

Synthesis of revised structure of klaivanolide (acetylmelodorinol)

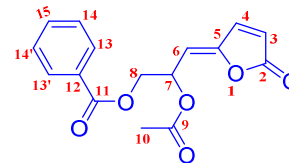
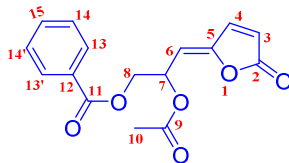
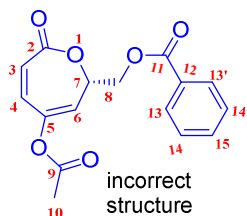
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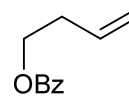
Dedicated to Dr. Jhillu Singh Yadav on the occasion of his 65th Birthday

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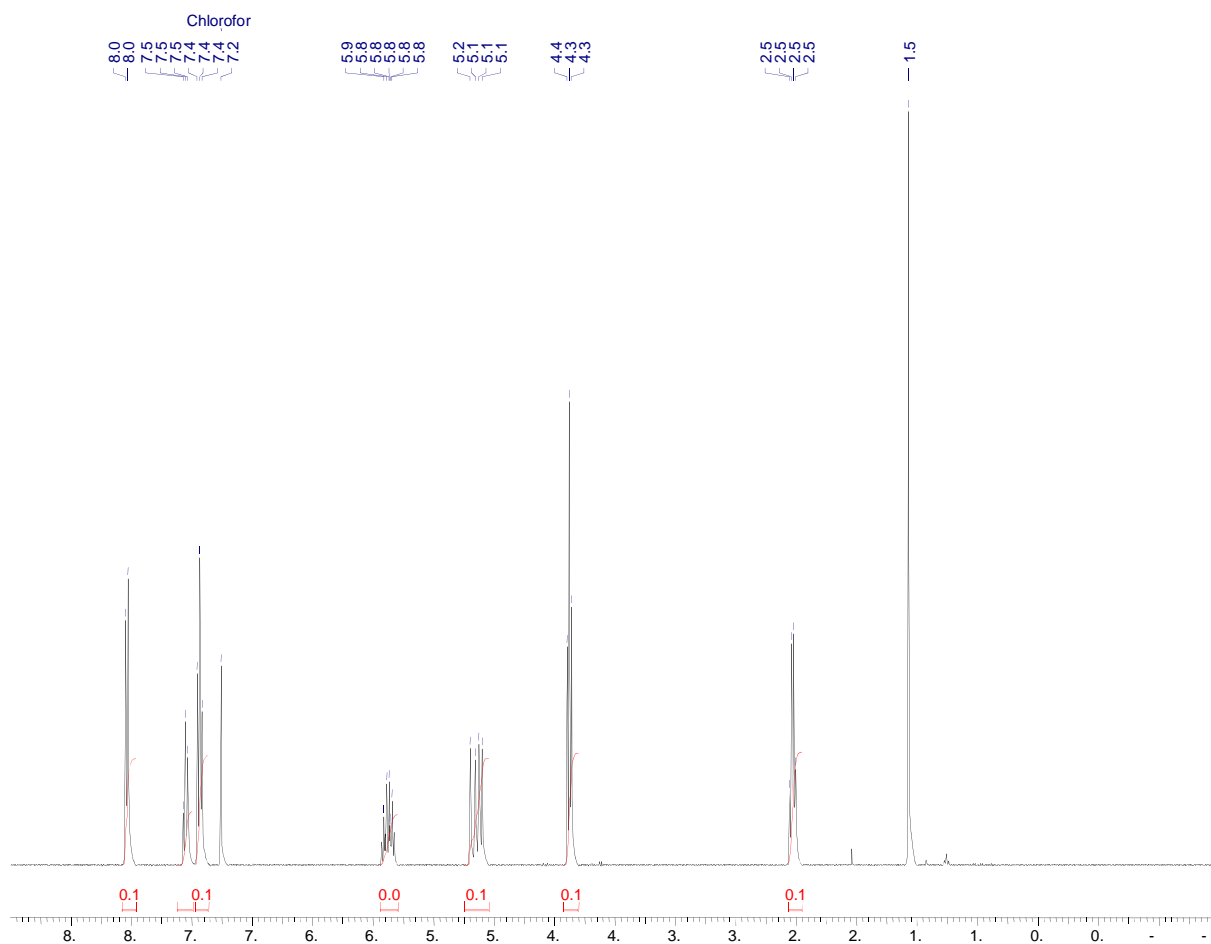
^1H & ^{13}C NMR Comparison Table of Klaivanolide and Acetylmelodorinol

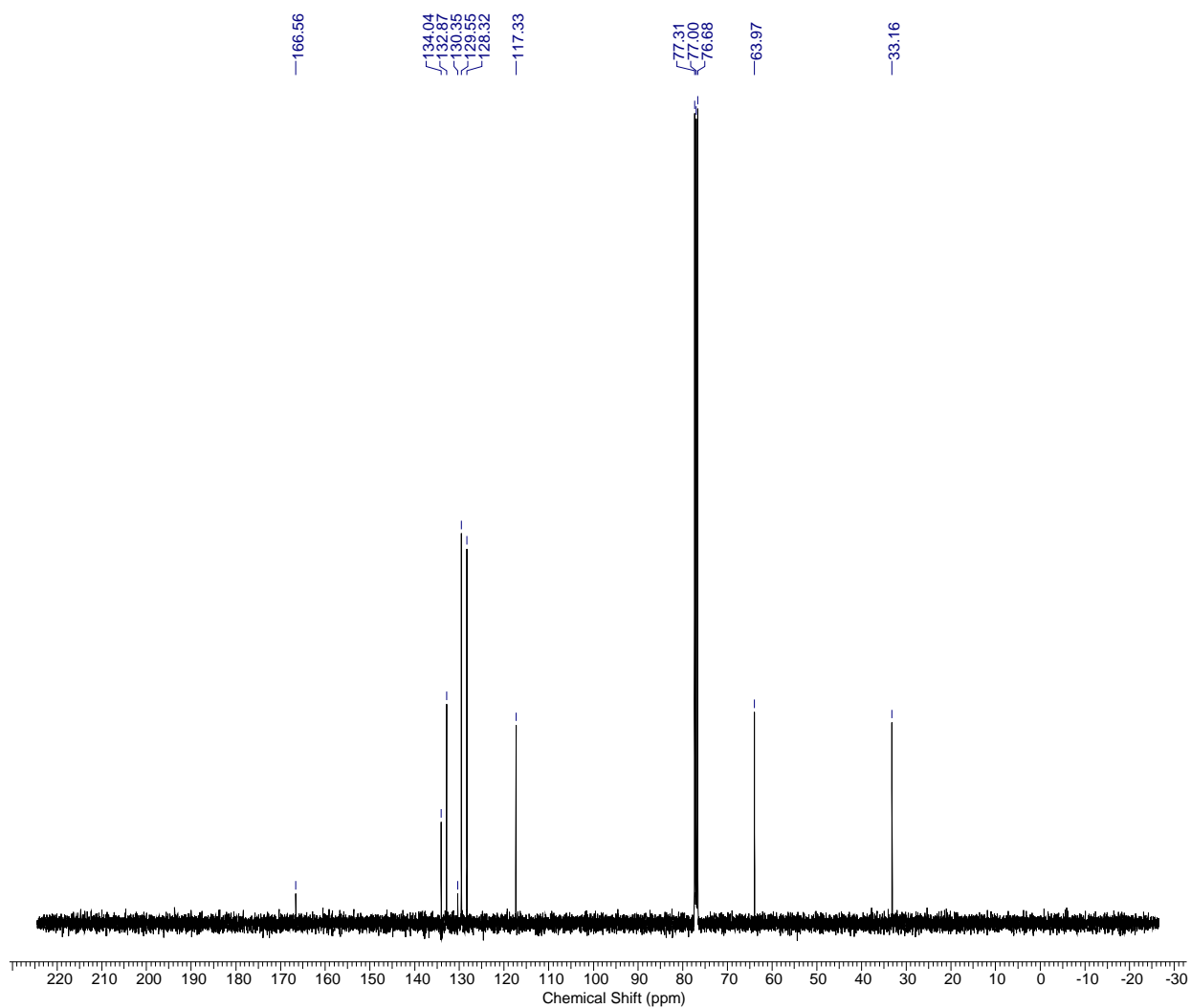
| | Klaivanolide <i>Phytochemistry</i> , 2002 , 59, 885 | | Acetylmelodorinol <i>Tetrahedron</i> 1990 , 46, 5043 | | Synthesized acetylmelodorinol (2) | |
|---------|--|------------------|--|------------------|---|------------------|
| | δH | δC | δH | δC | δH | δC |
| 1 | | | | | | |
| 2 | | 168.4 |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

¹H and ¹³C NMR spectra of compounds

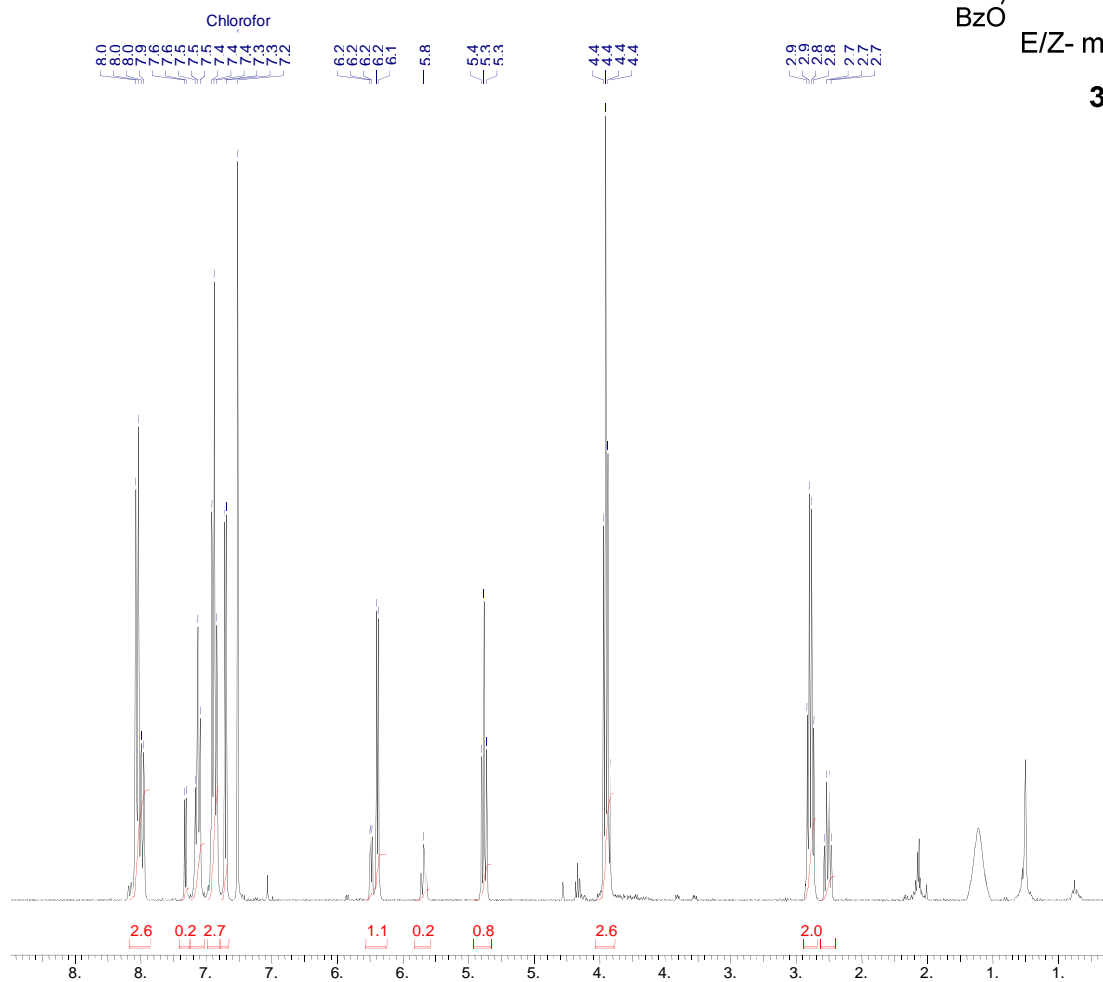
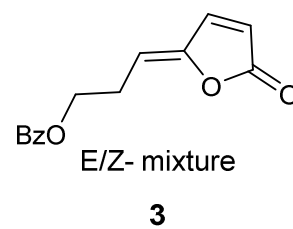


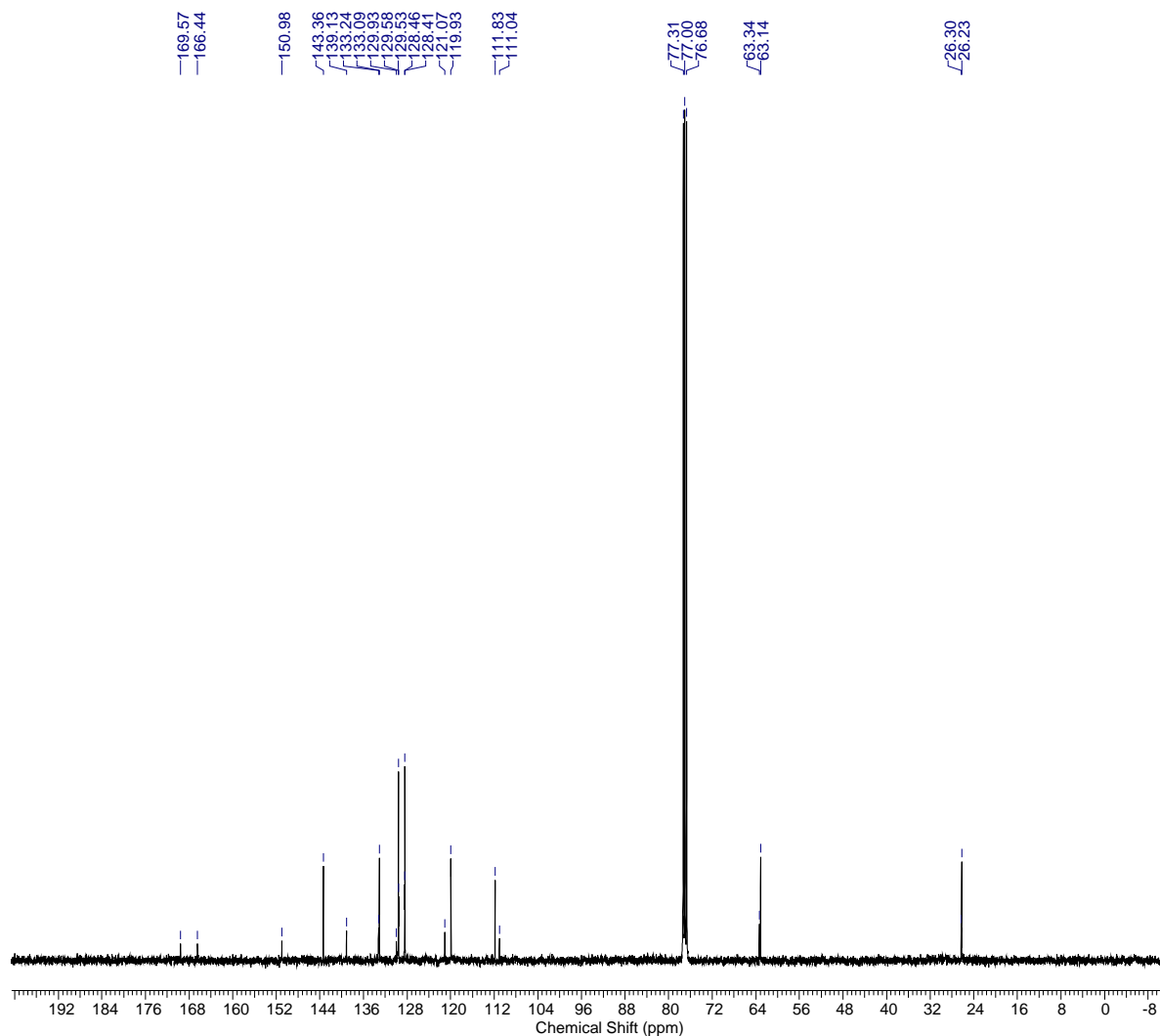
¹H NMR Spectra of 3-butenyl benzoate



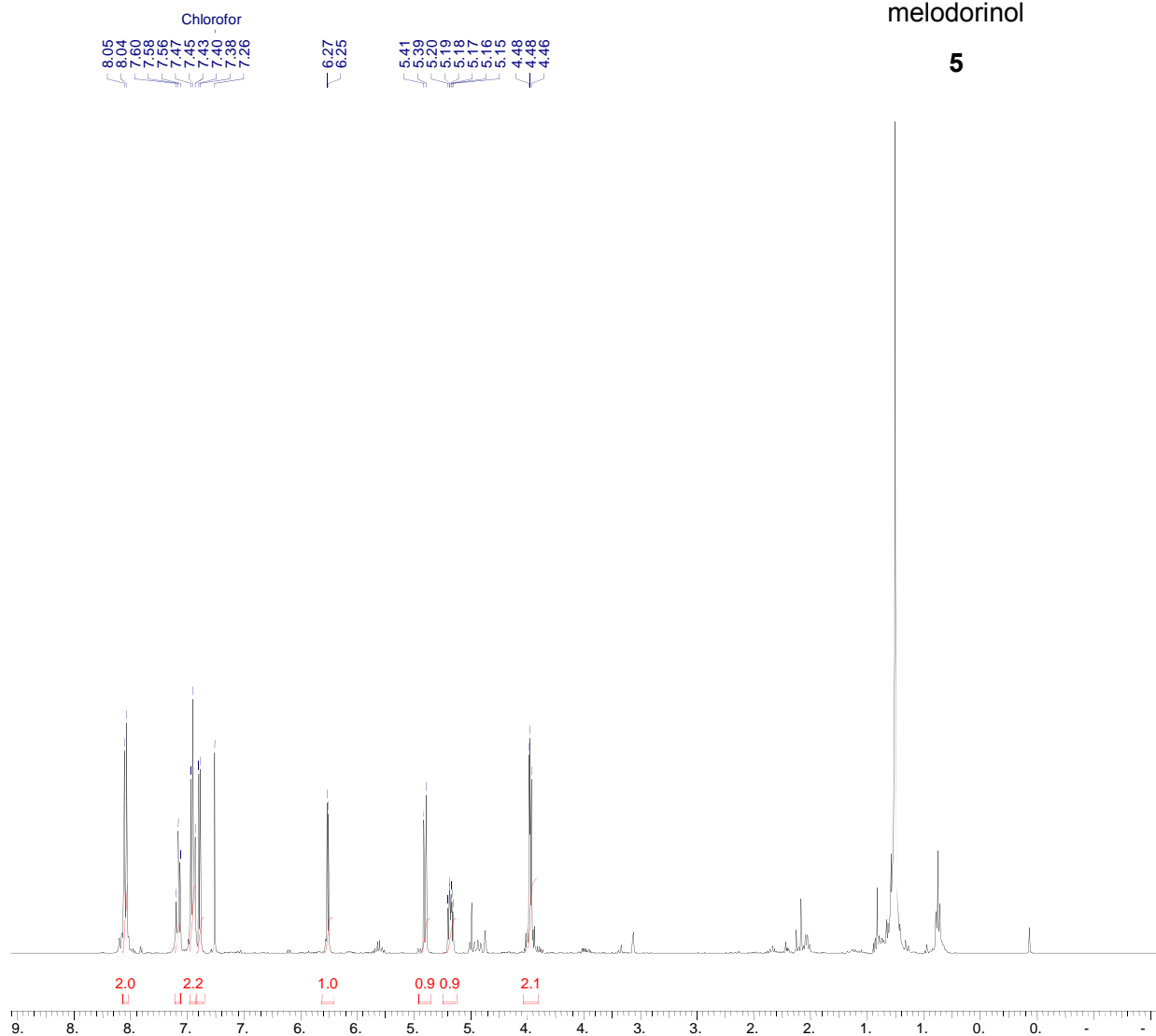
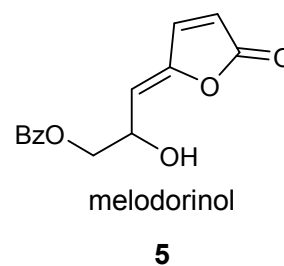
¹³CNMR Spectra of 3-butenyl benzoate

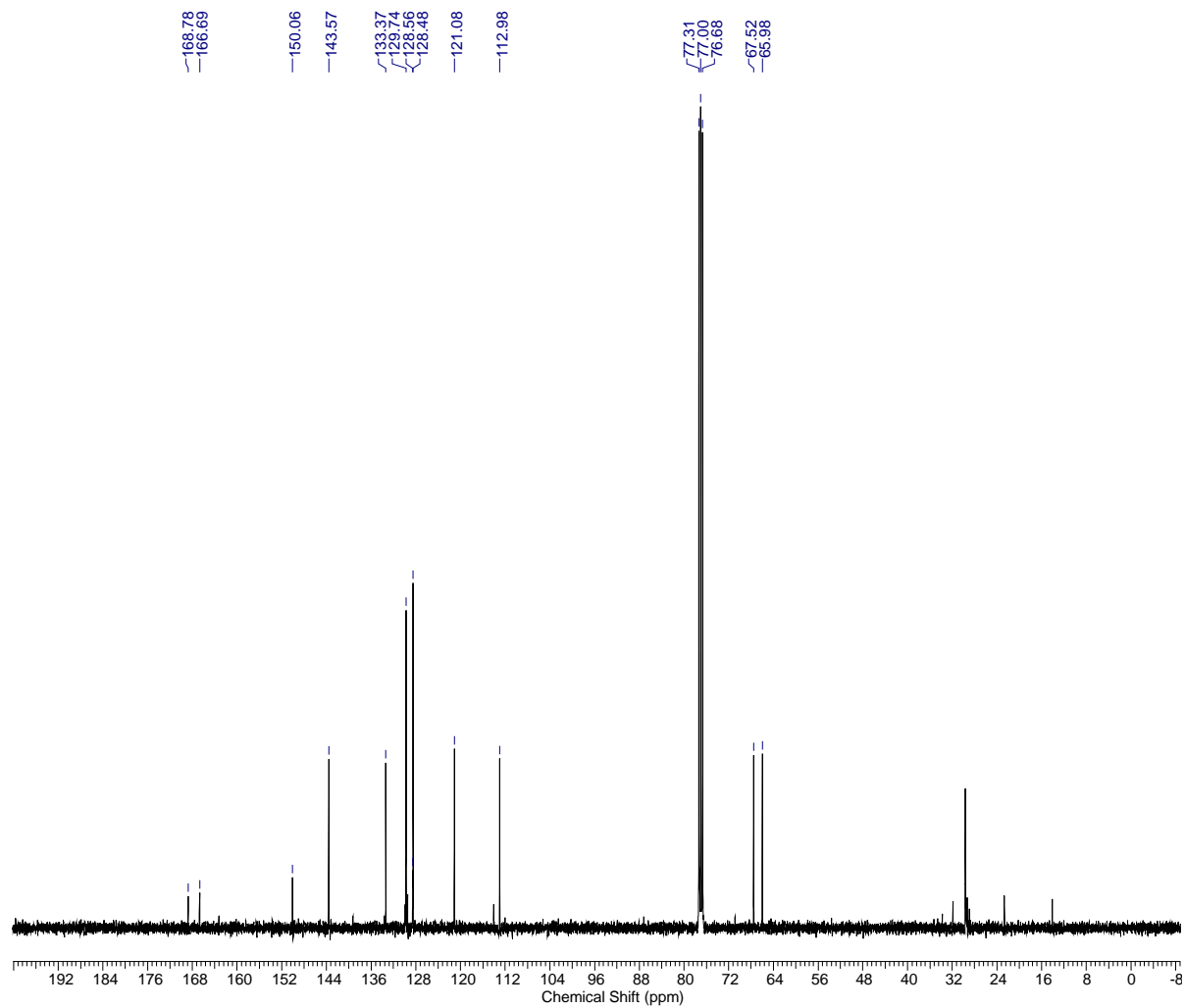
¹H NMR Spectra of Compound 3

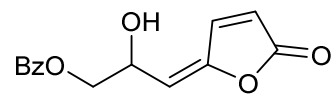
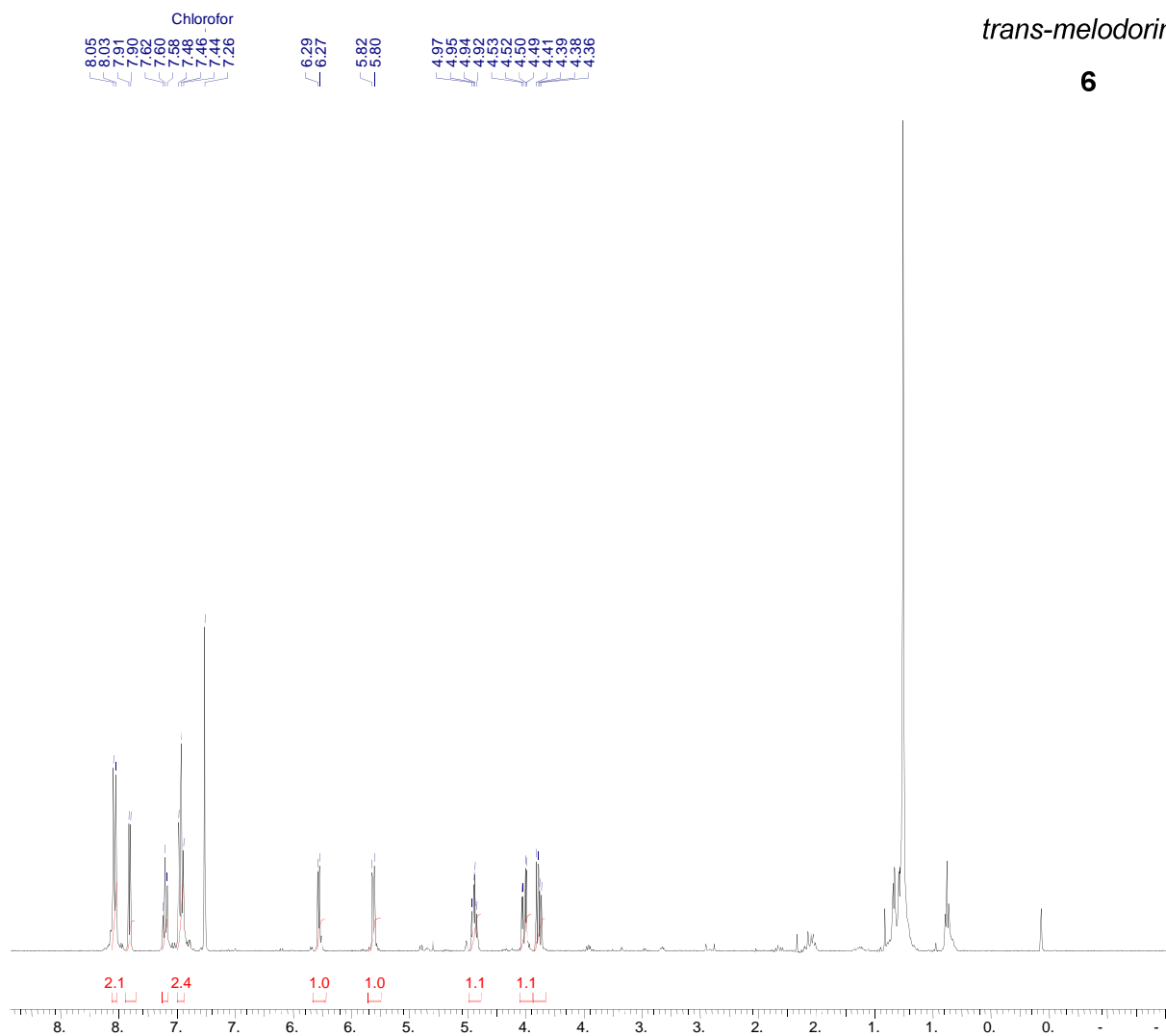


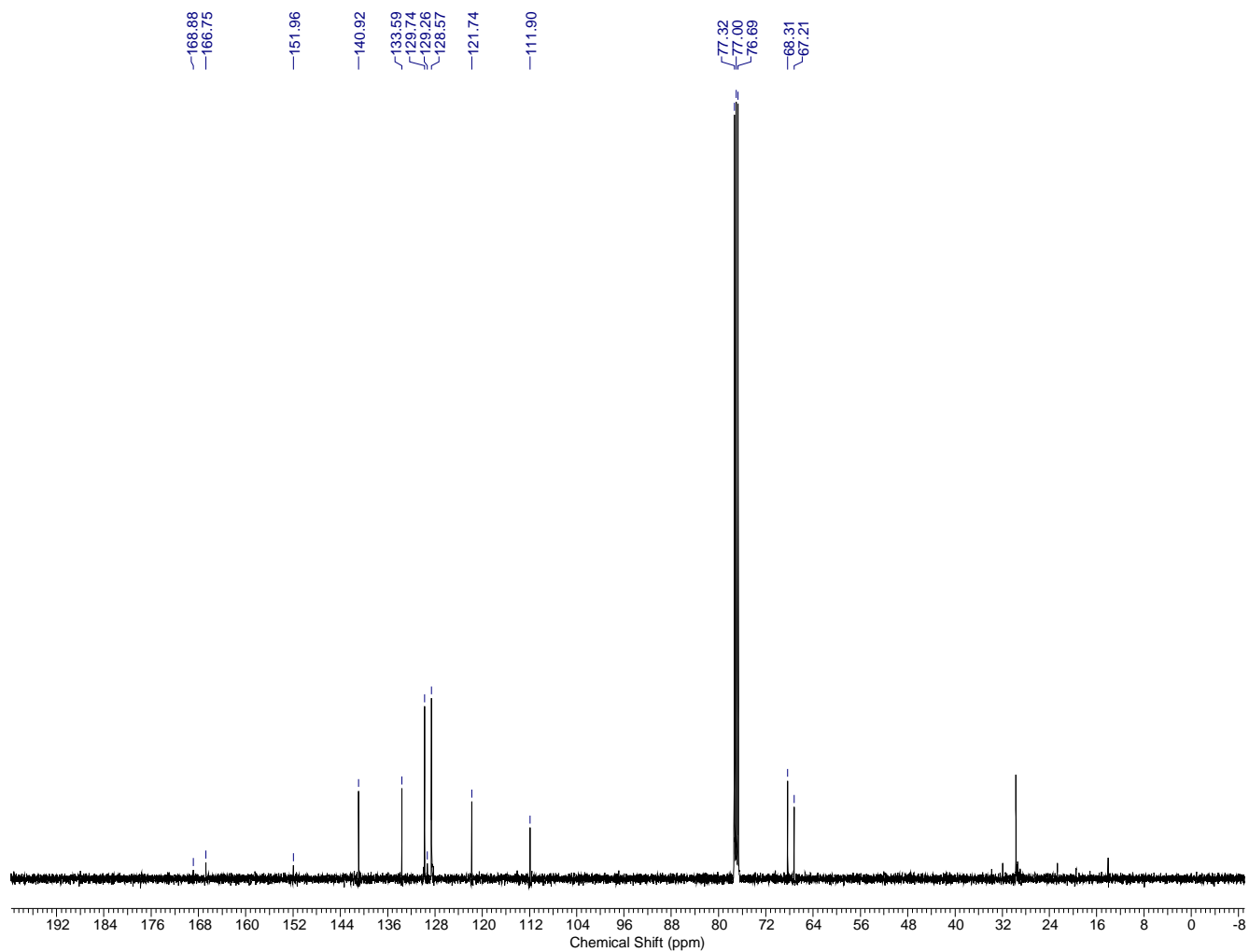
¹³C NMR Spectra of Compound 3

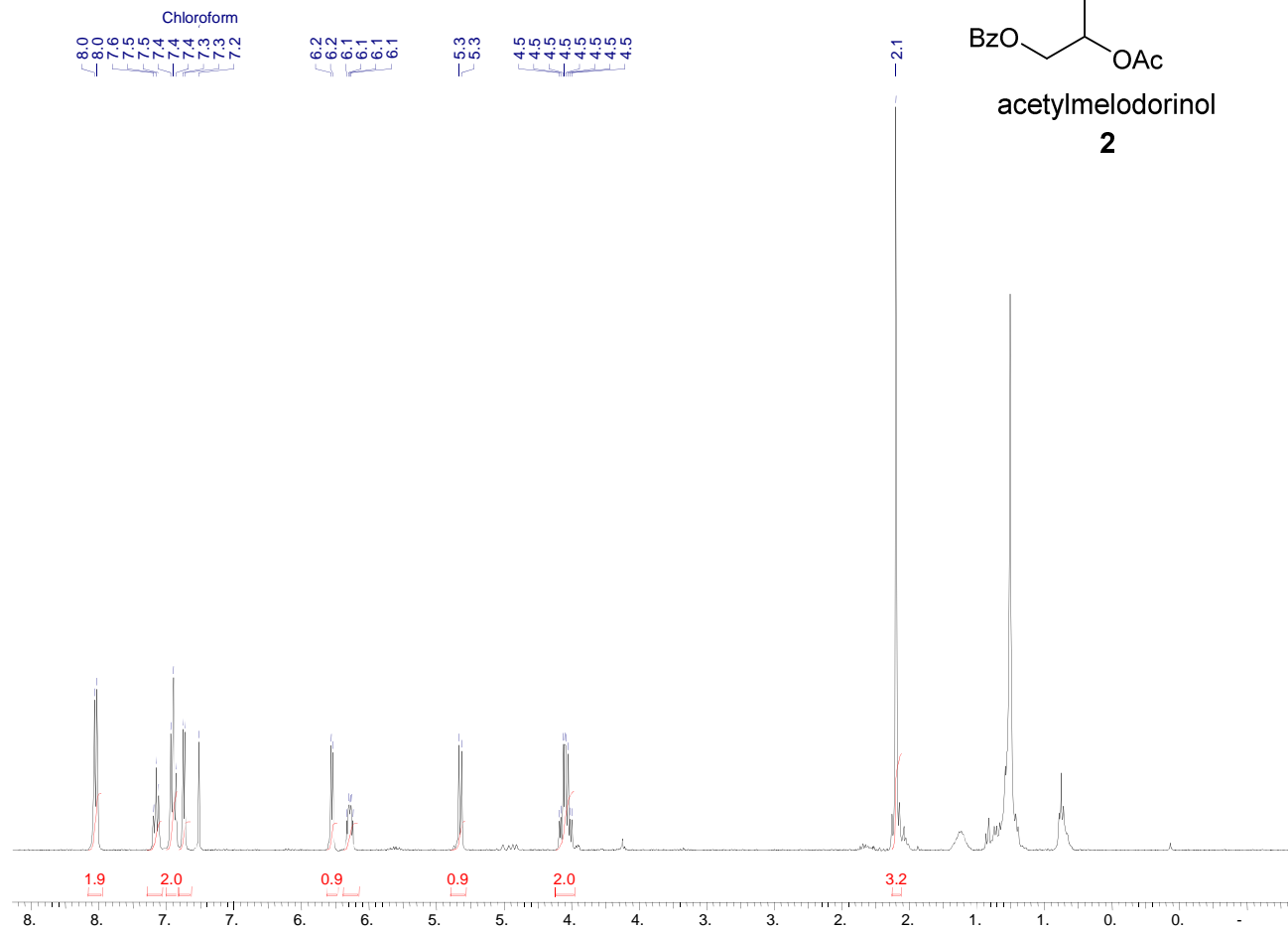
¹HNMR Spectra of Compound 5

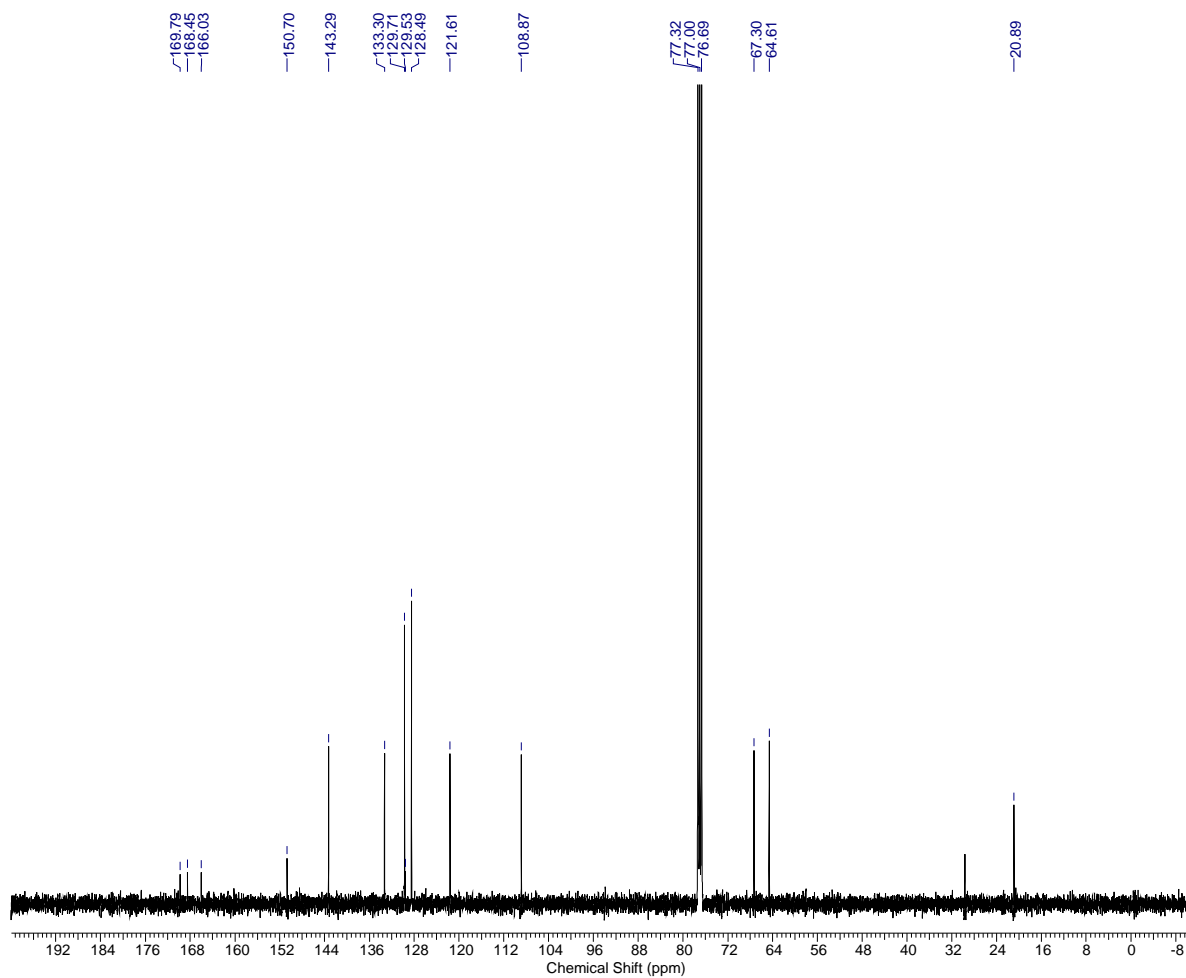


¹³CNMR Spectra of Compound 5

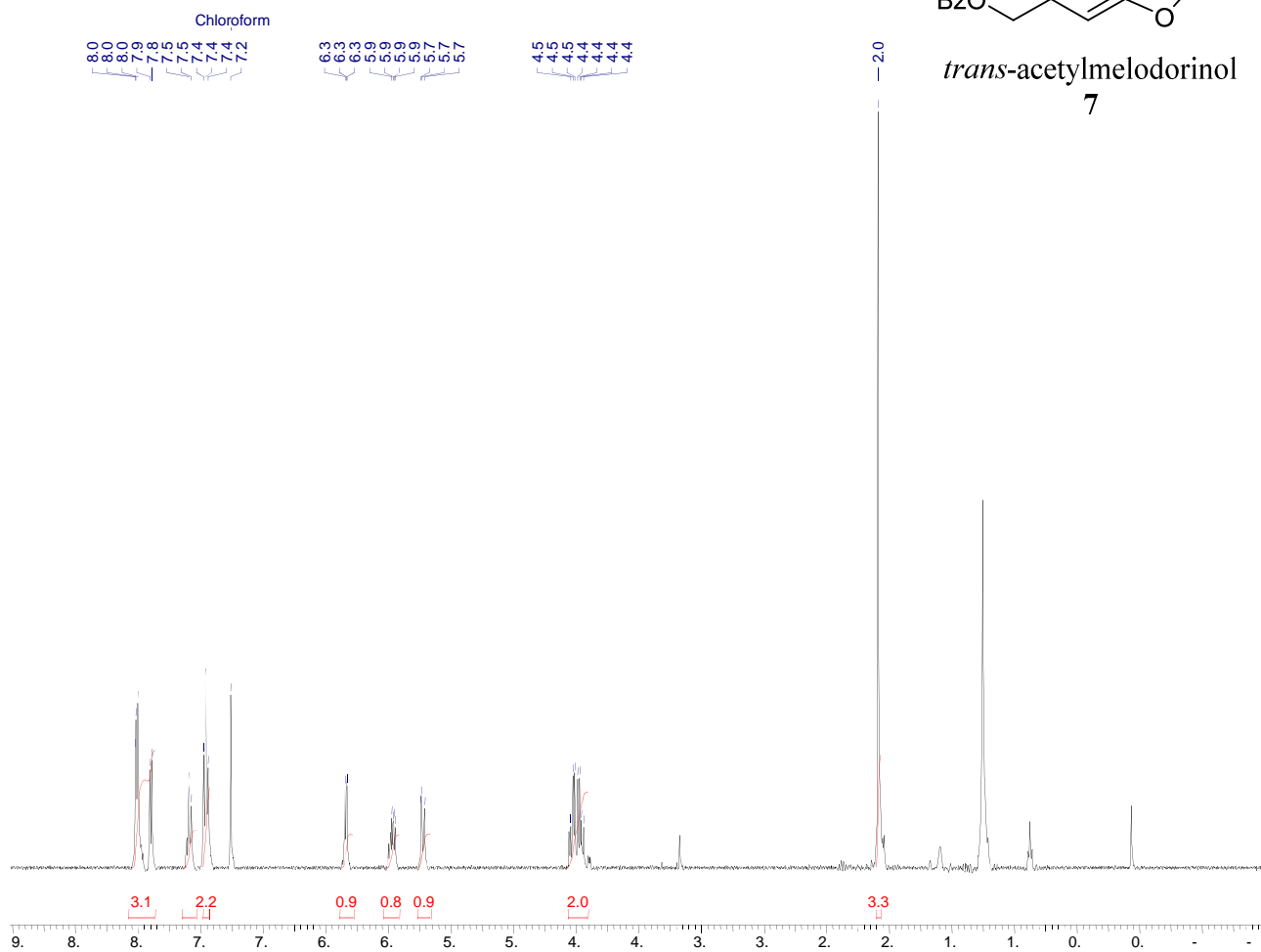
¹H NMR Spectra of Compound 6*trans*-melodorinol**6**

¹³CNMR Spectra of Compound 6

¹H NMR Spectra of Compound 2

¹³CNMR Spectra of Compound 2

¹H NMR Spectra of Compound 7



¹³C NMR Spectra of Compound 7