

Supplementary Materials: Design, Synthesis, DFT Study and Antifungal Activity of Pyrazolecarboxamide Derivatives

Jin-Xia Mu, Yan-Xia Shi, Ming-Yan Yang, Zhao-Hui Sun, Xing-Hai Liu, Bao-Ju Li and Na-Bo Sun

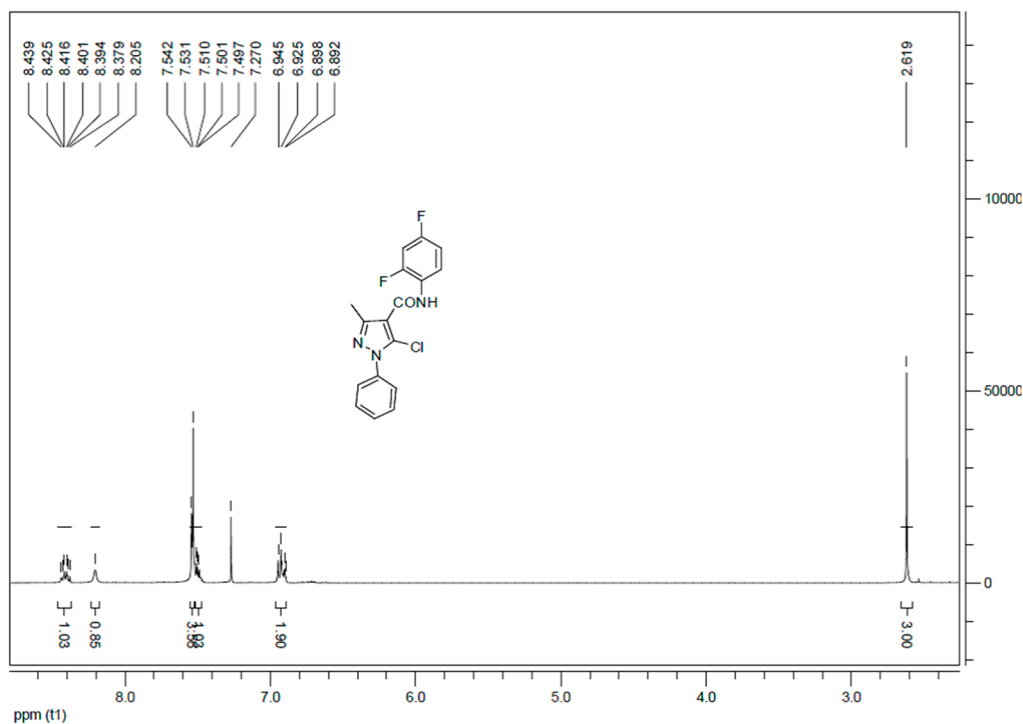


Figure S1. ¹H-NMR spectrum of compound 5a.

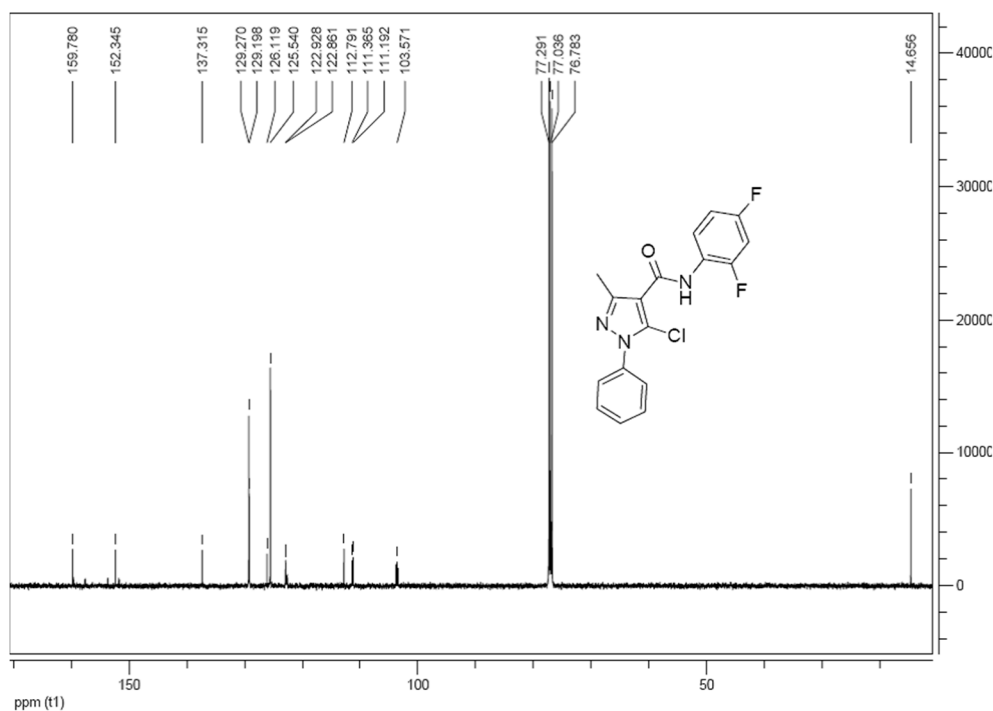
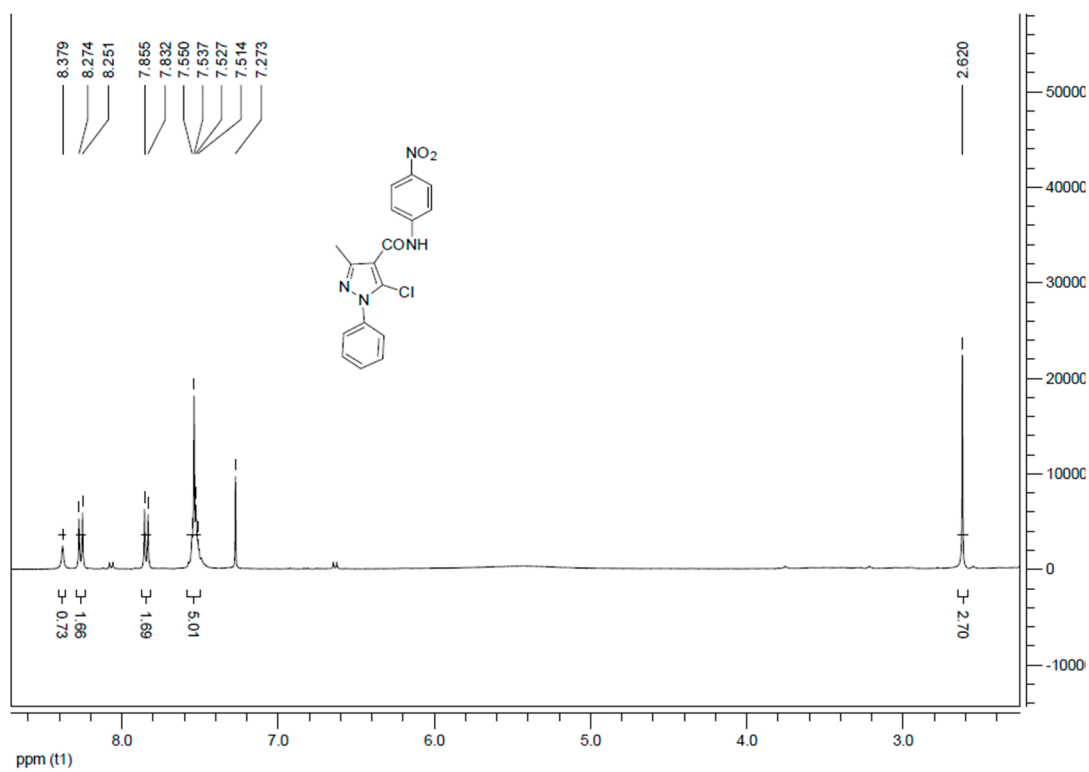
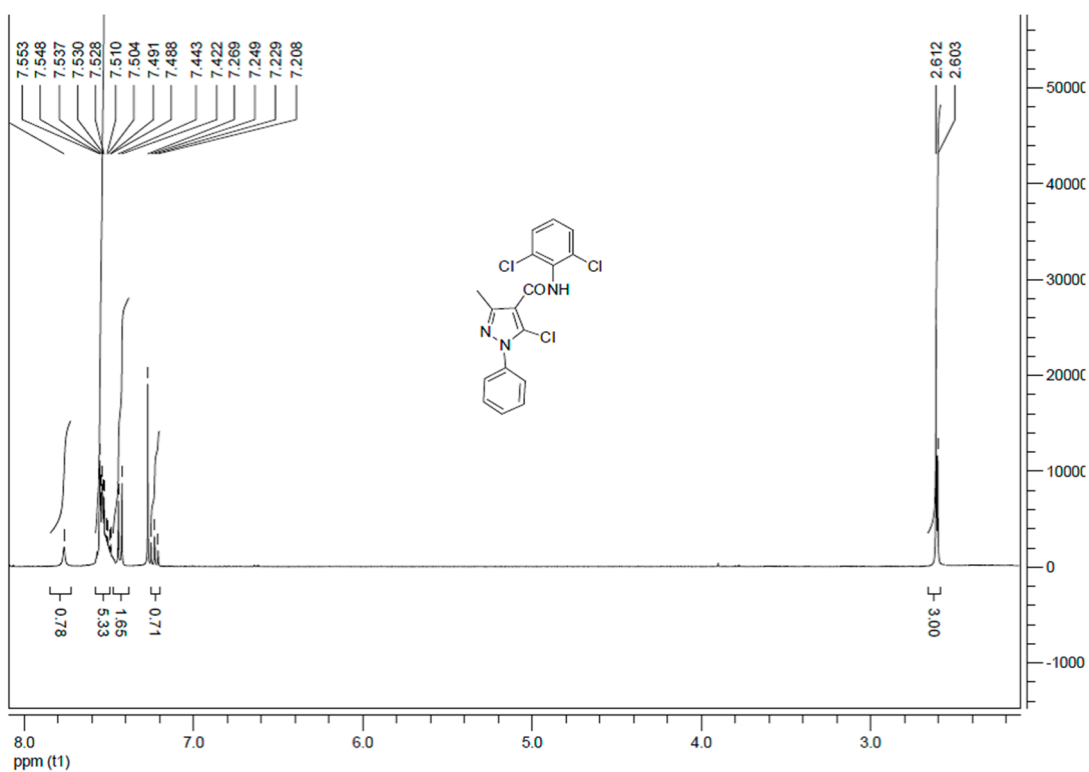
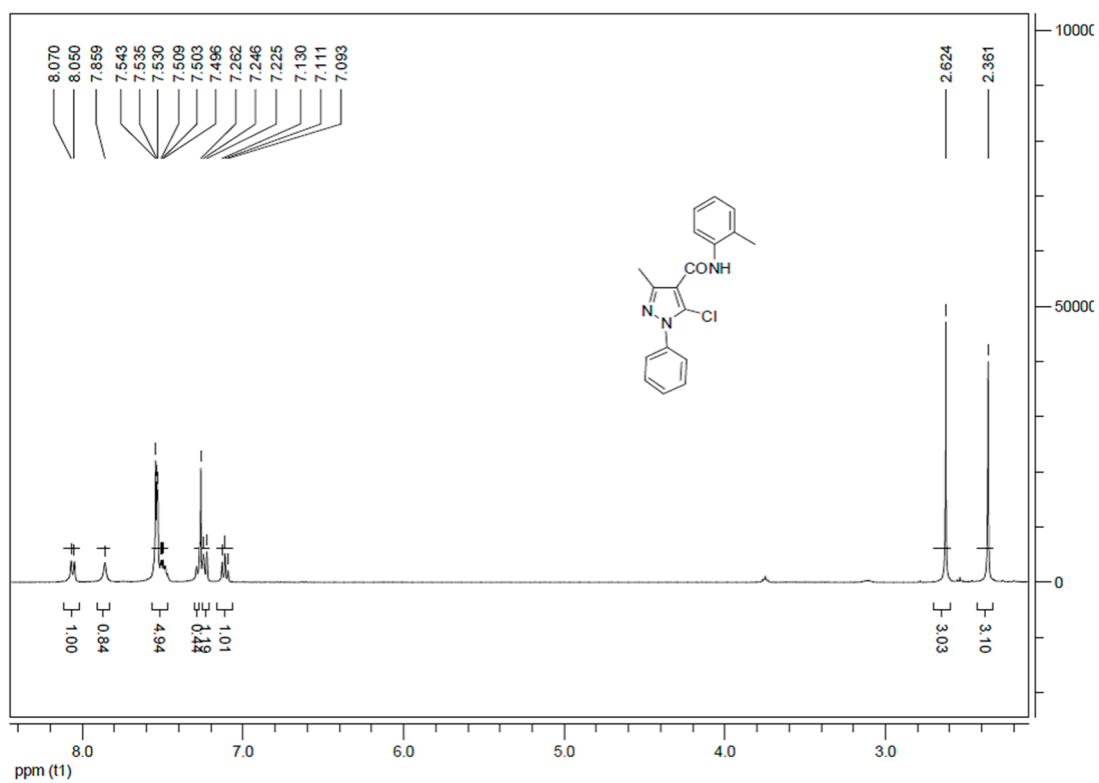
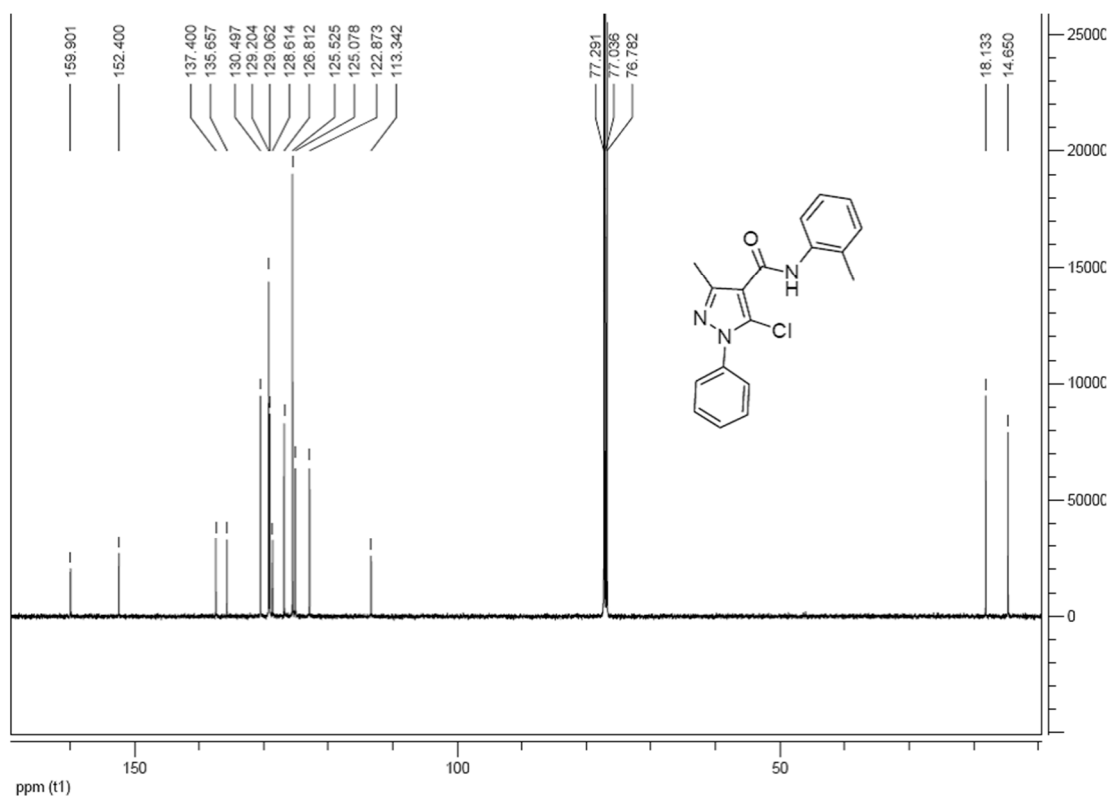
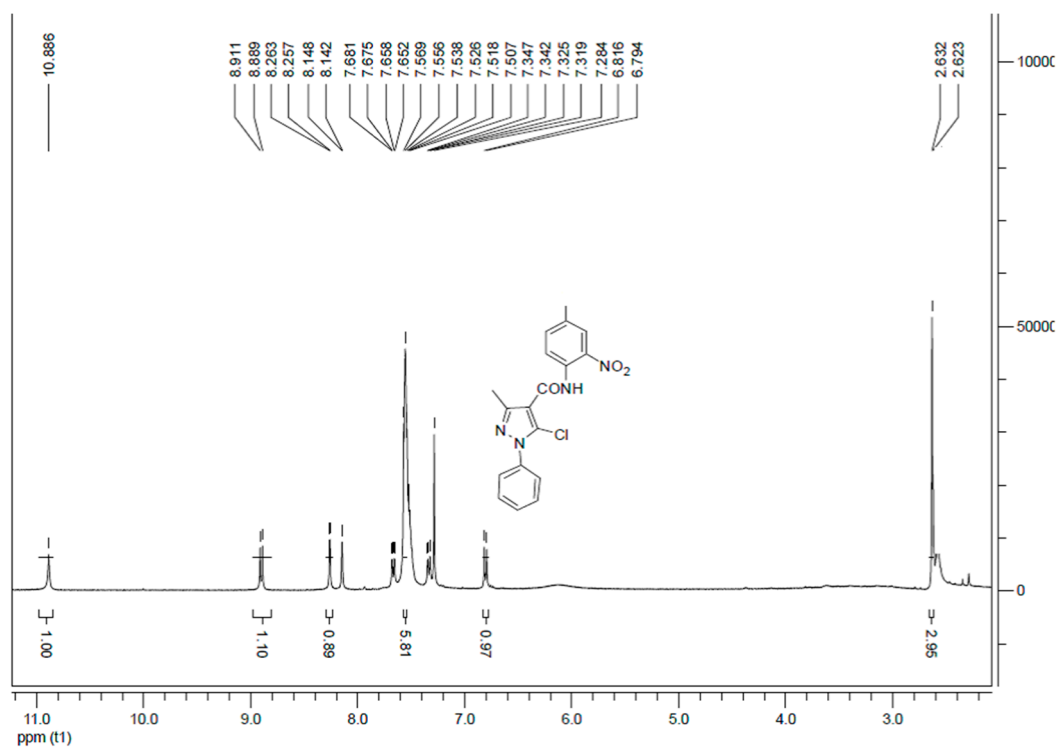
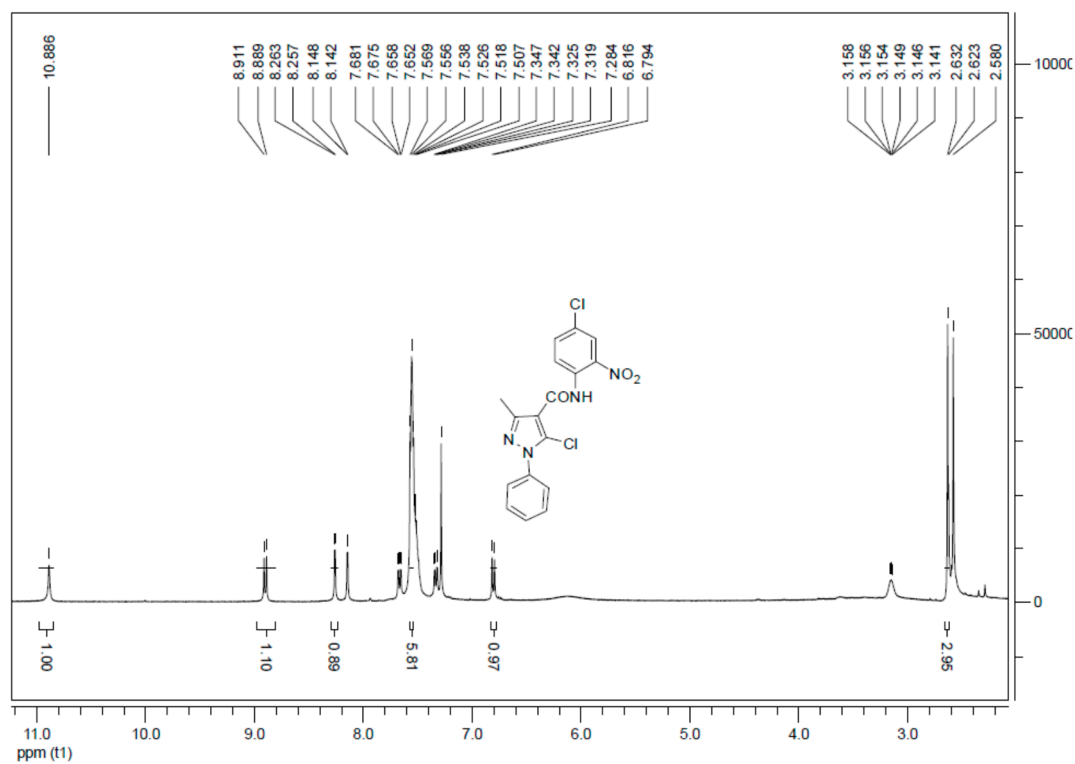
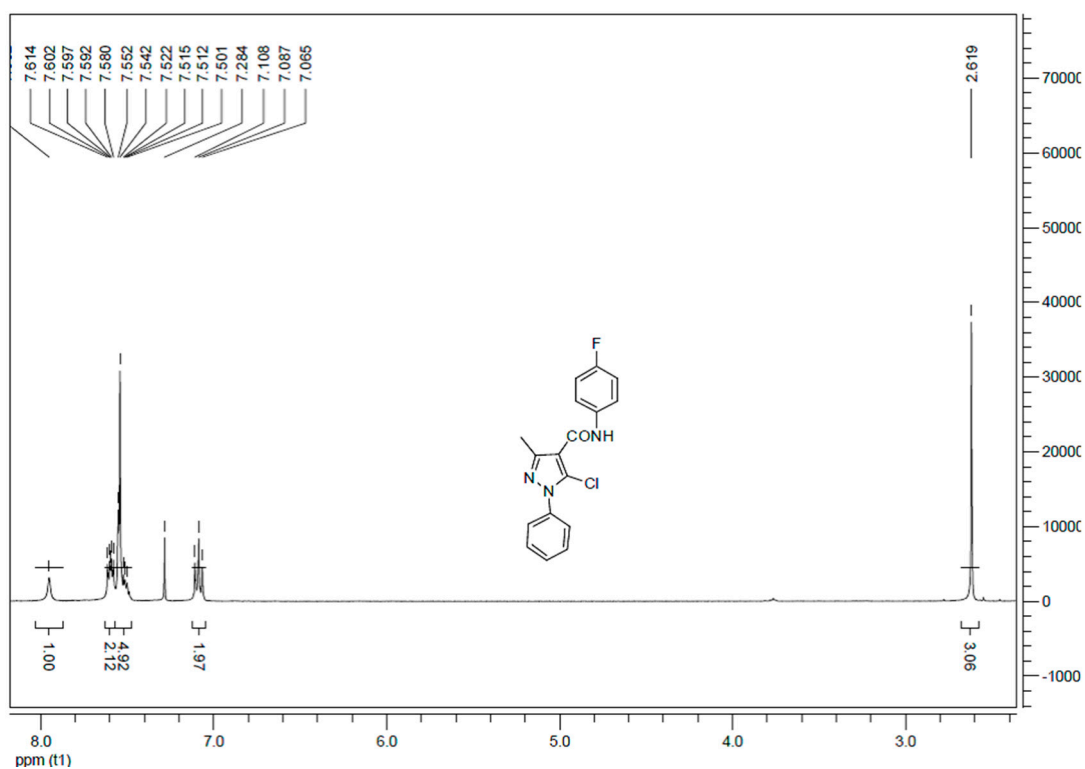
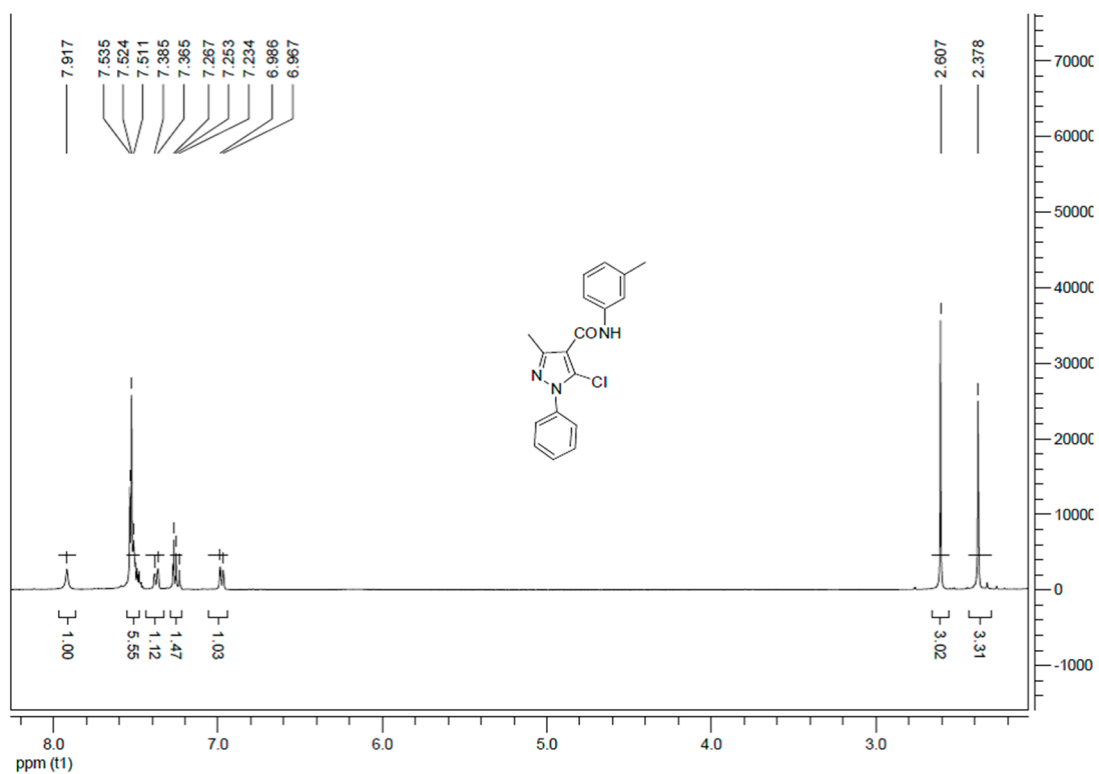


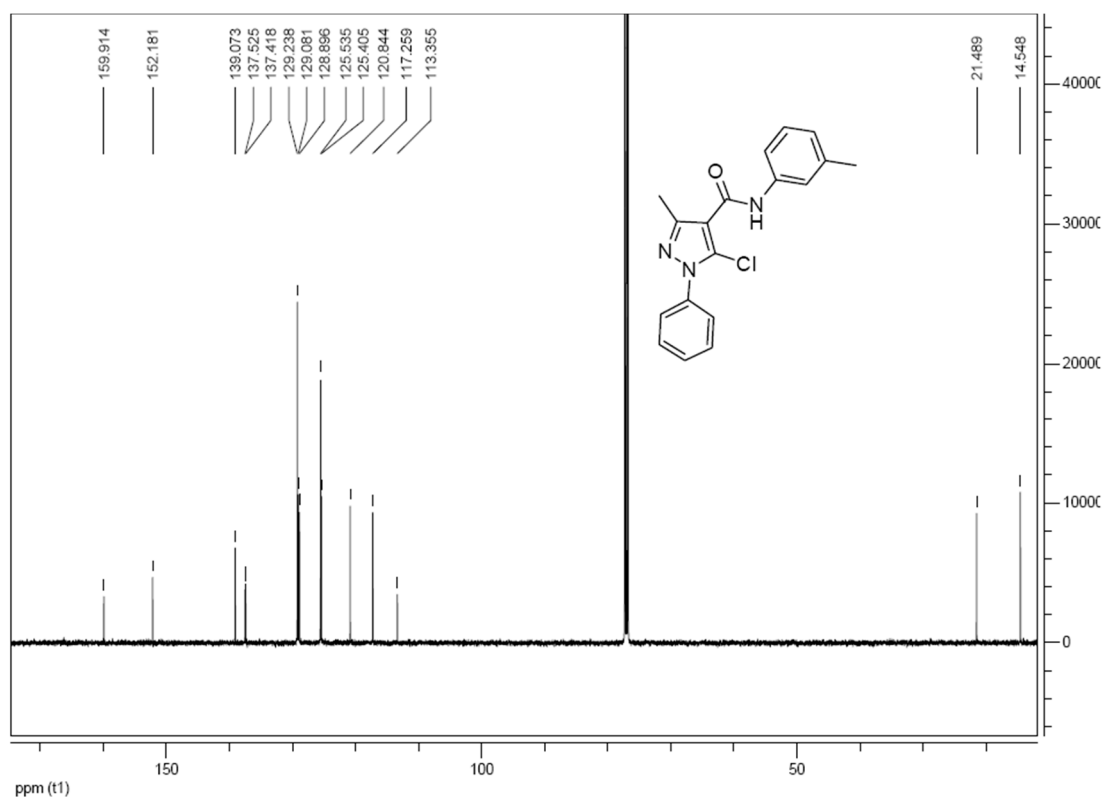
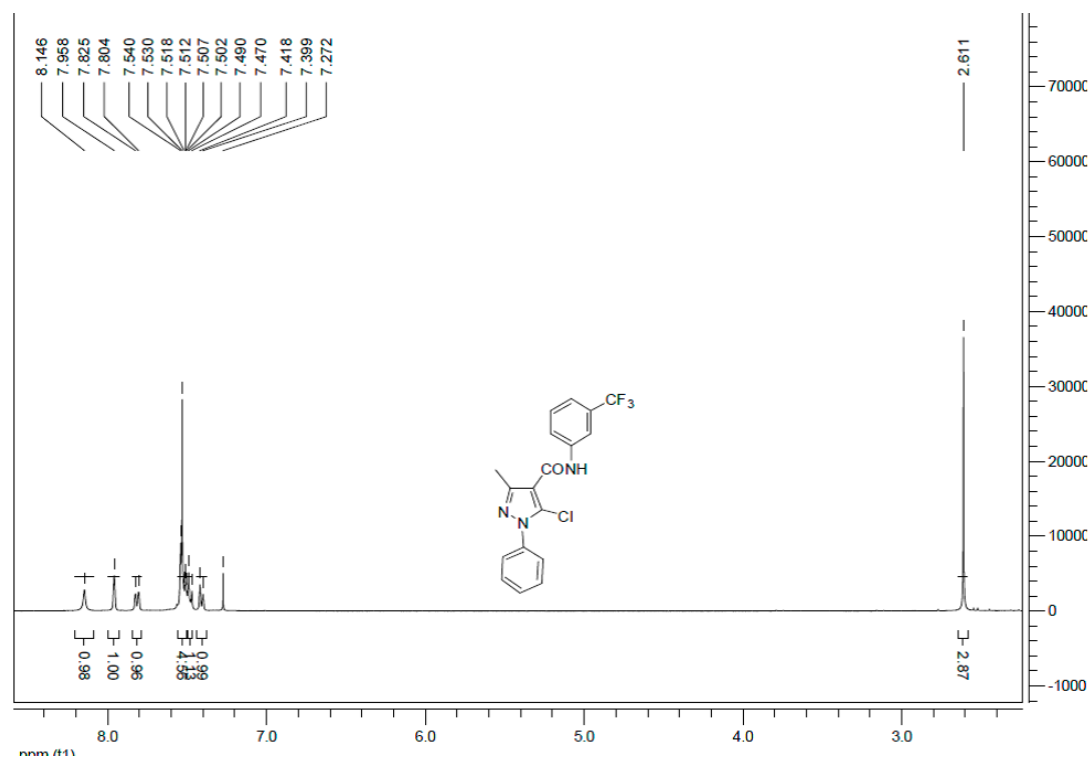
Figure S2. ¹³C-NMR spectrum of compound 5a.

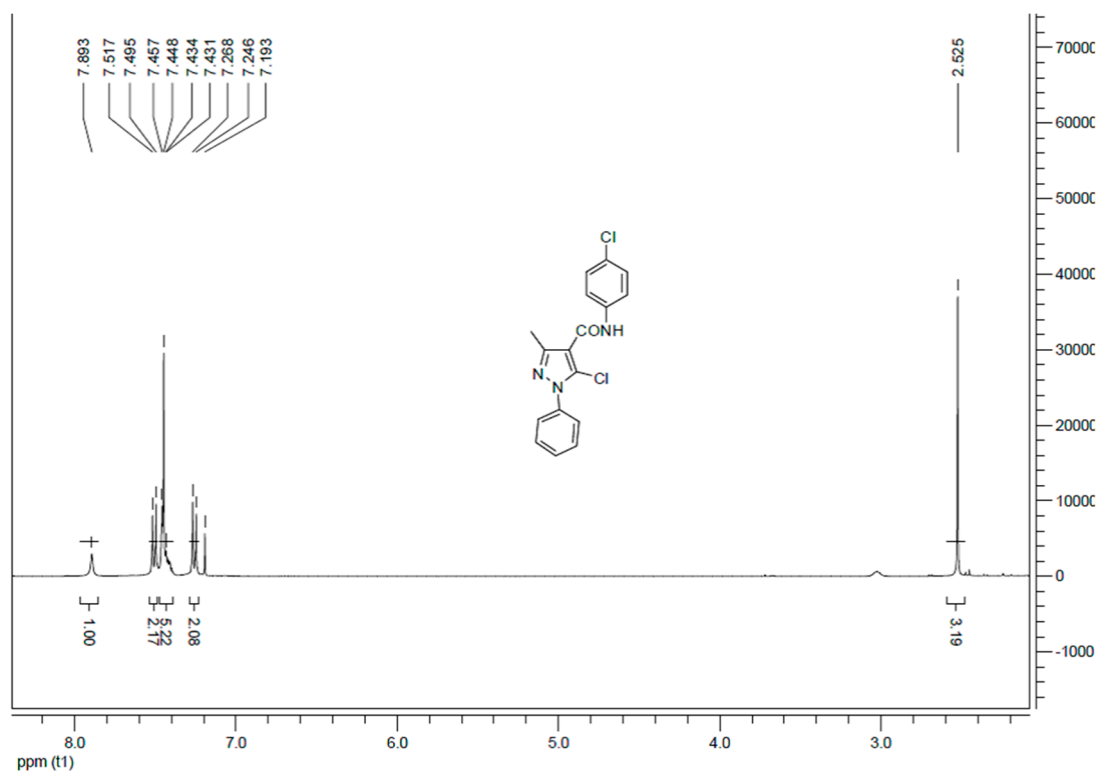
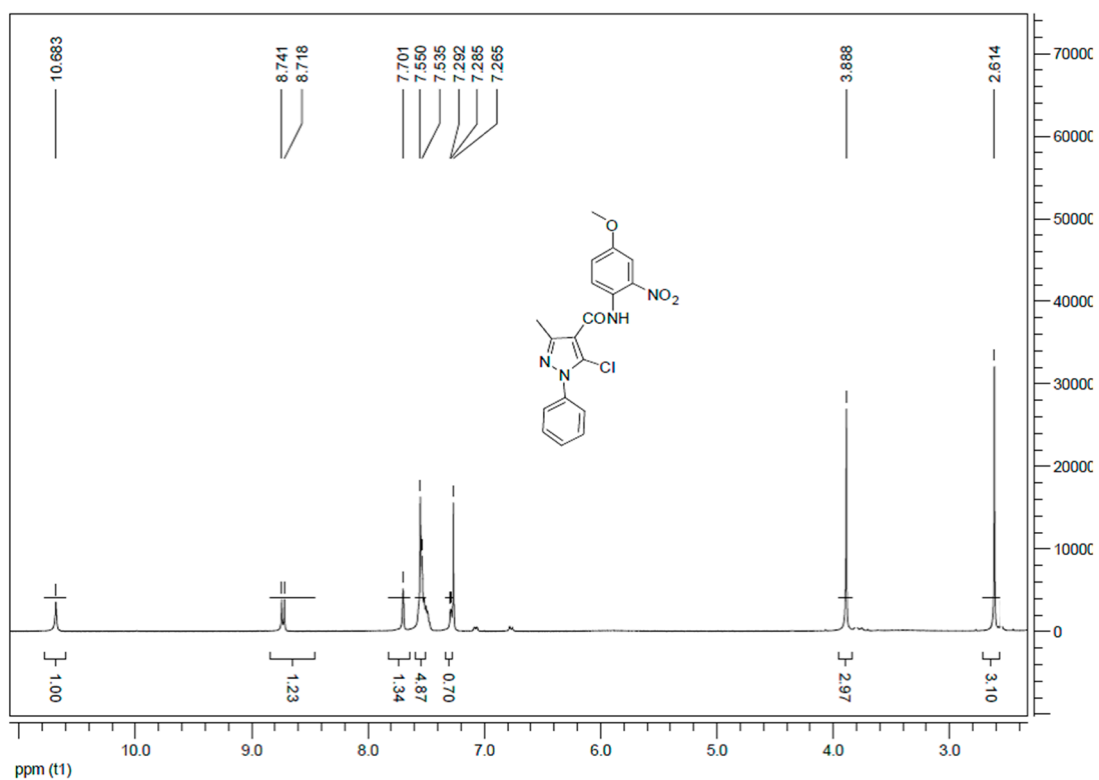
Figure S3. ¹H-NMR spectrum of compound 5b.Figure S4. ¹H-NMR spectrum of compound 5c.

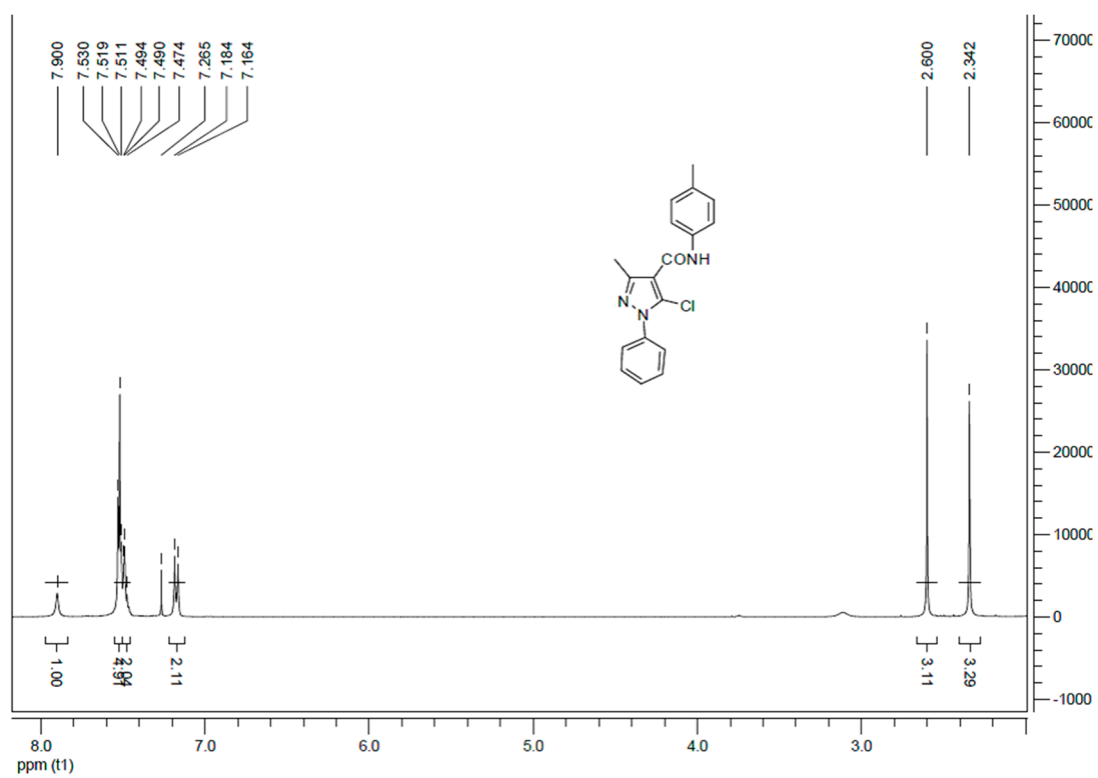
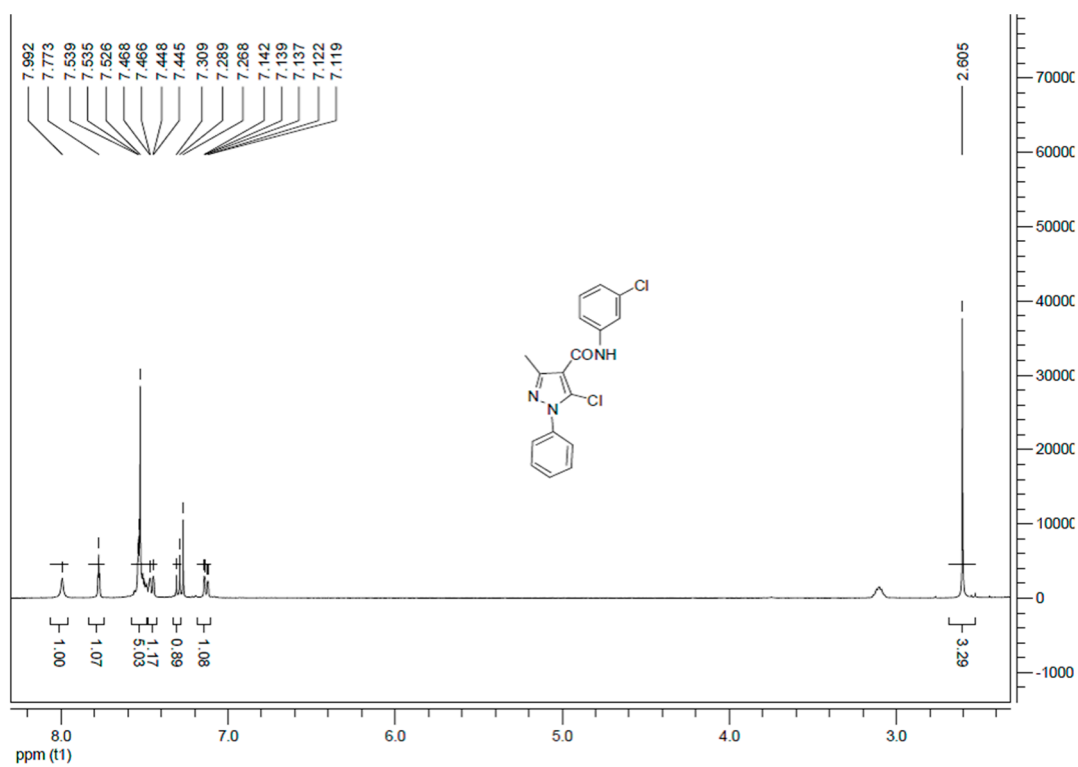
Figure S5. ¹H-NMR spectrum of compound 5d.Figure S6. ¹³C-NMR spectrum of compound 5d.

Figure S7. ¹H-NMR spectrum of compound 5e.Figure S8. ¹H-NMR spectrum of compound 5f.

Figure S9. ¹H-NMR spectrum of compound 5g.Figure S10. ¹H-NMR spectrum of compound 5h.

Figure S11. ¹³C-NMR spectrum of compound 5h.Figure S12. ¹H-NMR spectrum of compound 5i.

Figure S13. ¹H-NMR spectrum of compound 5j.Figure S14. ¹H-NMR spectrum of compound 5k.

Figure S15. ¹H-NMR spectrum of compound 5l.Figure S16. ¹H-NMR spectrum of compound 5m.

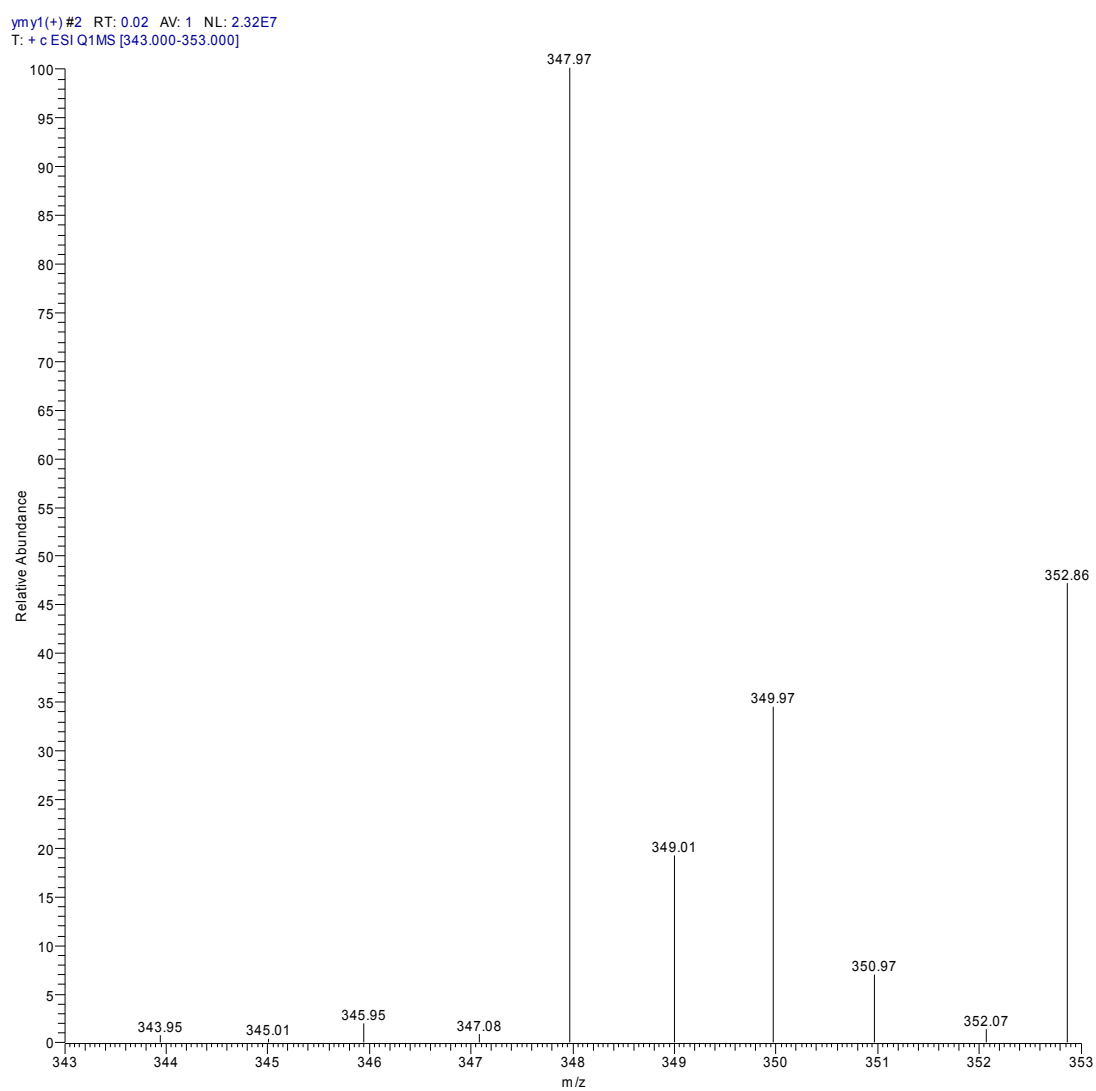


Figure S17. MS spectrum of compound 5a (+).

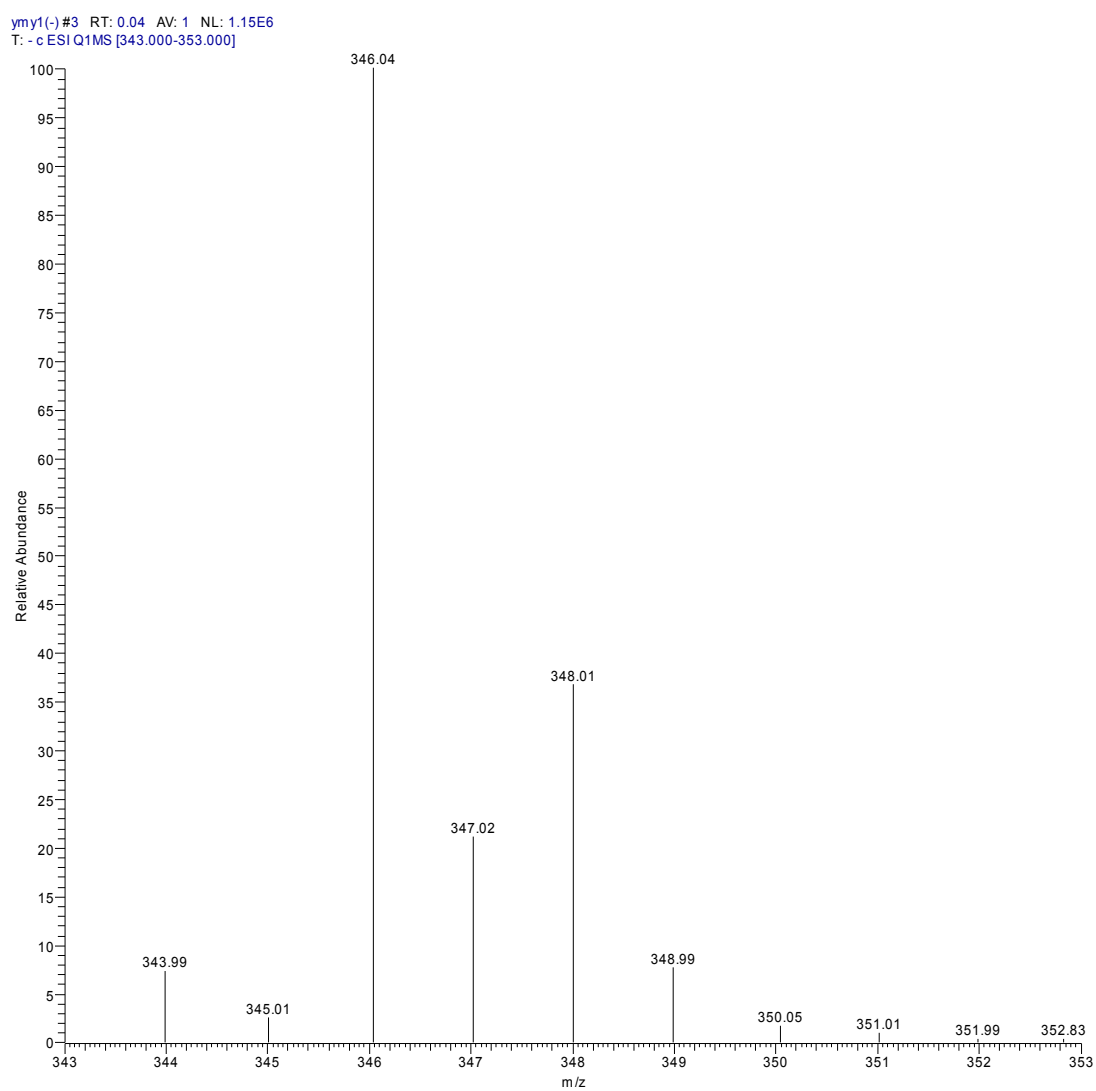


Figure S18. MS spectrum of compound 5a (-).

ymy2(+)#3 RT: 0.04 AV: 1 NL: 1.44E7
T: + c ESI Q1MS [350.000-360.000]

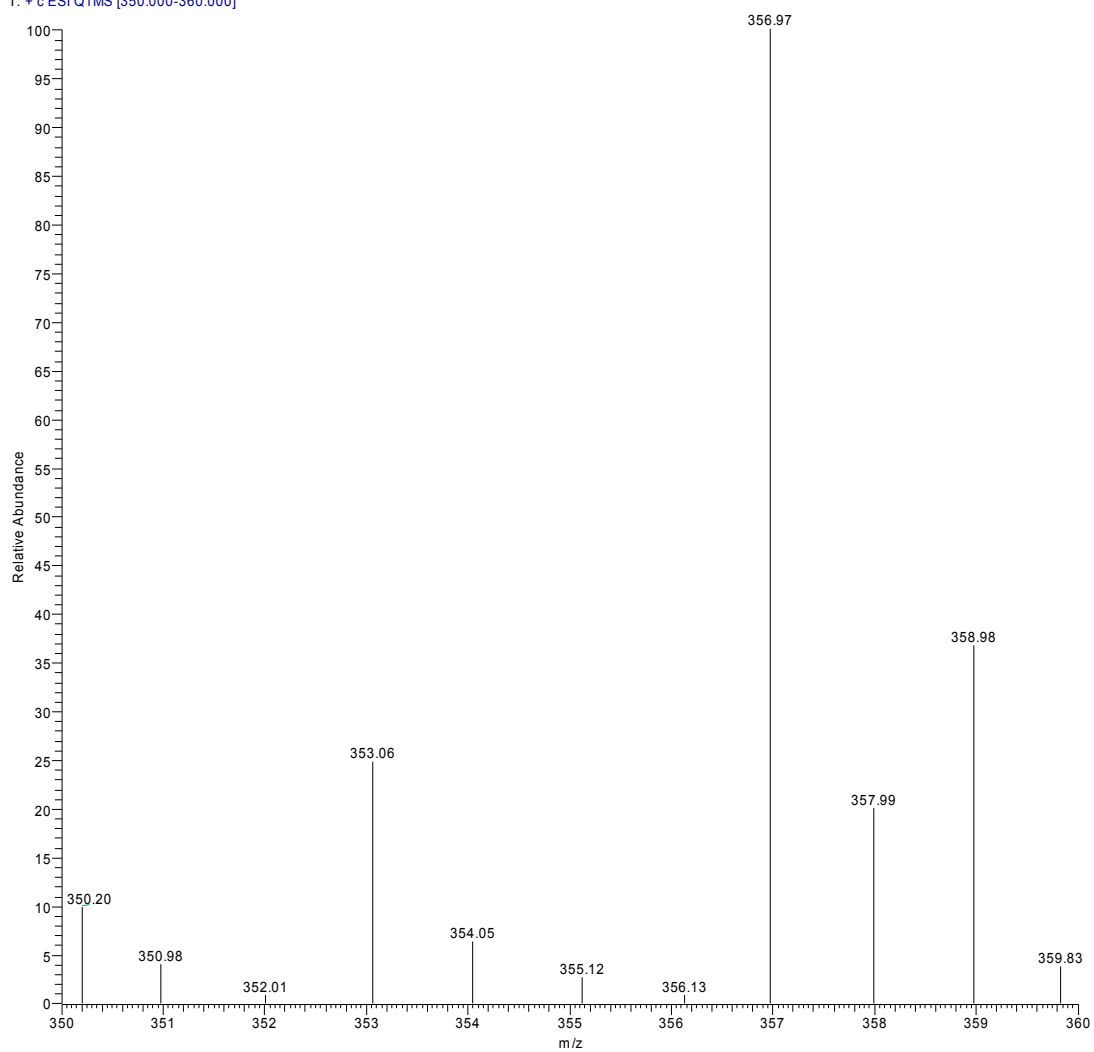


Figure S19. MS spectrum of compound 5b (+).

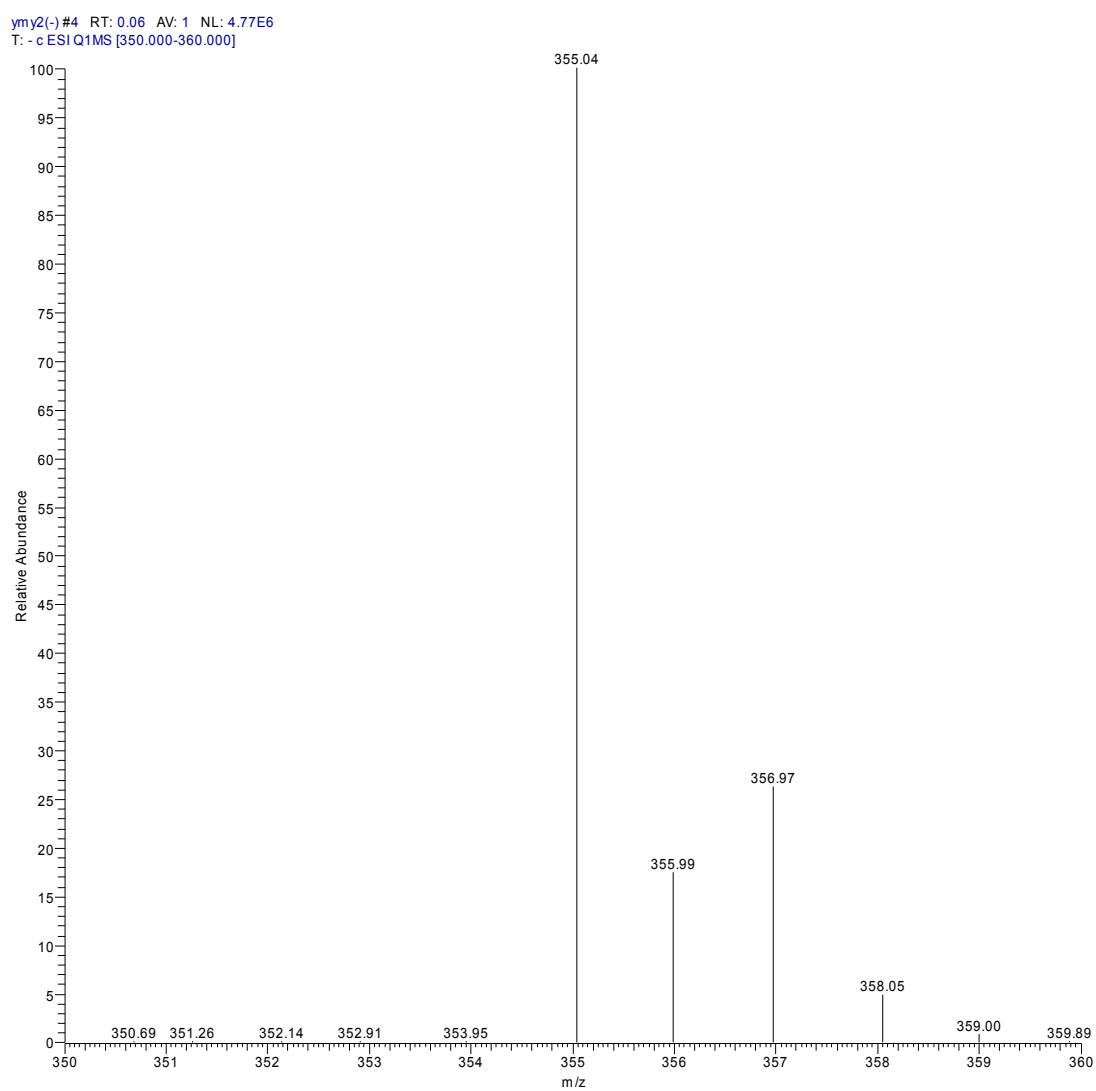


Figure S20. MS spectrum of compound **5b** (-).

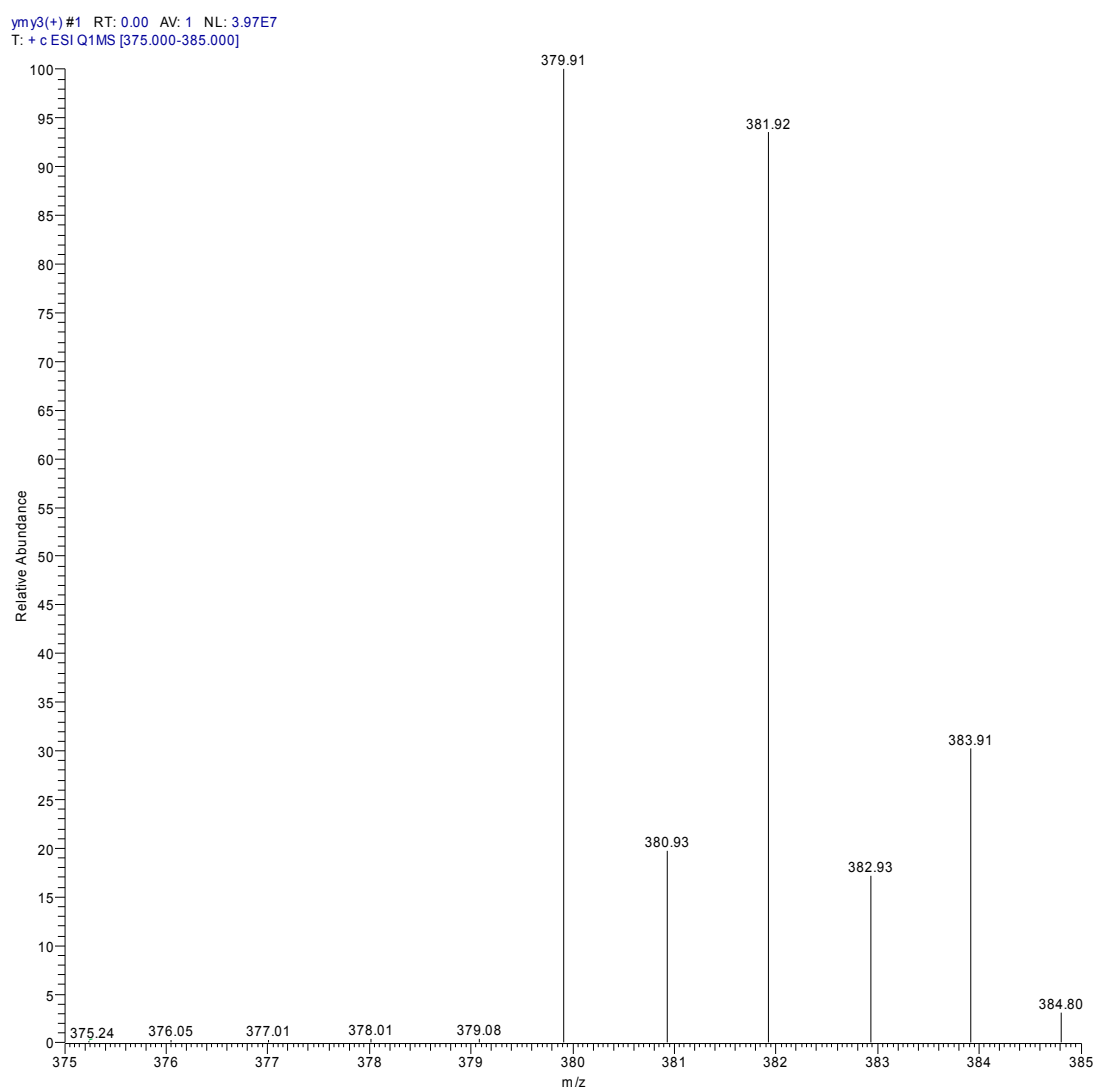


Figure S21. MS spectrum of compound 5c (+).

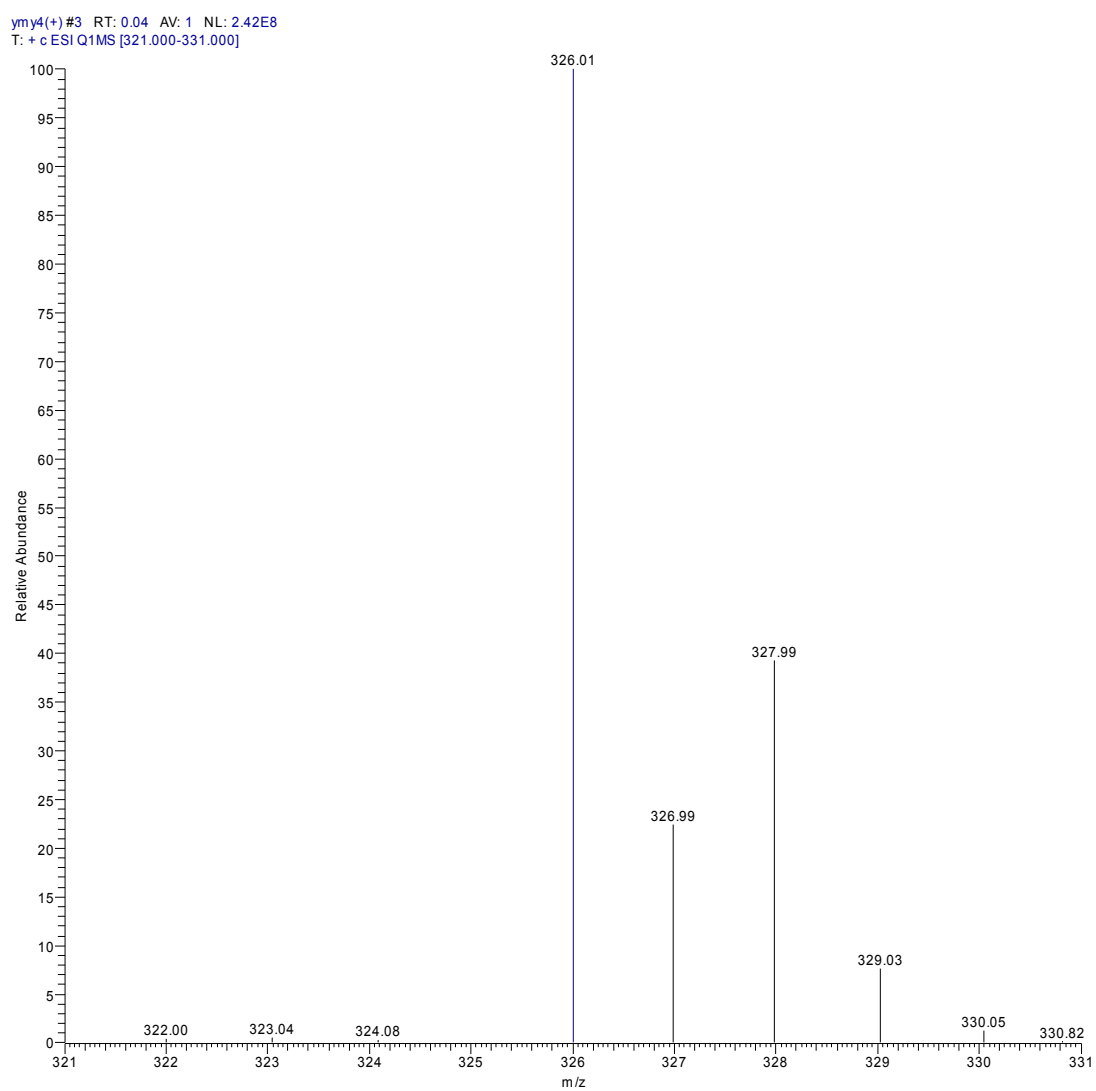


Figure S22. MS spectrum of compound 5d (+).

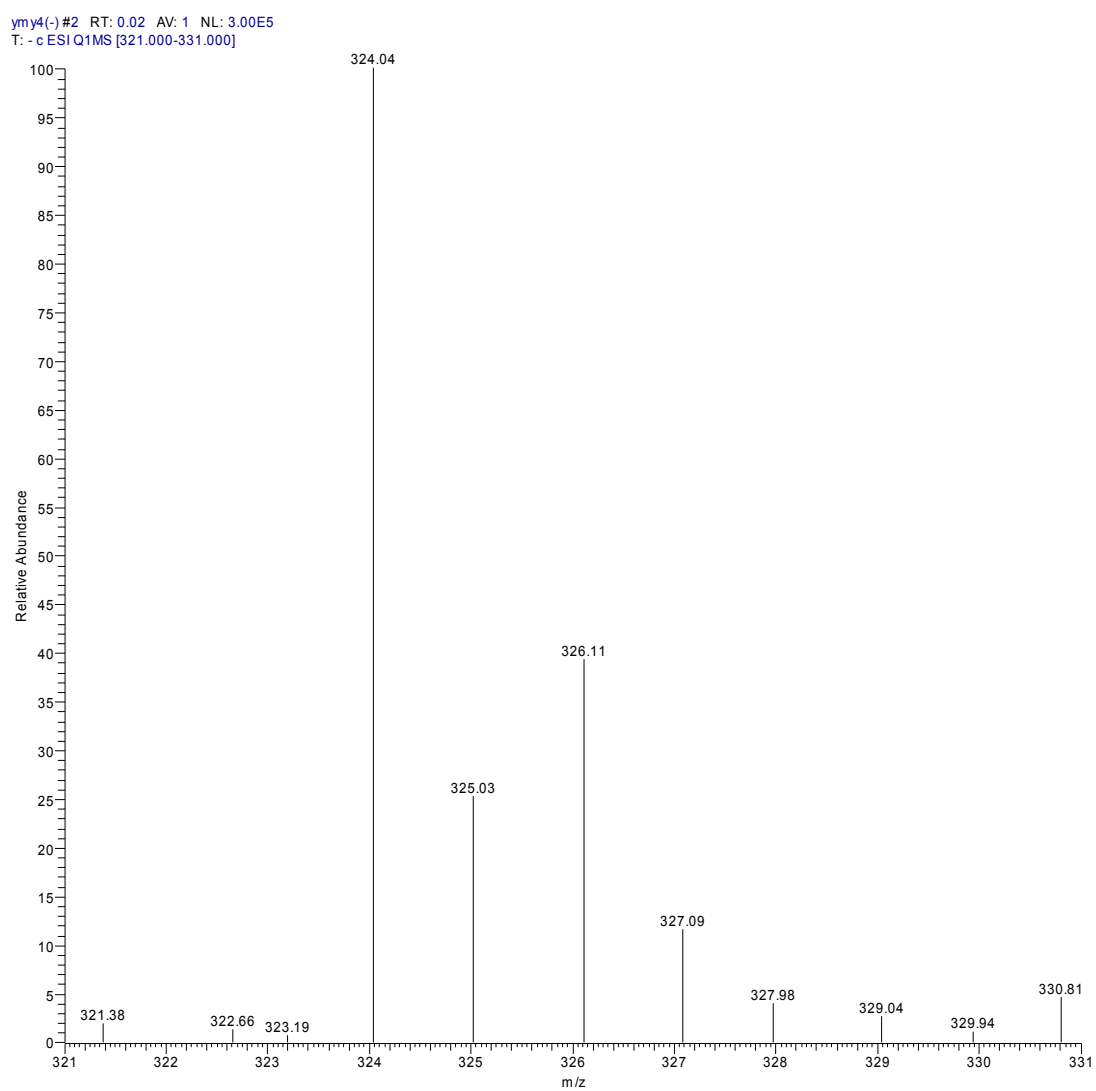


Figure S23. MS spectrum of compound 5d (-).

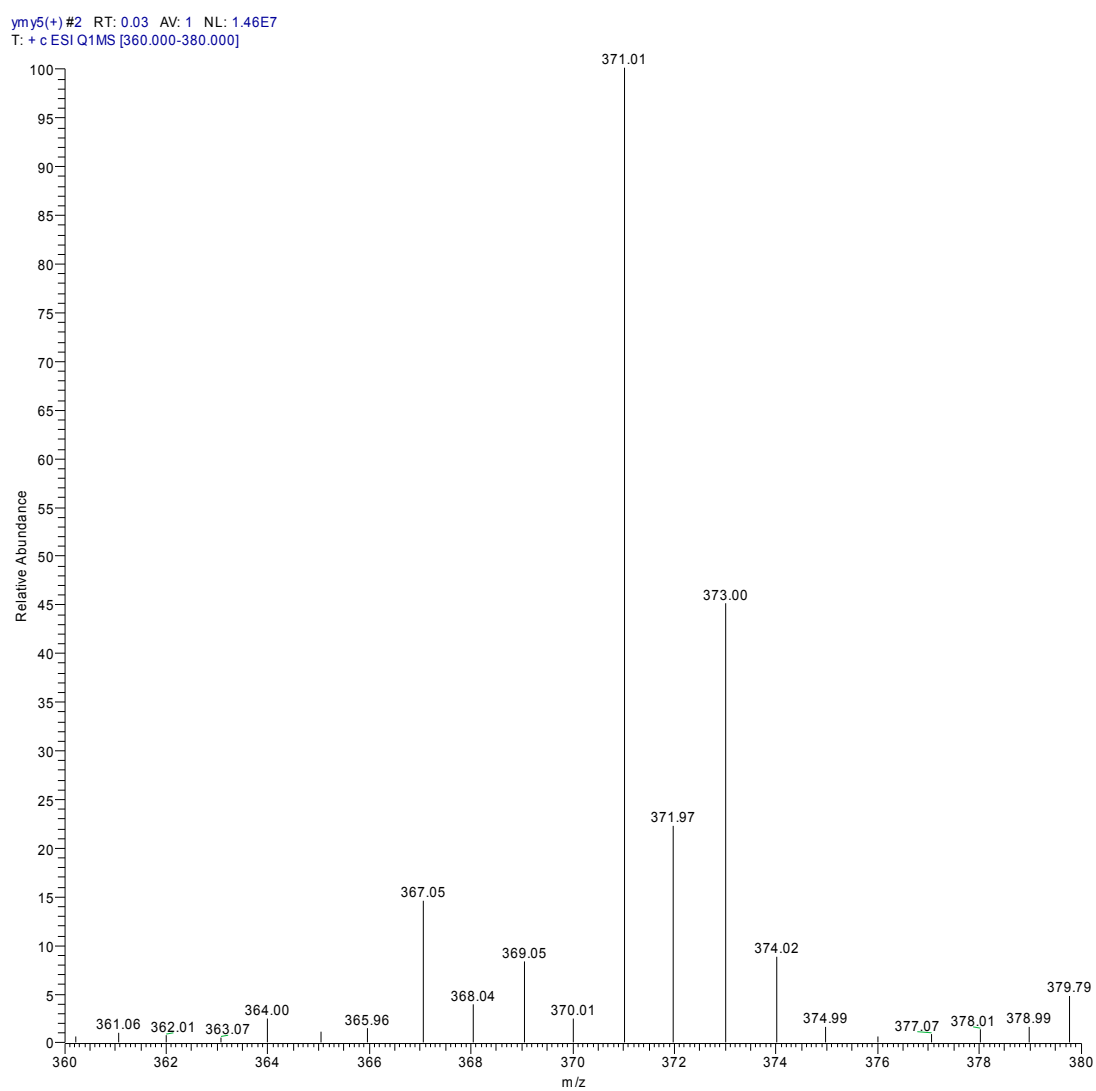


Figure S24. MS spectrum of compound 5e (+).

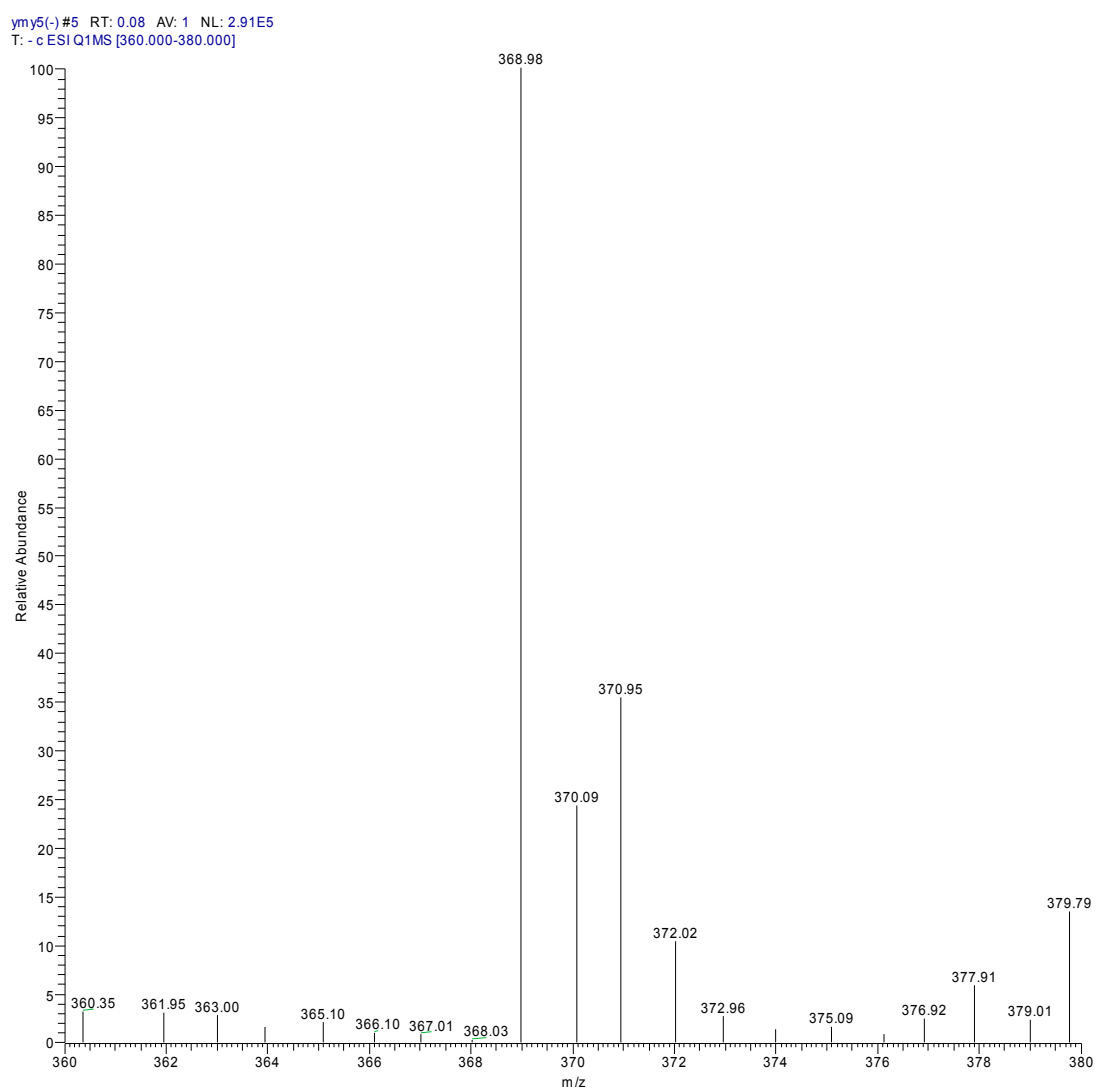


Figure S25. MS spectrum of compound 5e (-).

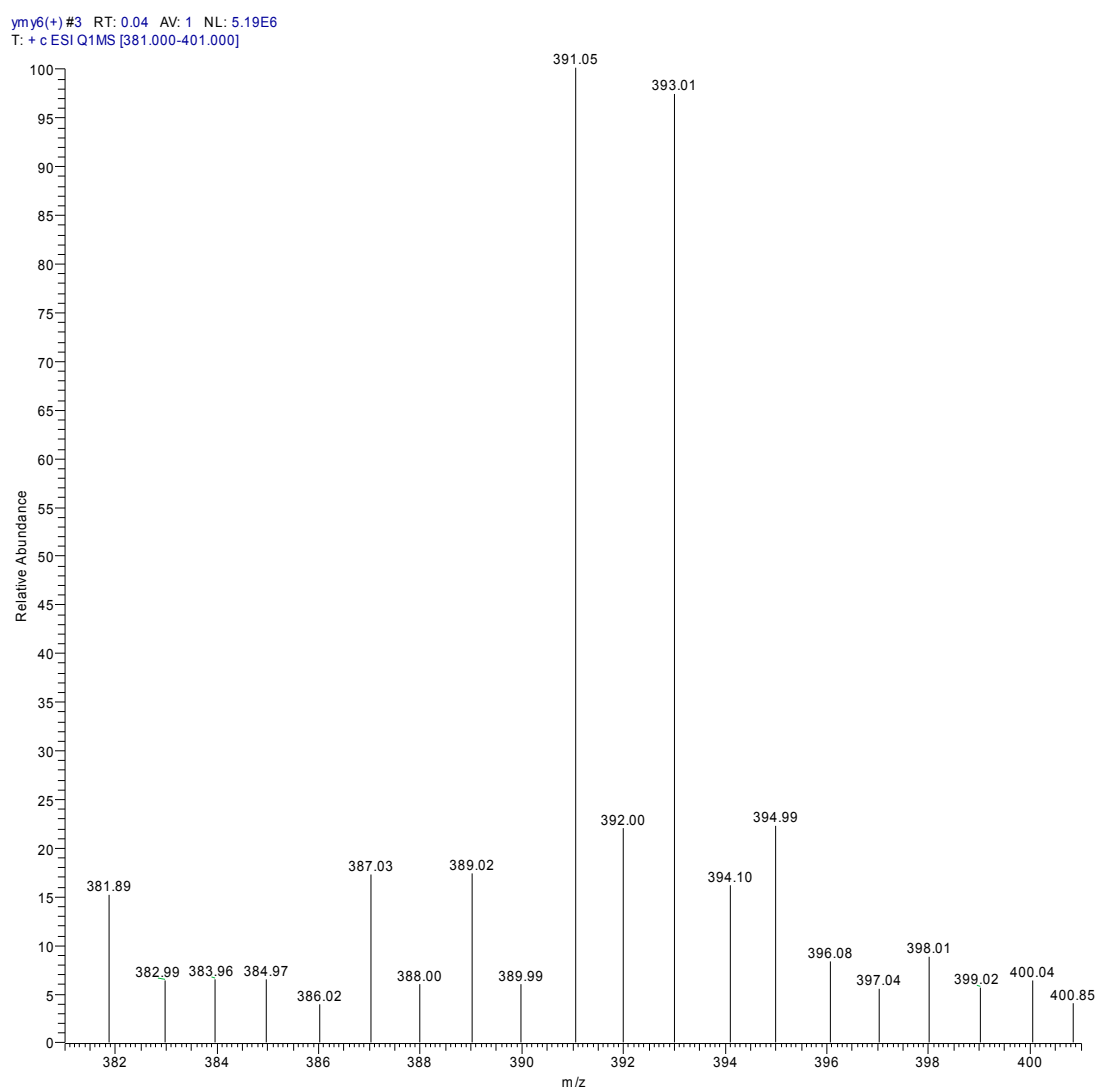


Figure S26. MS spectrum of compound 5f (+).

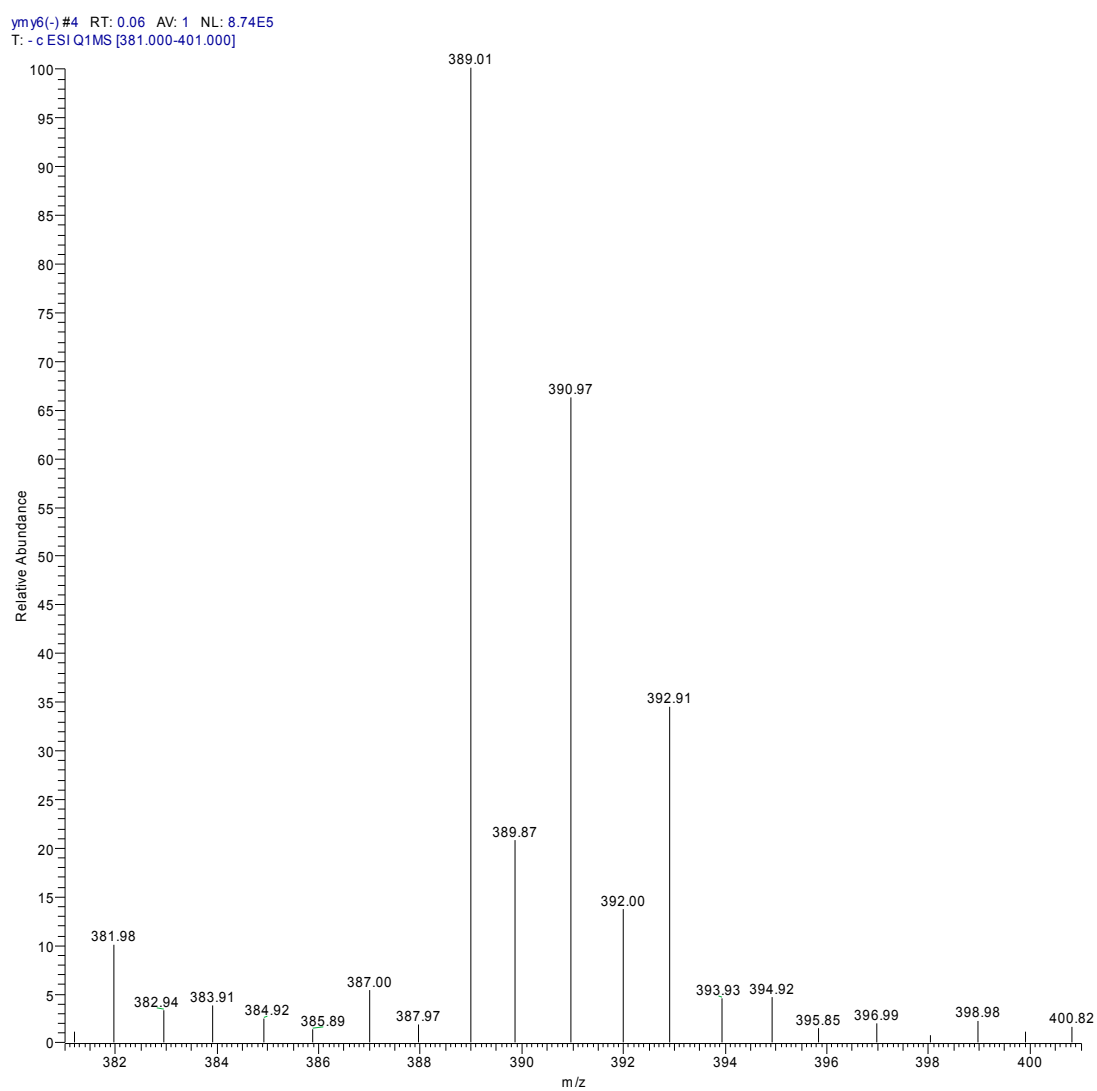


Figure S27. MS spectrum of compound 5f (-).

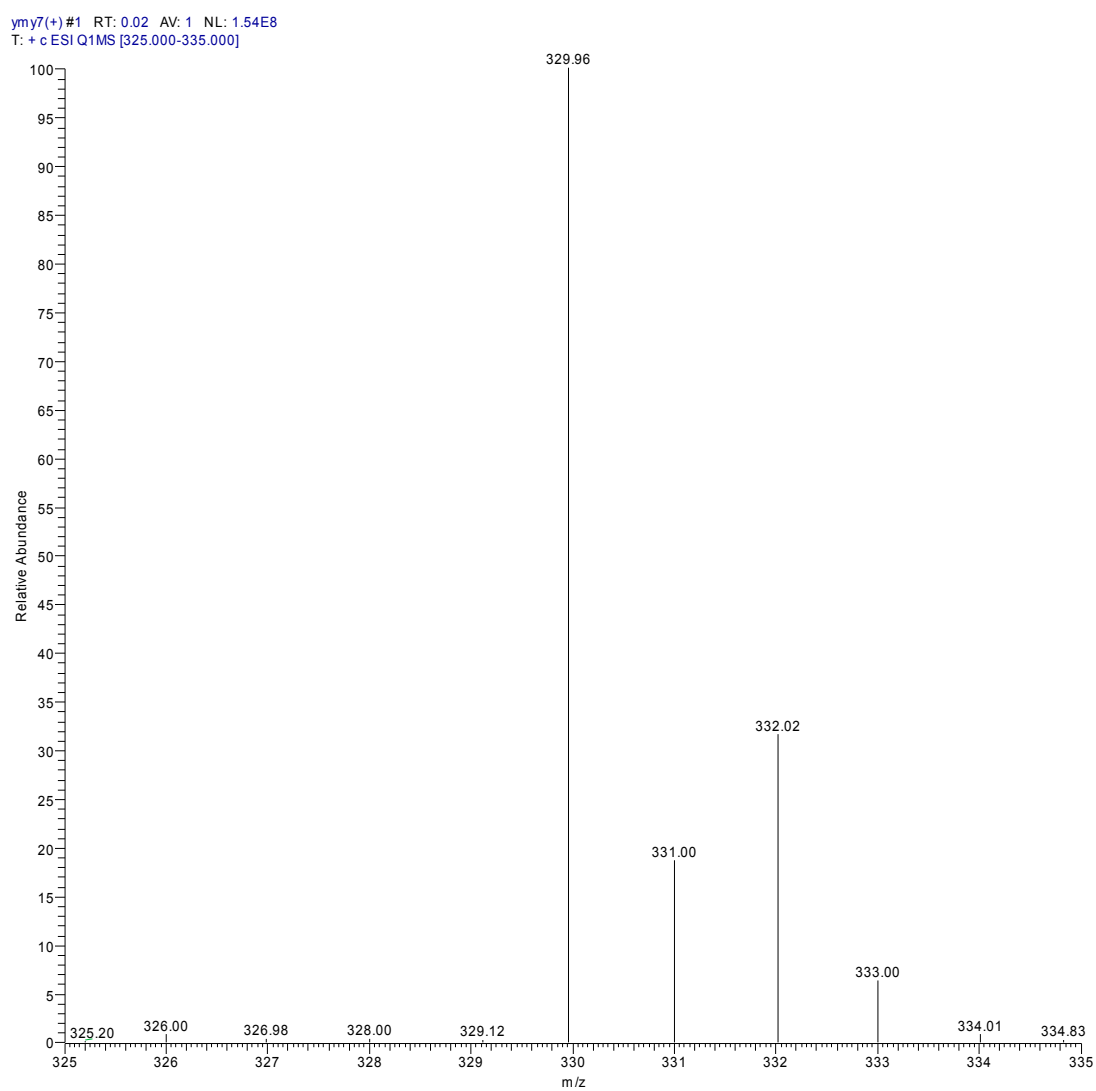


Figure S28. MS spectrum of compound 5g (+).

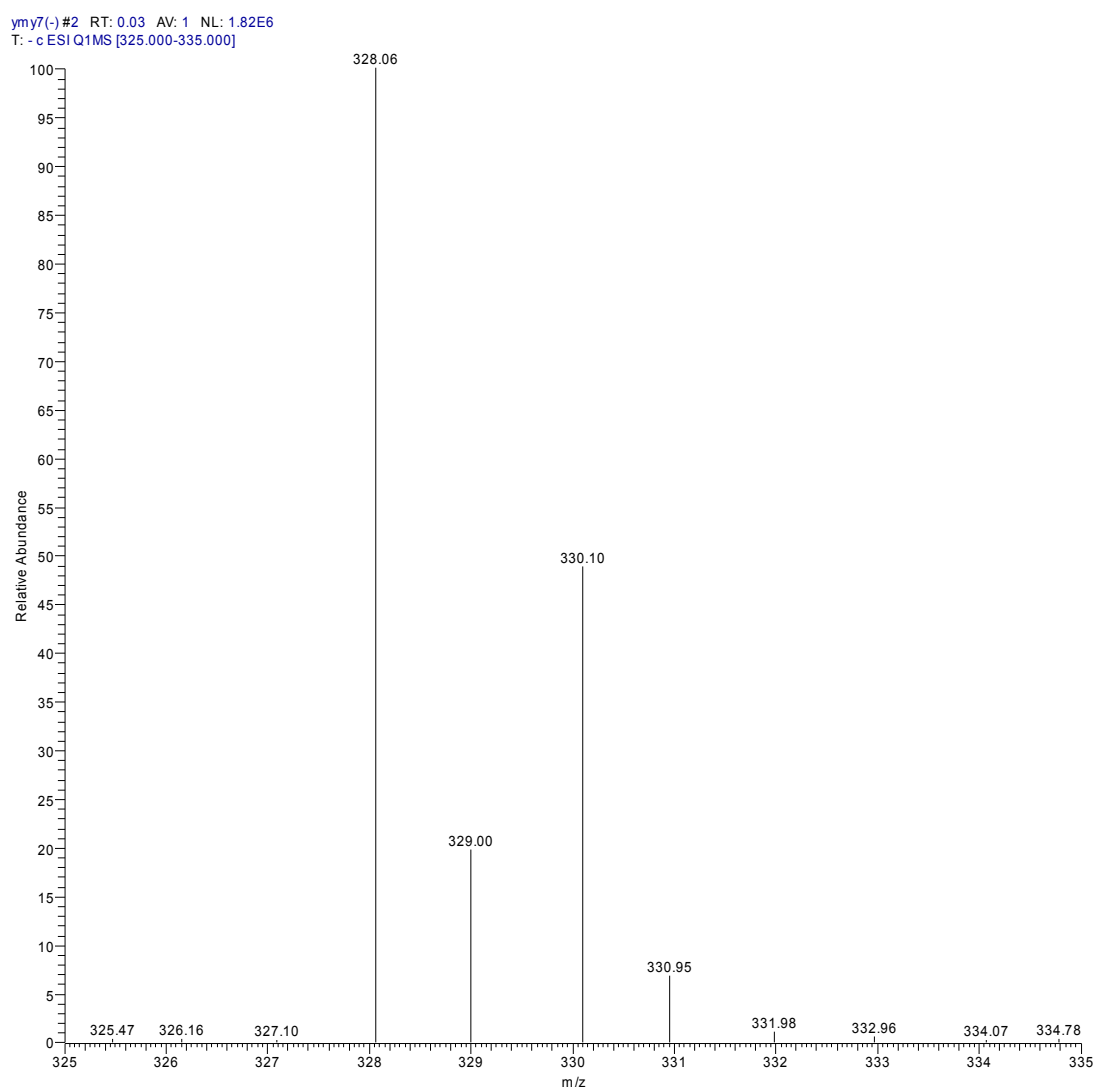


Figure S29. MS spectrum of compound 5g (-).

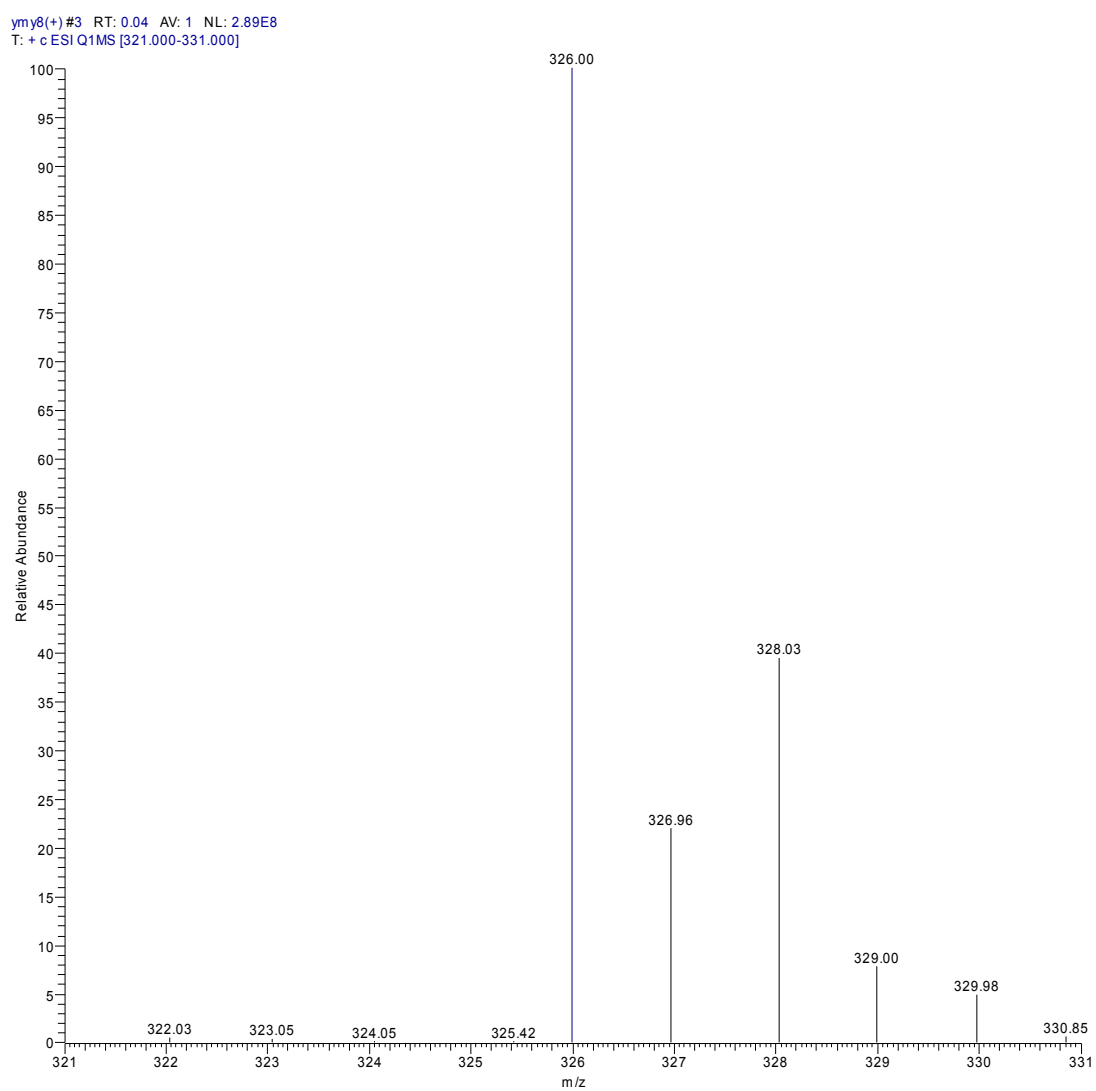


Figure S30. MS spectrum of compound 5h (+).

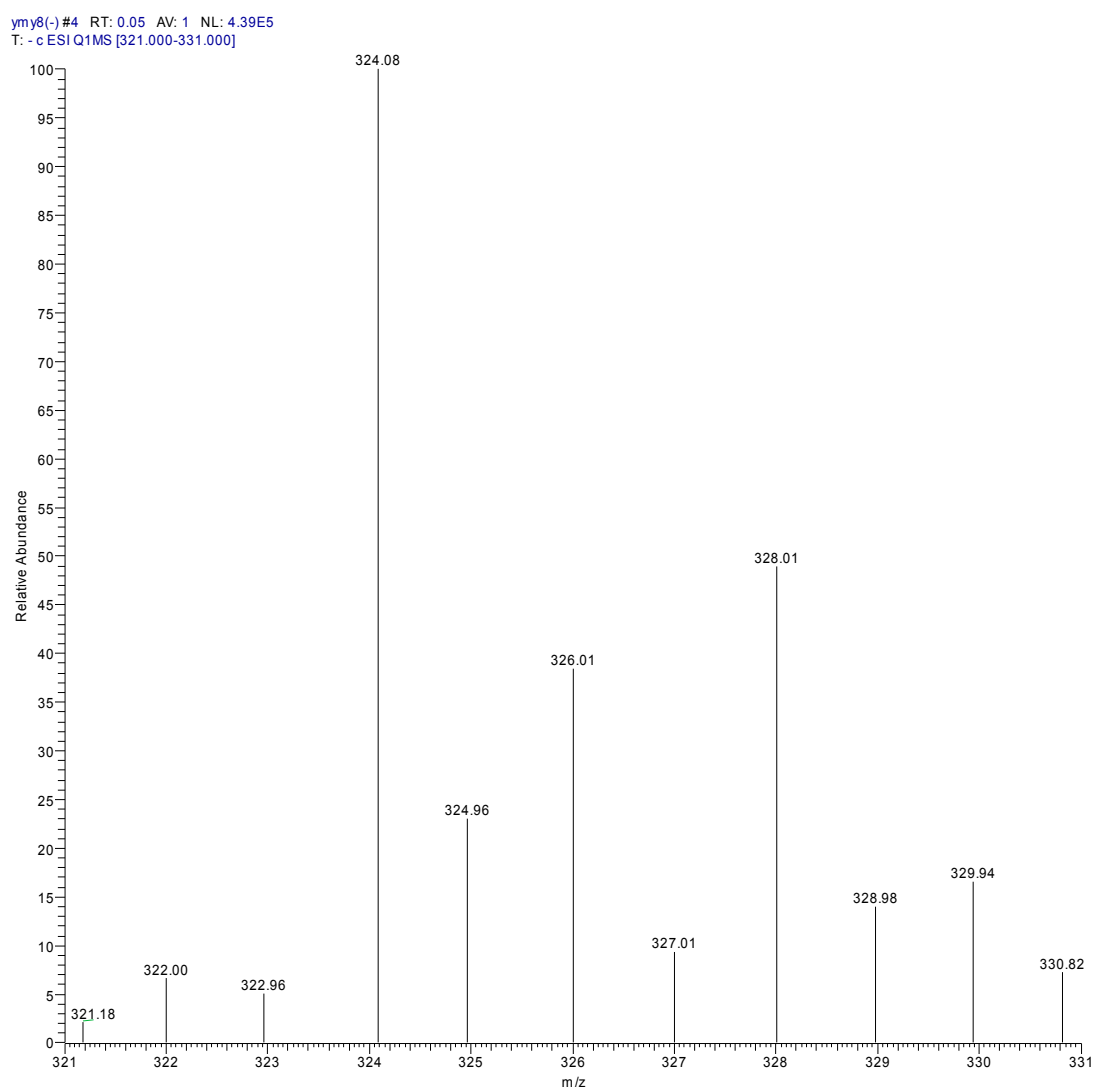


Figure S31. MS spectrum of compound 5h (-).

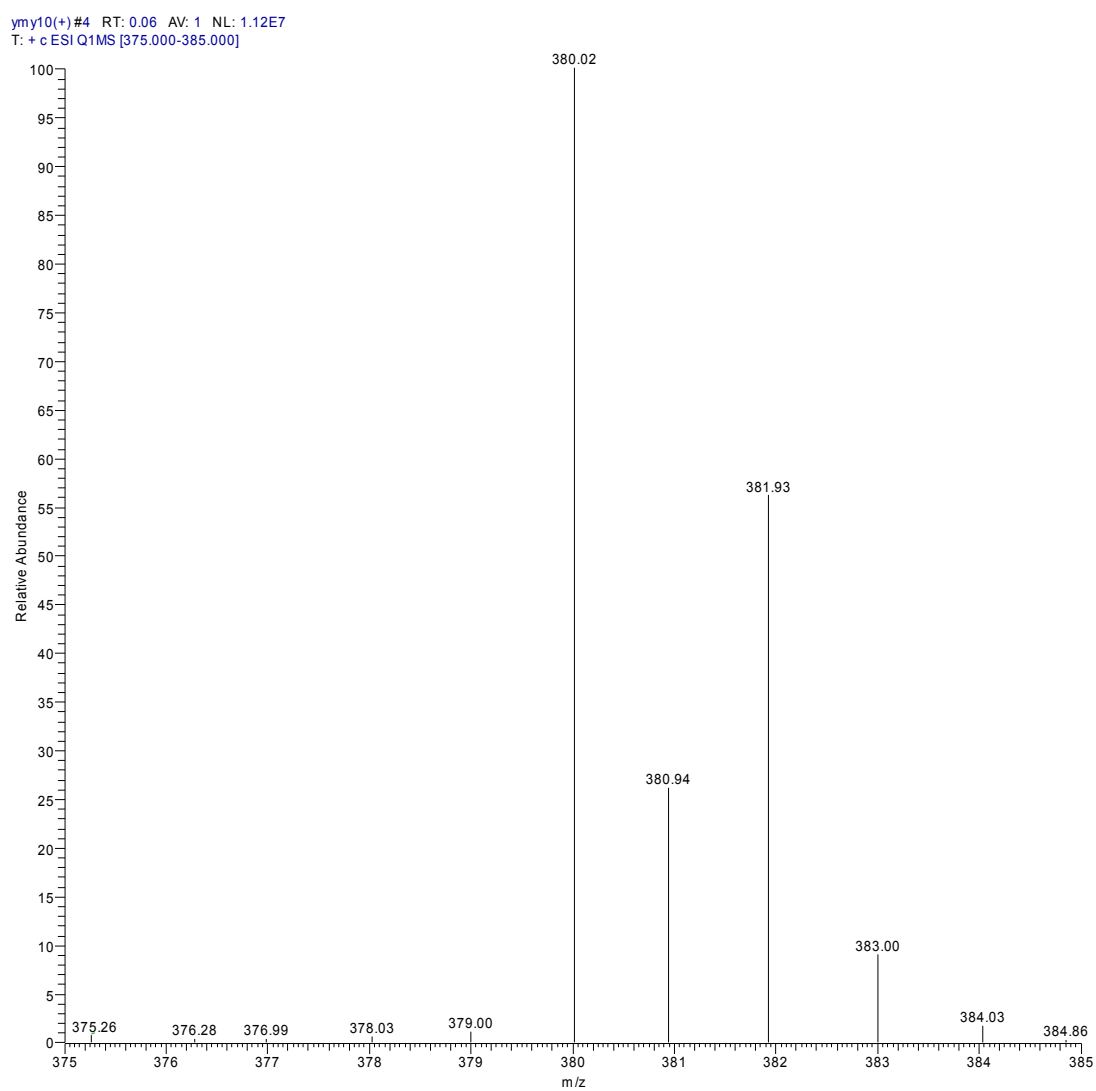


Figure S32. MS spectrum of compound **5i** (+).

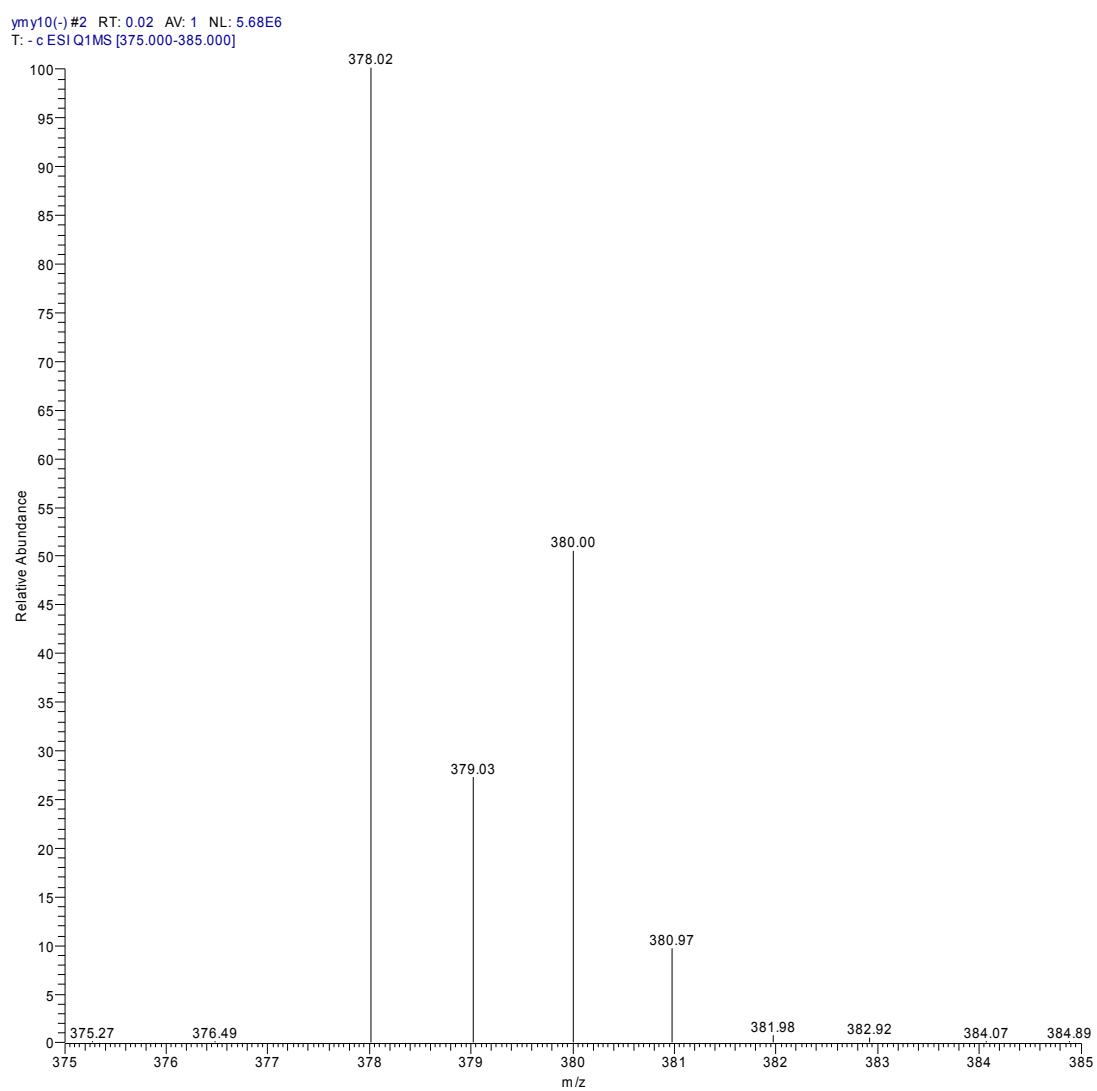


Figure S33. MS spectrum of compound **5i** (-).

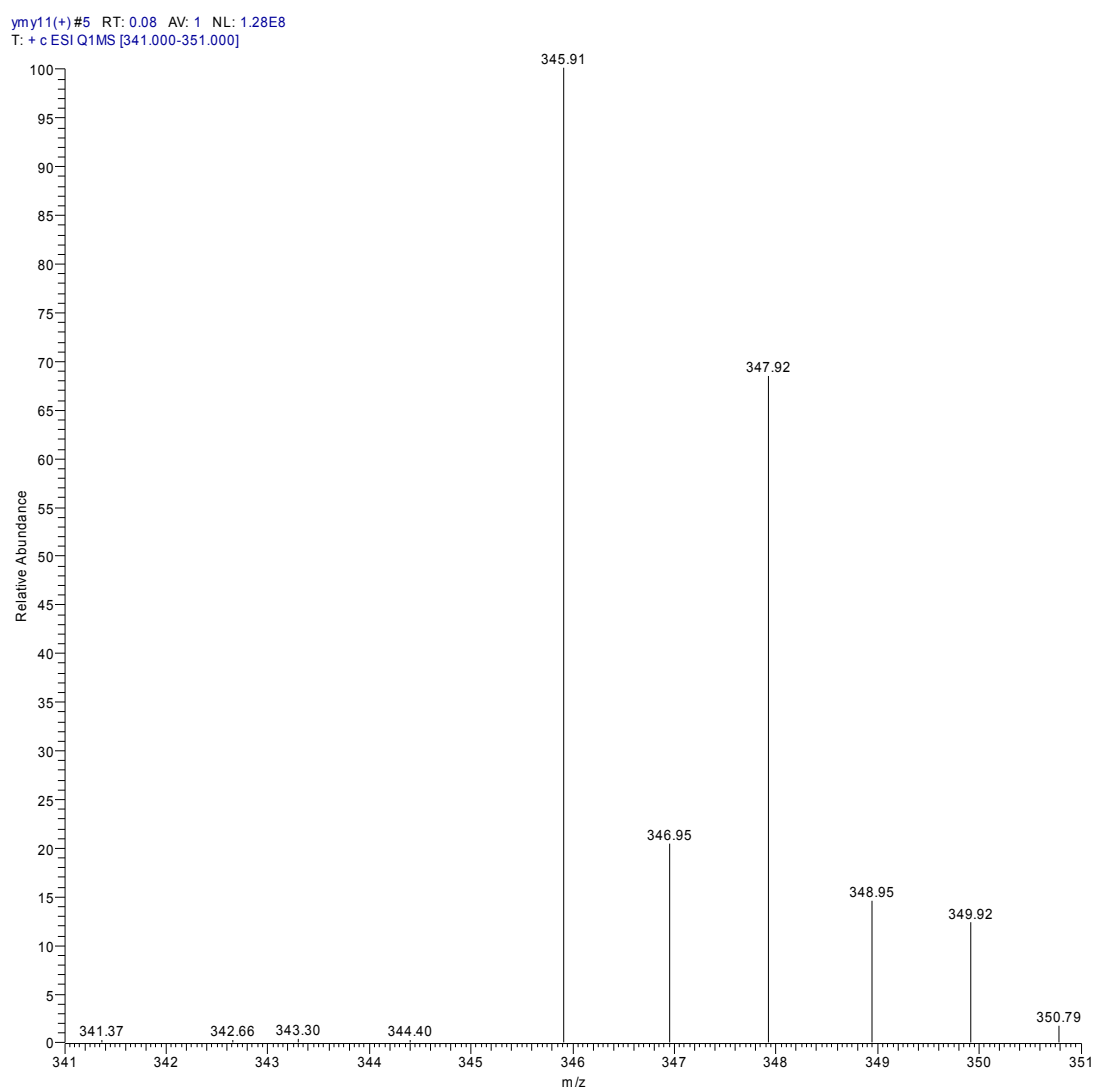


Figure S34. MS spectrum of compound 5j (+).

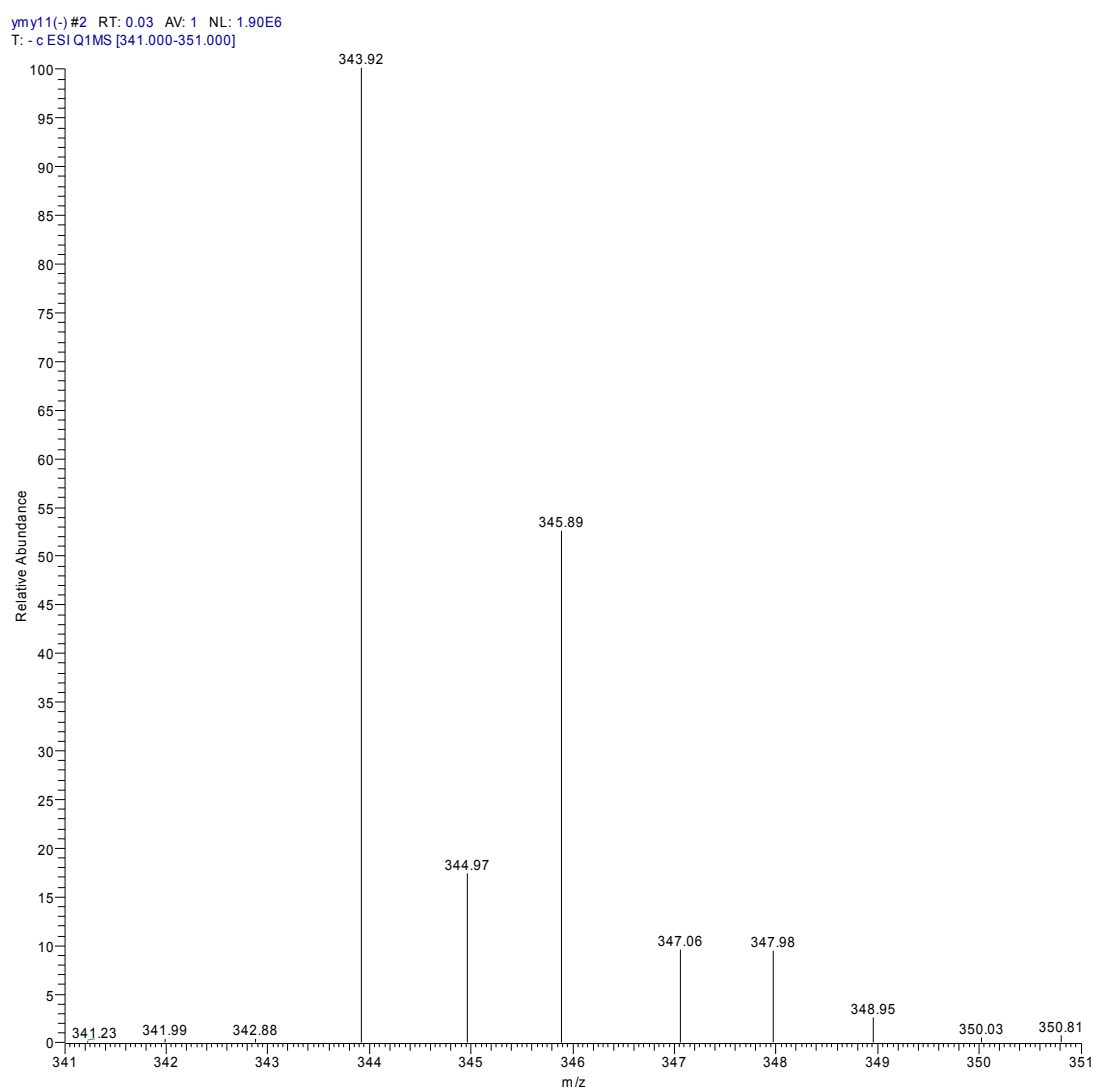


Figure S35. MS spectrum of compound 5j (-).

ymy12(+)#4 RT: 0.06 AV: 1 NL: 2.77E5
T: + c ESI Q1MS [382.000-392.000]

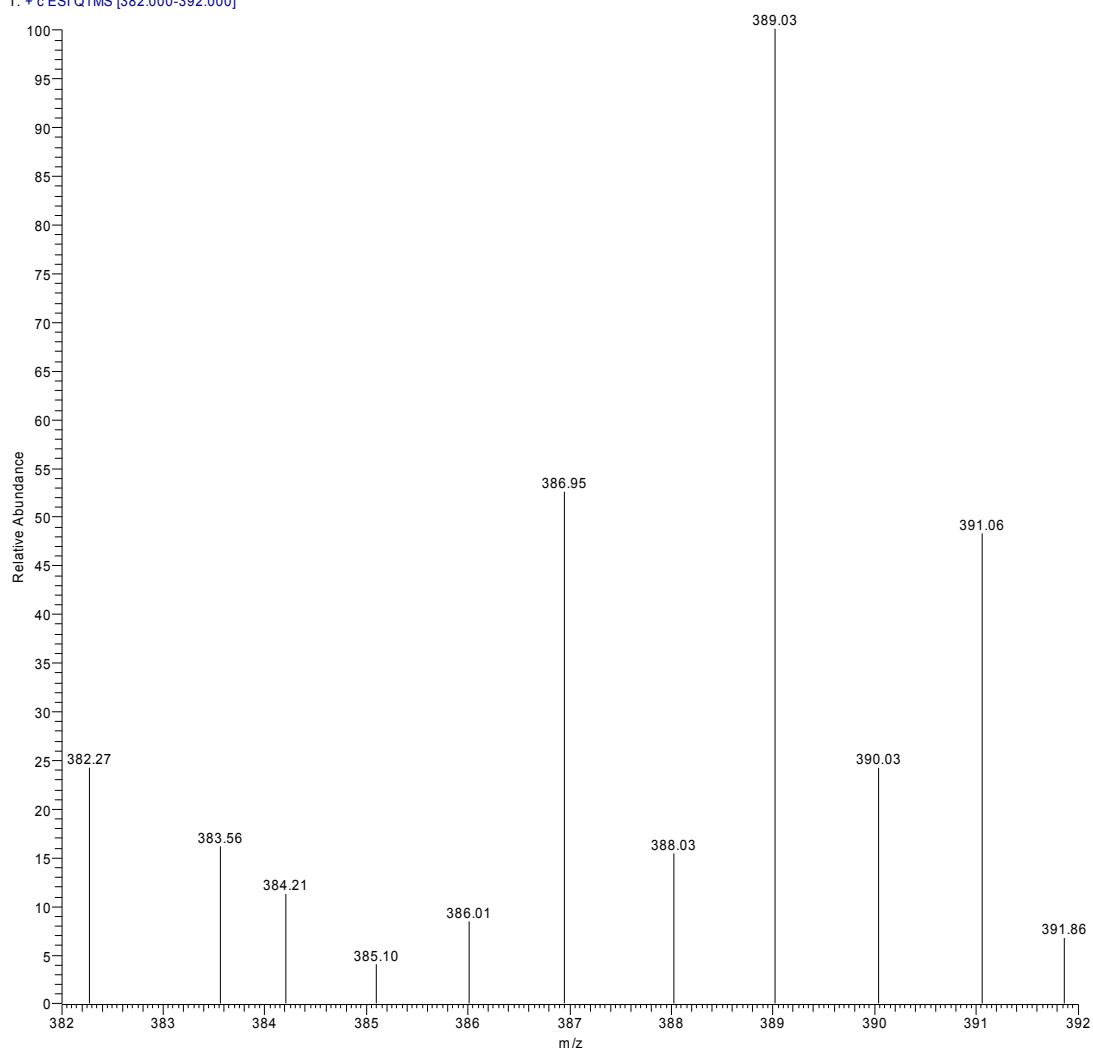


Figure S36. MS spectrum of compound 5k (+).

ymy12(-)#2 RT: 0.03 AV: 1 NL: 9.59E4
T: -c ESI Q1MS [382.000-392.000]

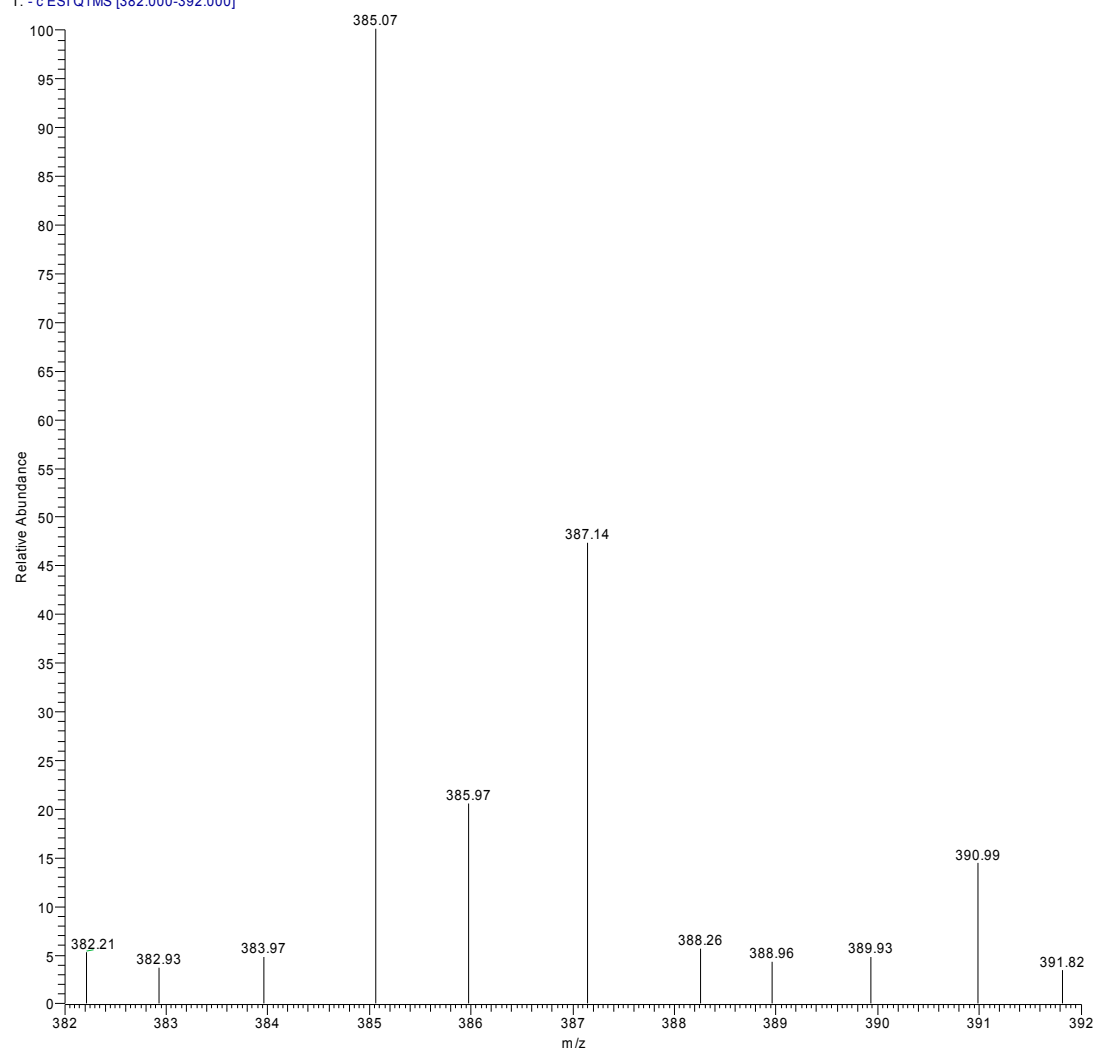


Figure S37. MS spectrum of compound 5k (-).

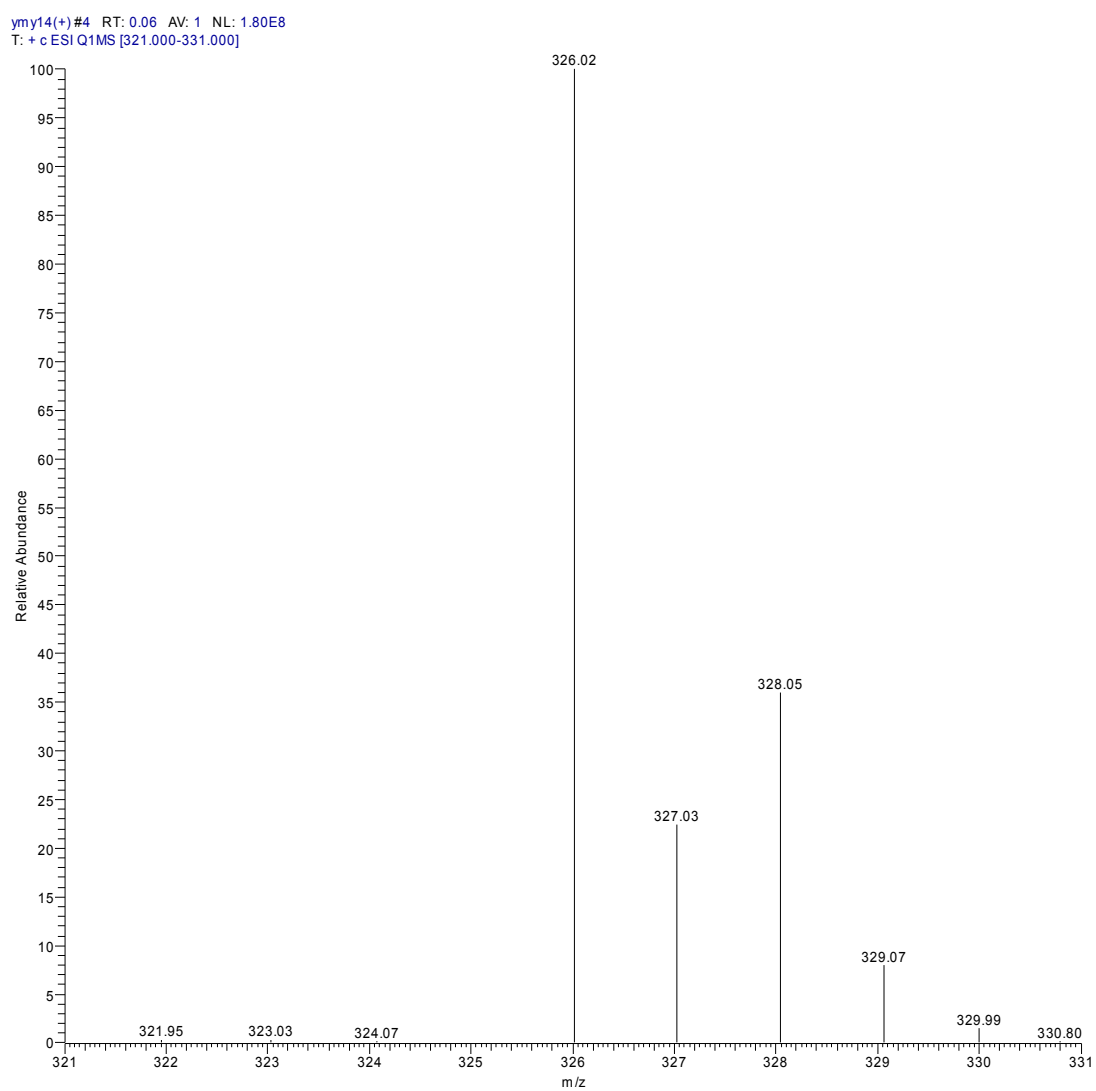


Figure S38. MS spectrum of compound 51 (+).

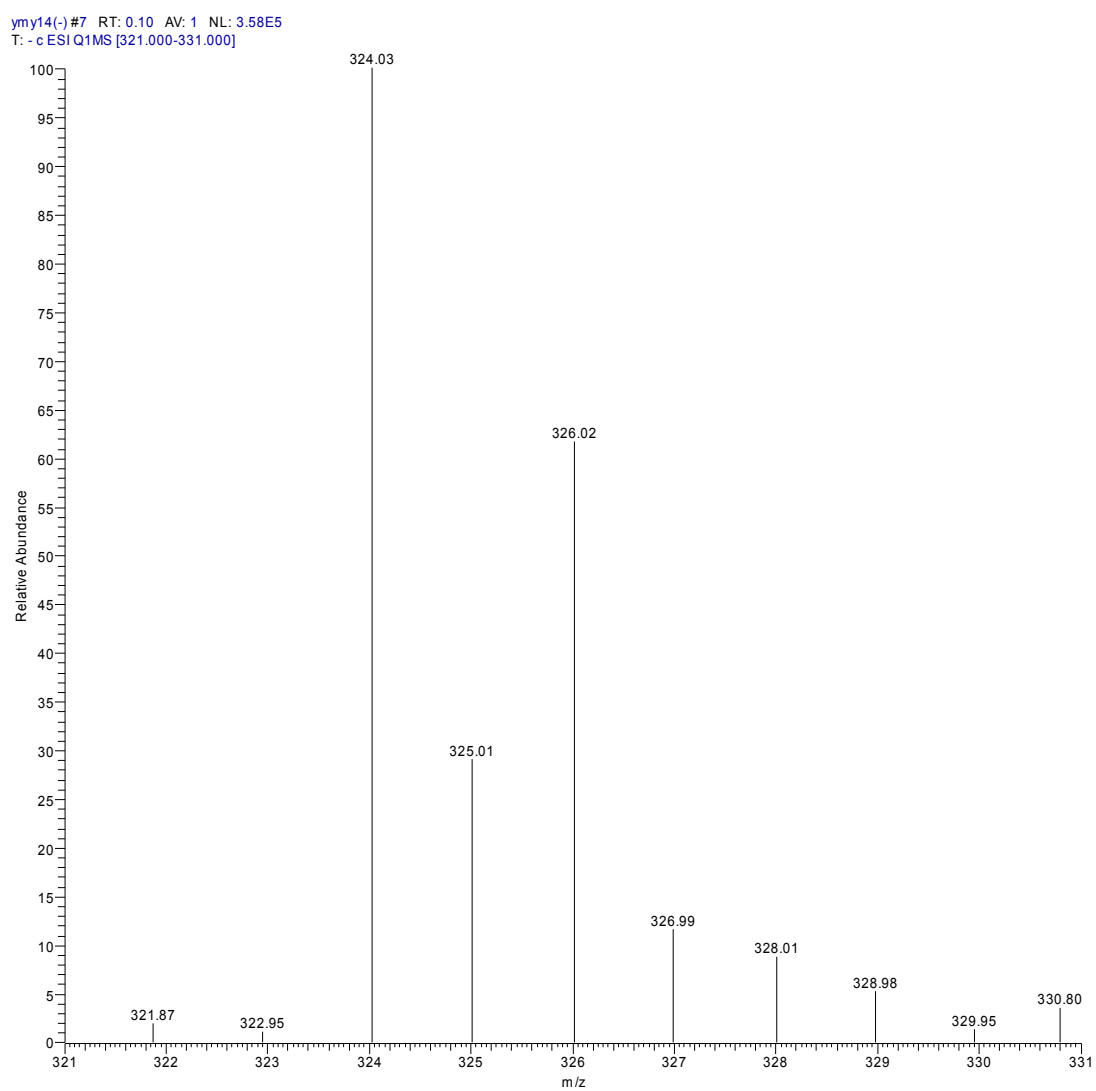


Figure S39. MS spectrum of compound 51 (-).

ymy15(+)#2 RT: 0.03 AV: 1 NL: 1.45E8
T: + c ESI Q1MS [341.000-351.000]

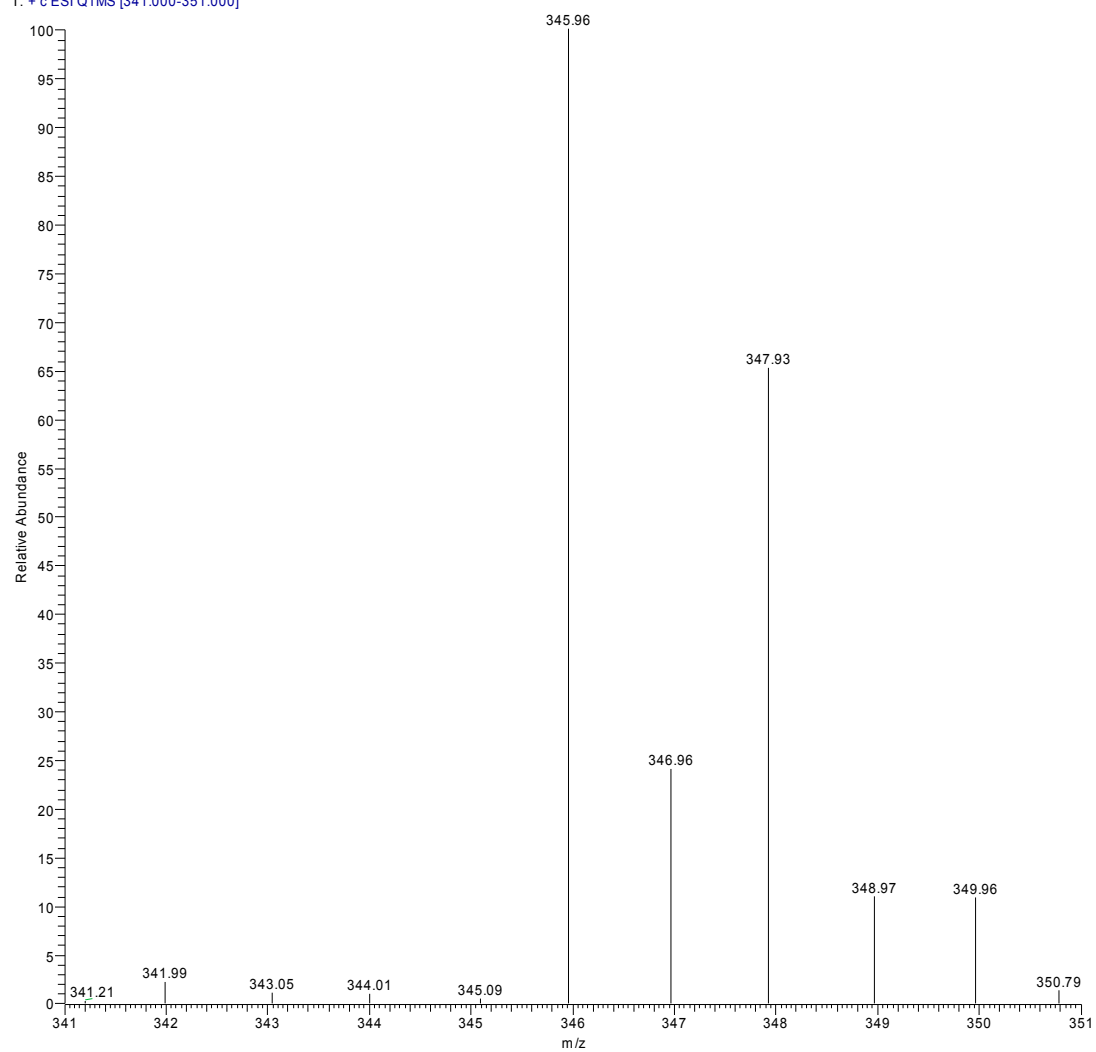


Figure S40. MS spectrum of compound 5m (+).

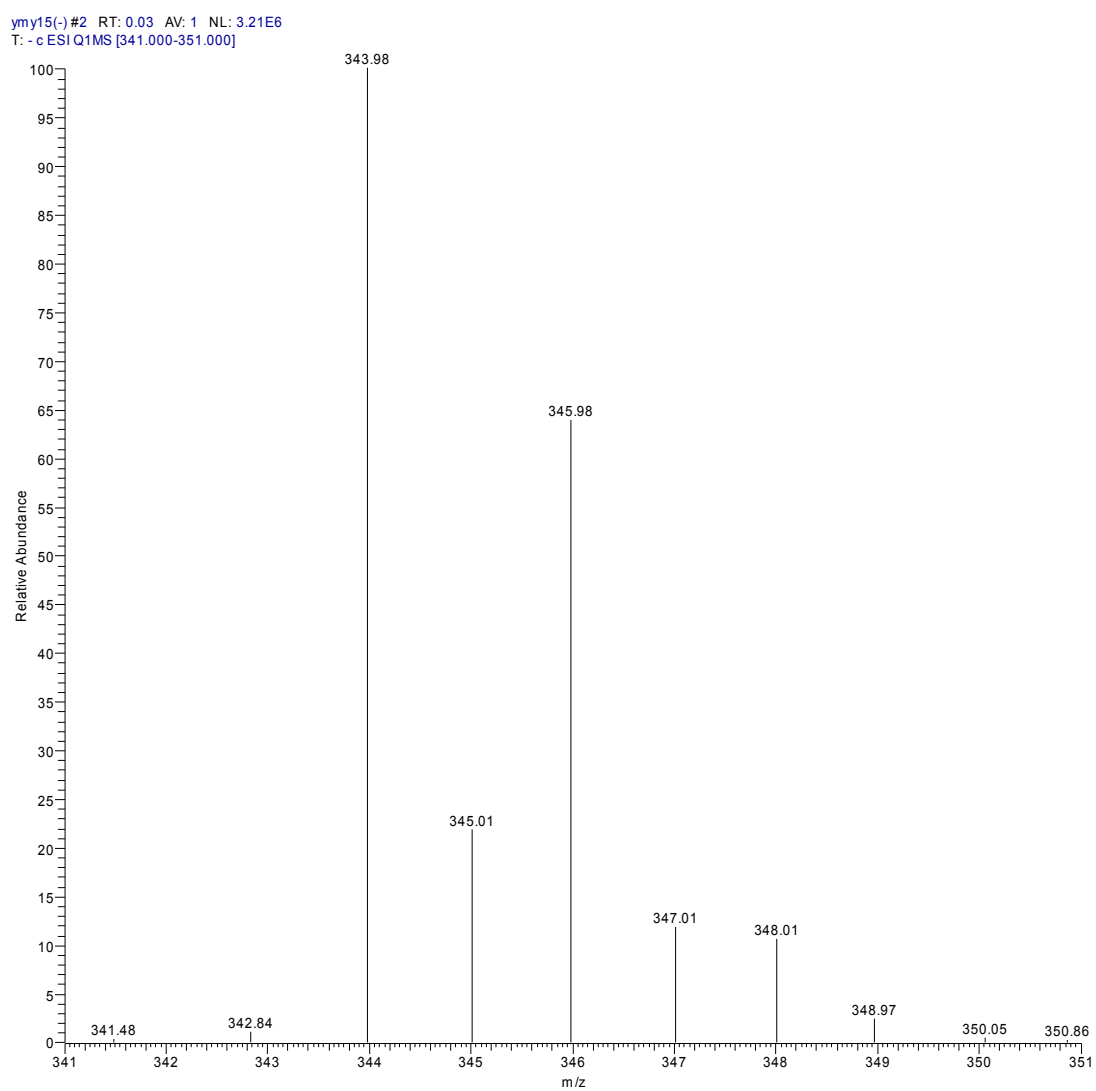


Figure S41. MS spectrum of compound 5m (-).