

Chemoselective and metal-free reduction of α,β -unsaturated ketones by in-situ produced benzeneselenol from O-(tert-Butyl) Se-phenyl selenocarbonate

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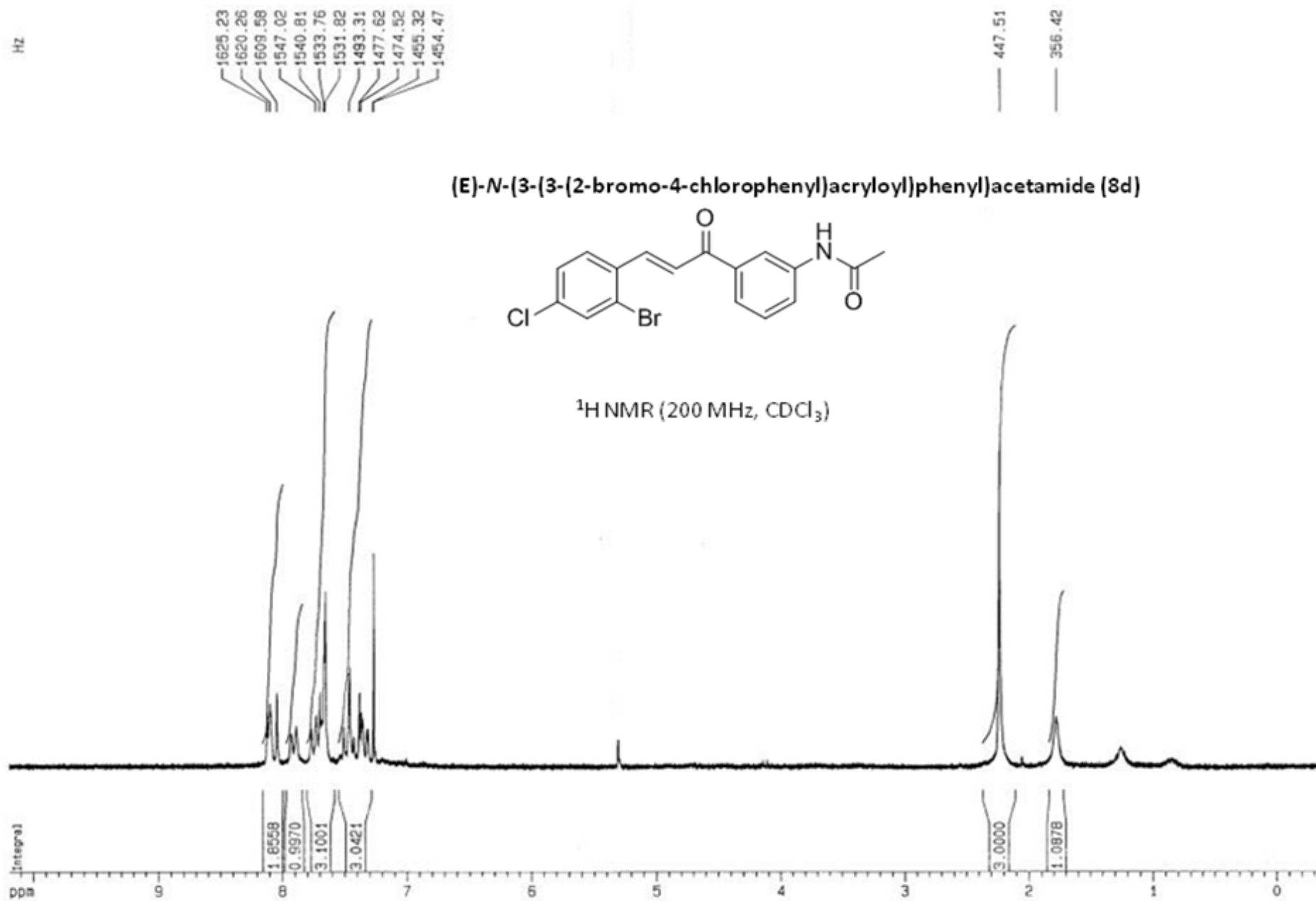
** Corresponding author e-mail: andrea.temperini@unipg.it*

Supporting Information

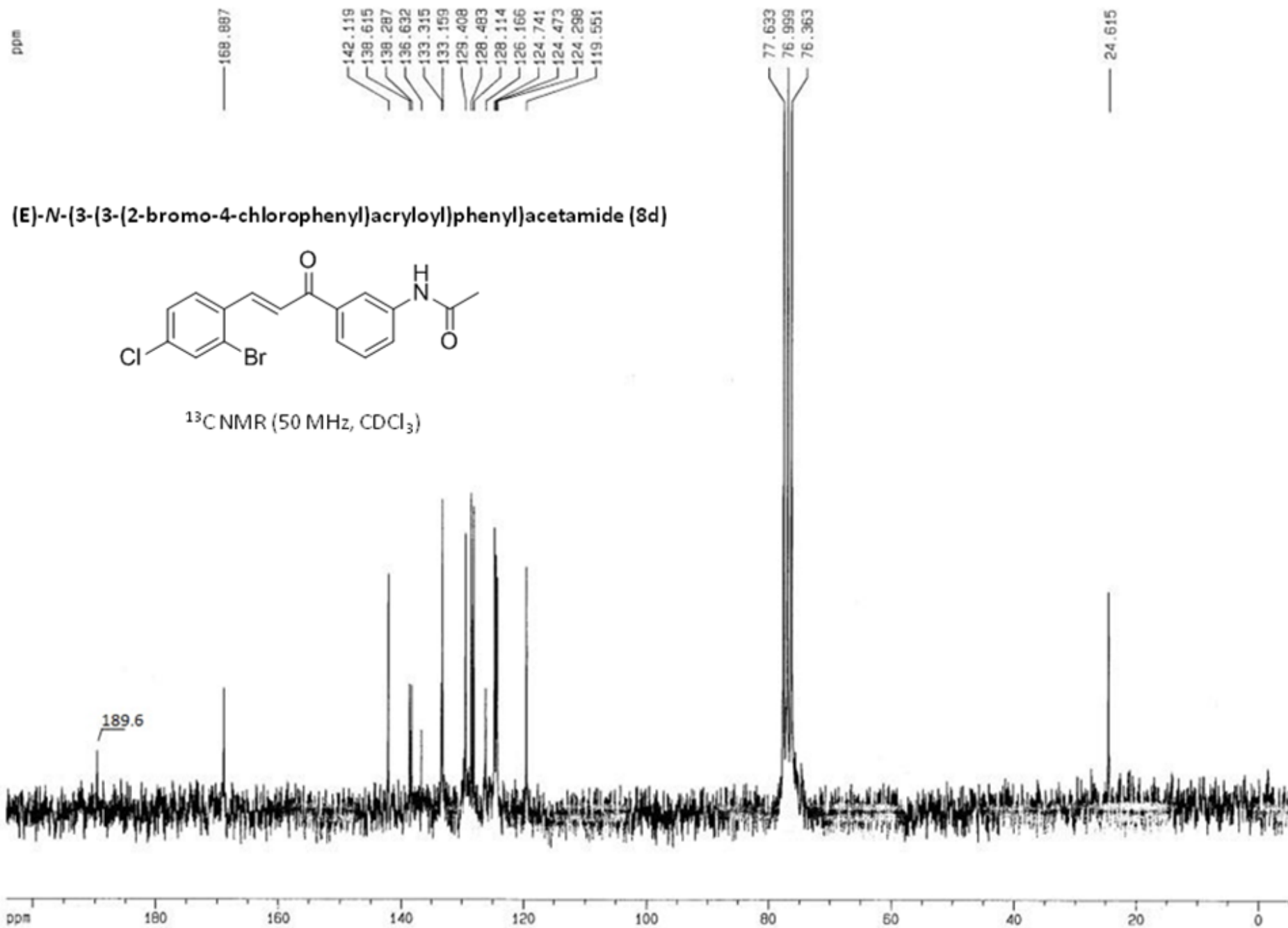
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NMR Spectra of compounds 15, 16 and 17	SI	48

SI 3

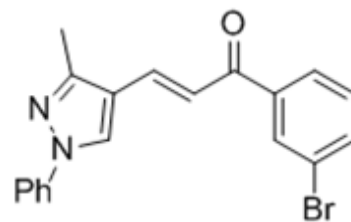


SI 4



SI 5

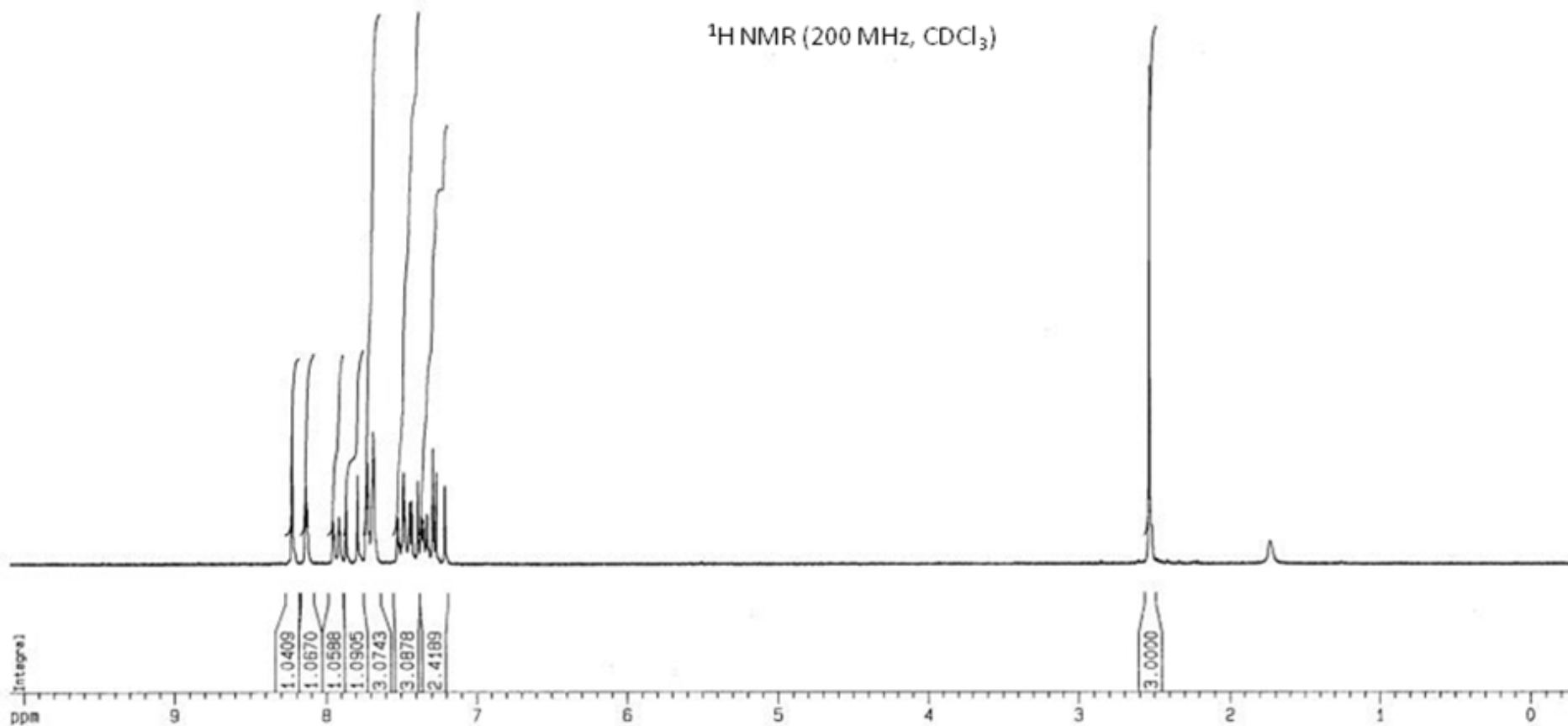
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7.86624
7.78806
7.73064
7.72619
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7.69627
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7.66265
7.46233
7.44200
7.42905
7.36957
7.29005
7.26780
7.21175



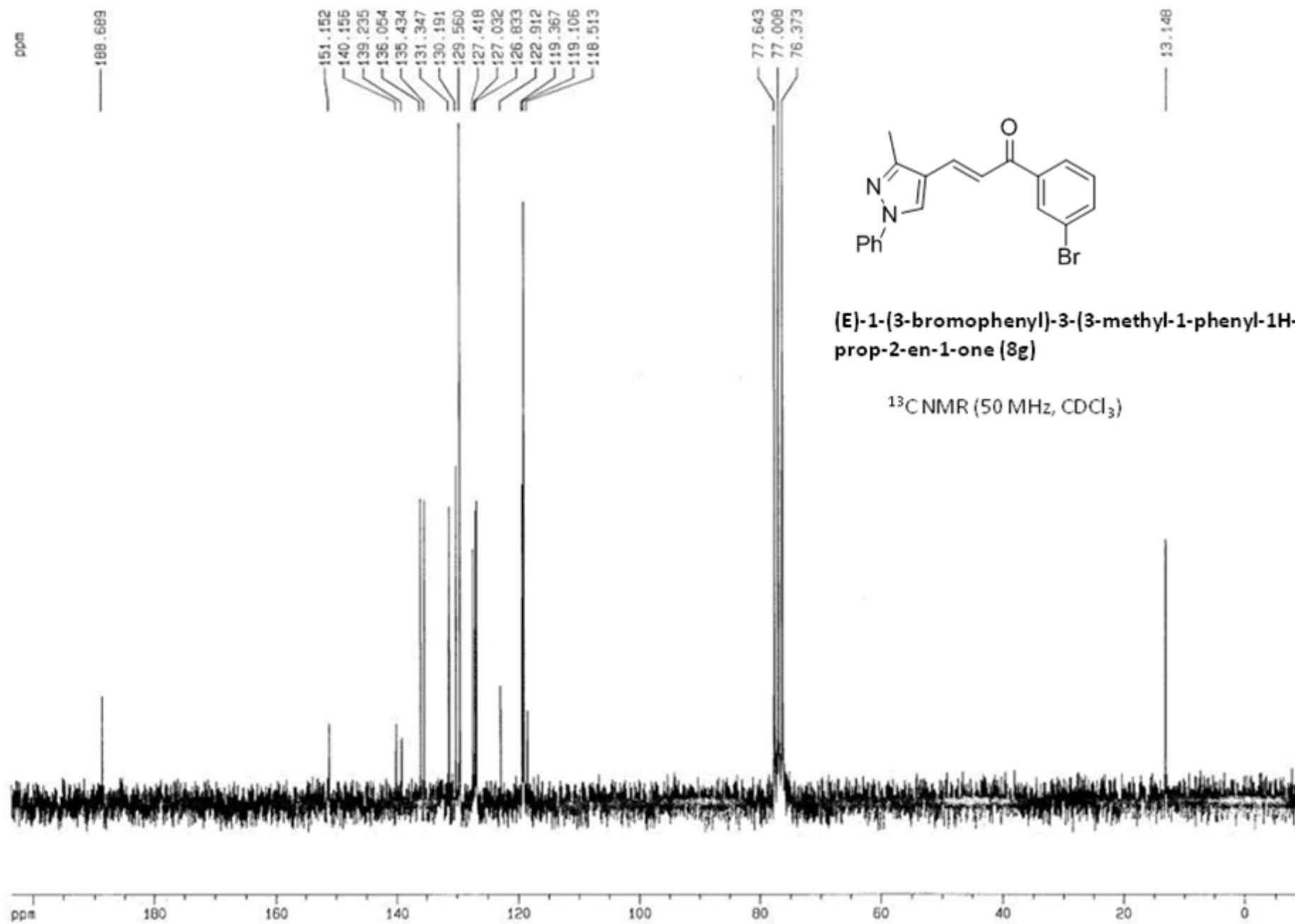
2.53559

(E)-1-(3-bromophenyl)-3-(3-methyl-1-phenyl-1H-pyrazol-4-yl)prop-2-en-1-one (8g)

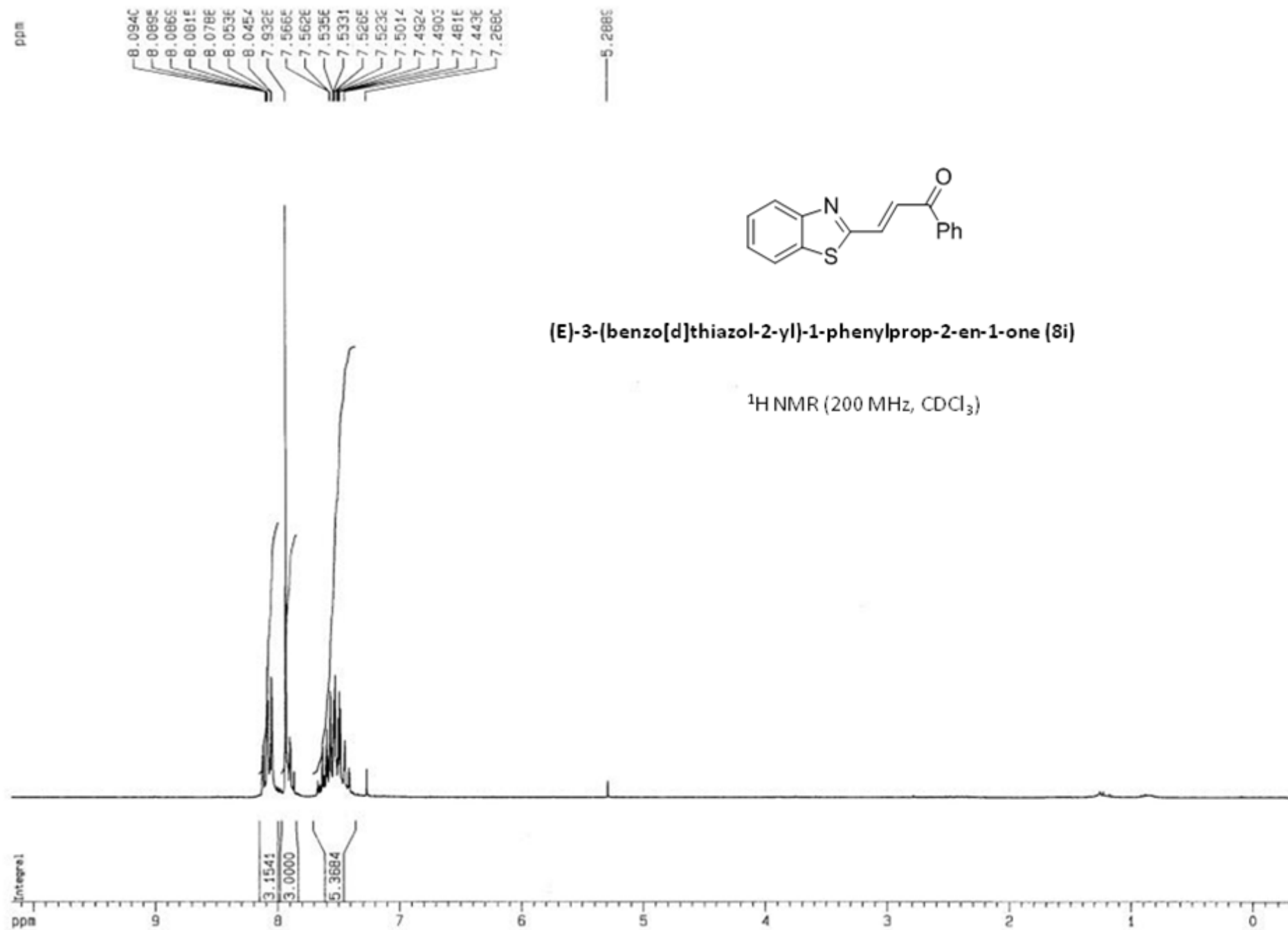
$^1\text{H NMR}$ (200 MHz, CDCl_3)



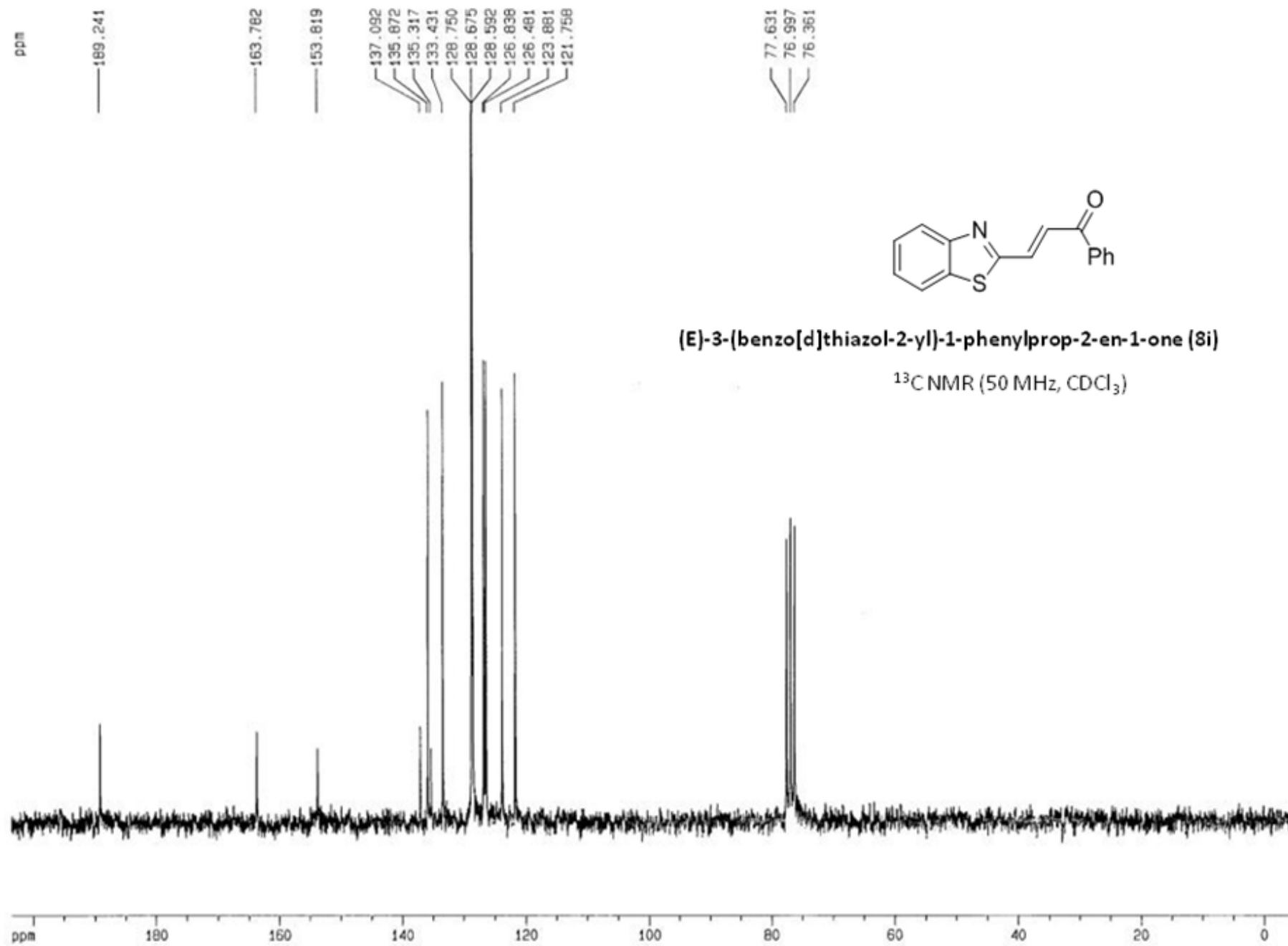
SI 6



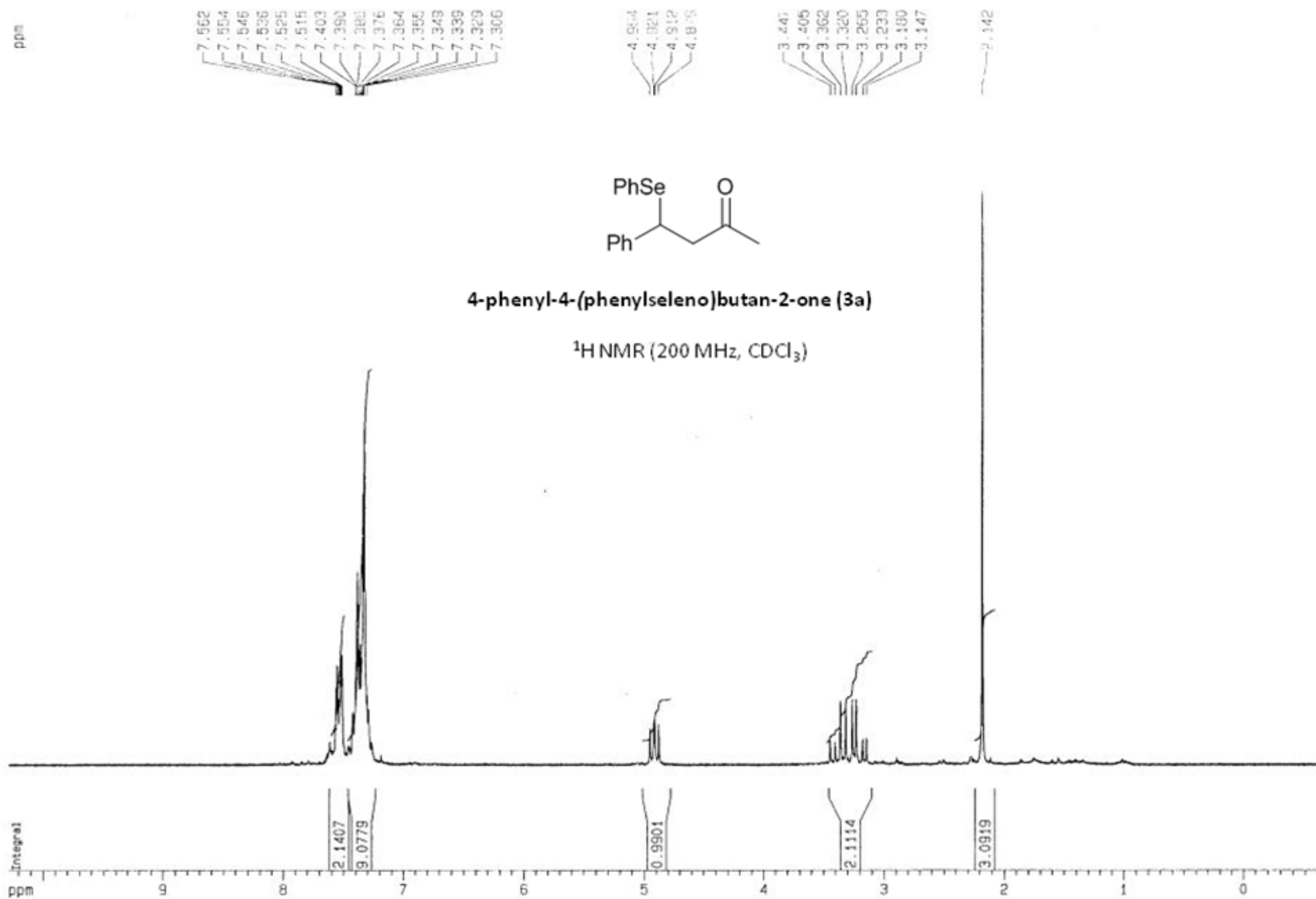
SI 7



SI 8



SI 9

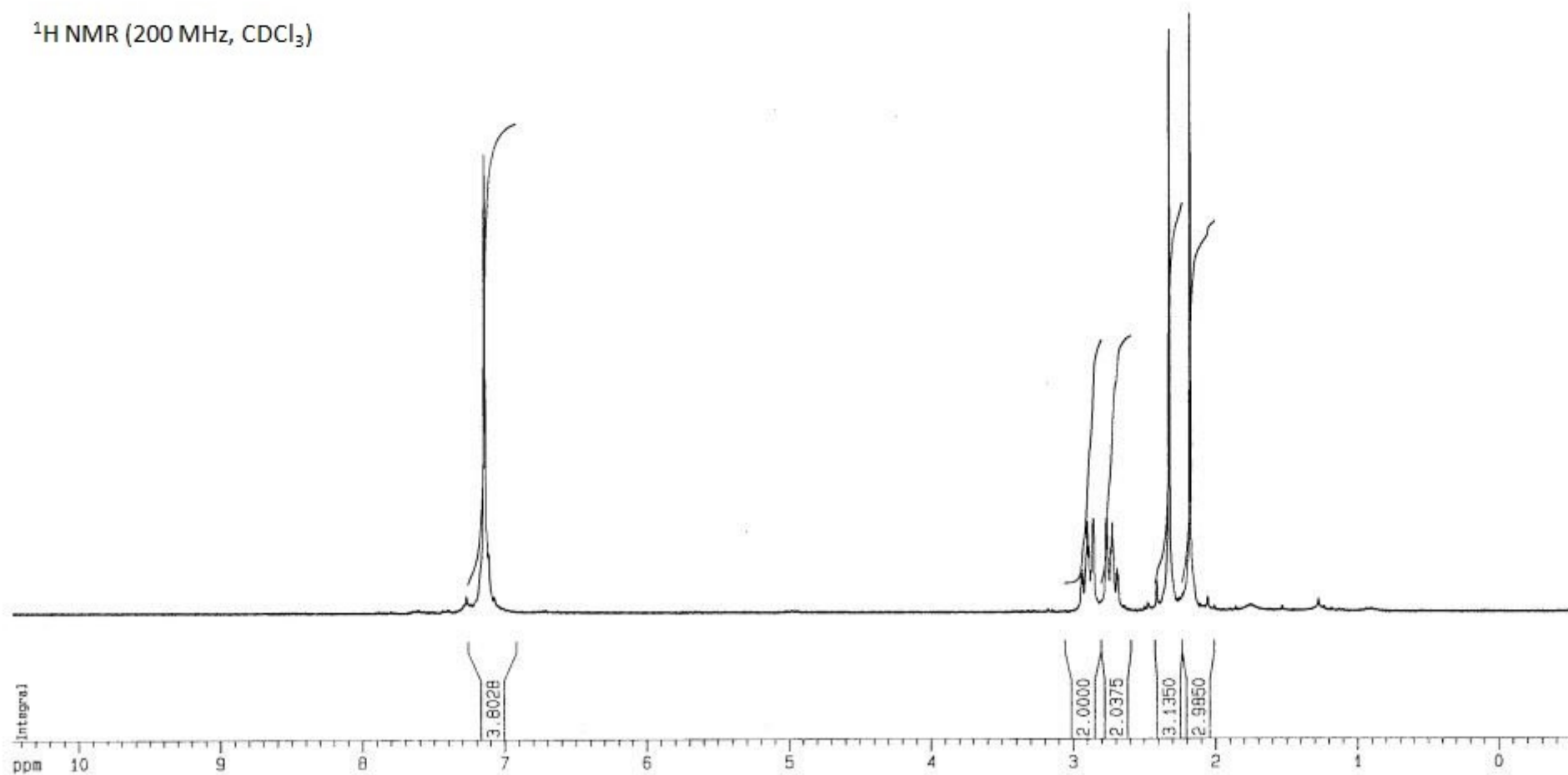


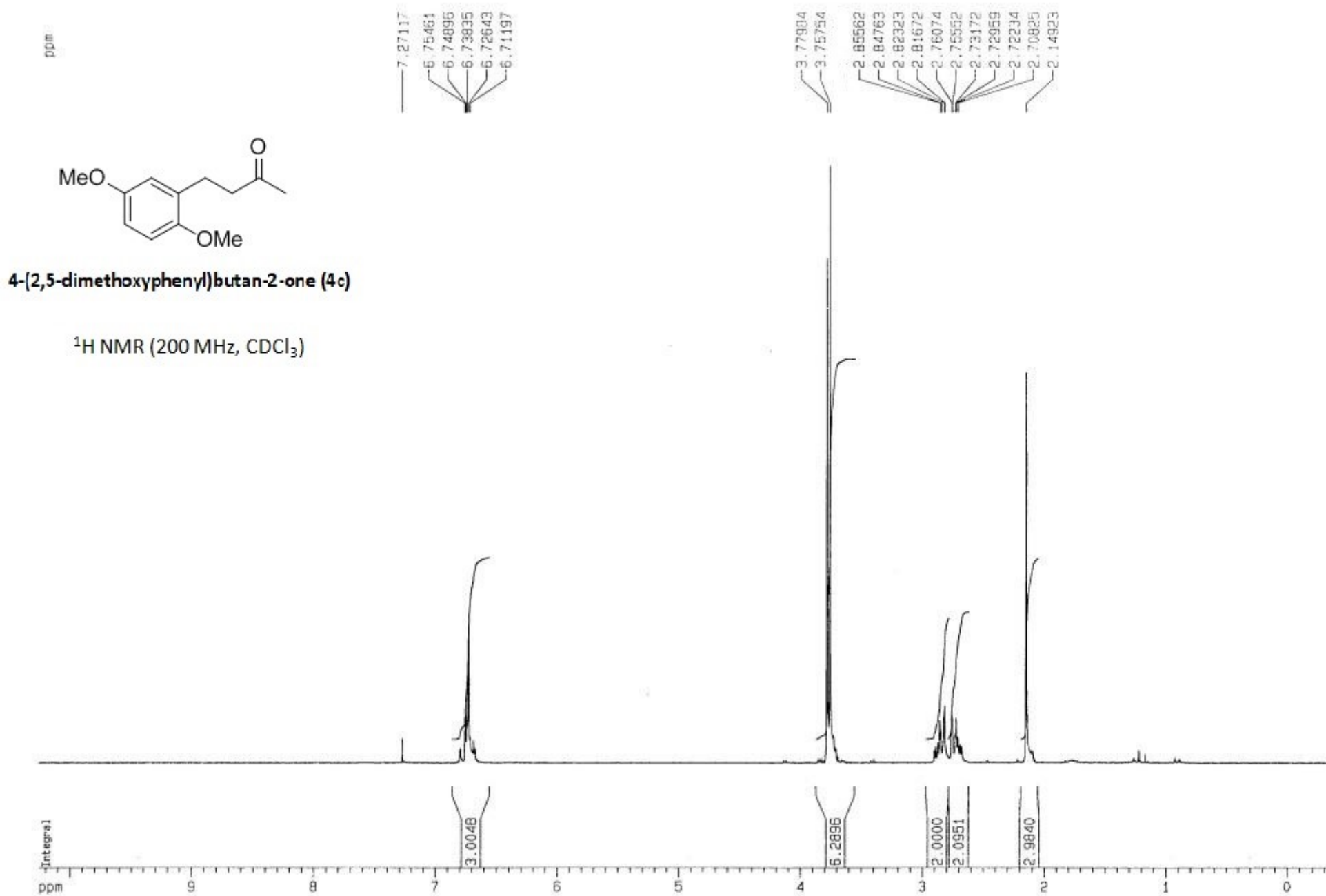
SI 10



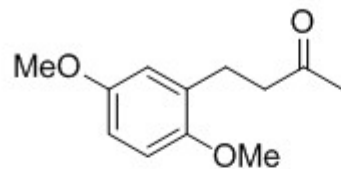
4-(2-methylphenyl)butan-2-one (4b)

^1H NMR (200 MHz, CDCl_3)





SI 12

ppm
208.590153.319
151.592

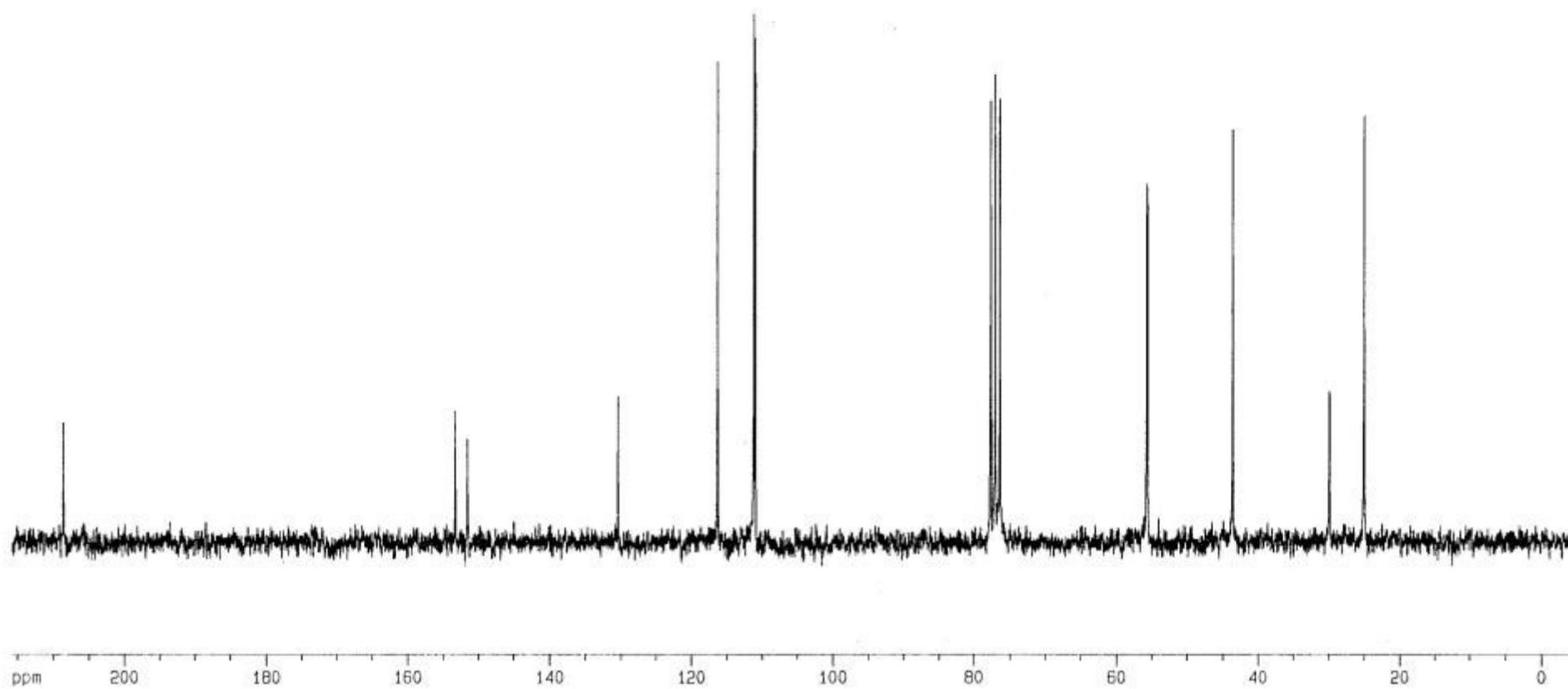
130.383

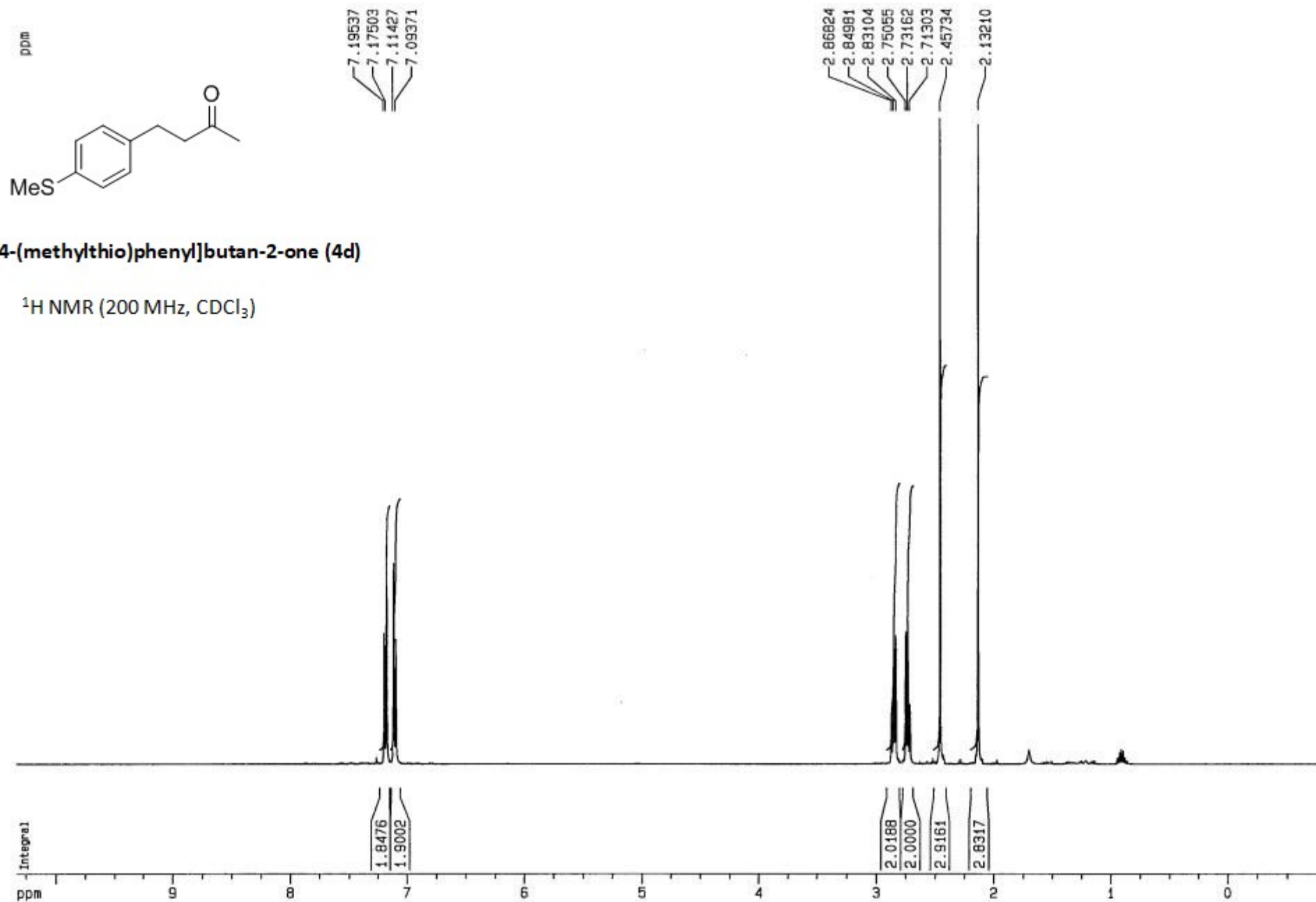
116.270
111.201
110.99777.634
76.999
76.36555.695
55.597

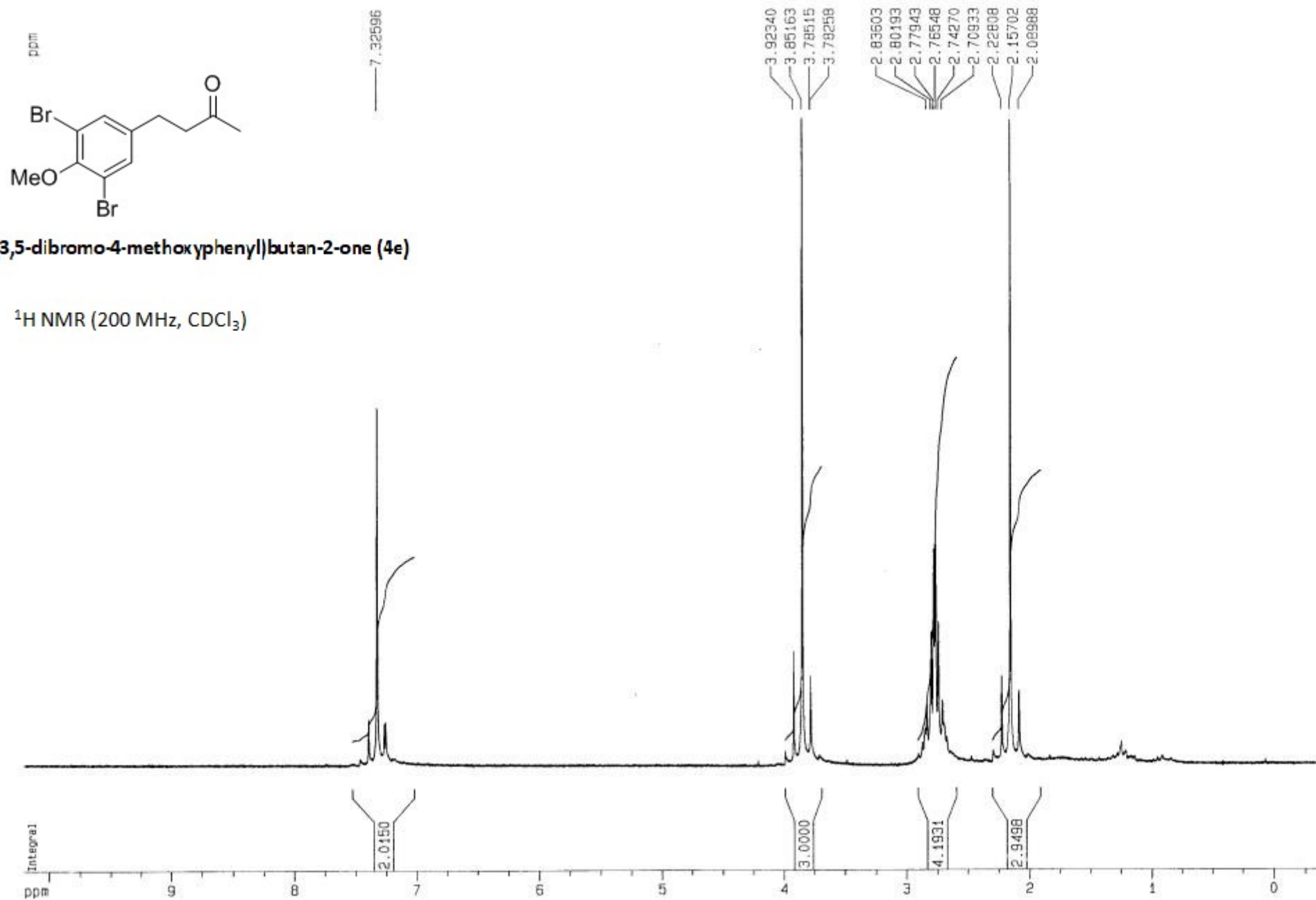
43.623

29.673
25.064

4-(2,5-dimethoxyphenyl)butan-2-one (4c)

 ^{13}C NMR (50 MHz, CDCl_3)

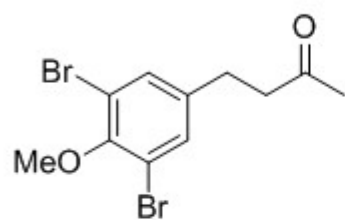




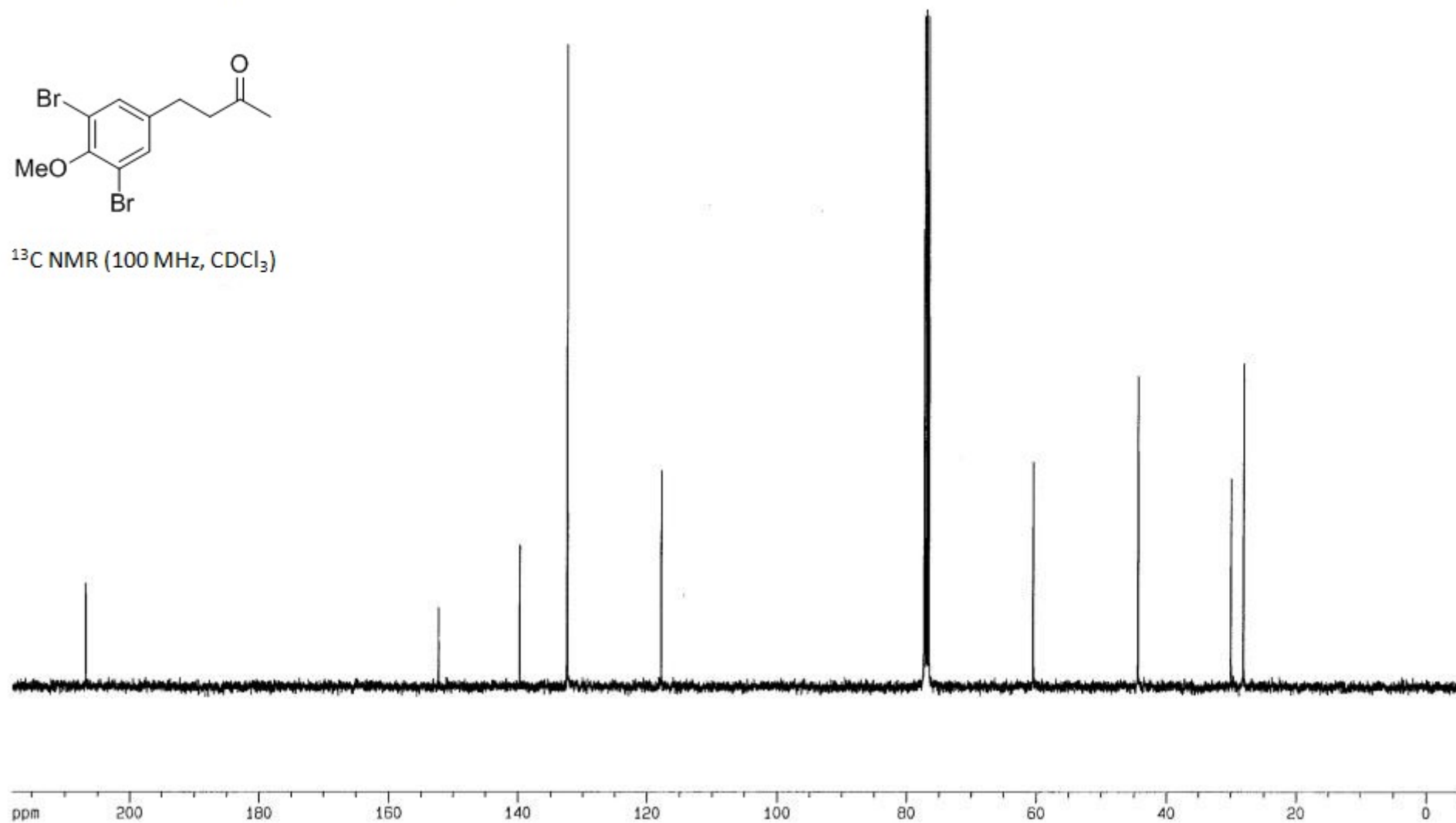
SI 15

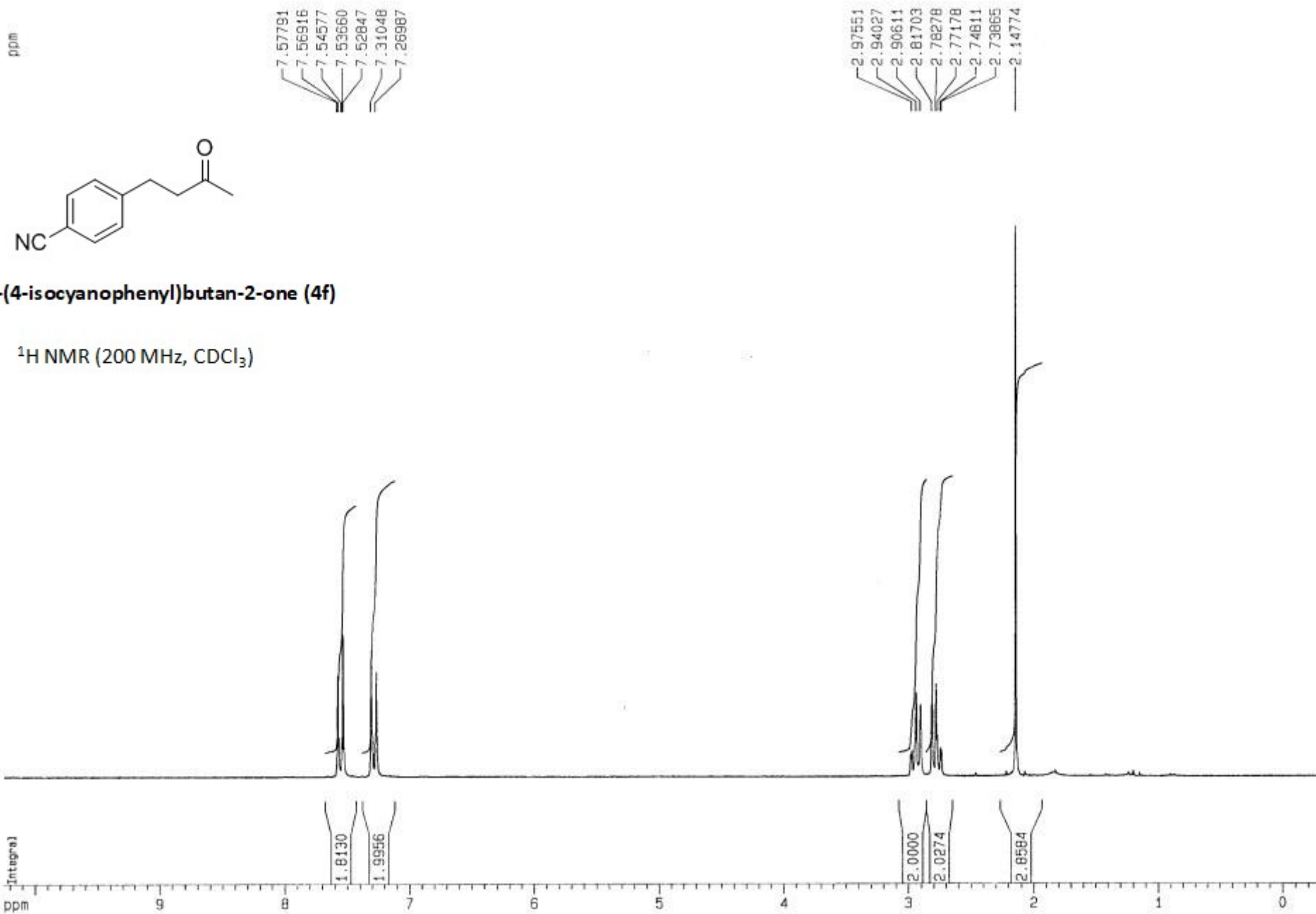


4-(3,5-dibromo-4-methoxyphenyl)butan-2-one (4e)

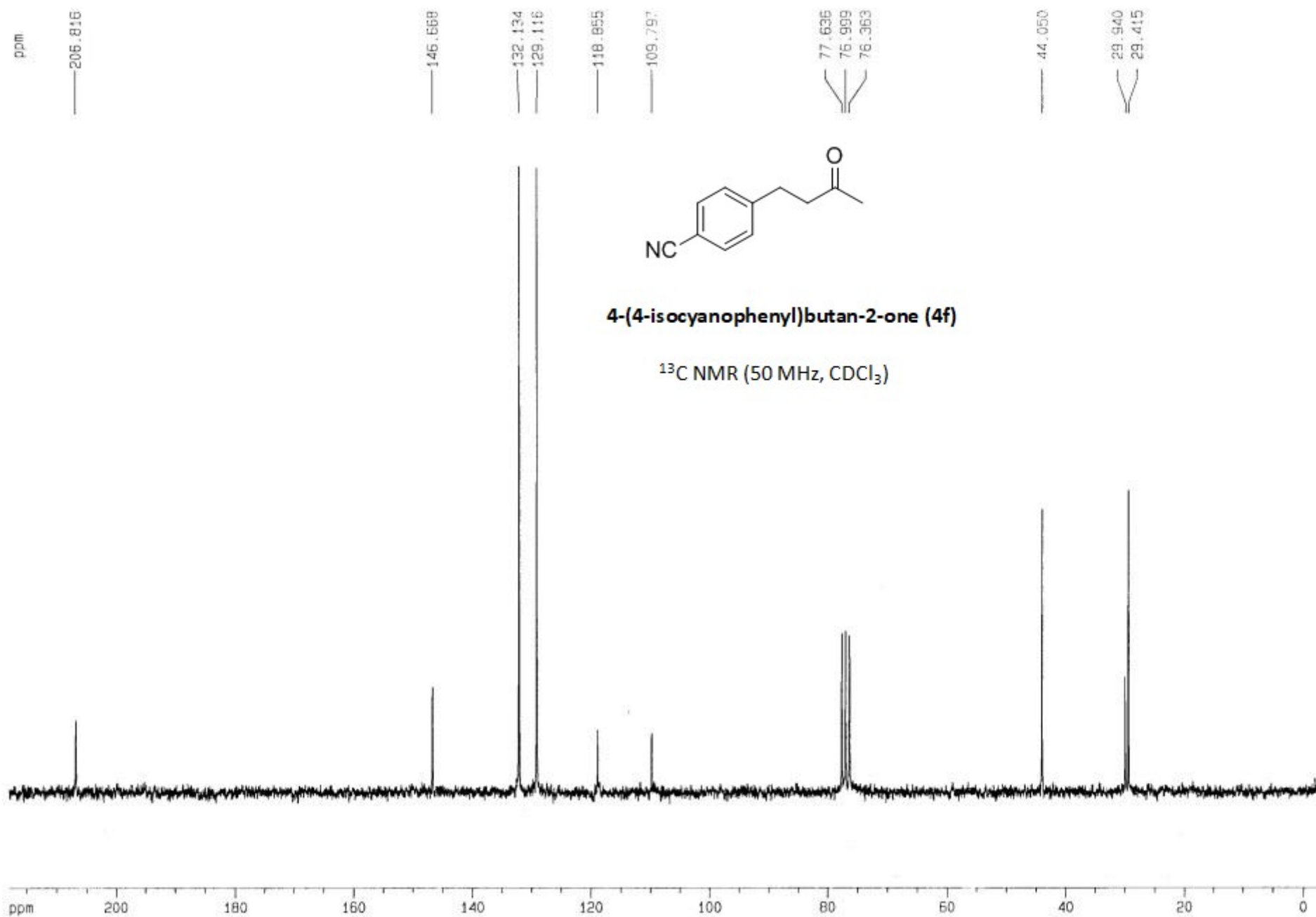


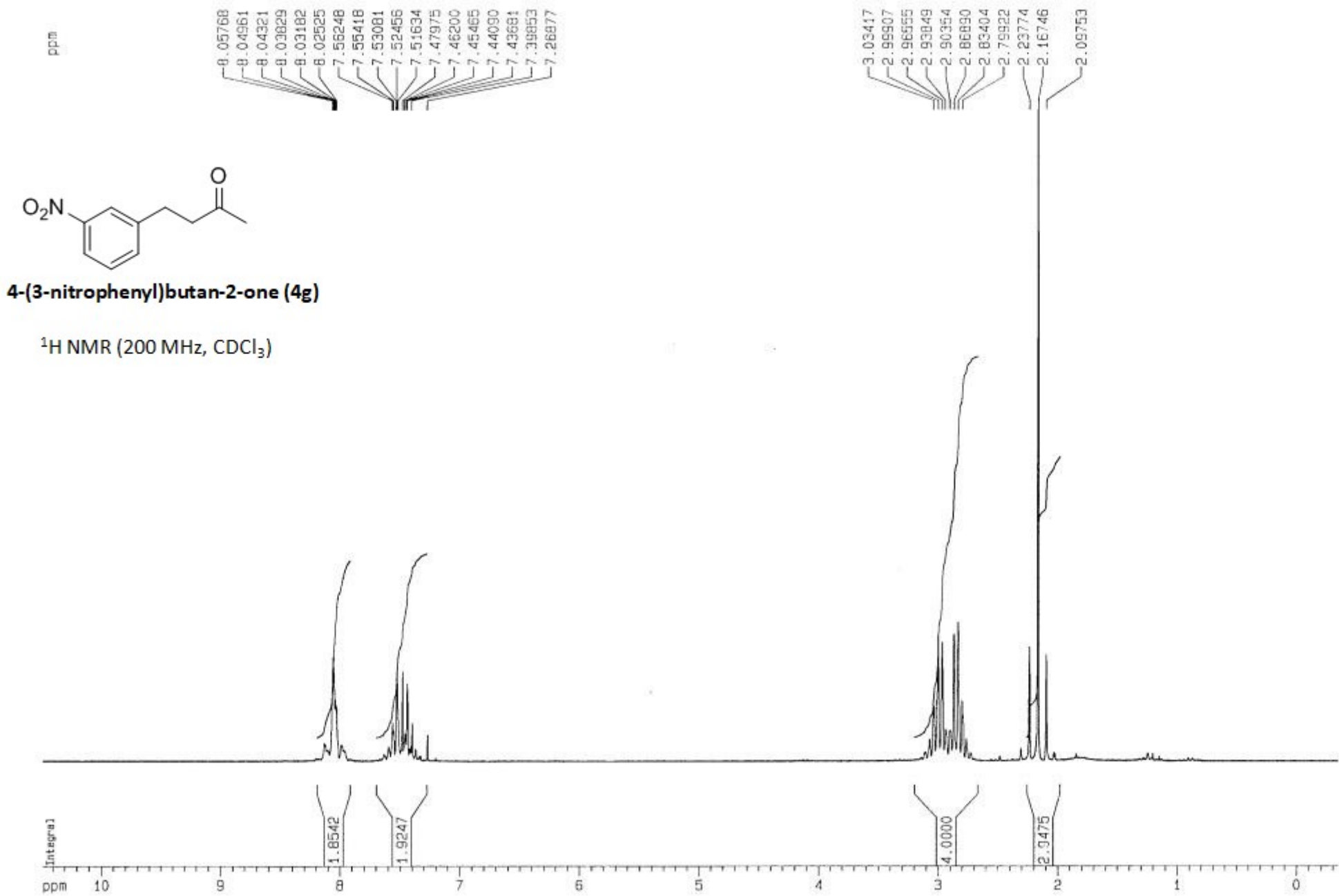
^{13}C NMR (100 MHz, CDCl_3)

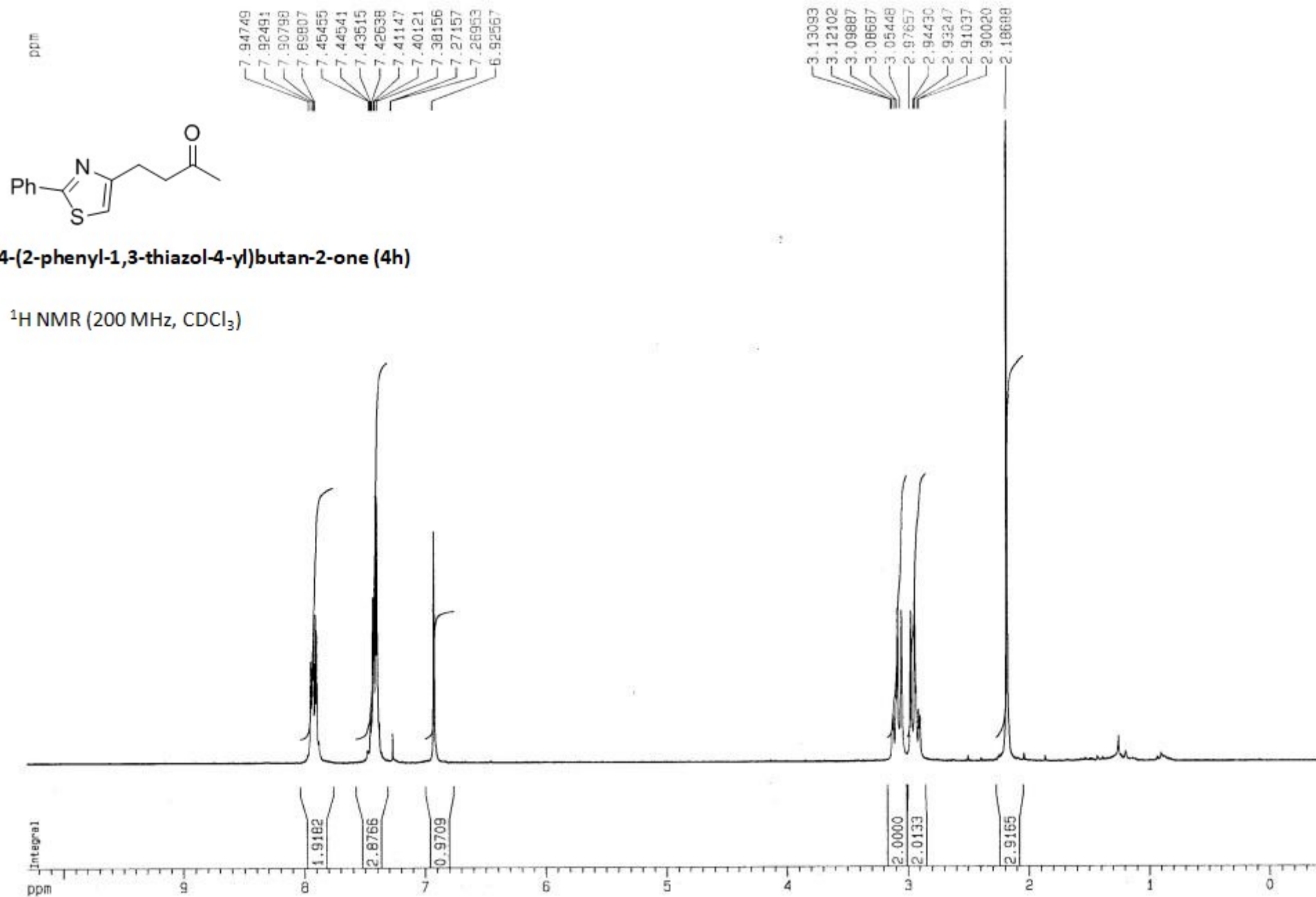




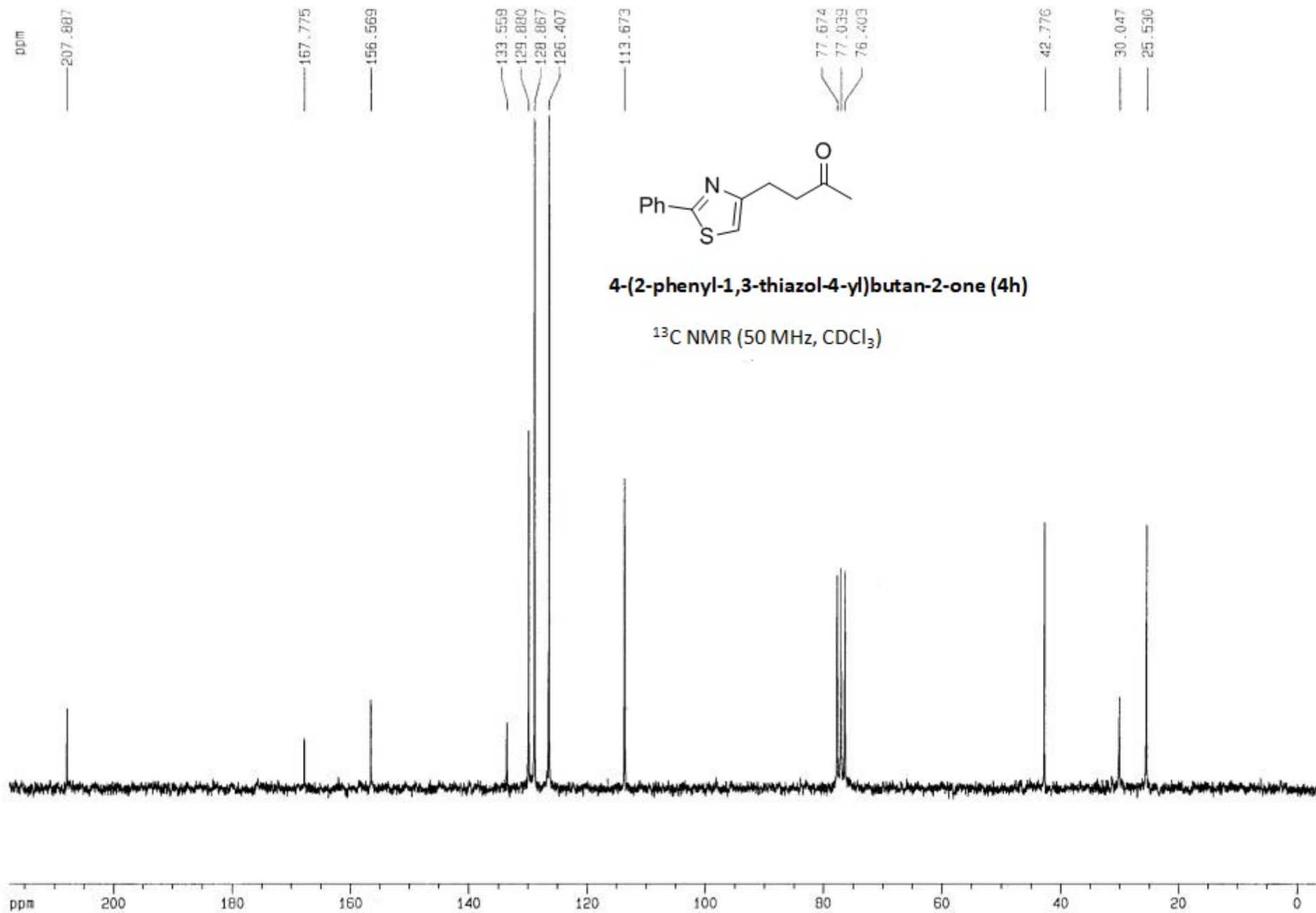
SI 17

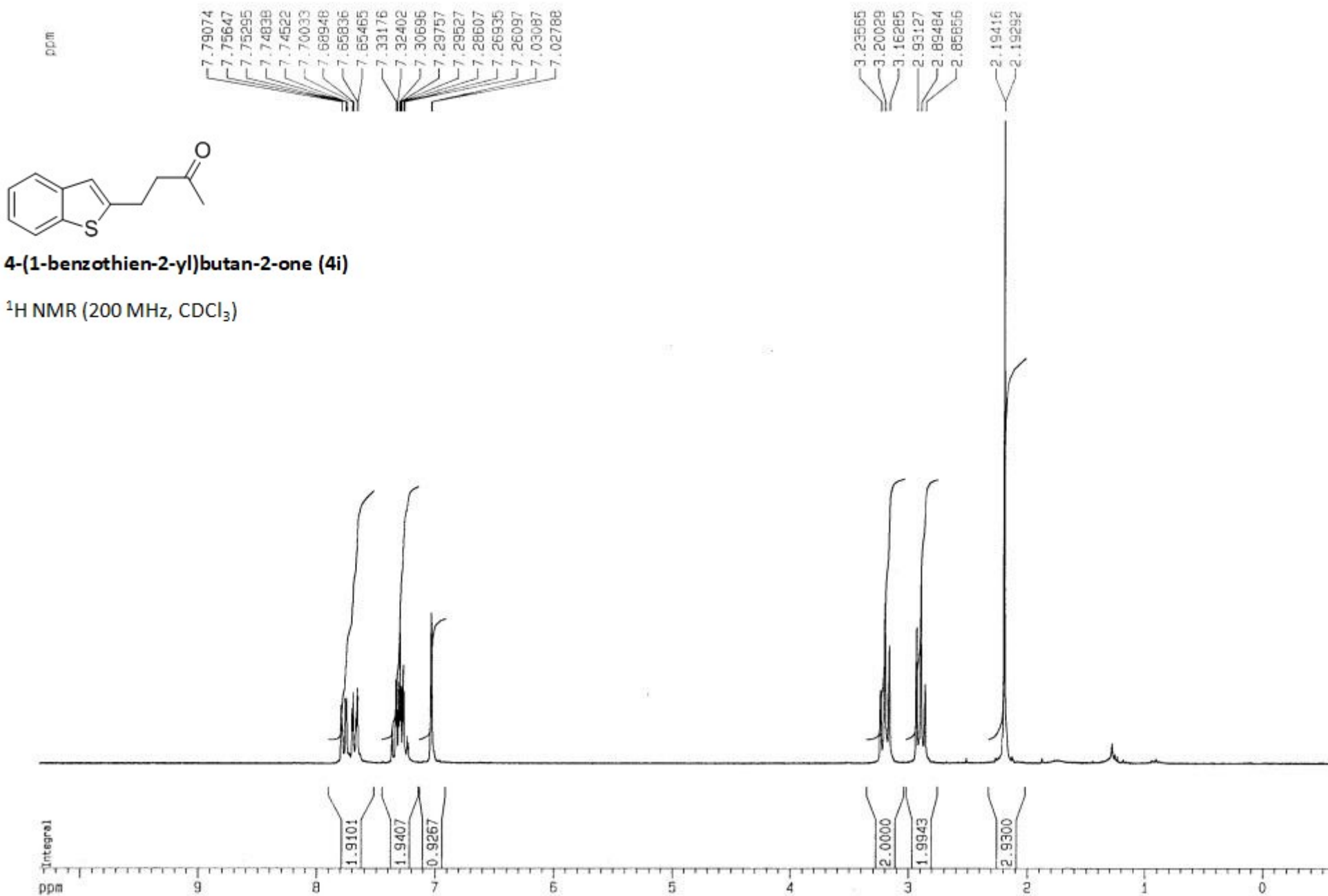




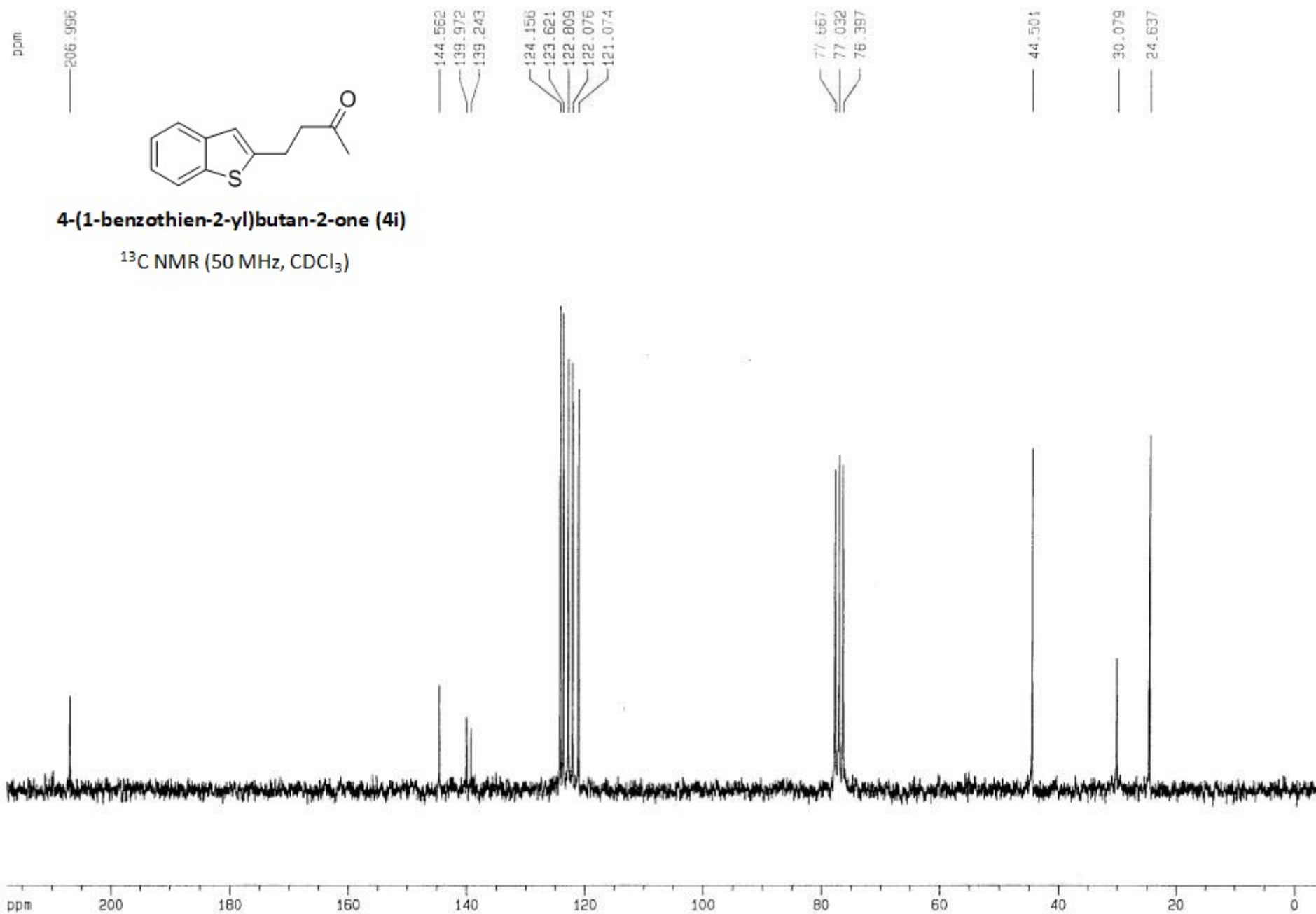


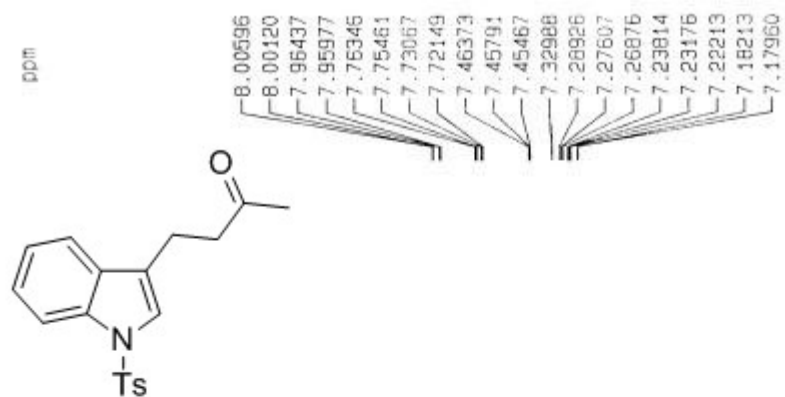
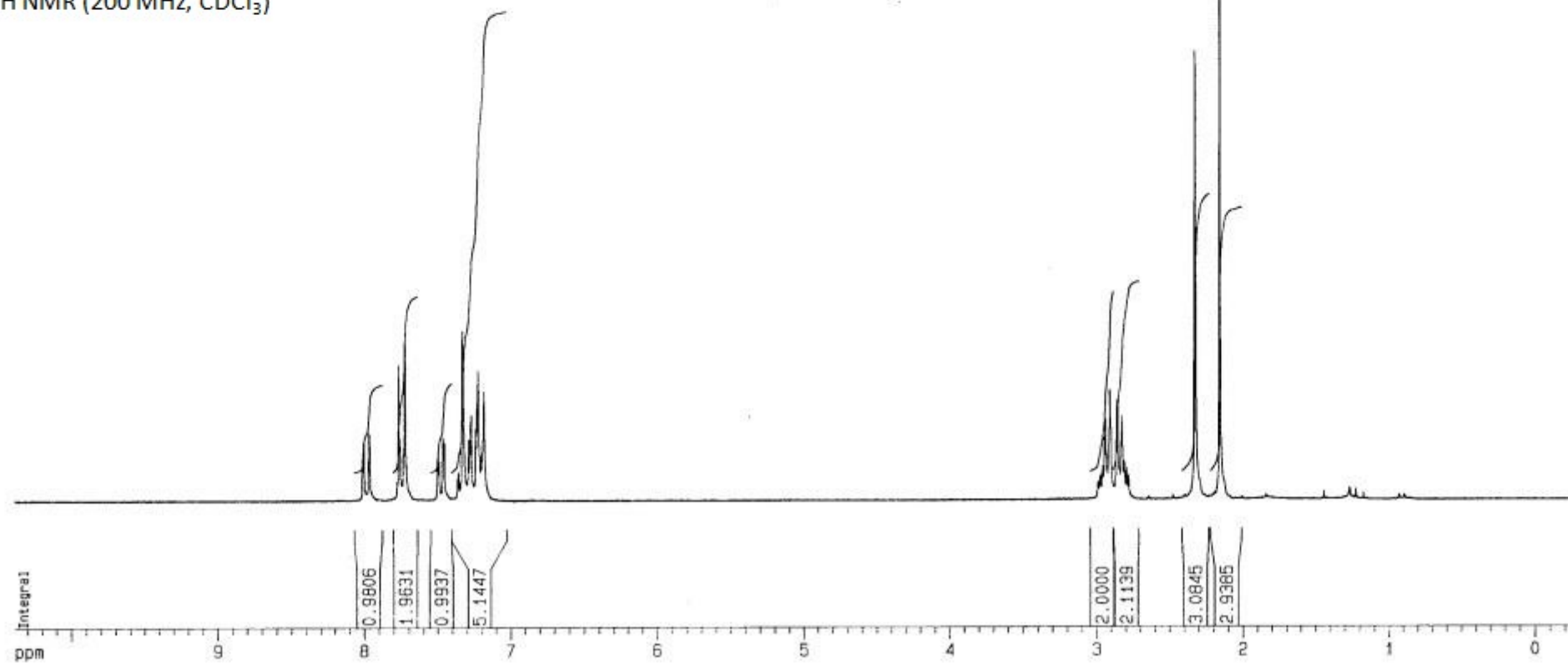
SI 20



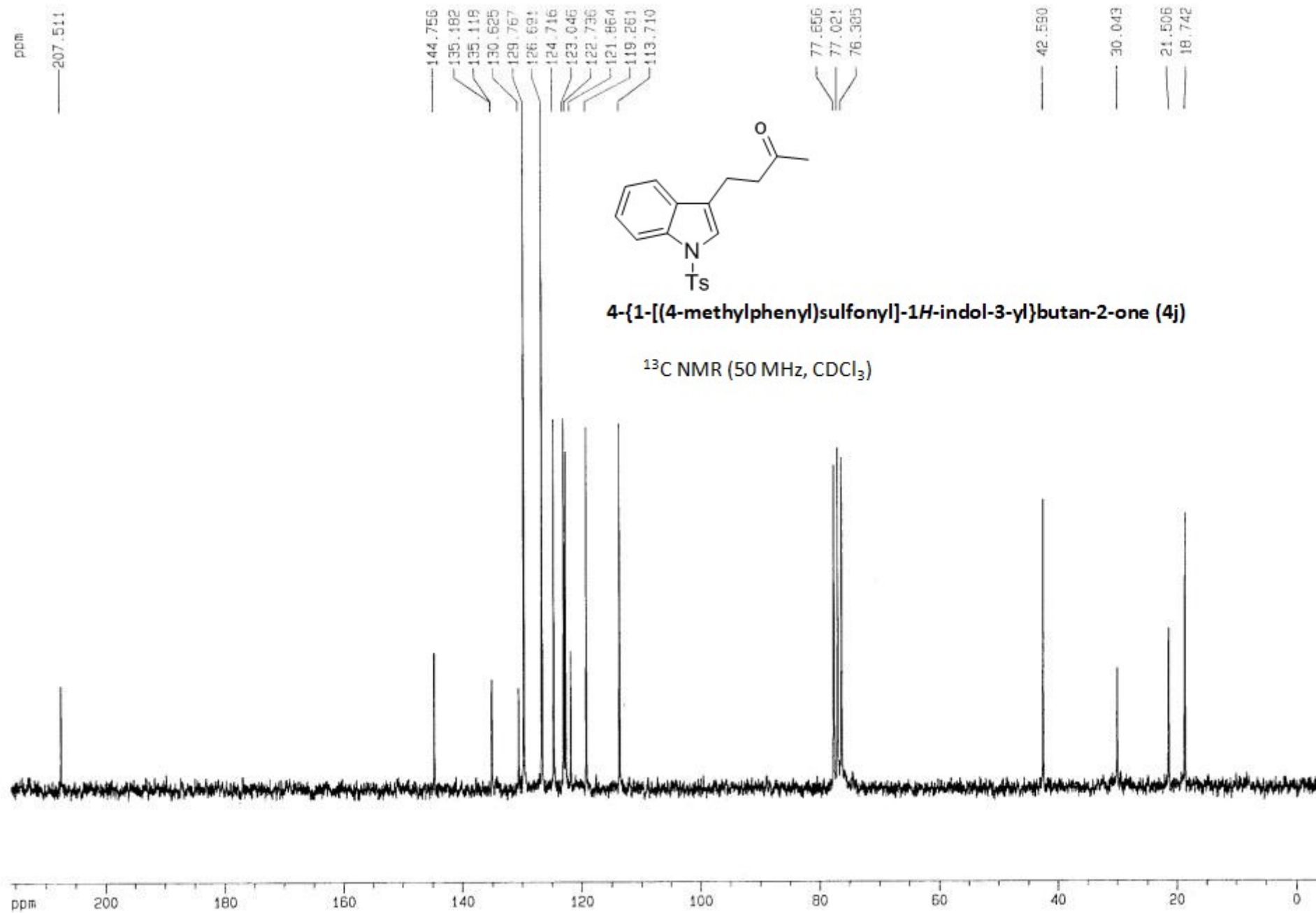


SI 22

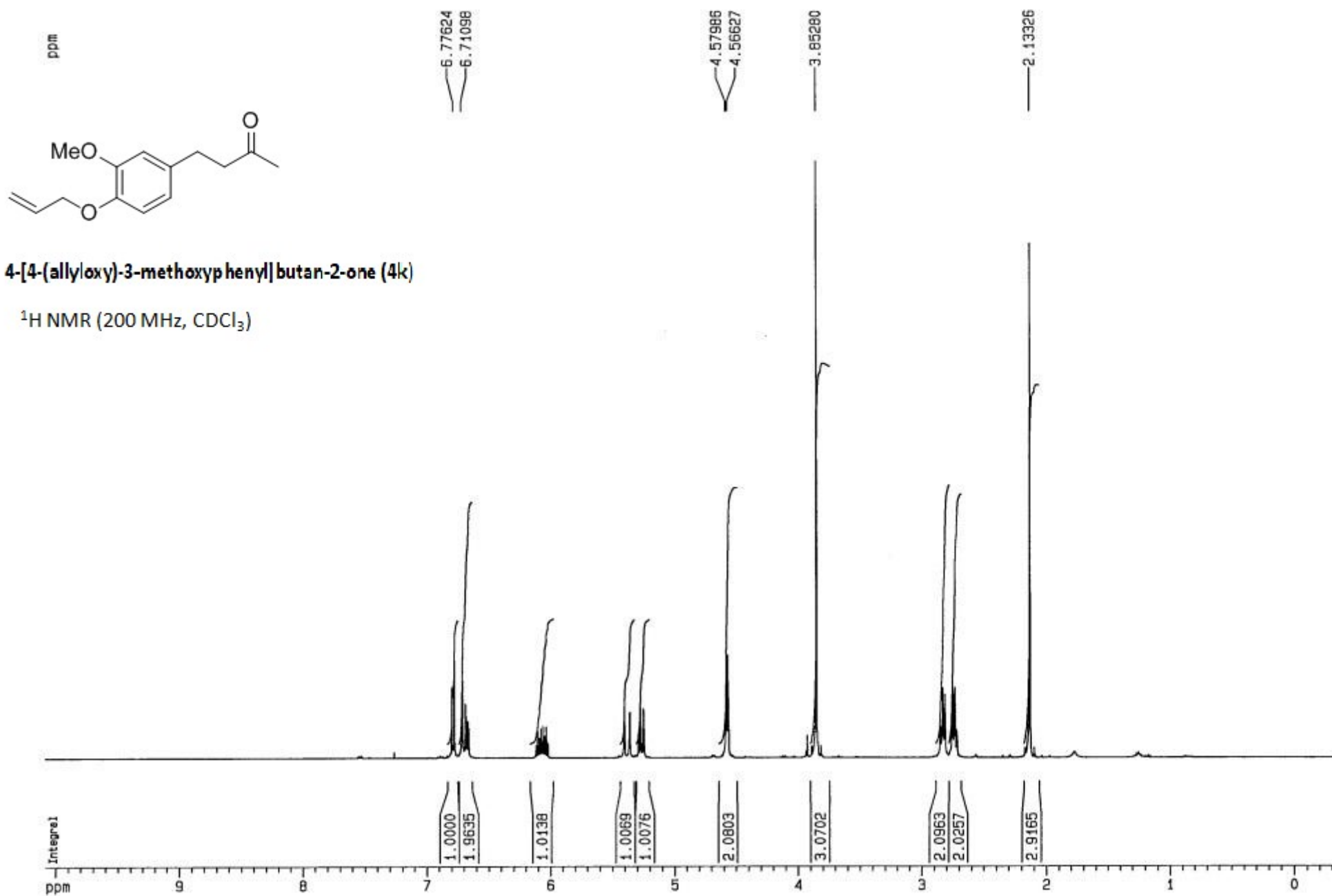


**4-{1-[(4-methylphenyl)sulfonyl]-1*H*-indol-3-yl}butan-2-one (4j)**¹H NMR (200 MHz, CDCl₃)

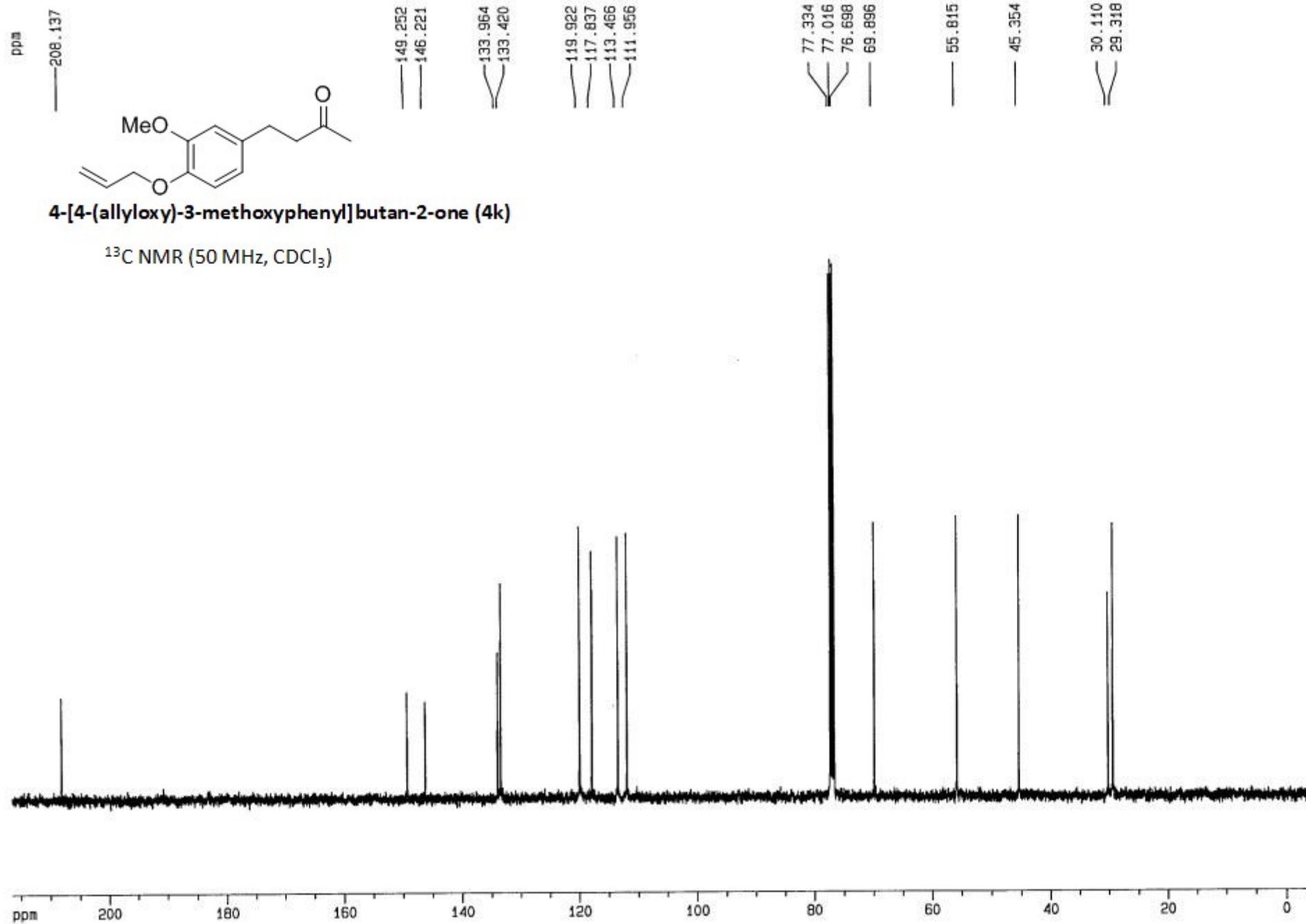
SI 24



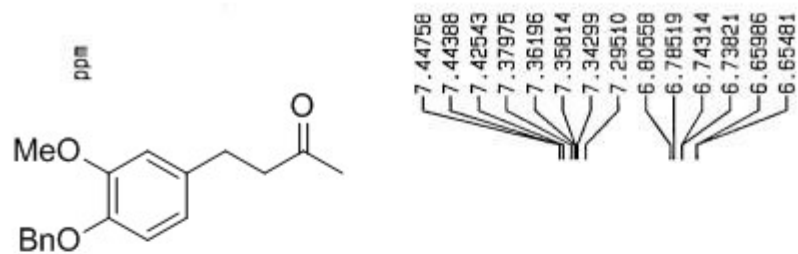
SI 25



SI 26

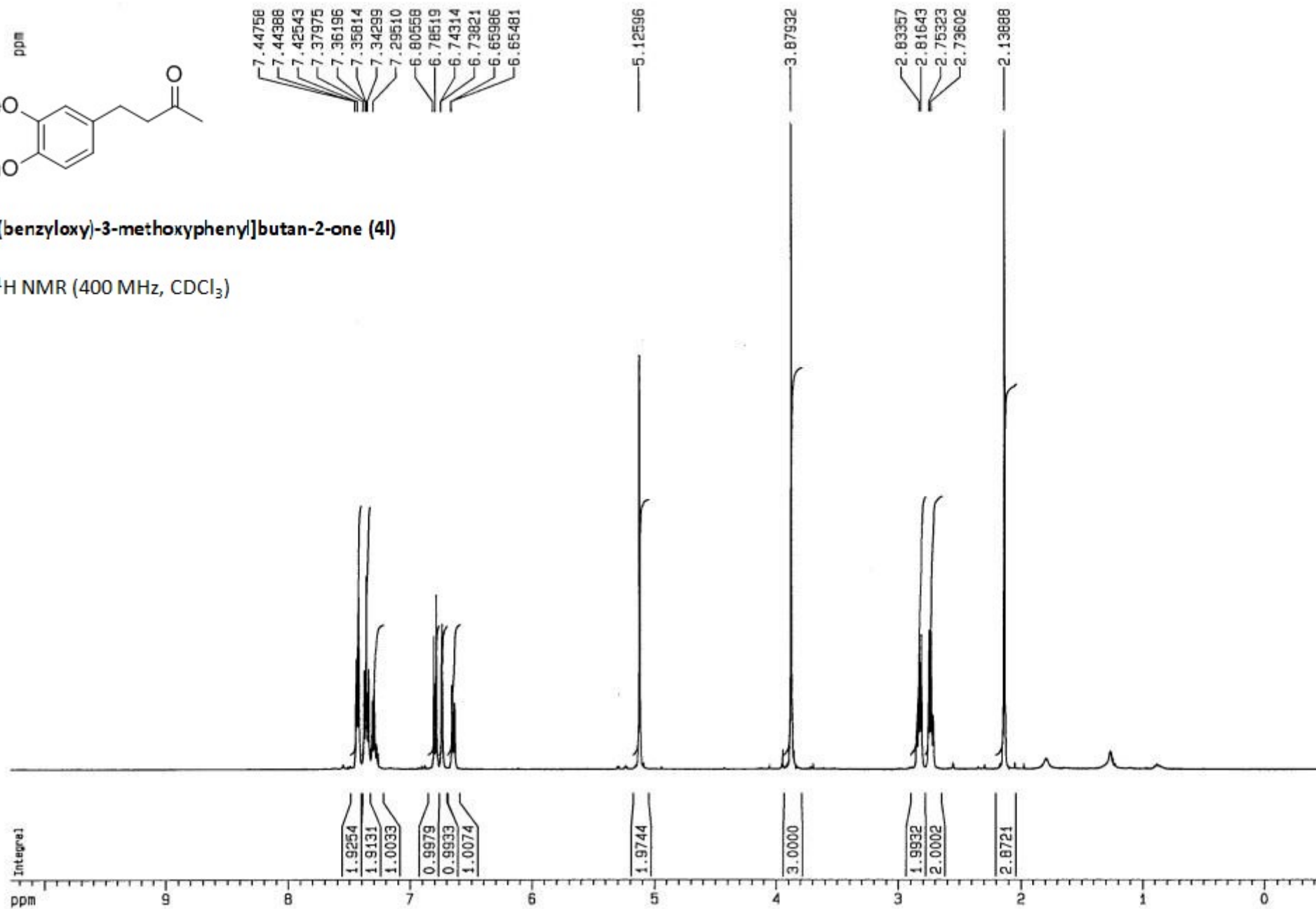


SI 27

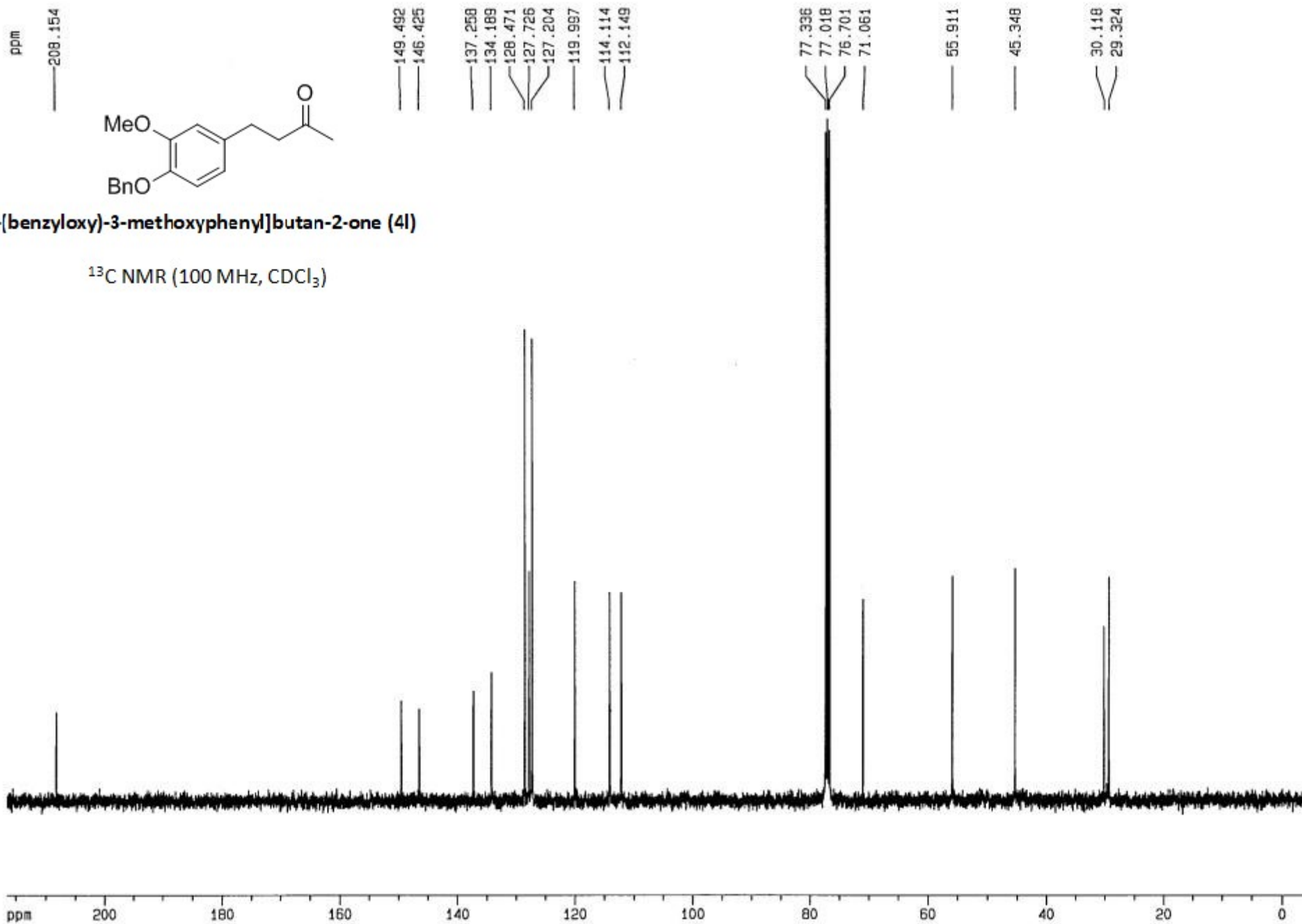


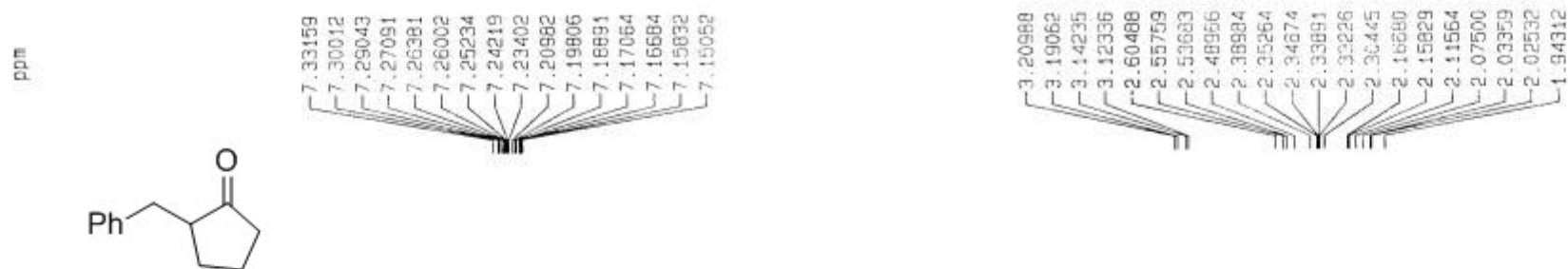
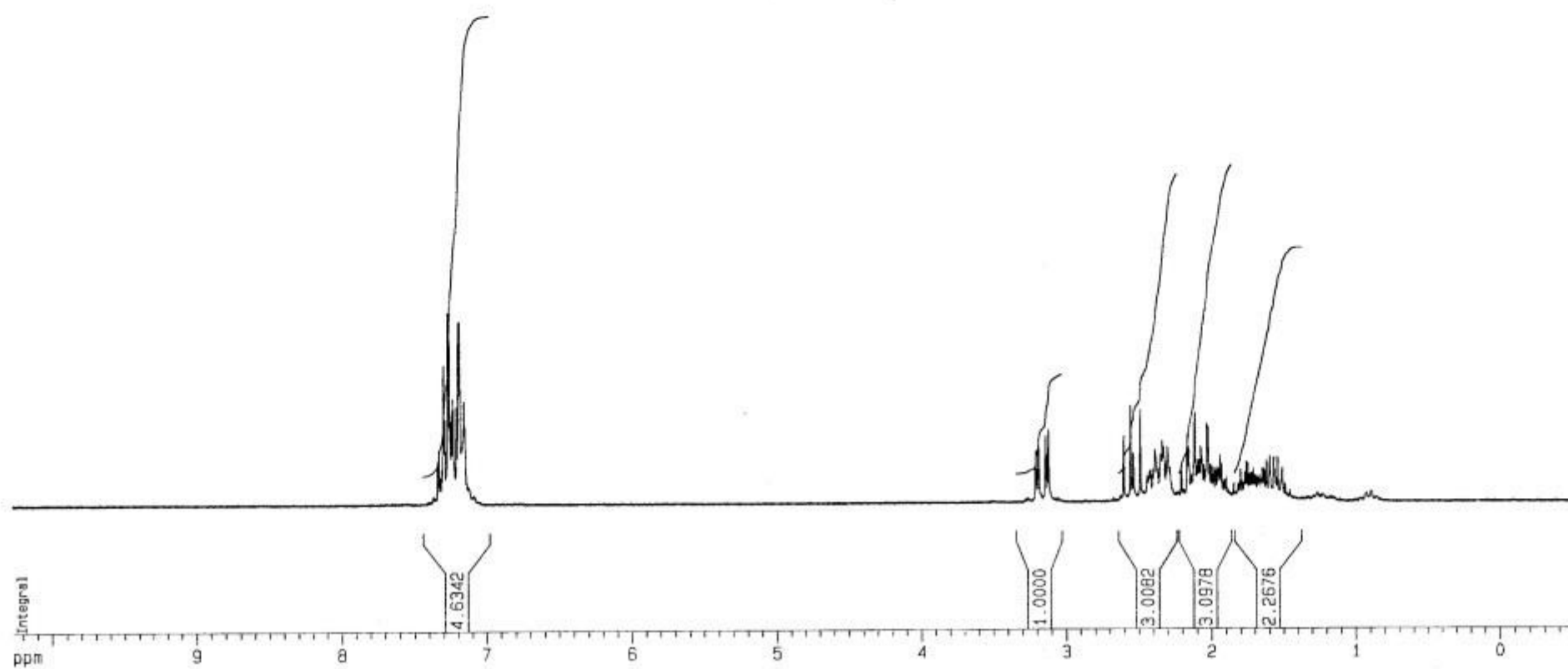
4-[4-(benzyloxy)-3-methoxyphenyl]butan-2-one (4)

^1H NMR (400 MHz, CDCl_3)



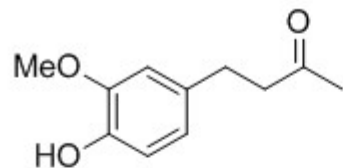
SI 28



**2-benzylcyclopentanone (4m)** ^1H NMR (200 MHz, CDCl_3)

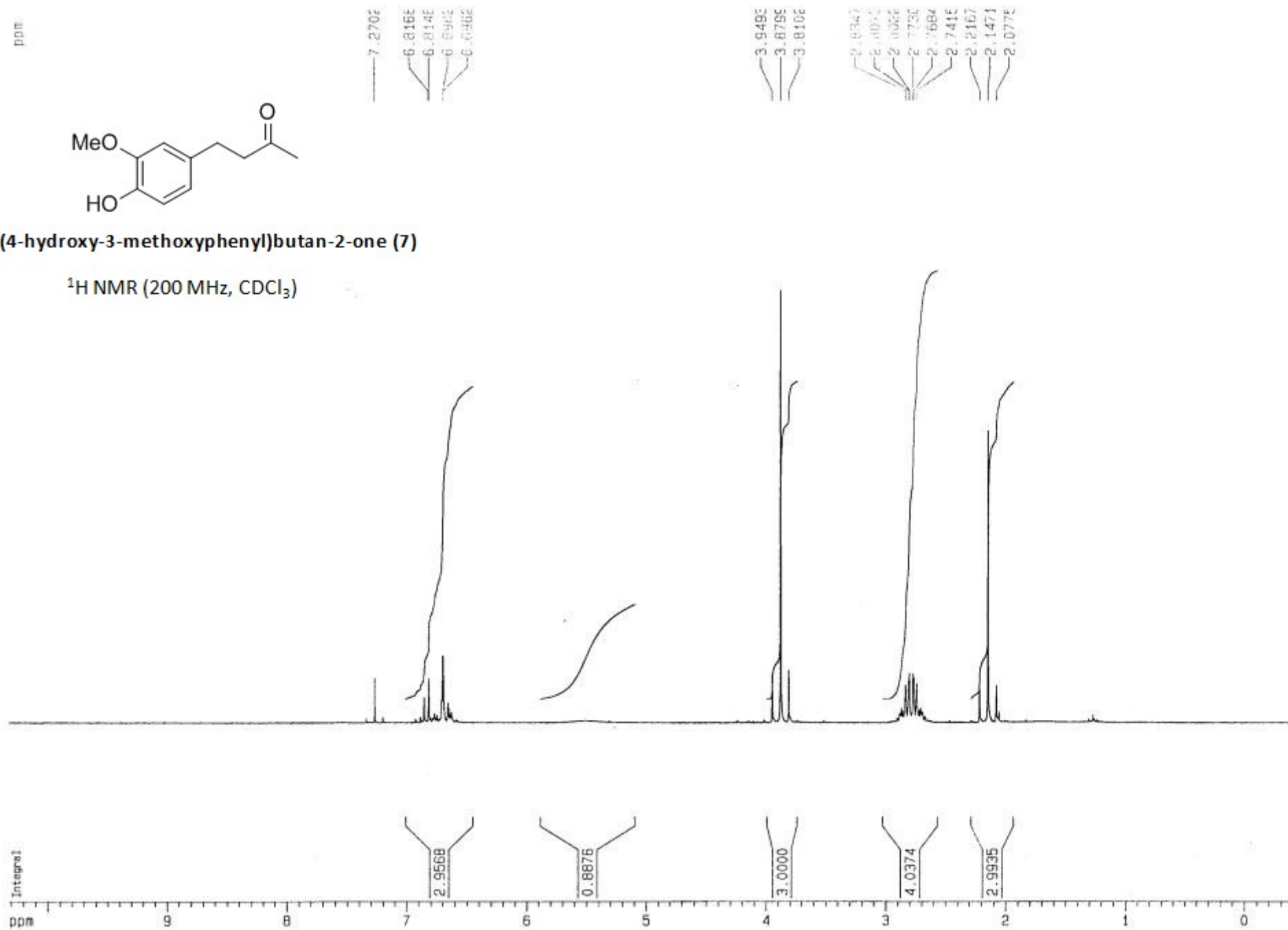
SI 30

ppm

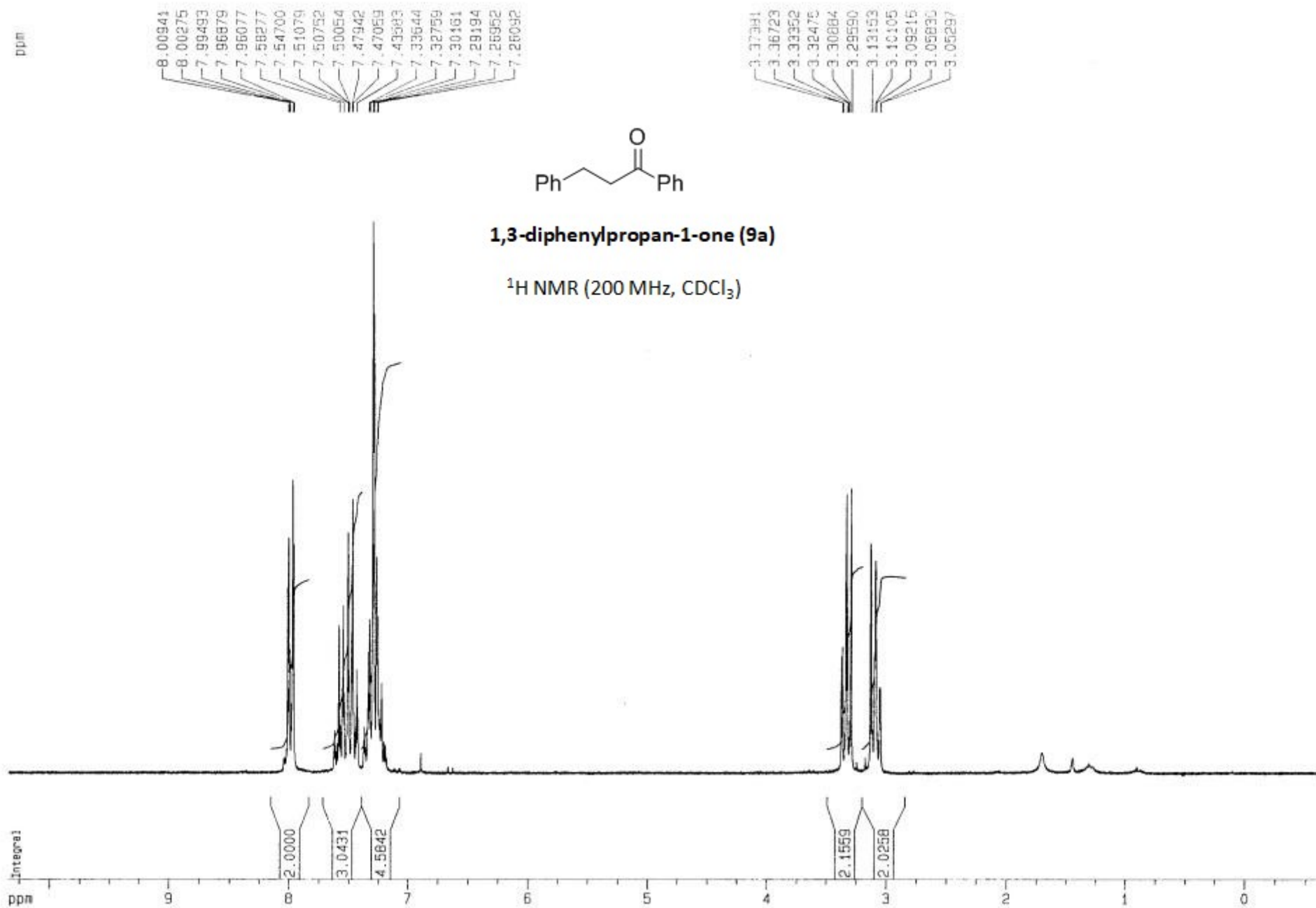


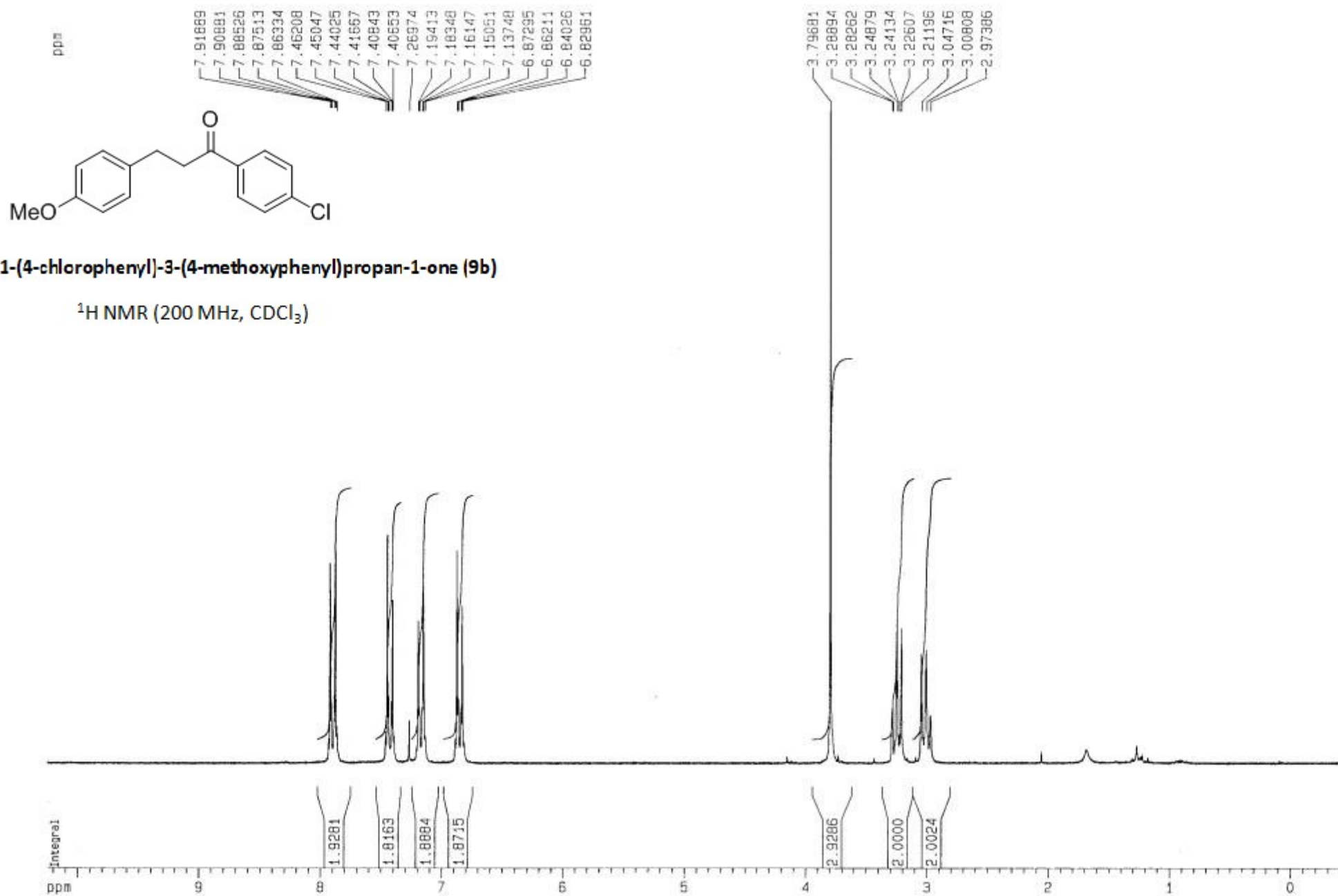
4-(4-hydroxy-3-methoxyphenyl)butan-2-one (7)

^1H NMR (200 MHz, CDCl_3)

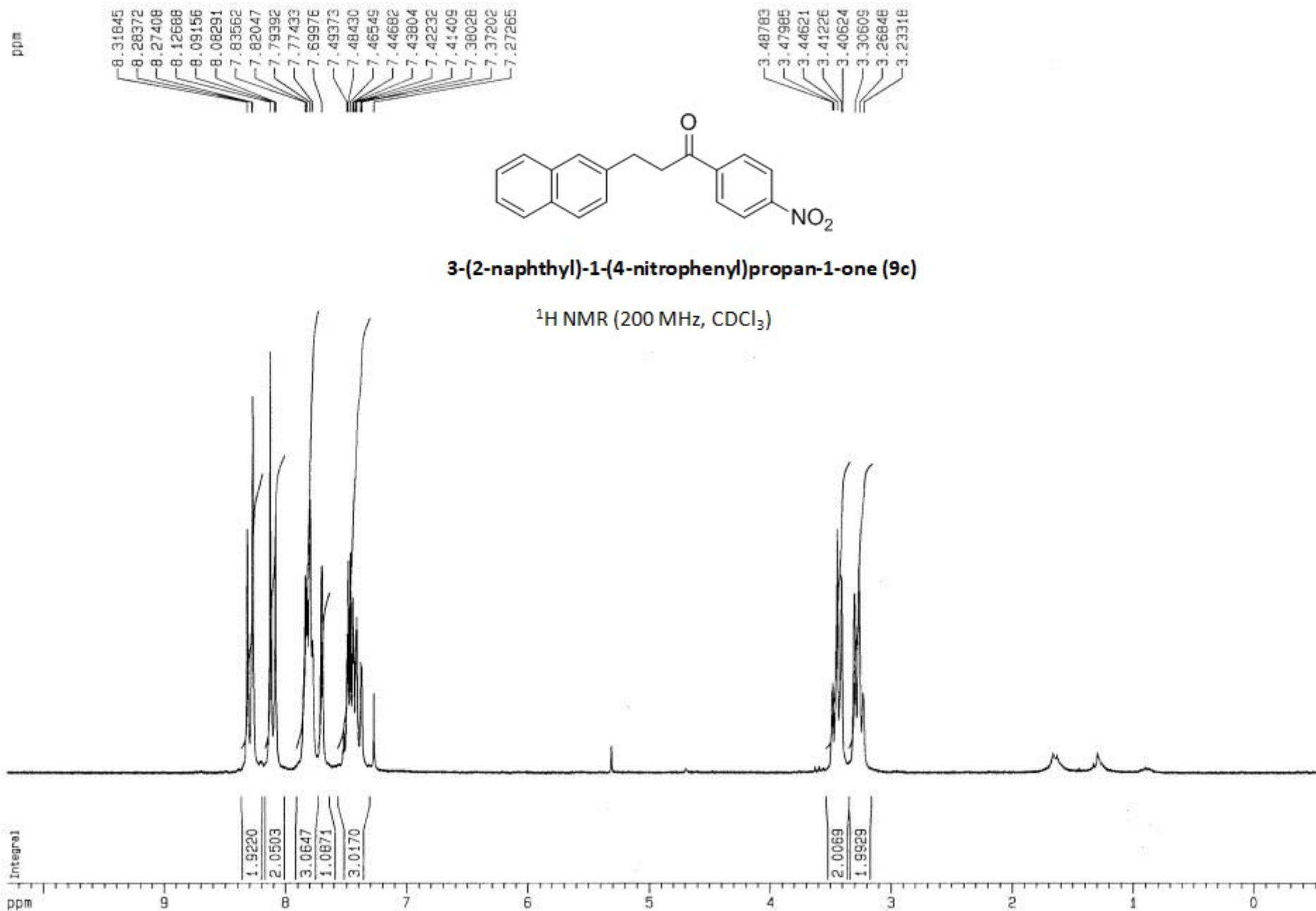


SI 31

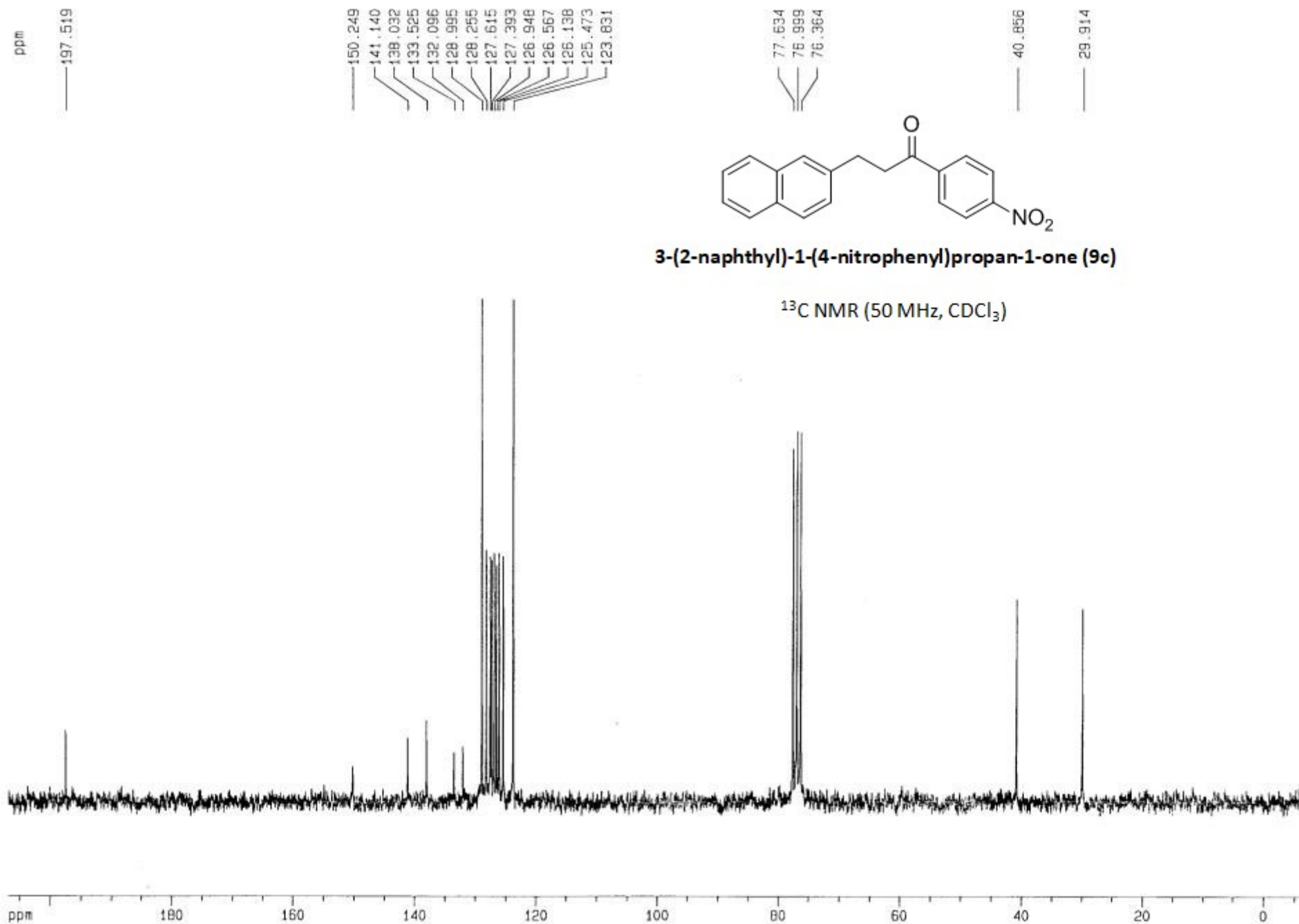




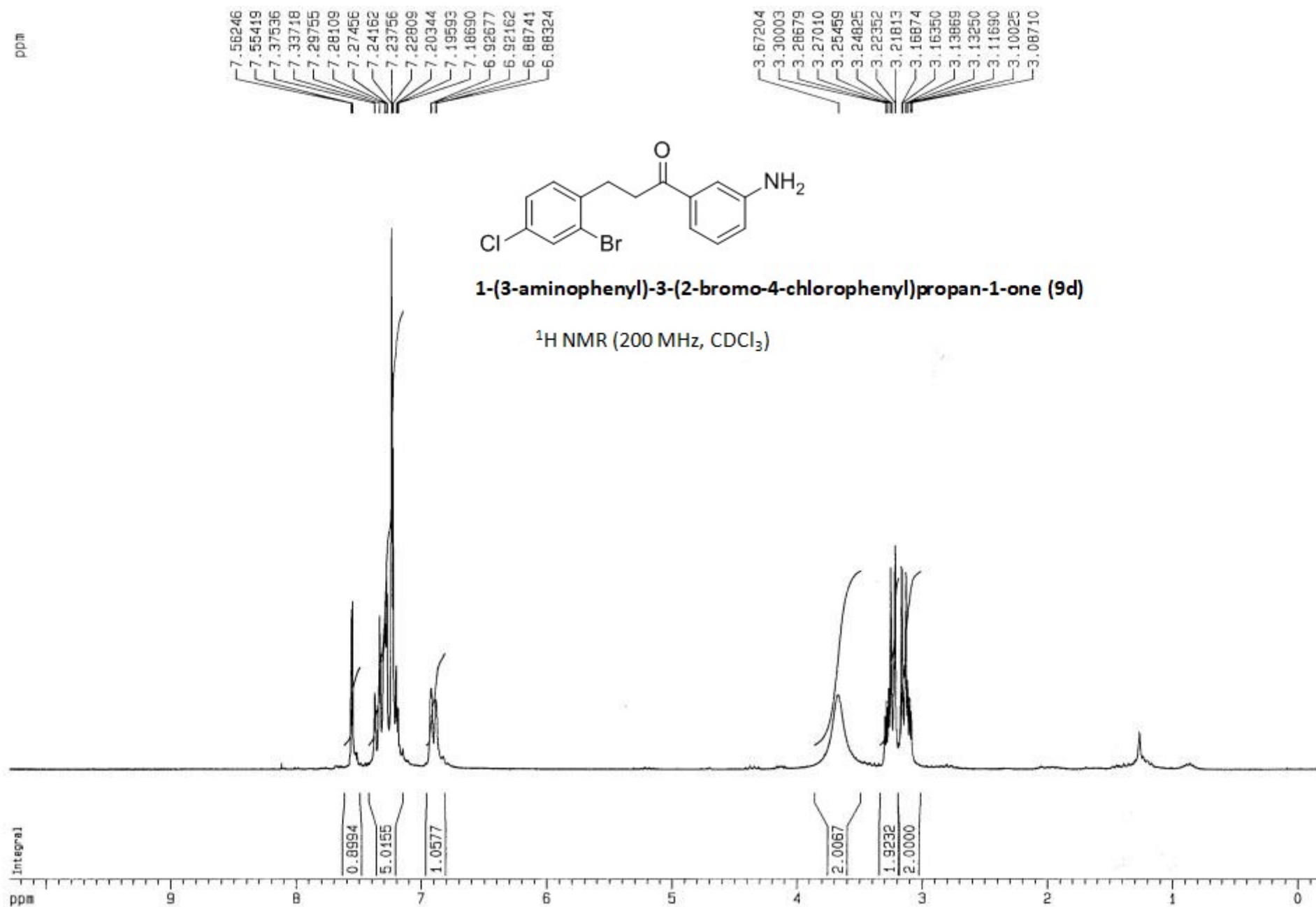
SI 33



SI 34



SI 35



SI 36

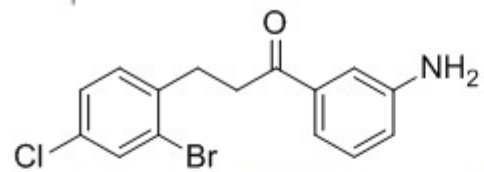
ppm
198.752

146.219
139.127
137.668
132.616
132.308
131.480
129.505
127.725
124.486
119.969
118.702
114.085

77.637
77.001
76.366

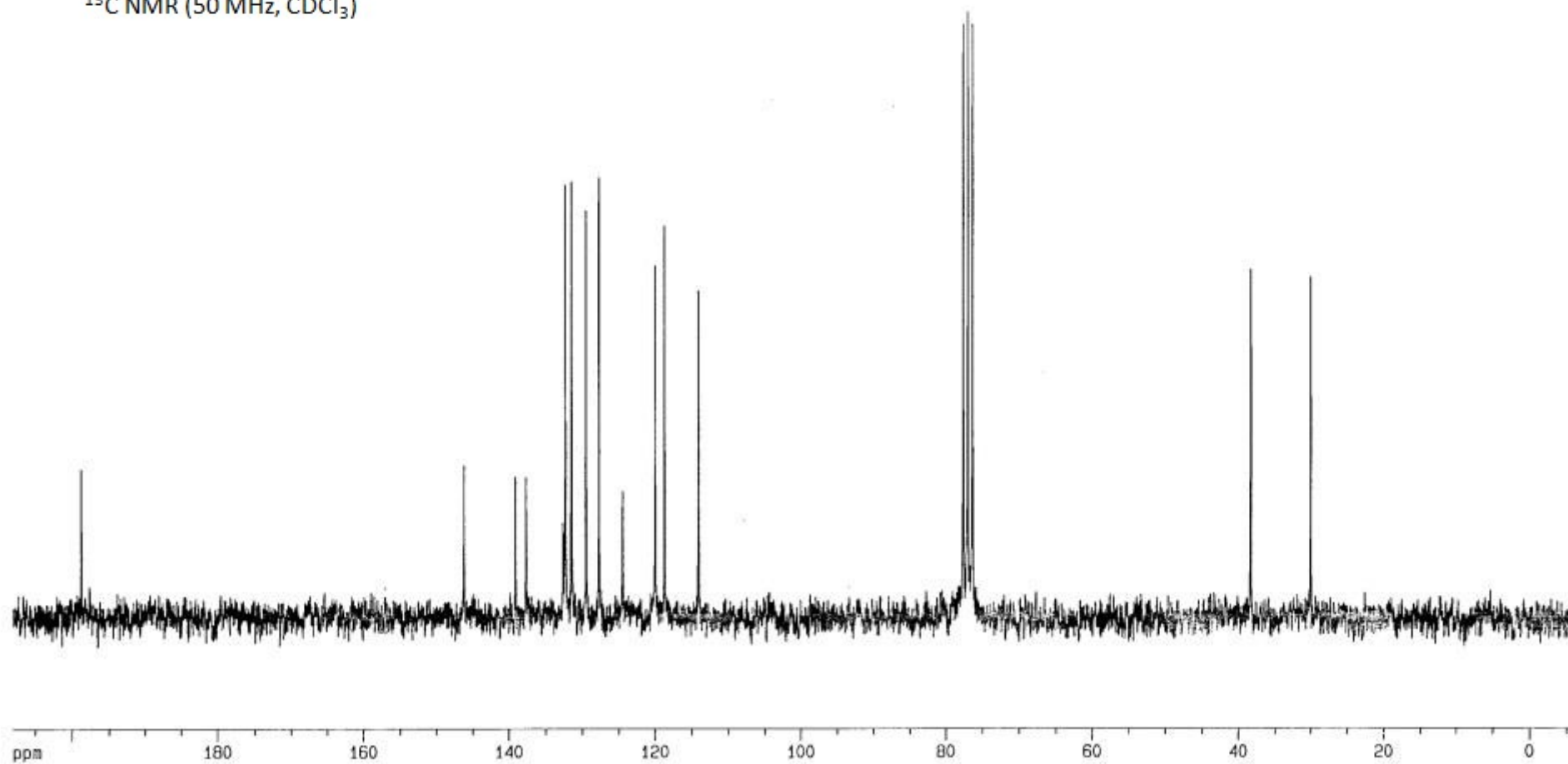
38.330

30.072

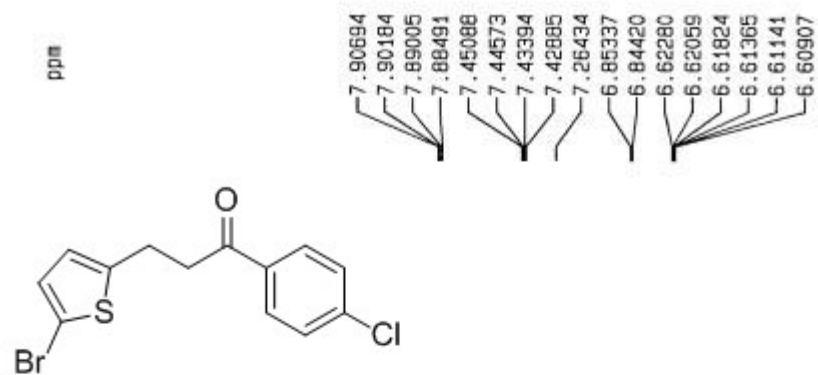


1-(3-aminophenyl)-3-(2-bromo-4-chlorophenyl)propan-1-one (9d)

^{13}C NMR (50 MHz, CDCl_3)

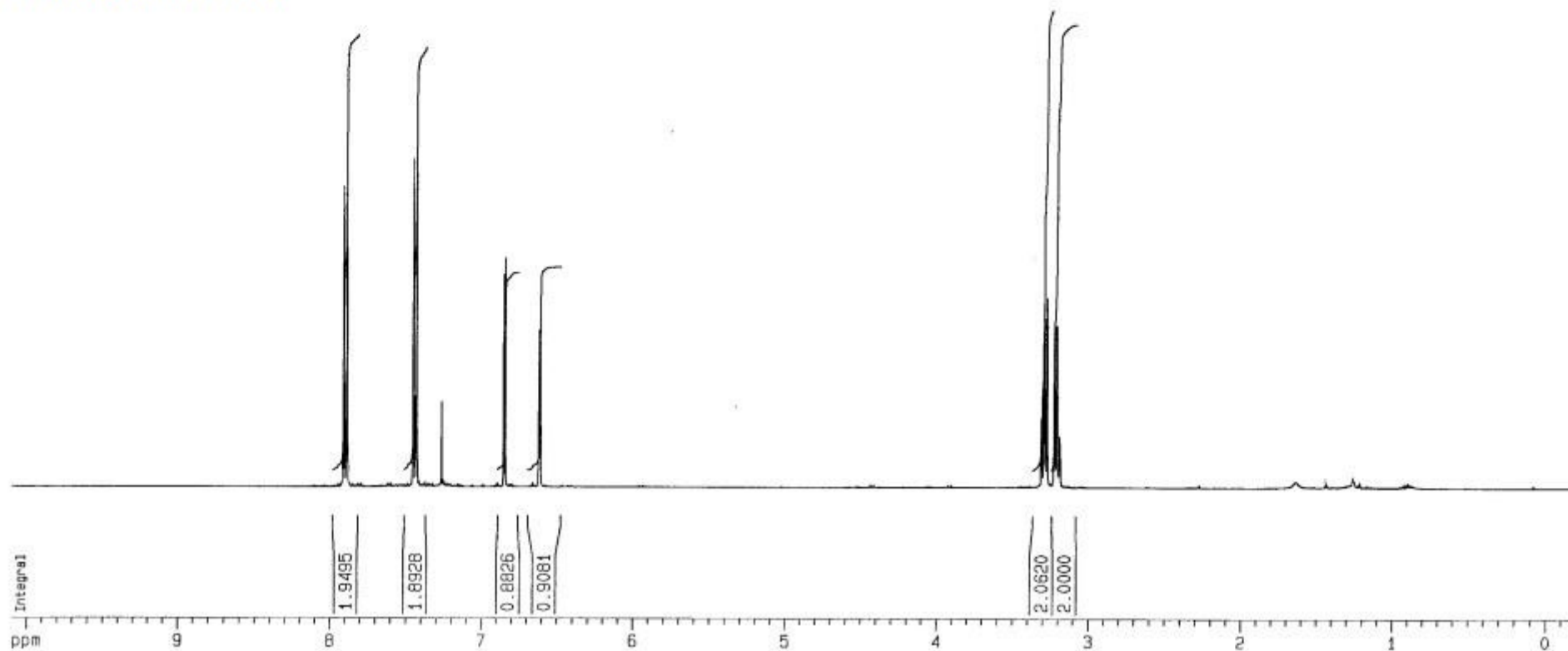


SI 37



3-(5-bromo-2-thienyl)-1-(4-chlorophenyl)propan-1-one (9e)

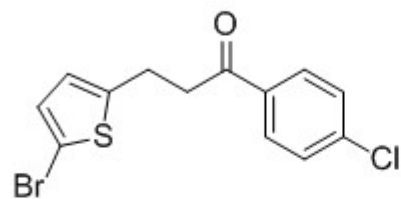
^1H NMR (200 MHz, CDCl_3)



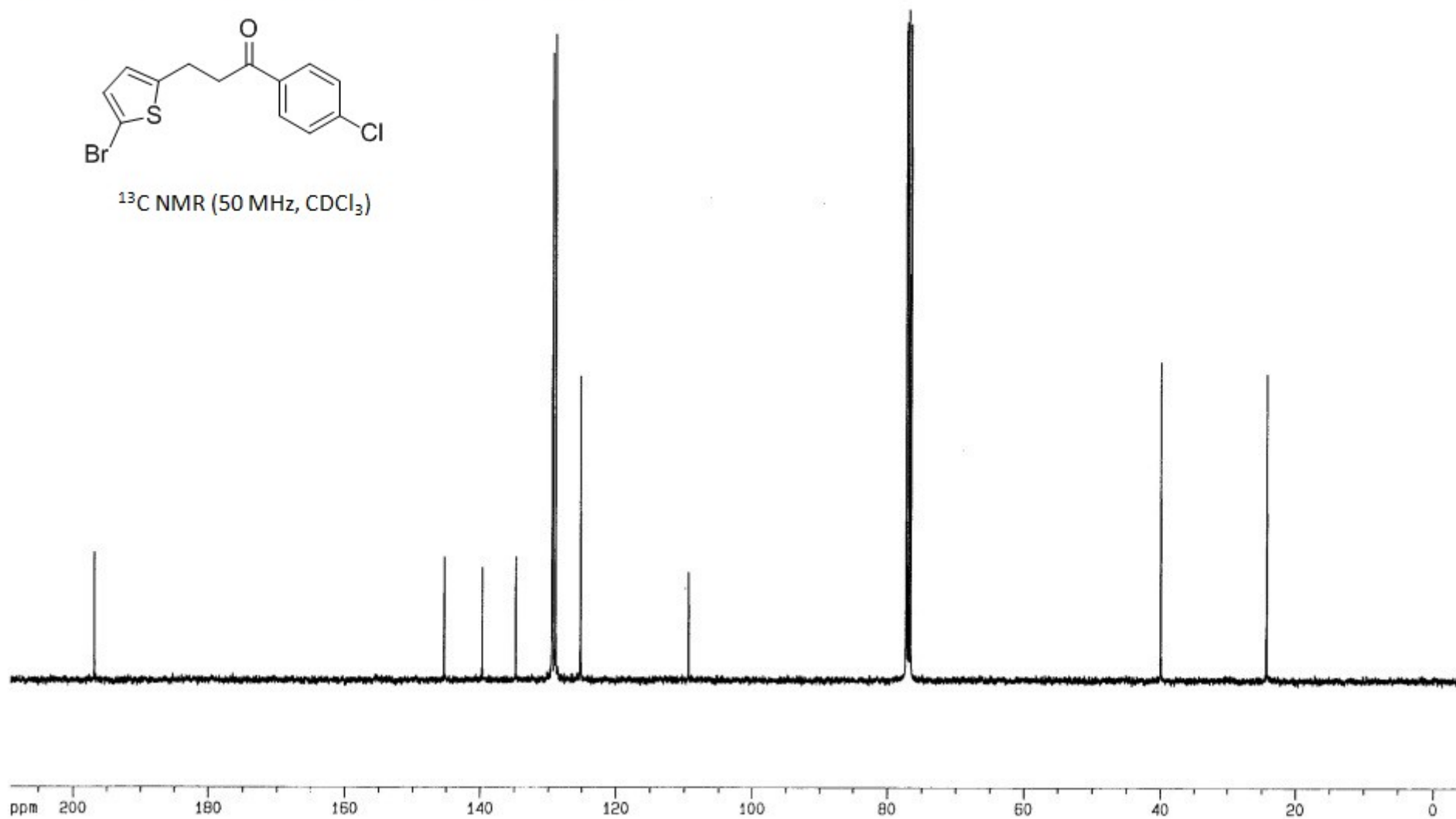
SI 38

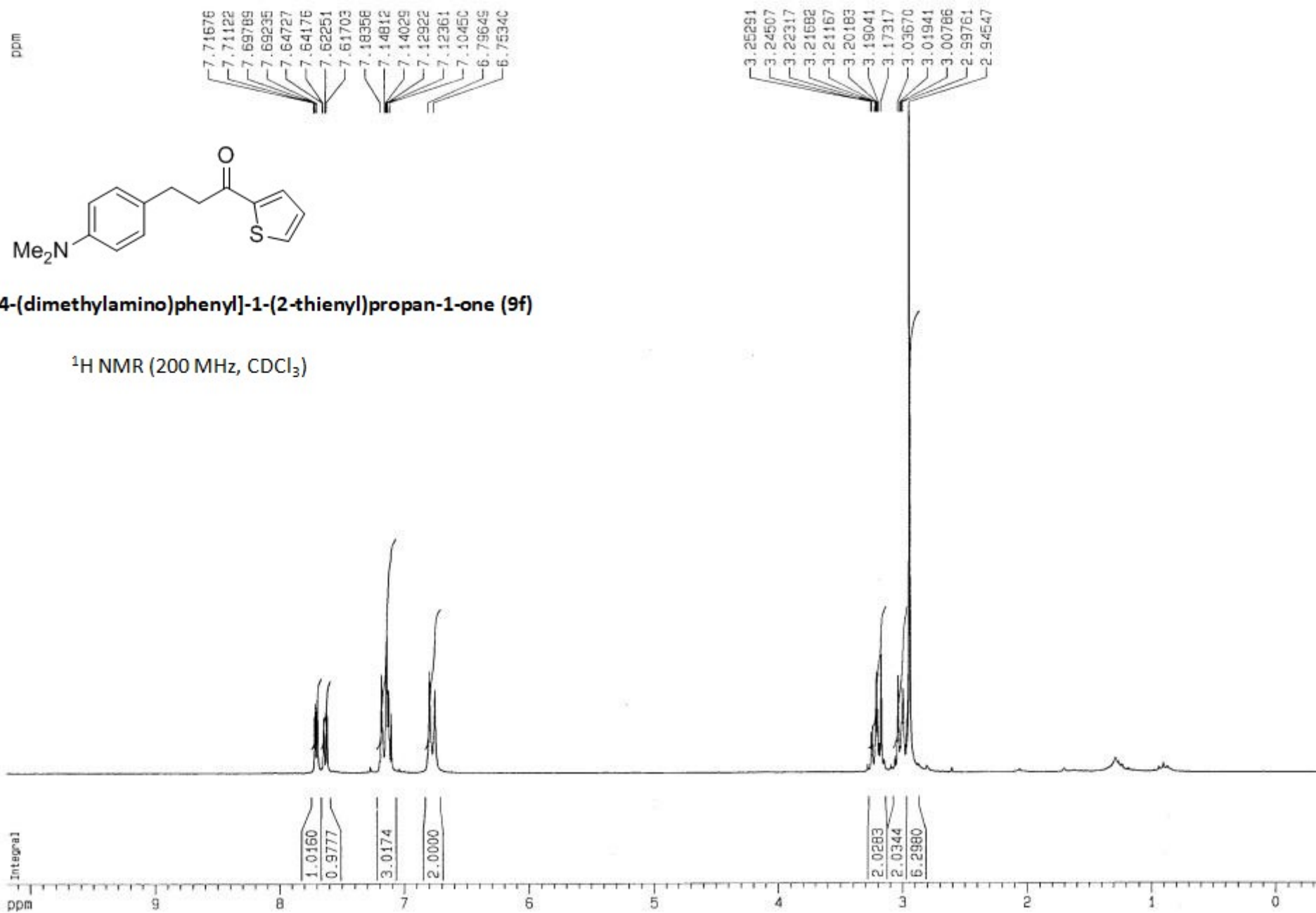


3-(5-bromo-2-thienyl)-1-(4-chlorophenyl)propan-1-one (9e)

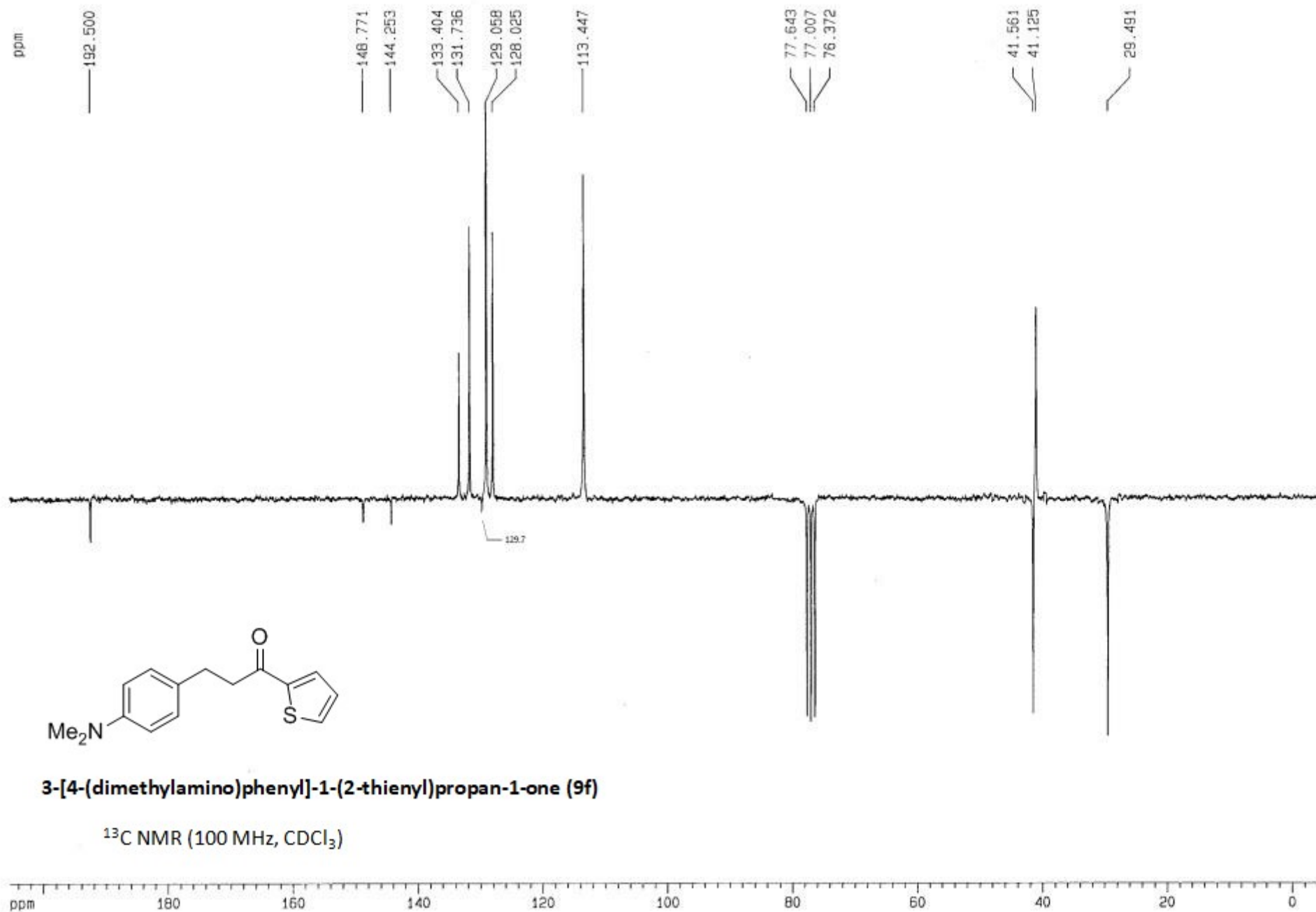


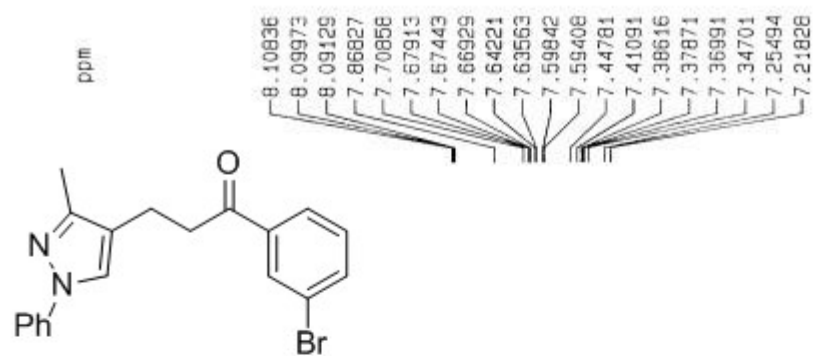
^{13}C NMR (50 MHz, CDCl_3)





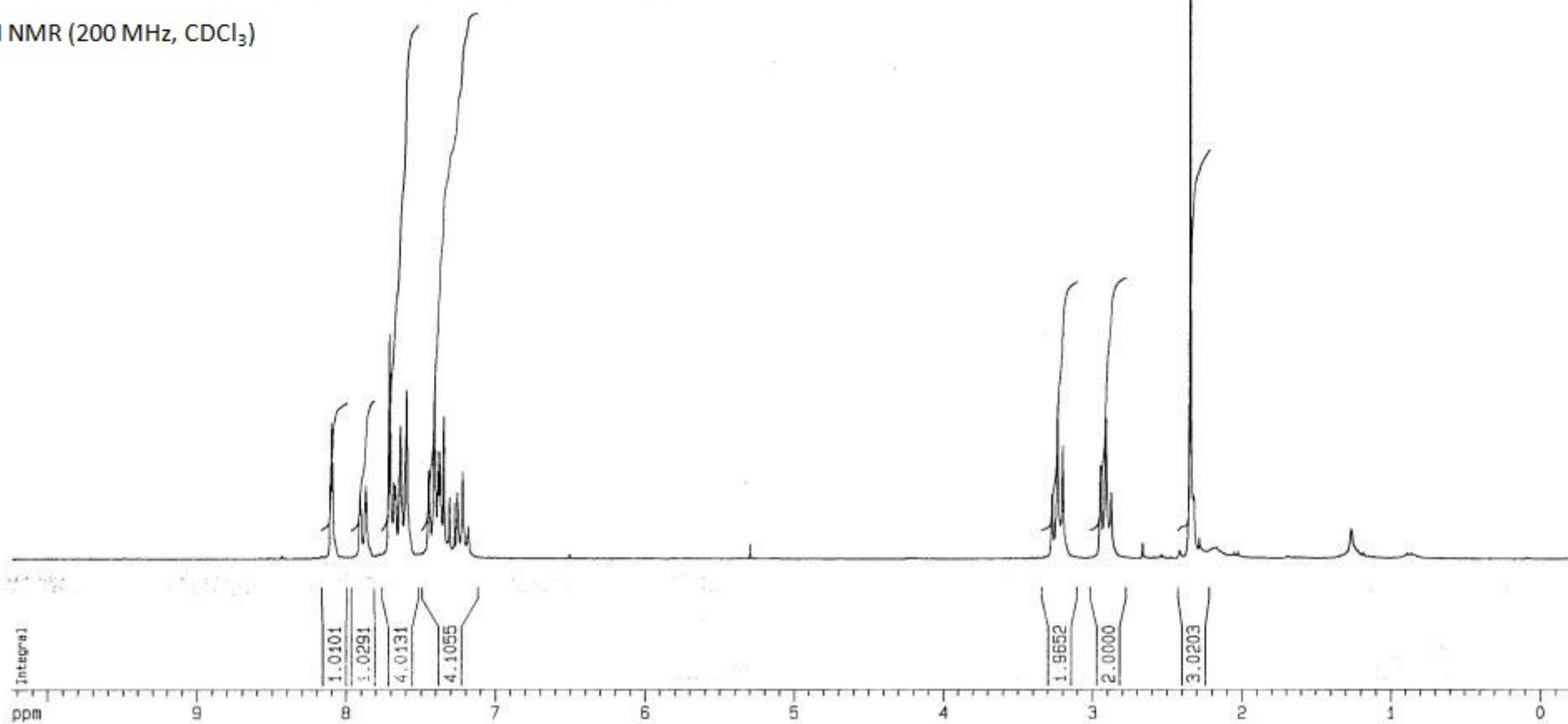
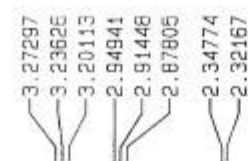
SI 40



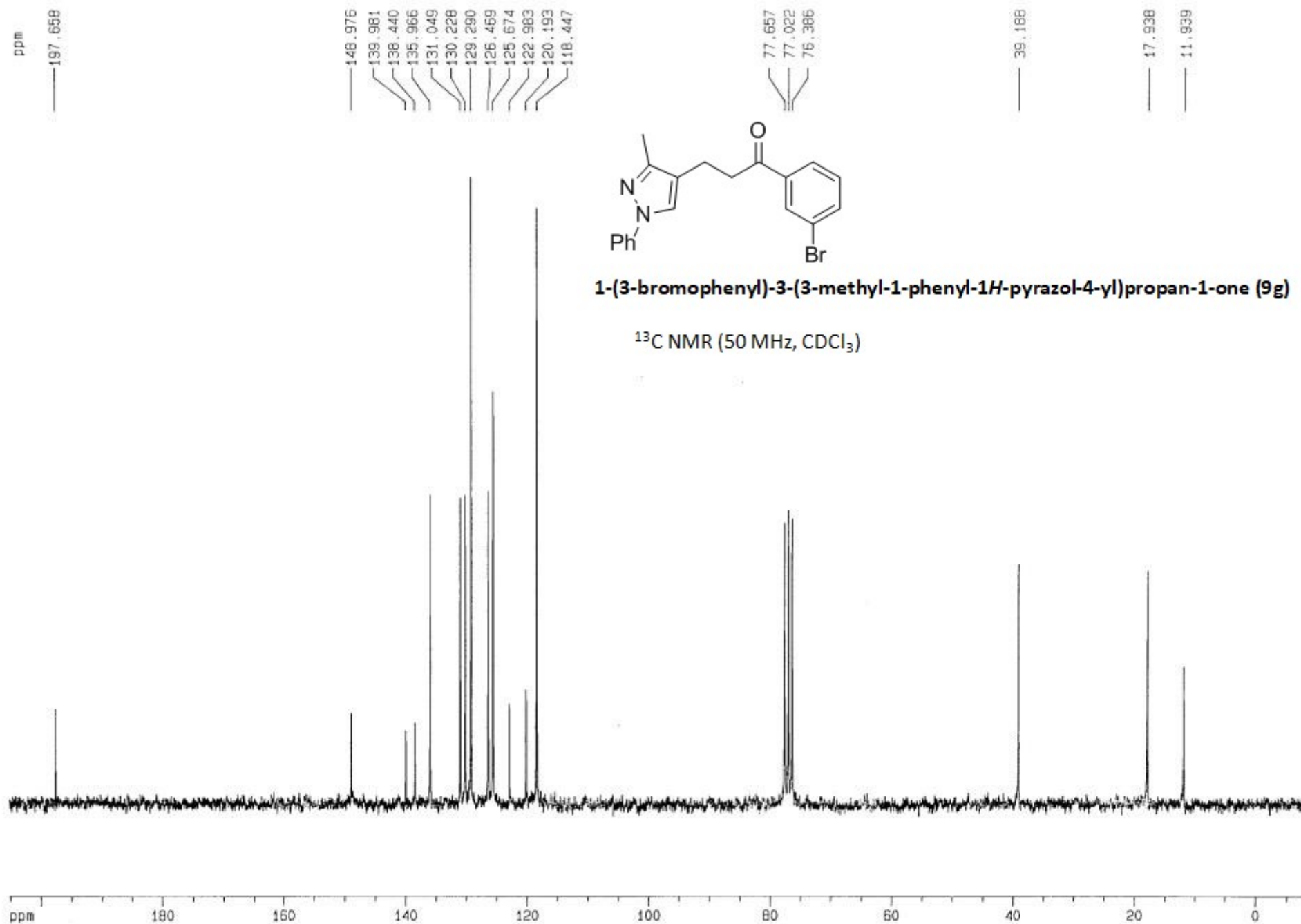


1-(3-bromophenyl)-3-(3-methyl-1-phenyl-1H-pyrazol-4-yl)propan-1-one (9g)

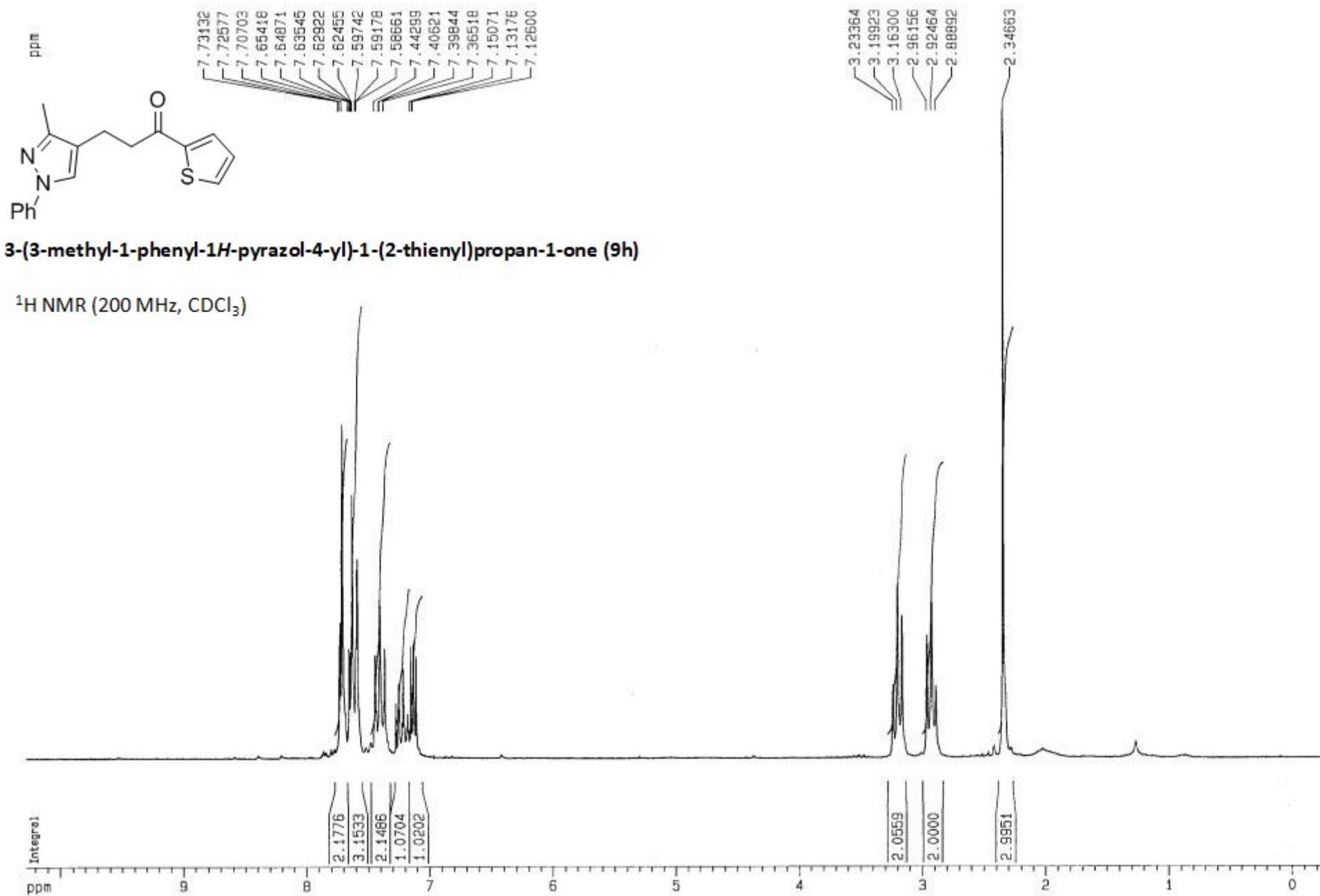
^1H NMR (200 MHz, CDCl_3)



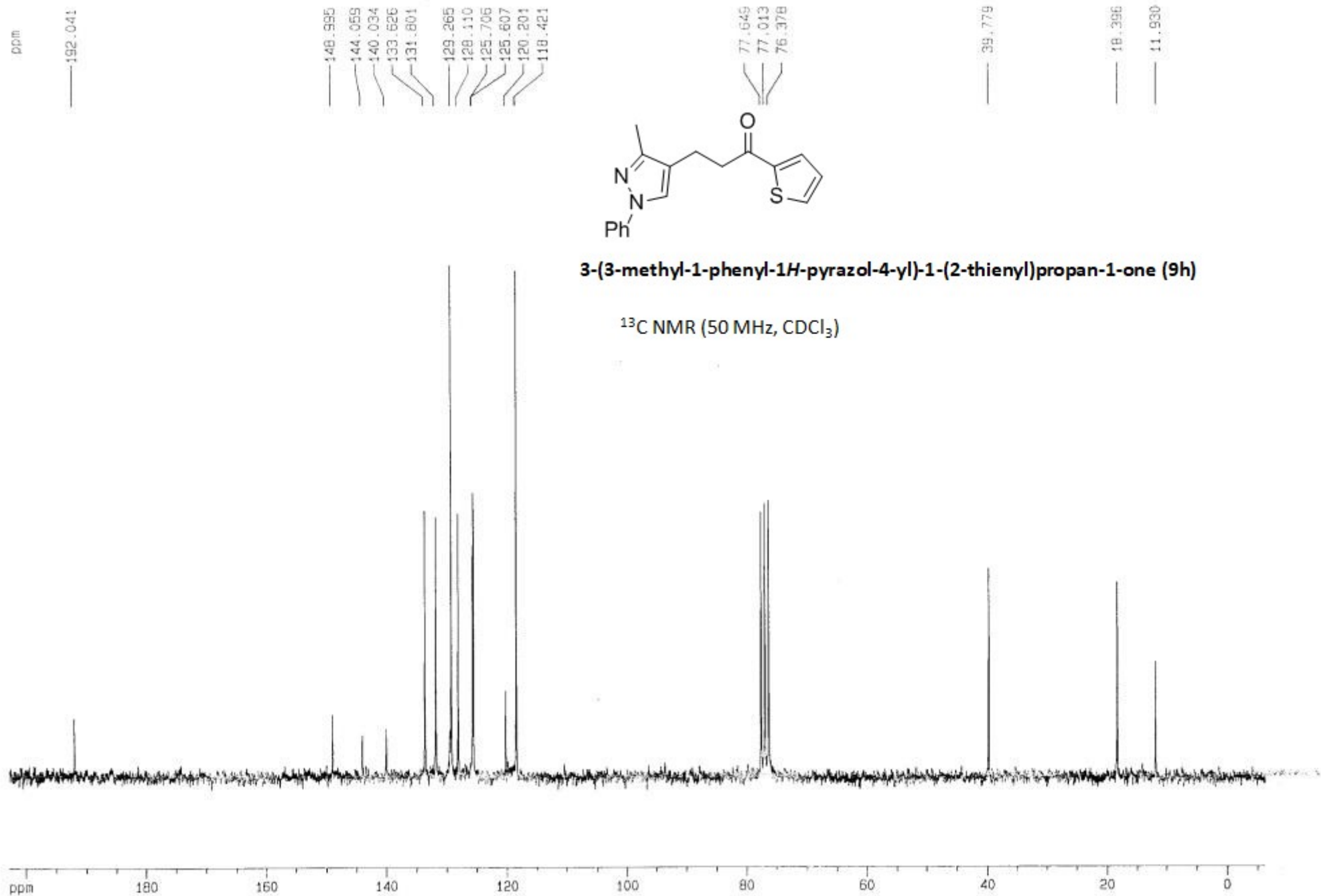
SI 42



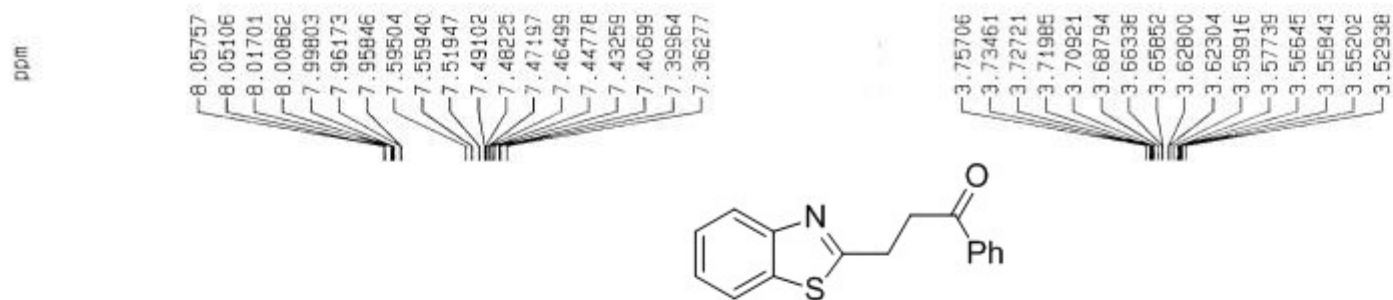
SI 43



SI 44

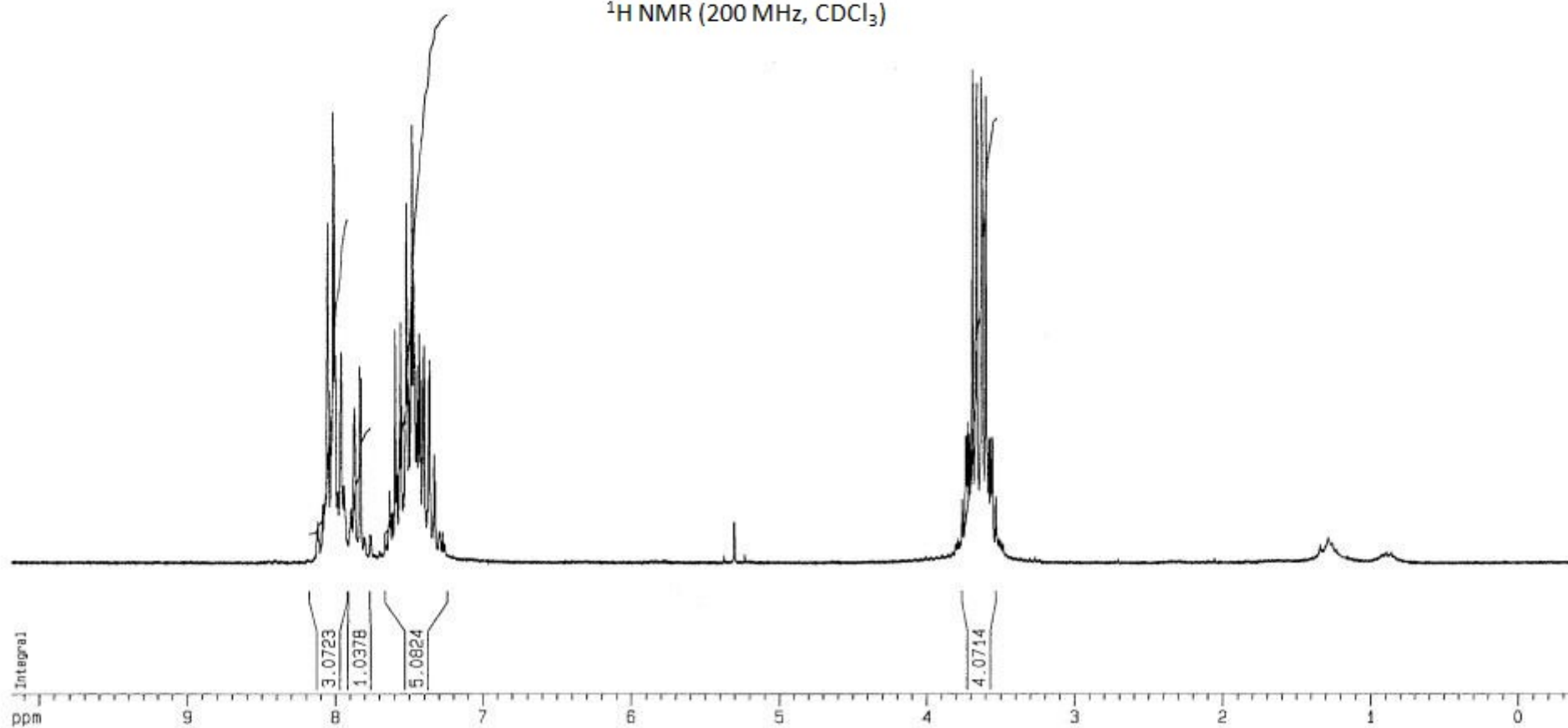


SI 45



3-(1,3-benzothiazol-2-yl)-1-phenylpropan-1-one (9i)

^1H NMR (200 MHz, CDCl_3)

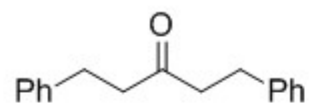


SI 46

ppm

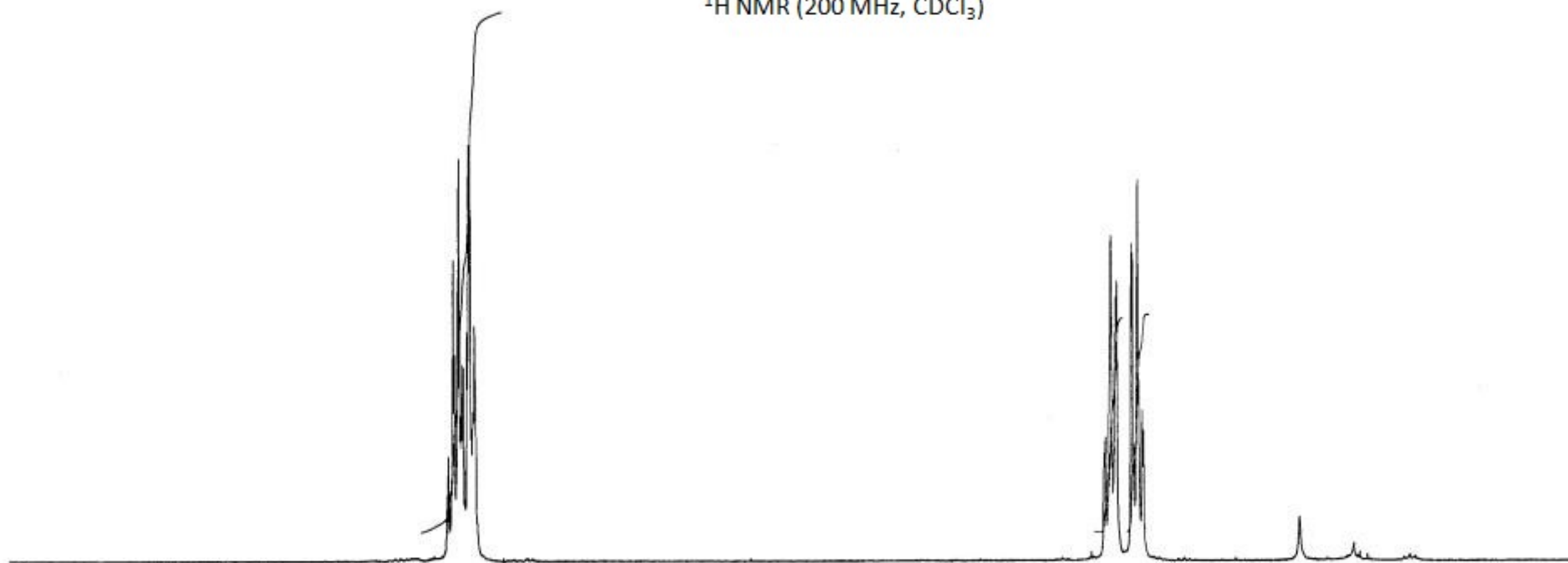
7.3307
7.2990
7.2897
7.2691
7.2621
7.2502
7.2391
7.2302
7.205E
7.195E
7.185E
7.1754
7.160E
7.1534
7.155E
7.145E

2.949E
2.9414
2.907E
2.873E
2.86E
2.780E
2.761E
2.732E
2.727E
2.720E
2.693E
2.604E



1,5-diphenylpentan-3-one (9j)

¹H NMR (200 MHz, CDCl₃)



Integrat
ppm

9.7632

4.0000
4.0701

9 8 7 6 5 4 3 2 1 0

SI 47

