Supporting Information

Synthesis of Well-Defined Tower-Shaped 1,3,5-Trisubstituted Adamantanes Incorporating a Macrocyclic Trilactam Ring System

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General Information. All reagents were purchased from commercial suppliers and used without further purification unless otherwise stated. Tetrahydrofuran (99.9%, anhydrous, inhibitor free), triethylamine (99.5%) and chlorobenzene (99.8%, anhydrous) were used as received. Solvents were well deoxygenated with N_2 before use in Sonogashira coupling reactions or macrocyclization reactions. Brine refers to a saturated aqueous solution of NaCl. Melting points are uncorrected. A decomposition point is indicated by dec. PHB means that the sample was placed in a preheated block just below the decomposition temperature. ^{1}H and ^{13}C NMR spectra were recorded at 300 and 75 MHz, respectively, in $CDCl_3$ unless otherwise noted (e.g. 500 and 125 MHz). Chemical shifts are in δ units (ppm) with the residual solvent peak (^{1}H $CHCl_3$, δ 7.26; ^{13}C $CDCl_3$, δ 77) as the internal standard. Coupling constants (*J*) are reported in hertz (Hz). NMR splitting patterns are designated as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; and br, broad. Column chromatography was carried out on silica gel (60–200 mesh). Analytical TLC was performed on commercially coated 60 mesh F_{254} plastic plates. Spots were rendered visible by exposing the plate to UV light. Radial chromatography (RC) was performed using 1, 2 and 4 mm disks covered with silica gel 60PF$_{254}$ containing gypsum. Fluorescence spectra were acquired at 25 °C on a fluorescence spectrometer with 5 nm and 10 nm excitation and emission slit widths, respectively, using a 10 mm path quartz cuvette. Mass spectra other than FAB mass spectra were measured by LC-MS.

1,3,5-Triethynyladamantane (8). Colorless crystals, mp 84-86 °C (Lit.[1] 84-86°C); ^{1}H NMR δ 1.78 (d, *J* = 3.0 Hz, 6H), 1.95 (s, 6H), 2.11 (t, *J* = 3.3 Hz, 1H), 2.14 (s, 3H); ^{13}C NMR δ 27.79, 29.76, 40.39, 46.15, 68.15, 90.02; MS calcd for $C_{16}H_{15}$ (M-1) 207.1, found 207.1. Anal. Calcd for $C_{16}H_{16}$: C, 92.26; H, 7.74. Found: C, 92.11; H, 7.77.

Pyrrolidin-1-yl-(4-trimethylsilanylethynylphenyl)diazene (11). Light yellow crystals, which were pure by TLC and NMR: mp 110-112 °C (lit.[2] mp 101 °C); ^{1}H NMR δ 0.24 (s, 9H), 2.02 (t, *J* = 6.3 Hz, 4H), 3.79 (brs, 4H), 7.34 (d, *J* = 8.9 Hz, 2H), 7.42 (d, *J* = 8.9 Hz, 2H); ^{13}C NMR δ 0.04, 23.75, 93.57, 105.71, 119.28, 120.12, 132.73, 151.32; MS calcd for $C_{15}H_{21}N_3Si$ (M) 271.1, found 271.0. Anal. Calcd for $C_{15}H_{21}N_3Si \cdot 1/4H_2O$: C, 65.29; H, 7.79; N, 15.23. Found: C, 65.49; H, 7.95; N, 15.31.

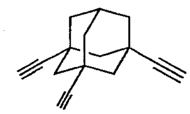
(4-Iodophenylethynyl)trimethylsilane (13). Colorless crystals, which were pure by TLC and NMR: mp 68-70 °C (lit.[3] mp 56-58 °C); ^{1}H NMR δ 0.24 (S, 9H), 7.18 (d, *J* = 8.7 Hz, 2H), 7.63 (d, *J* = 8.7 Hz, 2H); ^{13}C NMR δ -0.15, 94.46, 95.86, 103.95, 122.59, 133.41, 137.34; MS calcd for $C_{11}H_{12}ISi$ (M-1) 299.0, found 299.0. Anal. Calcd for $C_{11}H_{13}ISi$: C, 44.01; H, 4.36. Found: C, 43.72; H, 4.16.

Thioacetic Acid *S*-(4-Iodobenzyl) Ester (16). Colorless solid,[4] which was pure by TLC and NMR: mp 41-42 °C (lit.[5] mp 40-41 °C); ^{1}H NMR δ 2.34 (s, 3H), 4.04 (s, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR δ 30.30, 32.85, 92.65, 130,75, 137.44, 137.64, 194.82; MS calcd for C_9H_9IOSNa 314.94, found 315.0.

3,5-Bis(acetylsulfanylmethyl)iodobenzene (17). Colorless solid,[6] which was pure by TLC and NMR: mp 39-41 °C (lit.[6] no mp); ^{1}H NMR δ 2.35 (s, 6H), 4.00 (s, 4H), 7.15 (s, 1H), 7.50 (d, *J* = 1.5 Hz, 2H); ^{13}C NMR δ 30.31, 32.39, 94.40, 128.65, 136.55, 140.17, 194.64.

Thioacetic Acid *S*-(4-Trimethylsilanylethynylbenzyl) Ester (27). A light yellow solid, which was pure by TLC and NMR: mp 41-42 °C (lit.[5] mp 41-42 °C); ^{1}H NMR δ 0.27 (s, 9H), 2.37 (s, 3H), 4.12 (s, 2H), 7.24 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR δ -0.08, 30.27, 33.18, 94.38, 104.71, 122.05, 128.66, 132.13, 138.09, 194.83; MS calcd for $C_{14}H_{19}OSSi$ (M+1) 263.1, found 263.1. Anal. Calcd for $C_{14}H_{18}OSSi$: C, 64.07; H, 6.91. Found: C, 63.94; H, 6.73.

1-[4-(*S*-Acetylthiomethyl)phenyl]acetylene (28). A yellow oil,[5] which was pure by TLC and NMR: ^{1}H NMR δ 2.35 (s, 3H), 3.08 (s, 1H), 4.01 (s, 2H), 7.25 (d, *J* = 8.6 Hz, 2H), 7.42 (d, *J* = 8.6 Hz, 2H); ^{13}C NMR δ 30.23, 33.09, 77.00, 83.26, 120.96, 128.74, 132.28, 138.49, 194.74; MS calcd for $C_{11}H_9OS$ (M-1) 189.0, found 189.0. Anal. Calcd for $C_{11}H_{10}OS$: C, 69.44; H, 5.30. Found: C, 69.65; H, 5.31.



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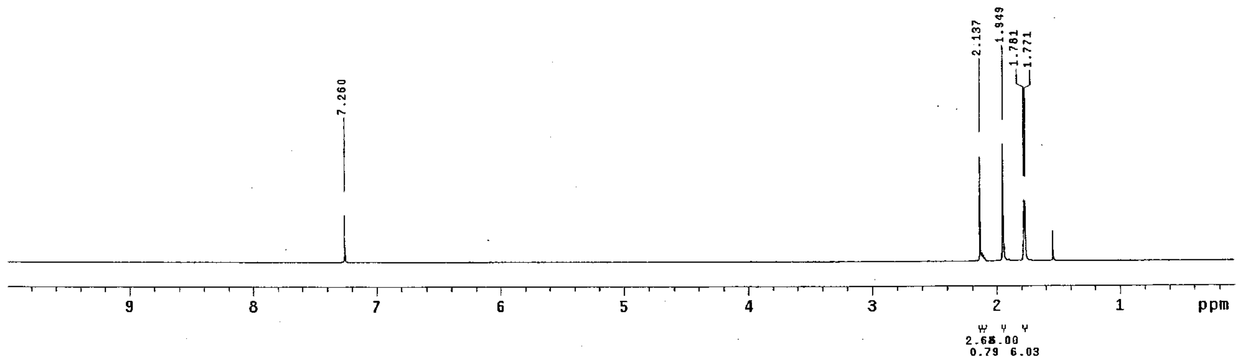

qli-256

Pulse Sequence: s2pul

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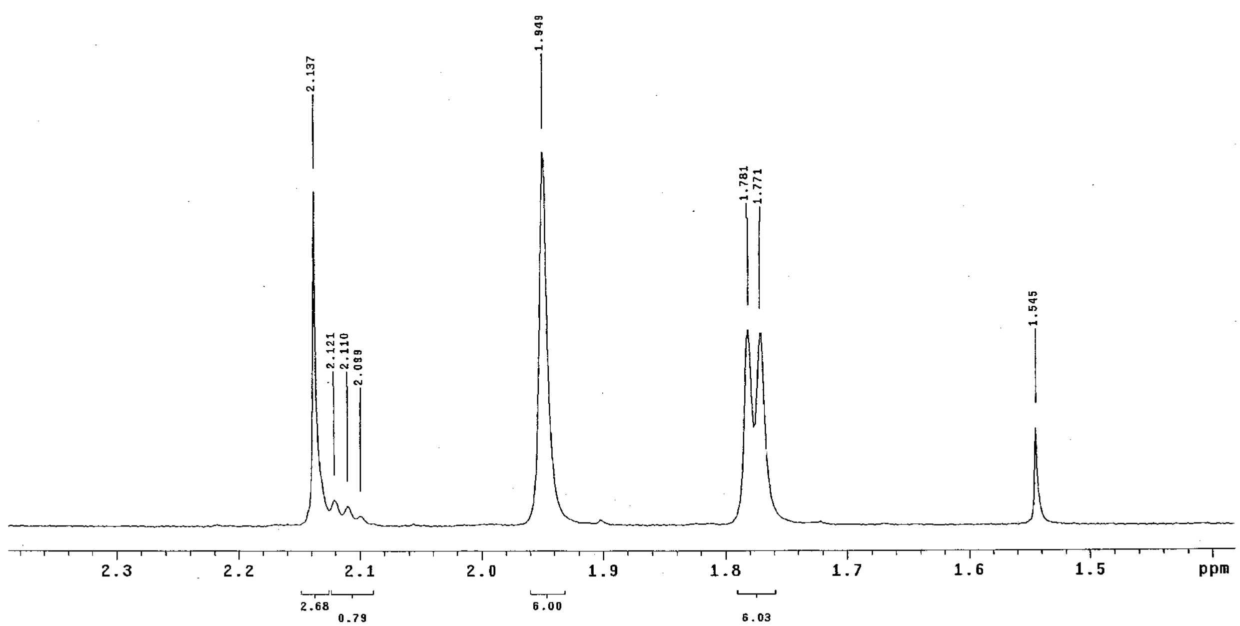
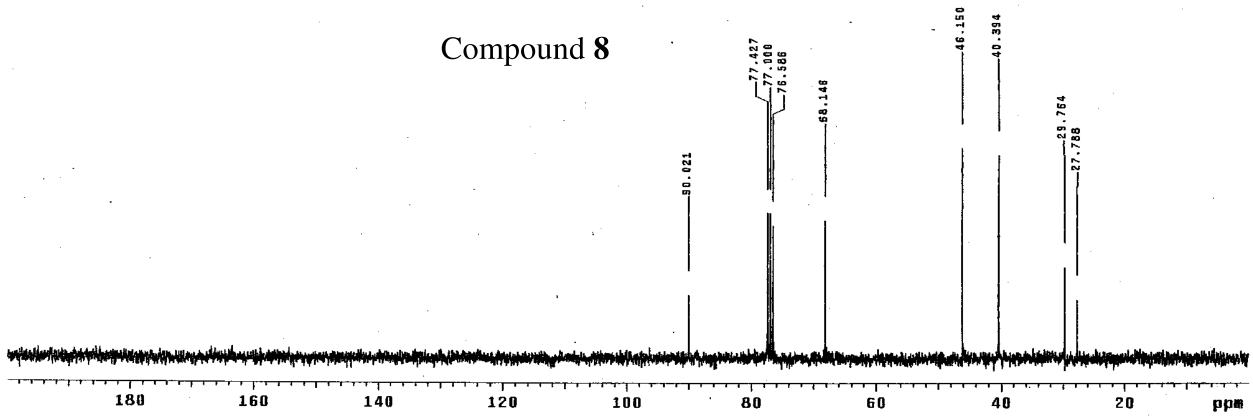
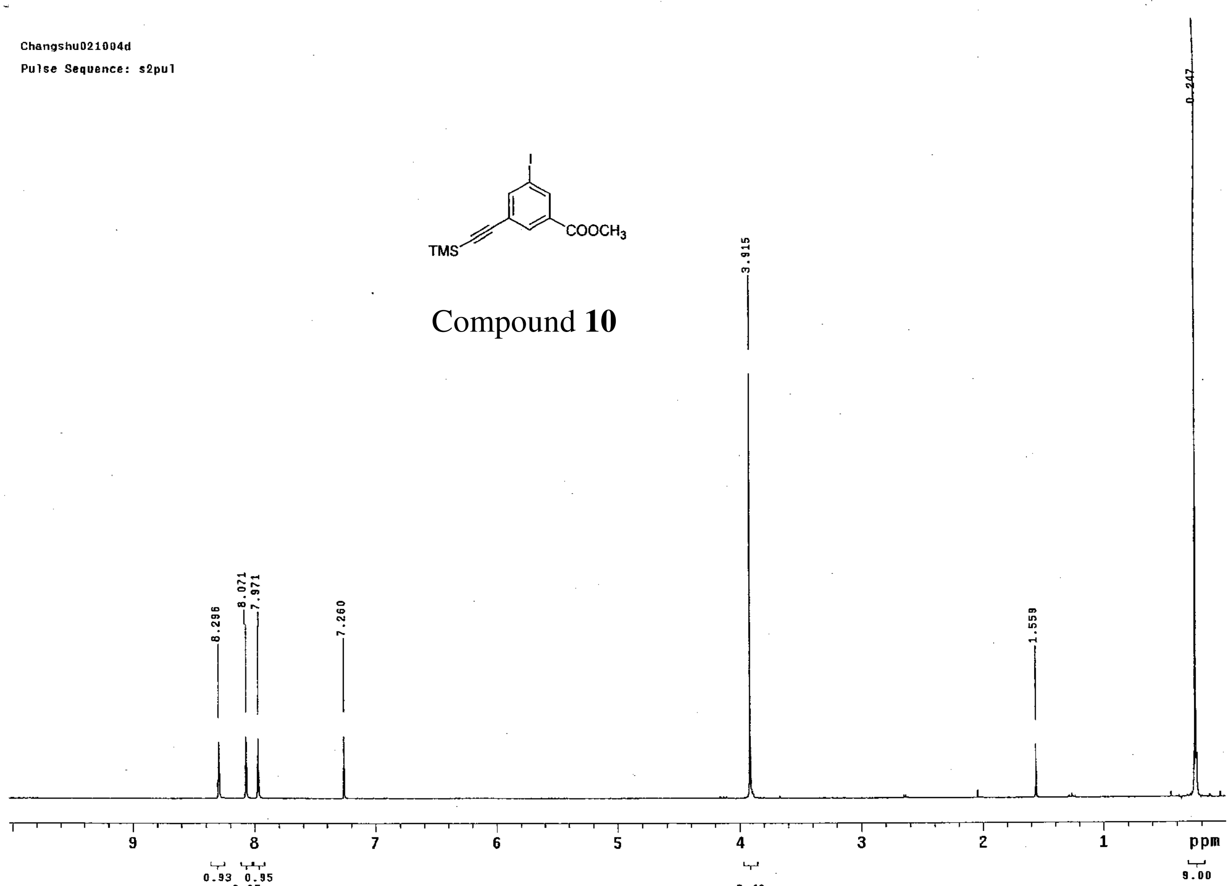


Compound **8**





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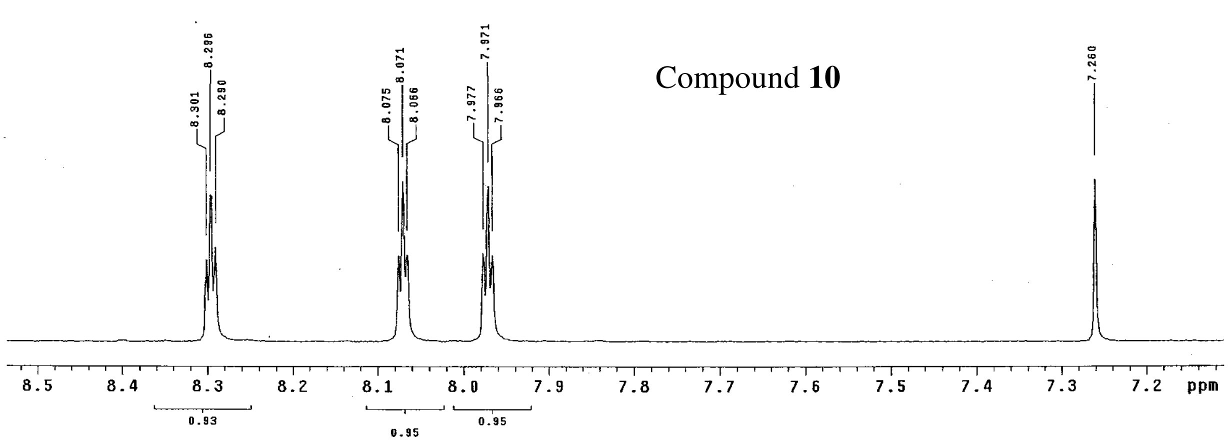

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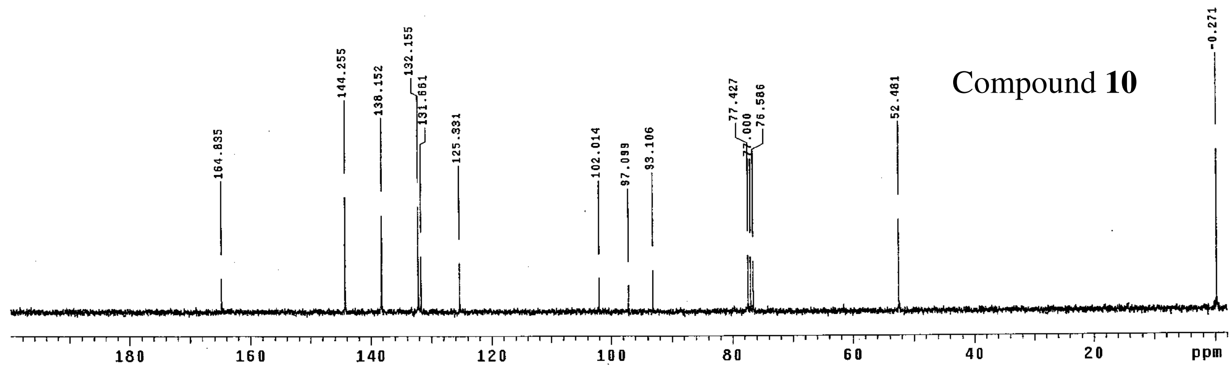

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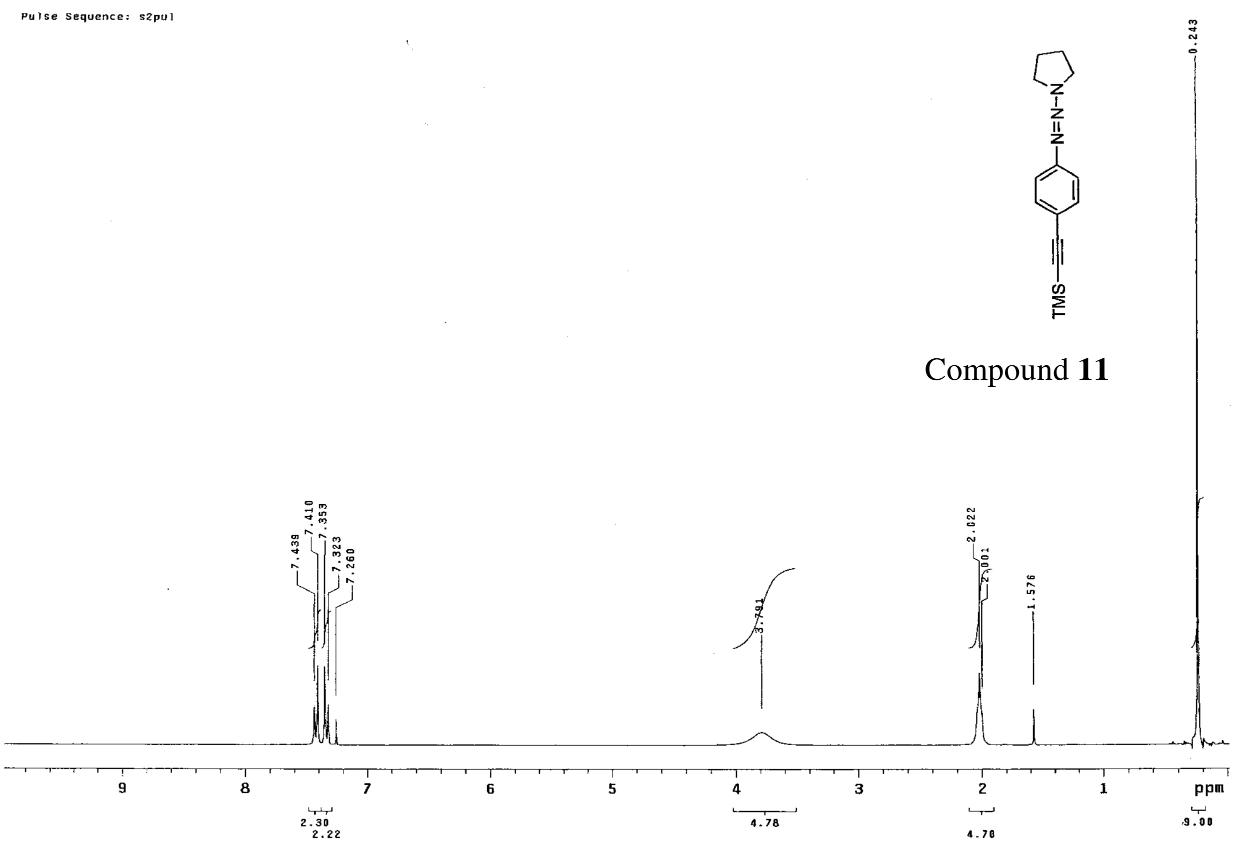

Compound **11**

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 Pulse 42.6 degrees
 Acq. time 0.599 sec
 Width 16501.7 Hz
 256 repetitions
OBSERVE  C13,  75.4216991 MHz
DECOUPLE  H1, 299.9478514 MHz
 Power 32 dB
 continuously on
 WALTZ-16 modulated
DATA PROCESSING
 Line broadening 1.0 Hz
FT size 32768
Total time 6 min, 42 sec
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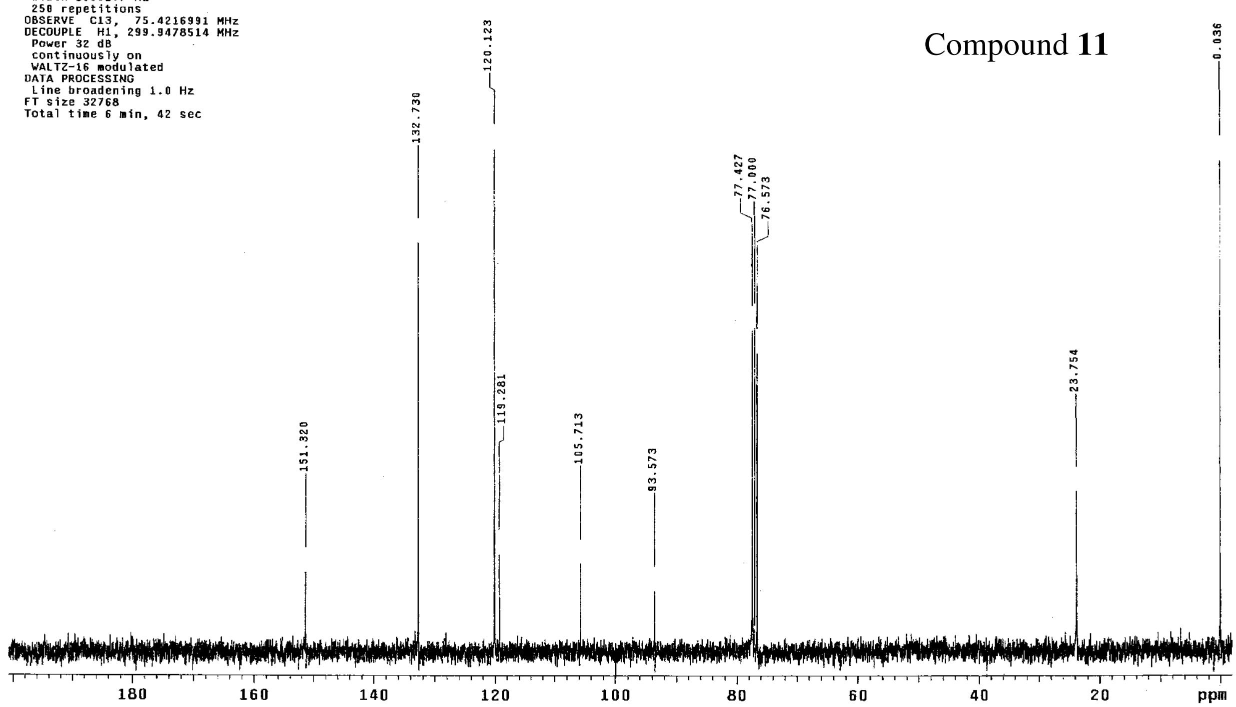
Compound **11**

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 Solvent: CDCl3
 Ambient temperature
File: quanli020207a
INOVA-500  "acetone"
PULSE SEQUENCE
 Relax. delay 1.000 sec
 Pulse 37.9 degrees
 Acq. time 2.500 sec
 Width 4799.0 Hz
 8 repetitions
OBSERVE H1, 299.9468689 MHz
DATA PROCESSING
 Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec
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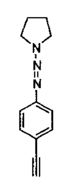

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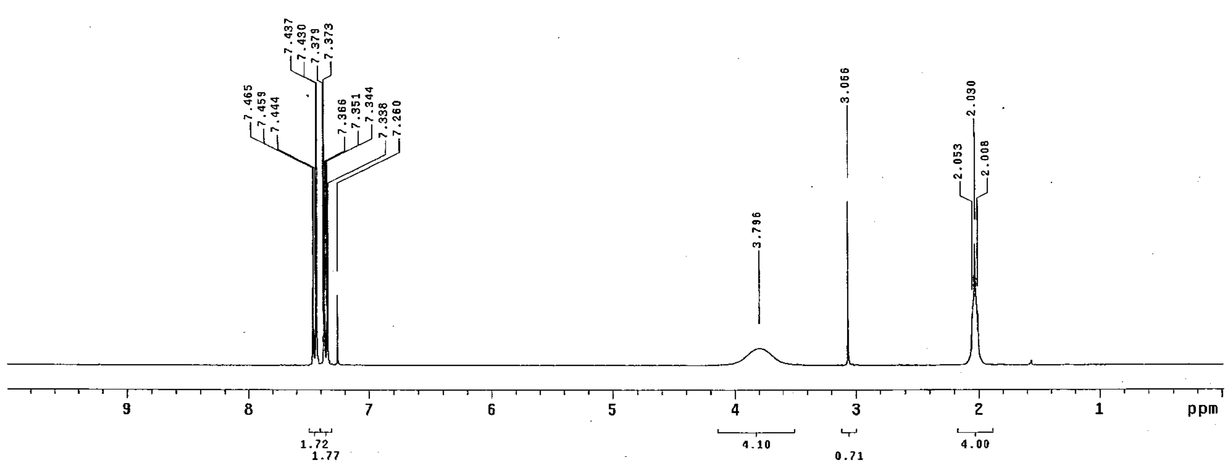

quanli020207a

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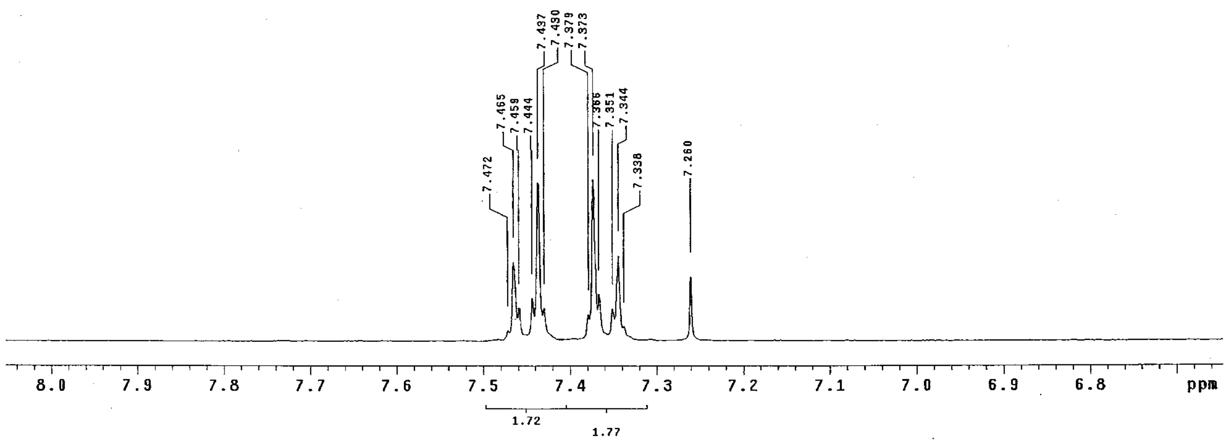
Solvent: CDCl3
Ambient temperature
File: quanli020207a
INOVA-500 "acetone"

PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.500 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9468689 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec

Compound **12**



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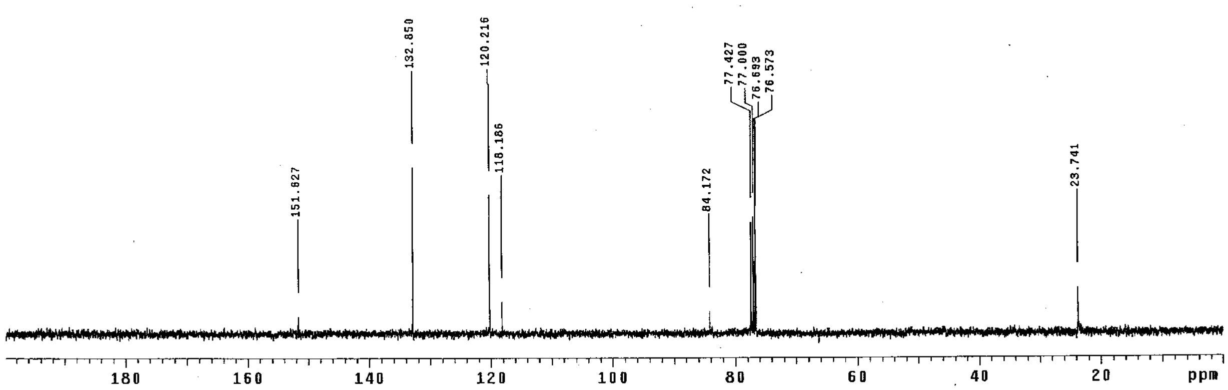
Ambient temperature
File: quanli020207b
INOVA-500 "acetone"

PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 42.6 degrees
Acq. time 0.599 sec
Width 16501.7 Hz
300 repetitions
OBSERVE C13, 75.4216995 MHz
DECOUPLE H1, 299.9478455 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 8 min, 3 sec

Compound **12**



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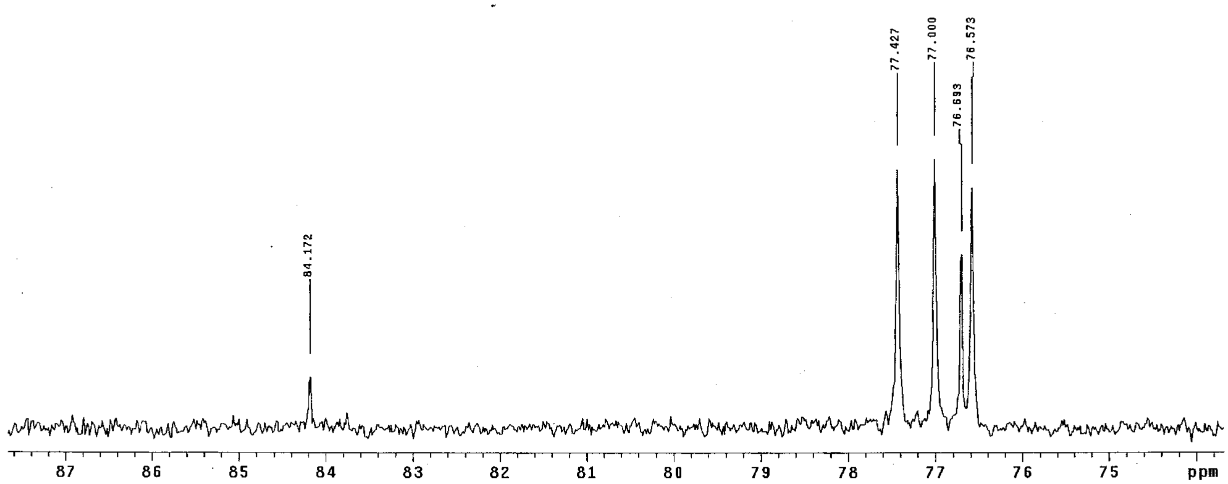
Solvent: CDCl3
Ambient temperature
File: quanli020207b
INOVA-500 "acetone"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 42.6 degrees
Acq. time 0.599 sec
Width 16501.7 Hz
300 repetitions
OBSERVE C13, 75.4216995 MHz
DECOUPLE H1, 299.9478455 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 8 min, 3 sec

Compound **12**



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INOVA-500 "acetone"
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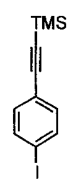
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.500 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9468689 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec



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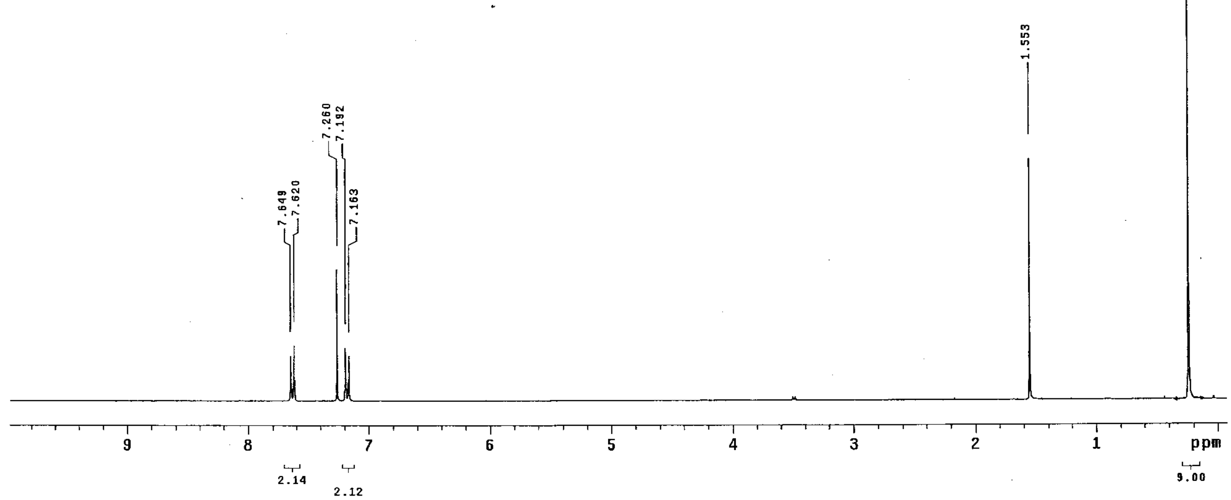


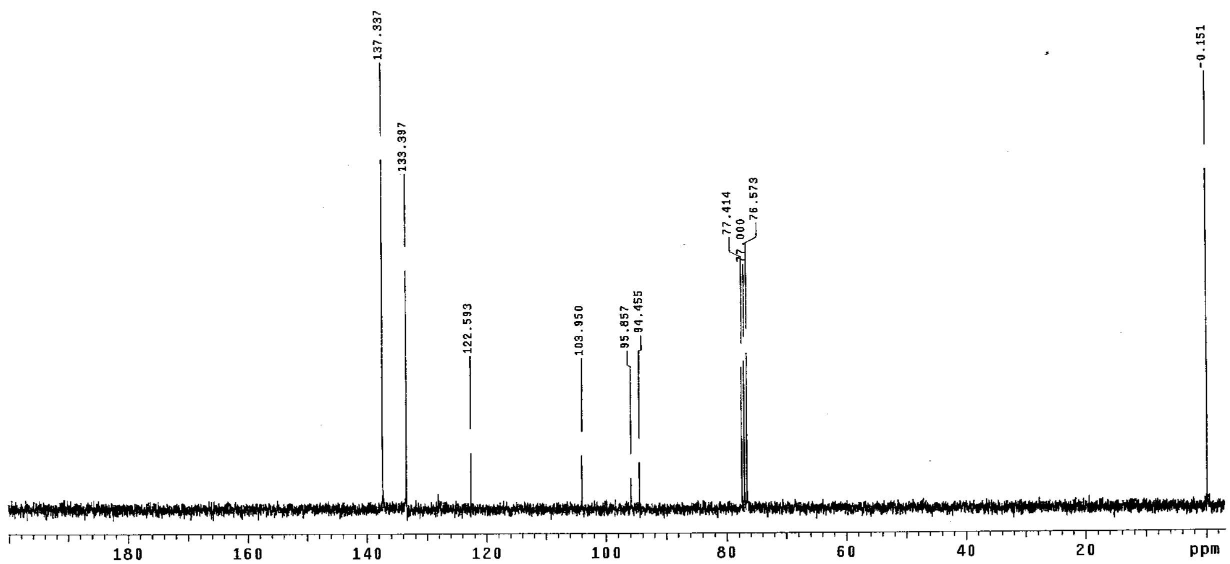
quanli011127b

Pulse Sequence: s2pul

Solvent: CDCl3
Ambient temperature
File: qli011127b
INOVA-500 "acetone"

PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 42.6 degrees
Acq. time 0.599 sec
Width 16501.7 Hz
200 repetitions
OBSERVE C13, 75.4216995 MHz
DECOUPLE H1, 299.9478455 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 5 min, 22 sec

Compound **13**



qli-280

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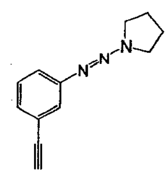

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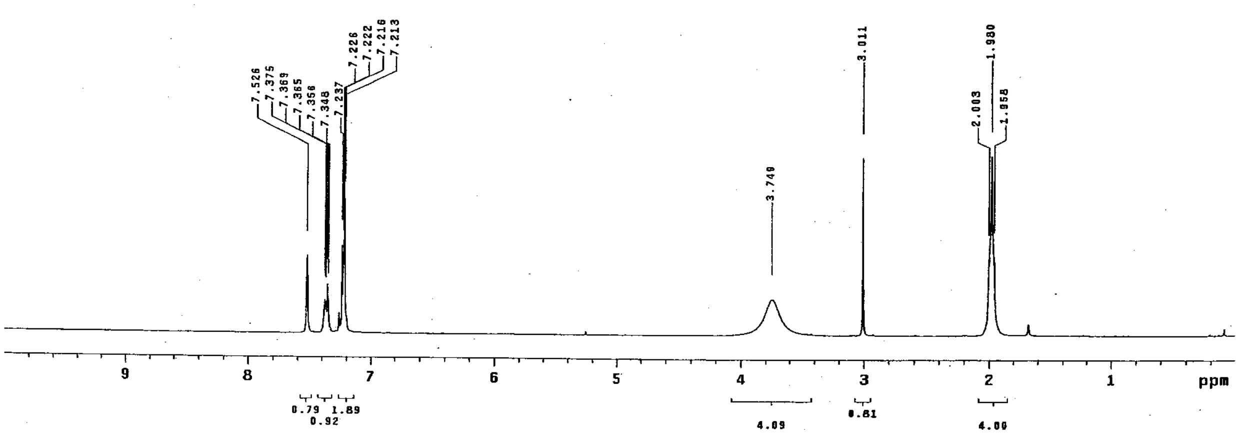

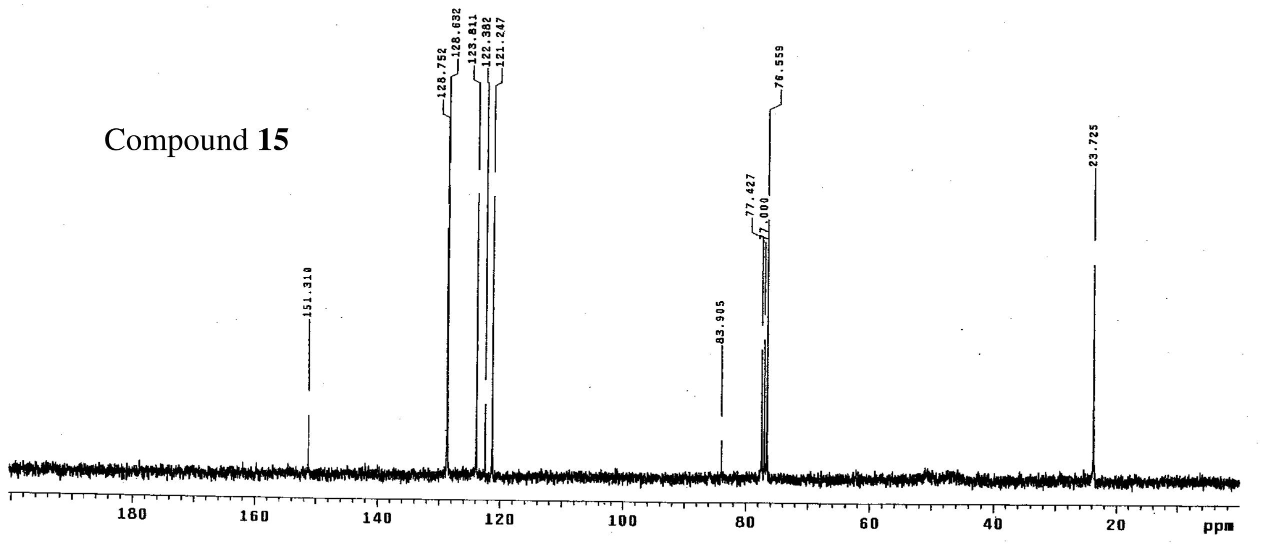
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121.247
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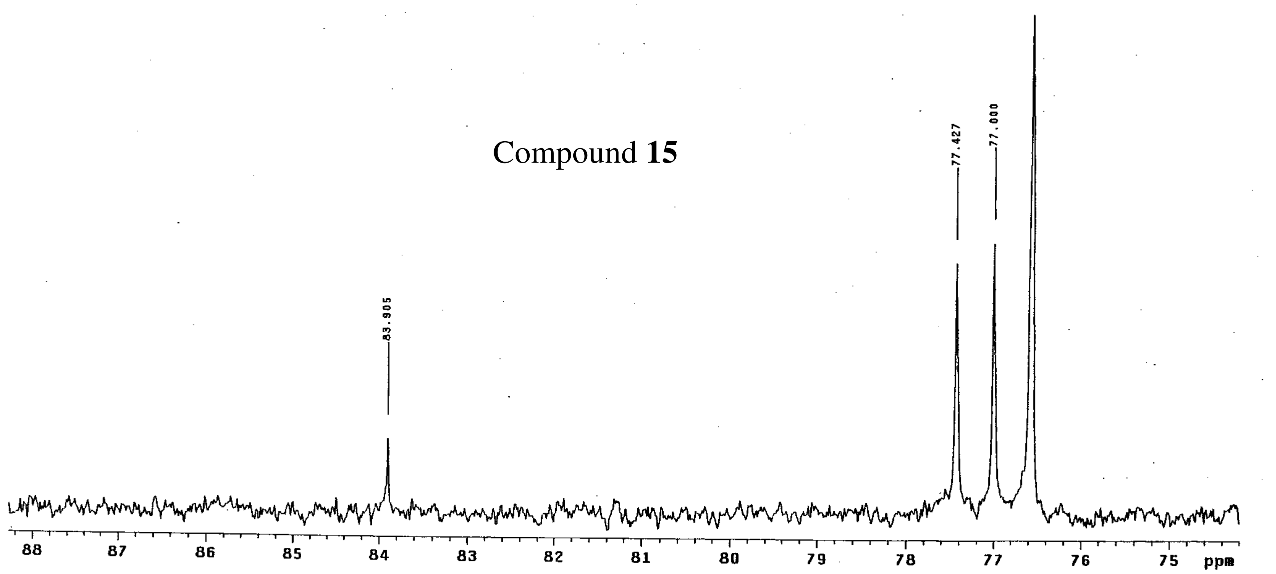
140
120
100
80
60
40
20
ppm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83
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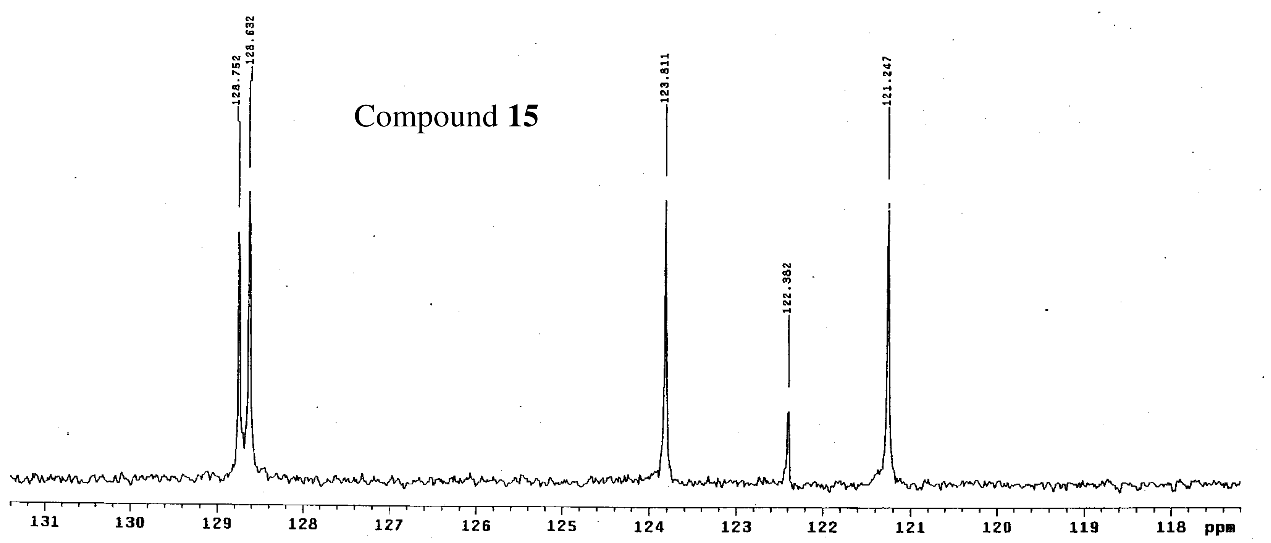
77
76
75
ppm


128.752
128.632
123.811
121.247
Compound 15
122.382
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127
126
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124
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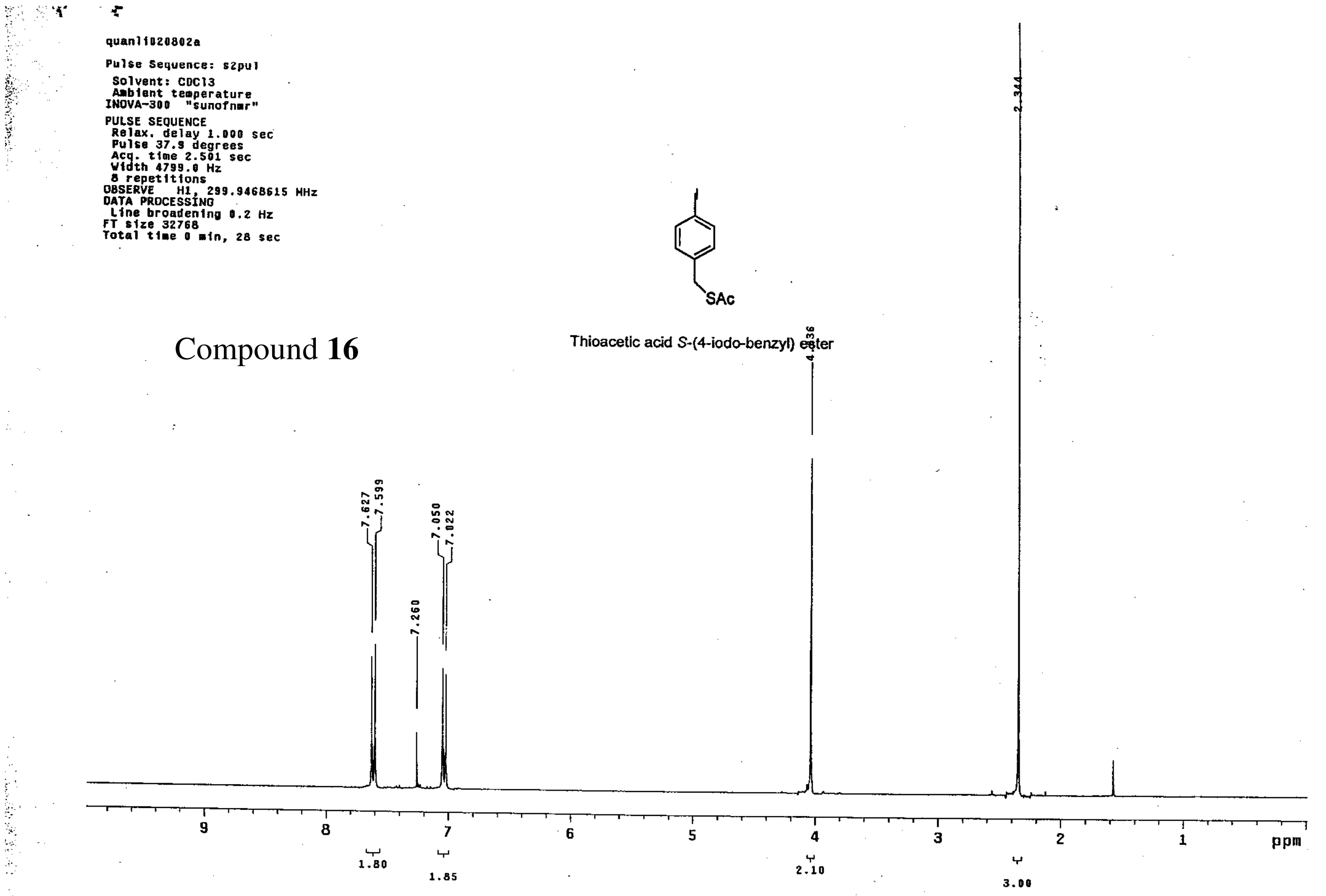
121
120
119
118
ppm


quanli020802a
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Solvent: CDCl3
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Pulse 37.9 degrees
Acq. time 2.501 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9468615 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec
SAc
Thioacetic acid S-(4-iodo-benzyl) ester
Compound **16**
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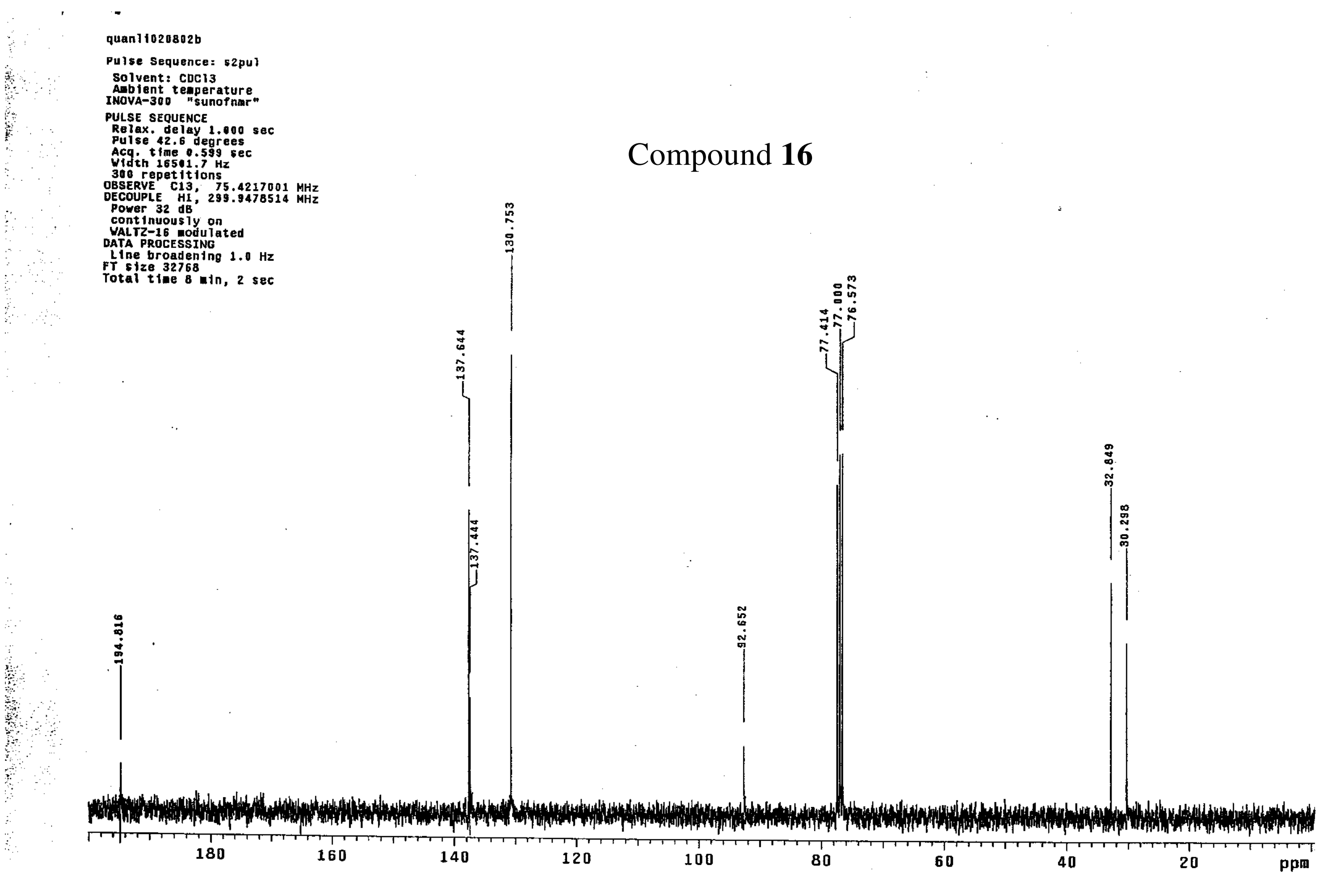
7.599
7.260
7.050
7.022
4.036
2.344
1.80
1.85
2.10
3.00
ppm


quanli020802b
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 42.6 degrees
Acq. time 0.599 sec
Width 16501.7 Hz
300 repetitions
OBSERVE C13, 75.4217001 MHz
DECOUPLE H1, 299.9478514 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 8 min, 2 sec
Compound **16**
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130.753
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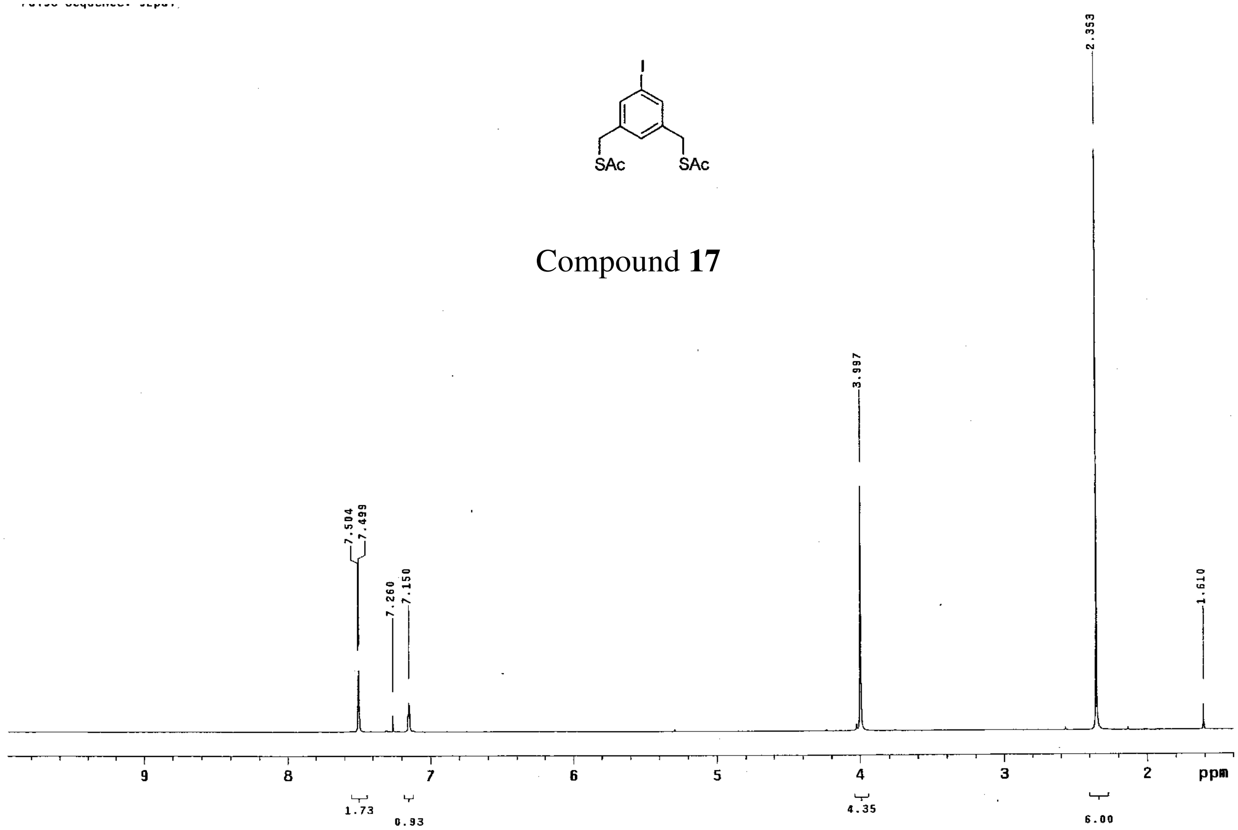
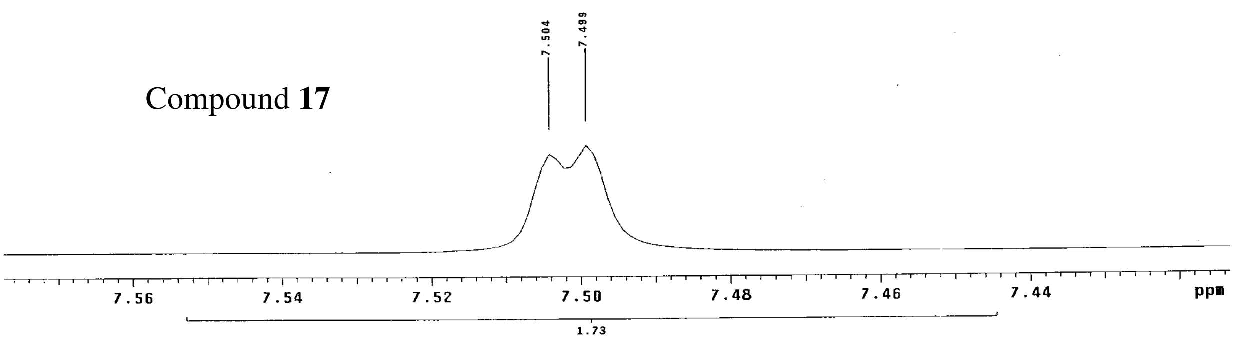
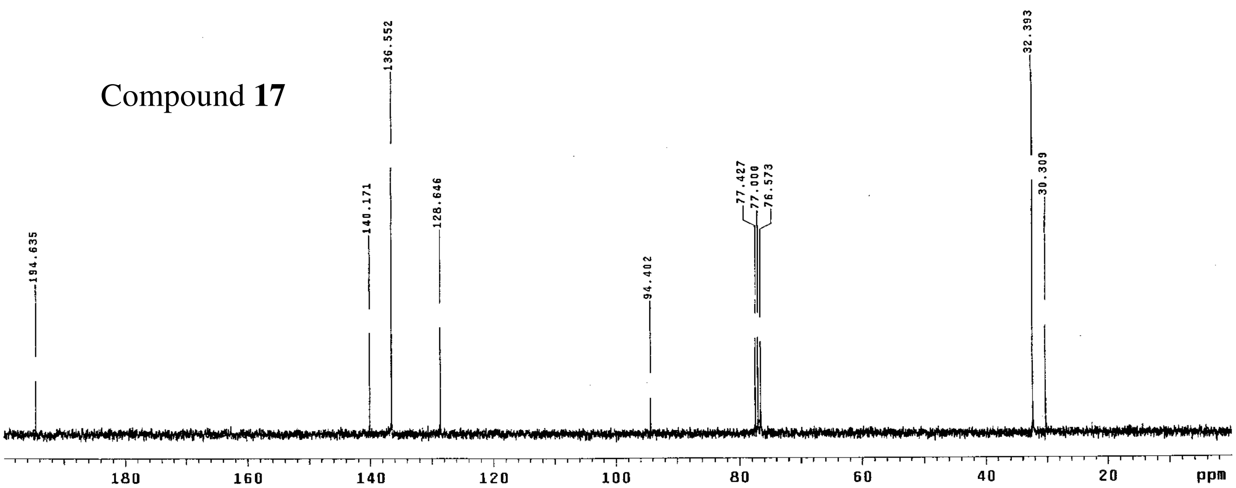
32.849
30.298
ppm



Compound **17**



Compound **17**



Compound **17**

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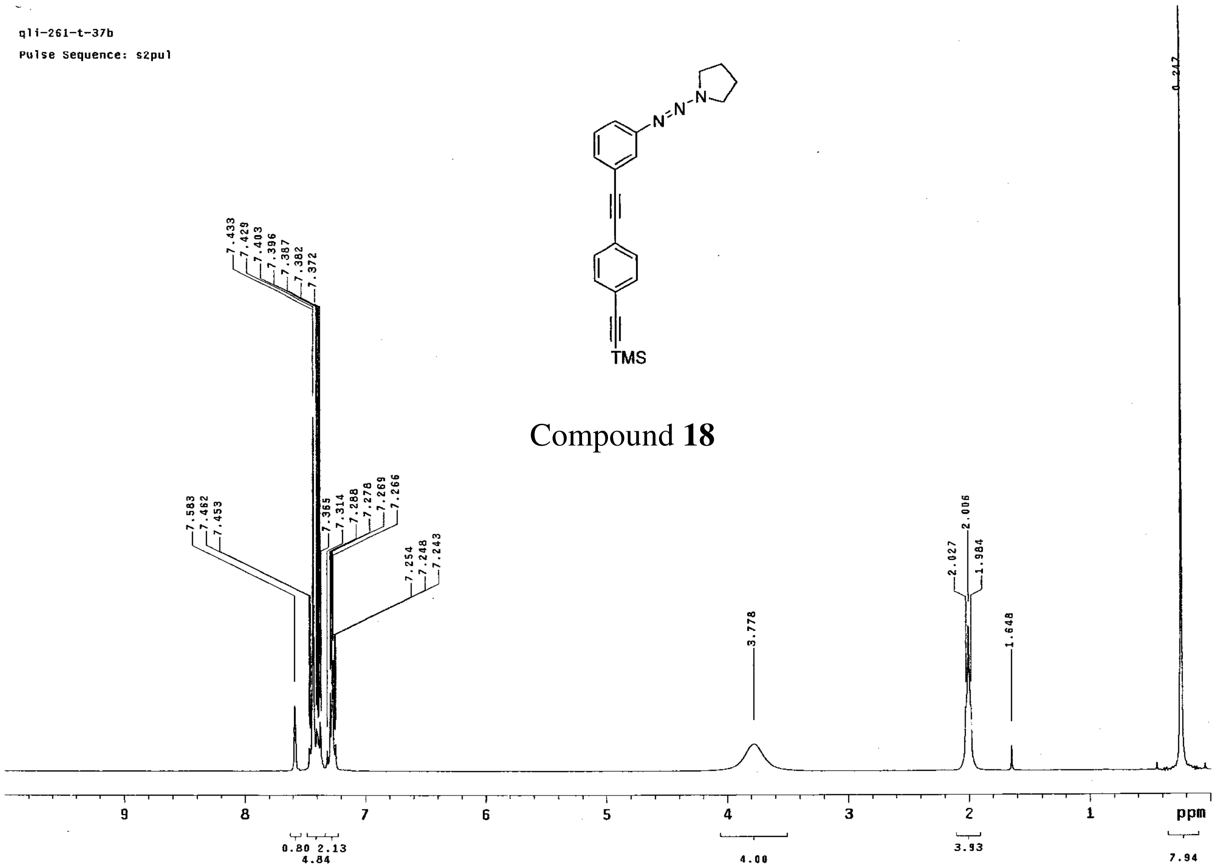
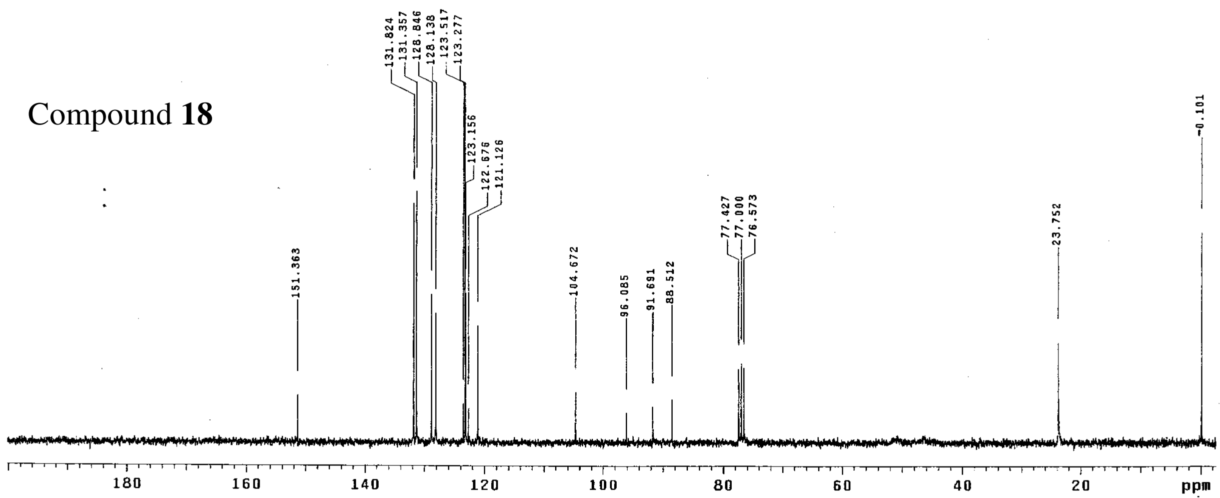
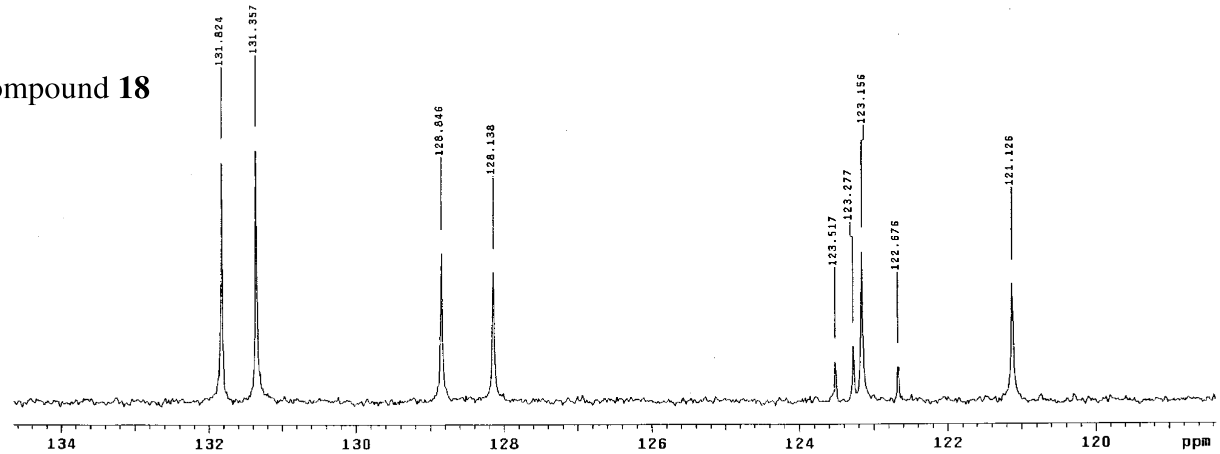


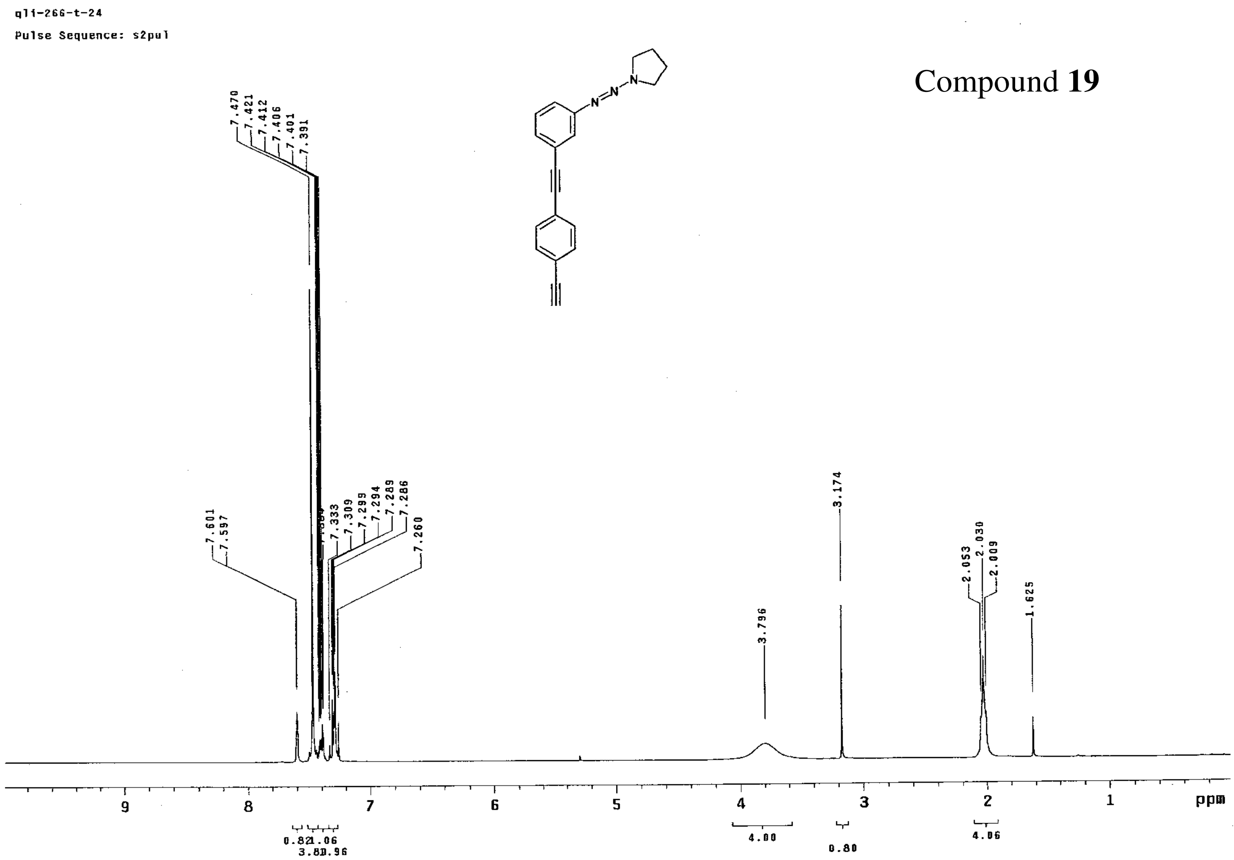
Compound **18**

Compound **18**



Compound **18**





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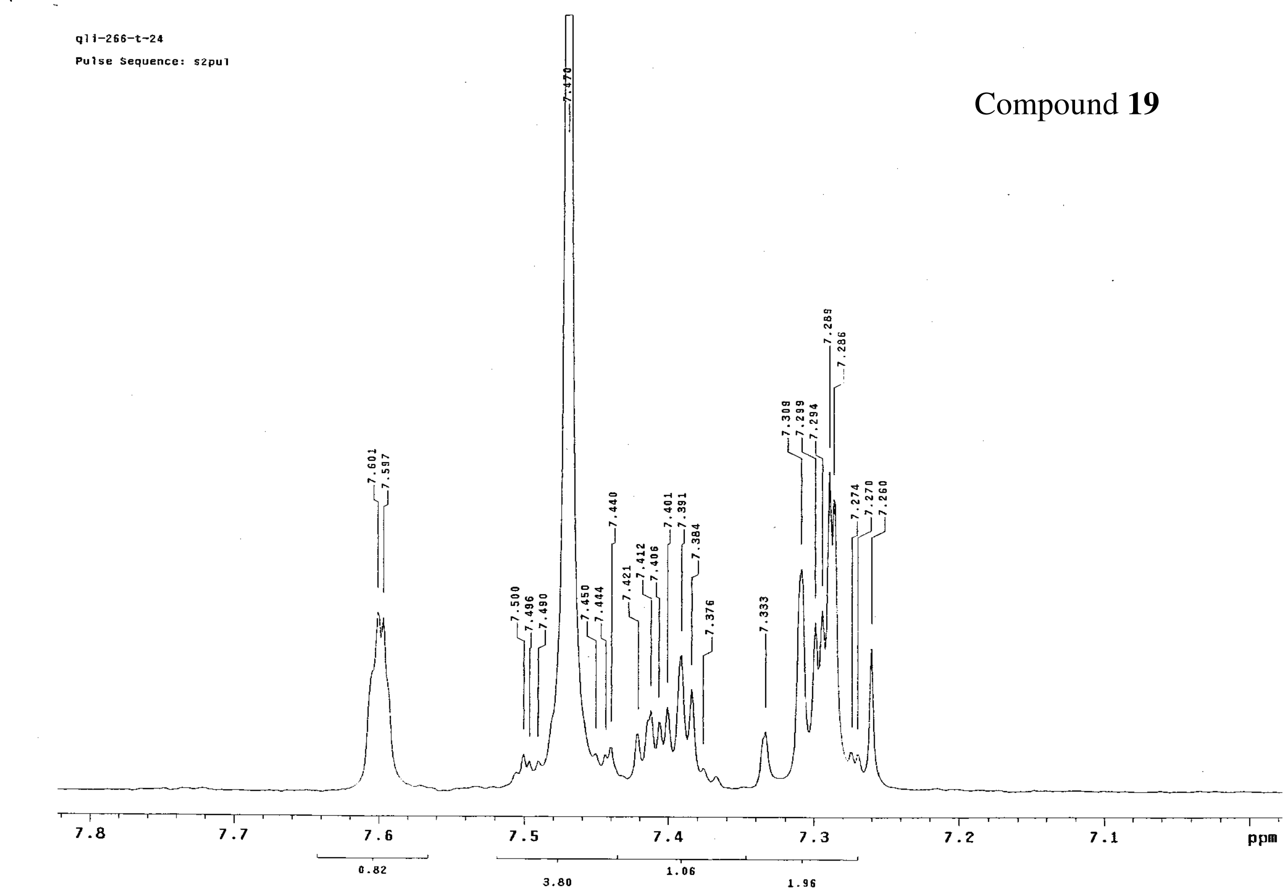
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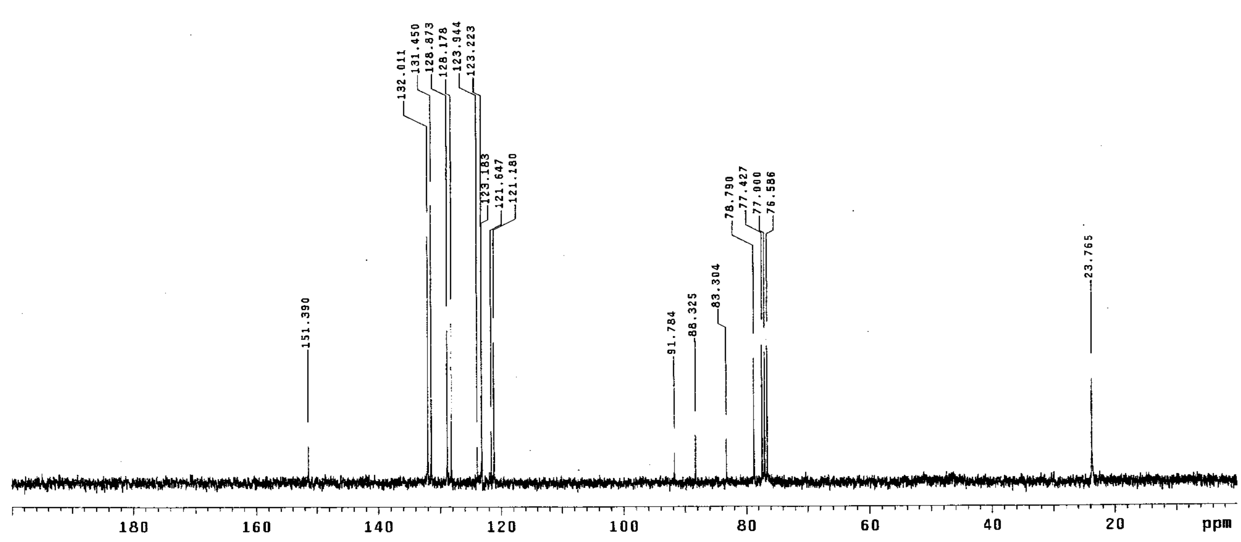
Compound 19
7.470
7.601
7.597
7.500
7.496
7.490
7.450
7.444
7.440
7.421
7.412
7.406
7.401
7.391
7.384
7.376
7.333
7.309
7.299
7.294
7.289
7.286
7.274
7.270
7.260
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
ppm
0.82
3.80
1.06
1.96


Compound 19
151.390
132.011
131.450
128.873
128.178
123.944
123.223
123.183
121.647
121.180
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88.325
83.304
78.790
77.427
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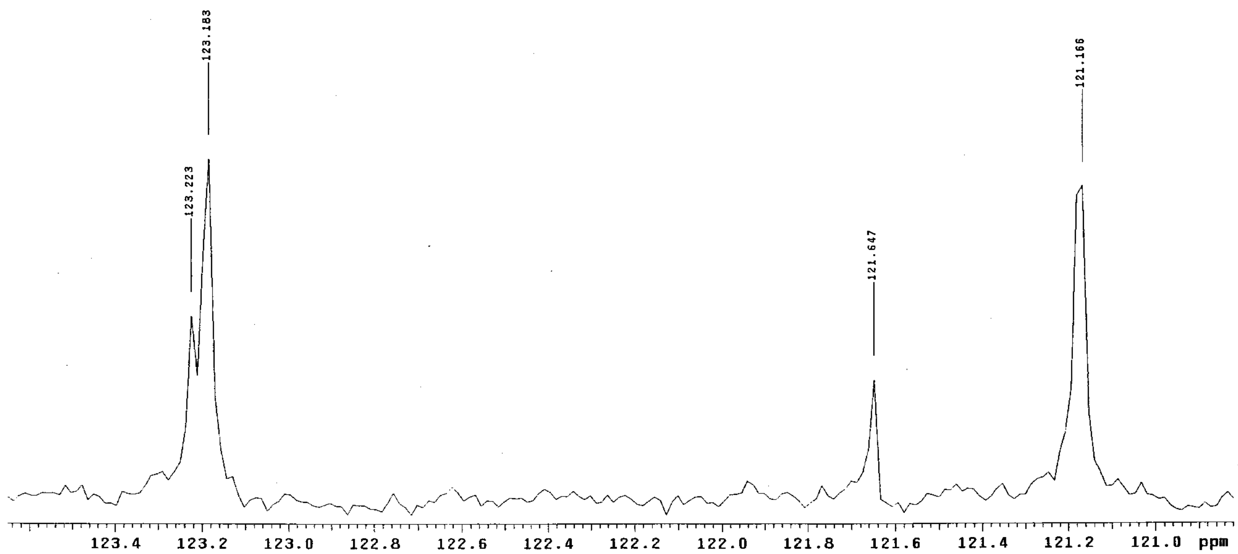
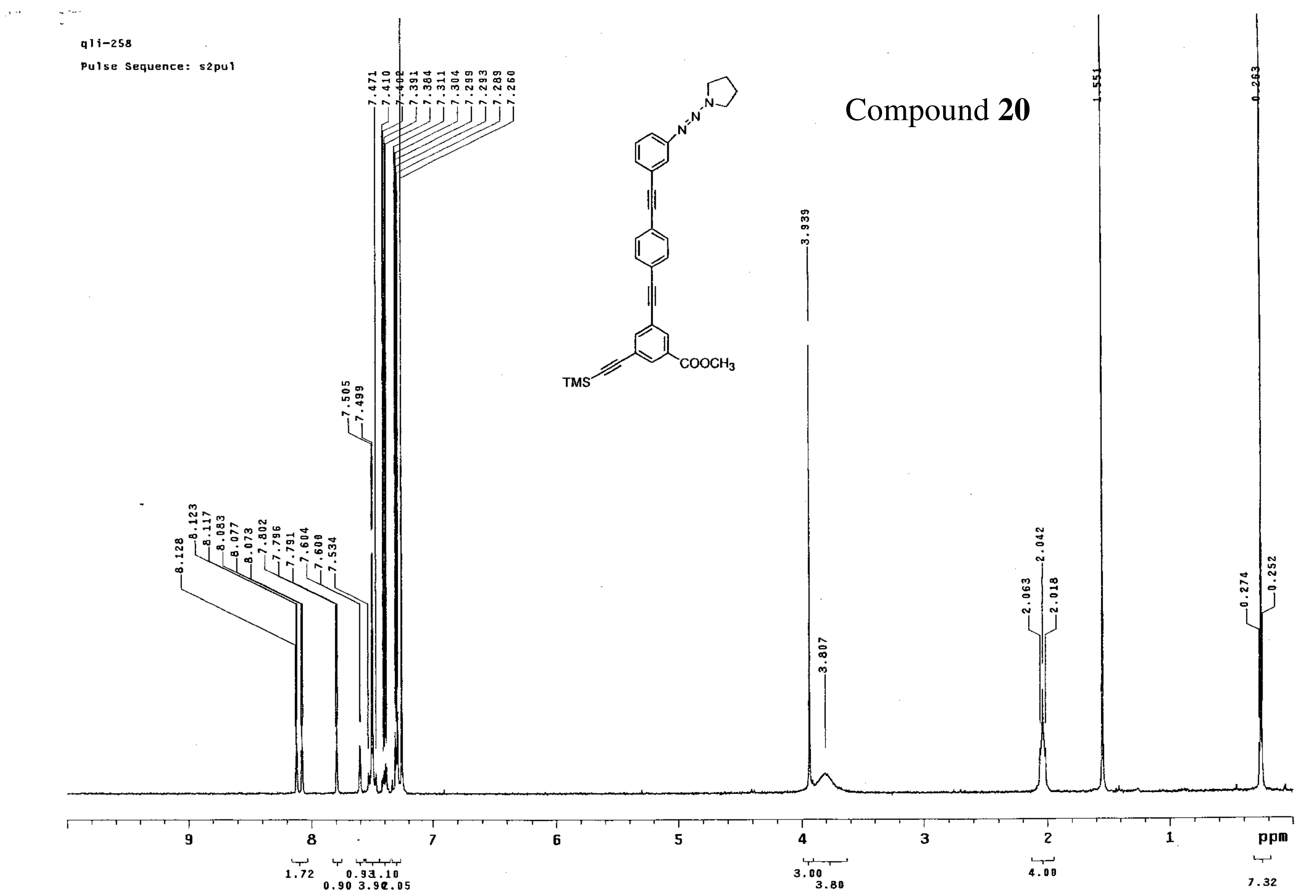
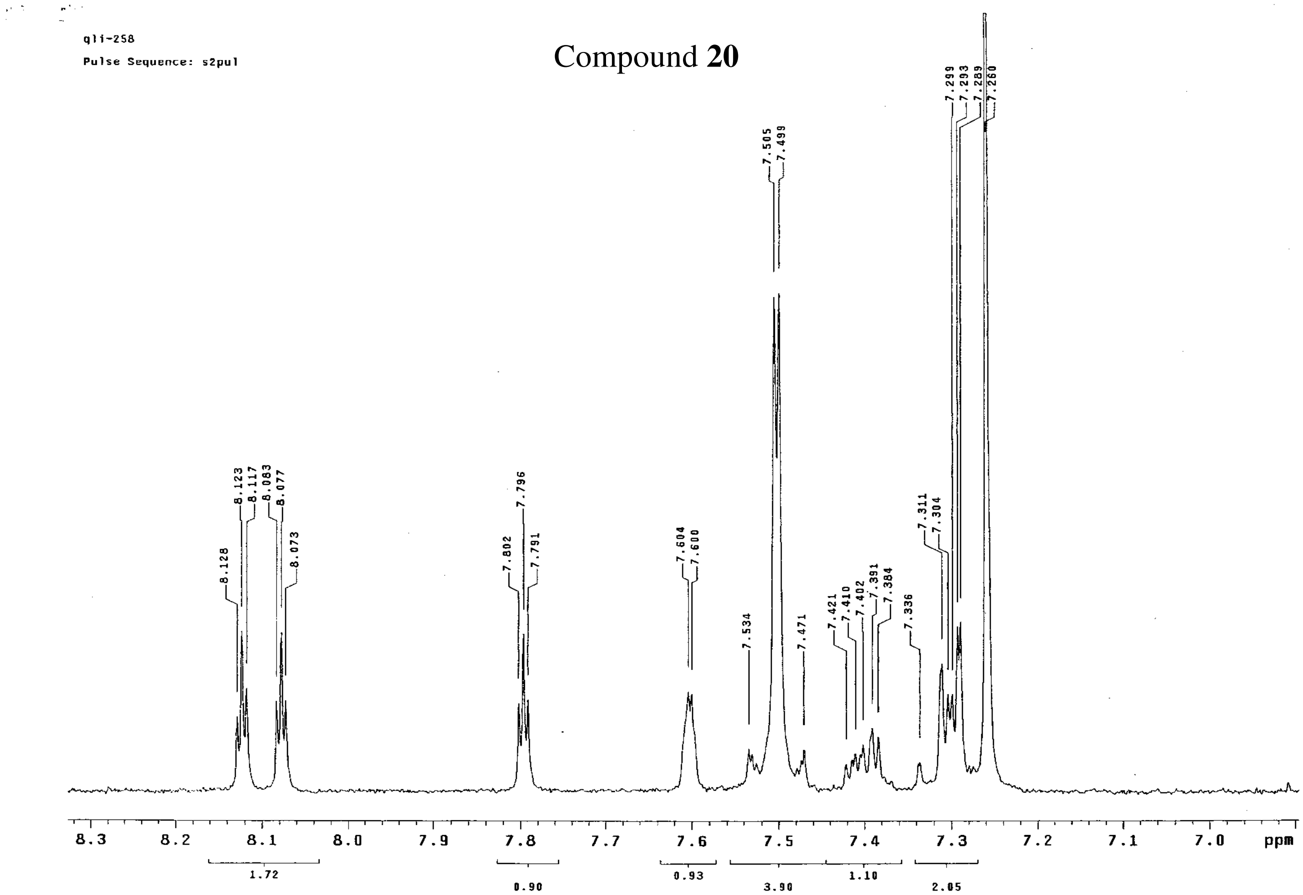
76.586
23.765
180
160
140
120
100
80
60
40
20
ppm

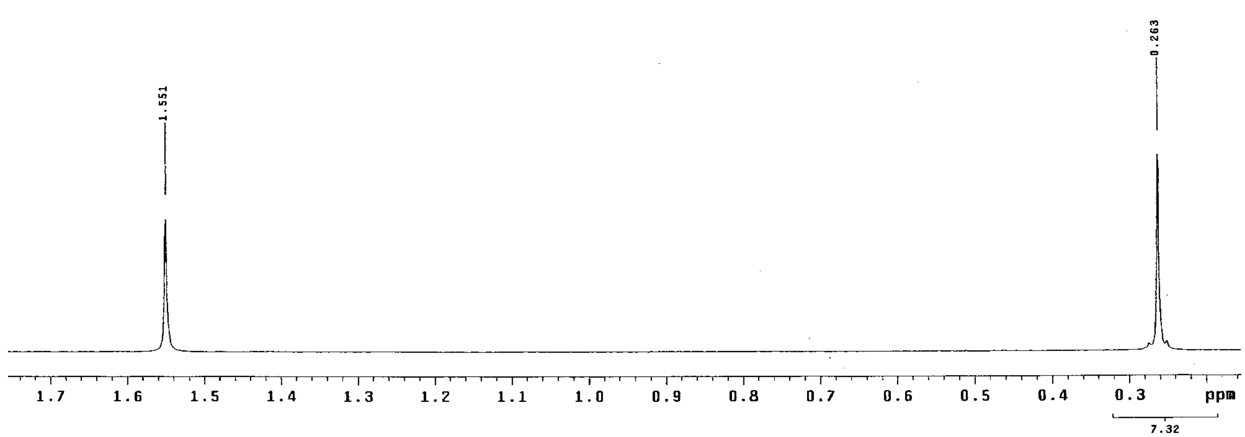
Compound **19**



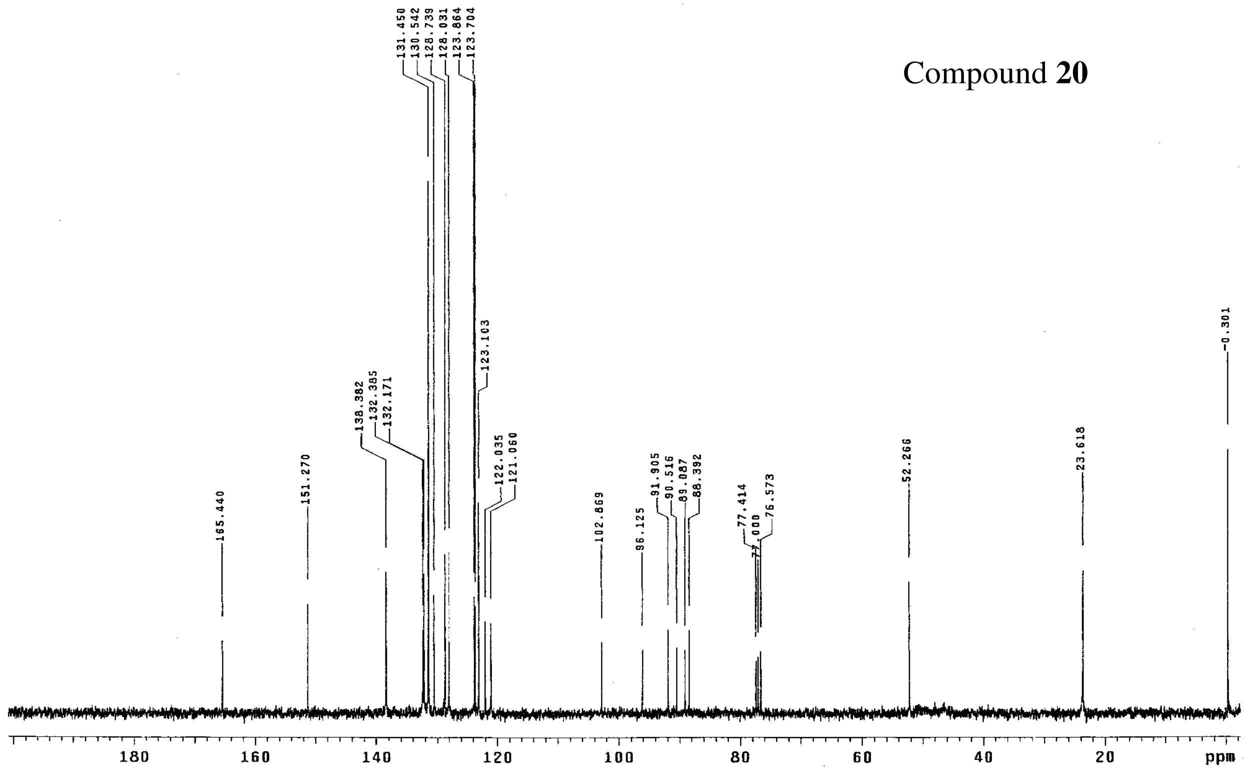




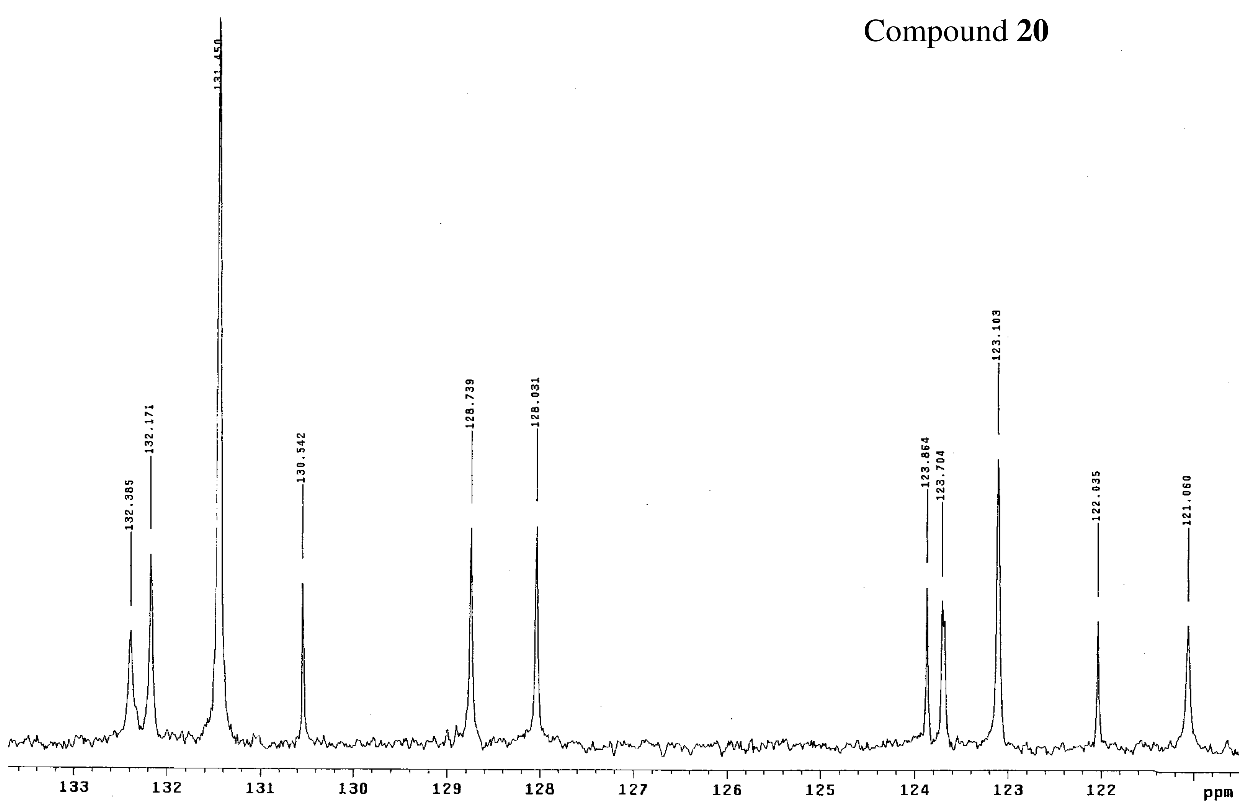
Compound **20**



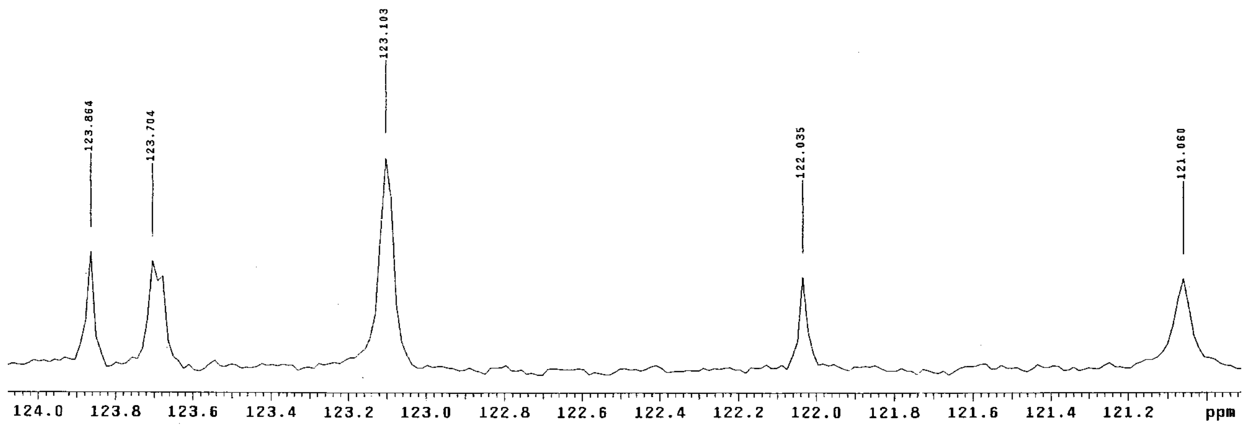
Compound **20**



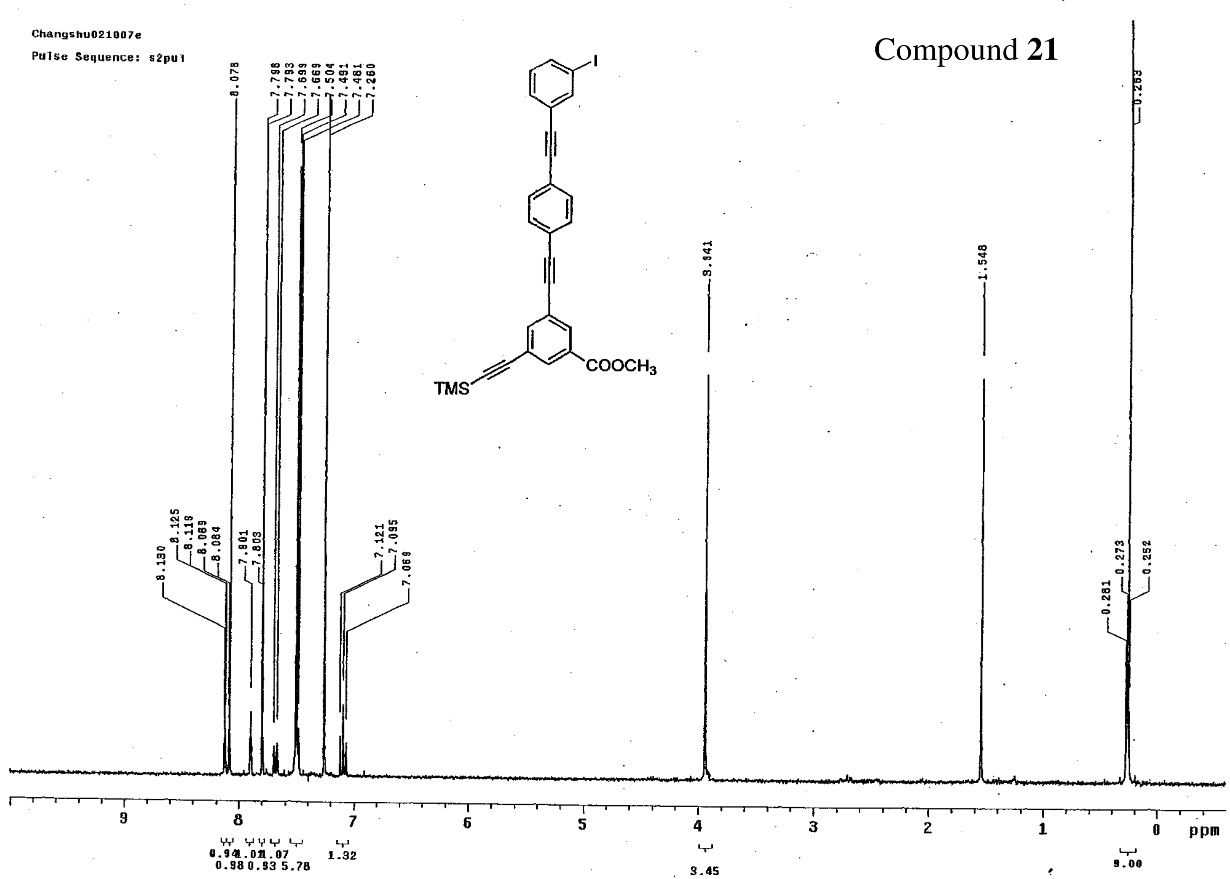
Compound **20**

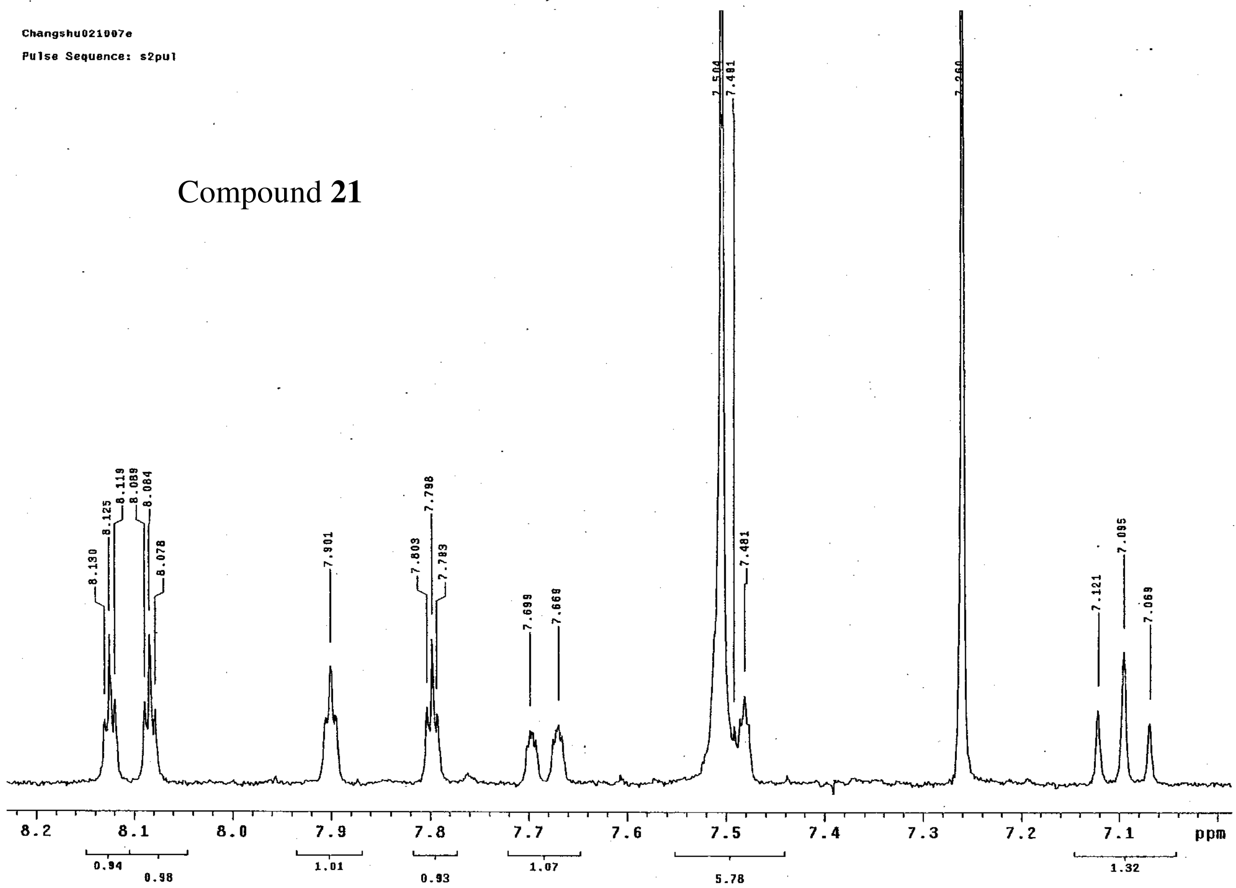


Compound **20**

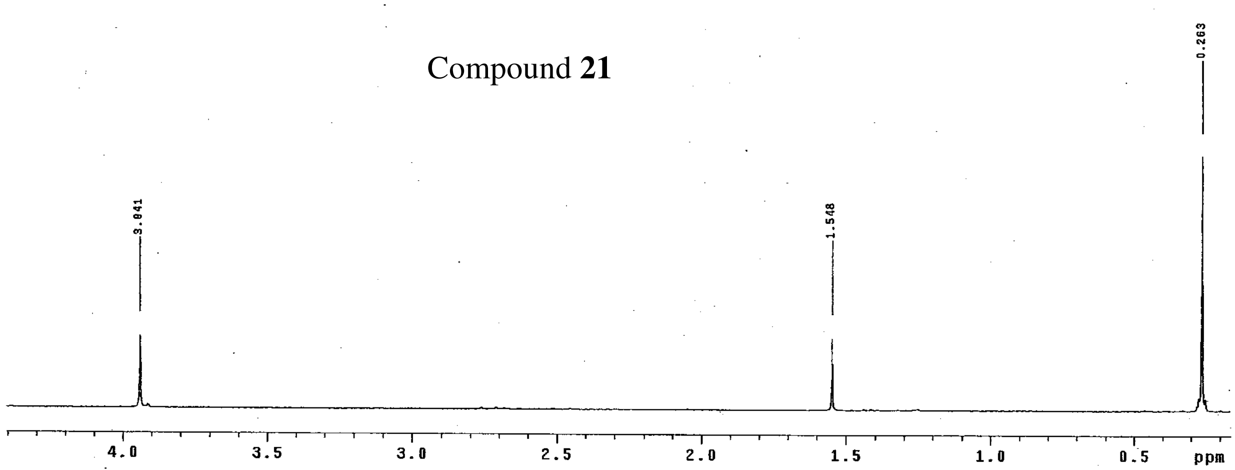


Compound **21**





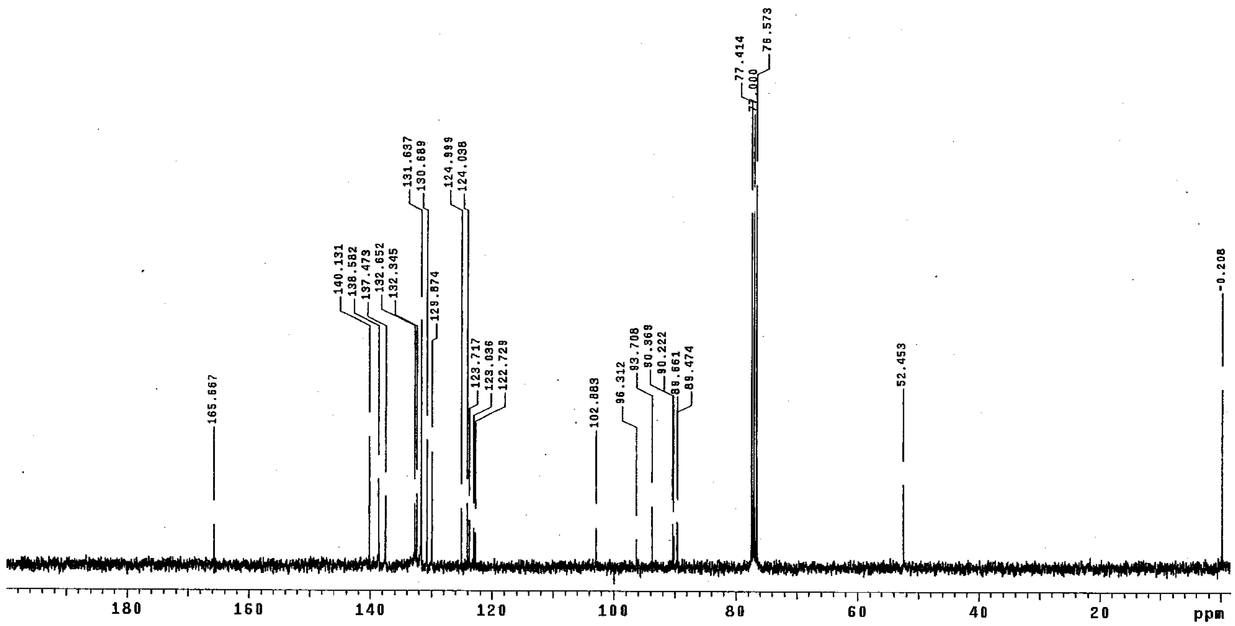
Compound **21**



Compound **21**

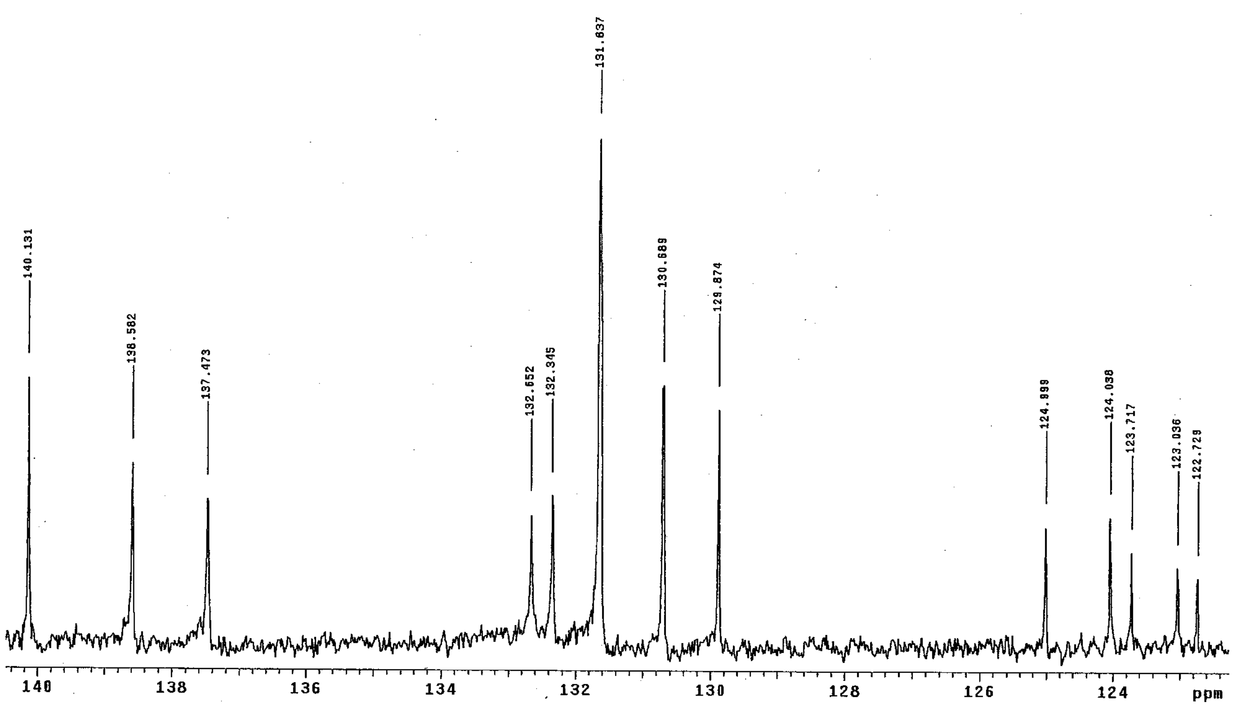
changshu021007
Pulse Sequence: s2pul

Compound **21**

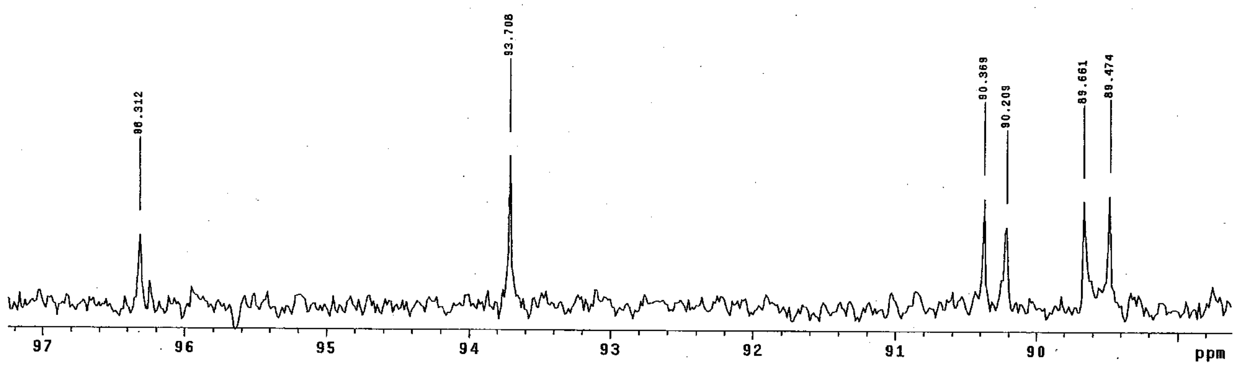


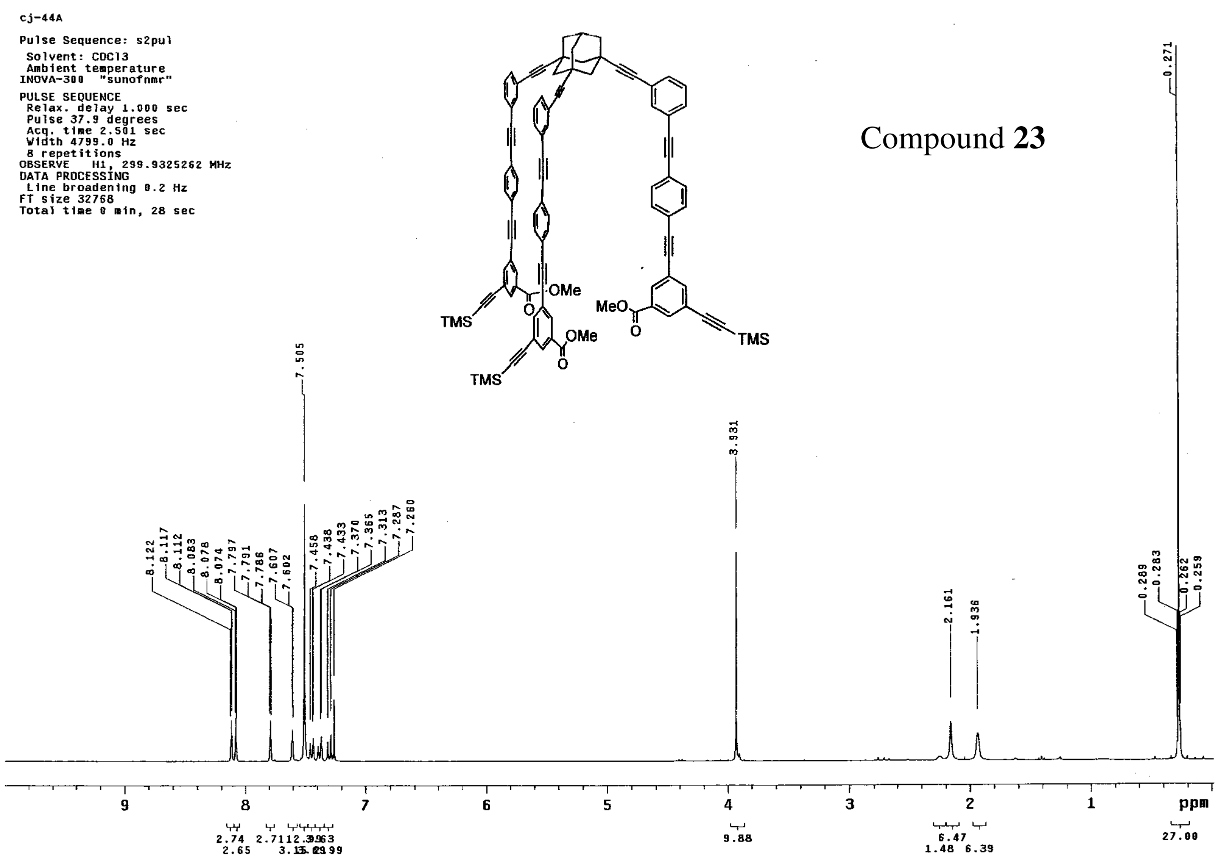
changshu021007
Pulse Sequence: s2pul

Compound **21**

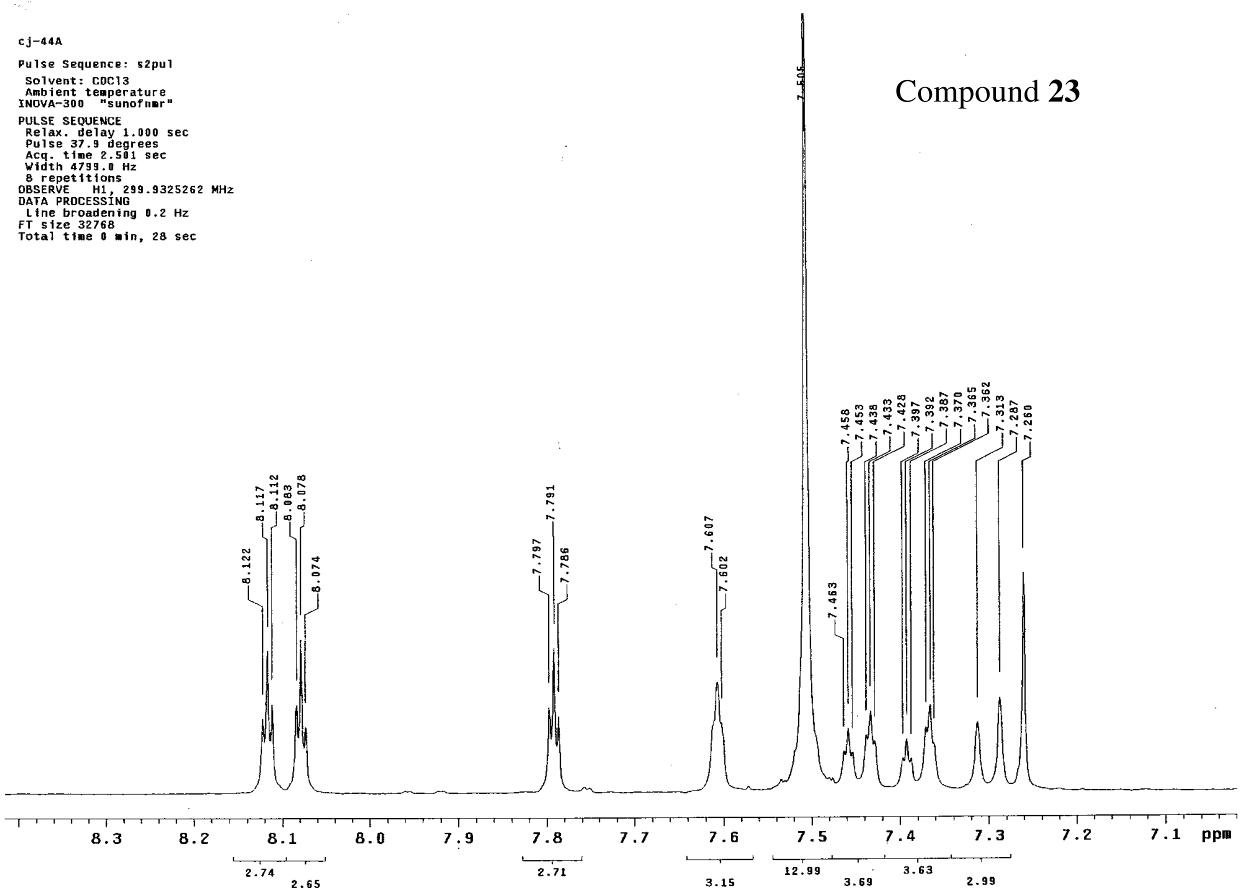


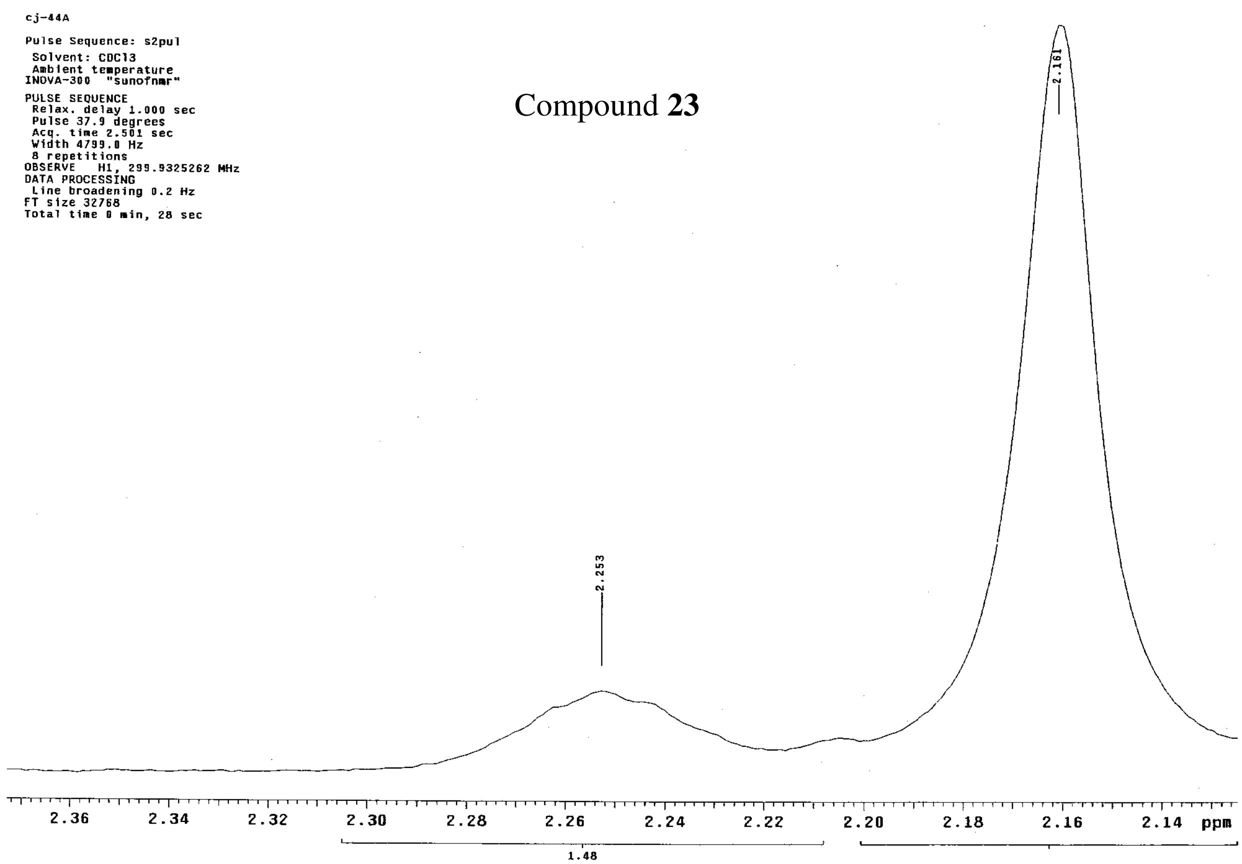
Compound **21**





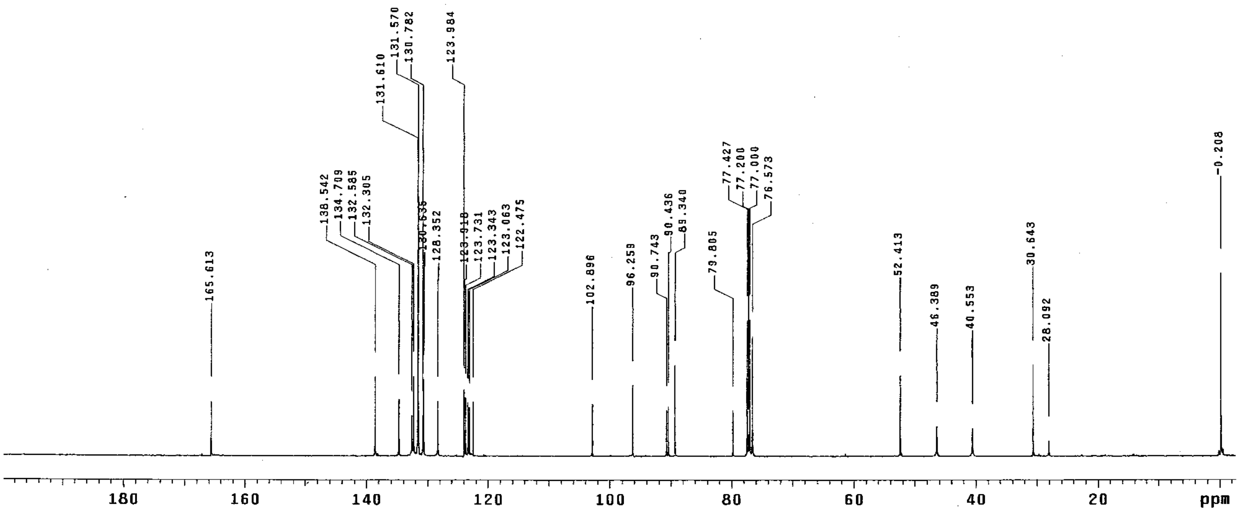
Compound **23**


cj-44A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.501 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9325262 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec
Compound 23
ppm

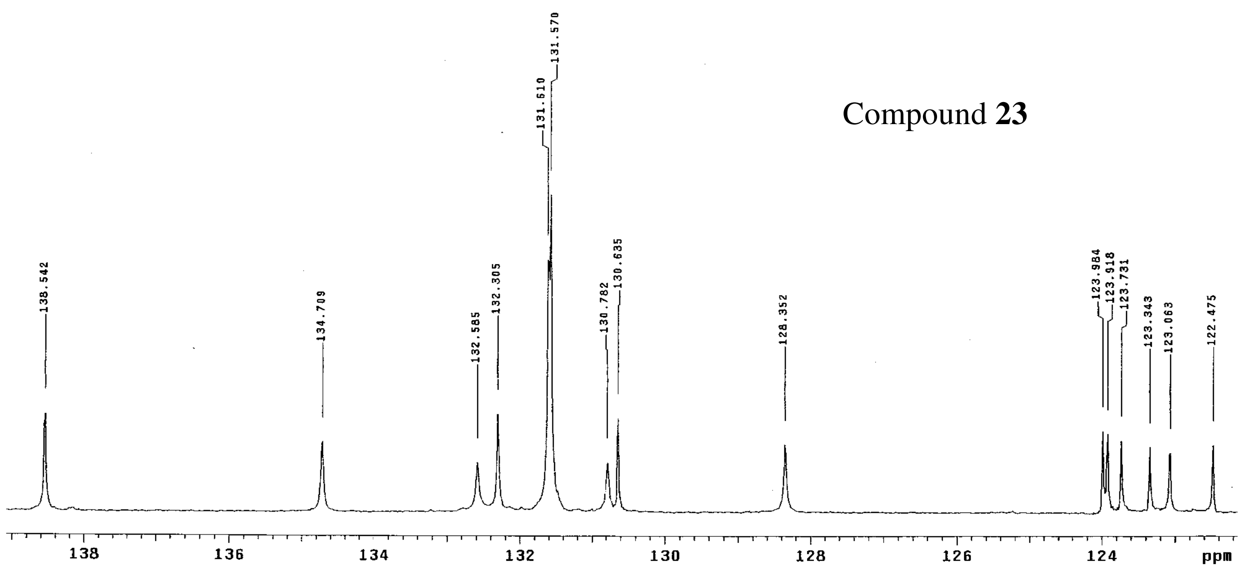

cj-44A
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.501 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9325262 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec
Compound 23
ppm

Ambient temperature
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 42.6 degrees
Acq. time 0.599 sec
Width 16501.7 Hz
28592 repetitions
OBSERVE C13, 75.4180974 MHz
DECOUPLE H1, 299.9335198 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 14 hr, 44 min, 25 sec

Compound **23**



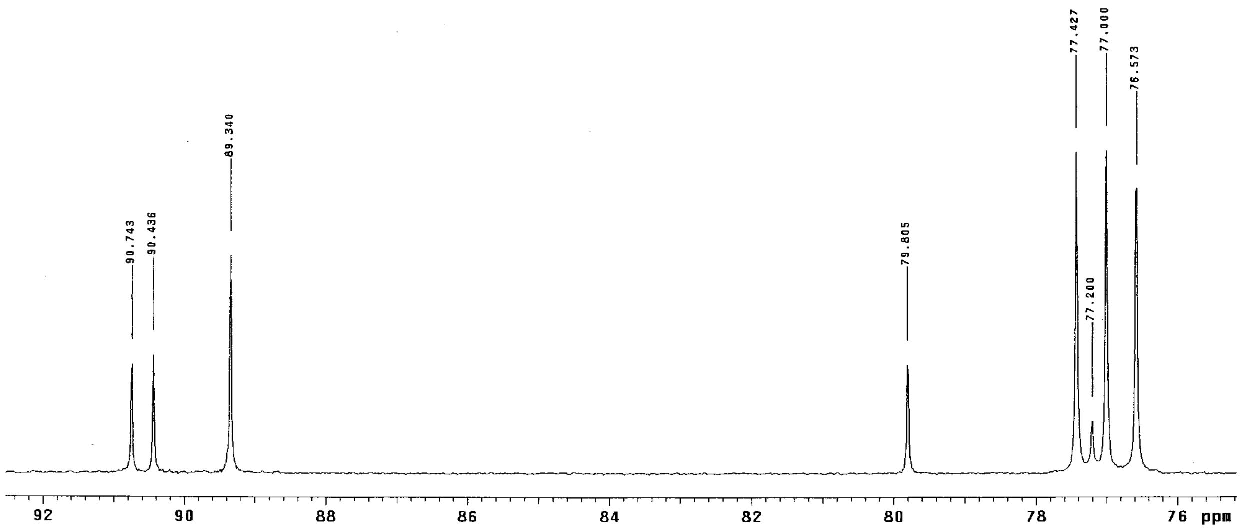
Compound **23**



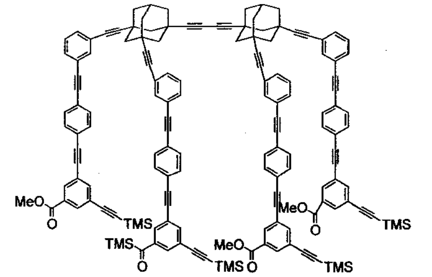
cj-44A

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 42.6 degrees
Acq. time 0.599 sec
Width 16501.7 Hz
28592 repetitions
OBSERVE C13, 75.4180974 MHz
DECOUPLE H1, 299.9335198 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 14 hr, 44 min, 25 sec

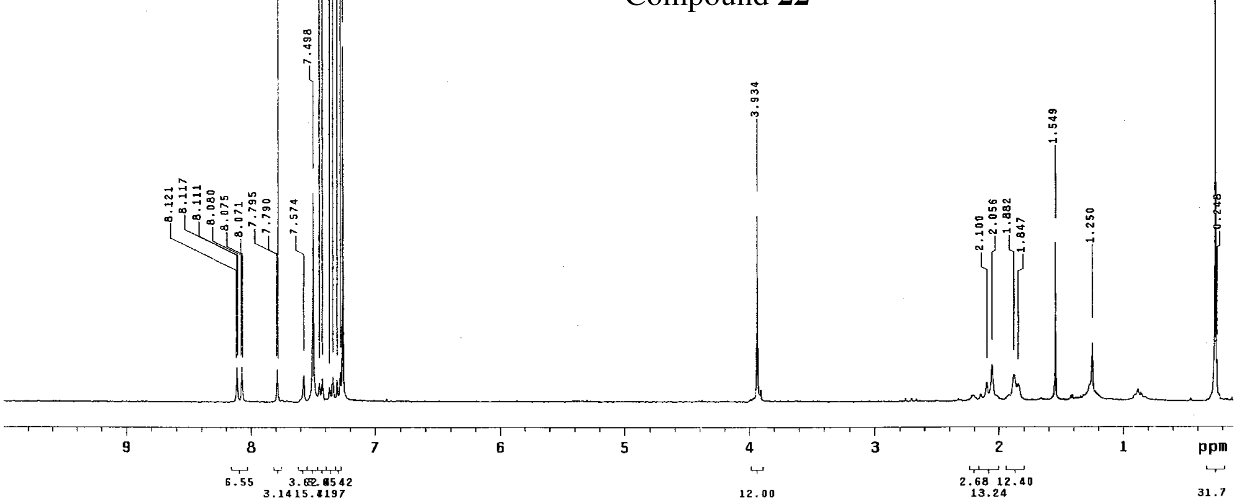
Compound **23**

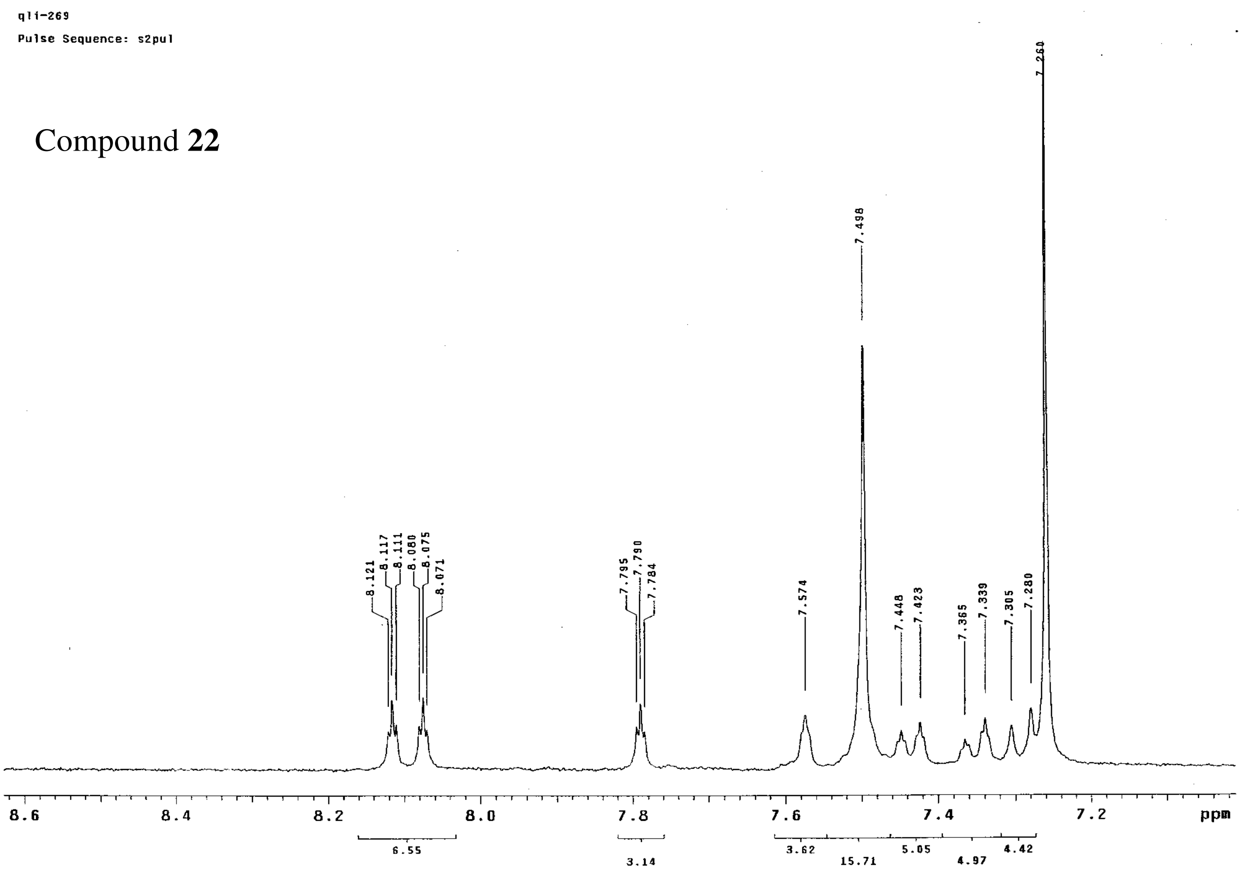


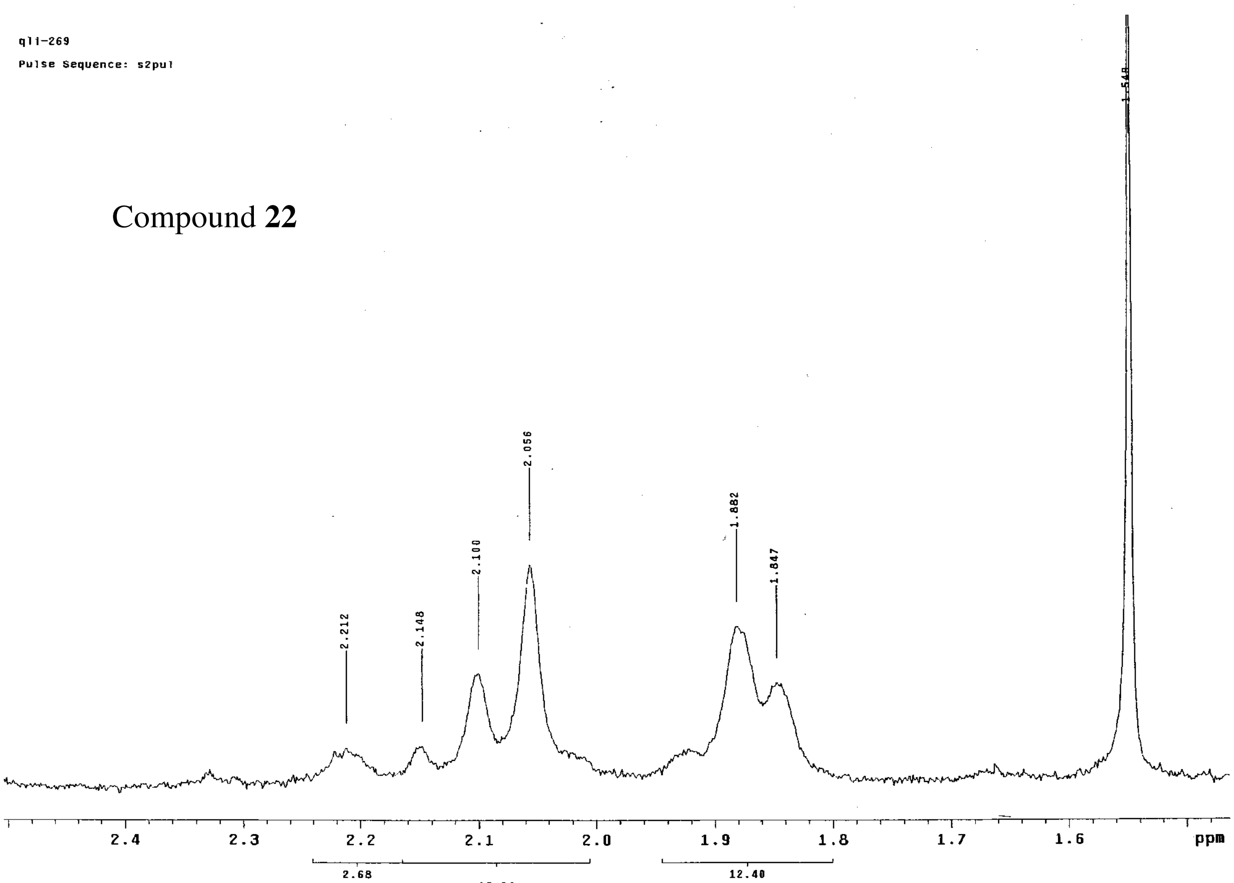
qli-269
Pulse Sequence: s2pul



Compound **22**

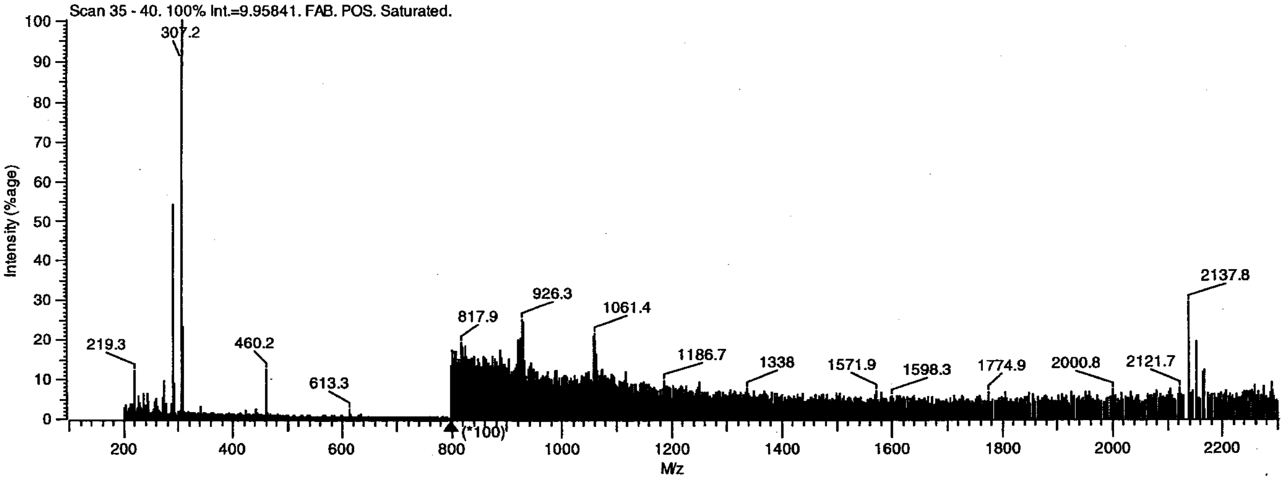



qli-269
Pulse Sequence: s2pul
Compound **22**
8.121 8.117 8.111 8.080 8.075 8.071
7.795 7.790 7.784
7.574 7.498 7.448 7.423 7.365 7.339 7.305 7.280 7.260
8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 ppm
6.55 3.14 3.62 15.71 5.05 4.97 4.42

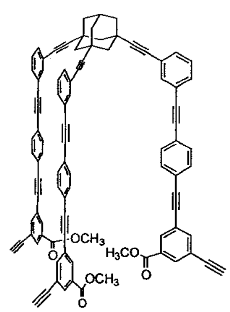

qli-269
Pulse Sequence: s2pul
Compound **22**
2.212 2.148 2.100 2.056 1.882 1.847 1.548
2.4 2.3 2.2 2.1 2.0 1.9 1.8 1.7 1.6 ppm
2.68 13.24 12.40

Quan Li
Sample: Qli-269 dimer

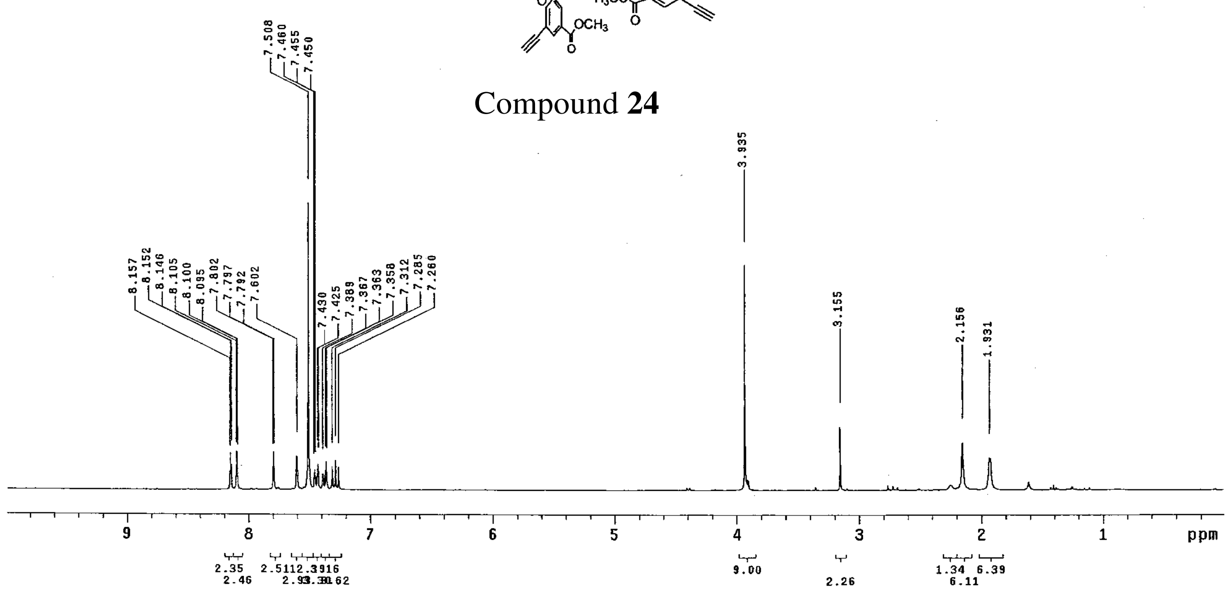
Compound **22**



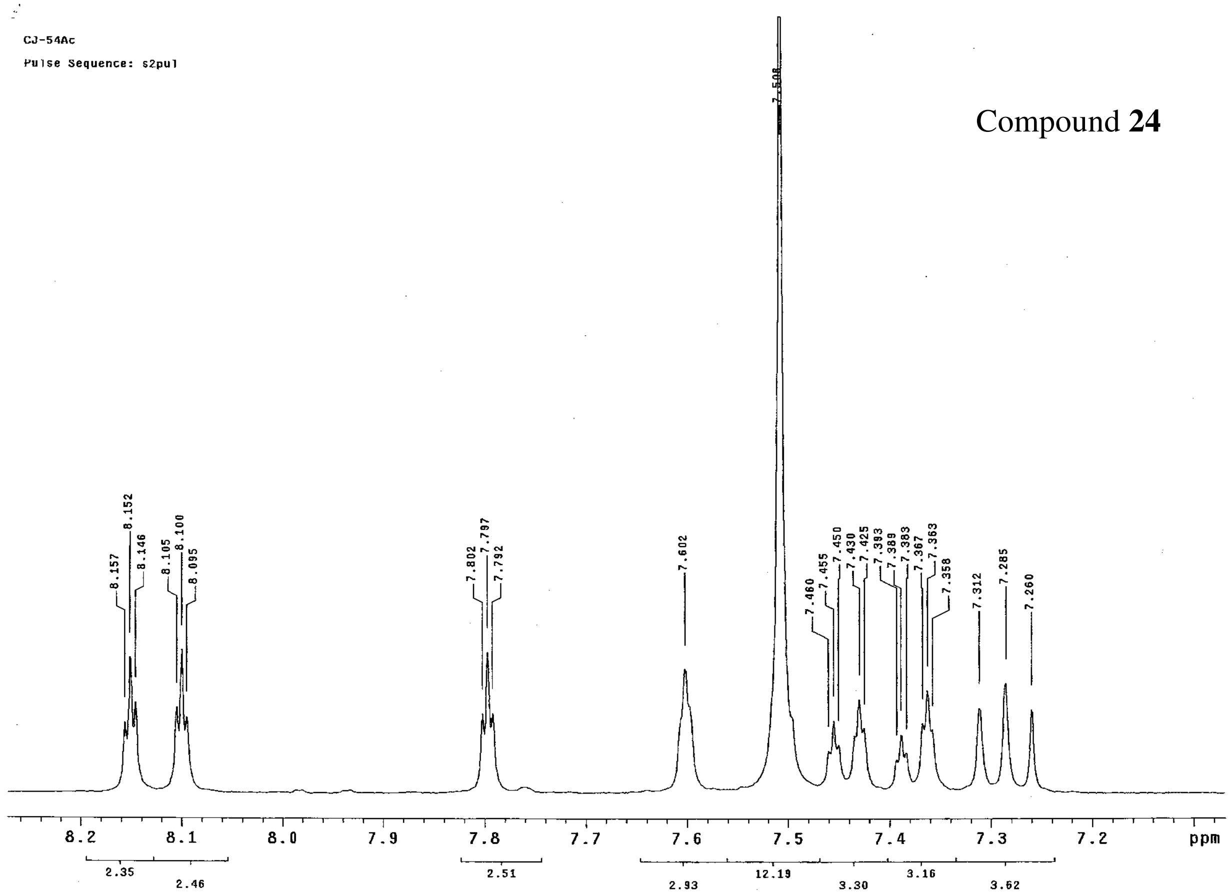
CJ-54Ac
Pulse Sequence: s2pul



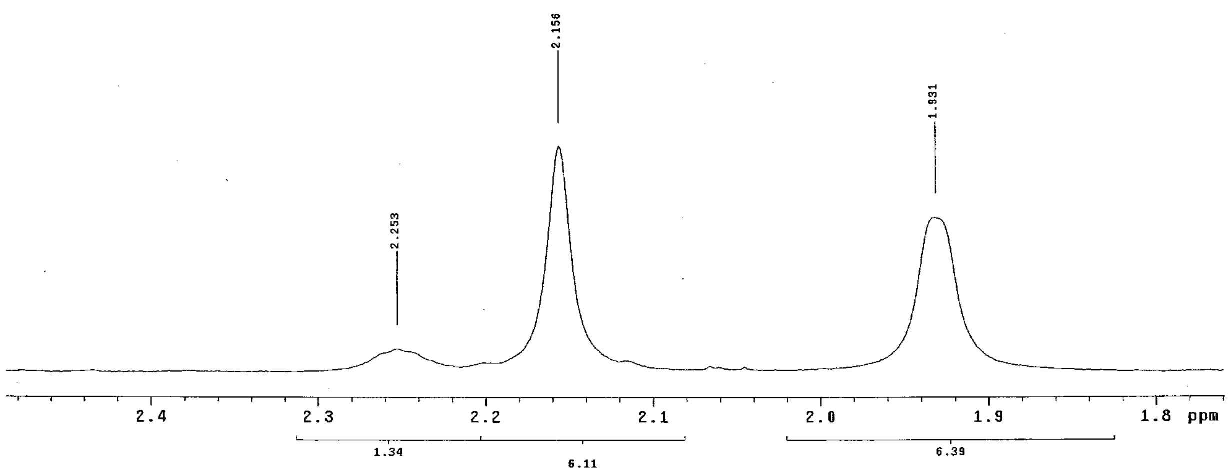
Compound **24**



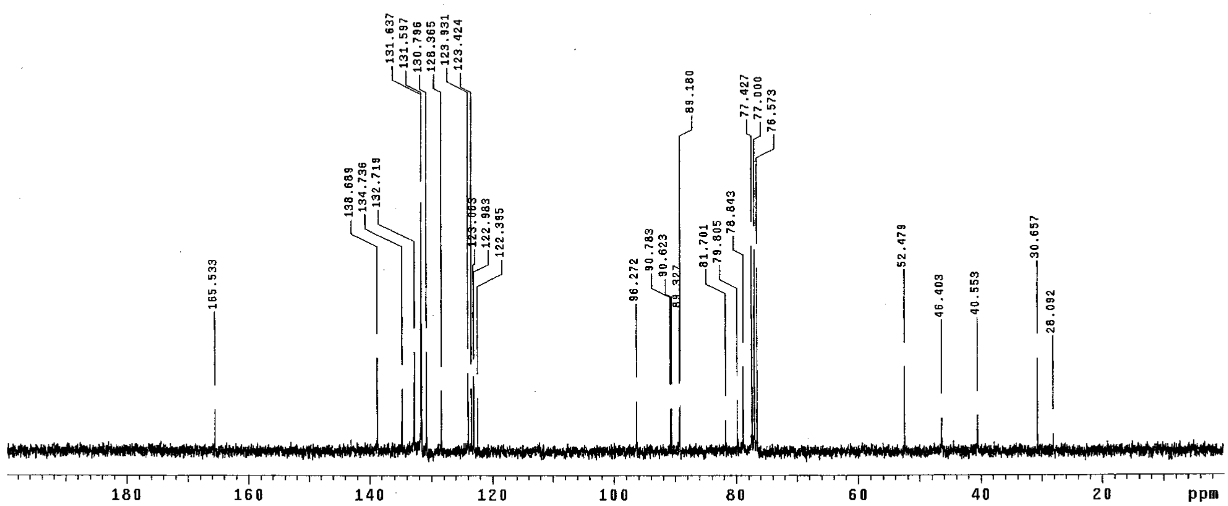
Compound **24**



Compound **24**

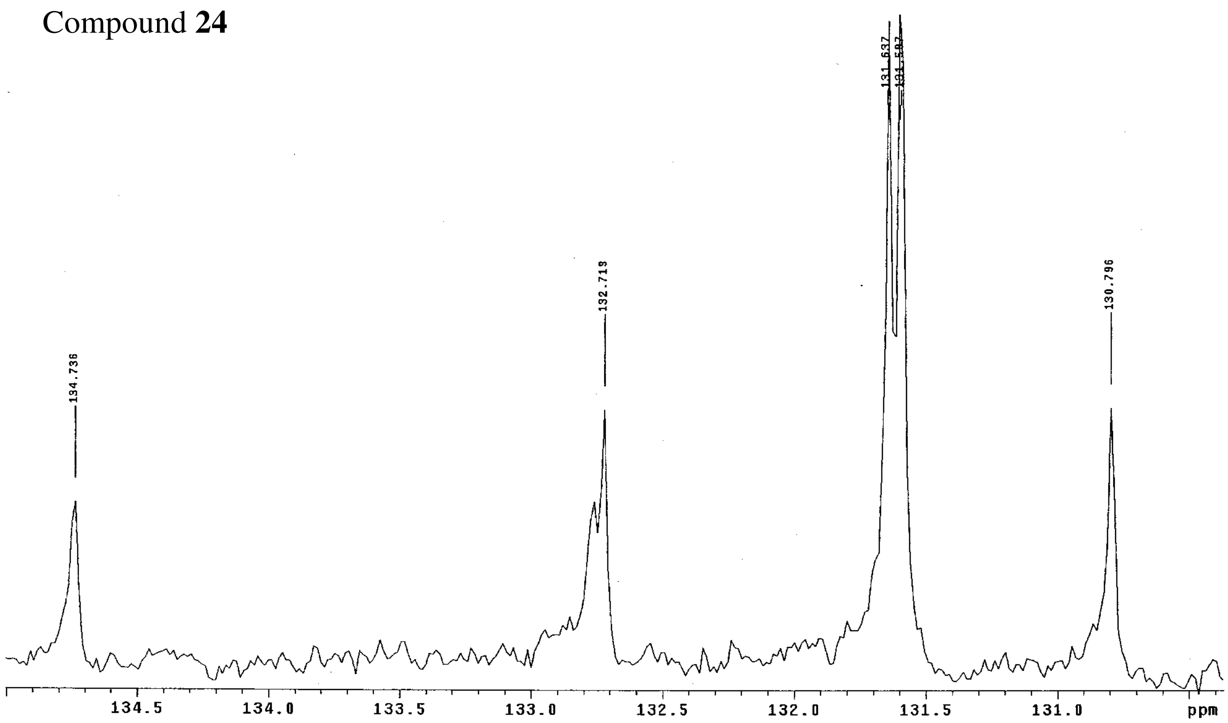


Compound **24**

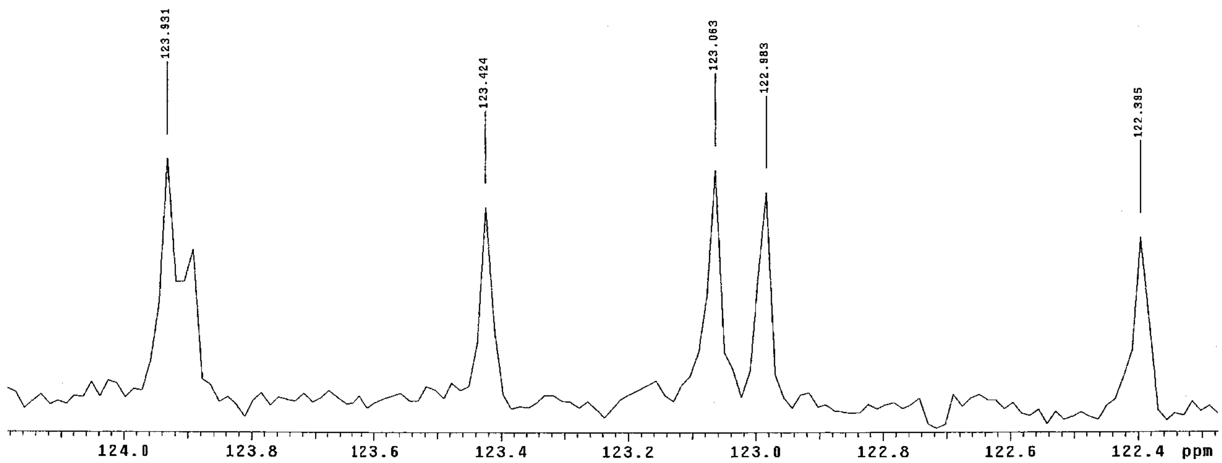


CJ-54Ac
Pulse Sequence: s2pul

Compound **24**

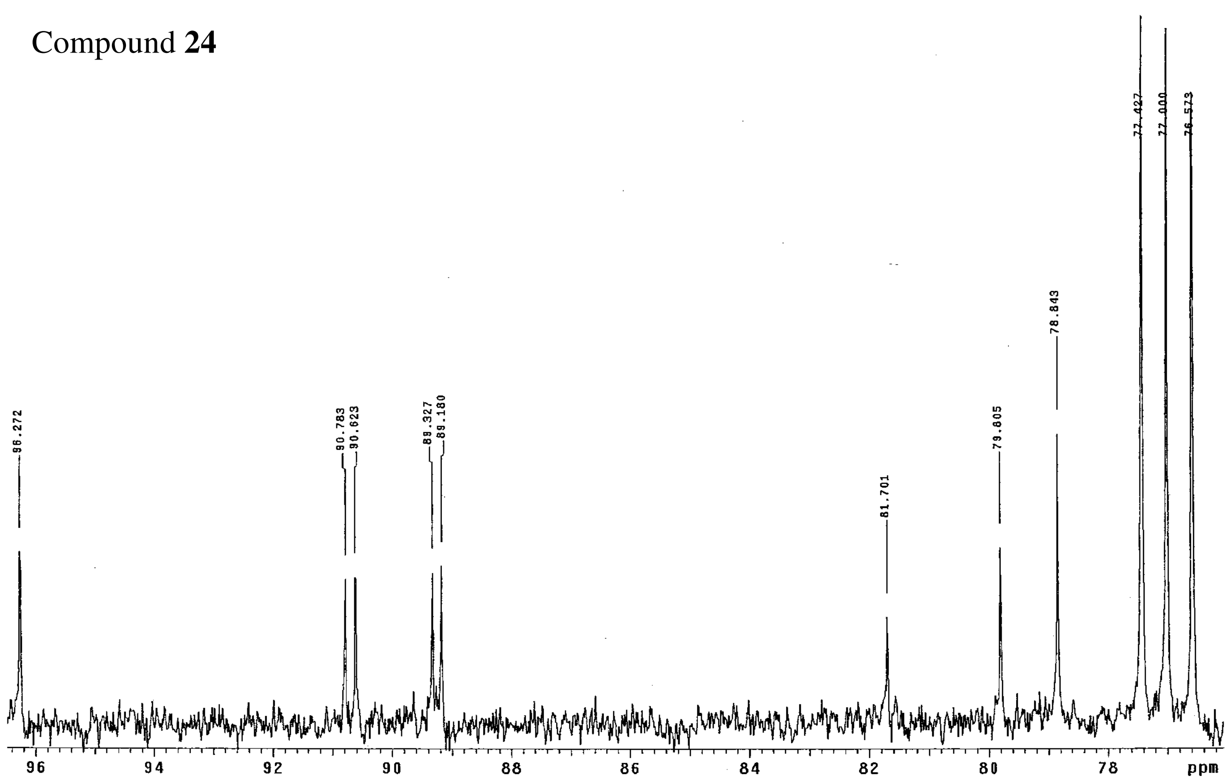


Compound **24**



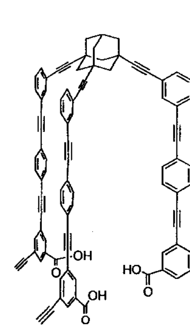
CJ-54Ac
Pulse Sequence: s2pul

Compound **24**

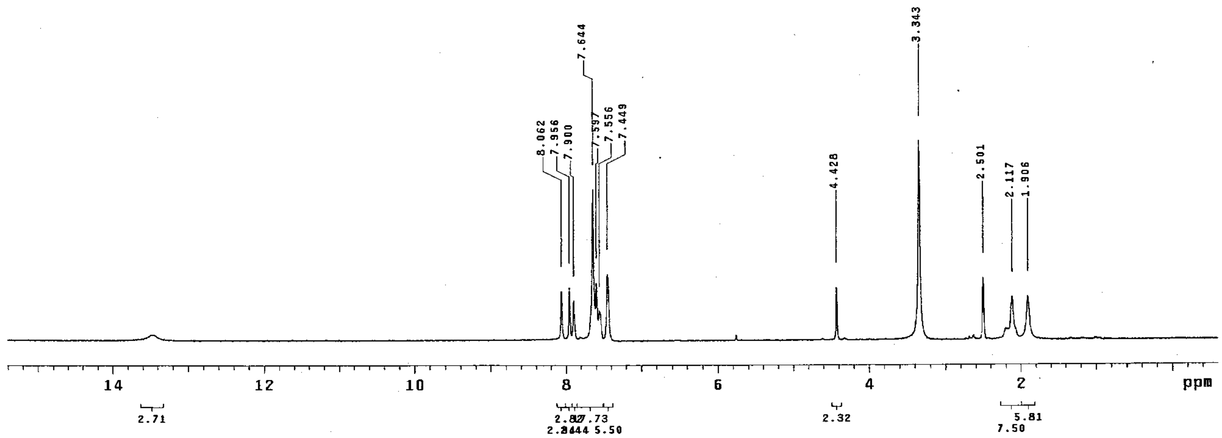


STANDARD 1H OBSERVE

Pulse Sequence: s2pul
Solvent: DMSO
Ambient temperature
File: cj-74
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.501 sec
Width 4799.0 Hz
16 repetitions
OBSERVE H1, 299.9339470 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 56 sec



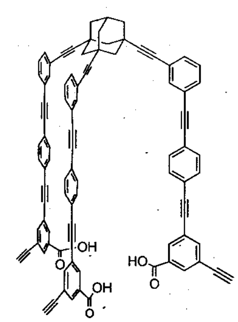
Compound **25**



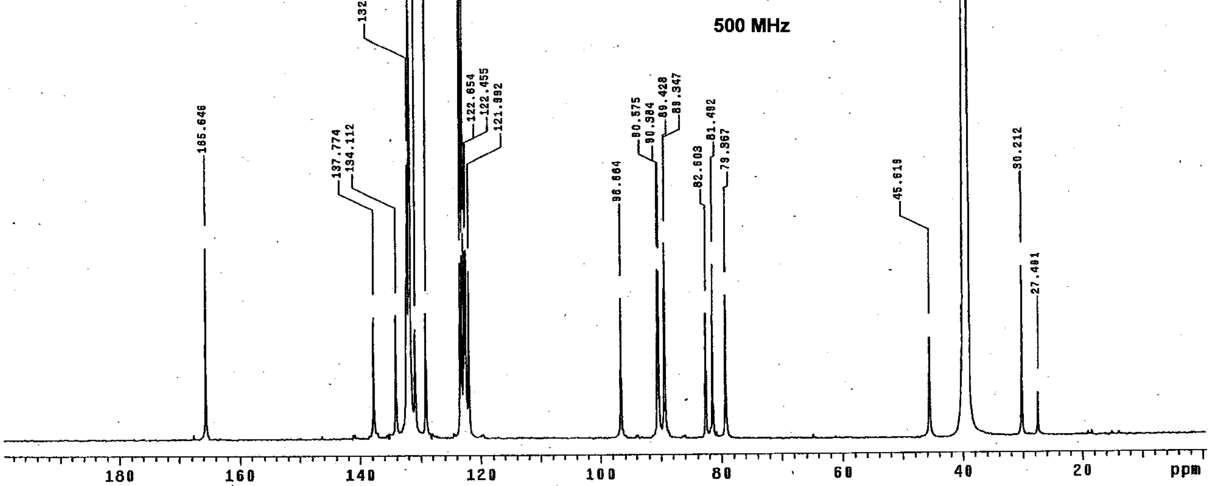
Mac-23

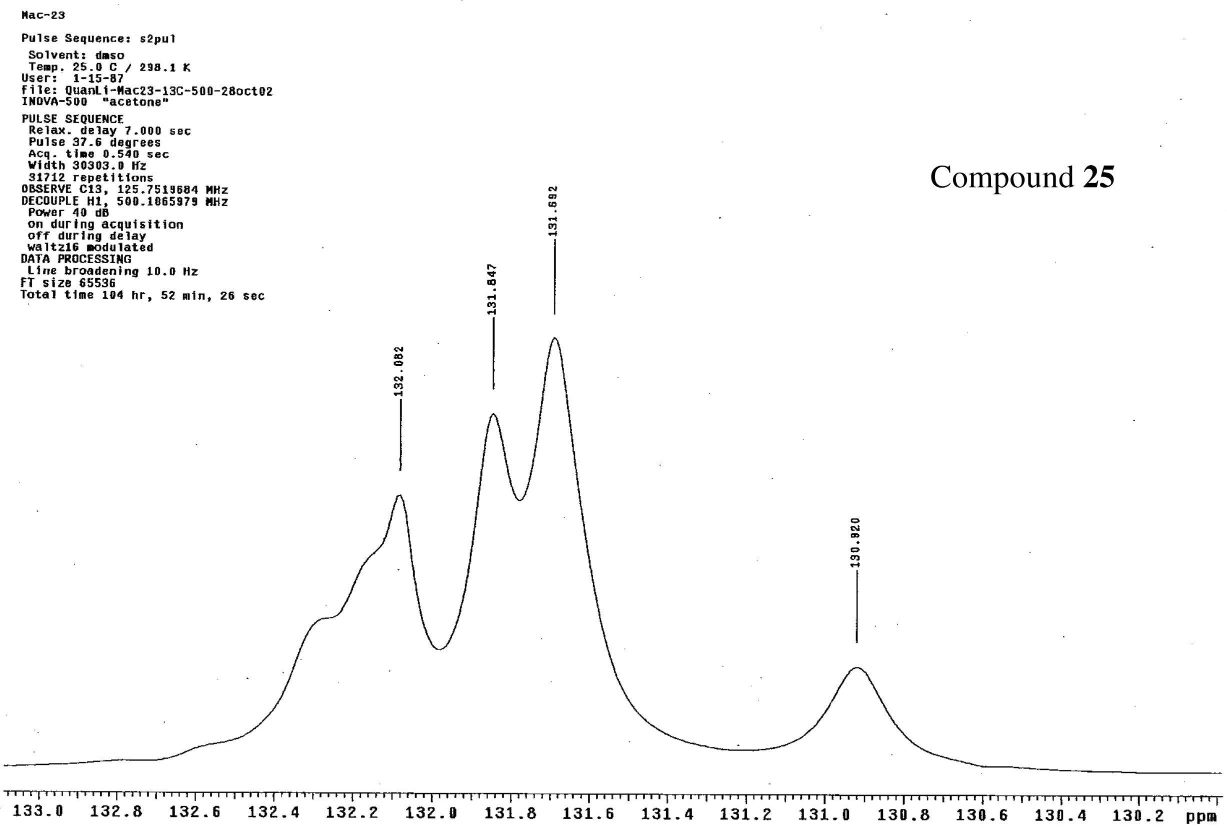
Pulse Sequence: s2pul
Solvent: dmso
Temp. 25.0 C / 298.1 K
User: 1-15-87
File: QuanLi-Mac23-13C-500-28oct02
INOVA-500 "acetone"
PULSE SEQUENCE
Relax. delay 7.000 sec
Pulse 37.6 degrees
Acq. time 0.540 sec
Width 30303.0 Hz
31712 repetitions
OBSERVE C13, 125.7519684 MHz
DECOUPLE H1, 500.1065979 MHz
Power 40 dB
on during acquisition
off during delay
waltz16 modulated
DATA PROCESSING
Line broadening 10.0 Hz
FT size 65536
Total time 104 hr, 52 min, 26 sec

Compound **25**

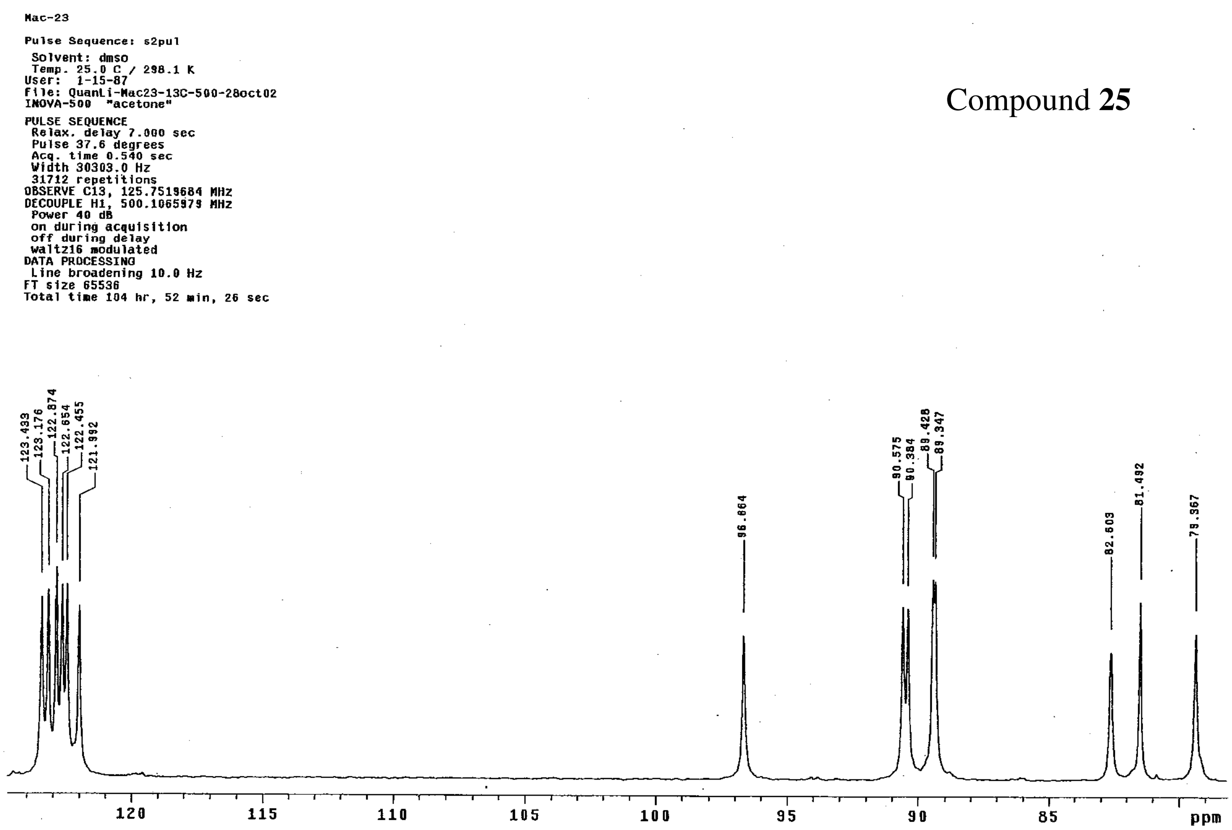


500 MHz

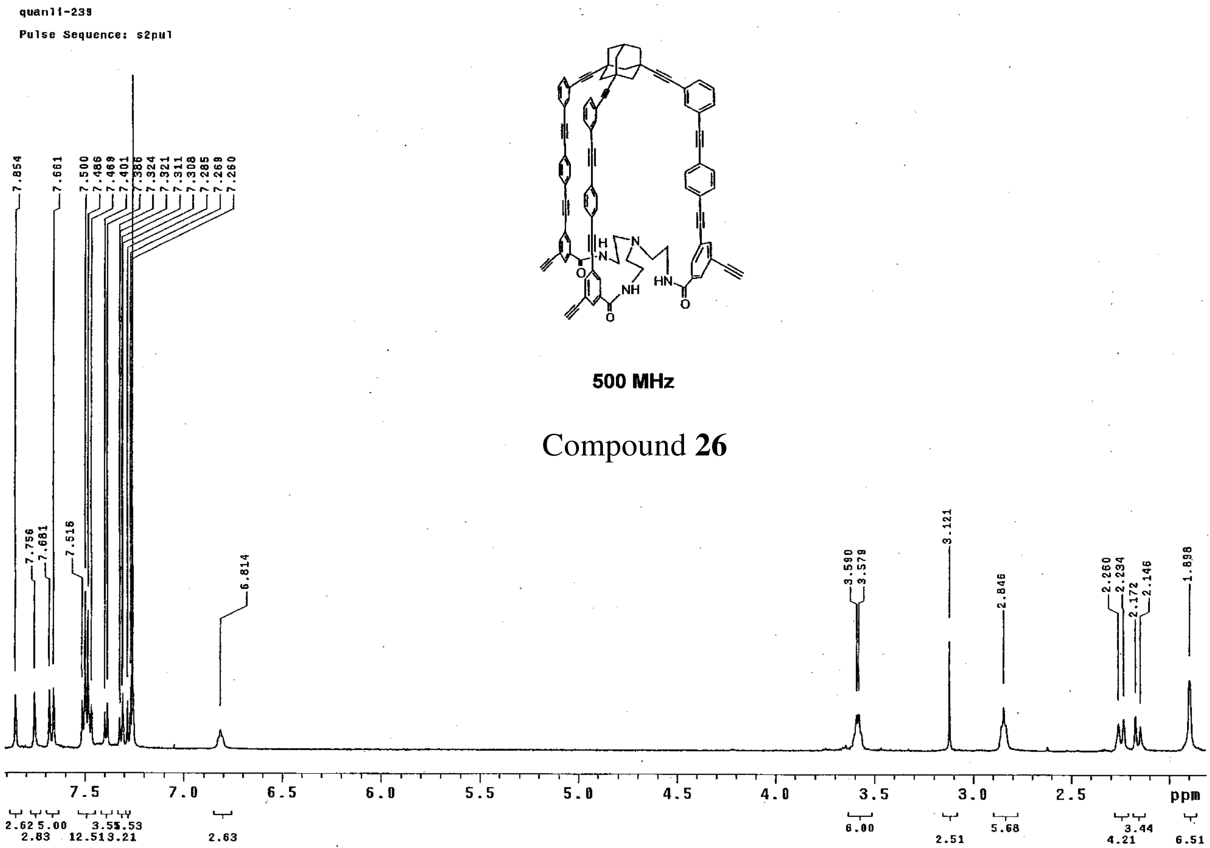




Compound **25**

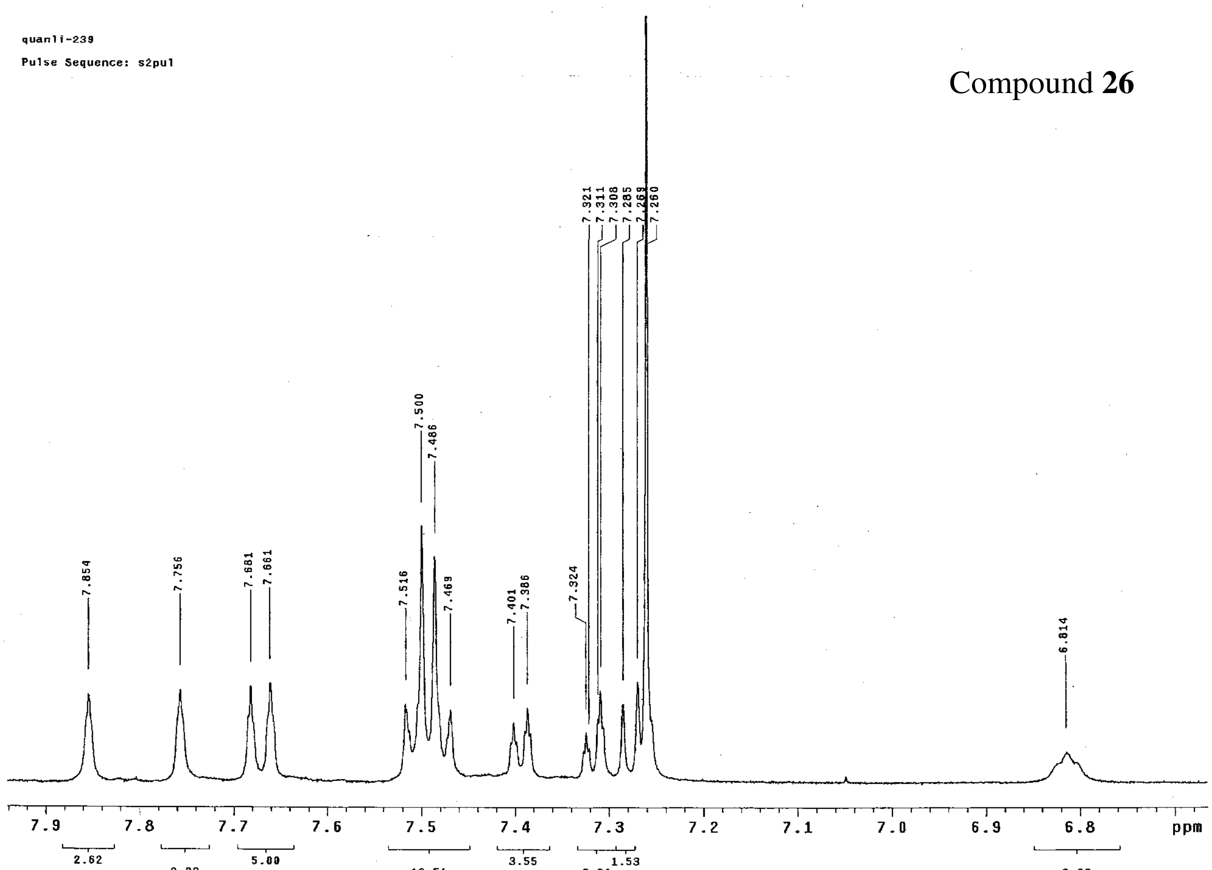


Compound **25**



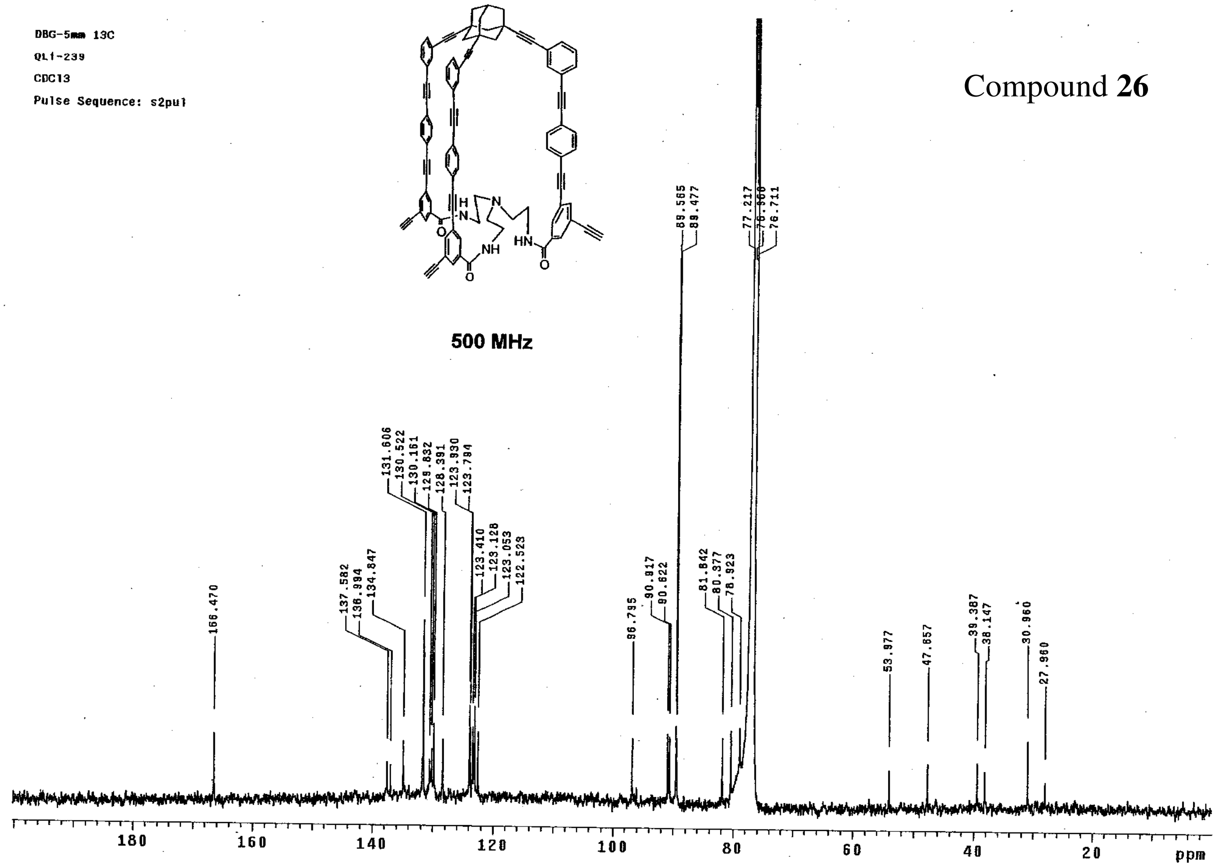
500 MHz

Compound **26**

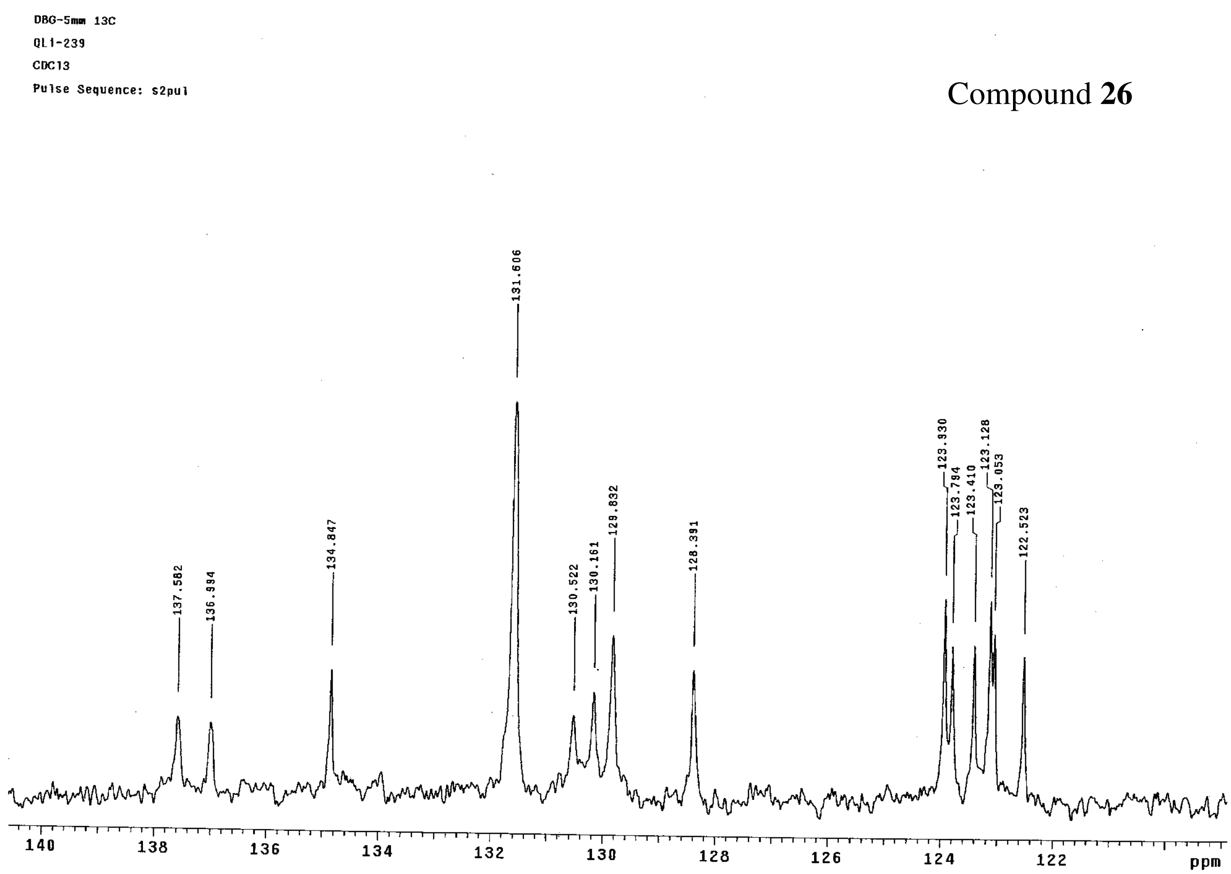


Compound **26**

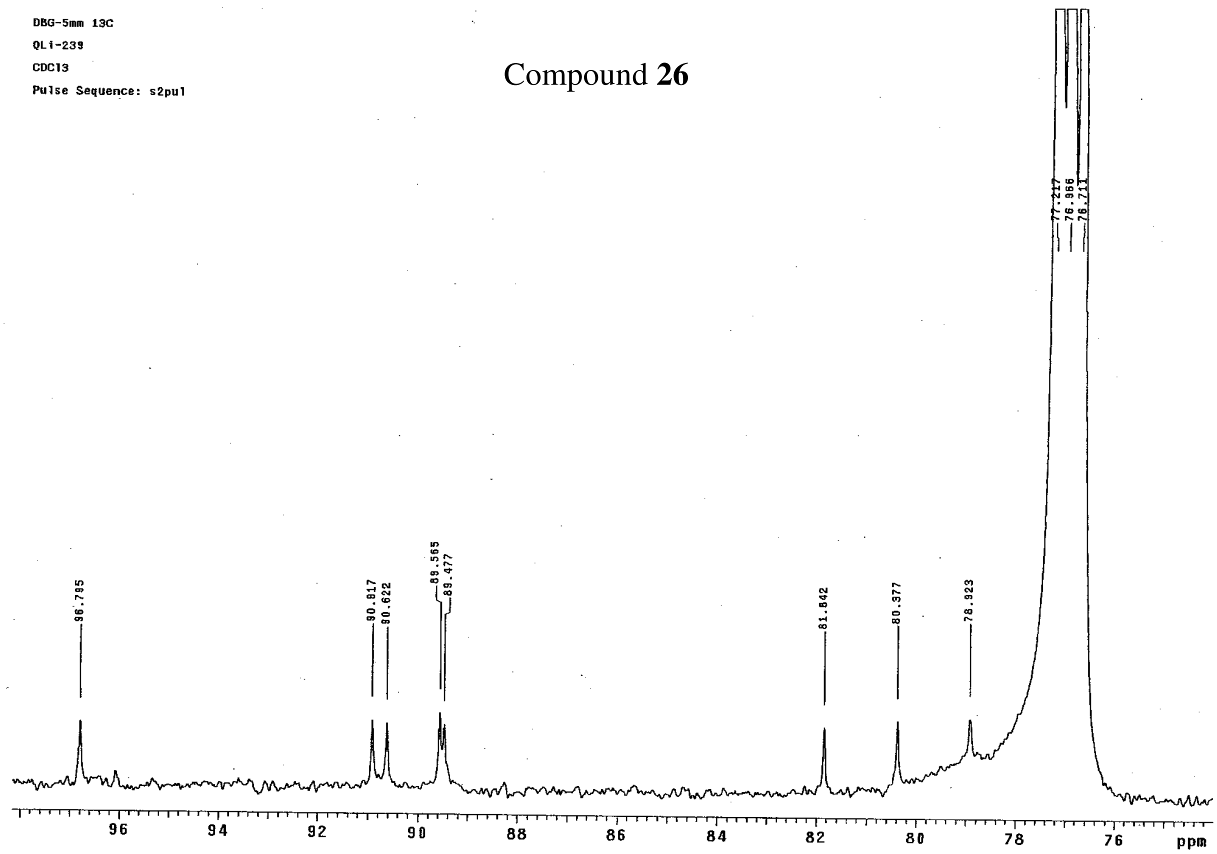
Compound **26**



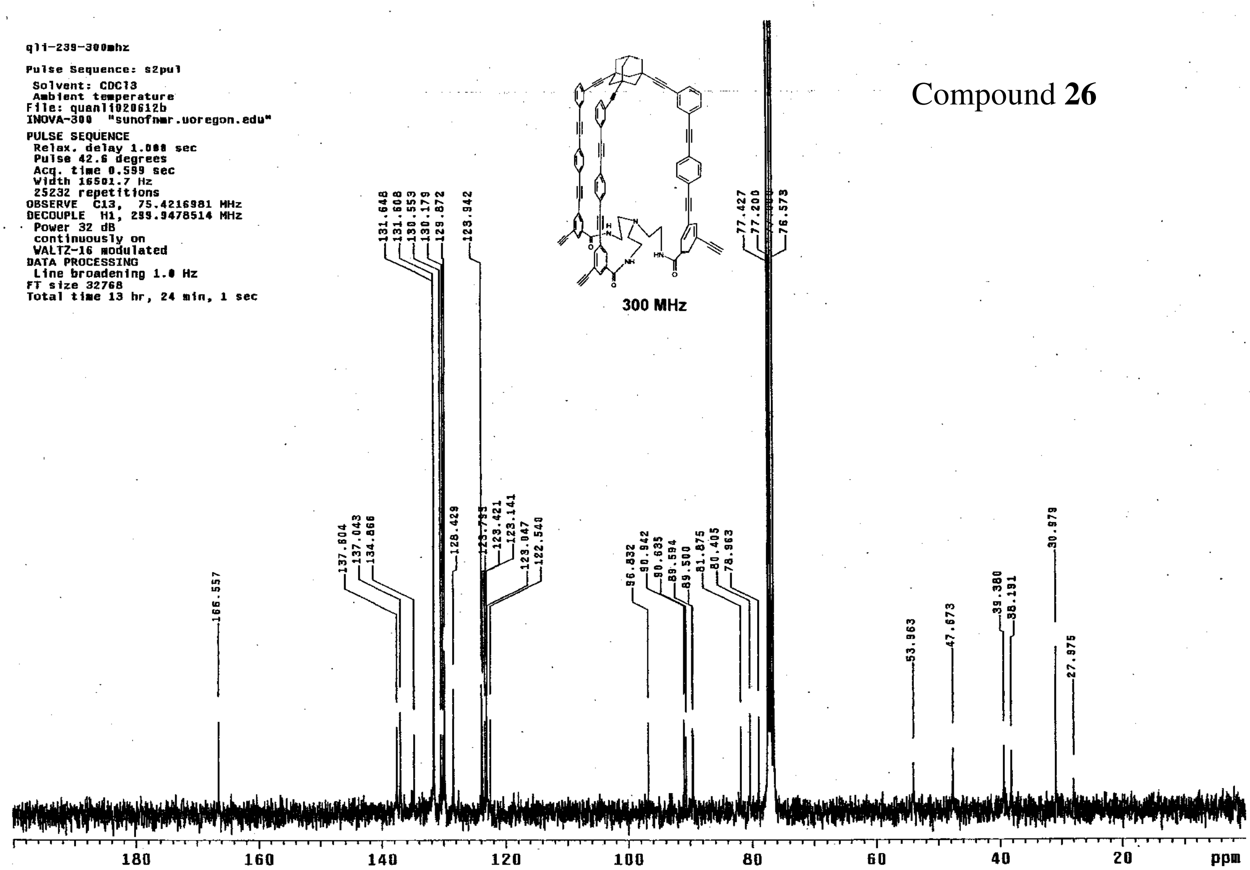
Compound **26**

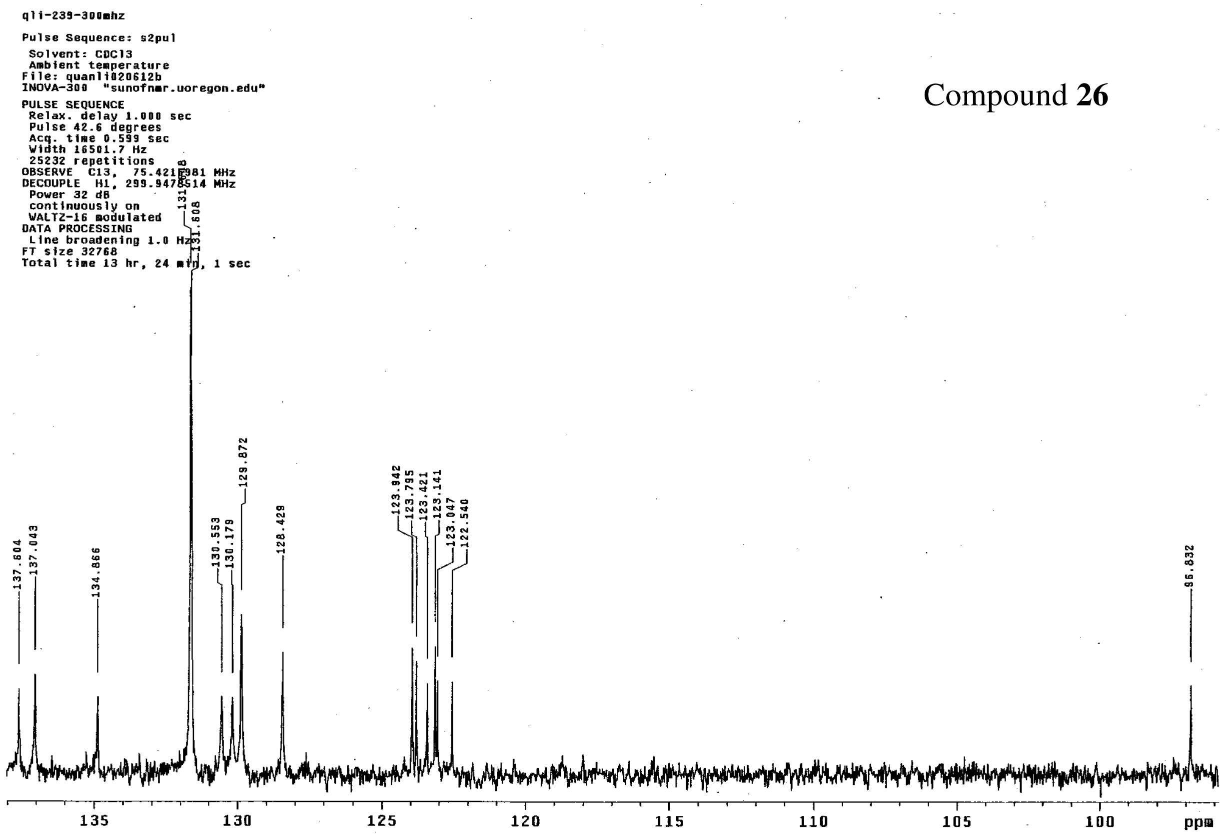


Compound **26**

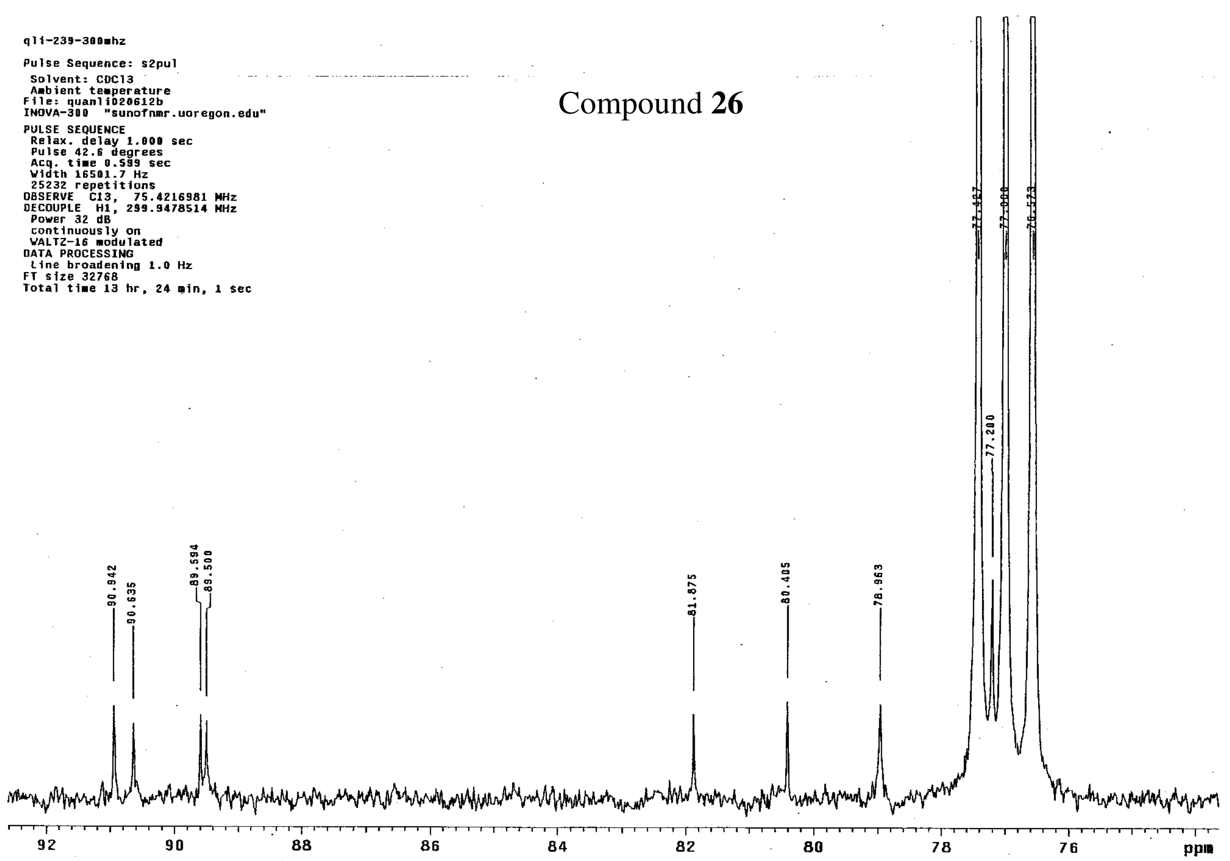


Compound **26**





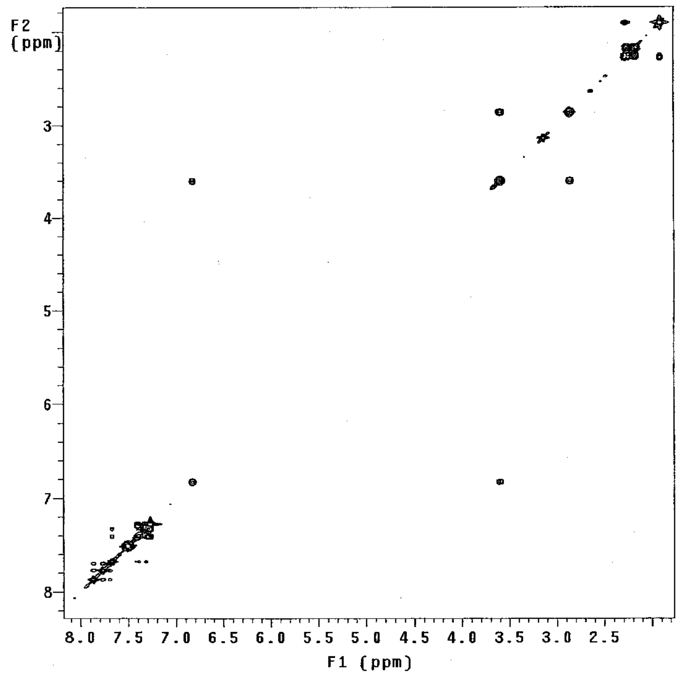
Compound **26**



Compound **26**

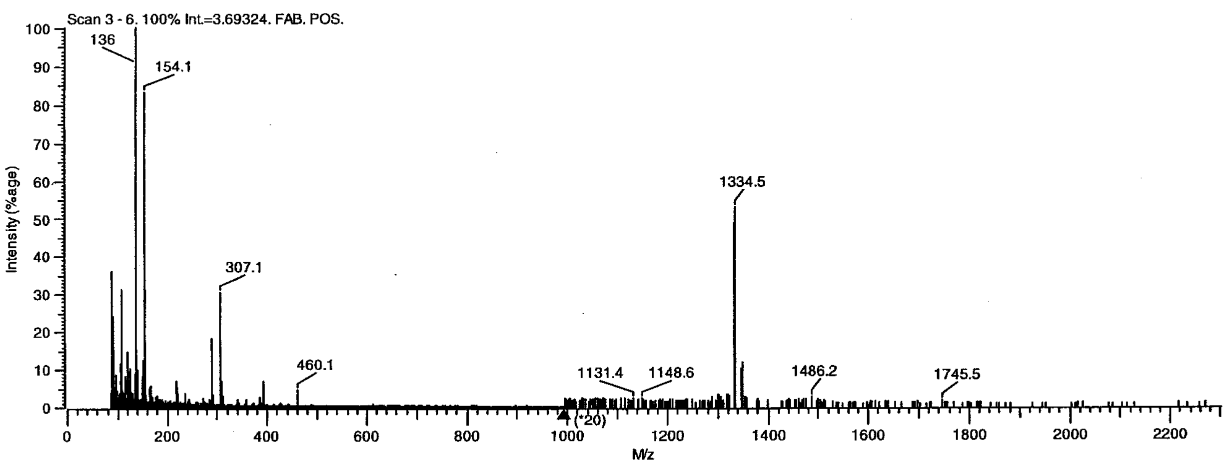
```
DBG-5mm
gCOSY
QLi-239
CDCl3

exp1  gcosy

        SAMPLE                 DEC. & VT
date   Feb 25 2003  dn               H1
solvent       cdcl3  dof               0
file /user4/people~ dm              nnn
/quanli/vnmrdata/5~ dmm               c
00/QLi-239-1H-500M~ dmf             200
Hz-gCOSY-25feb03.f~ homo              n
                 id  temp           25.0
   ACQUISITION
sfrq        500.106  lp              4.4
tn               H1  rp            105.3
at            0.465  rp1               0
np             4096  lp1               0
sw           4400.2      PROCESSING
fb             2000  lb             0.50
ss                2  sb            0.075
tpwr             57  sbs        not used
pw              9.5  proc             ft
p1             11.1  fn             8192
d1            1.000  math              i
tof          -406.9
nt                4  werr
ct                4  wexp
alock             n  wbs
gain             56  wnt
       FLAGS           2D PROCESSING
il                n  lb1            0.50
in                n  sb1           0.050
dp                y  sbs1       not used
hs               nn  proc1            ft
  2D ACQUISITION     fn1            4096
sw1          4400.2        DISPLAY
ni              512  sp            875.2
d2                0  wp           3263.3
     GRADIENTS       vs              459
gzlvl1         3000  sc                0
gt1        0.001900  wc              125
grise      0.000100  hzmm          35.20
gstab             0  is         83444.50
qlvl            1.0  rfl           115.5
    2D DISPLAY       rfp               0
sp1           881.9  th                4
wp1          3205.0  ins           1.000
sc2               0  ai     av
wc2             125
rfl1          115.5
rfp1              0
```

Compound **26**



Compound **26**

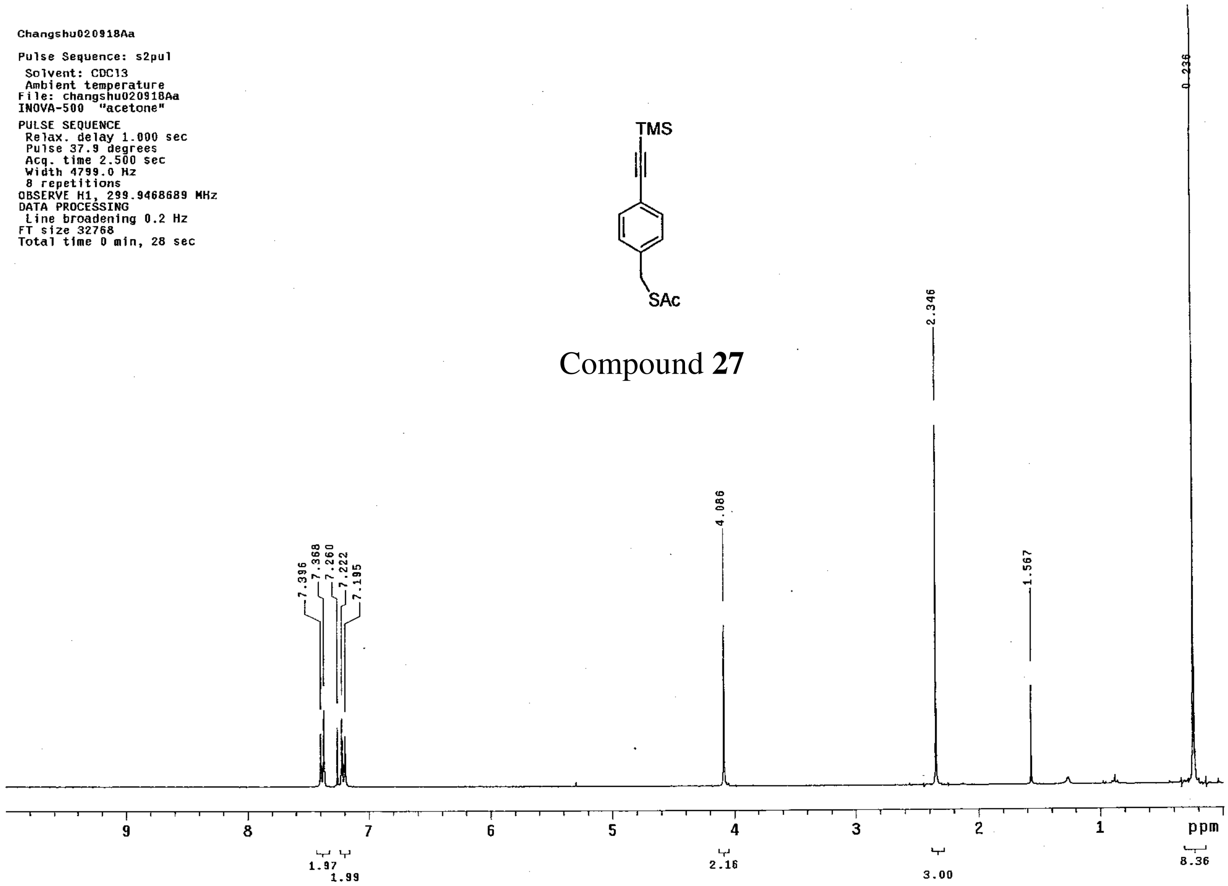
Sample:QLI-239
Quan Li



Changshu020918Aa

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: changshu020918Aa
INOVA-500 "acetone"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.500 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9468689 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec

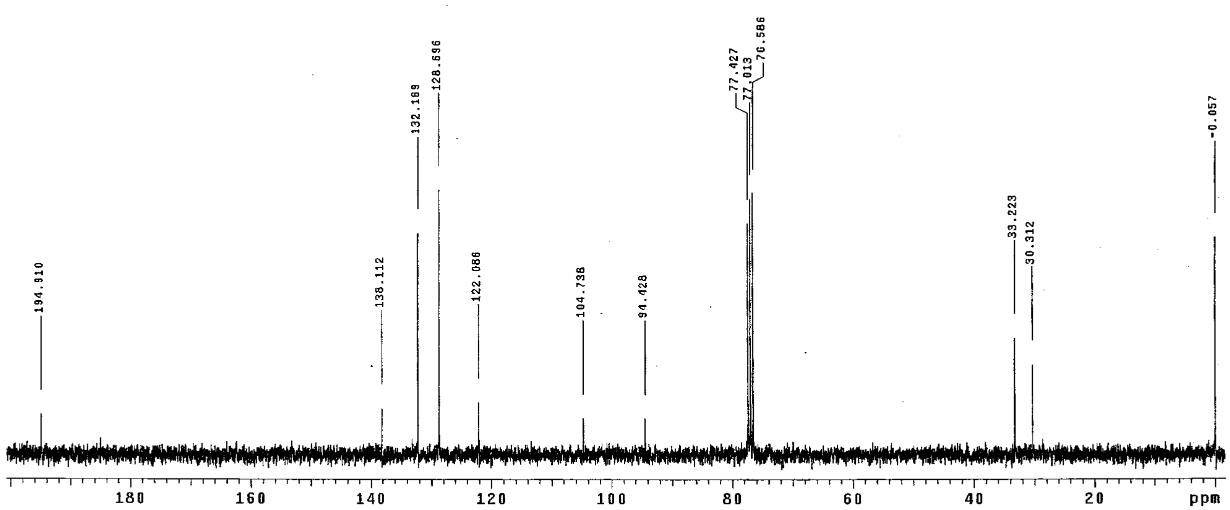
Compound **27**

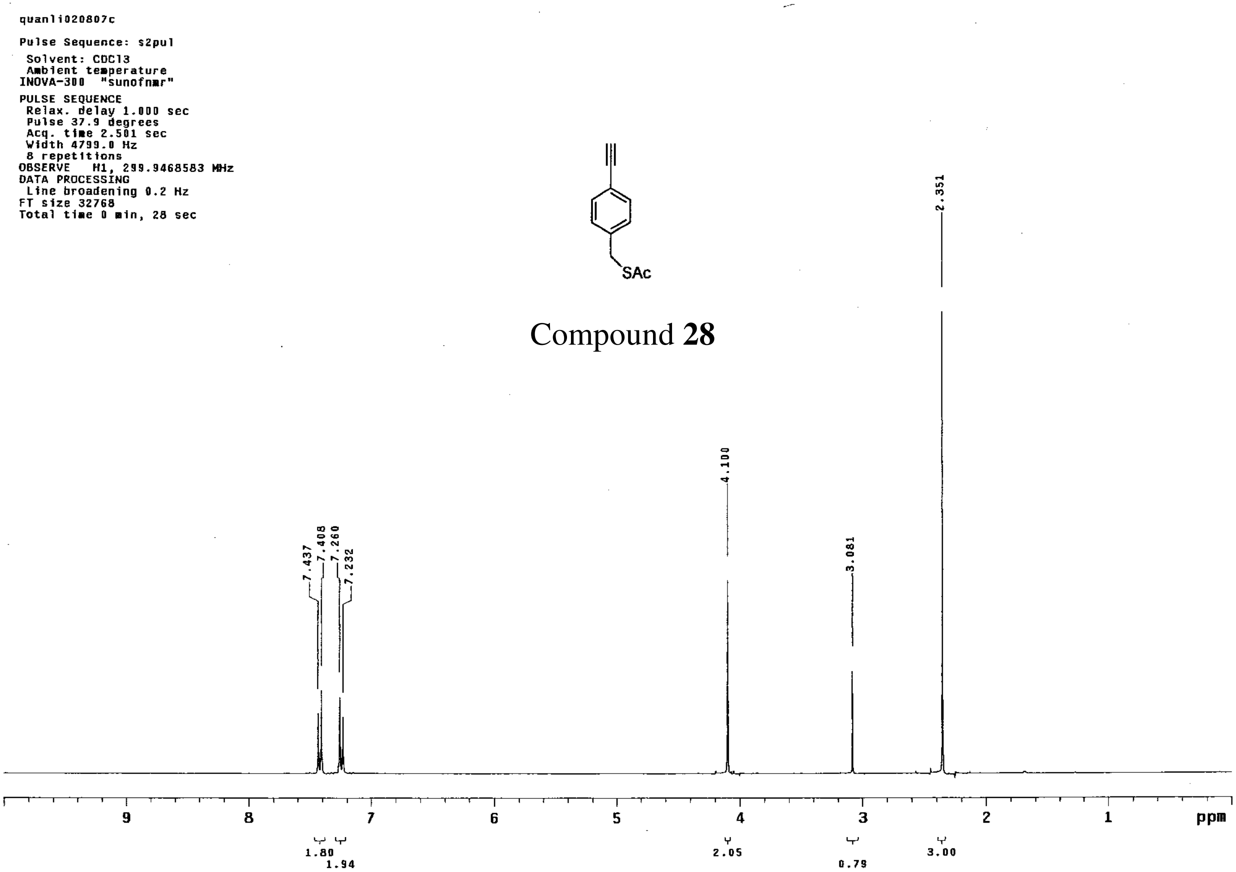


changshu020918Ab

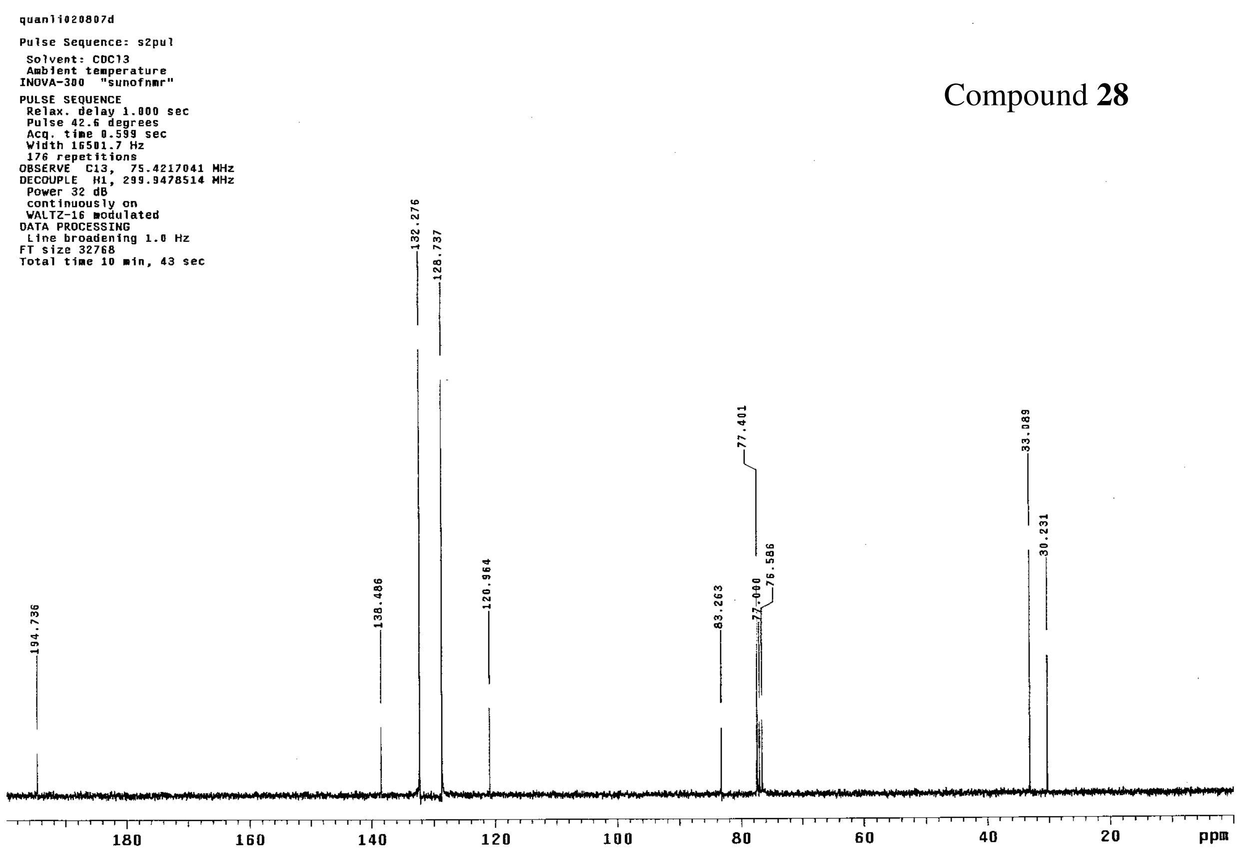
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
File: changshu020918Ab
INOVA-500 "acetone"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 42.6 degrees
Acq. time 0.599 sec
Width 16501.7 Hz
400 repetitions
OBSERVE C13, 75.4216995 MHz
DECOUPLE H1, 299.9478455 MHz
Power 32 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 32768
Total time 21 min, 28 sec

Compound **27**



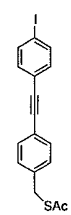


Compound **28**

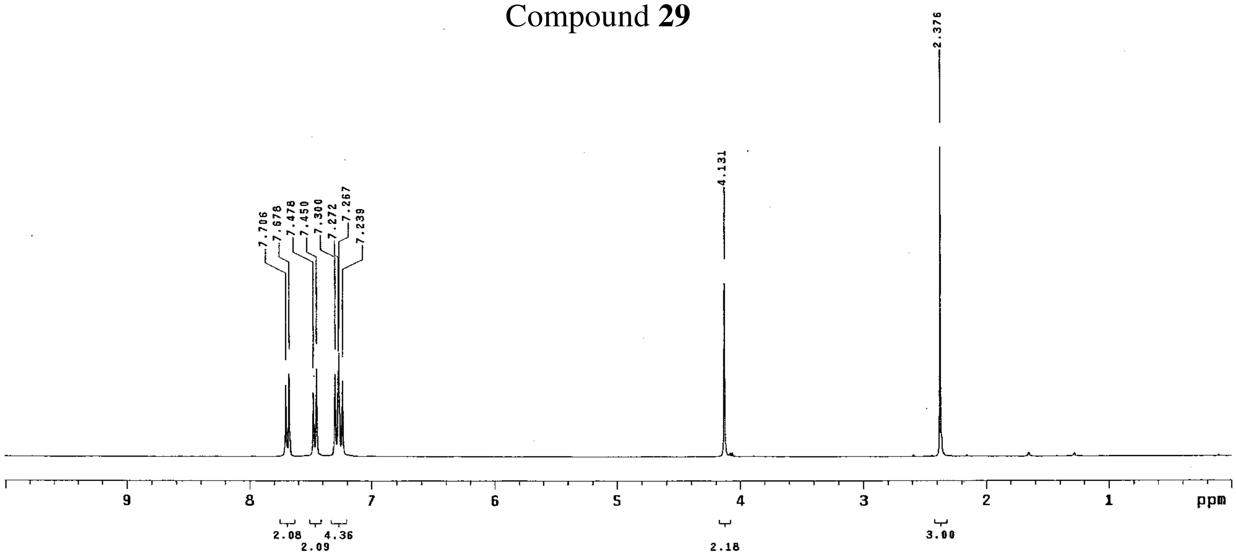


Compound **28**

qli-215
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.501 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9325201 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec

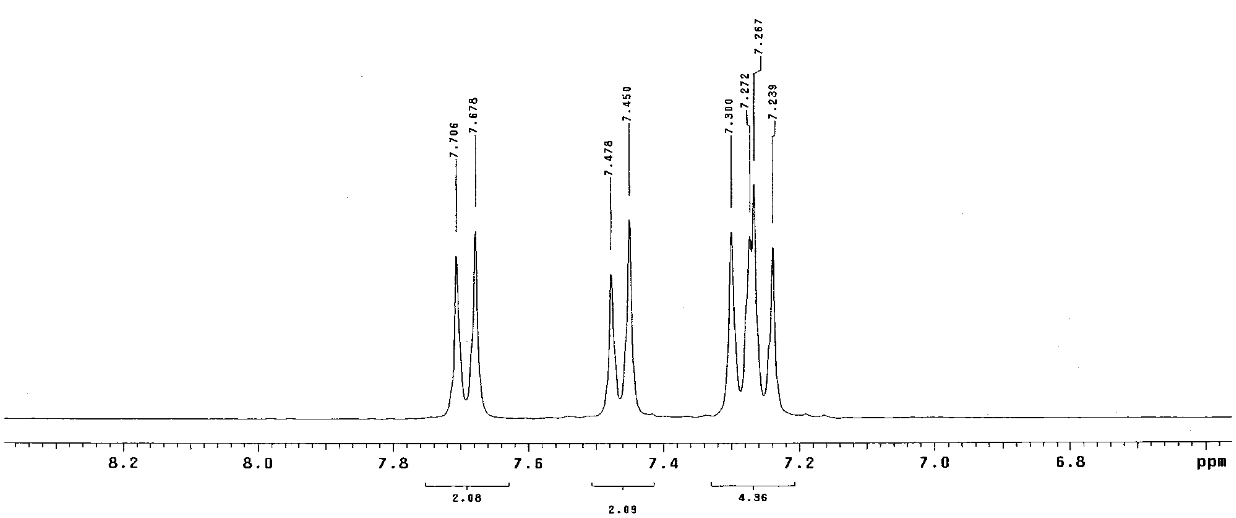


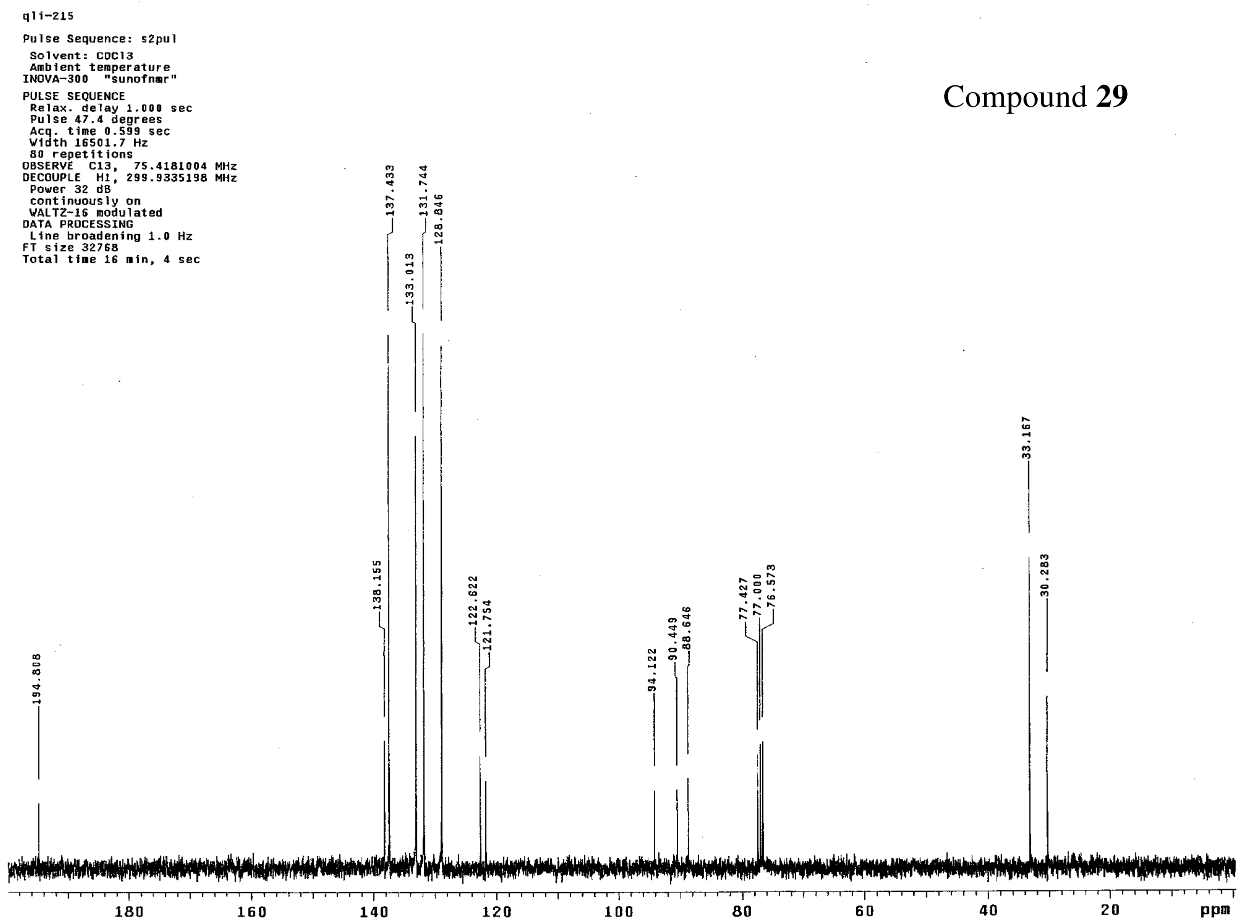
Compound **29**



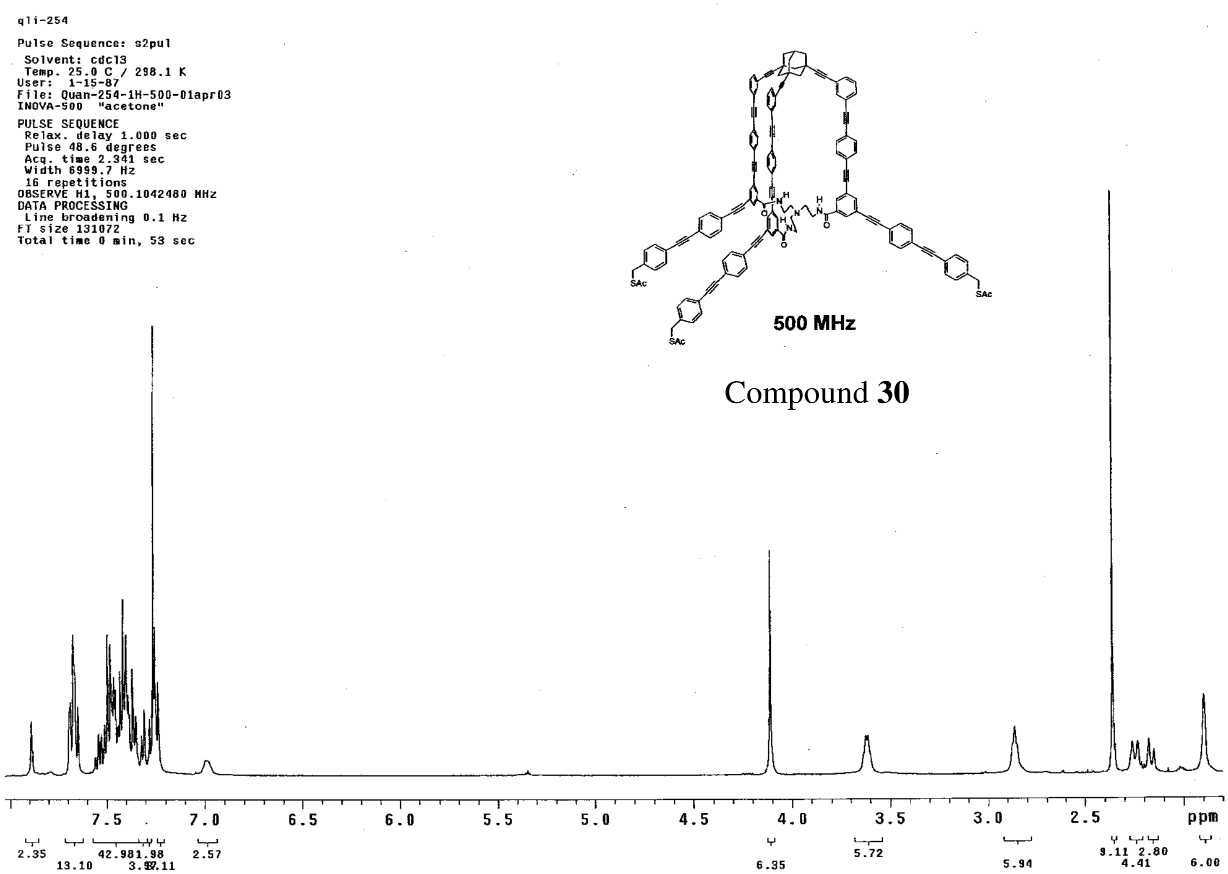
qli-215
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
INOVA-300 "sunofnmr"
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 37.9 degrees
Acq. time 2.501 sec
Width 4799.0 Hz
8 repetitions
OBSERVE H1, 299.9325201 MHz
DATA PROCESSING
Line broadening 0.2 Hz
FT size 32768
Total time 0 min, 28 sec

Compound **29**

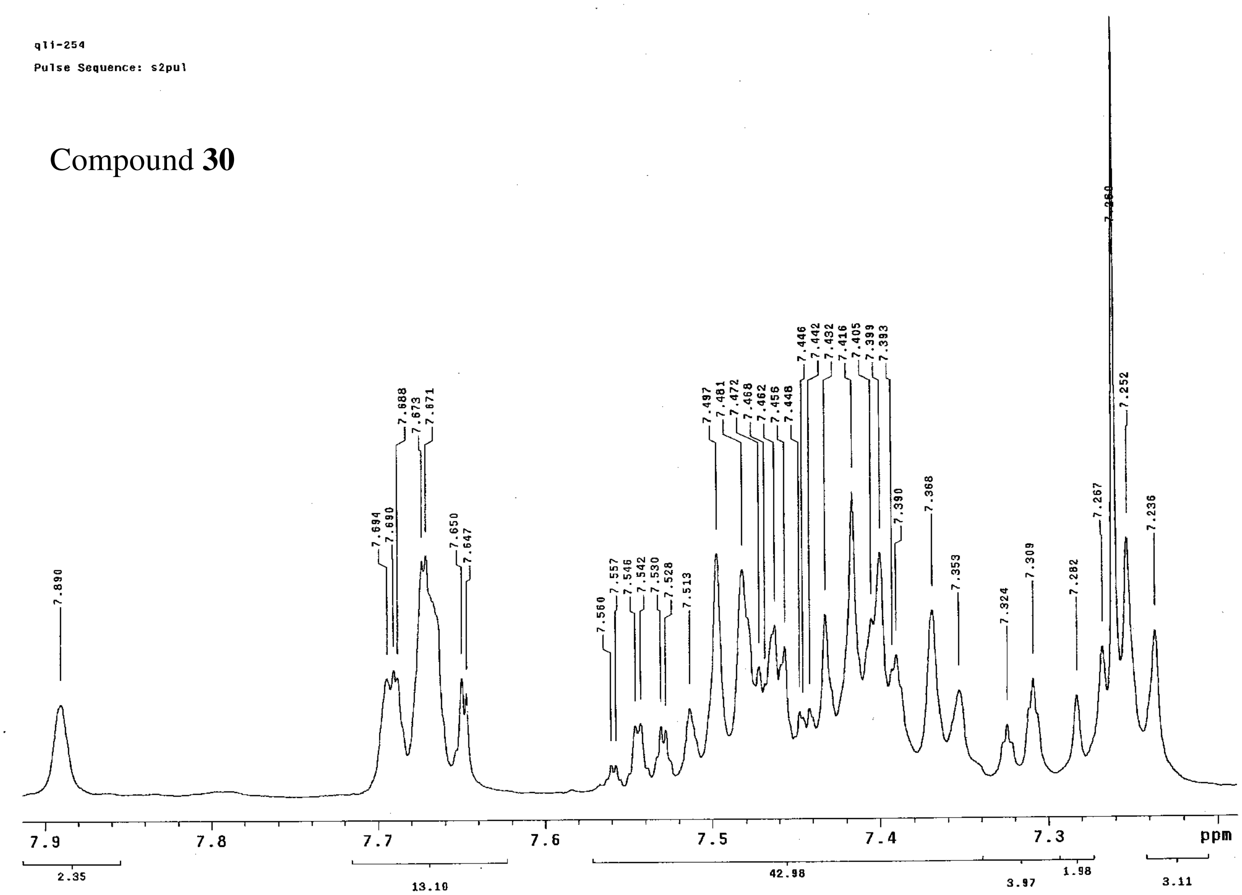




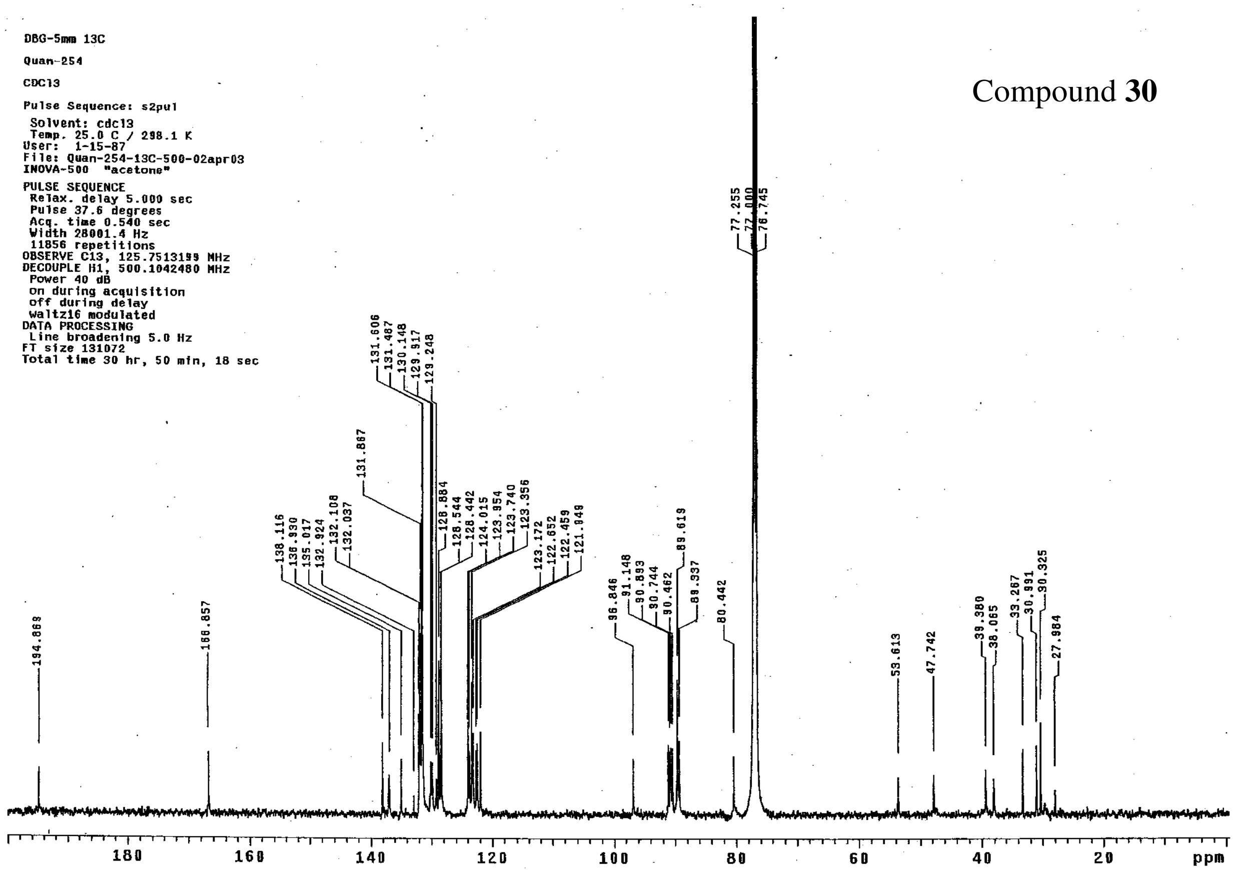
Compound **29**



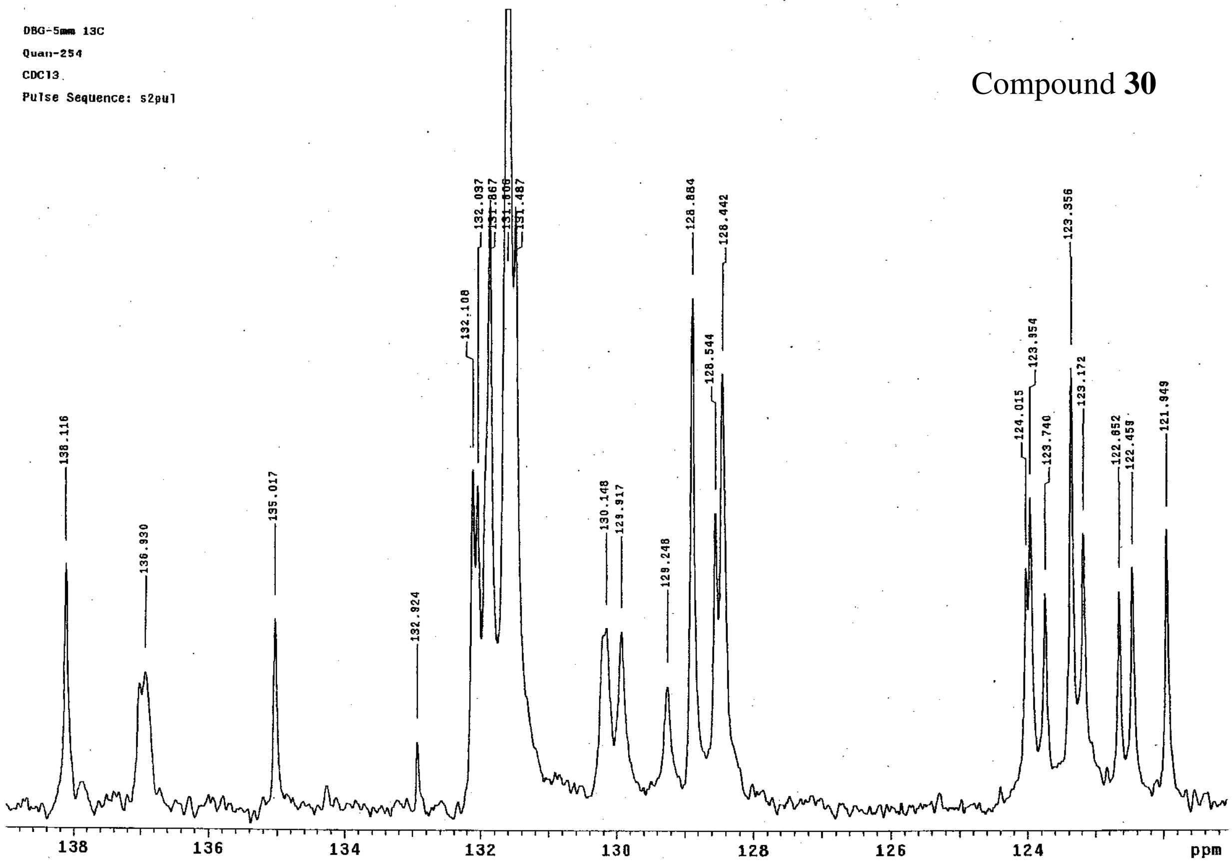
Compound **30**

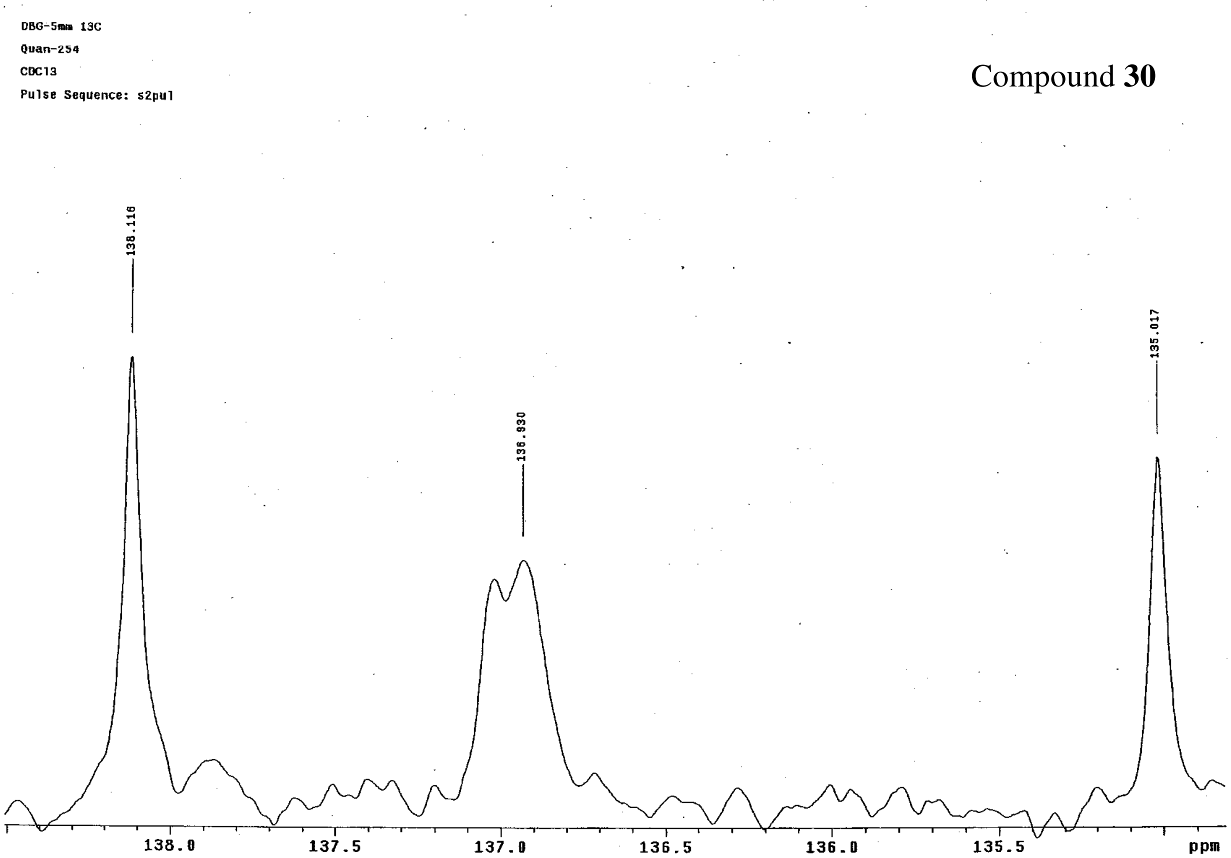


Compound **30**



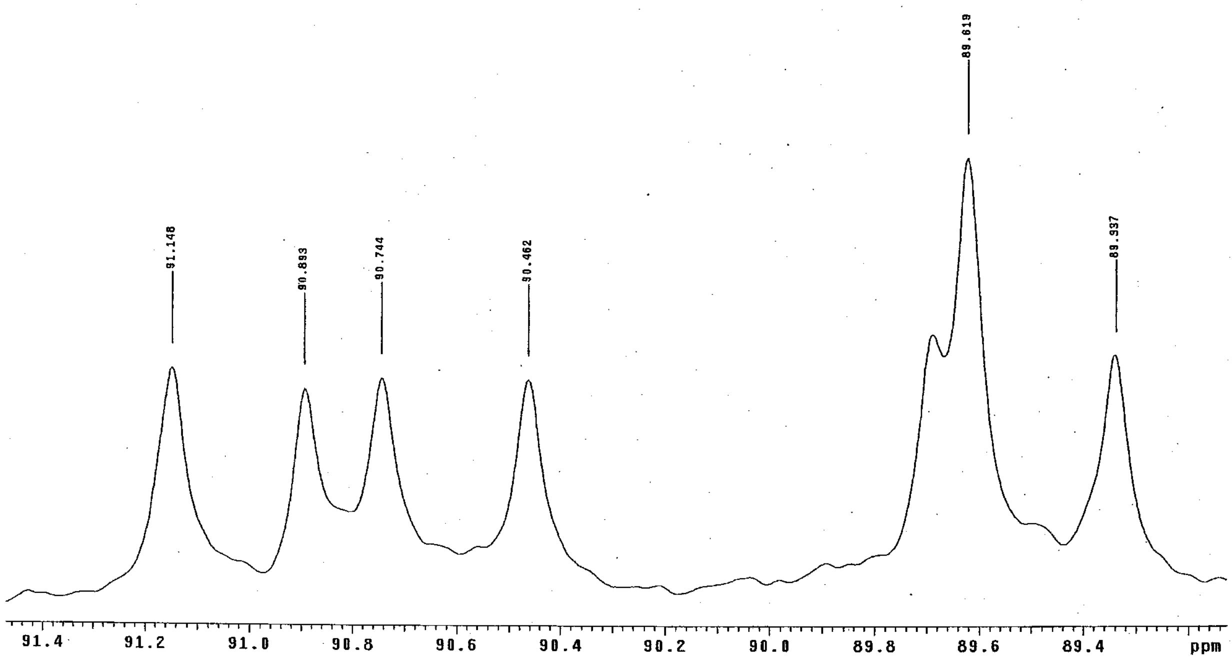
Compound **30**


DBG-5mm 13C
Quan-254
CDCl3
Pulse Sequence: s2pul
Compound 30
138.116
136.930
135.017
132.924
132.108
132.097
131.867
131.606
131.487
130.148
129.917
129.248
128.884
128.544
128.442
124.015
123.954
123.740
123.356
123.172
122.852
122.459
121.949
138
136
134
132
130
128
126
124
ppm


DBG-5mm 13C
Quan-254
CDCl3
Pulse Sequence: s2pul
Compound 30
138.116
136.930
135.017
138.0
137.5
137.0
136.5
136.0
135.5
ppm

DBG-5mm 13C
Quan-254
CDCl3
Pulse Sequence: s2pul

Compound **30**

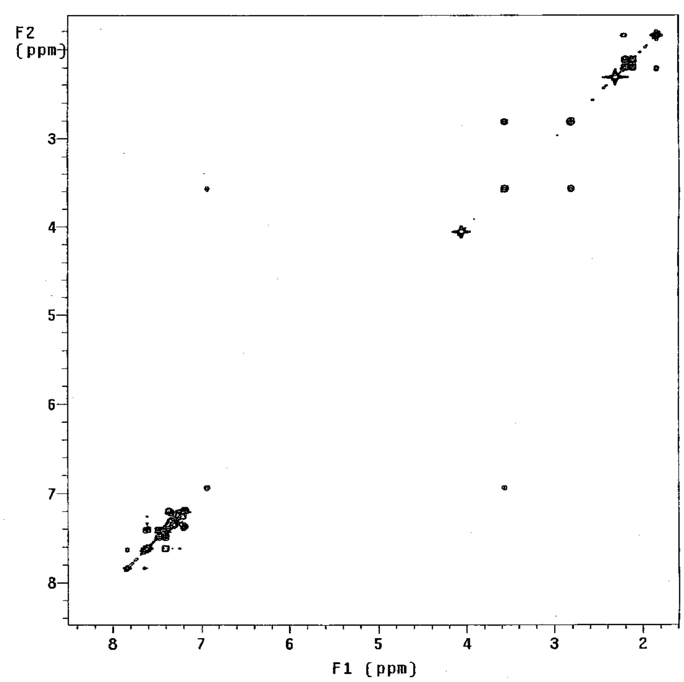


DBG-5mm
gCOSY
Quan-254
CDCl3

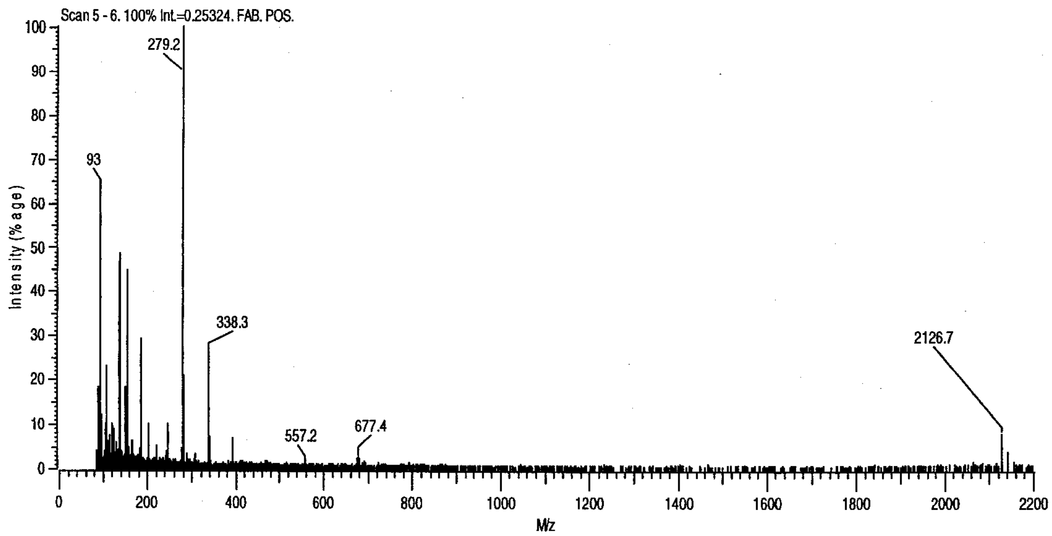
exp1 gcosy

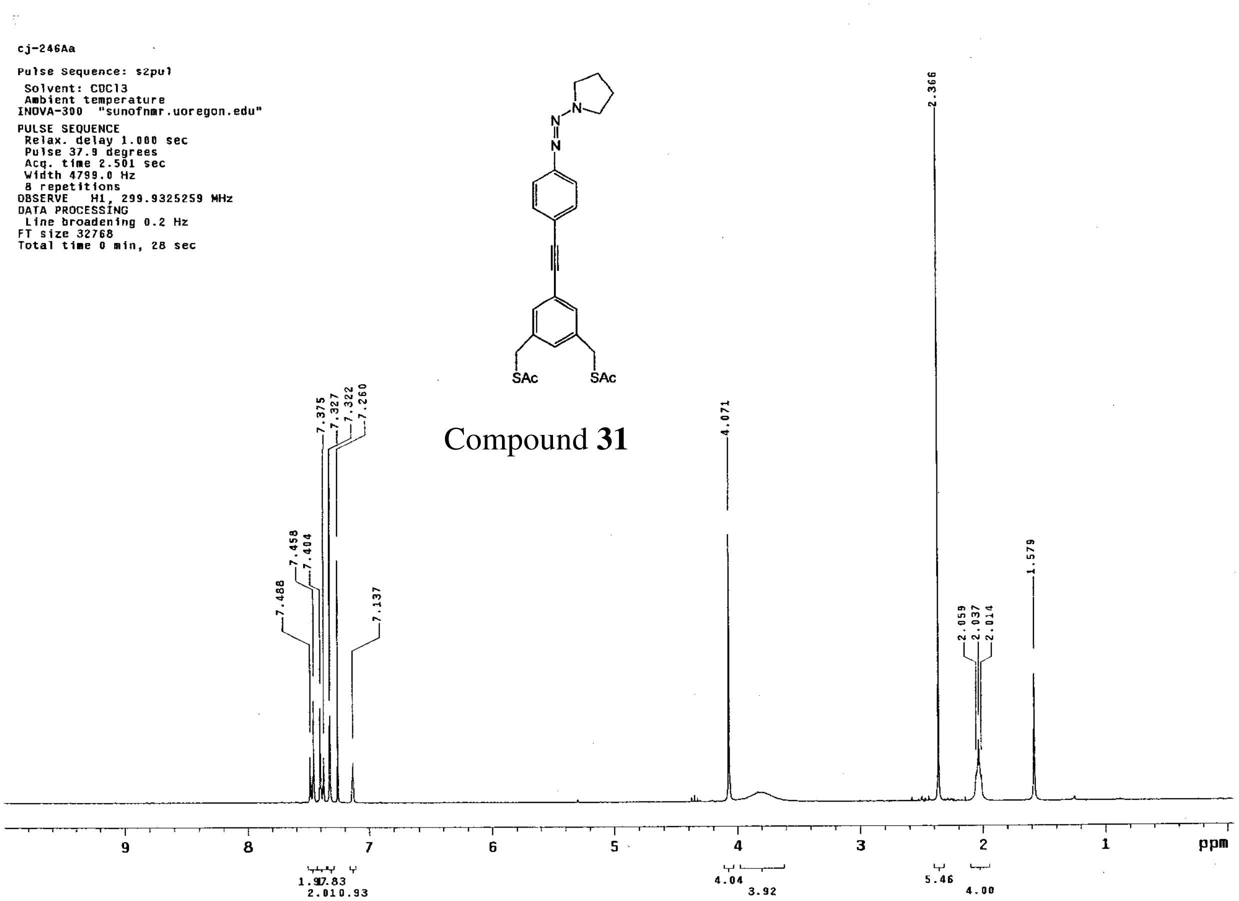
SAMPLE		DEC. & VT	
date	Apr 2 2003	dn	H1
solvent	cdcl3	dof	0
file /user4/people~		dm	nnn
/quanli/vnmrdata/5~		dmm	c
00/Quan-254-gCOSY-~		dmf	200
02Apr03.fid		homo	n
ACQUISITION		temp	25.0
sfrq	500.106		
tn	H1	lp	4.4
at	0.465	rp	105.3
np	4096	rp1	0
sw	4400.2	lp1	0
fb	2000	PROCESSING	
ss	2	lb	0.50
tpwr	57	sb	0.075
pw	9.5	sbs	not used
p1	11.1	proc	ft
d1	1.000	fn	8192
tof	-406.9	math	i
nt	4		
ct	4	werr	
alock	n	wexp	
gain	40	wbs	
FLAGS		wnt	
il	n	2D PROCESSING	
in	n	lb1	0.50
dp	y	sb1	0.050
hs	nn	sbs1	not used
2D ACQUISITION		proc1	ft
sw1	4400.2	fn1	4096
ni	512	DISPLAY	
d2	0	sp	812.0
GRADIENTS		wp	3423.5
gzlvl1	3000	vs	2081
gt1	0.001900	sc	0
grise	0.000100	wc	125
gstab	0	hzmm	35.20
qlvl	1.0	is	83444.50
2D DISPLAY		rfl	148.6
sp1	797.2	rfp	0
wp1	3452.2	th	3
sc2	0	ins	1.000
wc2	125	ai	av
rfl1	148.6		
rfp1	0		

Compound **30**



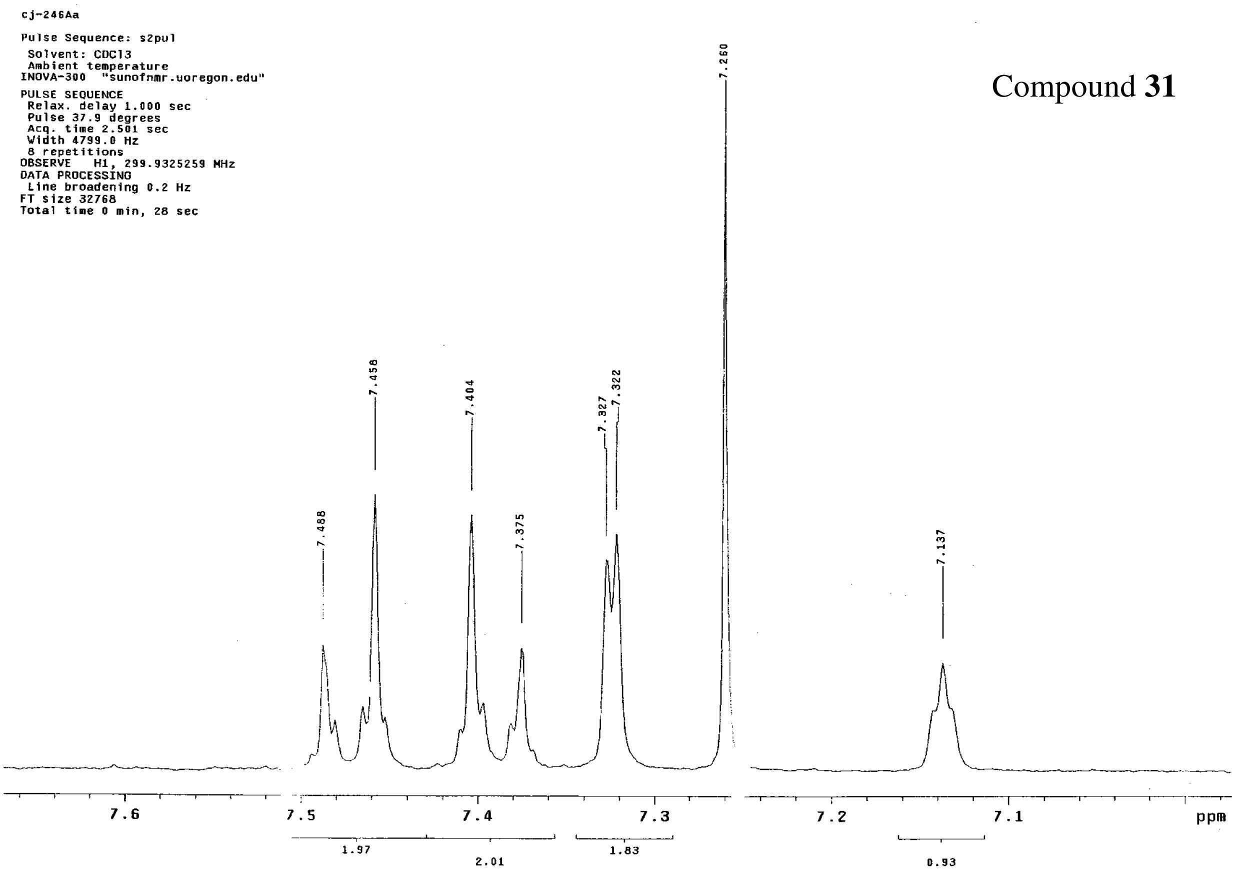
Compound **30**



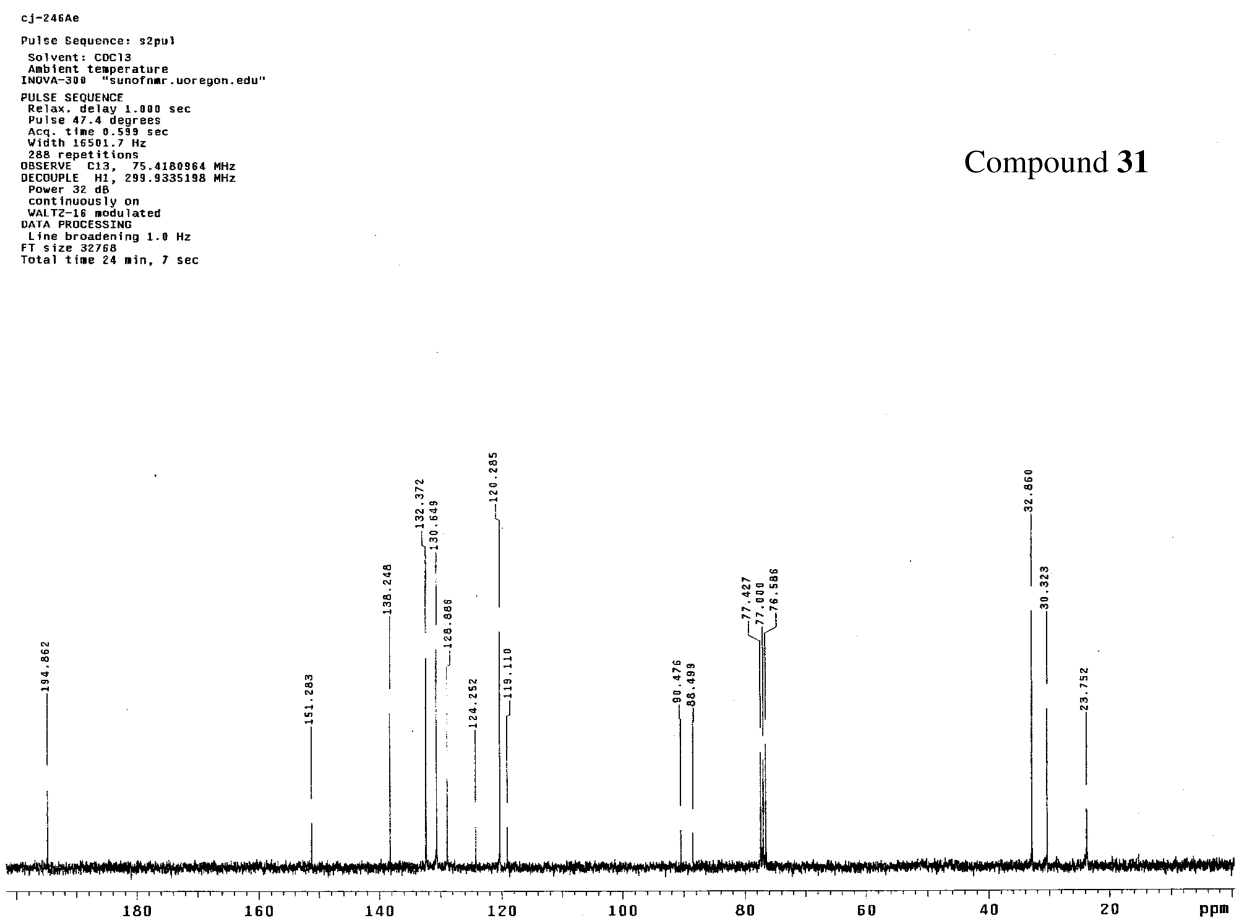


Compound **31**

Compound **31**

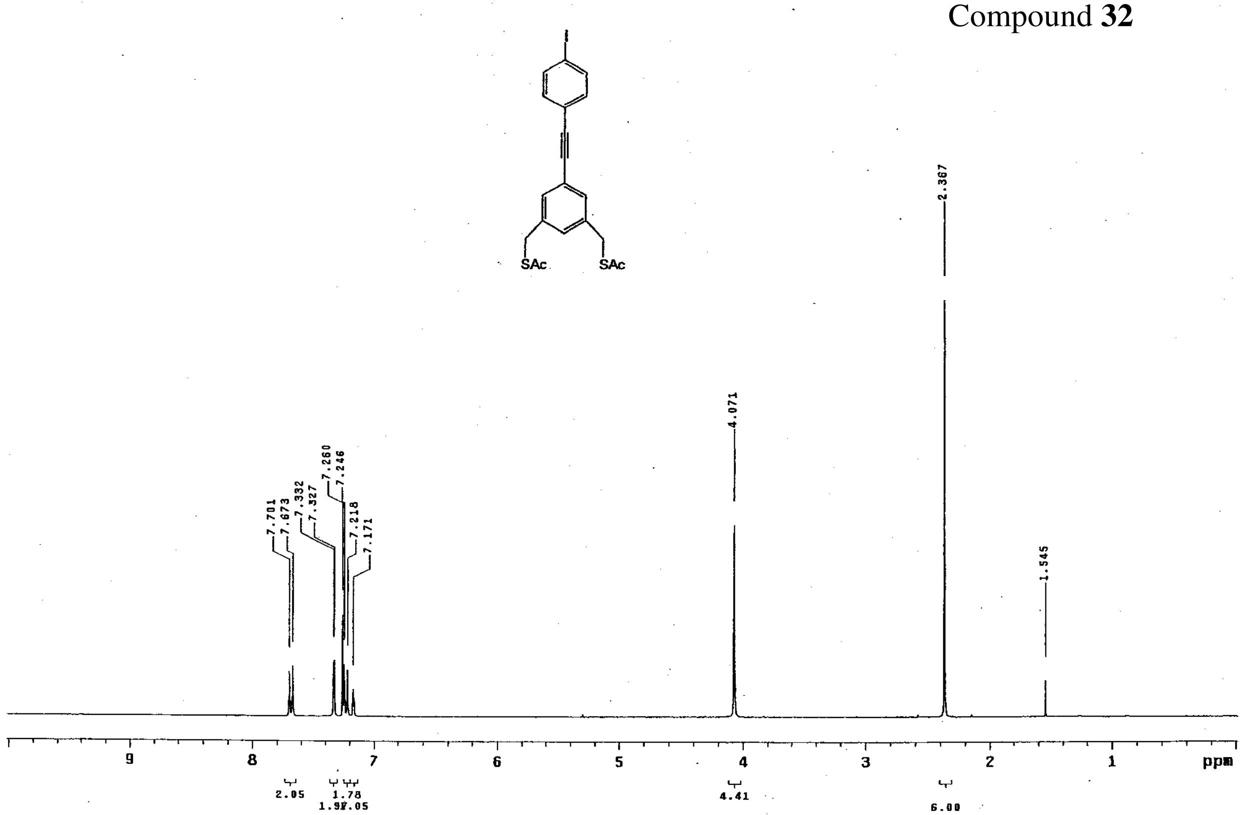


Compound **31**



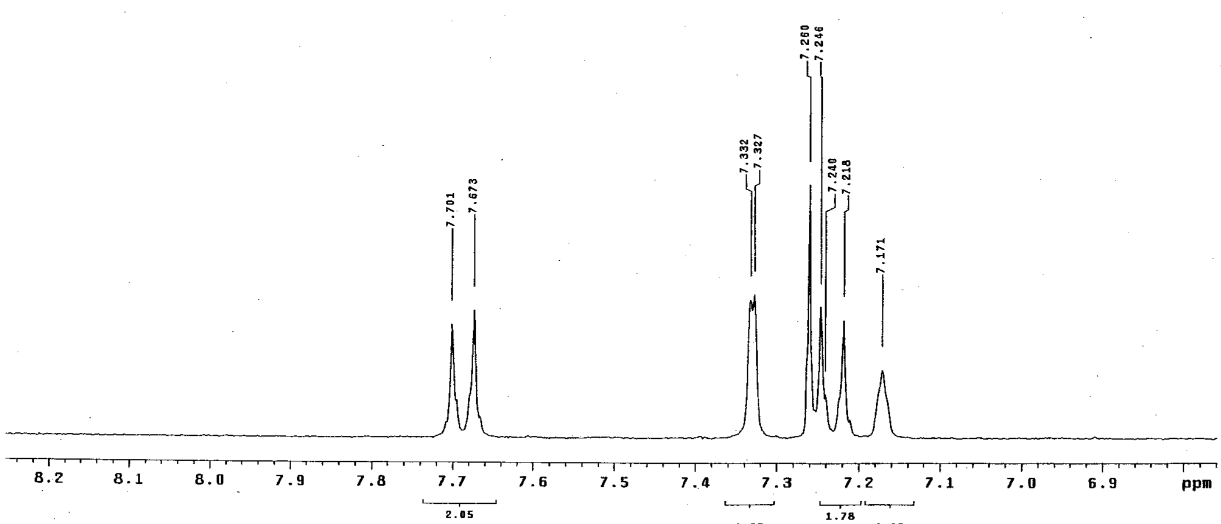
qli-278
Pulse Sequence: s2pul

Compound **32**

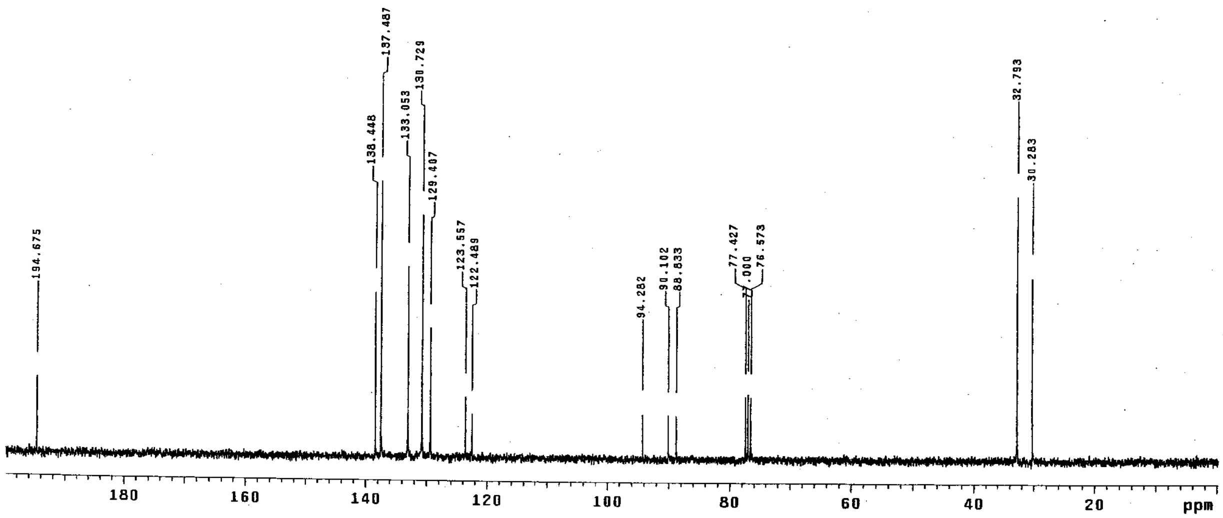


qli-278
Pulse Sequence: s2pul

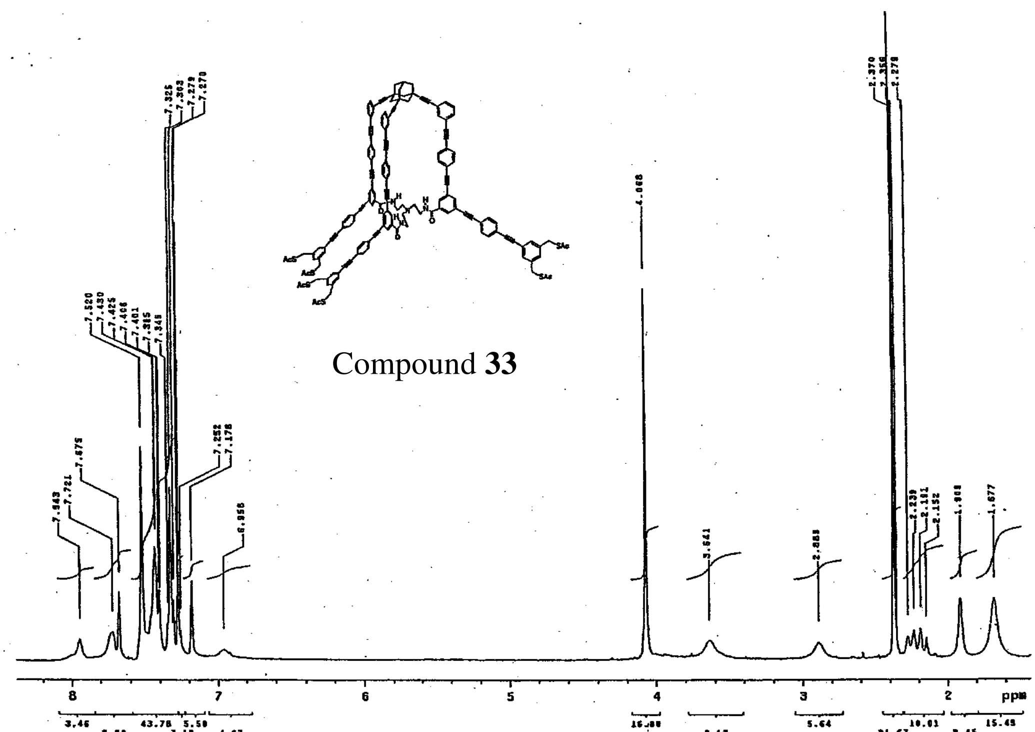
Compound **32**



Compound **32**



194.675
138.448
137.487
133.053
130.729
129.407
123.557
122.489
94.282
90.102
88.833
77.427
77.000
76.573
32.793
30.283
180
160
140
120
100
80
60
40
20
ppm



Compound 33
8
7
6
5
4
3
2
ppm

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