

Supplementary Materials

Identification of Antiprotozoal Compounds from *Buxus sempervirens* L. by PLS-Prediction

Lara U. Szabó ¹, Marcel Kaiser ^{2,3}, Pascal Mäser ^{2,3} and Thomas J. Schmidt ^{1,*}

¹ Institute of Pharmaceutical Biology and Phytochemistry (IPBP), University of Münster, PharmaCampus Corrensstraße 48, D-48149 Münster, Germany; lszabo@uni-muenster.de

² Swiss Tropical and Public Health Institute (Swiss TPH), Socinstrasse 57, CH-4051 Basel, Switzerland; marcel.kaiser@unibas.ch (M.K.); pascal.maeser@swisstph.ch (P.M.)

³ University of Basel, Petersplatz 1, CH-4003 Basel, Switzerland

* Correspondence: thomschm@uni-muenster.de; Tel.: +49-251-83-33378

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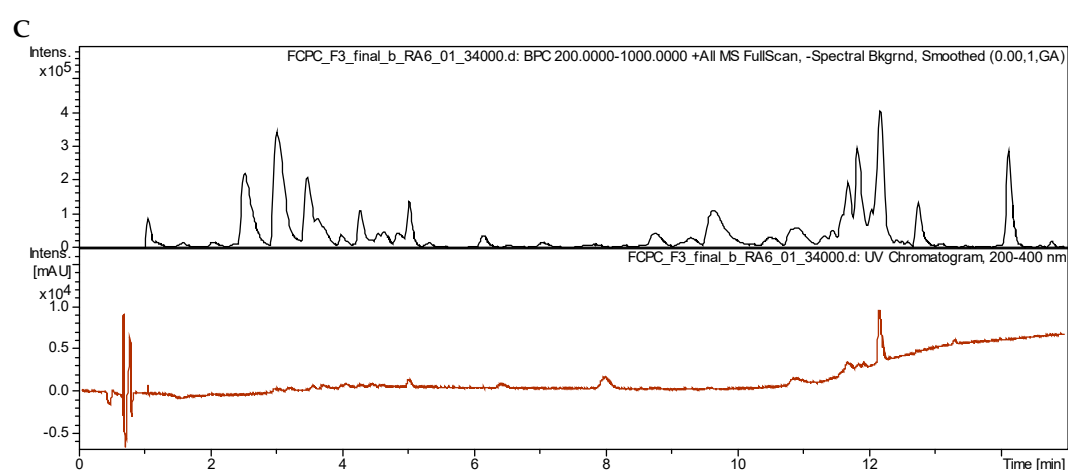
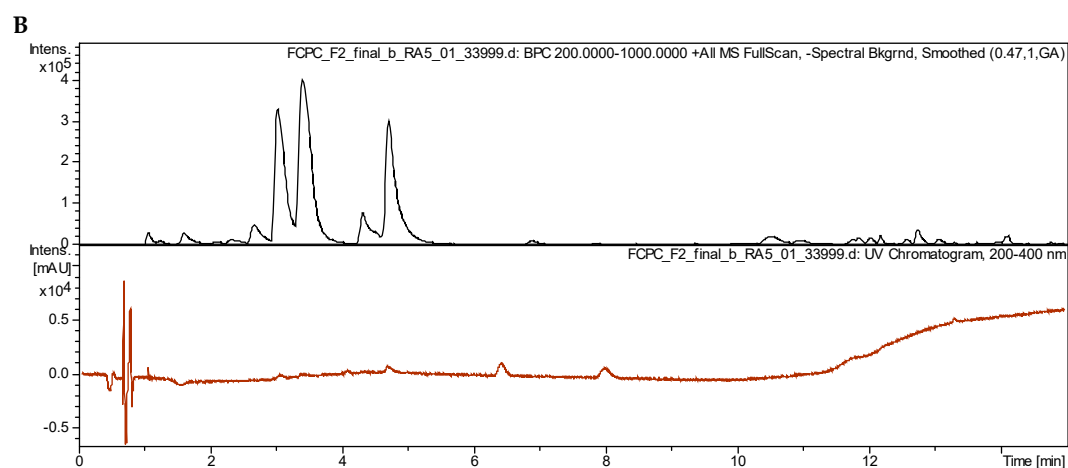
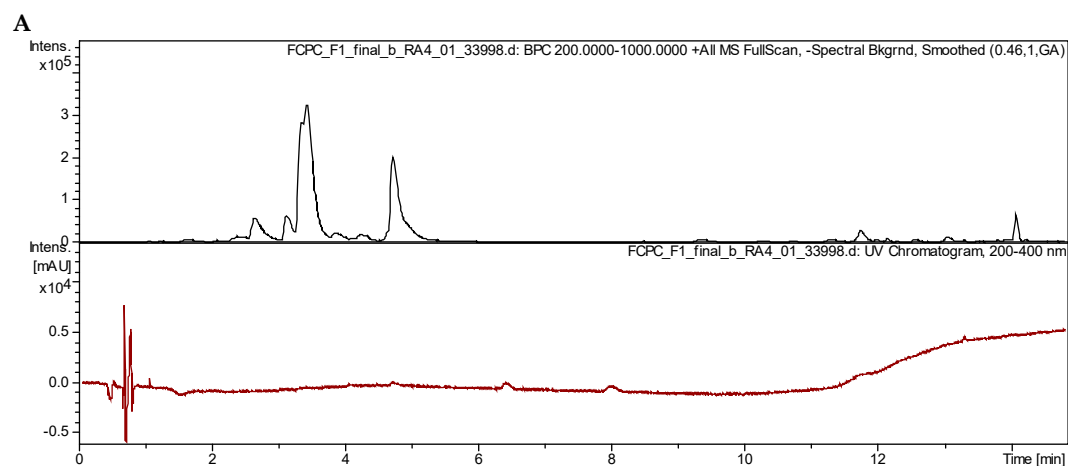
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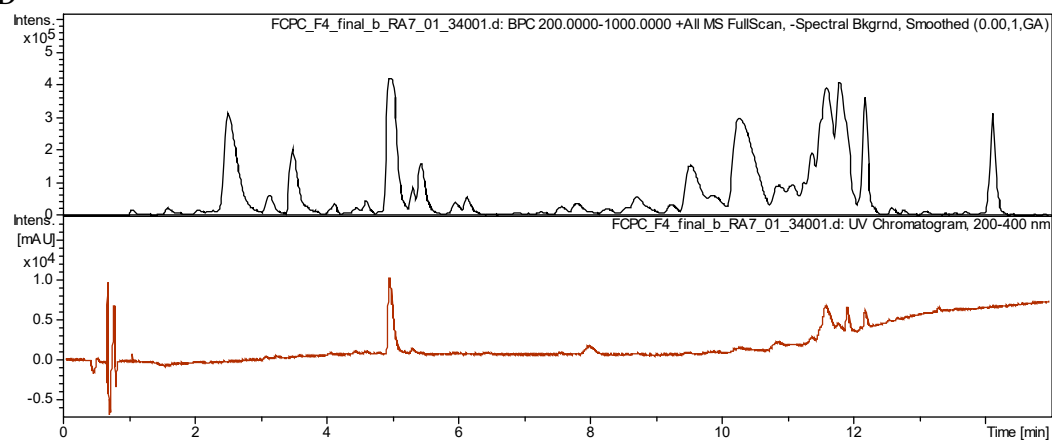
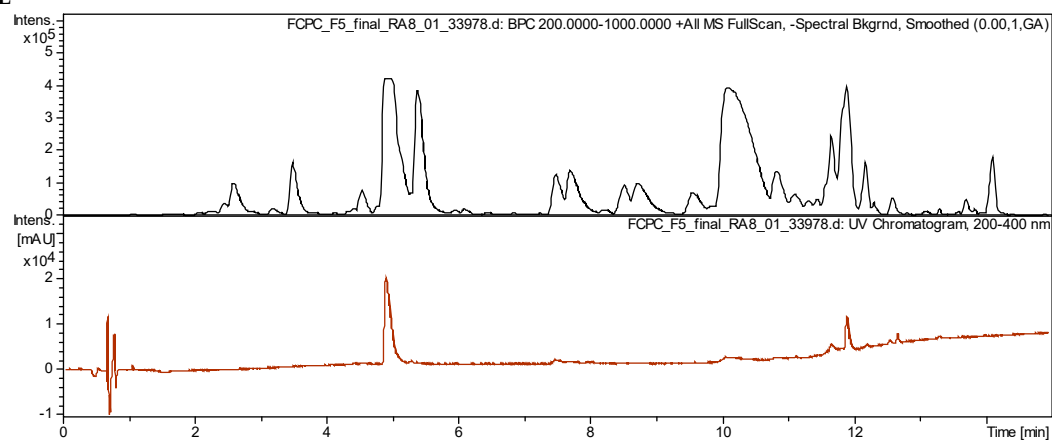
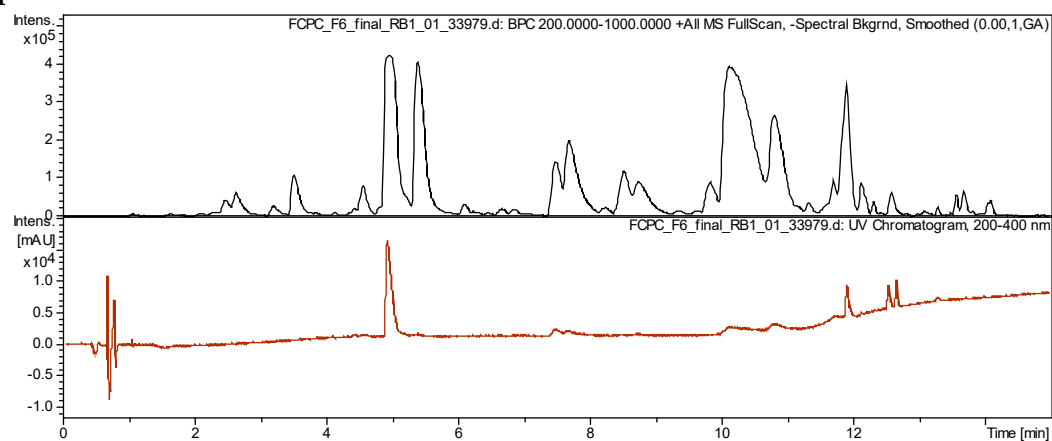
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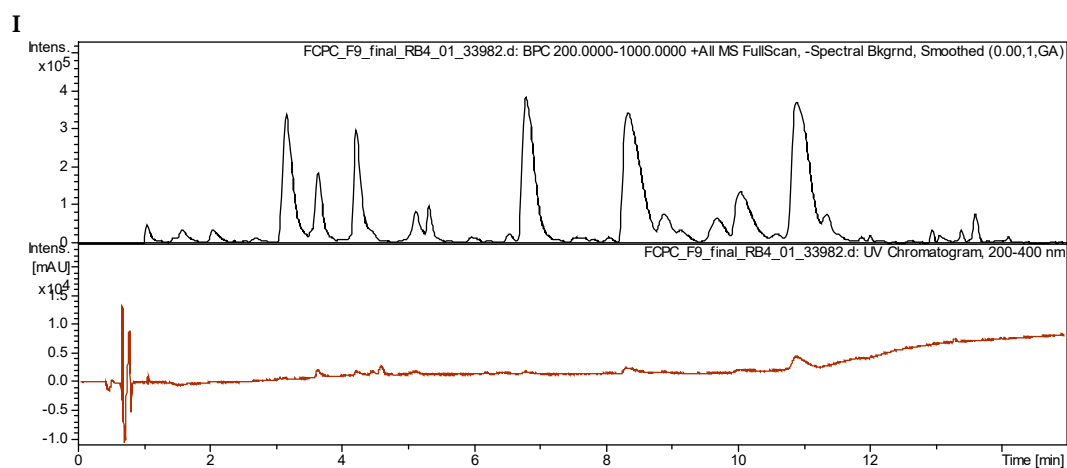
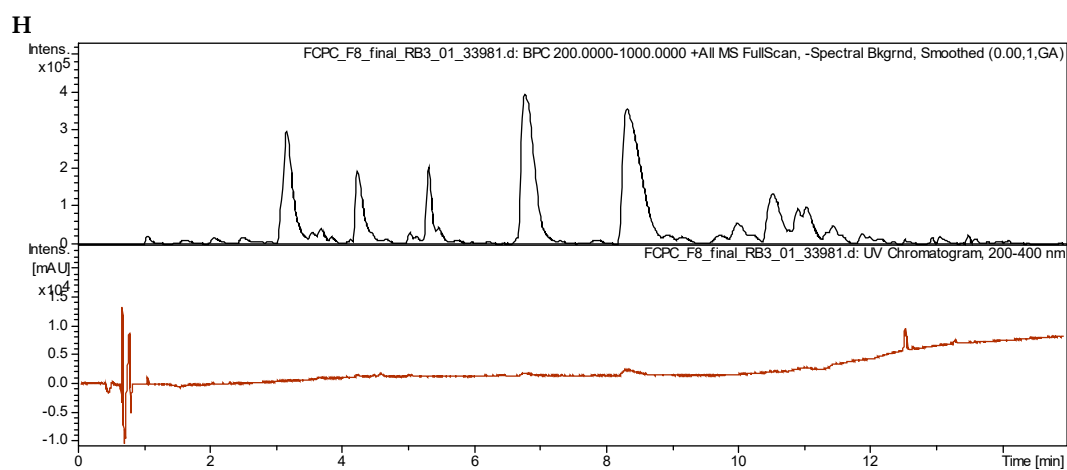
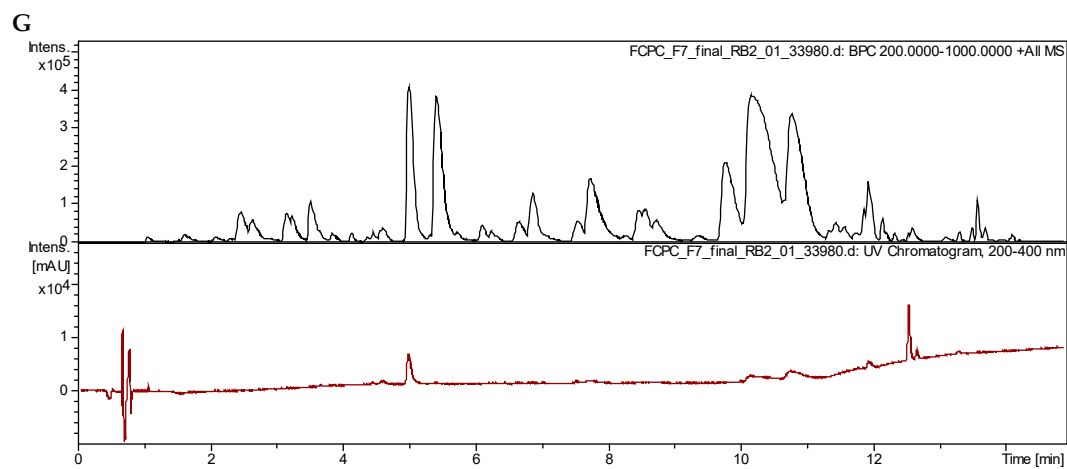
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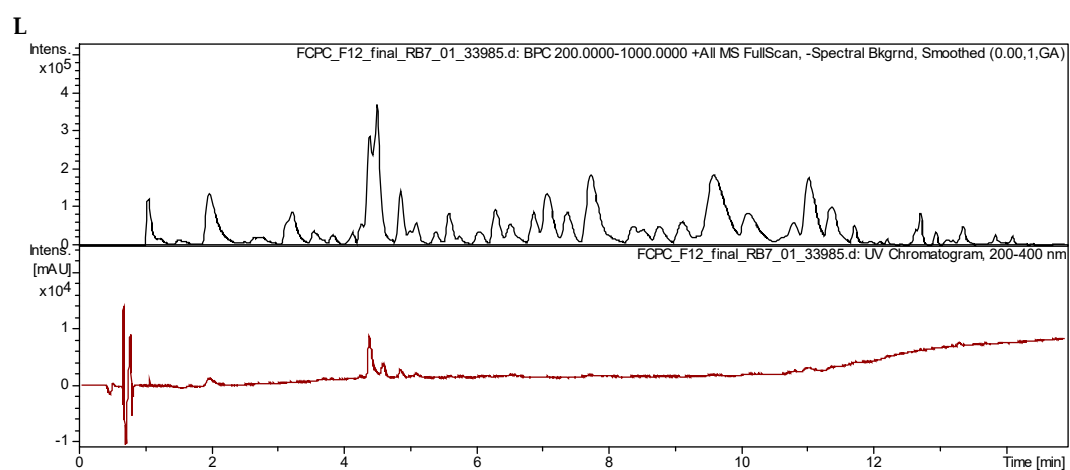
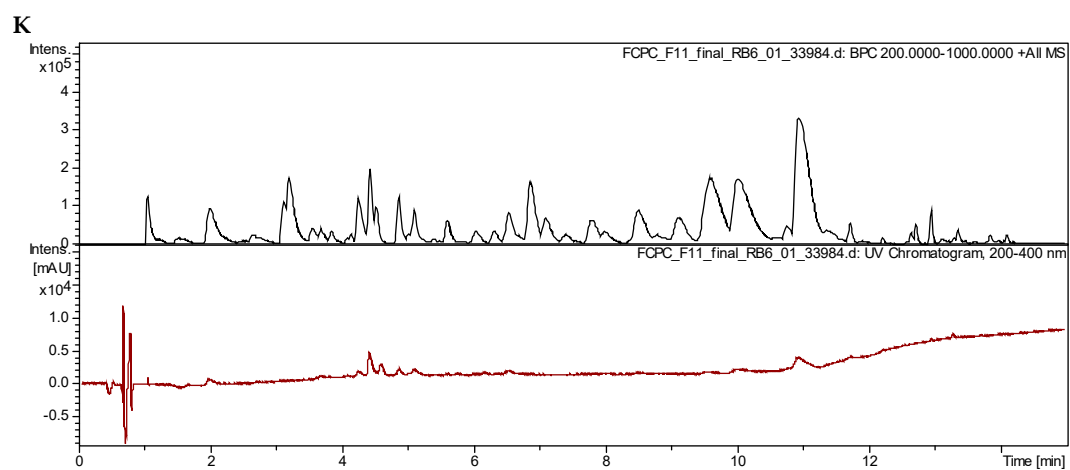
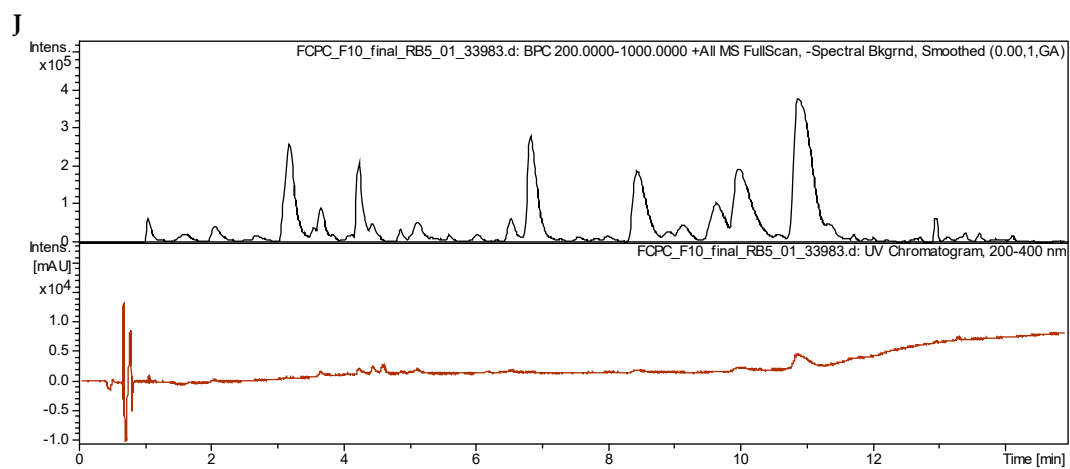


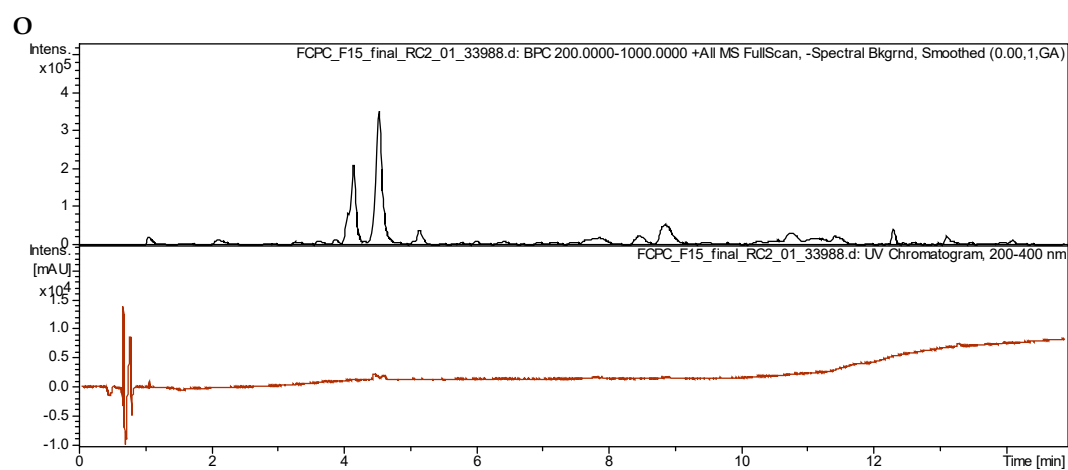
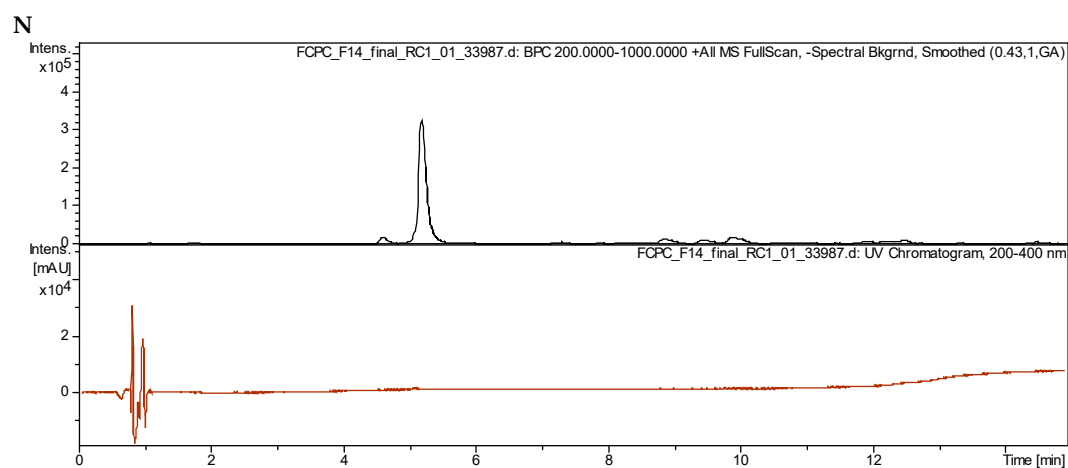
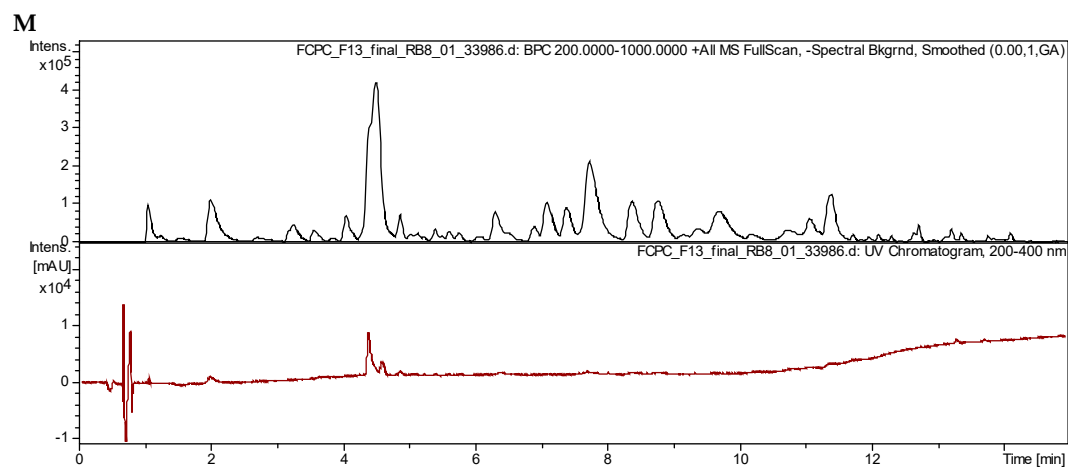
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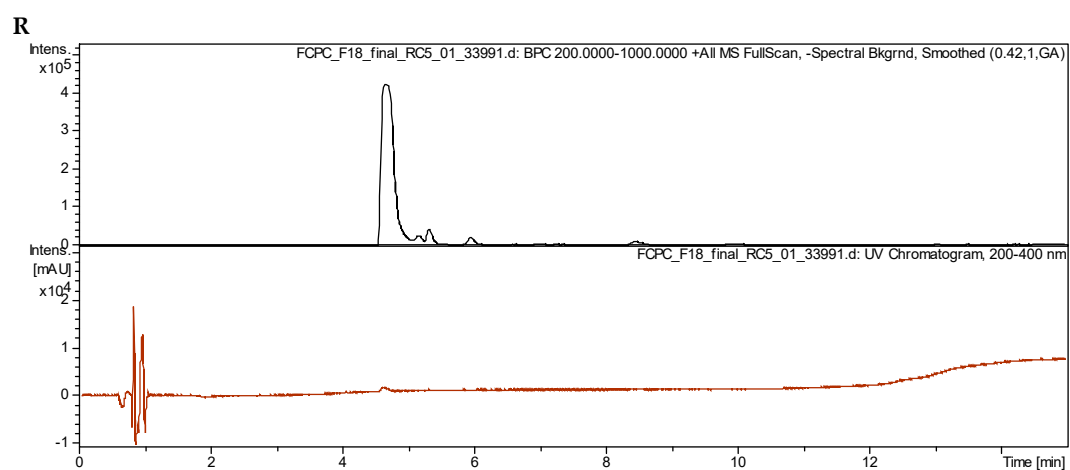
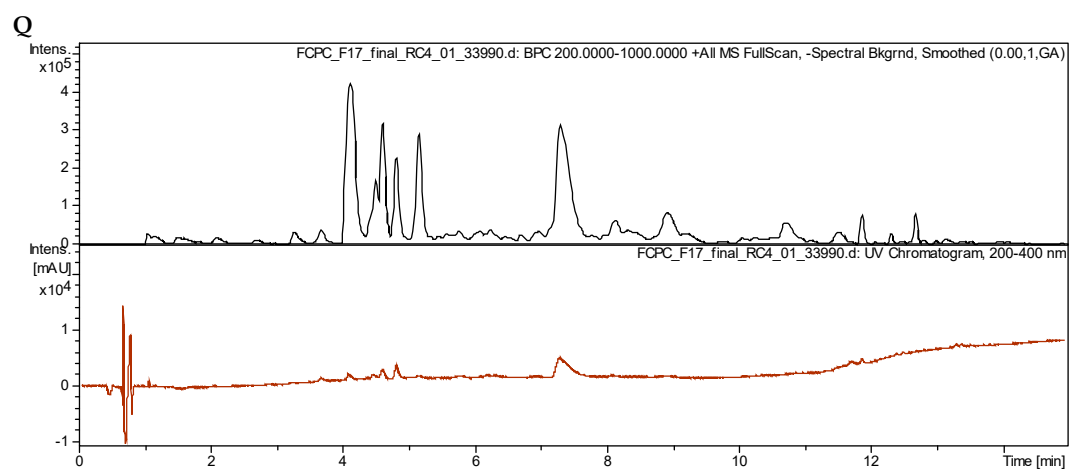
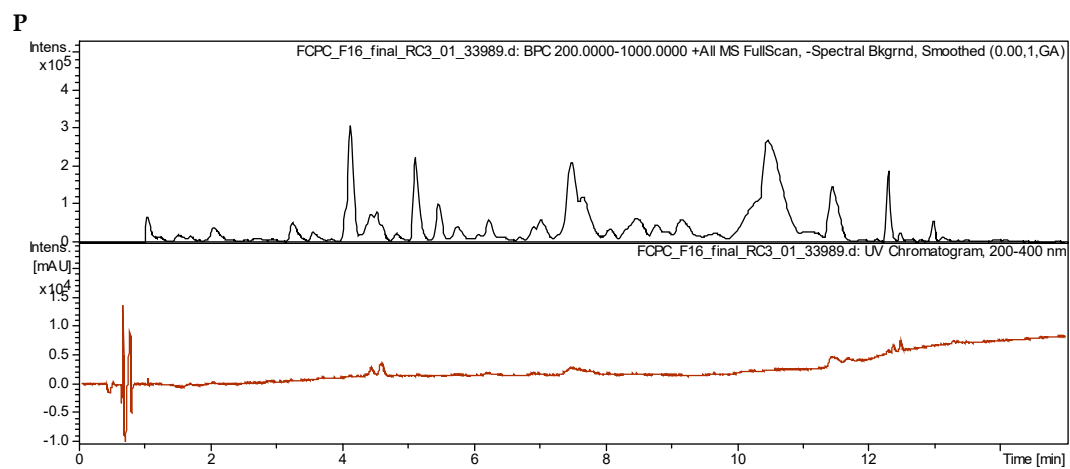


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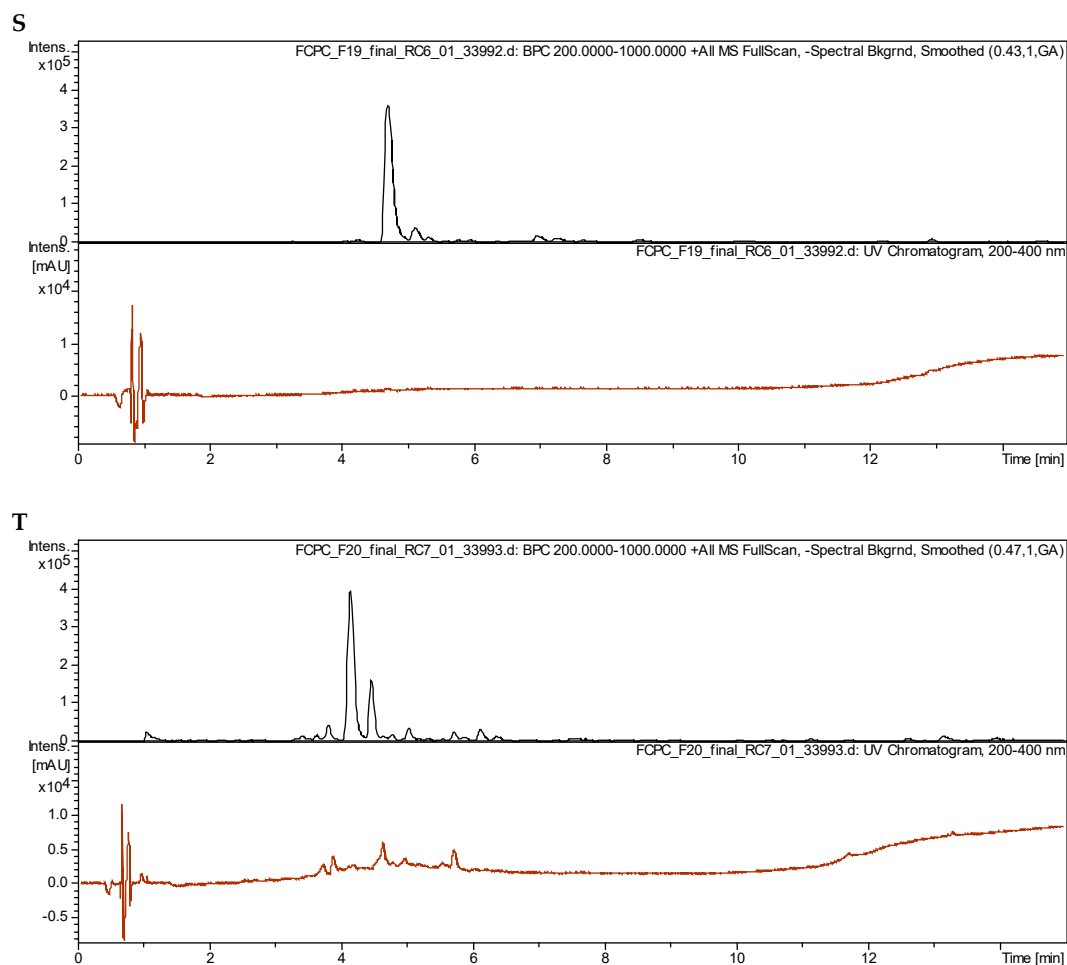


Figure S1. UHPLC/+ESI-QqTOF-MS/MS chromatograms of fractions 1-20. Base peak chromatogram 200.0000-1000.0000 +All MS (black); UV-Chromatogramm, 200-400 nm (red). **A:** Fraction (F) 1. **B:** F2. **C:** F3. **D:** F4. **E:** F5. **F:** F6. **G:** F7. **H:** F8. **I:** F9. **J:** F10. **K:** F11. **L:** F12. **M:** F13. **N:** F14. **O:** F15. **P:** F16. **Q:** F17. **R:** F18. **S:** F19. **T:** F20.

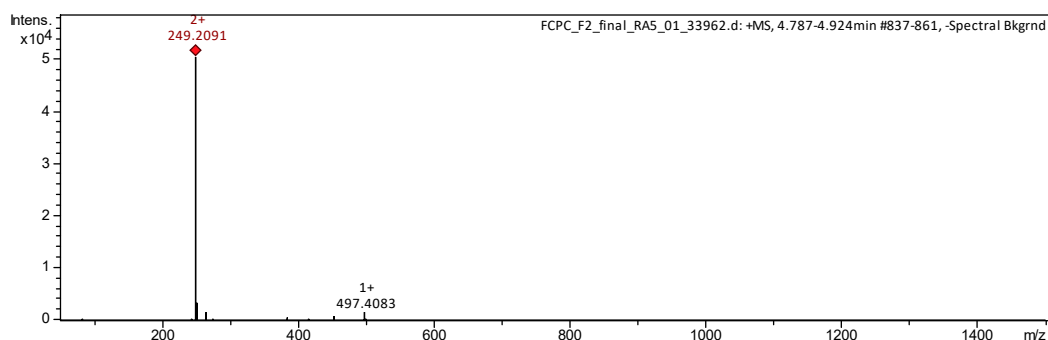


Figure S2. +ESI-QqTOF MS spectrum of compound **1** (O-tigloylcyclovirobuxine-B [4,9]); m/z 249.2091 [M+2H]²⁺ and 497.4083 [M+H]⁺.

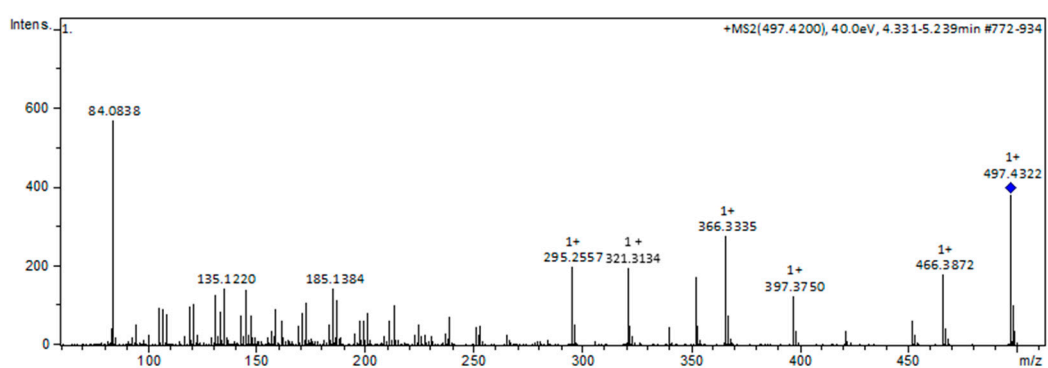


Figure S3. +ESI-QqTOF MS/MS spectrum of compound **1** (O-tigloylcyclovirobuxine-B [4,9]). The fragmentation pathway was already reported in [9].

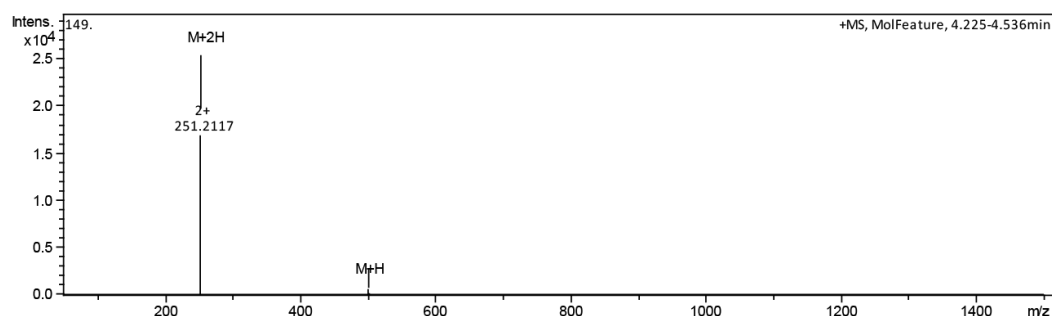


Figure S4. +ESI-QqTOF MS spectrum of compound 2; m/z 251.2117 $[M+2H]^{2+}$ and 501.4149 $[M+H]^+$.

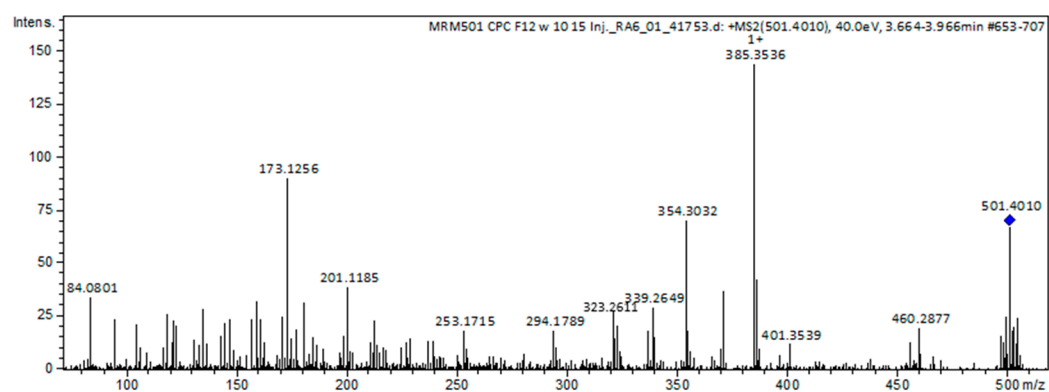


Figure S5. +ESI-QqTOF MS/MS spectrum of compound 2.

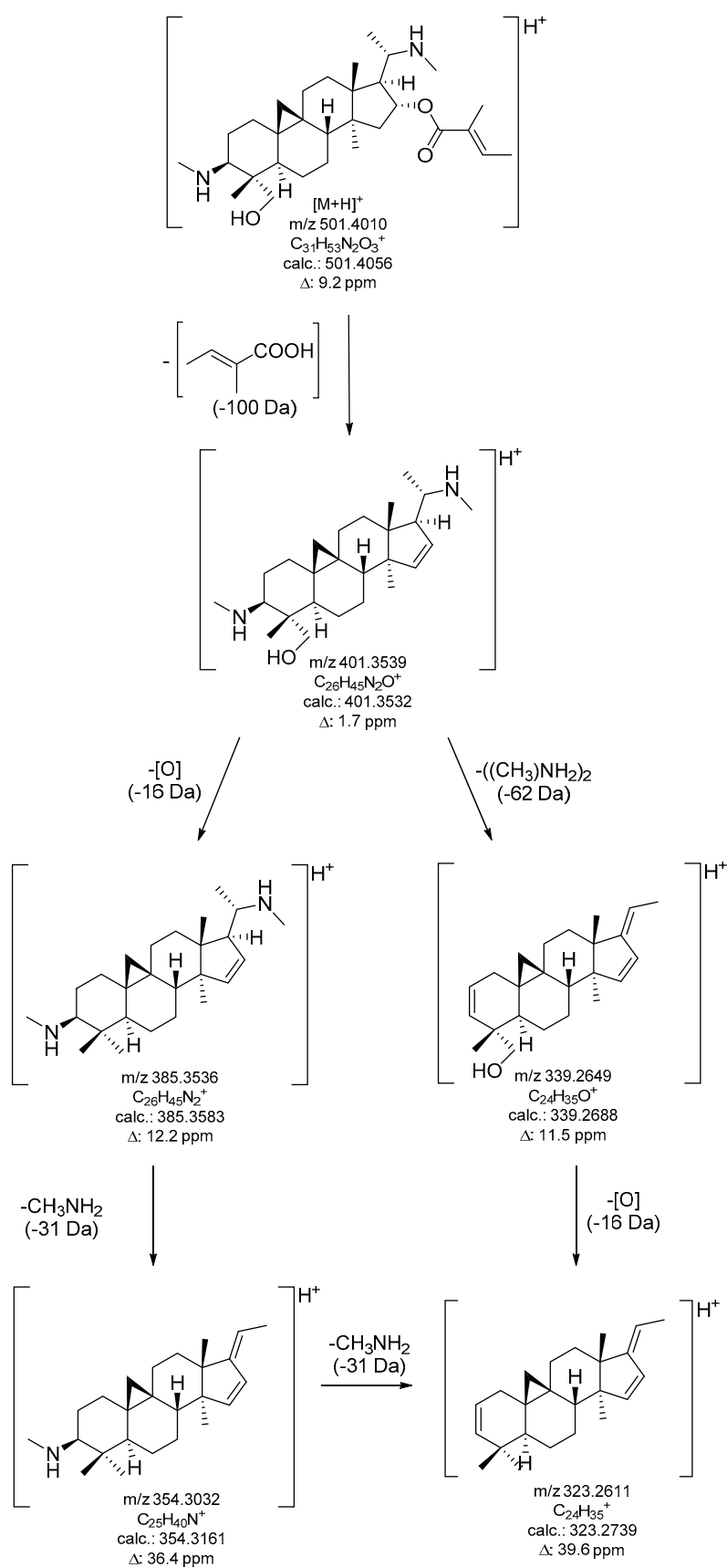


Figure S6. Possible fragmentation pathway of the $[M + H]^+$ ion of compound 2. (The postulated position of the hydroxyl- and ester group is based on the already known structures of compound 1 and 4).

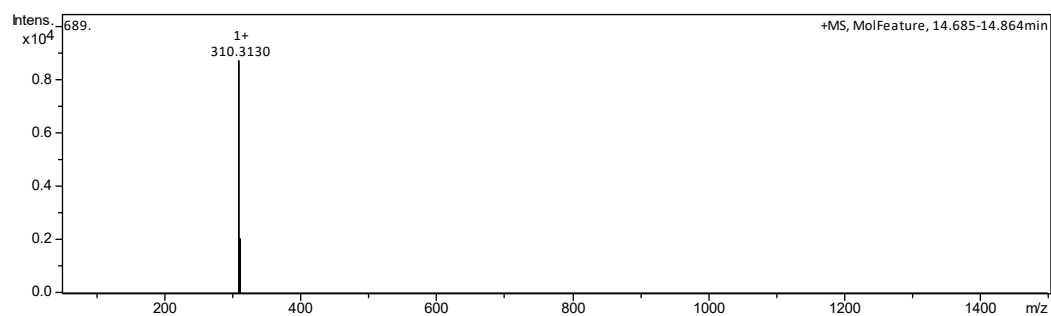


Figure S7. +ESI-QqTOF MS spectrum of compound **3**; 310.3130 [M+H]⁺.

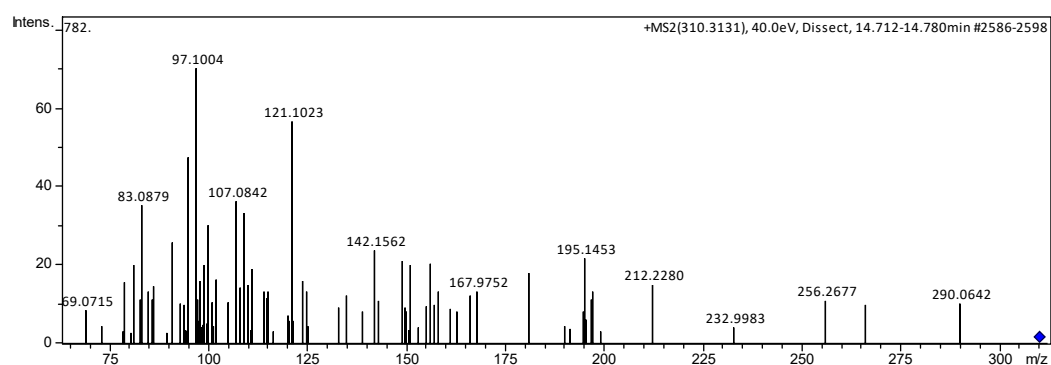


Figure S8. +ESI-QqTOF MS/MS spectrum of compound **3**.

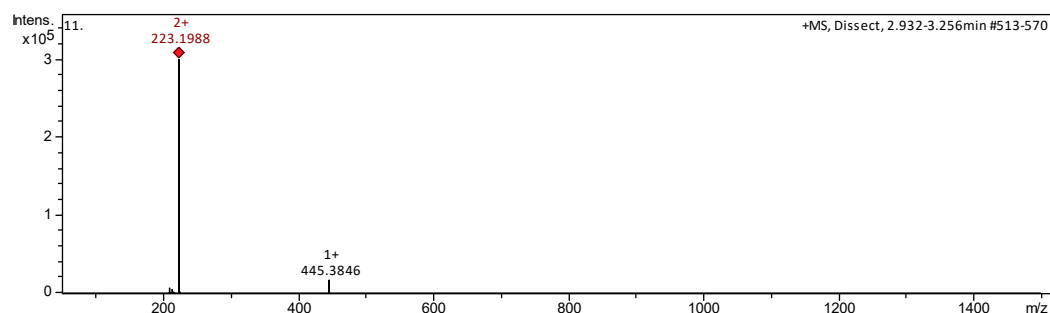


Figure S9. +ESI-QqTOF MS spectrum of compound **4** (cyclomicrophylline-A [4]); m/z 223.1988 $[M+2H]^{2+}$ and 445.3846 $[M+H]^+$.

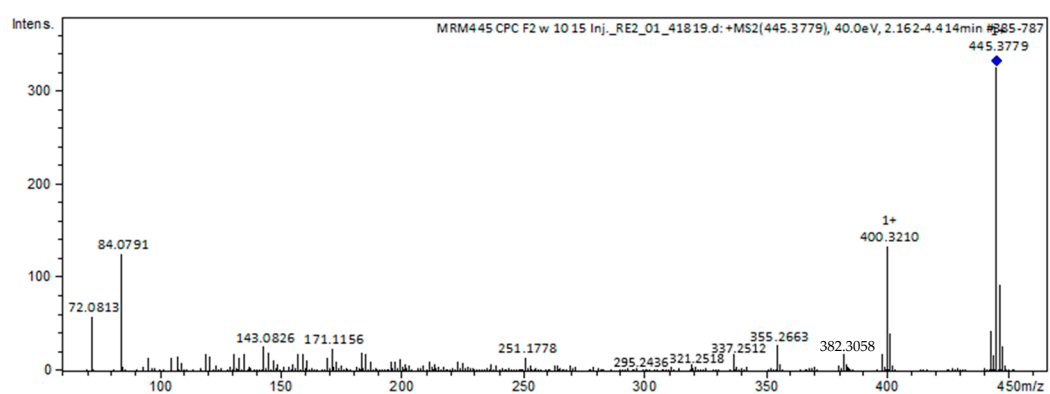


Figure S10. +ESI-QqTOF MS/MS spectrum of compound **4** (cyclomicrophylline-A [4]).

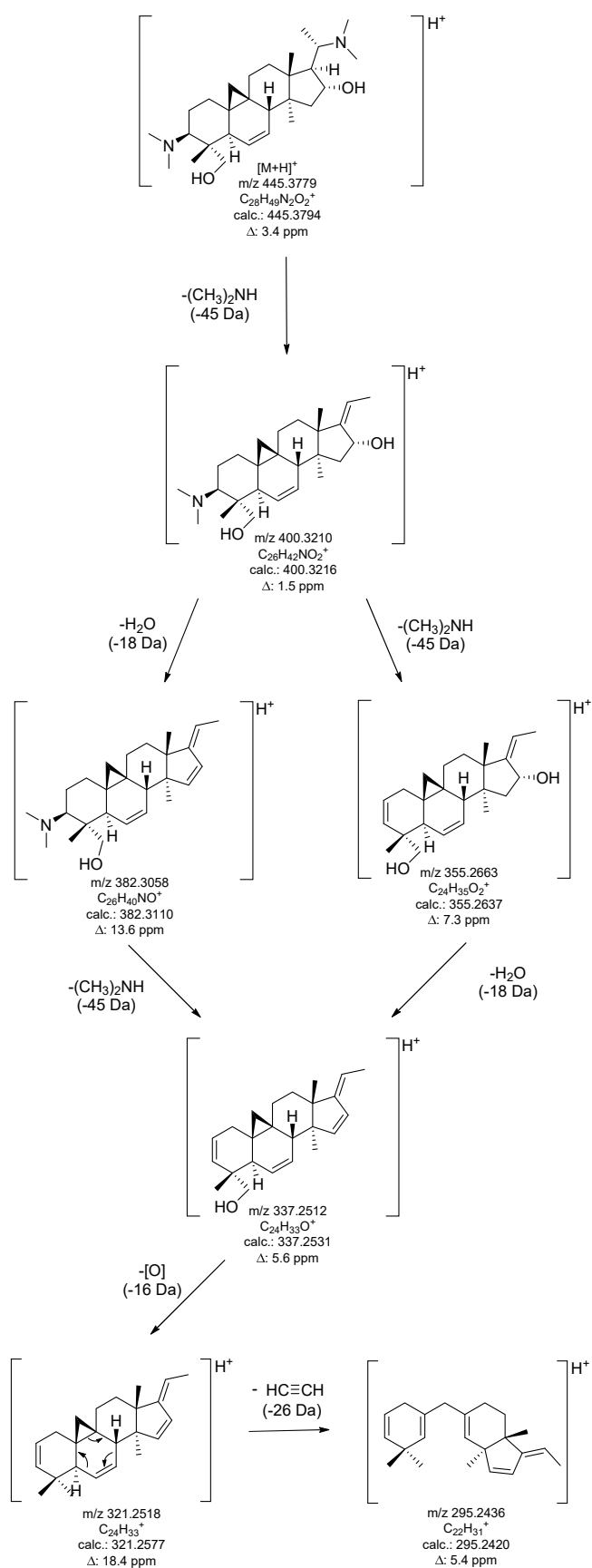


Figure S11. Possible fragmentation pathway of the $[M + H]^+$ ion of compound 4 (cyclomicrophyl-line-A).

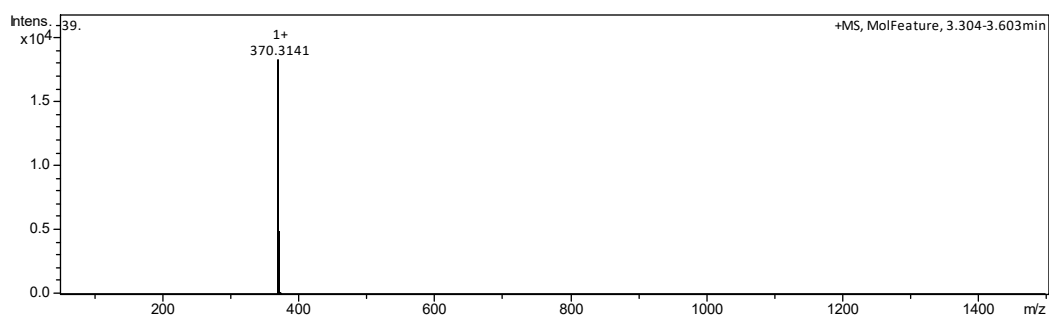


Figure S12. +ESI-QqTOF MS spectrum of compound **5**; 370.3141 [M+H]⁺.

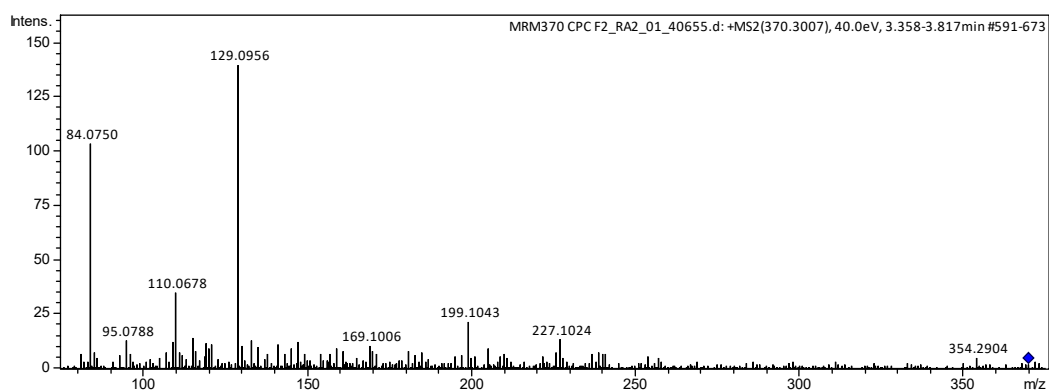


Figure S13. +ESI-QqTOF MS/MS spectrum of compound **5**.

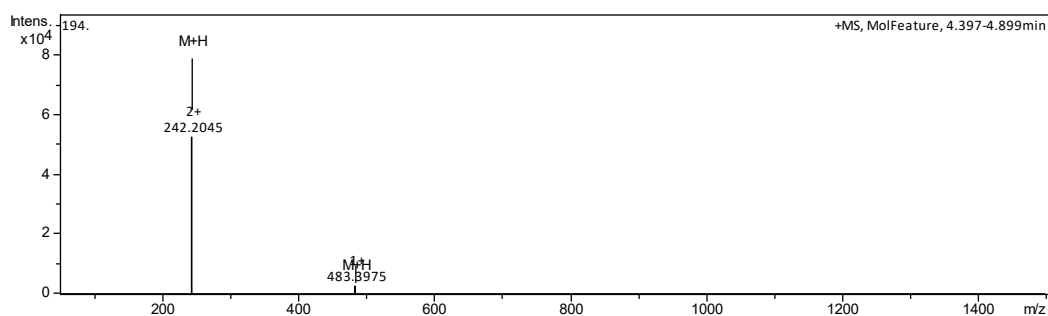


Figure S14. +ESI-QqTOF MS spectrum of compound 6; m/z 242.2045 [M+2H]²⁺ and 483.3975 [M+H]⁺.

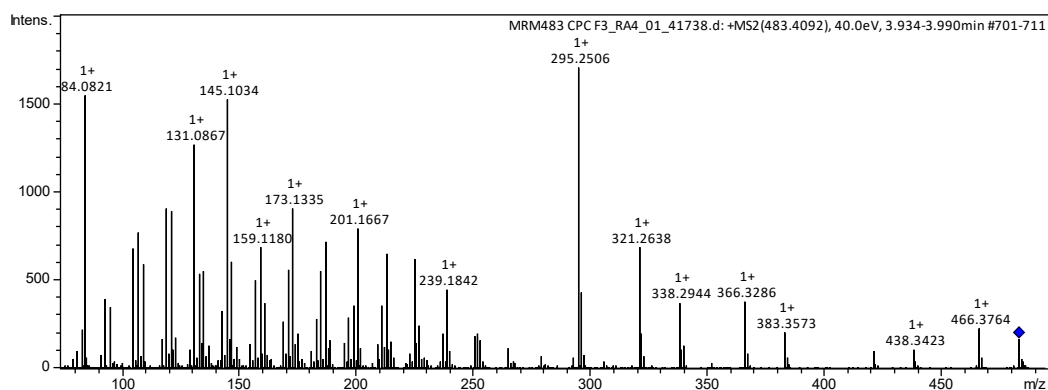


Figure S15. +ESI-QqTOF MS/MS spectrum of compound 6 (detailed in Figure S16).

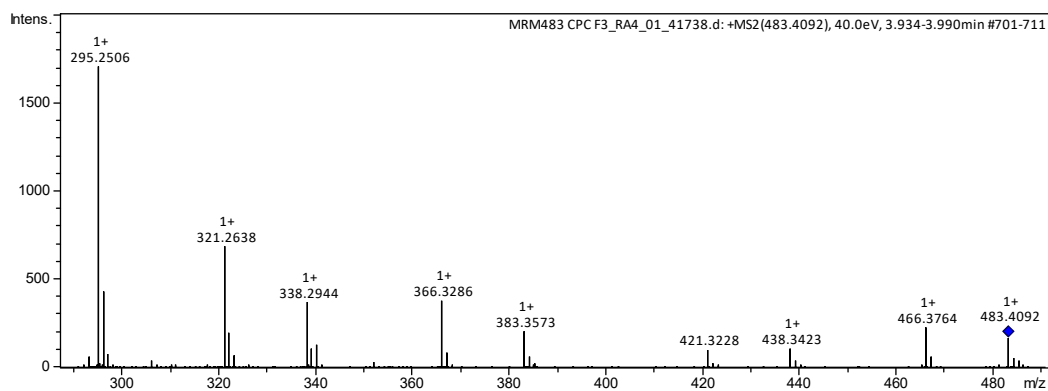


Figure S16. Detailed +ESI-QqTOF MS/MS spectrum of compound 6.

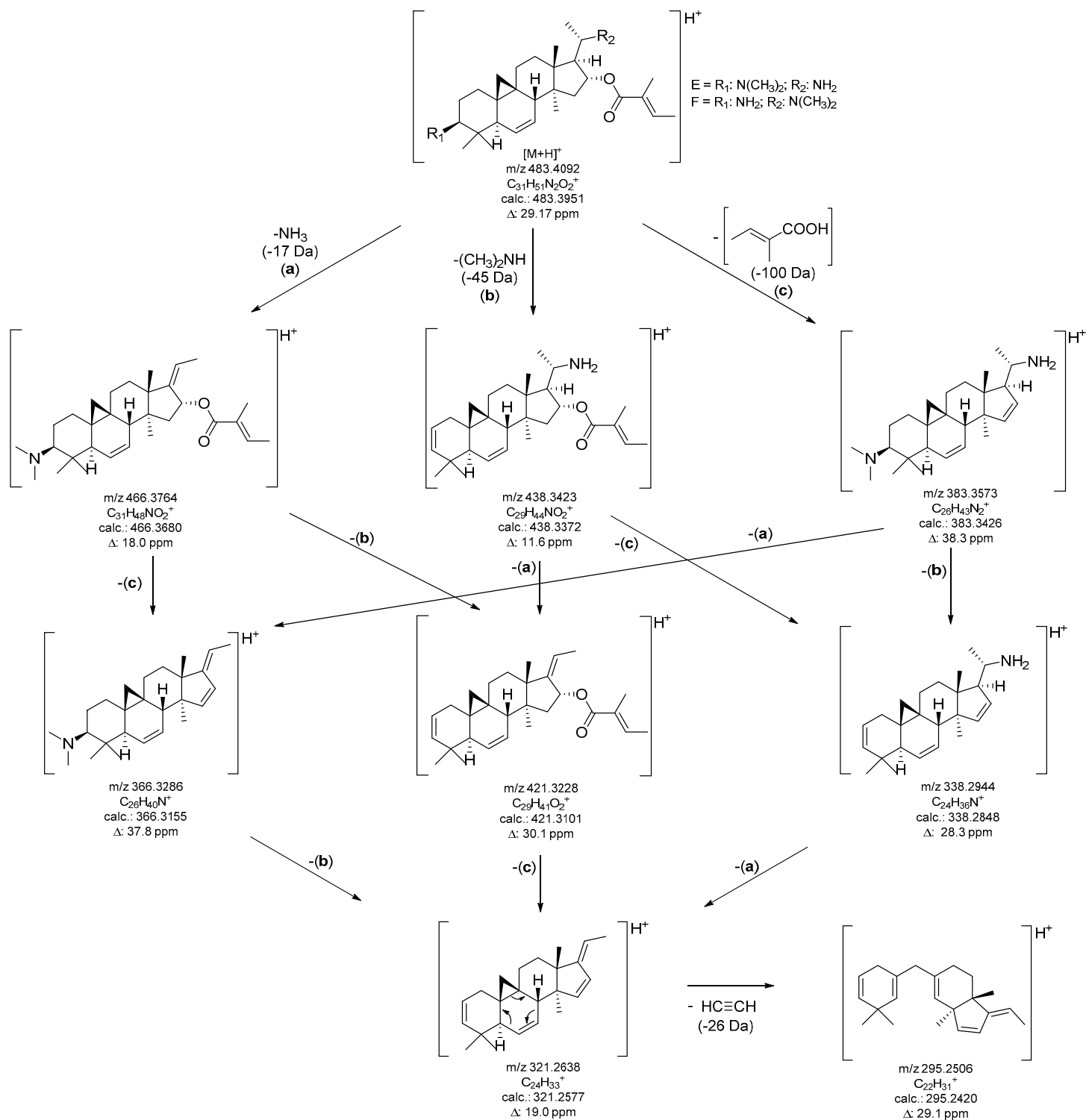


Figure S17. Possible fragmentation pathway of the $[M + H]^+$ ion of compound 6 (O-tigloylcyclovirobuxine-E or F; fragmentation exemplified for O-tigloylcyclovirobuxine-E).

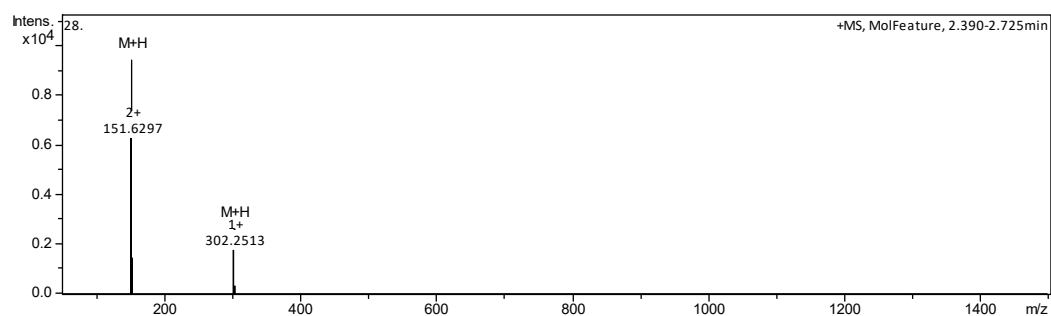


Figure S18. +ESI-QqTOF MS spectrum of compound 7; m/z 151.6297 [M+2H]²⁺ and 302.2513 [M+H]⁺.

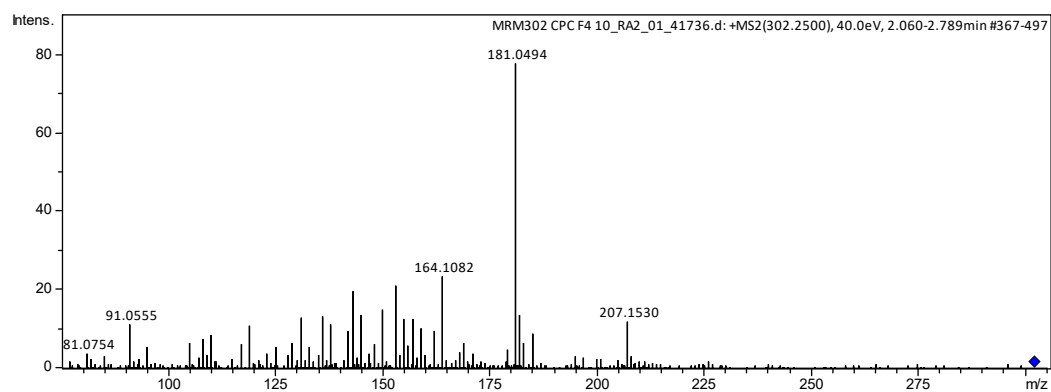


Figure S19. +ESI-QqTOF MS/MS spectrum of compound 7.

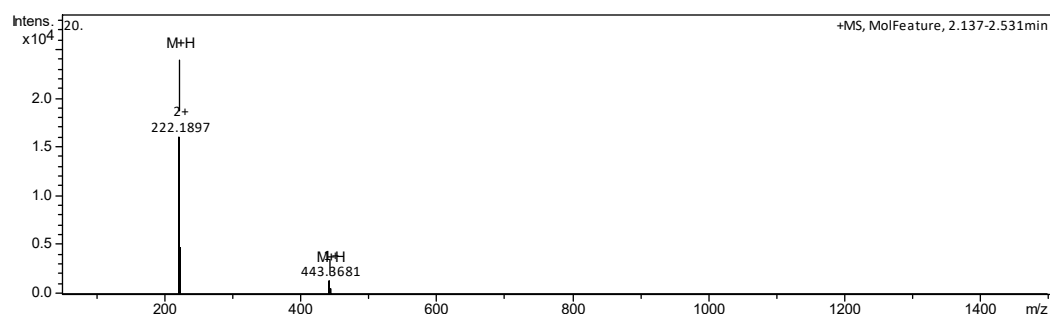


Figure S20. +ESI-QqTOF MS spectrum of compound 8 (N-formylcyclovirobuxine-B); m/z 222.1897 [M+2H]²⁺ and 443.3681 [M+H]⁺.

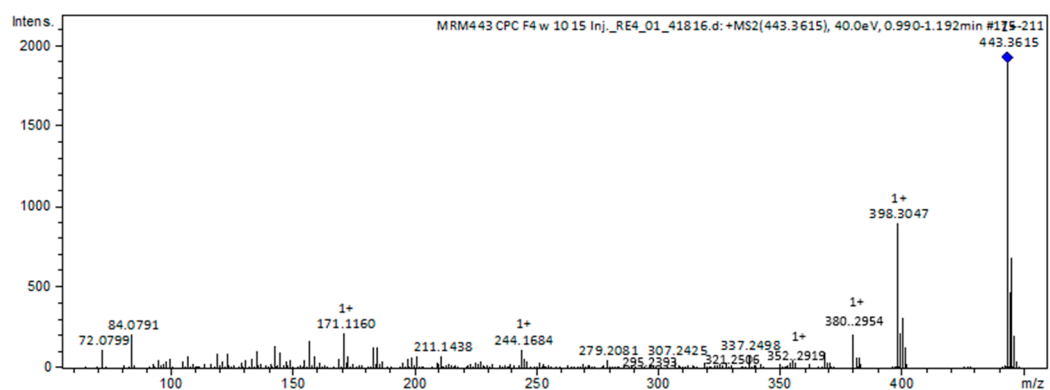


Figure S21. +ESI-QqTOF MS/MS spectrum of compound 8 (N-formylcyclovirobuxine-B).

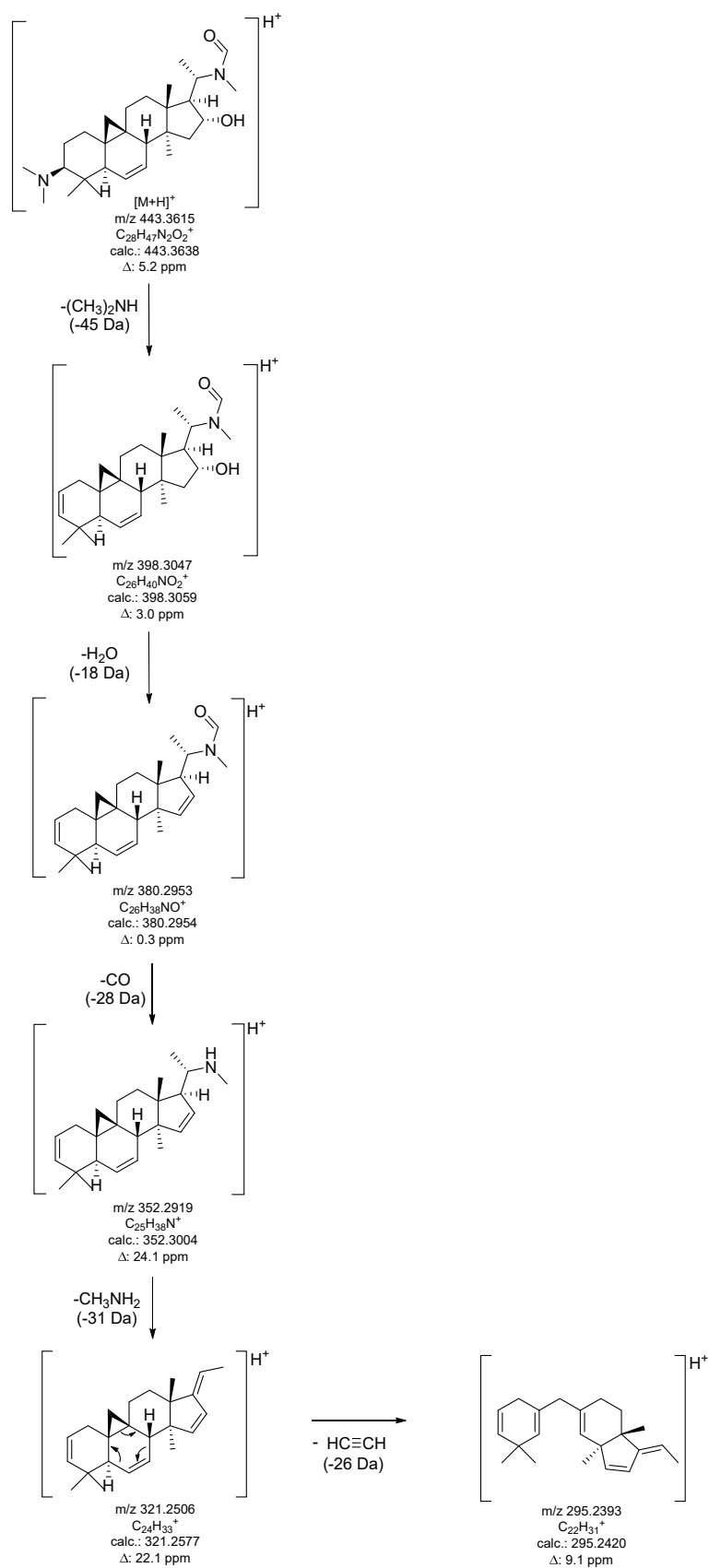


Figure S22. Possible fragmentation pathway of the $[M + H]^+$ ion of compound **8** (N-formylcyclovirobuxine-B).

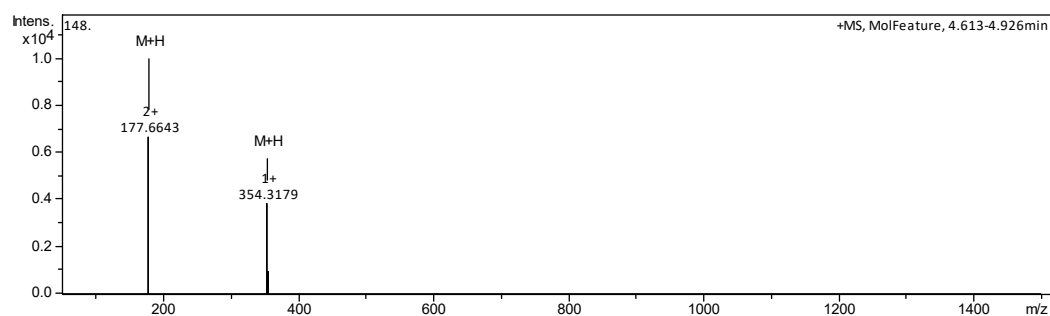


Figure S23. +ESI-QqTOF MS spectrum of compound **9**; m/z 177.6643 [M+2H]²⁺ and 354.3179 [M+H]⁺.

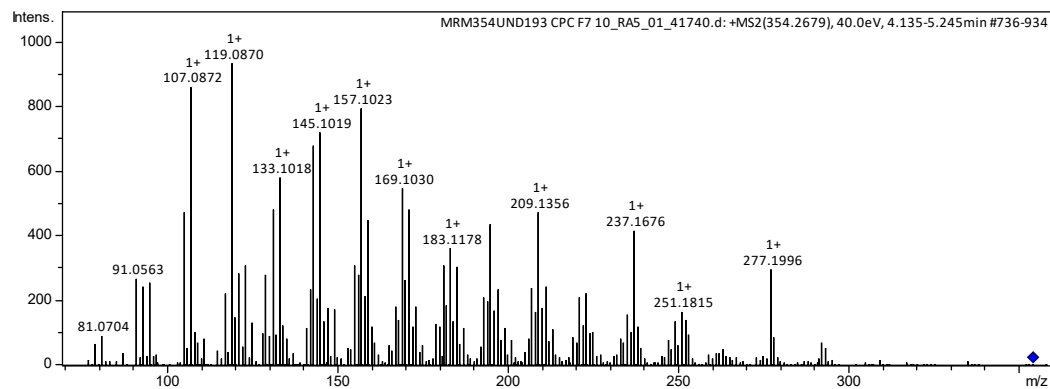


Figure S24. +ESI-QqTOF MS/MS spectrum of compound **9**.

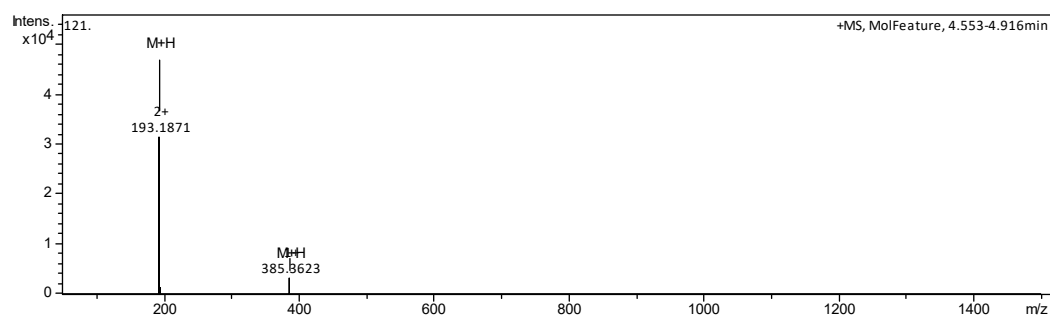


Figure S25. +ESI-QqTOF MS spectrum of compound **10**; m/z 193.1871 $[M+2H]^{2+}$ and 385.3623 $[M+H]^+$.

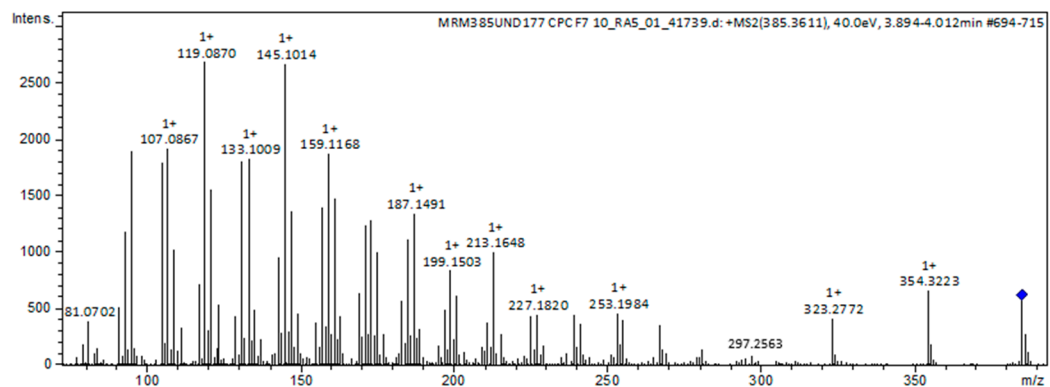


Figure S26. +ESI-QqTOF MS/MS spectrum of compound **10**.

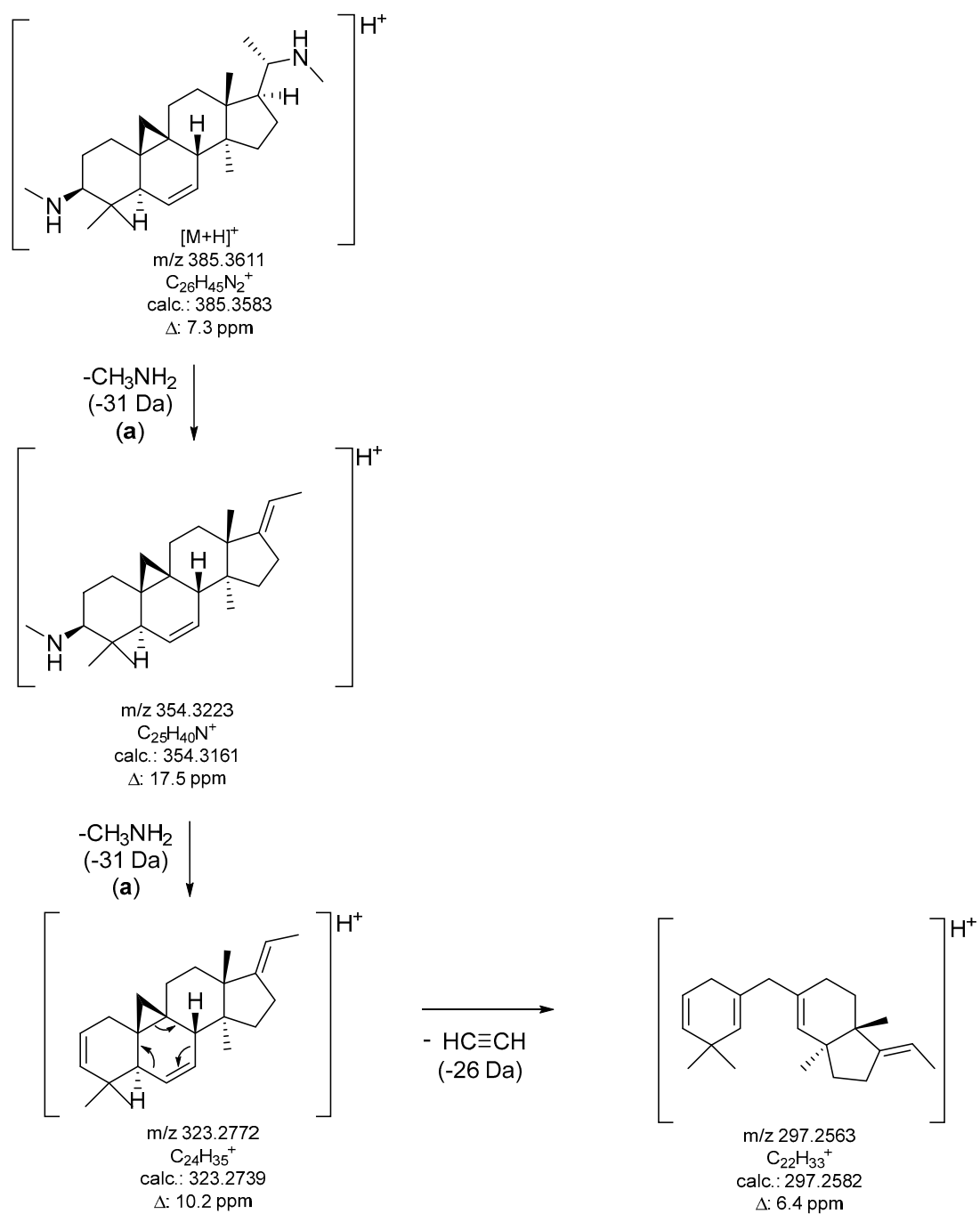


Figure S27. Possible fragmentation pathway of the $[M + H]^+$ ion of compound 10.

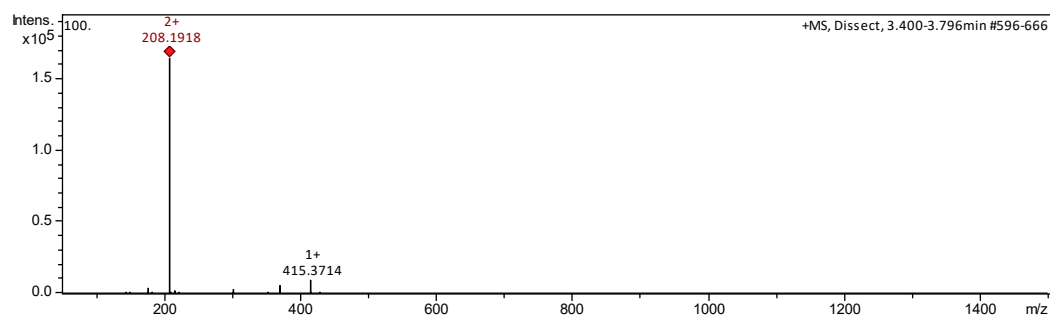


Figure S28. +ESI-QqTOF MS spectrum of compound **11** (cyclovirobuxine-B [4]); m/z 208.1918 $[M+2H]^{2+}$ and 415.3714 $[M+H]^+$.

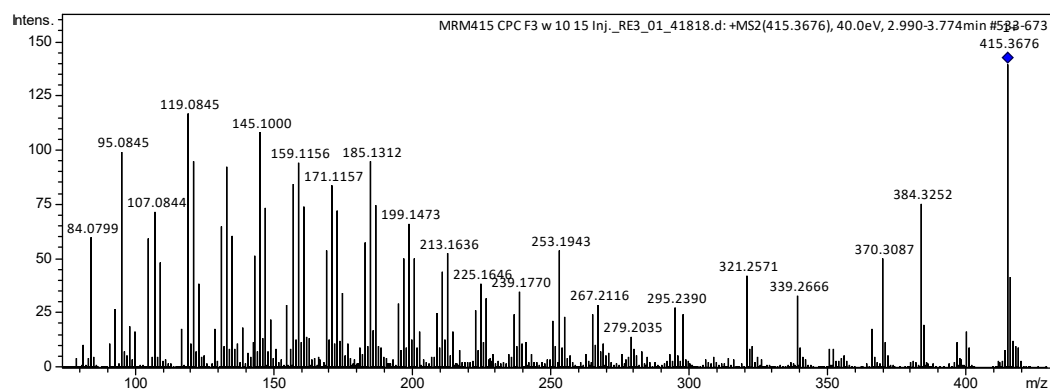


Figure S29. +ESI-QqTOF MS/MS spectrum of compound **11** (cyclovirobuxine-B [4]).

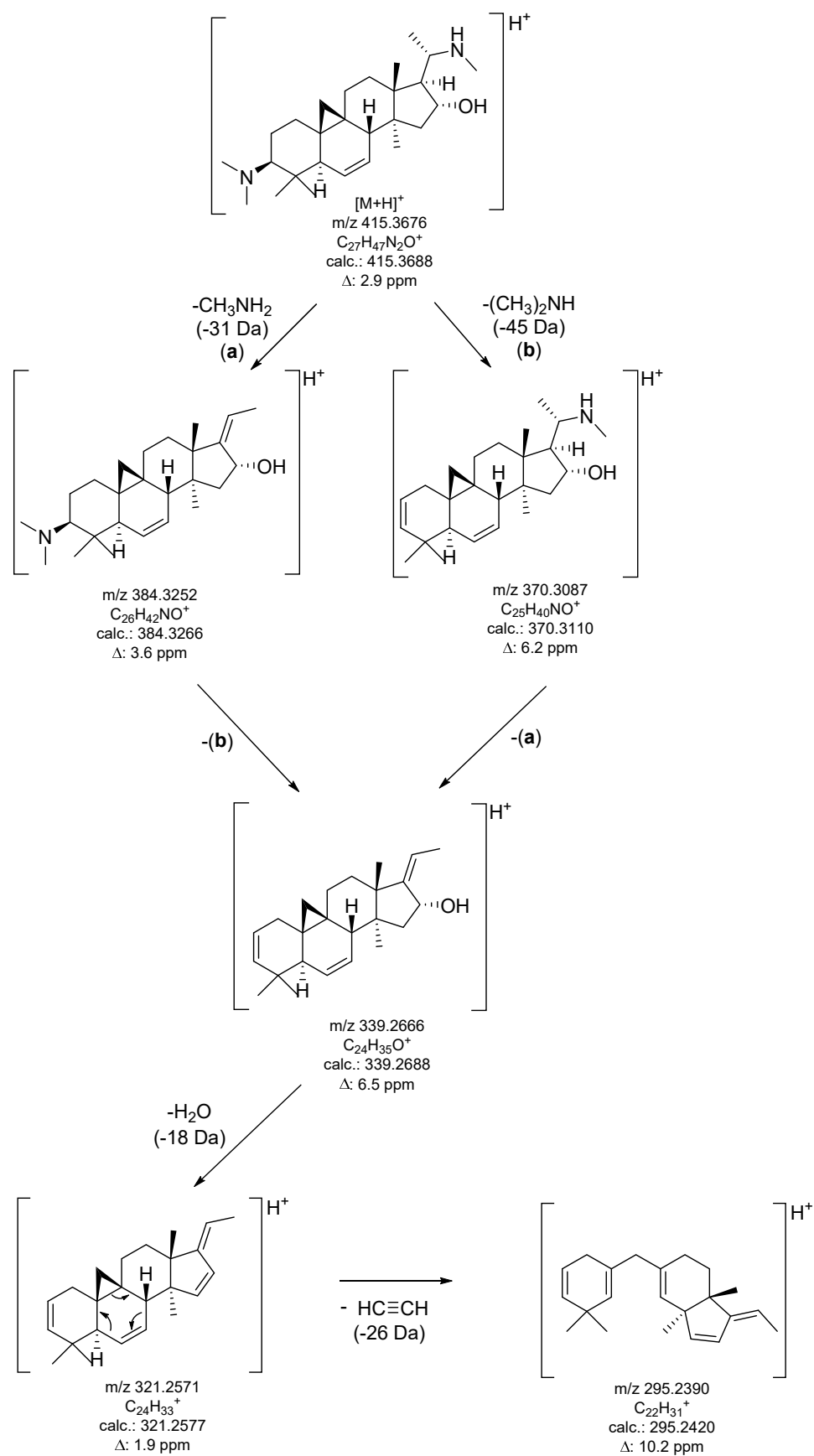


Figure S30. Possible fragmentation pathway of the $[M + H]^+$ ion of compound **11** (cyclovirobuxeine-B).