

Supplementary Material

From Sea Sponge to Clinical Trials I: Revealing the Journey of the Novel Compound PM742

Patricia G. Cruz,* Rogelio Fernández, Raquel Rodríguez-Acebes, Marta Martínez-Díez, Gema Santamaría-Núñez, Marta Pérez and Carmen Cuevas

Research and Development, PharmaMar S.A., Avda. de los Reyes 1, Pol. In. La Mina, 28770 - Colmenar Viejo, Madrid, Spain.

*Corresponding autor: pcruz@pharmamar.com

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Figure S1. ^1H NMR spectrum of **PM742**, (500 MHz, CD_3CN)

96159DMRP4H5H3-1H-2D

96159DMRP4H5H3

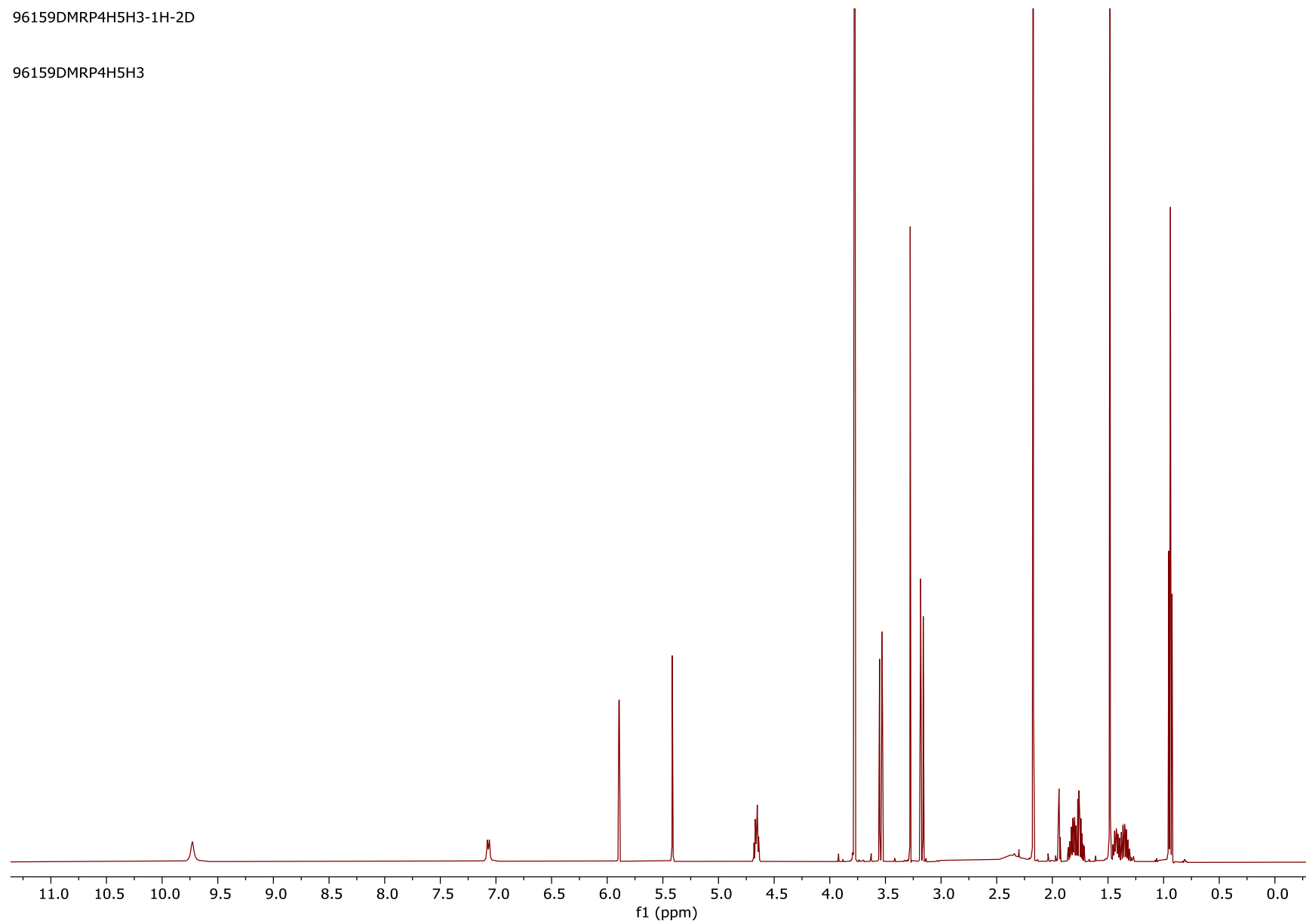


Figure S2. ^{13}C NMR spectrum **PM742**, (125 MHz, CD_3CN)

96159DMRP4H5H3-13C

96159DMRP4H5H3

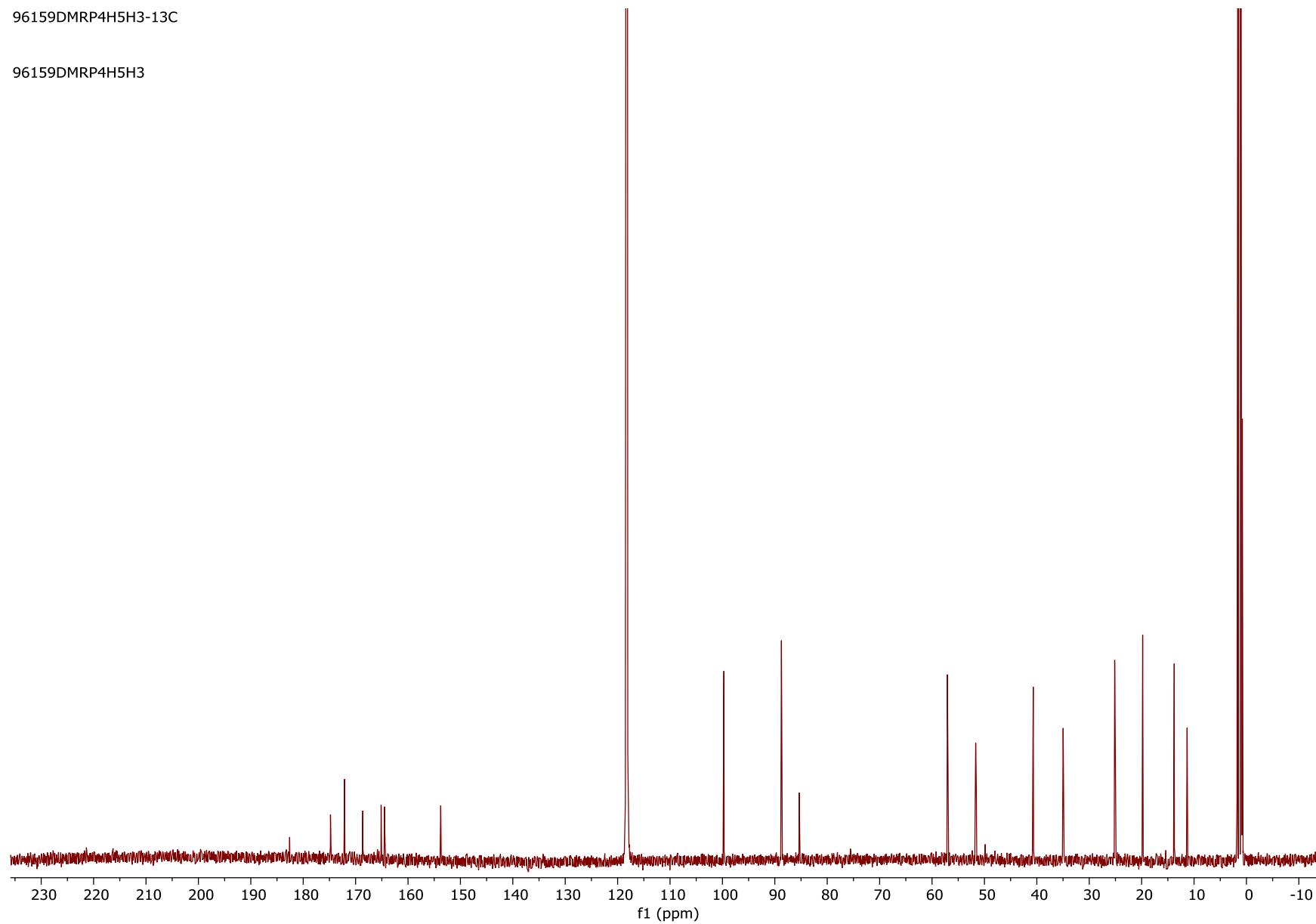


Figure S3. gCOSY spectrum **PM742**, (500 MHz, CD₃CN)

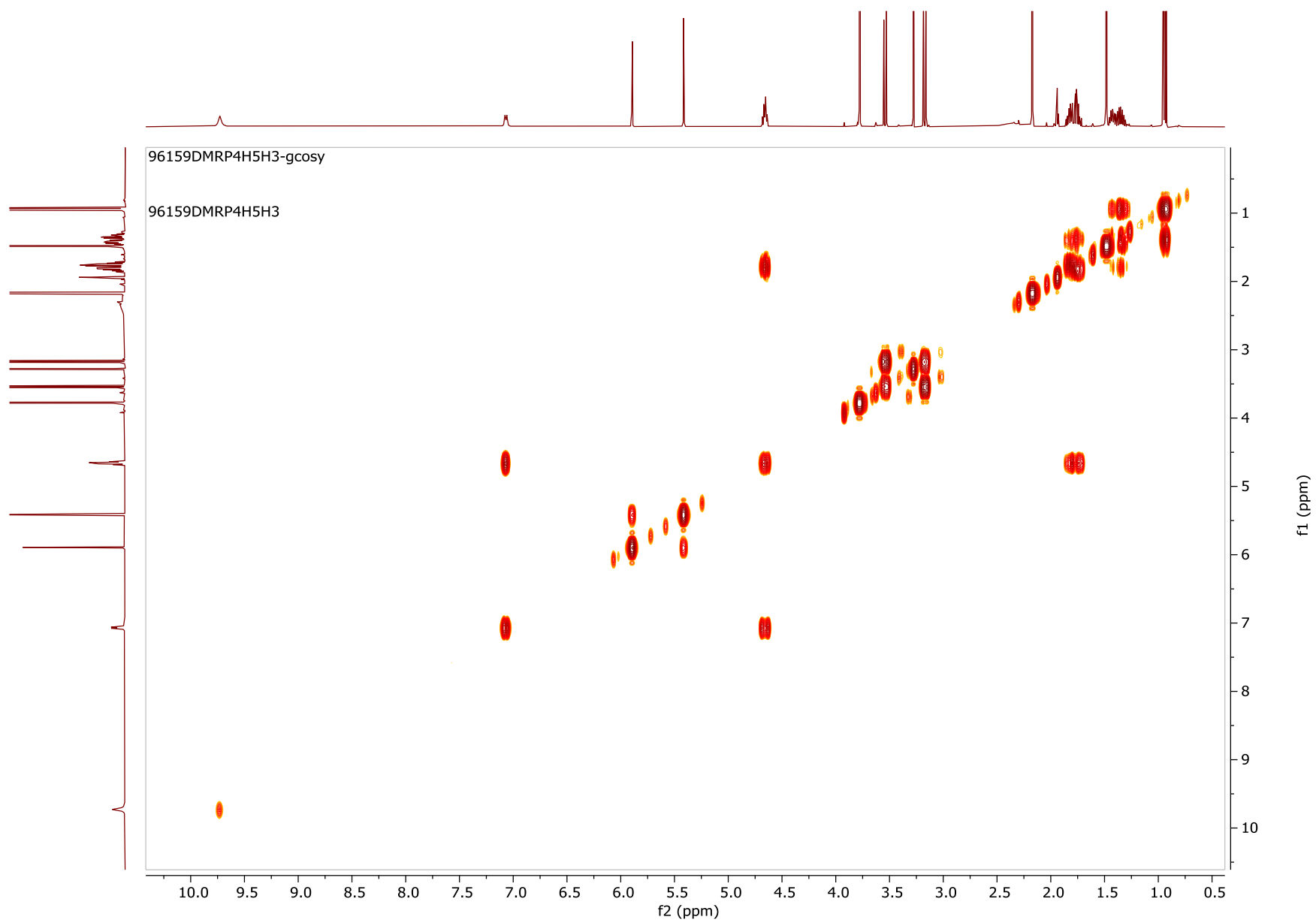


Figure S4. gHSQC spectrum **PM742**, (500 MHz, CD₃CN)

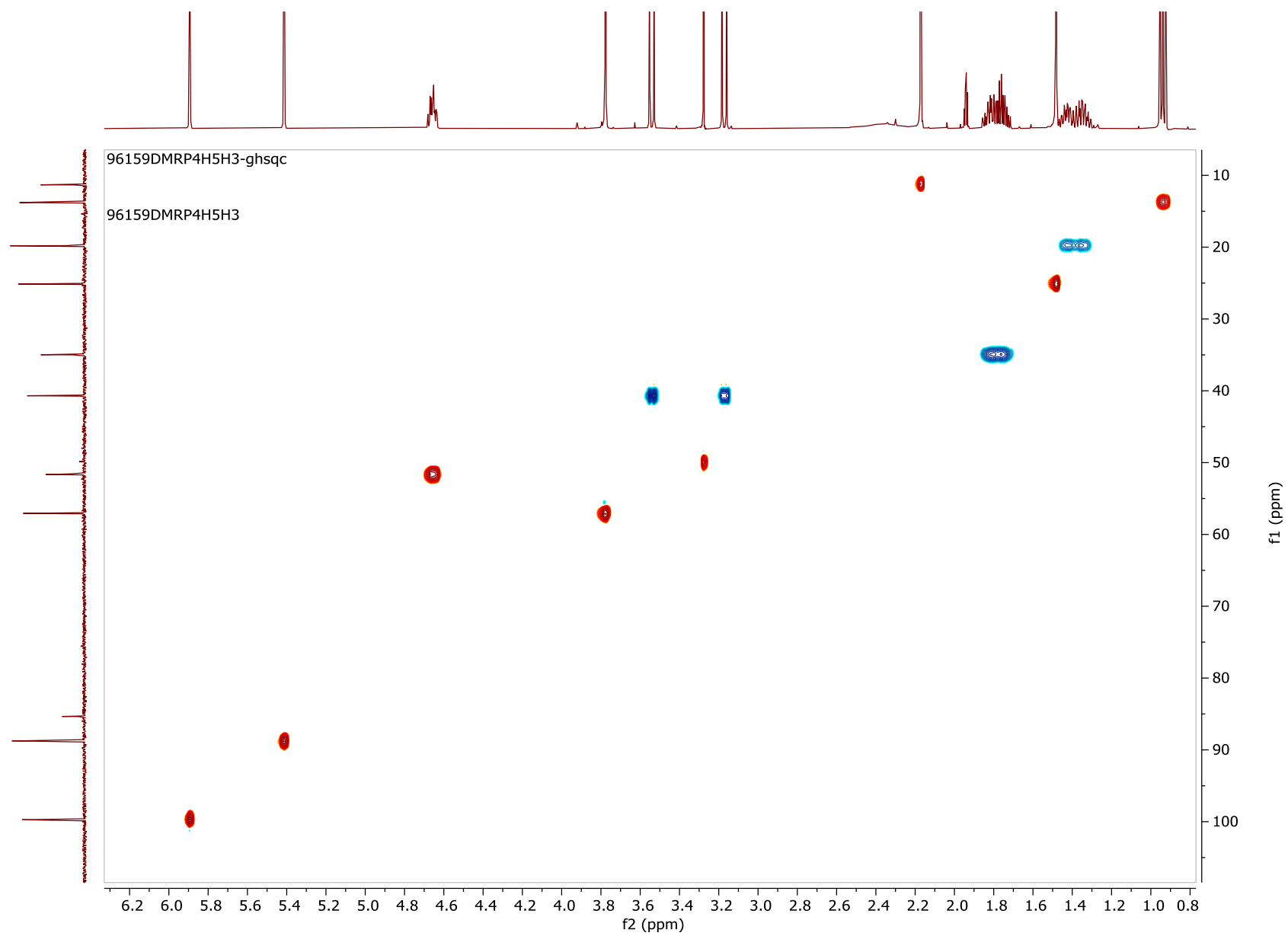


Figure S5. gHMBC spectrum **PM742**, (500 MHz, CD₃CN)

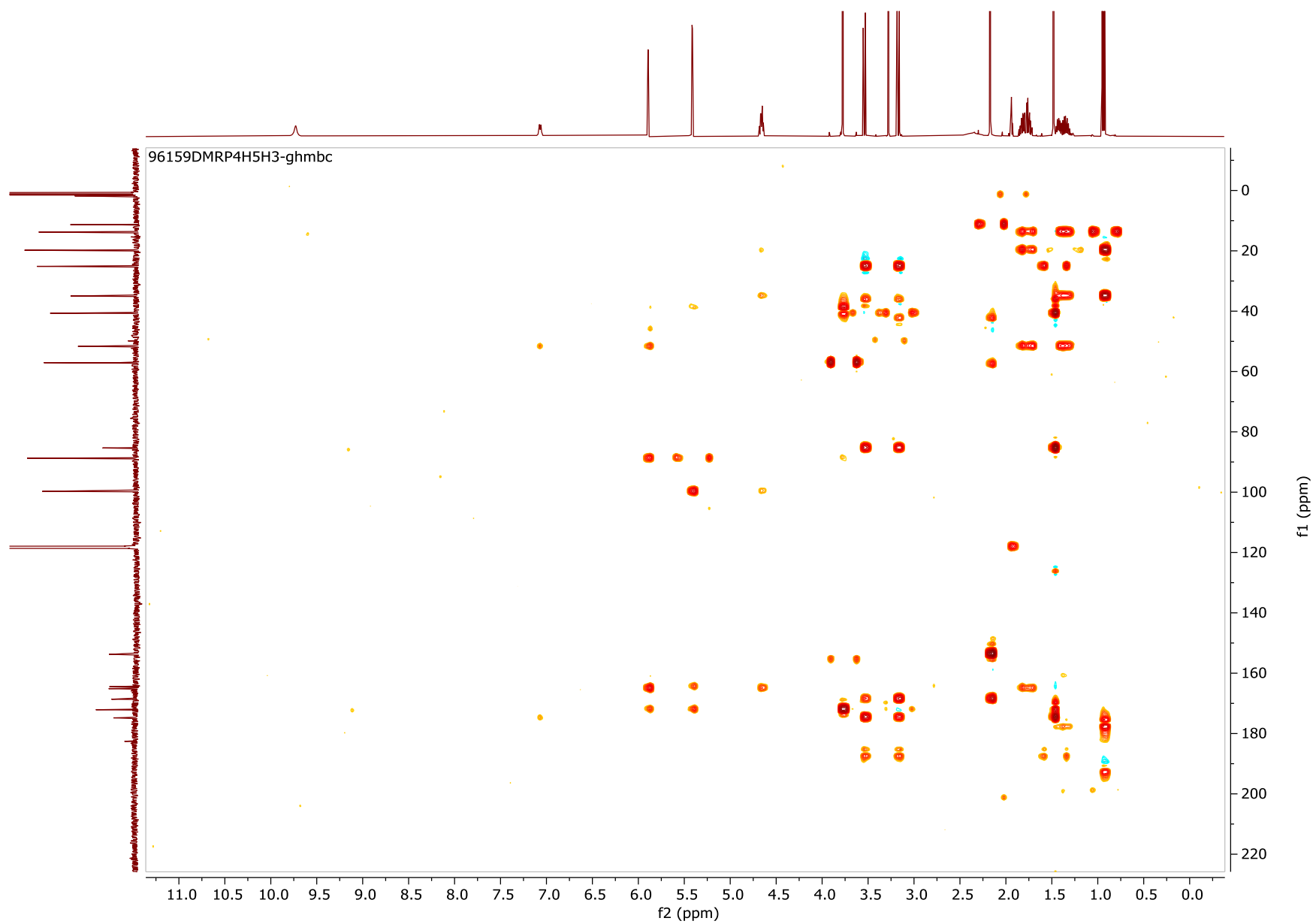


Figure S6. ROESY spectrum **PM742**, (500 MHz, CD₃CN)

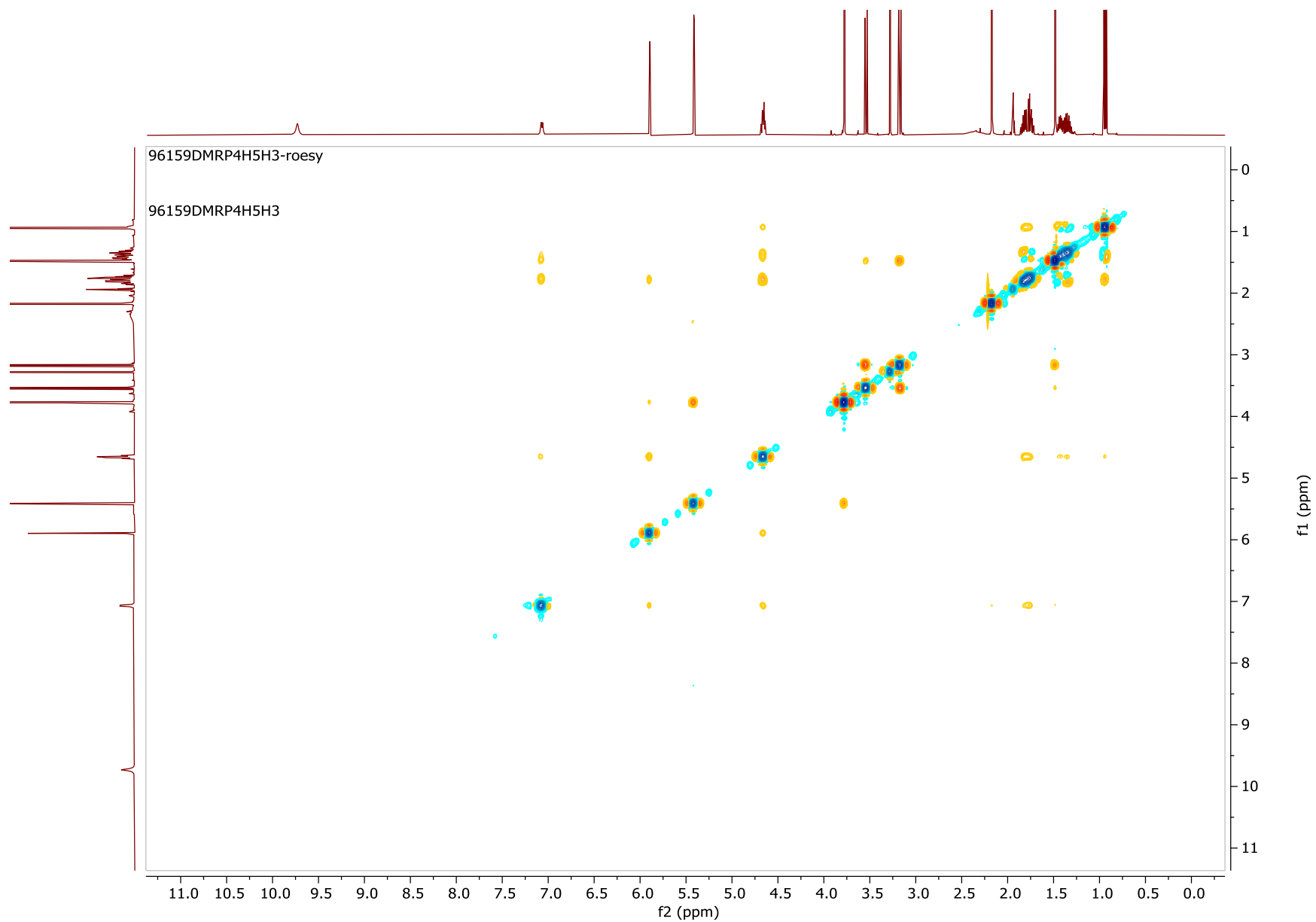


Figure S7. ^1H NMR spectrum of **PM742**, (500 MHz, CD_3OH)

96159DMRP4H5H3-MeOH-1H-presat

96159DMRP4H5H3

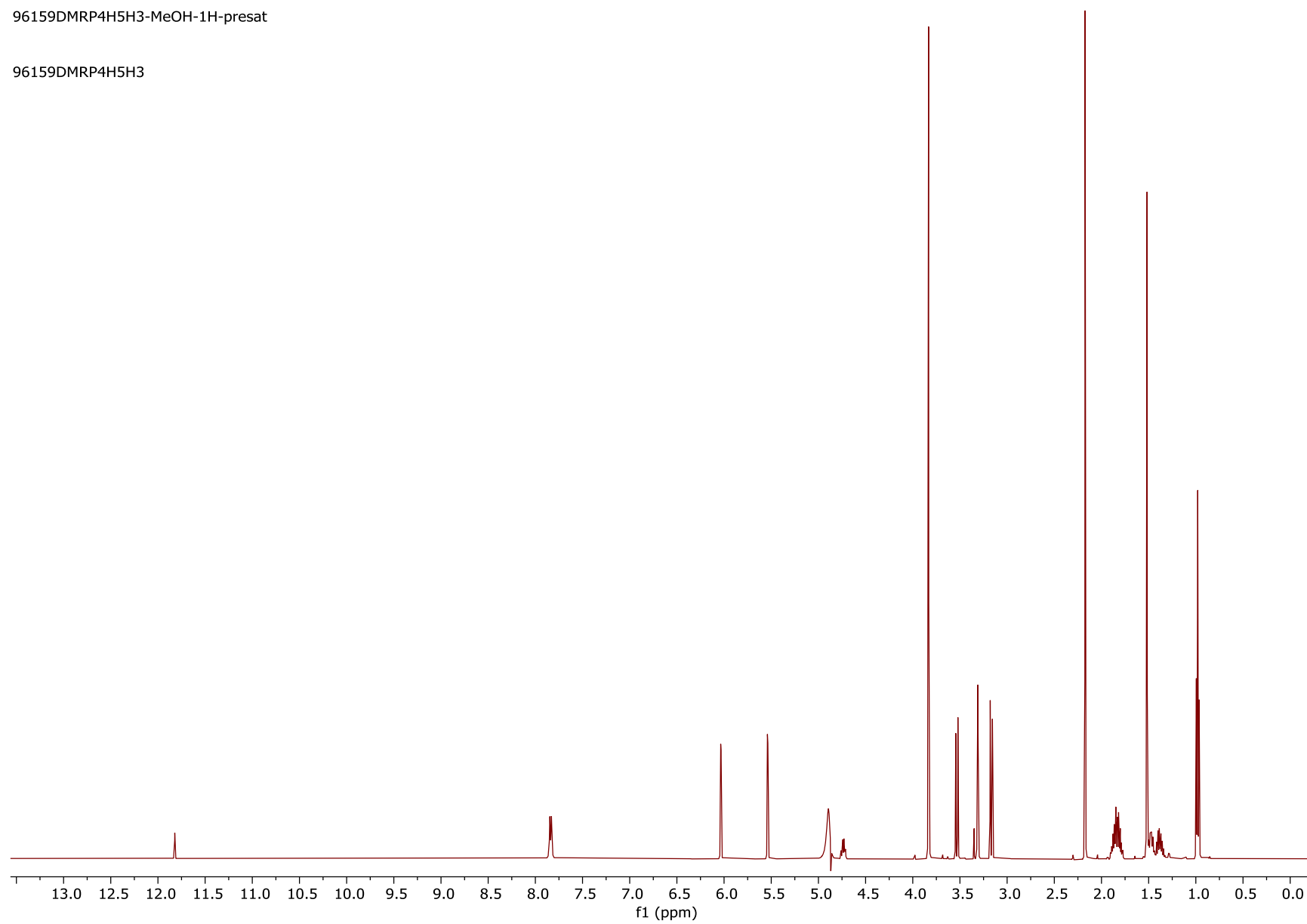


Figure S8. ^{13}C NMR spectrum **PM742**, (125 MHz, CD_3OH)

96159DMRP4H5H3-MeOH-13C

96159DMRP4H5H3

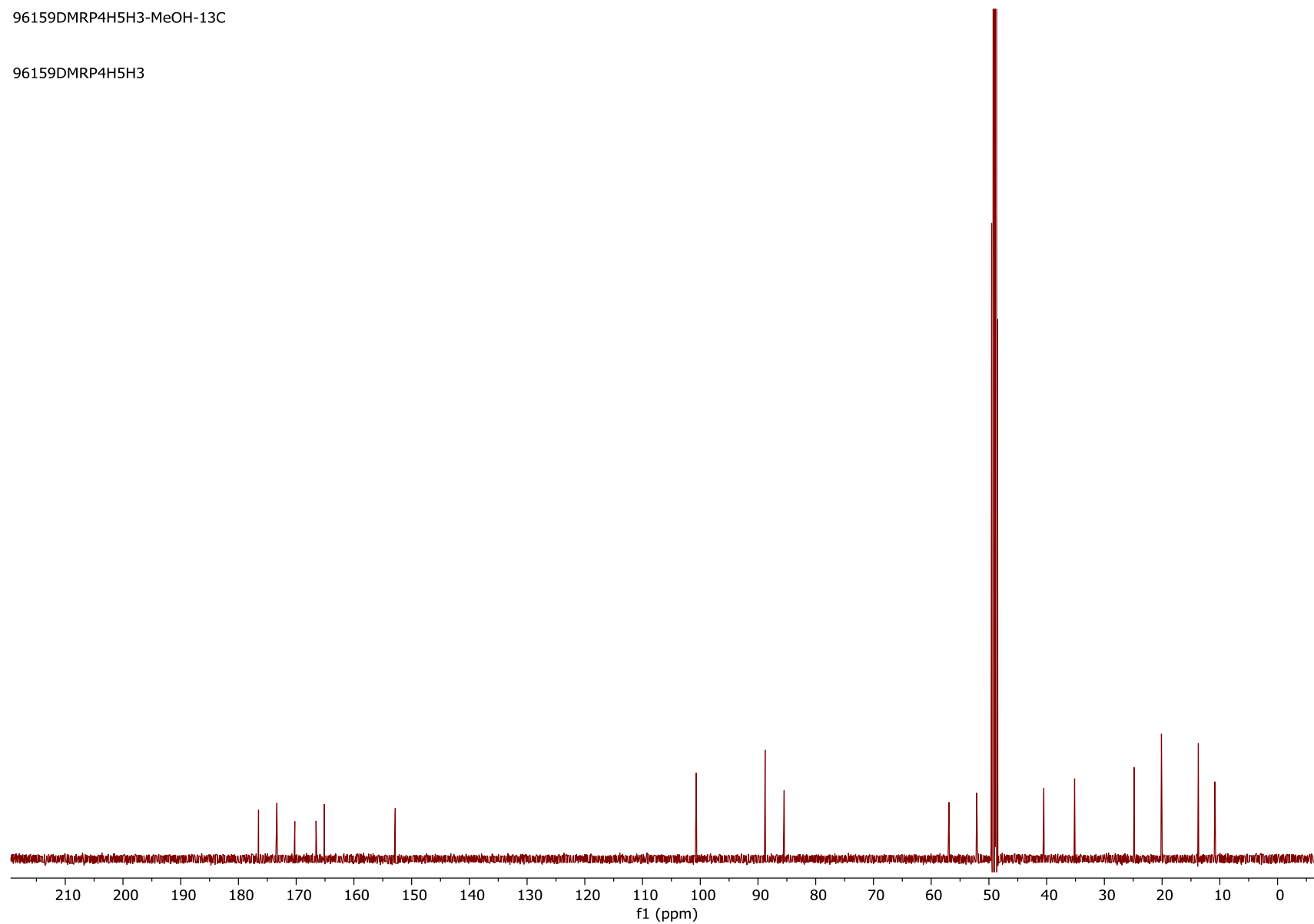


Figure S9. gHMBC spectrum **PM742**, (500 MHz, CD₃OH)

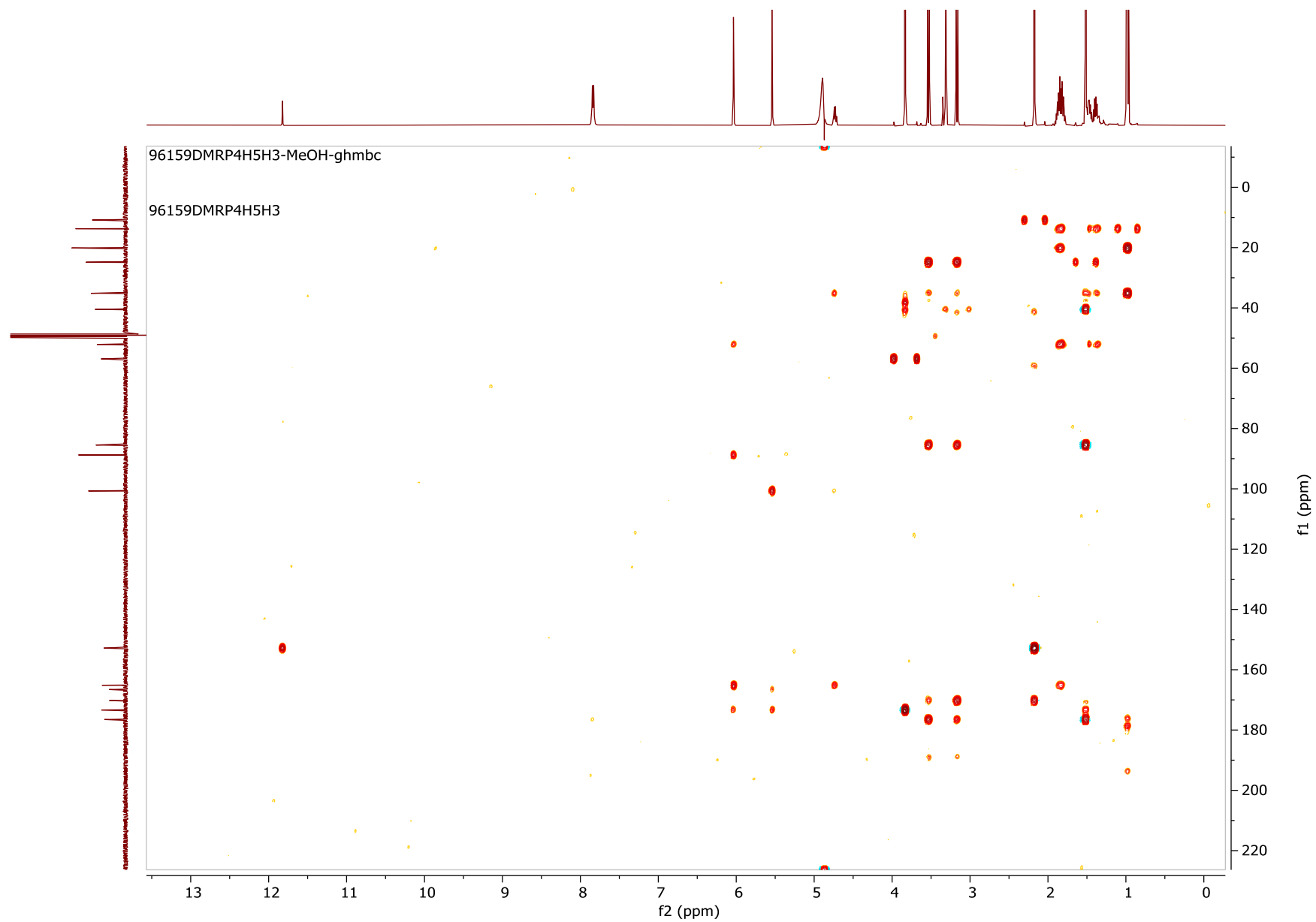


Figure S10. ROESY spectrum **PM742**, (500 MHz, CD₃OH)

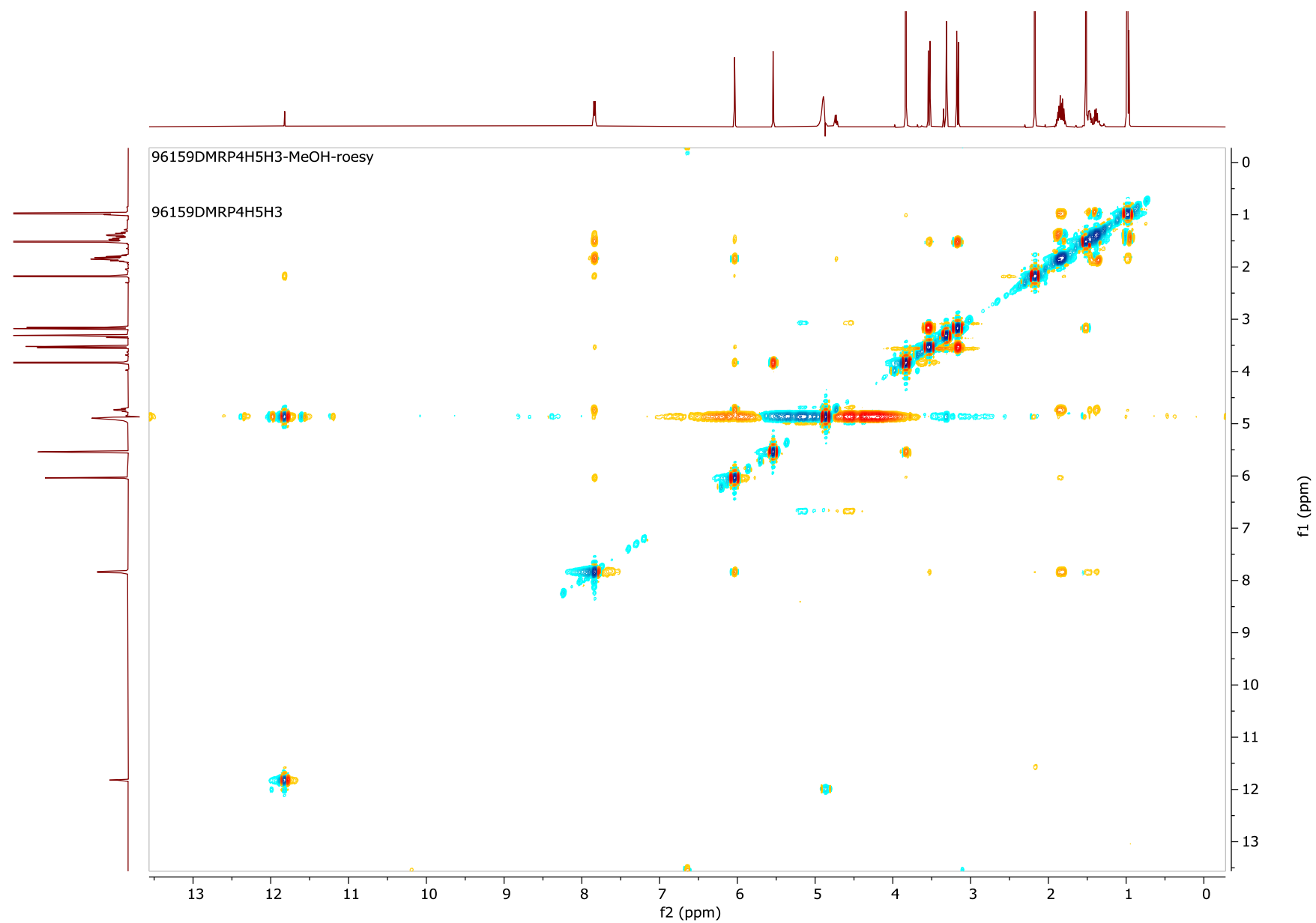


Figure S11. (+)-HRESITOFMS spectrum of **1**

User Spectrum Plot Report



Name	PM110742	Rack Pos.		Instrument	Instrument 1	Operator	sg
Inj. Vol. (ul)	1	Plate Pos.		IRM Status	All ions missed		
Data File	PM110742.d	Method (Acq)	TOF-DDMG.m	Comment		Acq. Time (Local)	11/23/2011 11:22:42 PM (UTC+02:00)

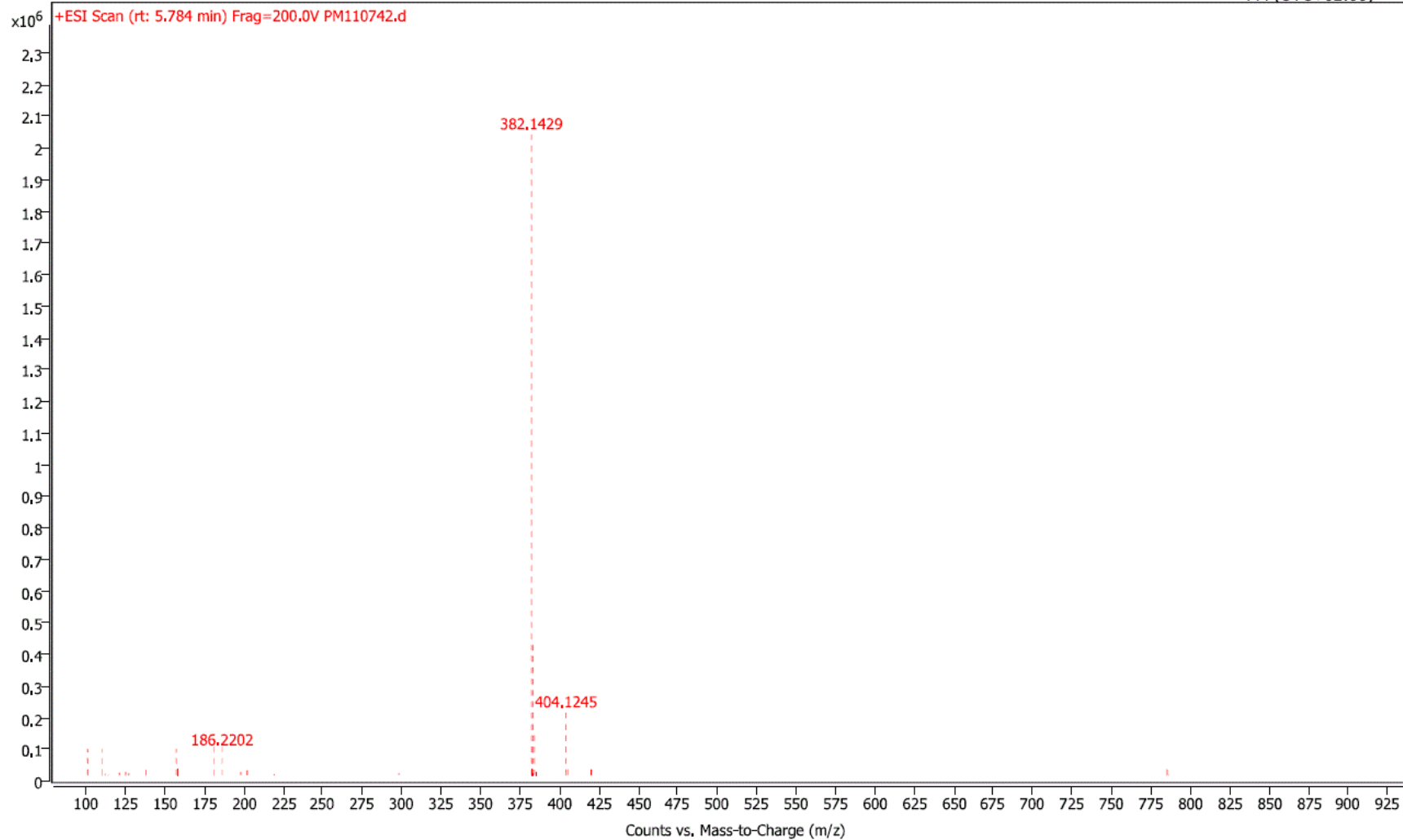


Figure S12. (+)ESIMS of hydrolysis of **1**

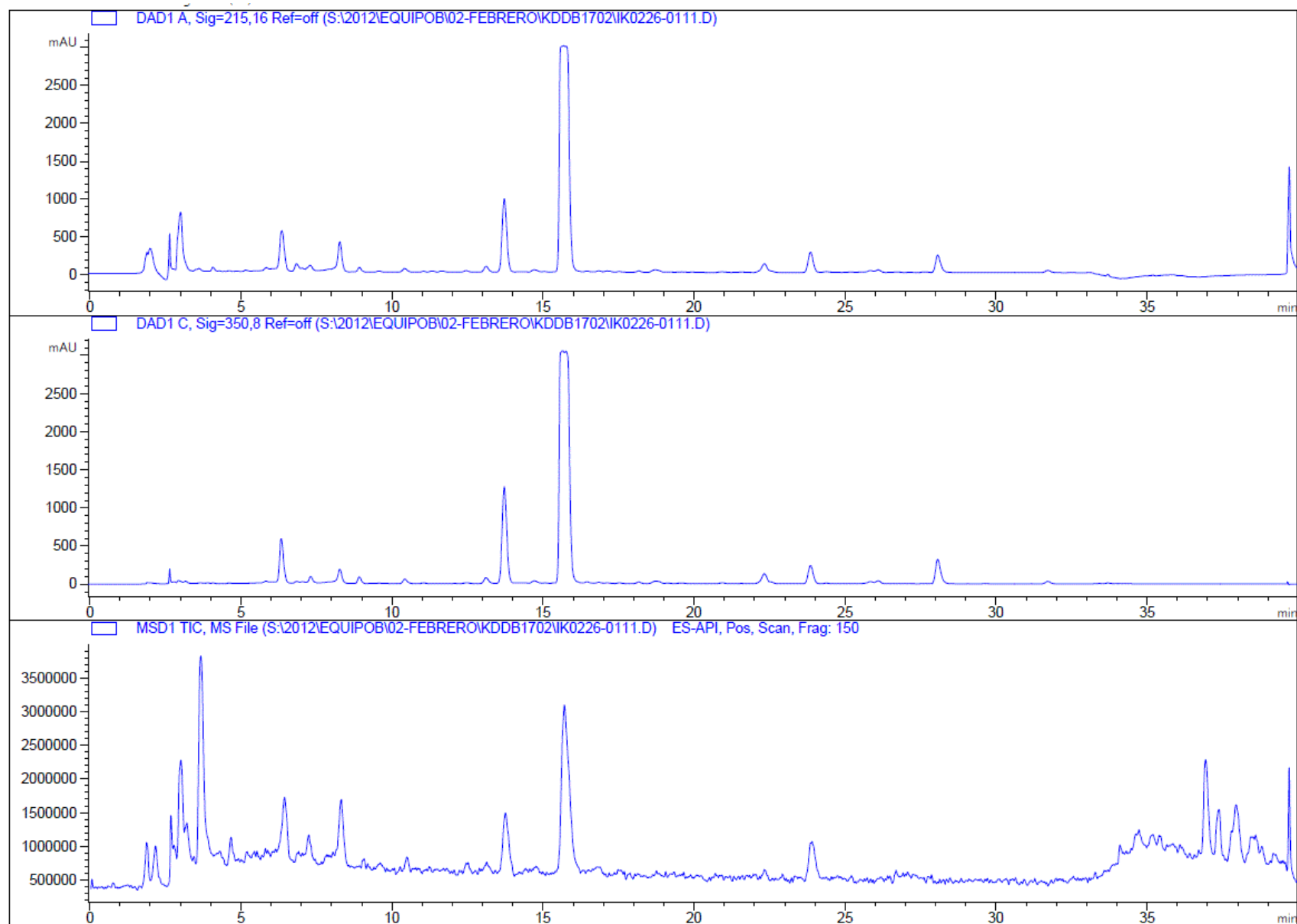


Figura S13. (+)ESIMS of hydrolysis of **1** after ozonolysis

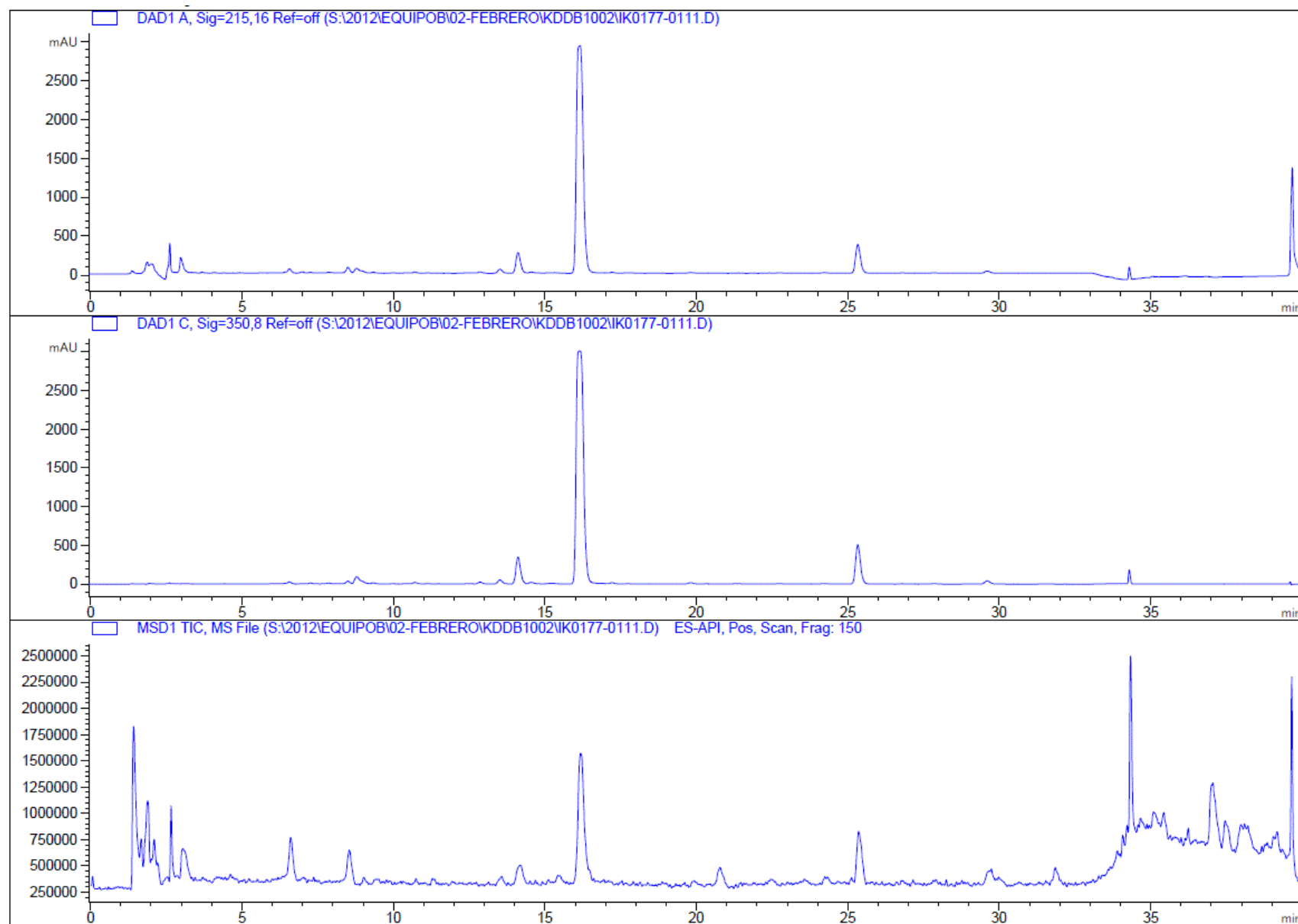


Figure S14. Extracted ion chromatogram of L-FDAA derivatives for NorVal

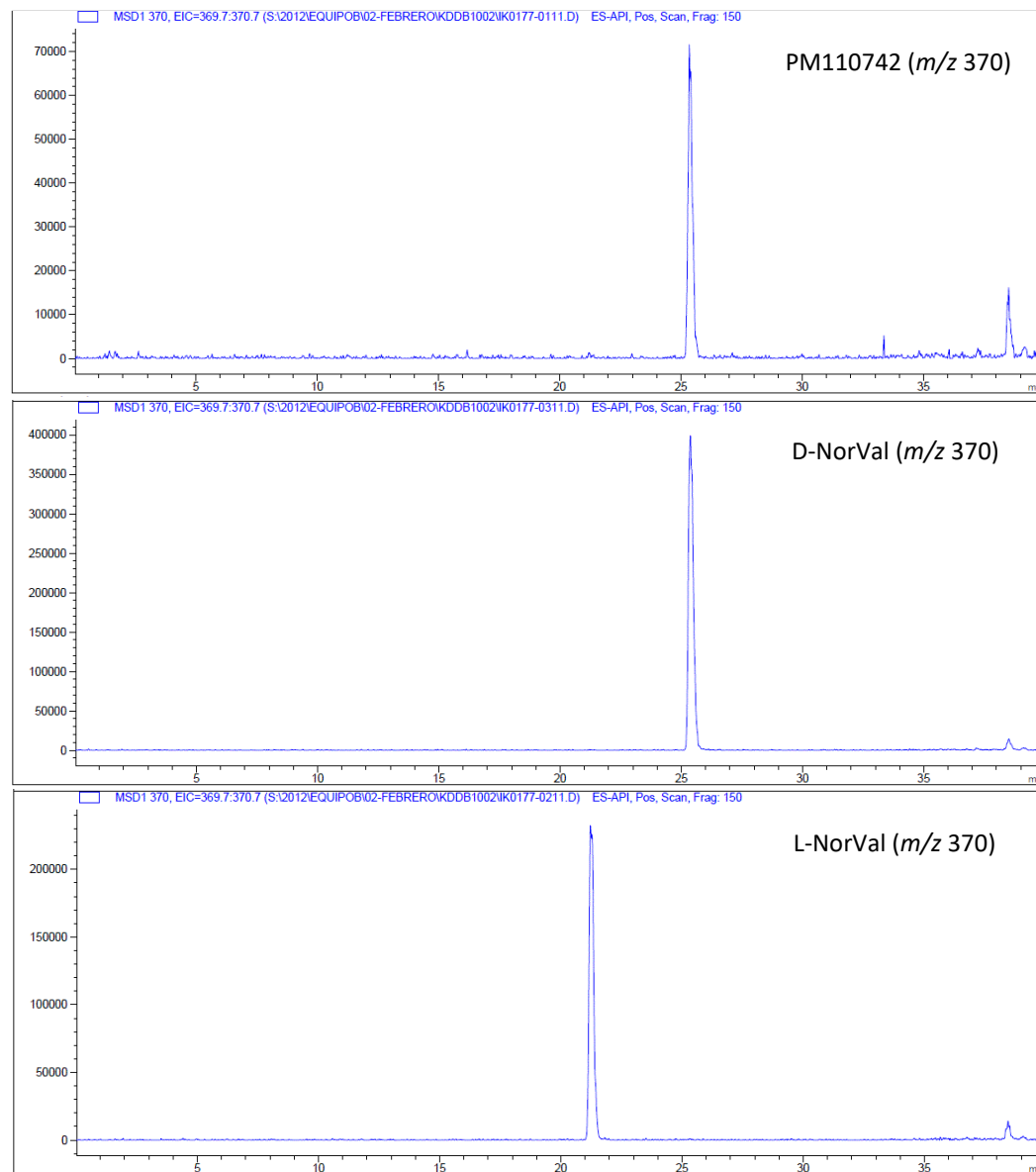


Figure S15. Extracted ion chromatogram of L-FDAA derivatives for MeCys

