

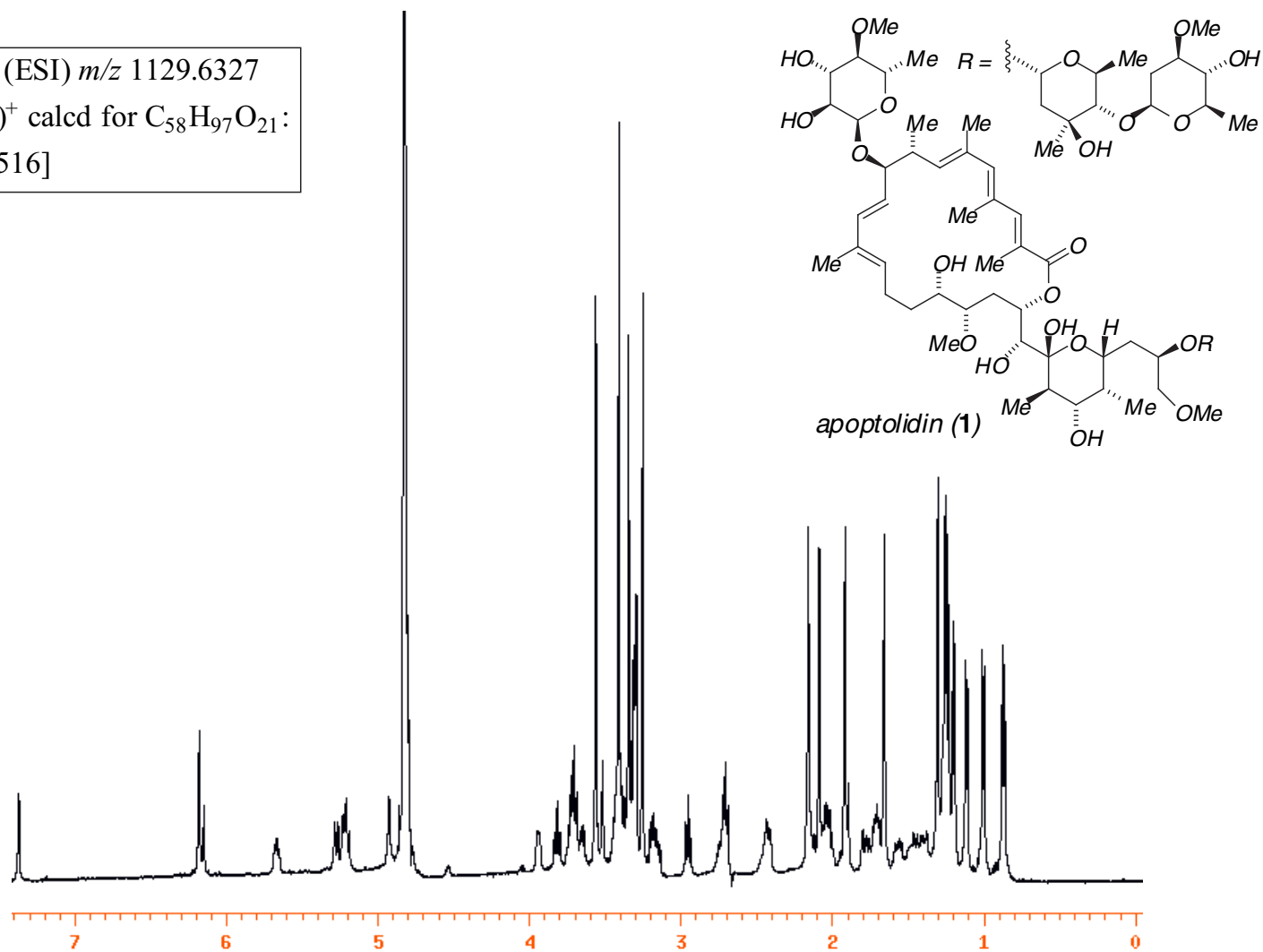
Supplementary Material for

Towards a Stable Apoptolidin Derivative: Identification of Iso-Apoptolidin and Selective Deglycosylation of Apoptolidin

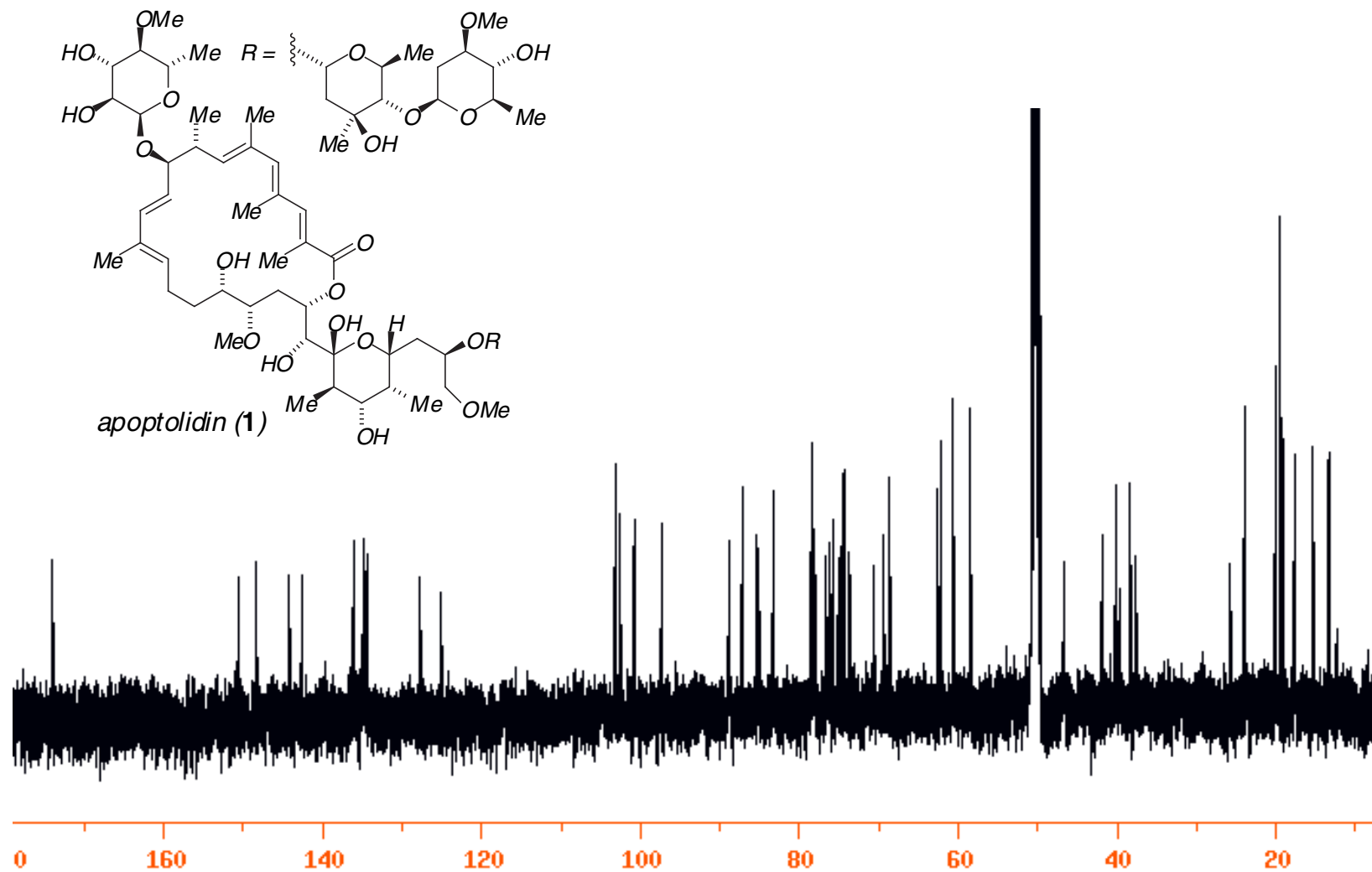
James D. Penington, Howard J. Williams, Arthur R. Salomon[‡] and Gary A. Sulikowski*

Department of Chemistry, Texas A&M University, College Station, Texas 77842.

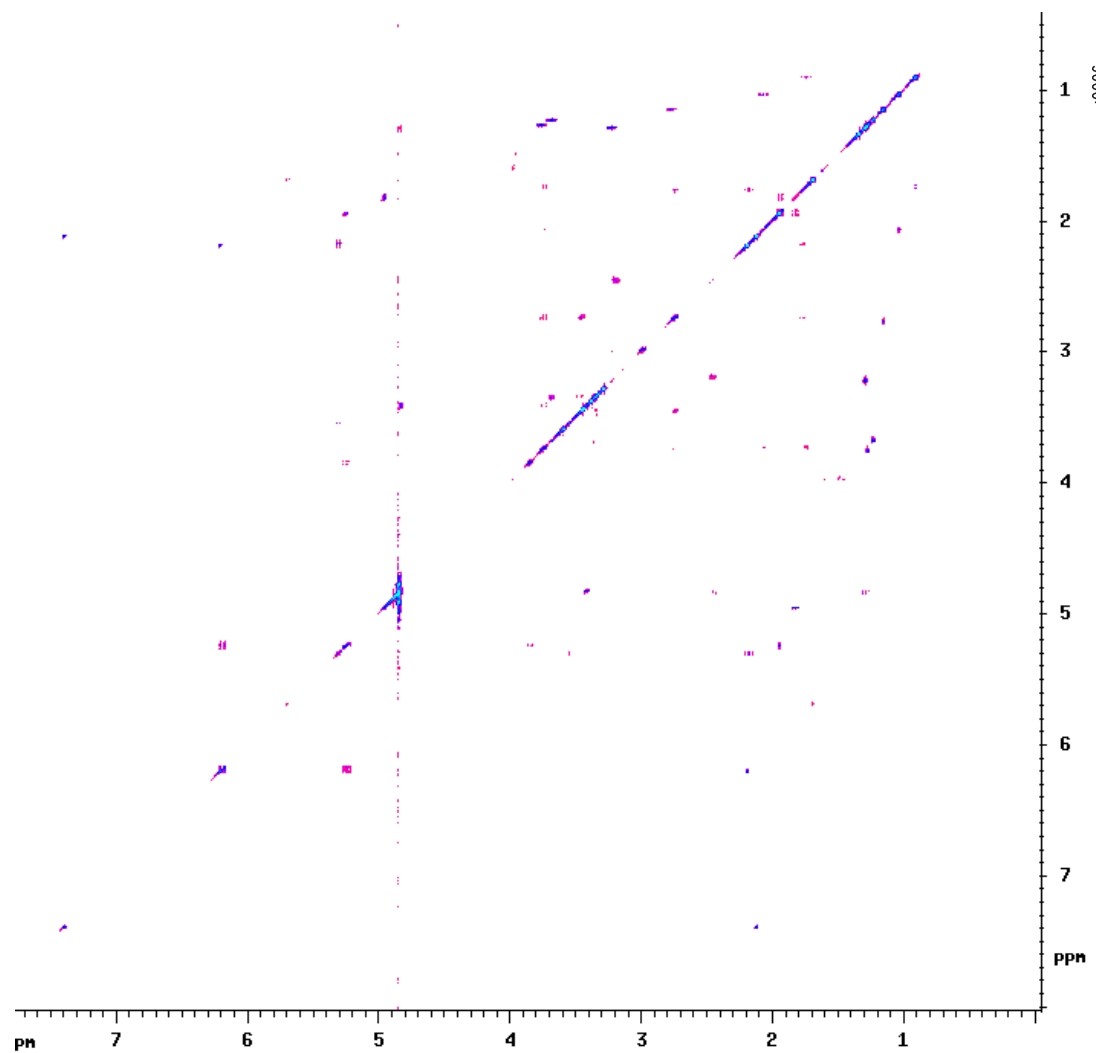
HRMS (ESI) m/z 1129.6327
[(M+H)⁺ calcd for C₅₈H₉₇O₂₁:
1129.6516]



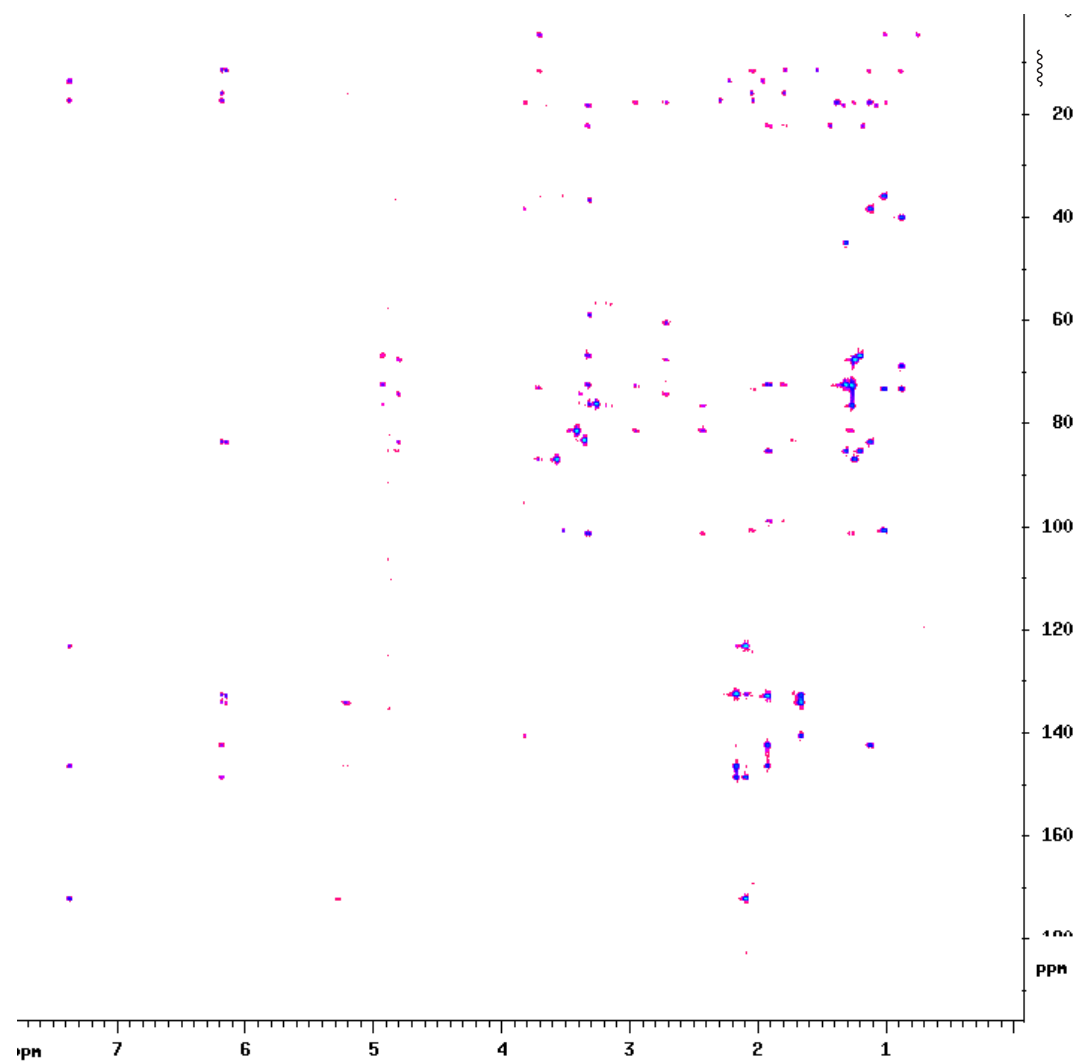
¹H NMR of apoptolidin recorded at 500 MHz in CD₃OD.



^{13}C NMR of apoptolidin recorded at 125 MHz in CD_3OD .

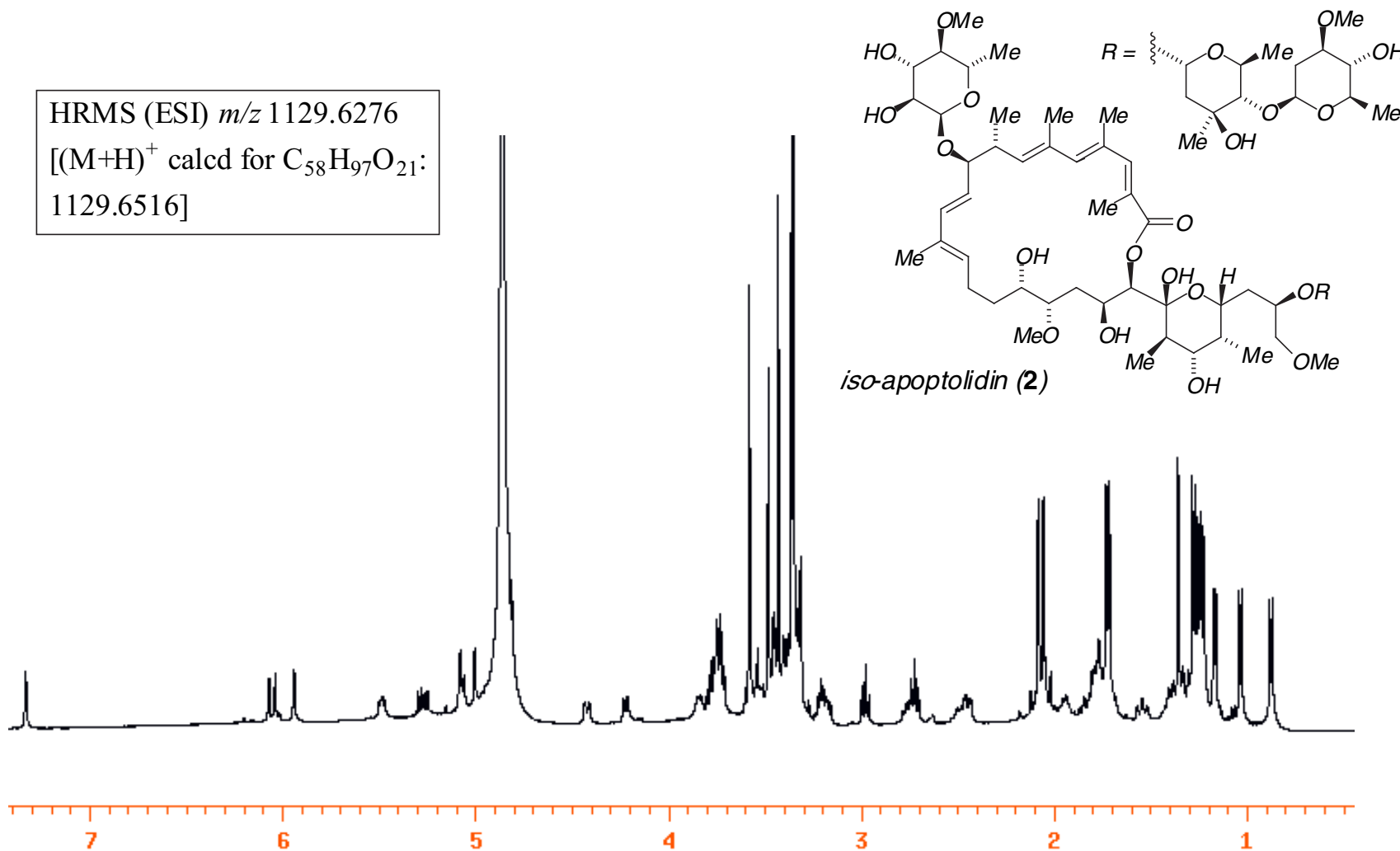


COSY spectrum of apoptolidin in CD₃OD.

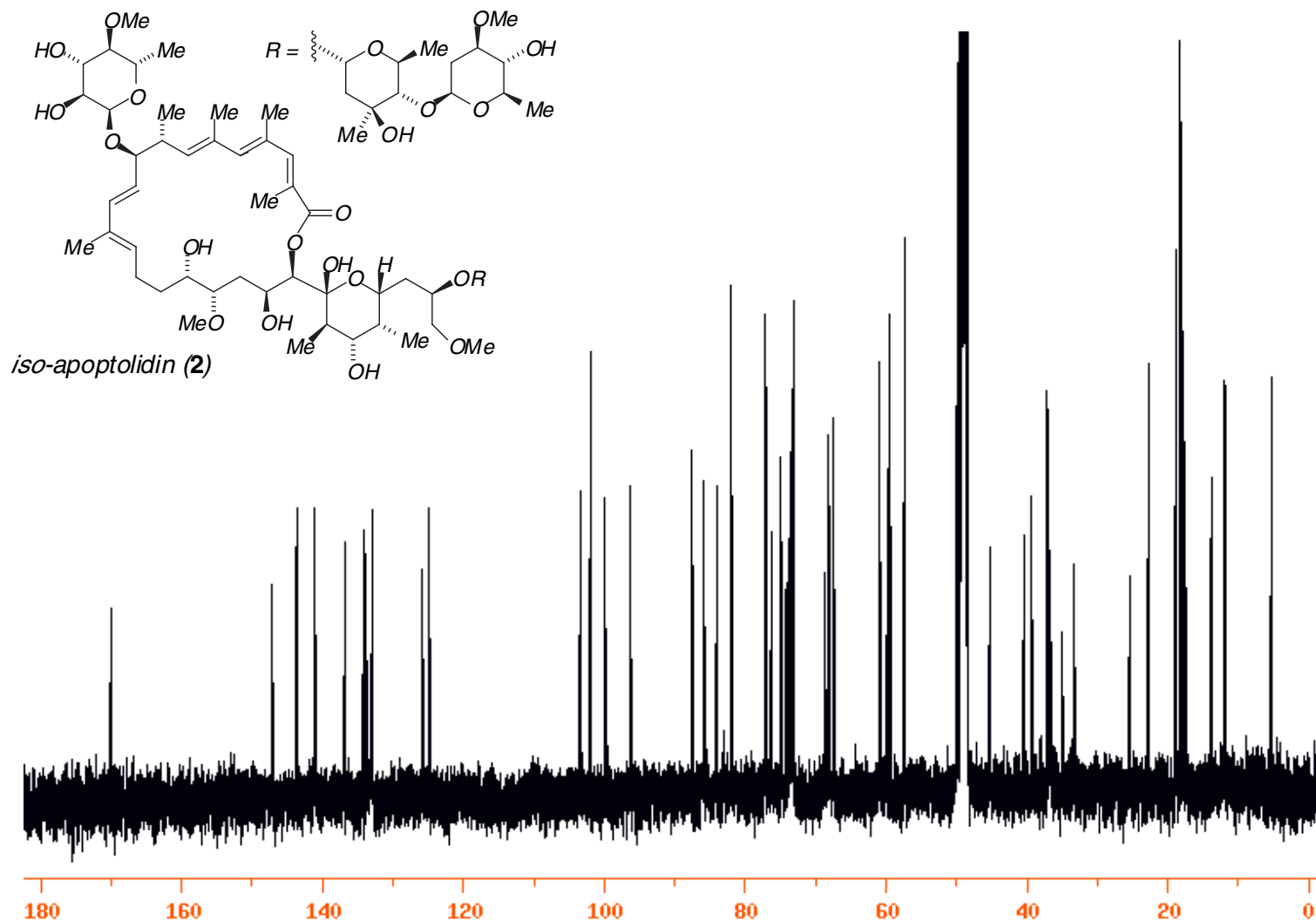


HMBC spectrum of apoptolidin in CD₃OD.

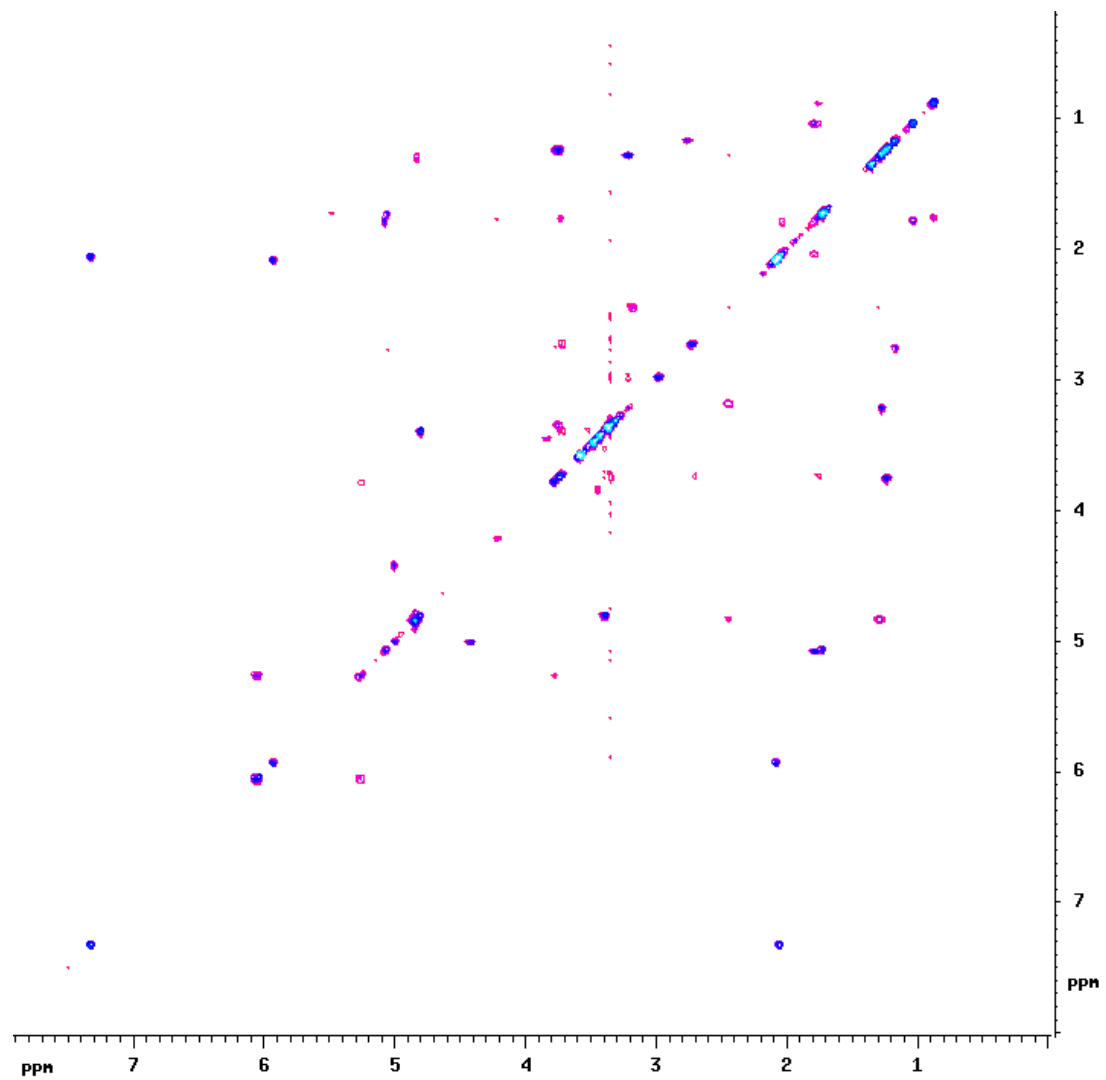
HRMS (ESI) m/z 1129.6276
[(M+H)⁺ calcd for C₅₈H₉₇O₂₁:
1129.6516]



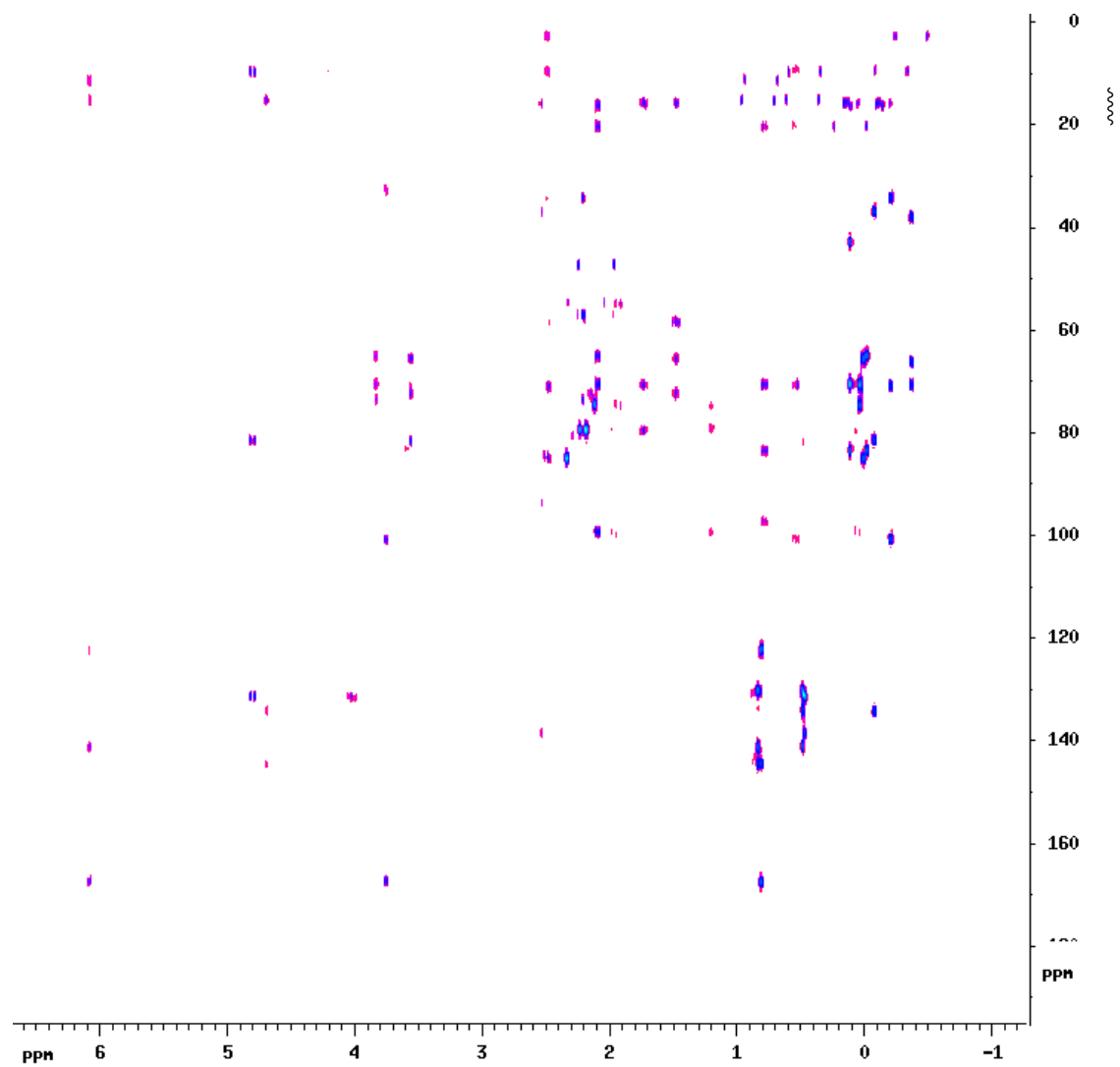
¹H NMR of *iso-apoptolidin* recorded at 500 MHz in CD₃OD.



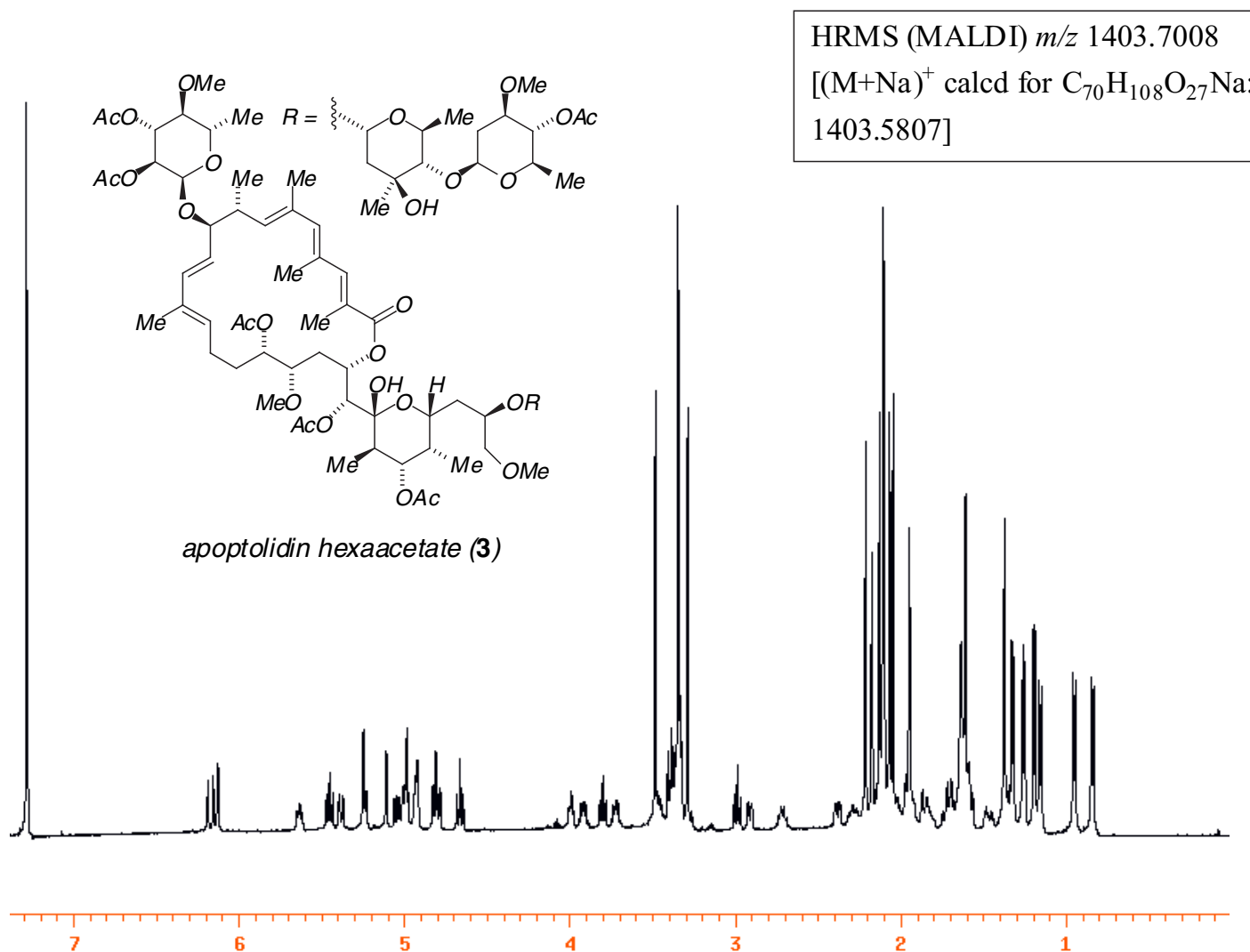
^{13}C NMR of *iso-apoptolidin* recorded at 500 MHz in CD_3OD .



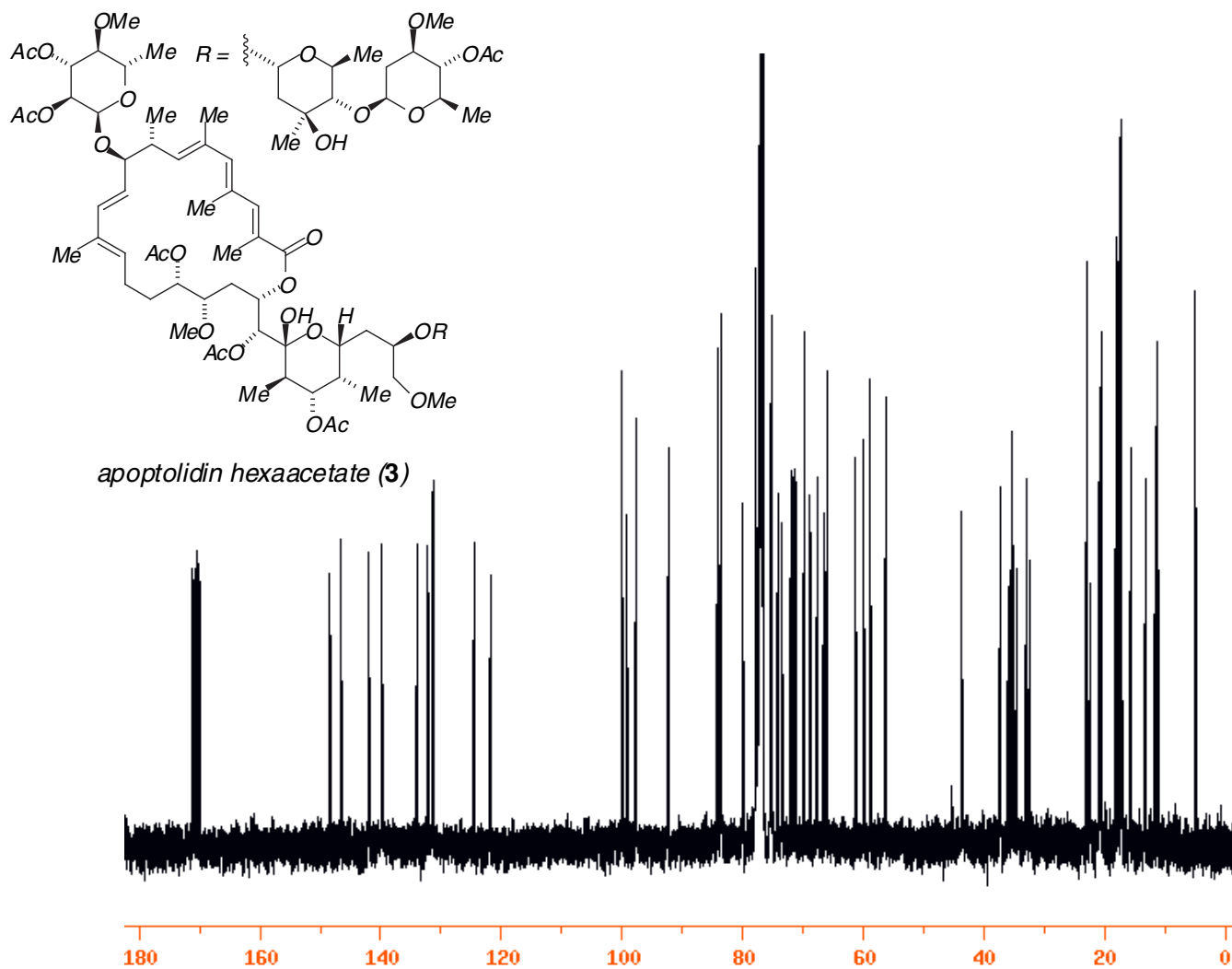
COSY spectrum of iso-apoptolidin in CD₃OD.



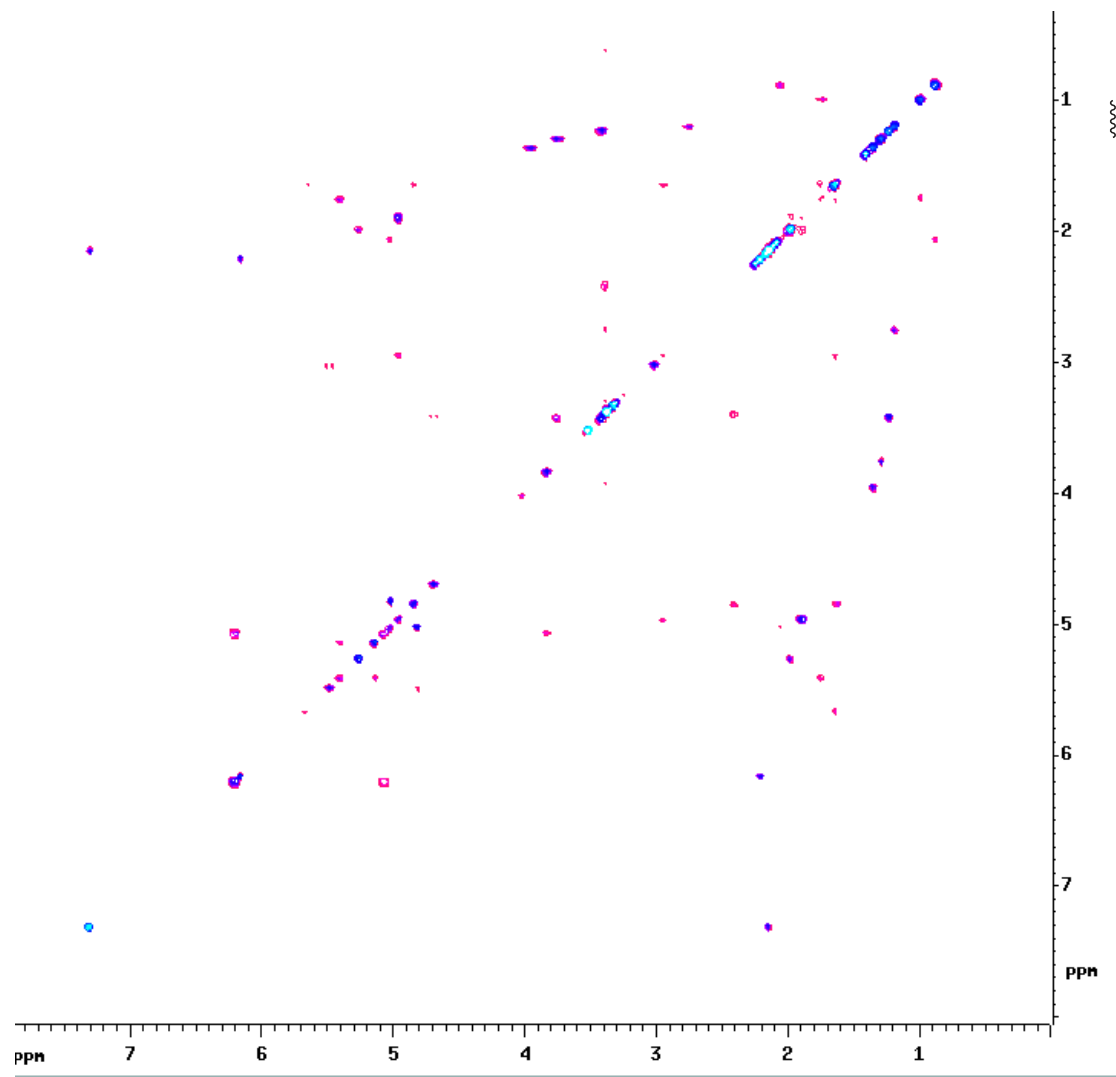
HMBC spectrum of iso-apoptolidin in CD₃OD.



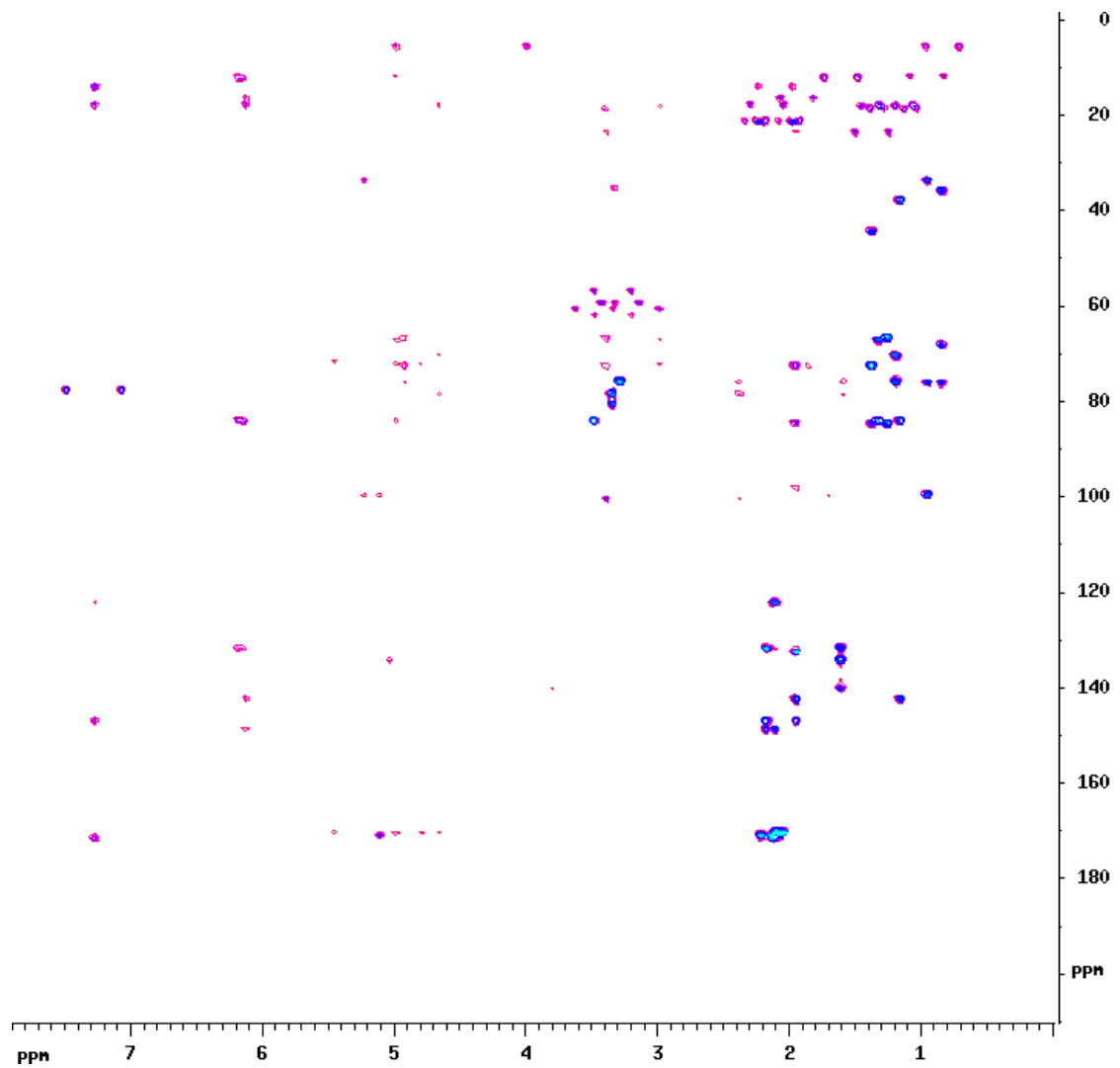
¹H NMR of *apoptolidin hexaacetate* recorded at 500 MHz in CDCl₃.



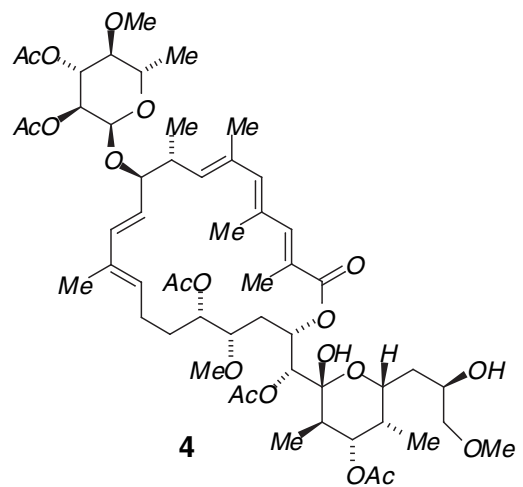
^{13}C NMR of apoptolidin hexaacetate recorded at 125 MHz in CDCl_3 .



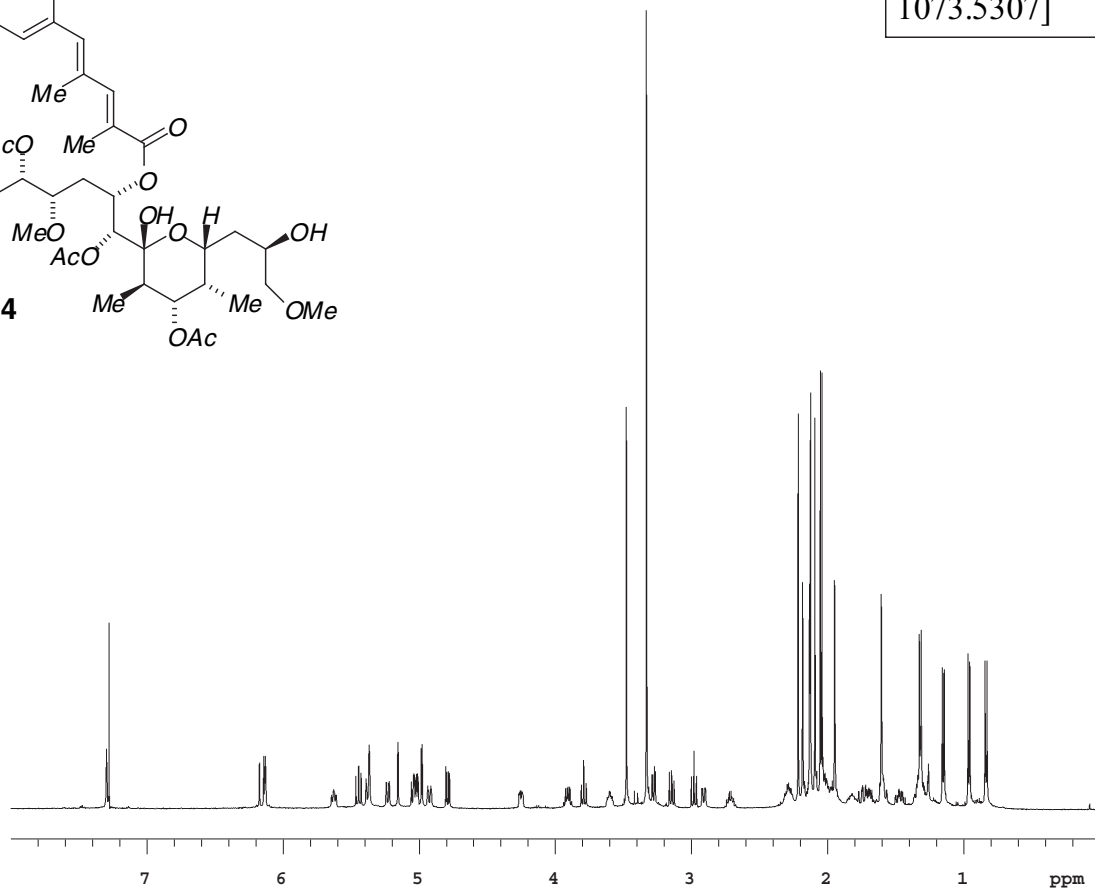
COSY spectrum of apoptolidin hexaacetate in CDCl₃.



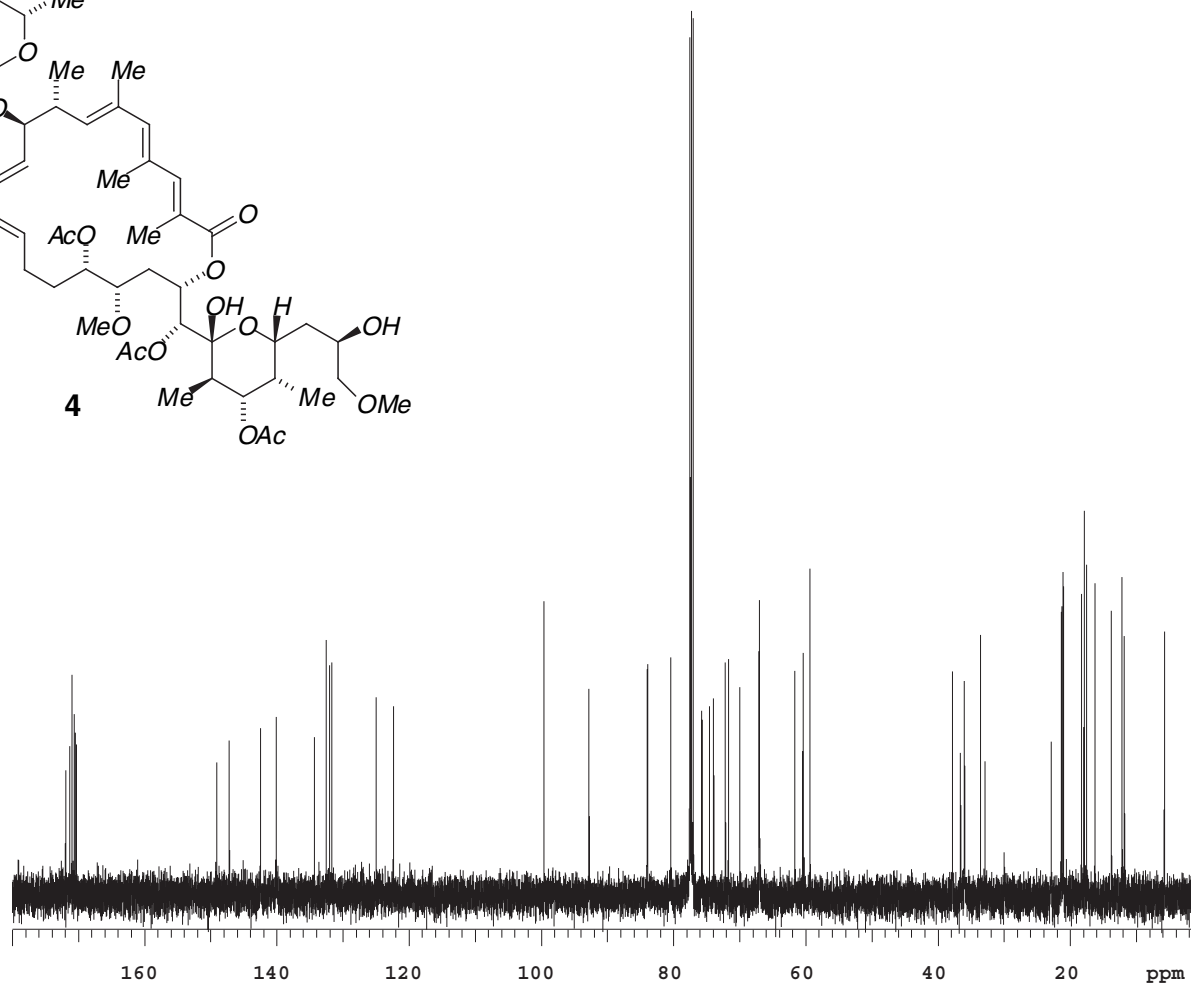
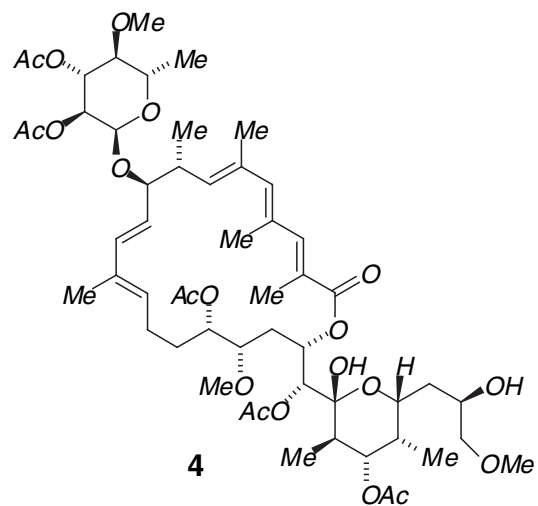
HMBC spectrum of apoptolidin hexaacetate in CDCl₃.



HRMS (MALDI) m/z 1073.5326
[[M+Na]⁺ calcd for C₅₄H₈₂O₂₀Na:
1073.5307]



¹H NMR of pseudoaglycone **4** recorded at 500 MHz in CDCl₃.



^{13}C NMR of pseudoaglycone **4** recorded at 125 MHz in CDCl_3 .