

**Enantiomeric scaffolding of α -tetralone and related scaffolds by
EKR (Enzymatic Kinetic Resolution) and stereoselective
ketoreduction with ketoreductases**

Rajib Bhuniya and Samik Nanda*

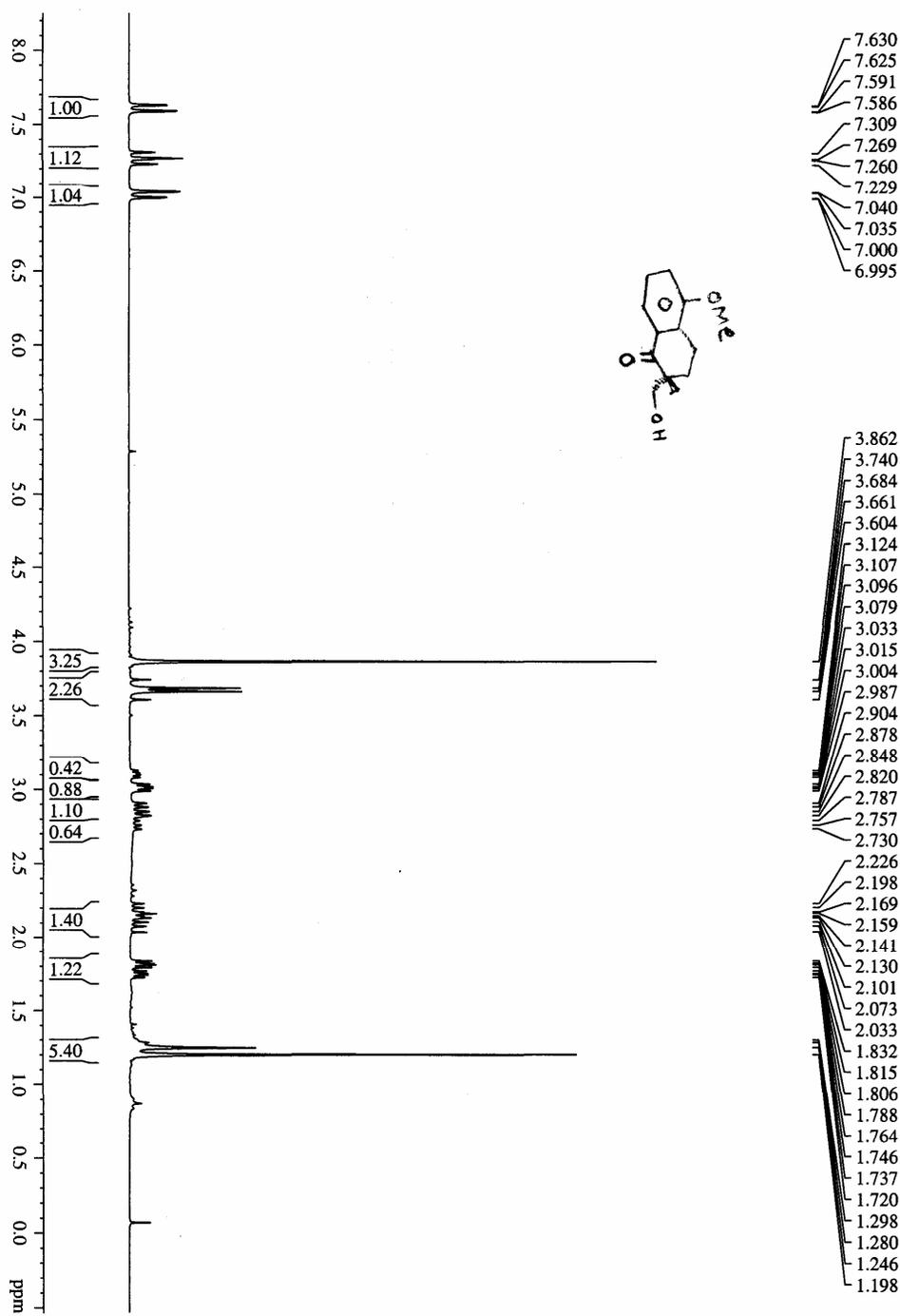
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Supporting Information Part I

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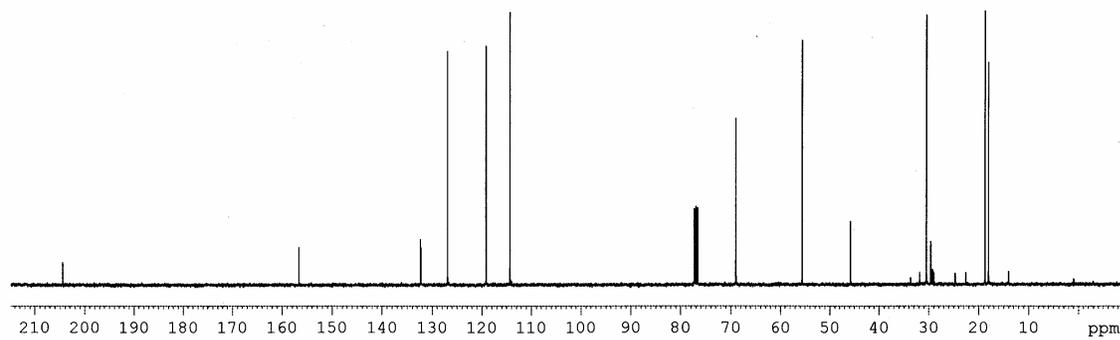
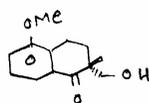
¹H NMR of compound 2



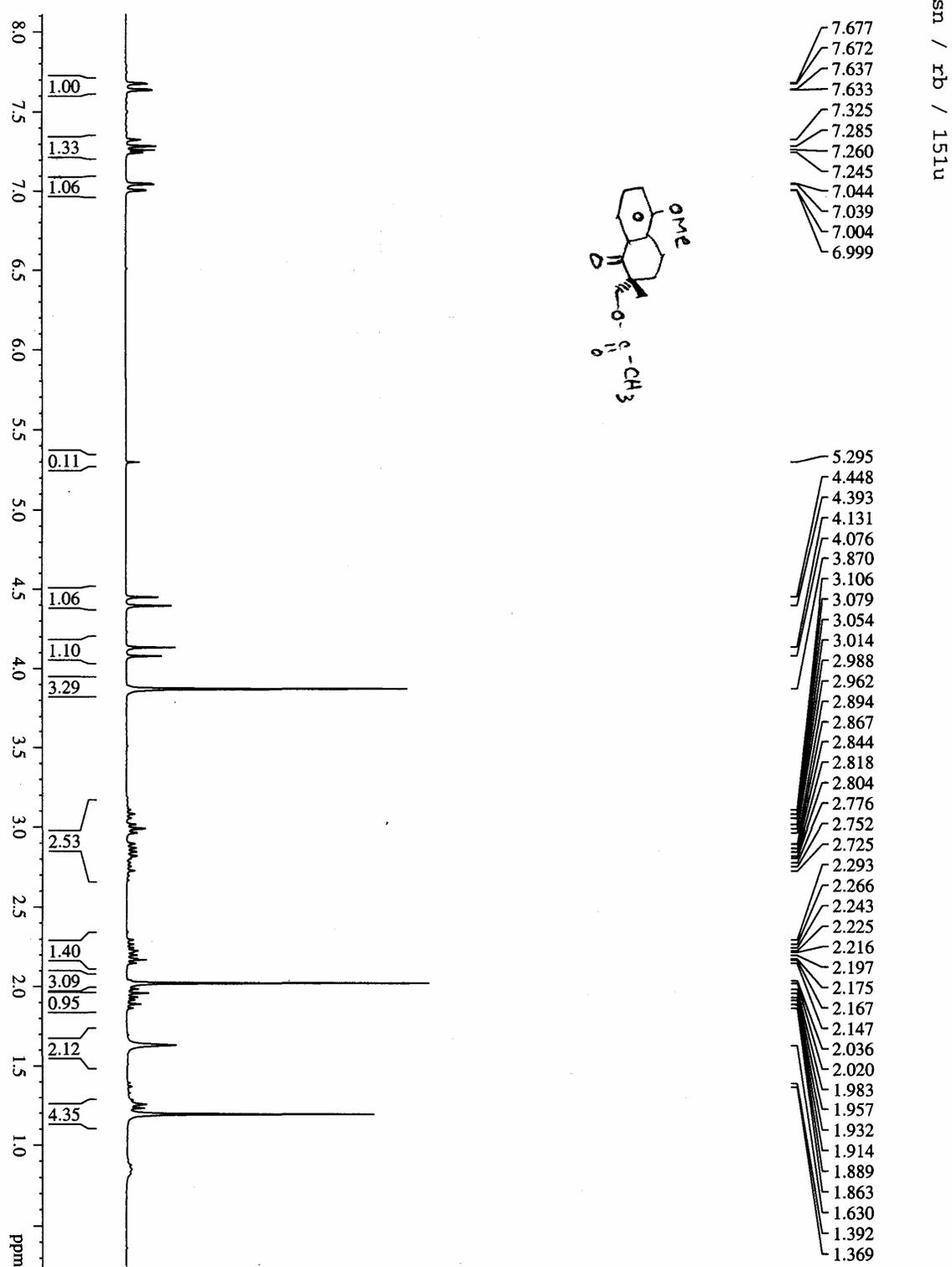
sn / r1b / 1511

¹³C NMR of compound 2

sn / rb / rn - 151 - 1 - 13c

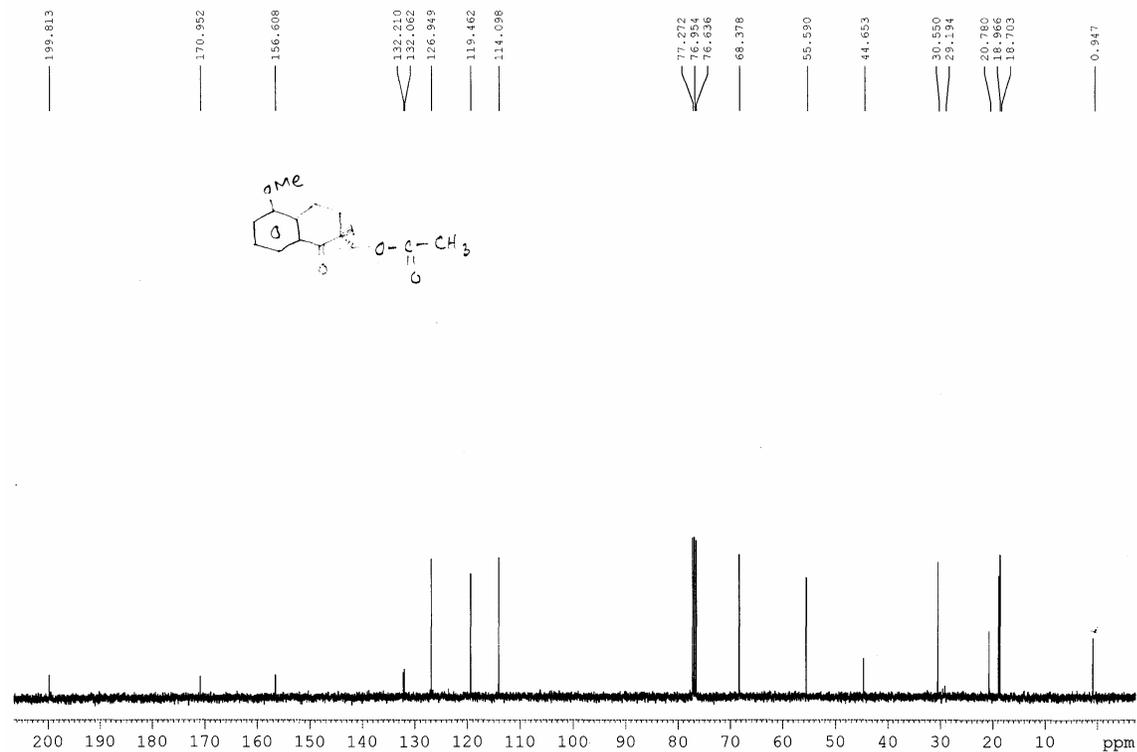


¹H NMR of acetate derivative of 2

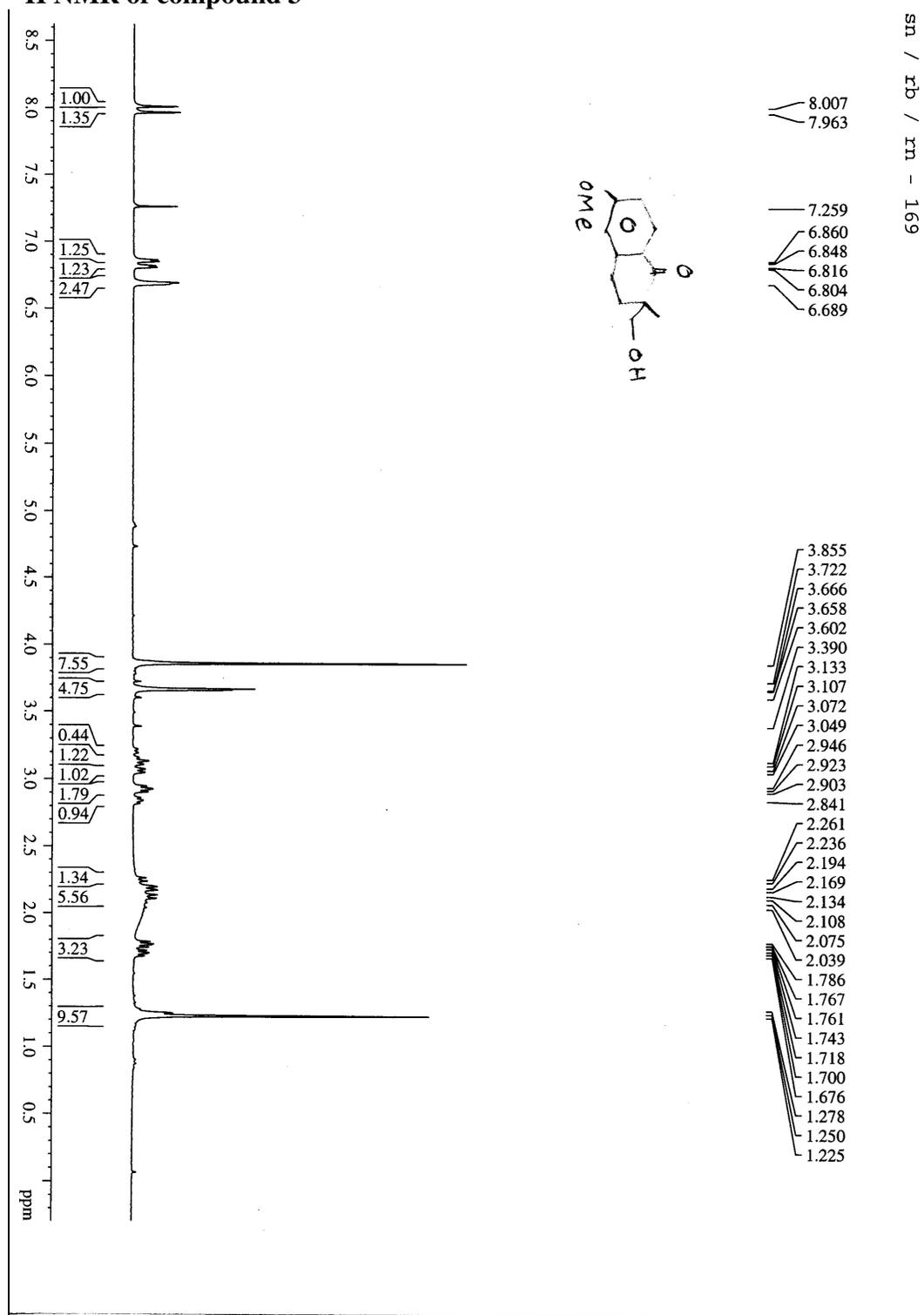


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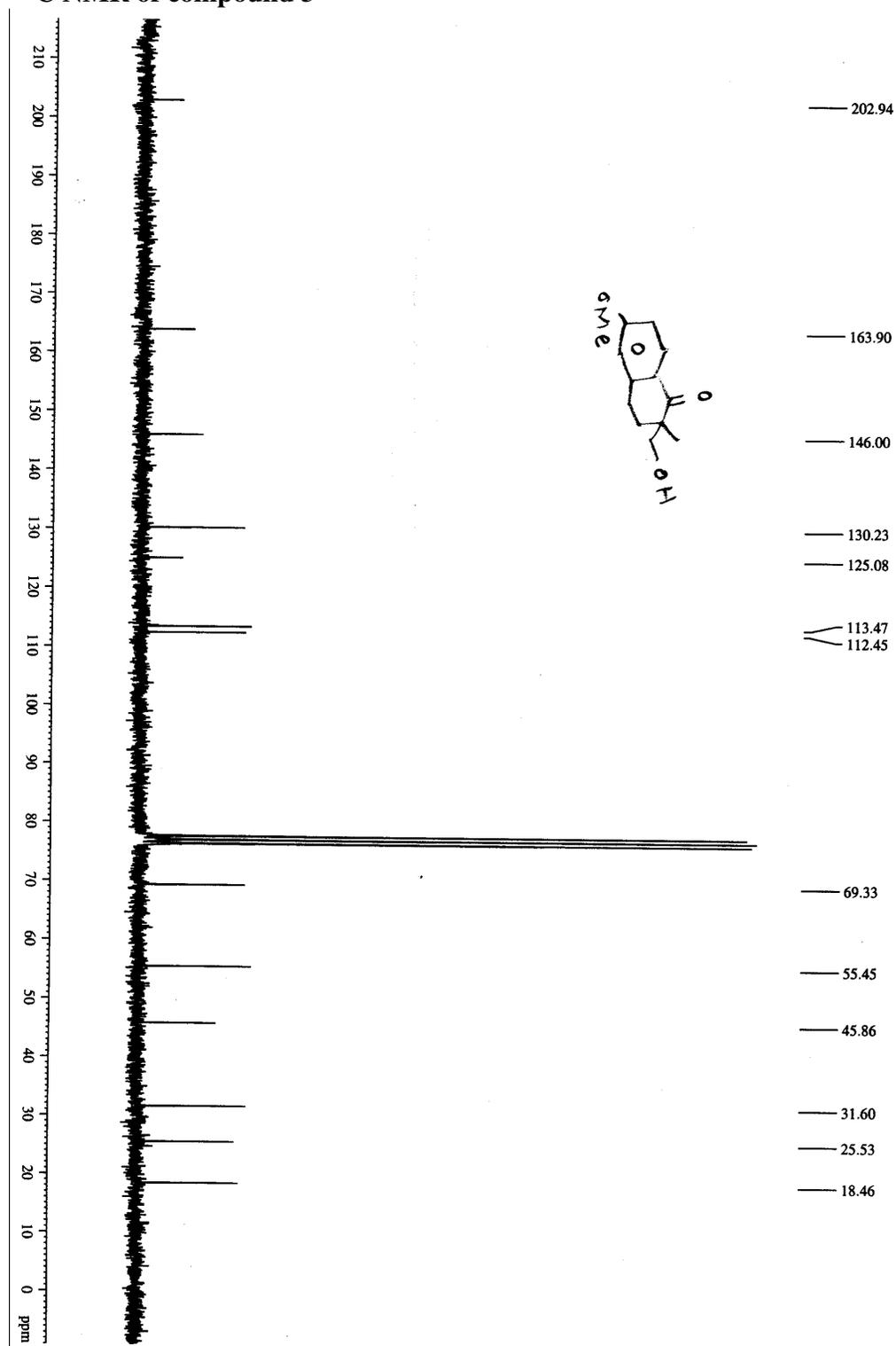
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¹H NMR of compound 3

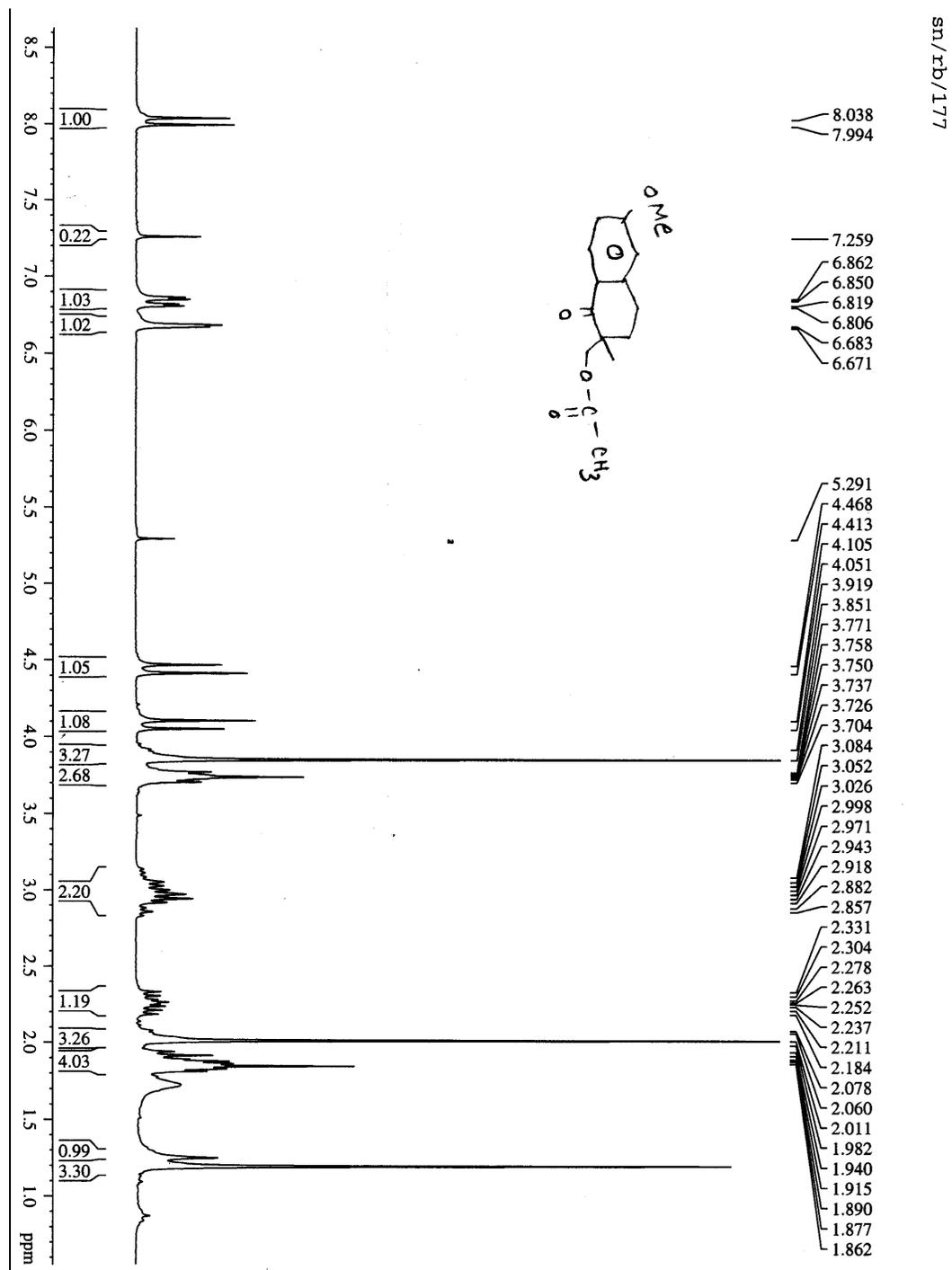


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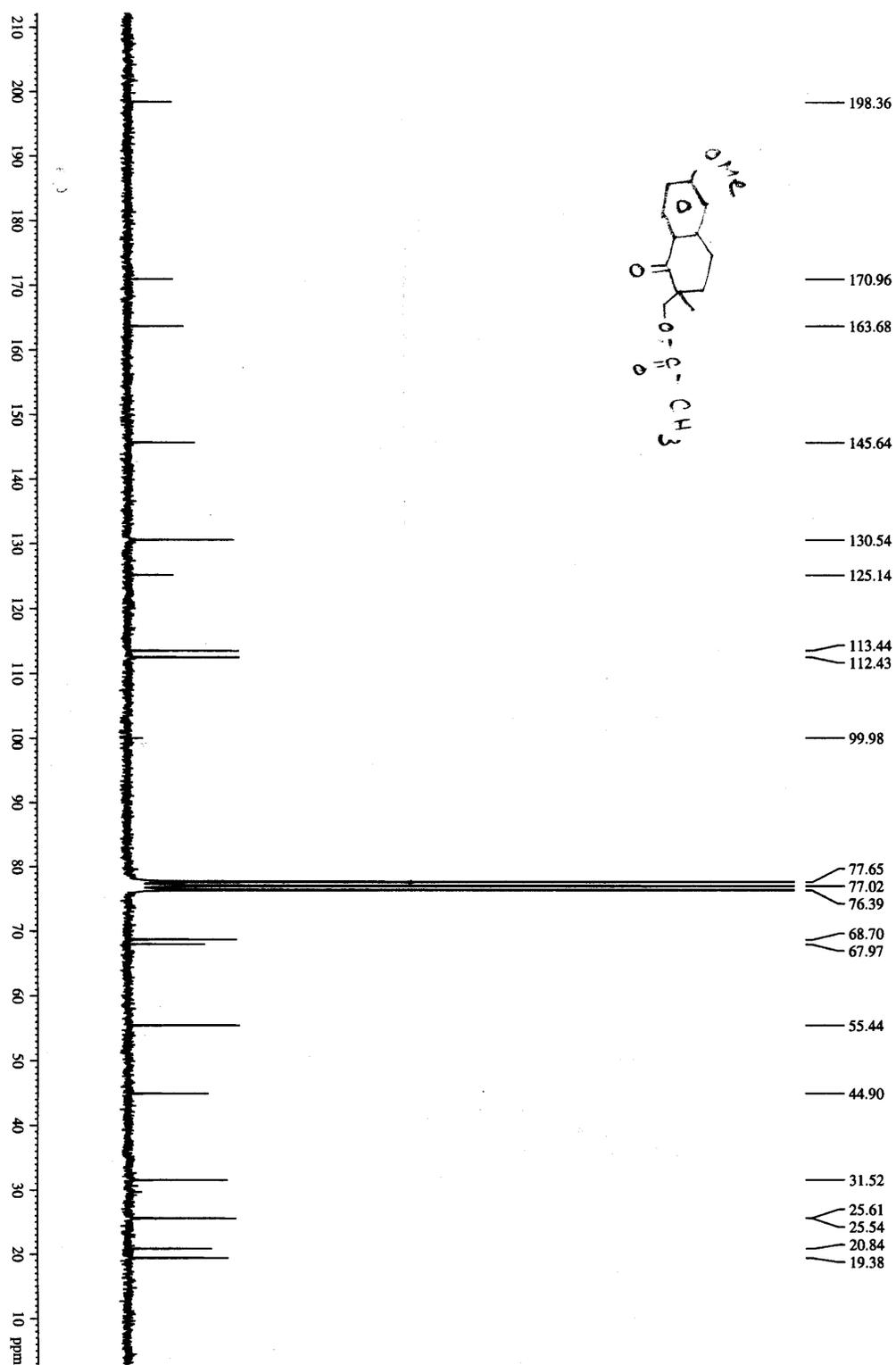


sn / rb / 169
C13CPD CDC13 D:\ IITK 2

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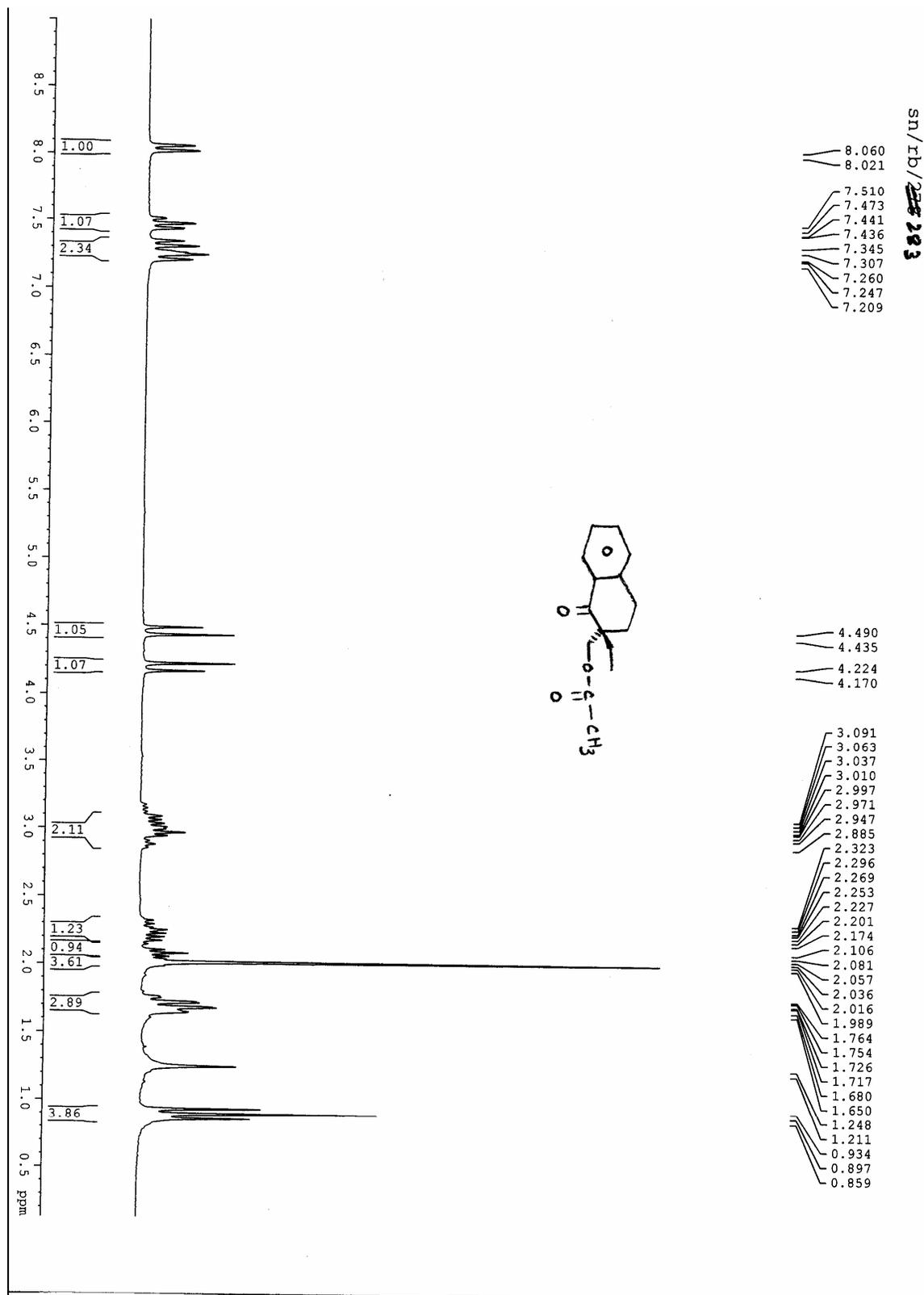


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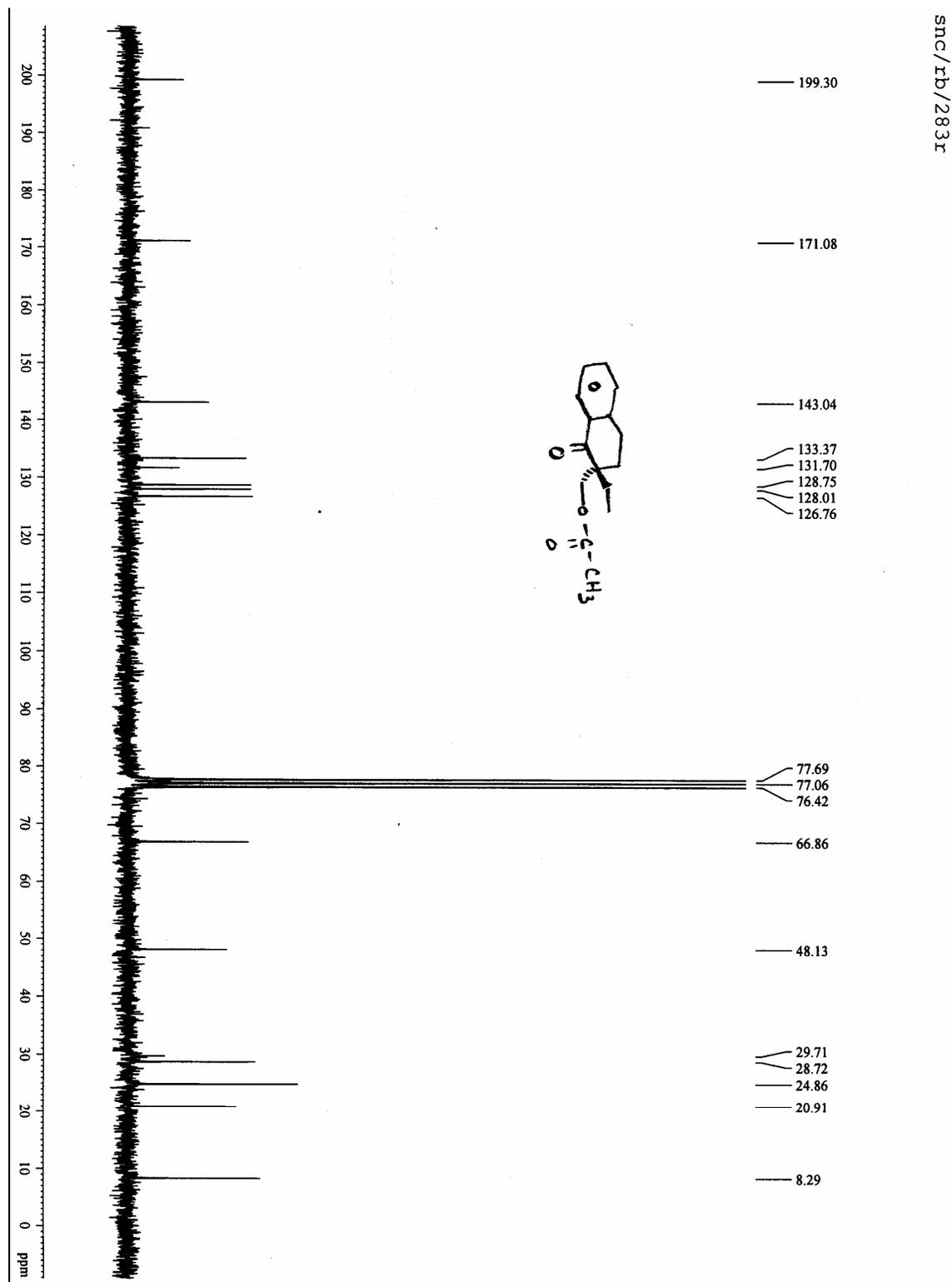


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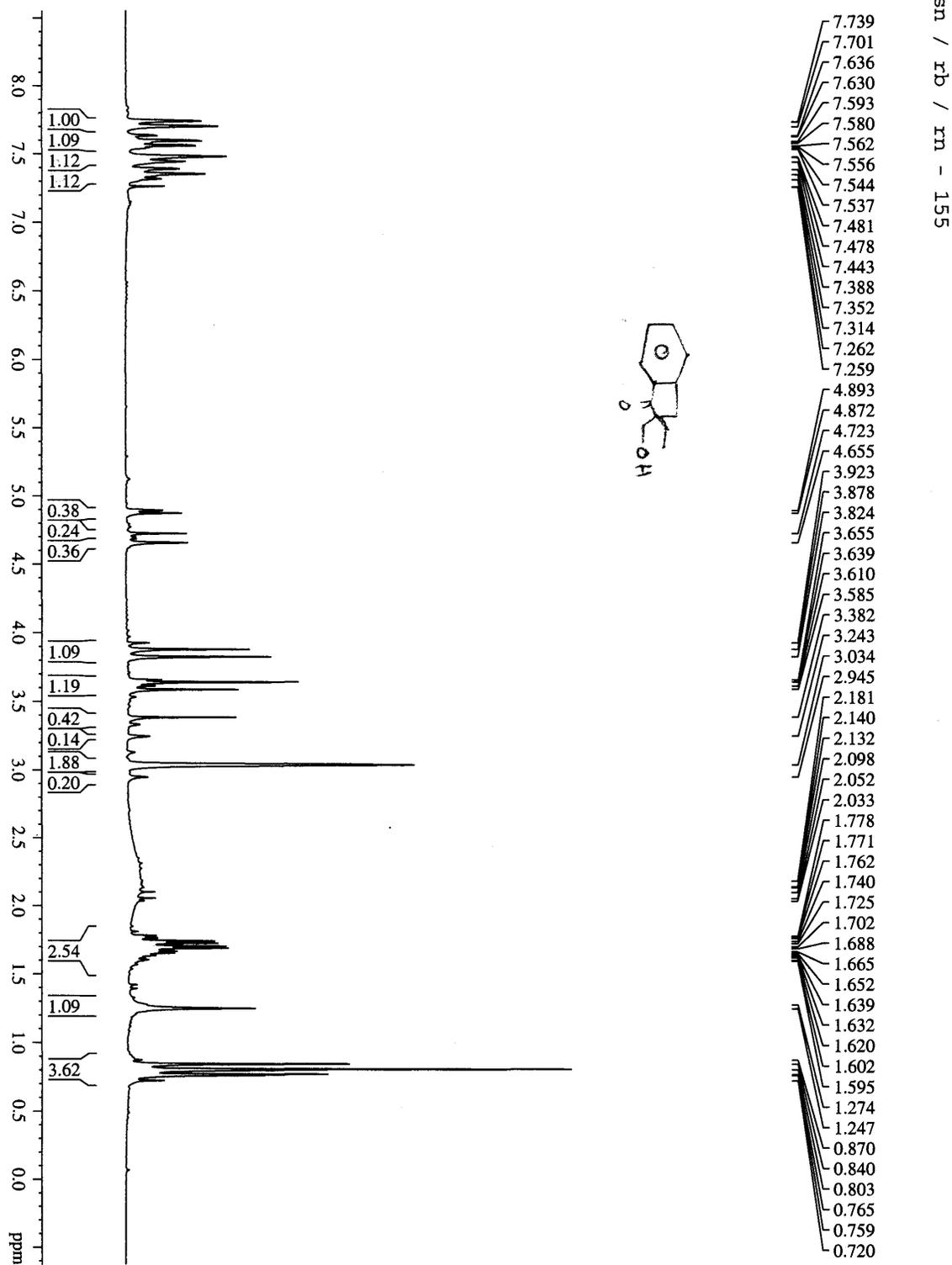
¹H NMR of acetate derivative of 4



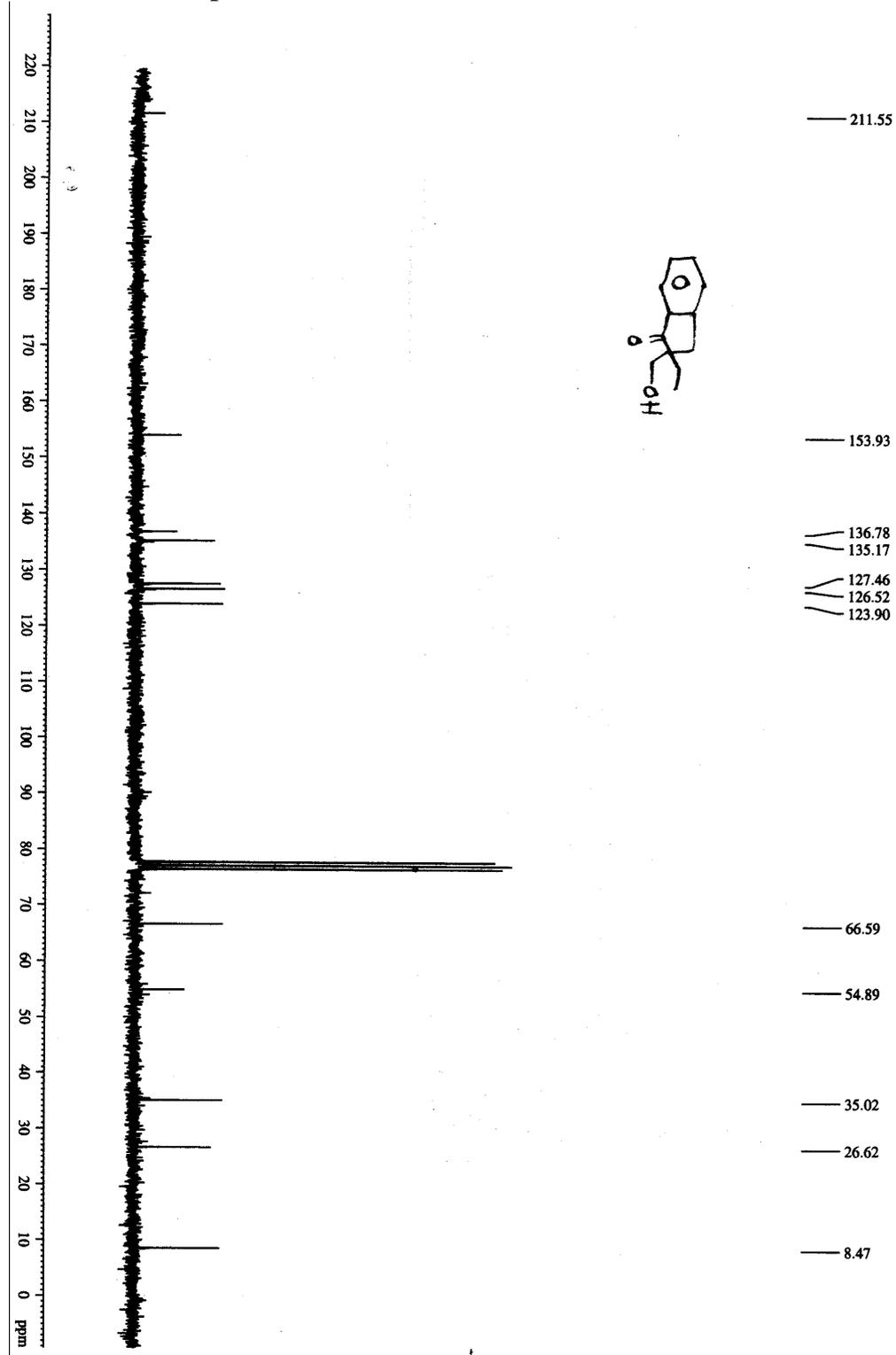
^{13}C NMR of acetate derivative of 4



¹H NMR of compound 7

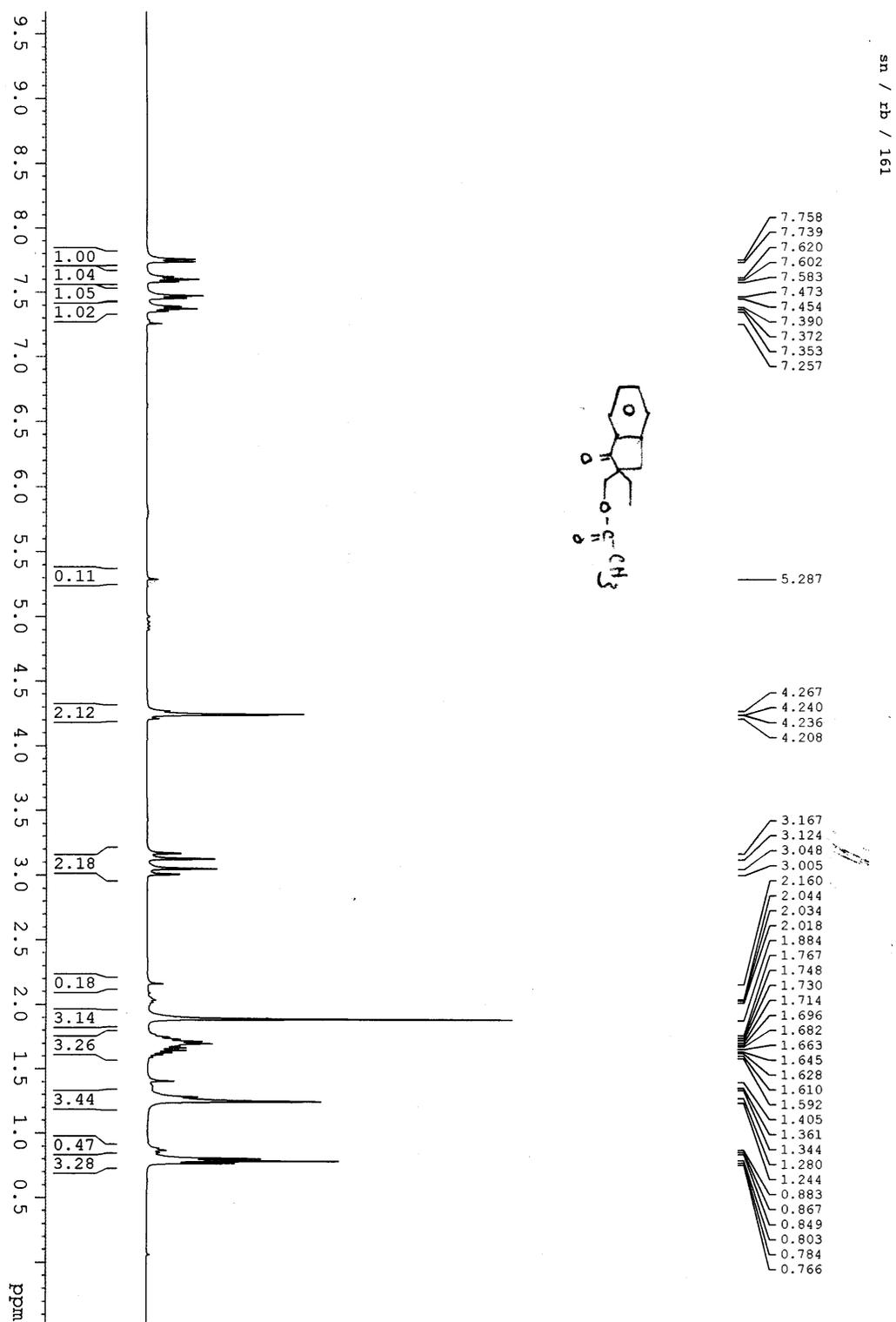


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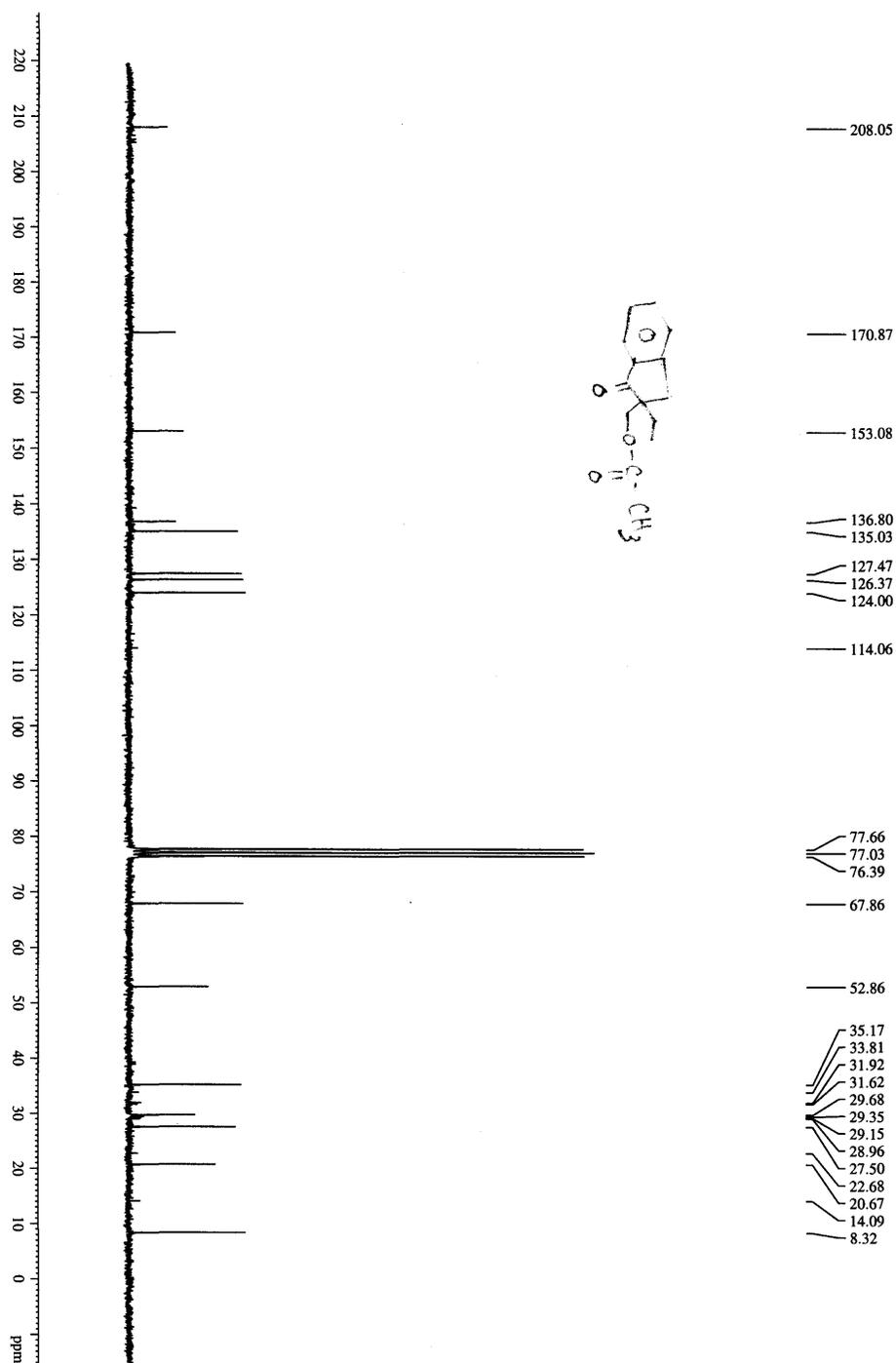


snc.rp155
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¹H NMR of acetate derivative of 7

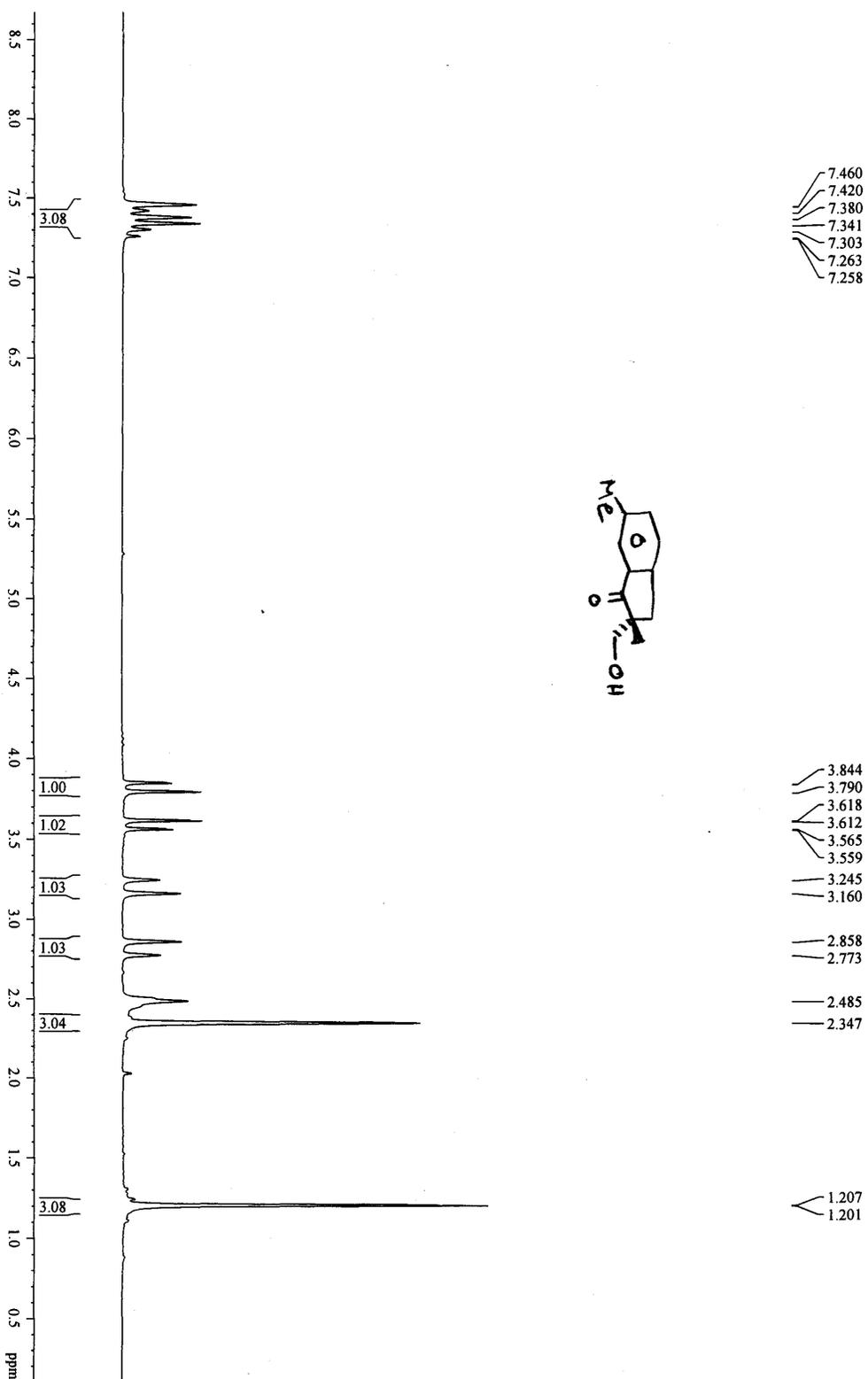


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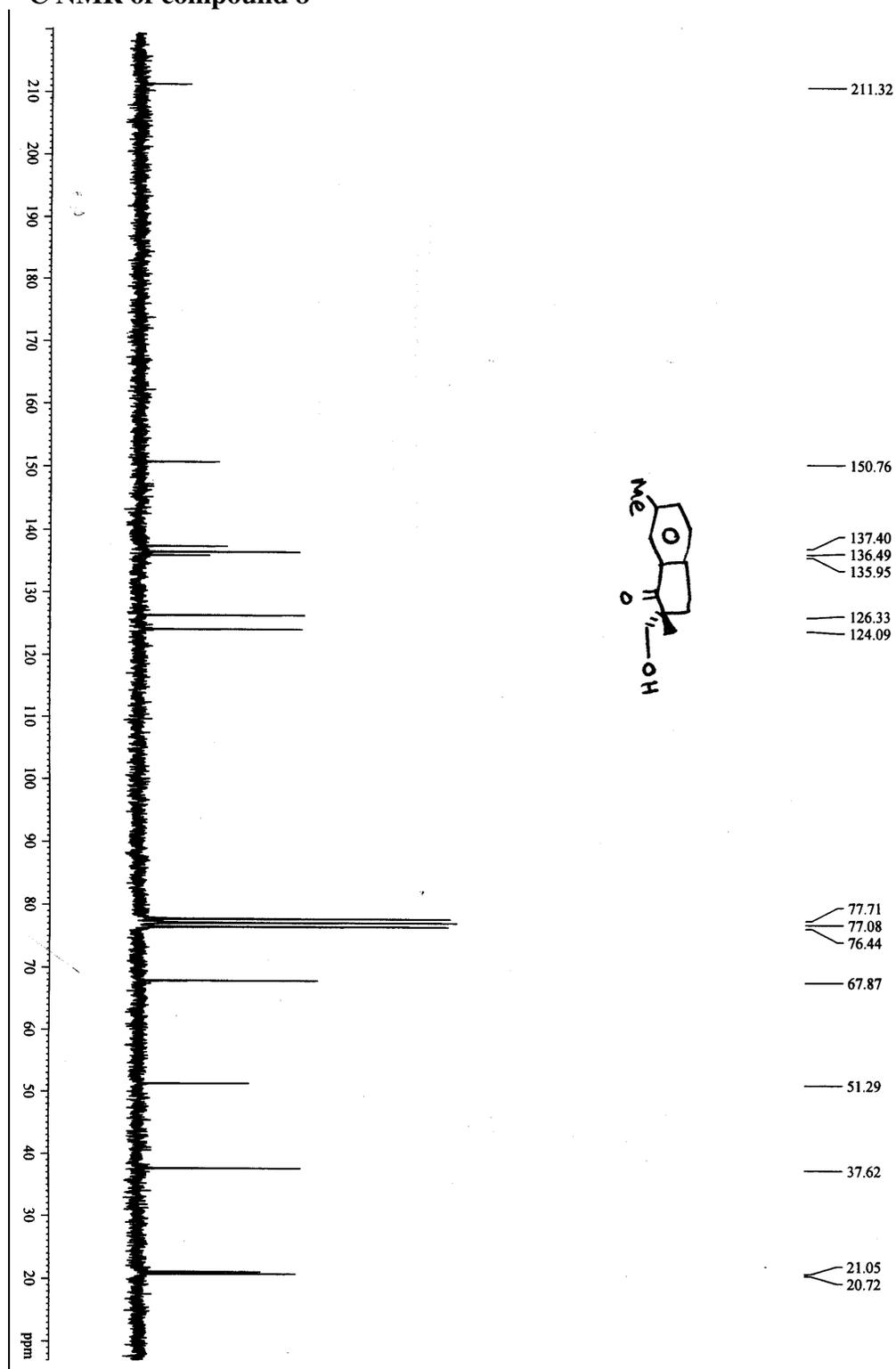
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¹H NMR of compound 8



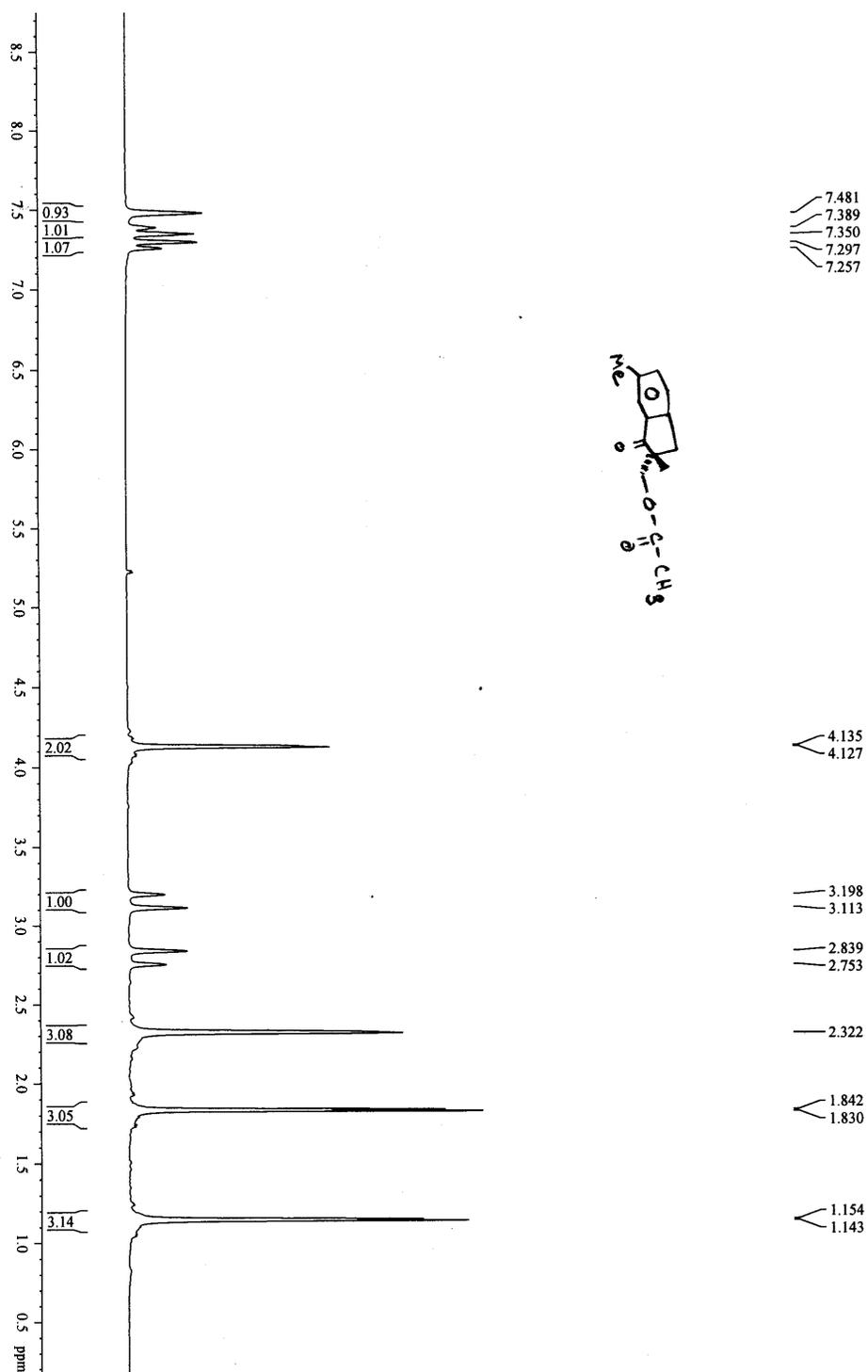
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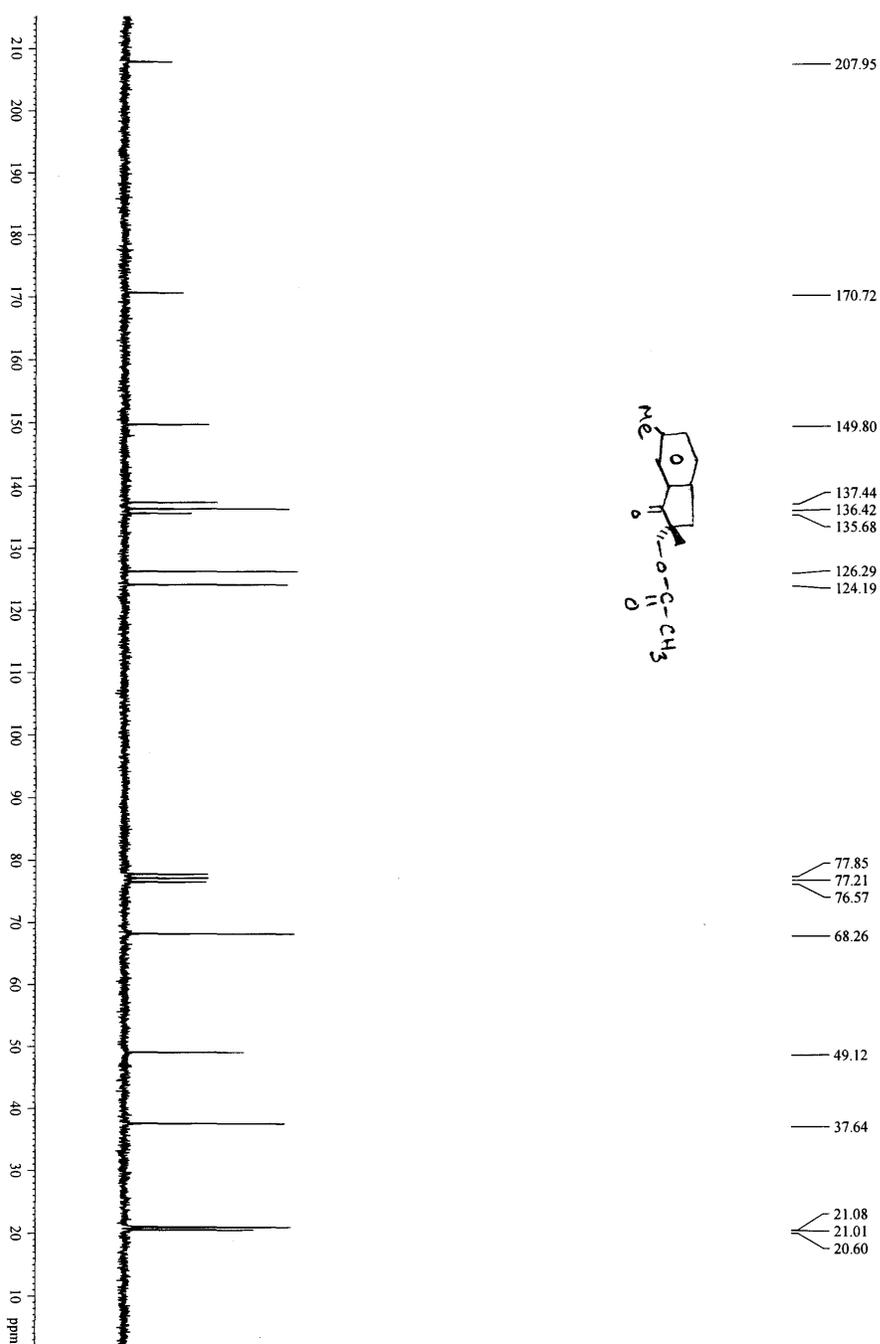
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¹H NMR of acetate derivative of 8



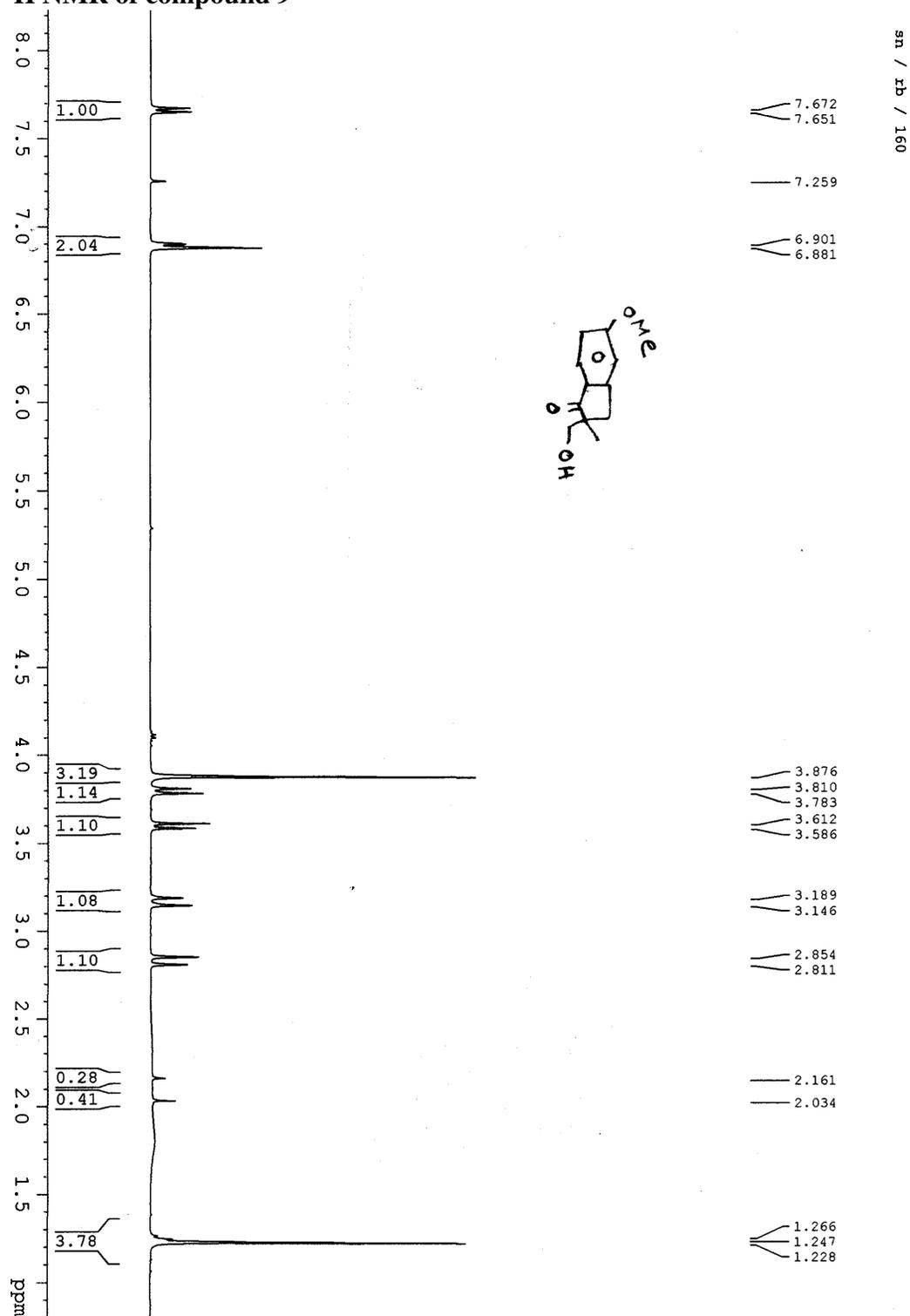
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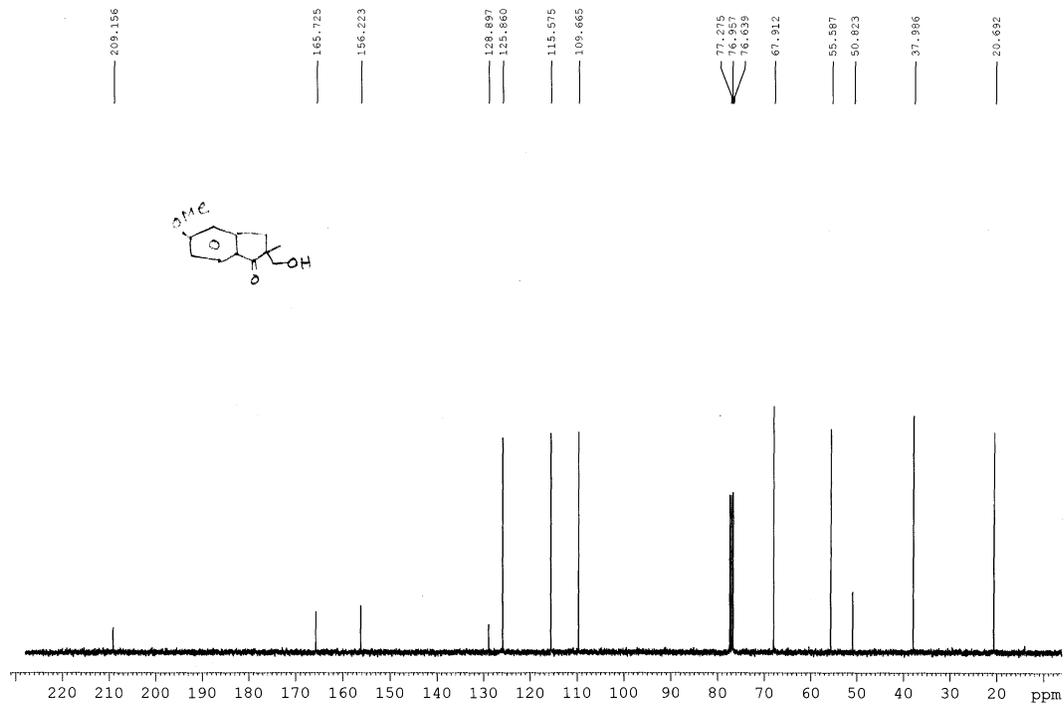
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¹H NMR of compound 9

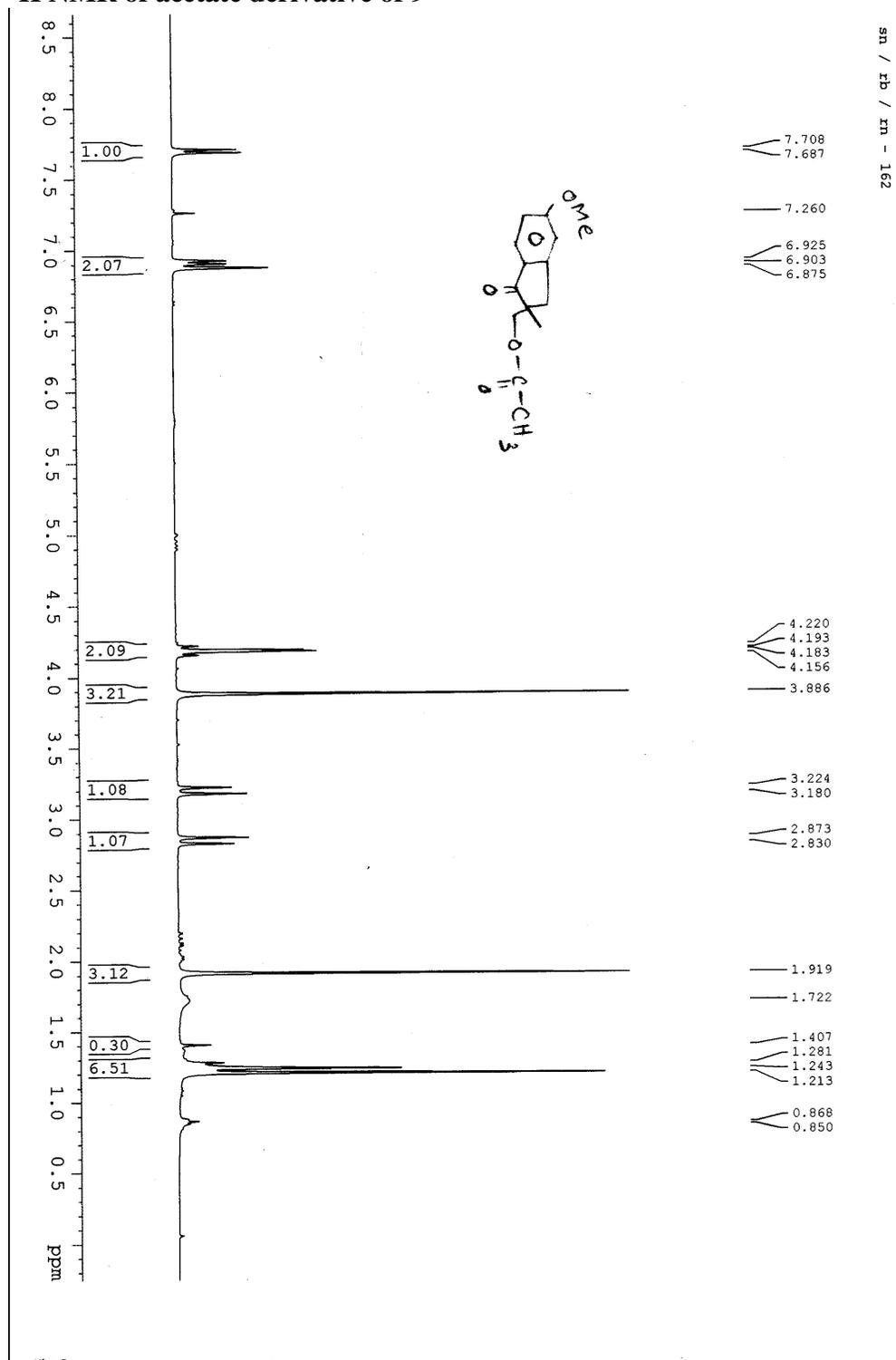


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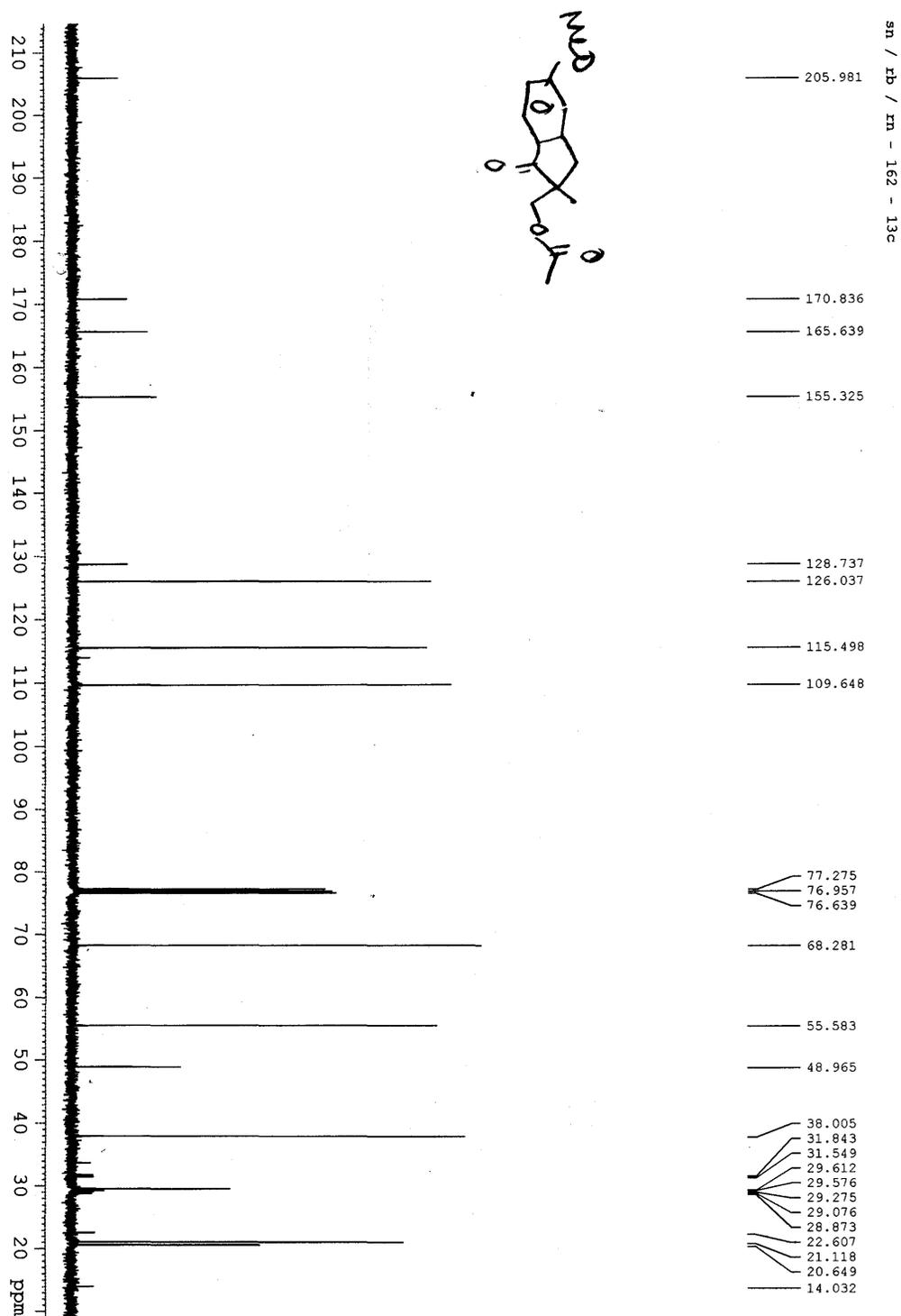
sn / rb / rn - 160 - 13c



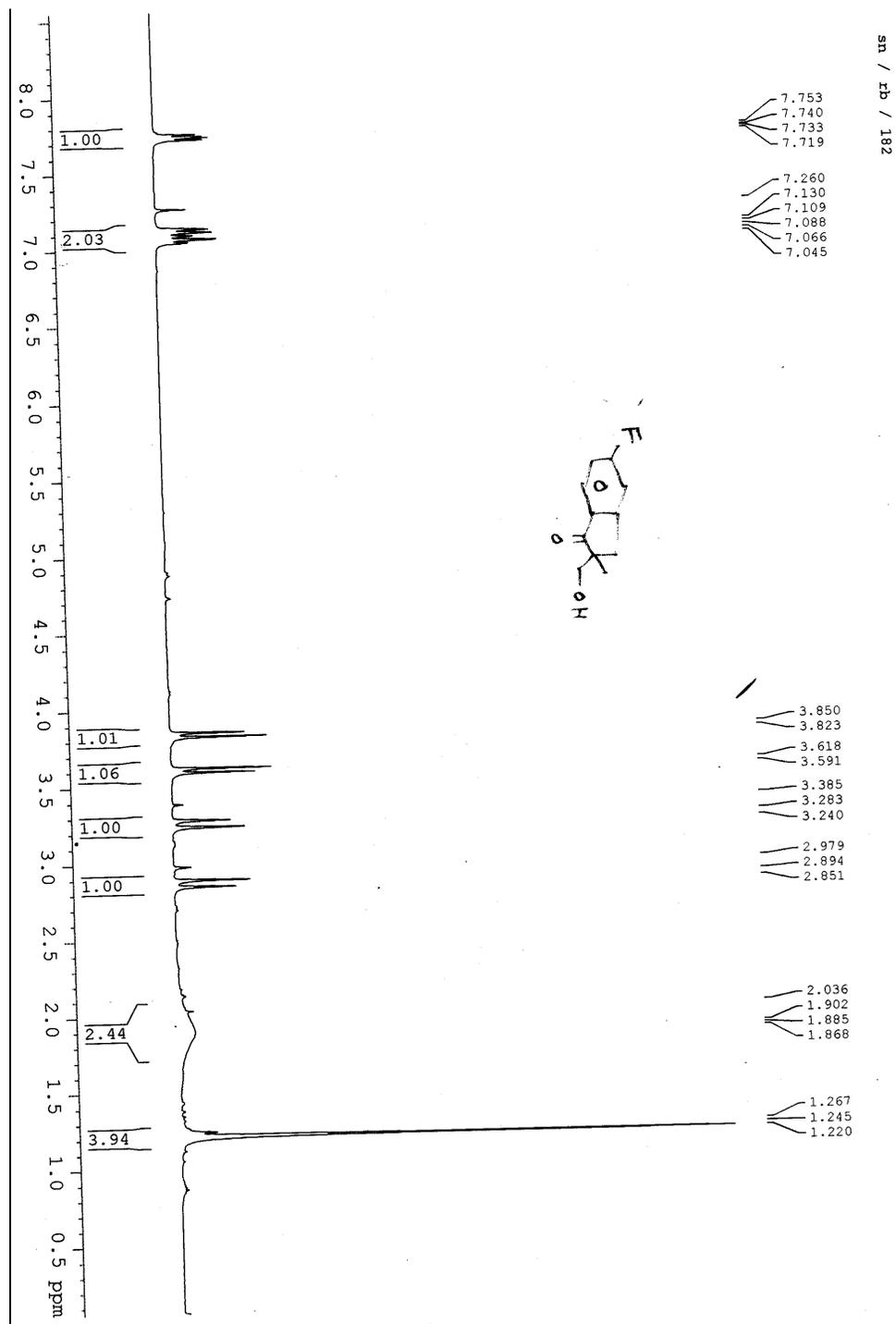
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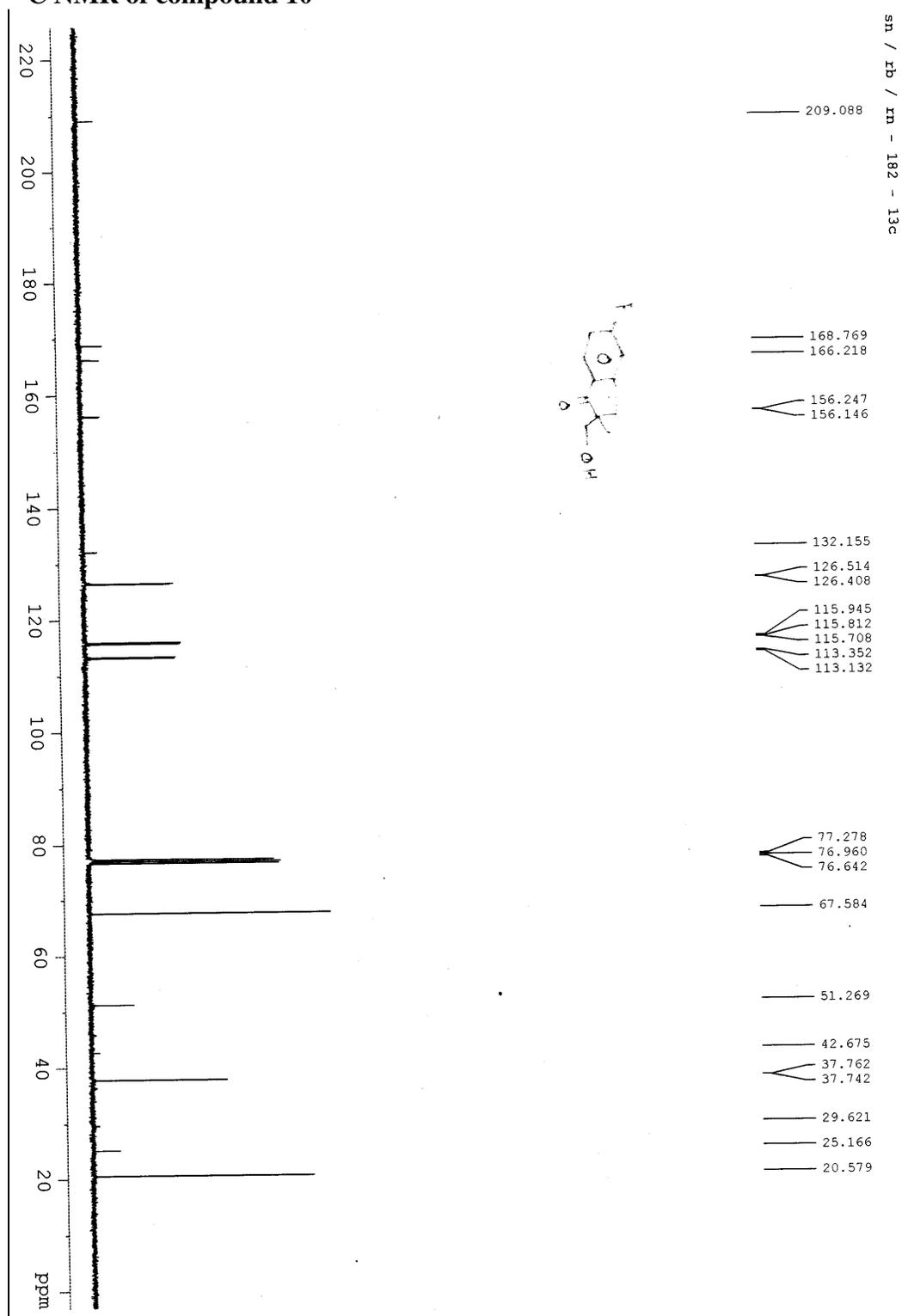
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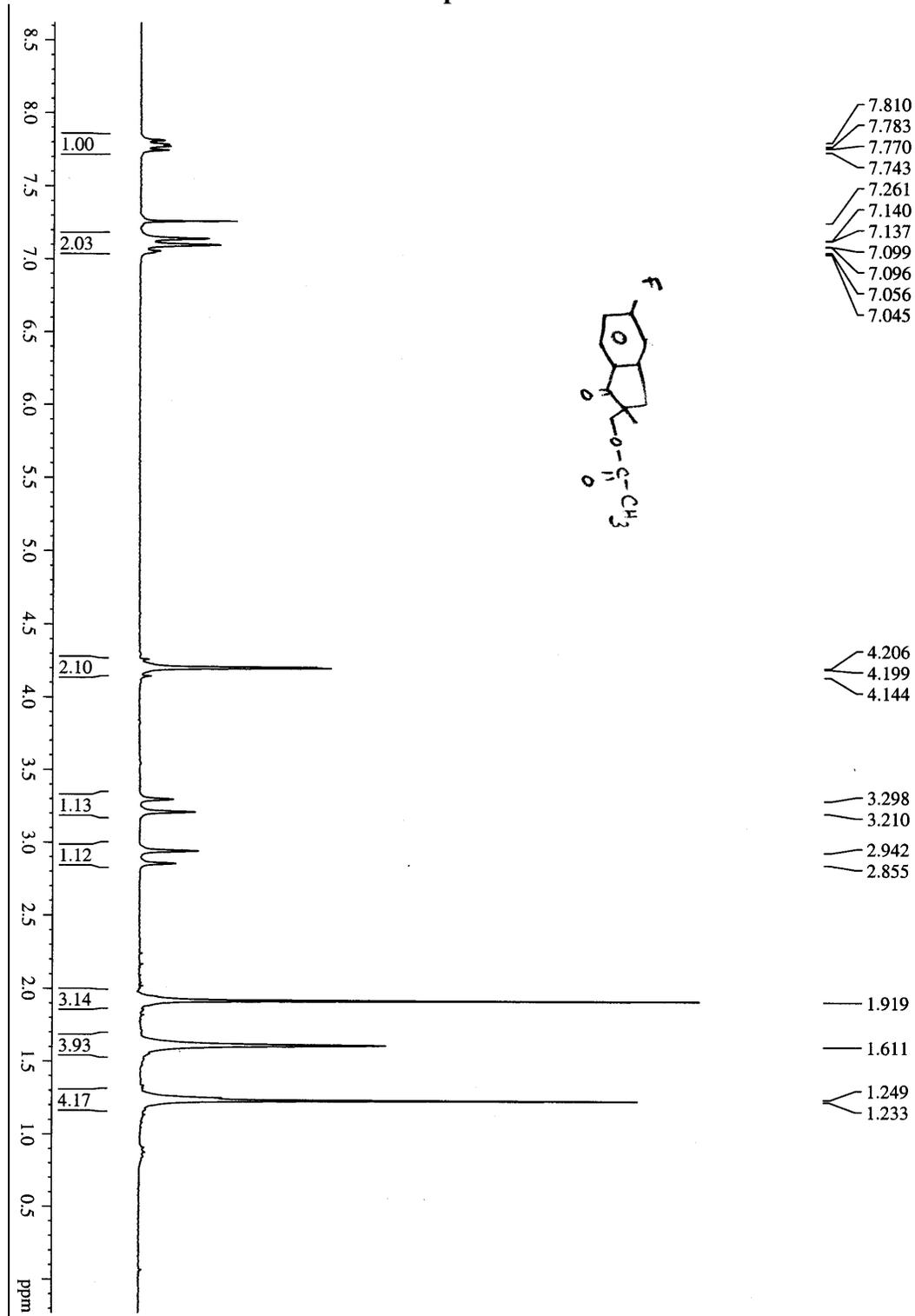
¹H NMR of compound 10



¹³C NMR of compound 10

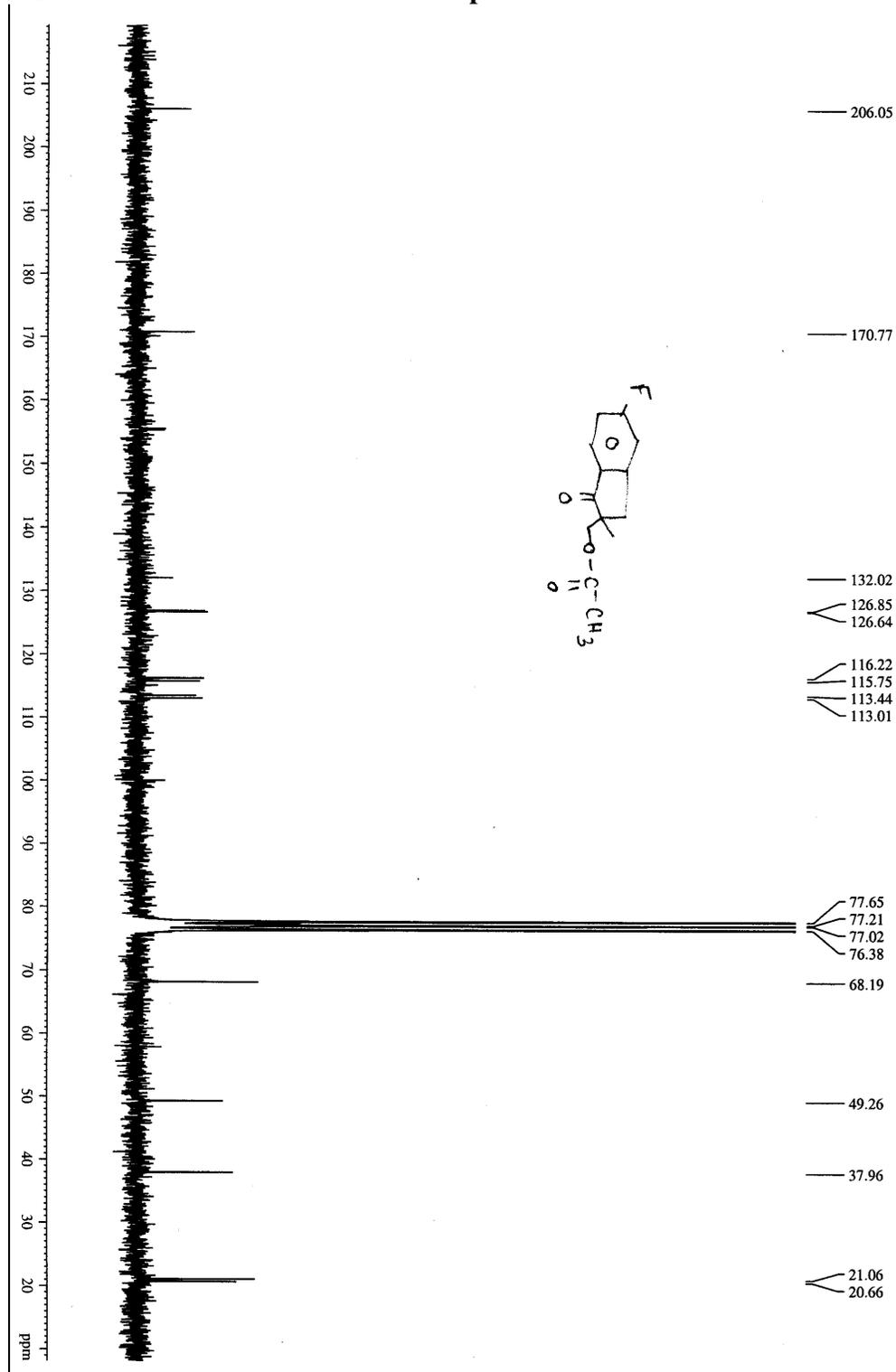


^1H NMR of acetate derivative of compound 10



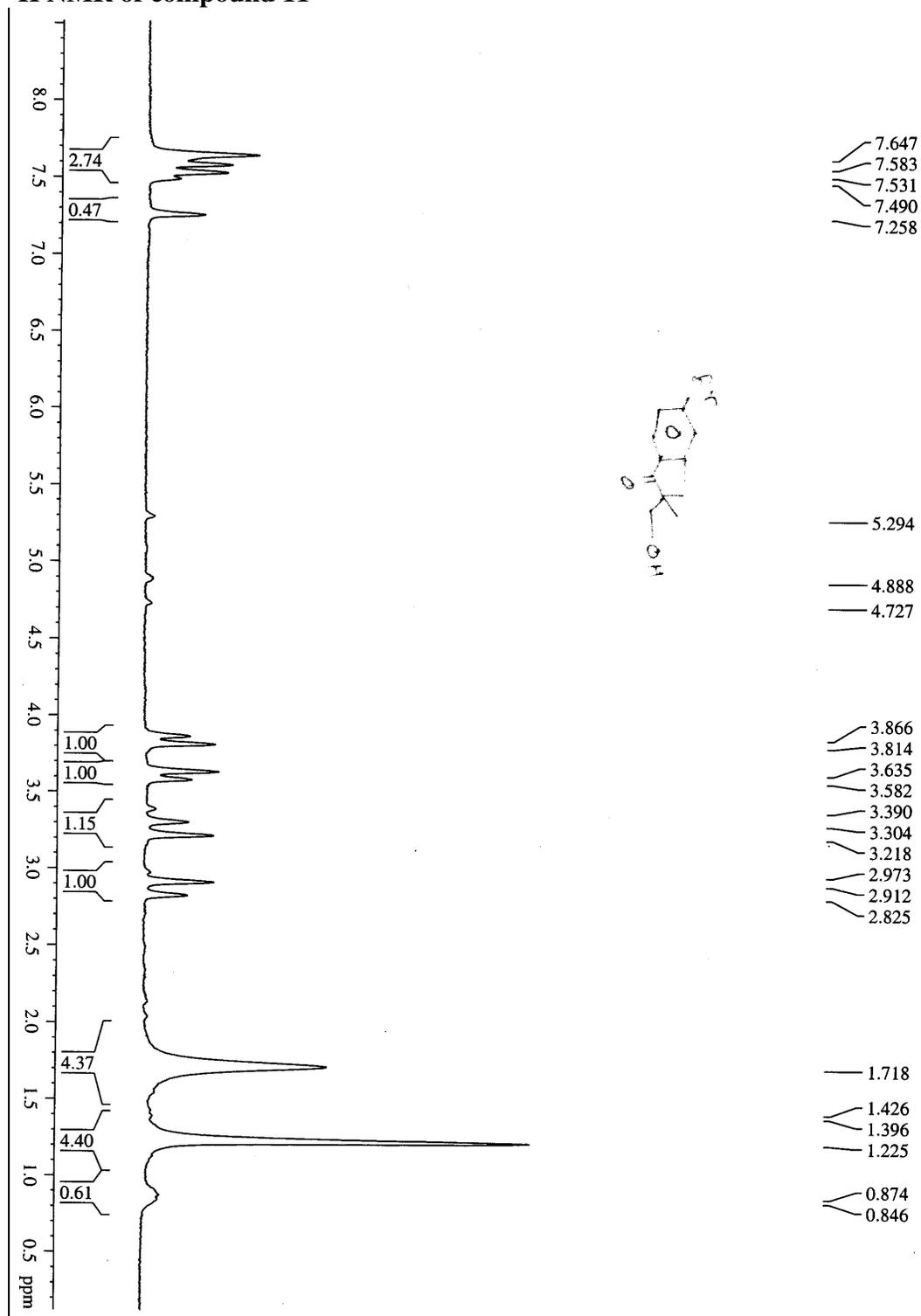
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¹³C NMR of acetate derivative of compound 10



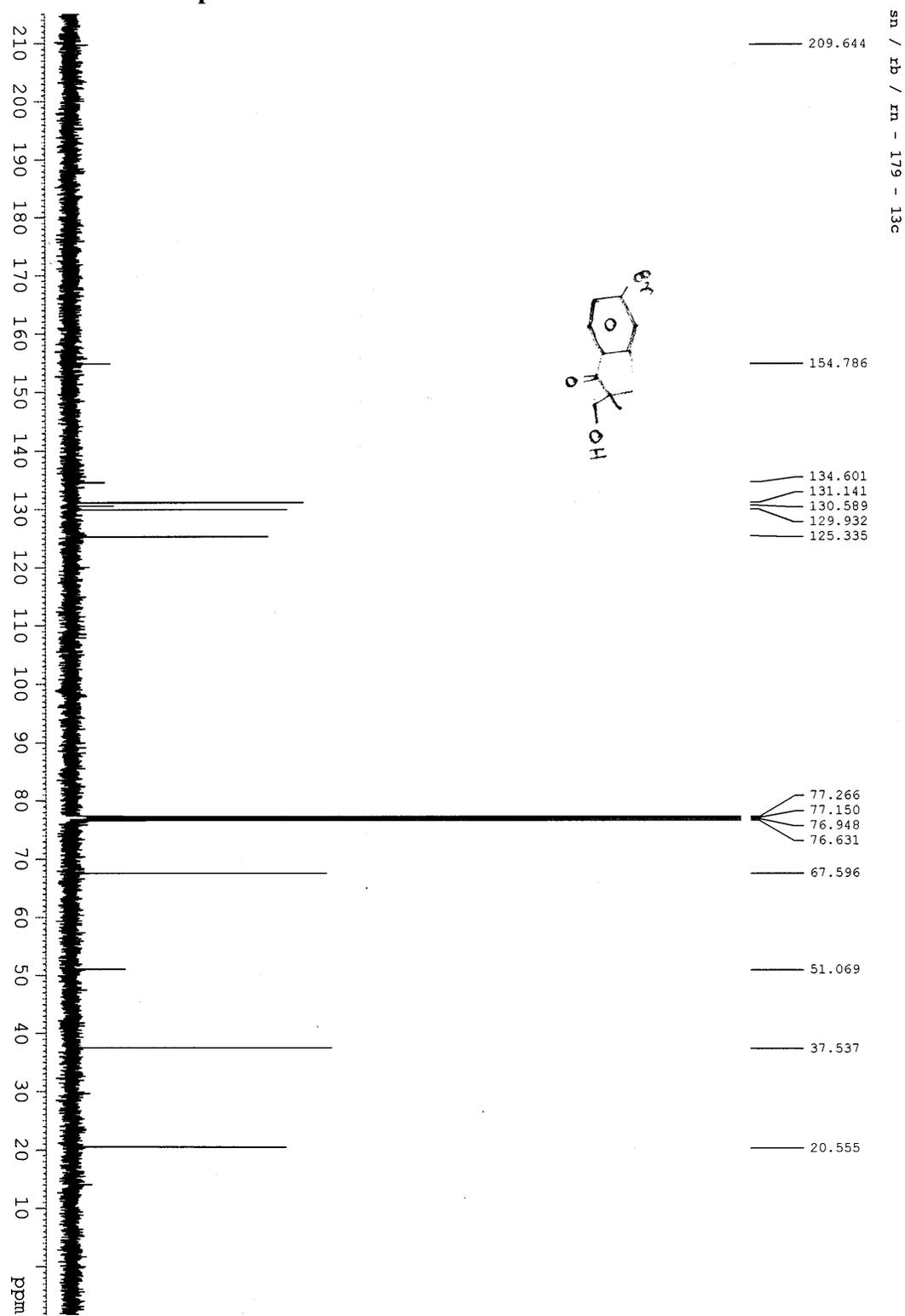
sn / ~~EA~~ / R8 / m188

¹H NMR of compound 11

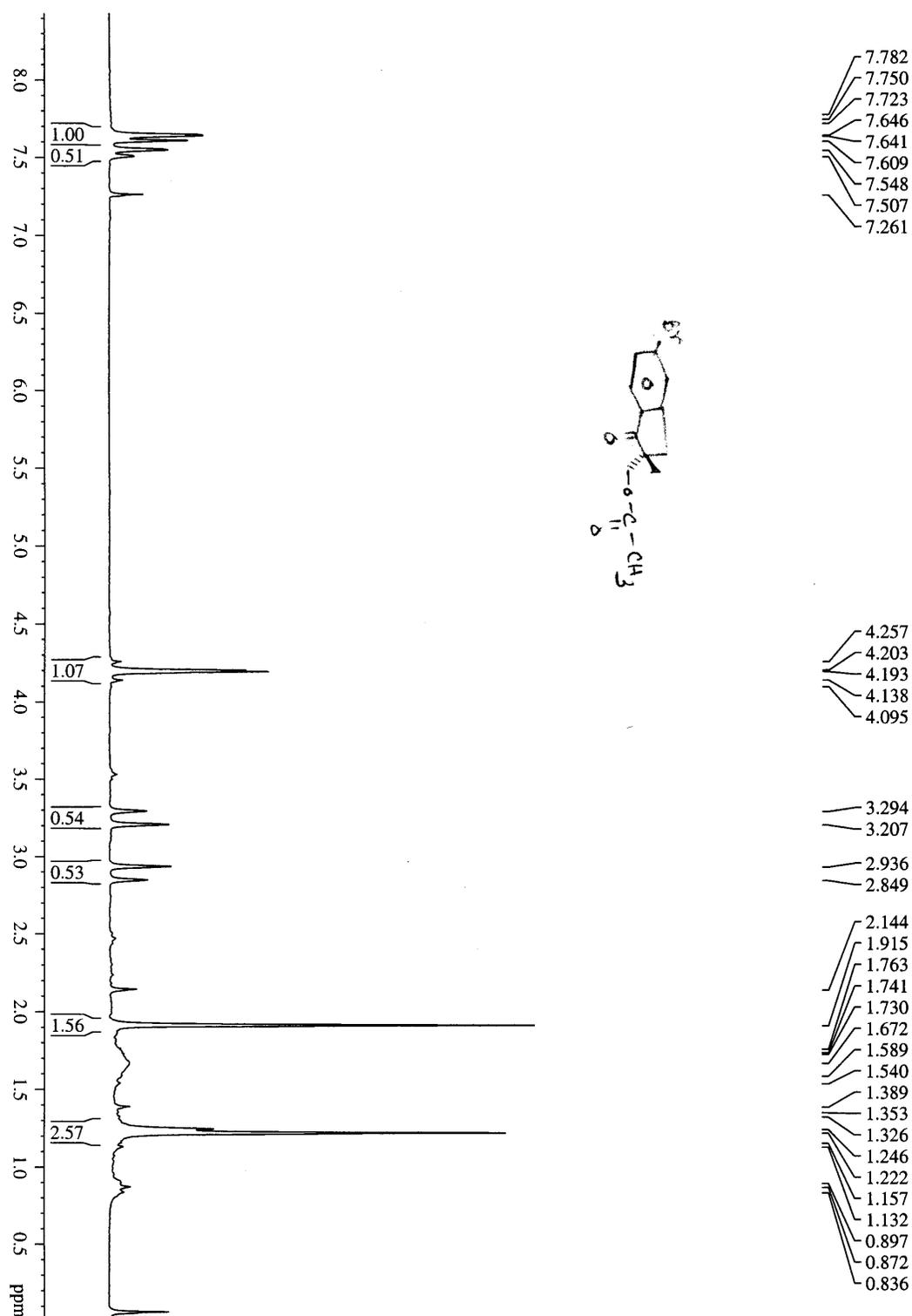


sn/rb/179

¹³C NMR of compound 11

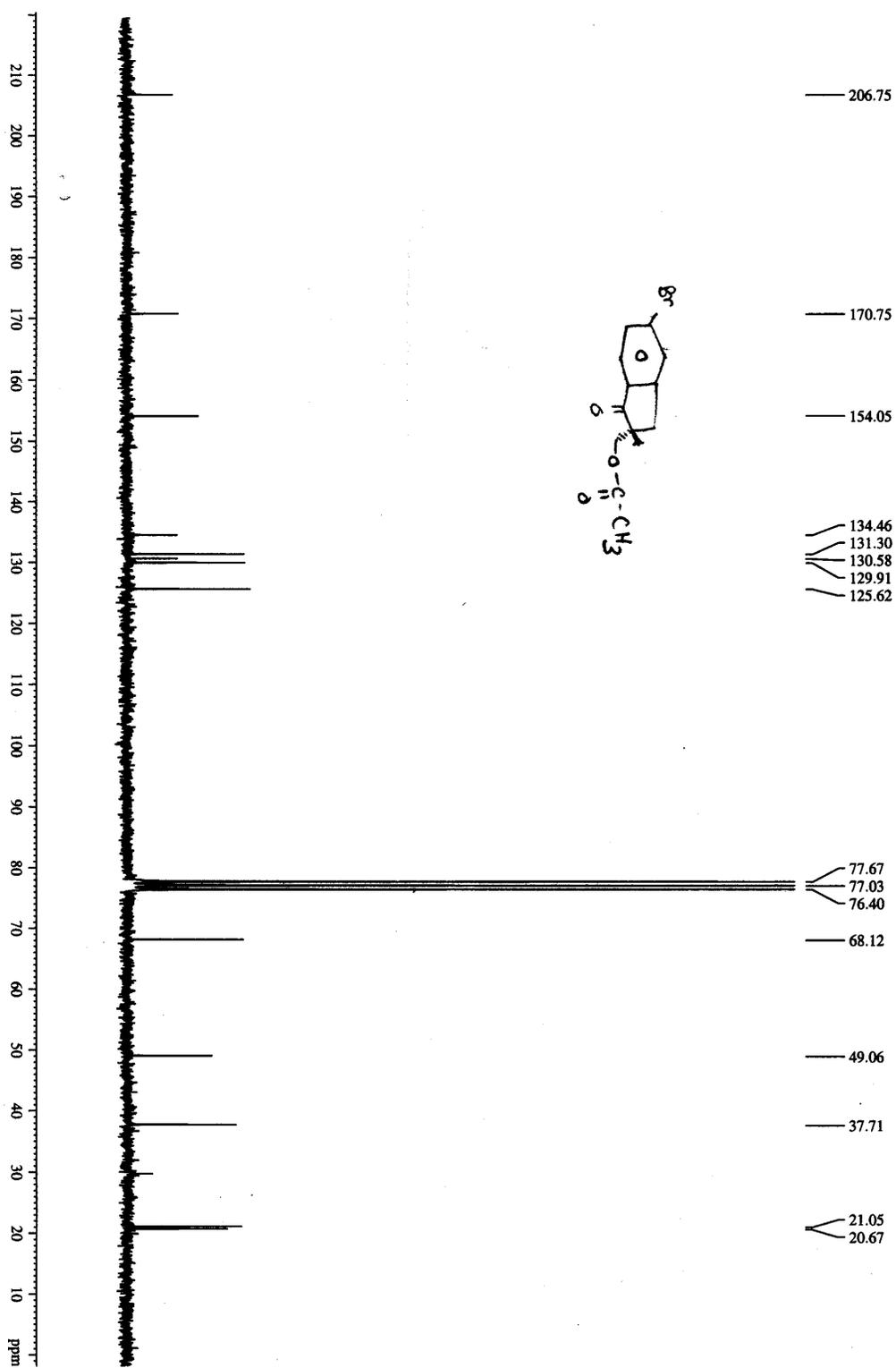


¹H NMR of acetate derivative of 11



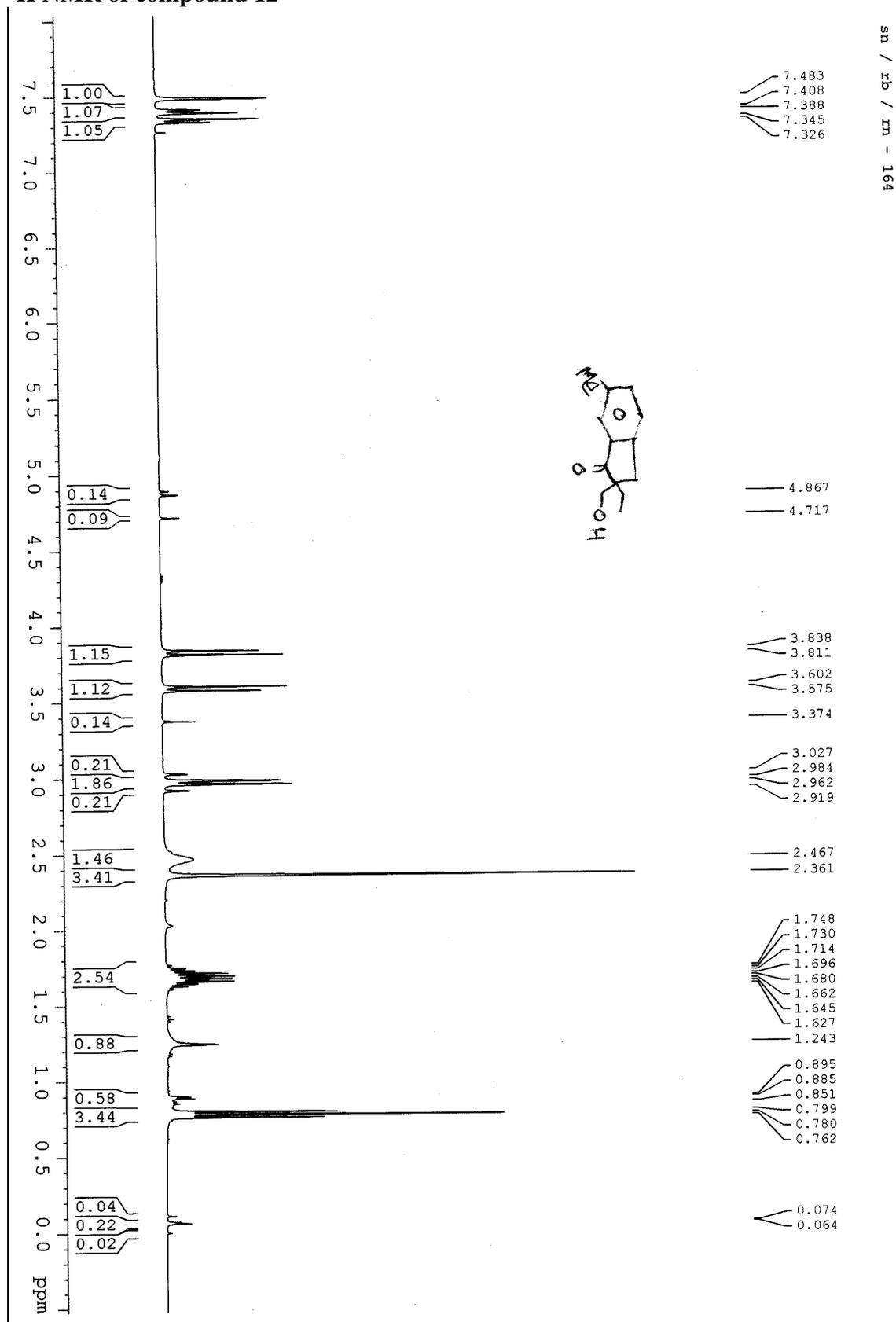
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¹³C NMR of acetate derivative of 11

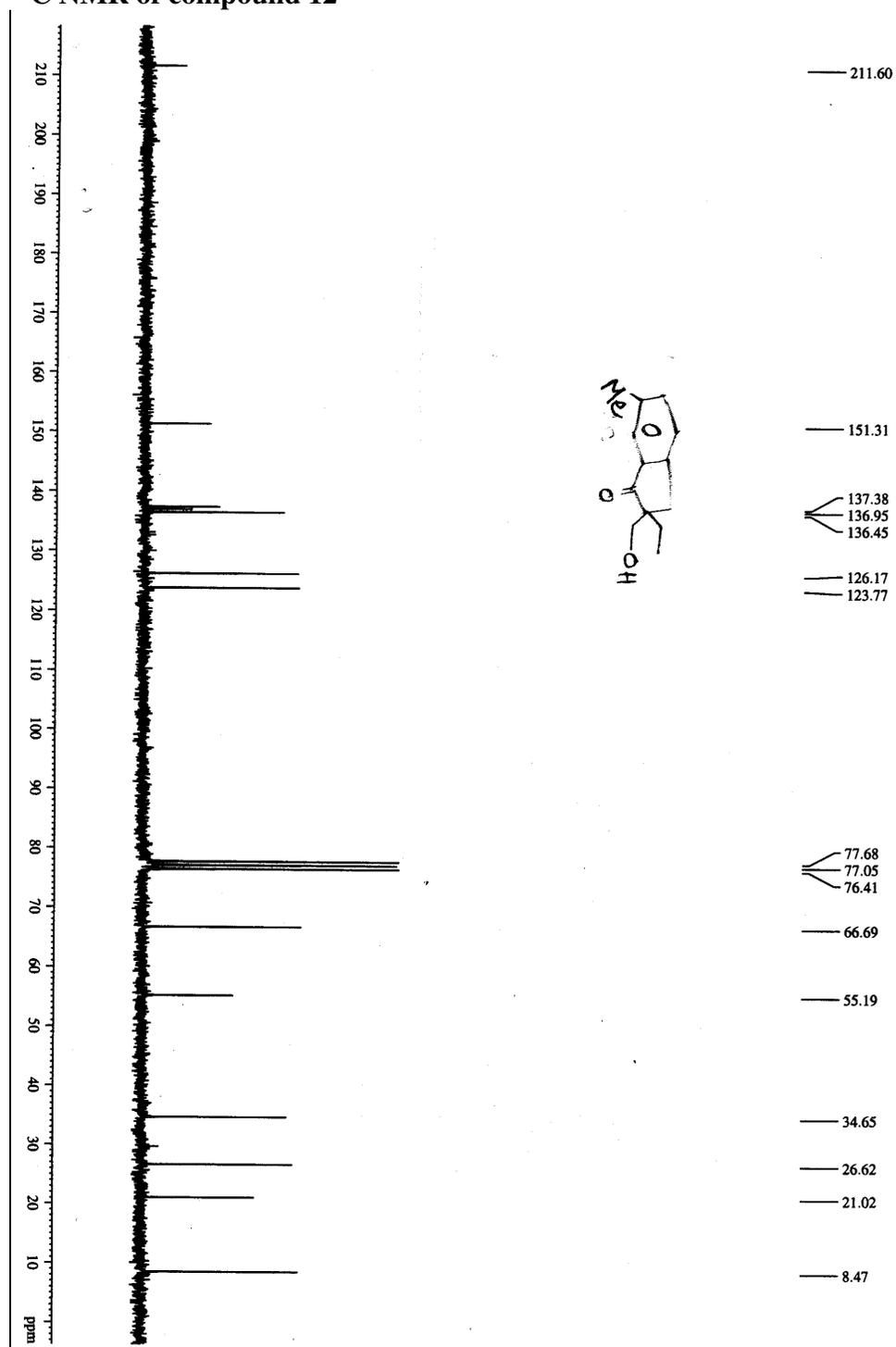


snc/rb/229
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¹H NMR of compound 12

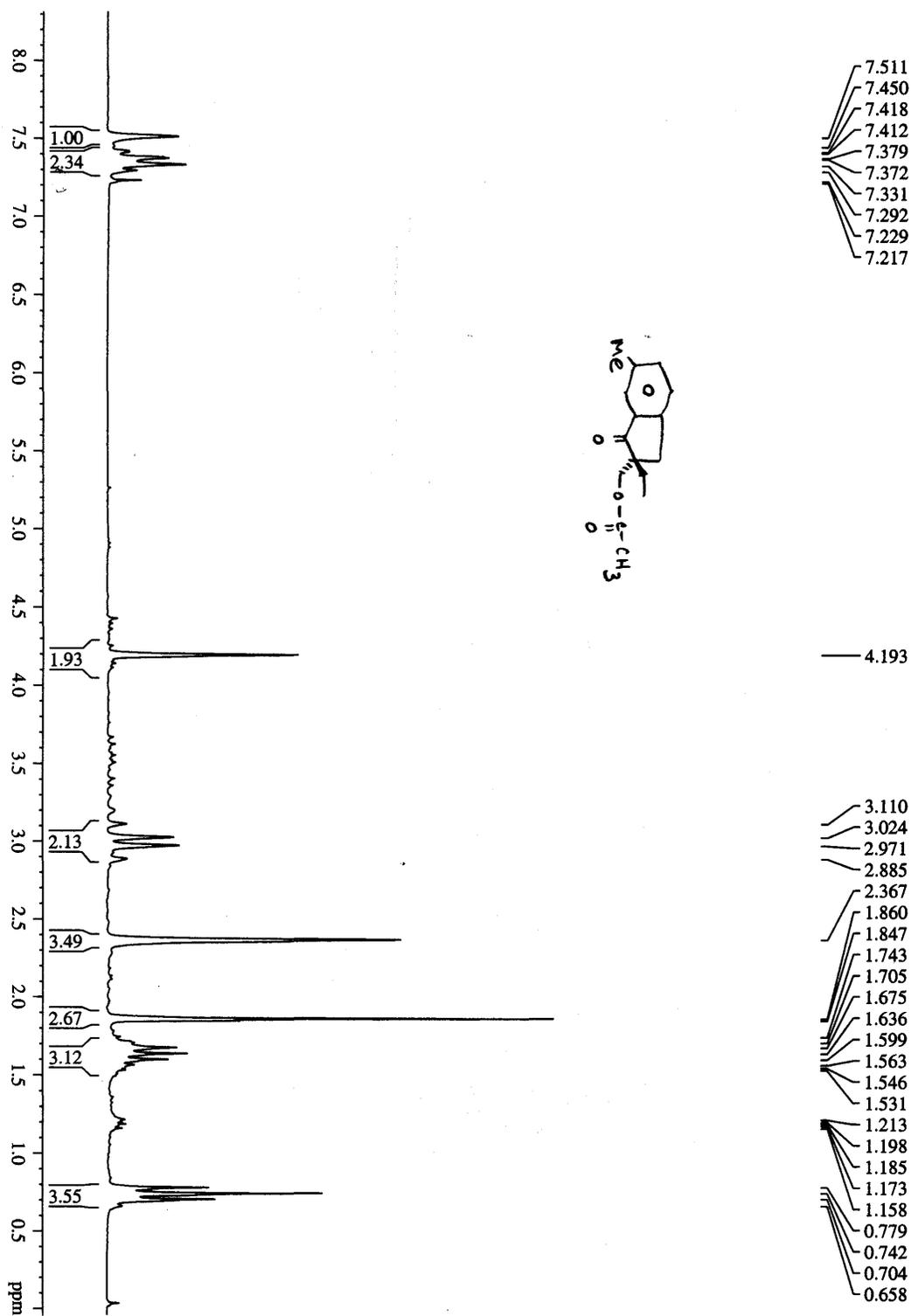


¹³C NMR of compound 12

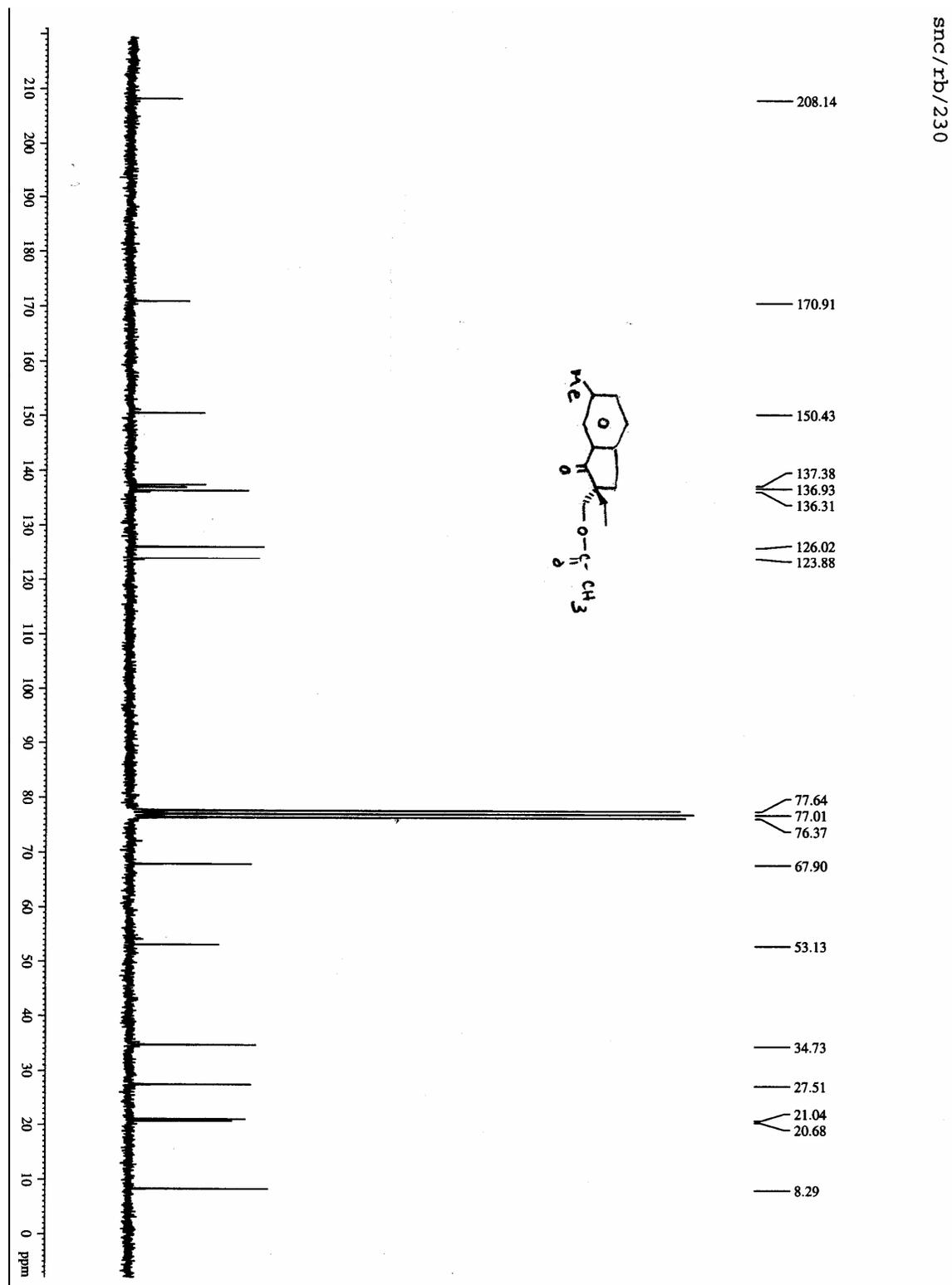


sn / rb/rn-164
¹³C

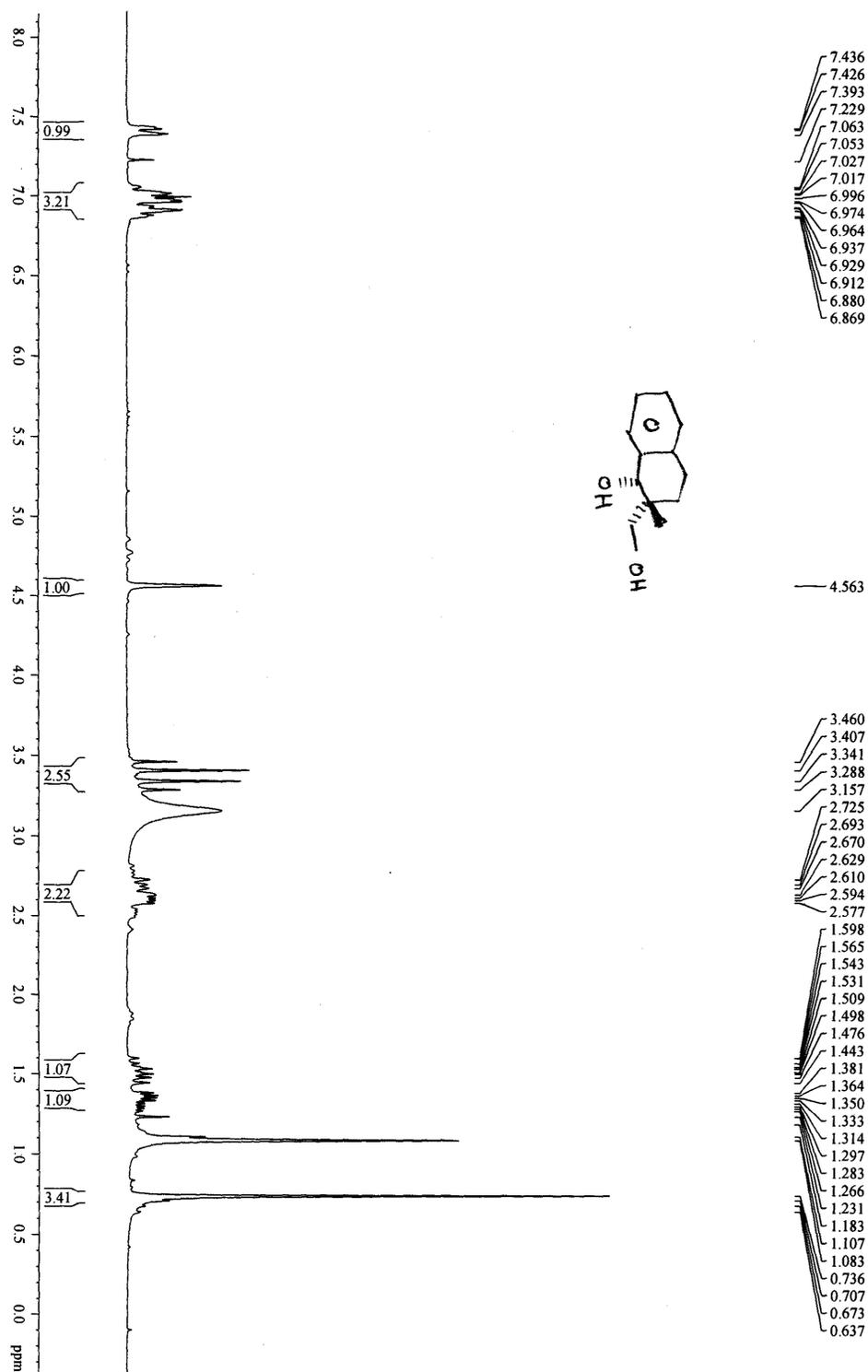
¹H NMR of acetate derivative of 12



¹³C NMR of acetate derivative of 12

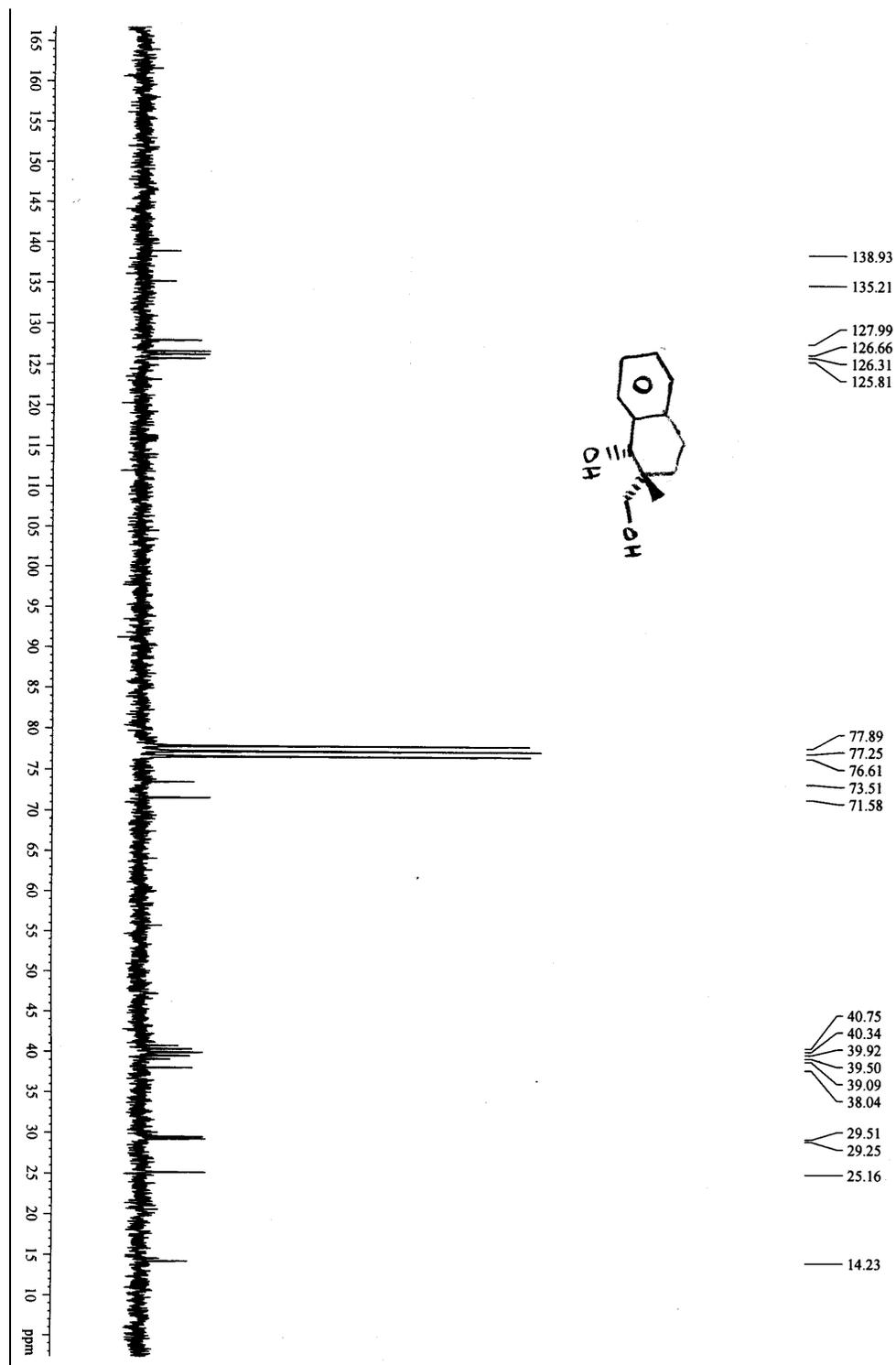


^1H NMR spectrum of 17



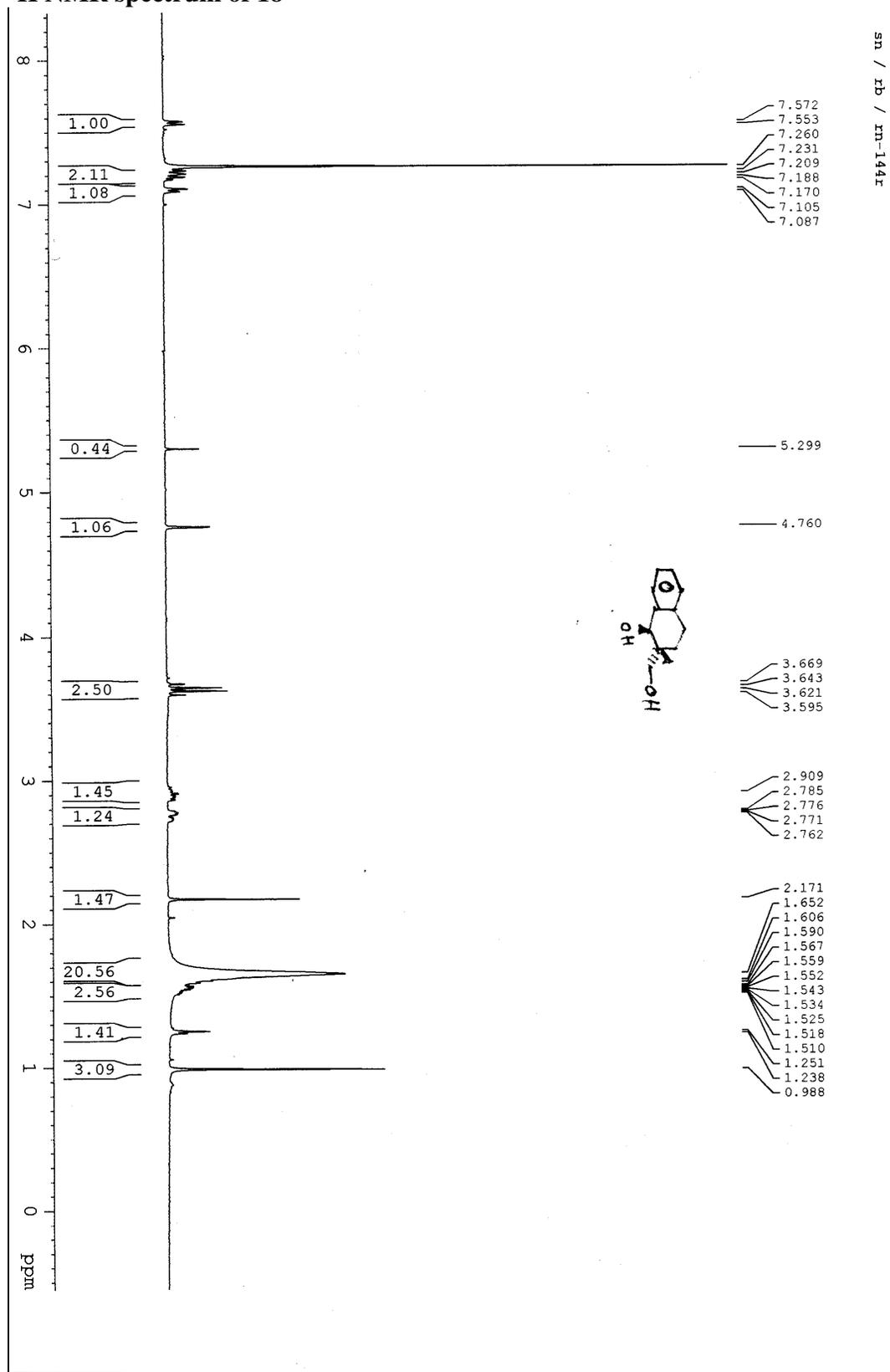
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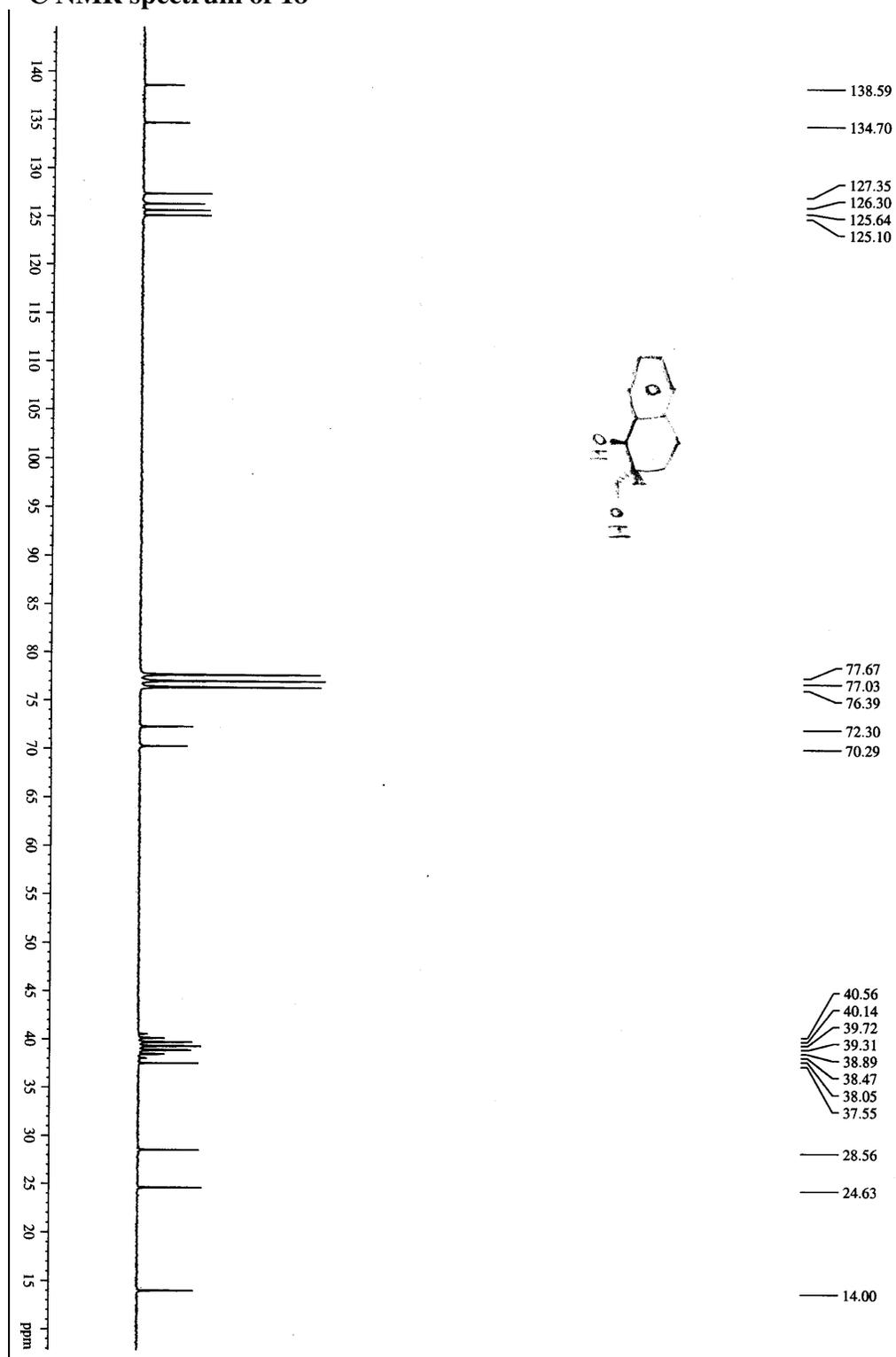


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¹H NMR spectrum of 18

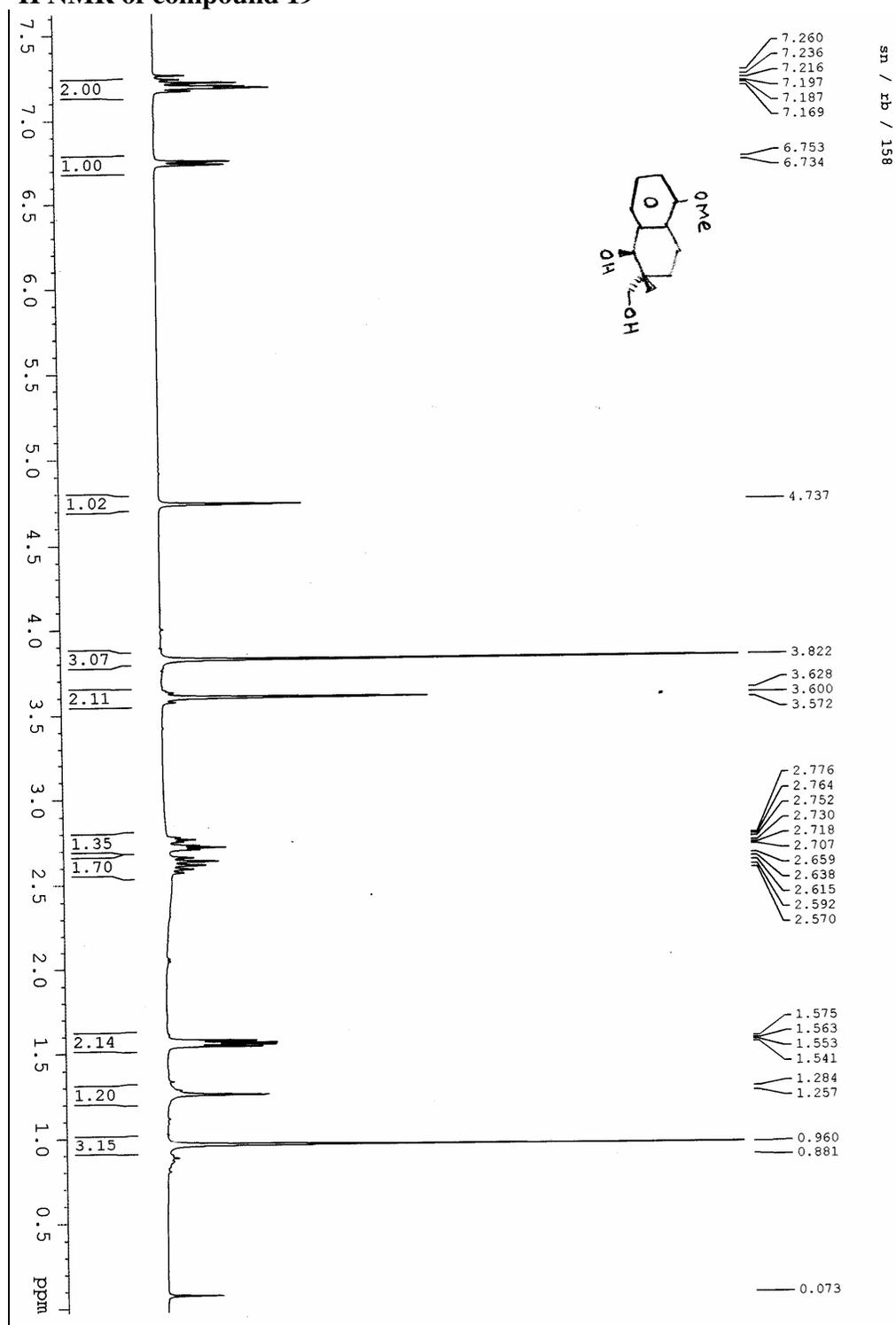


¹³C NMR spectrum of 18

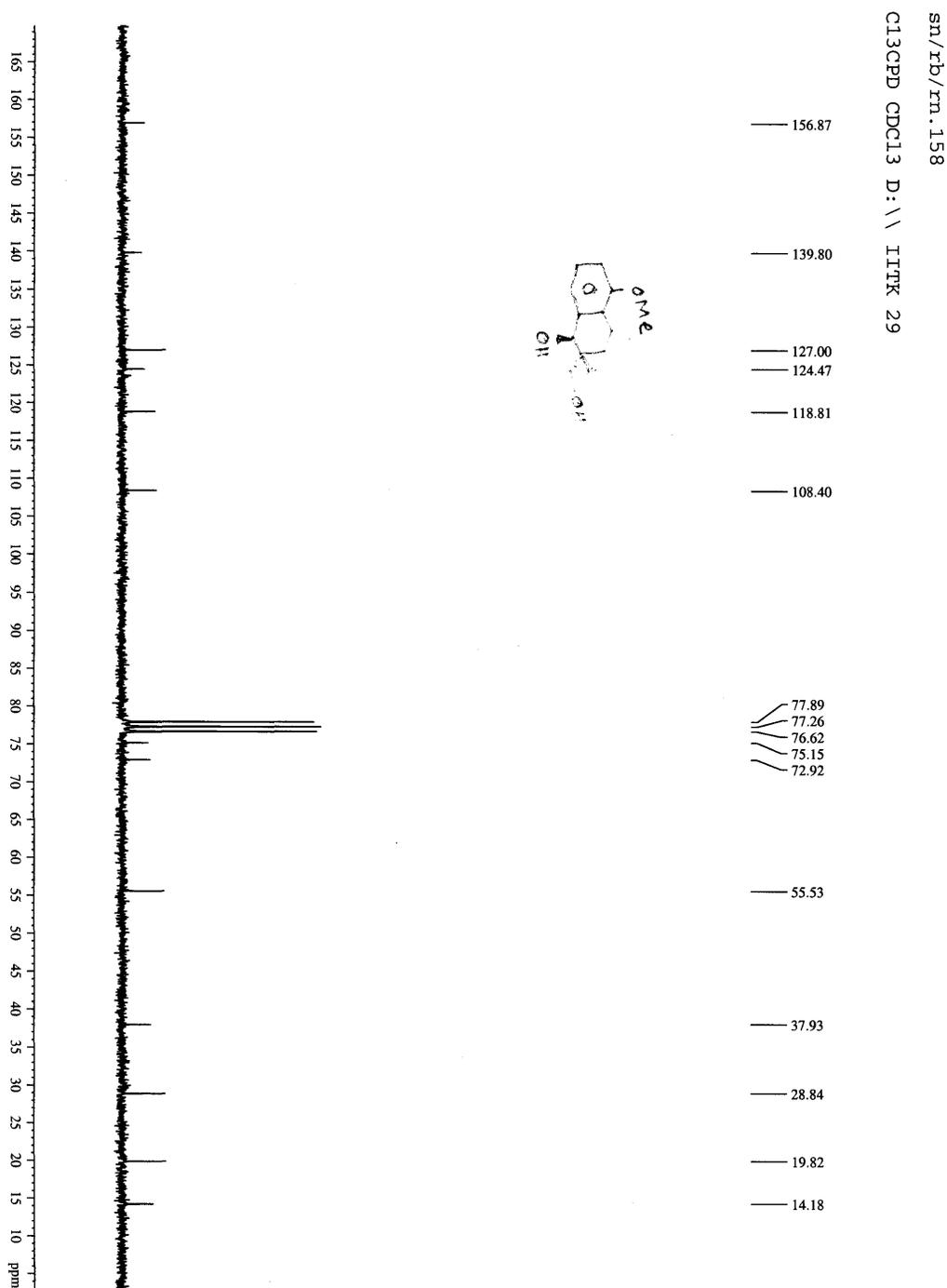


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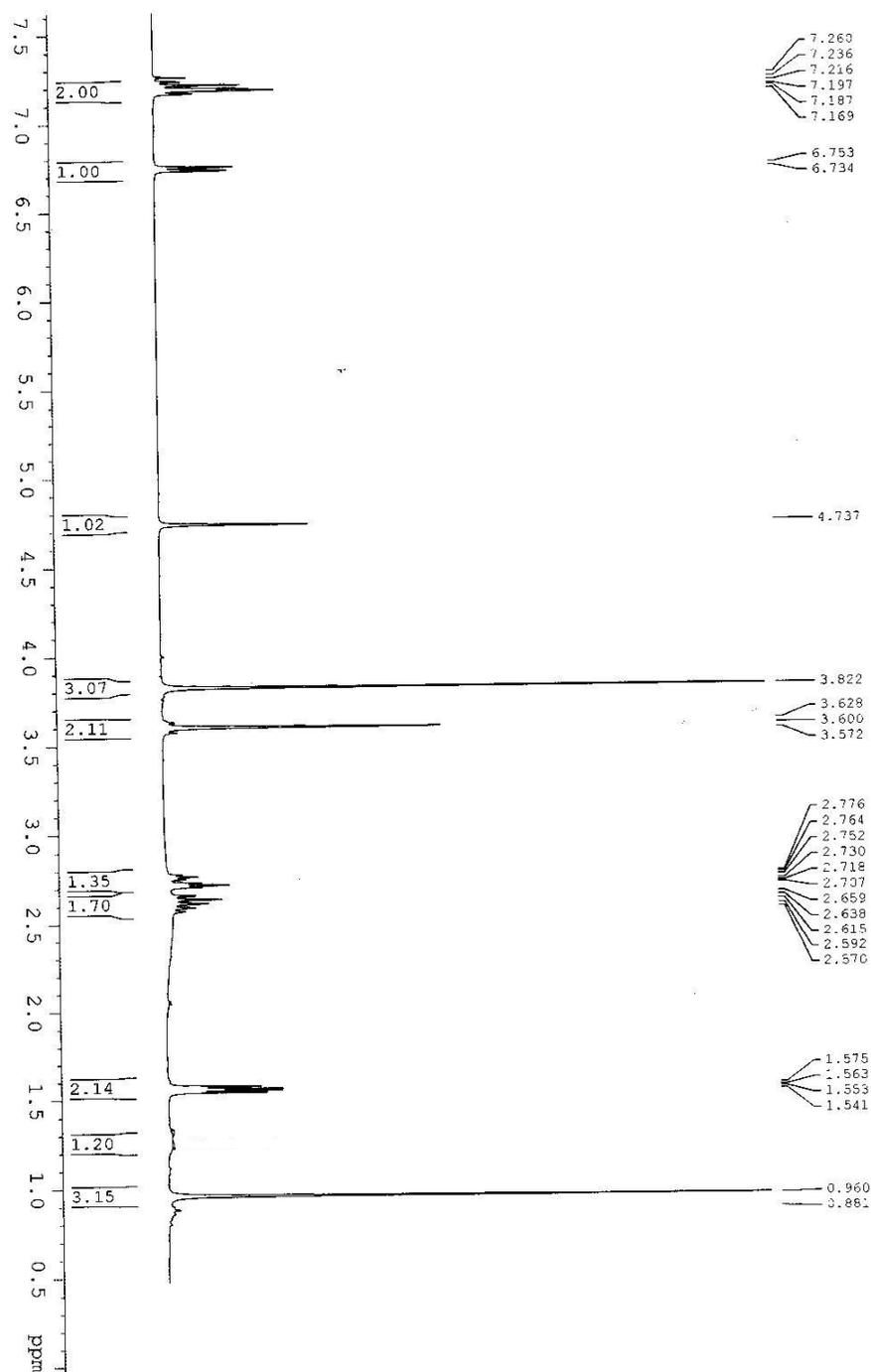
¹H NMR of compound 19



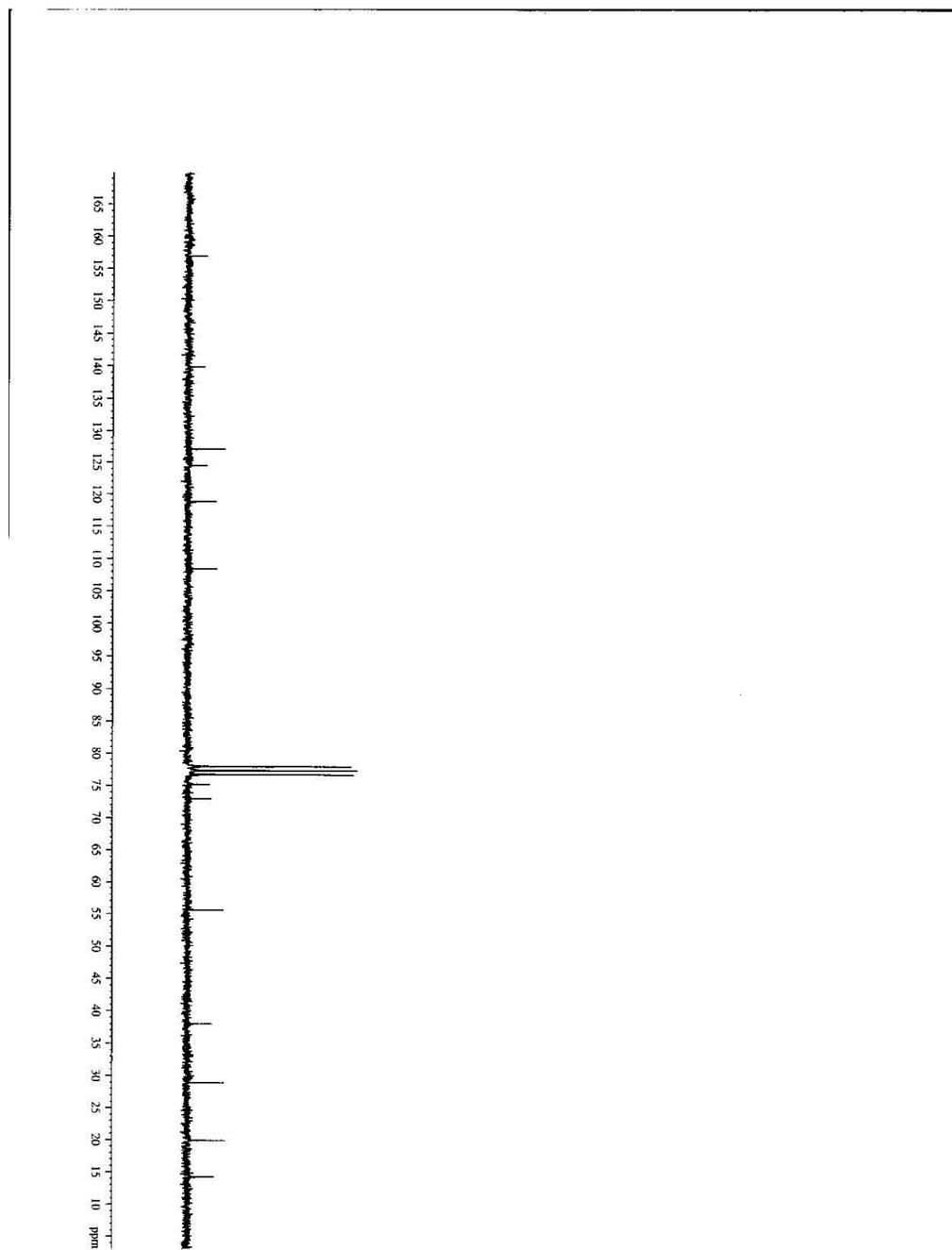
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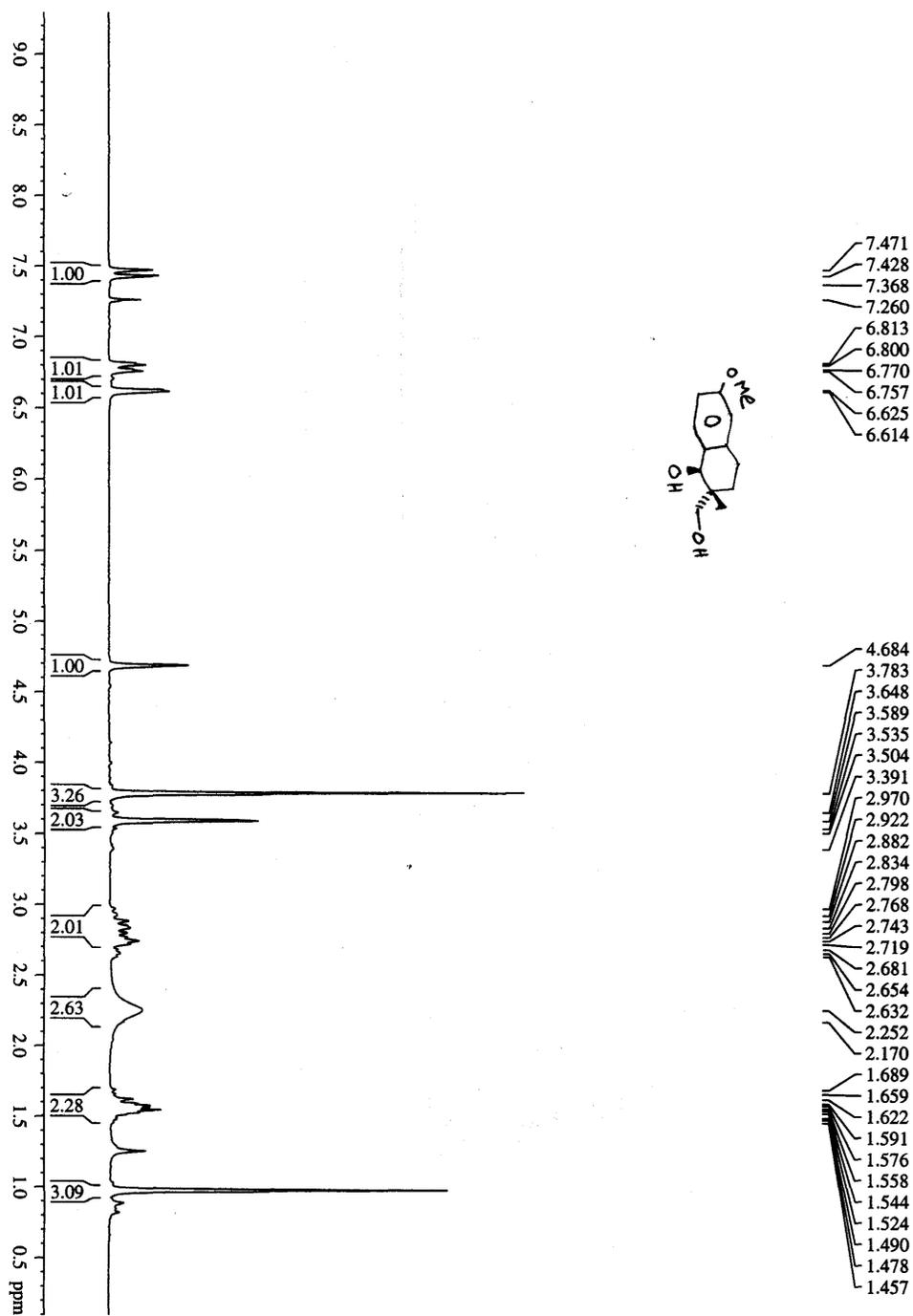
¹H NMR of compound 20



^{13}C NMR of compound 20

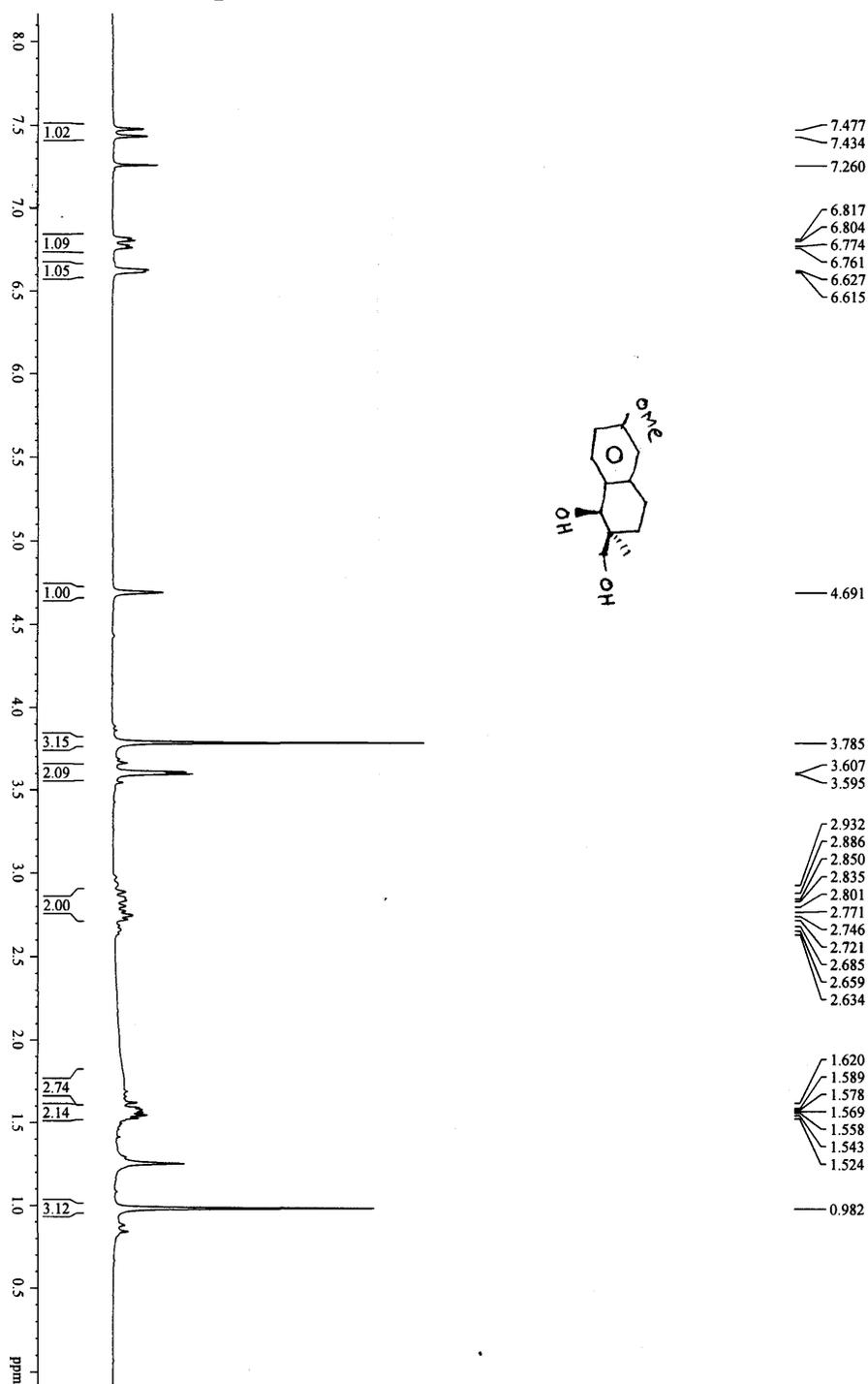


¹H NMR of compound 21



sn/rb/221

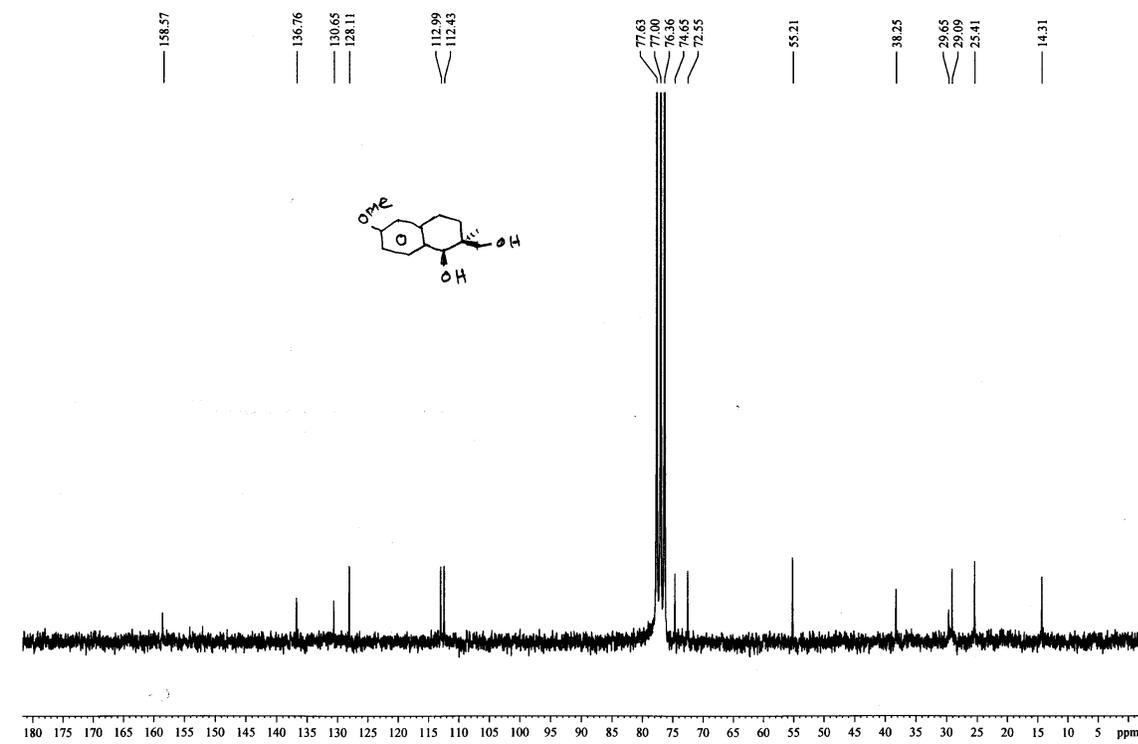
¹H NMR of compound ent-22



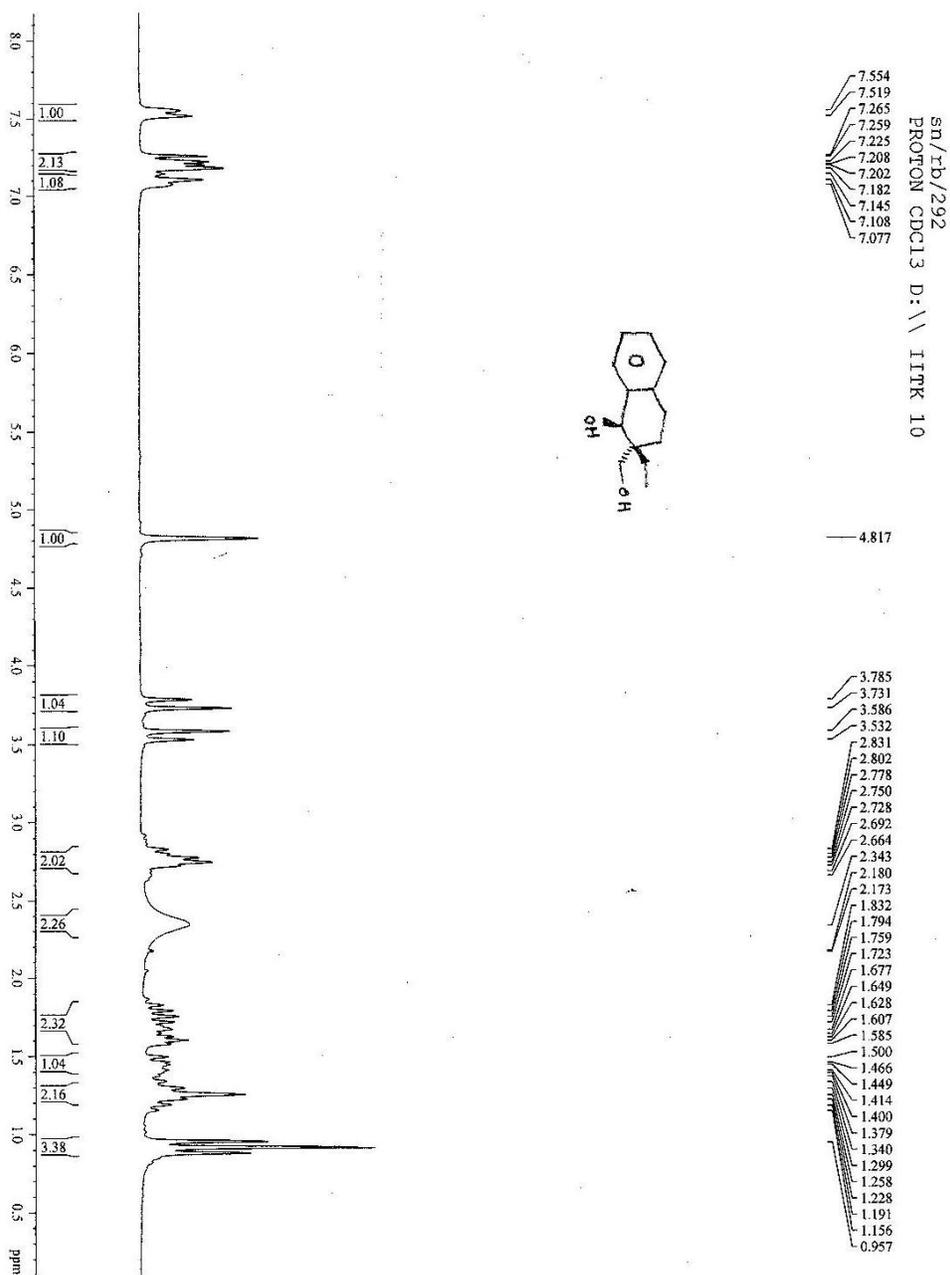
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PROTON CDCl3 D:\\ IITK 13

¹³C NMR of compound ent-22

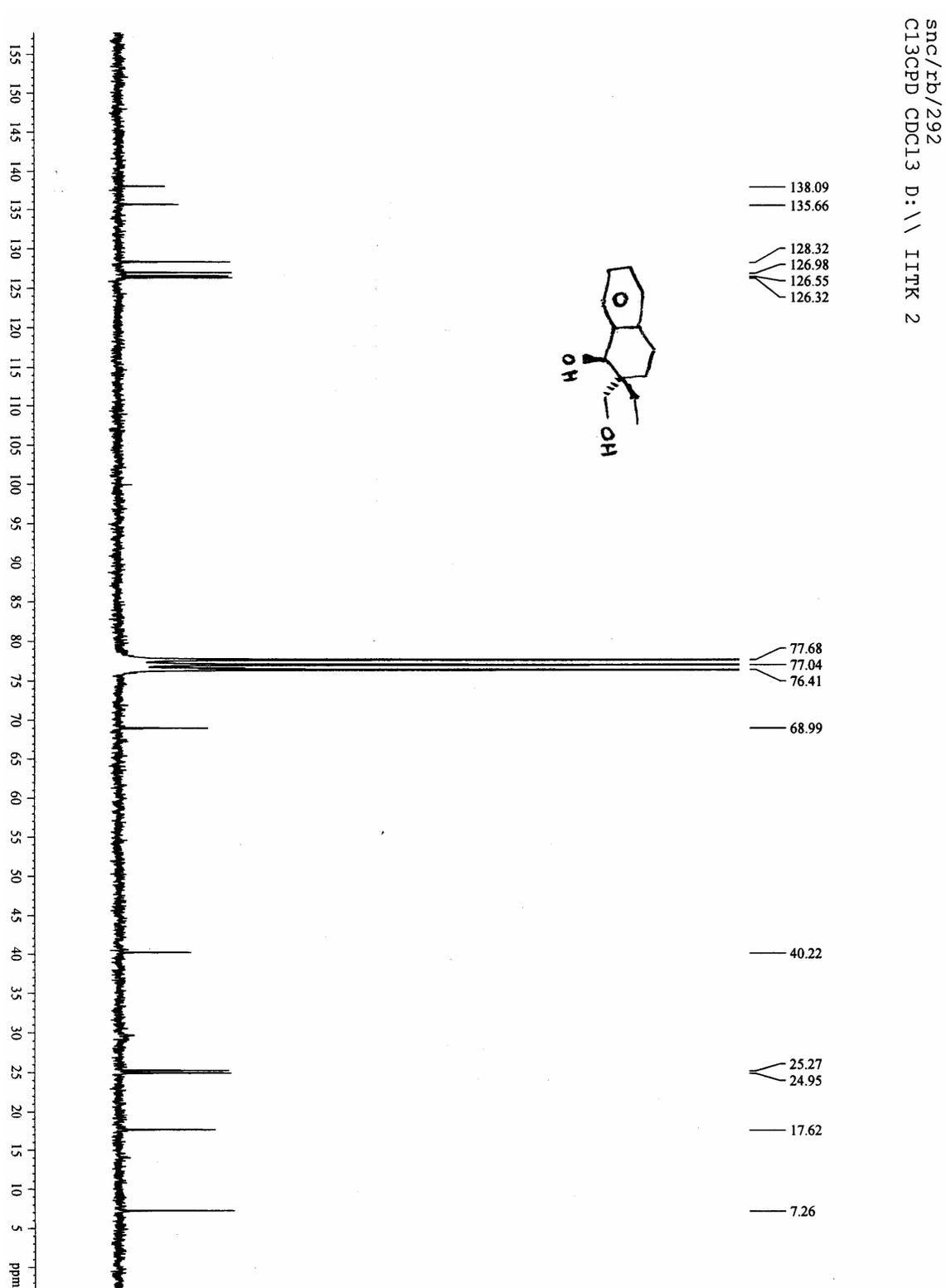
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C13CPD CDC13 D:\ IITK 2



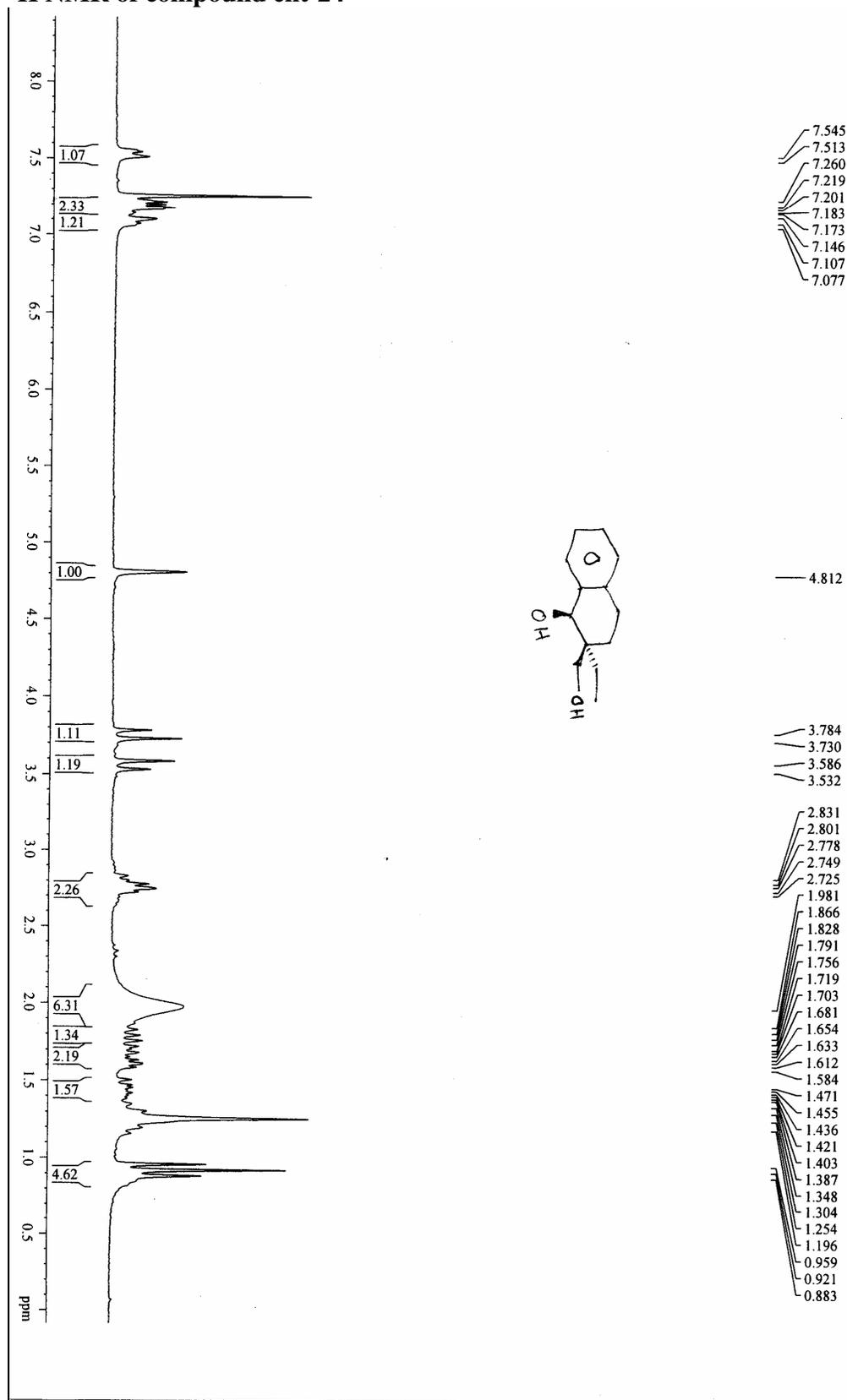
¹H NMR of compound 23



^{13}C NMR of compound 23

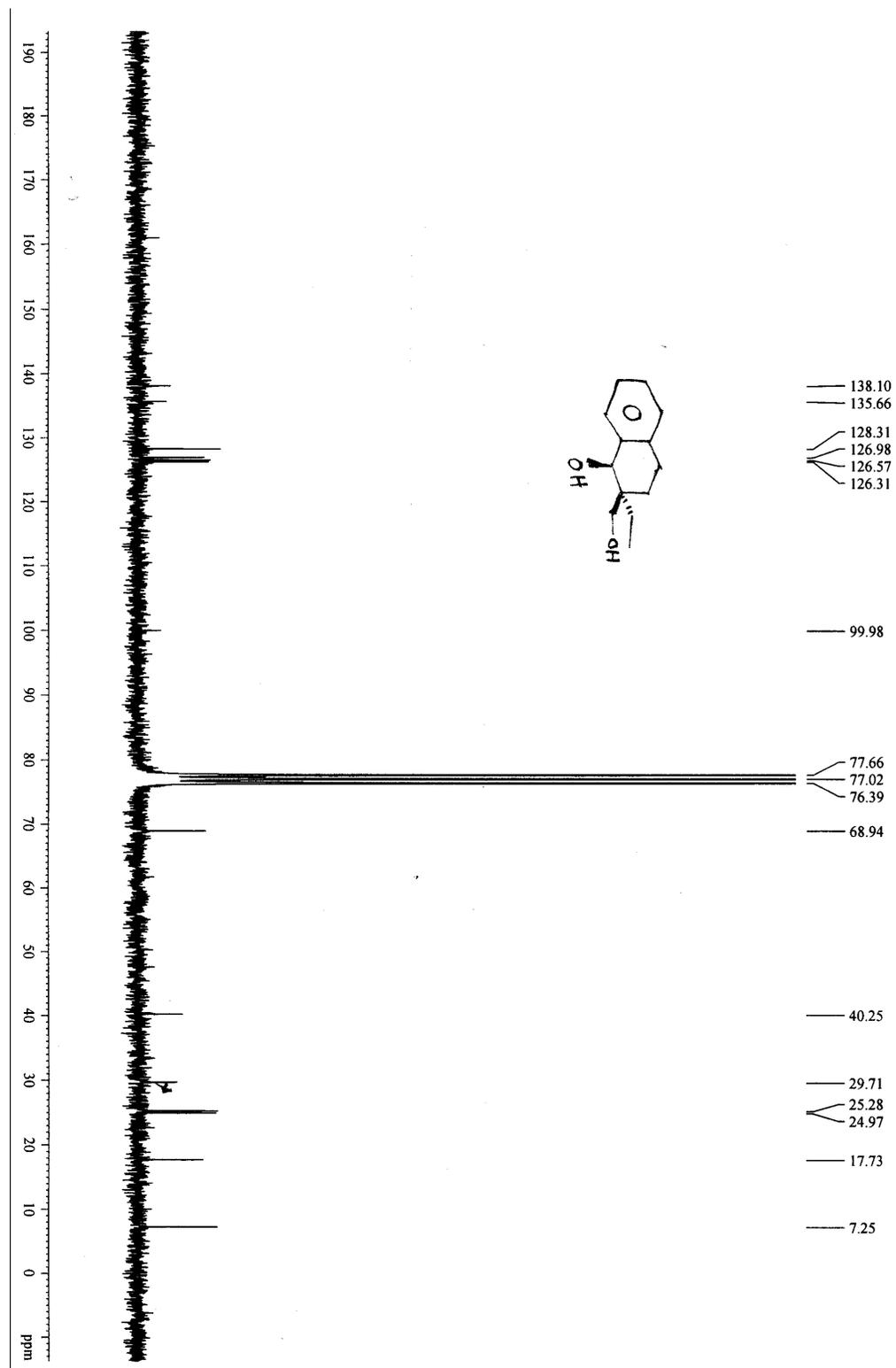


¹H NMR of compound ent-24



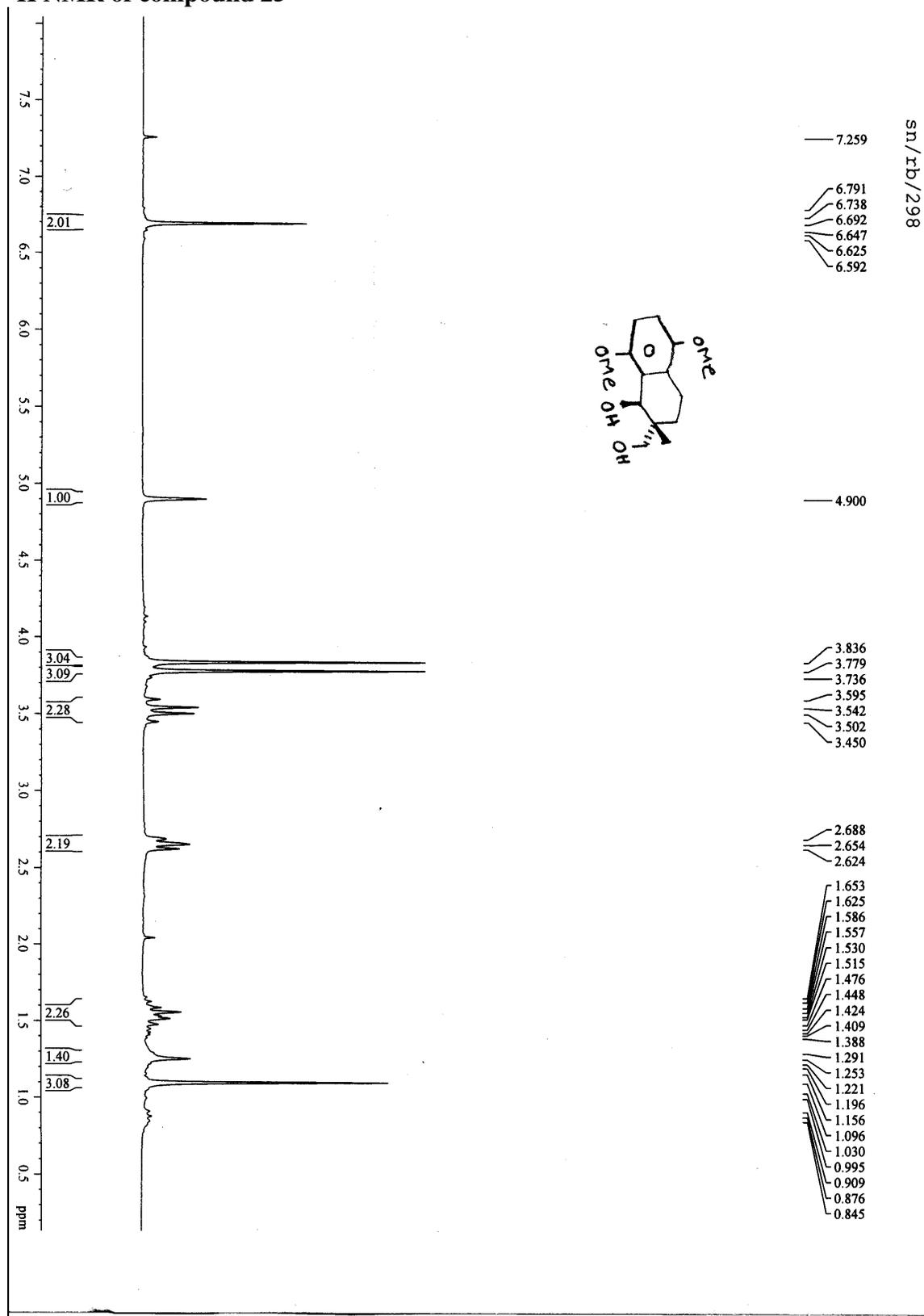
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^{13}C NMR of compound ent-24

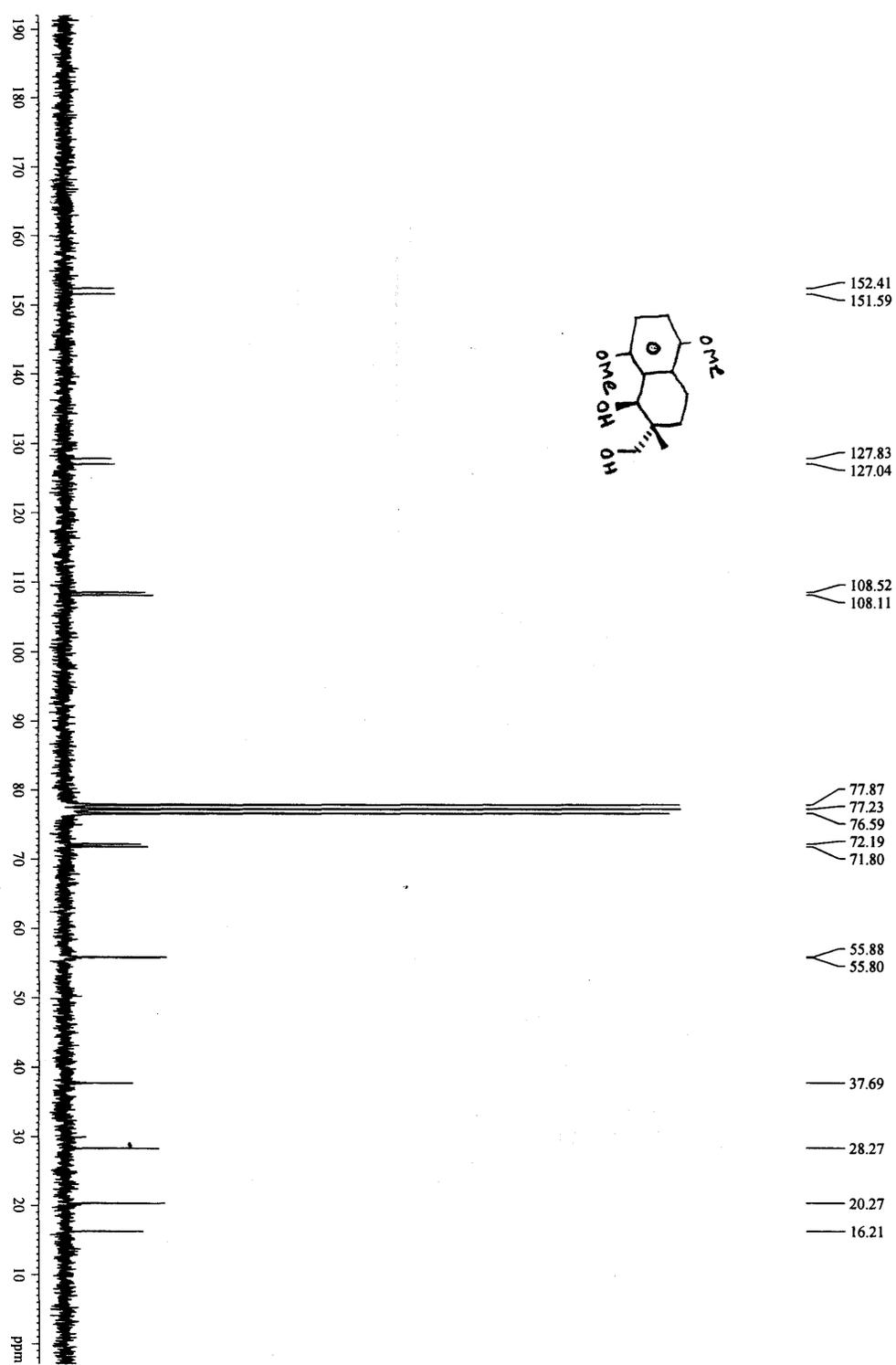


snc/rb/363

¹H NMR of compound 25

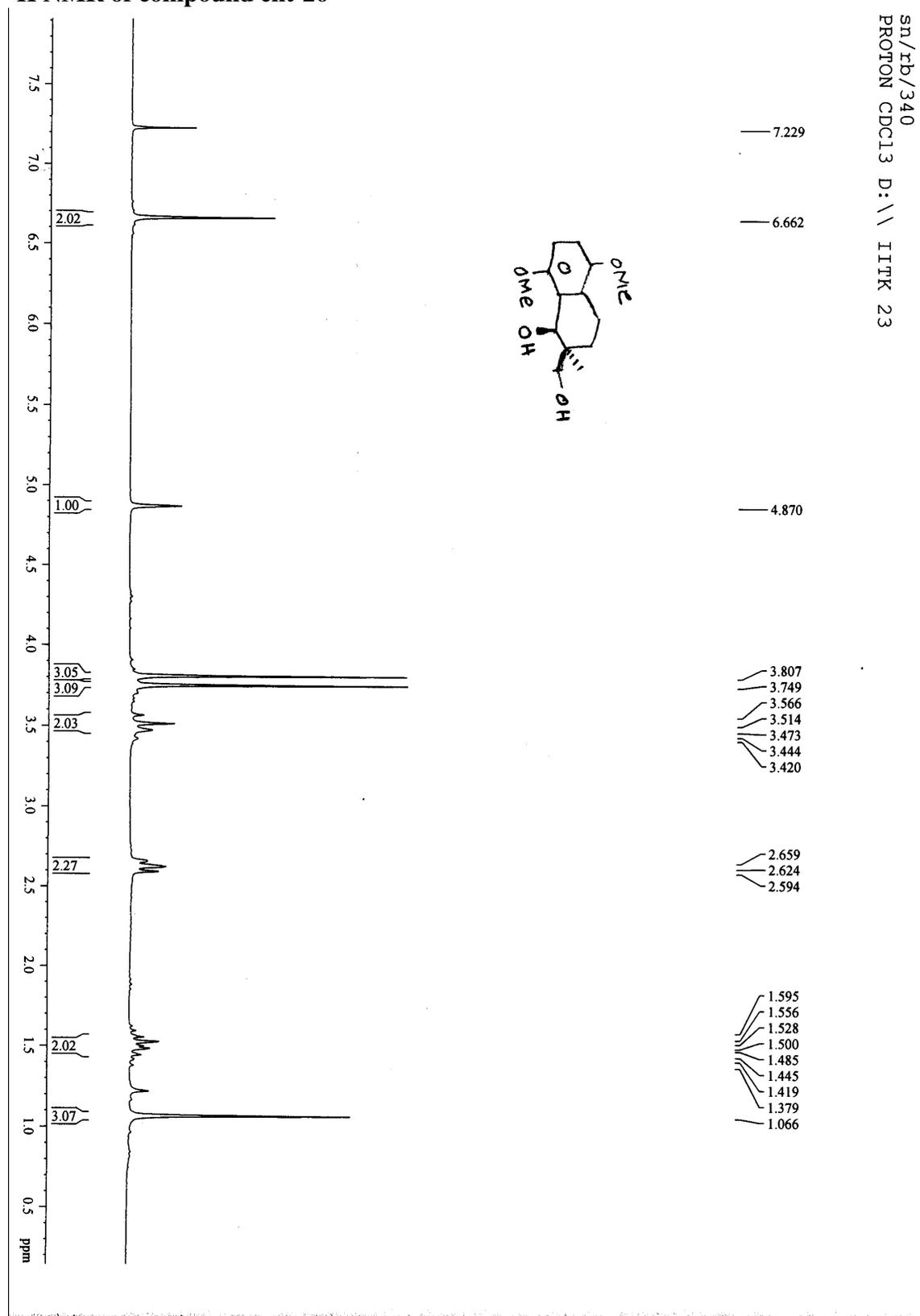


¹³C NMR of compound 25

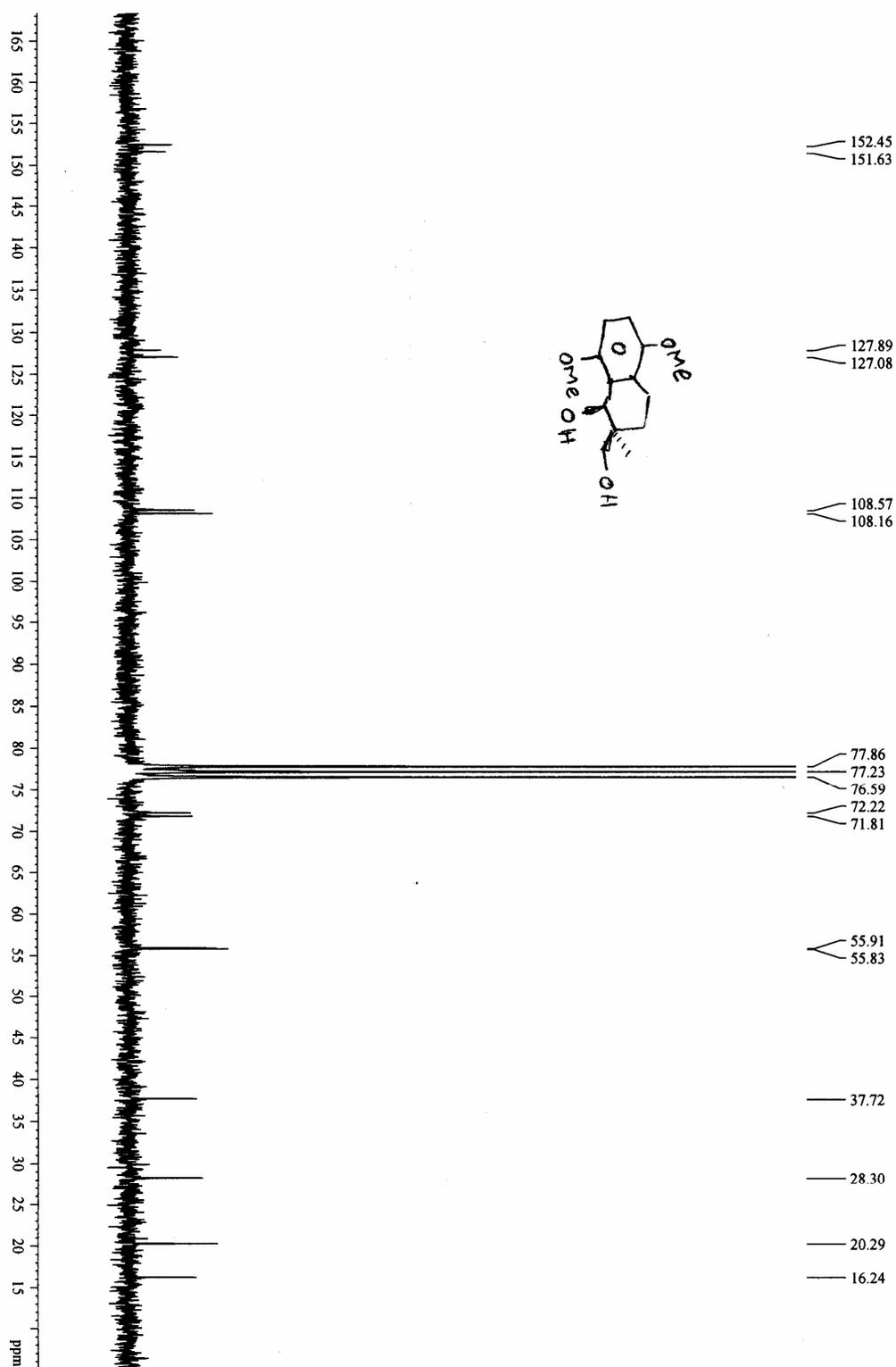


snc/rb/298
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^1H NMR of compound ent-26

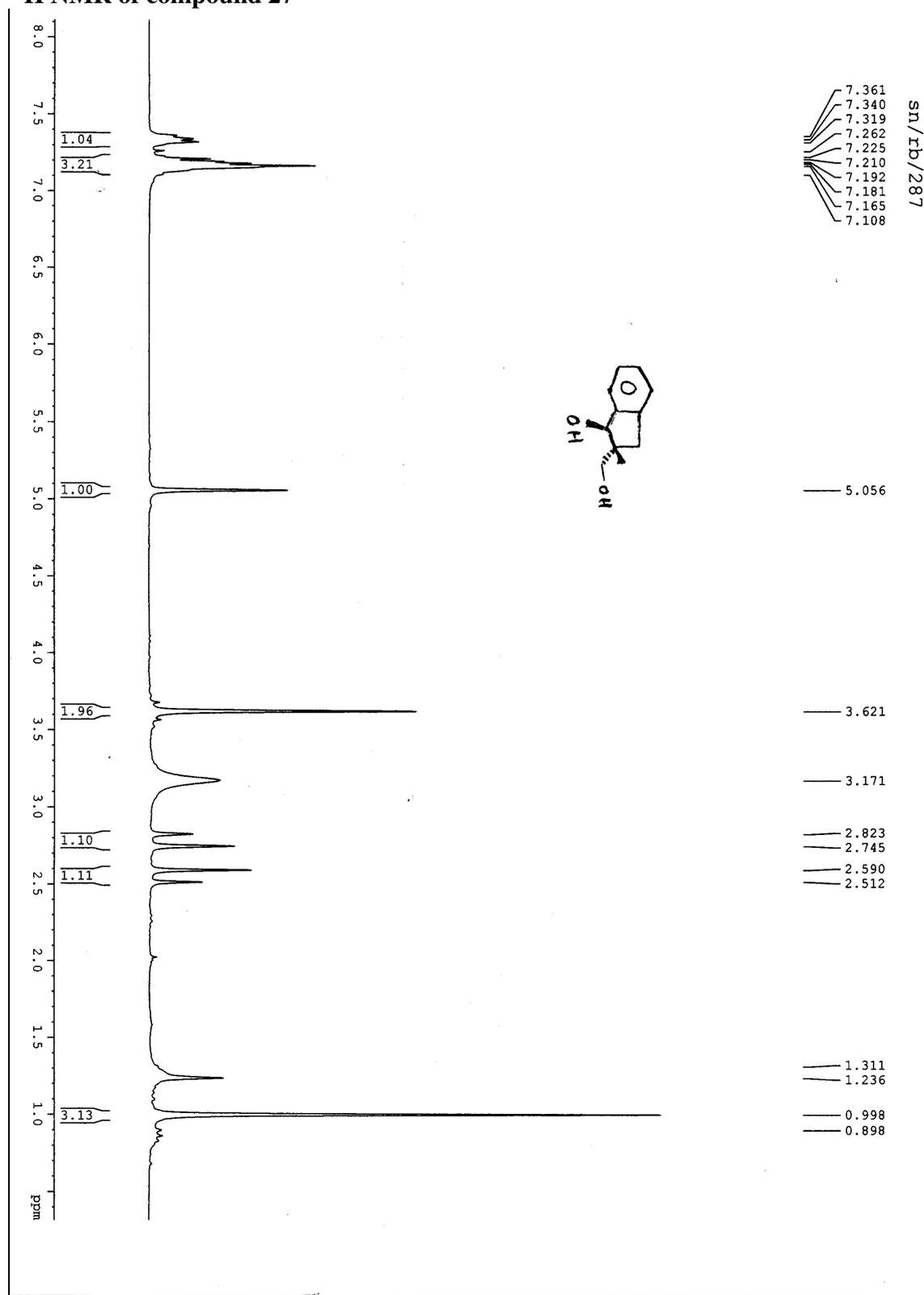


^{13}C NMR of compound ent-26



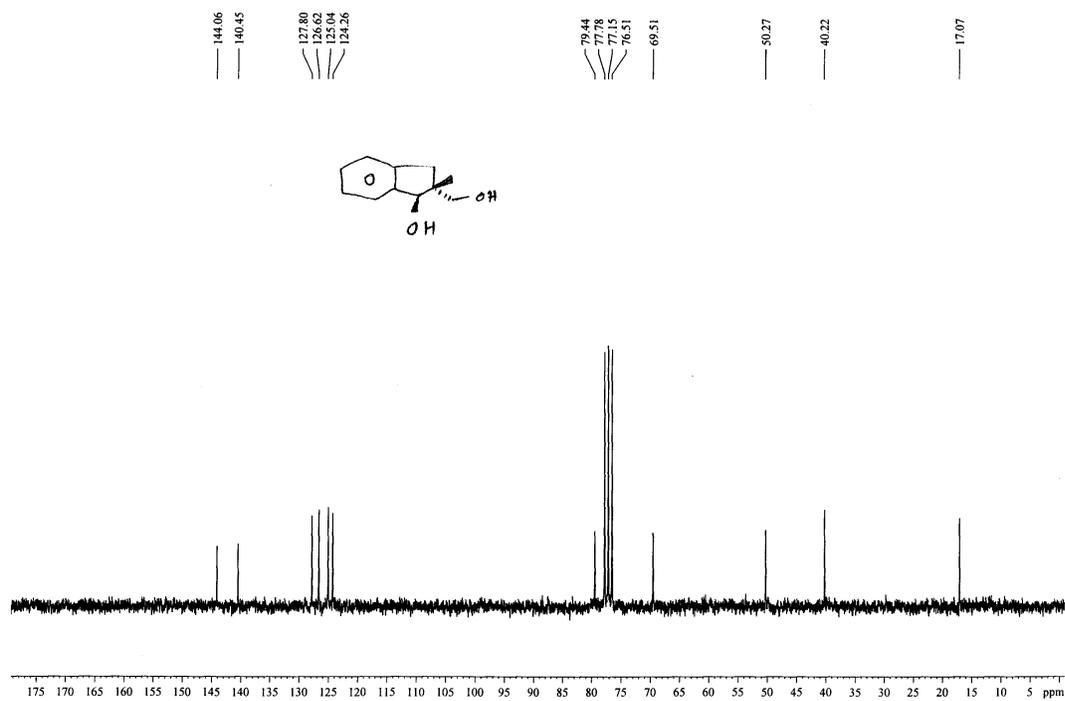
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¹H NMR of compound 27

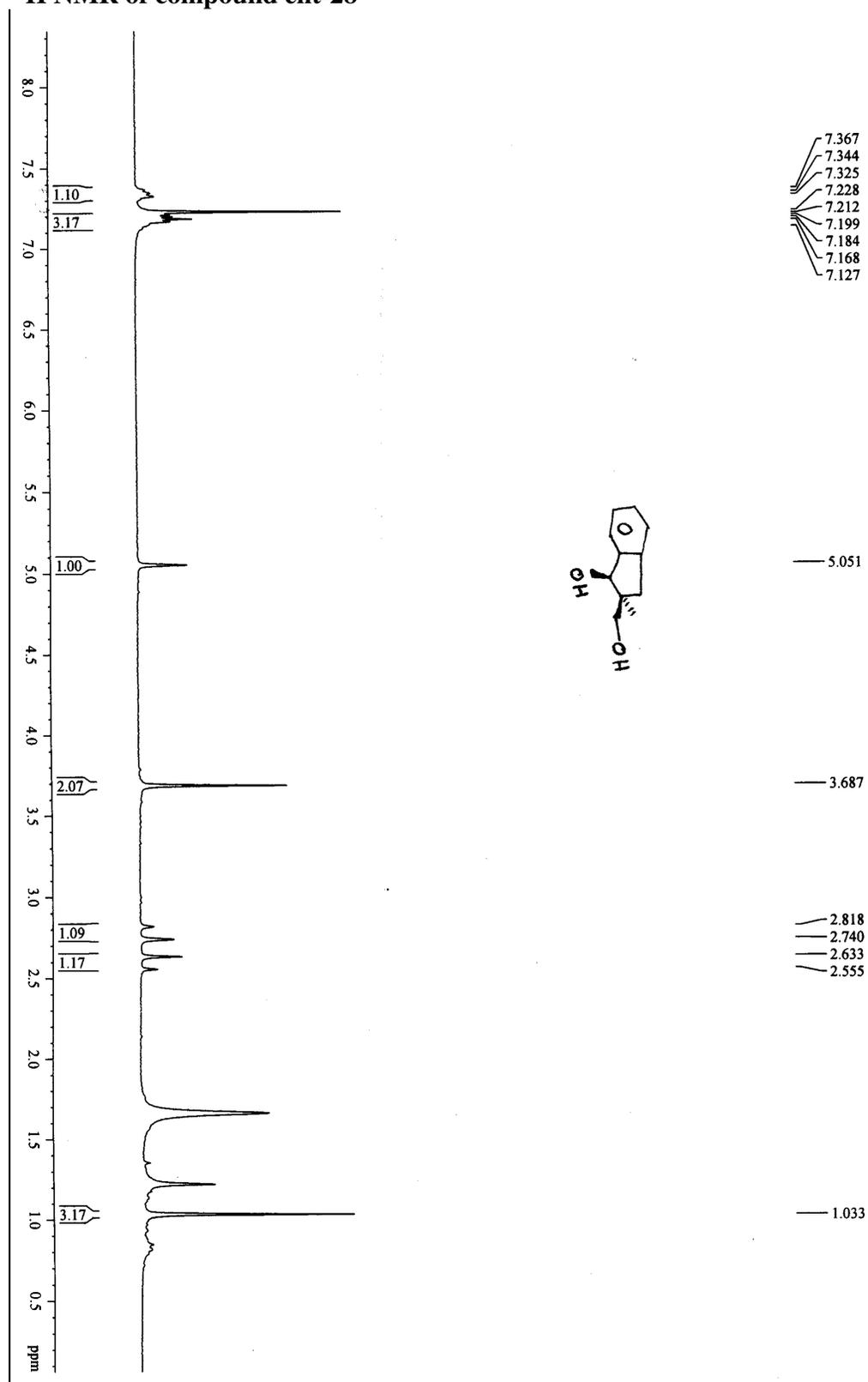


¹³C NMR of compound 27

snc/rb/287
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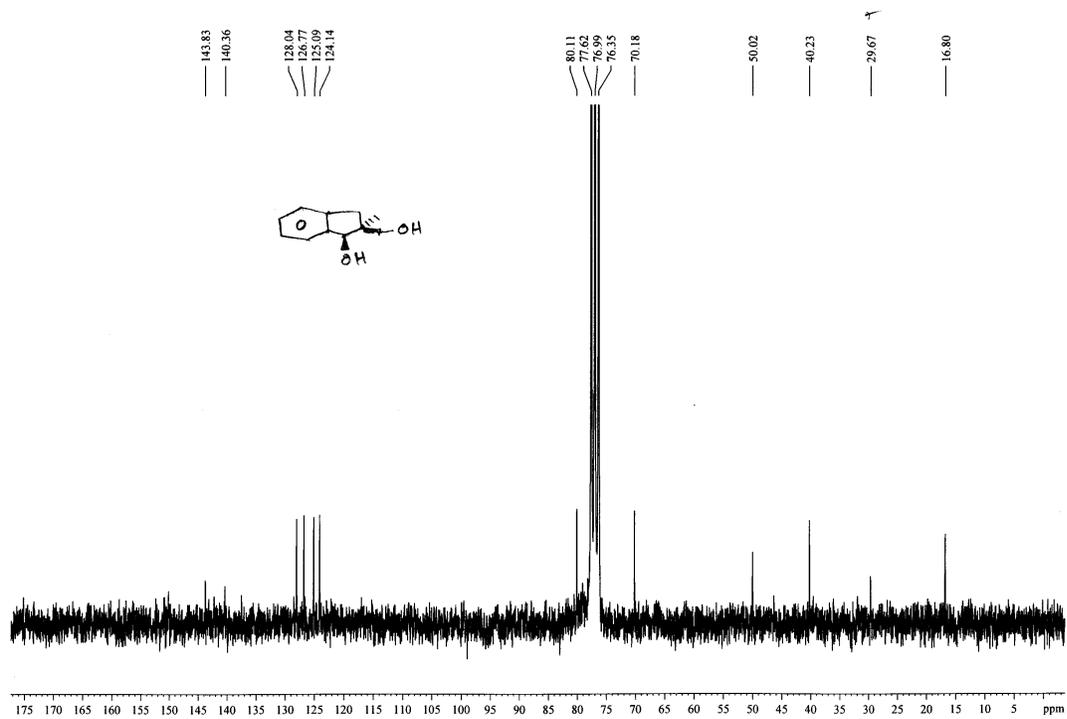
¹H NMR of compound ent-28



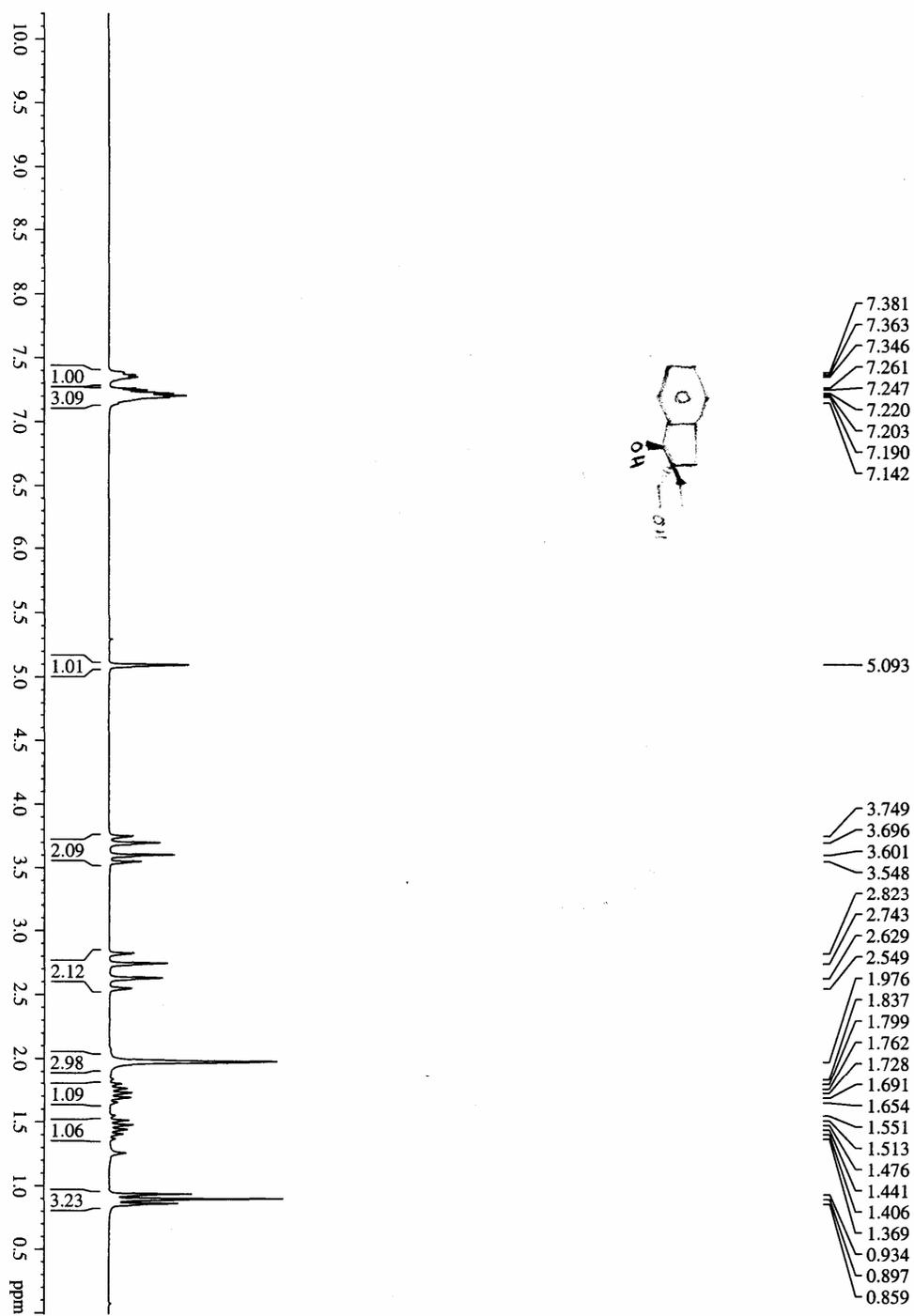
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¹³C NMR of compound ent-28

sn /rb/339

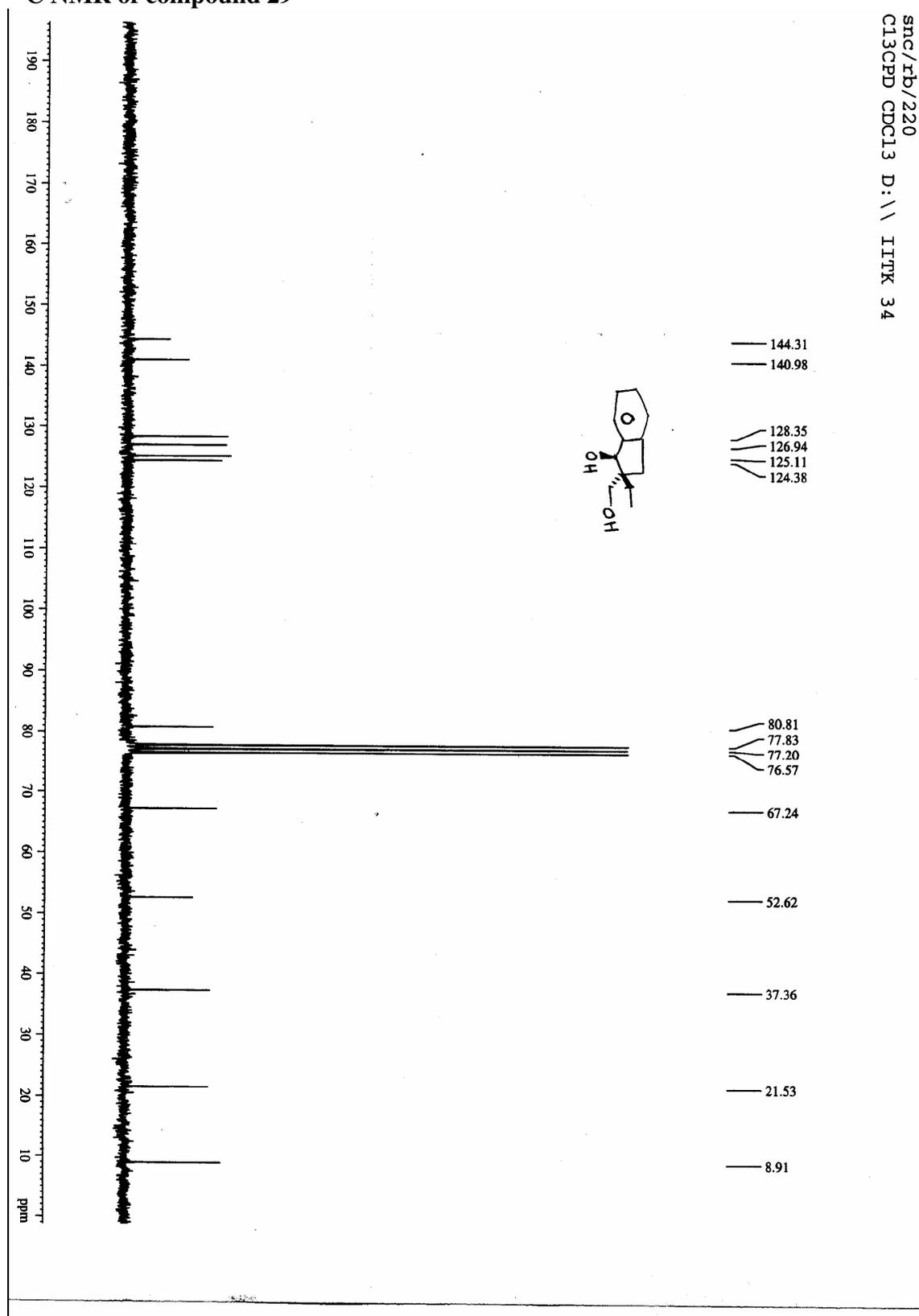


¹H NMR of compound 29

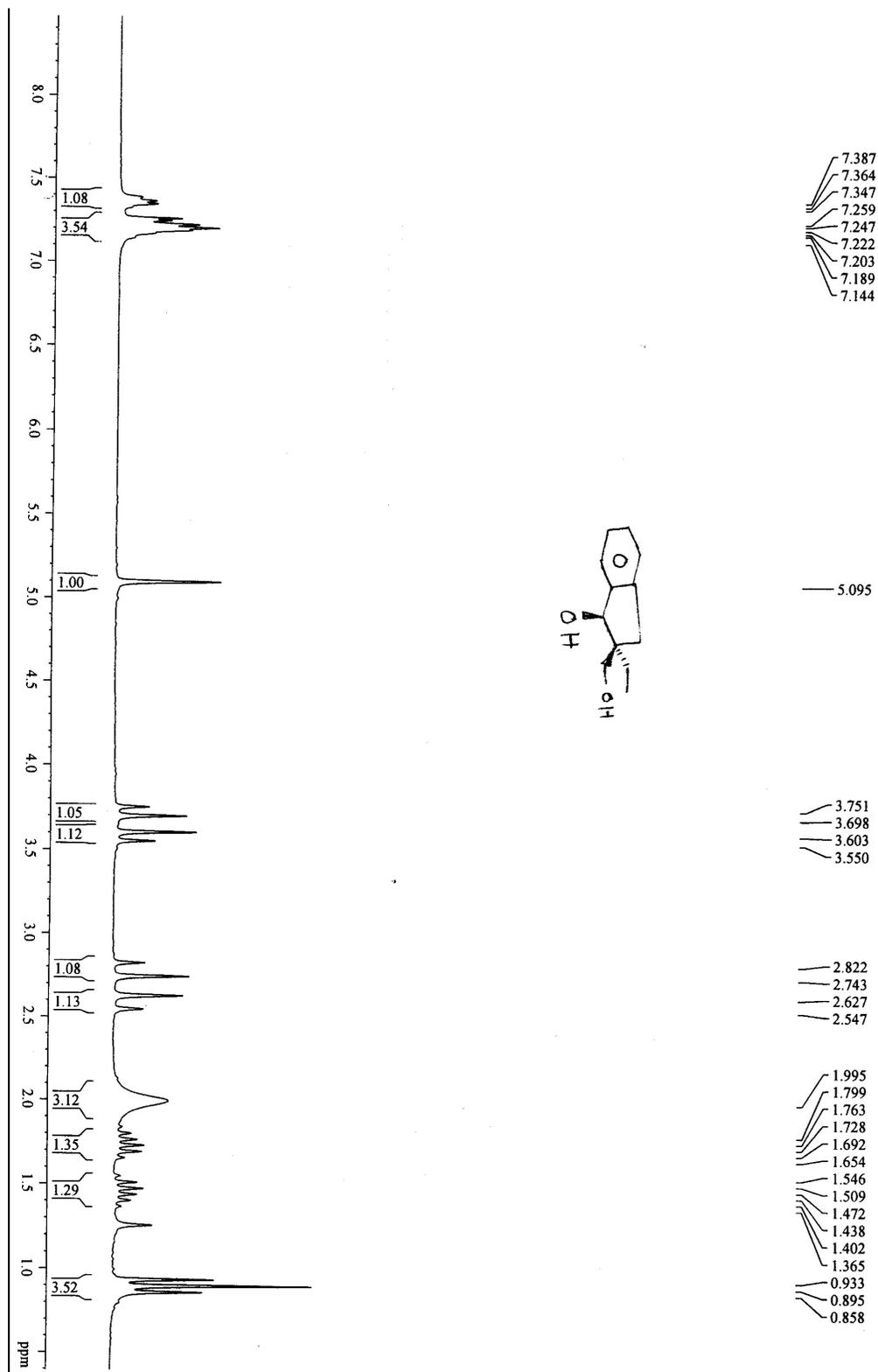


sm/rb/220

¹³C NMR of compound 29

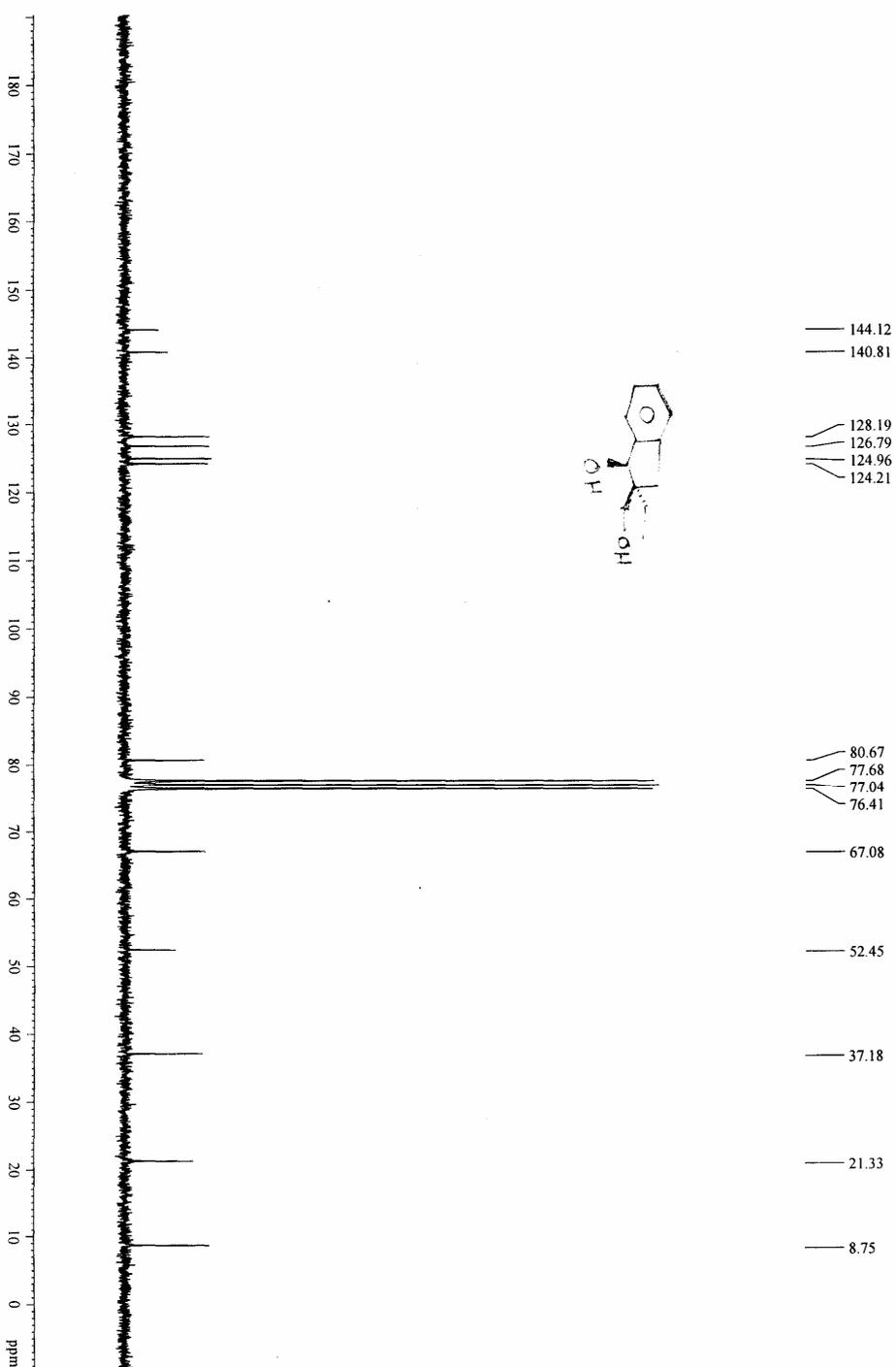


¹H NMR of compound ent-30



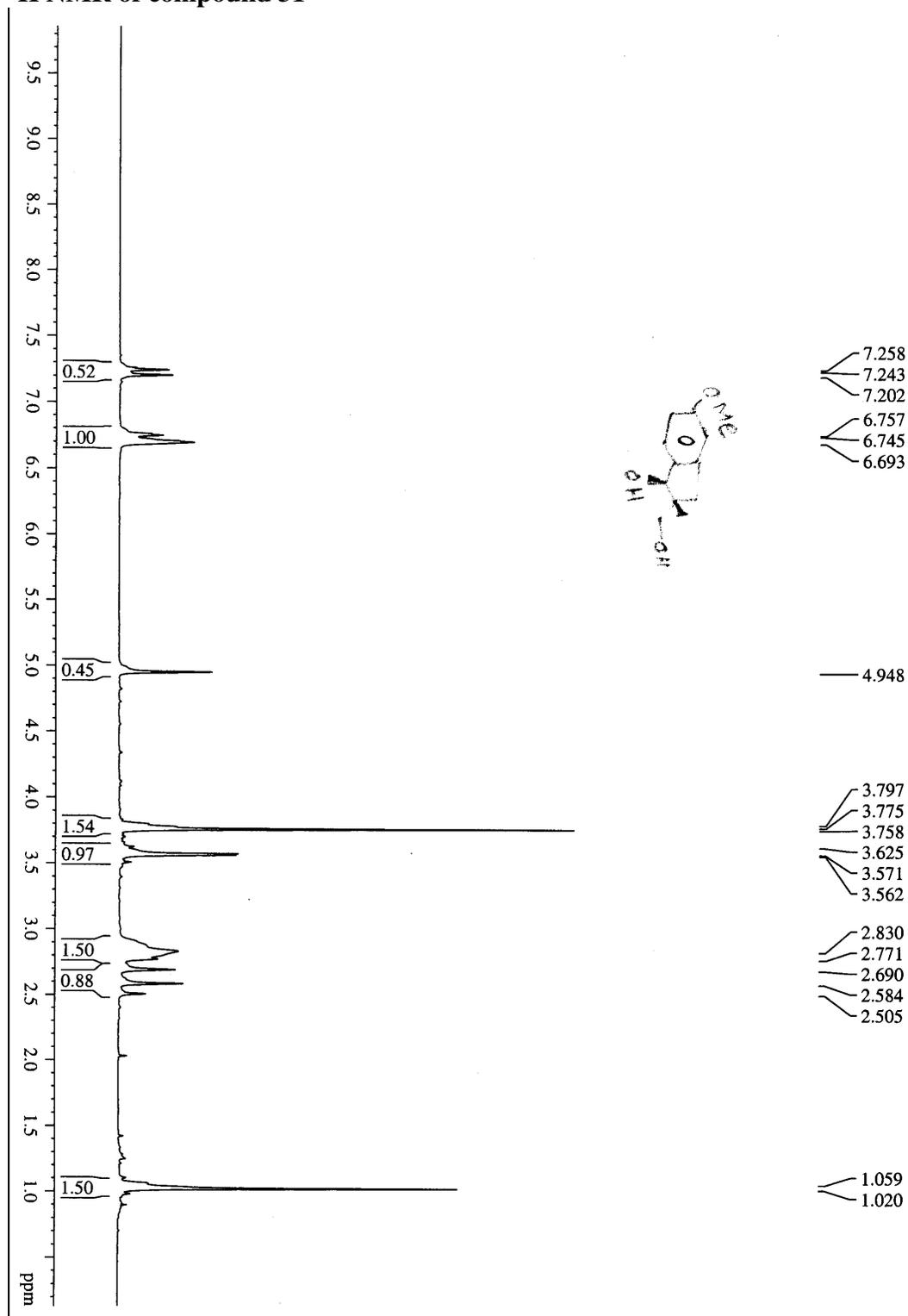
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^{13}C NMR of compound ent-30



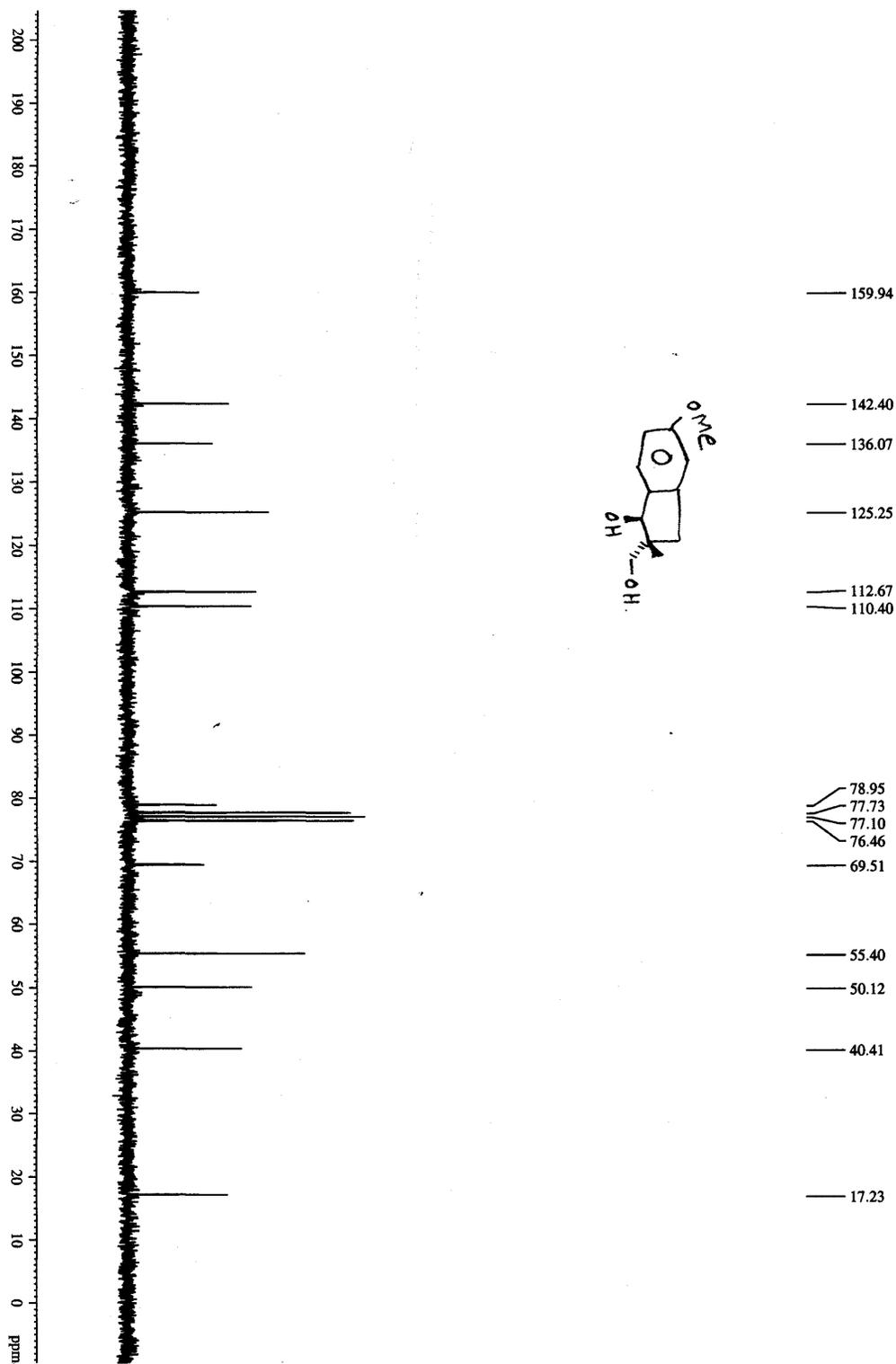
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¹H NMR of compound 31



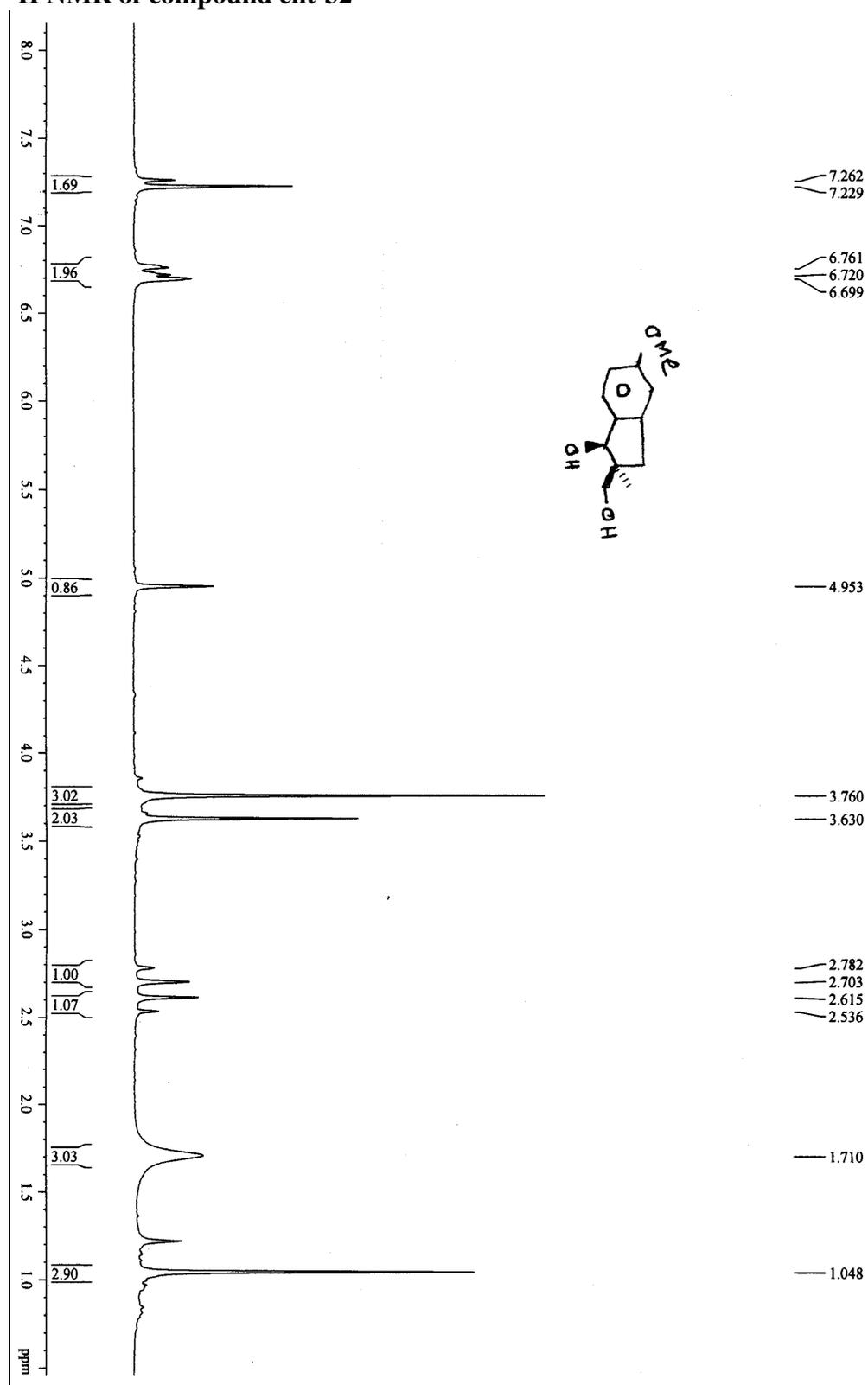
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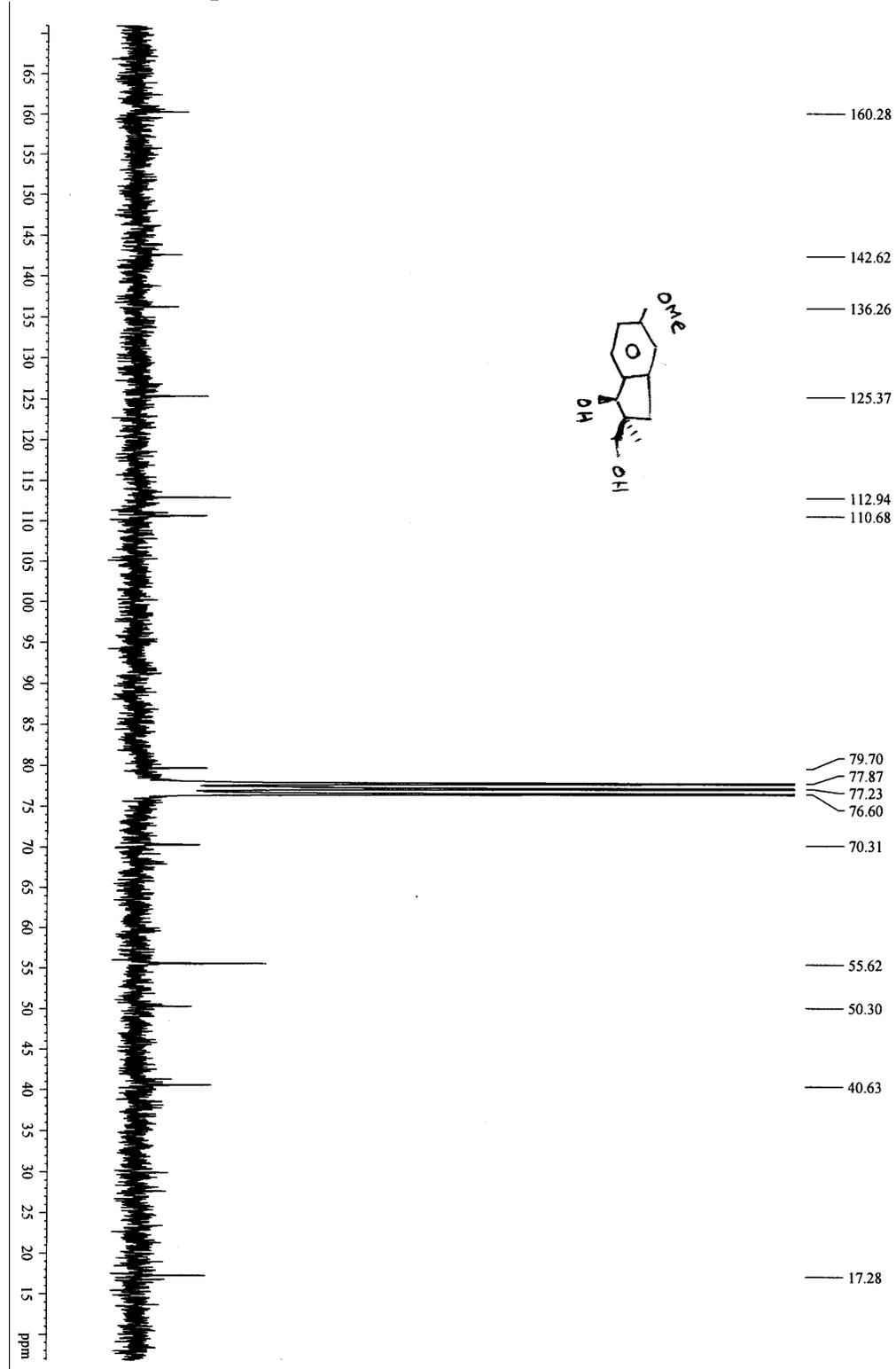
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C13CPD CDCl3 D: \\ IITK 2

¹H NMR of compound ent-32



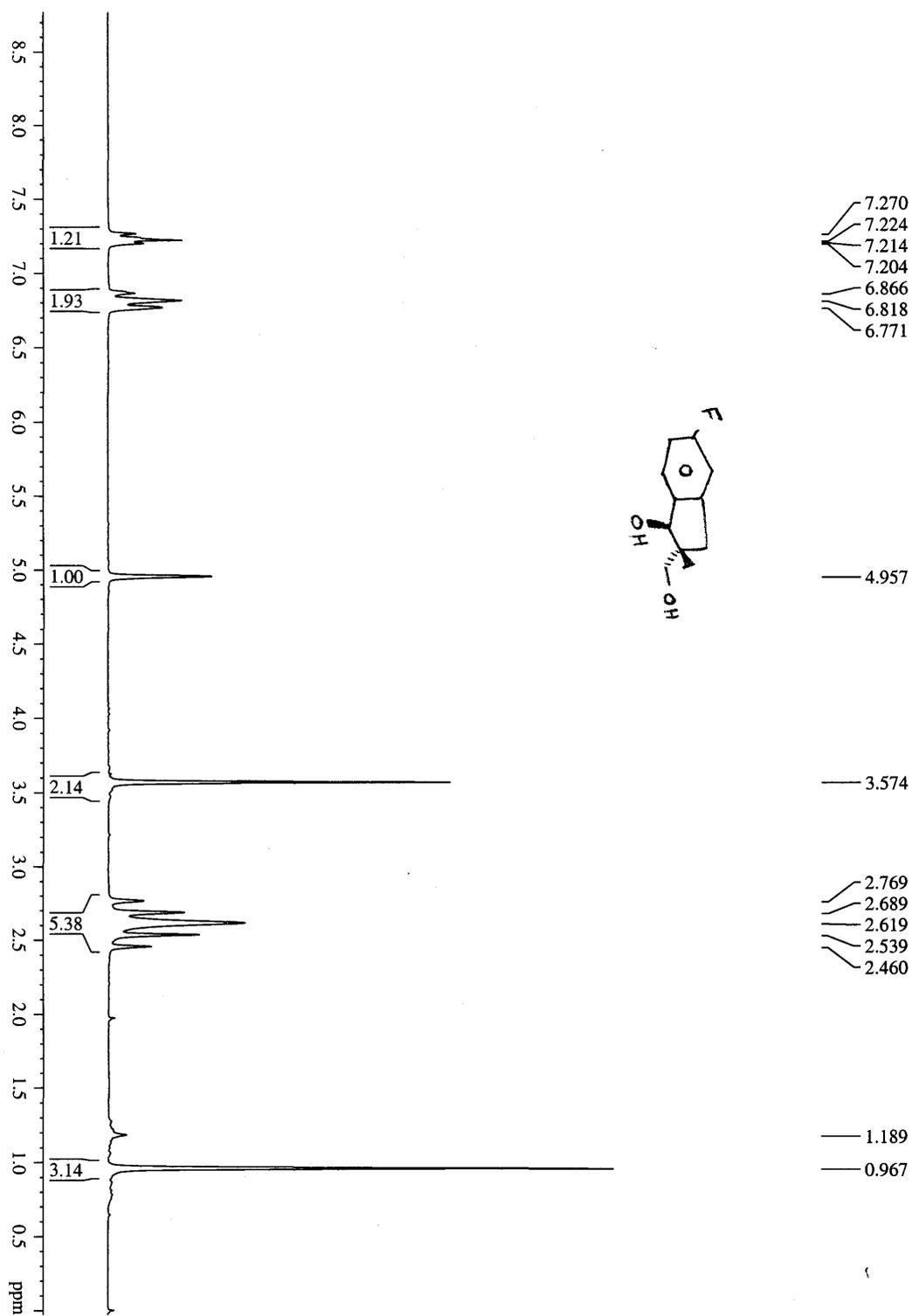
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^{13}C NMR of compound ent-32



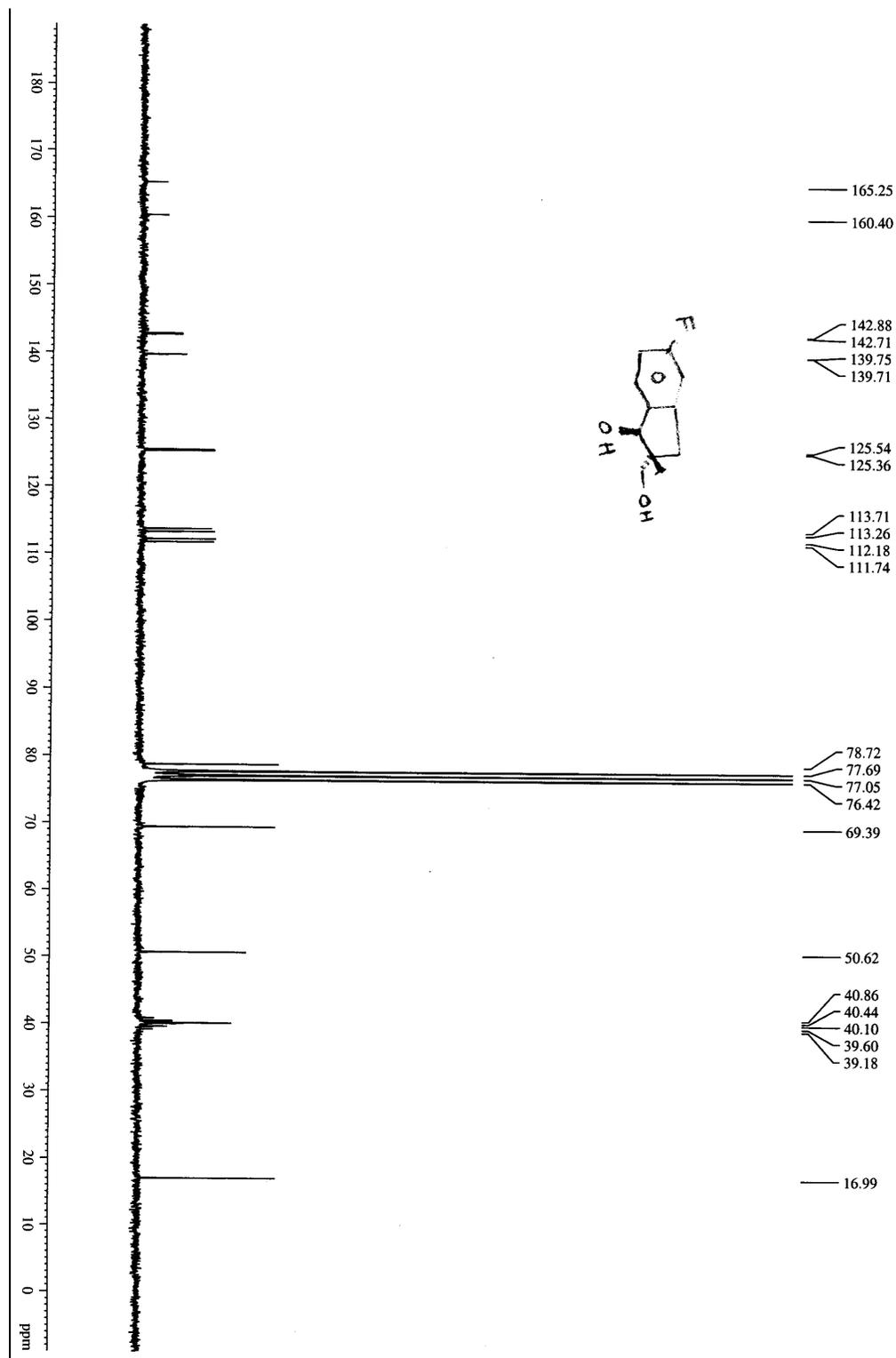
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C13CPD CDCl3 D:\ IITK 2

¹H NMR of compound 33



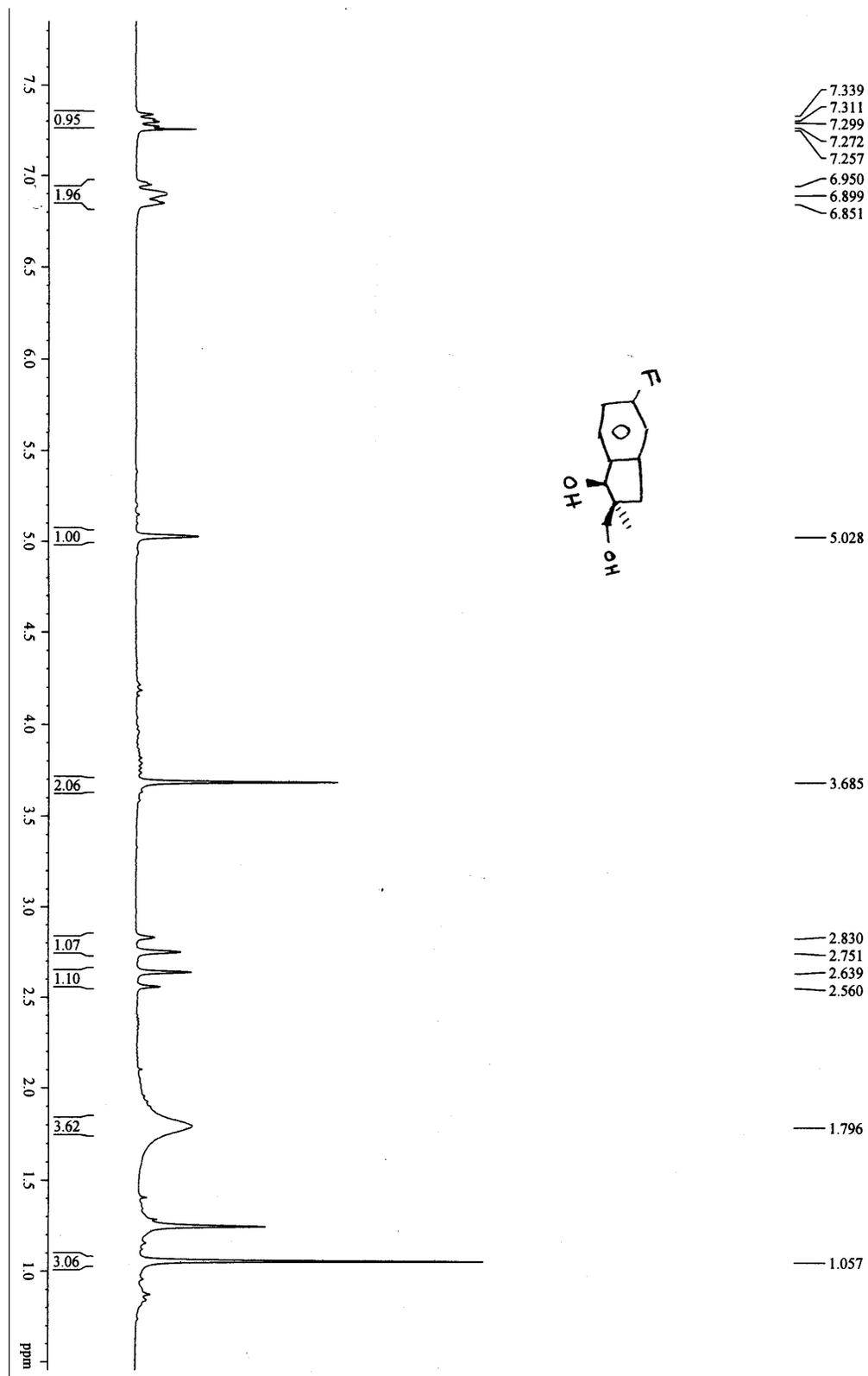
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^{13}C NMR of compound 33



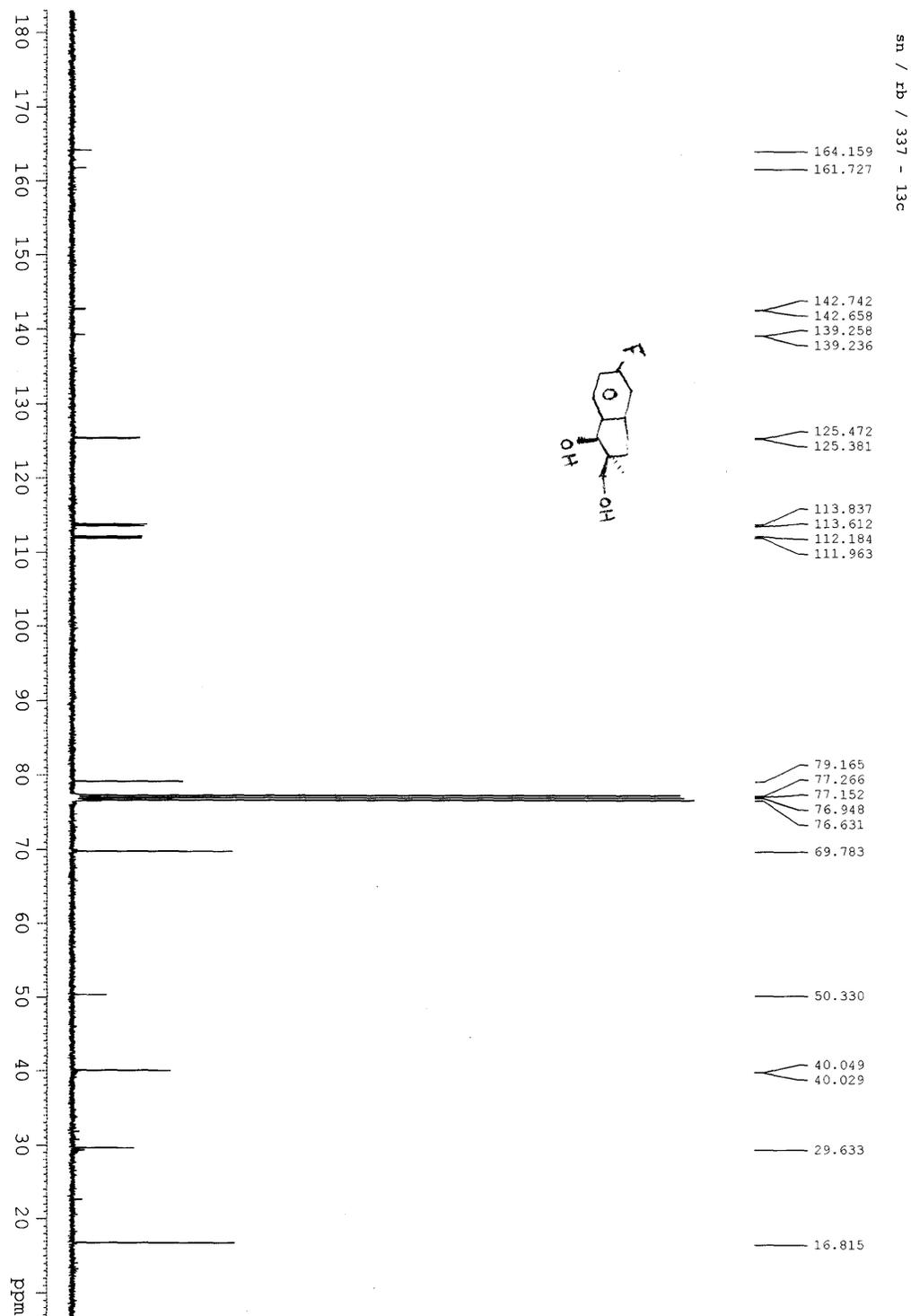
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¹H NMR of compound ent-34

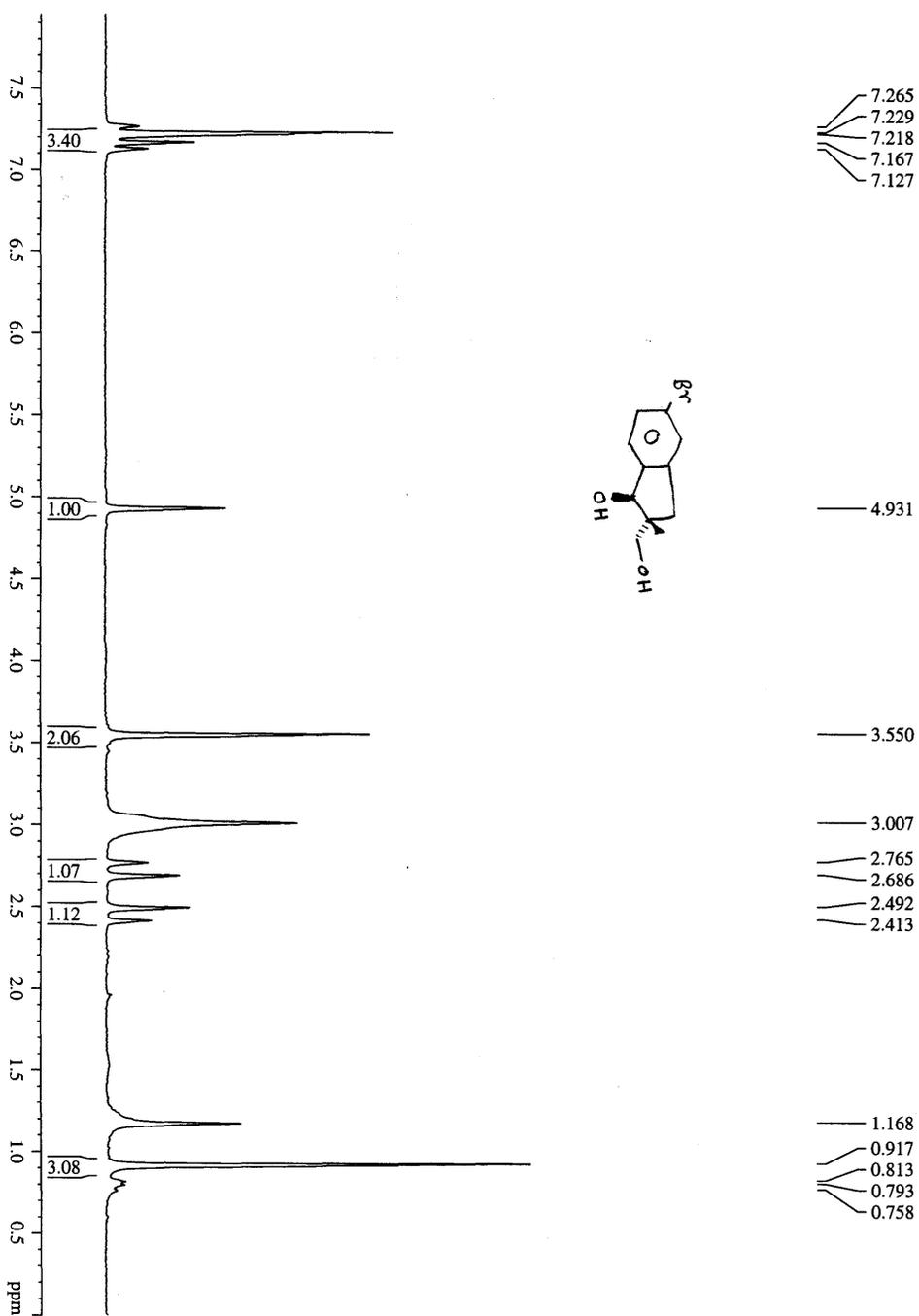


sn/rb/337
PROTON CDCl3 D:\\ IITK 23

^{13}C NMR of compound ent-34

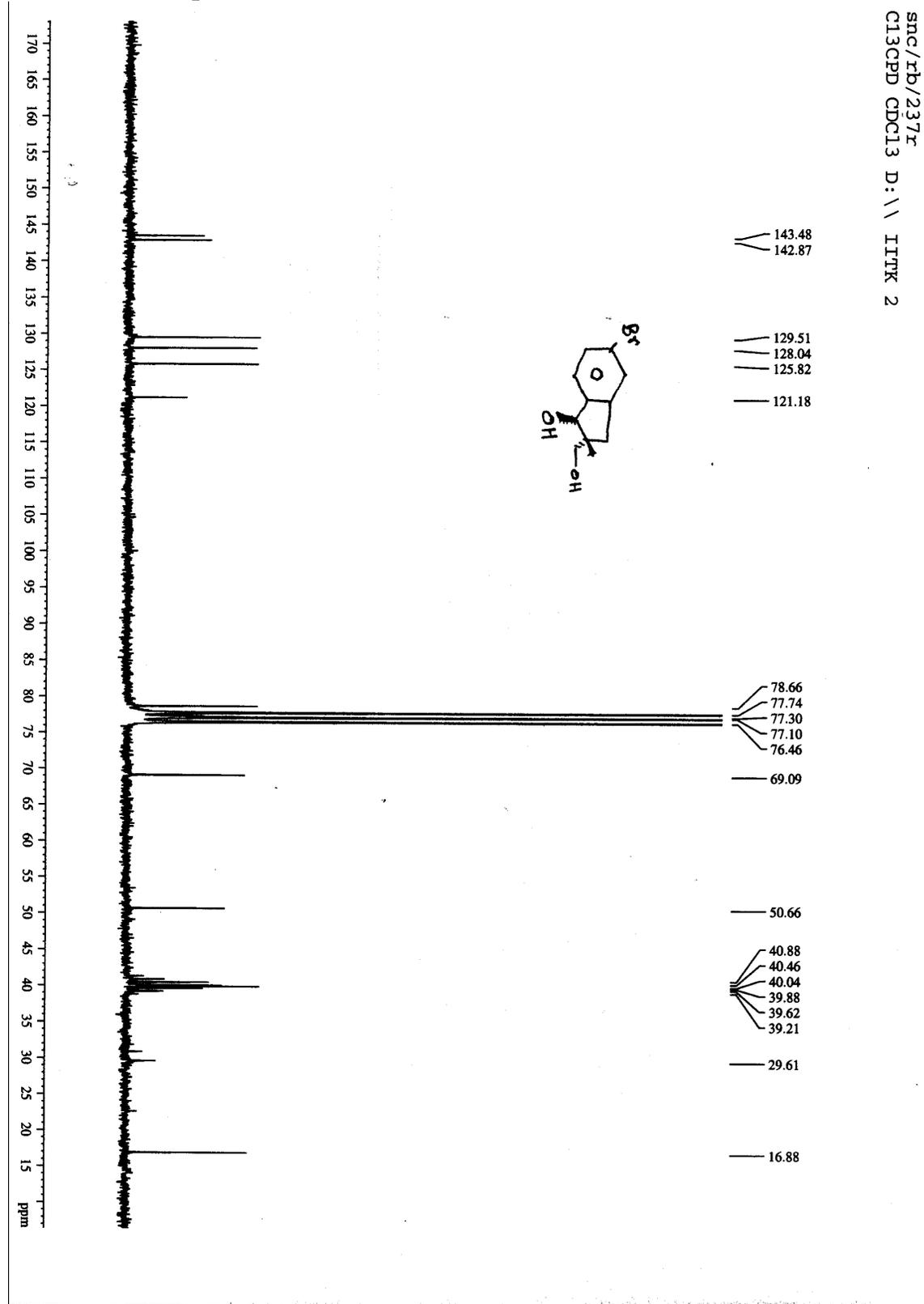


^1H NMR of compound 35

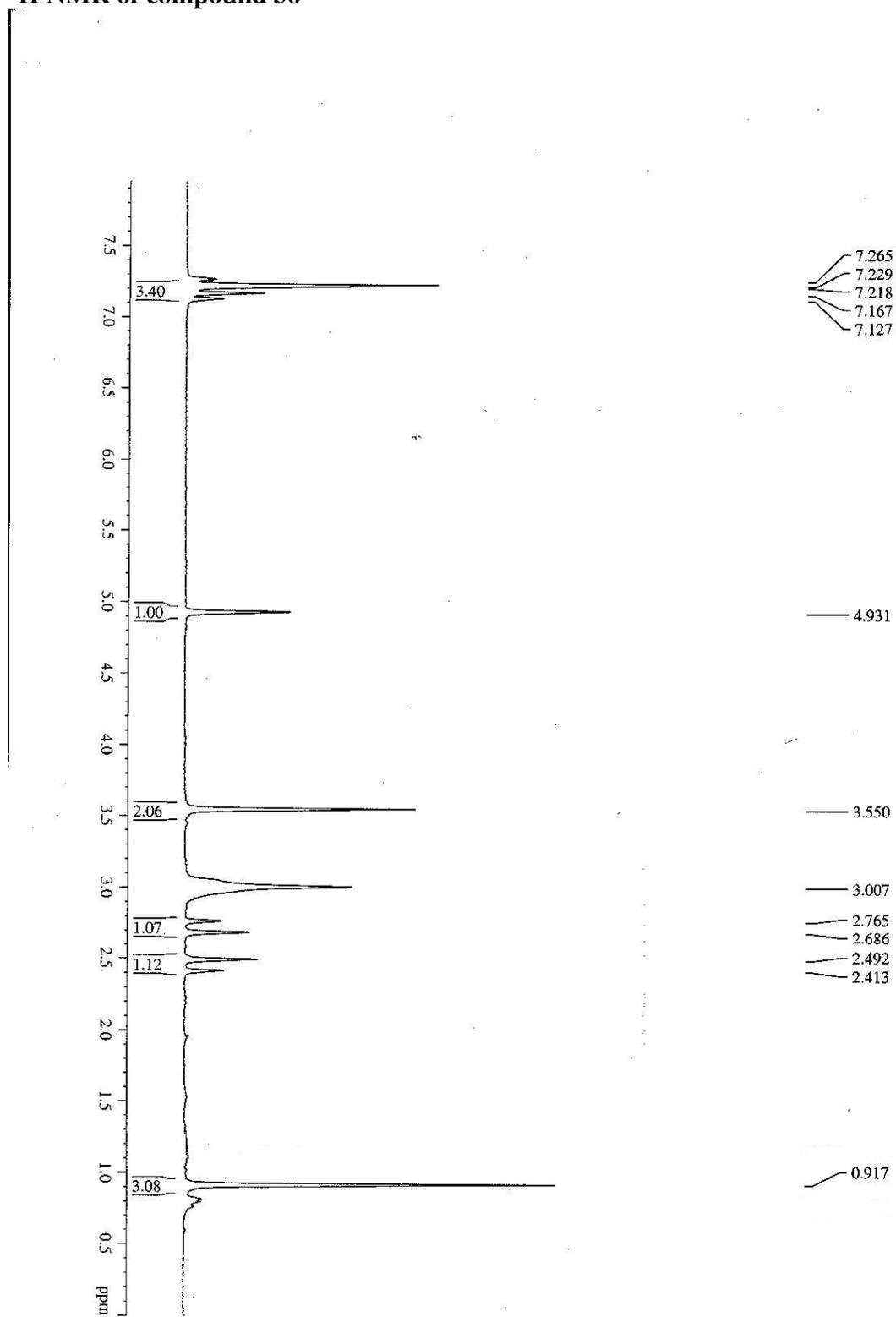


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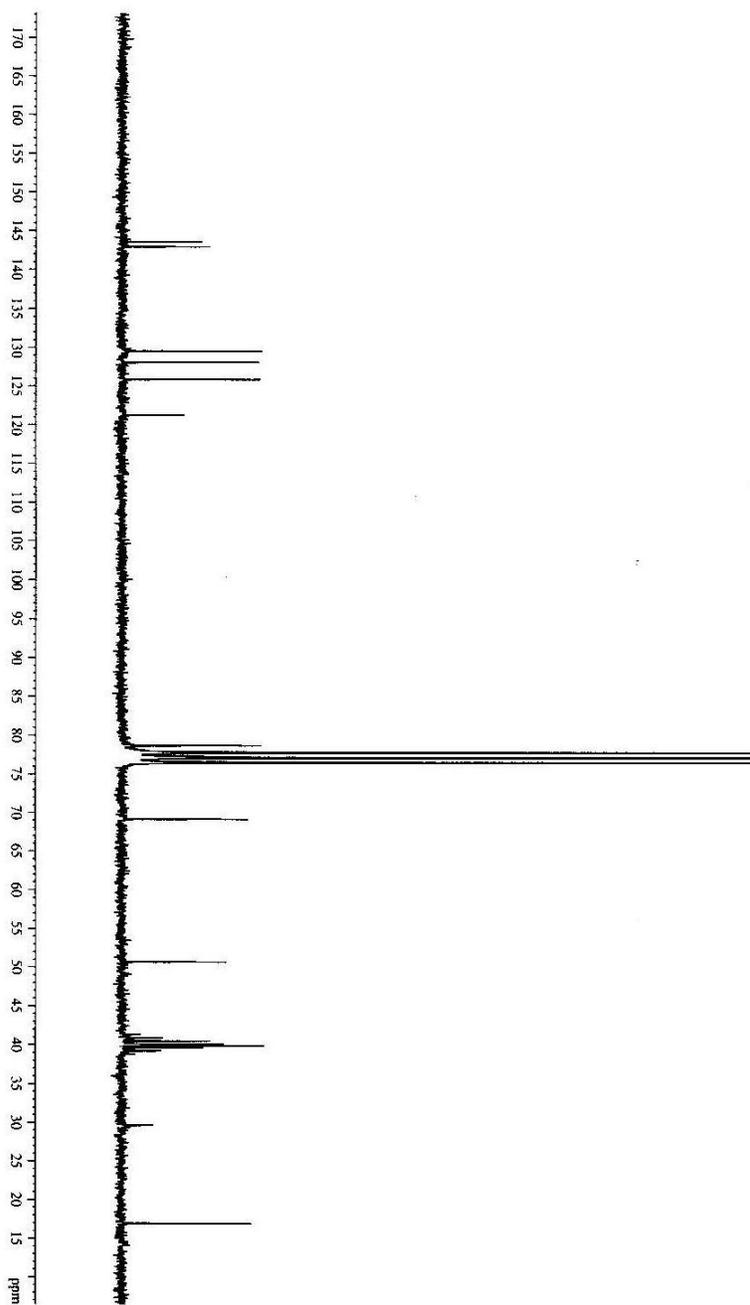
¹³C NMR of compound 35



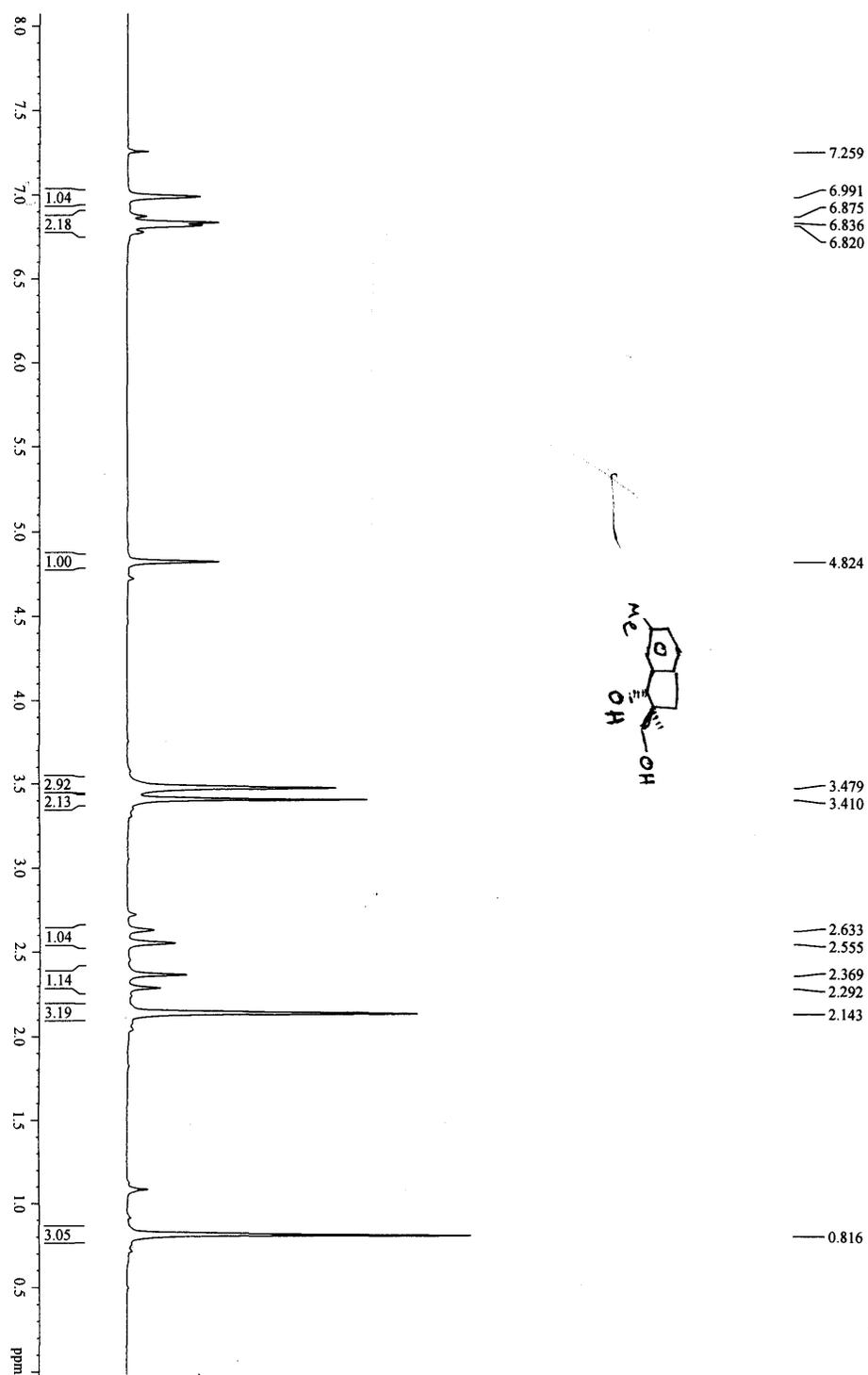
^1H NMR of compound 36



^{13}C NMR of compound 36

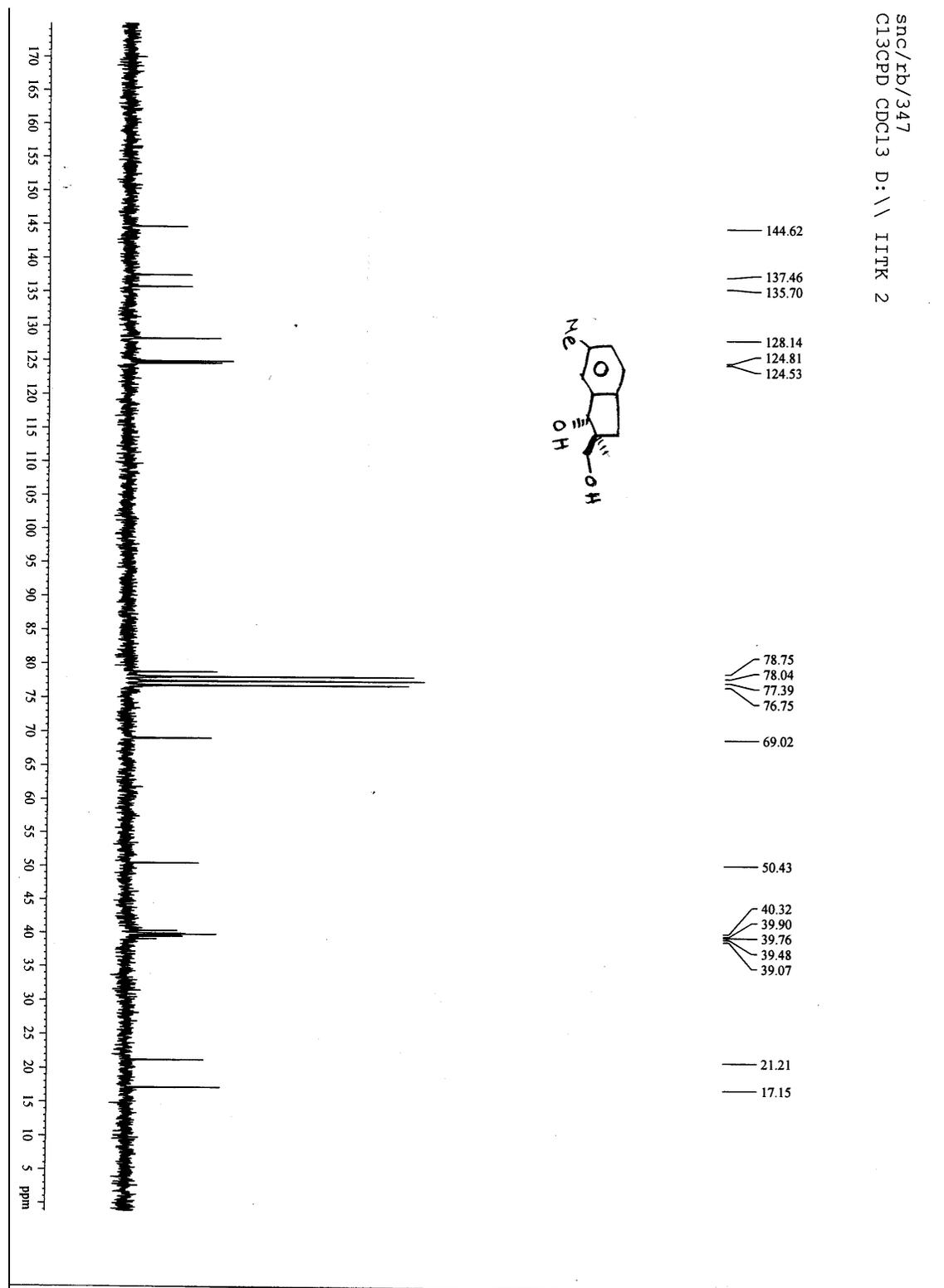


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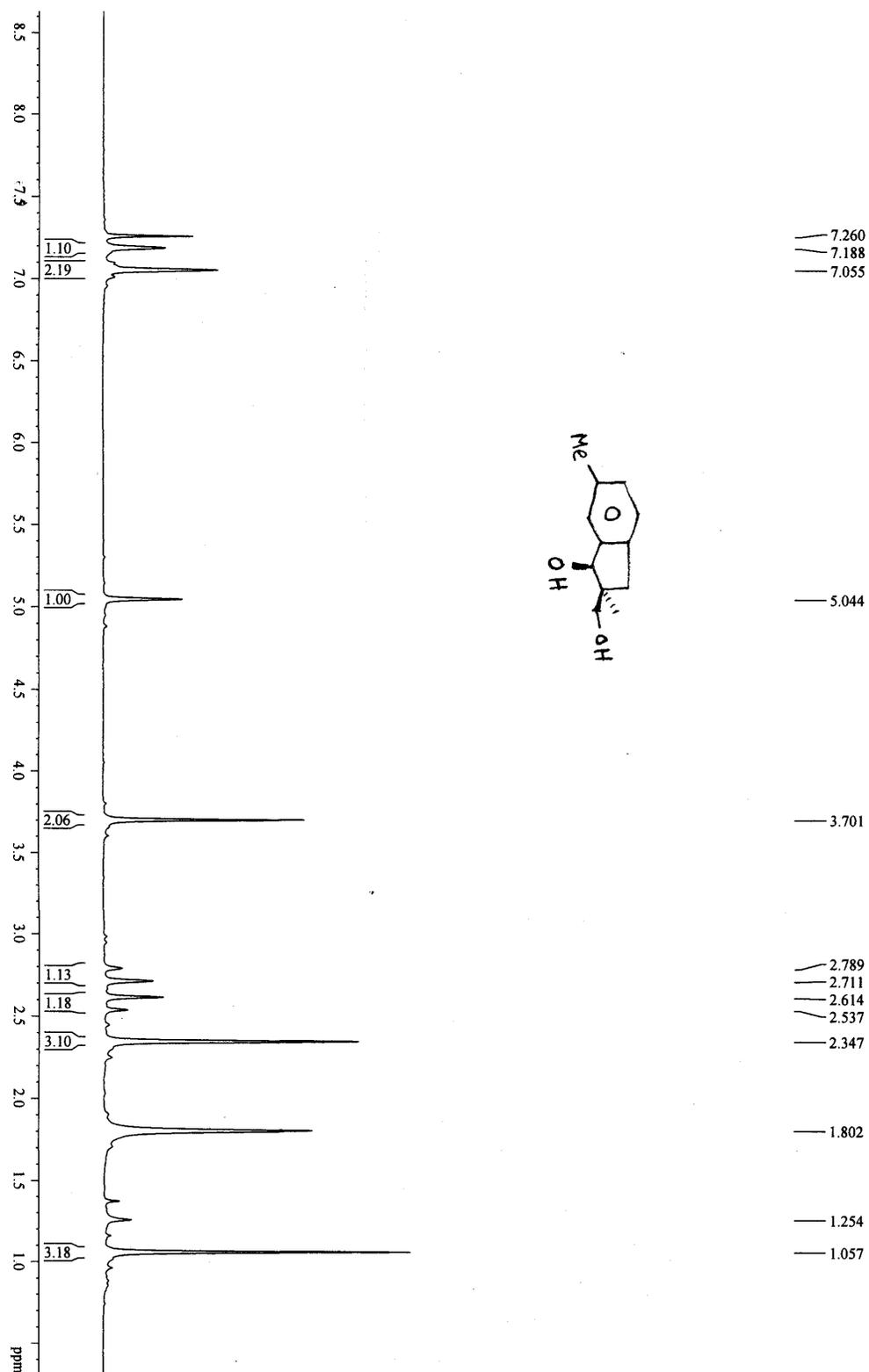


sn / rb / 347

^{13}C NMR of compound ent-37

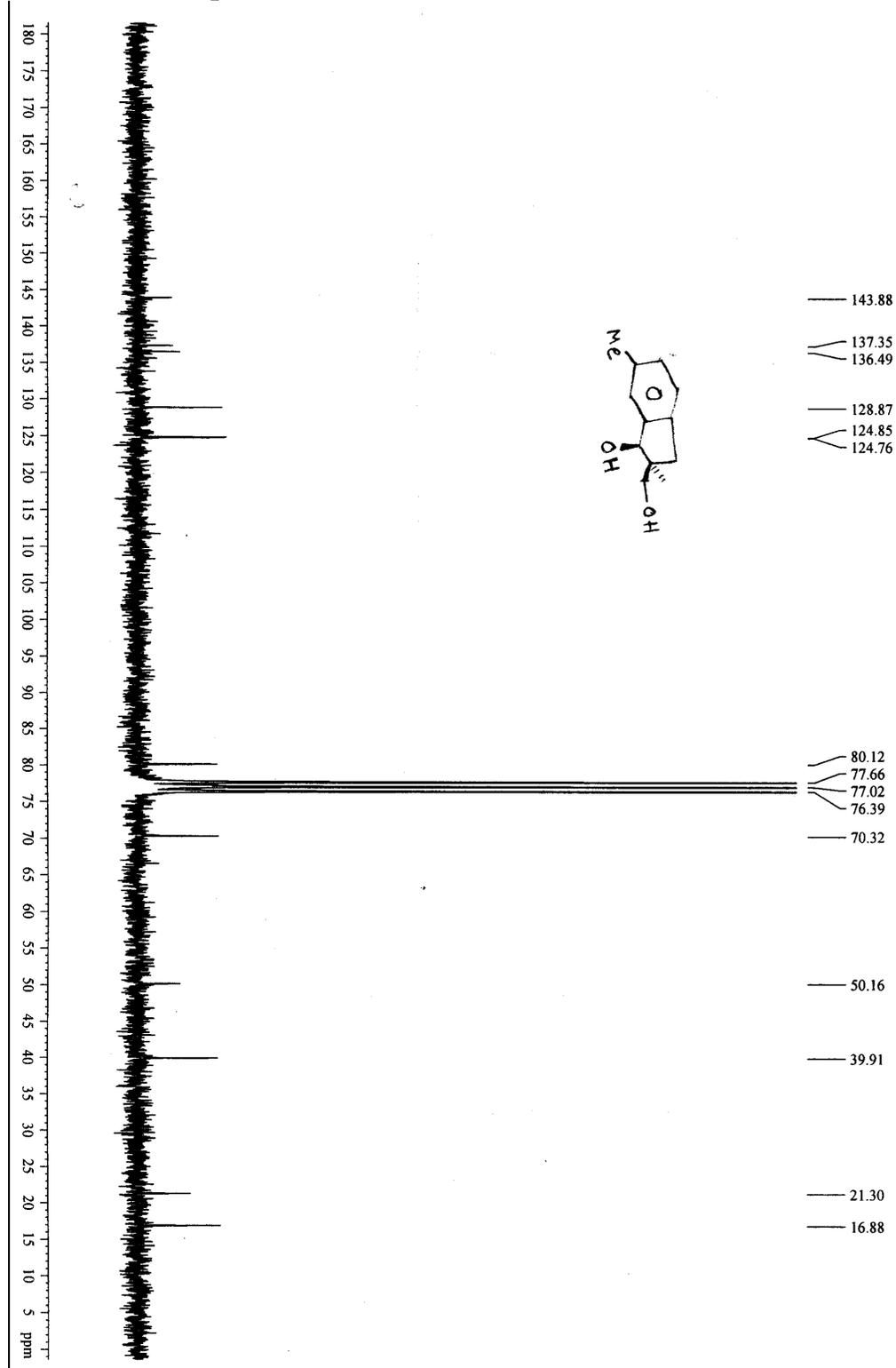


¹H NMR of compound ent-38



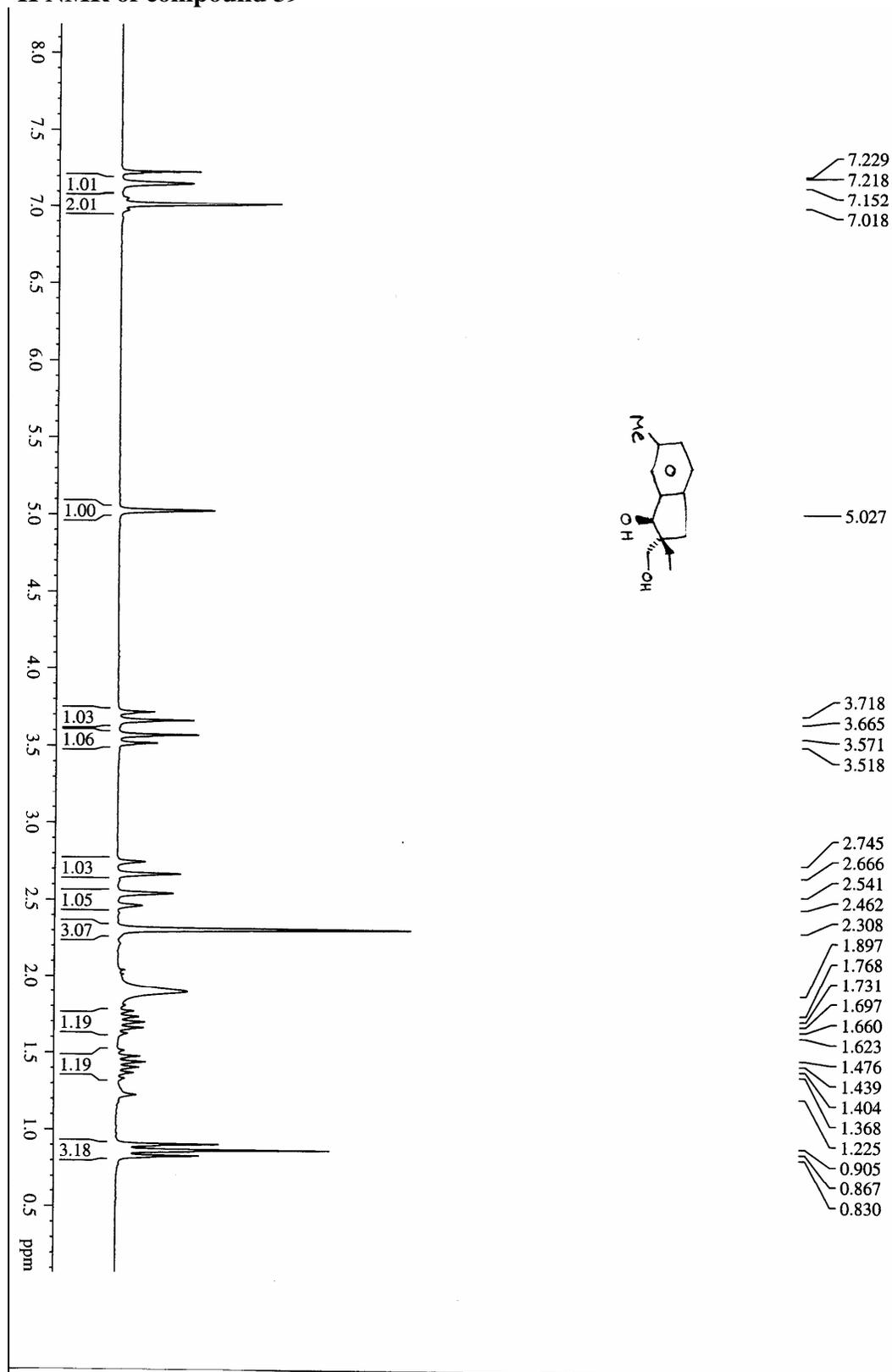
sn / rb / 348

^{13}C NMR of compound ent-38



snc/tp/348
C13CPD CDCl3 D:\ IITK 2

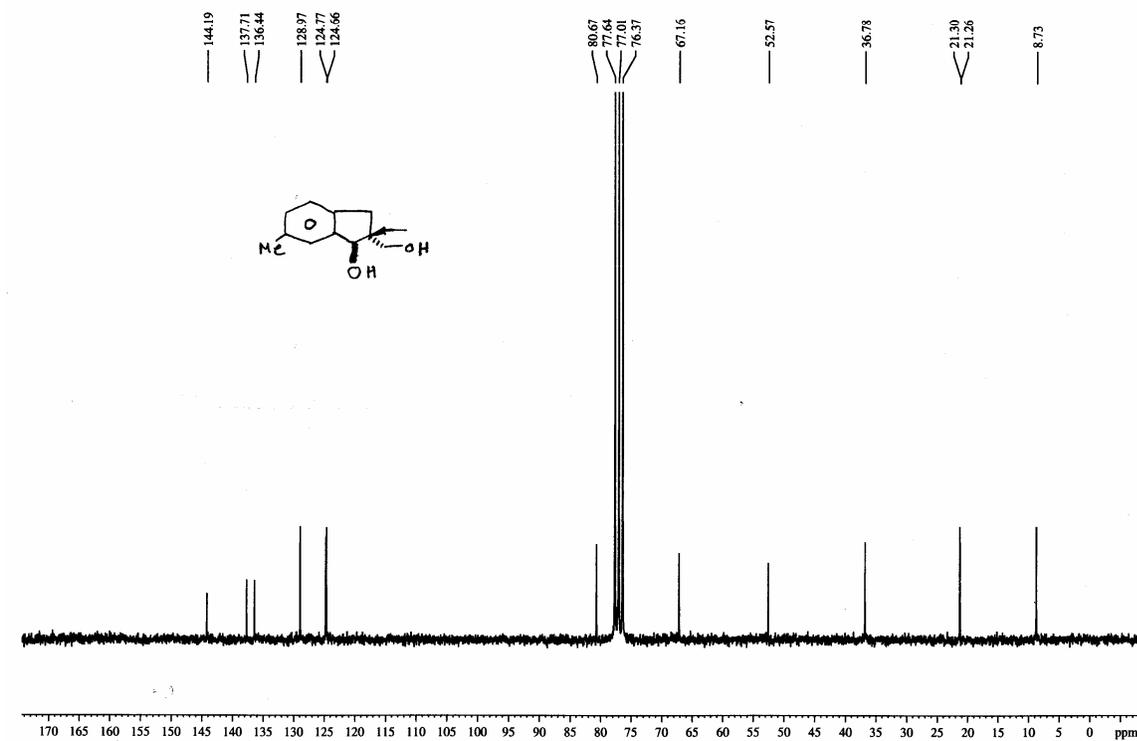
¹H NMR of compound 39



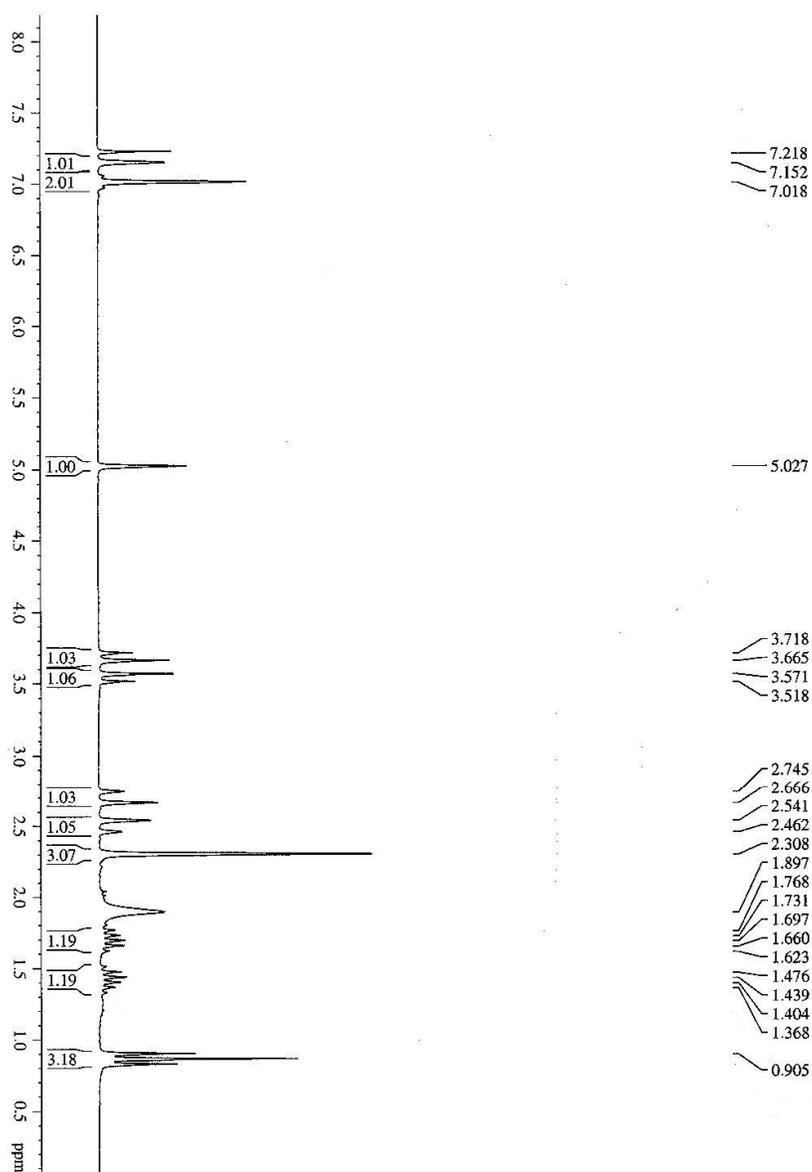
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¹³C NMR of compound 39

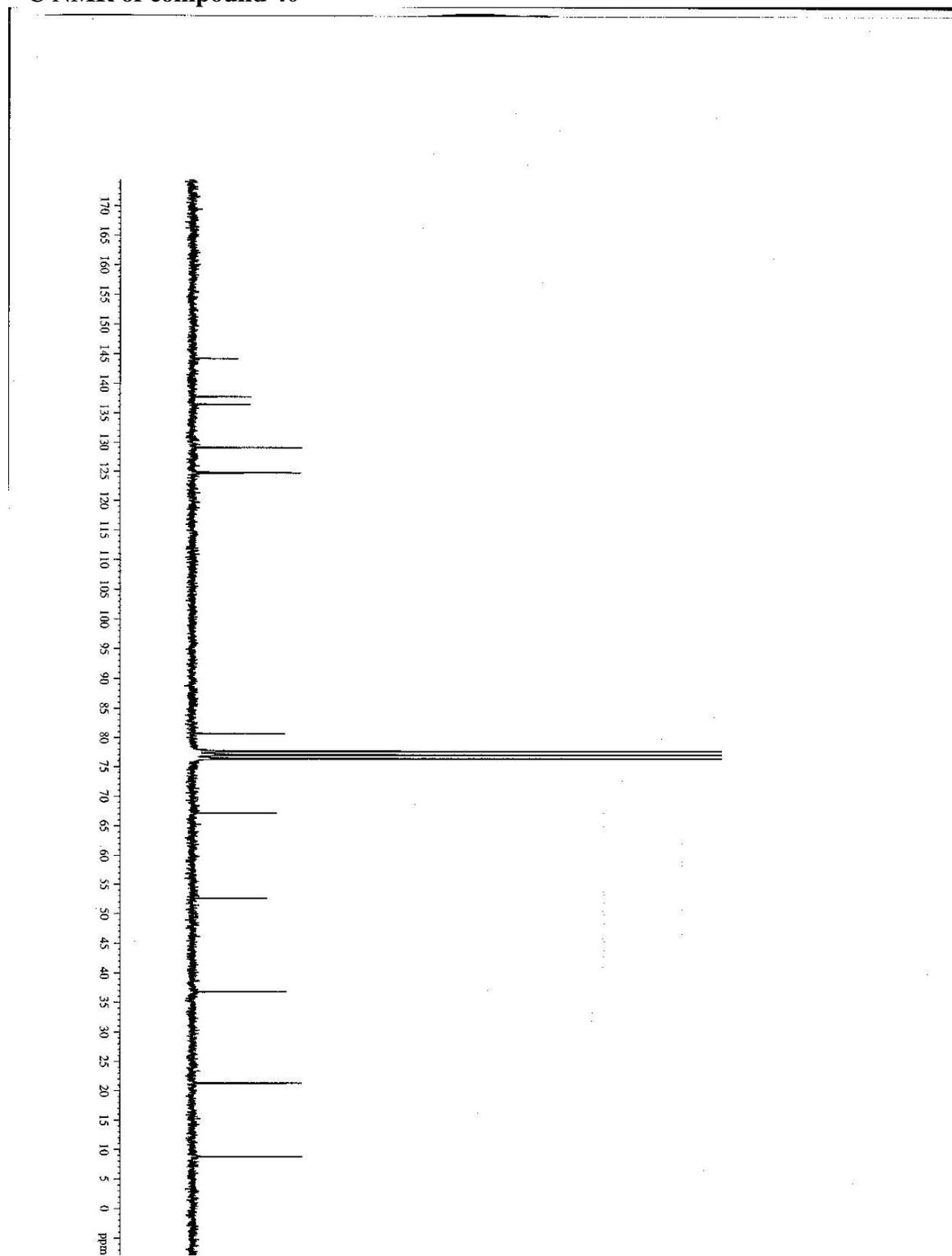
snc/rb/240
C13CPD CDCl3 D:\ IITK 2



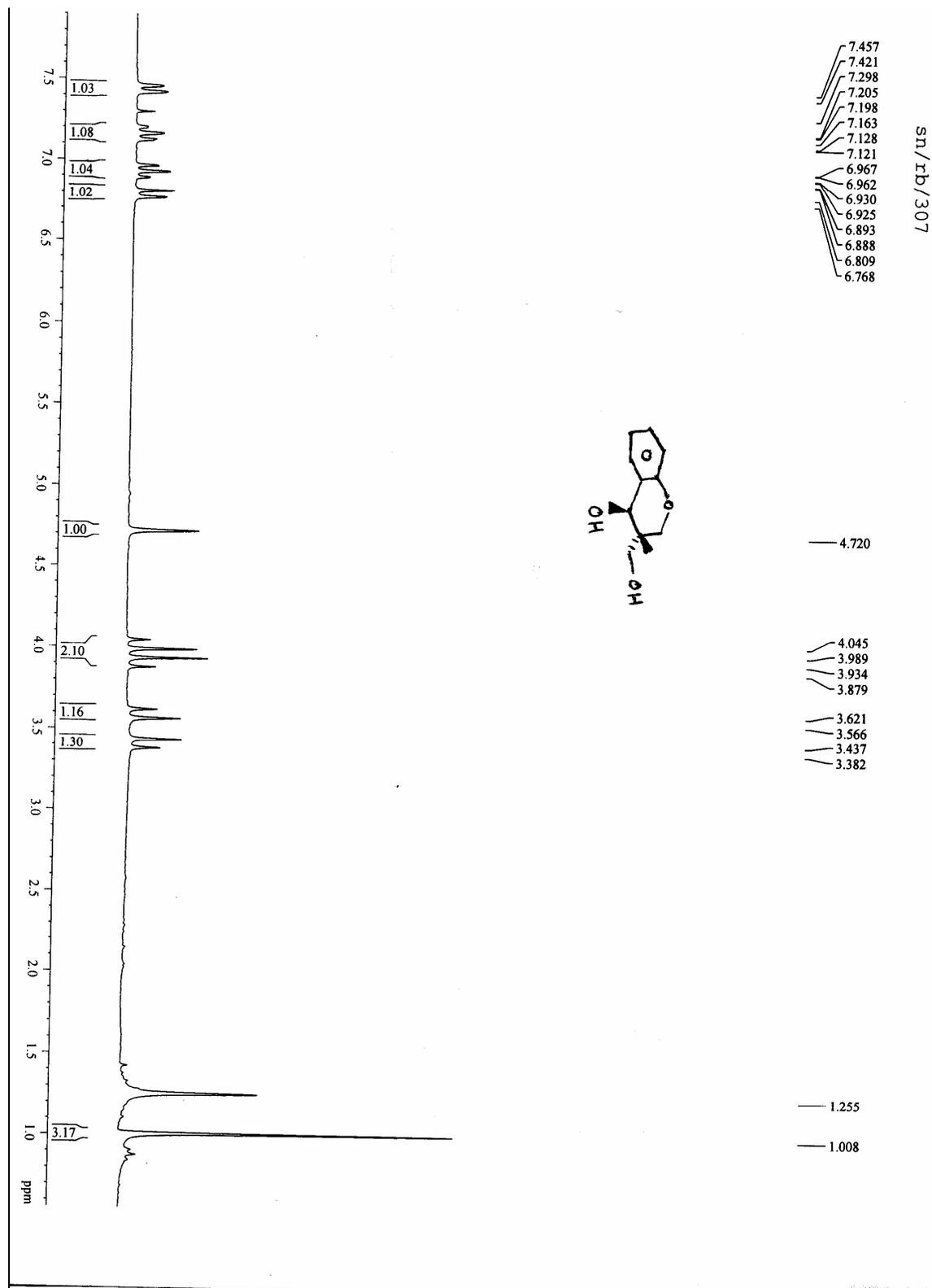
^1H NMR of compound 40



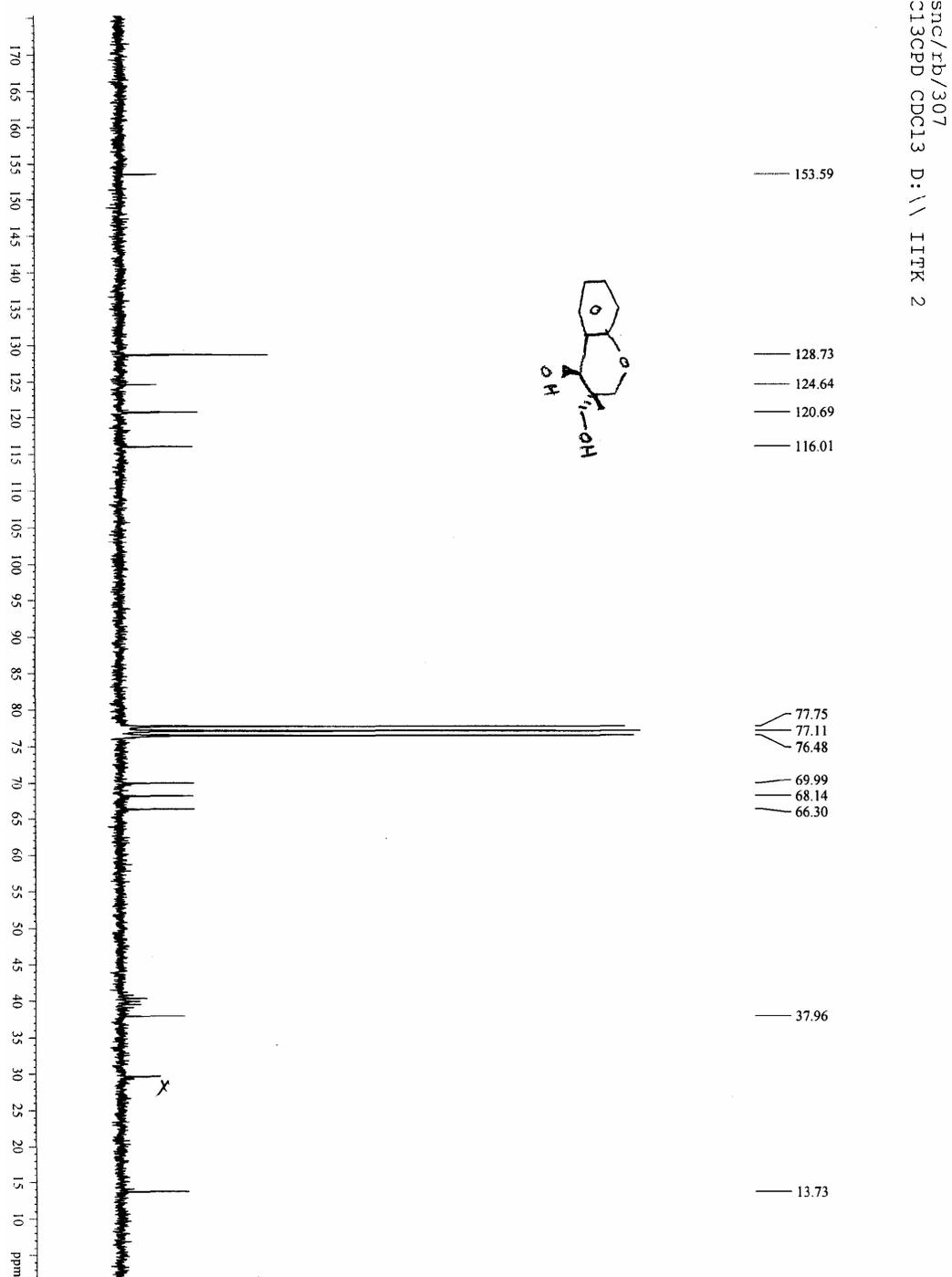
¹³C NMR of compound 40



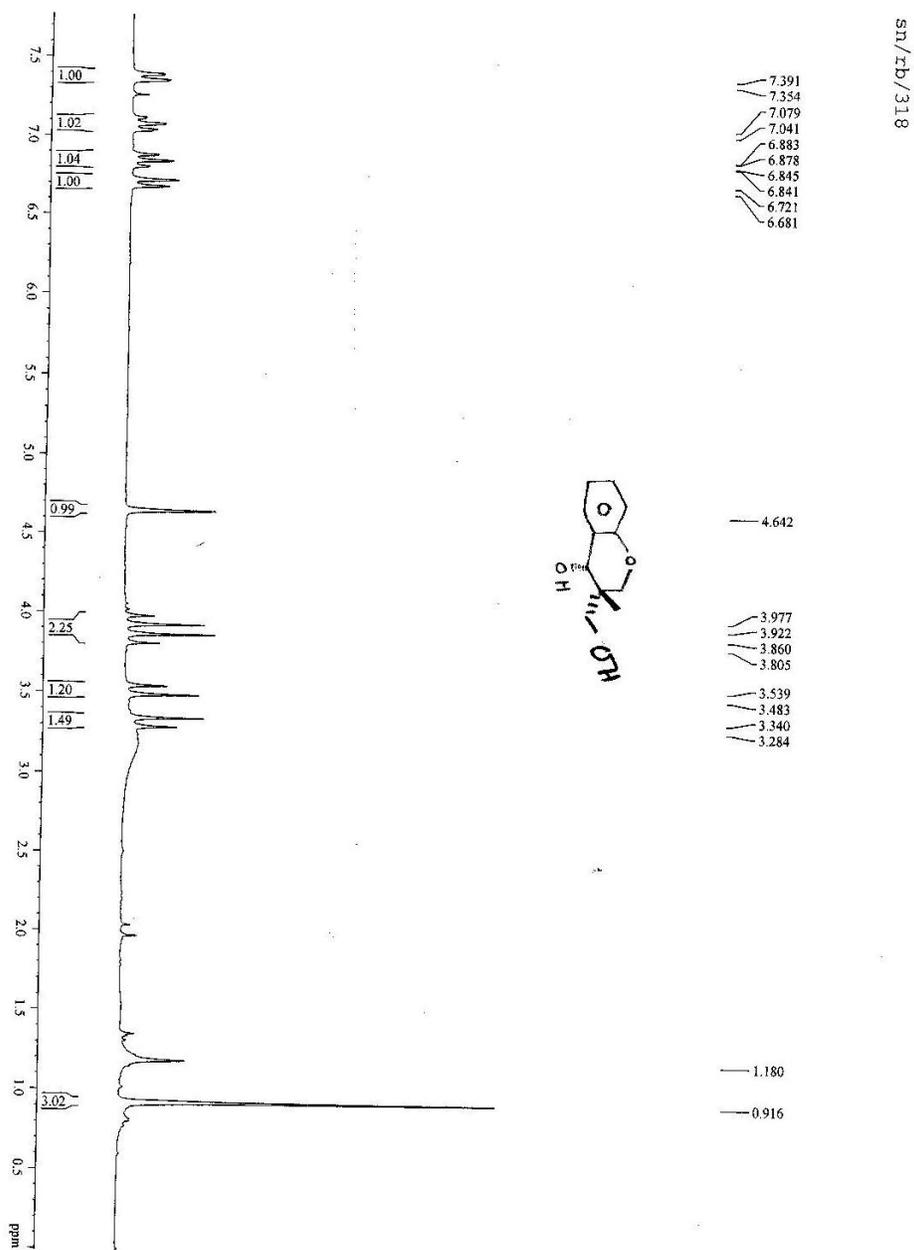
¹H NMR of compound 41



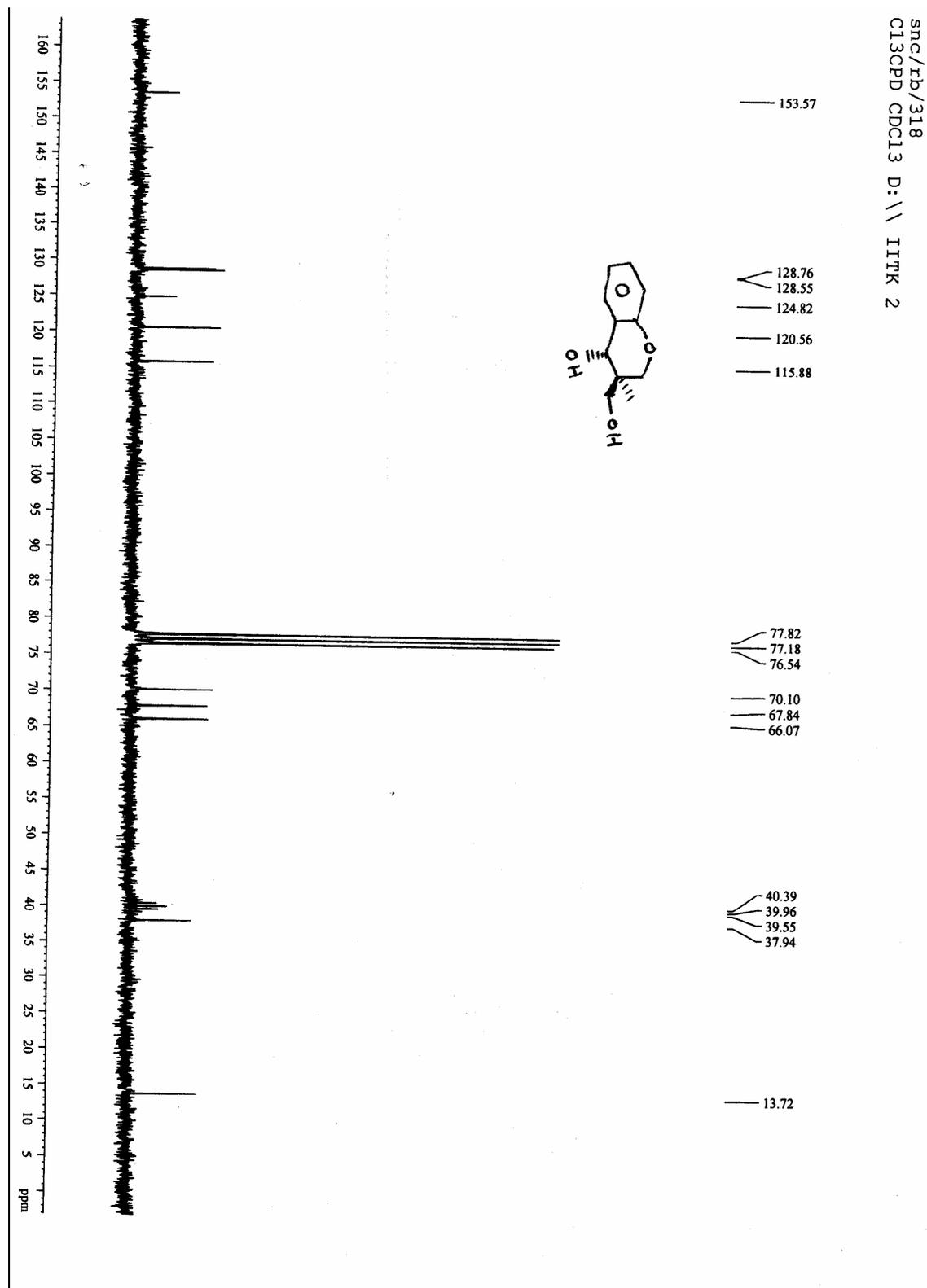
¹³C NMR of compound 41



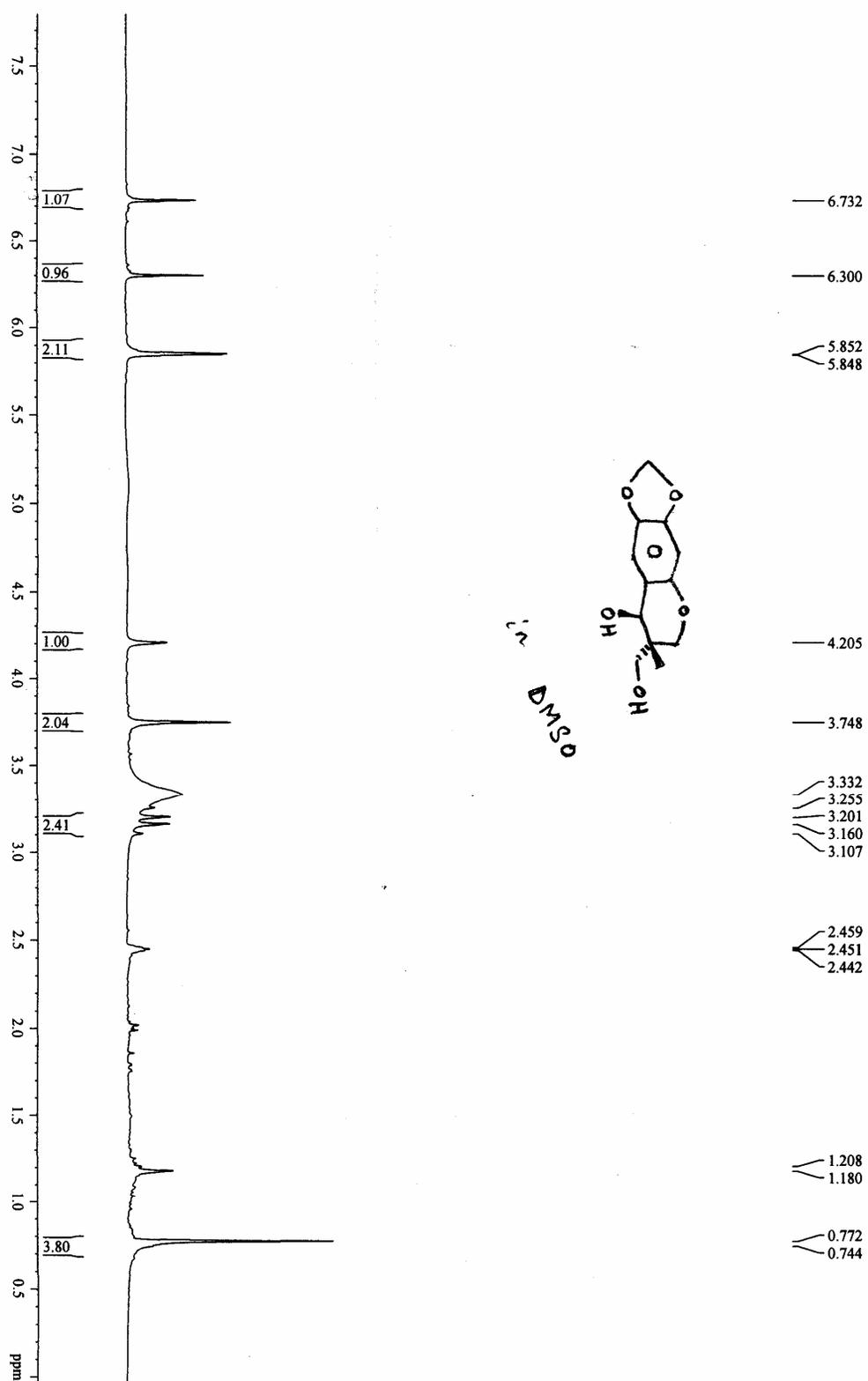
¹H NMR of compound 42



¹³C NMR of Compound 42

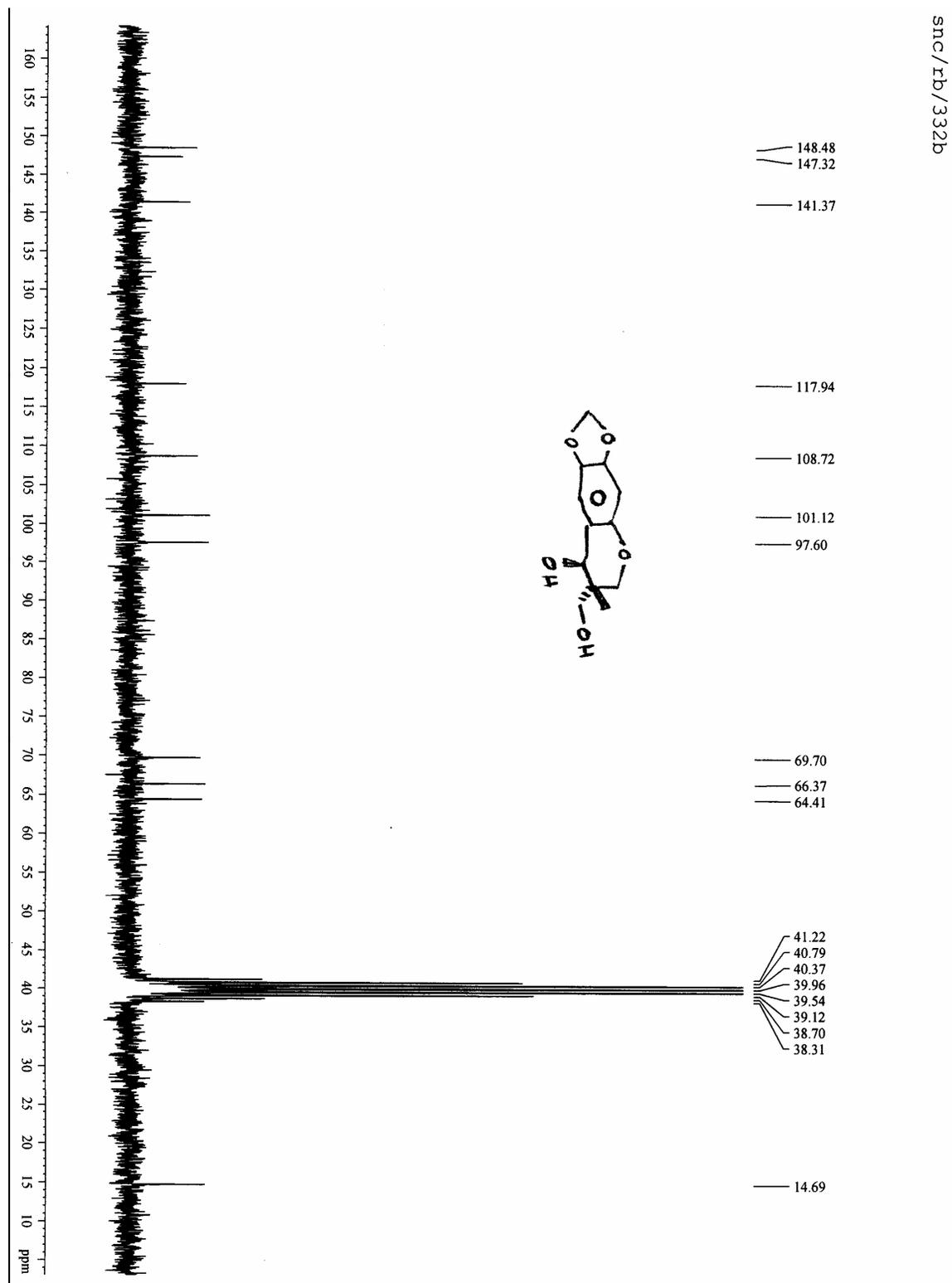


¹H NMR of compound 43

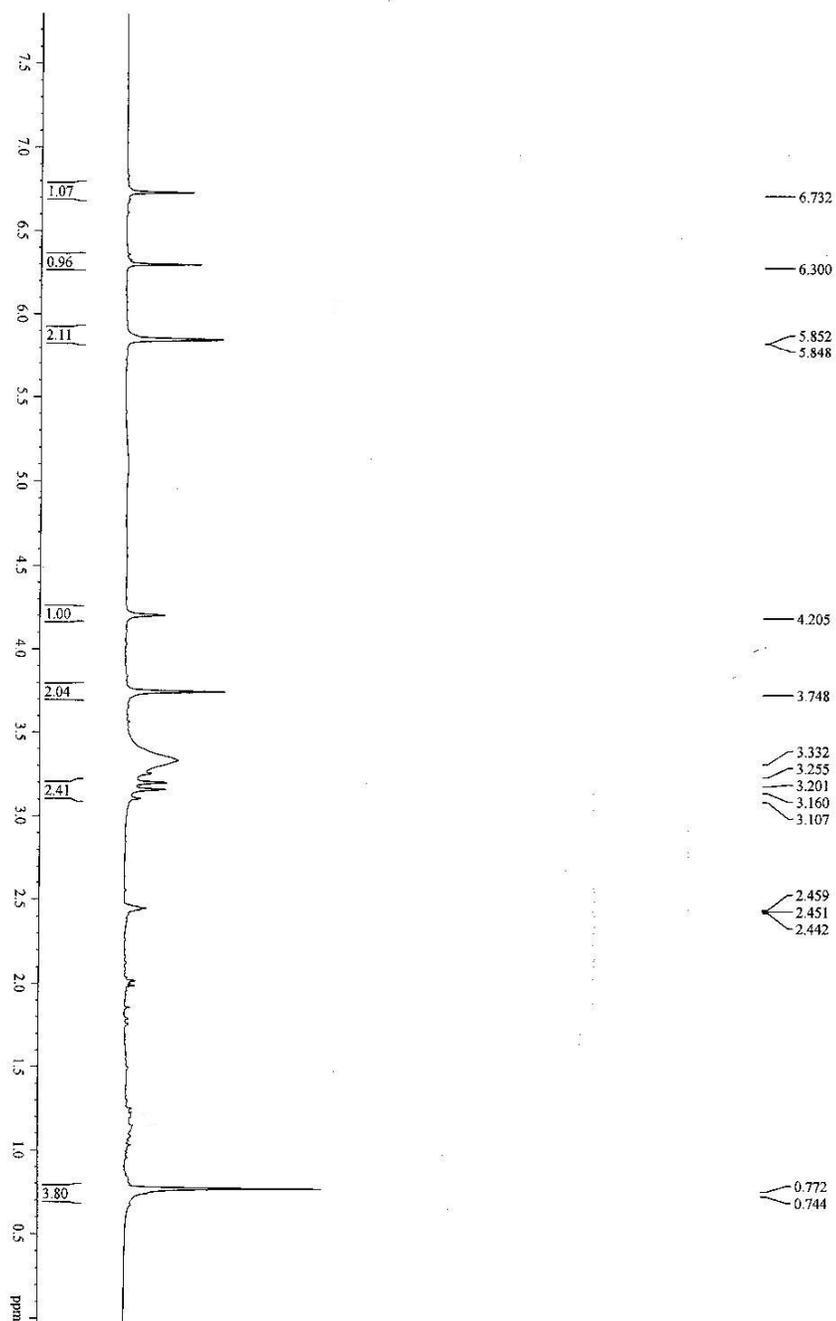


sn/rb/332b

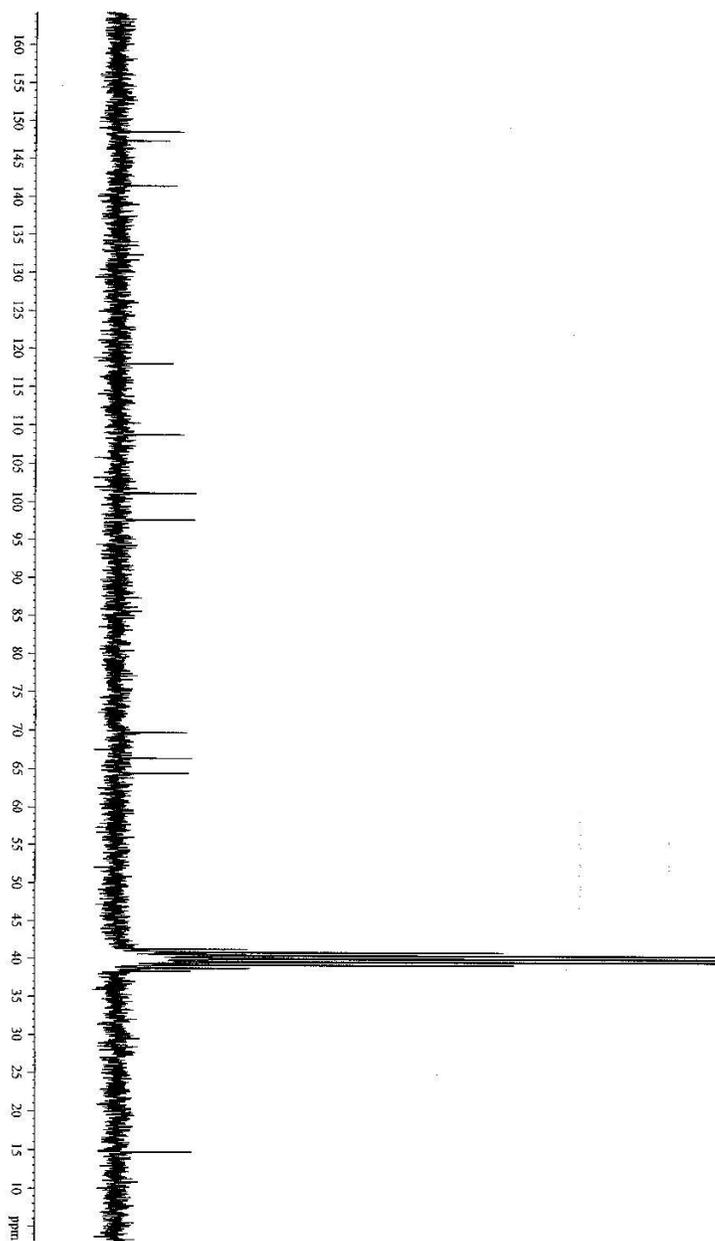
¹³C NMR of compound 43



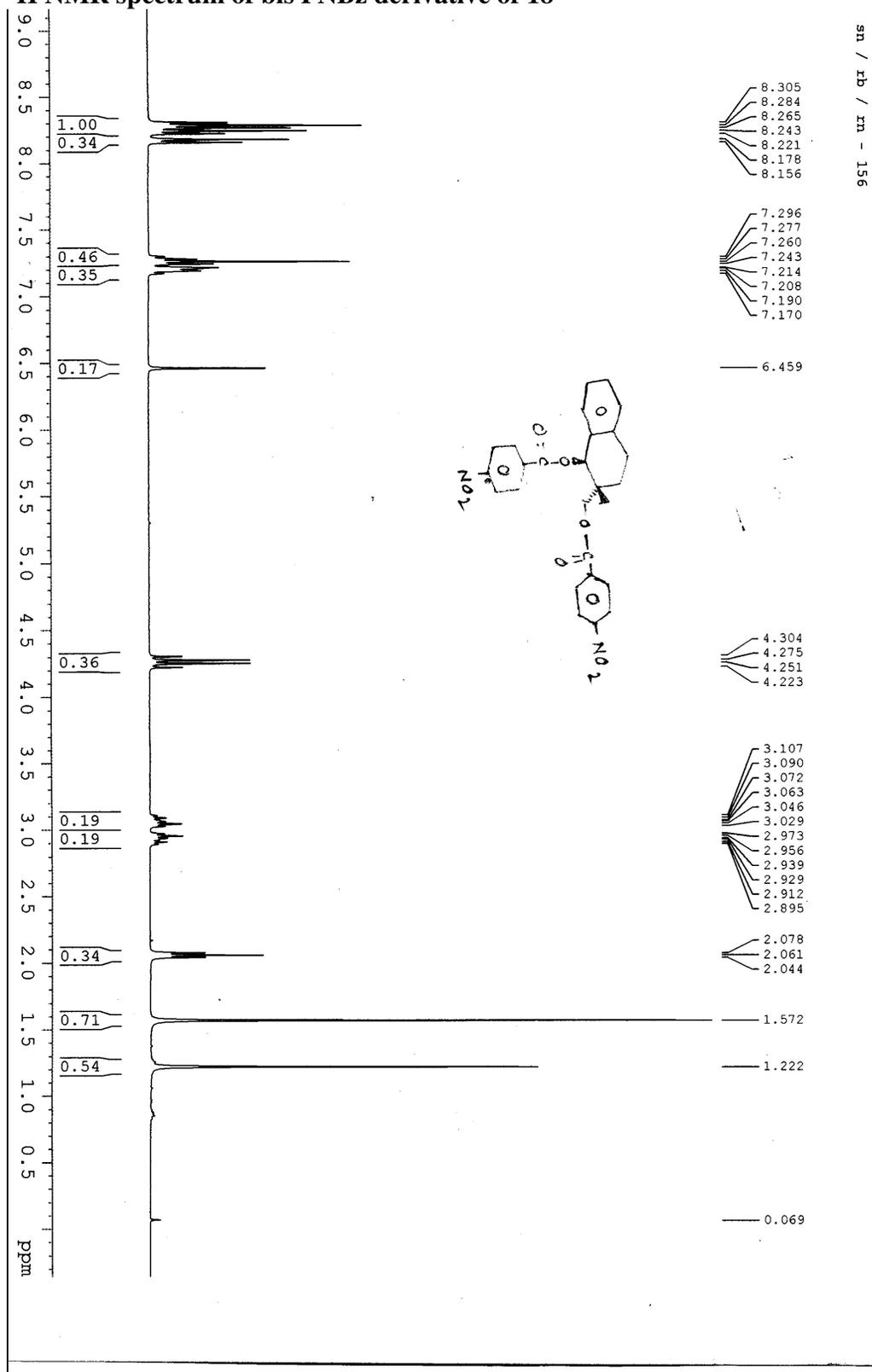
¹H NMR of compound 44



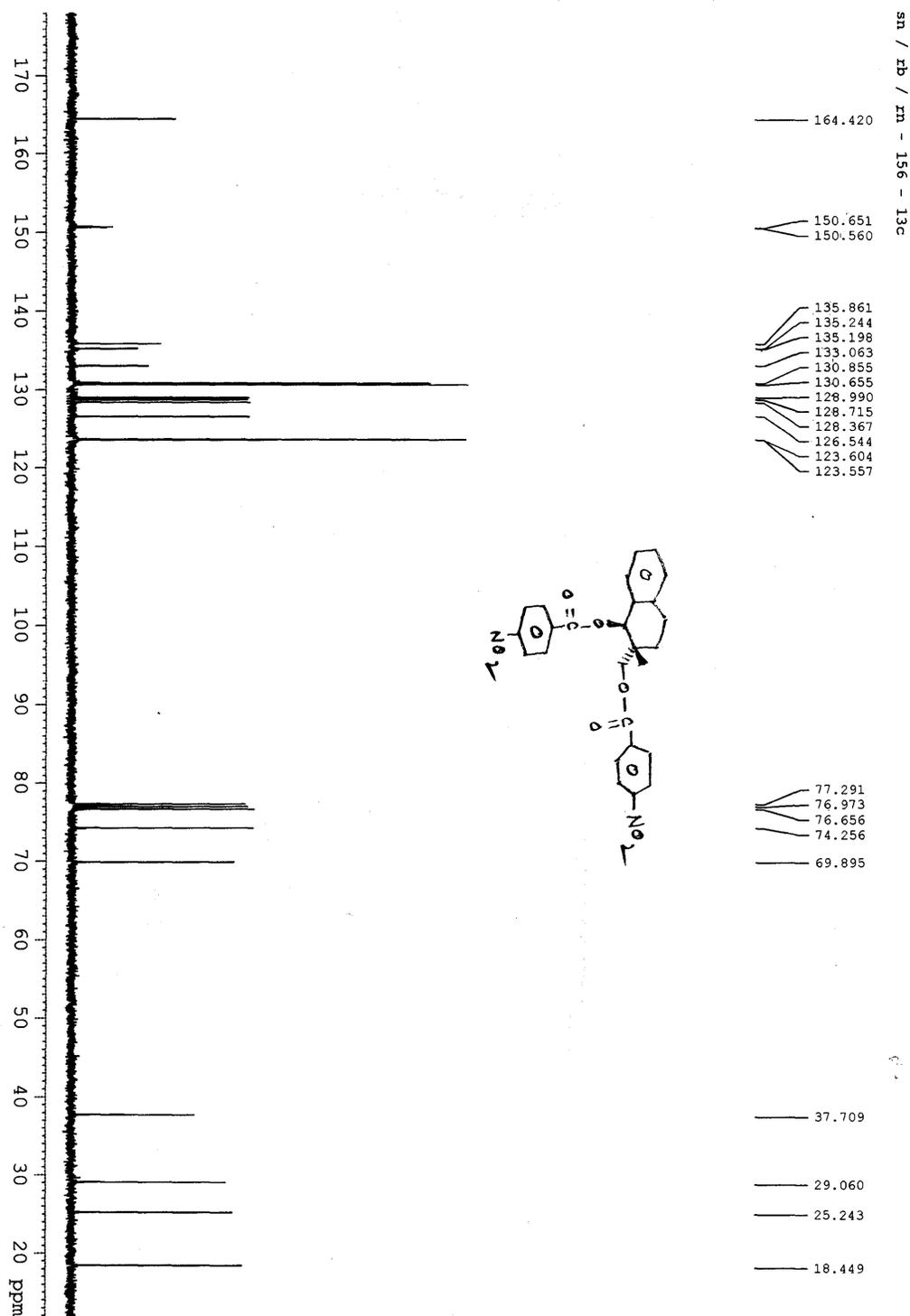
^{13}C NMR of compound 44



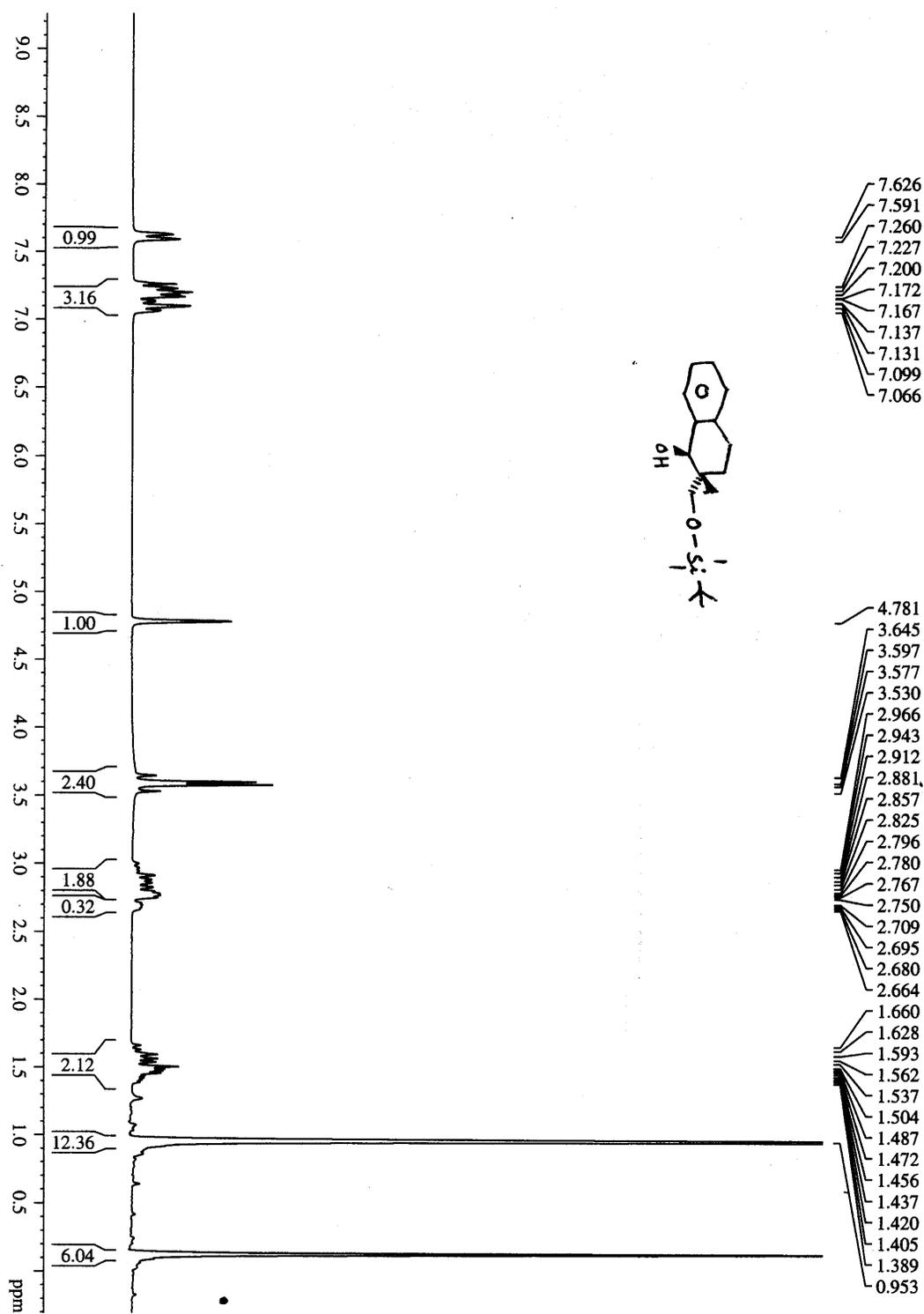
¹H NMR spectrum of bis PNBz derivative of 18



¹³C NMR spectrum of bis PNBz derivative of 18

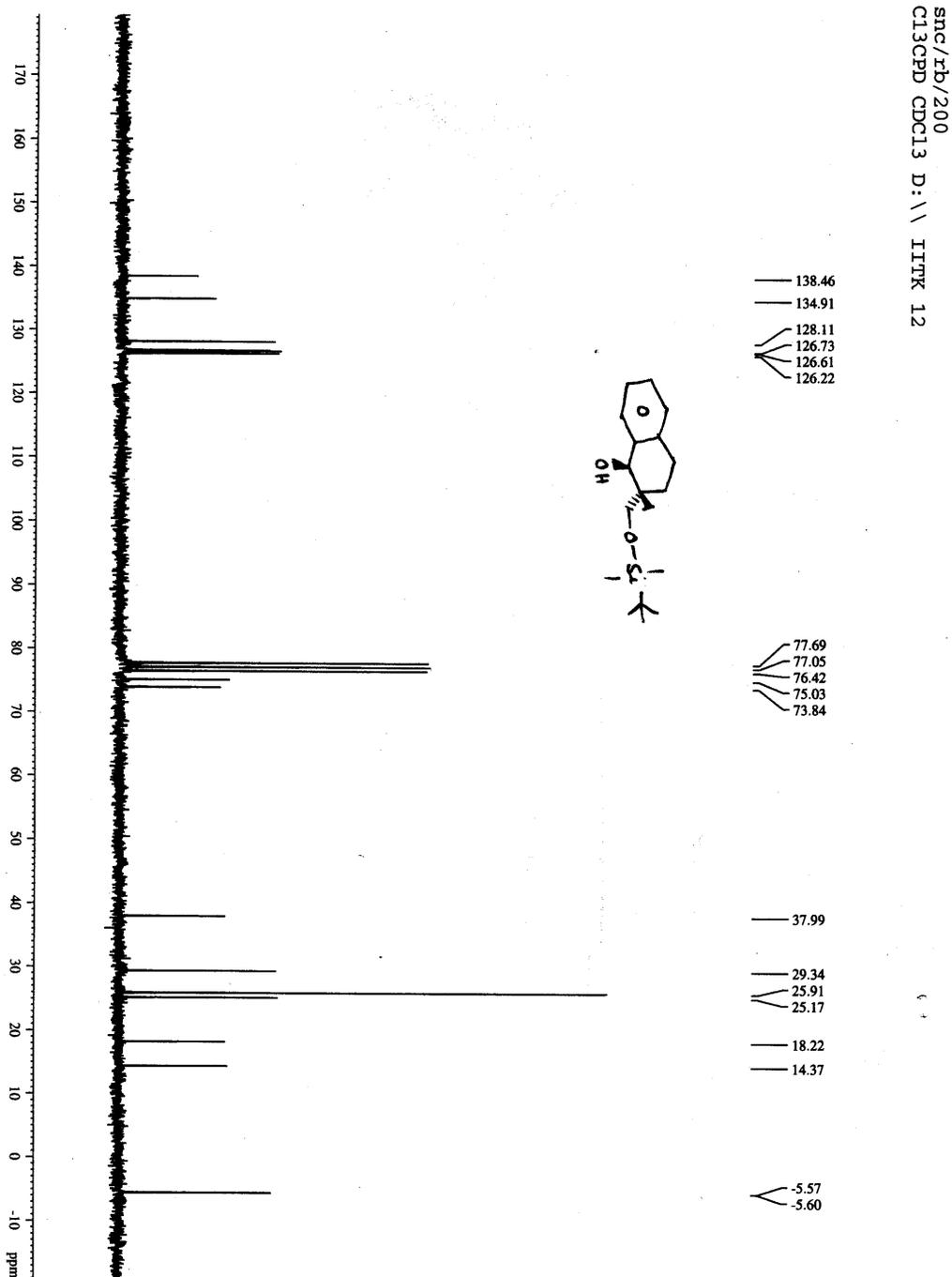


¹H NMR of compound 45

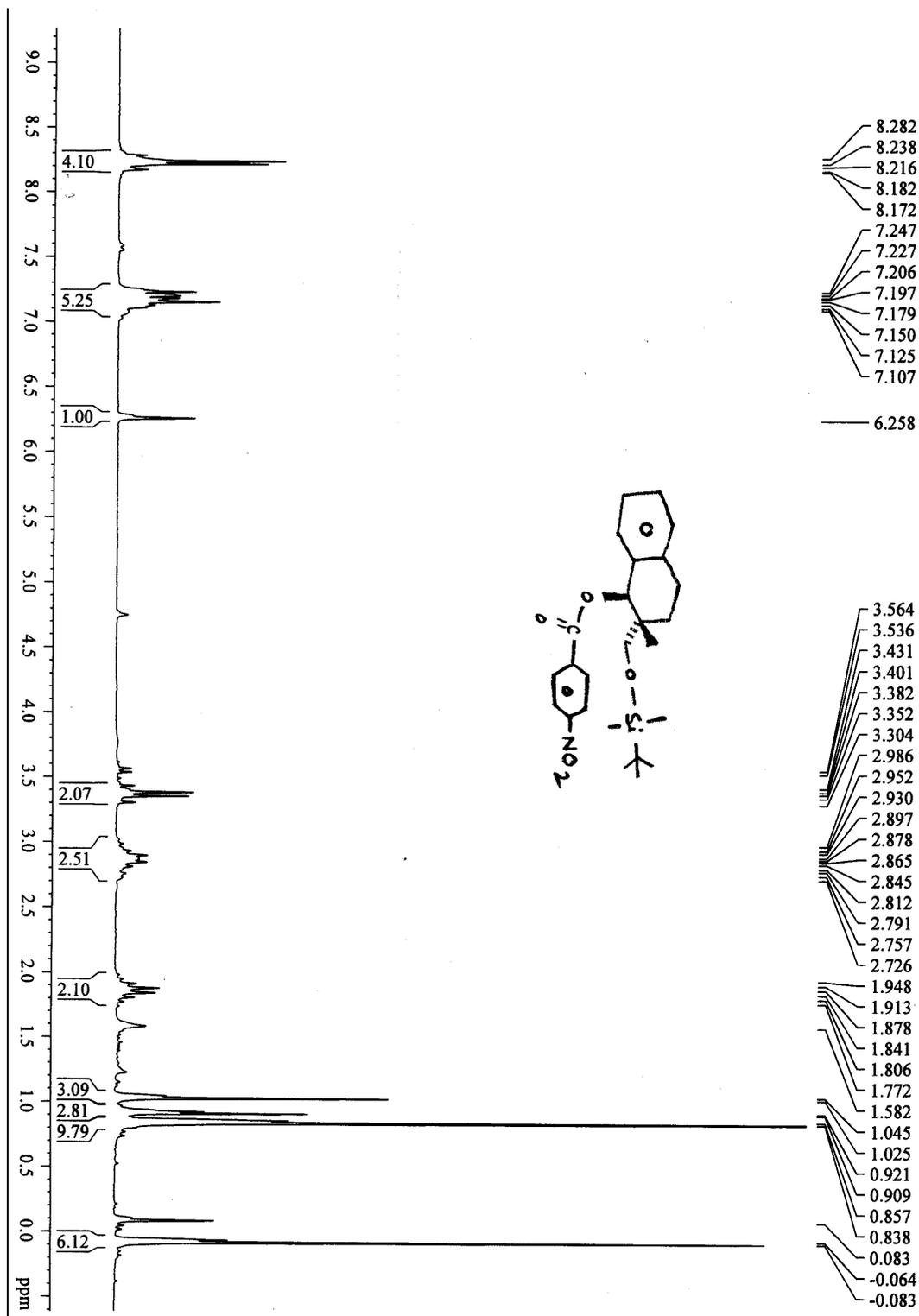


sn / rb-200

¹³C NMR of compound 45

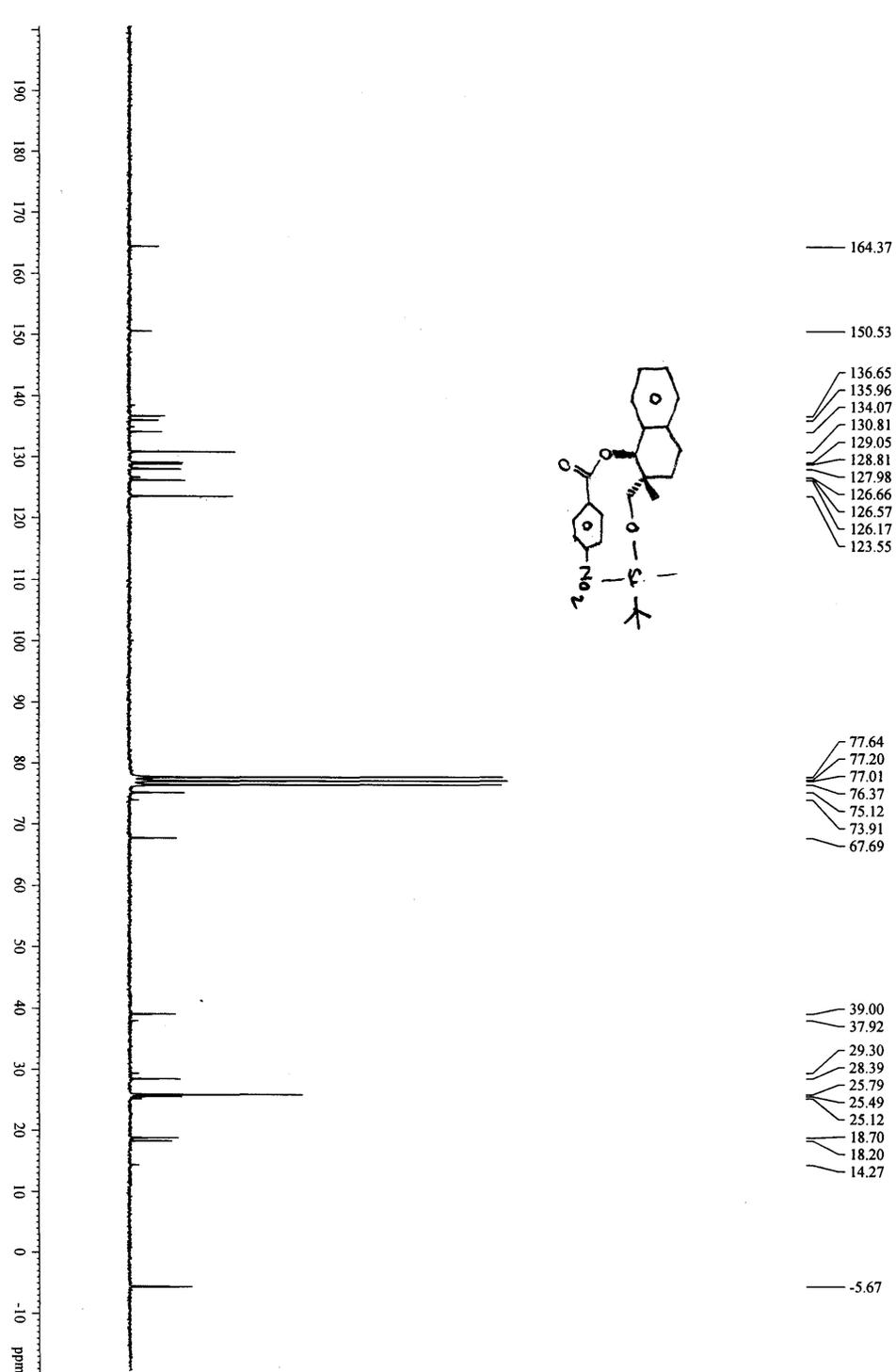


¹H NMR of compound 46



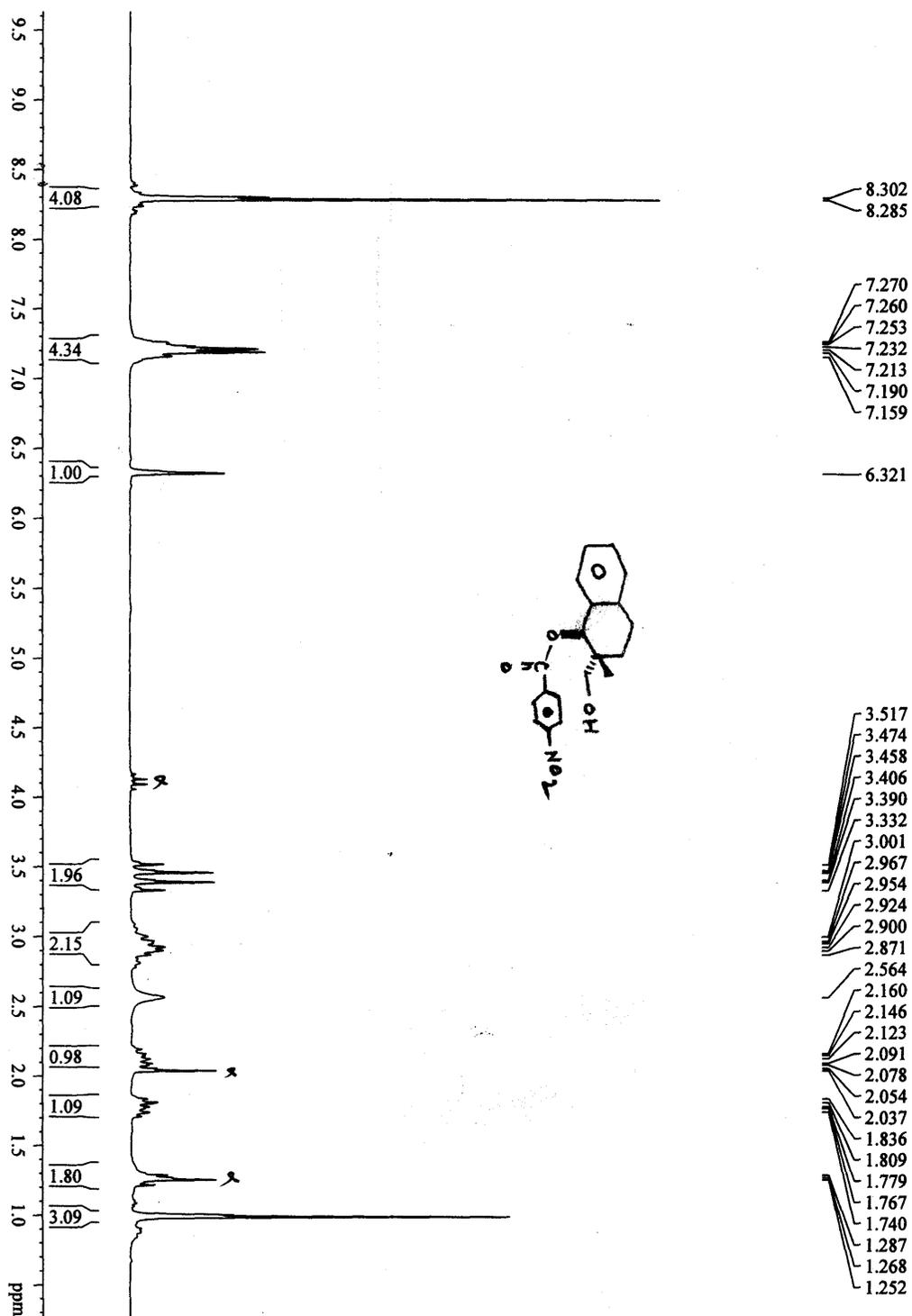
sn/rb/256

¹³C NMR of compound 46



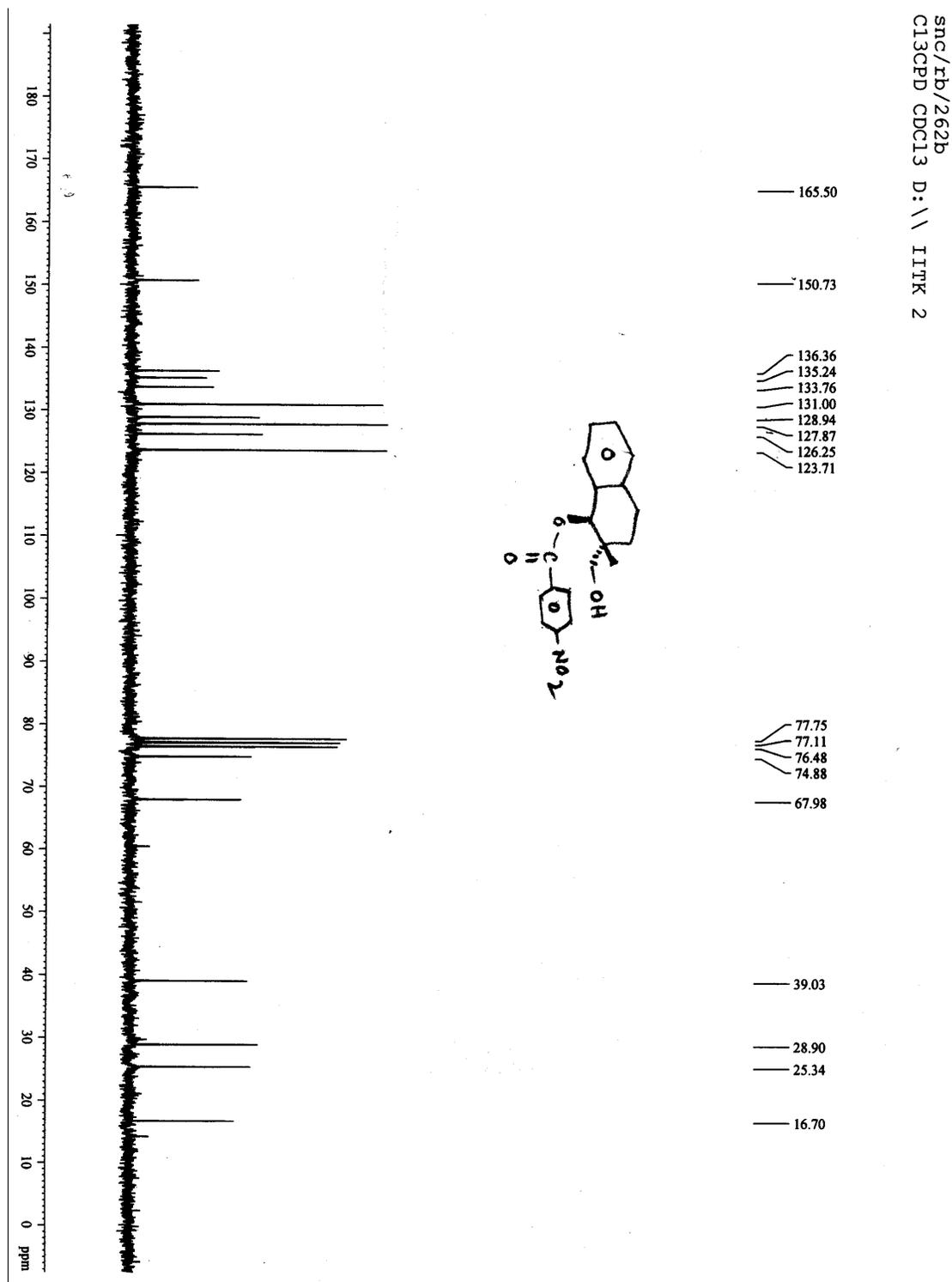
snc/rb/256
C13CPD CDCl3 D: \\ ITRK 2

^1H NMR of compound 47

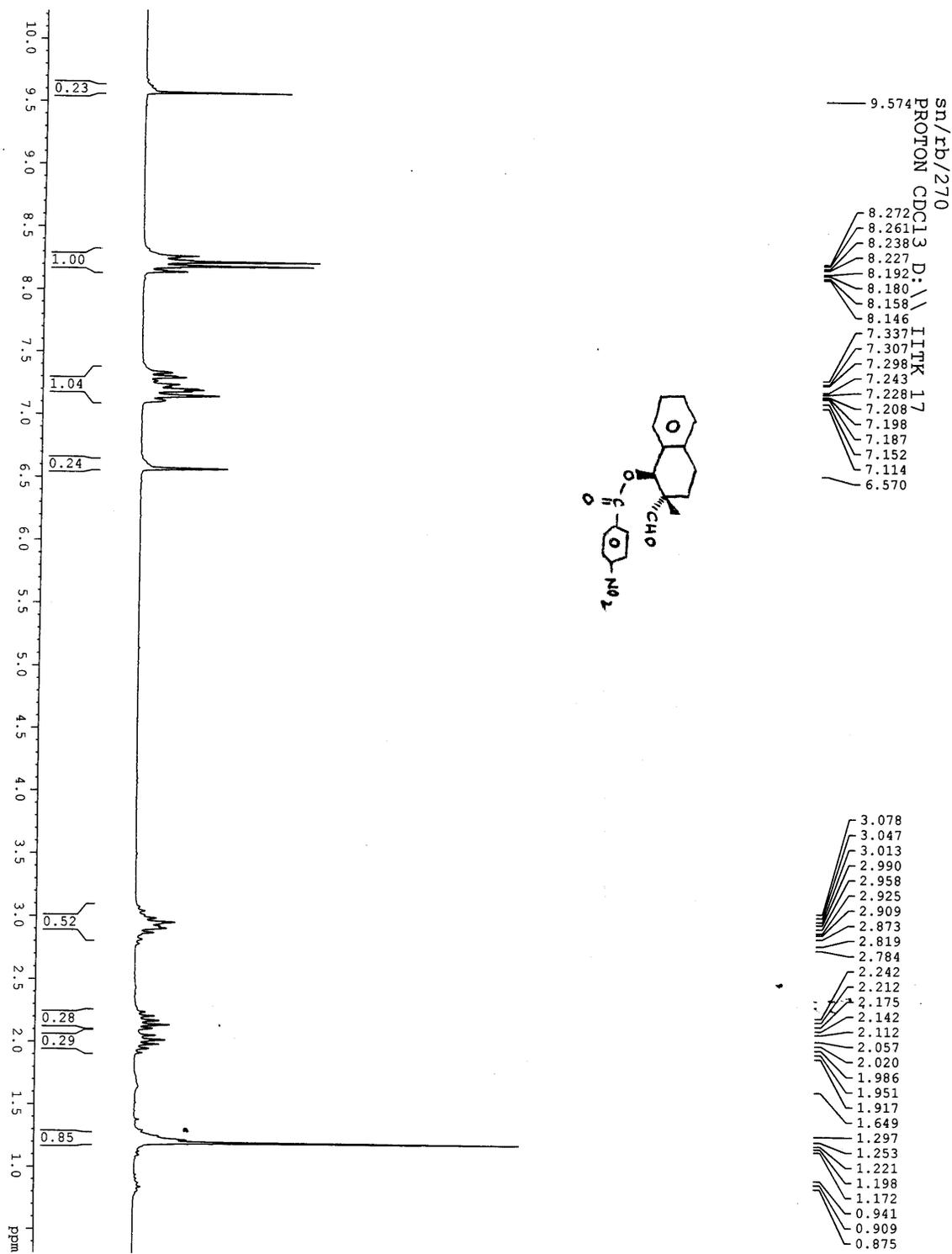


sn/rb/262b

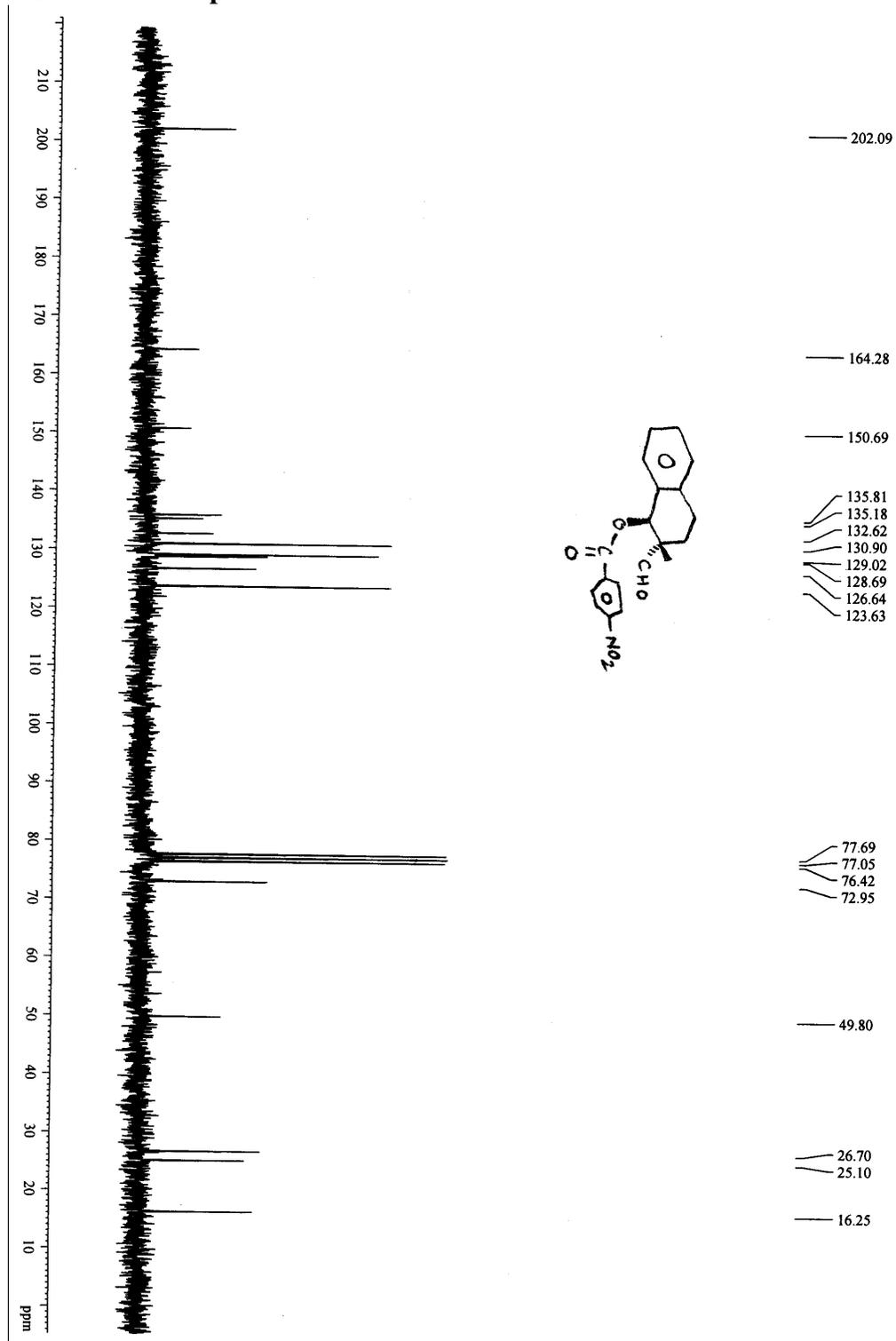
¹³C NMR of compound 47



¹H NMR of compound 48

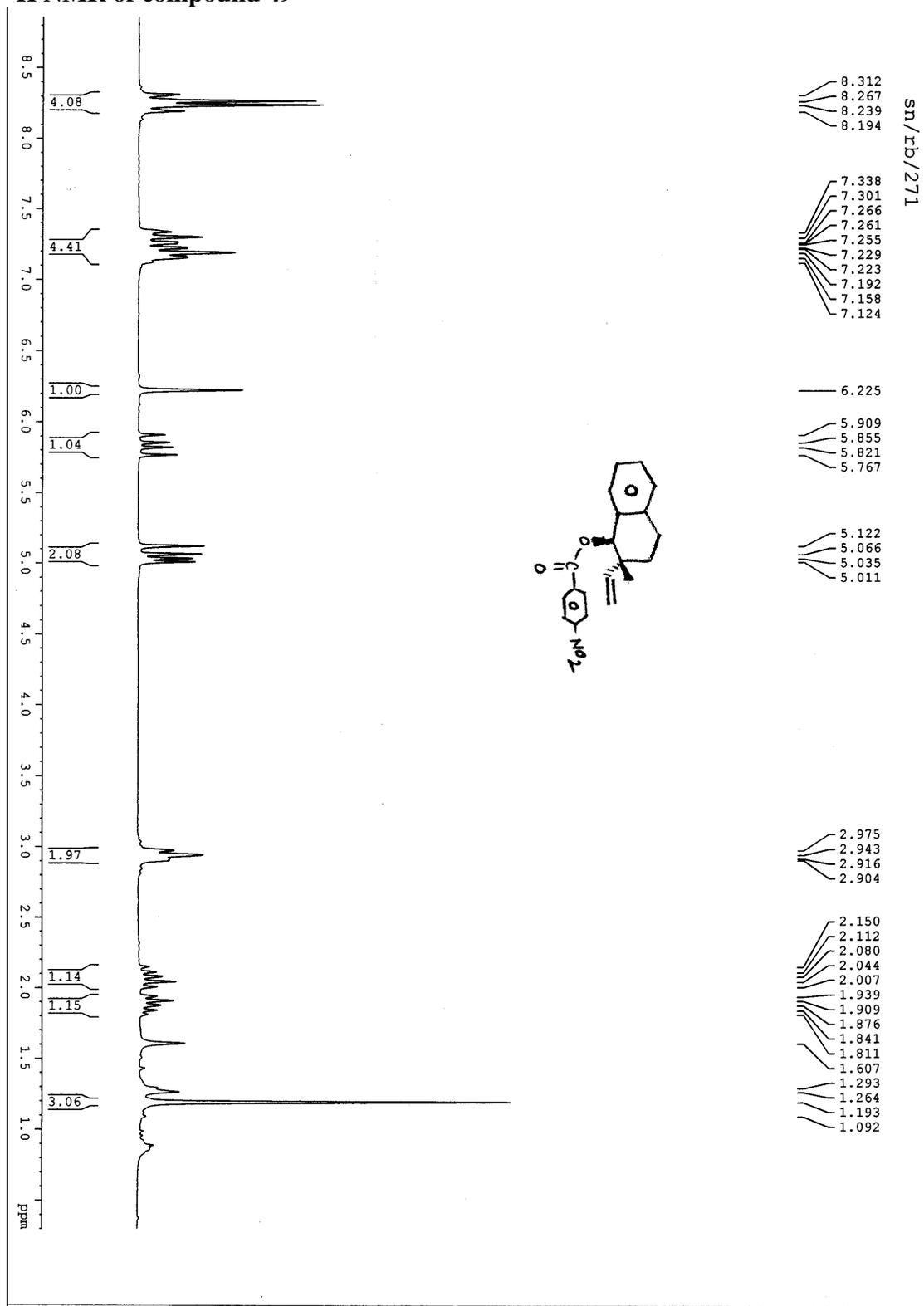


¹³C NMR of compound 48

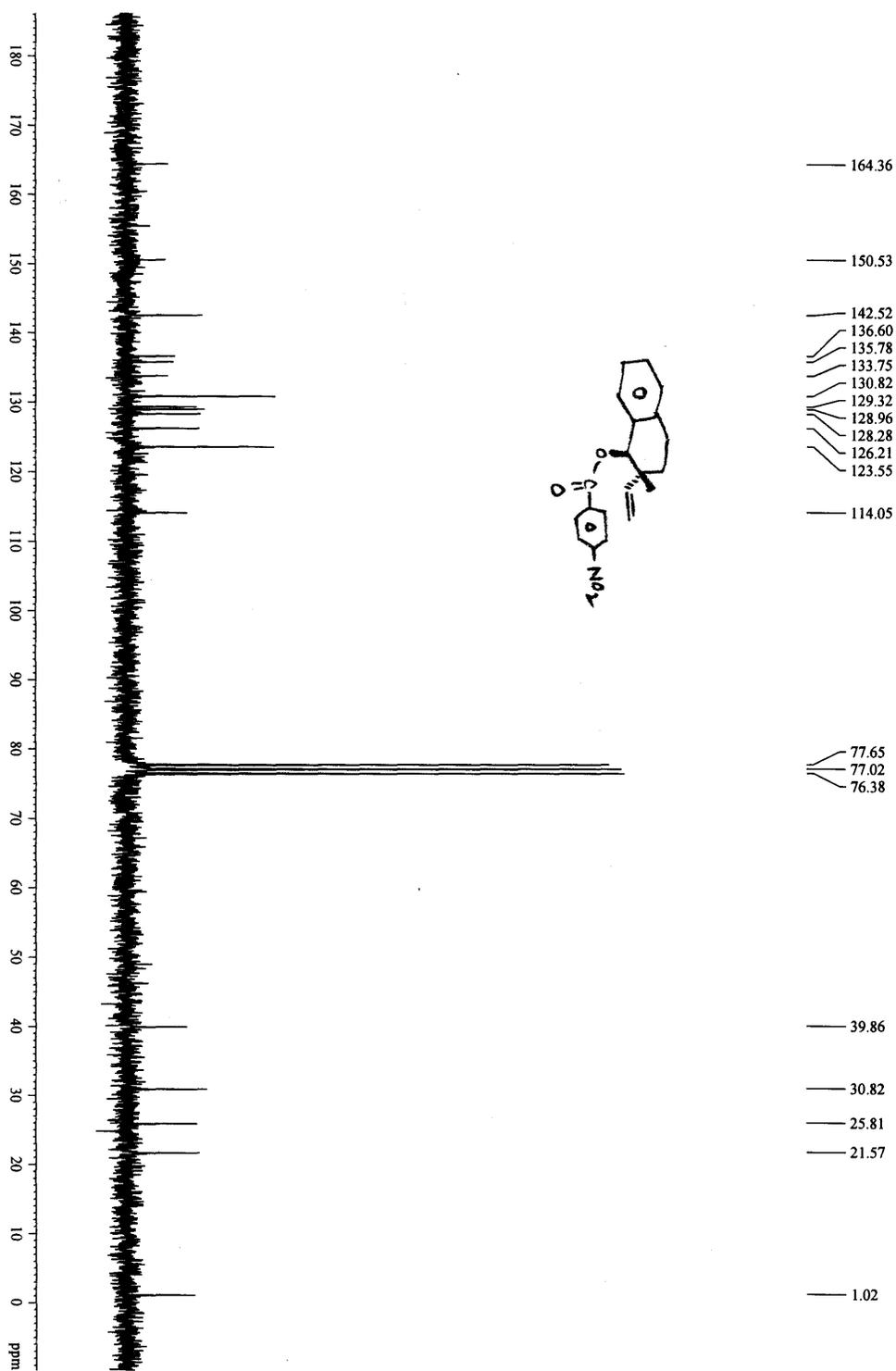


snc/rb/270
C13CPD CDCl3 D:\ IITK 2

¹H NMR of compound 49

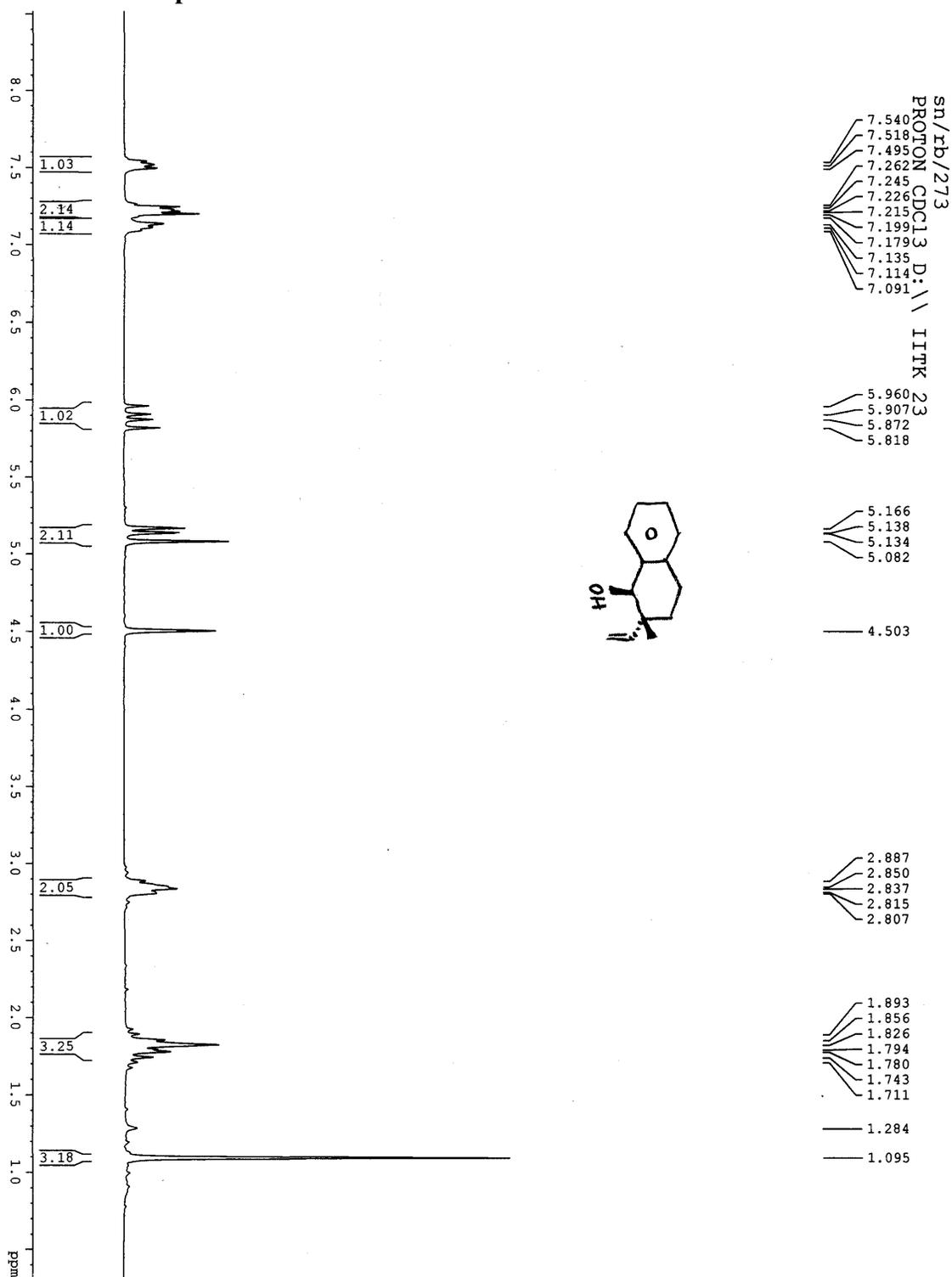


¹³C NMR of compound 49



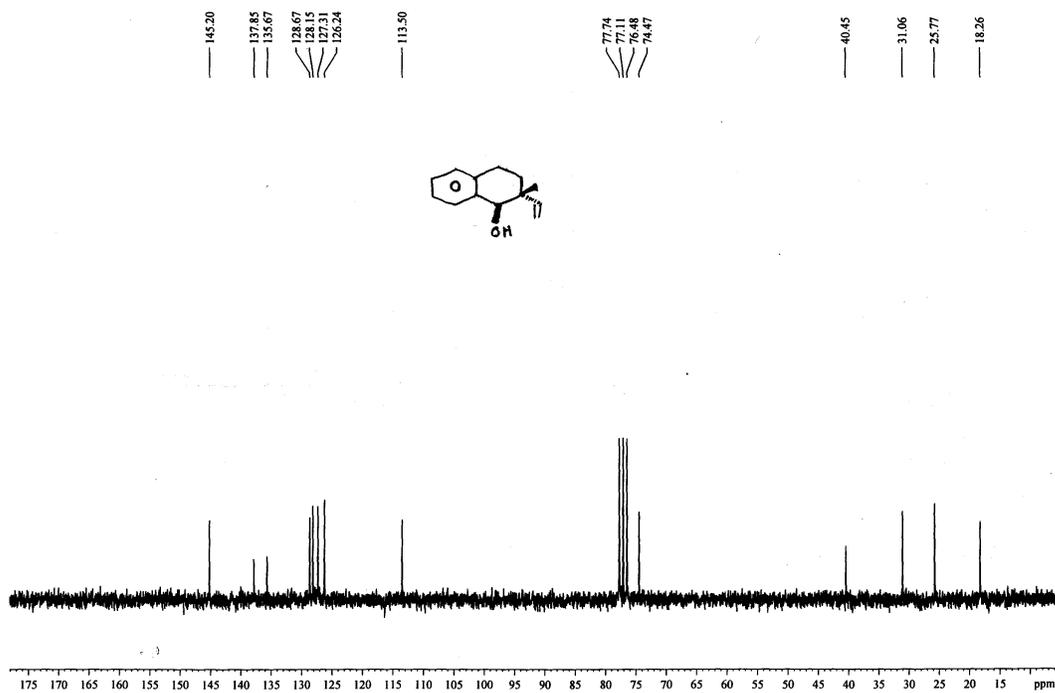
snc/rb/271
C13CPD CDC13 D:\ IITK 2

¹H NMR of compound 50

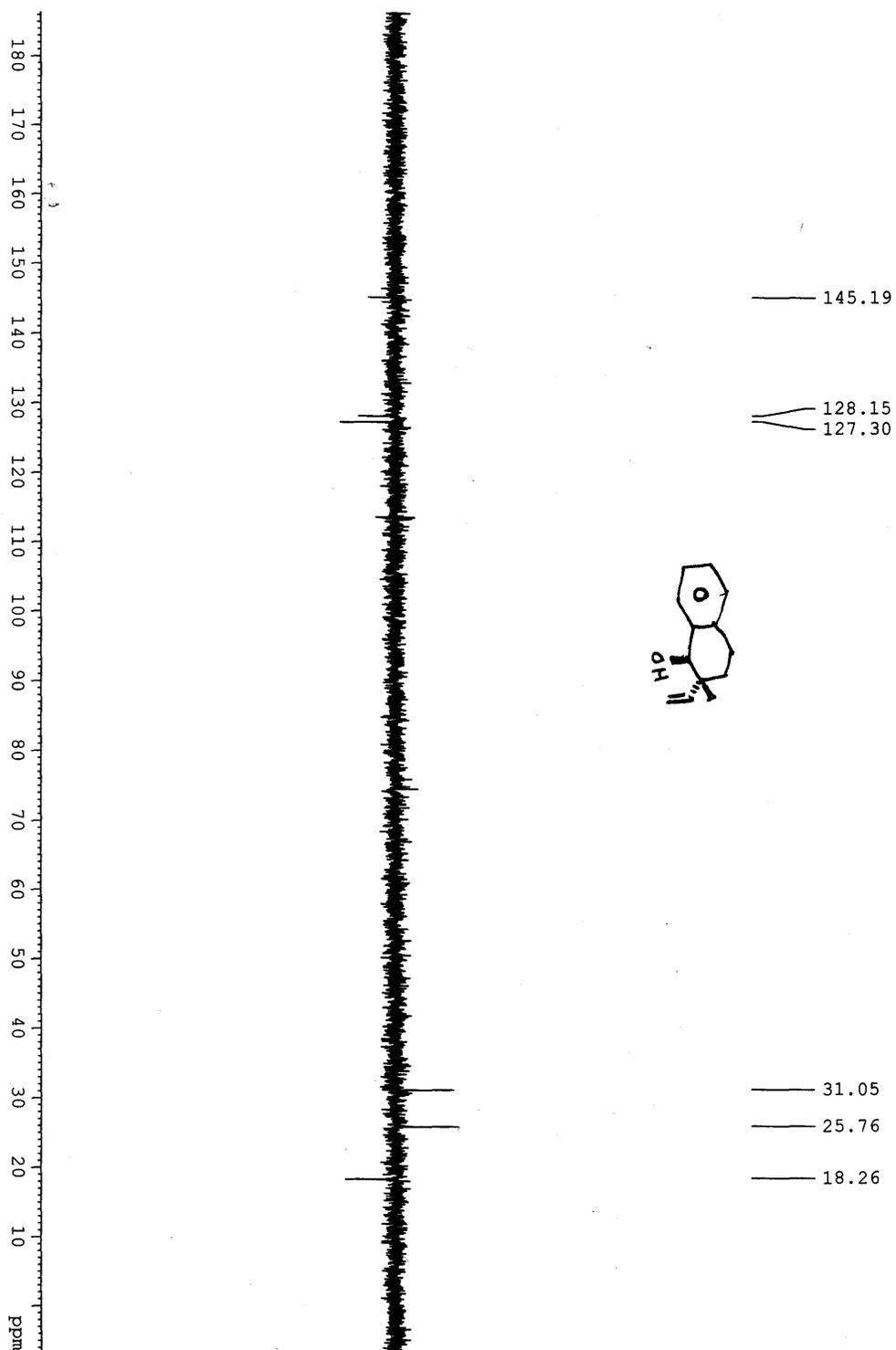


¹³C NMR of compound 50

snc/rb/273
C13CPD CDC13 D:\ IITK 2

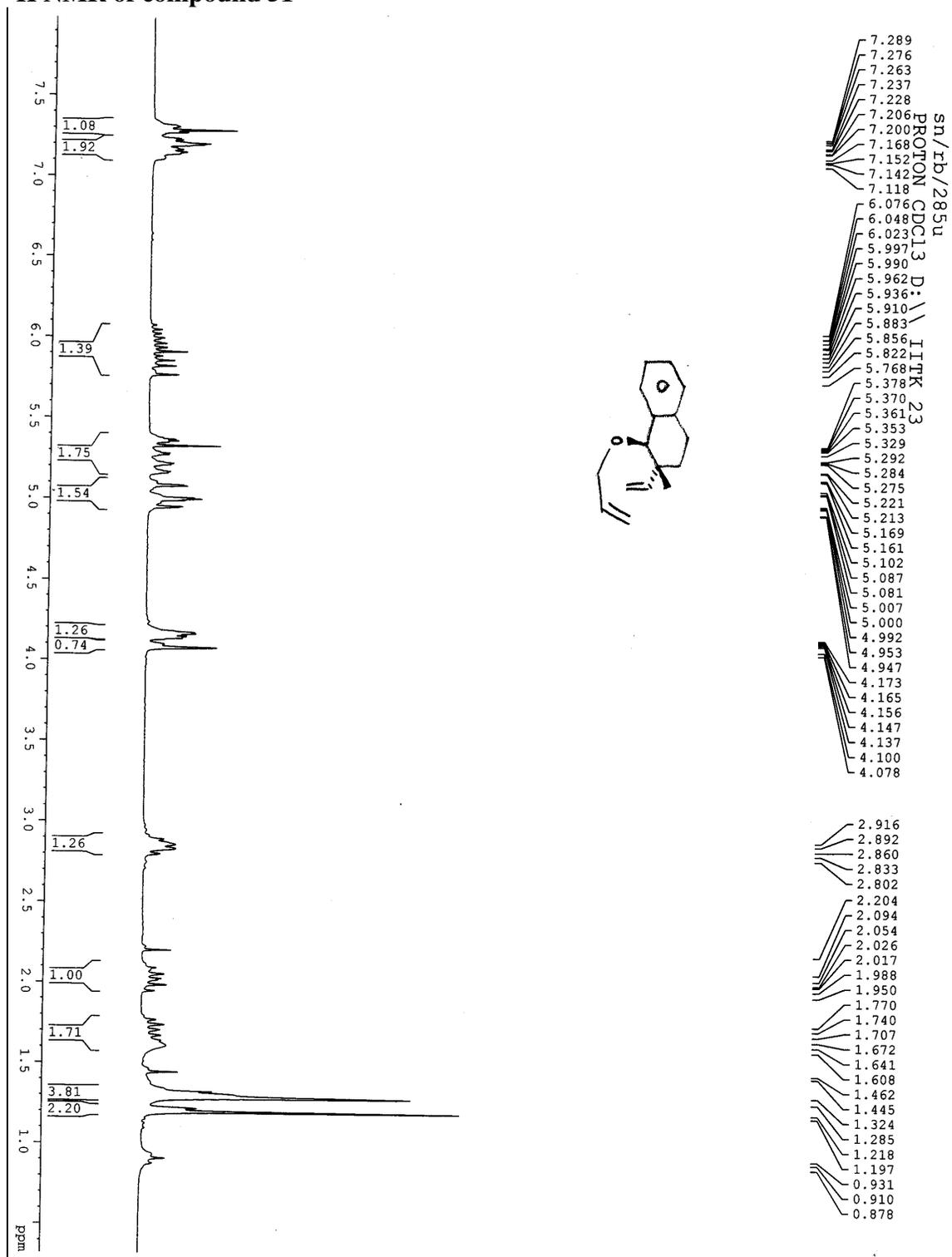


DEPT 135 of compound 50

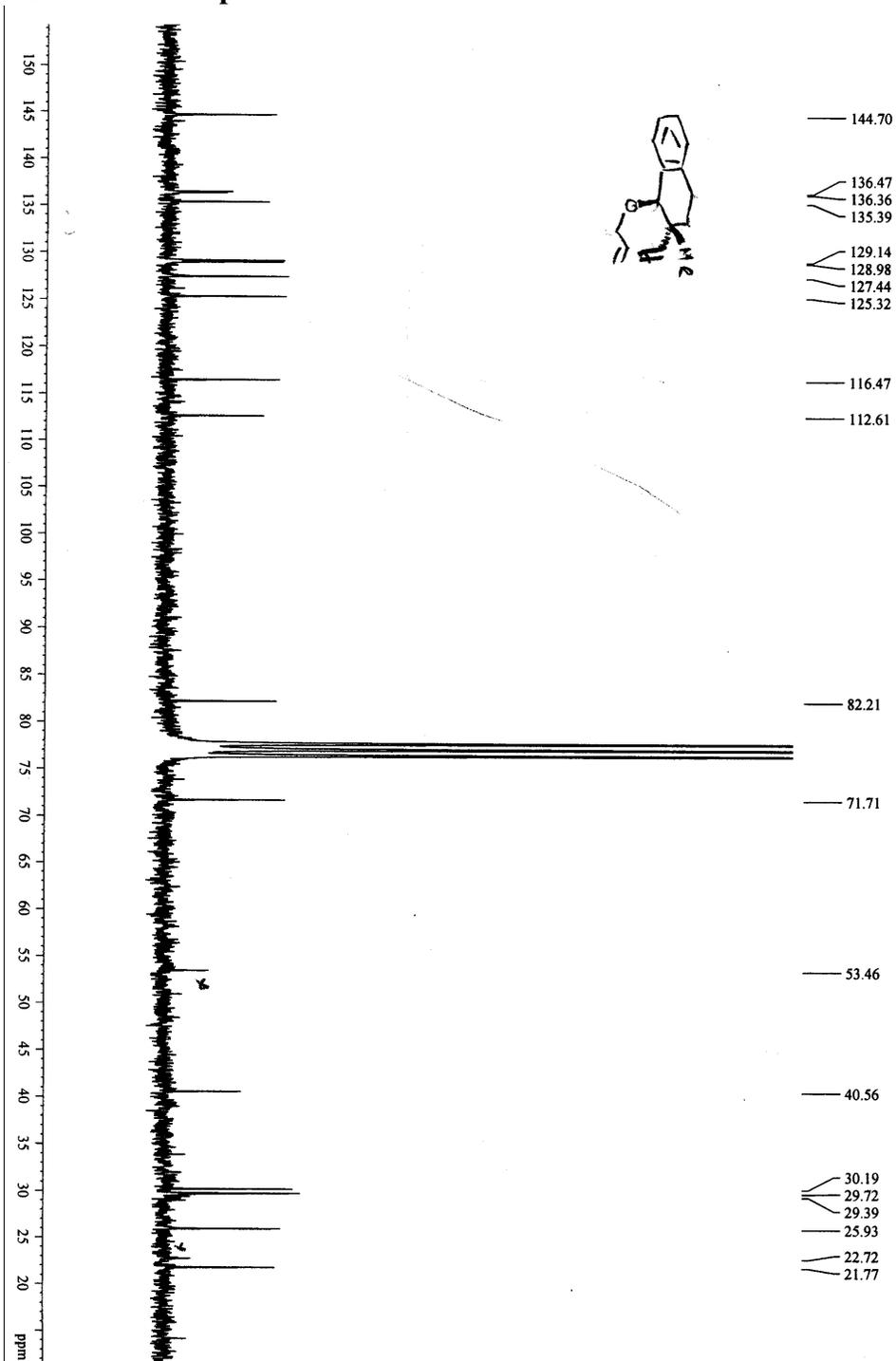


snd/rb/273
PROTON CDCl3 D:\ IITK 2

¹H NMR of compound 51

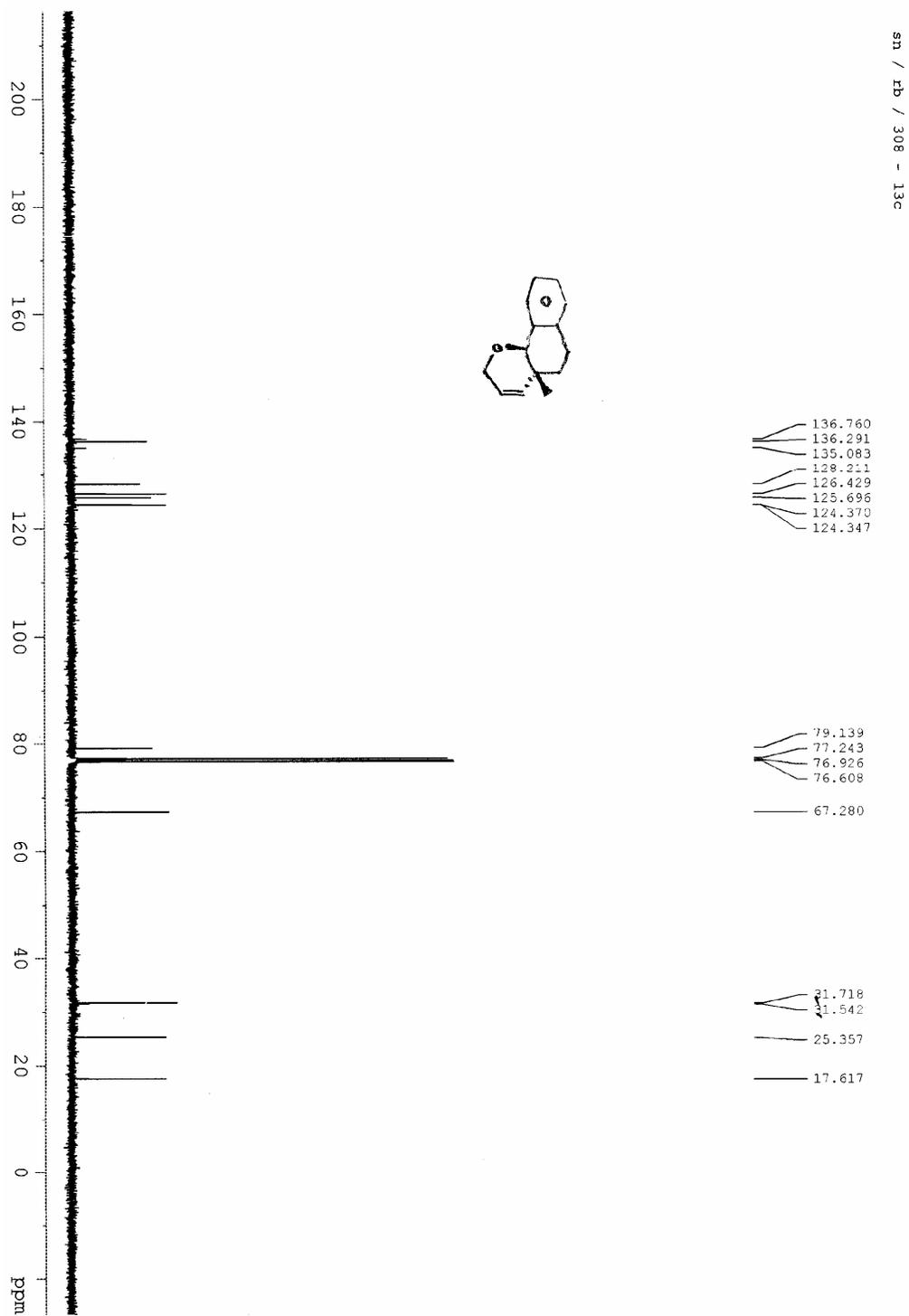


¹³C NMR of compound 51

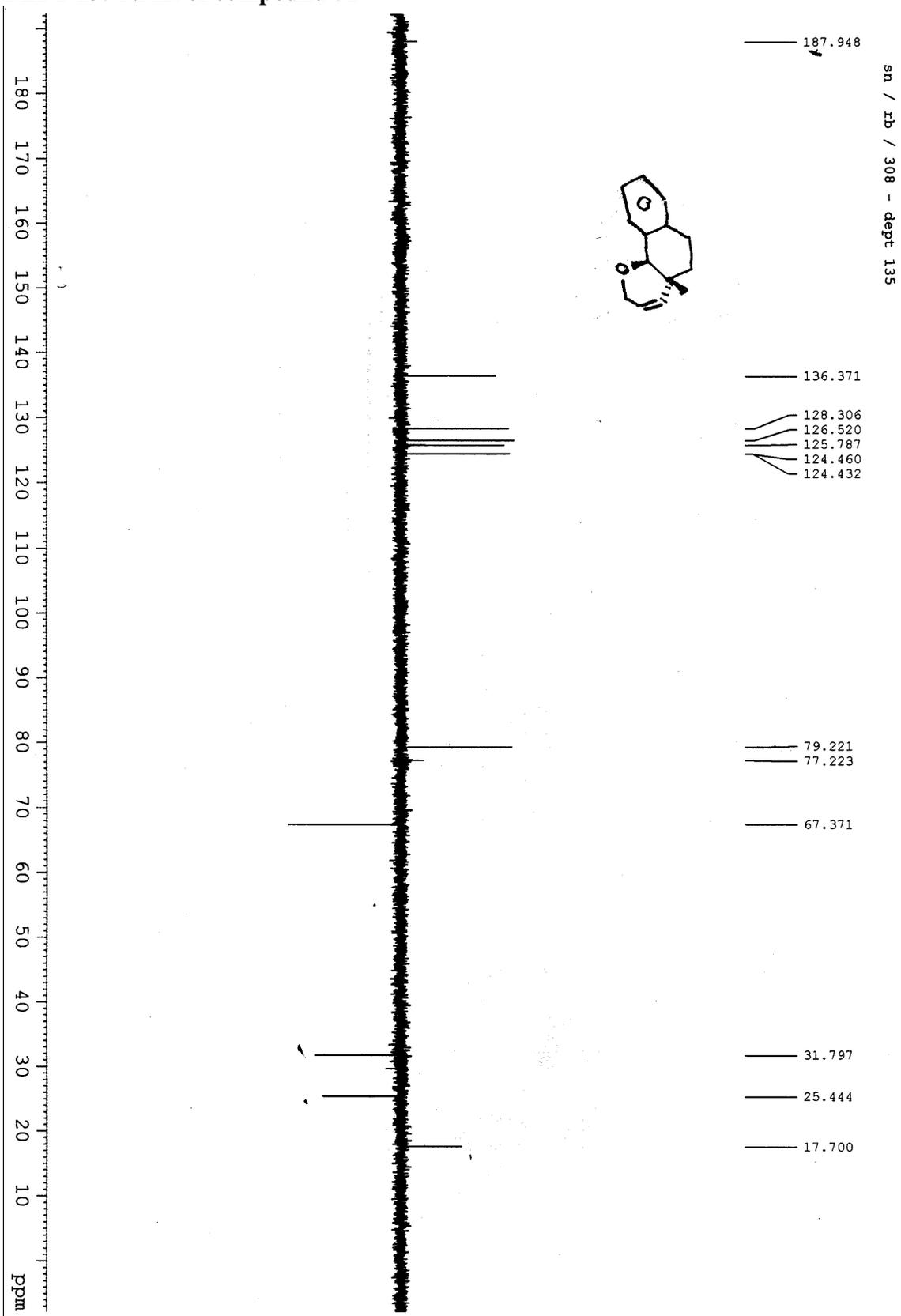


snc/rb/285u
C13CPD CDCl3 D:\ ITR 2

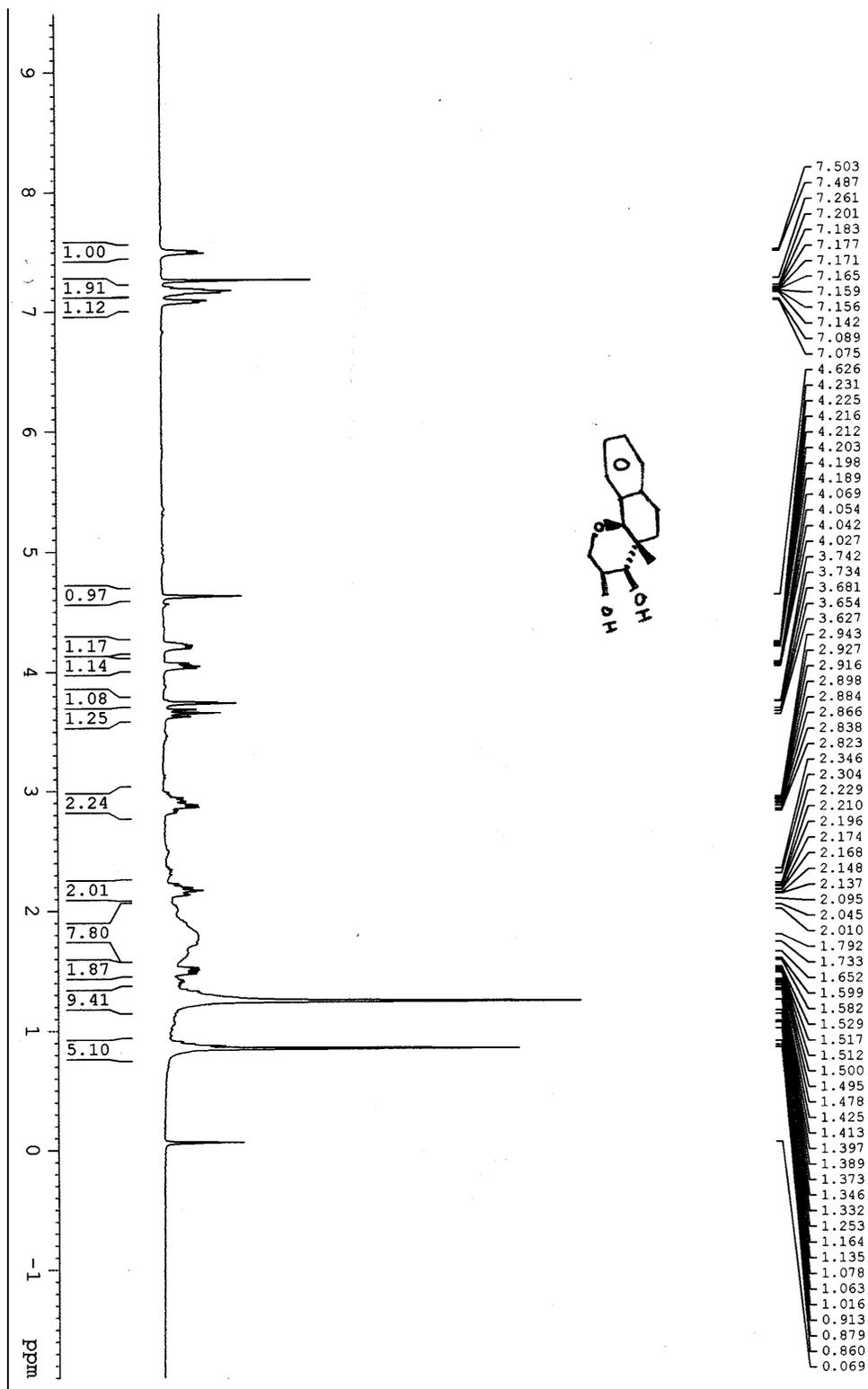
¹³C NMR of compound 52



DEPT 135 NMR of compound 52

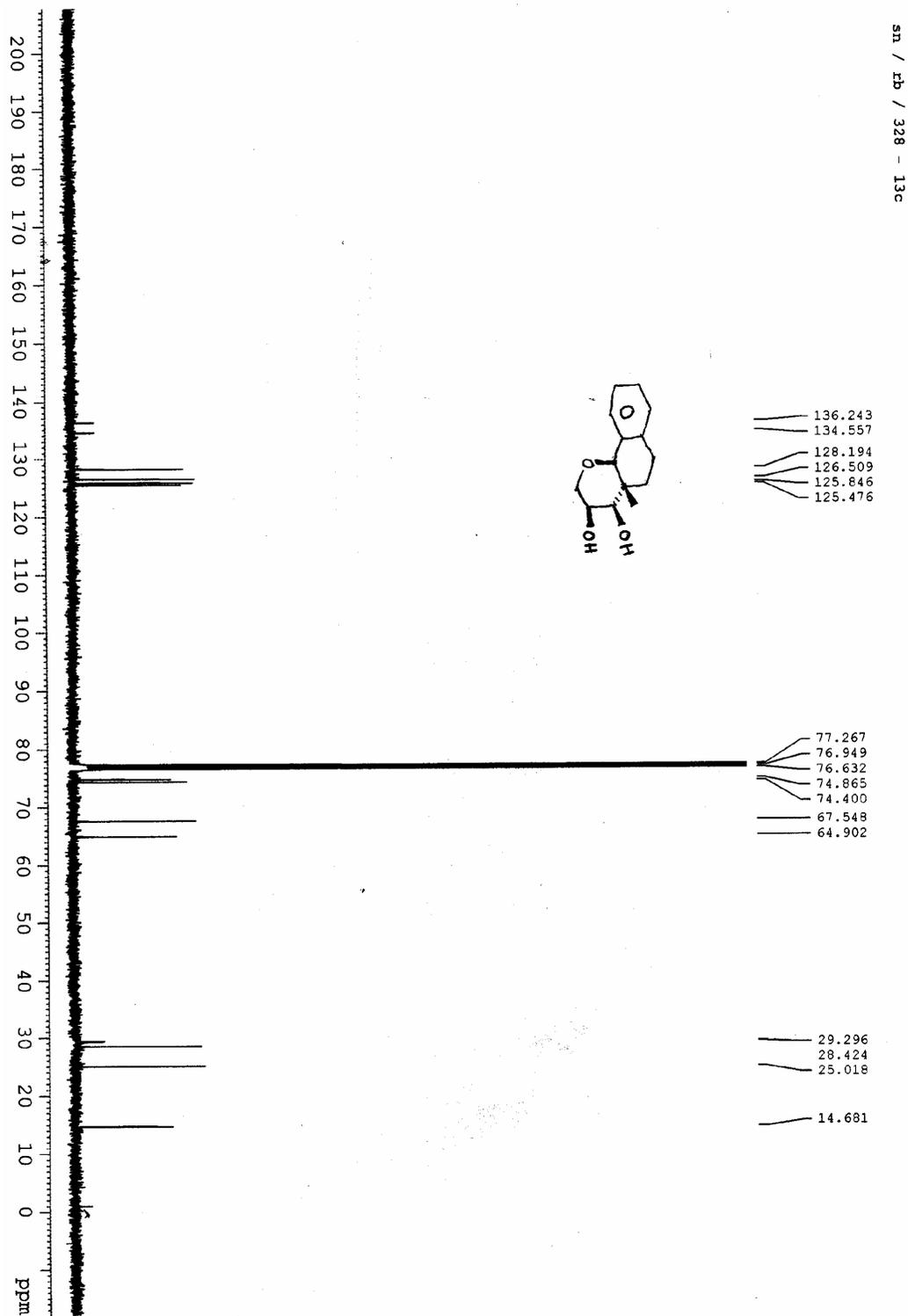


^1H NMR of compound 53

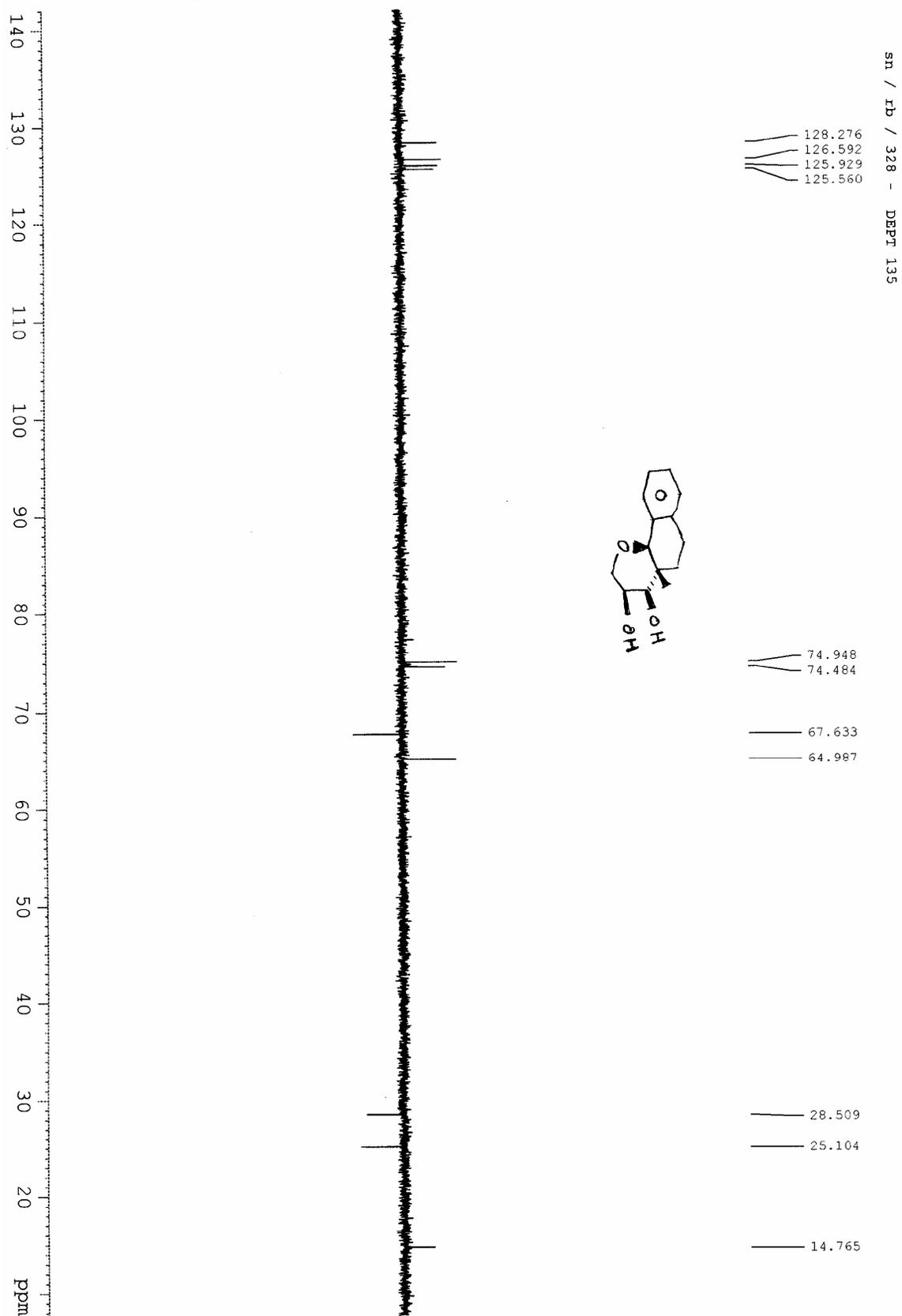


sn / rd / 328

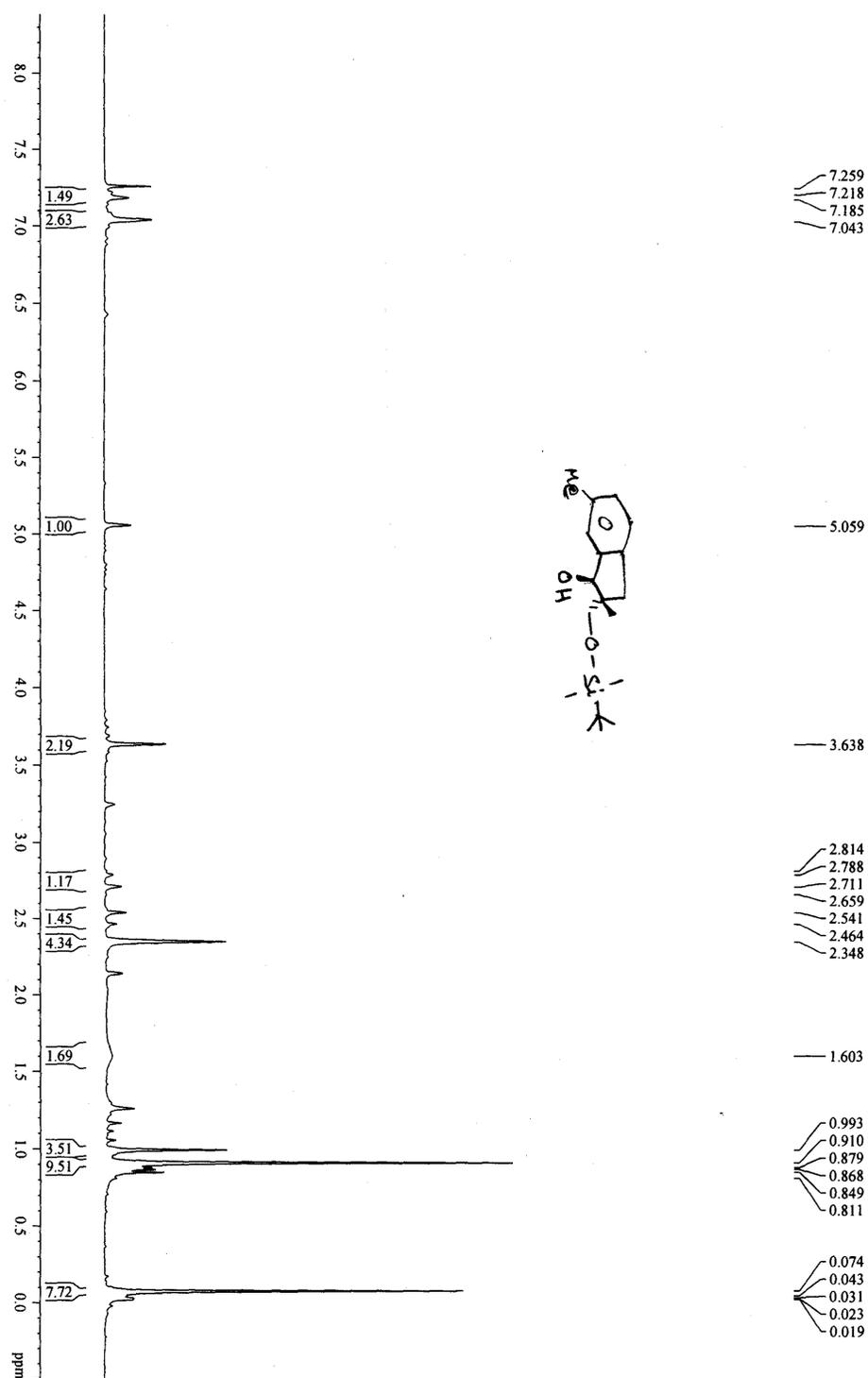
¹³C NMR of compound 53



DEPT 135 of compound 53

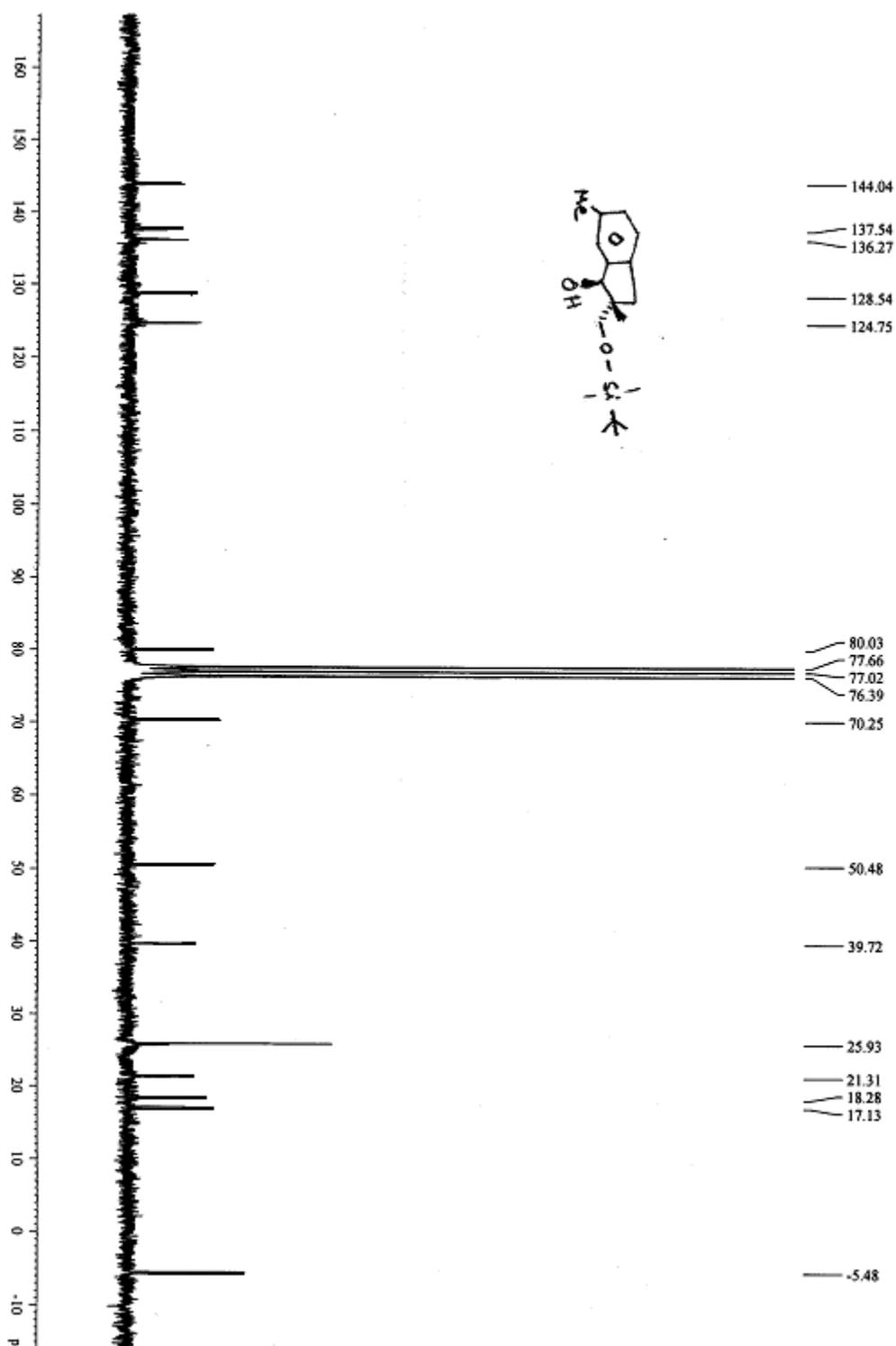


¹H NMR of compound 54



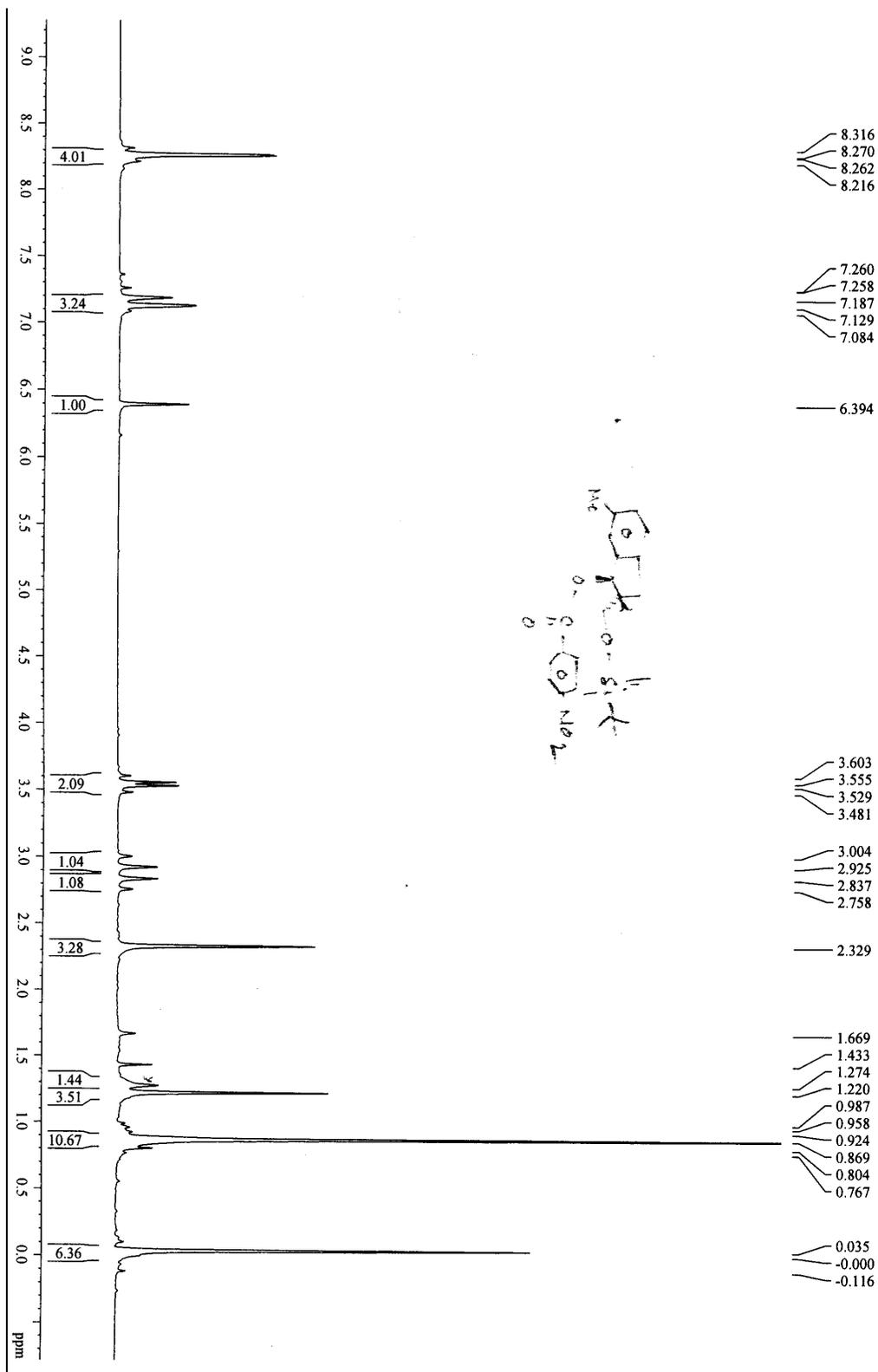
sn/rb/351
PROTON CDCl3 D:\ ITRK 2

¹³C NMR of compound 54



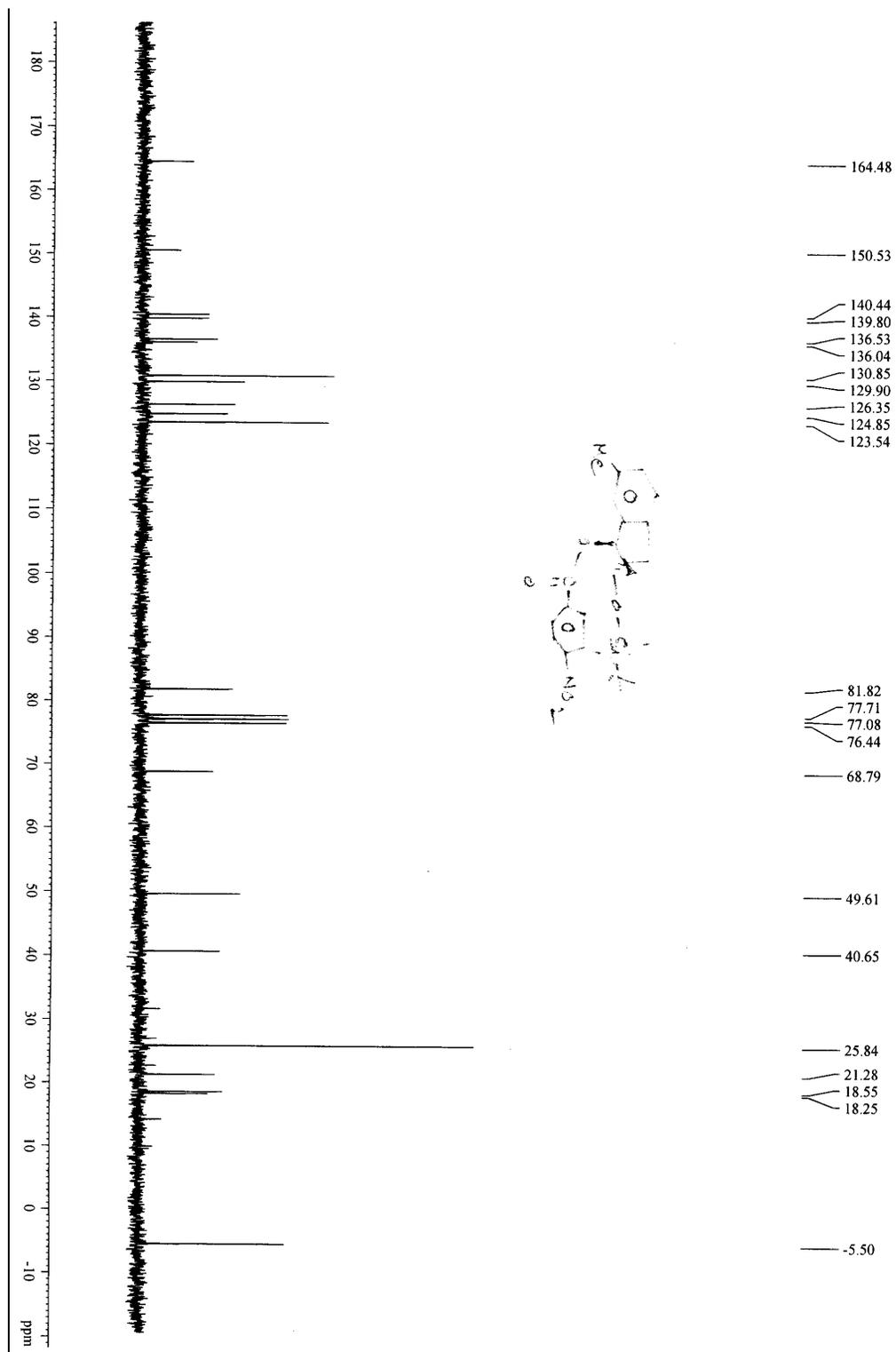
snc/rb/351

¹H NMR of compound 55



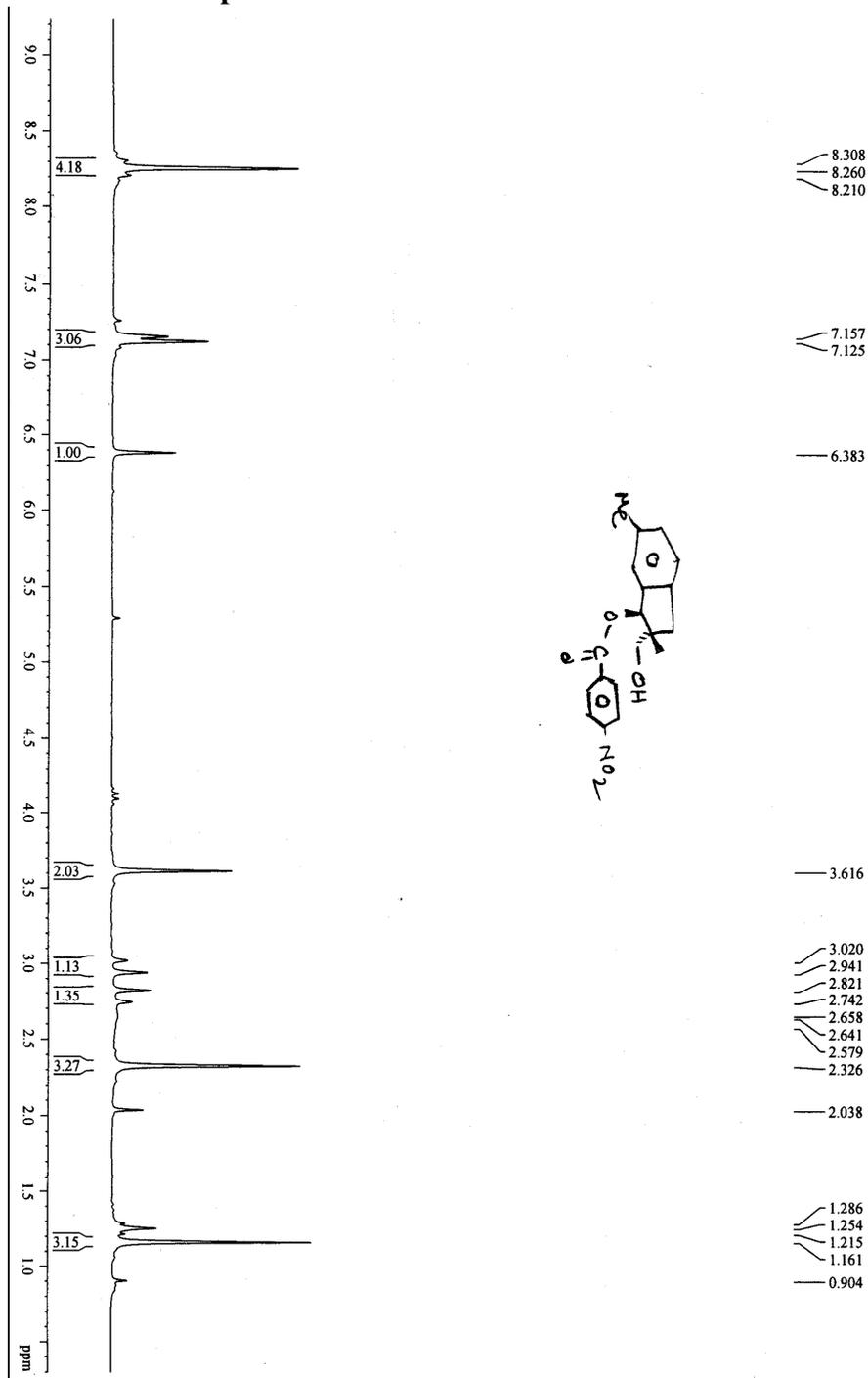
sn/rb/353

¹³C NMR of compound 55



snc/rb/353
C13CPD CDCl3 D:\ ITR 2

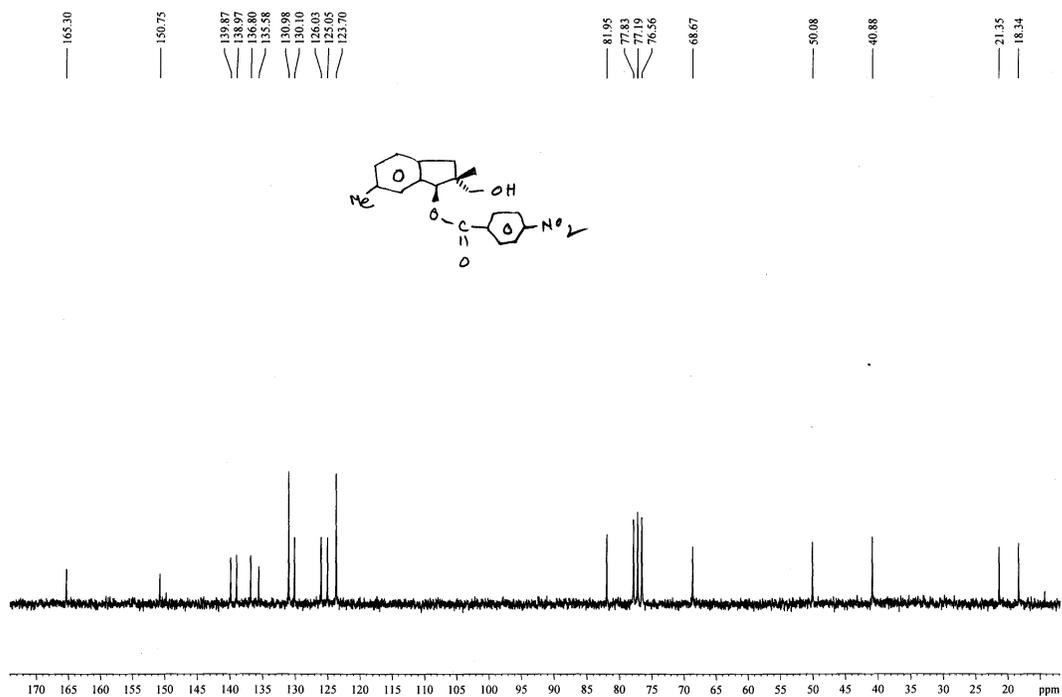
^1H NMR of compound 56



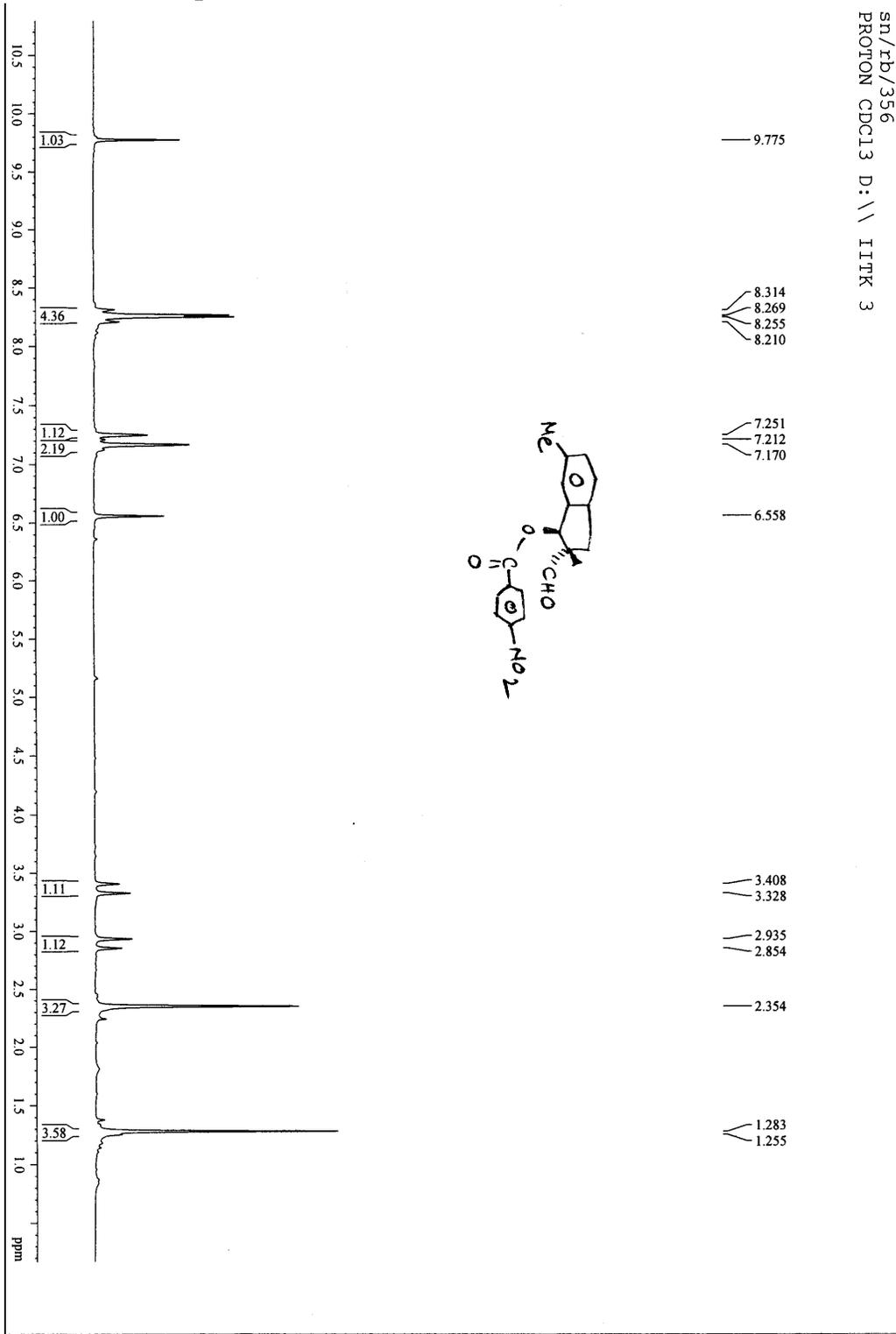
sn/rb/354

¹³C NMR of compound 56

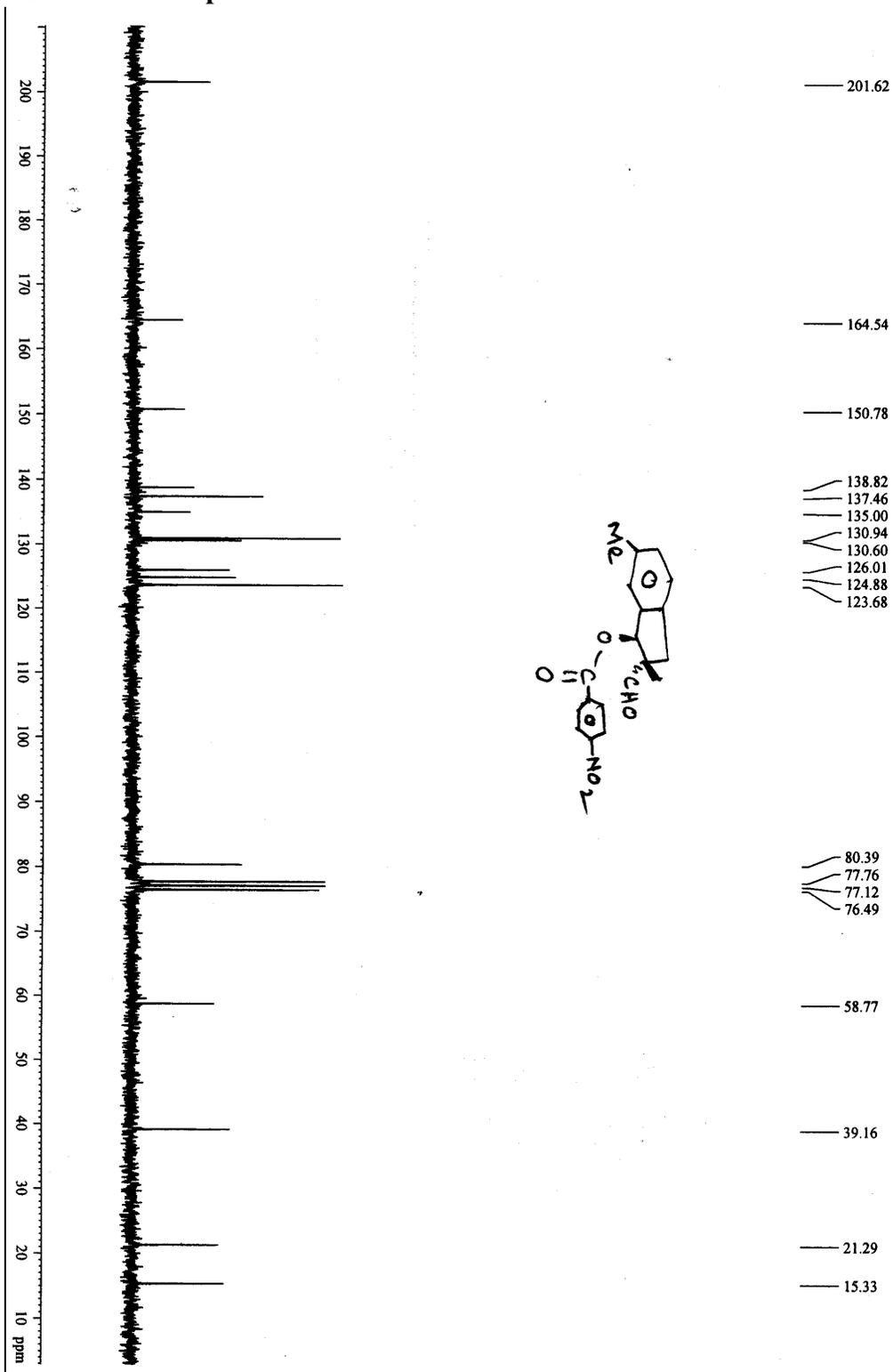
snc/rb/354
C13CPD CDC13 D:\ IITK 34



¹H NMR of compound 57

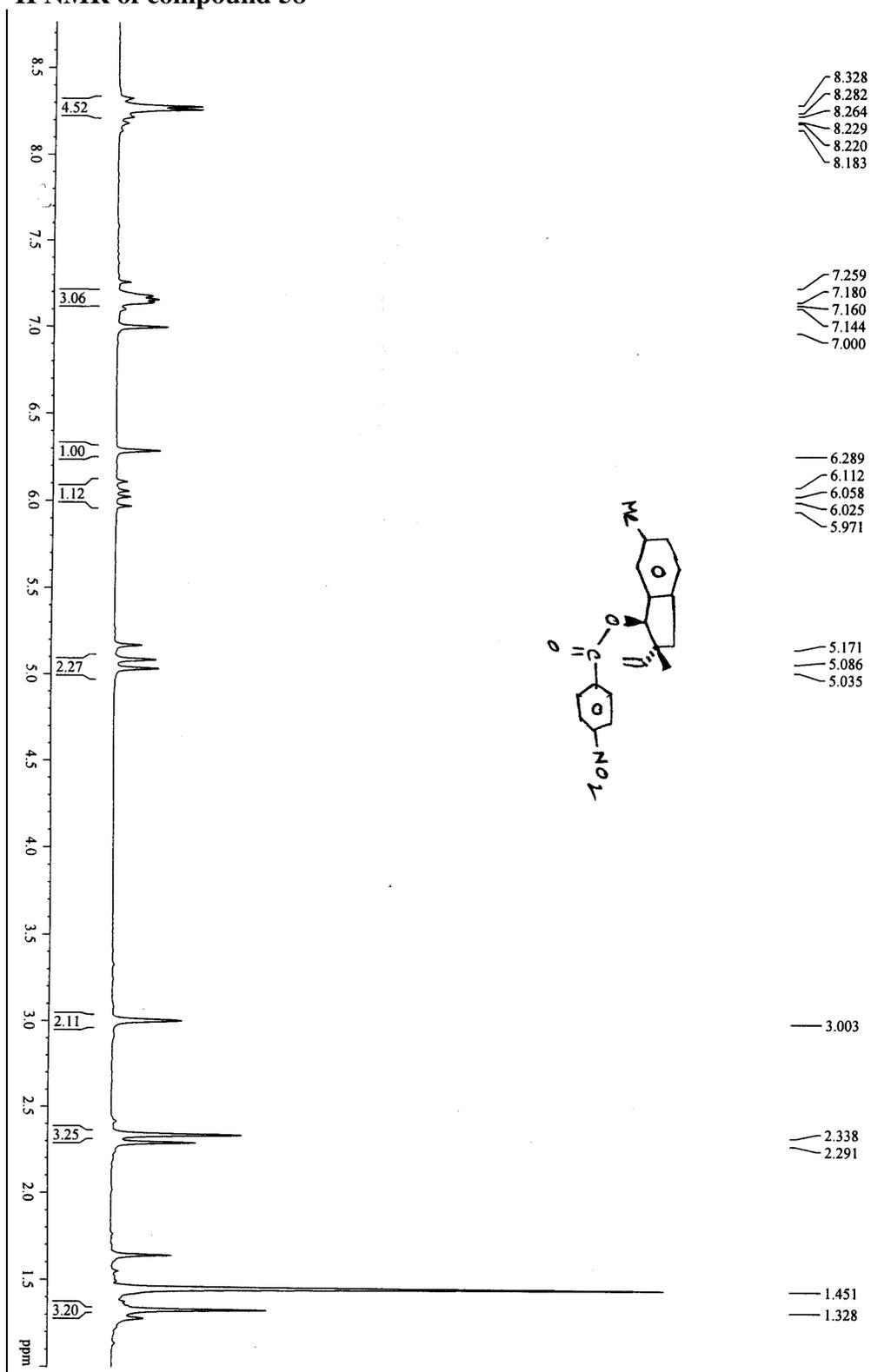


¹³C NMR of compound 57



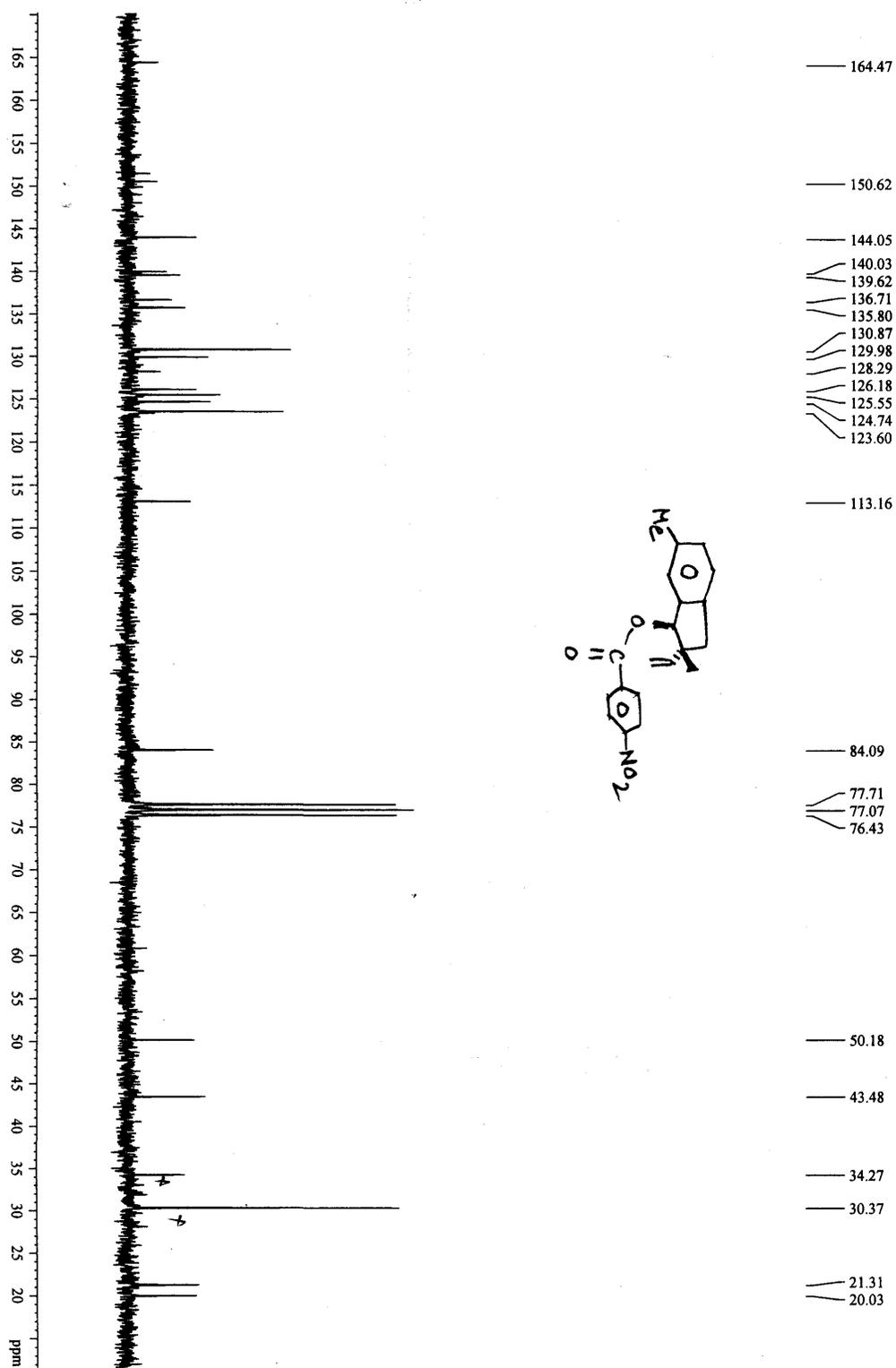
sn/rb/356
C13CPD CDCl3 D:\ IITK 23

¹H NMR of compound 58



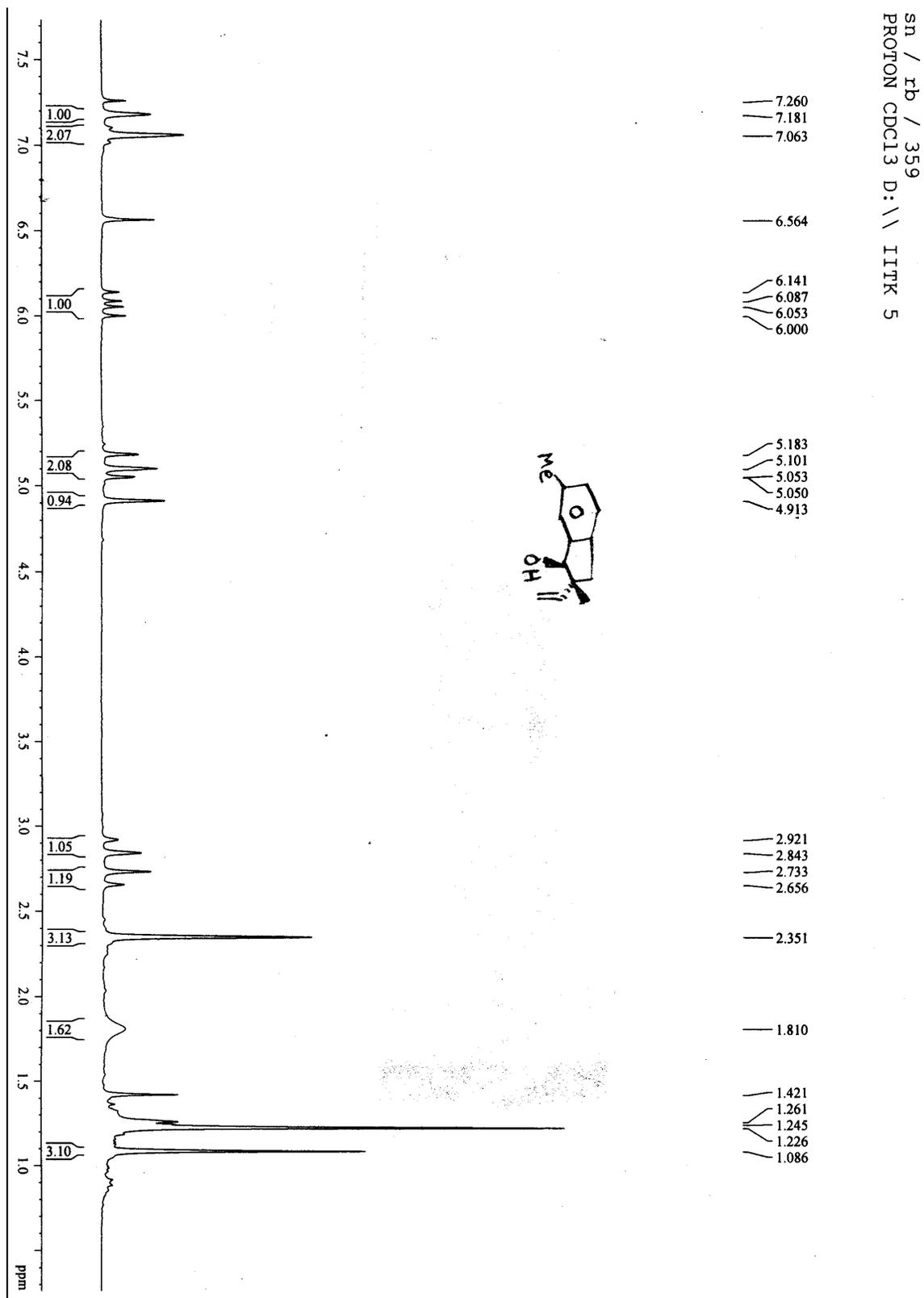
sn/rb/357

¹³C NMR of compound 58

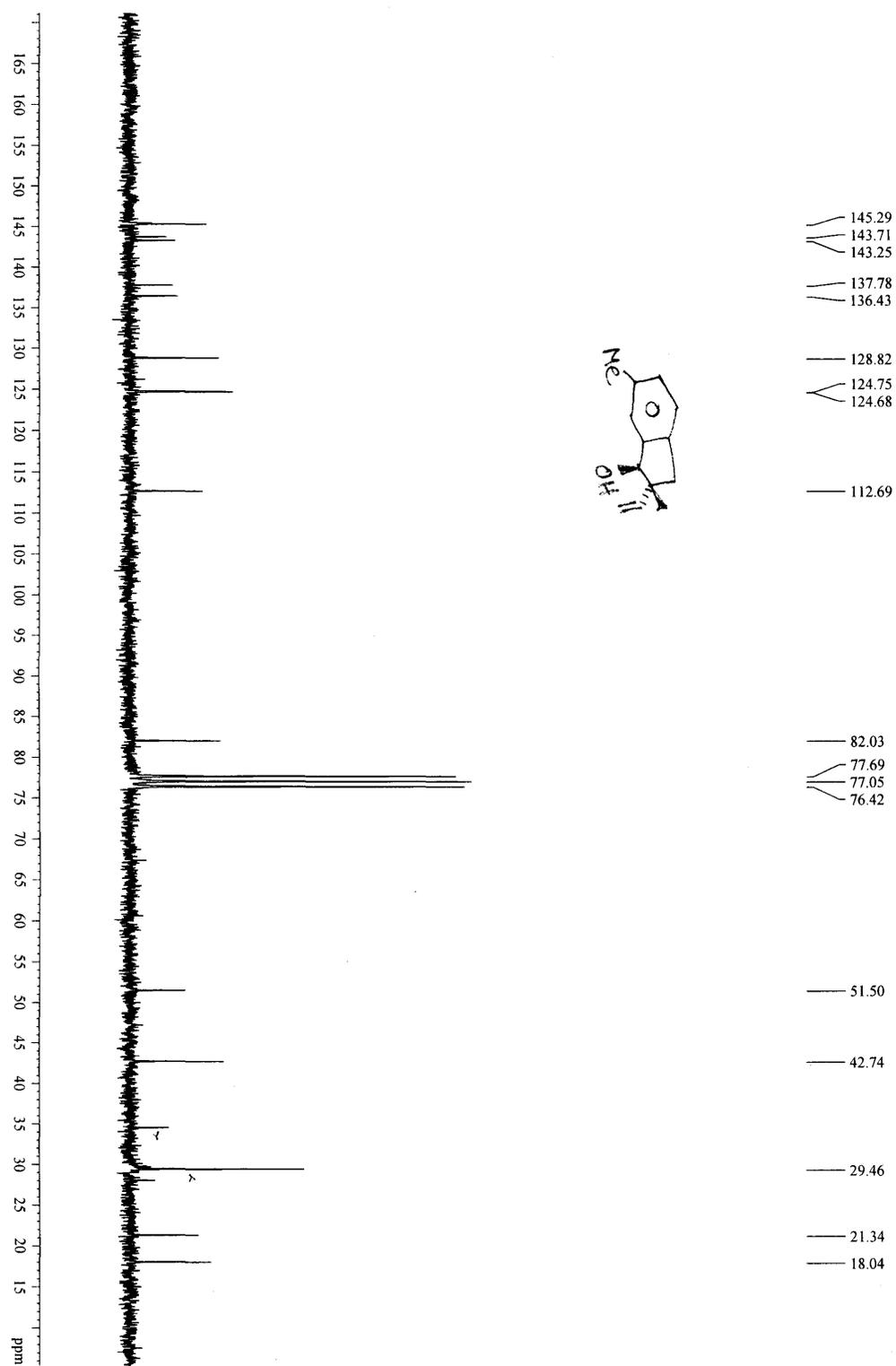


snc/rb/357
C13CPD CDCl3 D:\ IITK 2

¹H NMR of compound 59

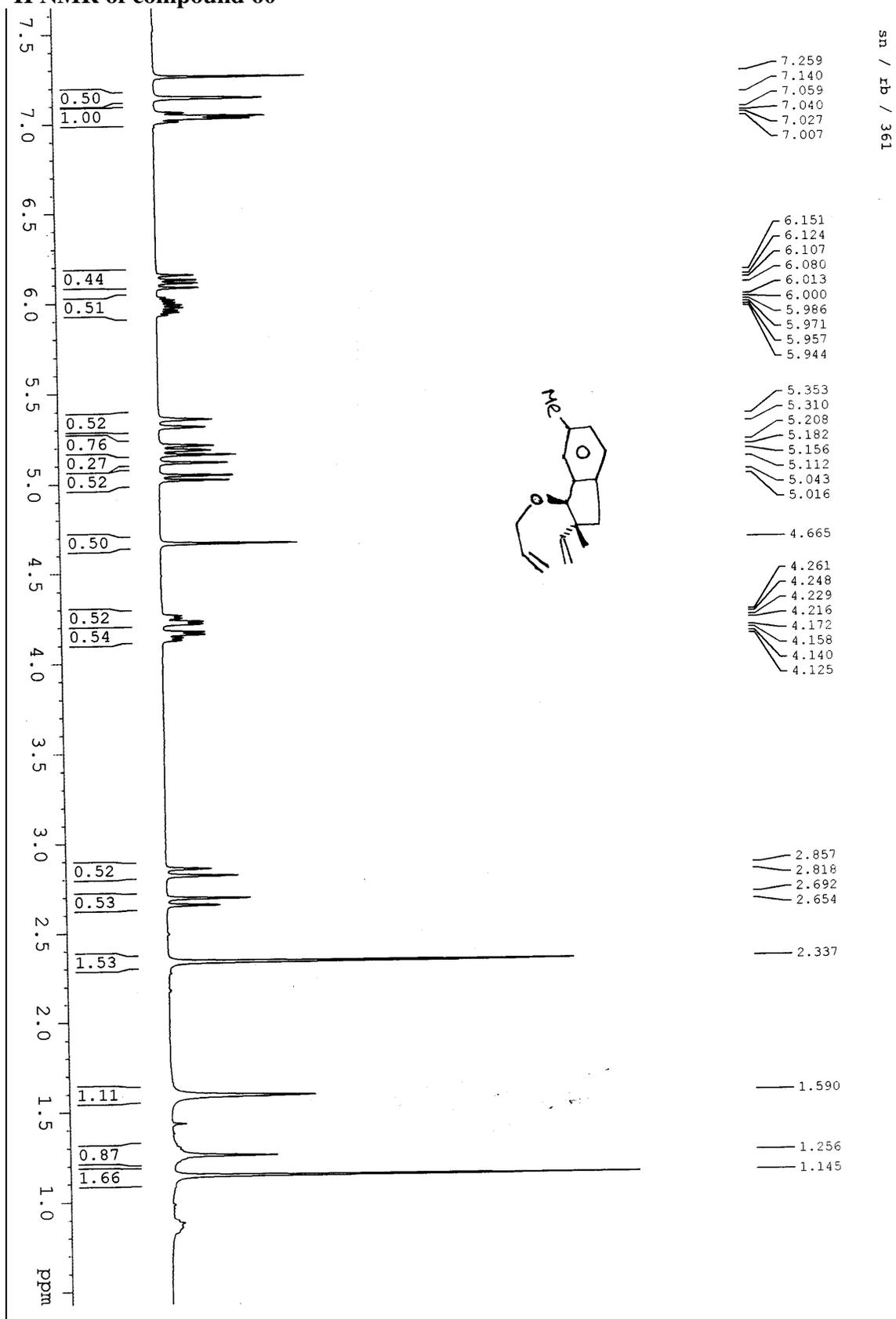


¹³C NMR of compound 59

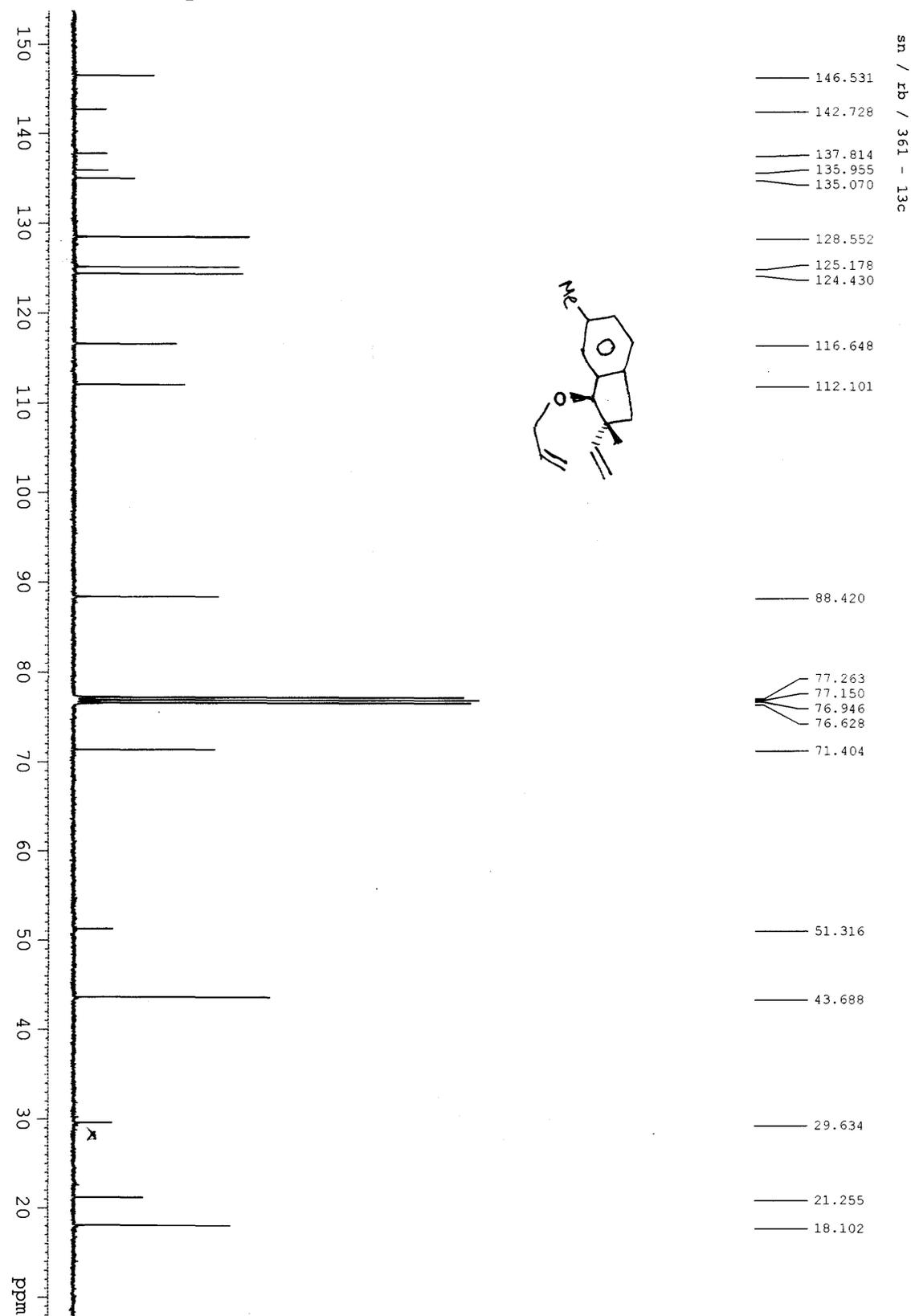


snc/rb/359
C13CPD CDCl3 D:\ IITK 2

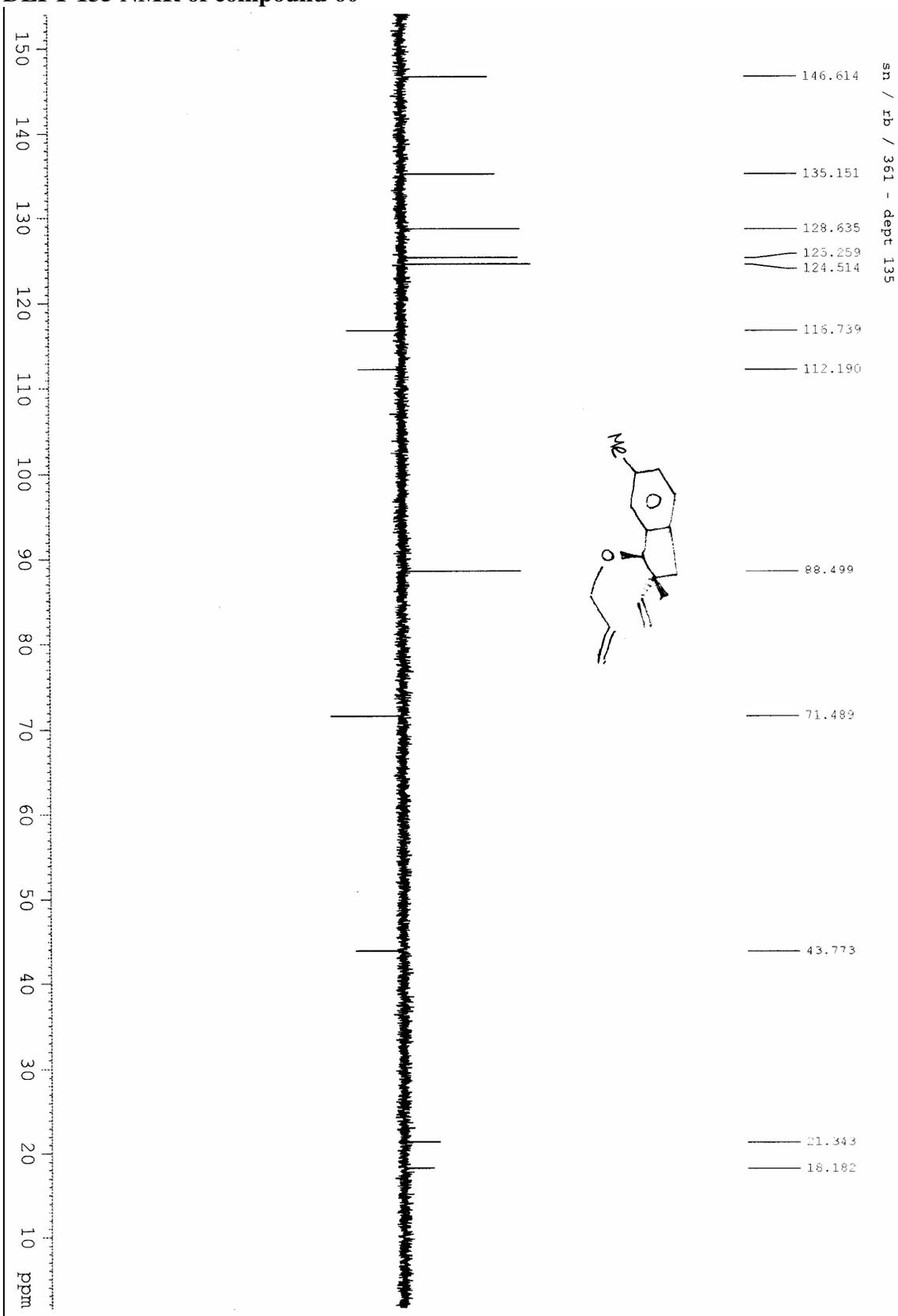
¹H NMR of compound 60



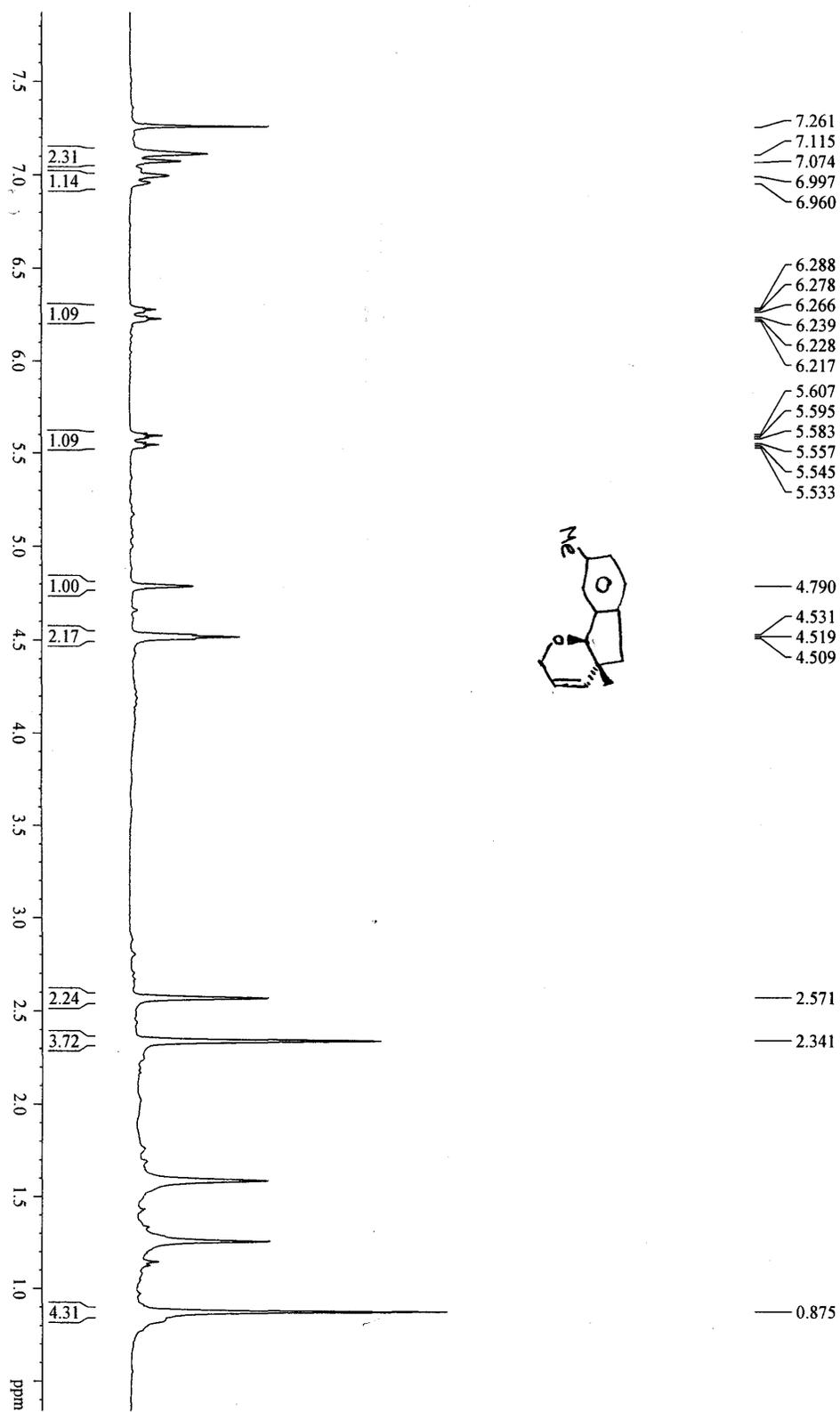
¹³C NMR of compound 60



DEPT 135 NMR of compound 60

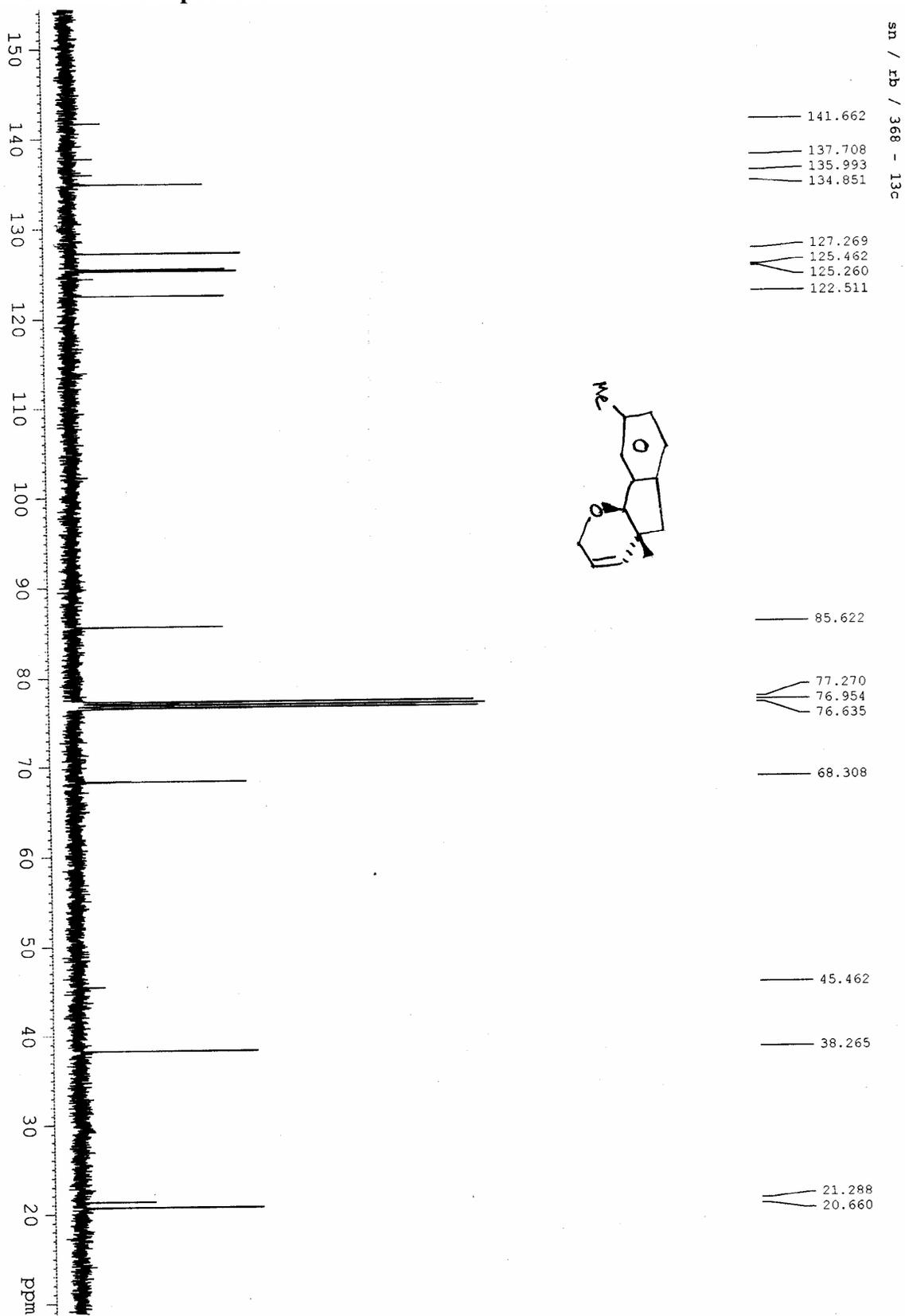


¹H NMR of compound 61

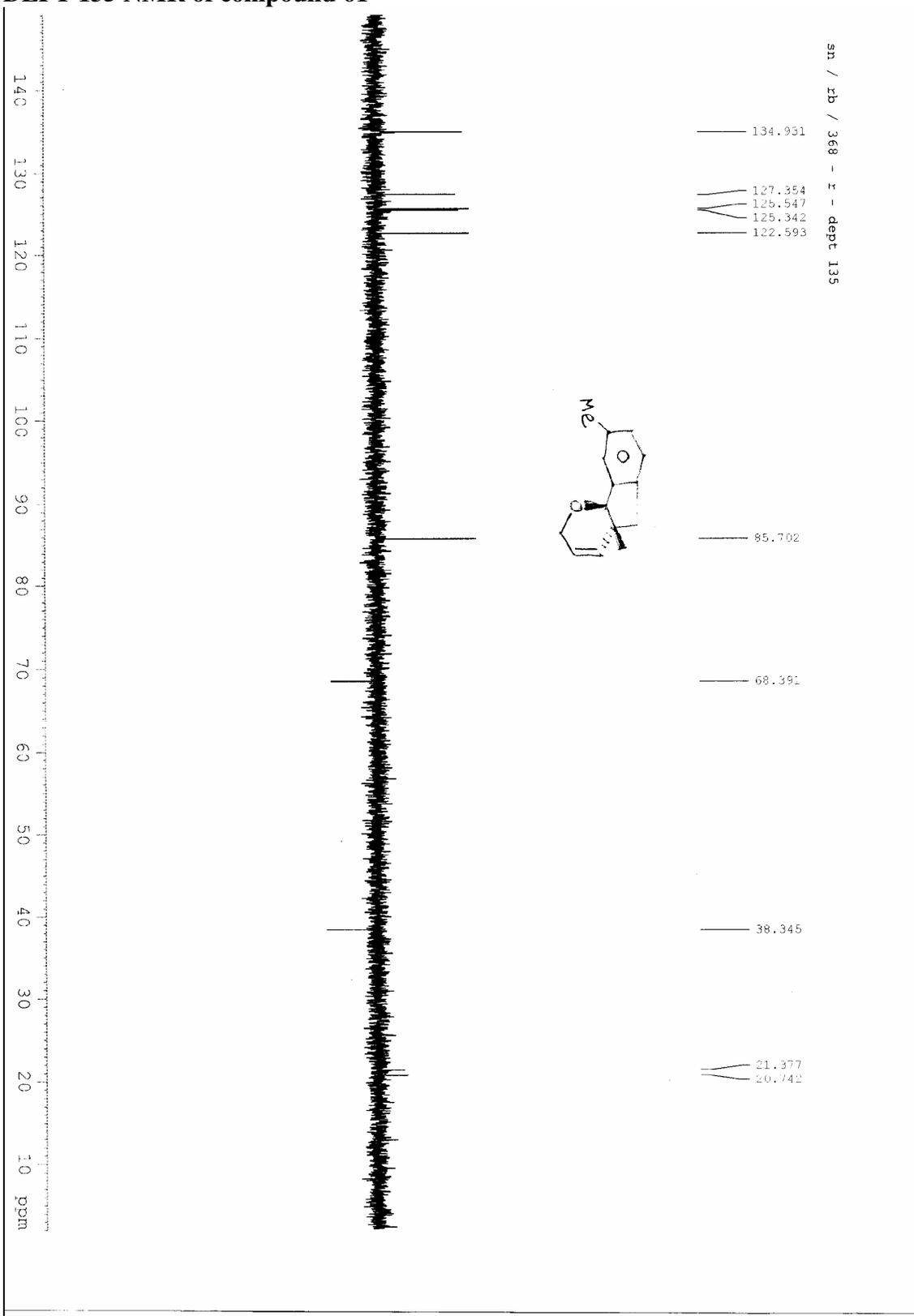


sn / rlb / 368

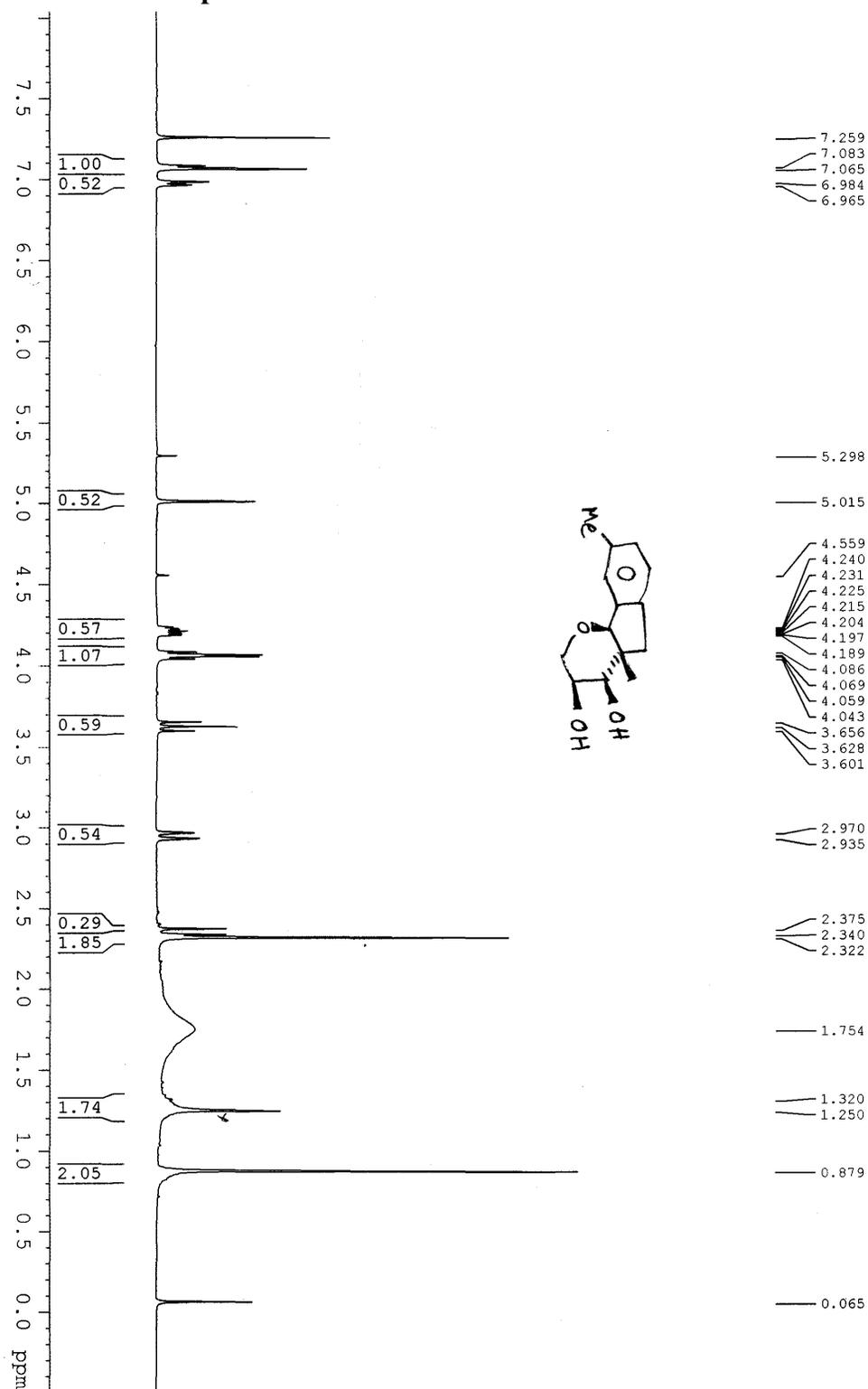
¹³C NMR of compound 61



DEPT 135 NMR of compound 61

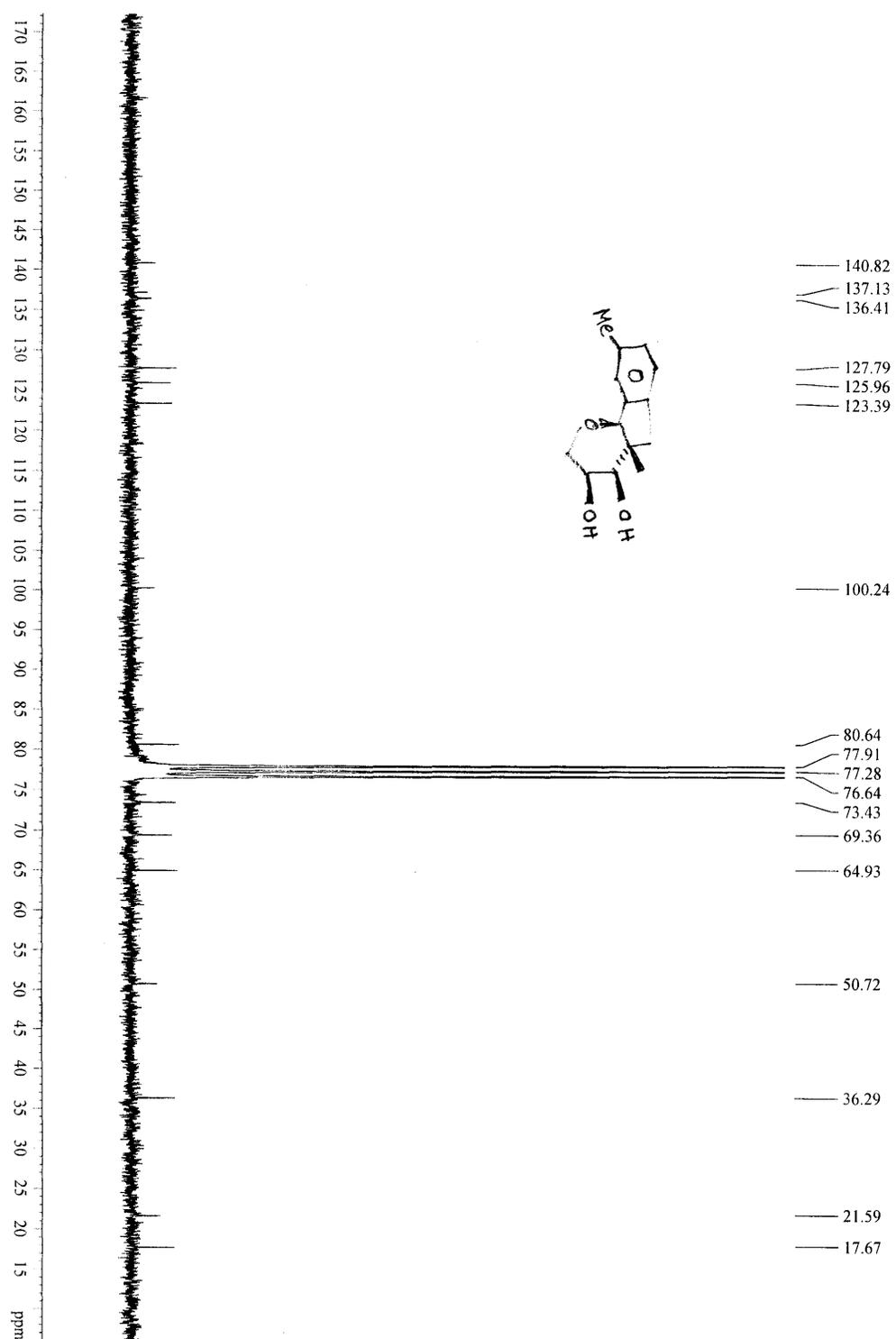


^1H NMR of compound 62



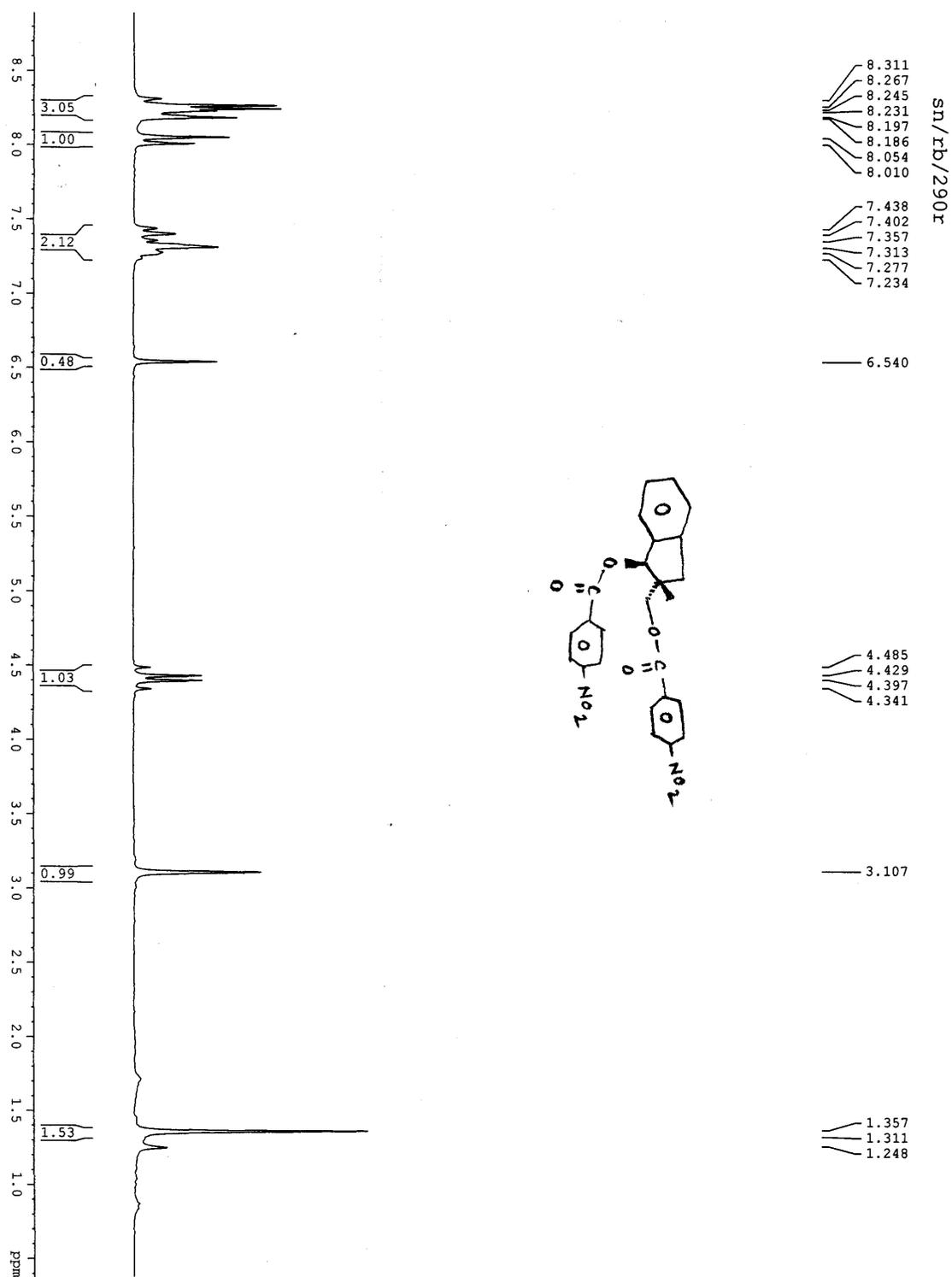
sm / hb / 372

¹³C NMR of compound 62

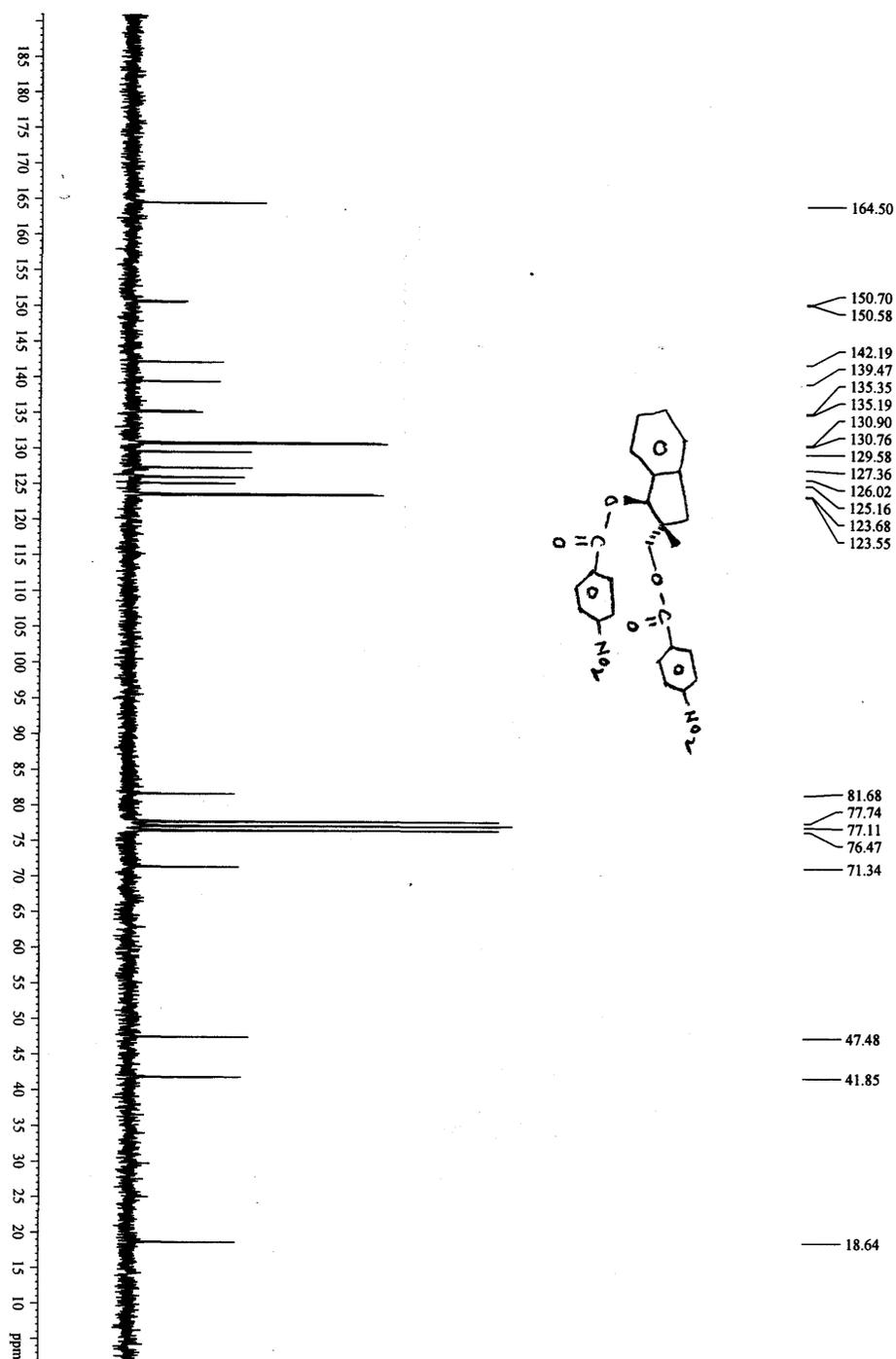


snc/rb/372
C13CPD CDCl3 D:\ IITK 2

¹H NMR of bis PNBz derivative of 27



¹³C NMR of bis PNBz derivative of 27



smc/ib/290r
C13CPD CDCl3 D:\ ITRK 2

- 164.50
- 150.70
- 150.58
- 142.19
- 139.47
- 135.35
- 135.19
- 130.90
- 130.76
- 129.58
- 127.36
- 126.02
- 125.16
- 123.68
- 123.55
- 81.68
- 77.74
- 77.11
- 76.47
- 71.34
- 47.48
- 41.85
- 18.64