# Malyngamide 2, an Oxidized Lipopeptide with Nitric Oxide Inhibiting Activity from a Papua New Guinea Marine Cyanobacterium

Karla L. Malloy,[†] Francisco A. Villa,[†] Niclas Engene,[†] Teatulohi Matainaho,[‡] Lena Gerwick[†] and William H. Gerwick[†,*]

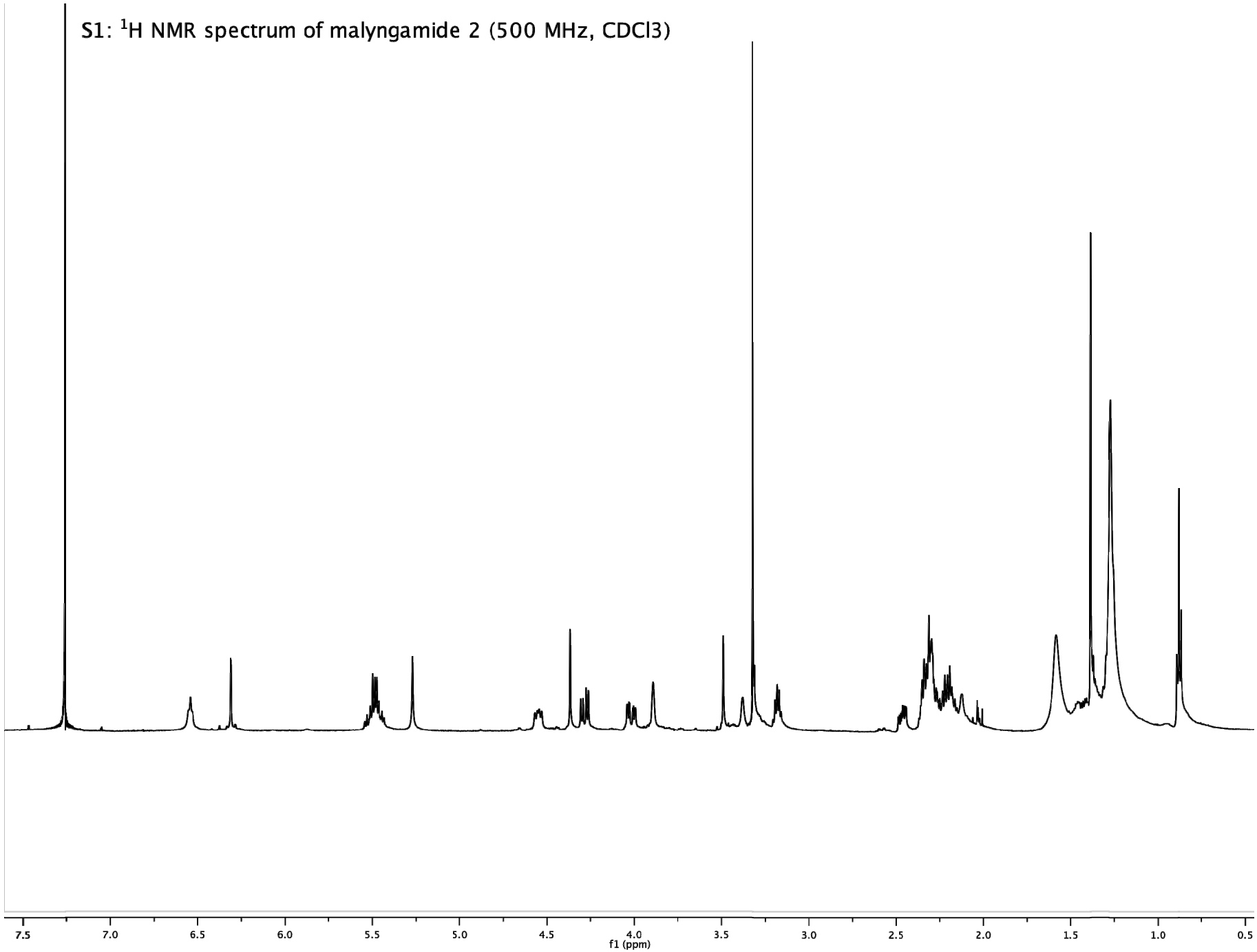
*Center for Marine Biotechnology and Biomedicine, Scripps Institution of Oceanography and Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California at San Diego, La Jolla, California 92093 and Discipline of Pharmacology, School of Medicine and Health Sciences, University of Papua New Guinea, National Capital District, Papua New Guinea*

## Supporting Information

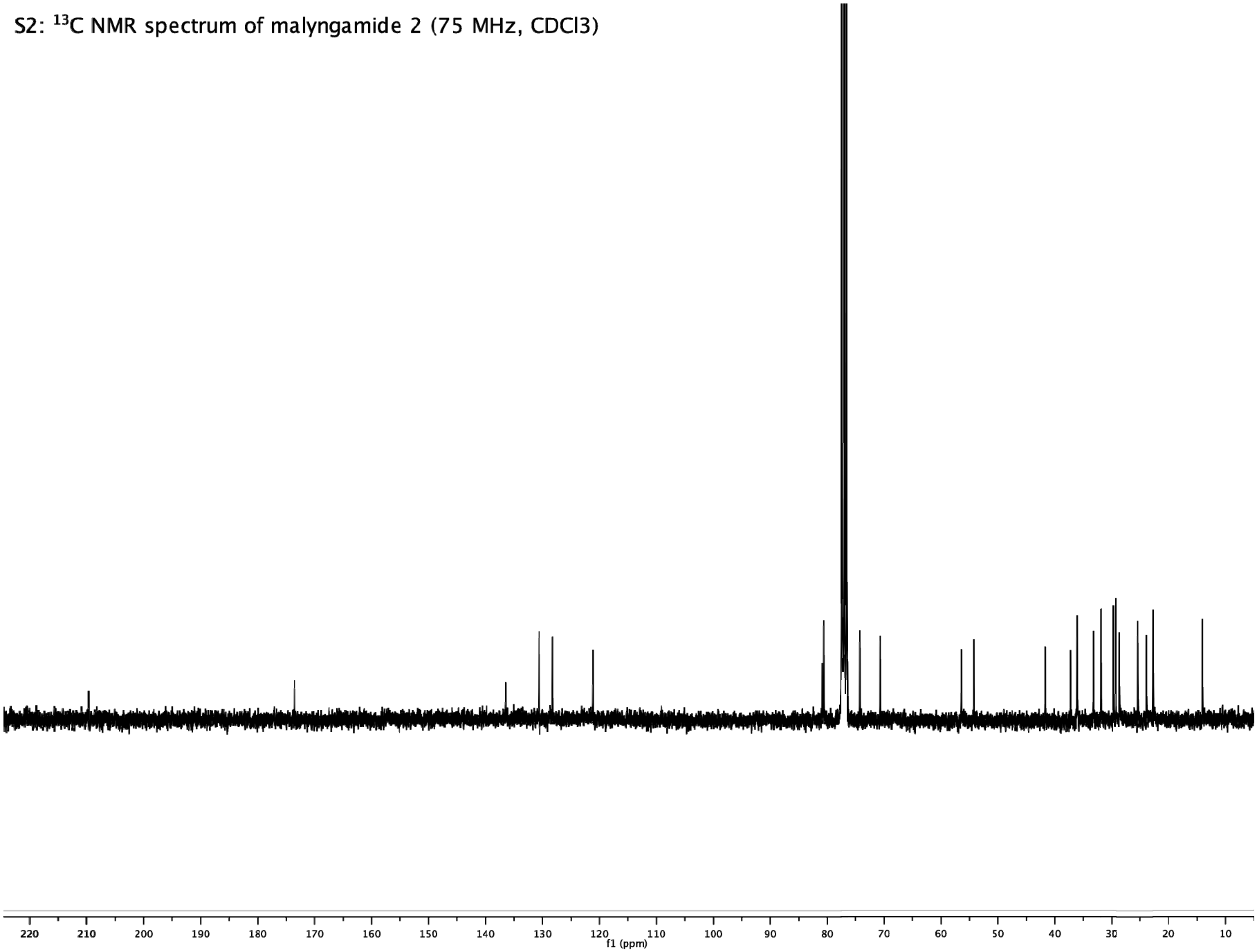
S7. Single best conformers for the 6*R**,8*R**,9*R**-triol and 7*R**,8*R**,9*R**-triol with calculated and observed $^{3}J_{HH}$ coupling constants.

S8. Comparison of the predicted $^{13}$C NMR shifts of two possible cyclohexanone core structures for malyngamide 2 (**1**) with experimentally determined $^{13}$C NMR shifts.

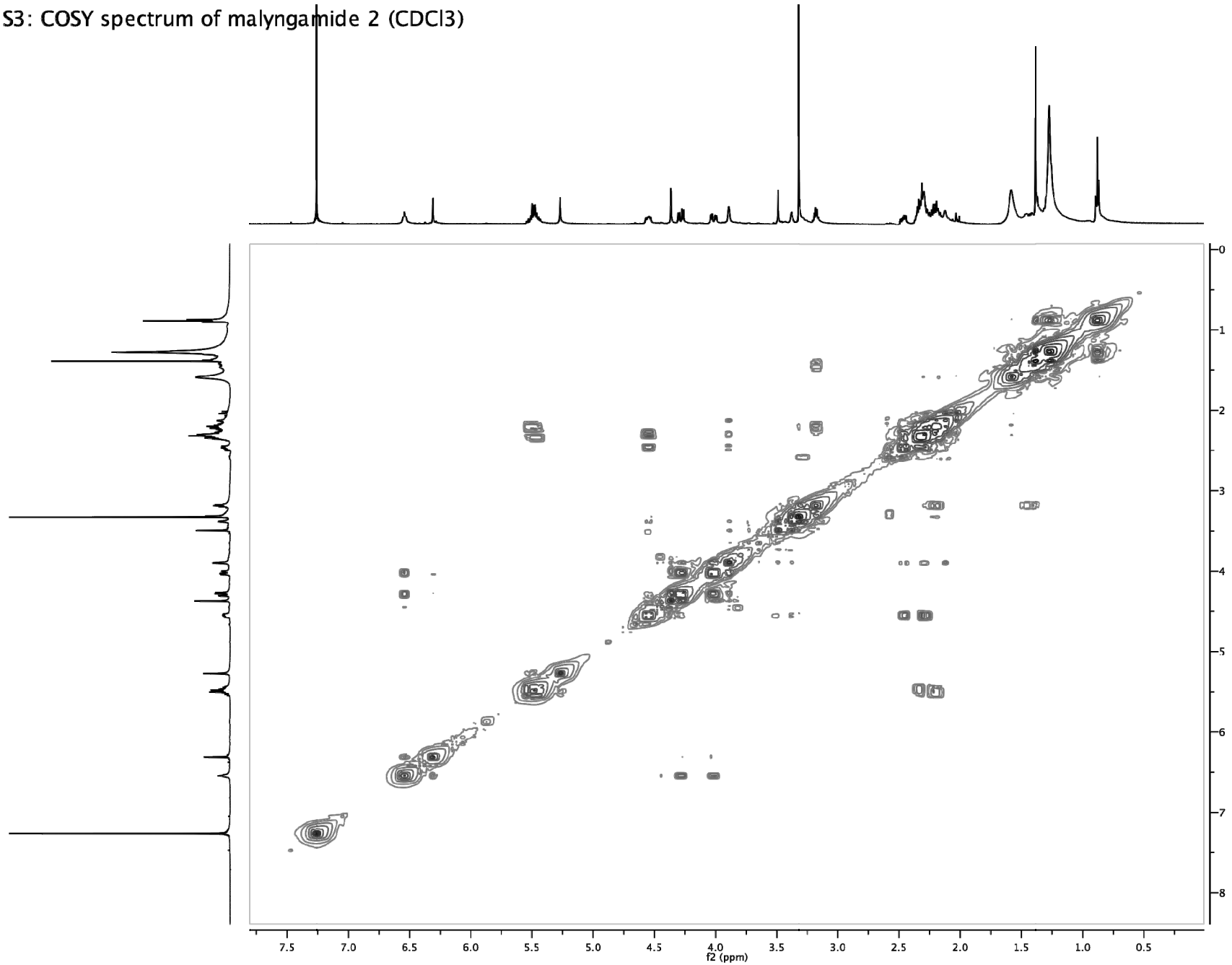
S1: $^{1}$H NMR spectrum of malyngamide 2 (500 MHz, CDCl3)



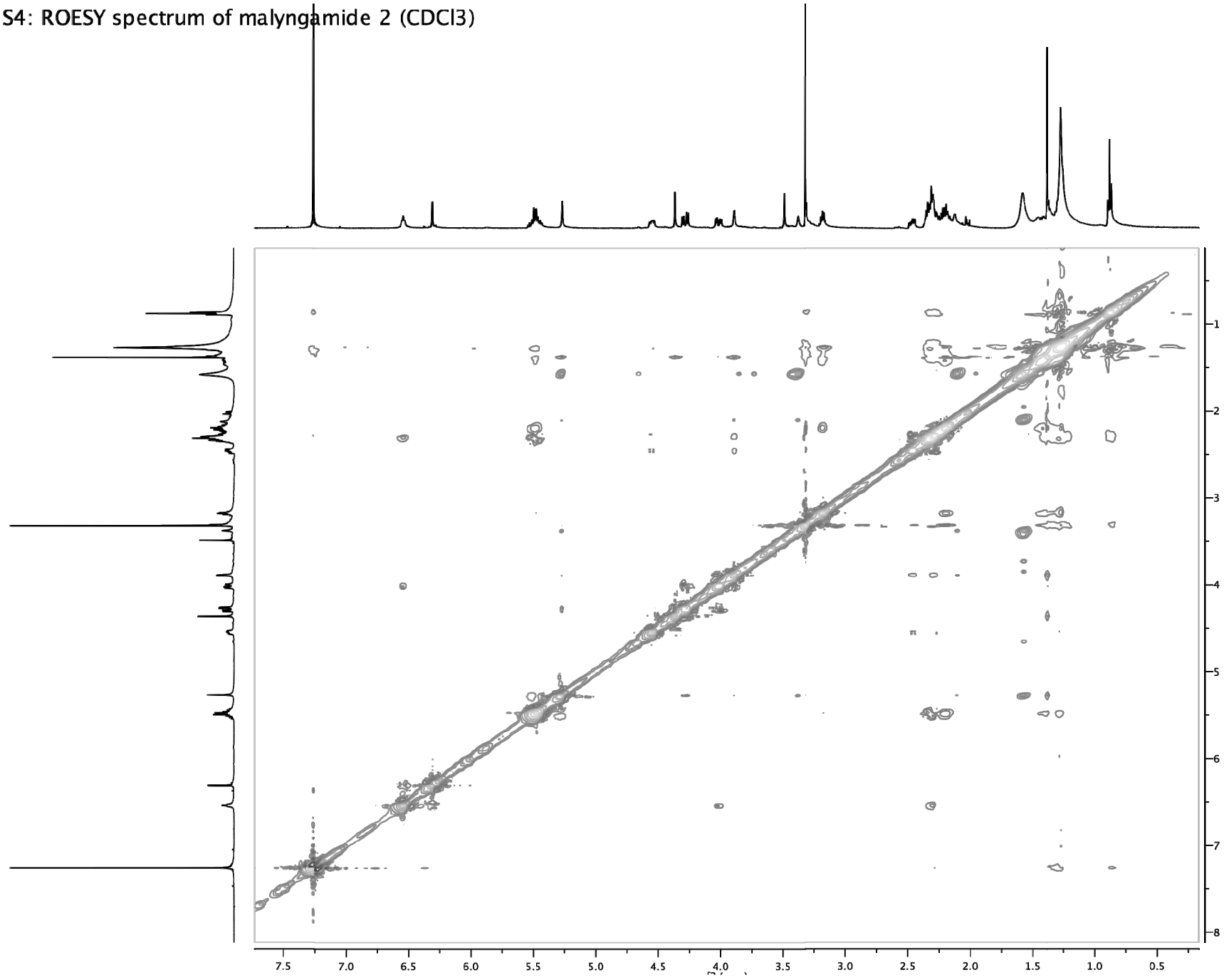
S2: $^{13}C$ NMR spectrum of malyngamide 2 (75 MHz, CDCl3)



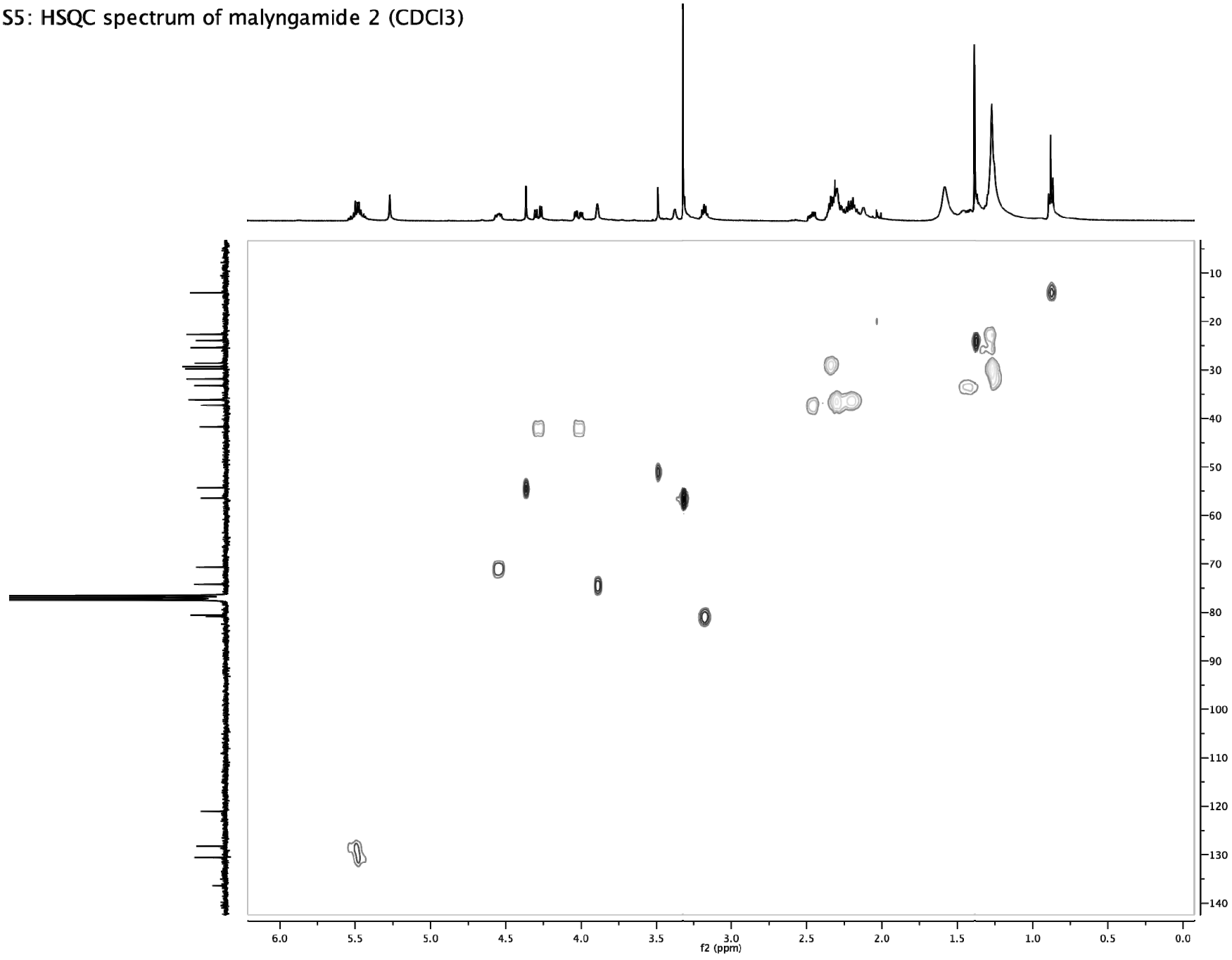
S3: COSY spectrum of malyngamide 2 (CDCl3)



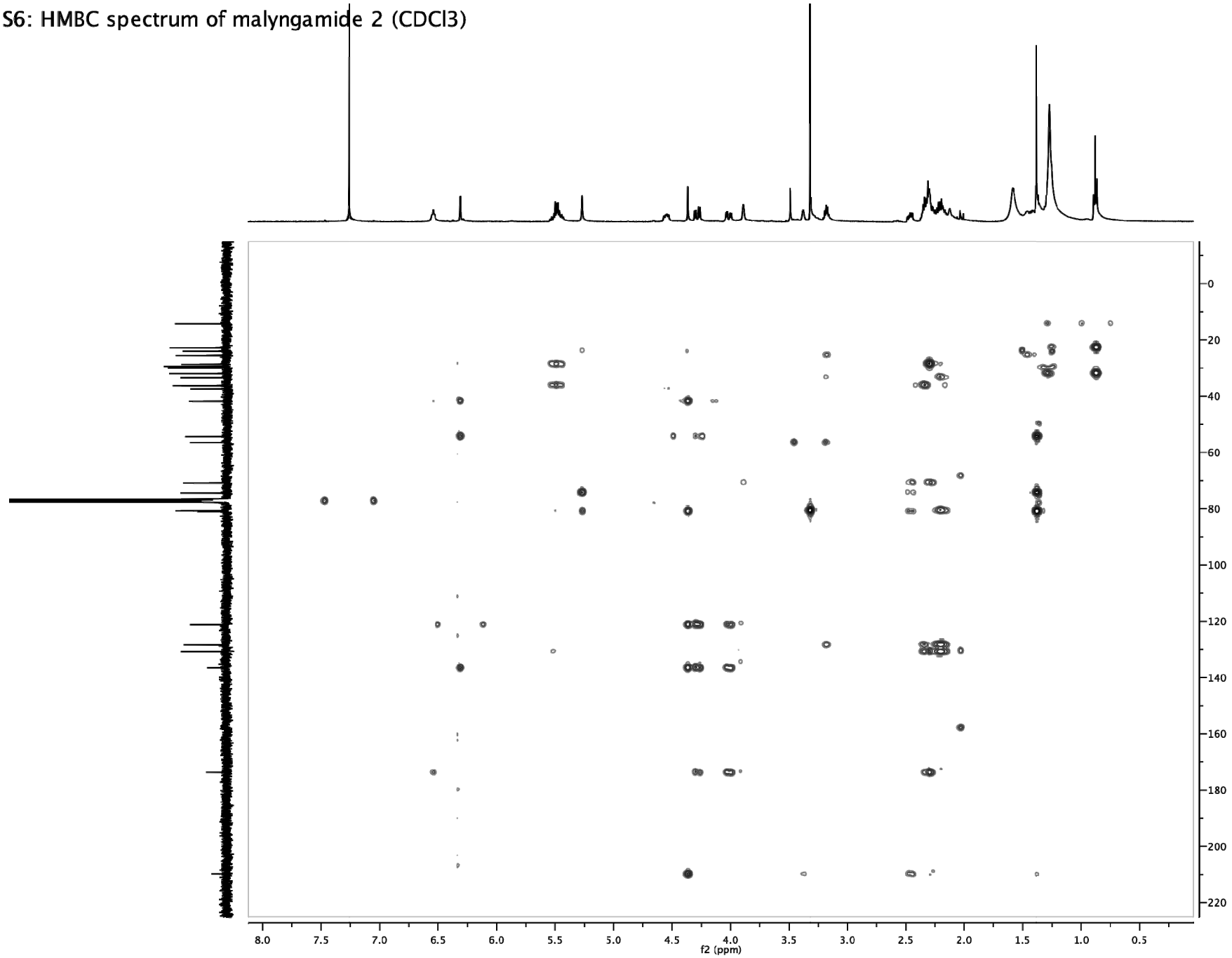
S4: ROESY spectrum of malyngamide 2 (CDCl3)

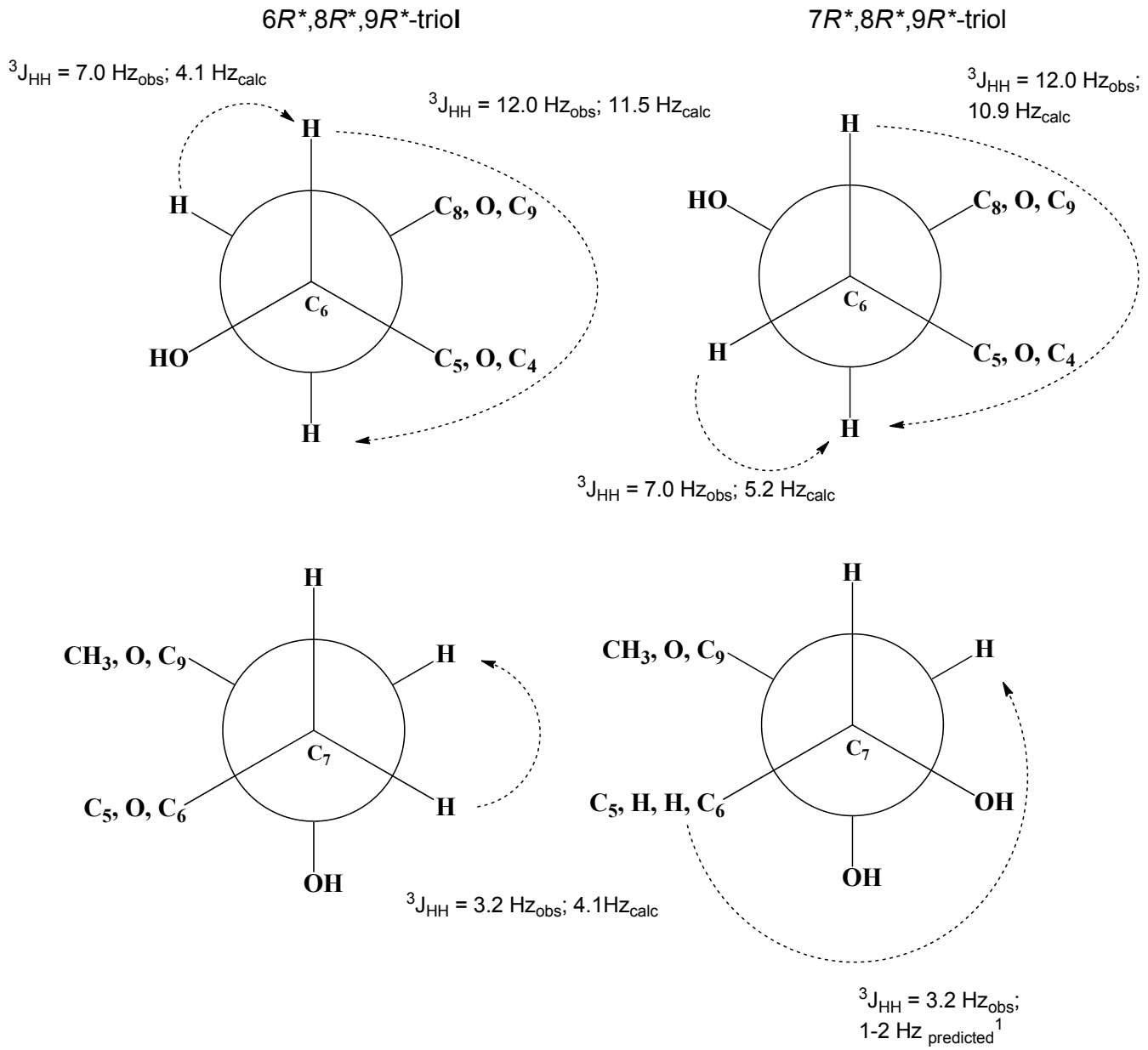


S5: HSQC spectrum of malyngamide 2 (CDCl3)



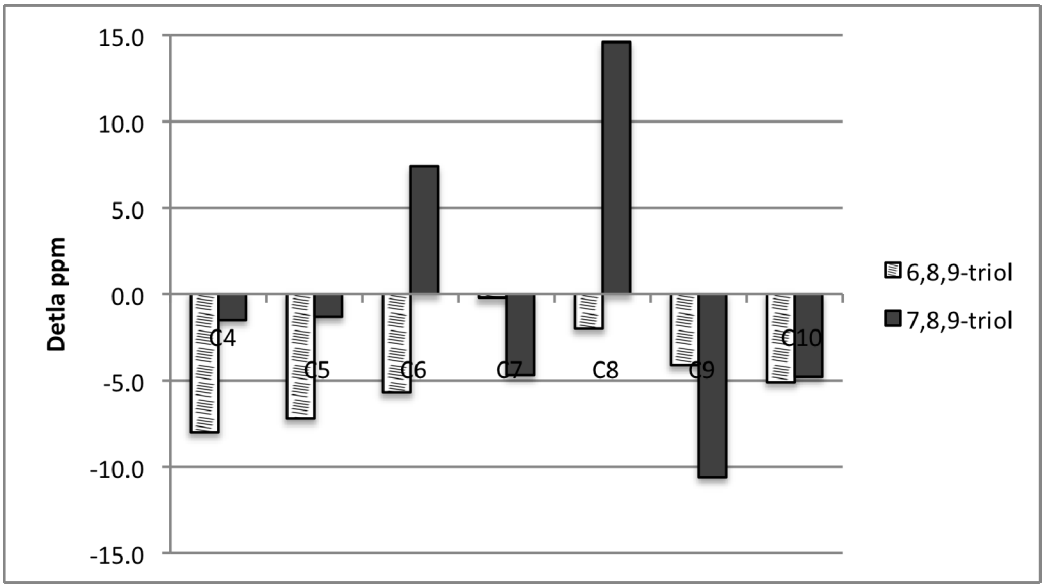
S6: HMBC spectrum of malyngamide 2 (CDCl3)






**S7.** Single best conformers for the 6*R**,8*R**,9*R**-triol and 7*R**,8*R**,9*R**-triol with calculated and observed $^{3}J_{HH}$ coupling constants.

Reference 1. Constantino, M. G.; Lacerda, V.; da Silva, G. V. J.; Tasic, L.; Rittner, R. *J. Mol. Struct.* **2001**, *597*, 129-136.




**S8.** Comparison of the predicted $^{13}C$ NMR shifts of two possible cyclohexanone core structures. In striped bars, the 6,8,9-triol is compared with the experimentally determined $^{13}C$ NMR shifts for malyngamide 2 (**1**) (mean deviation per carbon atom = 4.6 ± 2.8 ppm), and in solid bars, the 7,8,9-triol is compared (mean deviation per carbon atom = 6.4 ± 4.9 ppm).