

Hymenopsins A and B and a Macrophorin Analogue from a Fungicolous *Hymenopsis* sp.

Lori E. Schmidt,[†] Stephen T. Deyrup,[†] Jonas Baltrusaitis,[†] Dale C.

Swenson,[†] Donald T. Wicklow,[‡] and James B. Gloer^{*†}

[†]*Department of Chemistry, University of Iowa, Iowa City, IA, 52242*

[‡]*Mycotoxin Research Unit, Agricultural Research Service, USDA National Center for
Agricultural Utilization Research, USDA, Peoria, IL, 61604*

List of Supporting Information

Figure S1. ¹H NMR spectrum of hymenopsin A (**1**; 600 MHz, acetone-*d*₆)

Figure S2. ¹³C NMR spectrum of hymenopsin A (**1**; 75 MHz, methanol-*d*₄)

Figure S3. ¹H NMR spectrum of hymenopsin B (**2**; 400 MHz, CDCl₃)

Figure S4. ¹³C NMR spectrum of hymenopsin B (**2**; 75 MHz, CDCl₃)

Figure S5. ¹H NMR spectrum of 2',3'-epoxy-13-hydroxy-4'-oxomacrophorin A (**3**; 300 MHz, CDCl₃)

Figure S6. ¹³C NMR spectrum of 2',3'-epoxy-13-hydroxy-4'-oxomacrophorin A (**3**; 75 MHz, CDCl₃)

Figure S7. Lowest energy conformation of hymenopsin B (**2**) based on ORCA/RI-SCS-MP2/TZVP calculations viewed along the O=C bond on axes as employed in application of the octant rule.

Figure S8. Calculated, weighted-average CD spectrum of 10 lowest energy conformers of **2** showing negative Cotton effect in 320-330 range.

Figure S9. CD spectrum of **2** showing negative Cotton effect in 320-330 range.

*To whom correspondence should be addressed. Tel: 319-335-1361. Fax 319-335-1270.

E-mail: james-gloer@uiowa.edu.

[†]University of Iowa

[‡]USDA National Center for Agricultural Utilization Research

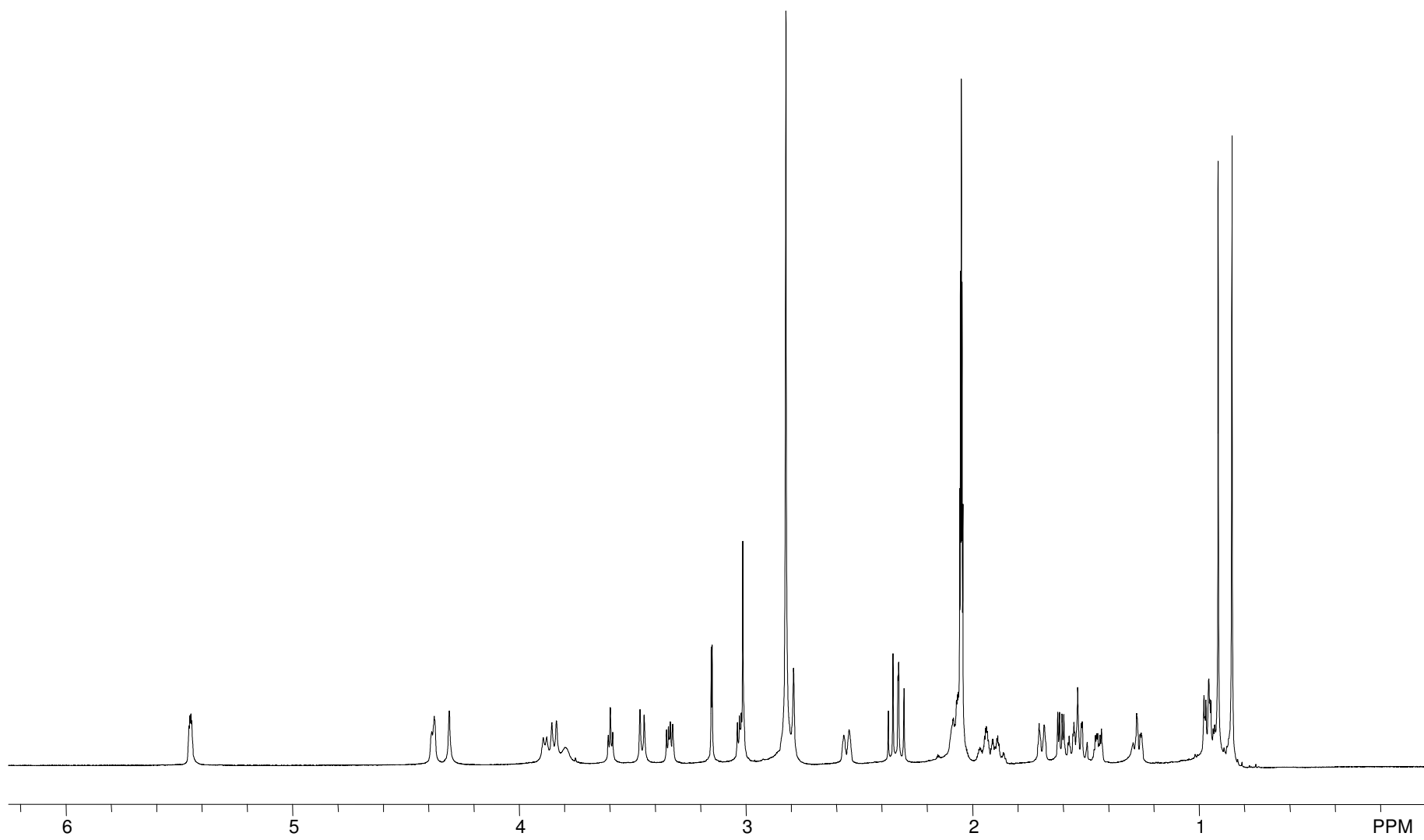


Figure S1. ^1H NMR spectrum of hymenopsin A (**1**; 600 MHz, acetone- d_6)

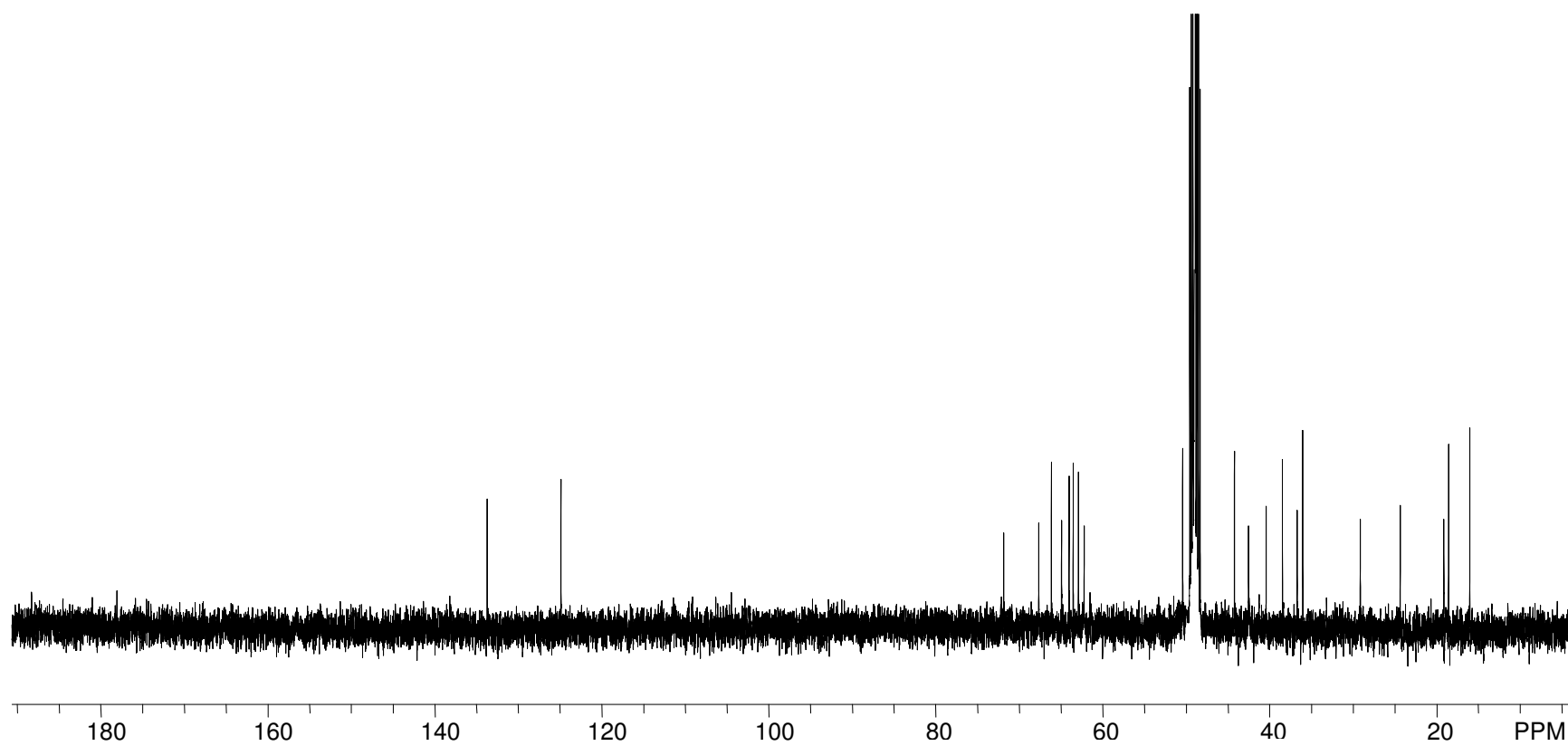


Figure S2. ^{13}C NMR spectrum of hymenopsin A (1; 75 MHz, $\text{methanol-}d_4$)

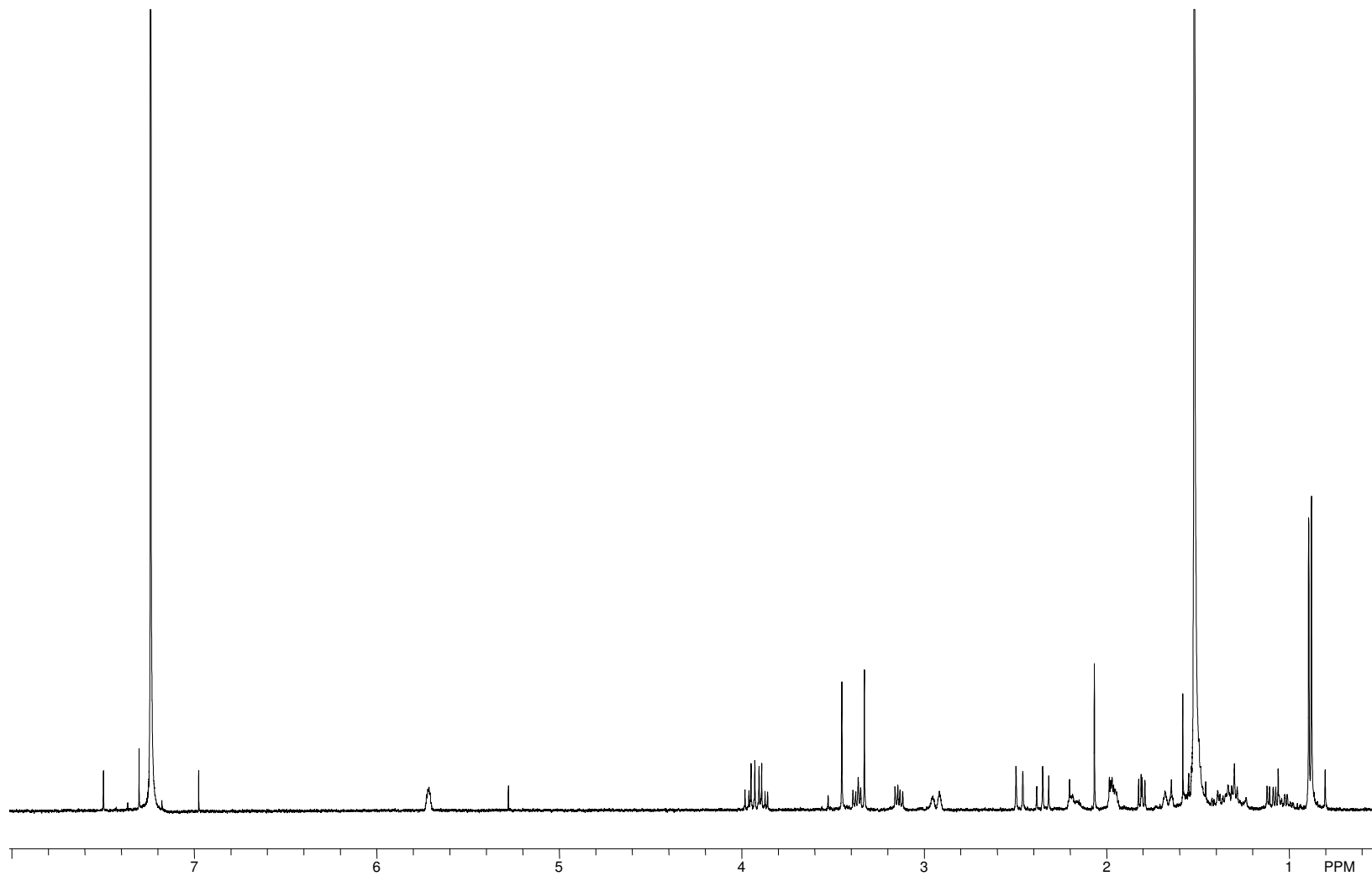


Figure S3. ^1H NMR spectrum of hymenopsin B (**2**; 400 MHz, CDCl_3)

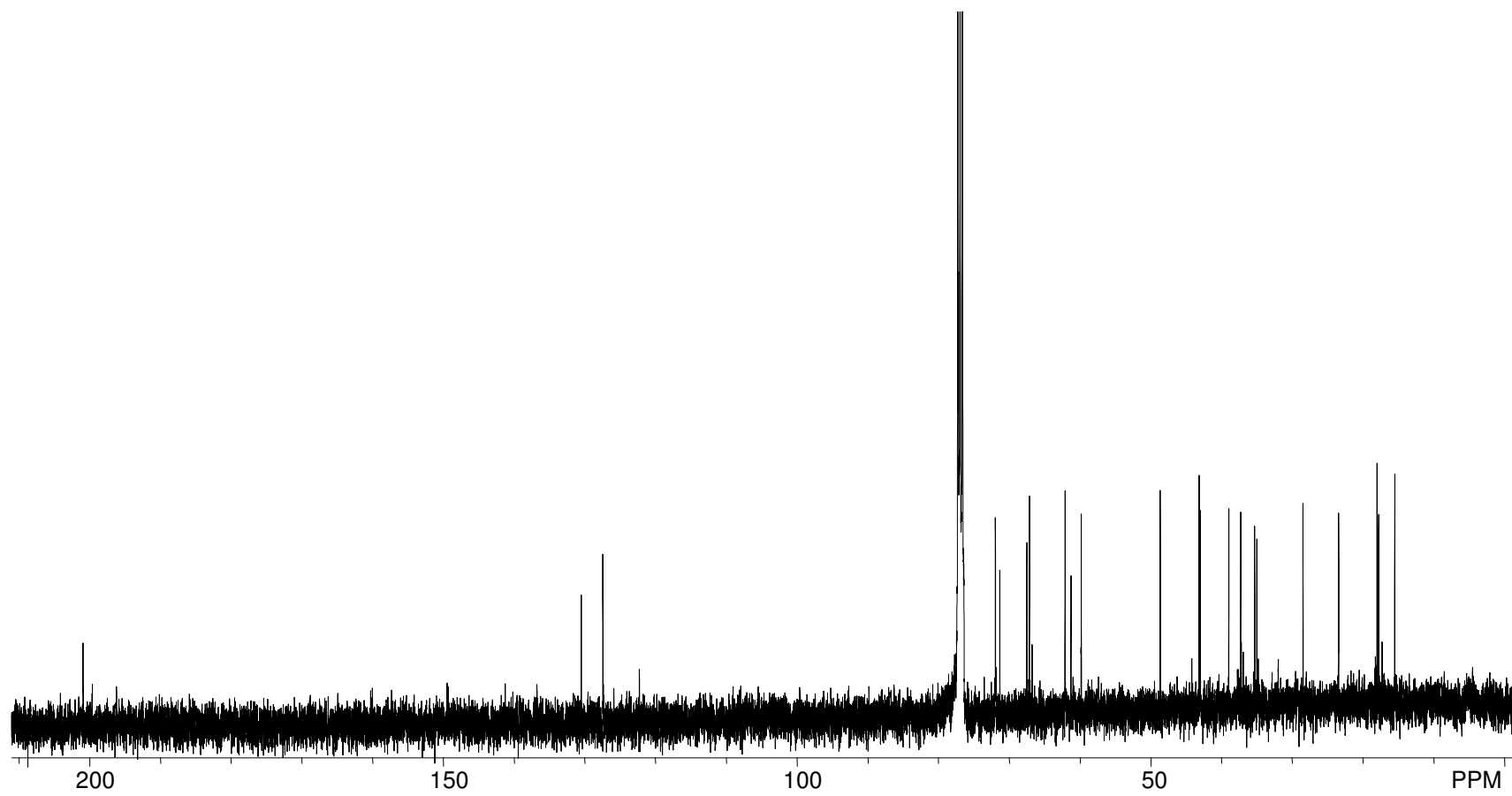


Figure S4. ^{13}C NMR spectrum of hymenopsin B (2; 75 MHz, CDCl_3)

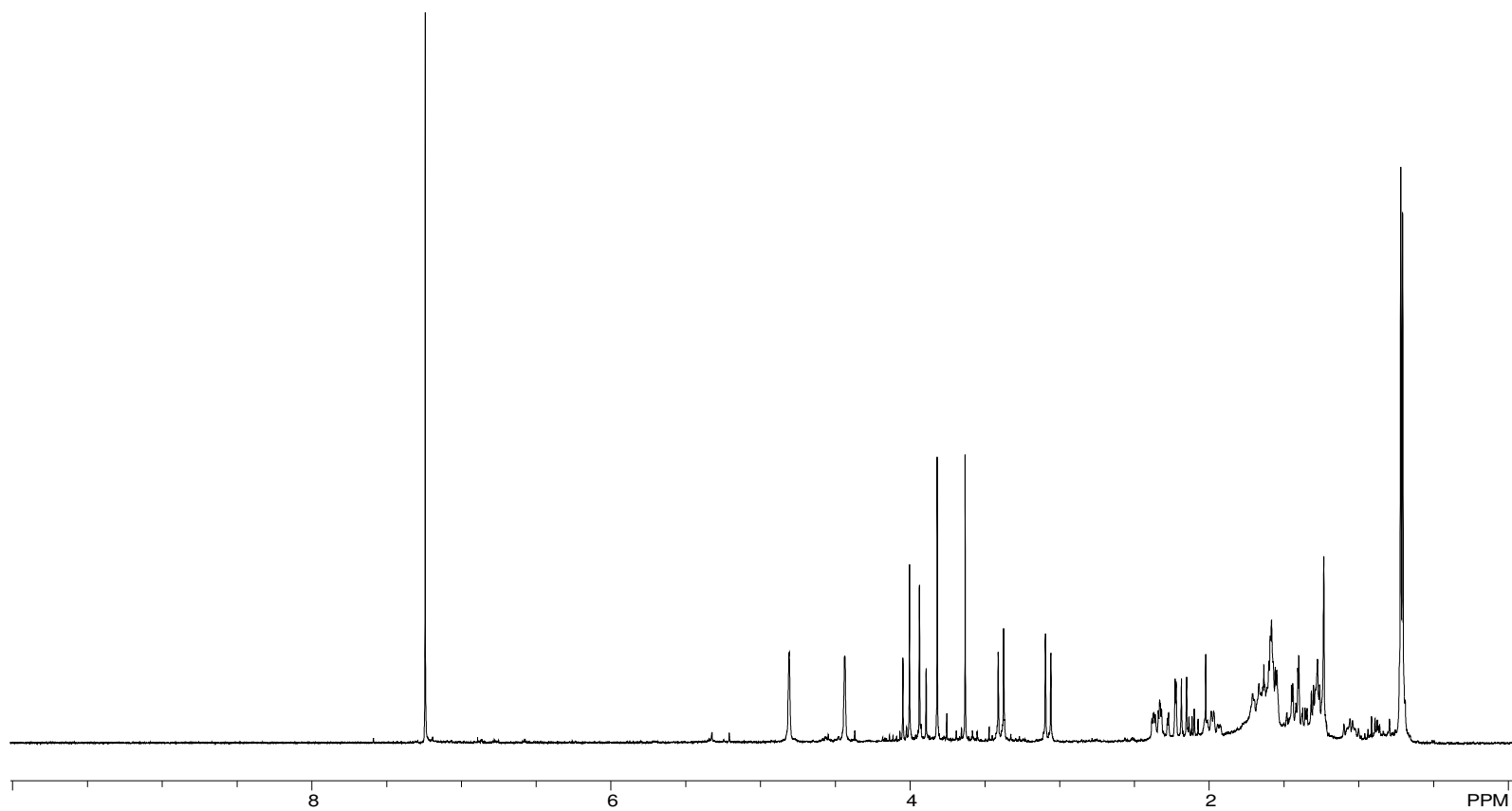


Figure S5. ¹H NMR spectrum of 2',3'-epoxy-13-hydroxy-4'-oxomacrophorin A (**3**; 300 MHz, CDCl₃)

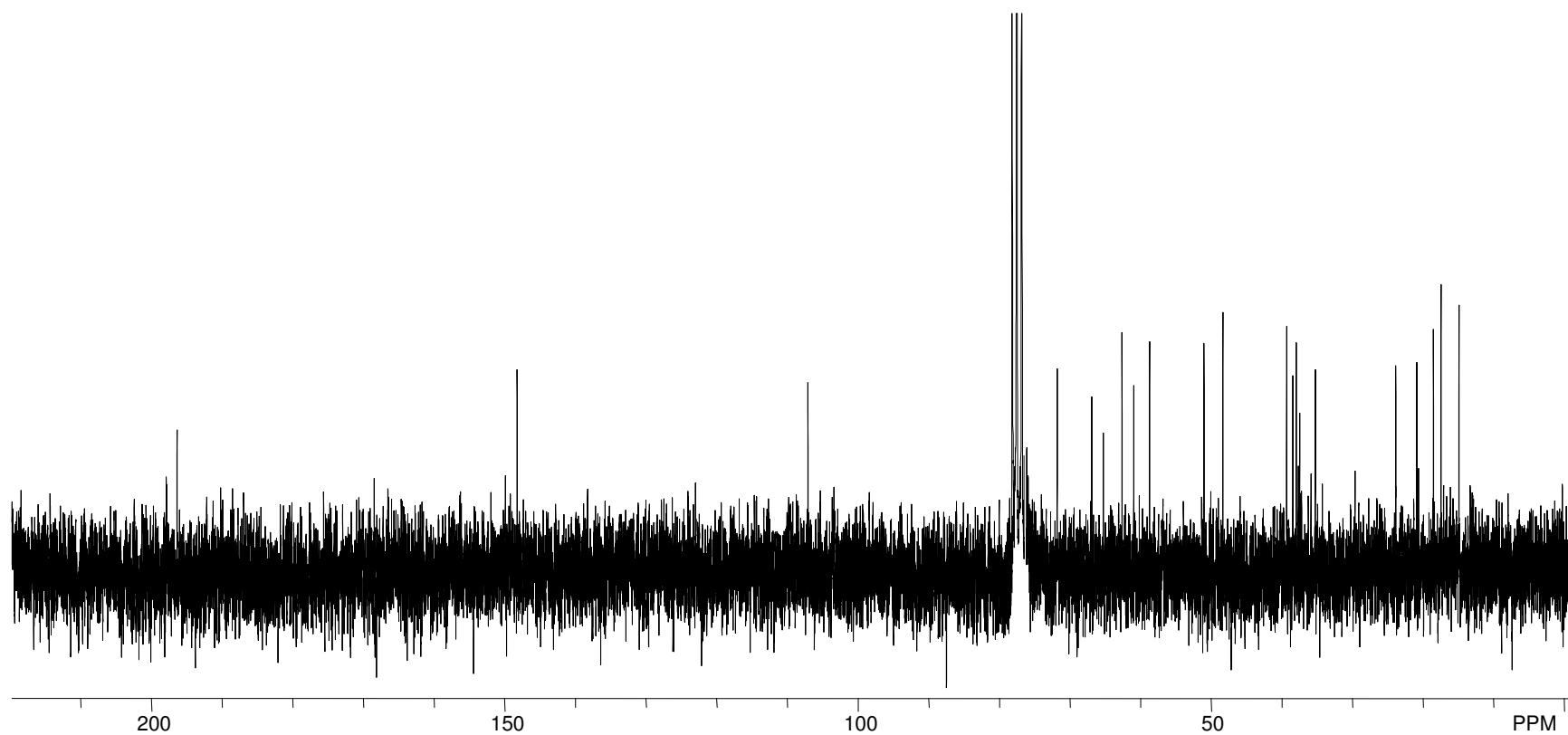


Figure S6. ^{13}C NMR spectrum of 2',3'-epoxy-13-hydroxy-4'-oxomacrophorin A (**3**; 75 MHz, CDCl_3)

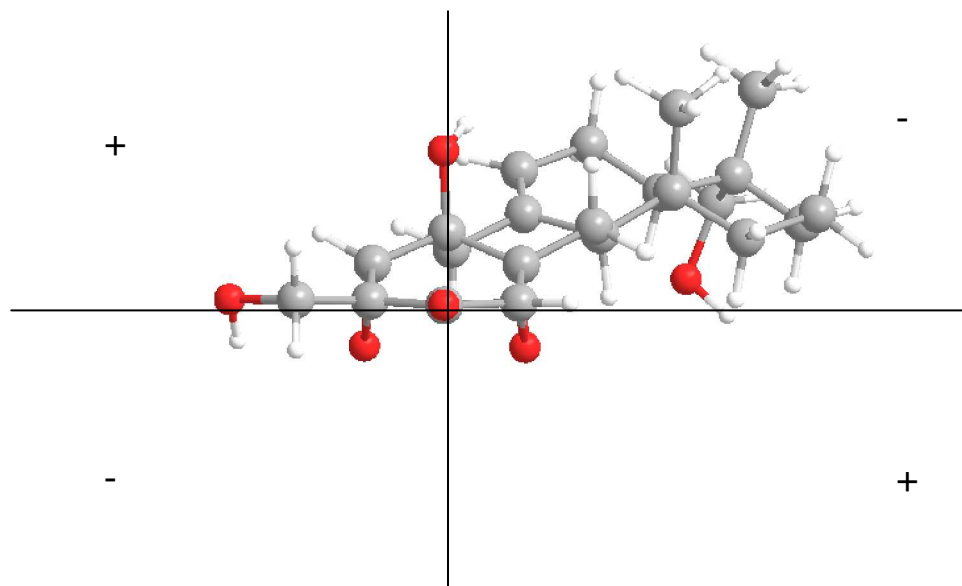


Figure S7. Lowest energy conformation of hymenopsin B (**2**) based on ORCA/RI-SCS-MP2/TZVP calculations viewed along the O=C bond on axes as employed in application of the octant rule.

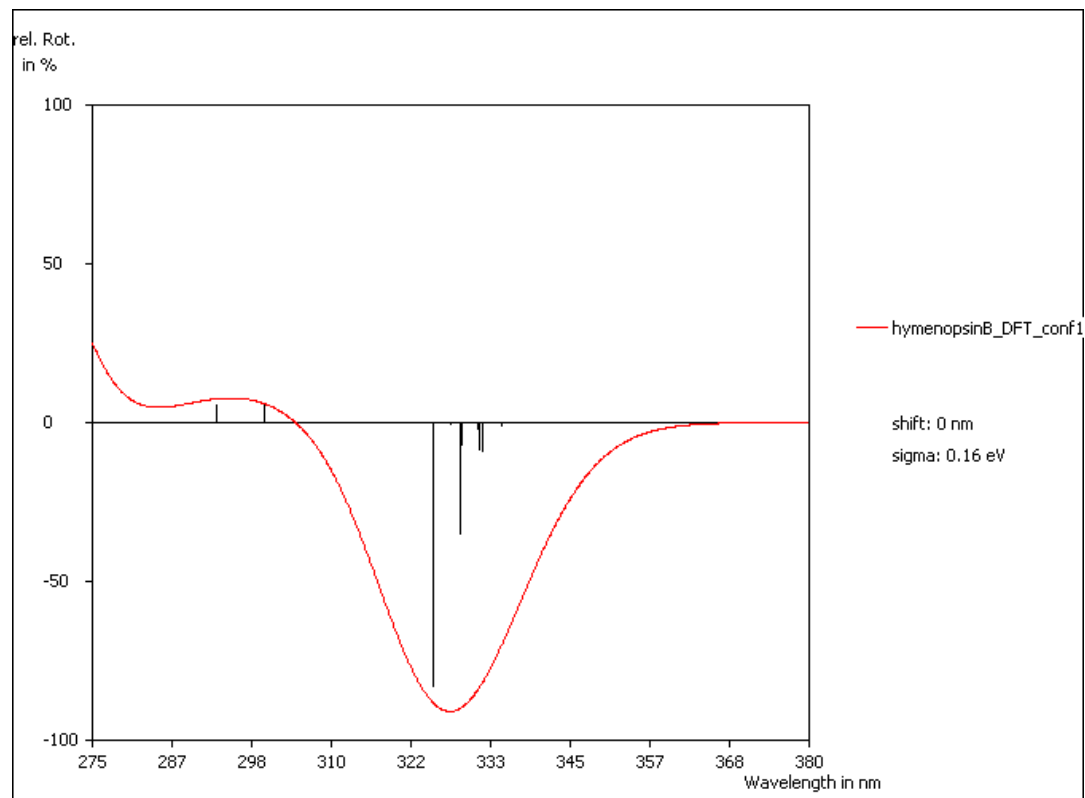


Figure S8. Calculated, weighted-average CD spectrum of 10 lowest energy conformers of **2** showing negative Cotton effect in 320-330 range.

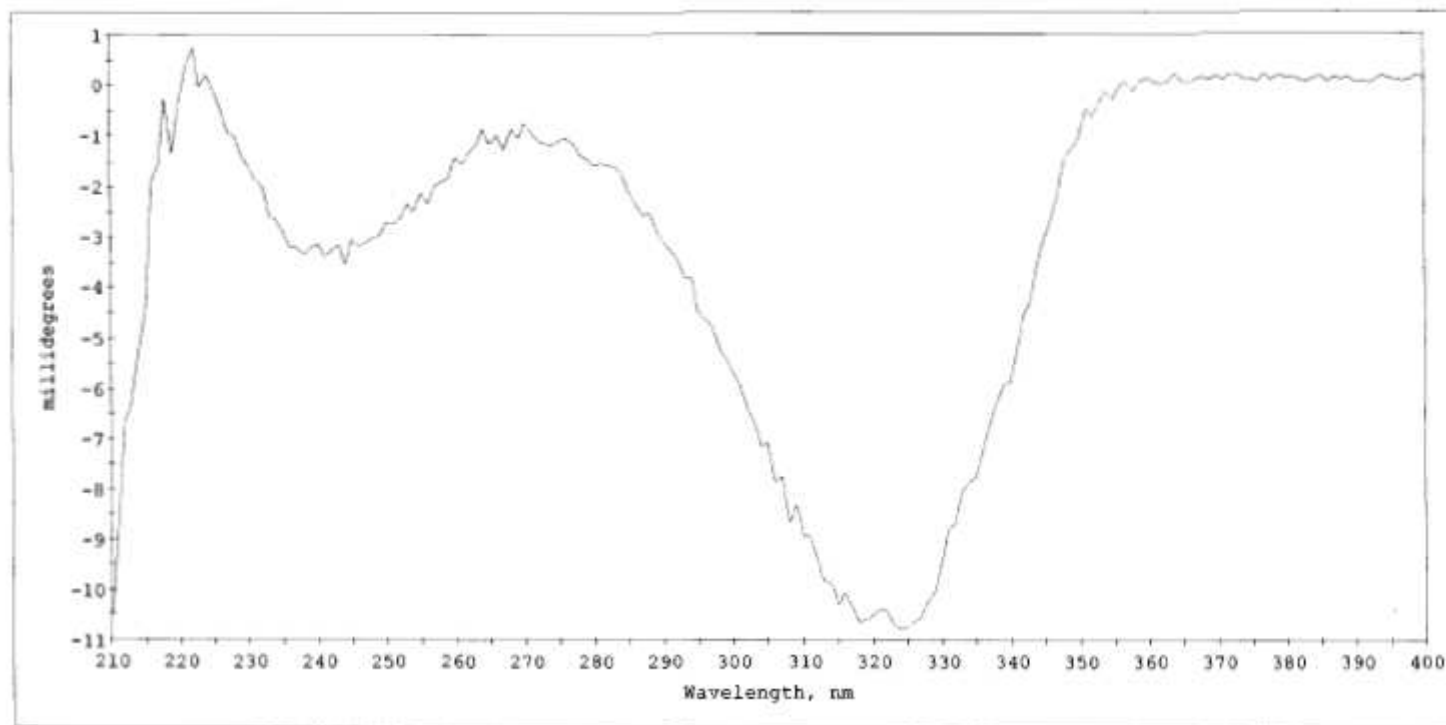


Figure S9. CD spectrum of **2** showing negative Cotton effect in 320-330 range.