

Supplementary Material

Photoinduced Cycloadditions in the Diversity-Oriented Synthesis Toolbox: Increasing Complexity with Straightforward Postphotochemical Modifications

*Weston J. Umstead, Olga A. Mukhina, N. N. Bhuvan Kumar and Andrei G. Kutateladze**

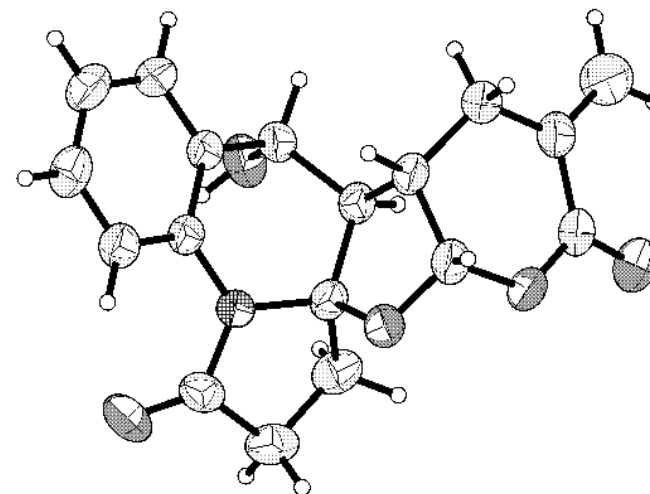
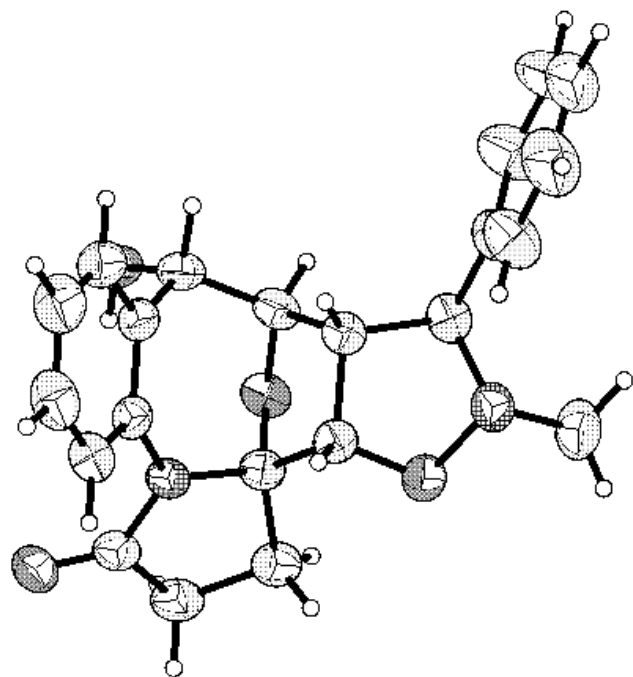
Department of Chemistry and Biochemistry, University of Denver, Denver, CO 80208

akutatel@du.edu

Contents

| | |
|--|---|
| Xray structures of compounds 7 and 12 " | 2 |
| ¹³ C NMR chemical shifts of compound 9 | 3 |
| NMR spectra of the products..... | 4 |

Xray structures of compounds 7 and 12''



7



^{13}C NMR chemical shifts of compound **9**

^{13}C NMR chemical shifts were calculated at the b3lyp/6-311+G(d,p)//b3lyp/6-31G(d) level of theory for both *exo*-COOR and *endo*-COOR stereoisomers of α -chloroester **9** and linearly corrected for the experimental chemical shift values. Figure S1 shows that the rmsd for the *endo* isomer was twice better than that of the *exo* isomer. The largest deviations were associated with the carbons most proximal to the C(Cl)COOR moiety.

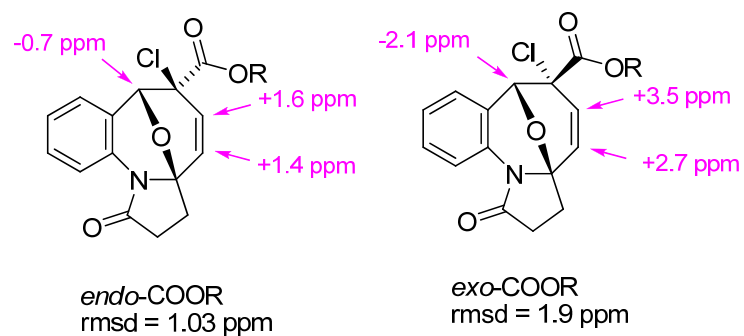
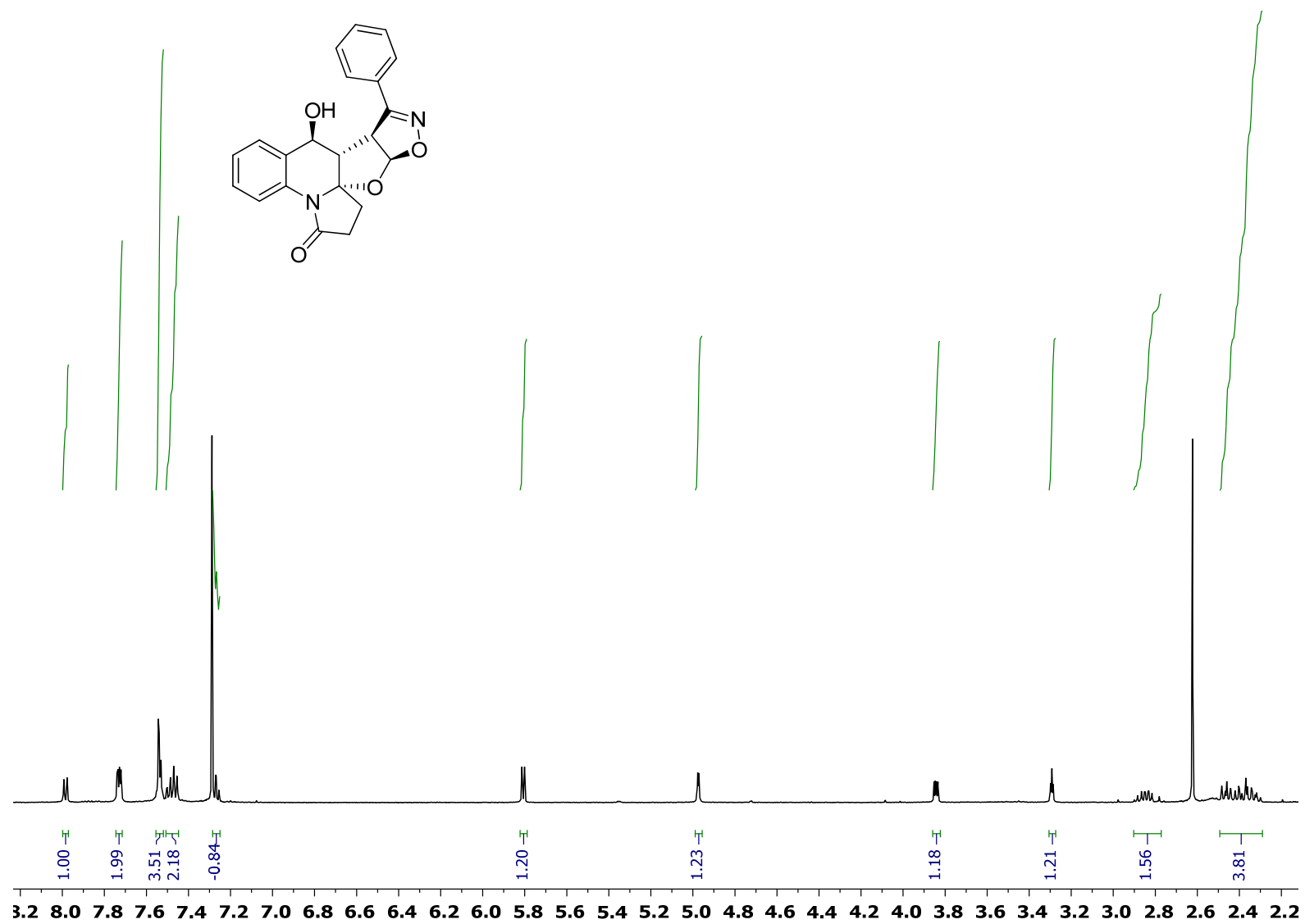
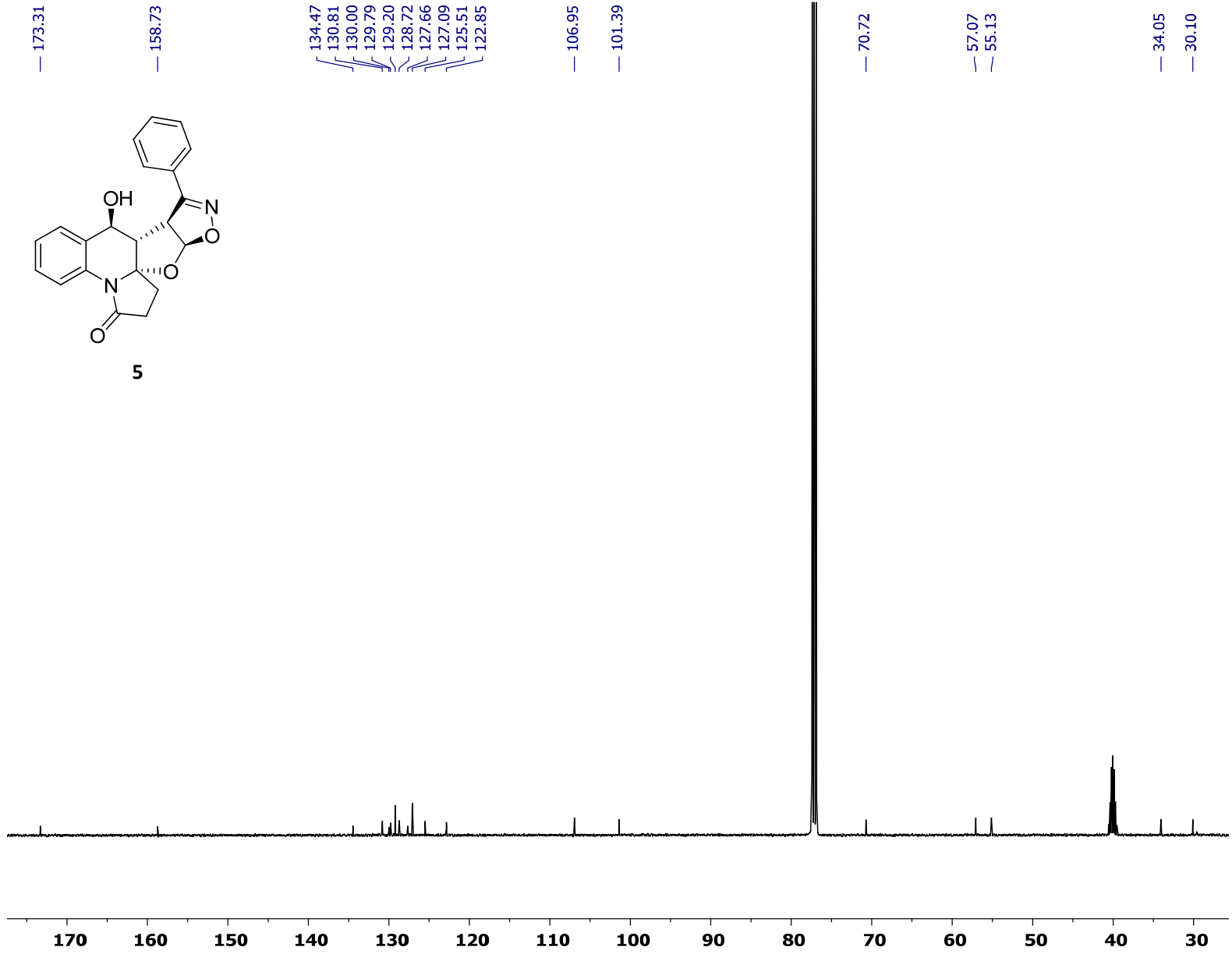
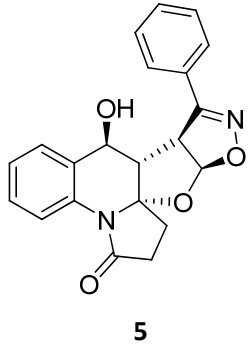
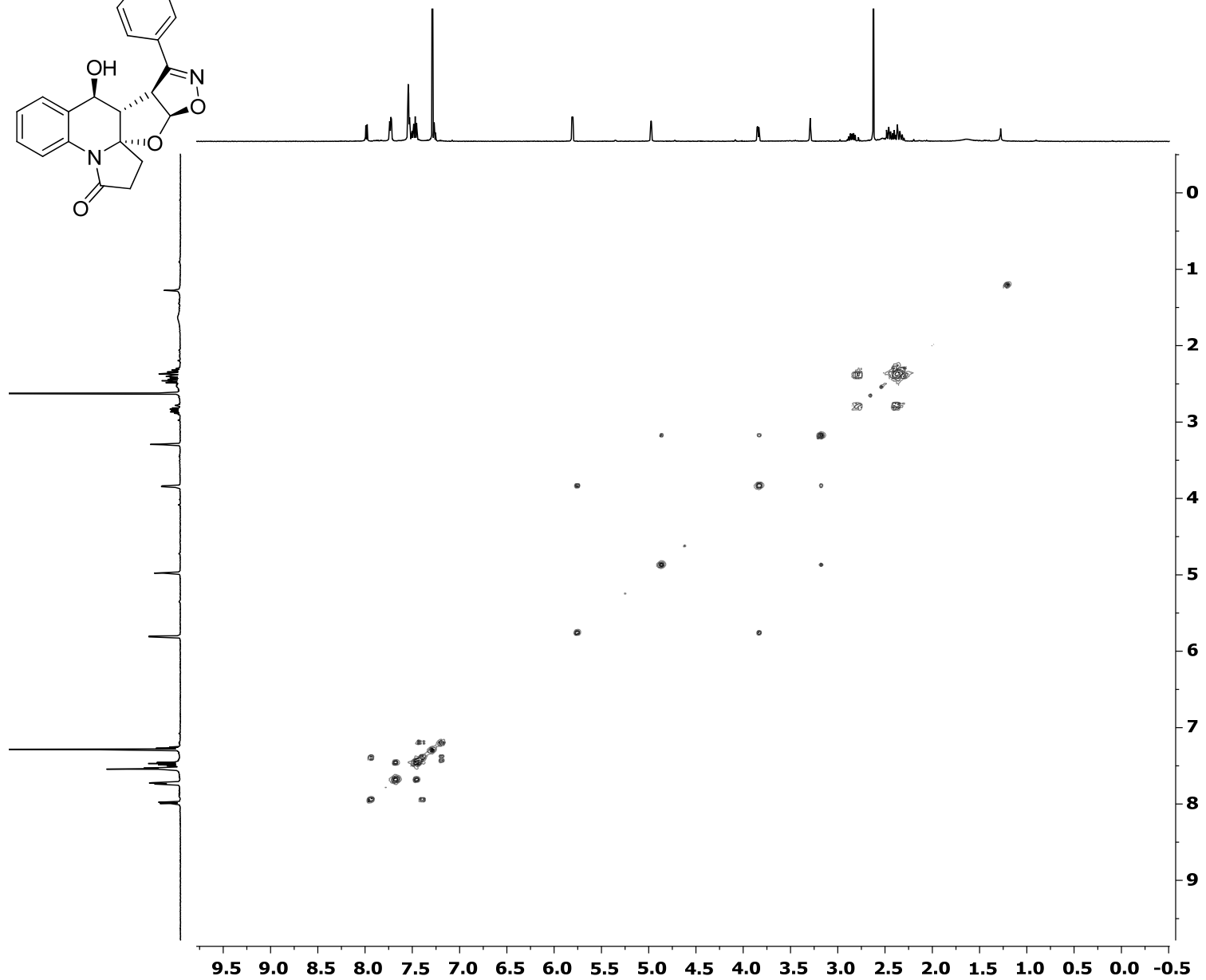
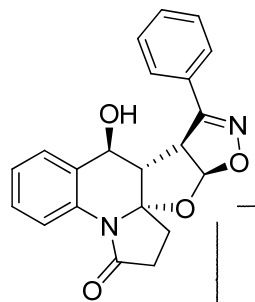


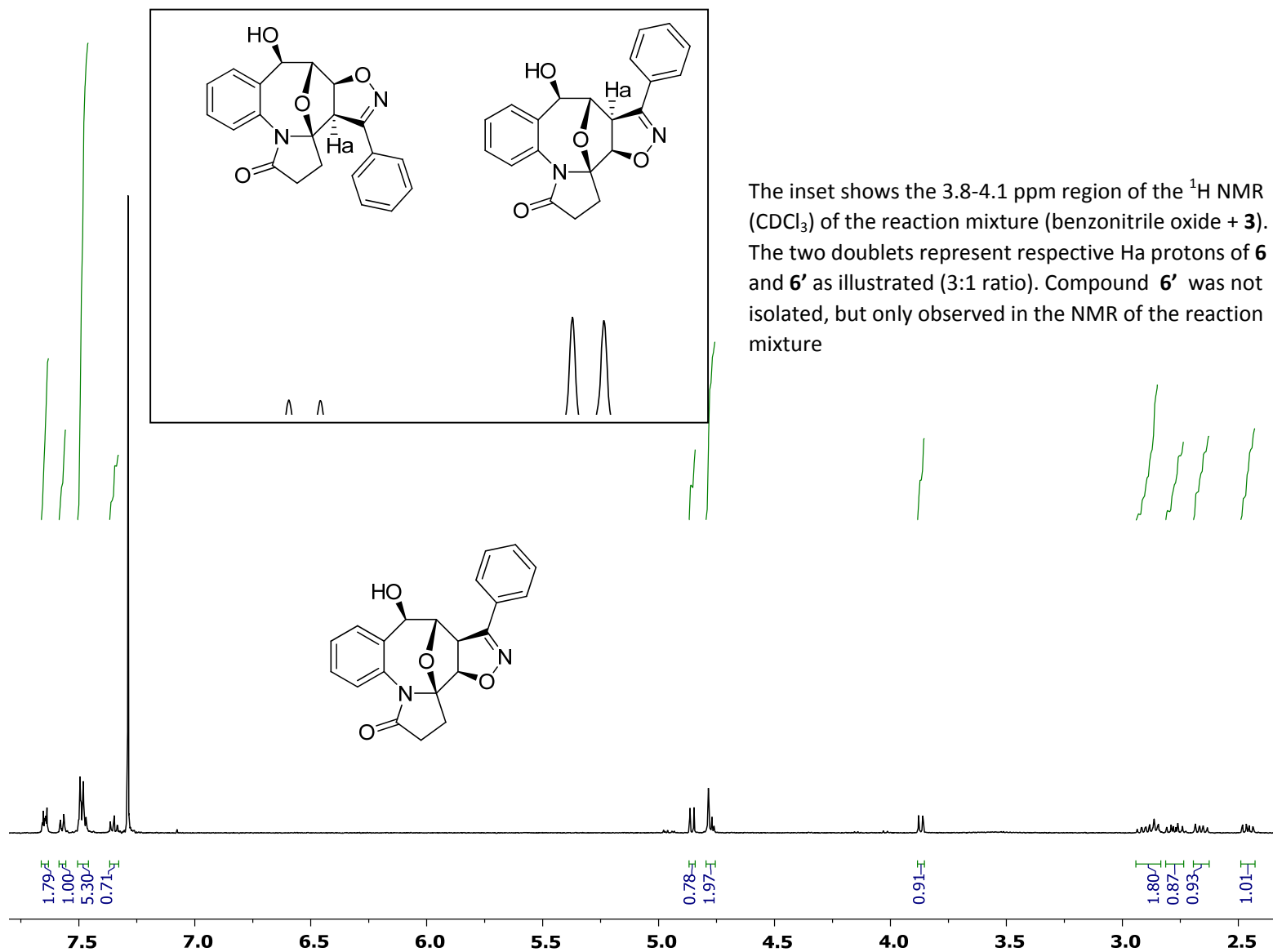
Figure S1. ^{13}C NMR chemical shifts computed for the *endo*-COOR stereoisomer fit experimental values much better (the largest deviations are shown in magenta).

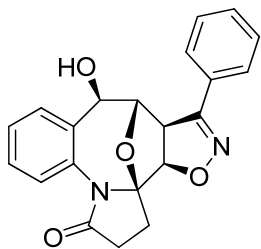
NMR spectra of the products



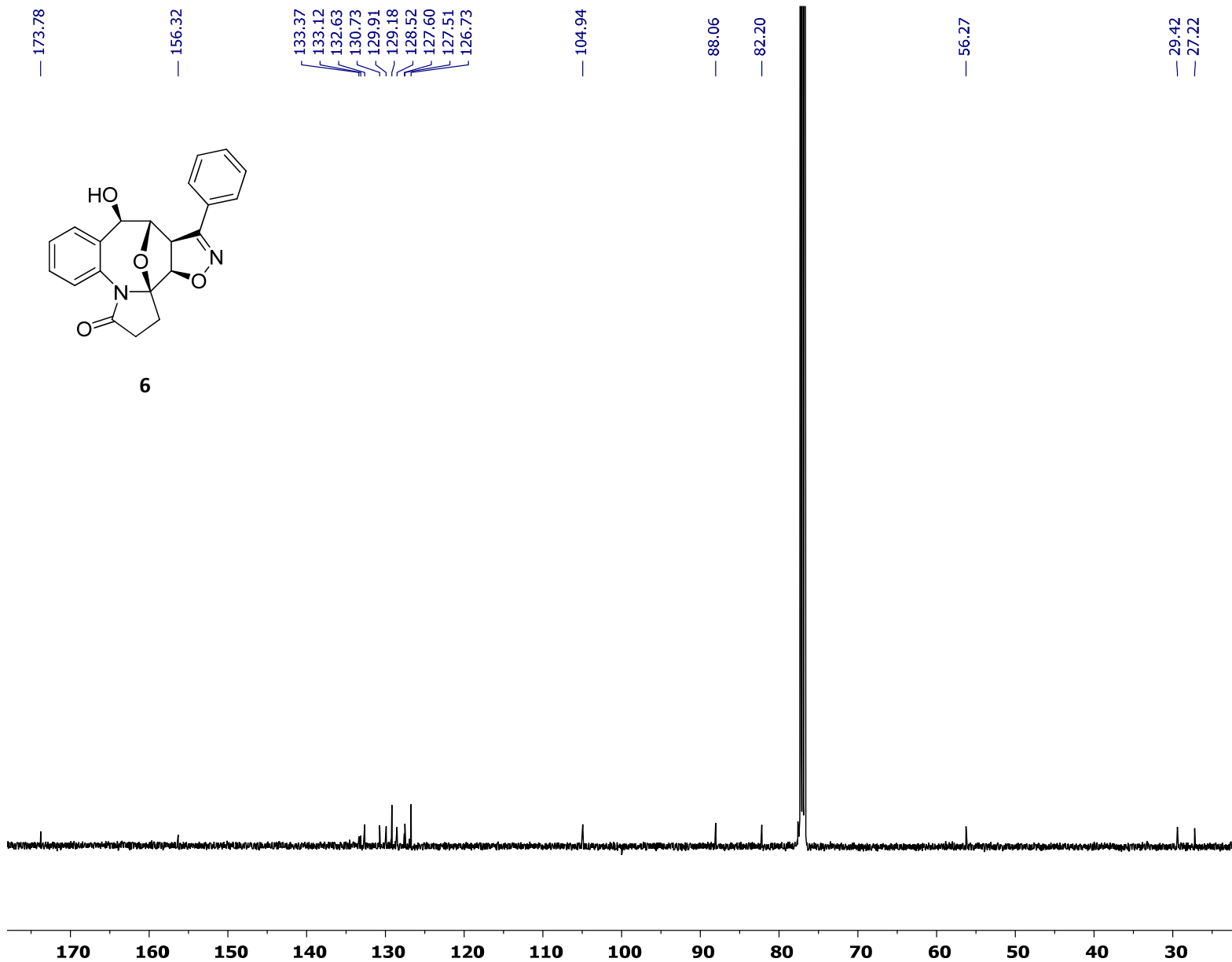


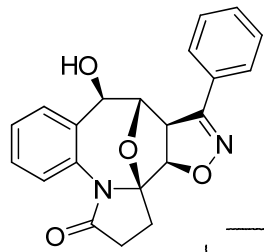




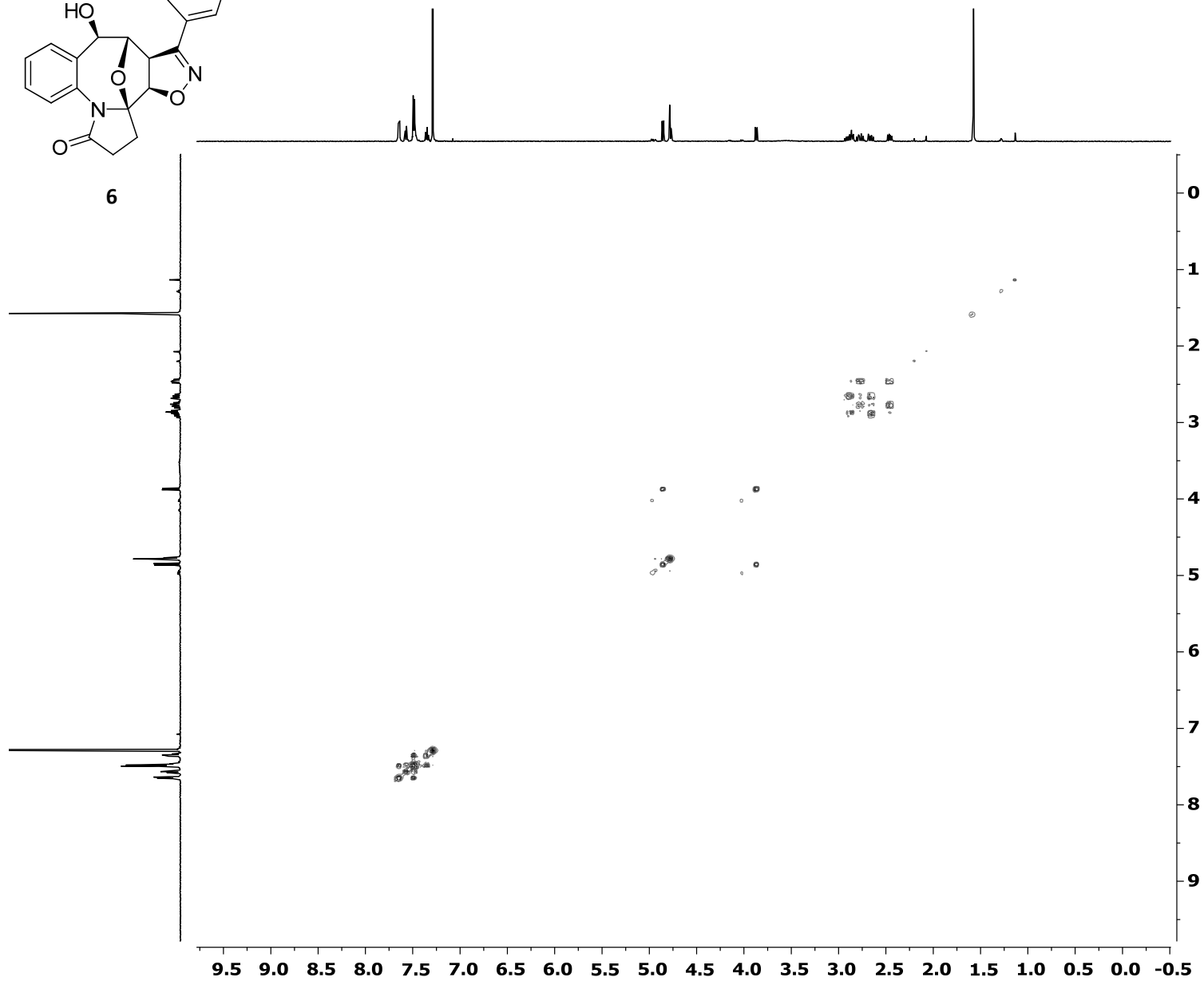


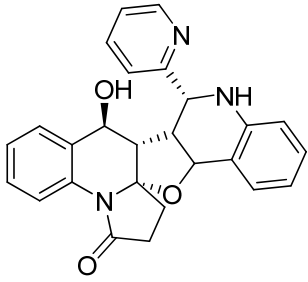
6



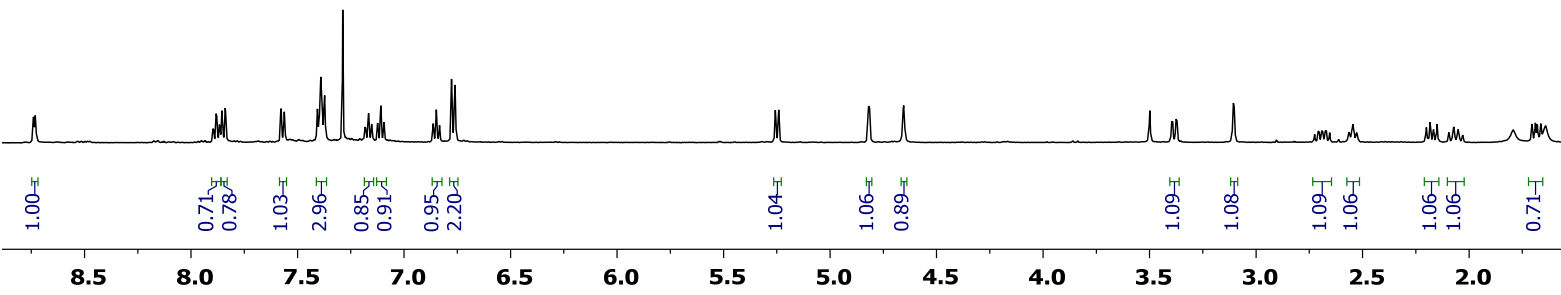
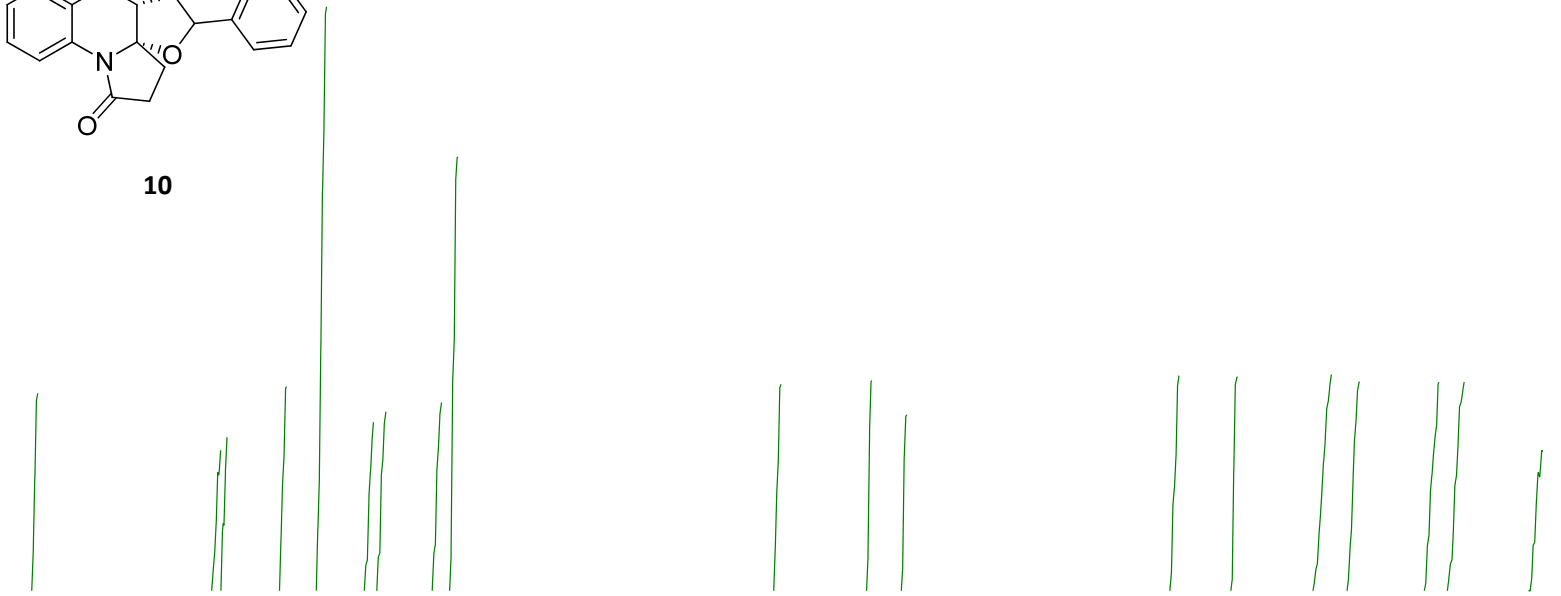


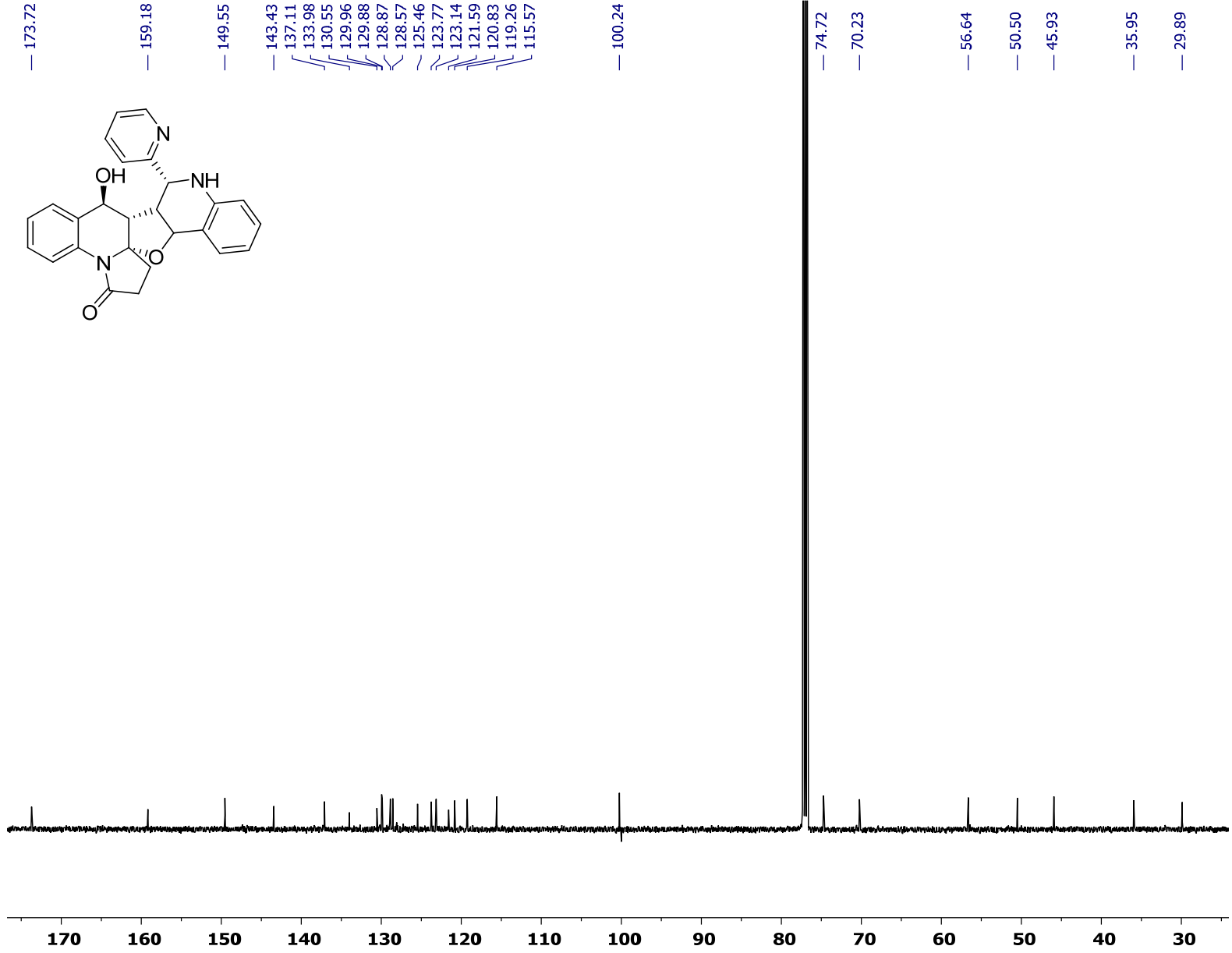
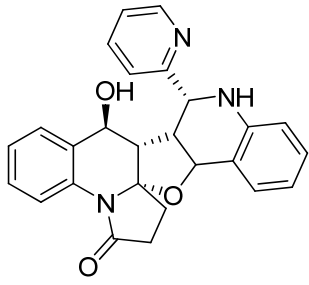
6

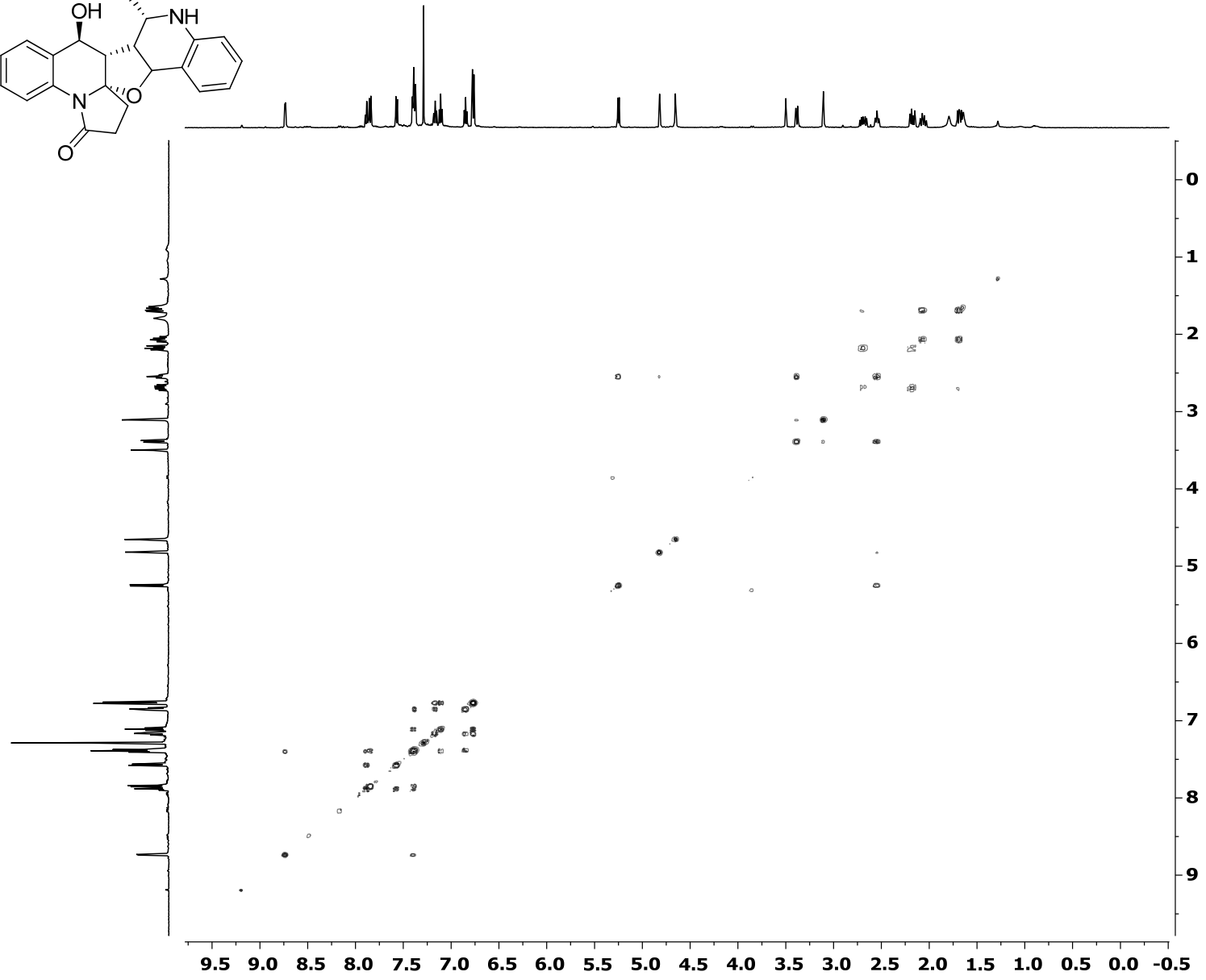
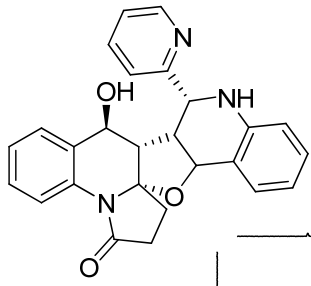


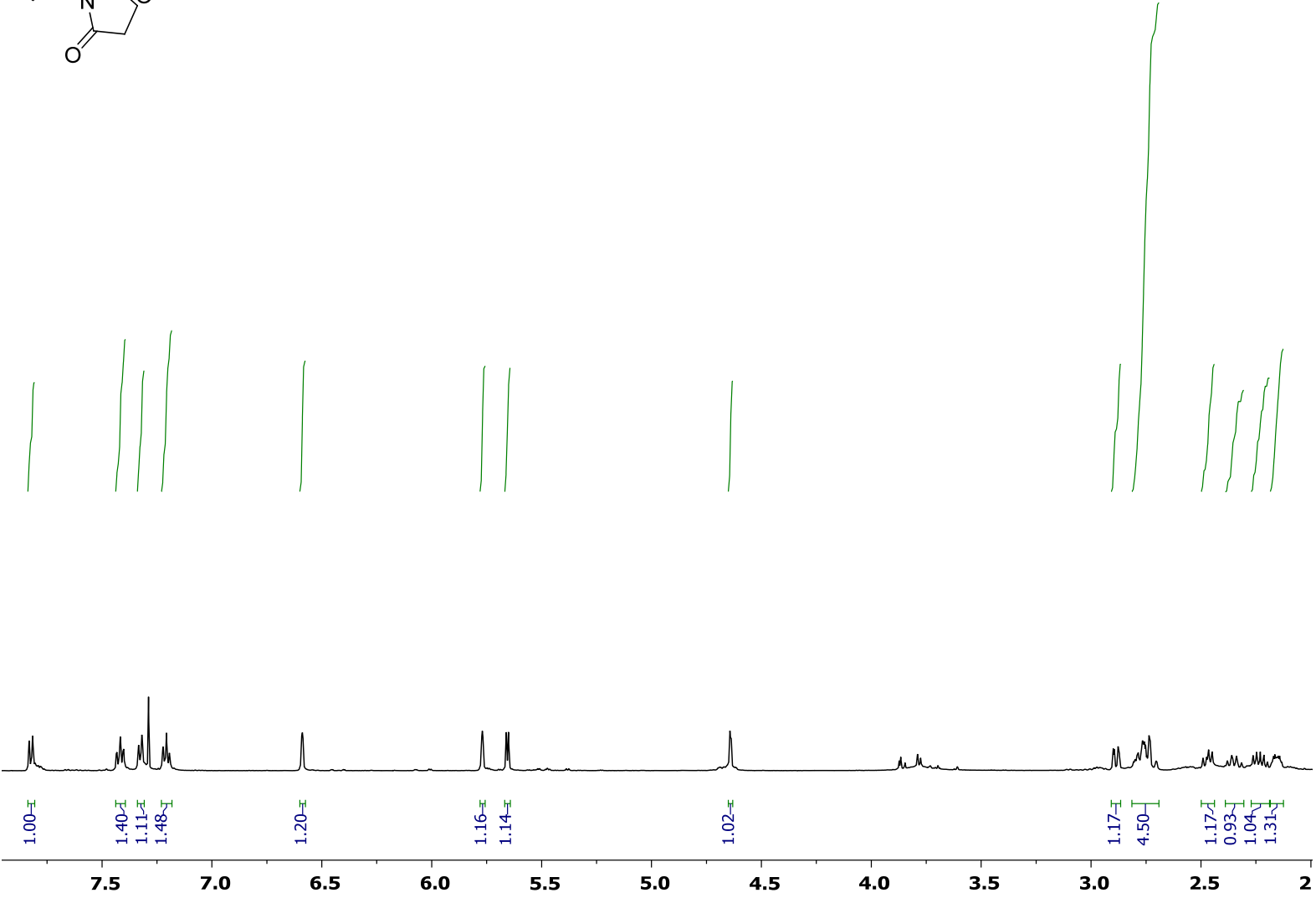
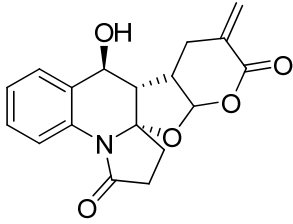


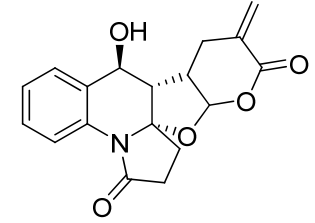
10











173.72
173.70

163.47

133.43
130.89
130.04
130.01
129.82
129.29
125.85
123.77

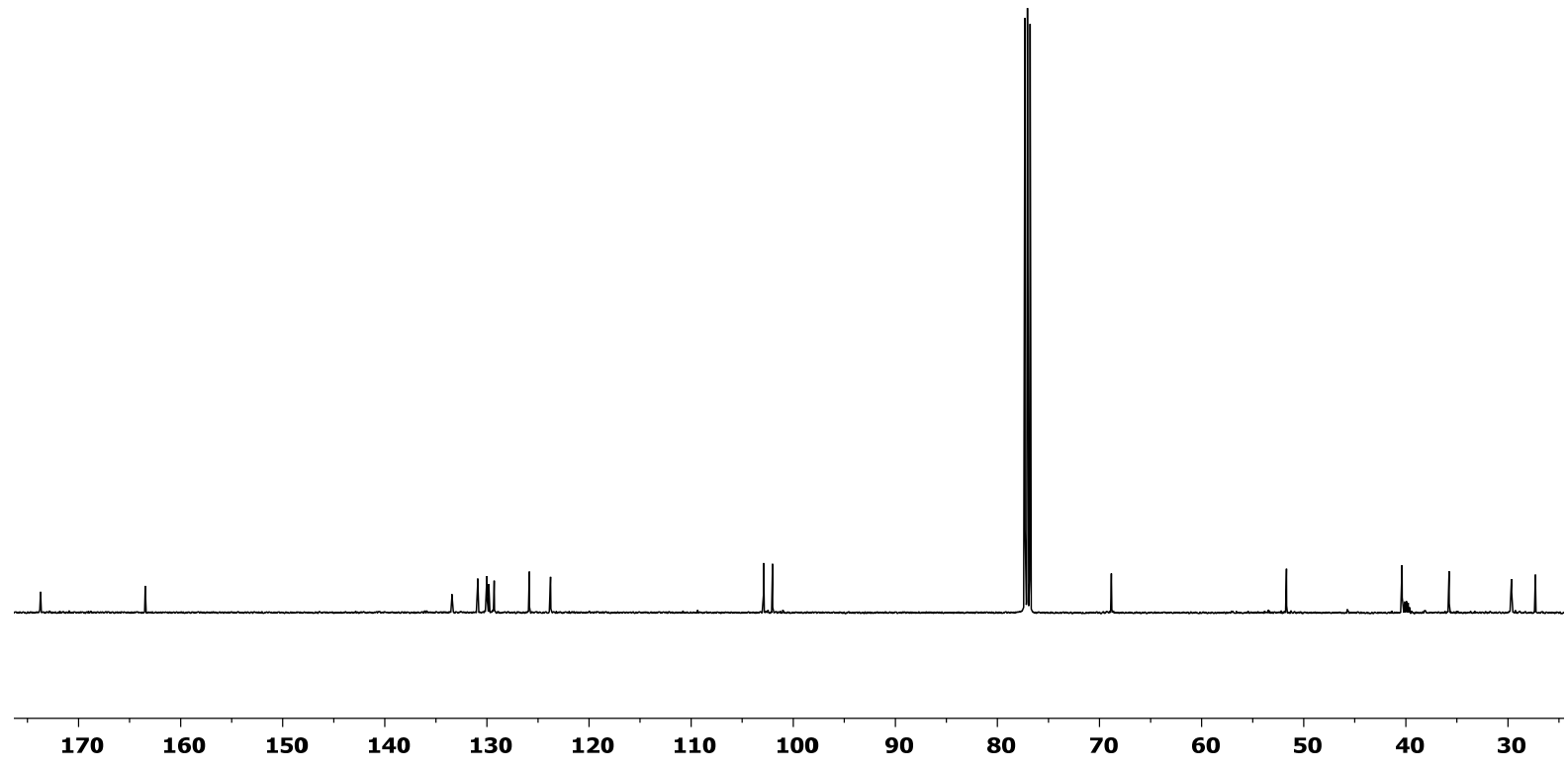
102.89
102.02

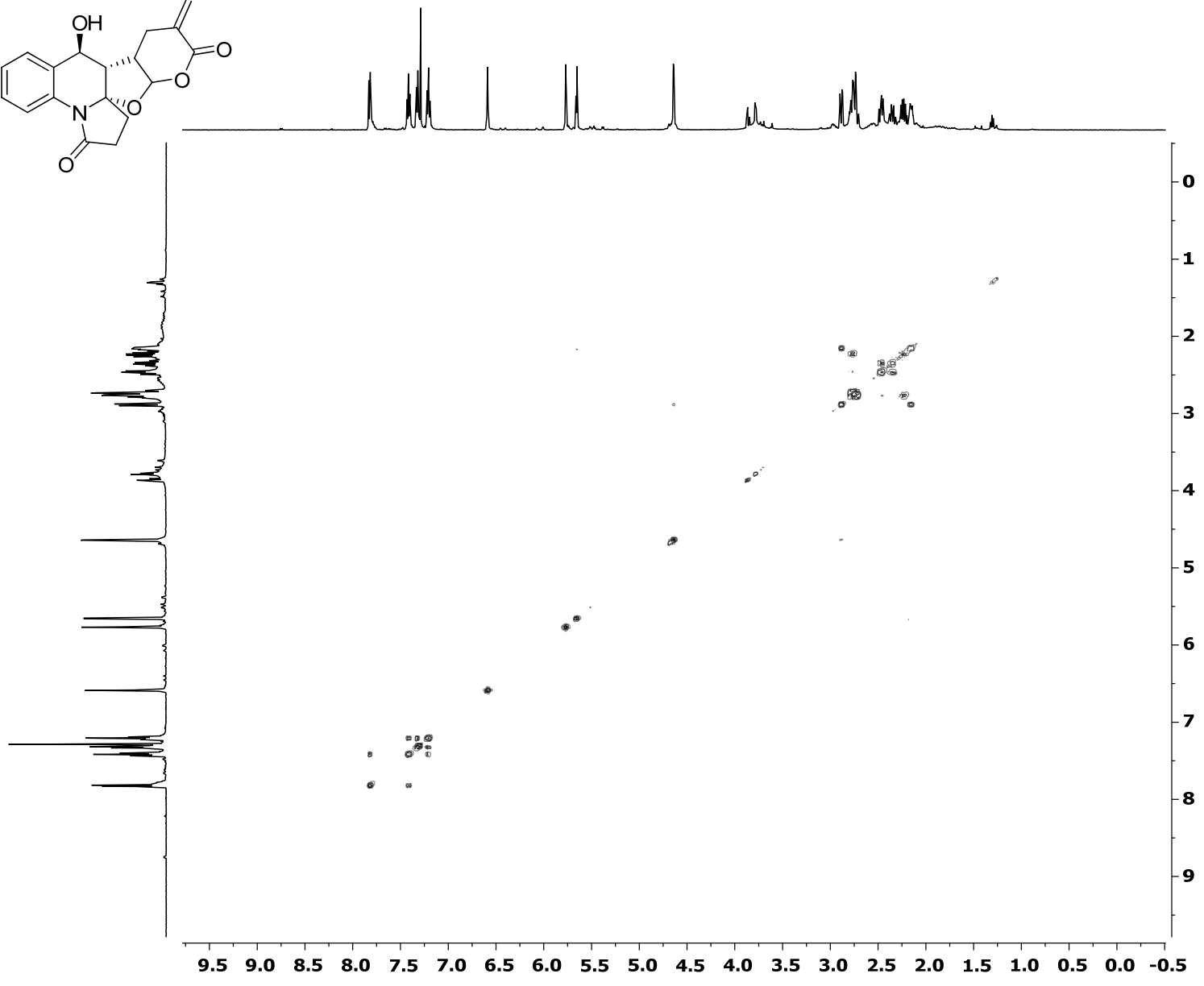
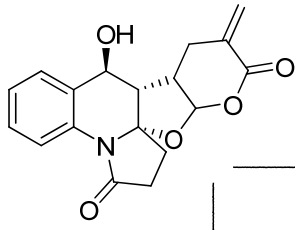
68.84

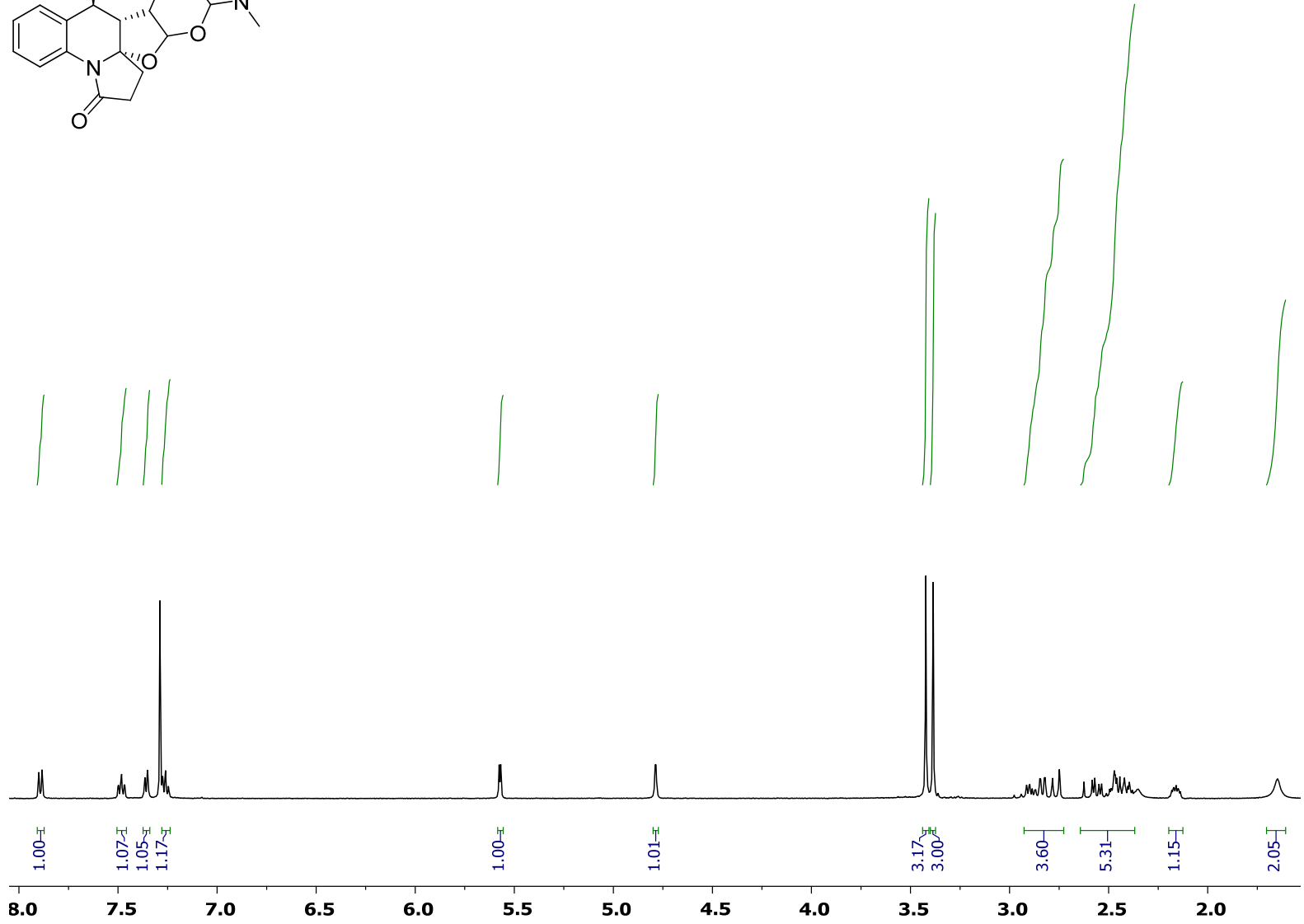
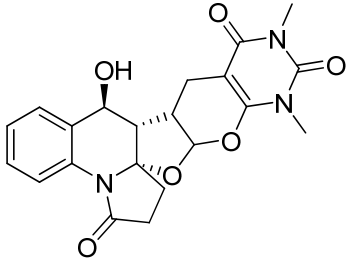
51.69

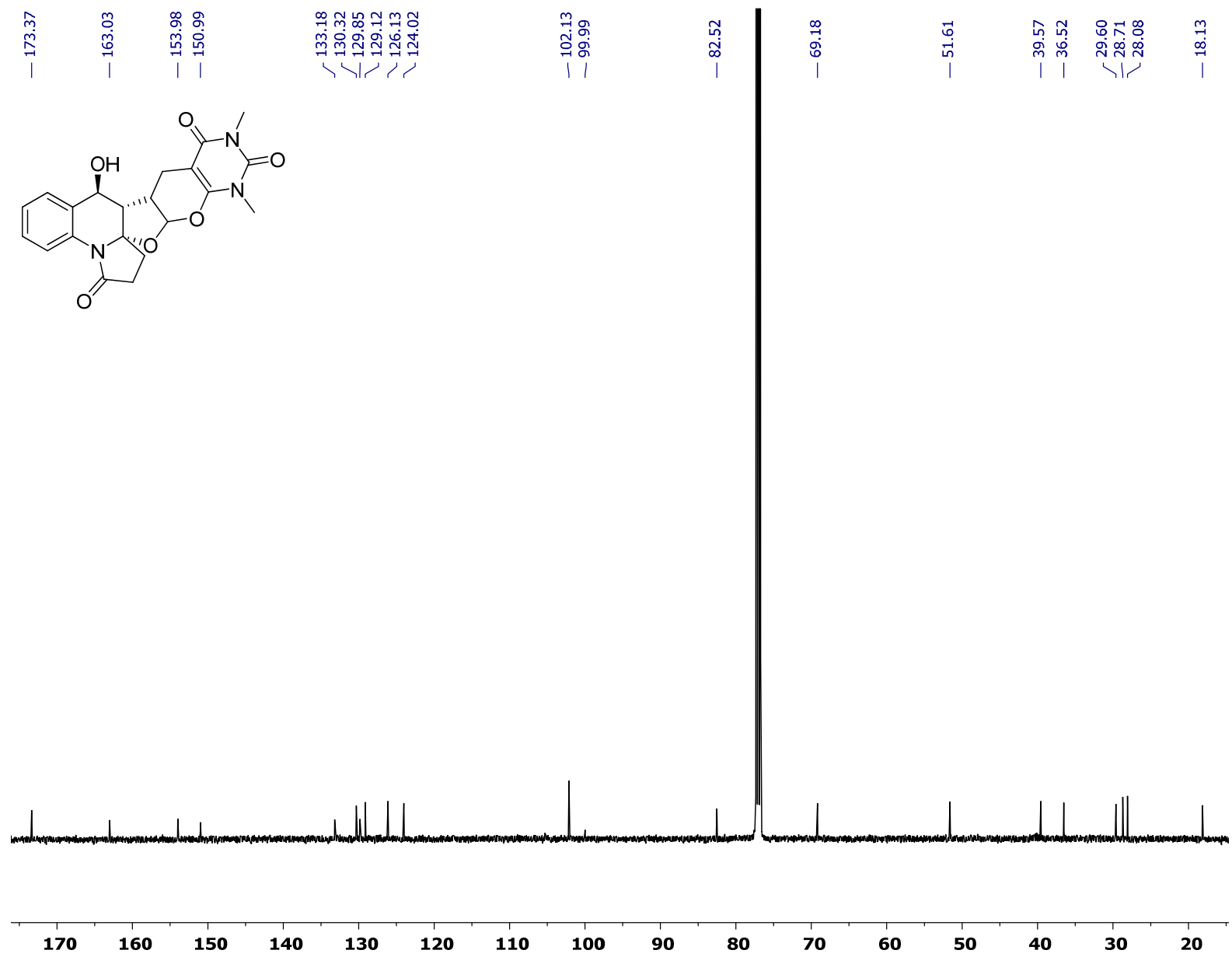
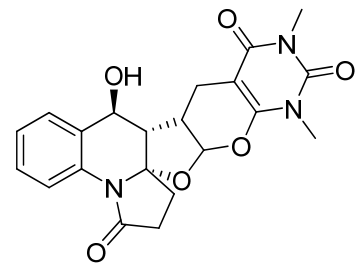
40.37
35.76

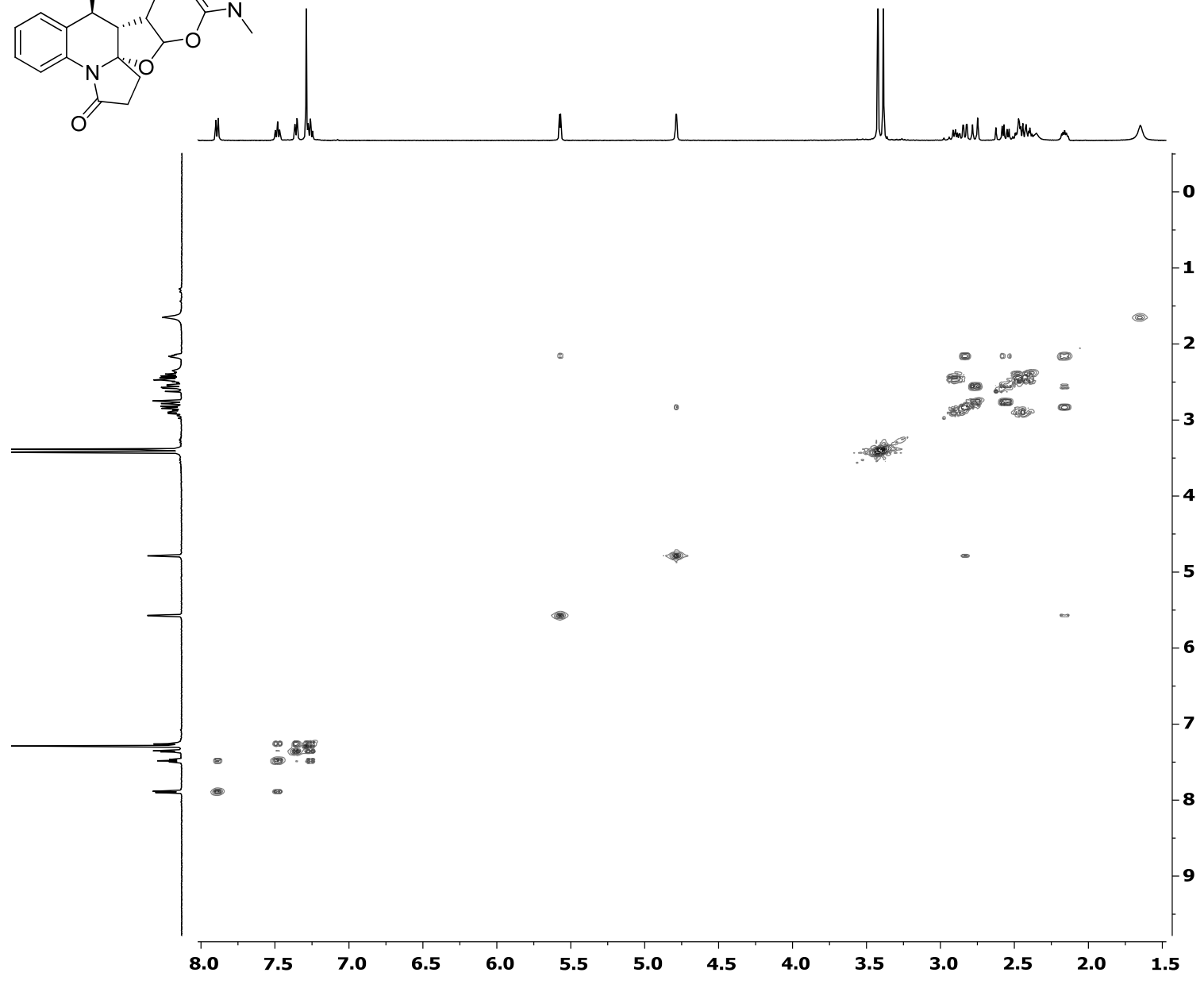
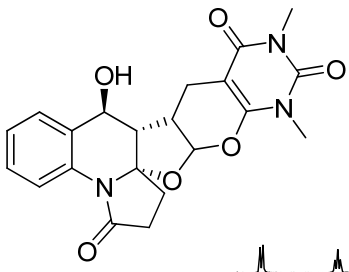
29.65
27.31

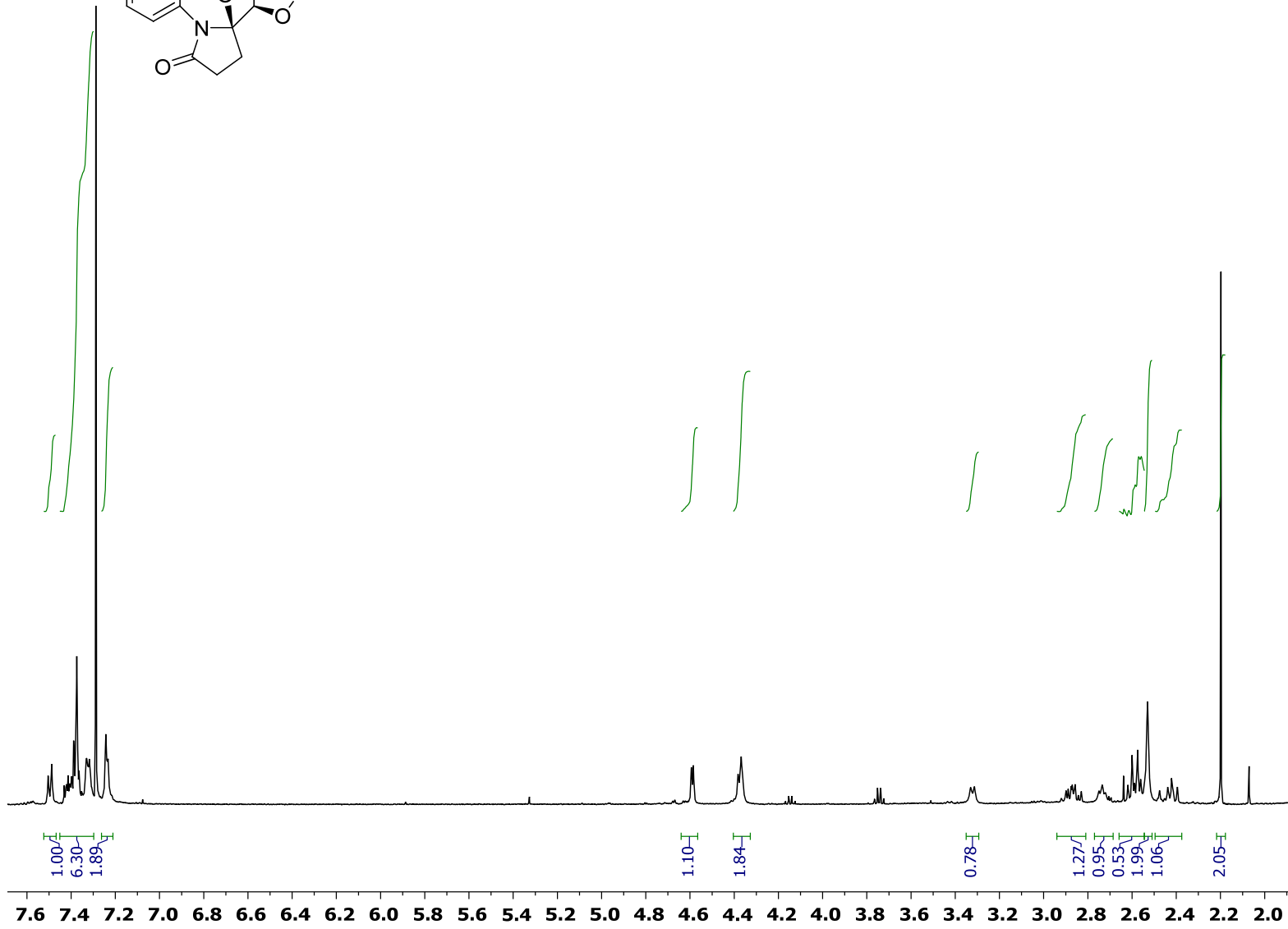
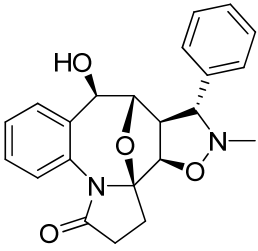












— 173.95

134.01
133.57
132.45
129.46
129.07
128.66
128.22
127.76
127.11

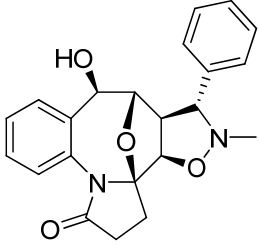
— 102.57

— 84.21
— 81.43
— 79.48

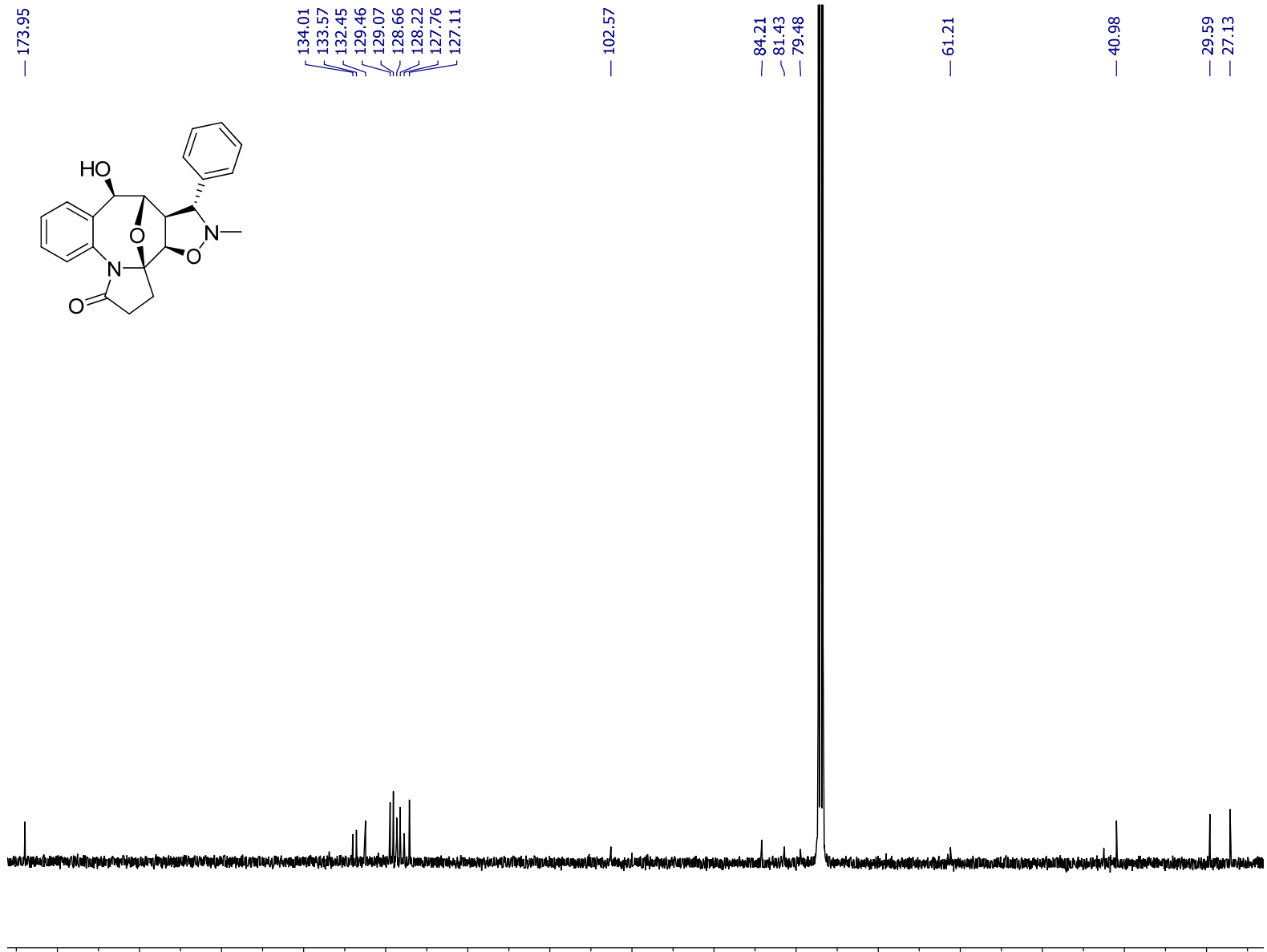
— 61.21

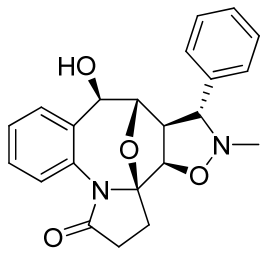
— 40.98

— 29.59
— 27.13

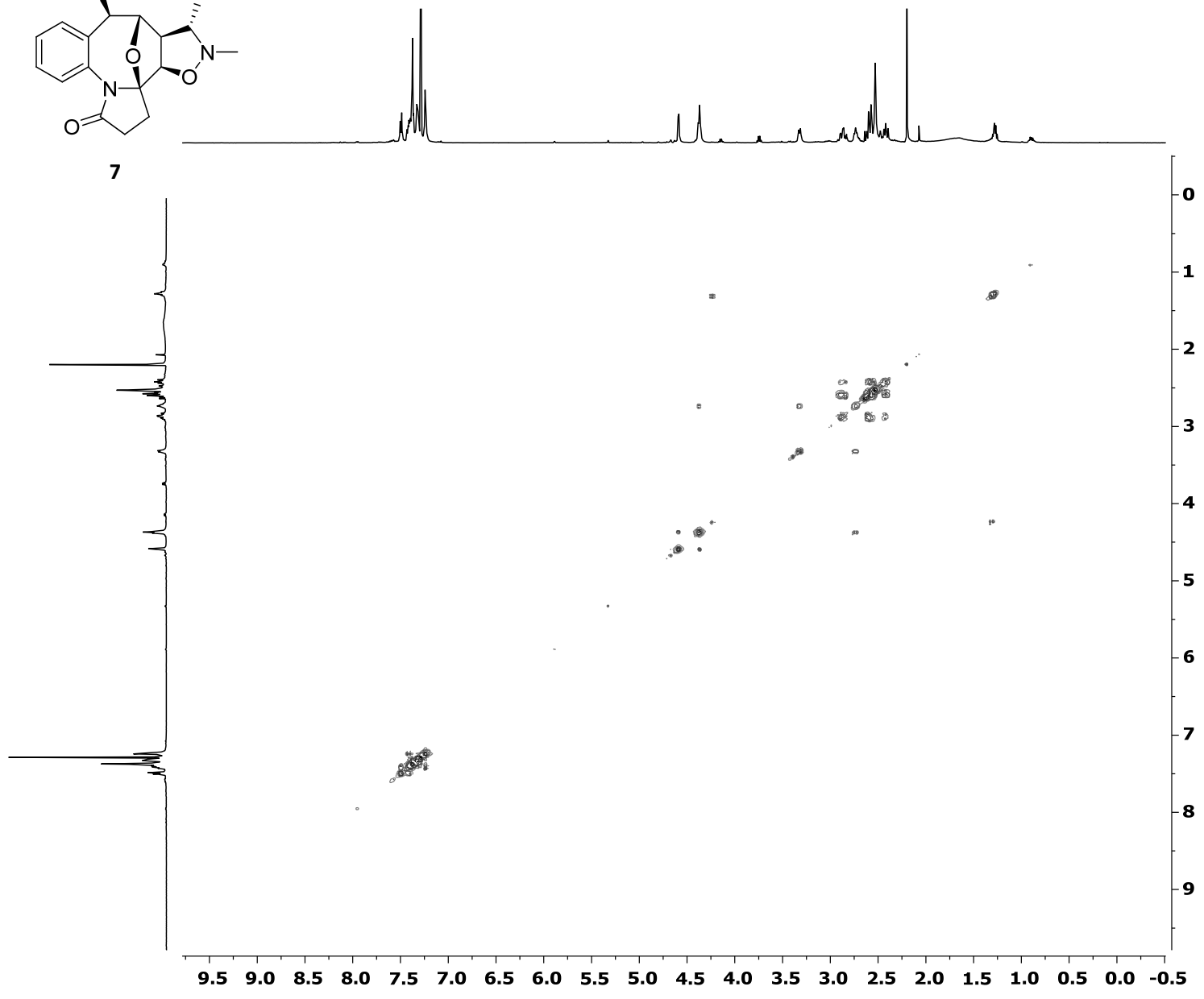


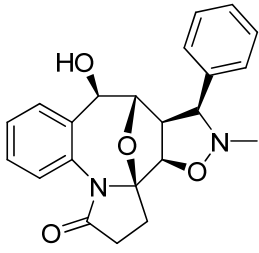
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30



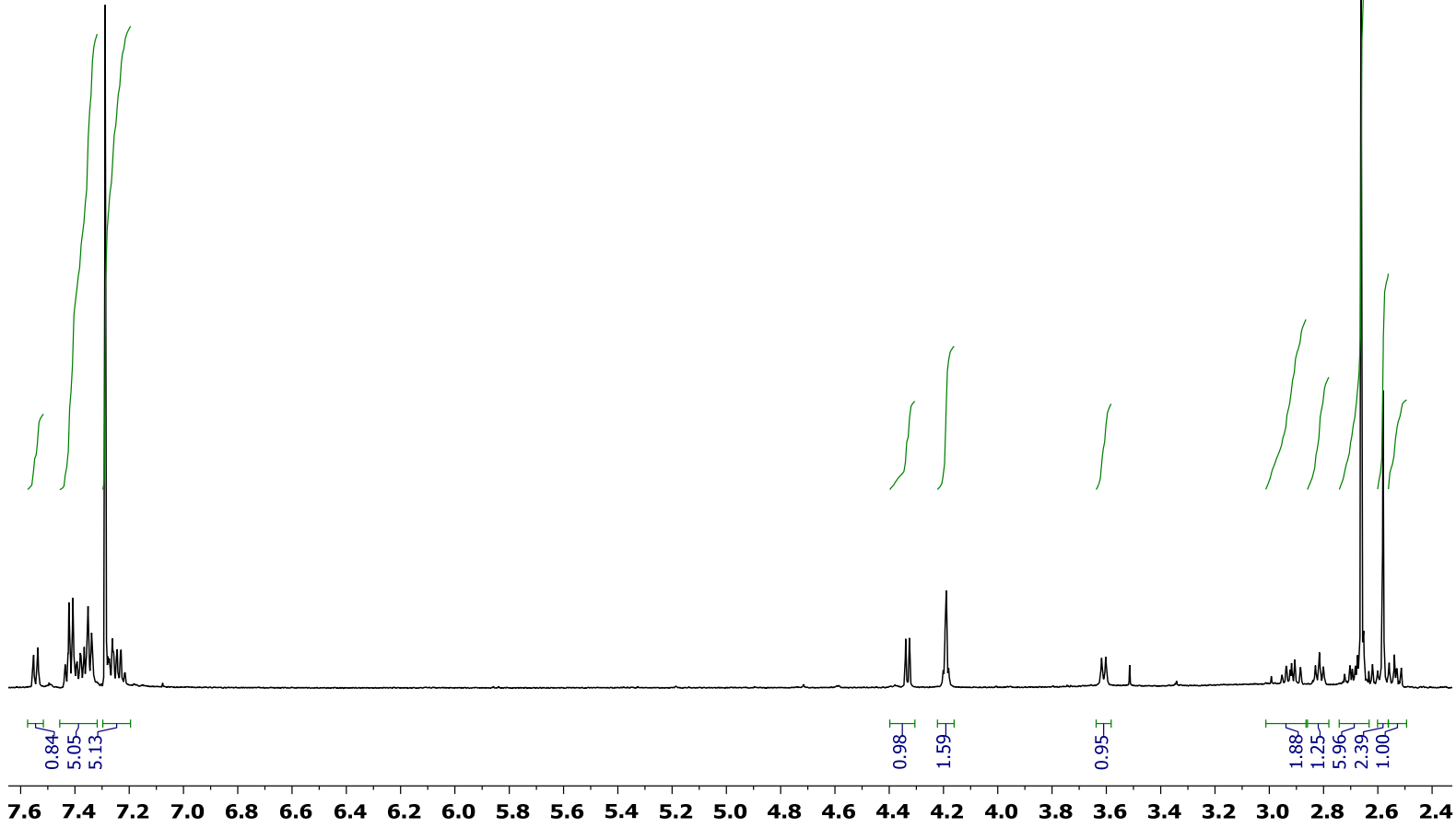


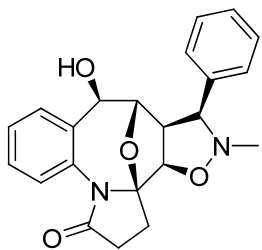
7



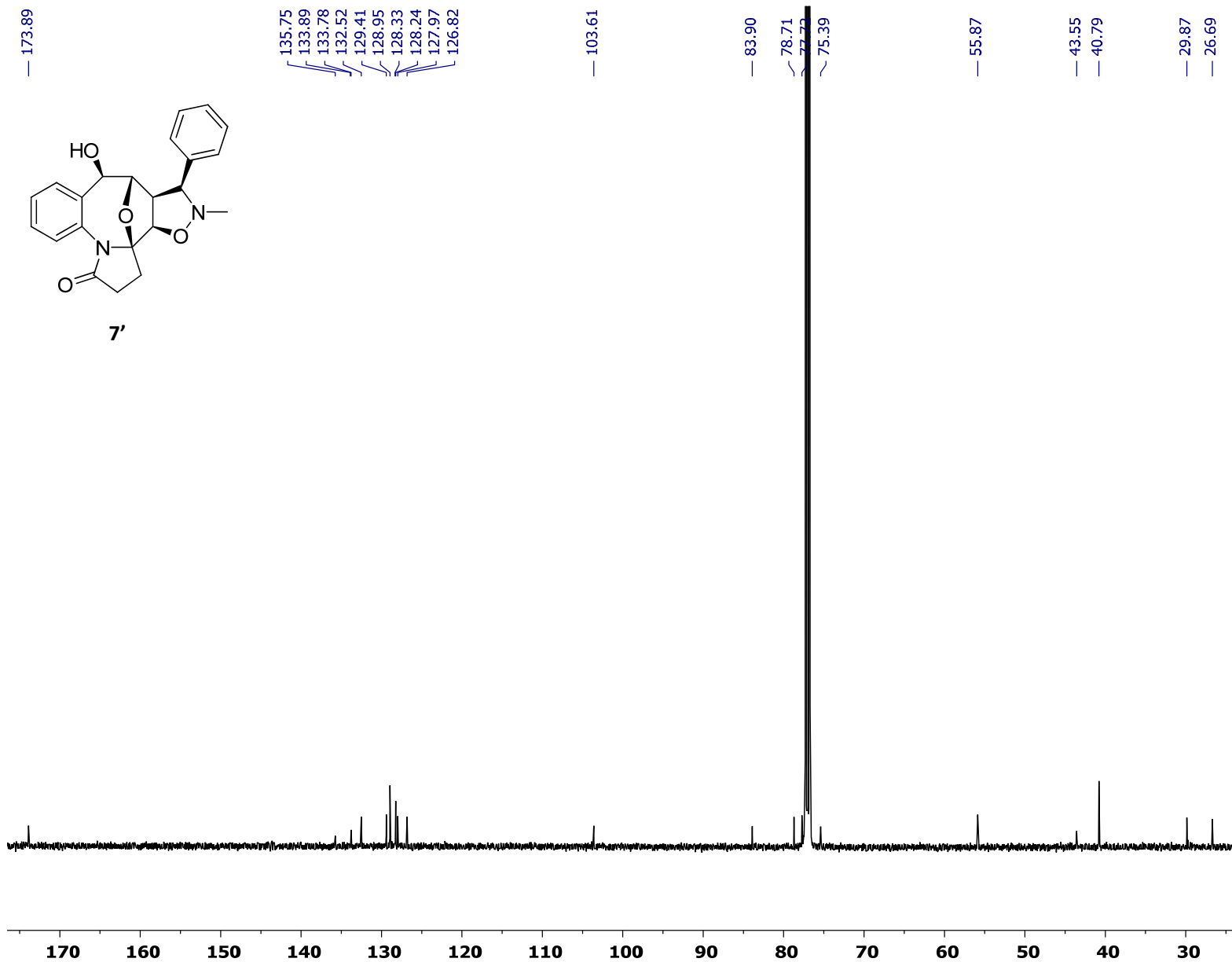


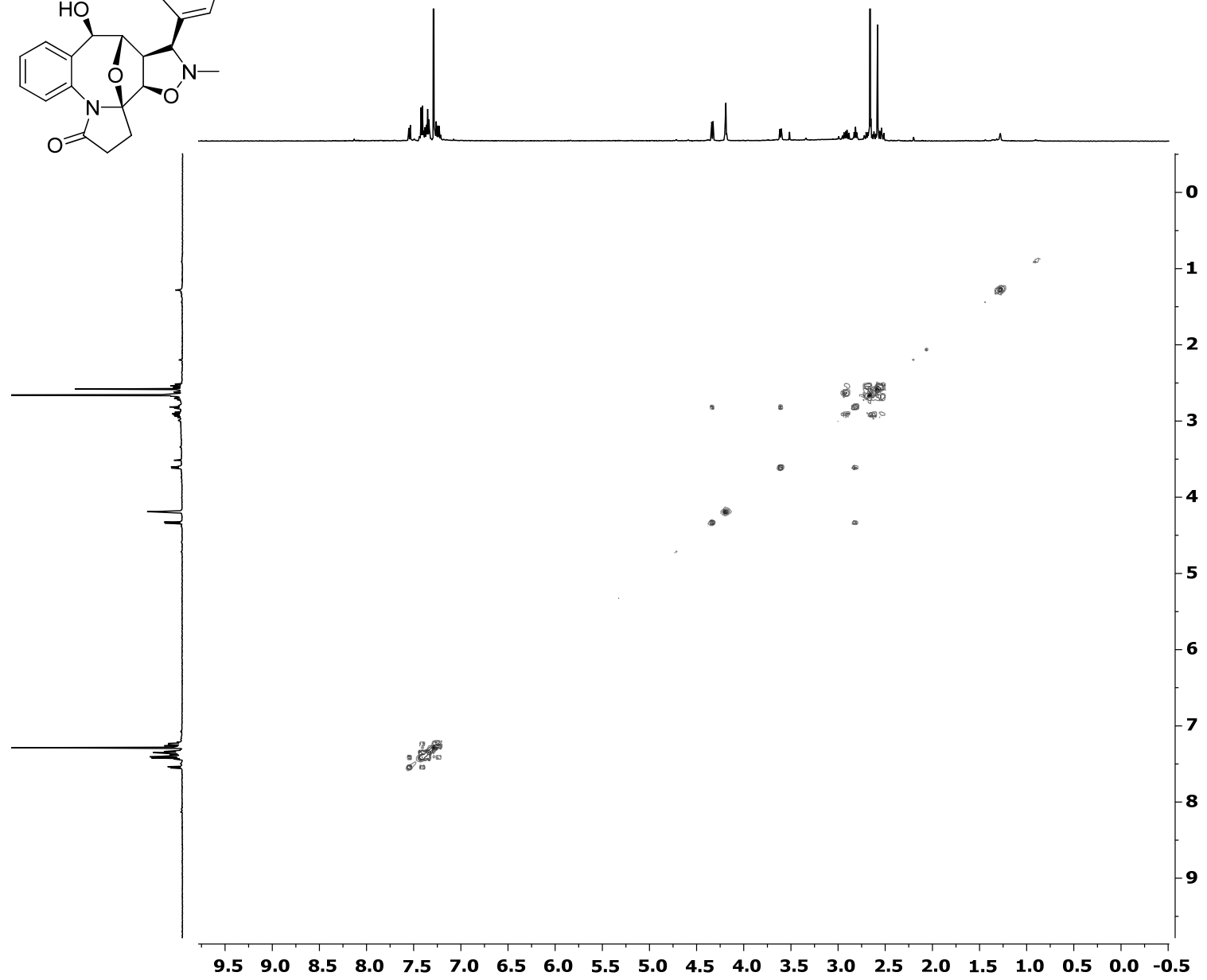
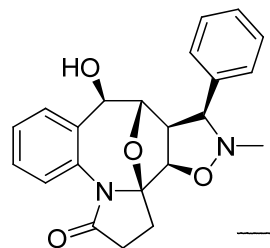
7'

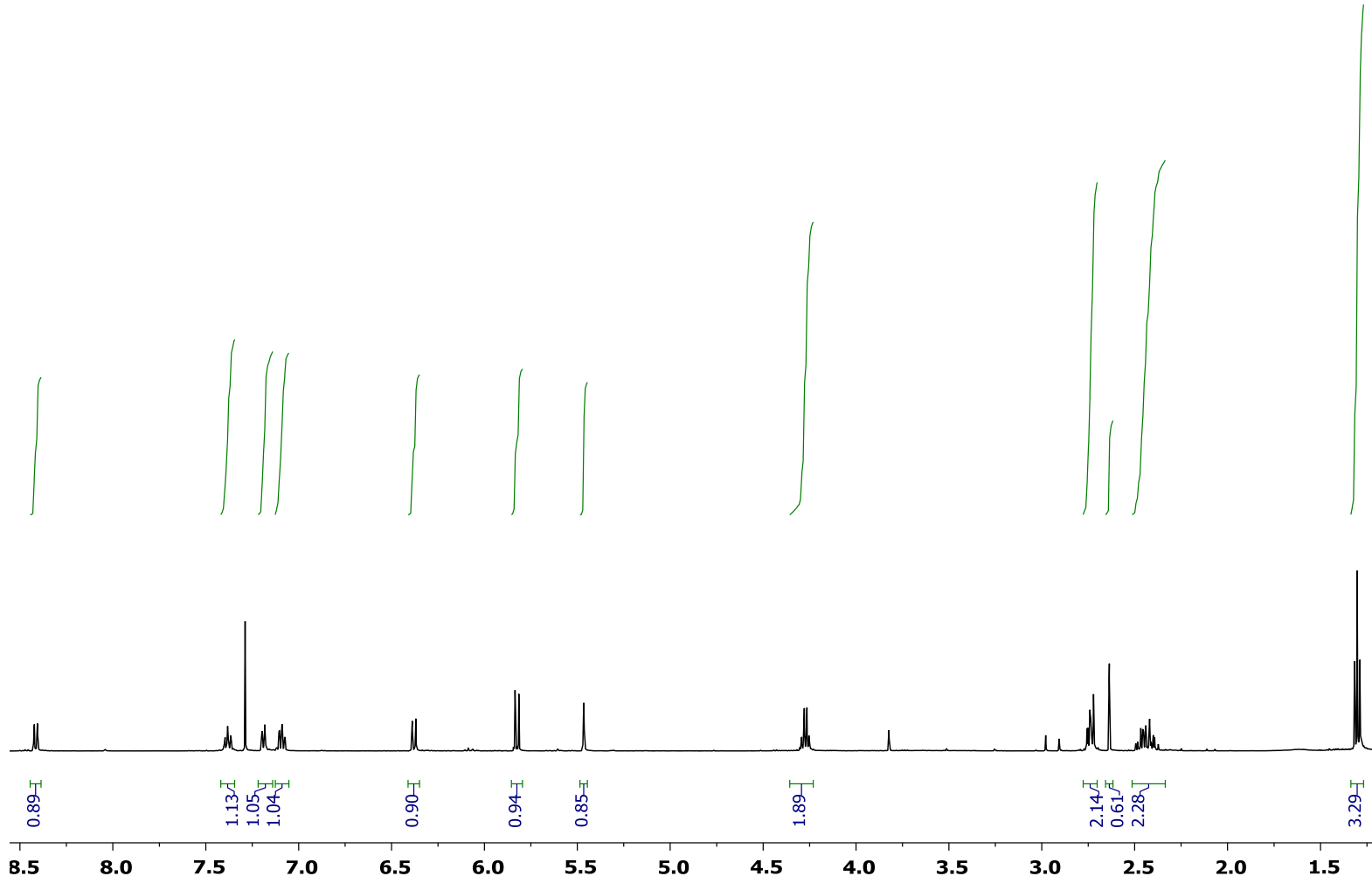
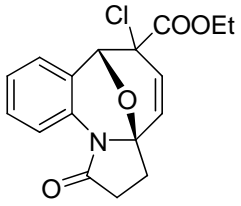




7'







— 170.83
— 167.34

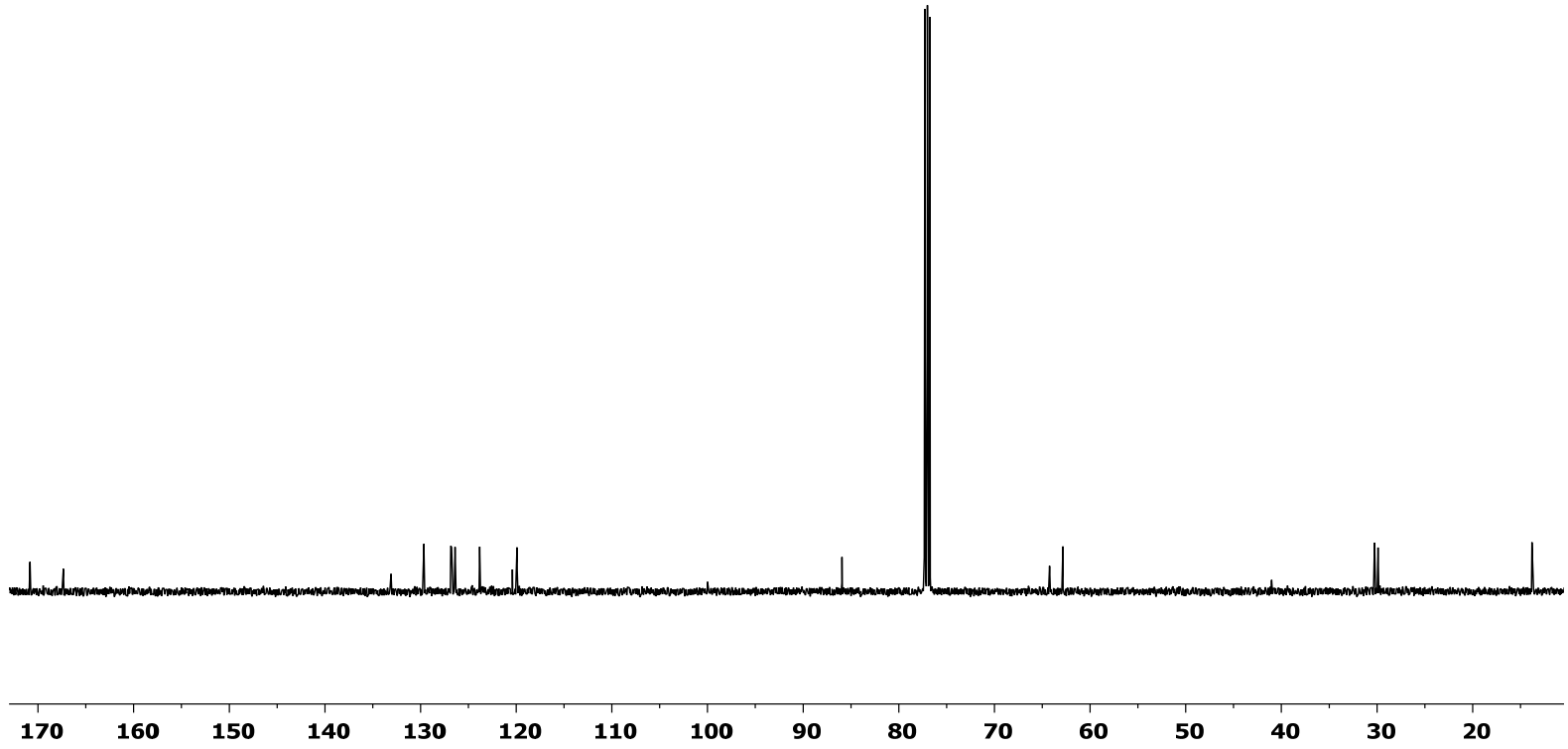
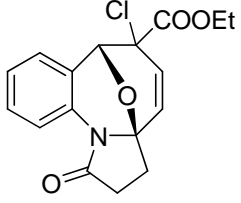
✓ 133.08
✓ 129.65
✓ 126.85
✓ 126.76
✓ 126.40
✓ 123.82
✓ 120.40
✓ 119.92

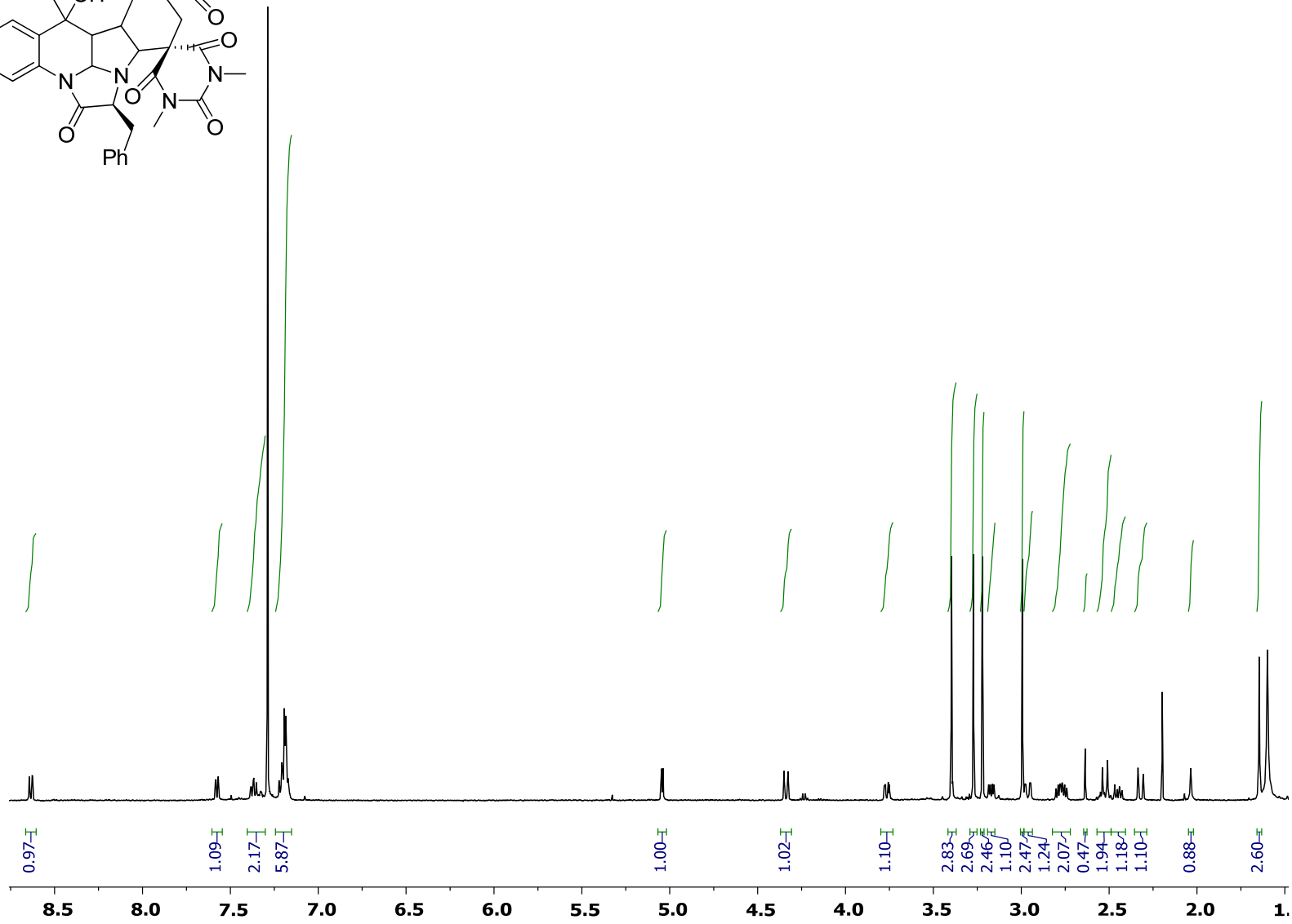
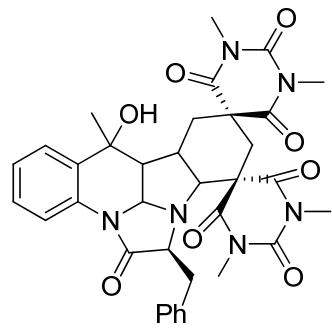
— 85.94

✓ 64.23
✓ 62.85

✓ 30.26
✓ 29.89

— 13.80





173.56
172.11
171.35
170.73
170.62

150.66
150.25

138.20
132.45
130.42
129.69
128.83
127.75
126.65
126.10
124.67
117.92

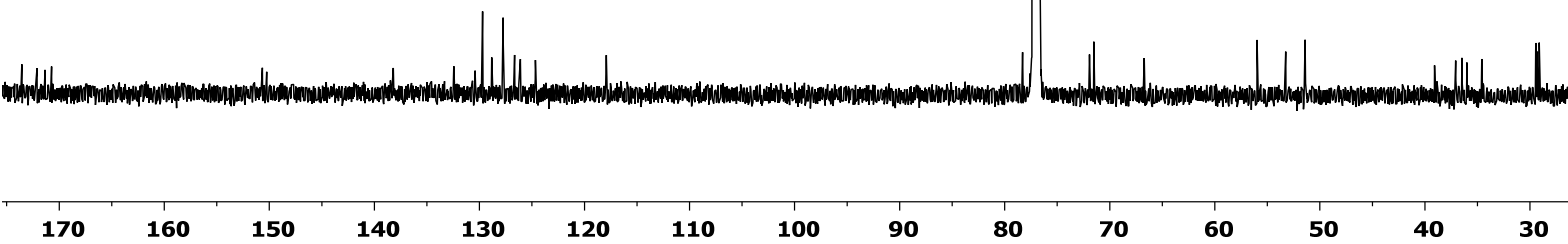
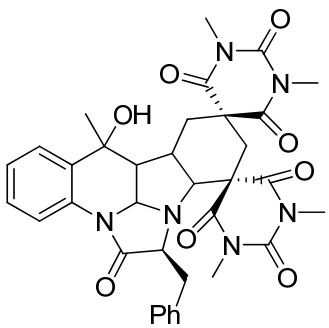
78.30

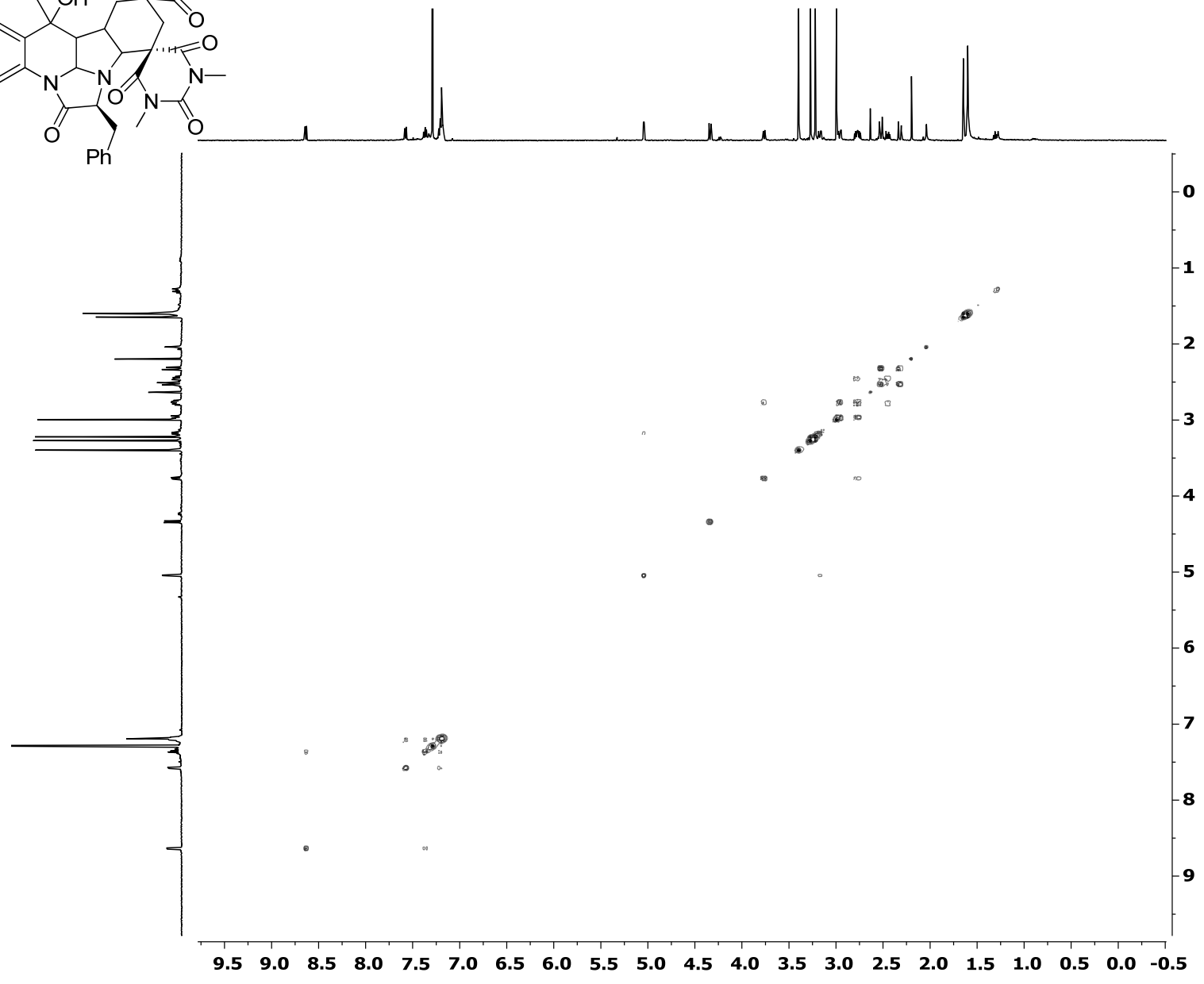
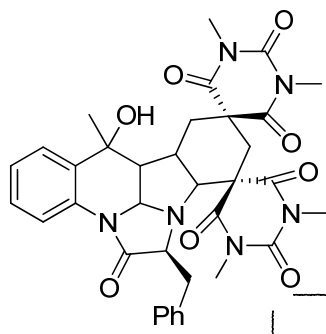
71.93
71.52

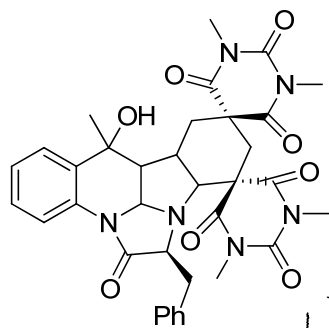
66.72

55.97
53.26
51.40

39.08
37.06
36.48
36.00
34.59
29.45
29.41
29.30
29.12

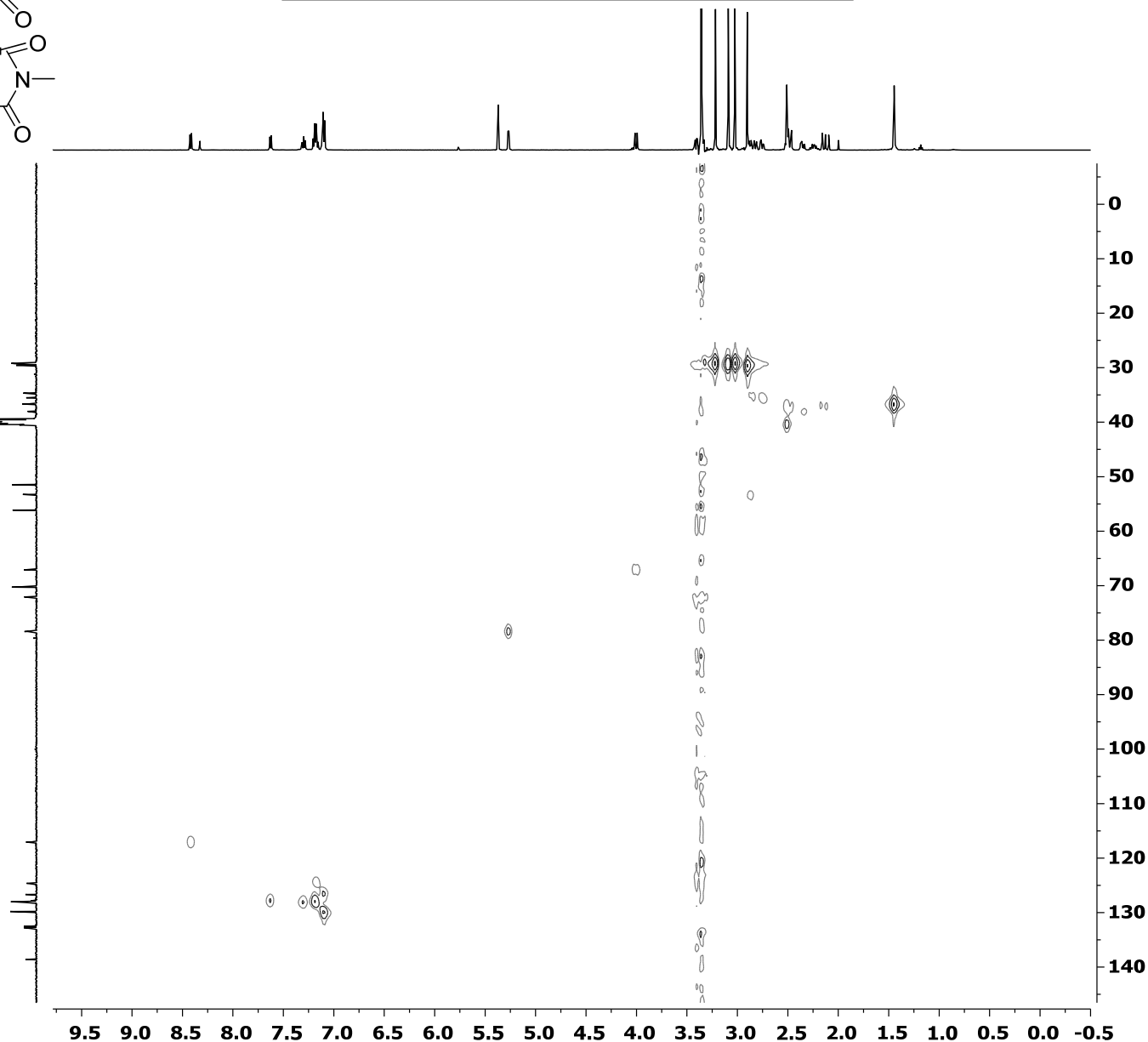


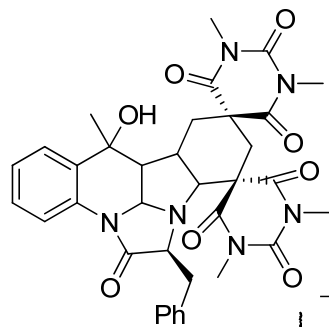




18

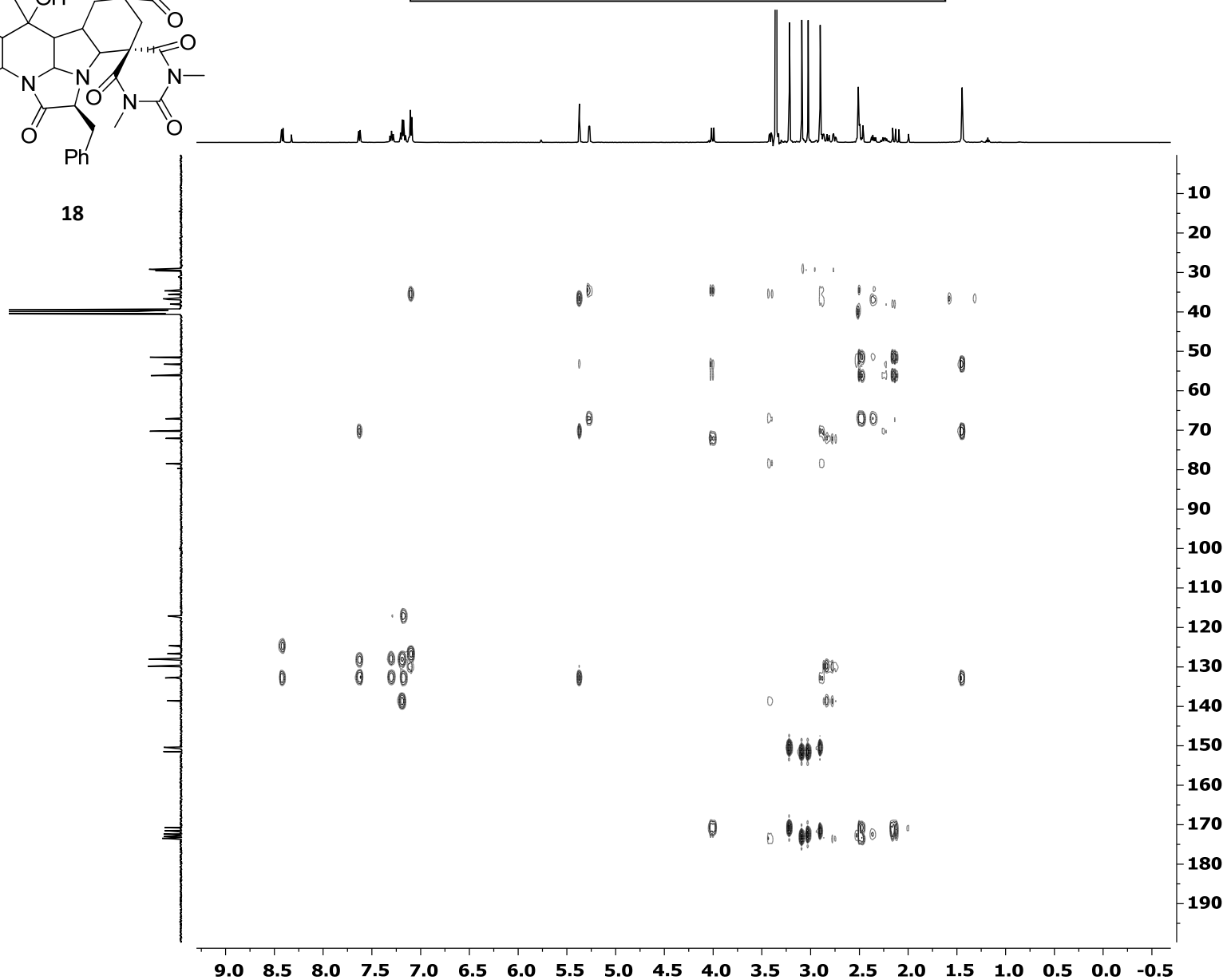
HMQC spectrum

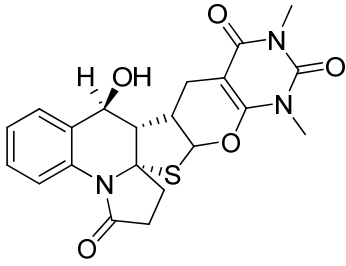




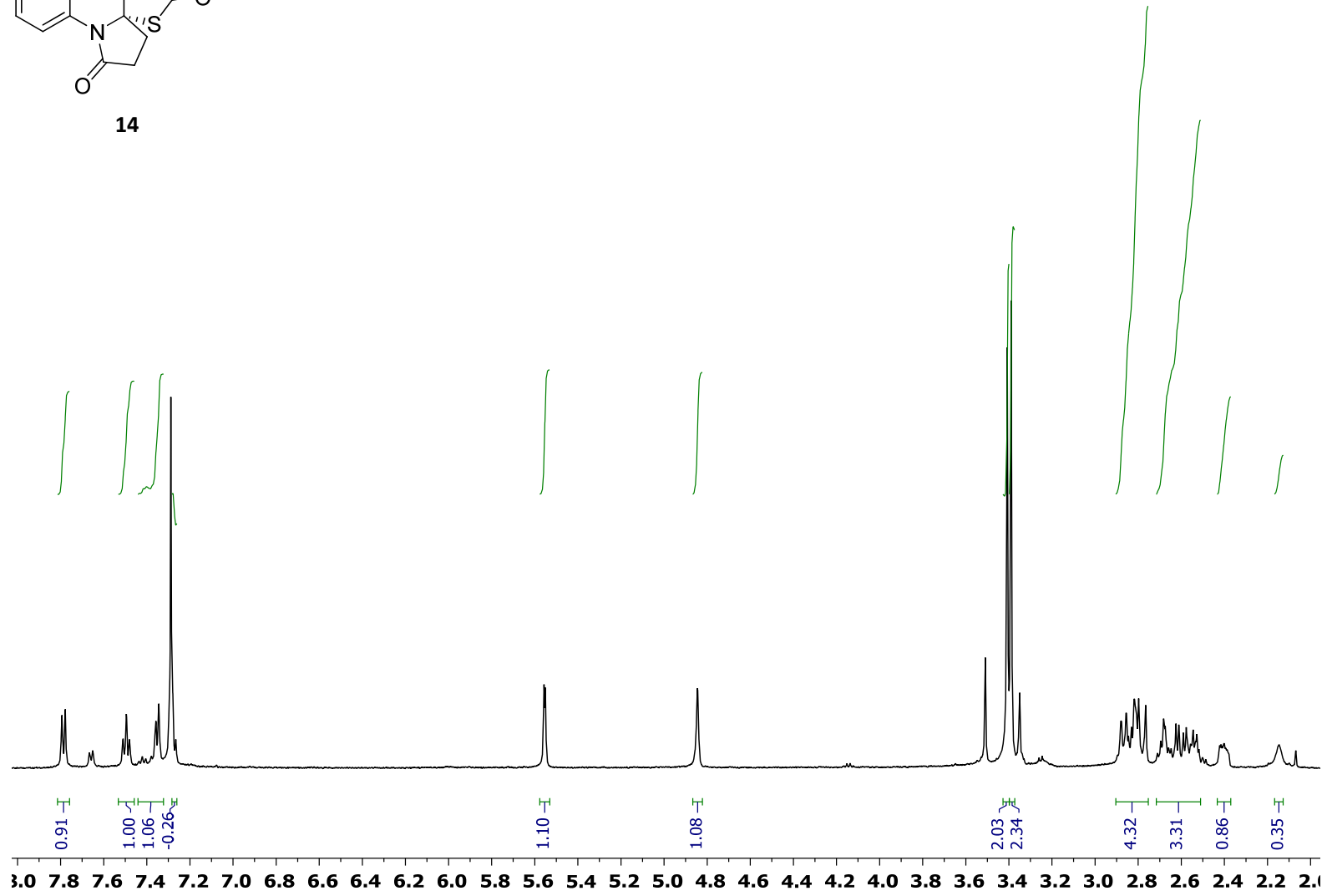
18

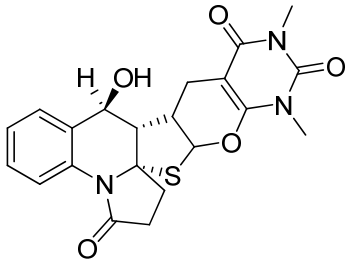
HMBC spectrum





14





14

