Four New Isocoumarins from *Cajanus cajan*

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Abstract

Four new isocoumarins, denominated Cajanolactone B, C, D1 and D2 (**1-4**), were isolated from ethanolic extract of the leaves of *Cajanus cajan.* The structural elucidation has been completed mainly depending on extensively spectroscopic analysis including UV, IR, NMR (1D and 2D), HRESIMS and chiral analysis. Notably, all these new isocoumarins were found to exist in racematic forms, among which compounds **3** and **4** share the same planar structure. This finding suggests that at least the biosynthesis of isocoumarin in *C. cajan* is chiral tolerant. A plausible biogenetic pathway of compounds **1-4** is proposed.

Supporting Information

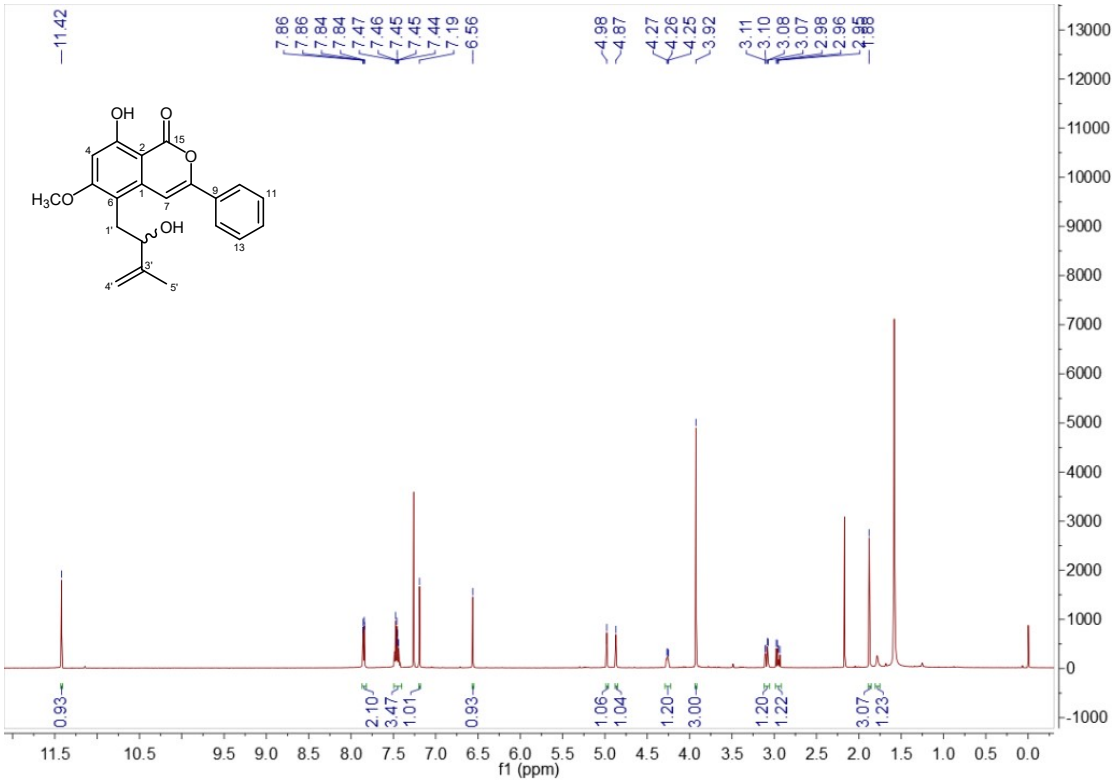

Figure S1. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **1**.

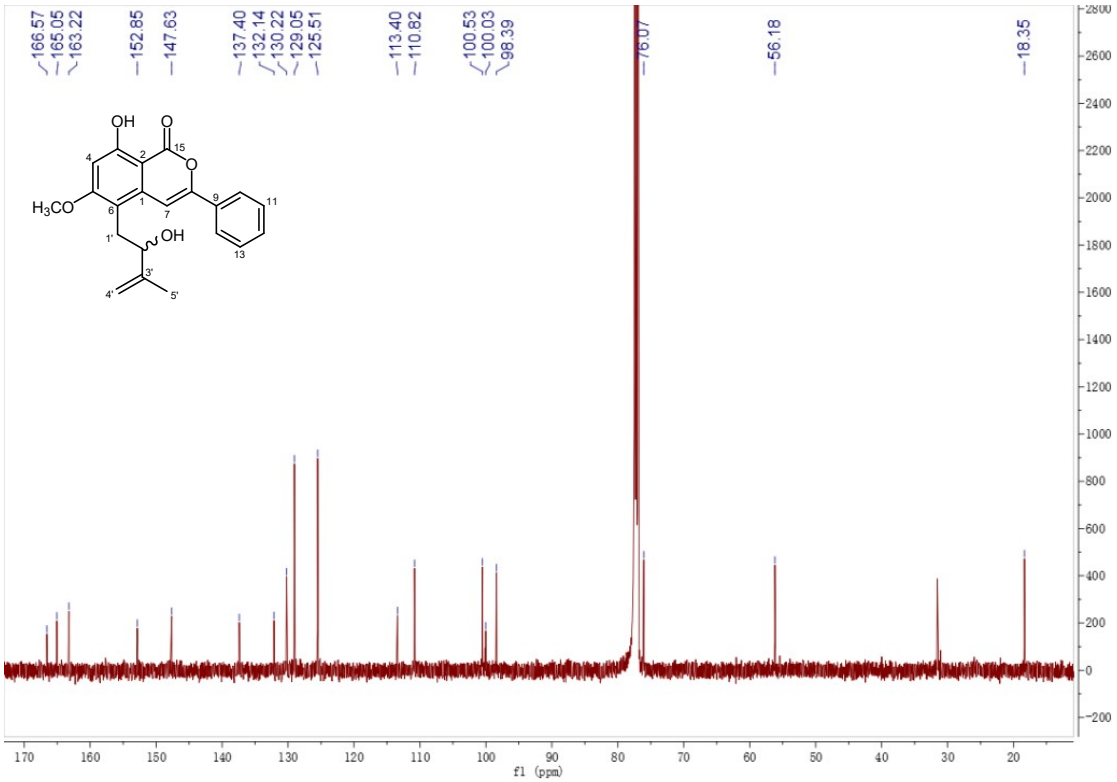

Figure S2. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **1**.

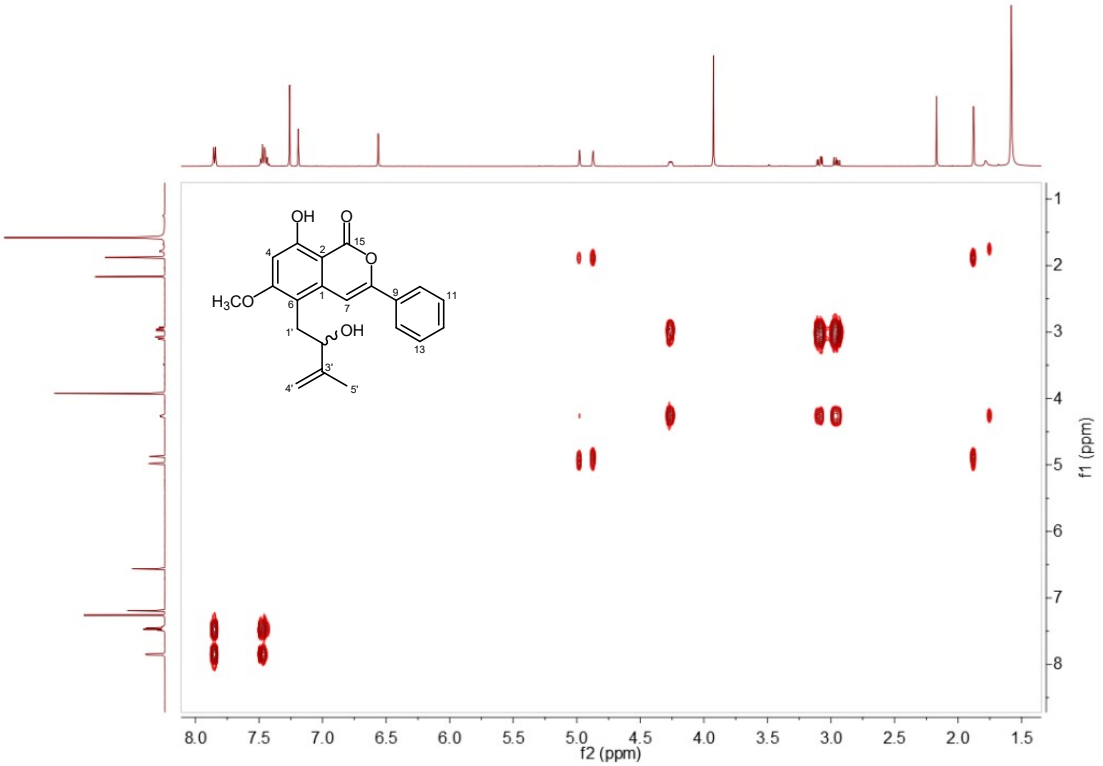

Figure S3. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **1**.

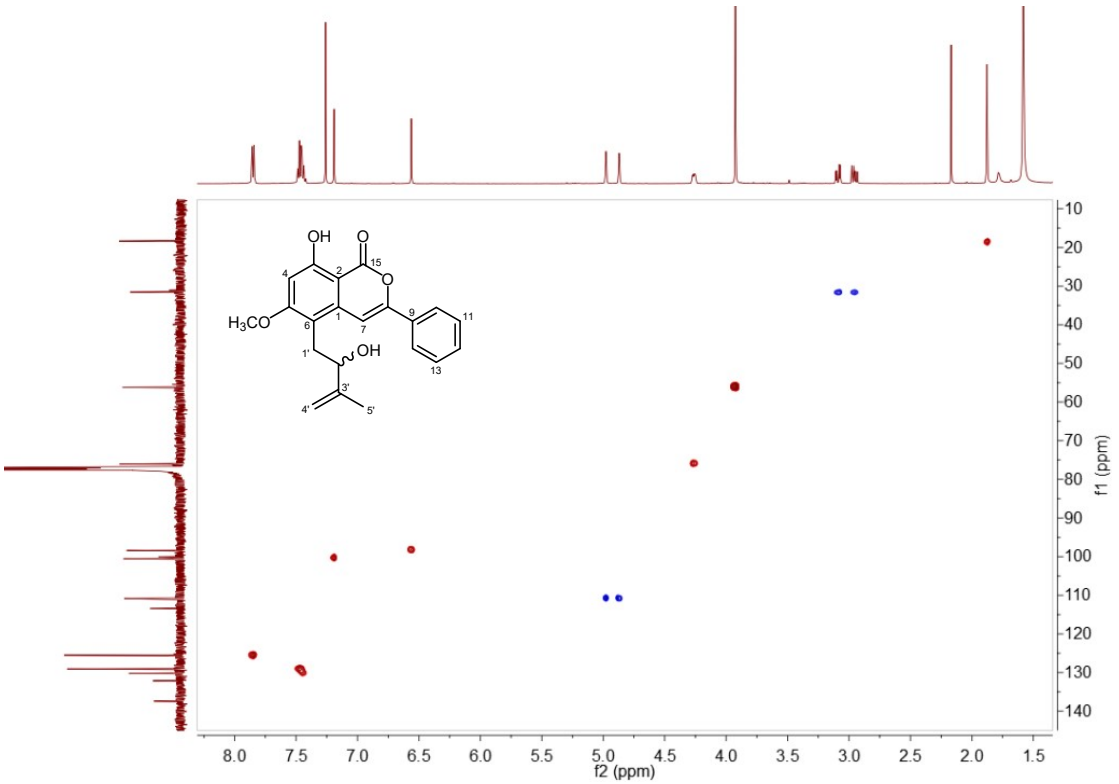

Figure S4. HSQC spectrum of **1**.

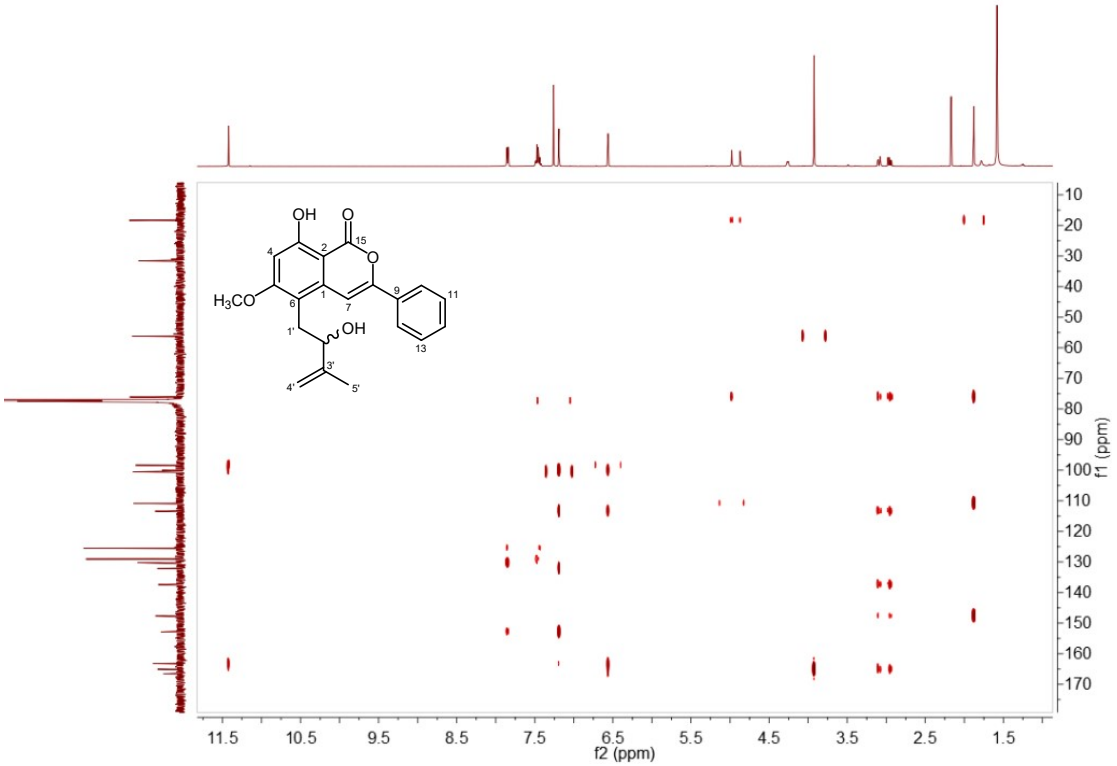

Figure S5. HMBC spectrum of **1**.

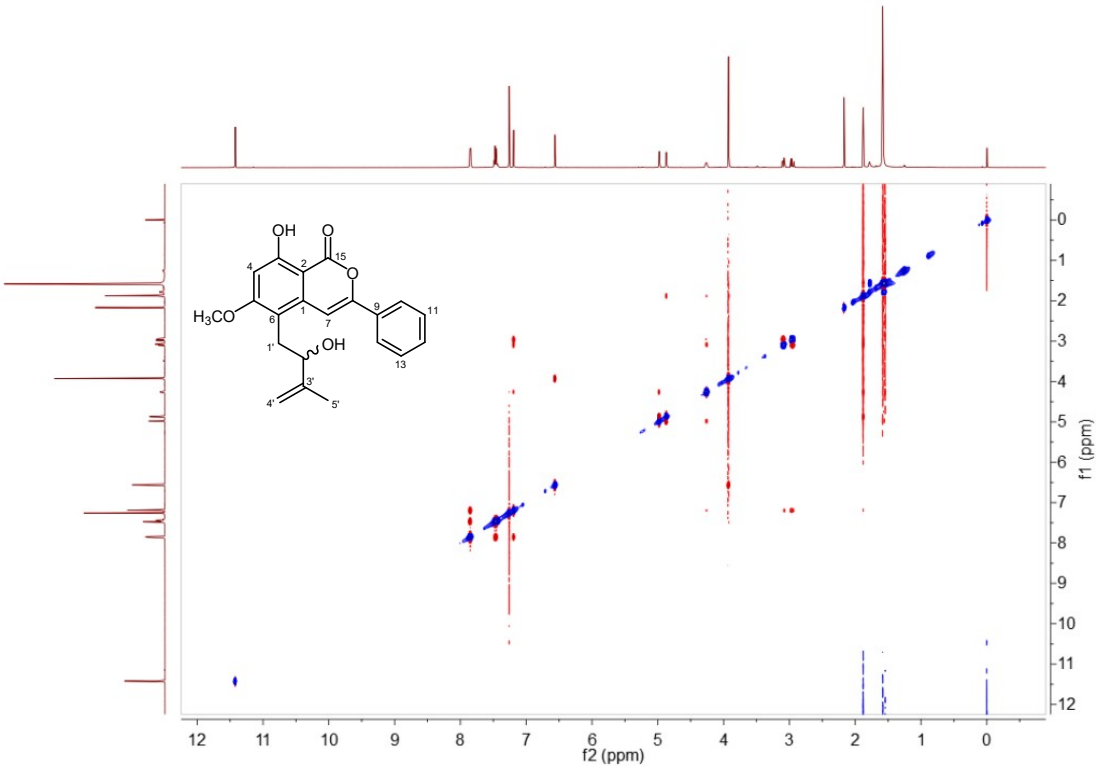

Figure S6. NOESY spectrum of **1**.

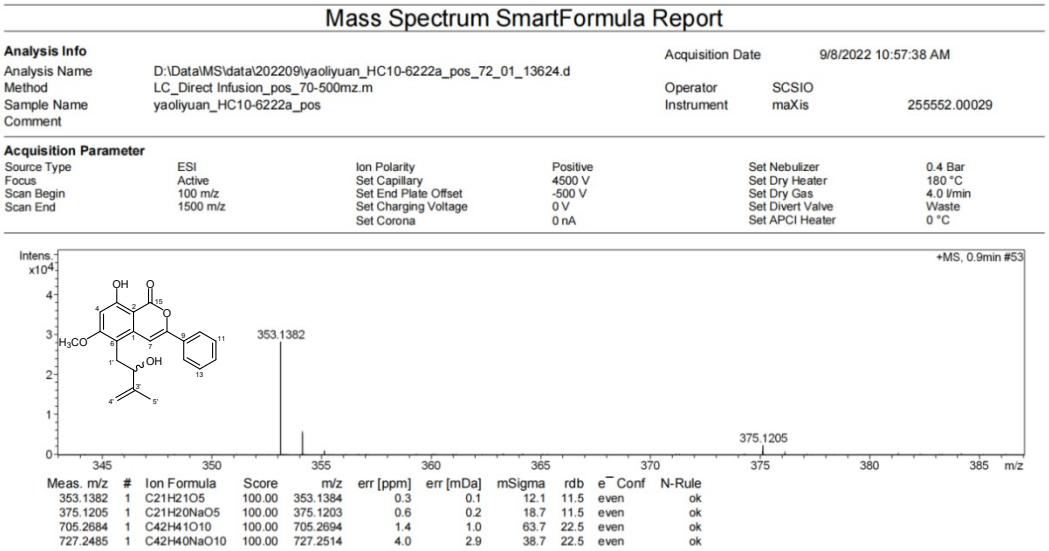

Figure S7. HRESIMS spectrum of **1**.

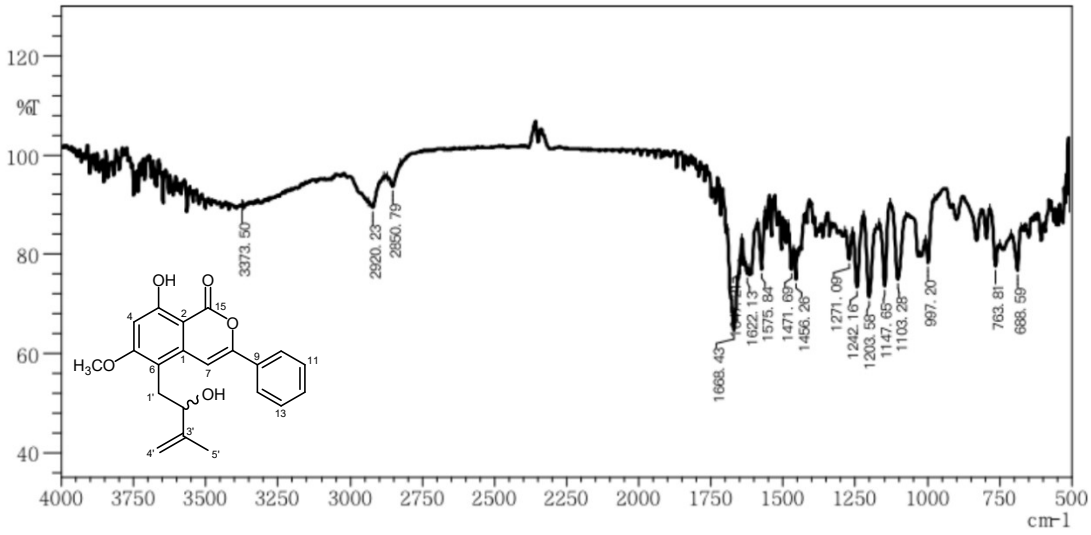

Figure S8. IR spectrum of **1**.

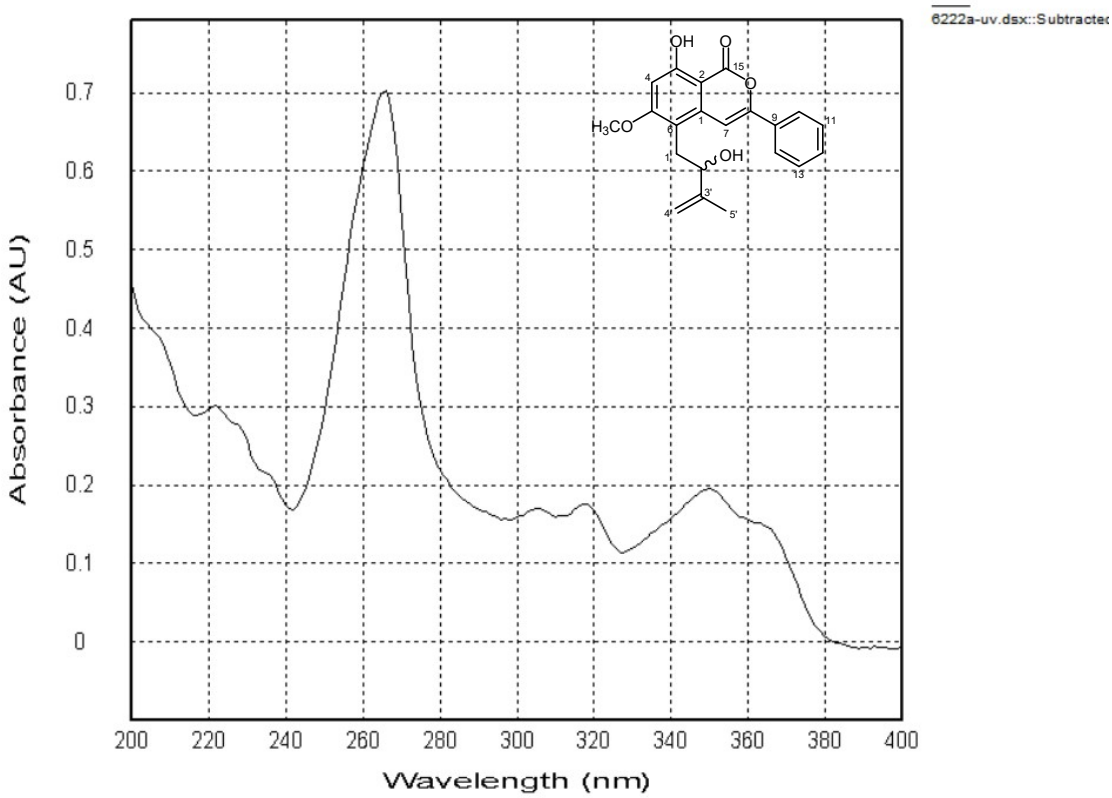

Figure S9. UV spectrum of **1**.

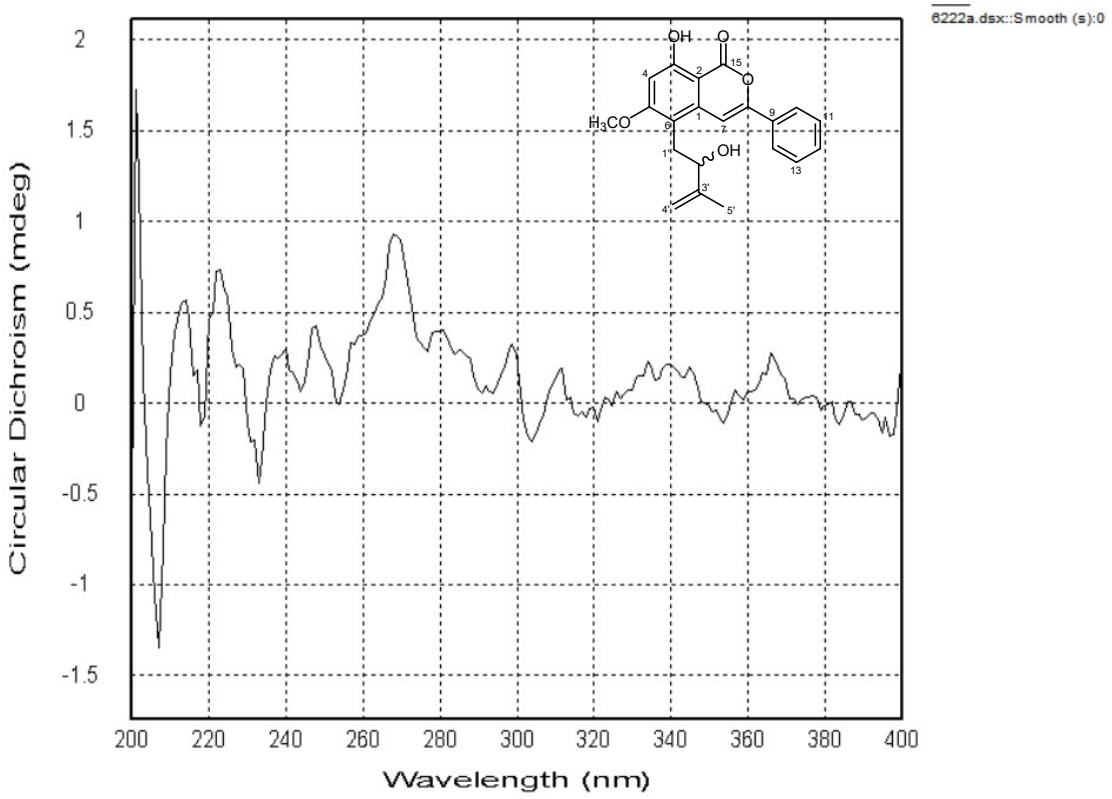

Figure S10. CD spectrum of **1**.

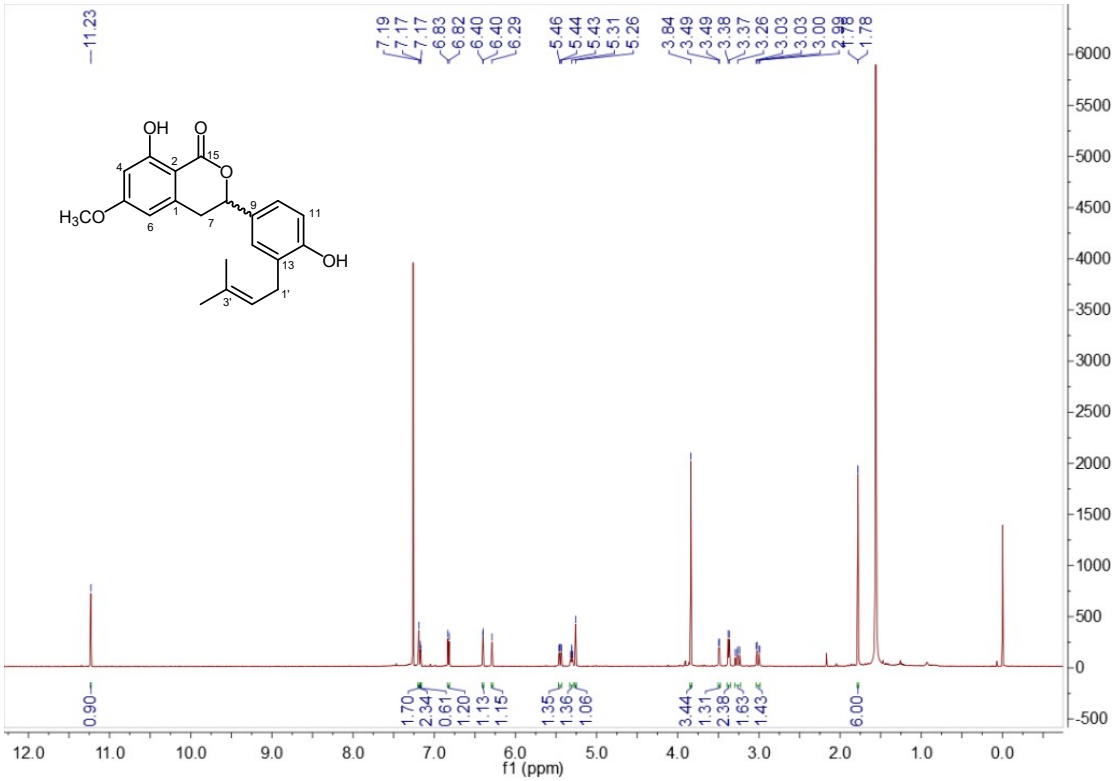

Figure S11. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **2**.

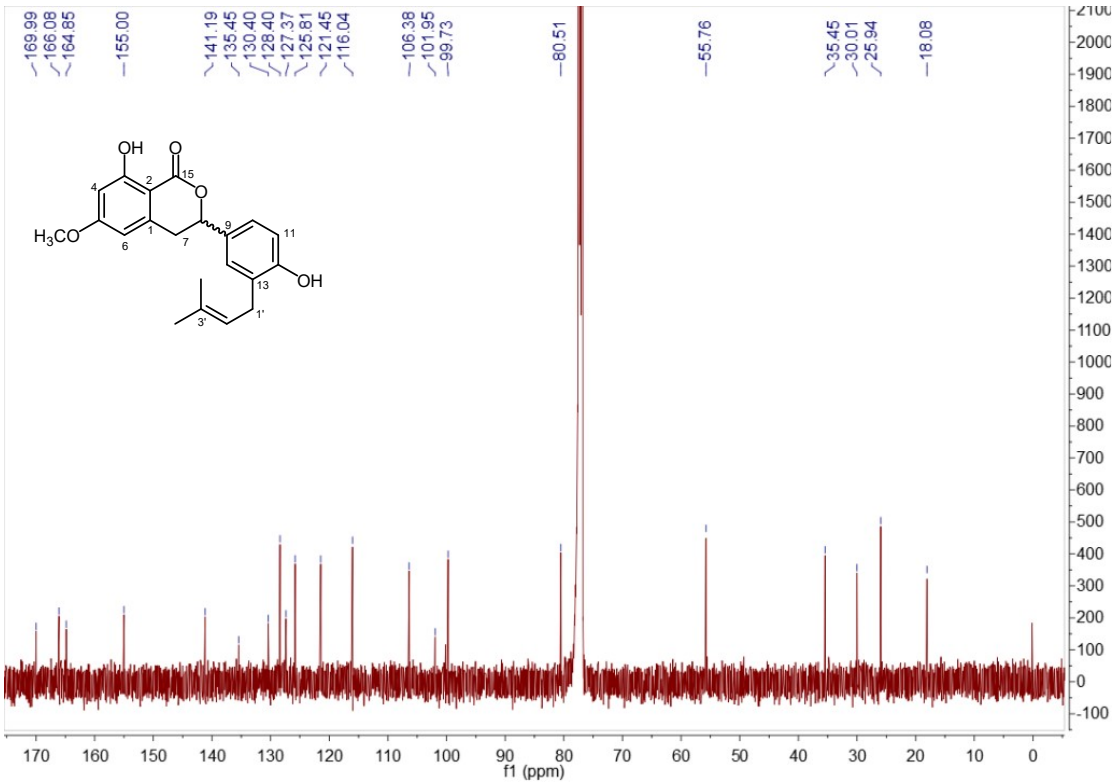

Figure S12. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **2**.

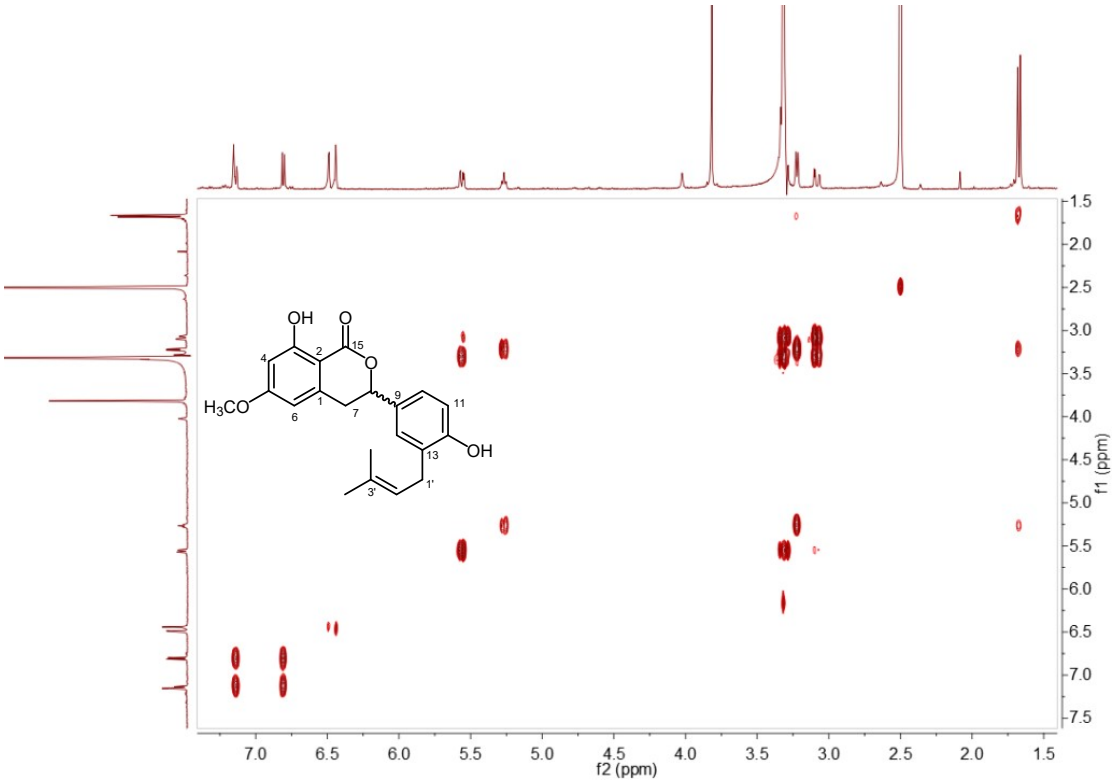

Figure S13. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **2**.

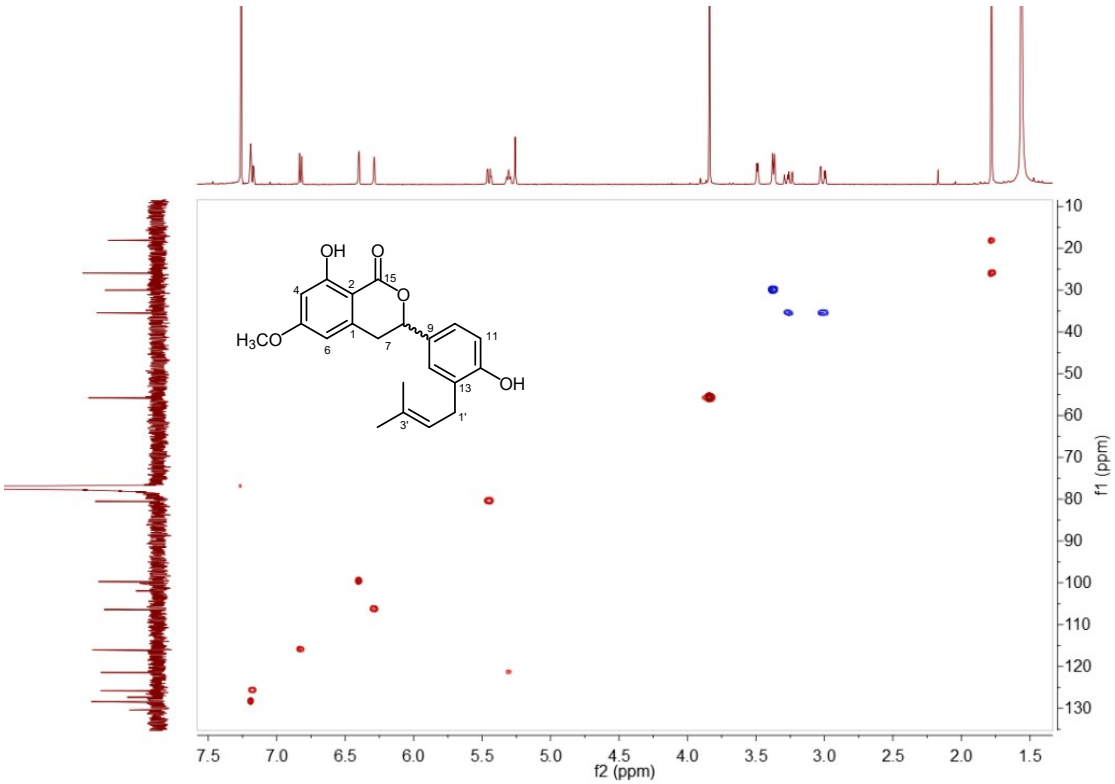

Figure S14. HSQC spectrum of **2**.

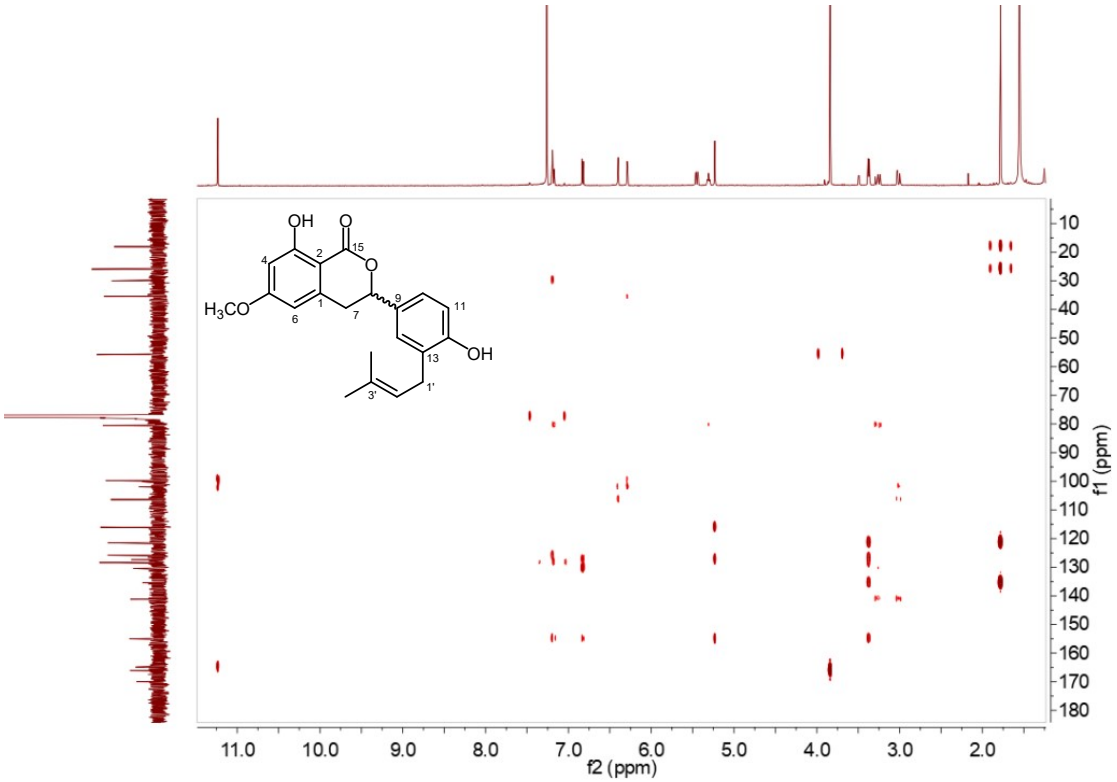

Figure S15. HMBC spectrum of **2**.

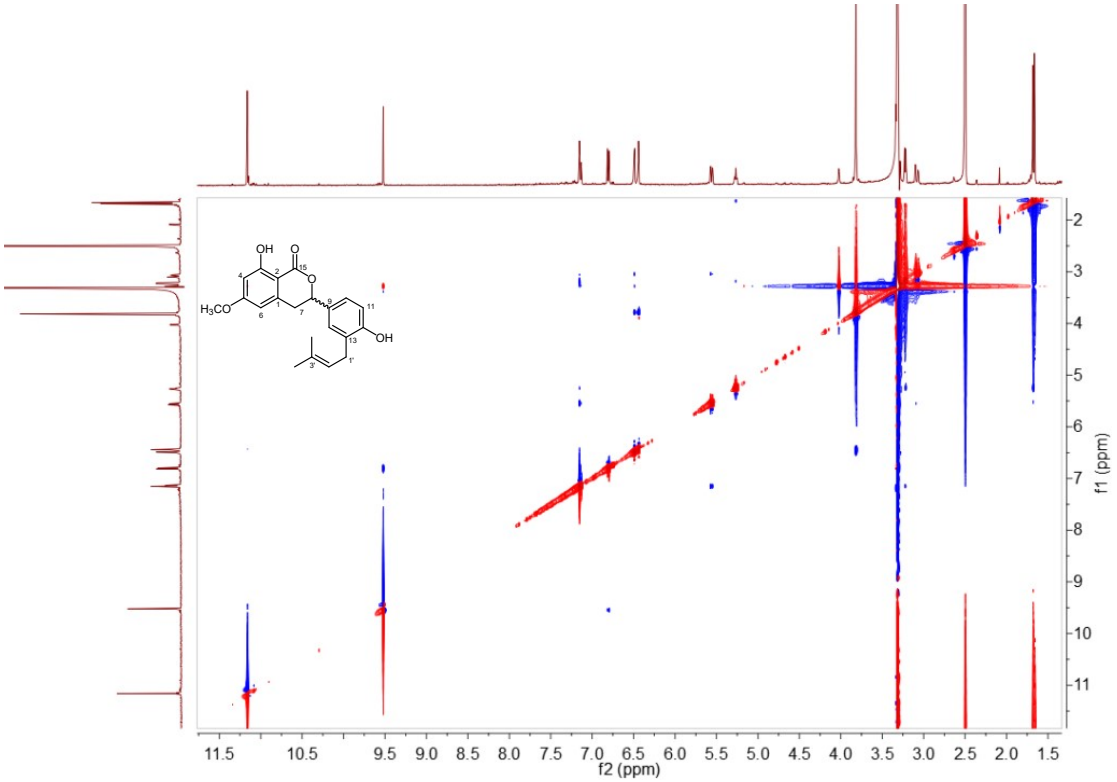

Figure S16. NOESY spectrum of **2**.

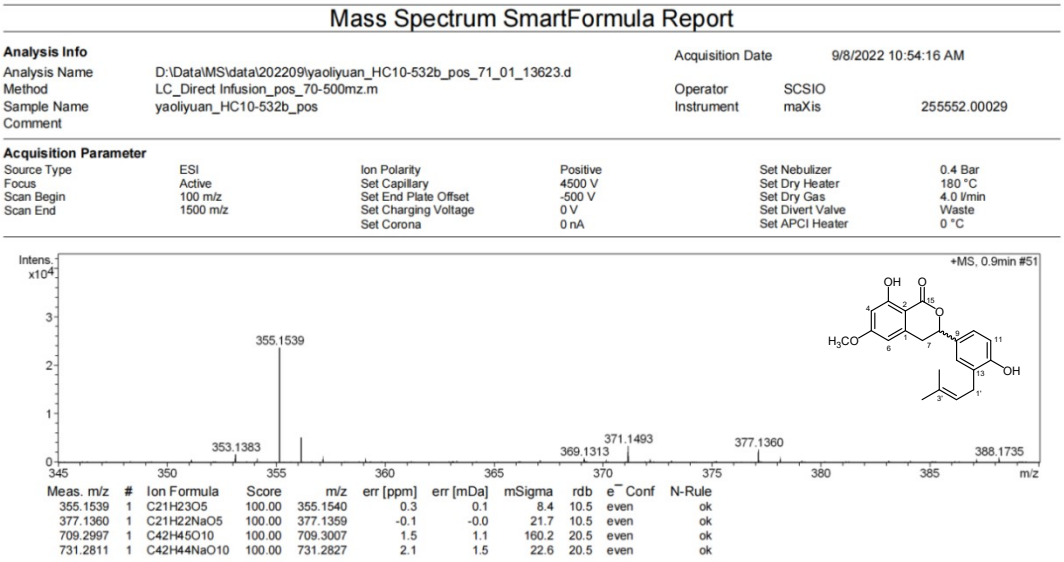

Figure S17. HRESIMS spectrum of **2**.

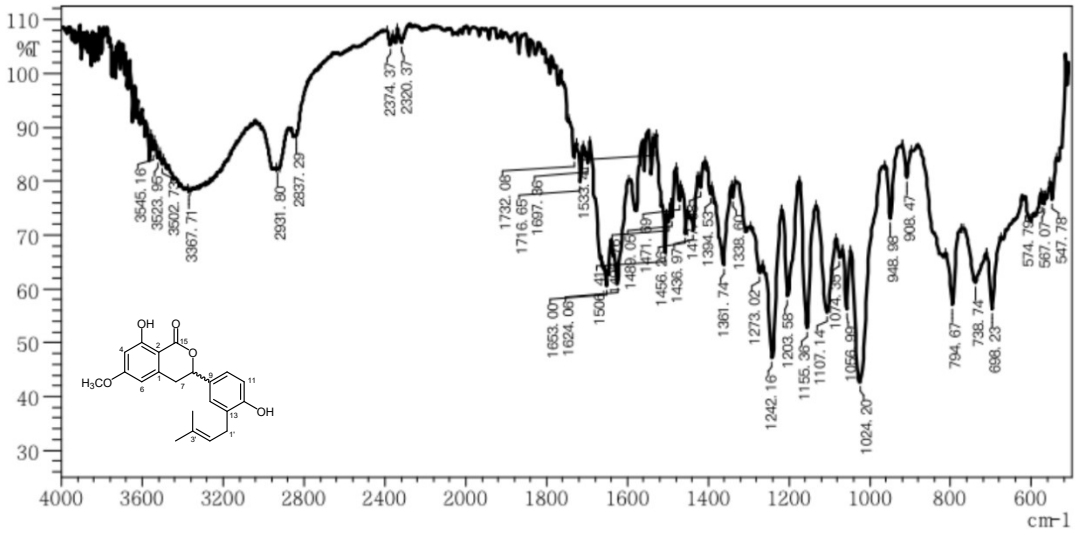

Figure S18. IR spectrum of **2**.

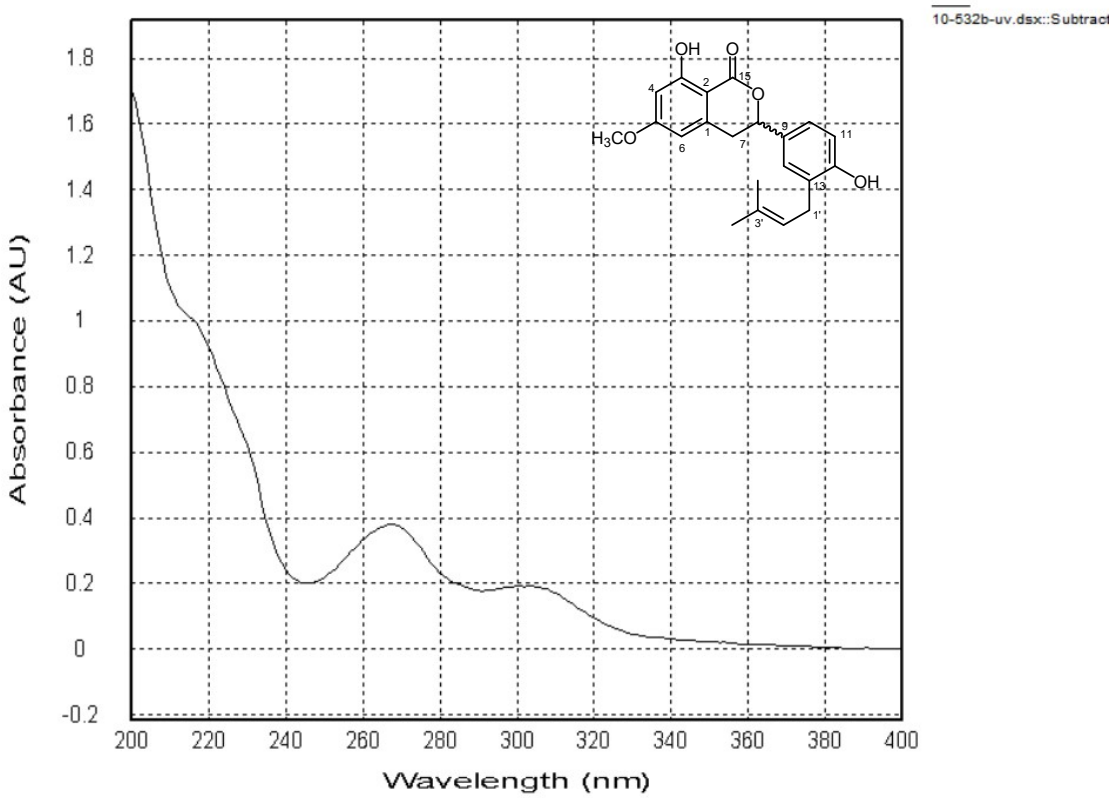

Figure S19. UV spectrum of **2**.

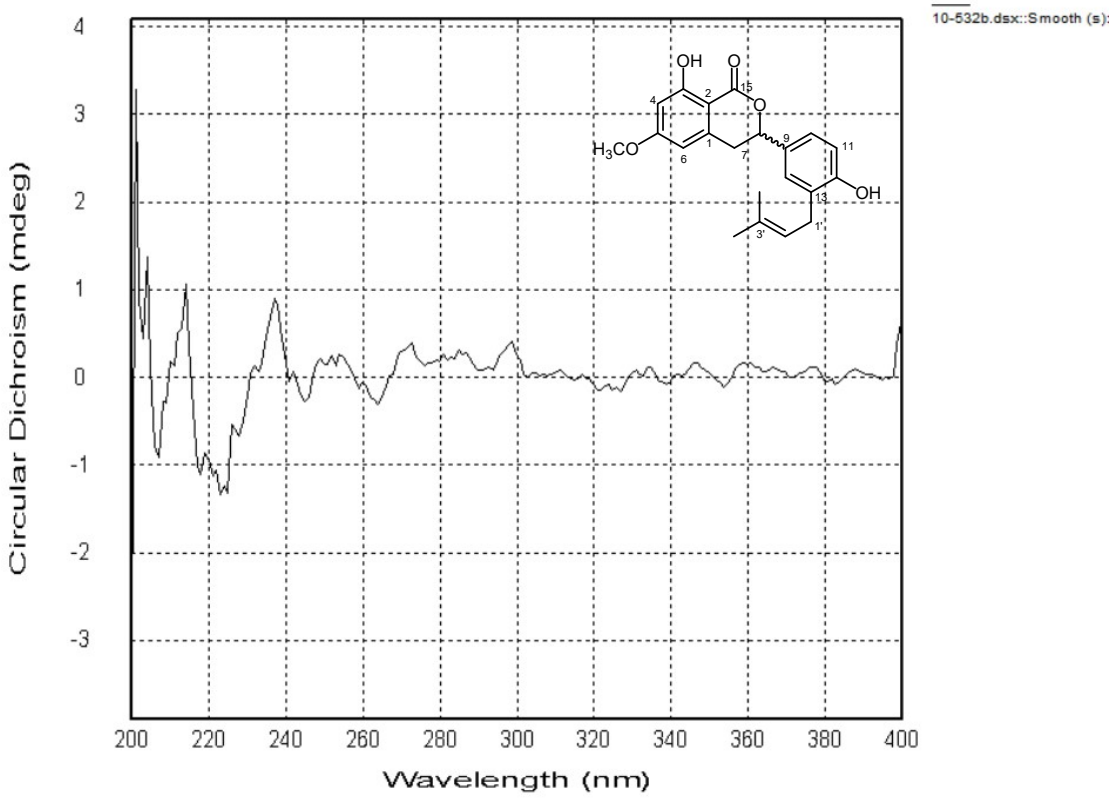

Figure S20. CD spectrum of **2**.

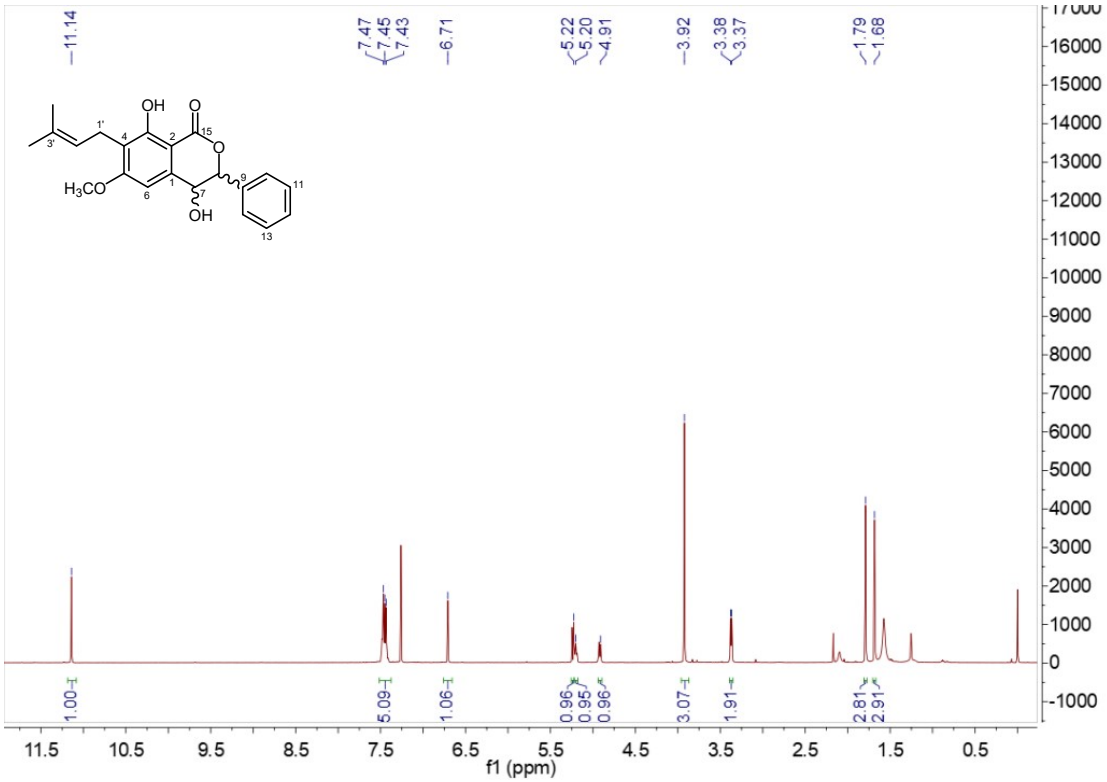

Figure S21. ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **3**.

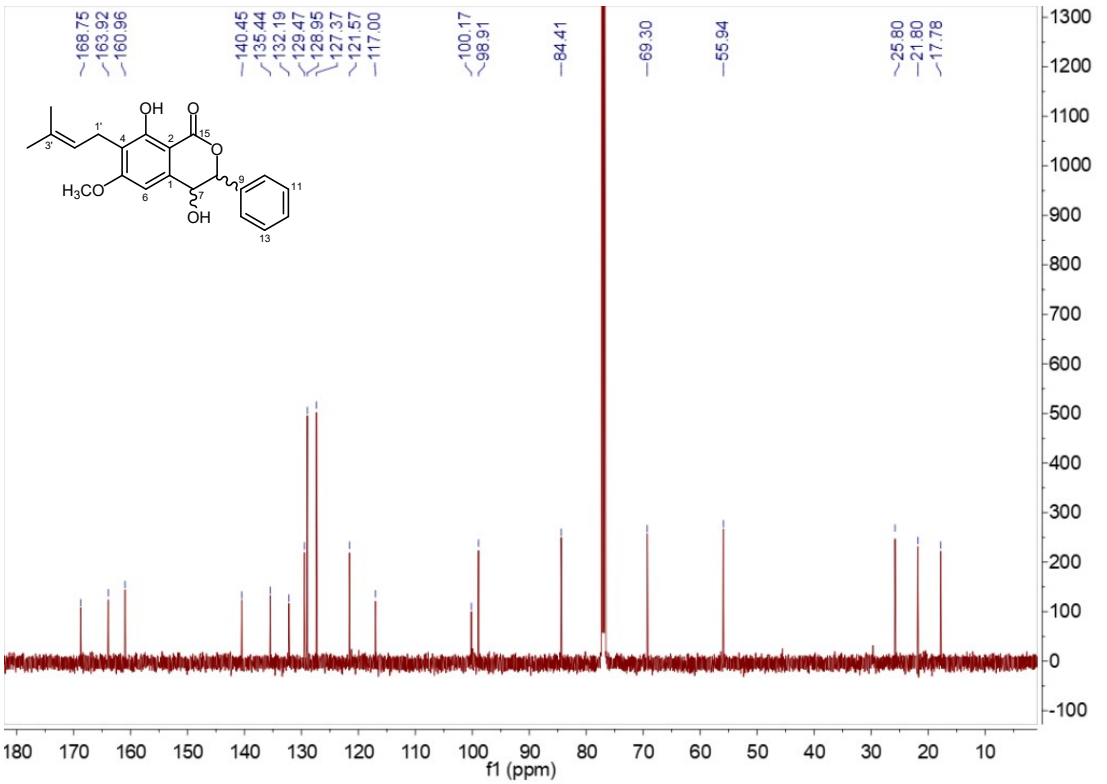

Figure S22. ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **3**.

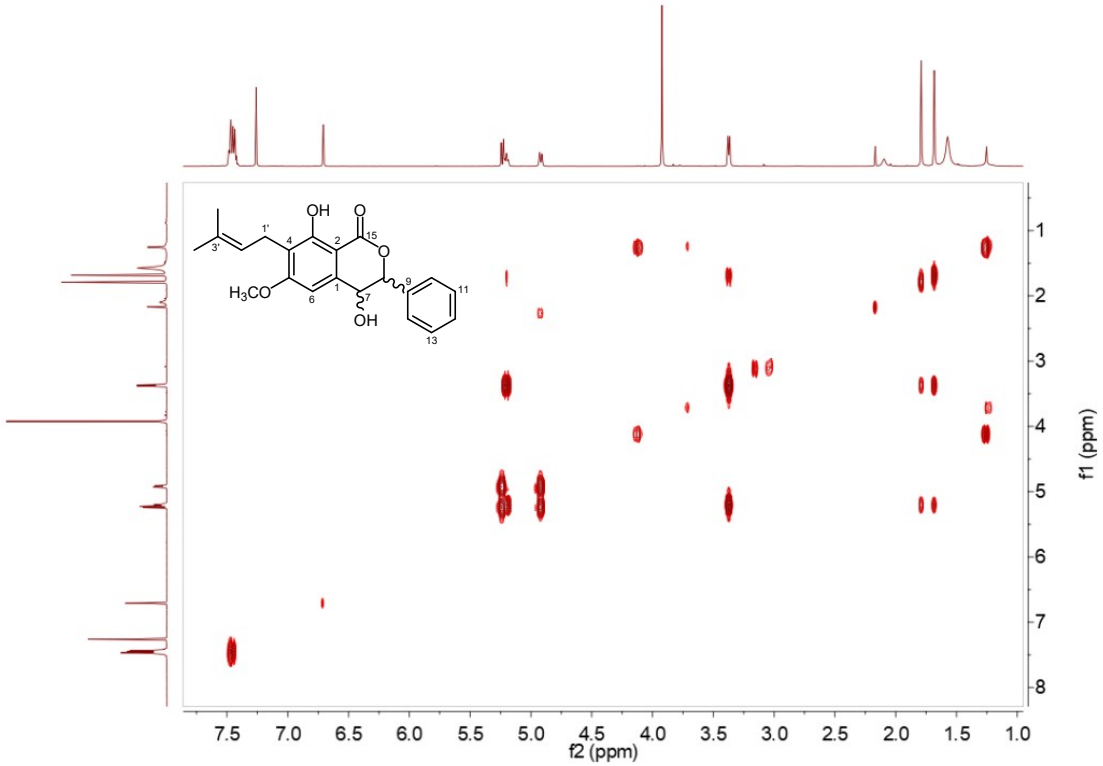

Figure S23. ^{1}H-^{1}H COSY spectrum (500 MHz, $CDCl_3$) of **3**.

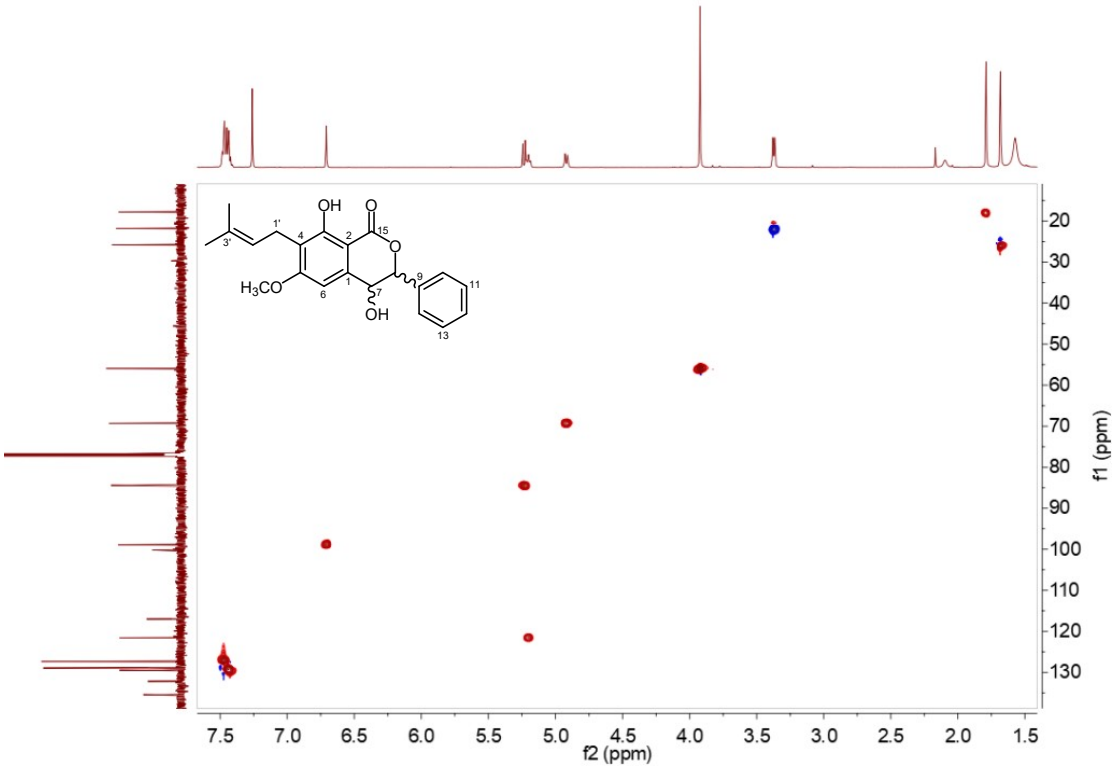

Figure S24. HSQC spectrum of **3**.

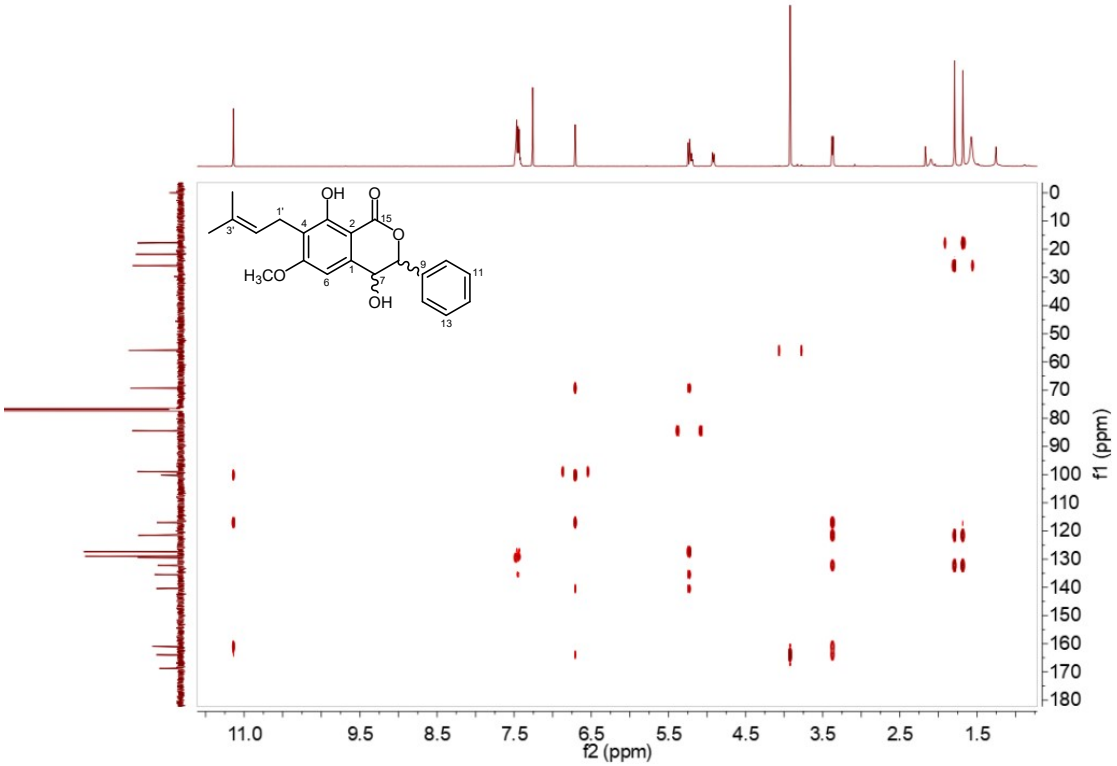

Figure S25. HMBC spectrum of **3**.

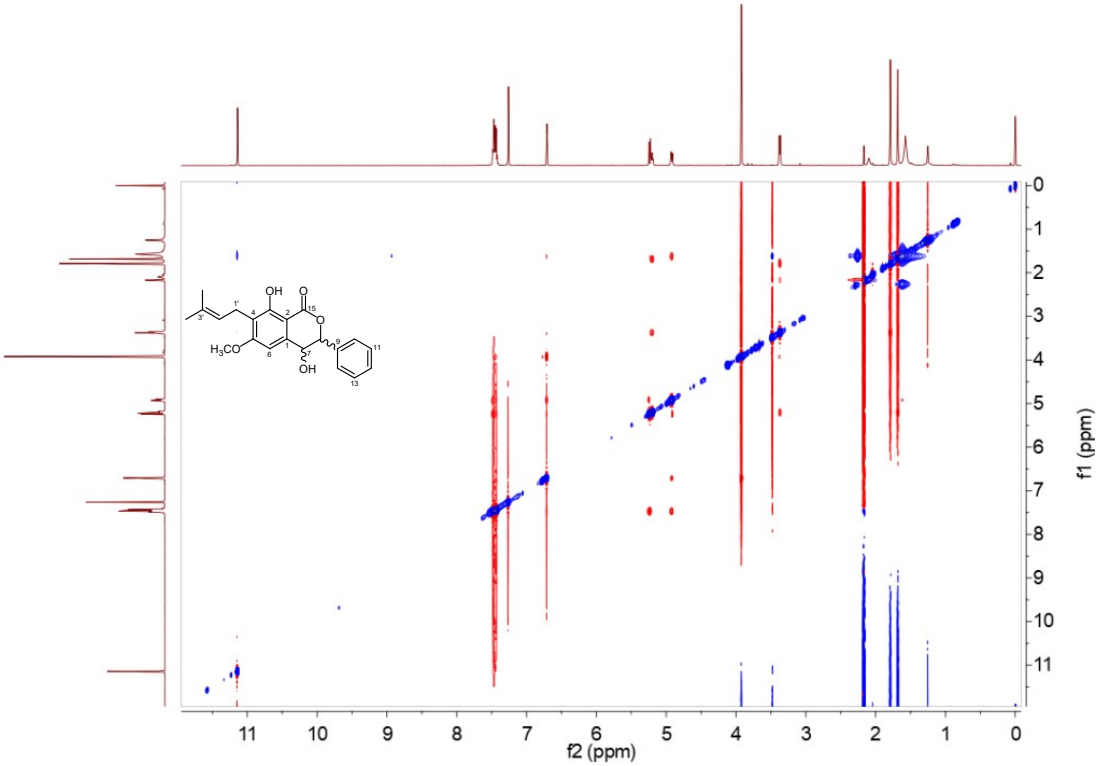

Figure S26. NOESY spectrum of **3**.

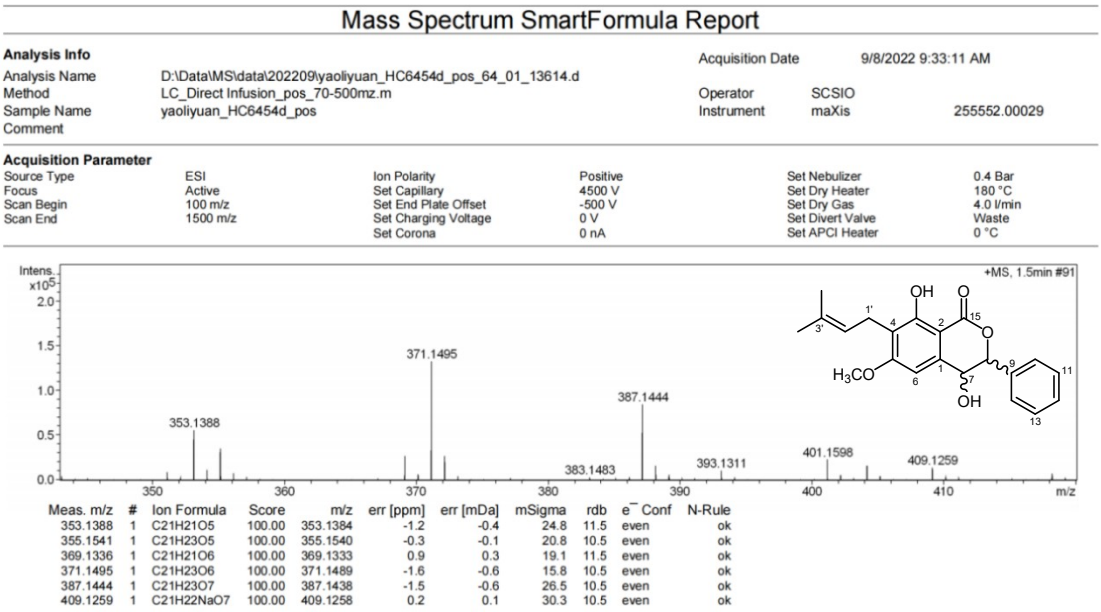

Figure S27. HRESIMS spectrum of **3**.

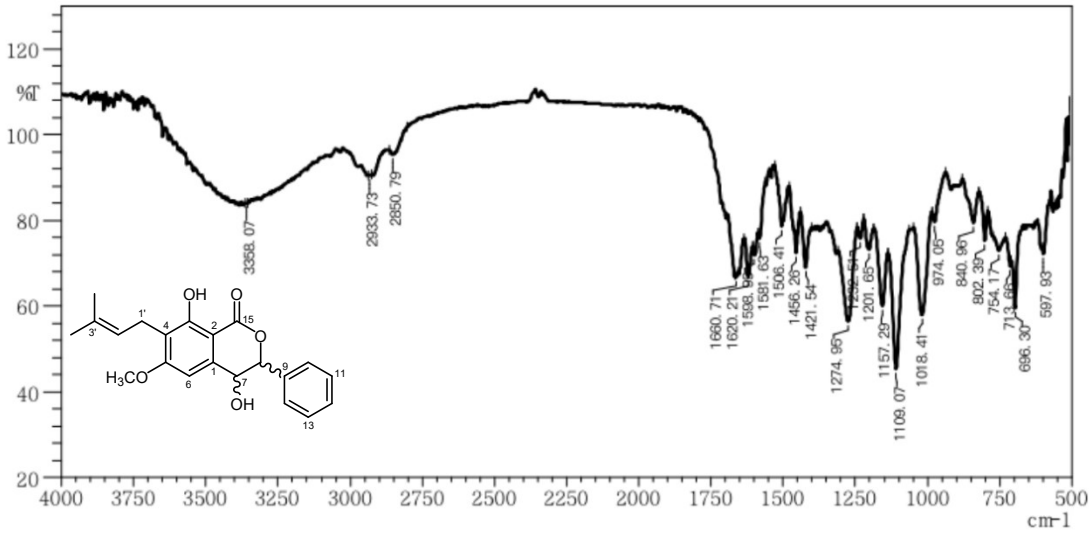

Figure S28. IR spectrum of **3**.

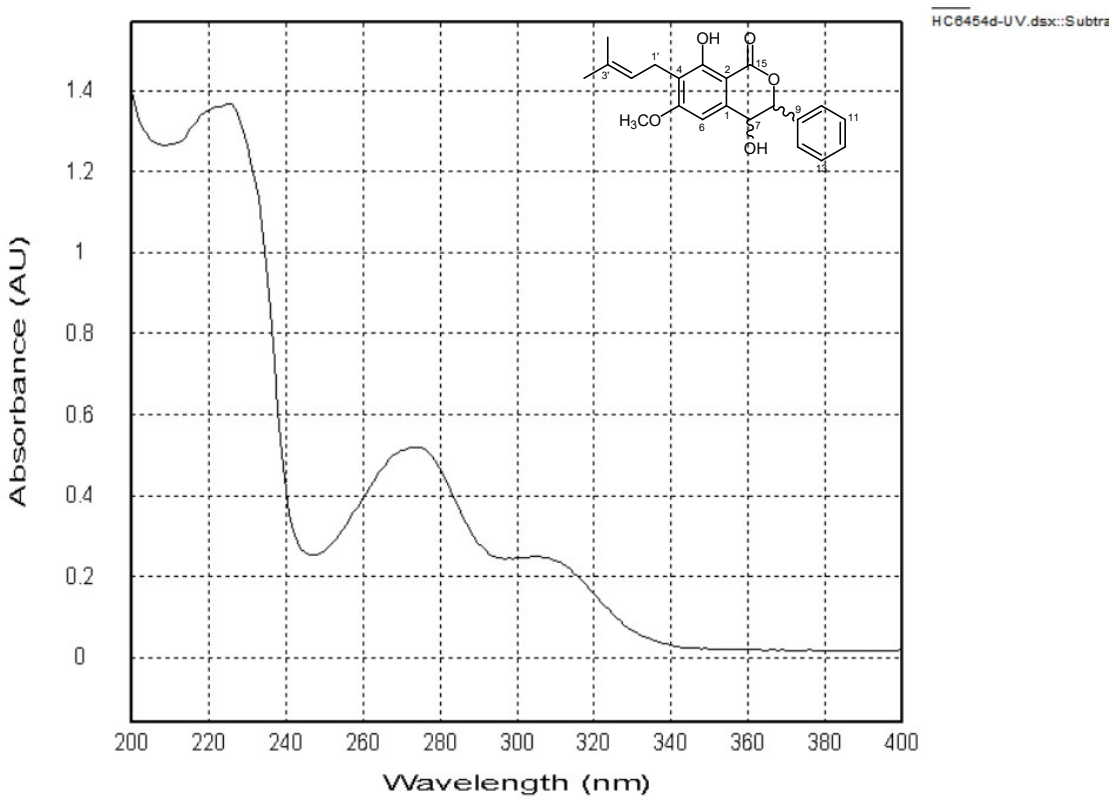

Figure S29. UV spectrum of **3**.

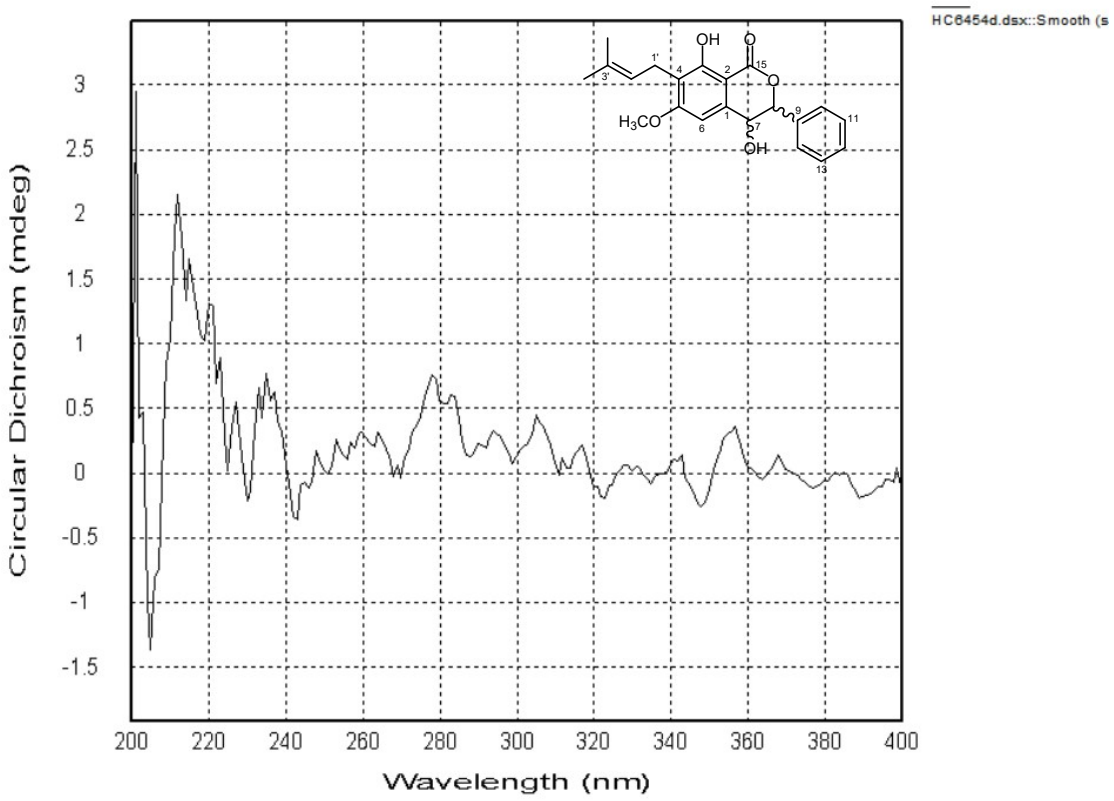

Figure S30. CD spectrum of **3**.

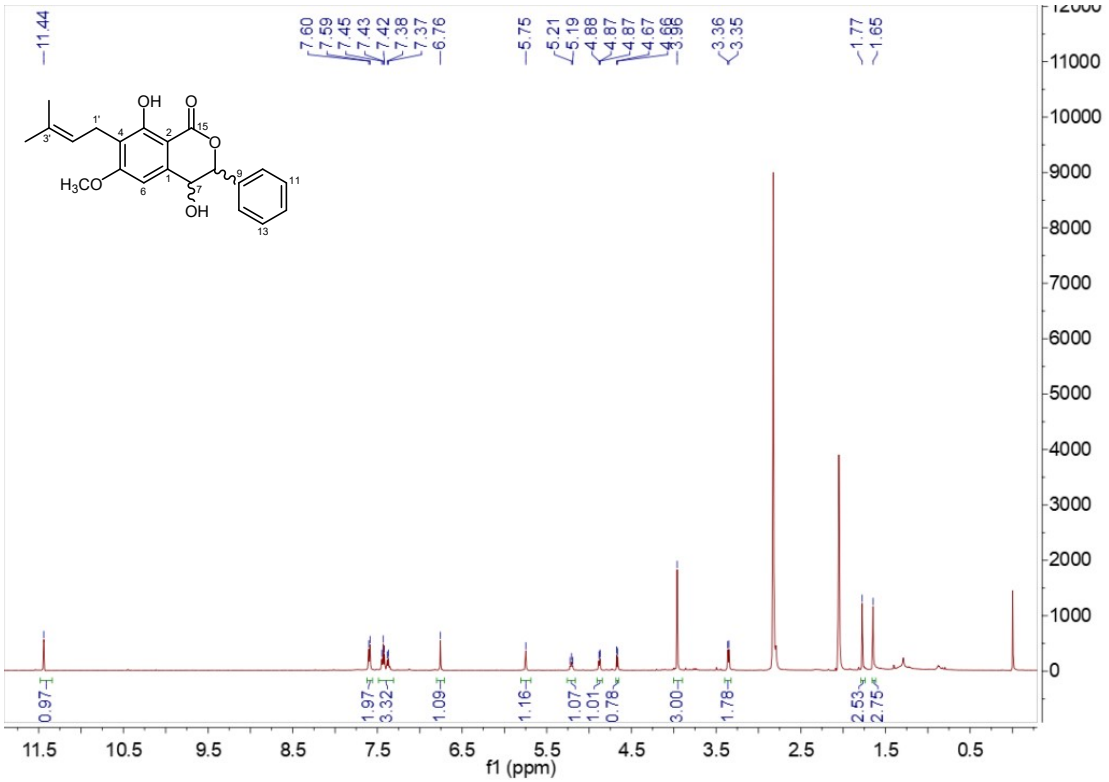

Figure S31. ^{1}H NMR spectrum (500 MHz, C_3D_6O) of **4**.

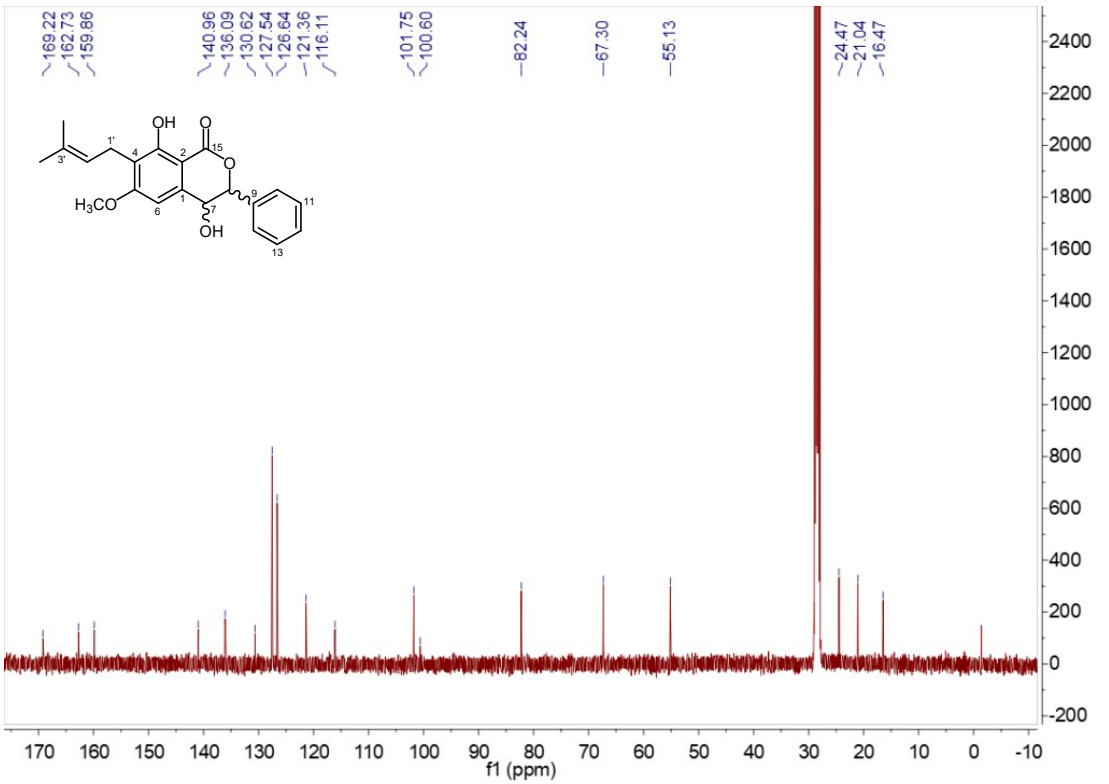

Figure S32. ^{13}C NMR spectrum (125 MHz, C_3D_6O) of **4**.

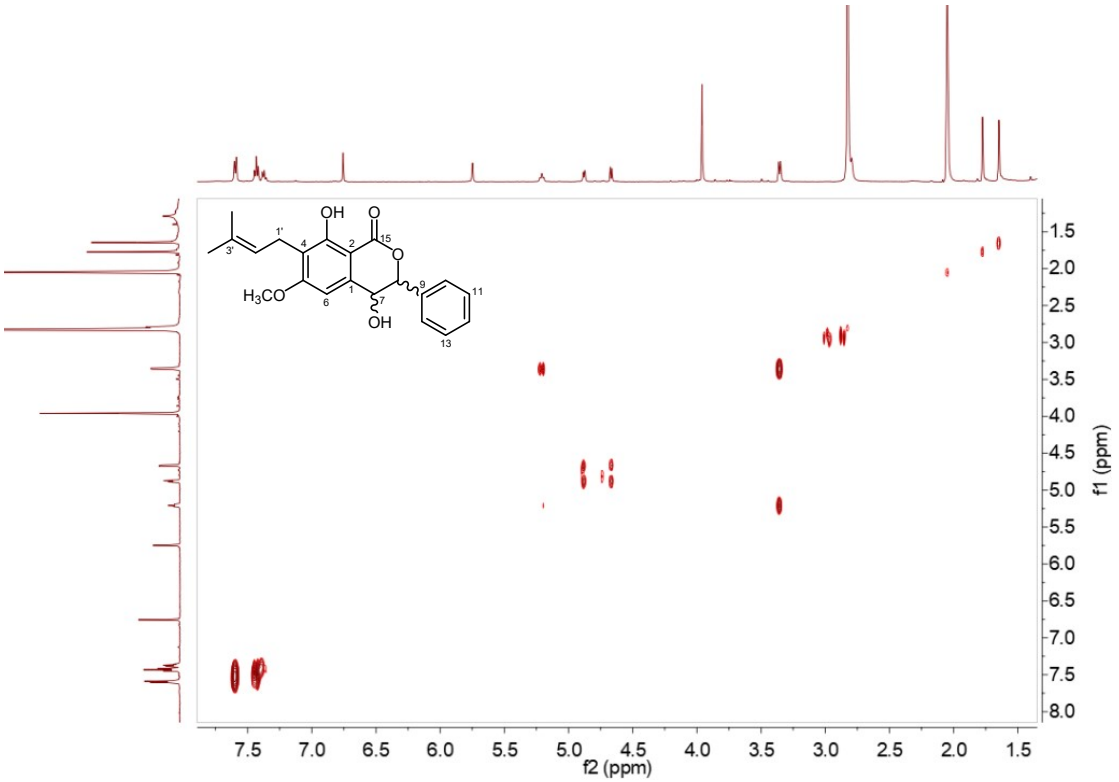

Figure S33. ^{1}H-^{1}H COSY spectrum (500 MHz, C_3D_6O) of **4**.

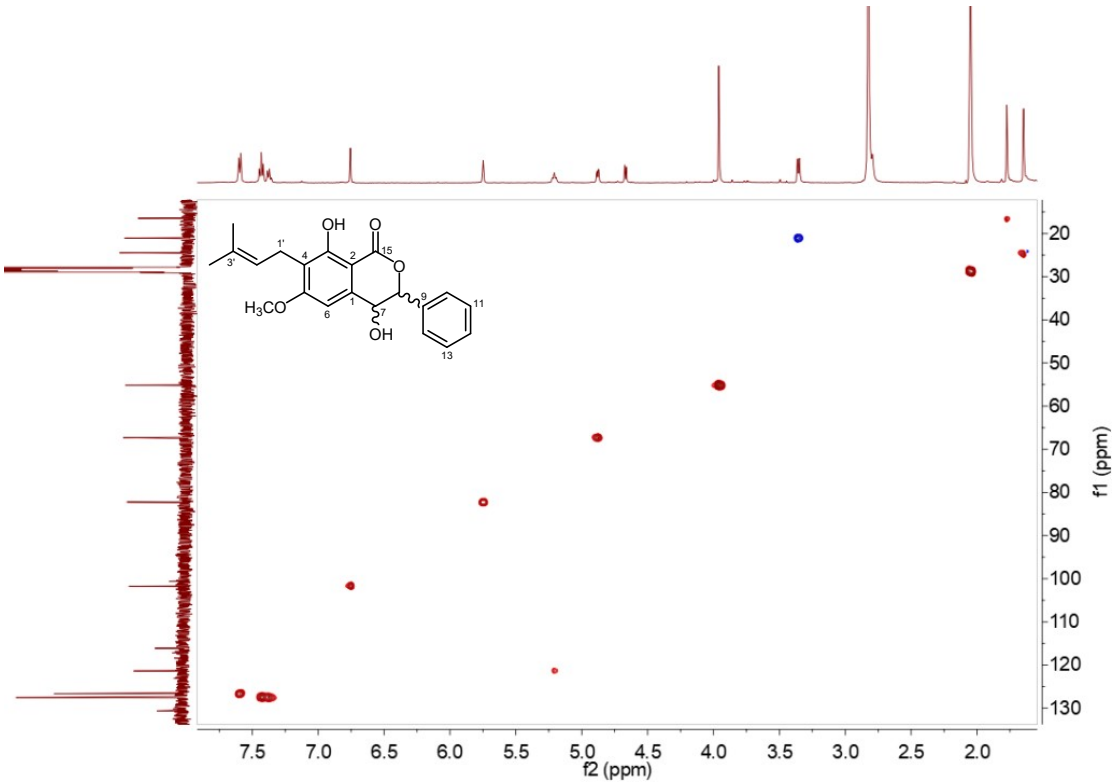

Figure S34. HSQC spectrum of **4**.

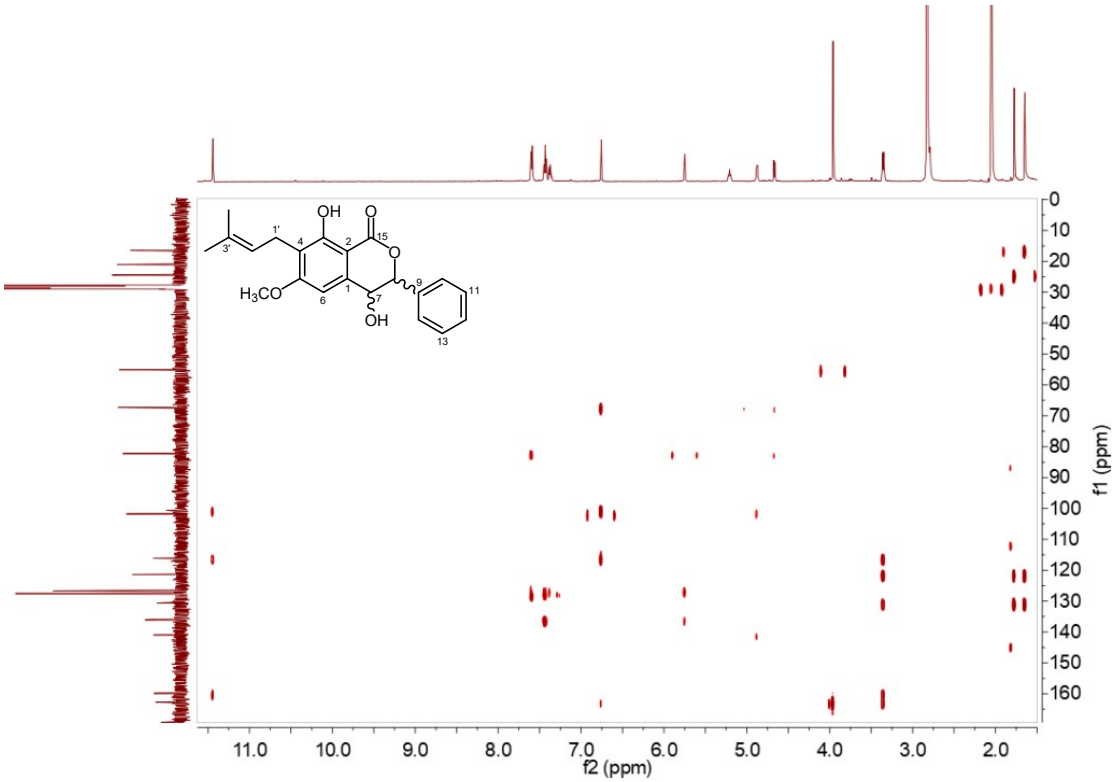

Figure S35. HMBC spectrum of **4**.

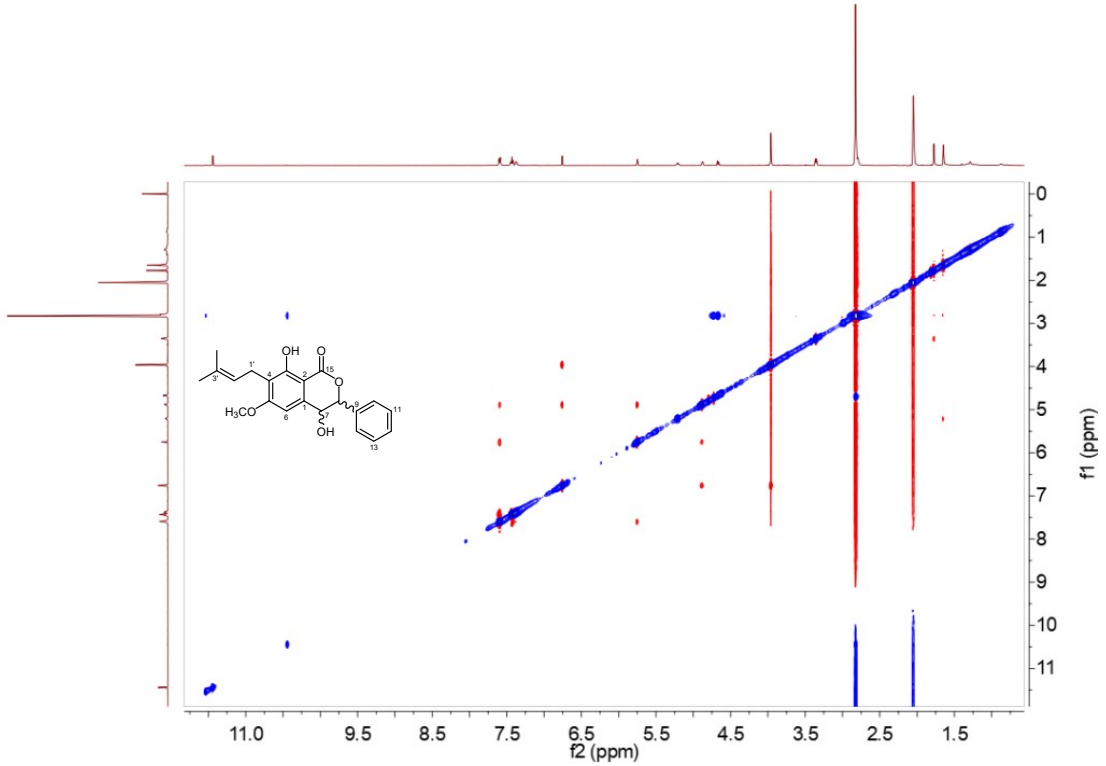

Figure S36. NOESY spectrum of **4**.

Mass Spectrum SmartFormula Report

Analysis Info

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Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	yaoliyuan_HC6454c_pos	Instrument	maXis 255552.00029
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
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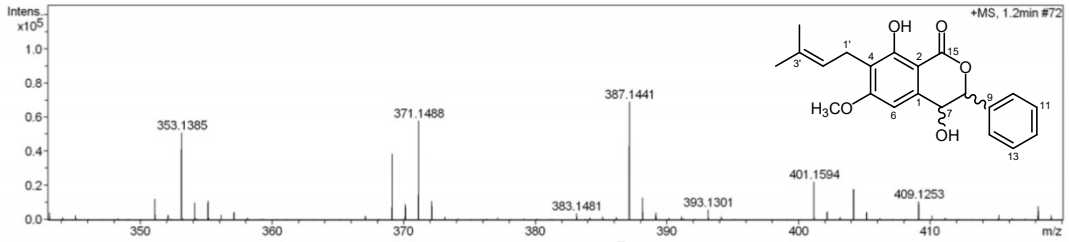
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
353.1385	1	C21H21O5	100.00	353.1384	-0.3	-0.1	92.4	11.5	even	ok
355.1531	1	C21H23O5	100.00	355.1540	-2.6	-0.9	23.4	10.5	even	ok
369.1332	1	C21H21O6	100.00	369.1333	0.1	0.0	19.1	11.5	even	ok
371.1488	1	C21H23O6	100.00	371.1489	-0.2	-0.1	22.7	10.5	even	ok
387.1441	1	C21H23O7	100.00	387.1438	0.8	0.3	26.0	10.5	even	ok
409.1253	1	C21H22NaO7	100.00	409.1258	-1.1	-0.5	31.7	10.5	even	ok

Figure S37. HRESIMS spectrum of **4**.

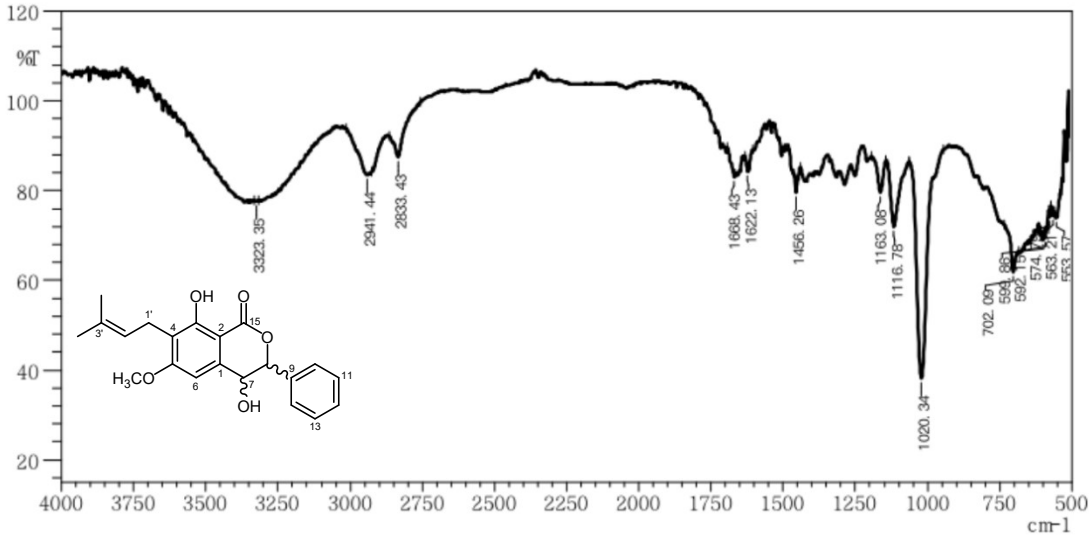


Figure S38. IR spectrum of **4**.

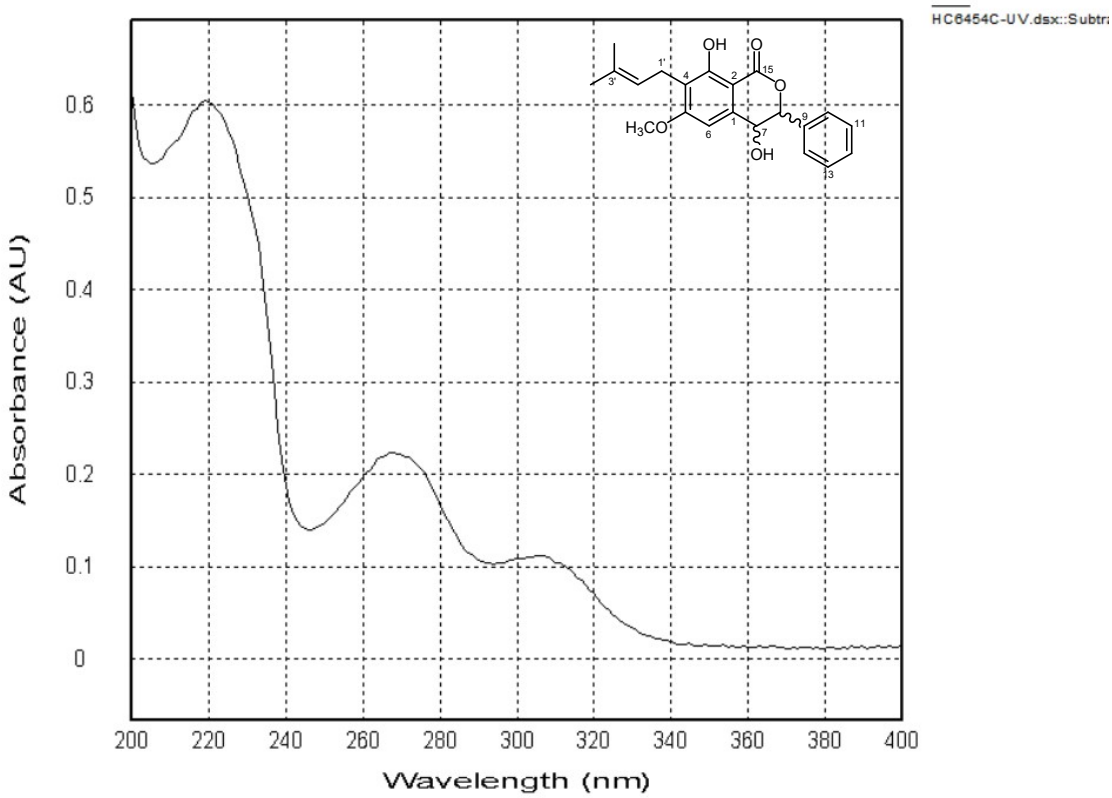


Figure S39. UV spectrum of **4**.

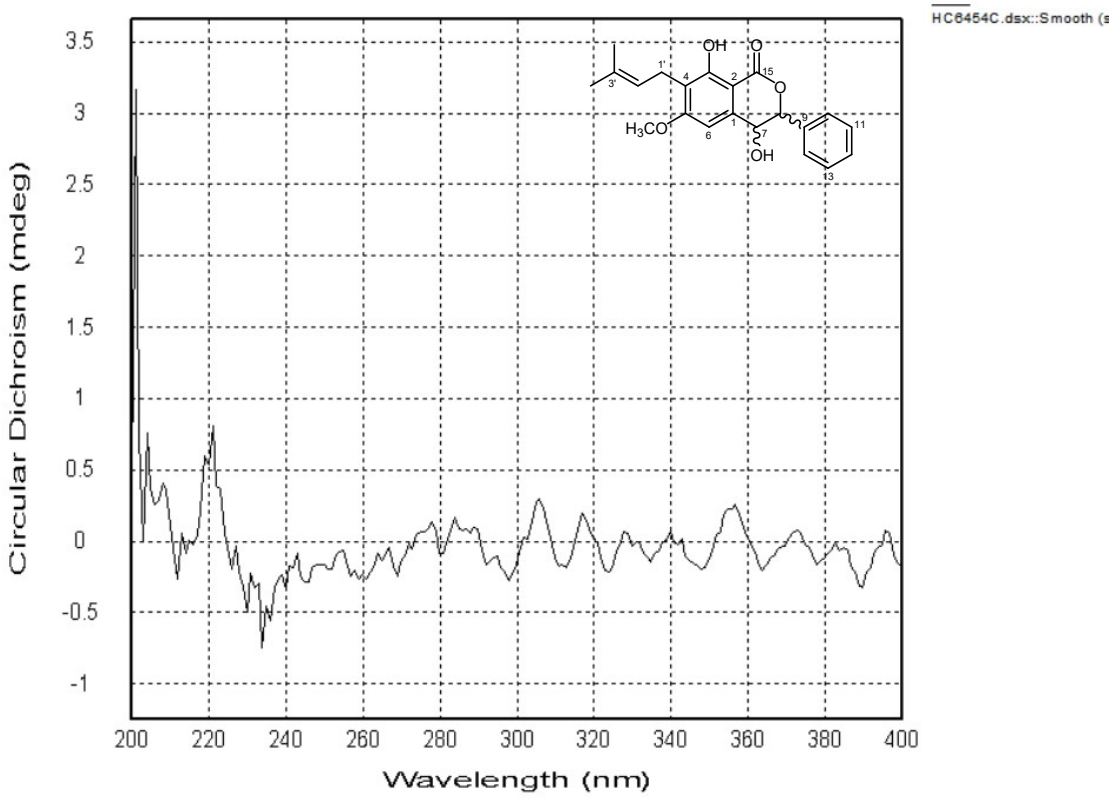


Figure S40. CD spectrum of **4**.