

Synthesis of revised structure of klaivanolide (acetylmelodorinol)

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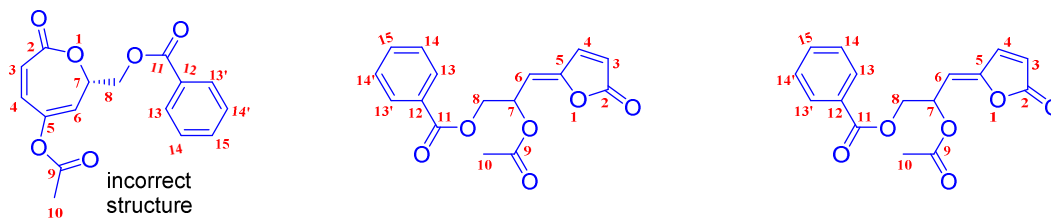
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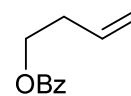
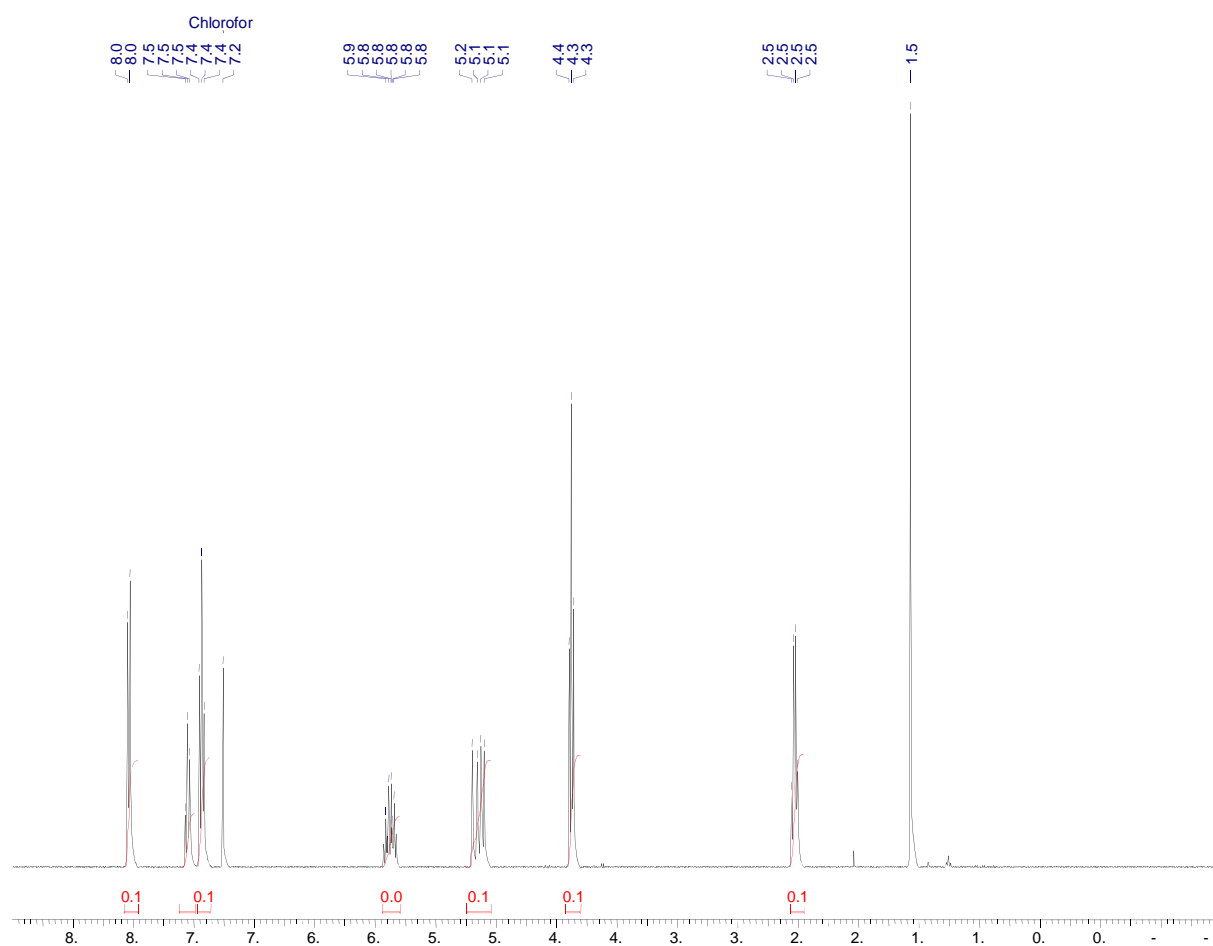
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Dedicated to Dr. Jhillu Singh Yadav on the occasion of his 65th Birthday

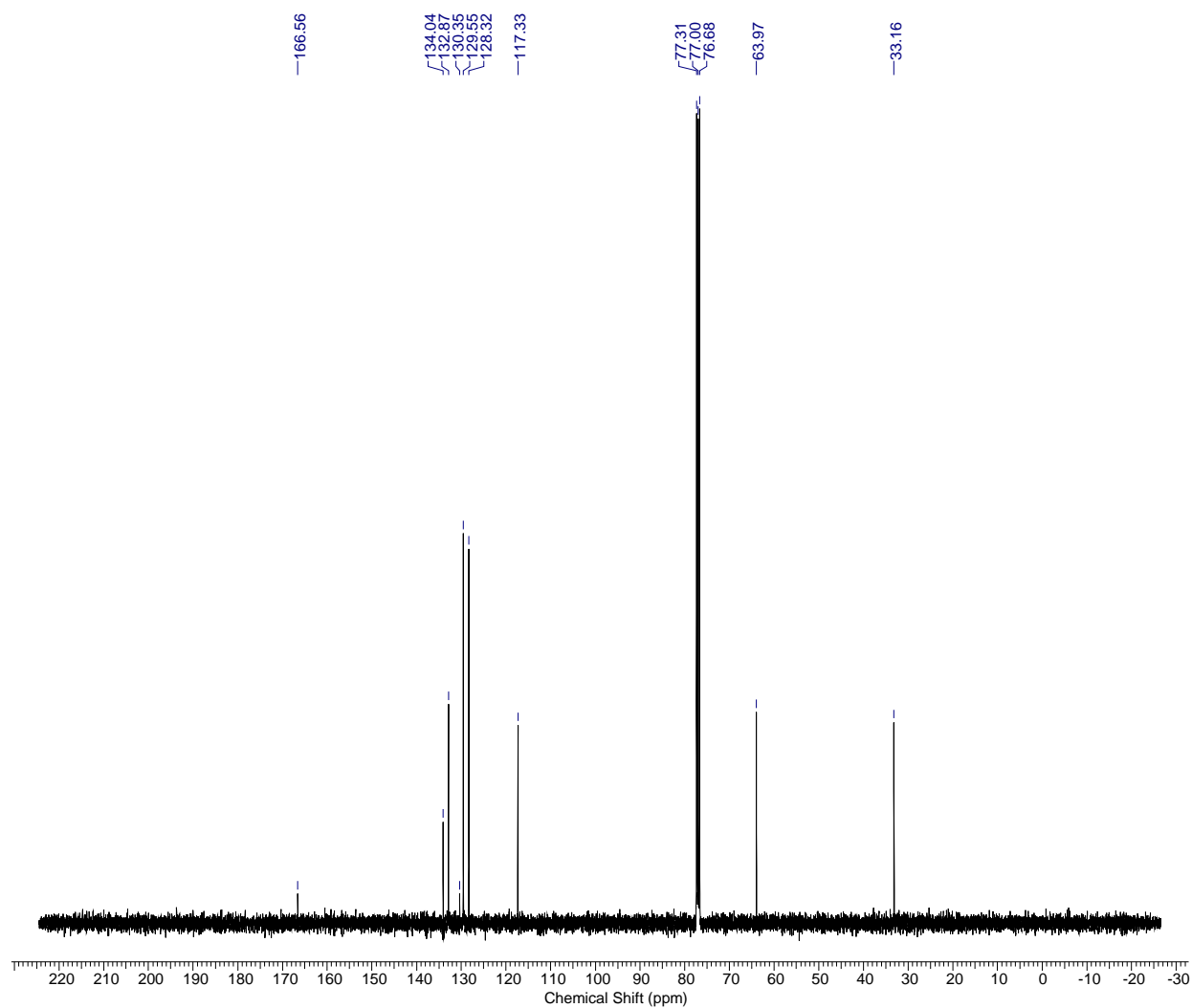
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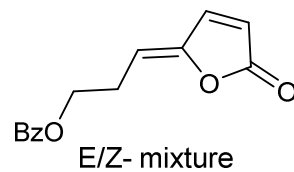
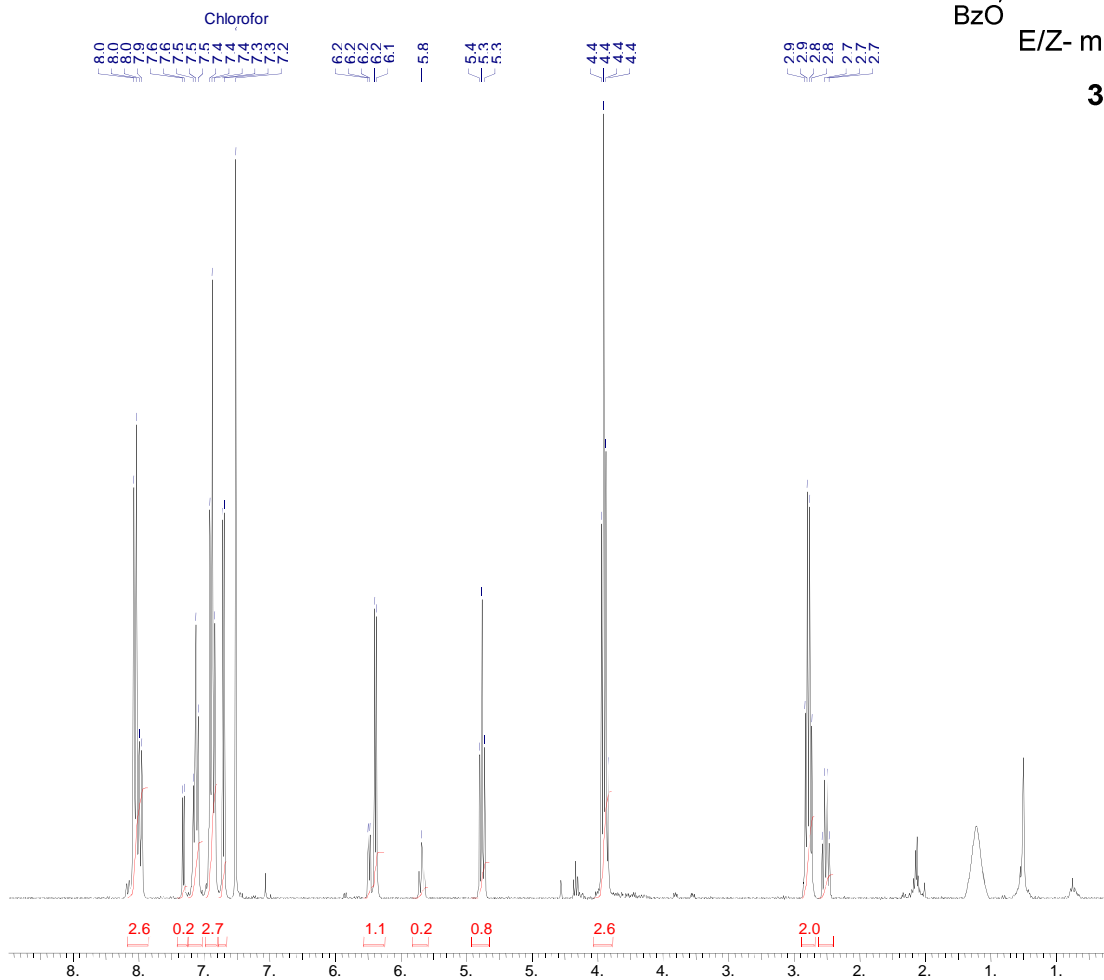
¹H & ¹³C NMR Comparison Table of Klaivanolide and Acetylmelodorinol

	Klaivanolide <i>Phytochemistry</i> , 2002 , 59, 885		Acetylmelodorinol <i>Tetrahedron</i> 1990 , 46, 5043		Synthesized acetylmelodorinol (2)	
	δ H	δ C	δ H	δ C	δ H	δ C
1						
2		168.4		168.4		168.5
3	6.27 (d, <i>J</i> 5.5 Hz, 1 H)	121.5	6.26 (dd, <i>J</i> 5.5, 0.5 Hz, 1 H)	121.4	6.28 (d, <i>J</i> 5.5 Hz, 1 H)	121.6
4	7.37 (d, <i>J</i> 5.5 Hz, 1 H)	143.3	7.36 (d, <i>J</i> 5.5 Hz, 1 H)	143.3	7.37 (d, <i>J</i> 5.5 Hz, 1 H)	143.3
5		150.7		150.6		150.7
6	5.32 (d, <i>J</i> 8.0 Hz, 1 H)	108.8	5.31 (dd, <i>J</i> 8.0, 0.5 Hz, 1 H)	108.8	5.32 (d, <i>J</i> 7.8 Hz, 1 H)	108.9
7	6.14 (ddd, <i>J</i> 4.2, 6.0, 8.0 Hz, 1 H)	67.2	6.12 (ddd, <i>J</i> 4.1, 6.1, 8.1 Hz, 1 H)	67.2	6.14 (ddd, <i>J</i> 4.4, 6.0, 7.9 Hz, 1 H)	67.3
8	4.57 (dd, <i>J</i> 11.7, 4.2 Hz) 4.52 (dd, <i>J</i> 11.7, 6.0 Hz)	64.6	4.55 (dd, <i>J</i> 11.7, 4.1 Hz) 4.50 (dd, <i>J</i> 11.7, 6.1 Hz)	64.6	4.59 - 4.50 (m, 2 H)	64.6
9		169.7		169.7		169.8
10	2.10 (s, 3H)	20.8	2.08 (s, 3H)	20.8	2.10 (s, 3 H)	20.9
11		165.9		165.9		166.0
12		129.5		129.5		129.5
13, 13'	8.02 (dd, <i>J</i> 1.3, 8.4 Hz, 2 H)	129.6	8.01 (dd, <i>J</i> 1.3, 8.2, 0.9 Hz, 2 H)	129.6	8.03 (d, <i>J</i> 7.3 Hz, 2 H)	129.7
14, 14'	7.45 (brt, <i>J</i> 8.0 Hz, 2 H)	128.4	7.43 (tt, <i>J</i> 8.2, 1.3 Hz, 2 H)	128.4	7.45 (t, <i>J</i> 7.7 Hz, 2 H)	128.5
15	7.58 (tt, <i>J</i> 7.4, 1.3 Hz, 1 H)	133.2	7.56 (tt, <i>J</i> 8.2, 1.3 Hz, 1 H)	133.2	7.58 (t, <i>J</i> 7.3 Hz, 1 H)	133.3

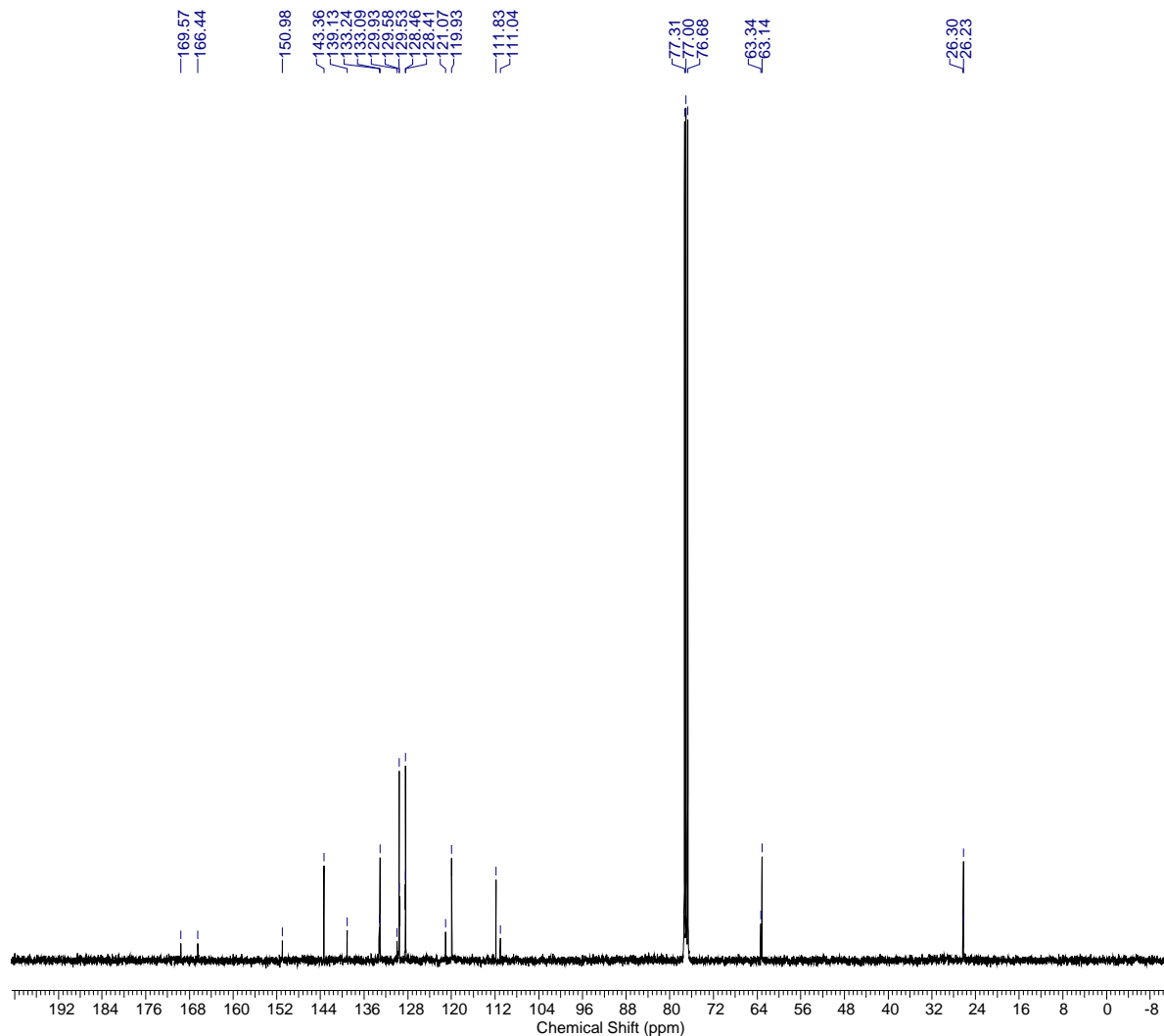
^1H and ^{13}C NMR spectra of compounds ^1H NMR Spectra of 3-butenyl benzoate

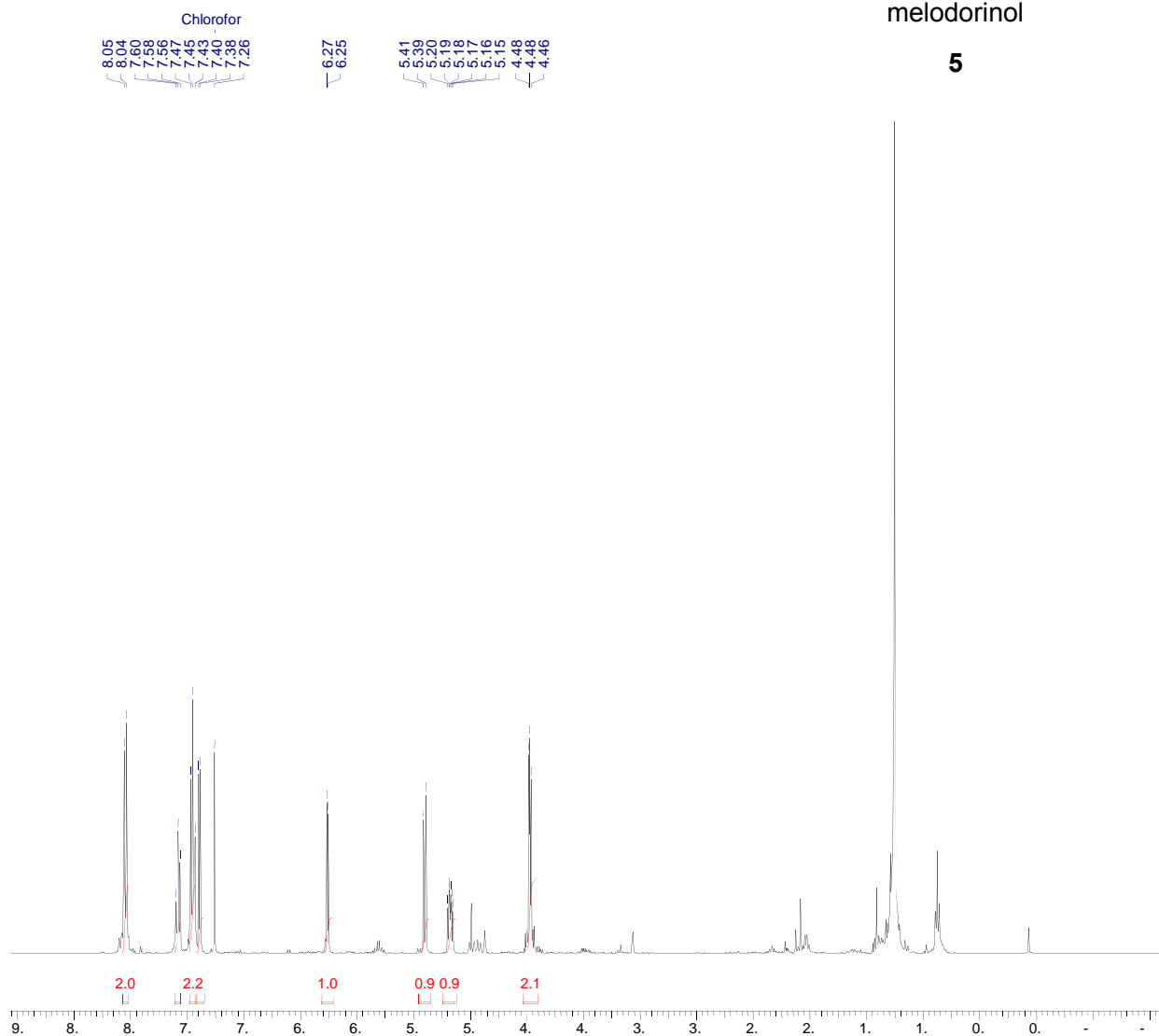
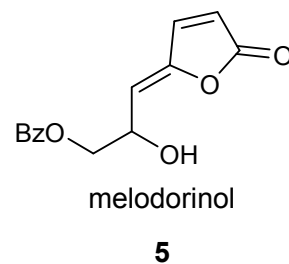
¹³CNMR Spectra of 3-butenyl benzoate



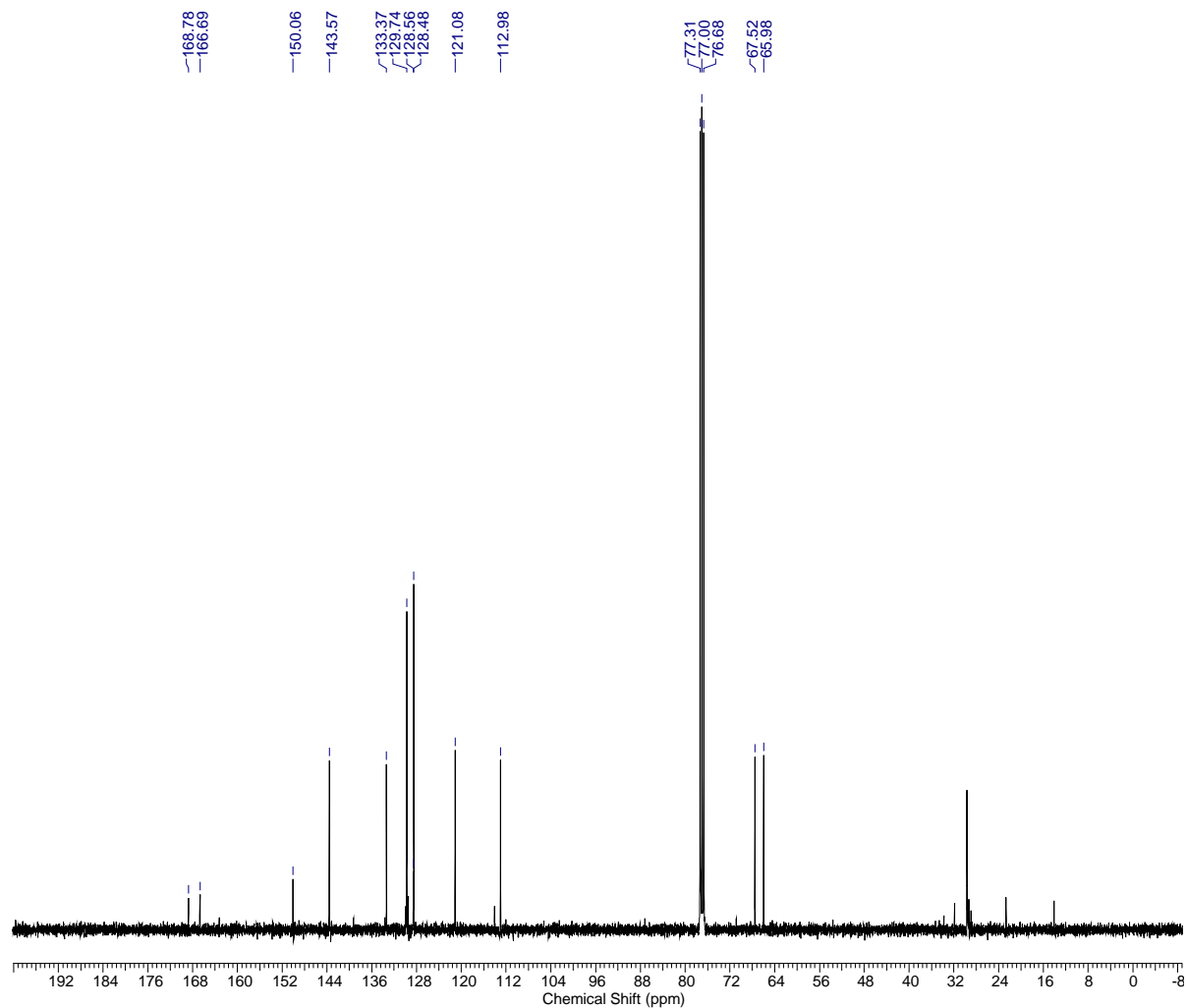
1 H NMR Spectra of Compound 3

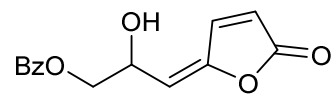
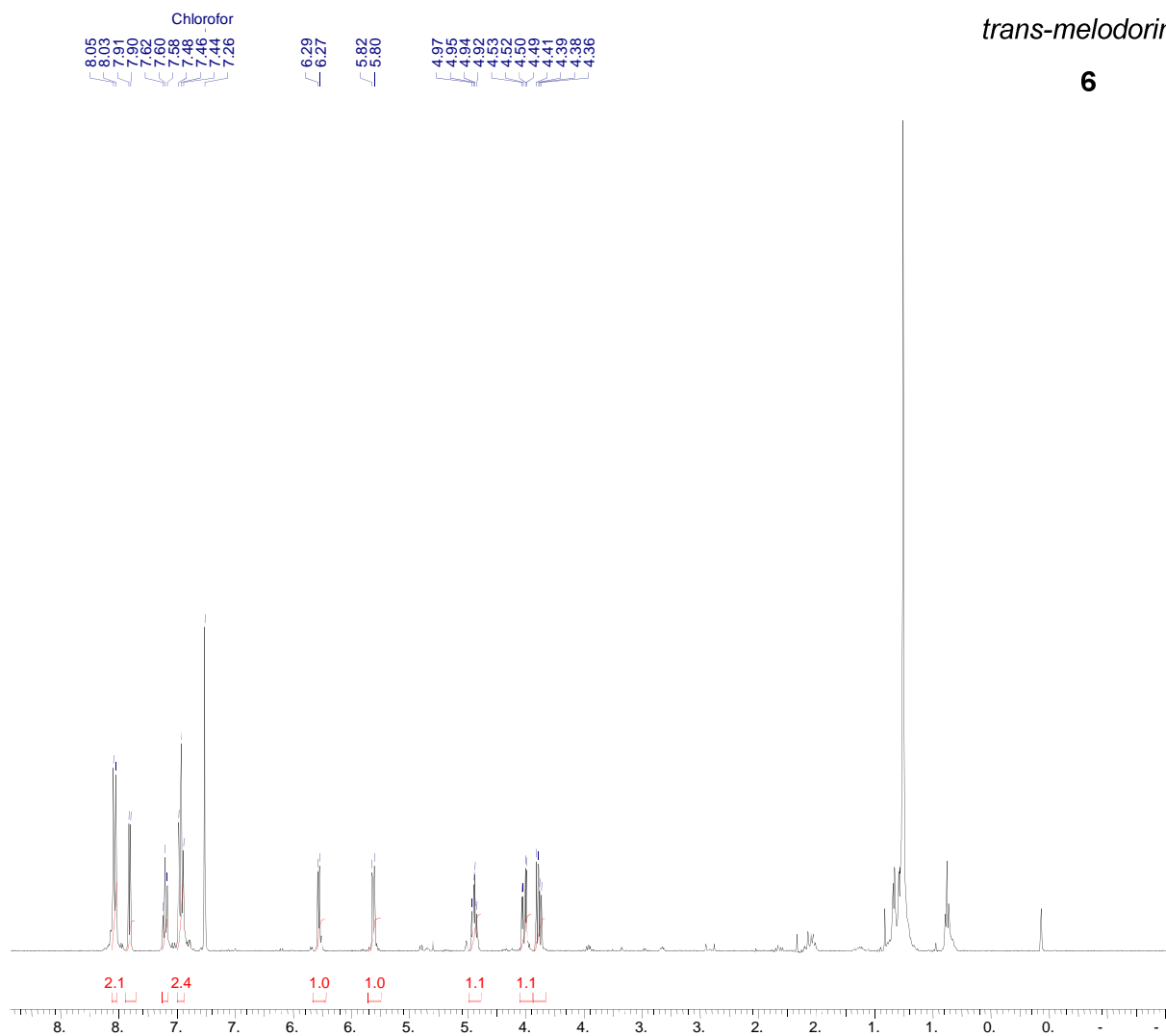
3

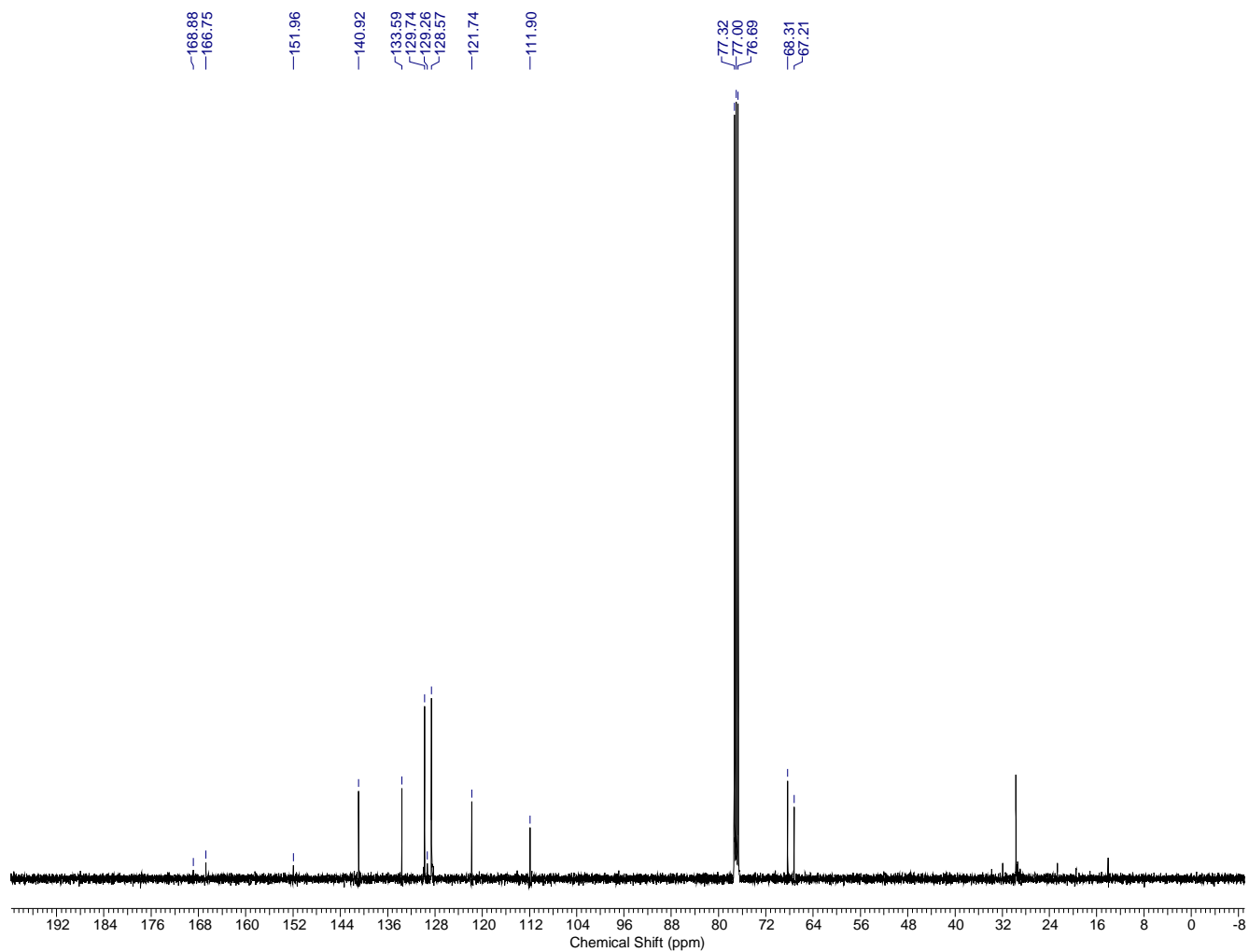
¹³C NMR Spectra of Compound 3

¹HNMR Spectra of Compound 5

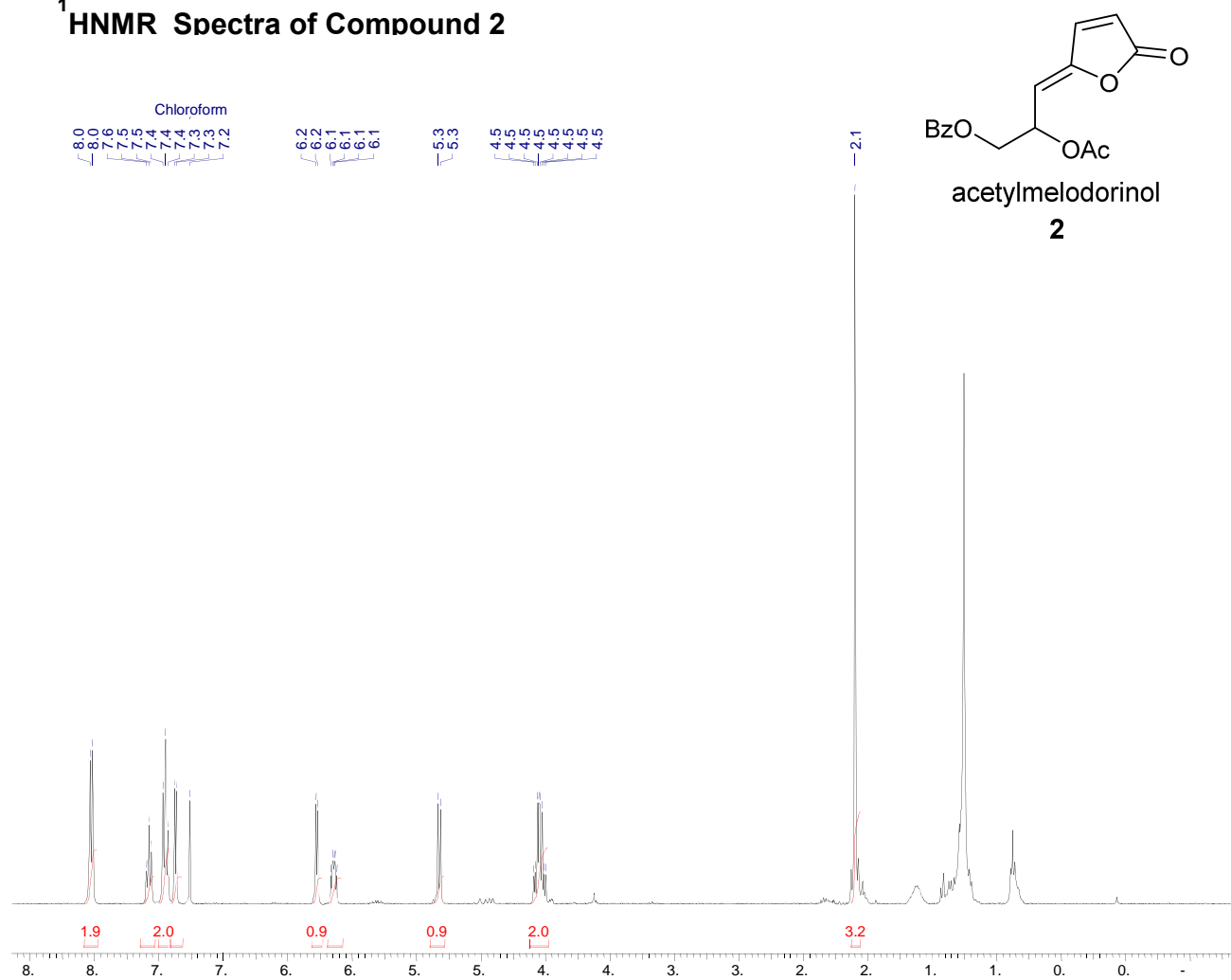
¹³CNMR Spectra of Compound 5

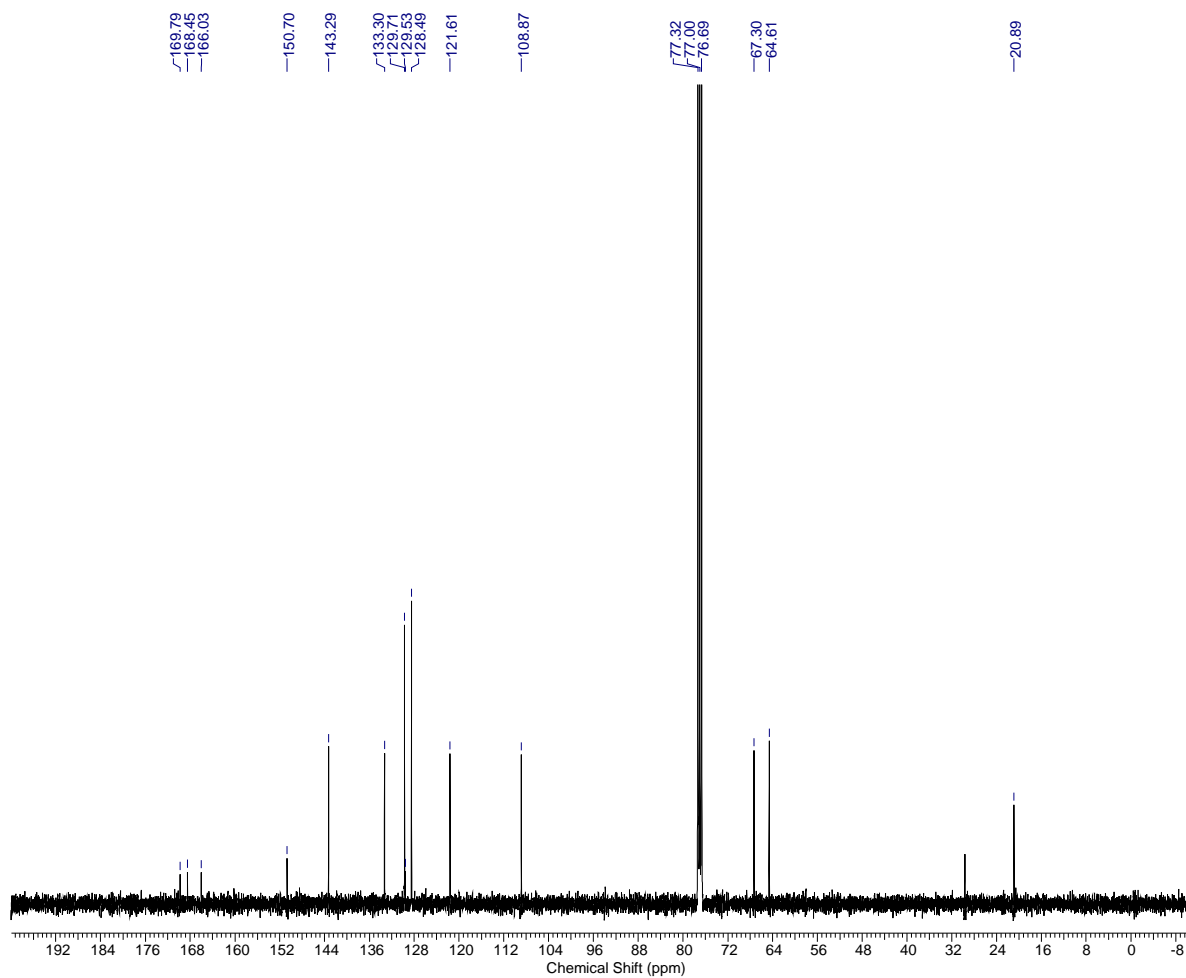


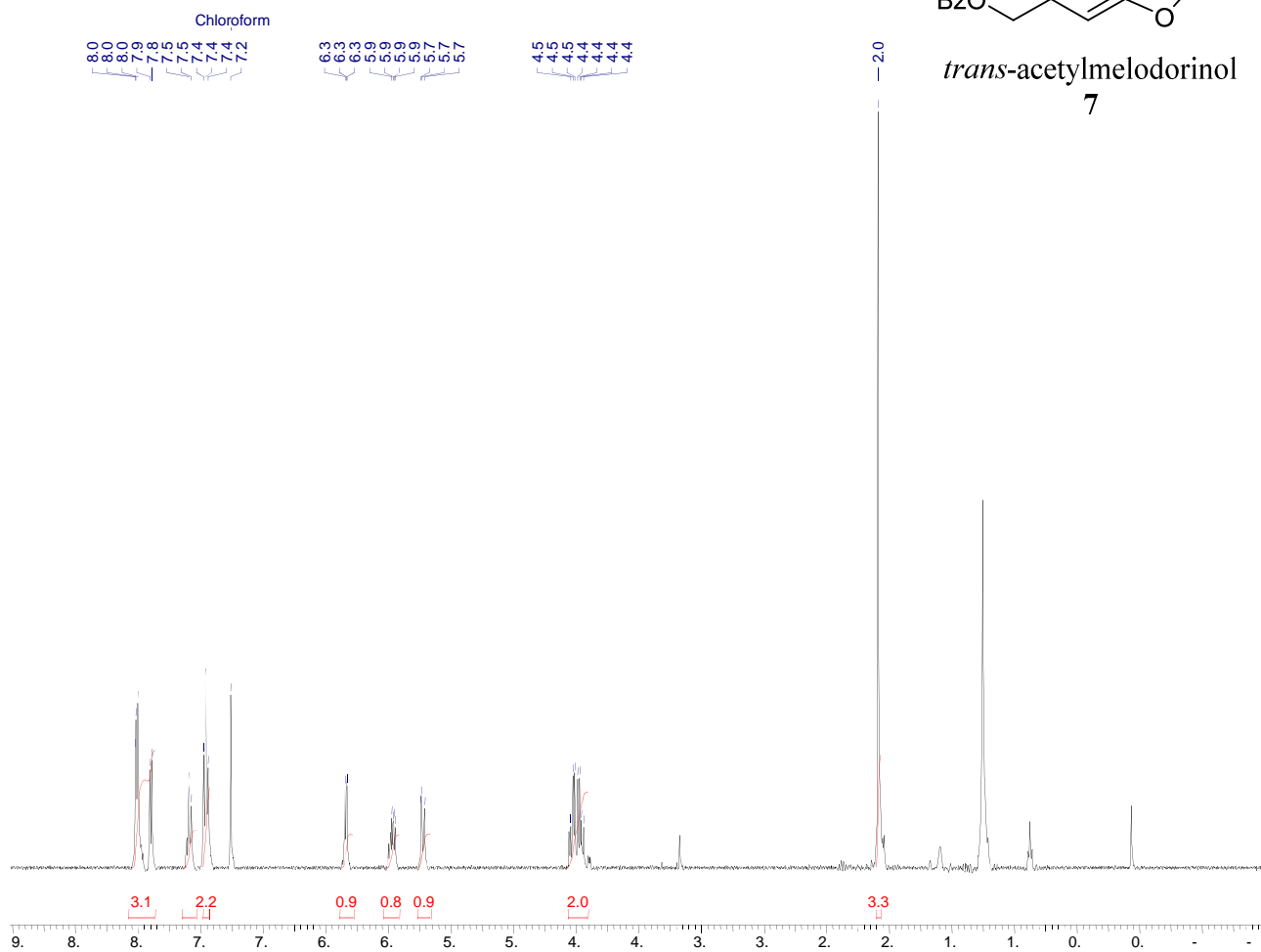
¹H NMR Spectra of Compound 6*trans*-melodorinol**6**

¹³CNMR Spectra of Compound 6

¹H NMR Spectra of Compound 2



¹³C NMR Spectra of Compound 2

¹H NMR Spectra of Compound 7

¹³C NMR Spectra of Compound 7