Supplementary Material (ESI) for Green Chemistry

Supporting Information

Aqueous Cross Coupling: Sustainable Protocol for Sonogashira Reactions of Heterocycles

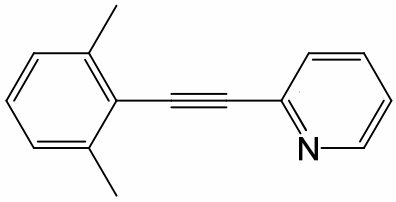
Christoph A. Fleckenstein and Herbert Plenio*

Anorganische Chemie im Zintl-Institut, TU Darmstadt, Petersenstr. 18, 64287 Darmstadt, Germany

plenio@tu-darmstadt.de

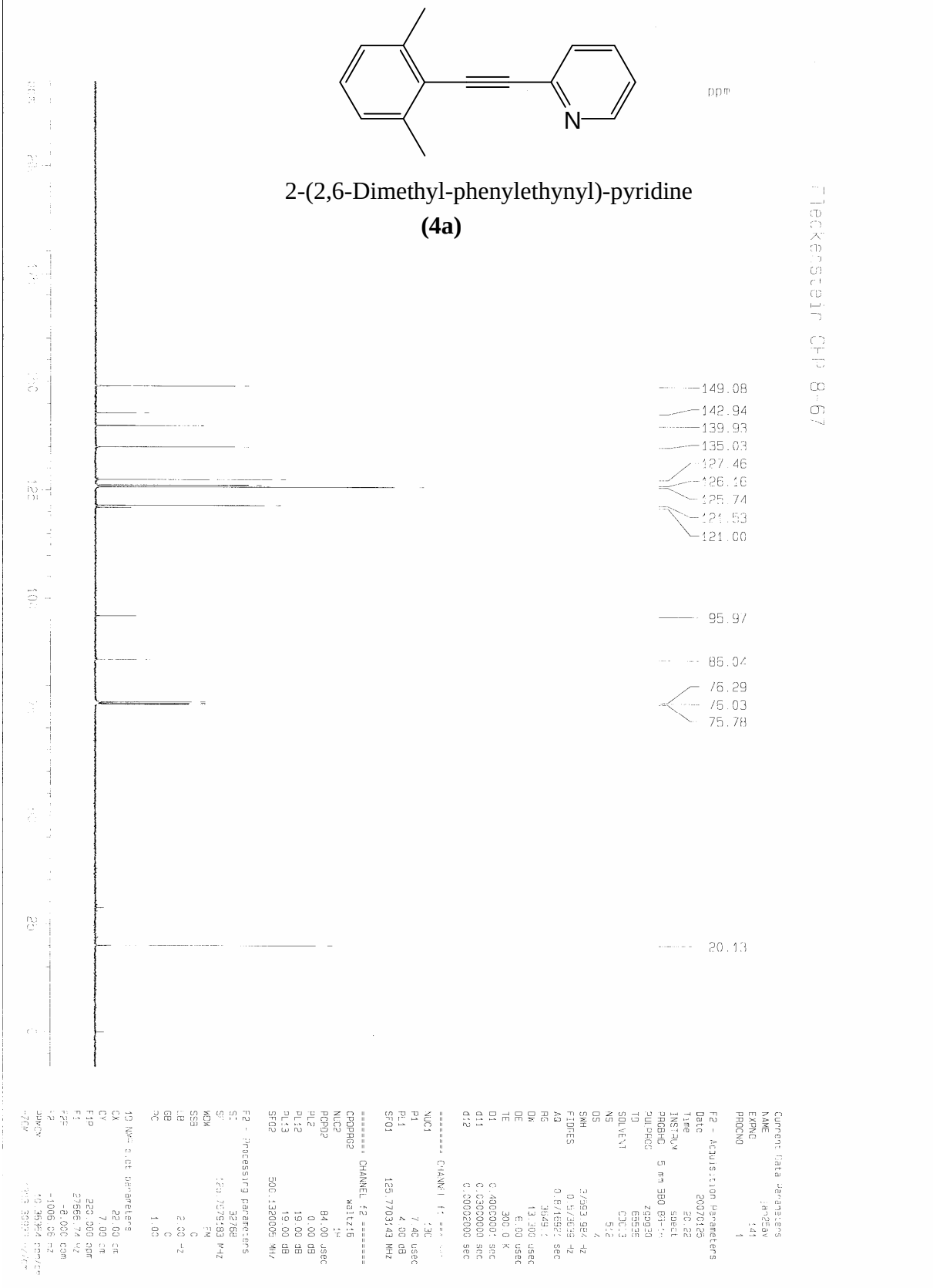
Table of Contents:

^{1}H-NMR



2-(2,6-Dimethyl-phenylethynyl)-pyridine
(4a)

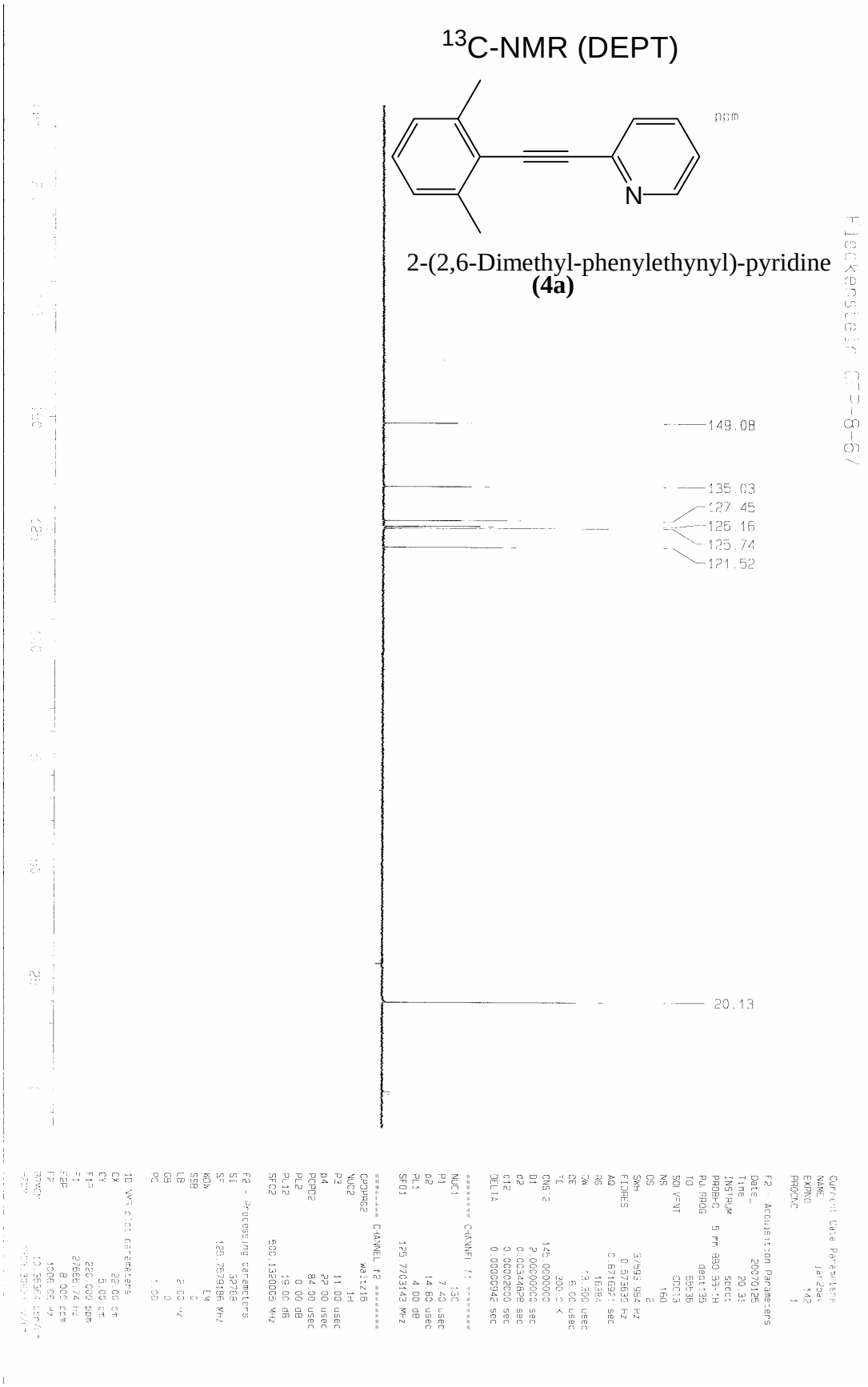
^{13}C-NMR



2-(2,6-Dimethyl-phenylethynyl)-pyridine

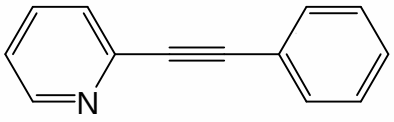
(4a)

^{13}C-NMR (DEPT)



2-(2,6-Dimethyl-phenylethynyl)-pyridine
(4a)

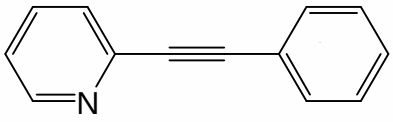
^{1}H-NMR



2-Phenylethynyl-pyridine

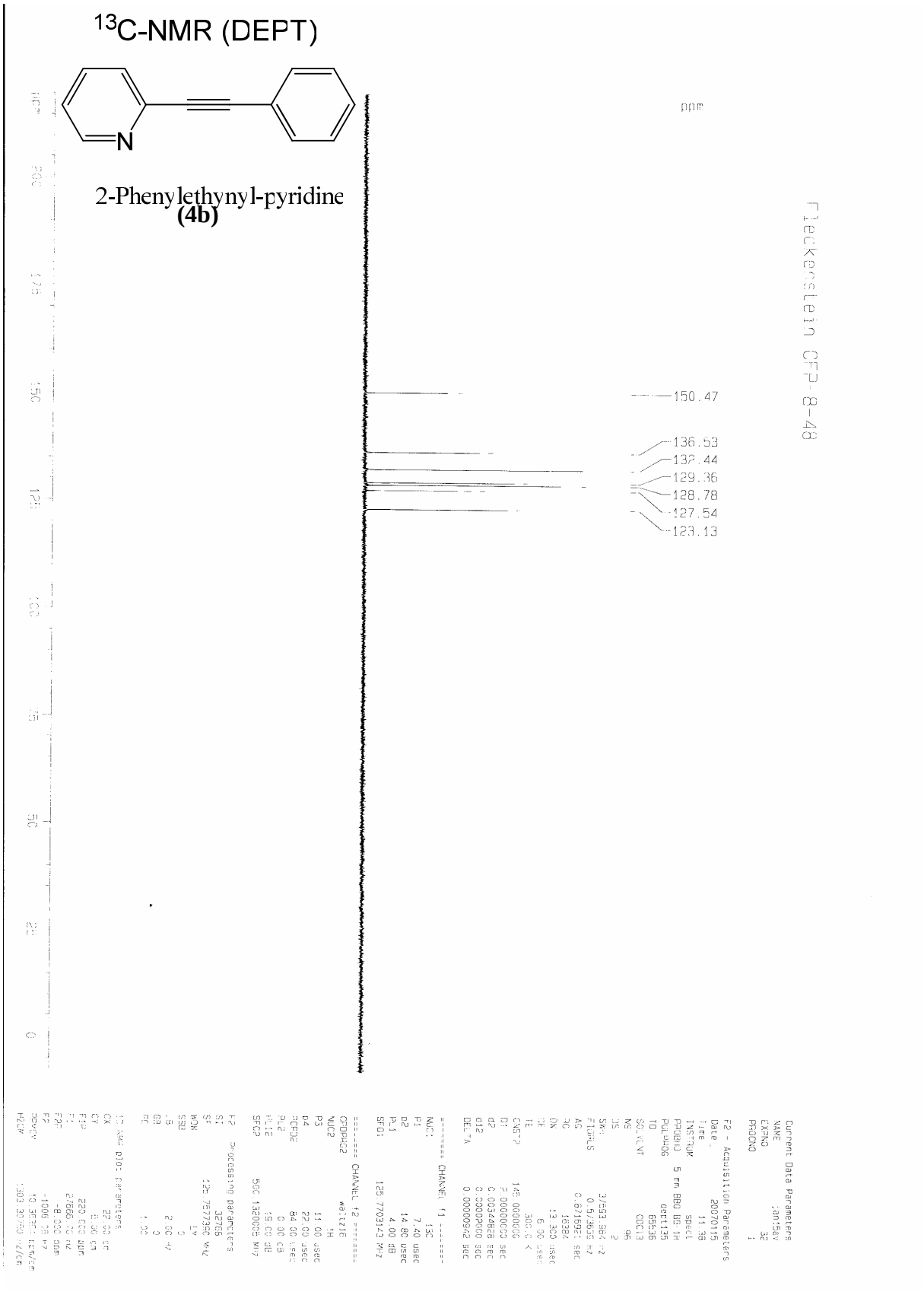
(4b)

^{13}C-NMR

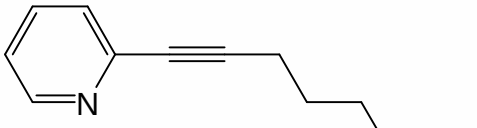


2-Phenylethynyl-pyridine

(4b)


13C-NMR (DEPT)
N
2-Phenylethynyl-pyridine
(4b)
ppm
150.47
136.53
132.44
129.36
128.78
127.54
123.13
Fleckenstein CFP-8-48

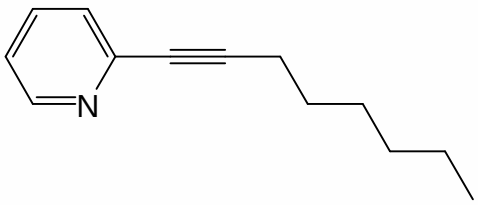
^{1}H-NMR



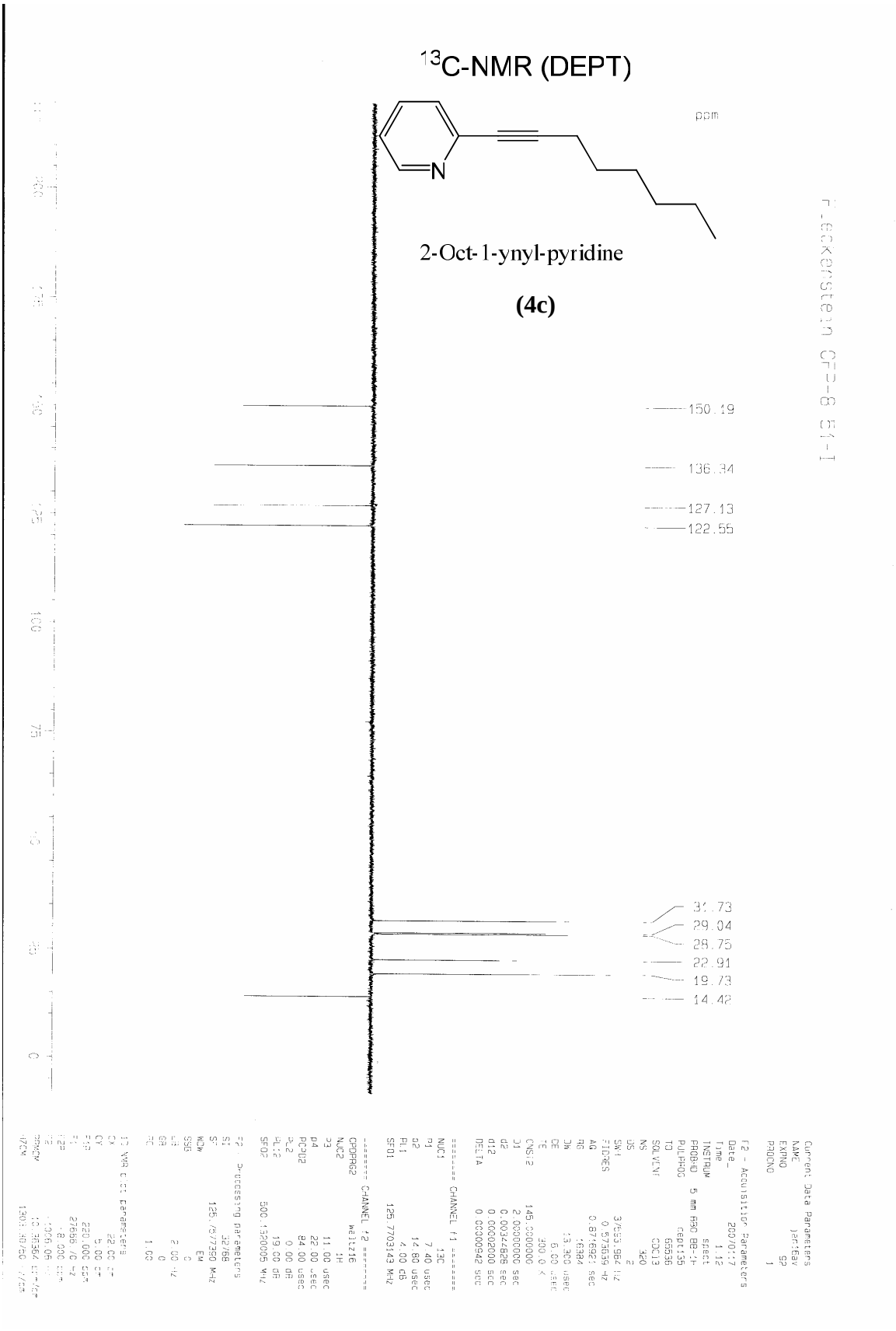
2-Oct-1-ynyl-pyridine

(4c)

^{13}C-NMR

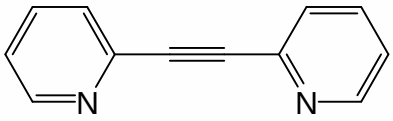


2-Oct-1-ynyl-pyridine
(4c)


^{13}C-NMR (DEPT)
ppm
N
2-Oct-1-ynyl-pyridine
(4c)
150.19
136.34
127.13
122.55
31.73
29.04
28.75
22.91
19.73
14.42

Fleckenstein CFP-8-56

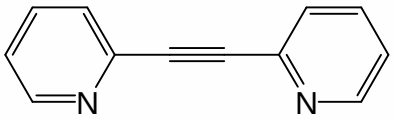
^{1}H-NMR



1,2-Di-(2,2'-pyridyl)-ethyne
(4d)


```
Current Data Parameters
NAME                  Jan19ac
EXPNO                     240
PROCNO                      1

F2 - Acquisition Parameters
Date_              20070119
Time                   15.20
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                zg30
TD                     32768
SOLVENT                CDCl3
NS                        32
DS                         2
SWH               6188.119 Hz
FIDRES            0.188846 Hz
AQ                2.6477044 sec
RG                       322
DW                  80.800 usec
DE                  10.00 usec
TE                  300.0 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     9.70 usec
PL1                   -3.00 dB
SFO1           299.9018520 MHz

F2 - Processing parameters
SI                     131072
SF           299.9000194 MHz
WDW                       EM
SSB                        0
LB                      0.10 Hz
GB                         0
PC                     50.00
```

^{13}C-NMR

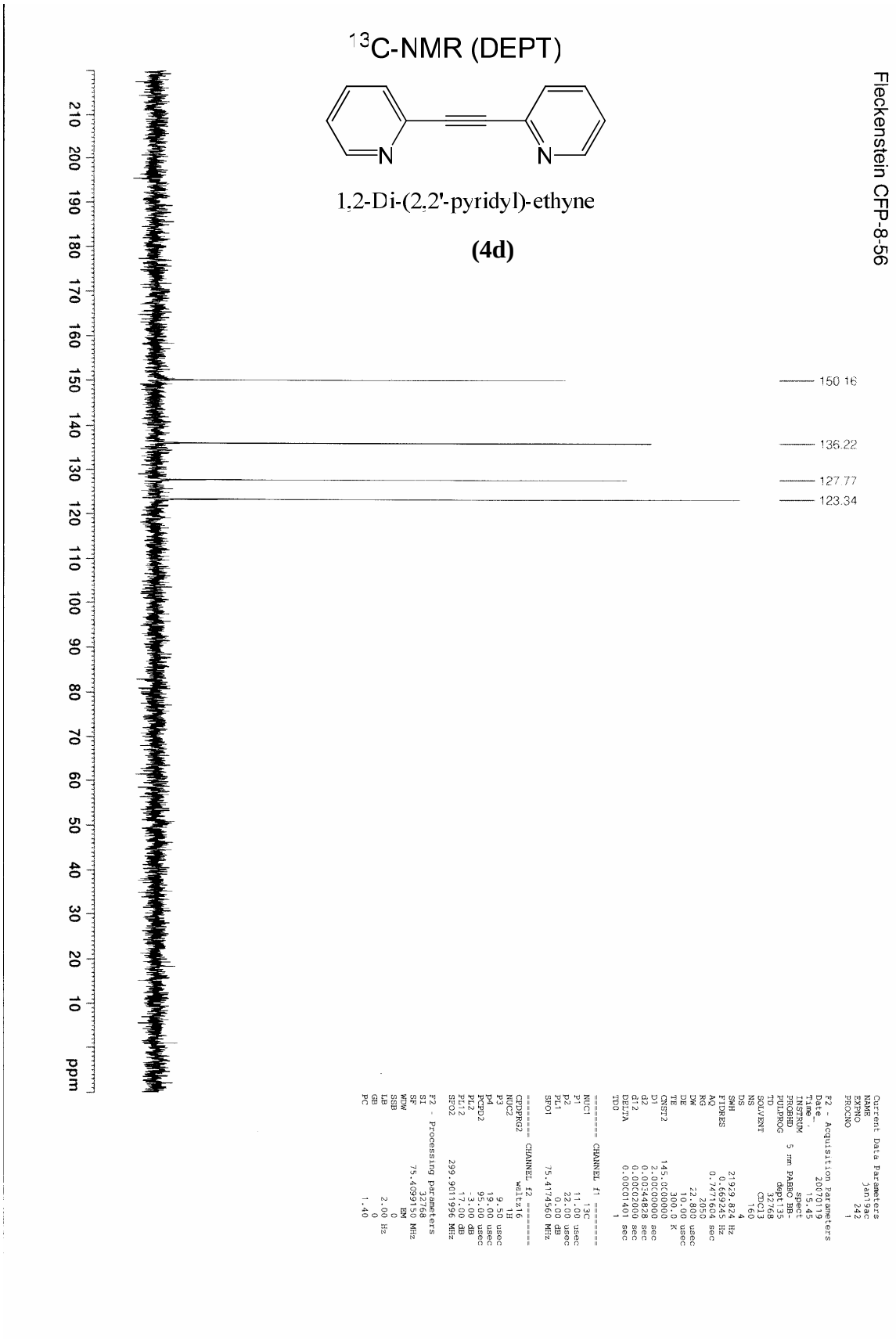


1,2-Di-(2,2'-pyridyl)-ethyne

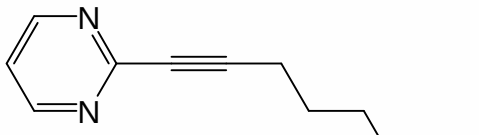
(4d)

Fleckenstein CFP-8-56


```
Current Data Parameters
NAME                  jan19ac
EXPNO                      241
PROCNO                       1

F2 - Acquisition Parameters
Date_              20070119
Time                   15.37
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG             zgpg30
TD                      32768
SOLVENT               CDCl3
NS                        512
DS                          4
SWH              29239.824 Hz
FIDRES           0.892242 Hz
AQ               0.7471744 sec
RG                       2054
DW                   22.800 usec
DE                    10.00 usec
TE                    300.0 K
D1                 1.00000000 sec
d11                0.03000000 sec
DELTA              0.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                     13C
P1                     11.00 usec
PL1                     0.00 dB
SFO1             75.4174560 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  95.00 usec
PL2                    13.00 dB
PL12                   17.00 dB
PL13                   23.00 dB
SFO2             299.9011996 MHz

F2 - Processing parameters
SI                       32768
SF               75.4099898 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.40
```


13C-NMR (DEPT)
1,2-Di-(2,2'-pyridyl)-ethyne
(4d)
Fleckenstein CFP-8-56
150.16
136.22
127.77
123.34
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

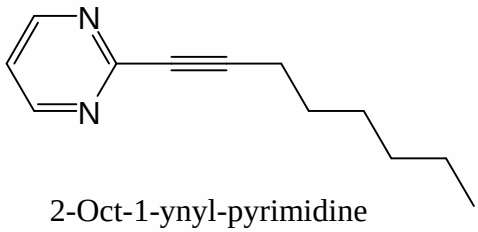
^{1}H-NMR



2-Oct-1-ynyl-pyrimidine

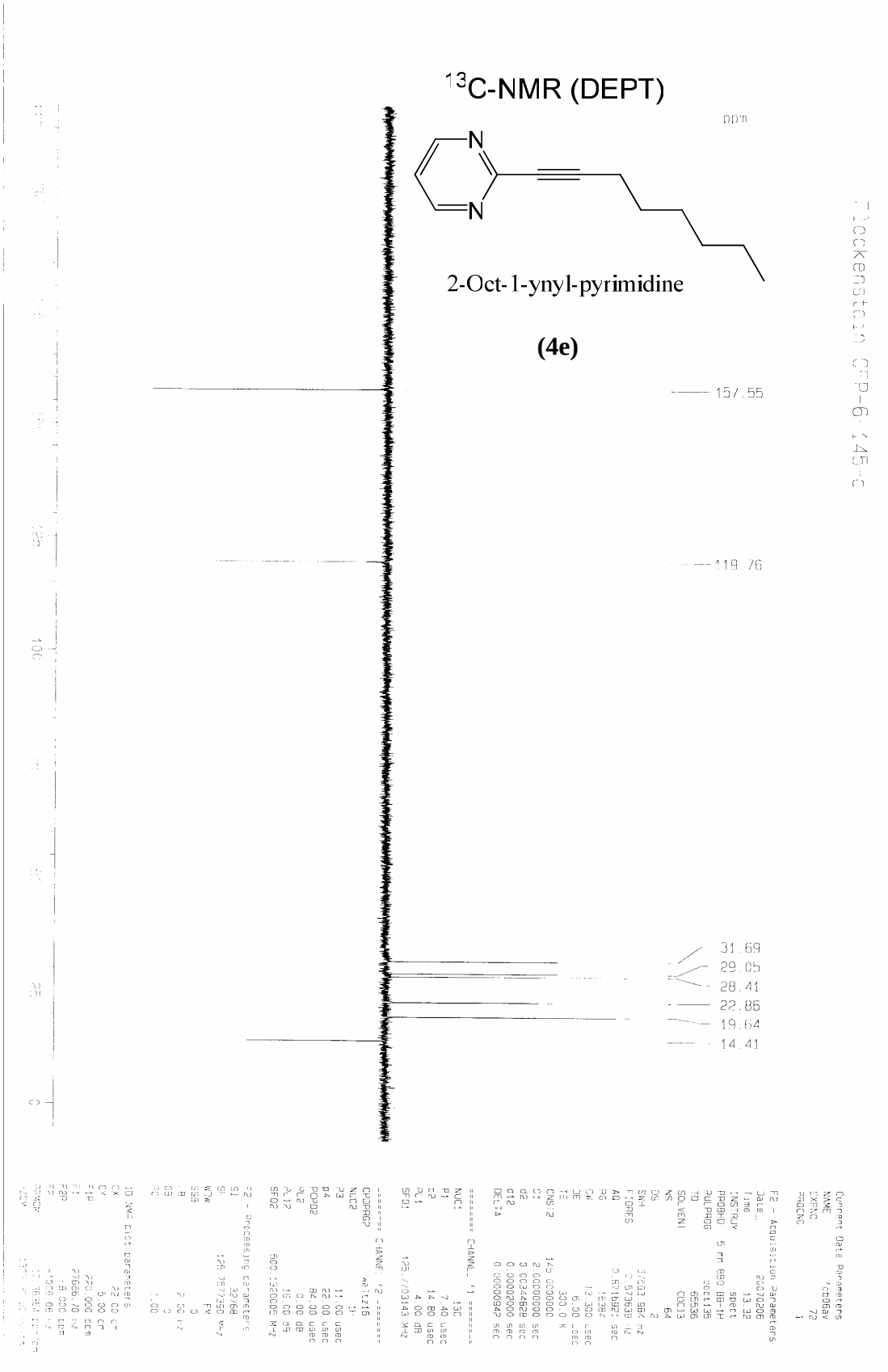
(4e)

^{13}C-NMR

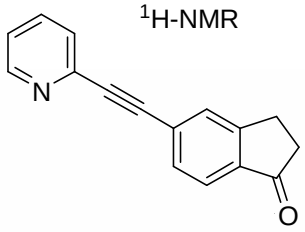


2-Oct-1-ynyl-pyrimidine

(4e)

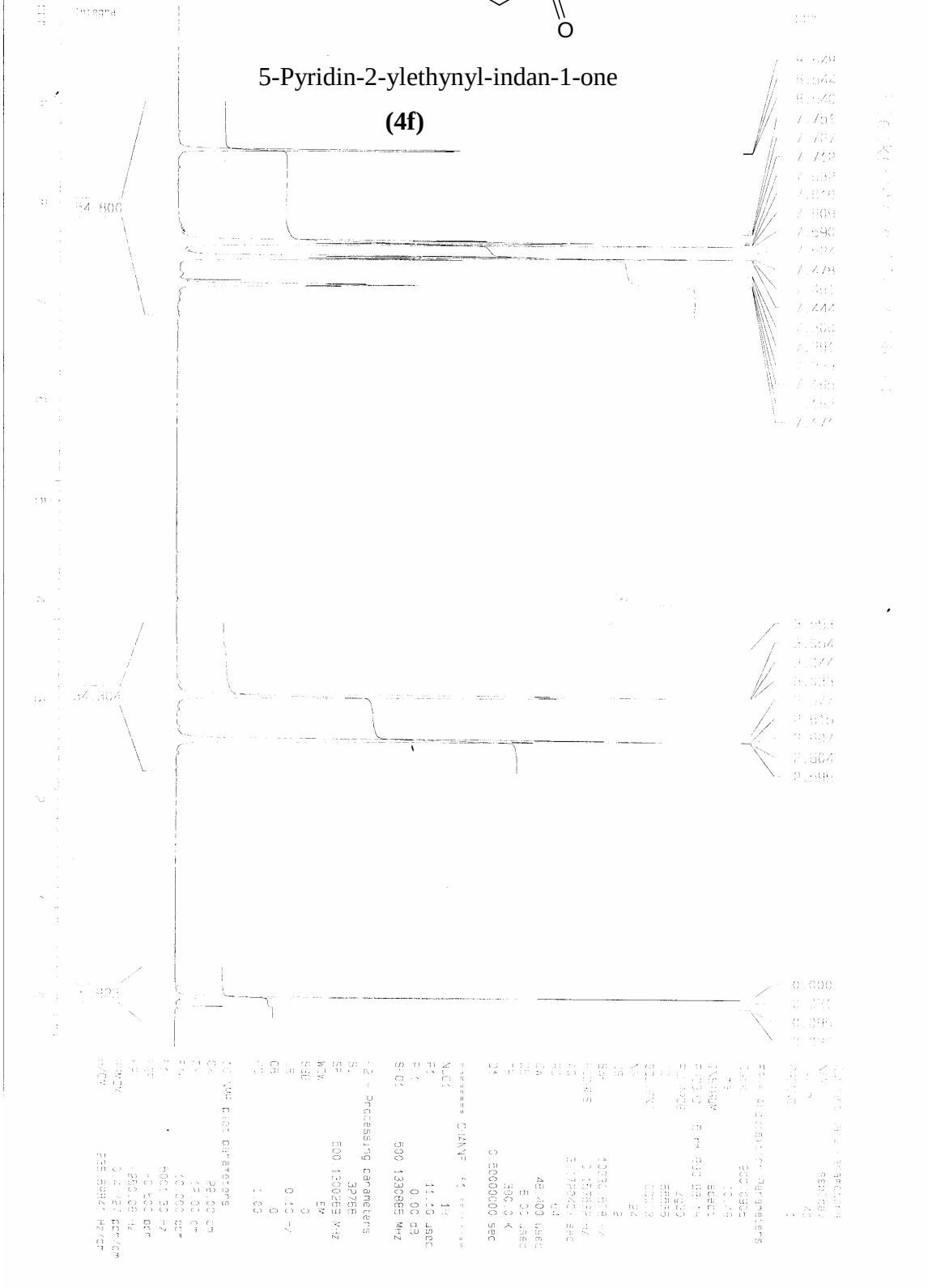

^{13}C-NMR (DEPT)
ppm
N
N
2-Oct-1-ynyl-pyrimidine
(4e)
157.55
119.76
31.69
29.05
28.41
22.86
19.64
14.41

^{1}H-NMR

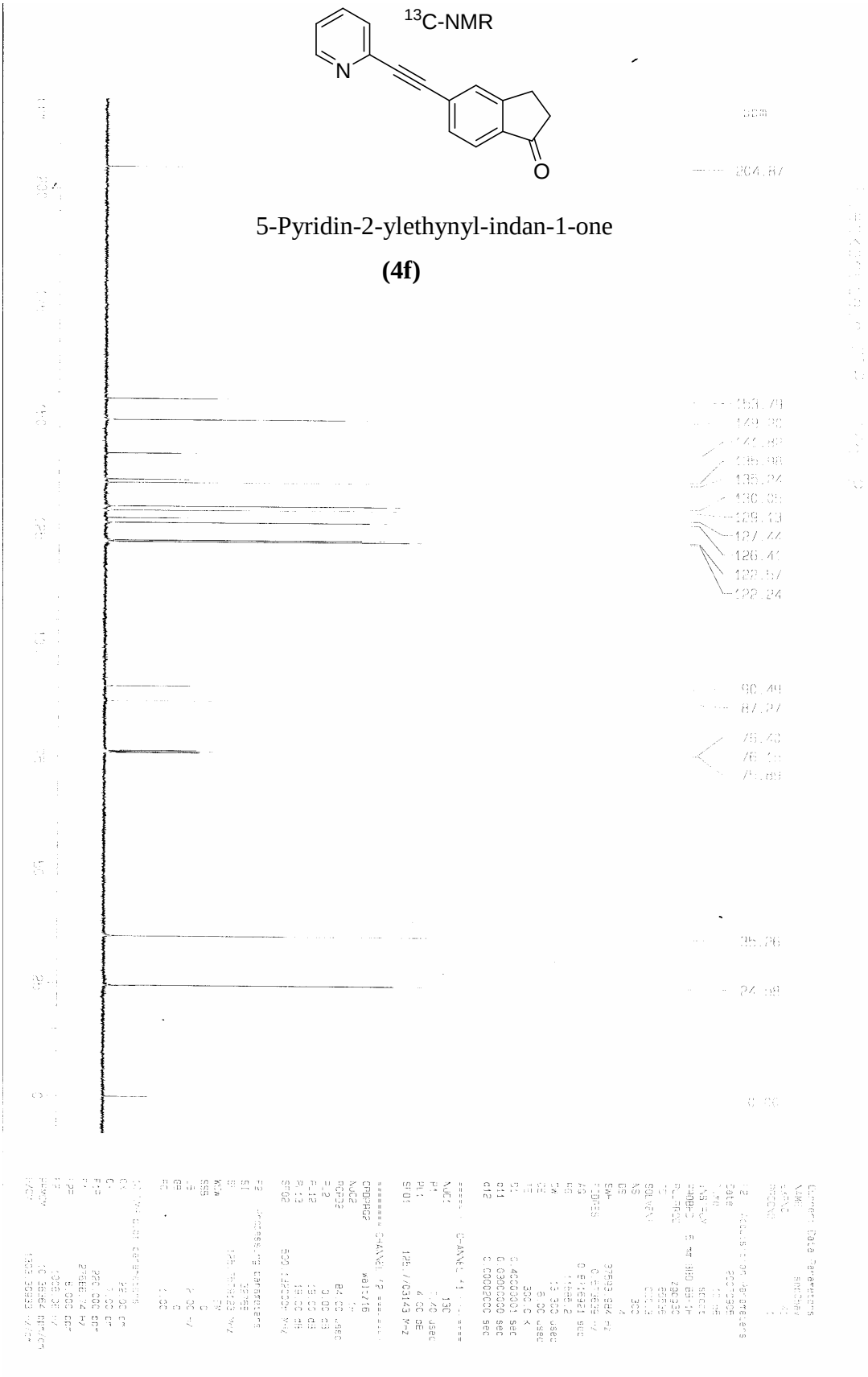


5-Pyridin-2-ylethynyl-indan-1-one

(4f)



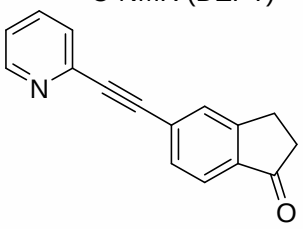
^{13}C-NMR



5-Pyridin-2-ylethynyl-indan-1-one

(4f)

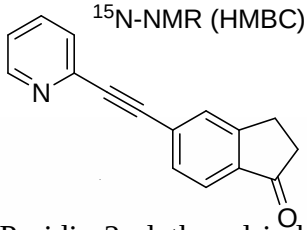
^{13}C-NMR (DEPT)



5-Pyridin-2-ylethynyl-indan-1-one

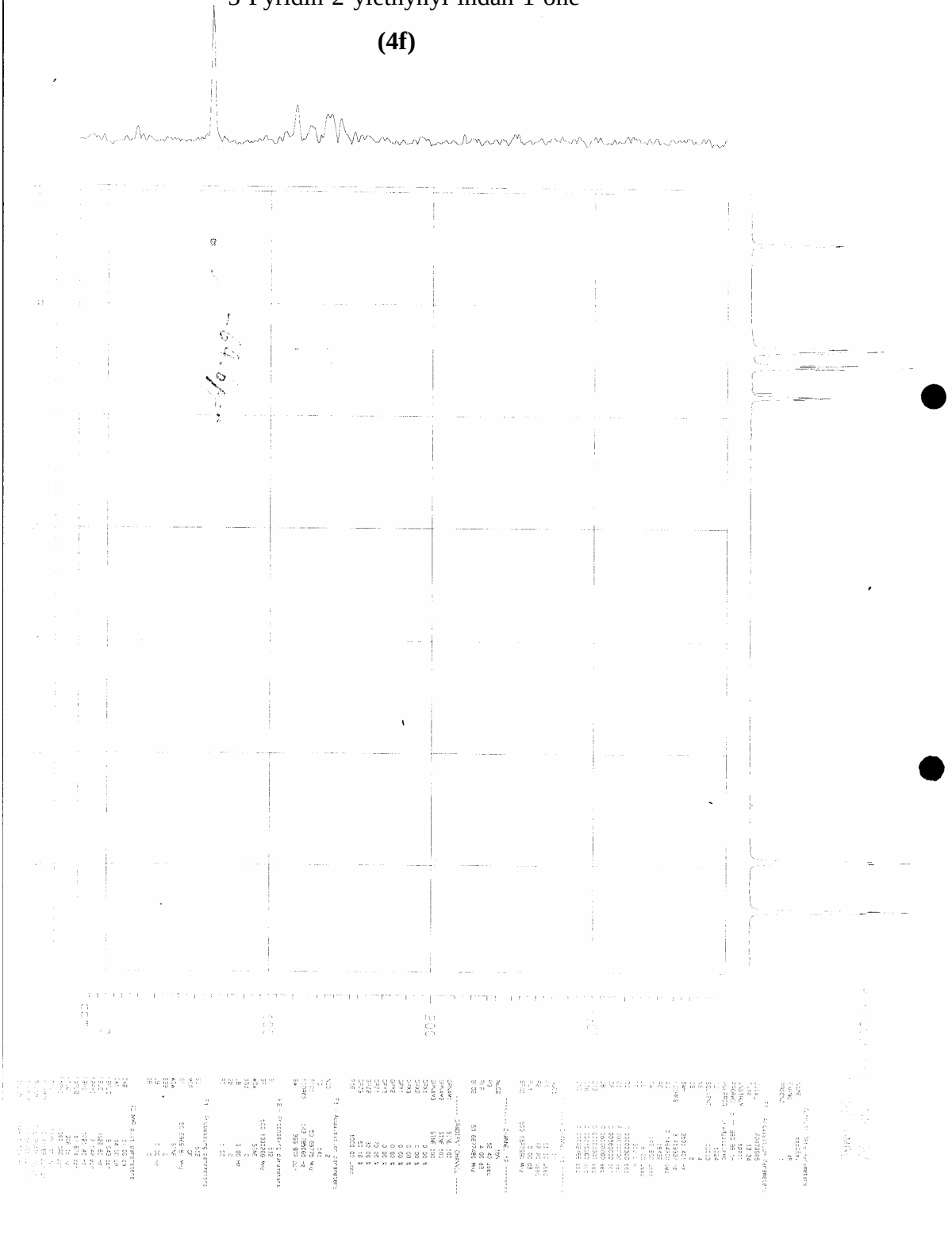
(4f)

^{15}N-NMR (HMBC)

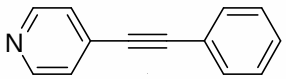


5-Pyridin-2-ylethynyl-indan-1-one

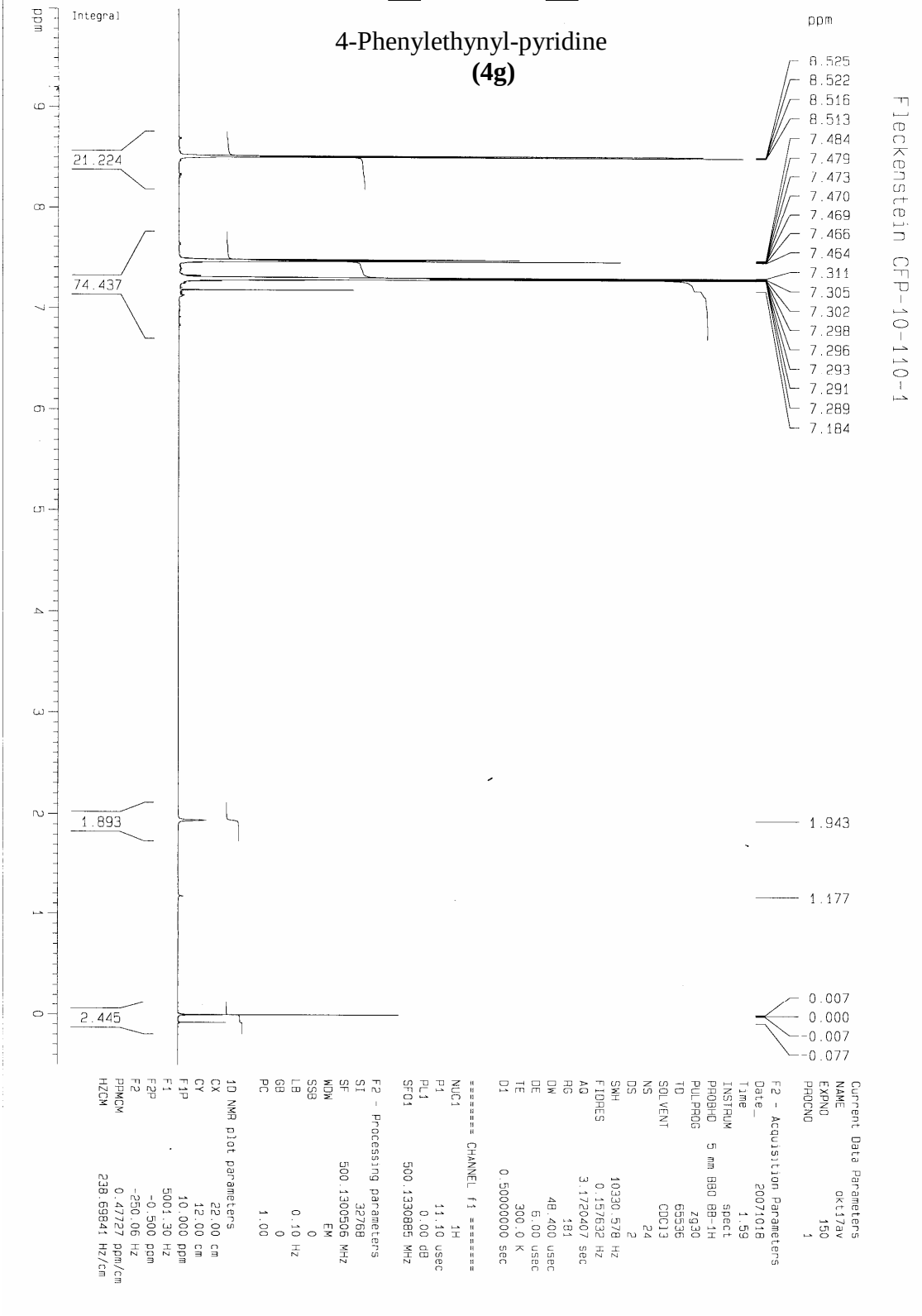
(4f)



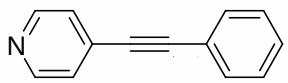
^{1}H-NMR



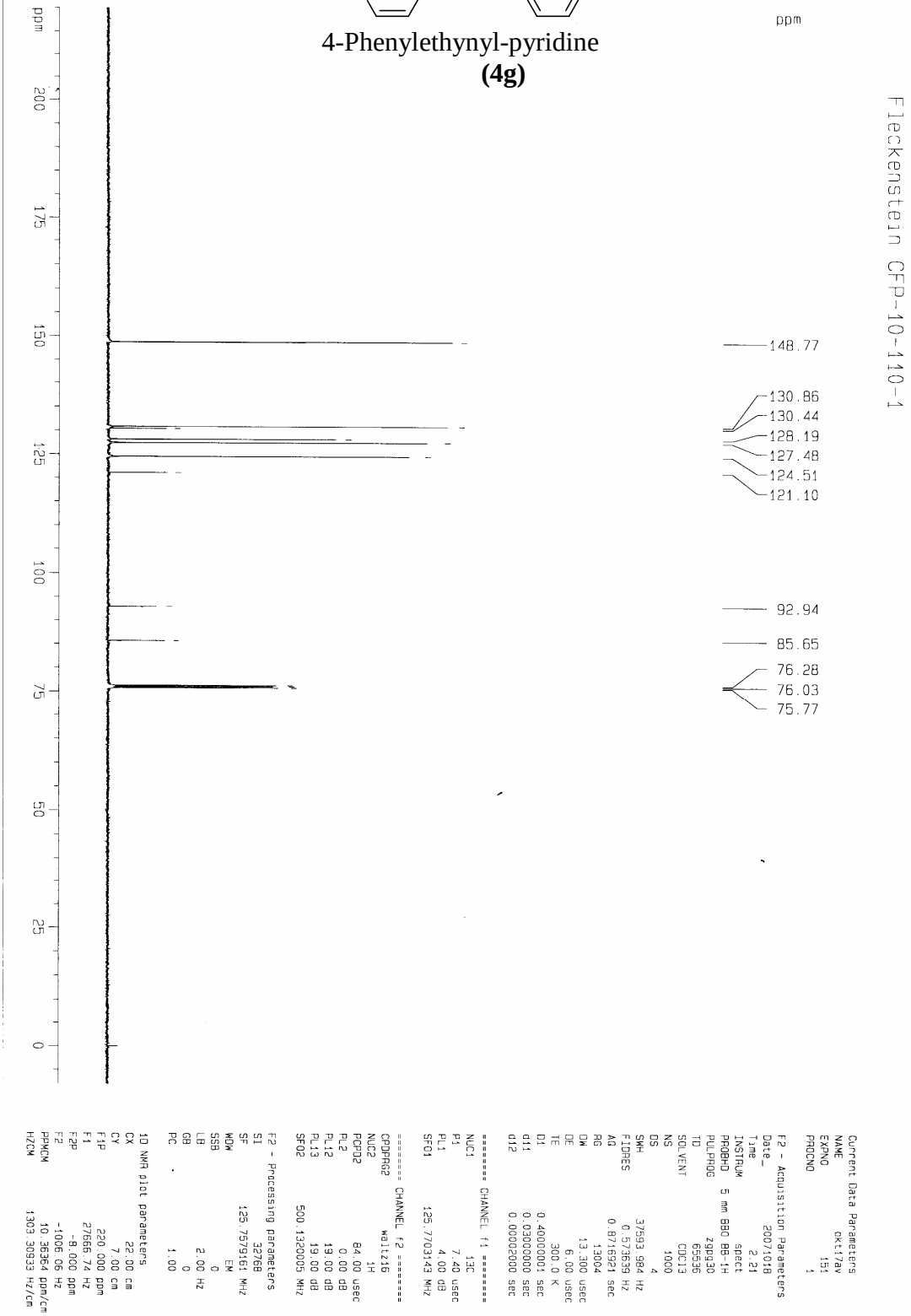
4-Phenylethynyl-pyridine
(4g)



^{13}C-NMR



4-Phenylethynyl-pyridine
(4g)



Current Data Parameters
NAME ckt17av
EXPNO 151
PROCNO 1

F2 - Acquisition Parameters
Date_ 20071018
Time_ 2.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 4
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8716821 sec
RG 13004
DW 13.300 usec
DE 6.00 usec
TE 300.0 K
D1 0.40000001 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
PL1 4.00 dB
SFO1 125.7703143 MHz

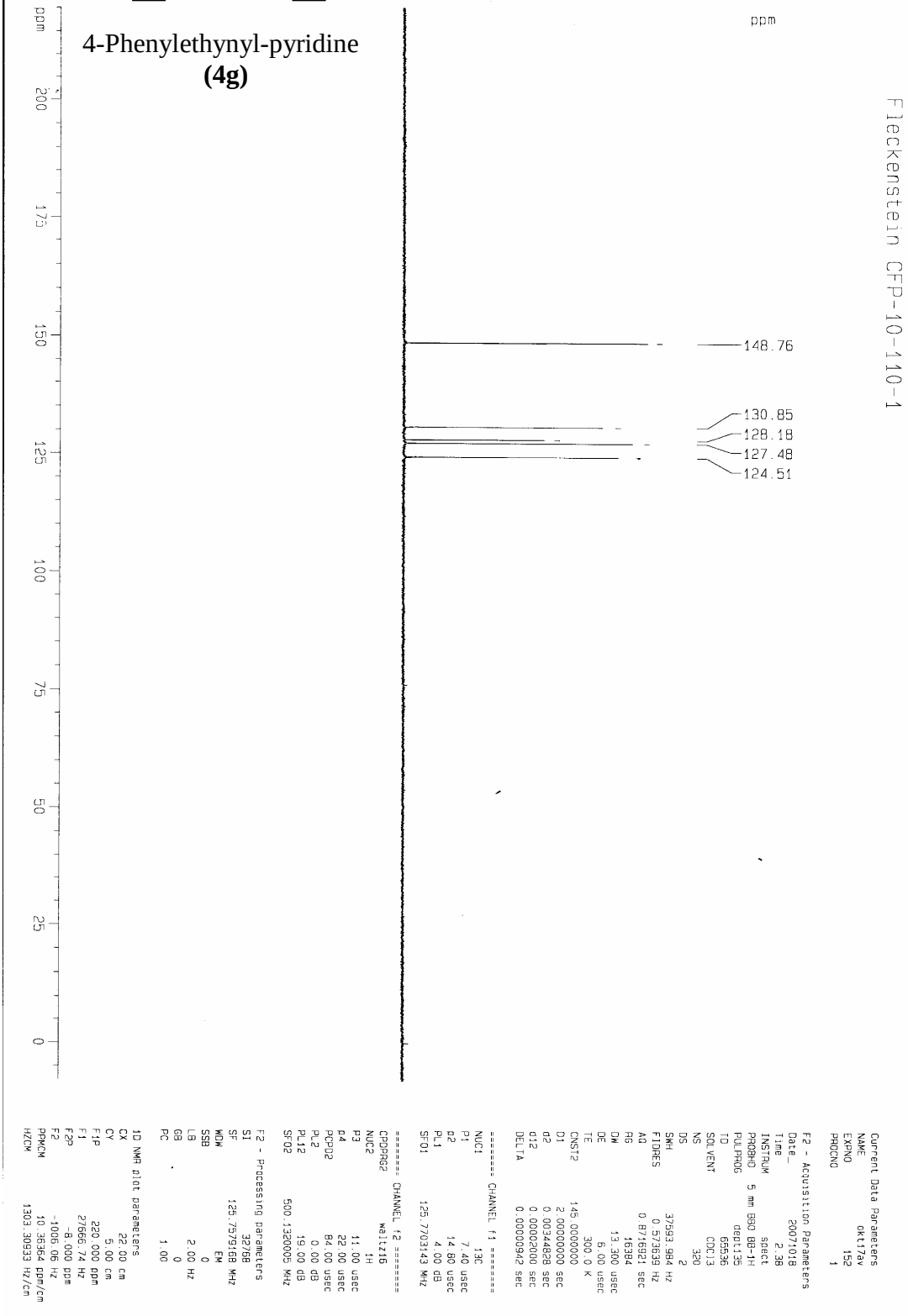
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7579161 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

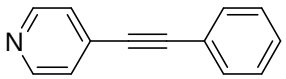
1D NMR plot parameters
CX 22.00 cm
CY 7.00 cm
F1P 220.000 ppm
F1 27666.74 Hz
F2P -8.000 ppm
F2 -1006.06 Hz
PPMCM 10.36364 ppm/cm
HZCM 1303.30933 Hz/cm

^{13}C-NMR (DEPT)

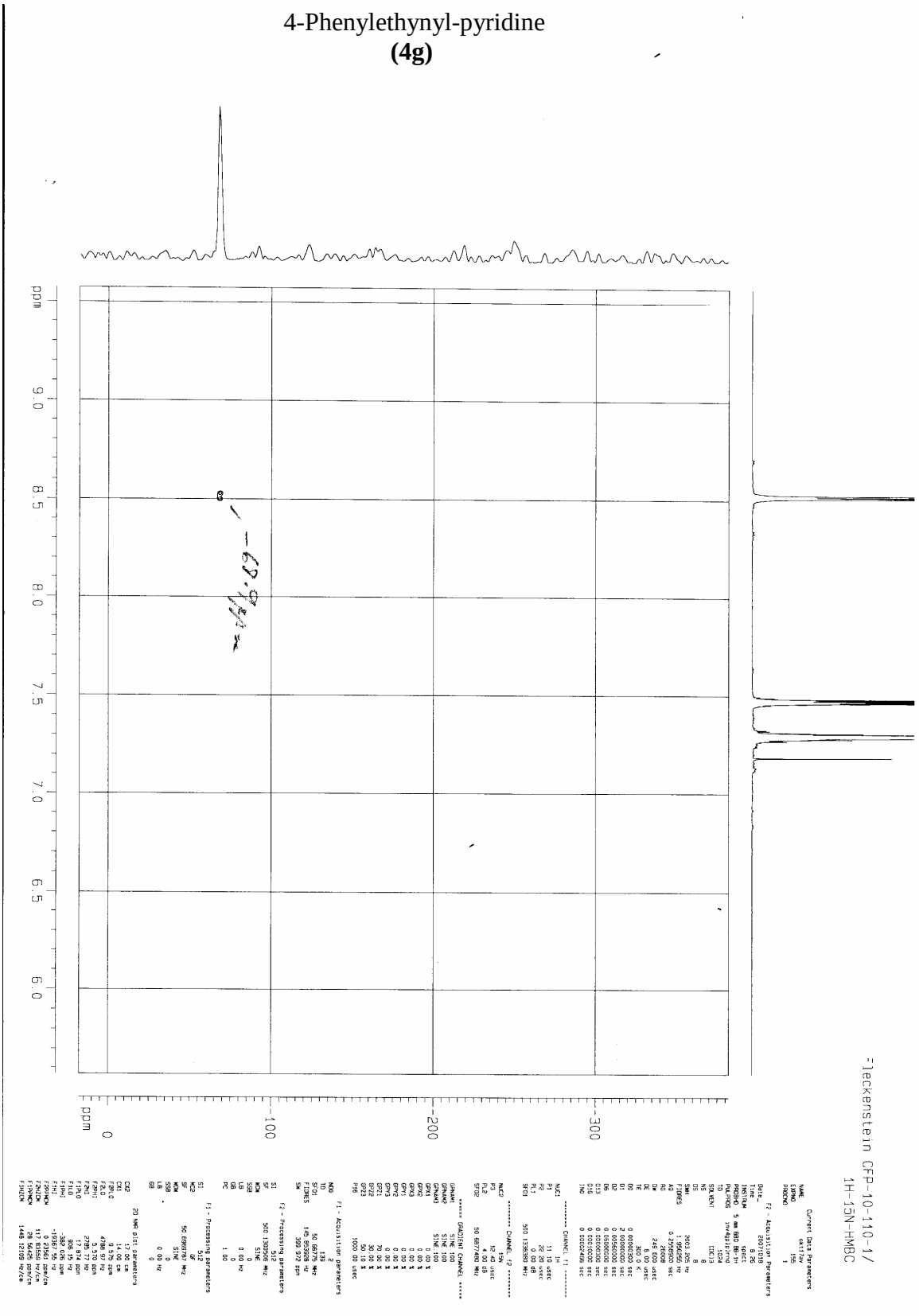
4-Phenylethynyl-pyridine
(4g)



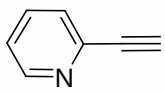
^{15}N-NMR (HMBC)



4-Phenylethynyl-pyridine
(4g)

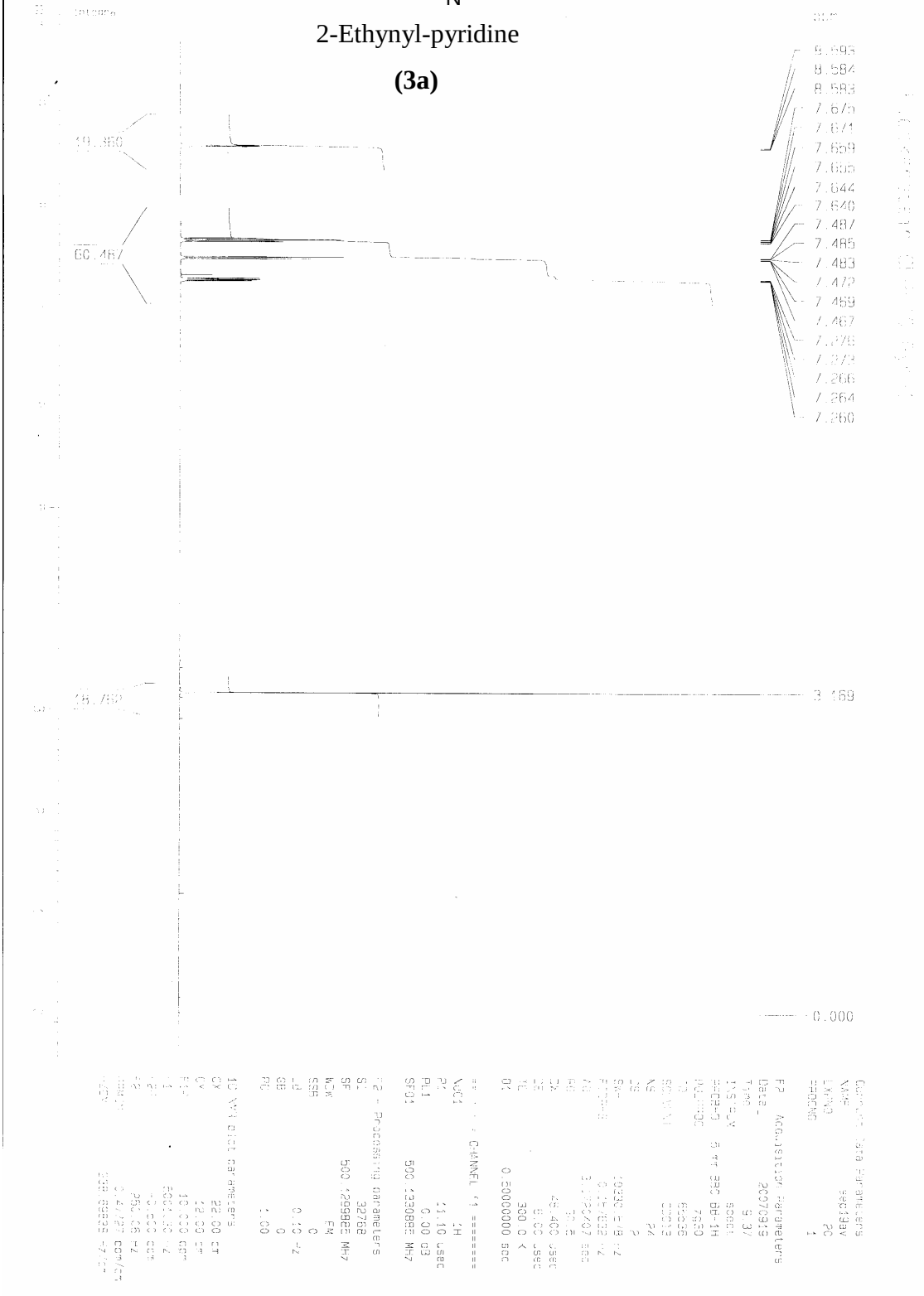


^{1}H-NMR

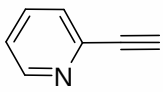


2-Ethynyl-pyridine

(3a)

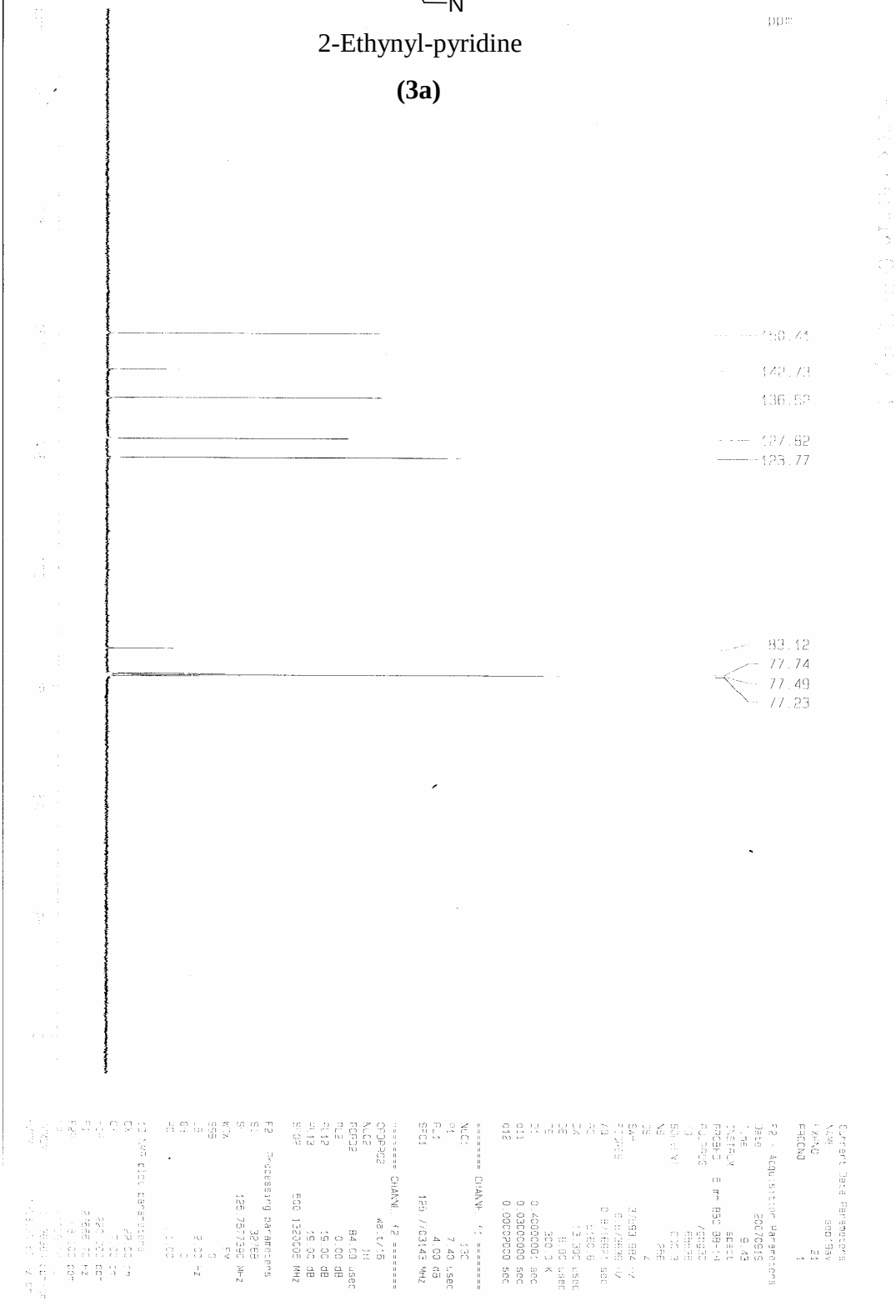


^{13}C-NMR

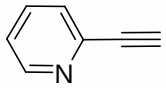


2-Ethynyl-pyridine

(3a)

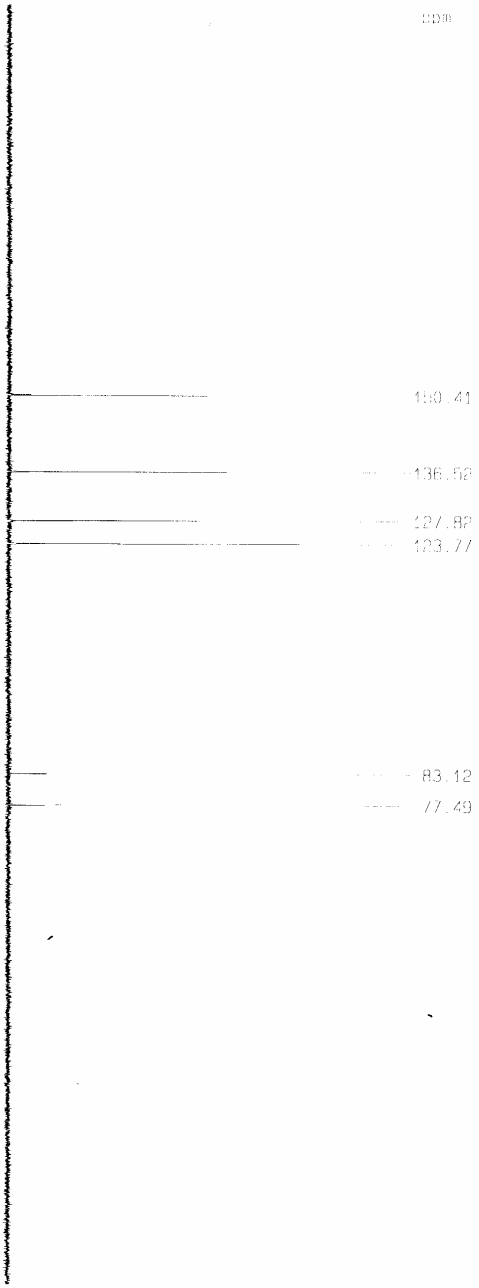


^{13}C-NMR (DEPT)

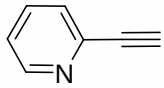


2-Ethynyl-pyridine

(3a)

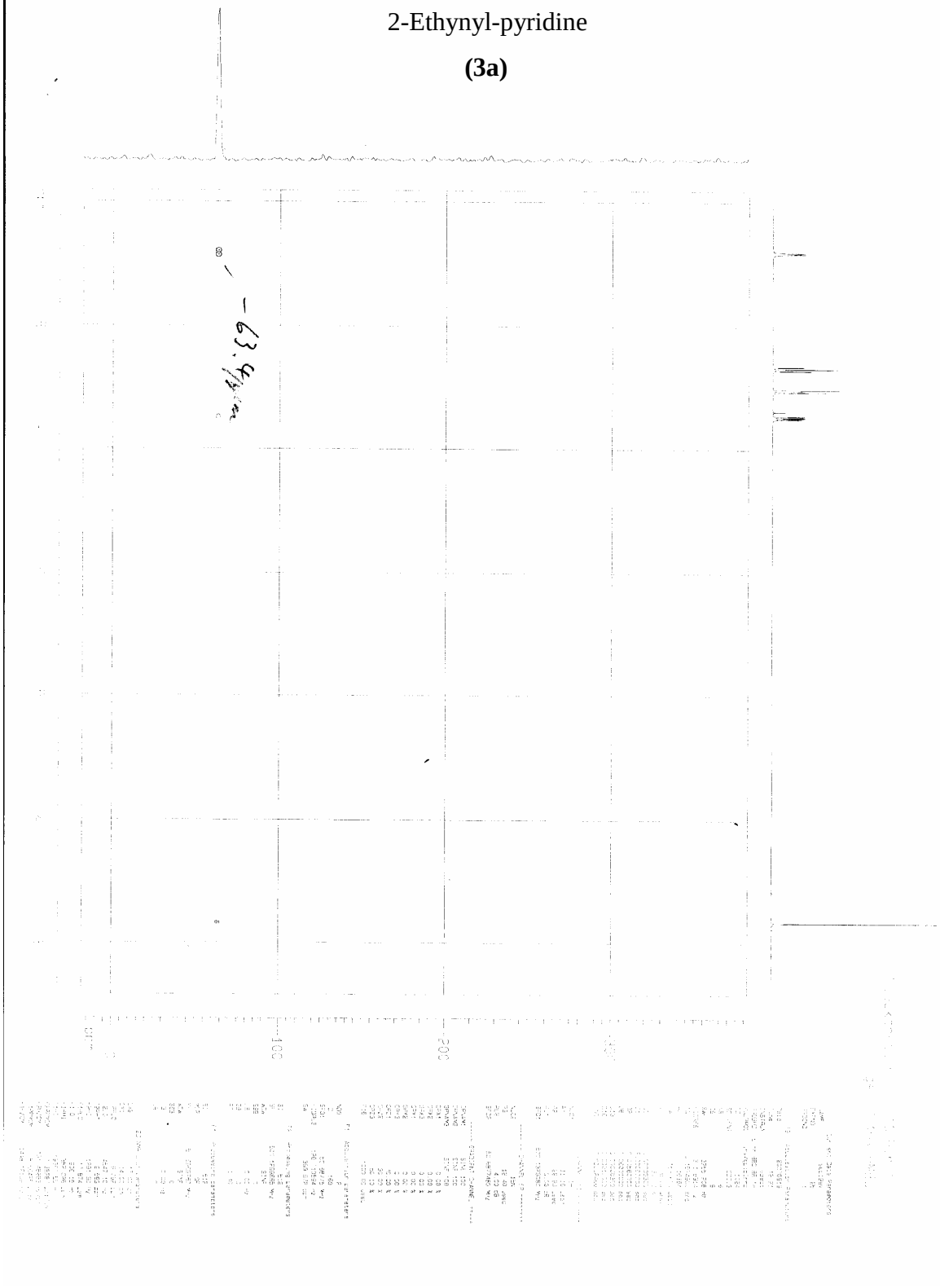


^{15}N-NMR (HMBC)

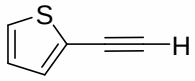


2-Ethynyl-pyridine

(3a)

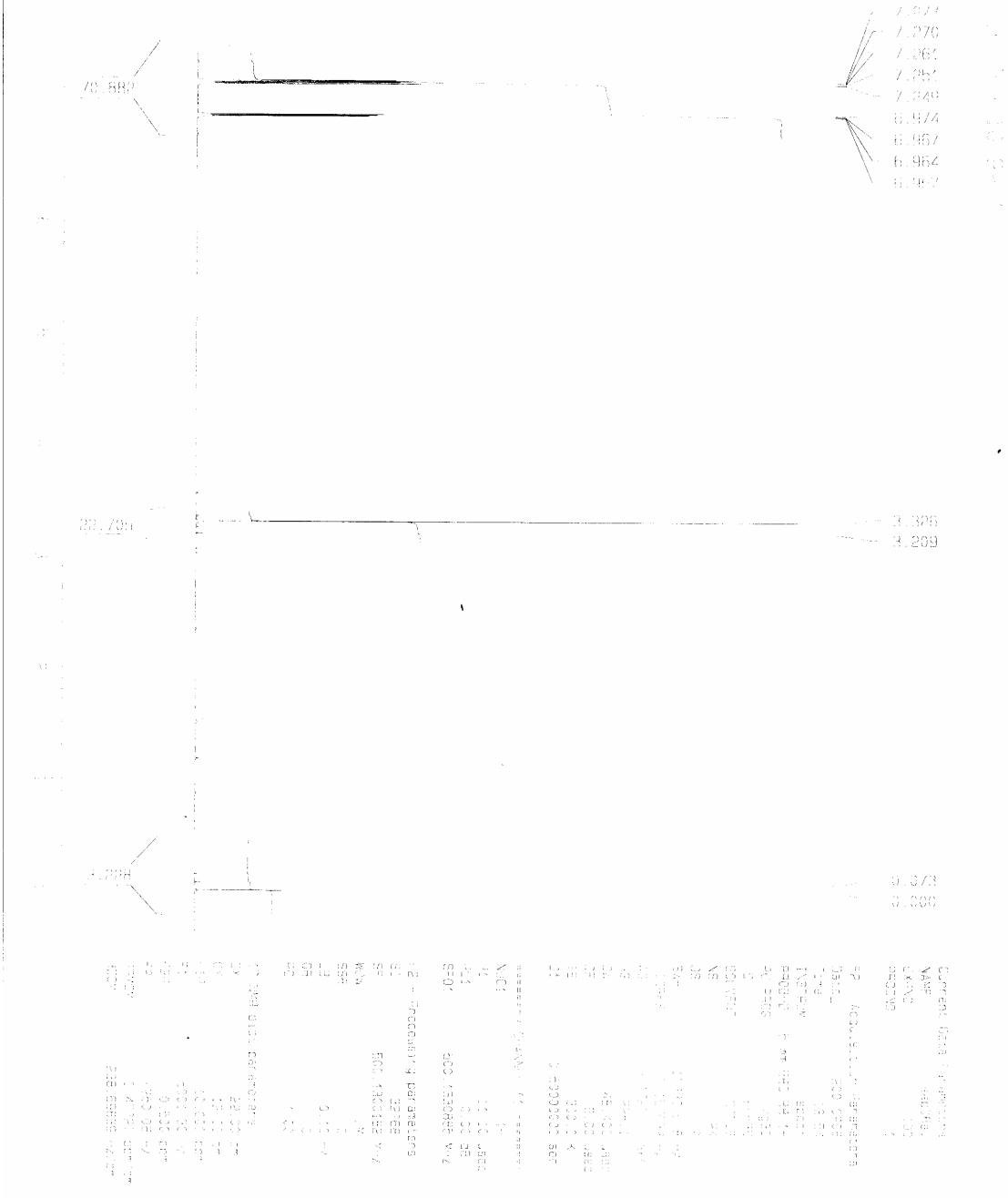


^{1}H-NMR

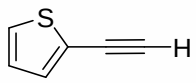


2-Ethynyl-thiophene

(3e)



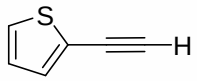
^{13}C-NMR



2-Ethynyl-thiophene

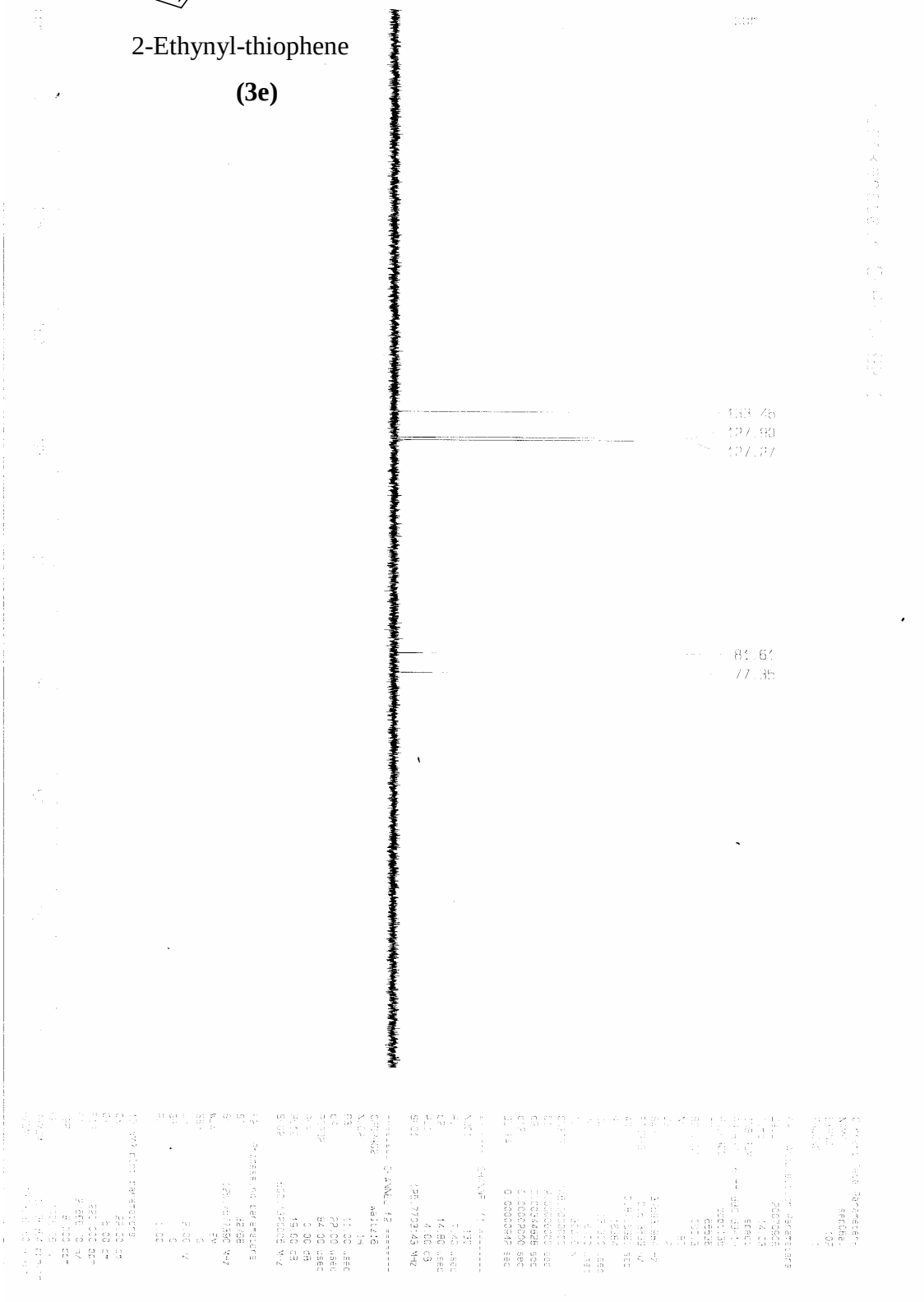
(3e)

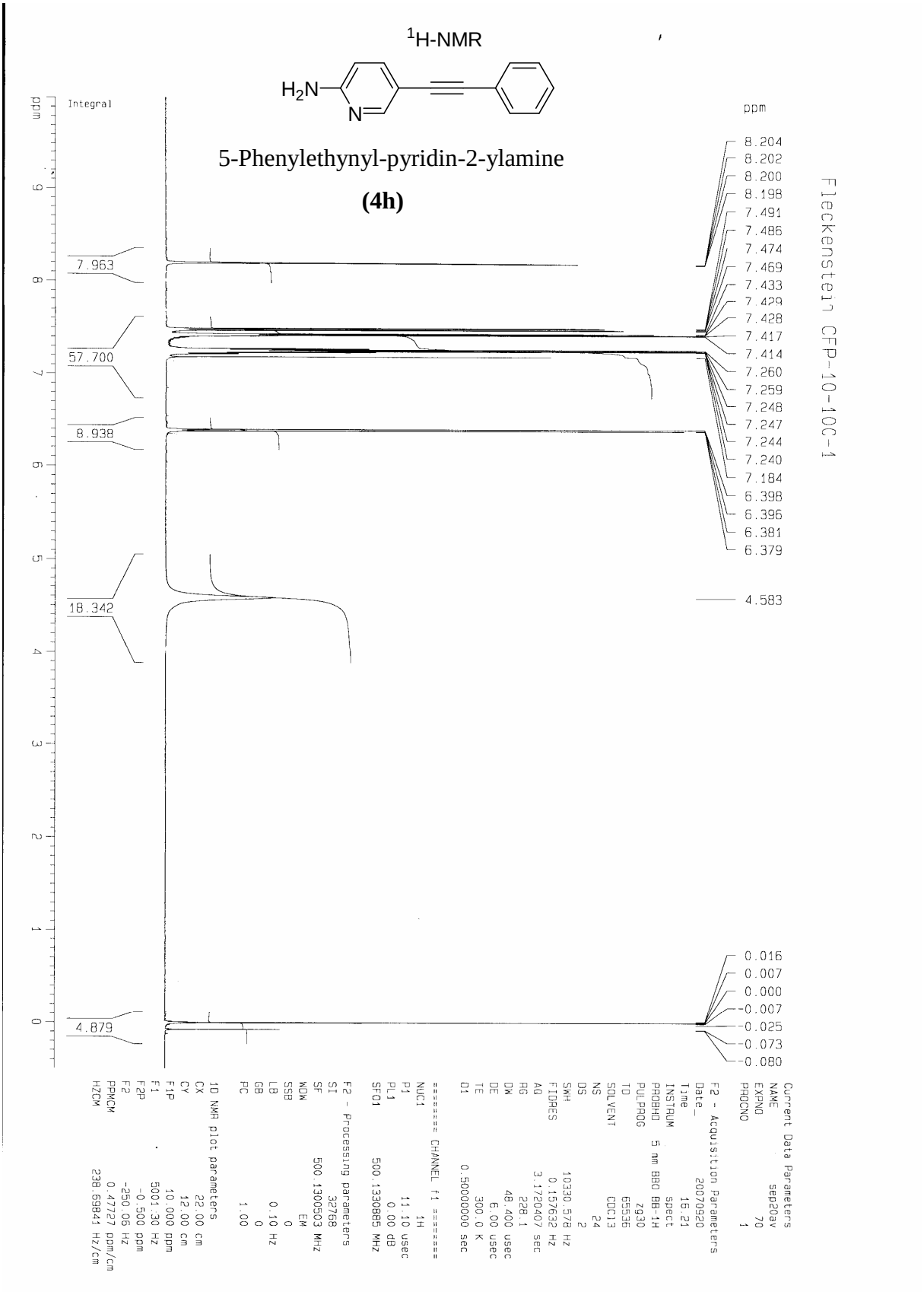
^{13}C-NMR (DEPT)

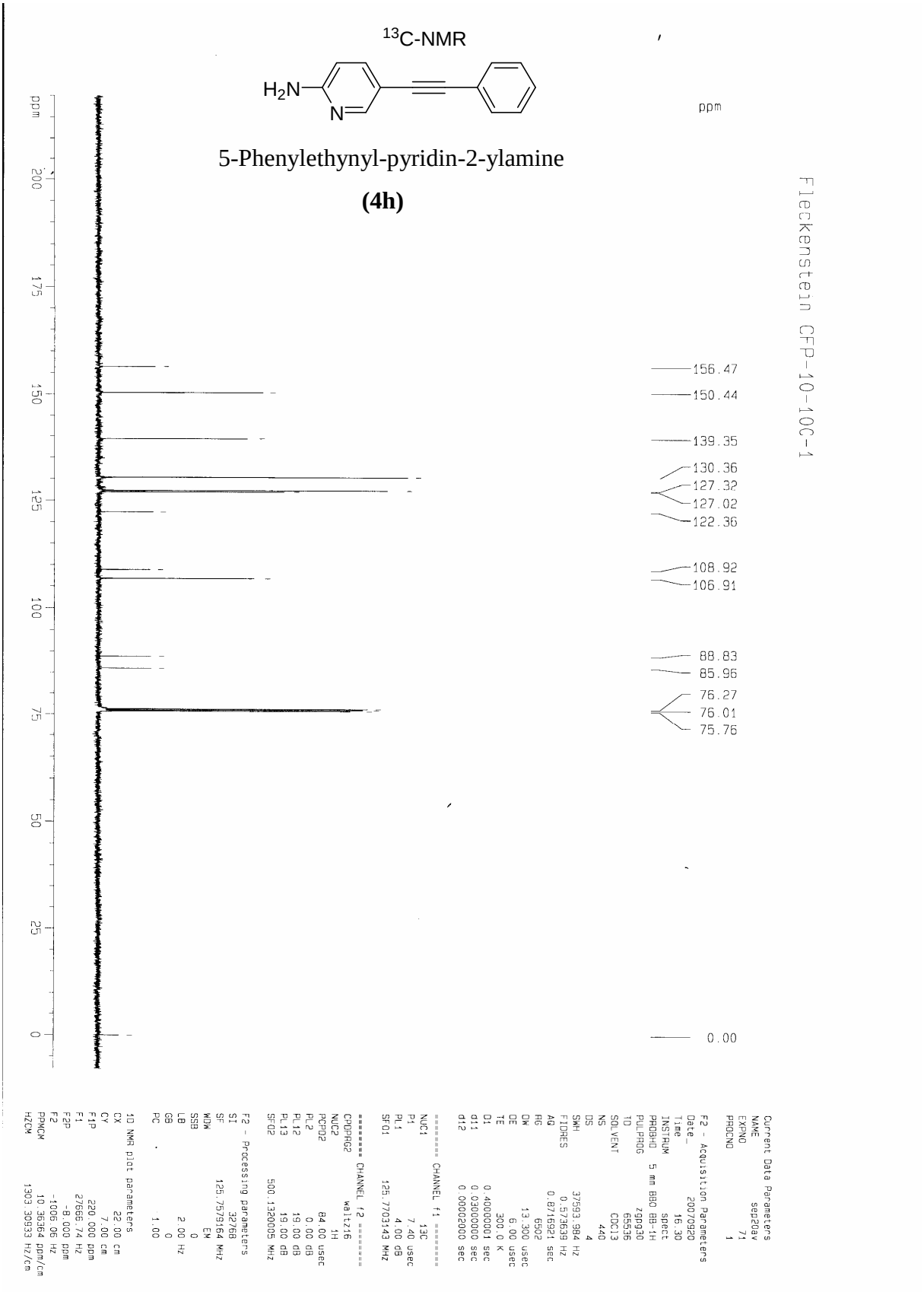


2-Ethynyl-thiophene

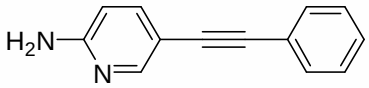
(3e)




^{1}H-NMR
H_2N
N
5-Phenylethynyl-pyridin-2-ylamine
(4h)
Fleckenstein CFP-10-10C-1
ppm
Integral
8.204
8.202
8.200
8.198
7.491
7.486
7.474
7.469
7.433
7.428
7.417
7.414
7.260
7.259
7.248
7.247
7.244
7.240
7.184
6.398
6.396
6.381
6.379
4.583
0.016
0.007
0.000
-0.007
-0.025
-0.073
-0.080
7.963
57.700
8.938
18.342
4.879
Current Data Parameters
NAME sep20av
EXPNO 70
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070920
Time 16.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 228.1
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.50000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.10 usec
PL1 0.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300503 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 12.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.05 Hz
PPMCM 0.47727 ppm/cm
HZCM 238.69841 Hz/cm


13C-NMR
H2N
N
ppm
5-Phenylethynyl-pyridin-2-ylamine
(4h)
Fleckenstein CFP-10-10C-1
156.47
150.44
139.35
130.36
127.32
127.02
122.36
108.92
106.91
88.83
85.96
76.27
76.01
75.76
0.00
Current Data Parameters
NAME sep20ay
EXPNO 71
PROCNO 1
F2 - Acquisition Parameters
Date_ 20070920
Time 16.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 440
DS 4
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8716921 sec
RG 6502
DW 13.300 usec
DE 6.00 usec
TE 300.0 K
D1 0.40000001 sec
D11 0.03000000 sec
D12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
PL1 4.00 dB
SFO1 125.7703143 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7579164 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 7.00 cm
F1P 220.000 ppm
F1 27666.74 Hz
F2P -8.000 ppm
F2 -1006.06 Hz
PPMCM 10.36364 ppm/cm
HZCM 1303.30933 Hz/cm

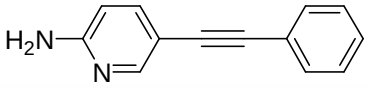
^{13}C-NMR (DEPT)



5-Phenylethynyl-pyridin-2-ylamine

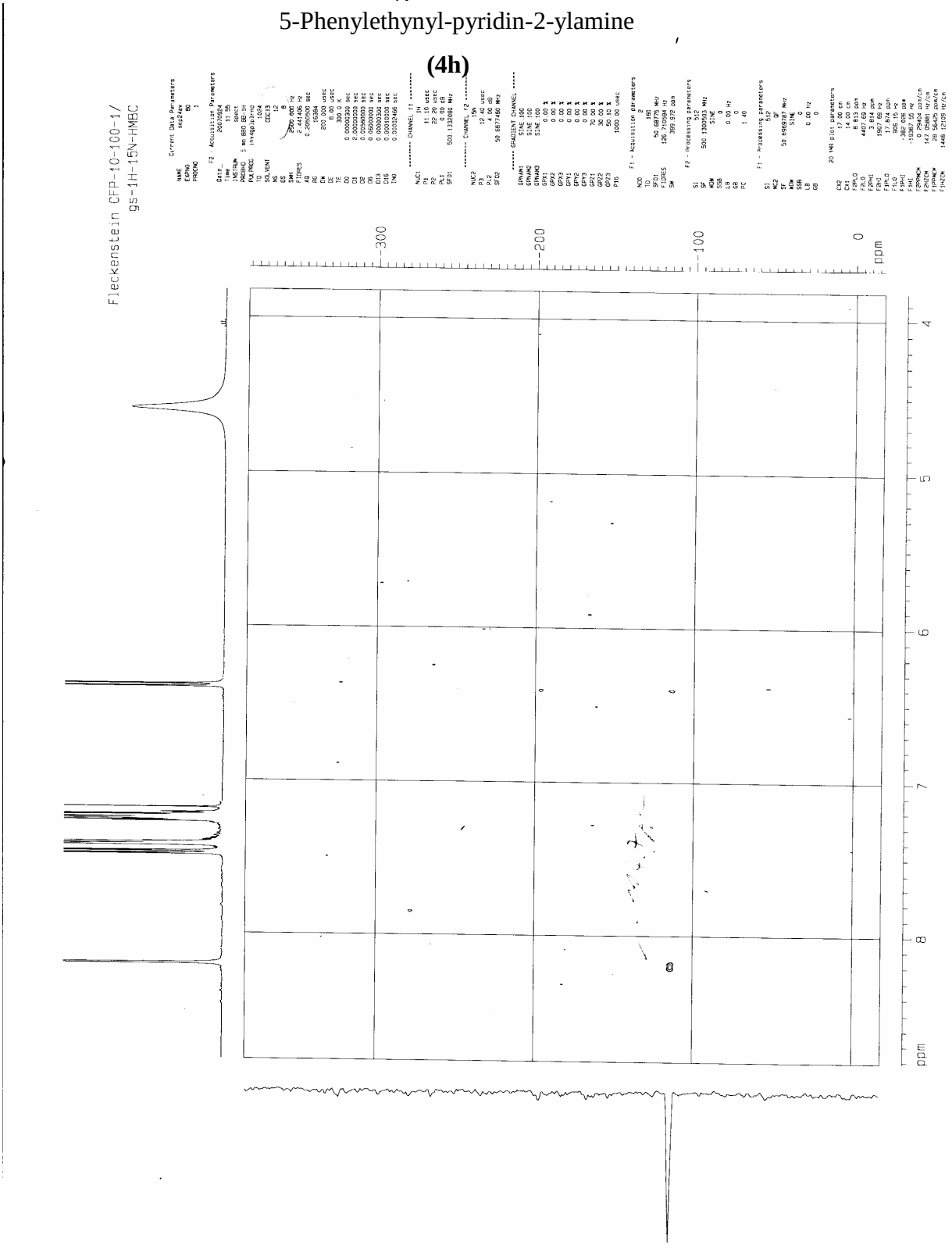
(4h)

^{15}N-NMR (HMBC)

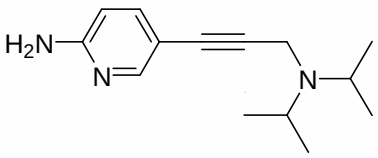


5-Phenylethynyl-pyridin-2-ylamine

(4h)



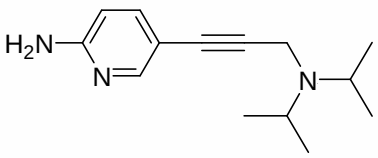
^{1}H-NMR



5-(3-Diisopropylamino-prop-1-ynyl)-pyridin-2-ylamine

(4i)

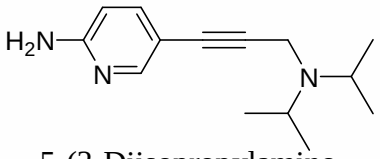
^{13}C-NMR



5-(3-Diisopropylamino-prop-1-ynyl)-pyridin-2-ylamine

(4i)

^{13}C-NMR (DEPT)



5-(3-Diisopropylamino-prop-1-ynyl)-pyridin-2-ylamine

(4i)

Fleckenstein CFP-10-103-1

Current Data Parameters
NAME Sep21ay
EXPNO 52
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070921
Time 11.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8716921 sec
RG 5502
DW 13.300 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000942 sec

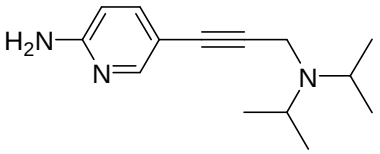
======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
p2 14.80 usec
PL1 4.00 dB
SFO1 125.7703143 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 11.00 usec
p4 22.00 usec
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

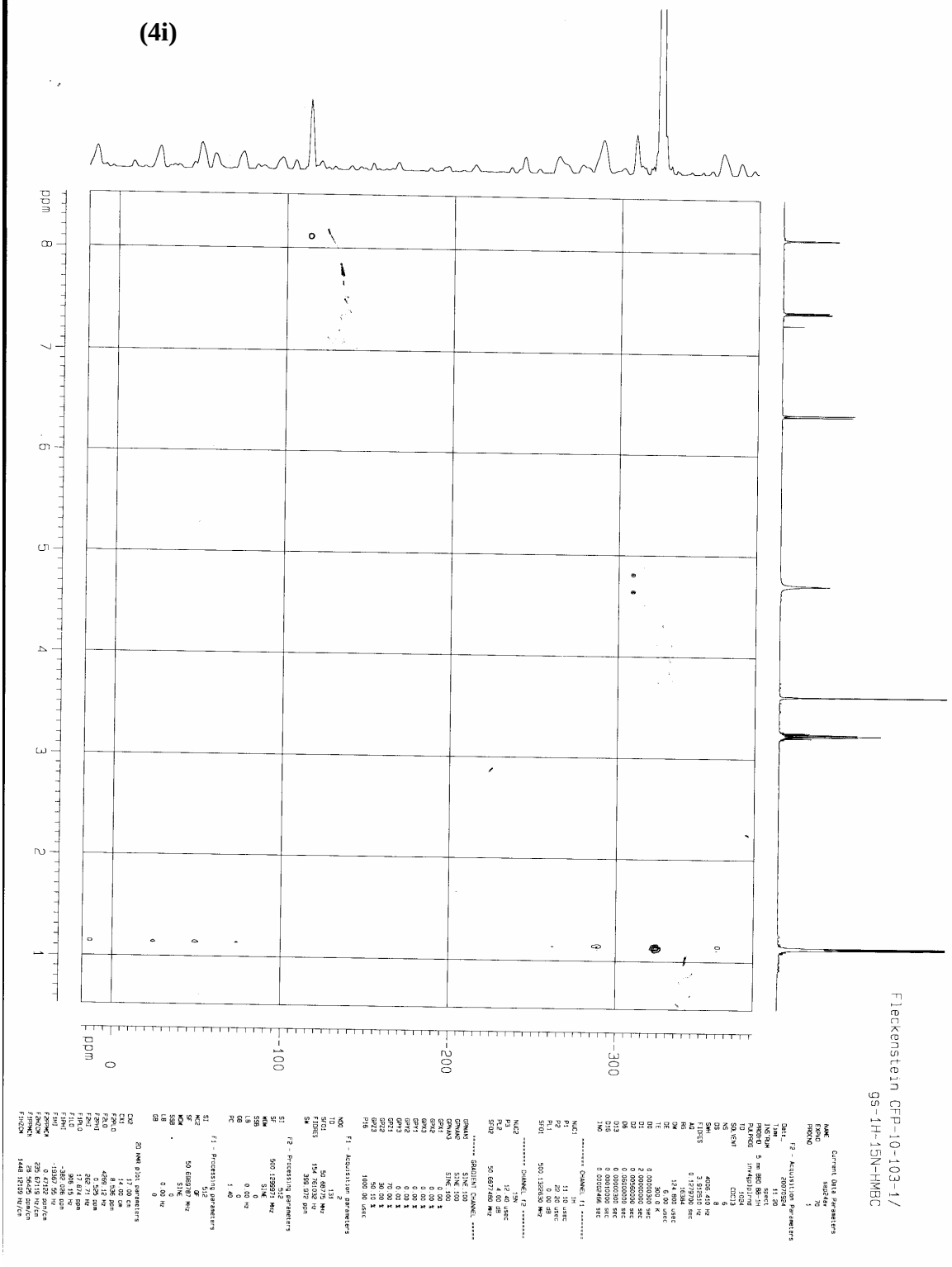
1D NMR plot parameters
CX 22.00 cm
CY 5.00 cm
F1P 220.000 ppm
F1 27666.70 Hz
F2P -8.000 ppm
F2 -1006.06 Hz
PPMCM 10.36364 ppm/cm
HZCM 1303.30750 Hz/cm

^{15}N-NMR (HMBC)

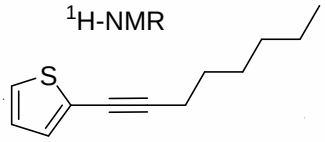


5-(3-Diisopropylamino-prop-1-ynyl)-pyridin-2-ylamine

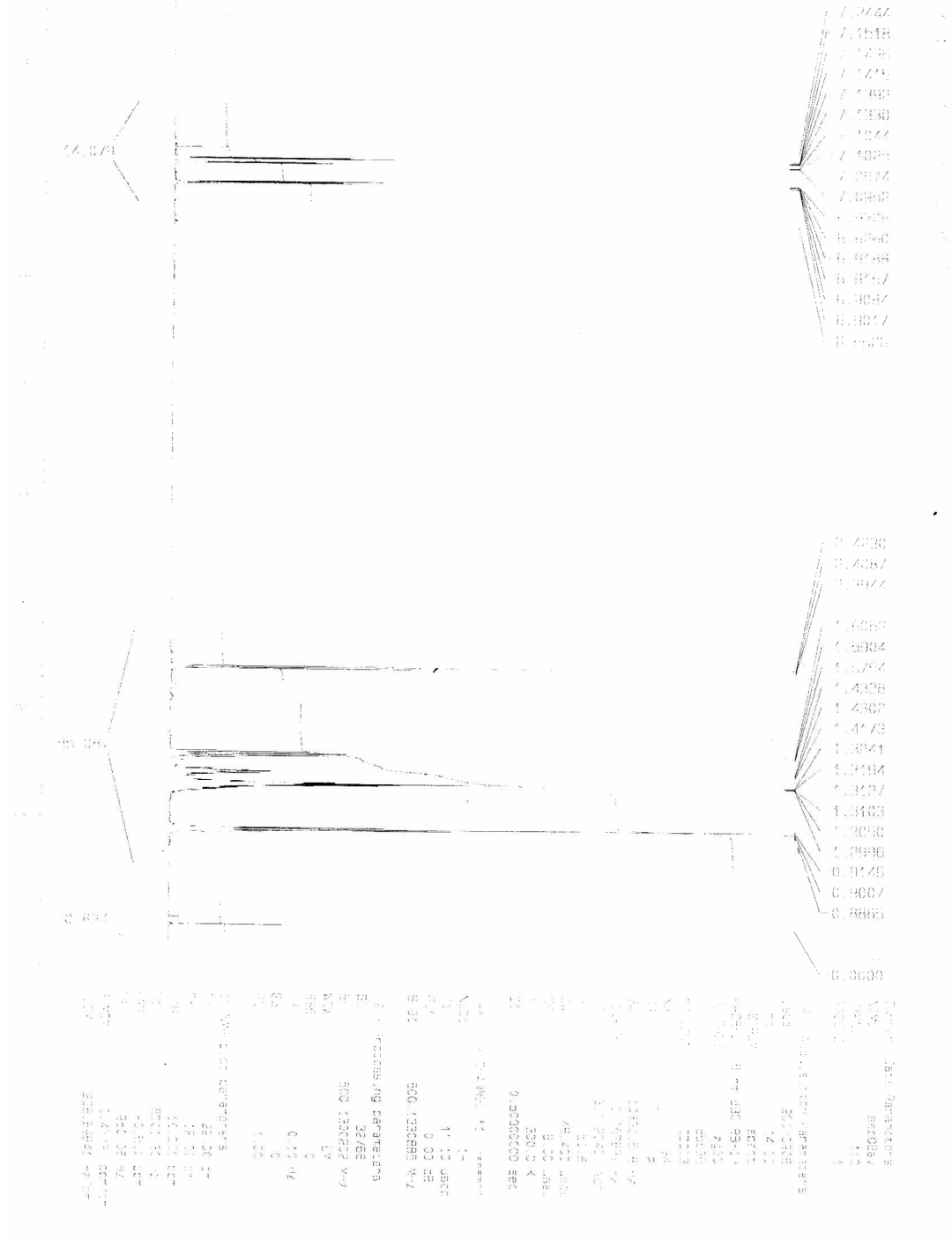
(4i)



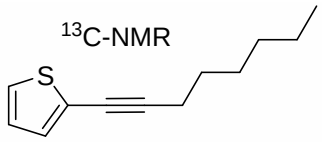
^{1}H-NMR



2-Oct-1-ynyl-thiophene
(4j)

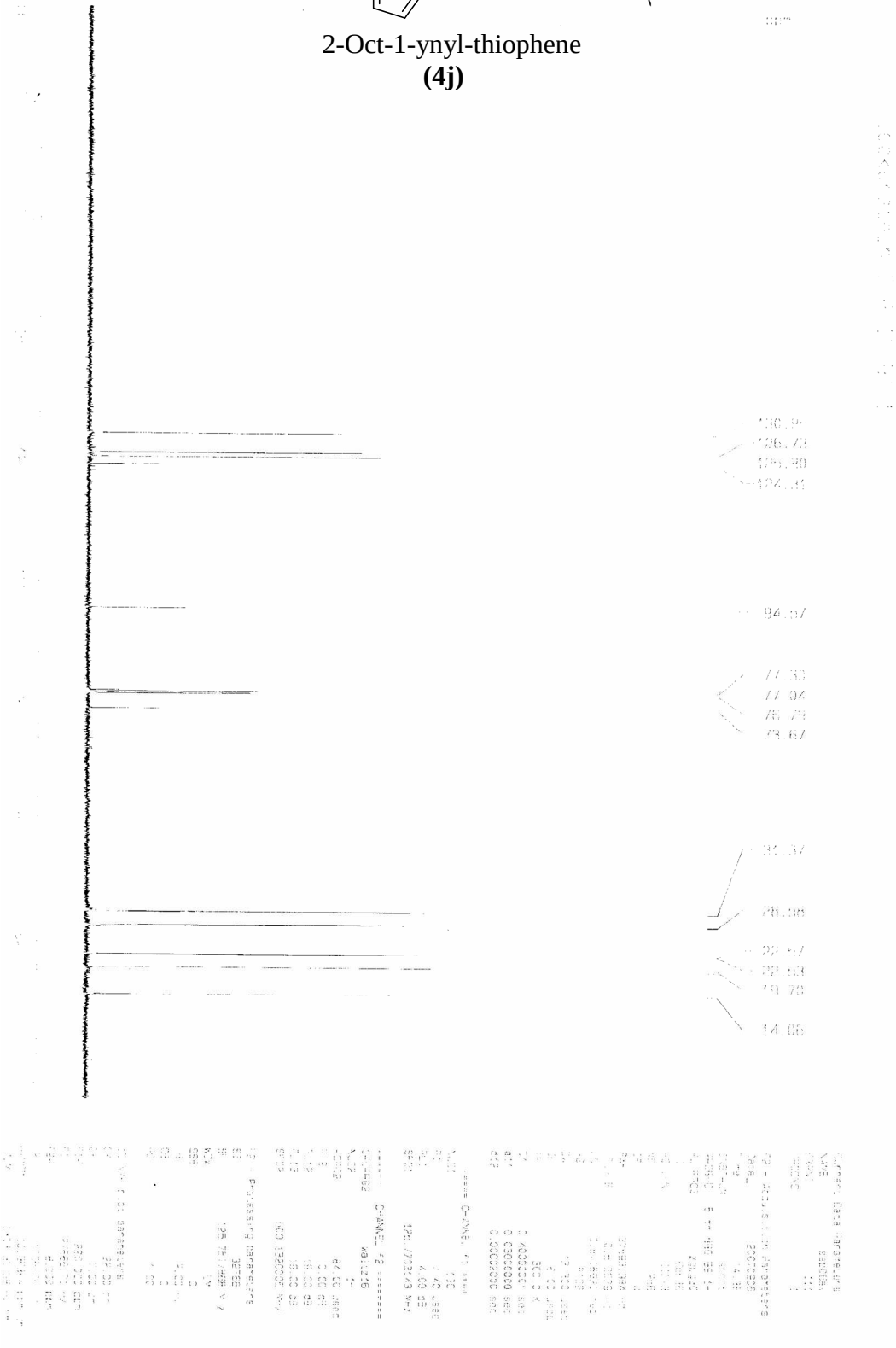


^{13}C-NMR

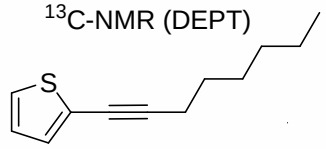


2-Oct-1-ynyl-thiophene

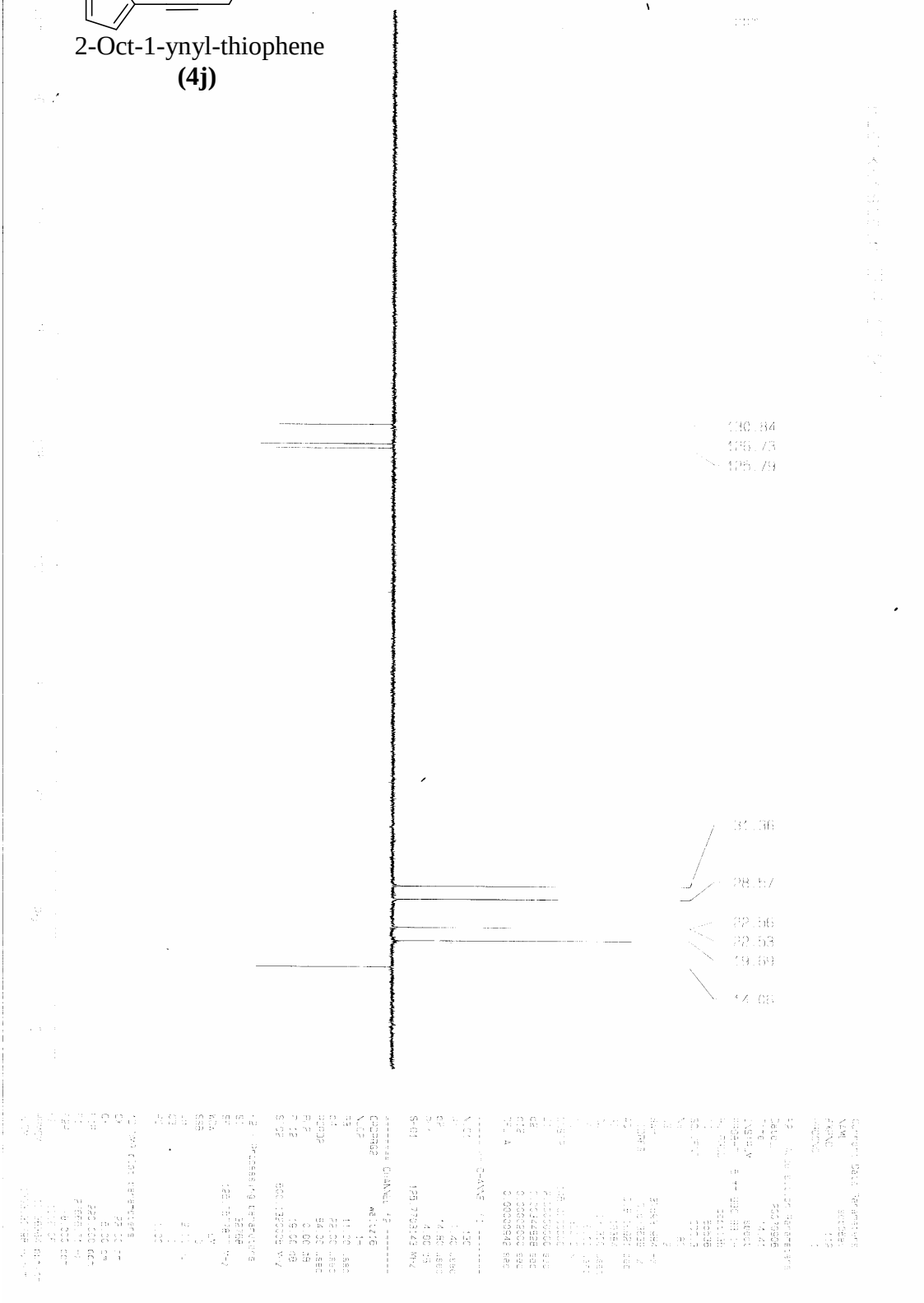
(4j)



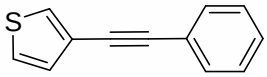
^{13}C-NMR (DEPT)



2-Oct-1-ynyl-thiophene
(4j)

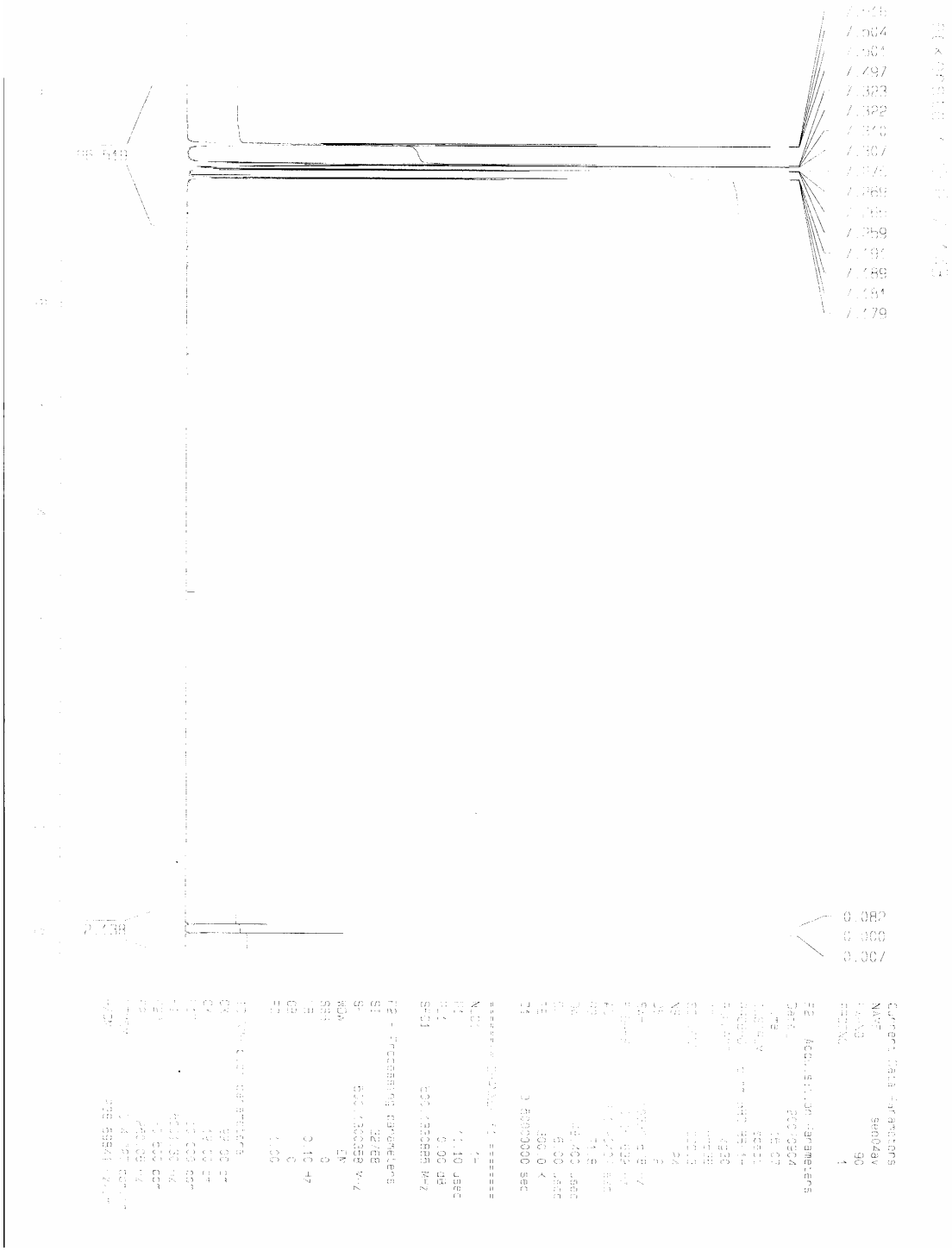


^{1}H-NMR

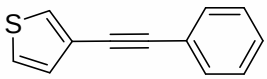


3-Phenylethynyl-thiophene

(4k)

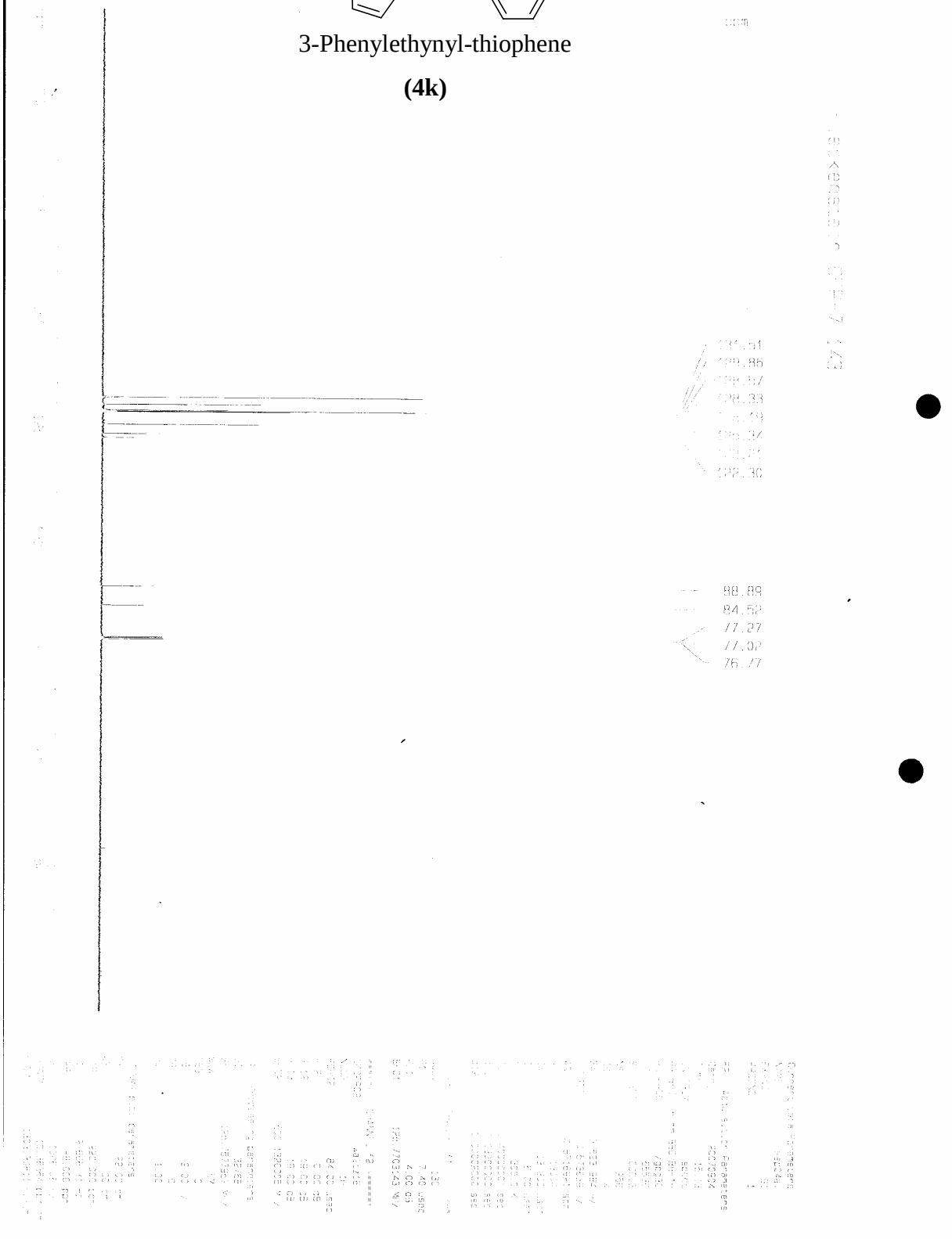


^{13}C-NMR

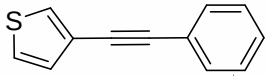


3-Phenylethynyl-thiophene

(4k)

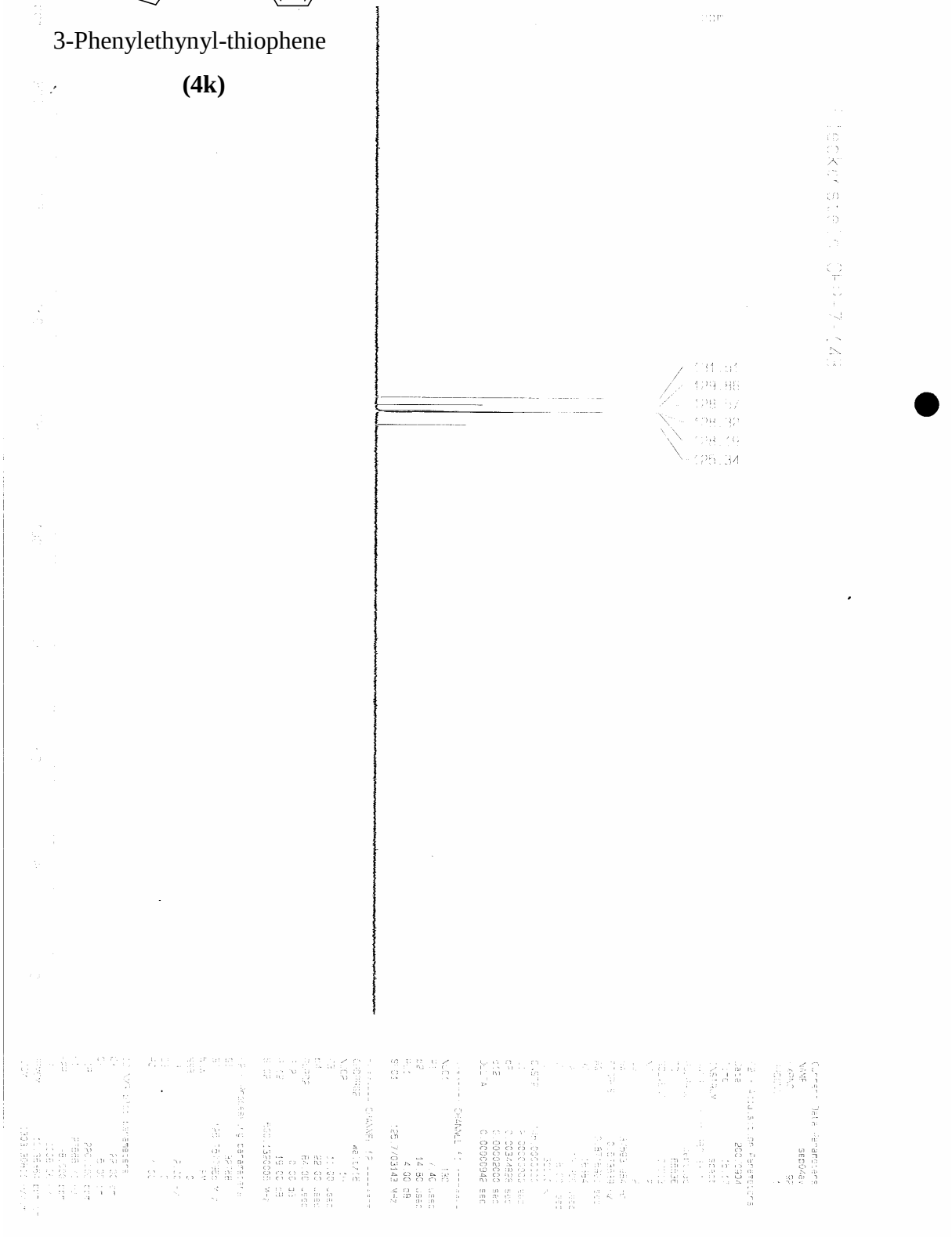


^{13}C-NMR (DEPT)

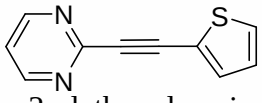


3-Phenylethynyl-thiophene

(4k)

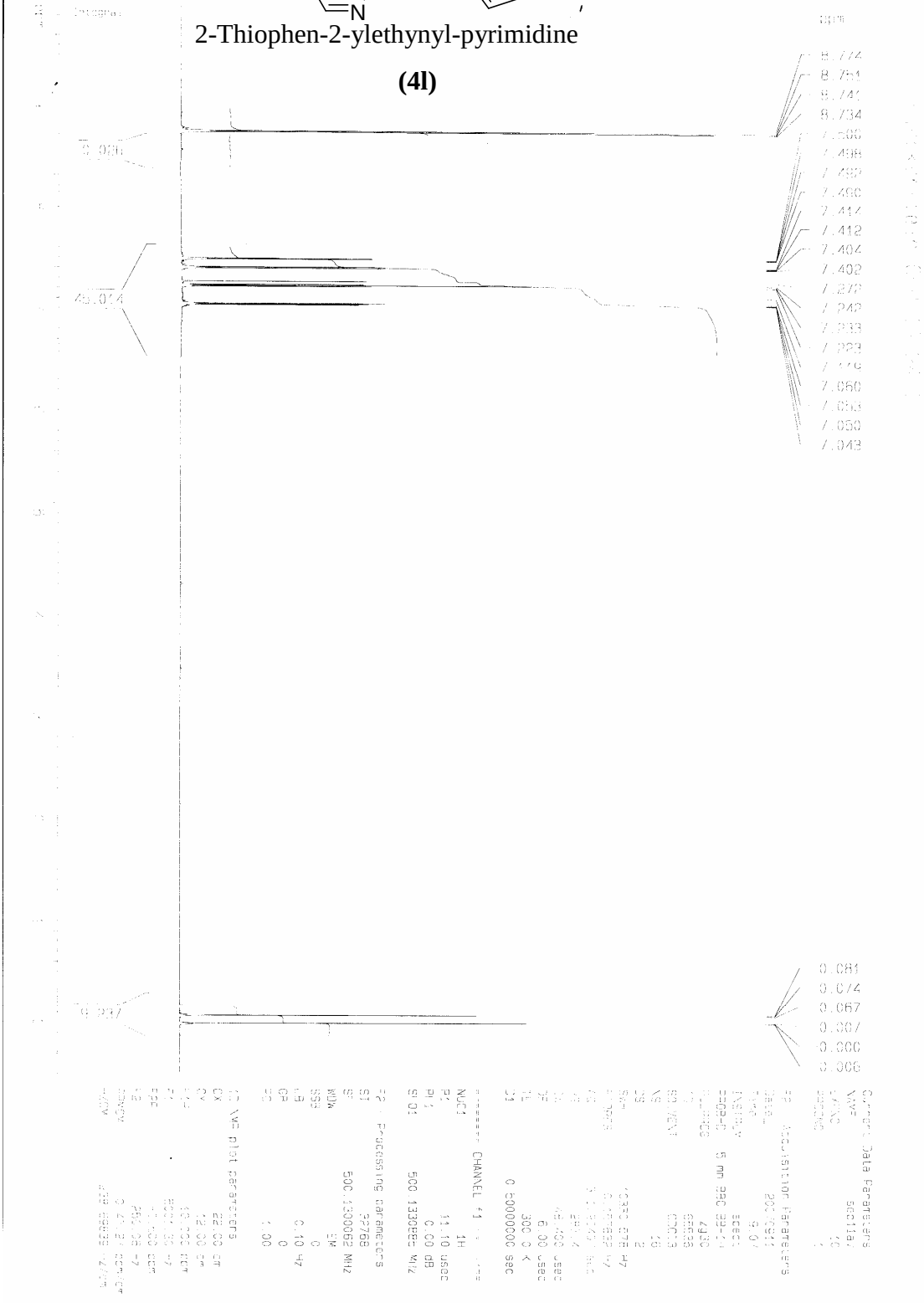


^{1}H-NMR

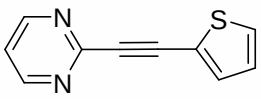


2-Thiophen-2-ylethynyl-pyrimidine

(4l)



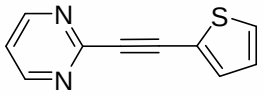
^{13}C-NMR



2-Thiophen-2-ylethynyl-pyrimidine

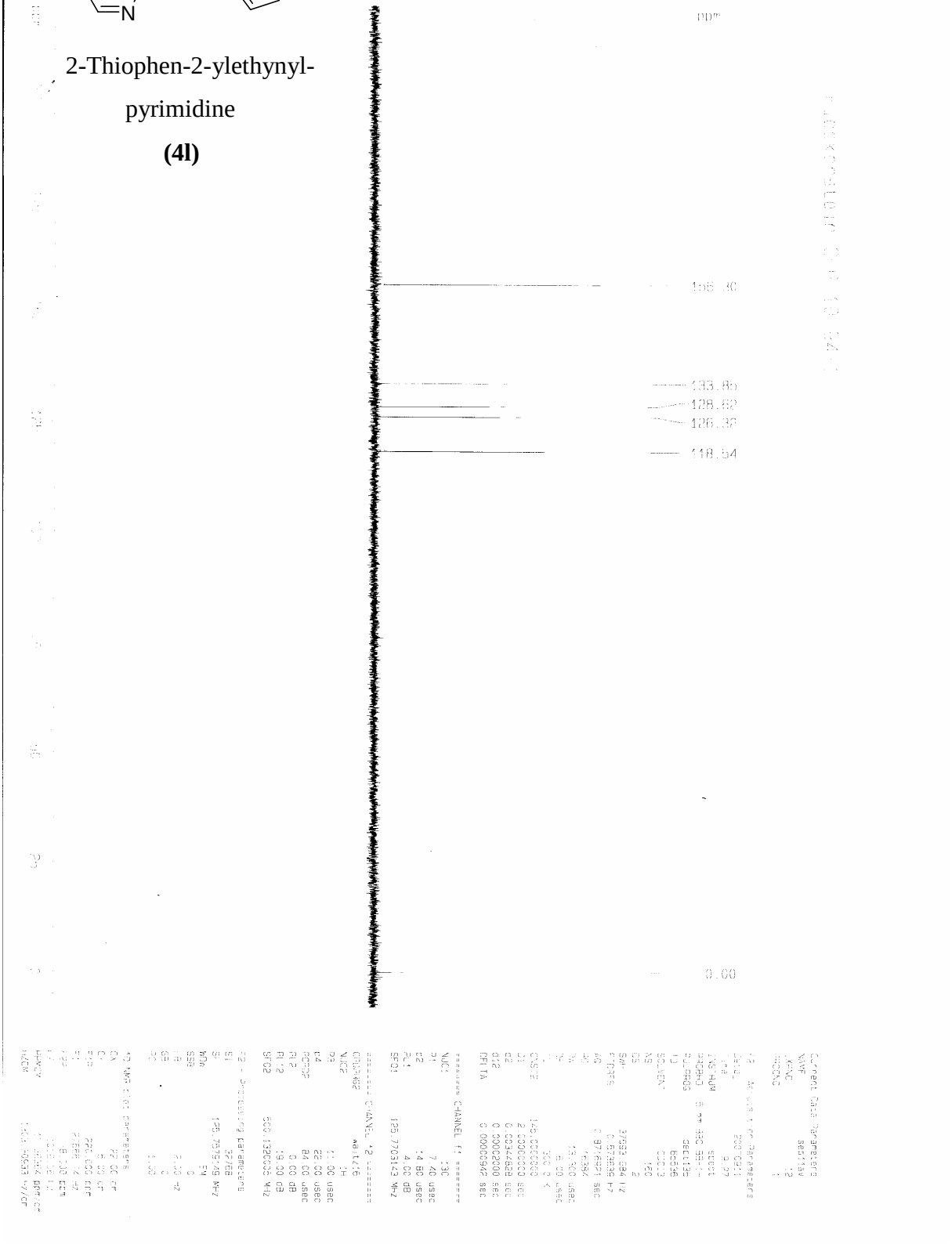
(4l)

^{13}C-NMR (DEPT)

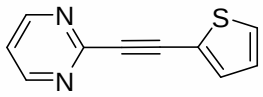


2-Thiophen-2-ylethynyl-pyrimidine

(4l)

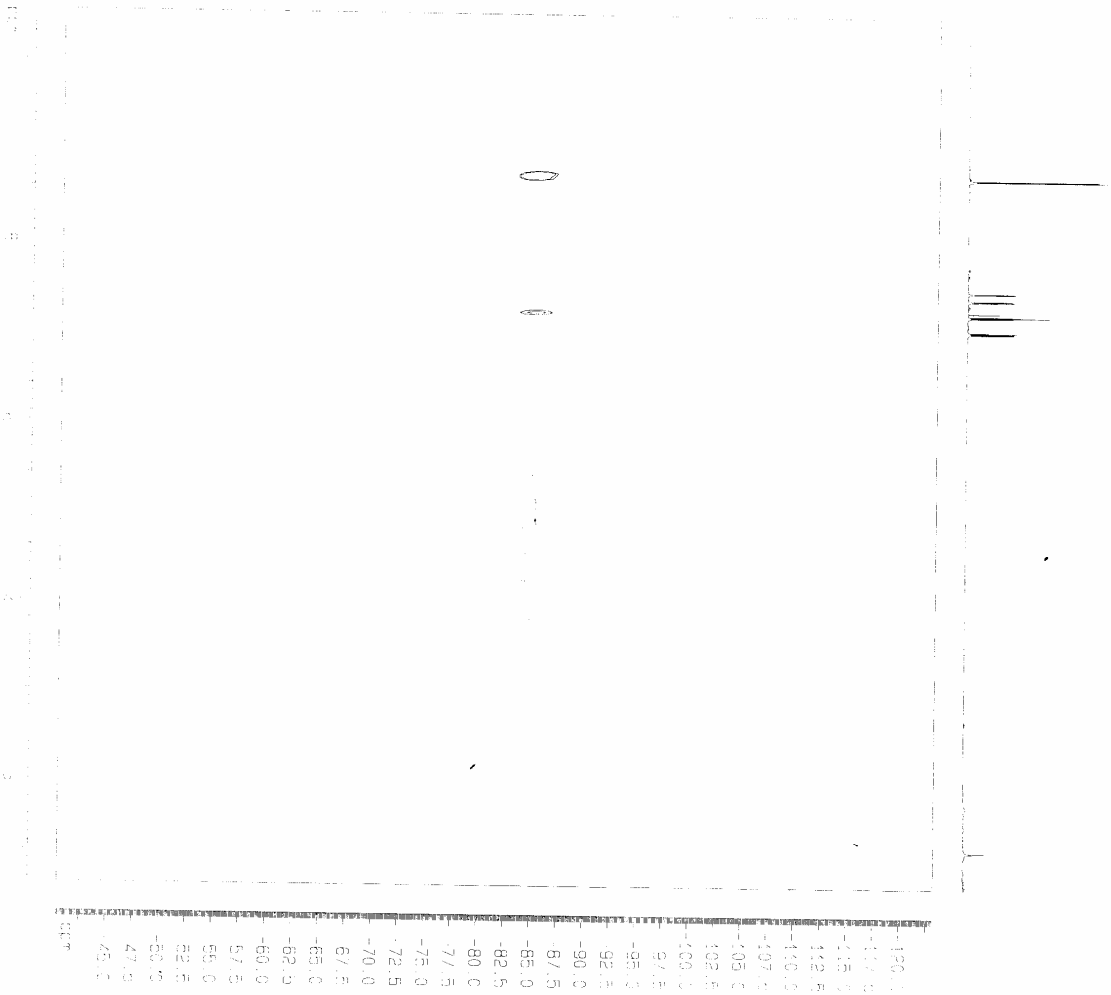


^{15}N-NMR (HMBC)

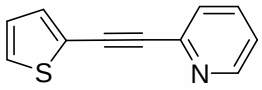


2-Thiophen-2-ylethynyl-pyrimidine

(4l)

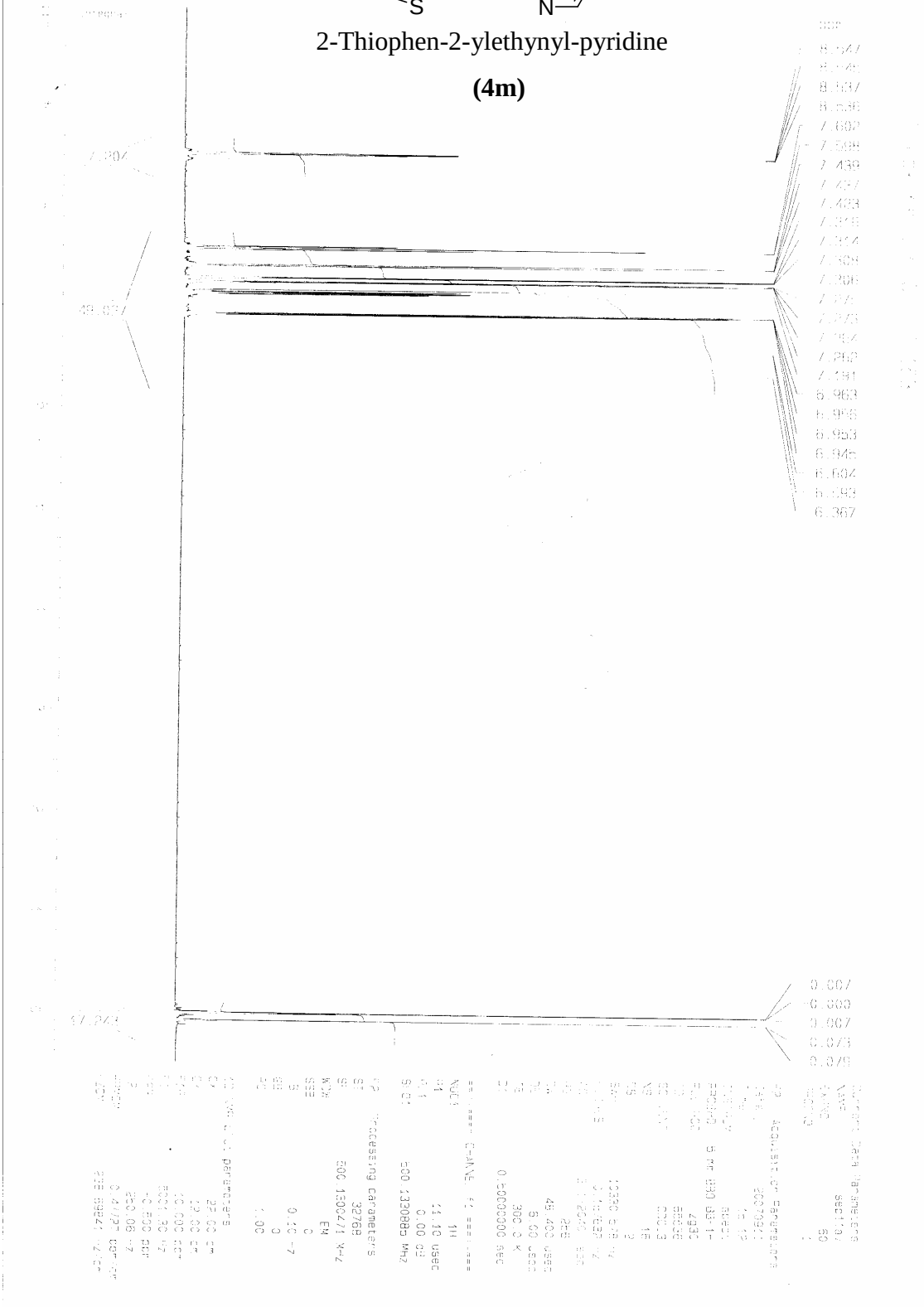


^{1}H-NMR

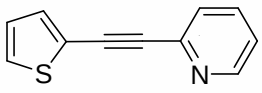


2-Thiophen-2-ylethynyl-pyridine

(4m)



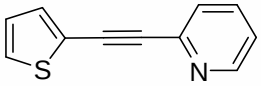
^{13}C-NMR



2-Thiophen-2-ylethynyl-pyridine

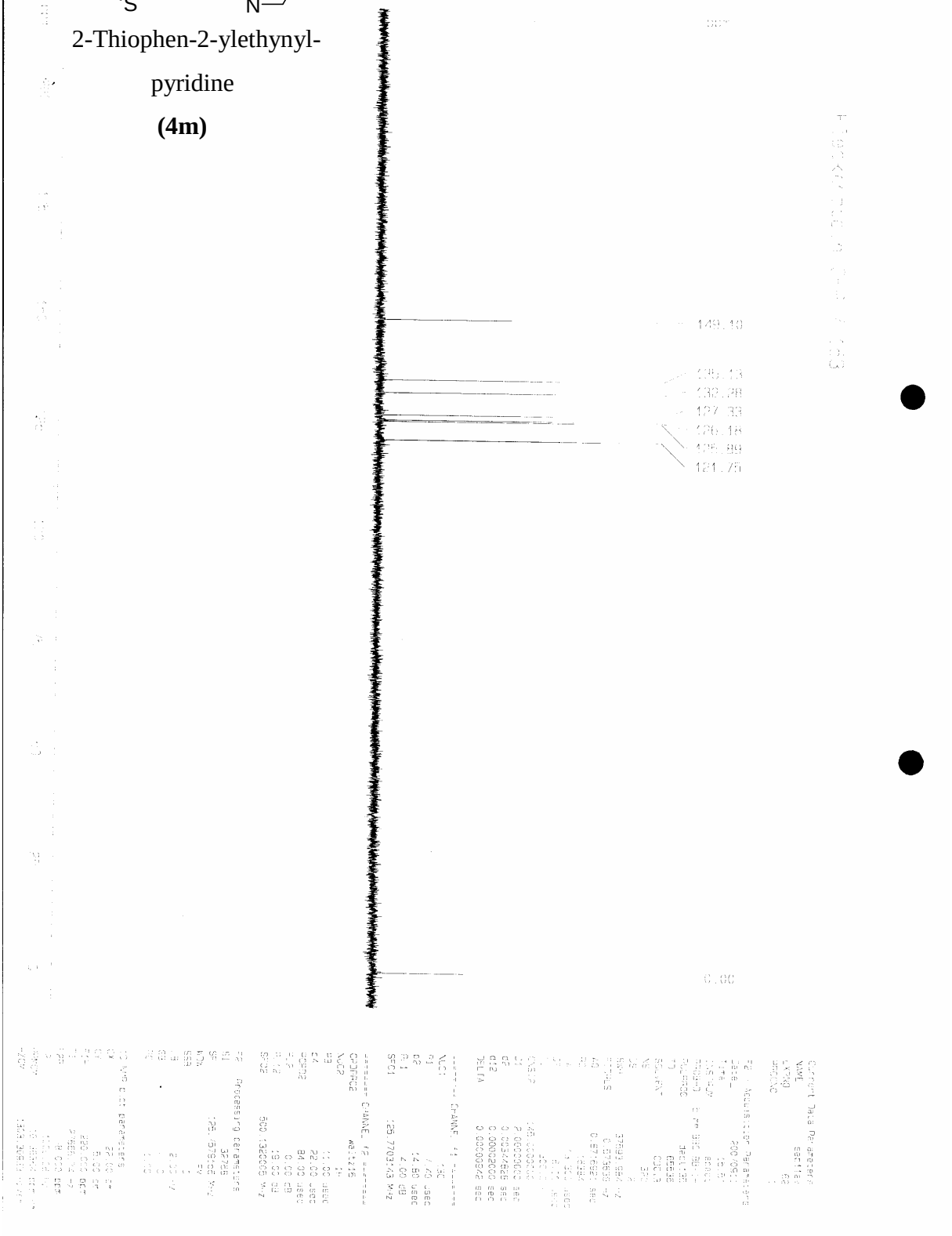
(4m)

^{13}C-NMR (DEPT)

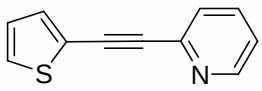


2-Thiophen-2-ylethynyl-pyridine

(4m)

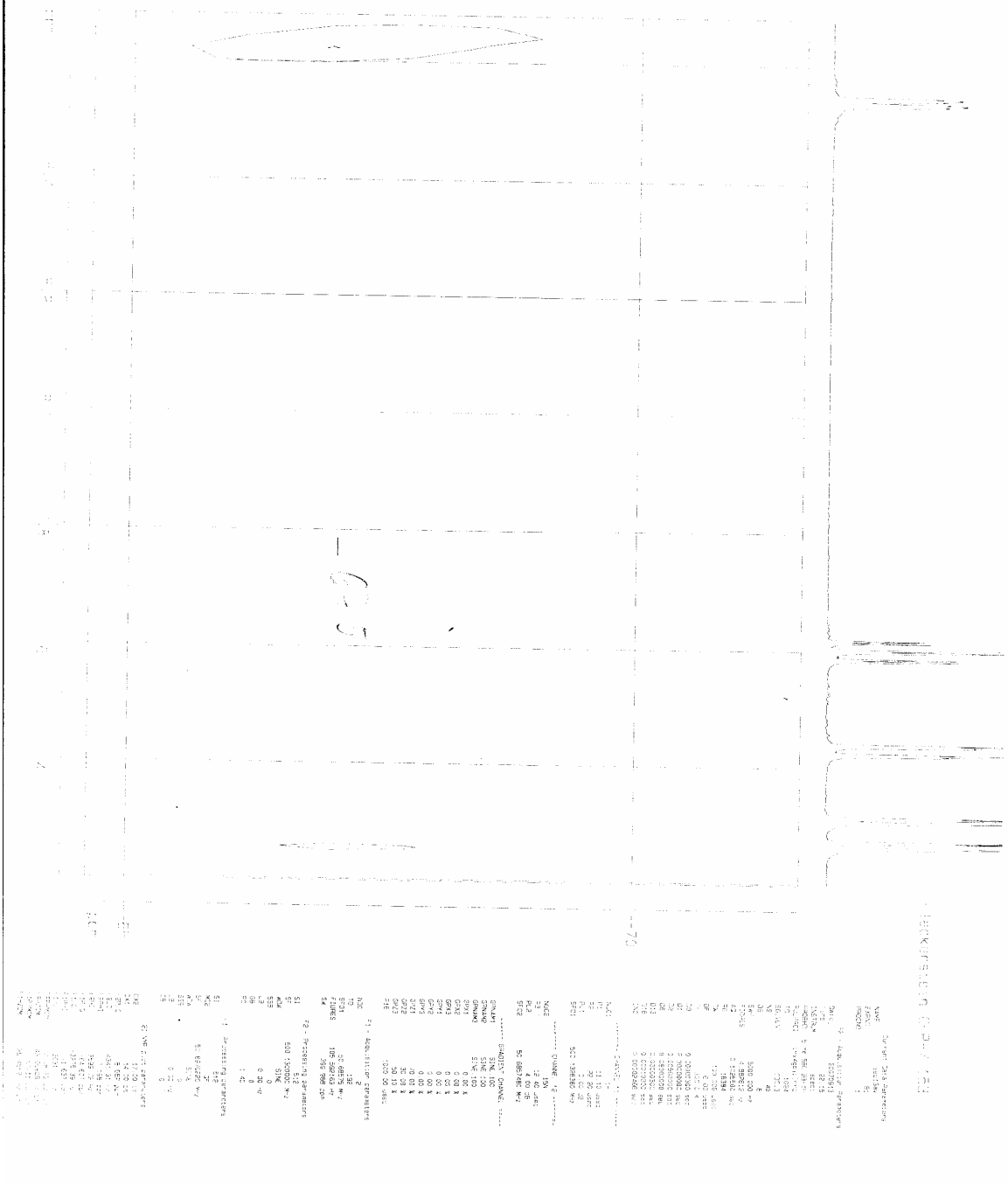


^{15}N-NMR (HMBC)

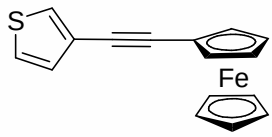


2-Thiophen-2-ylethynyl-pyridine

(4m)



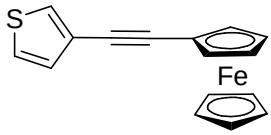
^{1}H-NMR



3-Ferrocenylethynyl-thiophene

(4n)

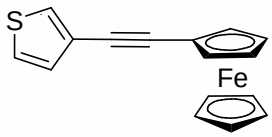
^{13}C-NMR



3-Ferrocenylethynyl-thiophene

(4n)

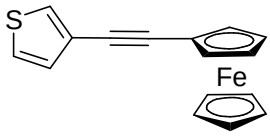
^{13}C-NMR (DEPT)



3-Ferrocenylethynyl-thiophene

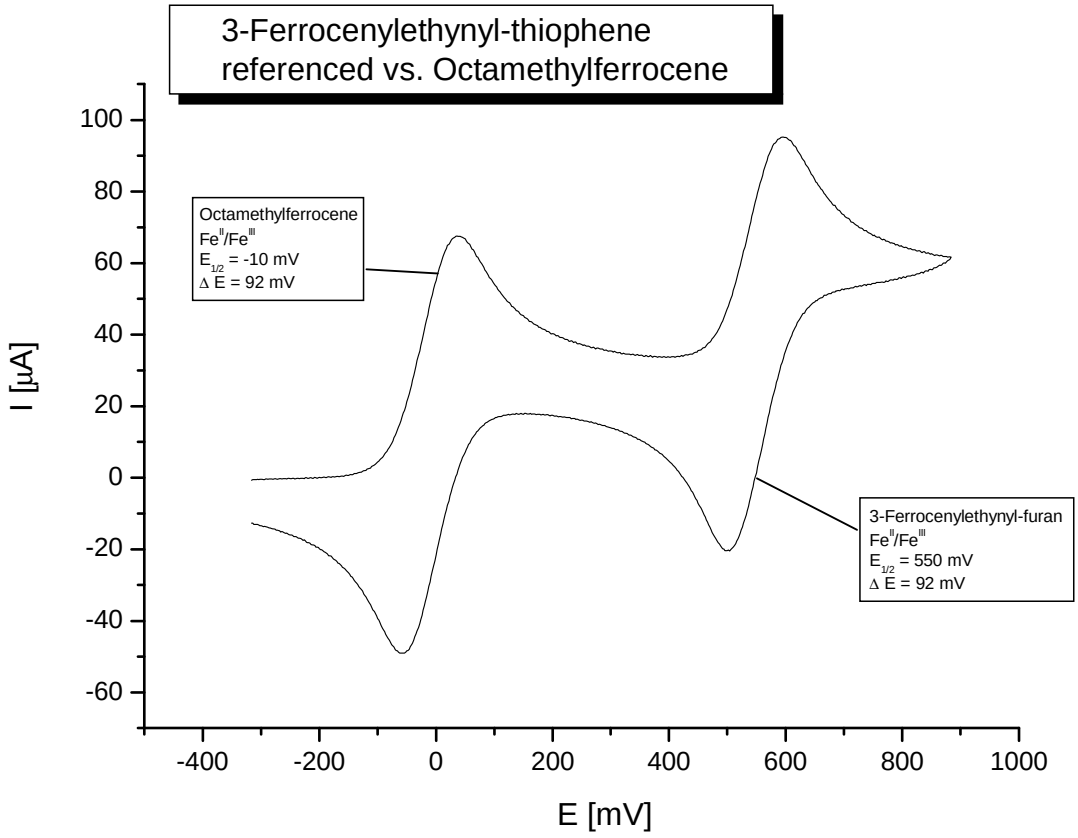
(4n)

Cyclovoltammogram

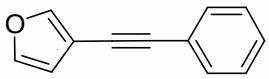


3-Ferrocenylethynyl-thiophene

(4n)

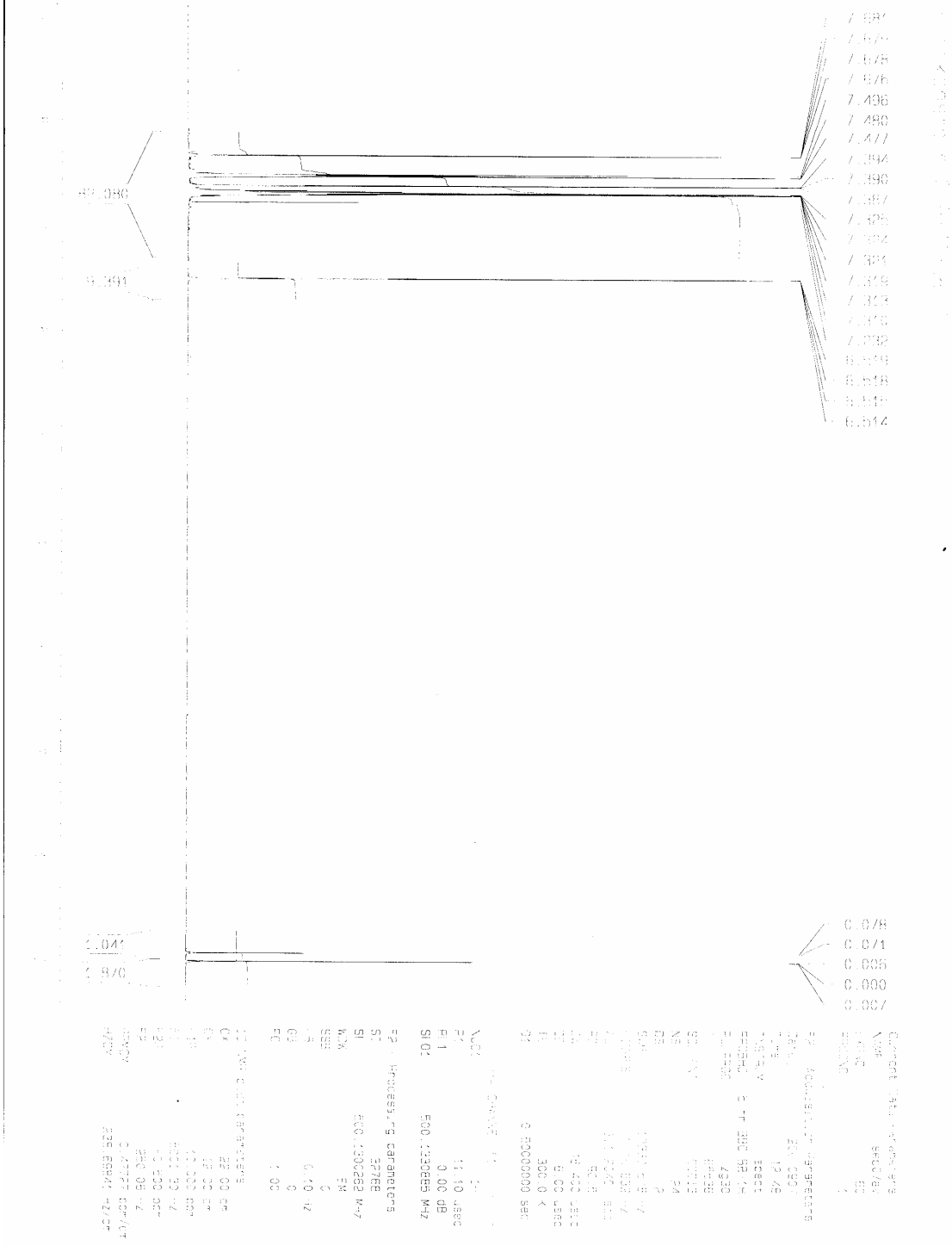


^{1}H-NMR

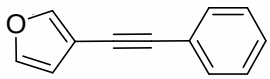


3-Phenylethynyl-furan

(4o)

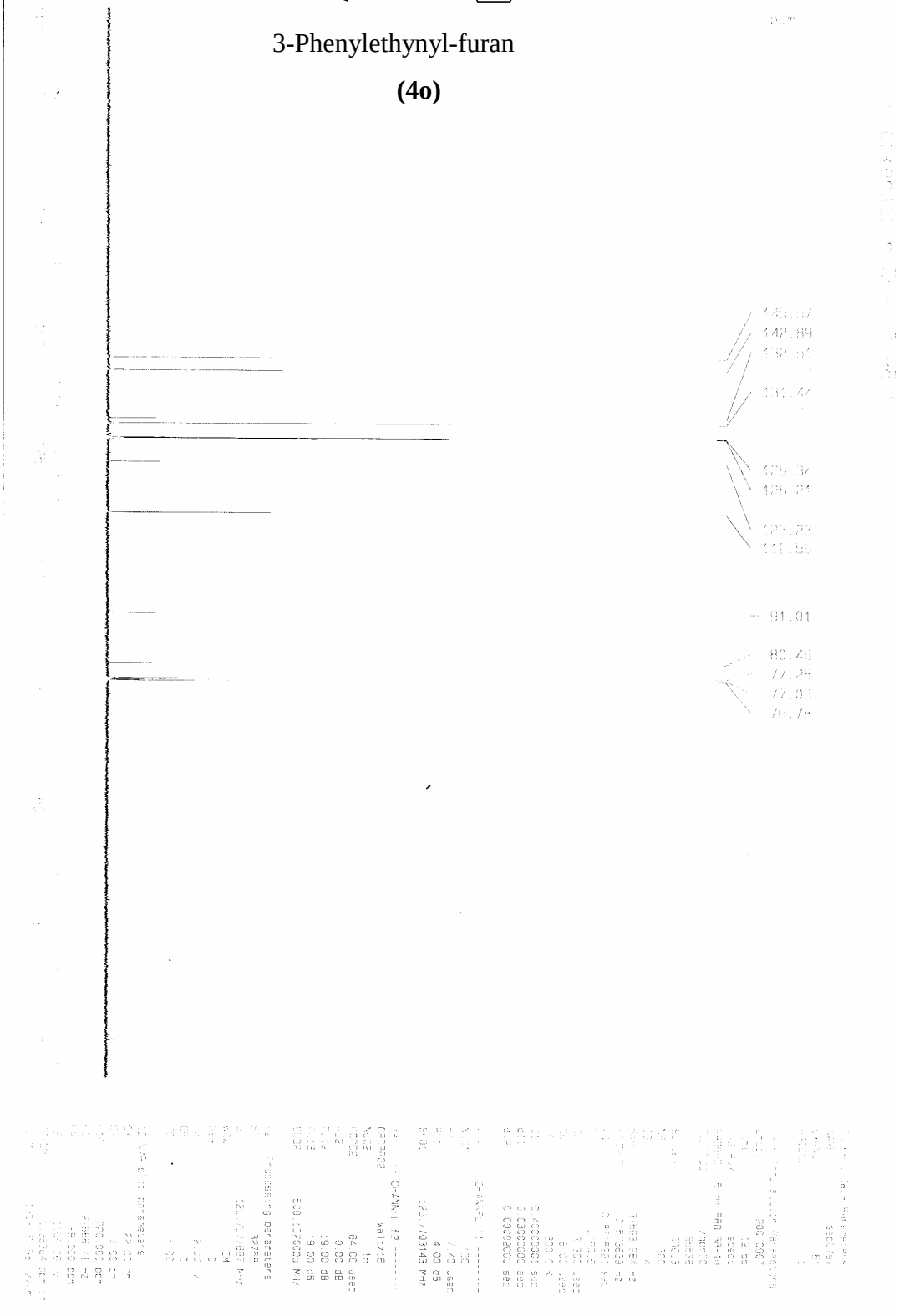


^{13}C-NMR

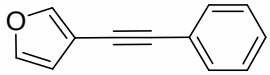


3-Phenylethynyl-furan

(4o)

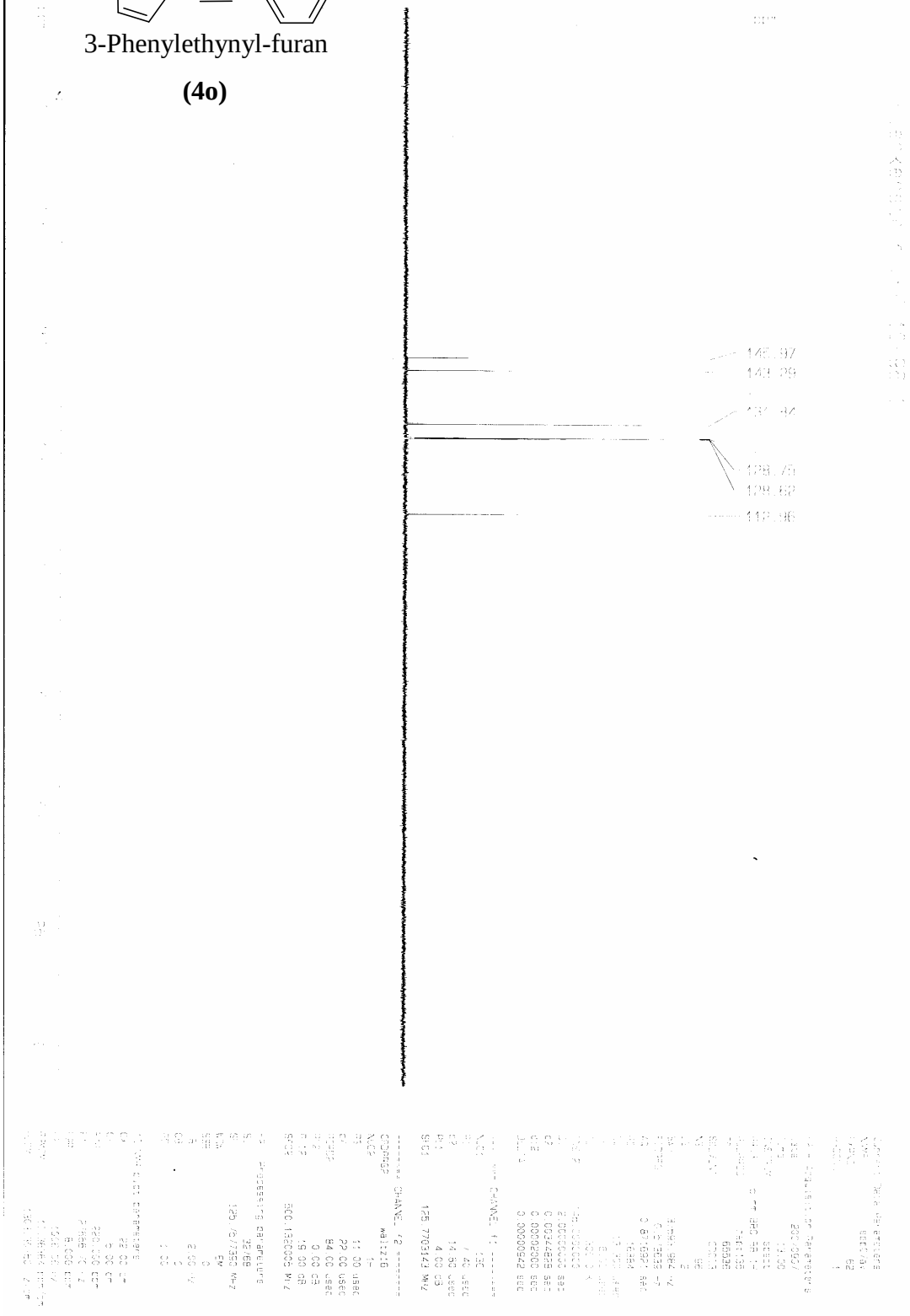


^{13}C-NMR (DEPT)

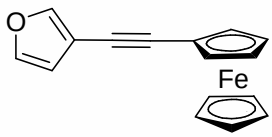


3-Phenylethynyl-furan

(4o)

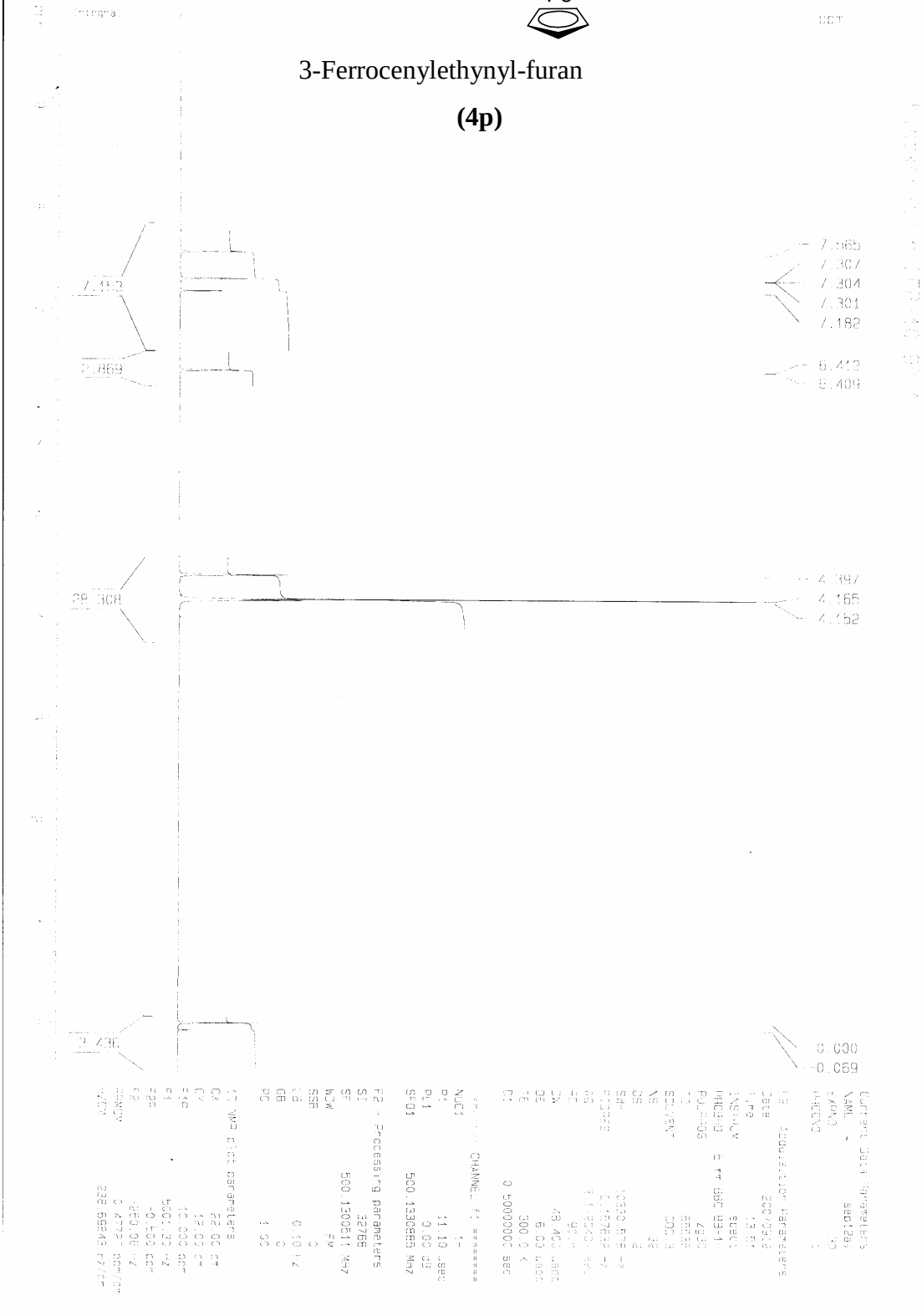


^{1}H-NMR

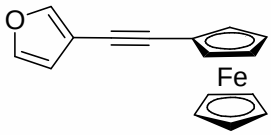


3-Ferrocenylethynyl-furan

(4p)



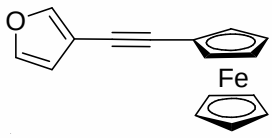
^{13}C-NMR



3-Ferrocenylethynyl-furan

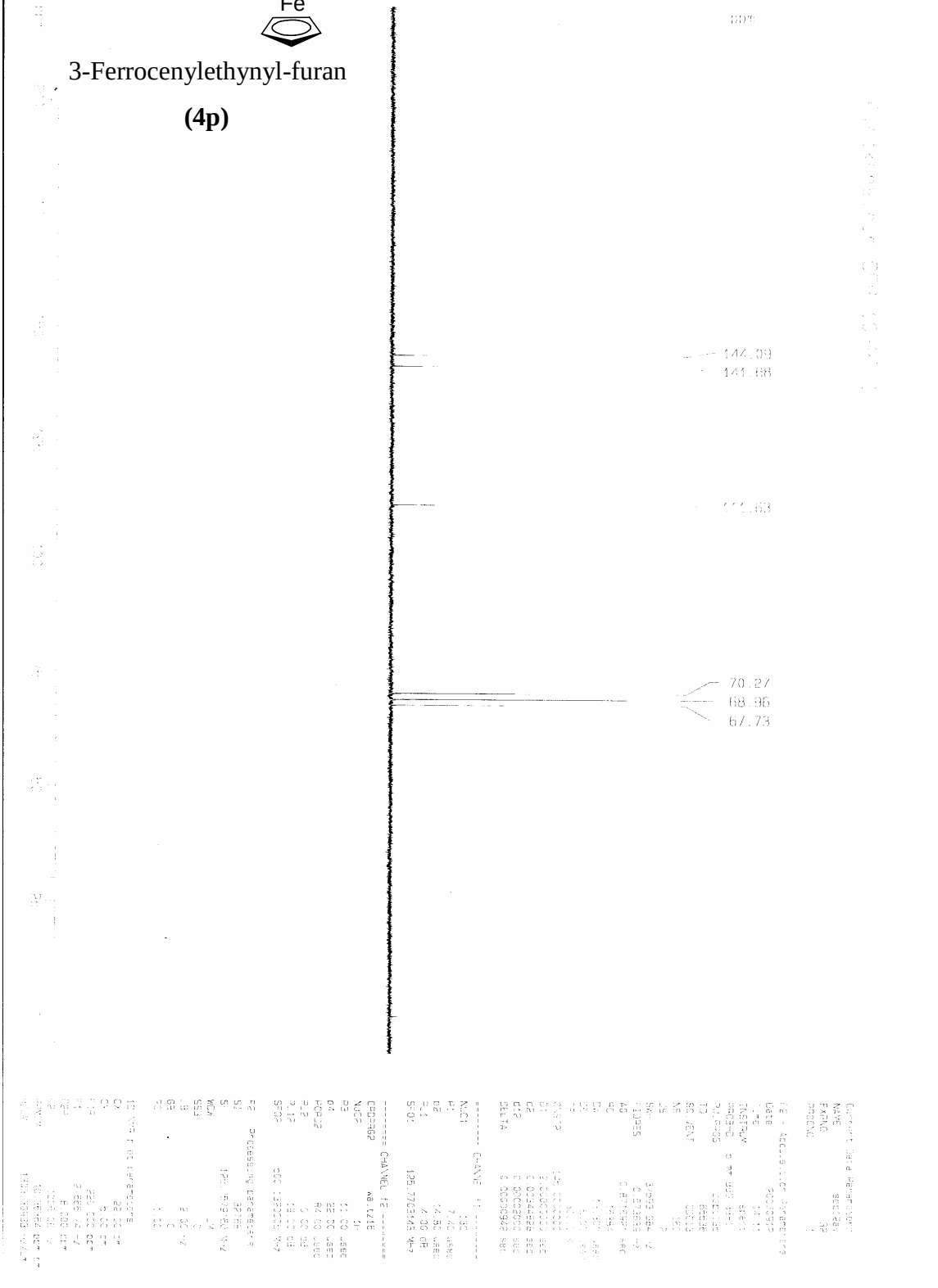
(4p)

^{13}C-NMR (DEPT)

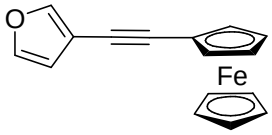


3-Ferrocenylethynyl-furan

(4p)

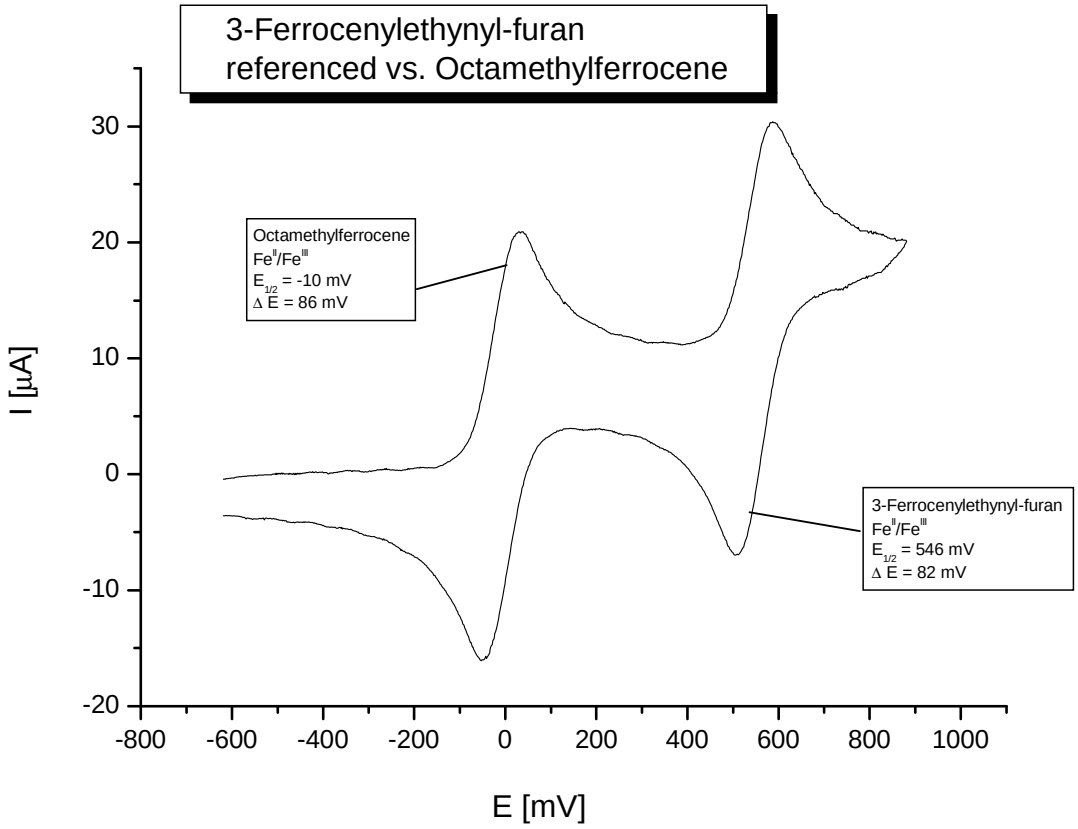


Cyclovoltammogram

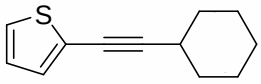


3-Ferrocenylethynyl-furan

(4p)



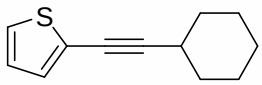
^{1}H-NMR



2-Cyclohexylethynyl-thiophene

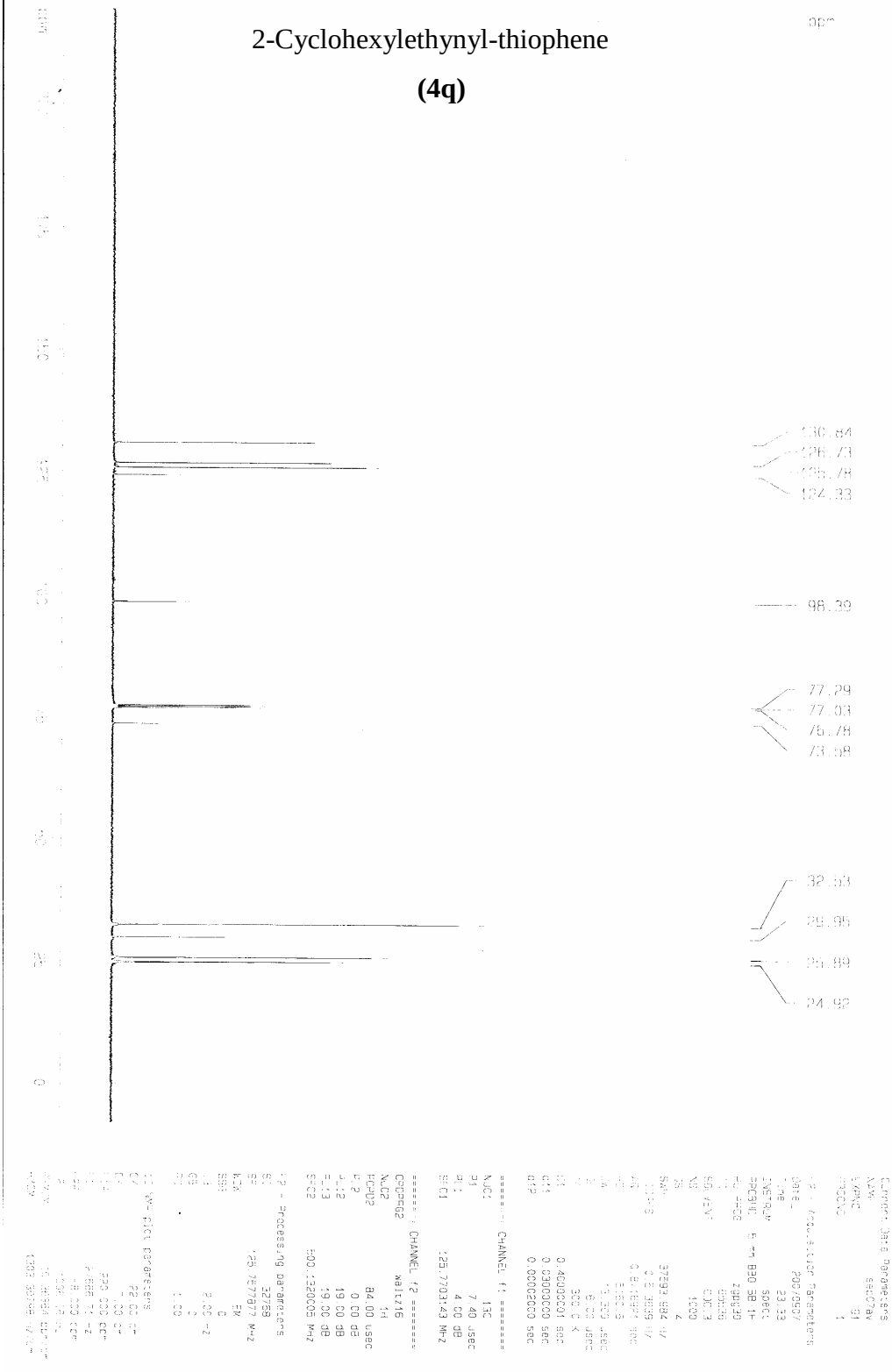
(4q)

^{13}C-NMR

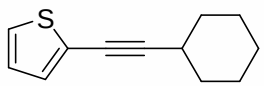


2-Cyclohexylethynyl-thiophene

(4q)

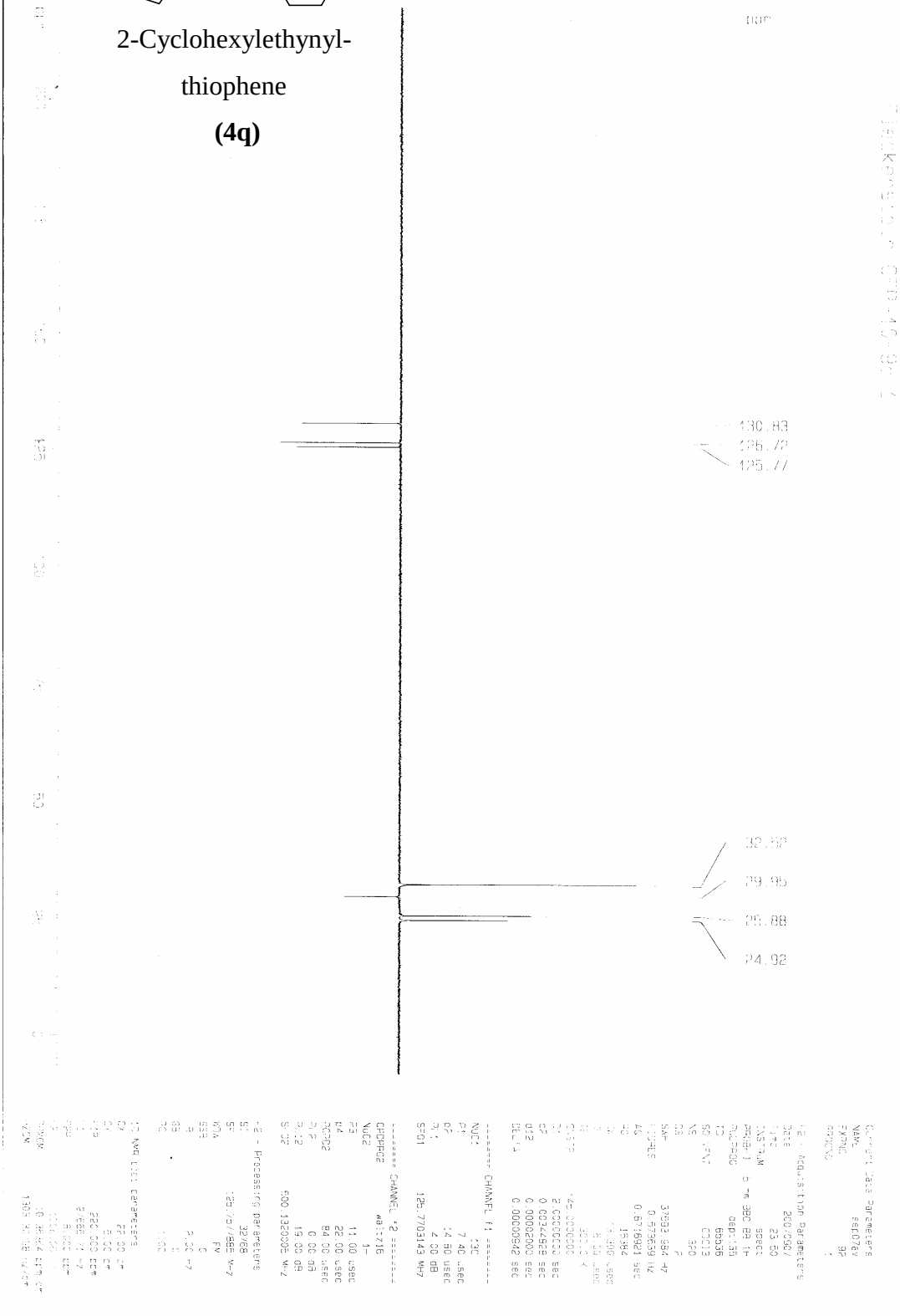


^{13}C-NMR (DEPT)

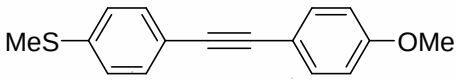


2-Cyclohexylethynyl-thiophene

(4q)



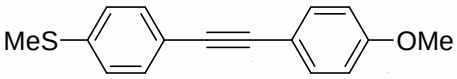
^{1}H-NMR



1-Methylsulfanyl-4-(4'-methoxy-phenylethynyl)-benzene

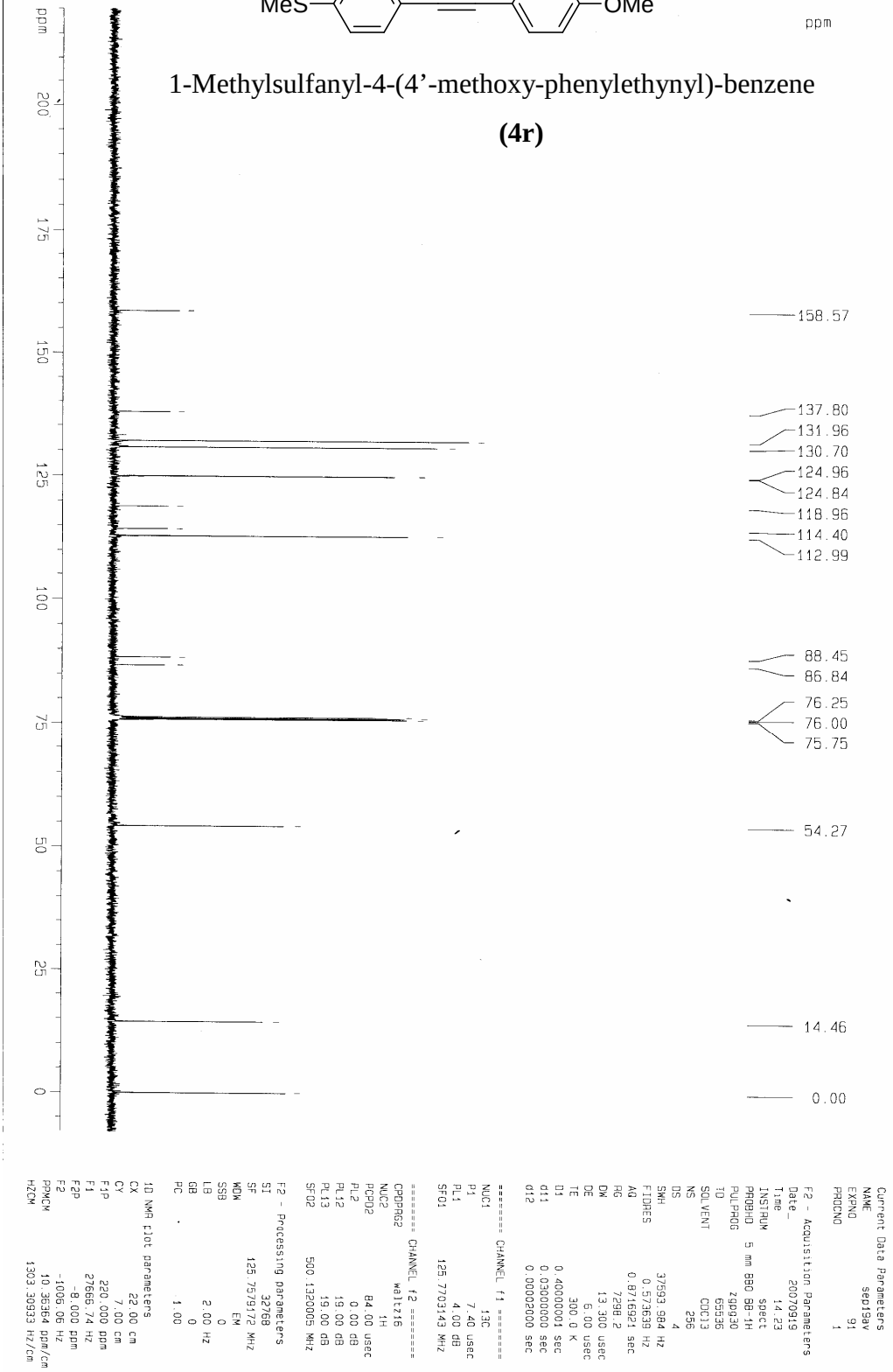
(4r)

^{13}C-NMR

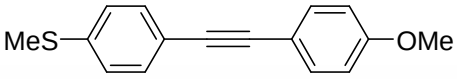


1-Methylsulfanyl-4-(4'-methoxy-phenylethynyl)-benzene

(4r)

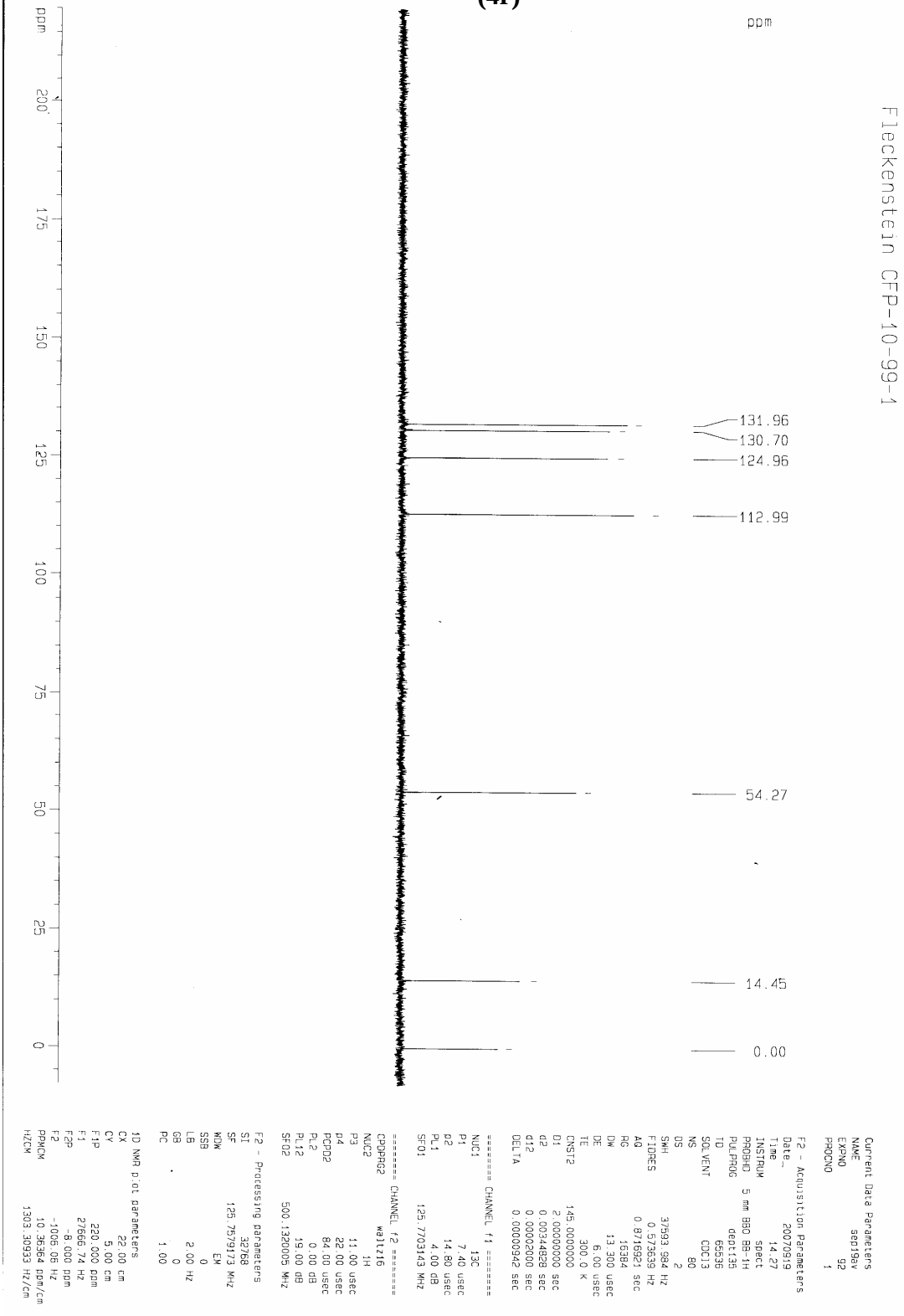


^{13}C-NMR (DEPT)

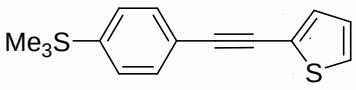


1-Methylsulfanyl-4-(4’-methoxy-phenylethynyl)-benzene

(4r)



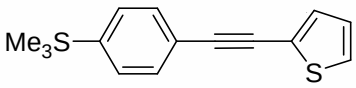
^{1}H-NMR



2-(4-Methylsulfanyl-phenylethynyl)-thiophene

(4s)

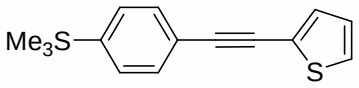
^{13}C-NMR



2-(4-Methylsulfanyl-phenylethynyl)-thiophene

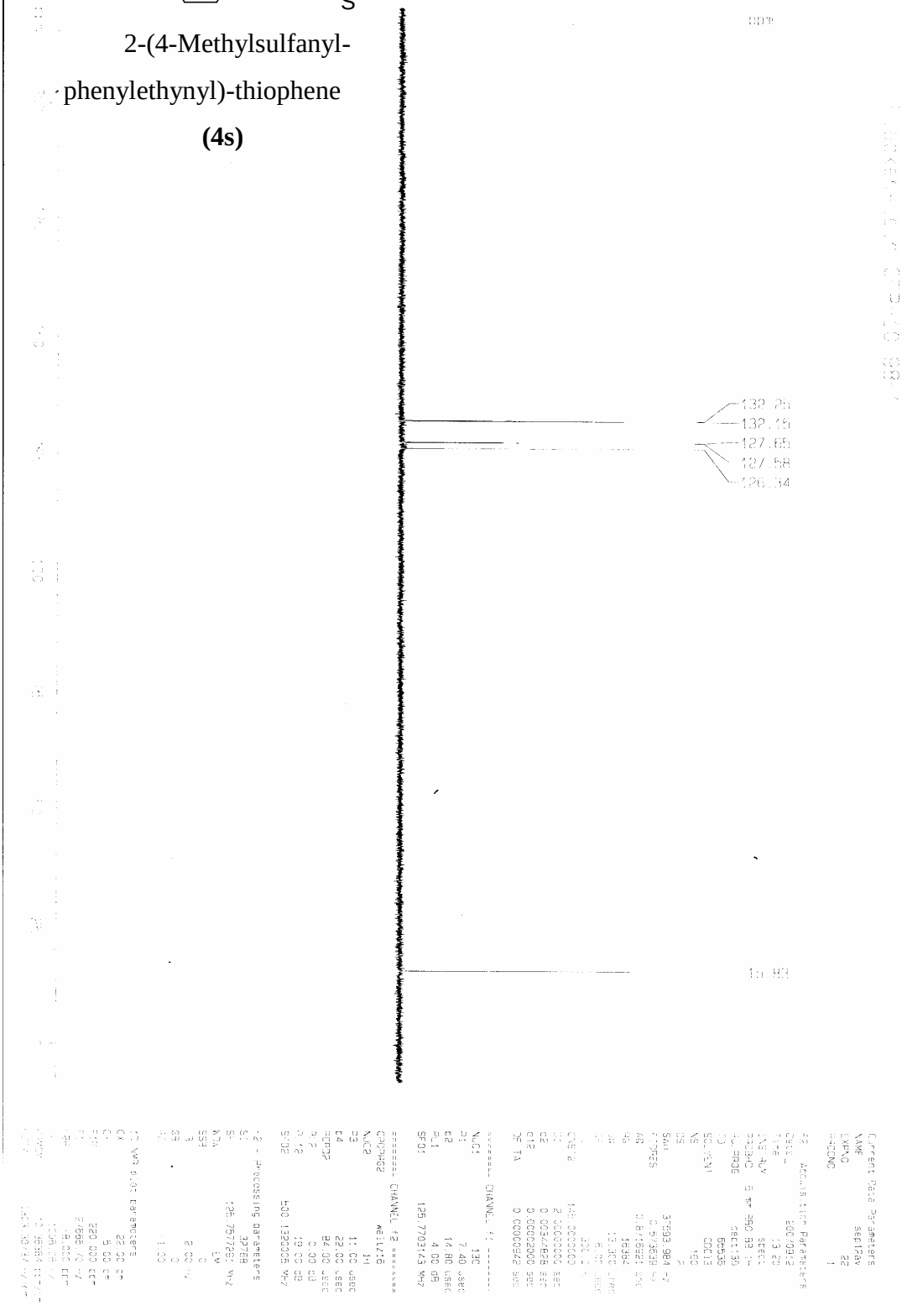
(4s)

^{13}C-NMR (DEPT)

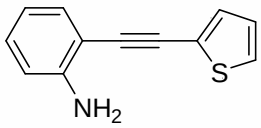


2-(4-Methylsulfanyl-phenylethynyl)-thiophene

(4s)



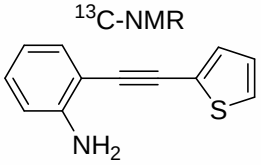
^{1}H-NMR



2-Thiophen-2-ylethynyl-phenylamine

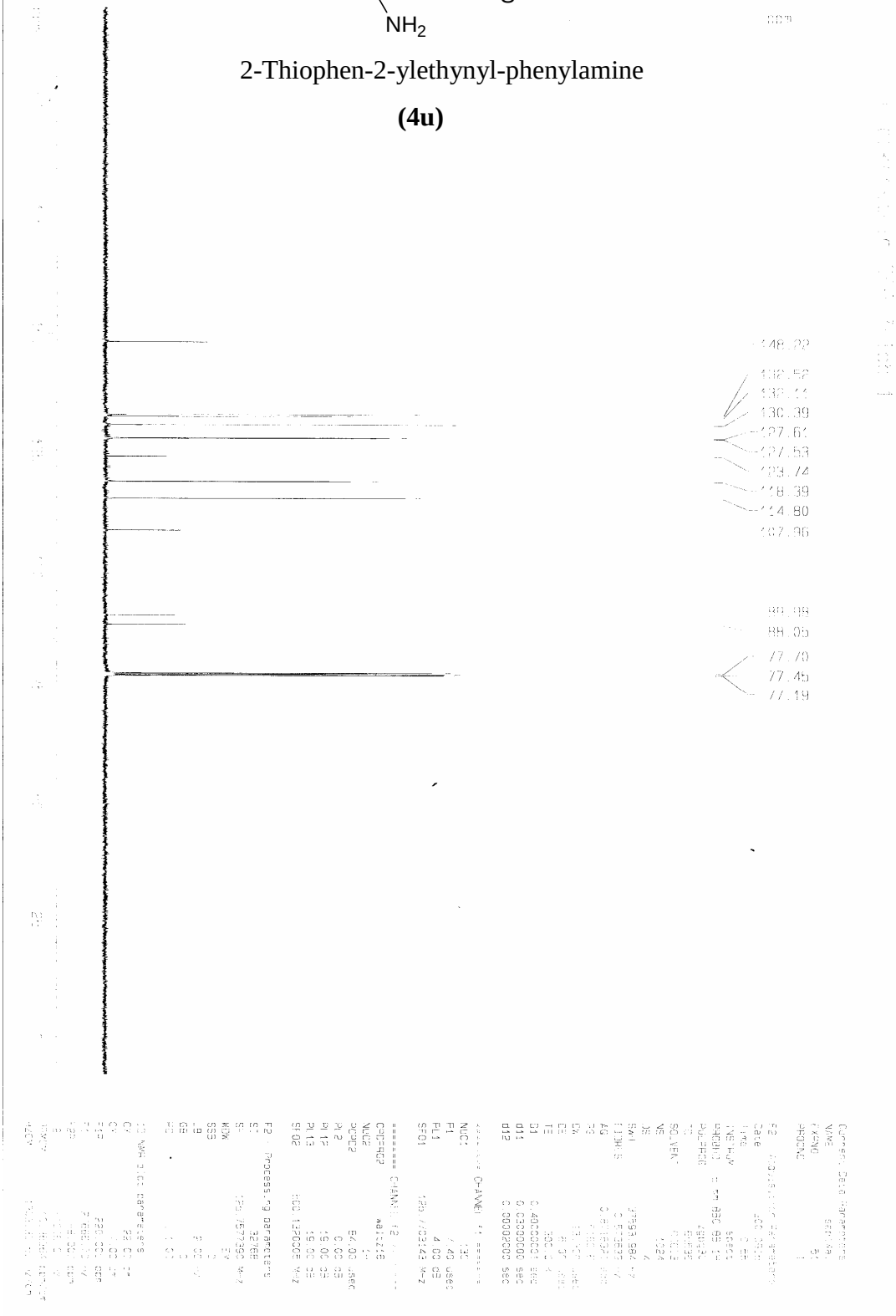
(4u)

^{13}C-NMR

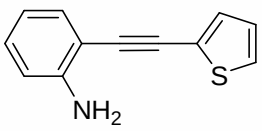


2-Thiophen-2-ylethynyl-phenylamine

(4u)

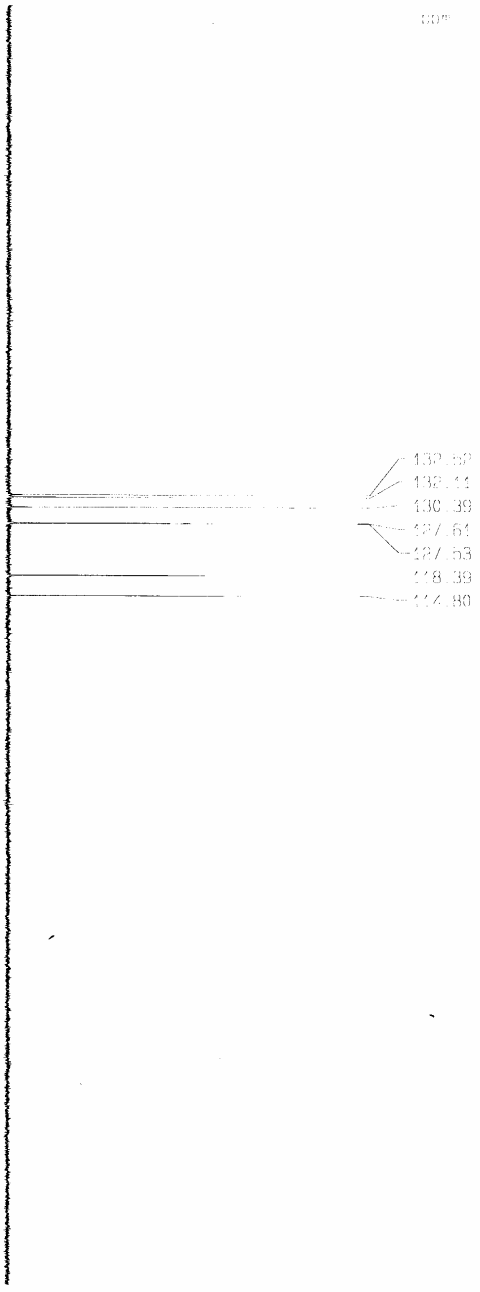


^{13}C-NMR (DEPT)

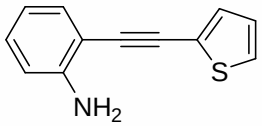


2-Thiophen-2-ylethynyl-phenylamine

(4u)

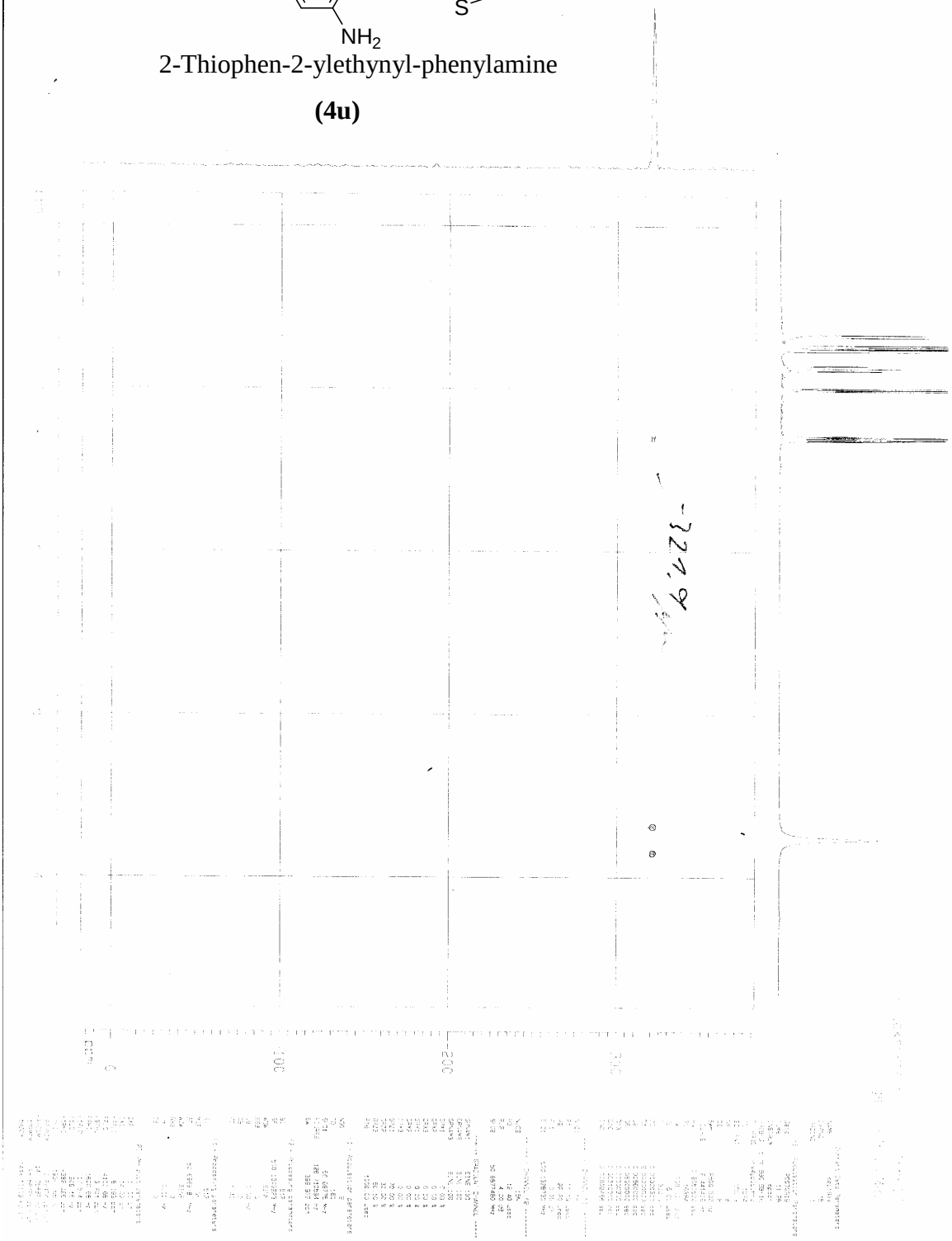


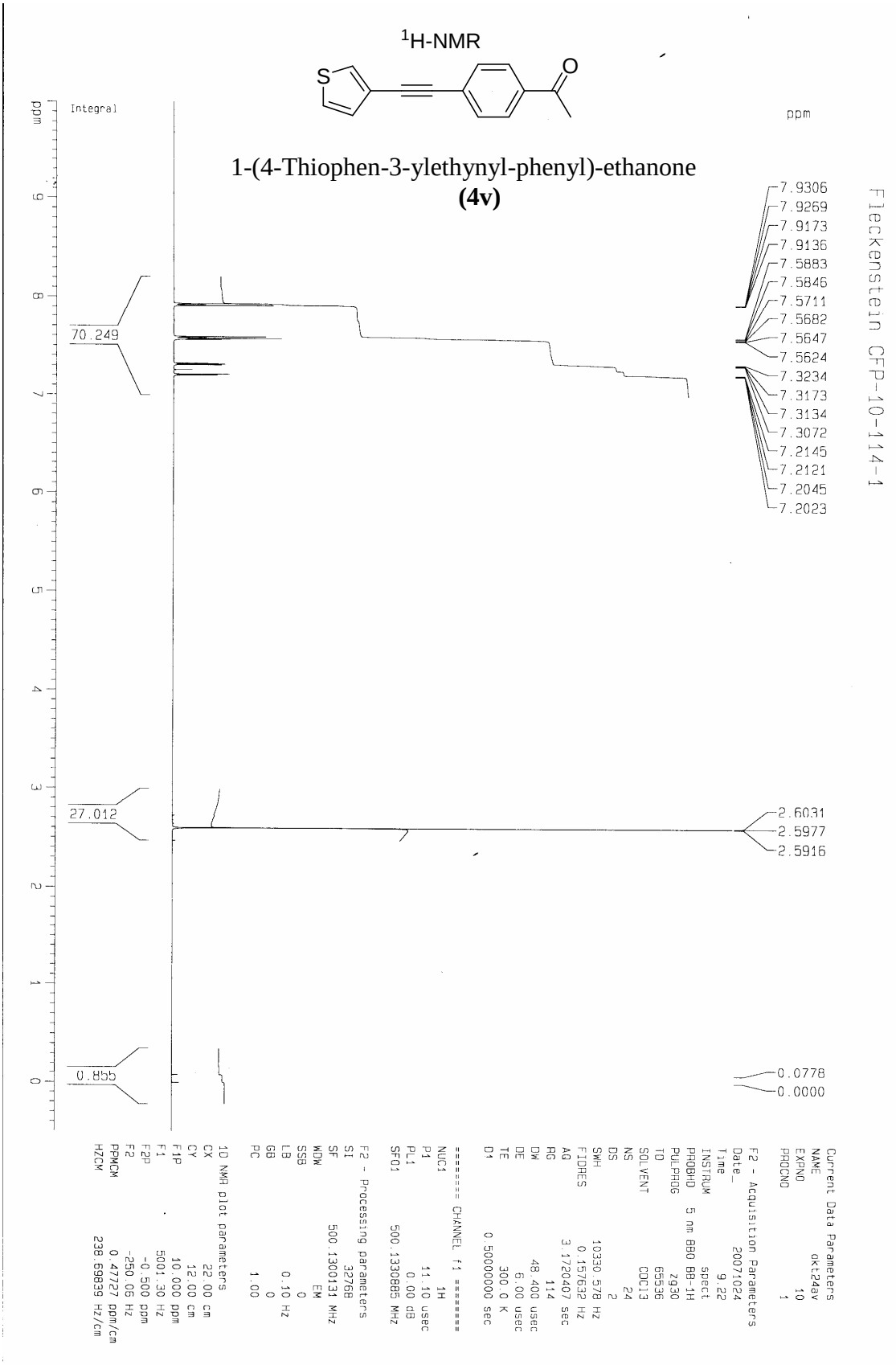
^{15}N-NMR (HMBC)



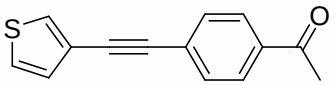
2-Thiophen-2-ylethynyl-phenylamine

(4u)



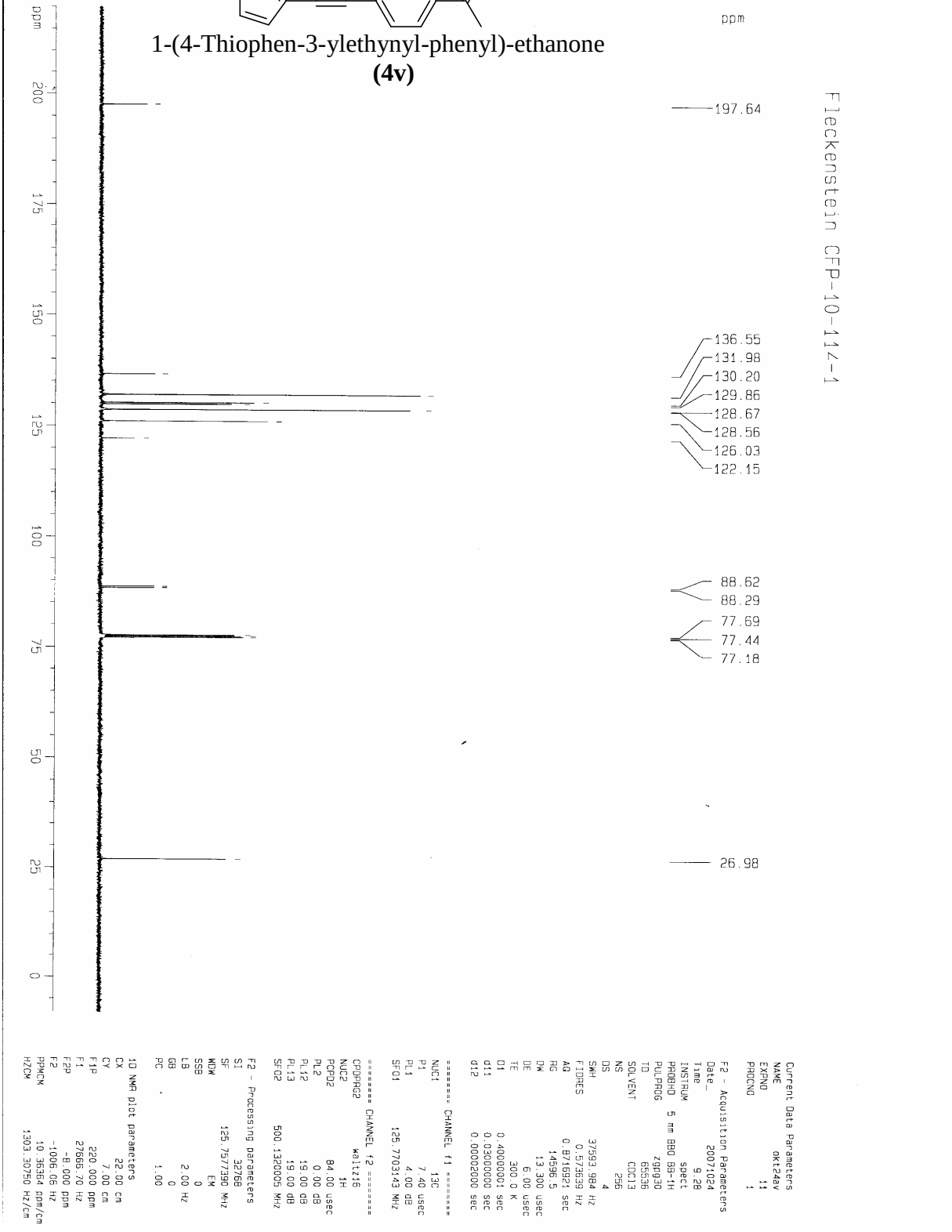

1H-NMR
S
O
1-(4-Thiophen-3-ylethynyl-phenyl)-ethanone
(4v)
Fleckenstein CFP-10-114-1
Integral
ppm
70.249
27.012
0.855
7.9306
7.9269
7.9173
7.9136
7.5883
7.5846
7.5711
7.5682
7.5647
7.5624
7.3234
7.3173
7.3134
7.3072
7.2145
7.2121
7.2045
7.2023
2.6031
2.5977
2.5916
0.0778
0.0000
Current Data Parameters
NAME
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071024
Time 9.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 24
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1720407 sec
RG 114
DW 48.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.50000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 11.10 usec
PL1 0.00 dB
SFO1 500.1330885 MHz
F2 - Processing parameters
SI 32768
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.00 cm
CY 12.00 cm
F1P 10.000 ppm
F1 5001.30 Hz
F2P -0.500 ppm
F2 -250.05 Hz
PPMCM 0.47727 ppm/cm
HZCM 238.69839 Hz/cm

^{13}C-NMR

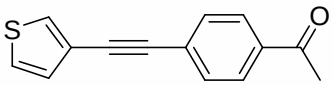


1-(4-Thiophen-3-ylethynyl-phenyl)-ethanone

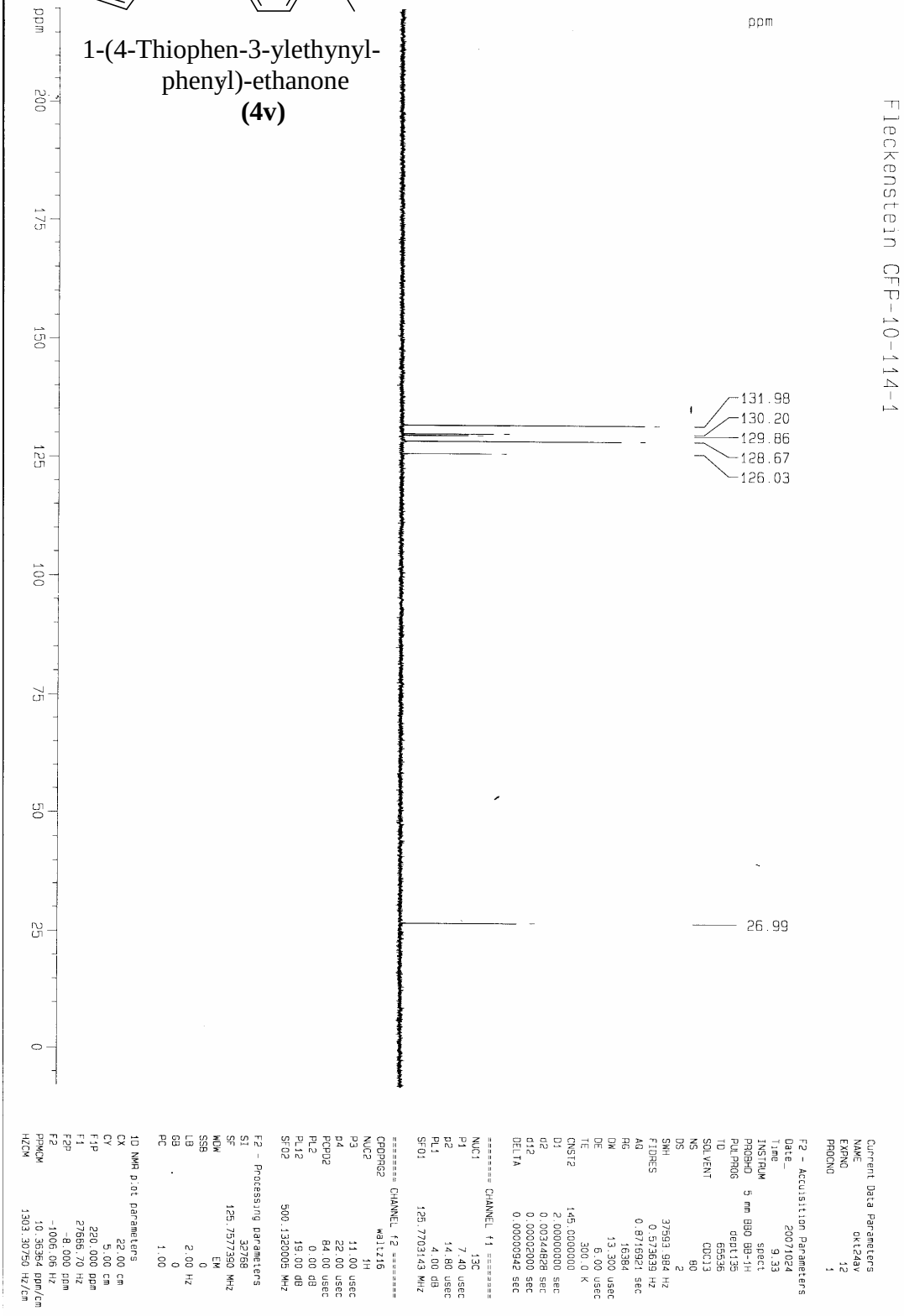
(4v)



^{13}C-NMR (DEPT)



1-(4-Thiophen-3-ylethynyl-phenyl)-ethanone
(4v)



Current Data Parameters
NAME ok124av
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date 20071024
Time 9.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 80
DS 2
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8715921 sec
RG 16384
DW 13.300 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000942 sec

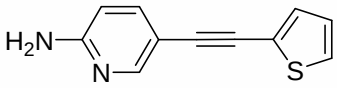
======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
p2 14.80 usec
PL1 4.00 dB
SFO1 125.7703143 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 11.00 usec
P4 22.00 usec
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
SFO2 500.1320005 MHz

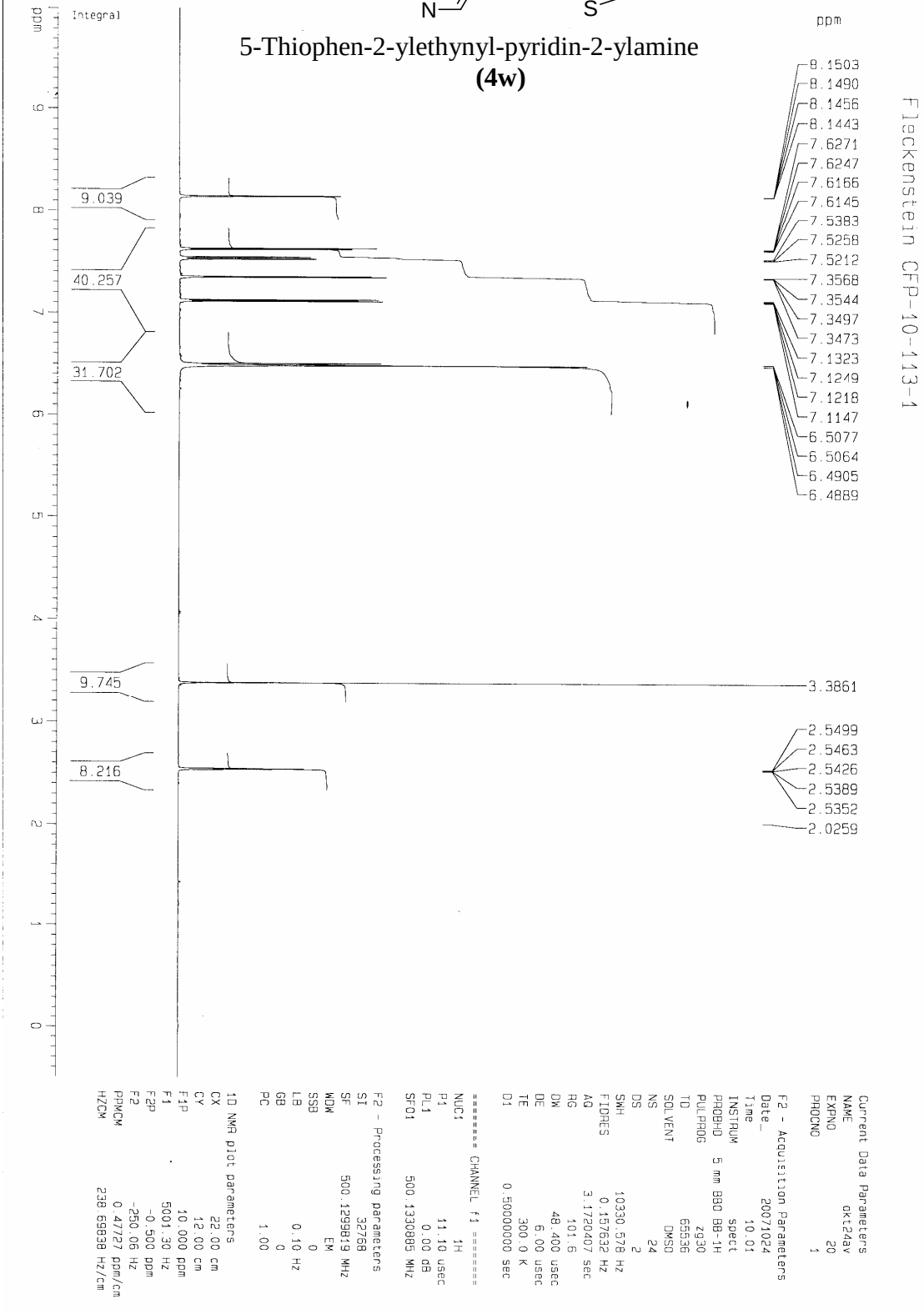
F2 - Processing parameters
SI 32768
SF 125.7577390 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 5.00 cm
F1P 220.000 ppm
F1 27666.70 Hz
F2P -8.000 ppm
F2 -1006.06 Hz
PPMCM 10.36364 ppm/cm
HZCM 1303.30750 Hz/cm

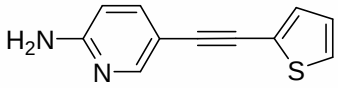
^{1}H-NMR



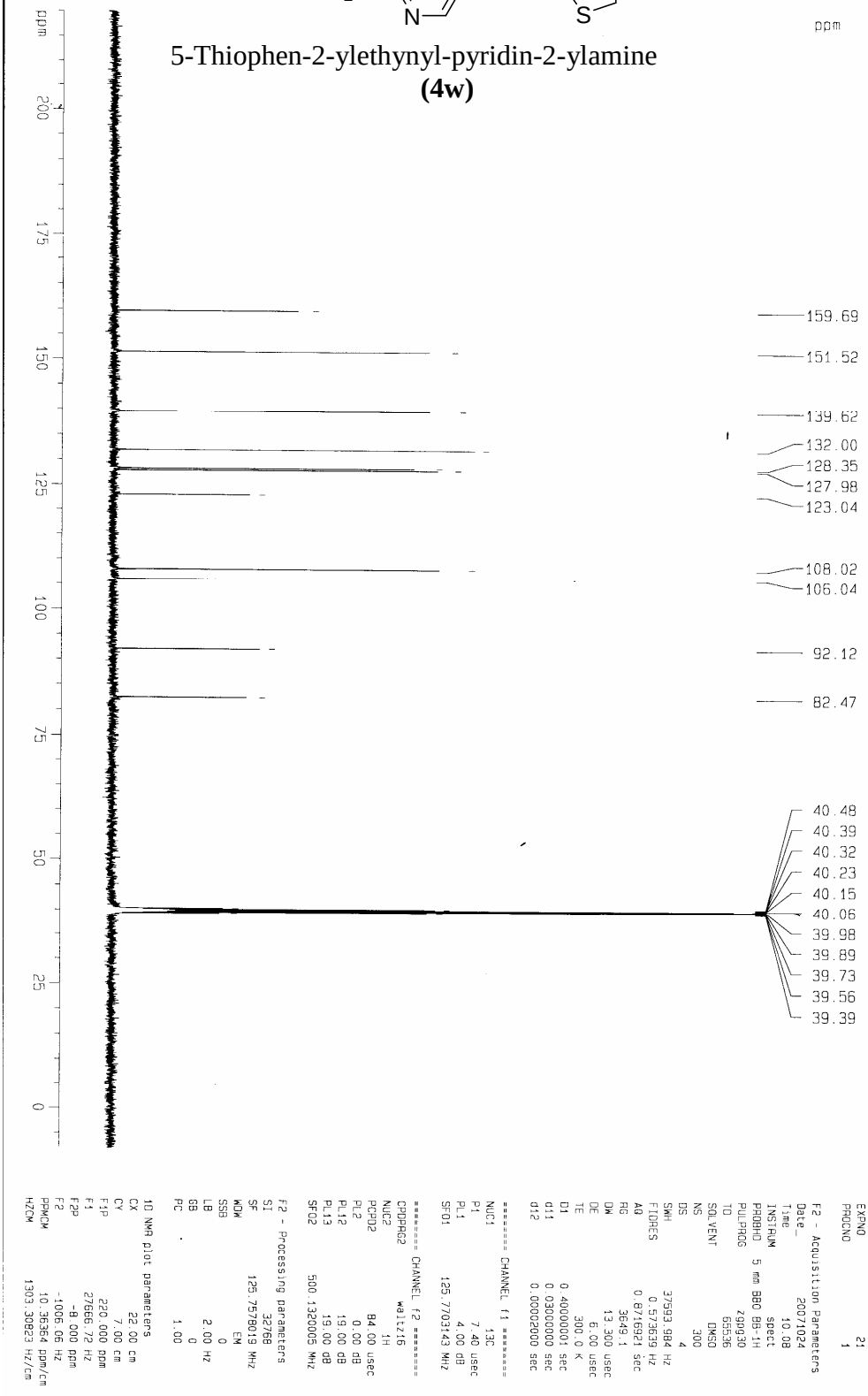
5-Thiophen-2-ylethynyl-pyridin-2-ylamine
(4w)

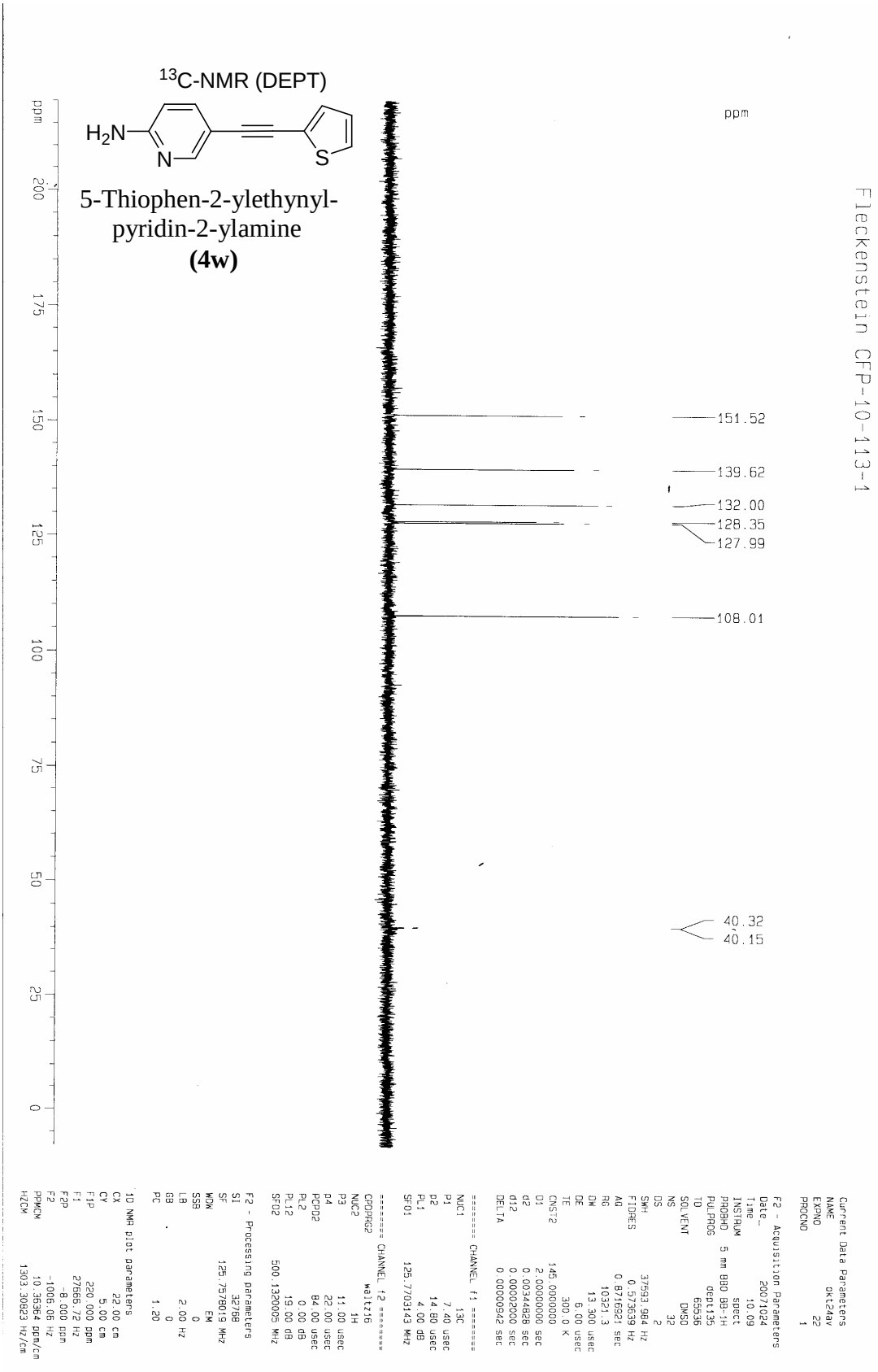


^{13}C-NMR

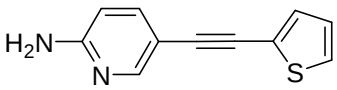


5-Thiophen-2-ylethynyl-pyridin-2-ylamine
(4w)




13C-NMR (DEPT)
H2N
N
S
5-Thiophen-2-ylethynyl-
pyridin-2-ylamine
(4w)
ppm
151.52
139.62
132.00
128.35
127.99
108.01
40.32
40.15
Fleckenstein CFP-10-113-1
Current Data Parameters
NAME dkt24ay
EXPNO 22
PROCNO 1
F2 - Acquisition Parameters
Date_ 20071024
Time_ 10.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8716921 sec
RG 10321.3
DW 13.300 usec
DE 6.00 usec
TE 300.0 K
CNST2 145.0000000
D1 2.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00000942 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.40 usec
P2 14.80 usec
PL1 4.00 dB
SFO1 125.7703143 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 11.00 usec
P4 22.00 usec
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7578019 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.20
1D NMR plot parameters
CX 22.00 cm
CY 5.00 cm
F1P 220.000 ppm
F1 27666.72 Hz
F2P -8.000 ppm
F2 -1006.06 Hz
PPMCM 10.35364 ppm/cm
HZCM 1303.30823 Hz/cm

^{15}N-NMR (HMBC)



5-Thiophen-2-ylethynyl-pyridin-2-ylamine
(4w)