

Associated content

Supporting Information

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Fig. S1 Accurate MS/MS spectrum of osthole and its proposed fragmentation pathway.

Fig. S2 MS/MS spectra and proposed fragmentation pathways of of M12, M33, M37, M41, M46, M56, M60 and M62.

Table S1 The involved biotransformation and mass change

Code	Description	Formula	Mass
1	Oxidation	+O	15.9949
2	Hydrogenation	+2H	2.0157
3	Hydrolysis	+H ₂ O	18.0106
4	Methylation	+CH ₂	14.0157
5	Demethylation	-CH ₂	-14.0157
6	Oxydrolisis	+H ₂ O ₂	34.0055
7	Loss of OCH ₂	-OCH ₂	-30.0106
8	Glucuronide Conjugation	+C ₆ H ₈ O ₆	176.0321
9	Sulfate Conjugation	+SO ₃	79.9568
10	Dehydrogenation	-2H	-2.0157
11	Loss of C ₅ H ₈	-C ₅ H ₈	-68.0626
12	Loss of C ₄ H ₈	-C ₄ H ₈	-56.0626
13	Loss of C ₃ H ₆	-C ₃ H ₆	-42.0470
14	Loss of C ₂ H ₄	-C ₂ H ₄	-28.0313
15	Loss of CO	-CO	-27.9949
16	Loss of H ₂ O	-H ₂ O	-18.0106
17	3,4-Epoxyde	+O	+15.9949
18	Aldehylation	-CO+2H	-25.9793
19	Phosphorylation	+HPO ₃	+79.9663
20	S-cysteine Conjugation	+C ₃ H ₅ NO ₂ S	+119.0041
21	N-acetylcysteine Conjugation	+C ₅ H ₇ NO ₃ S	+161.0147

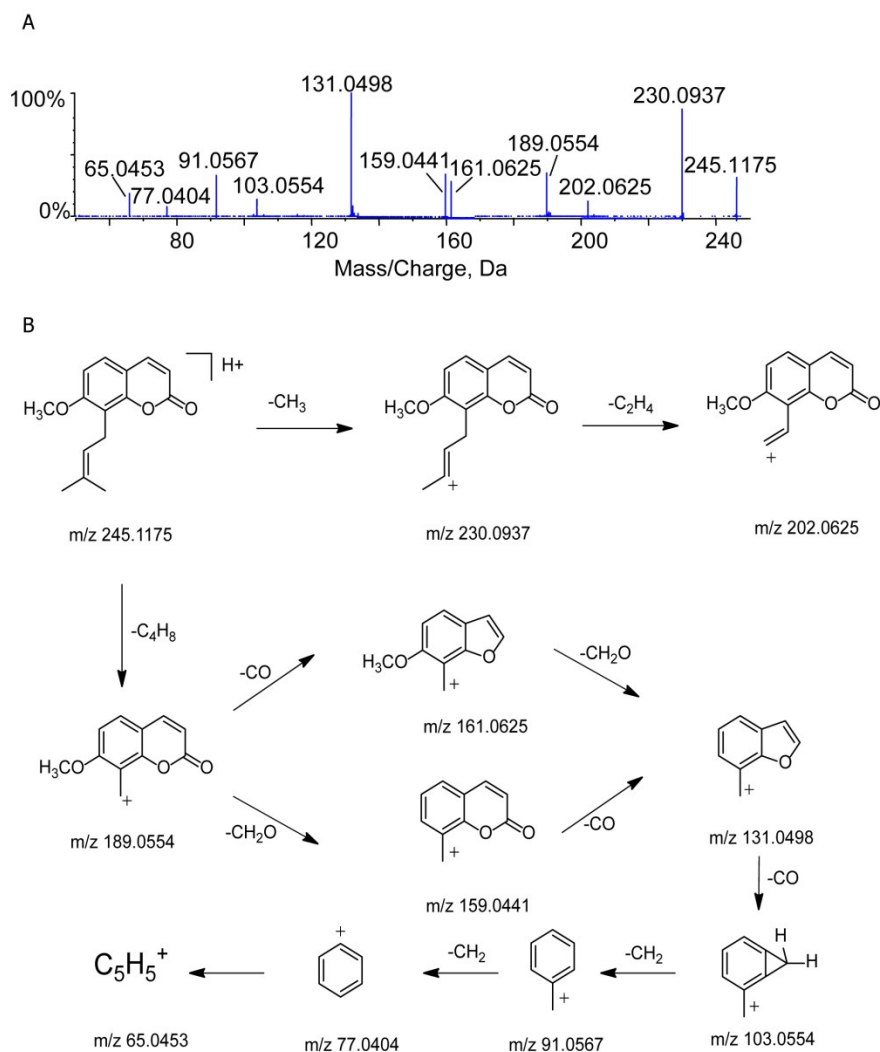


Fig. S1 Accurate MS/MS spectrum of osthole
and its proposed fragmentation pathway.

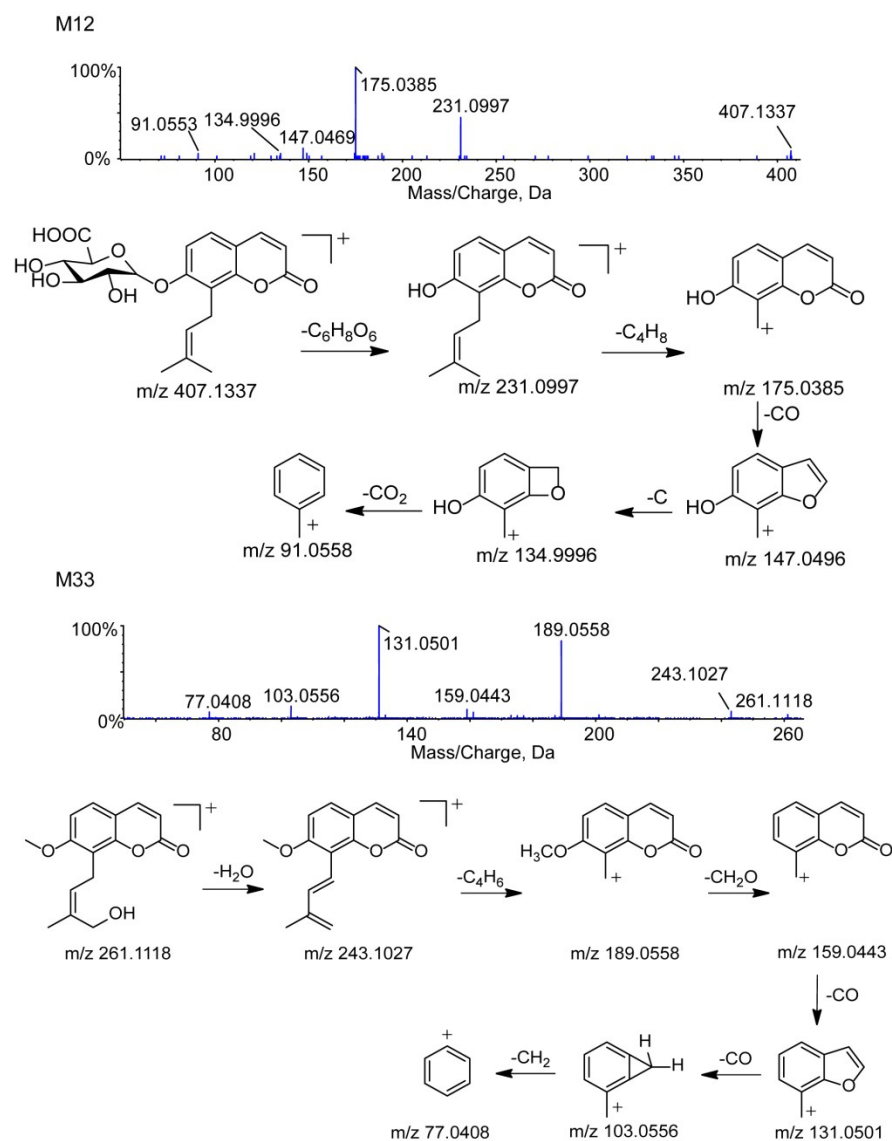


Fig. S2 MS/MS spectra and proposed fragmentation pathways of
of M12, M33, M37, M41, M46, M56, M60 and M62.

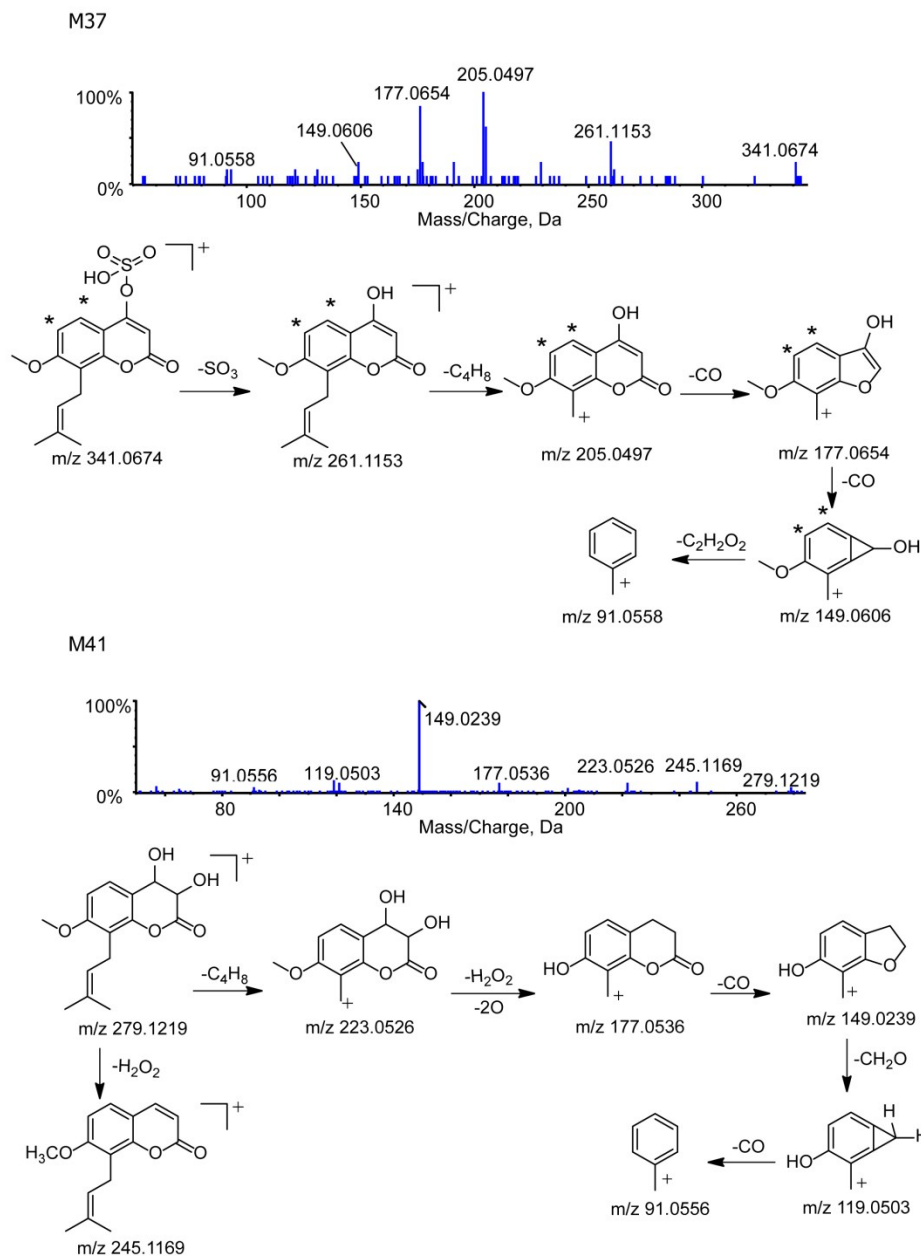
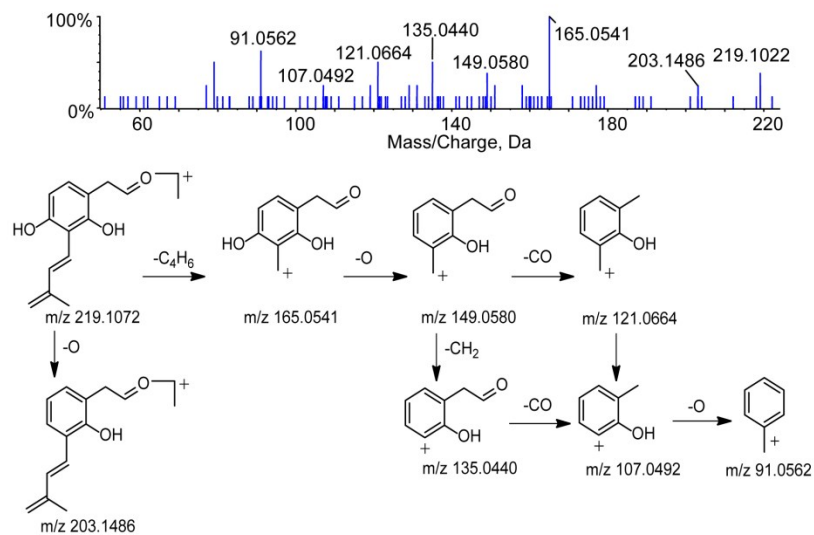


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M46



M56

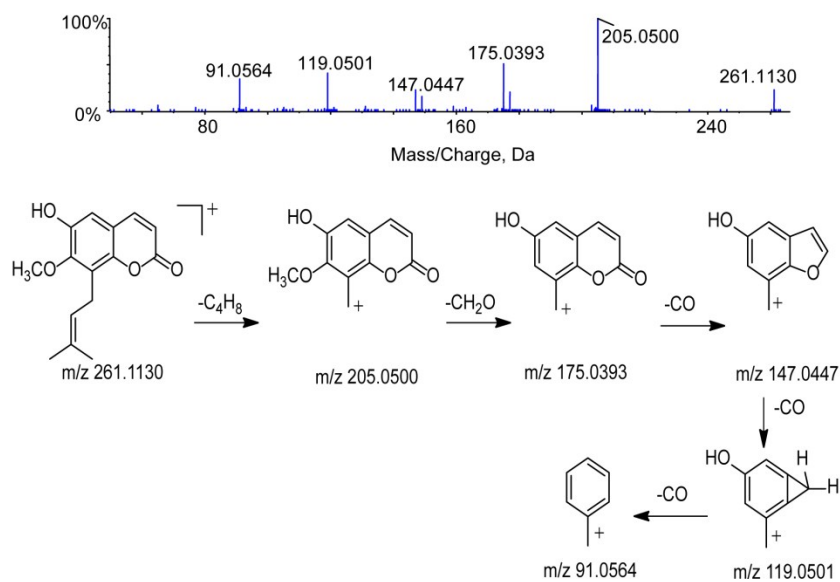


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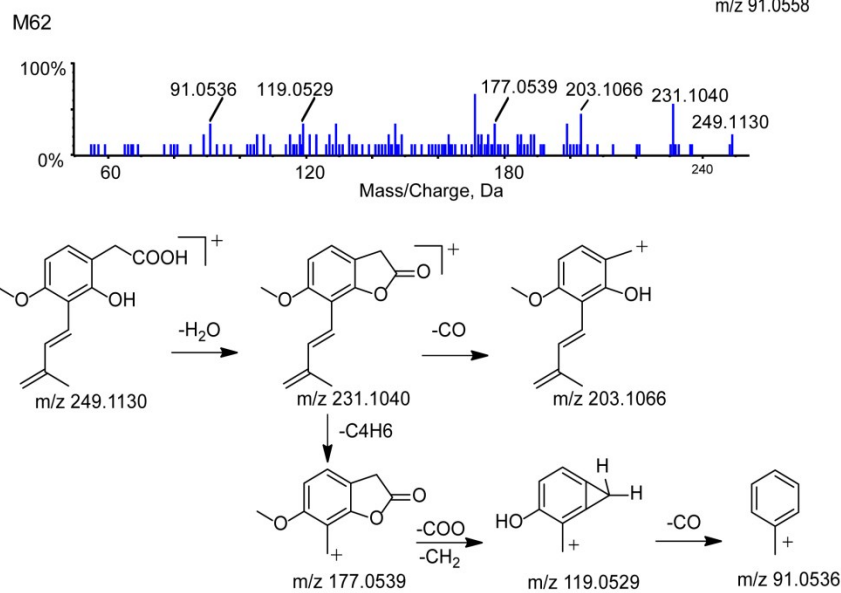
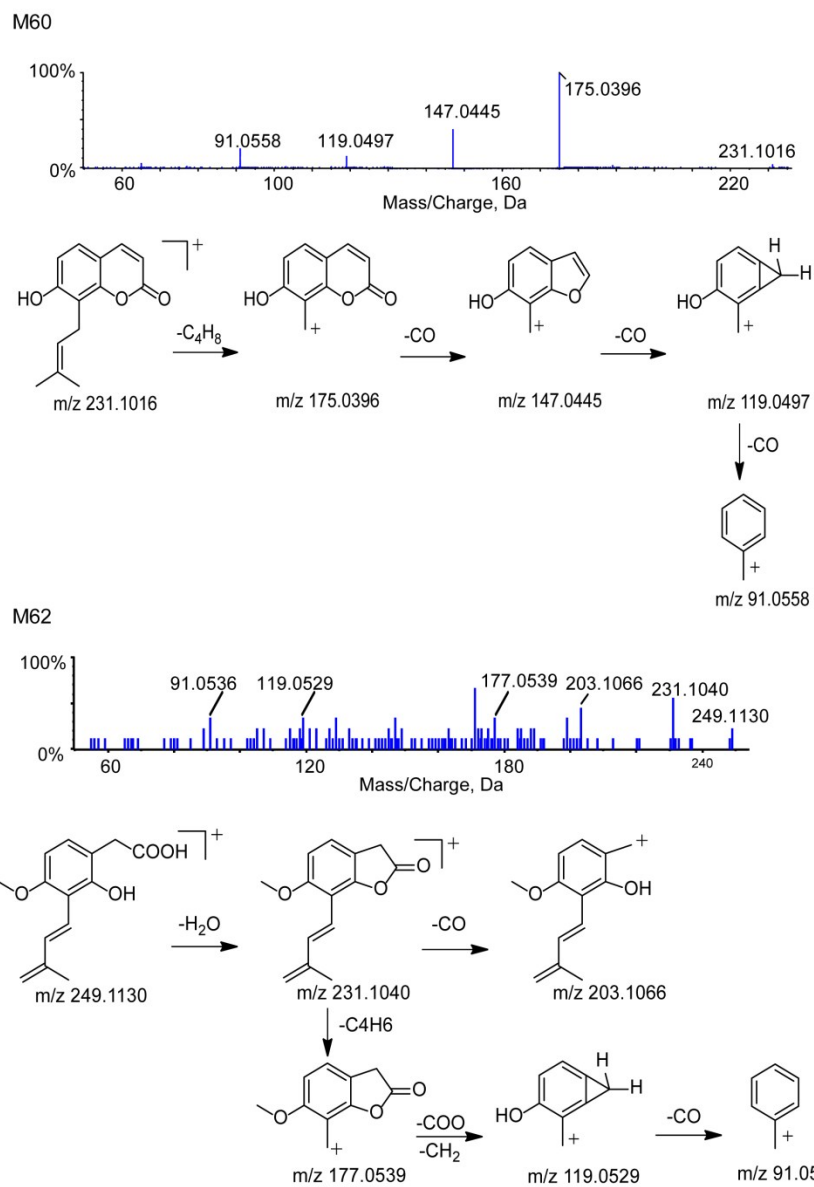


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