

Supporting Information

Aqueous Cross Coupling: Sustainable Protocol for Sonogashira Reactions of Heterocycles

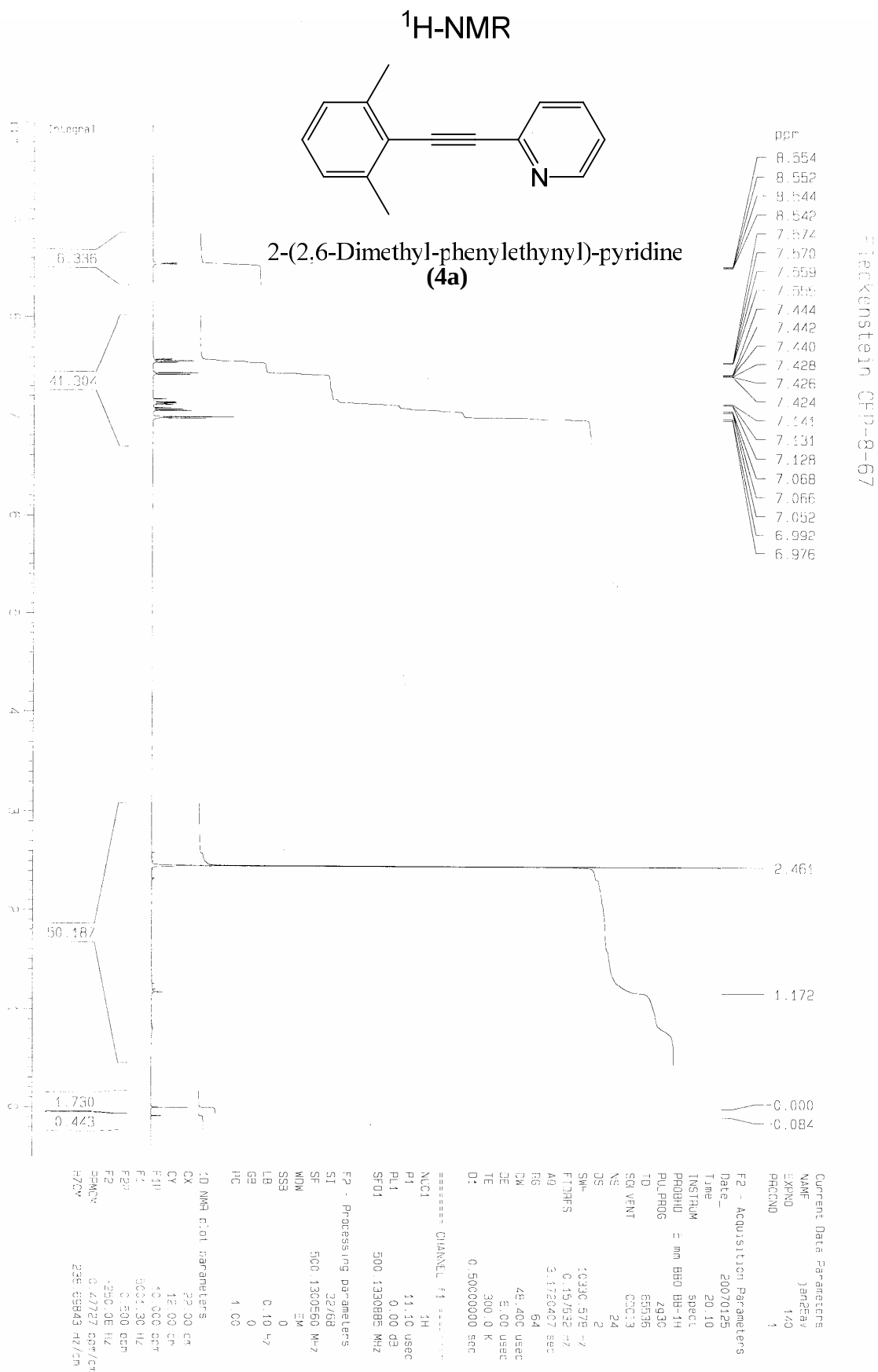
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*Anorganische Chemie im Zintl-Institut, TU Darmstadt, Petersenstr. 18,
64287 Darmstadt, Germany*

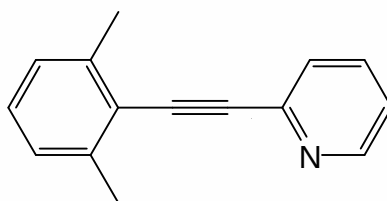
plenio@tu-darmstadt.de

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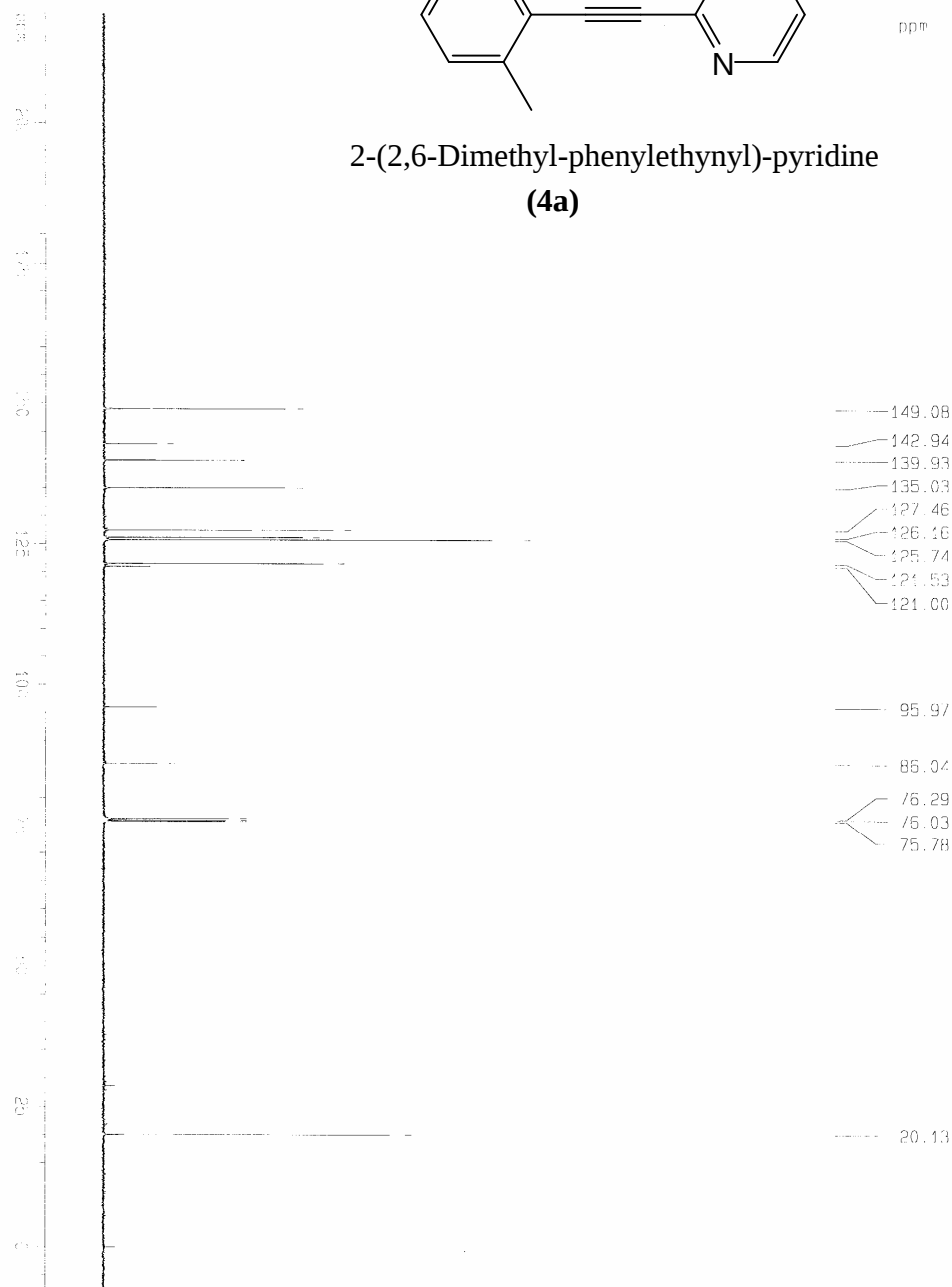
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¹³C-NMR



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



Current Data Parameters
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EXPNO 141
PROCNO 1

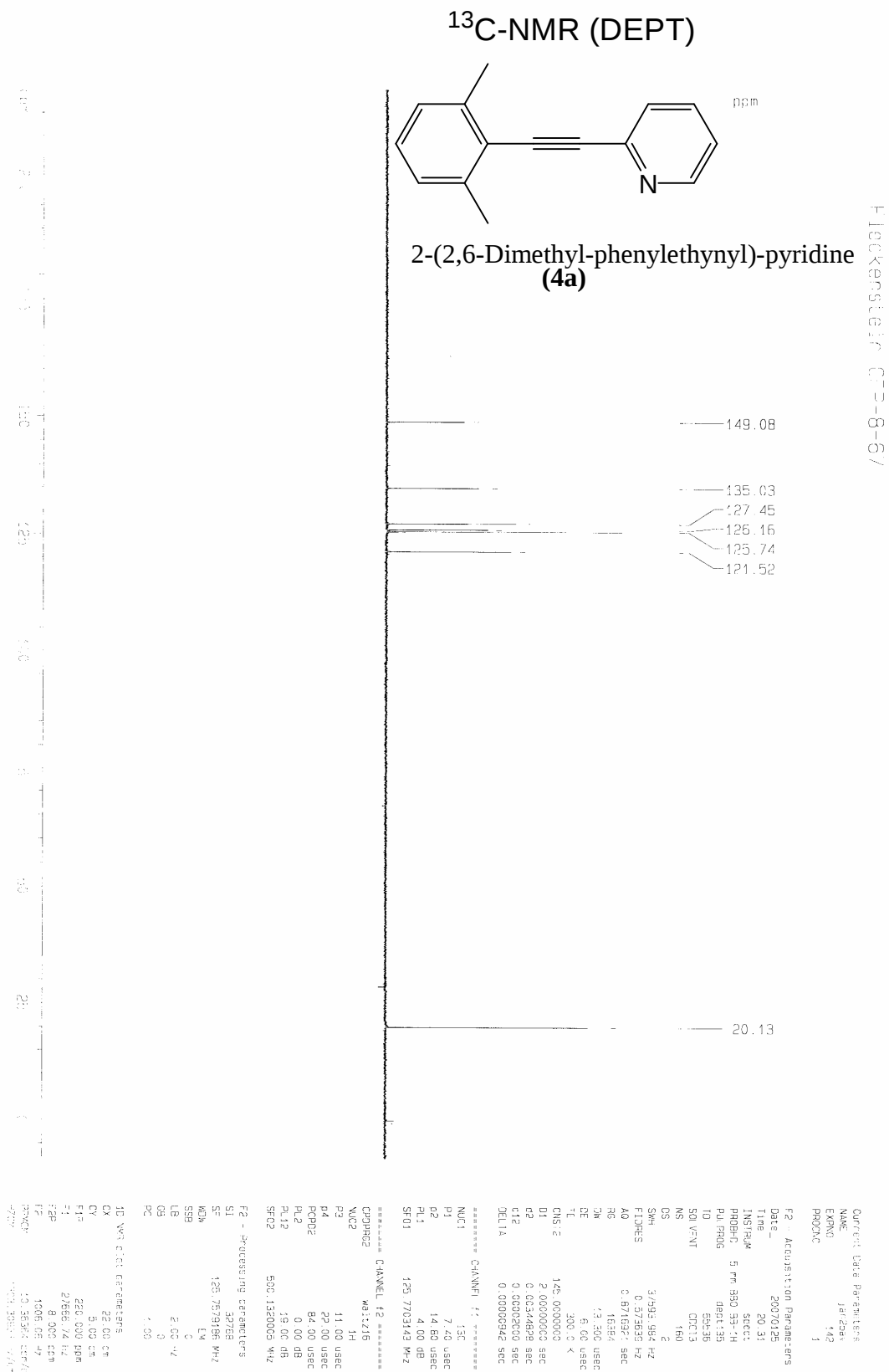
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Time 20.22
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NS 512
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FIDRES 0.173019 Hz
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DE 6.00 usec
TE 300.0 K
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d11 0.03000000 sec
d12 0.00020000 sec

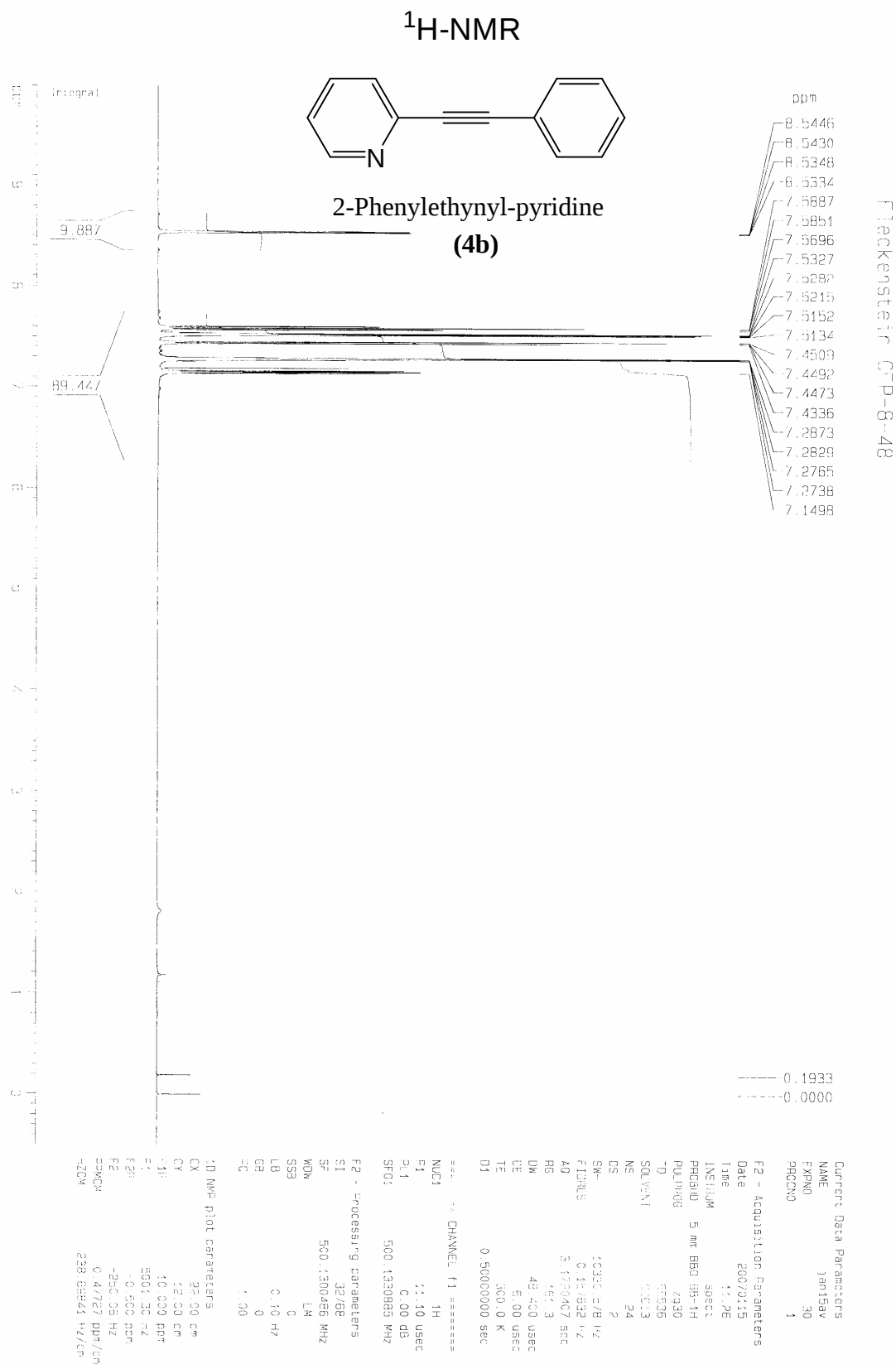
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PL1 4.00 dB
SFO1 125.770343 MHz

===== CHANNEL f2 =====
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NUC2 1H
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
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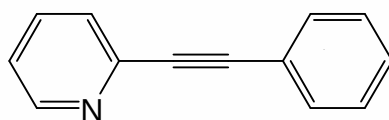
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WOK FM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

10 MHz offset parameters
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CY 7.00 cm
F1 220.000 cm
F1 27866.74 Hz
F2 -8.000 cm
F2 -1006.06 Hz
JQCX 10.3634 cm/s
JQCY 19.8393 cm/s



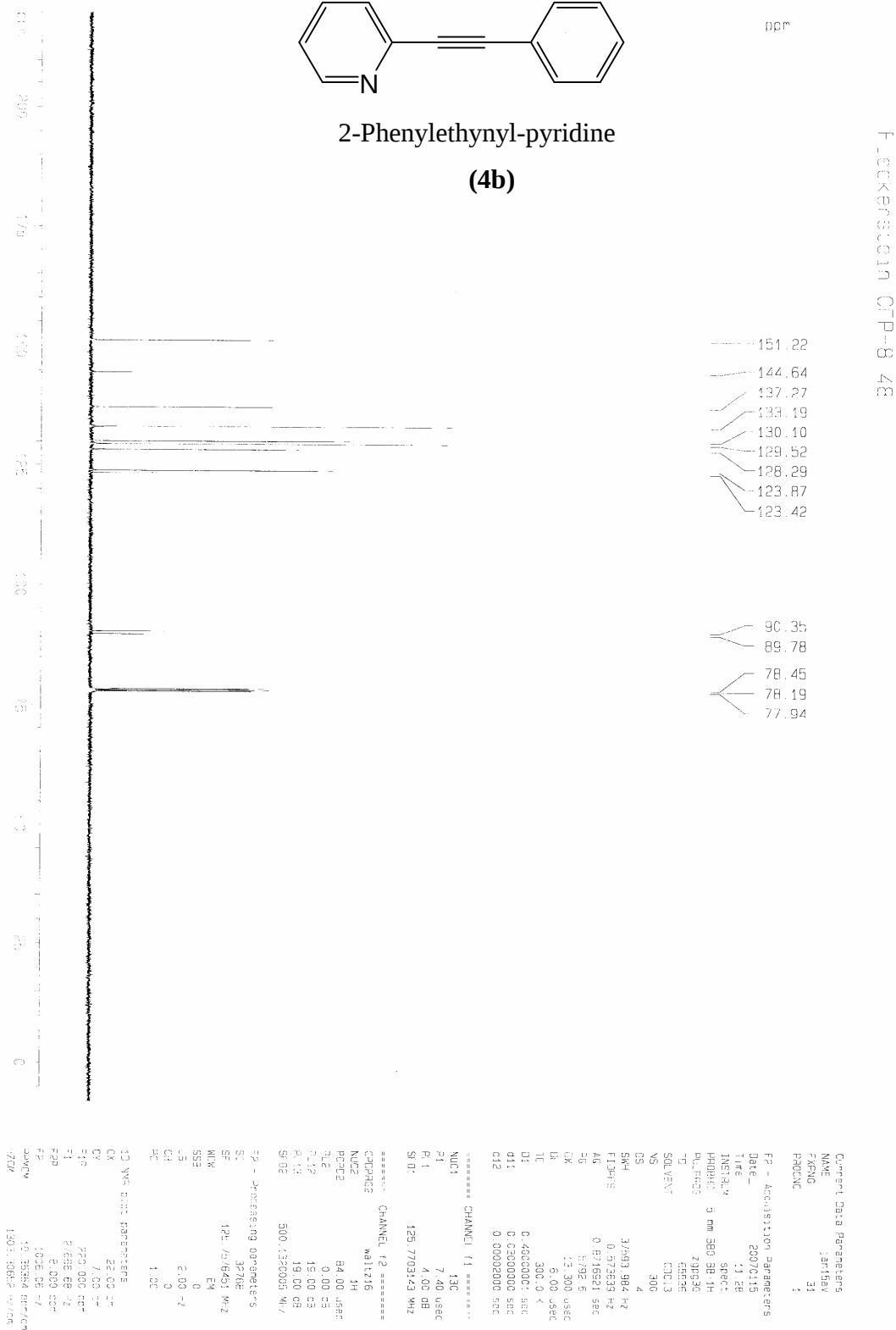


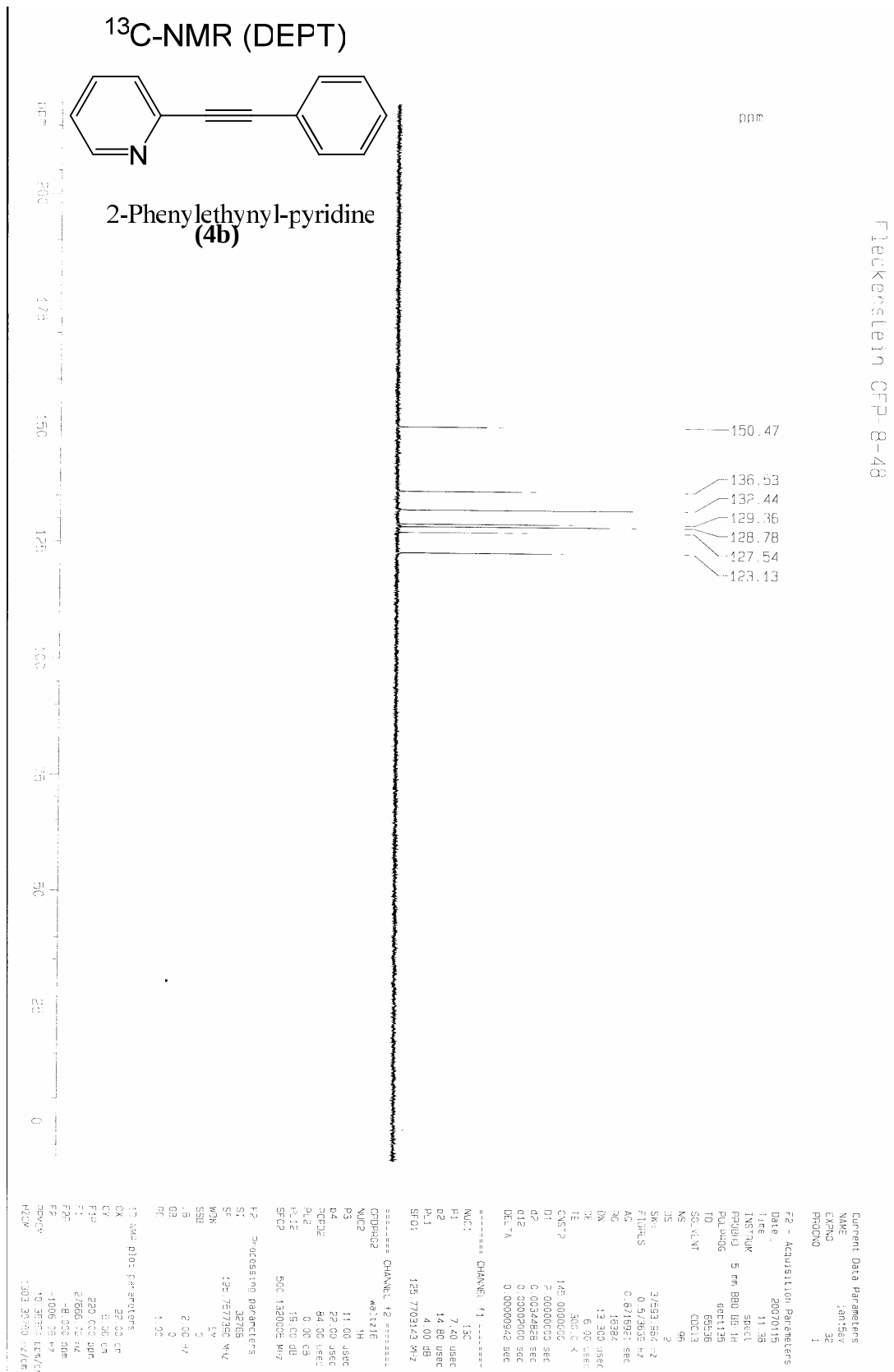
¹³C-NMR



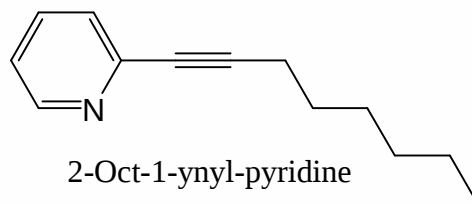
2-Phenylethynyl-pyridine

(4b)



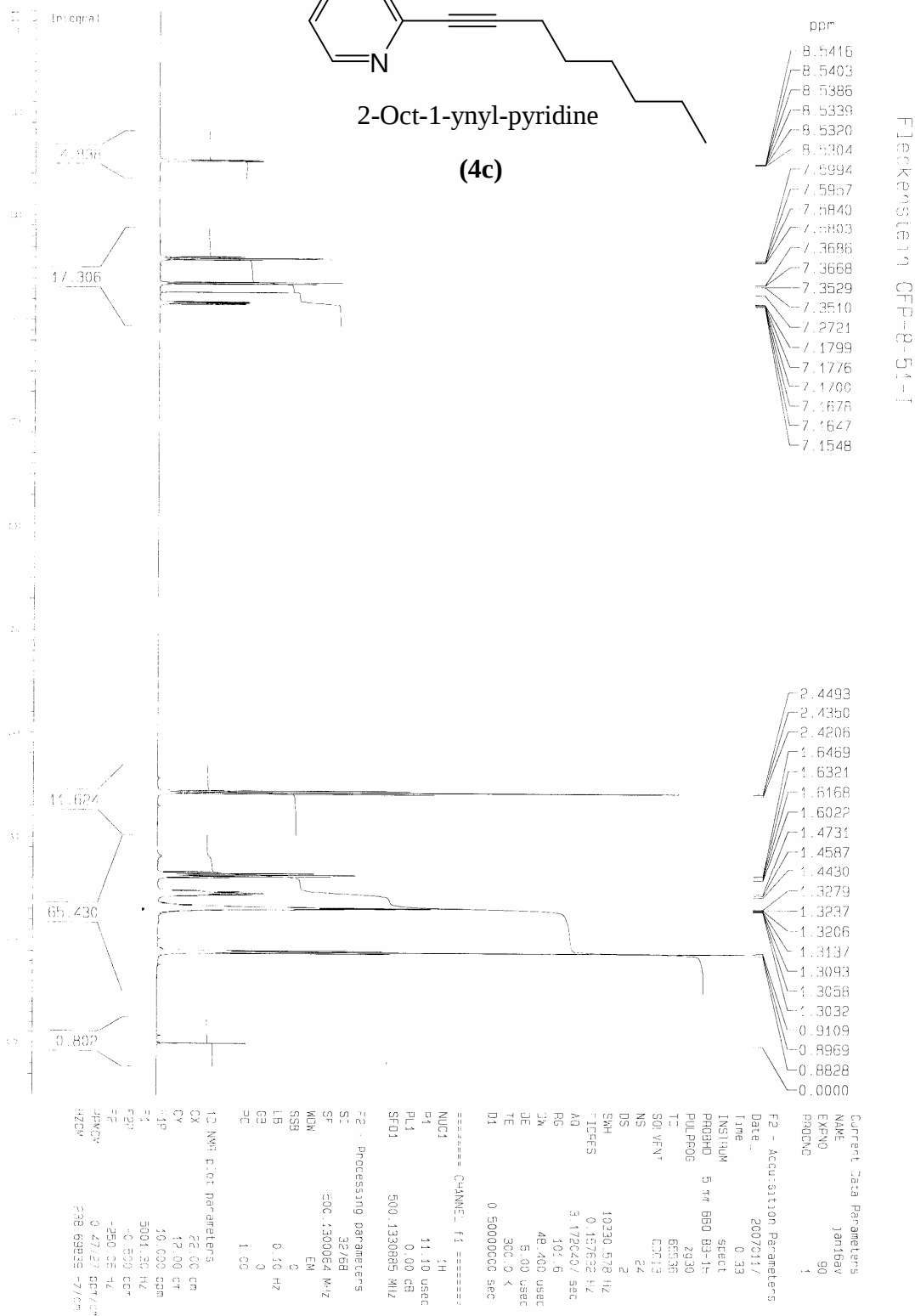


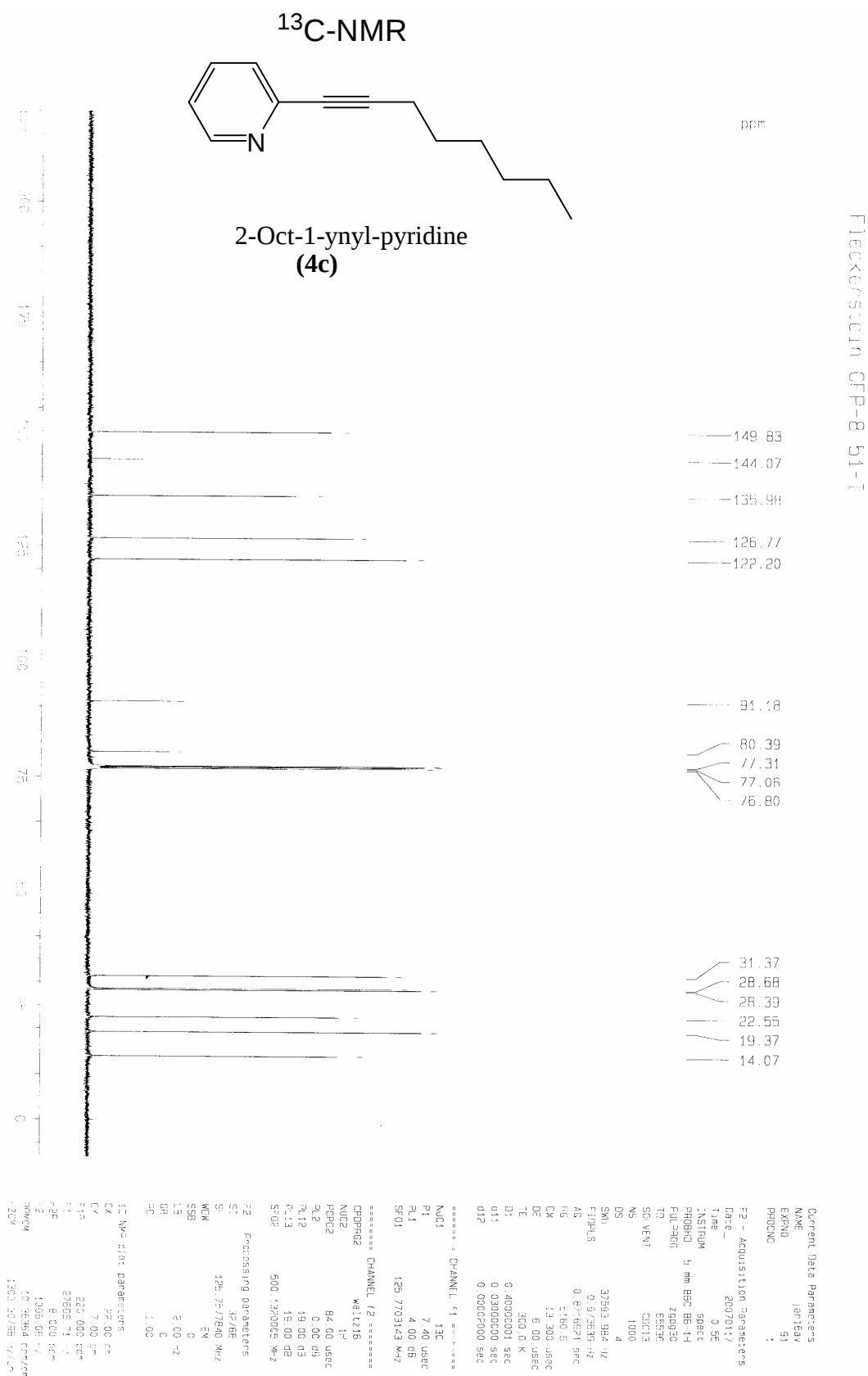
¹H-NMR

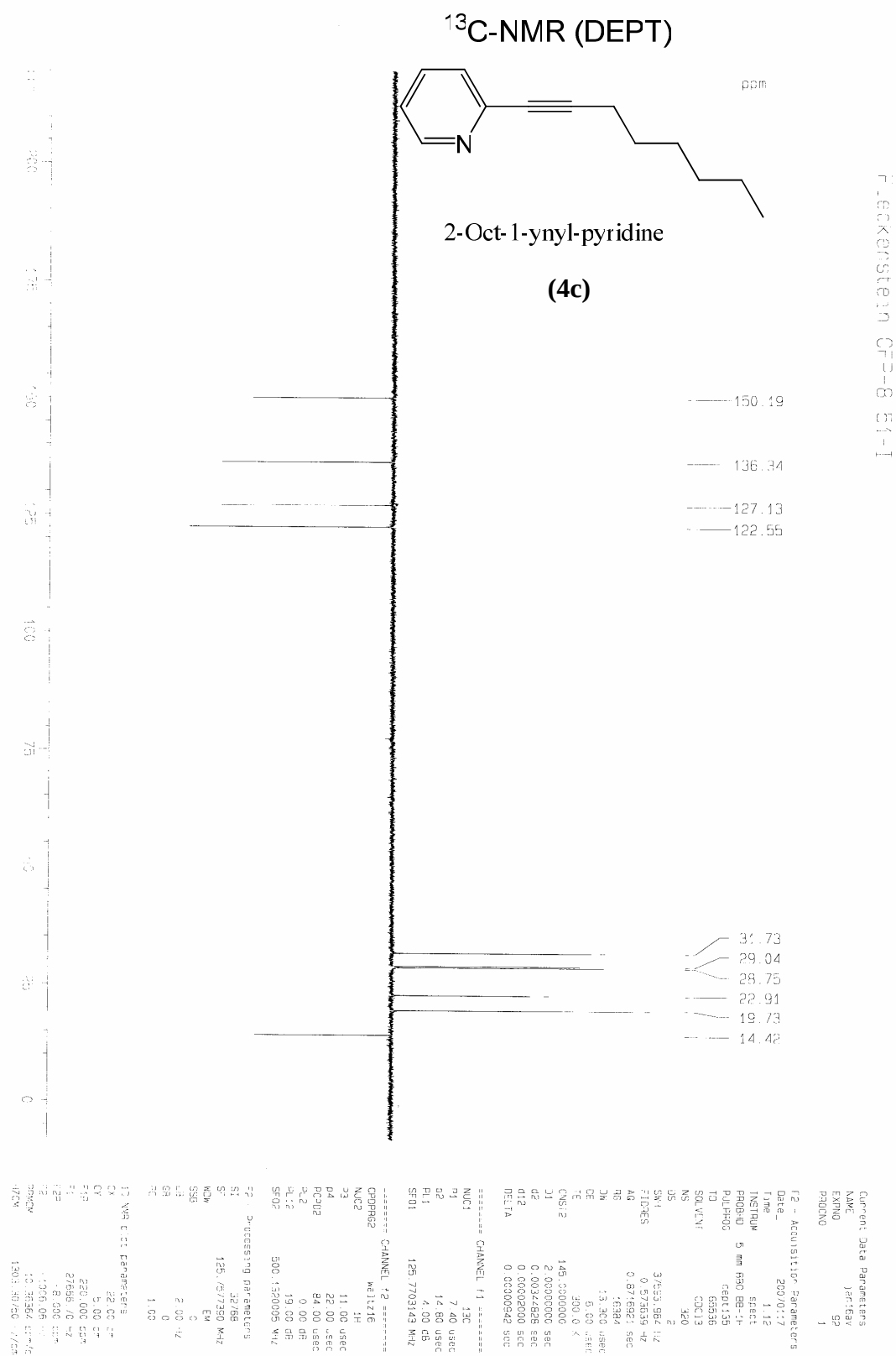


2-Oct-1-ynyl-pyridine

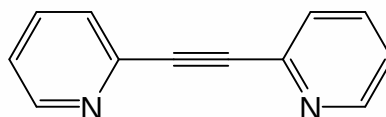
(4c)



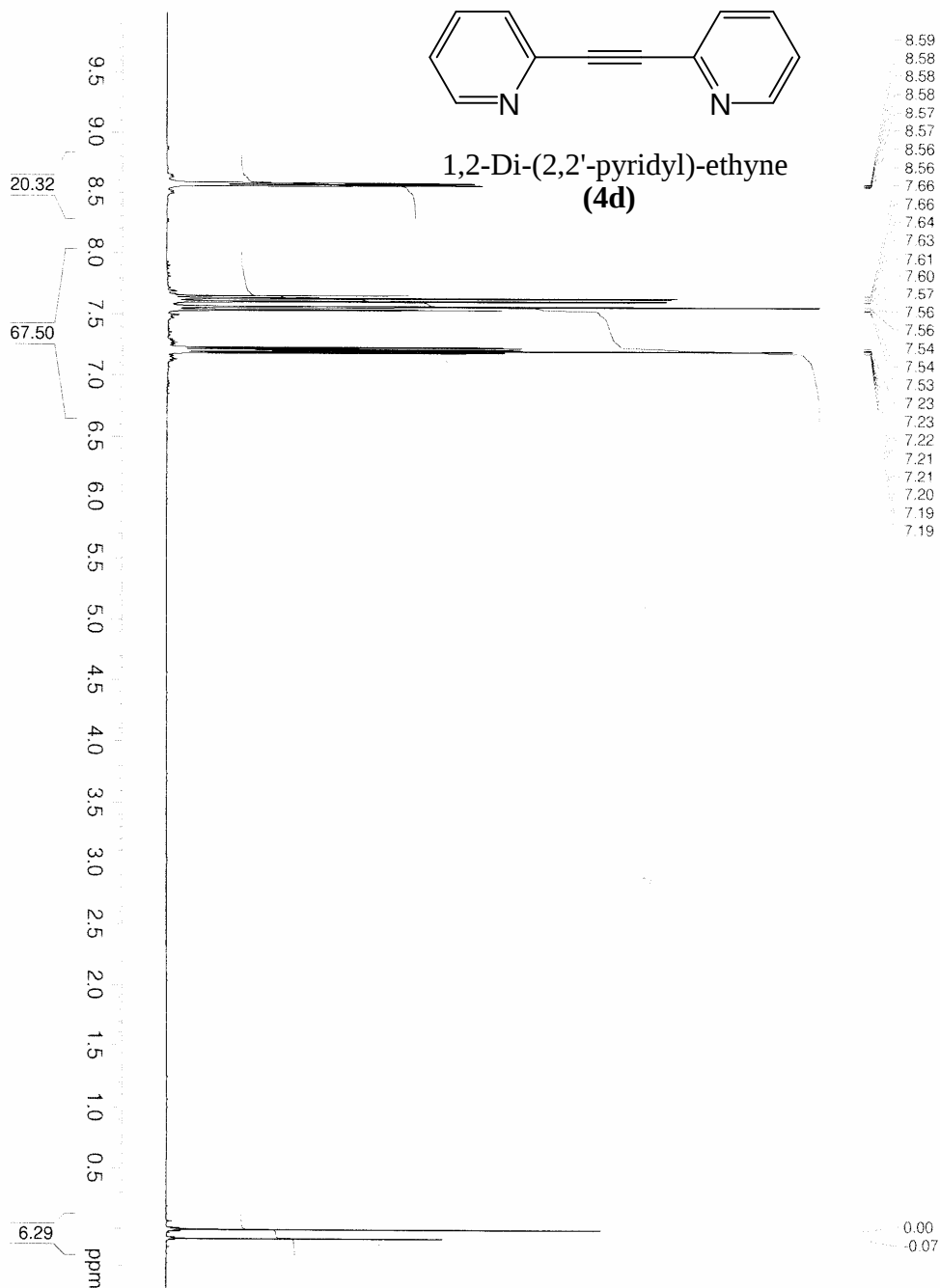




¹H-NMR



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



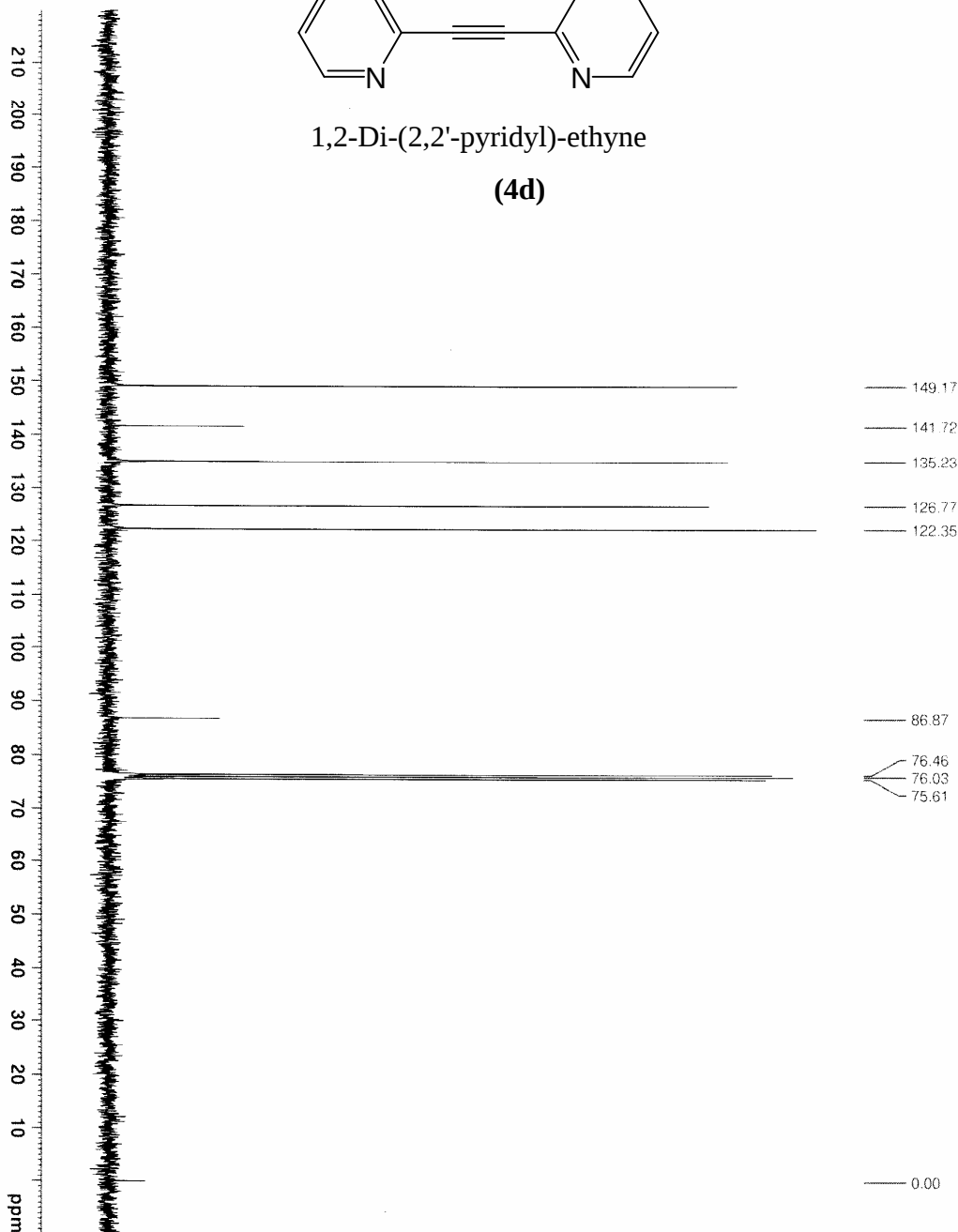
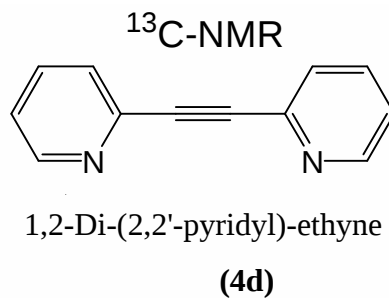
Fleckenstein CFP-8-56

8.59
8.58
8.58
8.58
8.57
8.57
8.56
8.56
7.66
7.66
7.64
7.63
7.61
7.60
7.57
7.56
7.56
7.54
7.54
7.53
7.23
7.23
7.22
7.21
7.21
7.20
7.19
7.19

0.00
-0.07

Current Data Parameters
NAME Jan19ac
EXNO 240
PROCNO 1
F2 - Acquisition Parameters
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Time 15.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
PCPDPR 32648
SOLVENT CDCl3
NS 32
DS 2
SWH 6188.119 Hz
FIDRES 0.188846 Hz
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RG 322
DE 80.800 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
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NUC1 1H
P1 9.70 usec
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PC 50.00

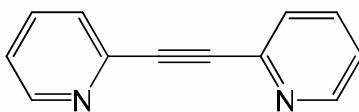
Fleckenstein CFP-8-56



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EXPNO 241
PROCNO 1
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Time 15.37
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PULPROG zgpg30
PCPDPR 326.63
SOLVENT CDCl3
NS 512
DS 4
SWH 27929.824 Hz
FIDRES 0.669245 Hz
AQ 0.7471624 sec
RG 327.250
DM 22.800 usec
DE 10.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.63939390 sec
TD0 1
===== CHANNEL f1 =====
NUC1 ¹³C
P1 1.00 usec
PL1 0.00 dB
SFO1 75.4174560 MHz
===== CHANNEL f2 =====
CDPRG2 waltz16
NUC2 ¹H
PCPD2 95.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 23.00 dB
SFO2 299.9011996 MHz
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SSB 0
LB 2.00 Hz
GB 0
PC 1.40

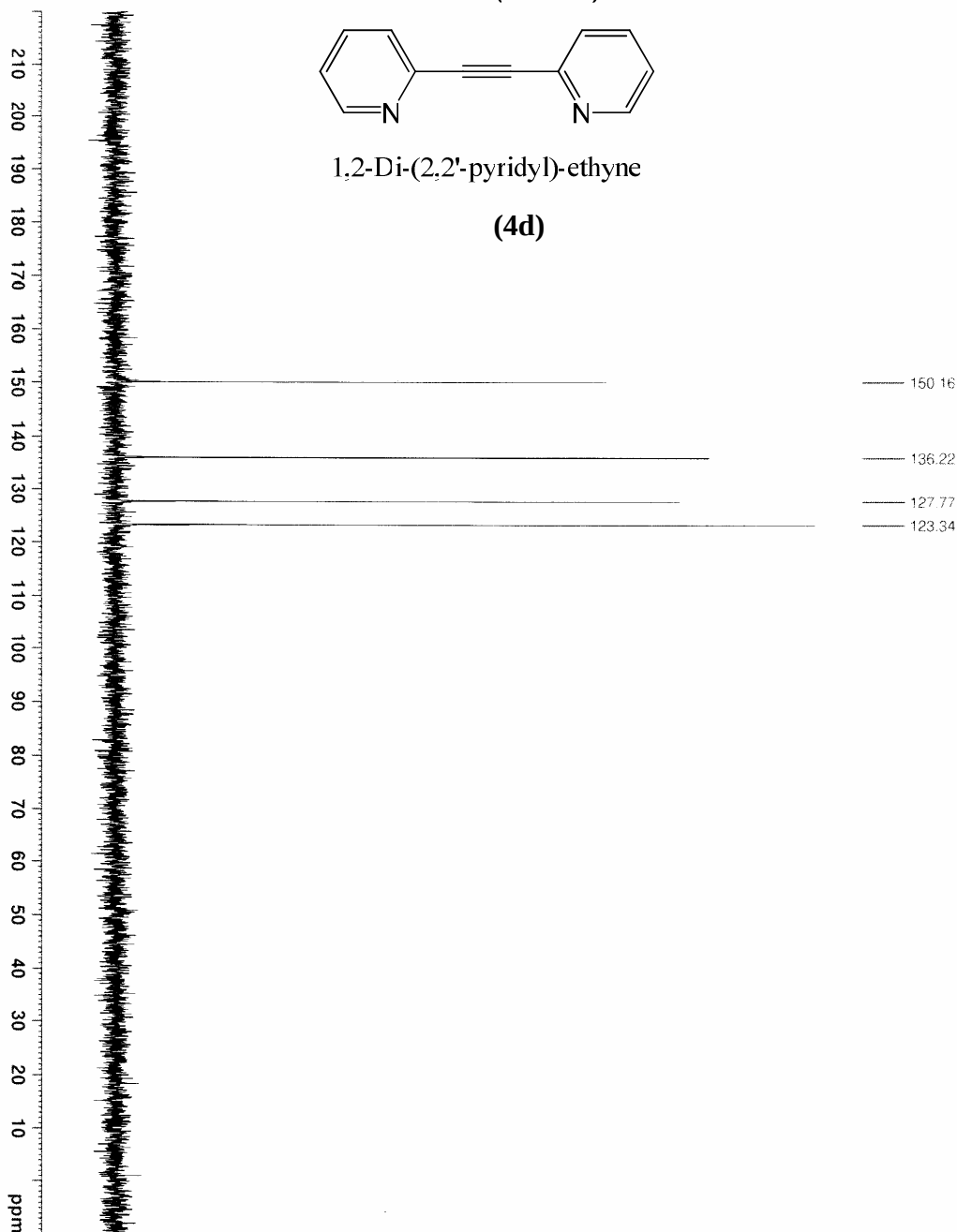
Fleckenstein CFP-8-56

¹³C-NMR (DEPT)

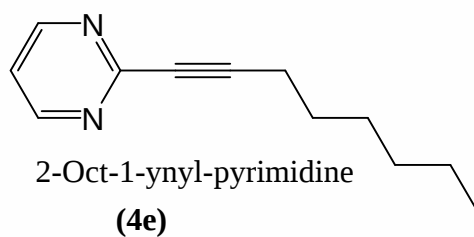


1,2-Di-(2,2'-pyridyl)-ethyne

(4d)



Current Data Parameters
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PROCNO 1
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Time 15.45
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 640
DS 4
SWH 21929.824 Hz
FIDRES 0.469245 Hz
AQ 0.747541 sec
RG 0.72050
DW 22.800 usec
DE 10.00 usec
TE 300.2 K
CARTZ2 145.070000
D1 2.0000000 sec
d12 0.00344828 sec
DELTA 0.0000000 sec
DELTA2 0.0000000 sec
TDO 0.0000000 sec
===== CHANNEL f1 =====
NUC1 13C
P1 11.00 usec
P2 22.00 usec
PL1 0.00 dB
SFO1 75.4174560 MHz
===== CHANNEL f2 =====
CDPRG2 waltz16
NUC2 1H
P3 9.00 usec
P4 19.00 usec
PCPD2 95.00 usec
PL2 -3.00 dB
PL12 17.00 dB
SFO2 299.901596 MHz
F2 - Processing parameters
SI 32768
SF 75.4099150 MHz
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LB 2.00 Hz
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PC 1.40

[illegible]

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Current Data Parameters
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PROCNO        1

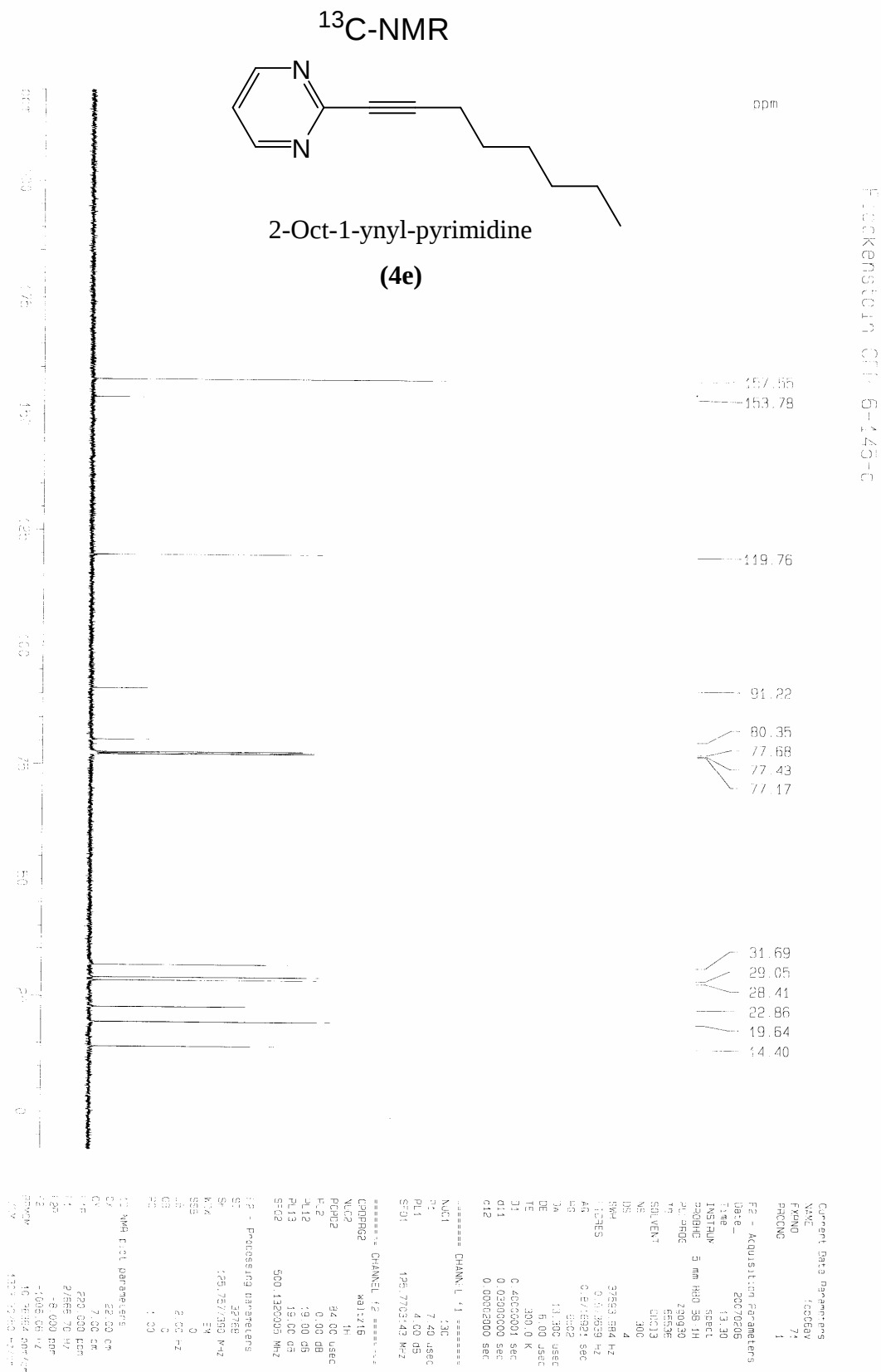
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Time          13.123
INSTRUM       spect
PROBHD        5 mm BBO 3B-1H
PULPROG       zg30
TD            65536
SOLVENT       CHCl3
NS            24
DS            2
SM            10330.00 Hz
F1CHS         0.150000 Hz
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DA            48.400 usec
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TE            300.0 K
D1            0.50000000 sec

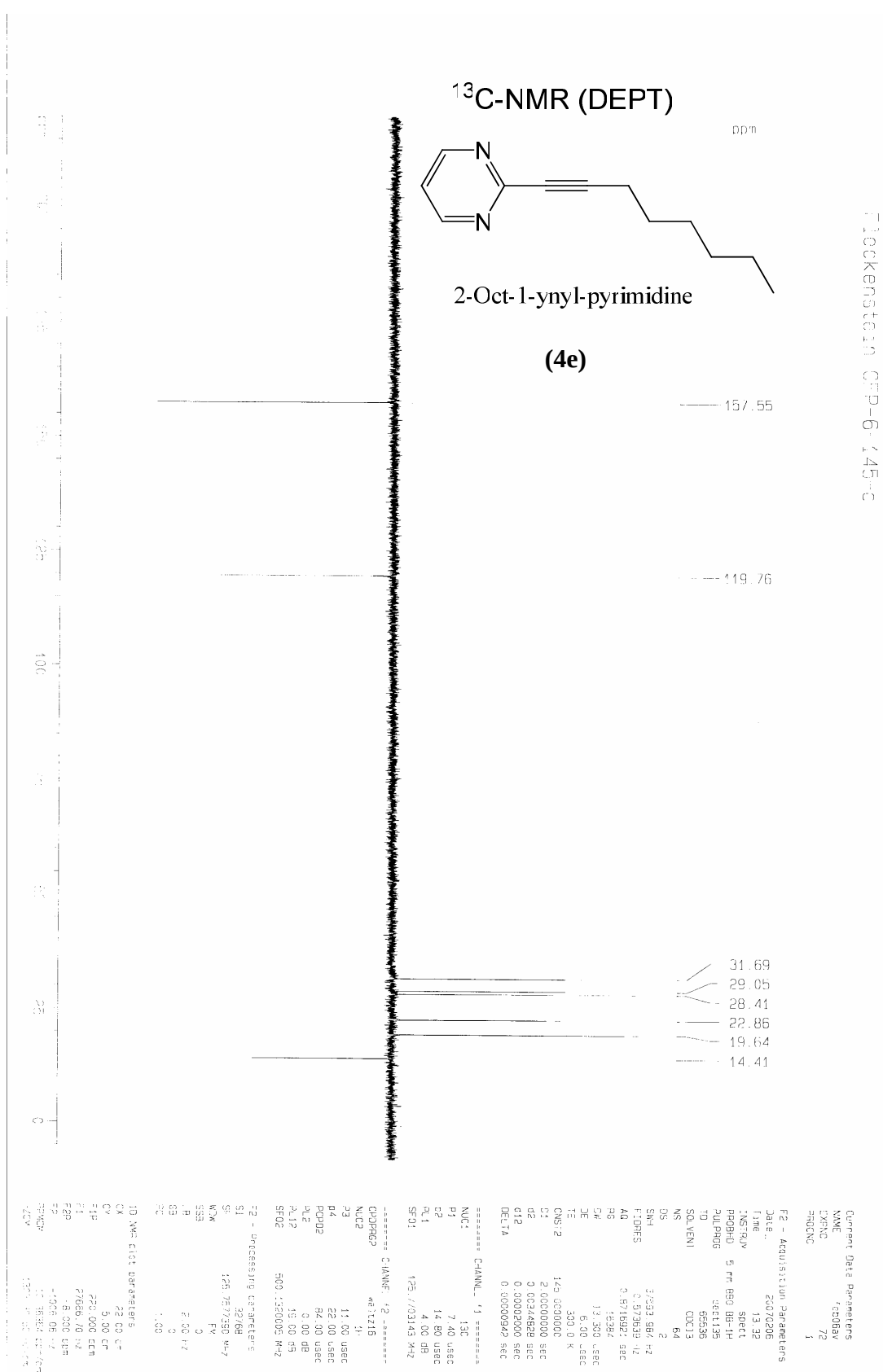
===== CHANNEL f1 =====
NUC1          1H
P1            11.10 usec
PL1           0.00 dB
SFO1          500.1330885 MHz

F2 - Processing parameters
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RB            0.10 Hz
GB            0
PC            1.00

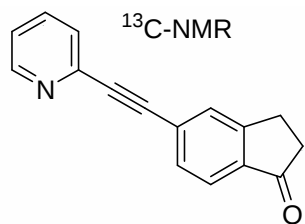
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CY            12.00 cm
F1-          10.000 MHz
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F2-          -250.00 Hz
SFO1          0.47727 Tmhz/cv
SFO1          238.09835 Hz/cm

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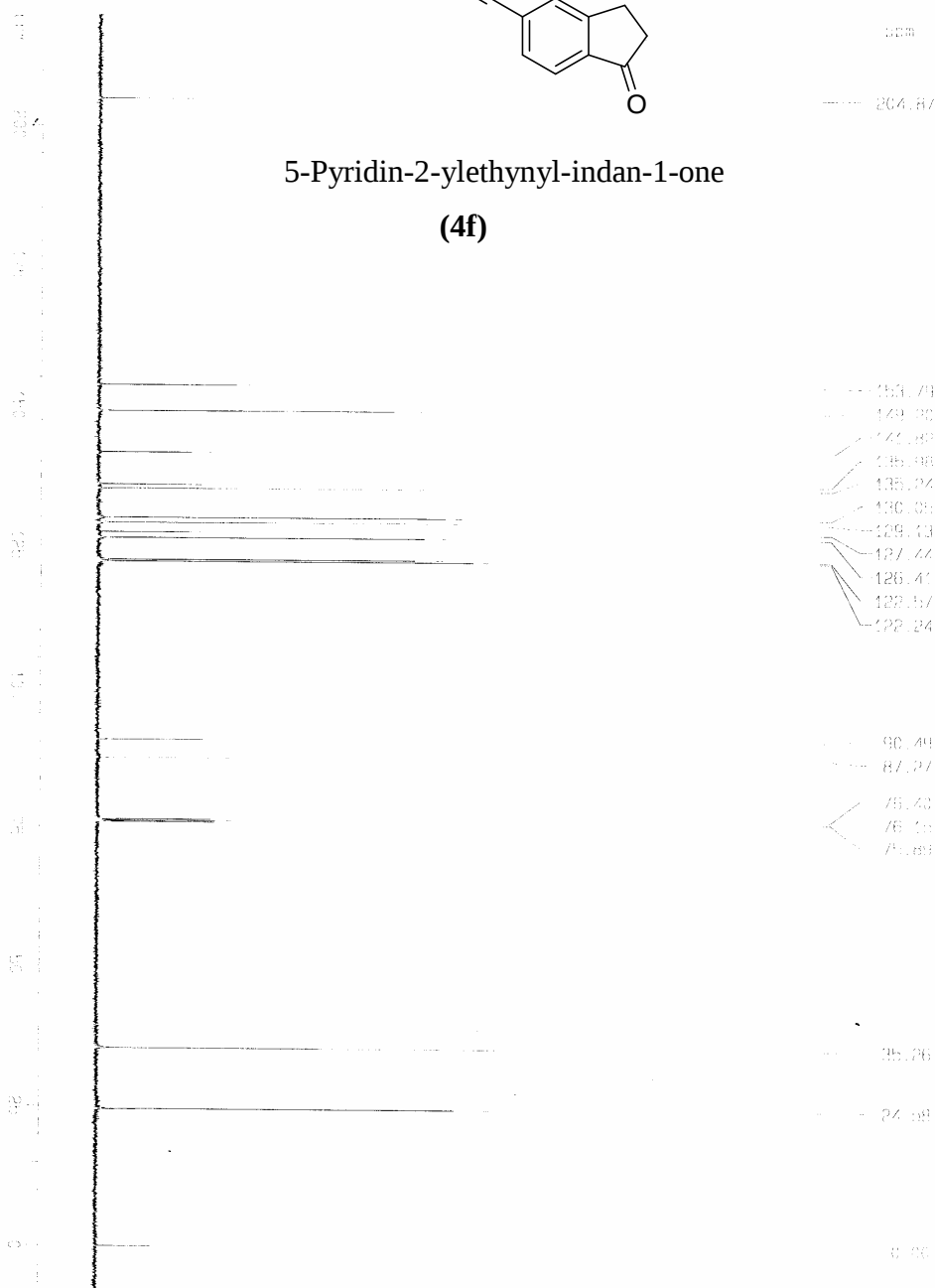




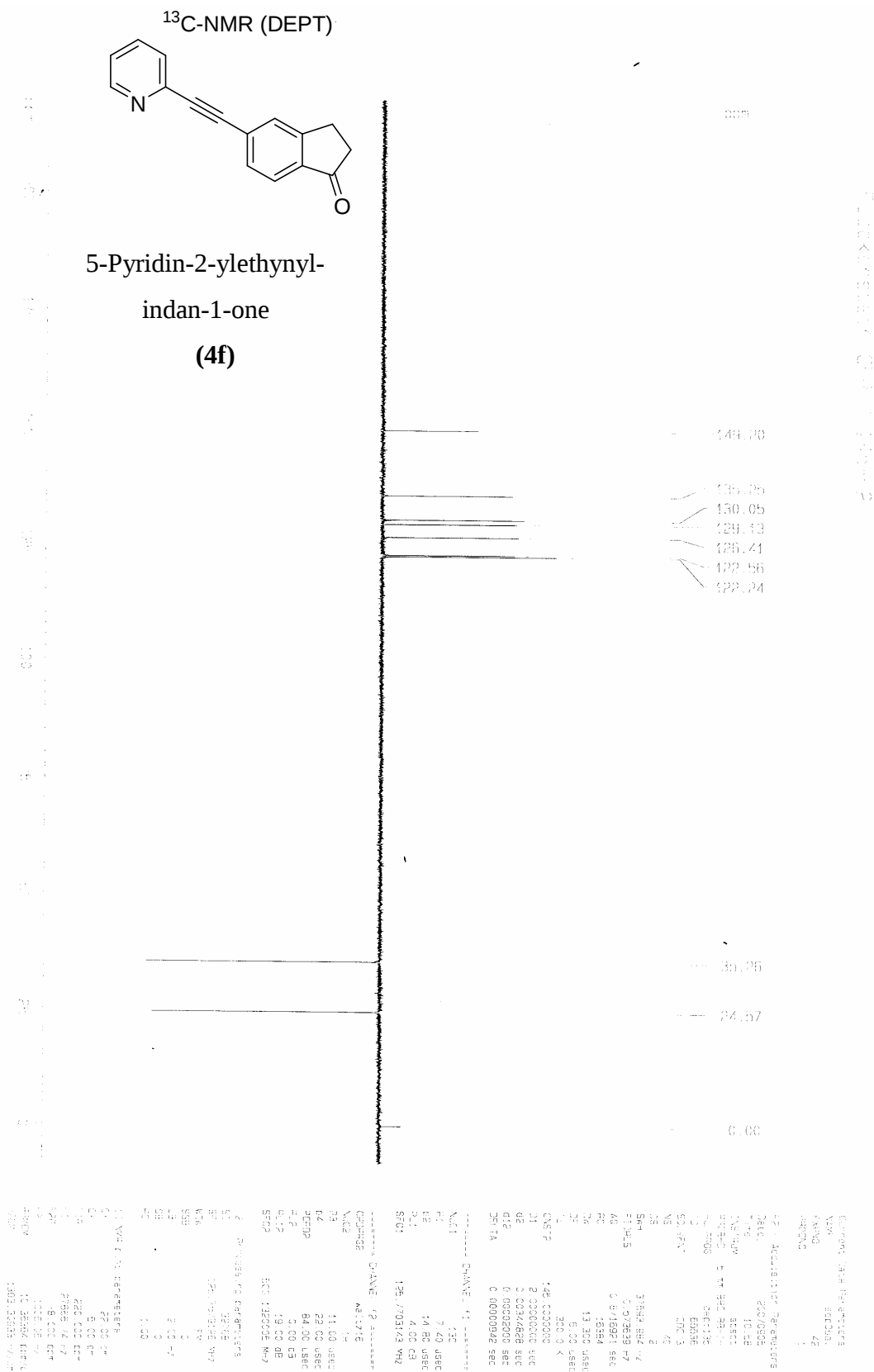




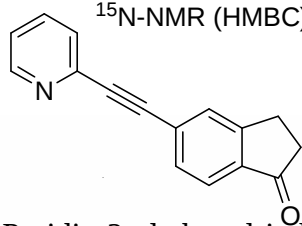
5-Pyridin-2-ylethynyl-indan-1-one
(4f)



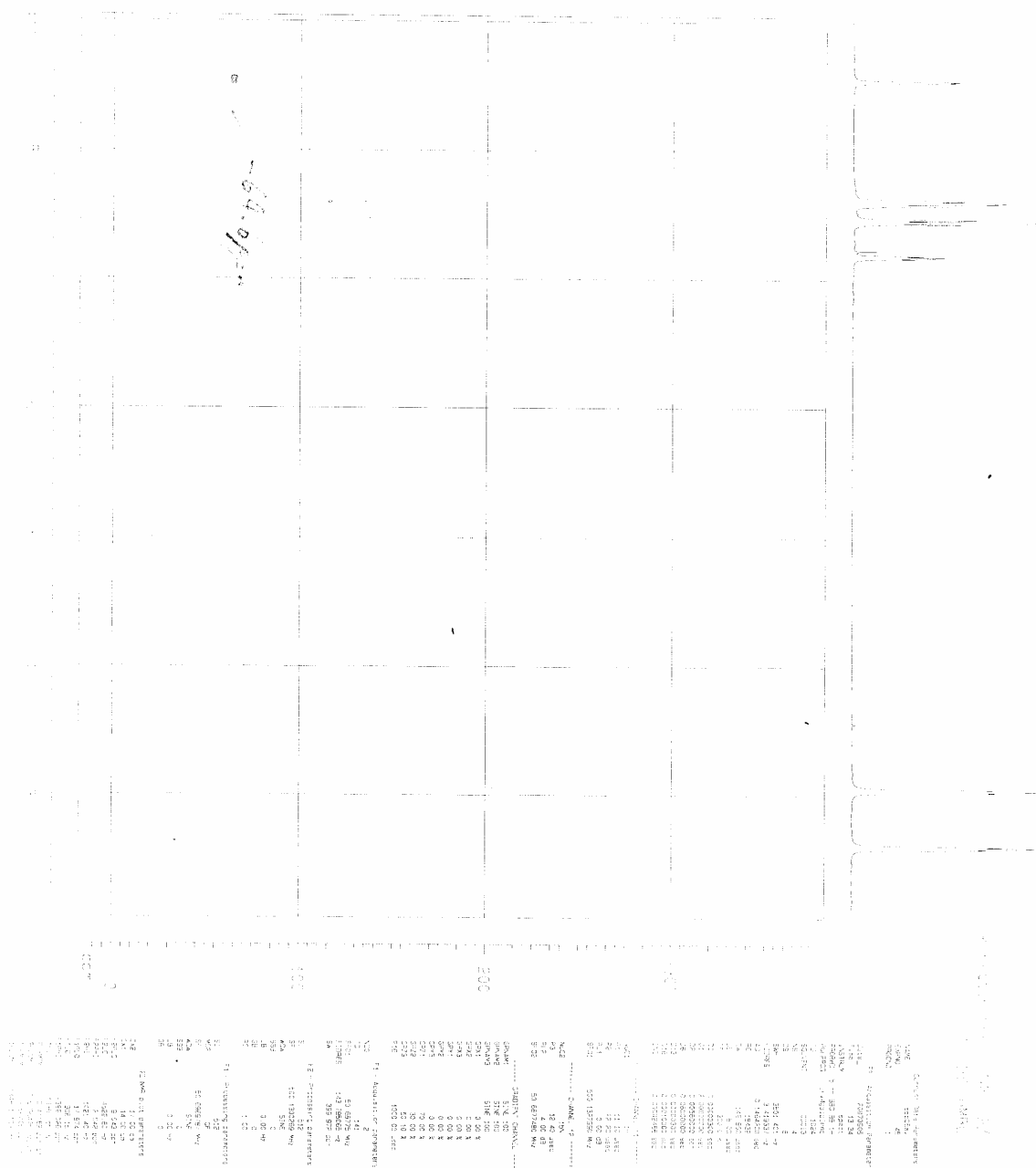
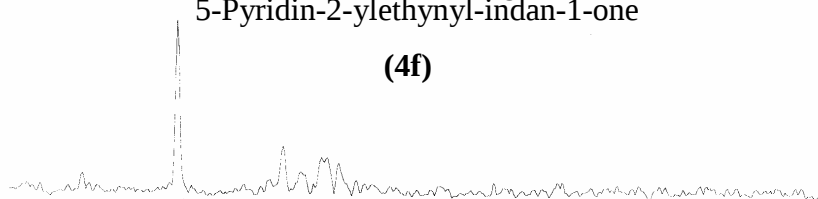
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Time: 15:05
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PULPROG: zgpg30
RG: 290.250
SI: 65536
SOLVENT: CDCl3
NS: 200
DS: 4
SWH: 37833.864 Hz
FIDRES: 0.674631 Hz
AQ: 0.811631 sec
RG: 1024.2
Wd: 13.330 usec
DE: 6.00 usec
TE: 300.2 K
D1: 2.00 usec
D2: 0.400000 sec
d11: 0.0300000 sec
d12: 0.0000000 sec
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NAME: 4f
EXPNO: 1
PROCNO: 1
Date_ Time: 09-08-2008 15:05:15
Date: 20080820
Time: 15:05
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
RG: 290.250
SI: 65536
SOLVENT: CDCl3
NS: 200
DS: 4
SWH: 37833.864 Hz
FIDRES: 0.674631 Hz
AQ: 0.811631 sec
RG: 1024.2
Wd: 13.330 usec
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TE: 300.2 K
D1: 2.00 usec
D2: 0.400000 sec
d11: 0.0300000 sec
d12: 0.0000000 sec

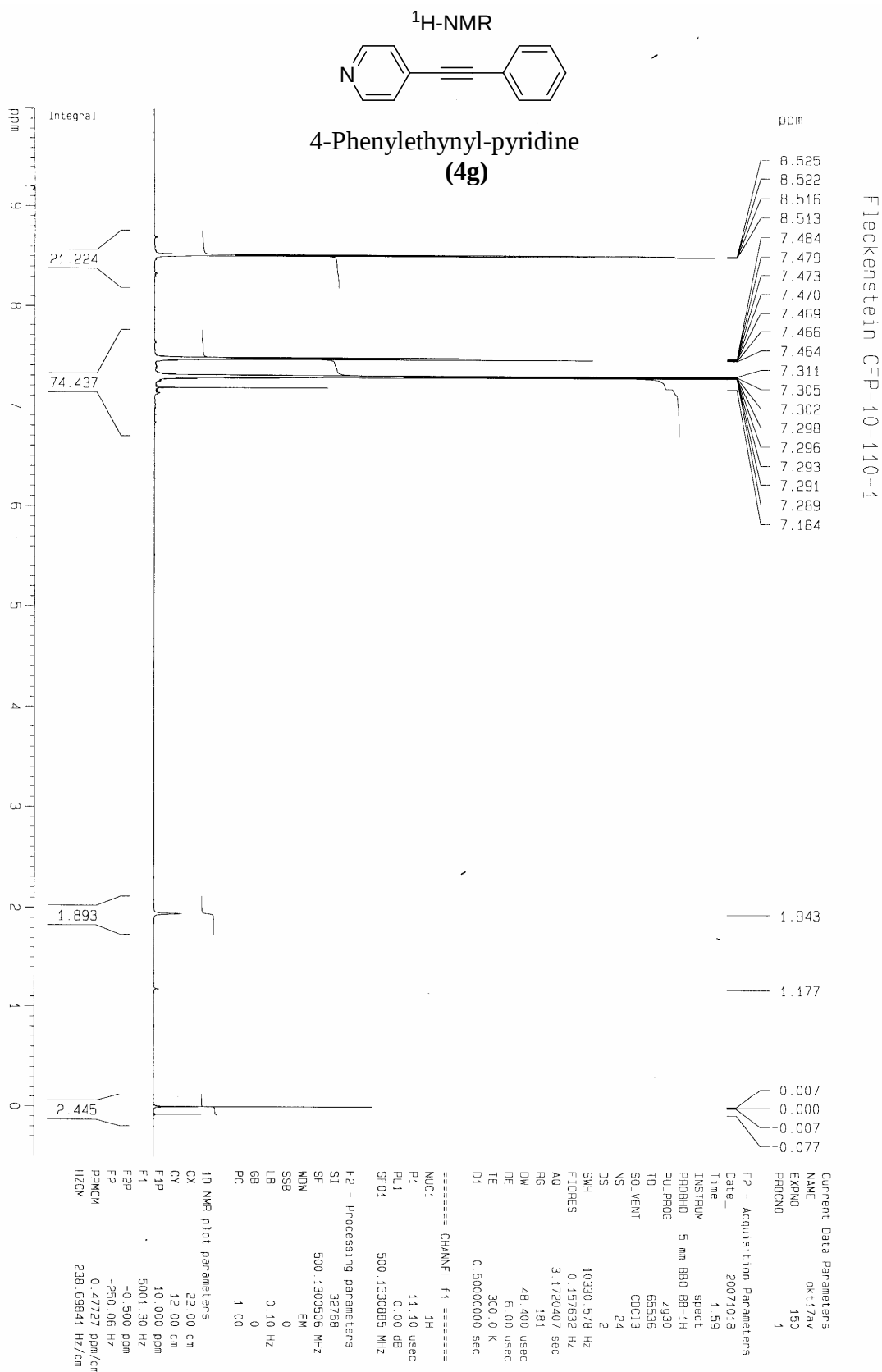


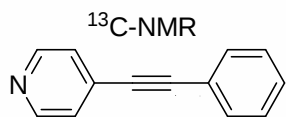
¹⁵N-NMR (HMBC)



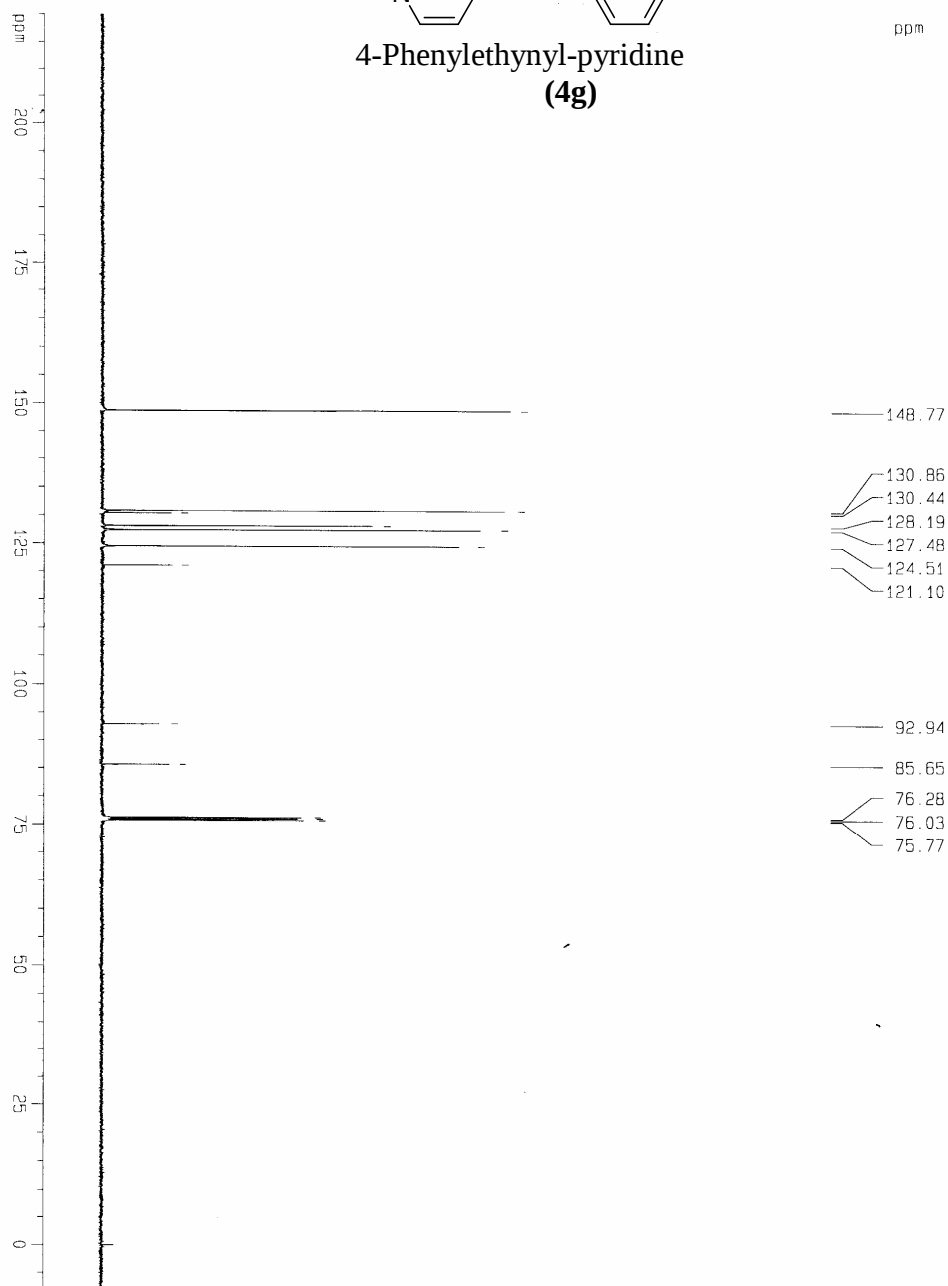
5-Pyridin-2-ylethynyl-indan-1-one
(4f)







**4-Phenylethynyl-pyridine
(4g)**



Fleckenstein CFP-10-110-1

Current Data Parameters
NAME OK17AV
EXPNO 151
PROCNO 1

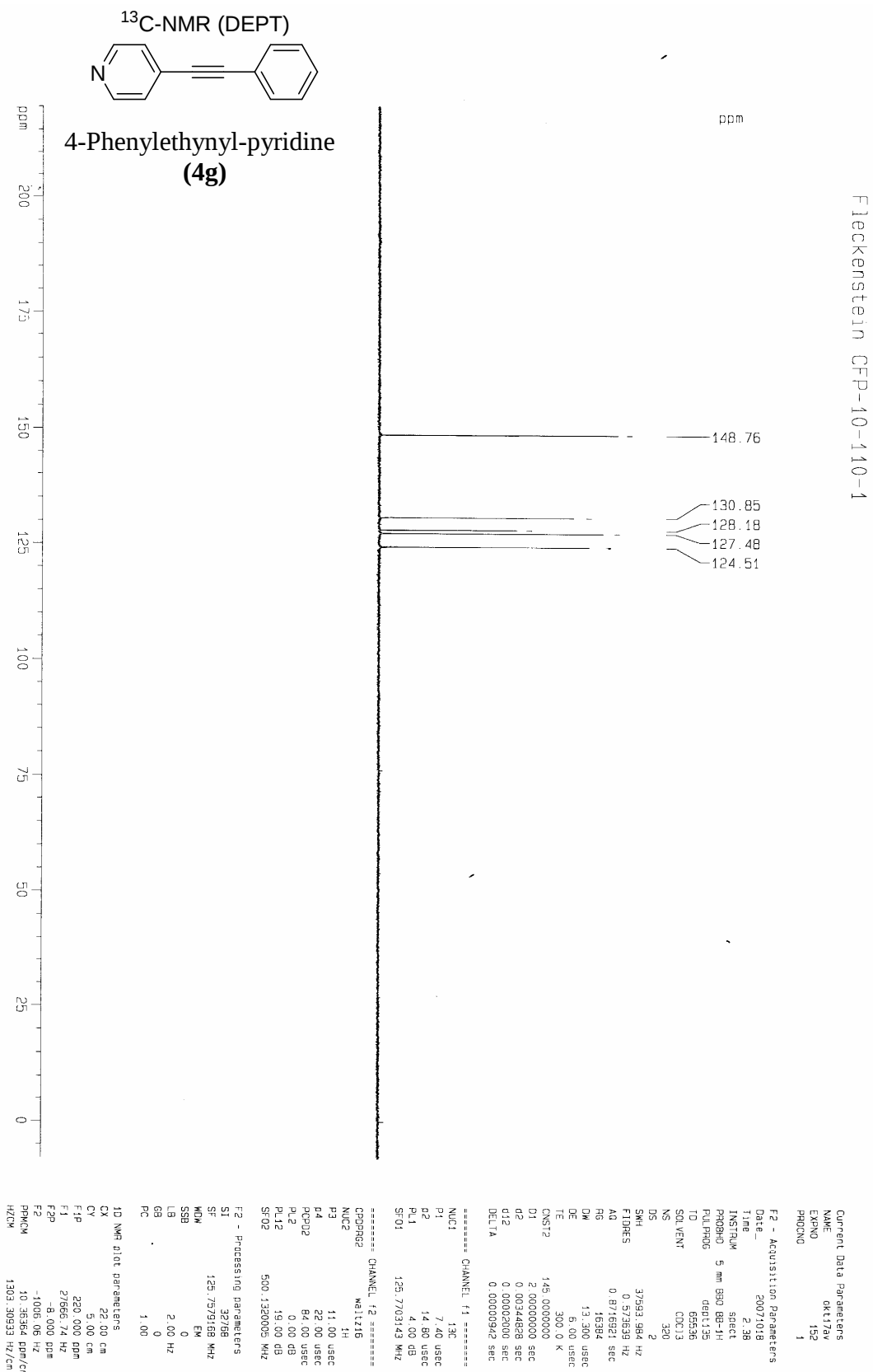
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Time 2.21
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 4
SWH 37593.984 Hz
FIDRES 0.573639 Hz
AQ 0.8716921 sec
RG 13004
DM 13.300 usec
DE 6.00 usec
TE 300.0 K
D1 0.4000001 sec
d11 0.0300000 sec
d12 0.0002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 7.40 usec
PL1 4.00 dB
SFO1 125.770343 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 84.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 19.00 dB
SFO2 500.132005 MHz

F2 - Processing parameters
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WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

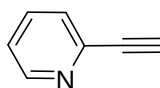
1D NMR plot parameters
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CY 7.00 cm
F1P 220.000 ppm
F1 2766.74 Hz
F2P -9.000 ppm
F2 -1006.06 Hz
PRCKN 10.36364 ppm/cm
HZCM 1305.30933 Hz/cm



(3a)



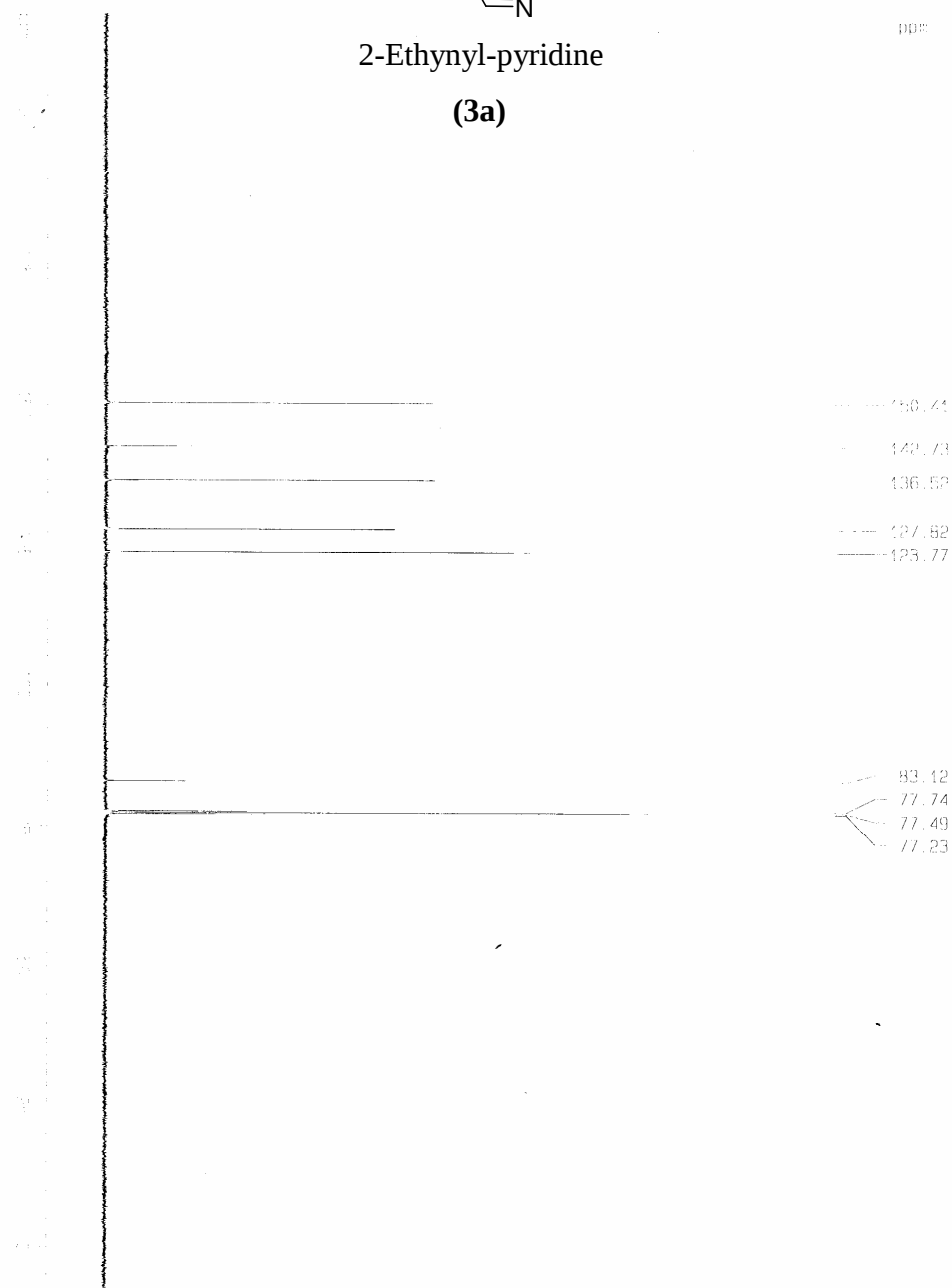
¹³C-NMR



2-Ethynyl-pyridine

(3a)

DDF

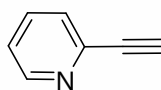


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Current Data Parameters
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EXPNO: 21
PROCNO: 1
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Time : 9.43
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
F2: 125.760 MHz
NUC1: 13C
NUC2: 1H
SFO1: 125.760 MHz
SFO2: 400.141 MHz
===== CHANNEL f2 =====
NUC1: 13C
P1: 7.40 usec
PL1: 4.00 dB
SFO1: 125.760 MHz
===== CHANNEL f2 =====
CTPPO2: 400.141 MHz
NUC2: 1H
P2: 14.00 usec
PL2: 0.00 dB
SFO2: 400.141 MHz
===== CHANNEL f2 =====
P2: Processing parameters
SI: 32768
SF: 125.760 MHz
WDW: EM
SSB: 0
GB: 0
EC: 0
LB: 0.30 Hz
GB: 0
PC: 1.00
=====
F2: Acquisition Parameters
Date_ : 20070515
Time : 9.43
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
F2: 125.760 MHz
NUC1: 13C
NUC2: 1H
SFO1: 125.760 MHz
SFO2: 400.141 MHz
===== CHANNEL f2 =====
NUC1: 13C
P1: 7.40 usec
PL1: 4.00 dB
SFO1: 125.760 MHz
===== CHANNEL f2 =====
CTPPO2: 400.141 MHz
NUC2: 1H
P2: 14.00 usec
PL2: 0.00 dB
SFO2: 400.141 MHz
===== CHANNEL f2 =====
P2: Processing parameters
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SF: 125.760 MHz
WDW: EM
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GB: 0
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PC: 1.00
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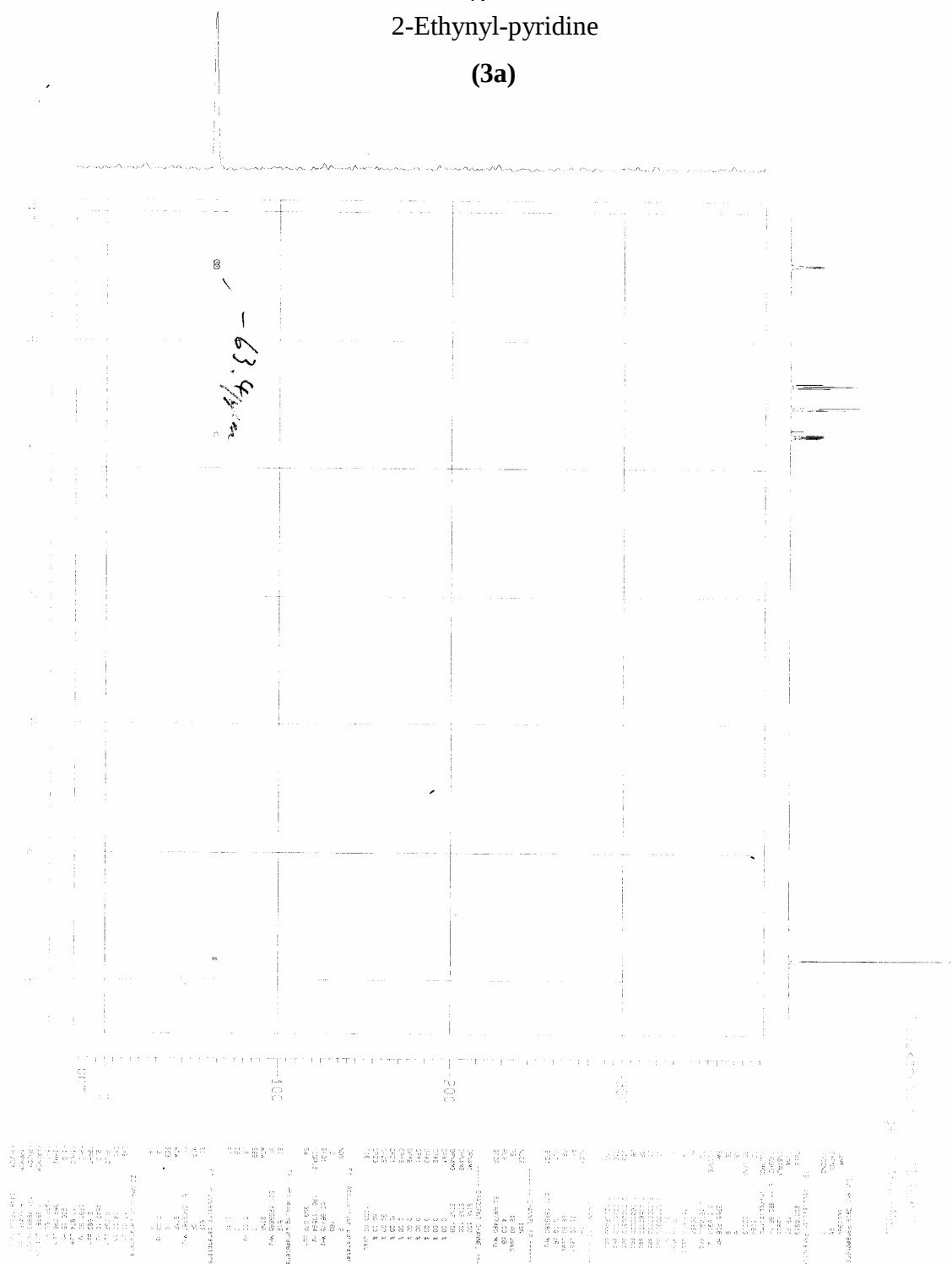
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¹⁵N-NMR (HMBC)

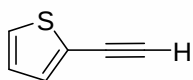


2-Ethynyl-pyridine

(3a)

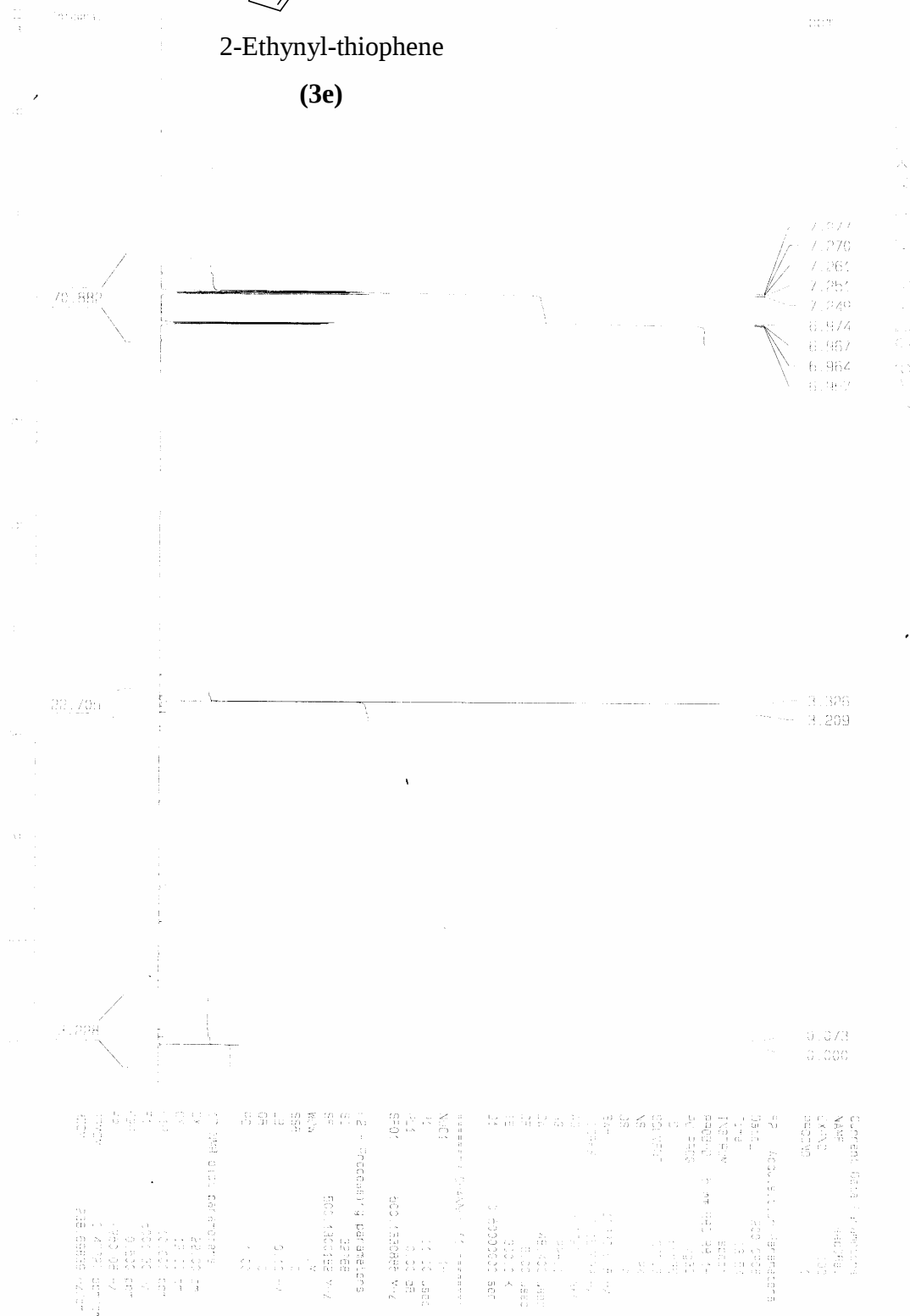


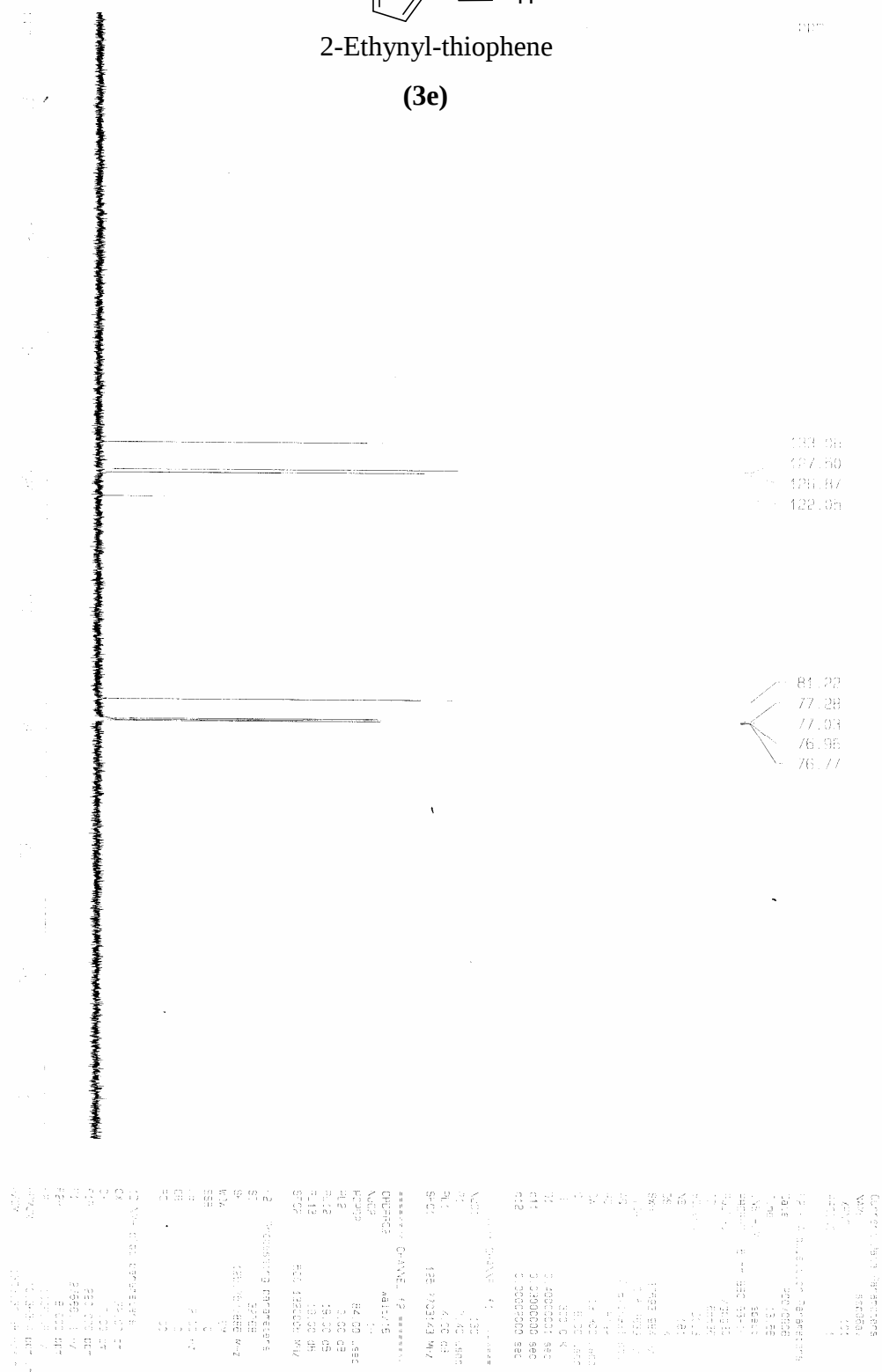
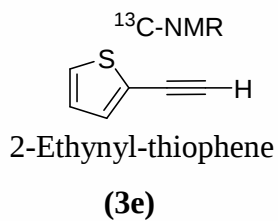
¹H-NMR

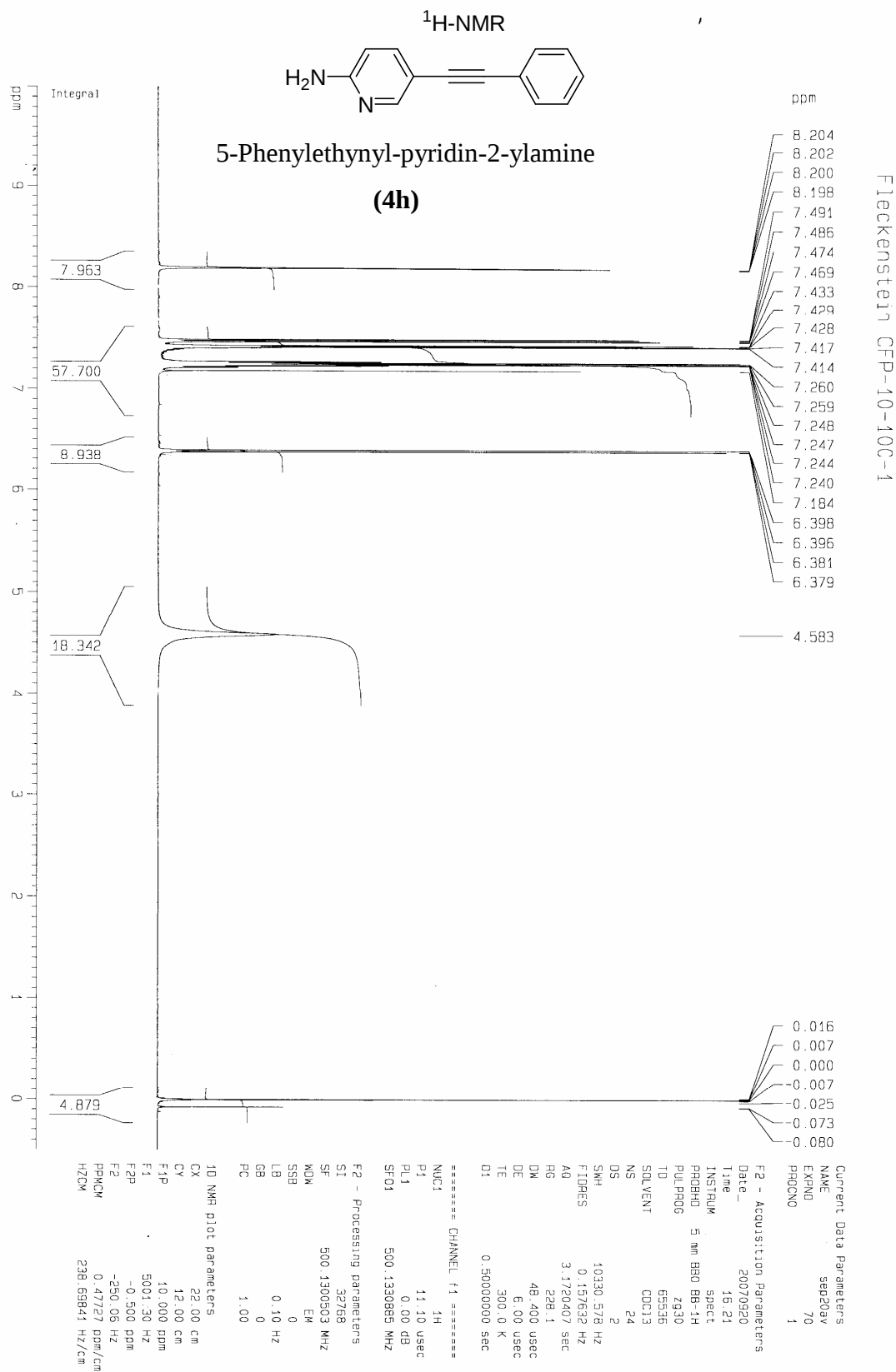


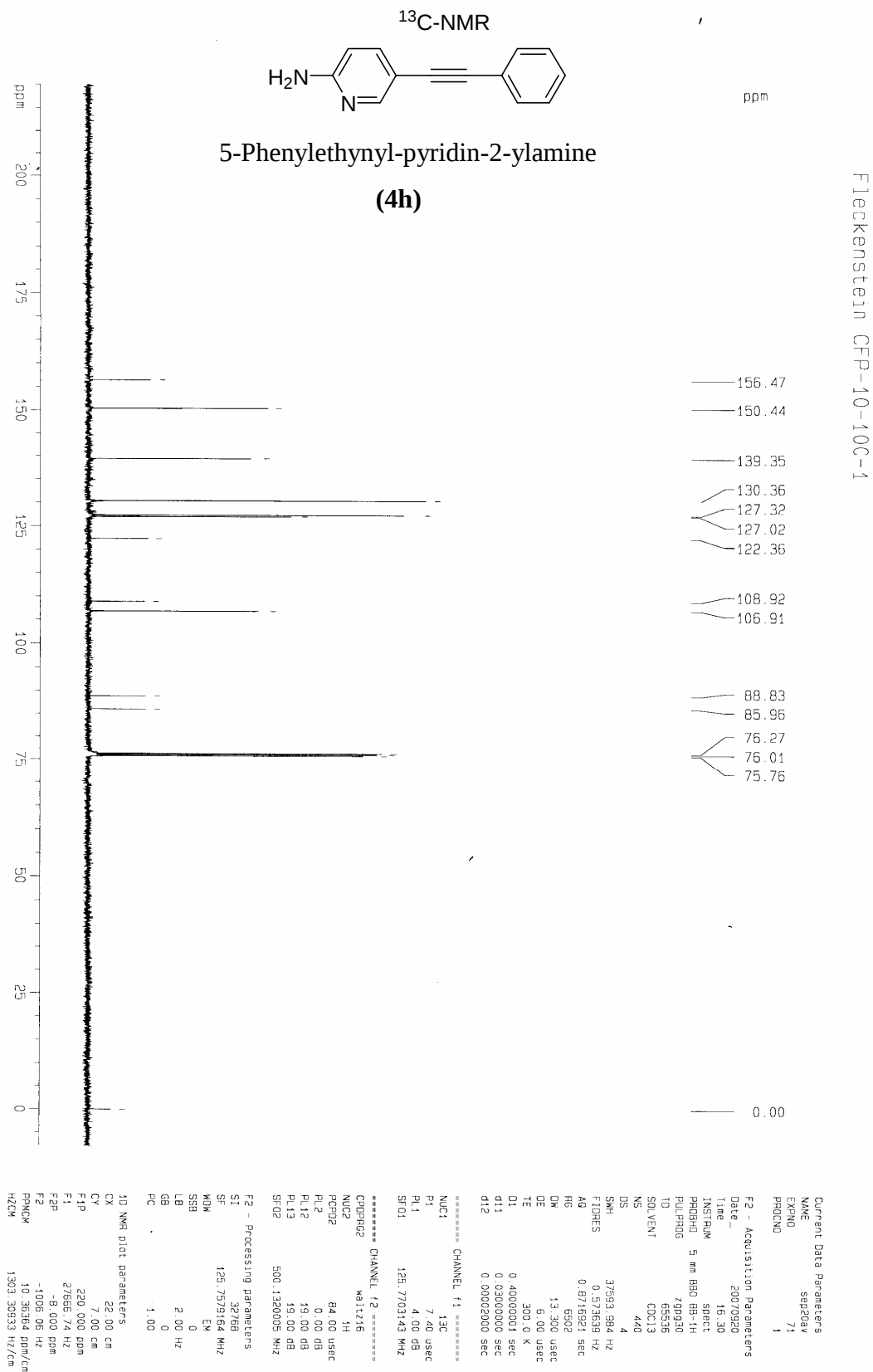
2-Ethynyl-thiophene

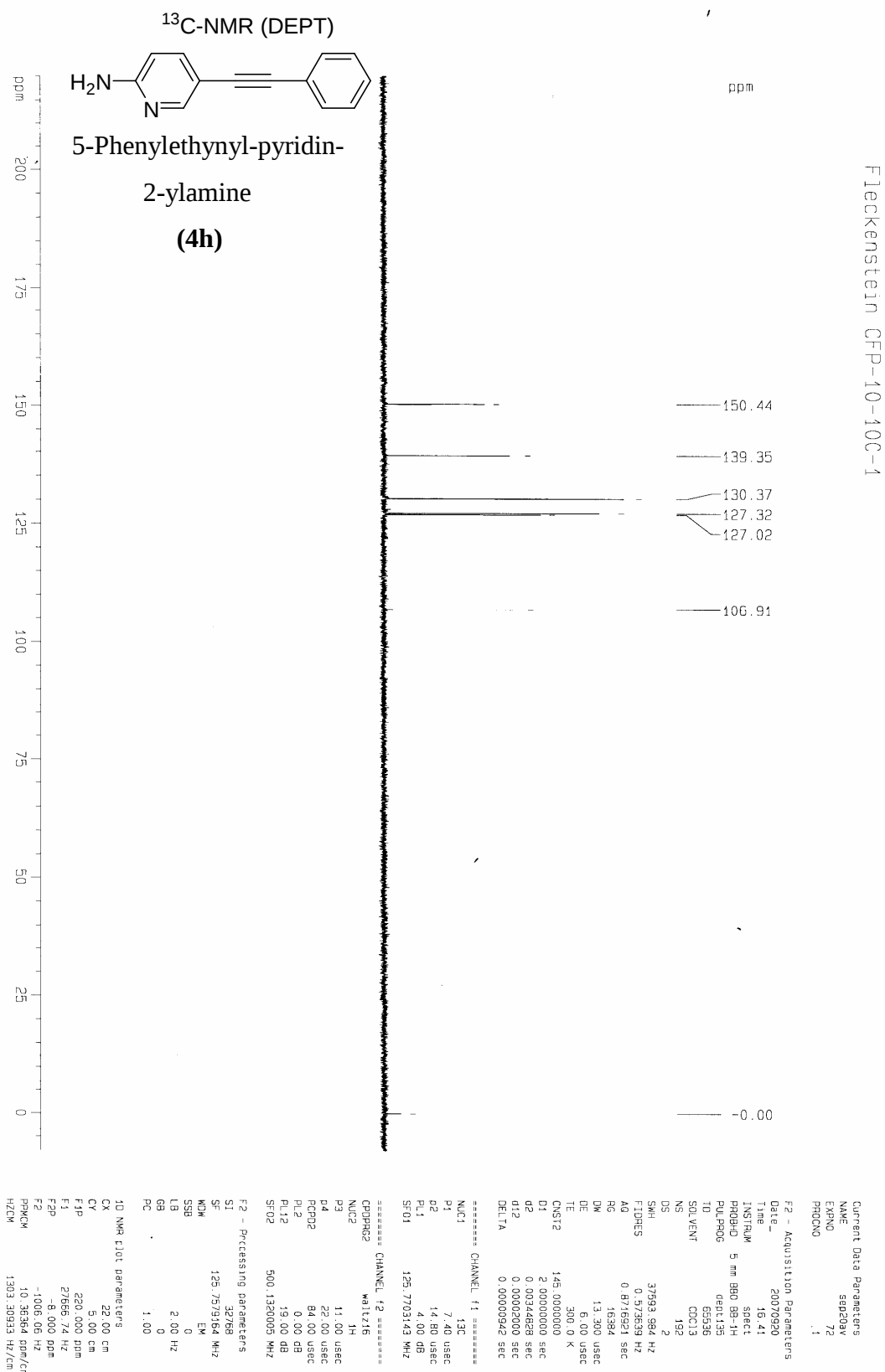
(3e)

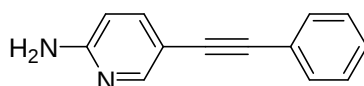






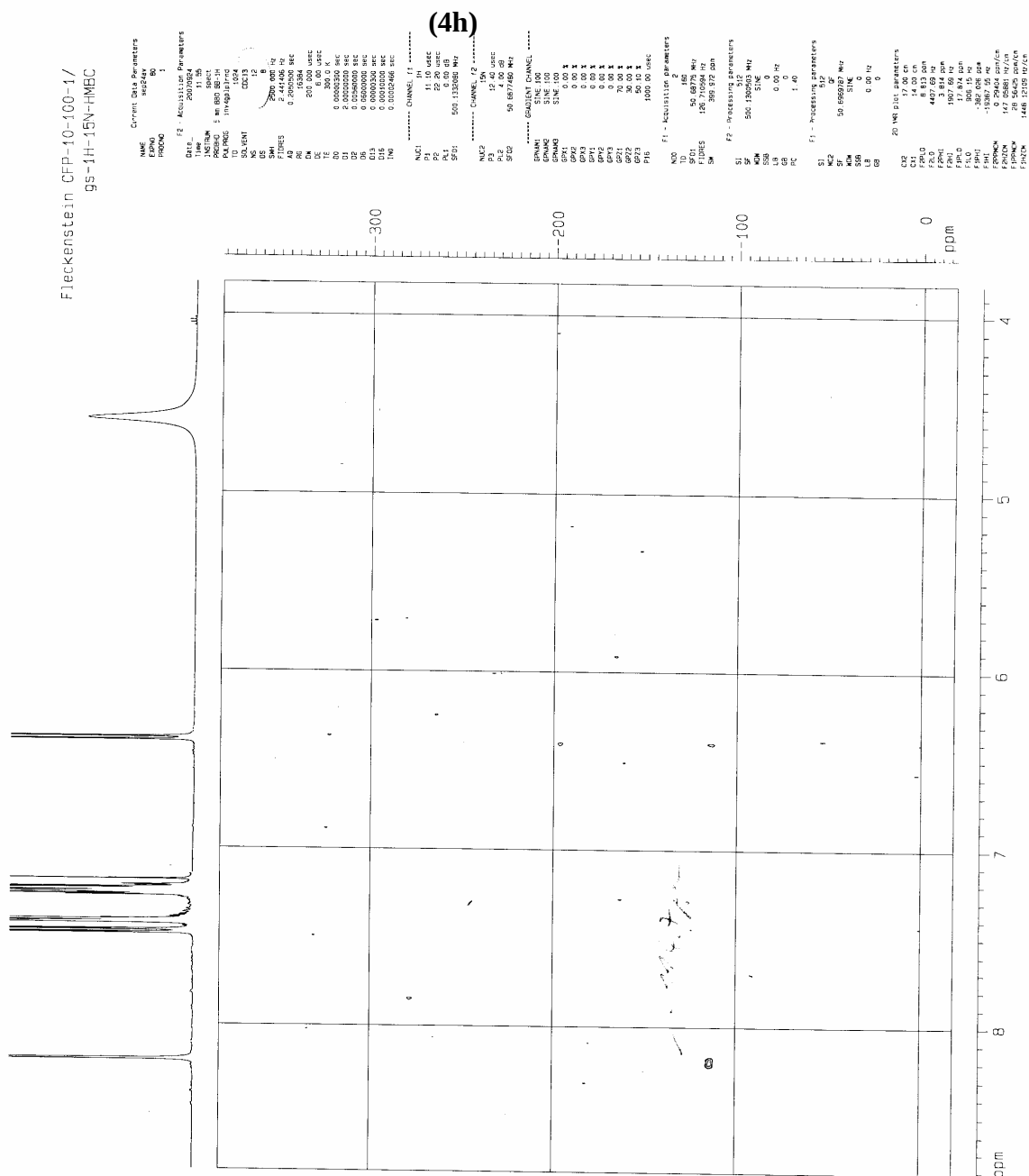


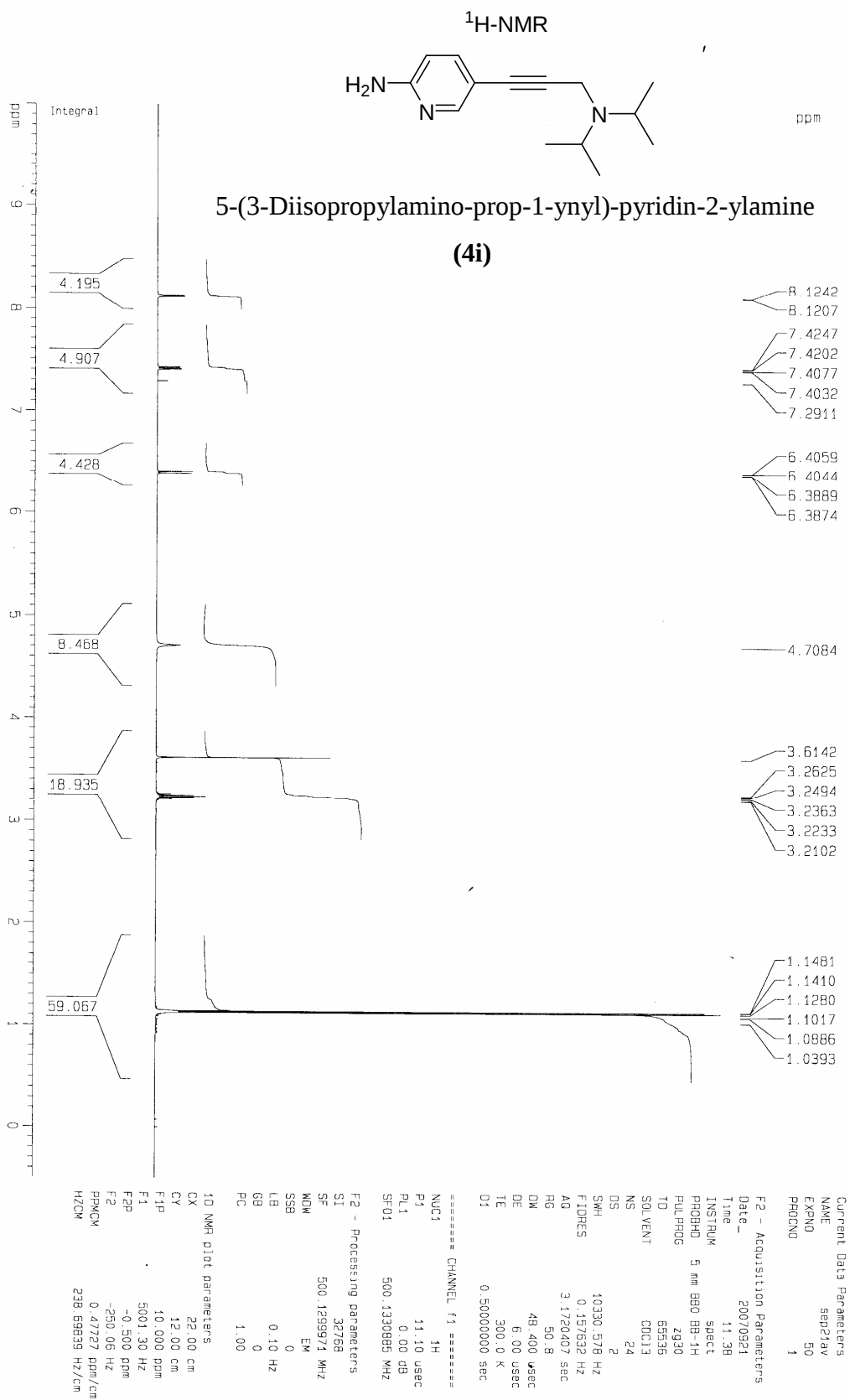




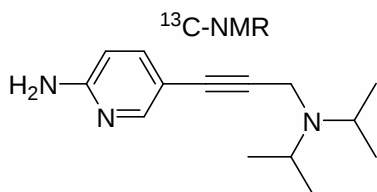
5-Phenylethynyl-pyridin-2-ylamine

Fleckenstein CFP-10-100-1/
gs-1H-15N-HMBC

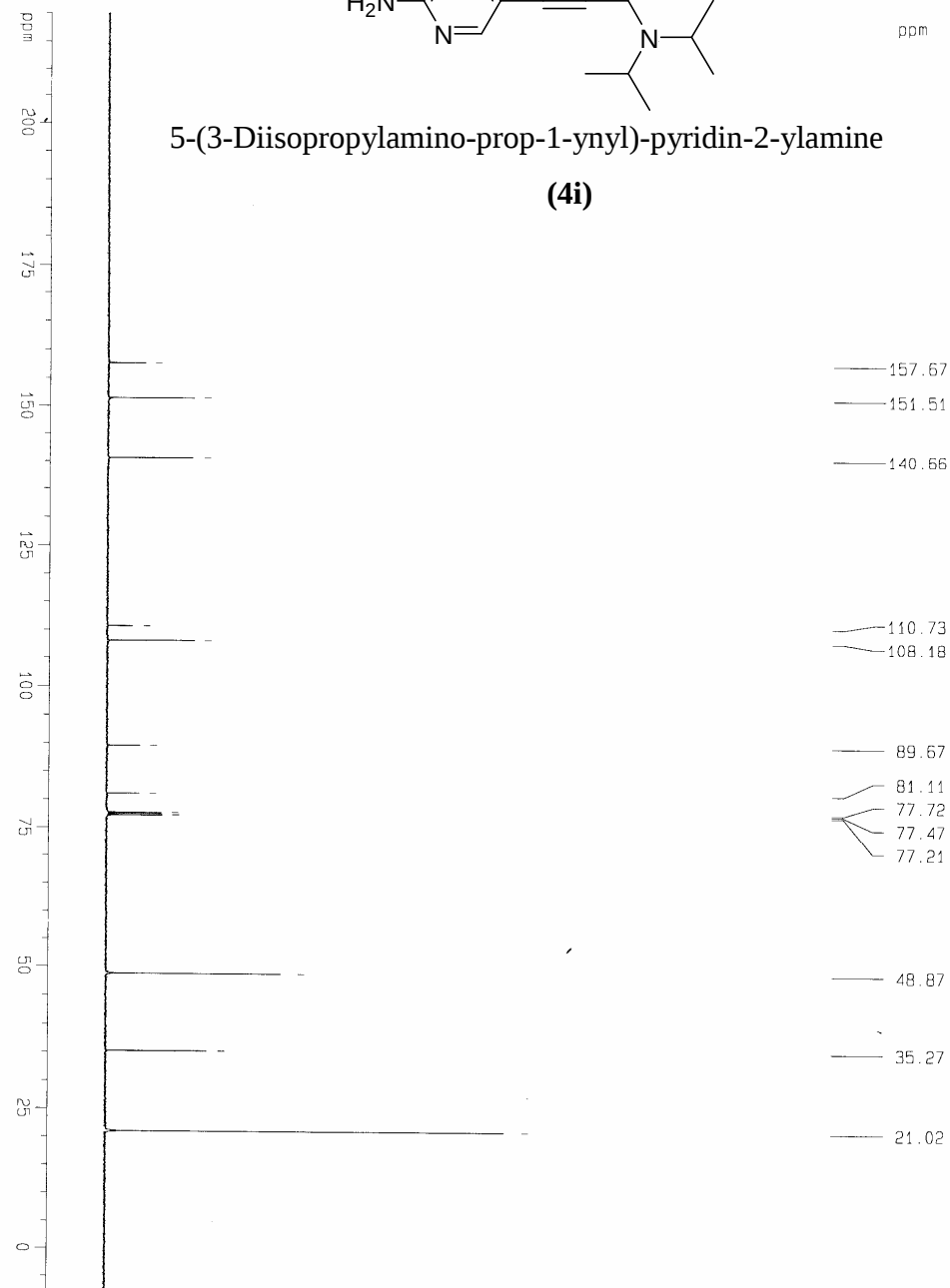




Fleckenstein CFP-10-103-1



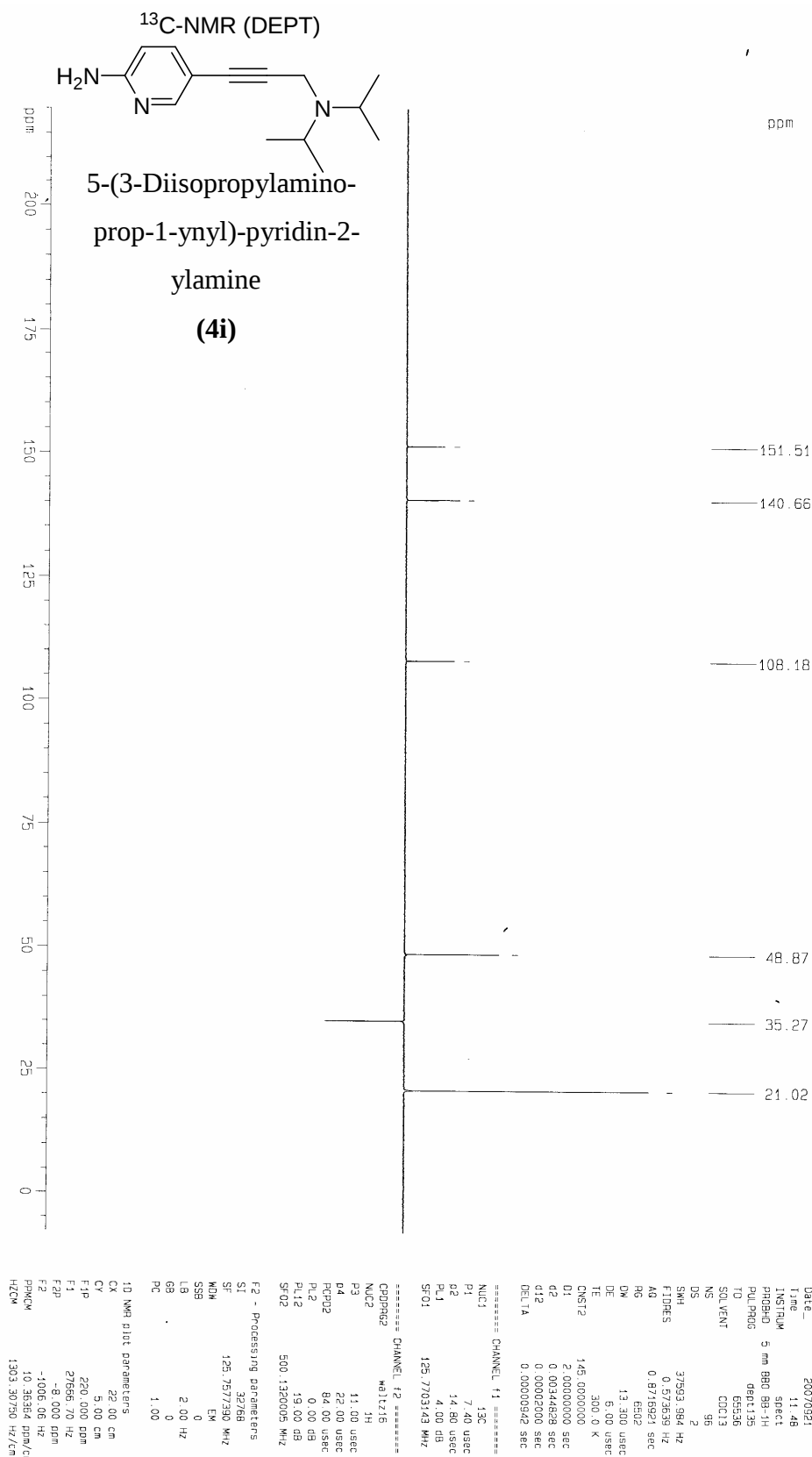
5-(3-Diisopropylamino-prop-1-ynyl)-pyridin-2-ylamine
(4i)



Fleckenstein CFP-10-103-1

Current Data Parameters
NAME: 20070921
EXPNO: 51
PROCNO: 1
F2 - Acquisition Parameters
Date_: 20070921
Time: 11:42
INSTRUM: spect
PROBHD: 5 mm BBO BB-41
PULPROG: zgpg30
TD: 65536
SOLVENT: CDCl3
NS: 165
DS: 4
SWH: 37593.984 Hz
FIDRES: 0.573639 Hz
AQ: 0.8716921 sec
RG: 5792.6
DE: 13.300 usec
TE: 300.0 K
D1: 0.4000001 sec
D11: 0.0300000 sec
D12: 0.0002000 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: 500.132005 MHz
F2 - Processing parameters
SI: 32768
SF: 125.7577390 MHz
WDW: EM
SSB: 0
LB: 2.00 Hz
GB: 0
PC: 1.00
10 MHz p.p.t. parameters
CY: 22.00 cm
CX: 7.00 cm
F1P: 220.000 ppm
F1: 27565.70 Hz
F2P: -8.000 ppm
F2: -1006.08 Hz
PRCKM: 10.36364 ppm/cm
HZCM: 1303.30750 Hz/cm

Fleckenstein CFP-10-103-1



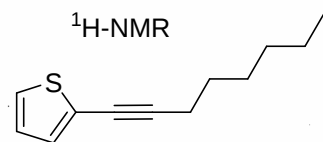
Fleckenstein CFP-10-103-1/
gs-1H-15N-HMBC

Current Data Parameters

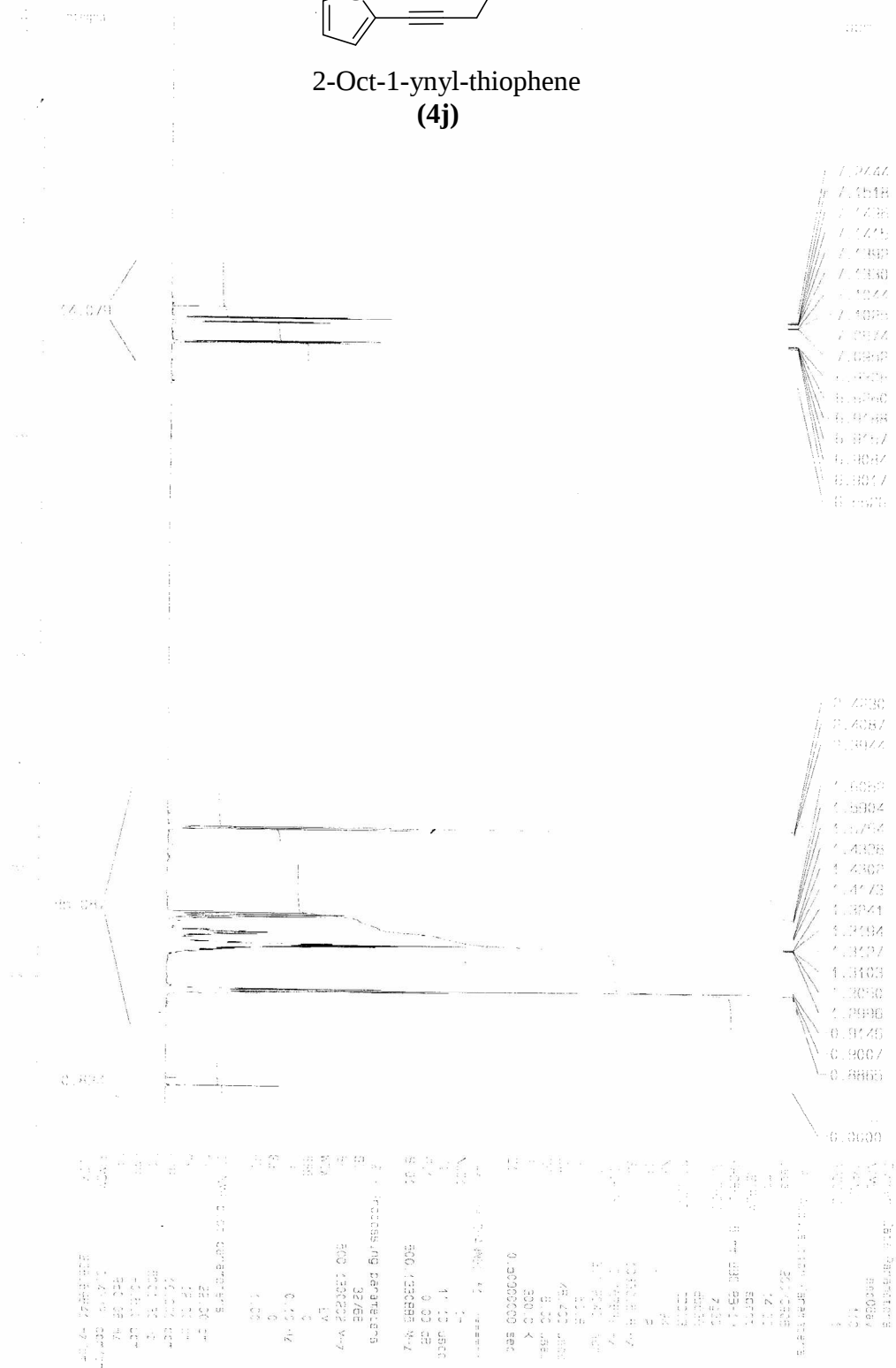
NAME	EXPNO	F2 - Acquisition Parameters
EXPNO	1	NAME
PROCNO	1	EXPNO
		PROCNO
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		PULPROG
		TD
		GB
		PC
		SD
		SI
		SR
		SWH
		F2
		F3
		F4
		F5
		F6
		F7
		F8
		F9
		F10
		F11
		F12
		F13
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		F96
		F97
		F98
		F99
		F100

1D 1H NMR Parameters

NAME	VALUE
NAME	1H
EXPNO	1
PROCNO	1
INSTRUM	nmr1
PROBHD	5mm QNP 1H/15N
PULPROG	zgpg30
TD	65536
GB	0
PC	1.00
SD	0
SI	32768
SR	1
SWH	10000.000 MHz
F2	500.136000 MHz
F3	125.760000 MHz
F4	101.623000 MHz
F5	101.623000 MHz
F6	101.623000 MHz
F7	101.623000 MHz
F8	101.623000 MHz
F9	101.623000 MHz
F10	101.623000 MHz
F11	101.623000 MHz
F12	101.623000 MHz
F13	101.623000 MHz
F14	101.623000 MHz
F15	101.623000 MHz
F16	101.623000 MHz
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F19	101.623000 MHz
F20	101.623000 MHz
F21	101.623000 MHz

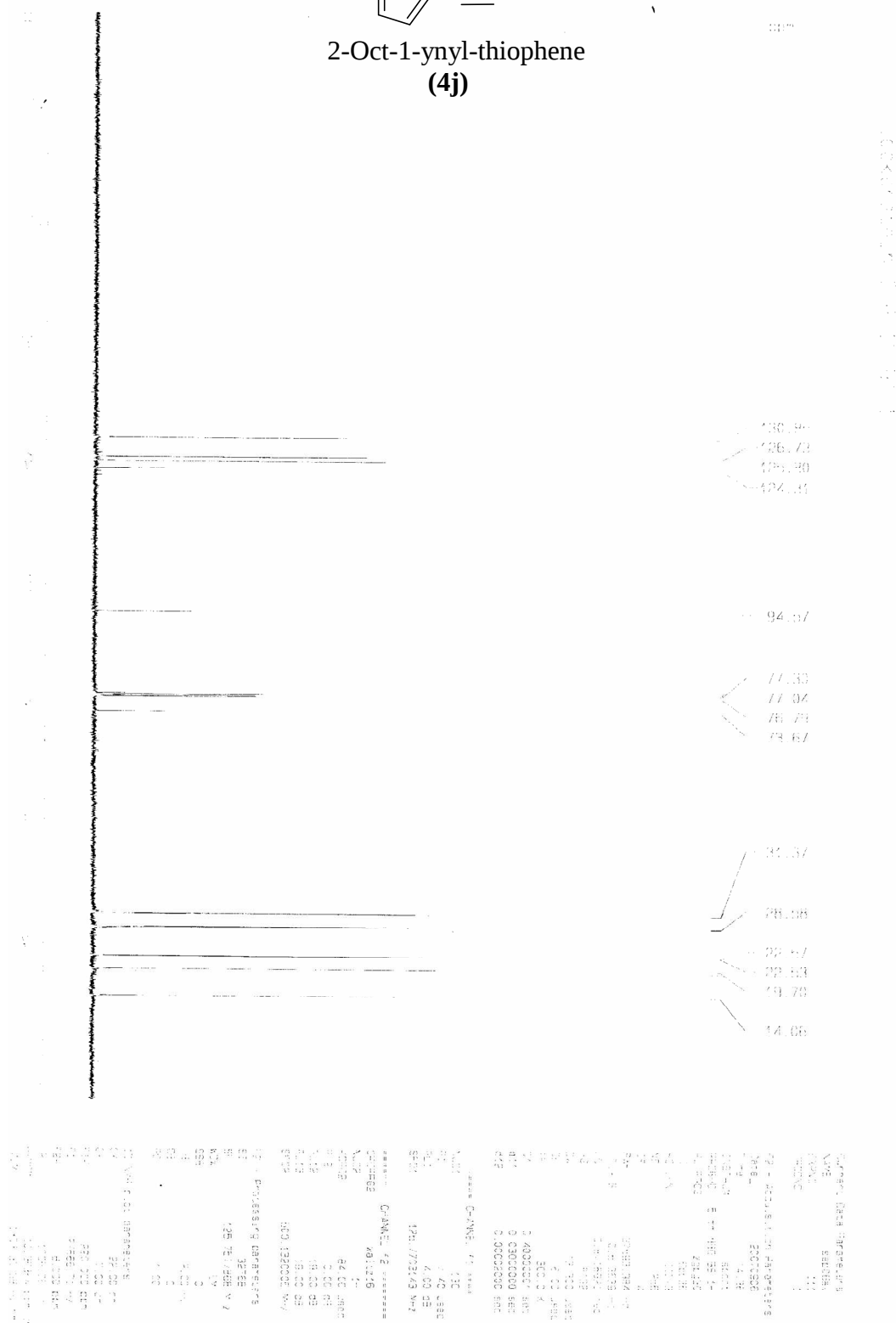


2-Oct-1-ynyl-thiophene
(4j)





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

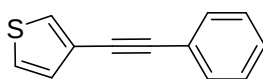




(4k)

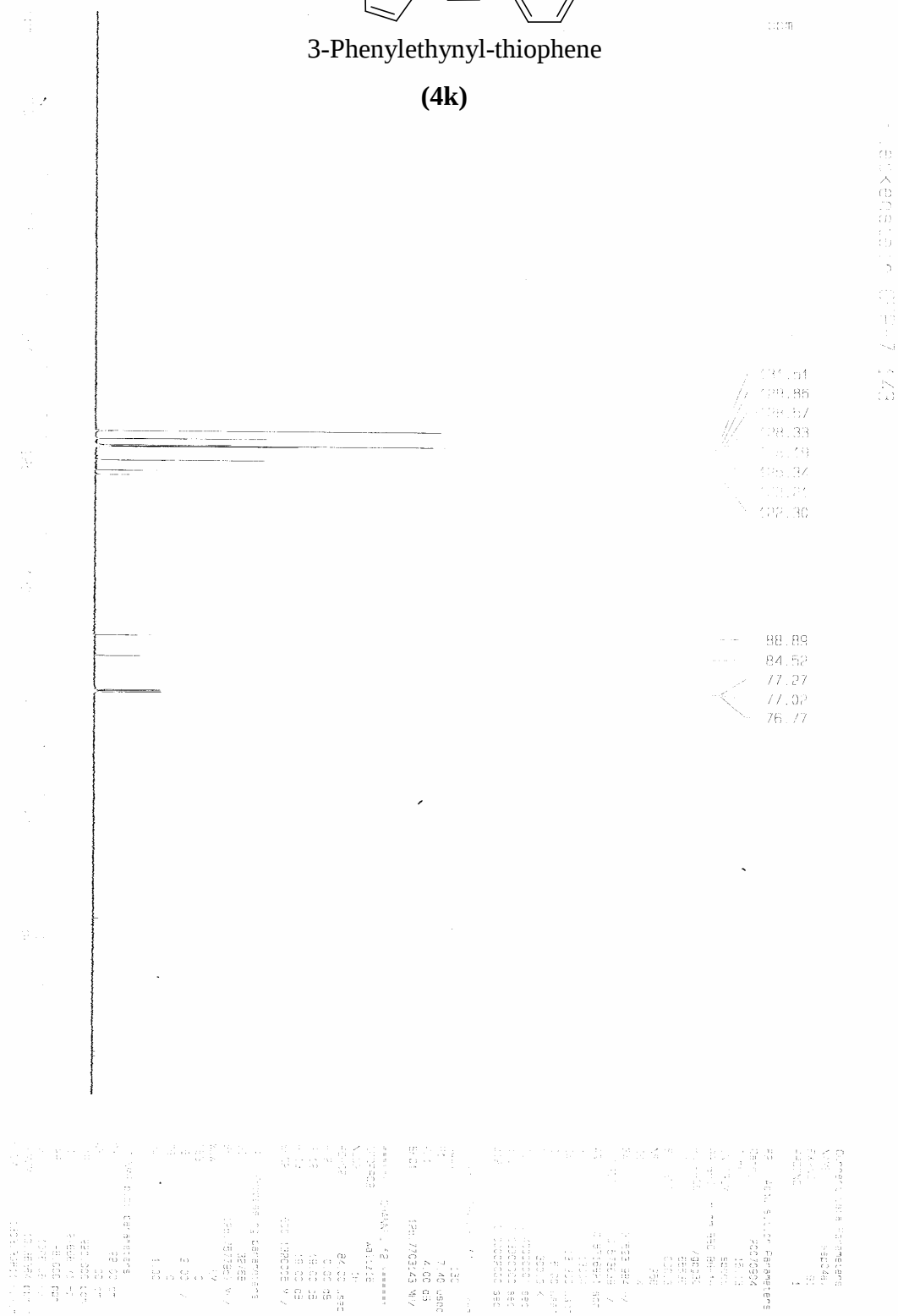


¹³C-NMR

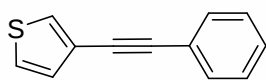


3-Phenylethynyl-thiophene

(4k)

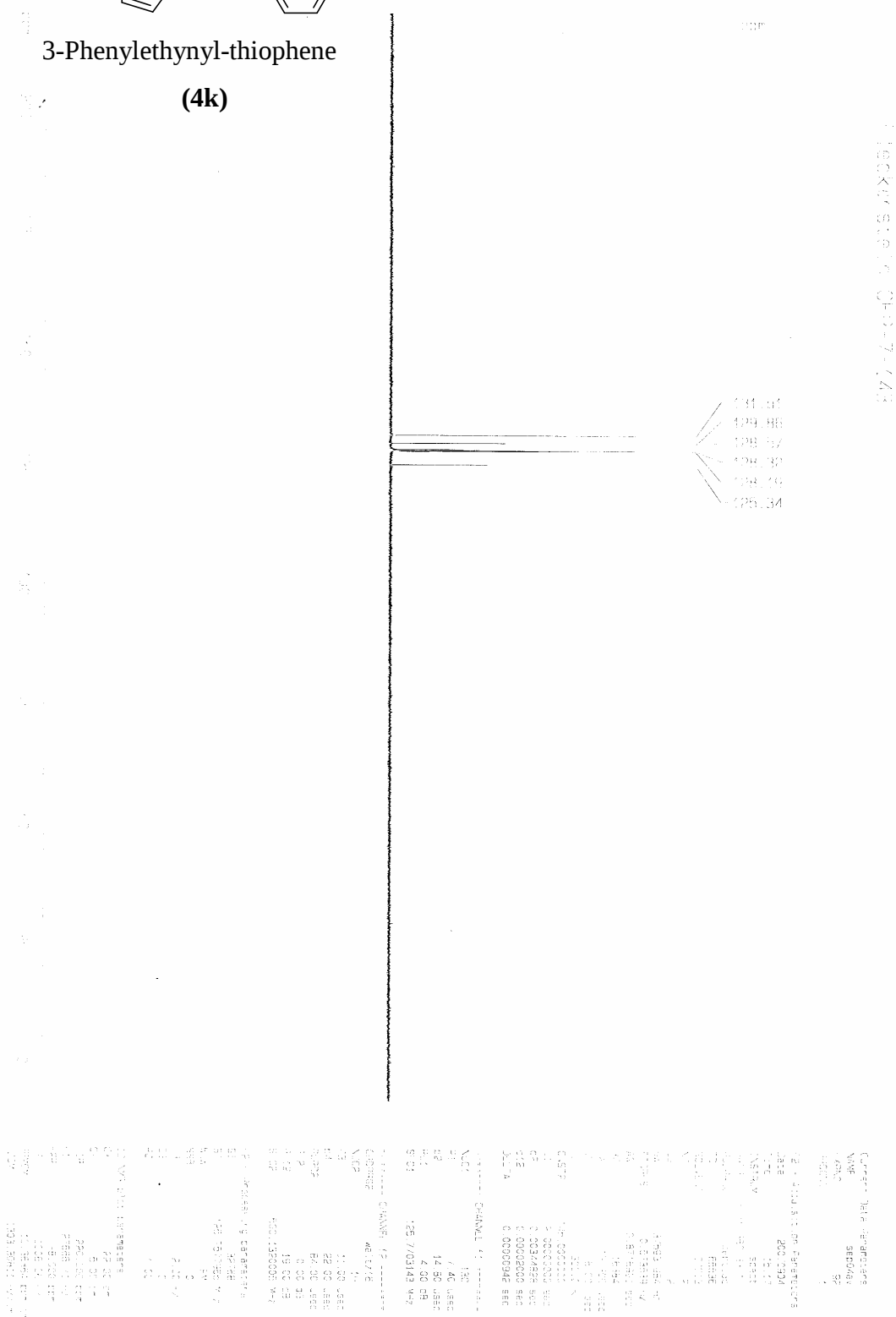


¹³C-NMR (DEPT)

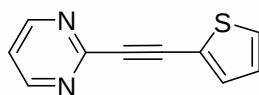


3-Phenylethynyl-thiophene

(4k)

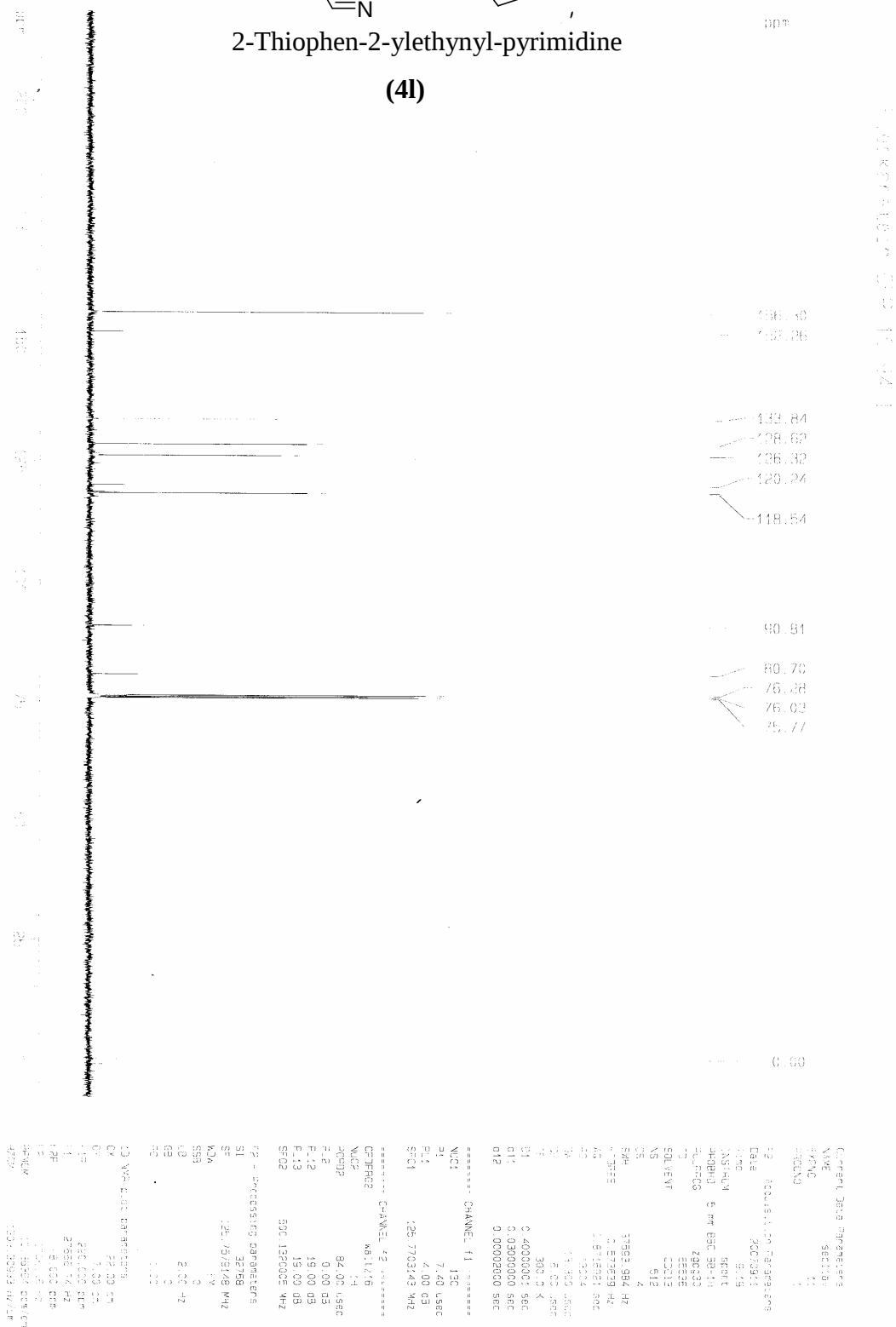


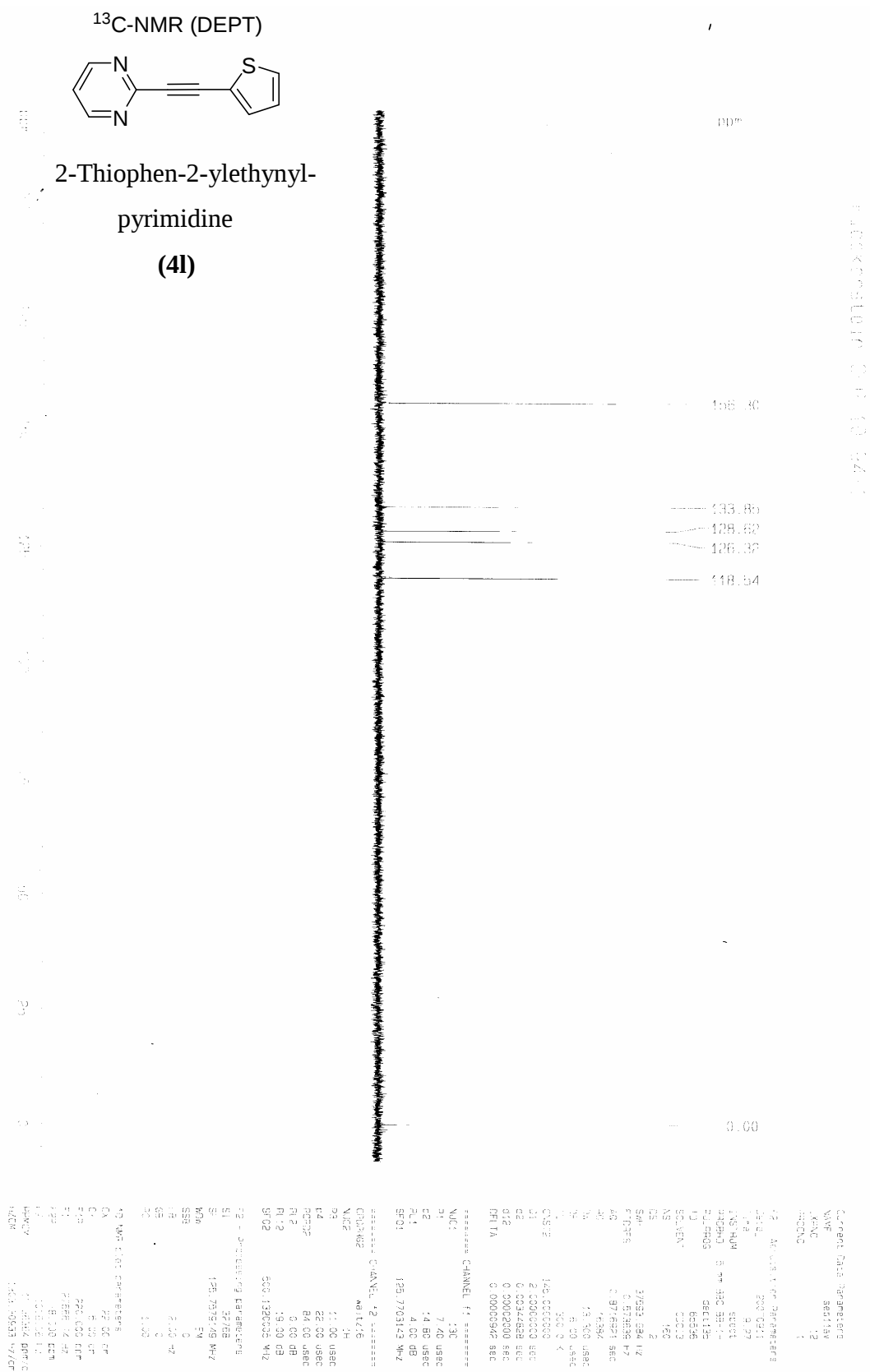
¹³C-NMR

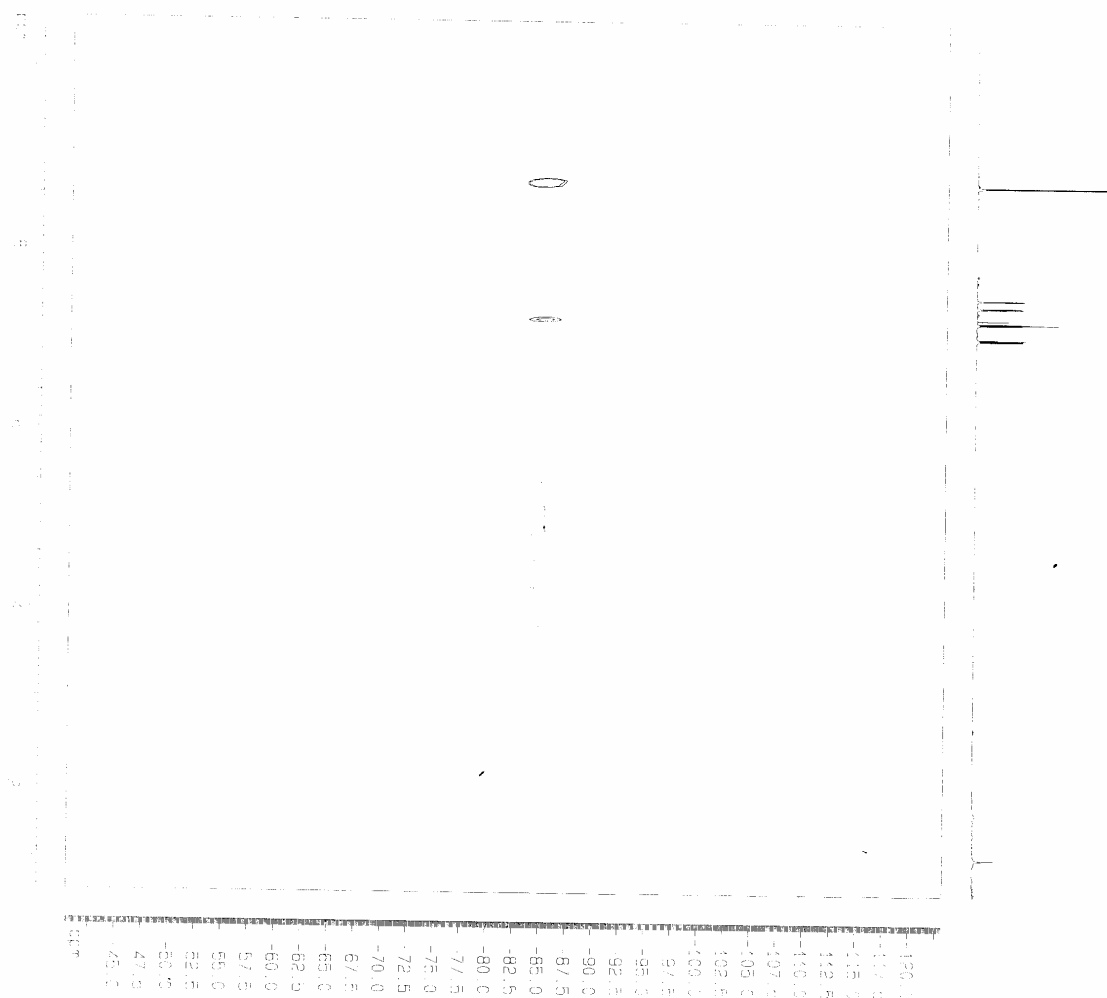
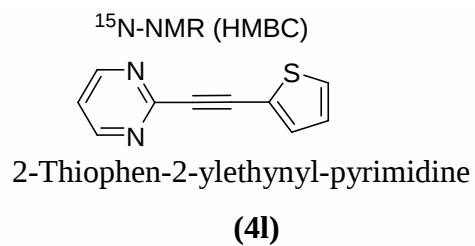


2-Thiophen-2-ylethynyl-pyrimidine

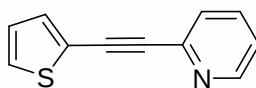
(4I)





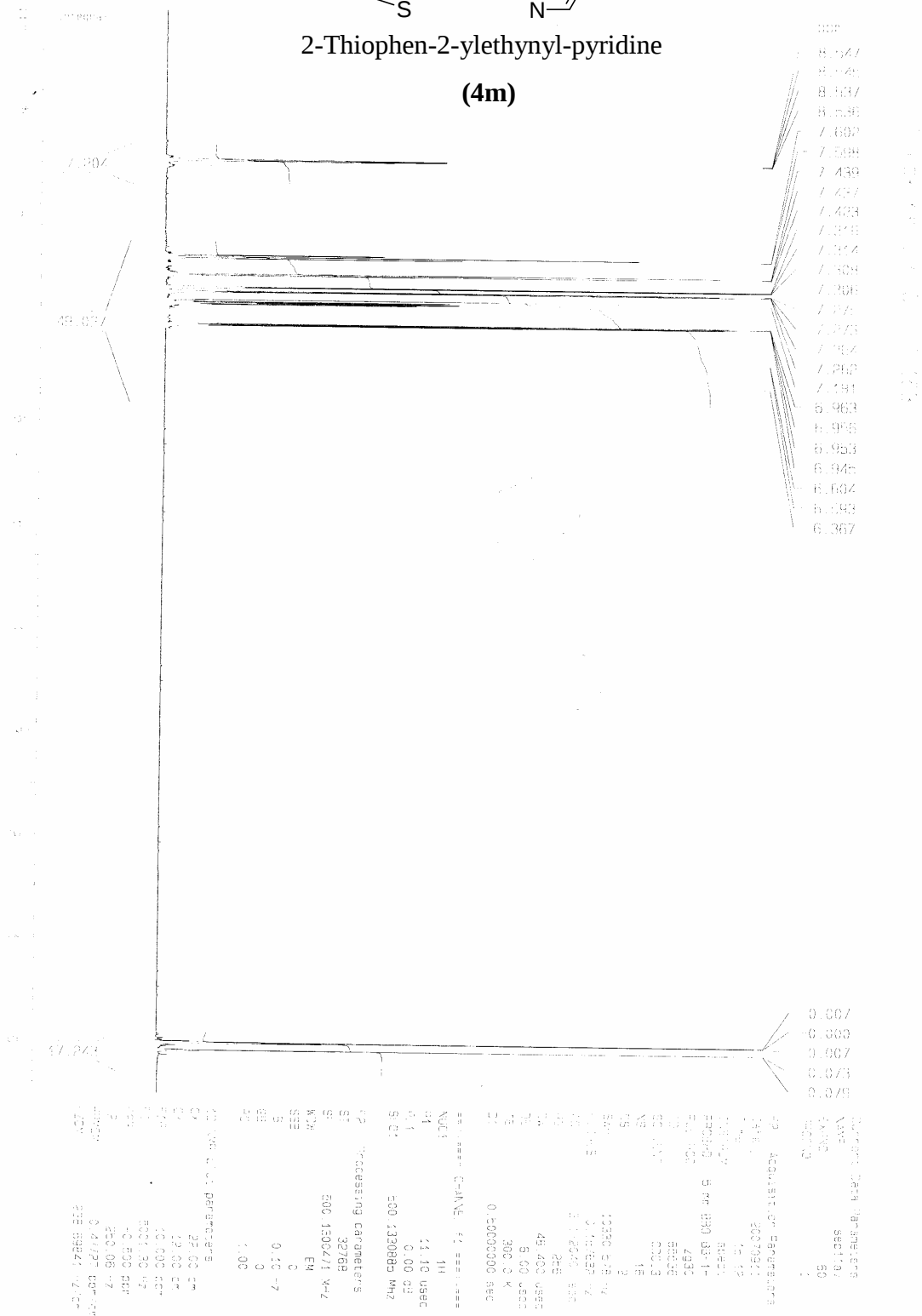


¹H-NMR

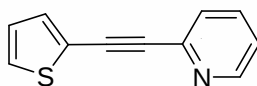


2-Thiophen-2-ylethynyl-pyridine

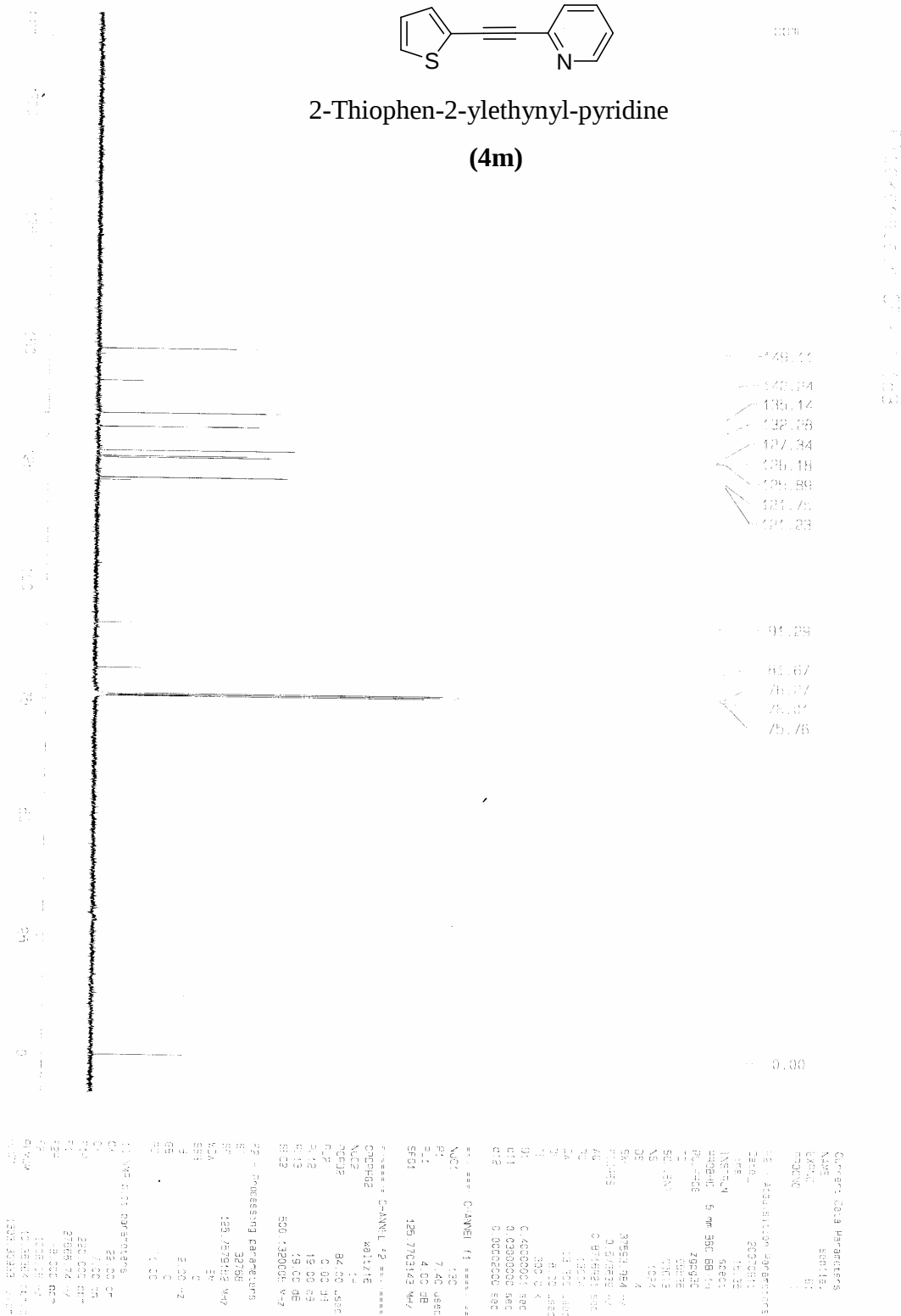
(4m)

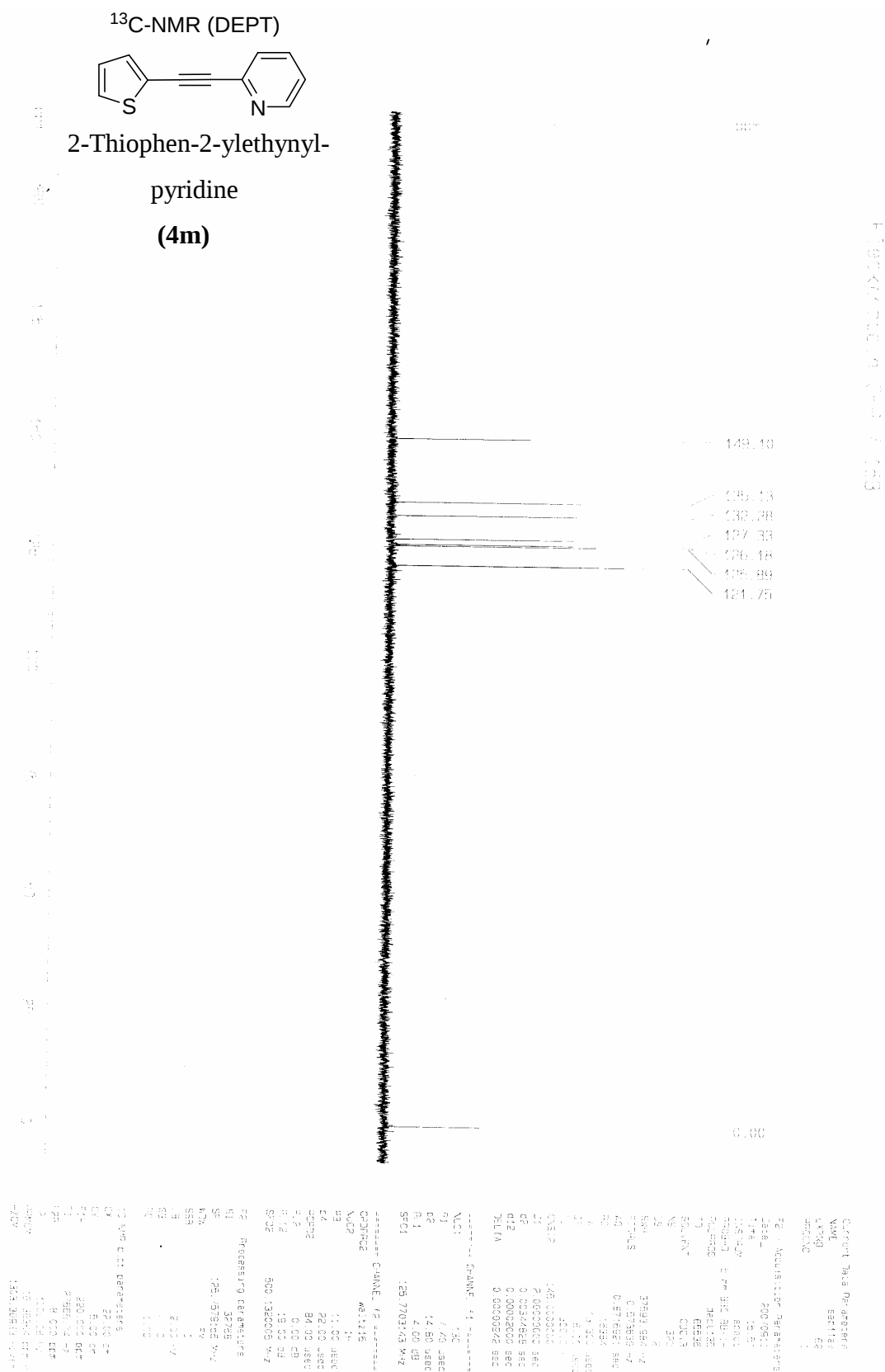


^{13}C -NMR

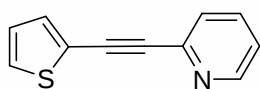


2-Thiophen-2-ylethynyl-pyridine
(4m)



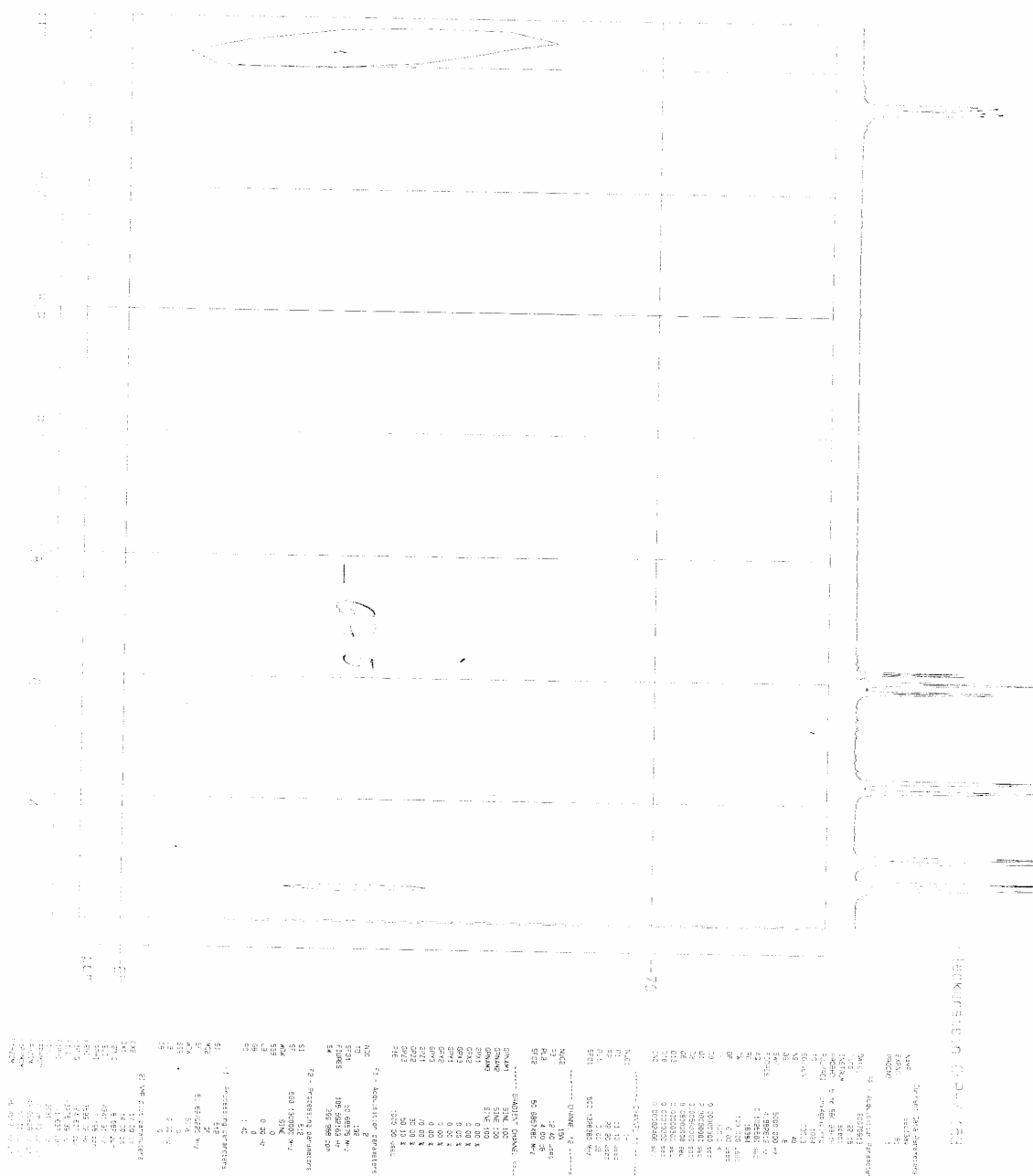


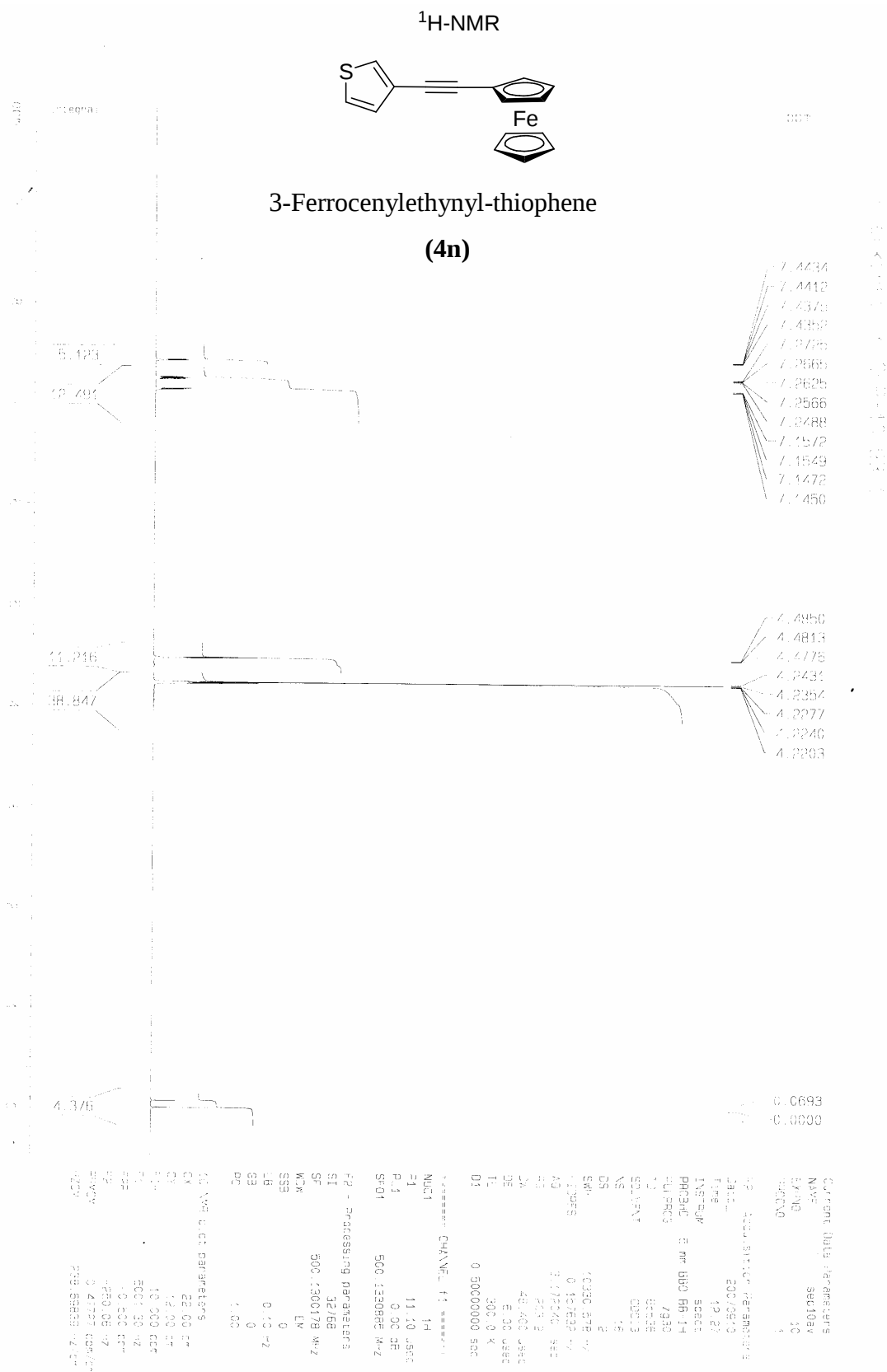
¹⁵N-NMR (HMBC)

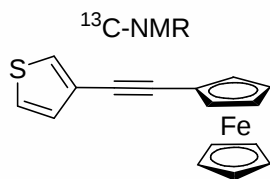


2-Thiophen-2-ylethynyl-pyridine

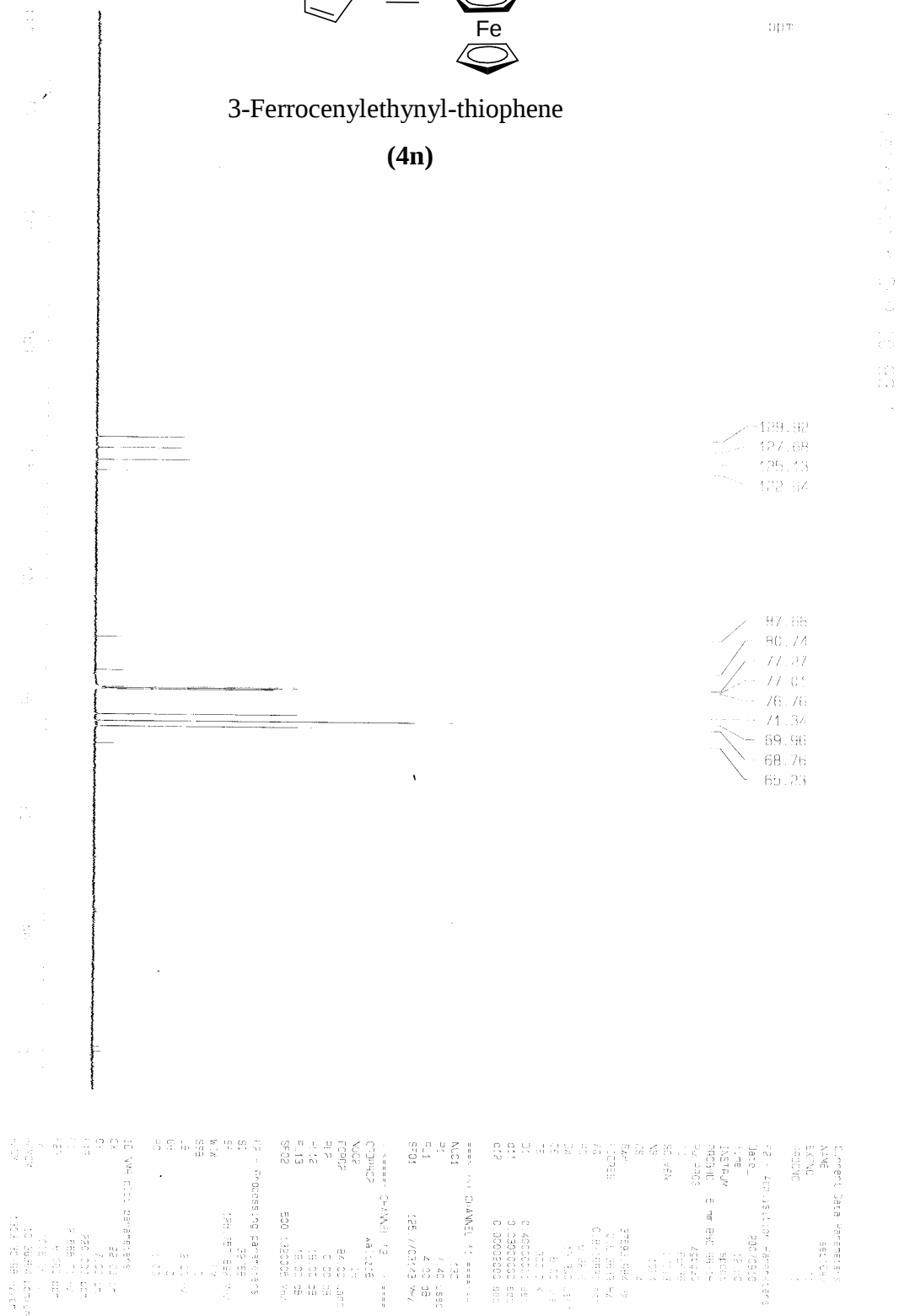
(4m)

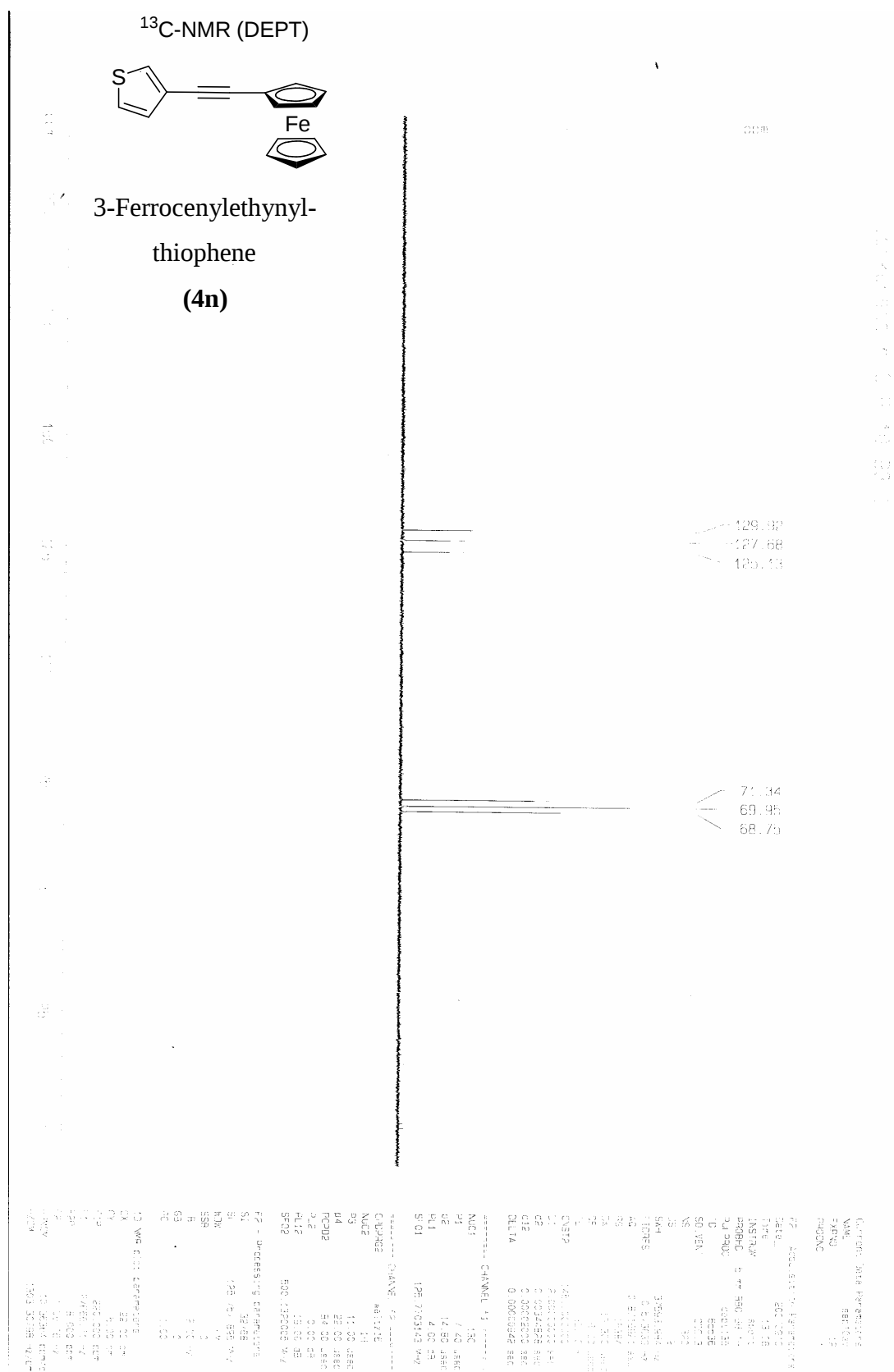




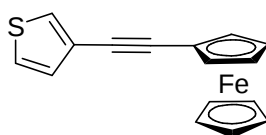


3-Ferrocenylethynyl-thiophene
(4n)

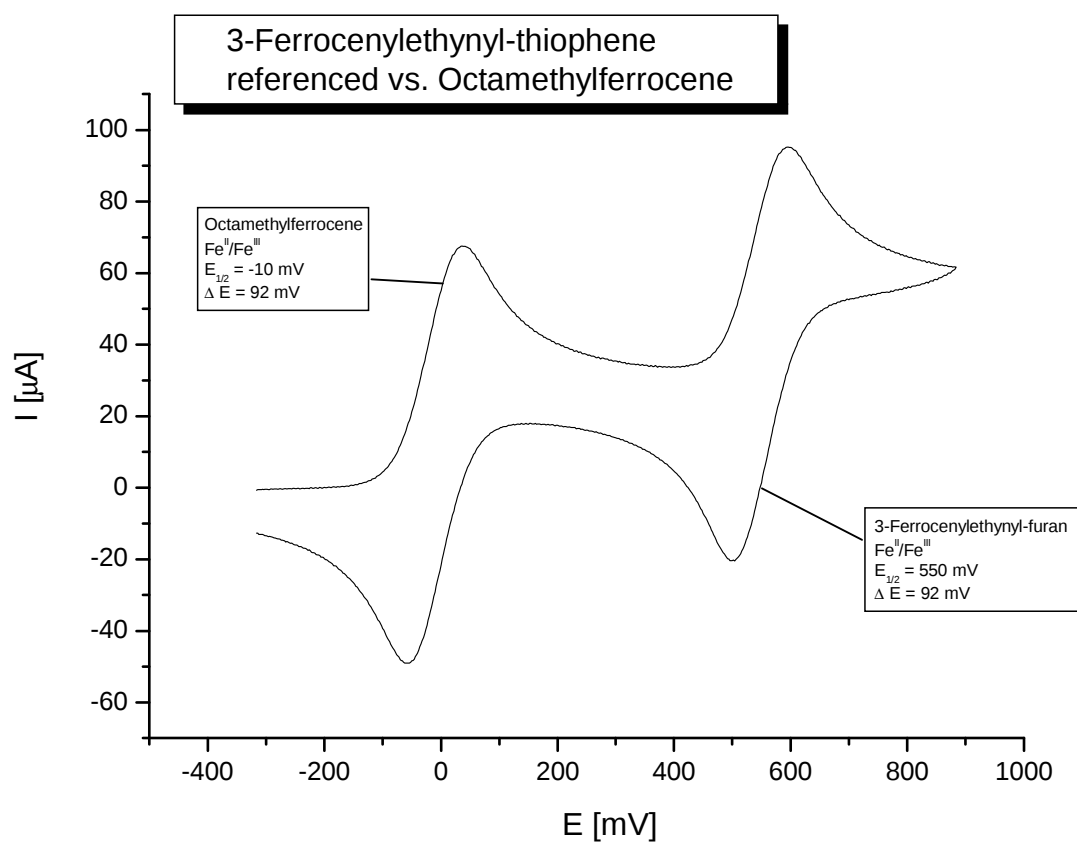




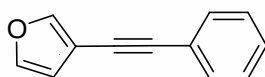
Cyclovoltammogram



3-Ferrocenylethynyl-thiophene
(4n)

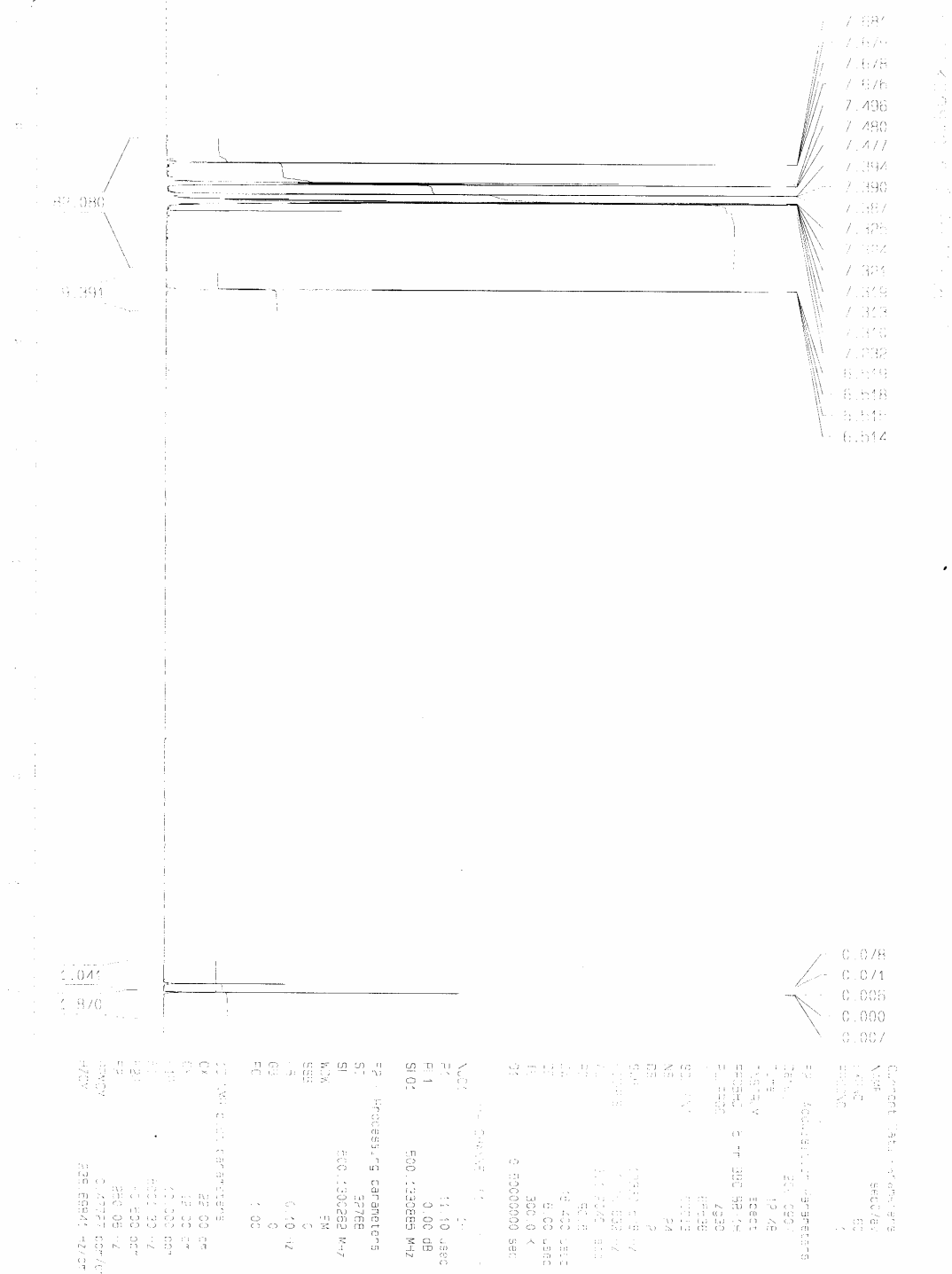


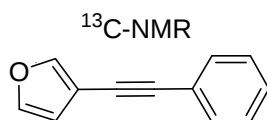
¹H-NMR



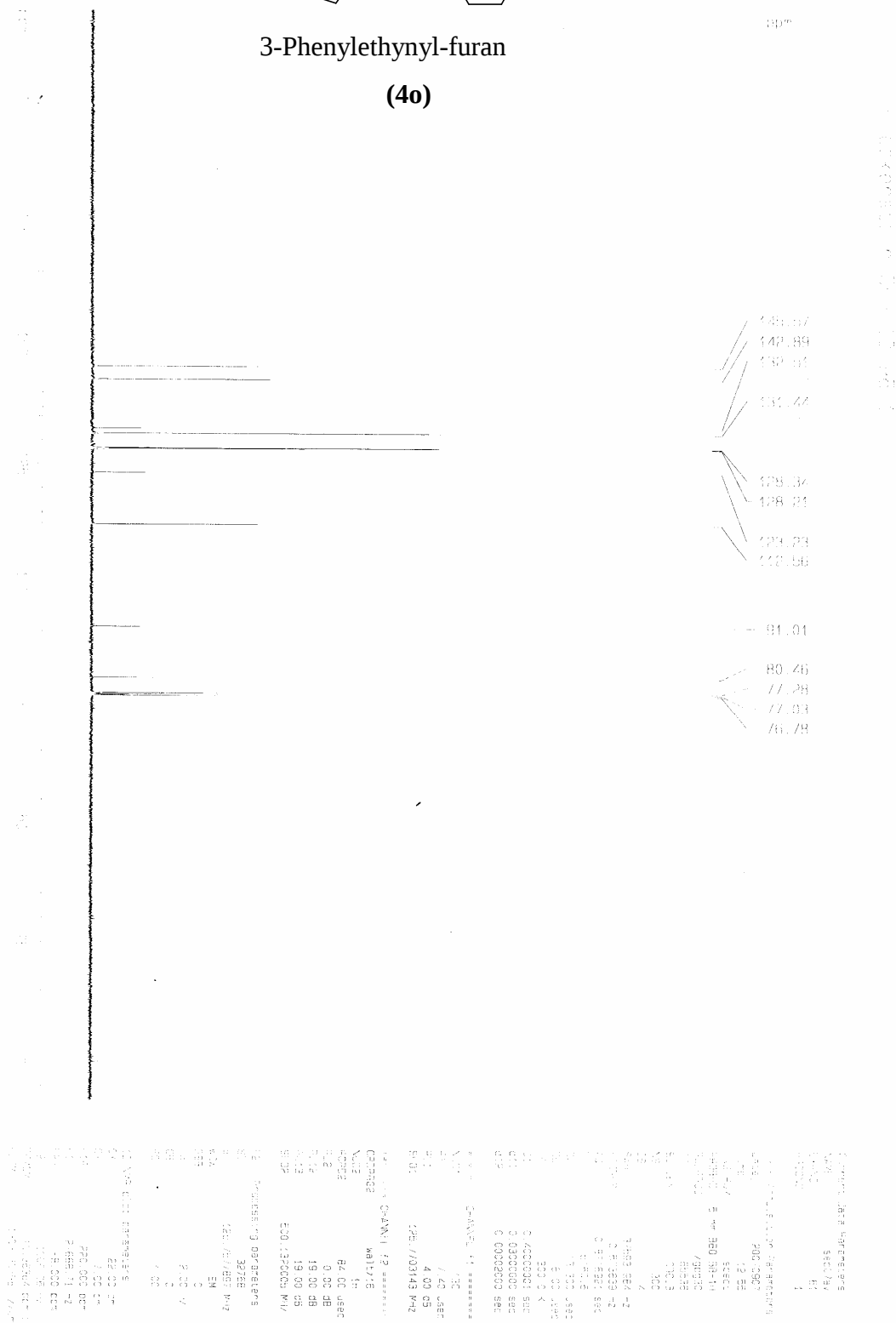
3-Phenylethynyl-furan

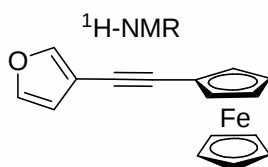
(4o)



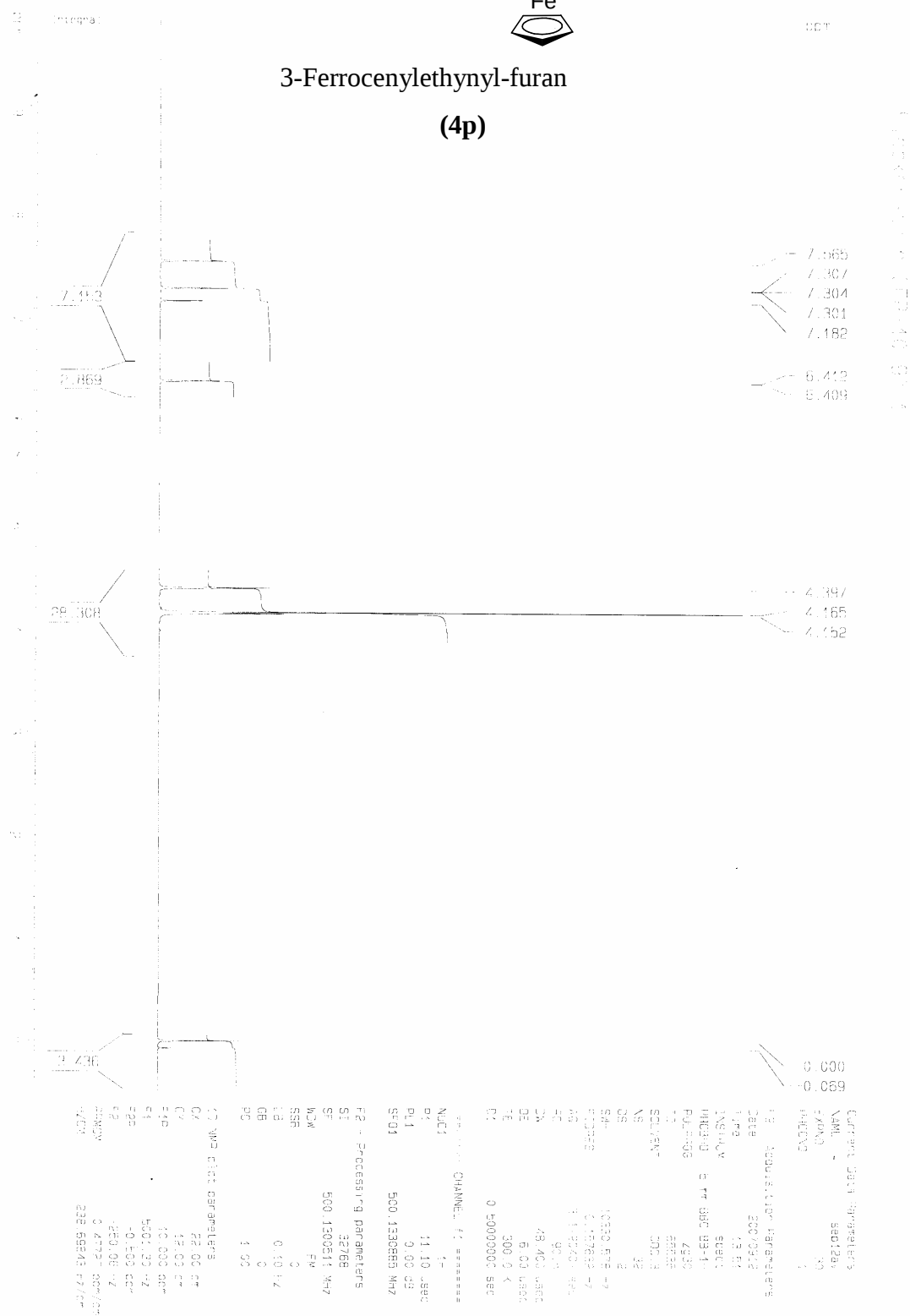


3-Phenylethynyl-furan
(40)



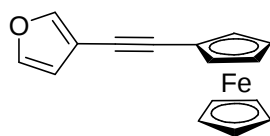


3-Ferrocenylethynyl-furan
(4p)

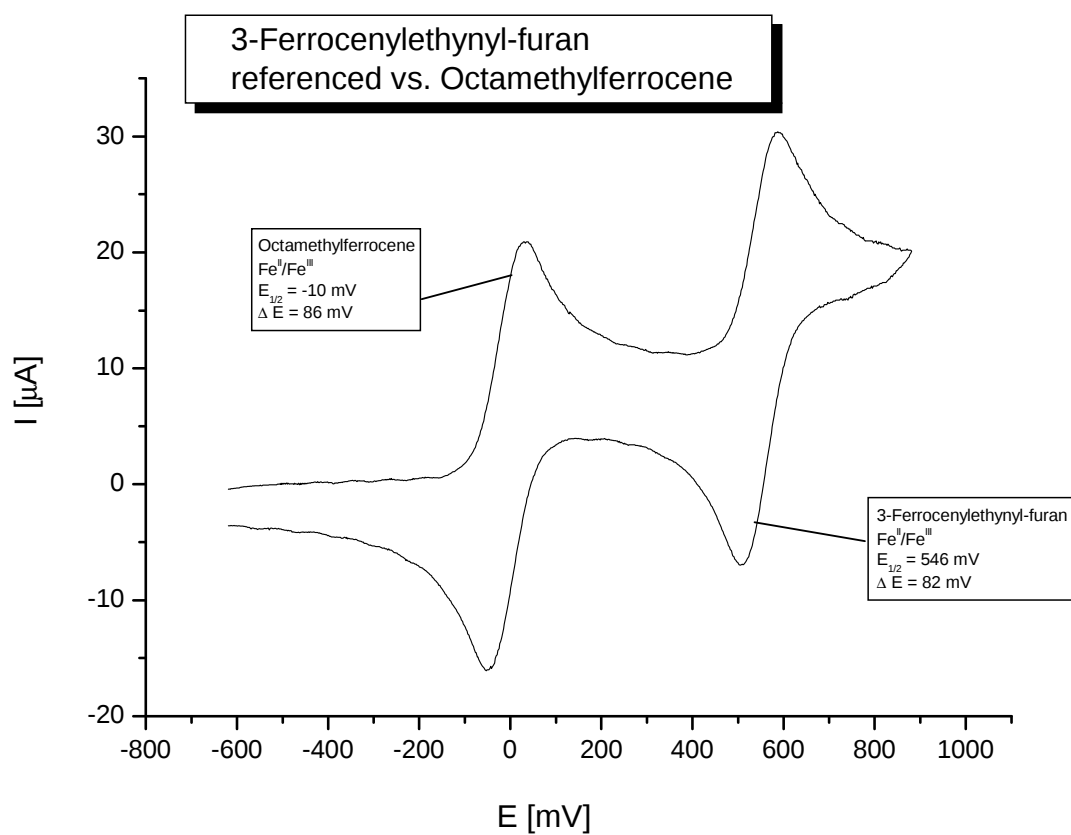


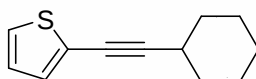
13C NMR spectrum of 3-Ferrocenylethynyl-furan (4p). The spectrum shows peaks at 144.09, 141.68, 141.63, 70.27, 68.96, and 67.73 ppm. The x-axis is labeled 'PPM' and ranges from 0 to 160. The y-axis is labeled 'Intensity'.

Cyclovoltammogram



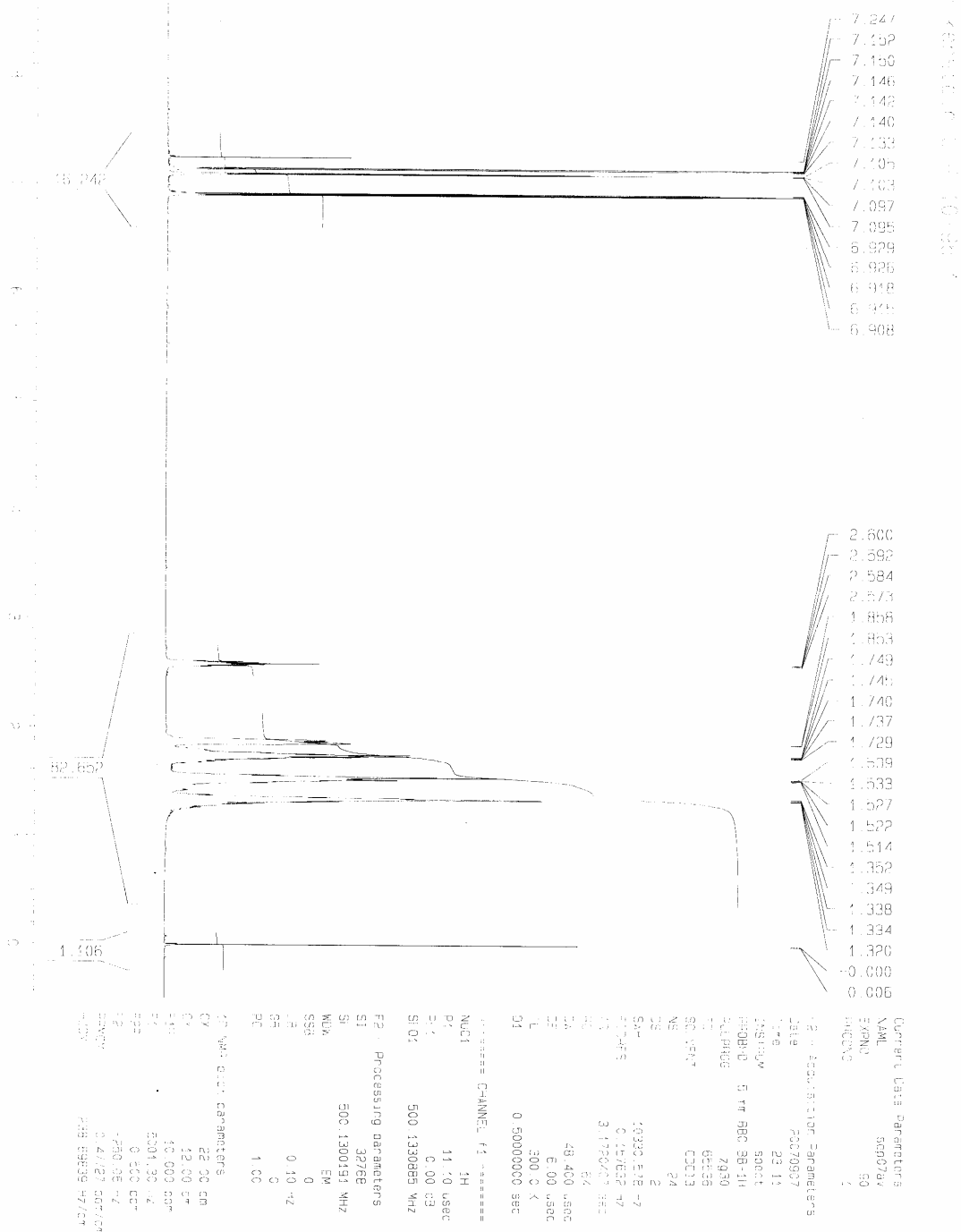
3-Ferrocenylethynyl-furan
(4p)



¹H-NMR

2-Cyclohexylethynyl-thiophene

(4q)



2-Cyclohexylethynyl-thiophene
(4q)

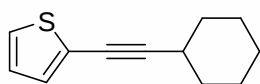
130.84
126.73
125.78
124.33

96.39

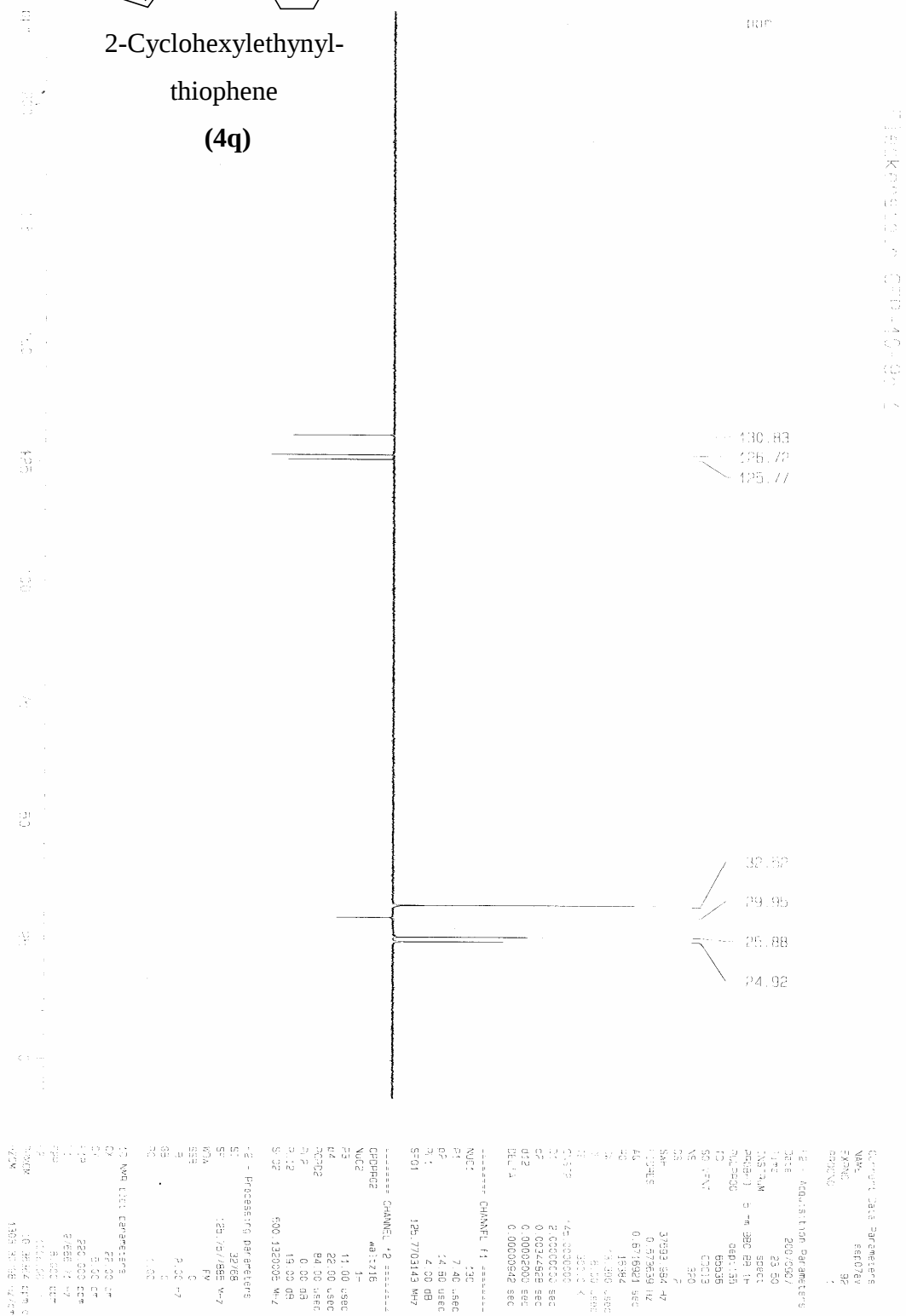
77.29
77.03
77.48

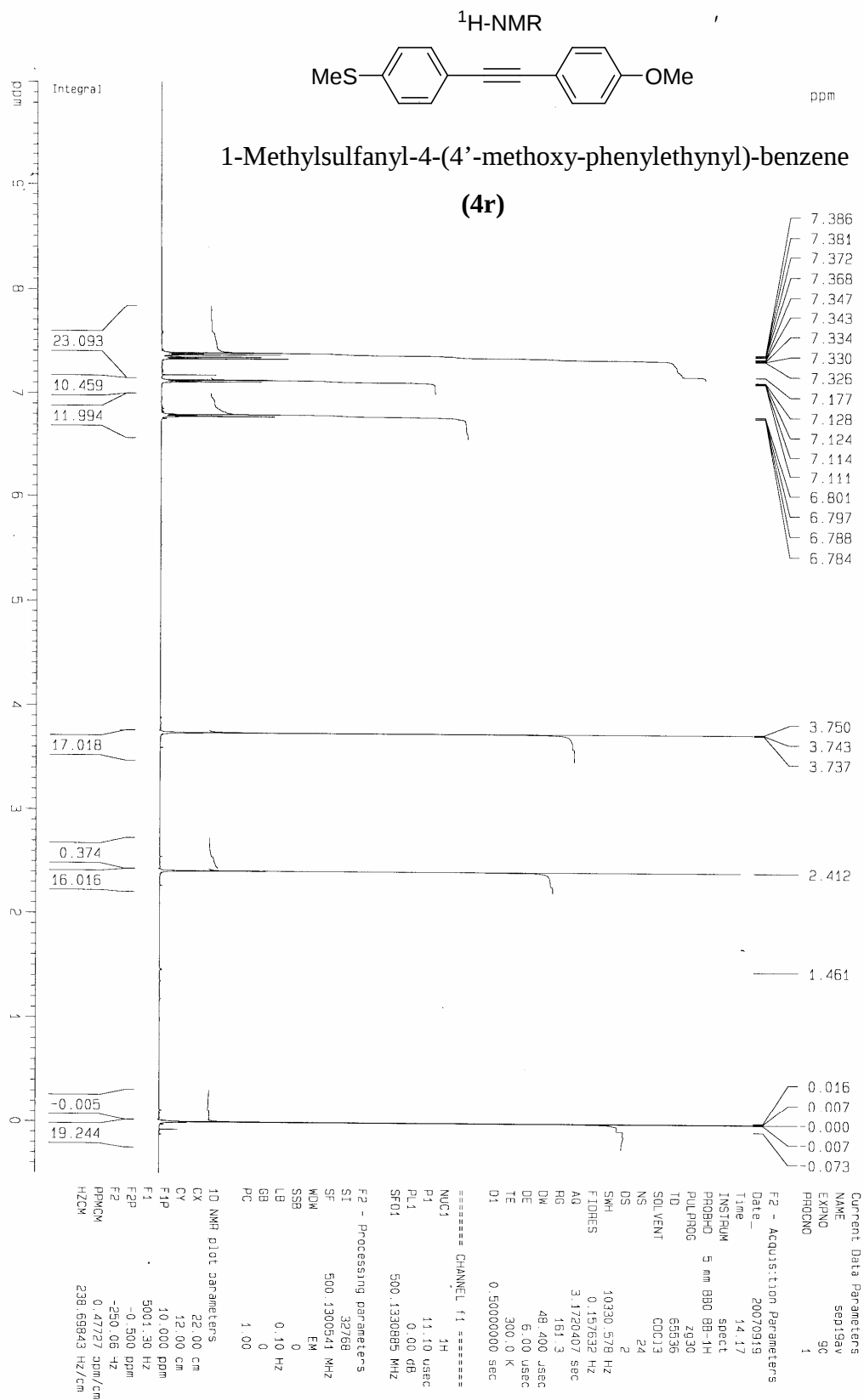
32.53
29.95
29.89
24.92

S 67

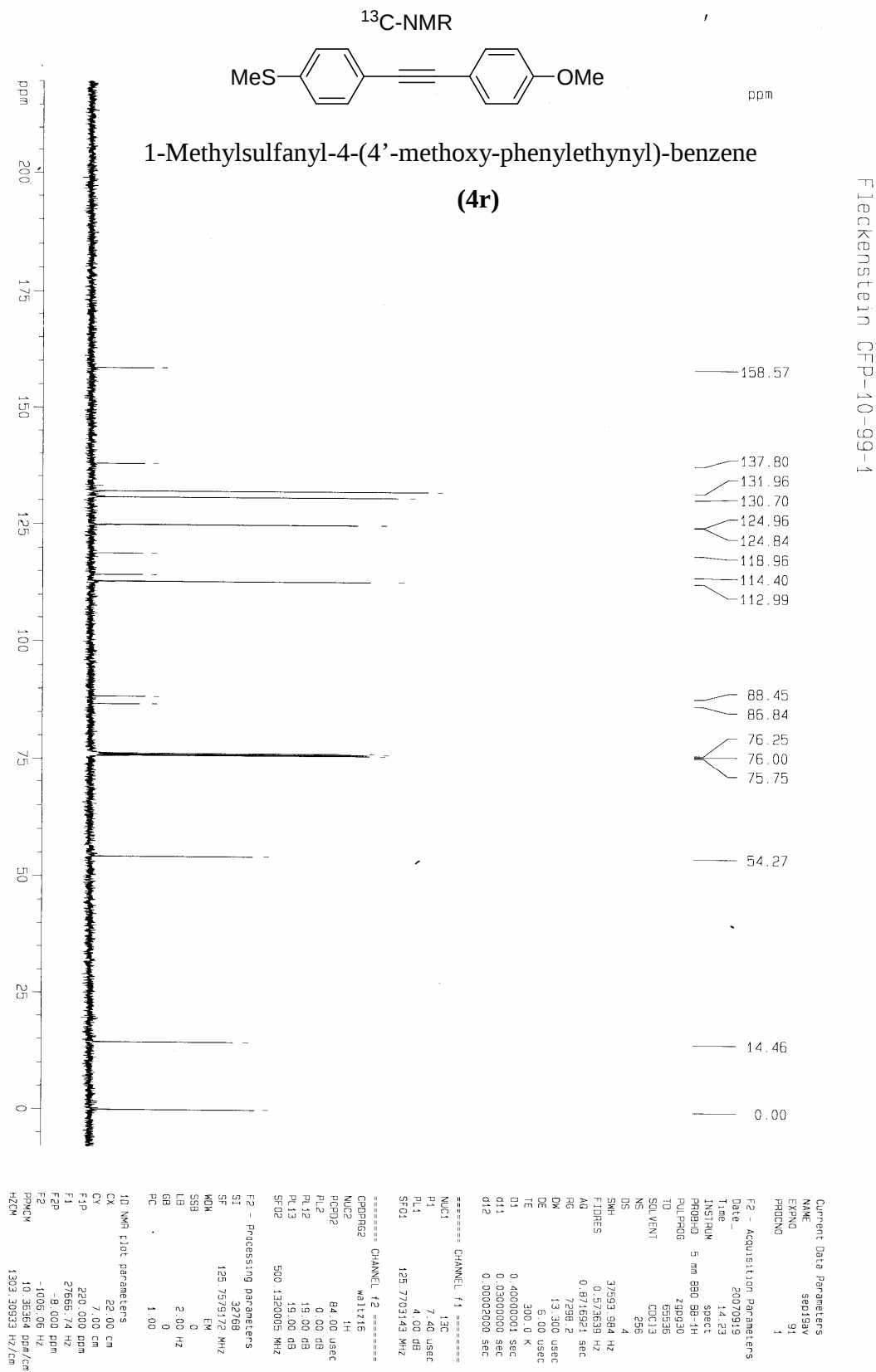
^{13}C -NMR (DEPT)

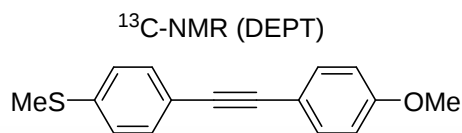
2-Cyclohexylethynyl-
thiophene
(4q)



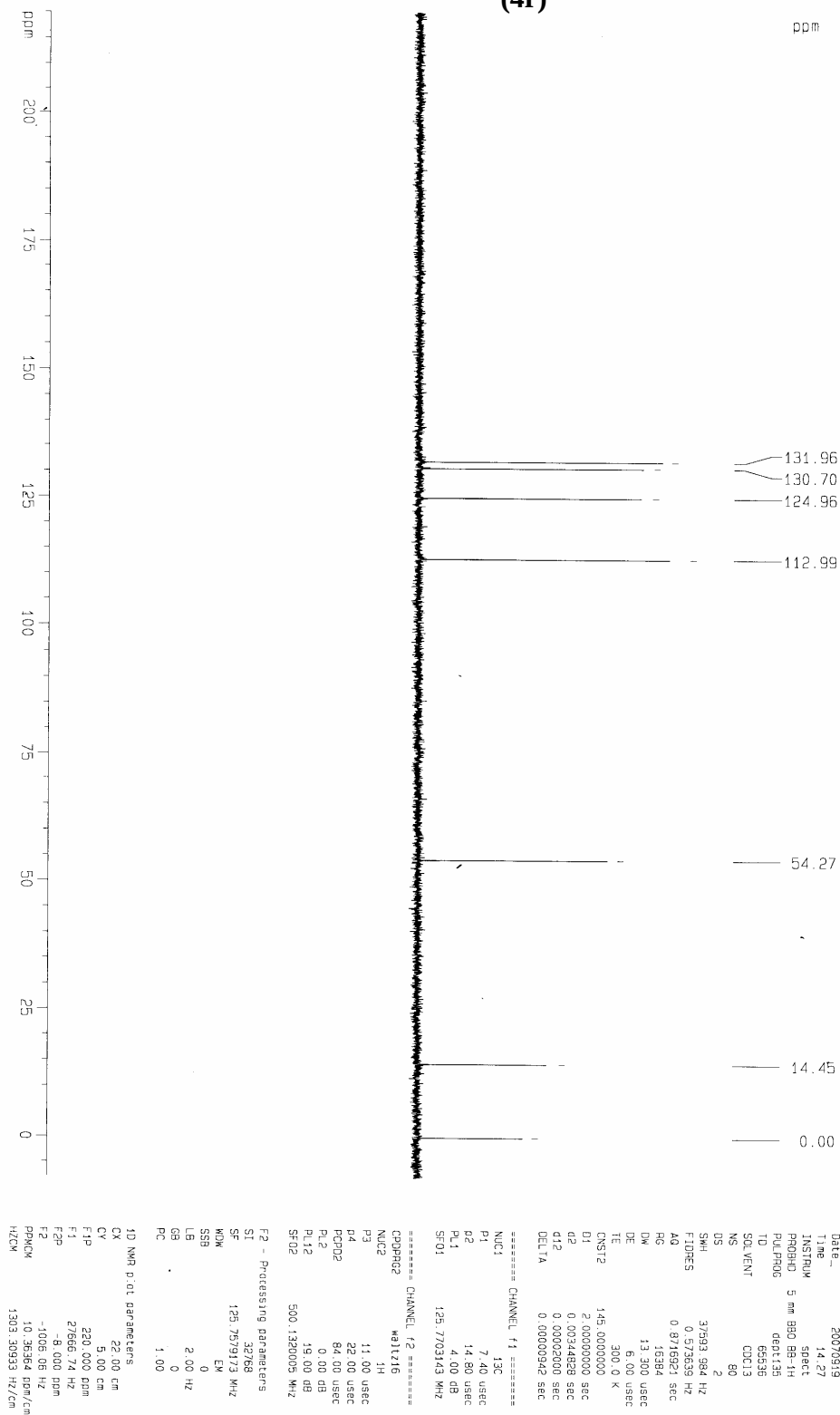


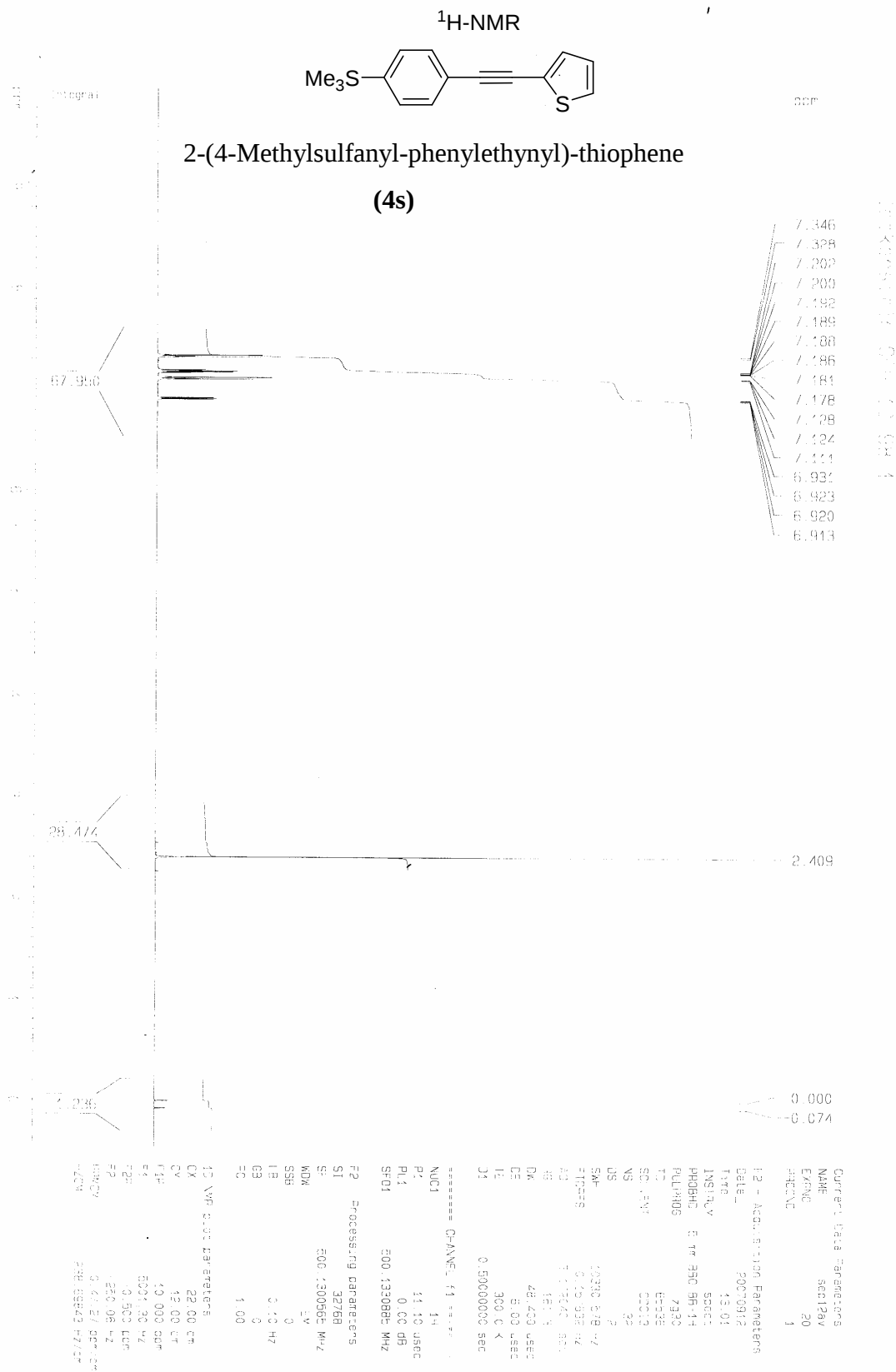
Fleckenstein GFP-10-99-1





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

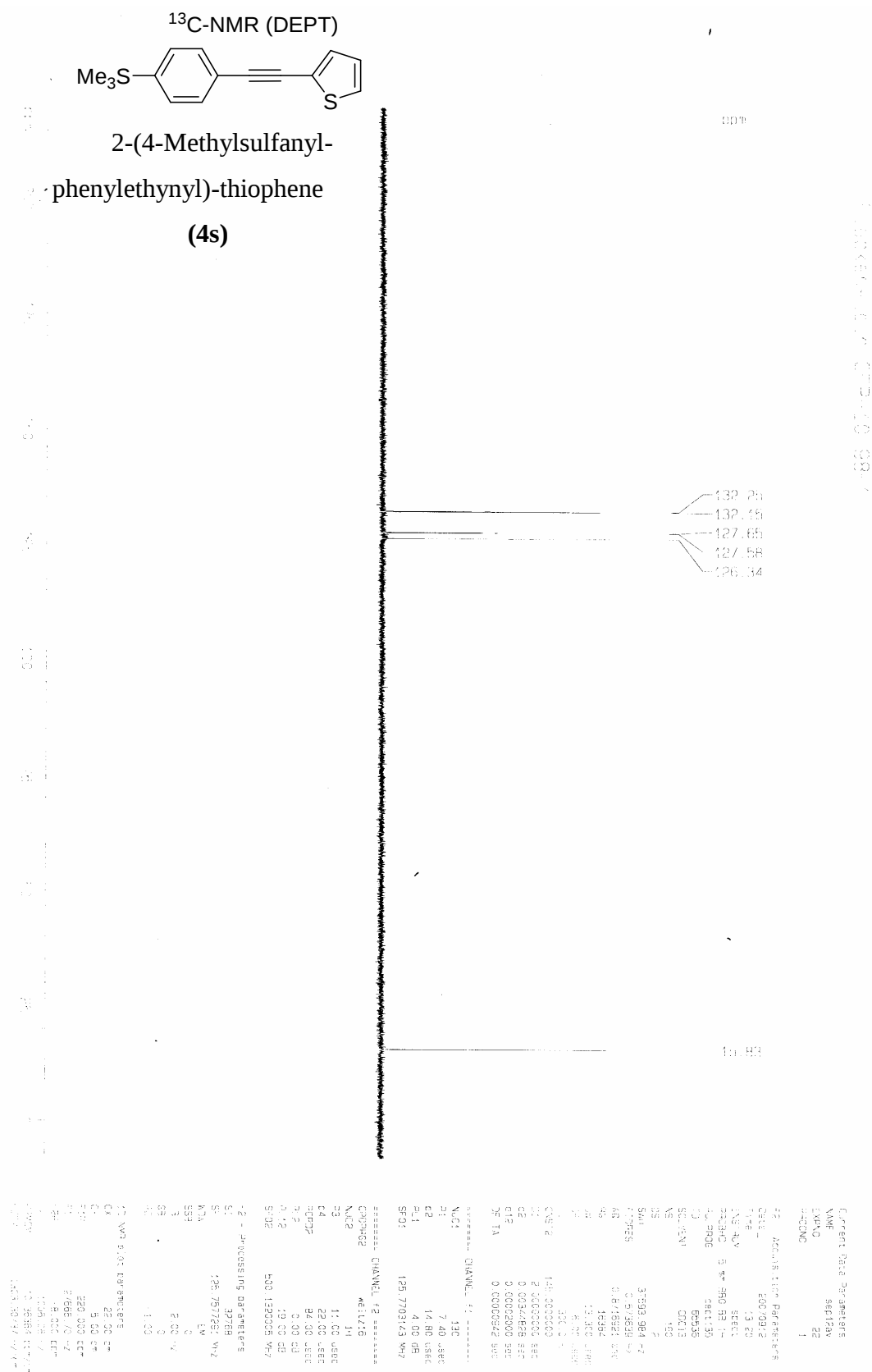


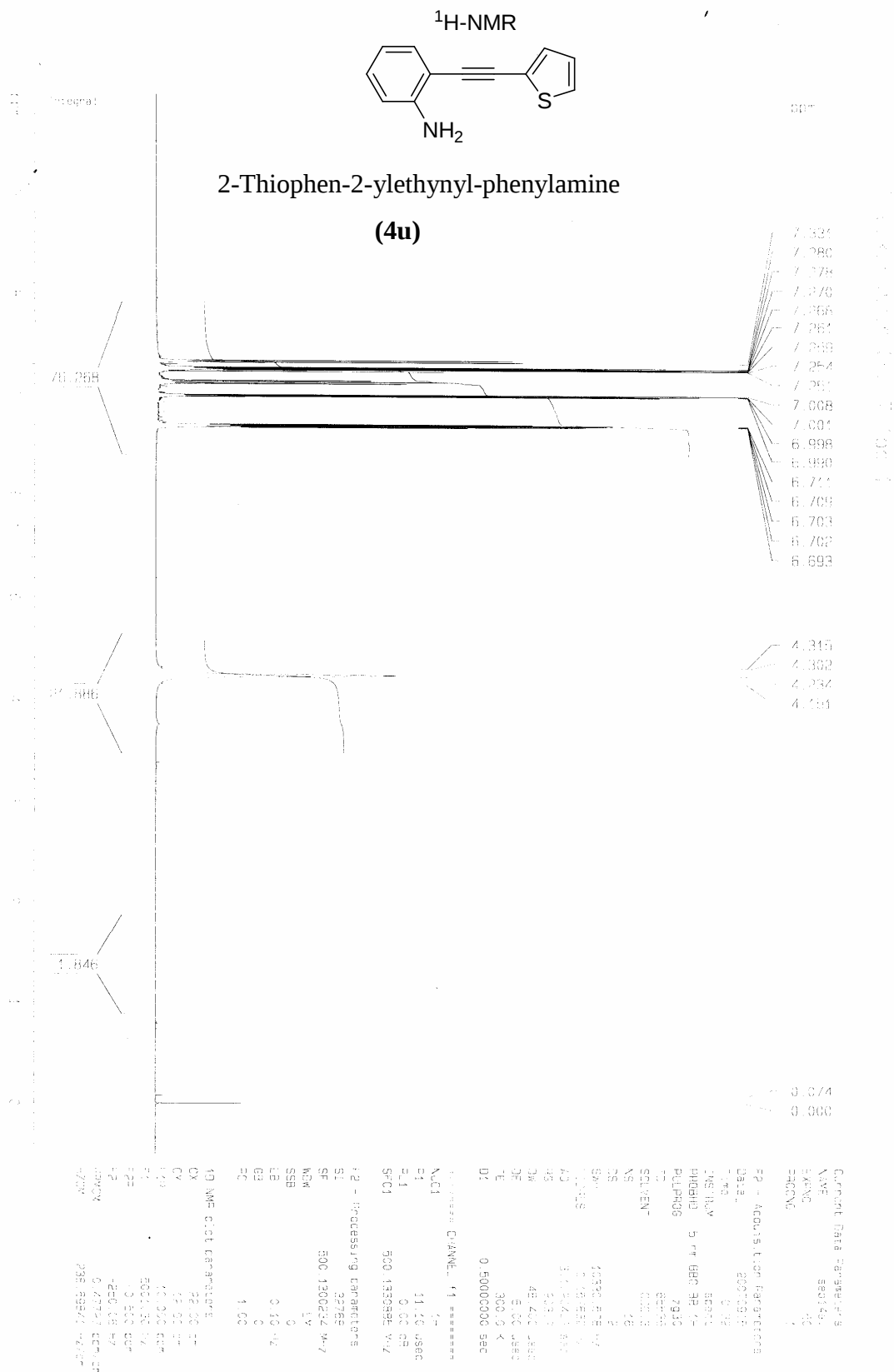


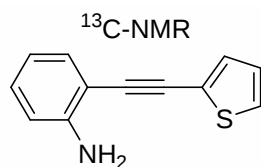
2-(4-Methylsulfanyl-phenylethynyl)-thiophene
(4s)

140.01
132.17
132.07
127.57
127.50
126.26
123.80
119.68
93.27
83.10
77.69
77.43
77.18
15.75

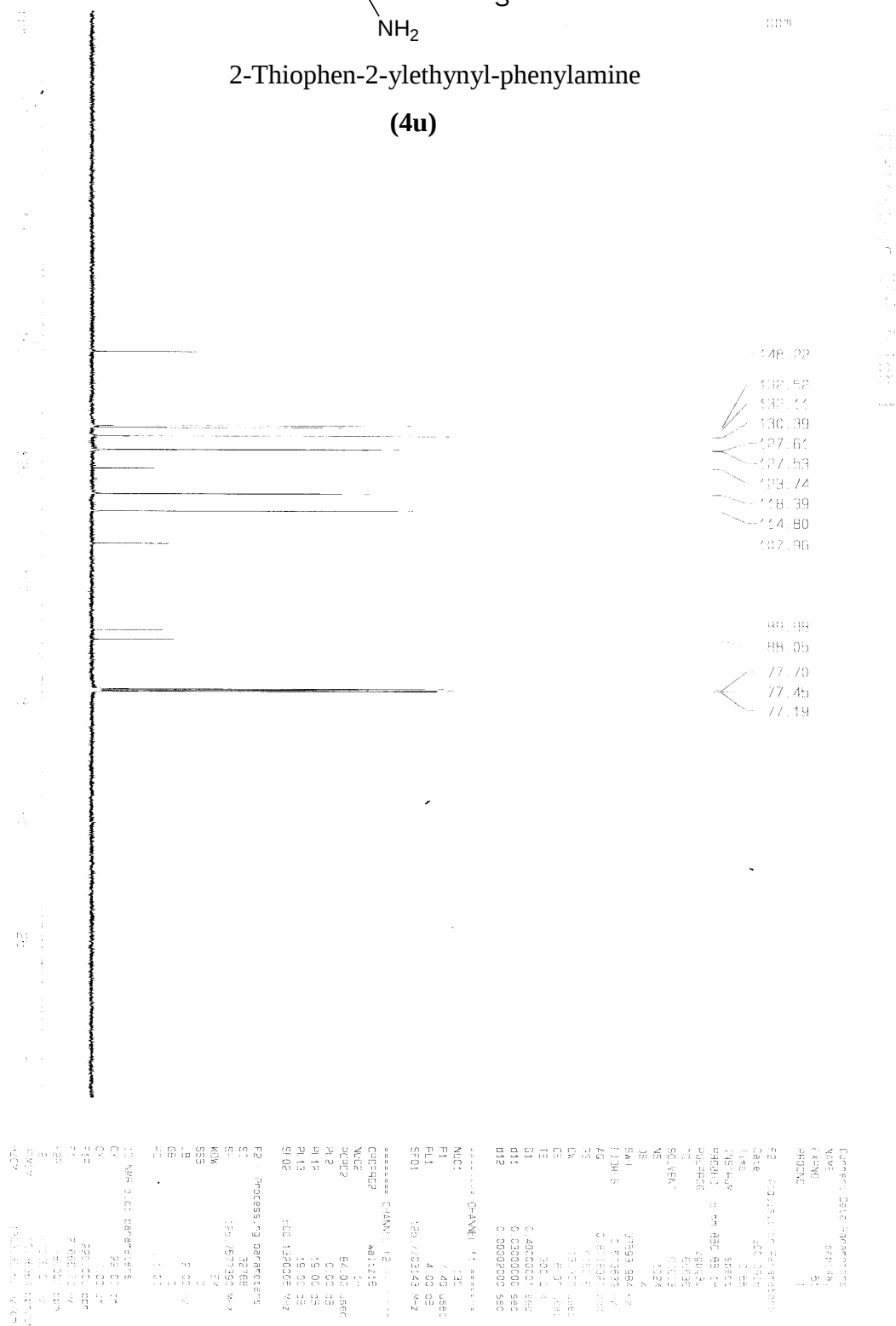
S 73



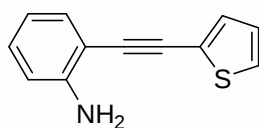




2-Thiophen-2-ylethynyl-phenylamine
(4u)



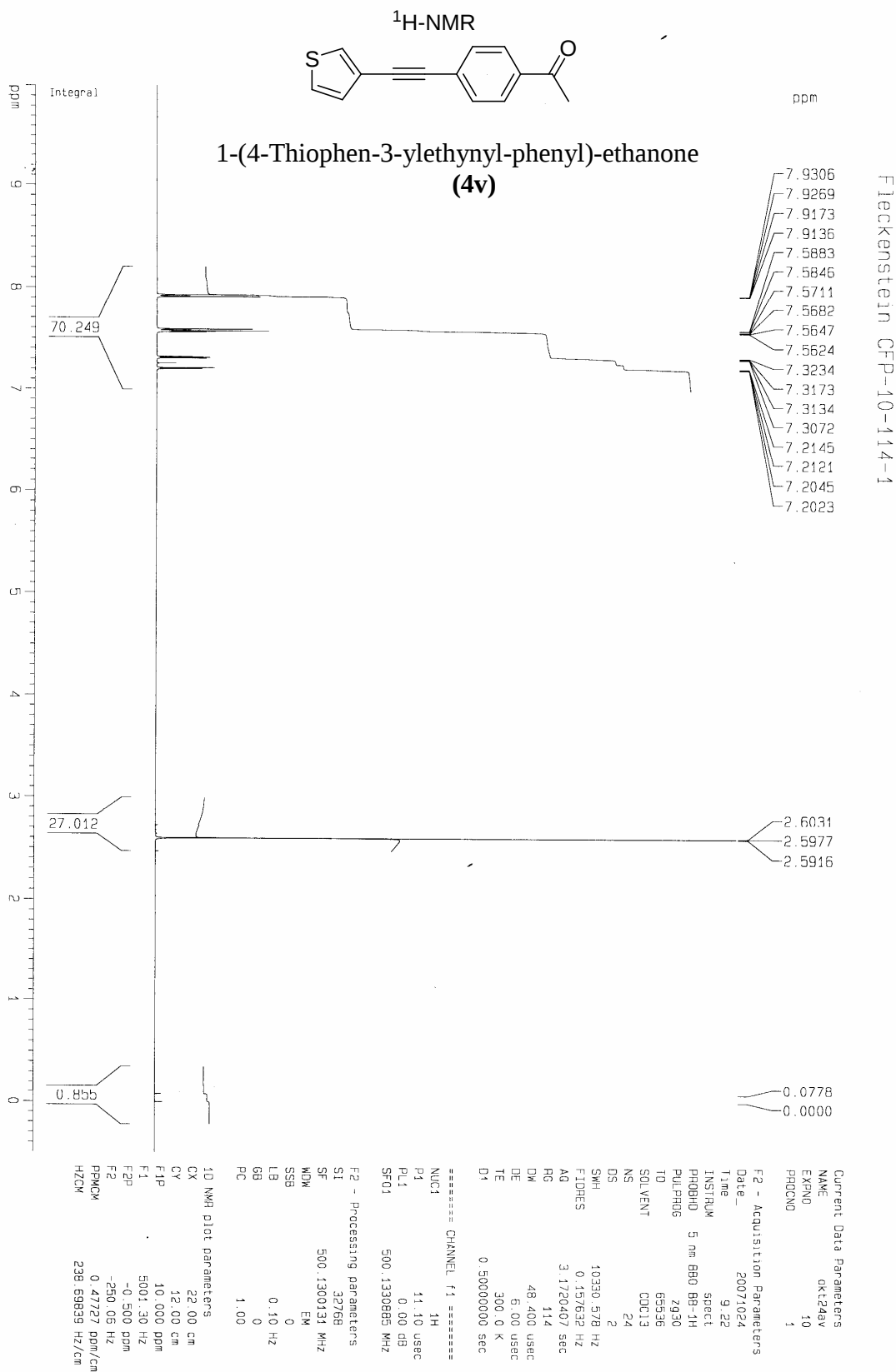
¹⁵N-NMR (HMBC)

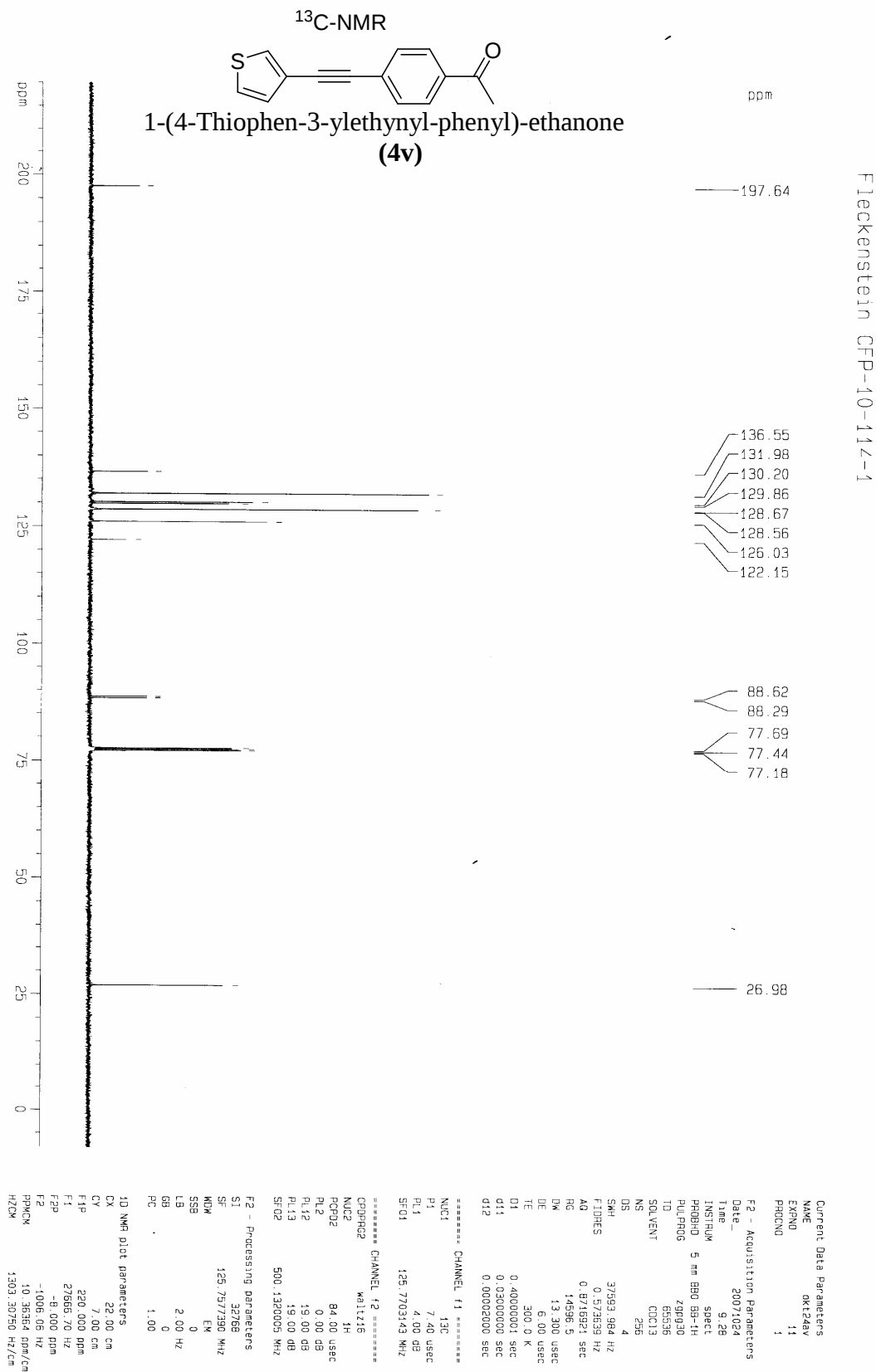


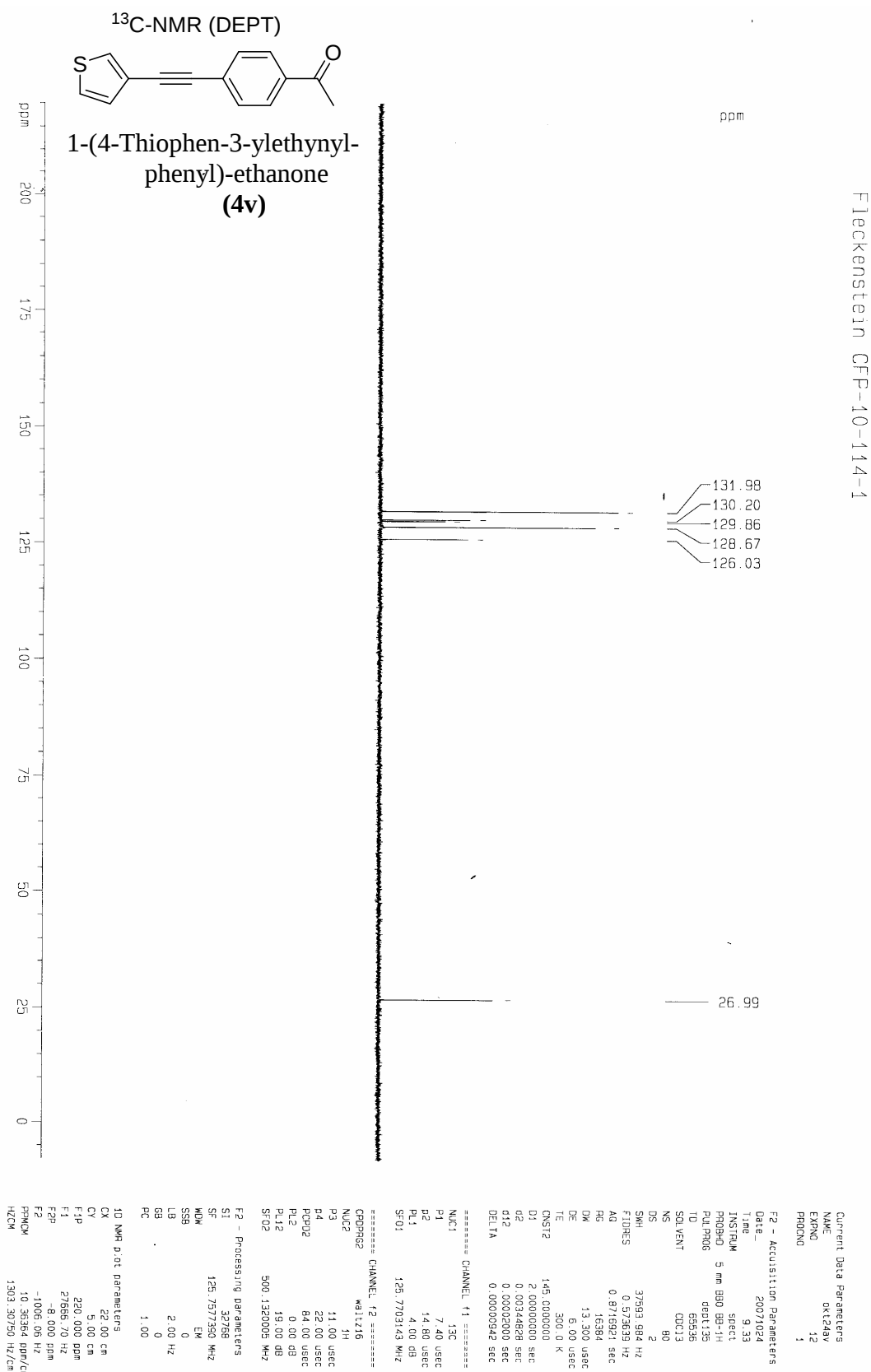
2-Thiophen-2-ylethynyl-phenylamine

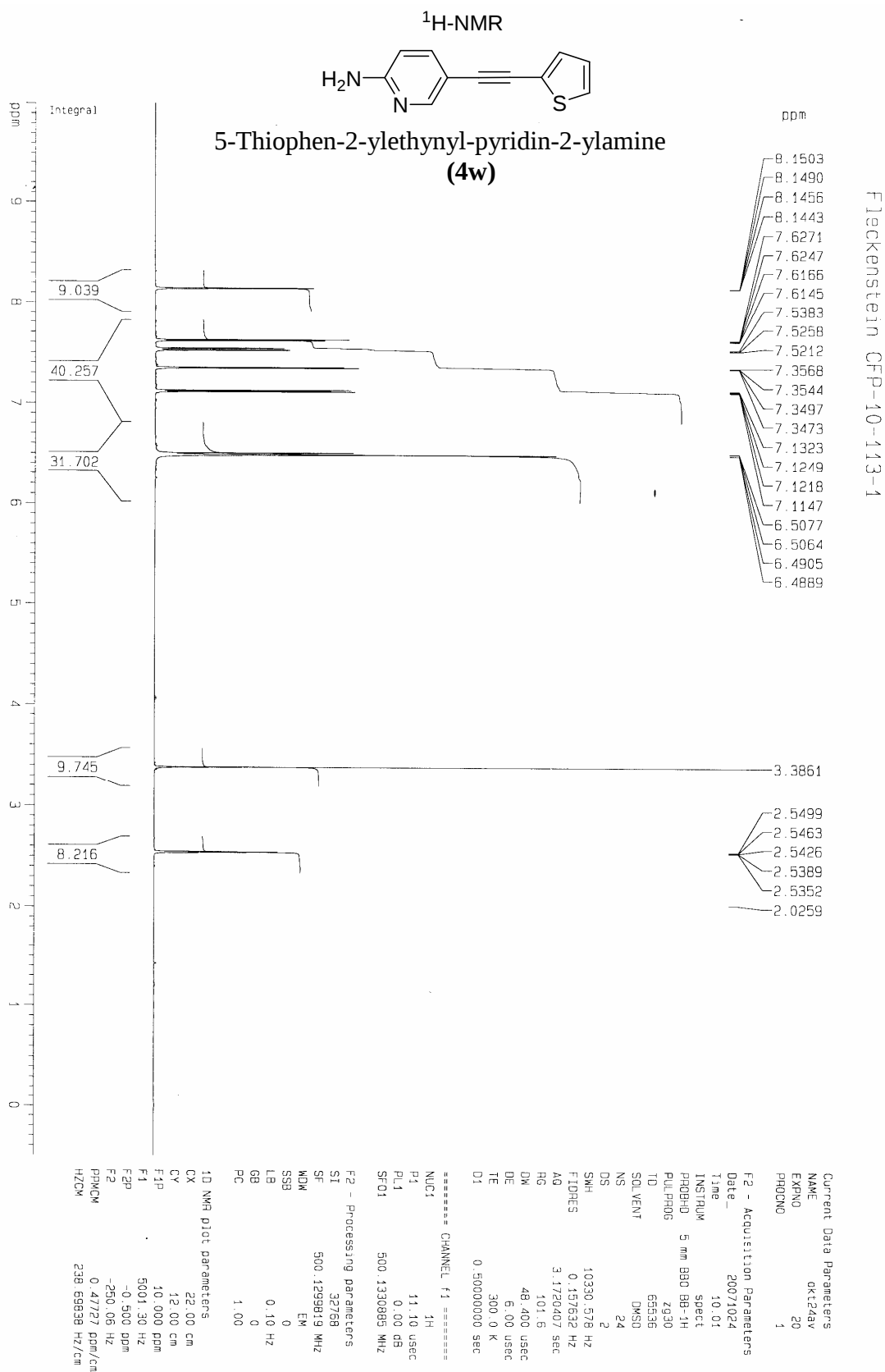
(4u)

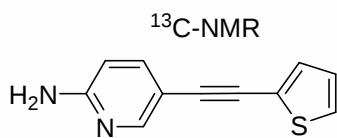




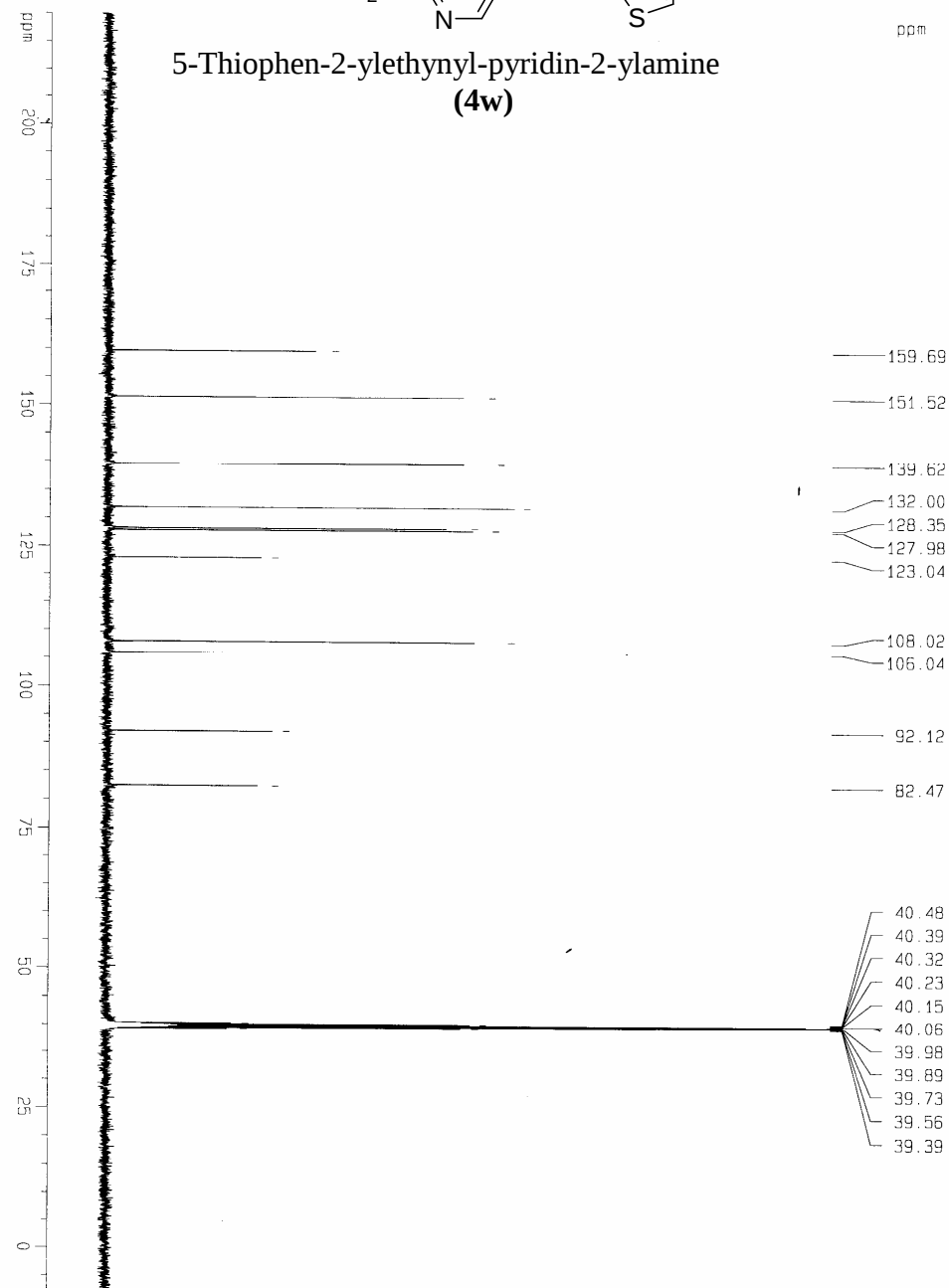








5-Thiophen-2-ylethynyl-pyridin-2-ylamine
(4w)



Current Data Parameters
NAME: 06124w
EXPNO: 21
PROCNO: 1

F2 - Acquisition Parameters
Date_: 20071024
Time: 10.08
INSTRUM: spect
PROBHD: 5 mm BBO BB-1H
PULPROG: zgpg30
TO: 65536
SOLVENT: DMSO
NS: 300
DS: 4
SWH: 37593.884 Hz
FIDRES: 0.572639 Hz
AQ: 0.8716921 sec
RG: 3649.1
DM: 13.308 usec
DE: 8.00 usec
TE: 300.0 K
D1: 0.4000001 sec
d11: 0.0300000 sec
d12: 0.0002000 sec

===== CHANNEL f1 =====
NUC1: 13C
P1: 7.40 usec
PL1: 4.00 dB
SFO1: 125.770343 MHz

===== CHANNEL f2 =====
CPRPRG2: waltz16
NUC2: 1H
PCPD2: 84.00 usec
PL2: 0.00 dB
PL12: 19.00 dB
PL13: 19.00 dB
SFO2: 500.132005 MHz

F2 - Processing parameters
SI: 32768
SF: 125.7578019 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: 27866.72 Hz
F2P: -8.000 ppm
F2: -1006.06 Hz
PPMCM: 10.36364 ppm/cm
HZCM: 1303.30823 Hz/cm

F]eckenstein CFP-10-113-1



13C NMR spectrum of 1,4-dichlorobenzene in CDCl₃. The spectrum shows a triplet for the solvent at 77.0 ppm and two main signals for the aromatic carbons at 128.5 ppm and 133.0 ppm. The x-axis ranges from 5.5 to 9.5 ppm.

Fleckenstein CFP-10-113-1/
1H-15N-HMBC

S 85