

Article

Characterization of Three Novel 4-Methylaminorex Derivatives Applied as Designer Drugs

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1. Supplementary materials

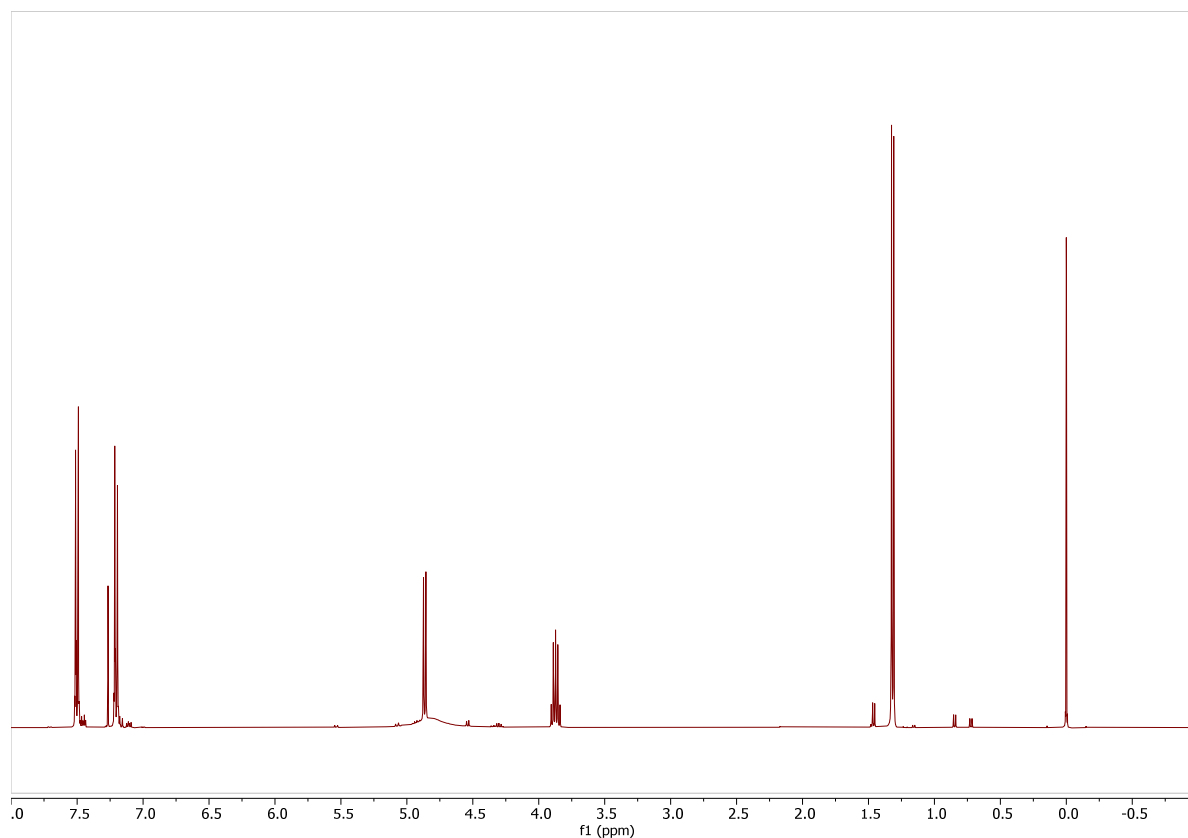


Figure S1. Proton NMR spectrum (400 MHz, CDCl_3) 4B-MAR.

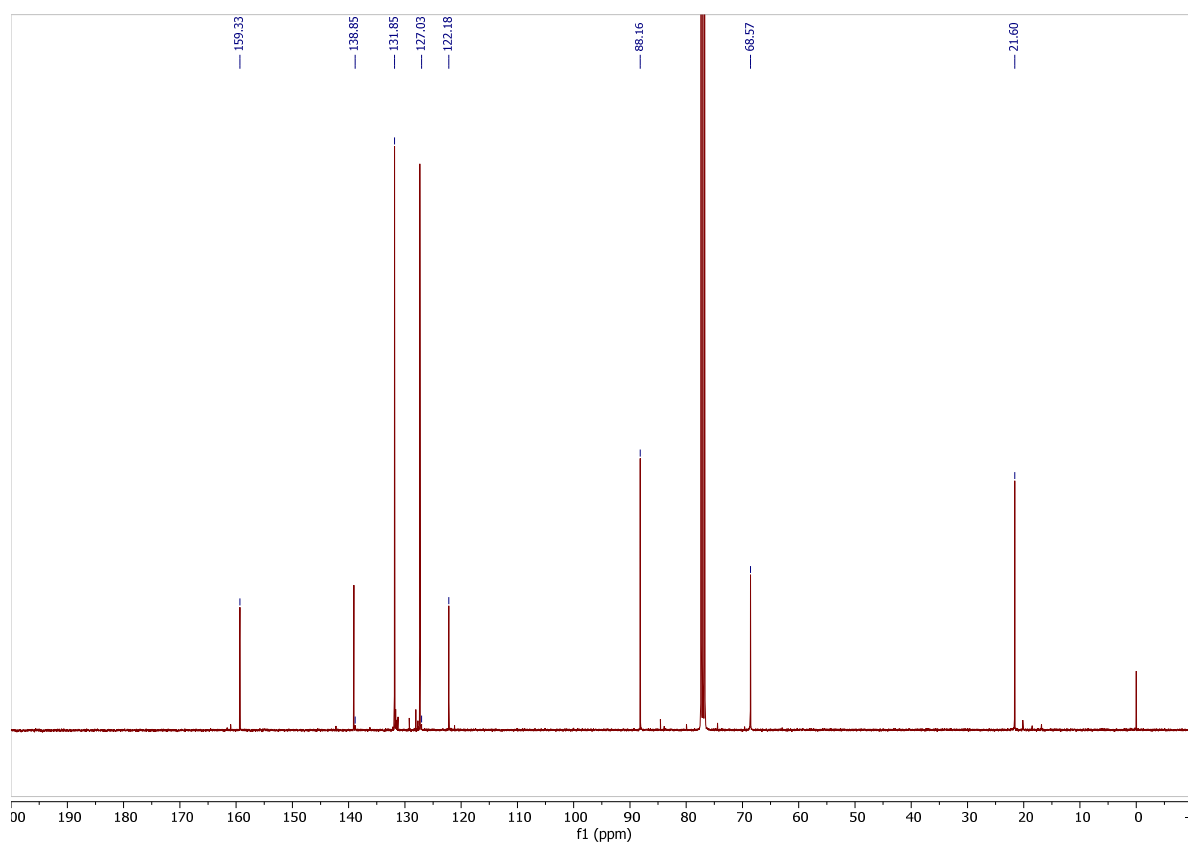


Figure S2. Carbon NMR spectrum (100 MHz, CDCl_3) 4B-MAR.

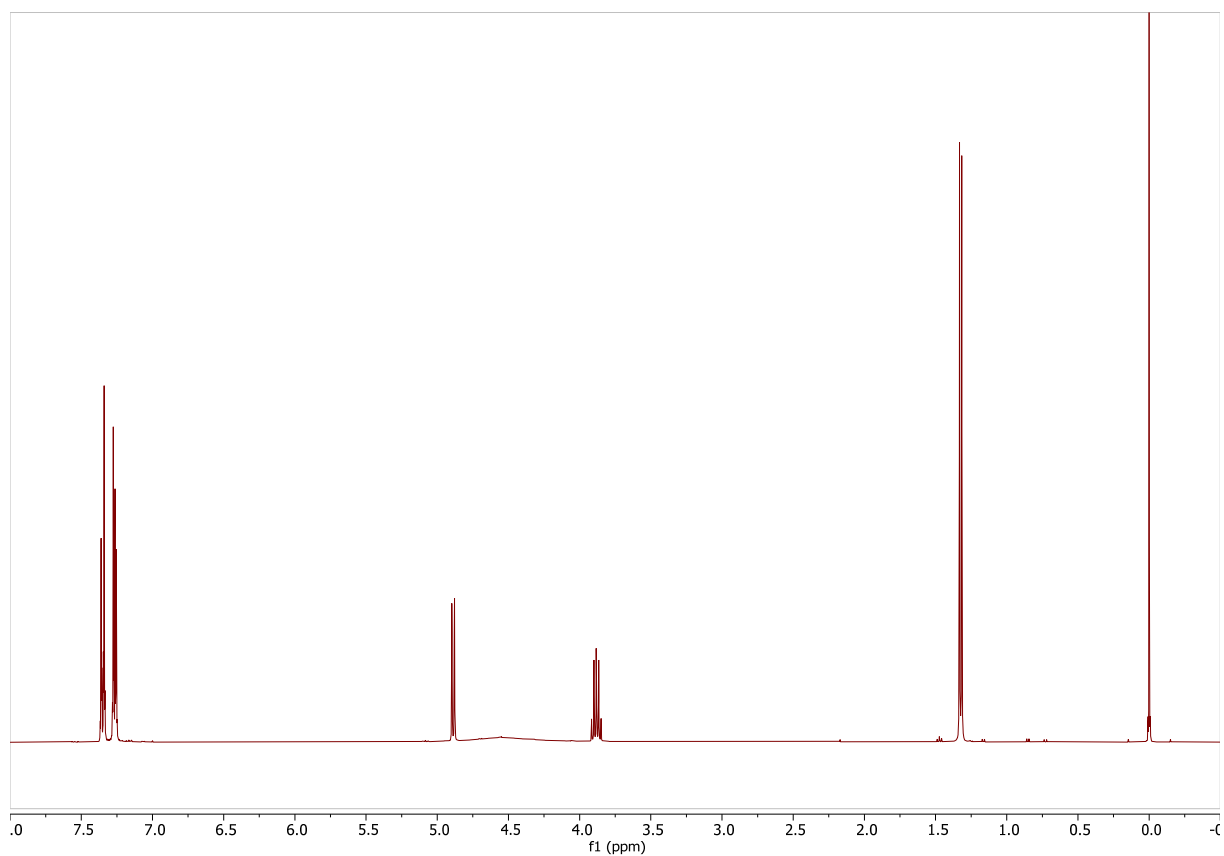


Figure S3. Proton NMR spectrum (400 MHz, CDCl_3) 4C-MAR.

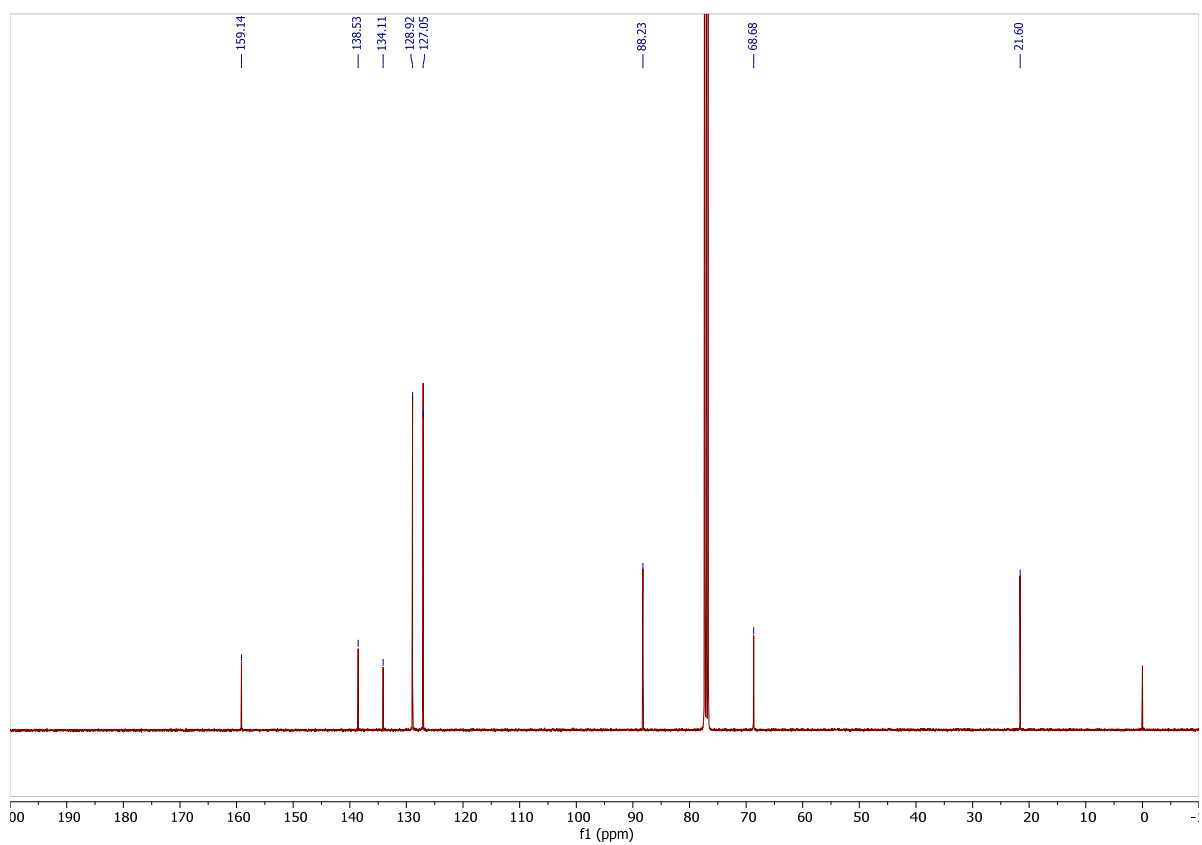


Figure S4. Carbon NMR spectrum (100 MHz, CDCl_3) 4C-MAR.

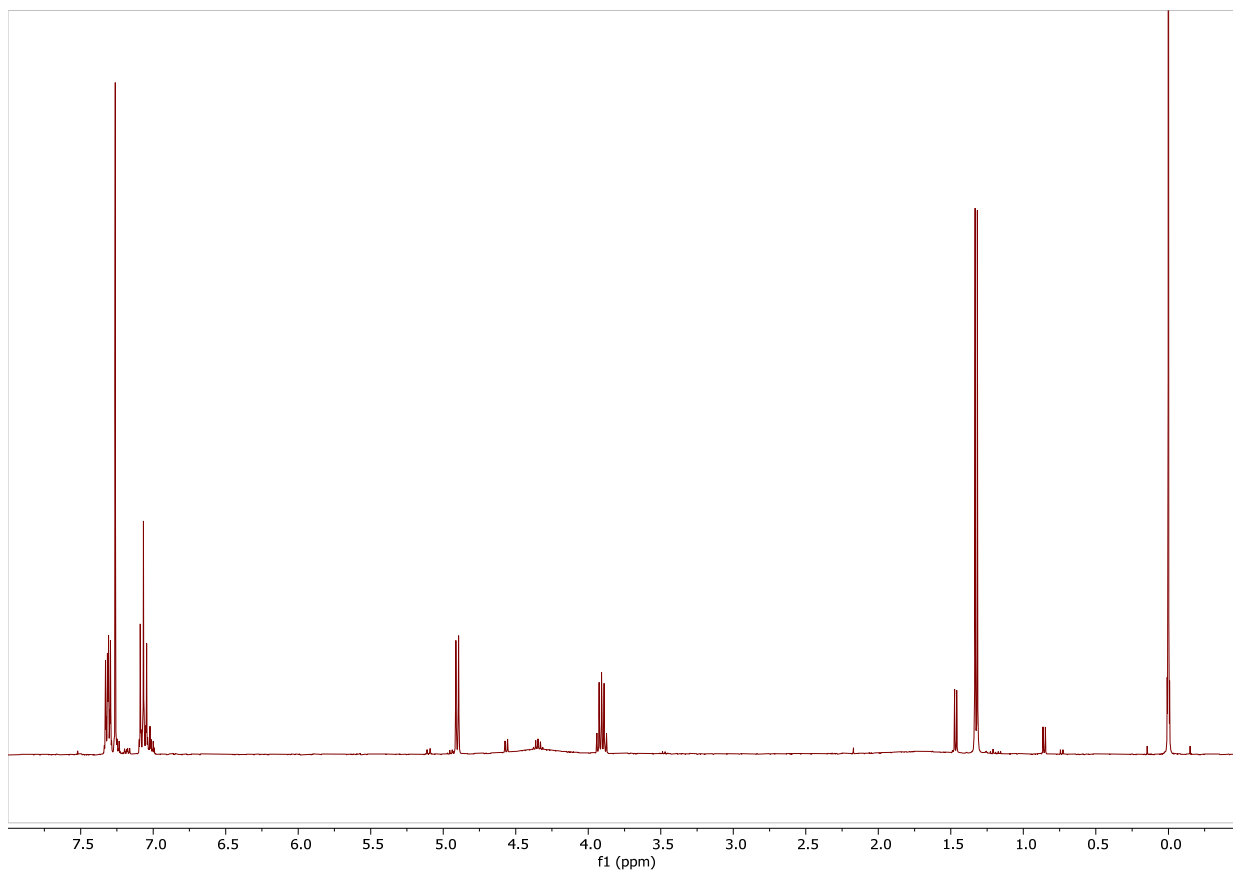


Figure S5. Proton NMR spectrum (400 MHz, CDCl_3) 4F-MAR.

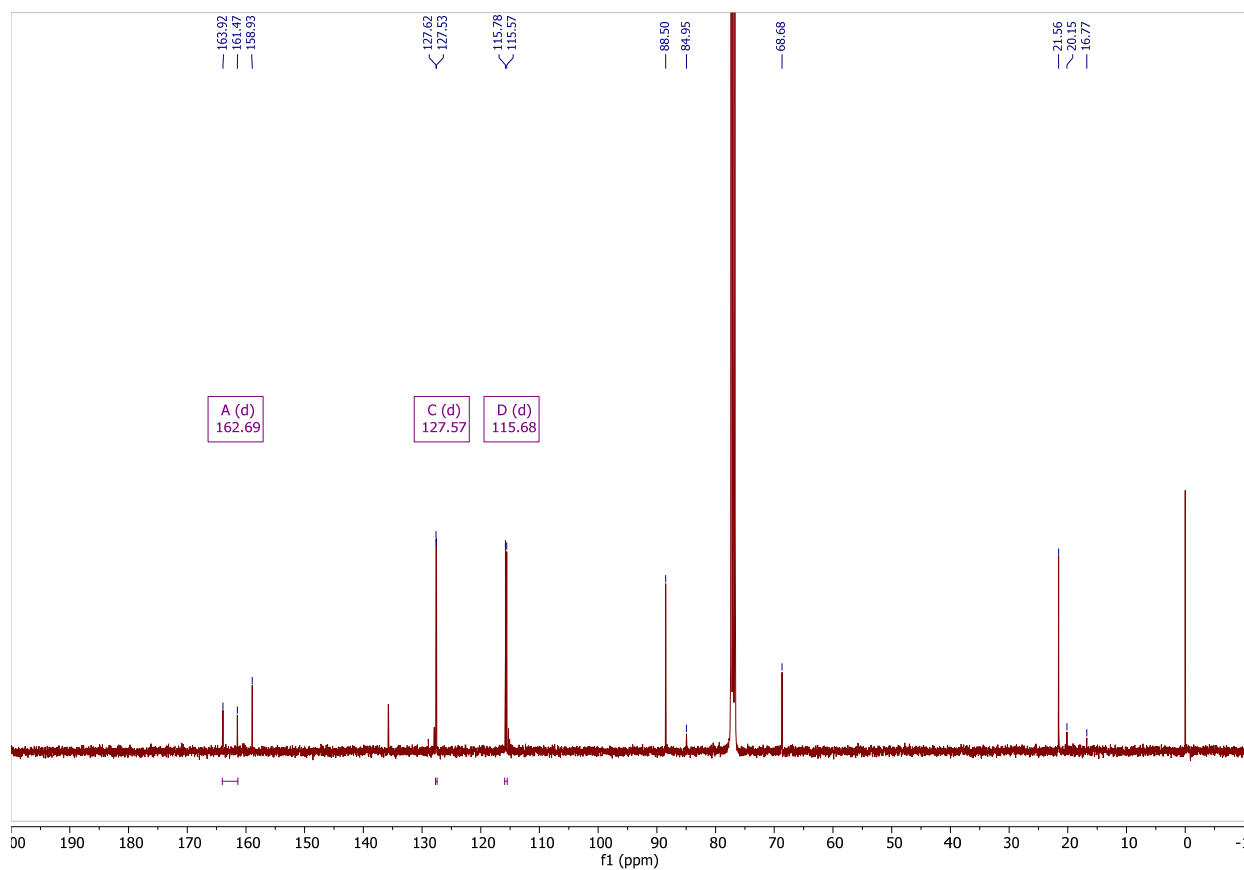


Figure S6. Carbon NMR spectrum (100 MHz, CDCl_3) 4F-MAR. The centers of the doublets caused by heteronuclear ^{19}F , ^{13}C - J -couplings are given in the boxes.

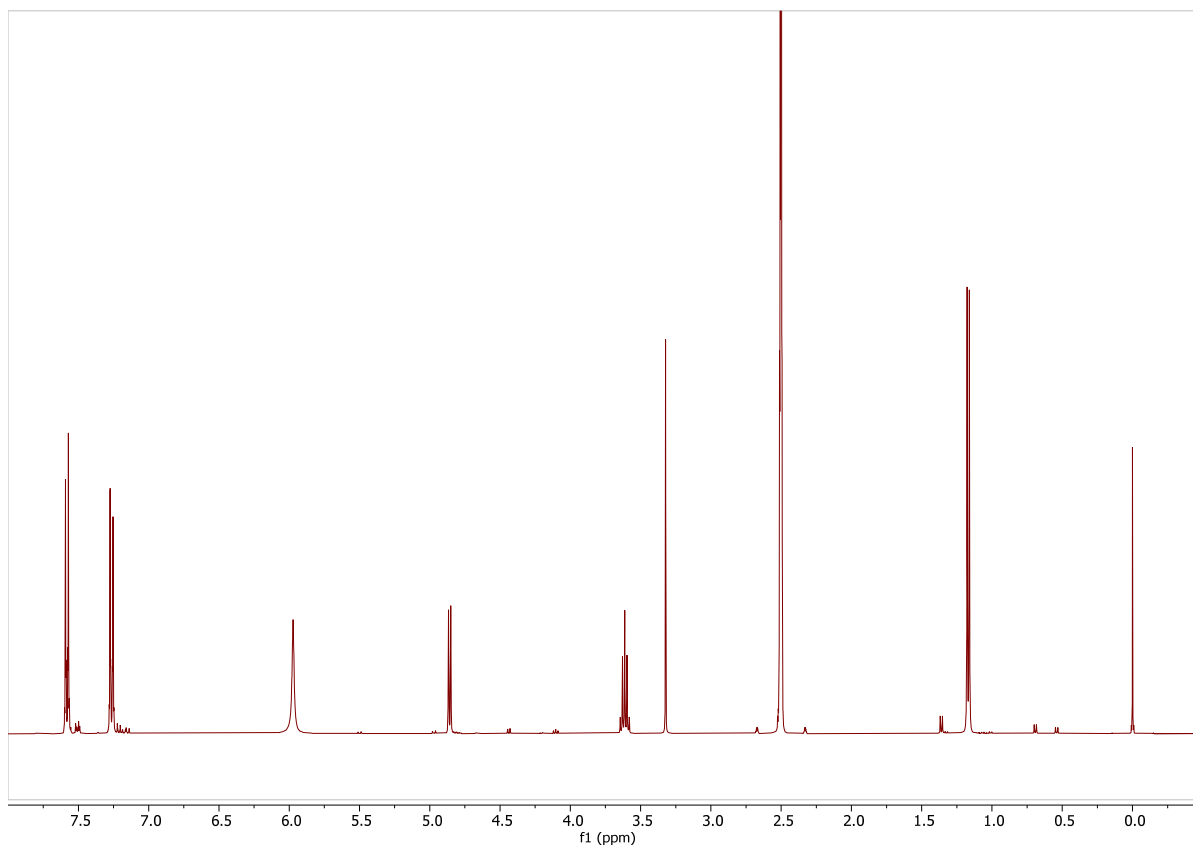


Figure S7. Proton NMR spectrum (400 MHz, DMSO-d₆) 4B-MAR.

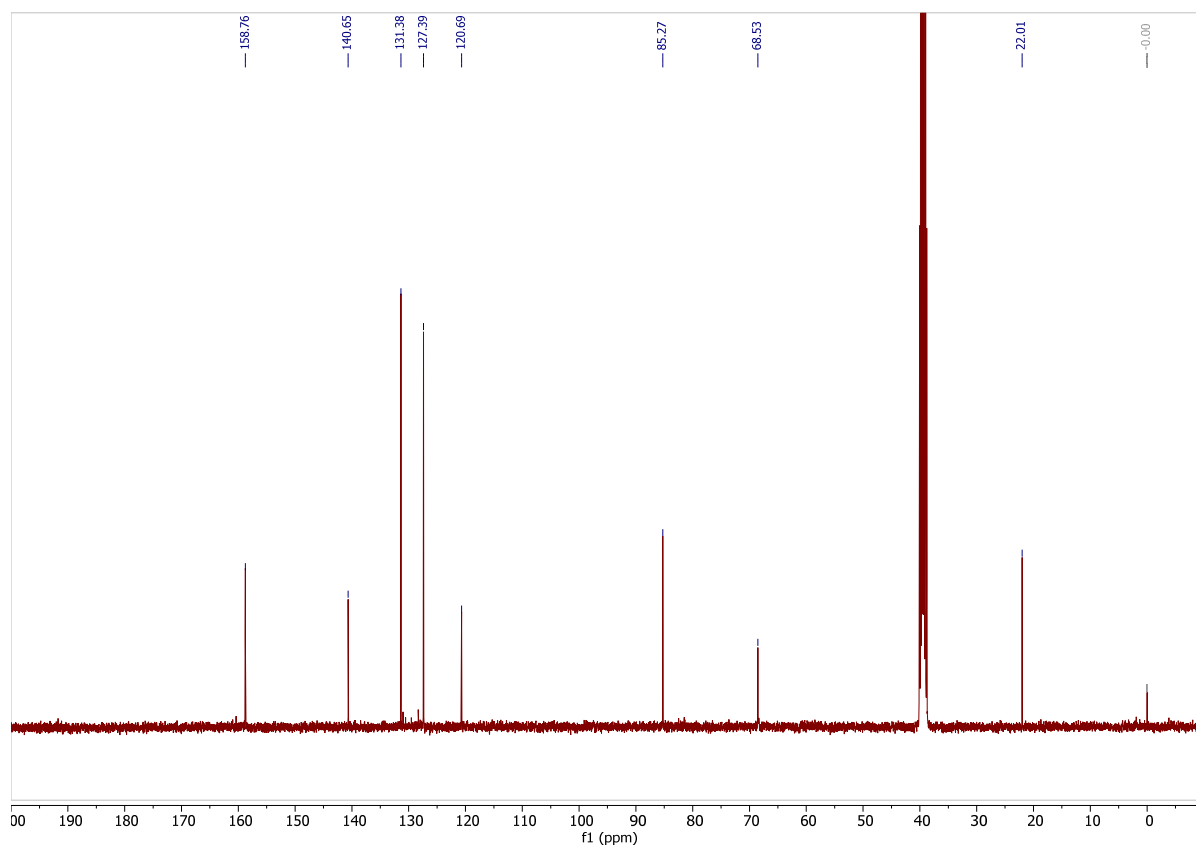


Figure S8. Carbon NMR spectrum (100 MHz, DMSO-d₆) 4B-MAR.

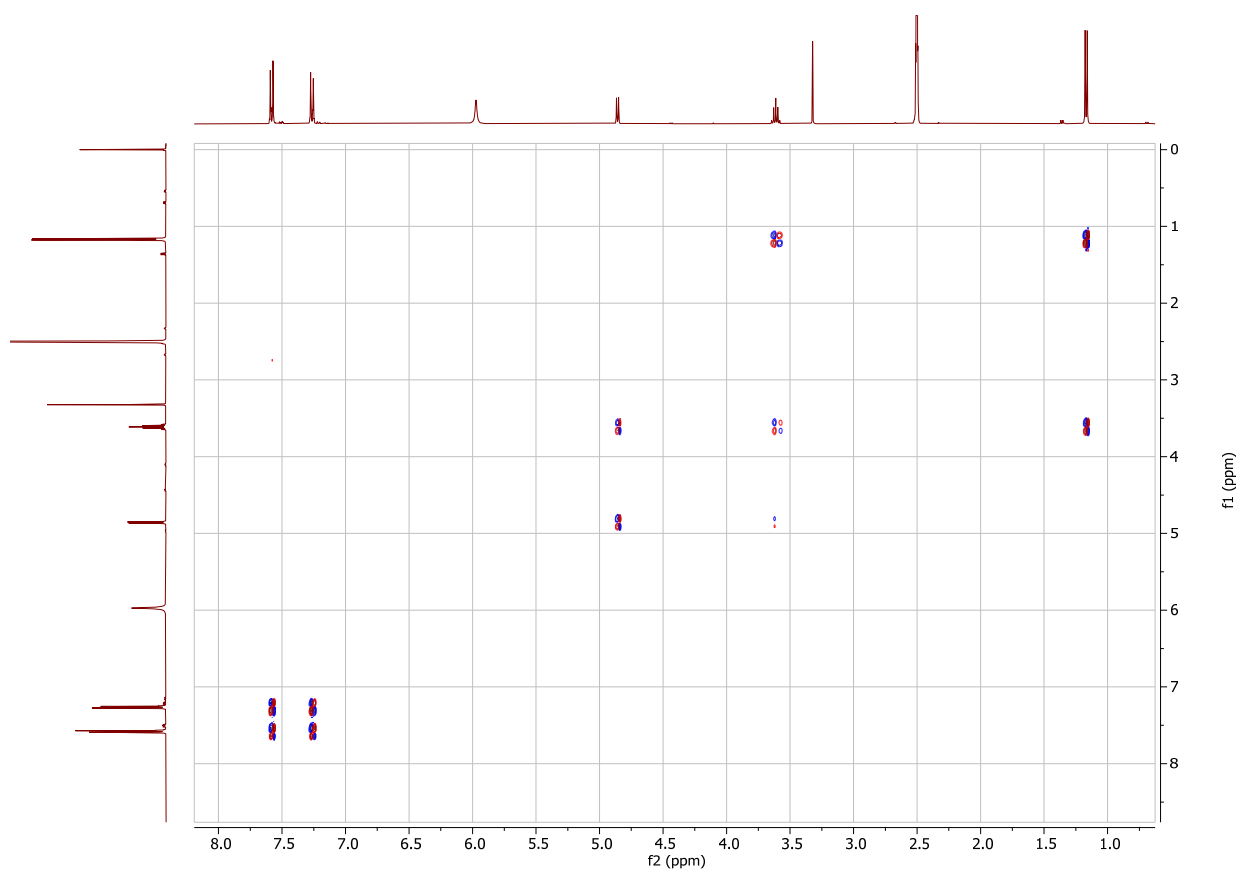


Figure S9. DQF-COSY NMR spectrum (400 MHz, DMSO-d₆) 4B-MAR.

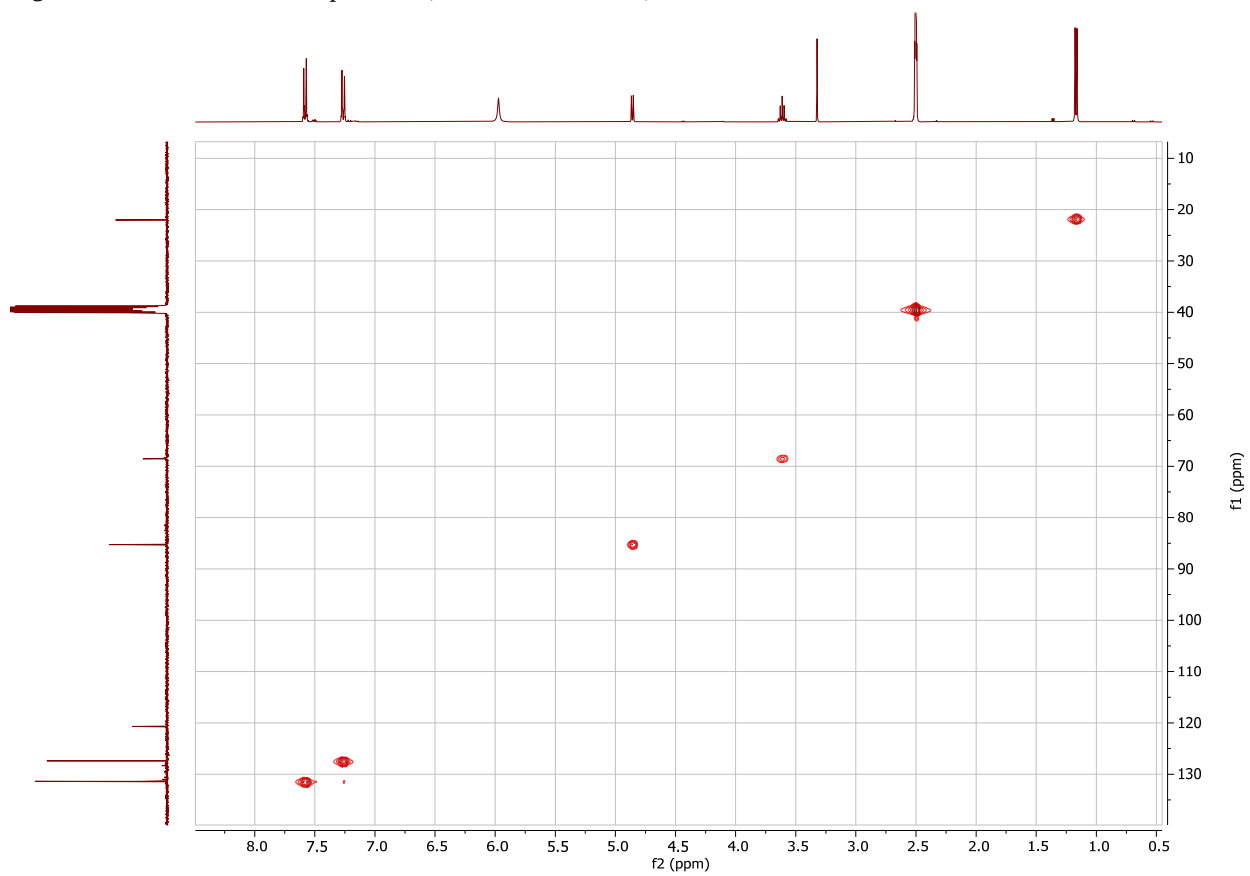


Figure S10. HSQC NMR spectrum (100/400 MHz, DMSO-d₆) 4B-MAR.

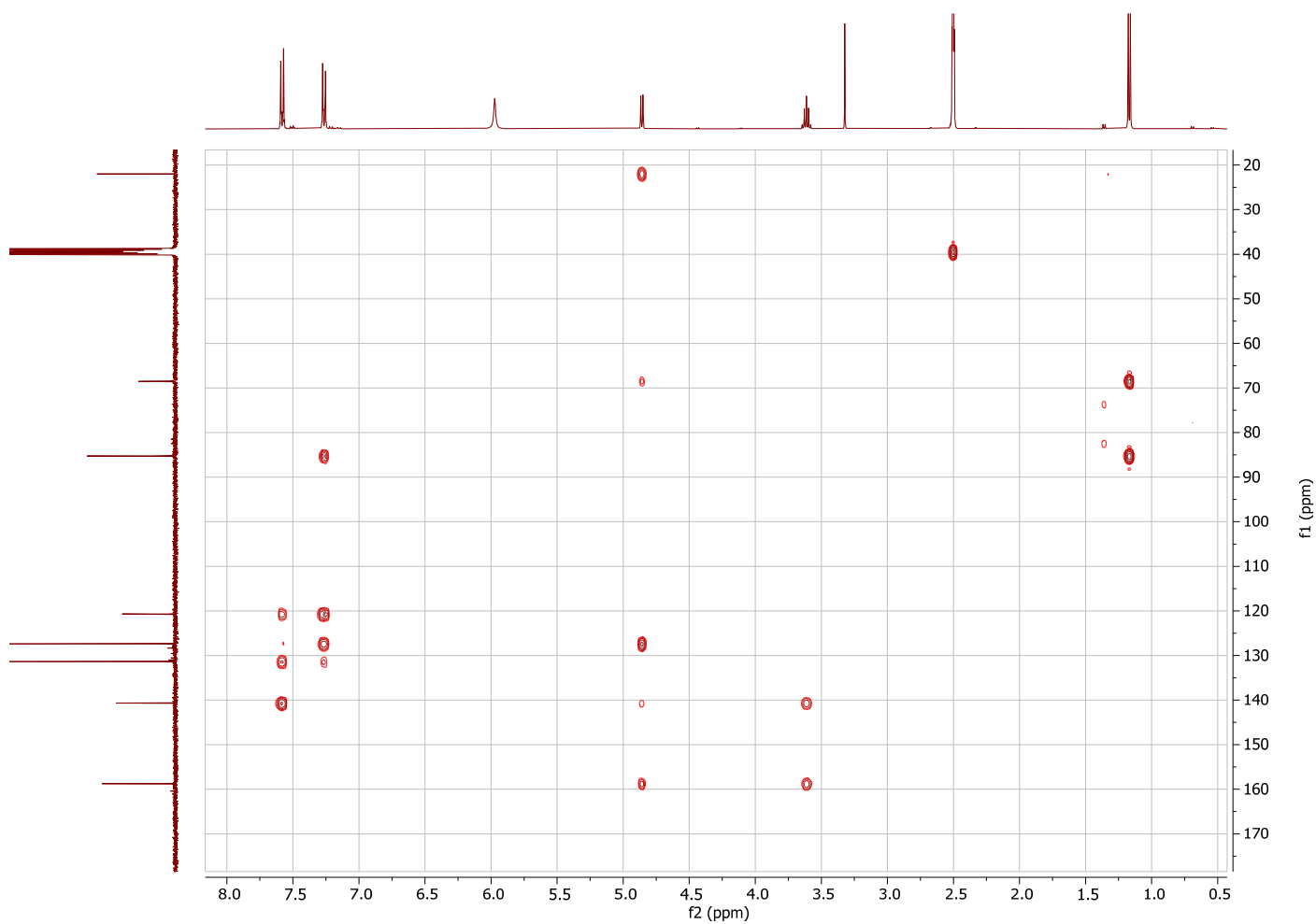


Figure S11. HMBC NMR spectrum (100/400 MHz, DMSO-d₆) 4B-MAR.

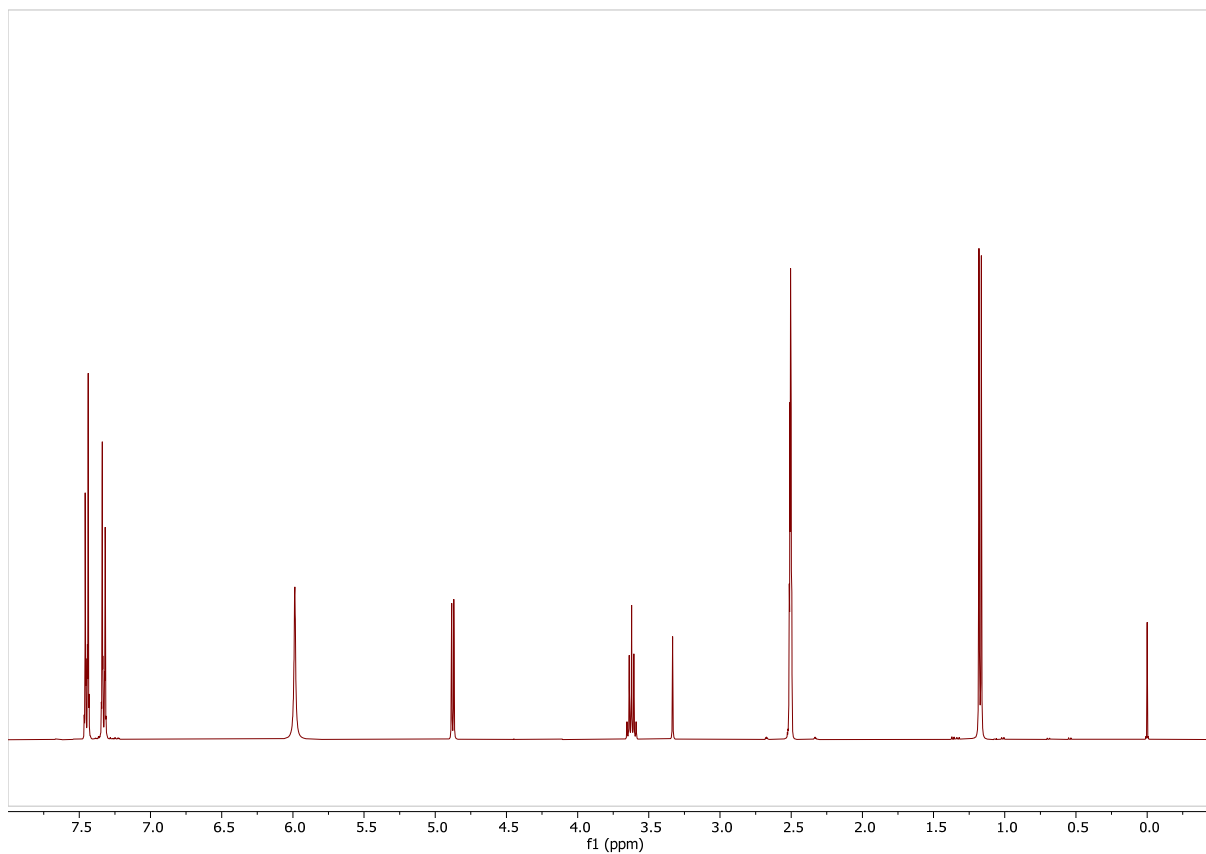


Figure S12. Proton NMR spectrum (400 MHz, DMSO-d₆) 4C-MAR.

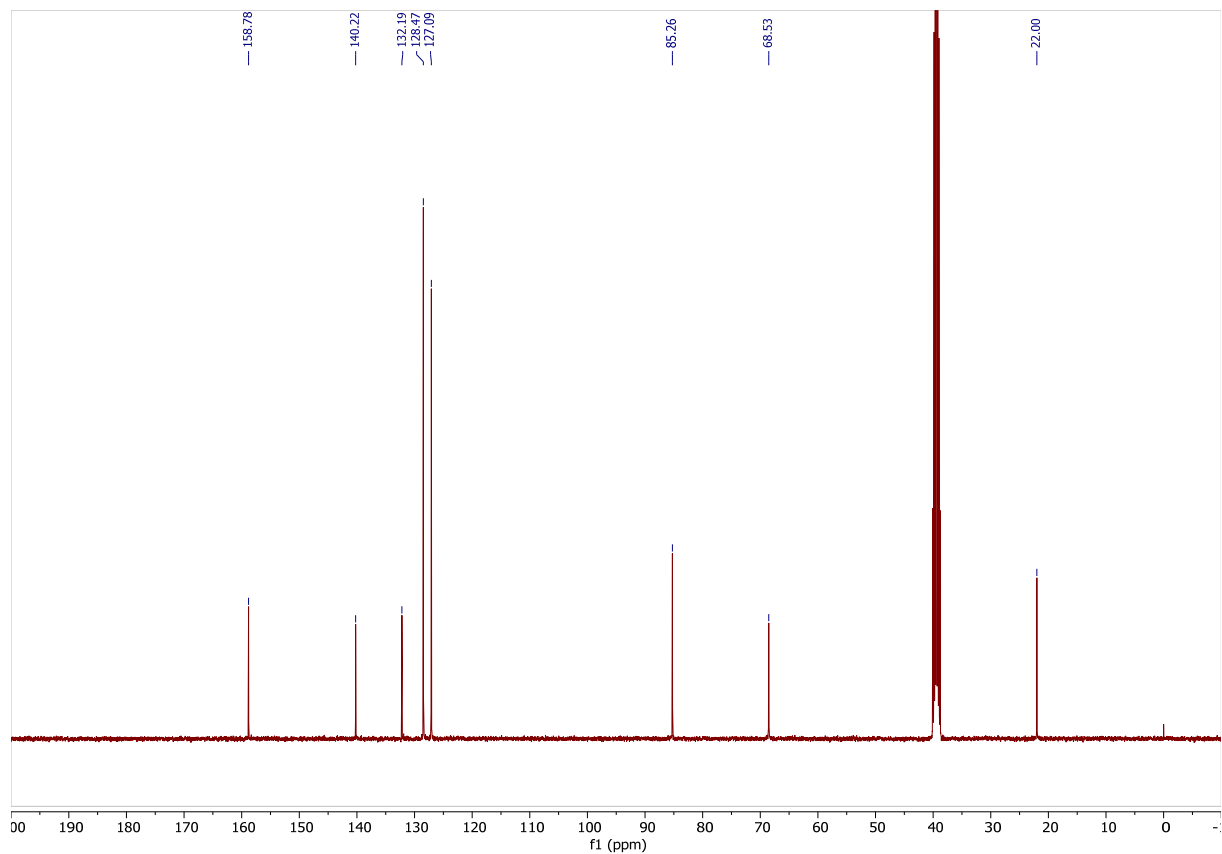


Figure S13. Carbon NMR spectrum (100 MHz, DMSO-d₆) 4C-MAR.

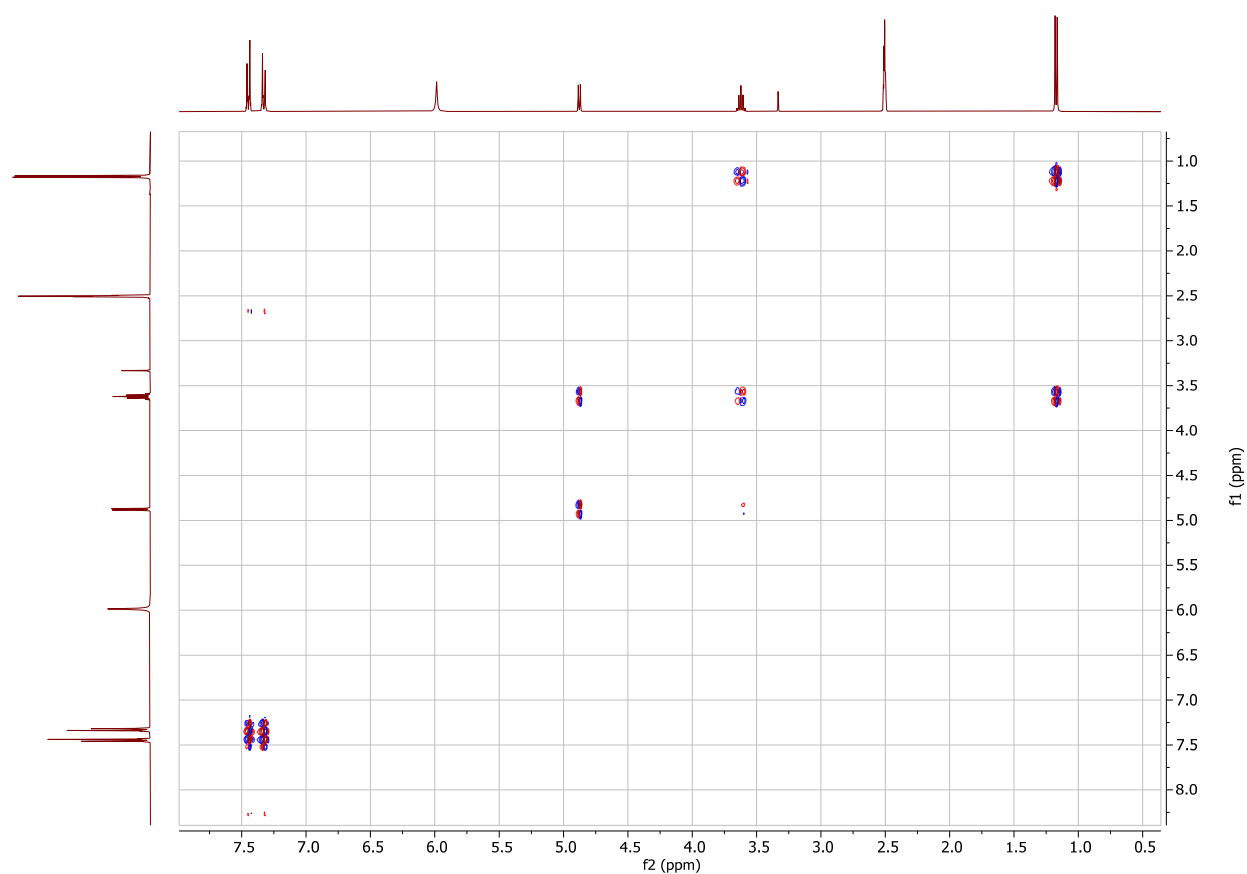


Figure S14. DQF-COSY NMR spectrum (400 MHz, DMSO-d₆) 4C-MAR.

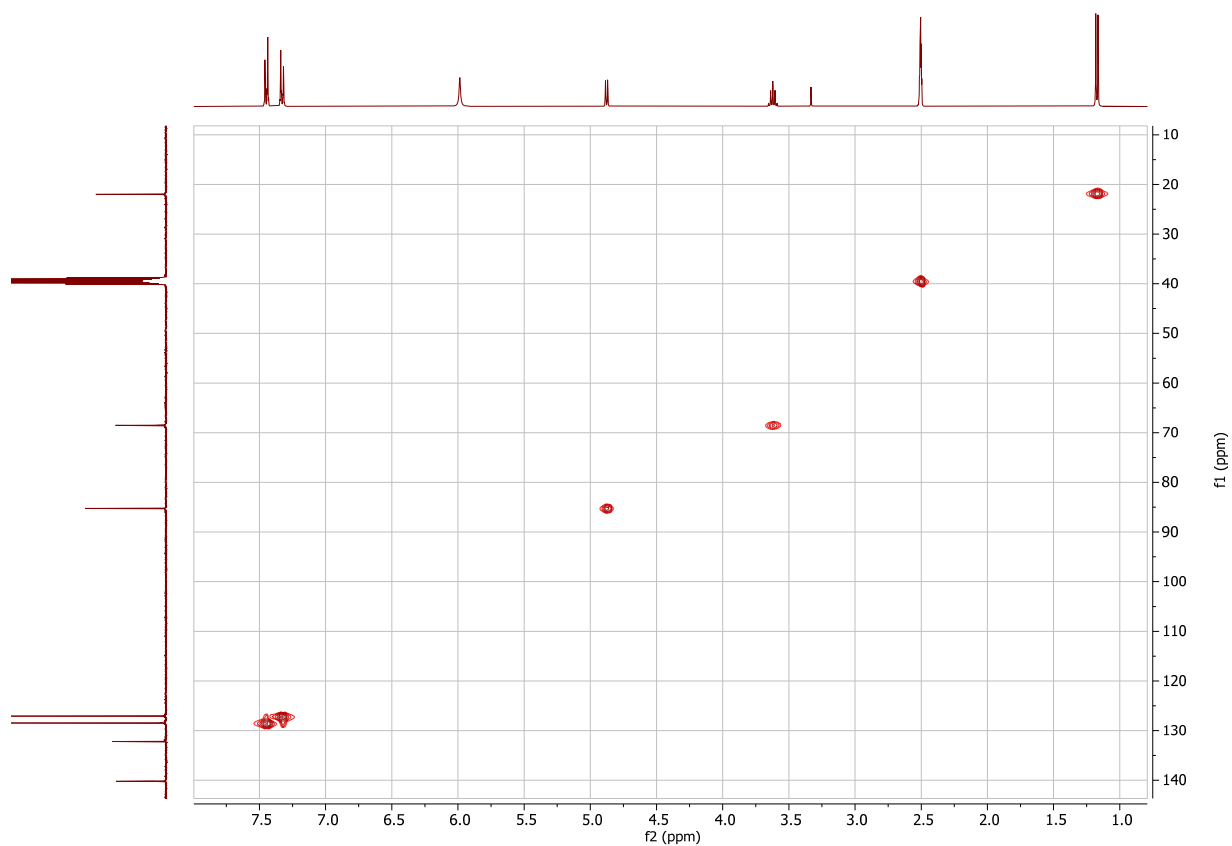


Figure S15. HSQC NMR spectrum (100/400 MHz, DMSO-d₆) 4C-MAR.

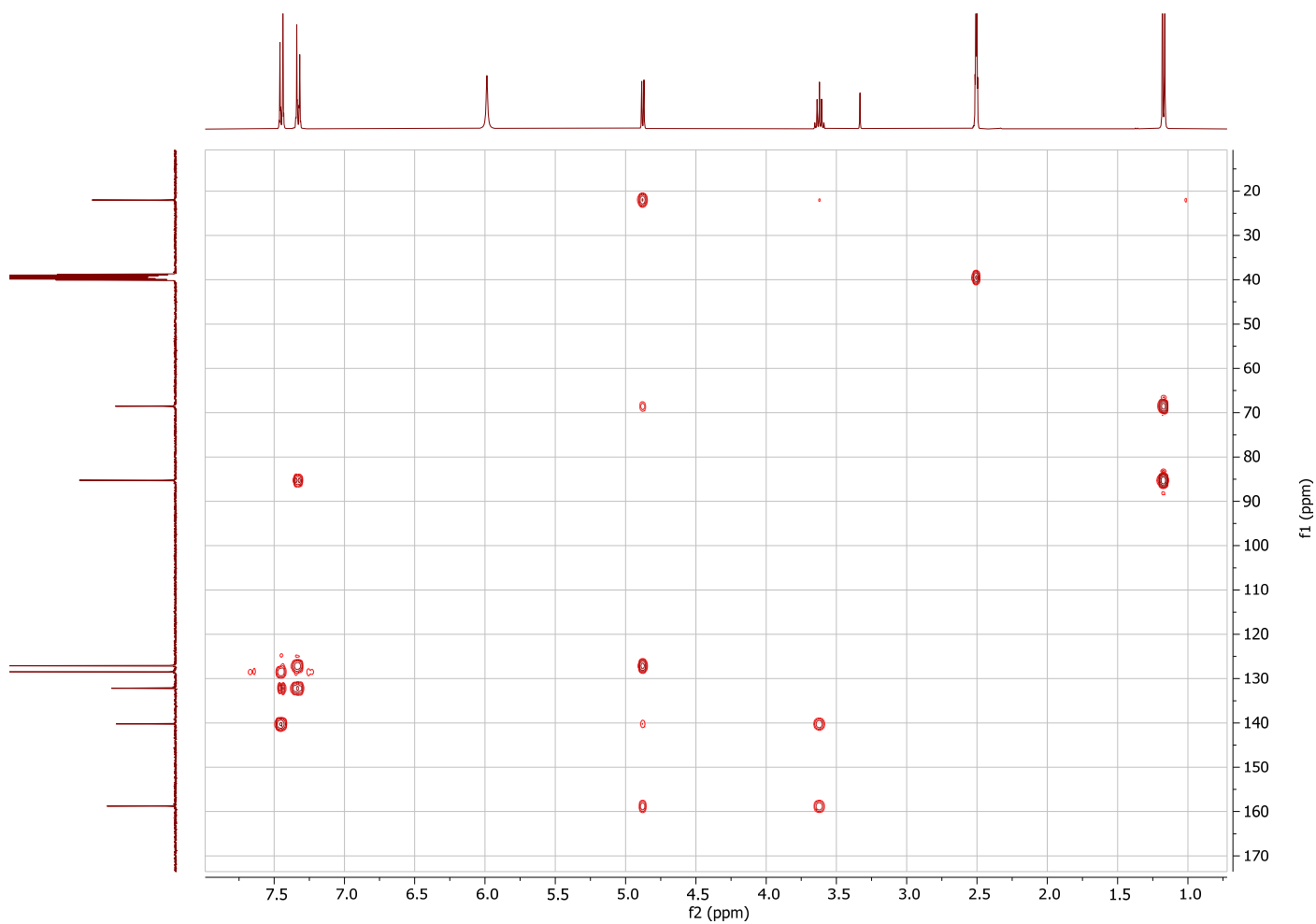


Figure S16. HMBC NMR spectrum (100/400 MHz, DMSO- d_6) 4C-MAR.

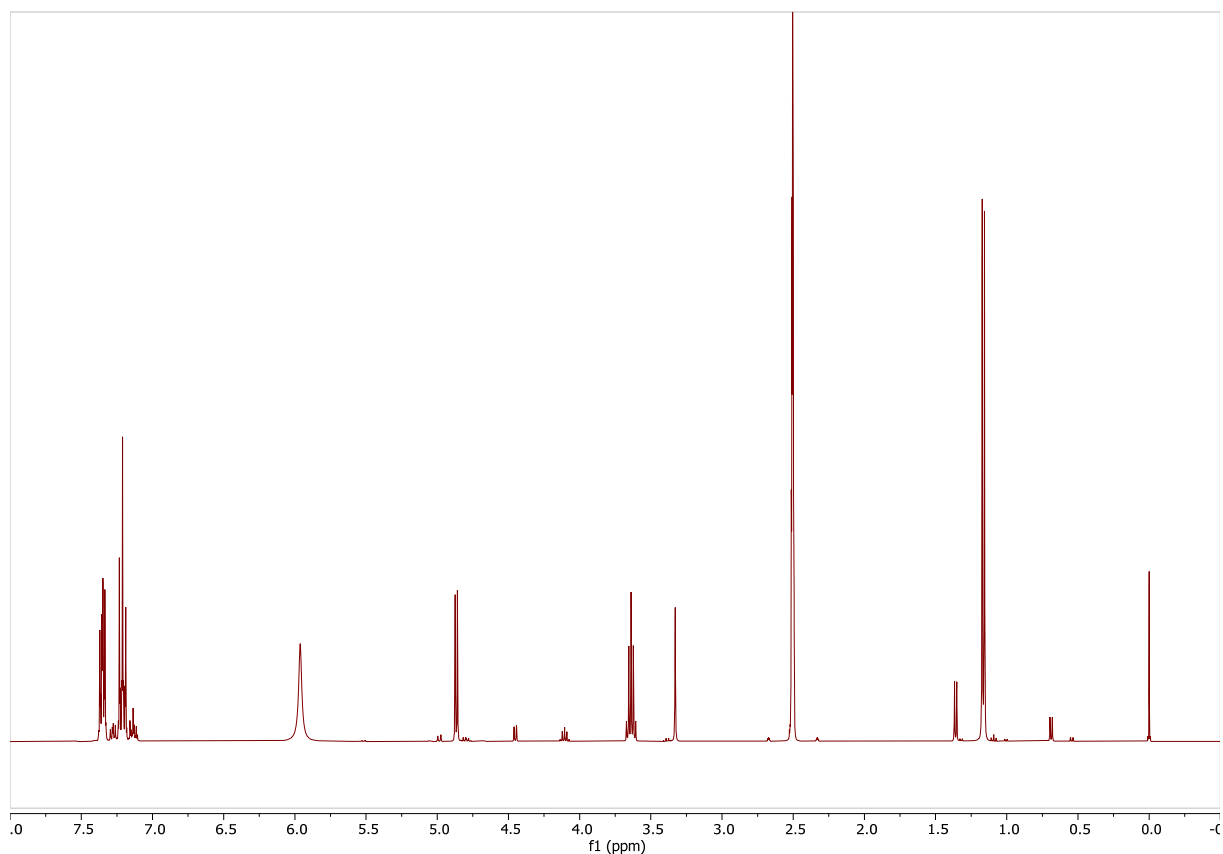


Figure S17. Proton NMR spectrum (400 MHz, DMSO- d_6) 4F-MAR.

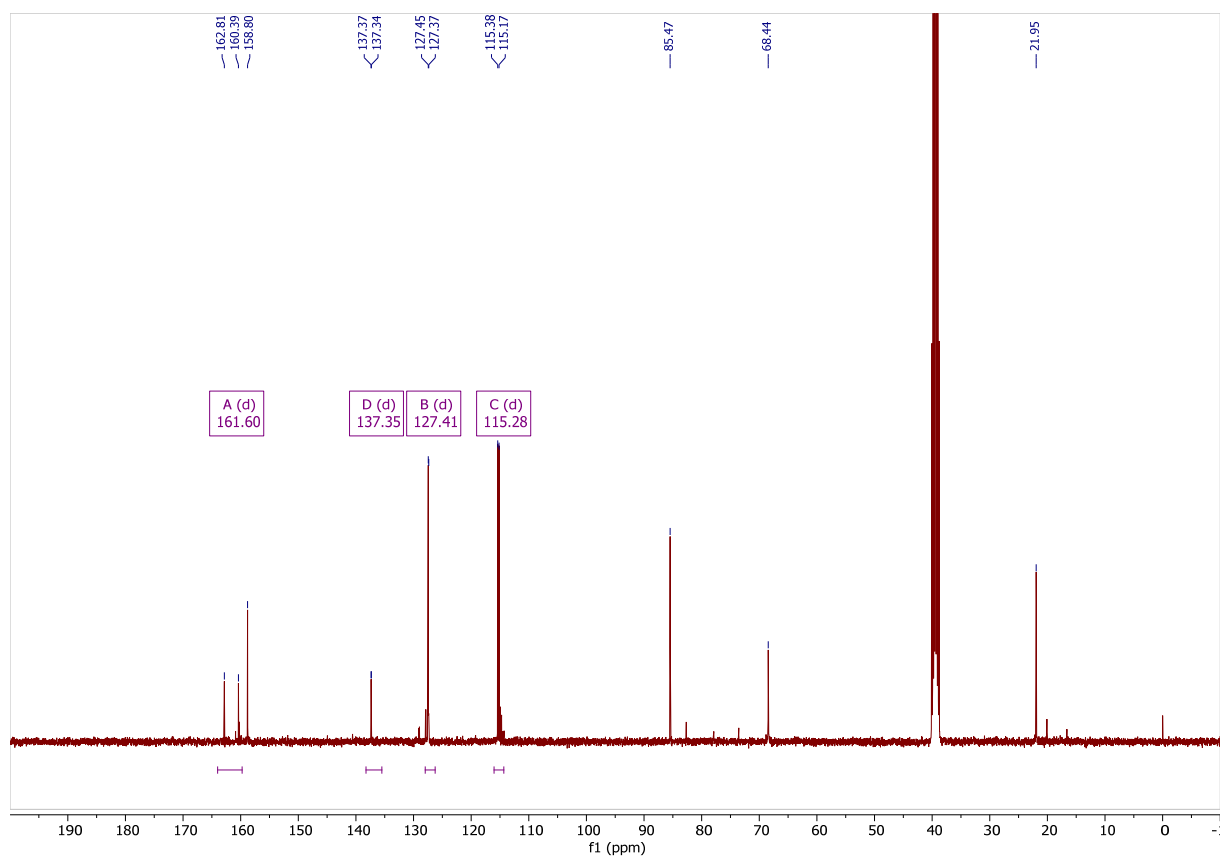


Figure S18. Carbon NMR spectrum (100 MHz, DMSO- d_6) 4F-MAR. The centers of the doublets caused by heteronuclear ^{19}F , ^{13}C - J -couplings are given in the boxes.

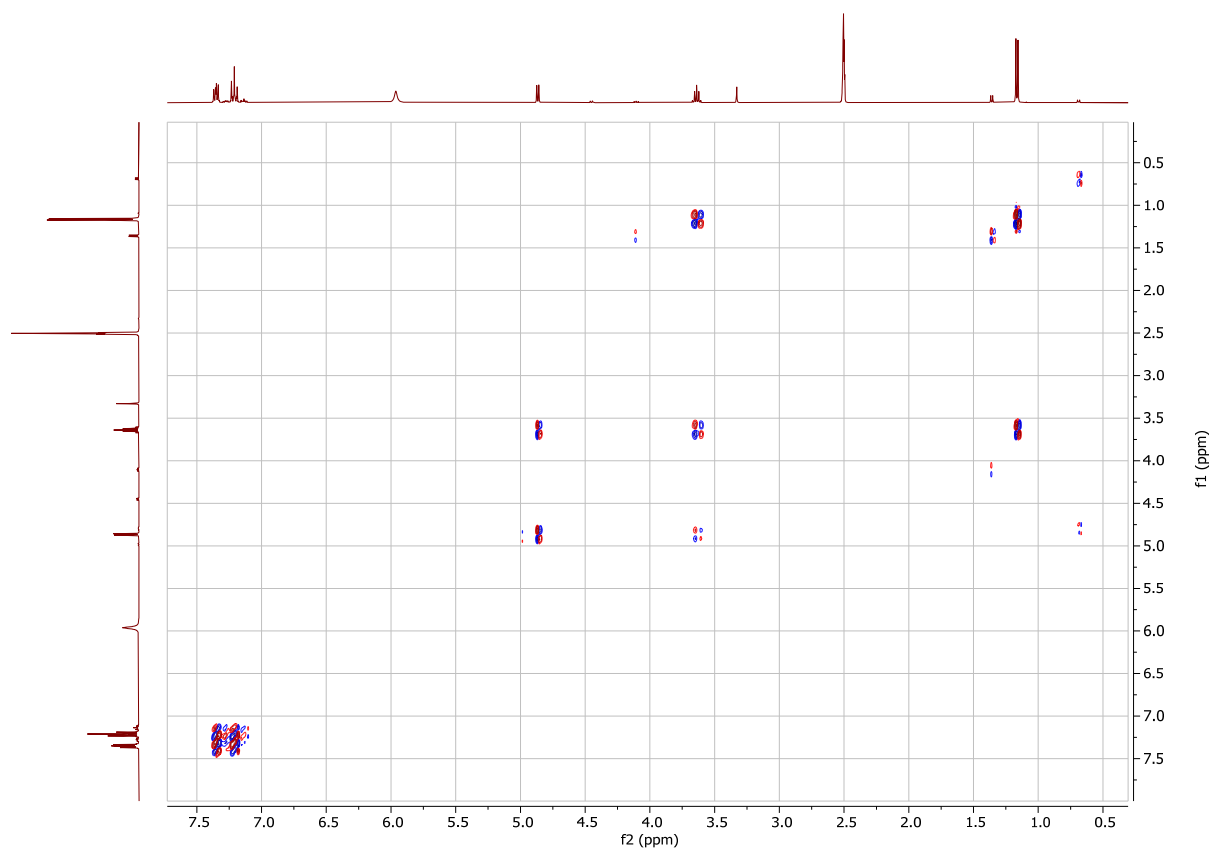


Figure S19. DQF-COSY NMR spectrum (400 MHz, DMSO-d₆) 4F-MAR.

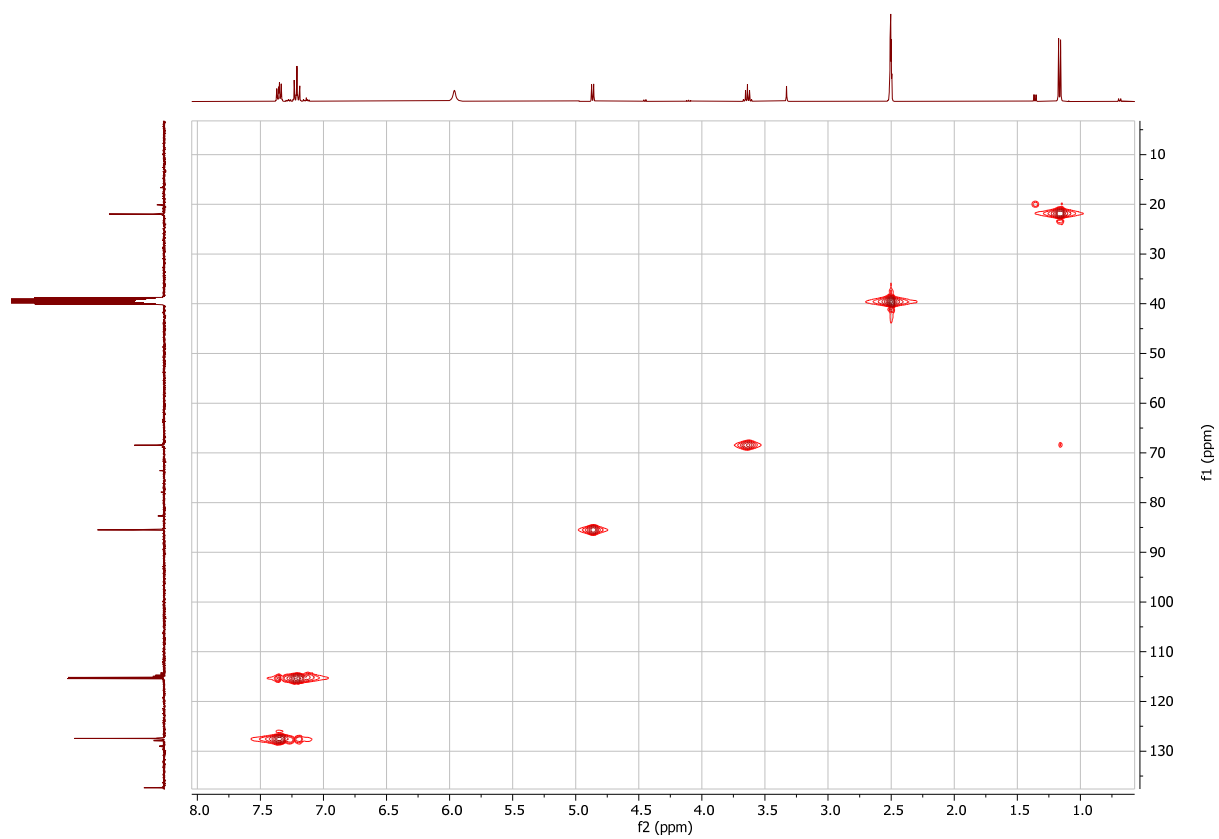


Figure S20. HSQC NMR spectrum (100/400 MHz, DMSO-d₆) 4F-MAR.

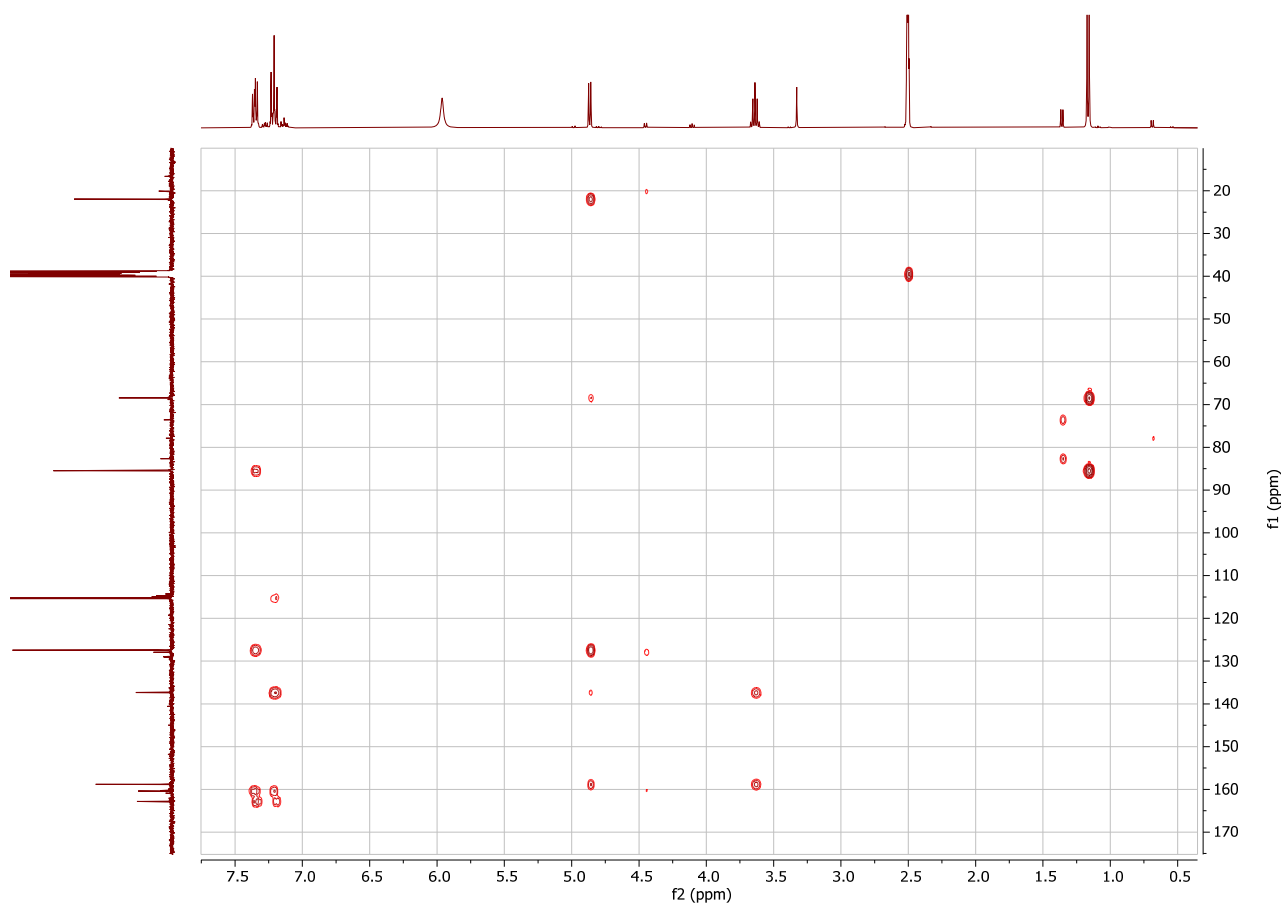


Figure S21. HMBC NMR spectrum (100/400 MHz, DMSO-d₆) 4F-MAR.

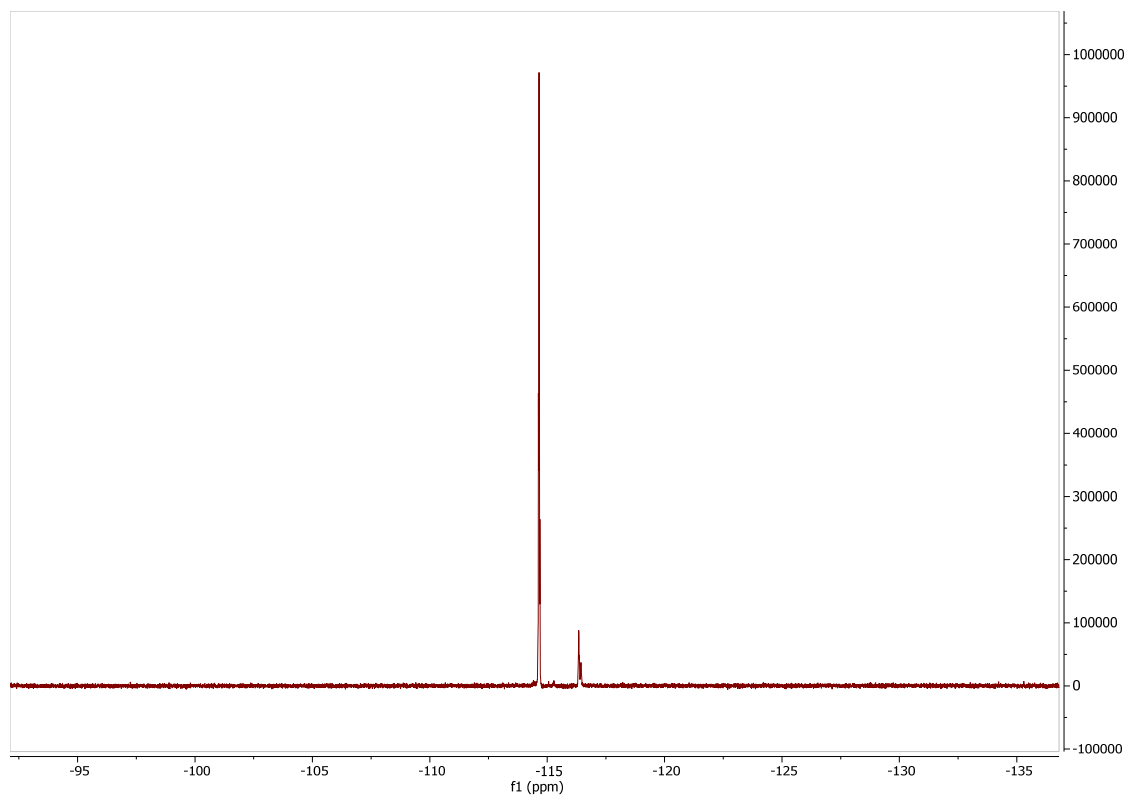


Figure S22. ¹⁹F NMR spectrum (377 MHz, DMSO-d₆) 4F-MAR

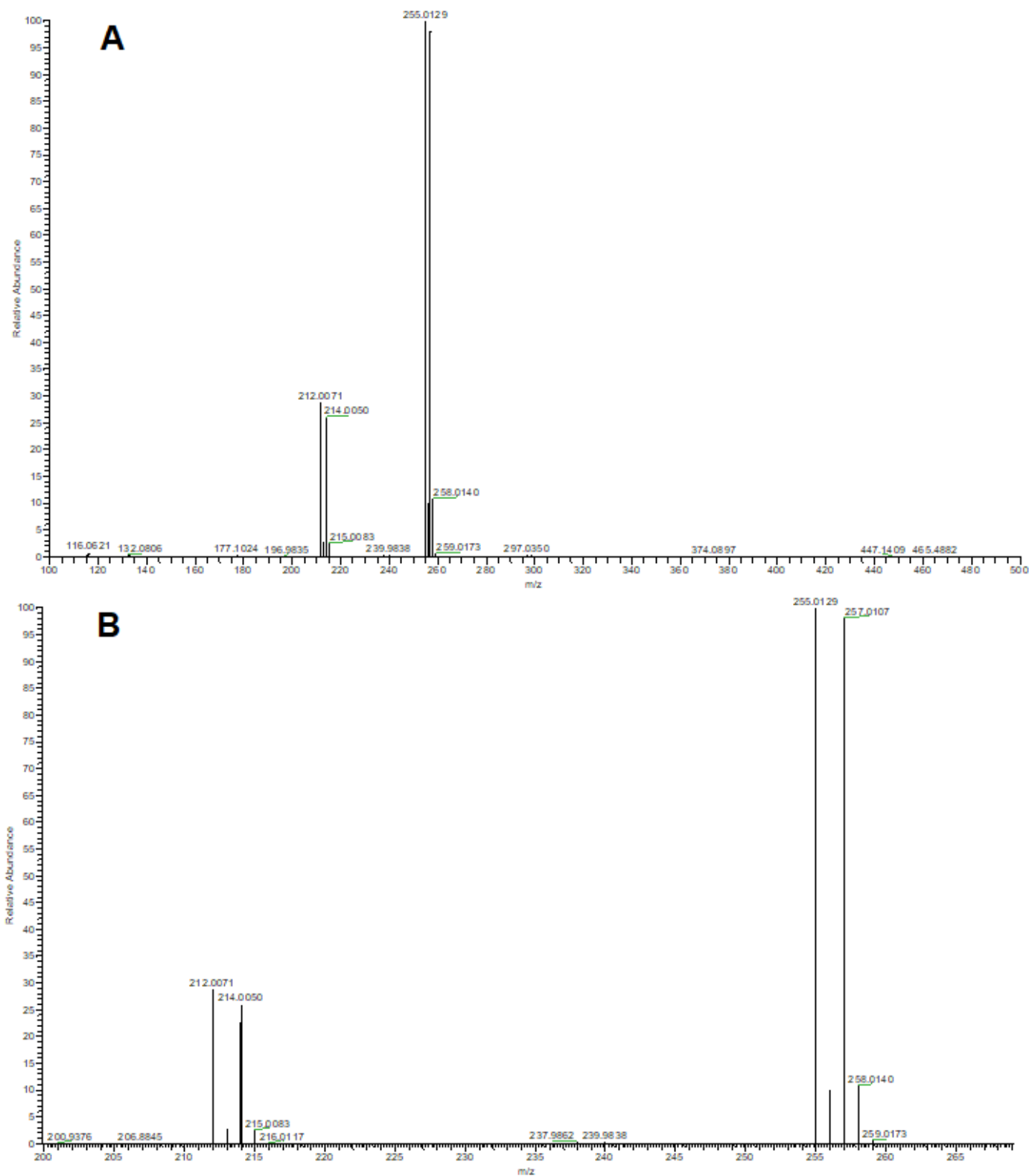


Figure S23. HESI positive mode full MS spectrum of 4B-MAR (A: full view, m/z 100-500, B: detailed view, m/z 200-270)

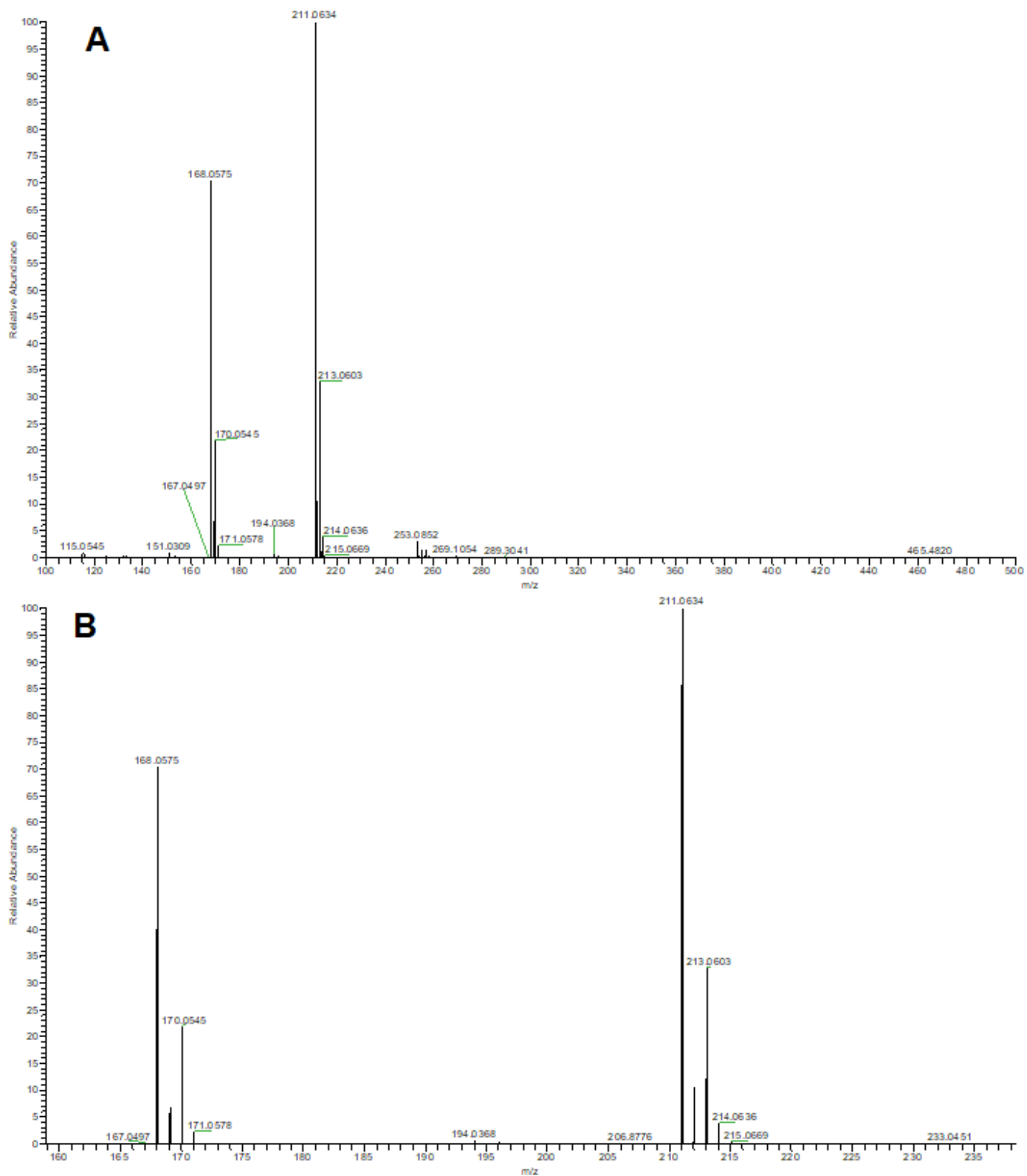


Figure S24. HESI positive mode full MS spectrum of 4C-MAR (A: full view, m/z 100-500, B: detailed view, m/z 160-240)

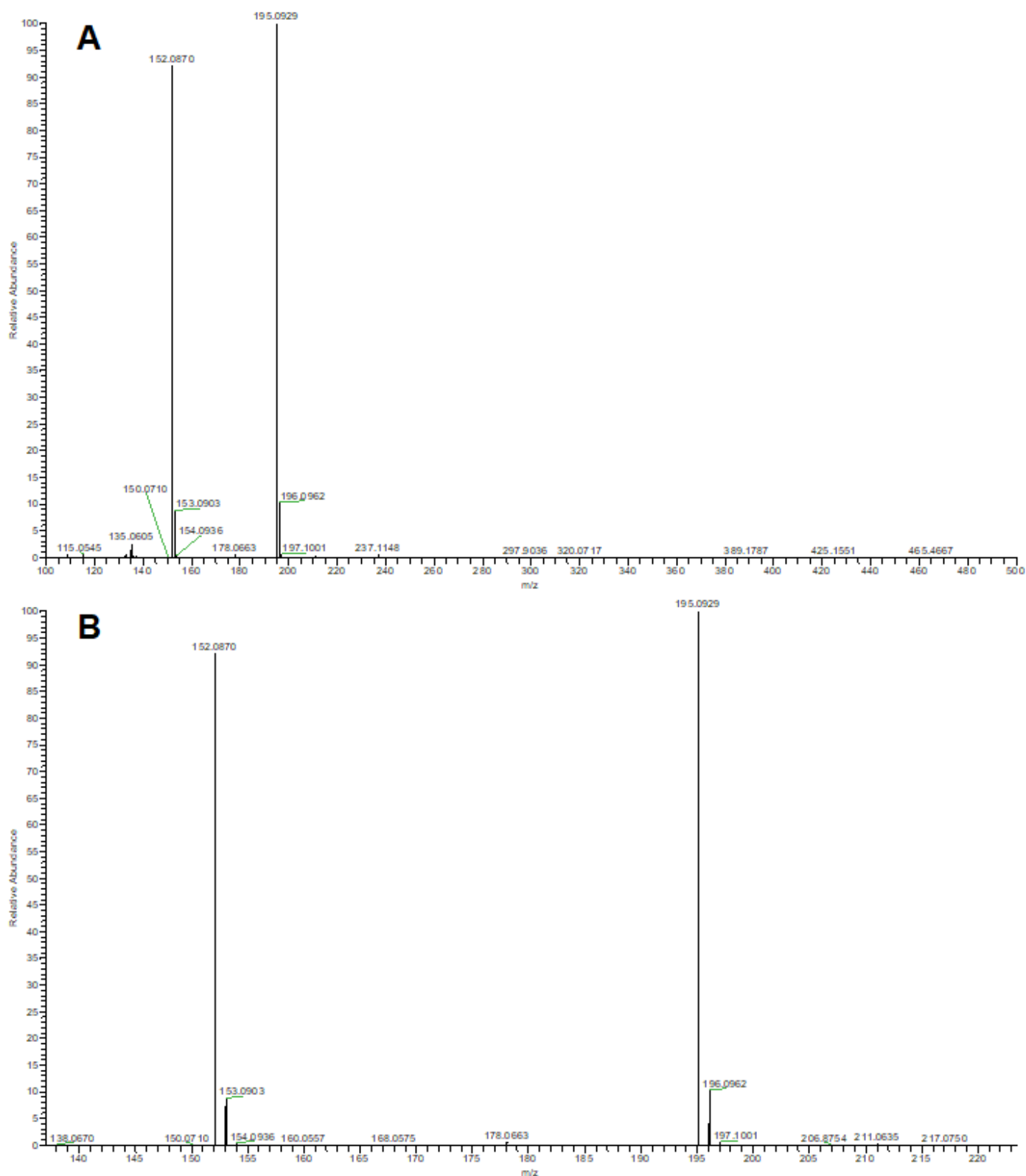


Figure S25. HESI positive mode full MS spectrum of 4F-MAR (A: full view, m/z 100-500, B: detailed view, m/z 140-220)

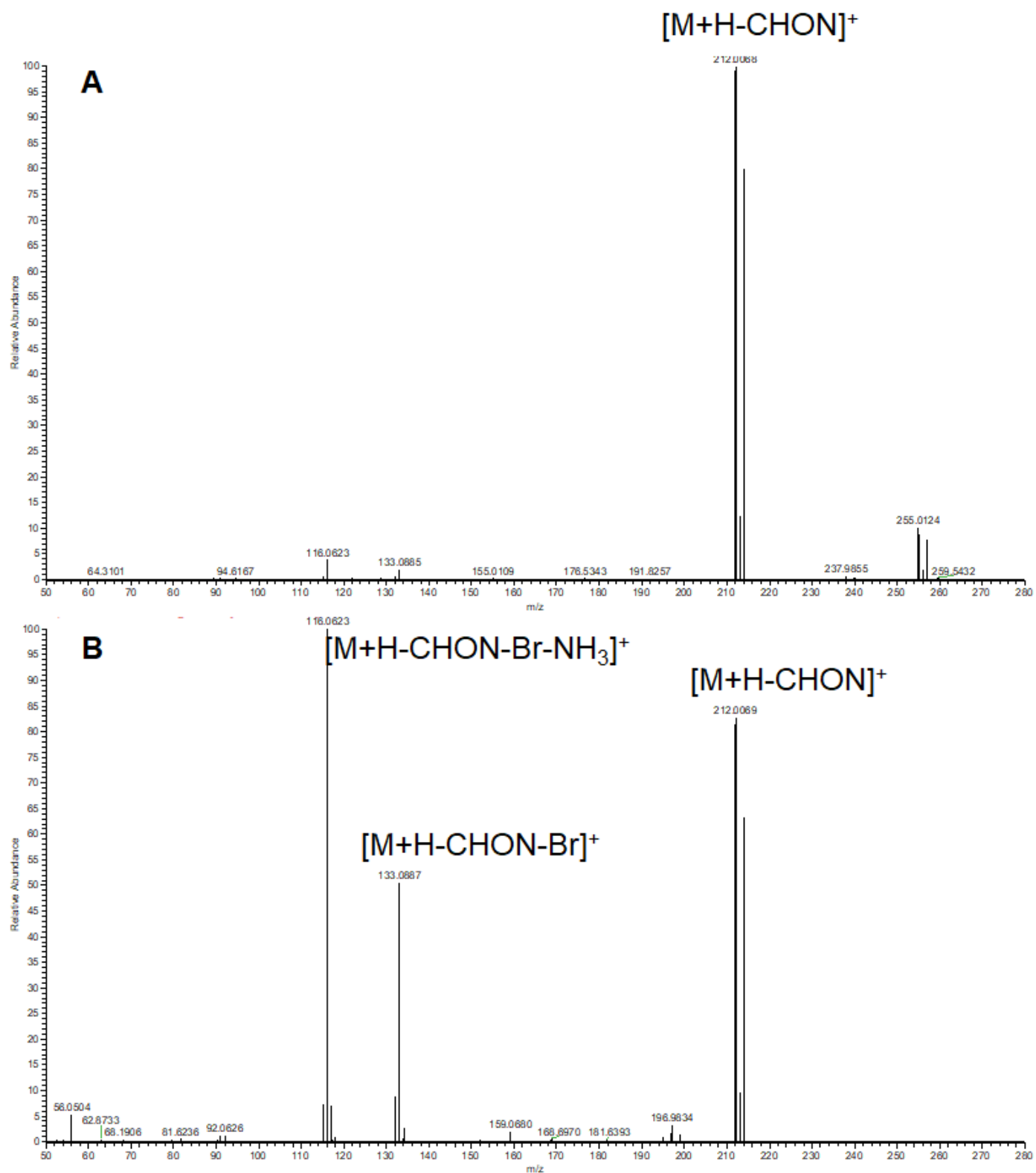


Figure S26. HESI positive mode MS/MS spectrum of 4B-MAR (A: normalized collision energy 18, B: normalized collision energy 45)

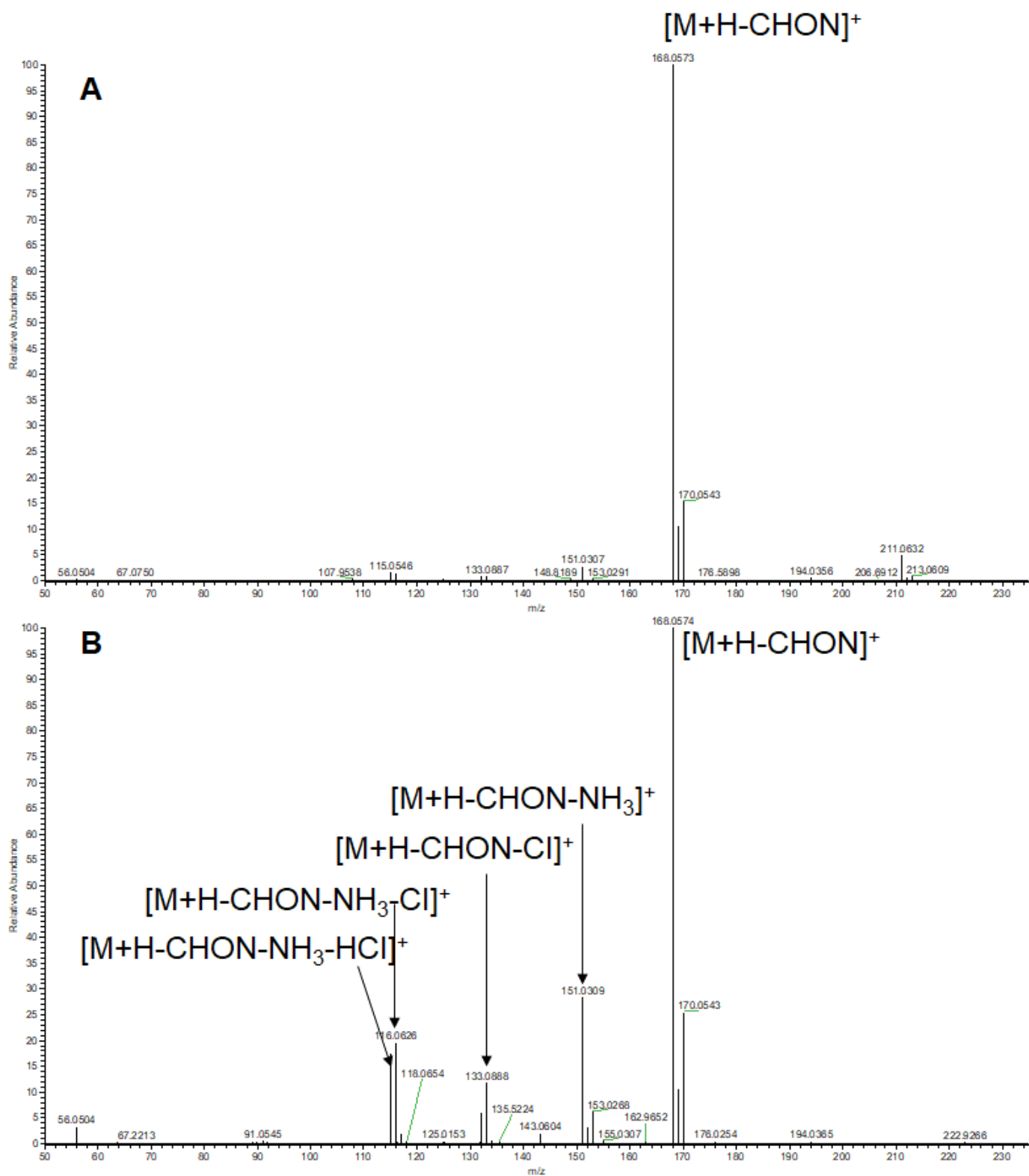


Figure S27. HESI positive mode MS/MS spectrum of 4C-MAR (A: normalized collision energy 18, B: normalized collision energy 45)

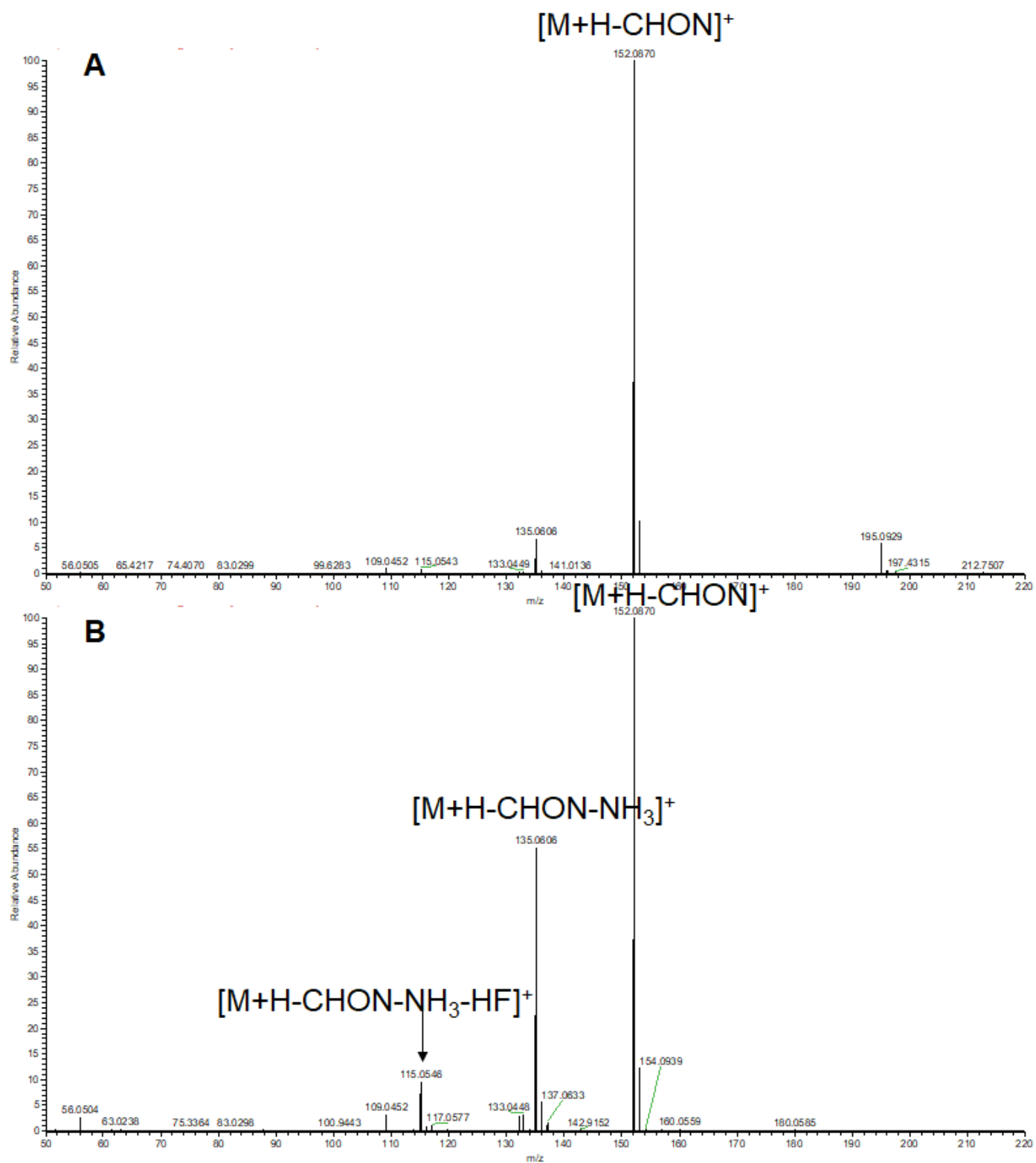


Figure S28. HESI positive mode MS/MS spectrum of 4F-MAR (A: normalized collision energy 18, B: normalized collision energy 45)