

Supplementary Materials:

Novel Flurbiprofen Derivatives as Antioxidant and Anti-inflammatory Agents: Synthesis, In silico, and In vitro Biological Evaluation

Iliyan Ivanov^{1*}, Stanimir Manolov^{1*}, Dimitar Bojilov¹, Gabriel Marc², Diyana Dimitrova¹, Smaranda Oniga³, Ovidiu Oniga², Paraskev Nedialkov⁴ and Maria Stoyanova¹

Table of Contents:

Figure S1. ¹ H-NMR spectrum of compound 4a	page 3
Figure S2. ¹ H-NMR spectrum of compound 4b	page 4
Figure S3. ¹ H-NMR spectrum of compound 4c	page 5
Figure S4. ¹ H-NMR spectrum of compound 4d	page 6
Figure S5. ¹ H-NMR spectrum of compound 4e	page 7
Figure S6. ¹³ C-NMR spectrum of compound 4a	page 8
Figure S7. ¹³ C-NMR spectrum of compound 4b	page 9
Figure S8. ¹³ C-NMR spectrum of compound 4c	page 10
Figure S9. ¹³ C-NMR spectrum of compound 4d	page 11
Figure S10. ¹³ C-NMR spectrum of compound 4e	page 12
Figure S11. UV spectrum of compound 4a	page 13
Figure S12. UV spectrum of compound 4b	page 14
Figure S13. UV spectrum of compound 4c	page 15
Figure S14. UV spectrum of compound 4d	page 16
Figure S15. UV spectrum of compound 4e	page 17

Figure S16. ESI-HRMS of compound 4a	page 18
Figure S17. Mass spectrum of 4a in positive ion ESI-MS/MS	page 19
Figure S18. Proposed fragmentation of protonated 4a	page 20
Figure S19. ESI-HRMS of compound 4b	page 21
Figure S20. Mass spectrum of 4b in positive ion ESI-MS/MS	page 22
Figure S21. Proposed fragmentation of protonated 4b	page 23
Figure S22. ESI-HRMS of compound 4c	page 24
Figure S23. Mass spectrum of 4c in positive ion ESI-MS/MS	page 25
Figure S24. Proposed fragmentation of protonated 4c	page 26
Figure S25. ESI-HRMS of compound 4d	page 27
Figure S26. Mass spectrum of 4d in positive ion ESI-MS/MS	page 28
Figure S27. Proposed fragmentation of protonated 4d	page 29
Figure S28. ESI-HRMS of compound 4e	page 30
Figure S29. Mass spectrum of 4e in positive ion ESI-MS/MS	page 31
Figure S30. Proposed fragmentation of protonated 4e	page 32

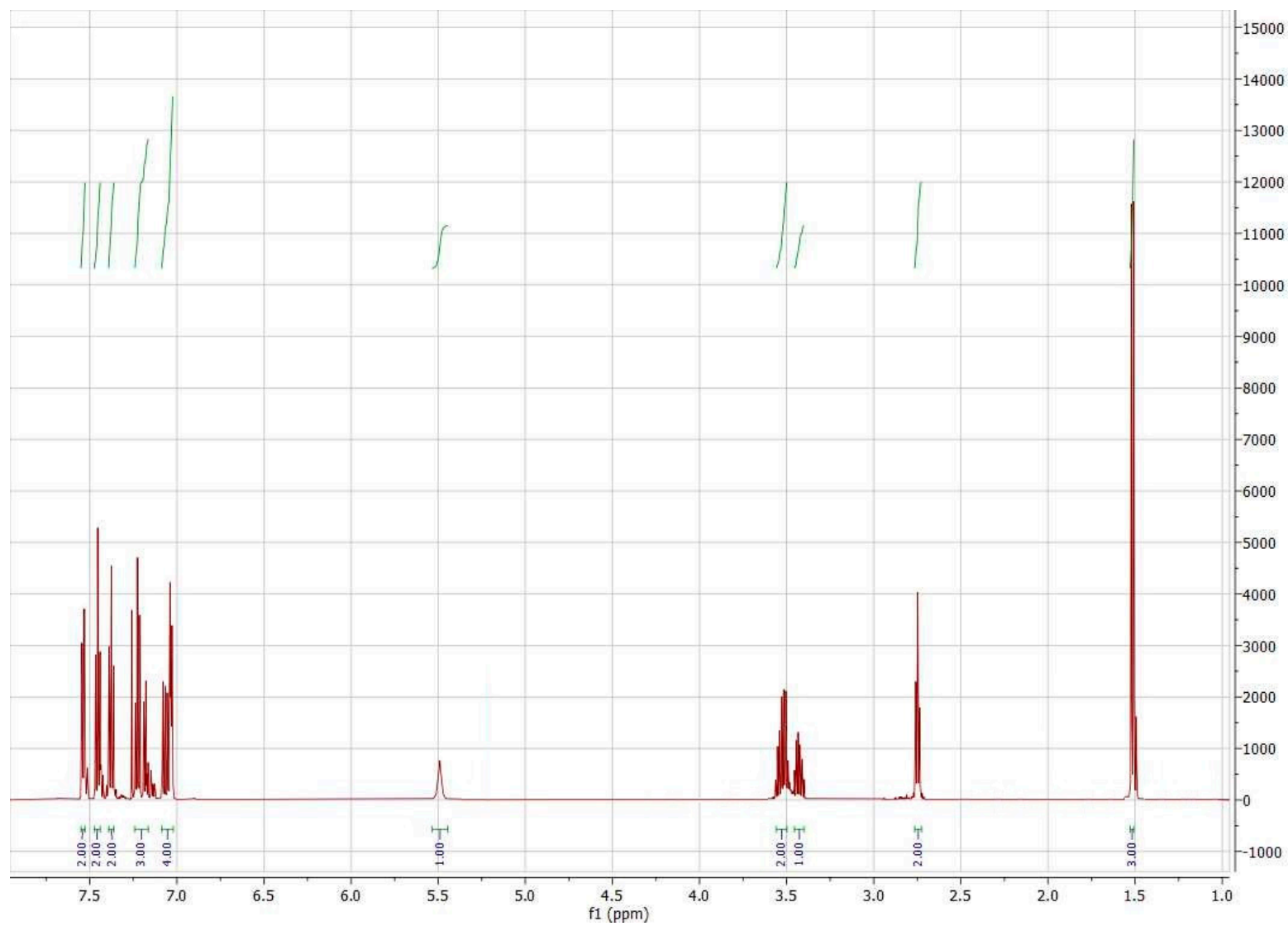


Figure S1. ^1H -NMR spectrum of compound 4a.

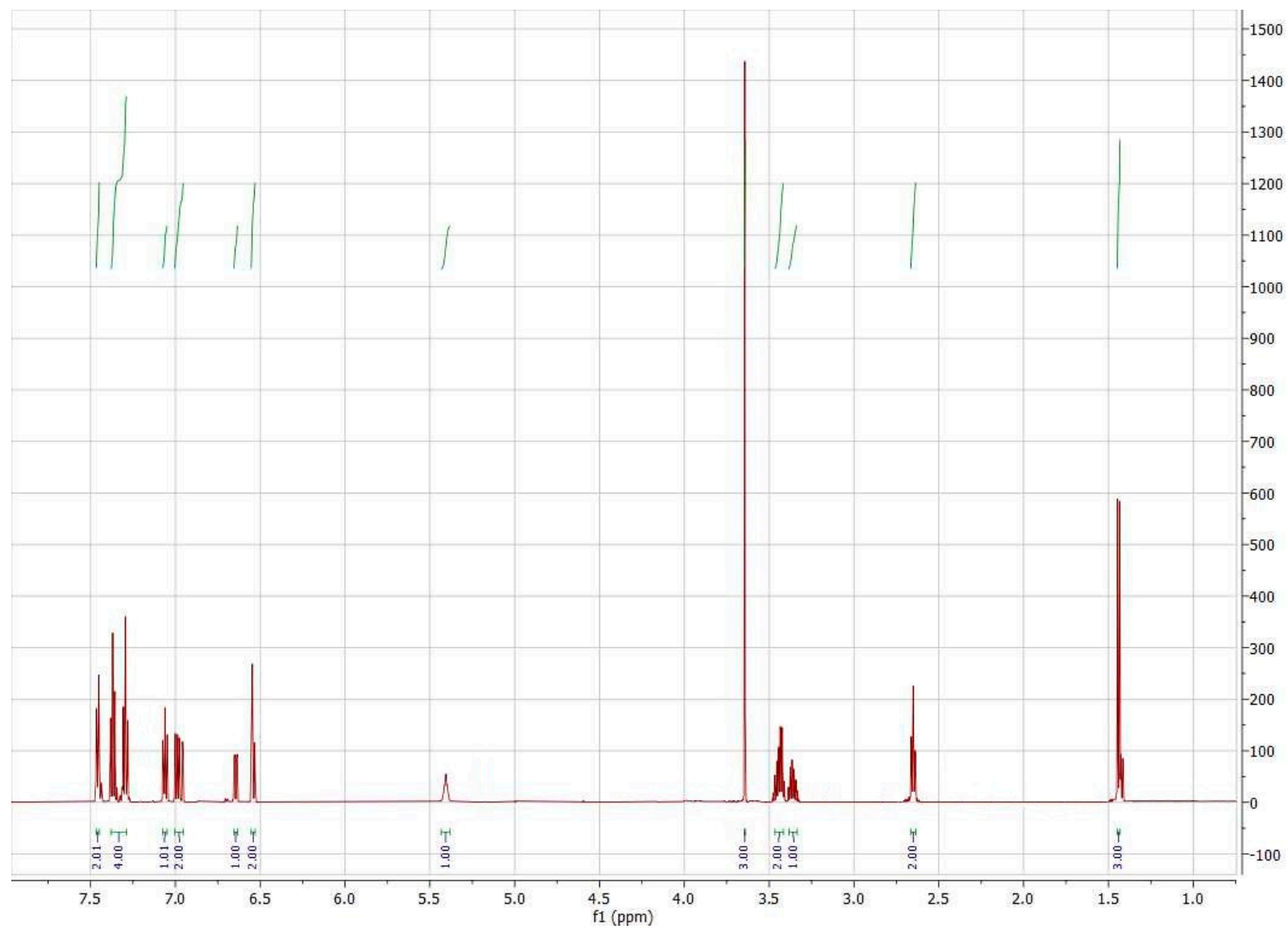


Figure S2. ^1H -NMR spectrum of compound **4b**.

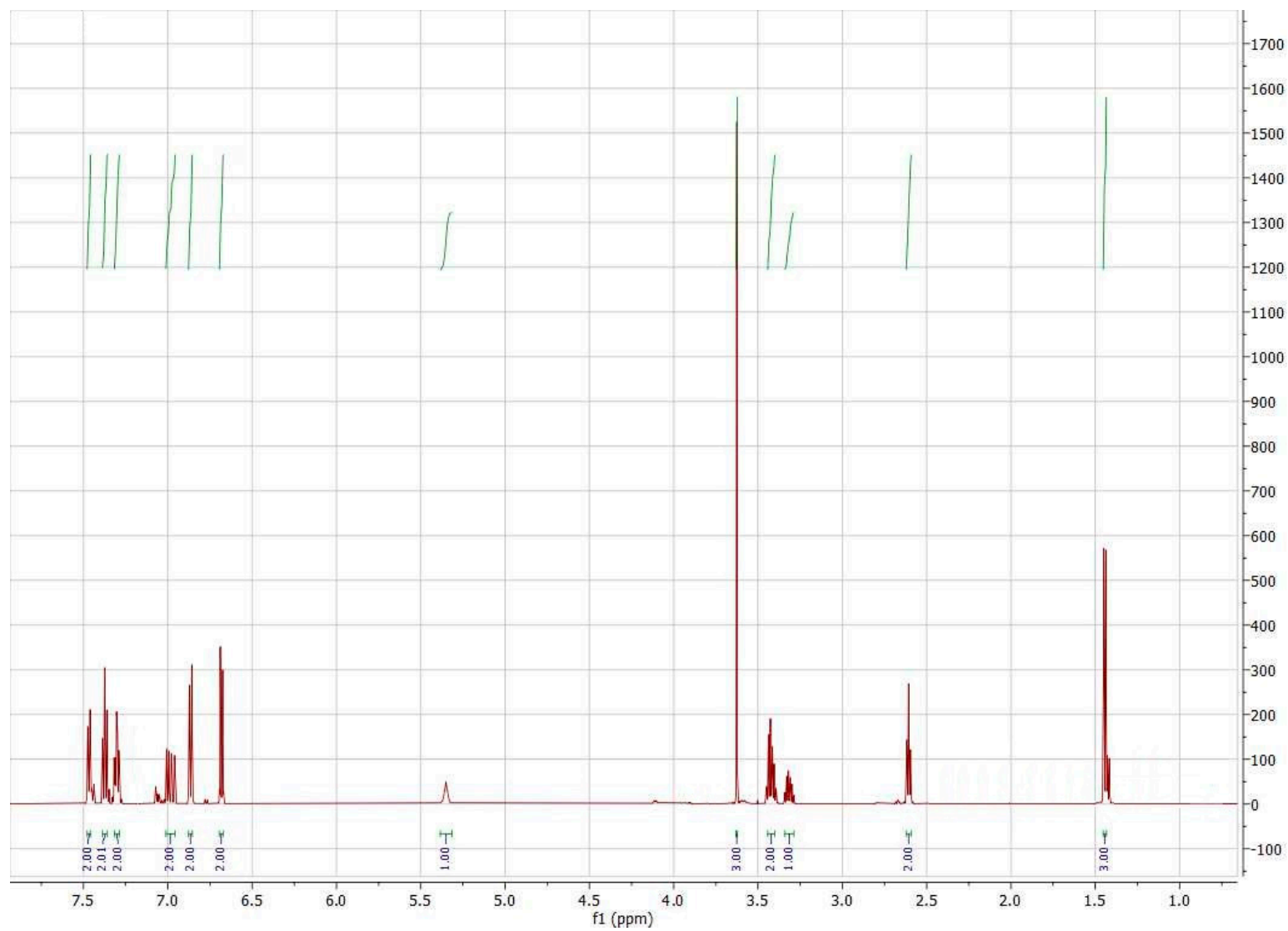


Figure S3. ^1H -NMR spectrum of compound **4c**.

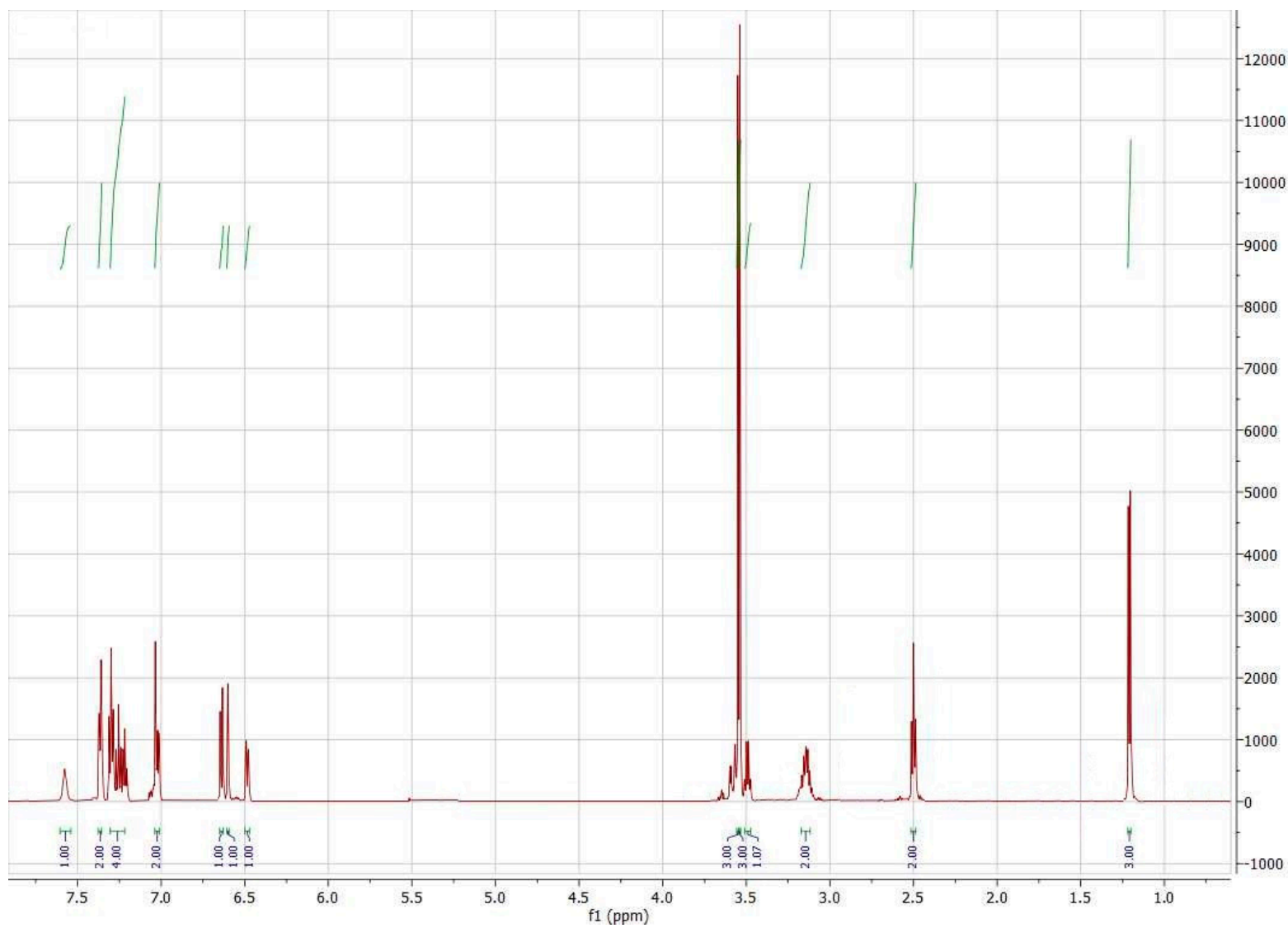


Figure S4. ^1H -NMR spectrum of compound **4d**.

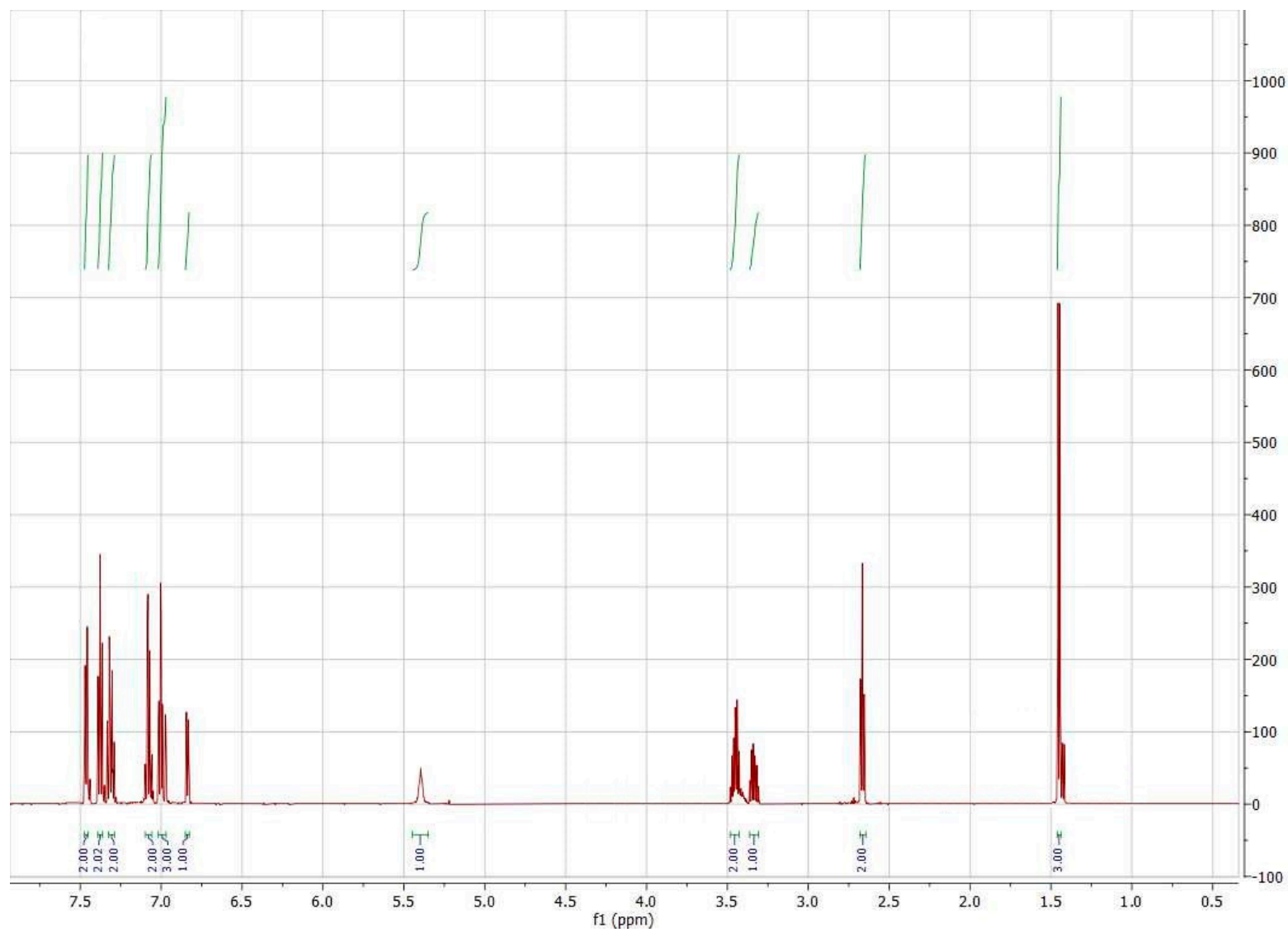


Figure S5. ^1H -NMR spectrum of compound **4e**.

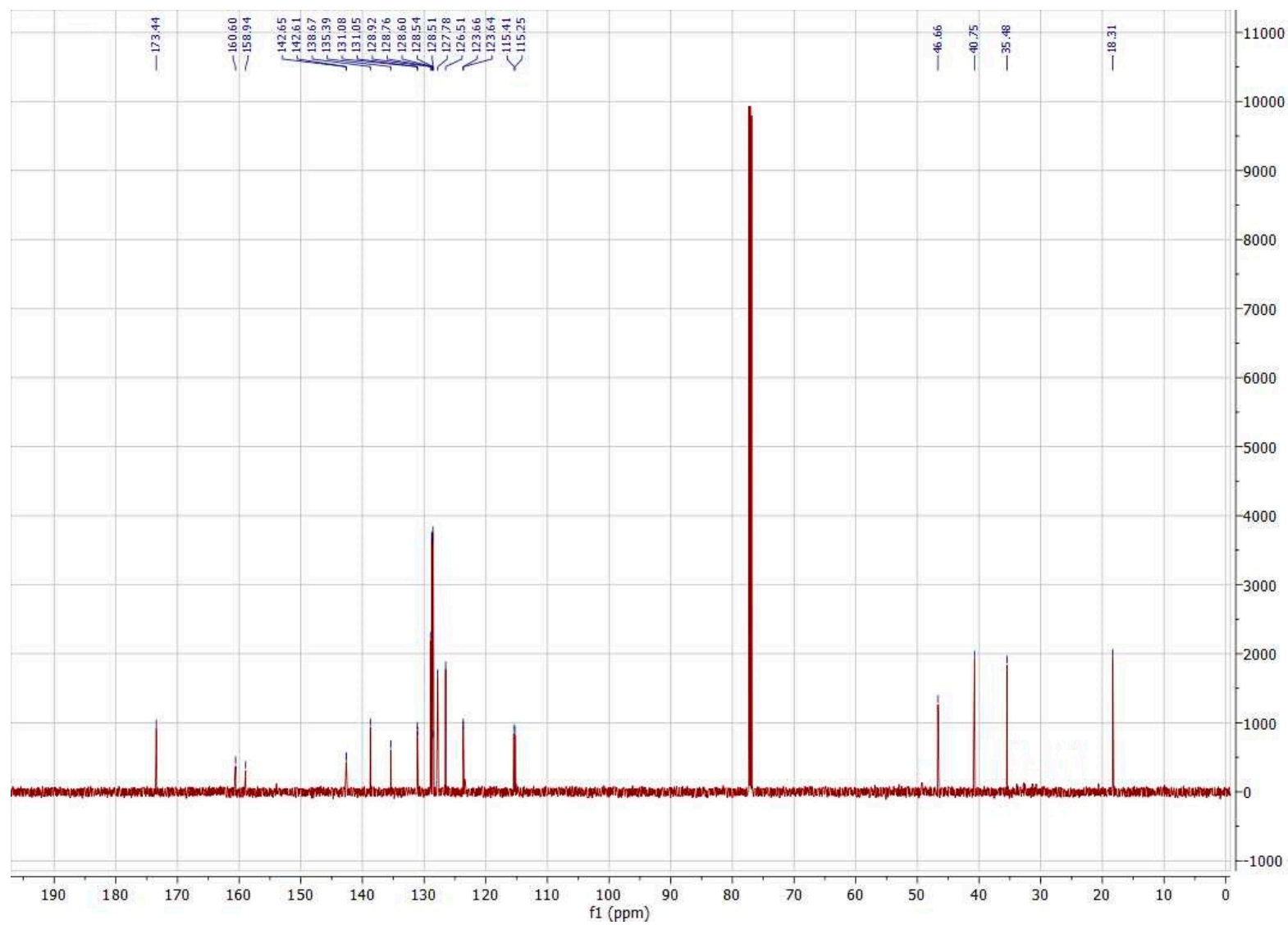


Figure S6. ^{13}C -NMR spectrum of compound **4a**.

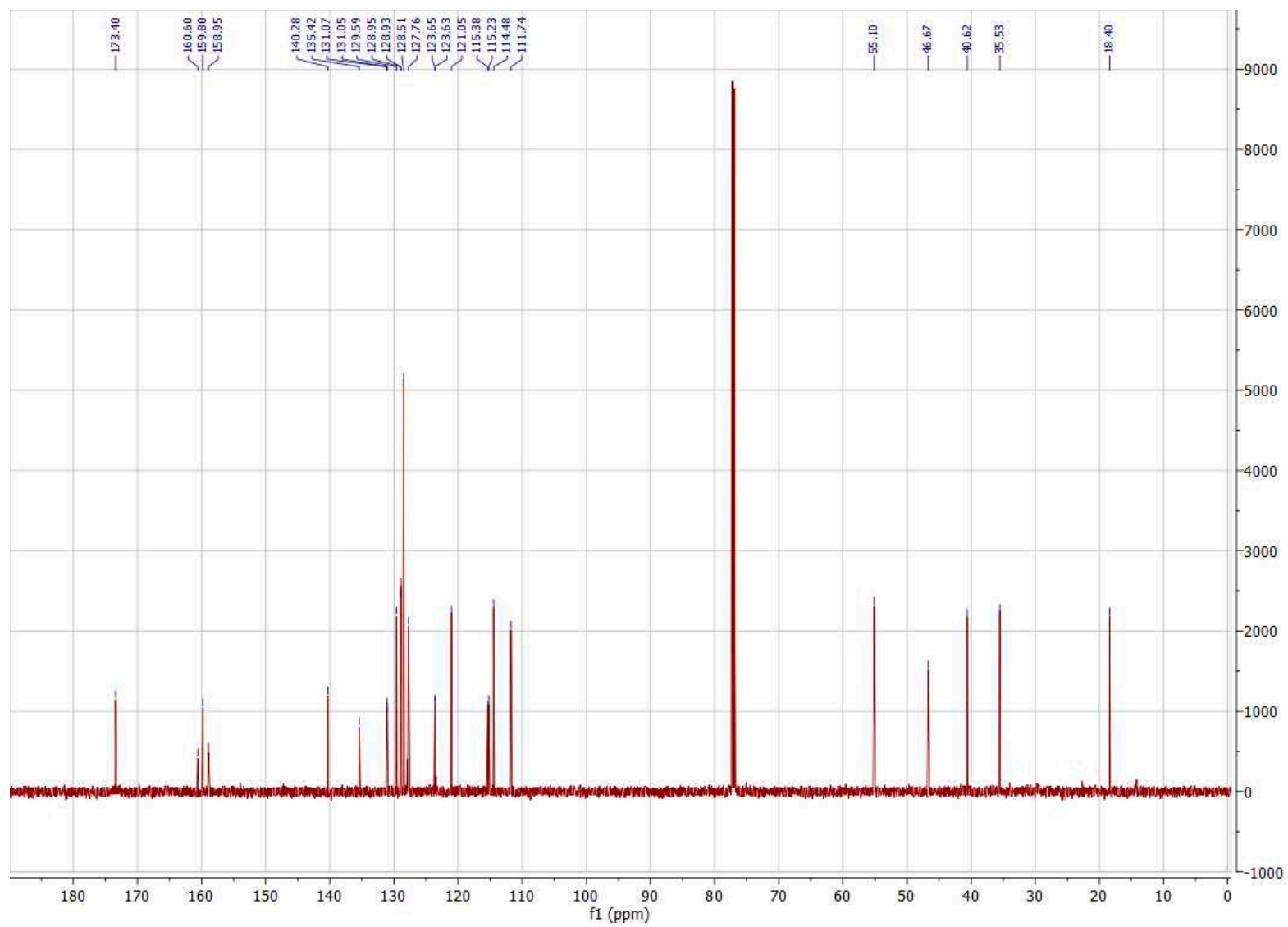


Figure S7. ¹³C-NMR spectrum of compound **4b**.

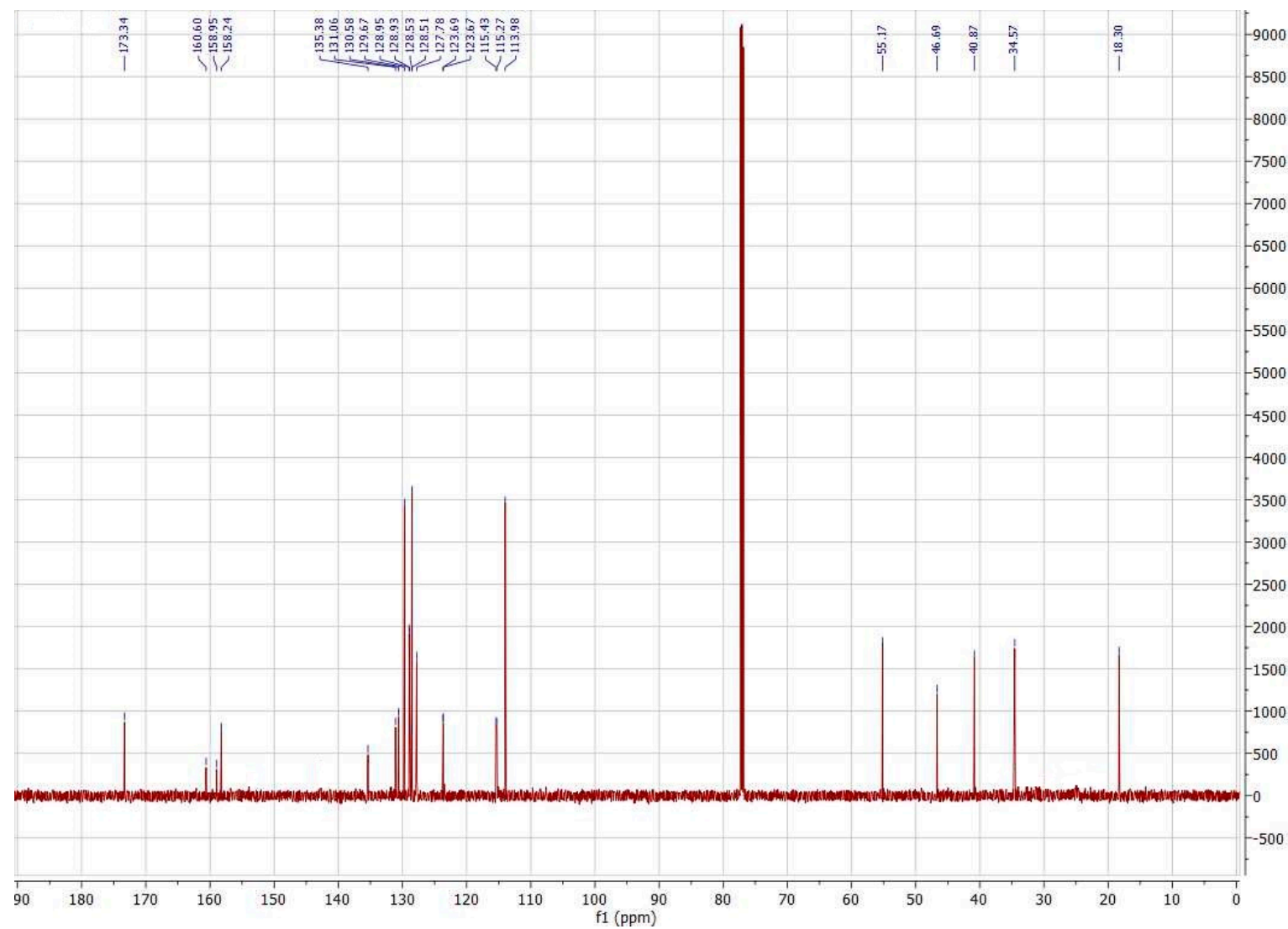


Figure S8. ¹³C-NMR spectrum of compound **4c**.

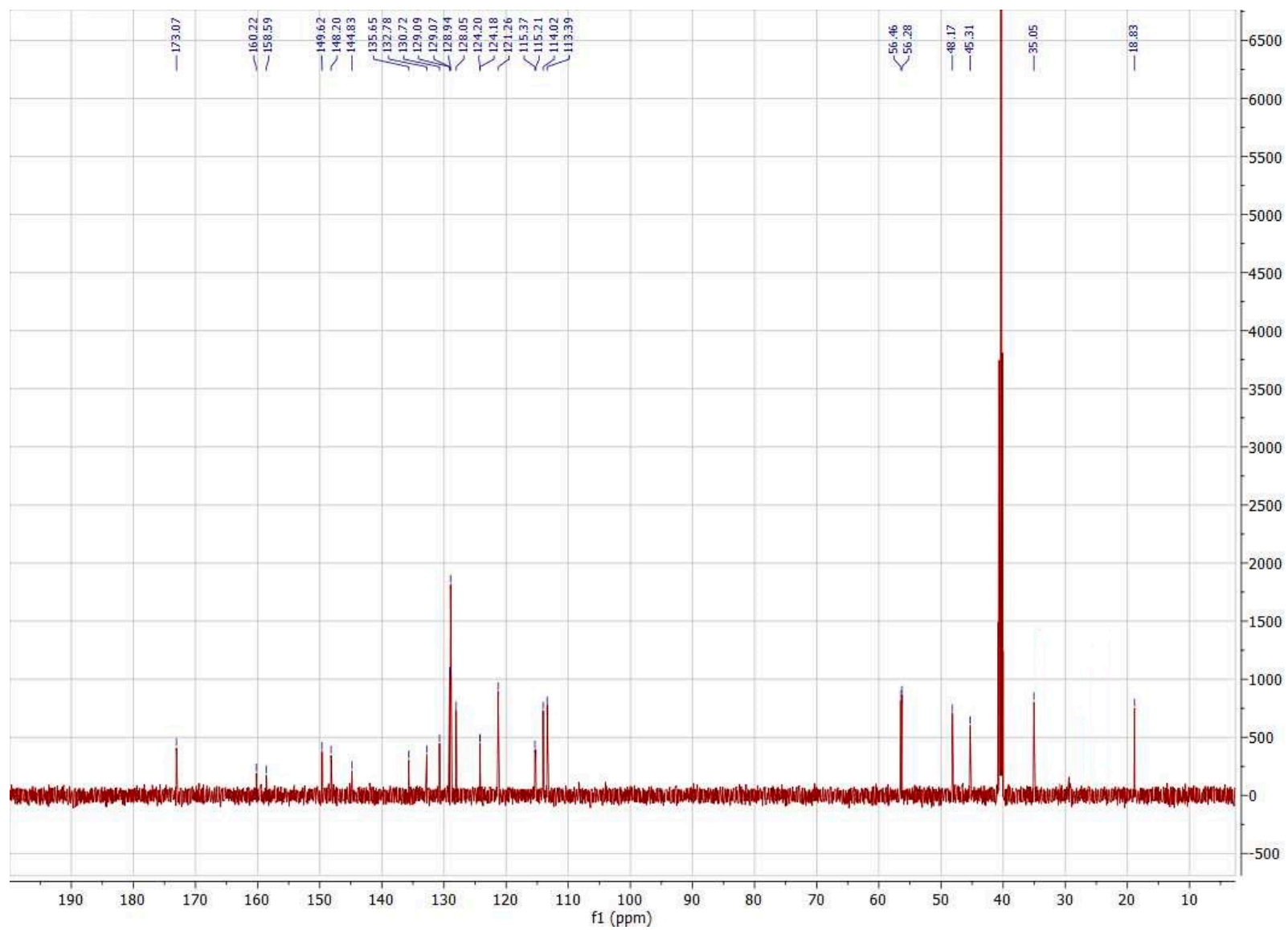


Figure S9. ¹³C-NMR spectrum of compound 4d.

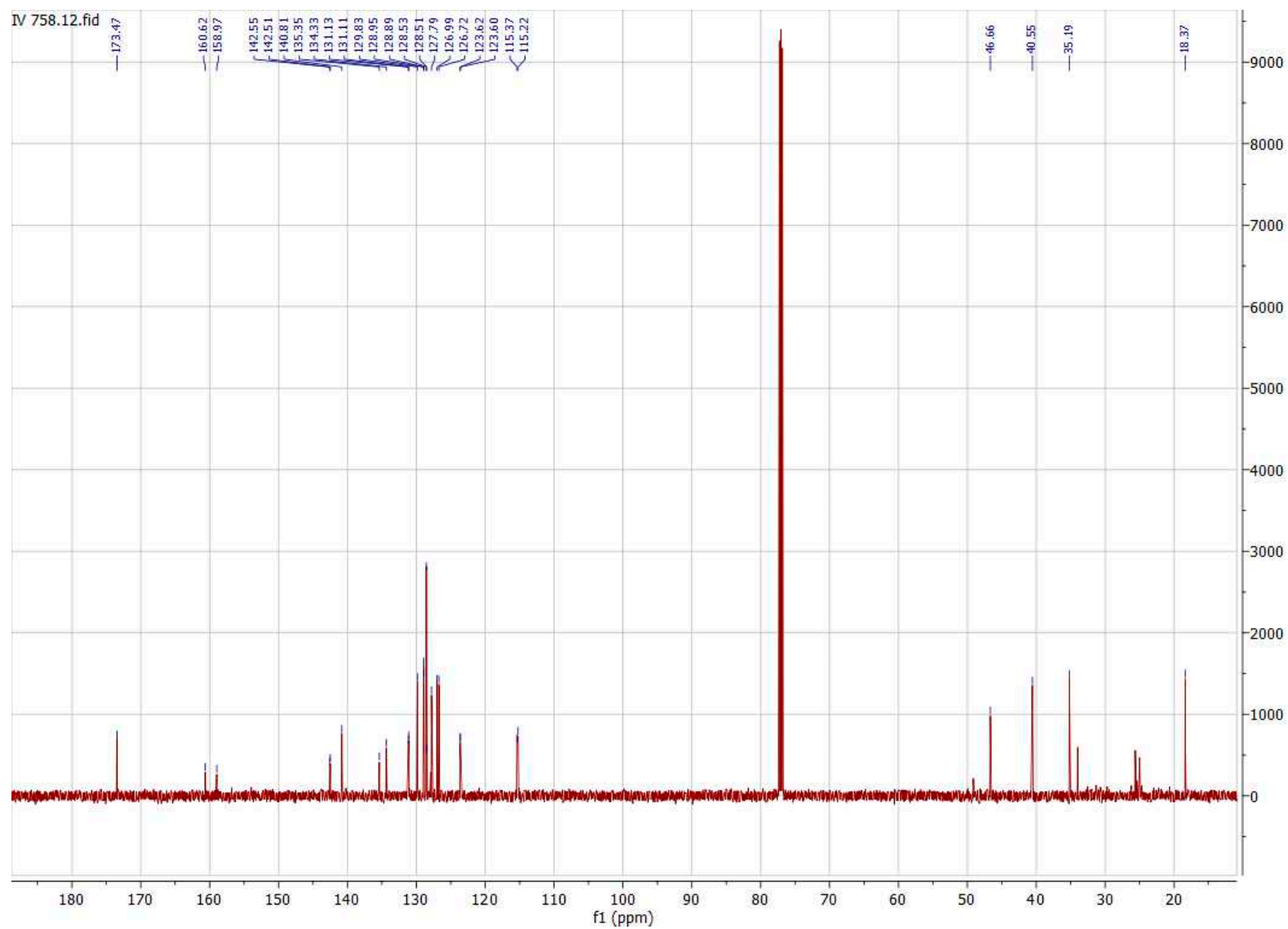


Figure S10. ^{13}C -NMR spectrum of compound 4e.

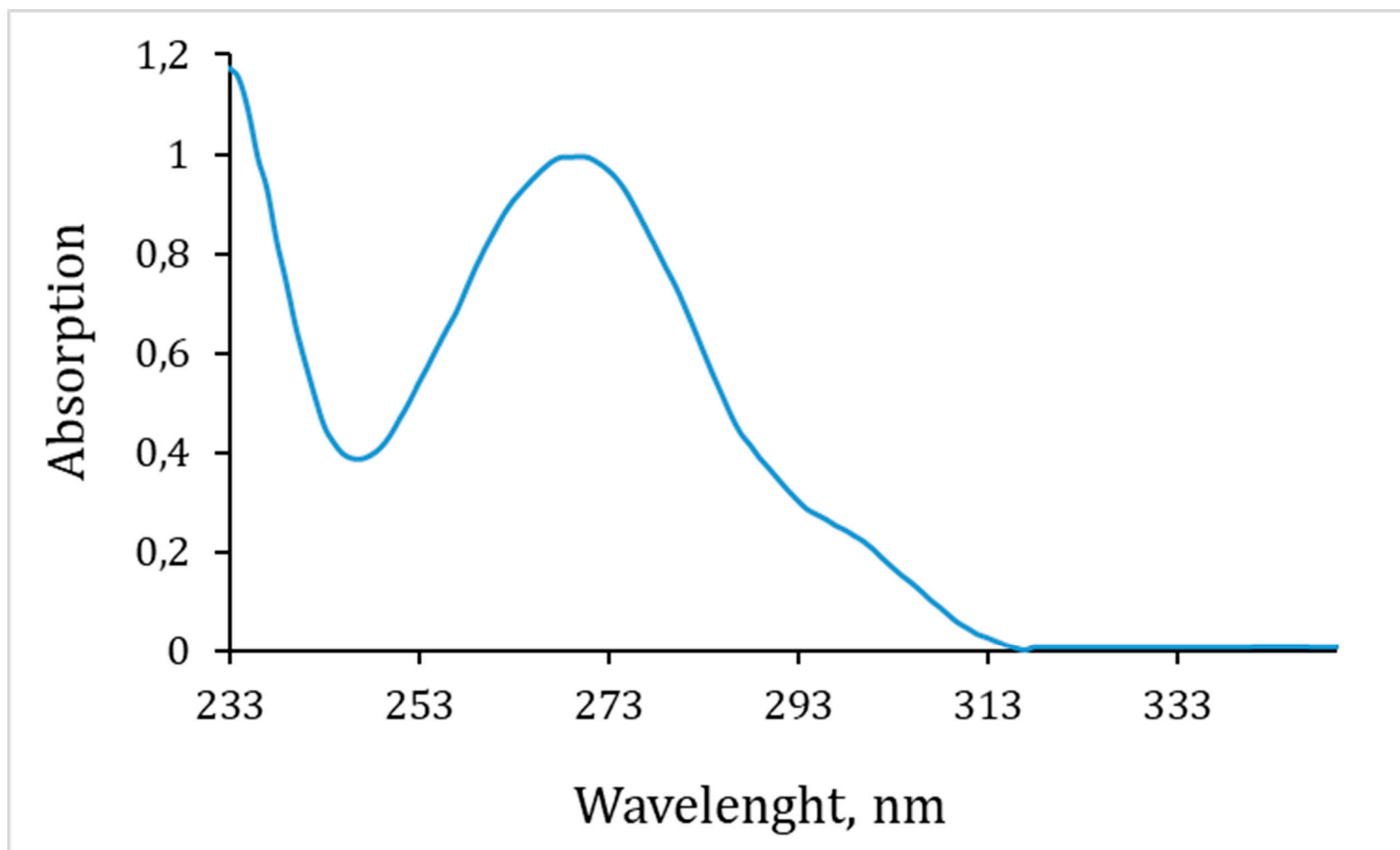


Figure S11. UV spectrum of compound **4a**.

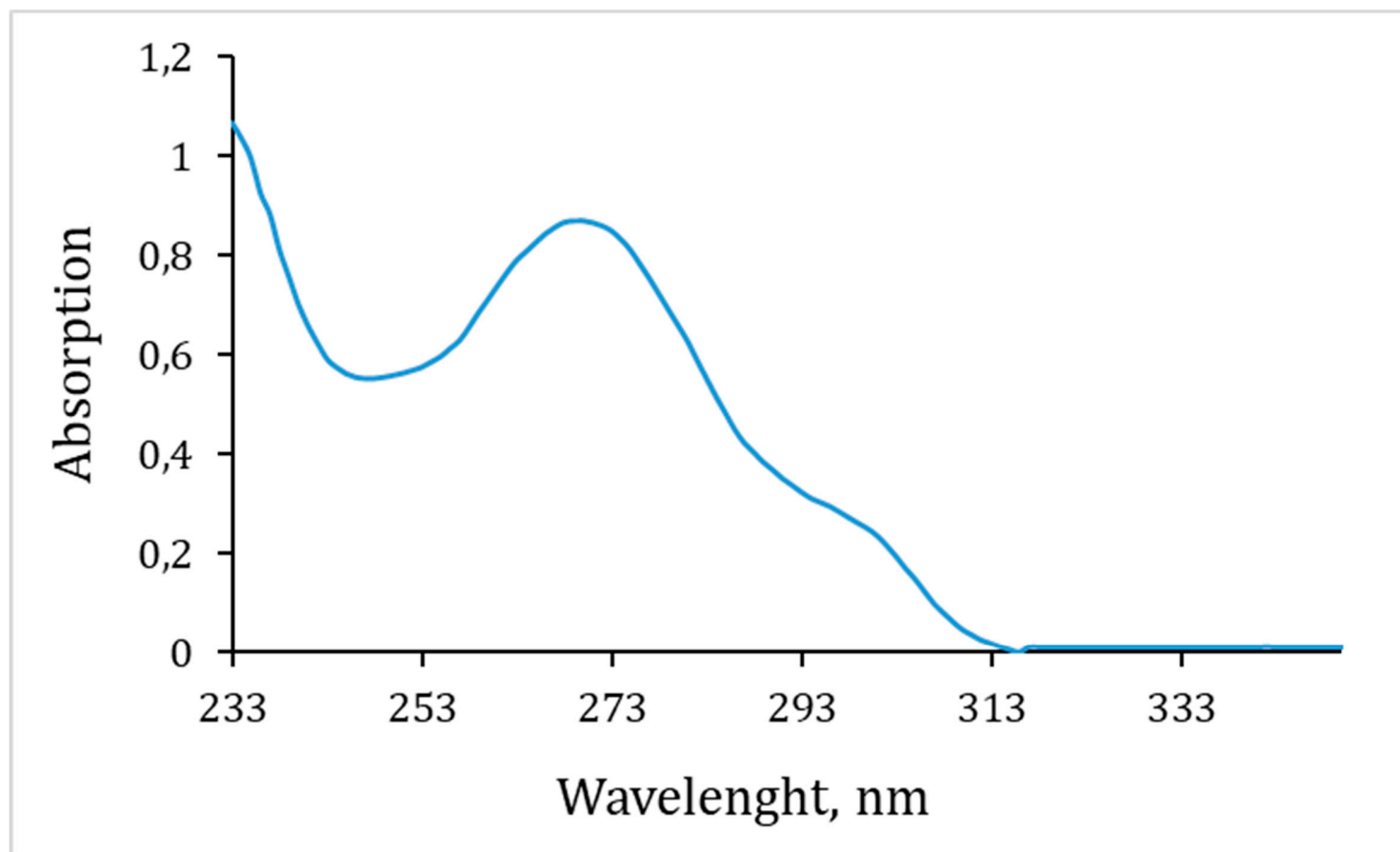


Figure S12. UV spectrum of compound **4b**.

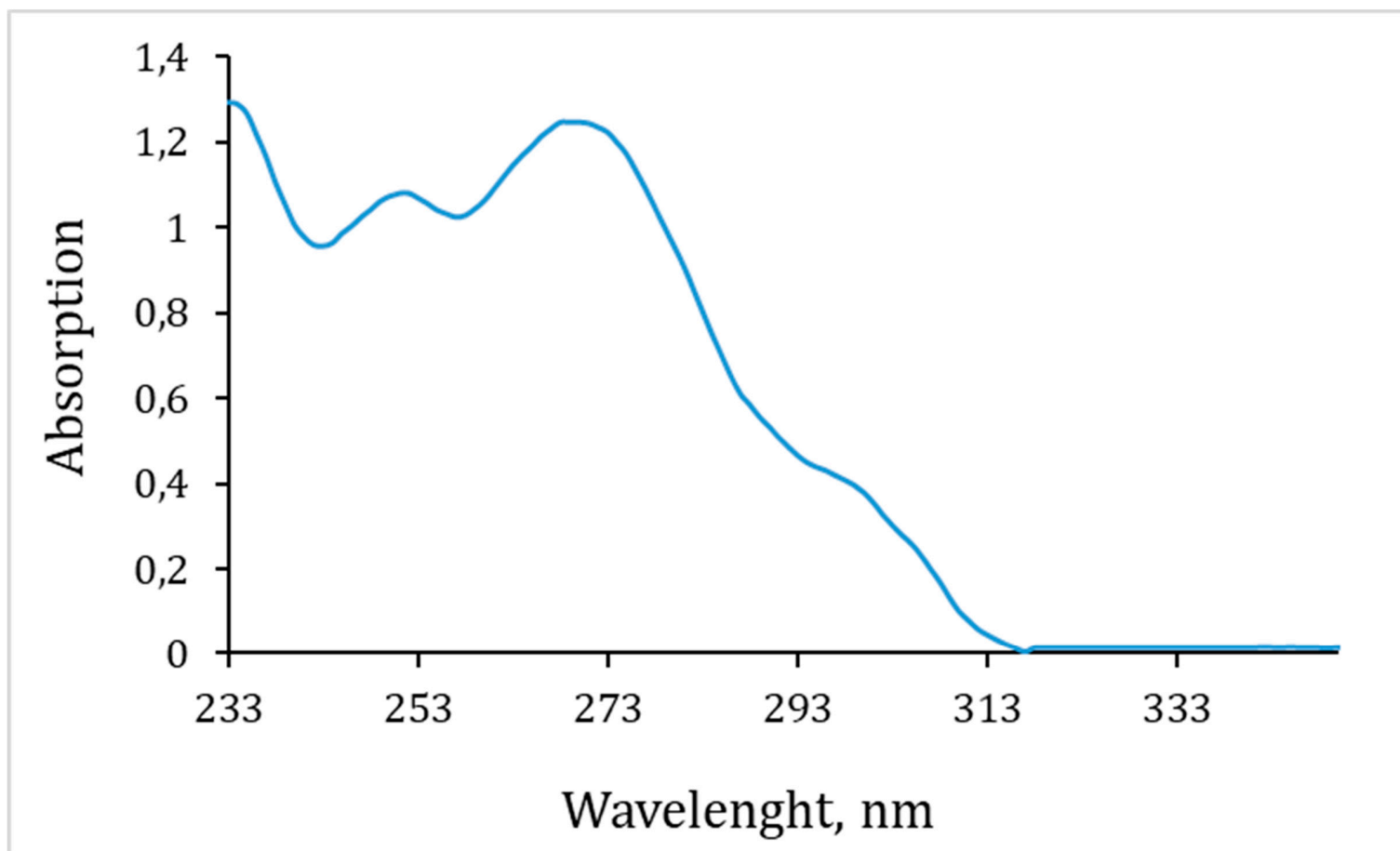


Figure S13. UV spectrum of compound **4c**.

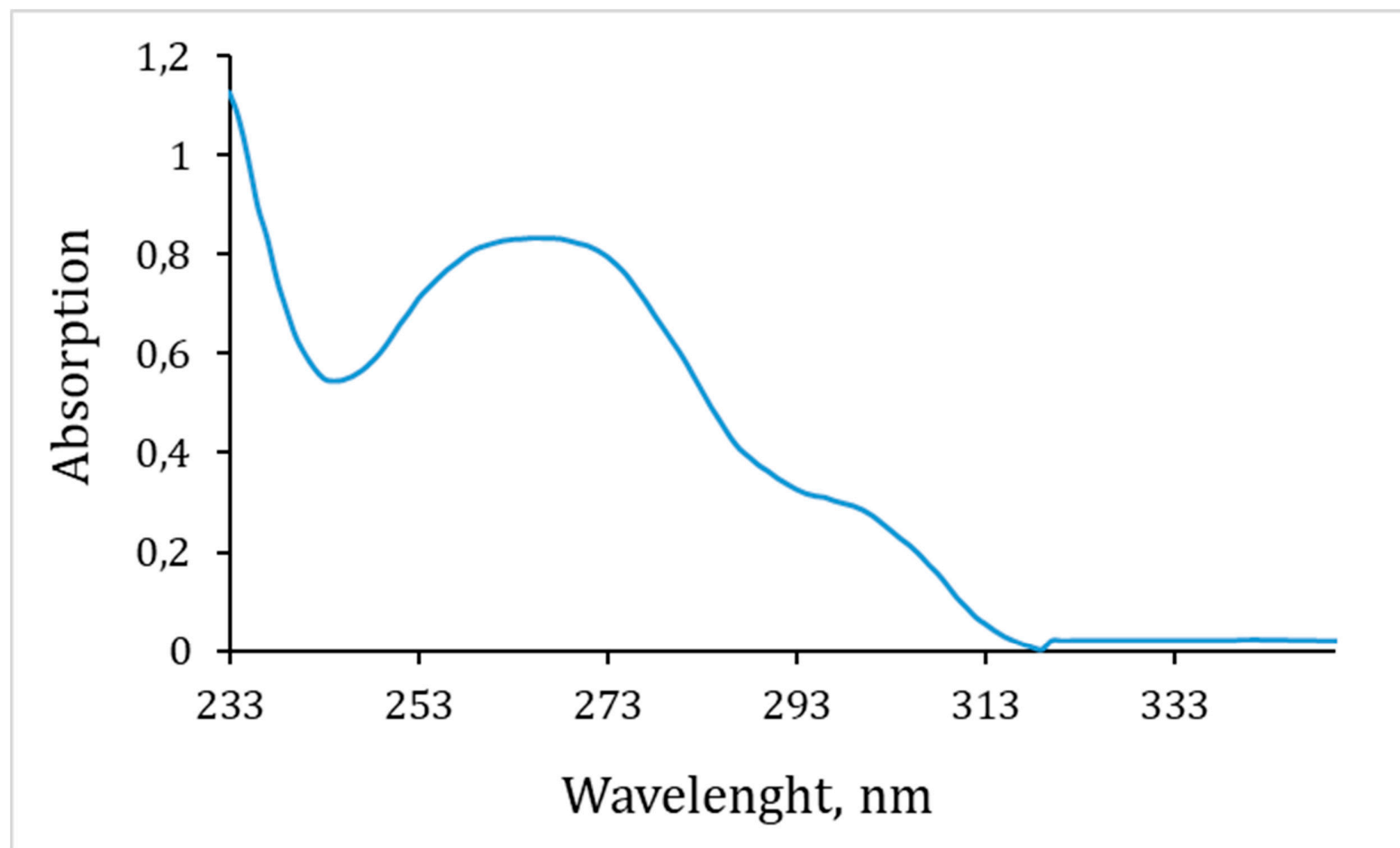


Figure S14. UV spectrum of compound **4d**.

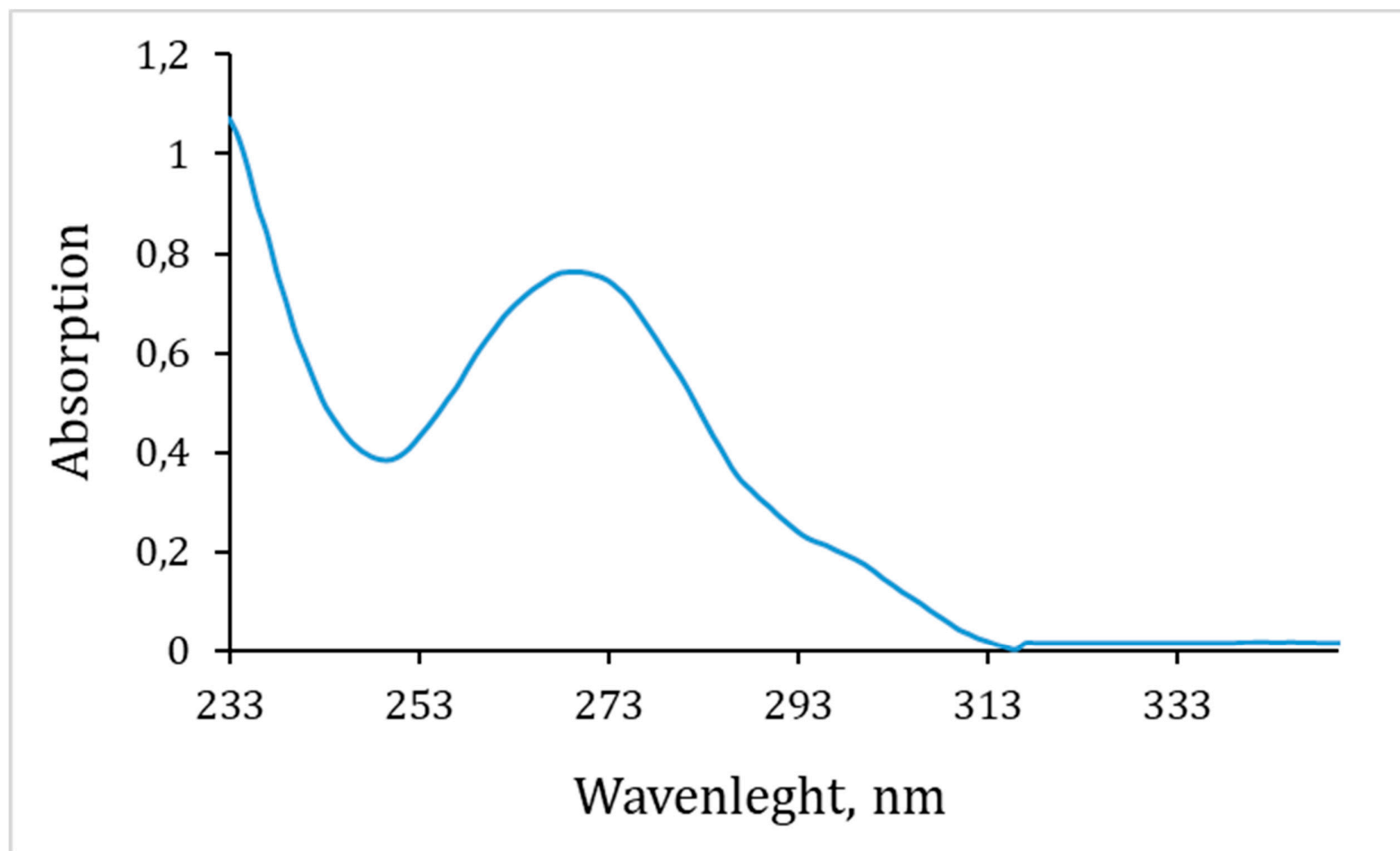


Figure S15. UV spectrum of compound **4e**.

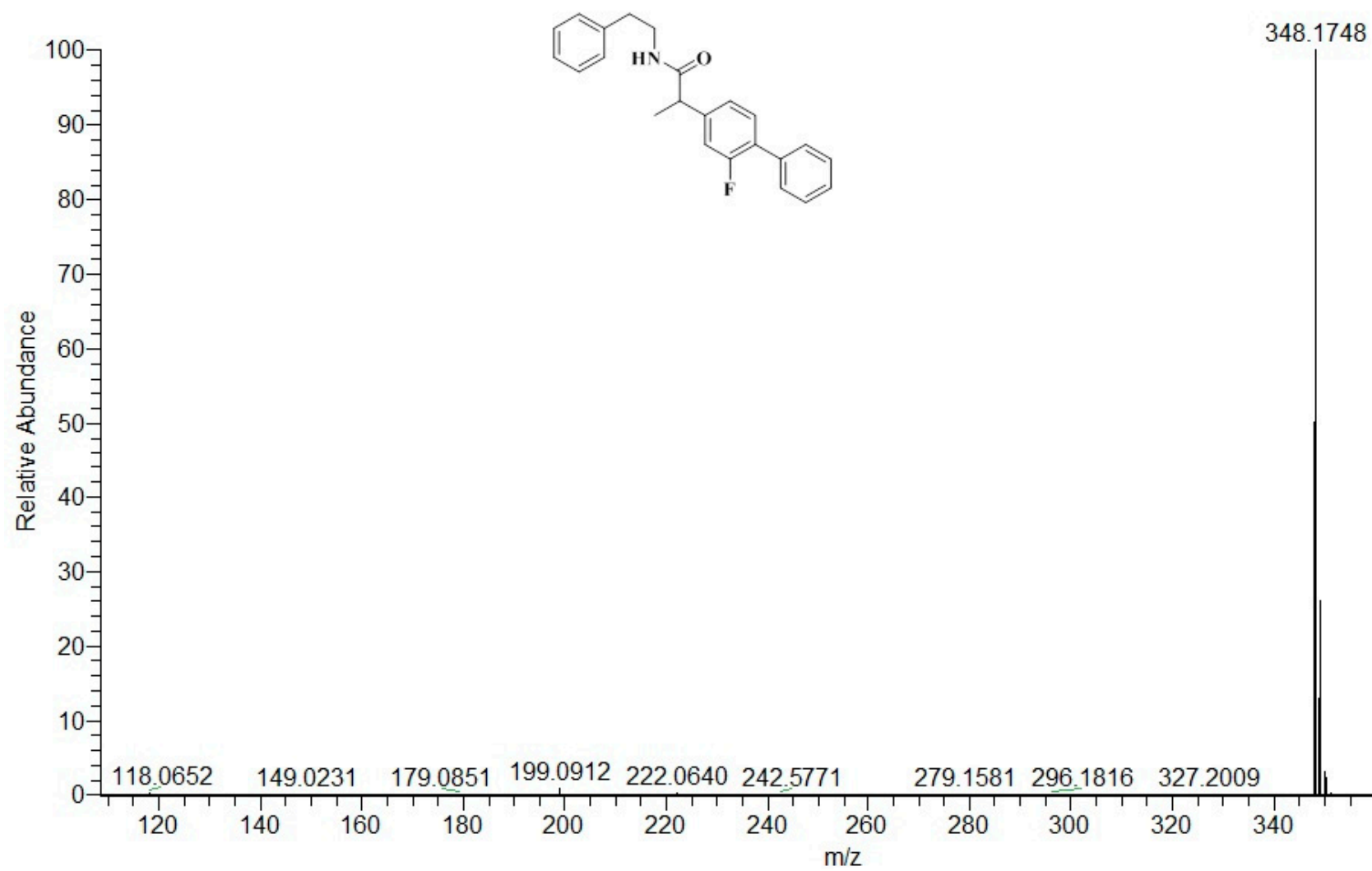


Figure S16. ESI-HRMS of compound 4a.

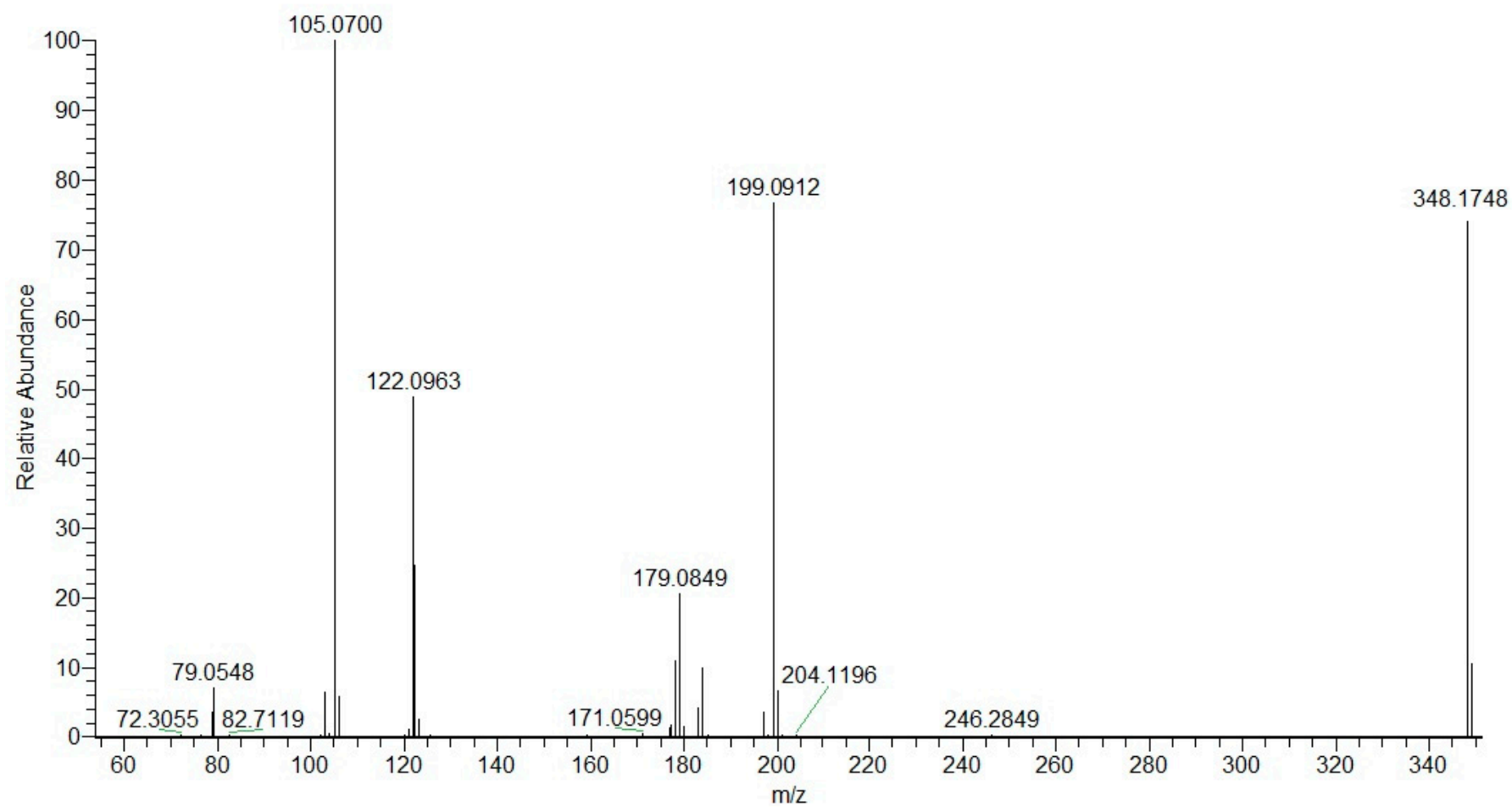


Figure S17. Mass spectrum of **4a** obtained by positive ion ESI-MS/MS.

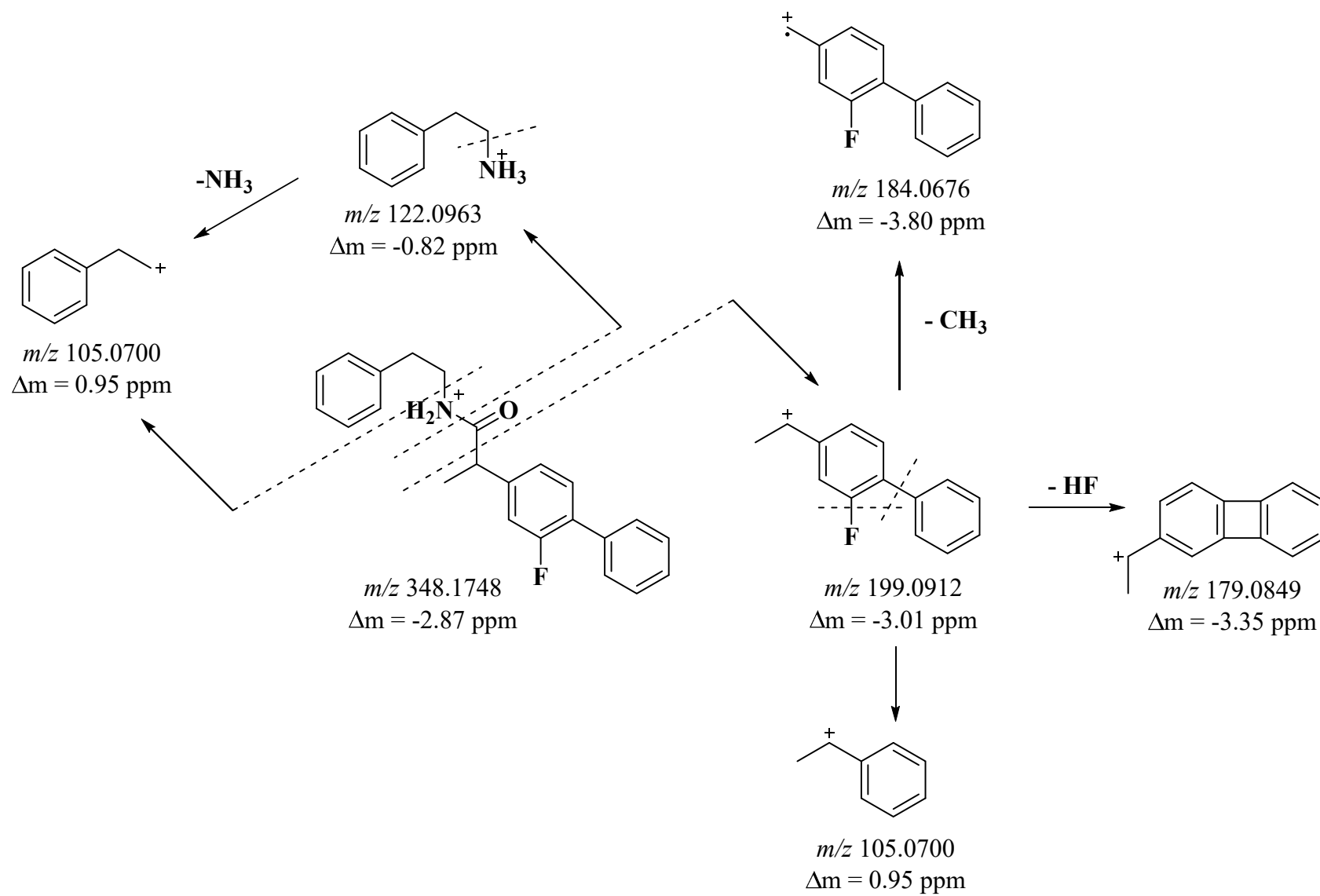


Figure S18. Proposed fragmentation of protonated **4a**.

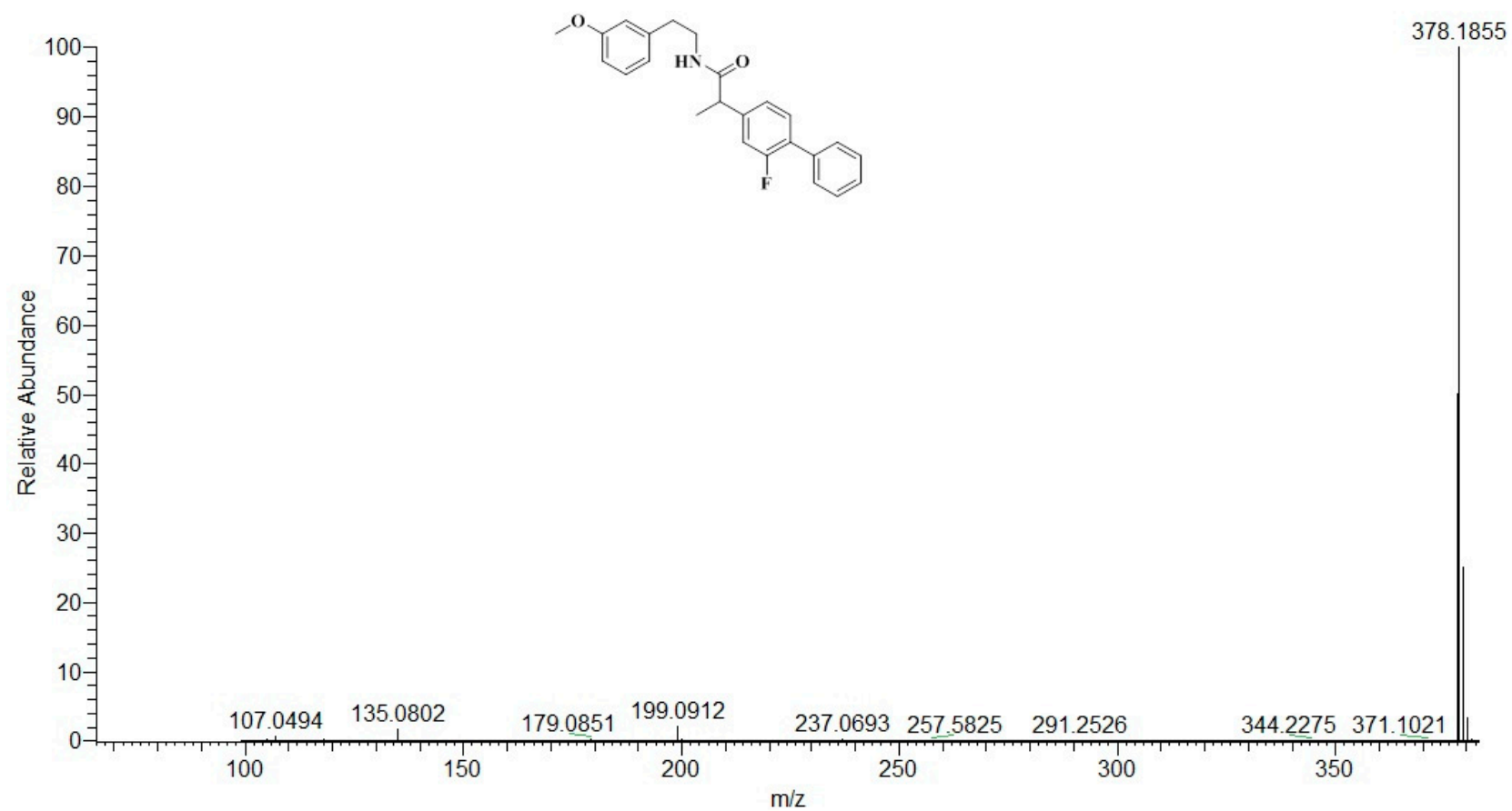


Figure S19. ESI-HRMS of compound **4b**.

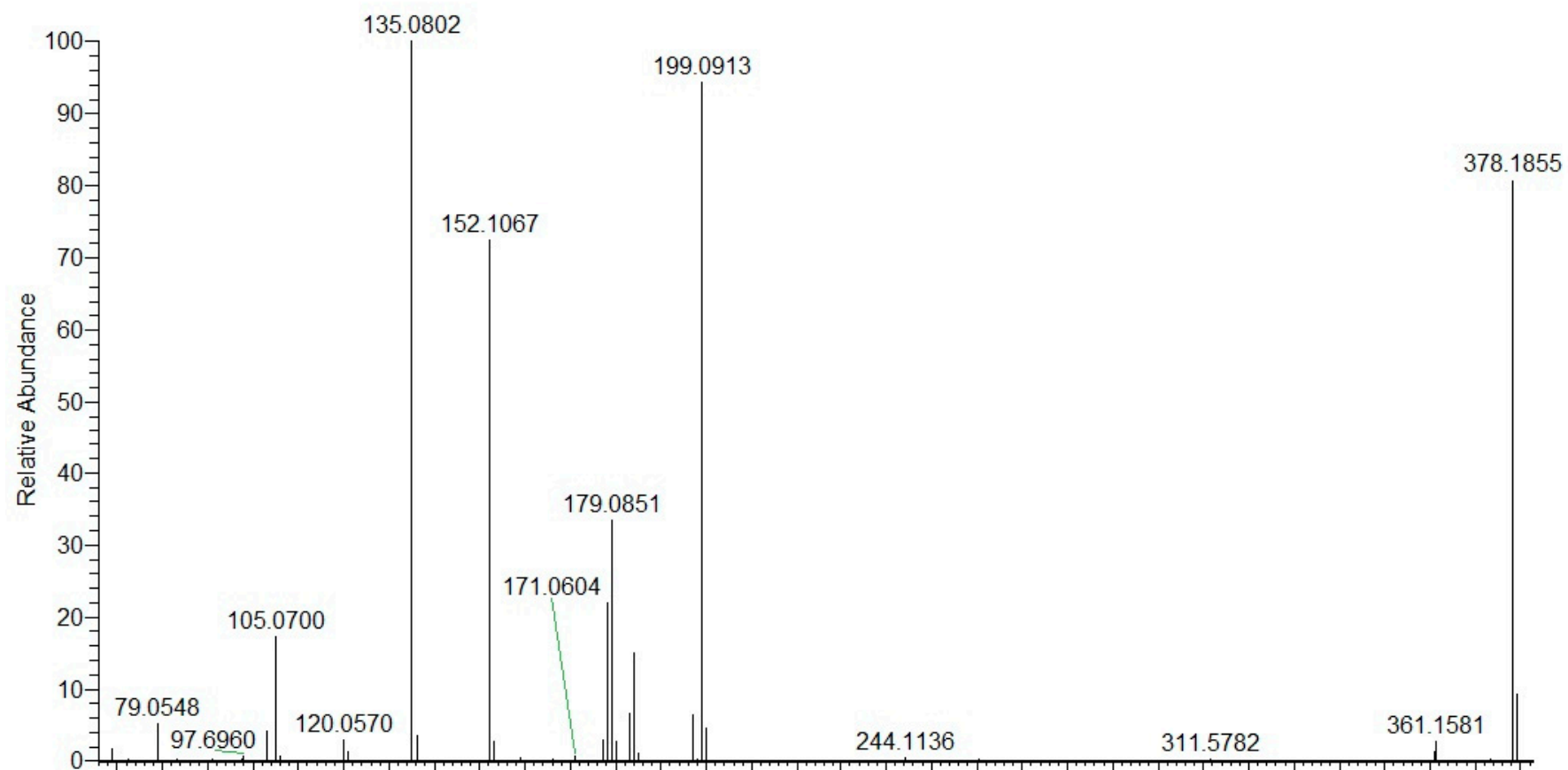


Figure S20. Mass spectrum of **4b** obtained by positive ion ESI-MS/MS.

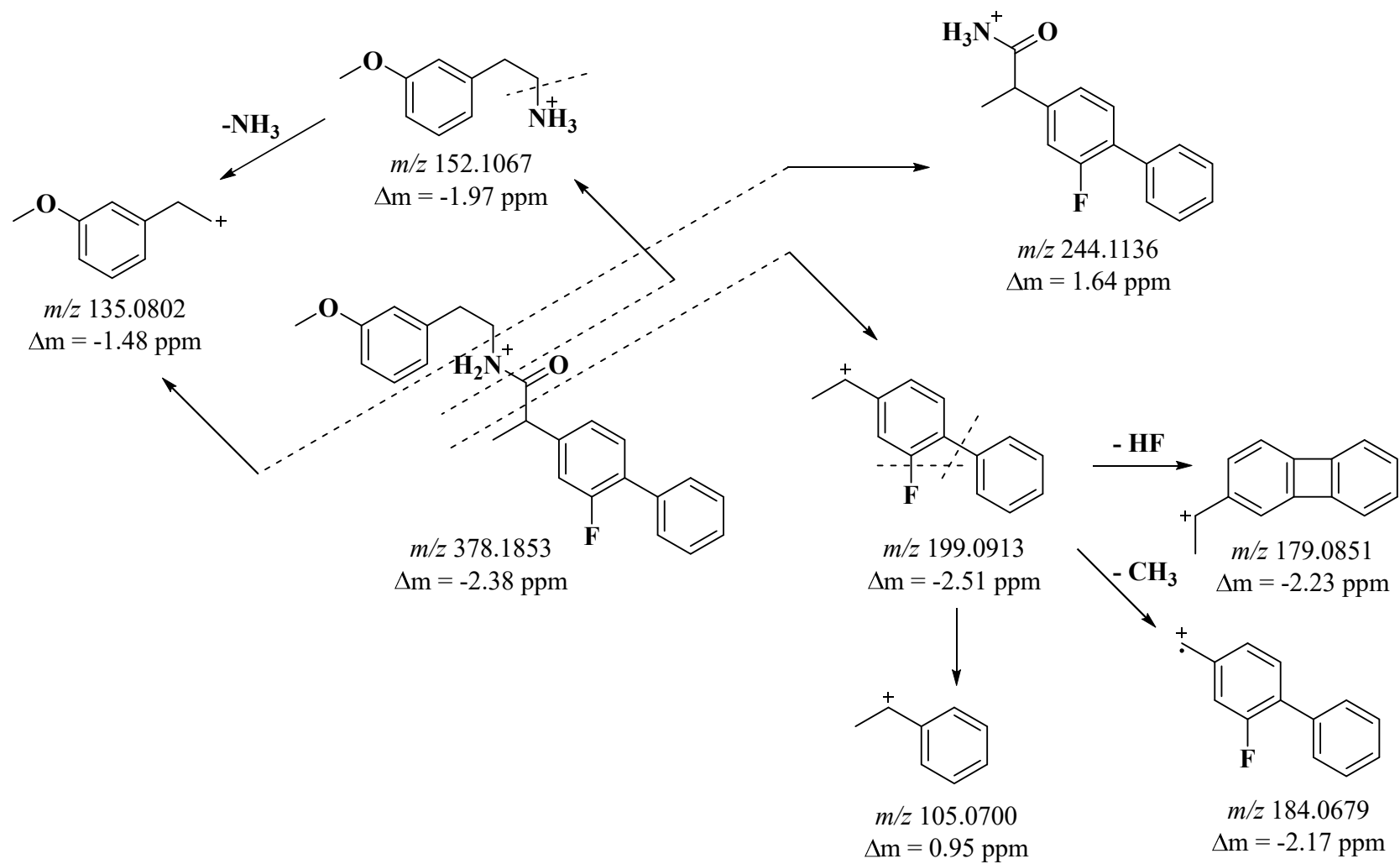


Figure S21. Proposed fragmentation of protonated **4b**.

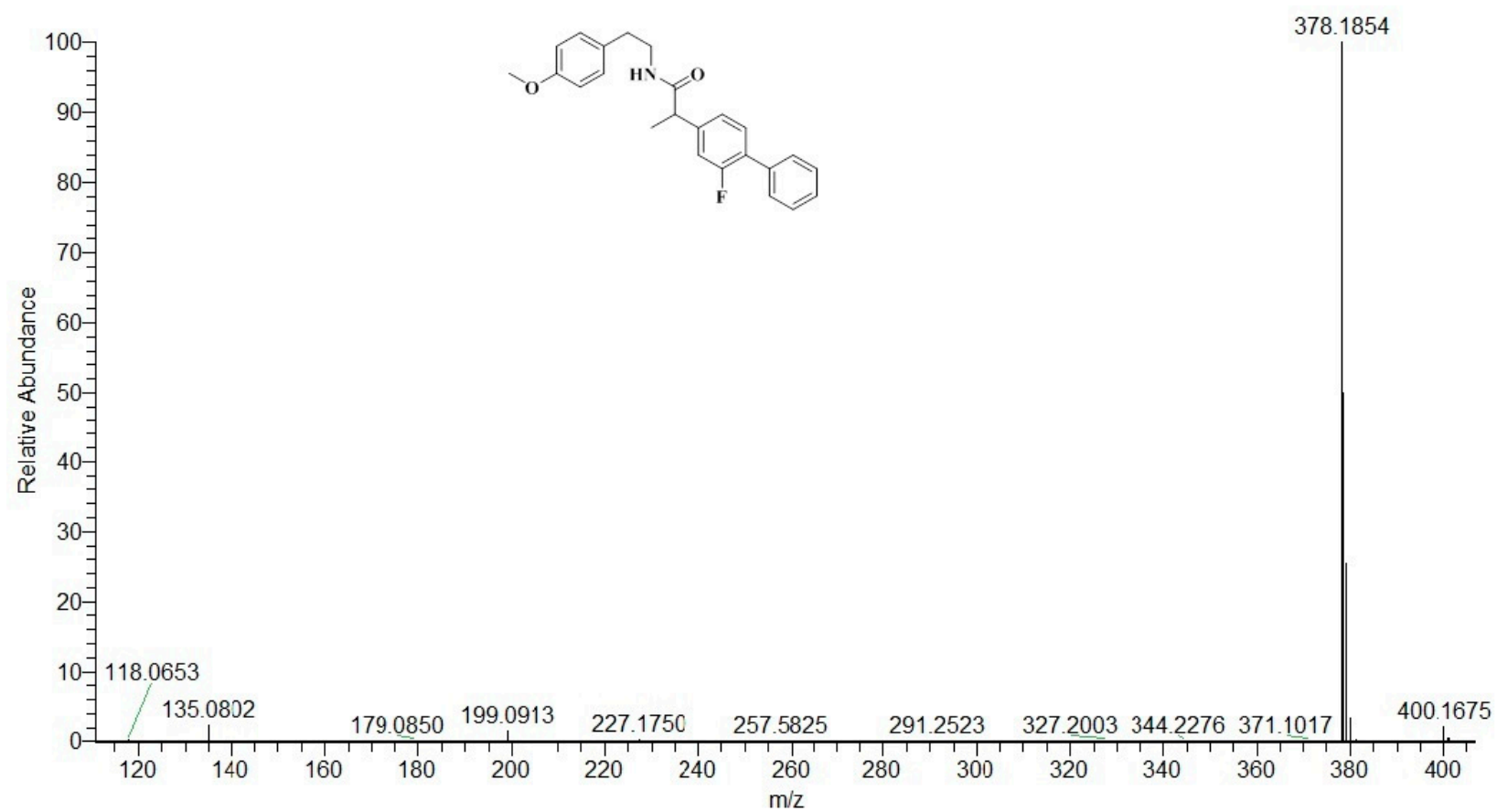


Figure S22. ESI-HRMS of compound **4c**.

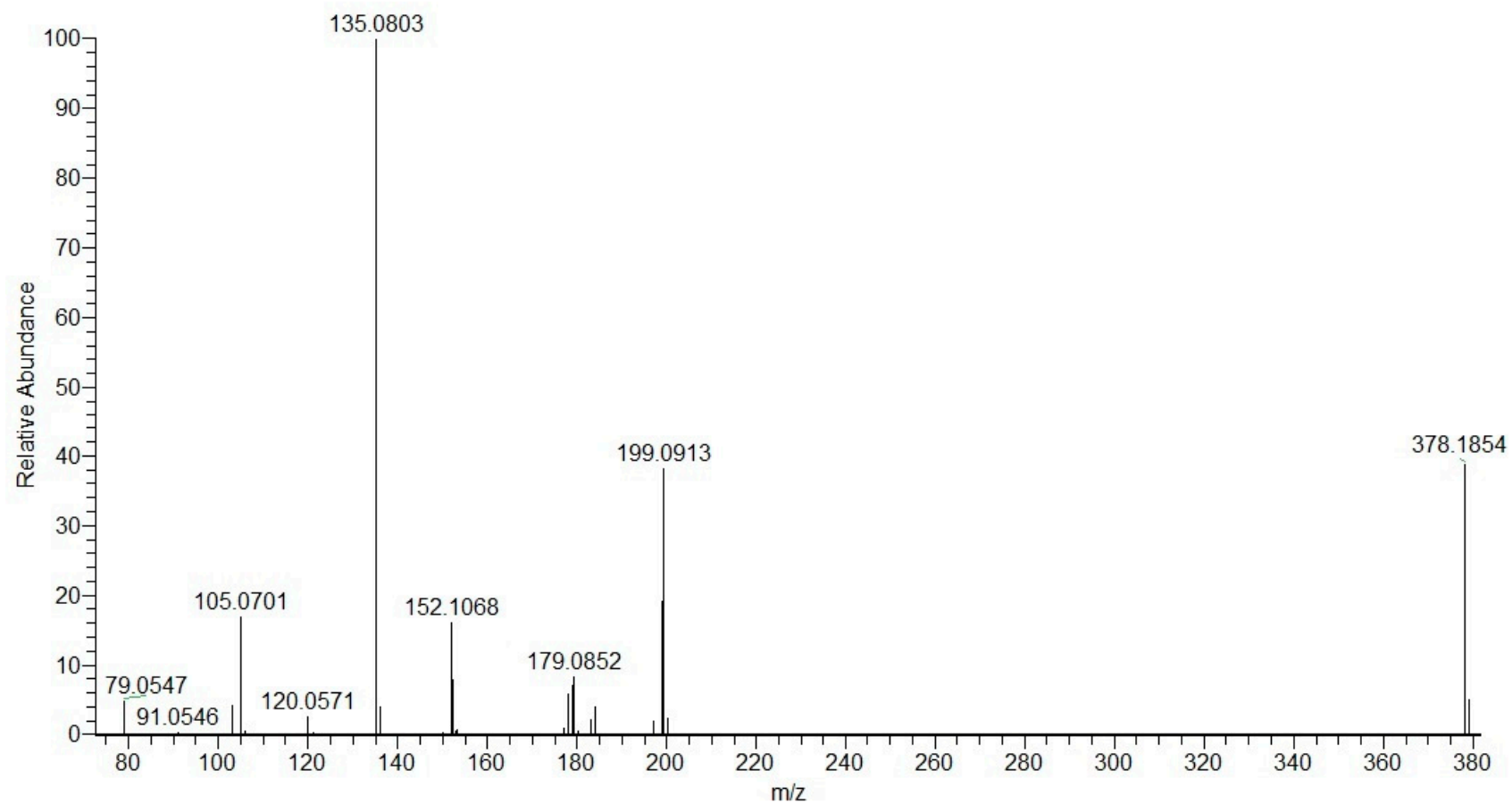


Figure S23. Mass spectrum of **4c** obtained by positive ion ESI-MS/MS.

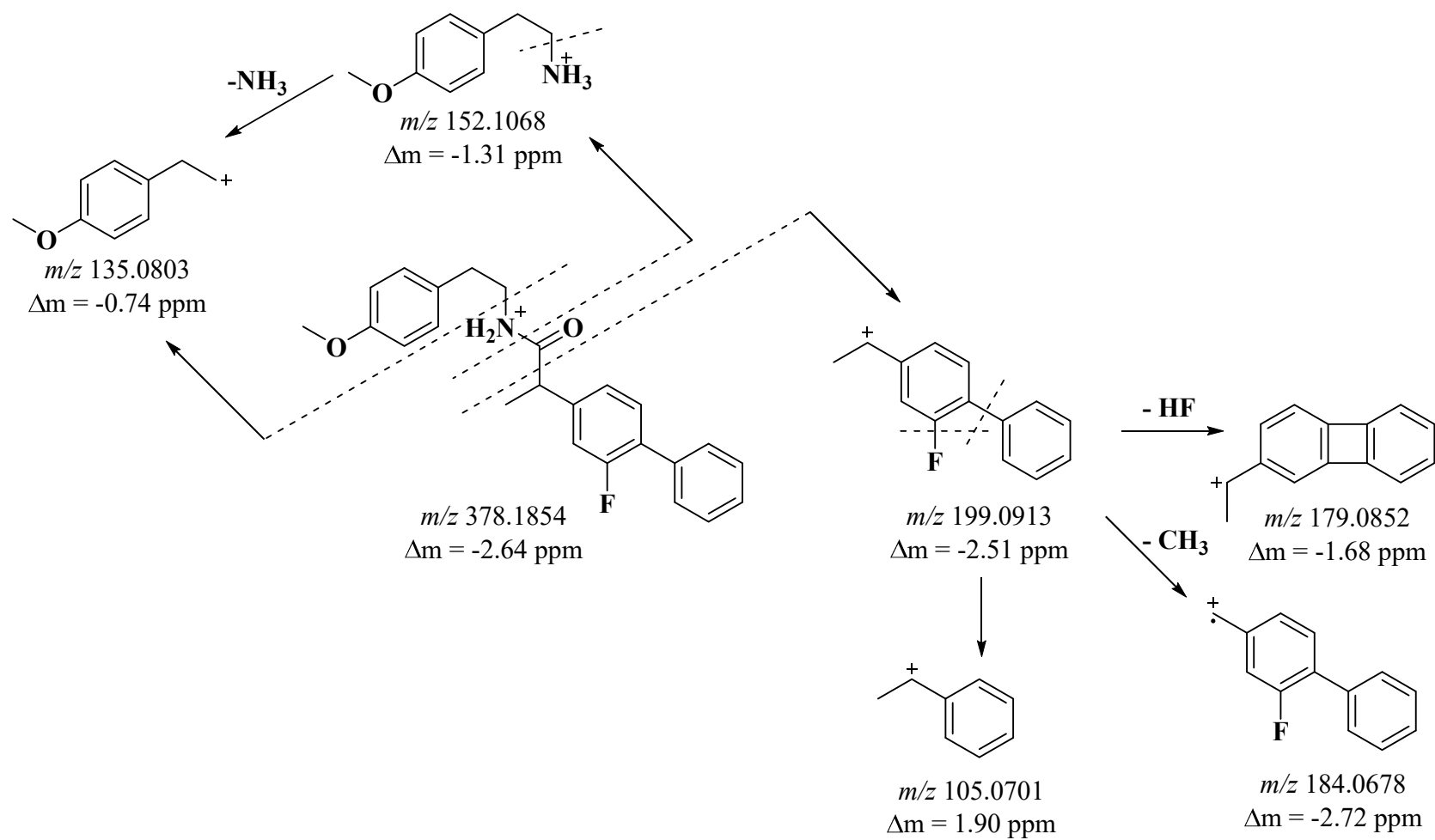


Figure S24. Proposed fragmentation of protonated **4c**.

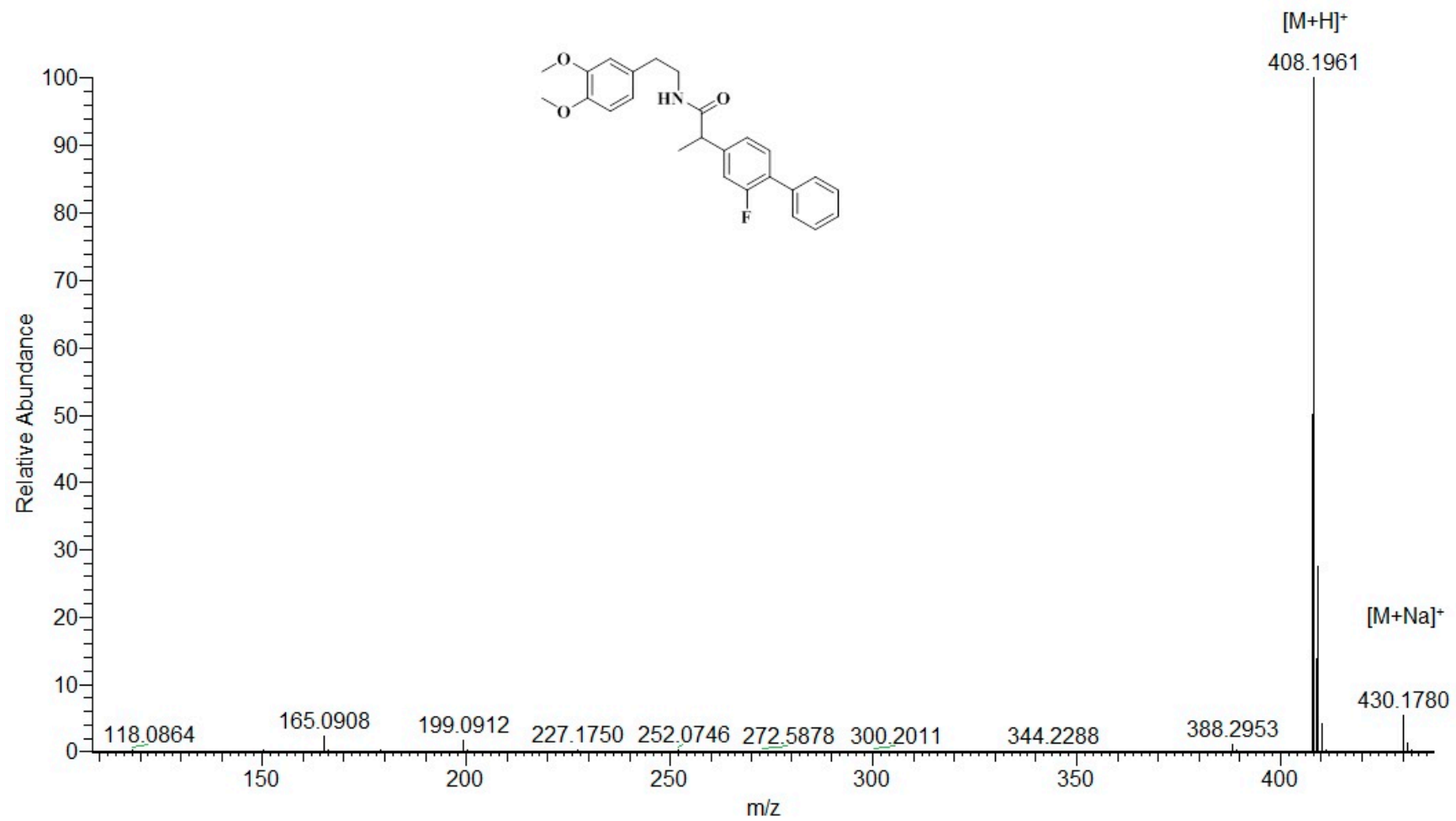


Figure S25. ESI-HRMS of compound **4d**.

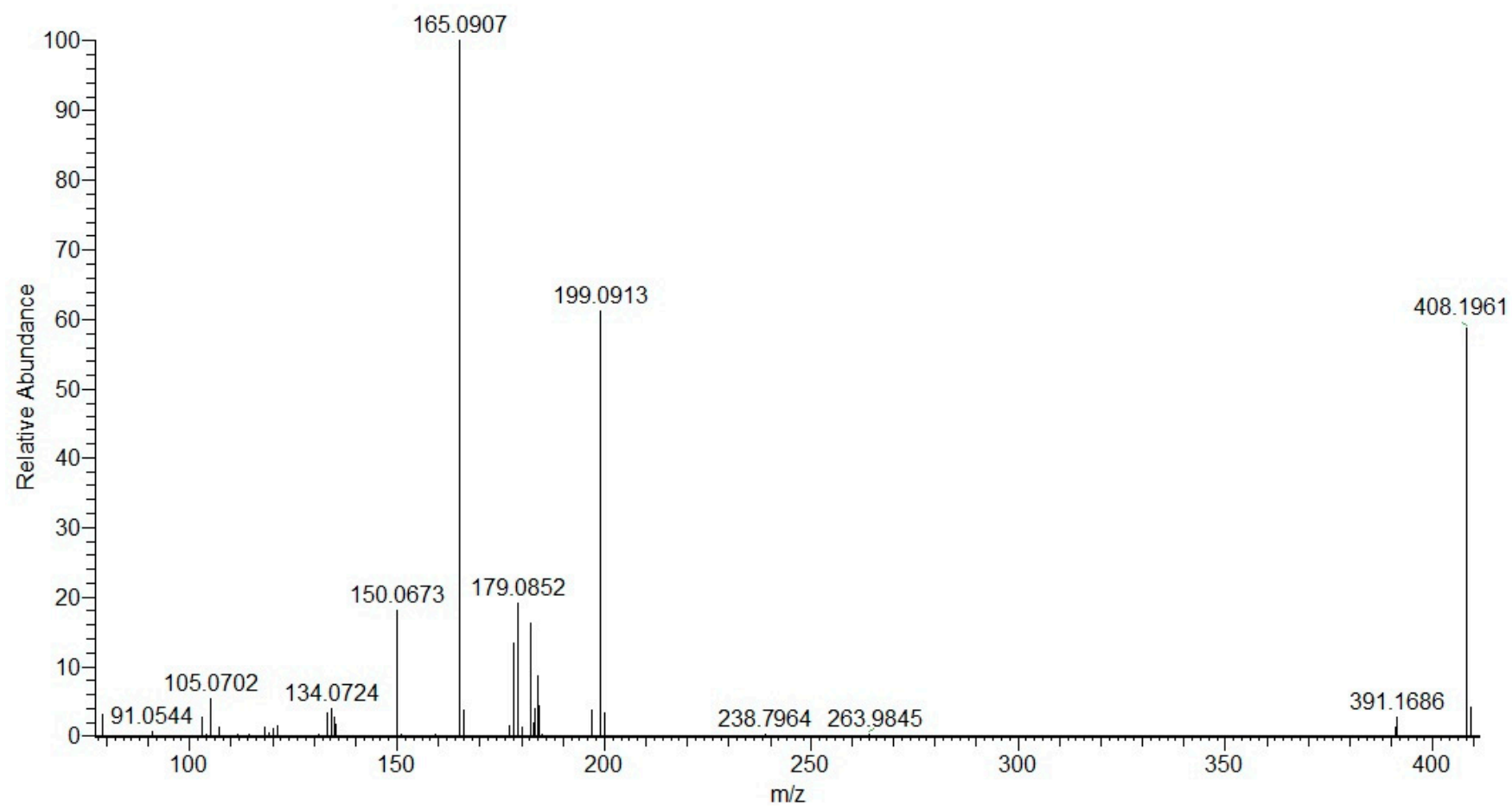


Figure S26. Mass spectrum of **4d** obtained by positive ion ESI-MS/MS.

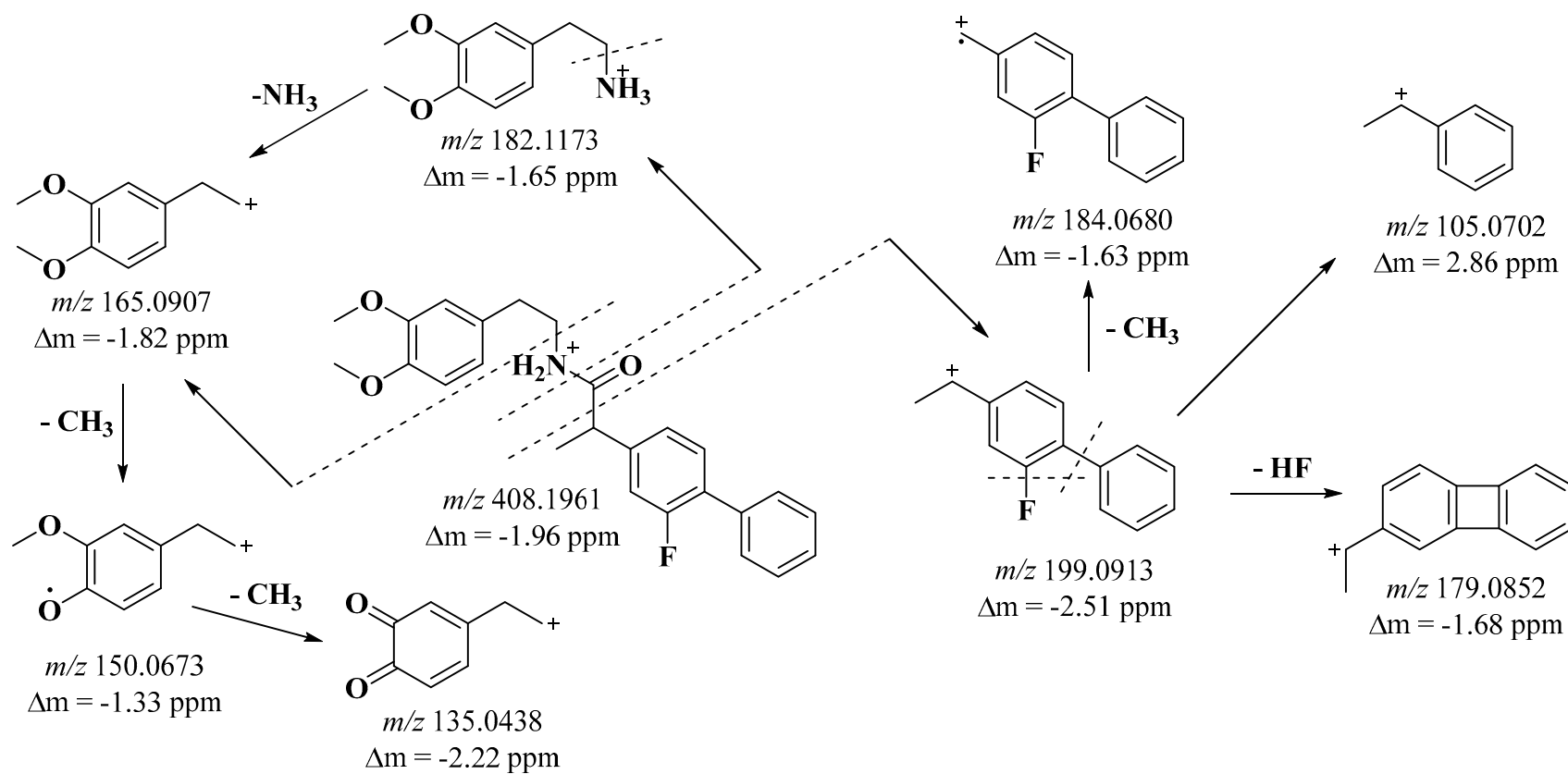


Figure S27. Proposed fragmentation of protonated **4d**.

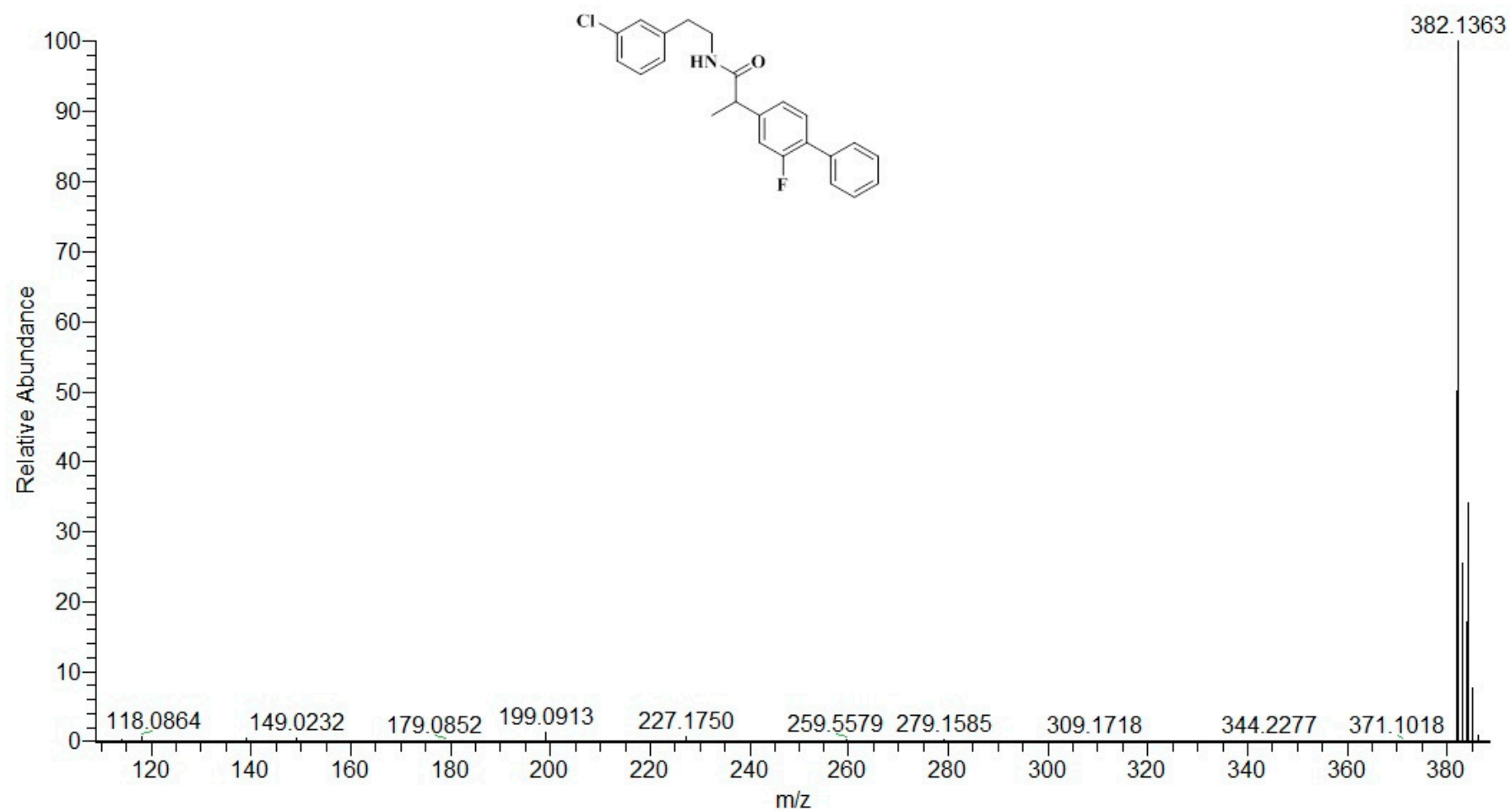


Figure S28. ESI-HRMS of compound **4e**.

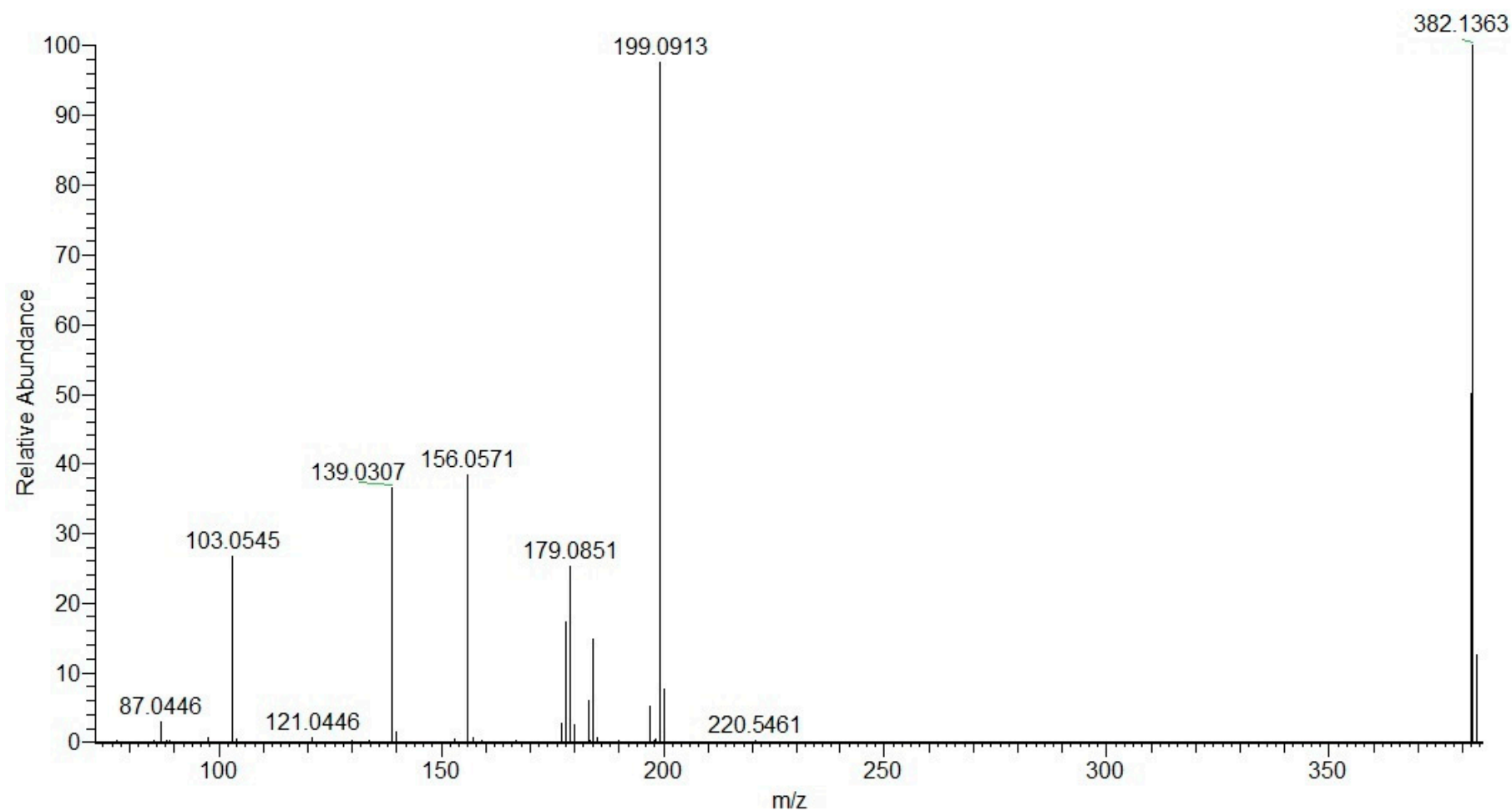


Figure S29. Mass spectrum of **4e** obtained by positive ion ESI-MS/MS.

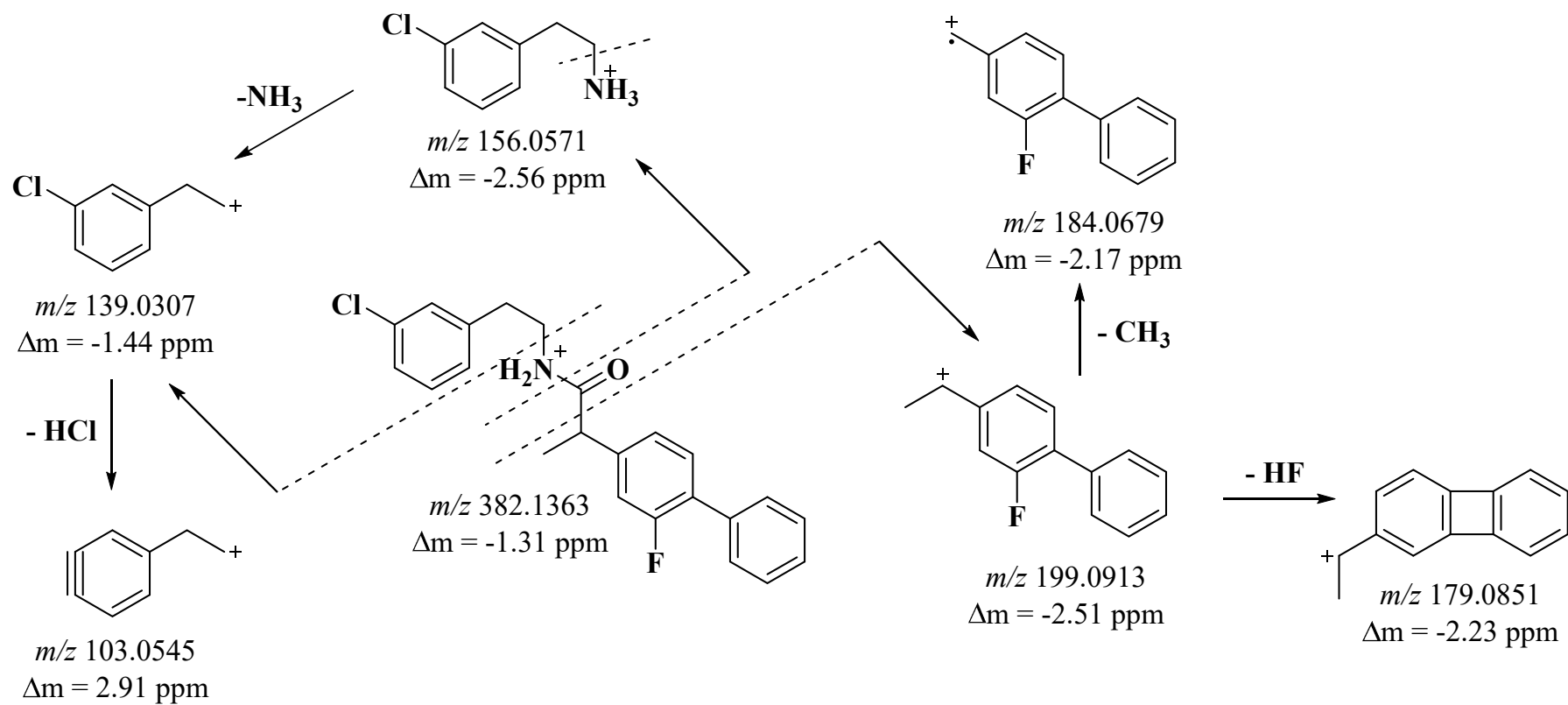


Figure S30. Proposed fragmentation of protonated **4e**.