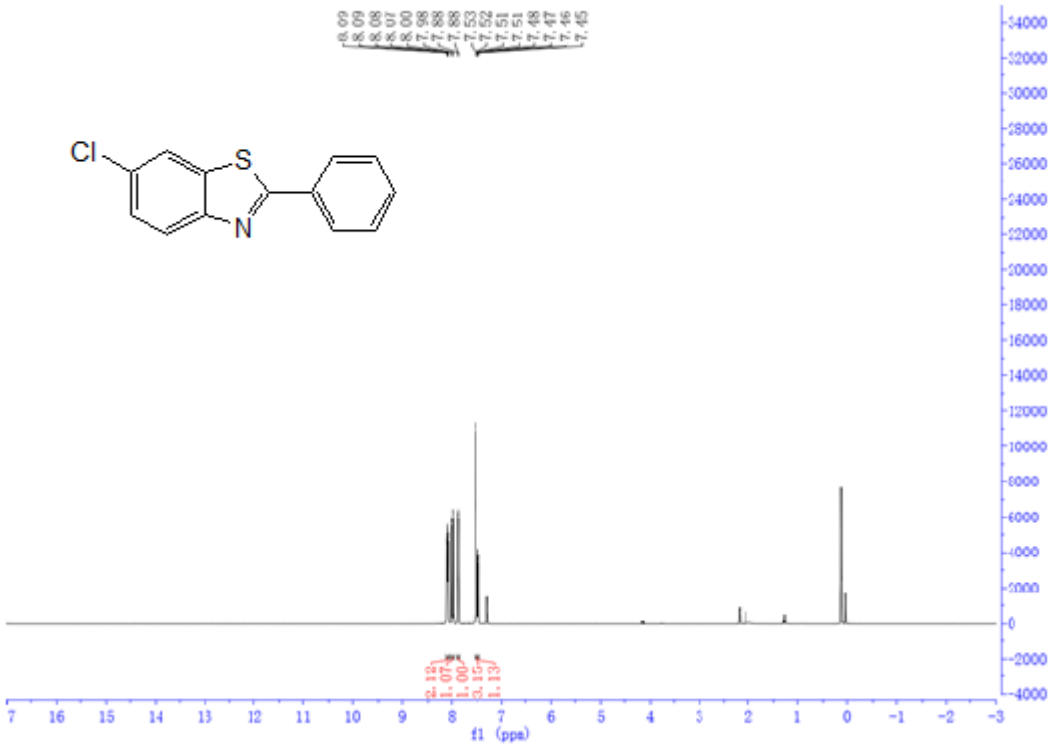


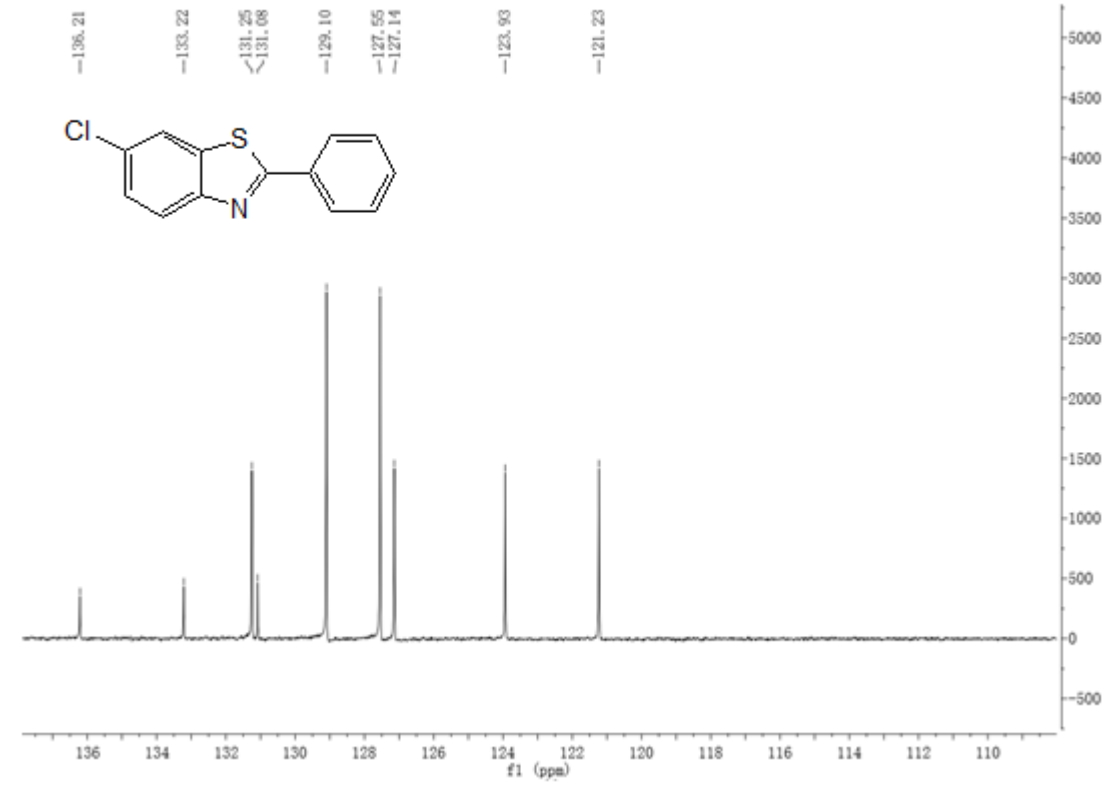

```
Current Data Parameters
NAME       20120530-YLT
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_           20120530
Time               19.54
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 128
DS                   0
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                2050
DW              20.800 usec
DE               6.50 usec
TE              300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                19.40 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             60.00 usec
PL12              11.09 dB
PL13              13.05 dB
PL2               -2.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

(14)6-methyl-2-phenylbenzothiazole

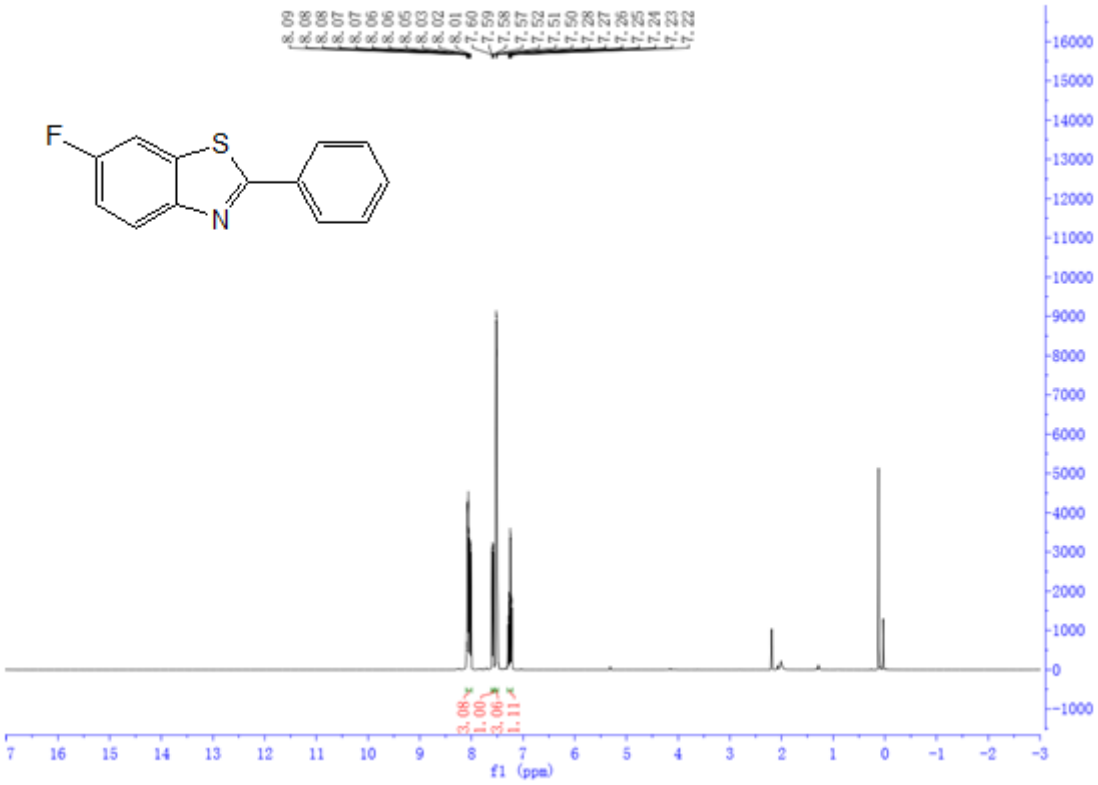


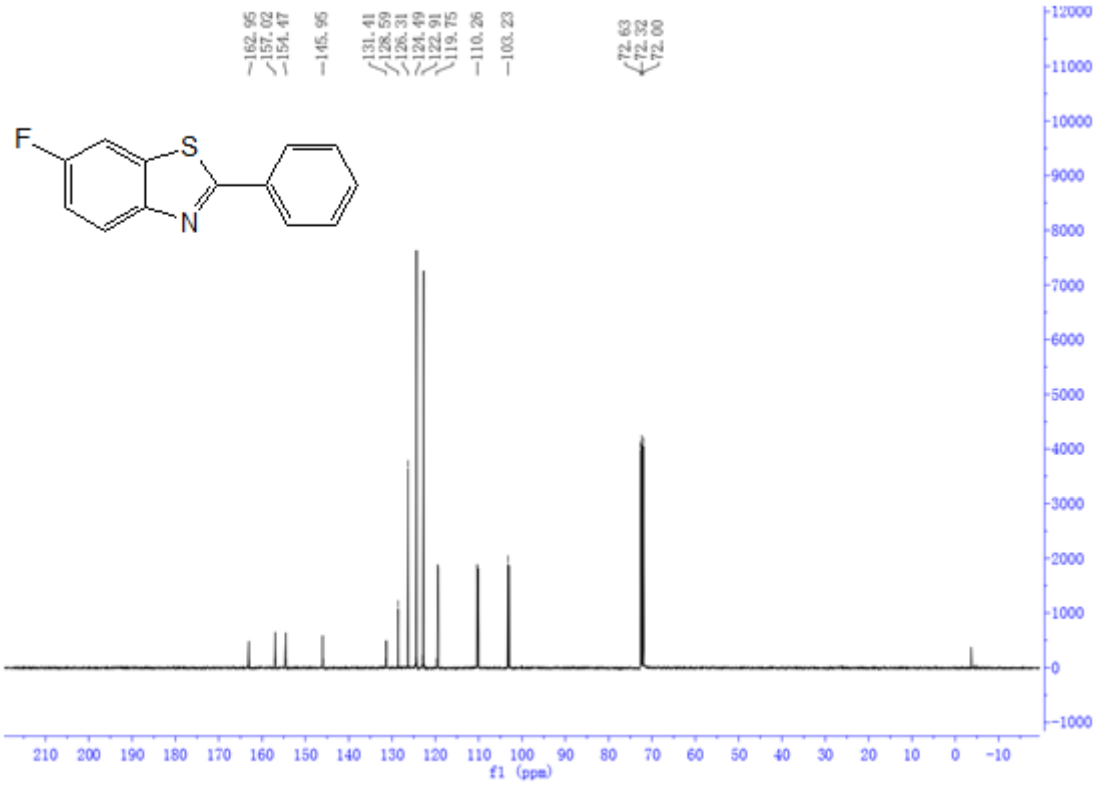
(15)6-chloro-2-phenylbenzothiazole



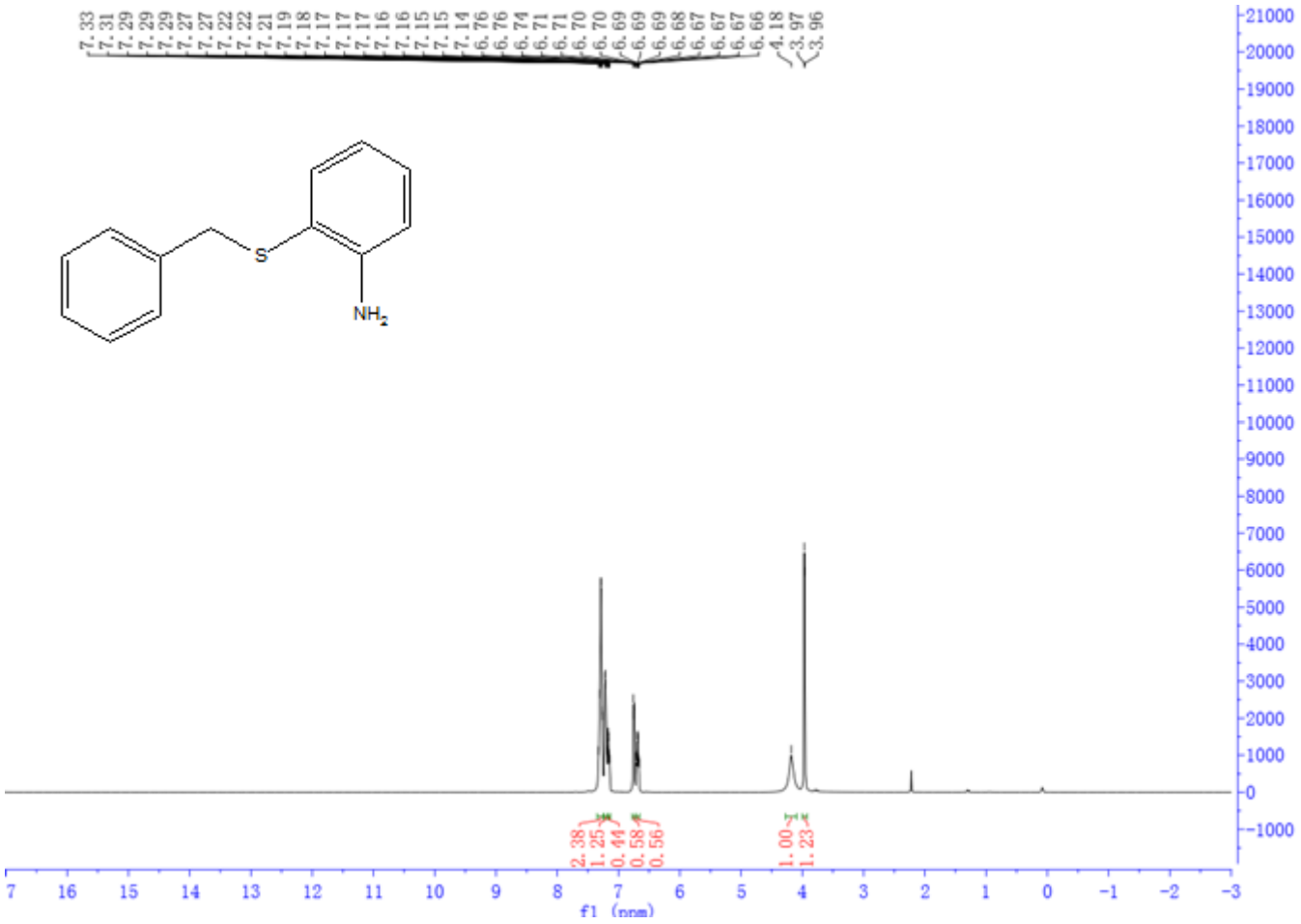


(16)6-fluoro-2-phenylbenzothiazole



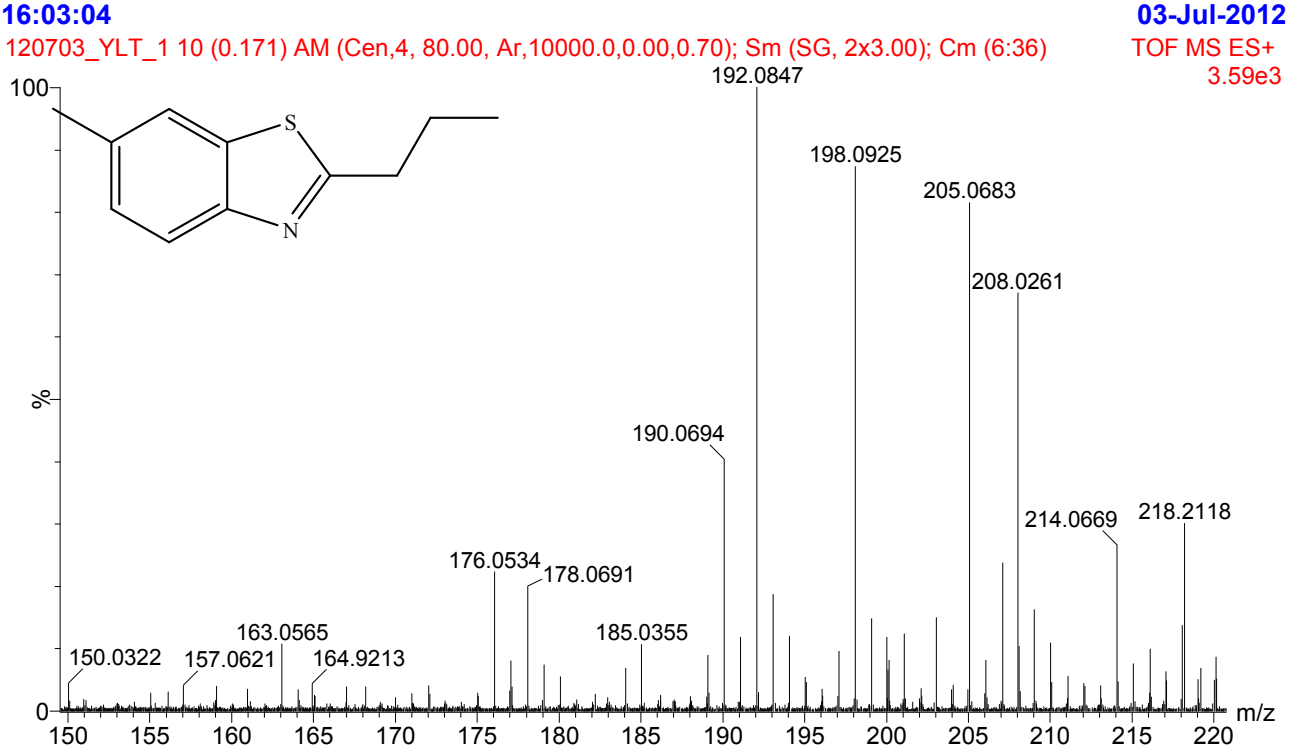


(17)2-Benzylsulfanyl-phenylamine

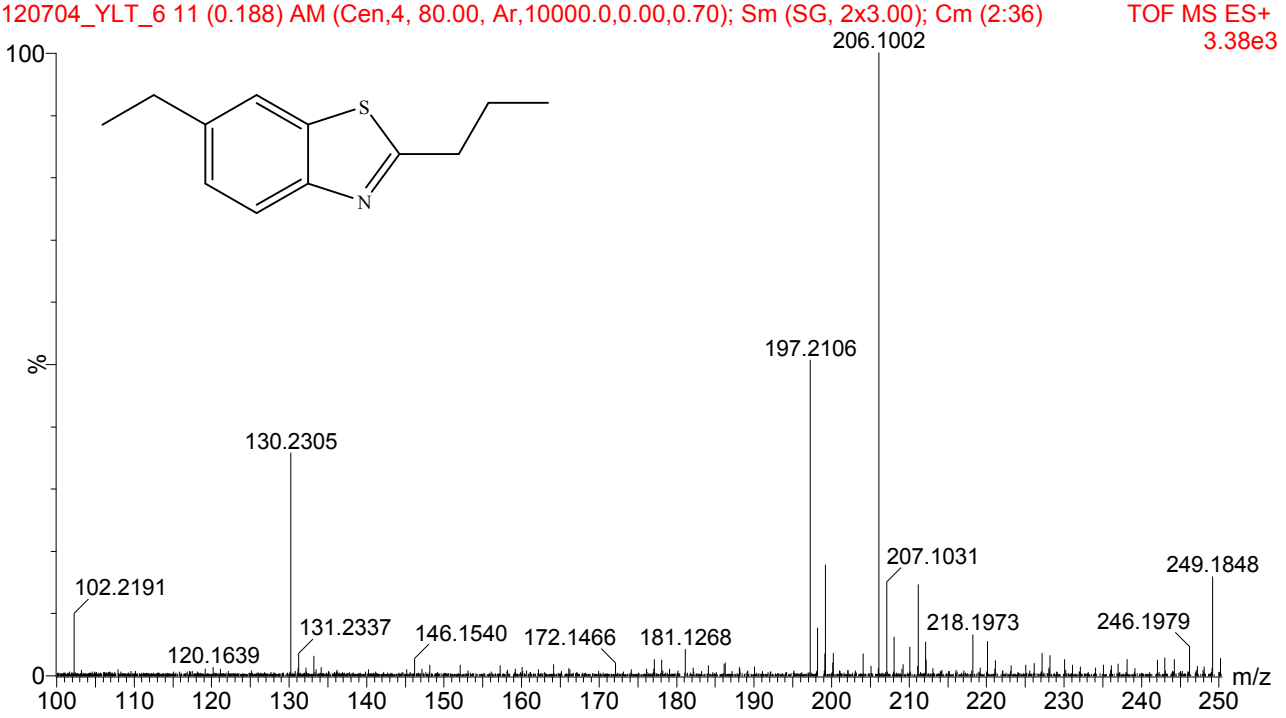


HRMS (ESI) spectra for the products

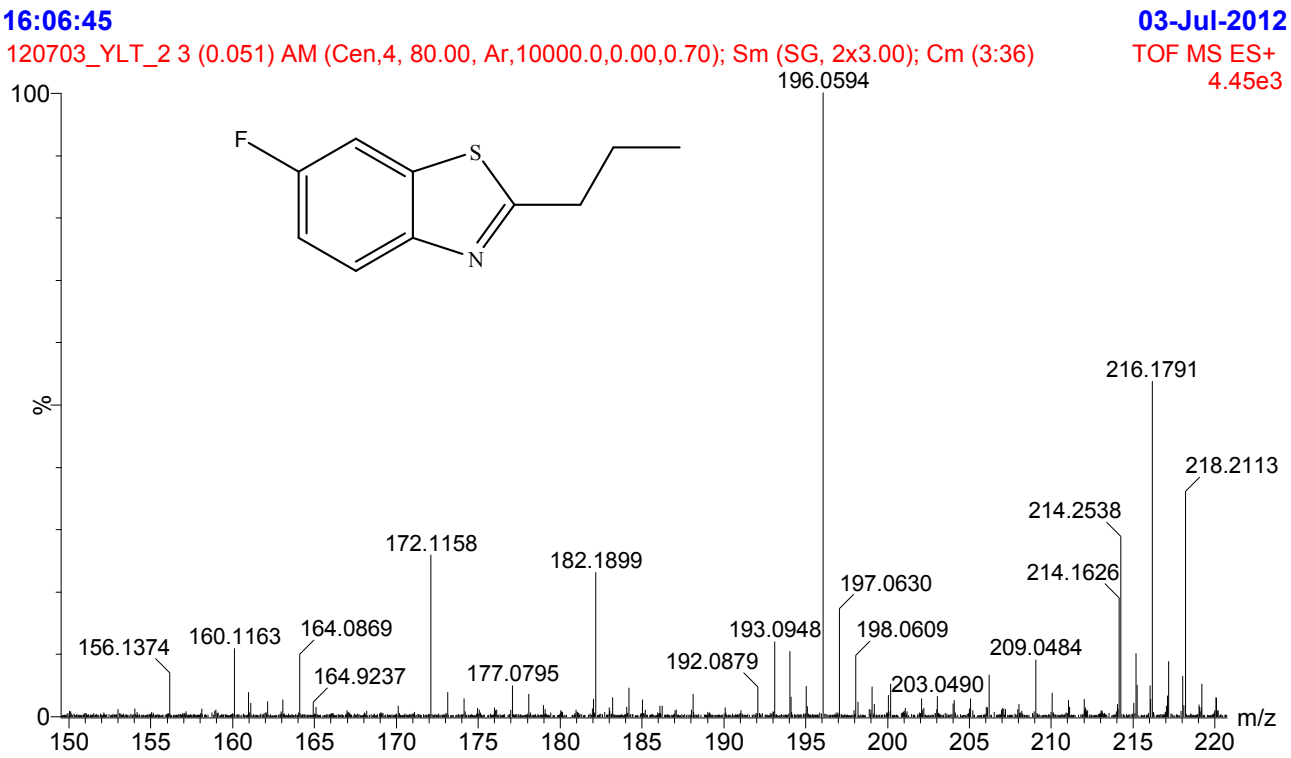
6-methyl-2-propylbenzothiazole



6-ethyl-2-propylbenzothiazole



6-fluoro-2-propylbenzothiazole



5-fluoro-2-propylbenzothiazole