

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

Rajib Bhuniya and Samik Nanda*

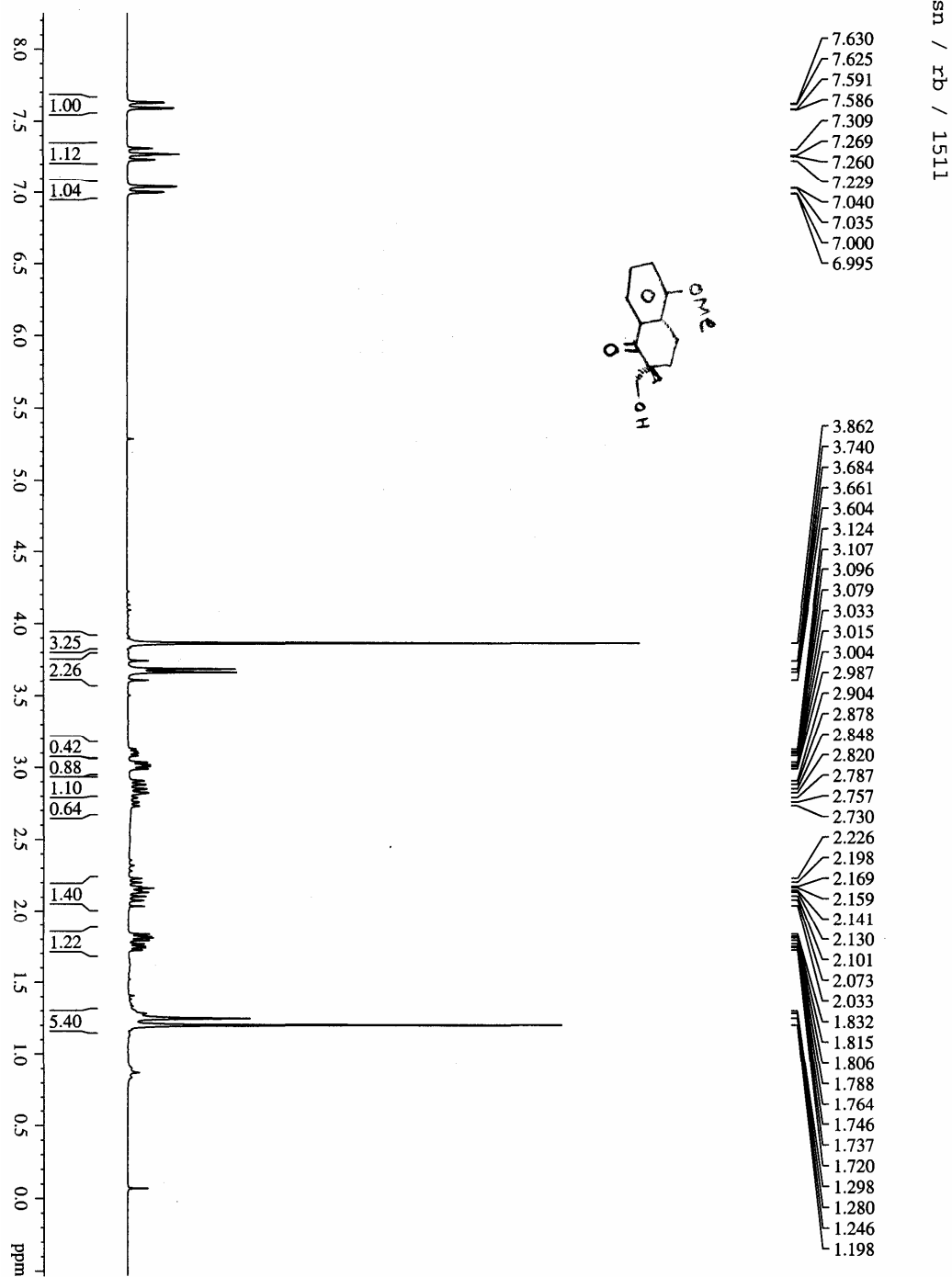
Department of Chemistry, Indian Institute of Technology, Kharagpur, 721302, India

snanda@chem.iitkgp.ernet.in

Supporting Information Part I

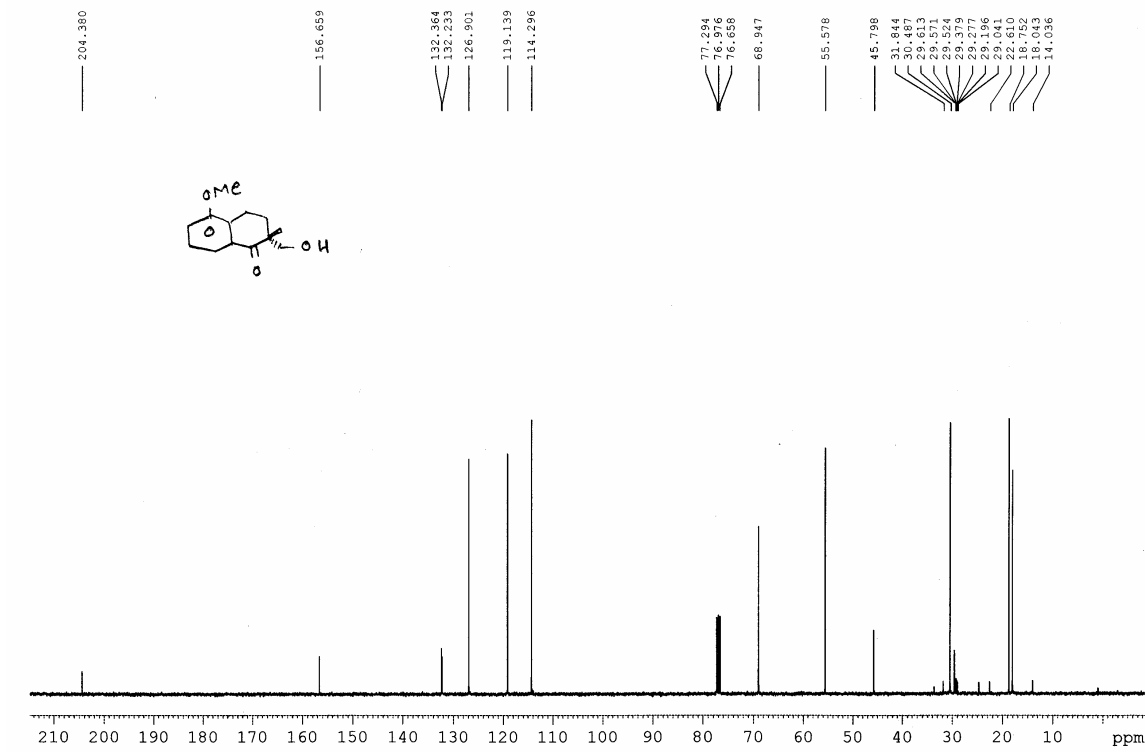
Contents	Page number
NMR spectra	2-134

¹H NMR of compound 2

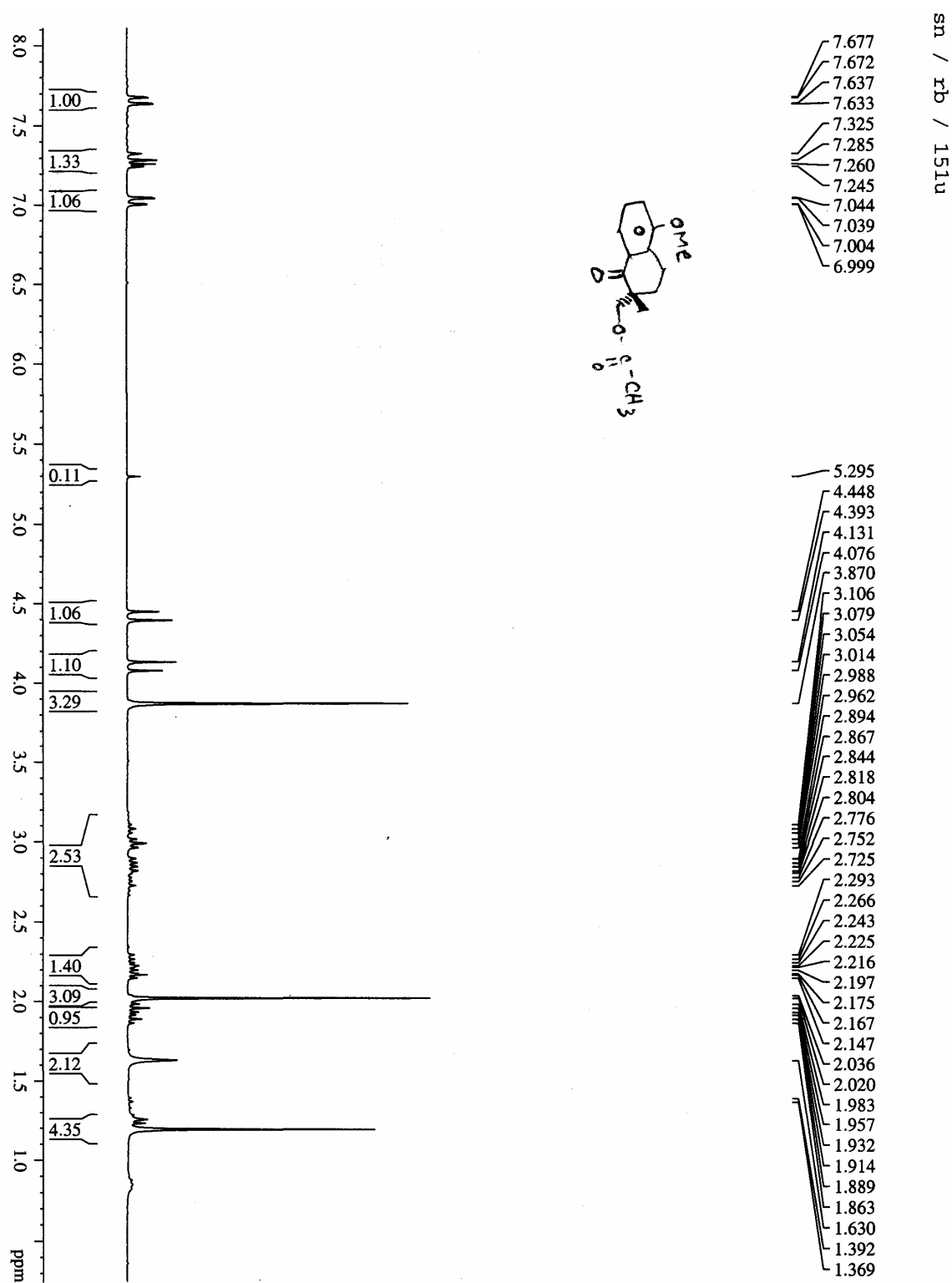


¹³C NMR of compound 2

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

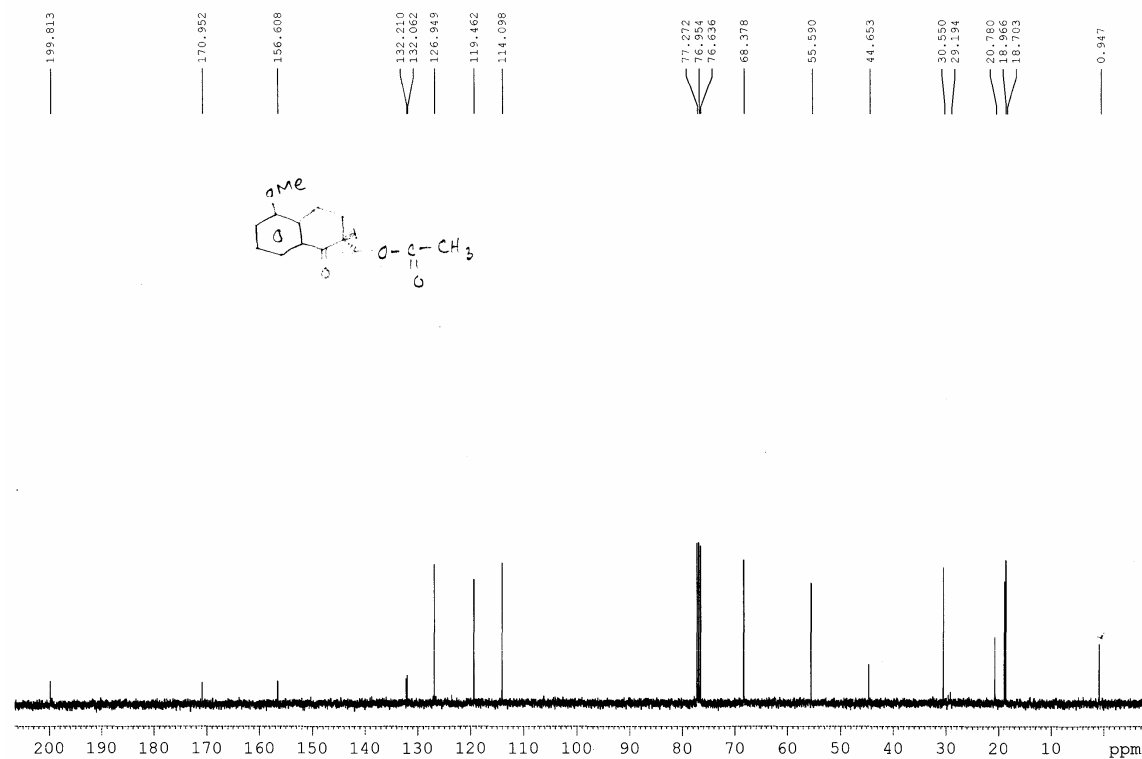


¹H NMR of acetate derivative of 2

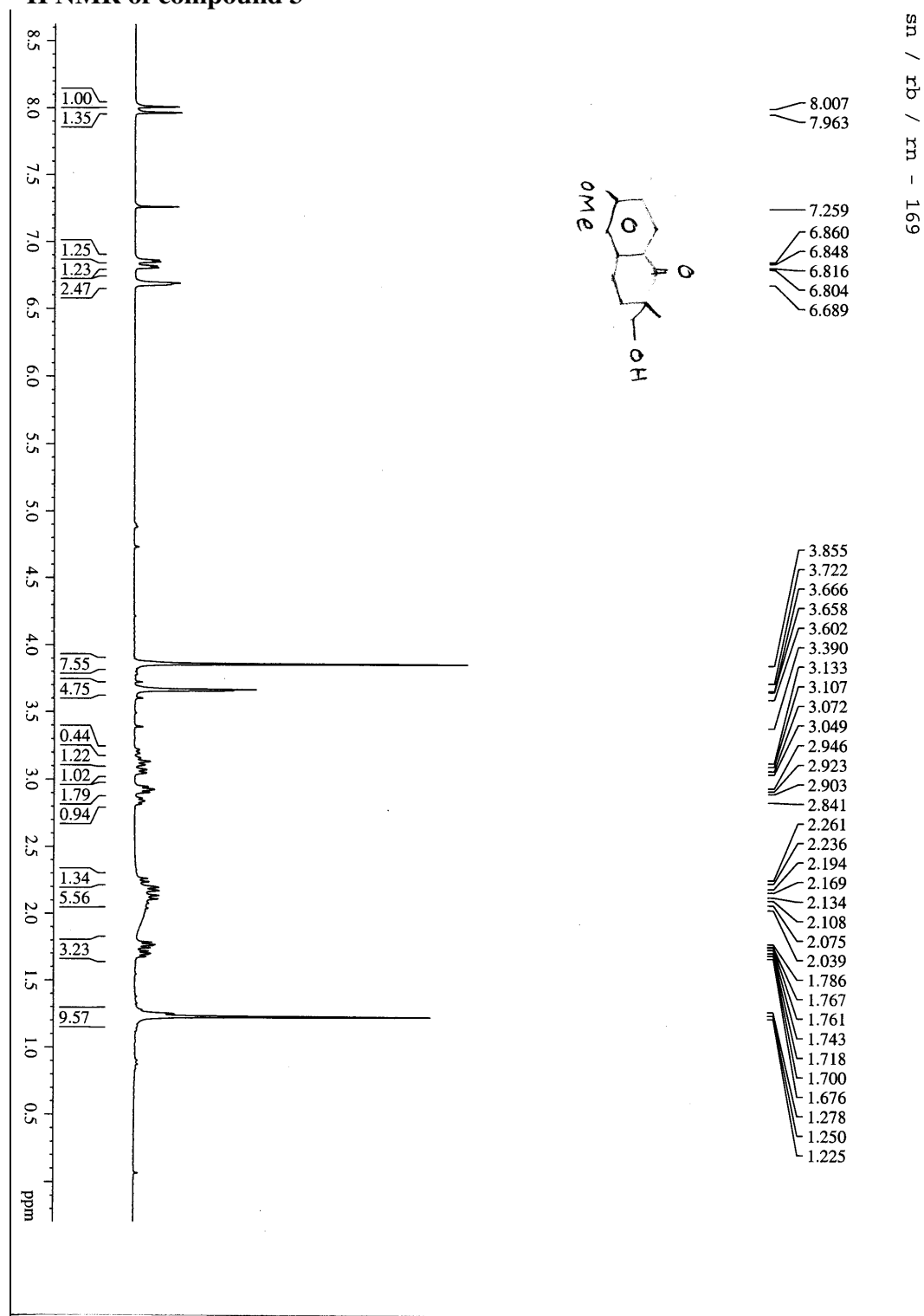


¹³C NMR of acetate derivative of 2

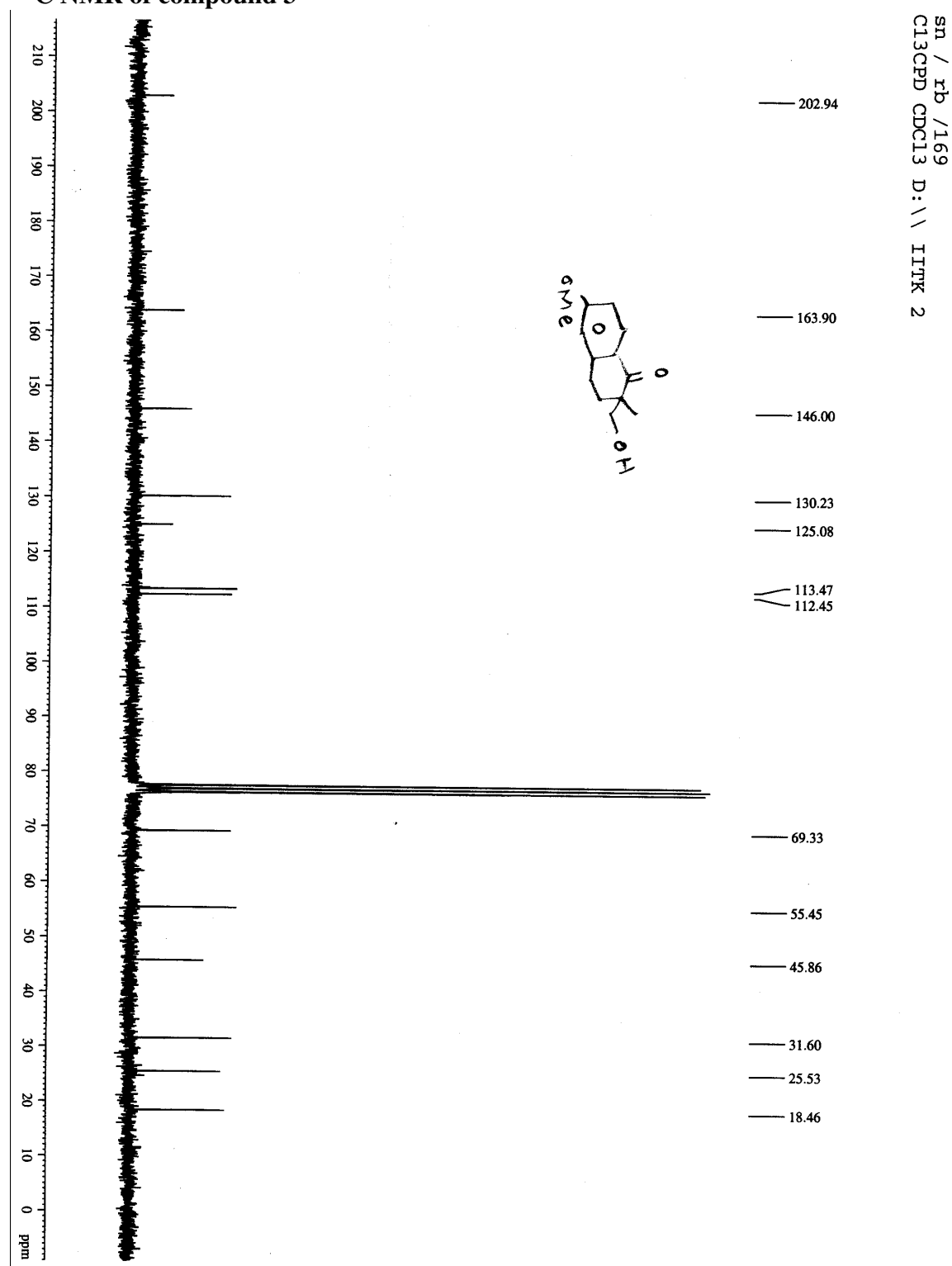
sn / rb / rn - 151 - 13c



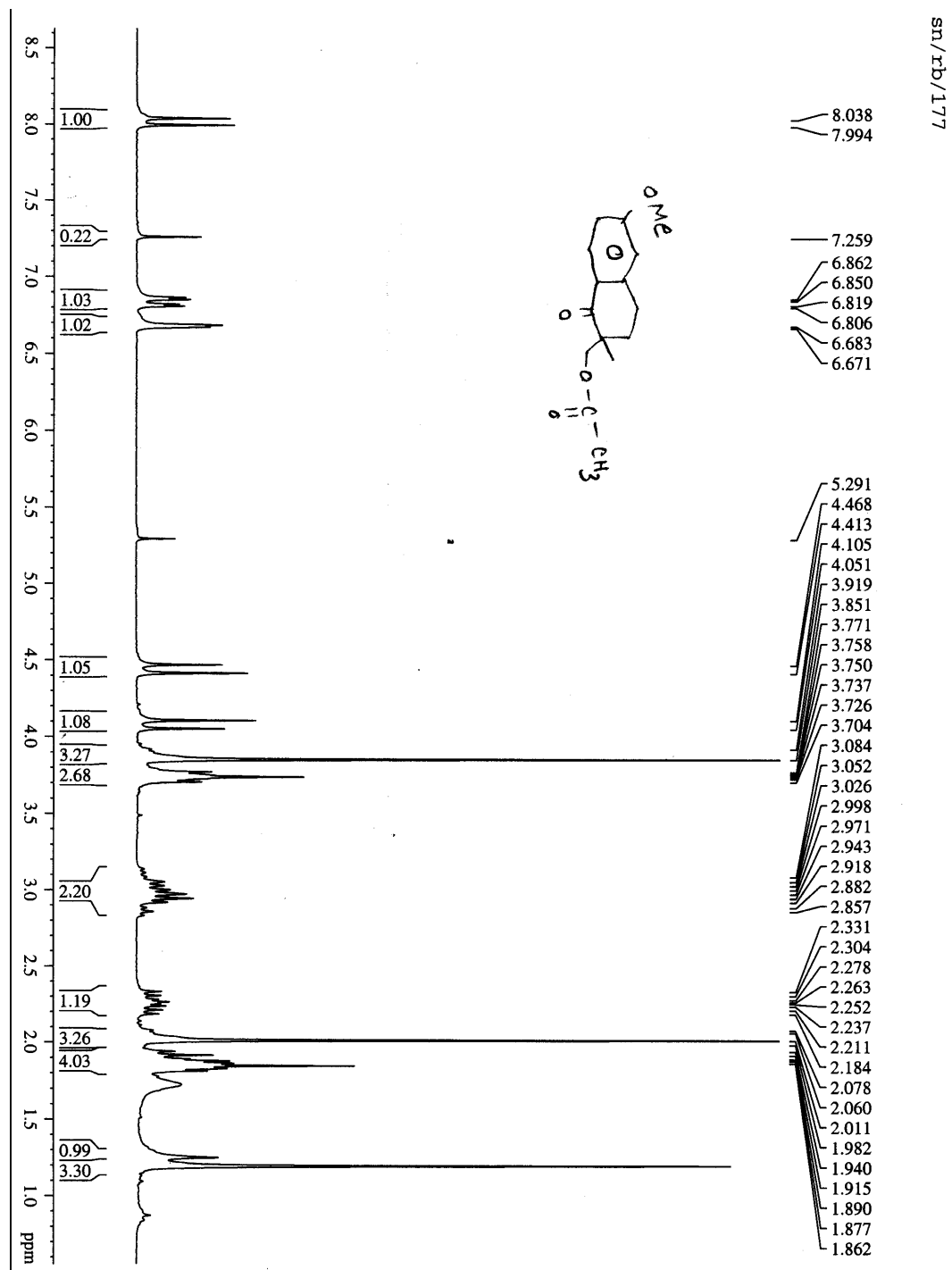
¹H NMR of compound 3



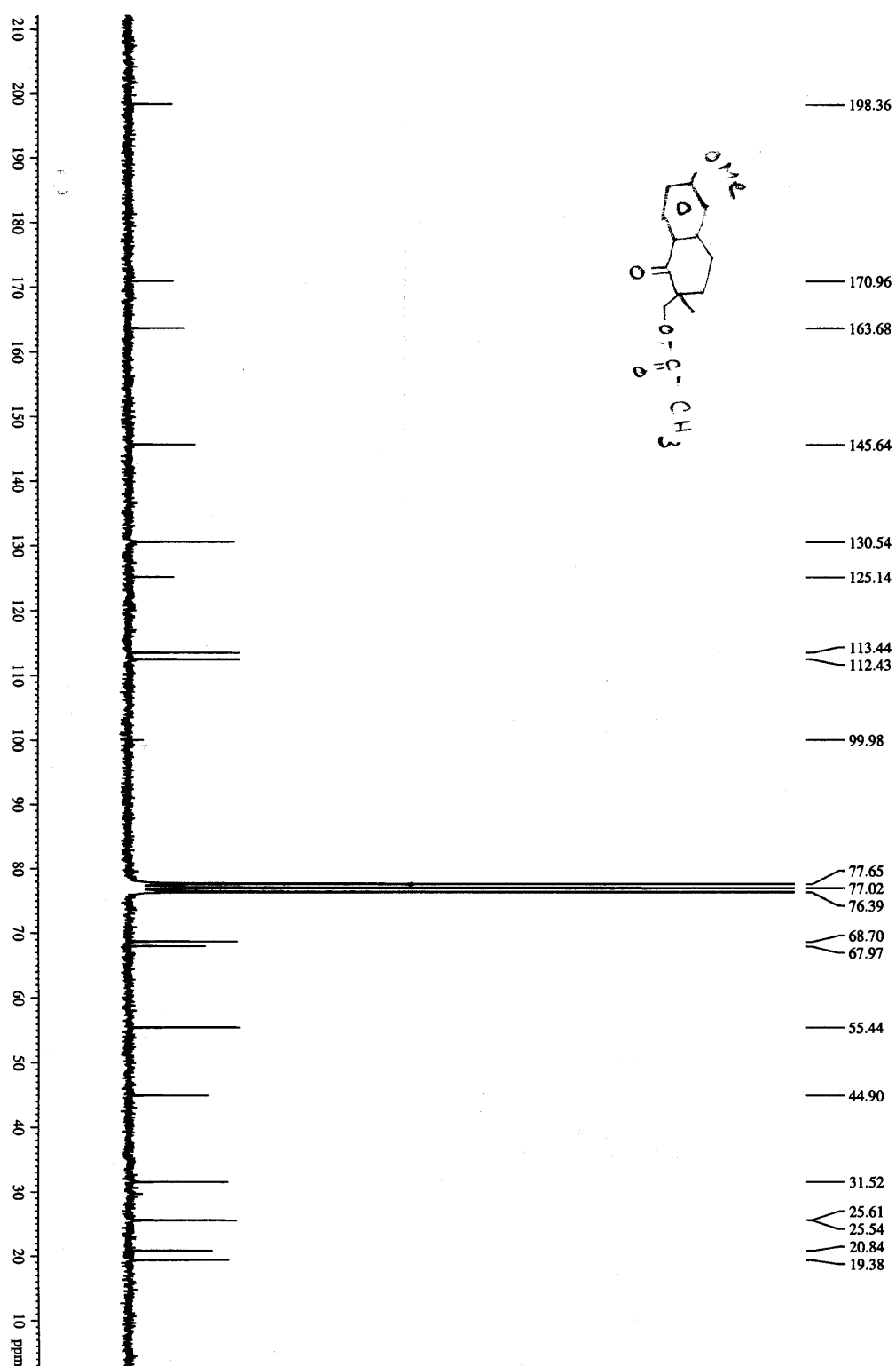
¹³C NMR of compound 3



¹H NMR of acetate derivative of 3

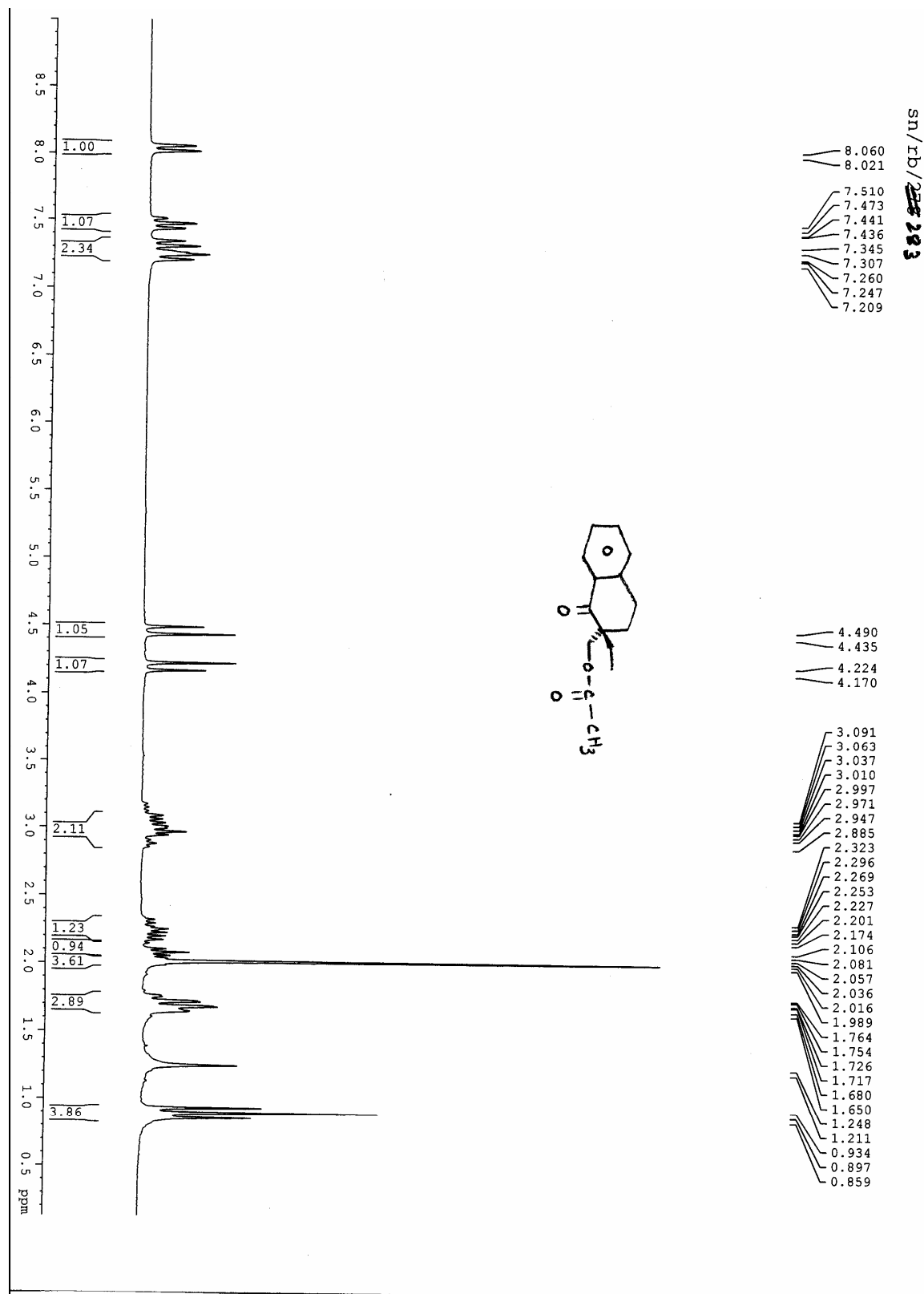


¹³C NMR of acetate derivative of 3

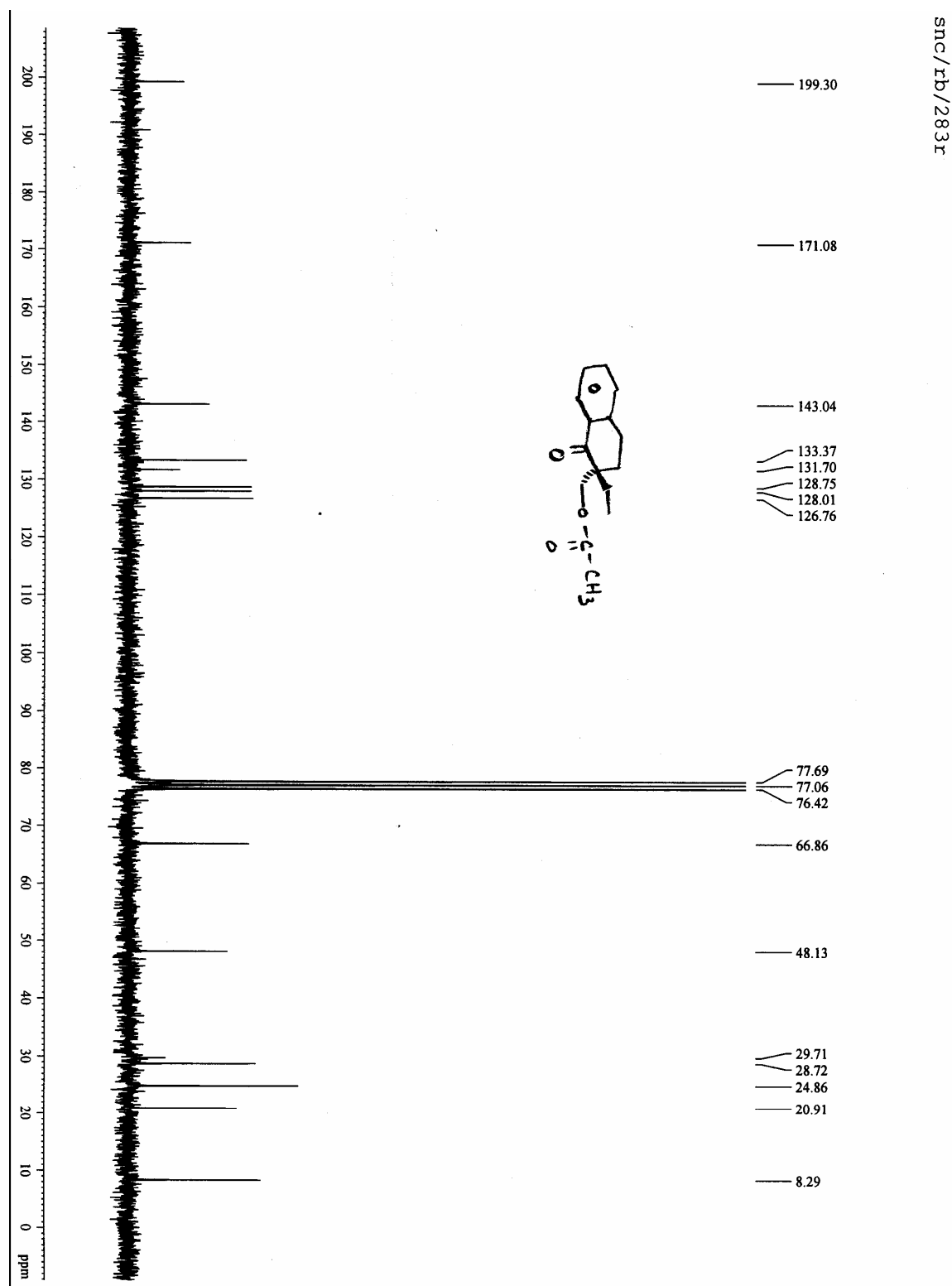


snc/rb/177
C13CPD CDCl3 D:\ IITK 12

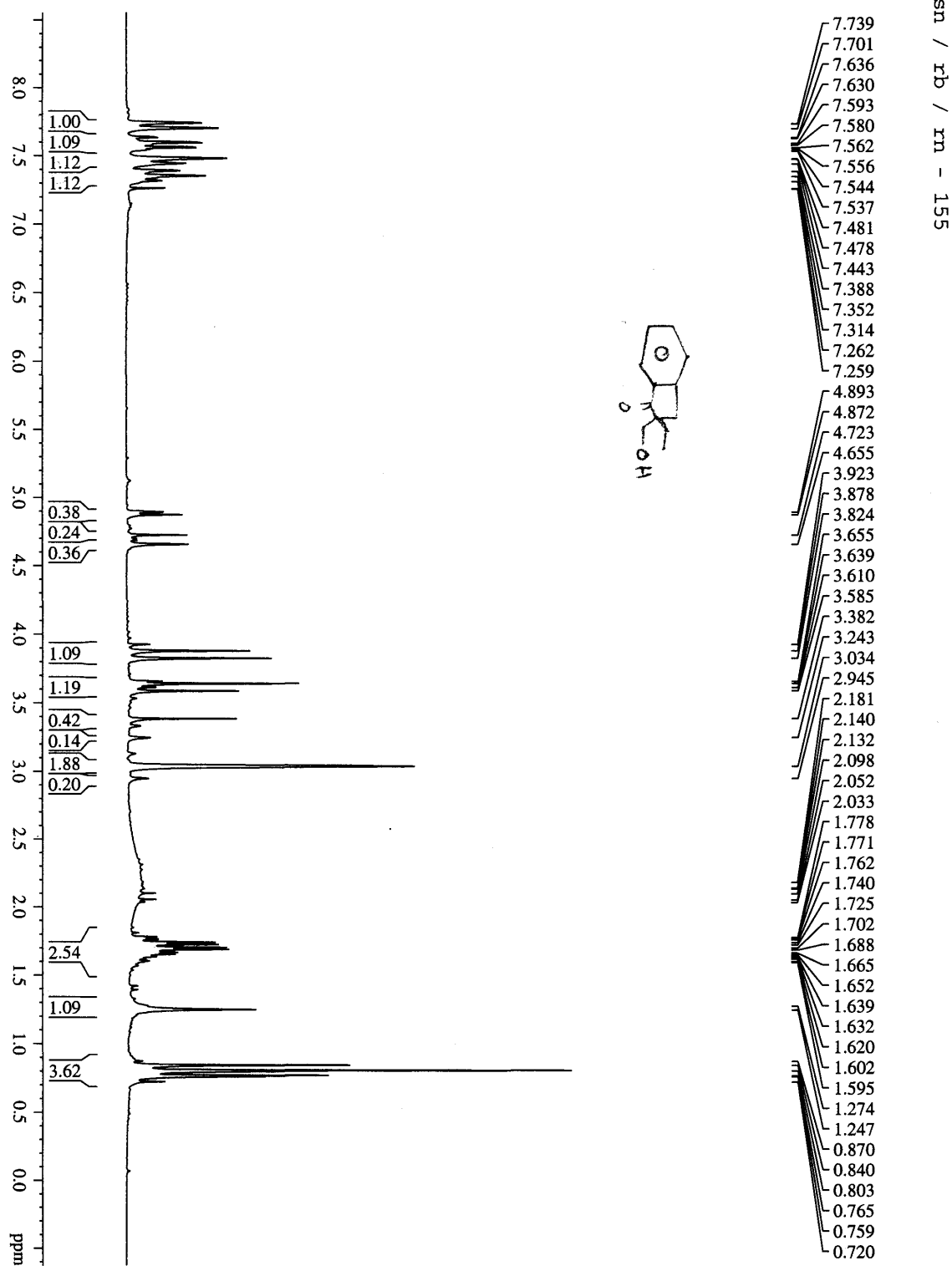
¹H NMR of acetate derivative of 4



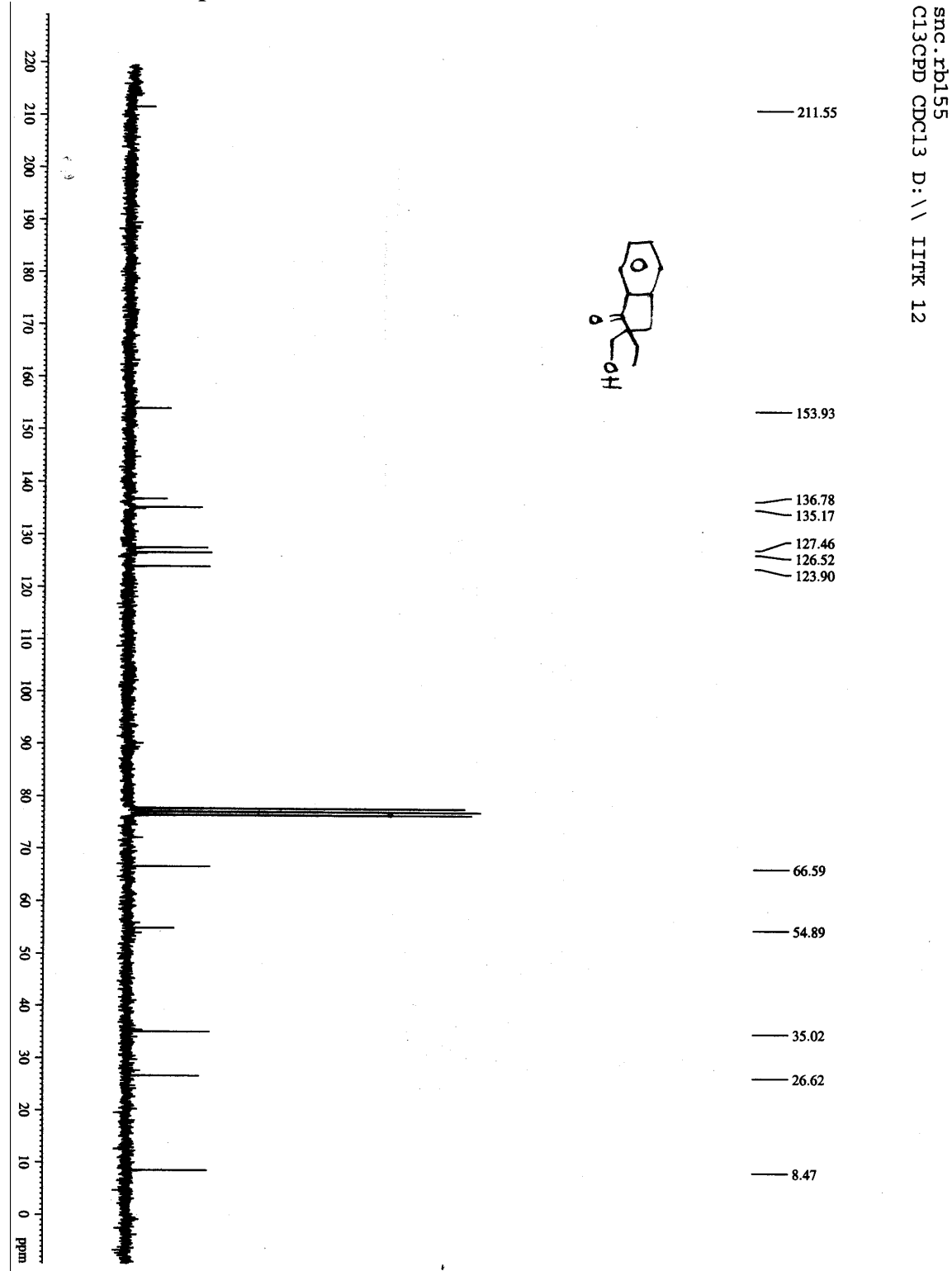
¹³C NMR of acetate derivative of 4



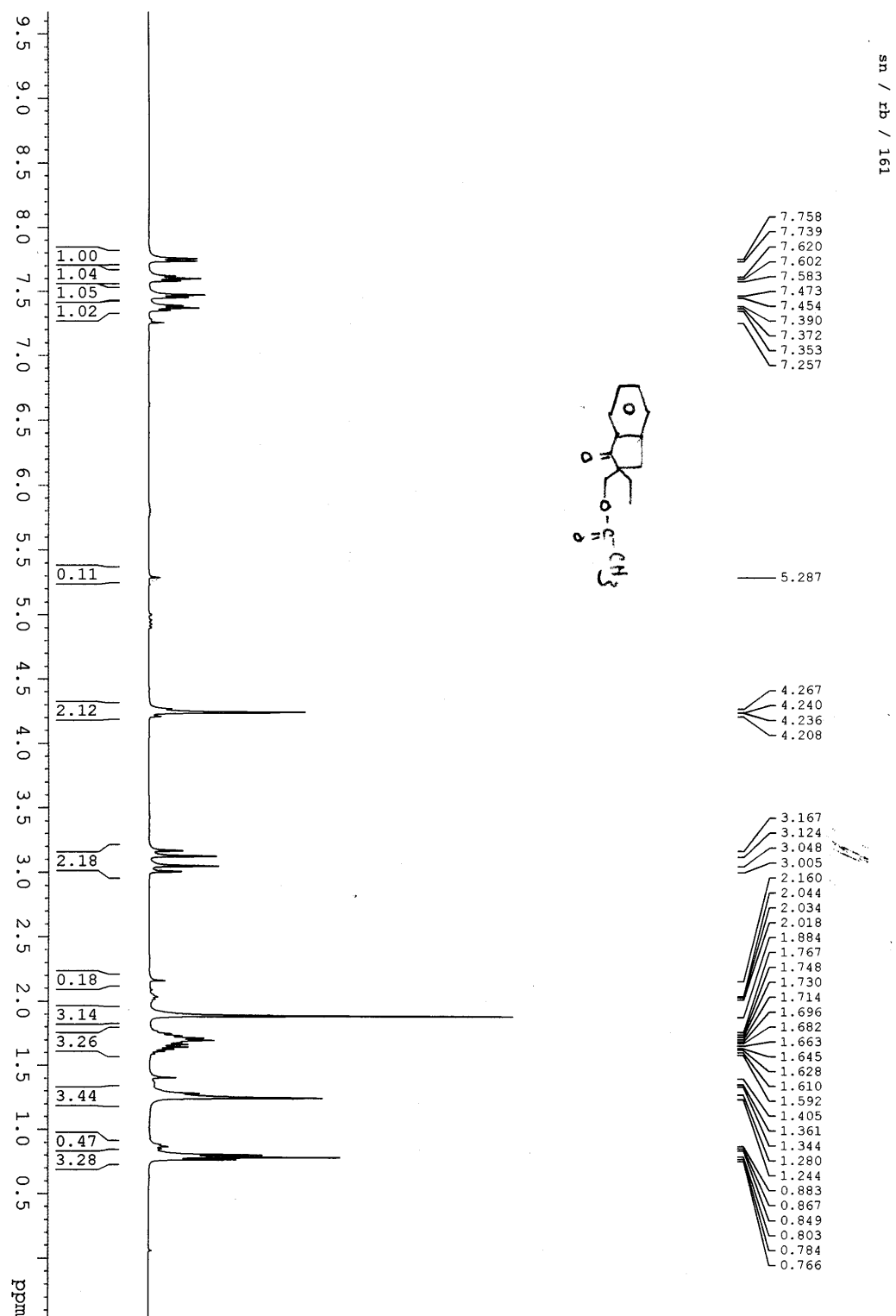
¹H NMR of compound 7



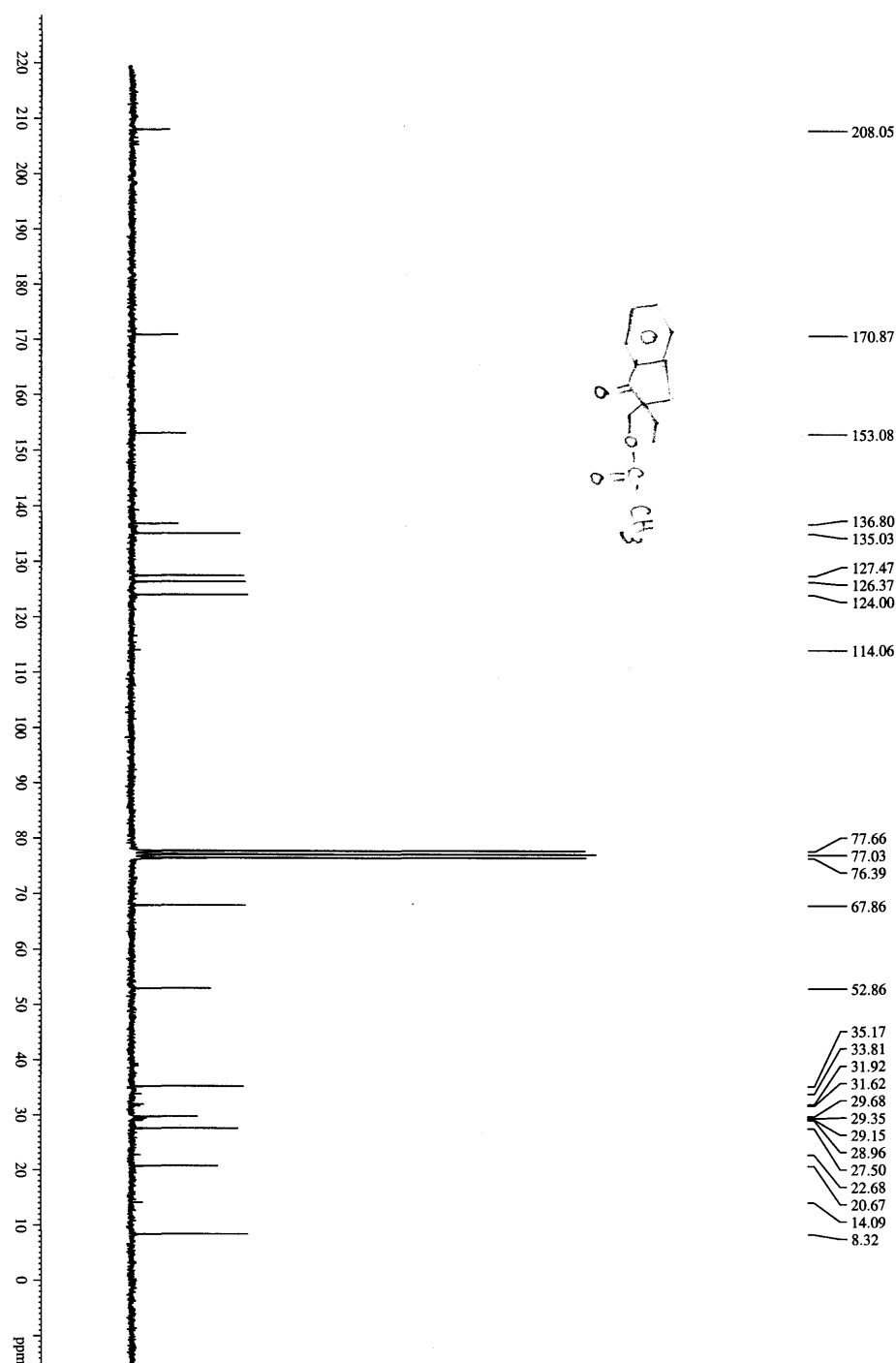
¹³C NMR of compound 7



¹H NMR of acetate derivative of 7

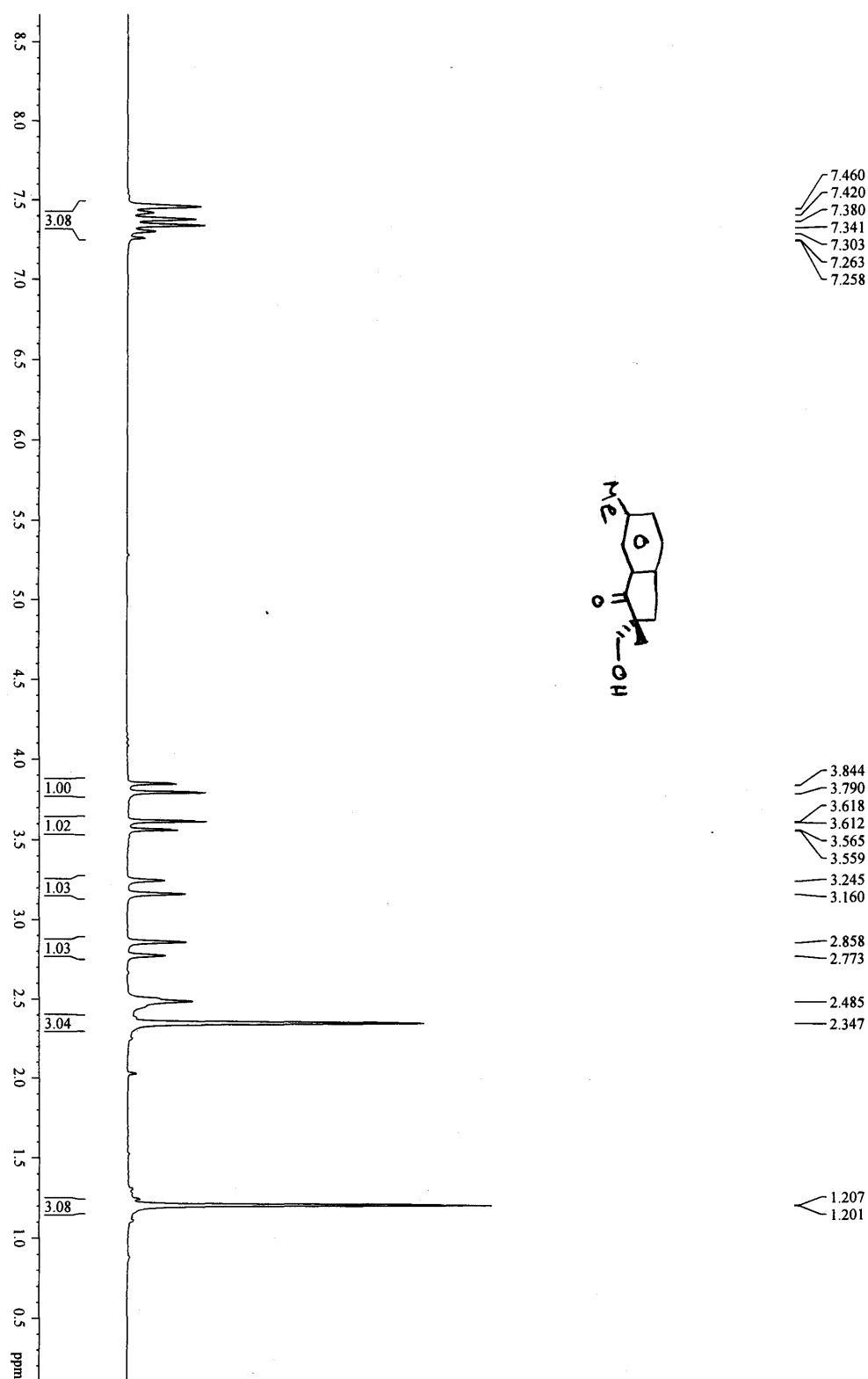


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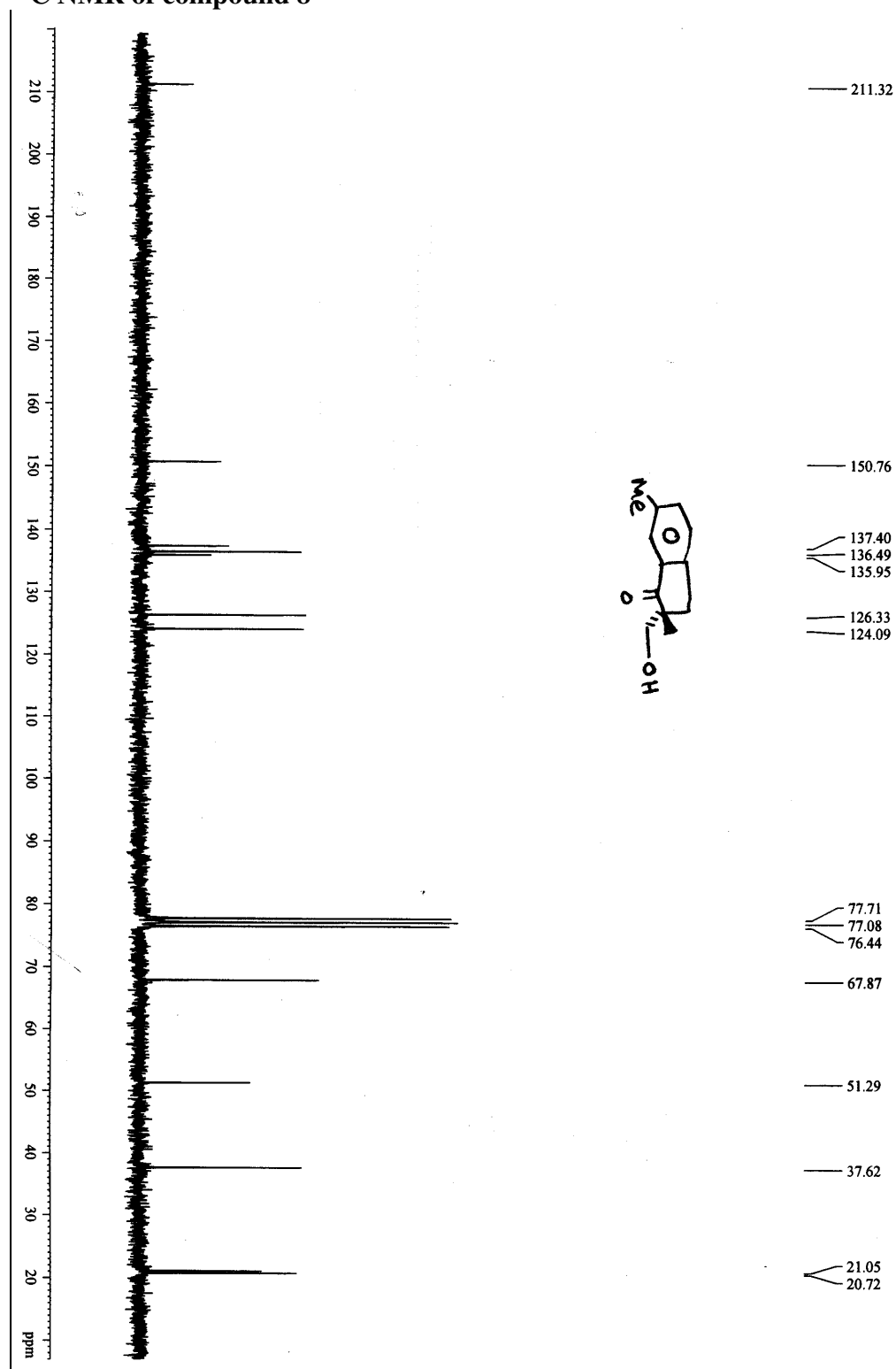
sn / rb / rn-161 - 13c

¹H NMR of compound 8



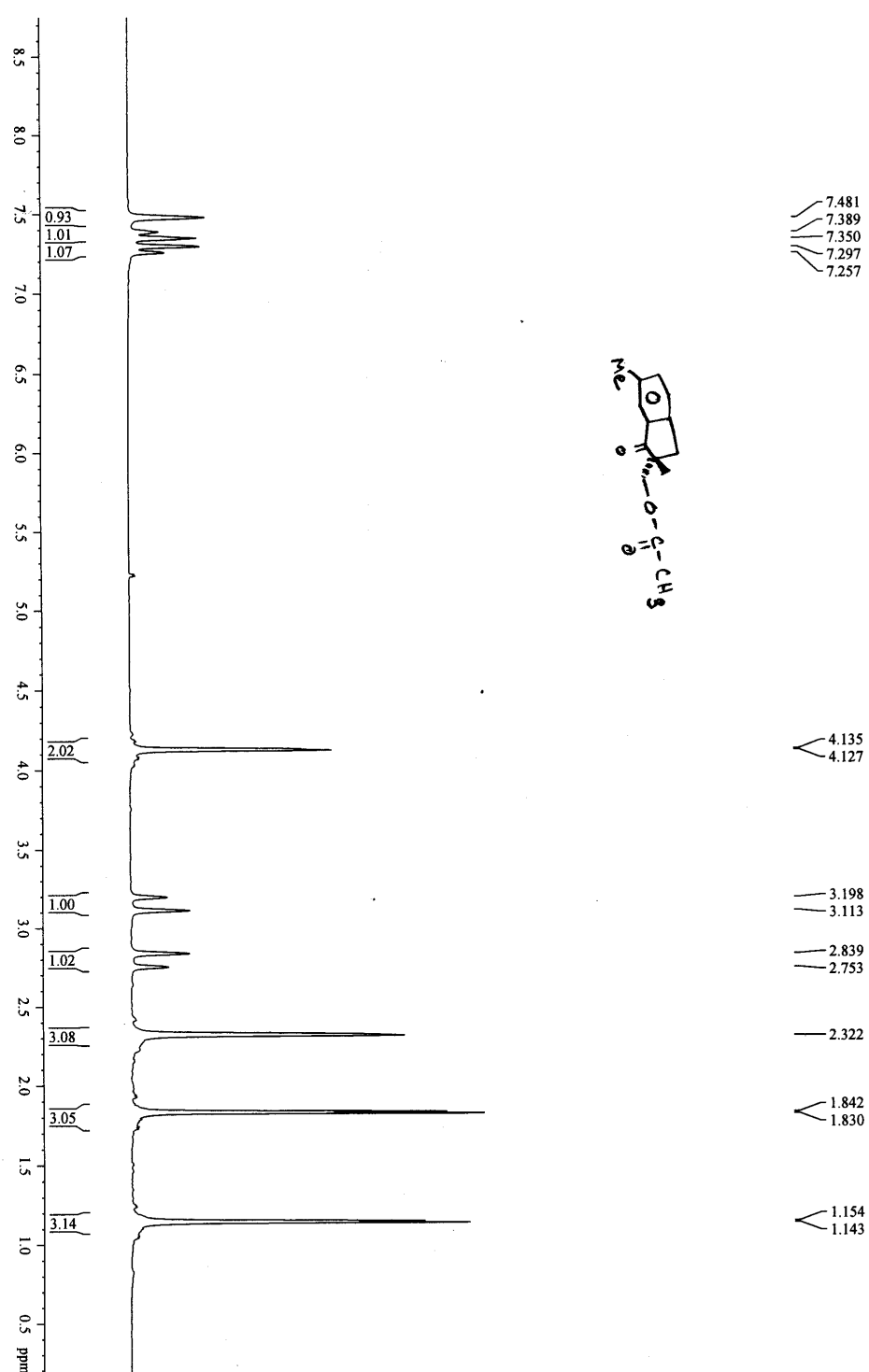
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¹³C NMR of compound 8



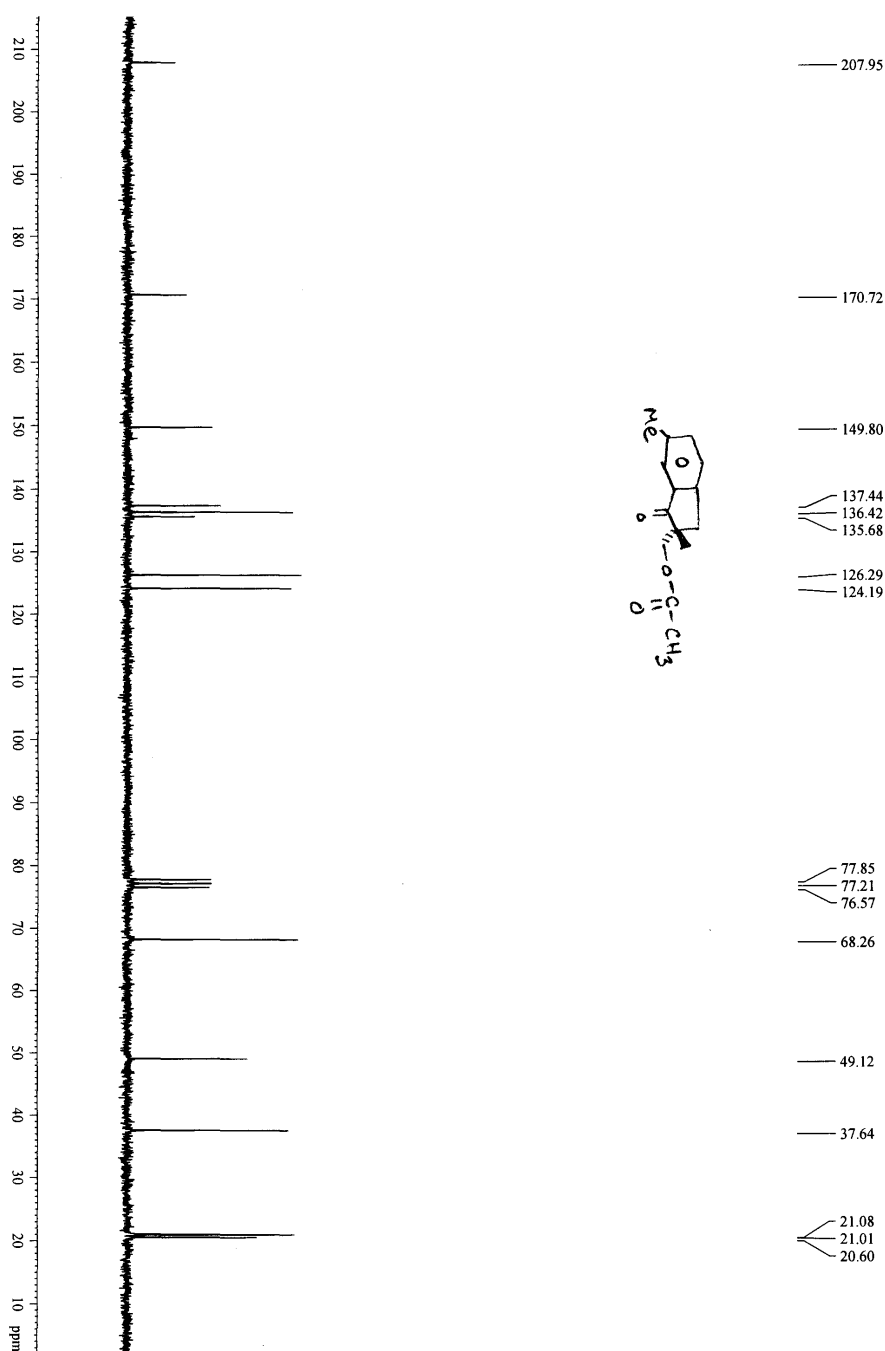
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C13CPD CDCl3 D:\ IITK 2

¹H NMR of acetate derivative of 8



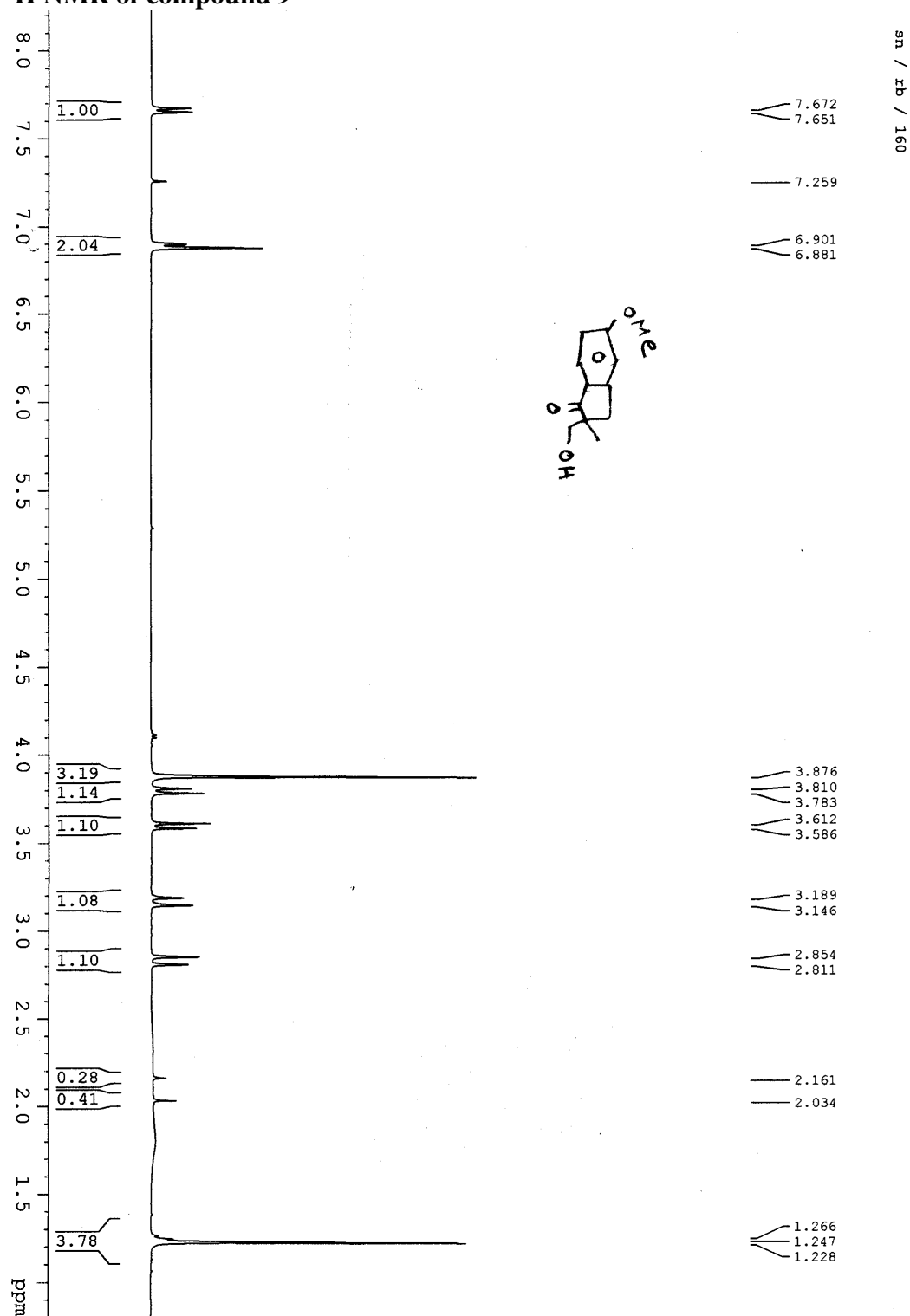
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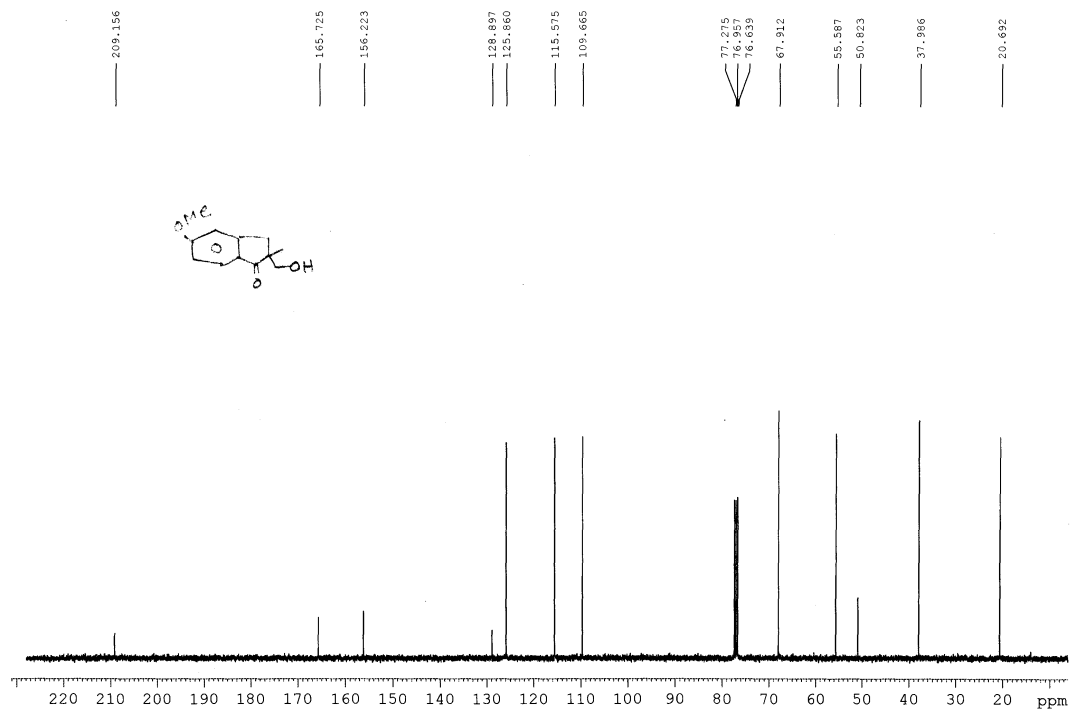
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¹H NMR of compound 9

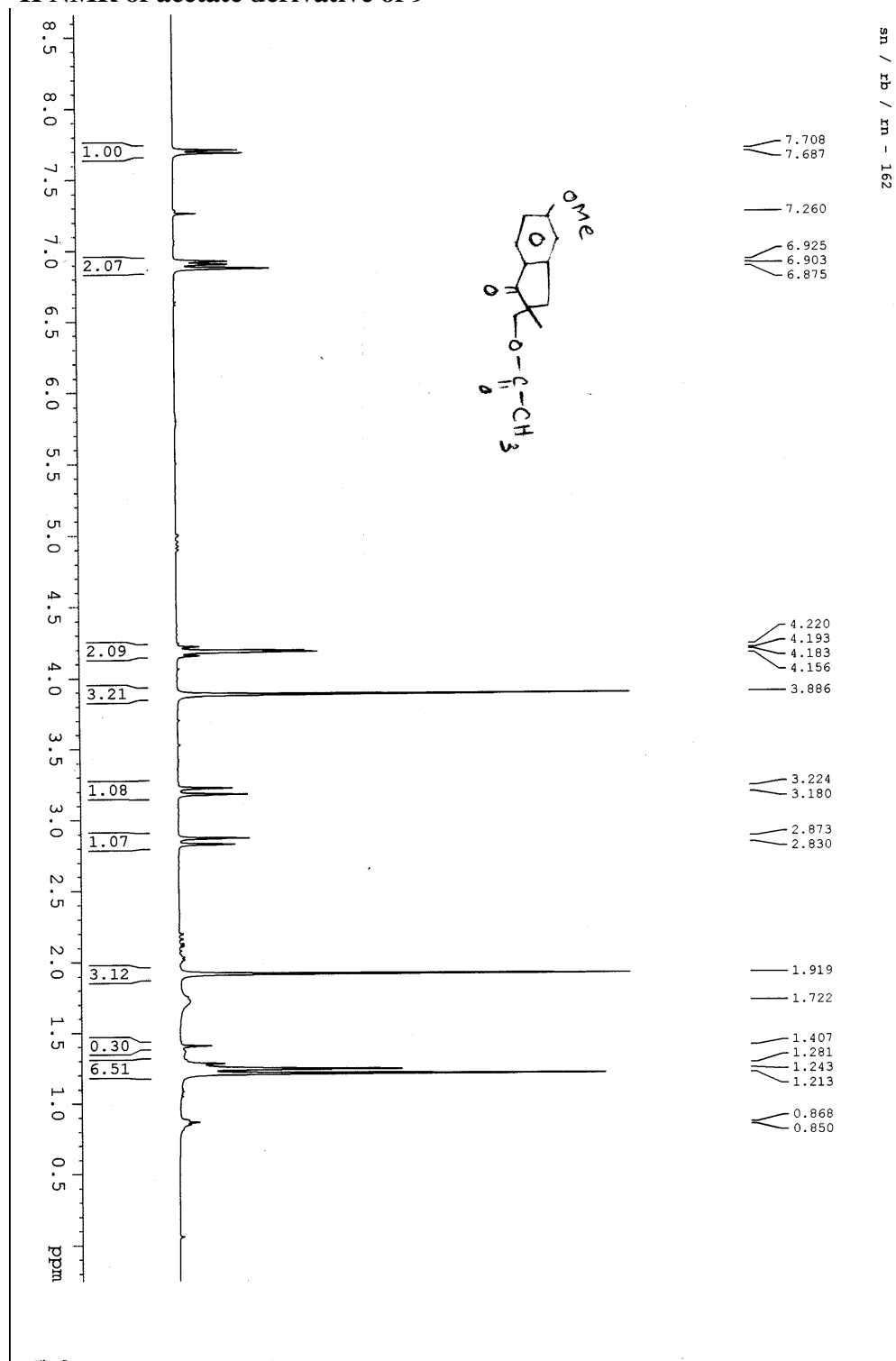


¹³C NMR of compound 9

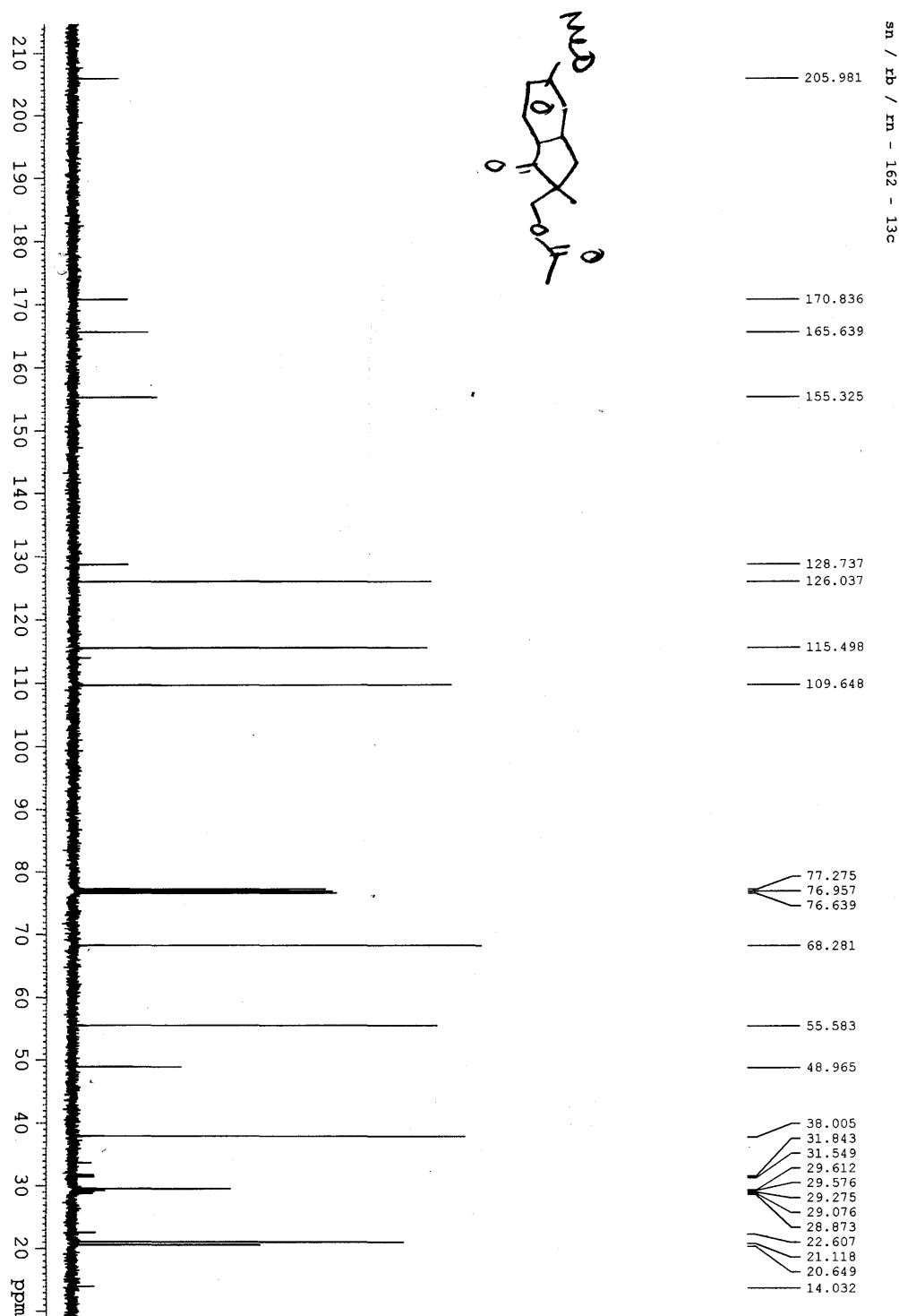
sn / rb / rn - 160 - 13c



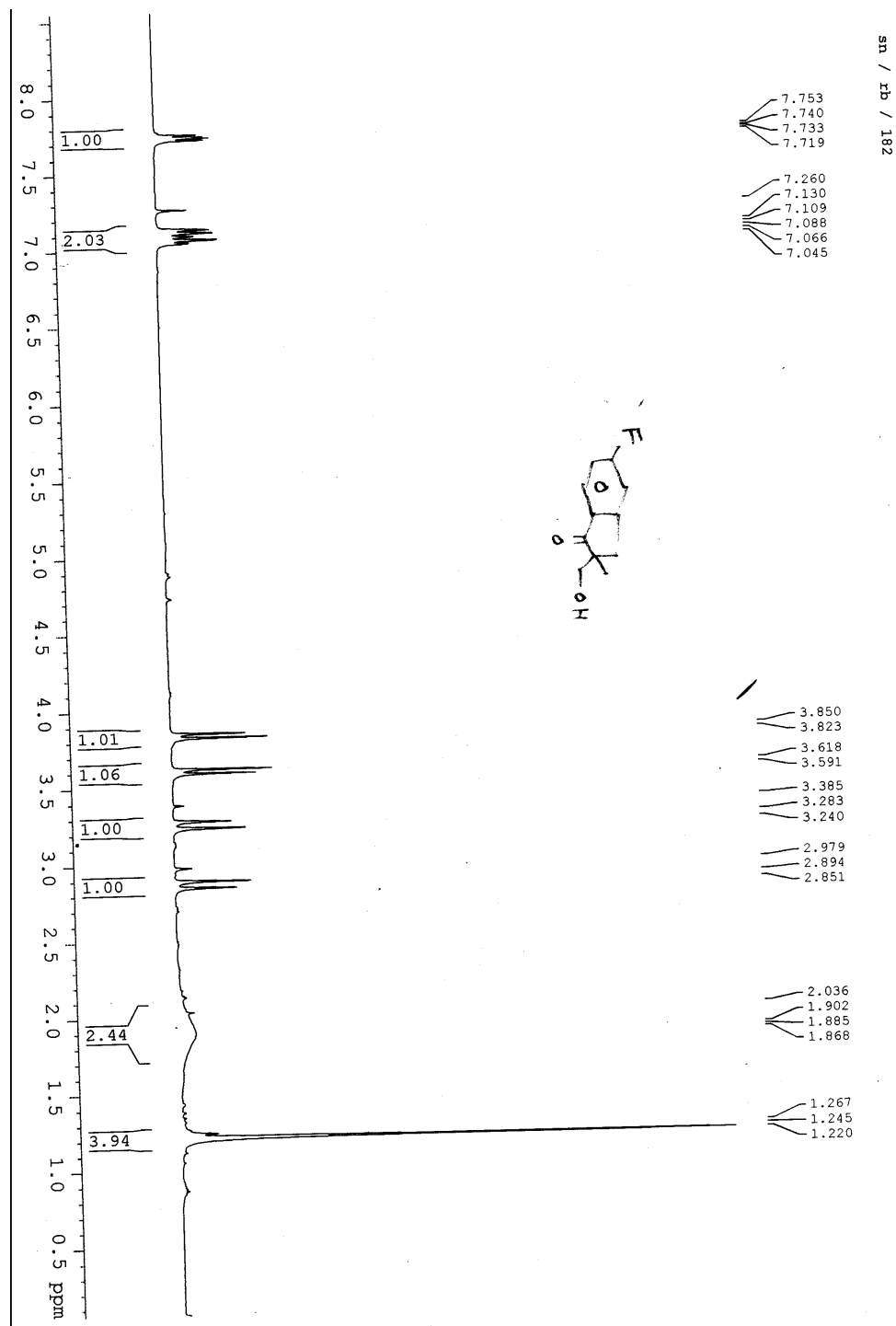
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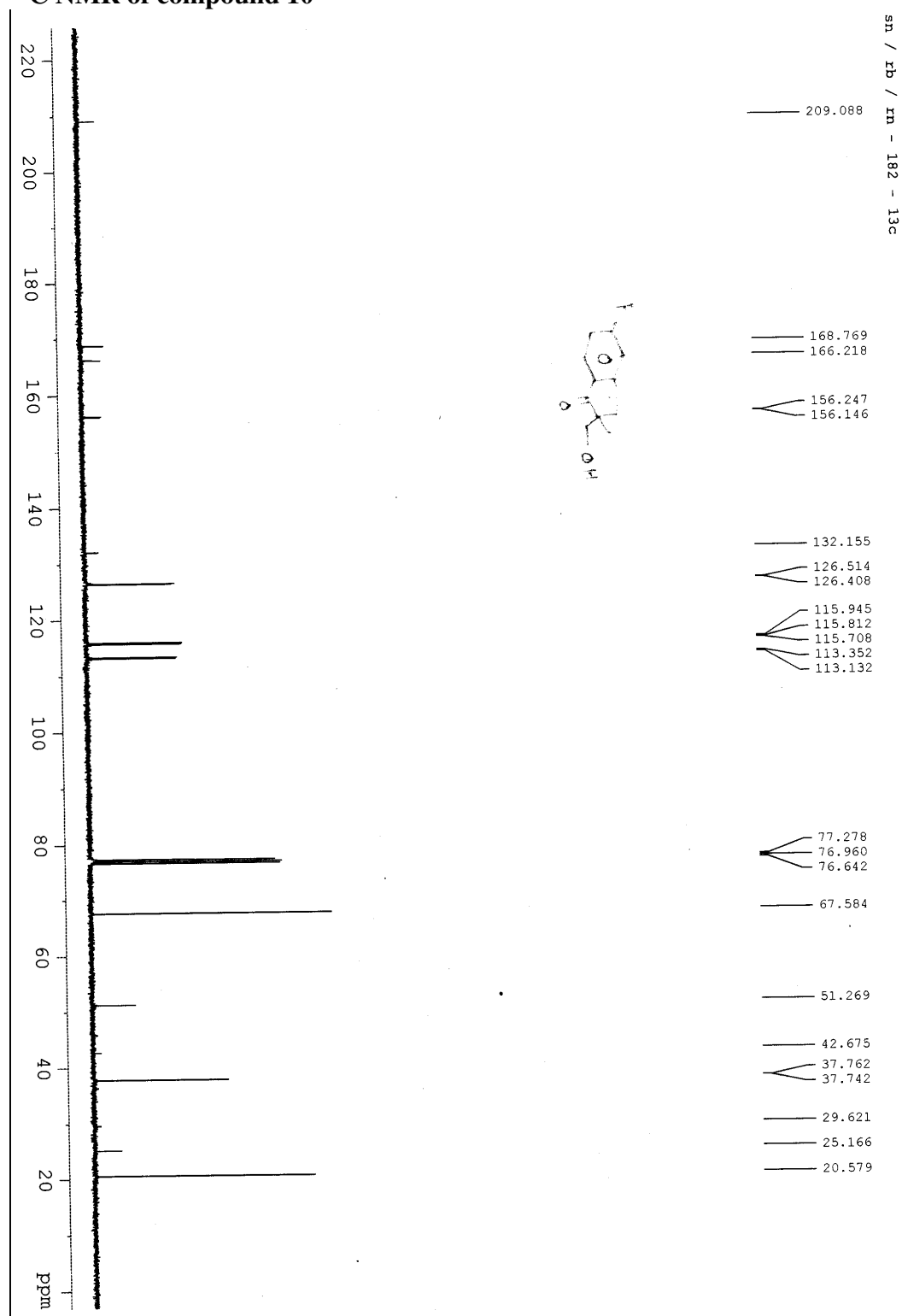
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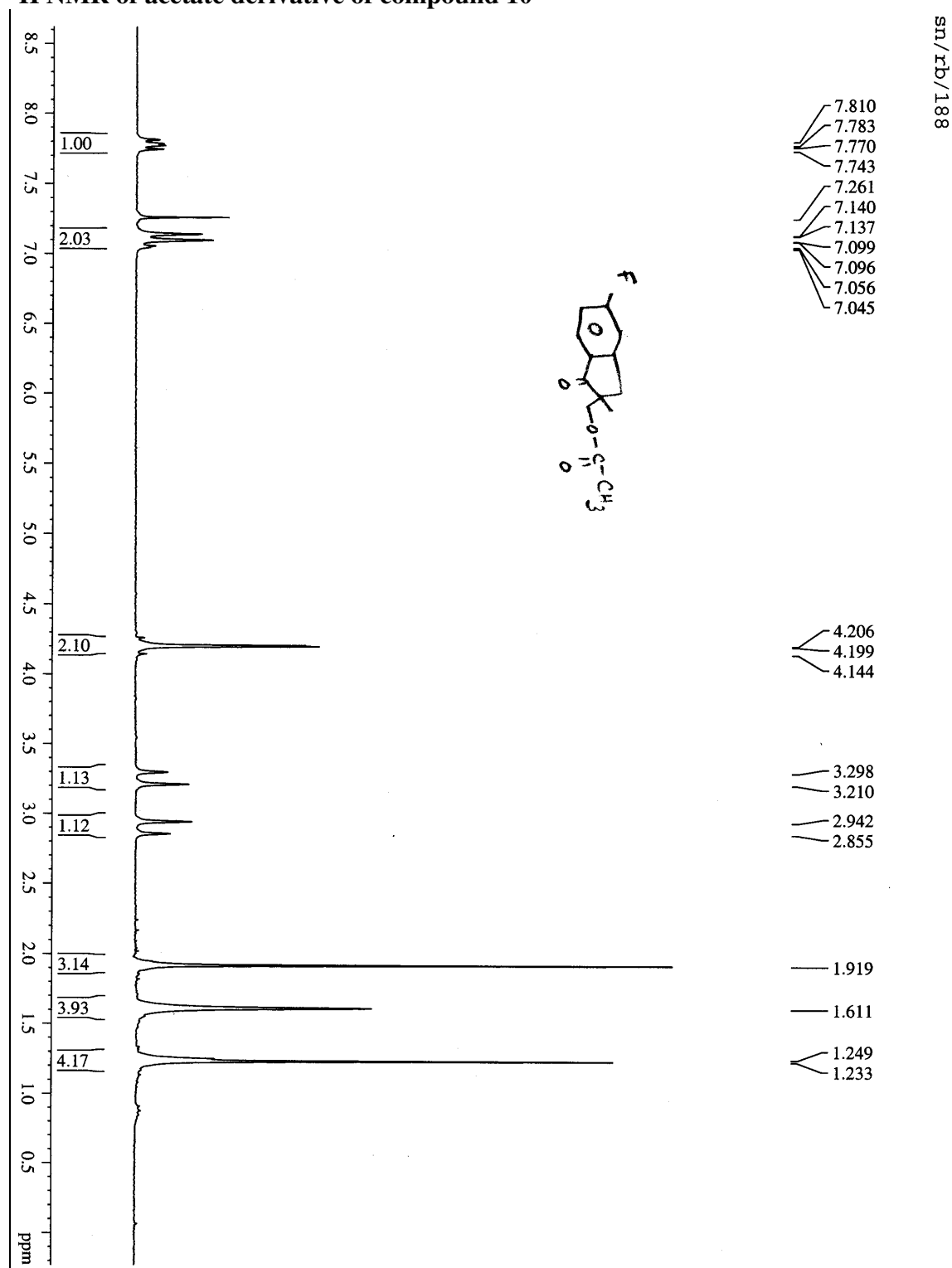
¹H NMR of compound 10



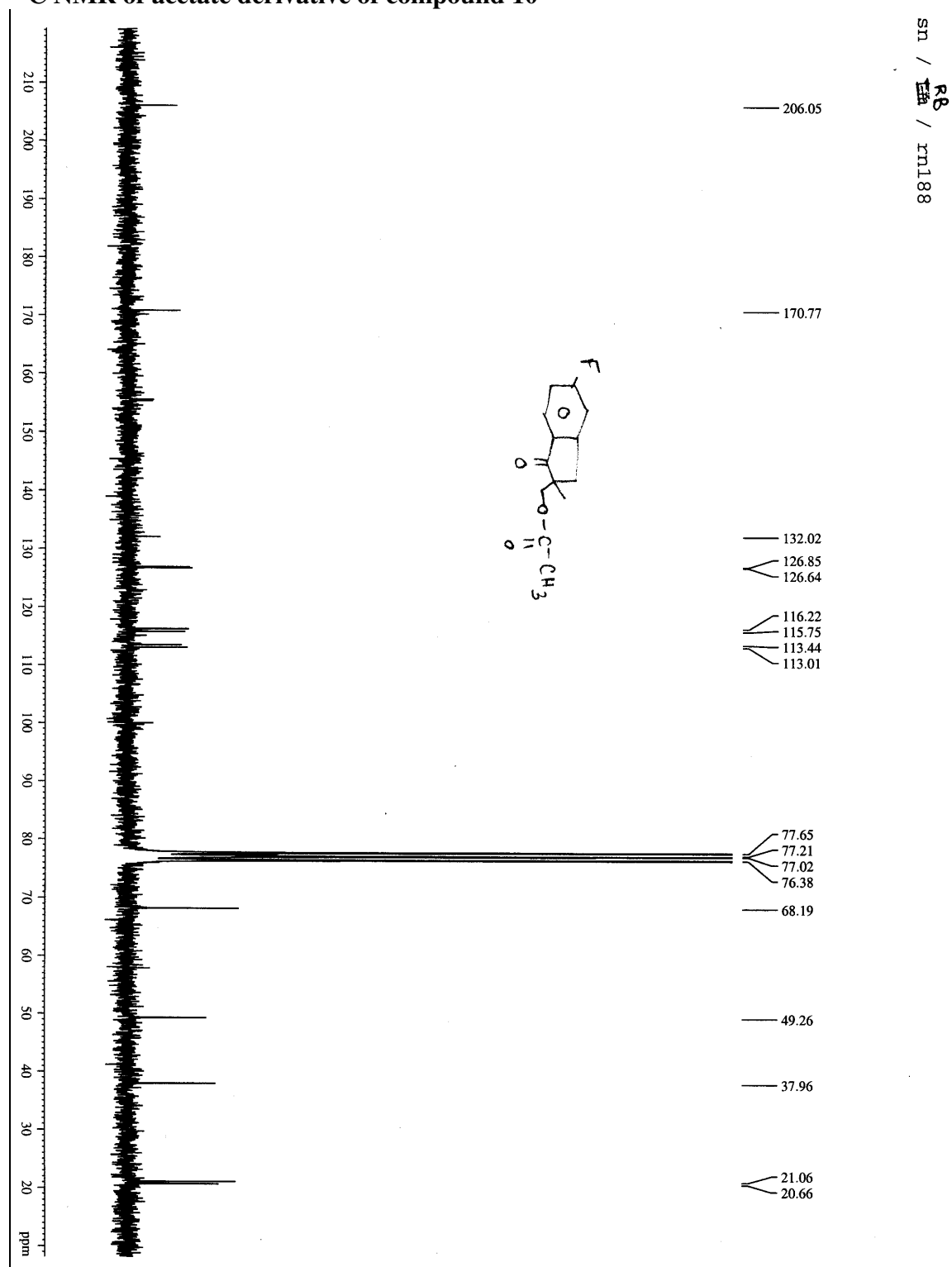
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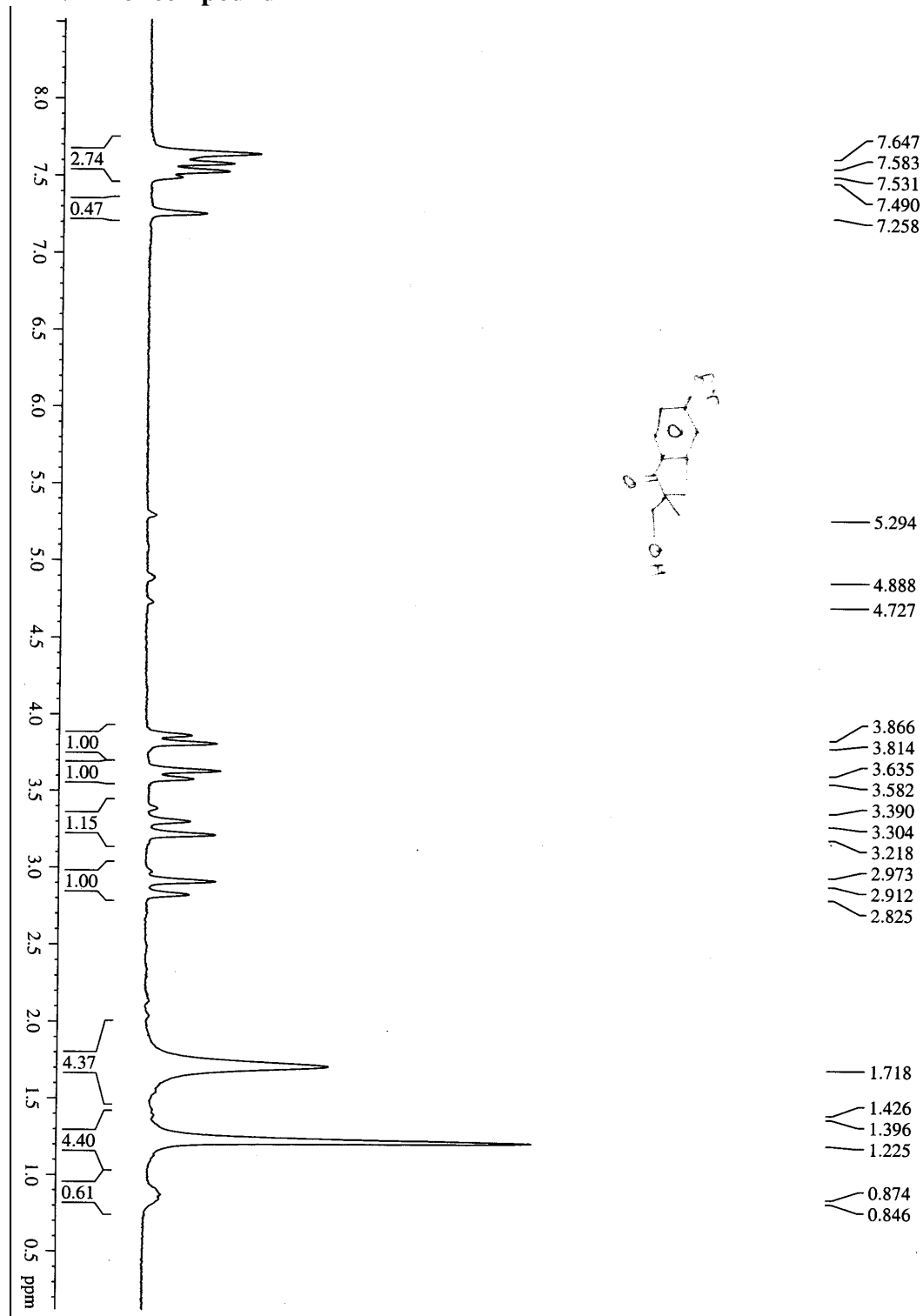
¹H NMR of acetate derivative of compound 10



¹³C NMR of acetate derivative of compound 10

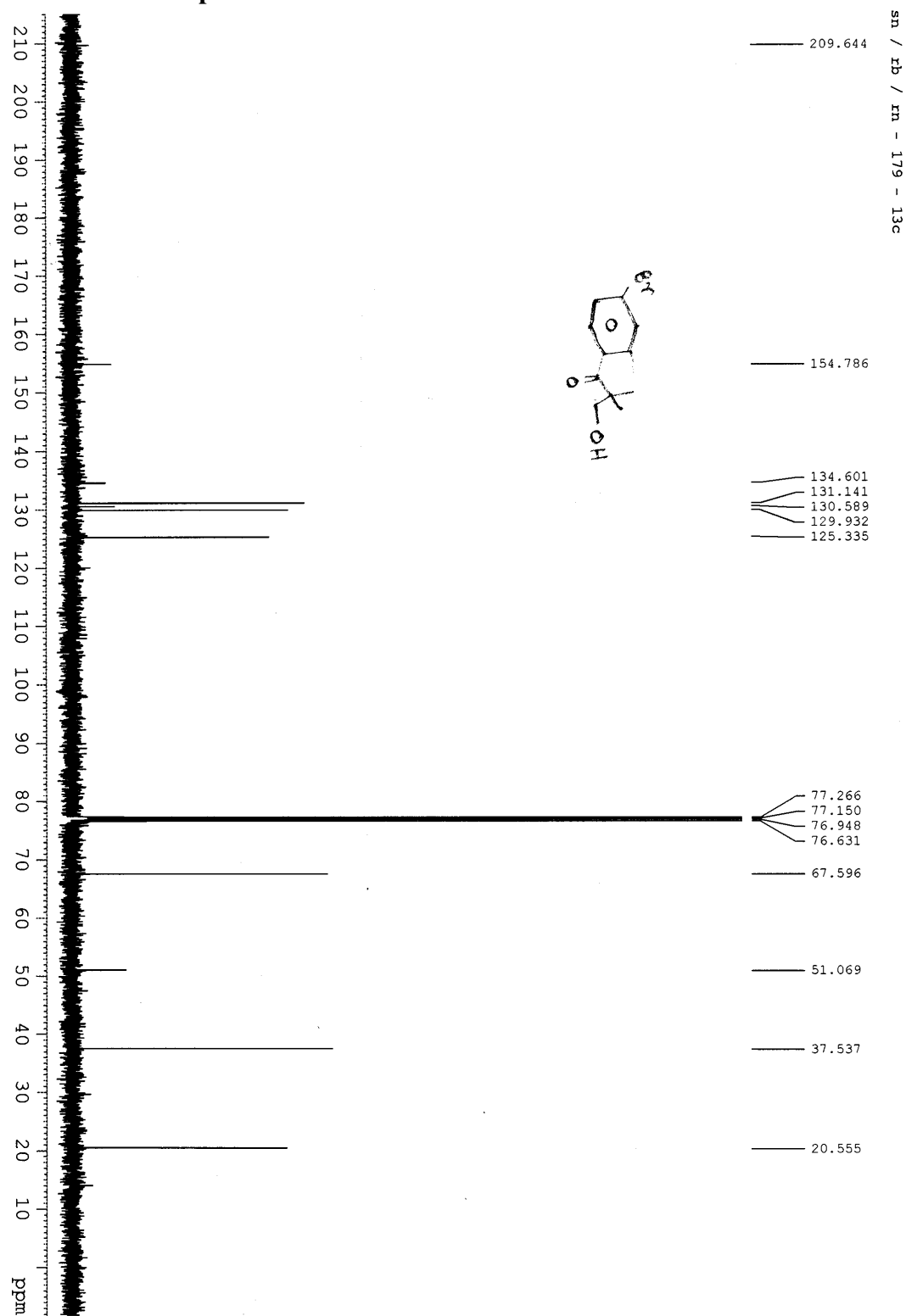


¹H NMR of compound 11

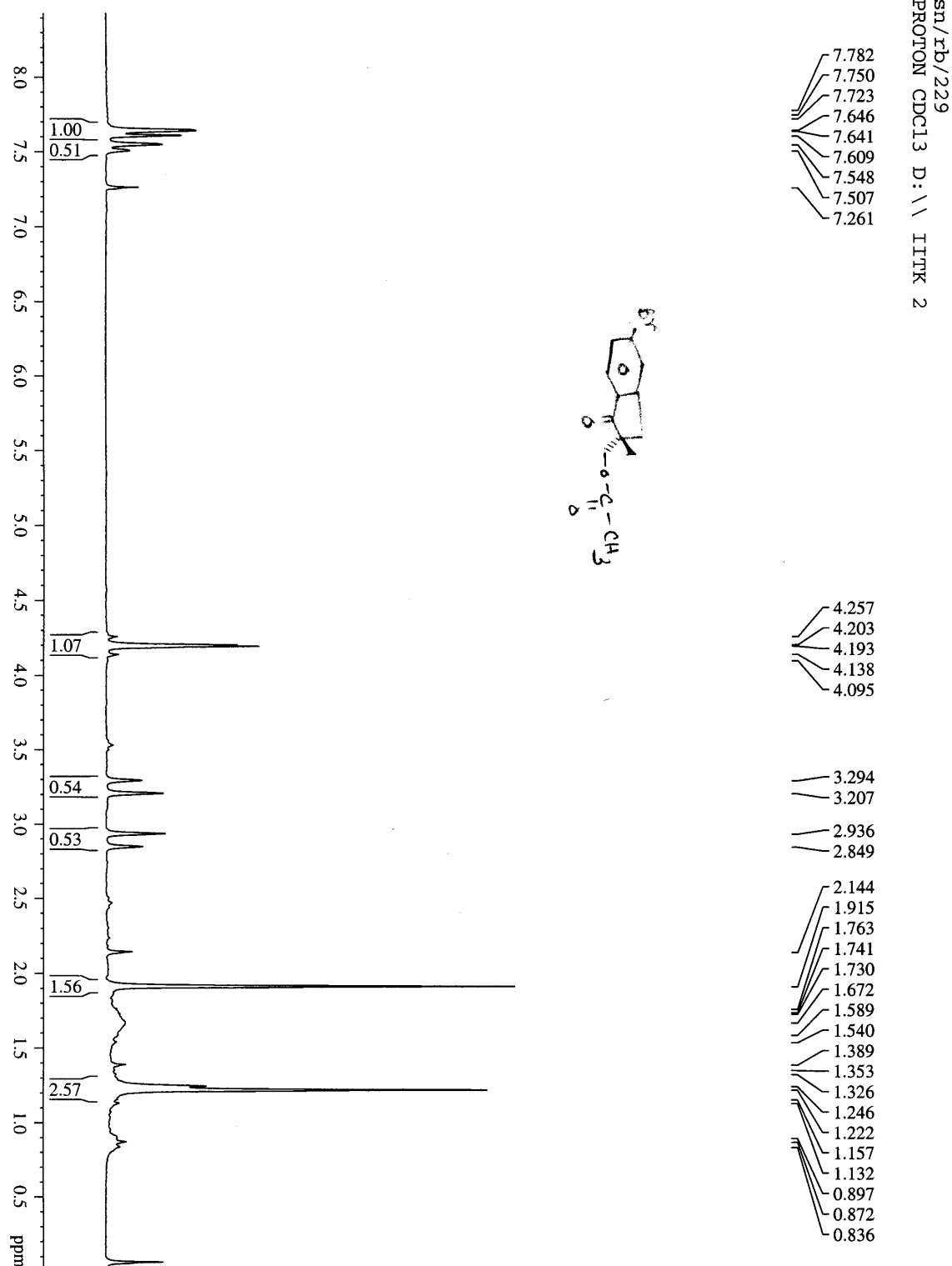


sn/rb/179

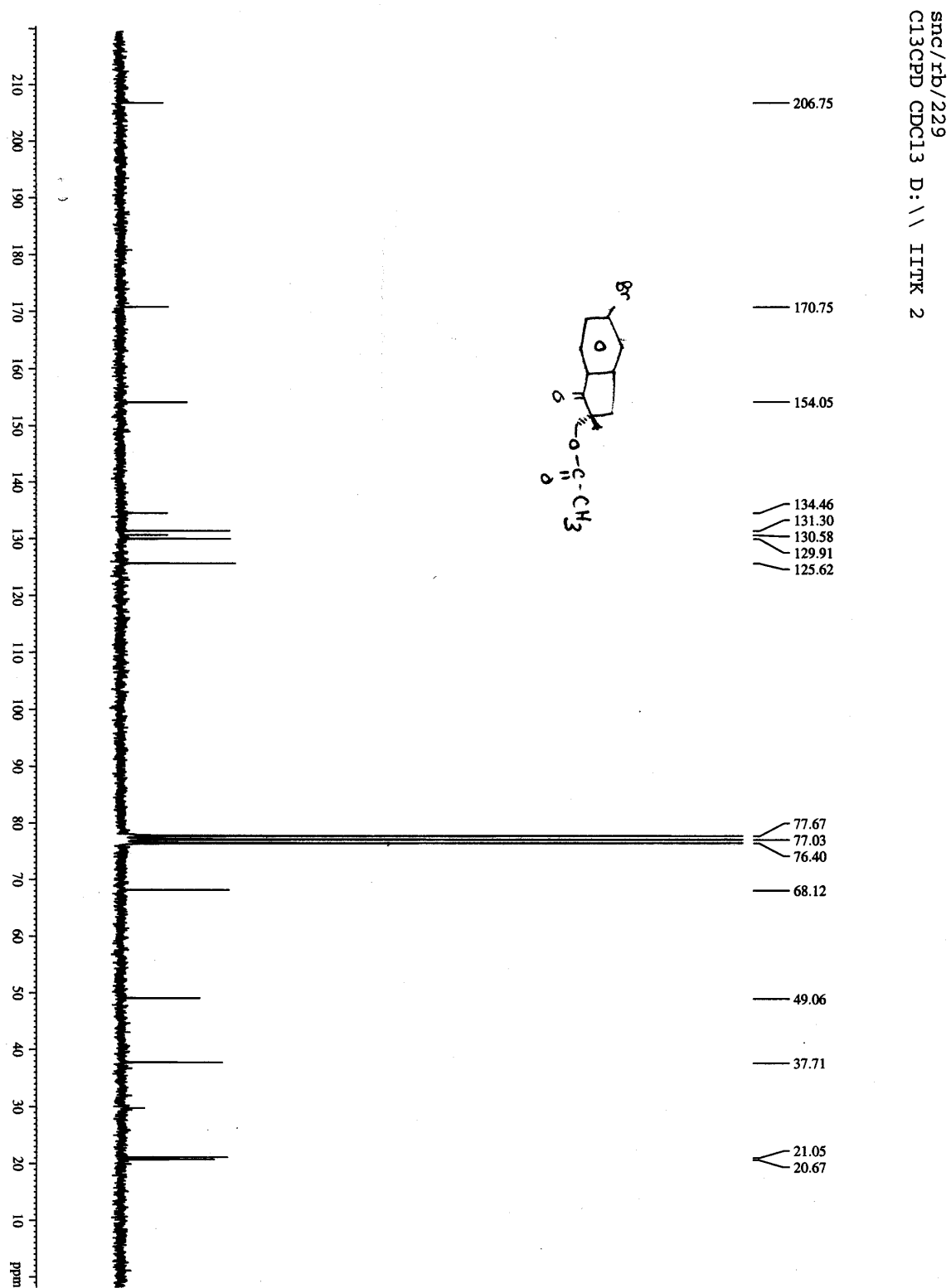
¹³C NMR of compound 11



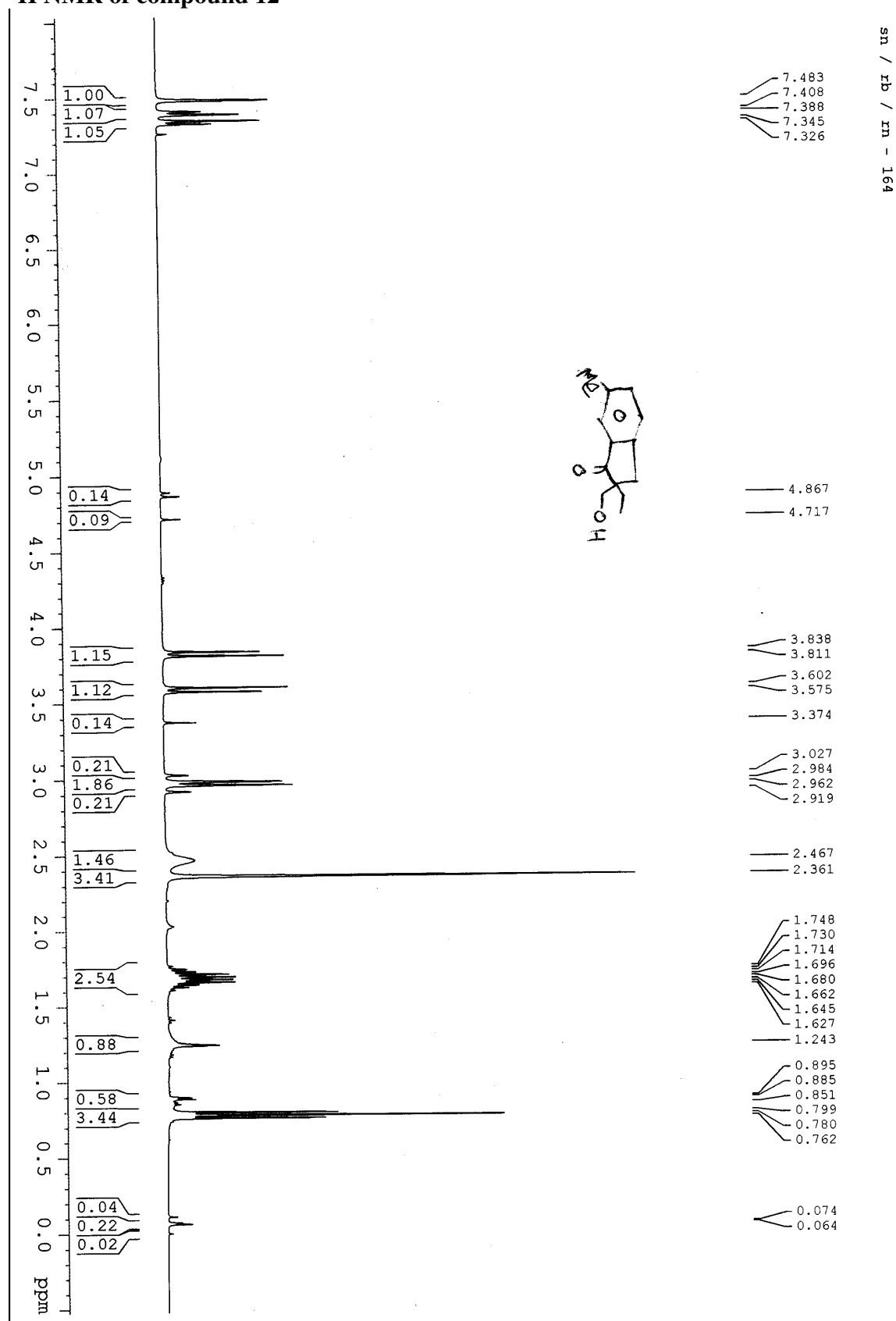
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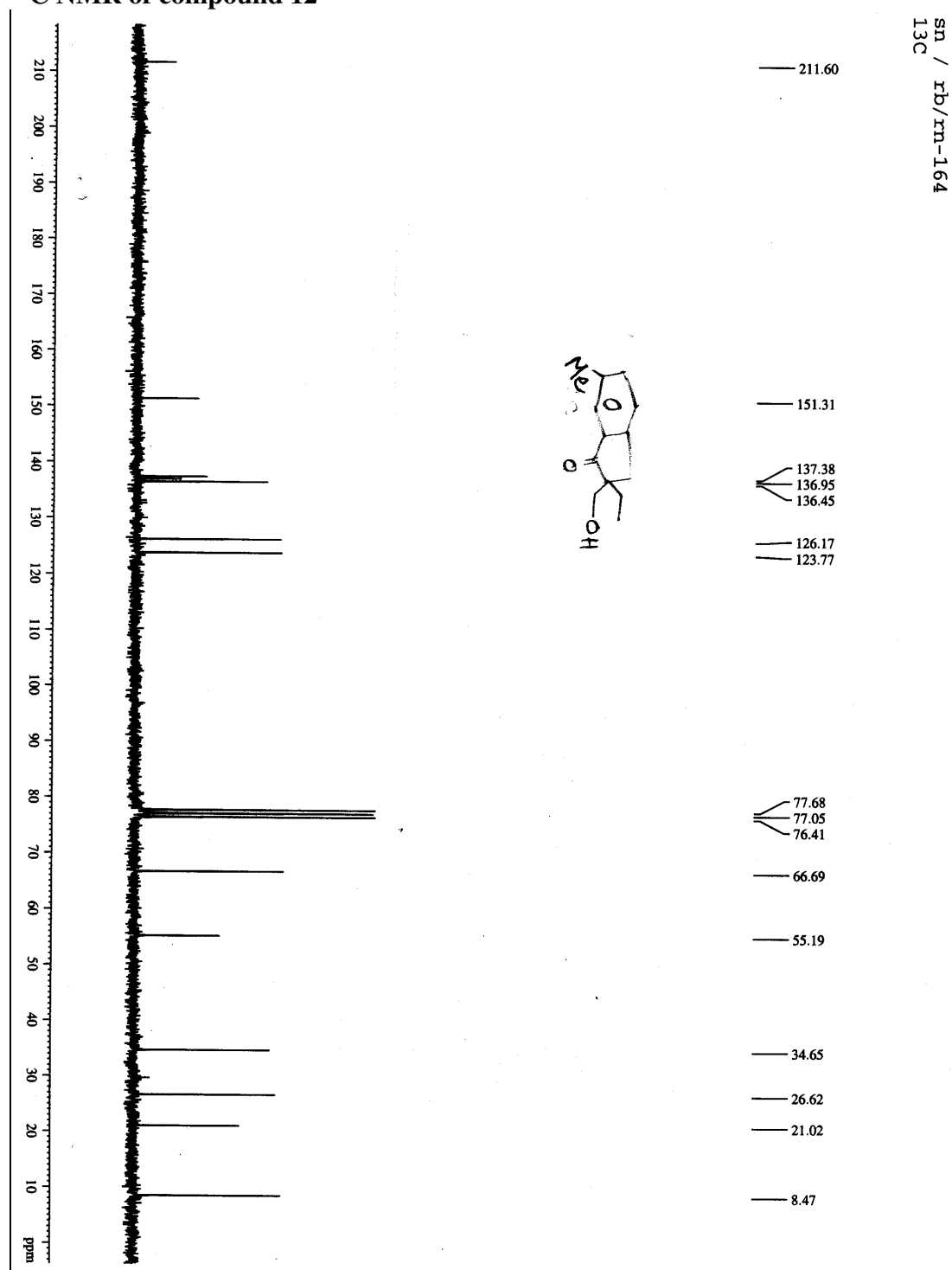
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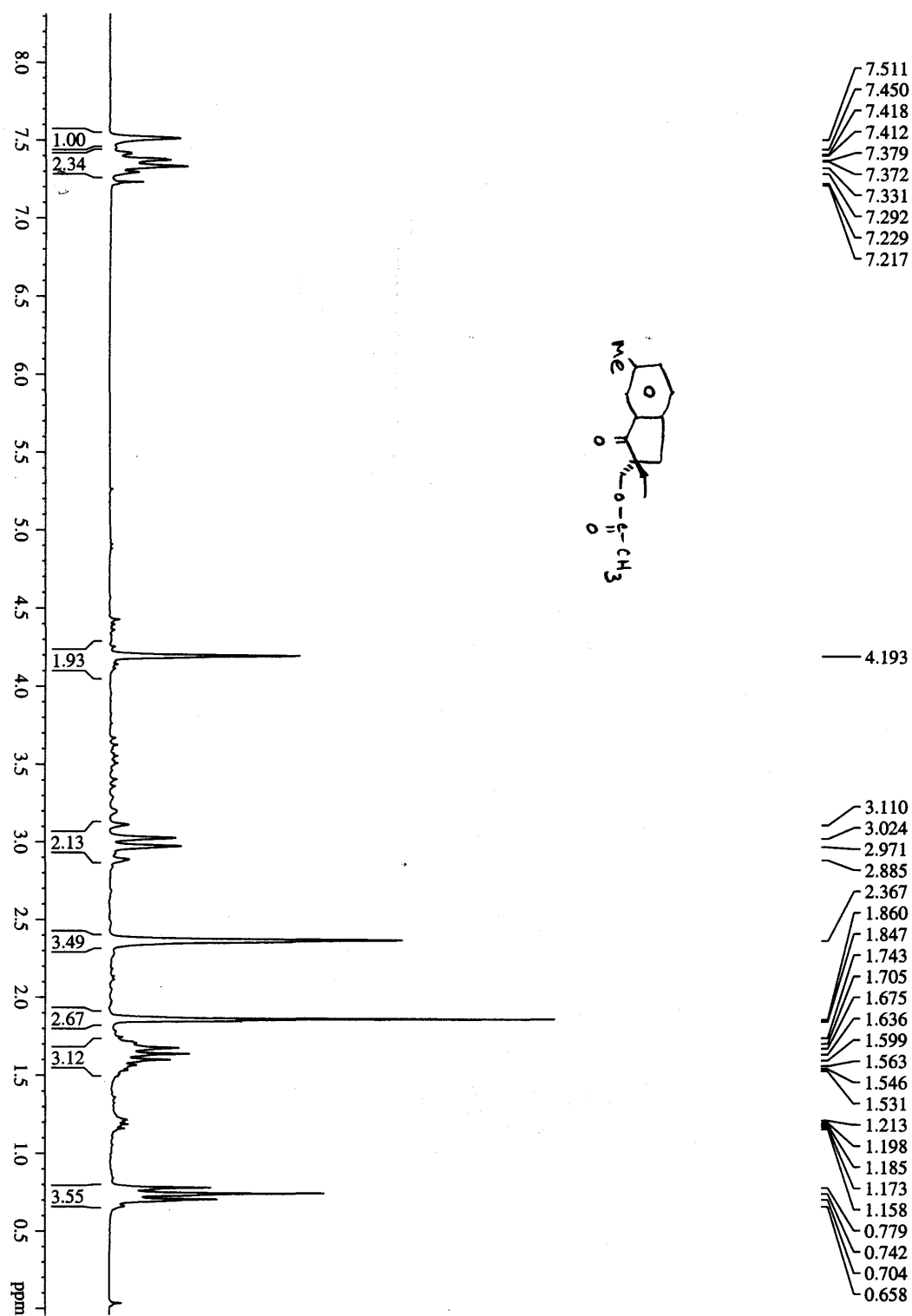
¹H NMR of compound 12



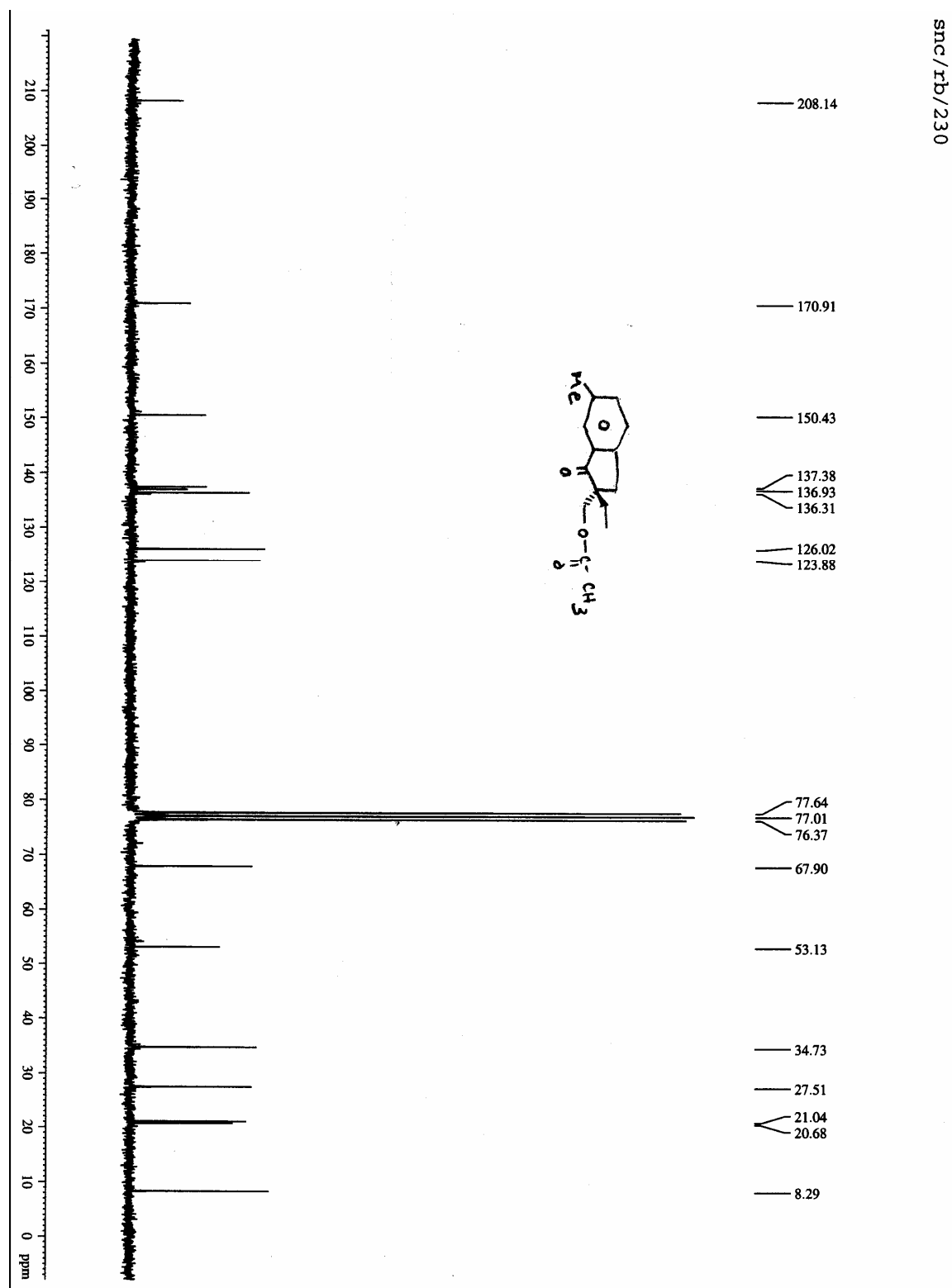
¹³C NMR of compound 12



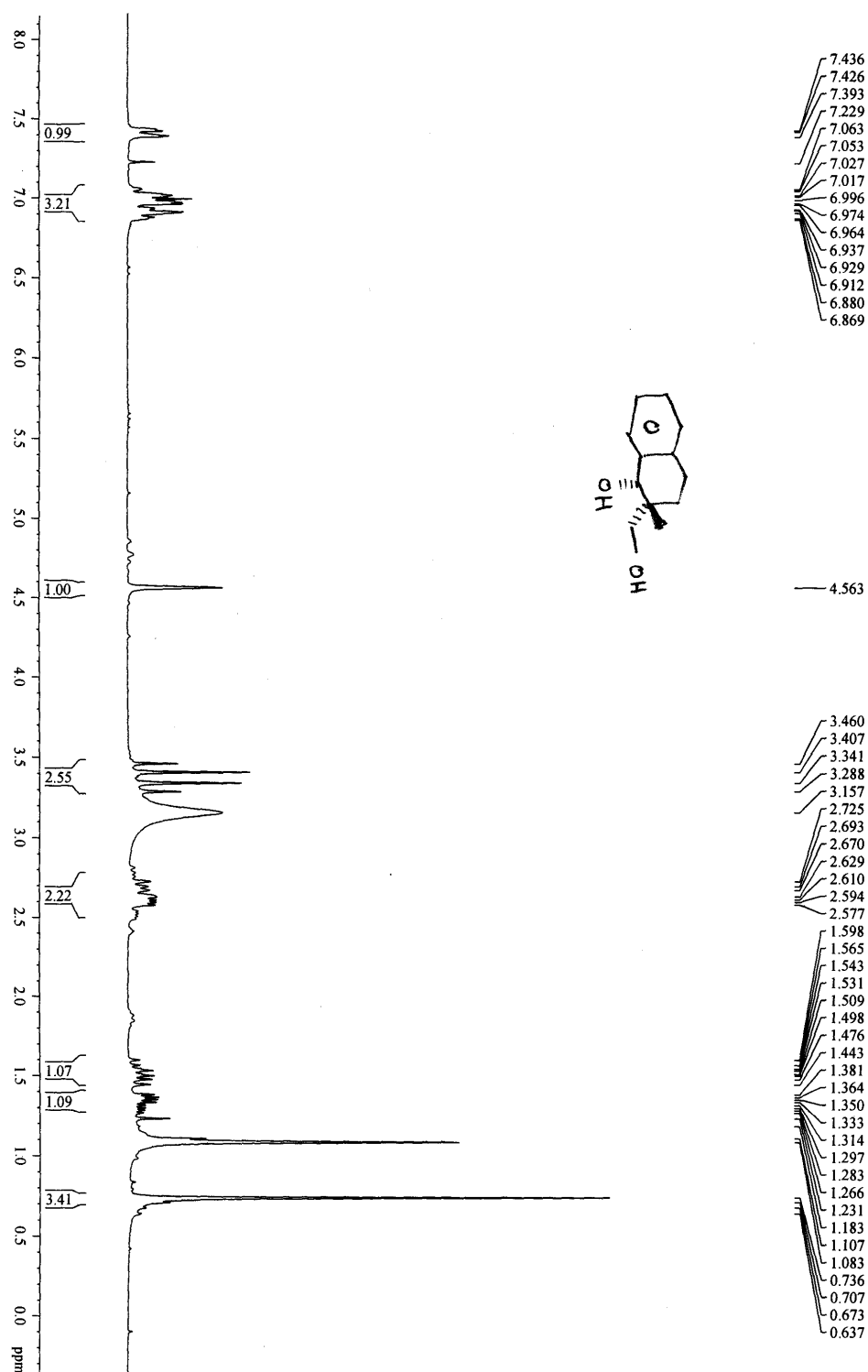
¹H NMR of acetate derivative of 12



¹³C NMR of acetate derivative of 12

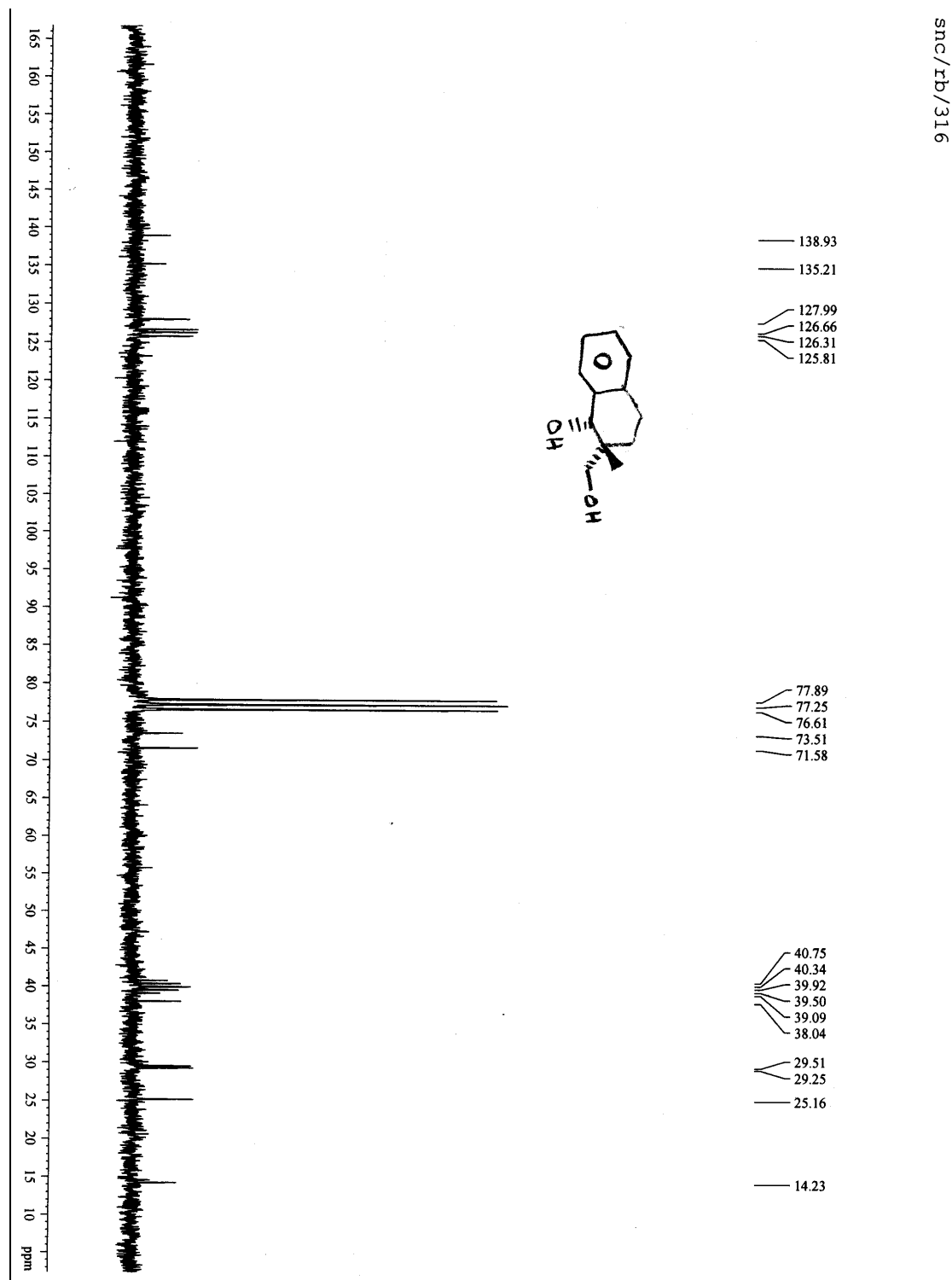


¹H NMR spectrum of 17

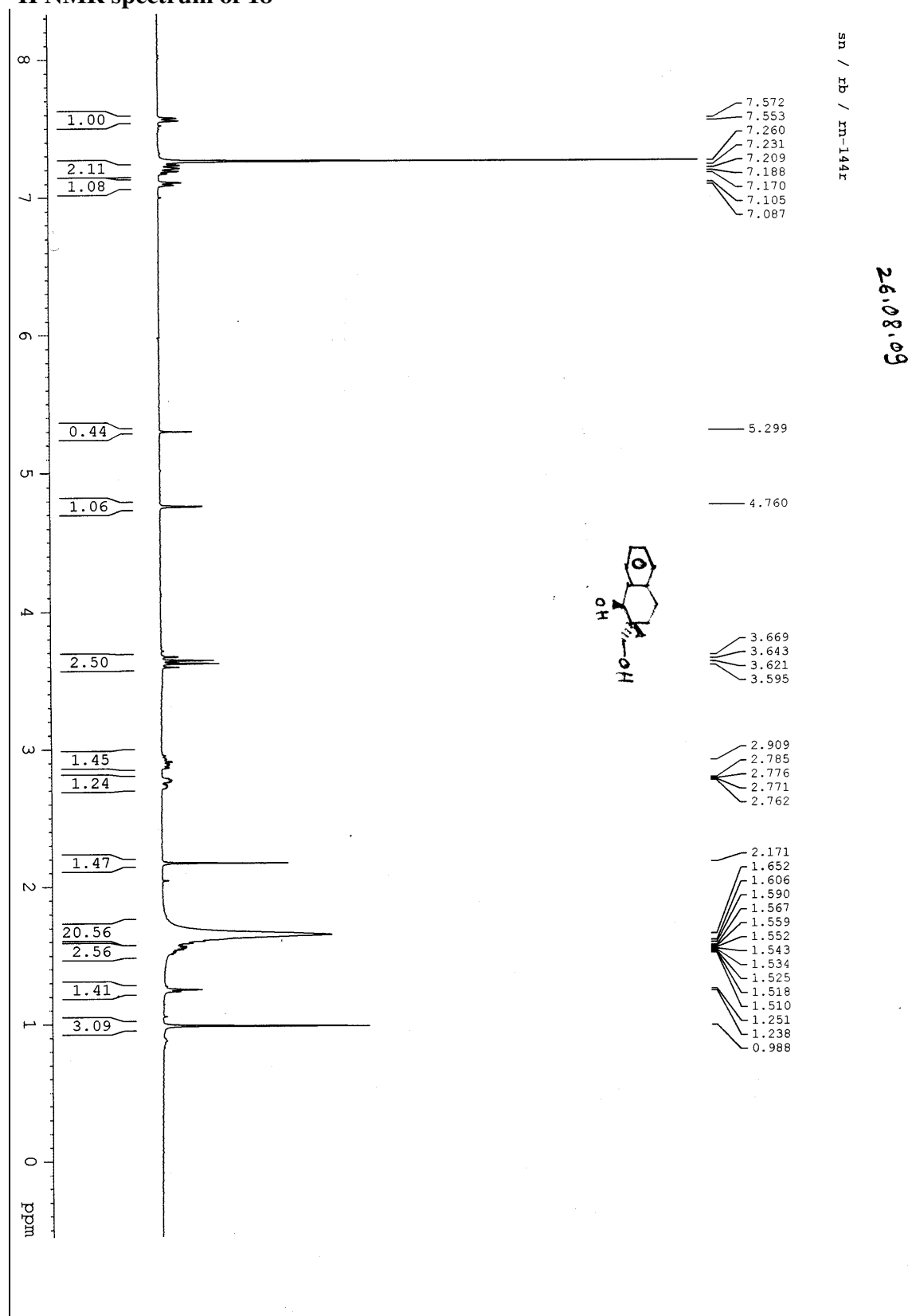


sn/rb/316

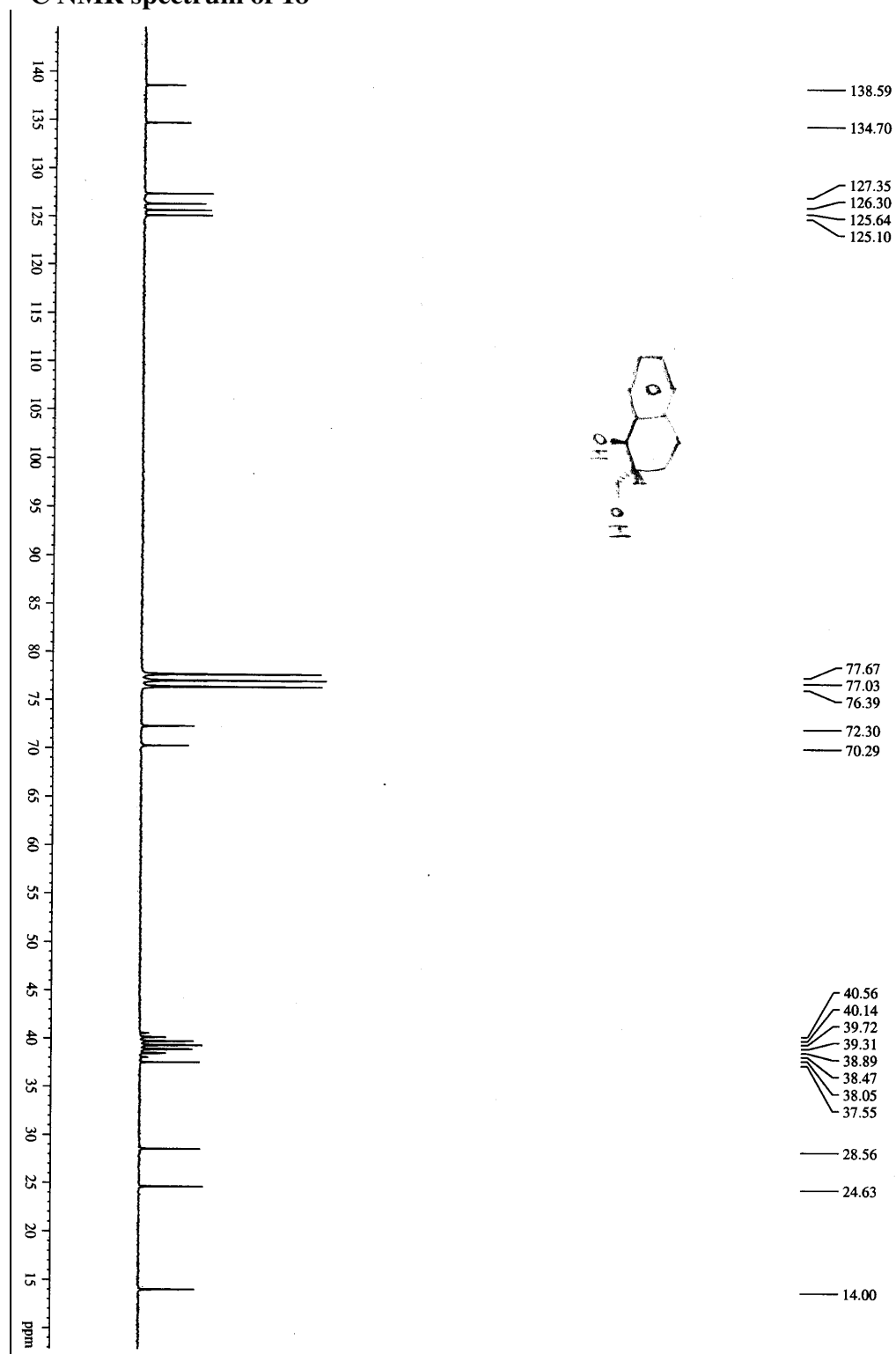
¹³C NMR spectrum of 17



¹H NMR spectrum of 18

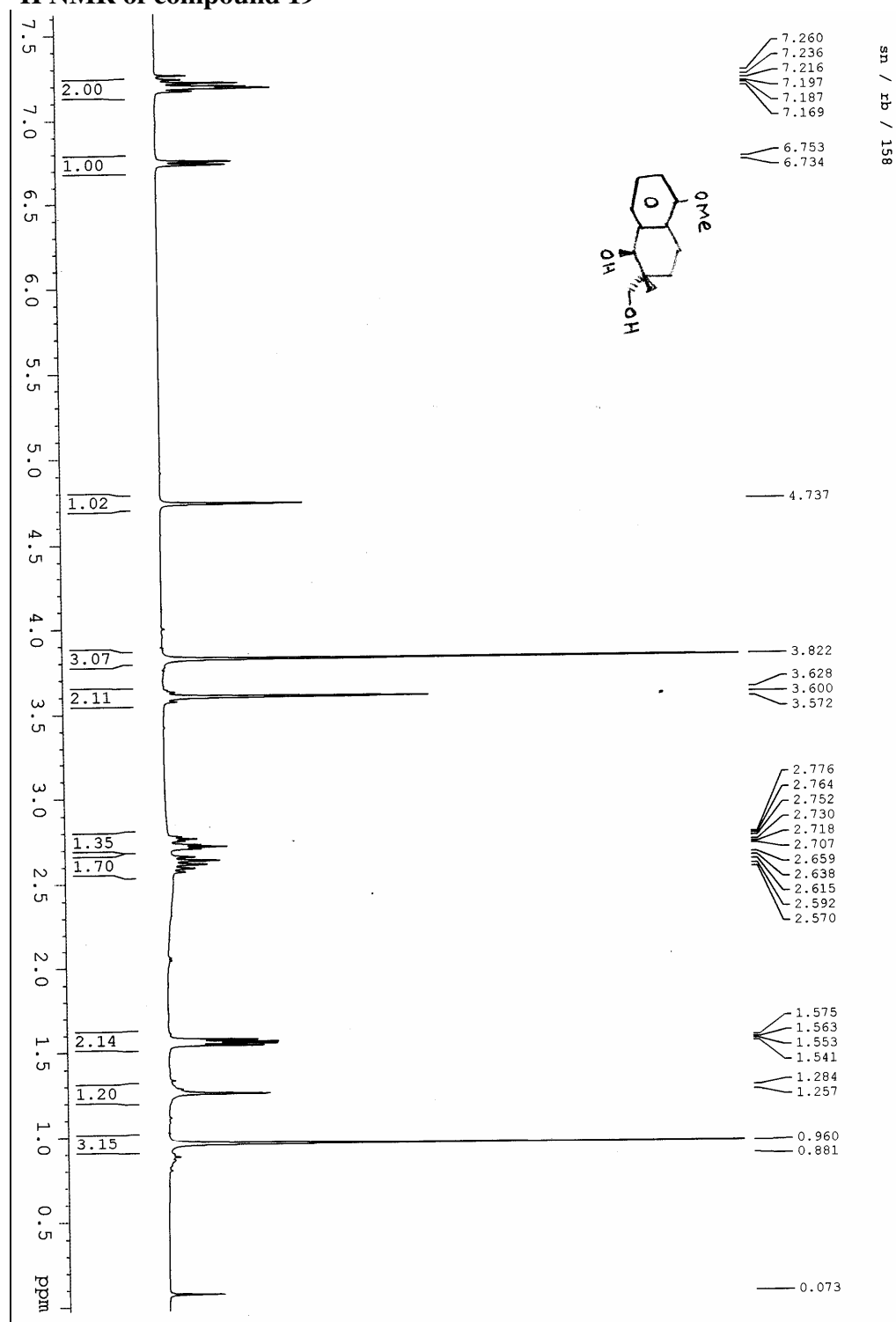


¹³C NMR spectrum of 18

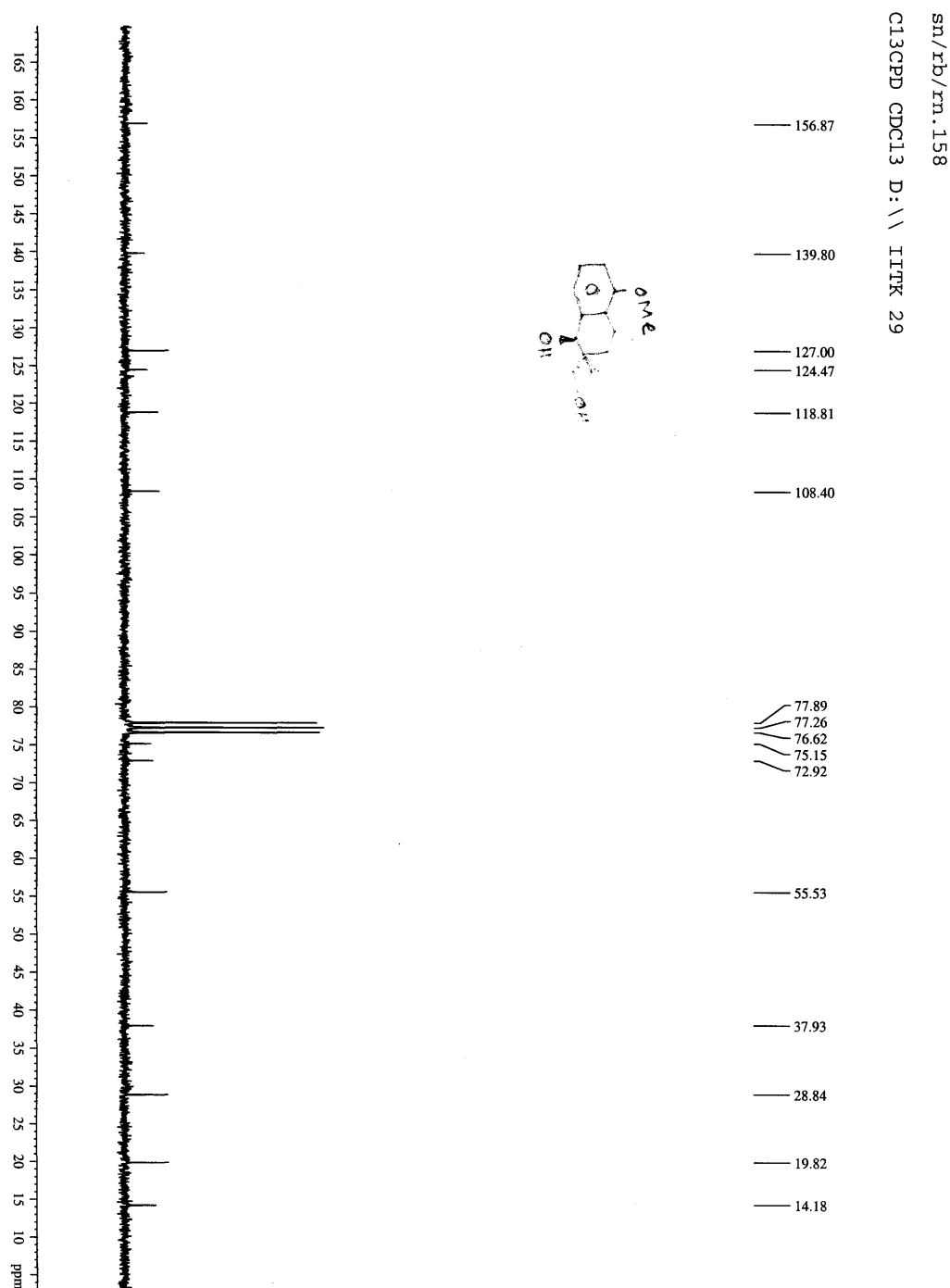


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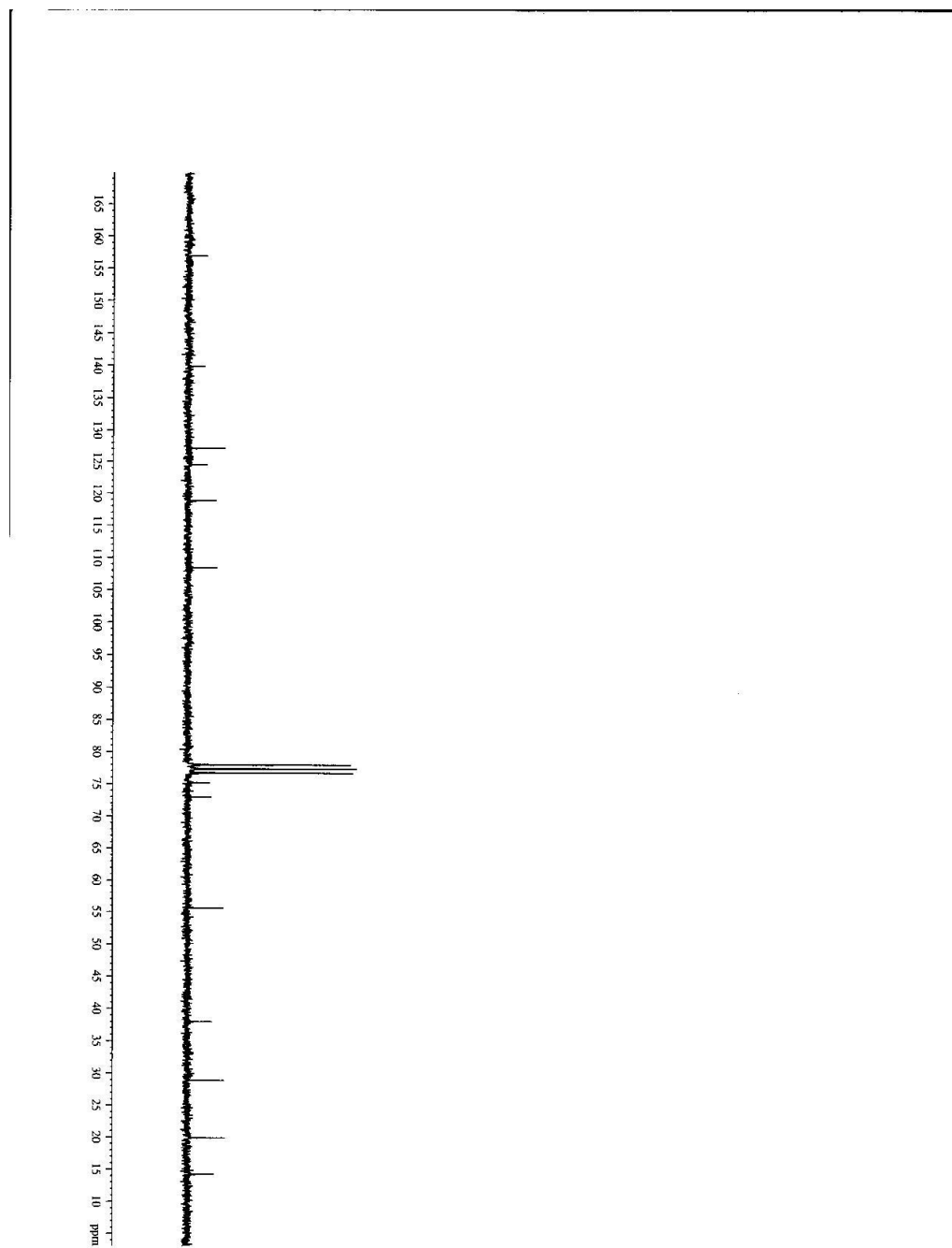
¹H NMR of compound 19



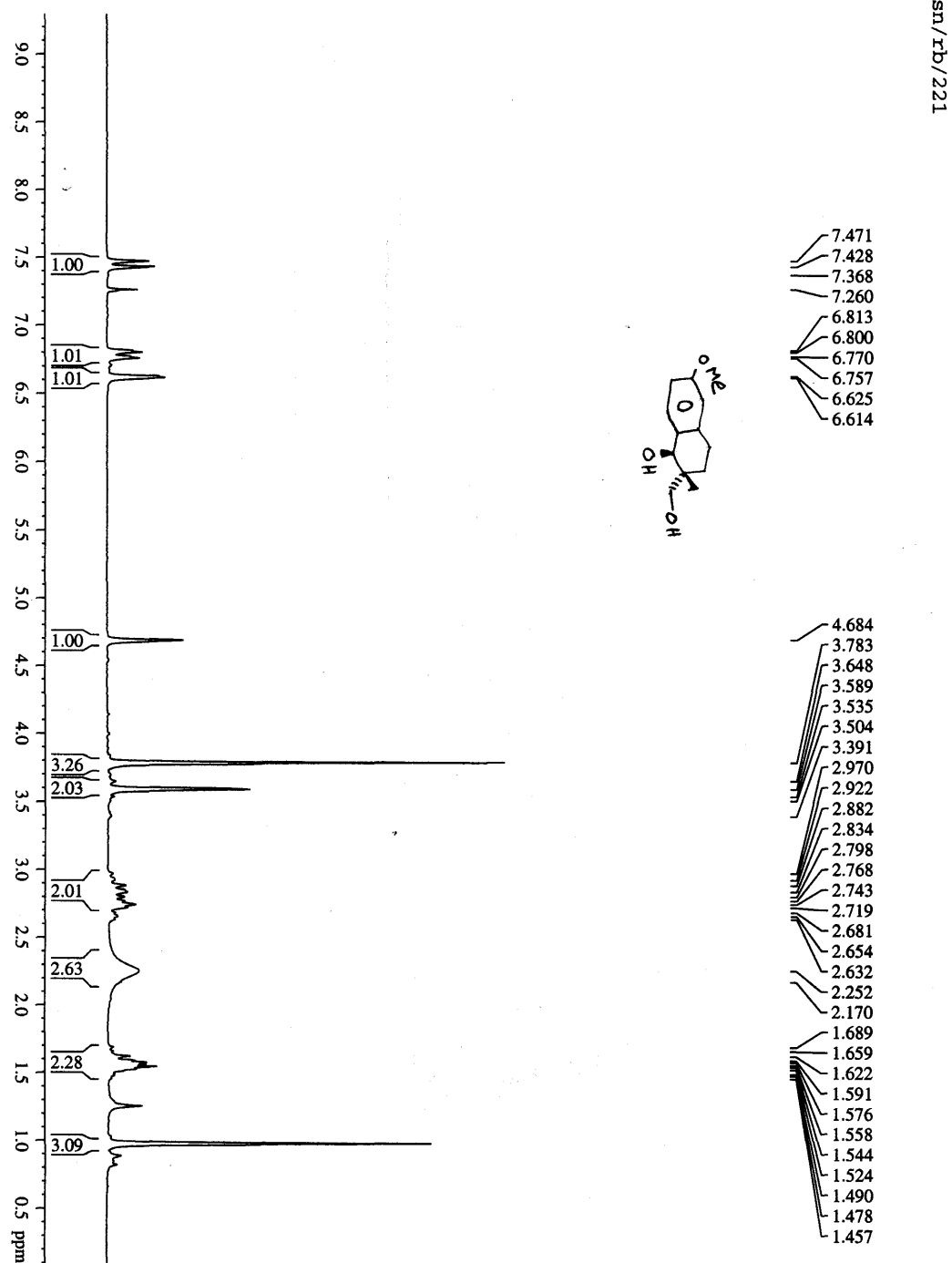
¹³C NMR of compound 19



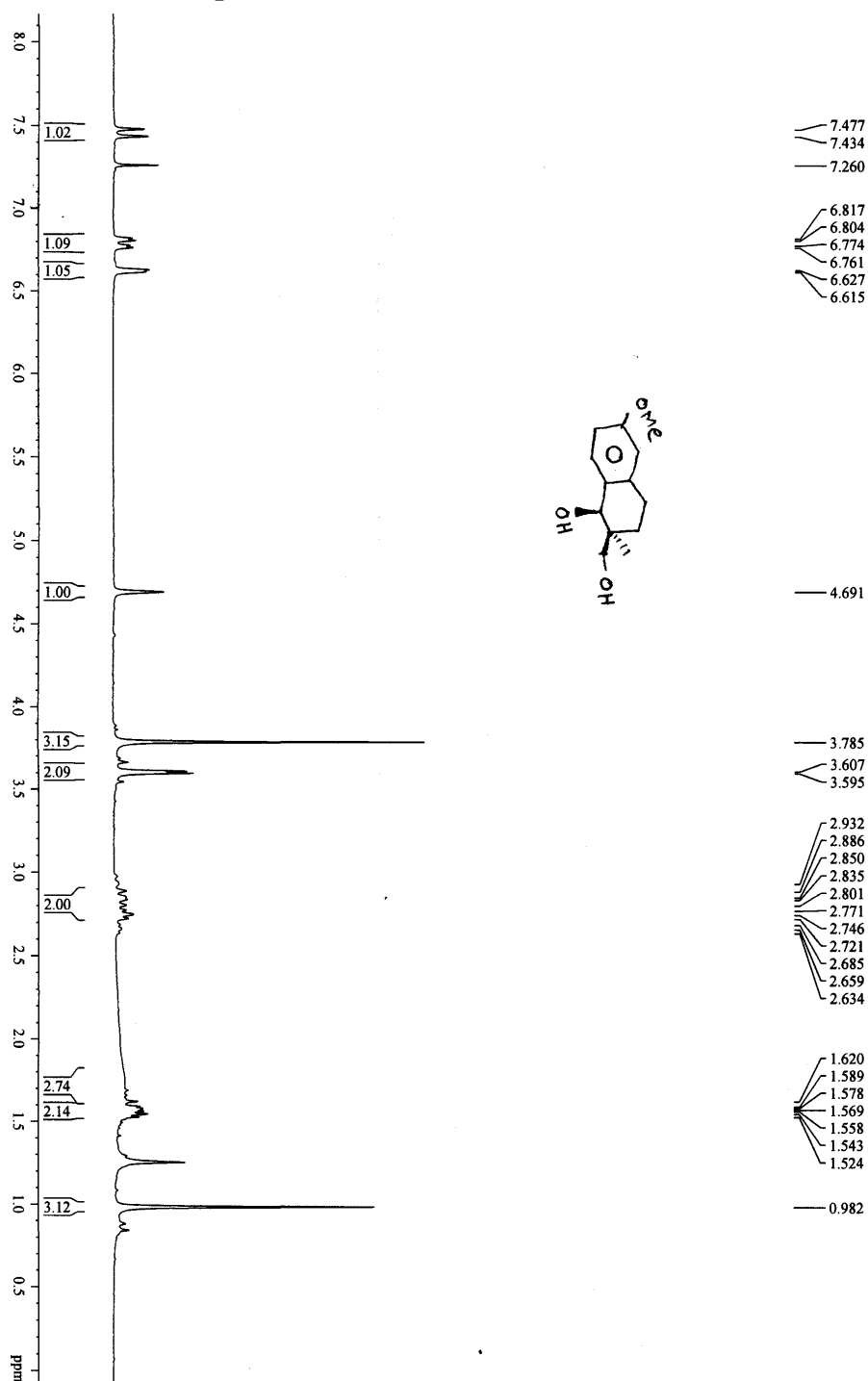
^{13}C NMR of compound 20



¹H NMR of compound 21



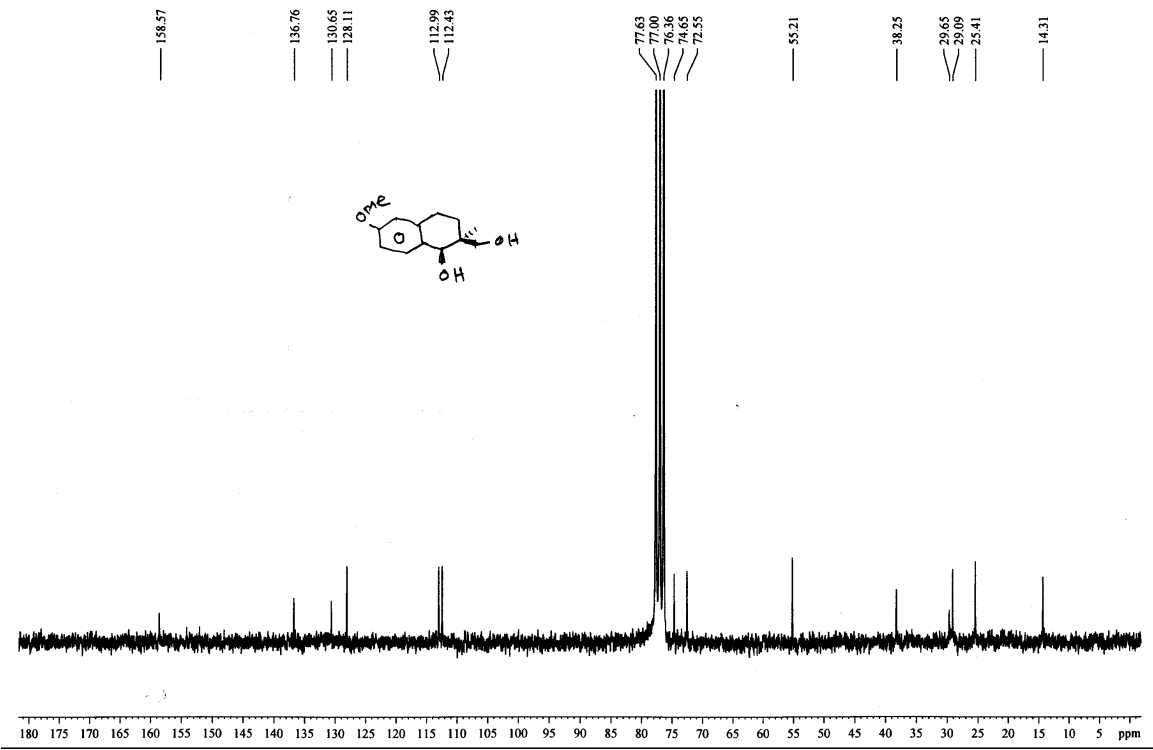
¹H NMR of compound ent-22



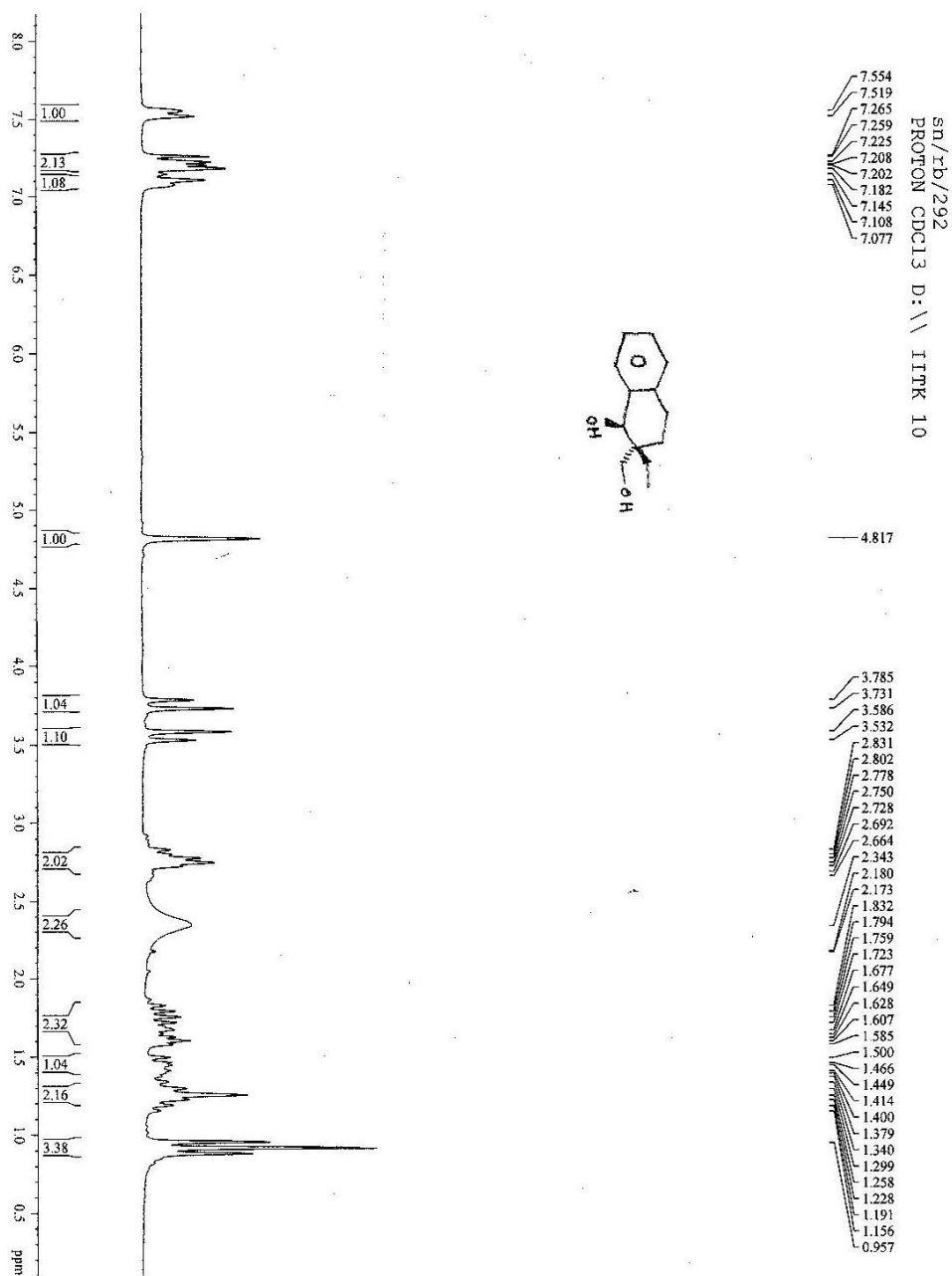
sn/rb/336
PROTON CDCl₃ D:\ IITK 13

¹³C NMR of compound ent-22

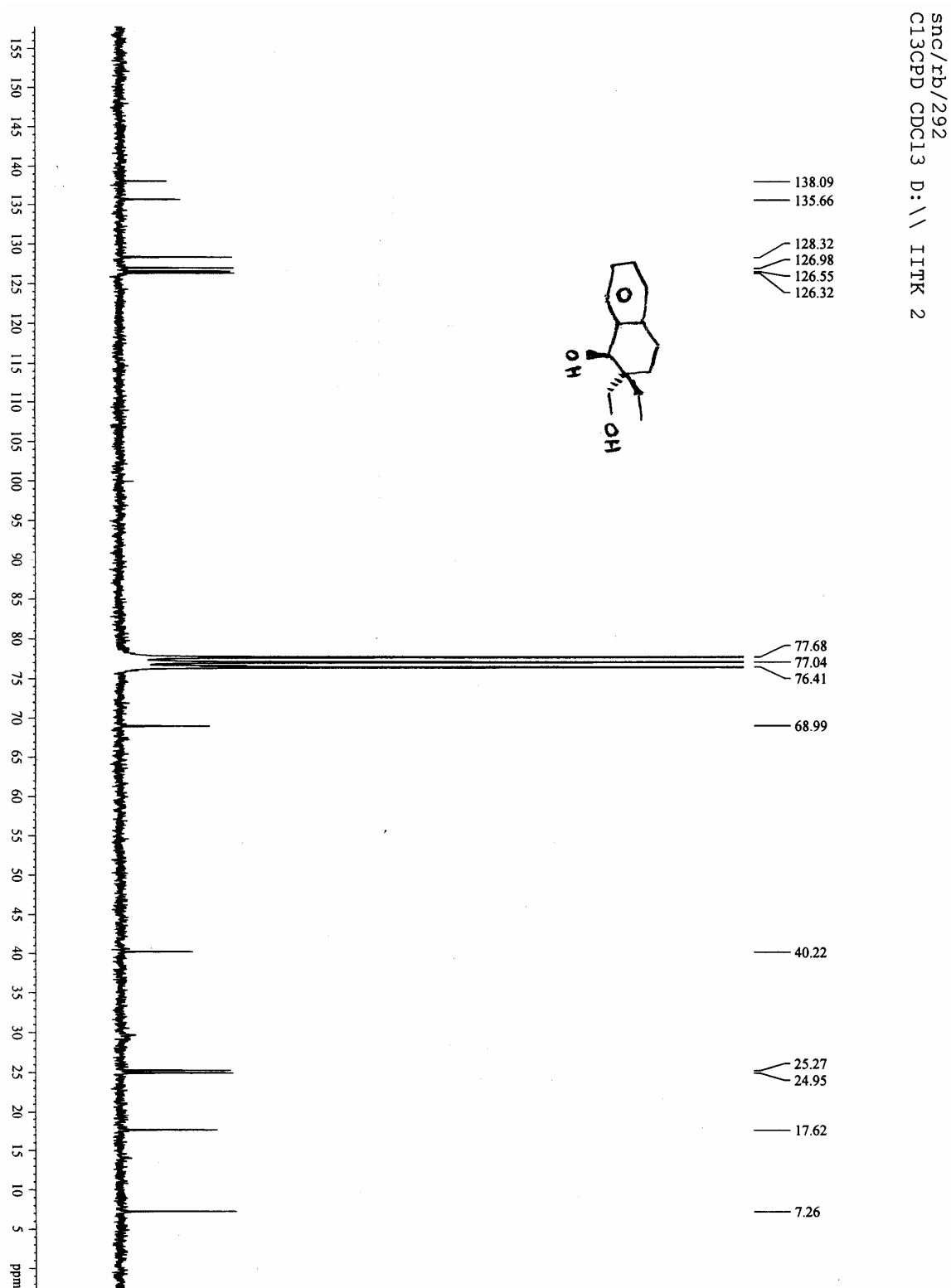
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C13CPD CDC13 D:\ IITK 2



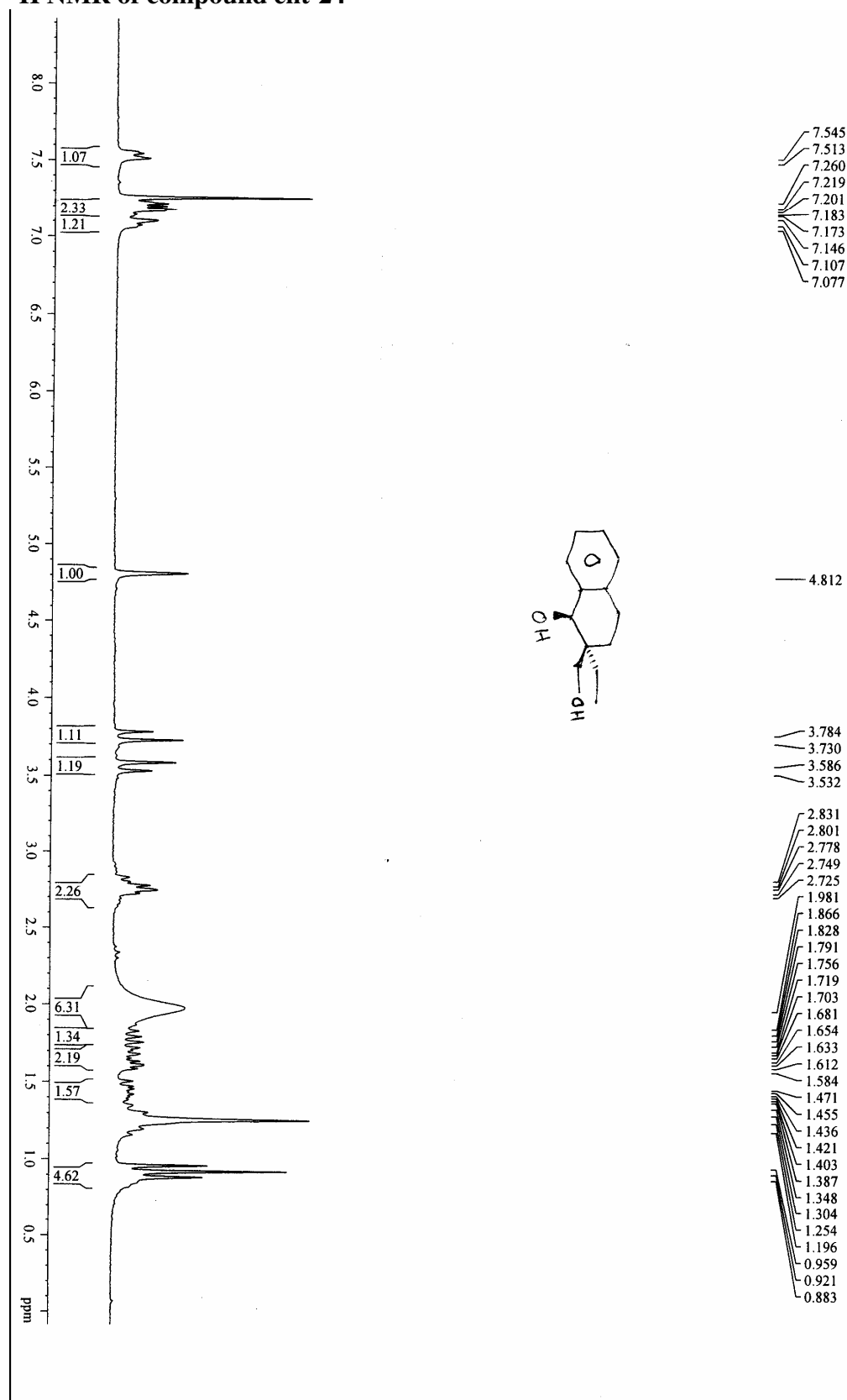
¹H NMR of compound 23



¹³C NMR of compound 23

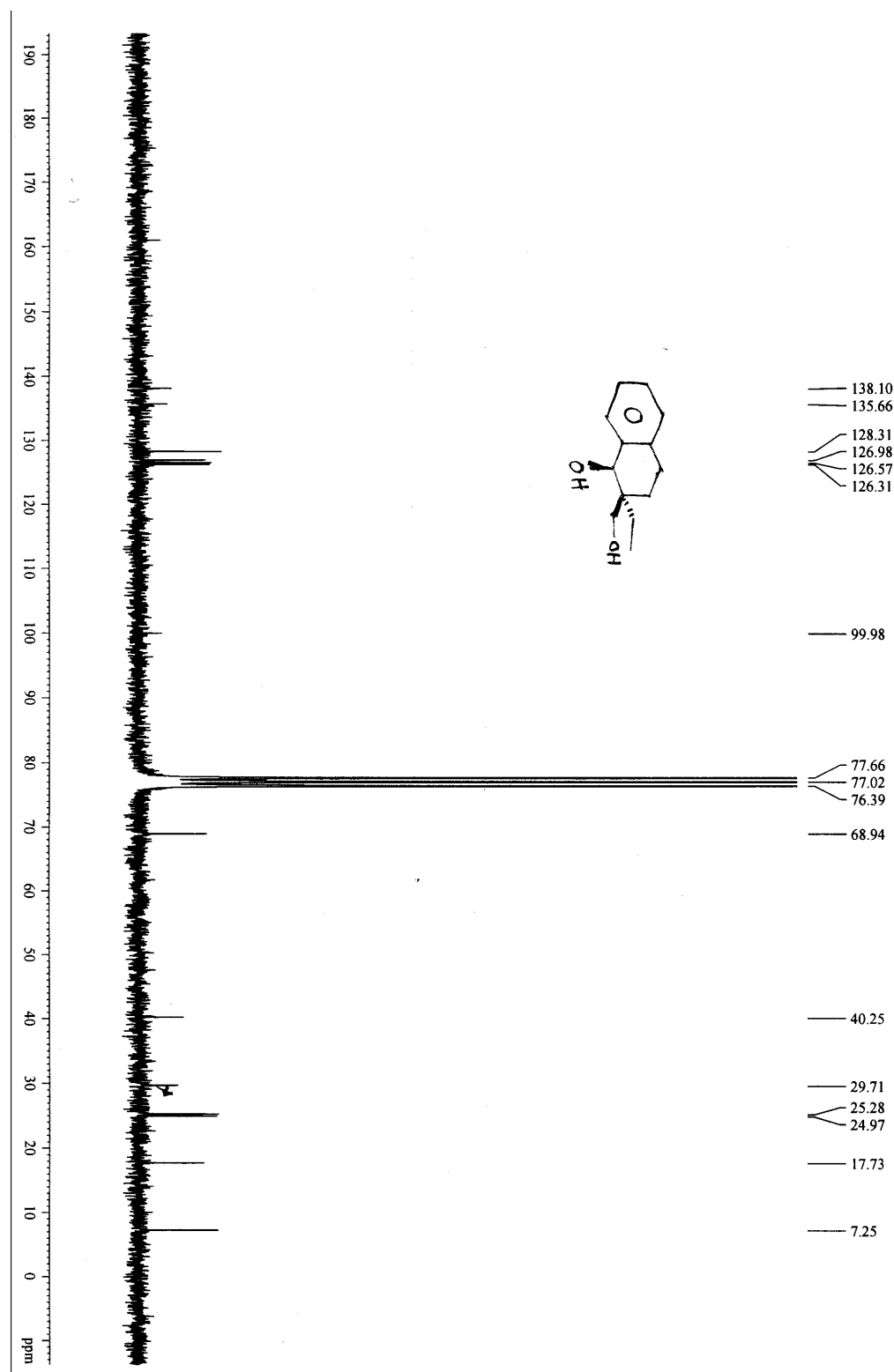


¹H NMR of compound ent-24



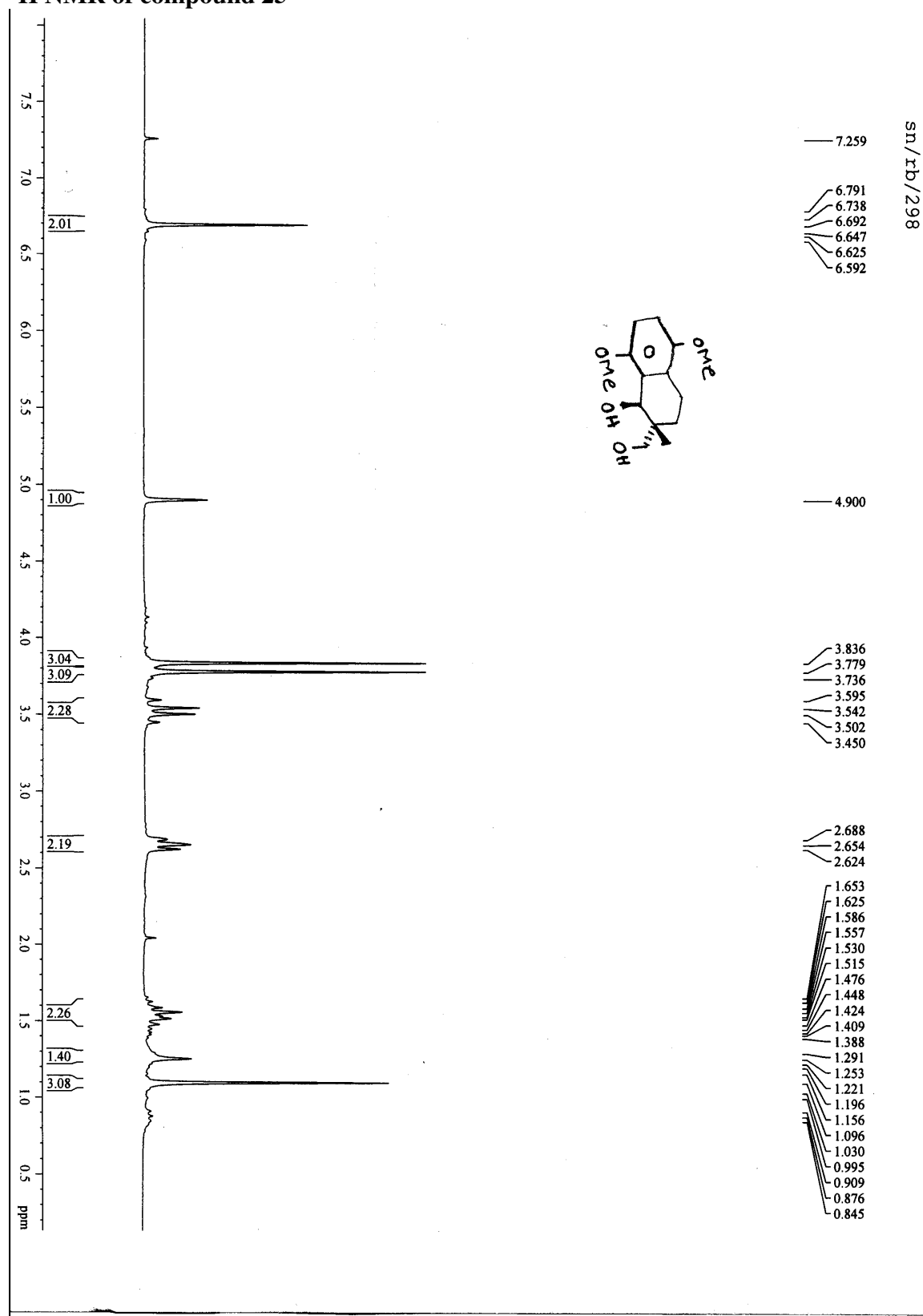
sn/rb/363

¹³C NMR of compound ent-24

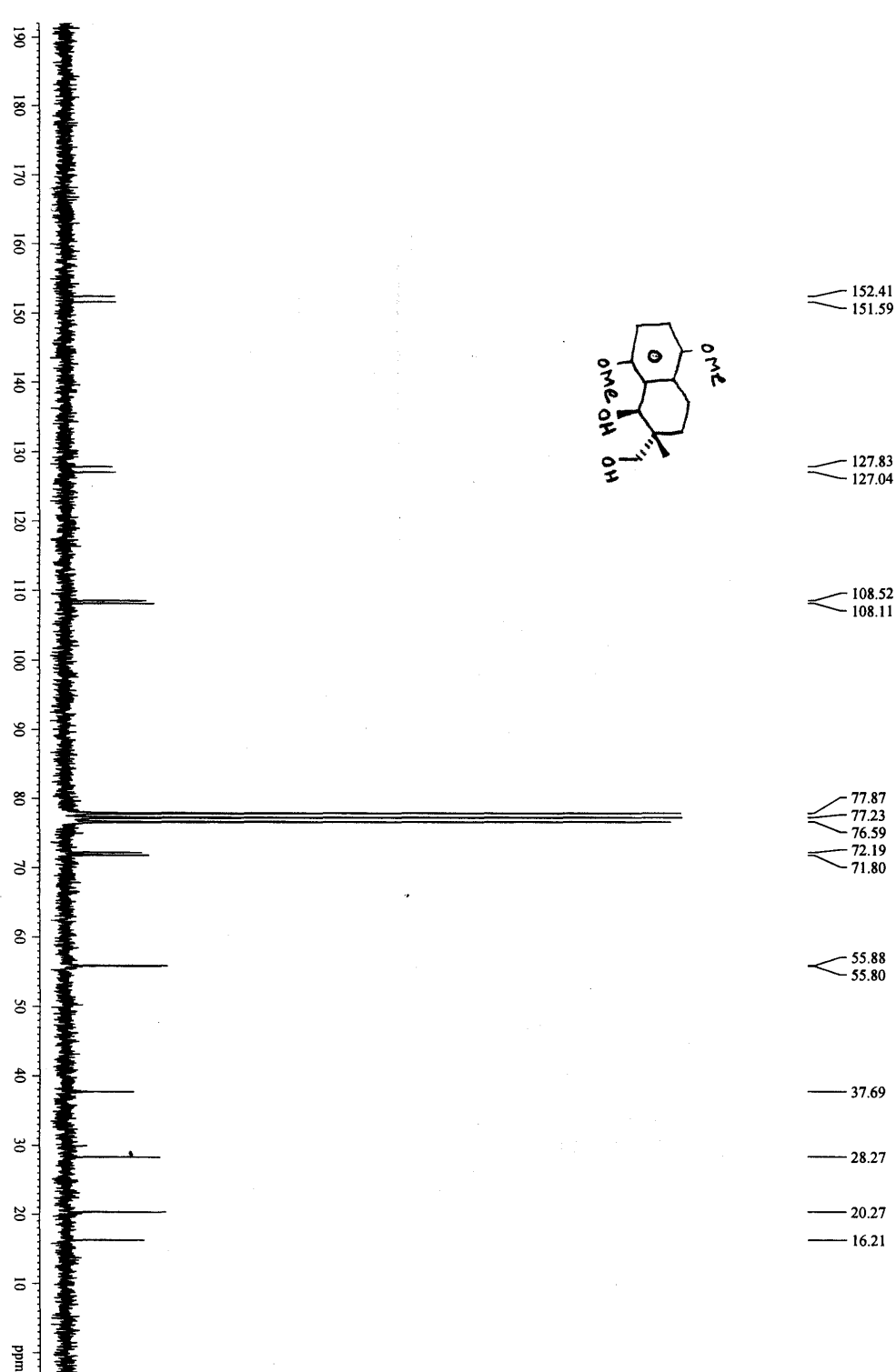


snc/rb/363

¹H NMR of compound 25

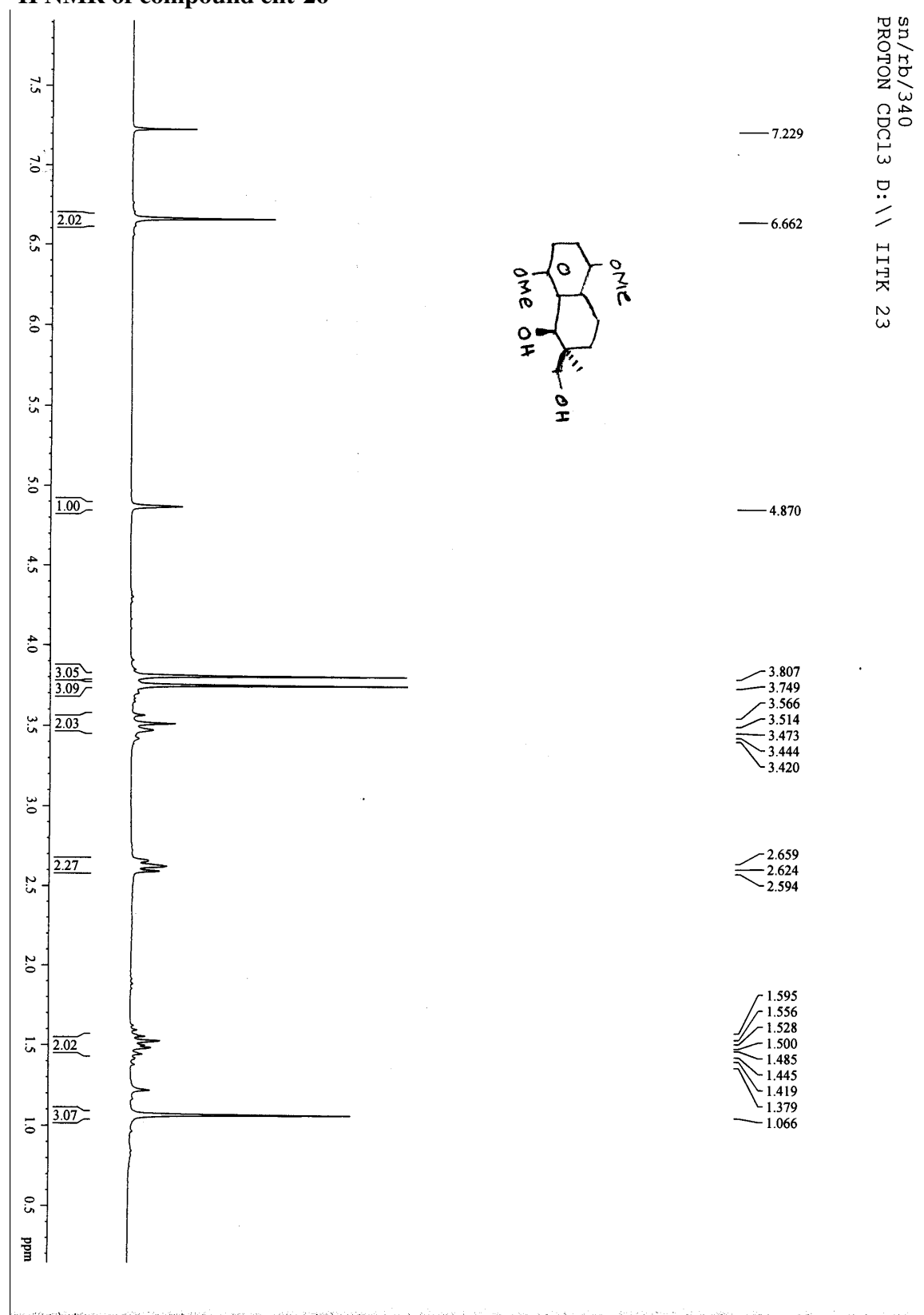


¹³C NMR of compound 25

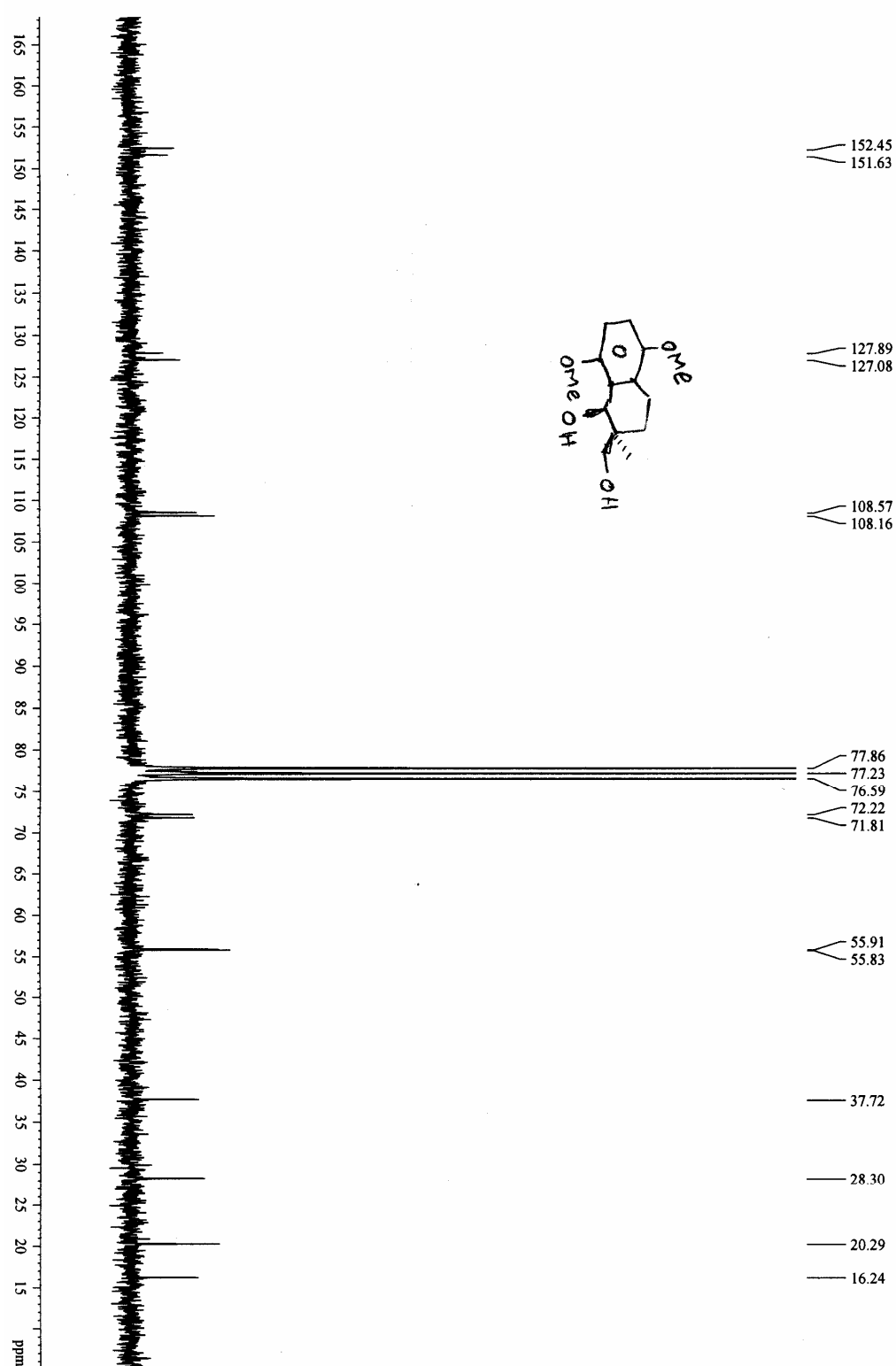


snc/rb/298
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¹H NMR of compound ent-26

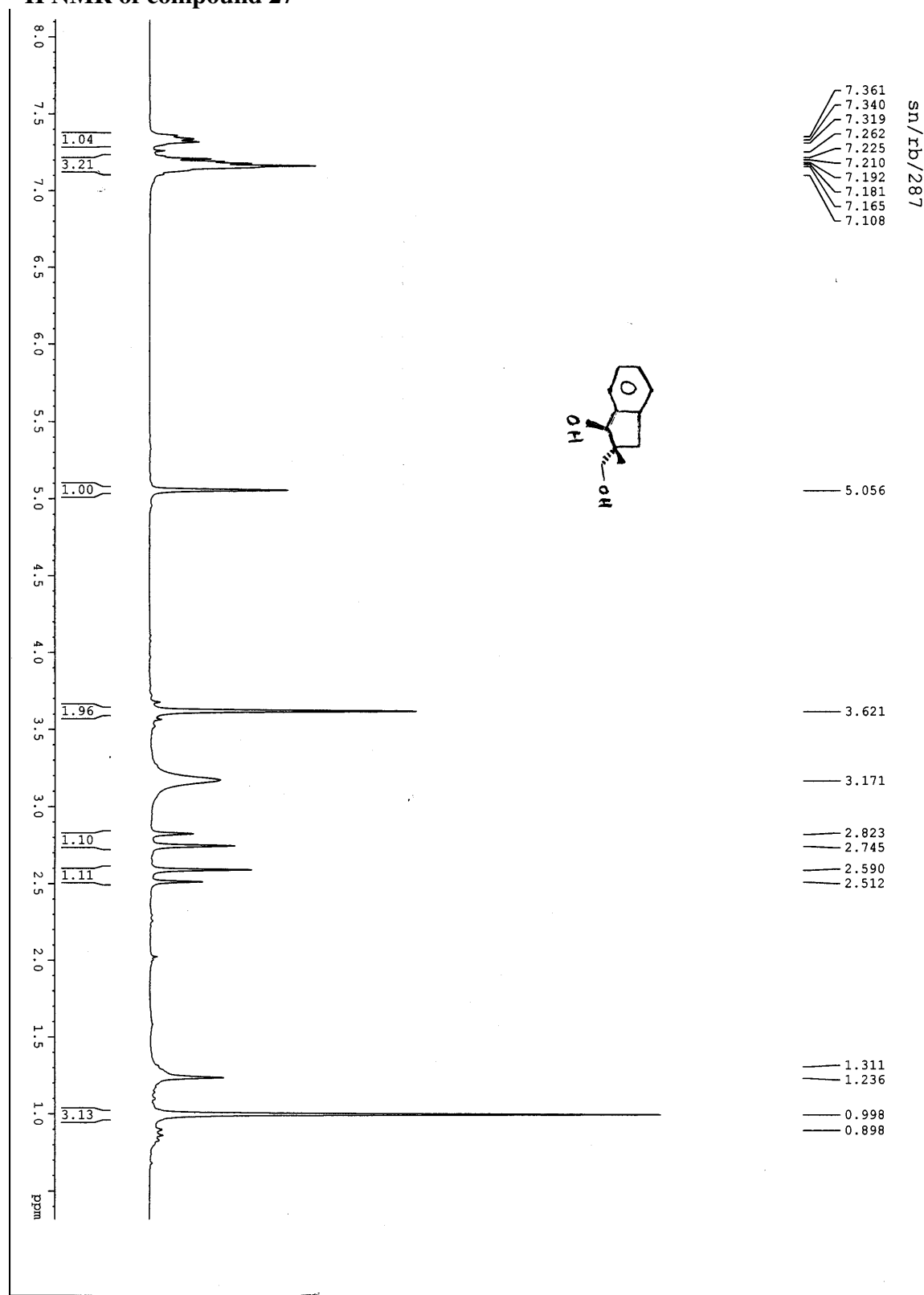


¹³C NMR of compound ent-26



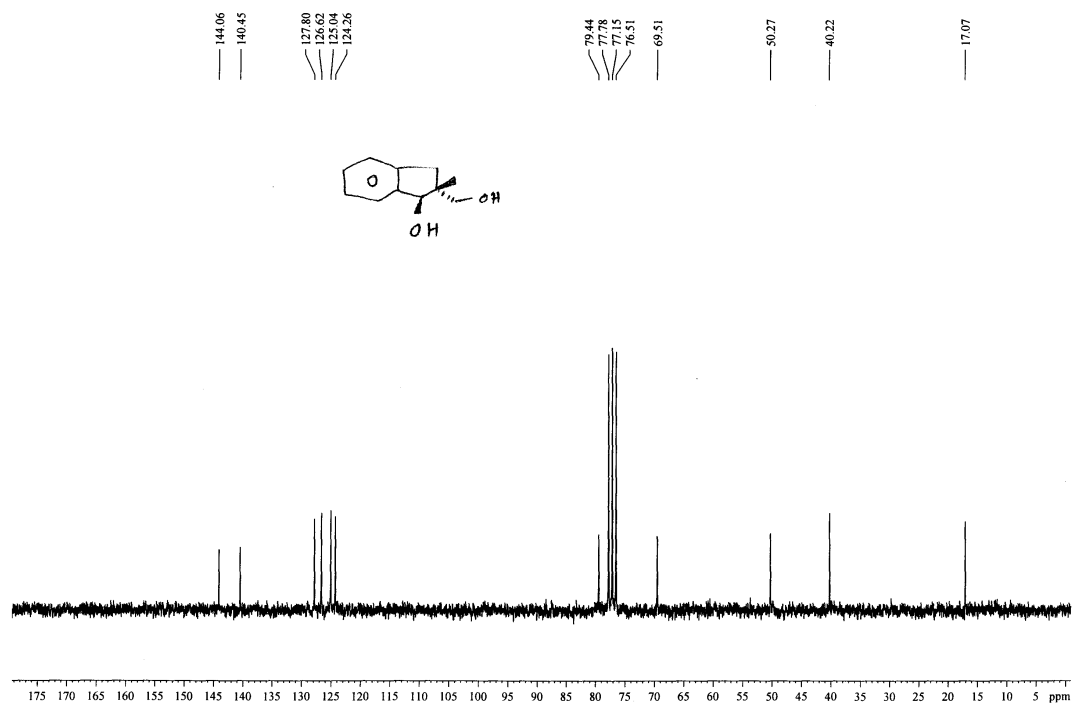
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¹H NMR of compound 27

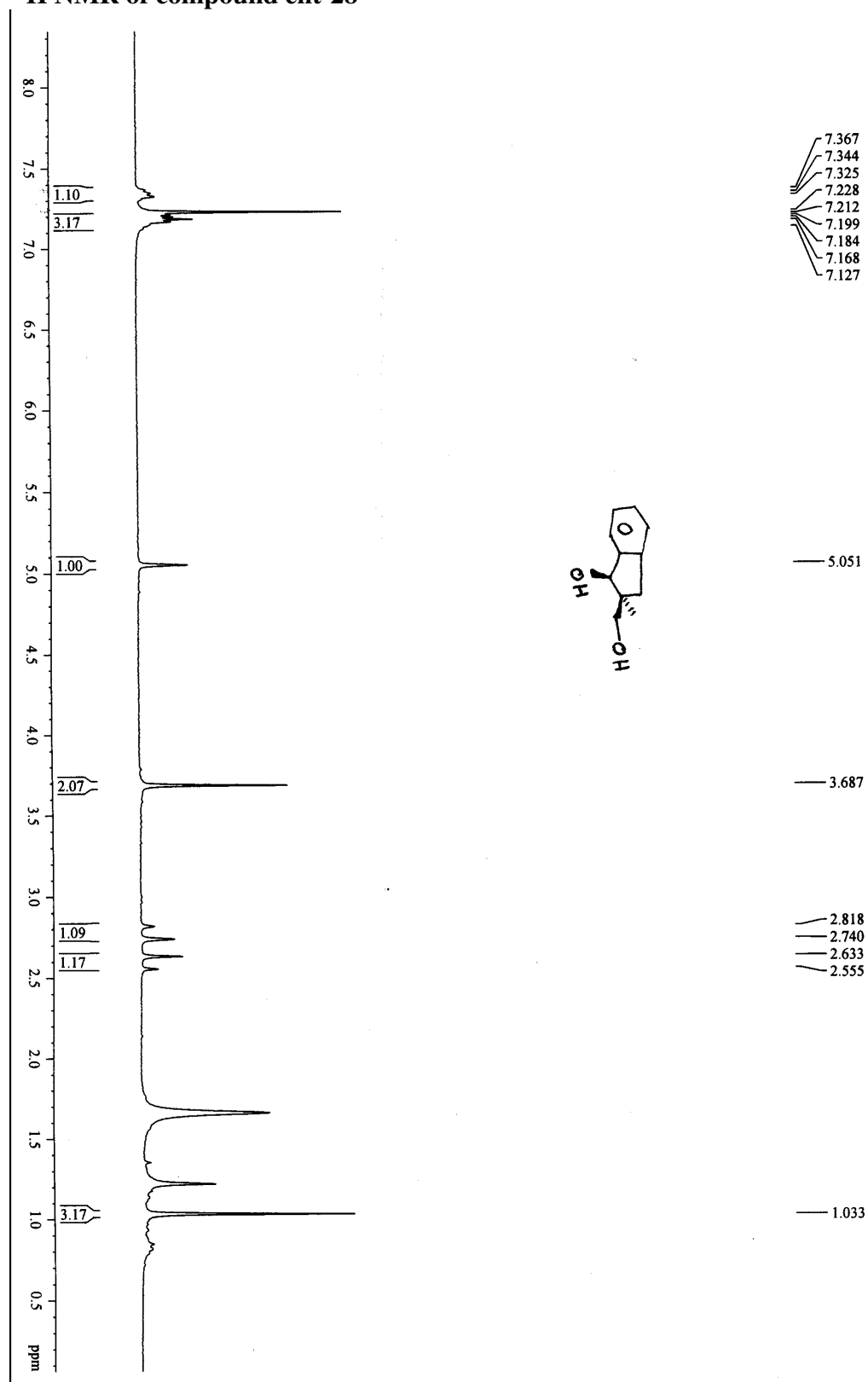


¹³C NMR of compound 27

snc/rb/287
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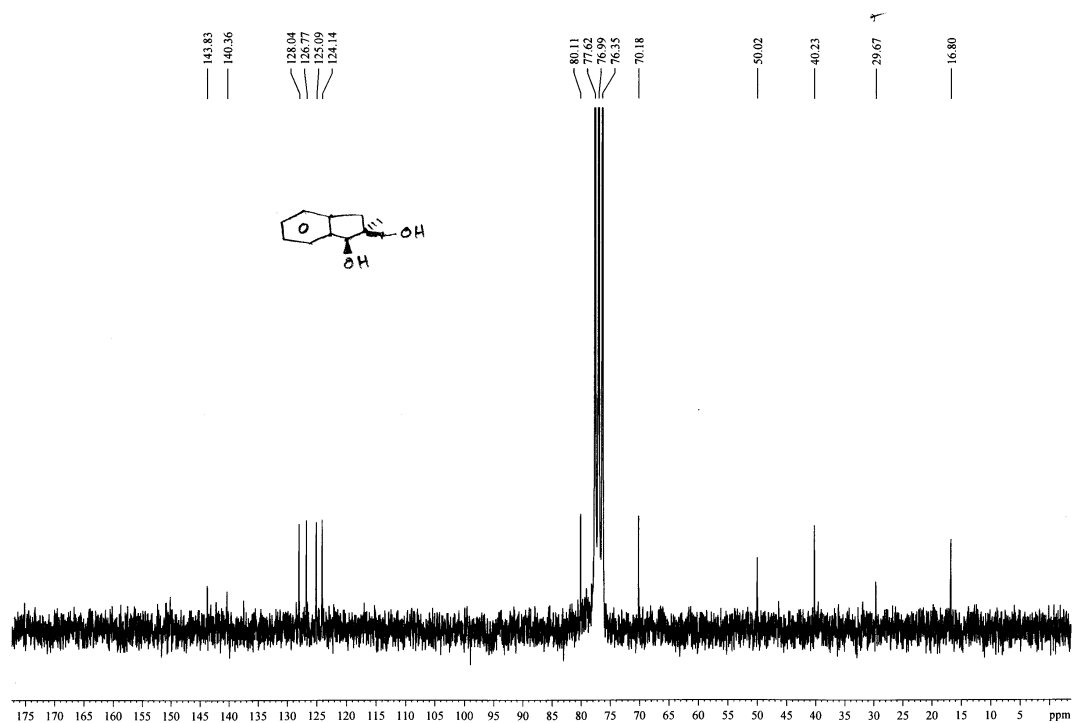
¹H NMR of compound ent-28



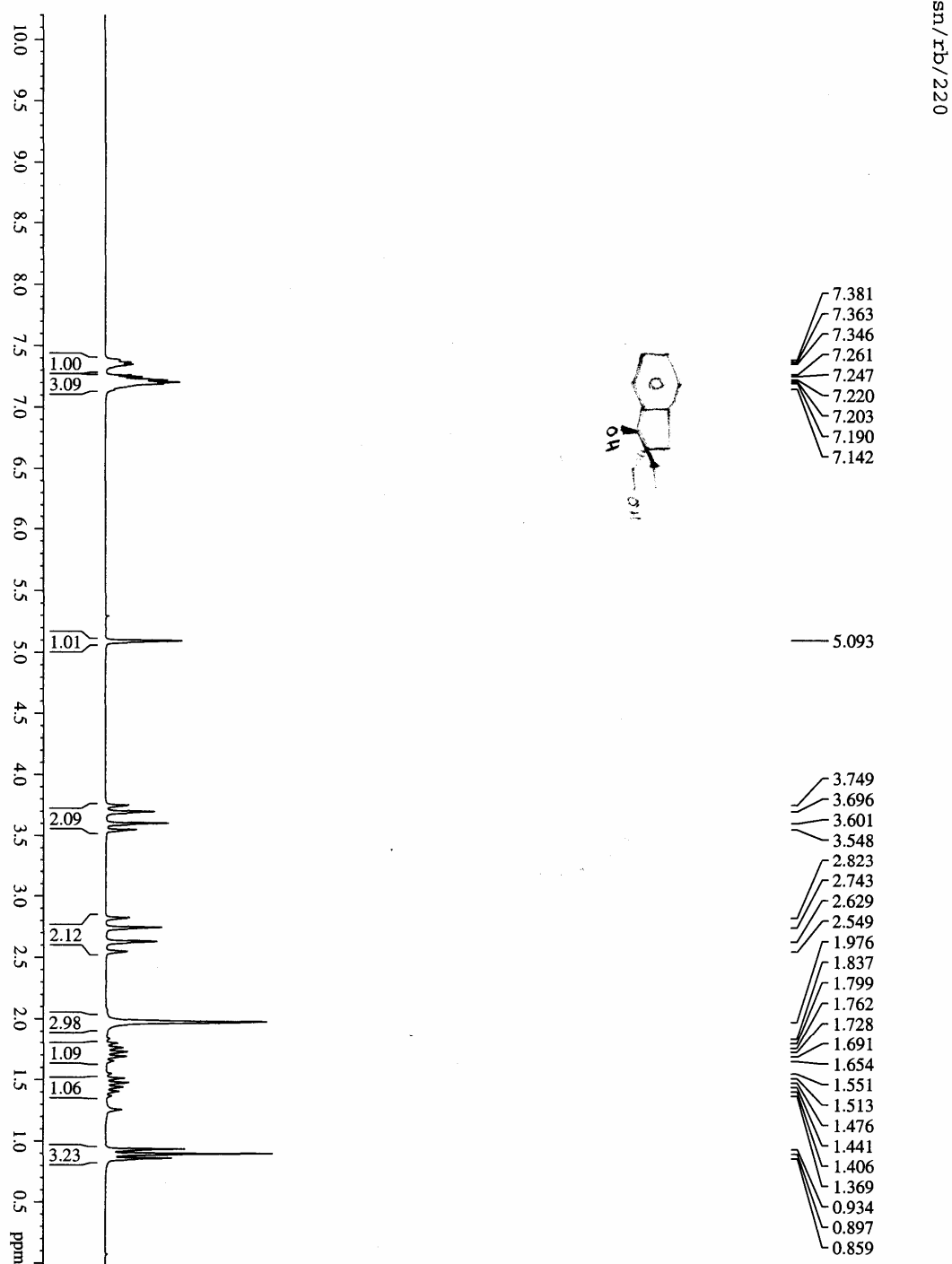
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¹³C NMR of compound ent-28

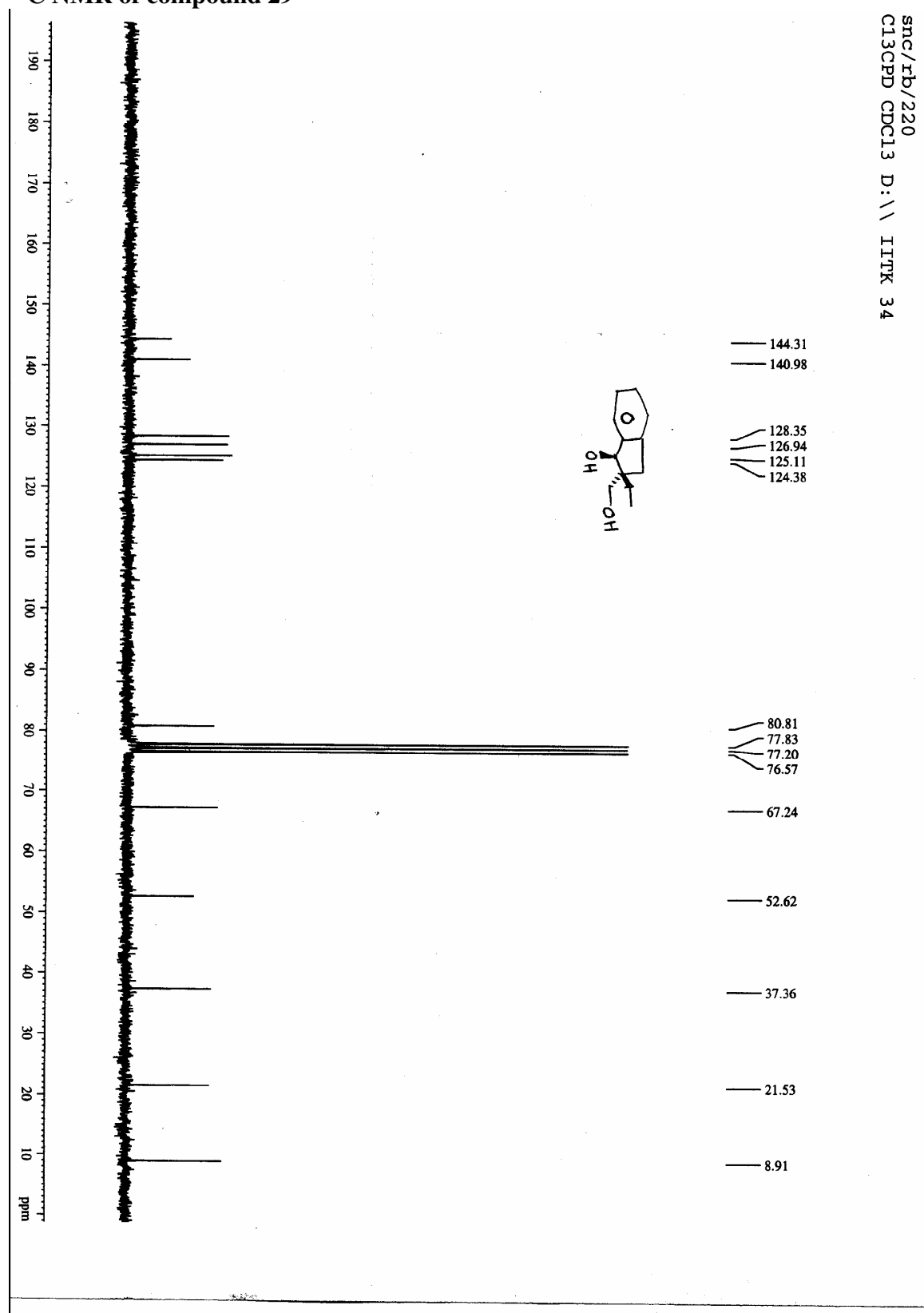
sn /rb/339



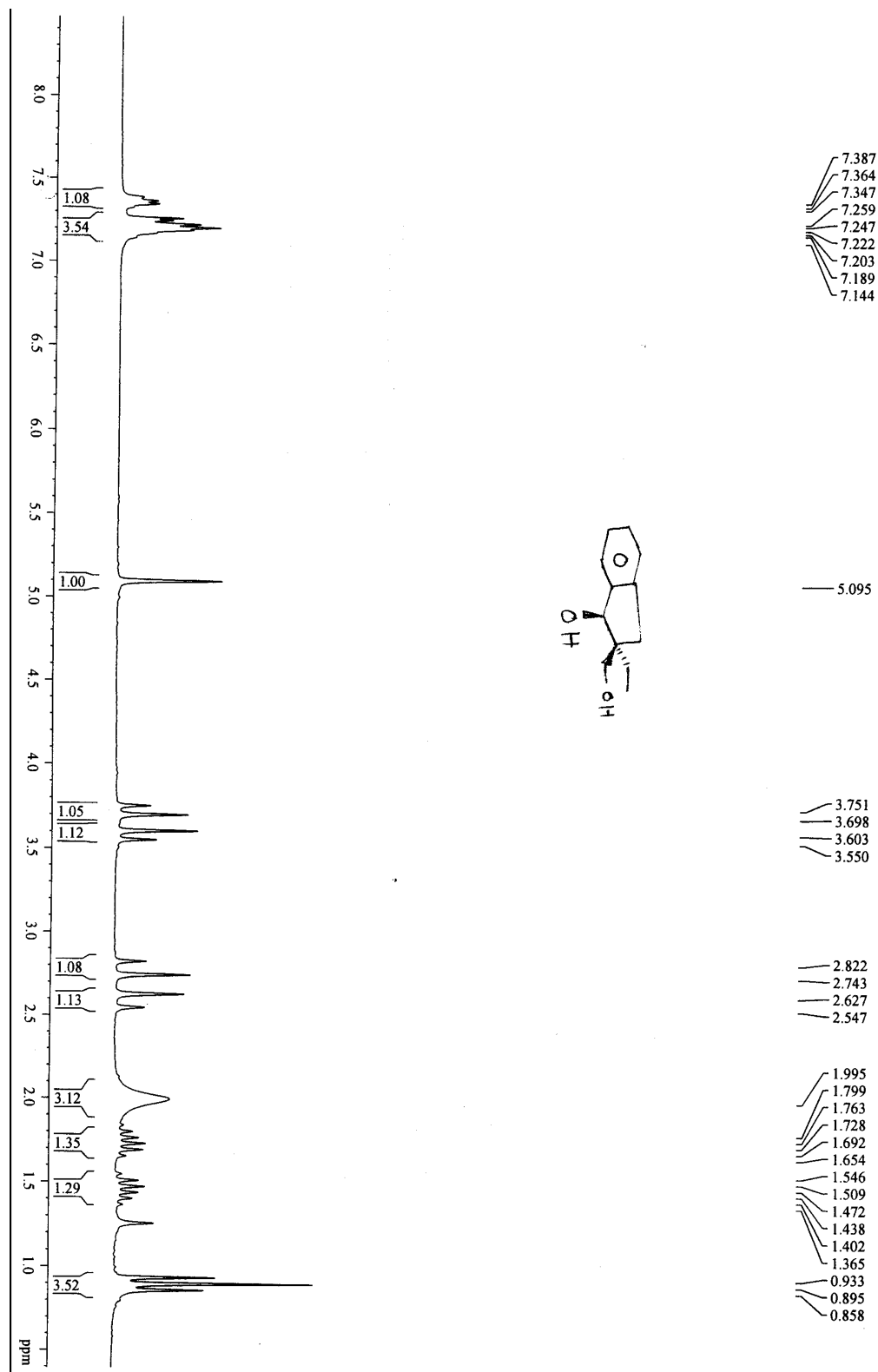
¹H NMR of compound 29



¹³C NMR of compound 29

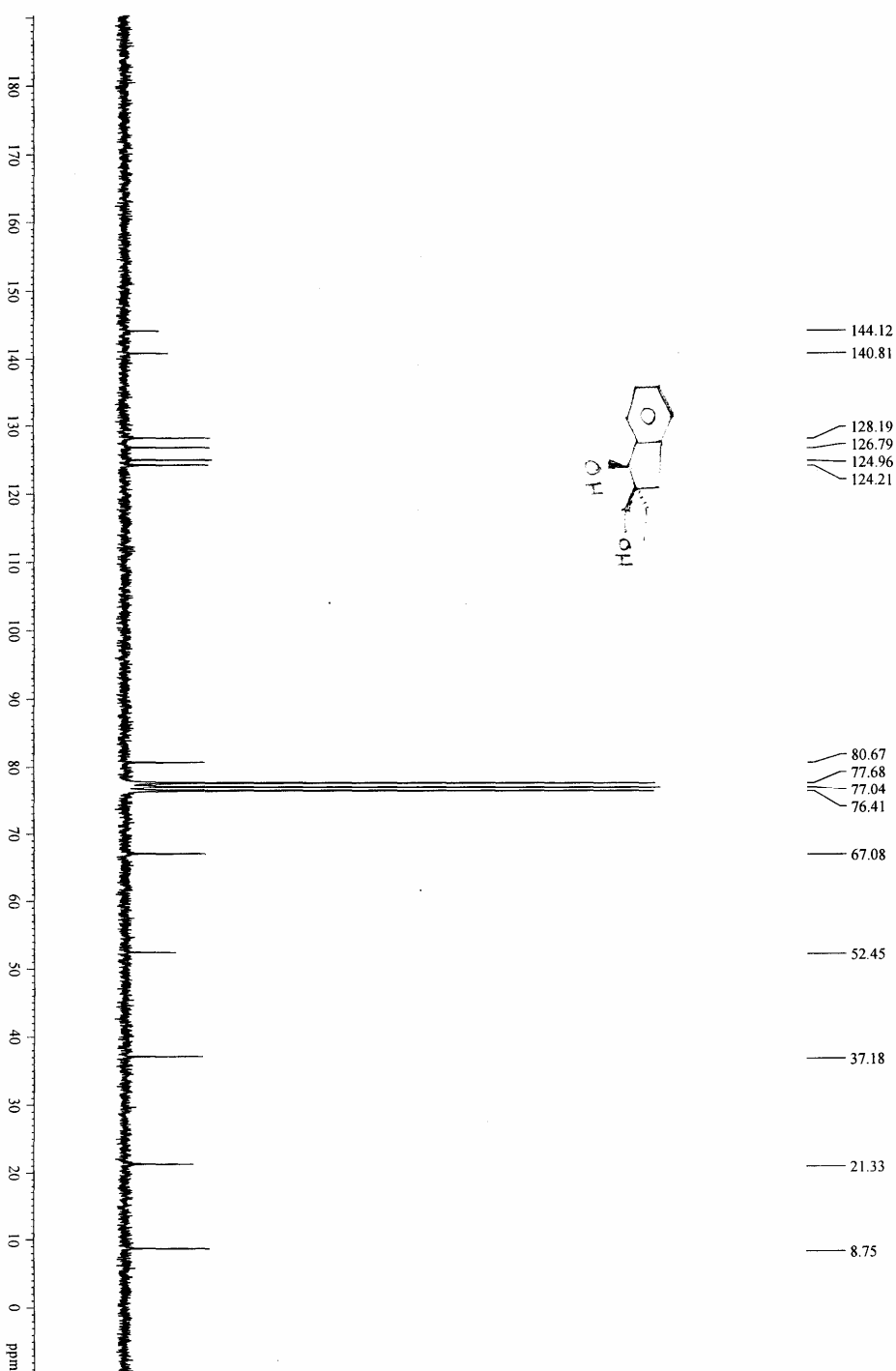


¹H NMR of compound ent-30



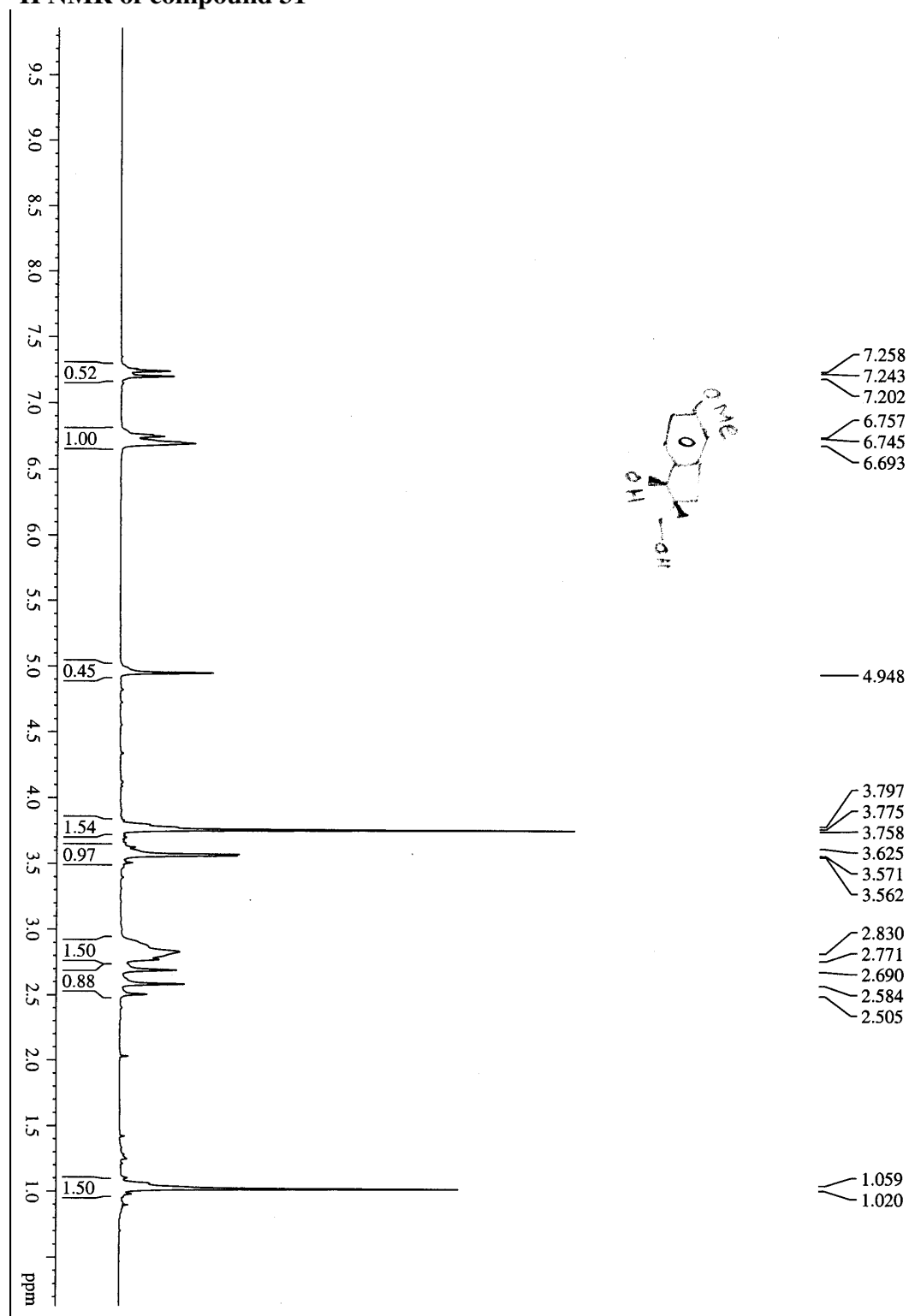
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¹³C NMR of compound ent-30



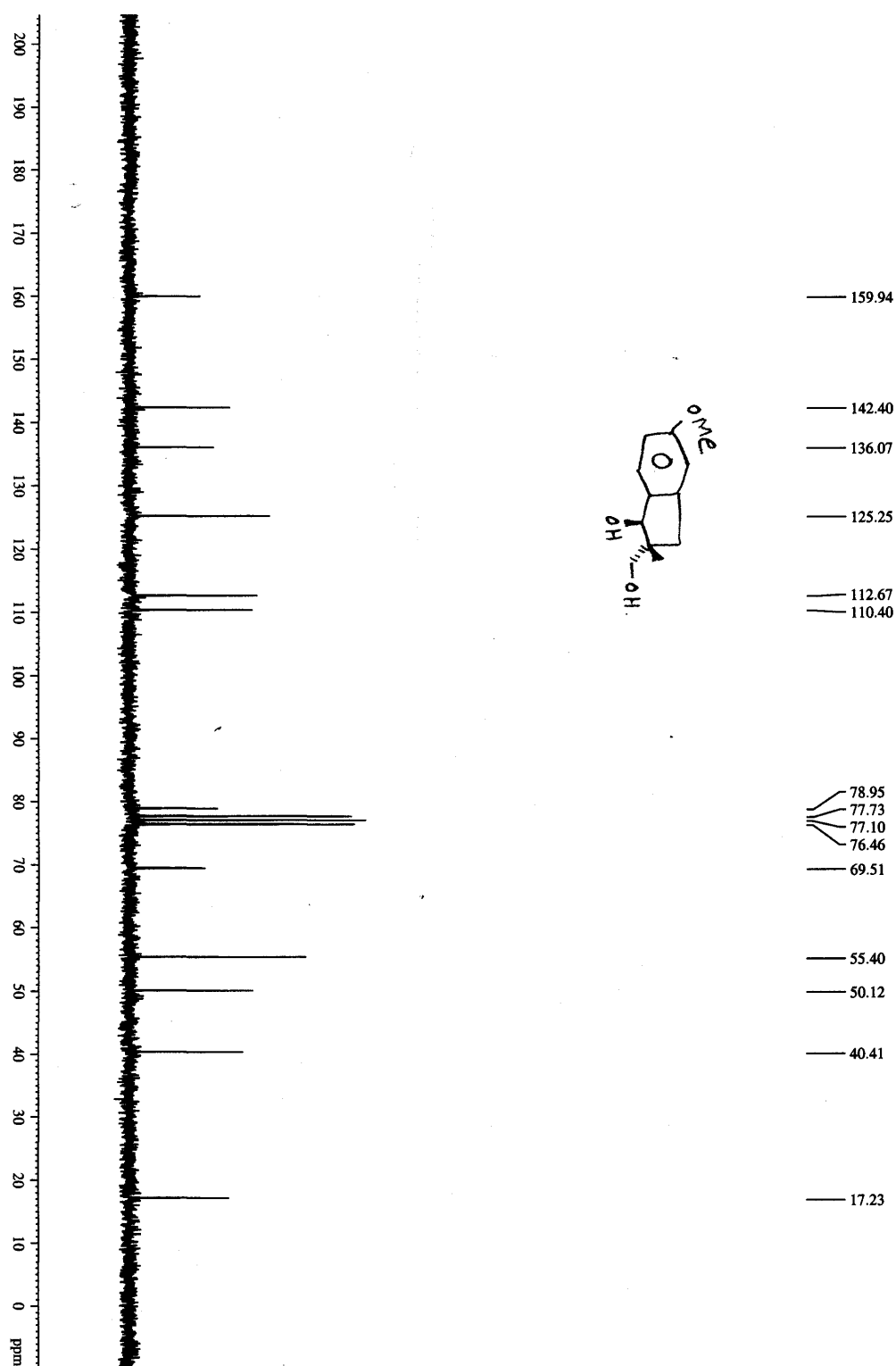
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¹H NMR of compound 31

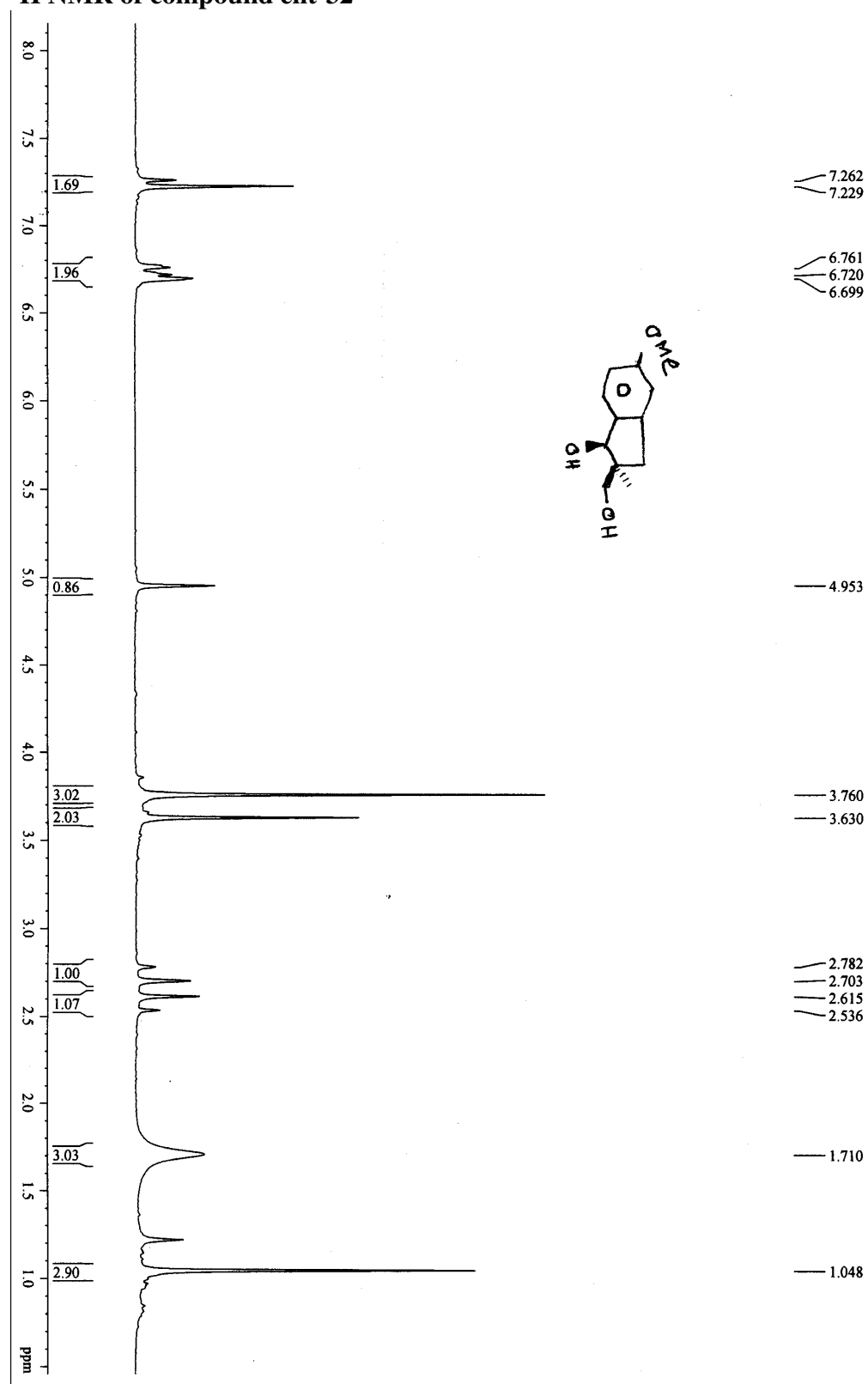


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¹³C NMR of compound 31

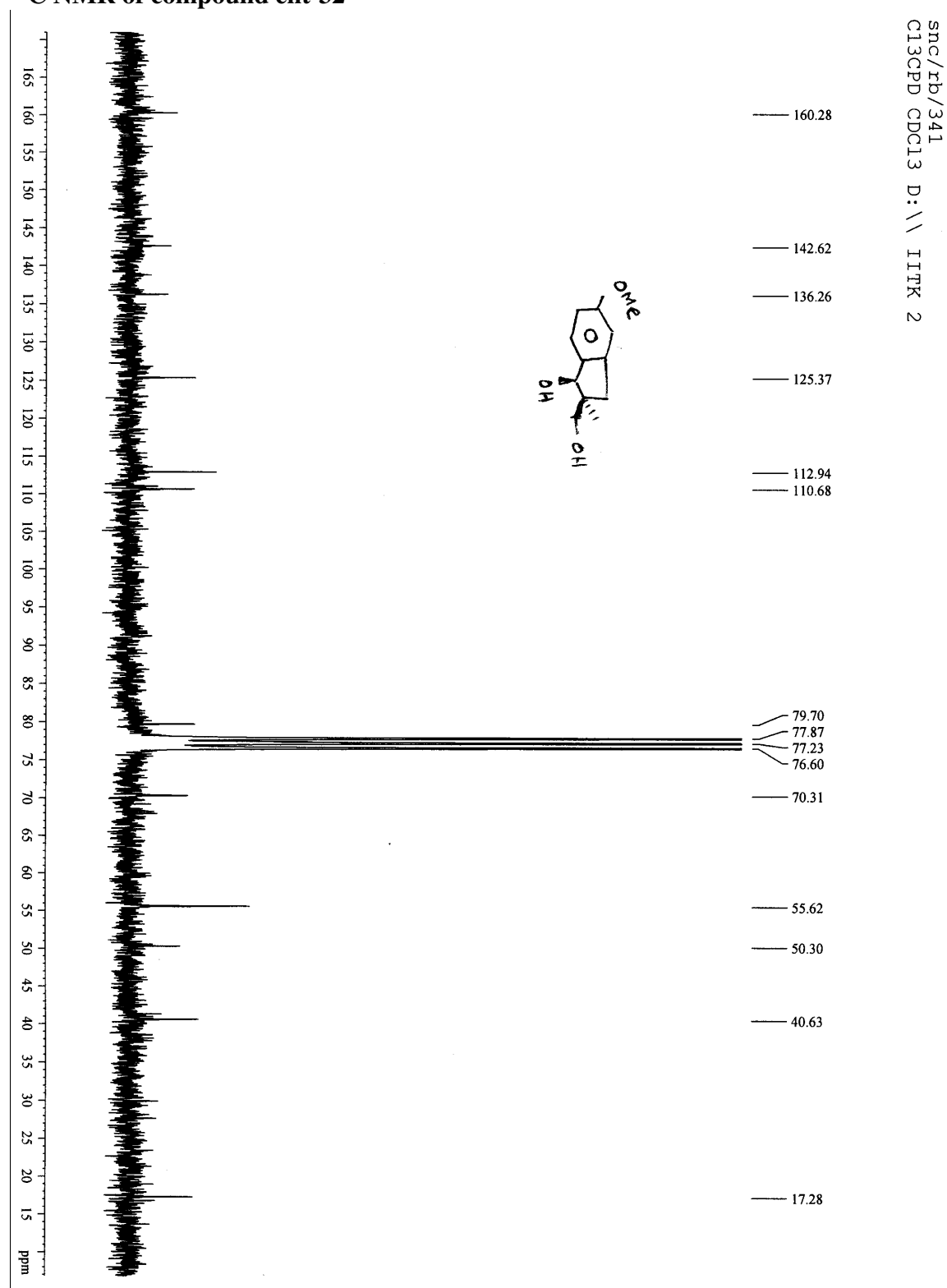


¹H NMR of compound ent-32

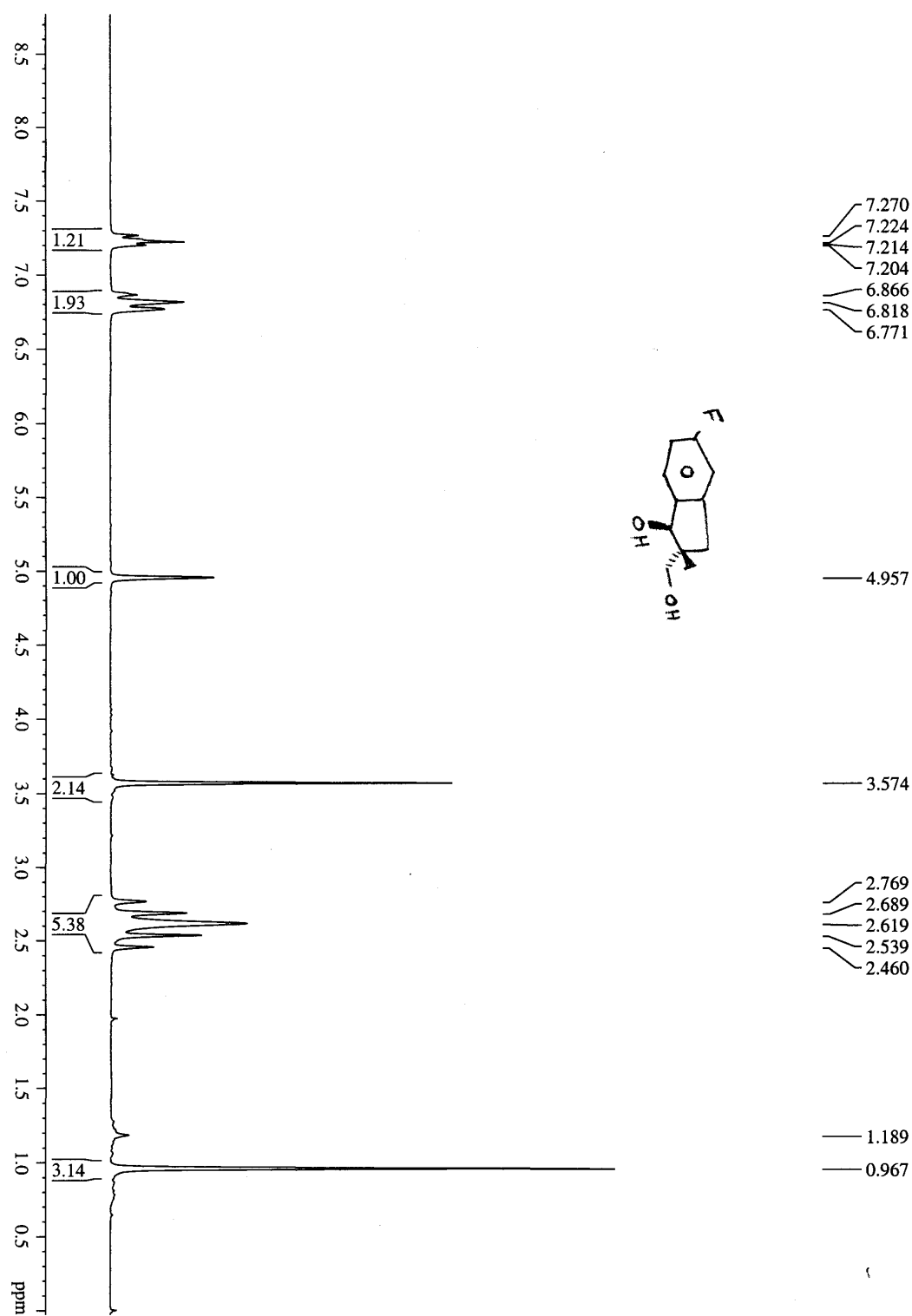


sn/rb/341
PROTON CDCl₃ D:\ IITK 2

¹³C NMR of compound ent-32

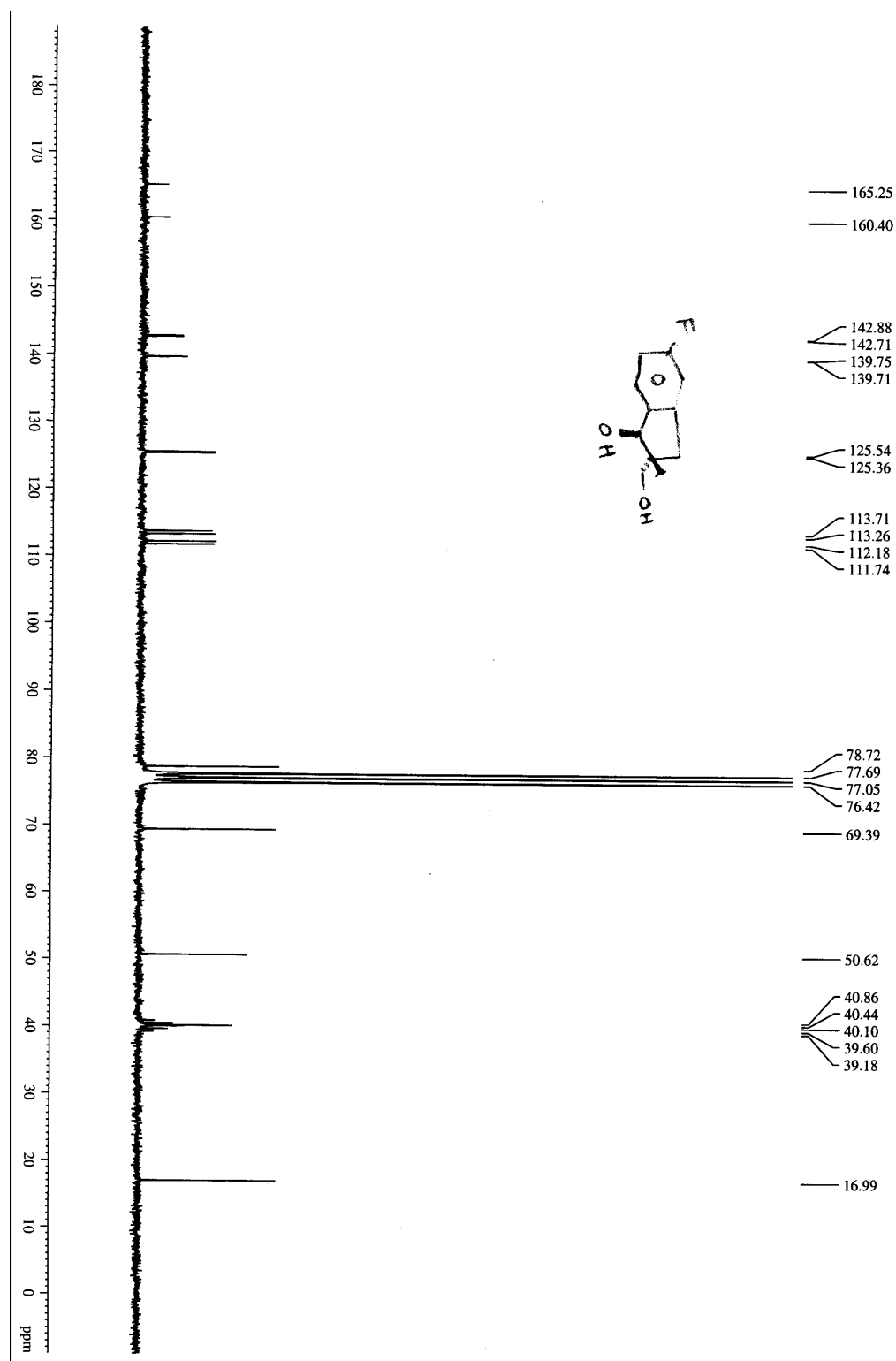


¹H NMR of compound 33



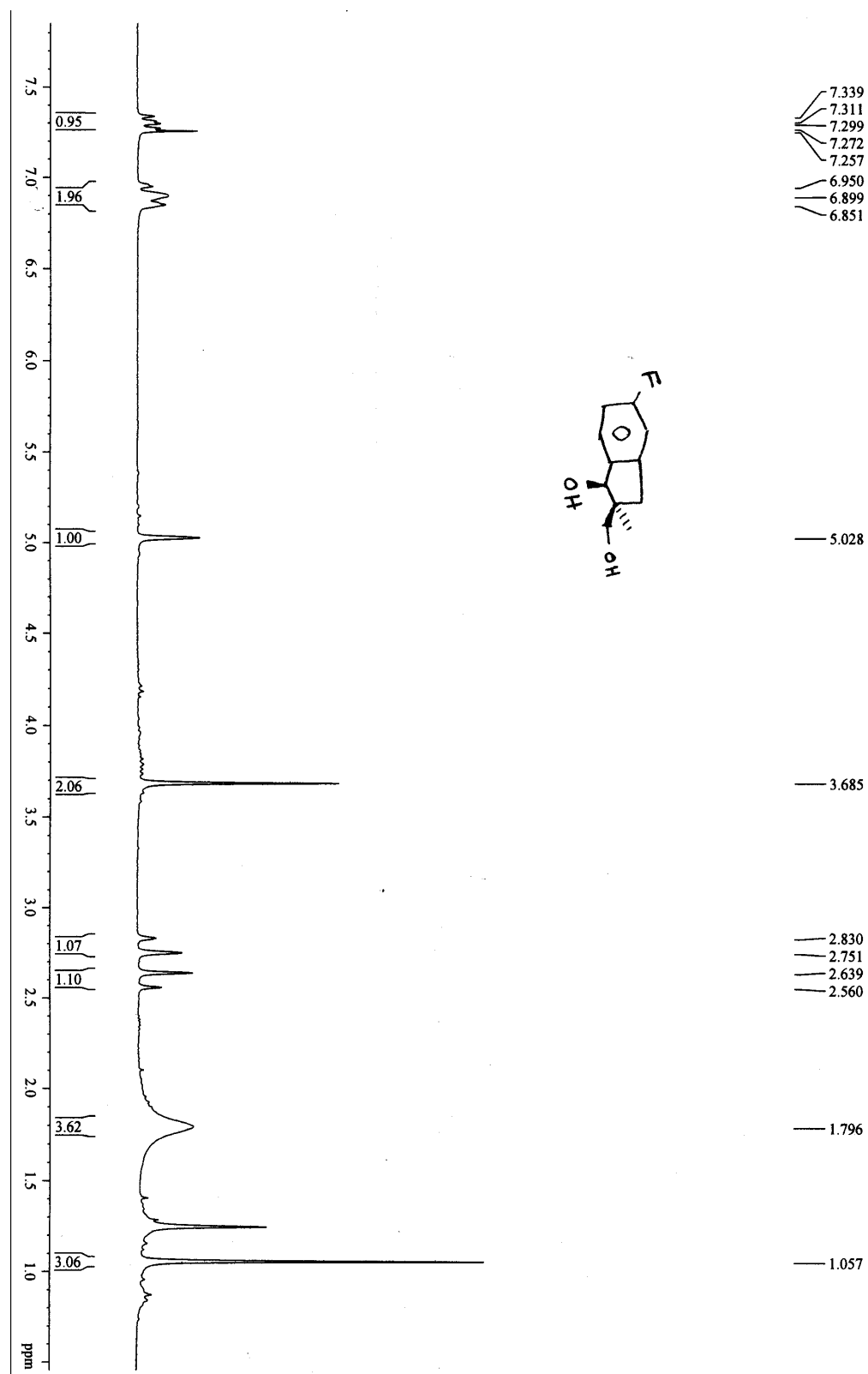
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¹³C NMR of compound 33

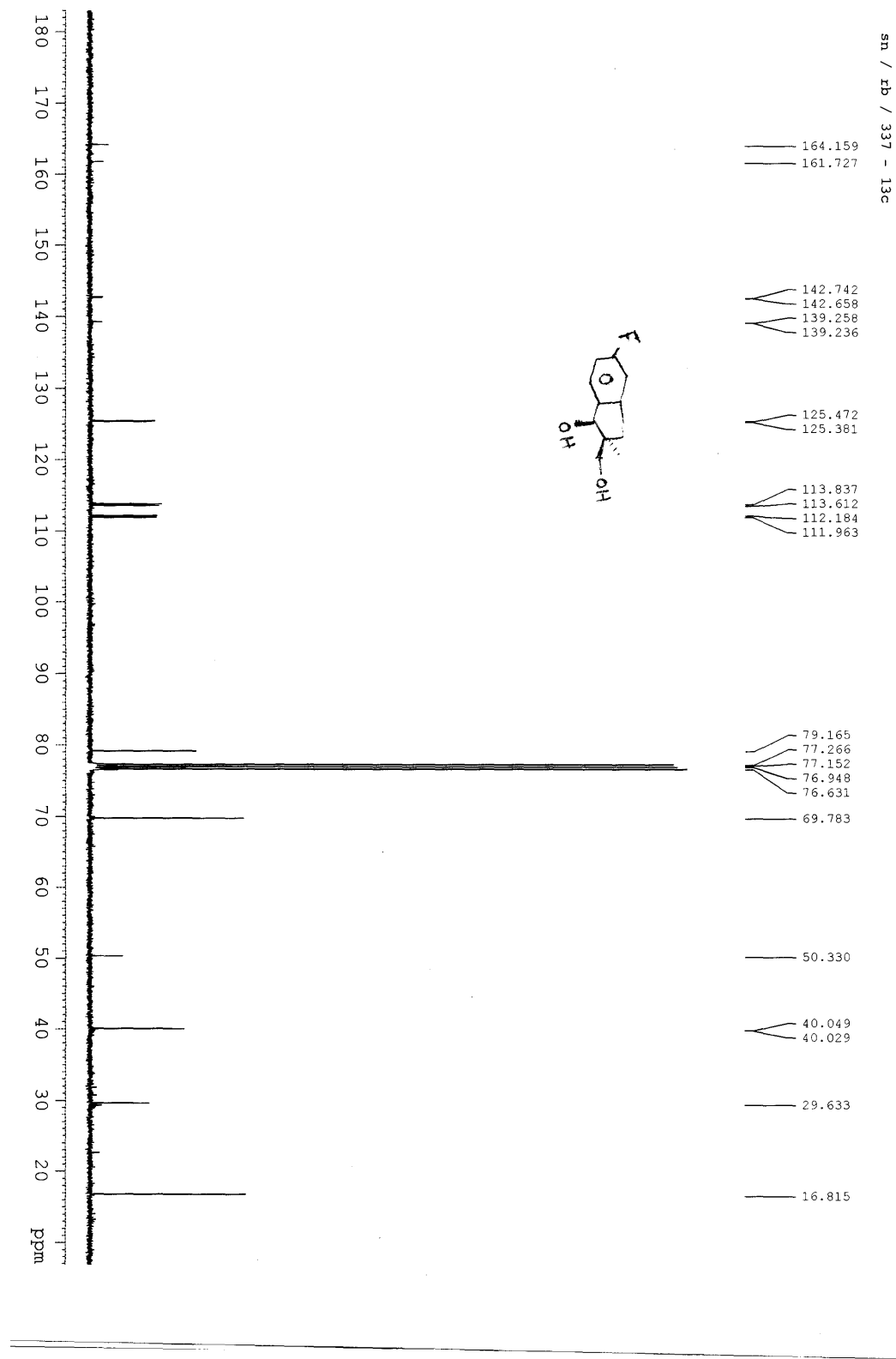


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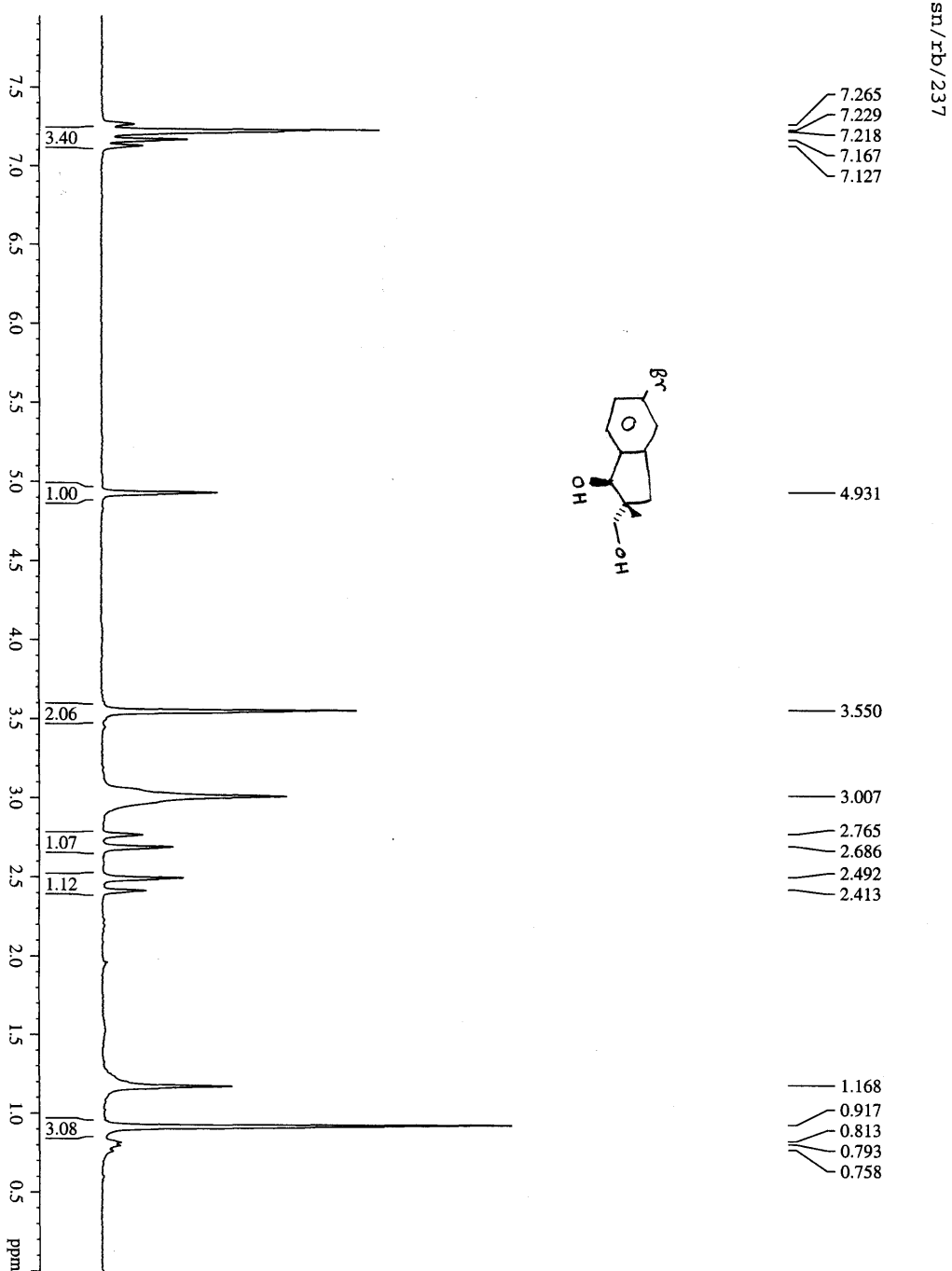
¹H NMR of compound ent-34



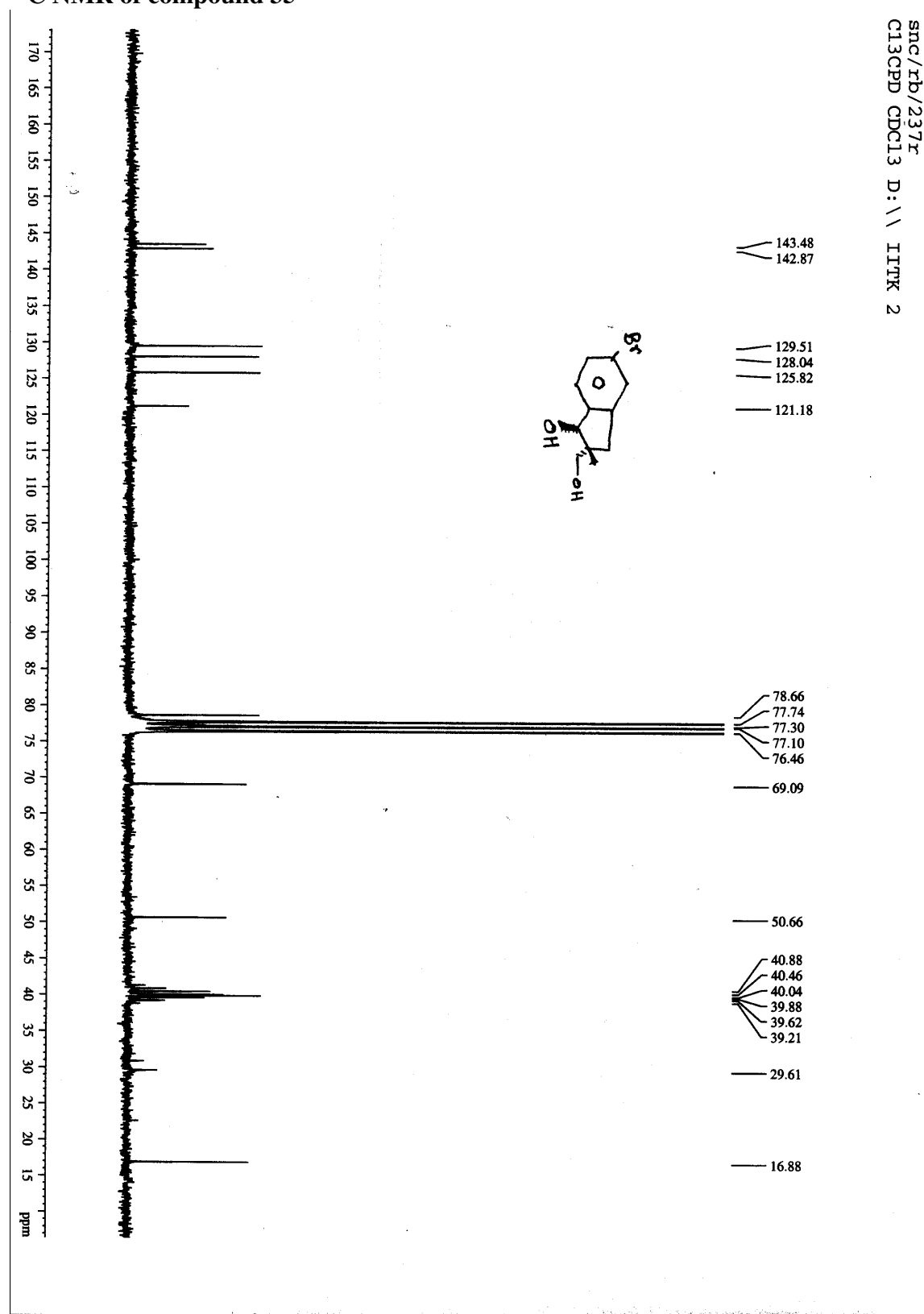
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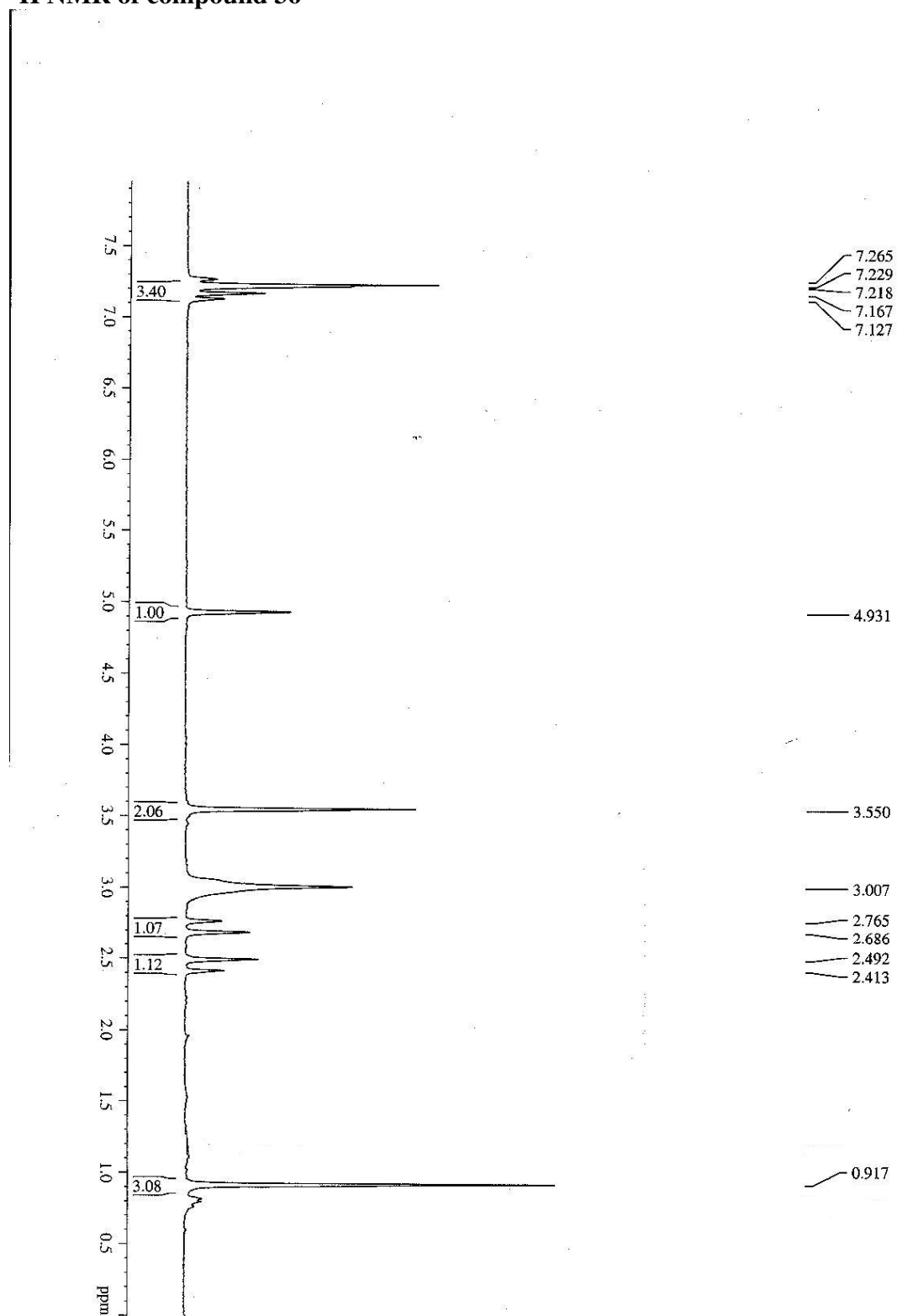
¹H NMR of compound 35



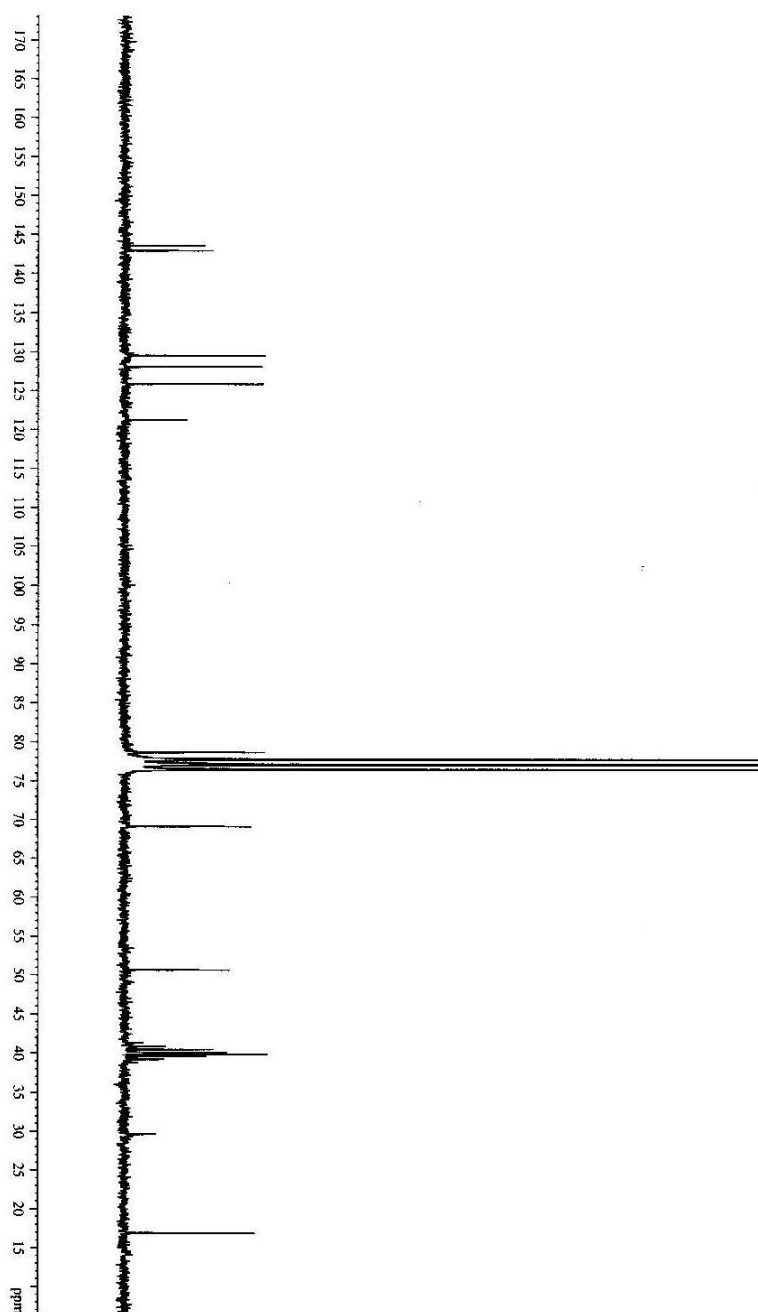
¹³C NMR of compound 35



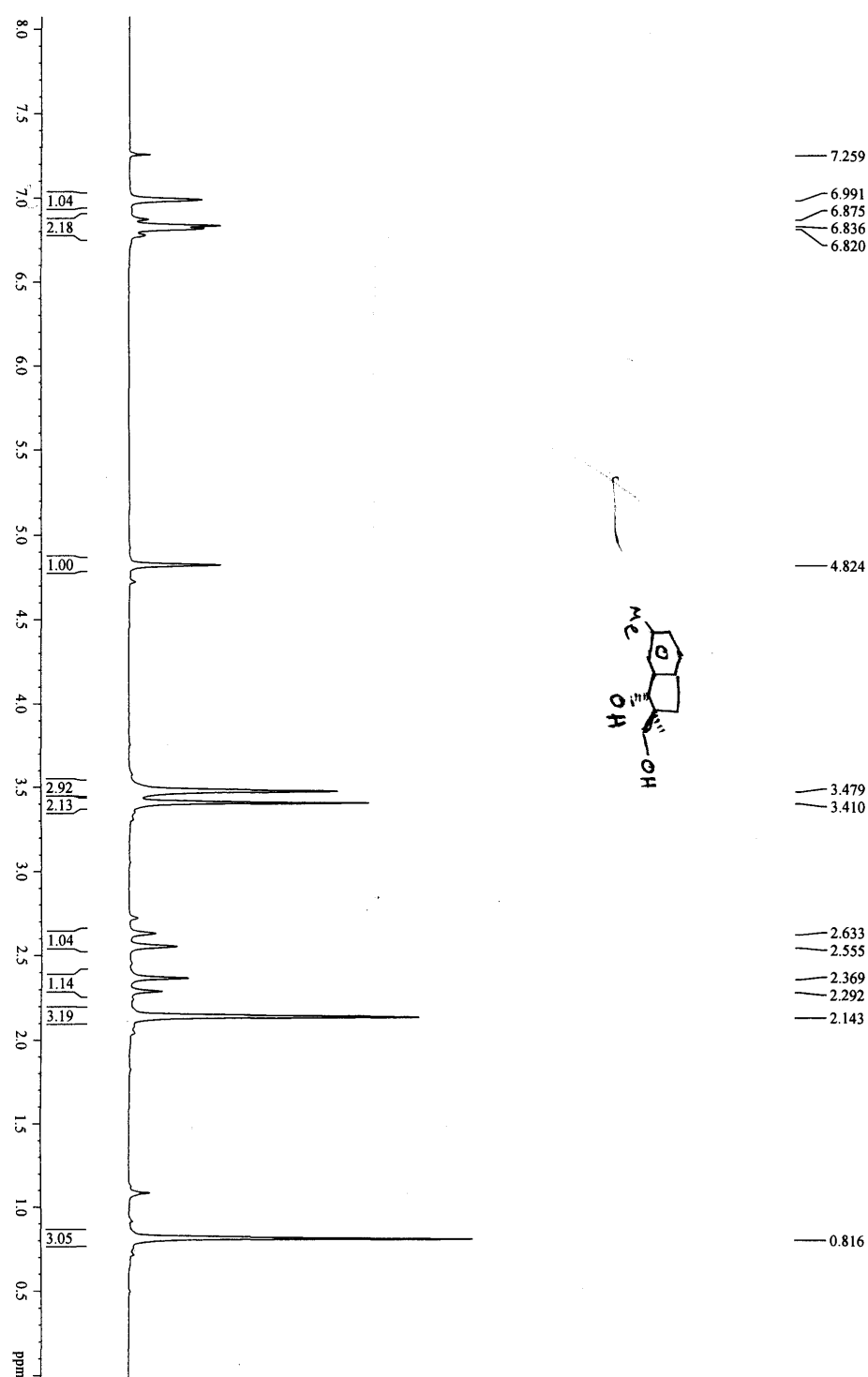
^1H NMR of compound 36



¹³C NMR of compound 36

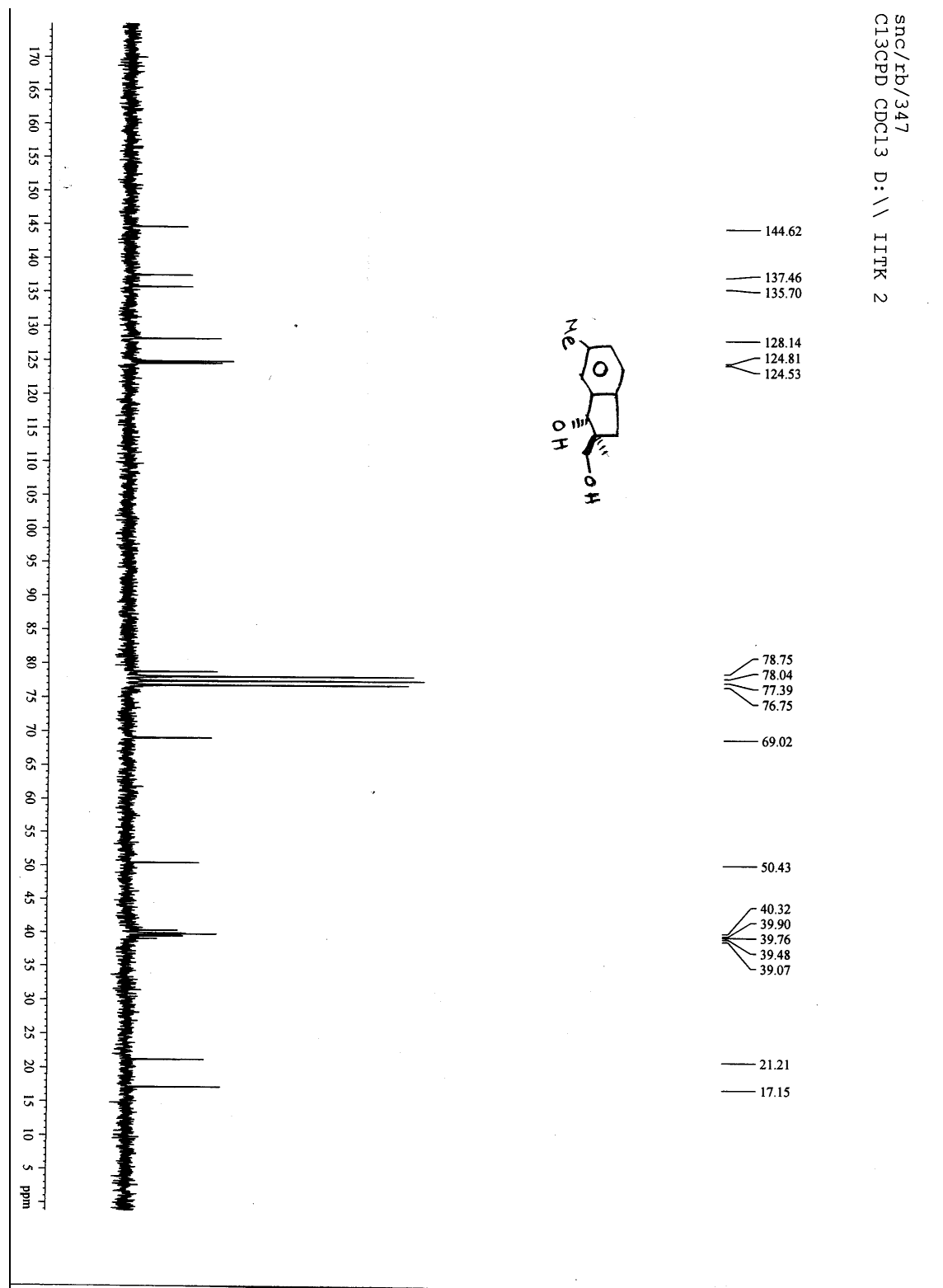


¹H NMR of compound ent-37

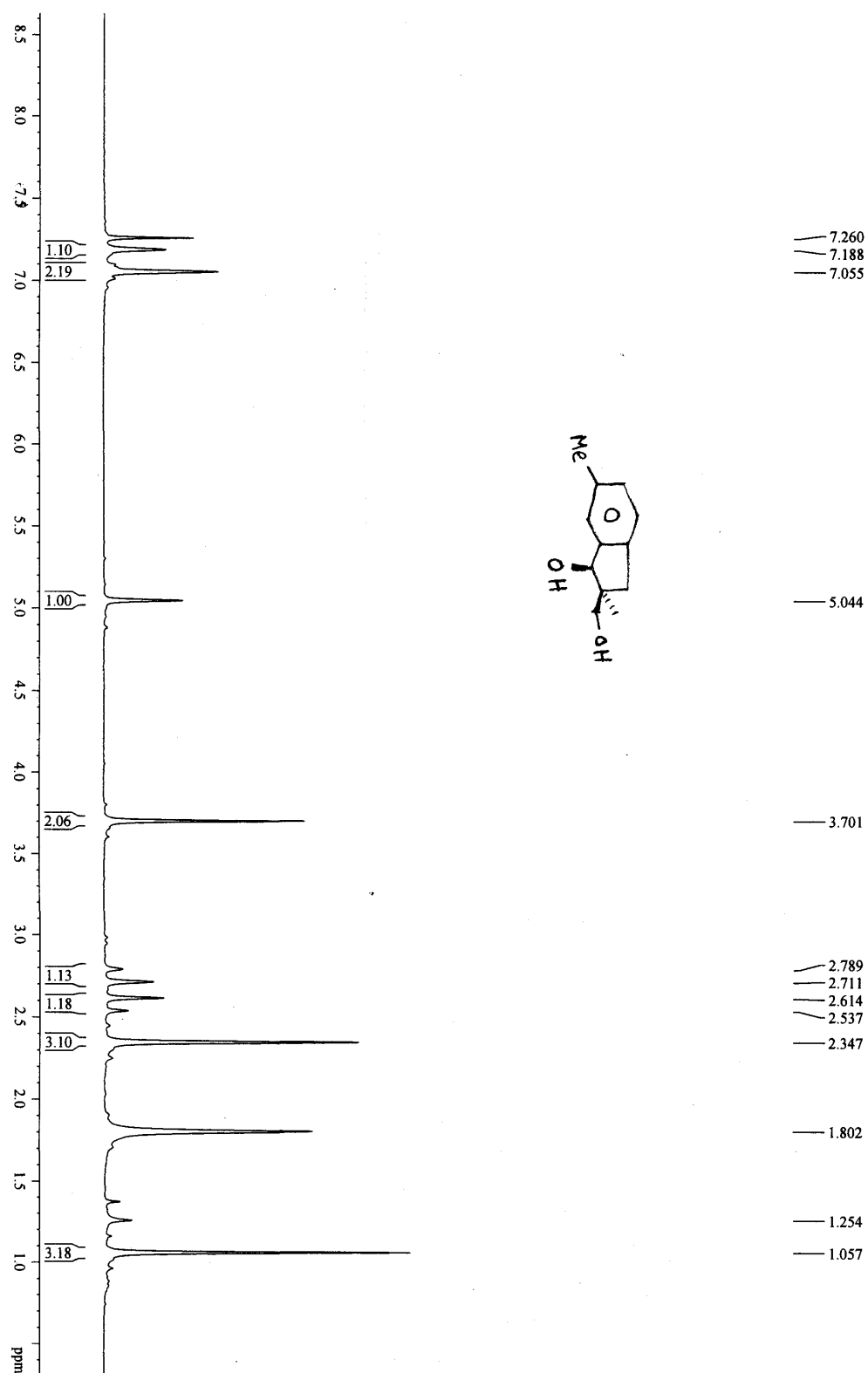


sn / rb / 347

¹³C NMR of compound ent-37

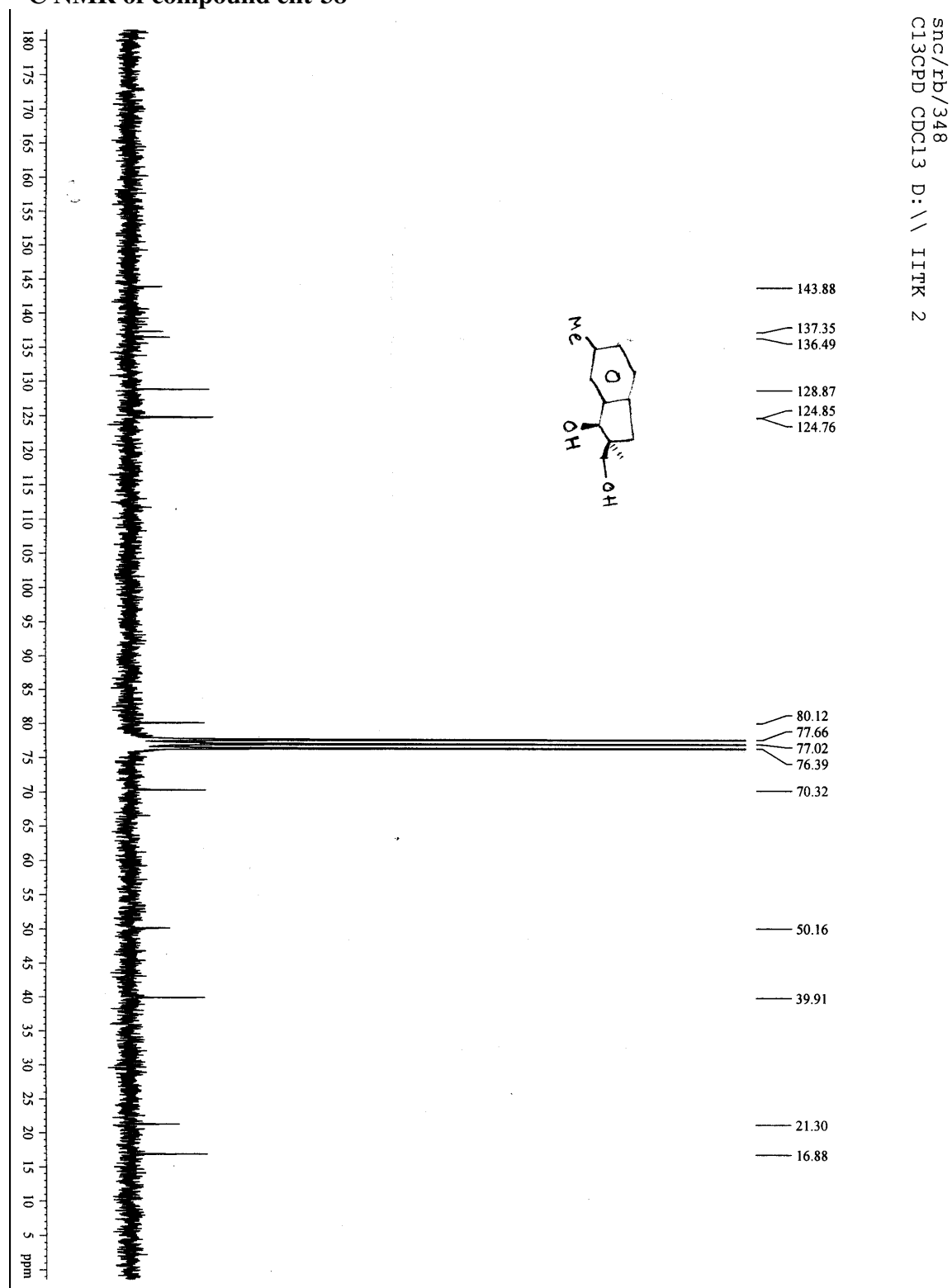


¹H NMR of compound ent-38

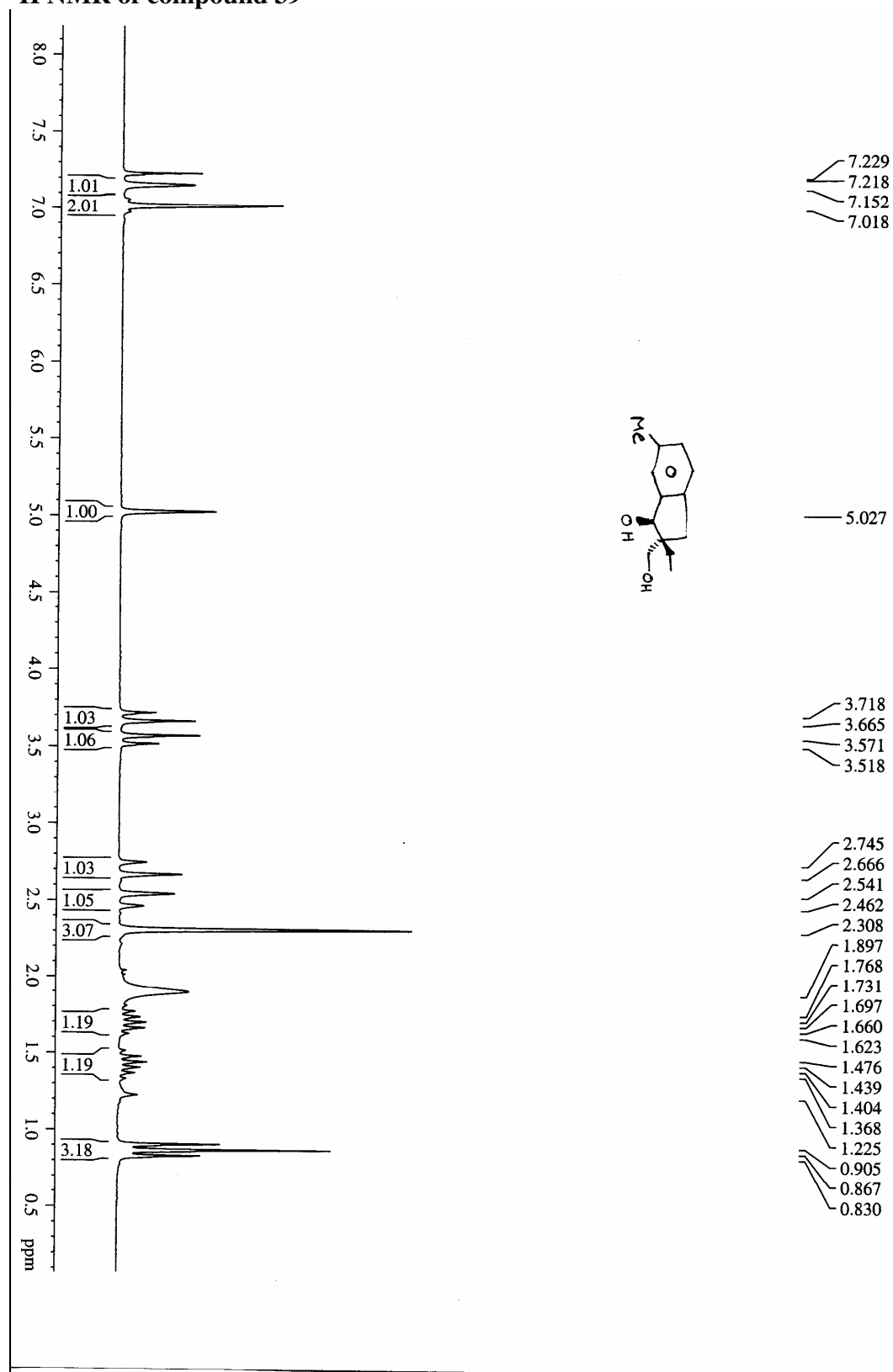


sn / rb / 348

¹³C NMR of compound ent-38

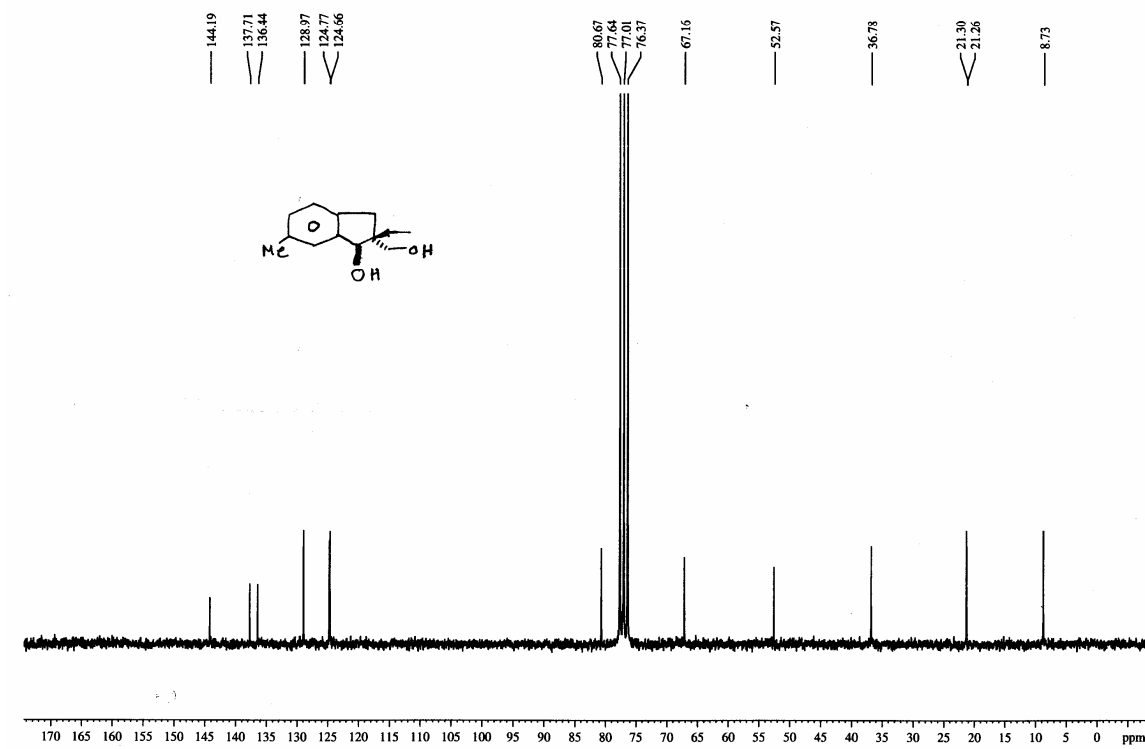


¹H NMR of compound 39

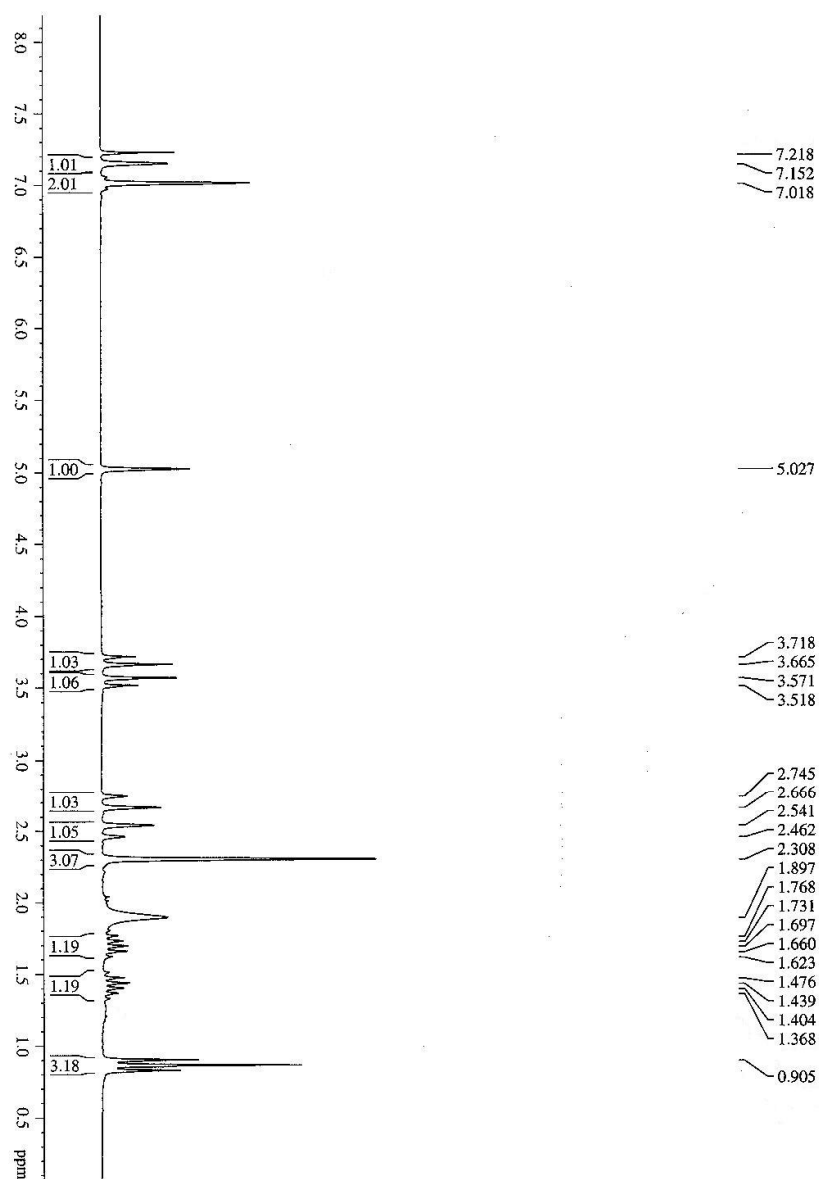


¹³C NMR of compound 39

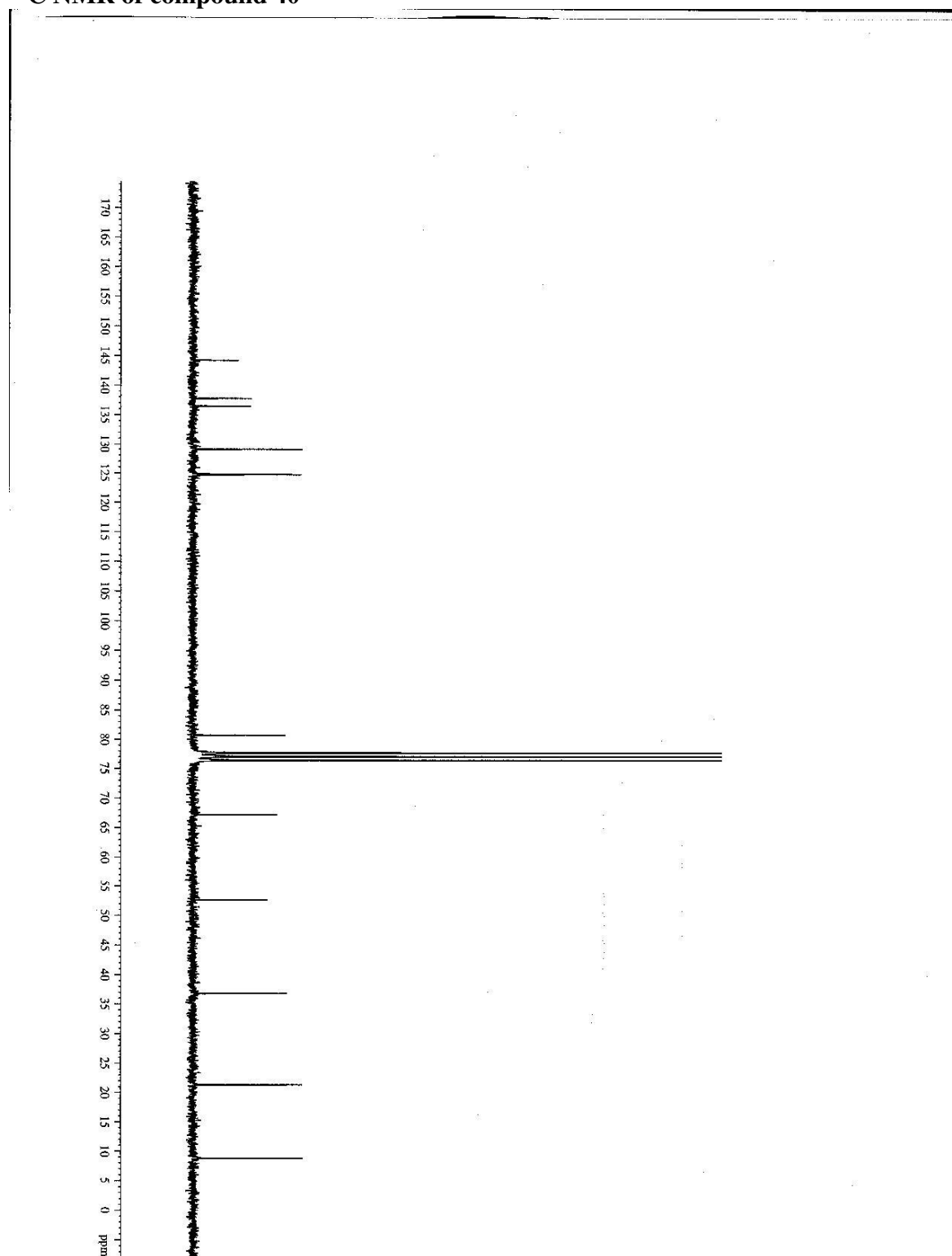
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C13CPD CDCl3 D:\ IITK 2



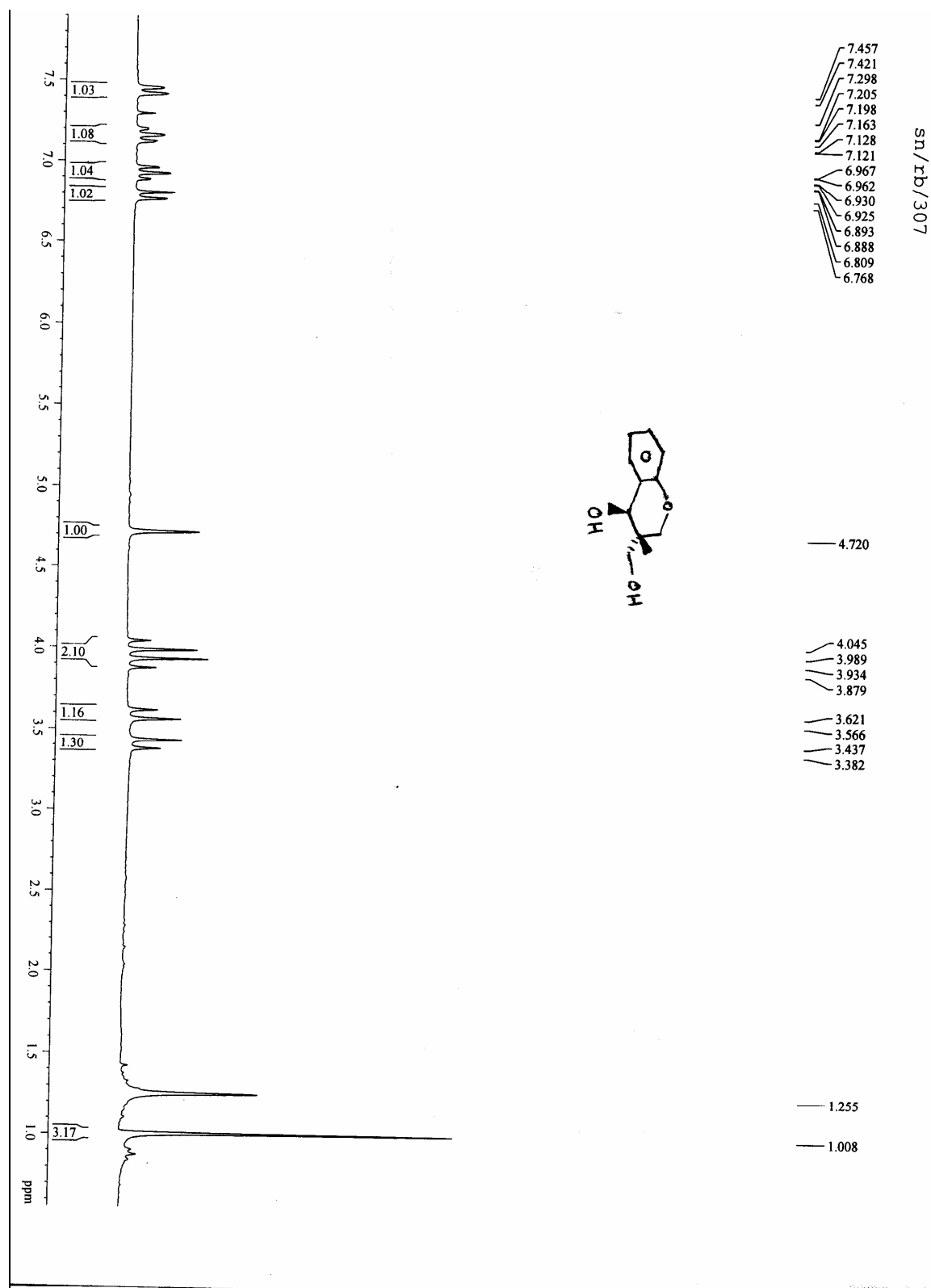
¹H NMR of compound 40



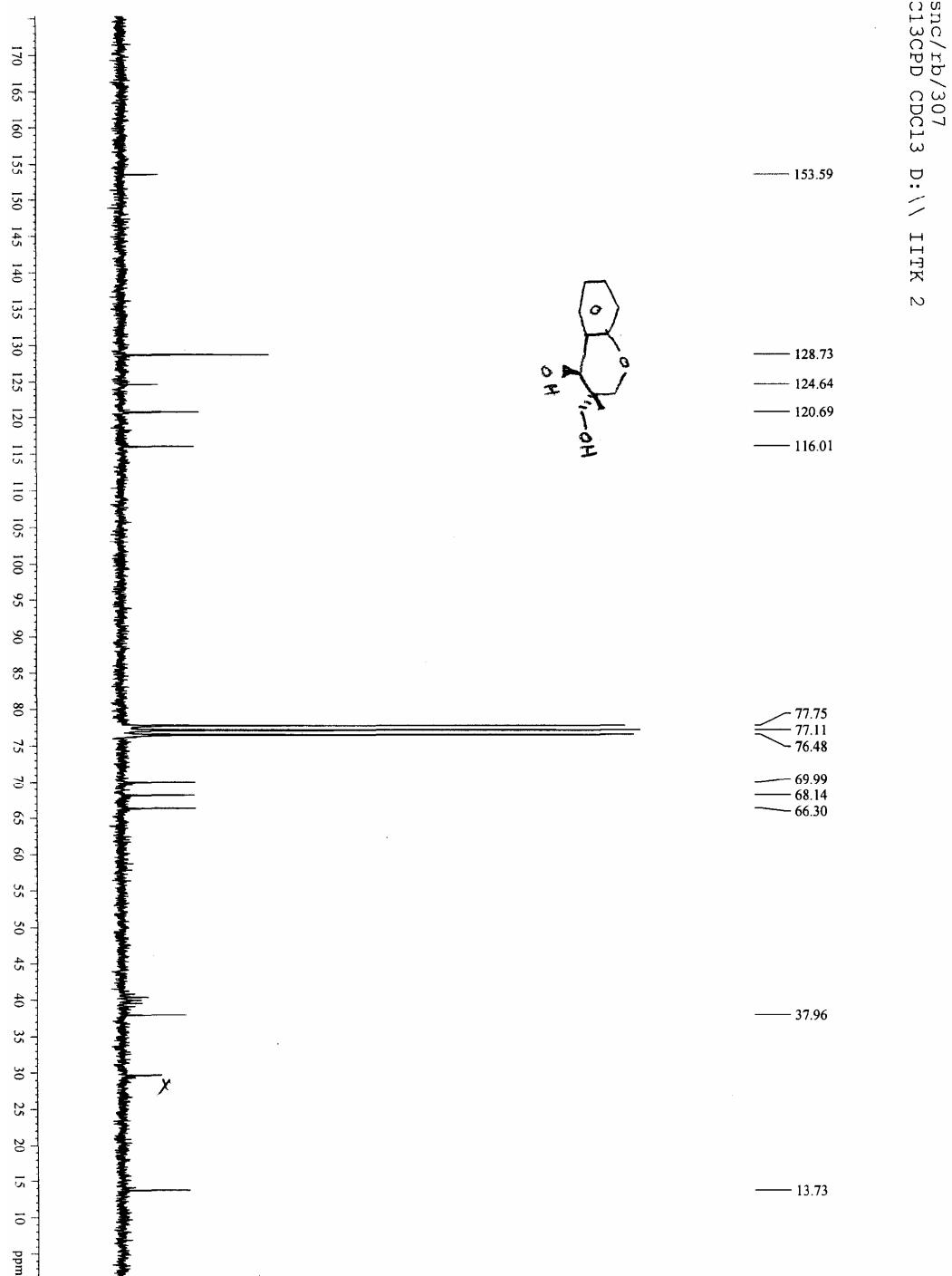
^{13}C NMR of compound 40



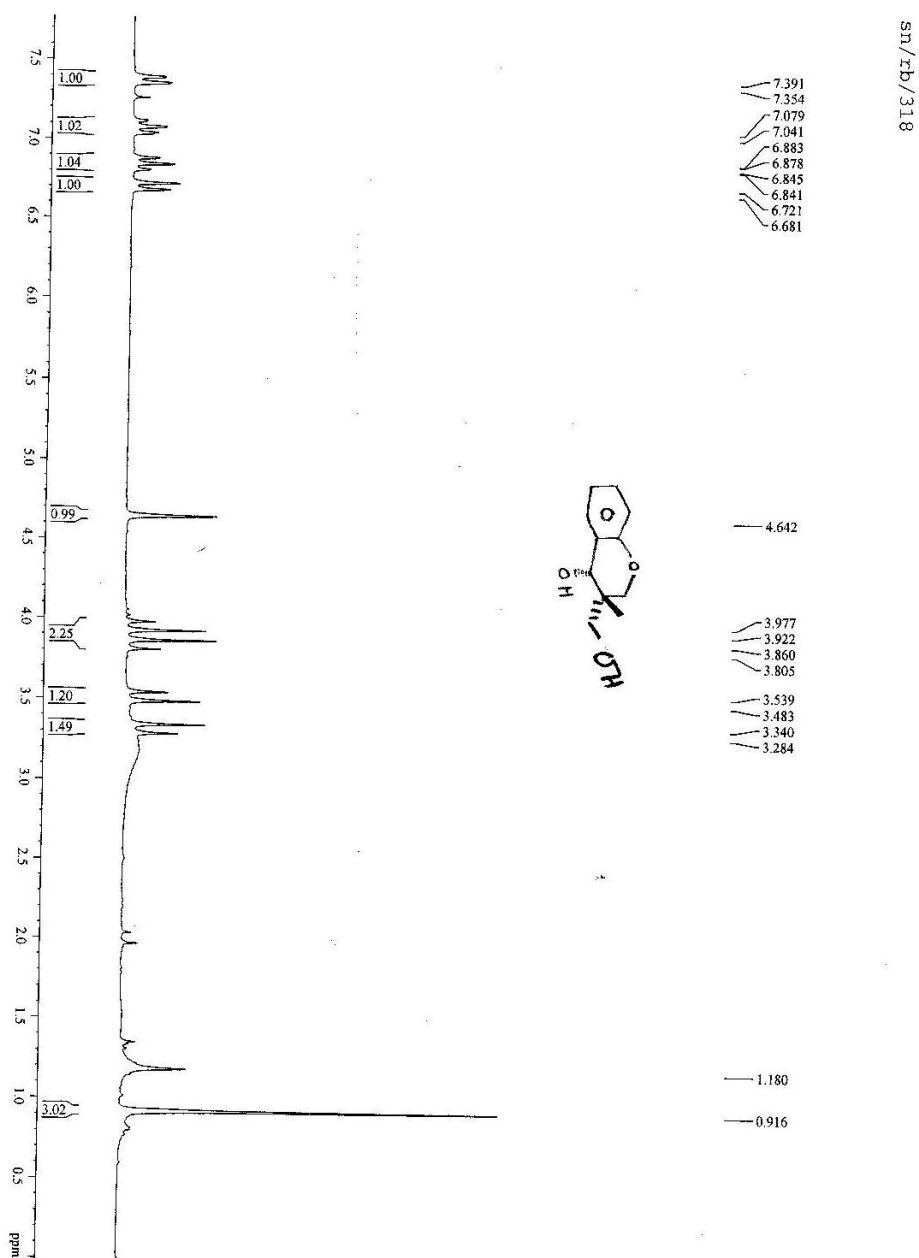
¹H NMR of compound 41



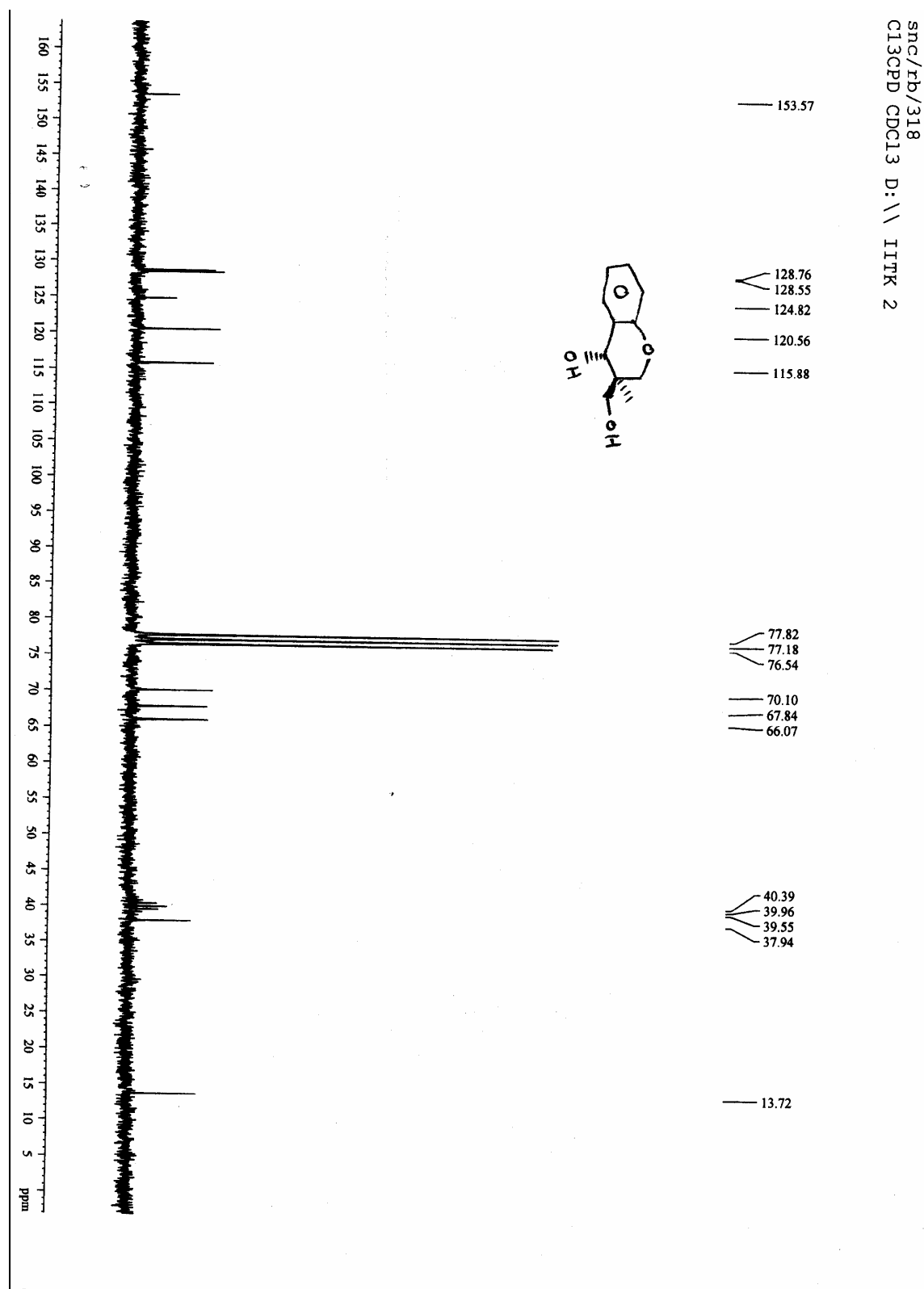
¹³C NMR of compound 41



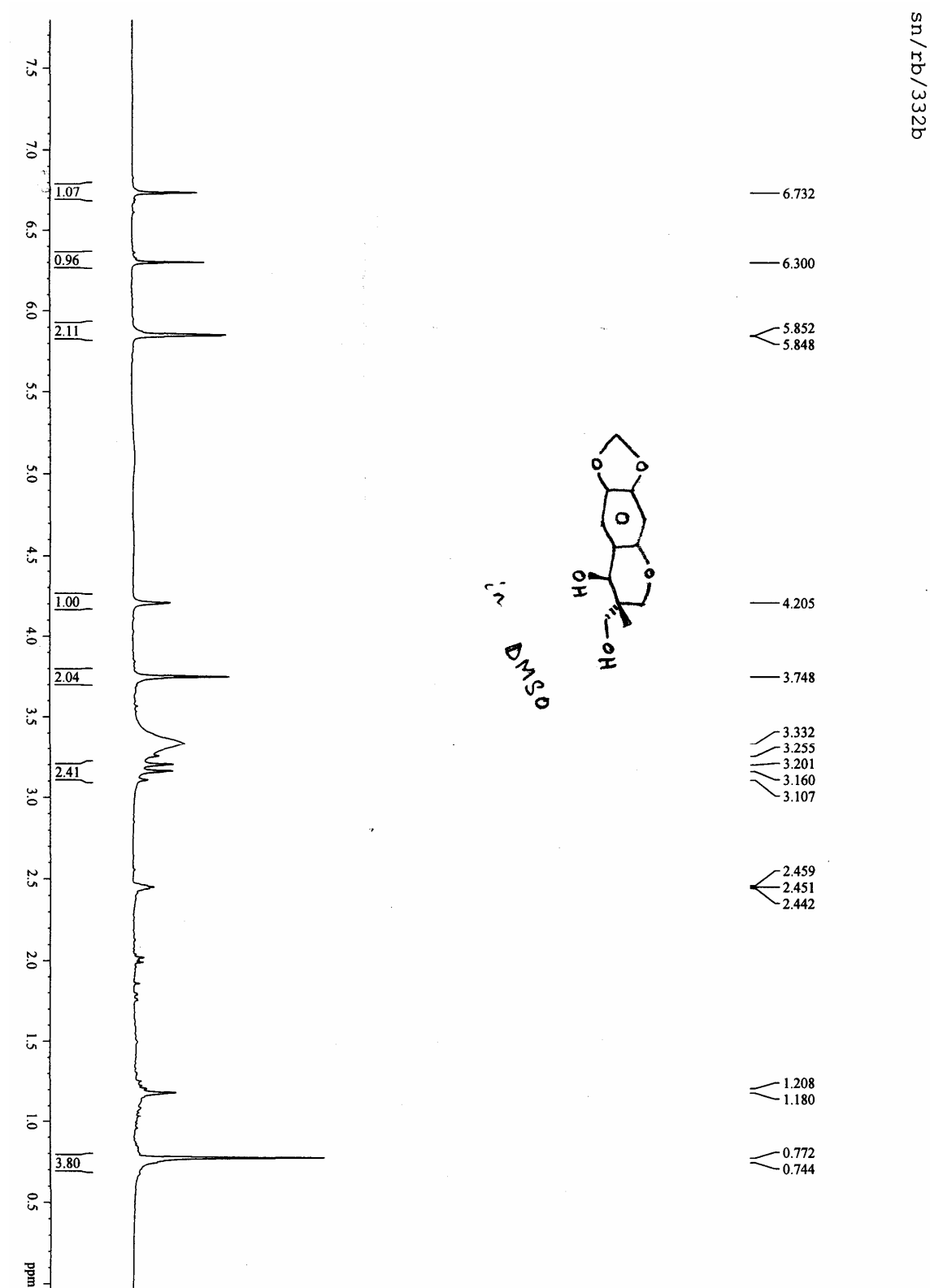
¹H NMR of compound 42



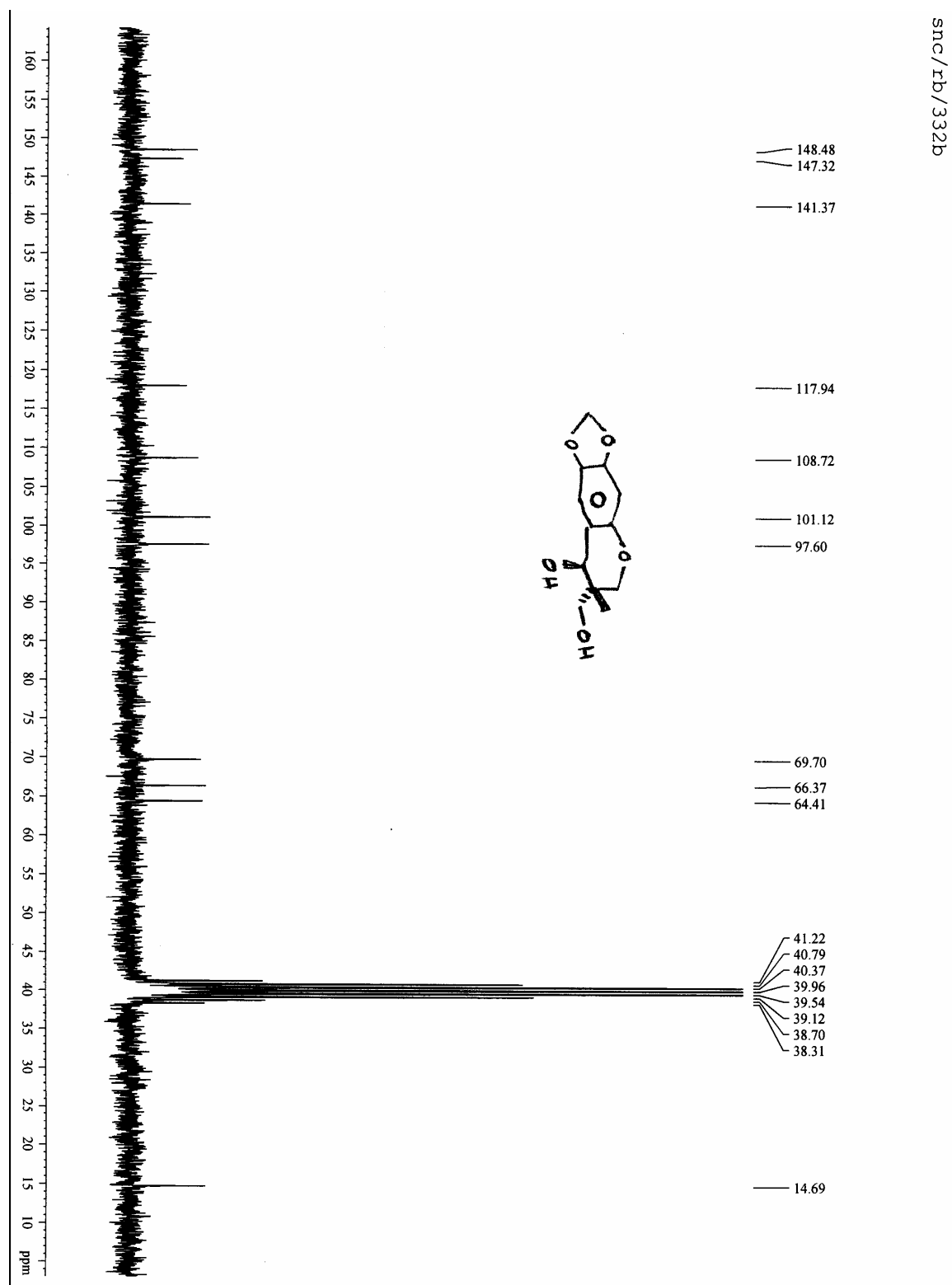
¹³C NMR of Compound 42



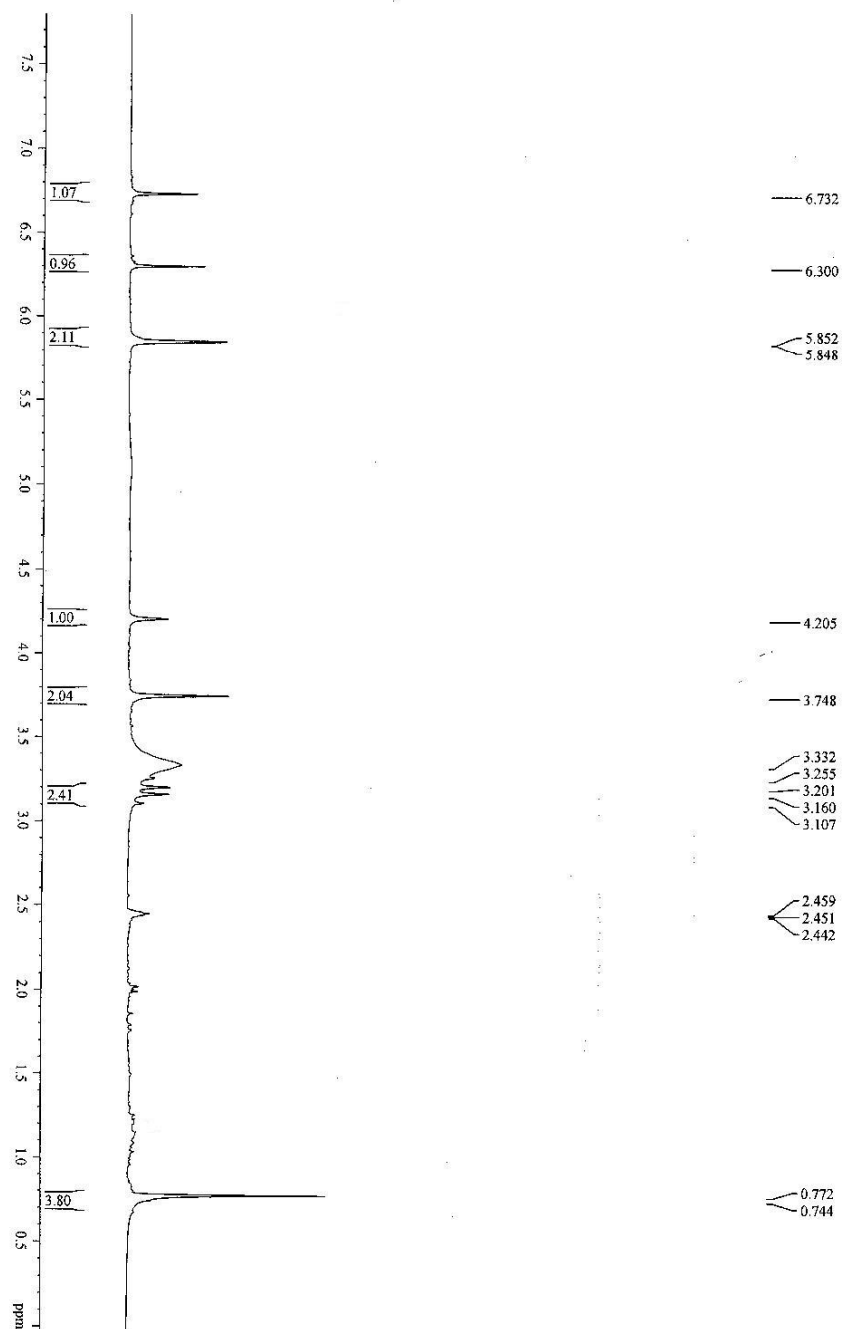
¹H NMR of compound 43



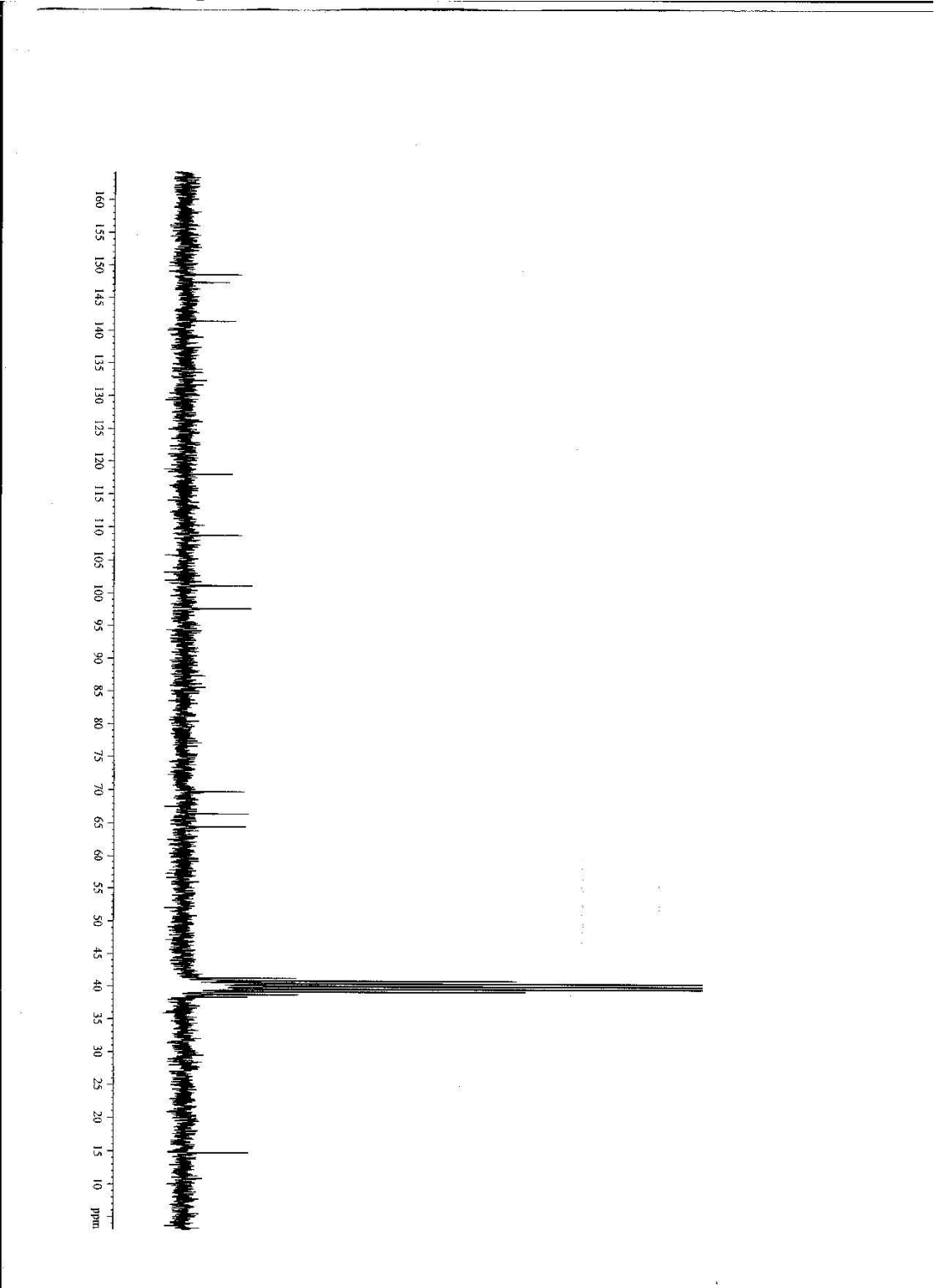
¹³C NMR of compound 43



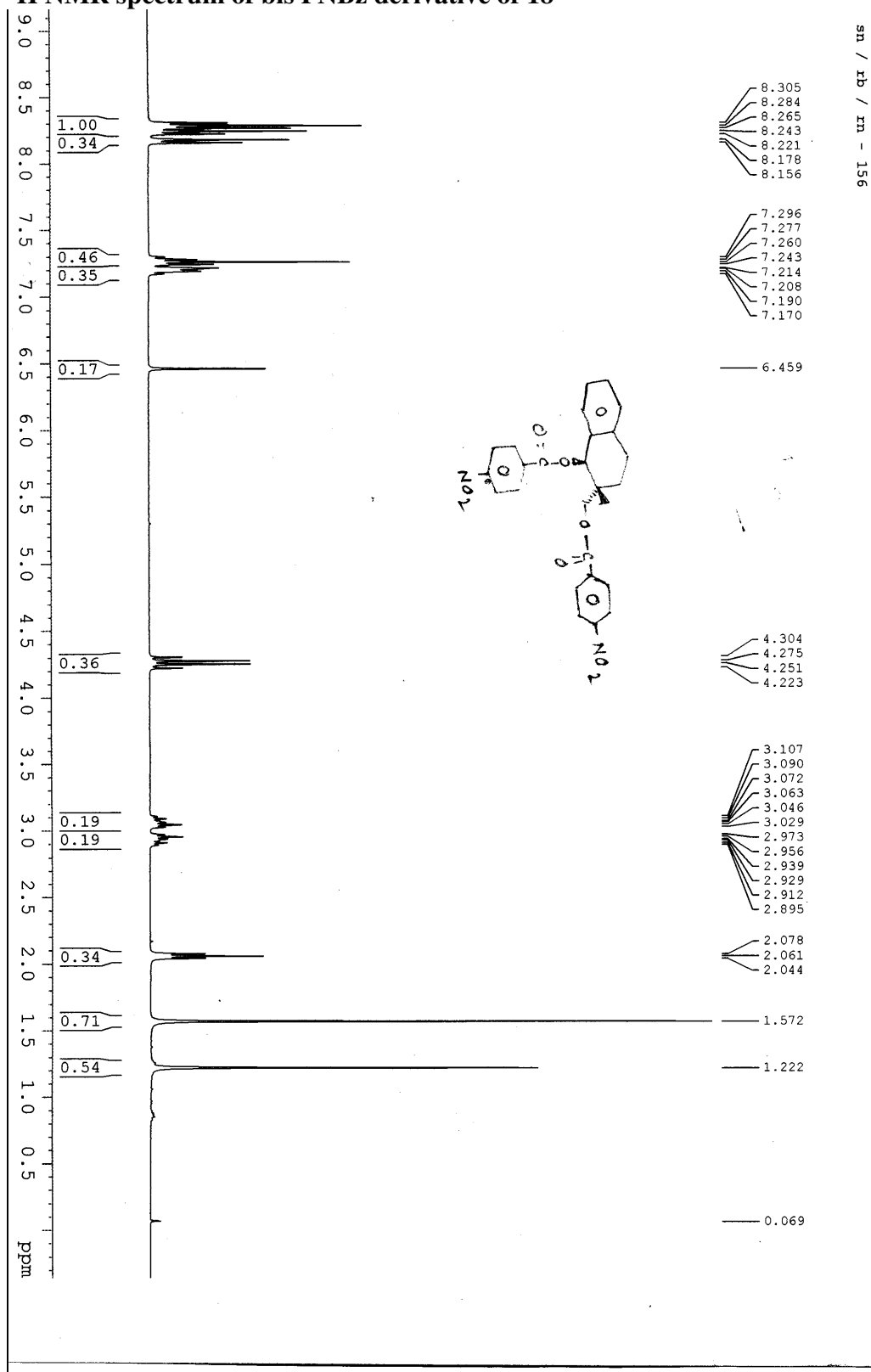
¹H NMR of compound 44



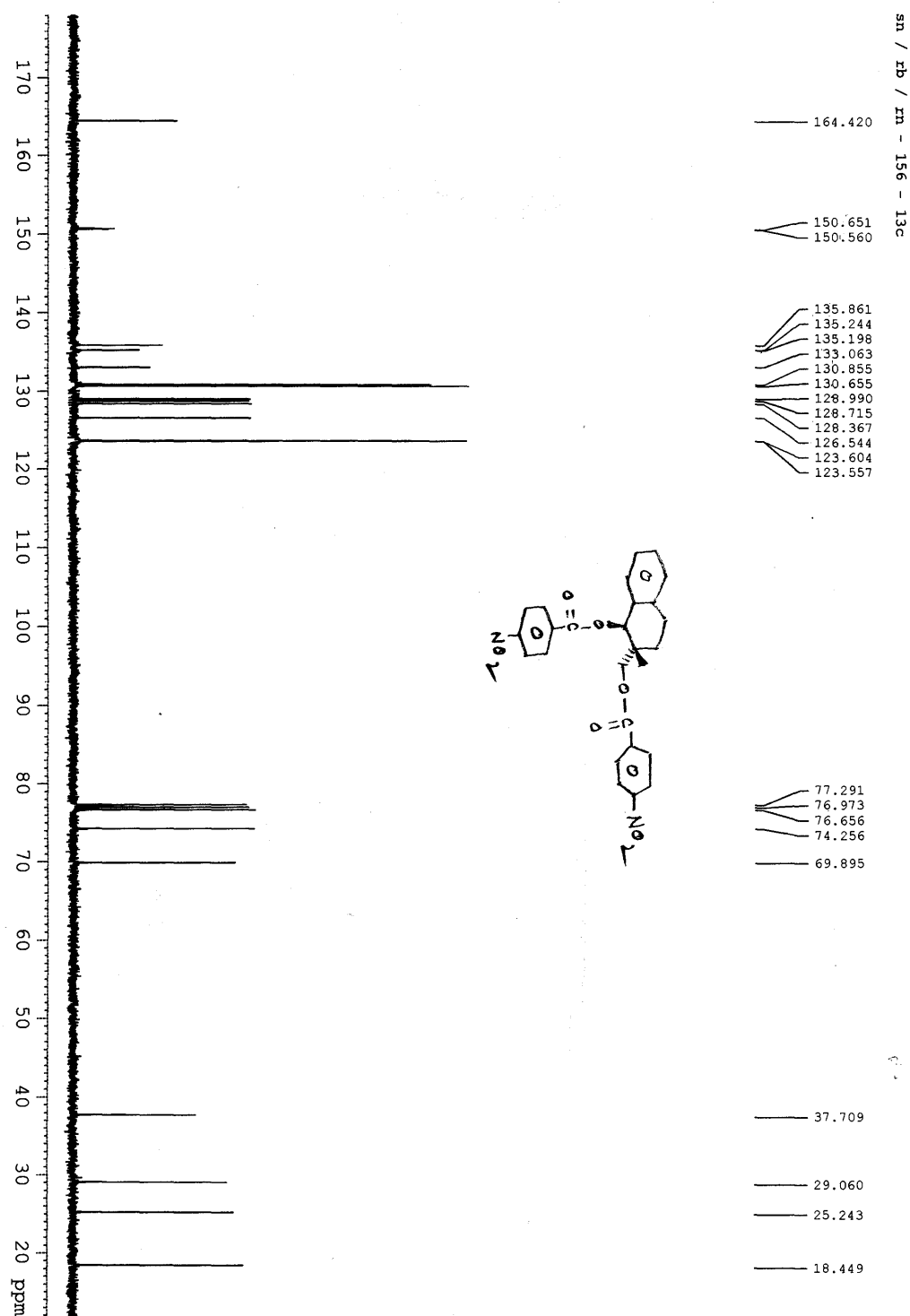
¹³C NMR of compound 44



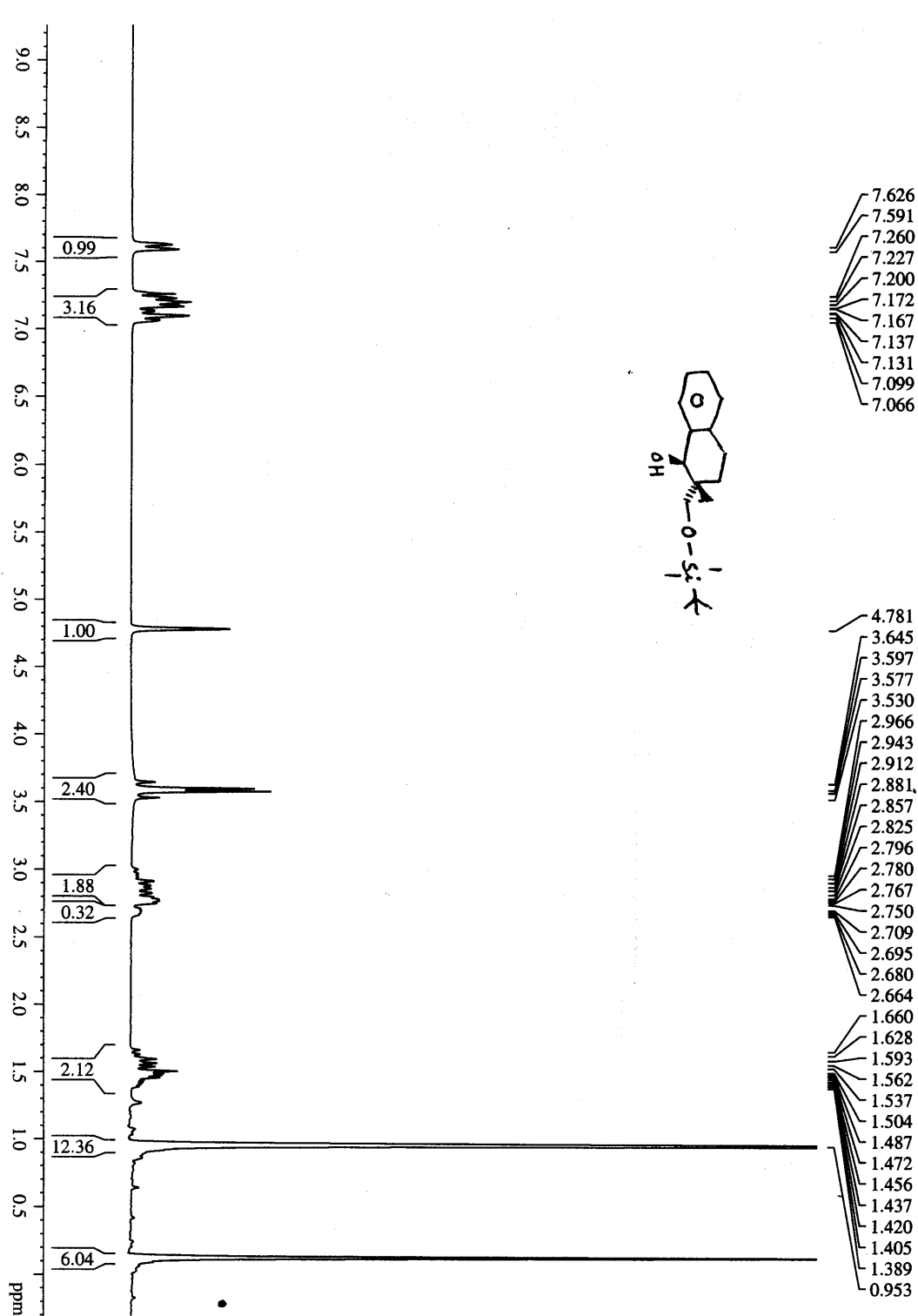
¹H NMR spectrum of bis PNBz derivative of 18



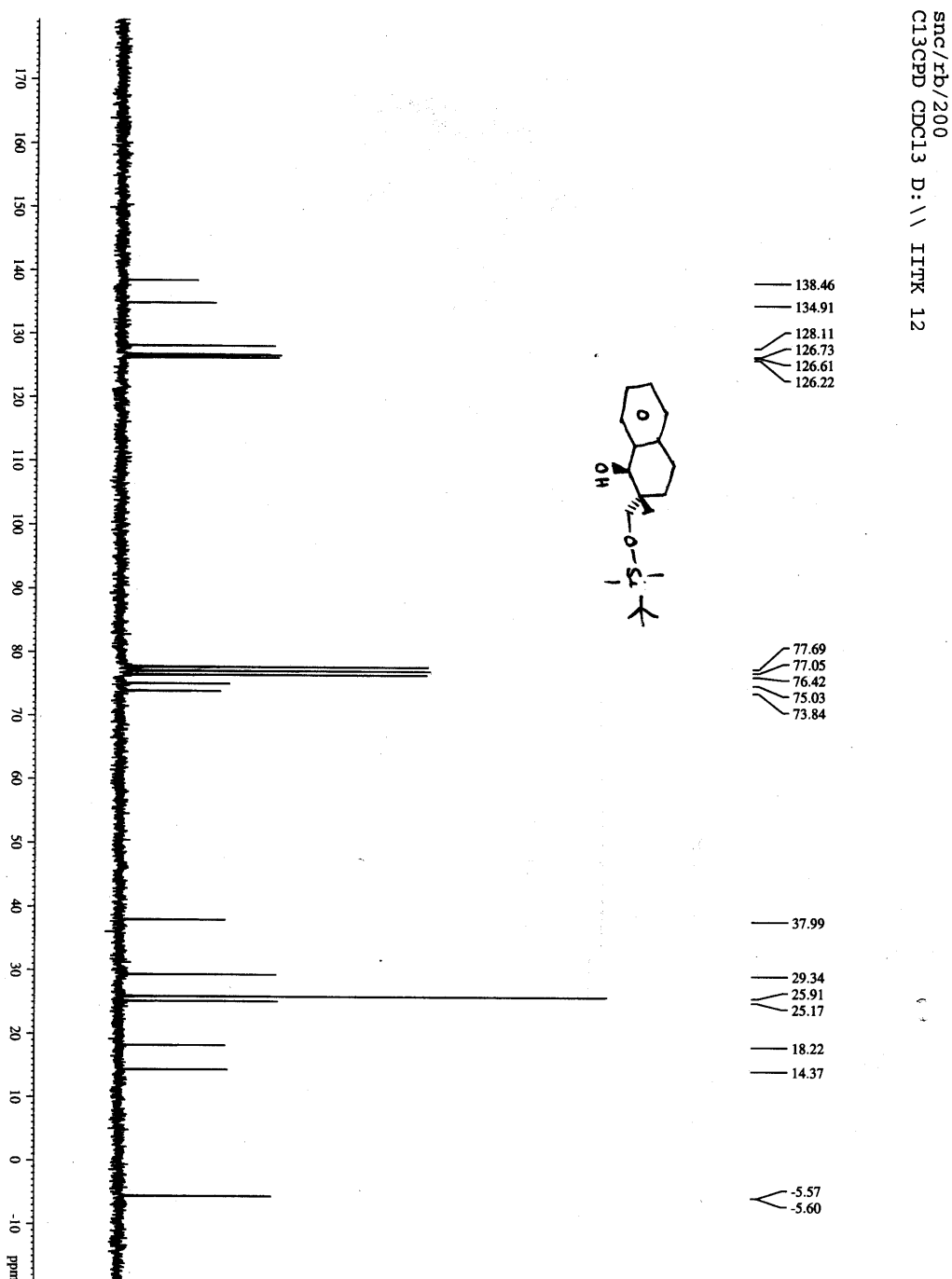
¹³C NMR spectrum of bis PNBz derivative of 18



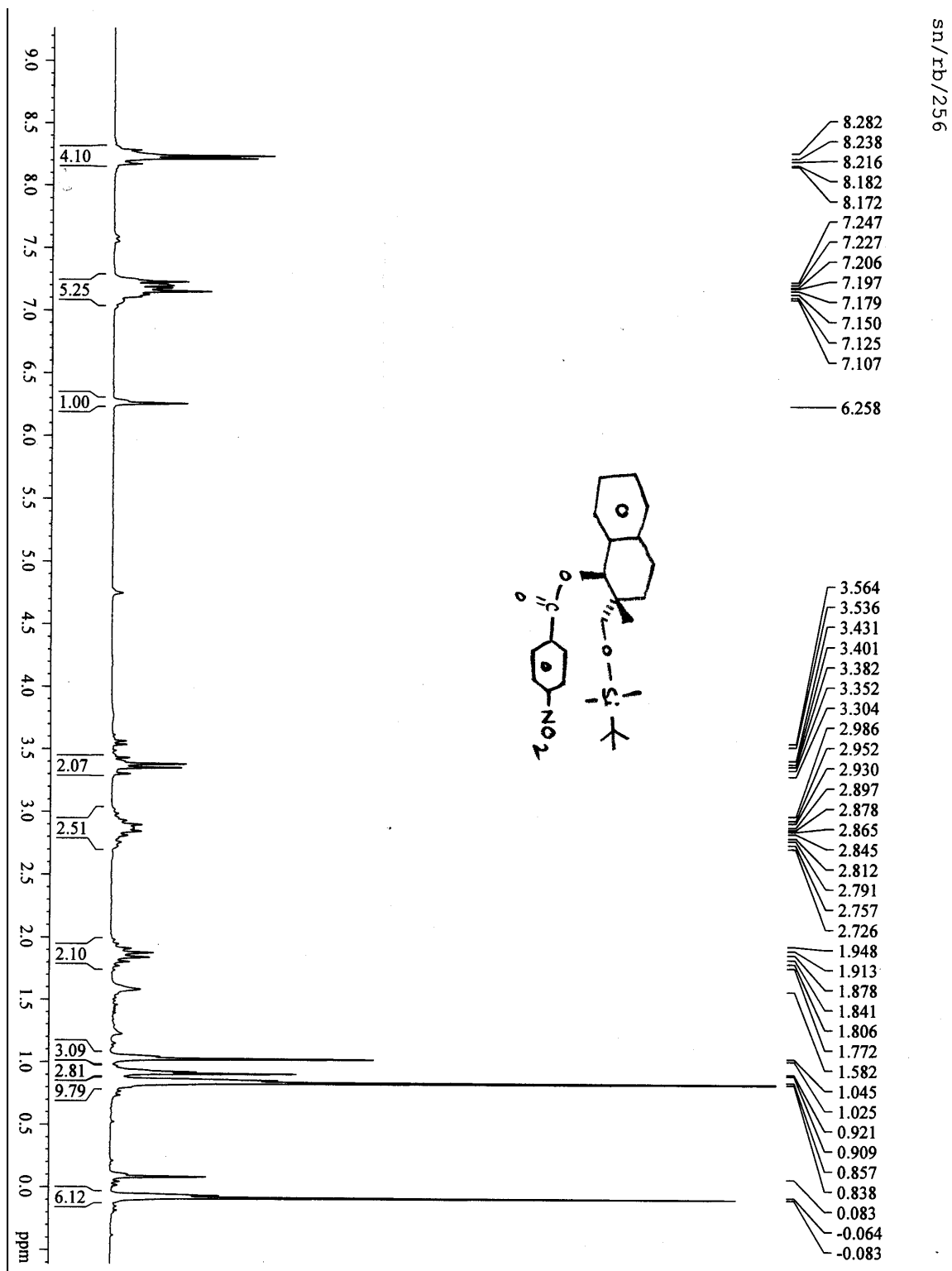
¹H NMR of compound 45



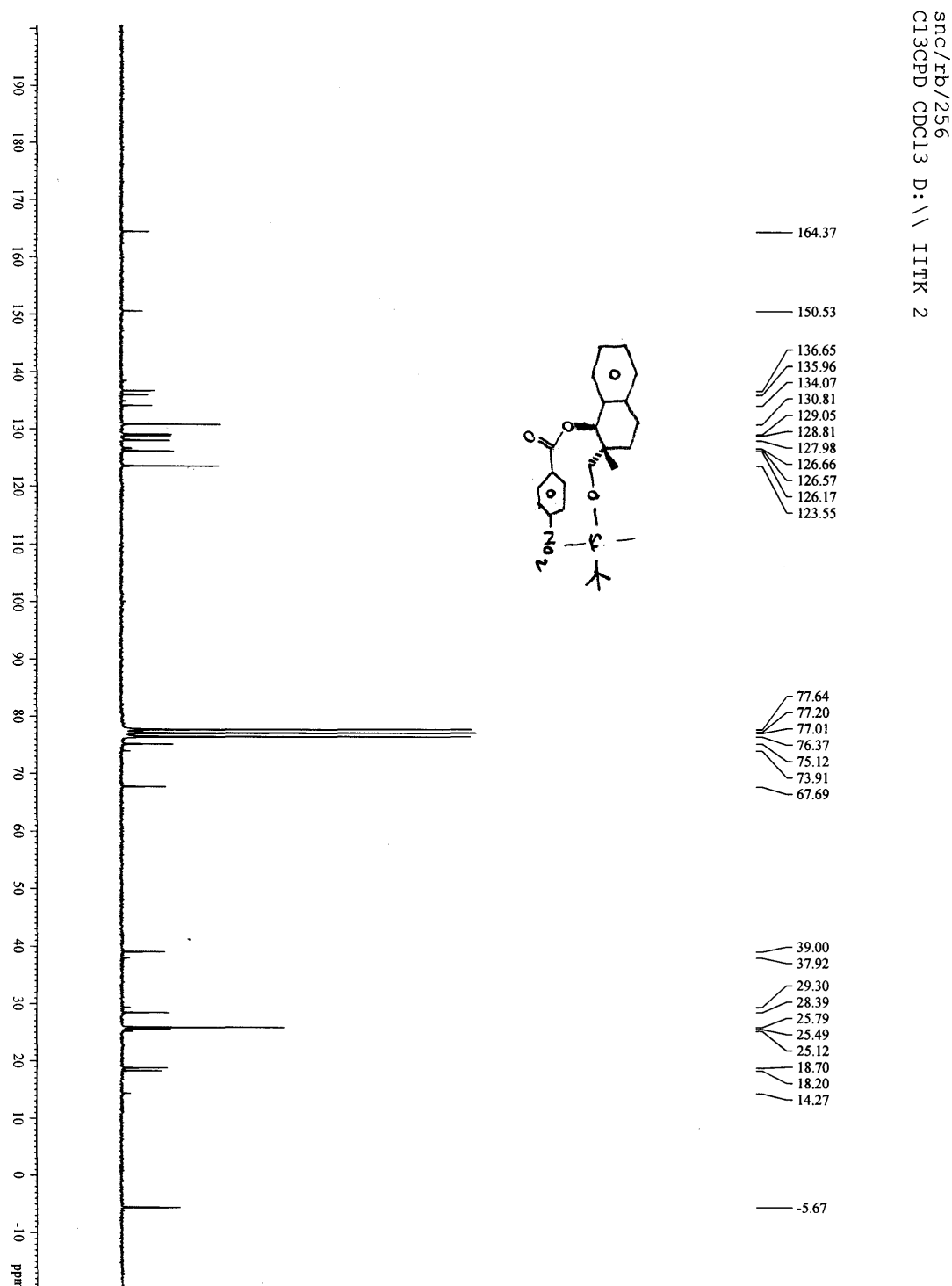
¹³C NMR of compound 45



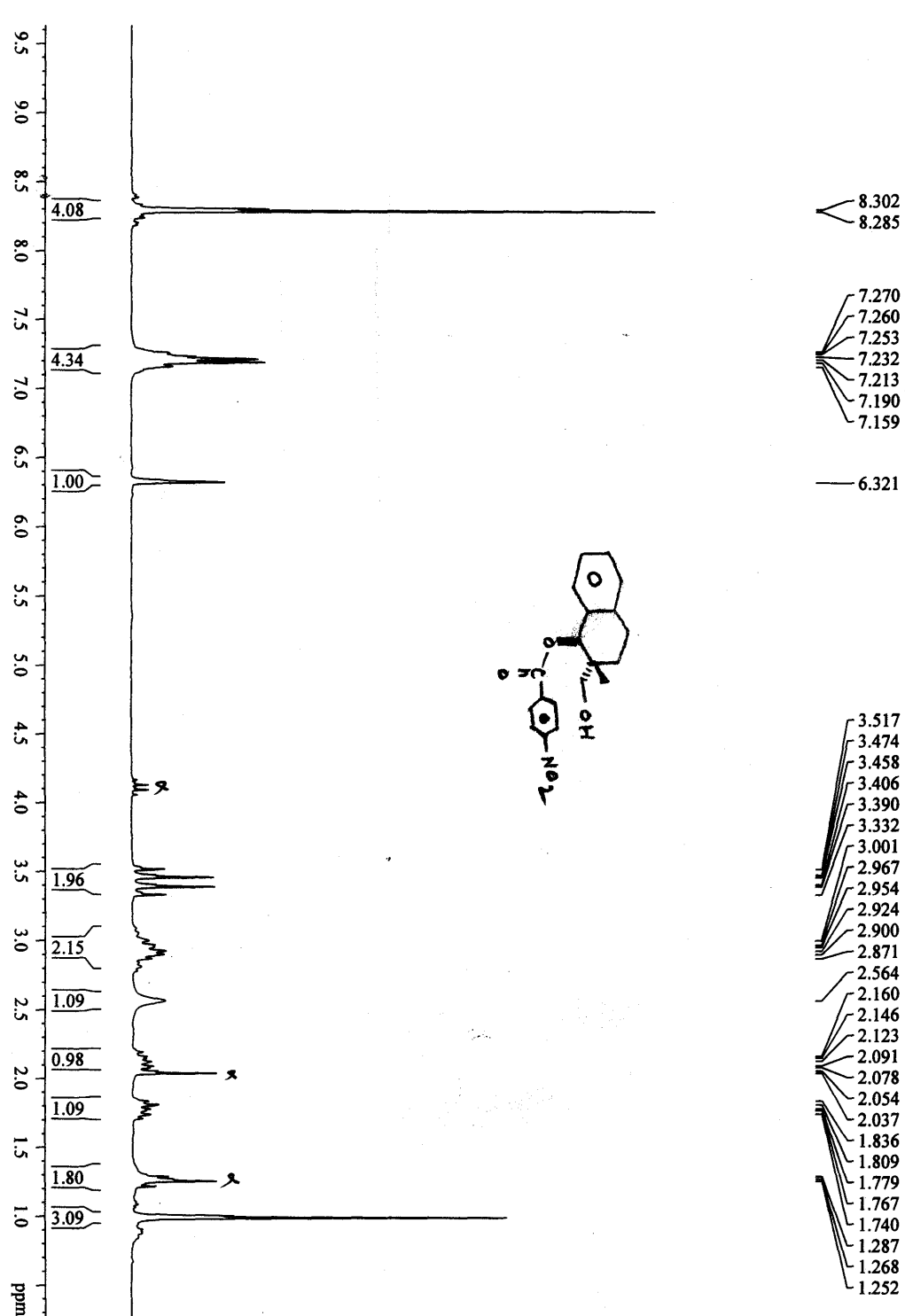
¹H NMR of compound 46



¹³C NMR of compound 46

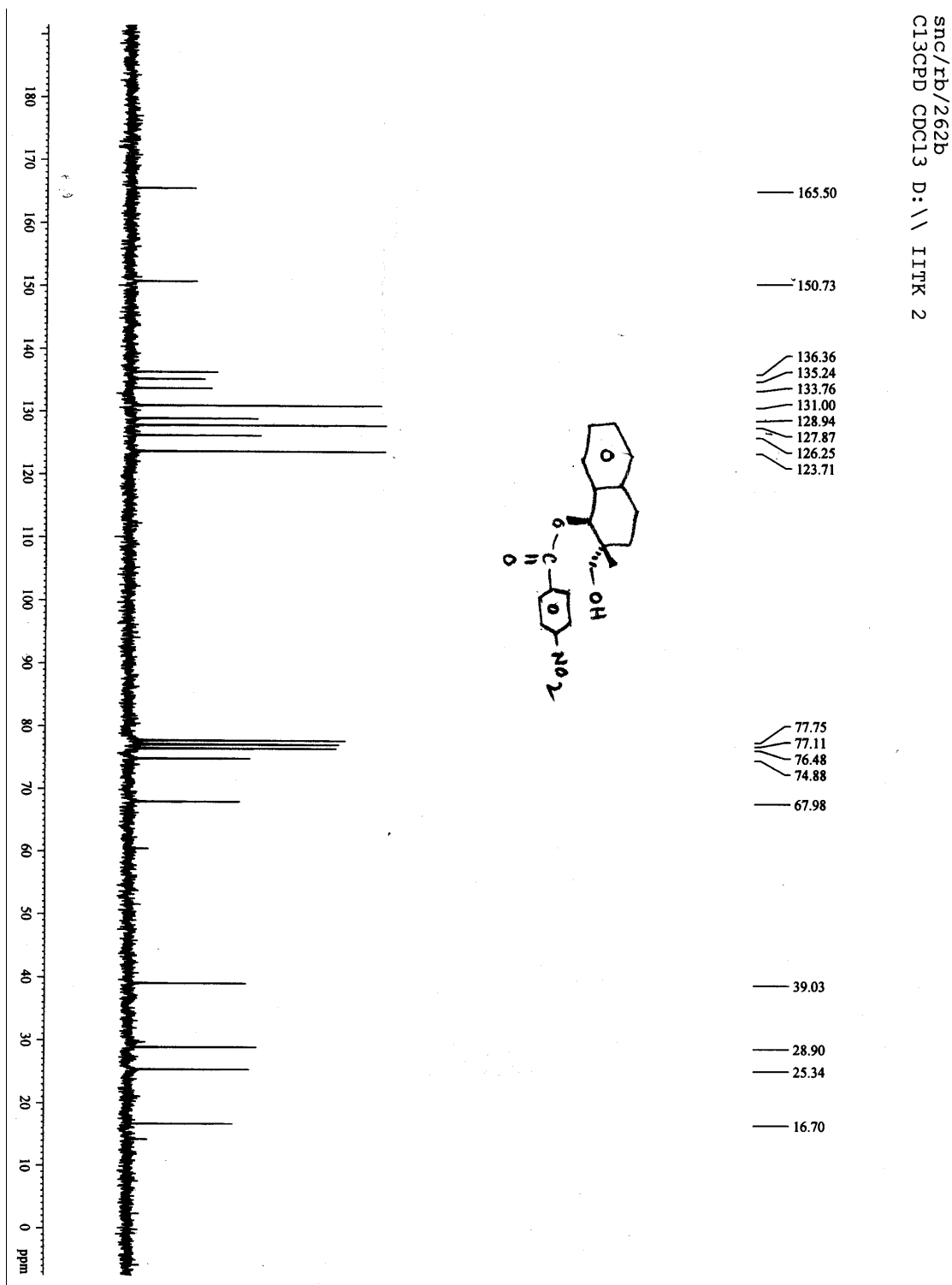


¹H NMR of compound 47

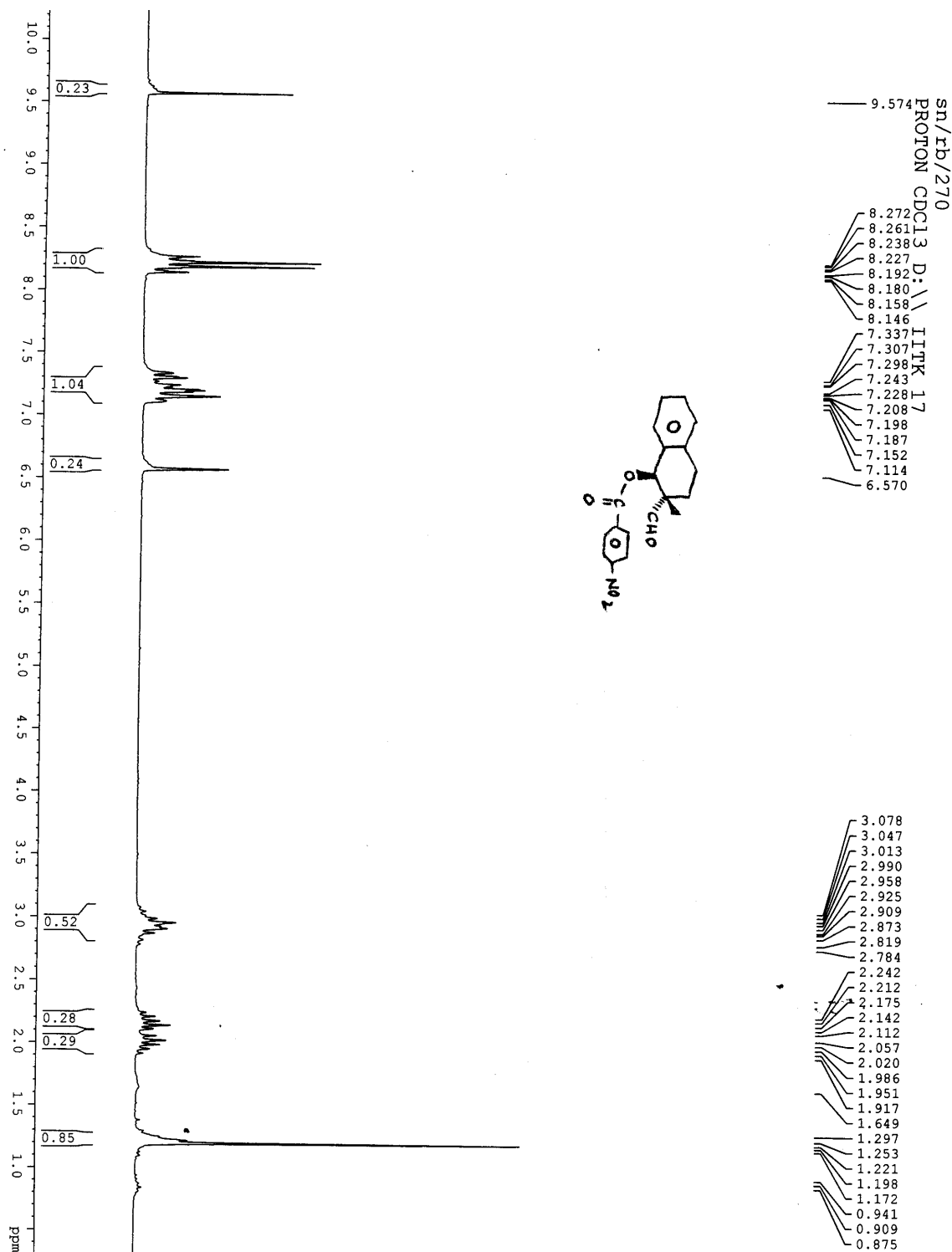


sn/rb/262b

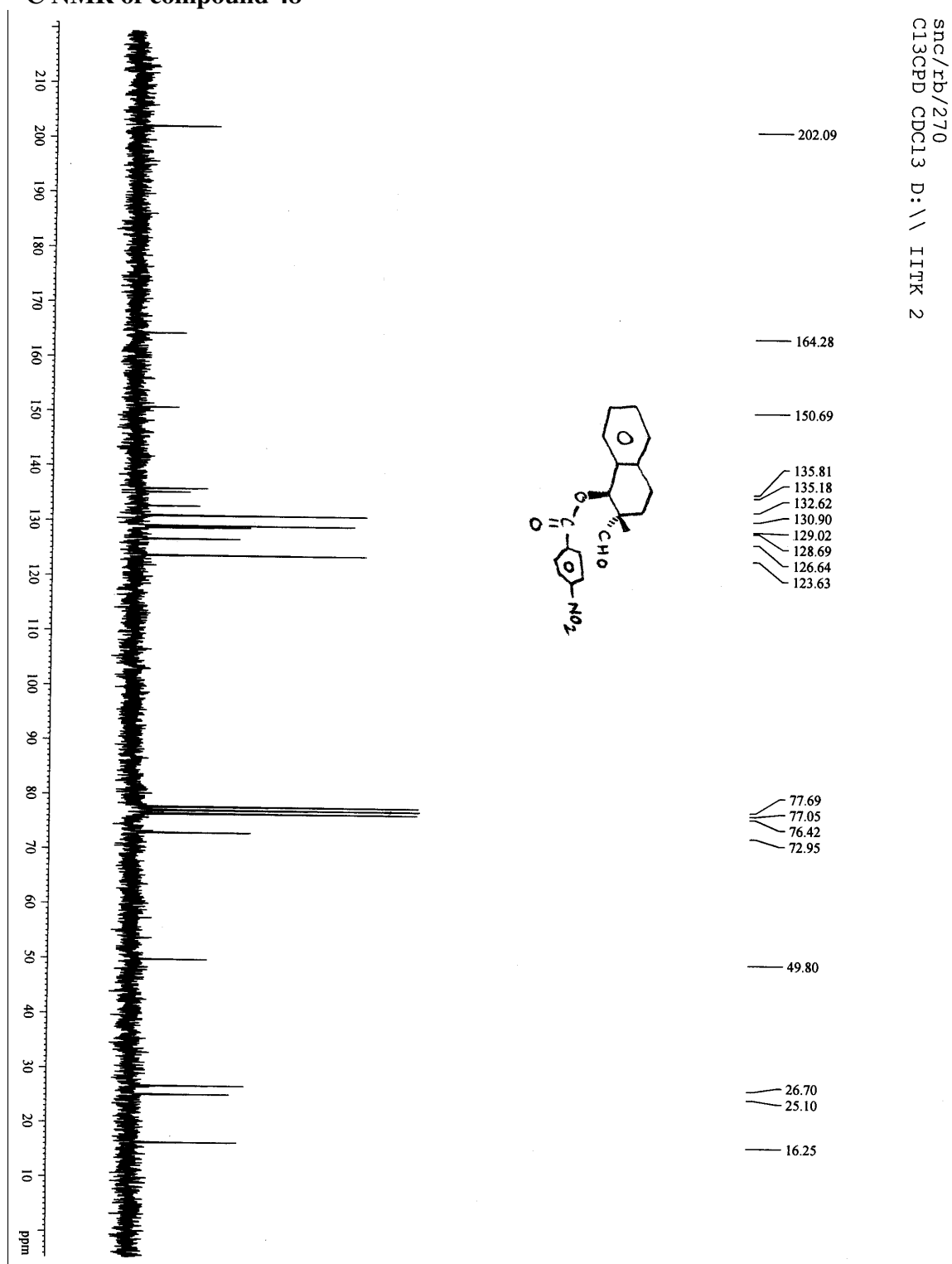
¹³C NMR of compound 47



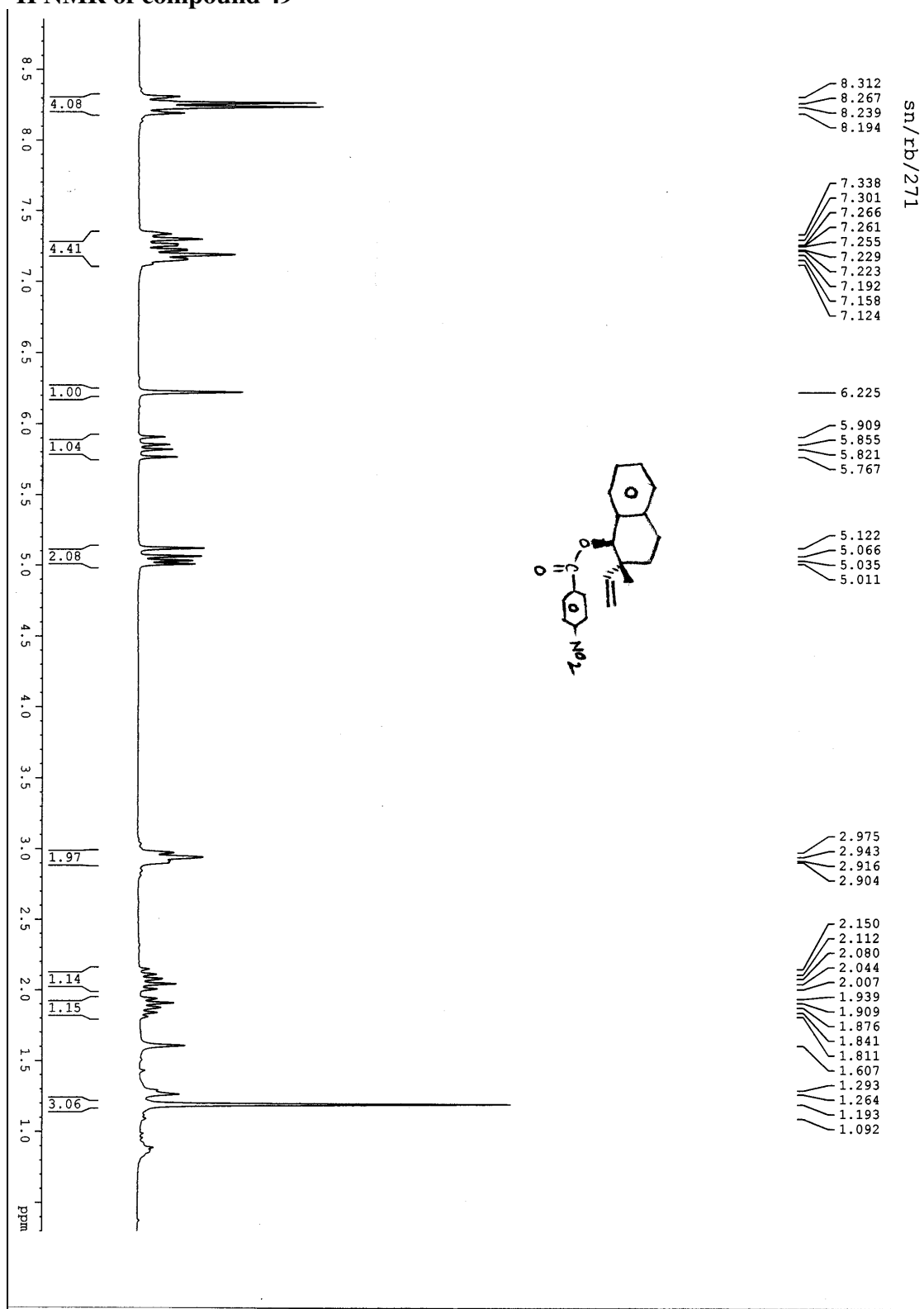
¹H NMR of compound 48



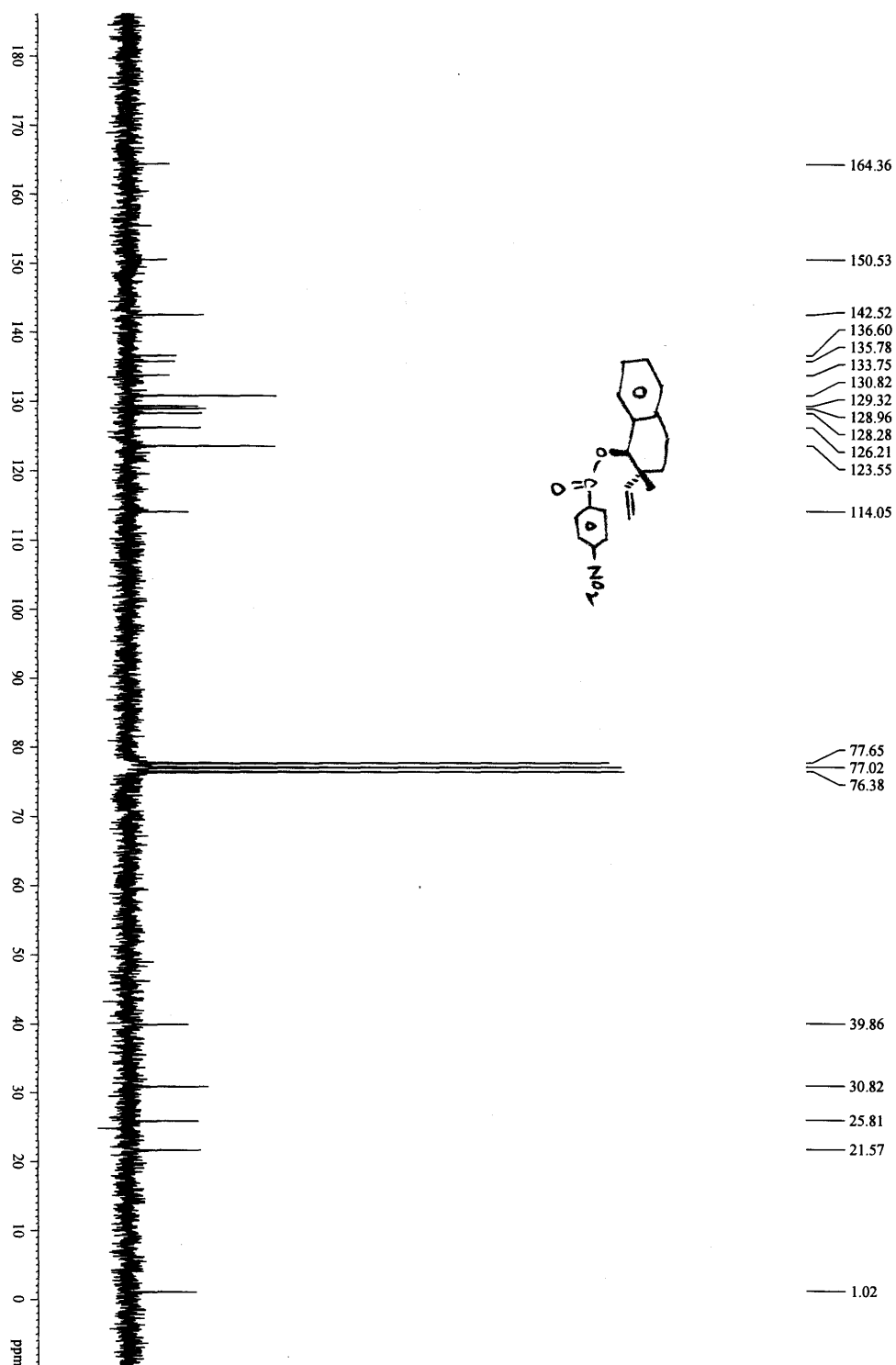
¹³C NMR of compound 48



¹H NMR of compound 49

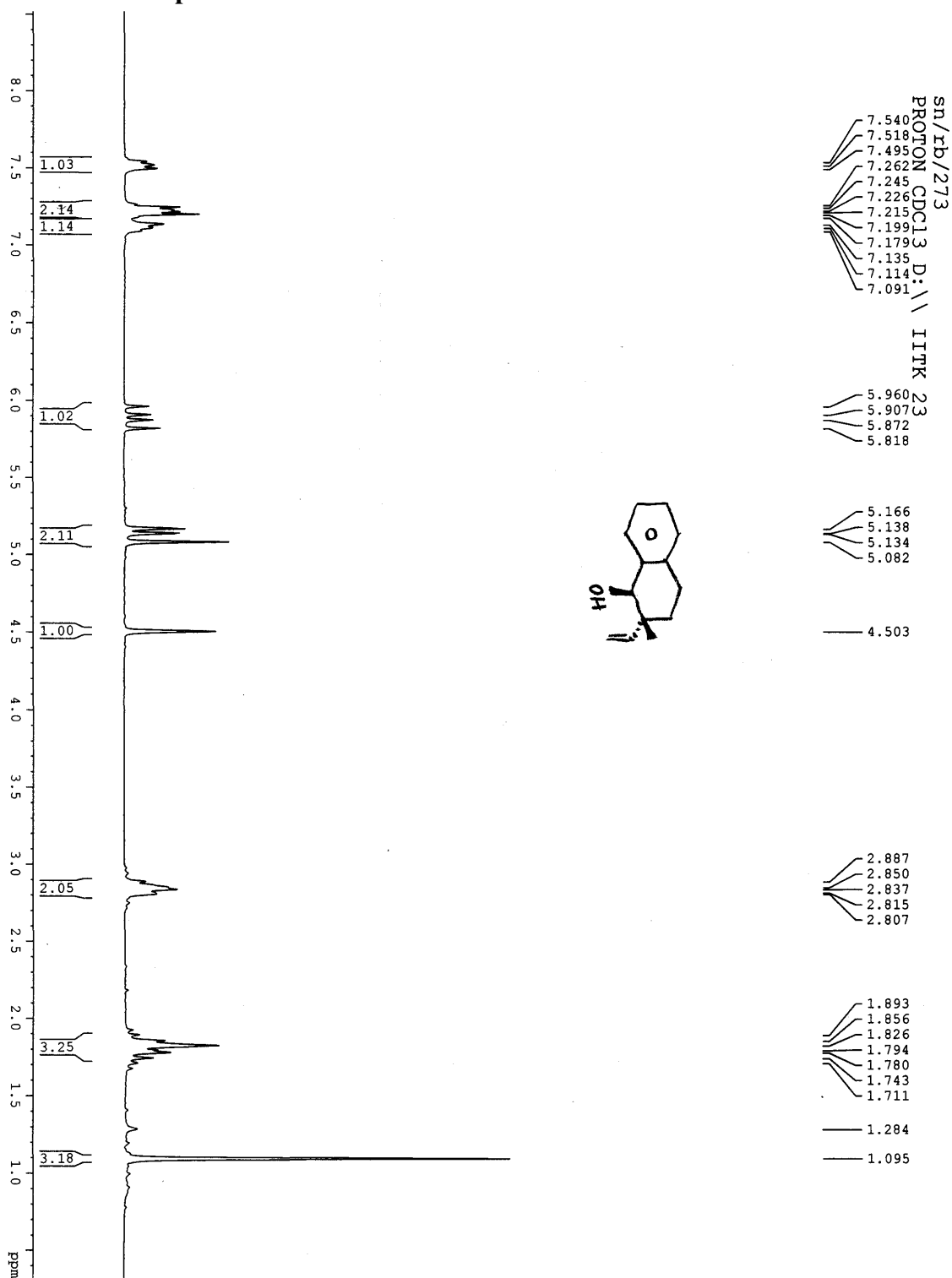


¹³C NMR of compound 49



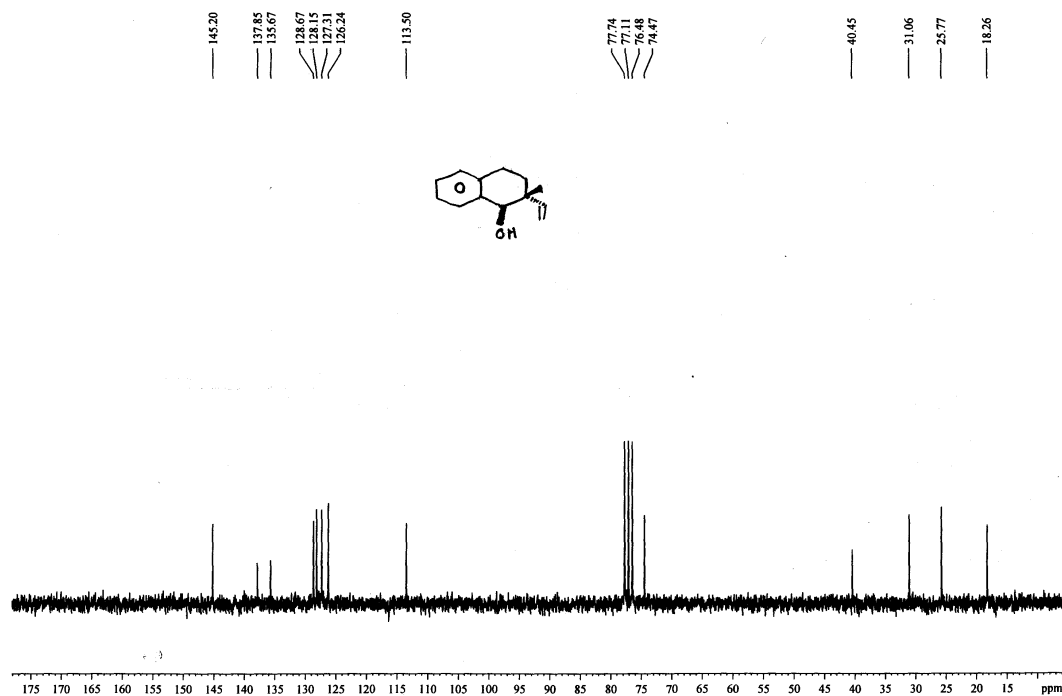
snc/rb/271
C13CPD CDCl3 D:\ IITK 2

¹H NMR of compound 50

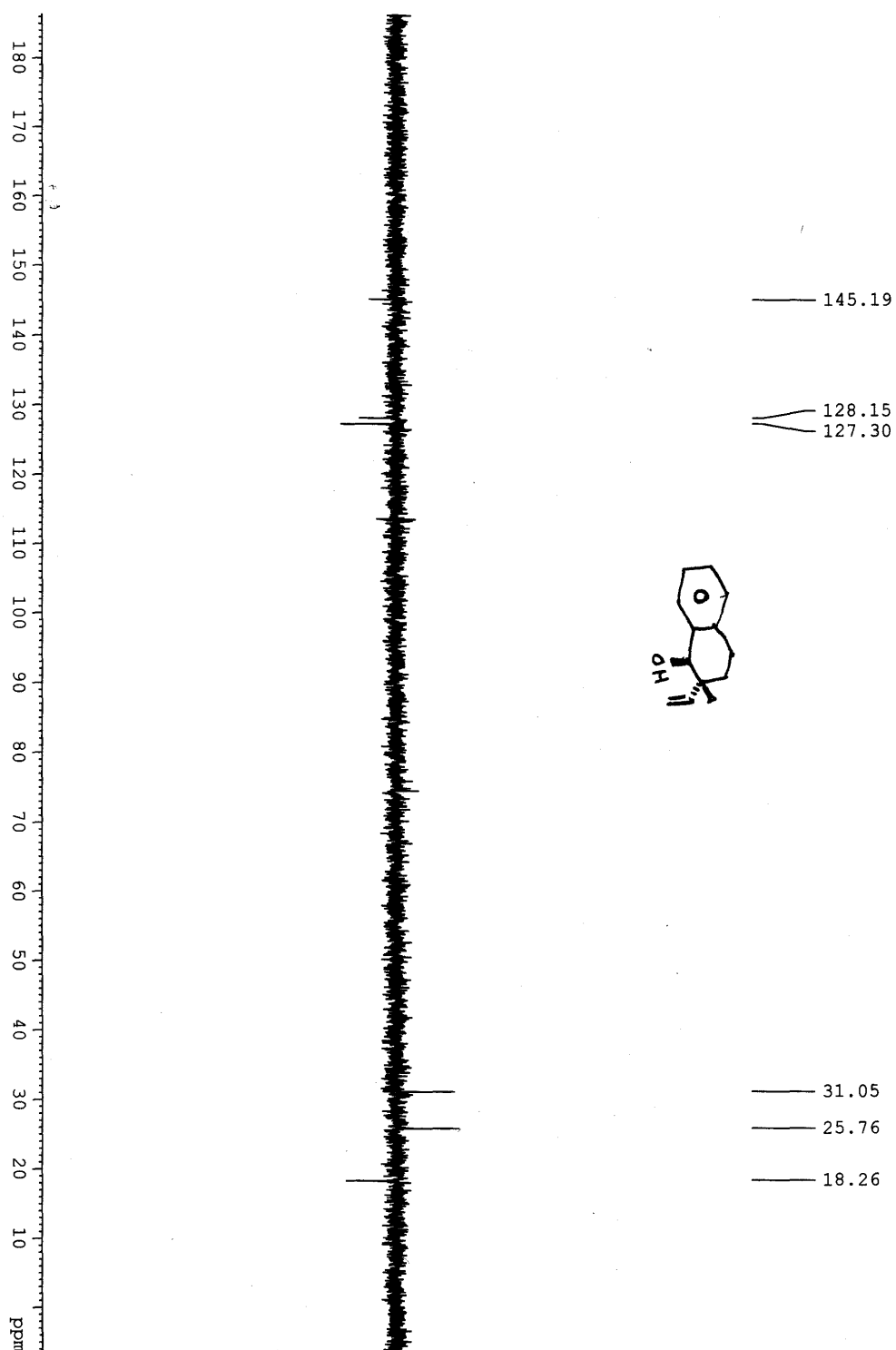


¹³C NMR of compound 50

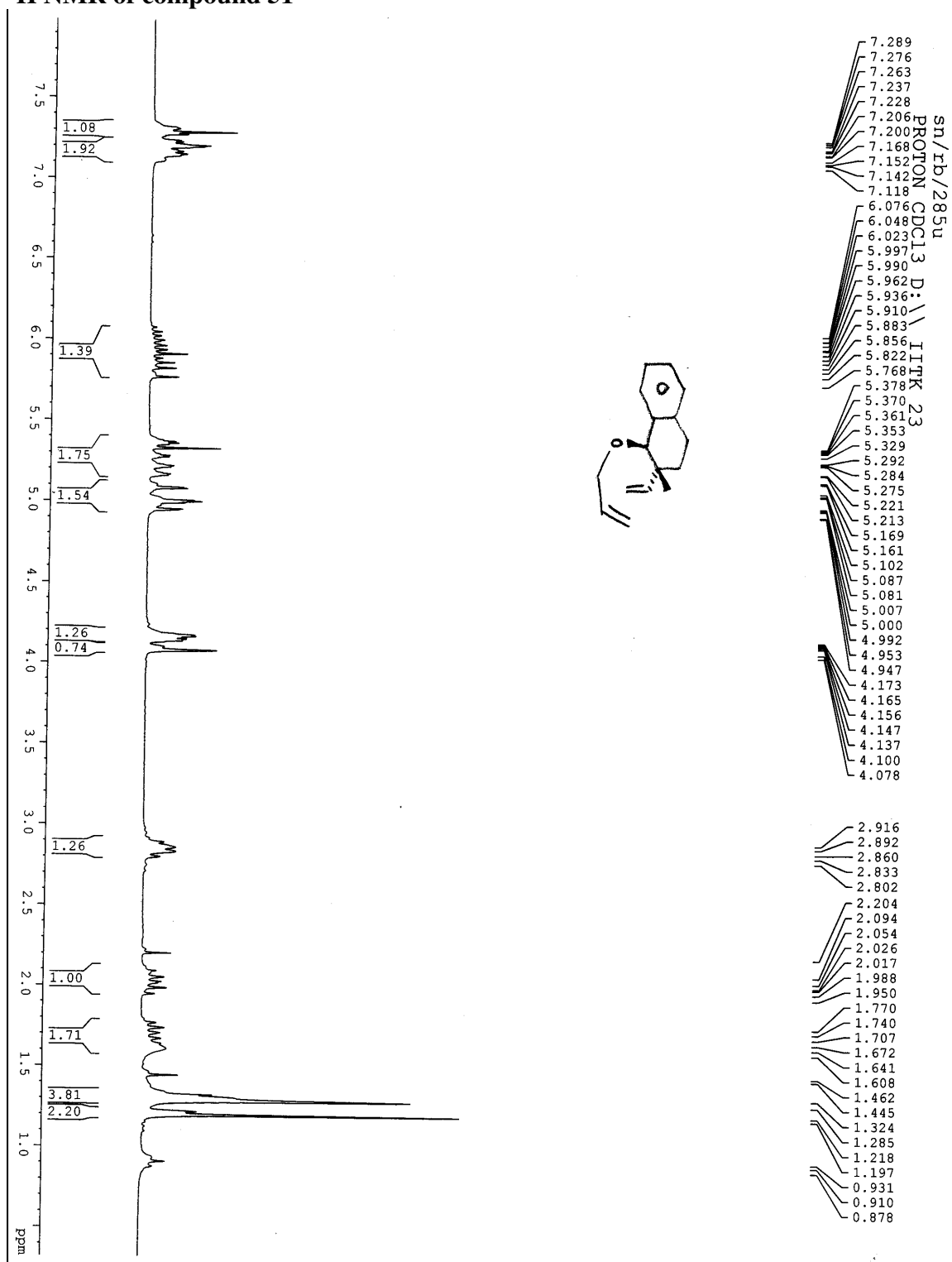
snc/rb/273
C13CPD CDC13 D:\ IITK 2



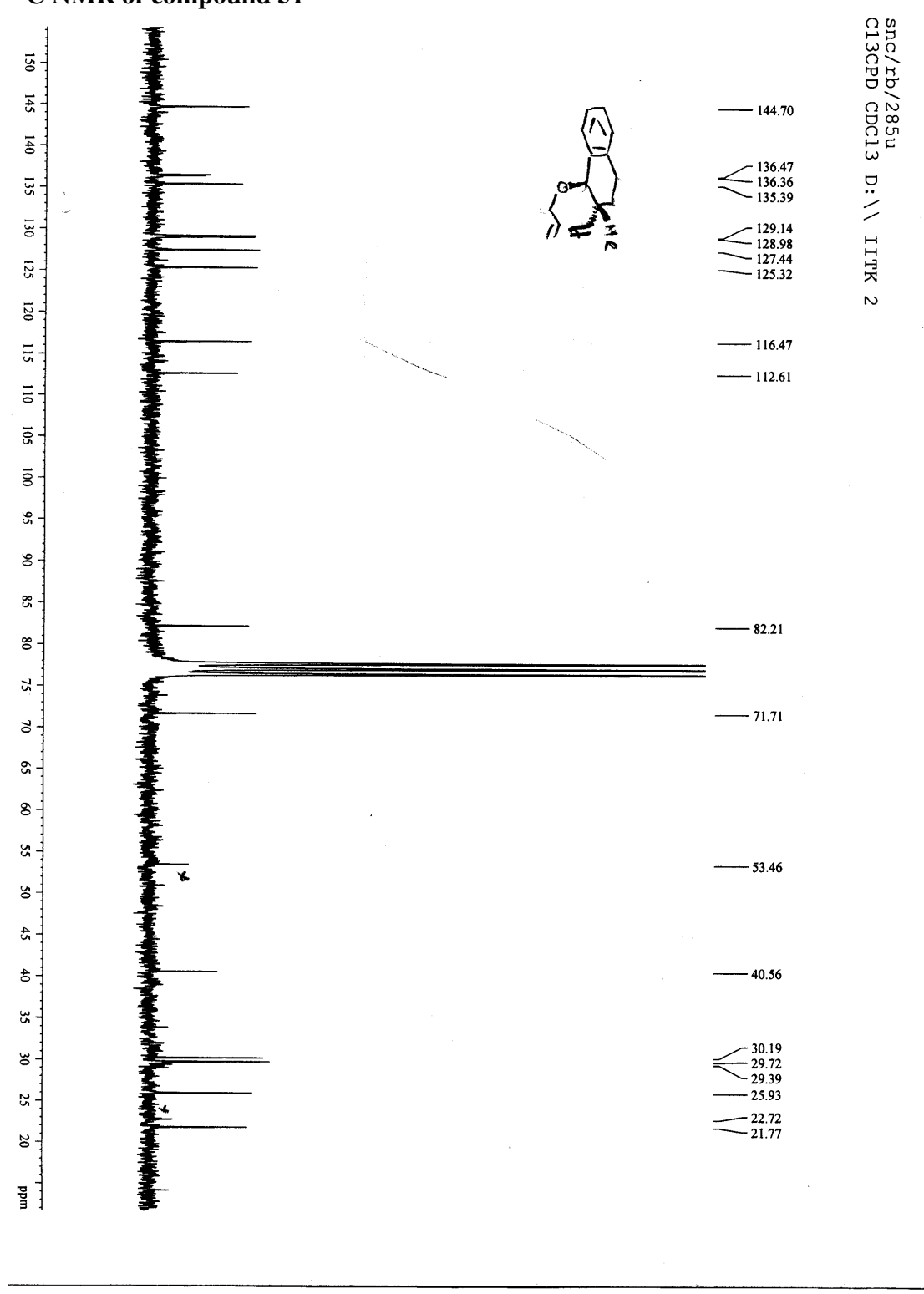
DEPT 135 of compound 50



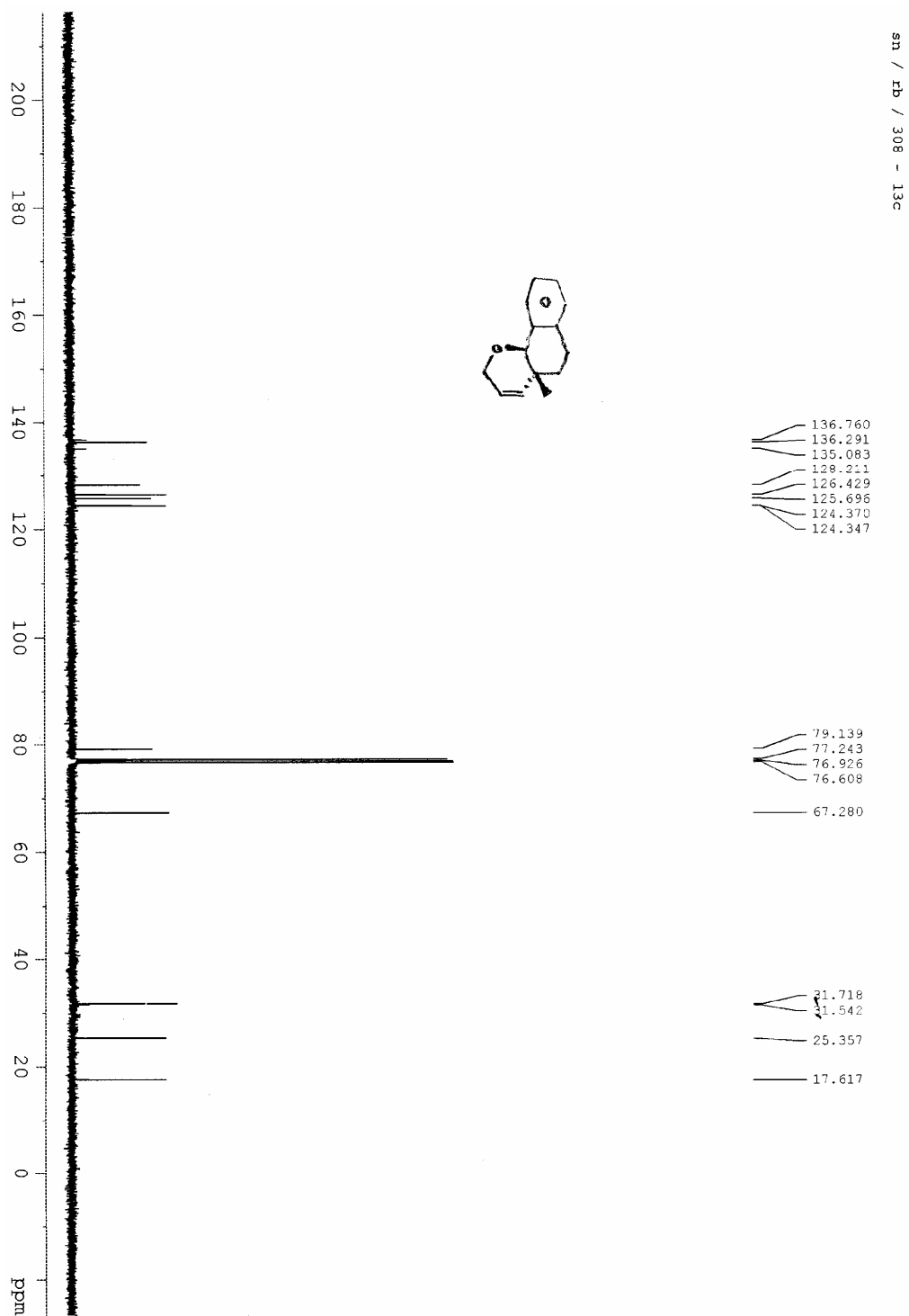
¹H NMR of compound 51



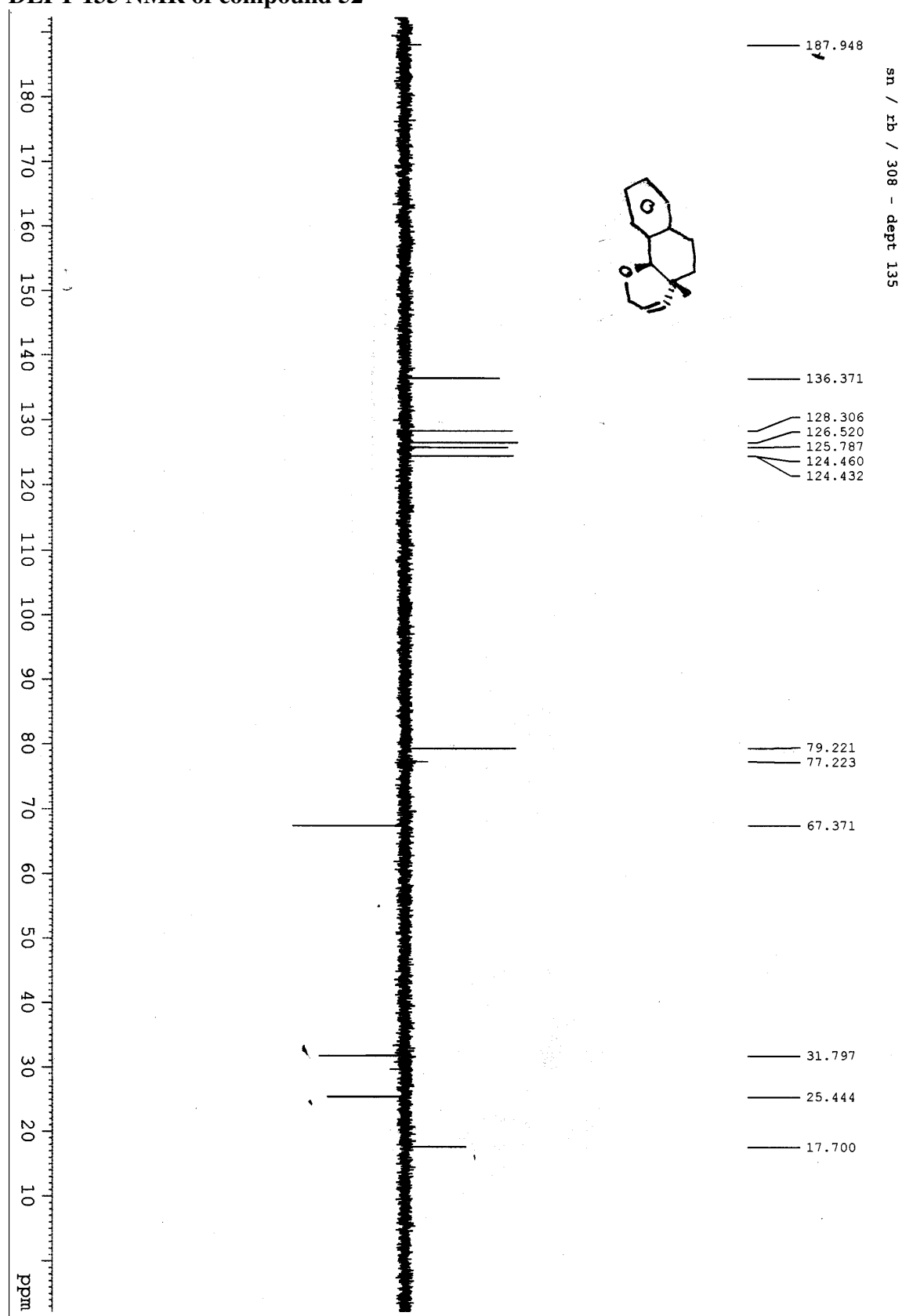
¹³C NMR of compound 51



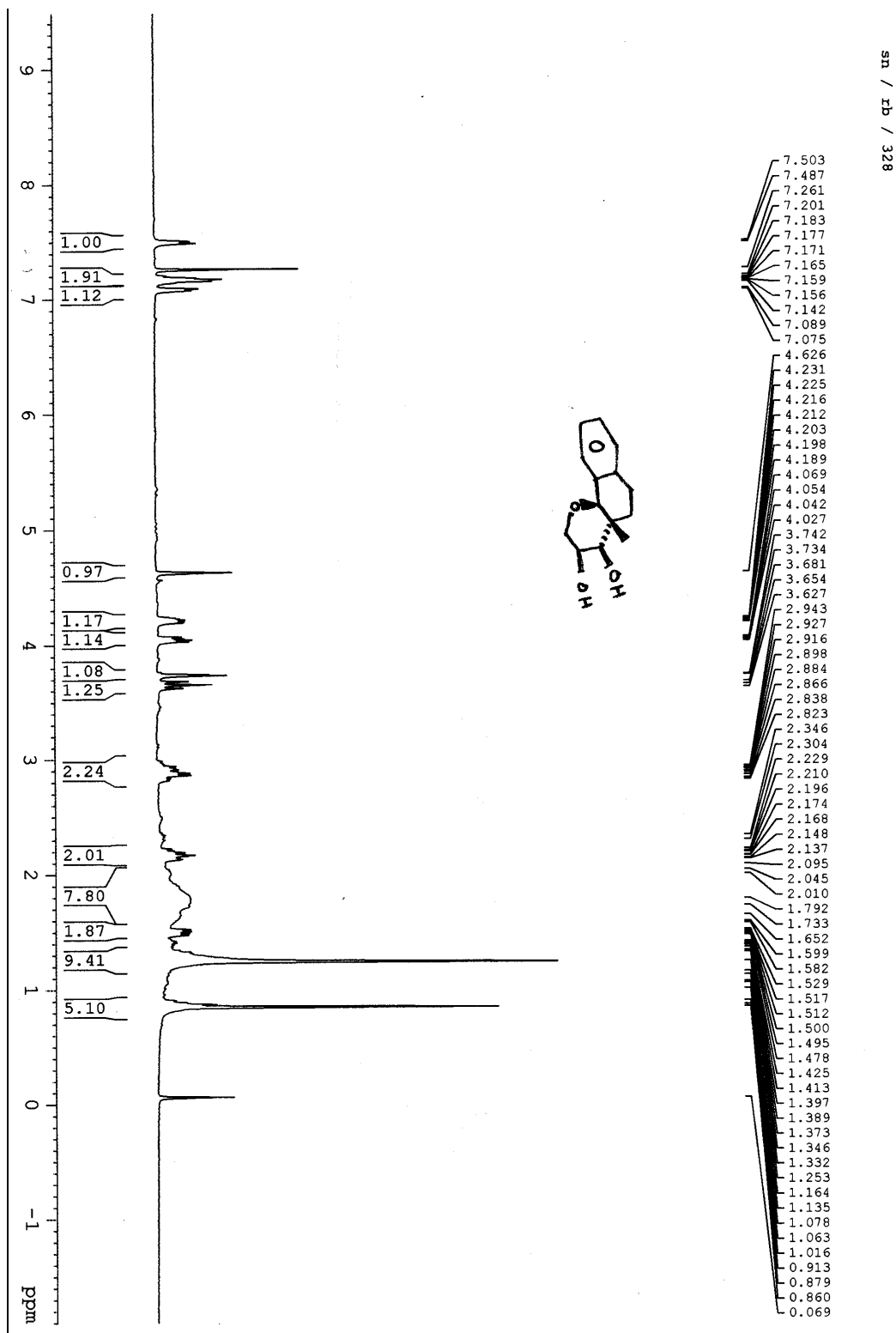
¹³C NMR of compound 52



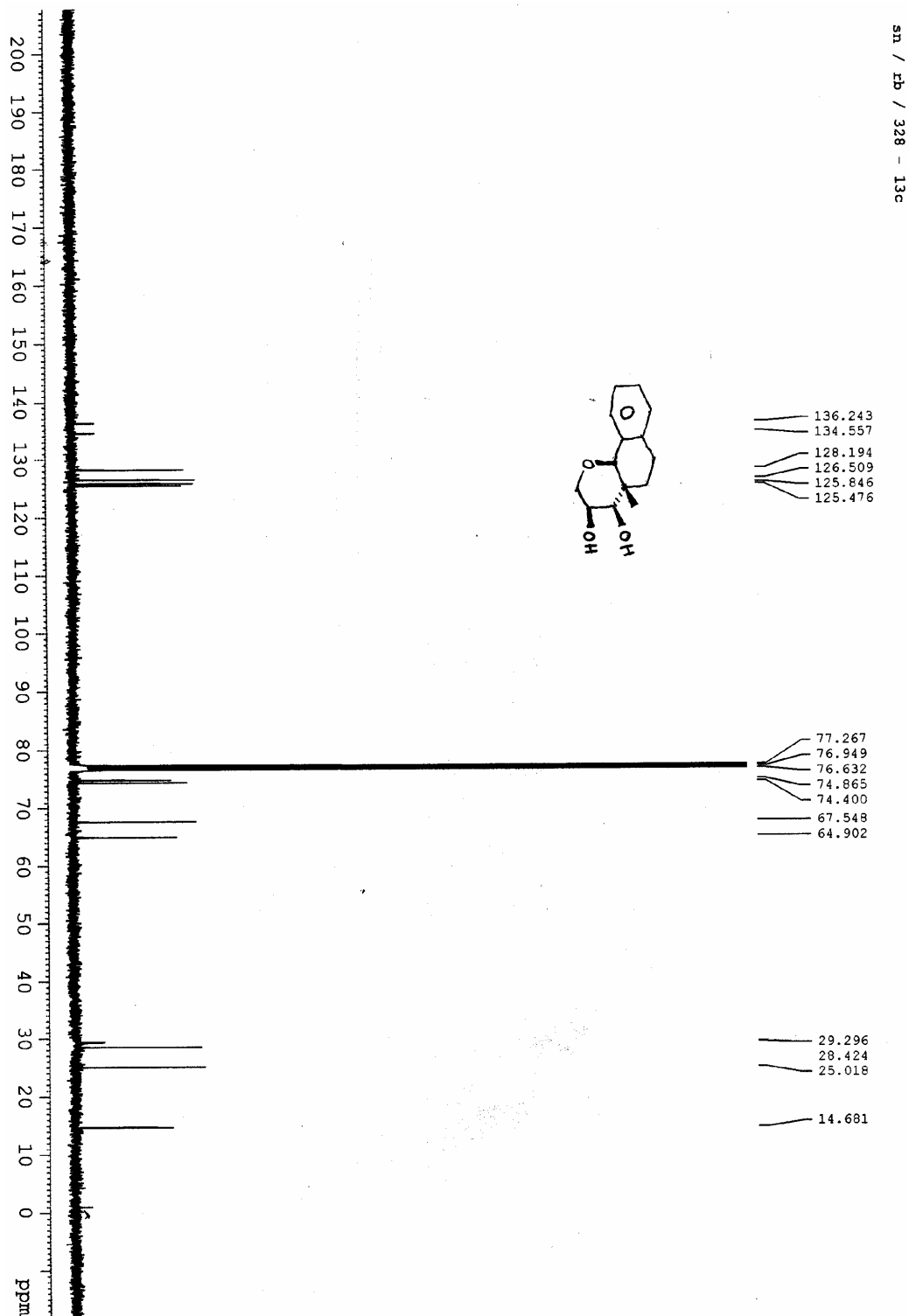
DEPT 135 NMR of compound 52



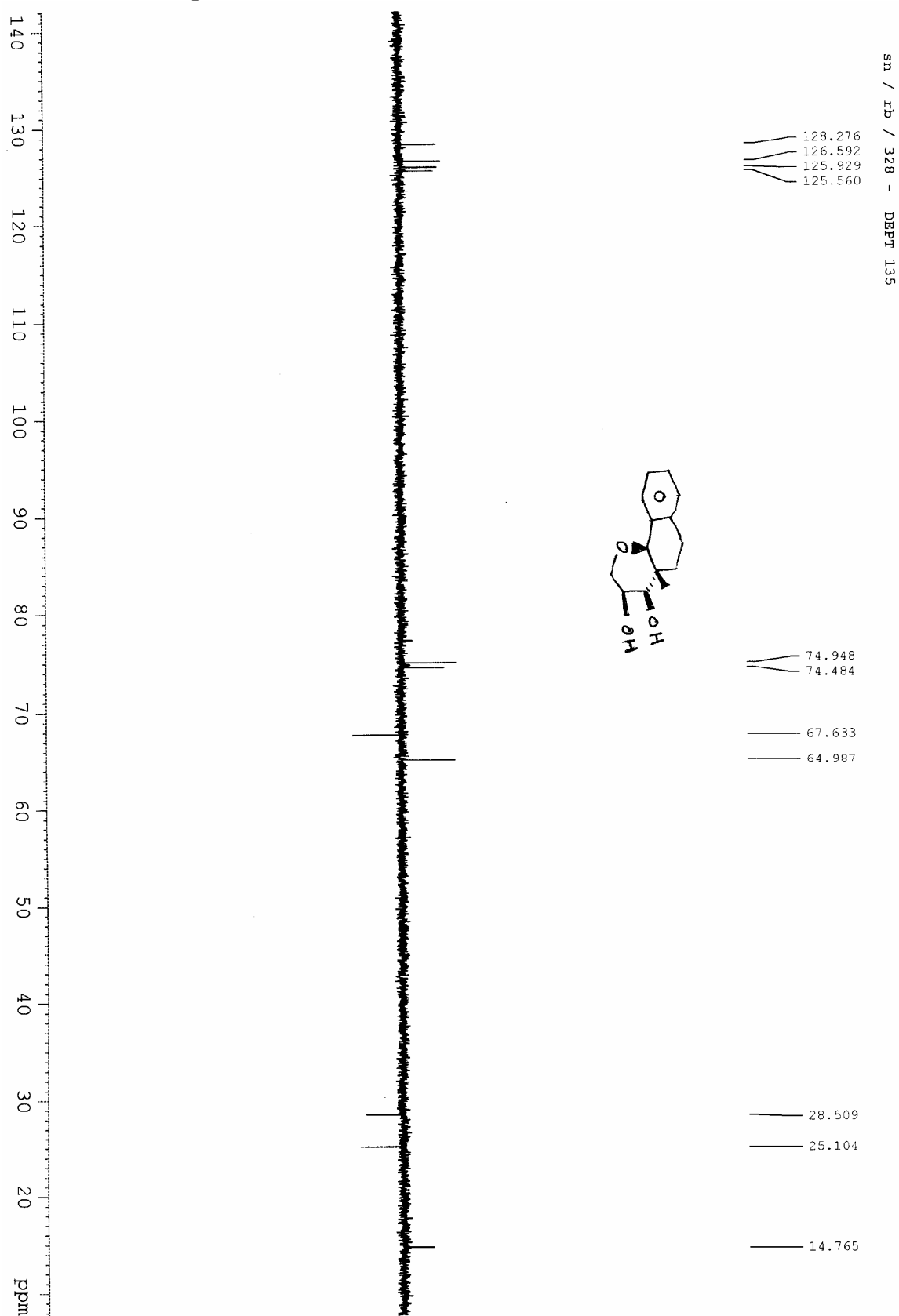
¹H NMR of compound 53



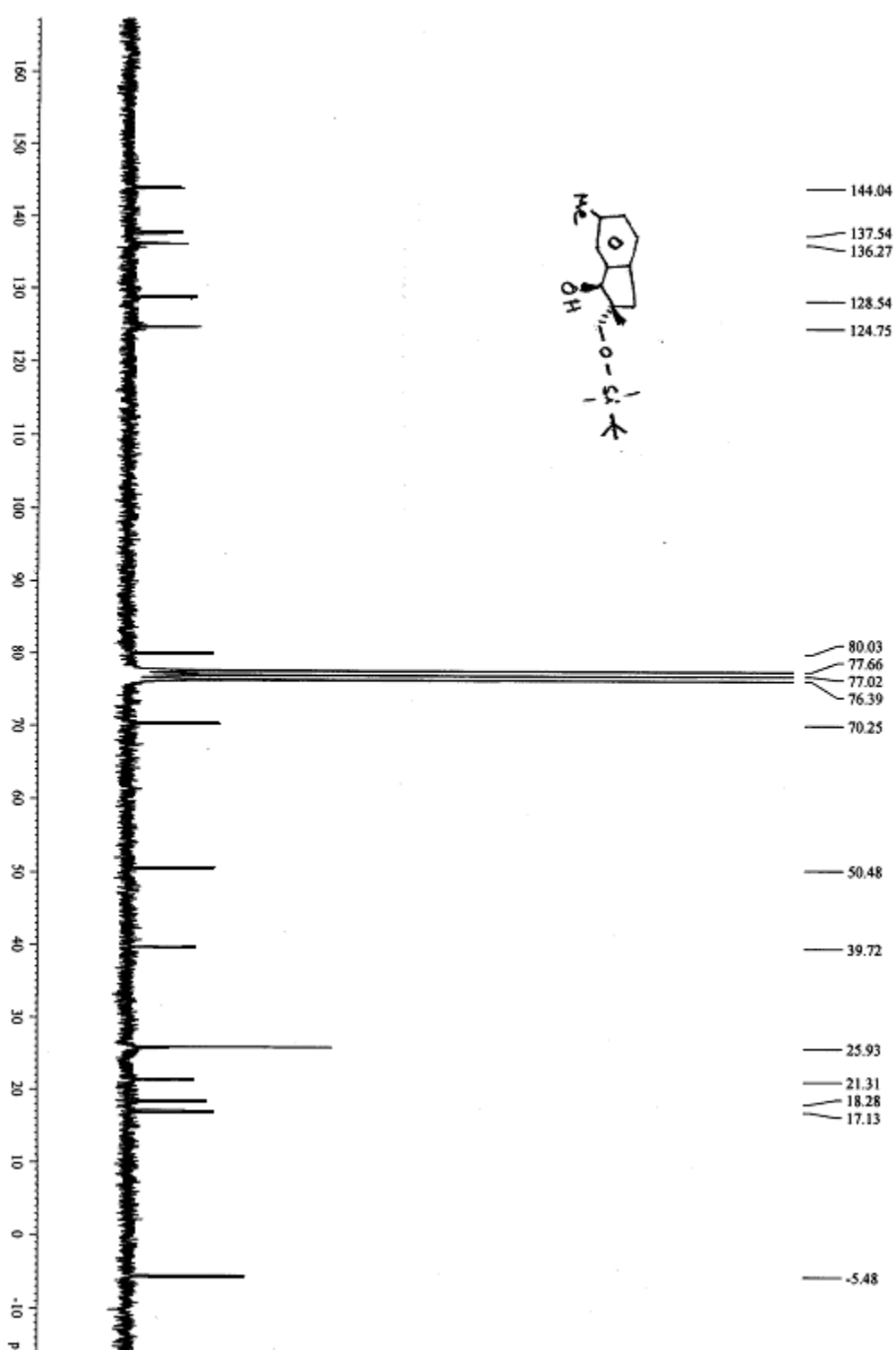
¹³C NMR of compound 53



DEPT 135 of compound 53

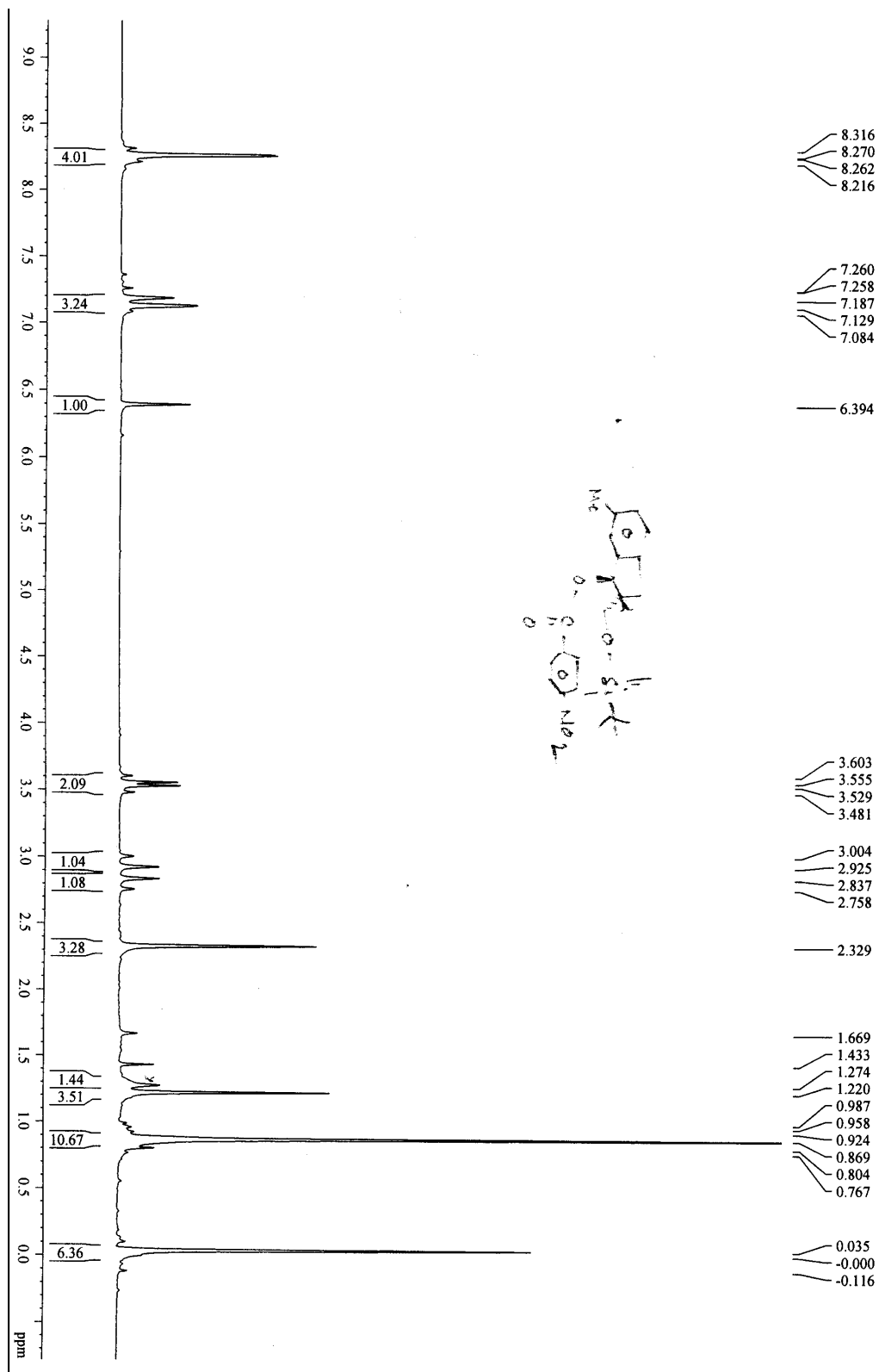


¹³C NMR of compound 54



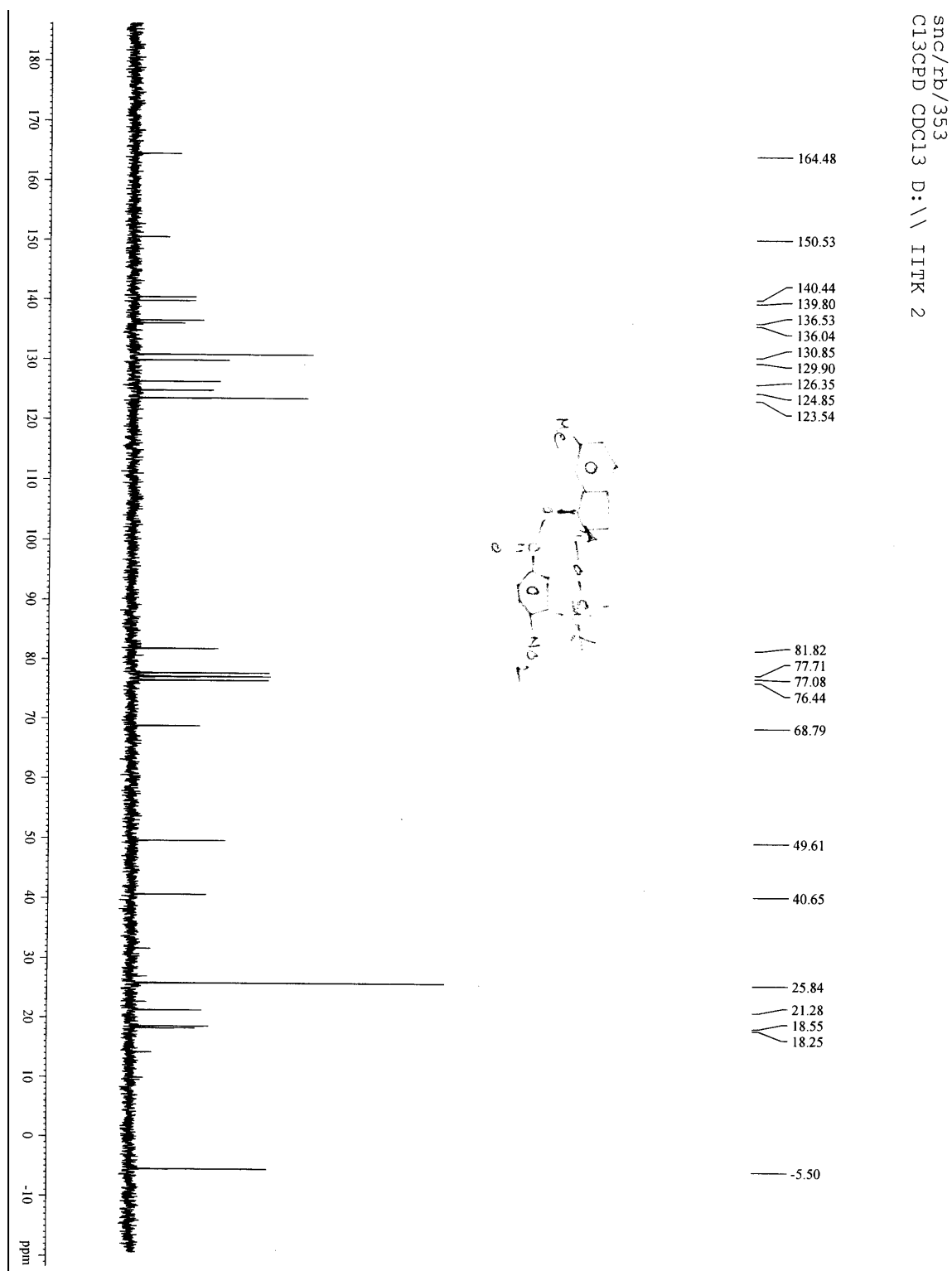
snc/rb/351

¹H NMR of compound 55

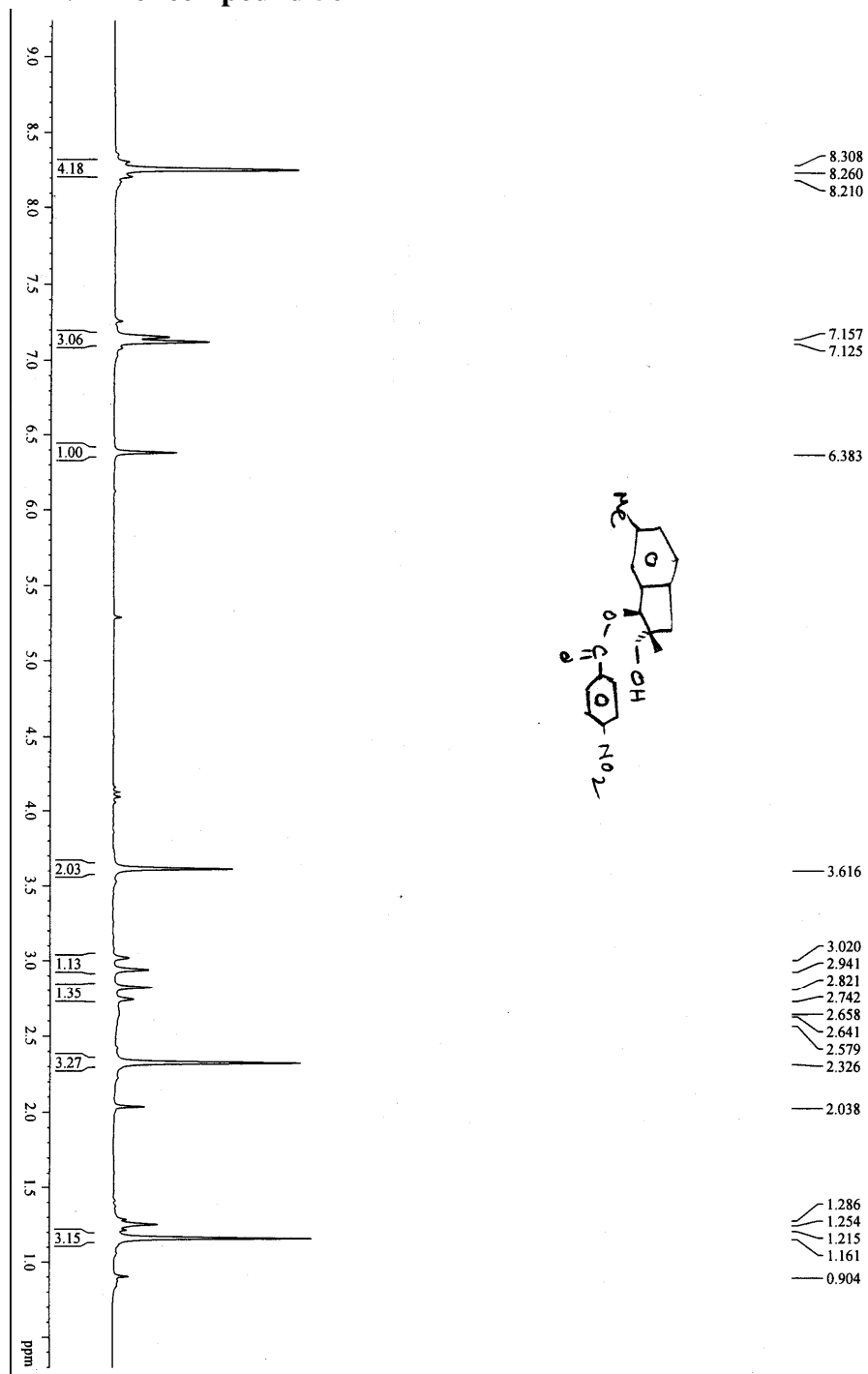


sn/rb/353

¹³C NMR of compound 55



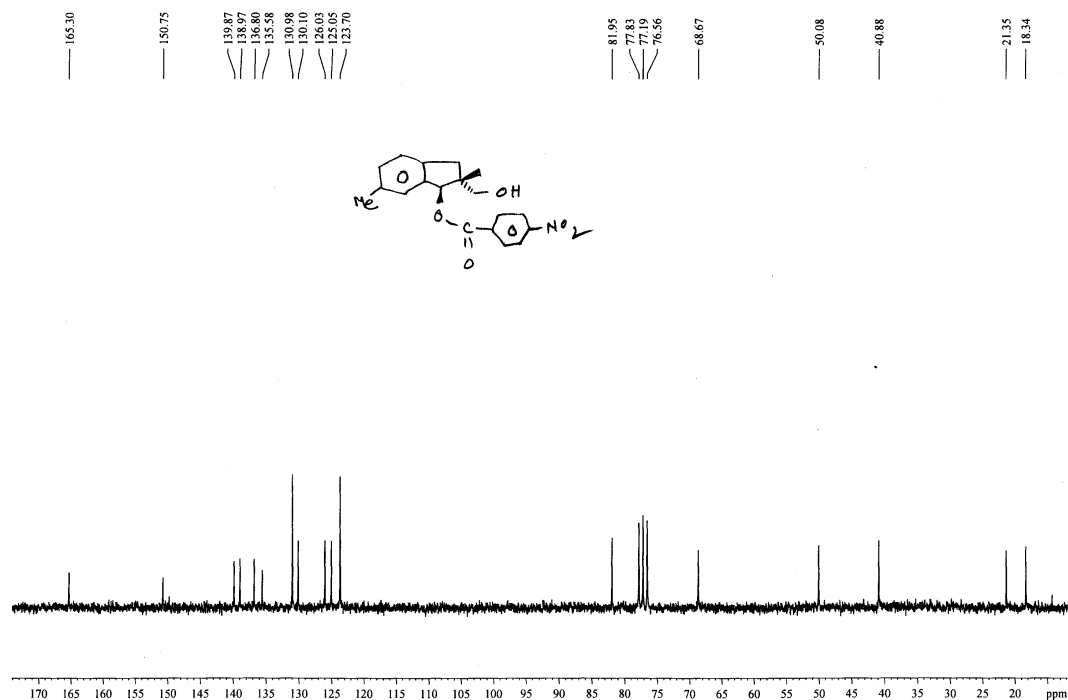
¹H NMR of compound 56



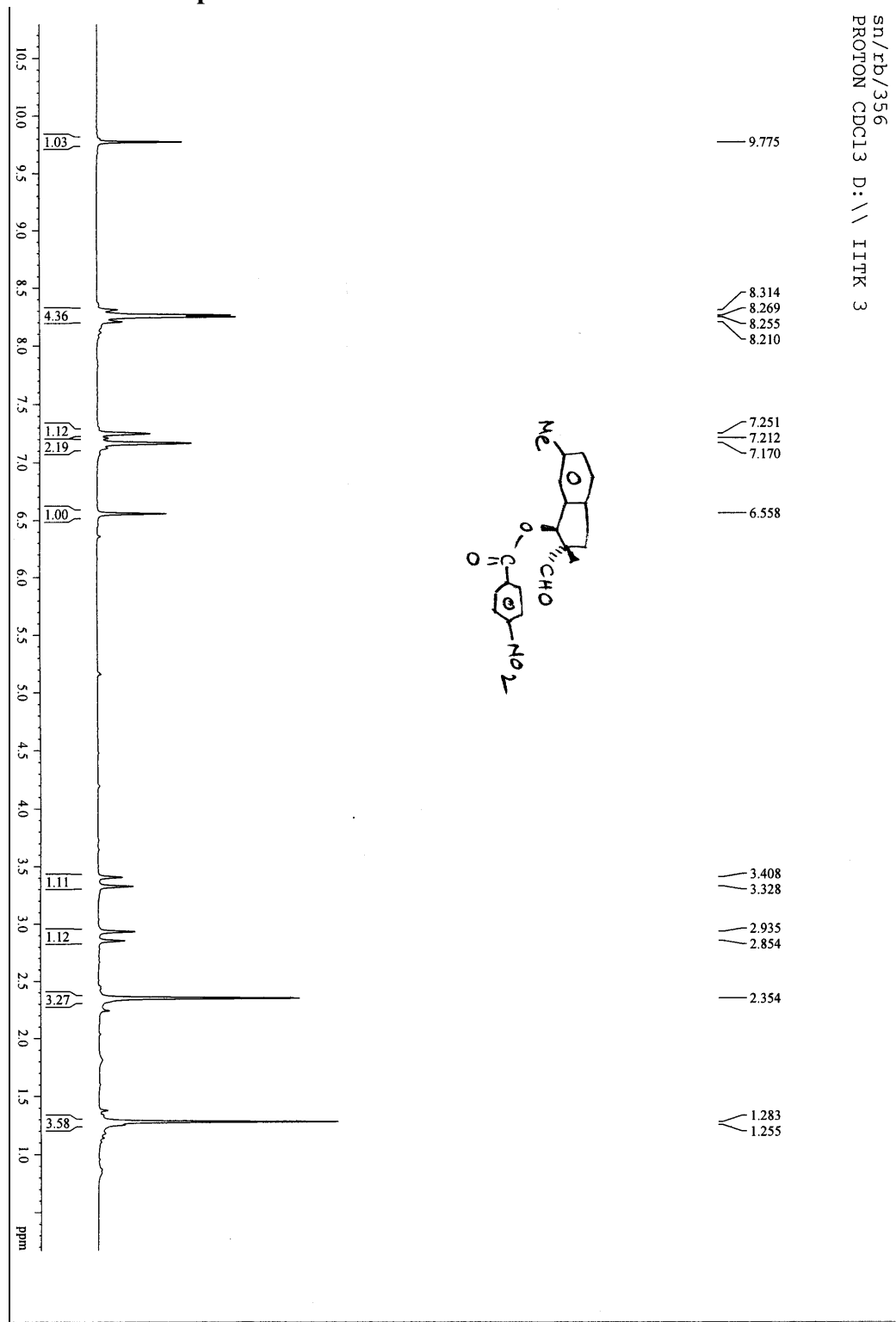
sn/rb/354

¹³C NMR of compound 56

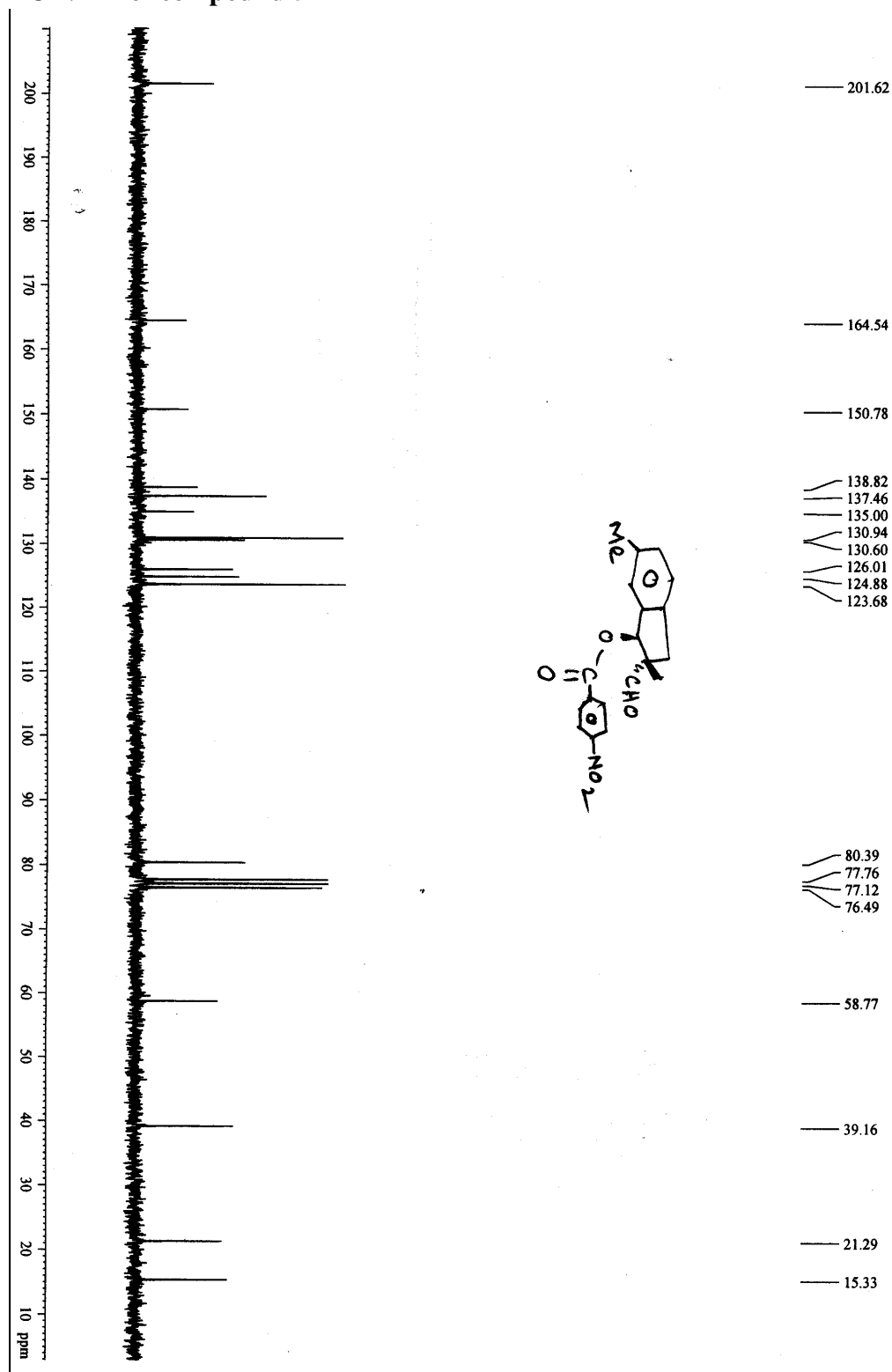
snc/rb/354
C13CPD CDC13 D:\ IITK 34



¹H NMR of compound 57

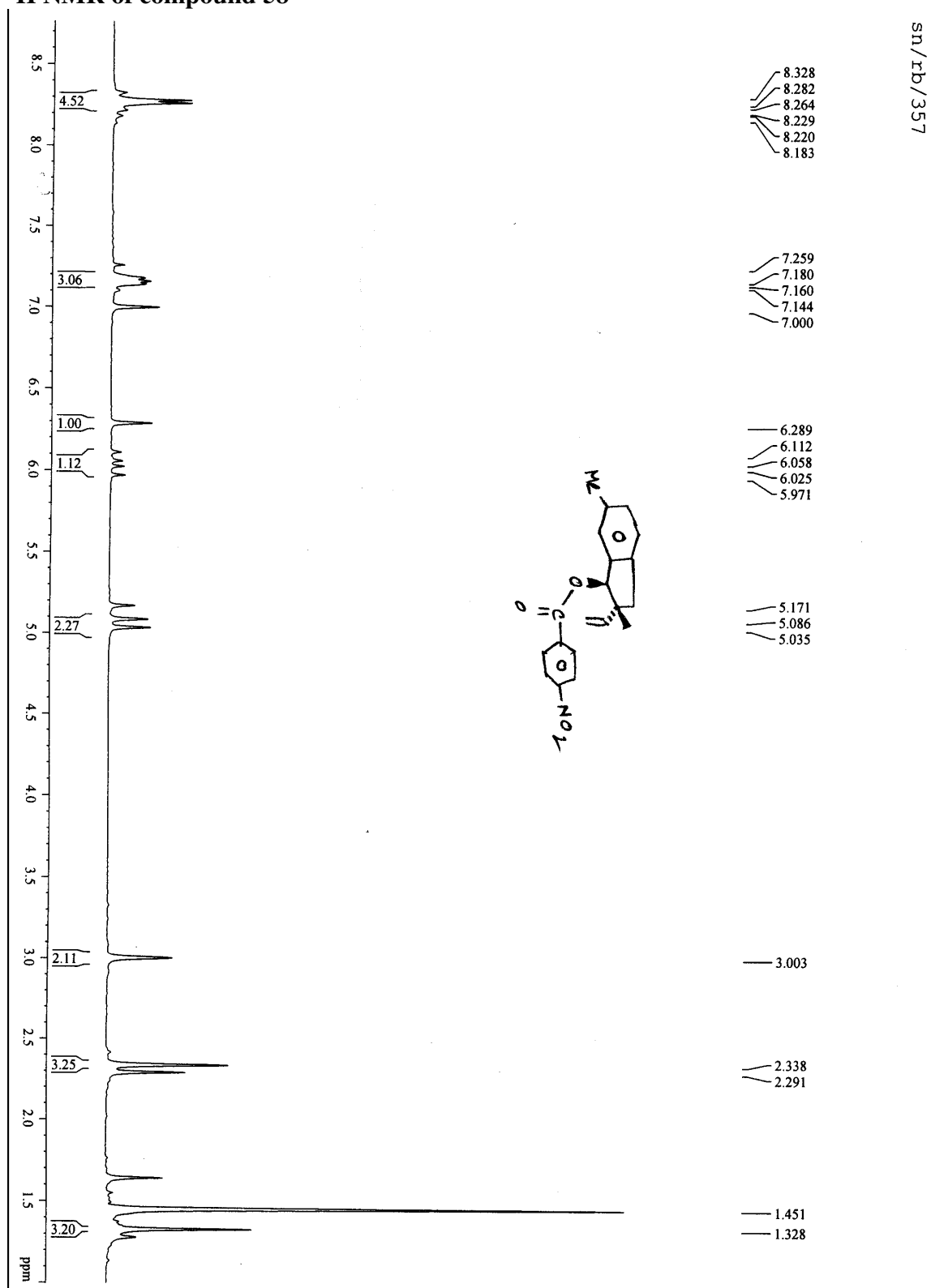


¹³C NMR of compound 57

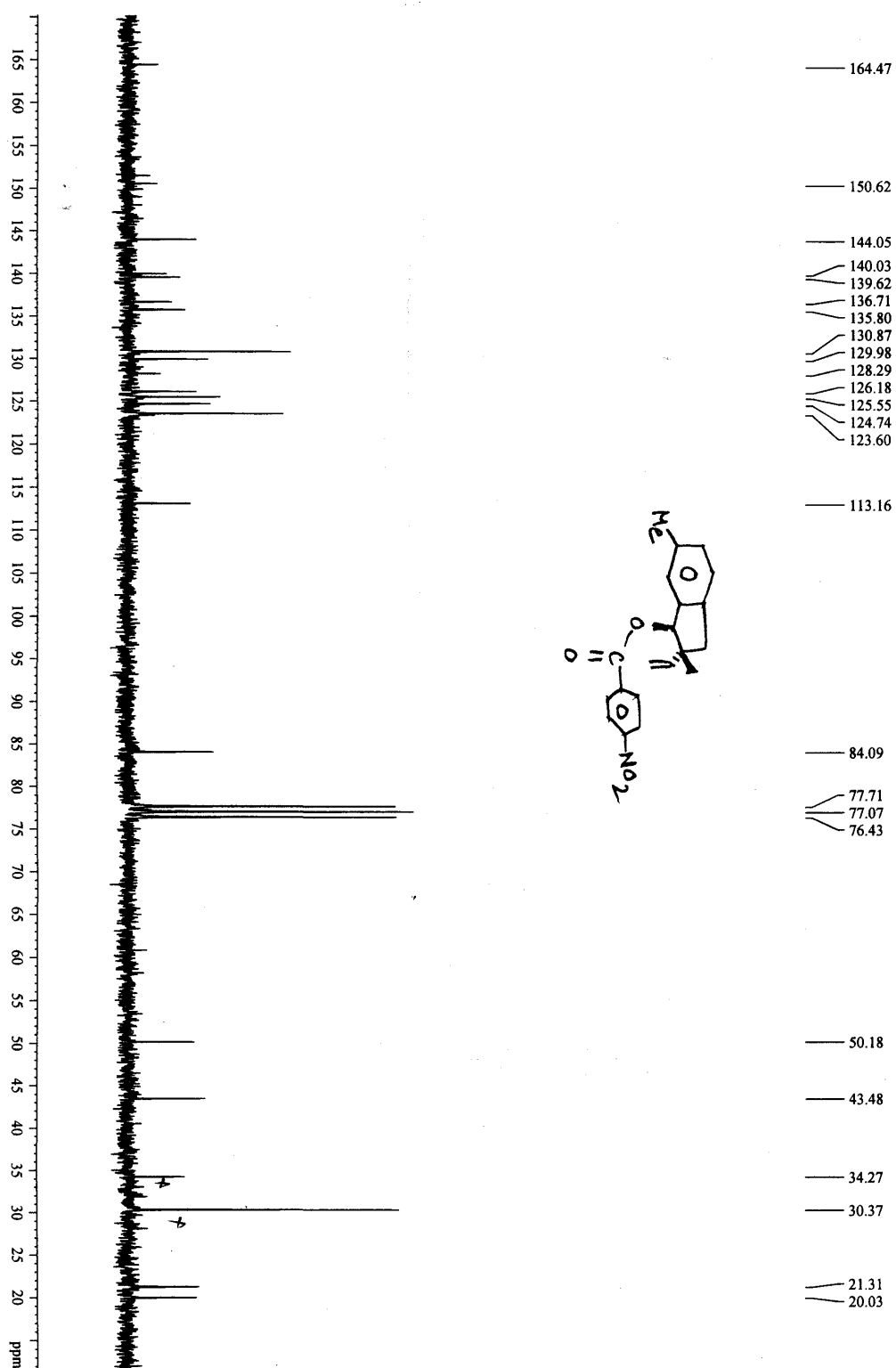


sn/rb/356
C13CPD CDCl3 D:\ IITK 23

¹H NMR of compound 58

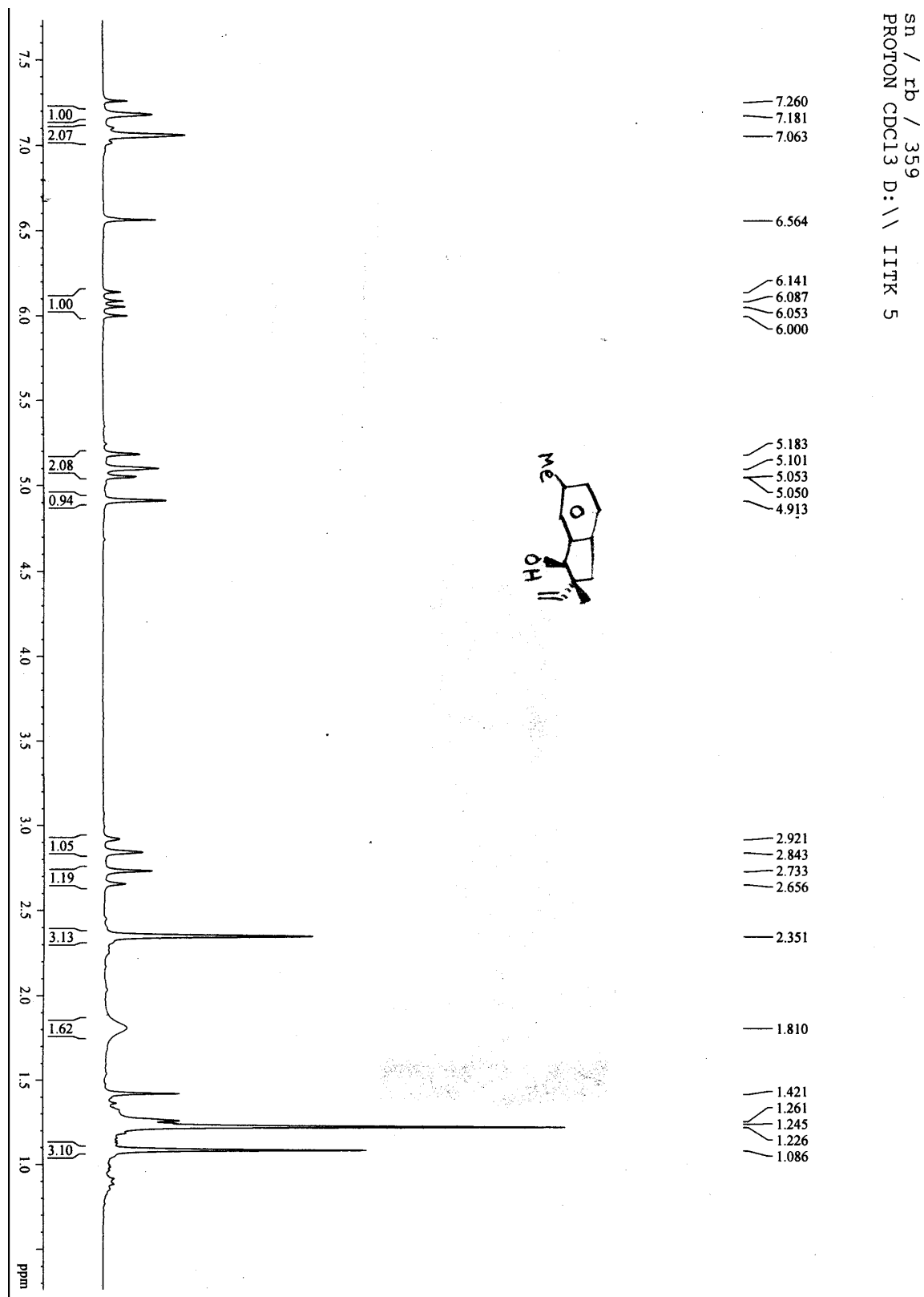


¹³C NMR of compound 58

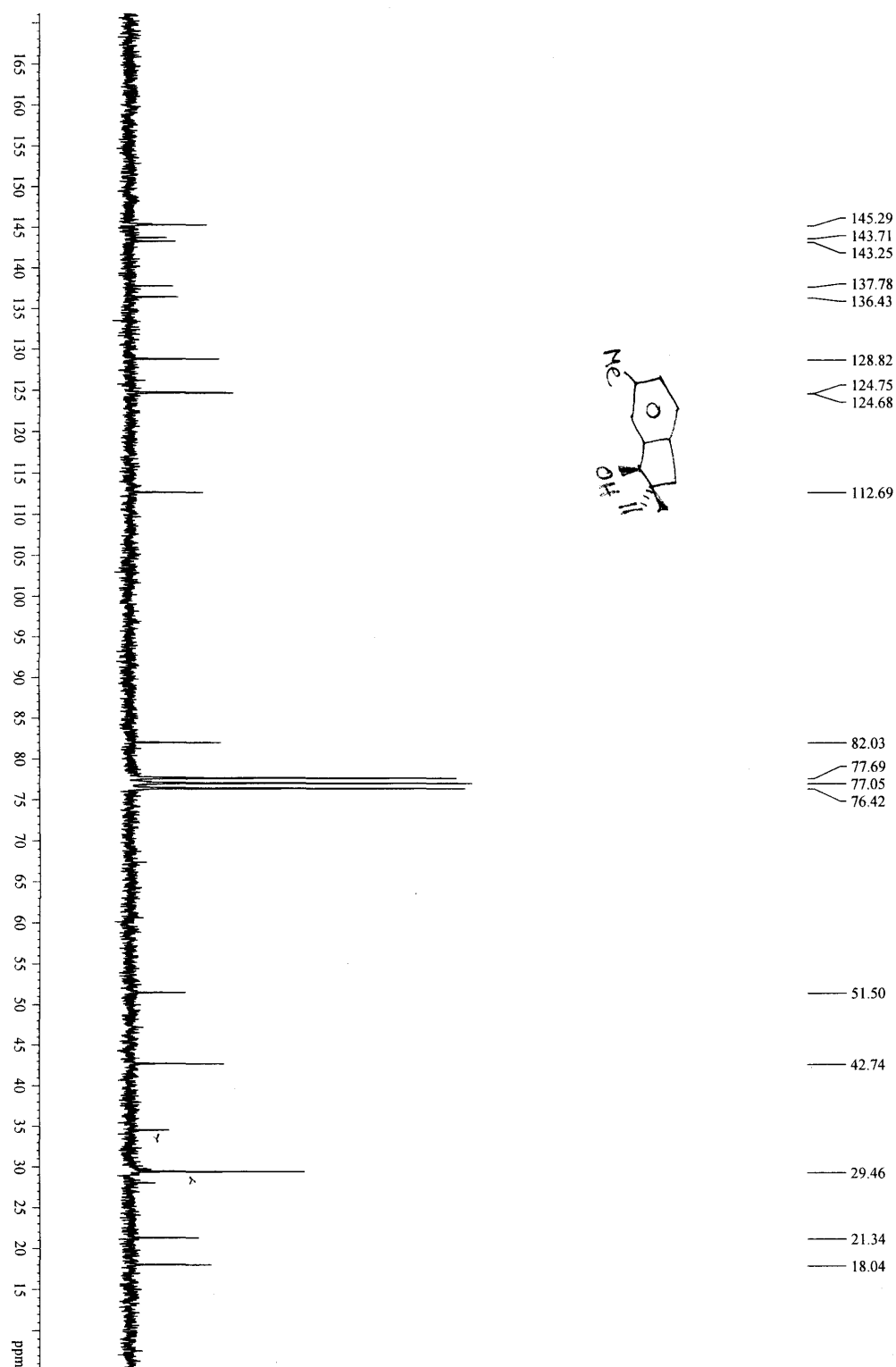


snc/rb/357
C13CPD CDCl3 D:\ IITK 2

¹H NMR of compound 59

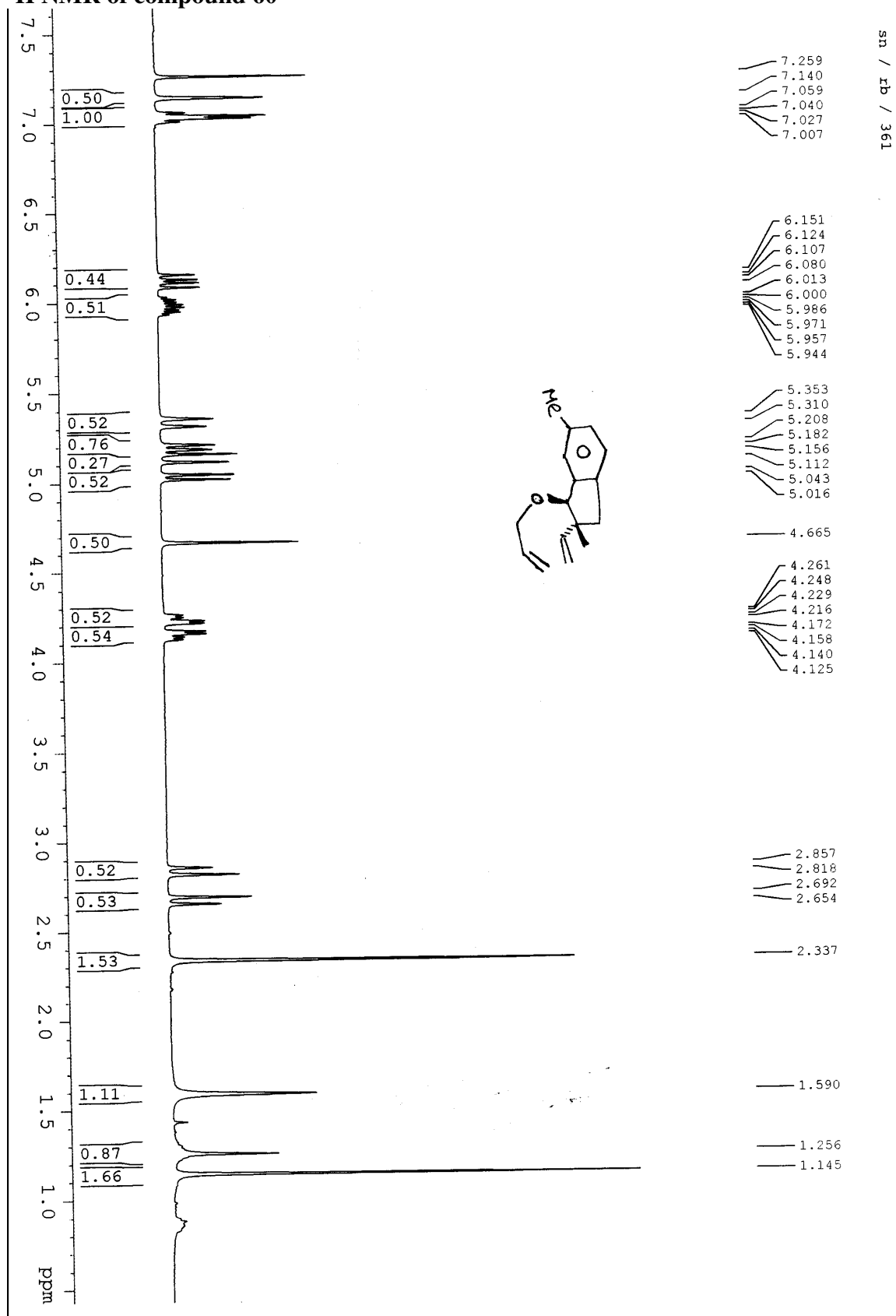


¹³C NMR of compound 59

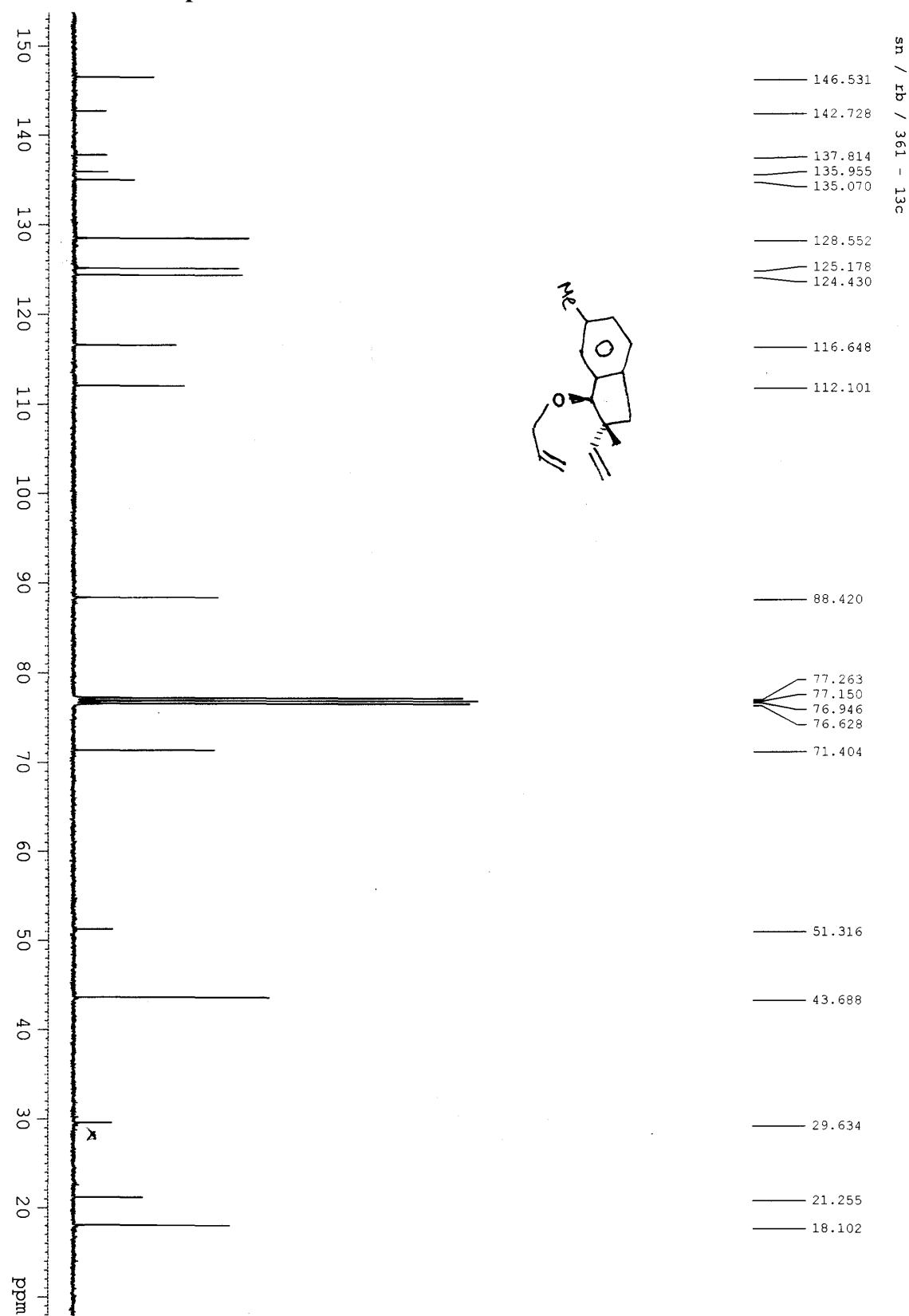


snc/rb/359
C13CPD CDCl3 D:\ IITK 2

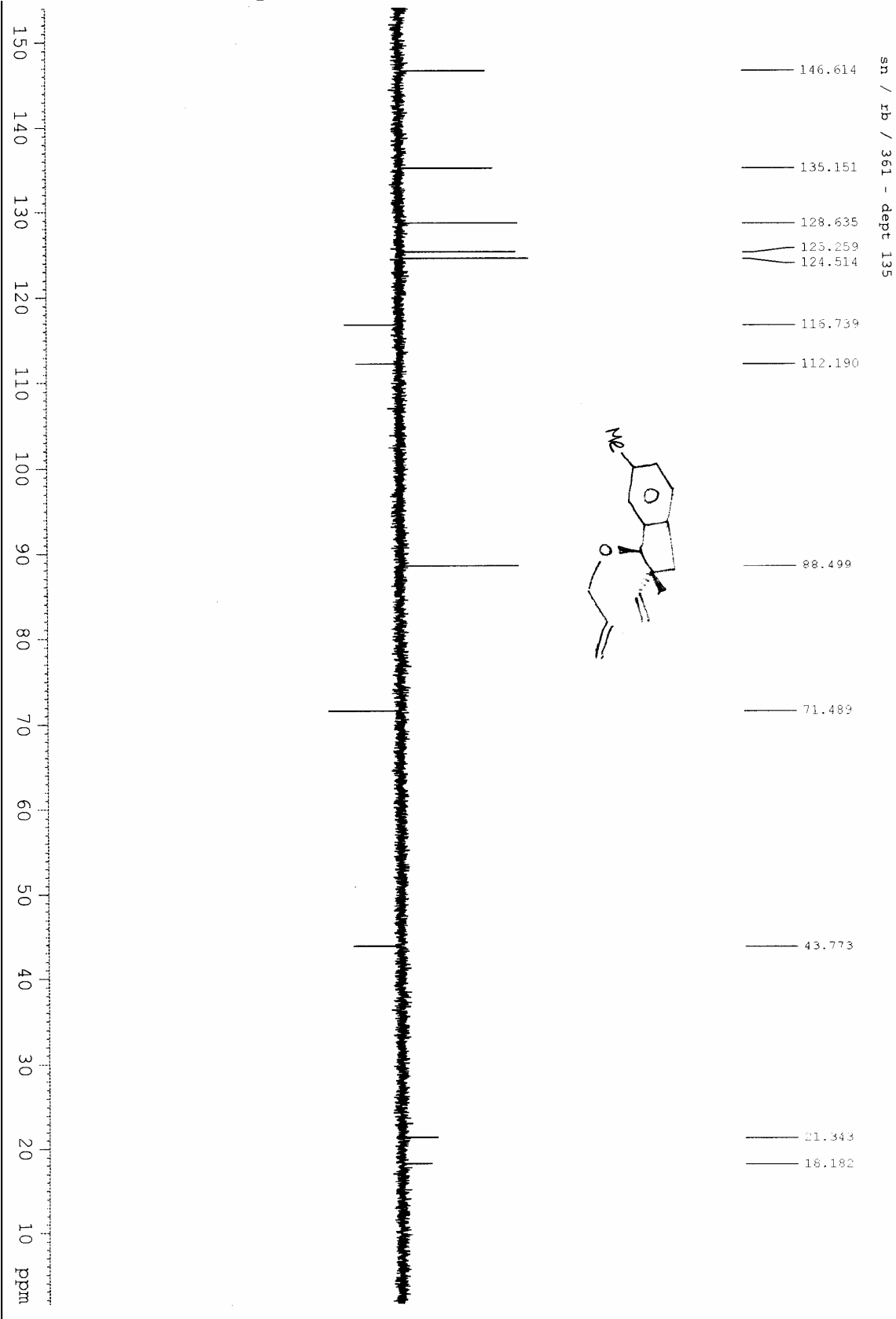
¹H NMR of compound 60



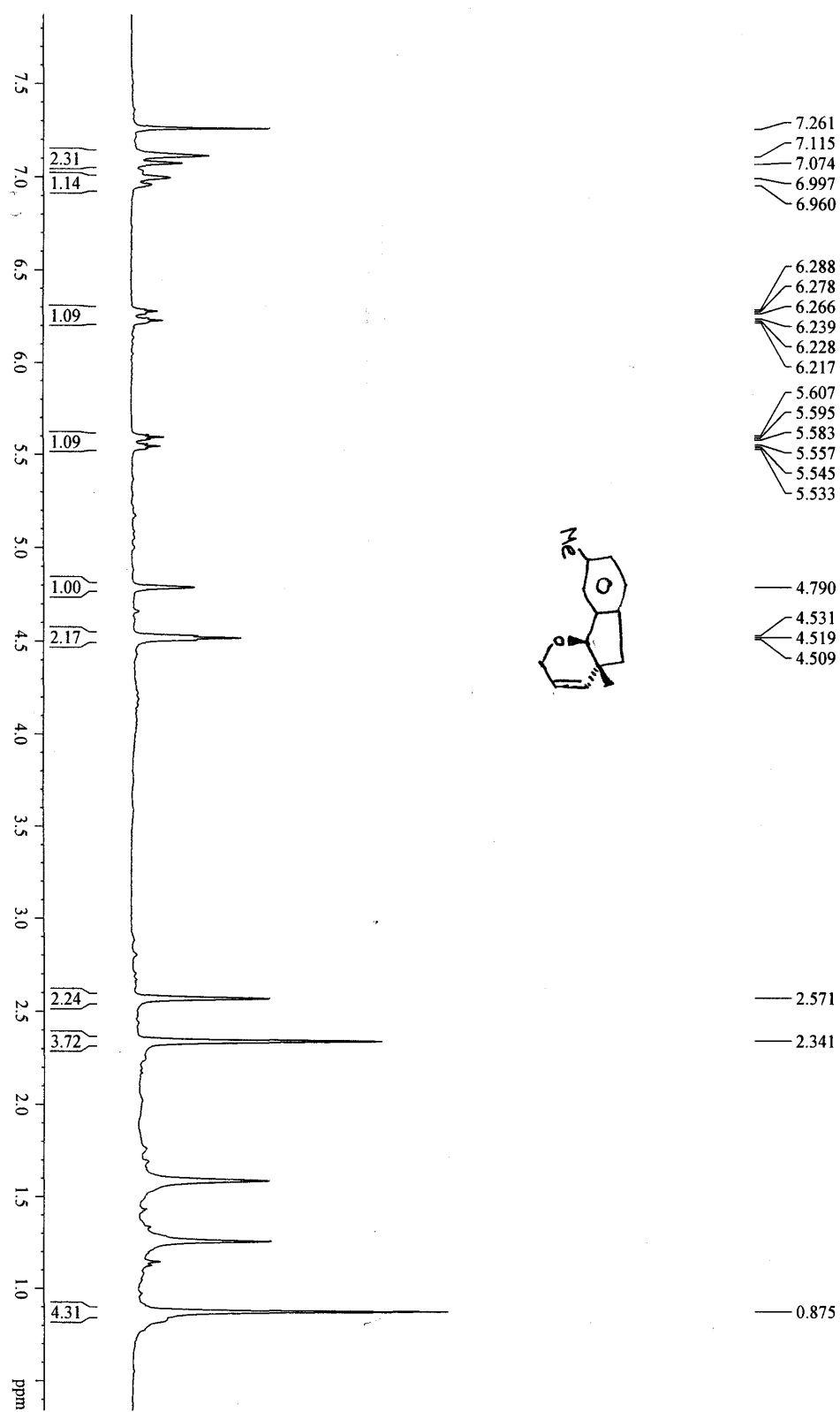
¹³C NMR of compound 60



DEPT 135 NMR of compound 60

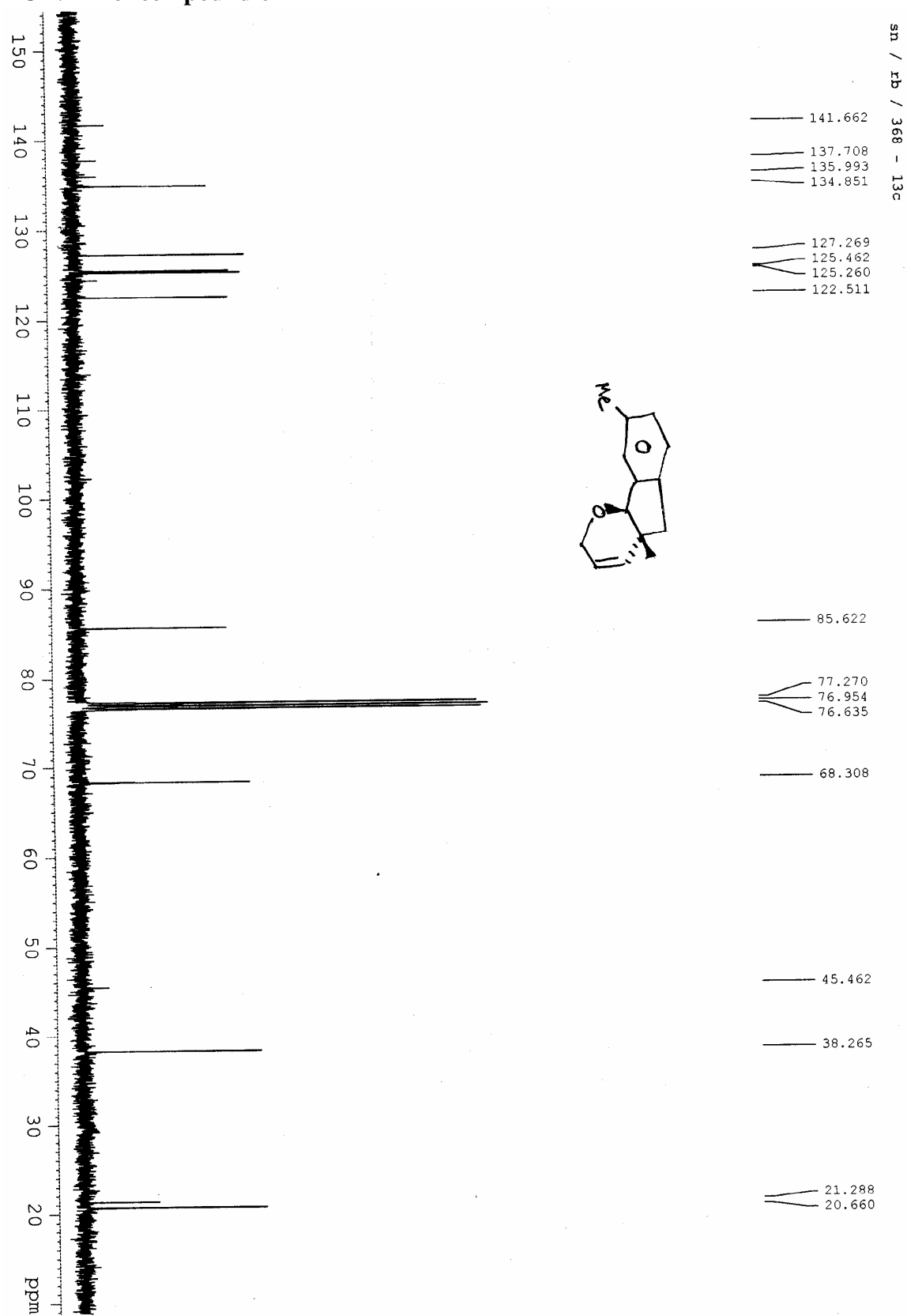


¹H NMR of compound 61

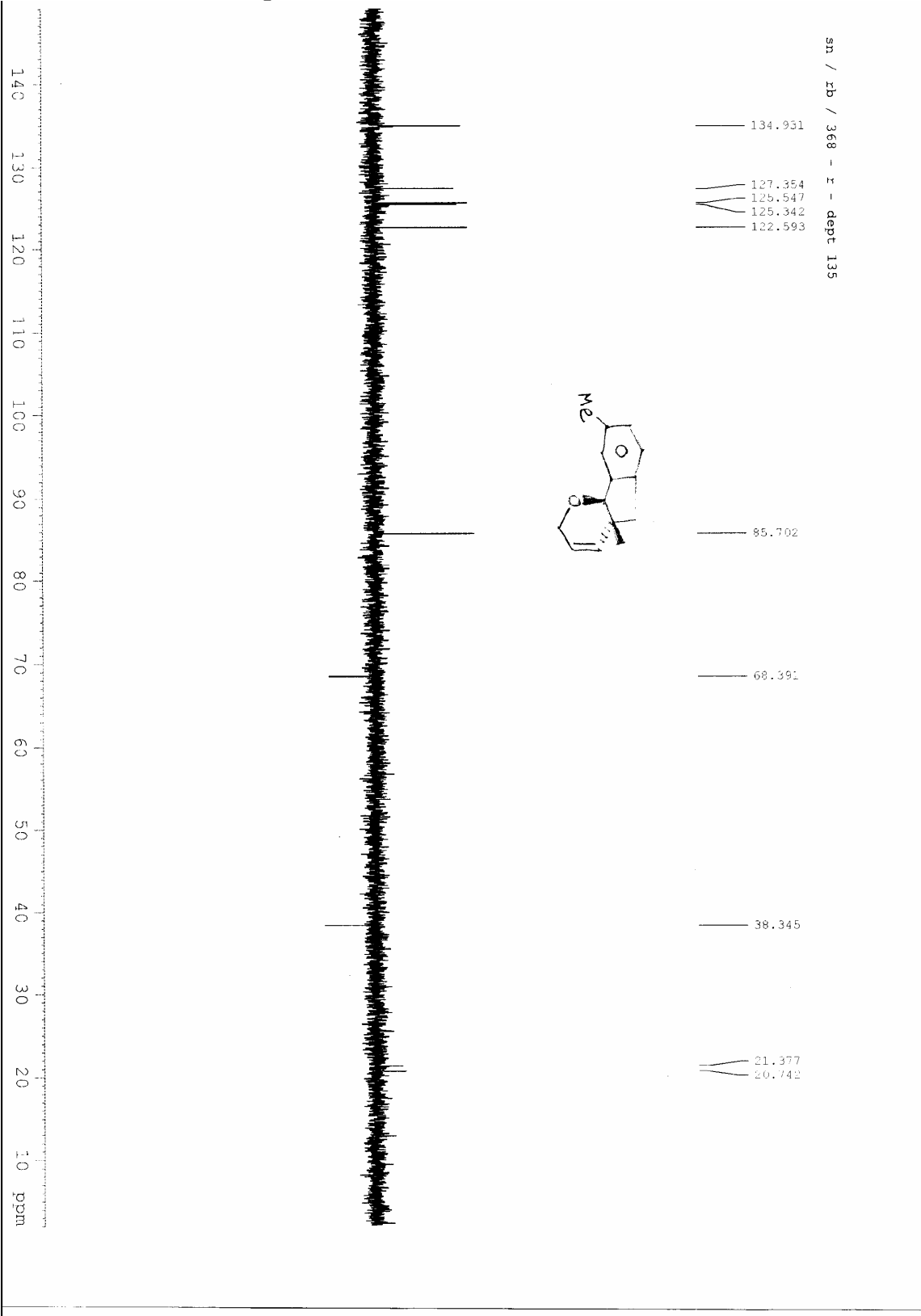


sn / rb / 368

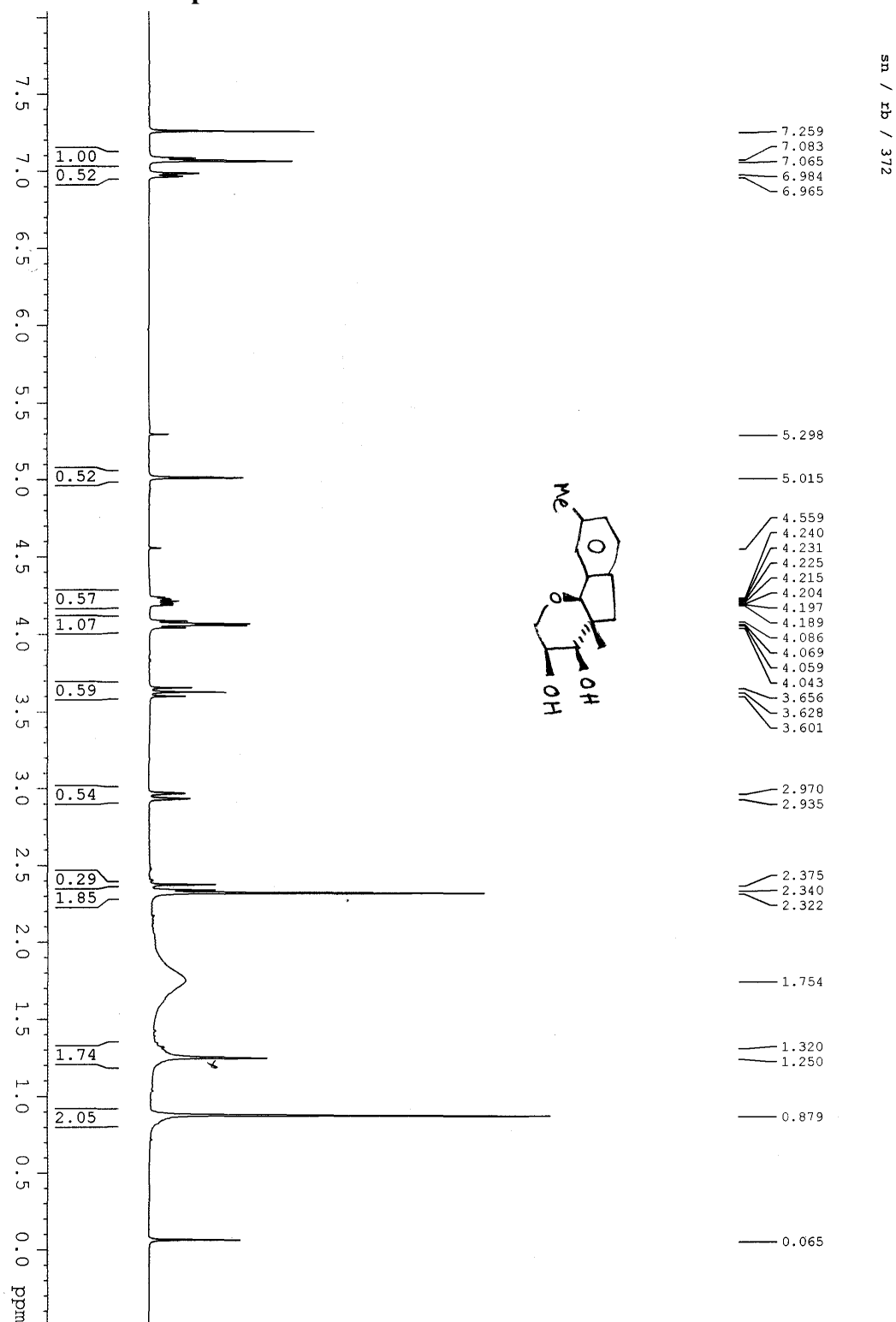
¹³C NMR of compound 61



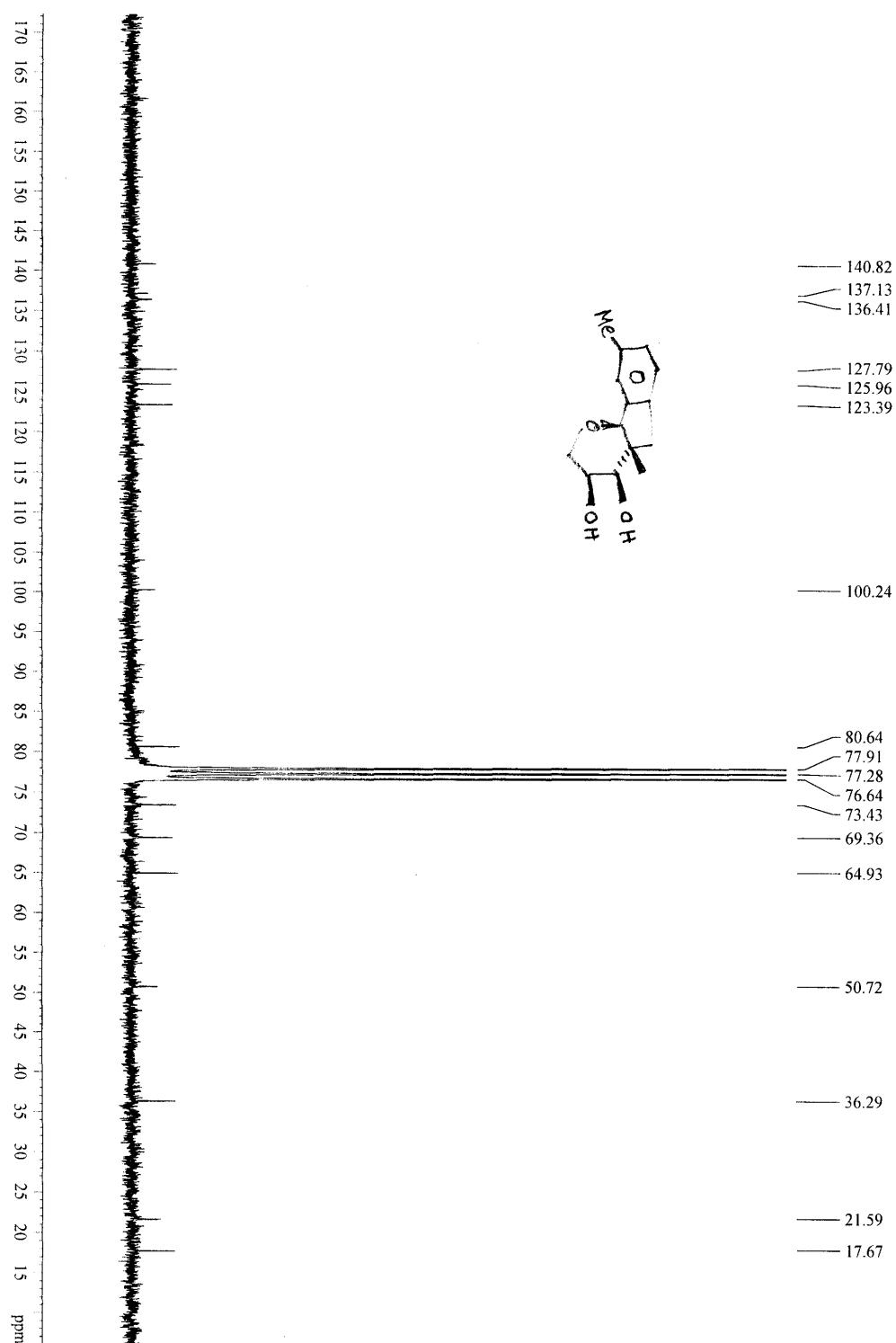
DEPT 135 NMR of compound 61



¹H NMR of compound 62

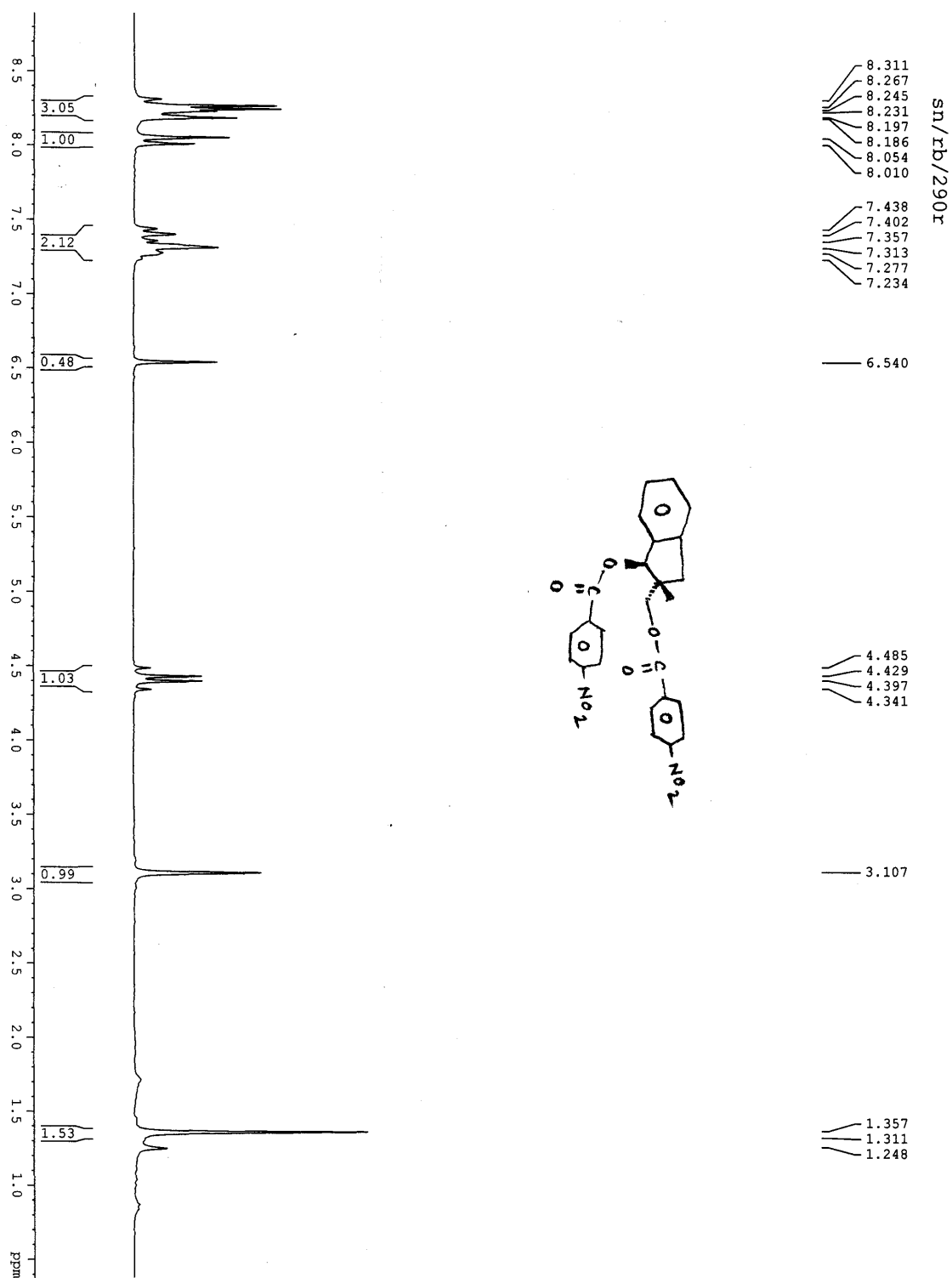


¹³C NMR of compound 62



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

¹H NMR of bis PNBz derivative of 27



¹³C NMR of bis PNBz derivative of 27

