Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Simple and Efficient Synthesis of Tetrahydro-β-Carbolines via the Pictet–Spengler Reaction in 1,1,1,3,3,3-Hexafluoro-2-Propanol (HFIP)

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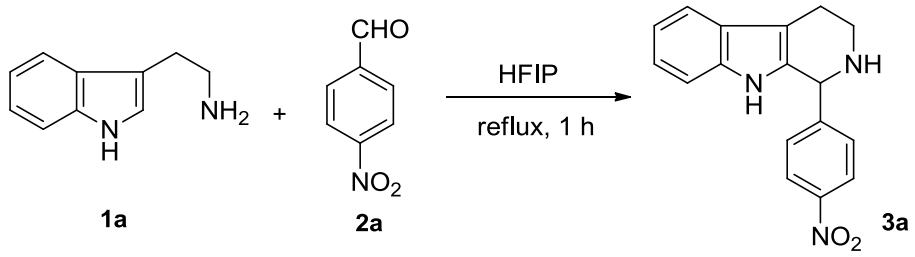
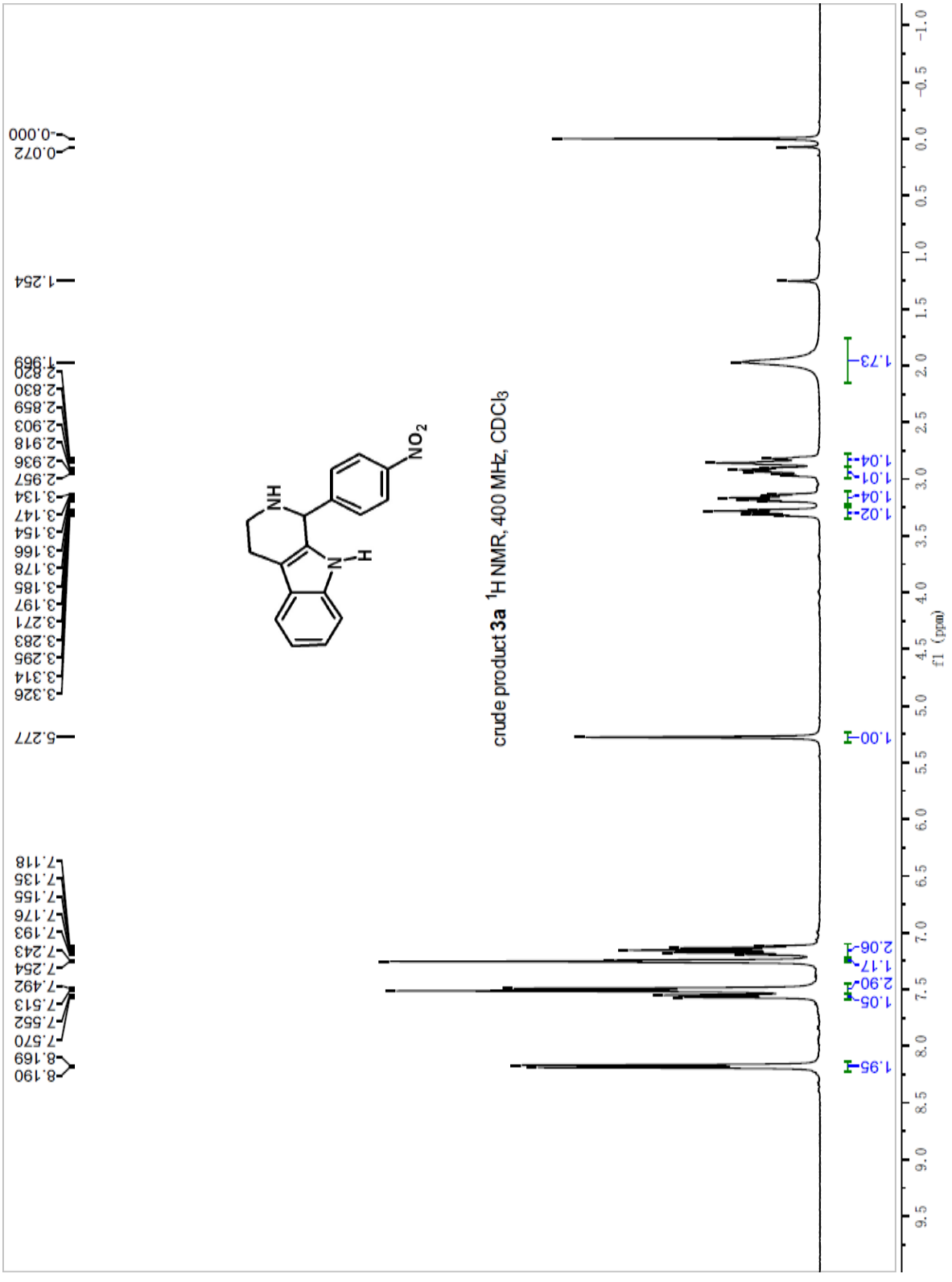
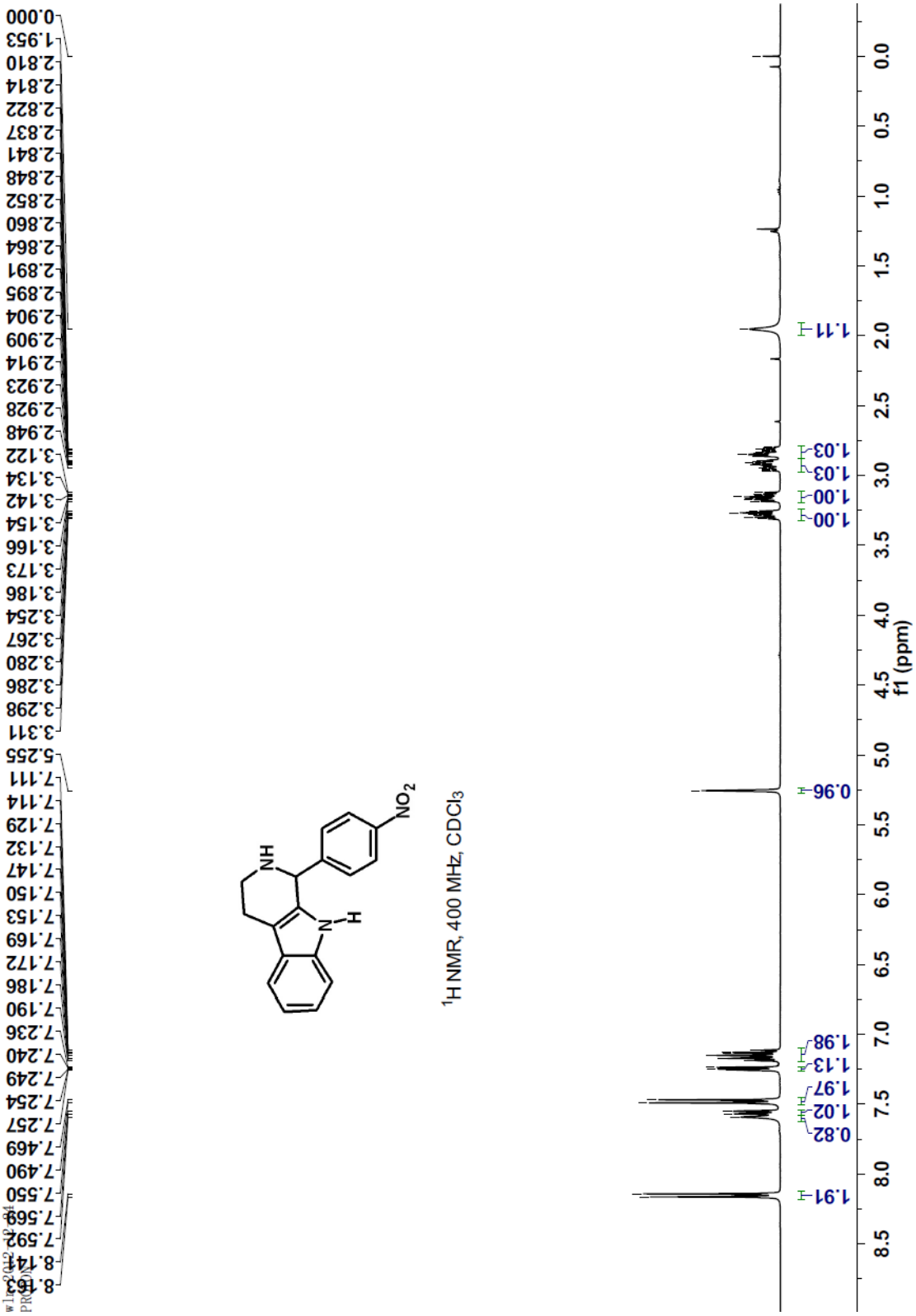


The ^{1}H NMR spectrum of the crude product after removal of solvent HFIP.

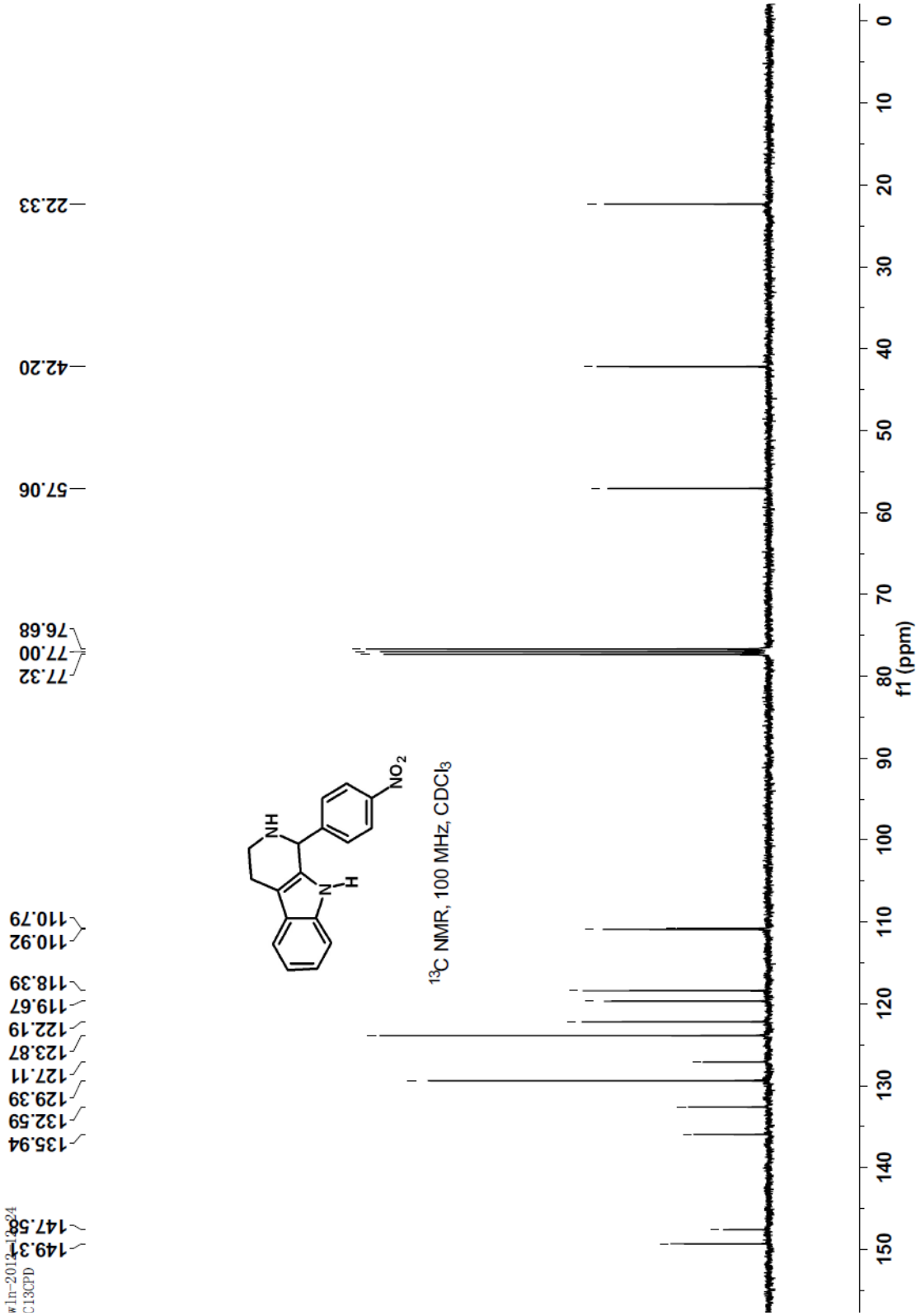


NMR spectra

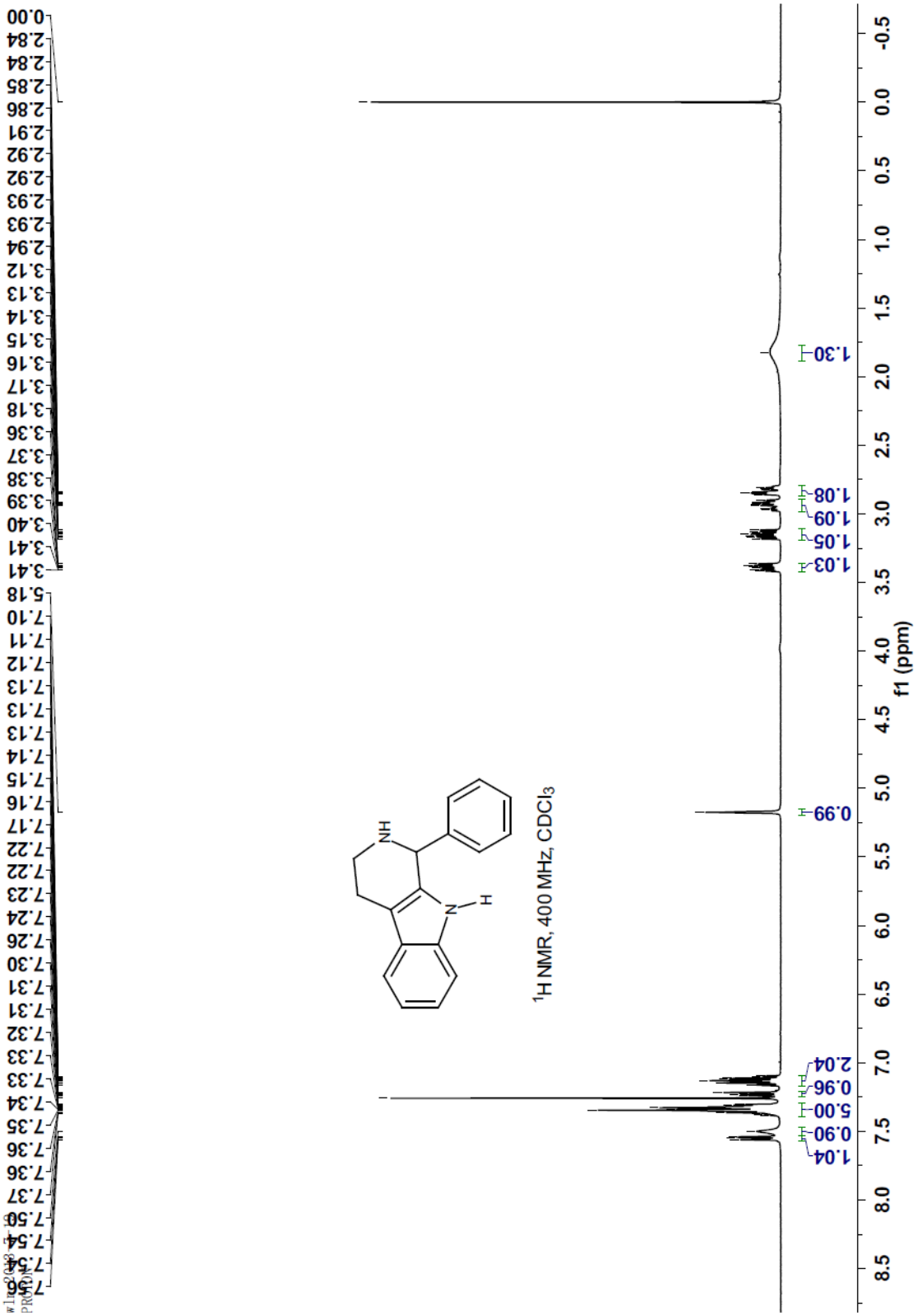
1-(4-Nitrophenyl)-1,2,3,4-tetrahydro-β-carboline (3a): ^{1}H NMR



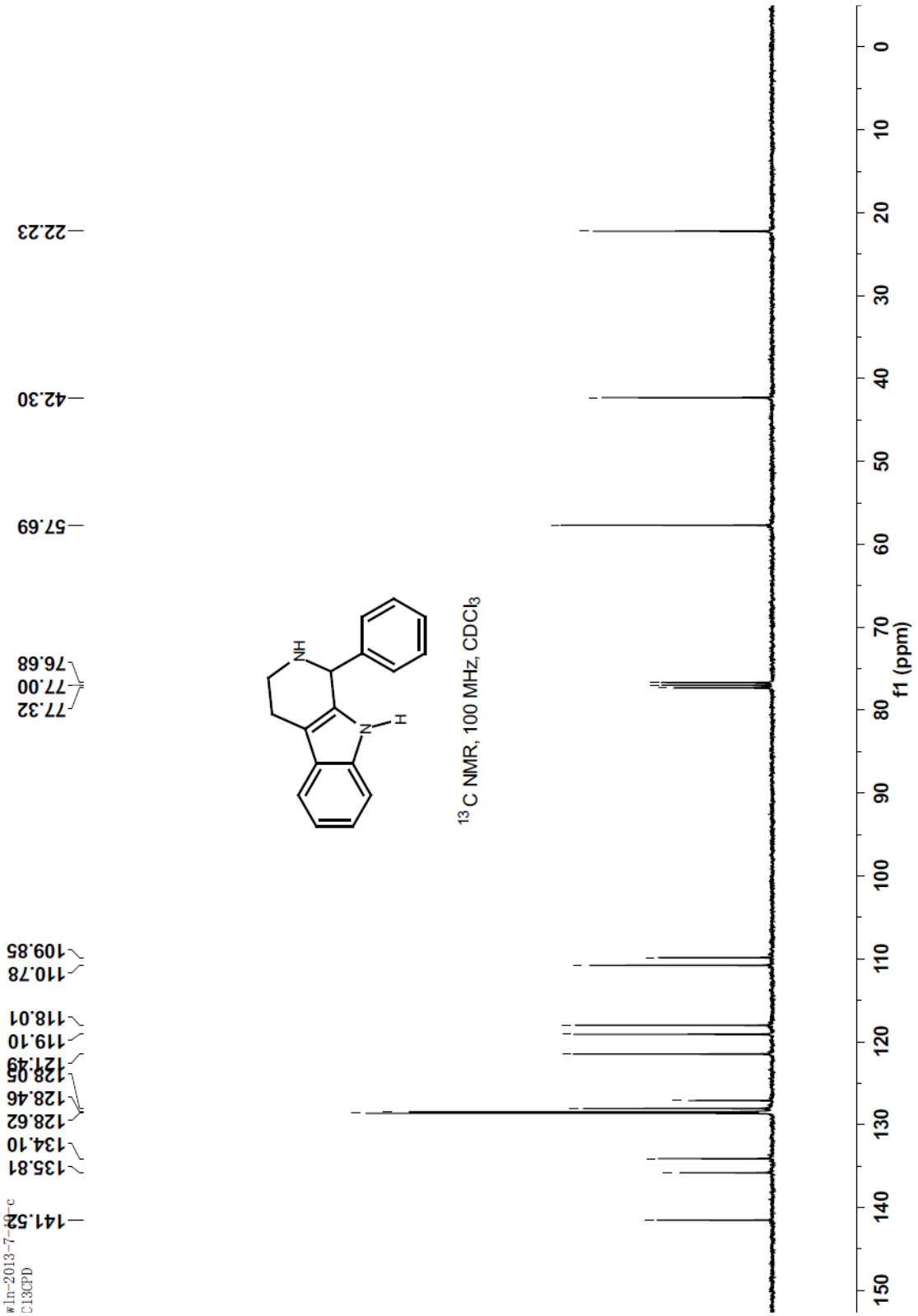
1-(4-Nitrophenyl)-1,2,3,4-tetrahydro-β-carboline (3a): ^{13}C NMR



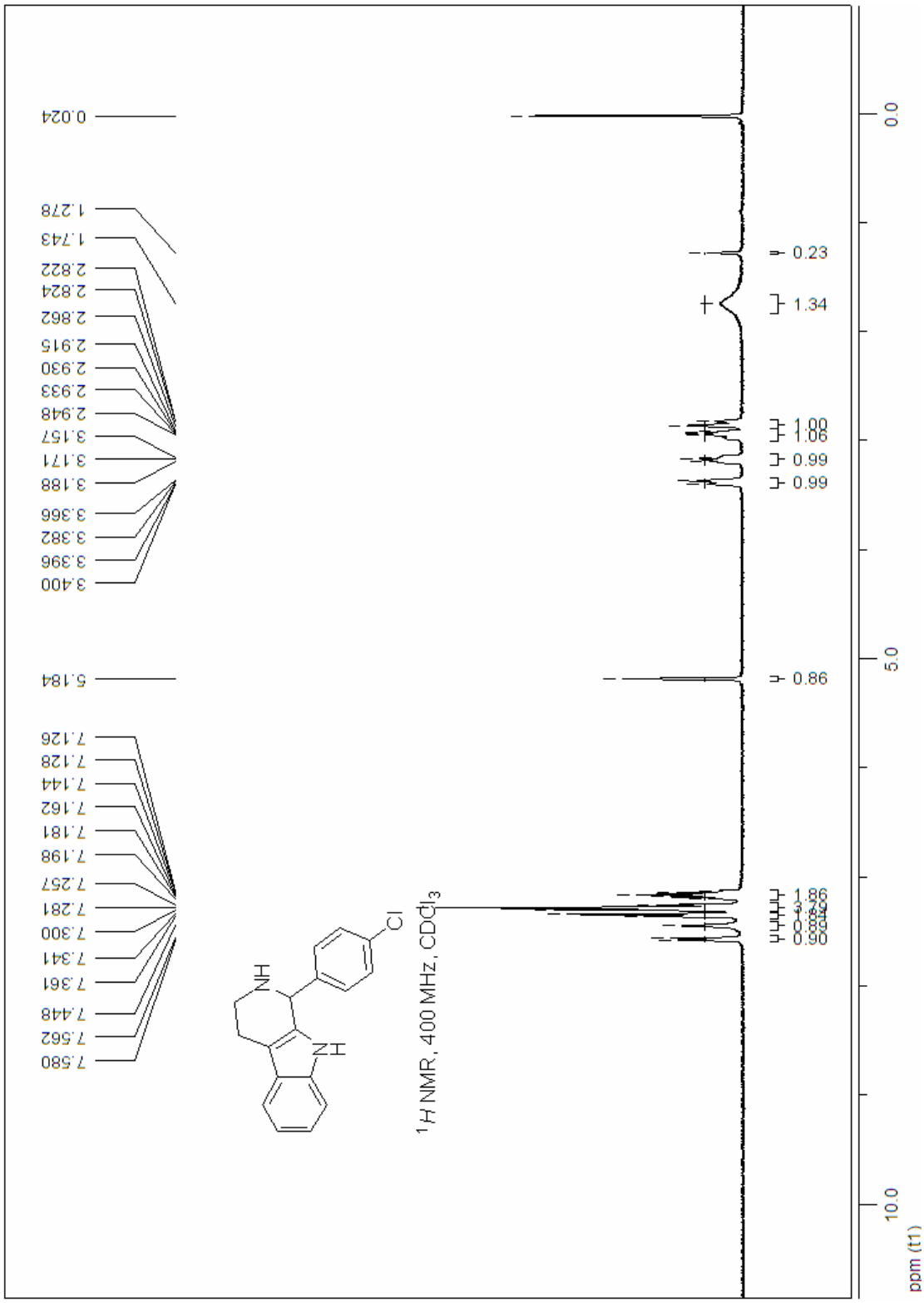
1-Phenyl-1,2,3,4-tetrahydro-β-carboline (3b): ^{1}H NMR



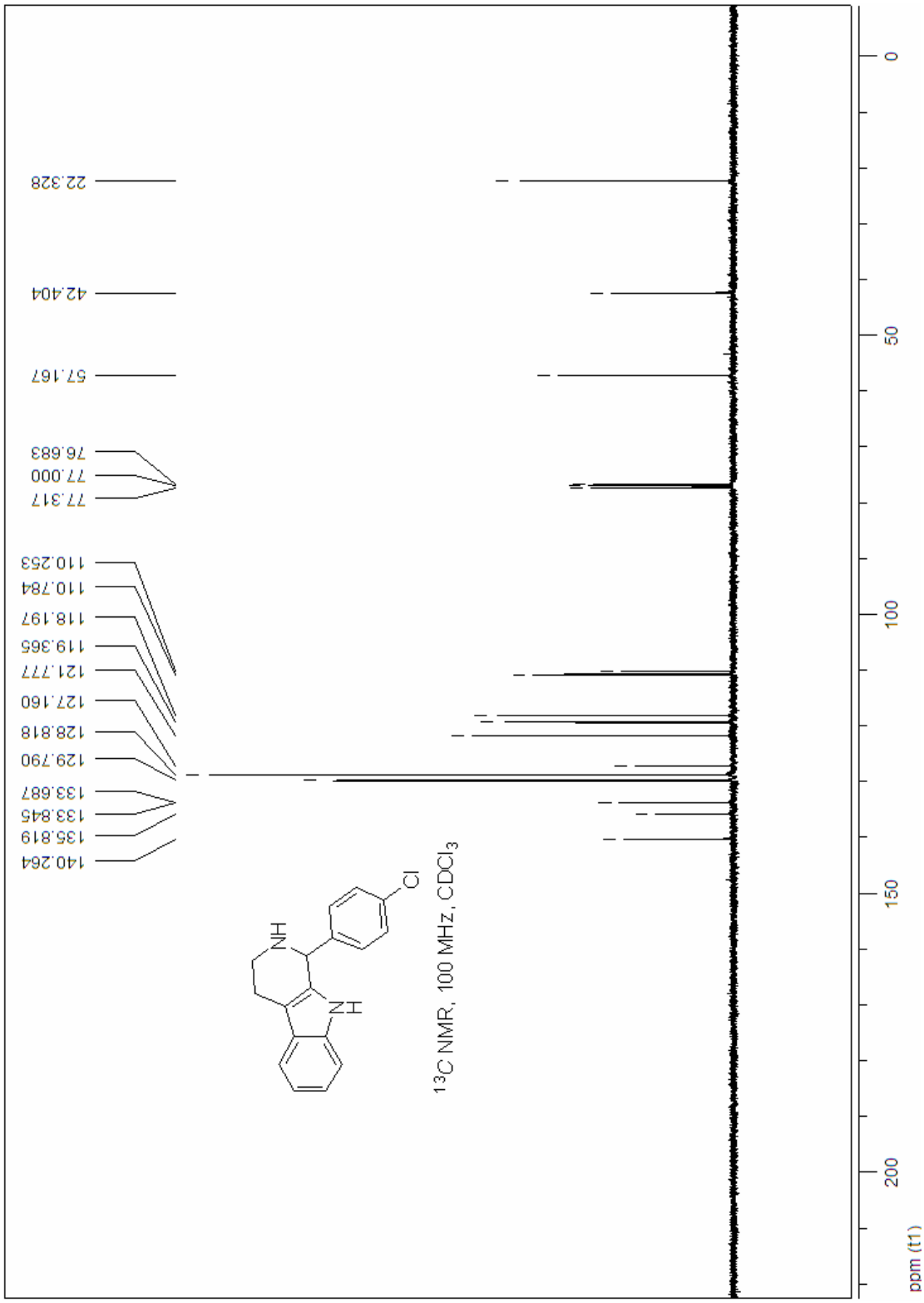
1-Phenyl-1,2,3,4-tetrahydro-β-carboline (3b): ^{13}C NMR



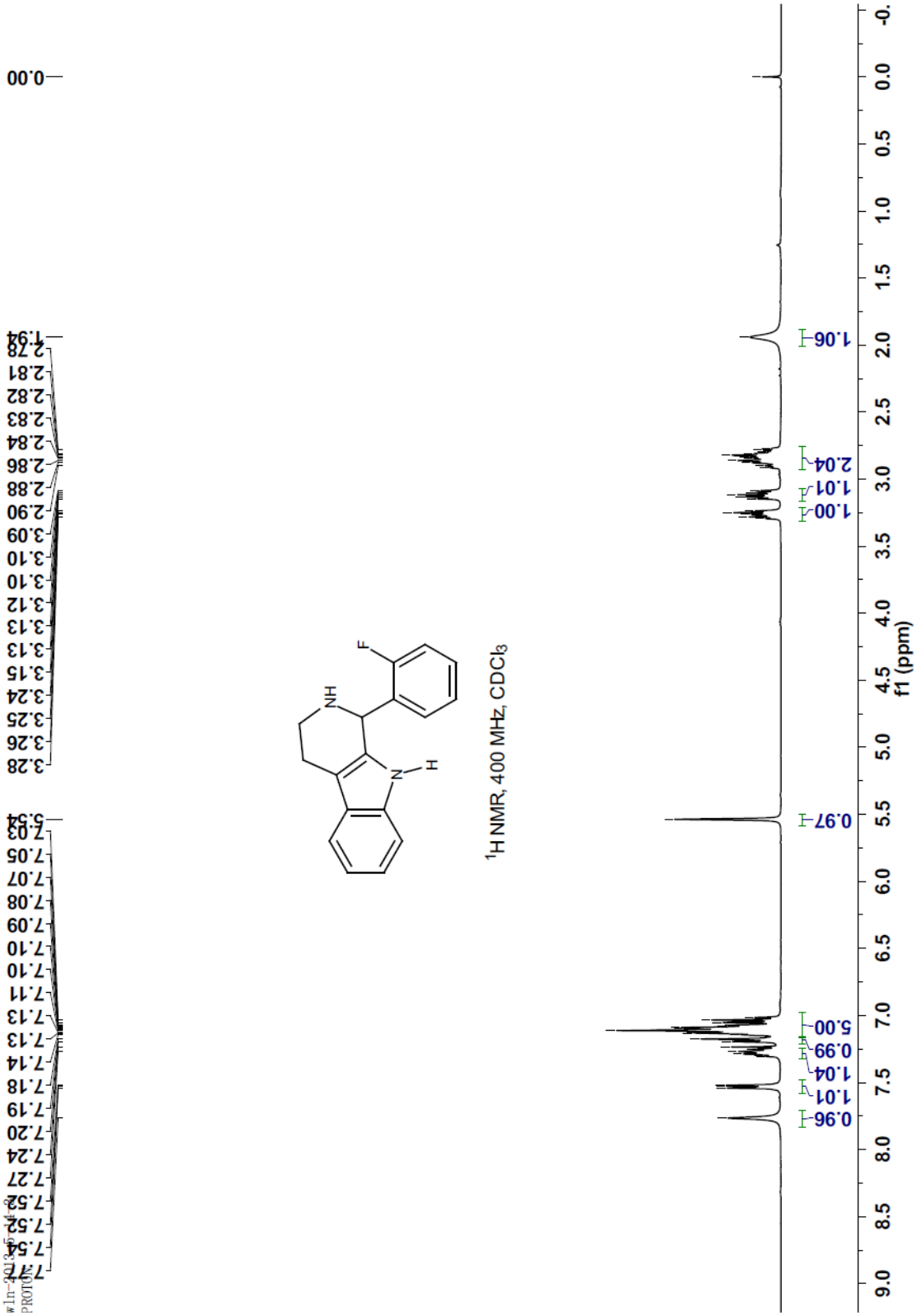
1-(4-Chlorophenyl)-1,2,3,4-tetrahydro-β-carboline (3c): ^{1}H NMR



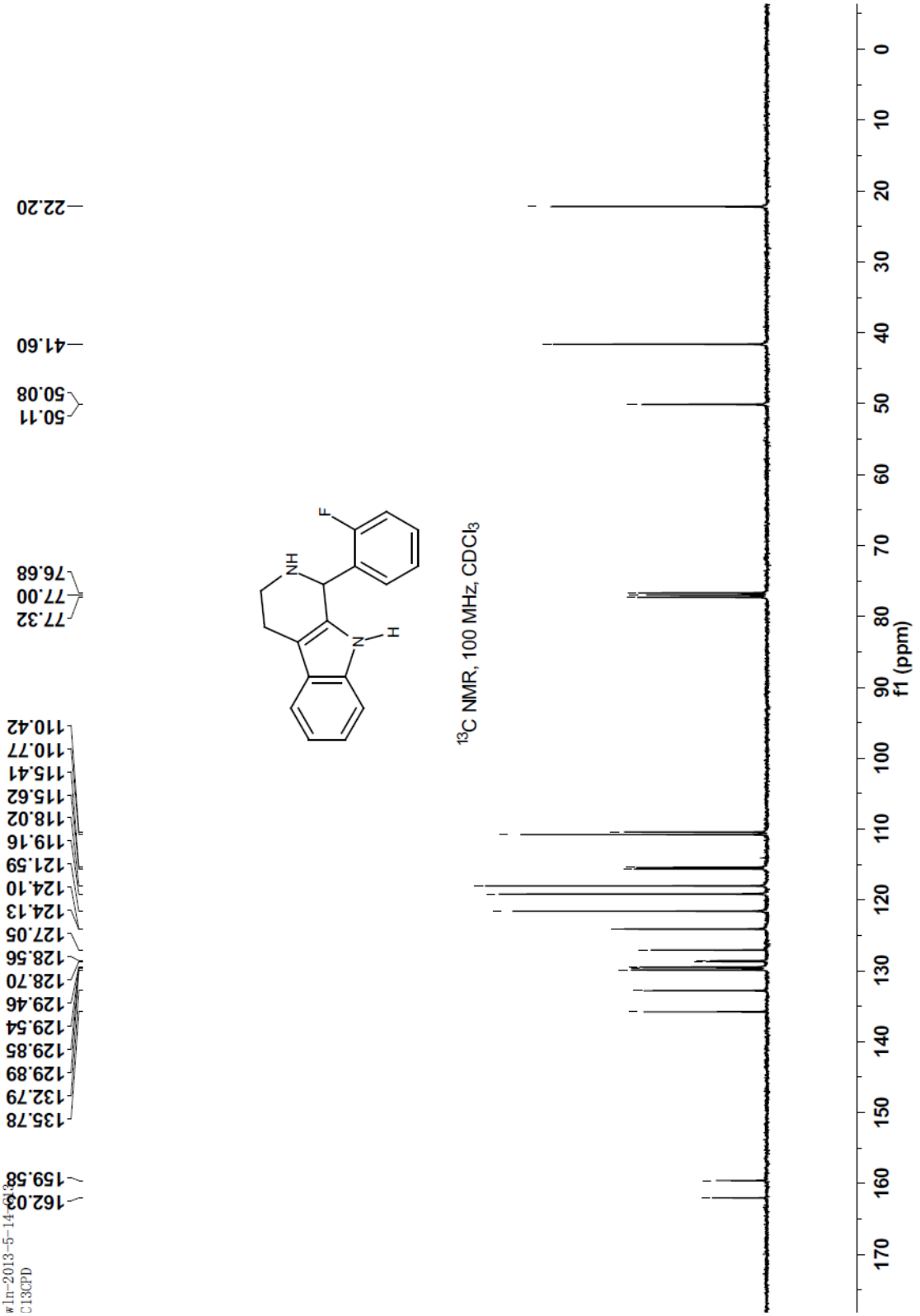
1-(4-Chlorophenyl)-1,2,3,4-tetrahydro-β-carboline (3c): ^{13}C NMR



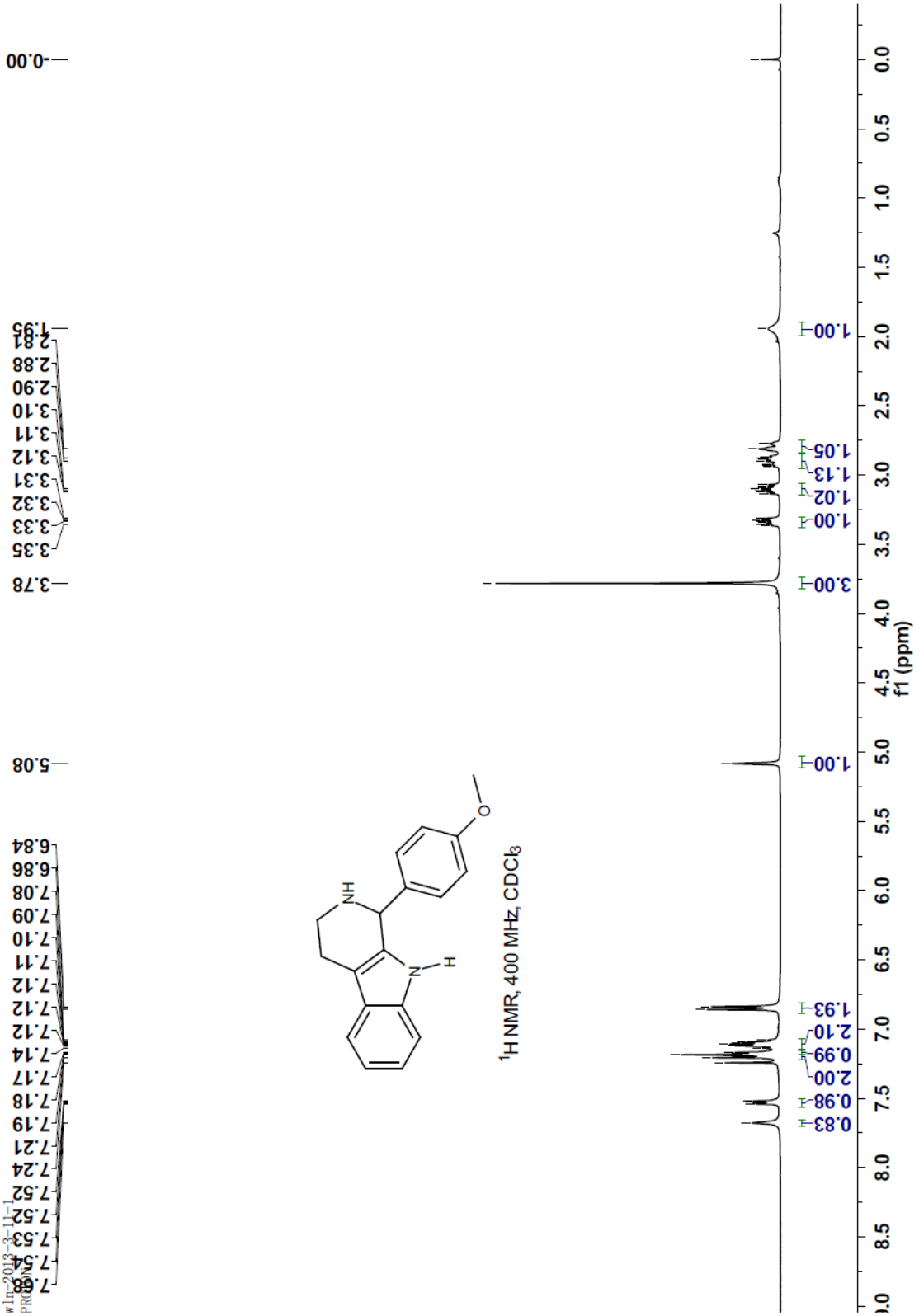
1-(2-Fluorophenyl)-1,2,3,4-tetrahydro-β-carboline (3d): ^{1}H NMR



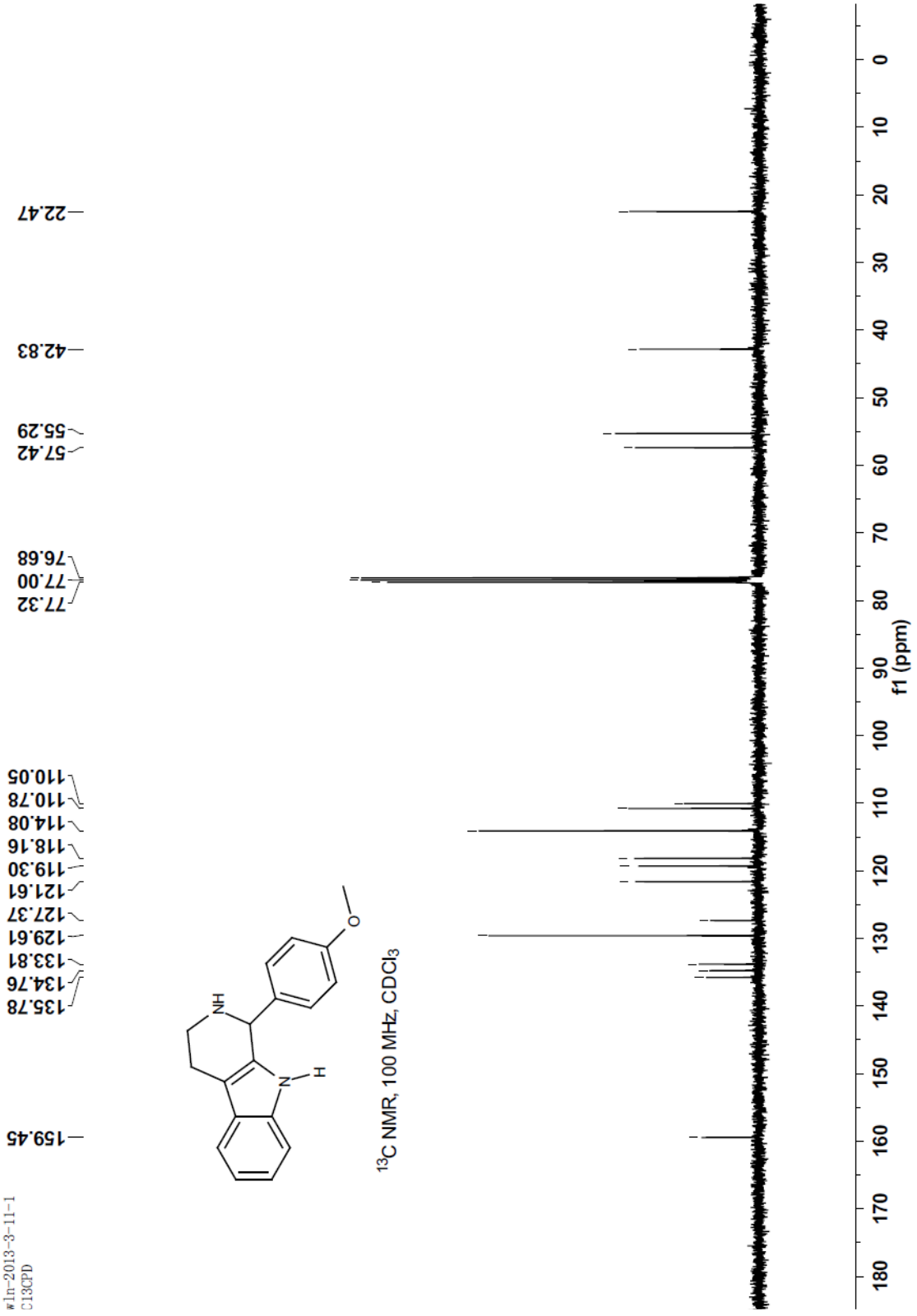
1-(2-Fluorophenyl)-1,2,3,4-tetrahydro-β-carboline (3d): ^{13}C NMR



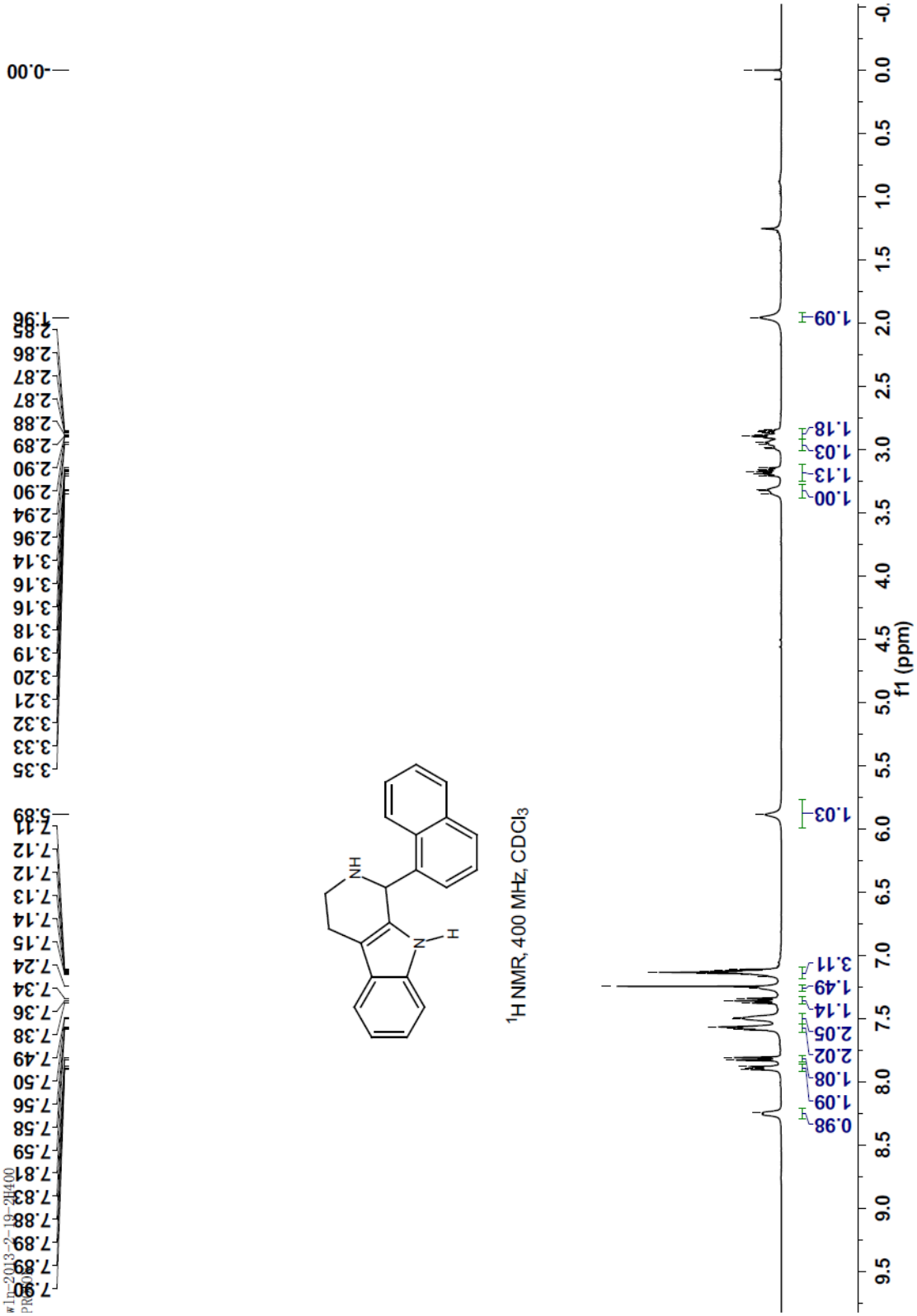
1-(*p*-Methoxyphenyl)-1,2,3,4-tetrahydro-β-carboline (3e): ^{1}H NMR



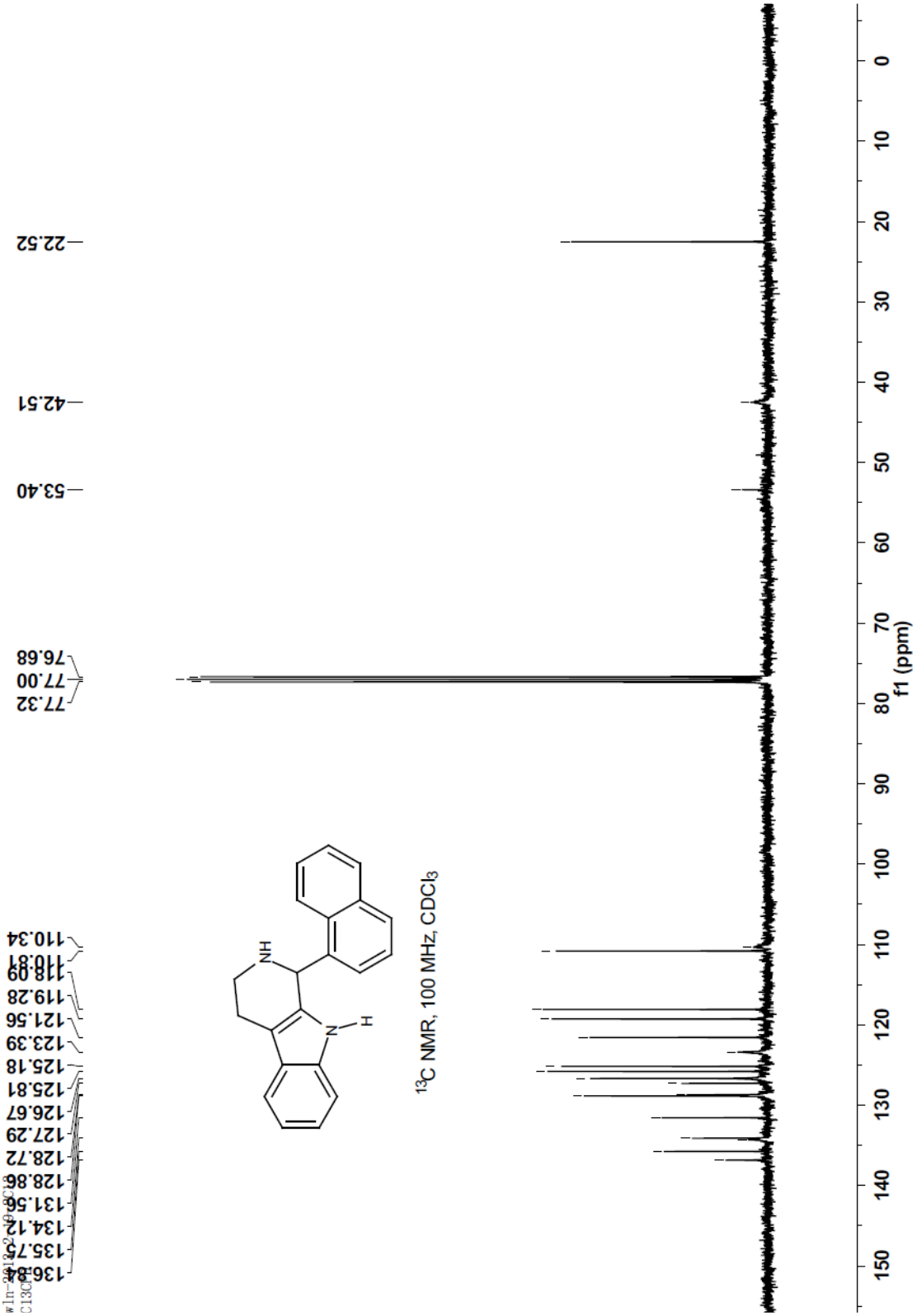
1-(*p*-Methoxyphenyl)-1,2,3,4-tetrahydro-β-carboline (3e): ^{13}C NMR



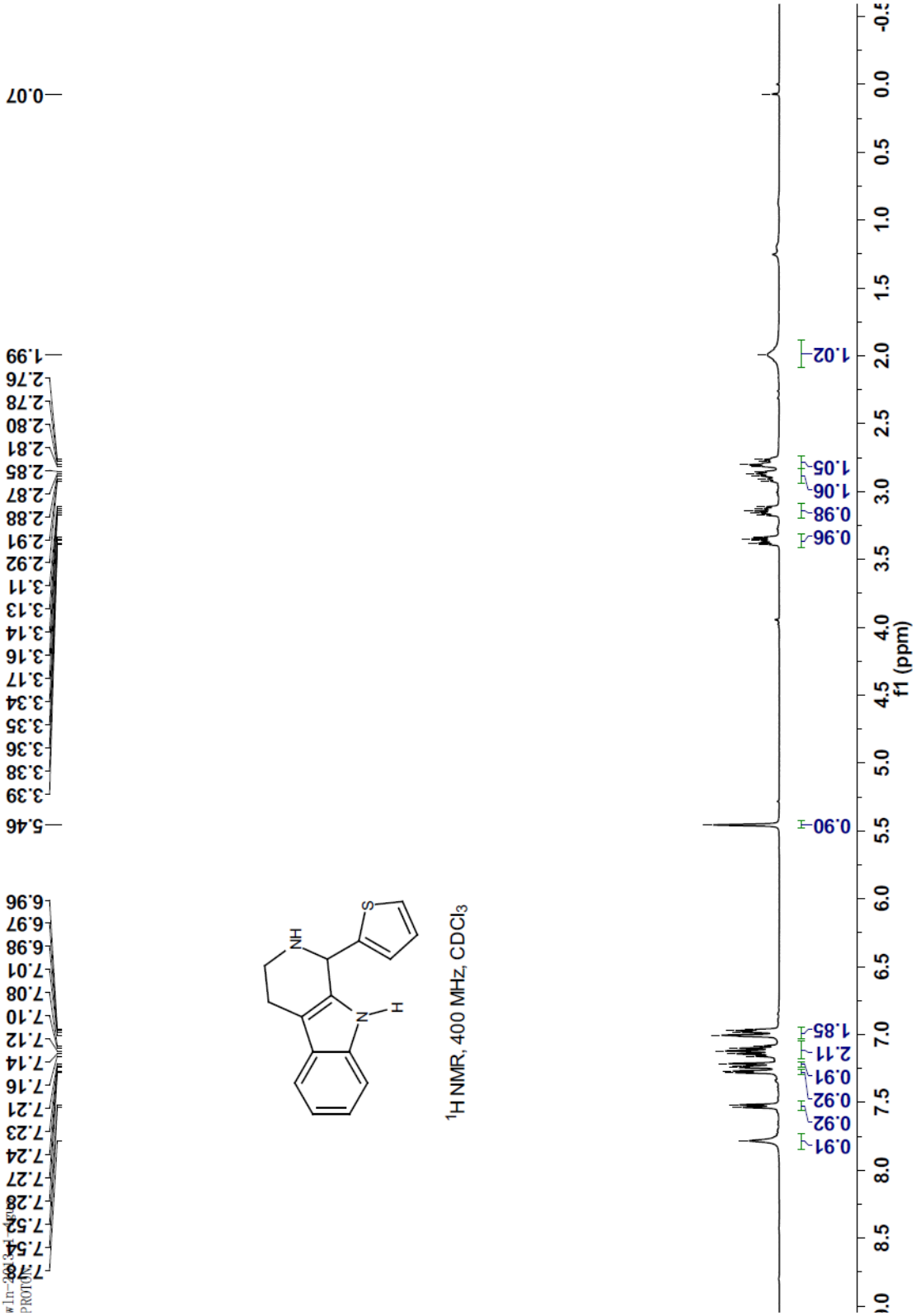
1-(Napthyl)-1,2,3,4-tetrahydro-β-carboline (3f): ^{1}H NMR



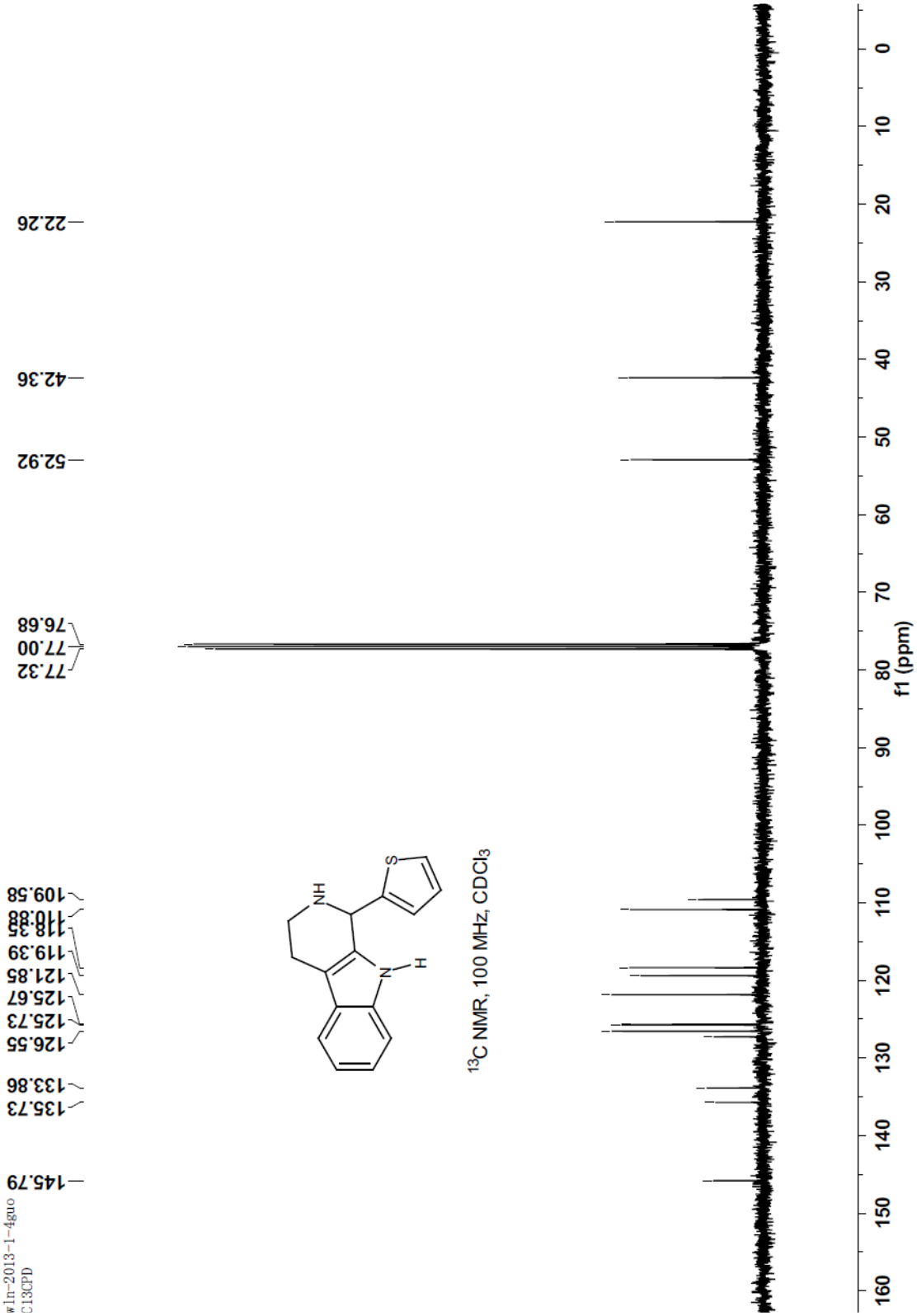
1-(Napthyl)-1,2,3,4-tetrahydro-β-carboline (3f): ^{13}C NMR



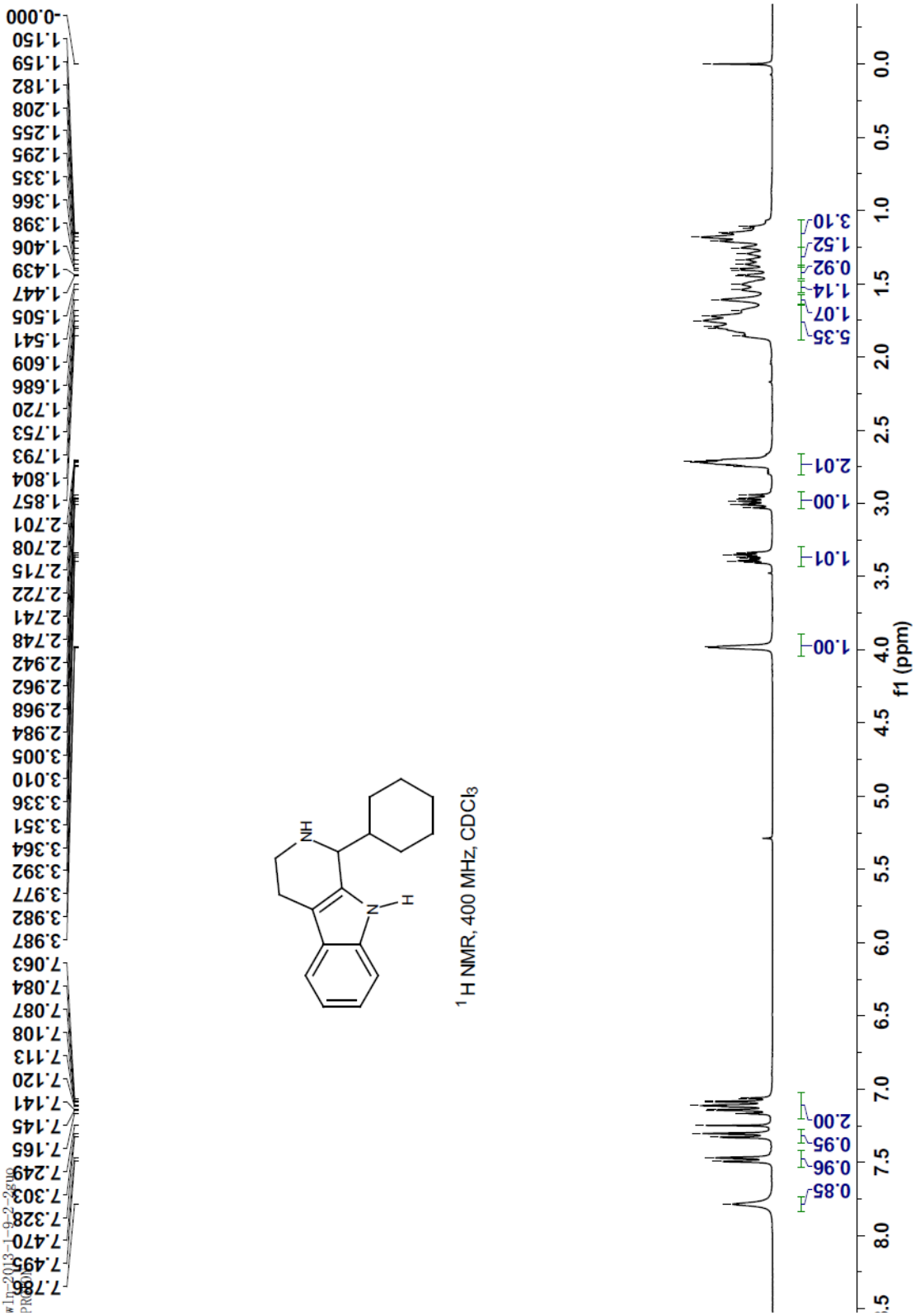
1-(2-Thienyl)-1,2,3,4-tetrahydro-β-carboline (3g): ^{1}H NMR



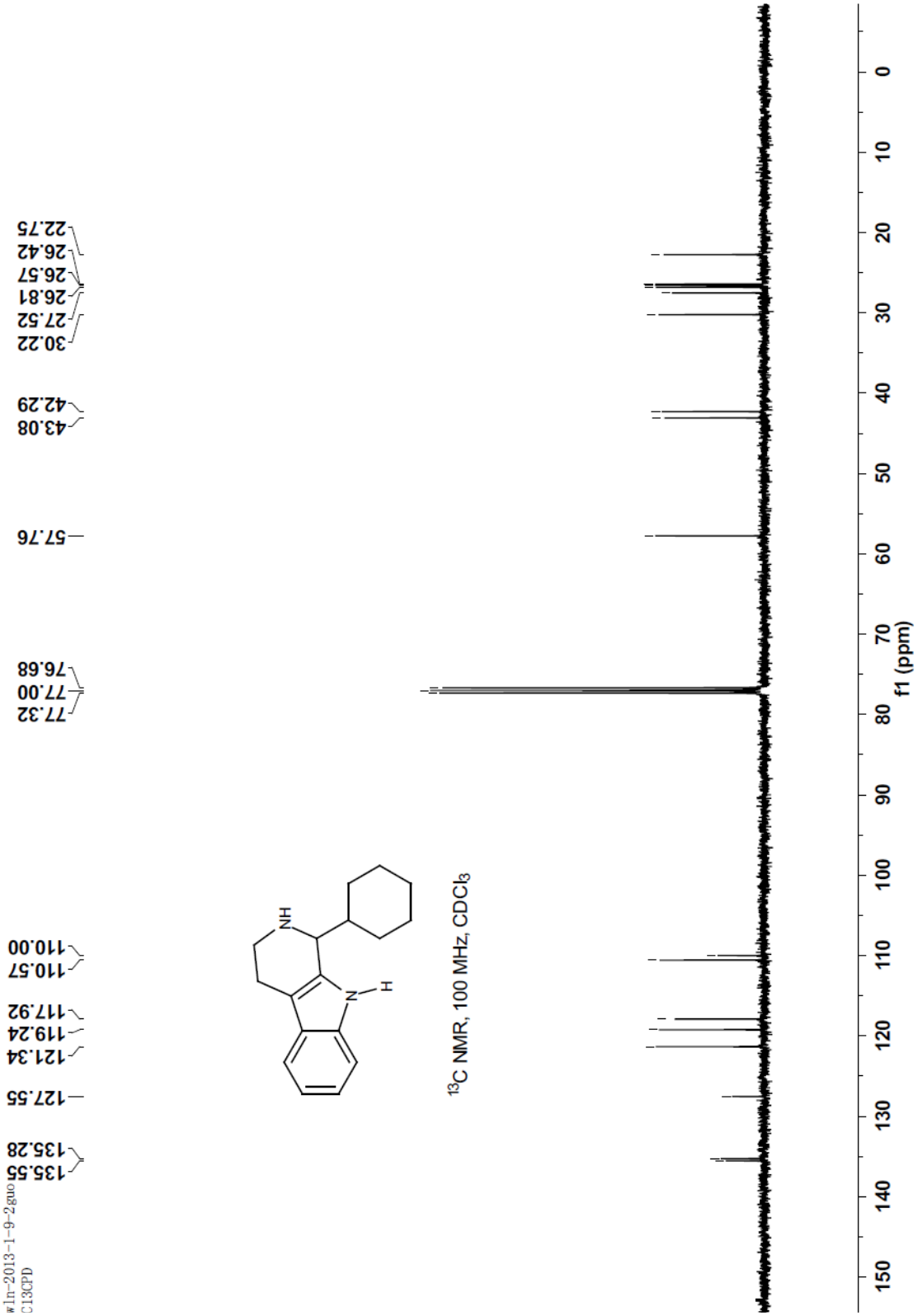
1-(2-Thienyl)-1,2,3,4-tetrahydro-β-carboline (3g): ^{13}C NMR



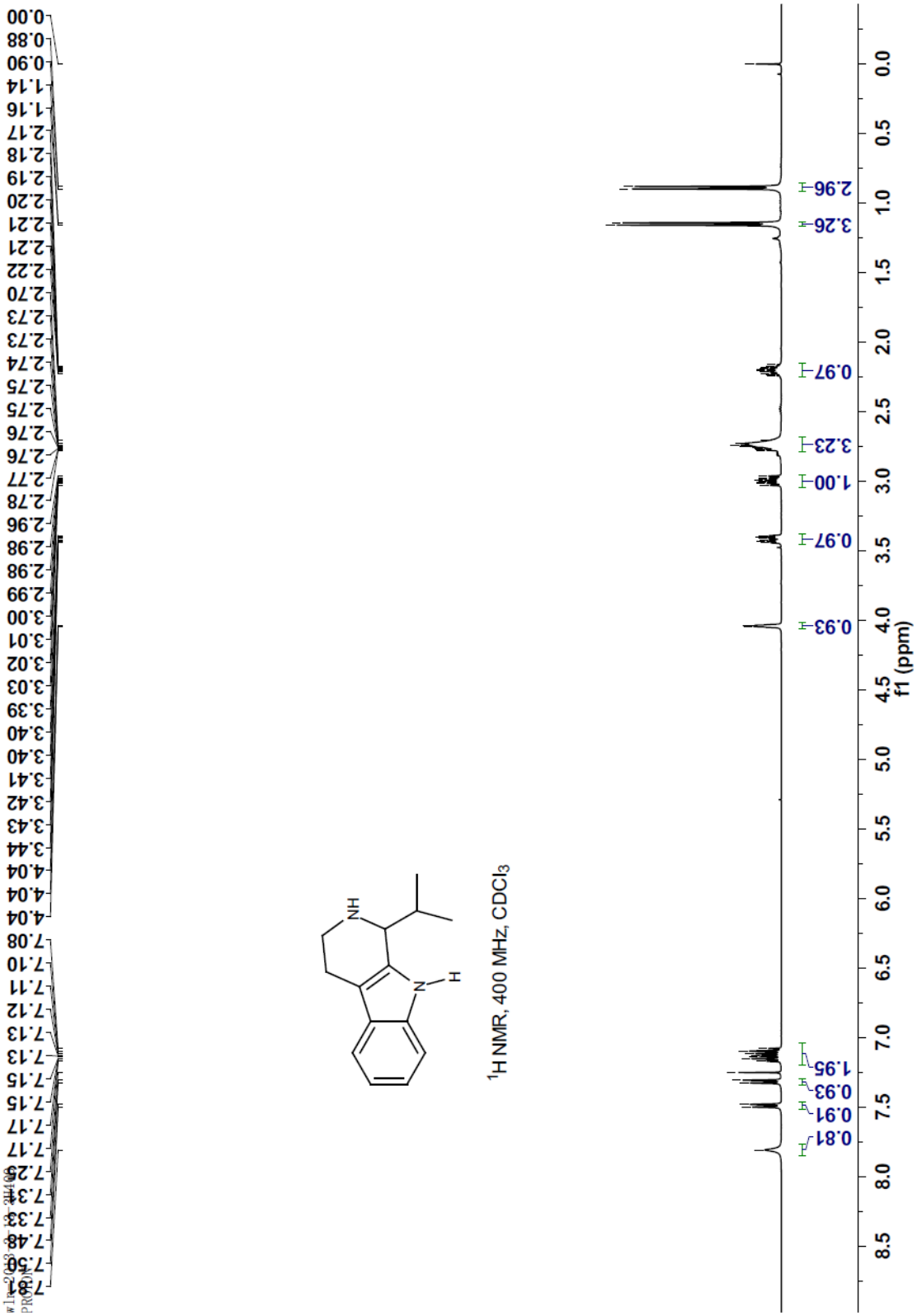
1-Cyclohexyl-1,2,3,4-tetrahydro-β-carboline (3h): ^{1}H NMR



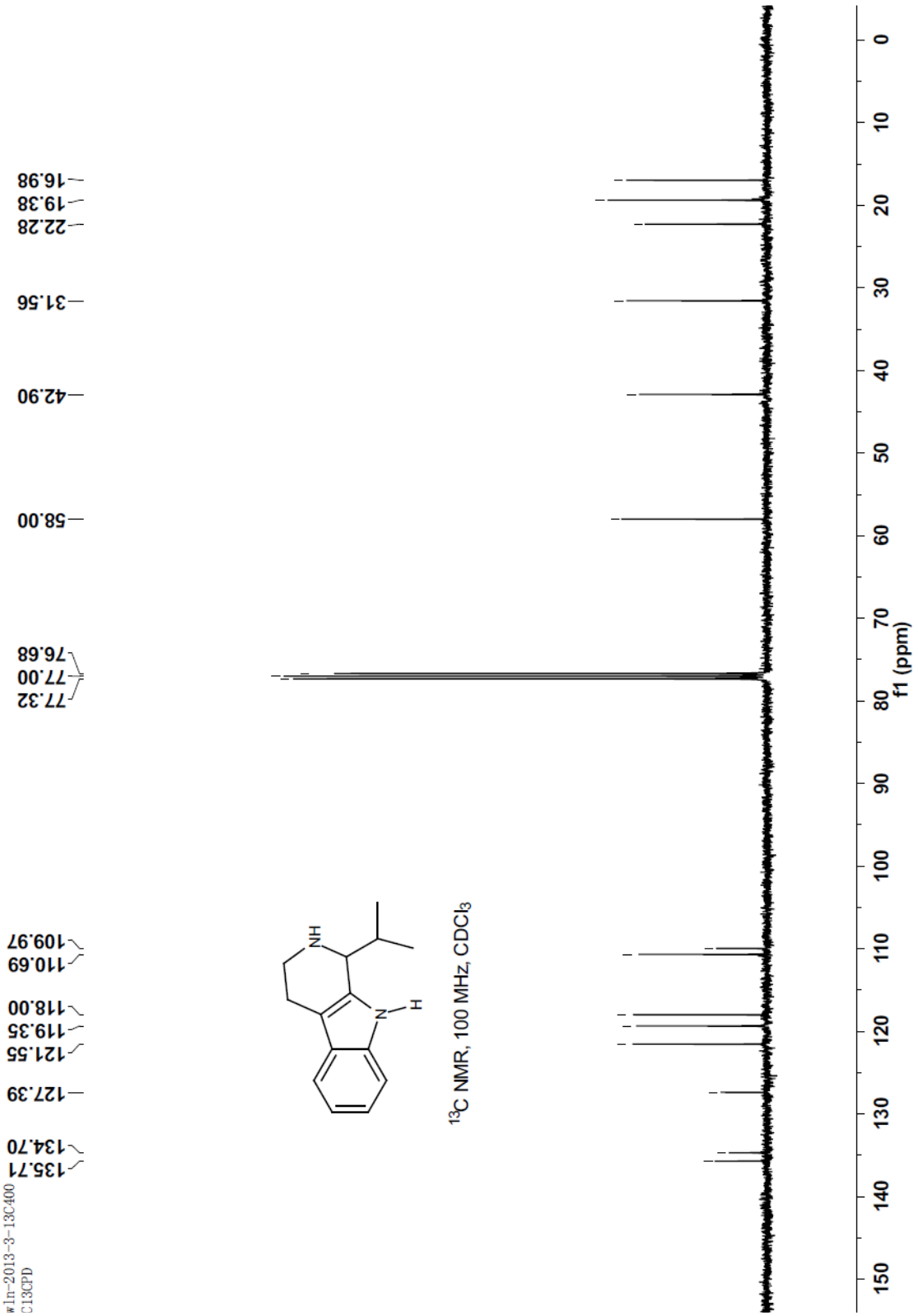
1-Cyclohexyl-1,2,3,4-tetrahydro-β-carboline (3h): ^{13}C NMR



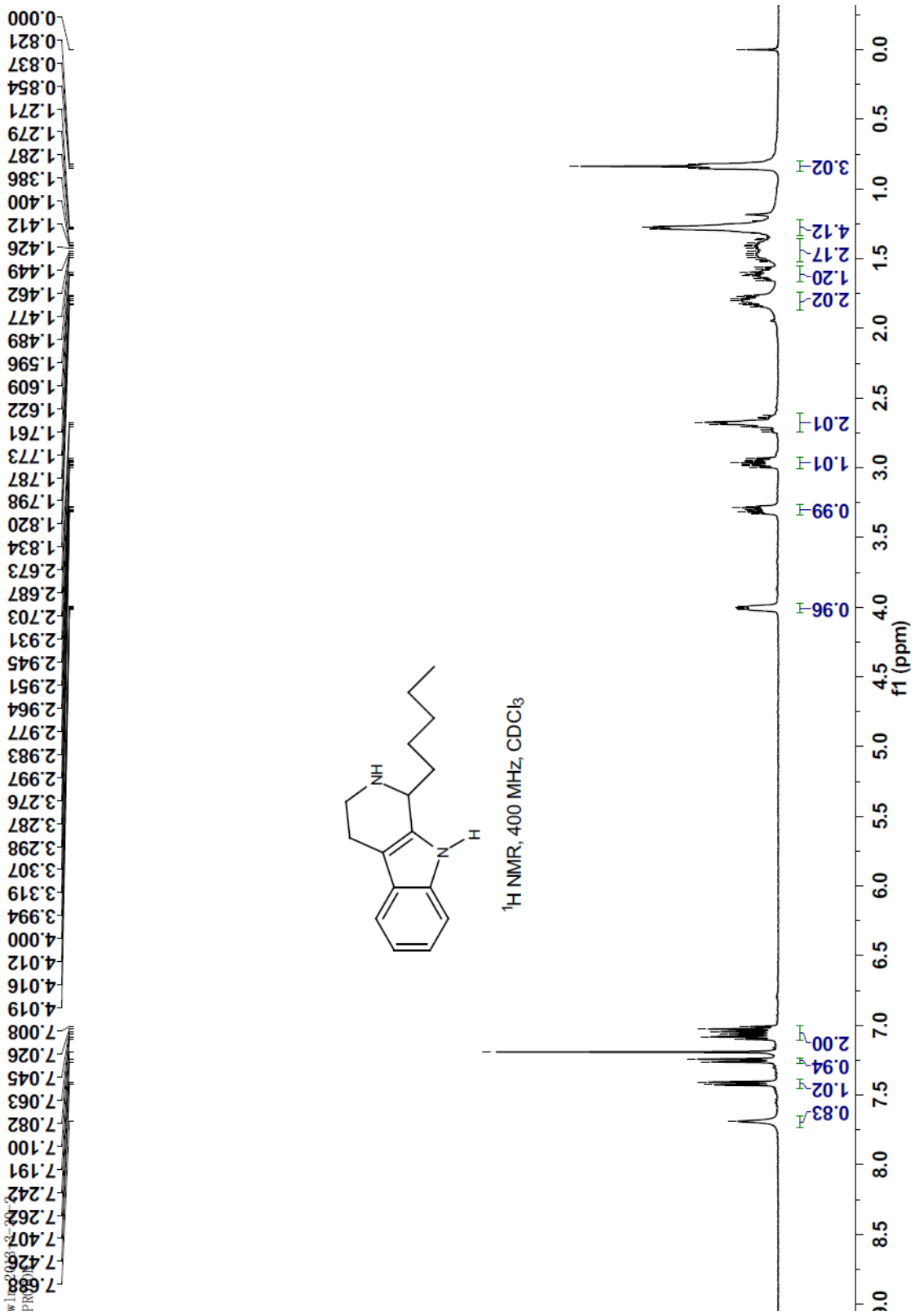
1-Isopropyl-1,2,3,4-tetrahydro-β-carboline (3i): ^{1}H NMR



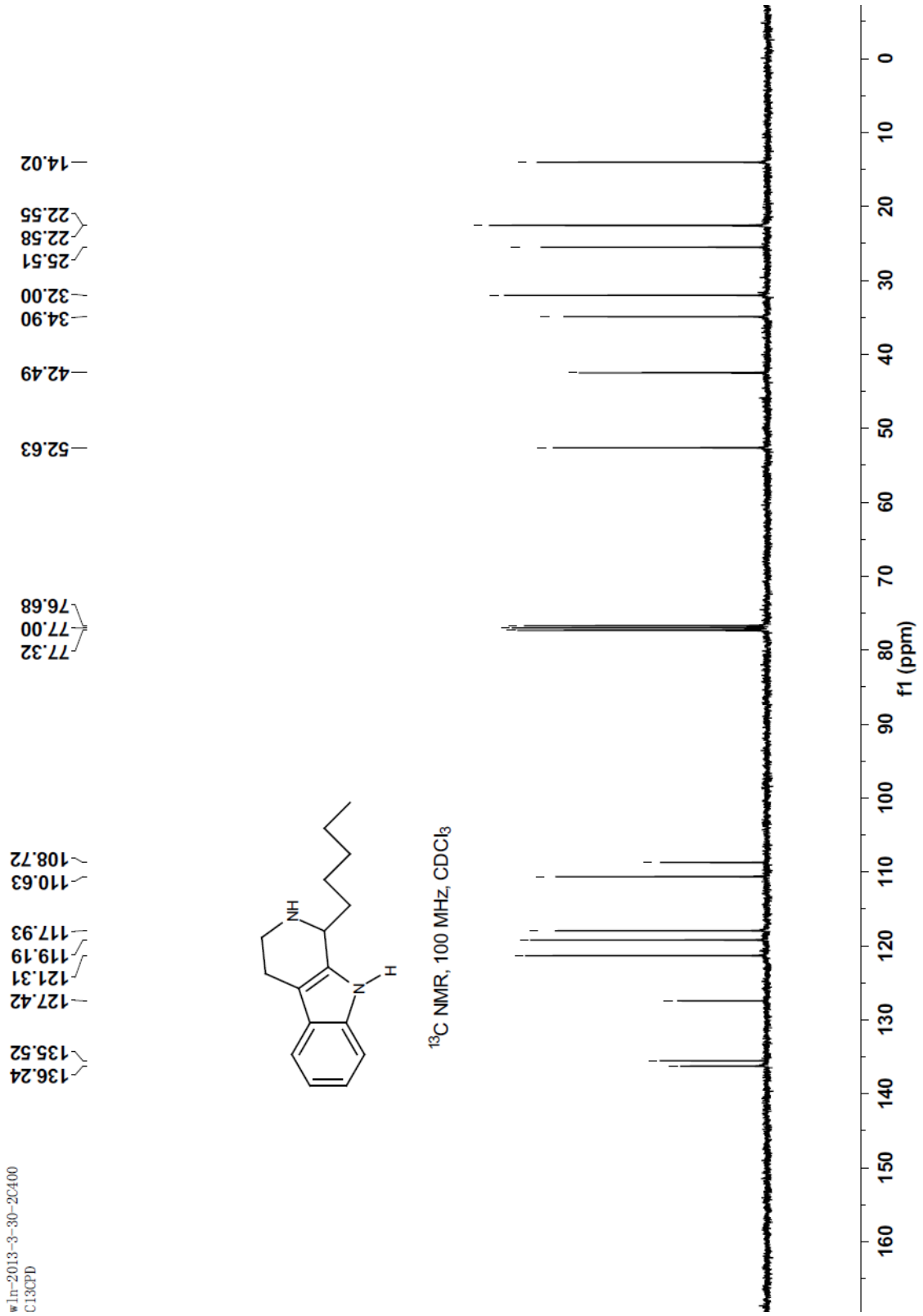
1-Isopropyl-1,2,3,4-tetrahydro-β-carboline (3i): ^{13}C NMR



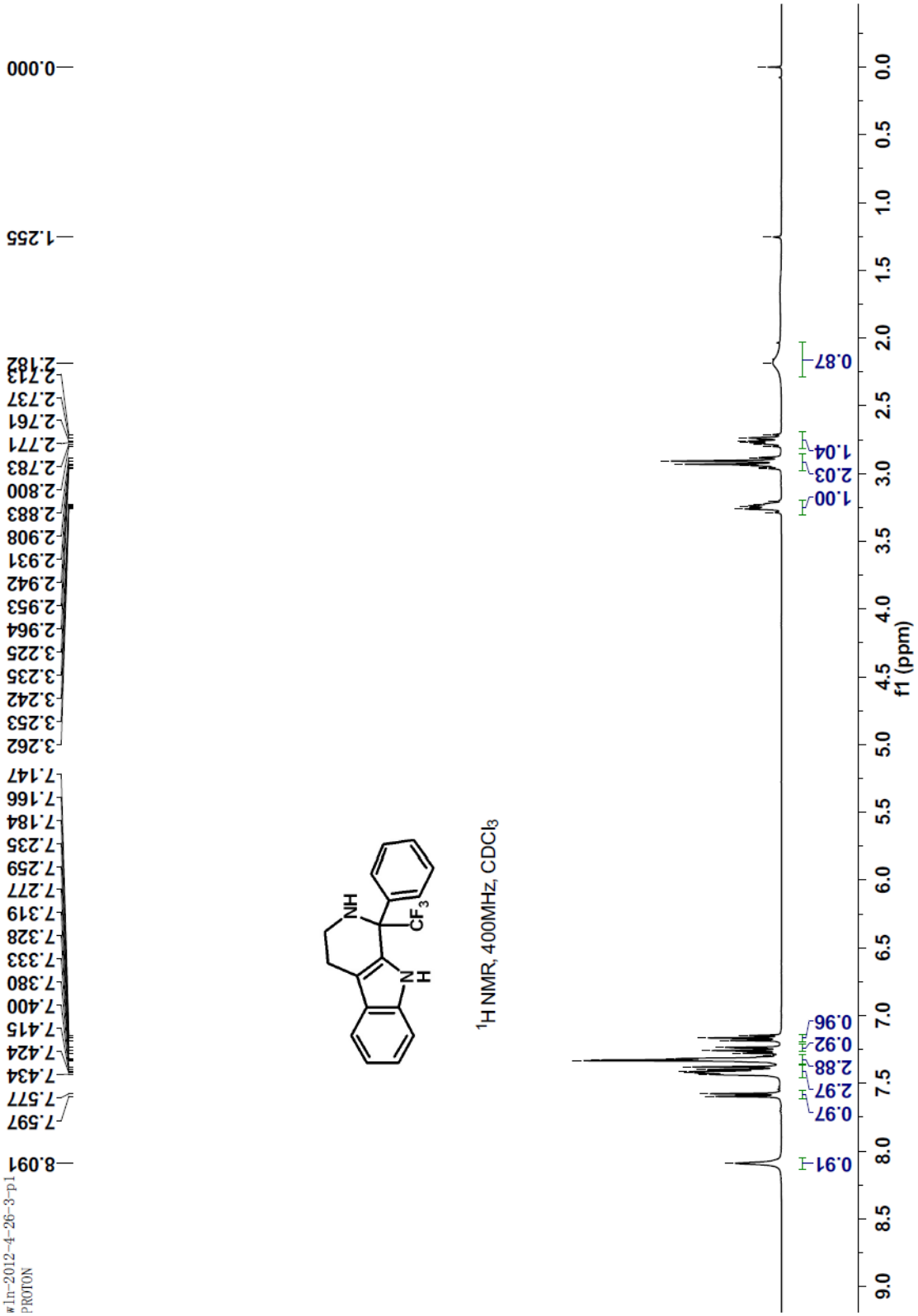
1-Pentyl-1,2,3,4-tetrahydro-β-carboline (3j): ^{1}H NMR



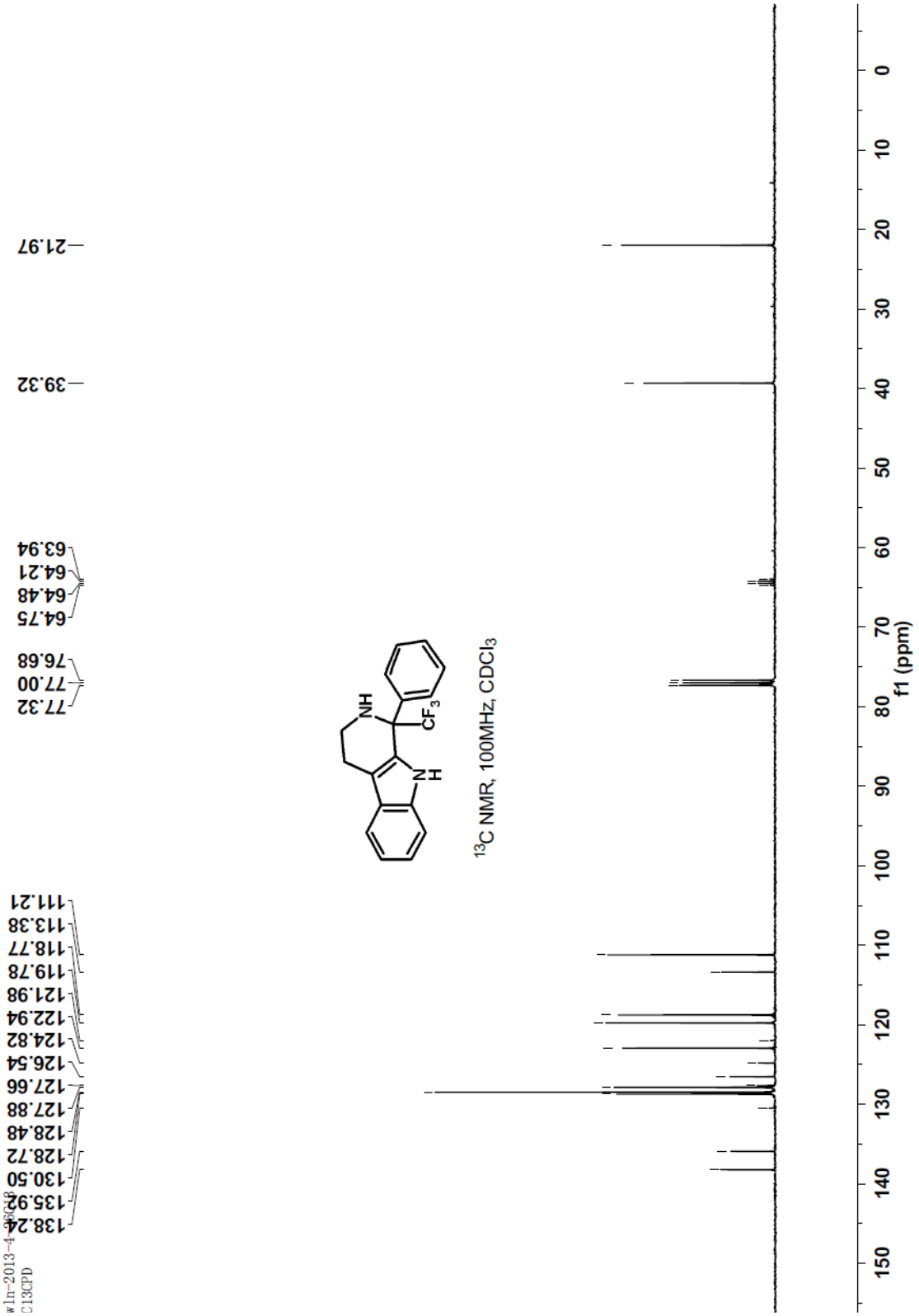
1-Pentyl-1,2,3,4-tetrahydro-β-carboline (3j): ^{13}C NMR



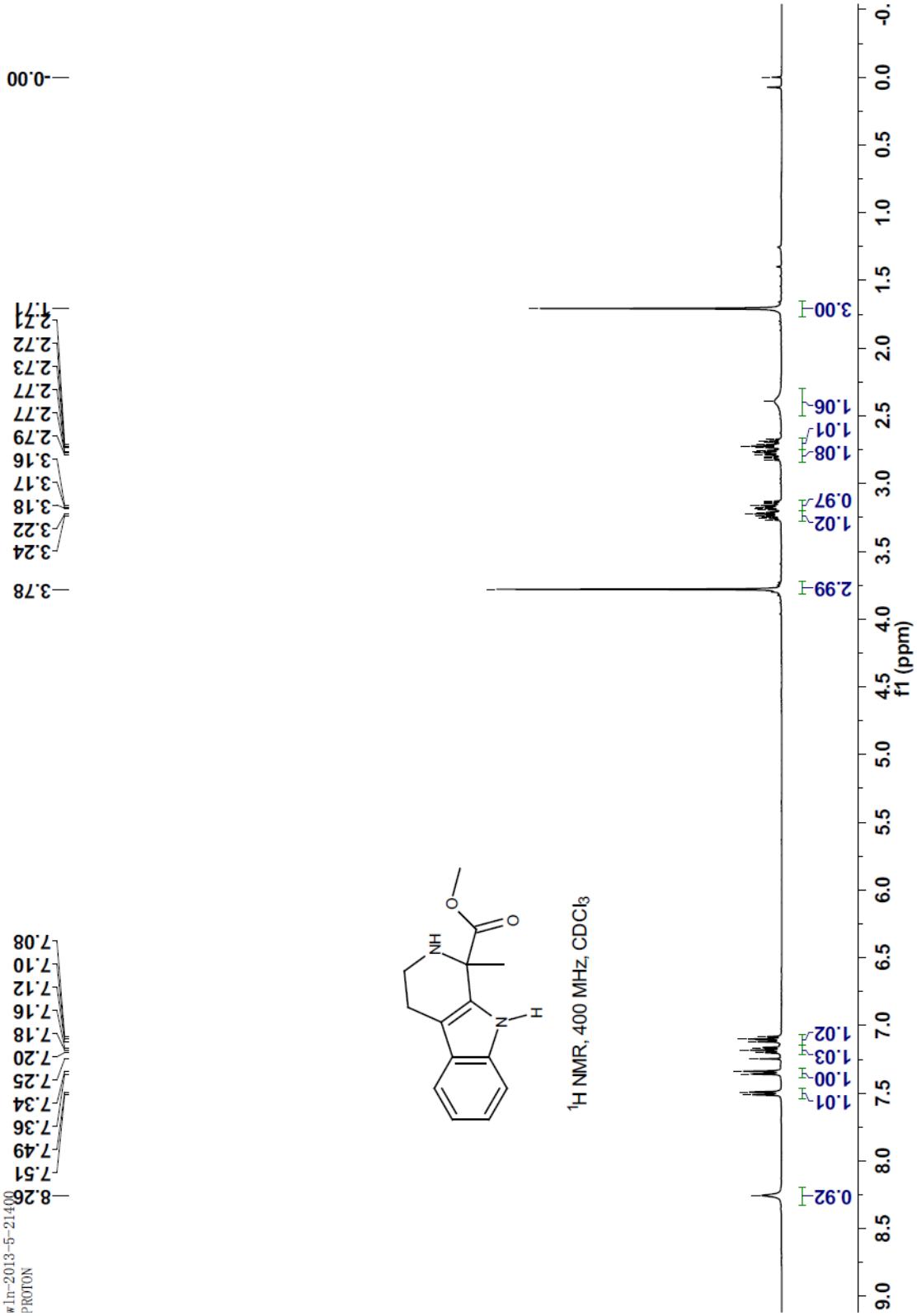
1-Phenyl-1-trifluoromethyl-1,2,3,4-tetrahydro-β-carboline (3k): ^{1}H NMR



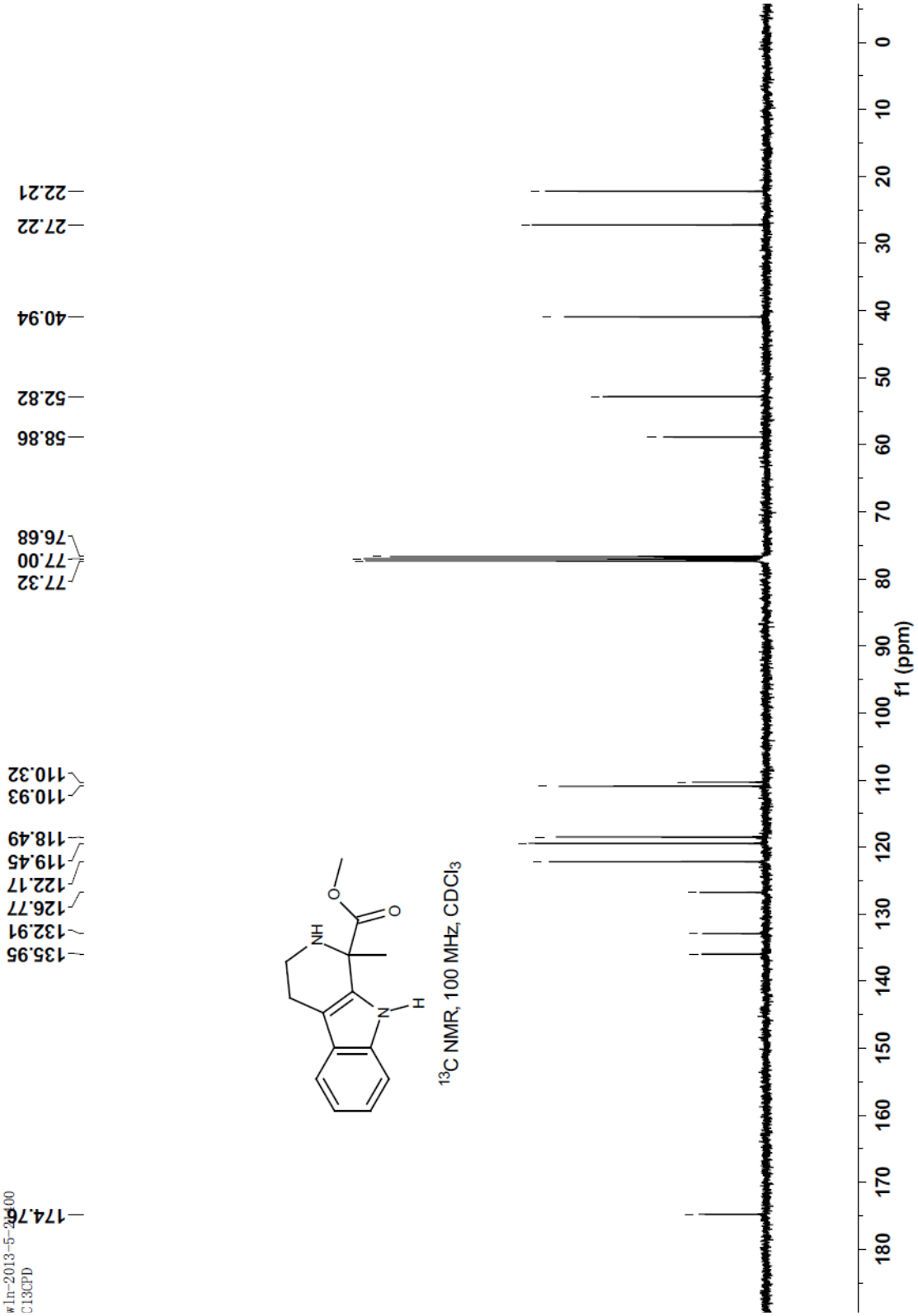
1-Phenyl-1-trifluoromethyl-1,2,3,4-tetrahydro-β-carboline (3k): ^{13}C NMR



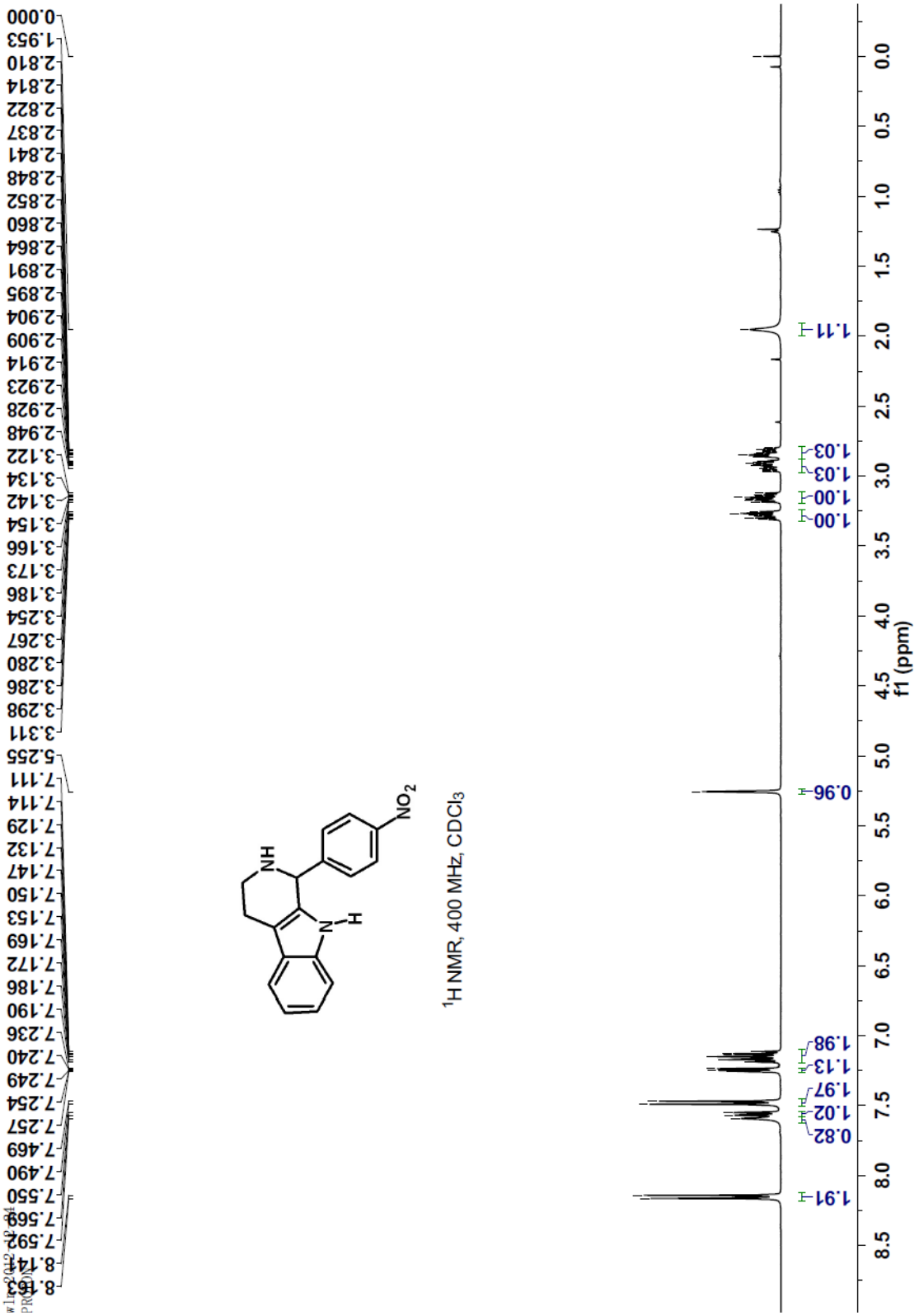
Methyl-(1-methyl-1,2,3,4-tetrahydro-β-carboline-1-yl) carboxylate (3l): ^{1}H NMR



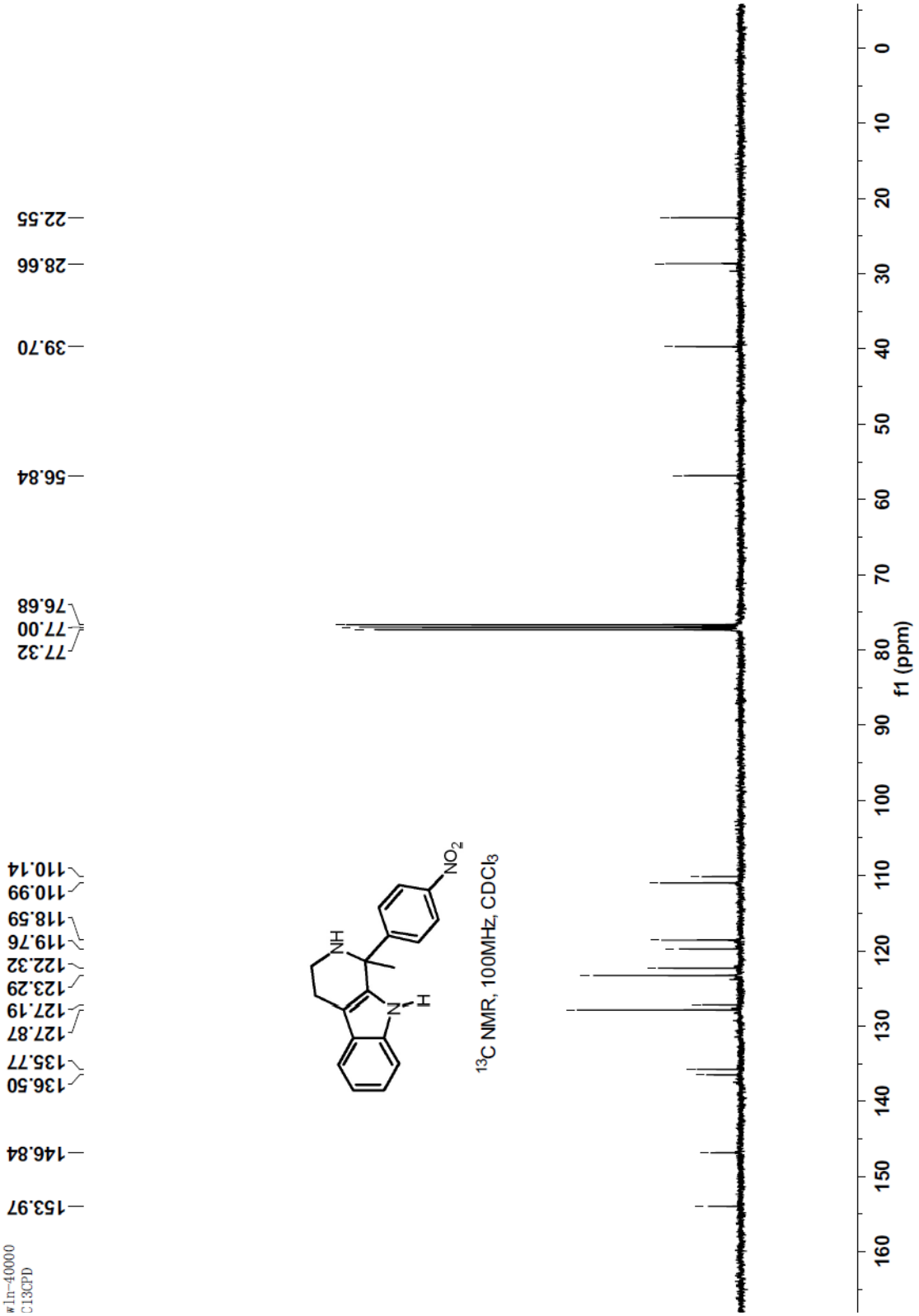
Methyl-(1-methyl-1,2,3,4-tetrahydro-β-carboline-1-yl) carboxylate (3l): ^{13}C NMR



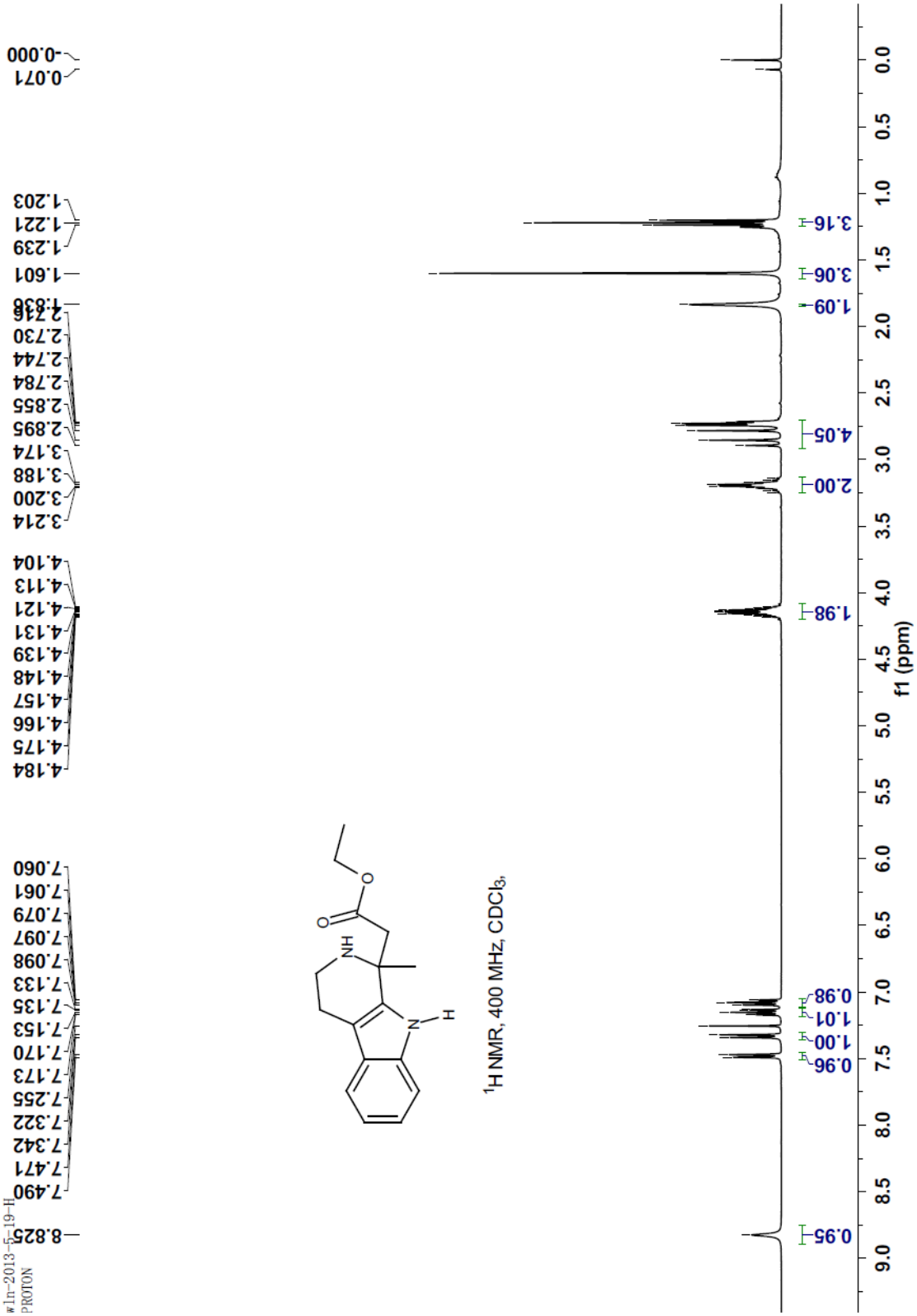
1-Methyl-1-(4-nitrophenyl)-1,2,3,4-tetrahydro-β-carboline (3m): ^{1}H NMR



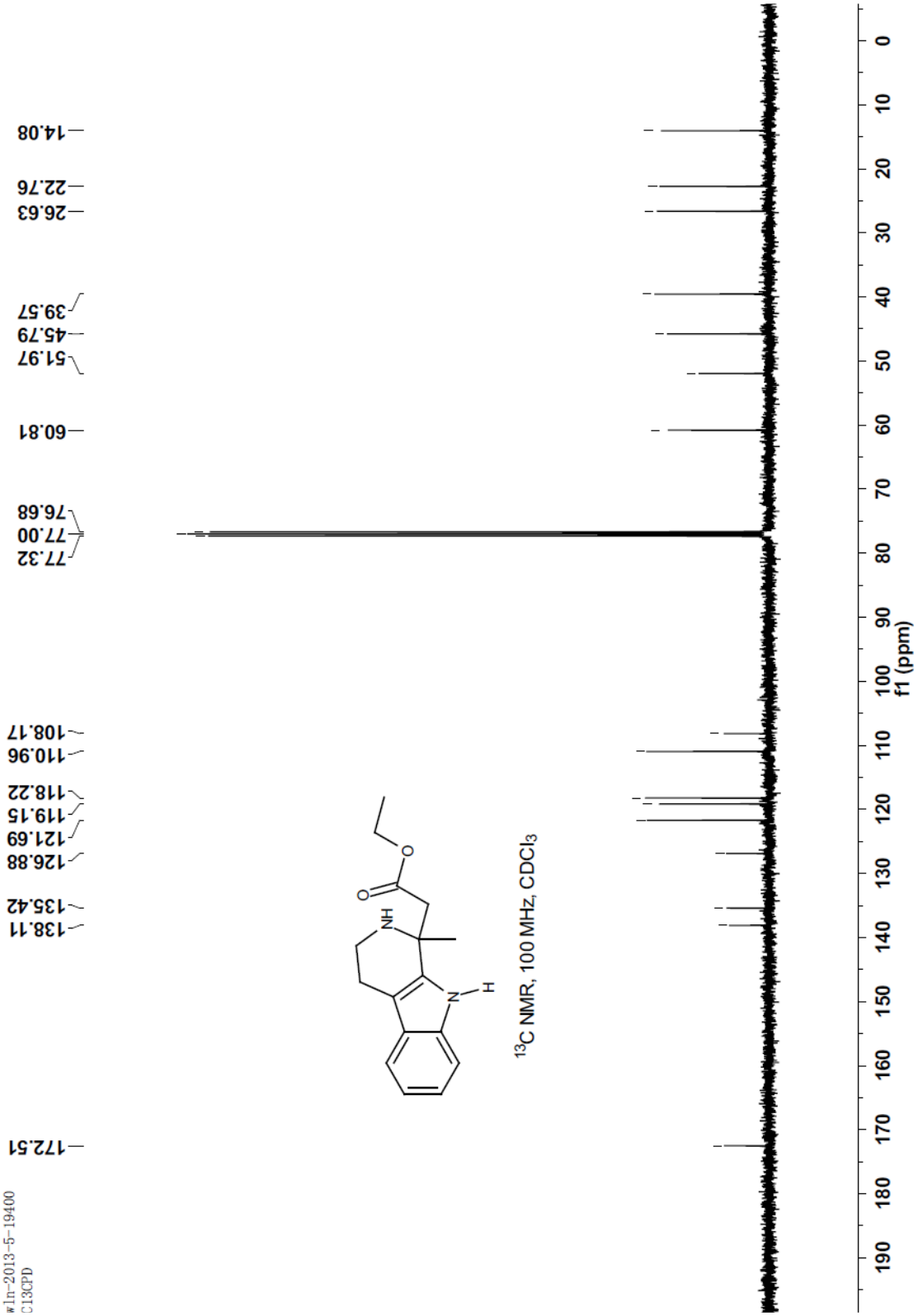
1-Methyl-1-(4-nitrophenyl)-1,2,3,4-tetrahydro-β-carboline (3m): ^{13}C NMR



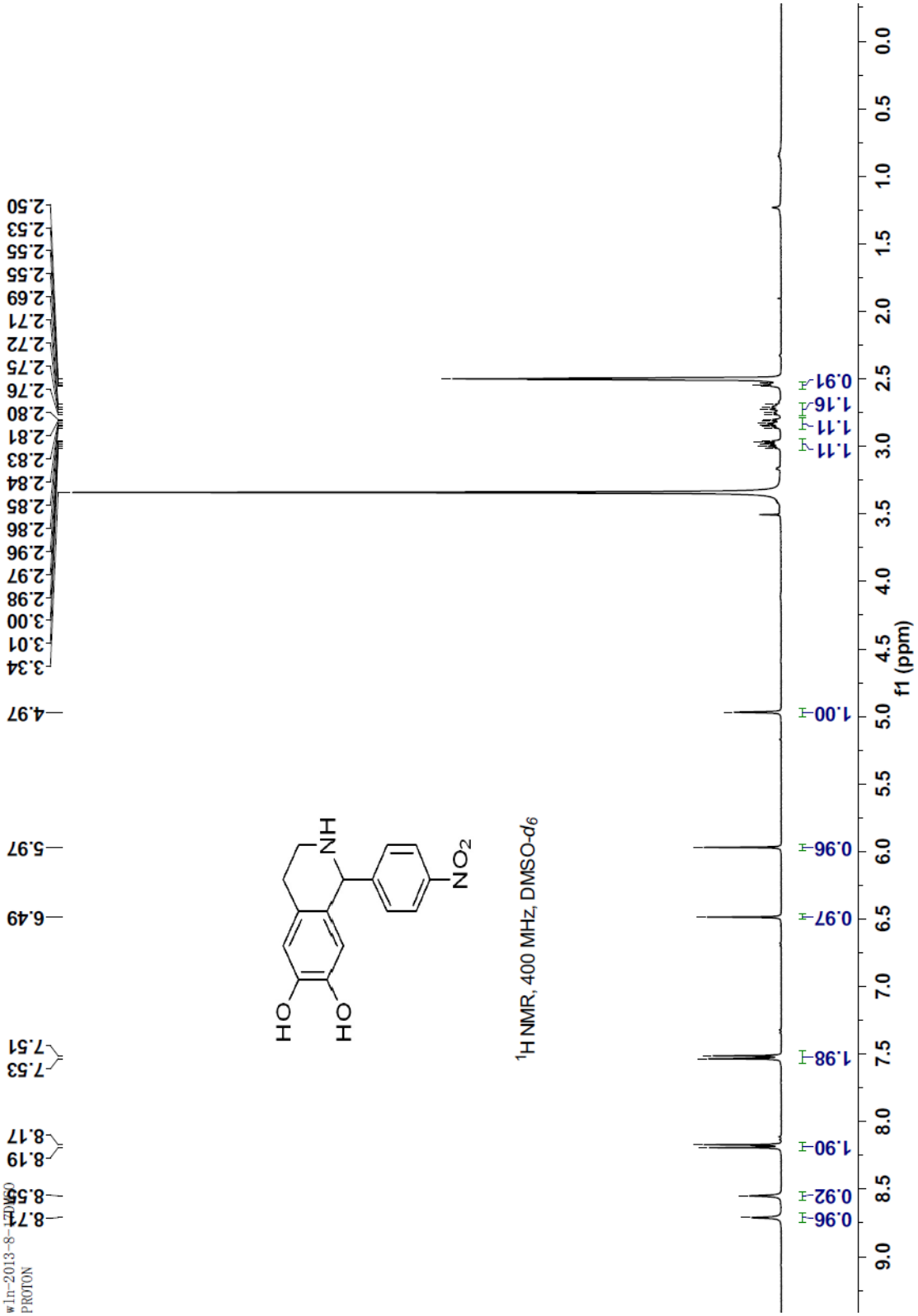
Ethyl-2-(1-methyl-1,2,3,4-tetrahydro-β-carboline-1-yl) acetate (3n): ^{1}H NMR



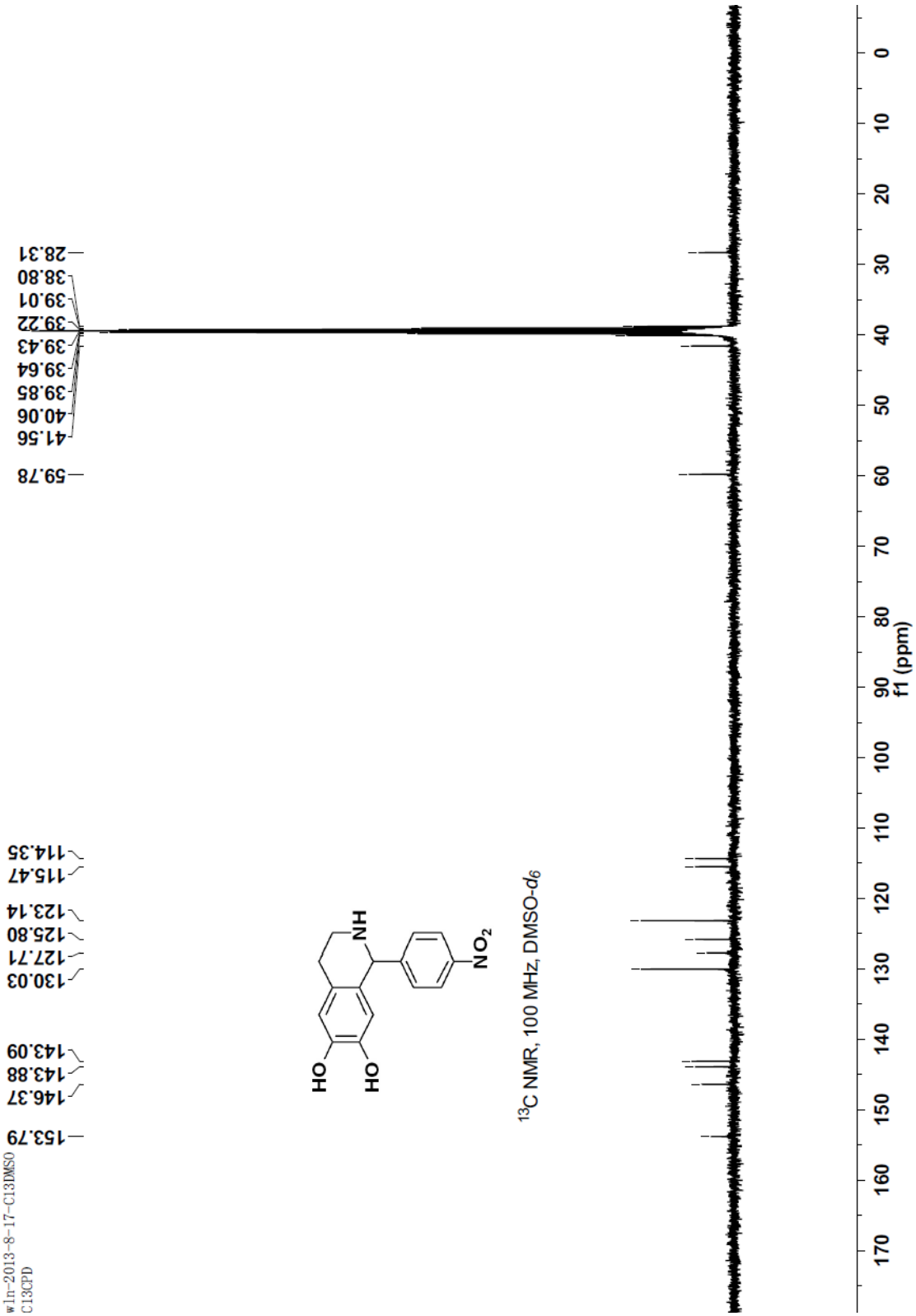
Ethyl-2-(1-methyl-1,2,3,4-tetrahydro-β-carboline-1-yl) acetate (3n): ^{13}C NMR



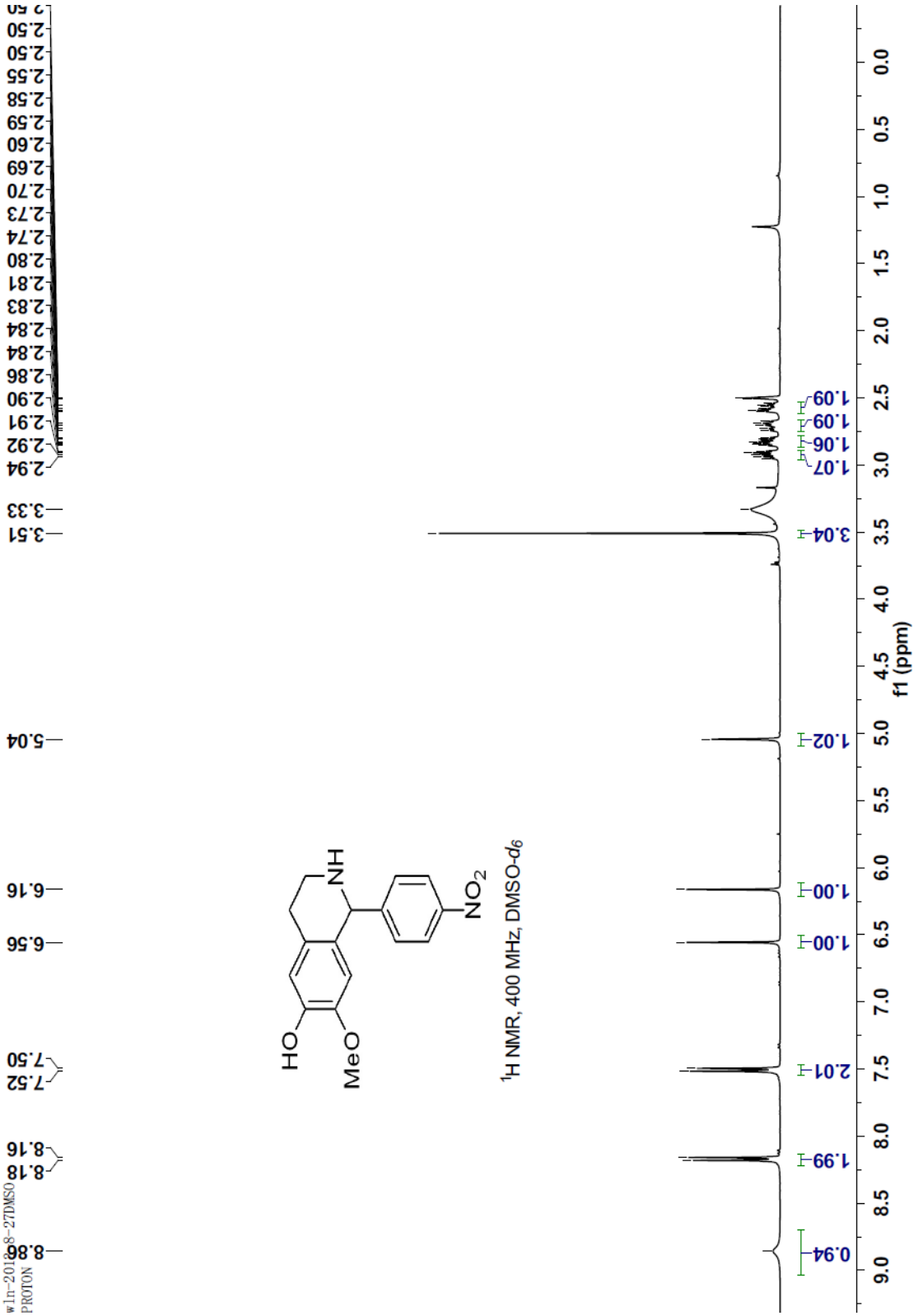
1-(4-Nitrophenyl)-1,2,3,4-tetrahydroisoquinoline-6,7-diol (3o): ^{1}H NMR



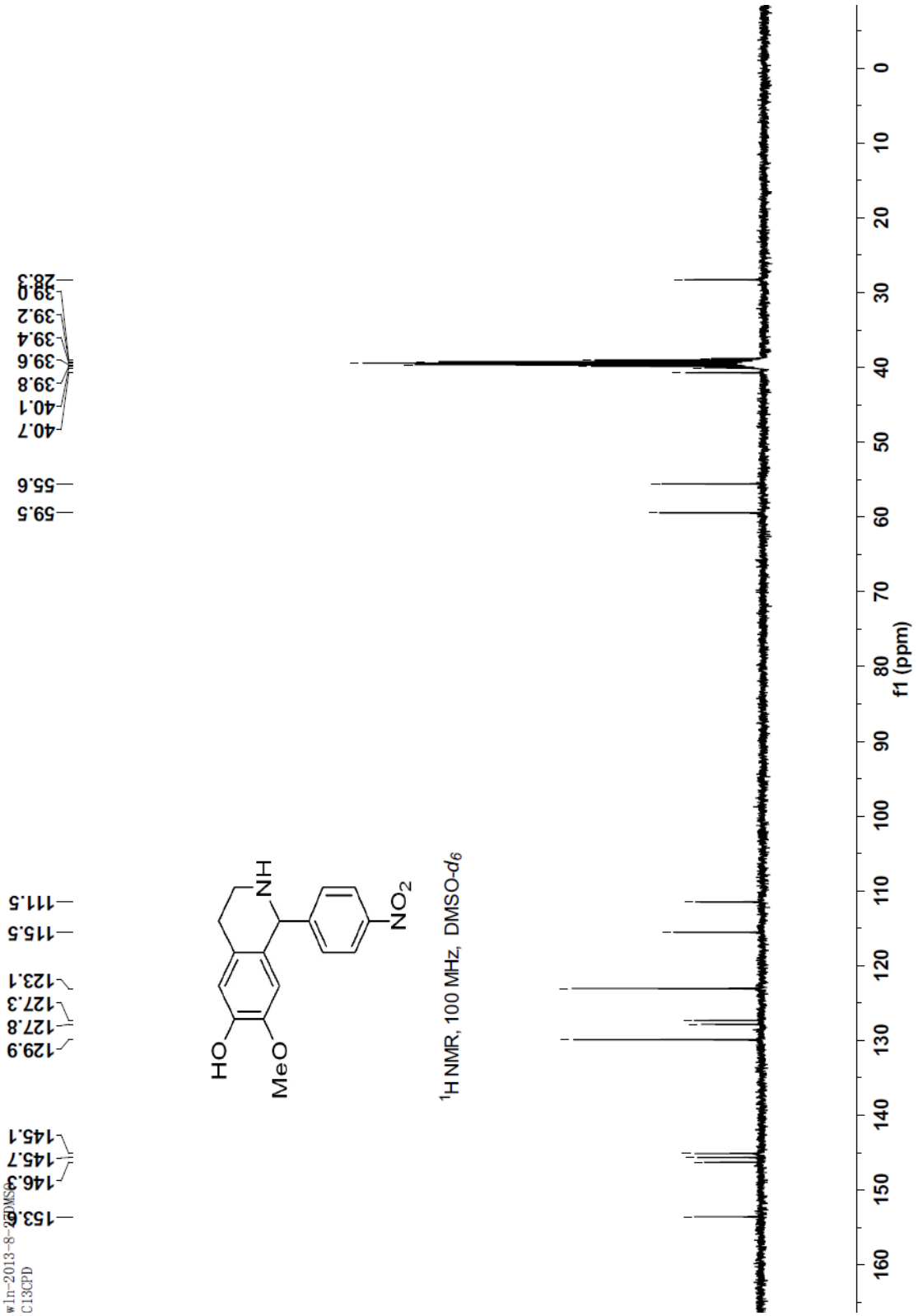
1-(4-Nitrophenyl)-1,2,3,4-tetrahydroisoquinoline-6,7-diol (3o) : ^{13}C NMR



1-(4-Nitrophenyl)-6-hydroxy-7-methoxy-1,2,3,4-tetrahydroisoquinoline (3p): ^{1}H NMR

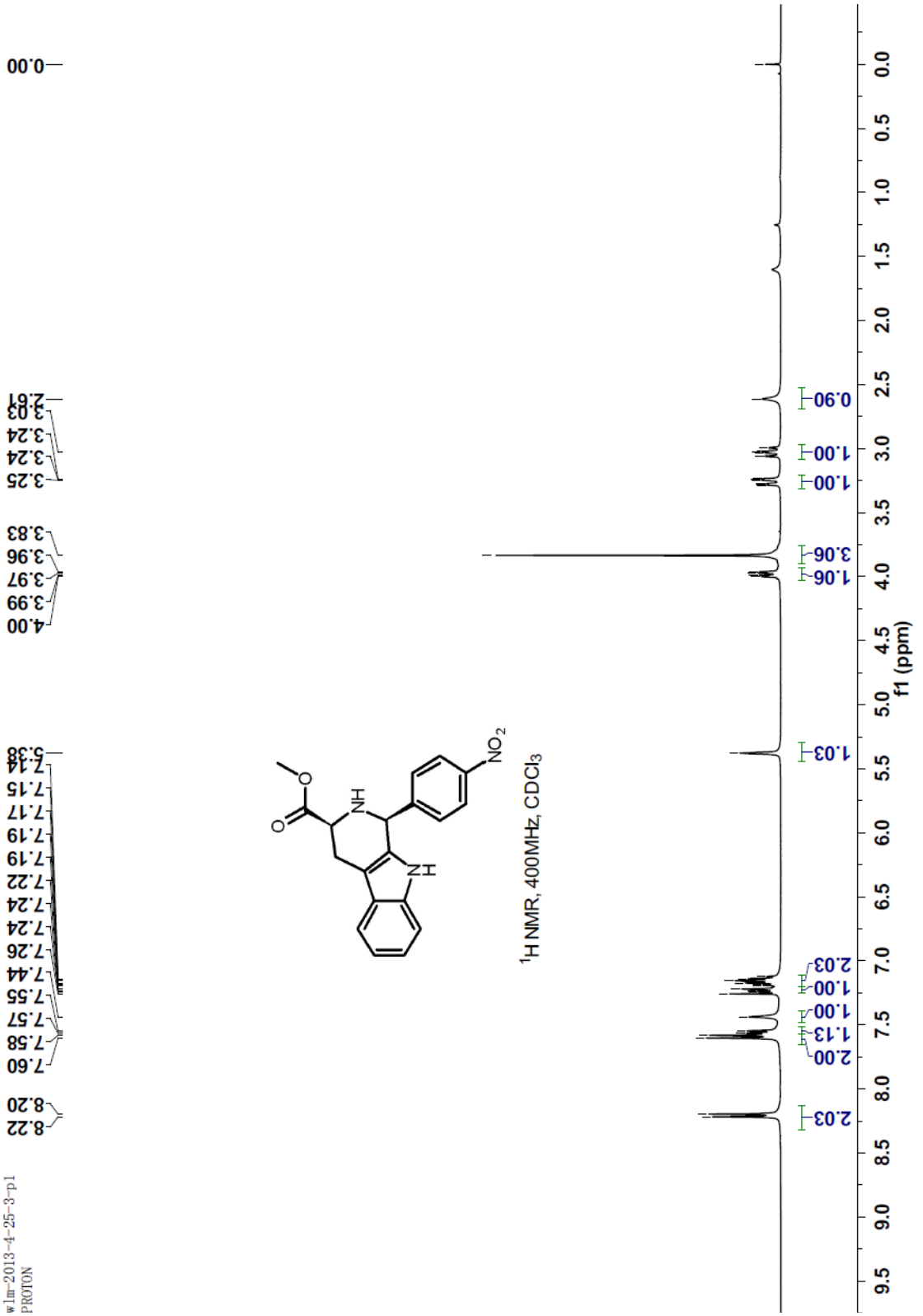


1-(4-Nitrophenyl)-6-hydroxy-7-methoxy-1,2,3,4-tetrahydroisoquinoline (3p): ^{13}C NMR

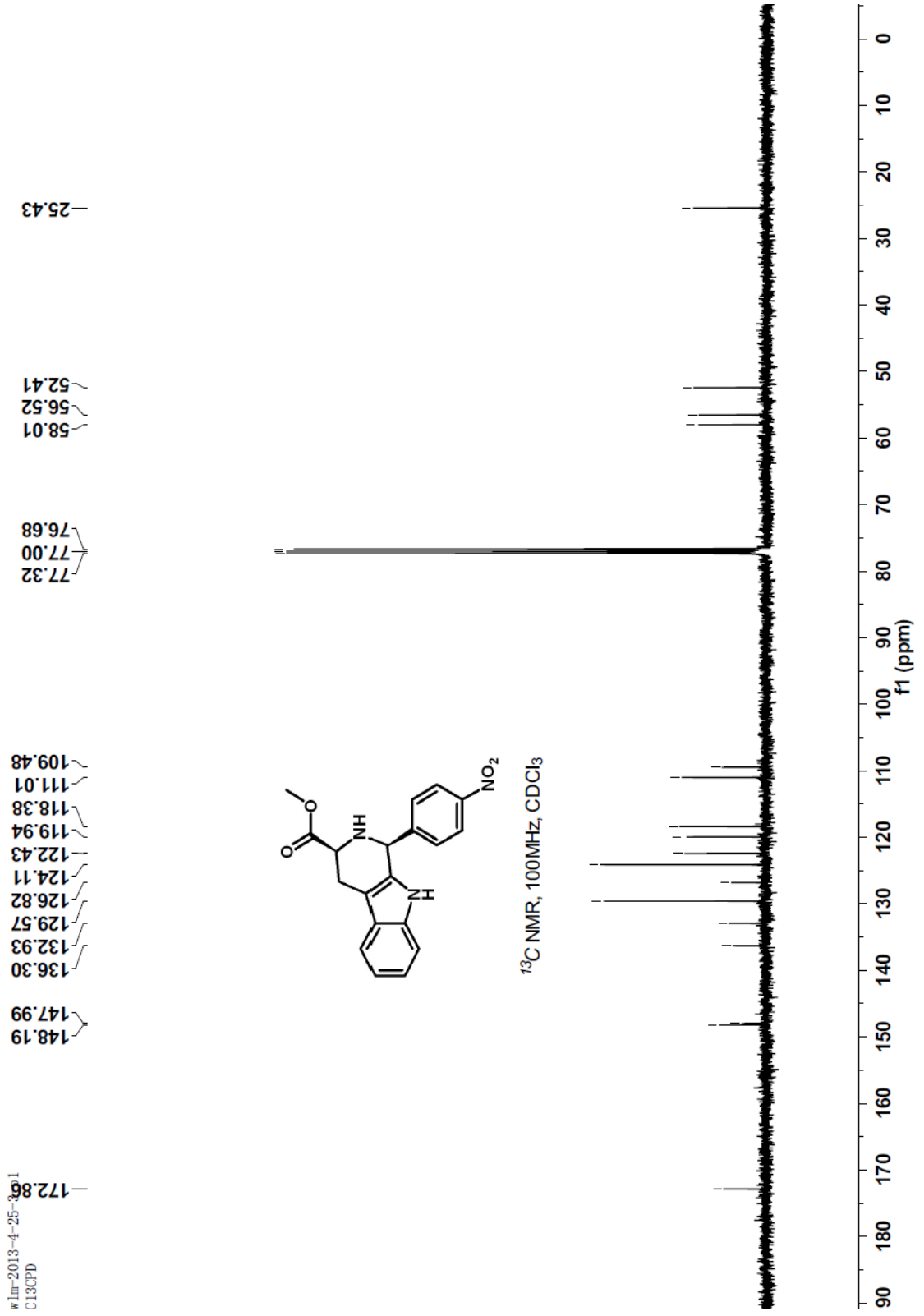


1-(*p*-Nitrophenyl)-3-methoxycarbonyl-1,2,3,4-tetrahydro-β-carboline (3q):

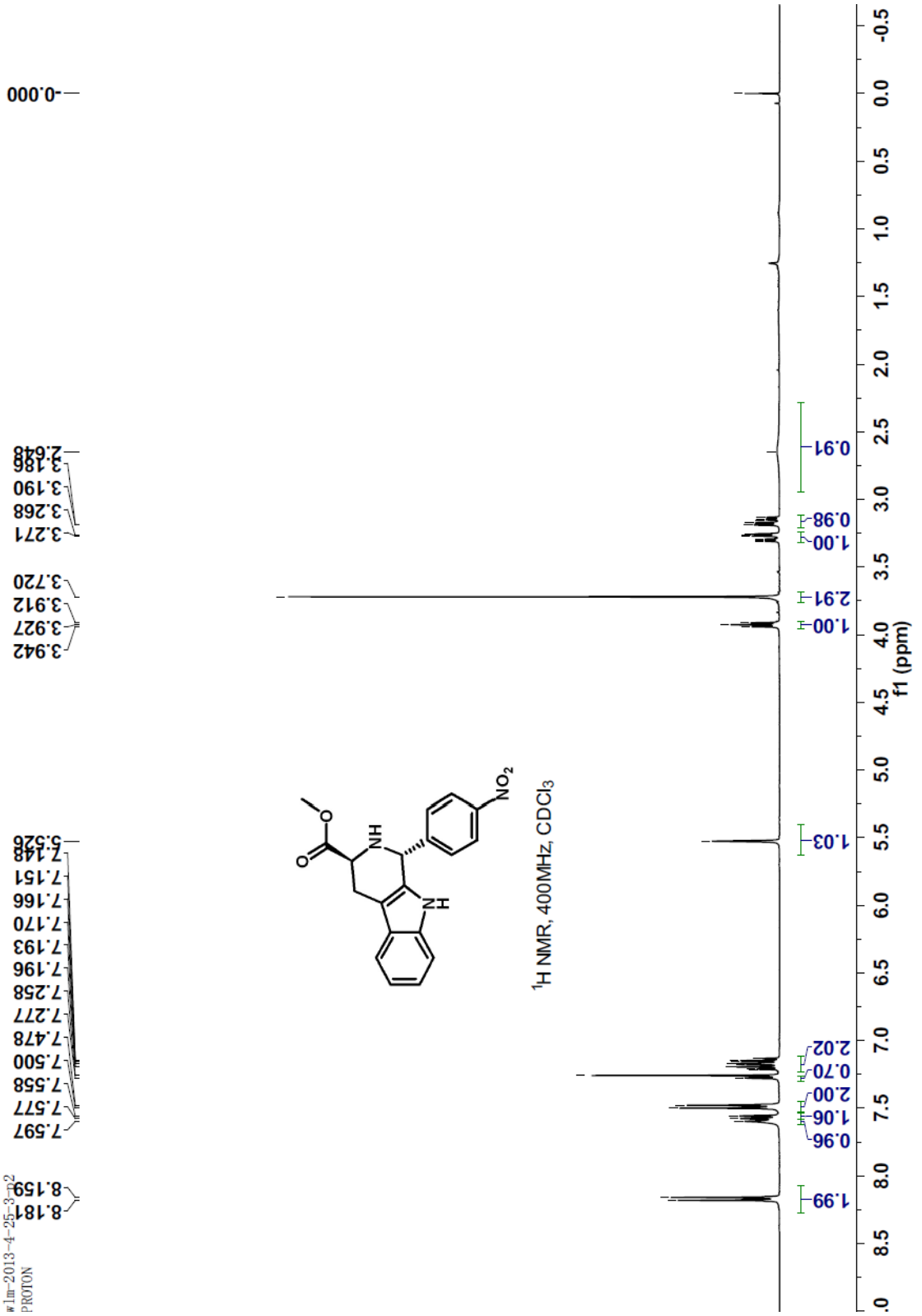
cis-**3q**: **^{1}H NMR**



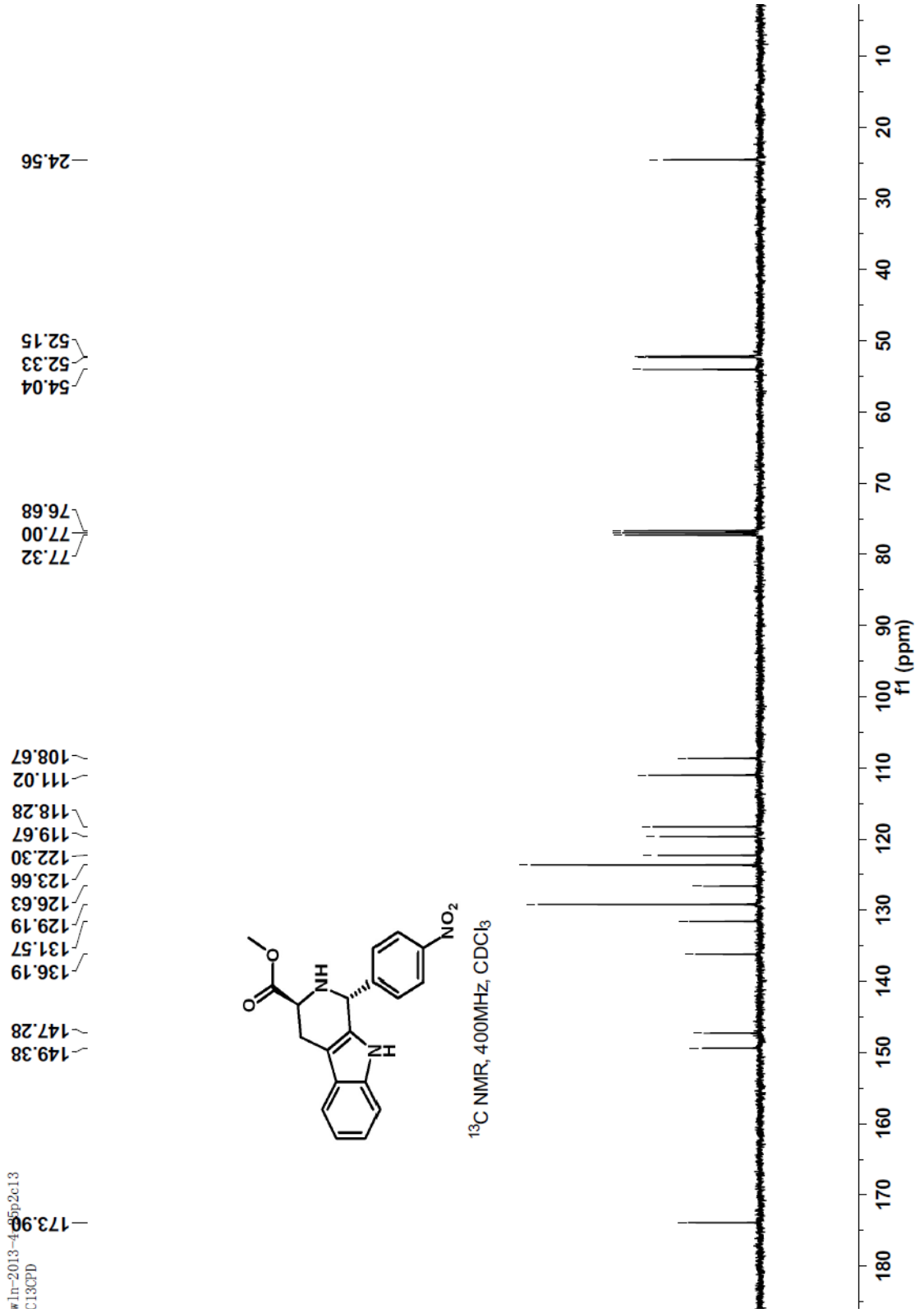
cis-**3q**: **^{13}C NMR**



trans-**3q**: **^{1}H NMR**

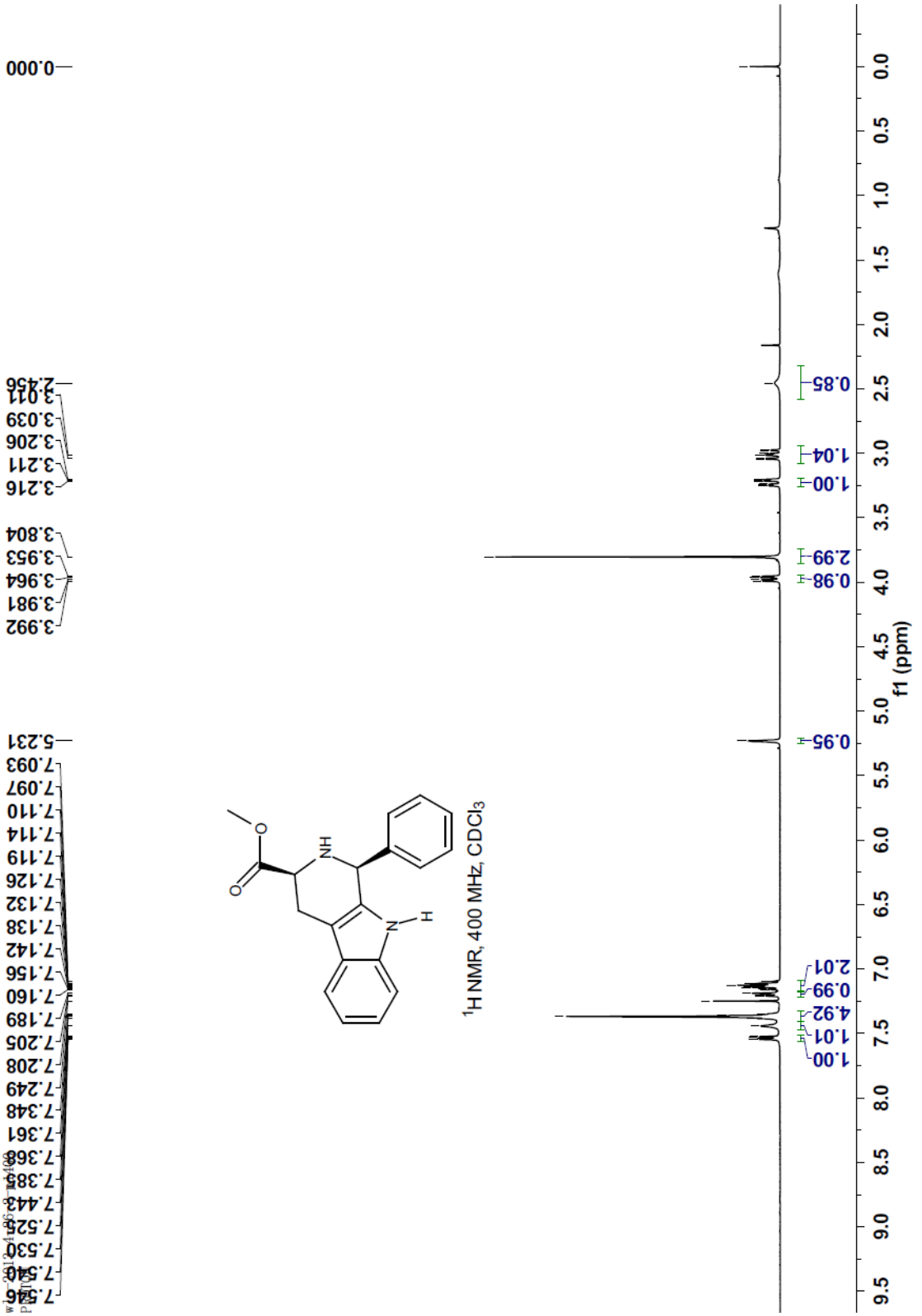


trans-**3q**: **^{13}C NMR**

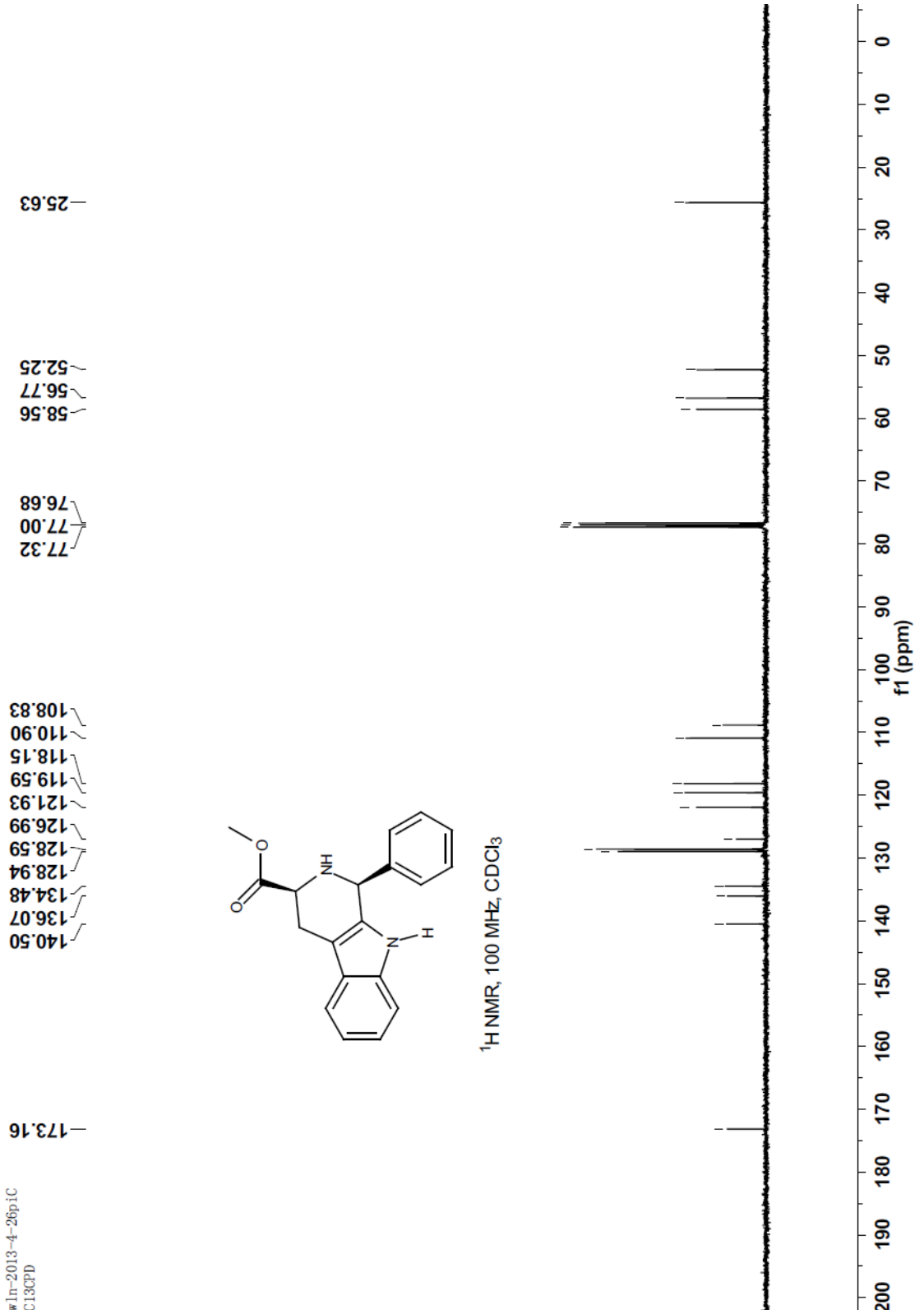


1-Phenyl-3-methoxycarbonyl-1,2,3,4-tetrahydro-β-carboline (3r):

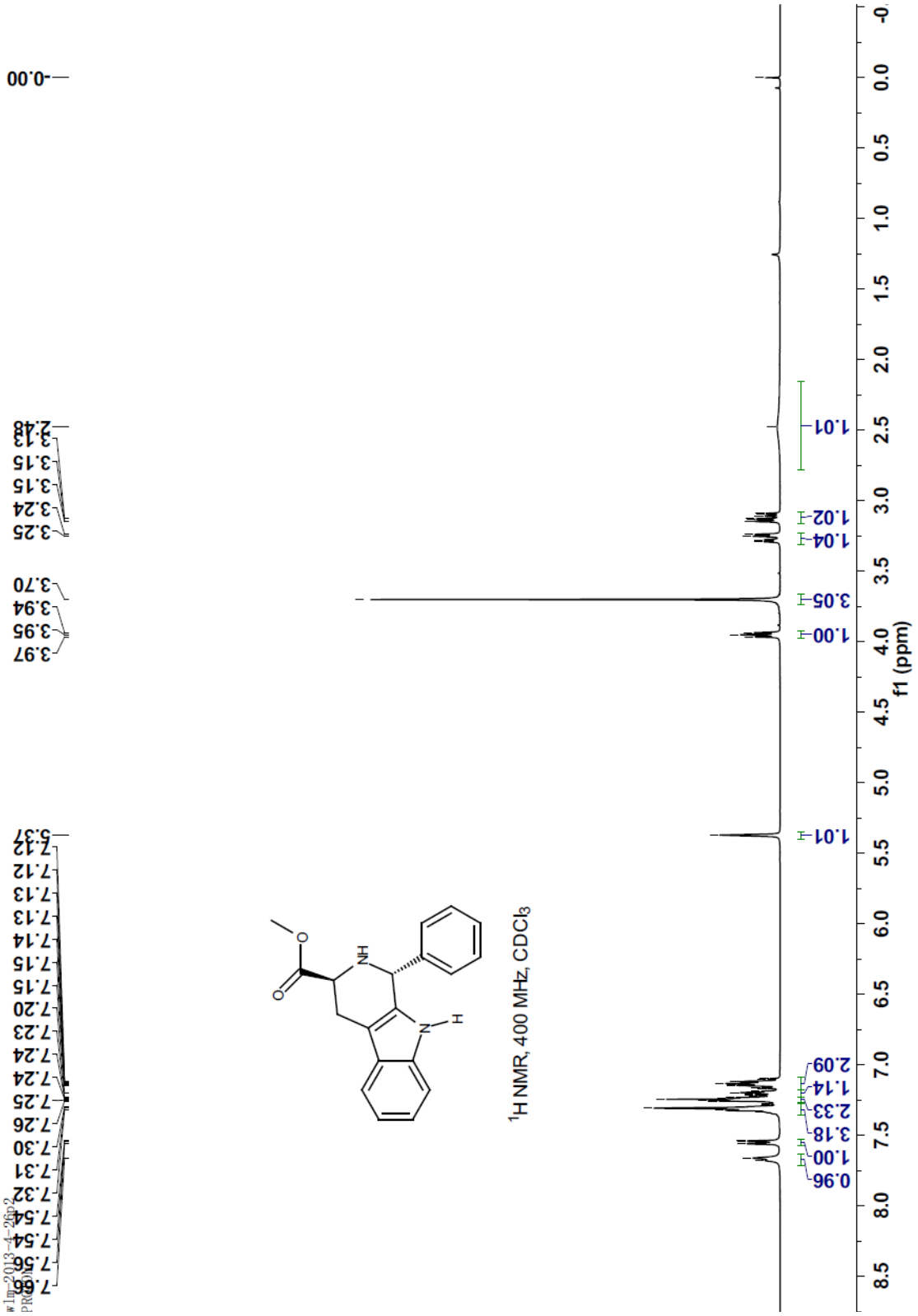
cis-**3r**: **^{1}H NMR**



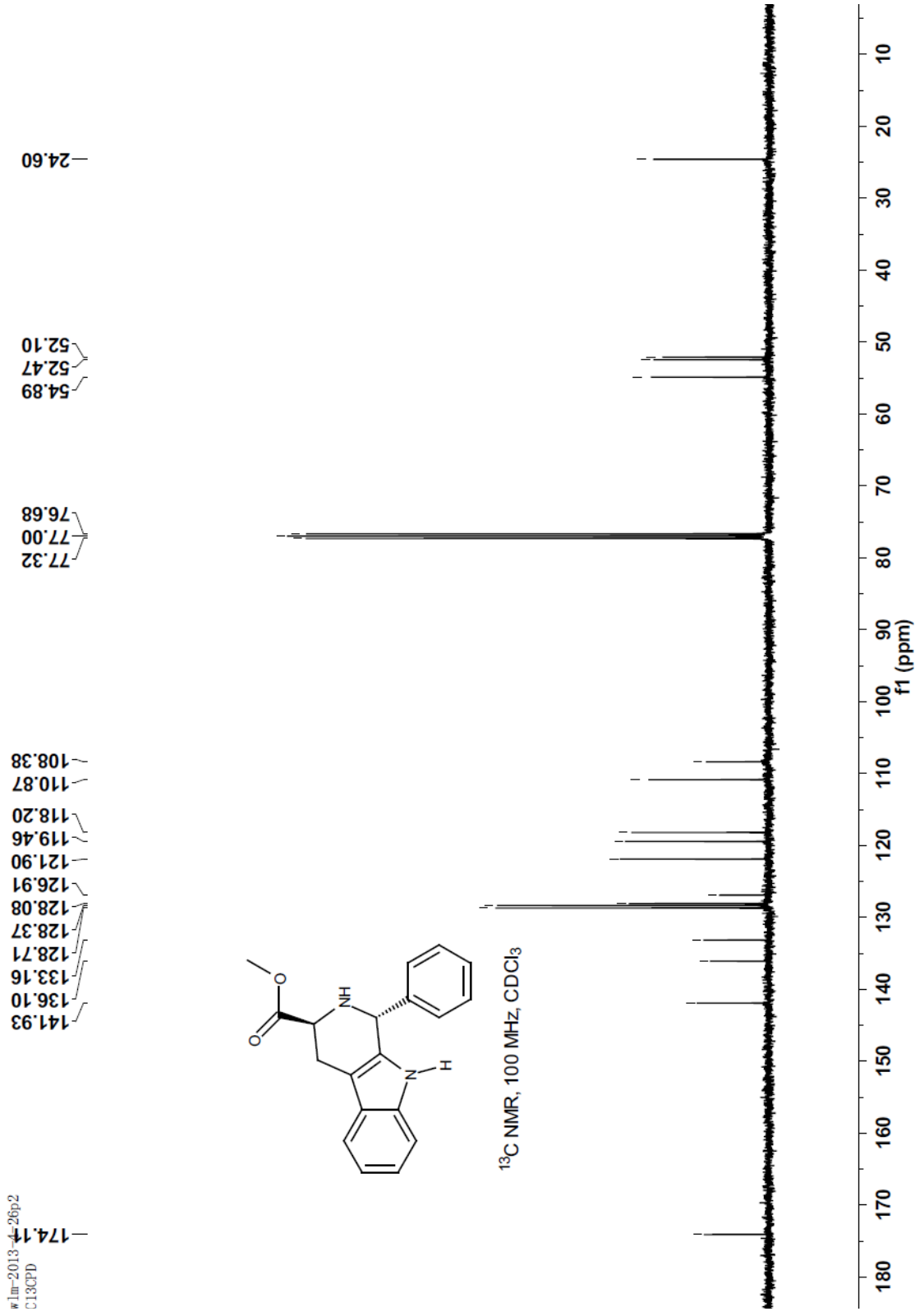
cis-**3r**: **^{13}C NMR**



trans-**3r**: **^{13}C NMR**

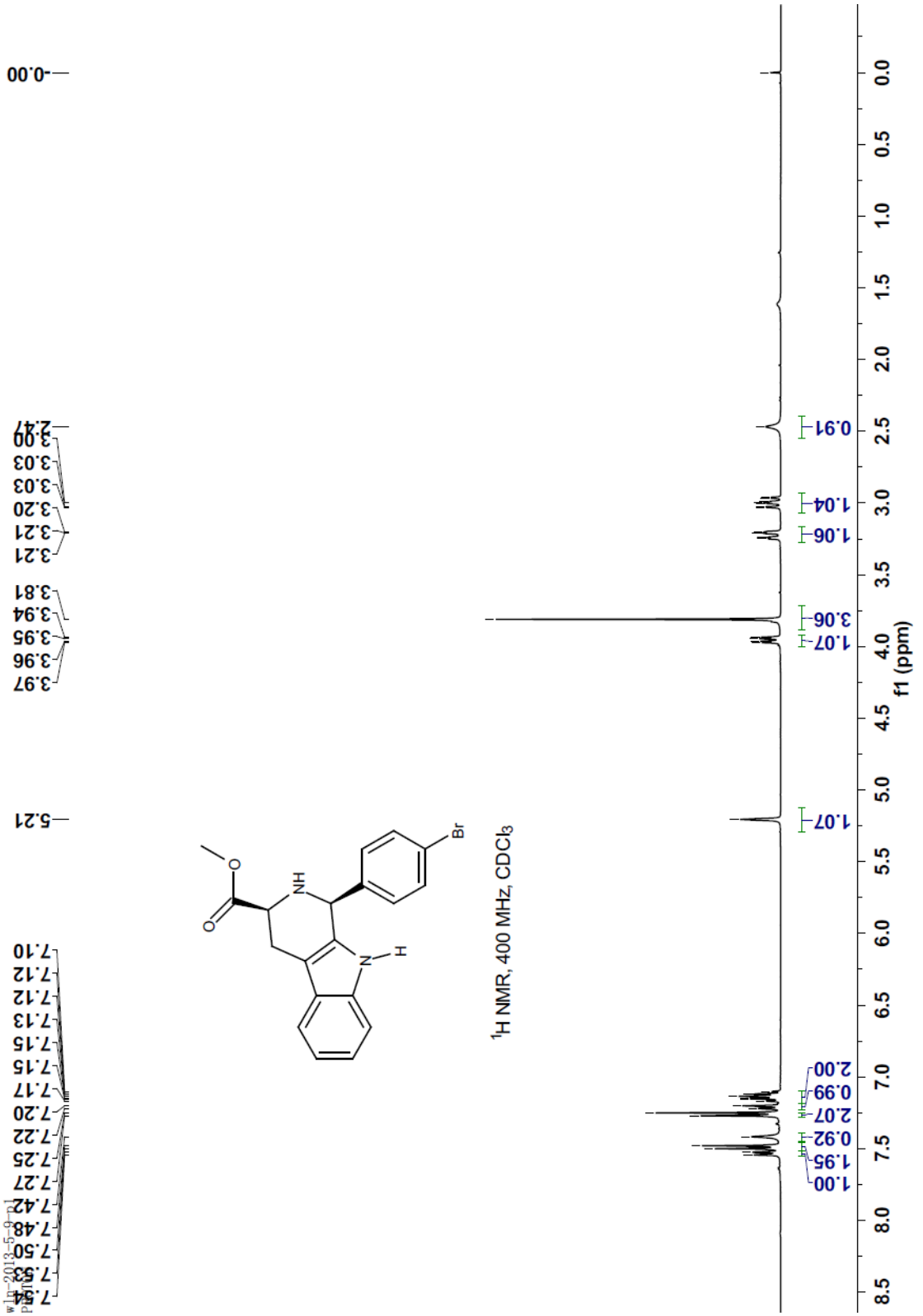


trans-**3r**: **^{13}C NMR**

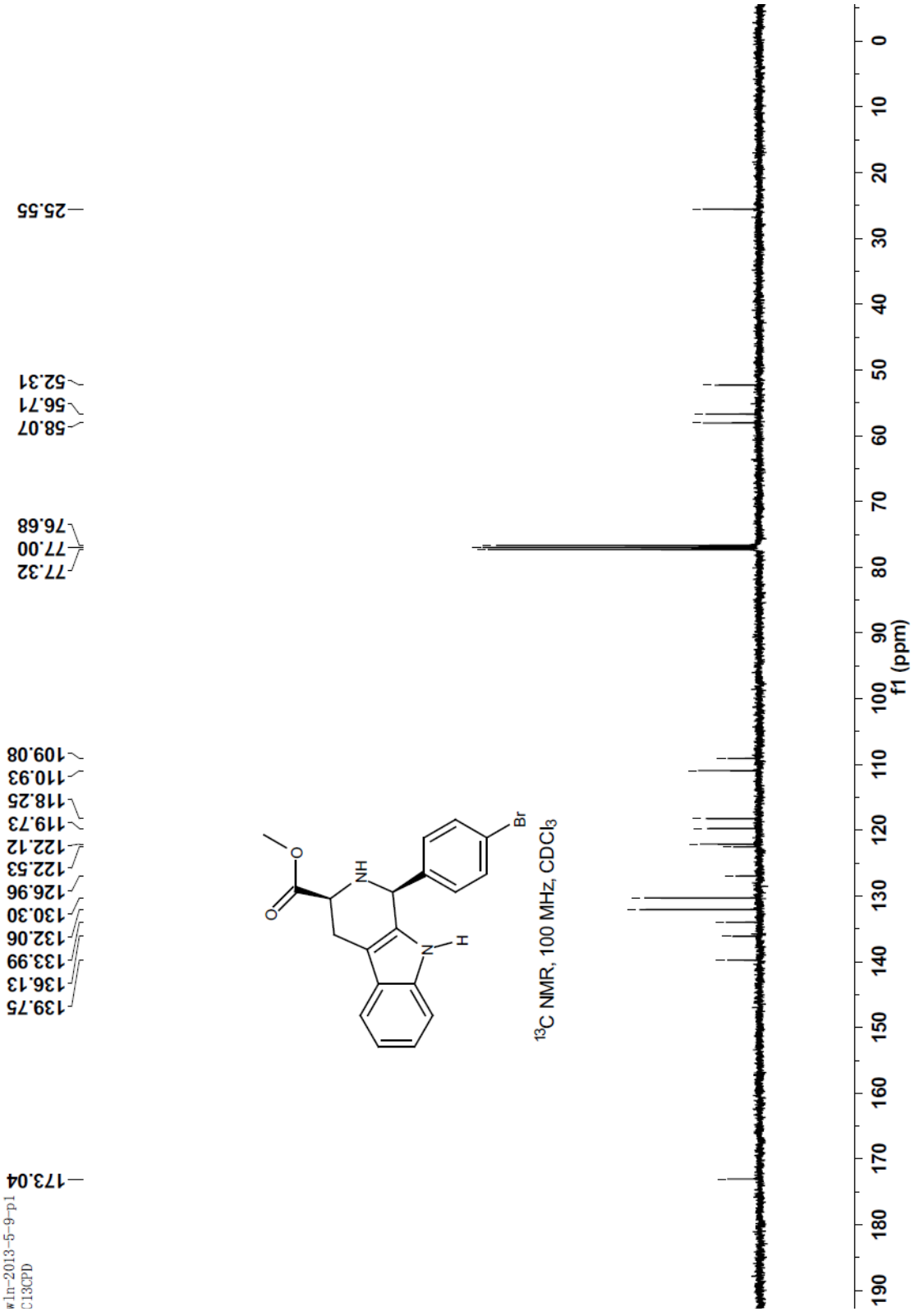


1-(*p*-Bromophenyl)-3-methoxycarbonyl-1,2,3,4-tetrahydro-β-carboline (3s):

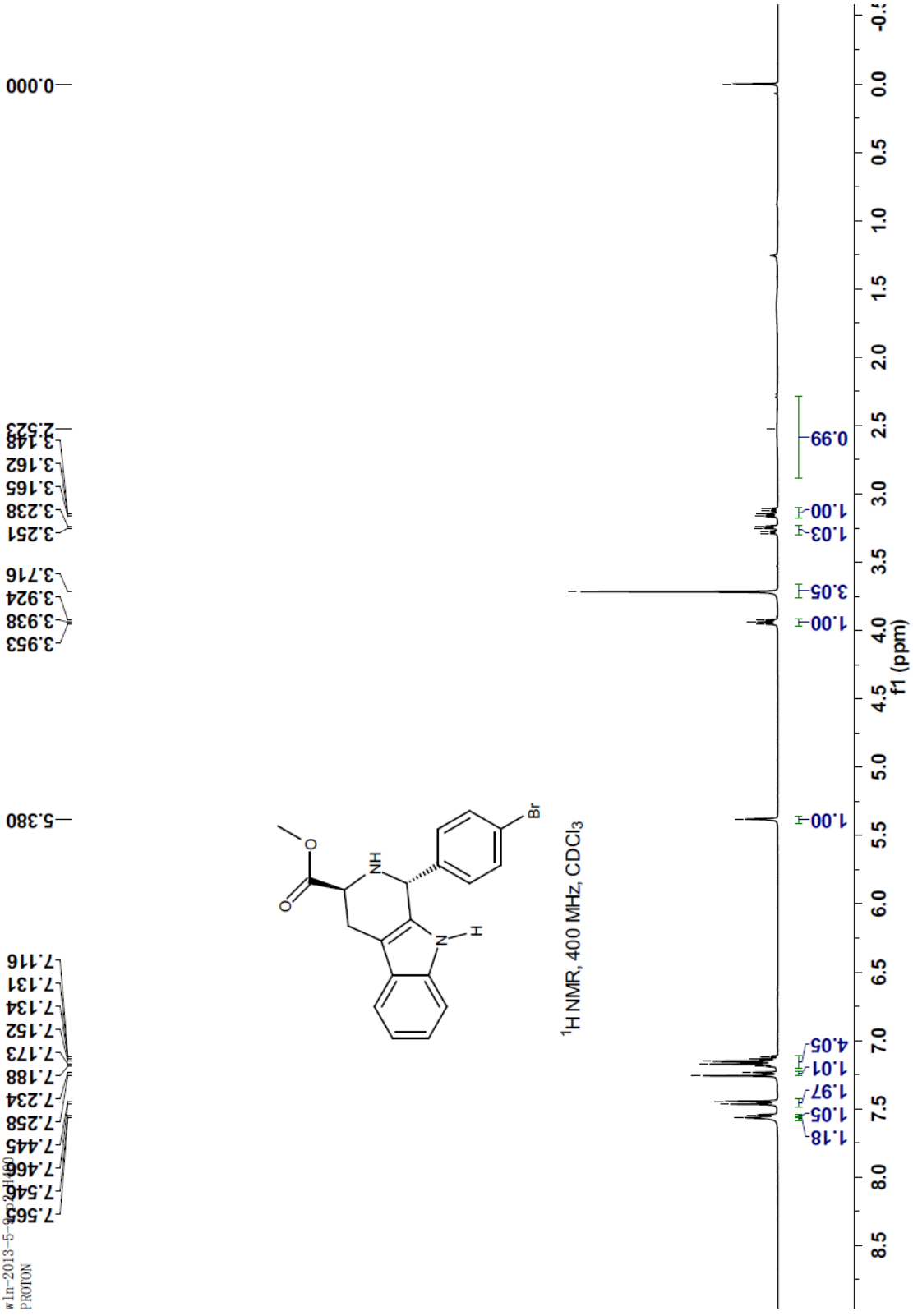
cis-**3s**: **^{1}H NMR**



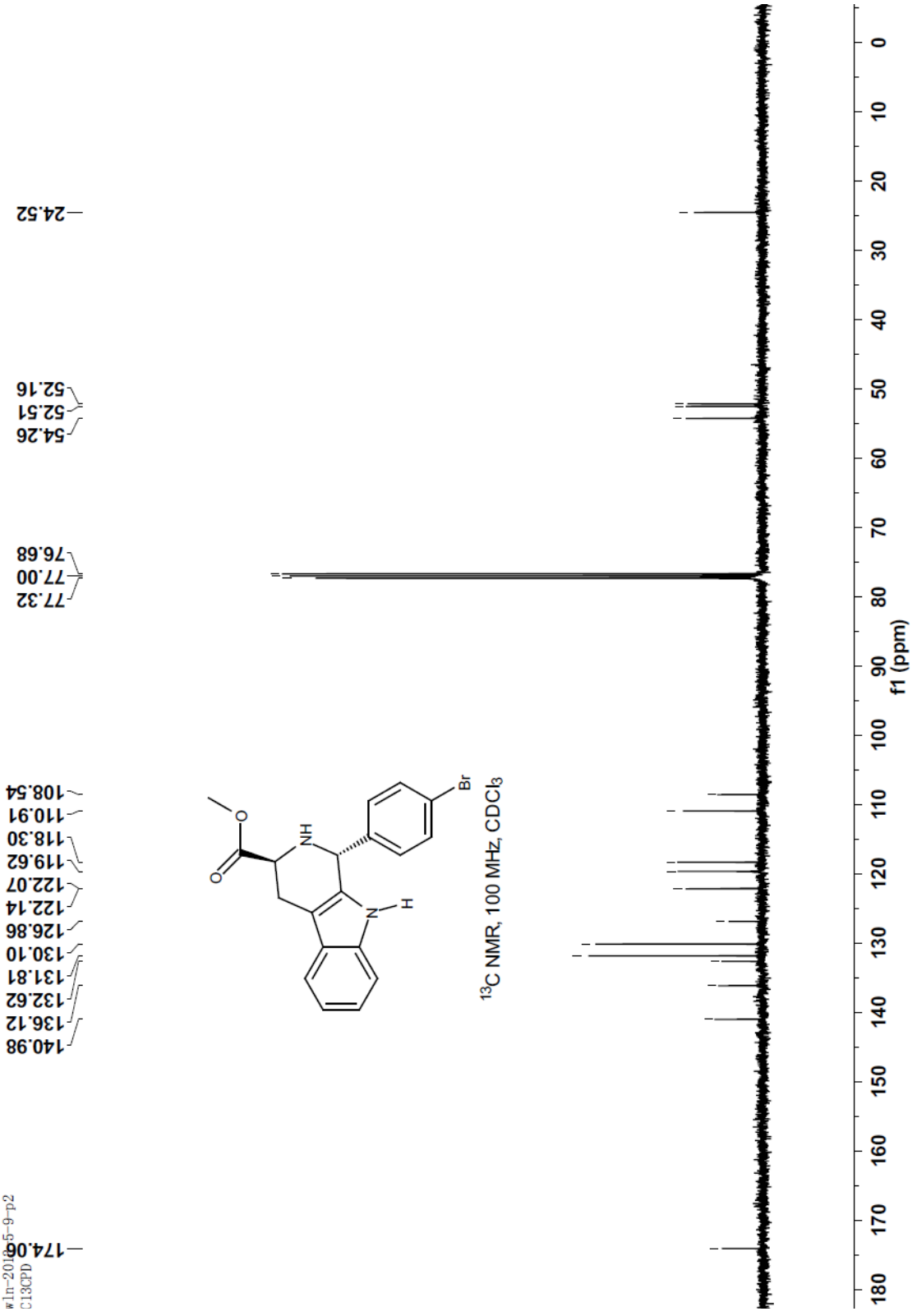
cis-**3s**: **^{13}C NMR**



trans-**3s**: **^{1}H NMR**

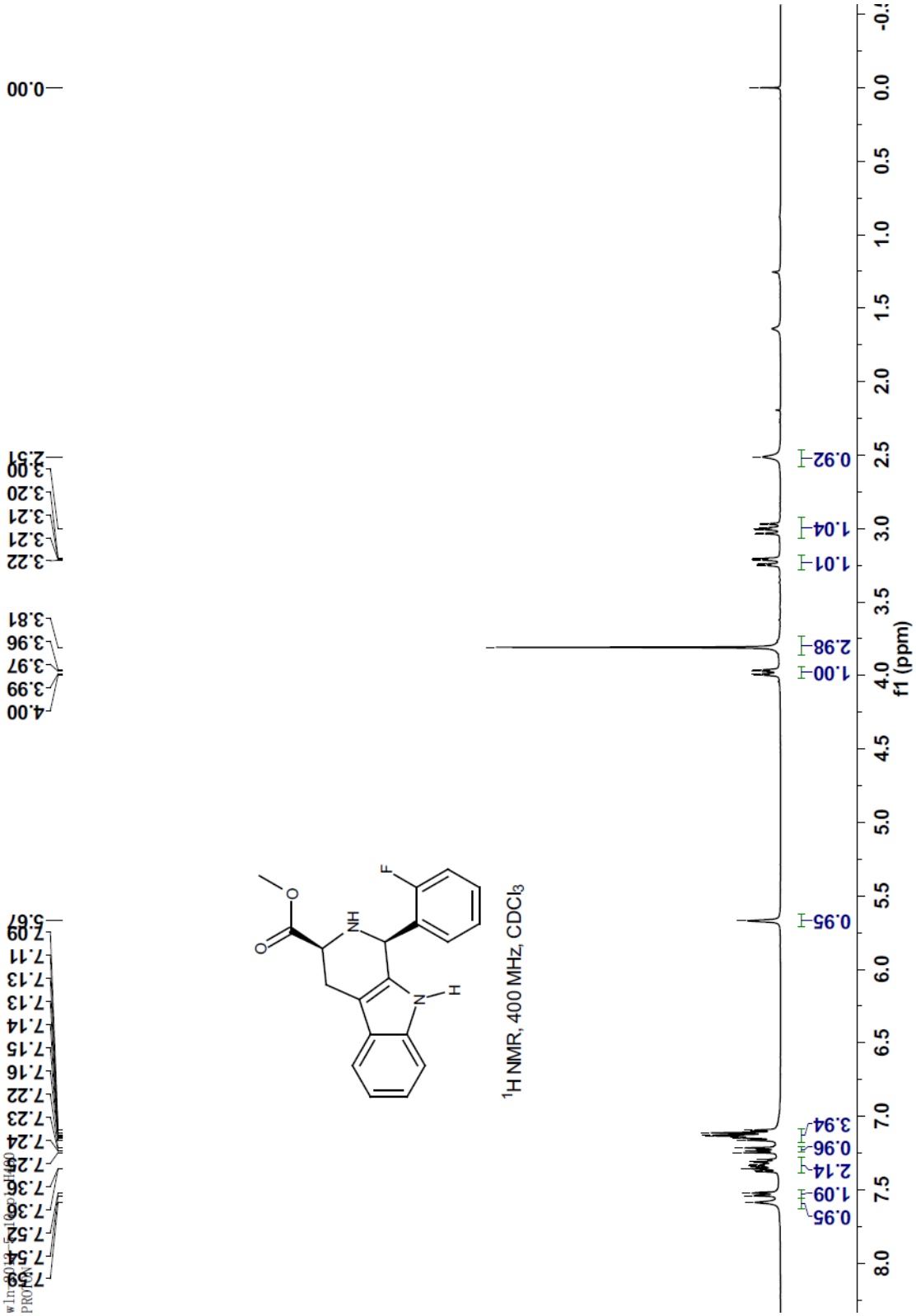


trans-**3s**: **^{13}C NMR**

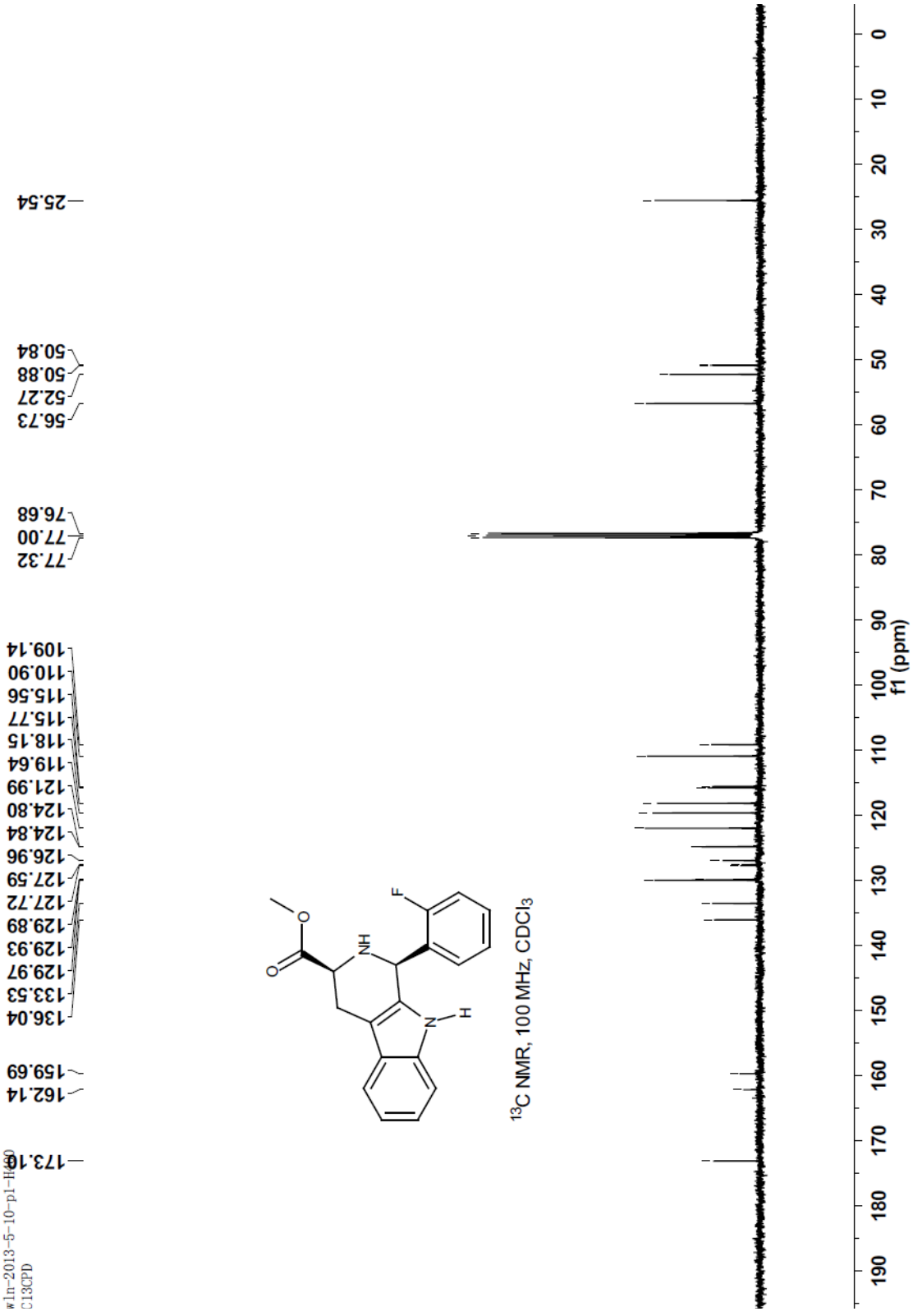


1-(2-Fluorophenyl)-3-methoxycarbonyl-1,2,3,4-tetrahydro-β-carboline (3t):

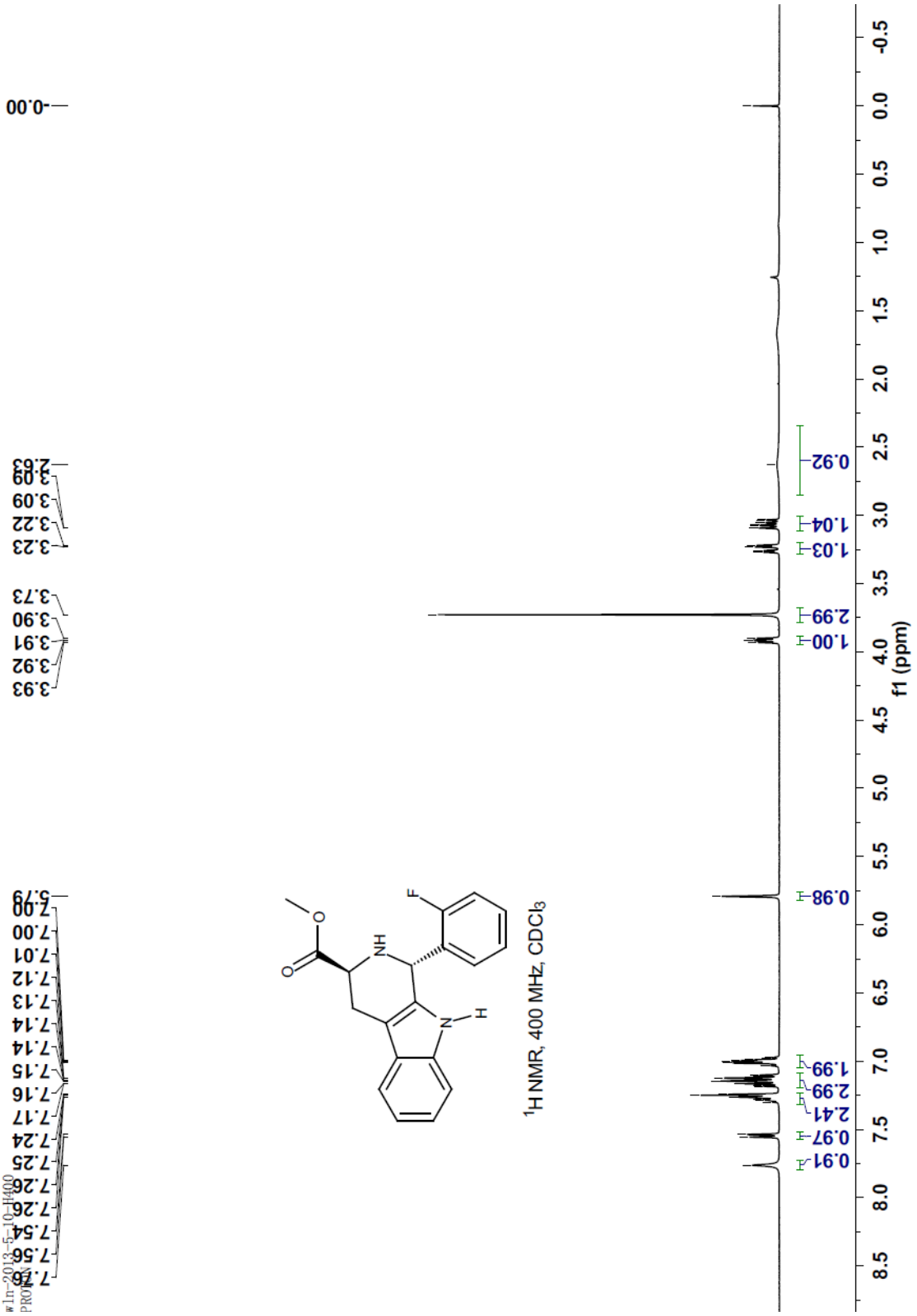
cis-**3t**: **^{1}H NMR**



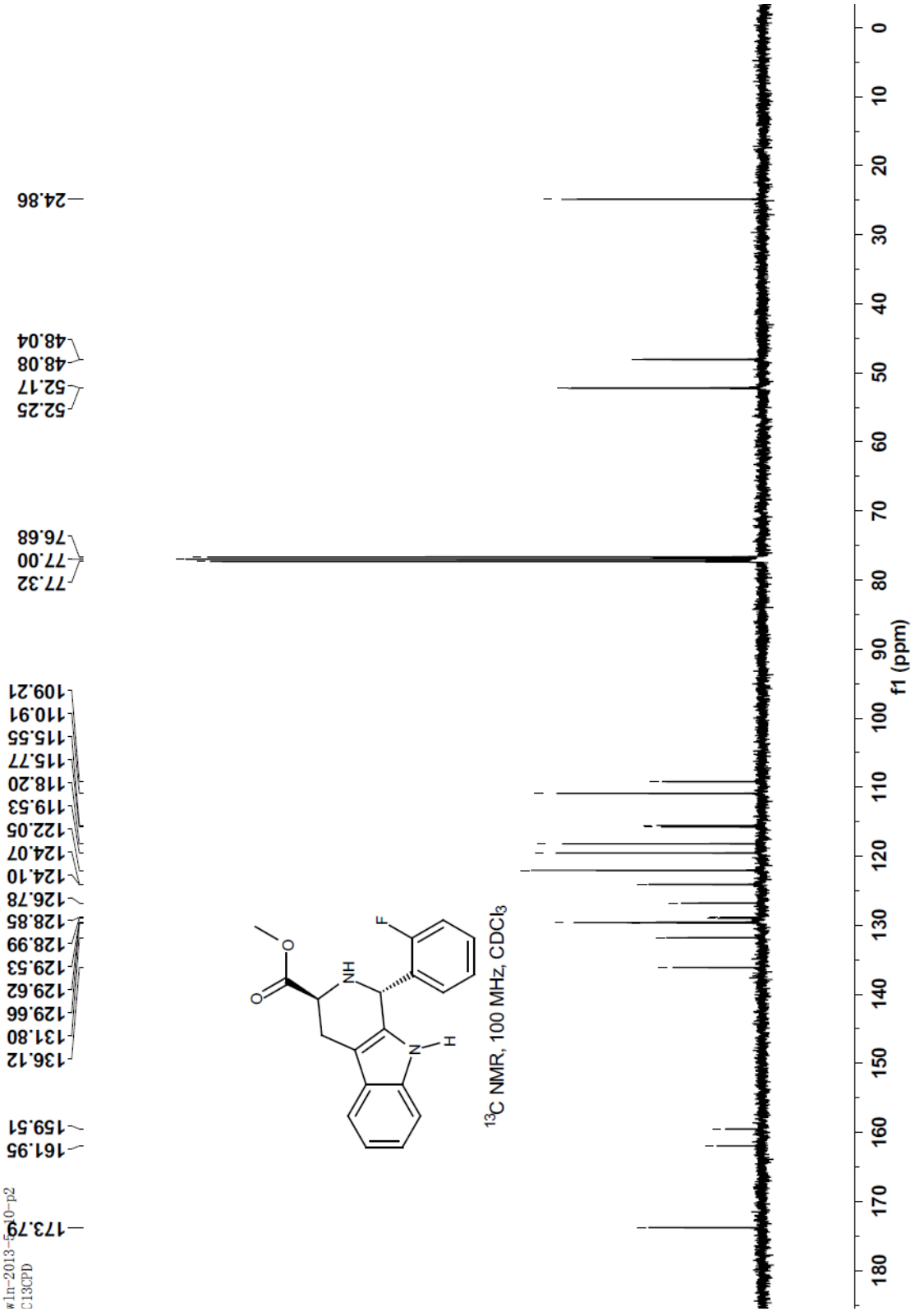
cis-**3t**: **^{13}C NMR**



trans-**3t**: **^{1}H NMR**

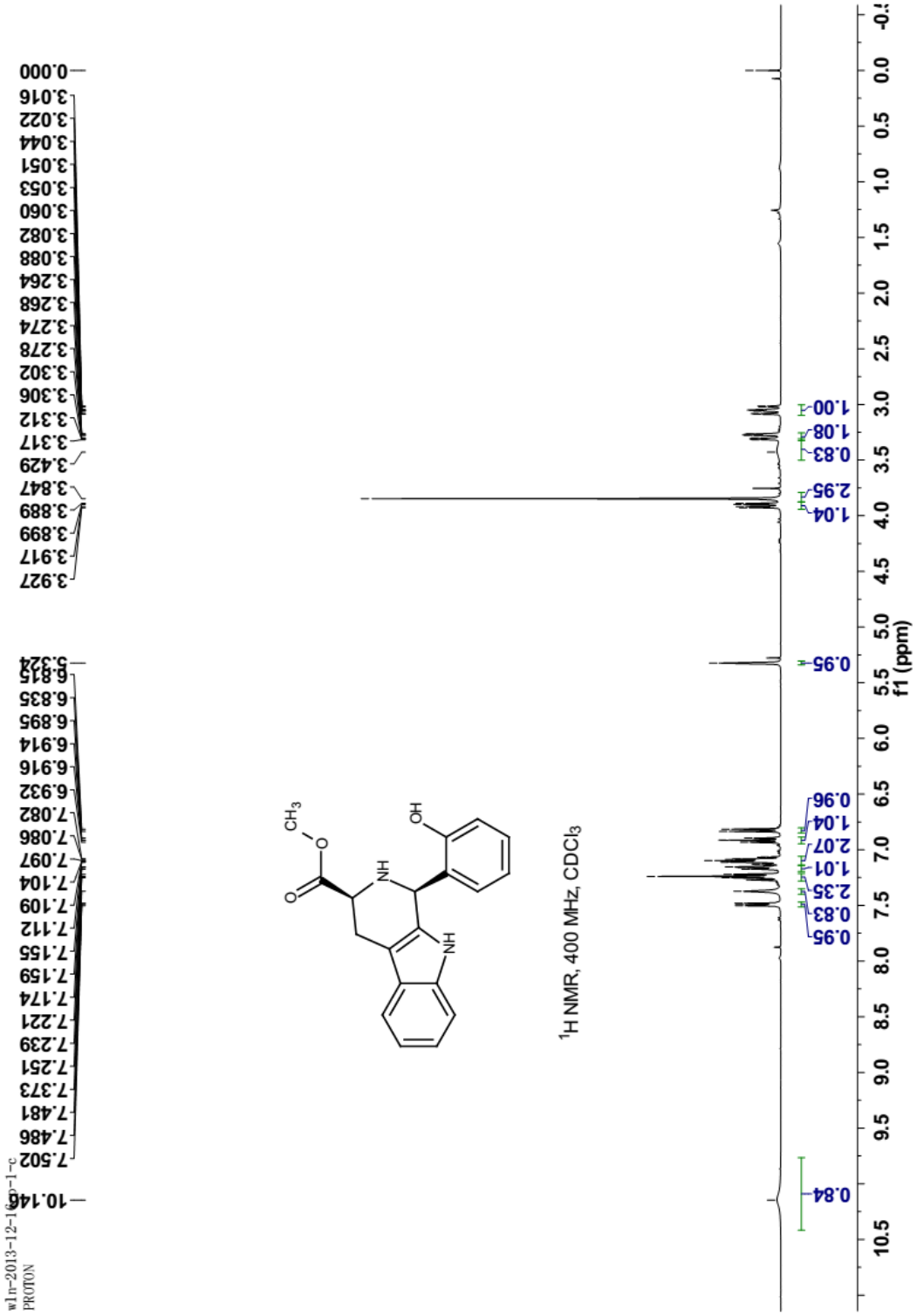


trans-**3t**: **^{13}C NMR**

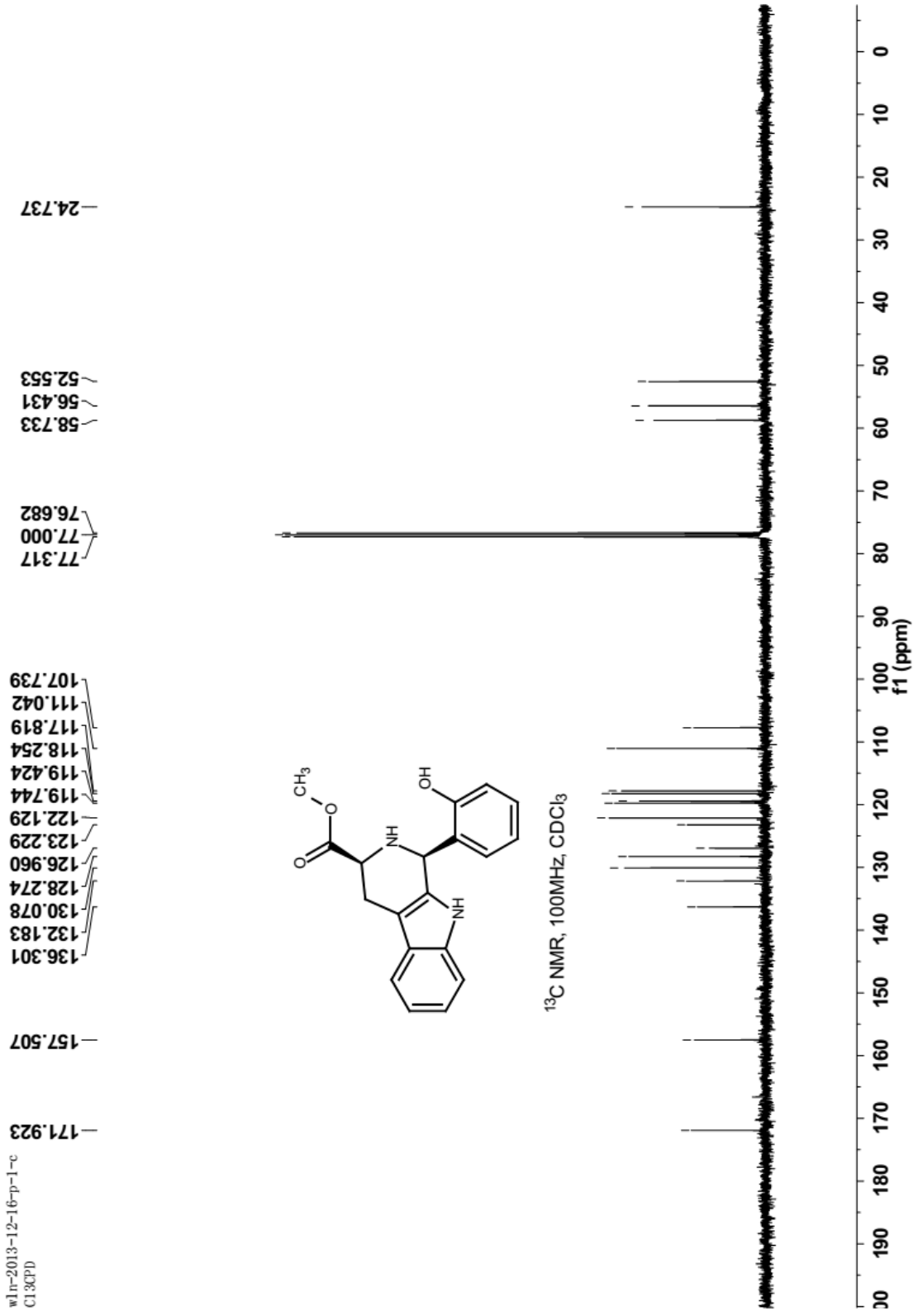


1-(2-Hydroxypheny)-3-methoxycarbonyl-1,2,3,4-tetrahydro-β-carboline (3u)

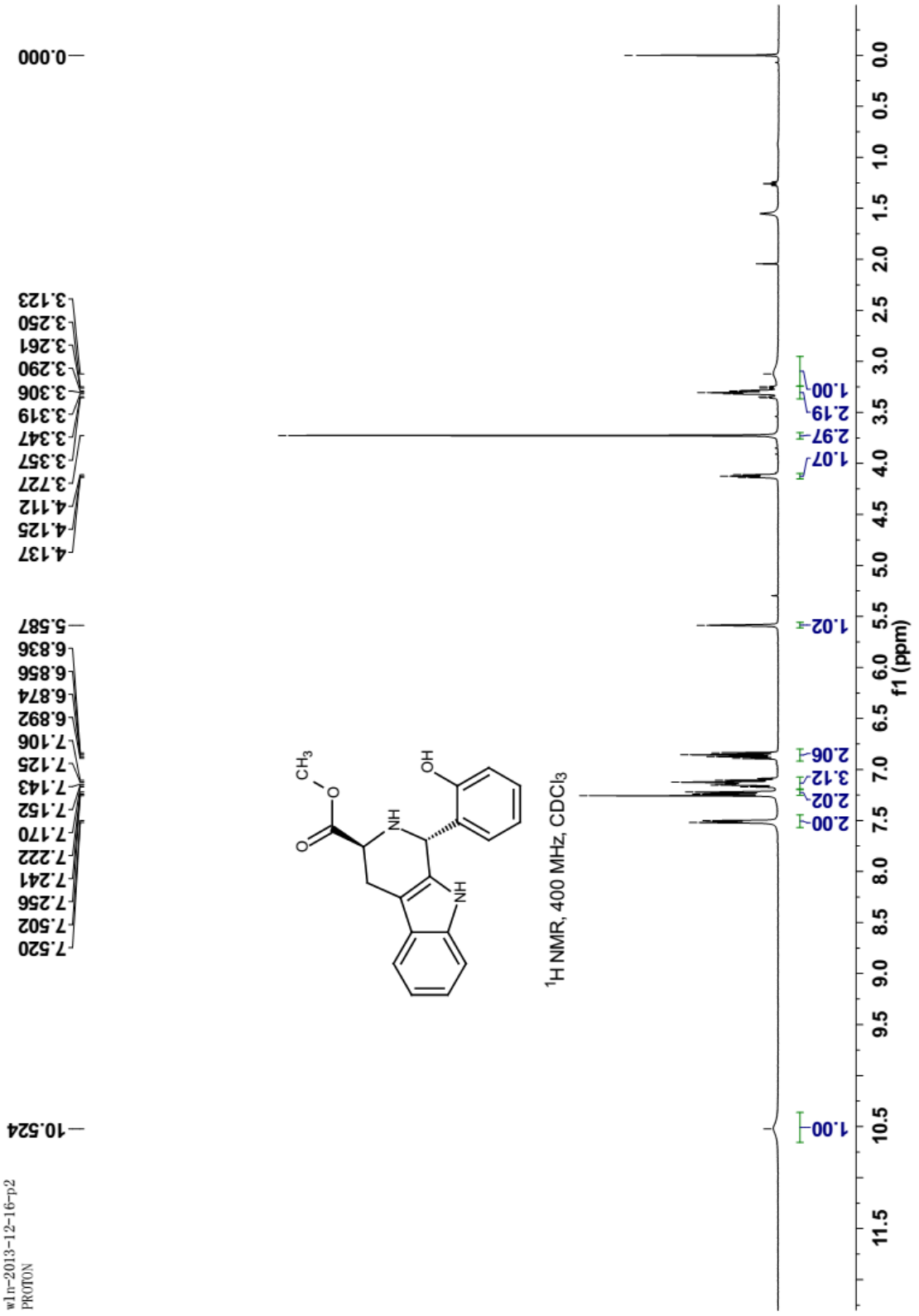
cis-**3u**: **^{1}H NMR**



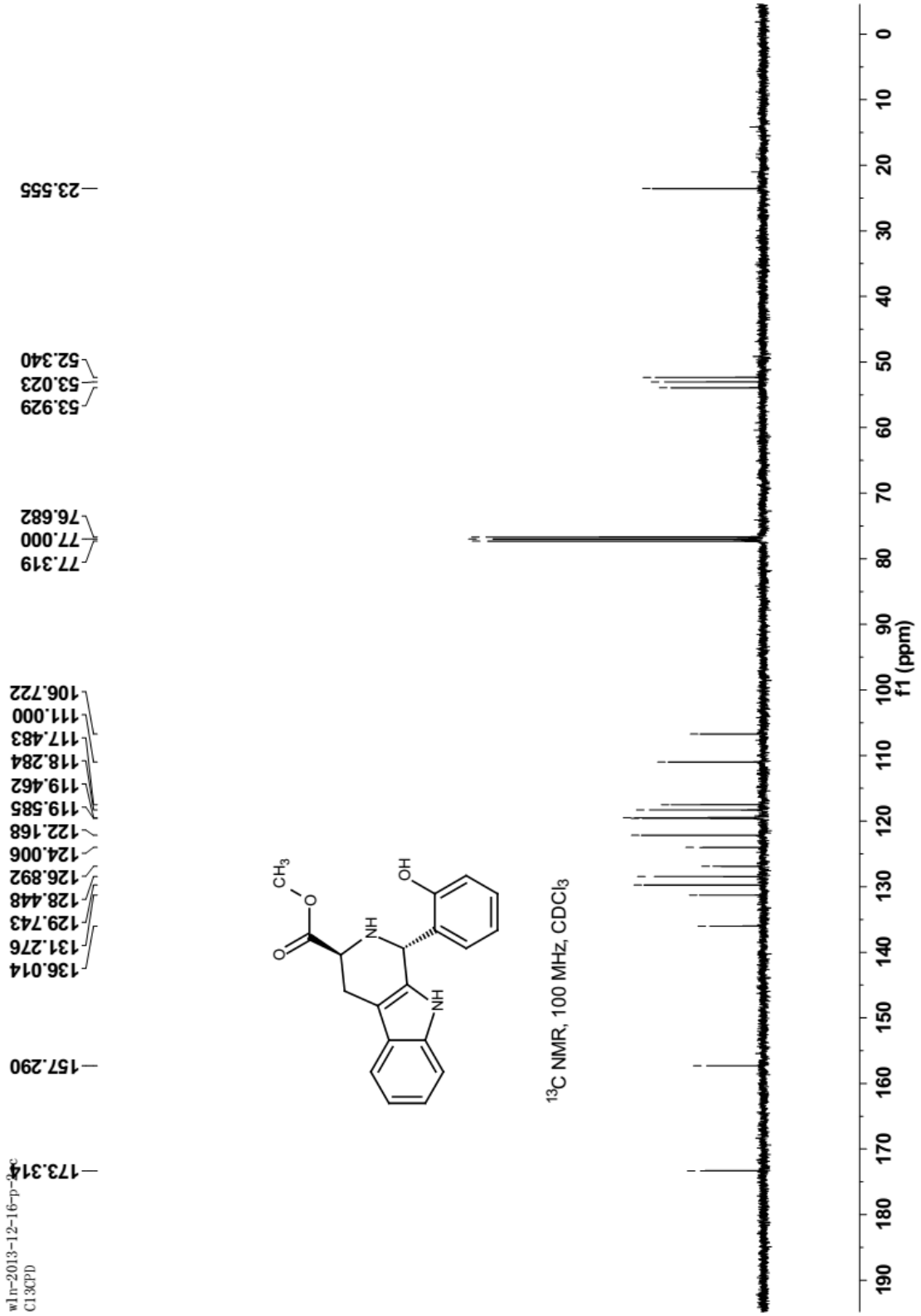
cis-**3u**: **^{13}C NMR**



trans-**3u**: **^{1}H NMR**

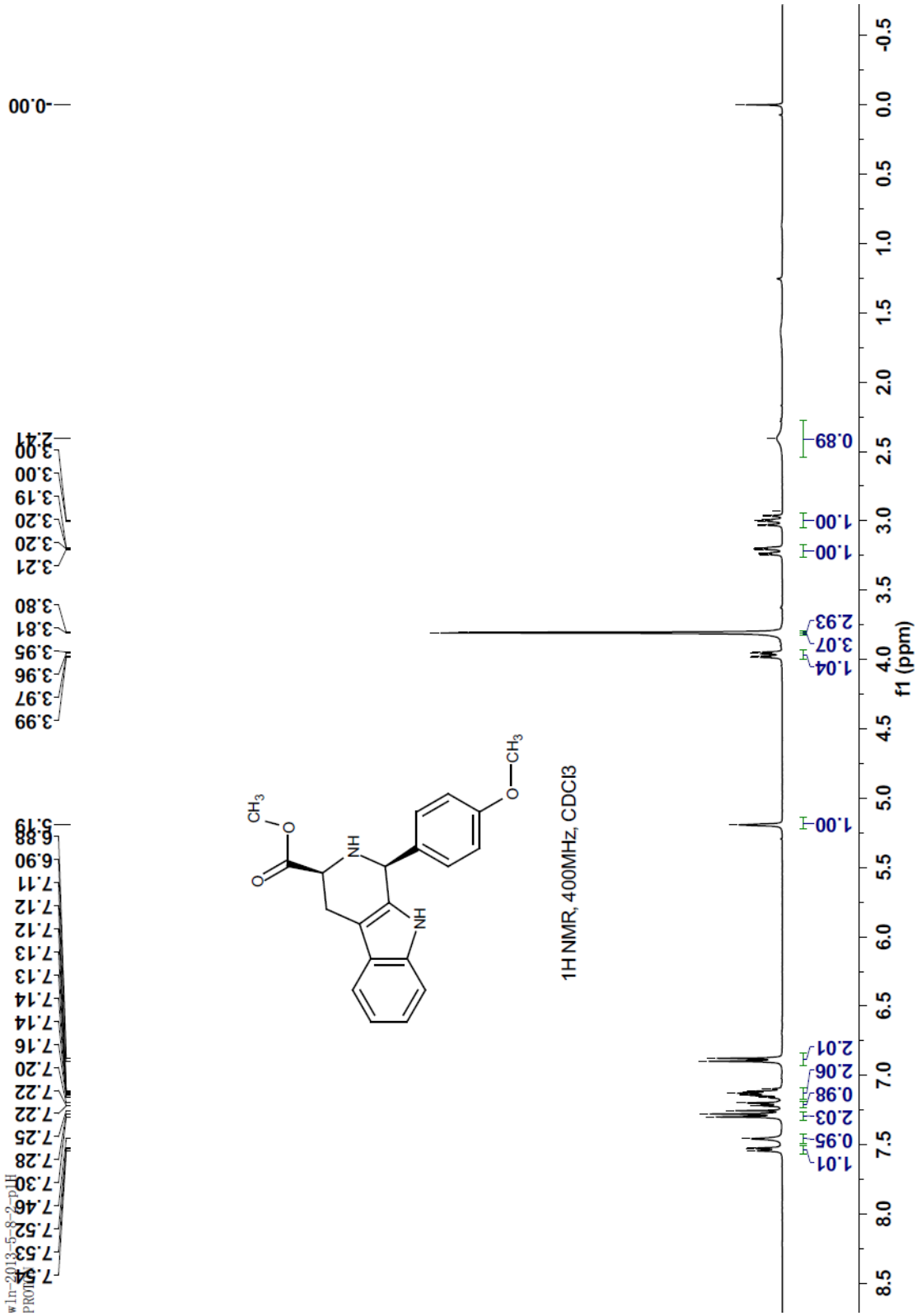


trans-**3u**: **^{13}C NMR**

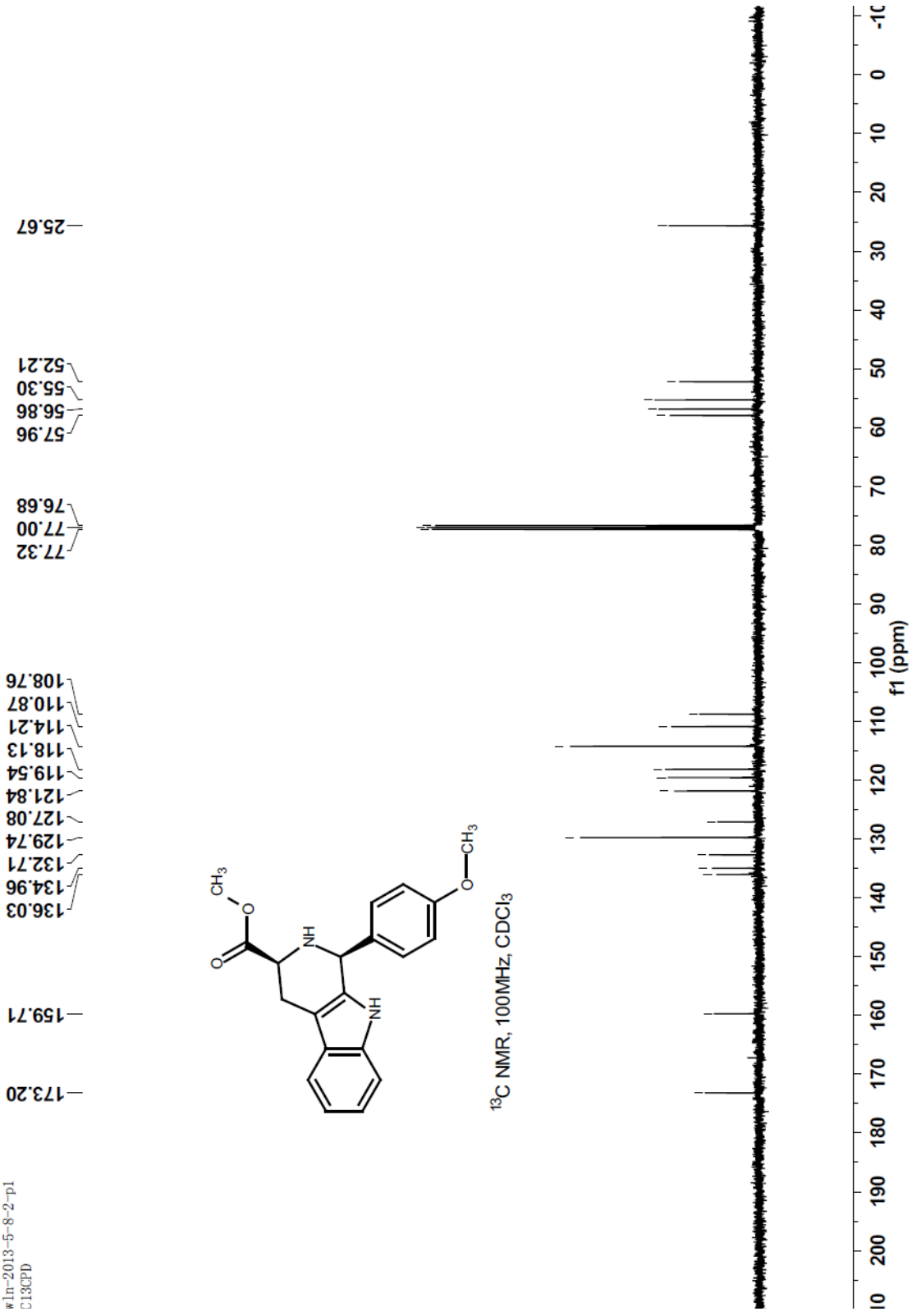


1-(4-Methoxyphenyl)-3-methoxycarbonyl-1,2,3,4-tetrahydro-β-carboline (3v):

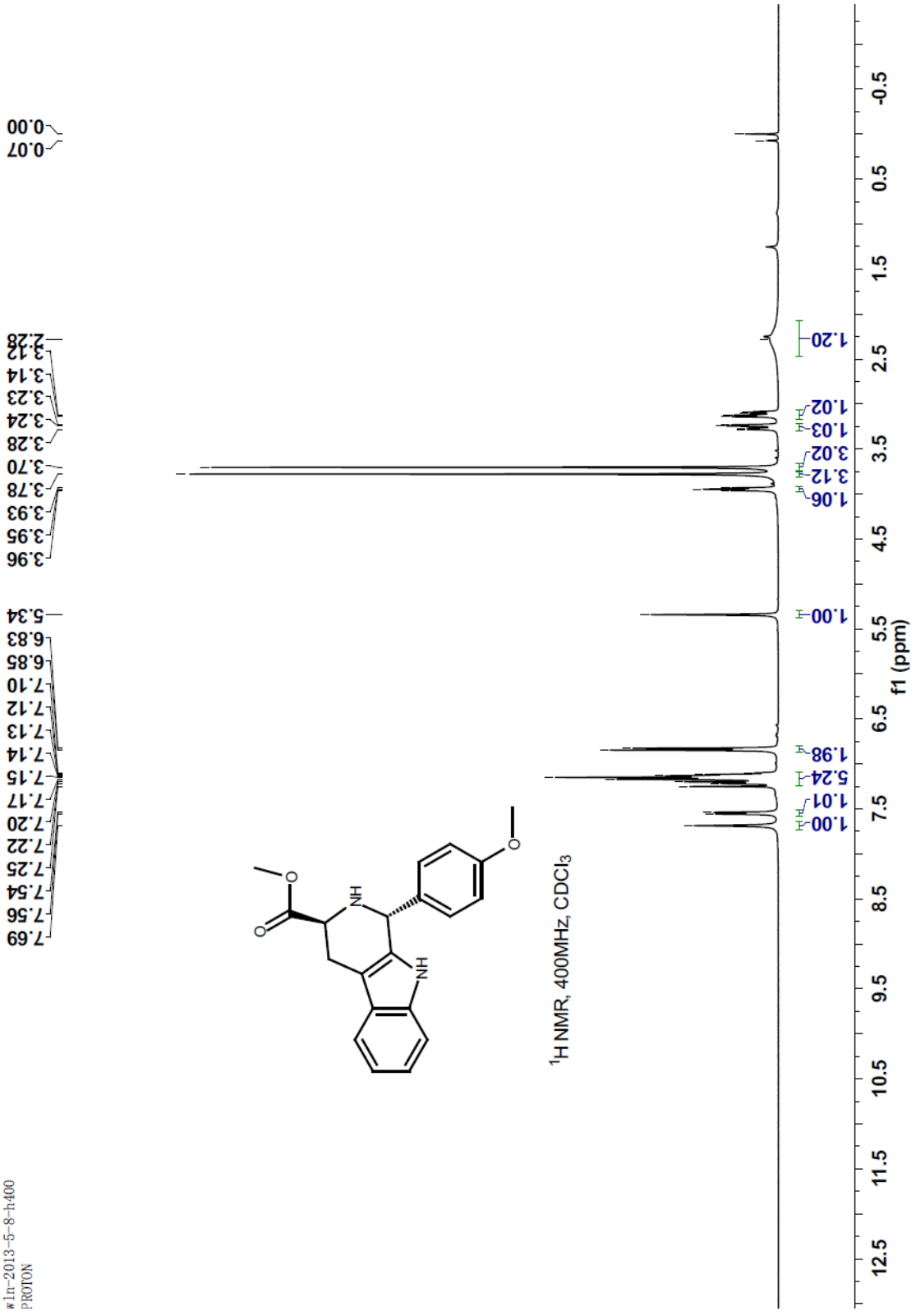
cis-**3v**: **^{1}H NMR**



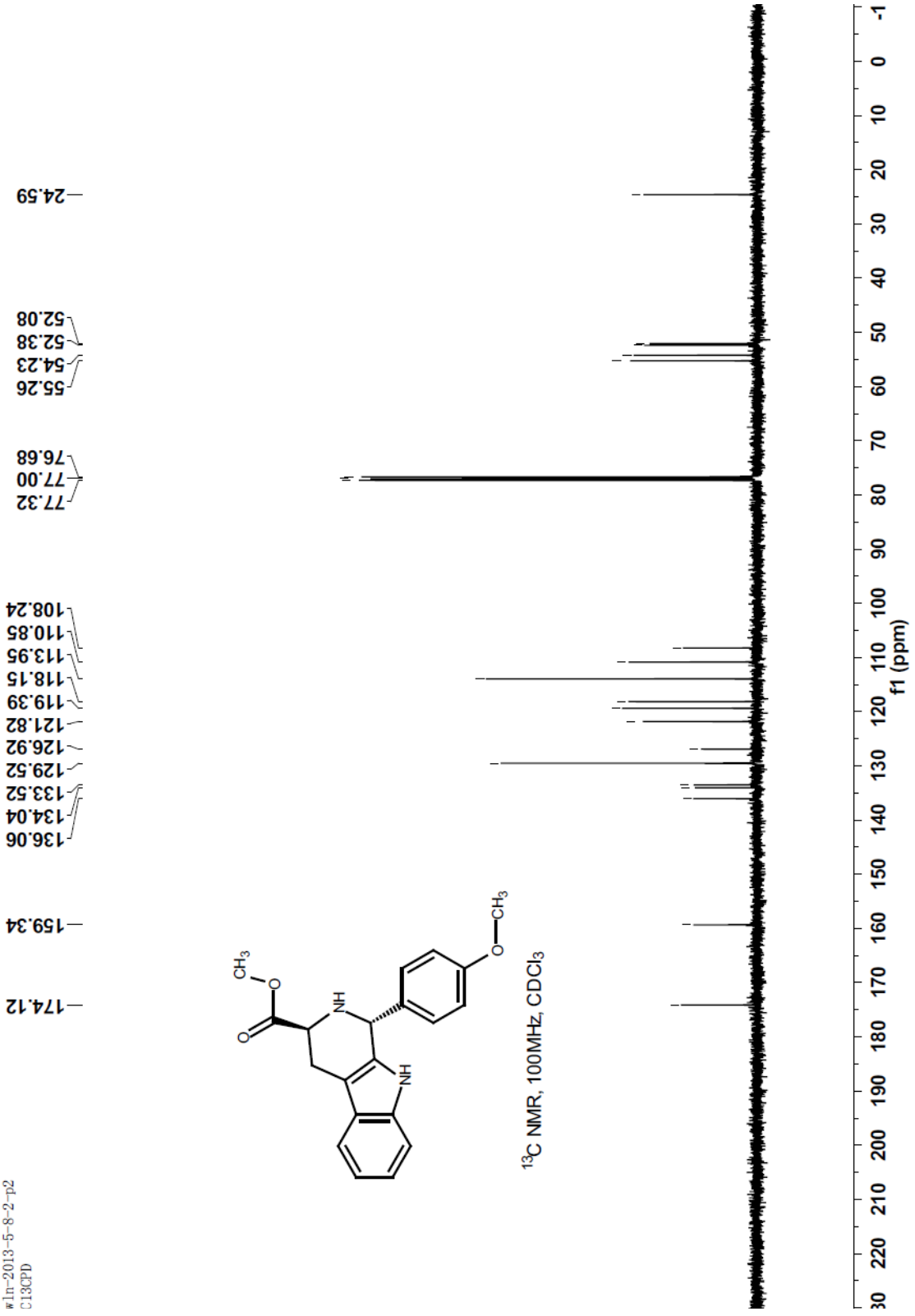
cis-**3v**: **^{13}C NMR**



trans-**3v**: **^{1}H NMR**

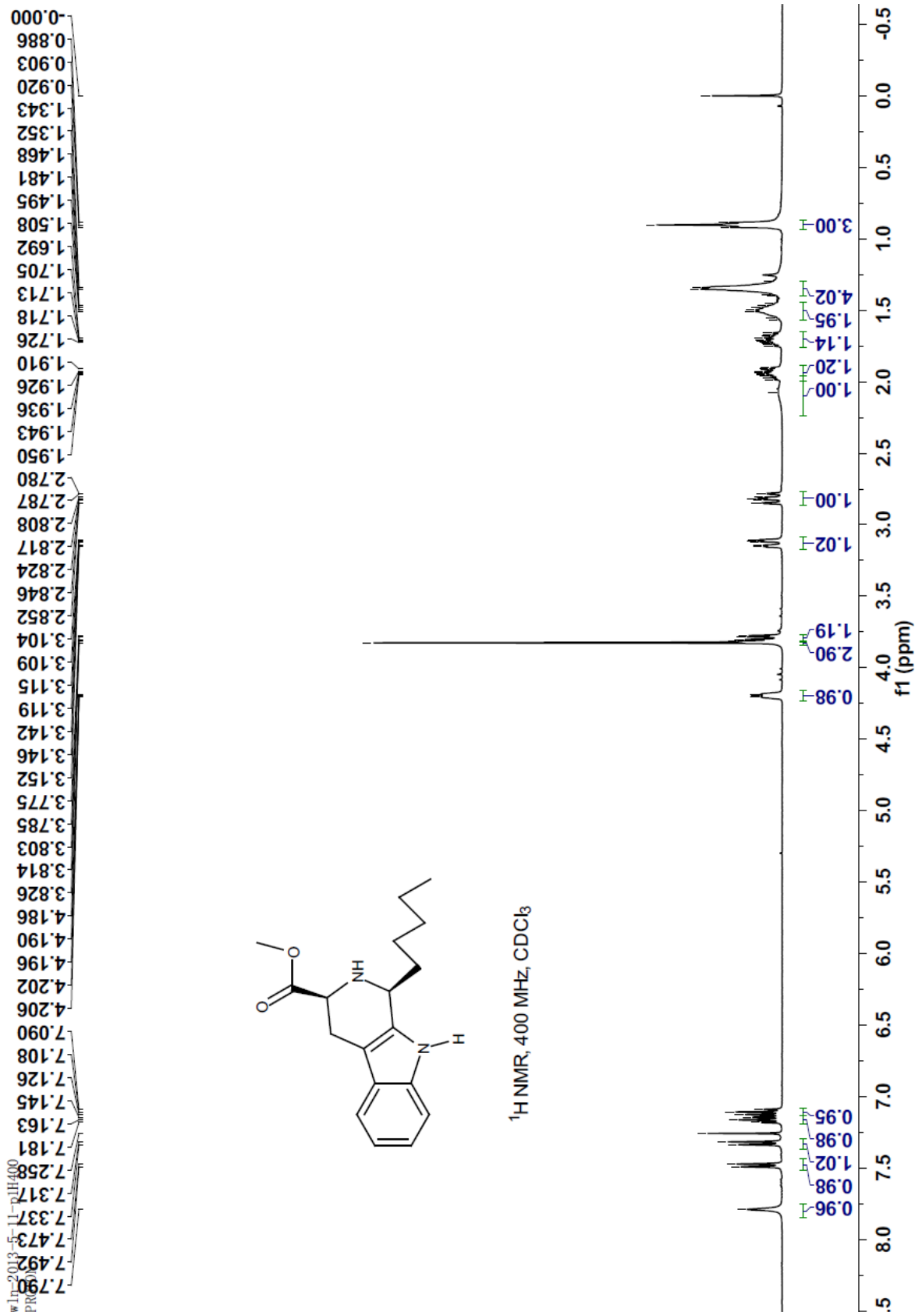


trans-**3v**: **^{13}C NMR**

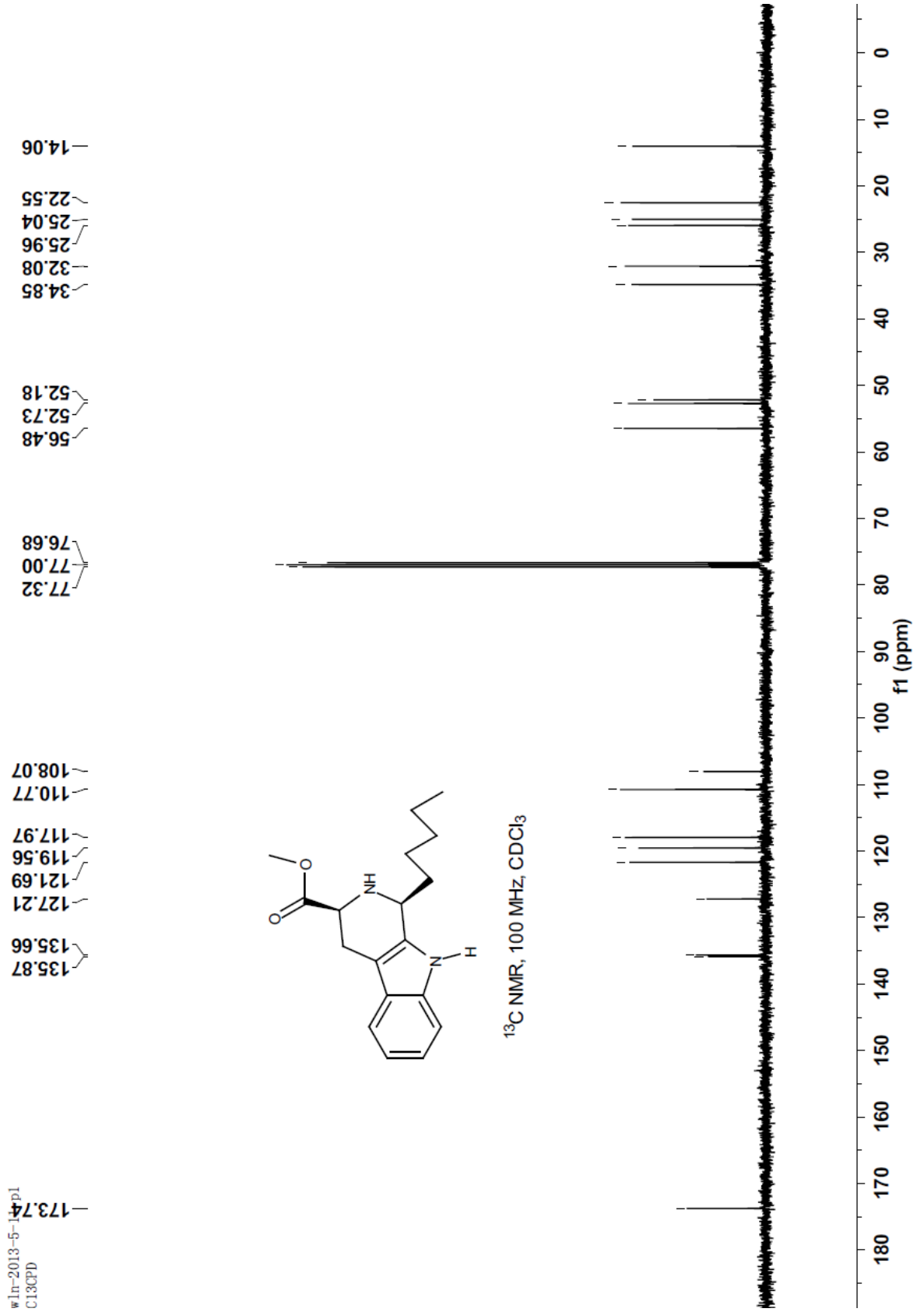


1-Pentyl-3-methoxycarbonyl-1,2,3,4-tetrahydro-*β*-carboline (3w):

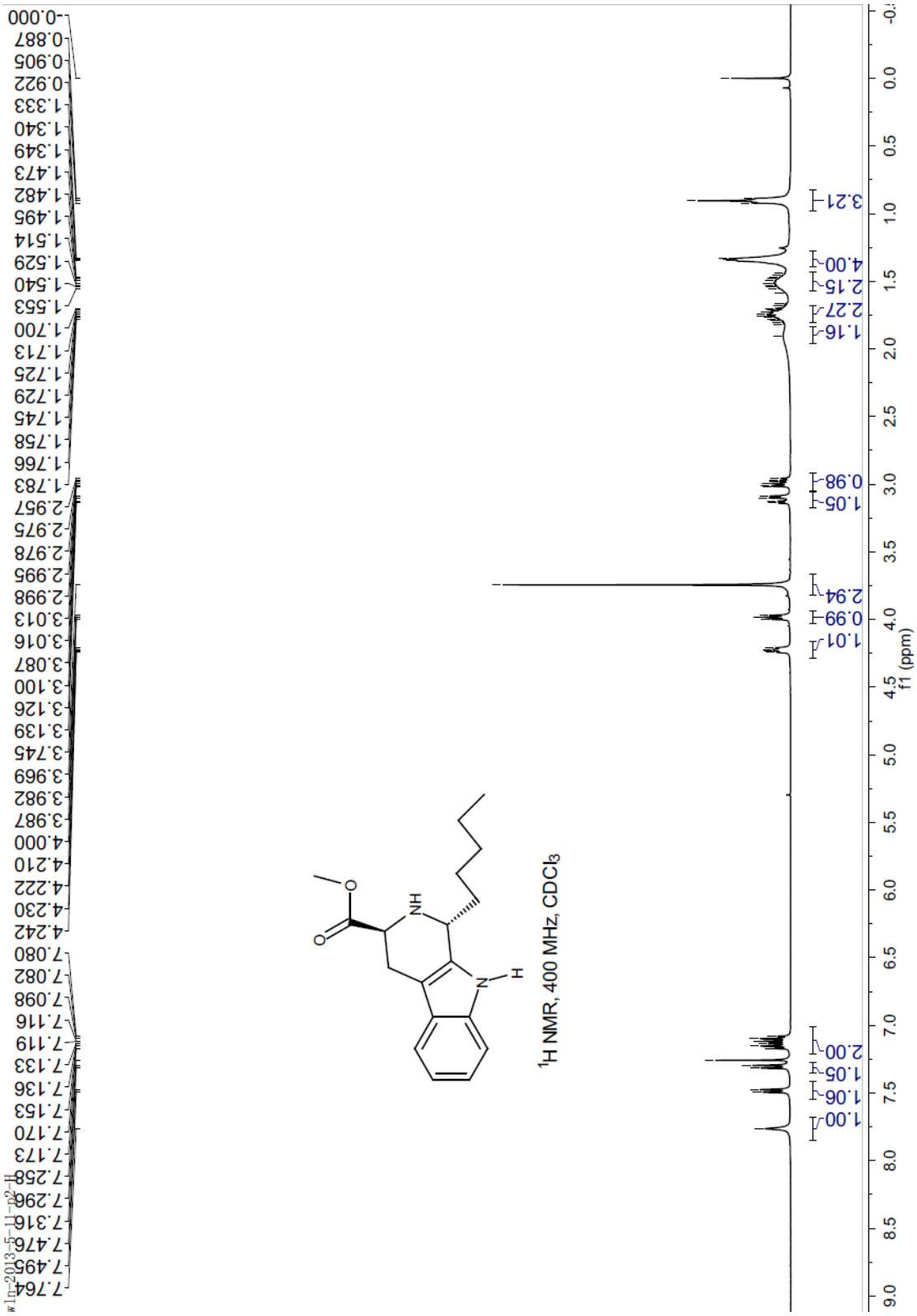
cis-**3w**: **^{1}H NMR**


wln-2013-5-11-pUH400
PROTON
-0.000
0.886
0.903
0.920
1.343
1.352
1.468
1.481
1.495
1.508
1.692
1.705
1.713
1.718
1.726
1.910
1.926
1.936
1.943
1.950
2.780
2.787
2.808
2.817
2.824
2.846
2.852
3.104
3.109
3.115
3.119
3.142
3.146
3.152
3.775
3.785
3.803
3.814
3.826
4.186
4.190
4.196
4.202
4.206
7.090
7.108
7.126
7.145
7.163
7.181
7.258
7.317
7.337
7.473
7.492
7.790
O
O
NH
N
H
^{1}H NMR, 400 MHz, CDCl$_3$
3.00
4.02
1.95
1.14
1.20
1.00
1.00
1.02
1.19
2.90
0.98
0.95
0.98
1.02
0.98
0.96
f1 (ppm)

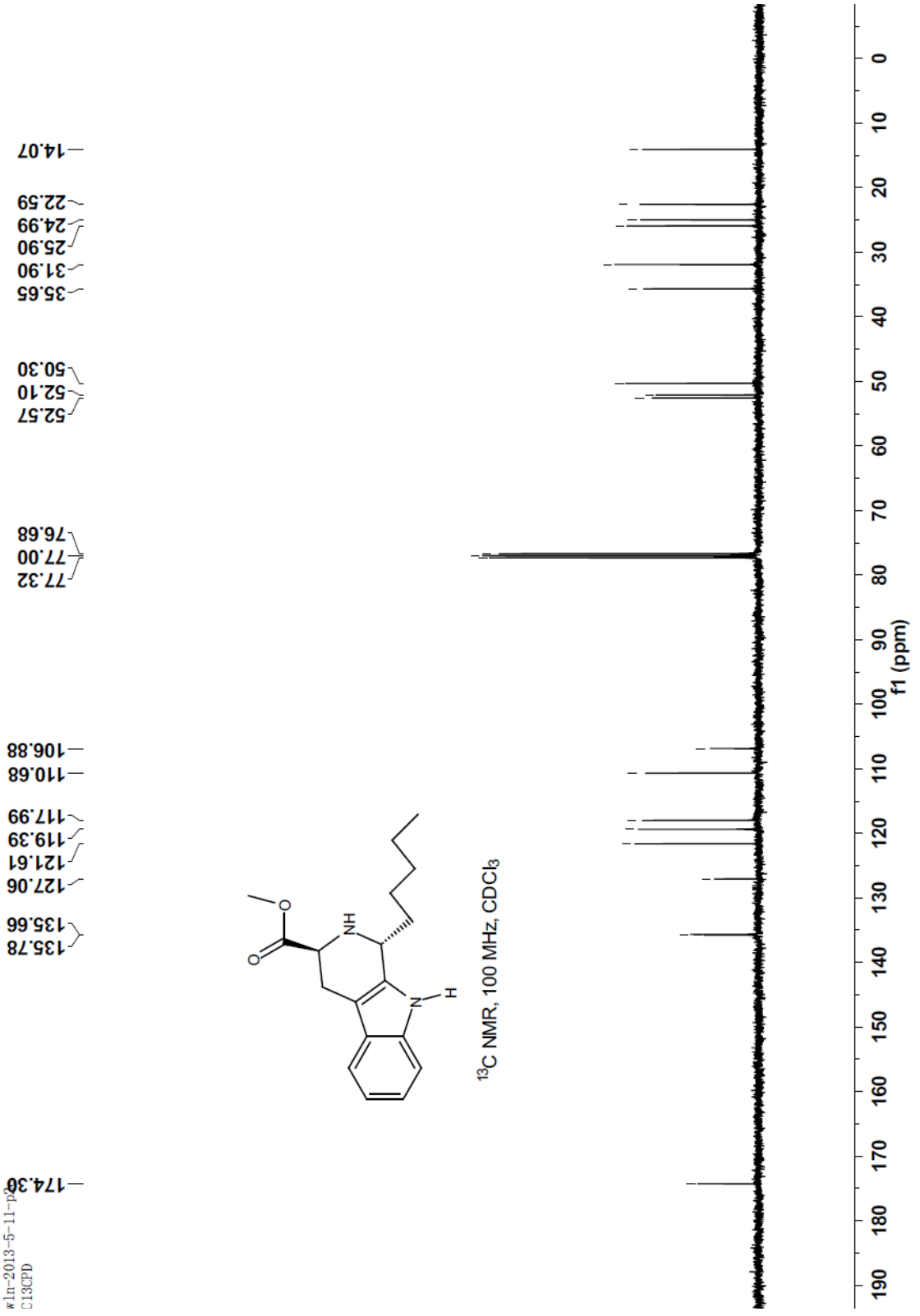
cis-**3w**: **^{13}C NMR**



trans-**3w: ^{1}H NMR**

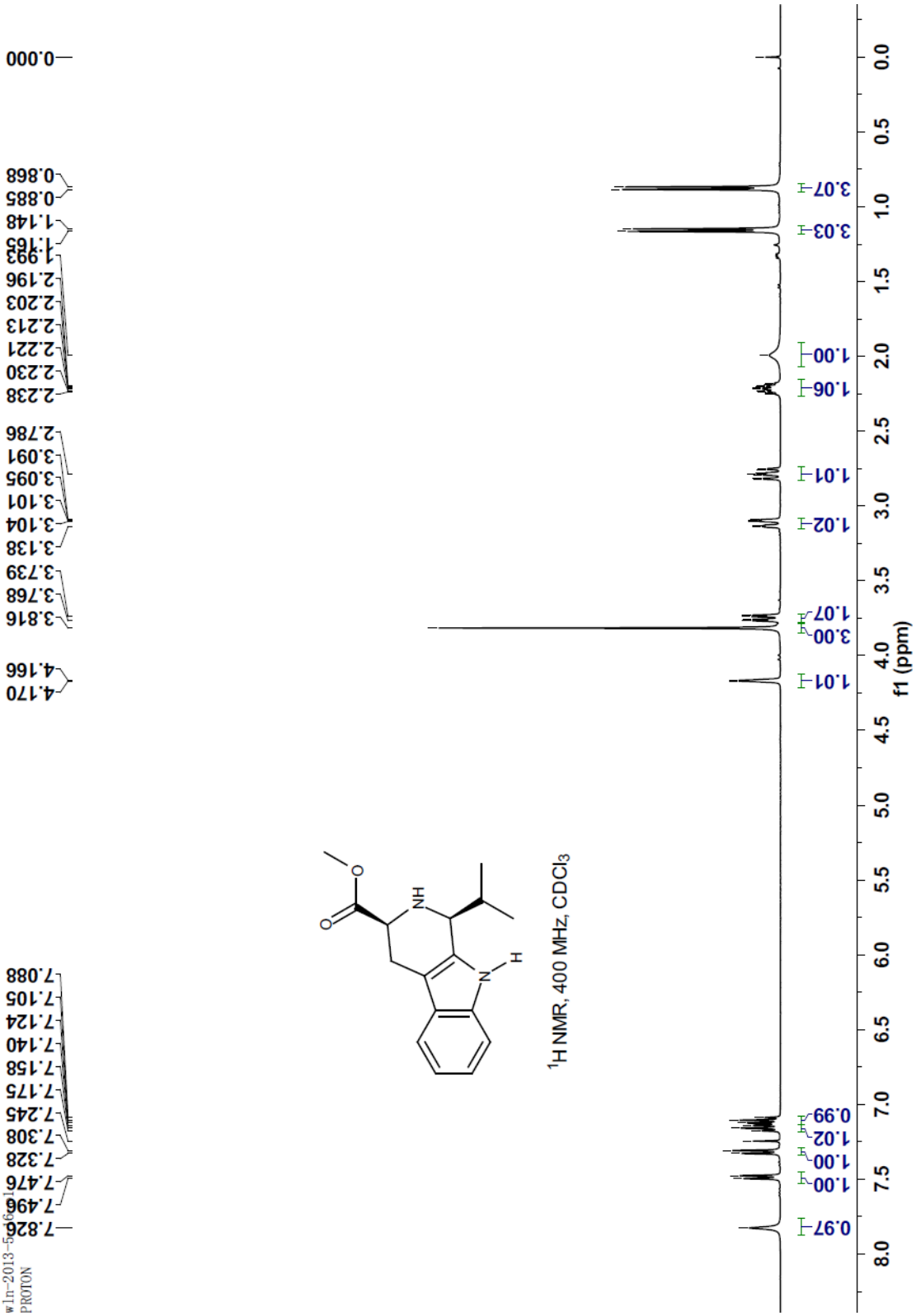


trans-**3w**: **^{13}C NMR**

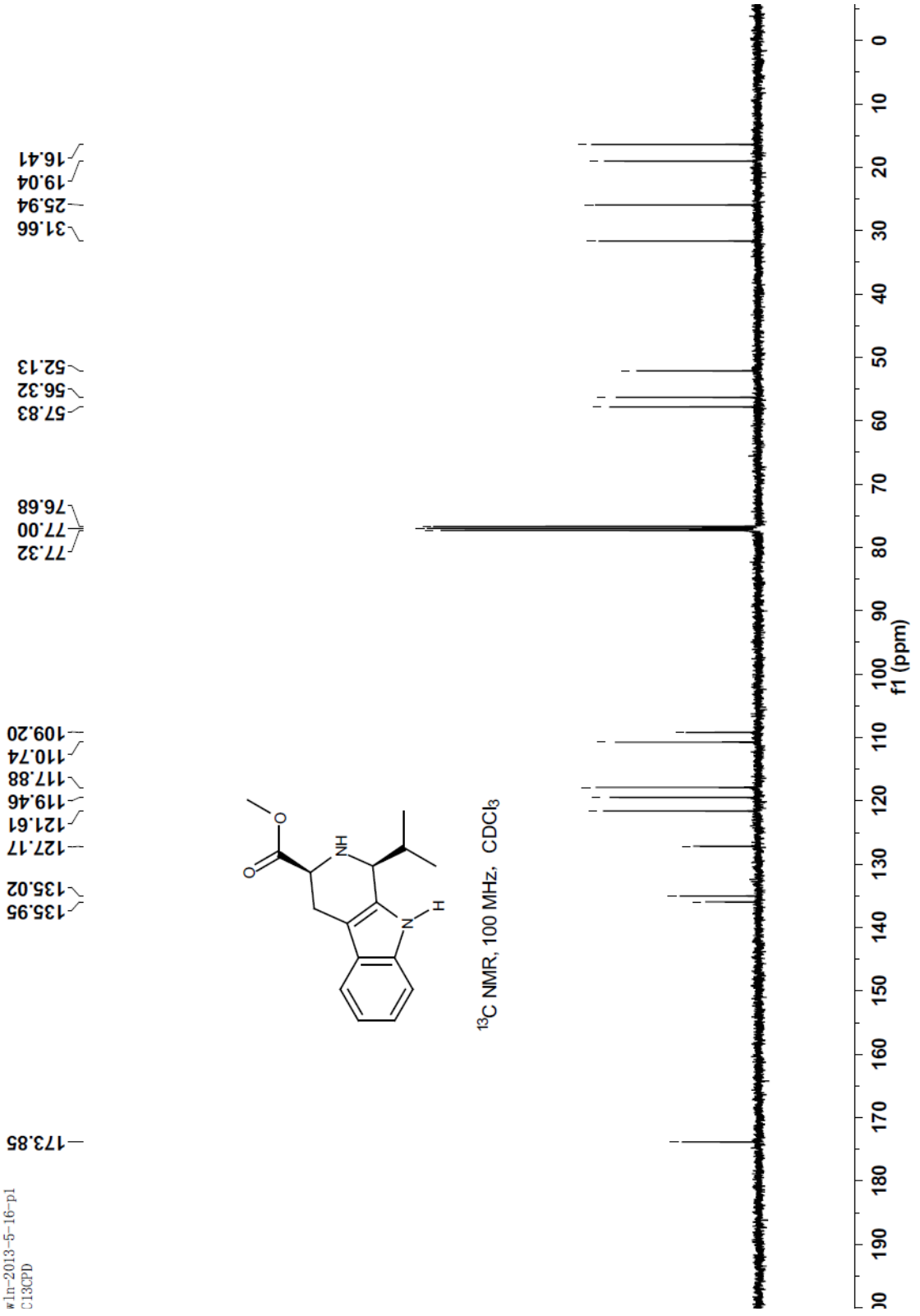


1-Isopropyl-3-methoxycarbonyl-1,2,3,4-tetrahydro-β-carboline (3x):

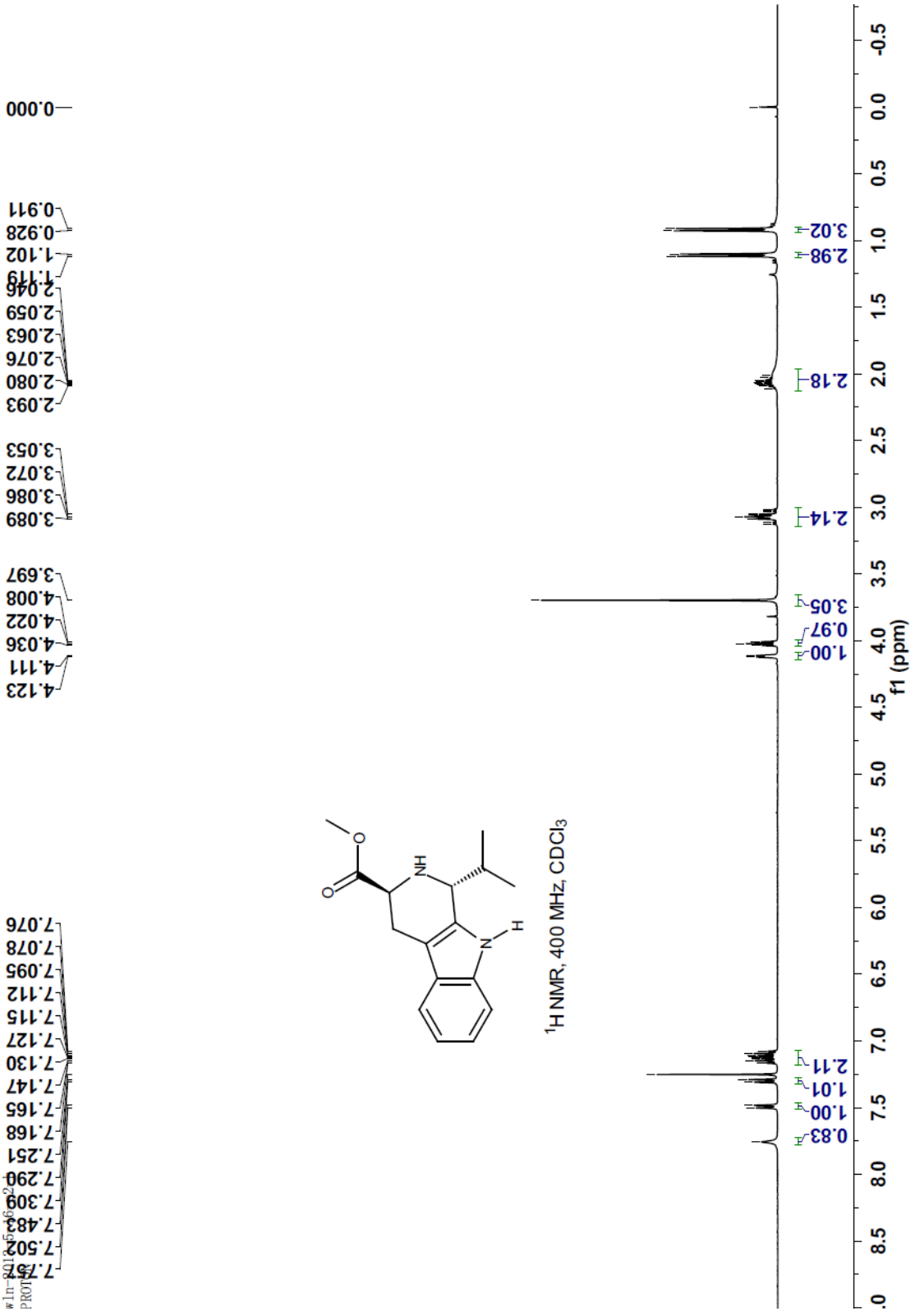
cis-**3x**: **^{1}H NMR**



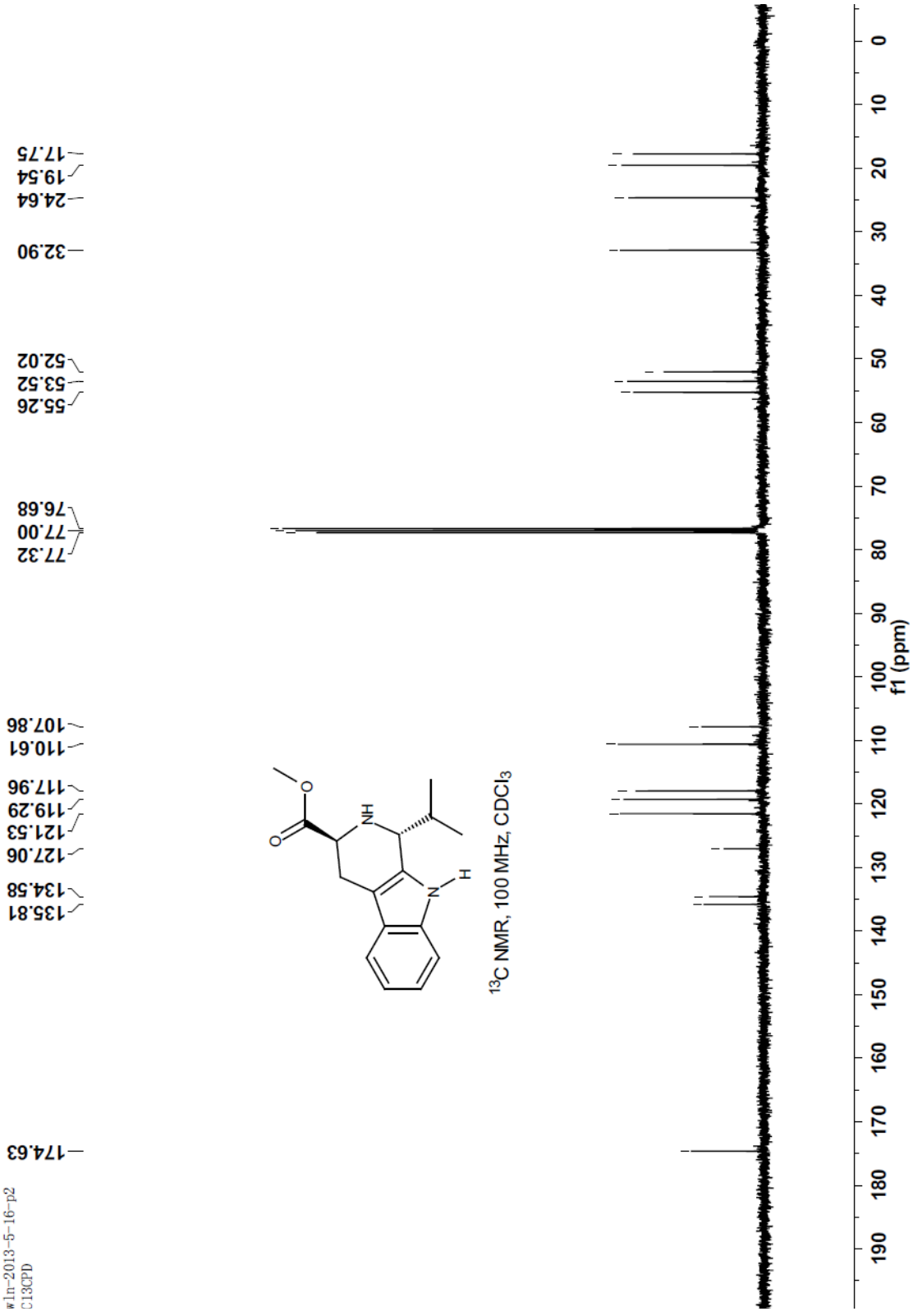
cis-**3x**: **^{13}C NMR**



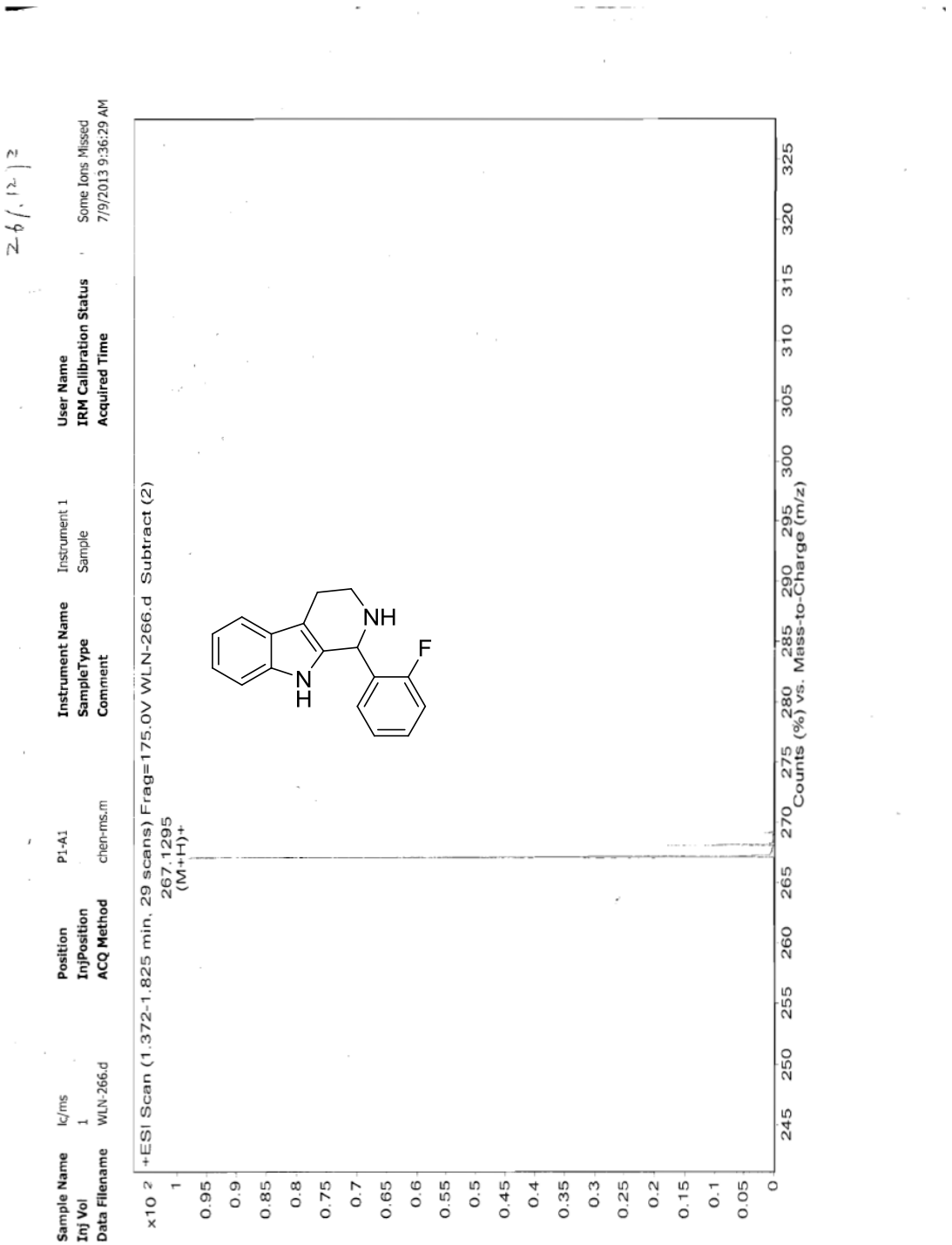
trans-**3x**: **^{1}H NMR**



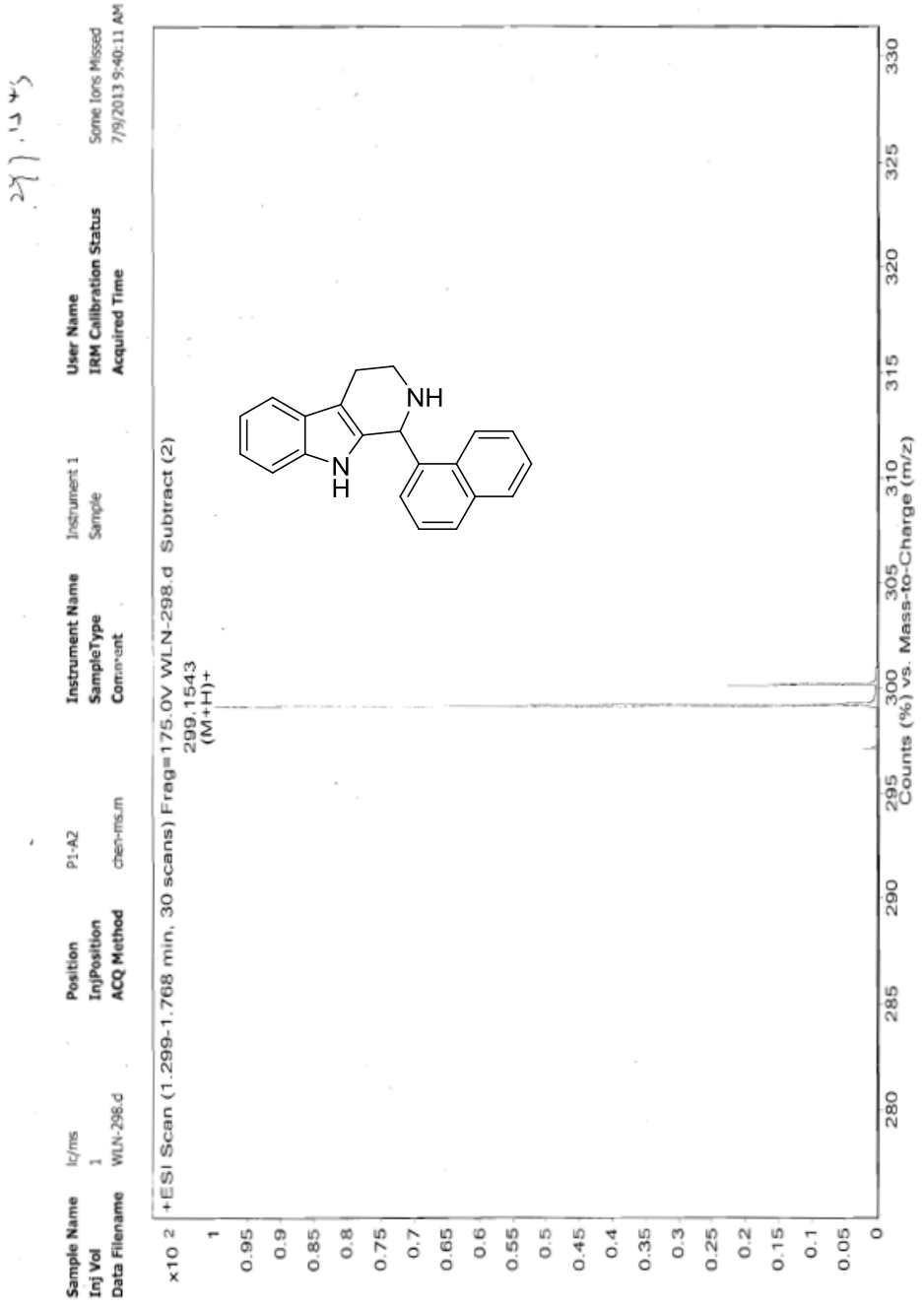
trans-**3x**: **^{13}C NMR**



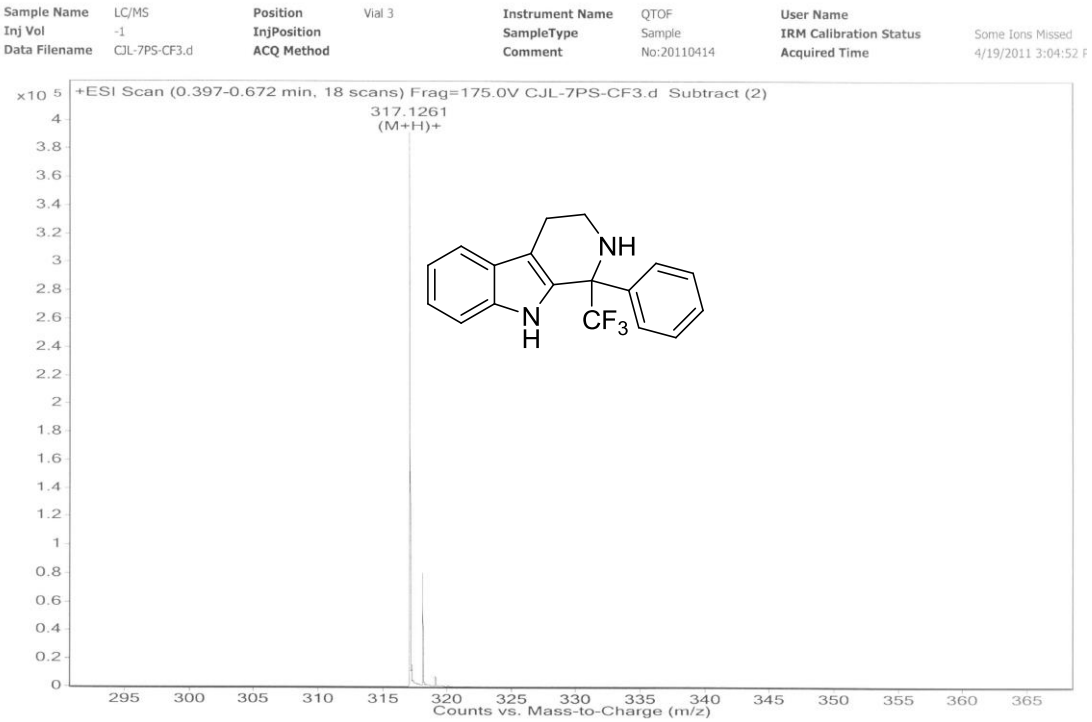
1-(2-Fluorophenyl)-1,2,3,4-tetrahydro-β-carboline (3d): HRMS



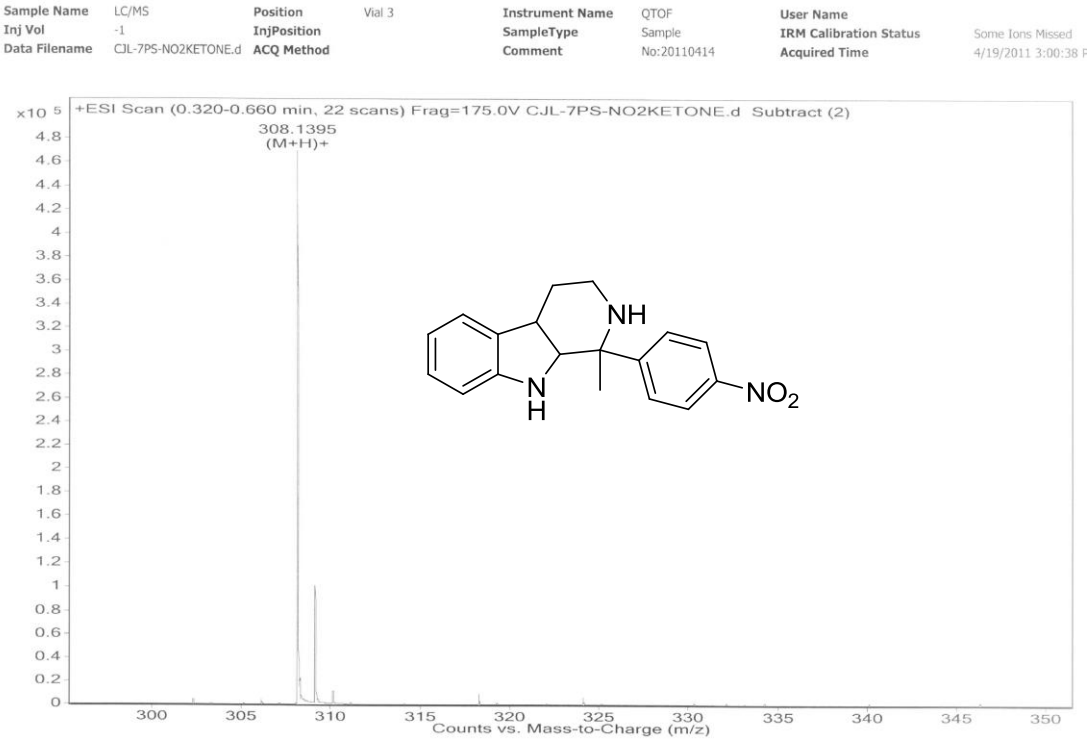
1-(Napthyl)-1,2,3,4-tetrahydro-β-carboline (3f): HRMS



1-Phenyl-1-trifluoromethyl-1,2,3,4-tetrahydro-β-carboline (3k): HRMS



1-Methyl-1-(4-nitrophenyl)-1,2,3,4-tetrahydro-β-carboline (3m): HRMS



Ethyl-2-(1-methyl-1,2,3,4-tetrahydro-β-carboline-1-yl) acetate (3n): HRMS

Sample Name	LC/MS	Position	Vial 3	Instrument Name	QTOF	User Name	
Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Some Ions Missed
Data Filename	CJL-7-PS-CH2CO2ET.d	ACQ Method		Comment		Acquired Time	4/19/2011 3:13:48 P