

Supporting Information

New Fusaric Acid Derivatives from the Endophytic Fungus *Fusarium oxysporum* and Their Phytotoxicity to Barley Leaves

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[†]Institute of Pharmaceutical Biology and Biotechnology, Heinrich-Heine-Universität Düsseldorf, Universitätsstrasse 1, 40225 Düsseldorf, Germany

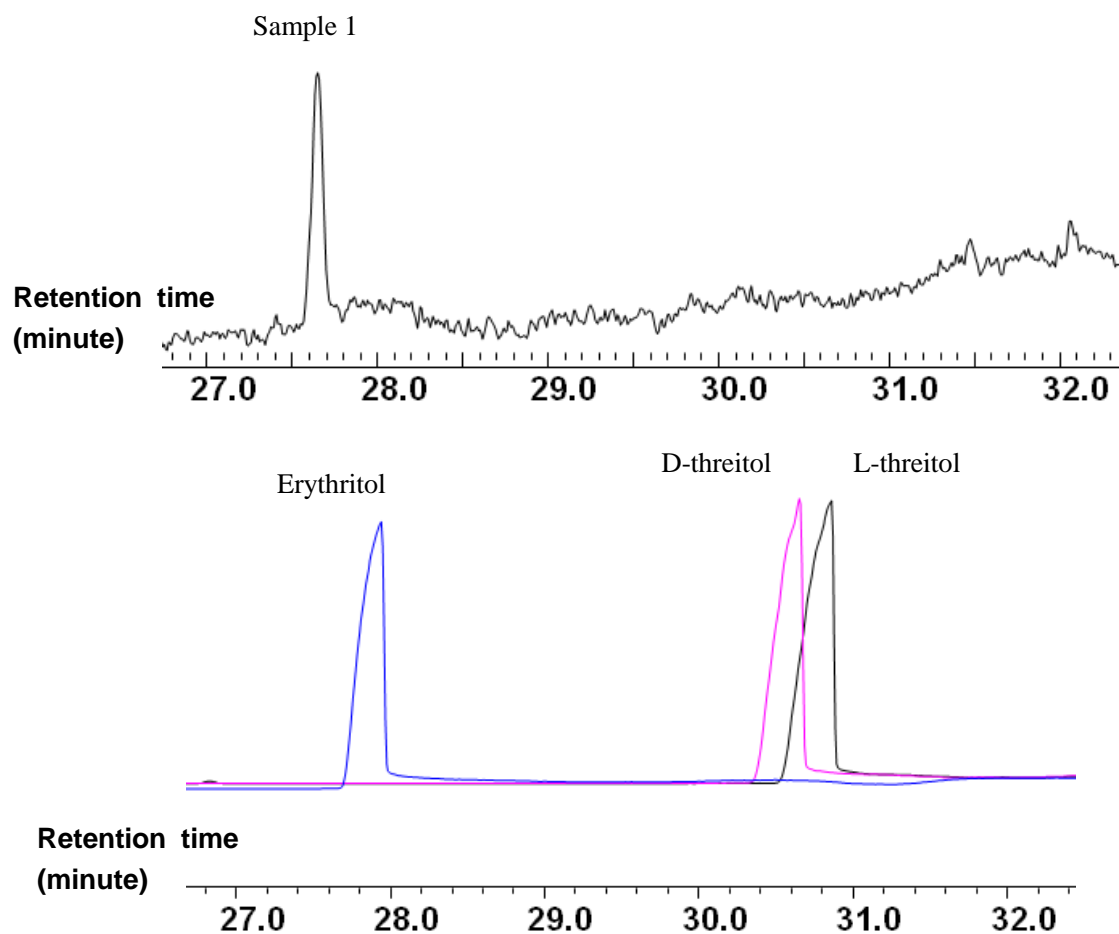
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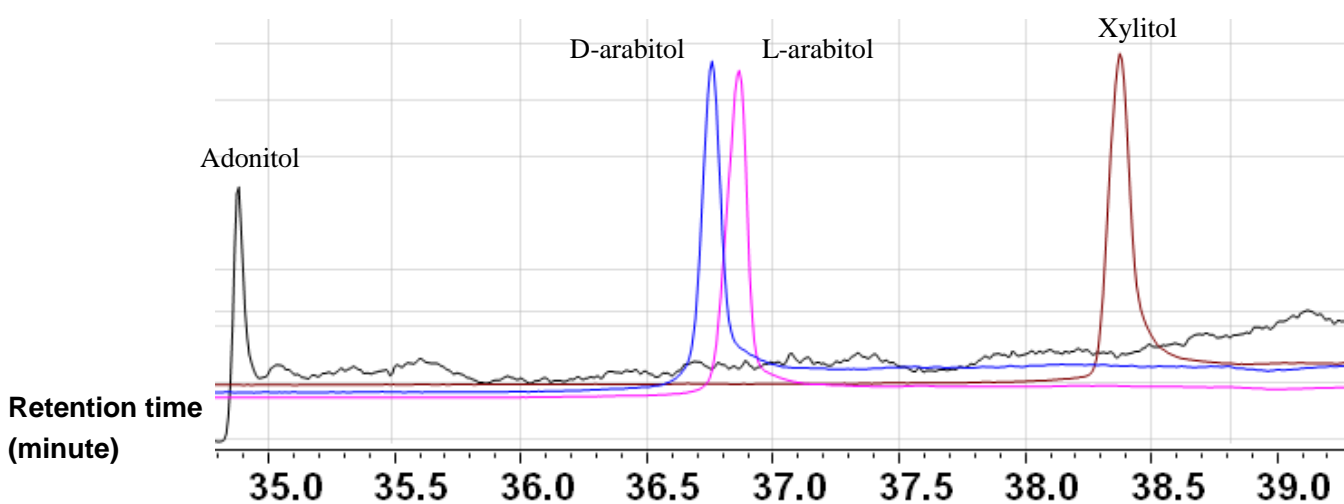
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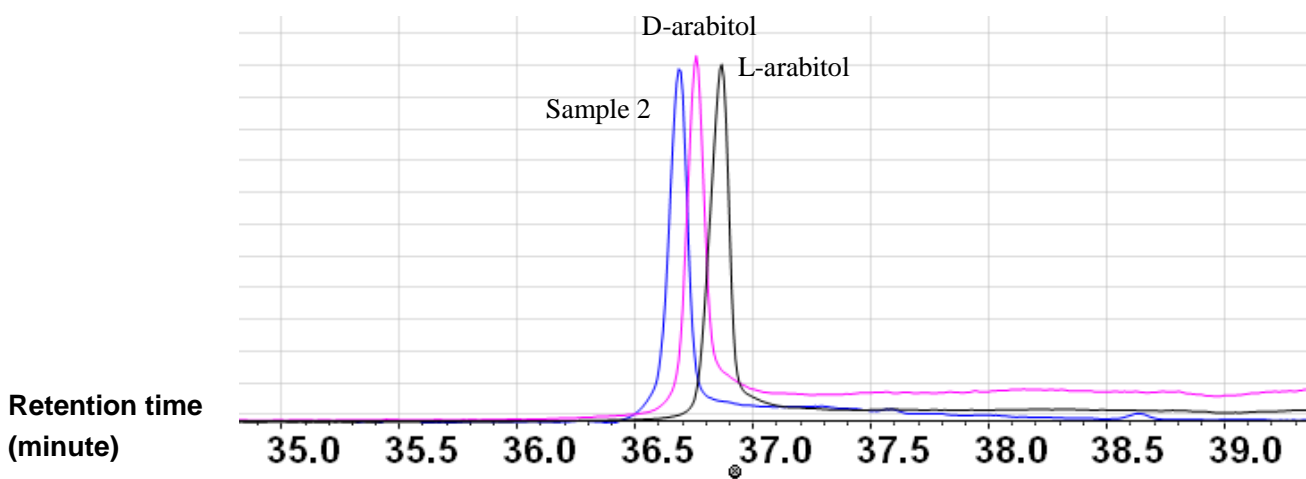
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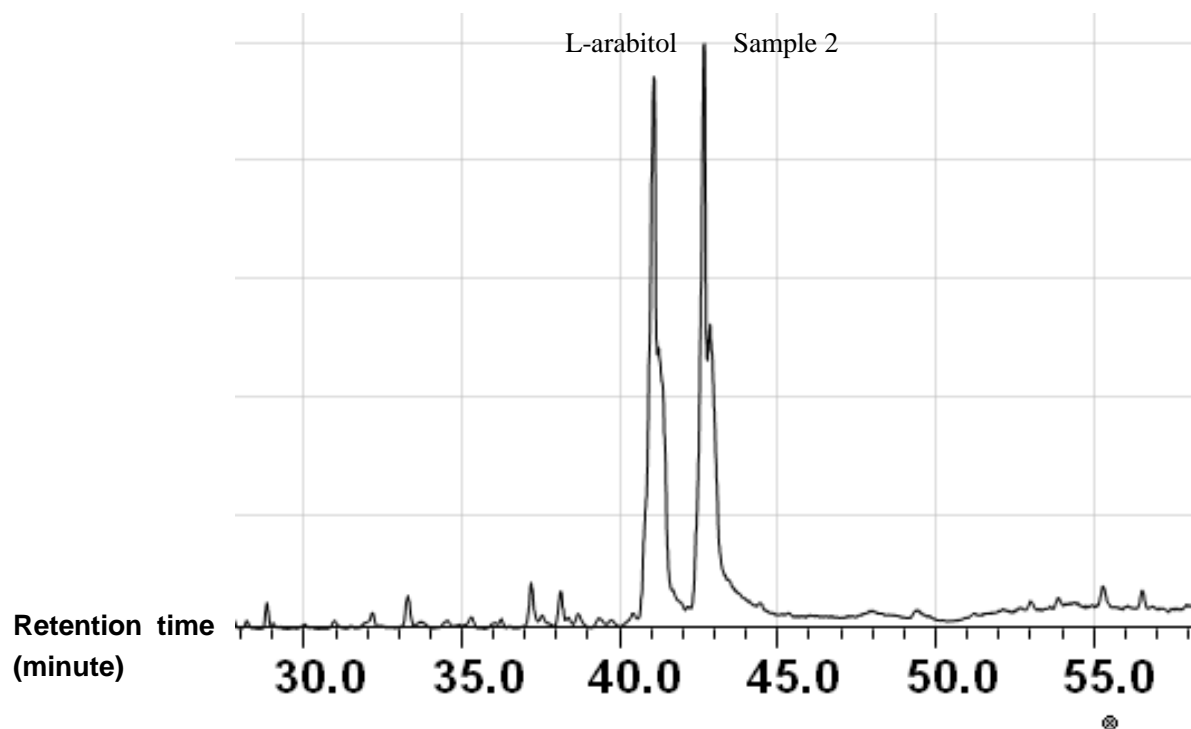
S1-A. Analysis of trifluoroacetyl sample 1 (degraded from compound **3**) and trifluoroacetyl tetritol standards by gas chromatography.



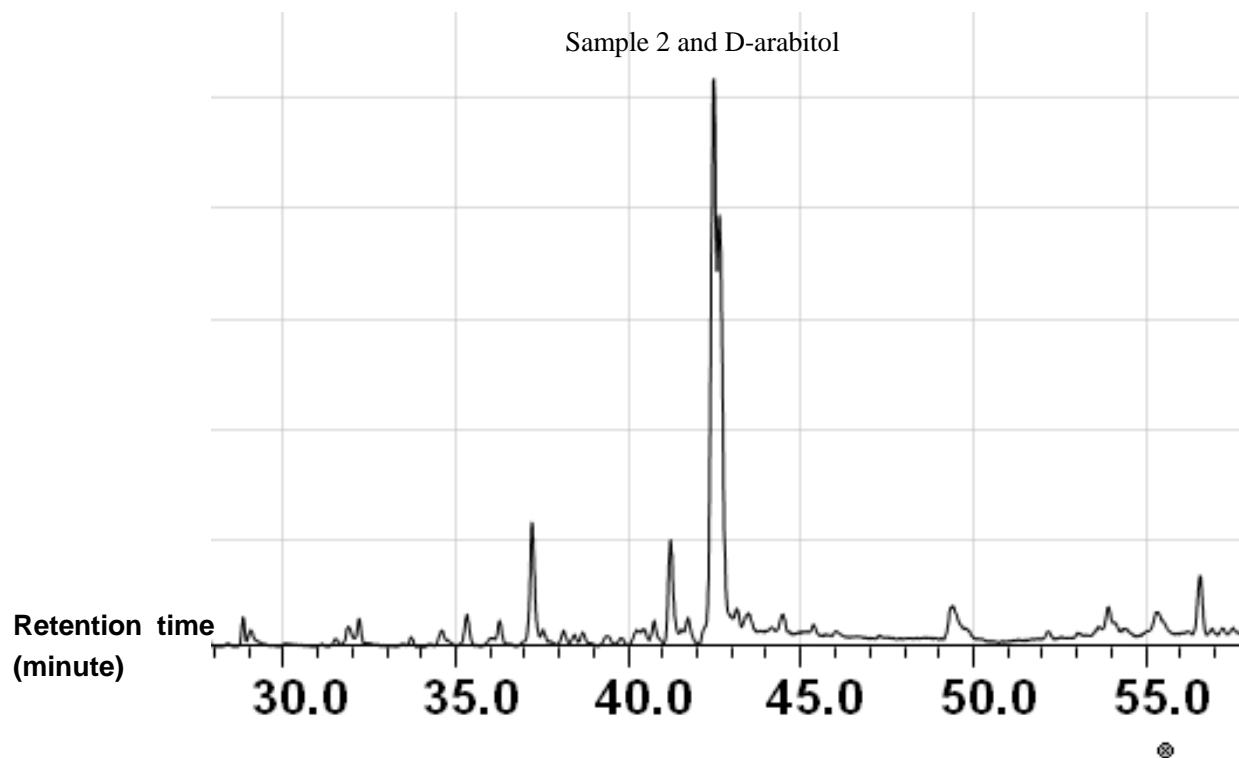
S1-B. Analysis of trifluoroacetyl pentitol standards by gas chromatography.



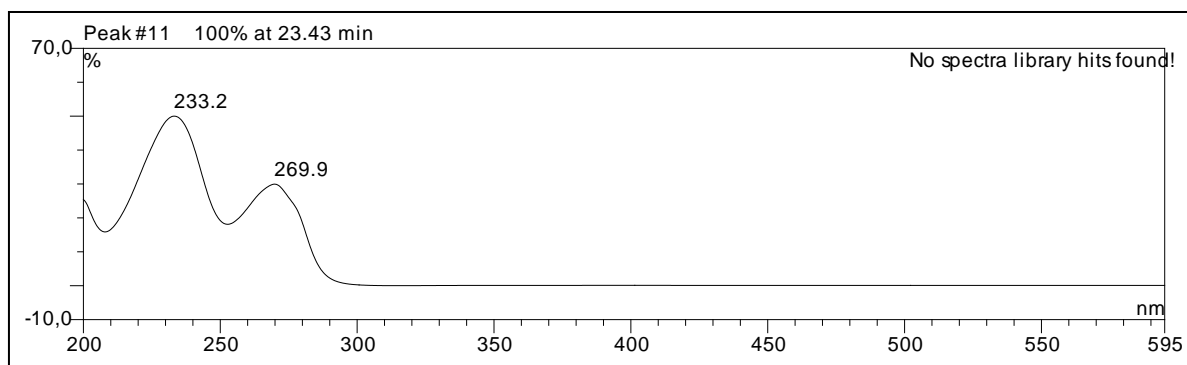
S1-C. Analysis of trifluoroacetyl sample 2 (degraded from mixture of compounds **4** and **5**) by gas chromatography.



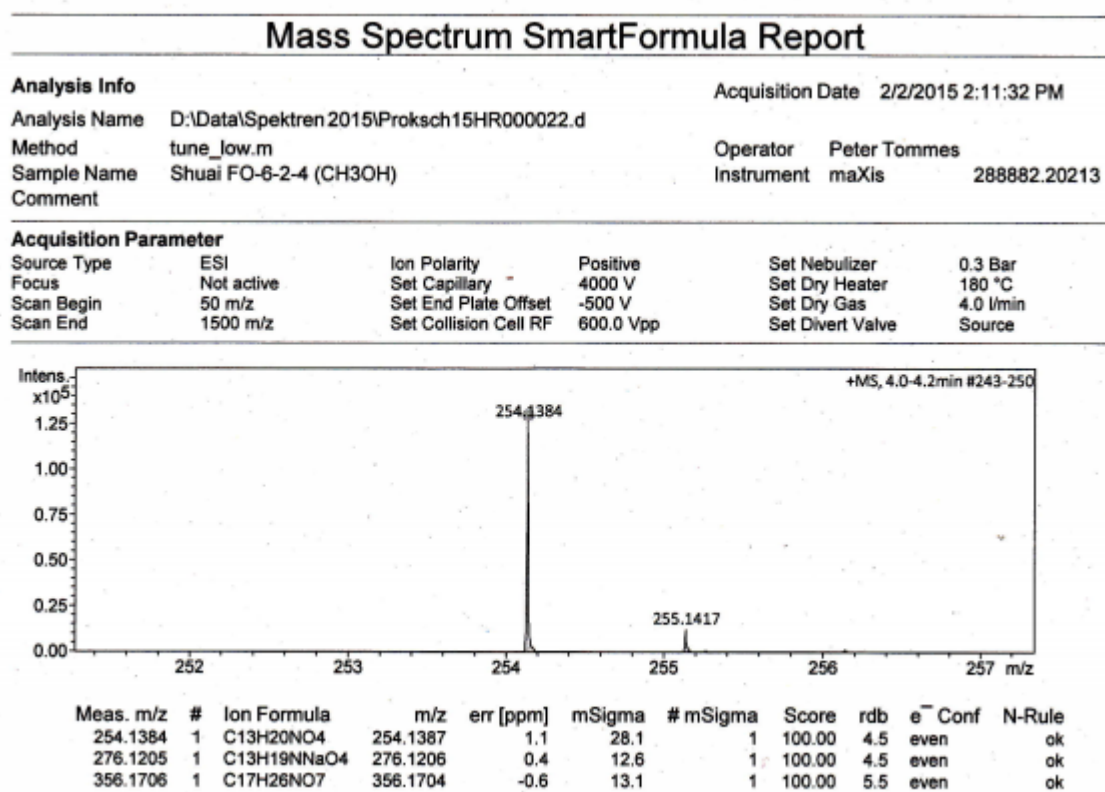
S1-D. Analysis of trifluoroacetyl sample 2 (degraded from mixture of compounds **4** and **5**) and L-arabitol in one injection by gas chromatography.



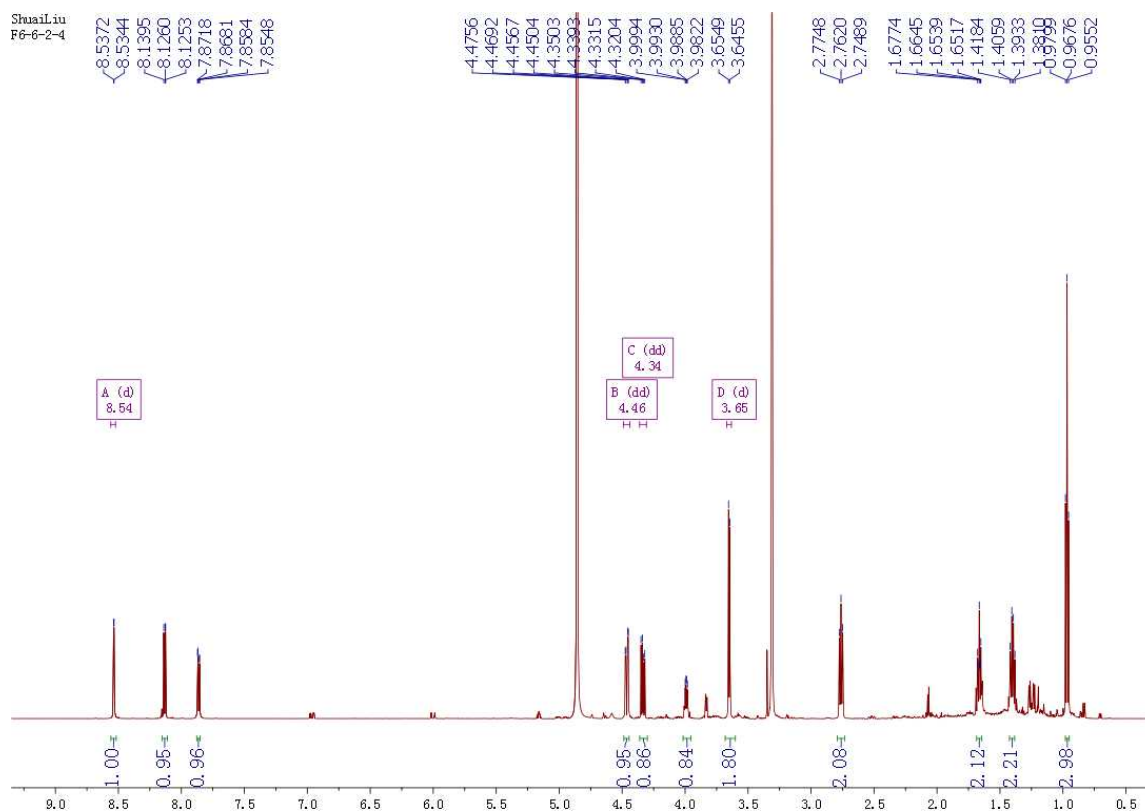
S1-E. Analysis of trifluoroacetyl sample 2 (degraded from mixture of compounds **4** and **5**) and D-arabitol in one injection by gas chromatography.



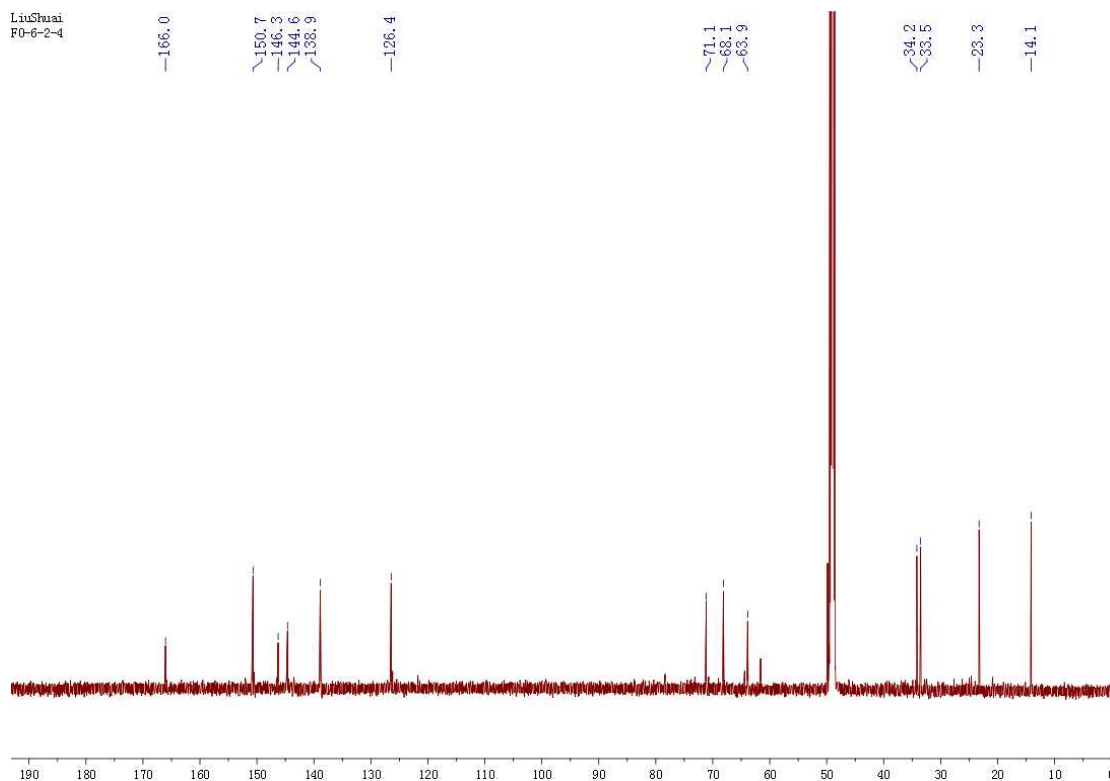
S2. UV spectrum of compound 1.



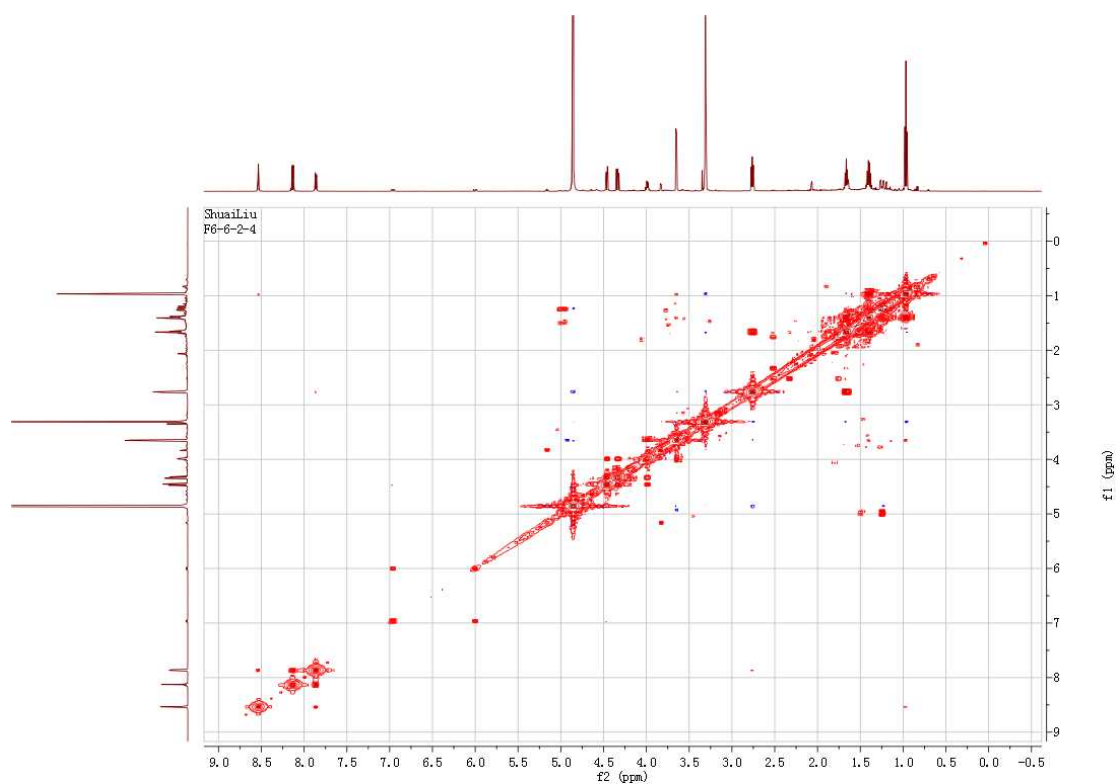
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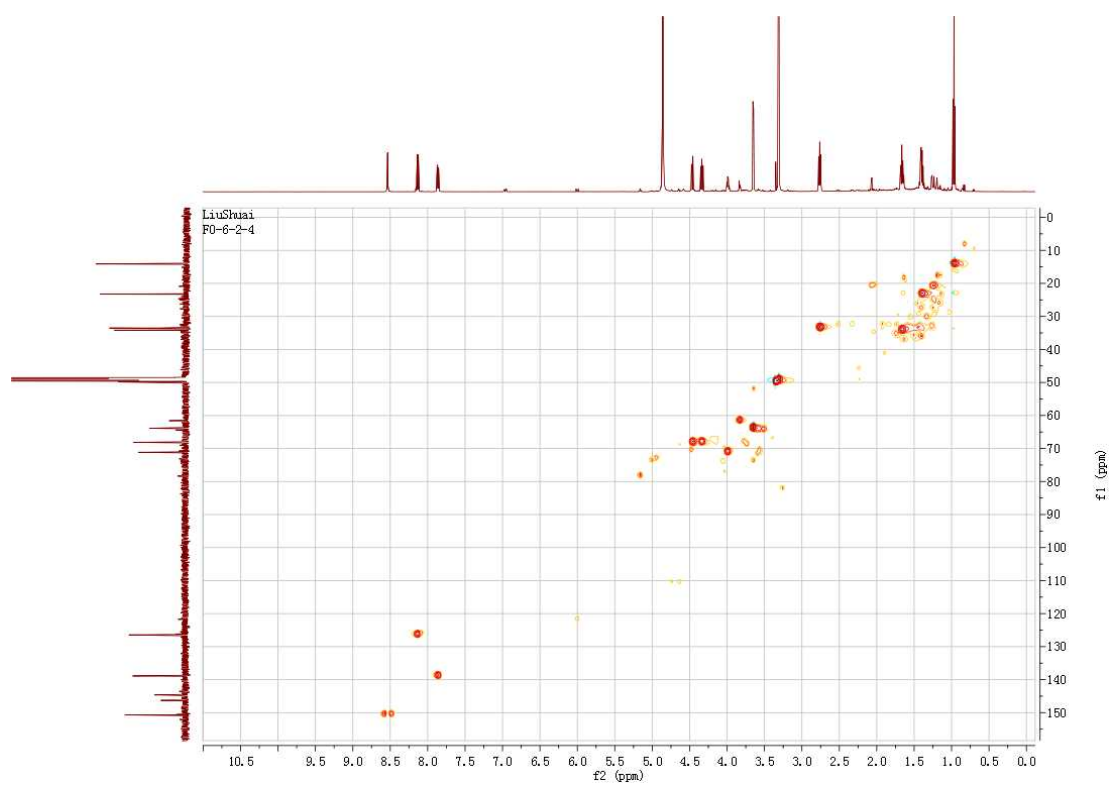
S4. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **1**.



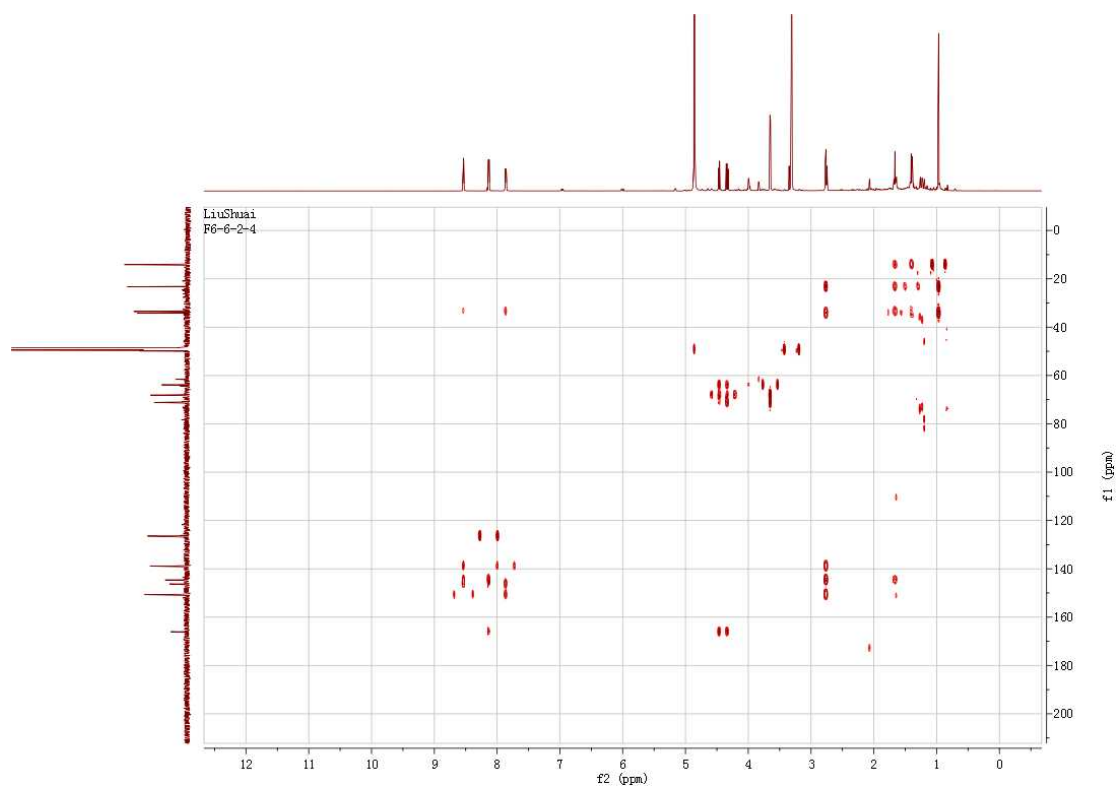
S5. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **1**.



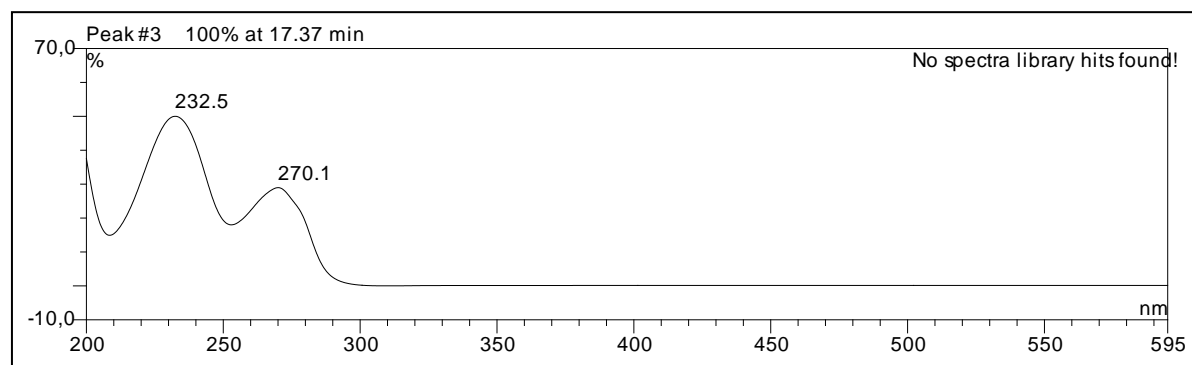
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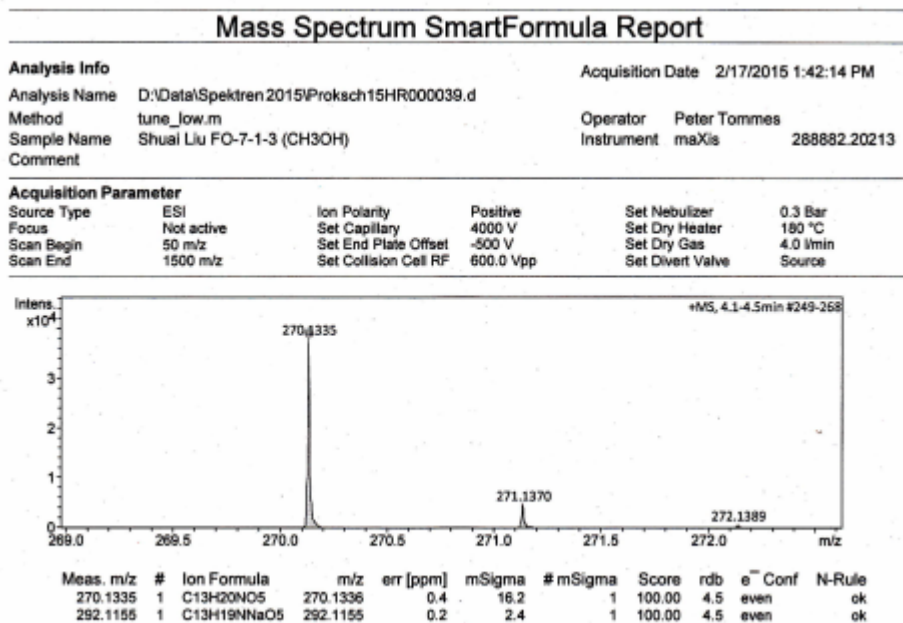
S7. HSQC (600 and 150 MHz, CD_3OD) spectrum of compound **1**.



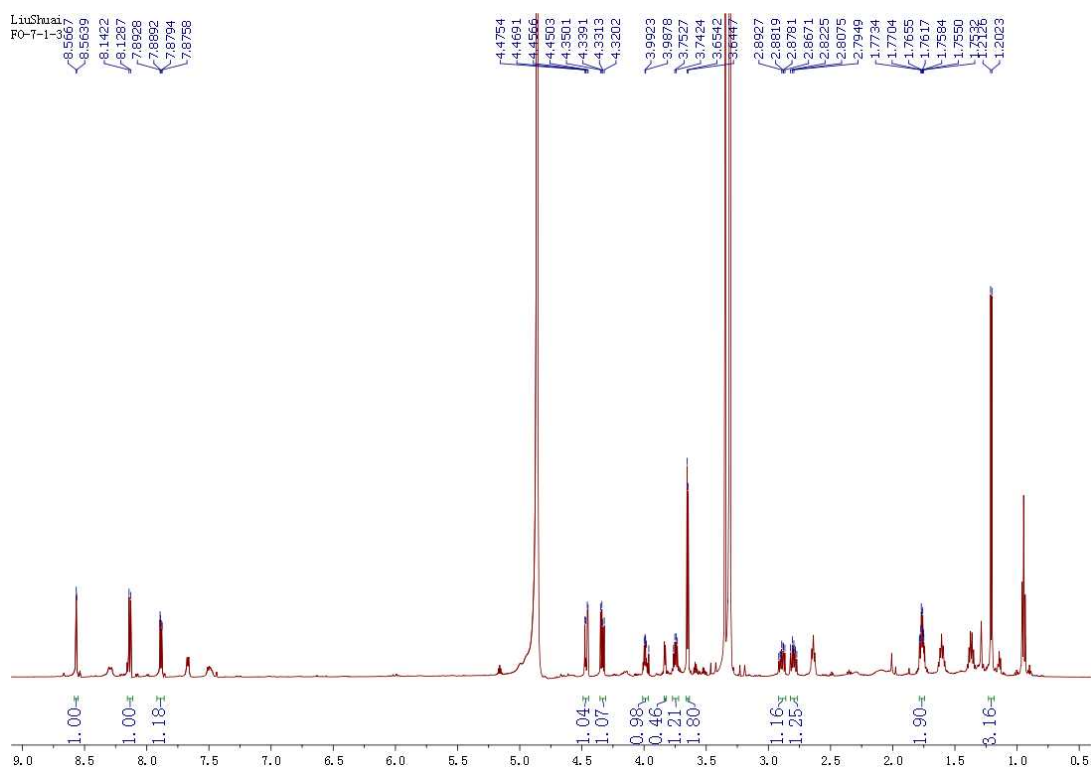
S8. HMBC (600 and 150 MHz, CD₃OD) spectrum of compound **1**.



S9. UV spectrum of compound **2**.

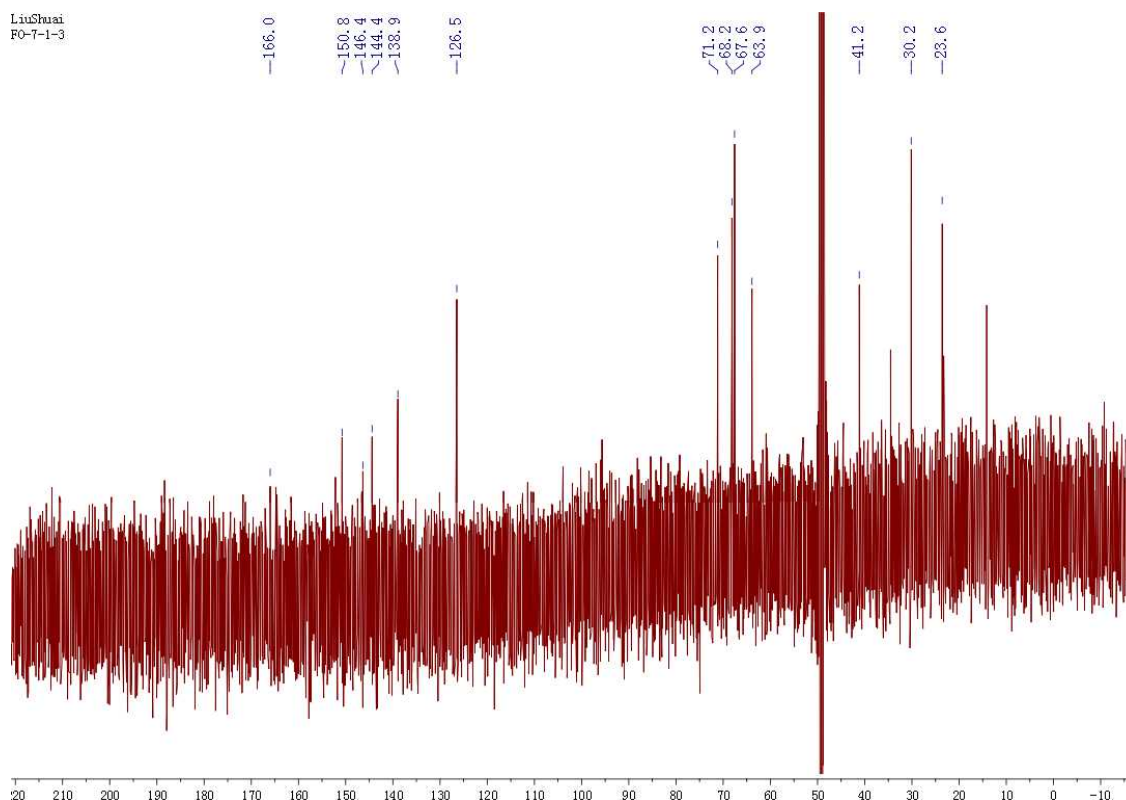


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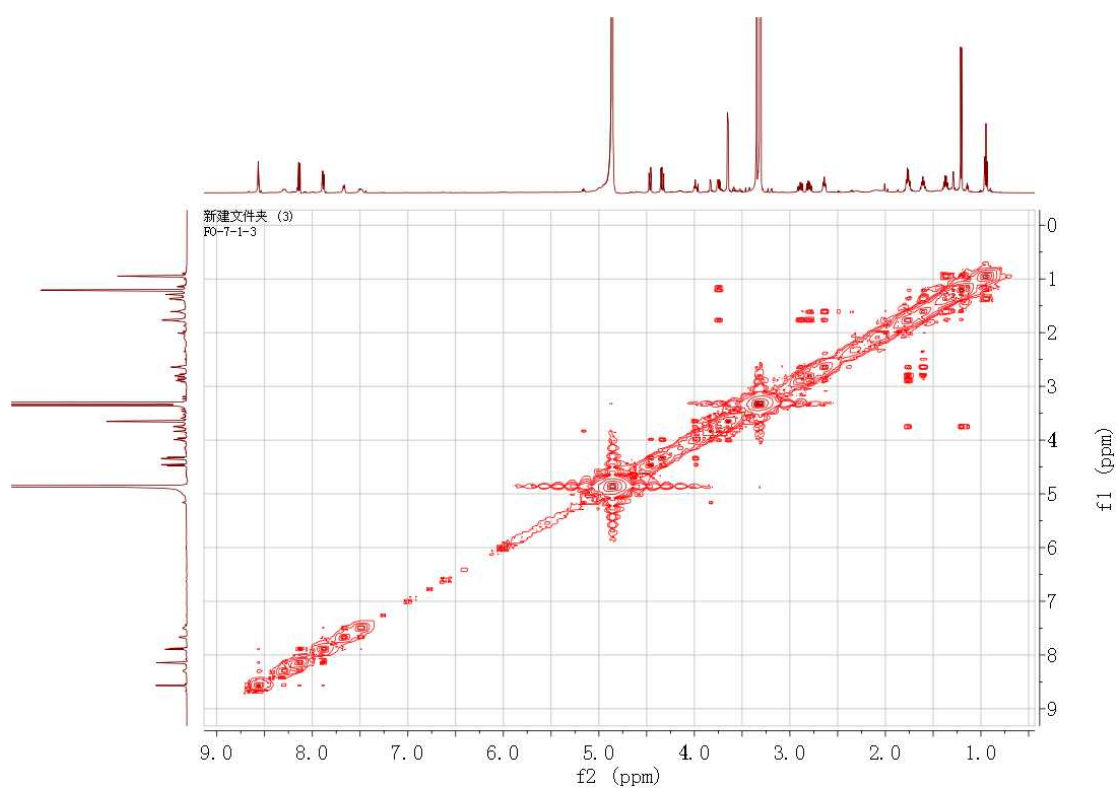


S11. ¹H NMR (600 MHz, CD₃OD) spectrum of compound **2**.

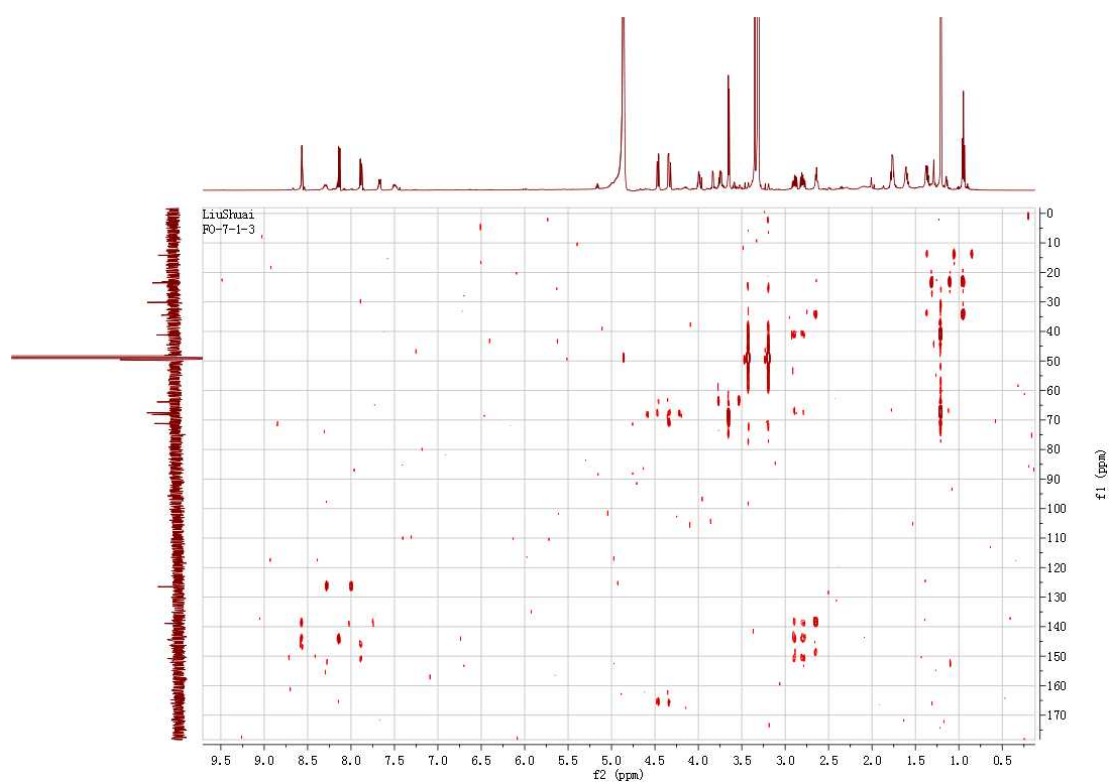
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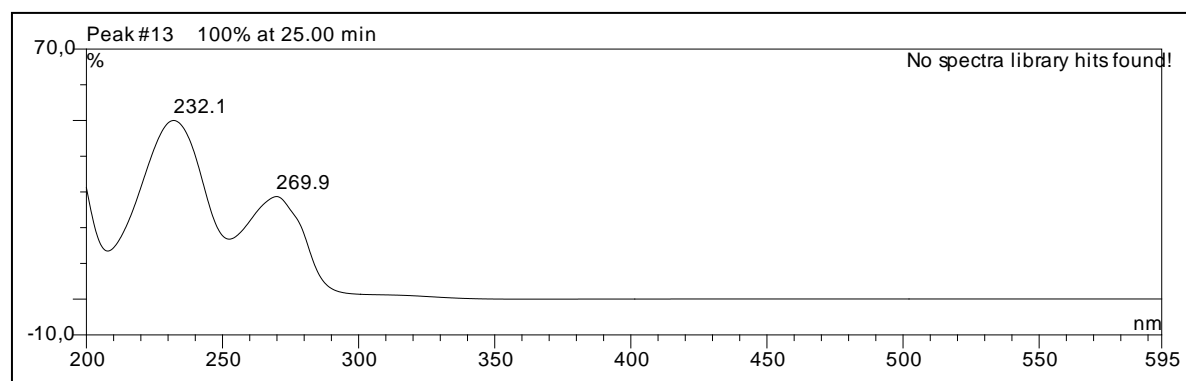
S12. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound **2**.



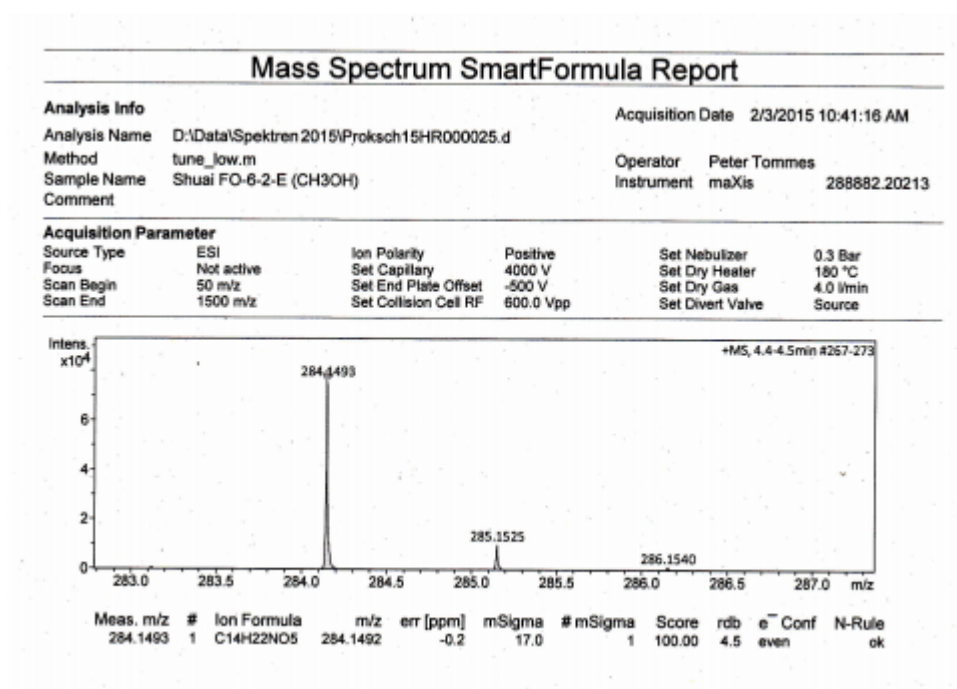
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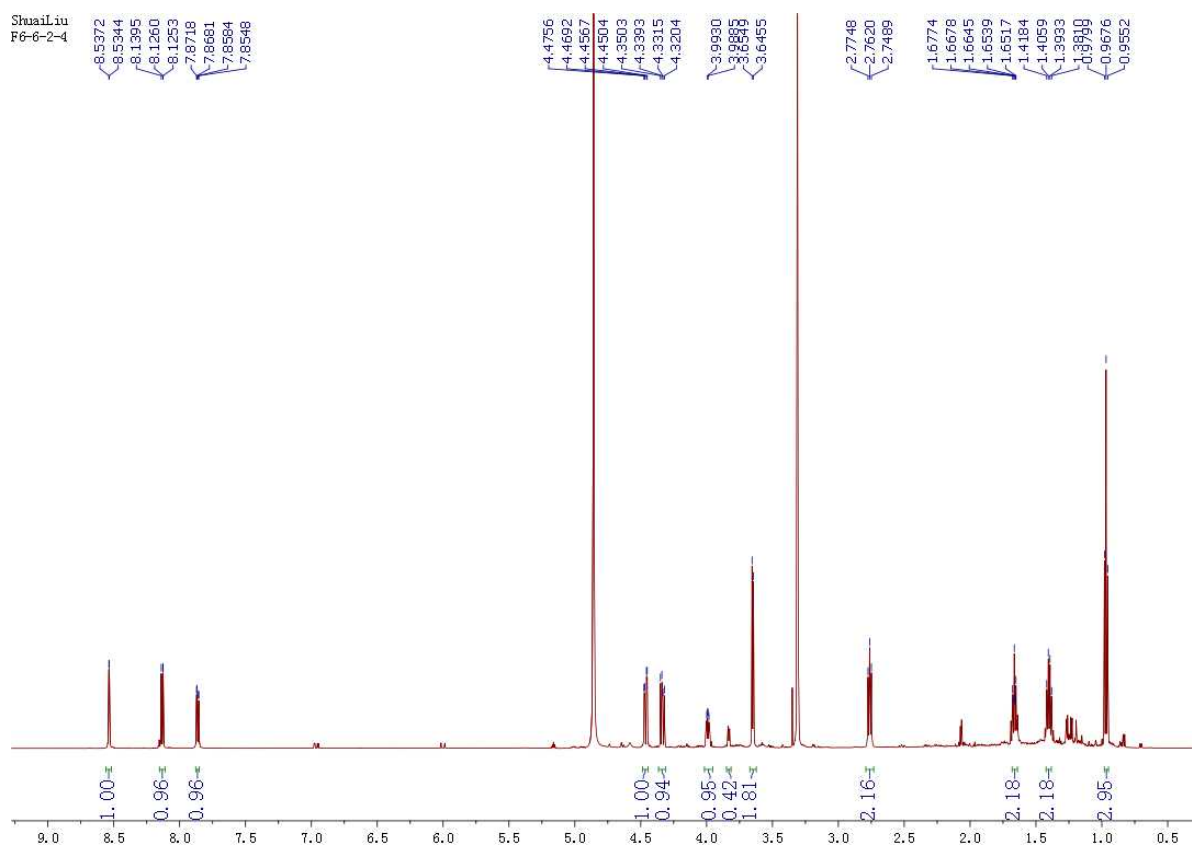
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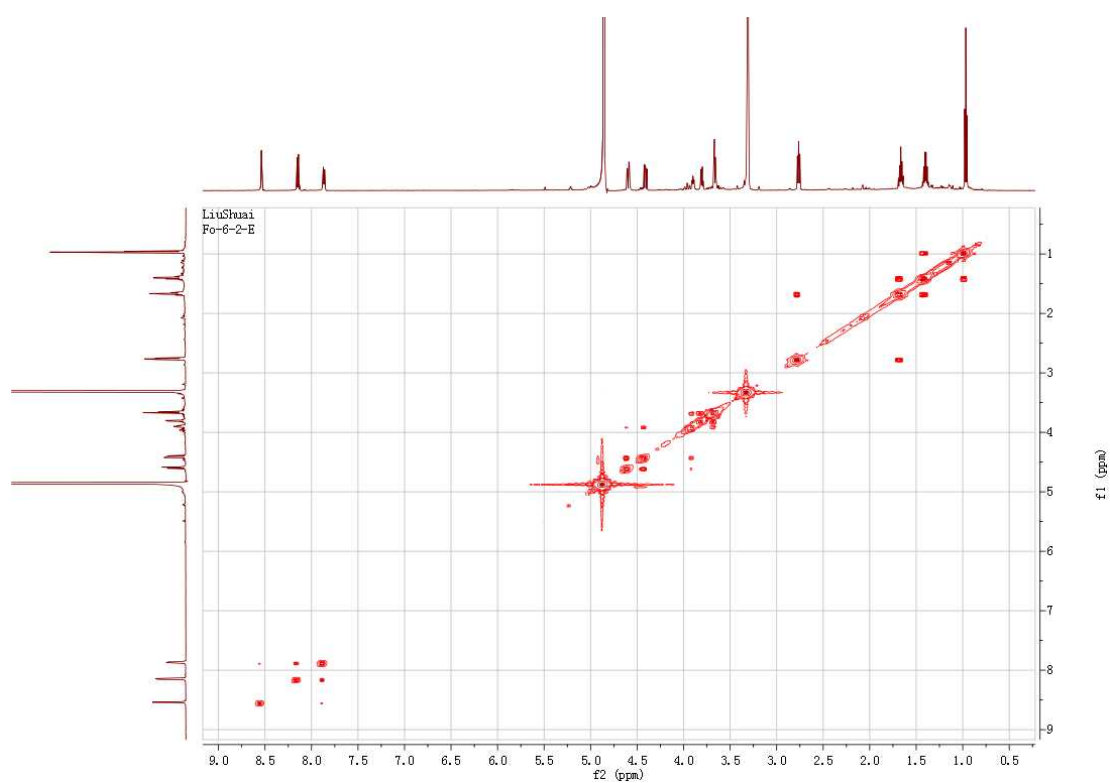
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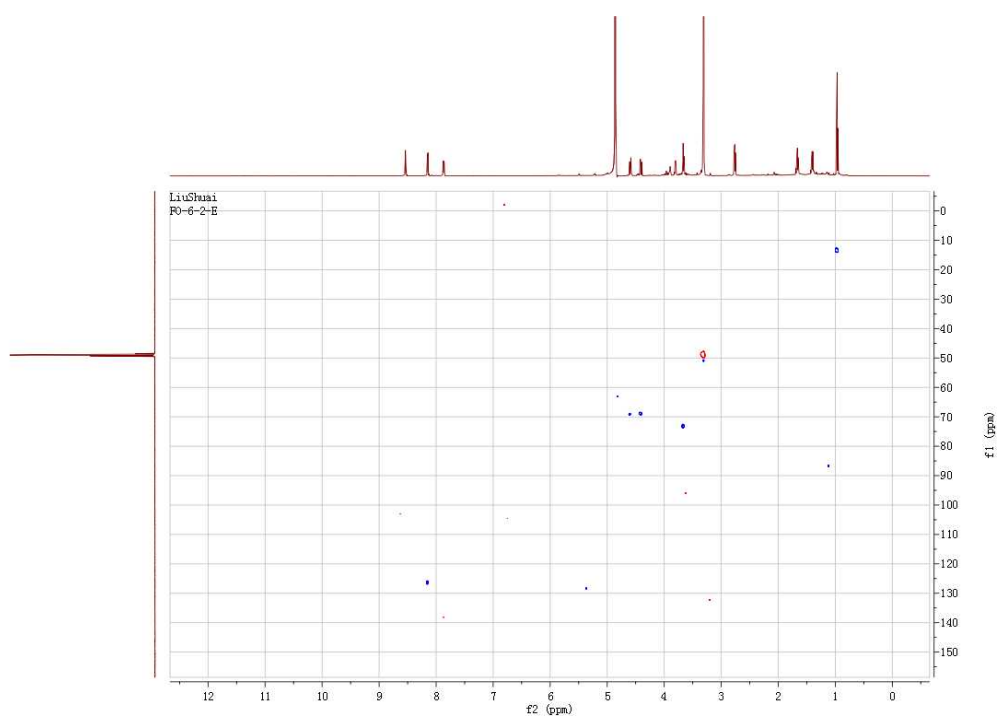
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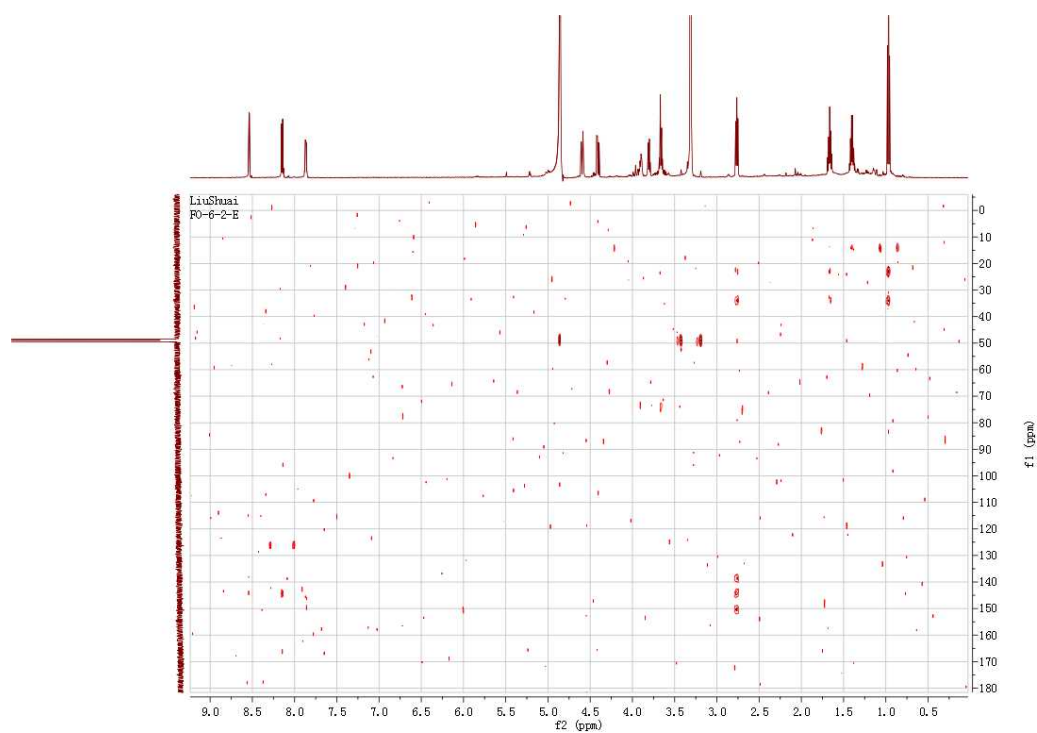
S17. ¹H NMR (600 MHz, CD₃OD) spectrum of compound **3**.



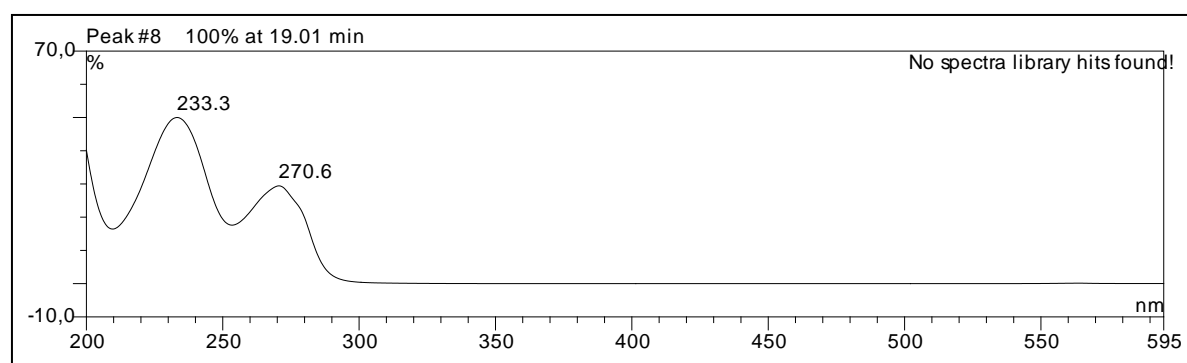
S18. ^1H - ^1H COSY (600 MHz, CD_3OD) spectrum of compound **3**.



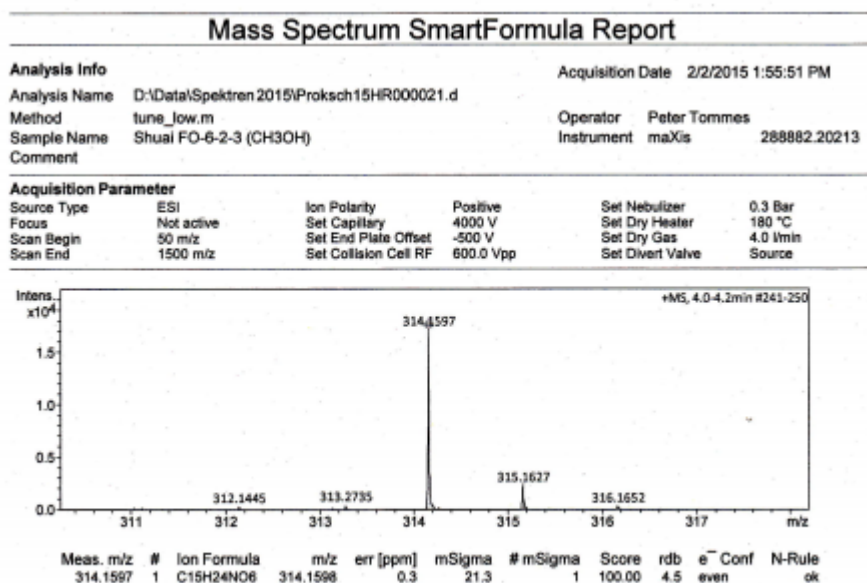
S19. HSQC (600 and 150 MHz, CD_3OD) spectrum of compound **3**.



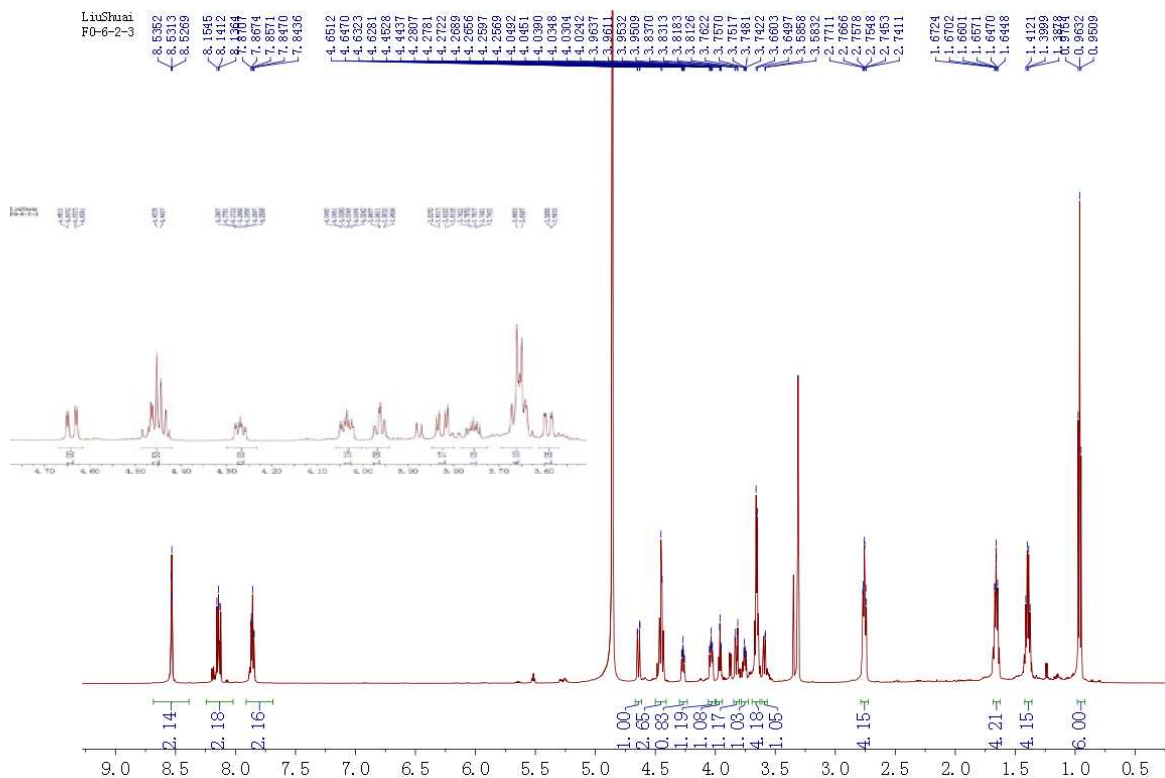
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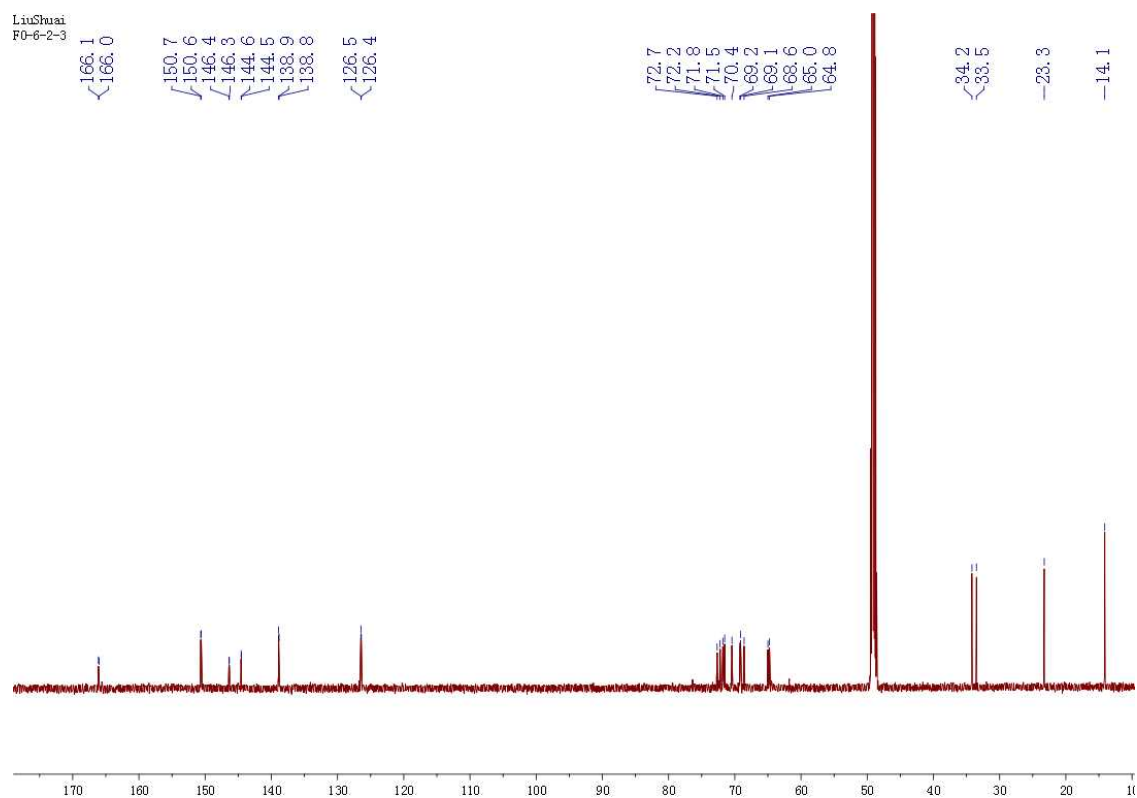
S21. UV spectrum of mixture of **4** and **5**.



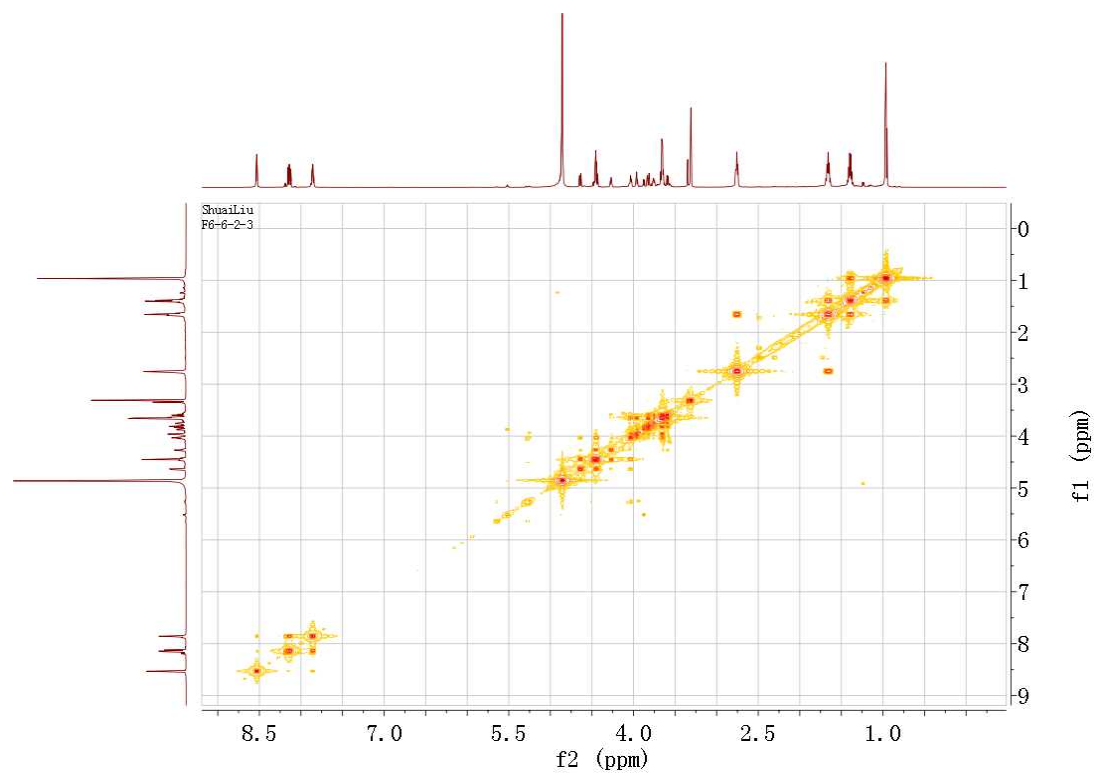
S22. HRESIMS spectrum of mixture of 4 and 5.



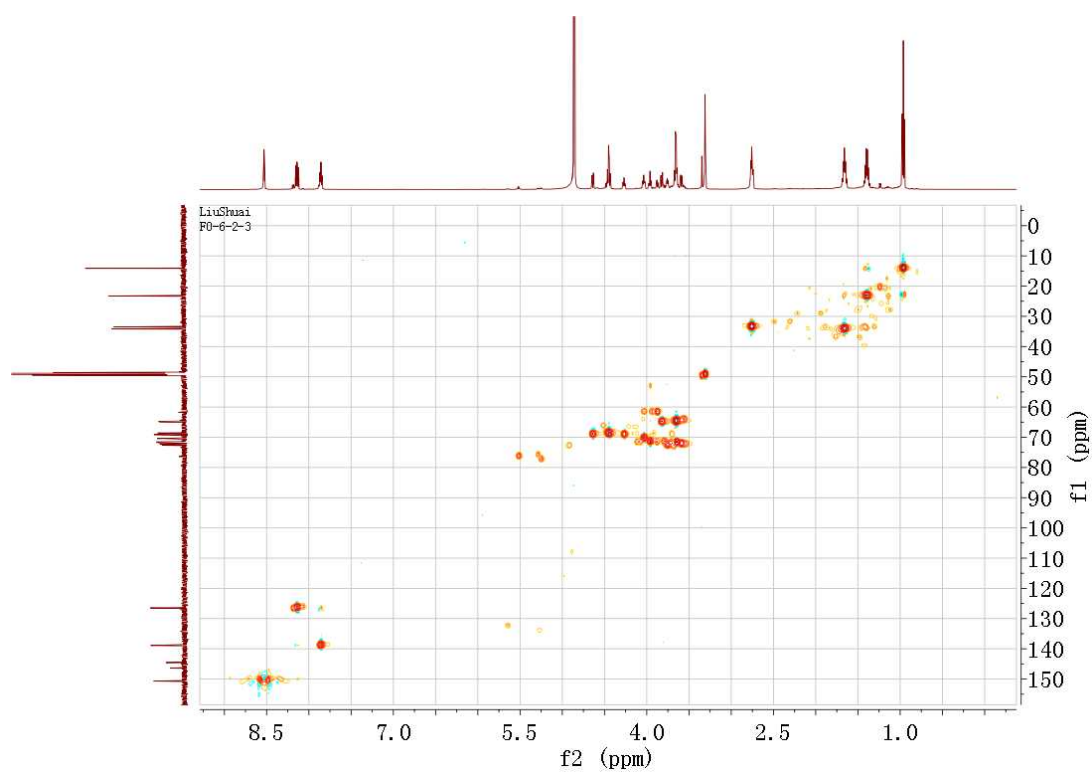
S23. ¹H NMR (600 MHz, CD₃OD) spectrum of mixture of 4 and 5.



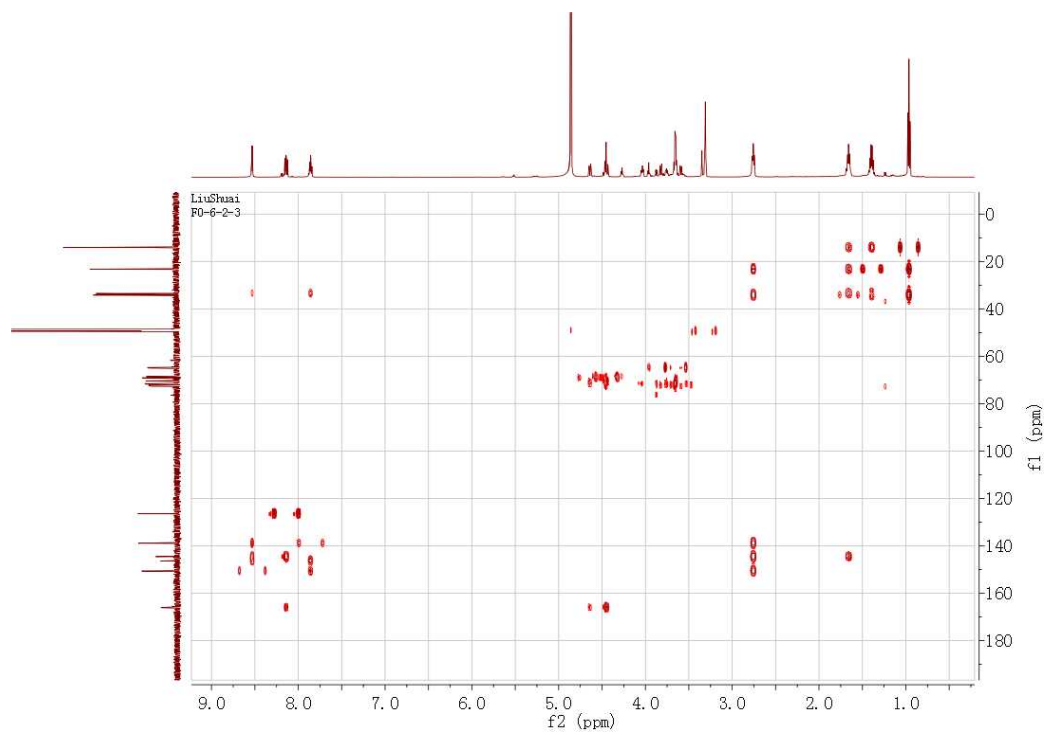
S24. ^{13}C NMR (150 MHz, CD_3OD) spectrum of mixture of **4** and **5**.



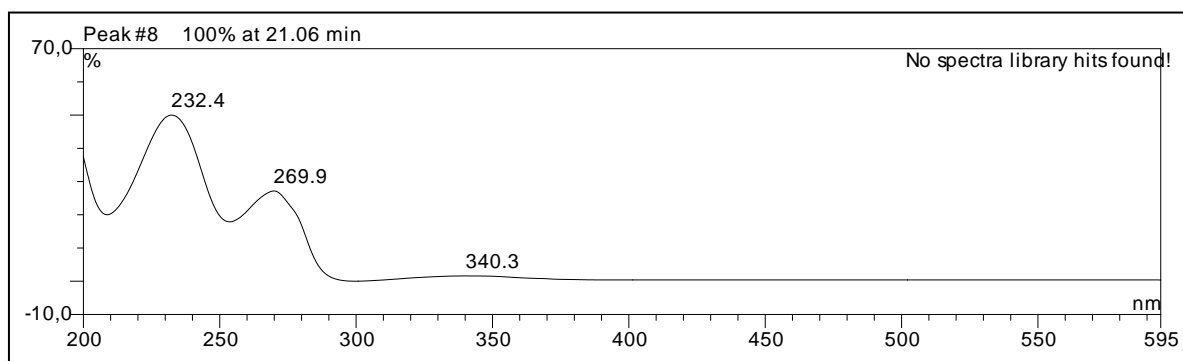
S25. ^1H - ^1H COSY (600 MHz, CD_3OD) spectrum of mixture of **4** and **5**.



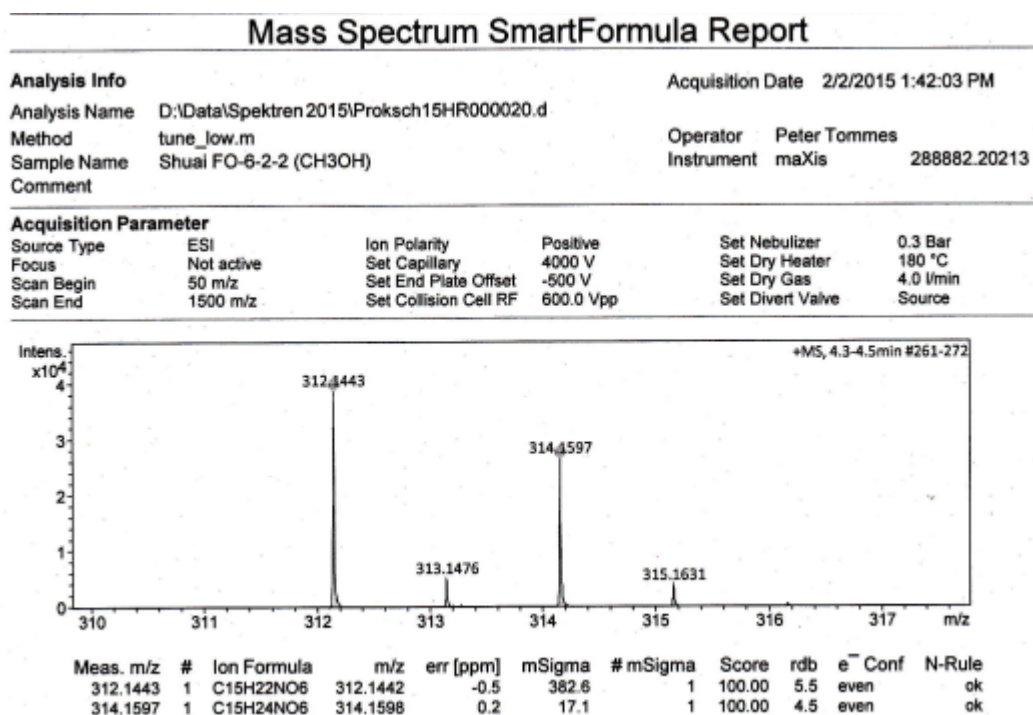
S26. HSQC (600 and 150 MHz, CD₃OD) spectrum of mixture of **4** and **5**.



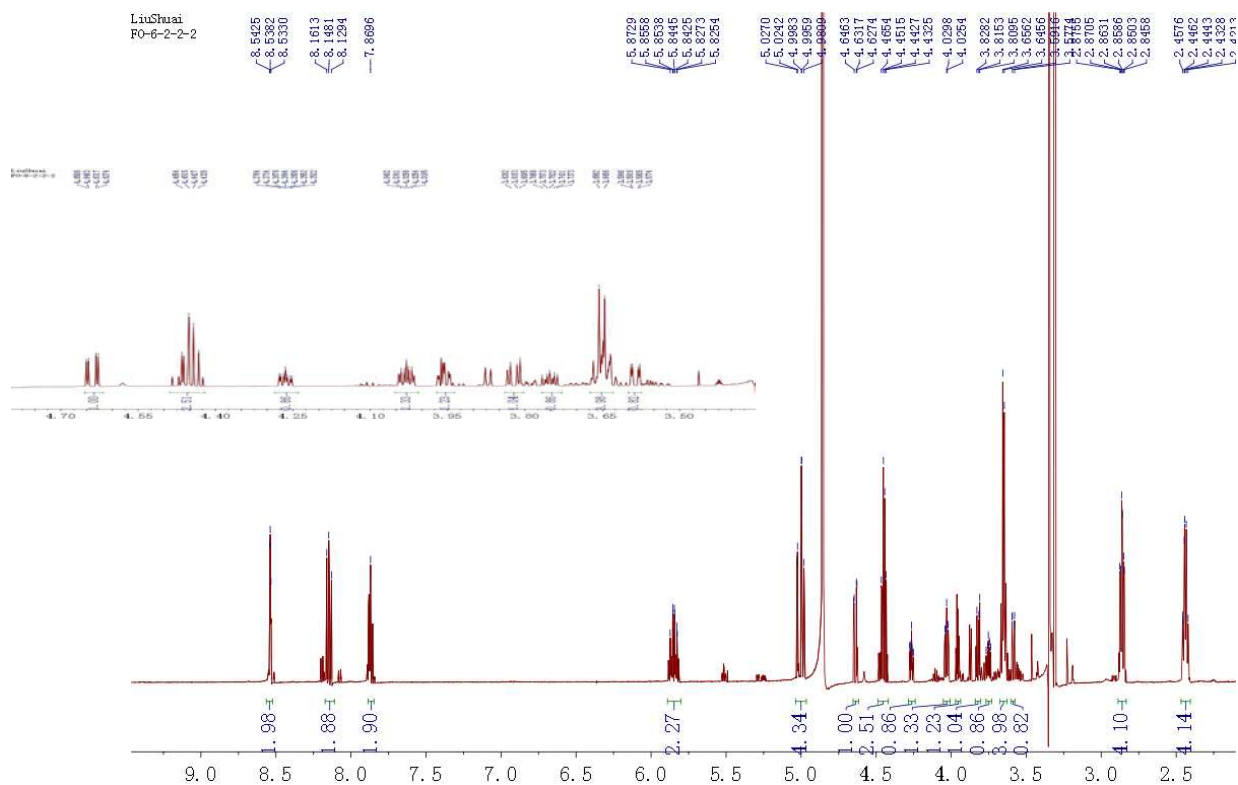
S27. HMBC (600 and 150 MHz, CD₃OD) spectrum of mixture of **4** and **5**.



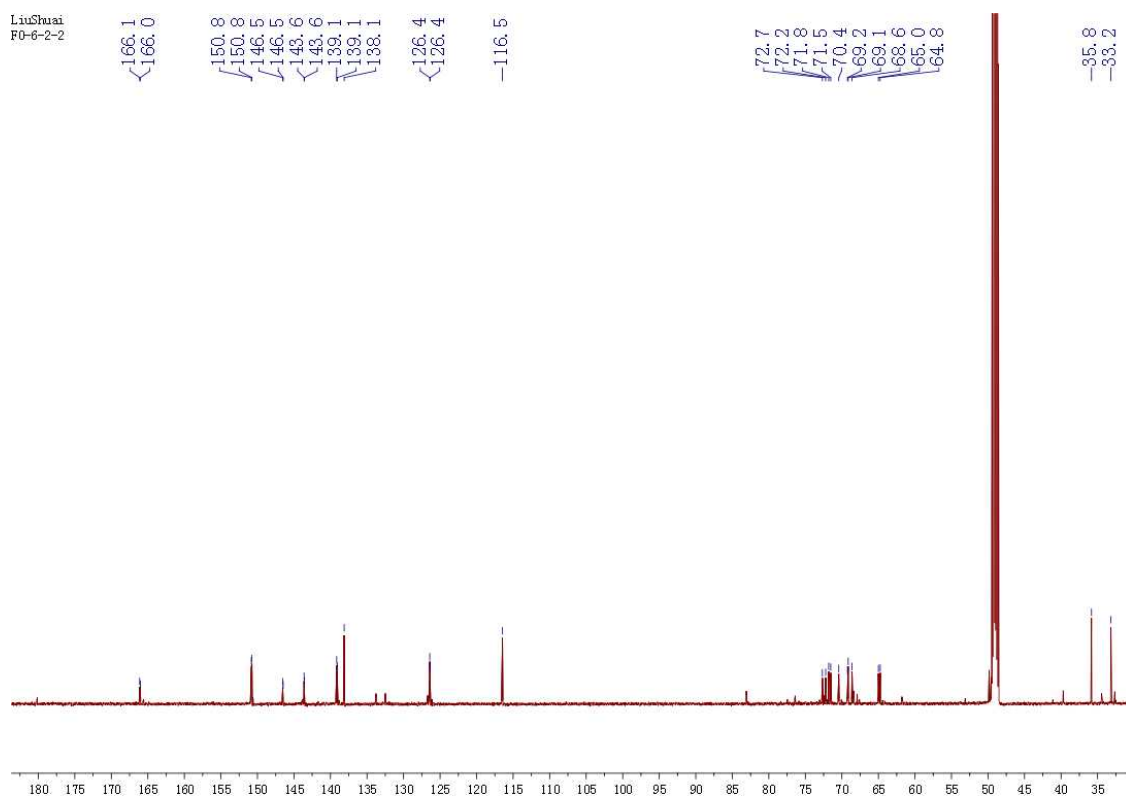
S28. UV spectrum of mixture of **6** and **7**.



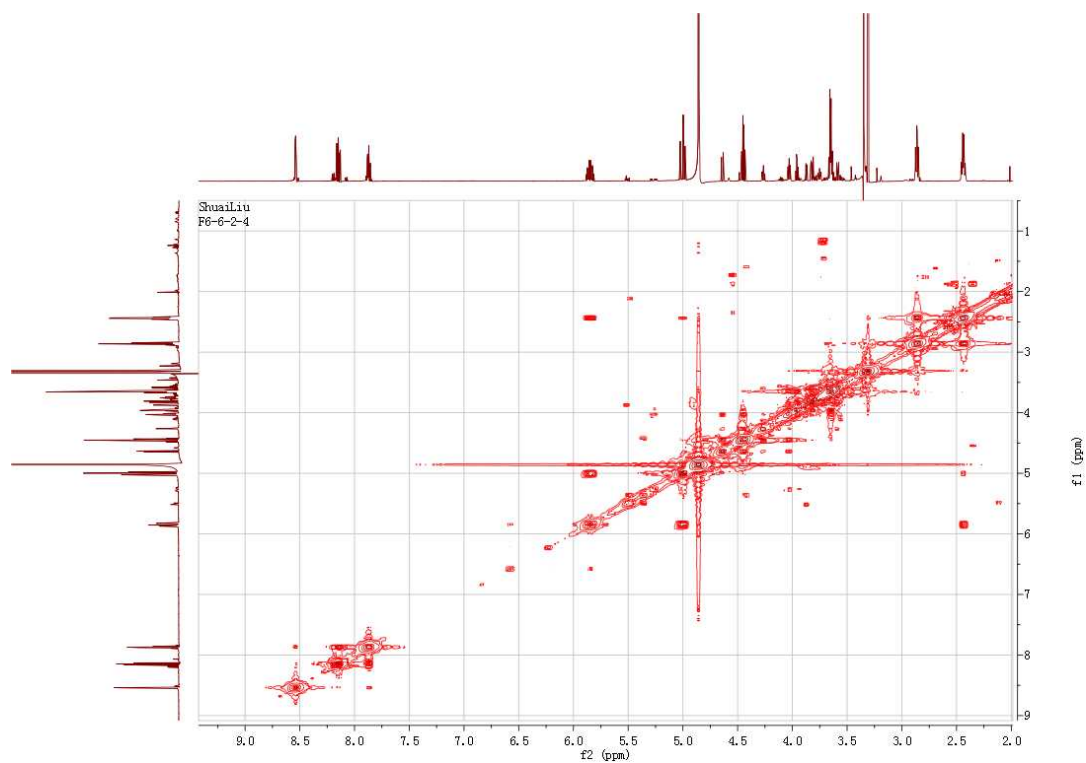
S29. HRESIMS spectrum of mixture of **6** and **7**.



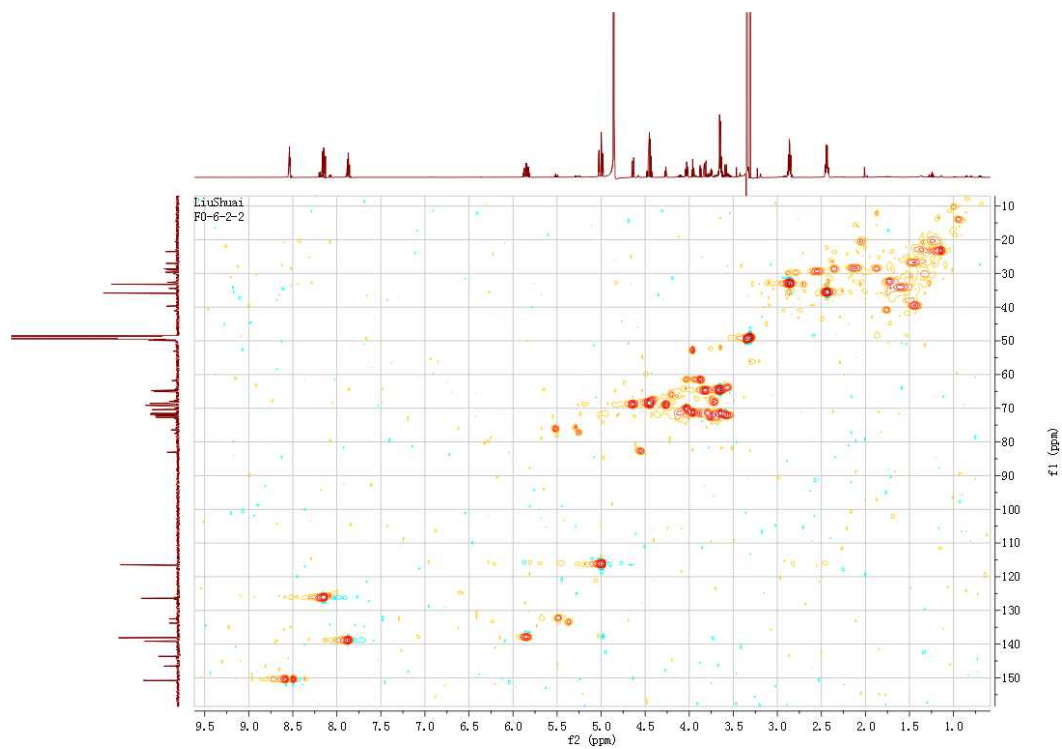
S30. ^1H NMR (600 MHz, CD_3OD) spectrum of mixture of **6** and **7**.



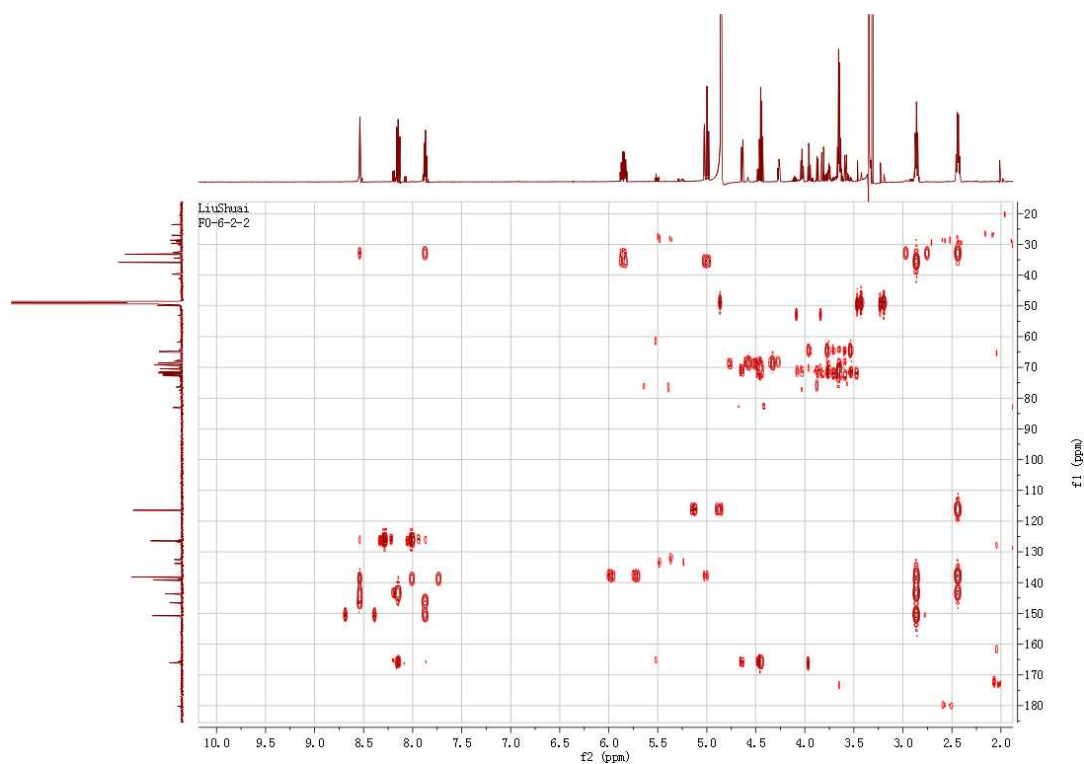
S31. ^{13}C NMR (150 MHz, CD_3OD) spectrum of mixture of **6** and **7**.



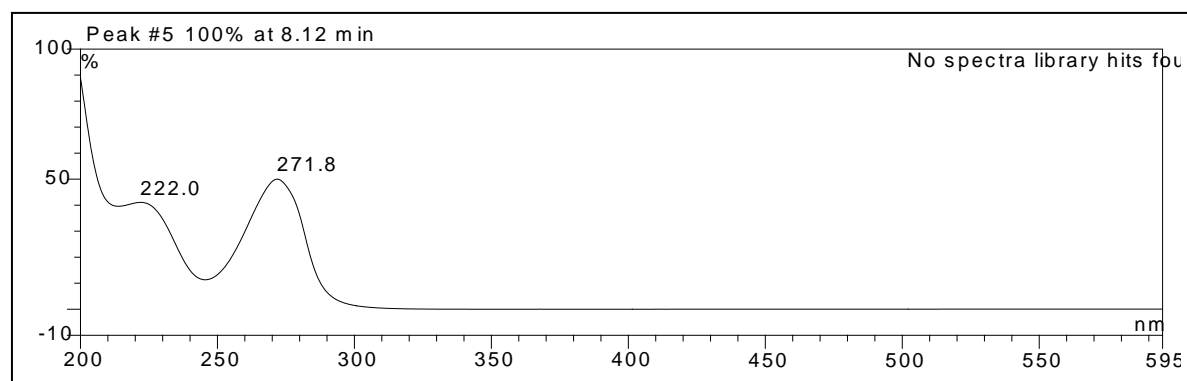
S32. ^1H - ^1H COSY (600 MHz, CD_3OD) spectrum of mixture of **6** and **7**.



S33. HSQC (600 and 150 MHz, CD_3OD) spectrum of mixture of **6** and **7**.



S34. HMBC (600 and 150 MHz, CD₃OD) spectrum of mixture of **6** and **7**.



S35. UV spectrum of compound **8**.

Mass Spectrum SmartFormula Report

Analysis Info

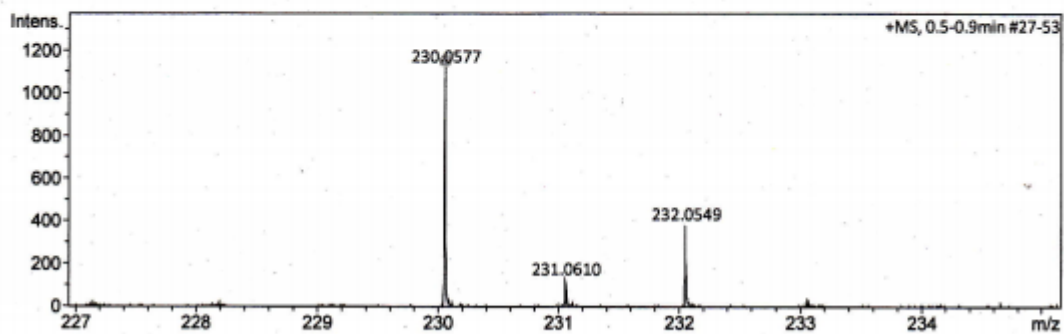
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 Sample Name Shuai FO-7-1-1 (CH₃OH)
 Comment

Acquisition Date 2/2/2015 3:41:04 PM

Operator Peter Tommes
 Instrument maXis 288882.20213

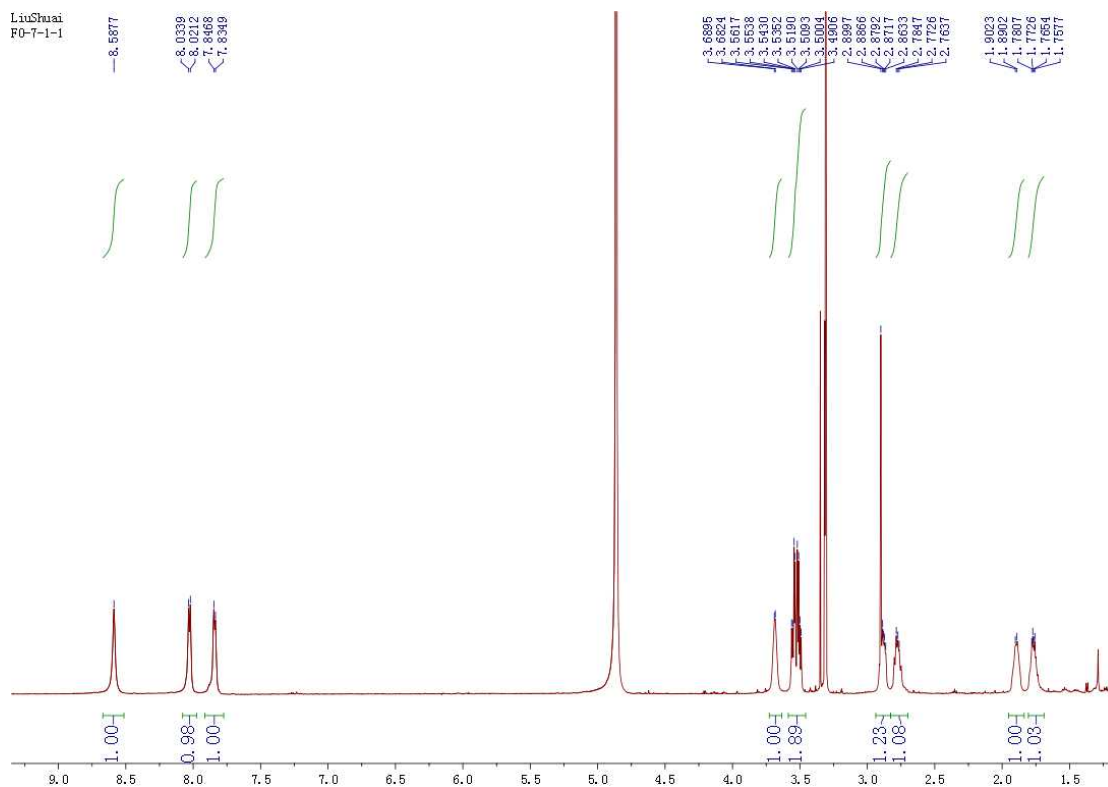
Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source

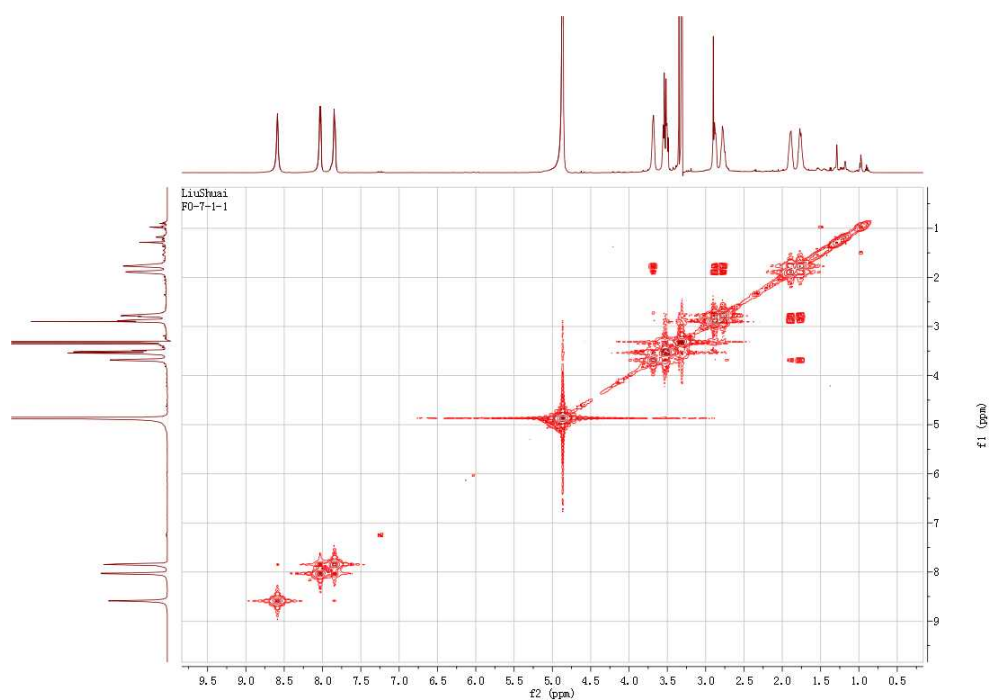


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
230.0577	1	C ₁₀ H ₁₃ CINO ₃	230.0578	0.8	19.4	1	100.00	4.5	even	ok

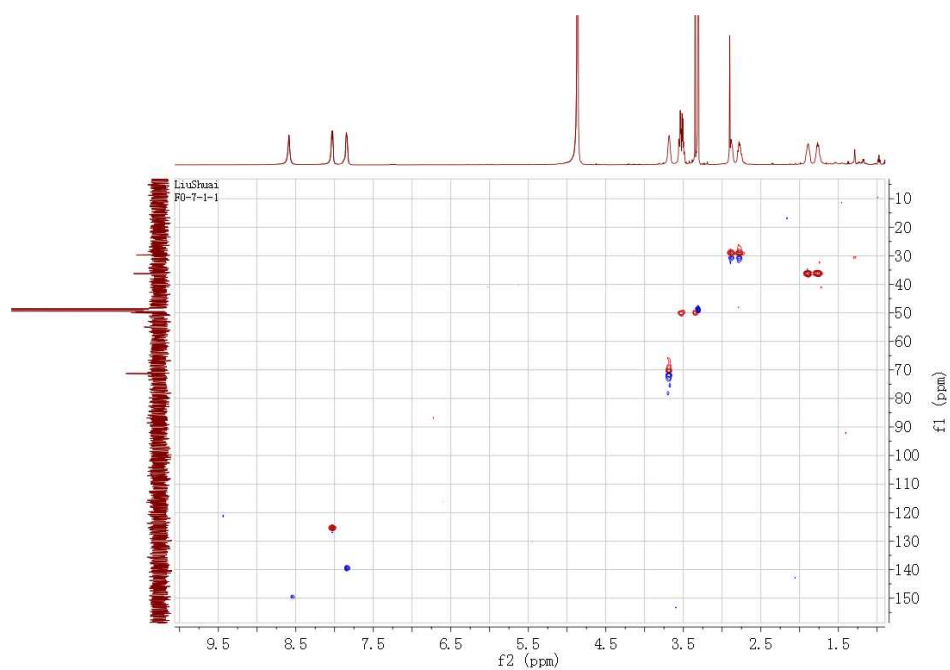
S36. HRESIMS spectrum of compound **8**.



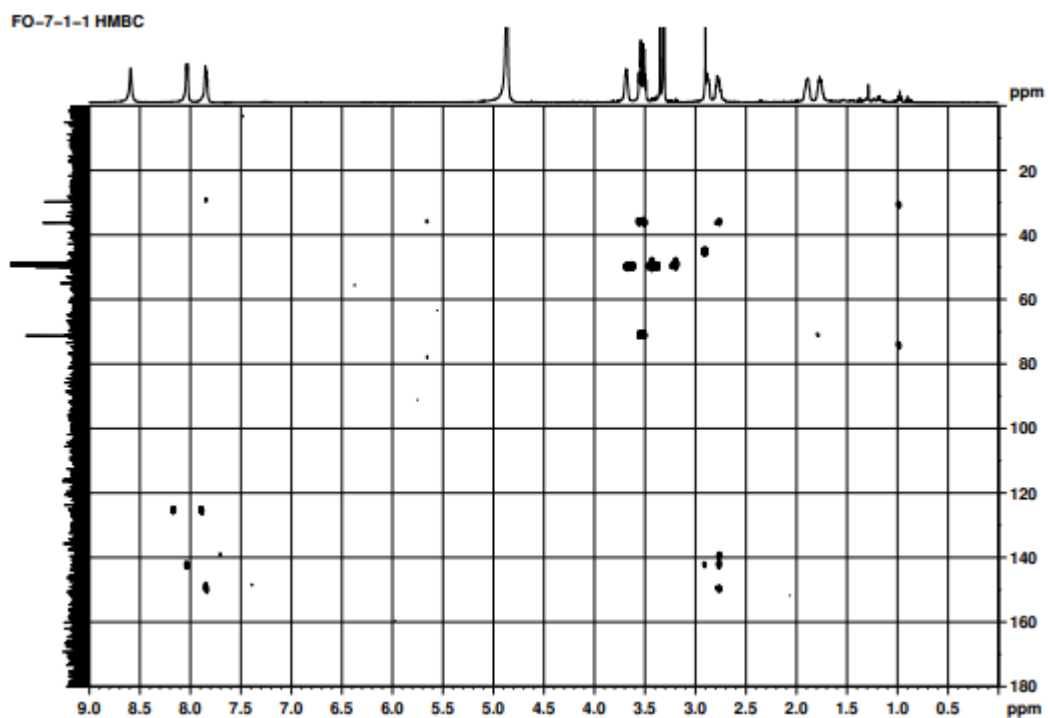
S37. ¹H NMR (600 MHz, CD₃OD) spectrum of compound **8**.



S38. ^1H - ^1H COSY (600 MHz, CD_3OD) spectrum of compound **8**.

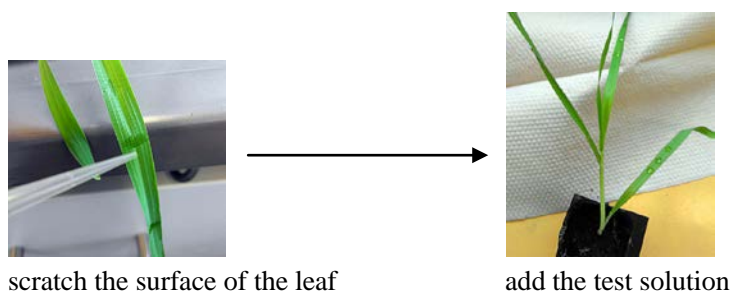


S39. HSQC (600 and 150 MHz, CD_3OD) spectrum of compound **8**.



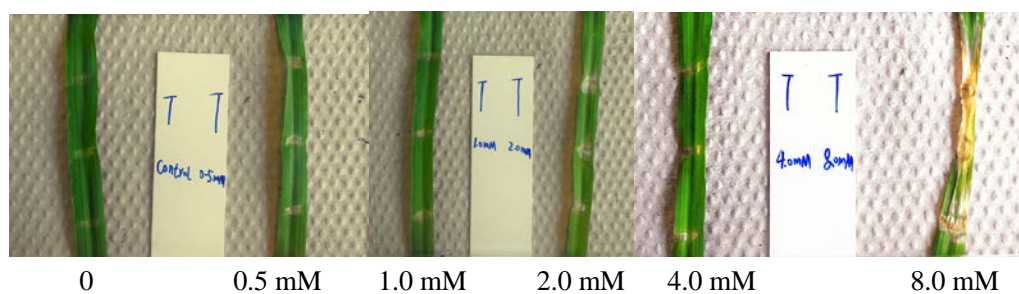
S40. HMBC (600 and 150 MHz, CD₃OD) spectrum of compound **8**.

S41. Phytotoxic bioassay for fusaric acid derivatives (20 μ L at three locations on barley leaf).

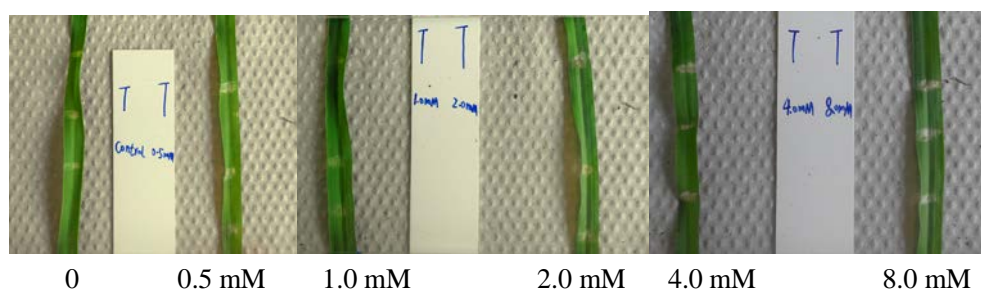


Score 0 1 2 3 4 5
 Visual rating: 0 = no necrosis (negative control); 5 = severe necrosis.

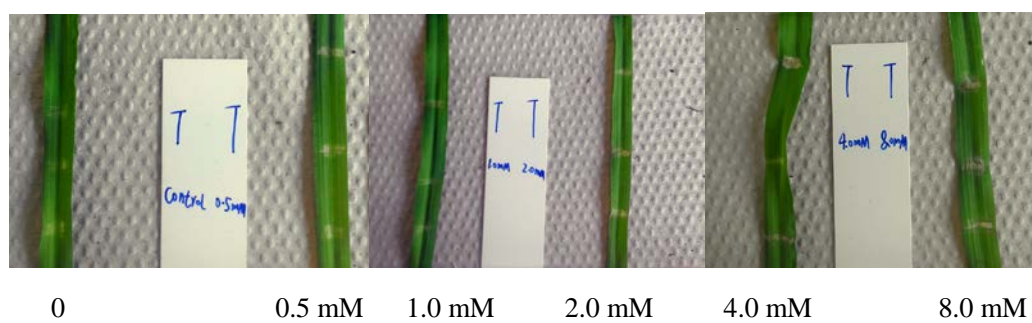
Compound 1



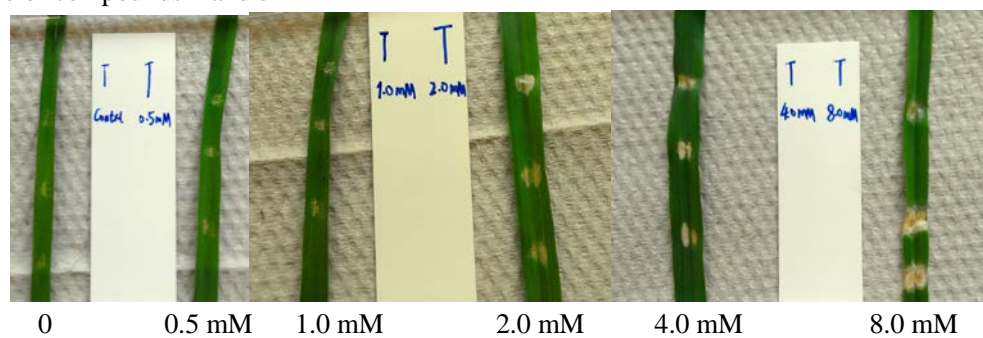
Compound 2



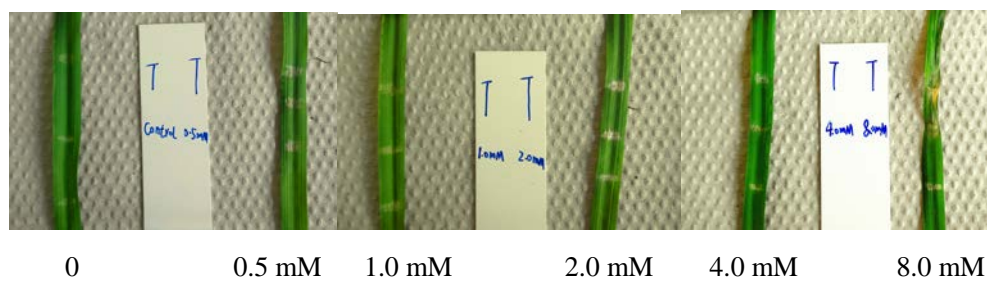
Compound 3



Mixture of compounds 4 and 5



Mixture of compounds 6 and 7



Compound 8

