CHEMISTRY
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Supporting Information

Highly efficient Suzuki-Miyaura Coupling of Heterocyclic Substrates through Rational Reaction Design

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plenio@tu-darmstadt.de

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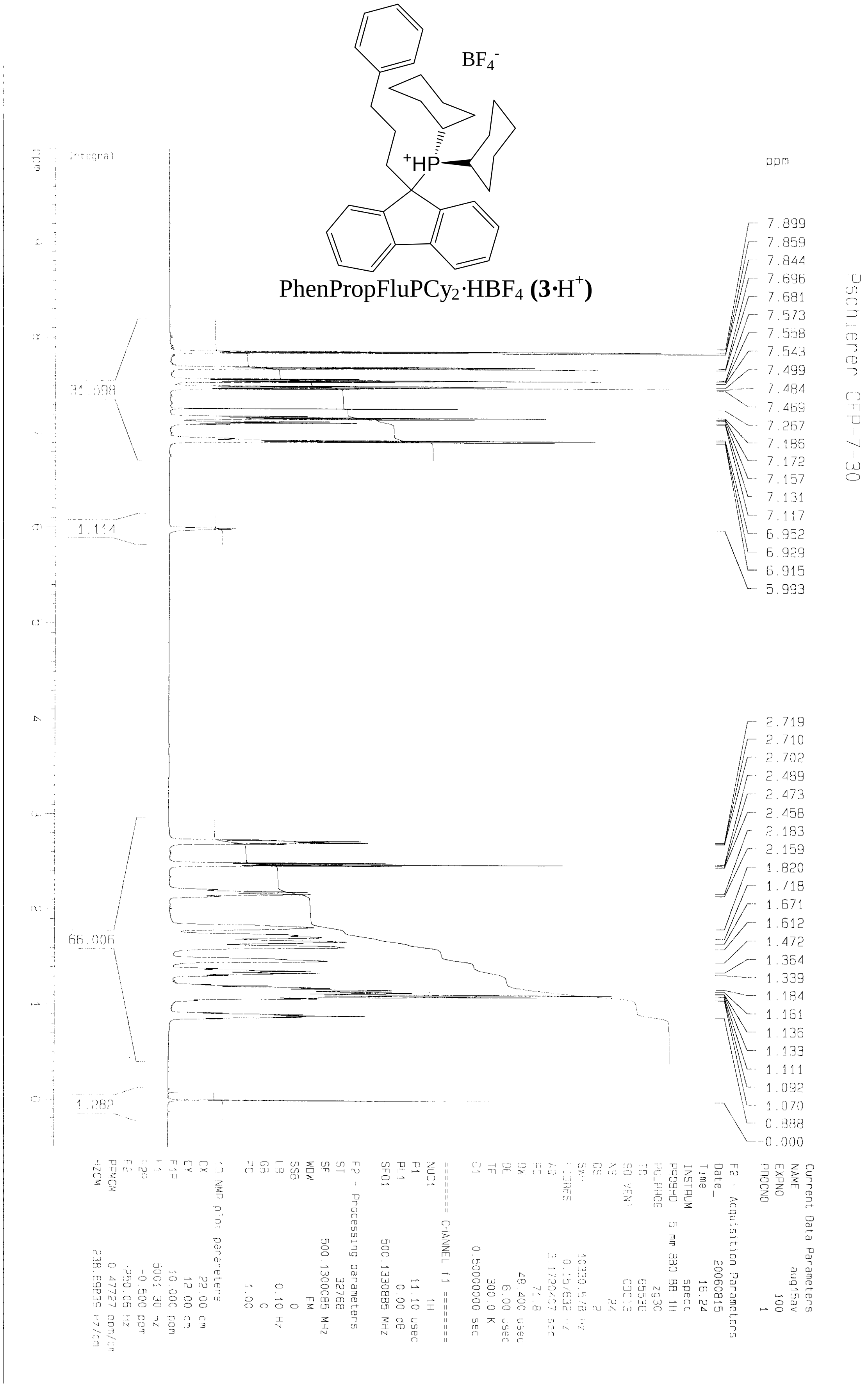
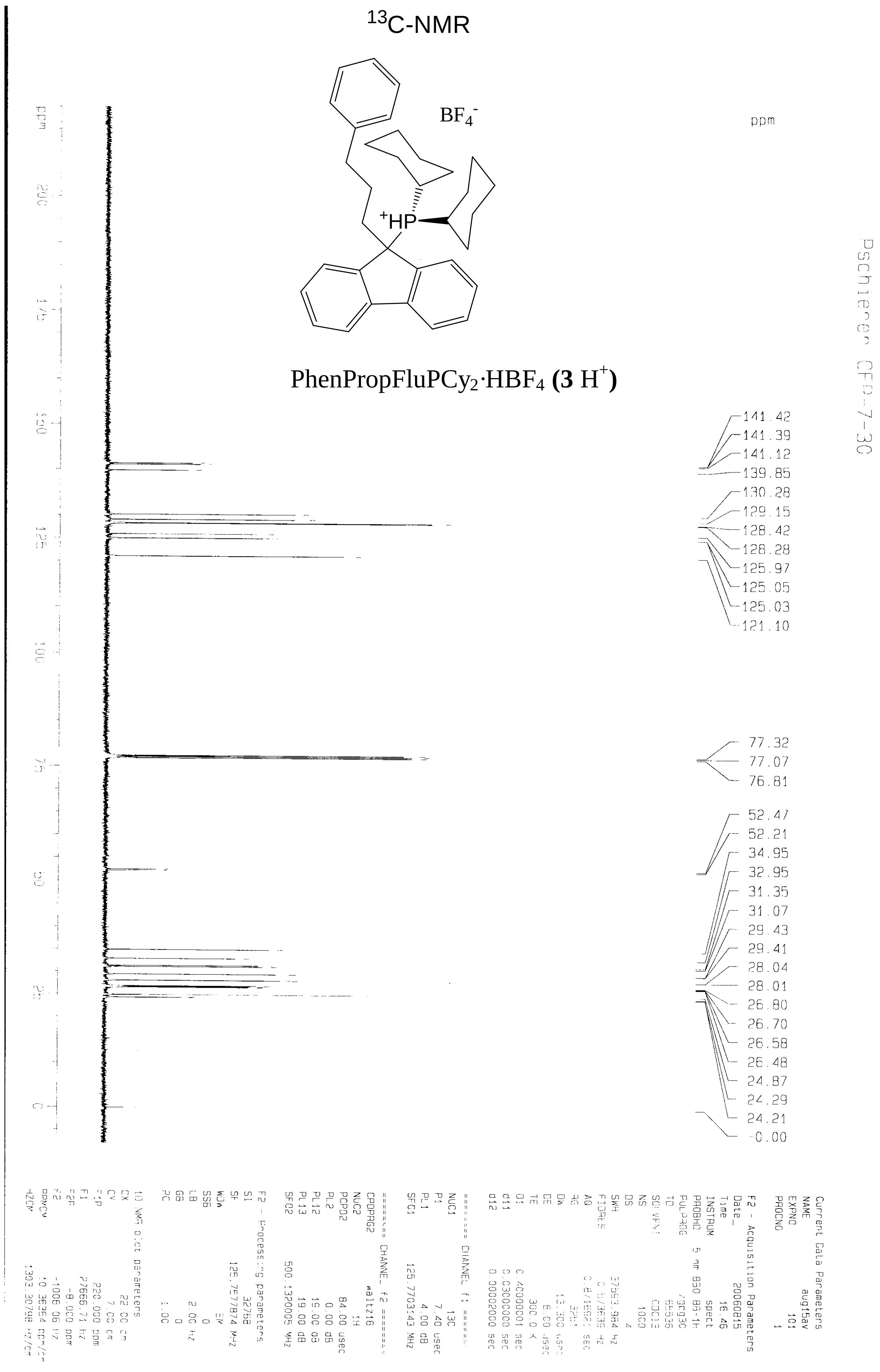
^{1}H-NMR



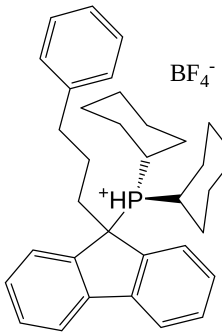
PhenPropFluPCy$_2$·HBF$_4$ (**3·H$^+$**)

^{13}C-NMR

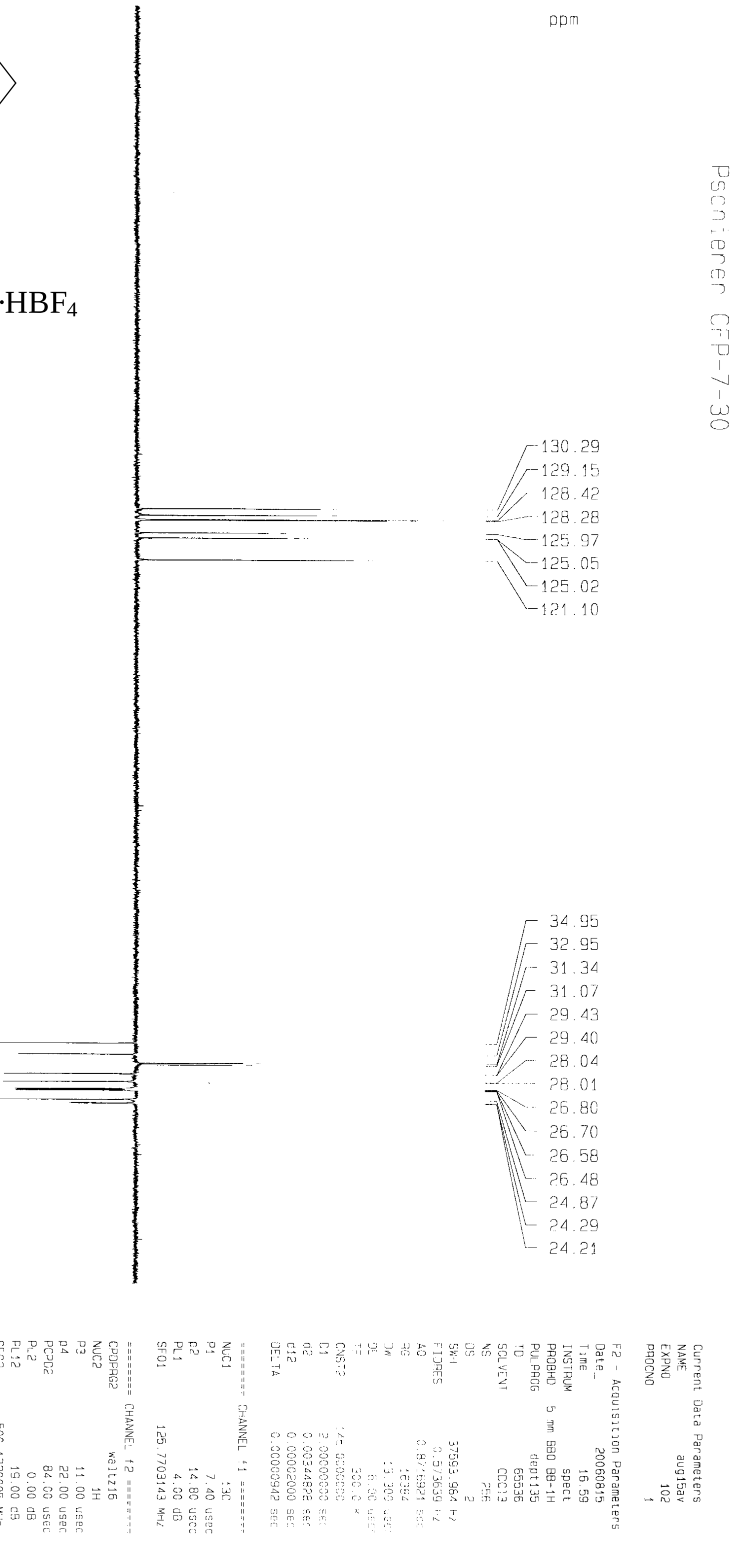


PhenPropFluPCy$_2$·HBF$_4$ (**3** H$^+$)

^{13}C-NMR (DEPT)



PhenPropFluPCy$_2$·HBF$_4$
(3 H$^+$)



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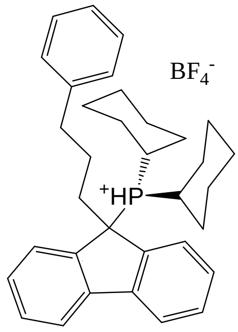

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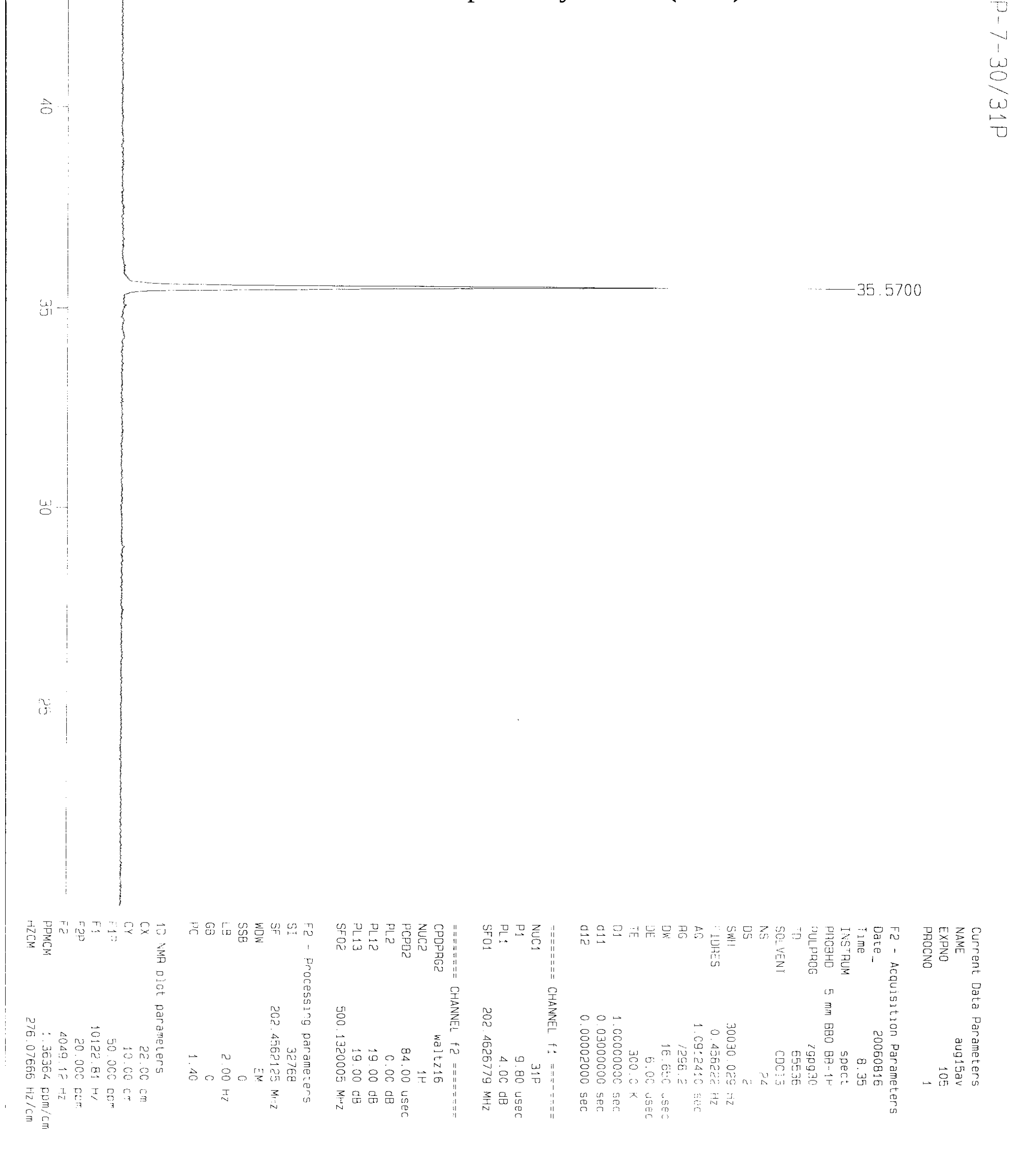

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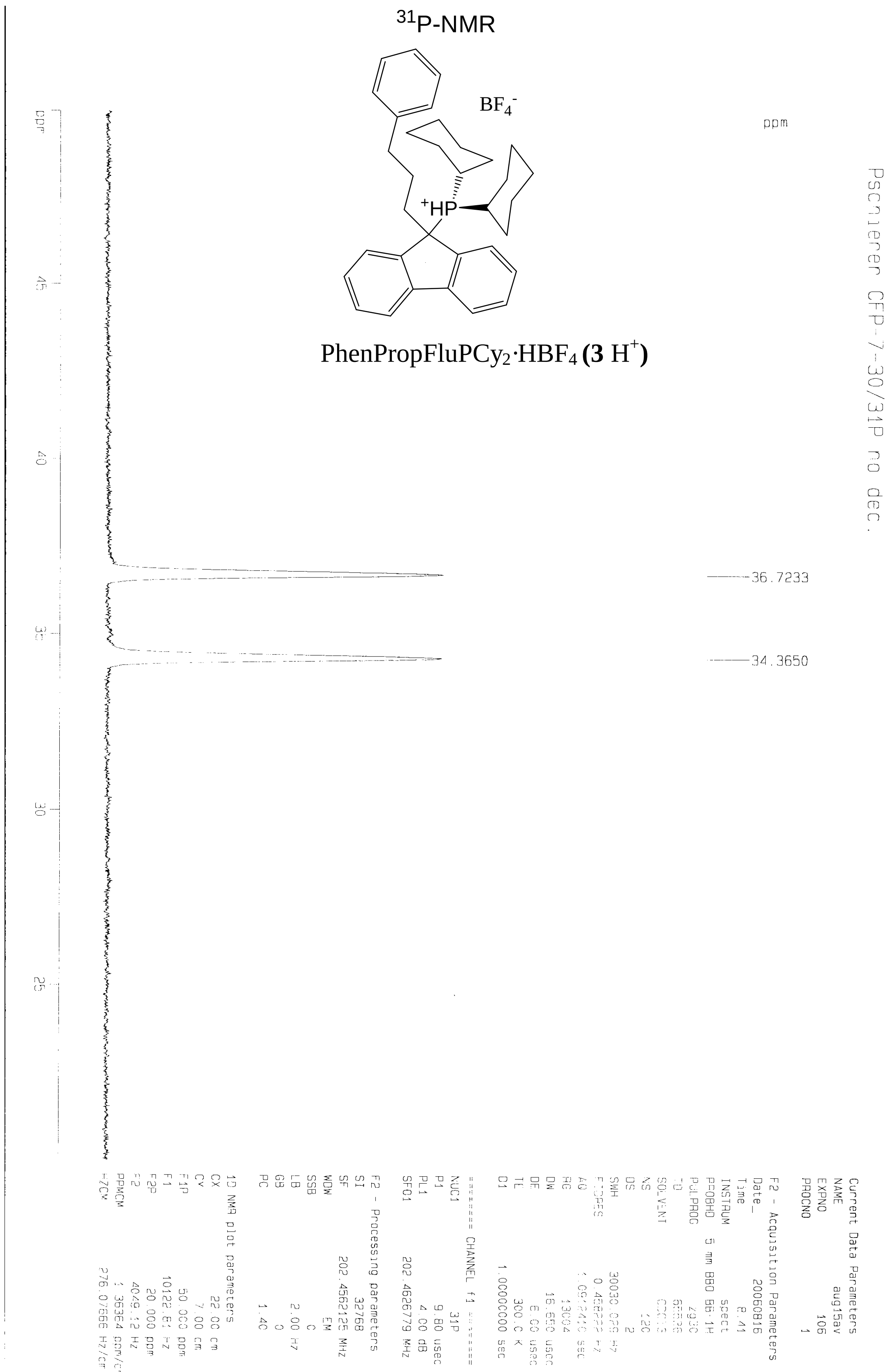

PhenPropFluPCy$_2$·HBF$_4$ (**3** H$^+$)

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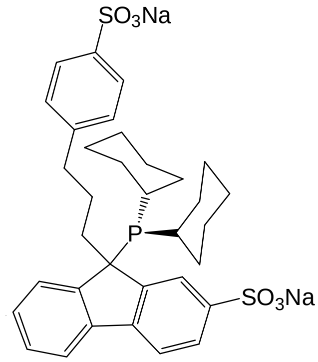

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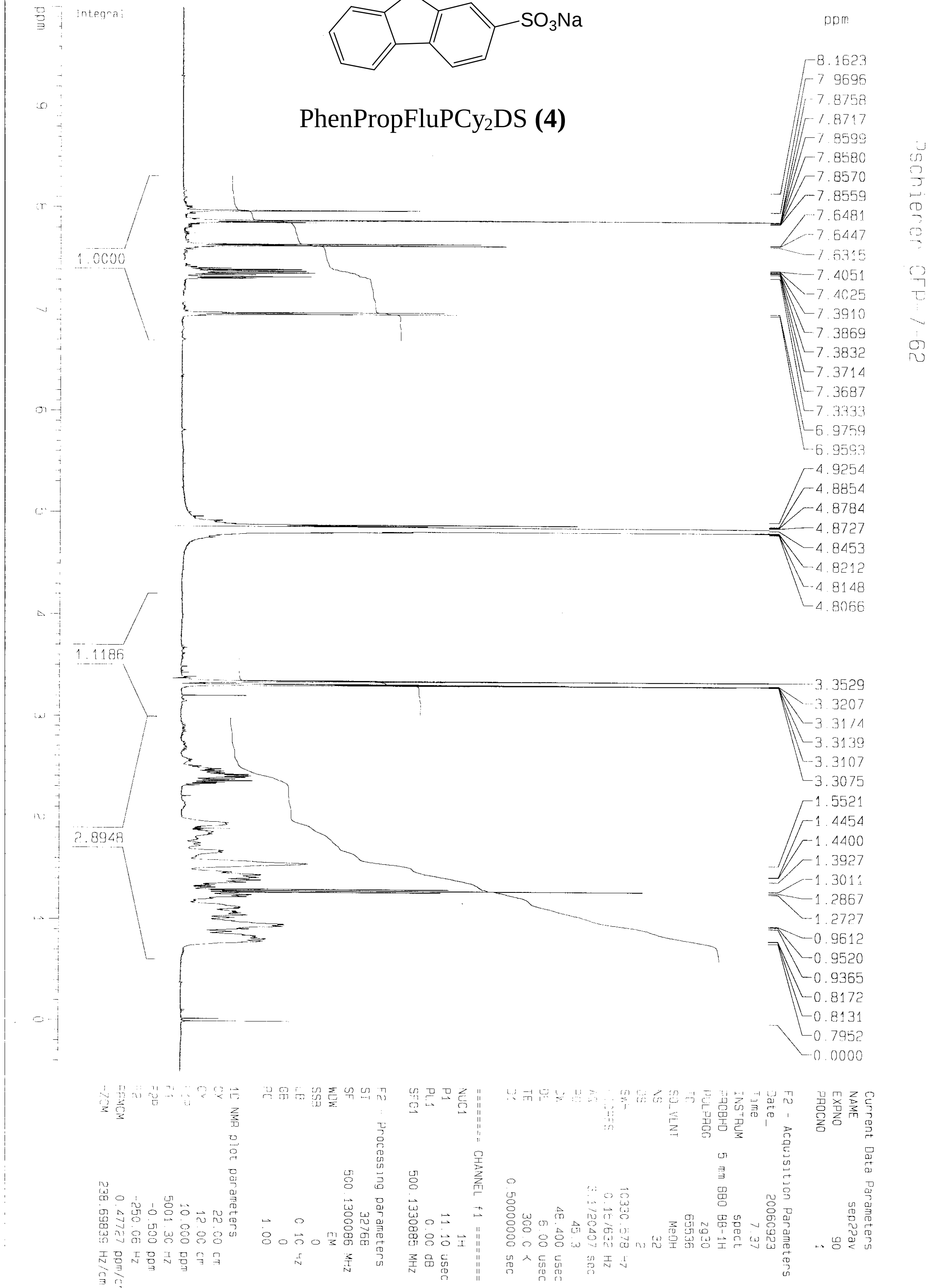

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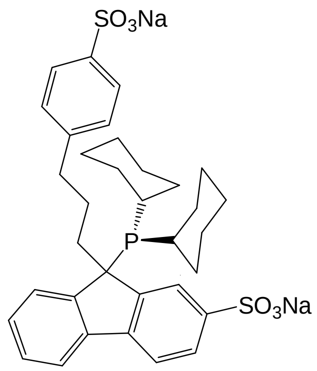

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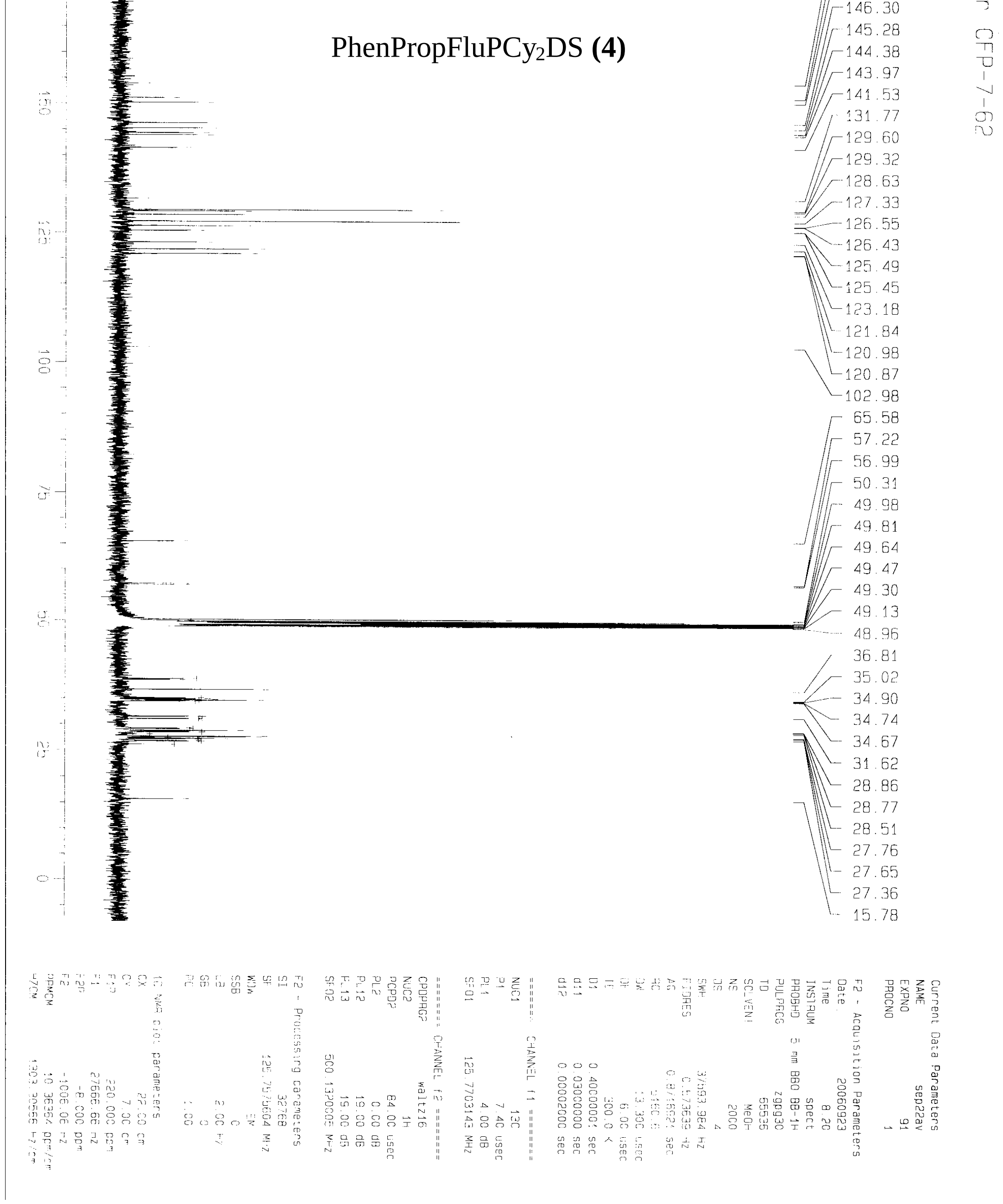

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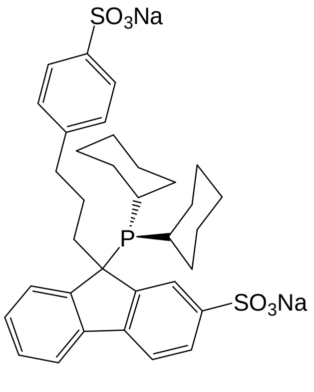

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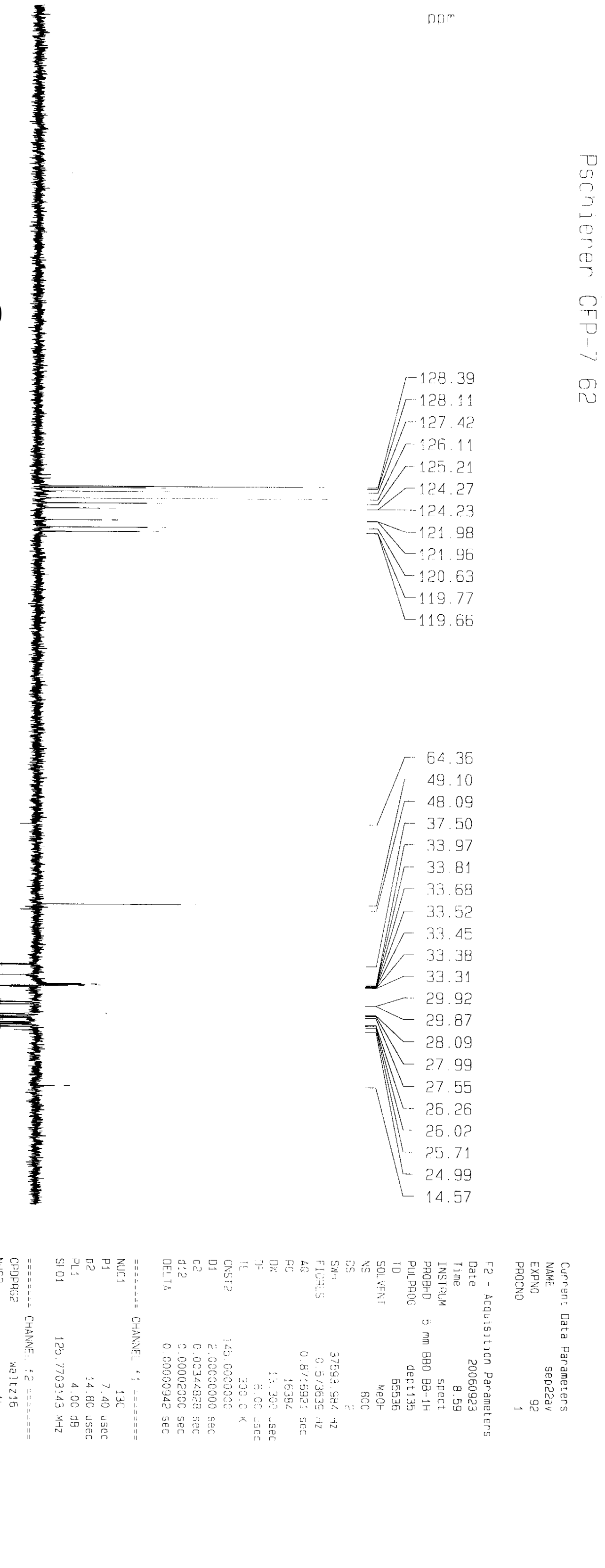

^{31}P-NMR {^{1}H}

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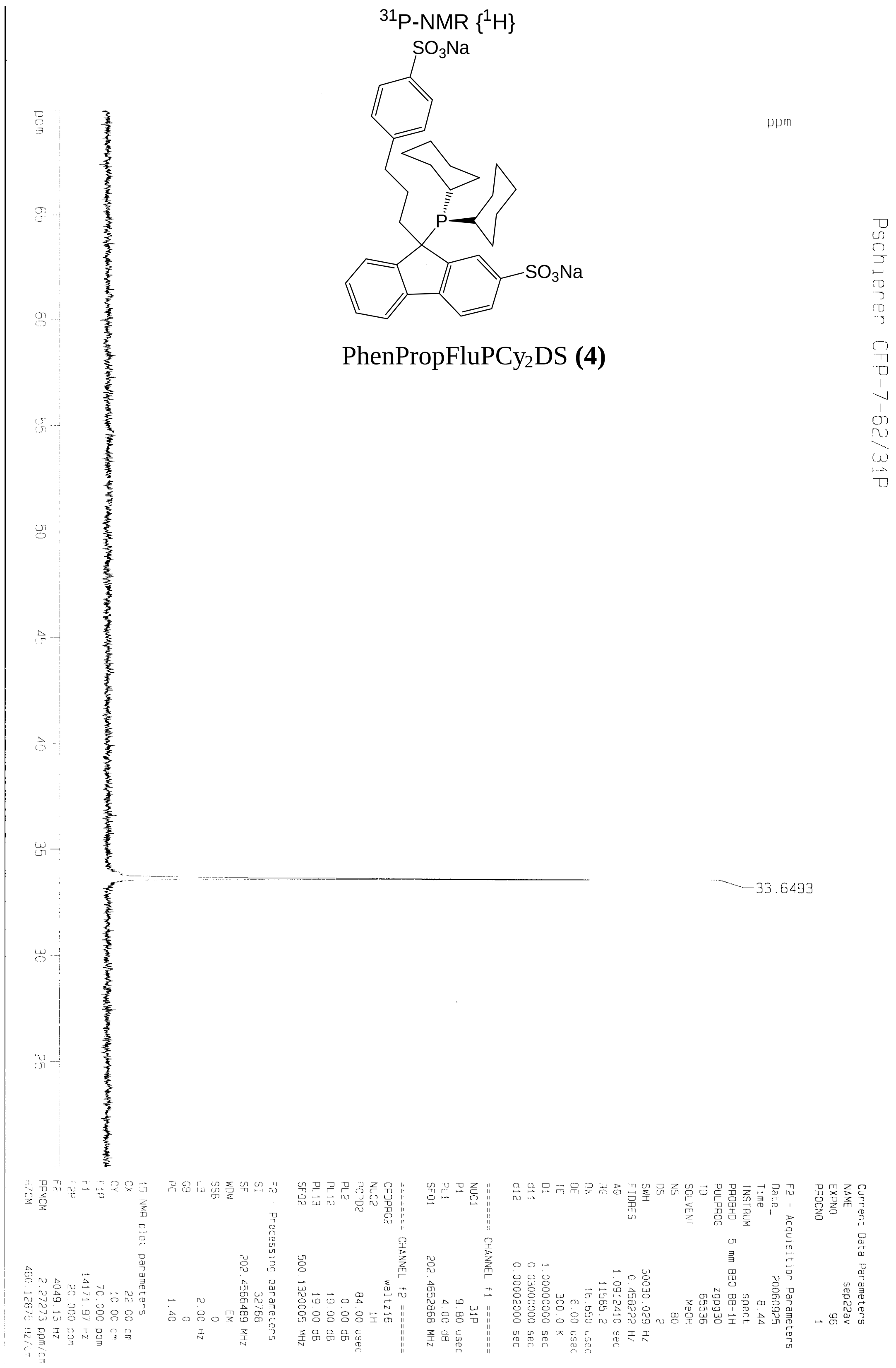

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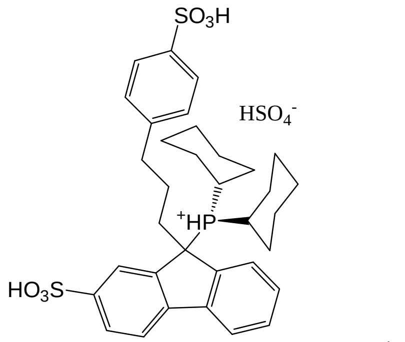

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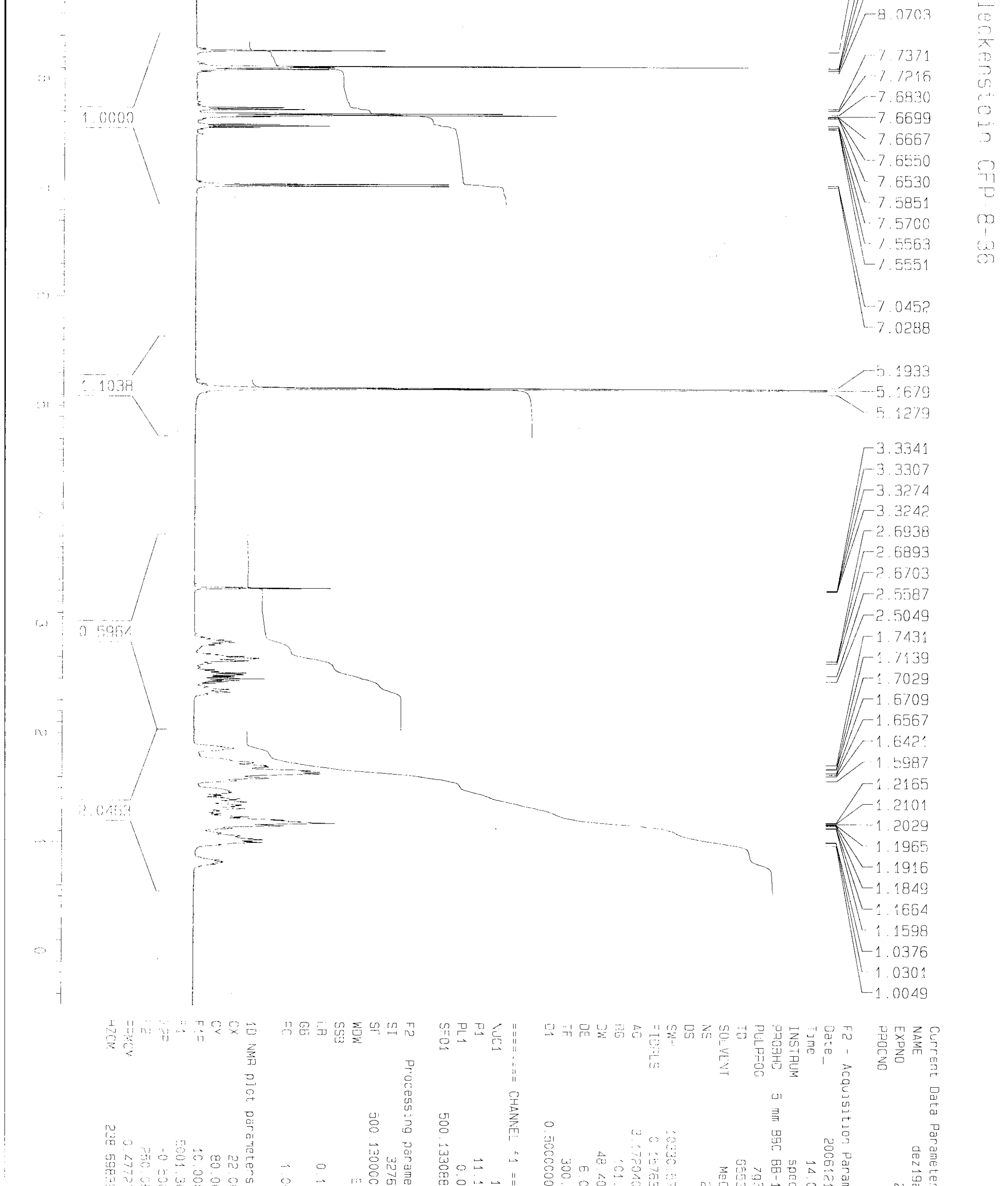

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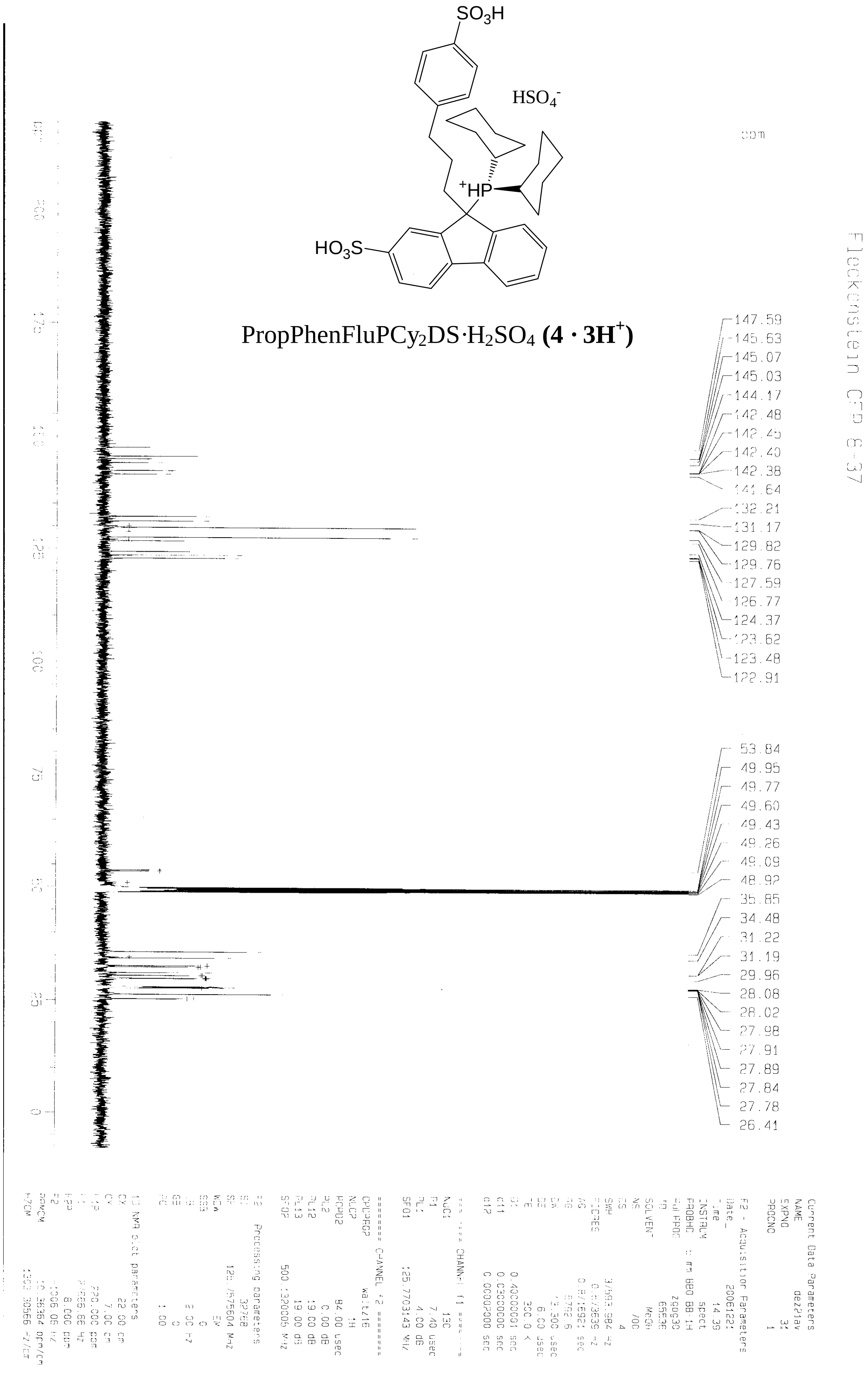

PropPhenFluPCy$_2$DS·H_2SO_4 **(4 · 3H$^+$)**

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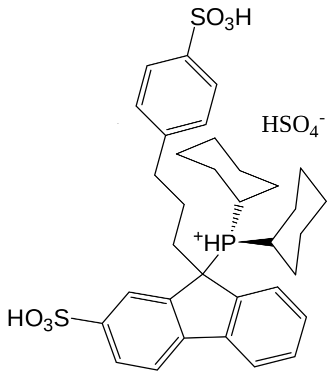
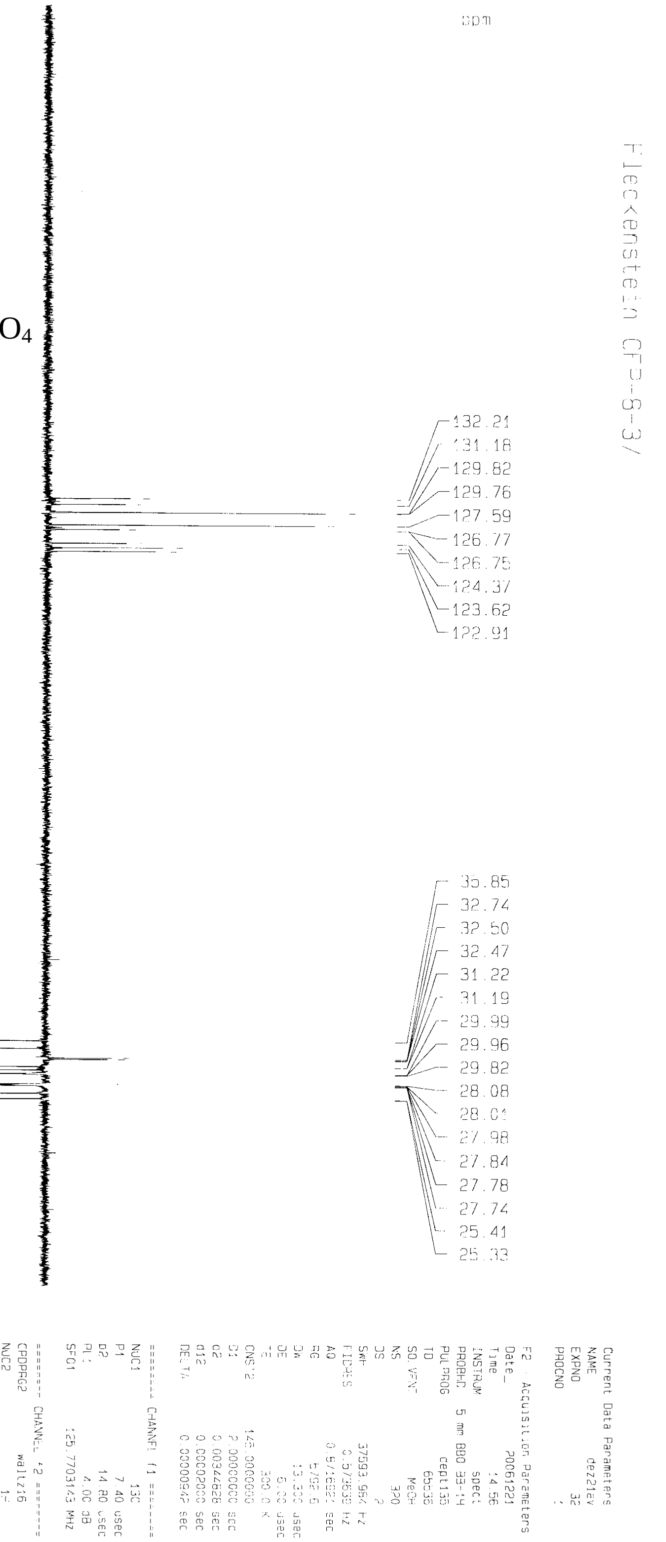
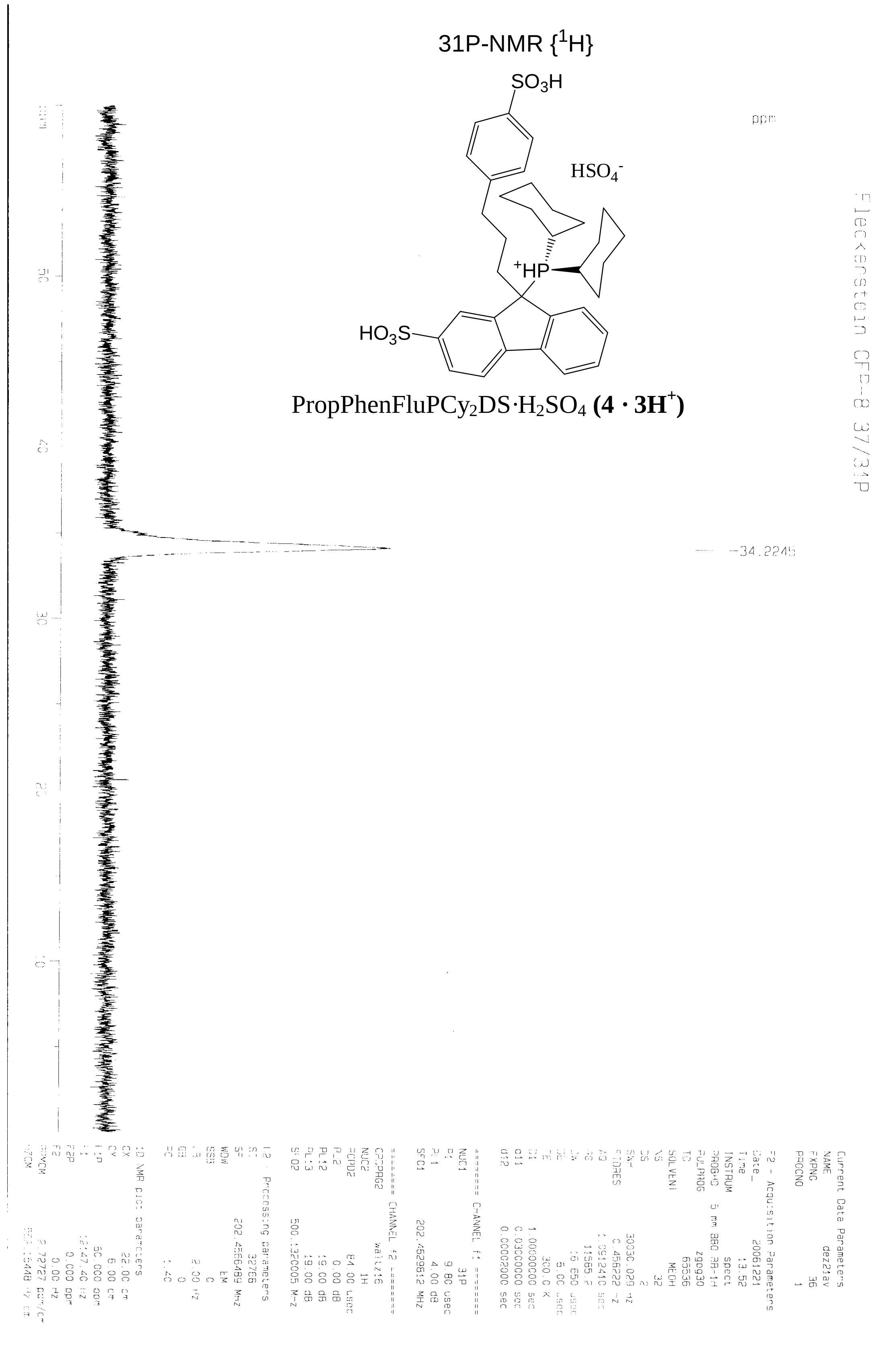


PropPhenFluPCy$_2$DS·H_2SO_4
(4 · 3H$^+$)



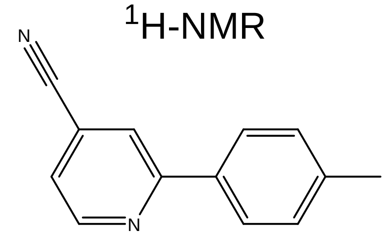
31P-NMR {^{1}H}



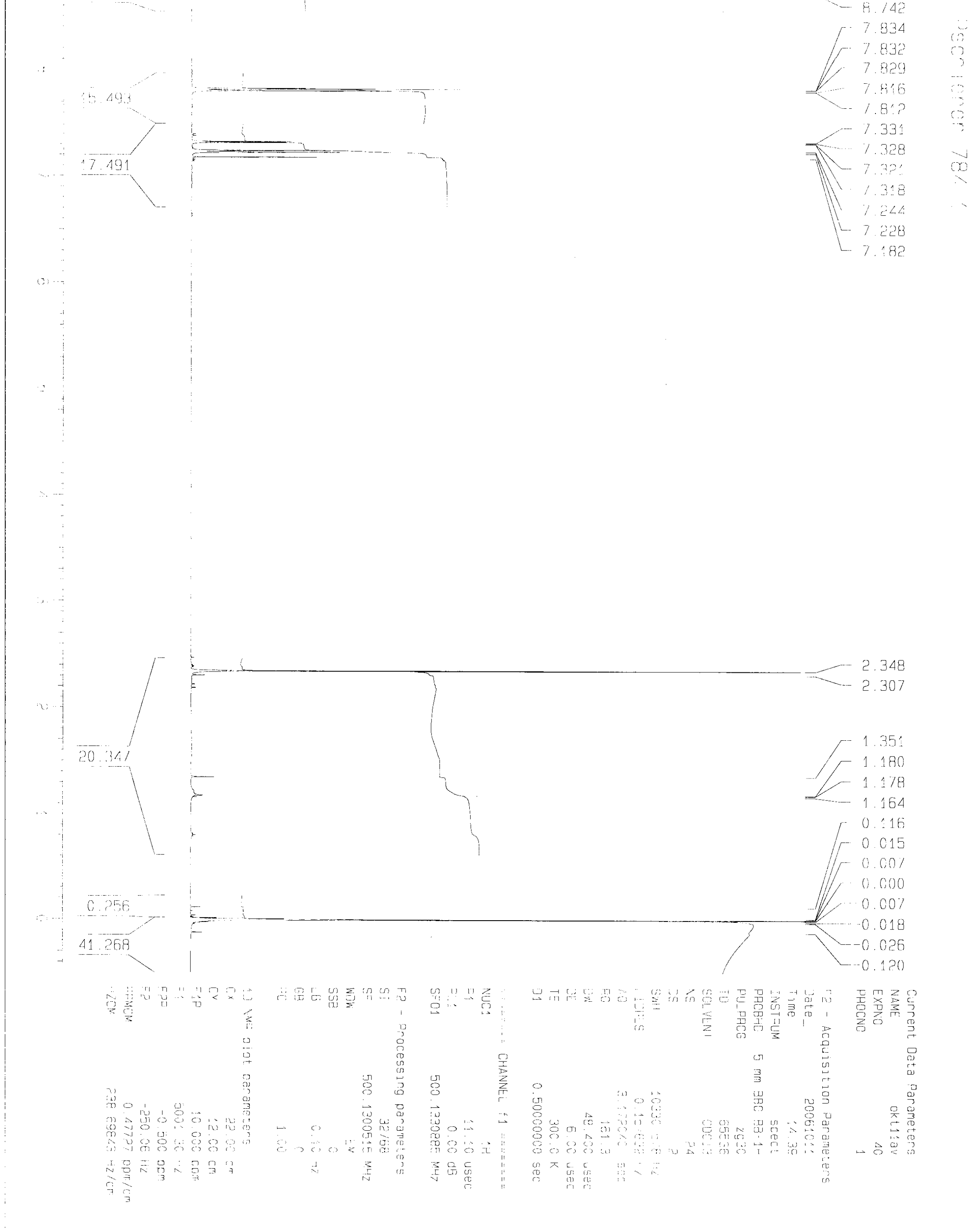
PropPhenFluPCy$_2$DS·H_2SO_4 **(4 · 3H$^+$)**

Suzuki Cross Coupling Products

^{1}H-NMR



2-*p*Tolyl-isonicotinonitrile



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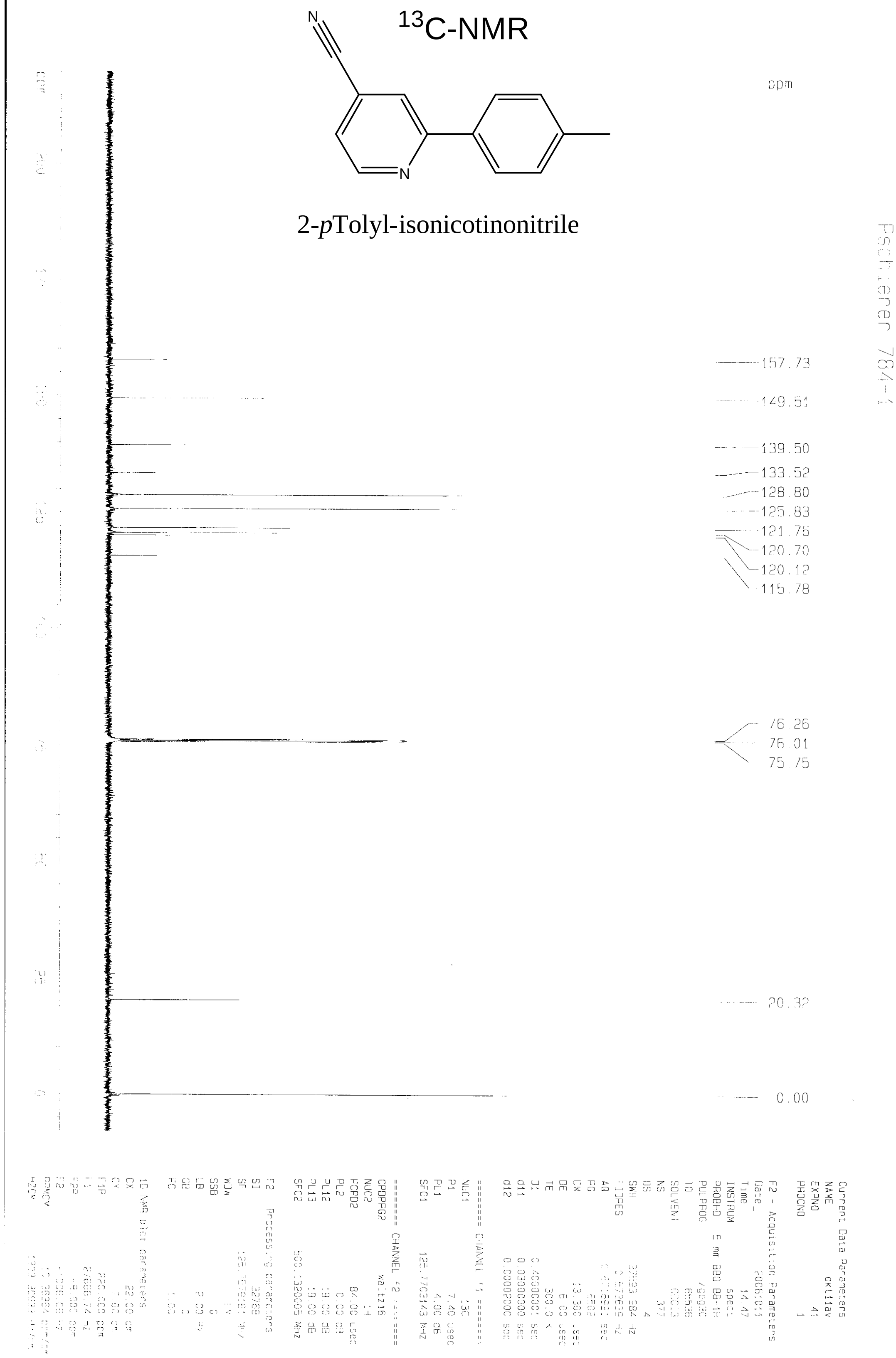

2-*p*Tolyl-isonicotinonitrile

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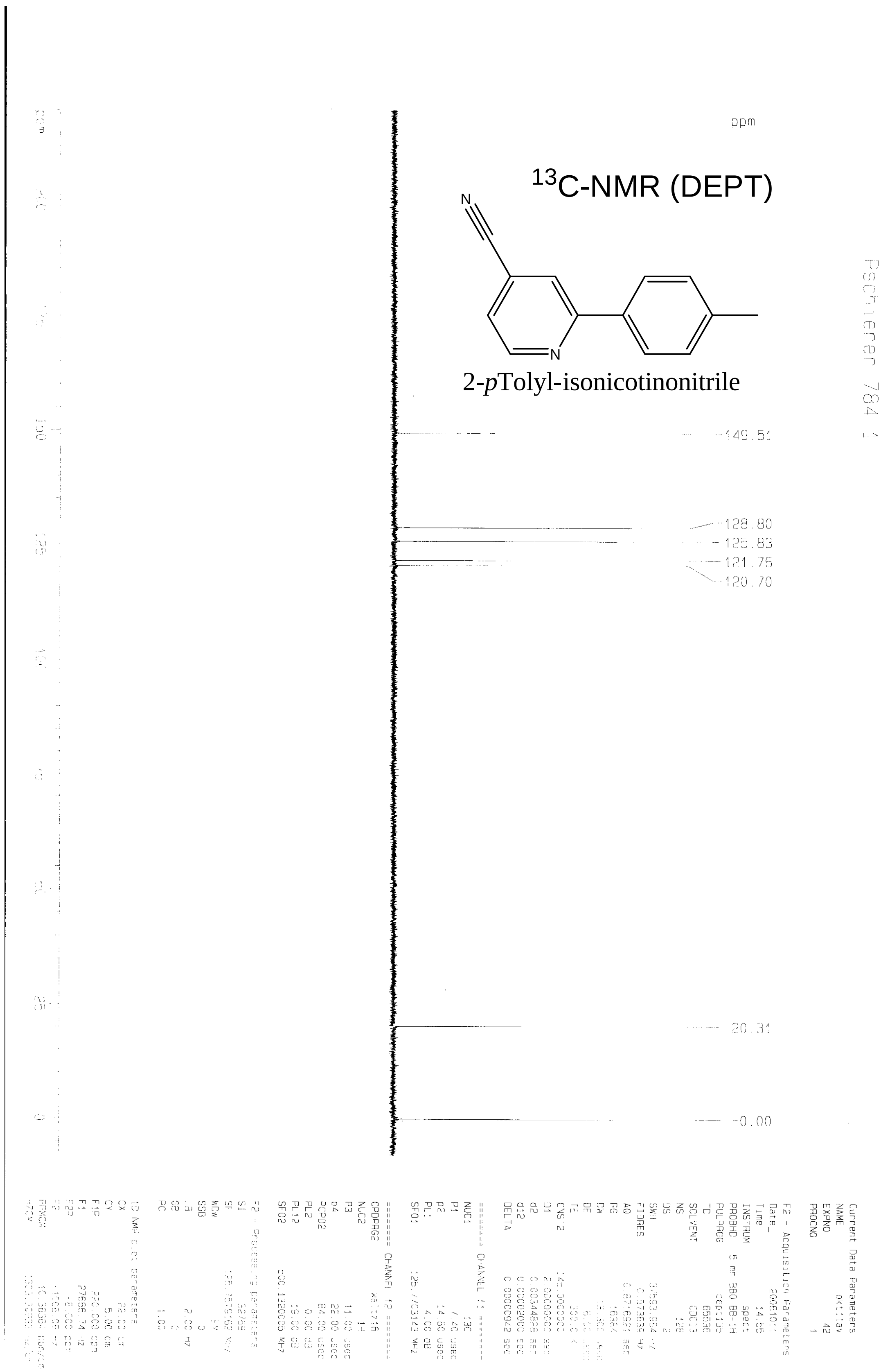
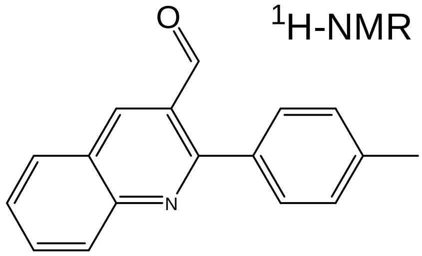
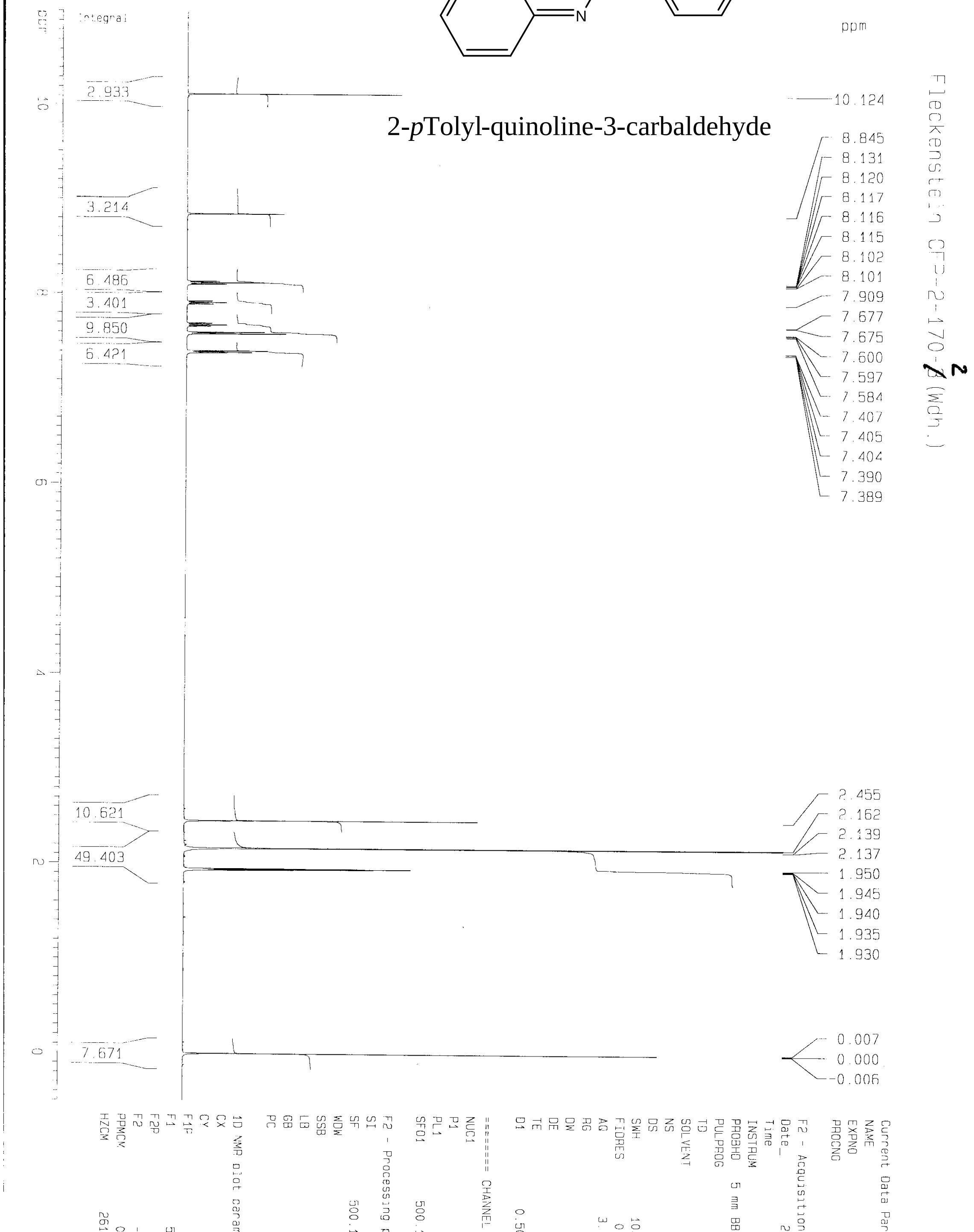


2-*p*Tolyl-isonicotinonitrile

^{1}H-NMR



2-*p*Tolyl-quinoline-3-carbaldehyde



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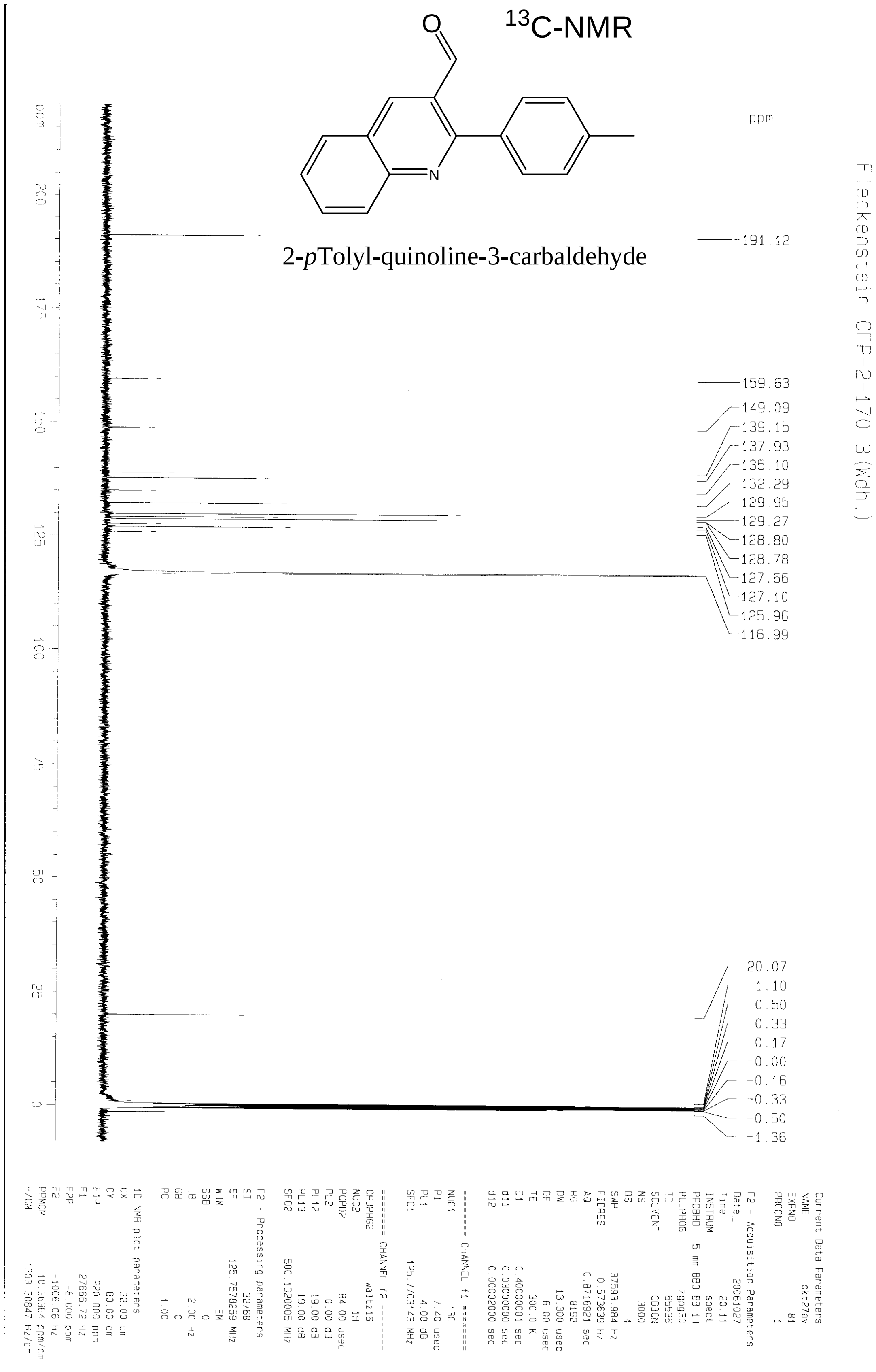
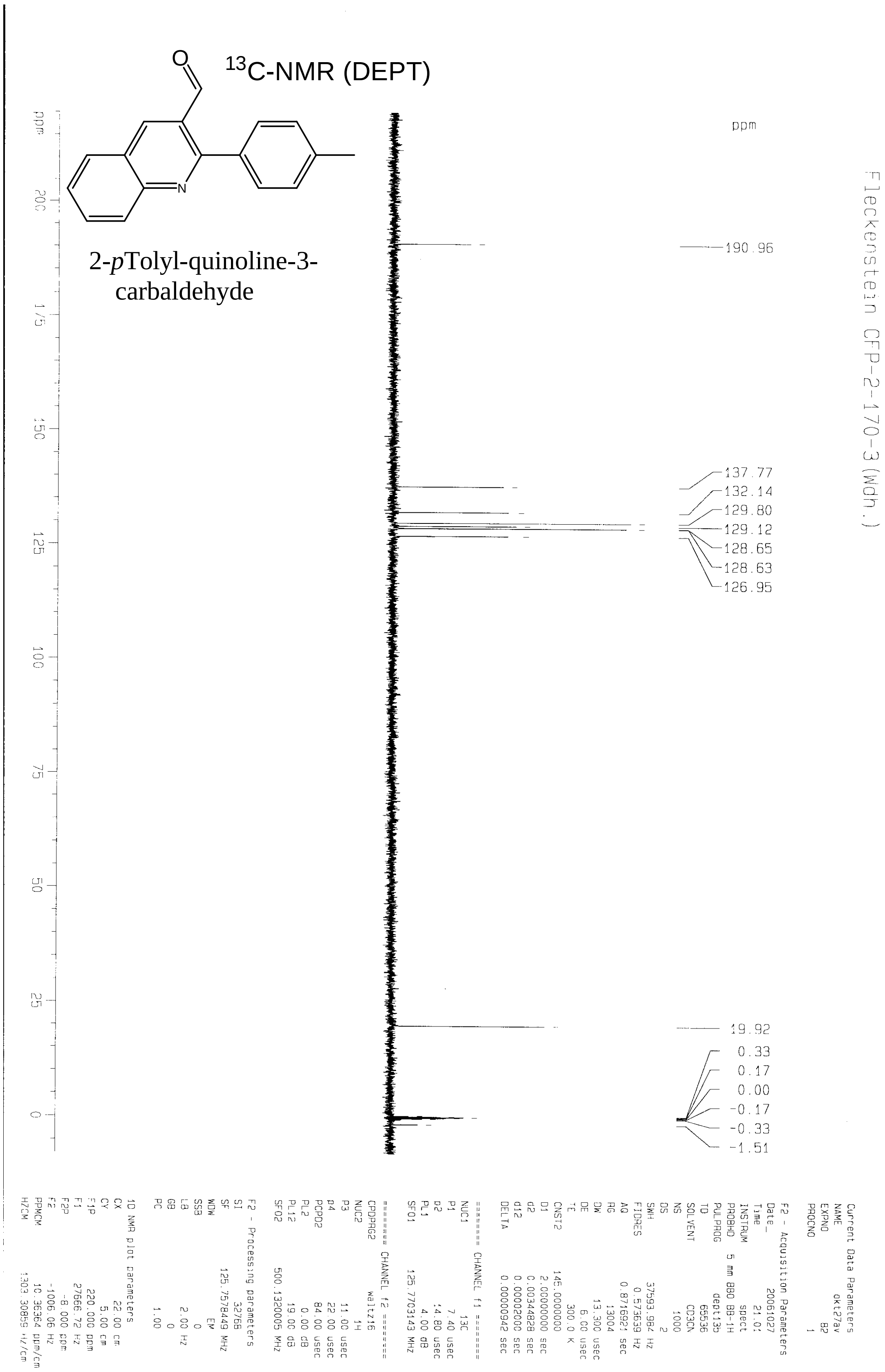


2-*p*Tolyl-quinoline-3-carbaldehyde

^{13}C-NMR (DEPT)

2-*p*Tolyl-quinoline-3-carbaldehyde



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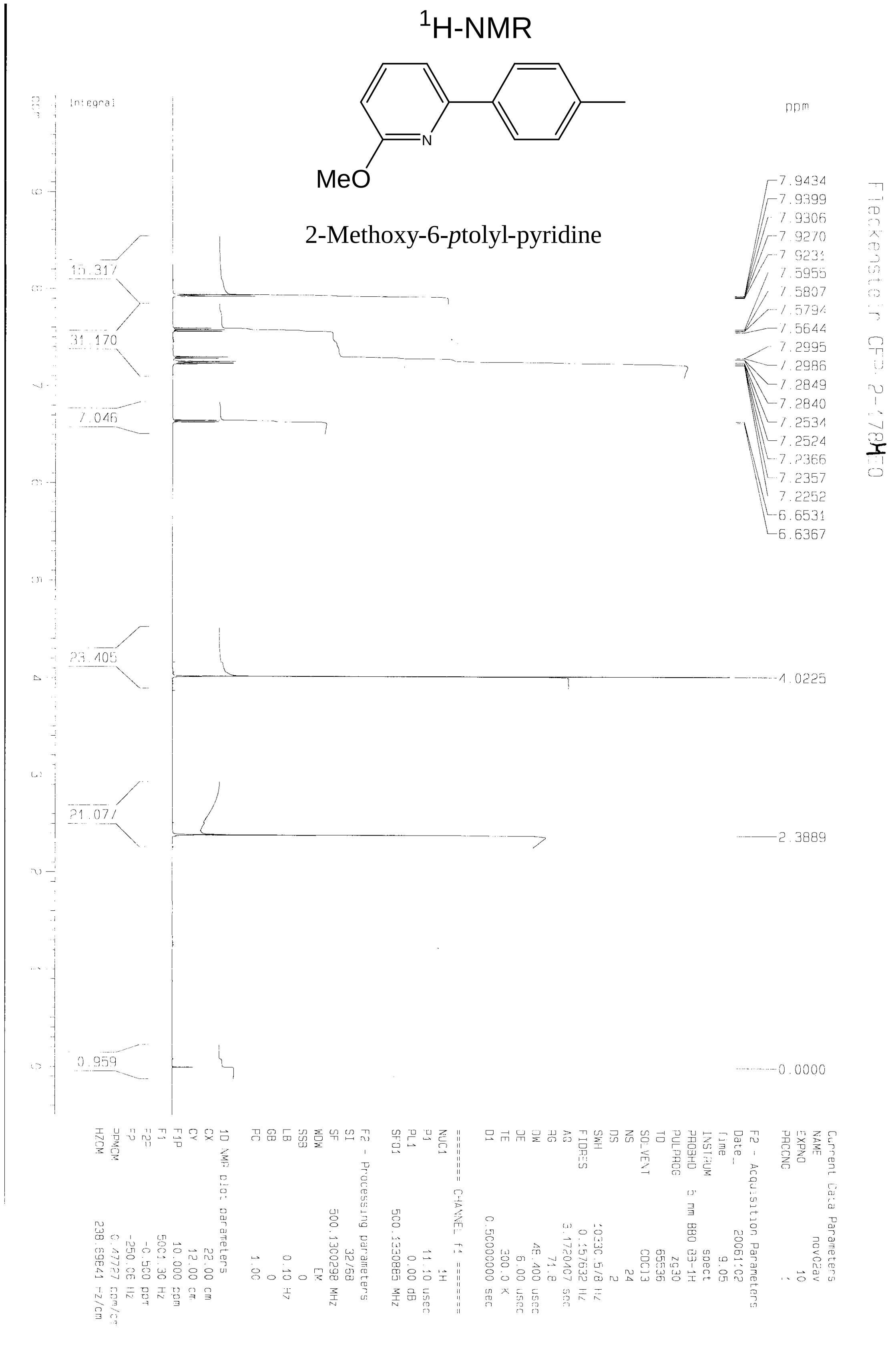

2-Methoxy-6-*p*tolyl-pyridine

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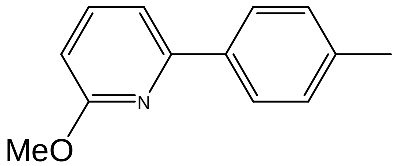

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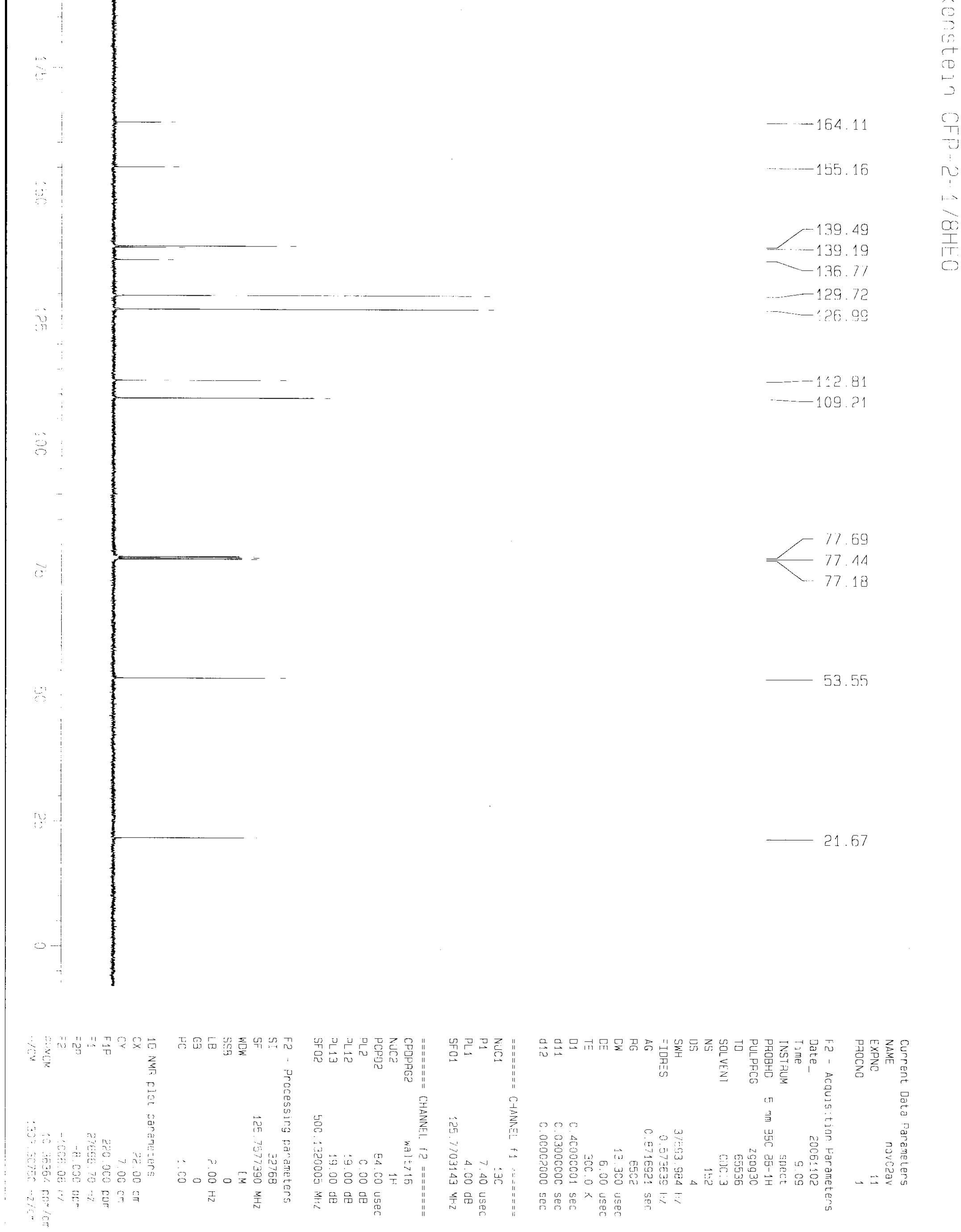
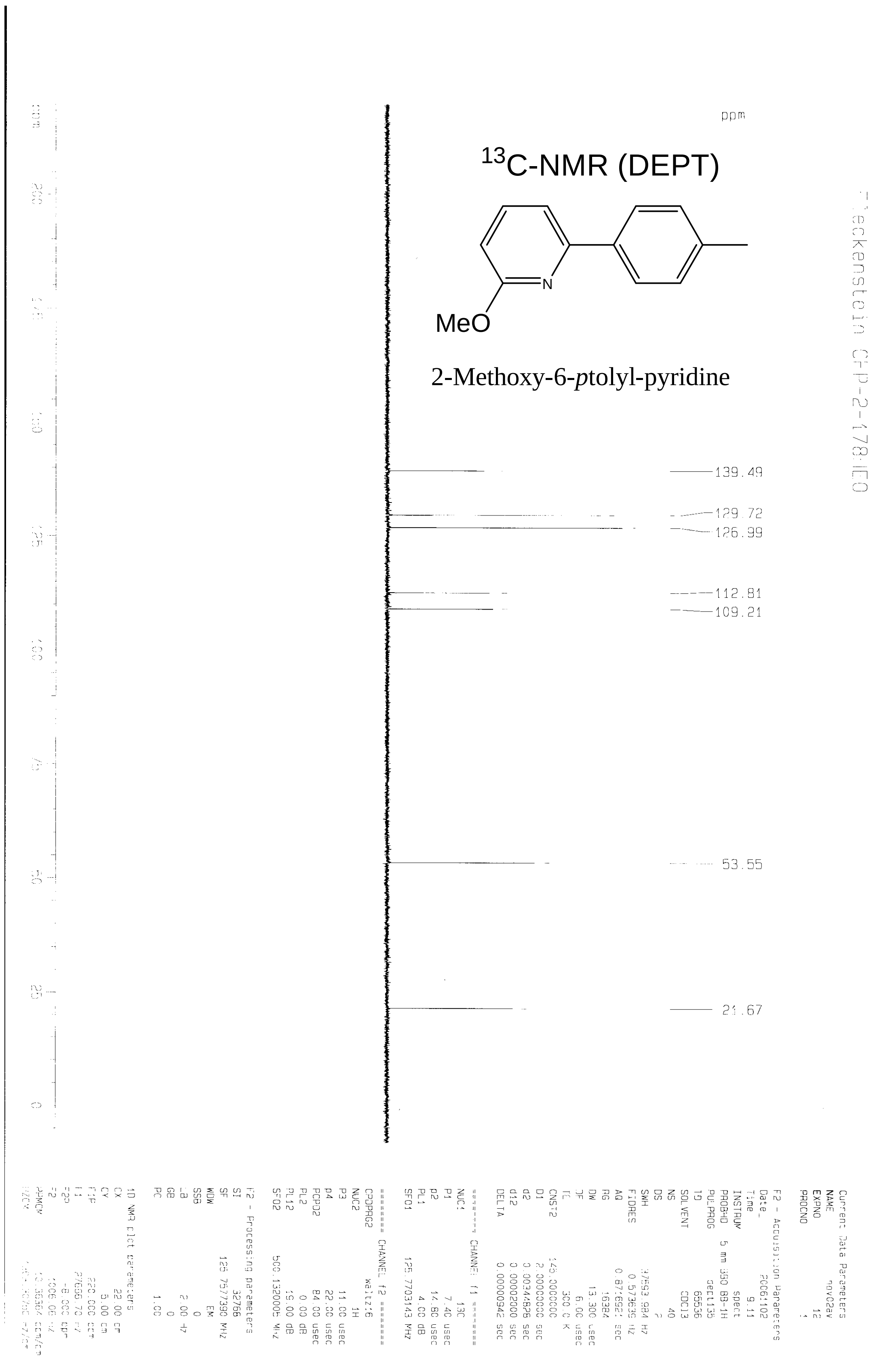
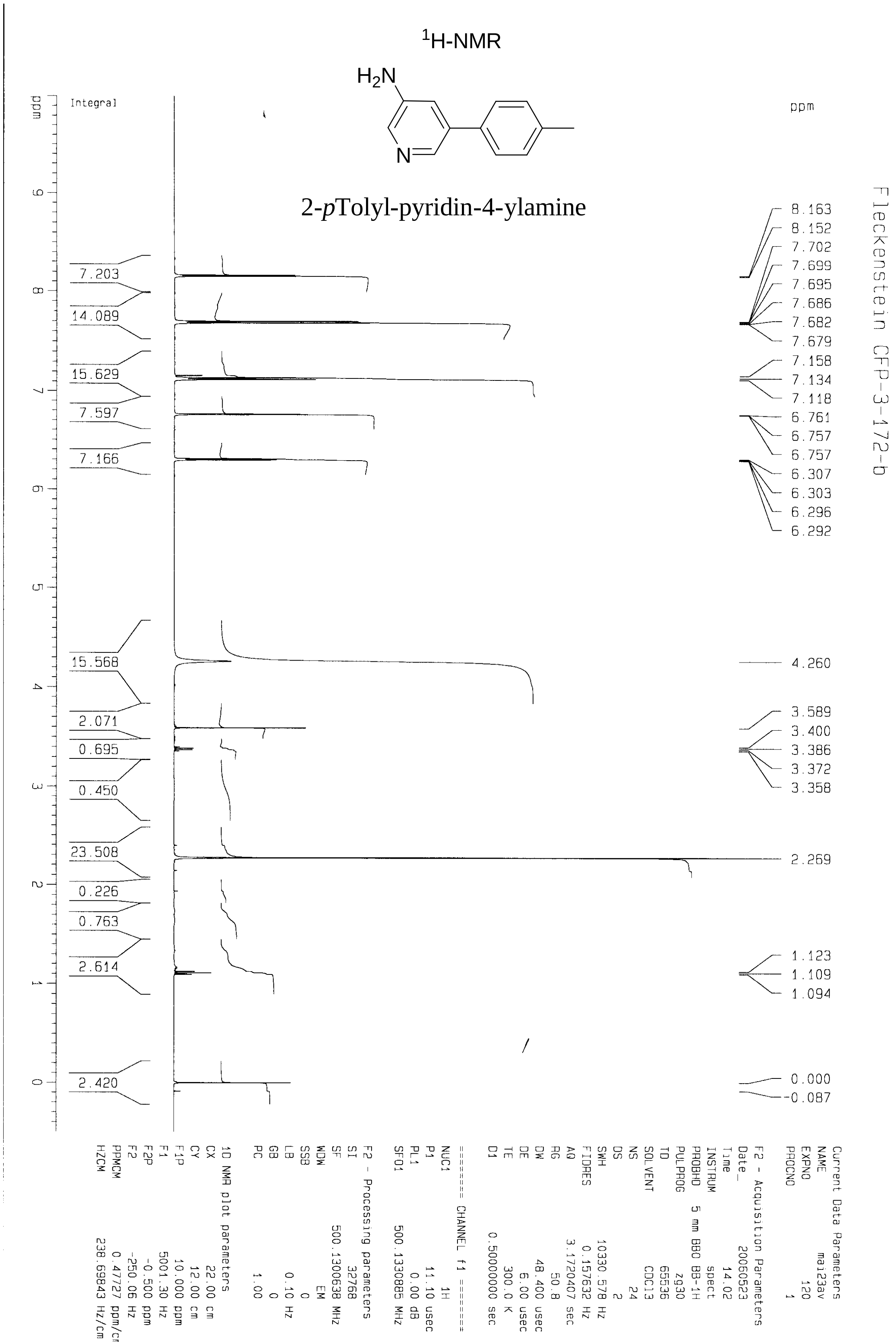




ppm
^{13}C-NMR (DEPT)
N
MeO
2-Methoxy-6-*p*tolyl-pyridine
139.49
129.72
126.99
112.81
109.21
53.55
21.67

^{1}H-NMR

2-*p*Tolyl-pyridin-4-ylamine



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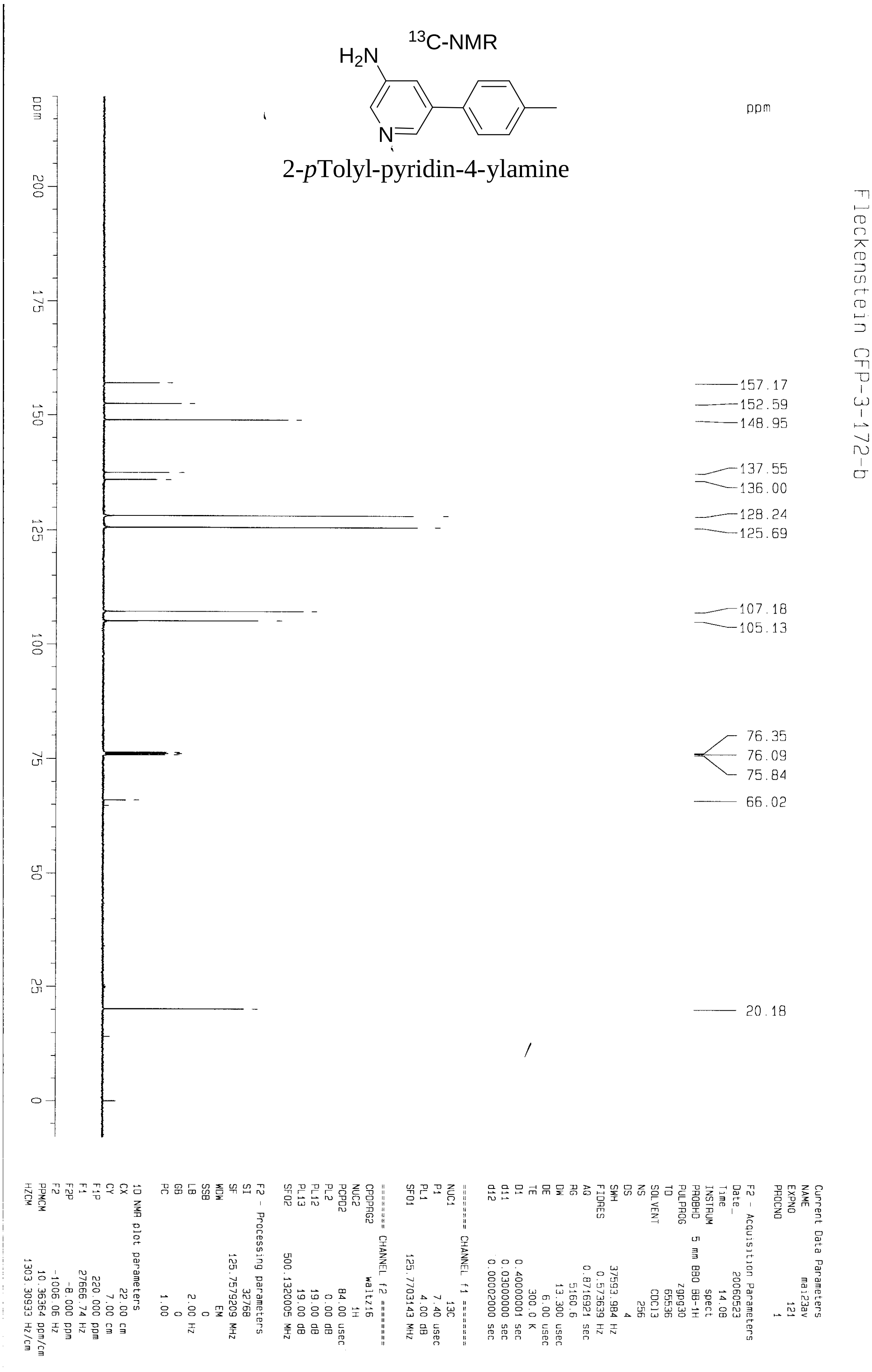
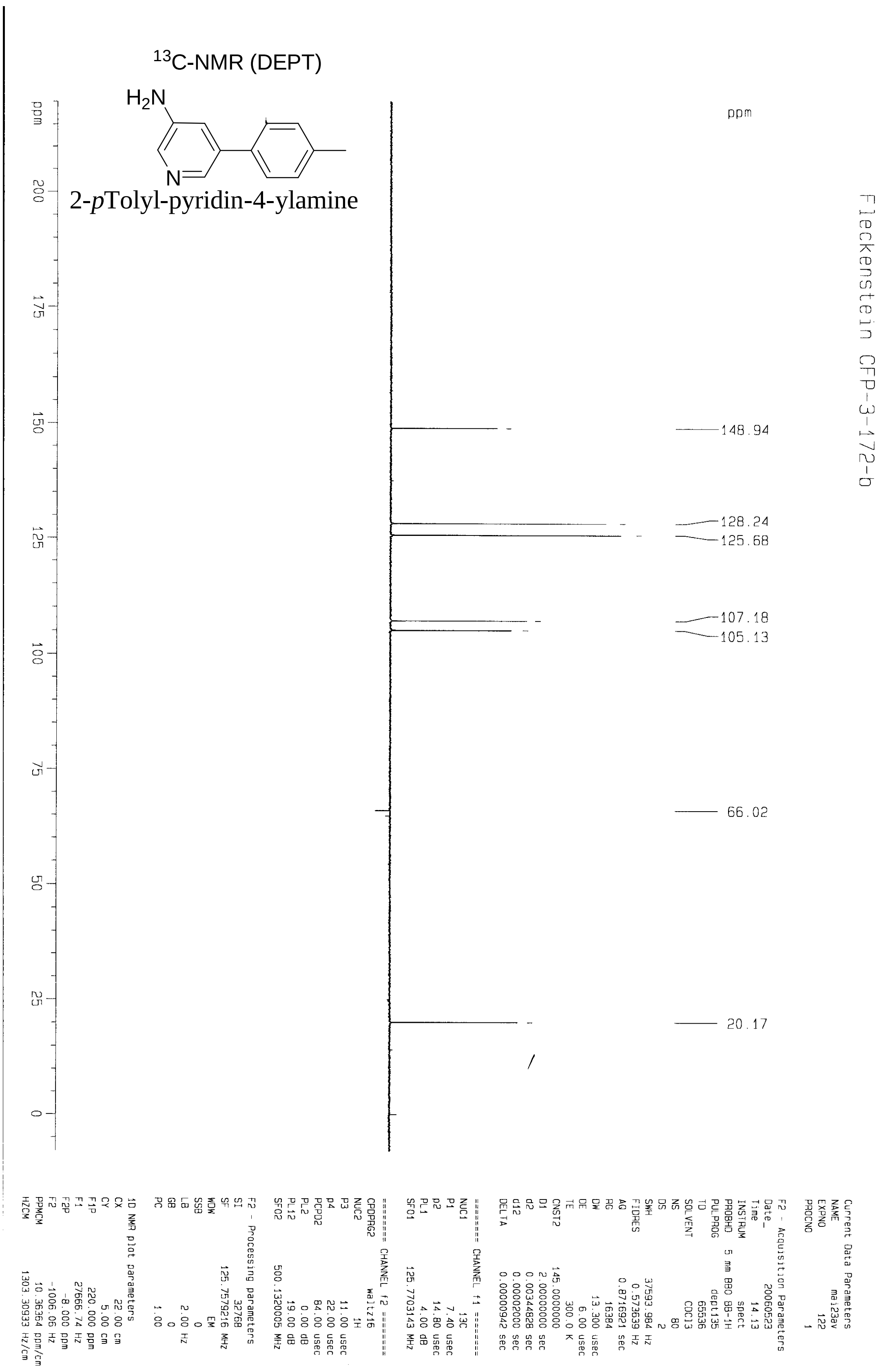


2-*p*Tolyl-pyridin-4-ylamine

^{13}C-NMR (DEPT)

2-*p*Tolyl-pyridin-4-ylamine



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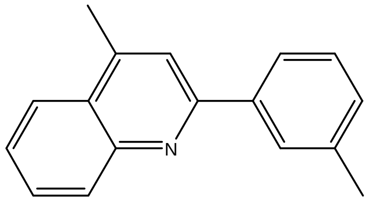
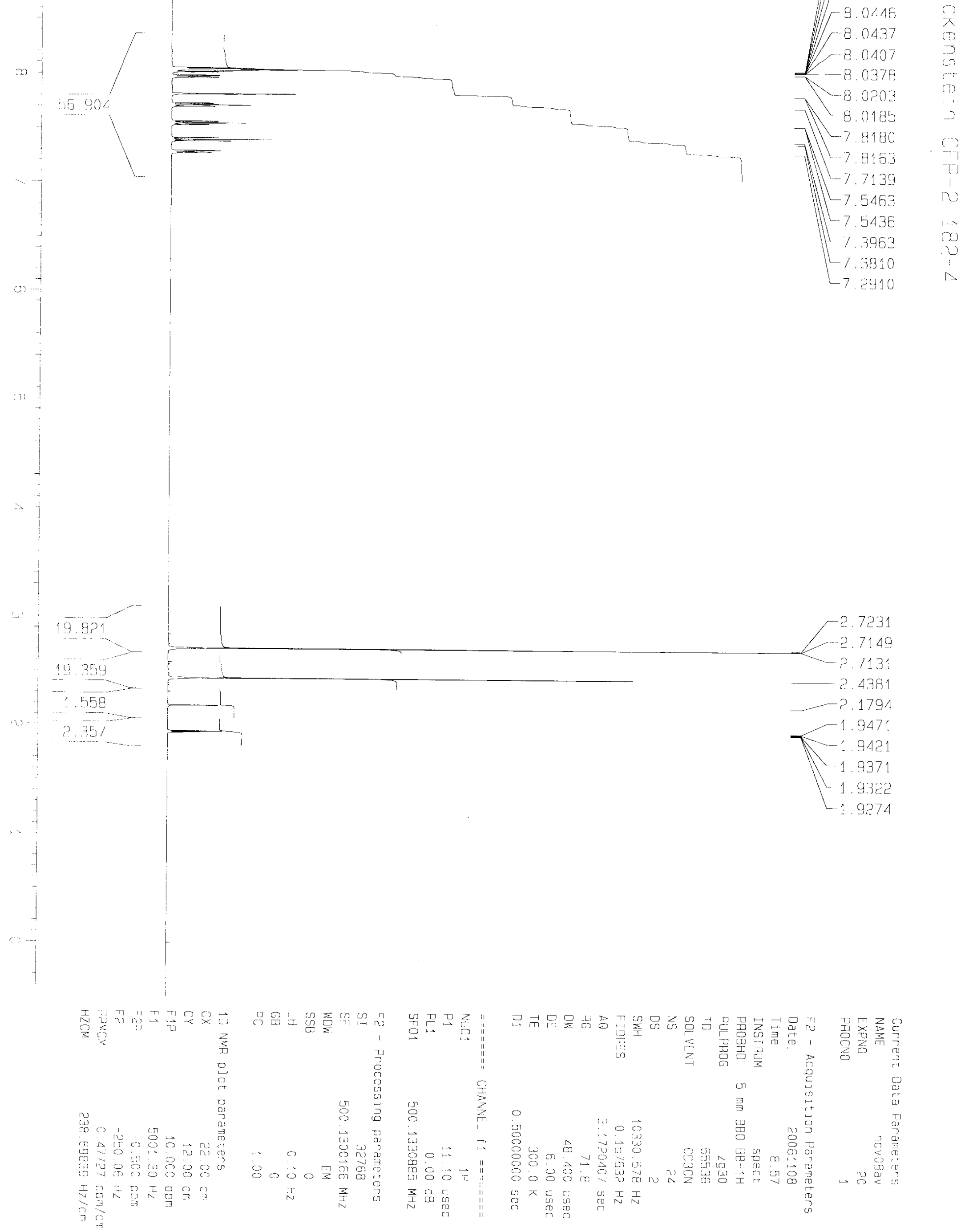


4-Methyl-2-*m*tolyl-quinoline



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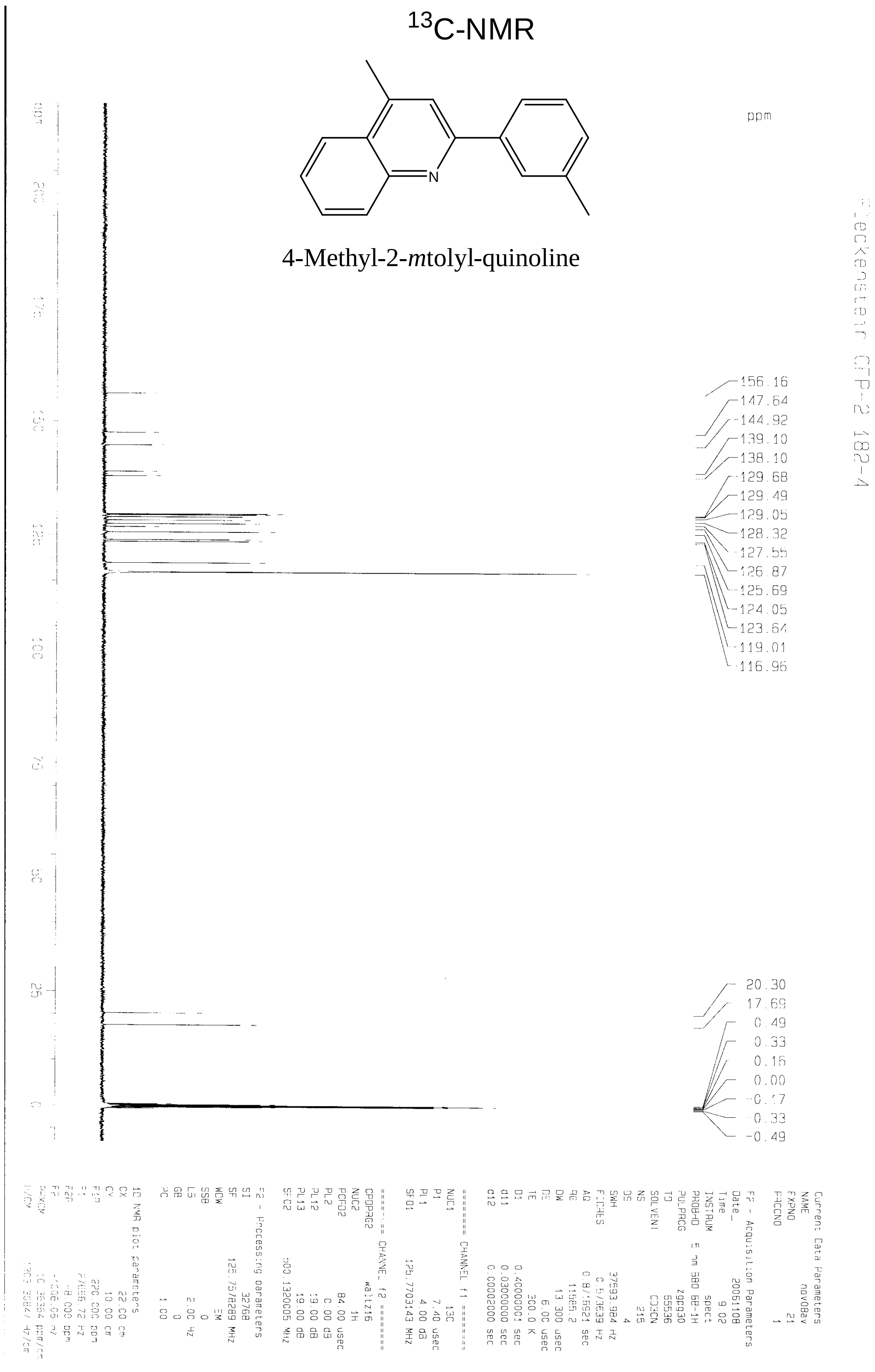

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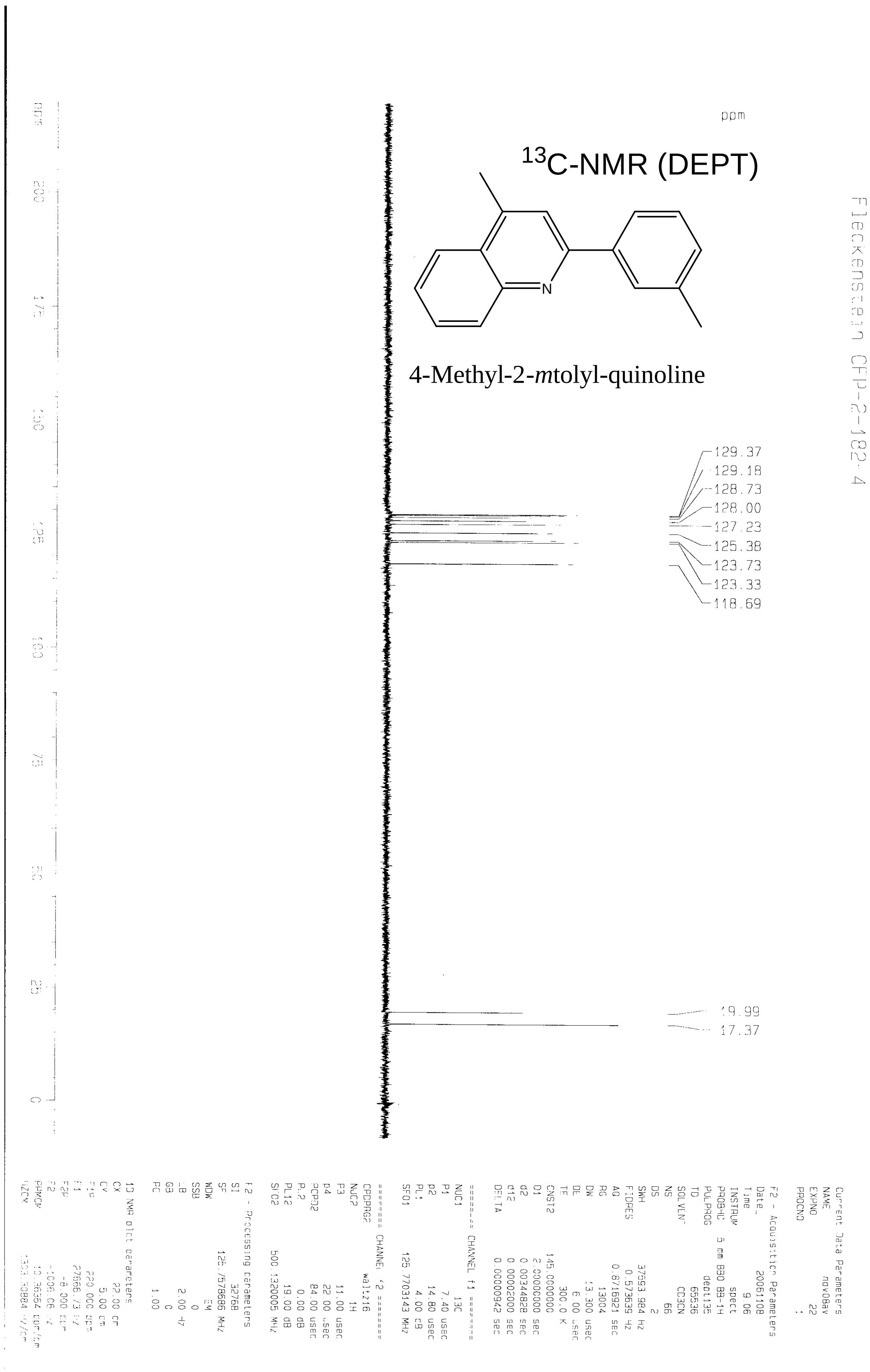
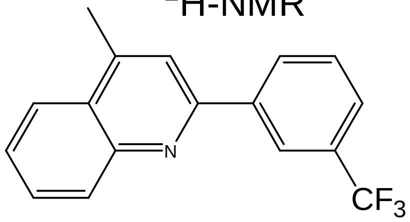


^{13}C-NMR (DEPT)

4-Methyl-2-*m*tolyl-quinoline

^{1}H-NMR



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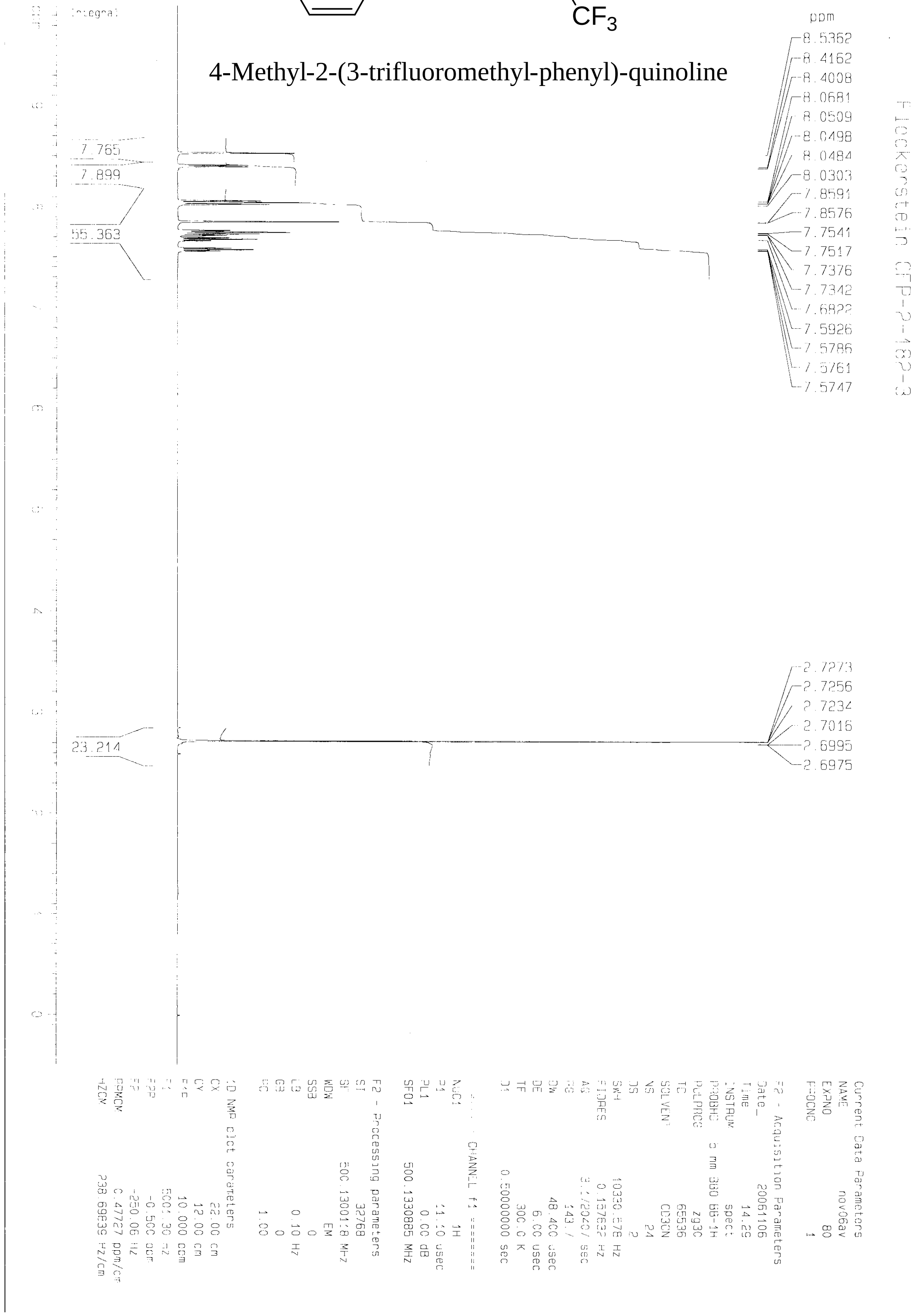

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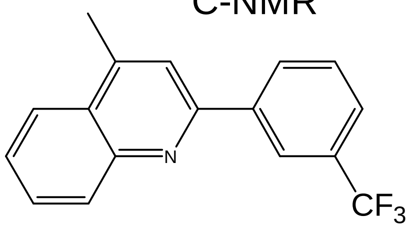

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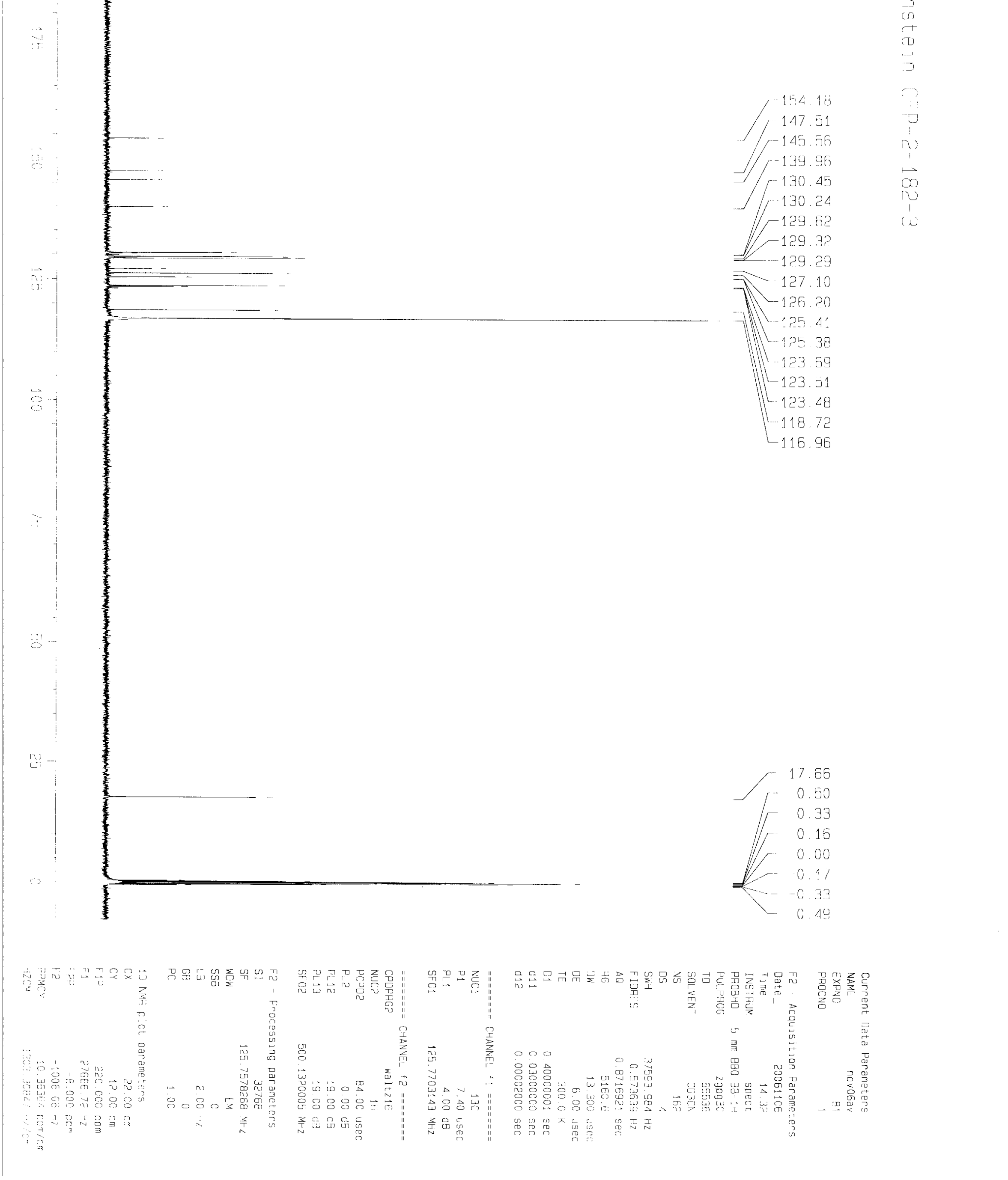

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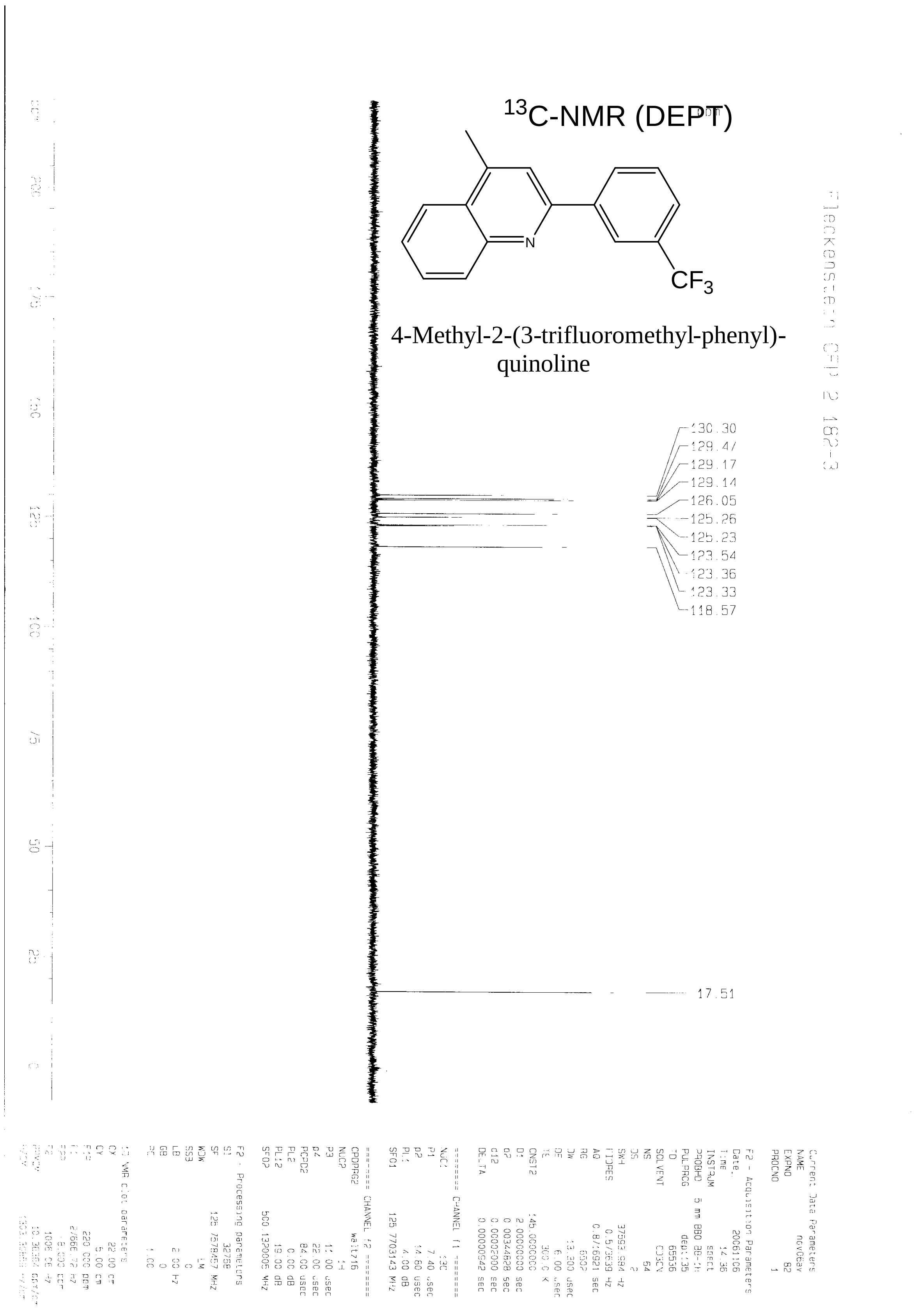

4-Methyl-2-(3-trifluoromethyl-phenyl)-quinoline

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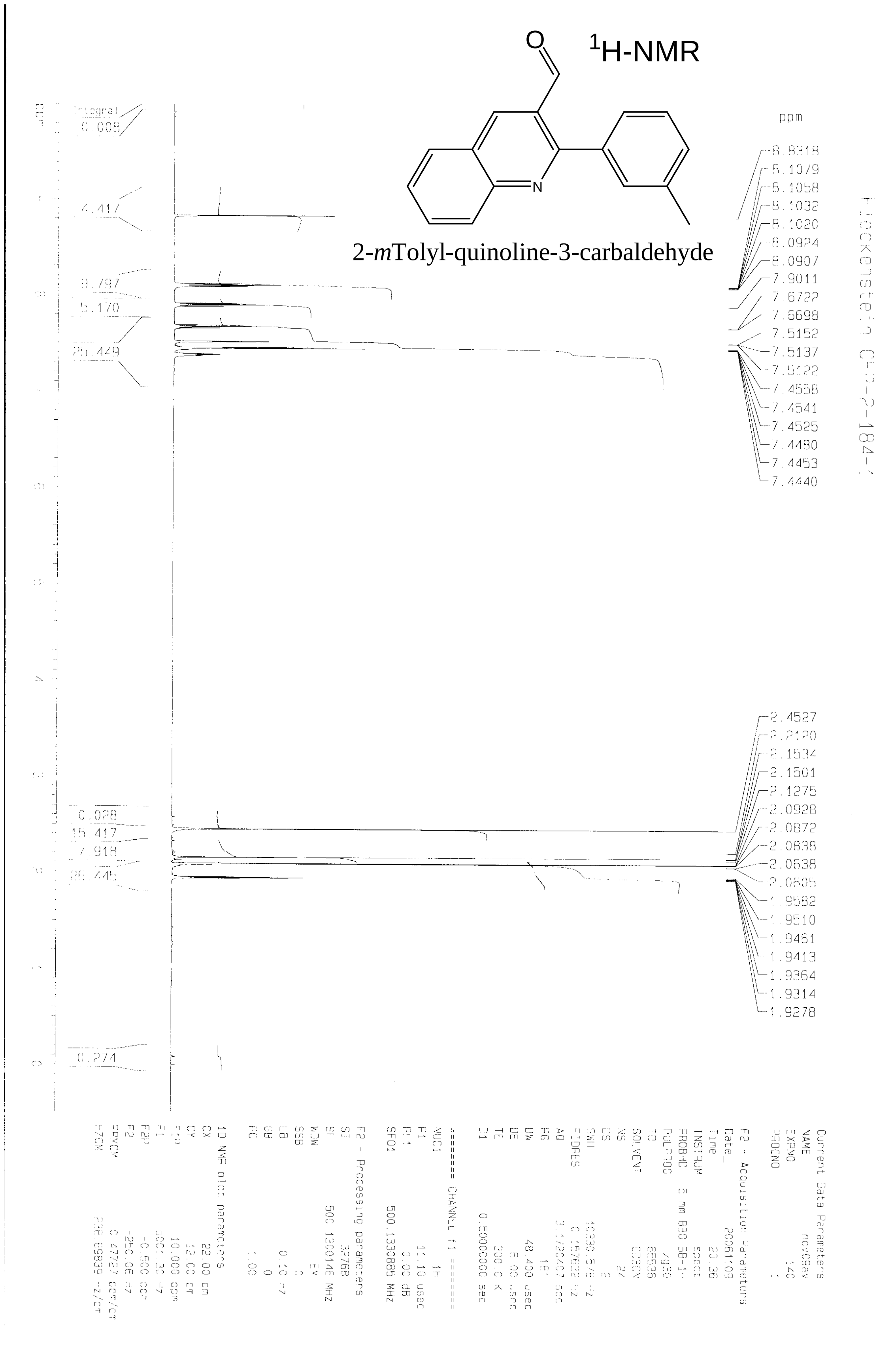
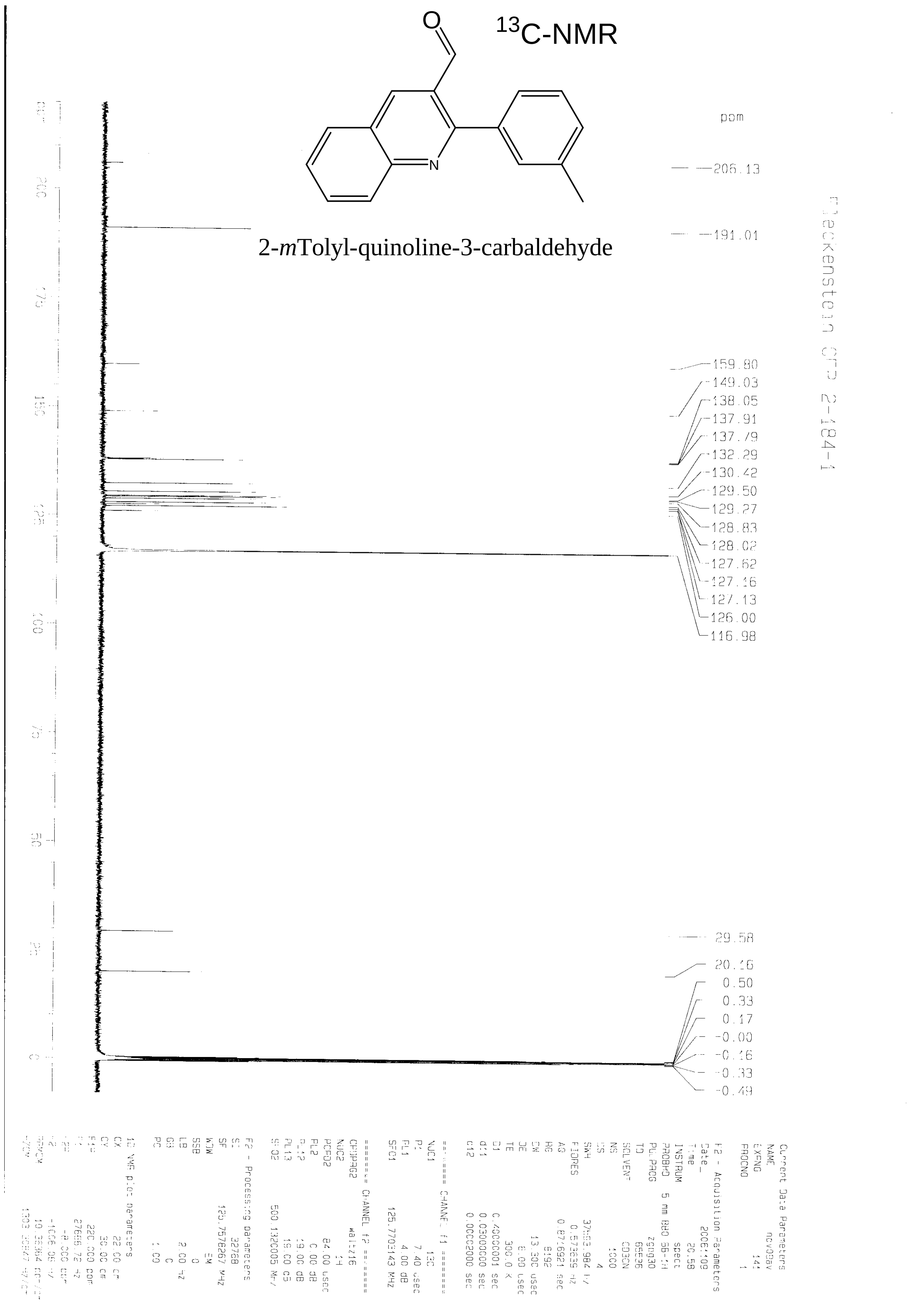


2-*m*Tolyl-quinoline-3-carbaldehyde



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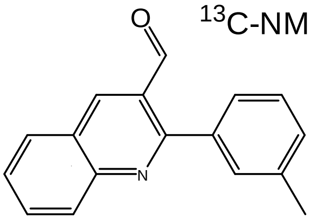

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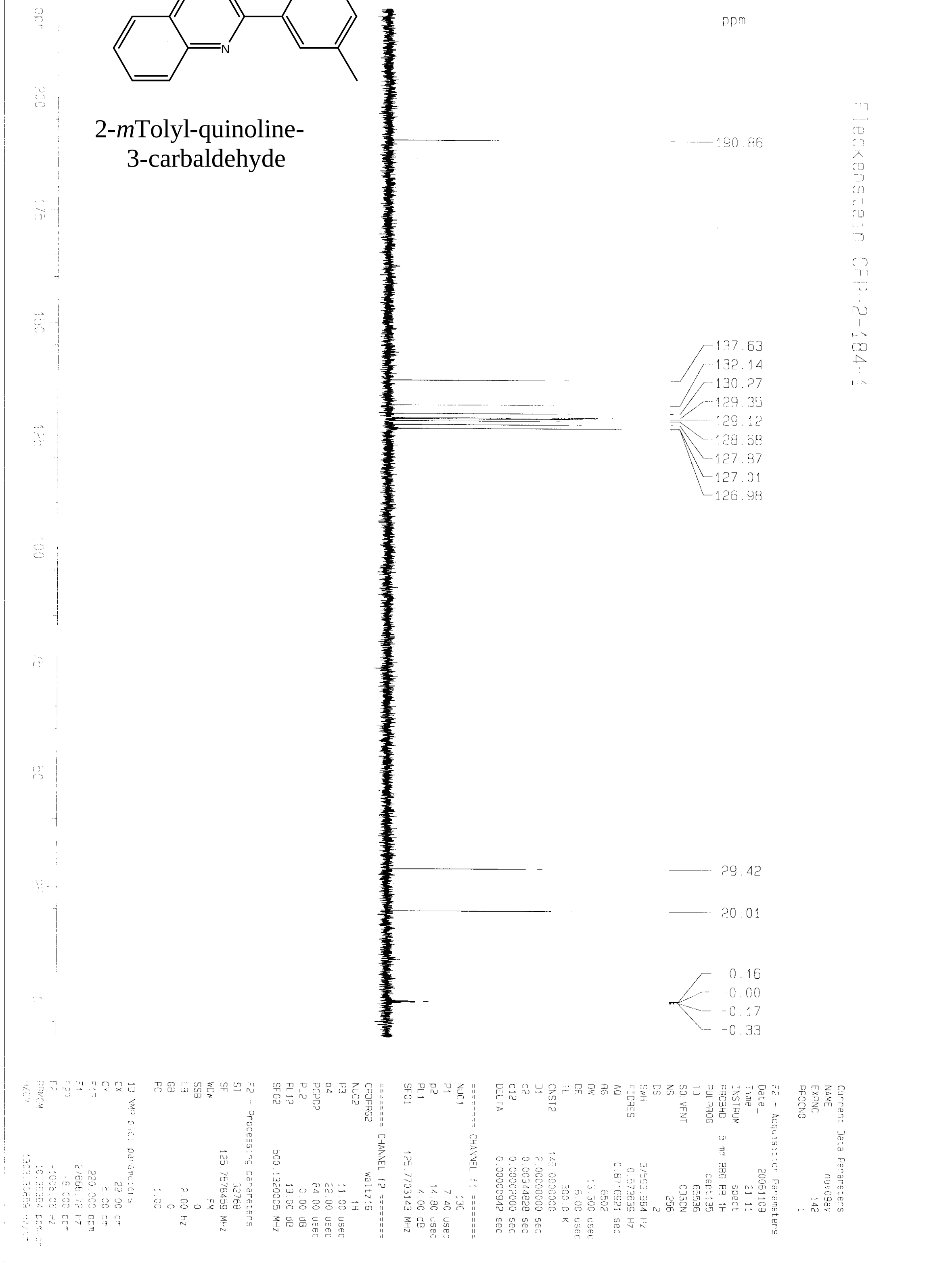
2-*m*Tolyl-quinoline-3-carbaldehyde



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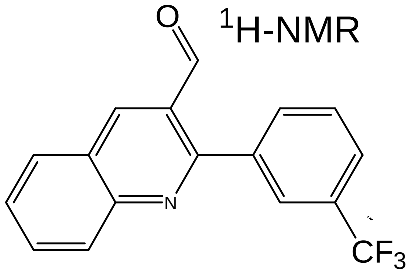

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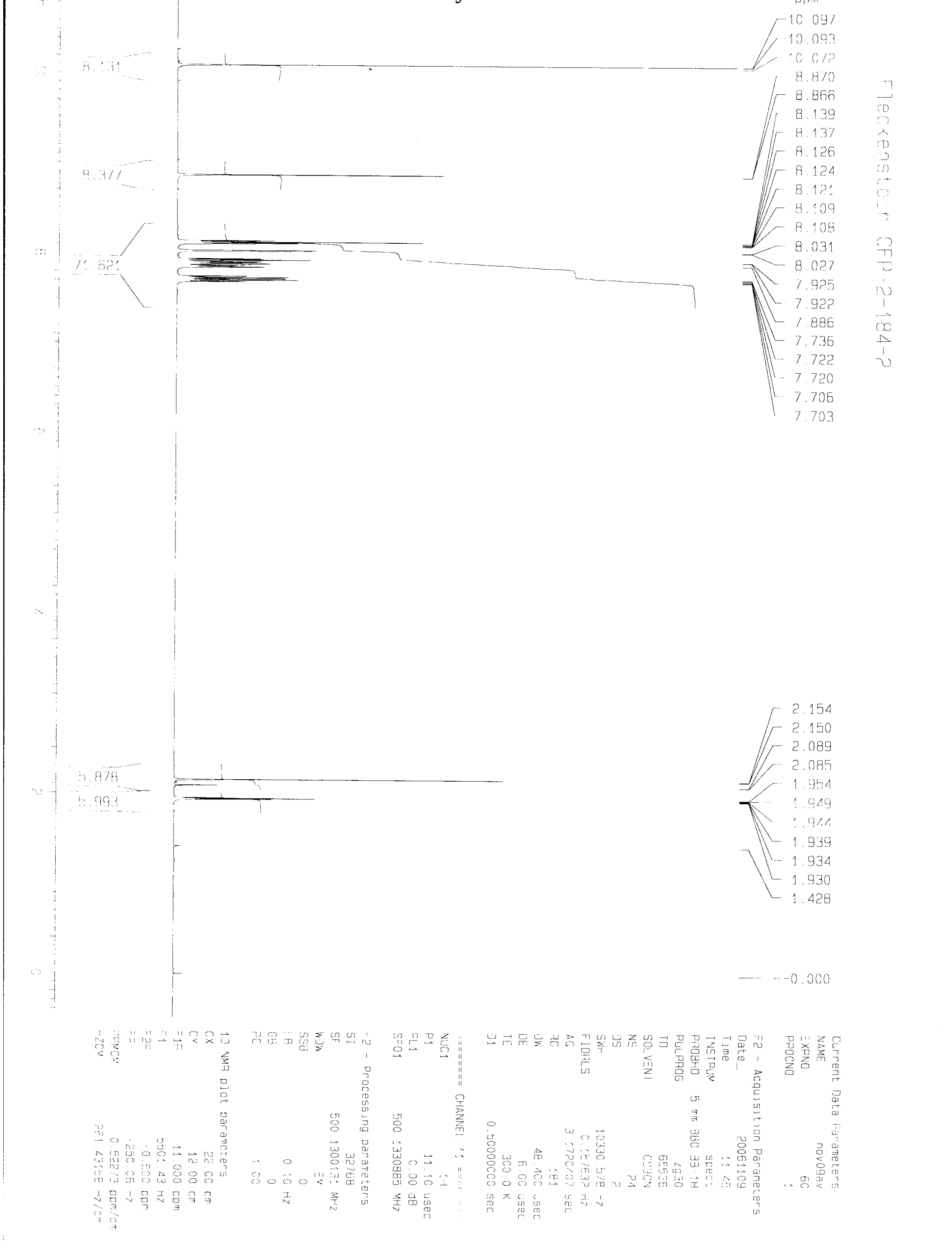

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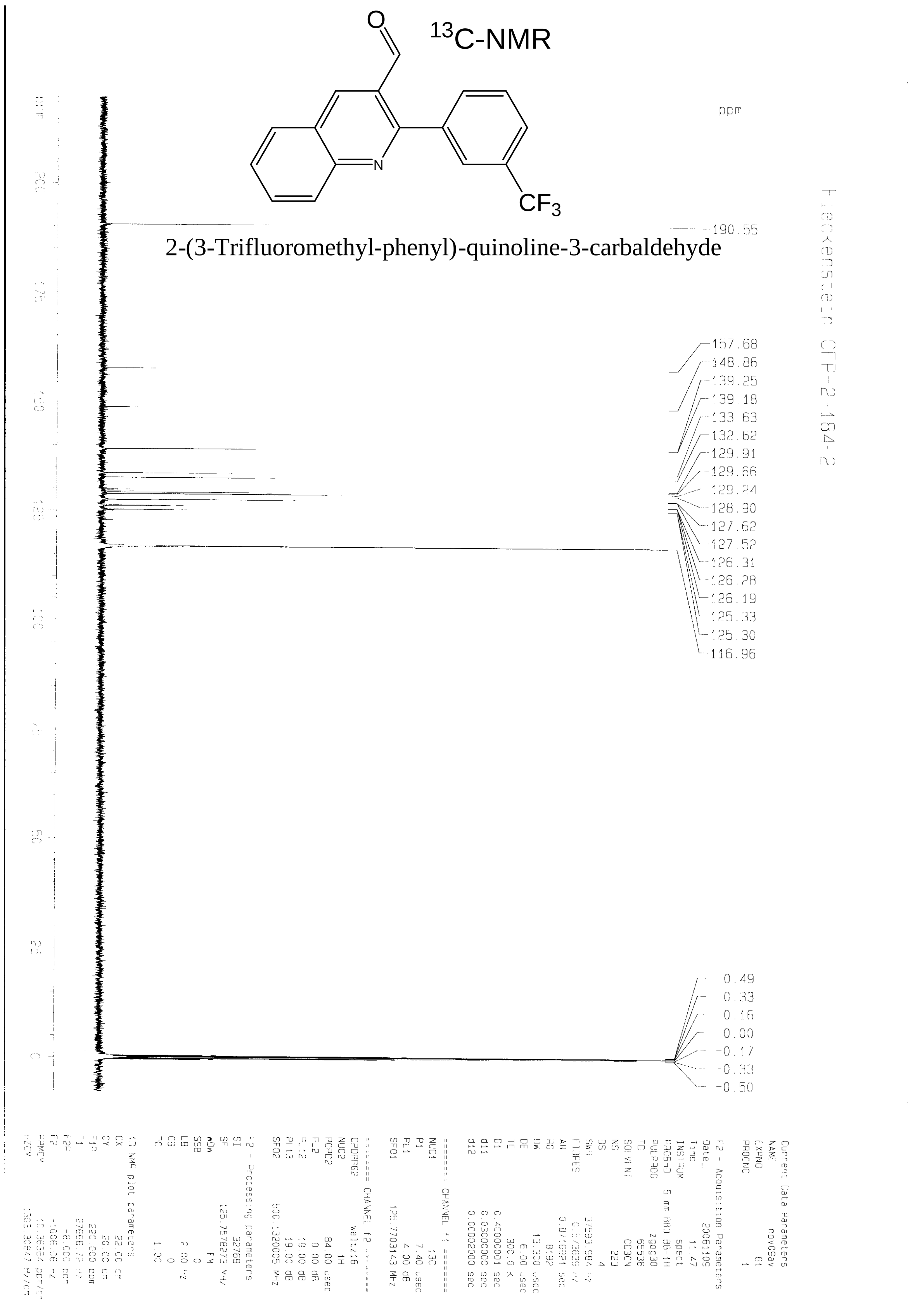

2-(3-Trifluoromethyl-phenyl)-quinoline-3-carbaldehyde

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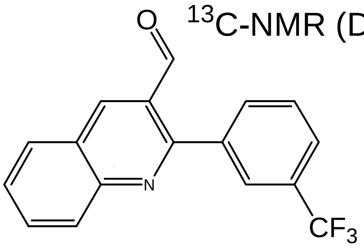
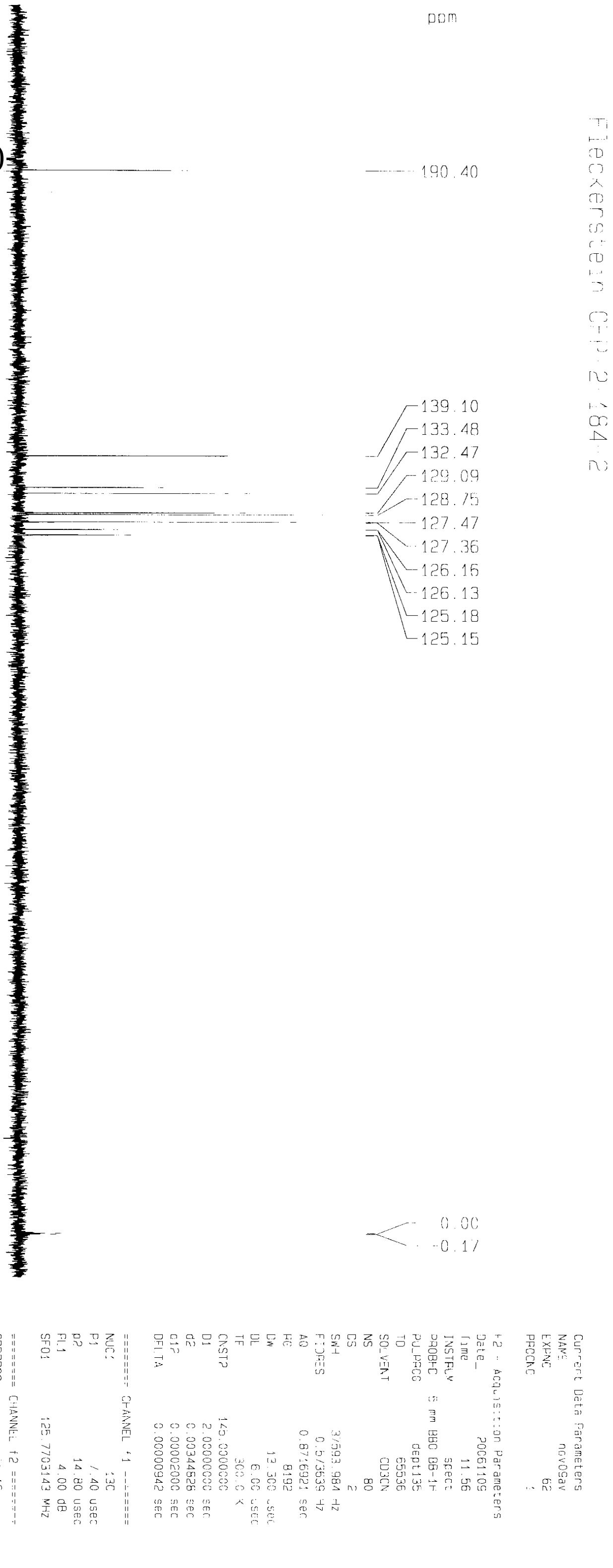
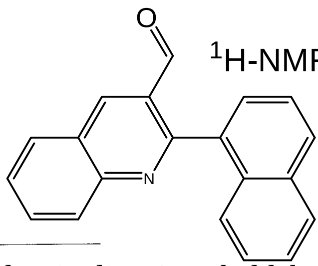


2-(3-Trifluoromethyl-phenyl)-quinoline-3-carbaldehyde





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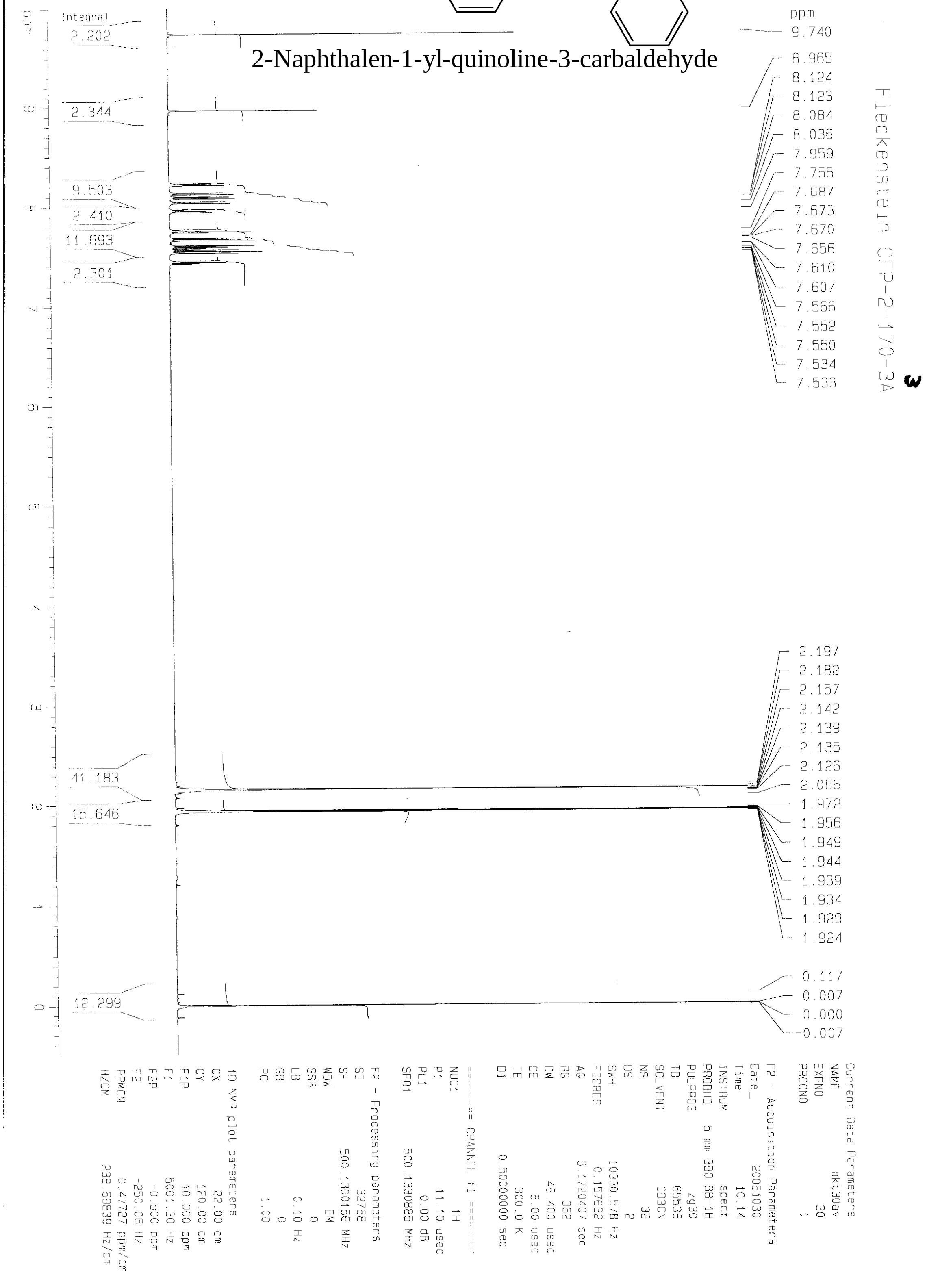
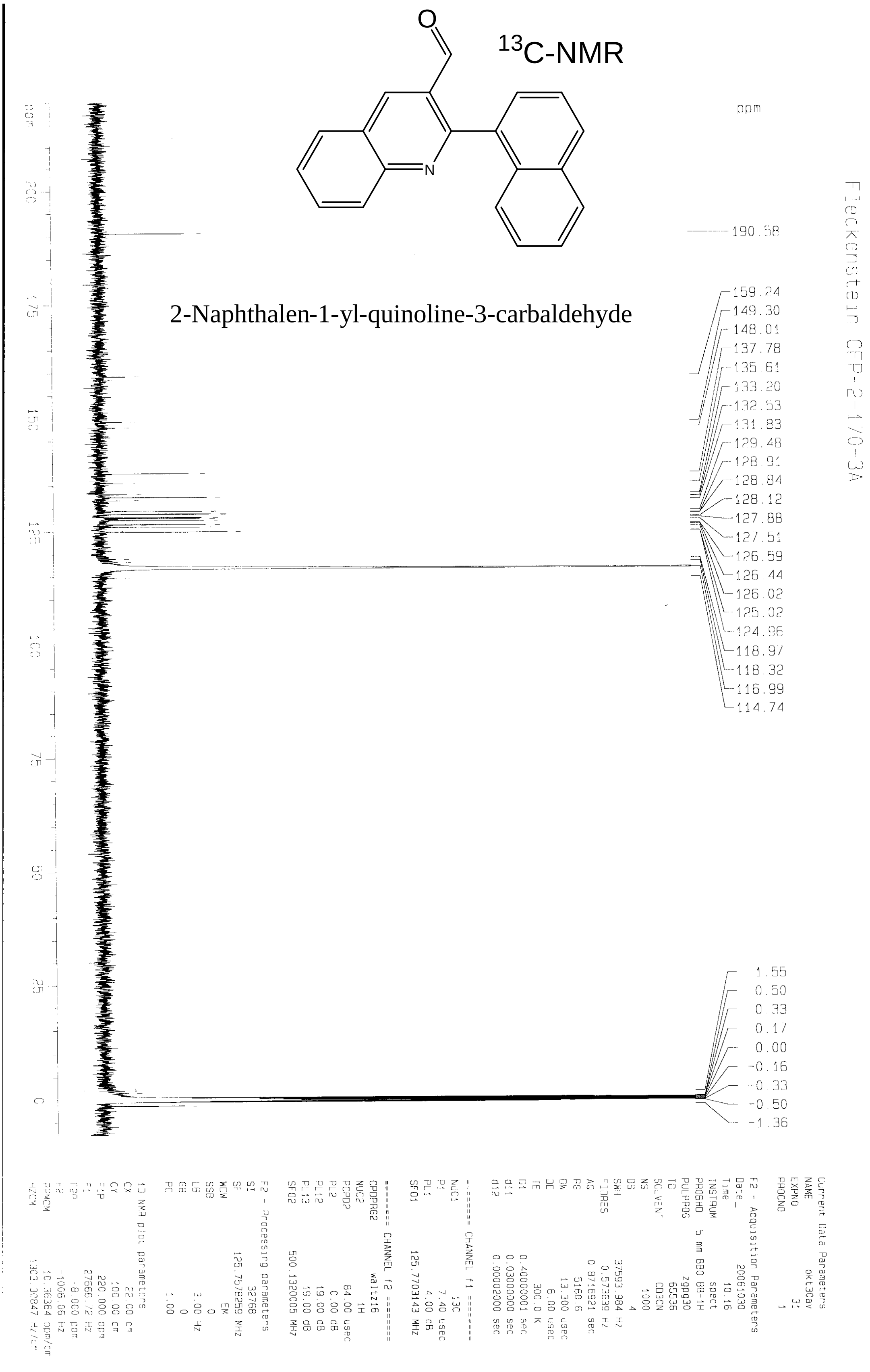


2-Naphthalen-1-yl-quinoline-3-carbaldehyde

^{13}C-NMR

2-Naphthalen-1-yl-quinoline-3-carbaldehyde



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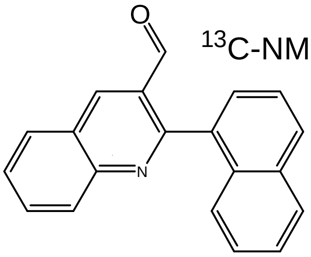
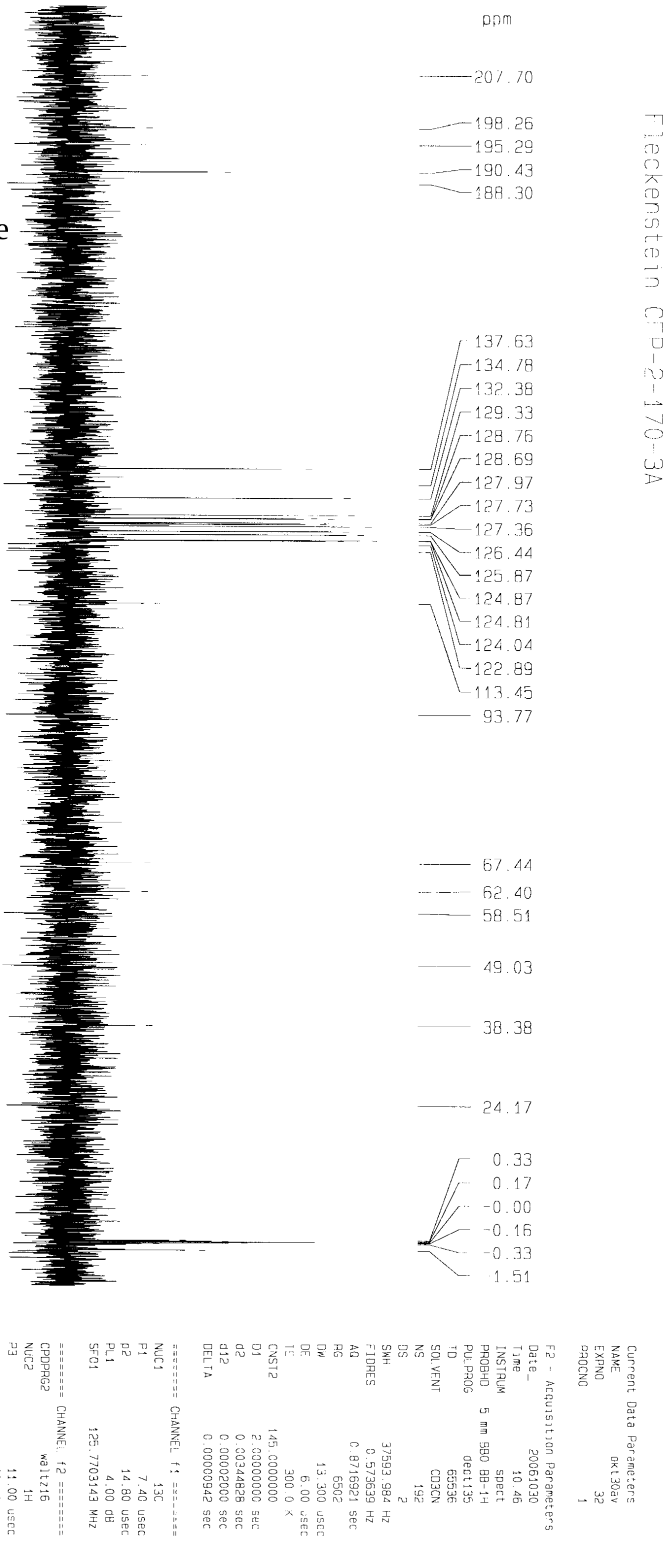


2-Naphthalen-1-yl-quinoline-3-carbaldehyde



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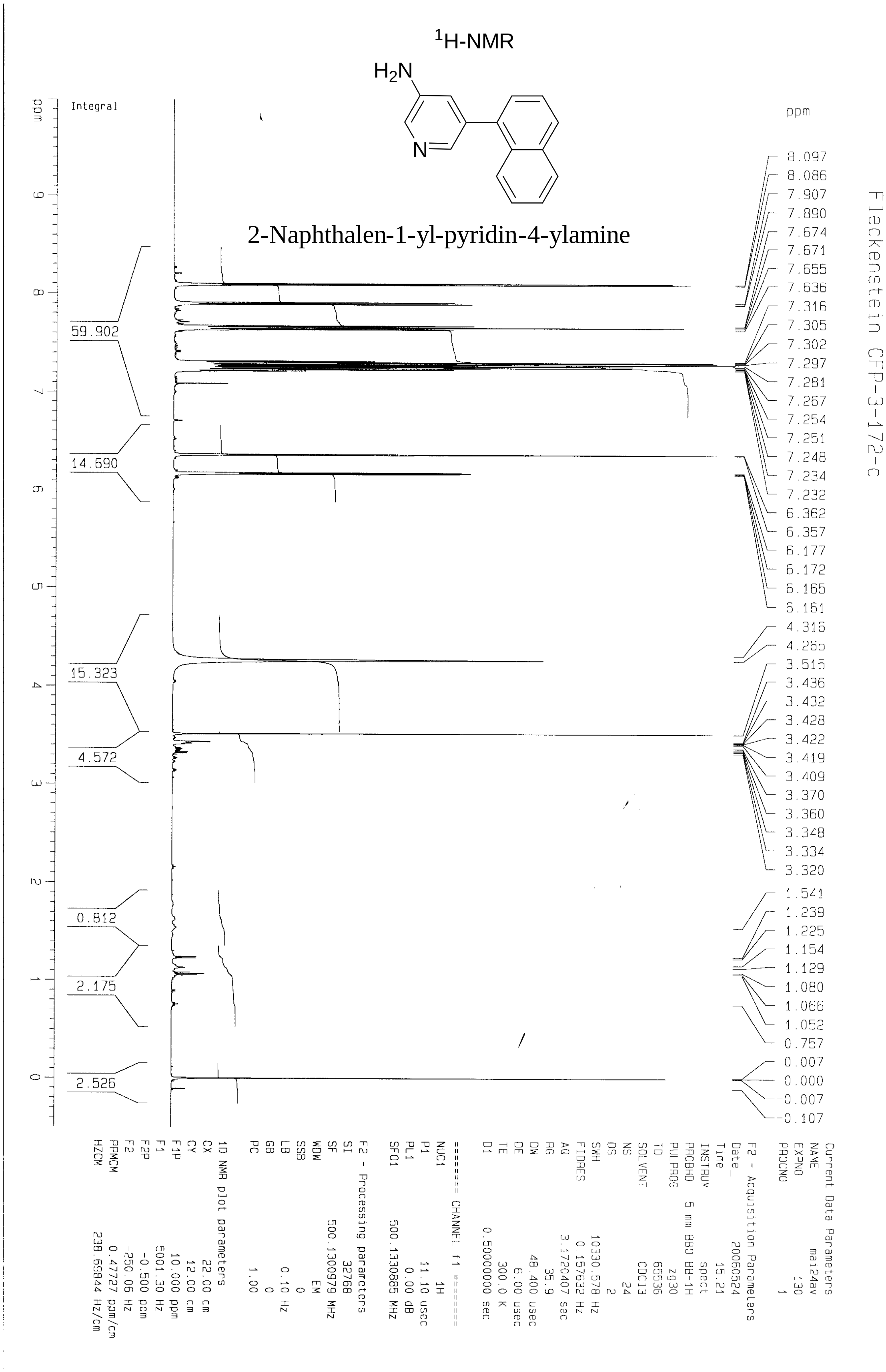

2-Naphthalen-1-yl-pyridin-4-ylamine

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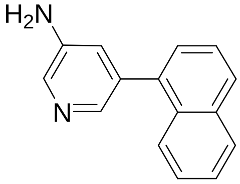
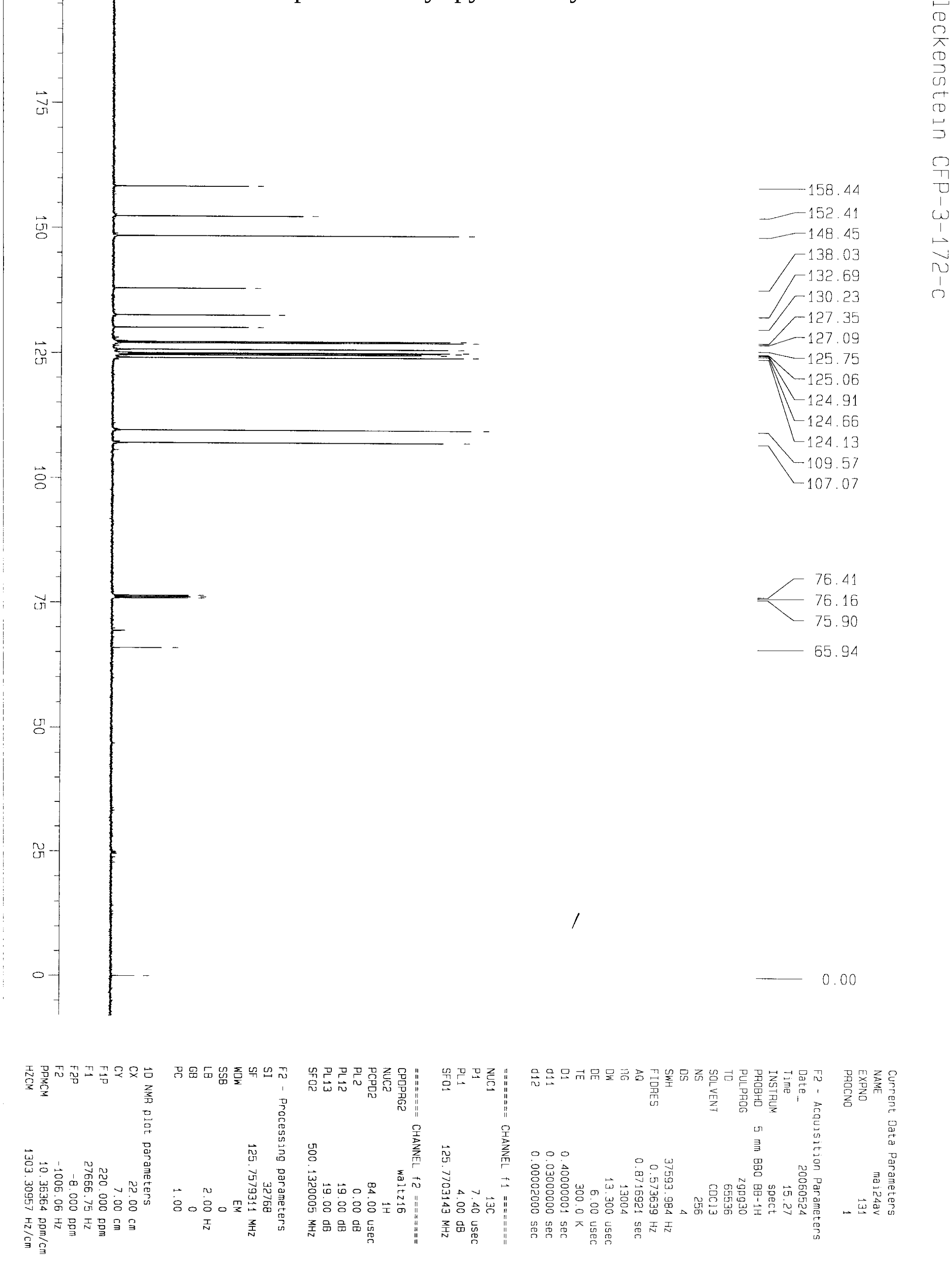


2-Naphthalen-1-yl-pyridin-4-ylamine



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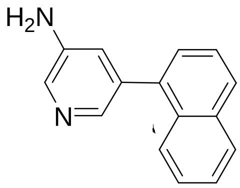

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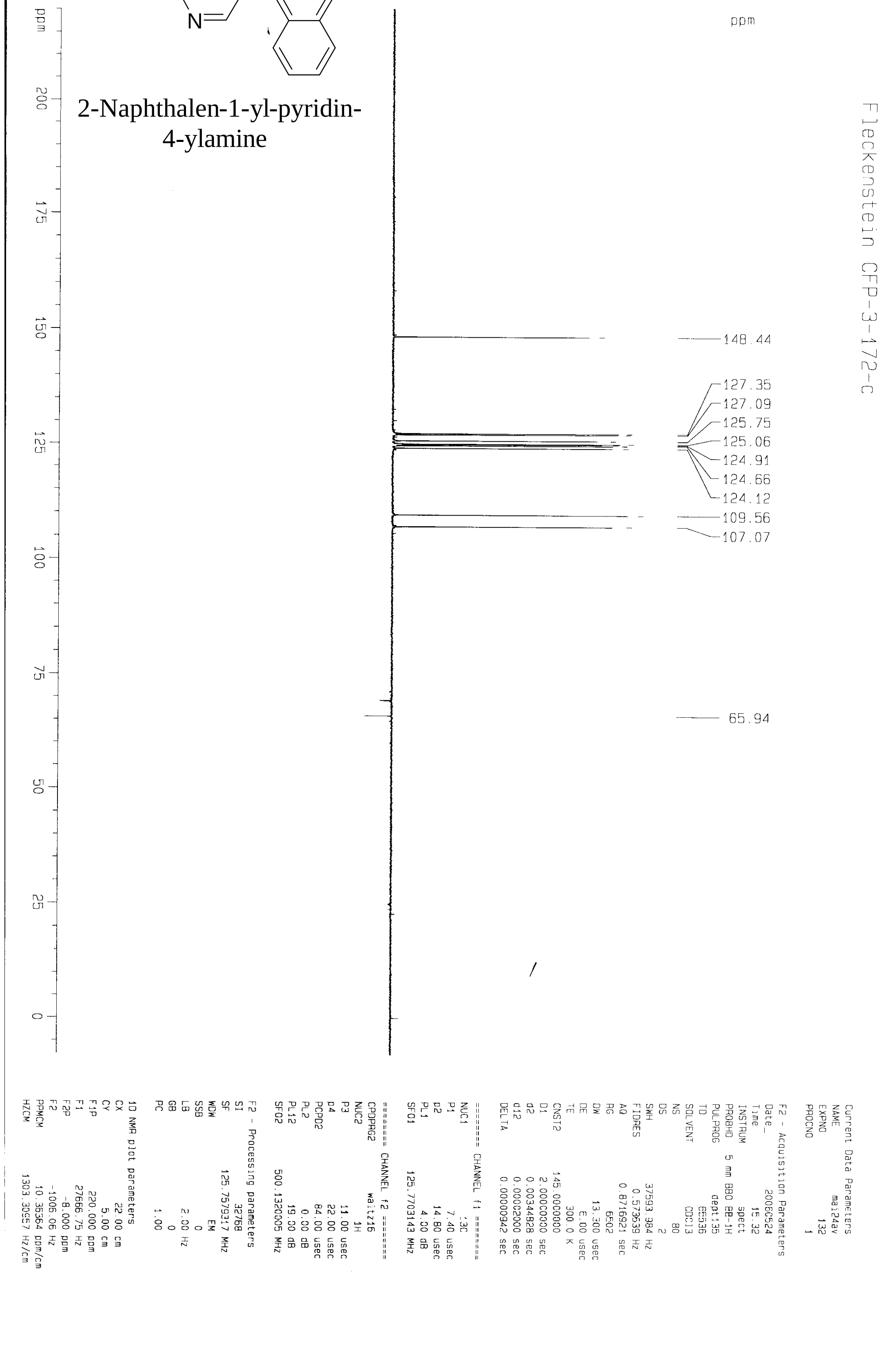
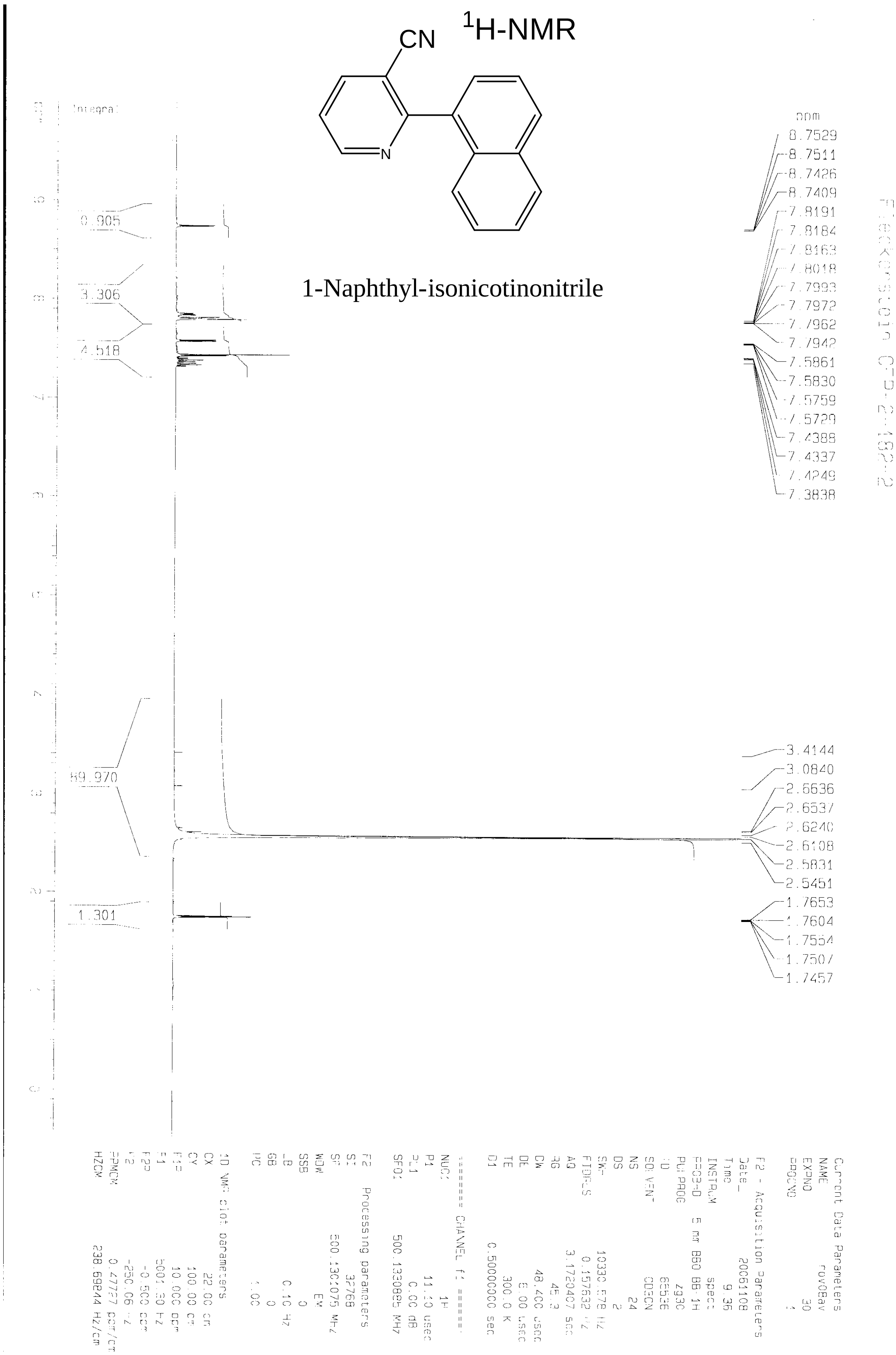
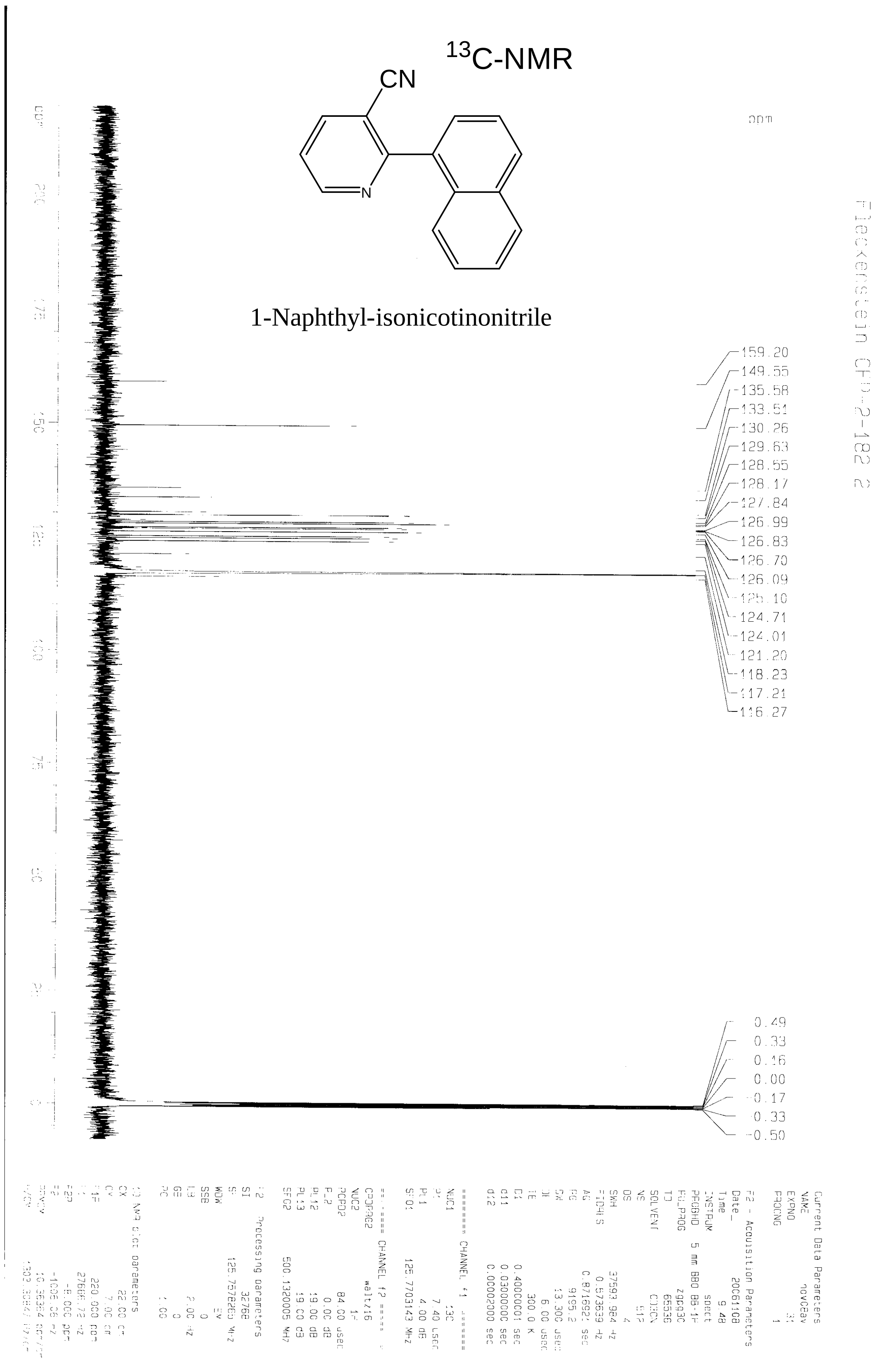


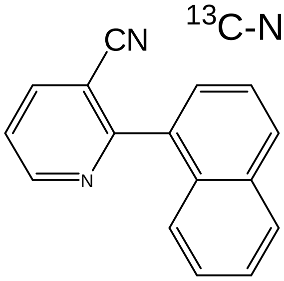


1-Naphthyl-isonicotinonitrile

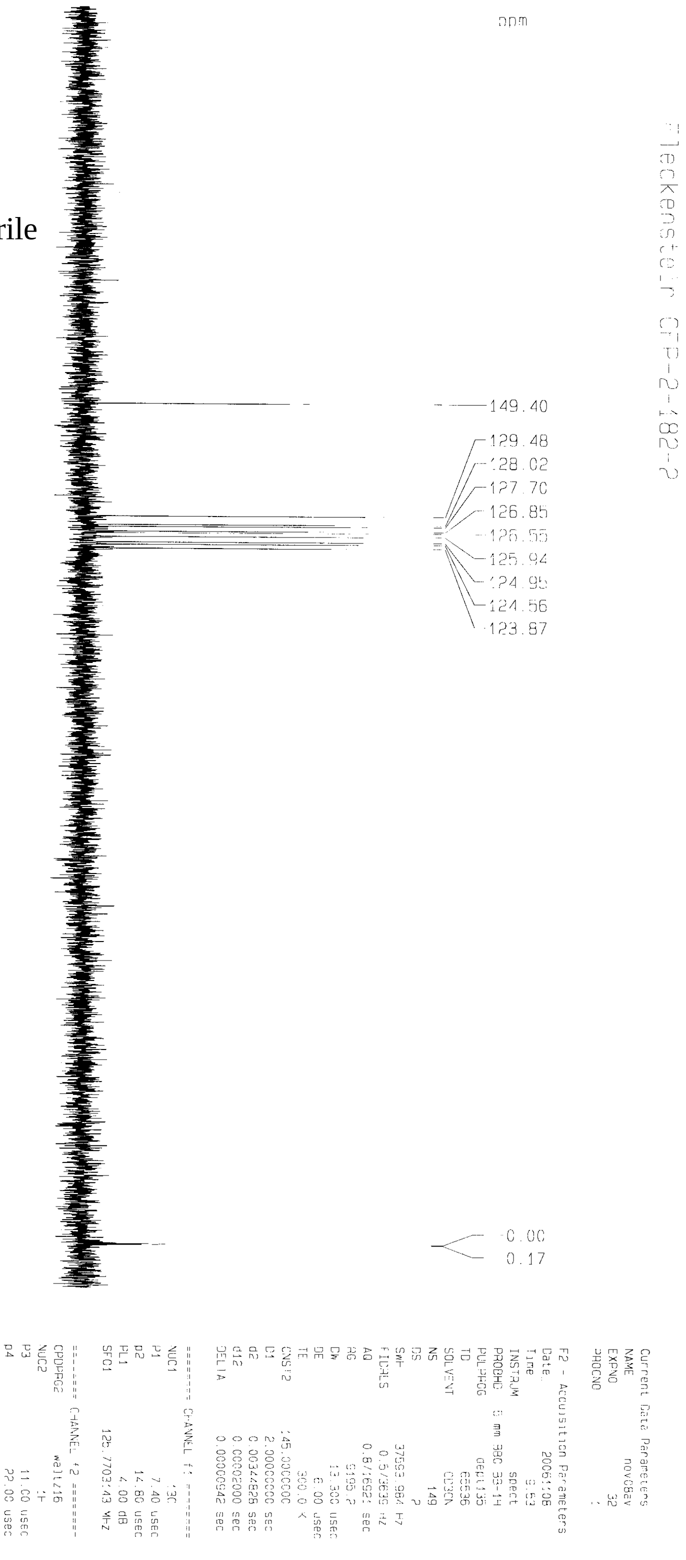


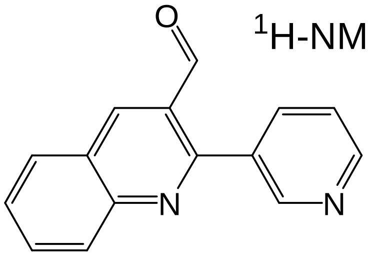
1-Naphthyl-isonicotinonitrile

^{13}C-NMR (DEPT)



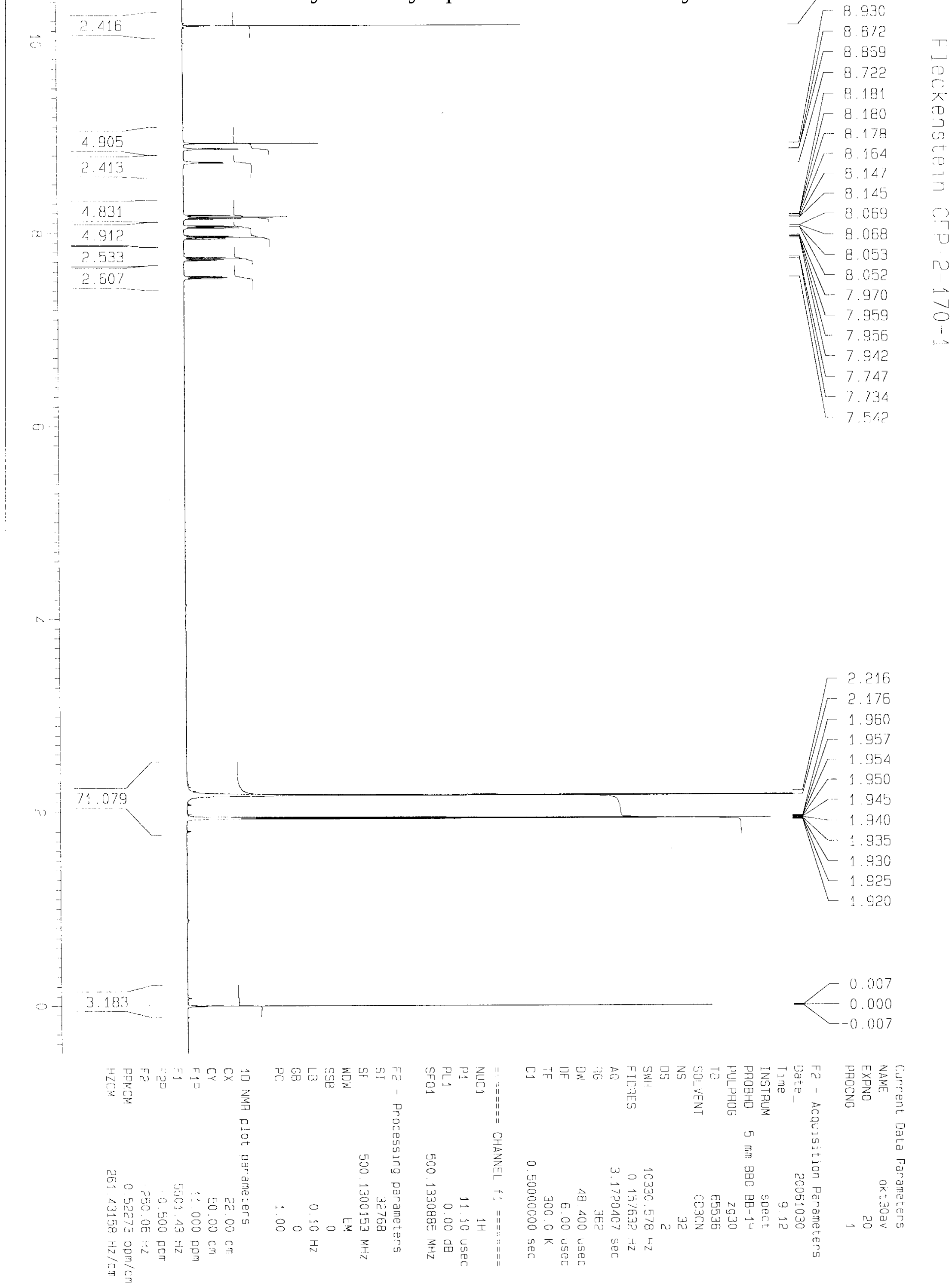
1-Naphthyl-isonicotinonitrile





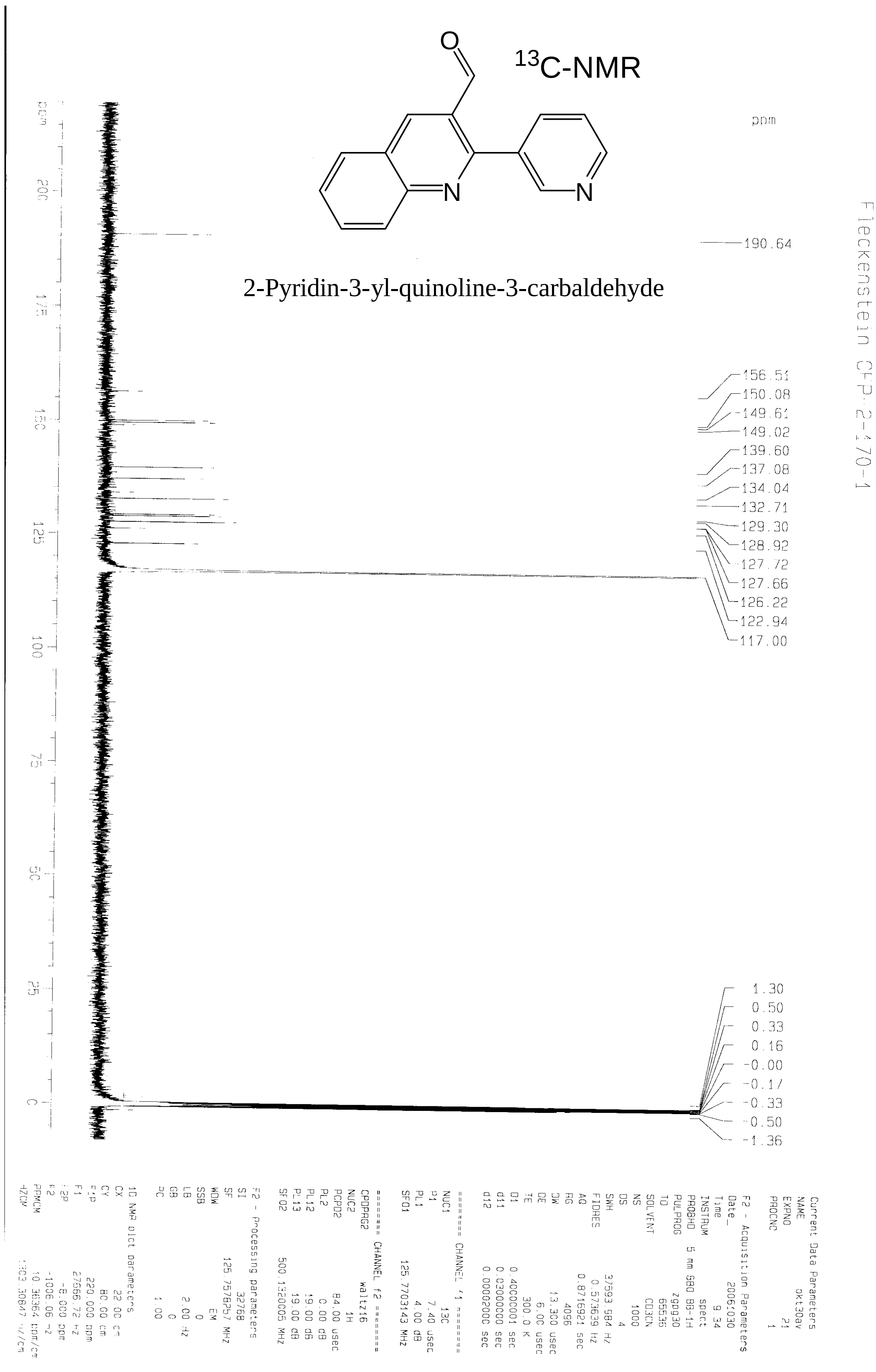
^{1}H-NMR

2-Pyridin-3-yl-quinoline-3-carbaldehyde

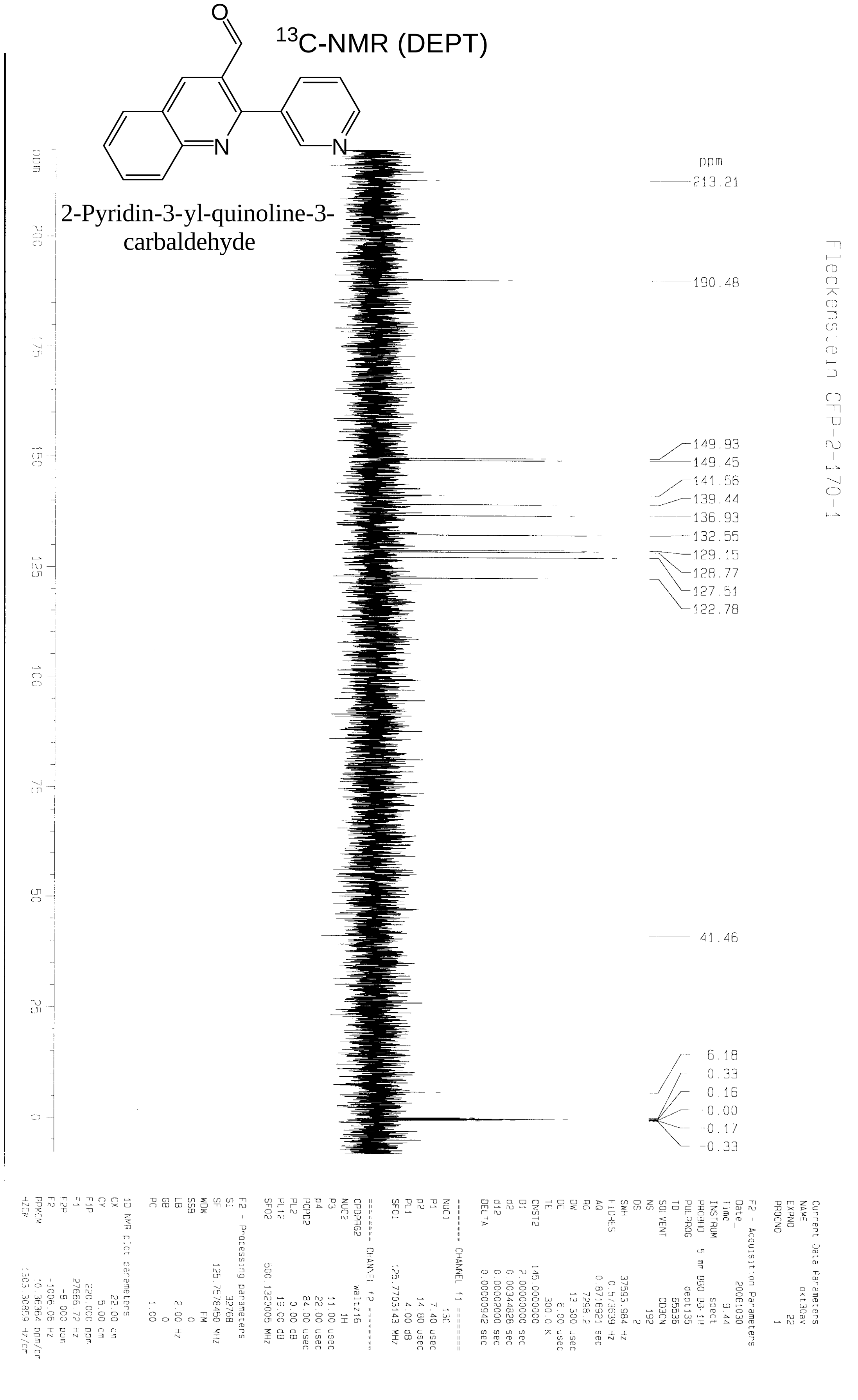


^{13}C-NMR

2-Pyridin-3-yl-quinoline-3-carbaldehyde

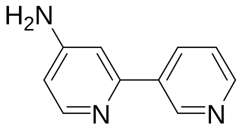


^{13}C-NMR (DEPT)

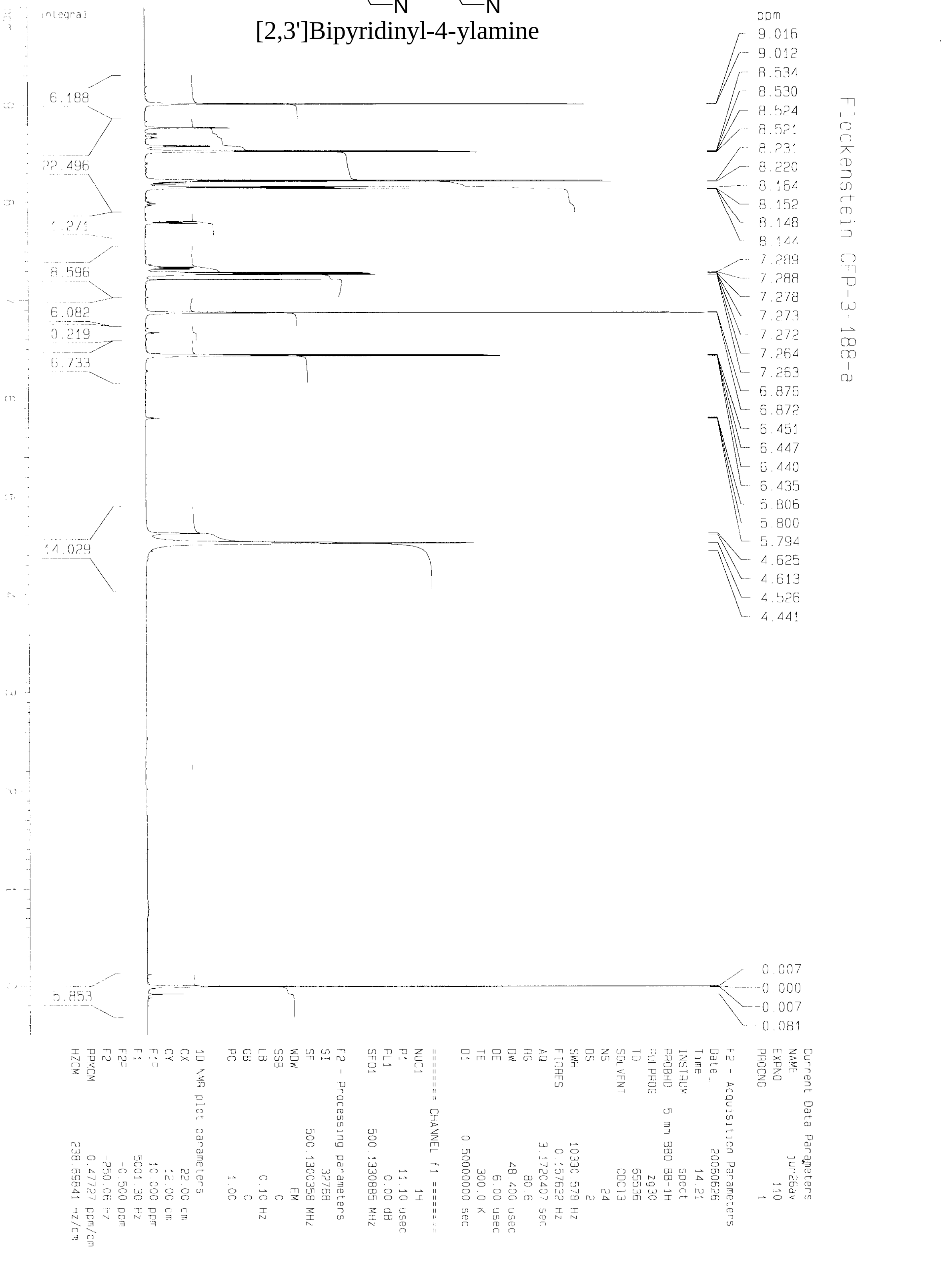


2-Pyridin-3-yl-quinoline-3-carbaldehyde

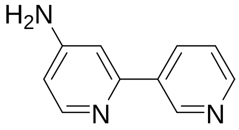
^{1}H-NMR



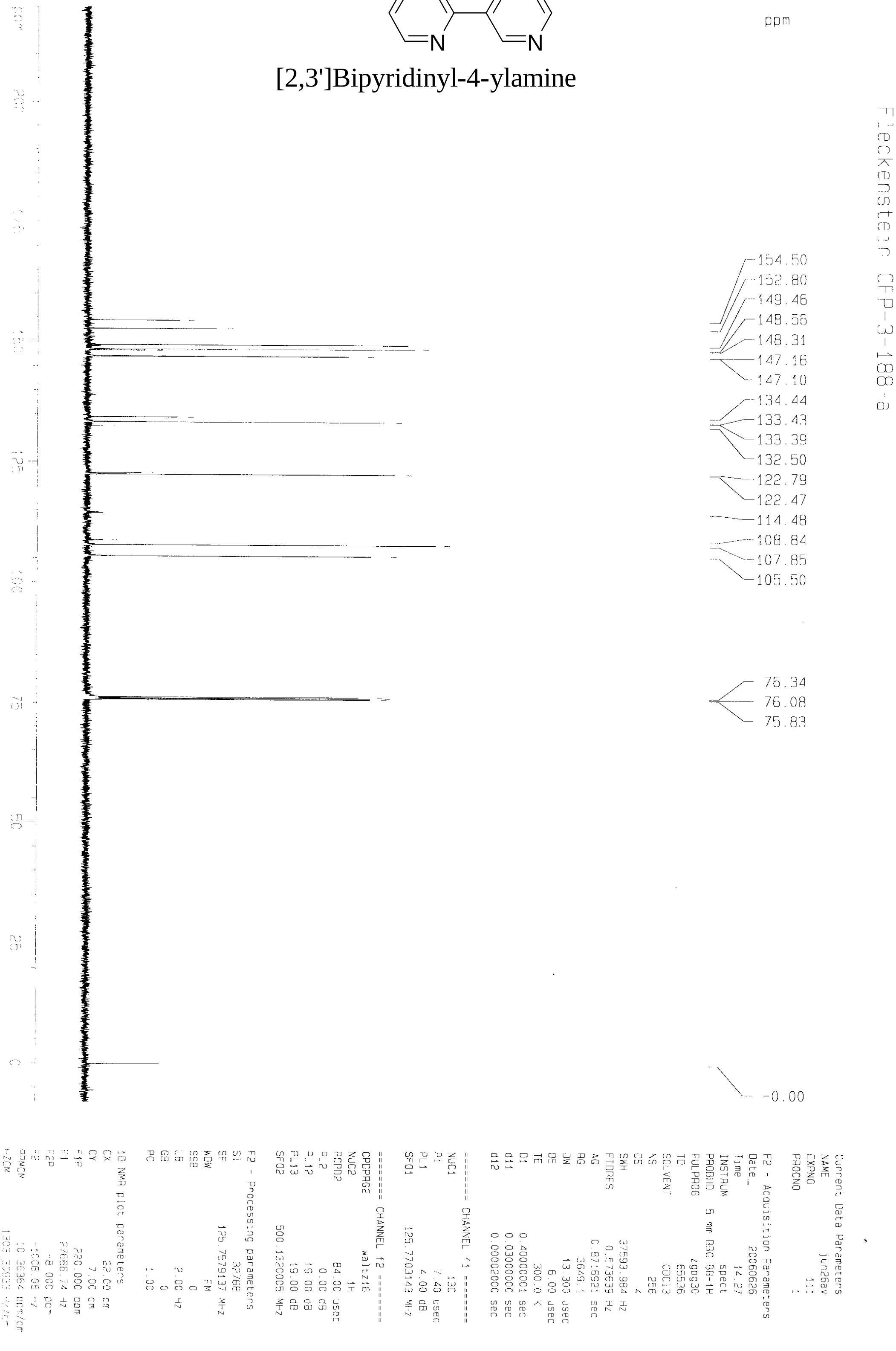
[2,3']Bipyridinyl-4-ylamine



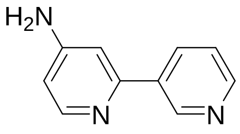
^{13}C-NMR



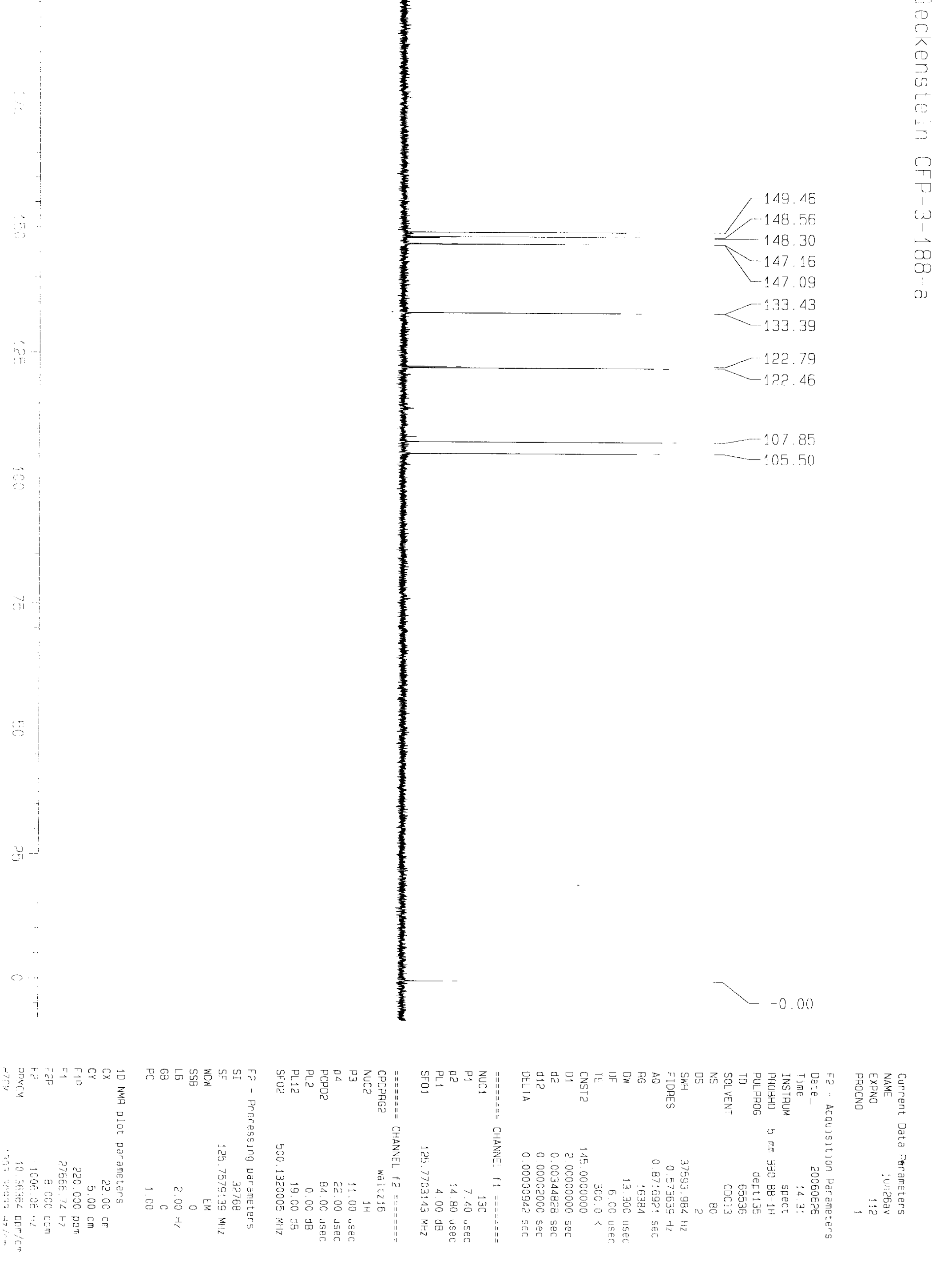
[2,3']Bipyridinyl-4-ylamine



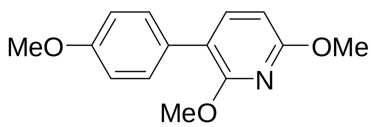
^{13}C-NMR (DEPT)



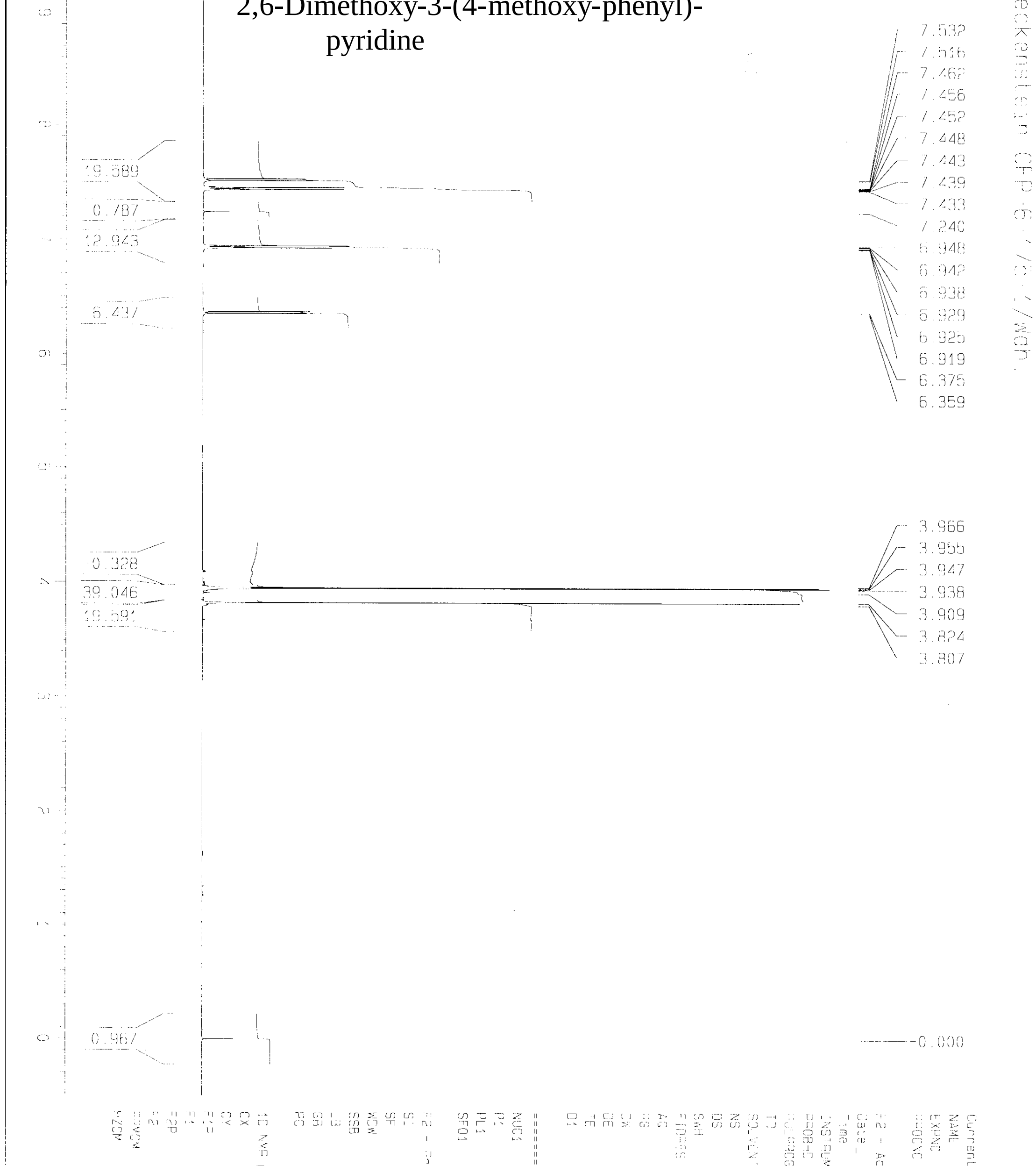
[2,3']Bipyridinyl-4-ylamine



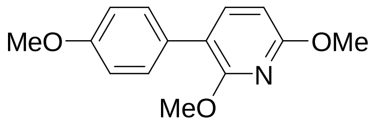
^{1}H-NMR



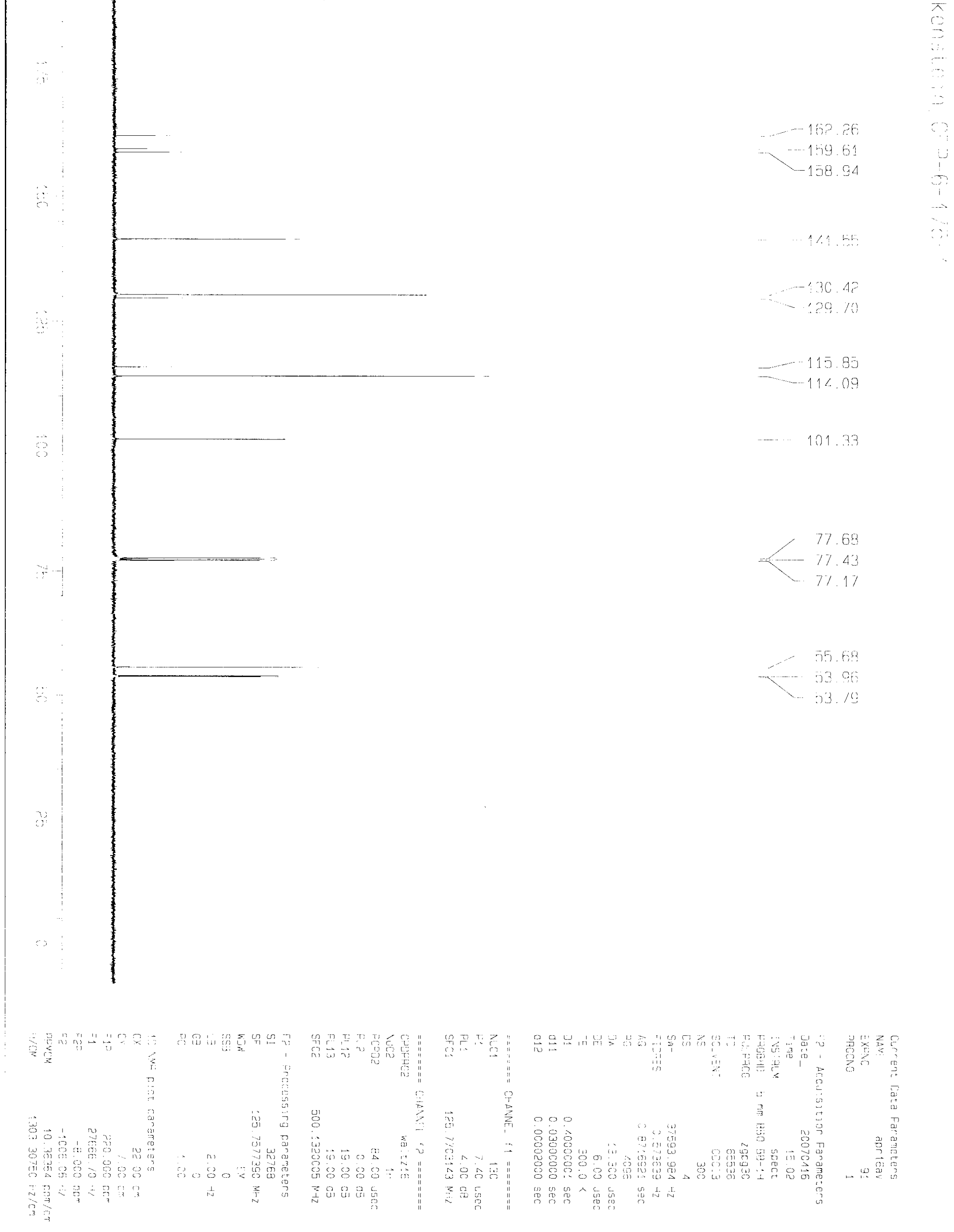
2,6-Dimethoxy-3-(4-methoxy-phenyl)-pyridine



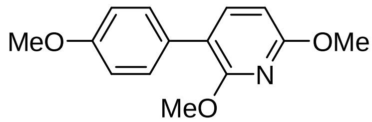
^{13}C-NMR



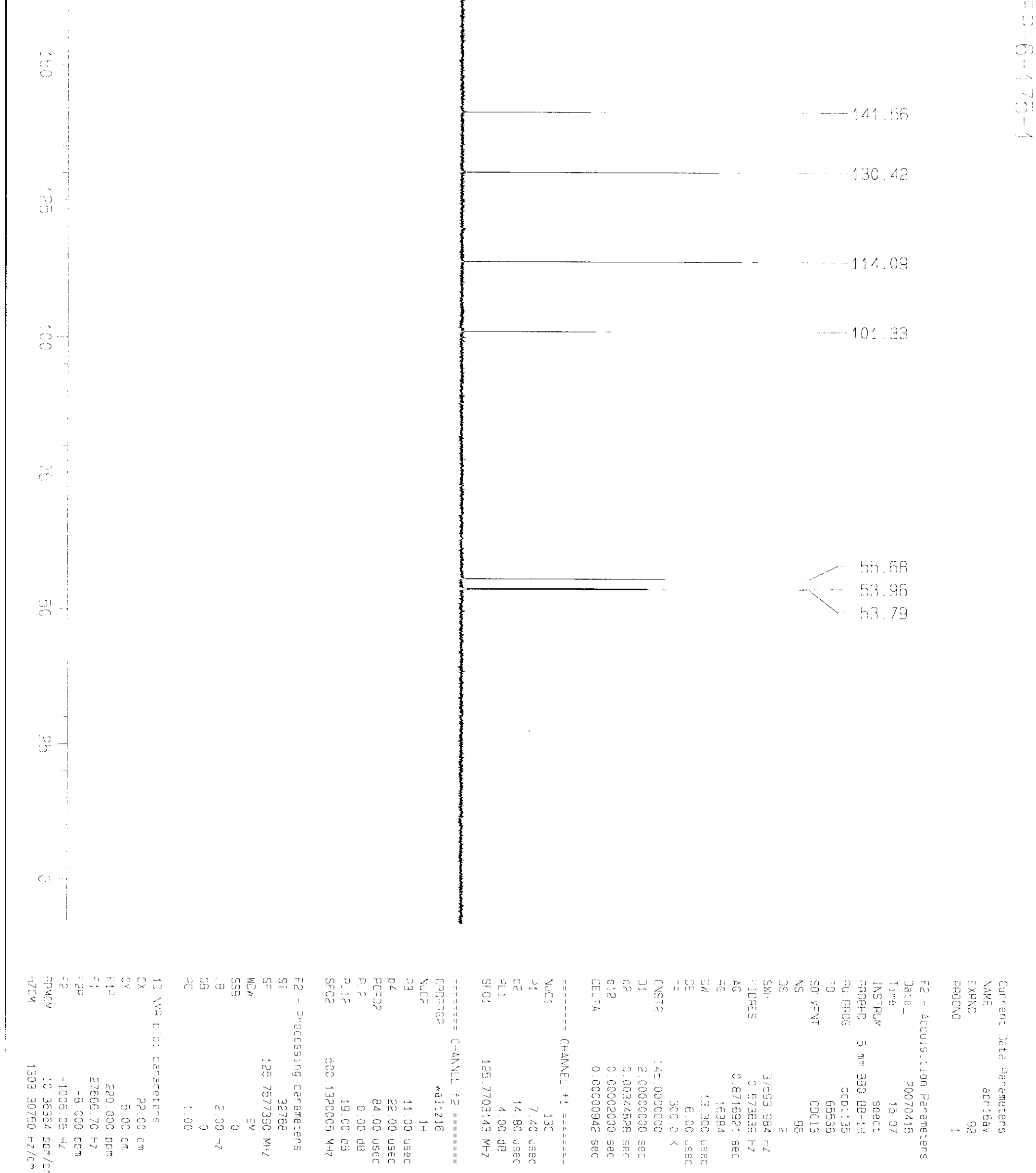
2,6-Dimethoxy-3-(4-methoxy-phenyl)-pyridine



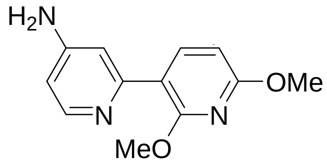
^{13}C-NMR (DEPT)



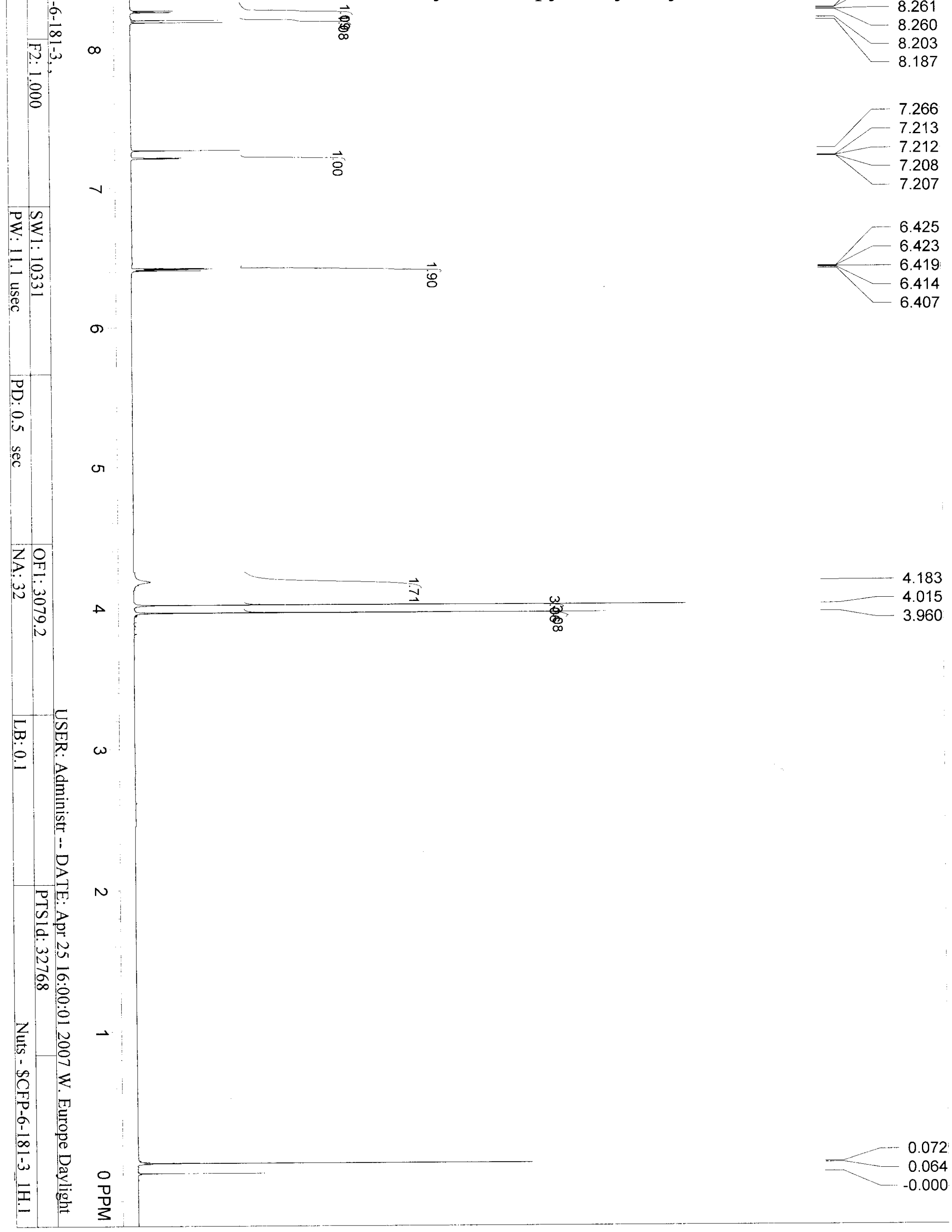
2,6-Dimethoxy-3-(4-methoxy-phenyl)-pyridine



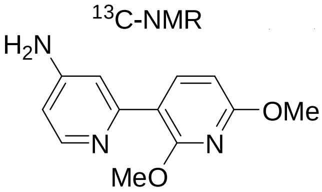
^{1}H-NMR



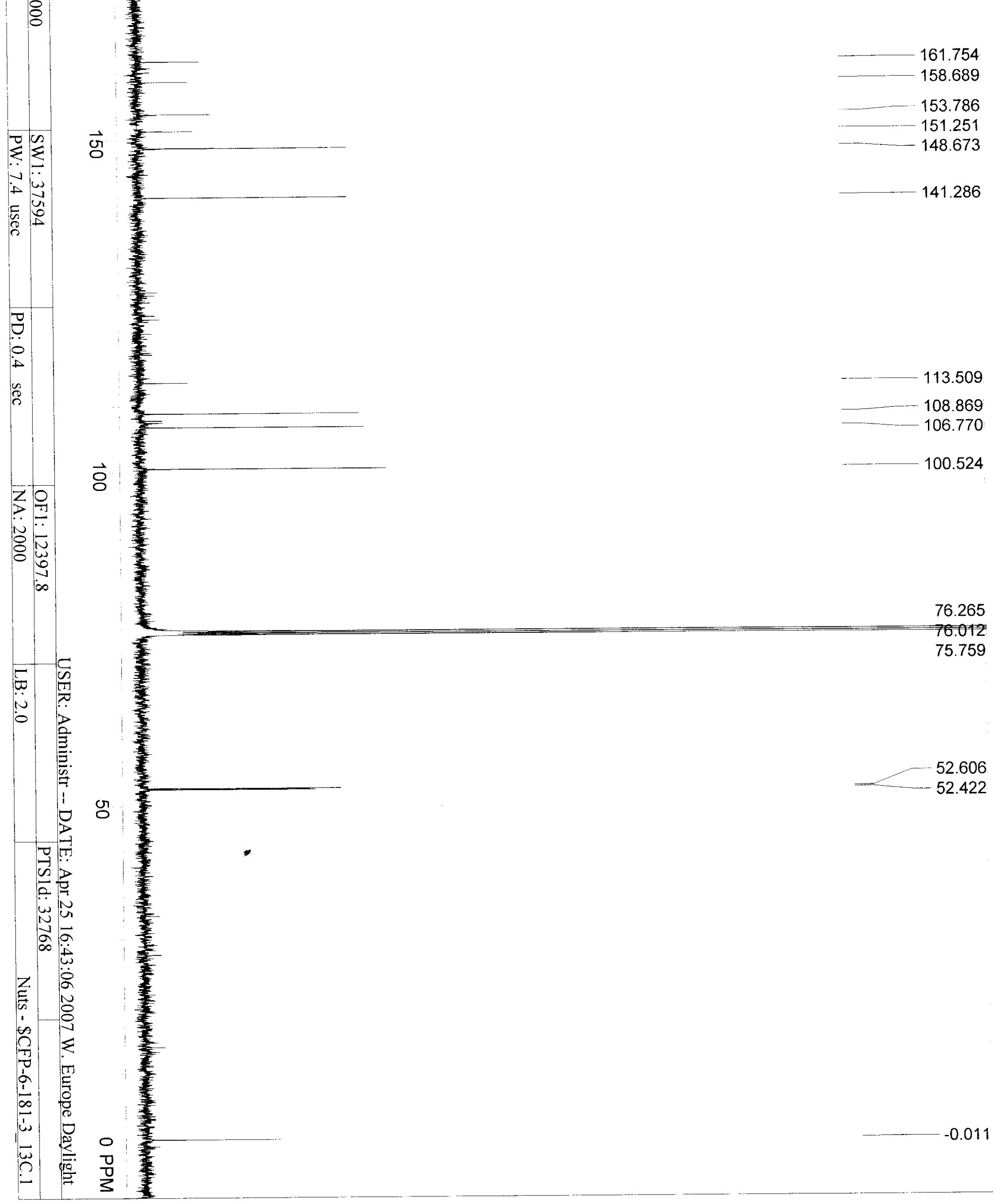
2',6'-Dimethoxy-[2,3']bipyridinyl-4-ylamine



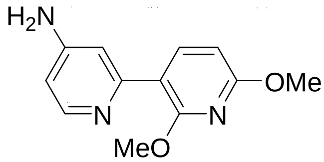
^{13}C-NMR



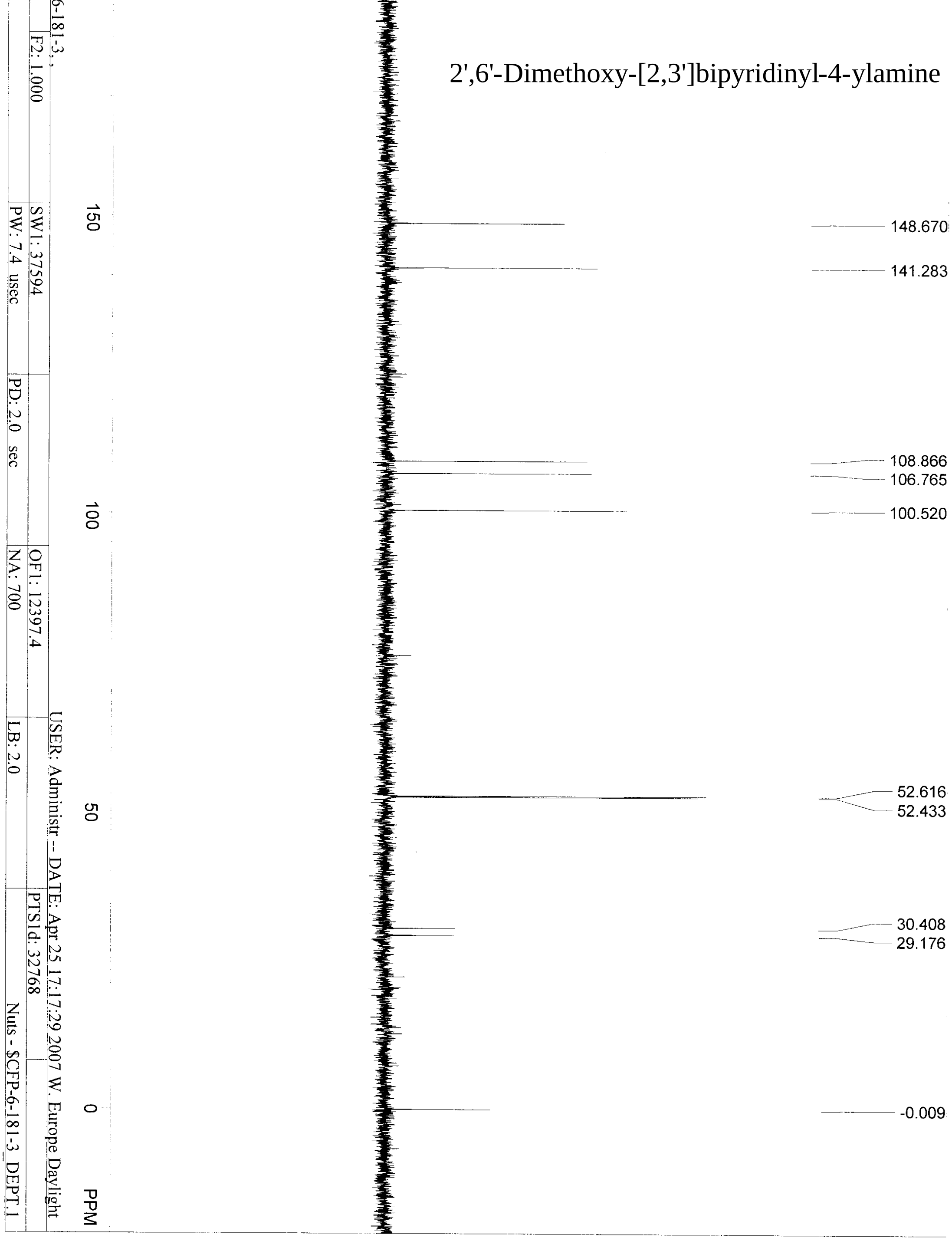
2',6'-Dimethoxy-[2,3']bipyridinyl-4-ylamine



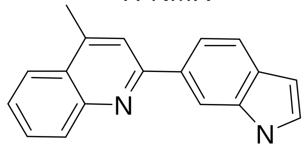
^{13}C-NMR (DEPT)



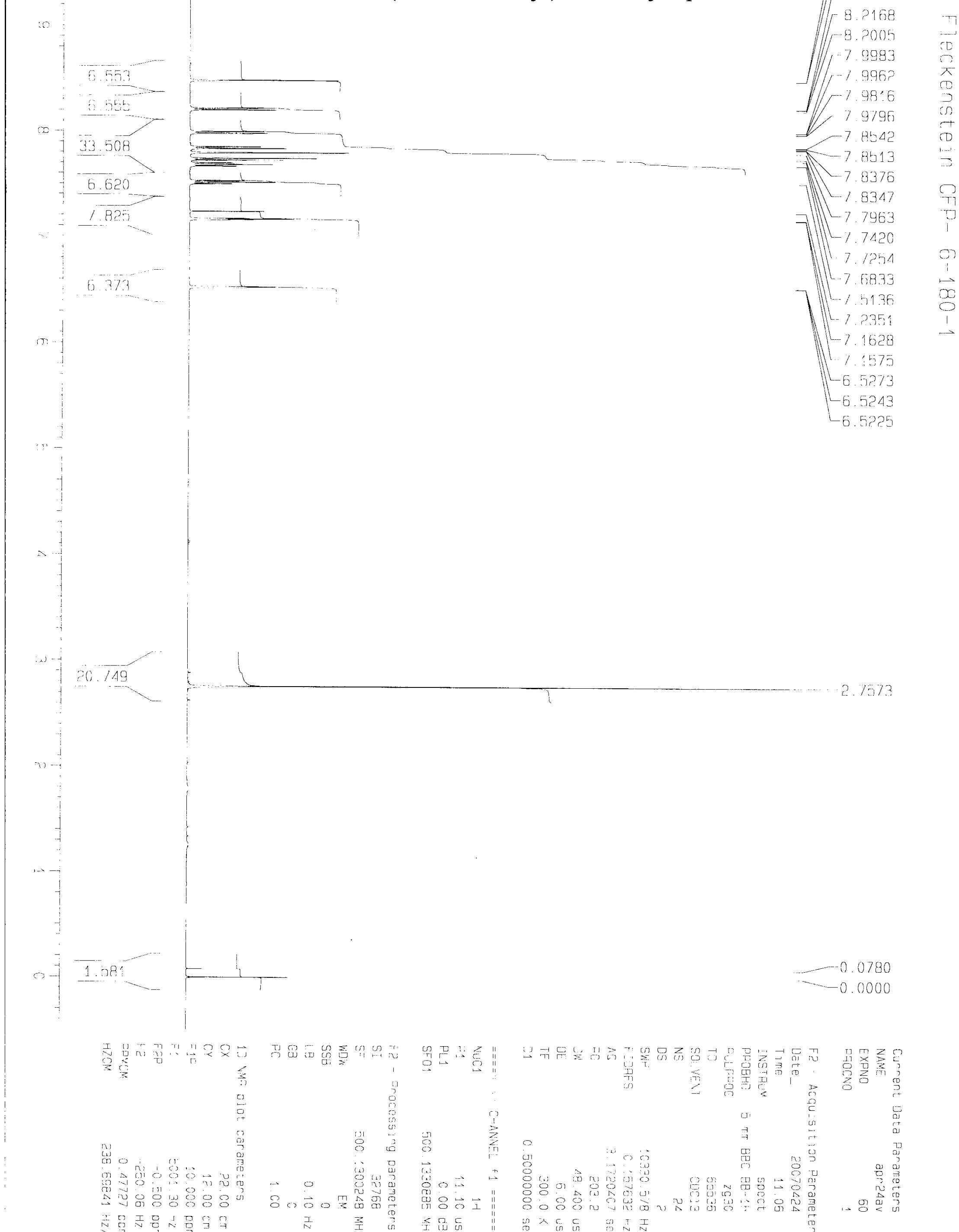
2',6'-Dimethoxy-[2,3']bipyridinyl-4-ylamine



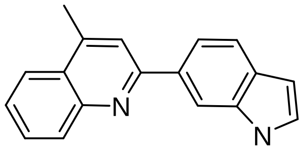
^{1}H-NMR



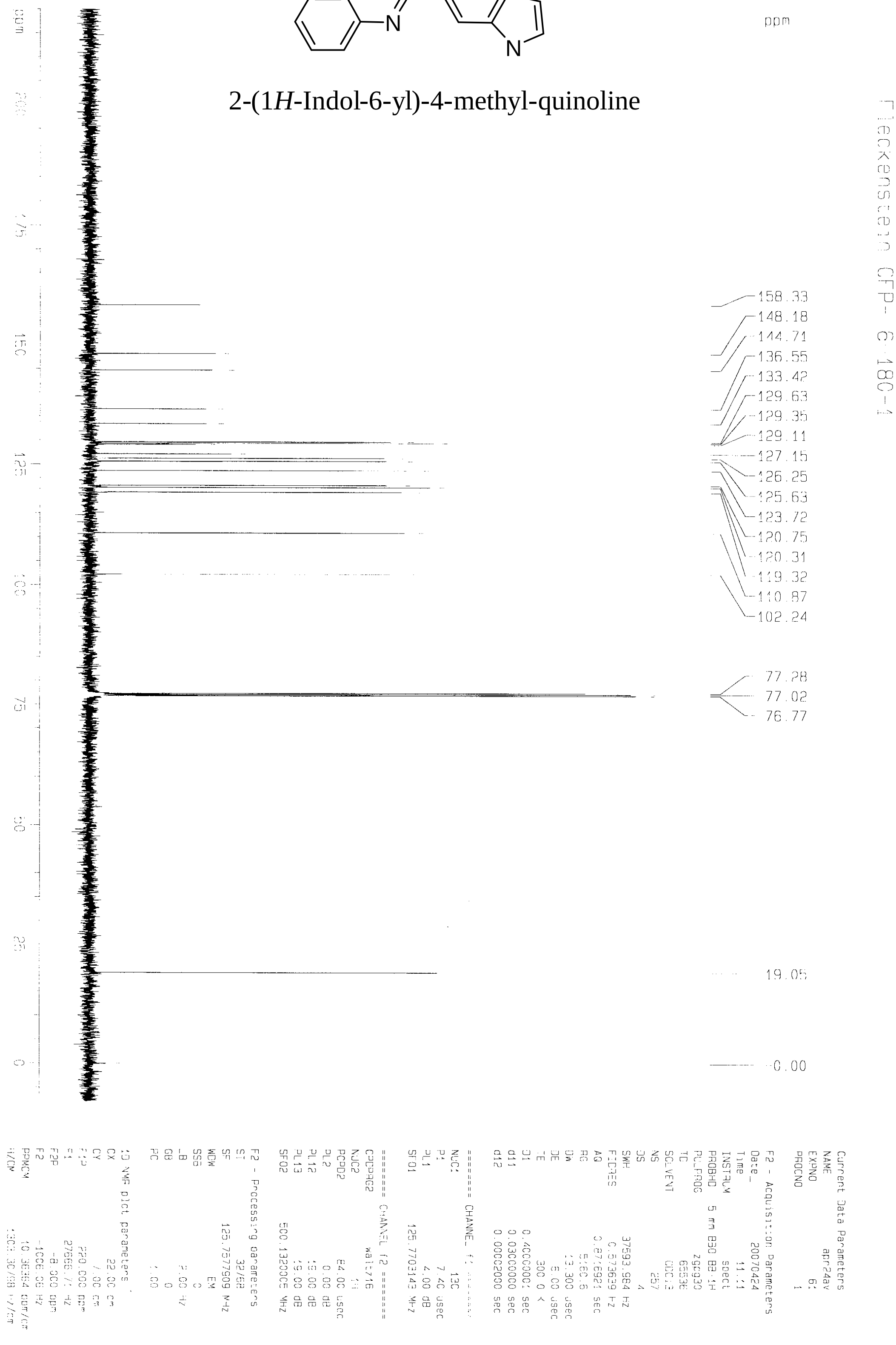
2-(1*H*-Indol-6-yl)-4-methyl-quinoline



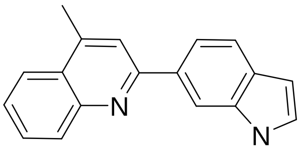
^{13}C-NMR



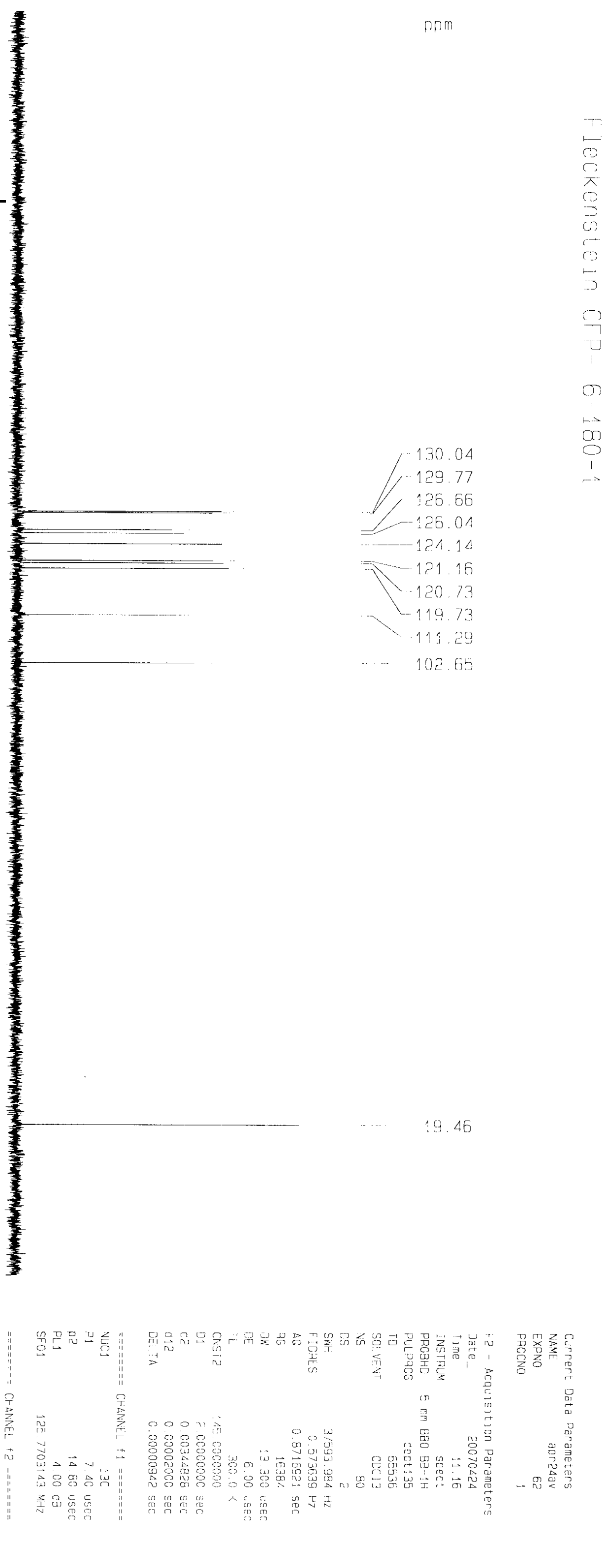
2-(1*H*-Indol-6-yl)-4-methyl-quinoline



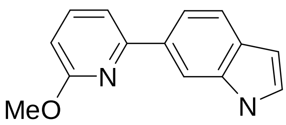
^{13}C-NMR (DEPT)



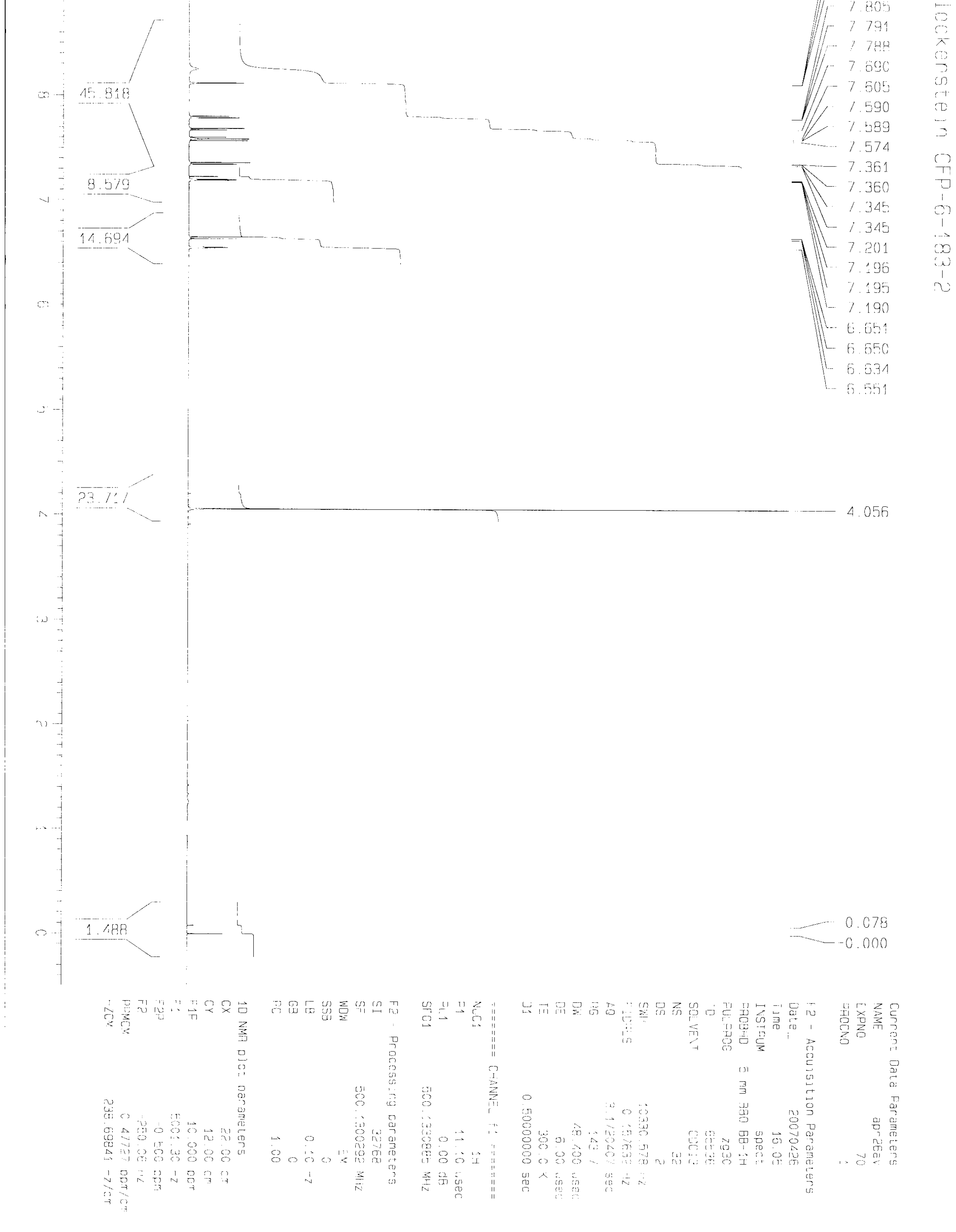
2-(1*H*-Indol-6-yl)-4-methyl-quinoline



^{1}H-NMR

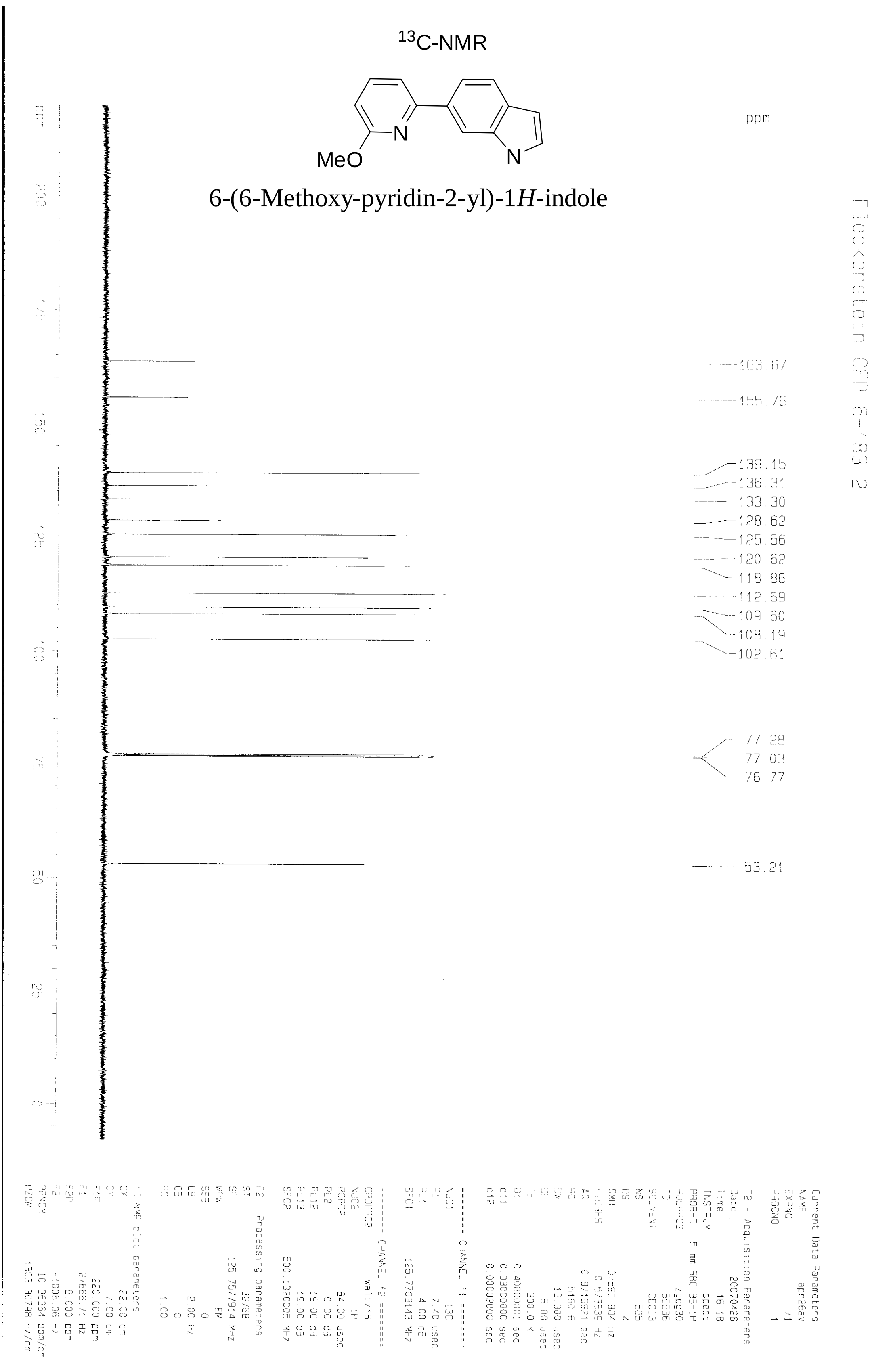


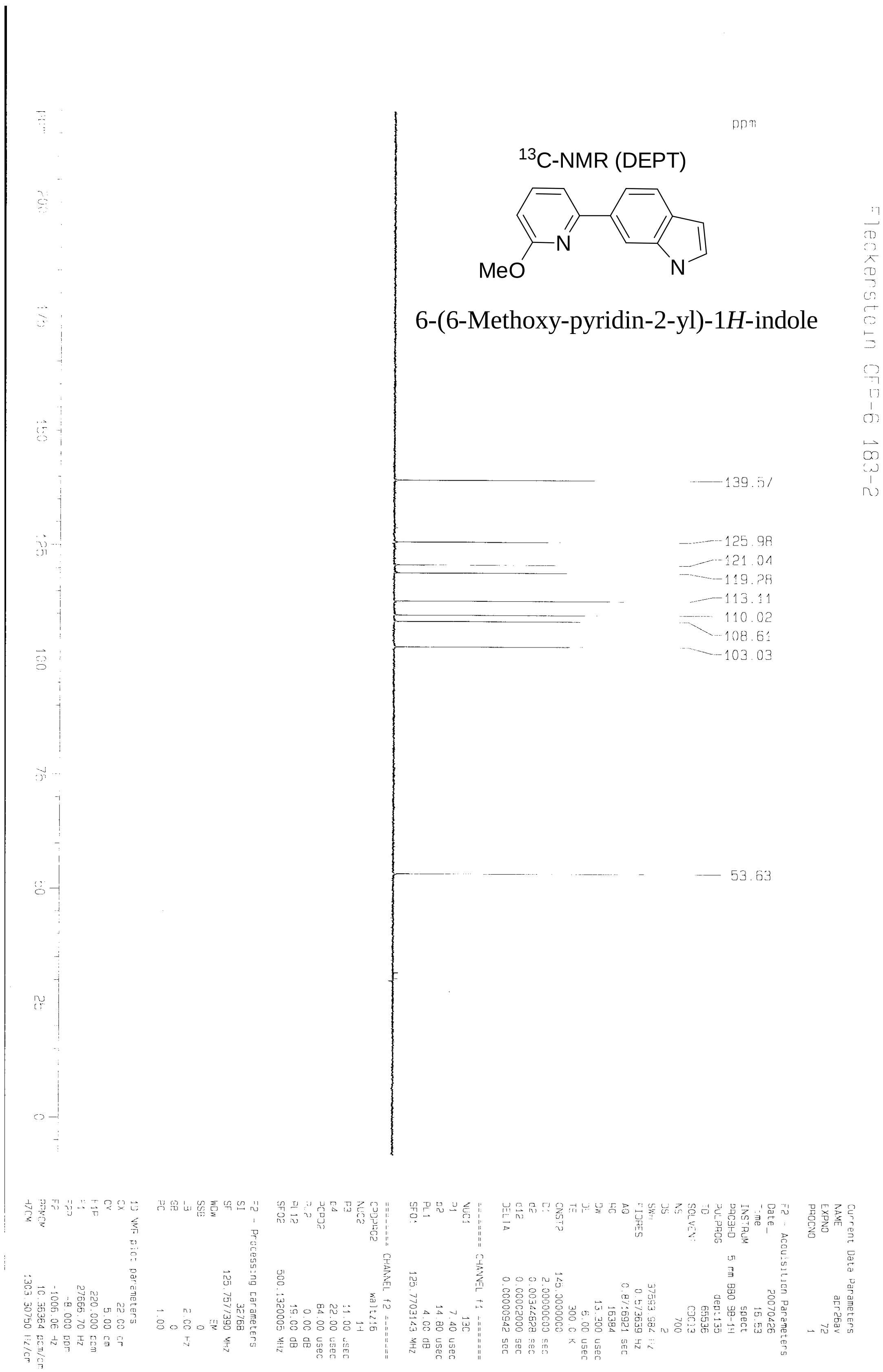
6-(6-Methoxy-pyridin-2-yl)-1*H*-indole



^{13}C-NMR

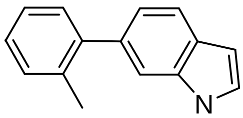
6-(6-Methoxy-pyridin-2-yl)-1*H*-indole



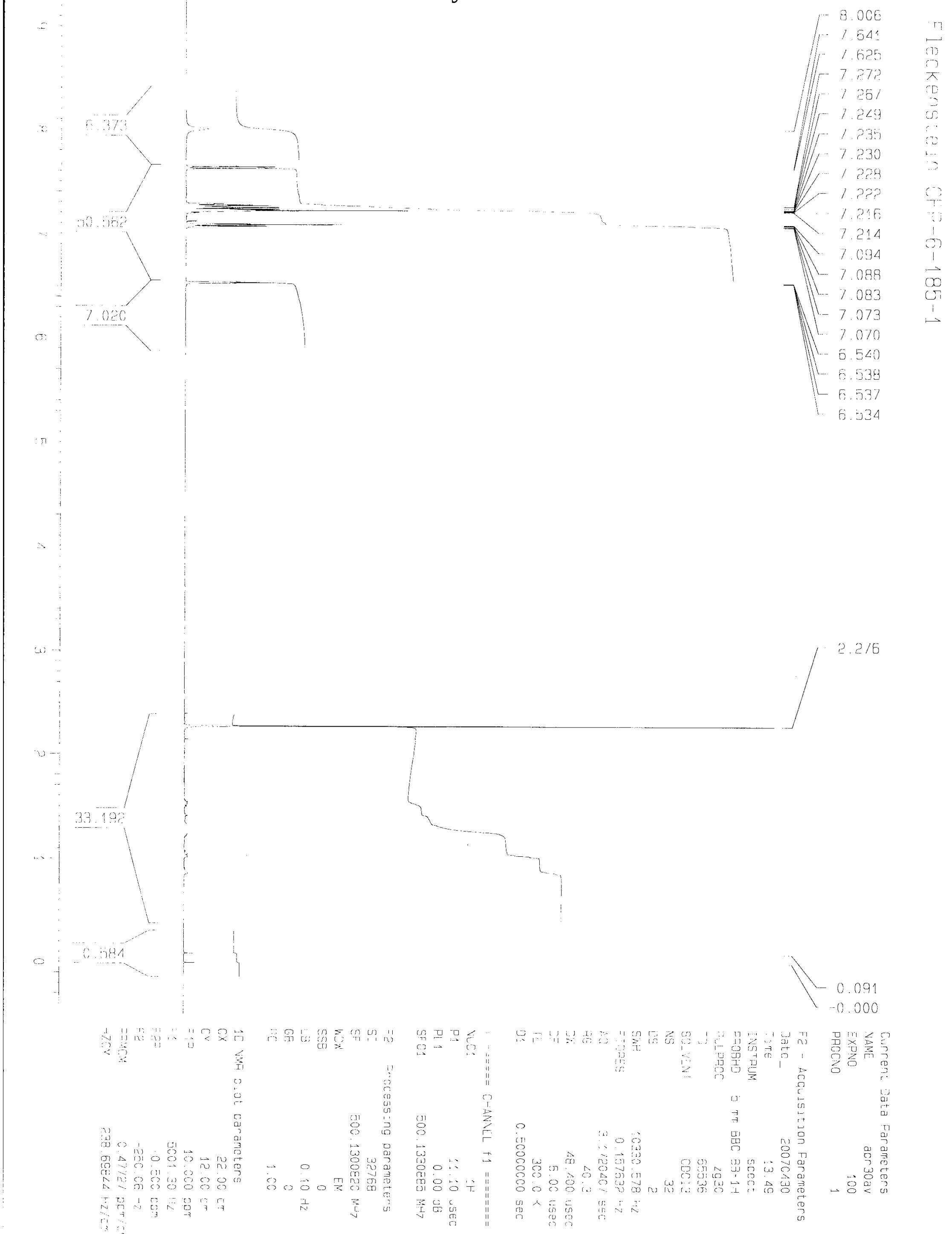


ppm
13C-NMR (DEPT)
MeO
N
N
6-(6-Methoxy-pyridin-2-yl)-1H-indole
139.57
125.98
121.04
119.28
113.11
110.02
108.61
103.03
53.63

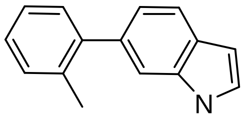
^{1}H-NMR



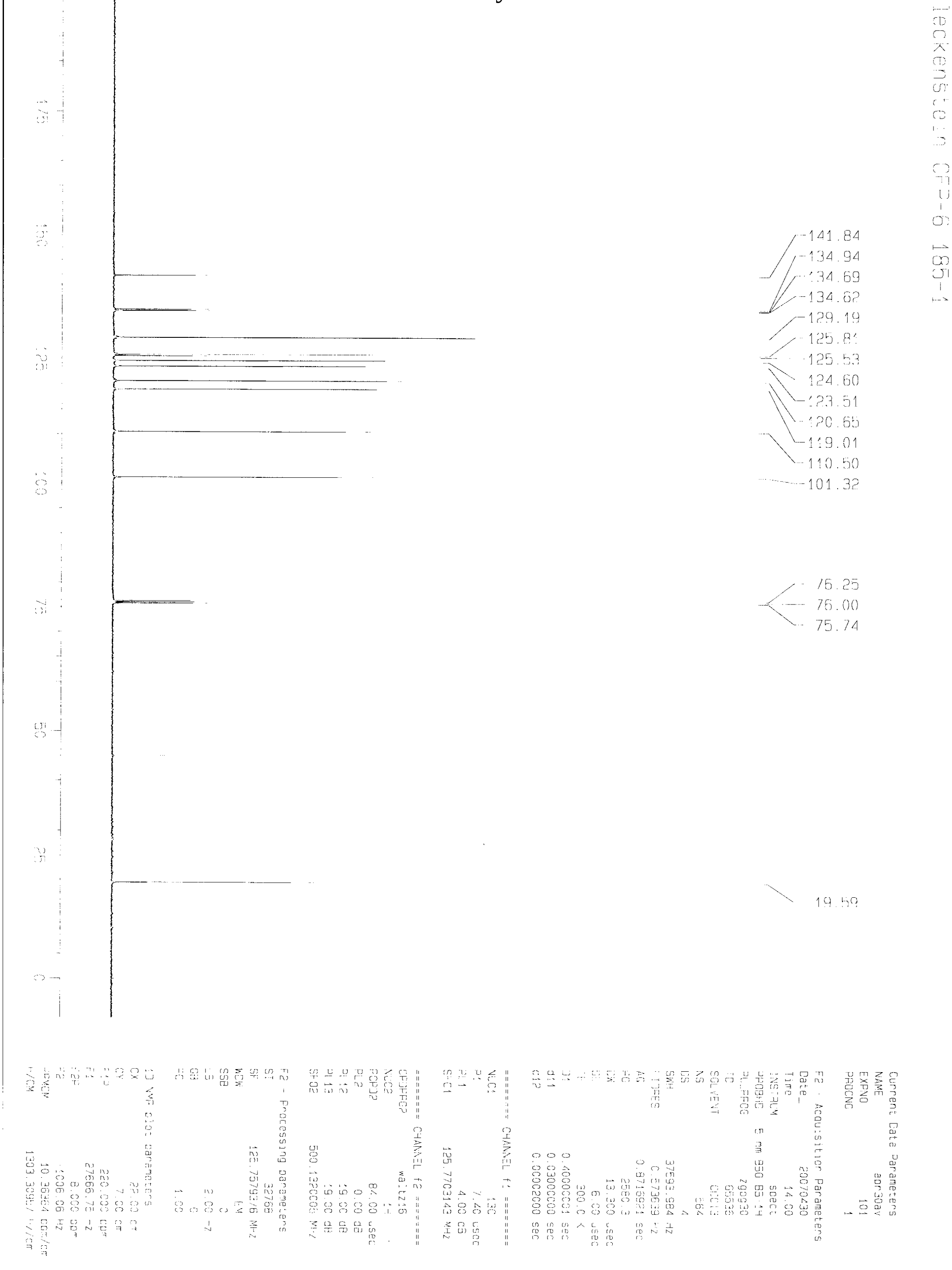
6-*o*Tolyl-1H-indole

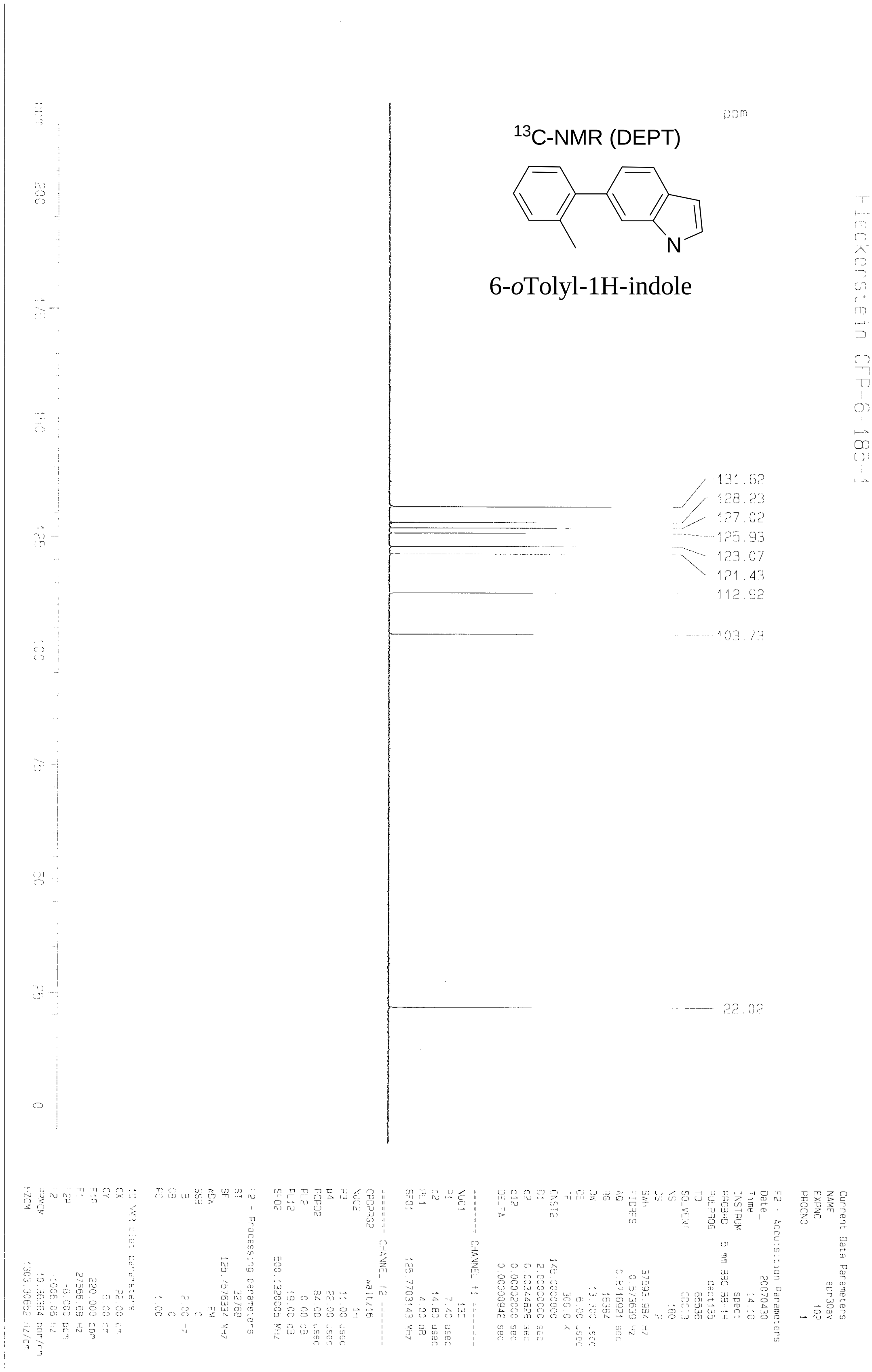


^{13}C-NMR

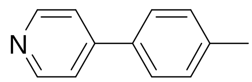


6-*o*Tolyl-1H-indole

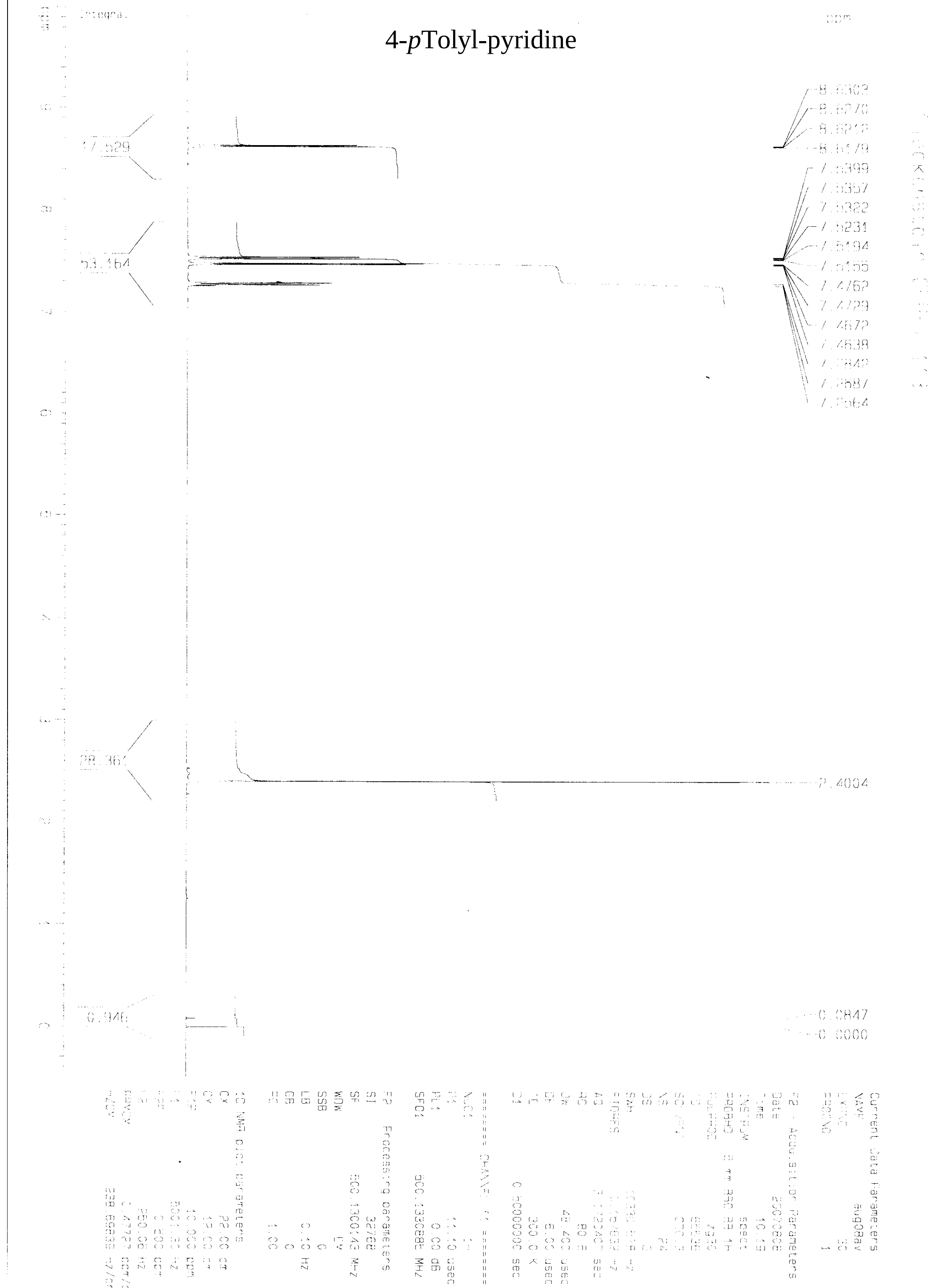



^{13}C-NMR (DEPT)
N
6-*o*Tolyl-1H-indole
131.62
128.23
127.02
125.93
123.07
121.43
112.92
103.73
22.02
ppm

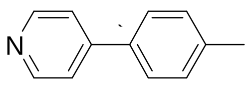
^{1}H-NMR



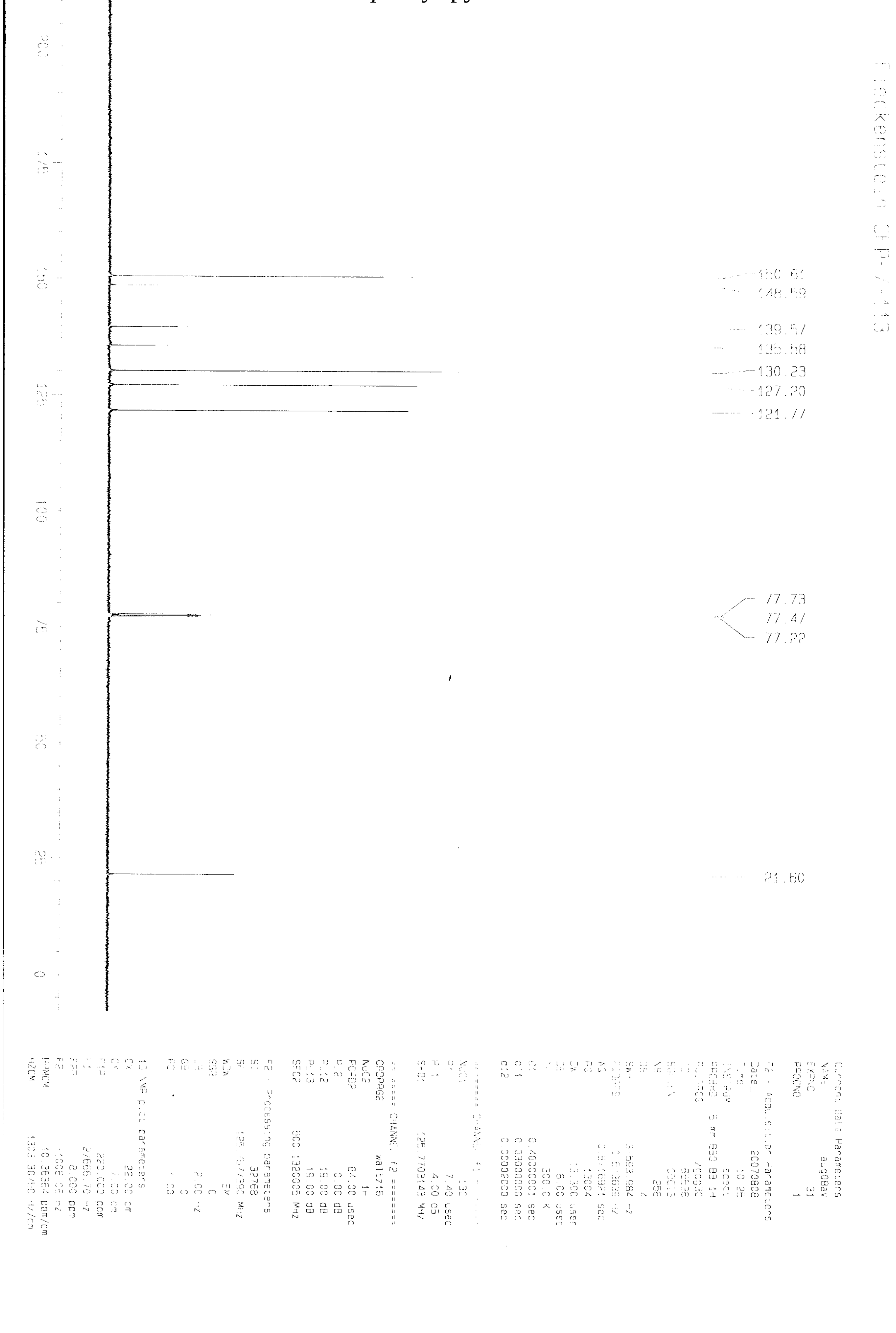
4-*p*Tolyl-pyridine



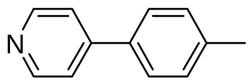
^{13}C-NMR



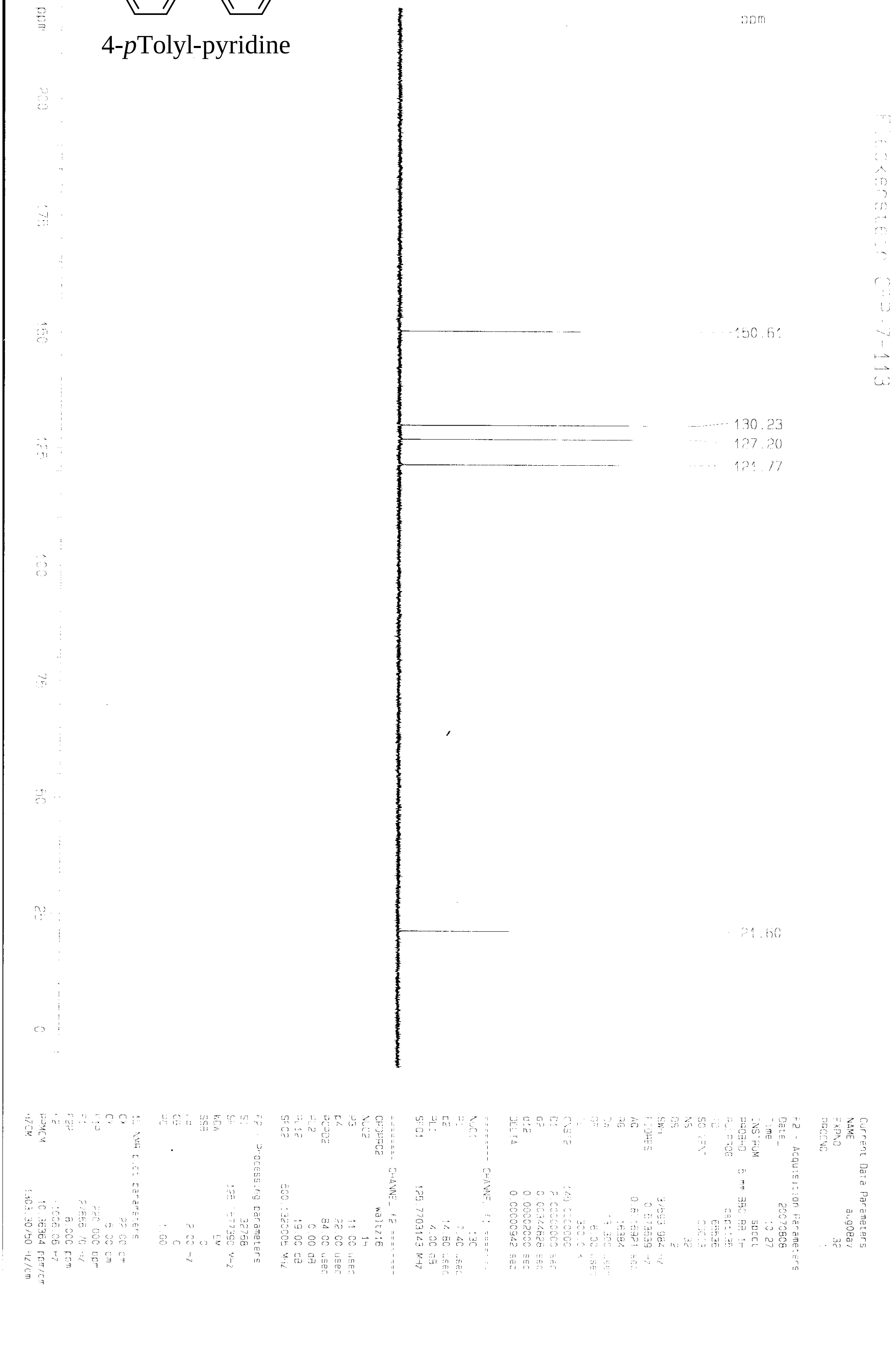
4-*p*Tolyl-pyridine



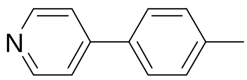
^{13}C-NMR (DEPT)



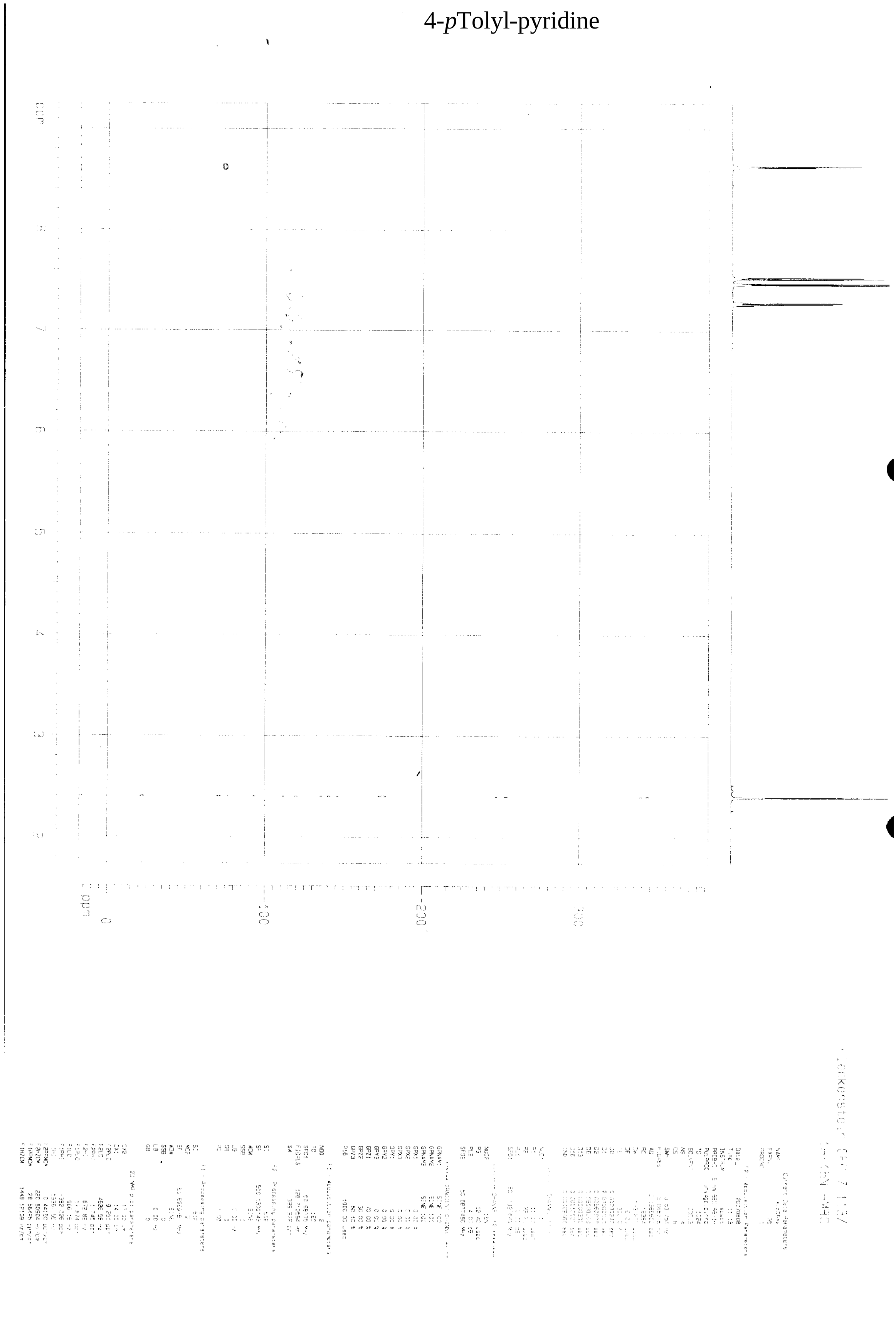
4-*p*Tolyl-pyridine



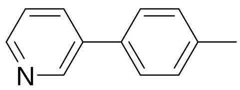
^{15}N-NMR (HMBC)



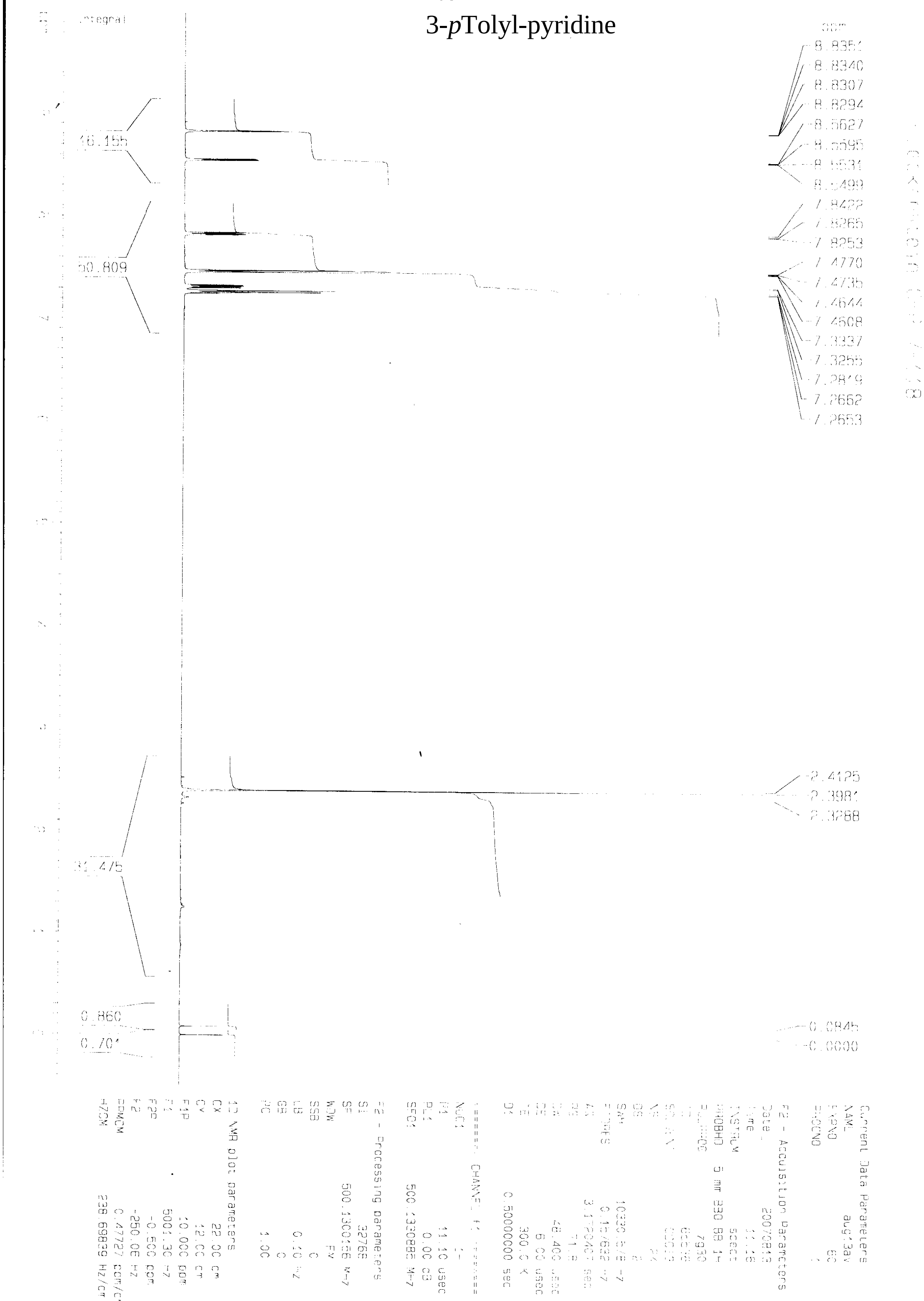
4-*p*Tolyl-pyridine



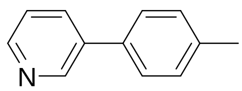
^{1}H-NMR



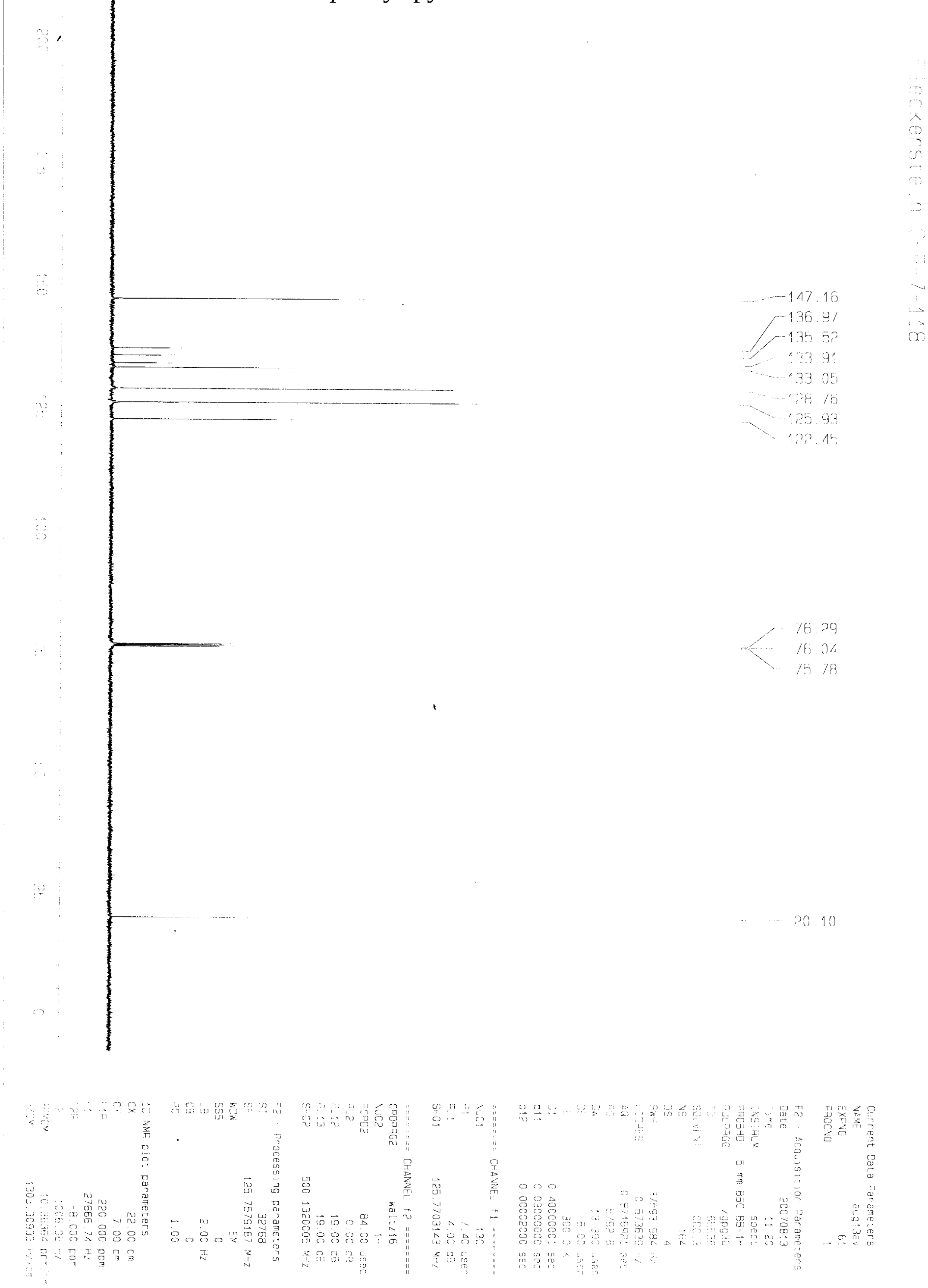
3-*p*Tolyl-pyridine



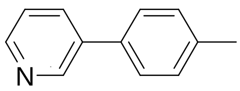
^{13}C-NMR



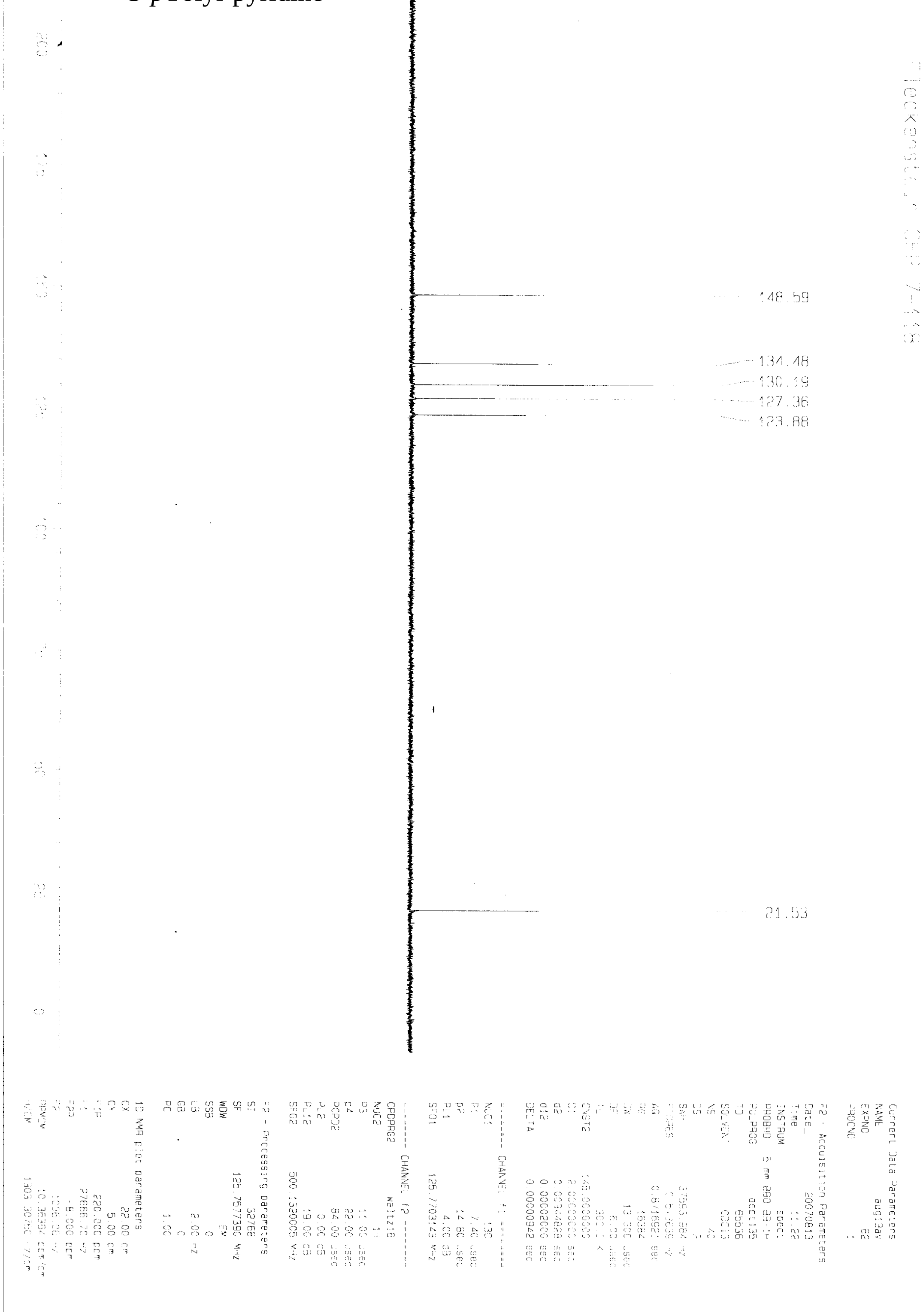
3-*p*Tolyl-pyridine



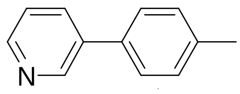
^{13}C-NMR (DEPT)



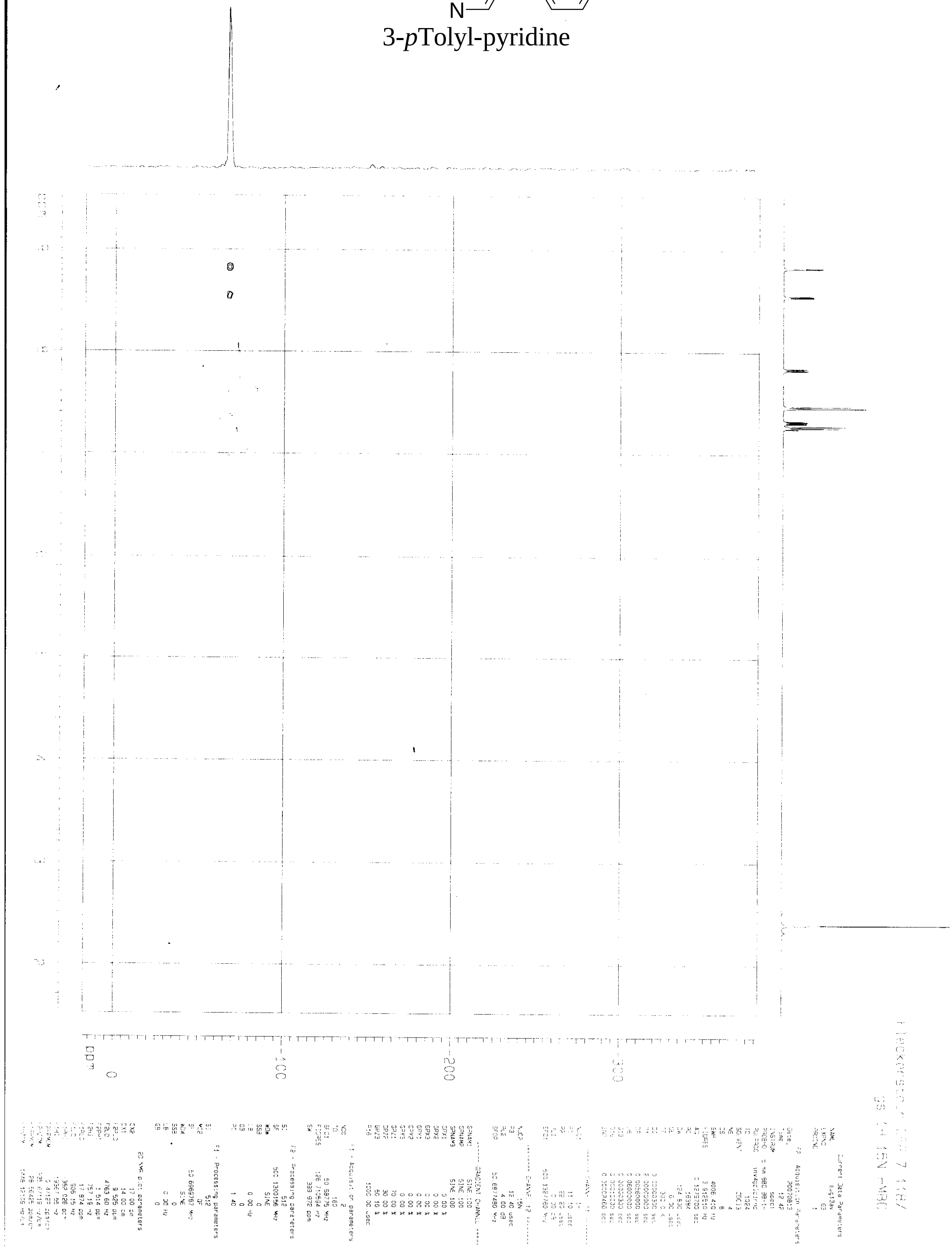
3-*p*Tolyl-pyridine



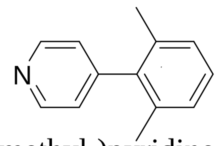
^{15}N-NMR (HMBC)



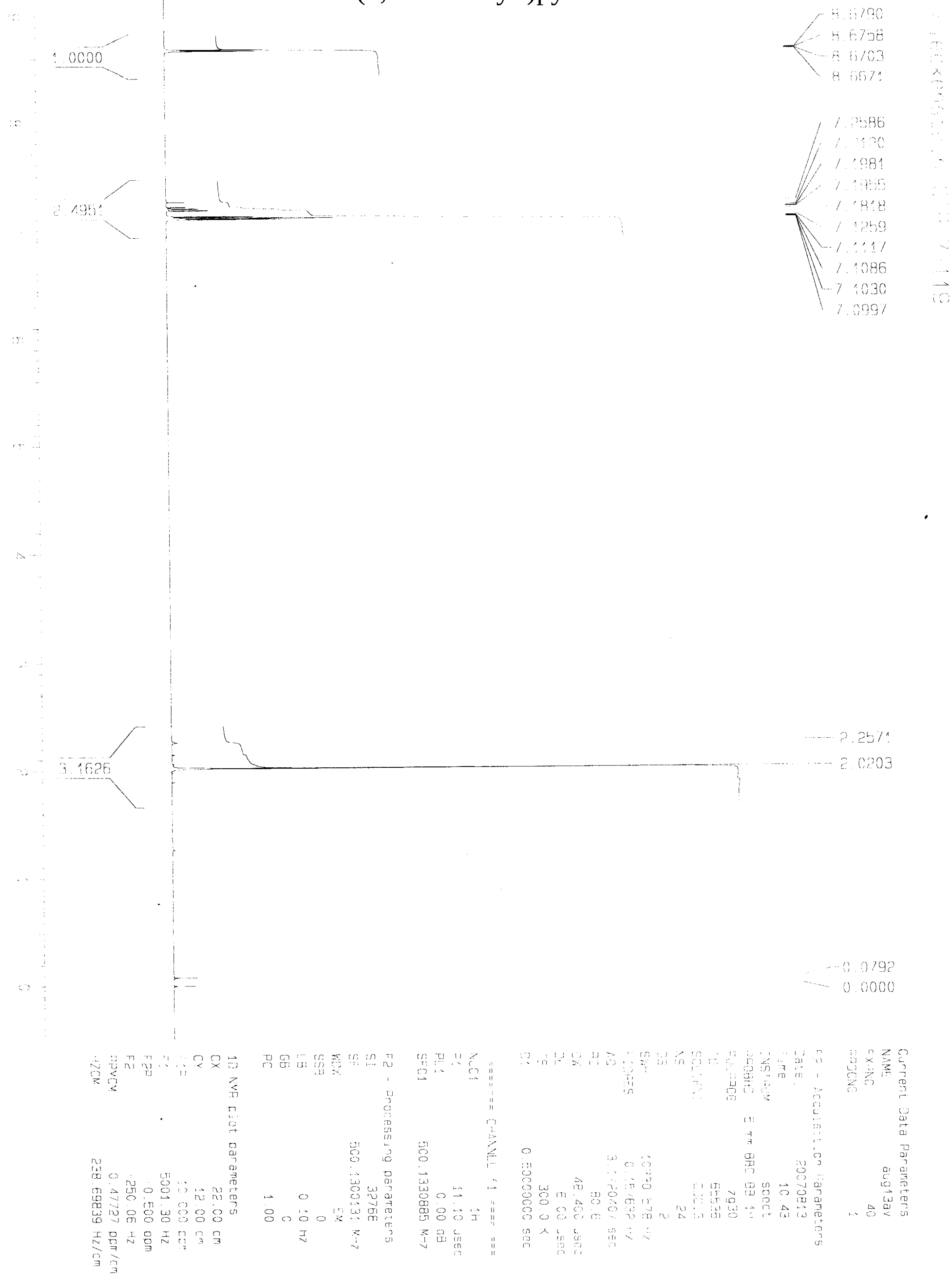
3-*p*Tolyl-pyridine



^{1}H-NMR

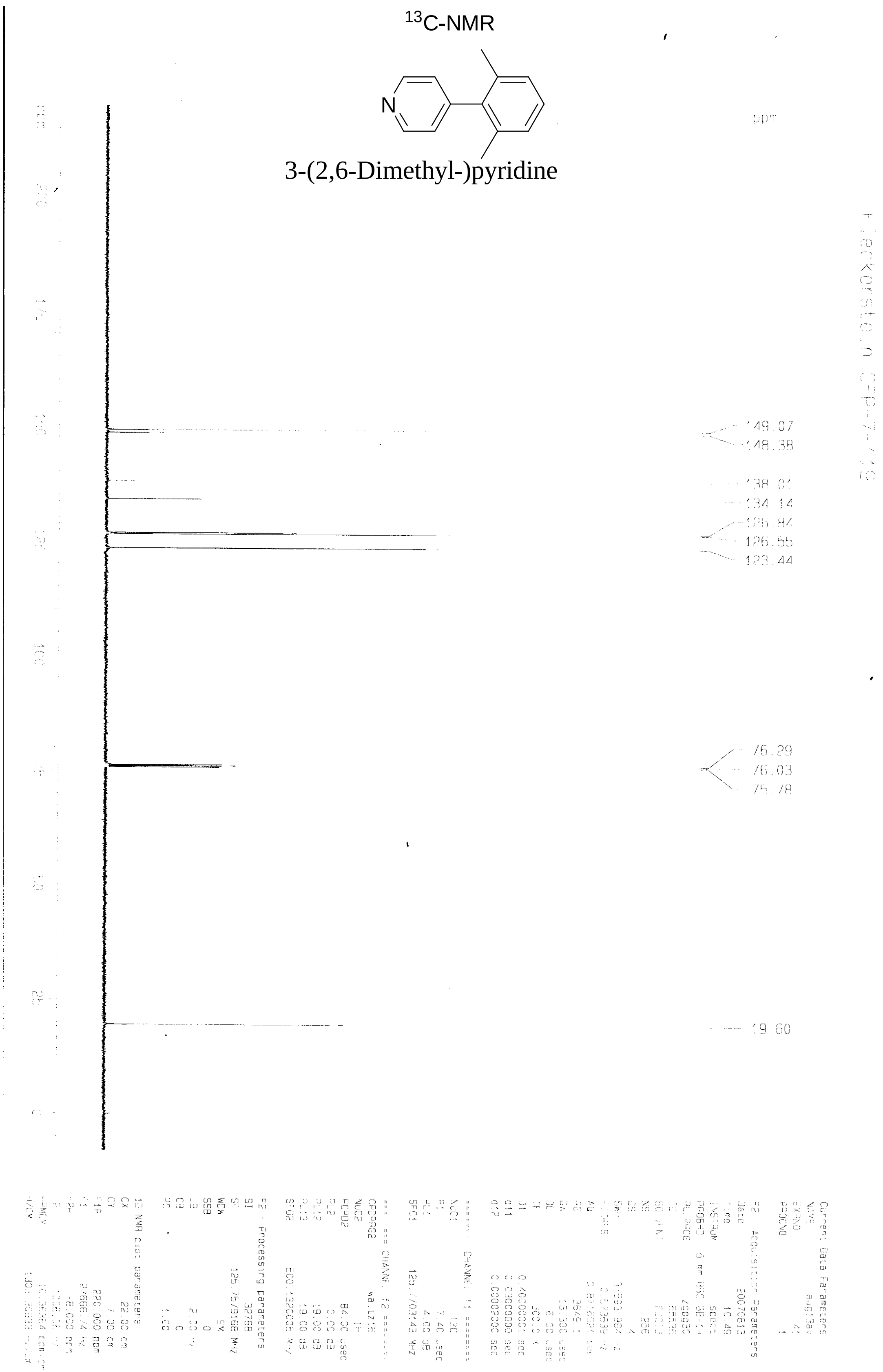


3-(2,6-Dimethyl-)pyridine

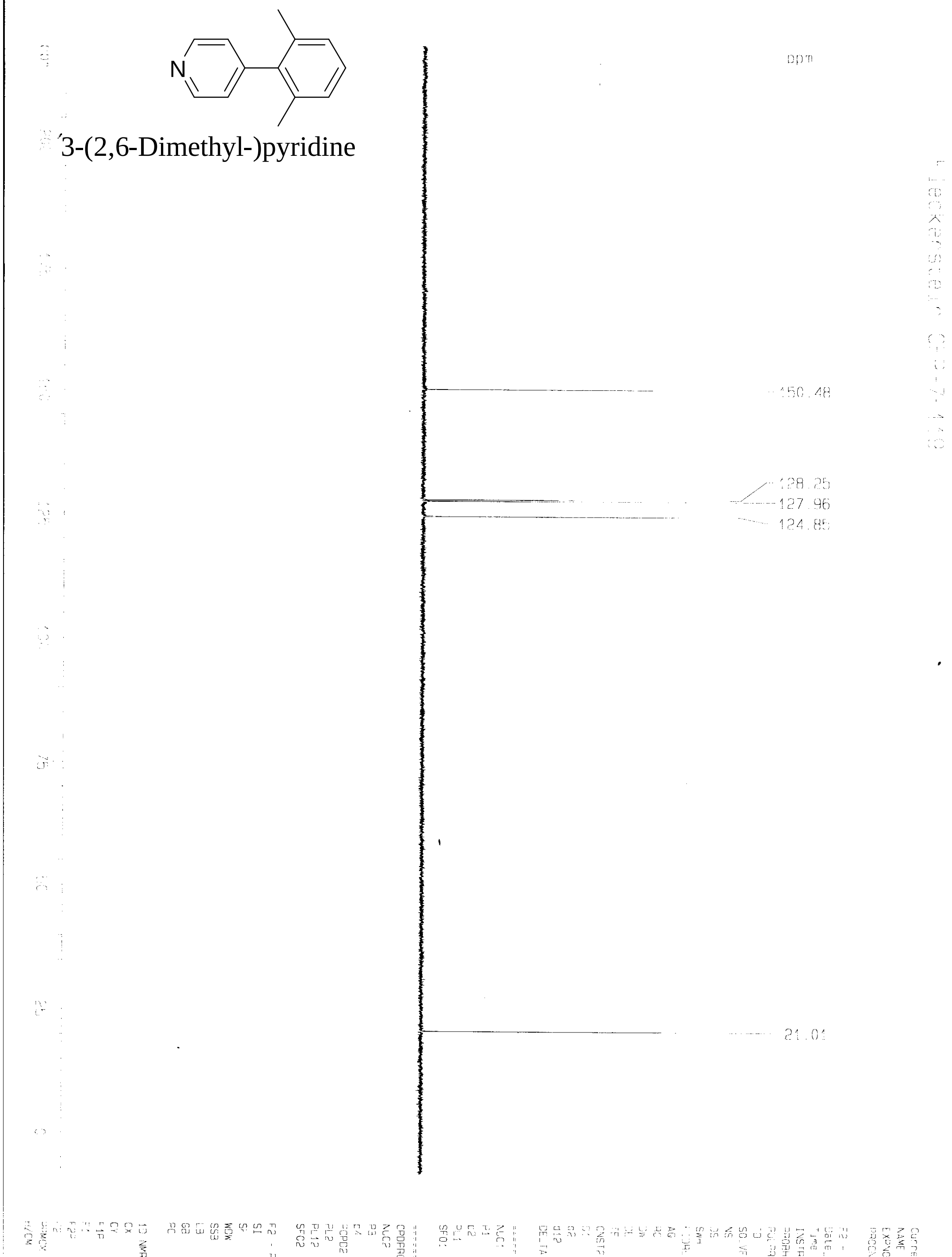


^{13}C-NMR

3-(2,6-Dimethyl-)pyridine

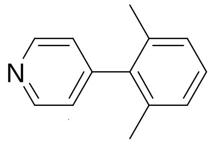


^{13}C-NMR (DEPT)

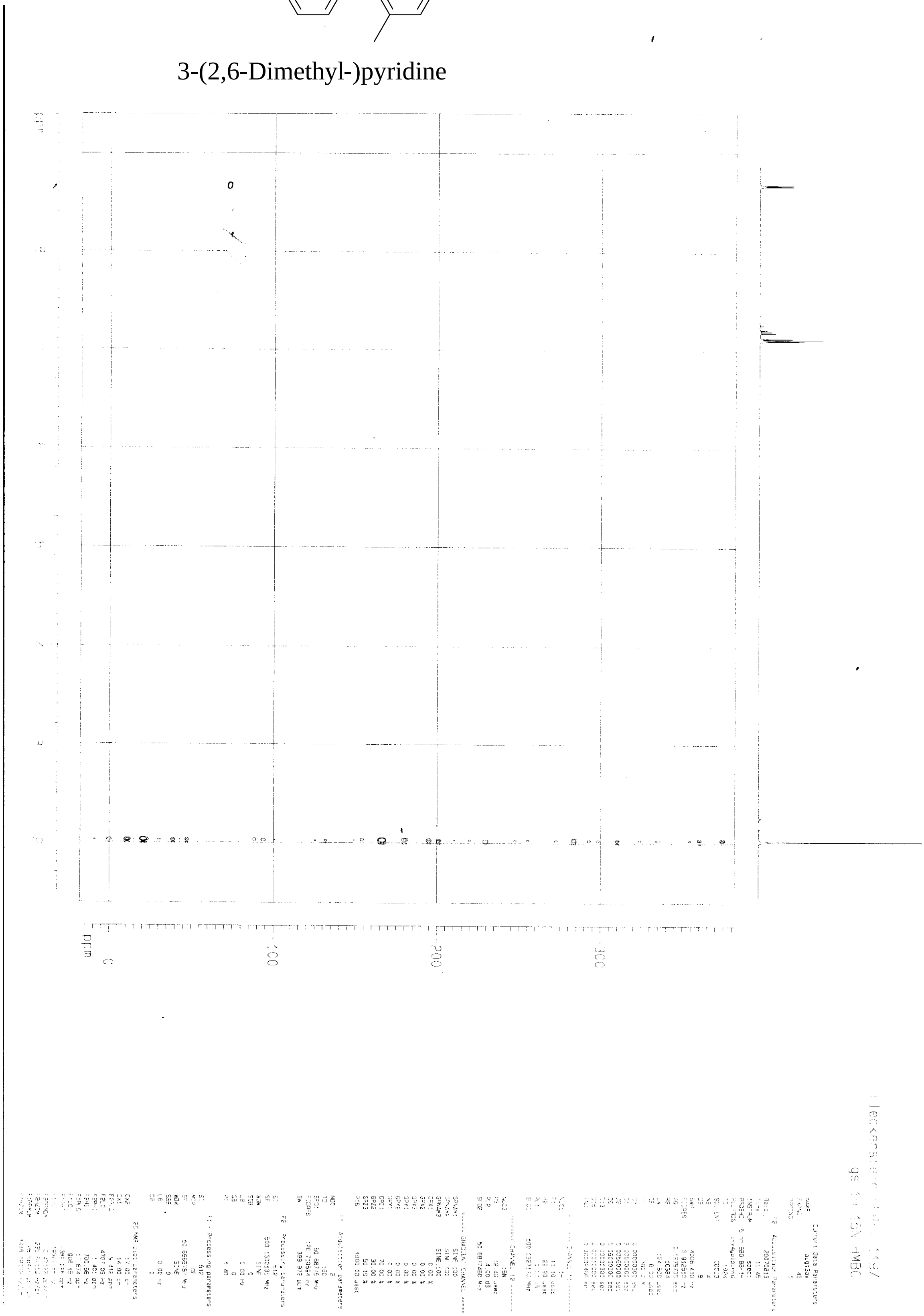


3-(2,6-Dimethyl-)pyridine

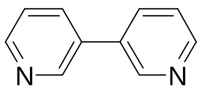
^{15}N-NMR (HMBC)



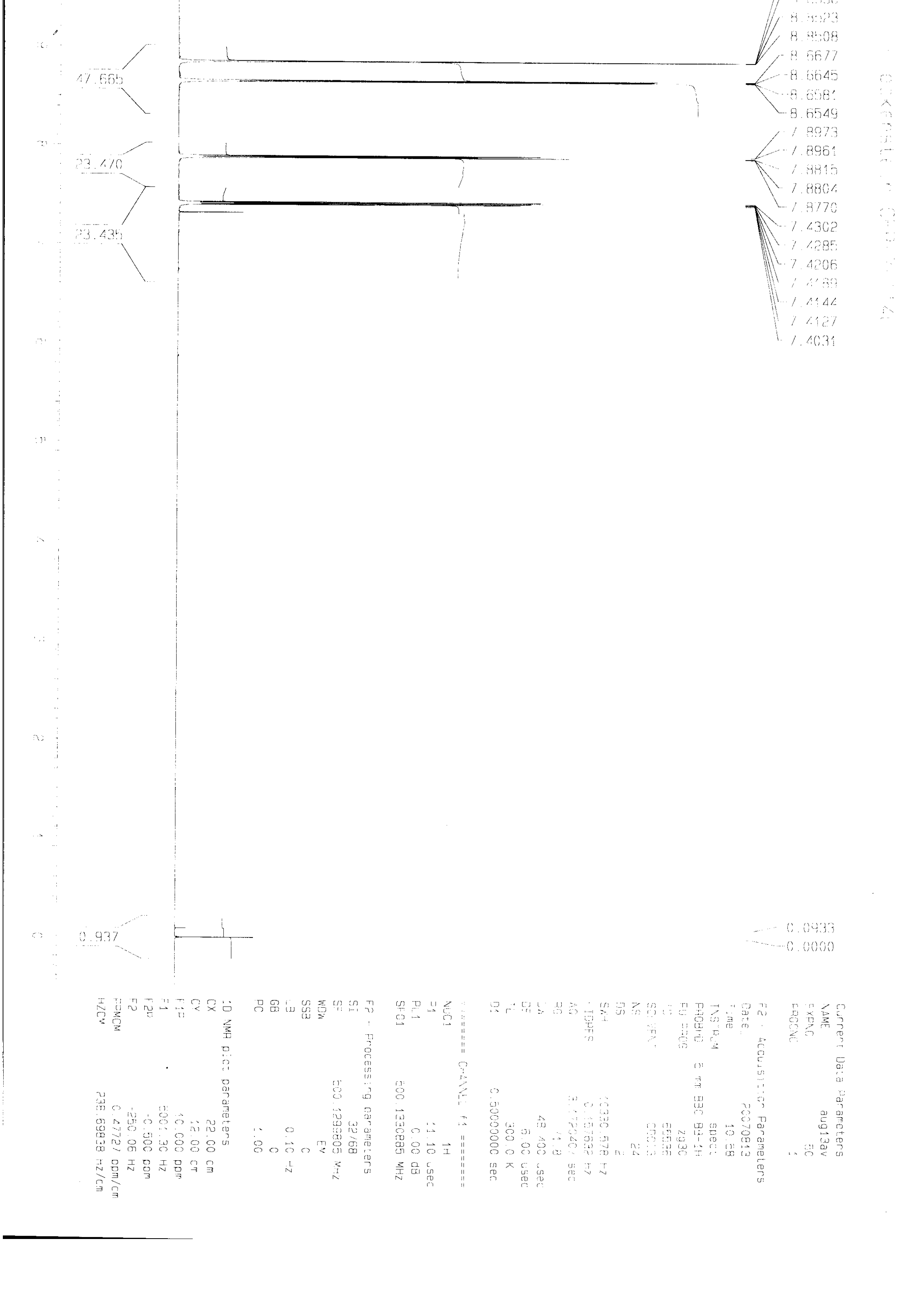
3-(2,6-Dimethyl-)pyridine



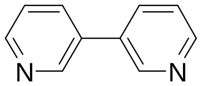
^{1}H-NMR



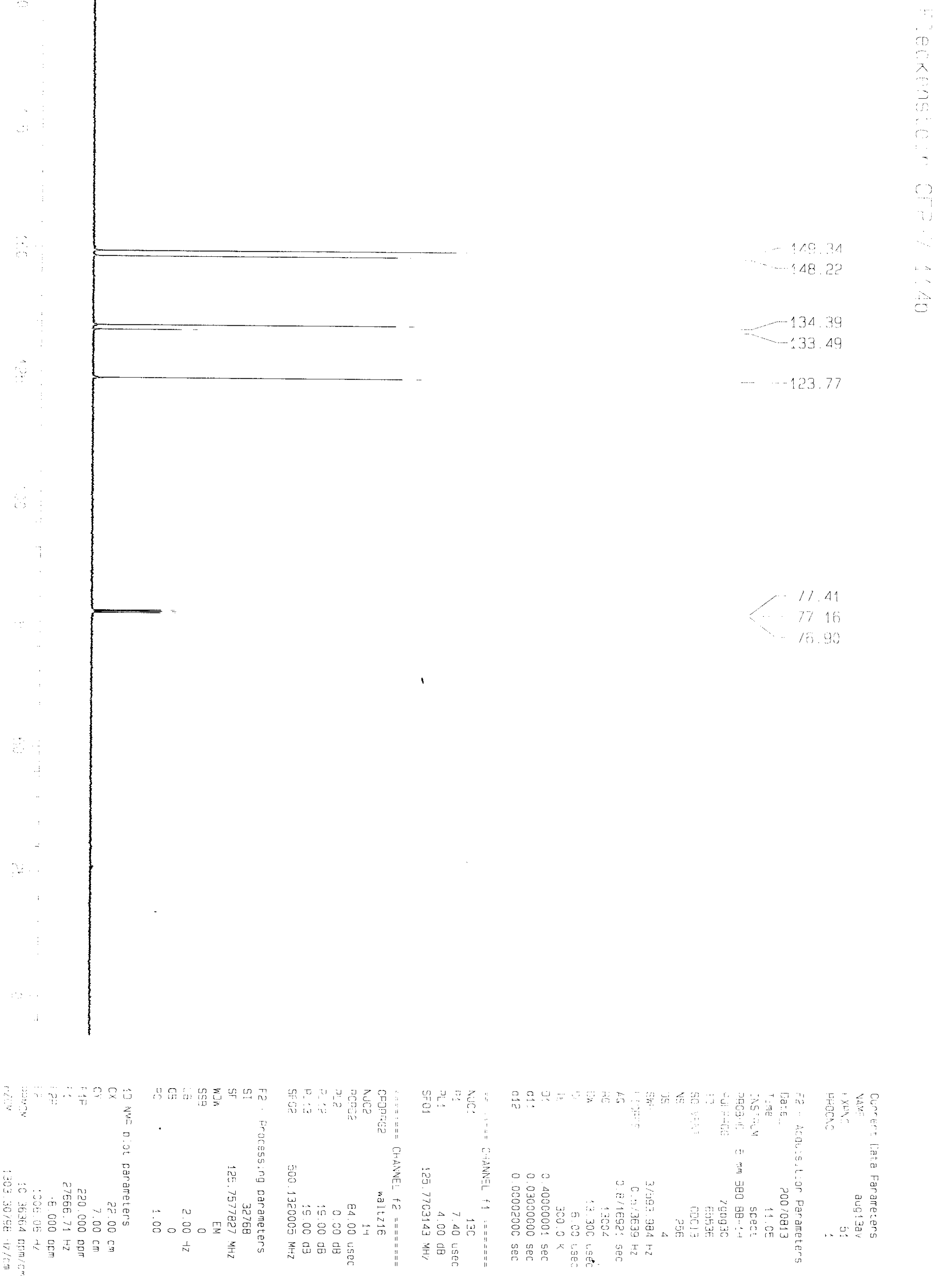
[3,3’]-Bipyridinyl



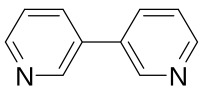
^{13}C-NMR



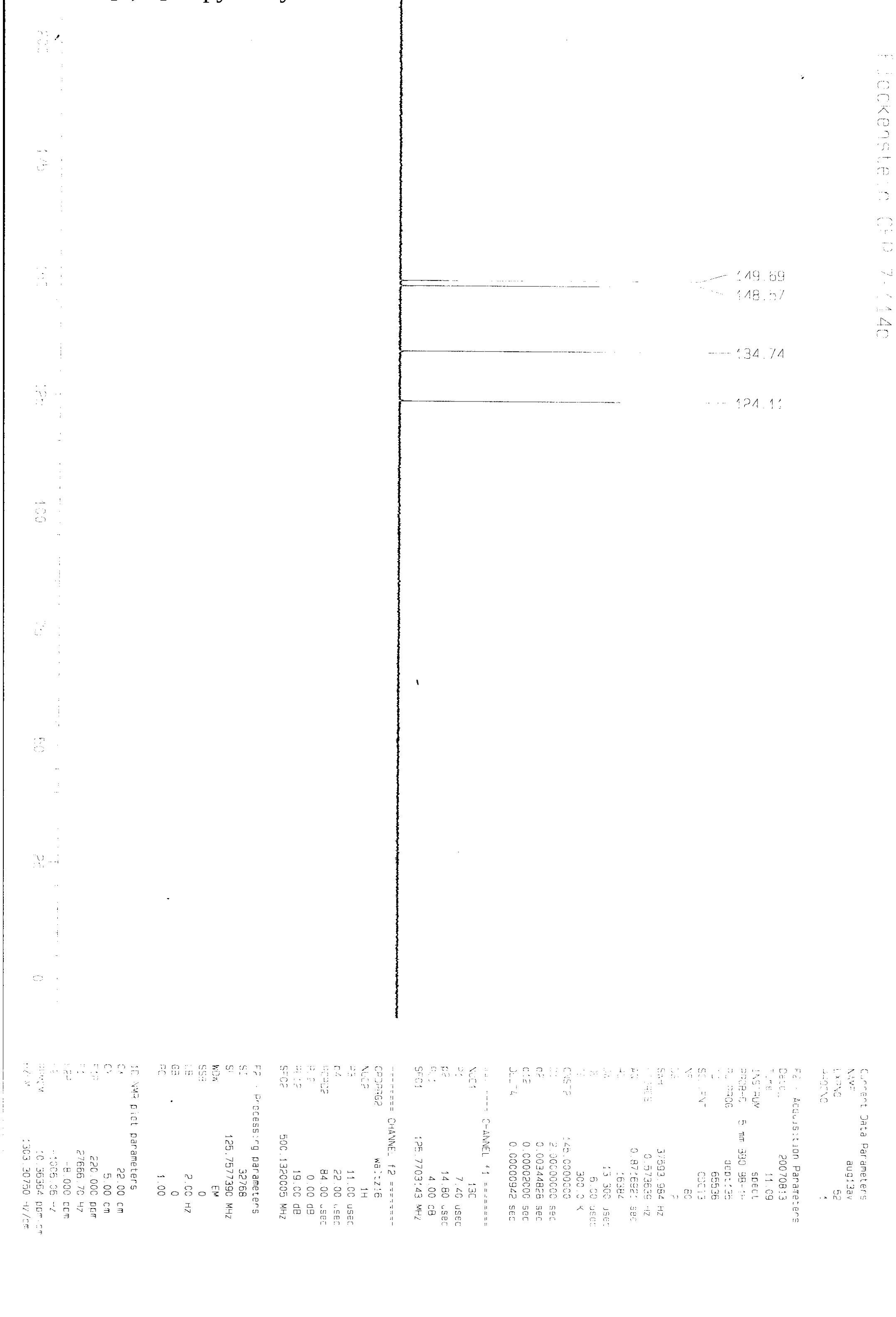
[3,3']-Bipyridinyl



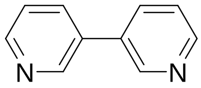
^{13}C-NMR (DEPT)



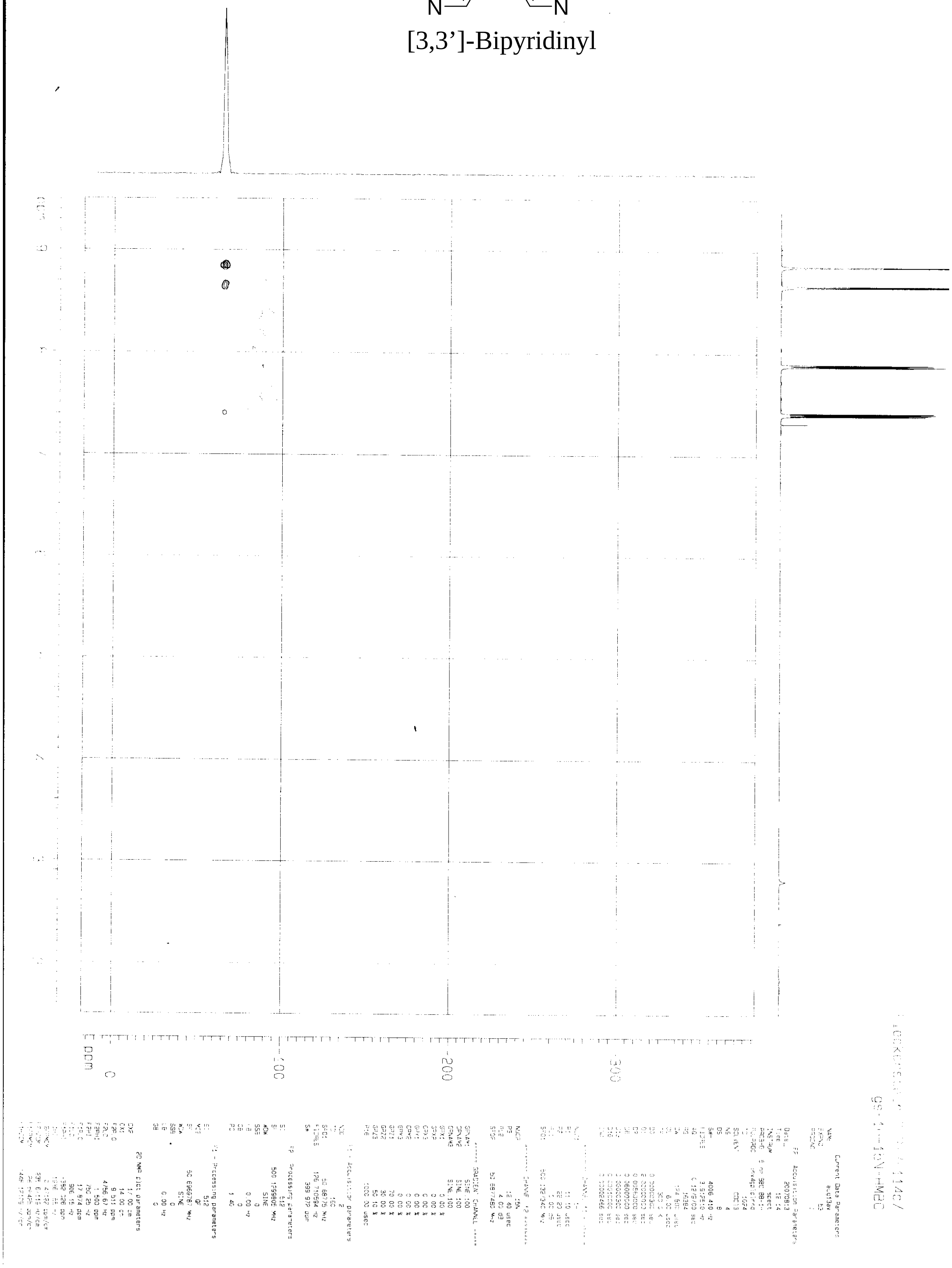
[3,3']-Bipyridinyl



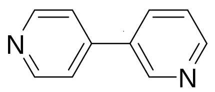
^{15}N-NMR (HMBC)



[3,3']-Bipyridinyl

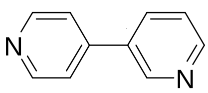


^{1}H-NMR

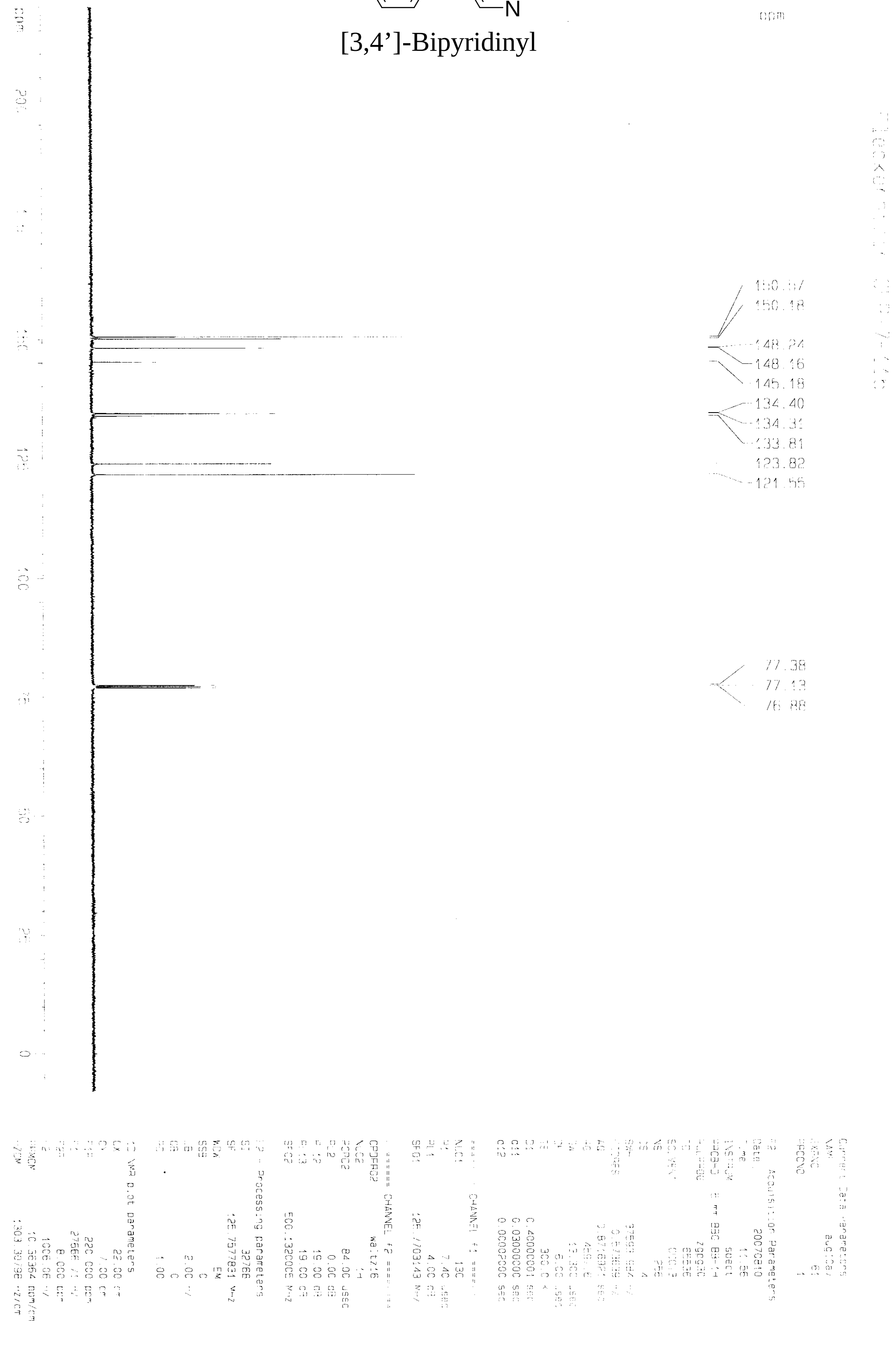


[3,4']-Bipyridinyl

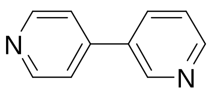
^{13}C-NMR



[3,4']-Bipyridinyl



^{13}C-NMR (DEPT)



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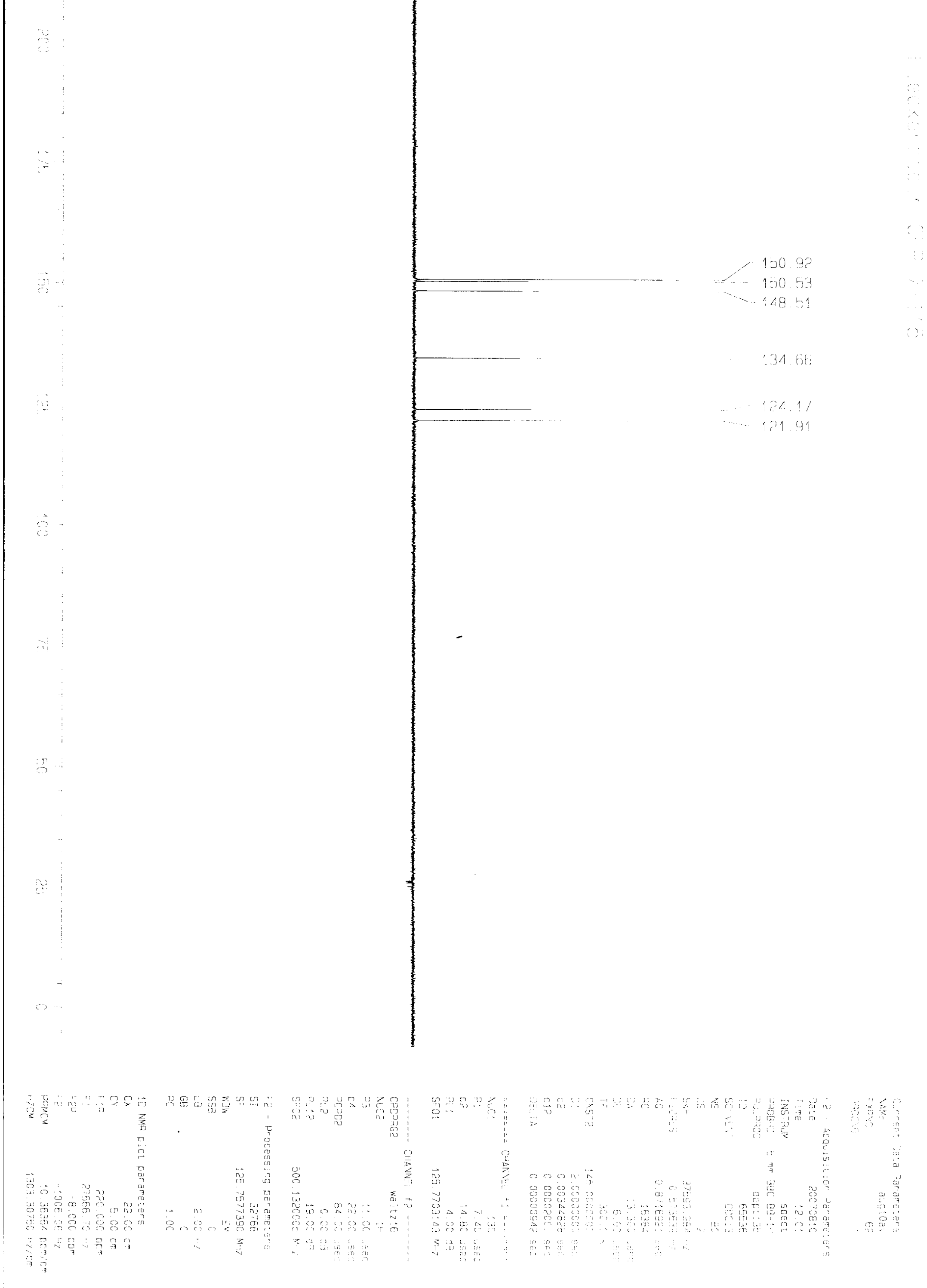

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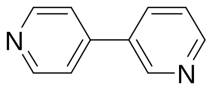
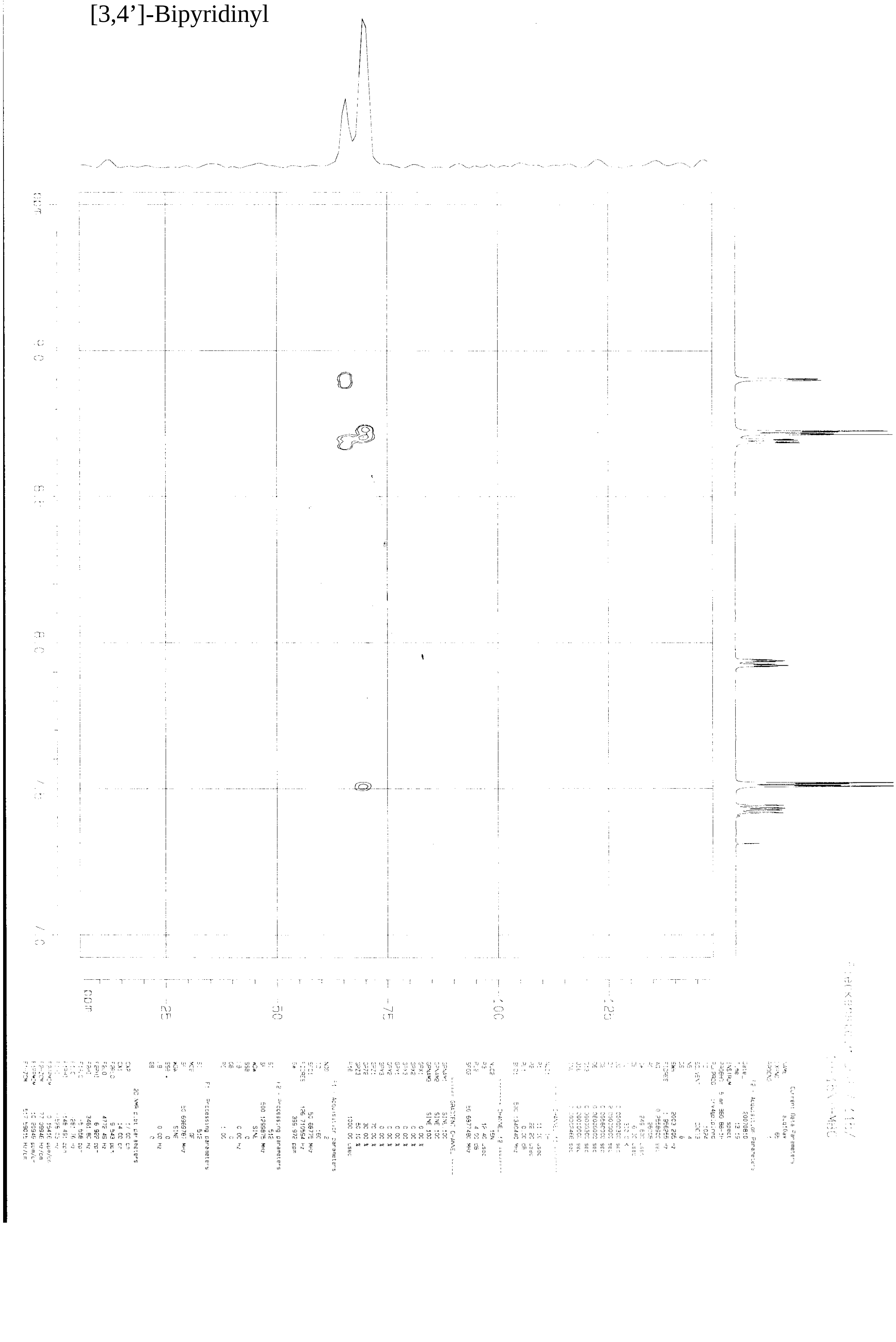


[3,4']-Bipyridinyl



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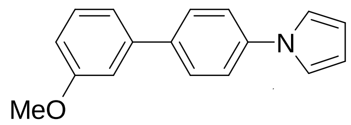
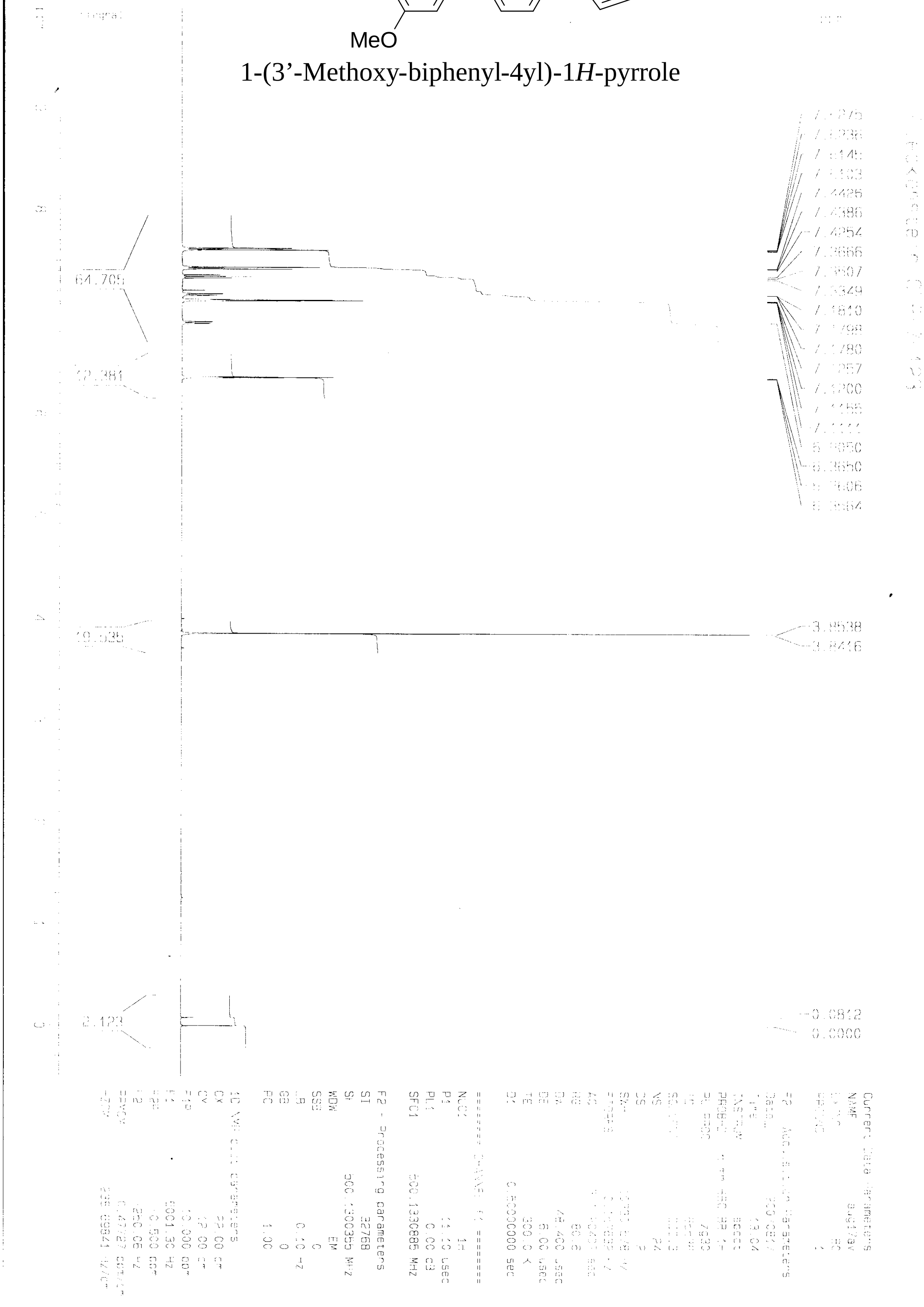
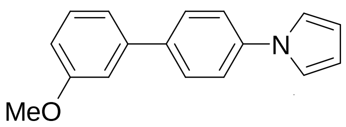


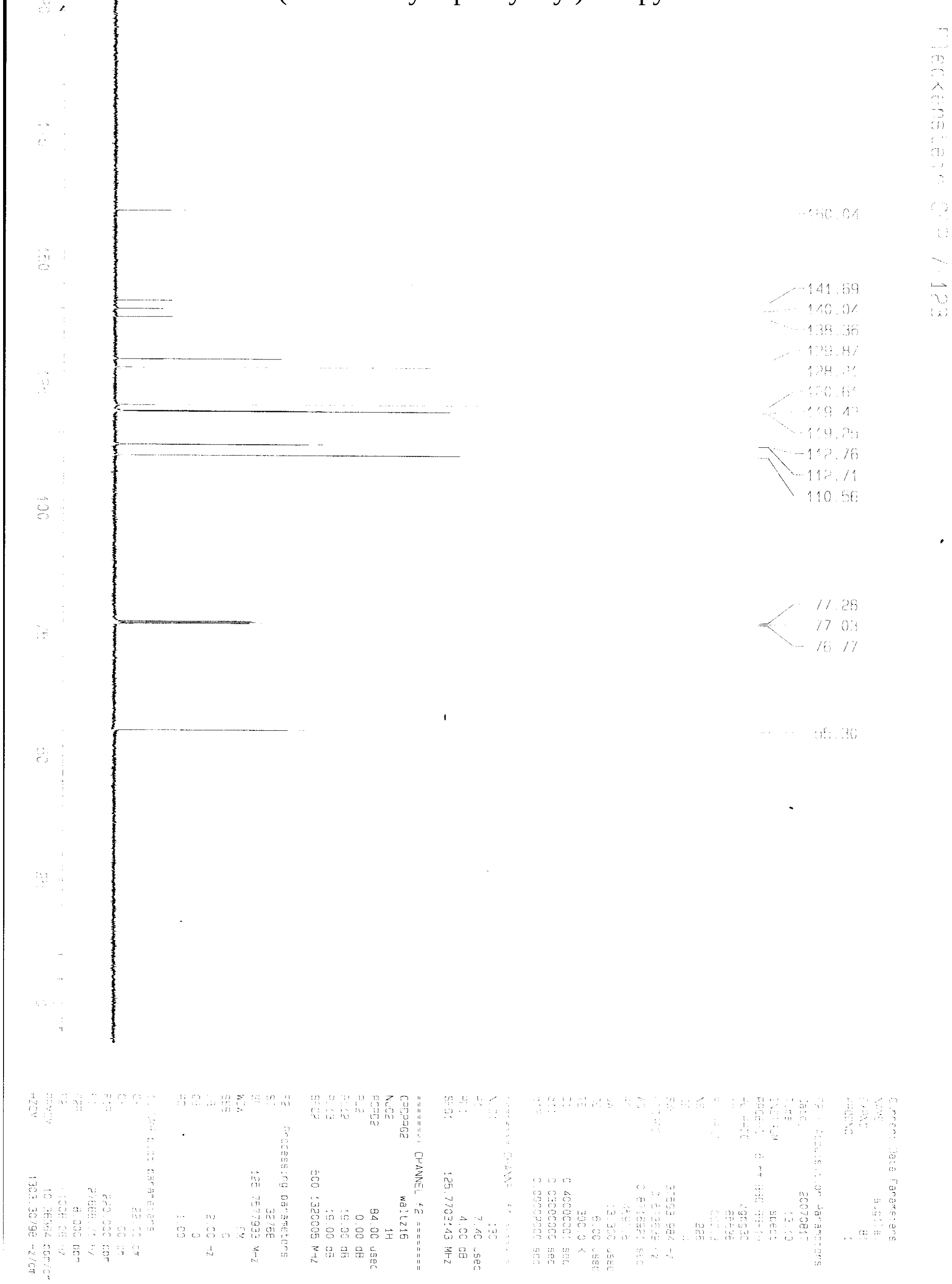
1-(3'-Methoxy-biphenyl-4yl)-1*H*-pyrrole



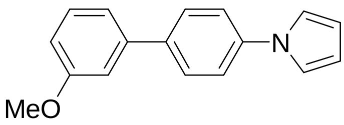
^{13}C-NMR



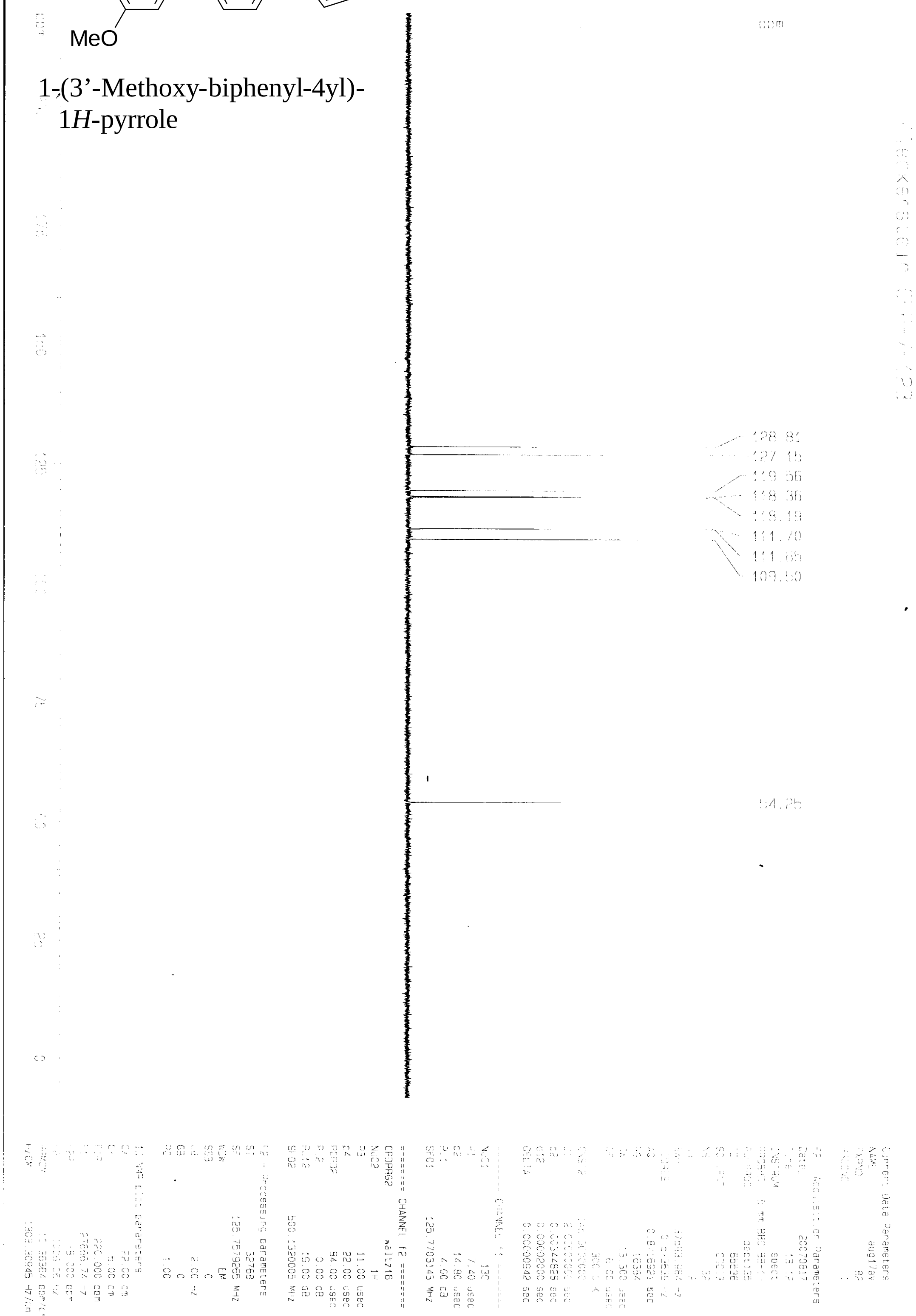
1-(3’-Methoxy-biphenyl-4yl)-1*H*-pyrrole



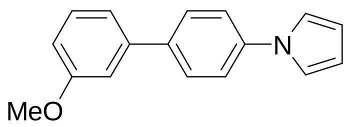
^{13}C-NMR (DEPT)



1-(3’-Methoxy-biphenyl-4yl)-1*H*-pyrrole

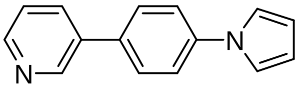


^{15}N-NMR (HMBC)

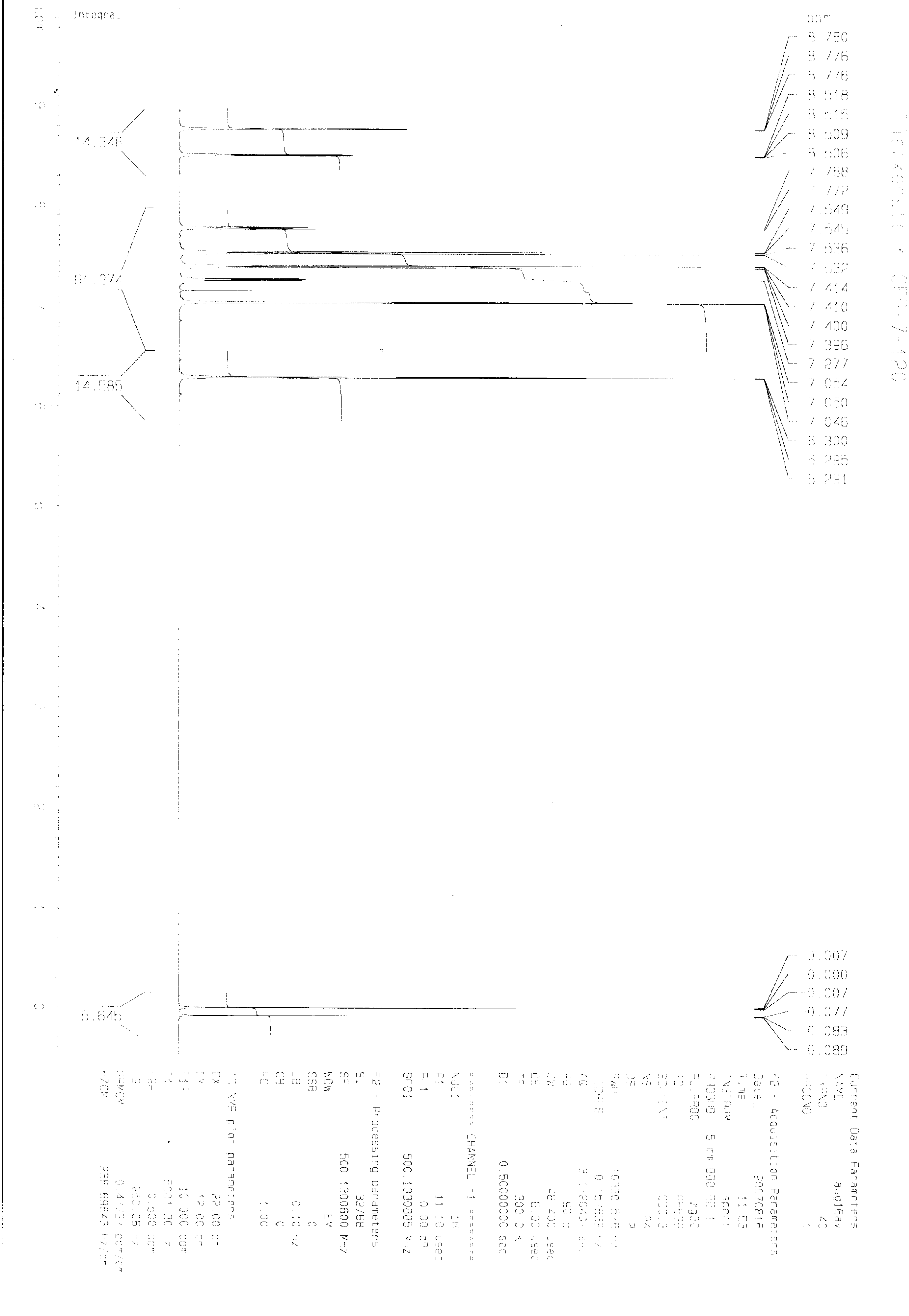


1-(3'-Methoxy-biphenyl-4yl)-1*H*-pyrrole

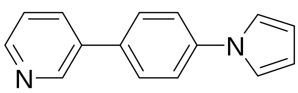
^{1}H-NMR



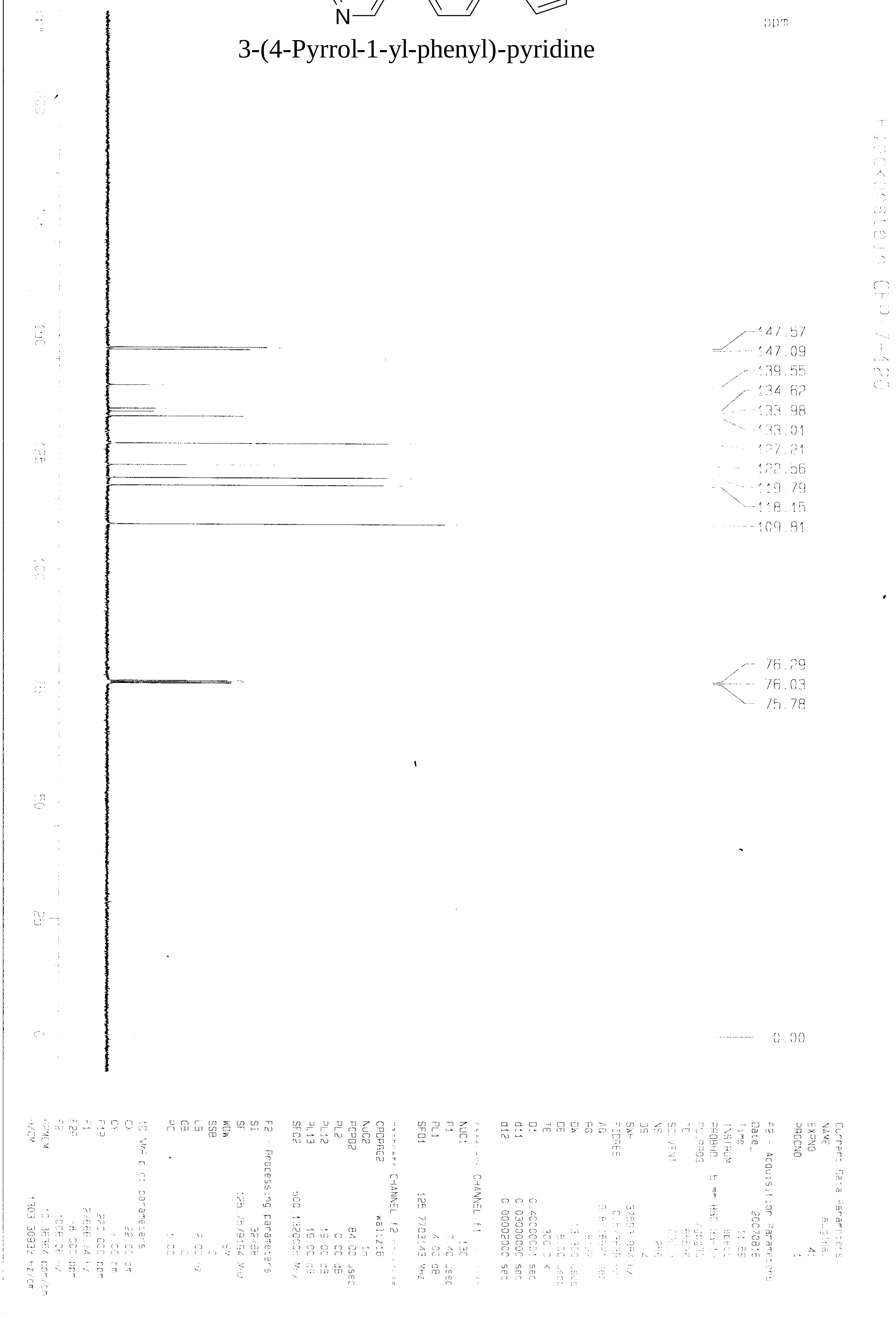
3-(4-Pyrrol-1-yl-phenyl)-pyridine



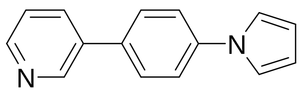
^{13}C-NMR



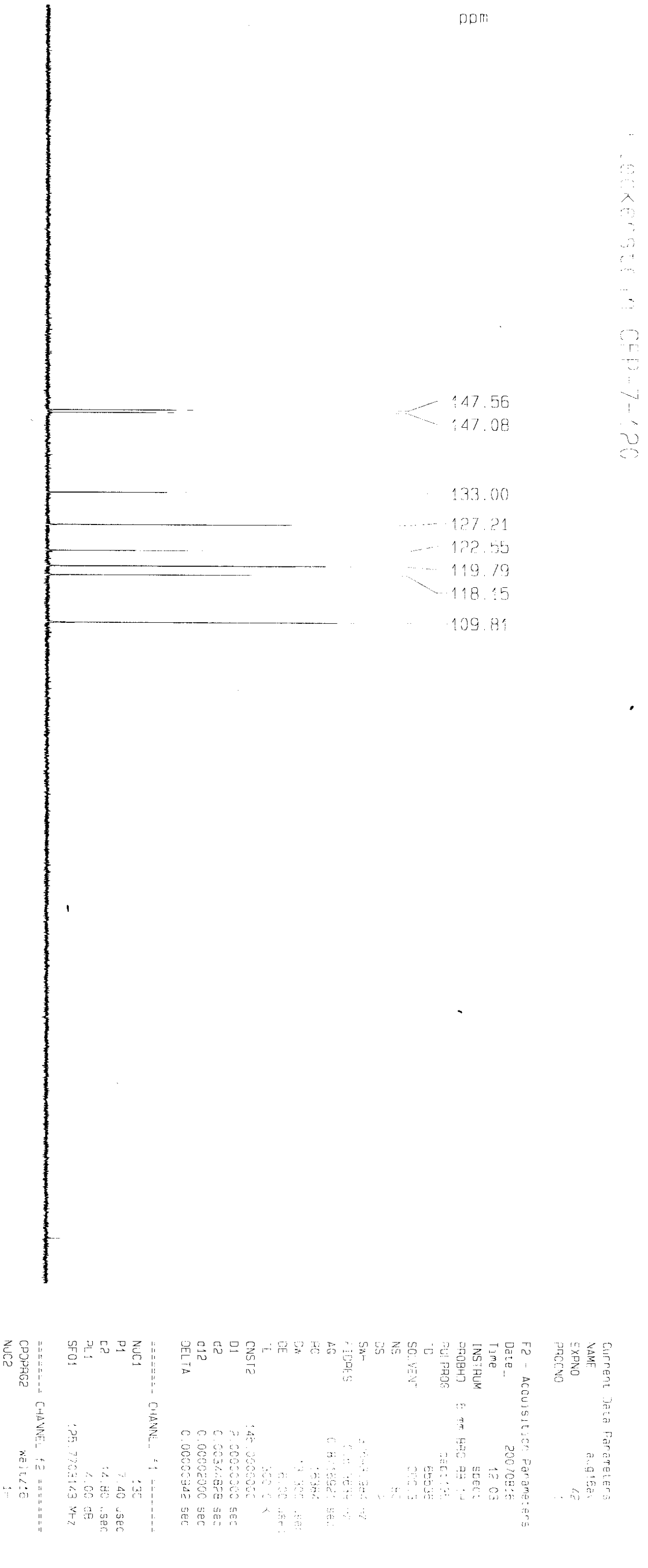
3-(4-Pyrrol-1-yl-phenyl)-pyridine



^{13}C-NMR (DEPT)



3-(4-Pyrrol-1-yl-phenyl)-pyridine



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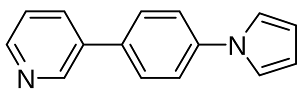
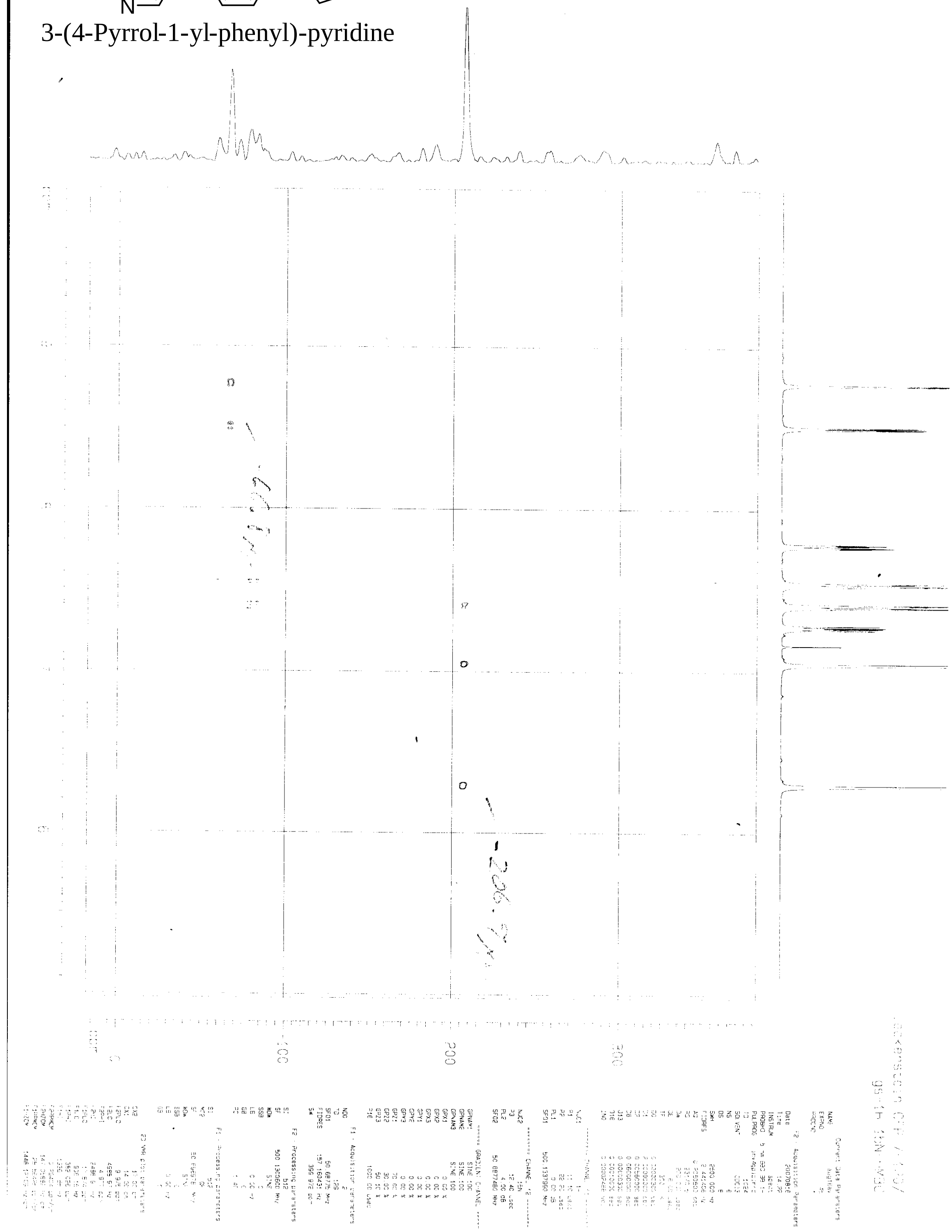
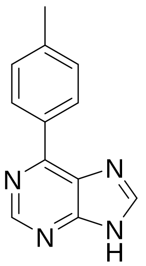


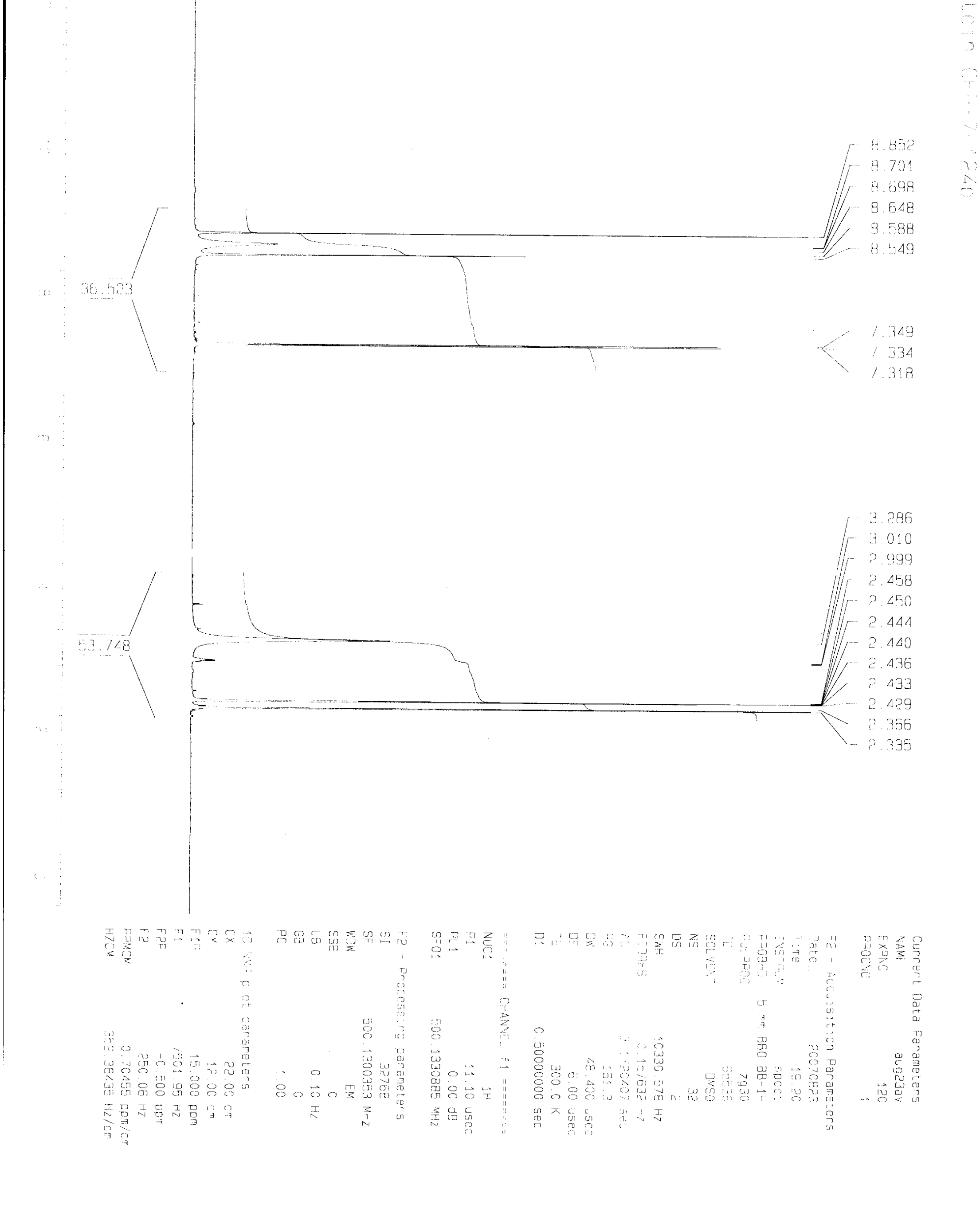
3-(4-Pyrrol-1-yl-phenyl)-pyridine

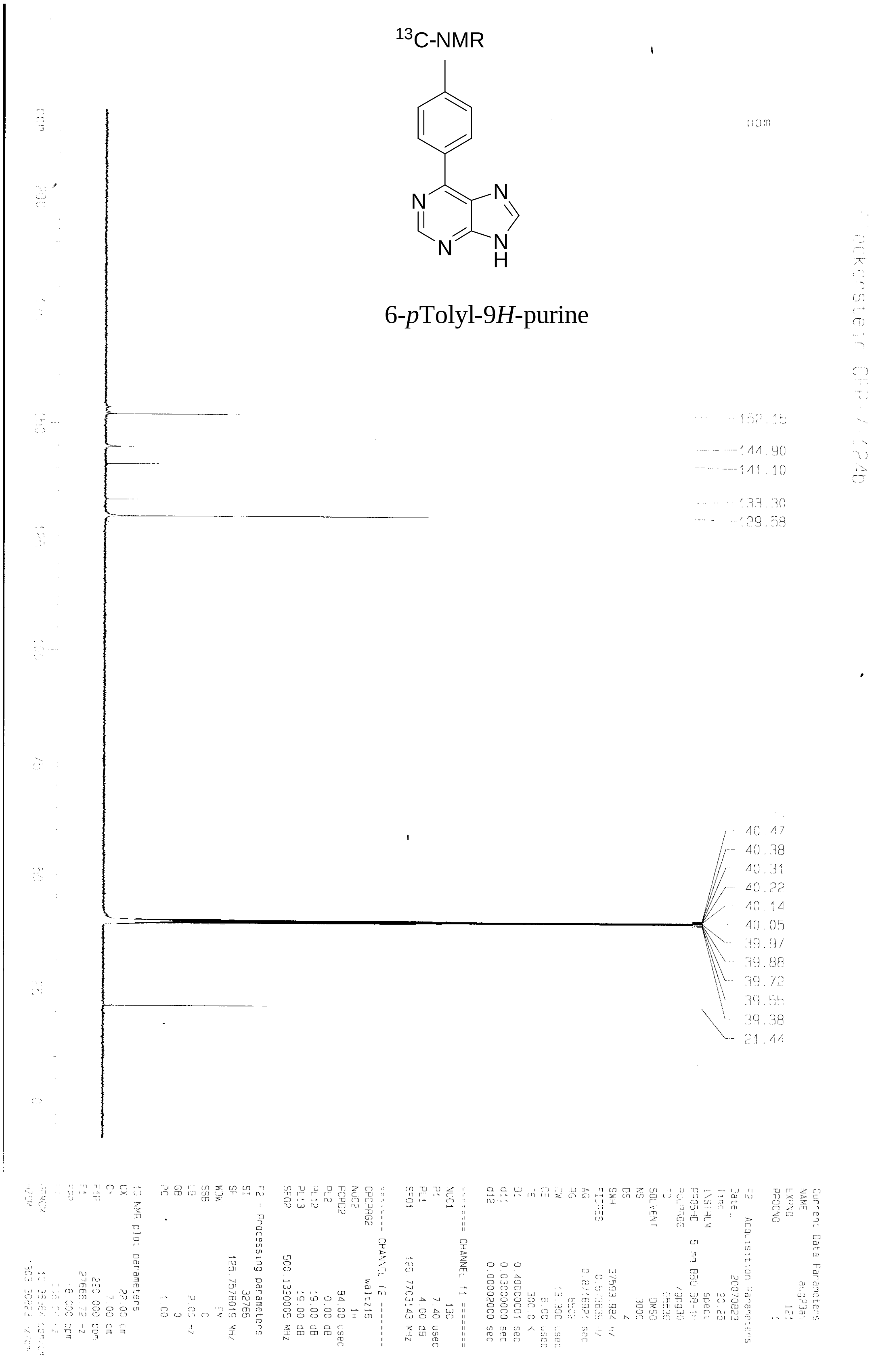


^{1}H-NMR



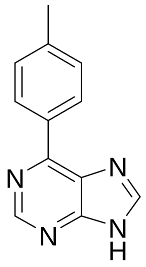
6-*p*Tolyl-9*H*-purine





6-*p*Tolyl-9*H*-purine

^{13}C-NMR (DEPT)



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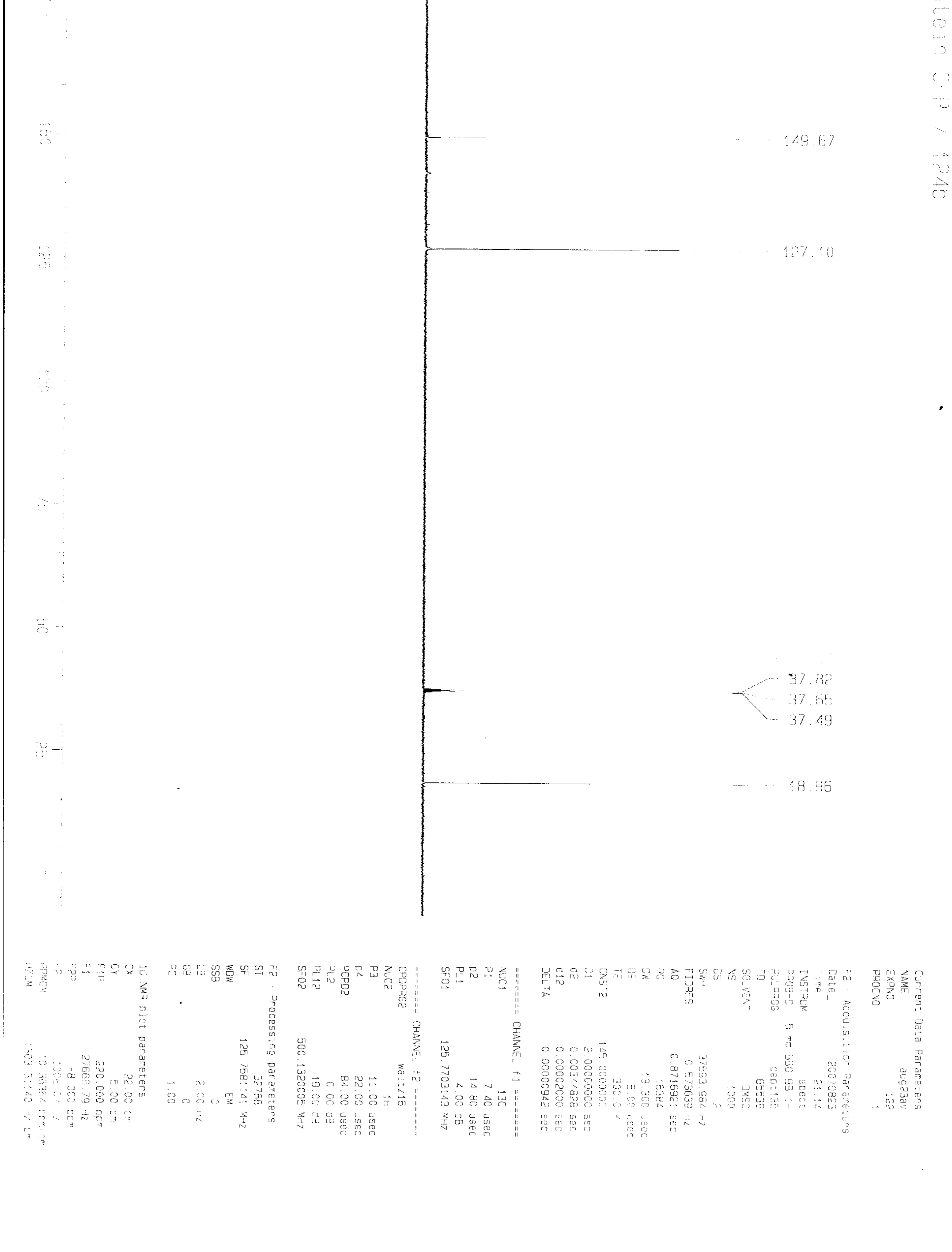

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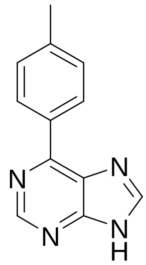

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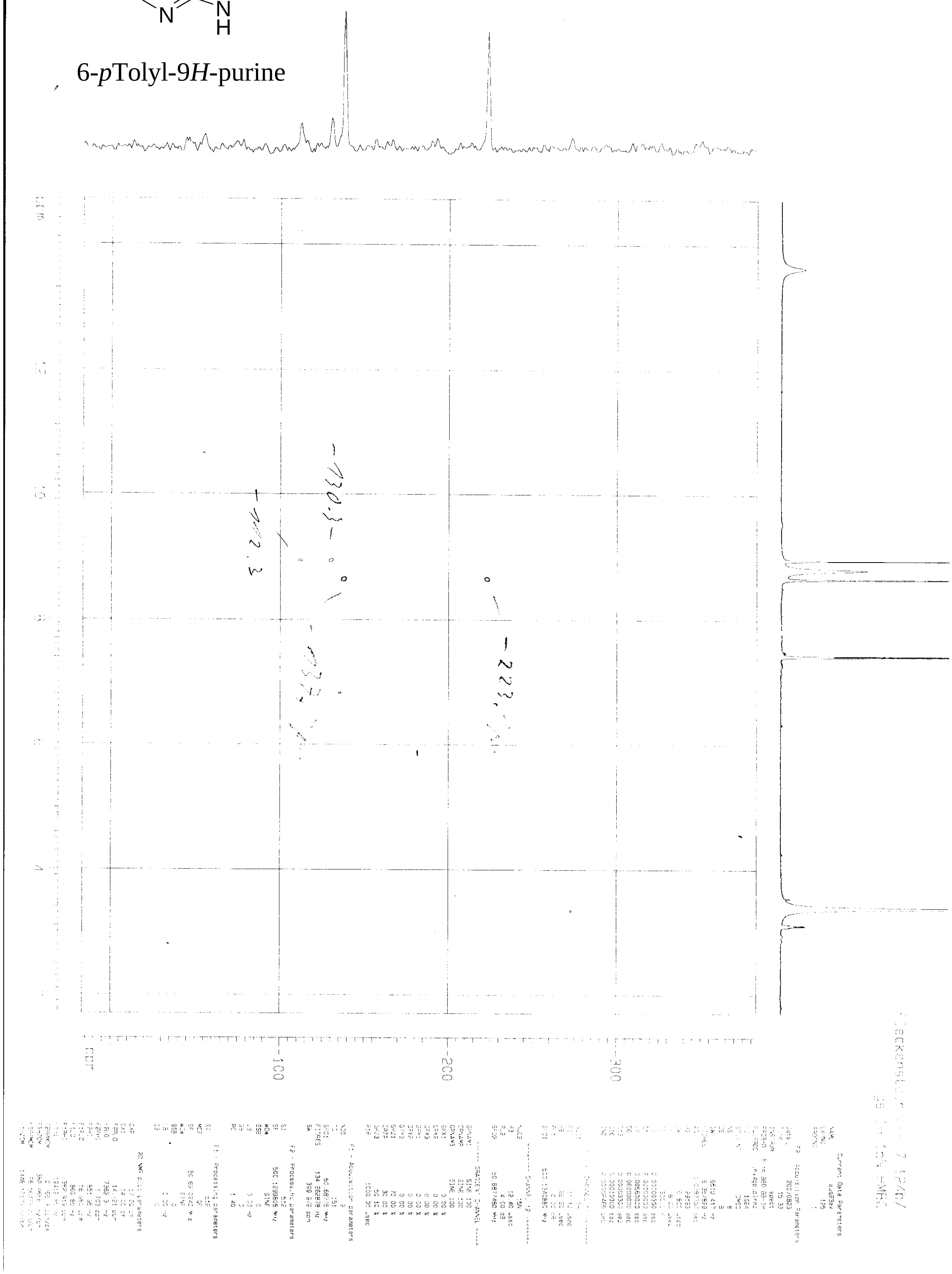
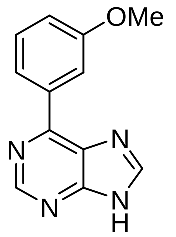
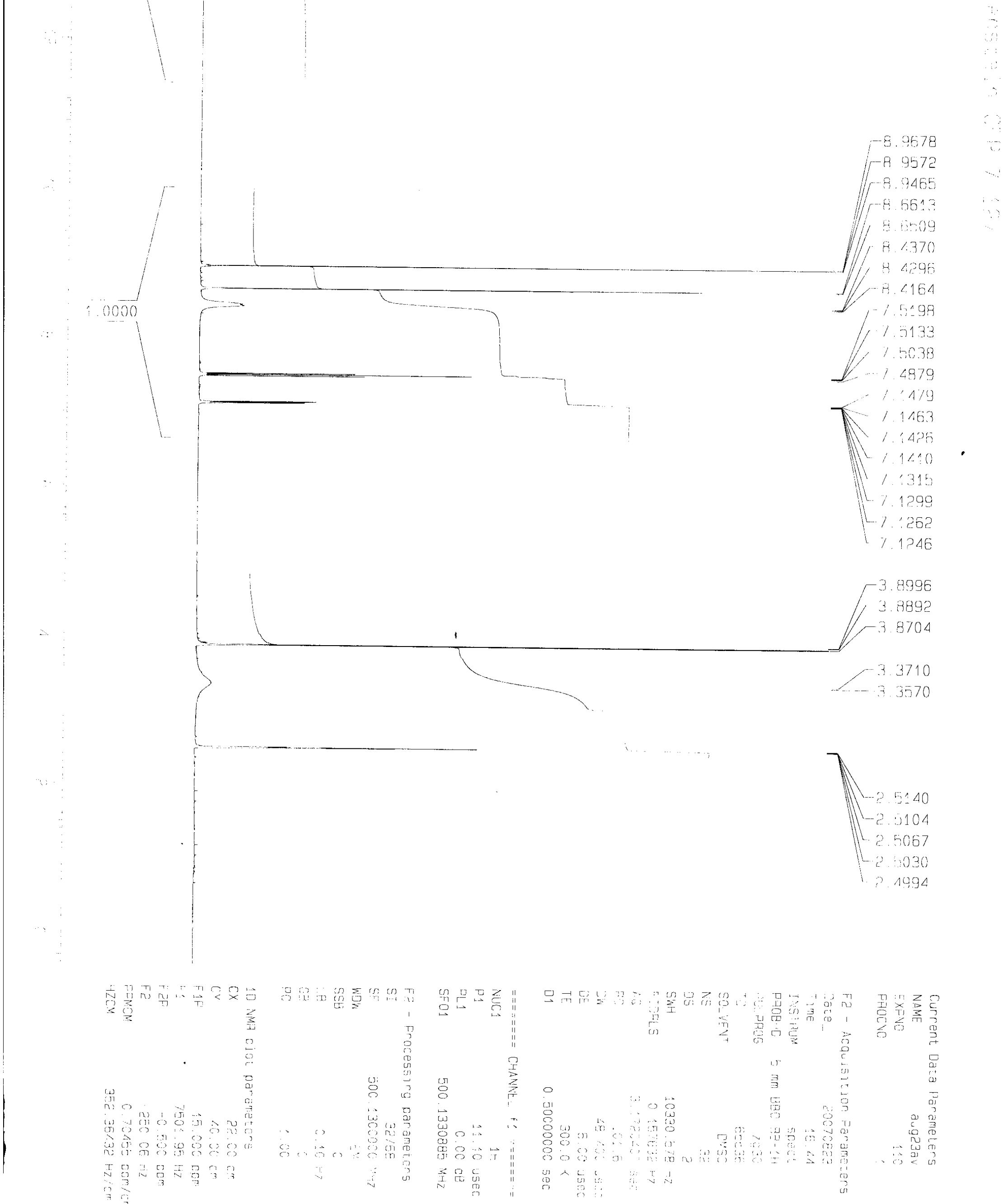


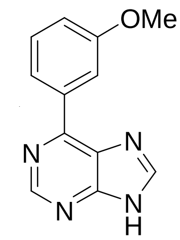
^{1}H-NMR



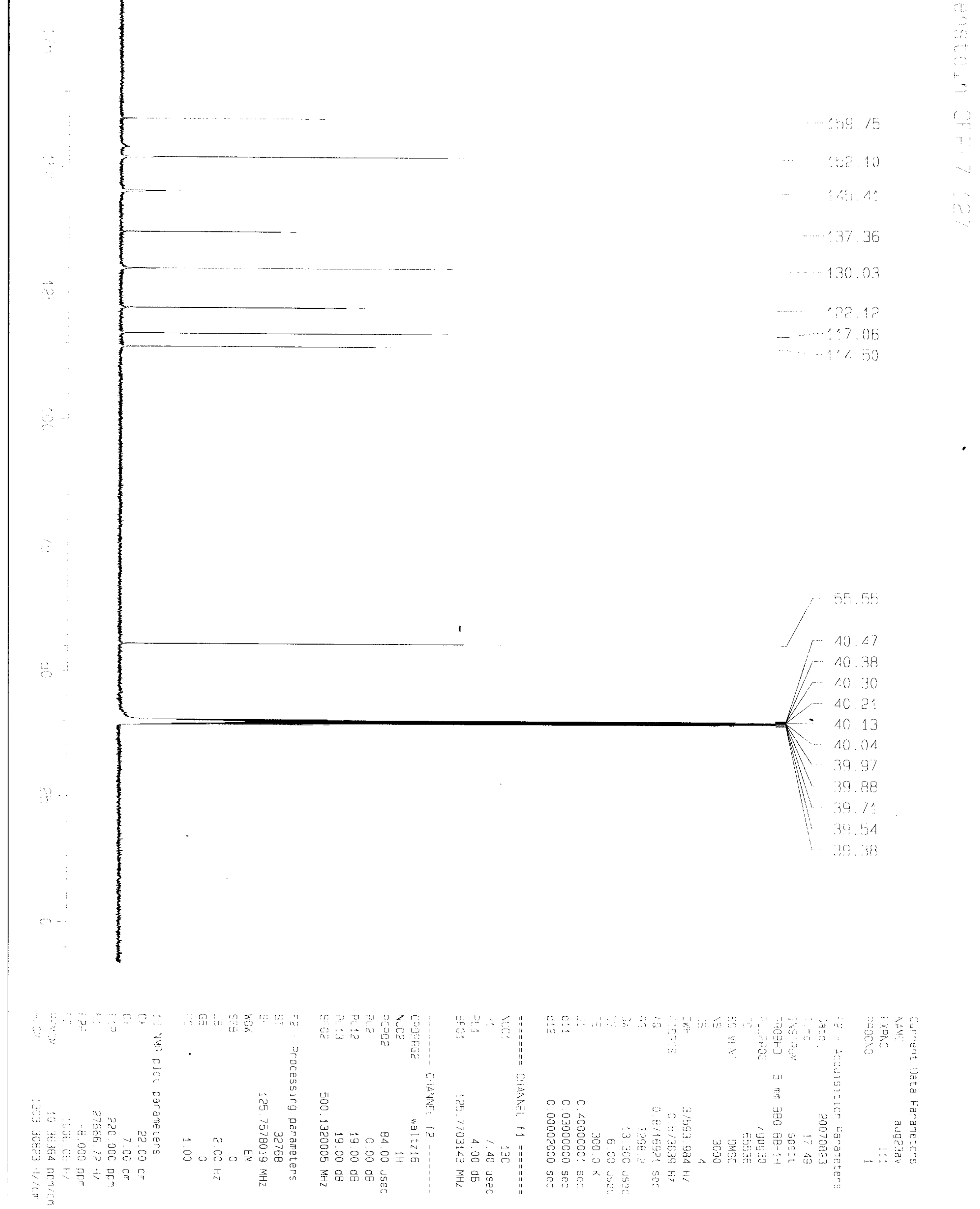
6-(3-Methoxy-phenyl-)9*H*-purine



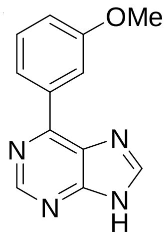
^{13}C-NMR



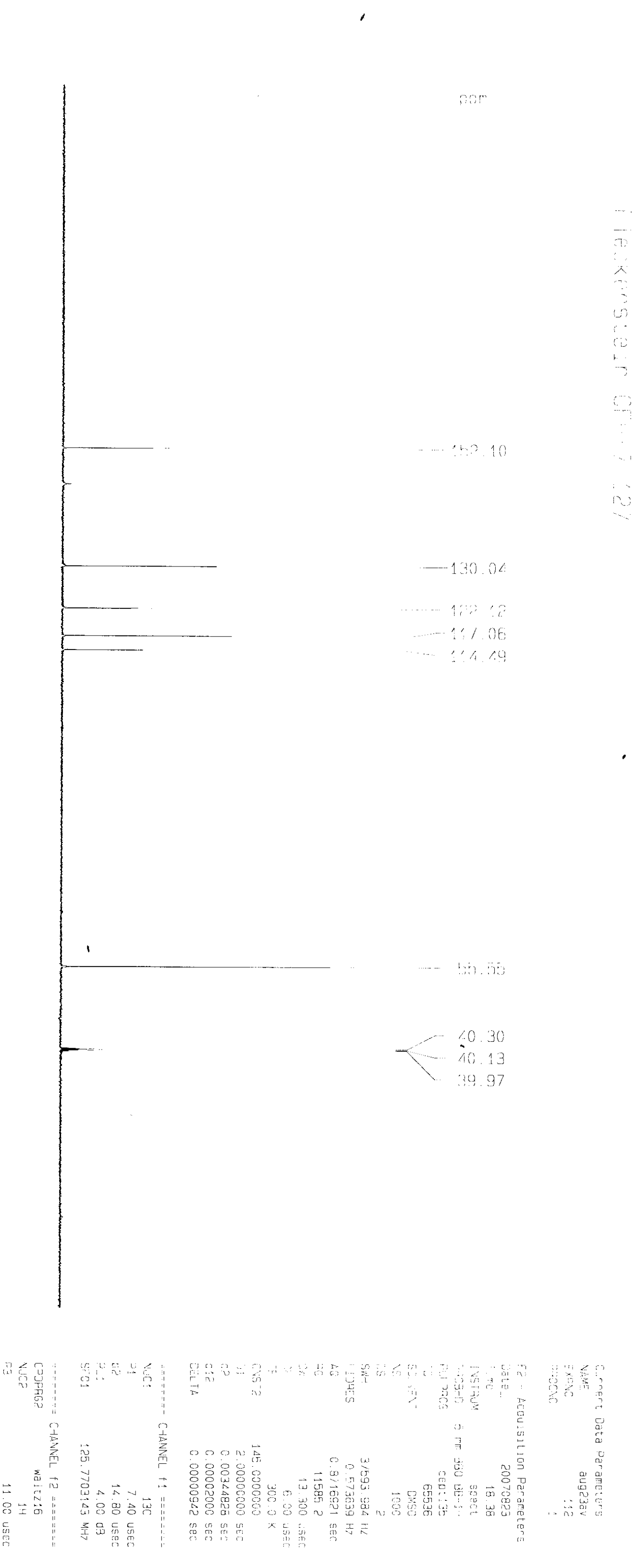
6-(3-Methoxy-phenyl-)9*H*-purine



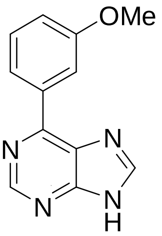
[13]C-NMR (DEPT)



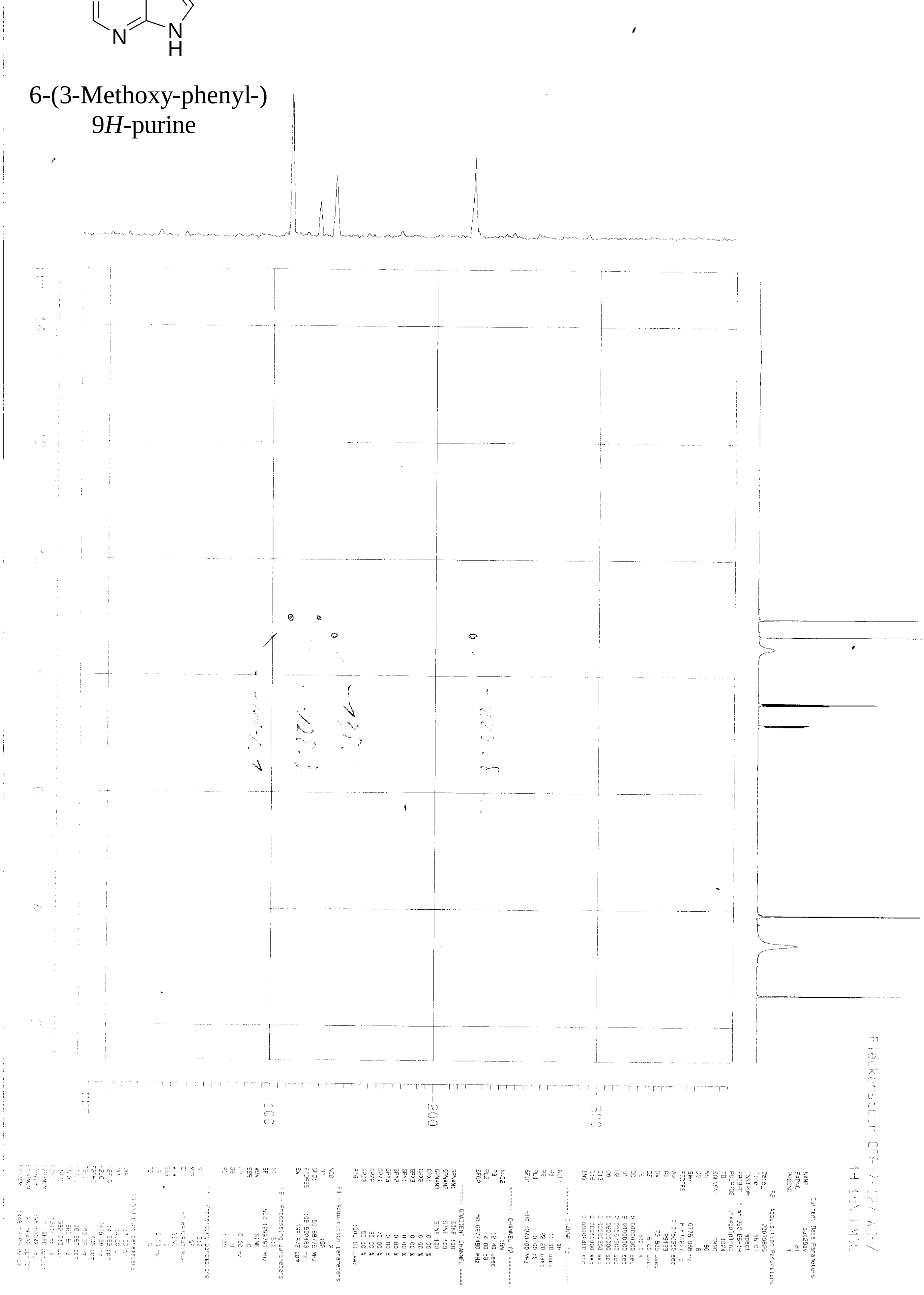
6-(3-Methoxy-phenyl-) 9*H*-purine



^{15}N-NMR (HMBC)

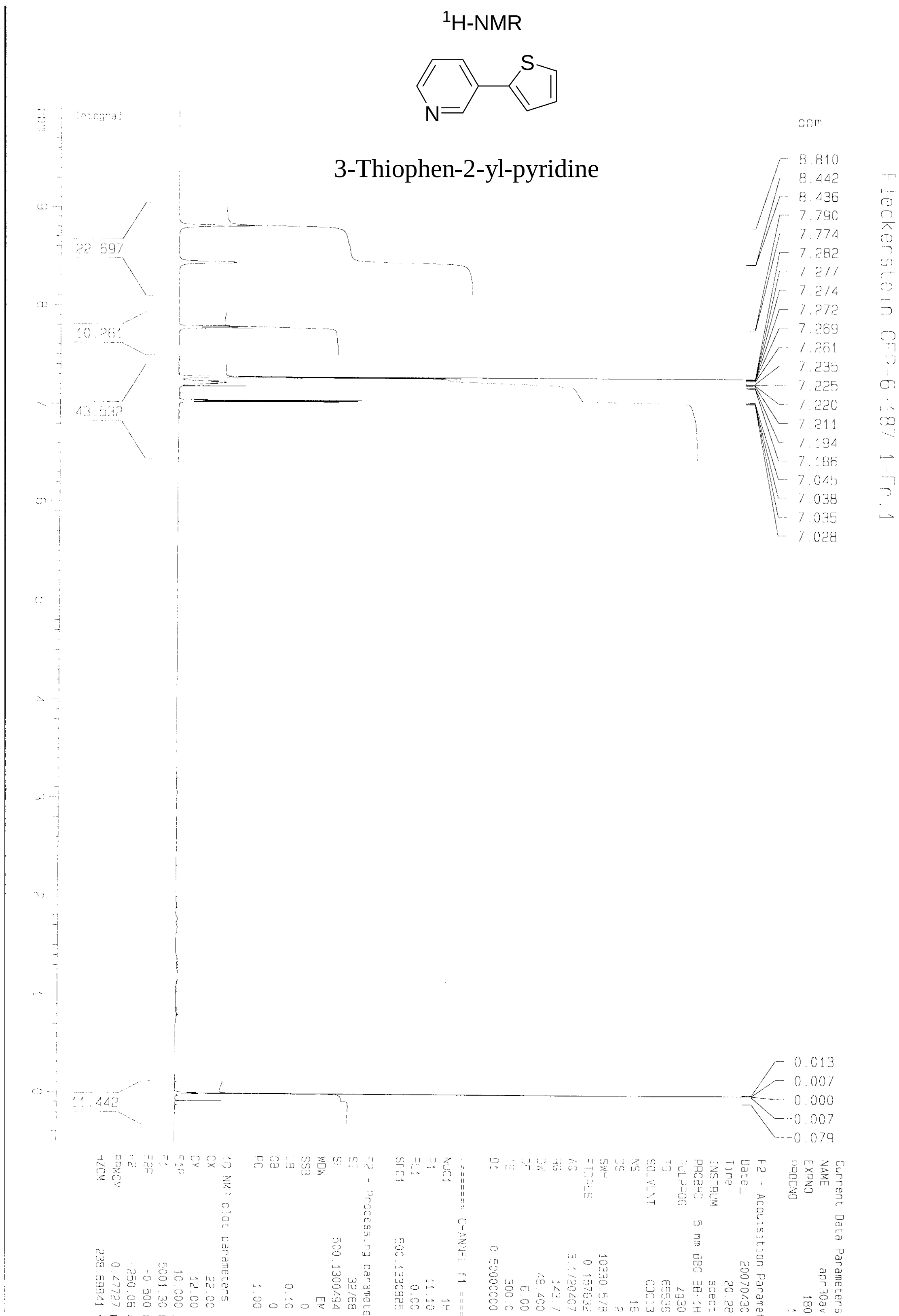


6-(3-Methoxy-phenyl-)
9*H*-purine

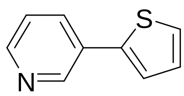


^{1}H-NMR

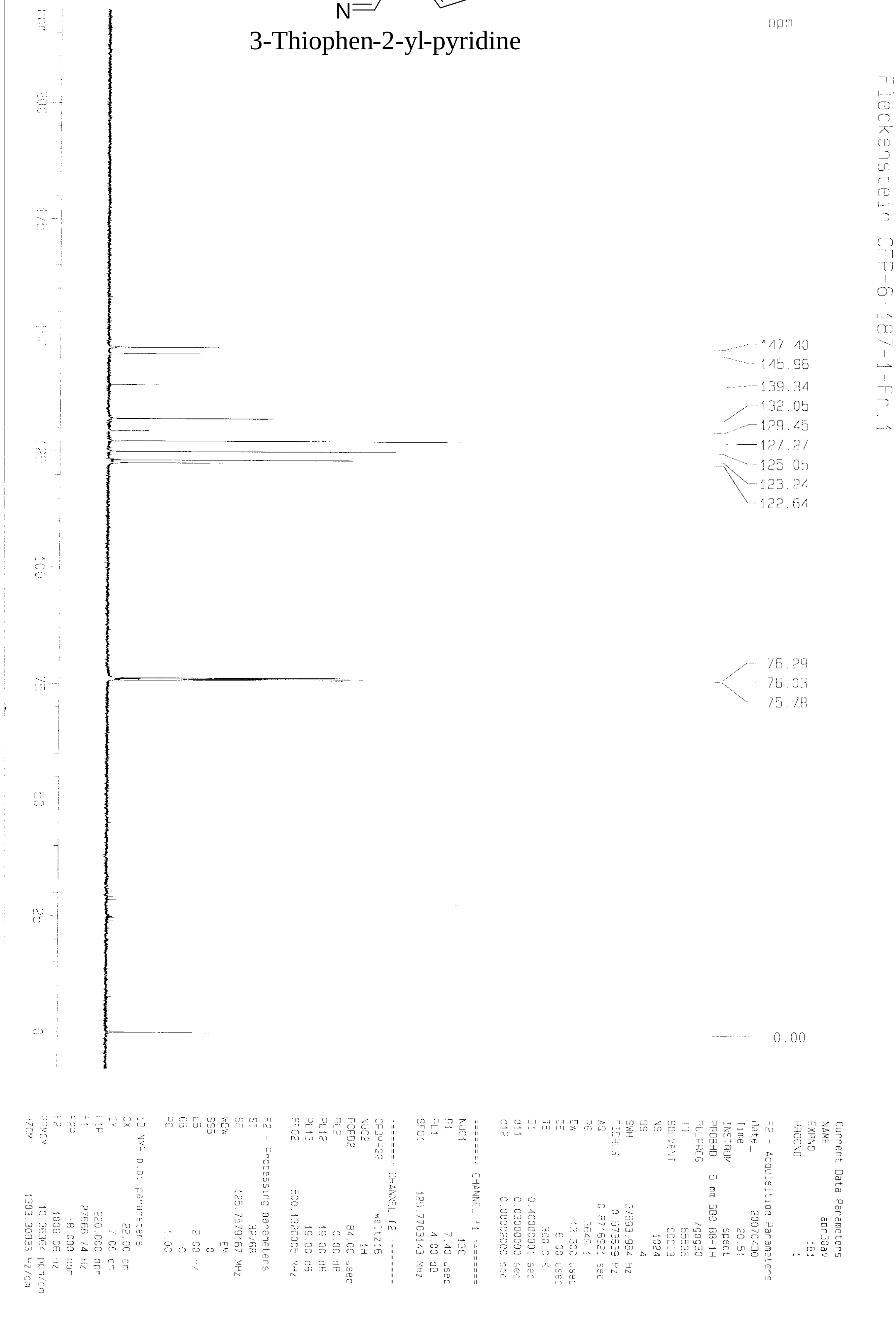
3-Thiophen-2-yl-pyridine



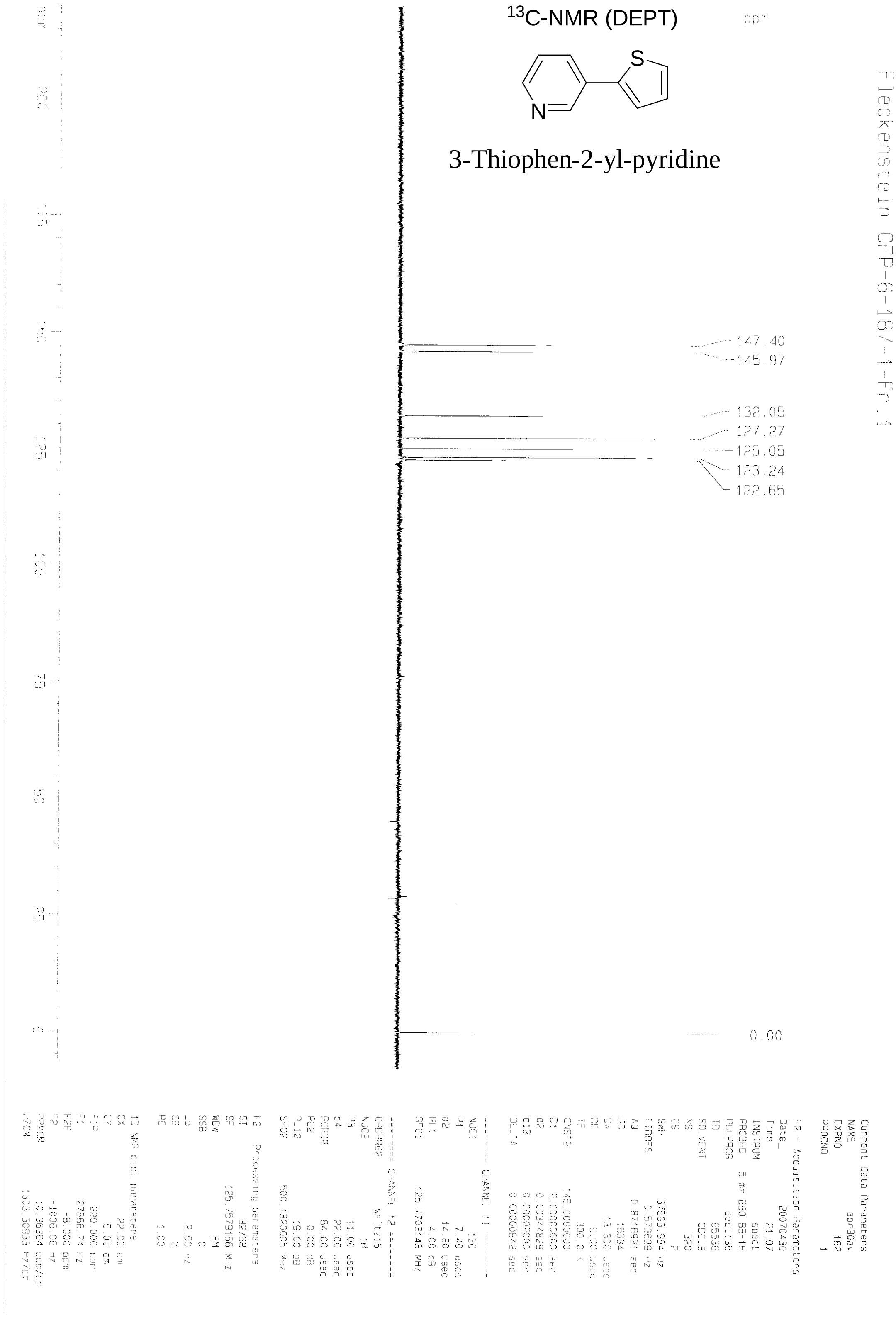
^{13}C-NMR



3-Thiophen-2-yl-pyridine

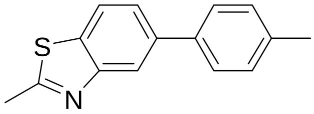


^{13}C-NMR (DEPT)

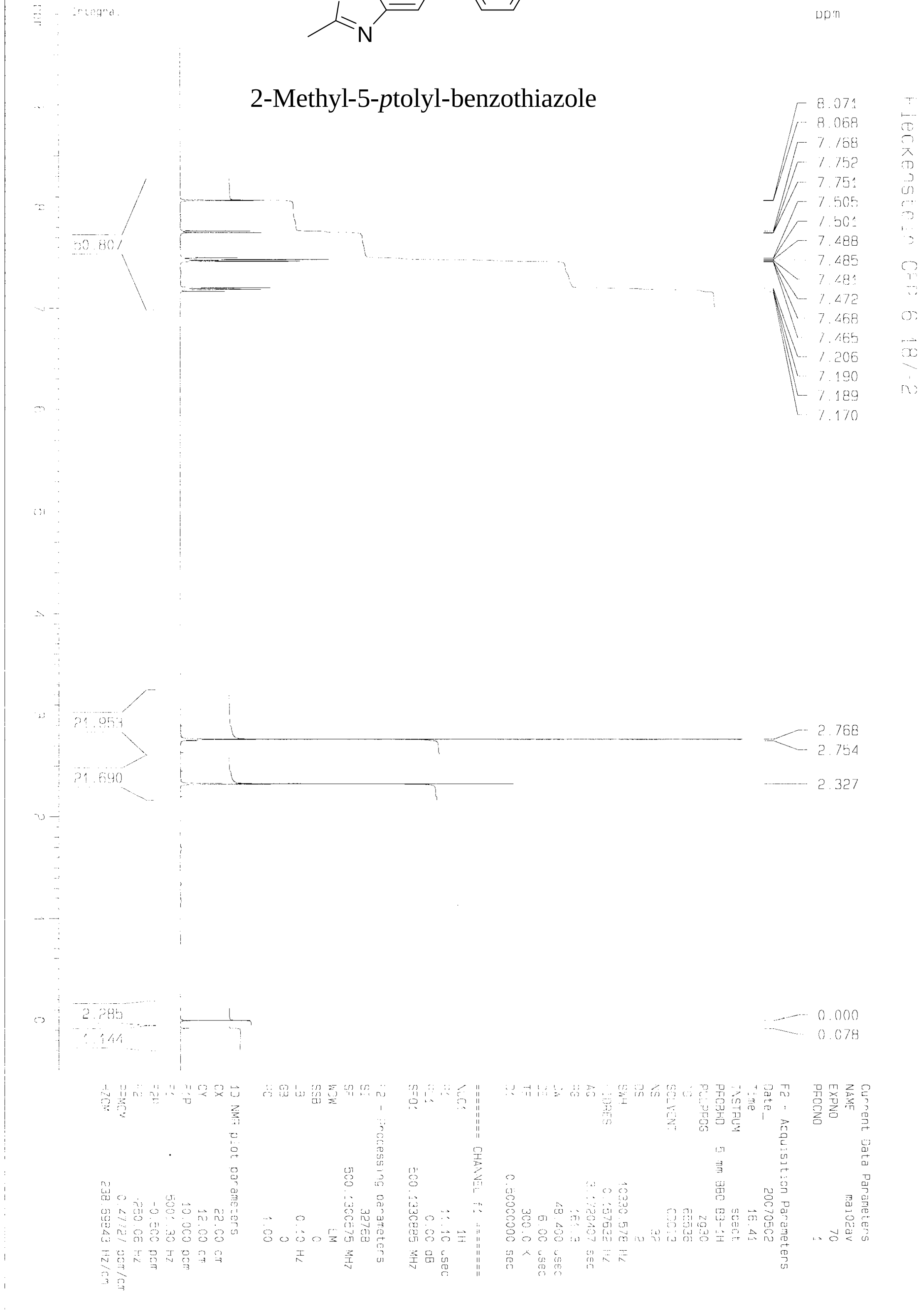


3-Thiophen-2-yl-pyridine

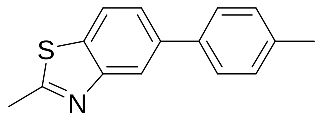
[1]H-NMR



2-Methyl-5-*p*tolyl-benzothiazole



^{13}C-NMR



2-Methyl-5-*p*tolyl-benzothiazole

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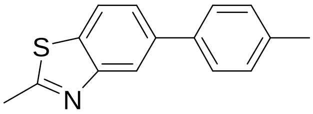
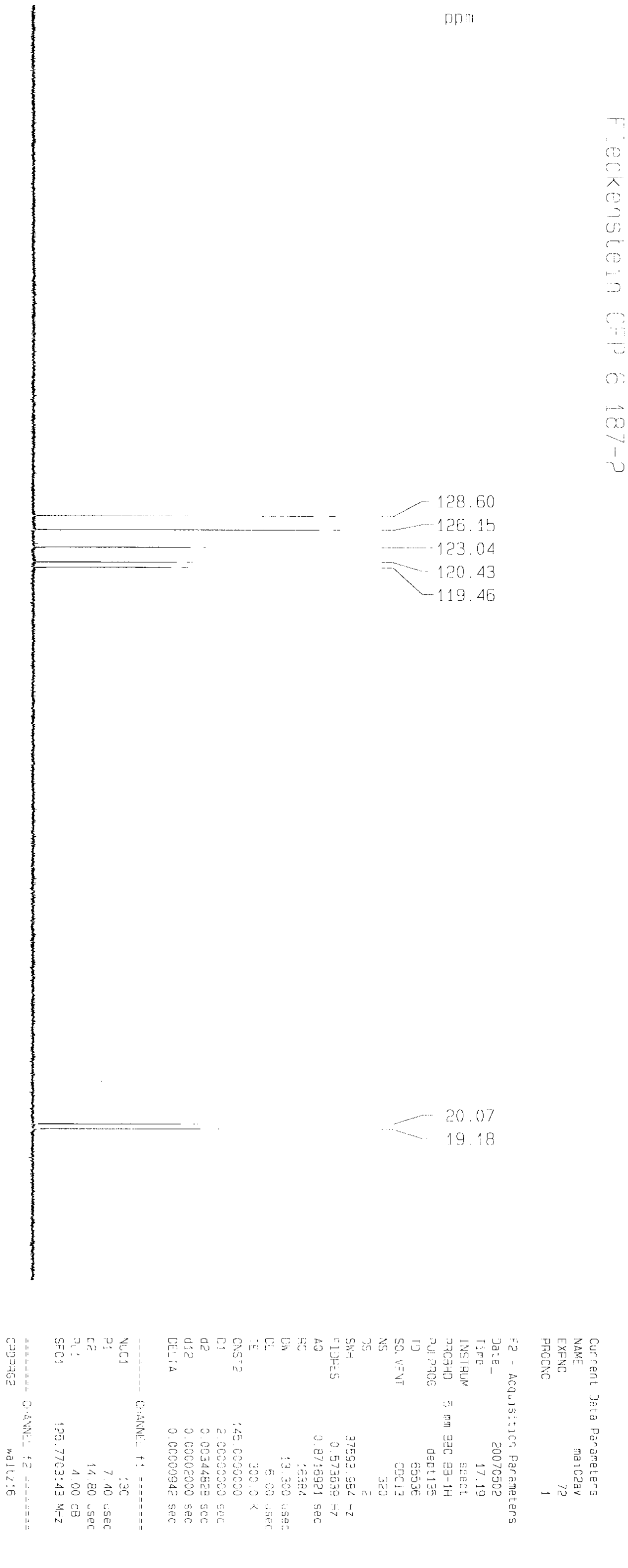
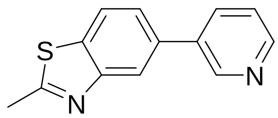


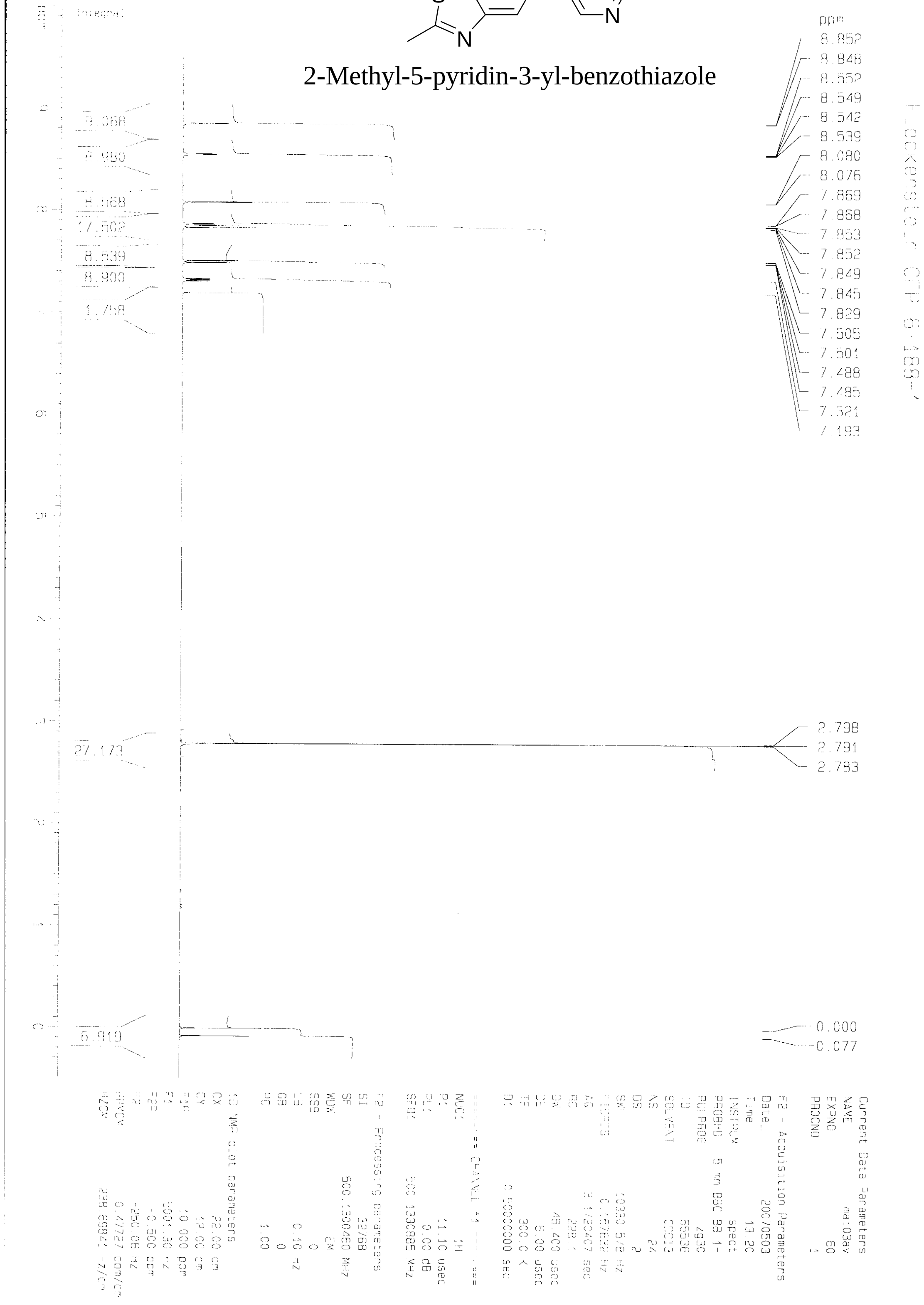
2-Methyl-5-*p*tolyl-benzothiazole



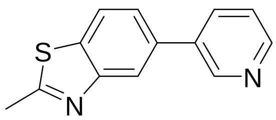
[1]H-NMR



2-Methyl-5-pyridin-3-yl-benzothiazole



^{13}C-NMR



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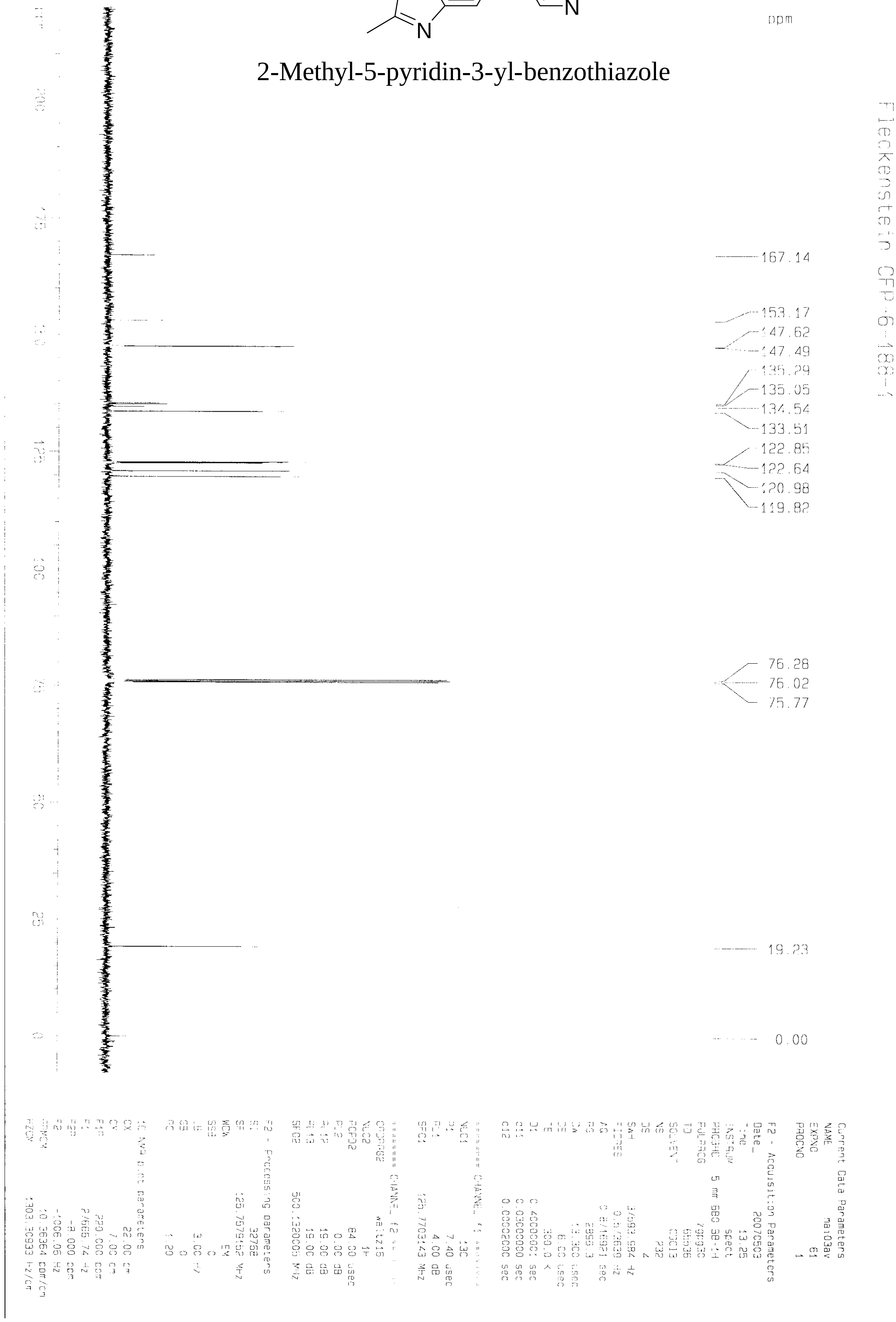

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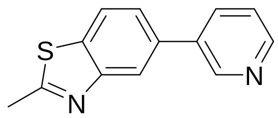

2-Methyl-5-pyridin-3-yl-benzothiazole