

Determination of the absolute configuration of bioactive indole-containing pyrazino[2,1-*b*]quinazoline-3,6-diones and study of their *in vitro* metabolic profile

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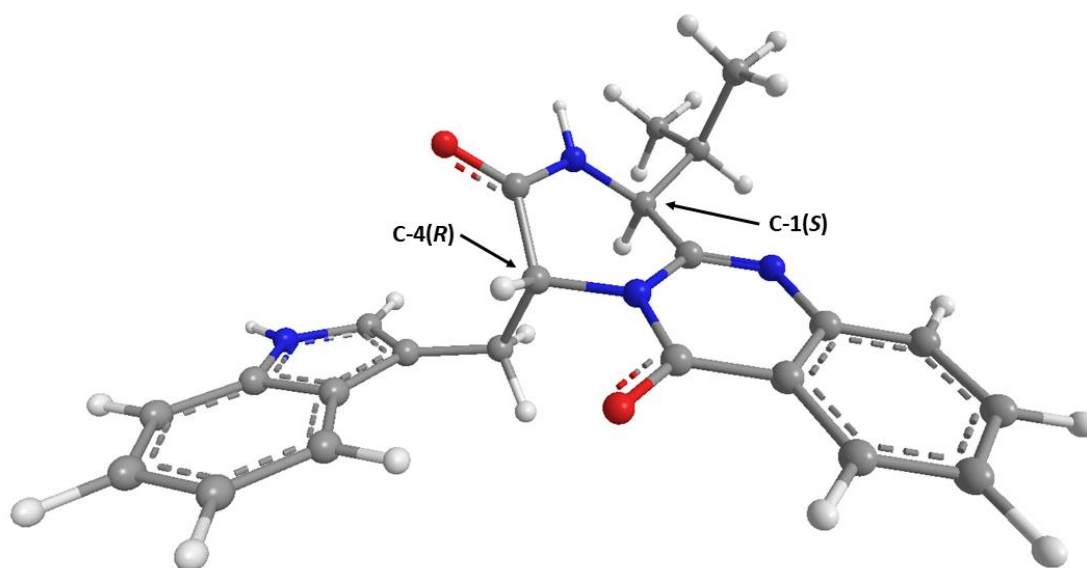


Figure S1. Model of the most abundant conformation of **1** (B3LYP/6-311+G(2d,p) lowest energy conformer accounting for 51% of conformer population) in its (1*S*,4*R*) configuration, as assigned by ECD.

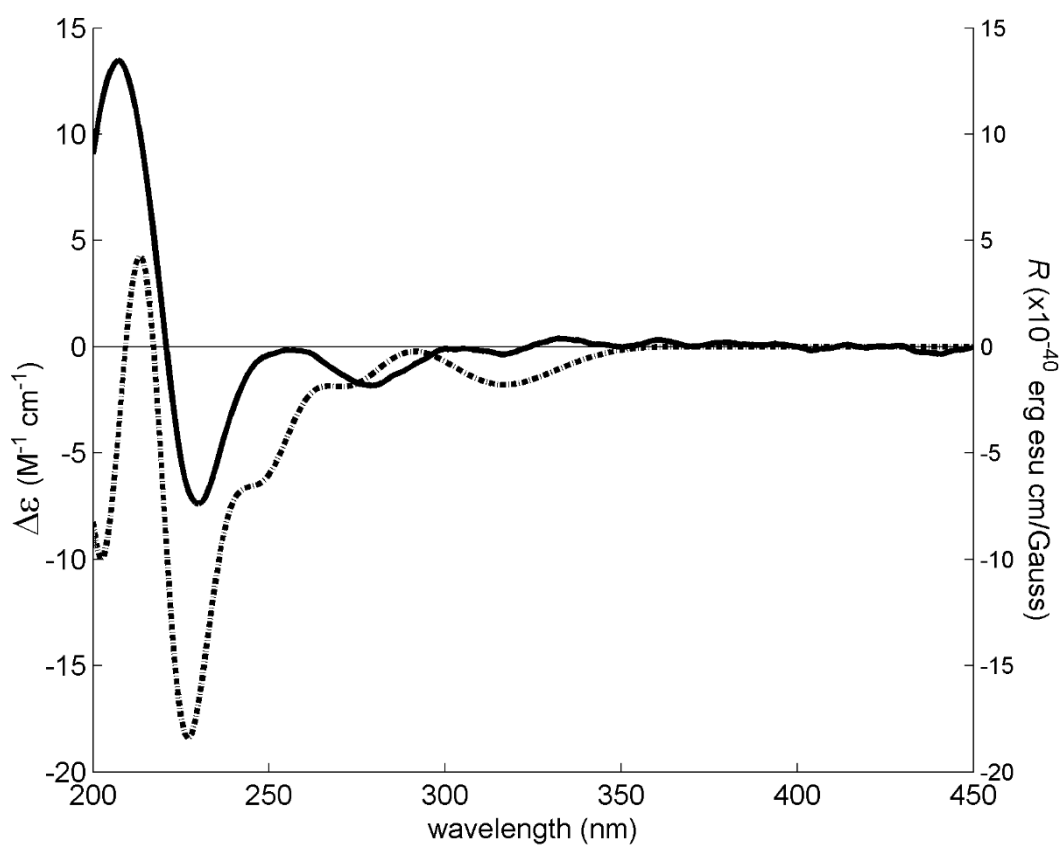


Figure S2. Experimental ECD spectrum (solid line, left axis) of (-)-**1** and theoretical ECD spectrum (dotted line, right axis) of (1*S*,4*R*)-**1** configuration.

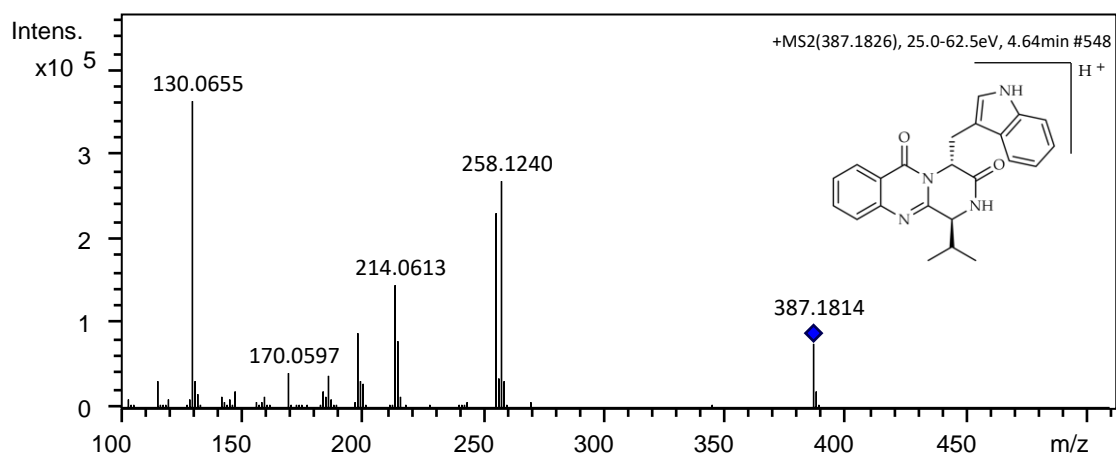


Figure S3. LC-HRMS/MS spectrum of fiscalin B (**1**), m/z 387.1826.

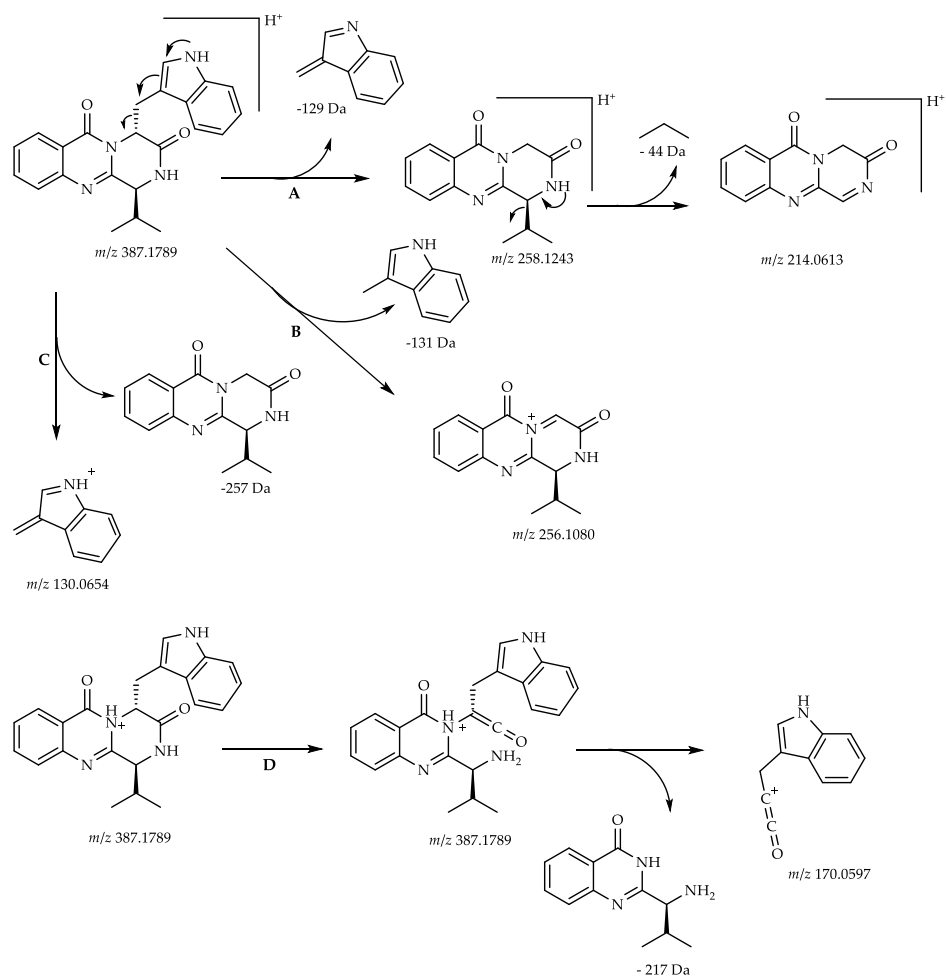


Figure S4. Proposed fragmentation pathways of fiscalin B (**1**) in positive ion mode.

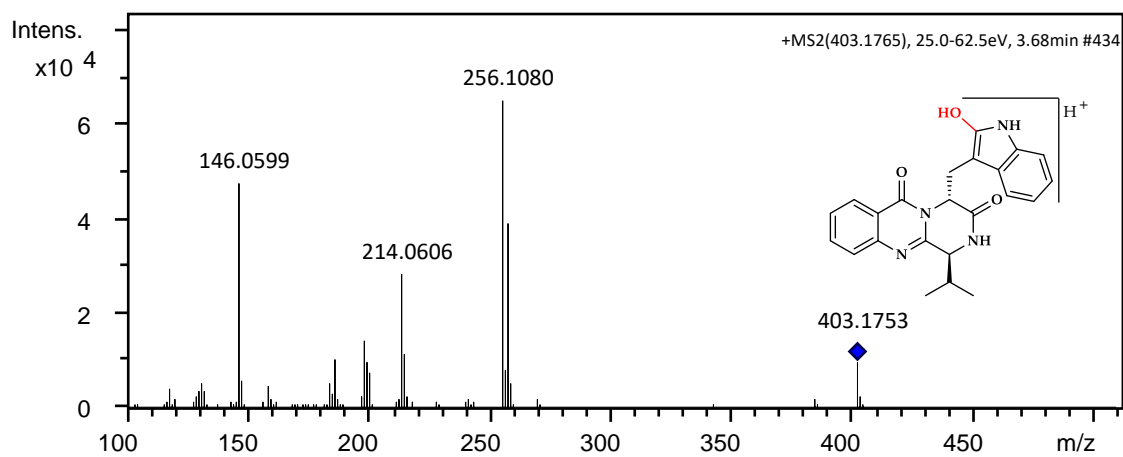


Figure S5. LC-HRMS/MS spectrum of M1, m/z 403.1765.

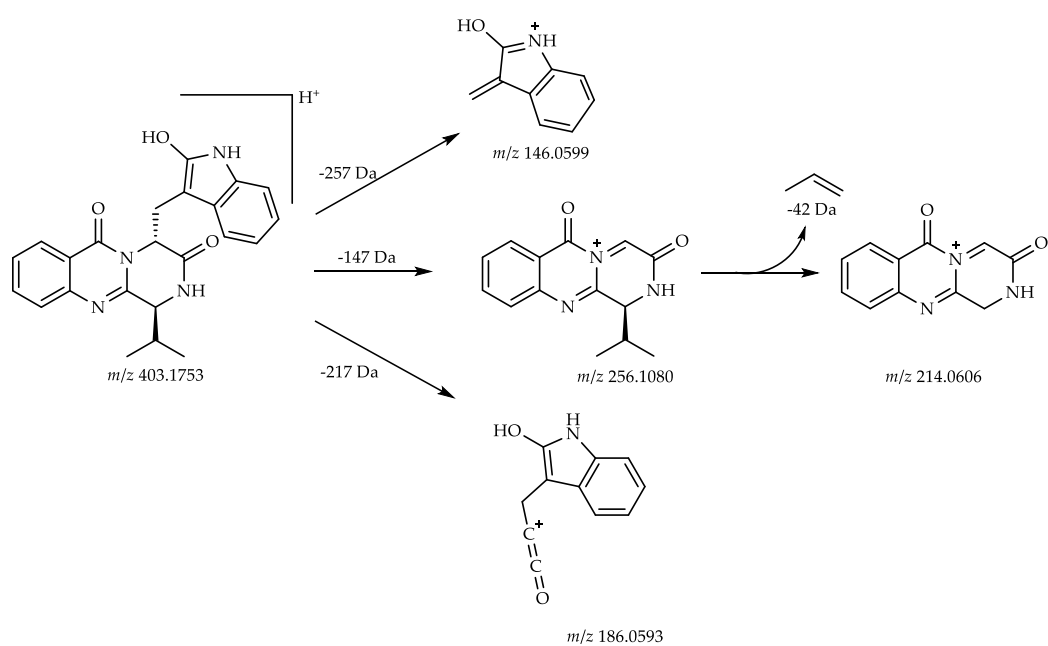


Figure S6. Proposed fragmentation pathways of metabolite M1.

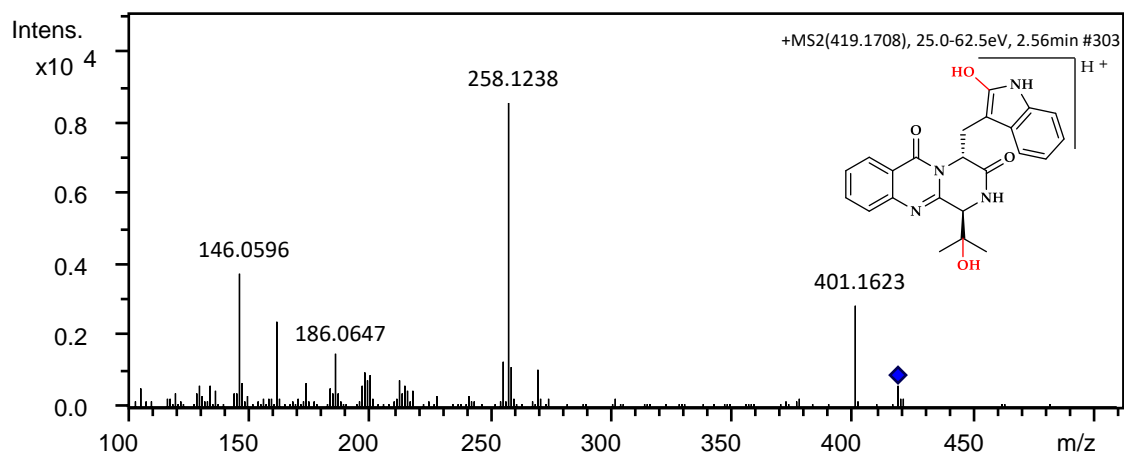


Figure S7. LC-HRMS/MS spectrum of M2, m/z 419.1708.

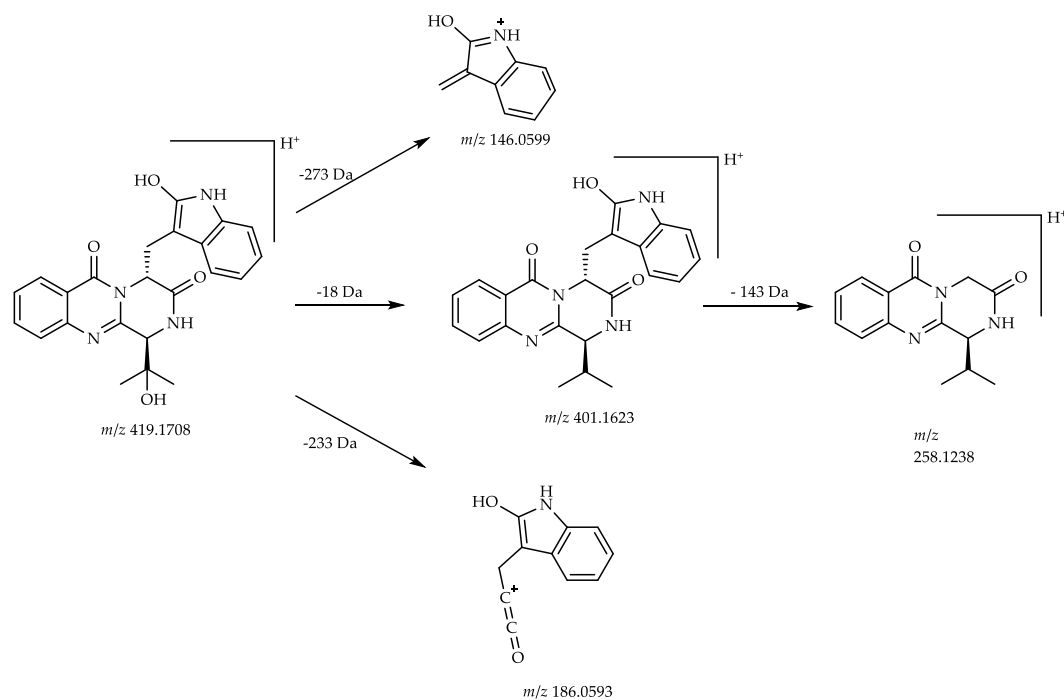


Figure S8. Proposed fragmentation pathways of metabolite M2.

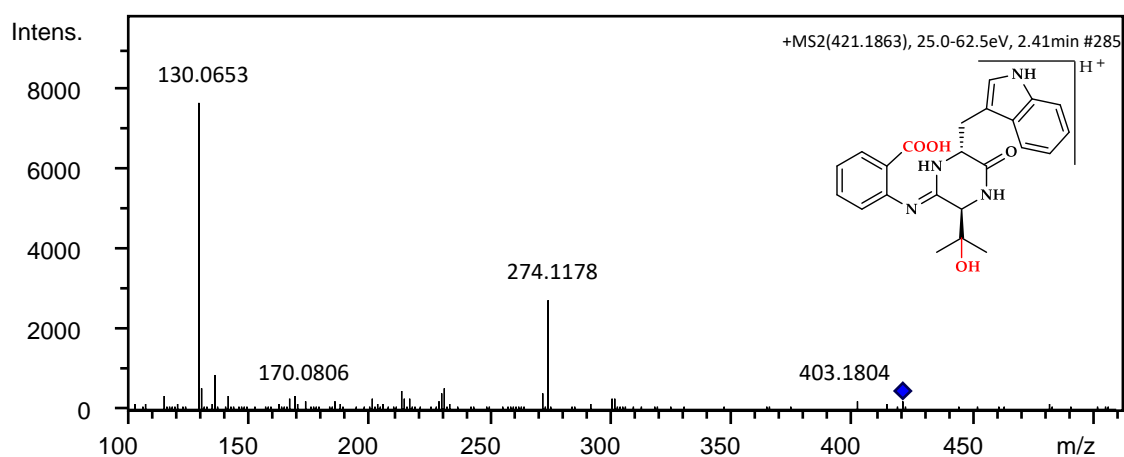


Figure S9. LC-HRMS/MS spectrum of M3, m/z 421.1863.

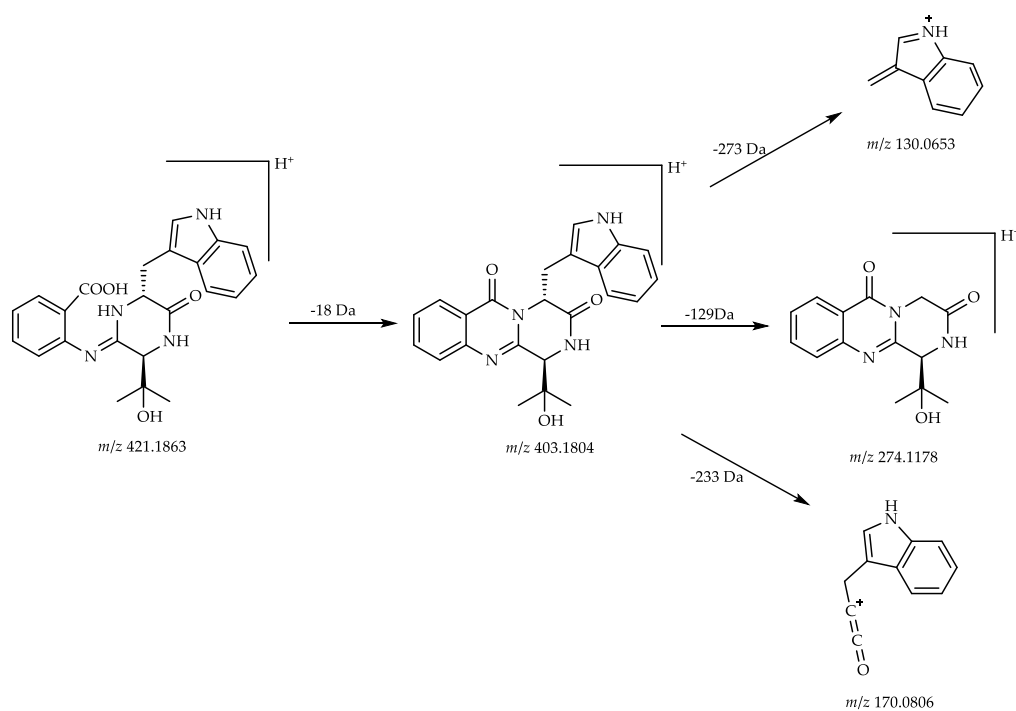


Figure S10. Proposed fragmentation pathways of metabolite M3.

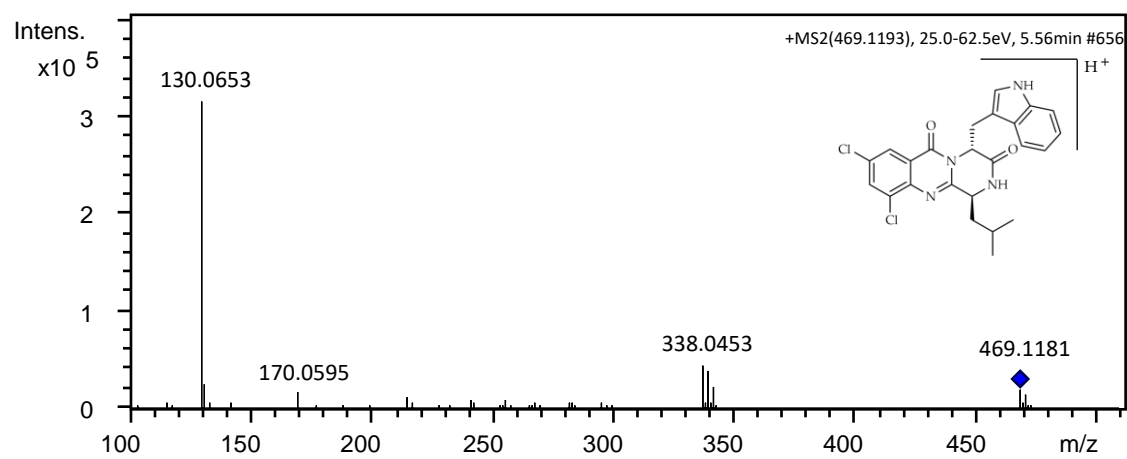


Figure S11. LC-HRMS/MS spectrum of fiscalin B chloro derivative (**2**), m/z 469.1193 in positive ion mode

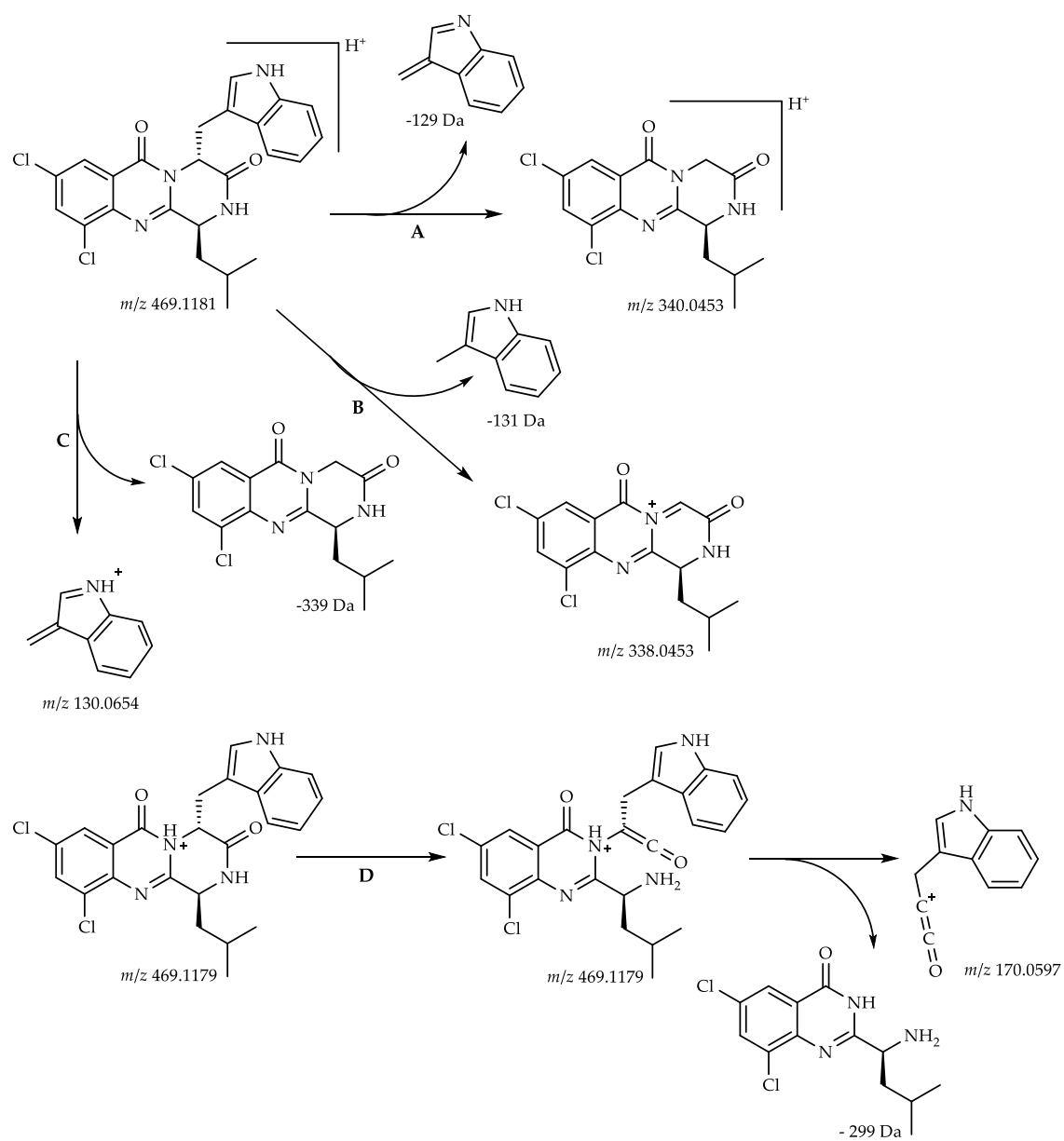


Figure S12. Proposed fragmentation pathways of fiscalin B chloro derivative (2).

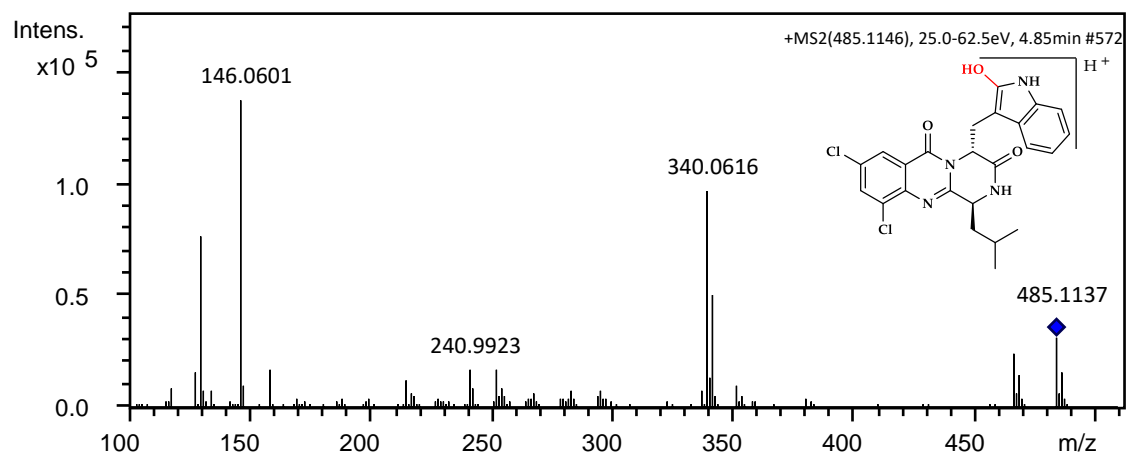


Figure S13. LC-HRMS/MS spectrum of M4, m/z 485.1146.

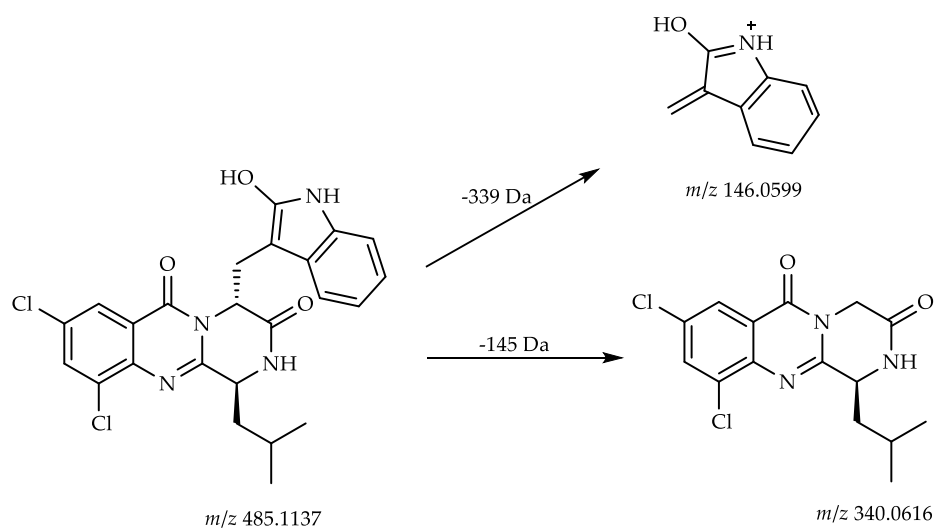


Figure S14. Proposed fragmentation pathways of metabolite M4.

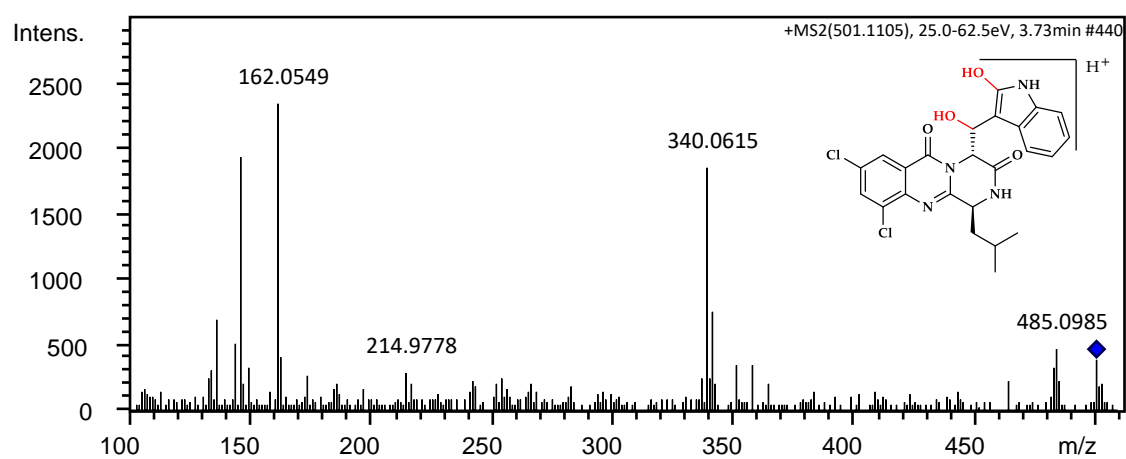


Figure S15. LC-HRMS/MS spectrum of M5, m/z 501.1105.

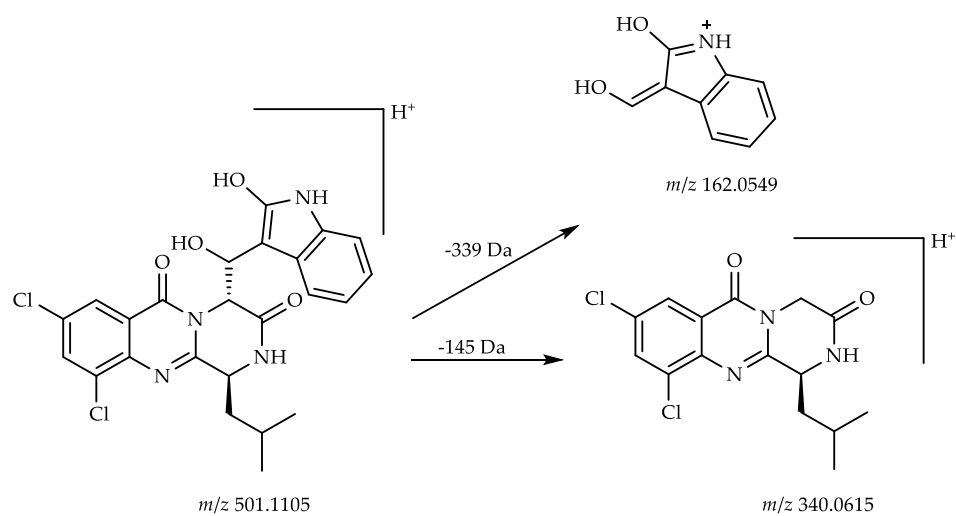


Figure S16. Proposed fragmentation pathways of metabolite M5.