

Supporting Information

Preparative separation of 1,1-diphenyl-2-picrylhydrazyl inhibitors originating from *Saxifraga sinomontana* employing medium-pressure liquid chromatography in combination with reversed-phase liquid chromatography

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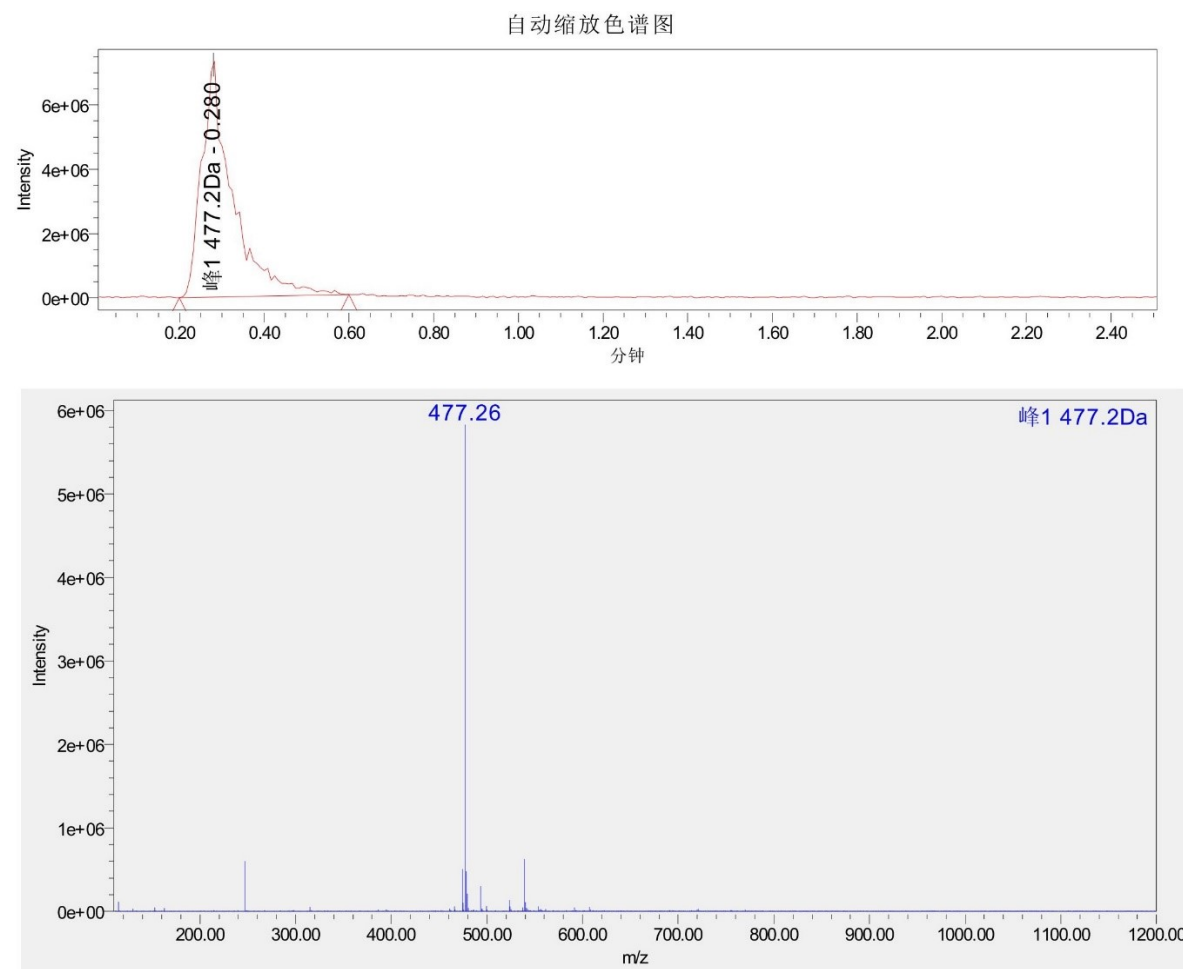


Figure S1. ESI+ of Peak Fr3-1 fraction (3-methoxy-4-hydroxyphenol-(6'-O-galloyl)-1-O- β -D-glucopyranoside)

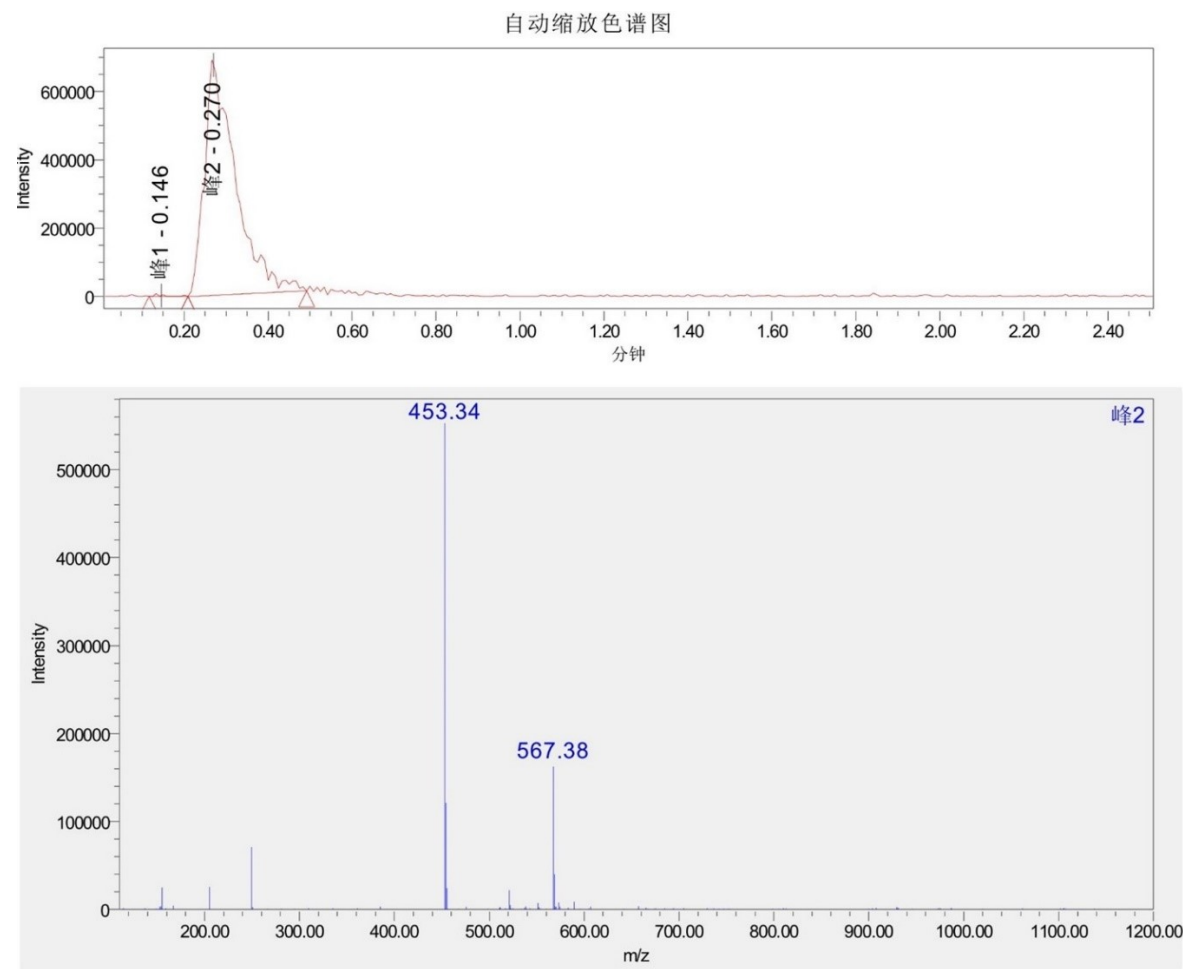


Figure S2. ESI- of Peak Fr3-1 fraction (3-methoxy-4-hydroxyphenol-(6'-O-galloyl)-1-O- β -D-glucopyranoside)

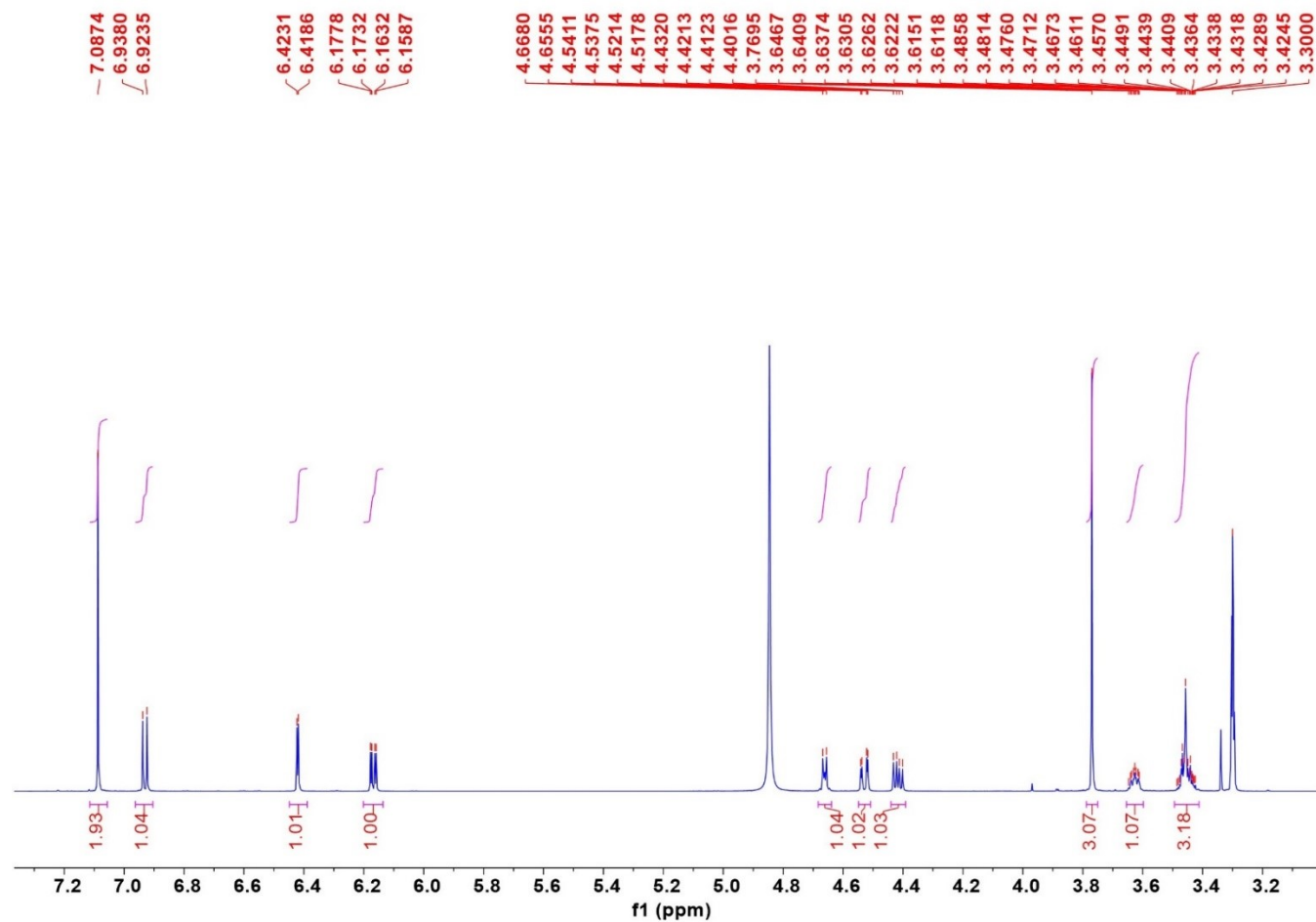


Figure S3. ¹H NMR Spectrum (600 MHz) of Peak Fr3-1 fraction (3-methoxy-4-hydroxyphenol-(6'-O-galloyl)-1-O-β-D-glucopyranoside) in MeOH-*d*₄

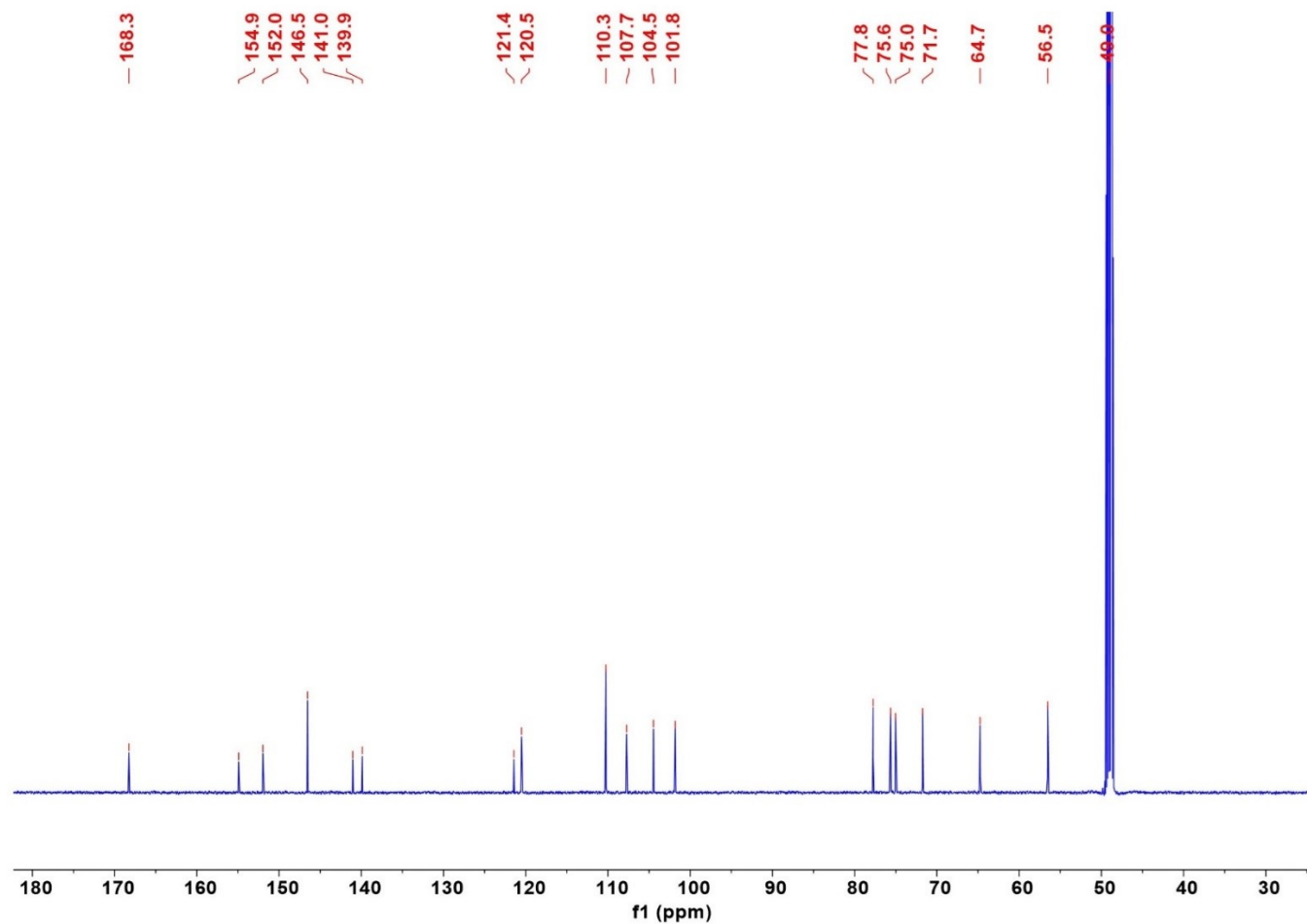


Figure S4. ^{13}C NMR Spectrum (151 MHz) of Peak Fr4-1-1 fraction (3-methoxy-4-hydroxyphenol-(6'-O-galloyl)-1-O- β -D-glucopyrano side) in $\text{MeOH-}d_4$

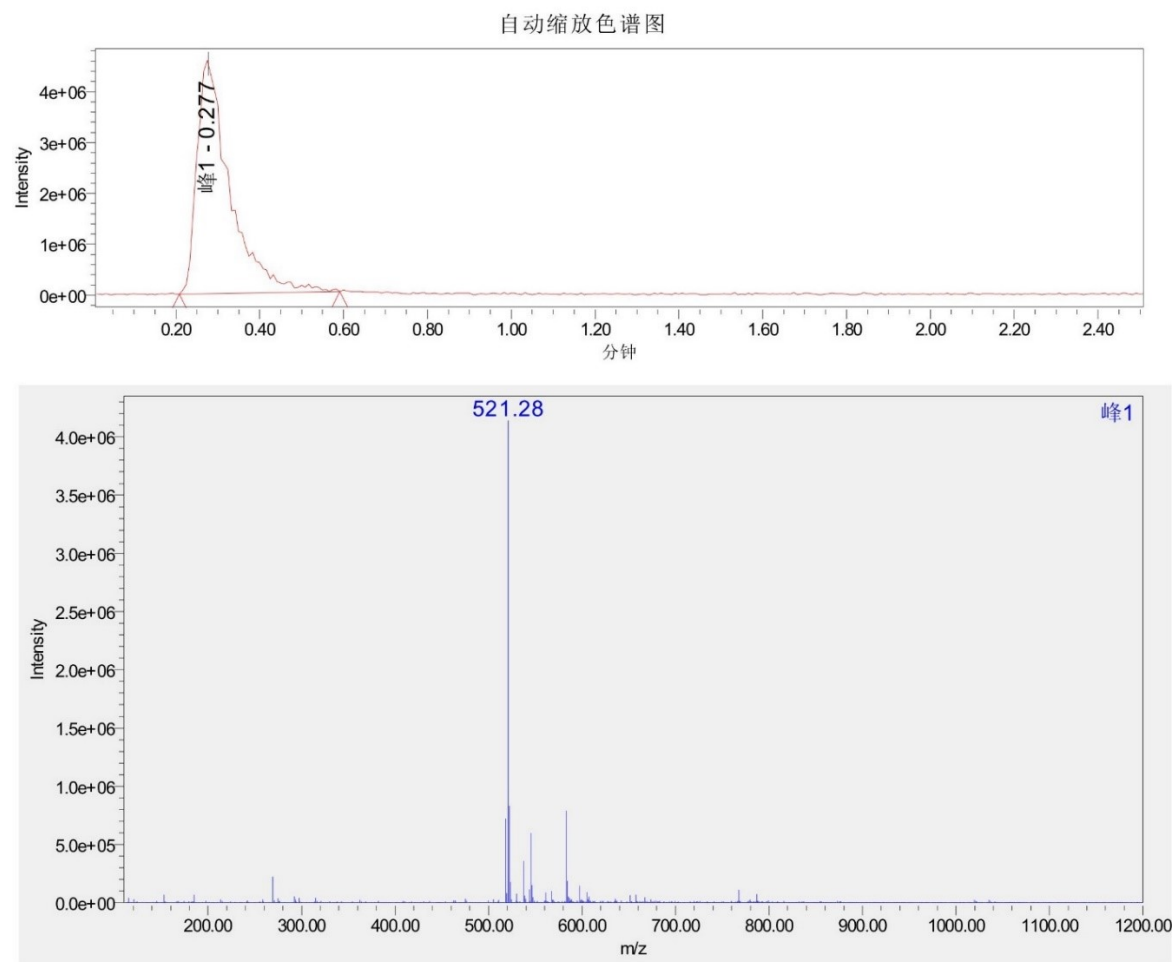


Figure S5. ESI+ of Peak Fr3-2 fraction (3,4,5-trimethoxyphenyl-(6'-O-galloyl)-1-O- β -D-glucopyranoside)

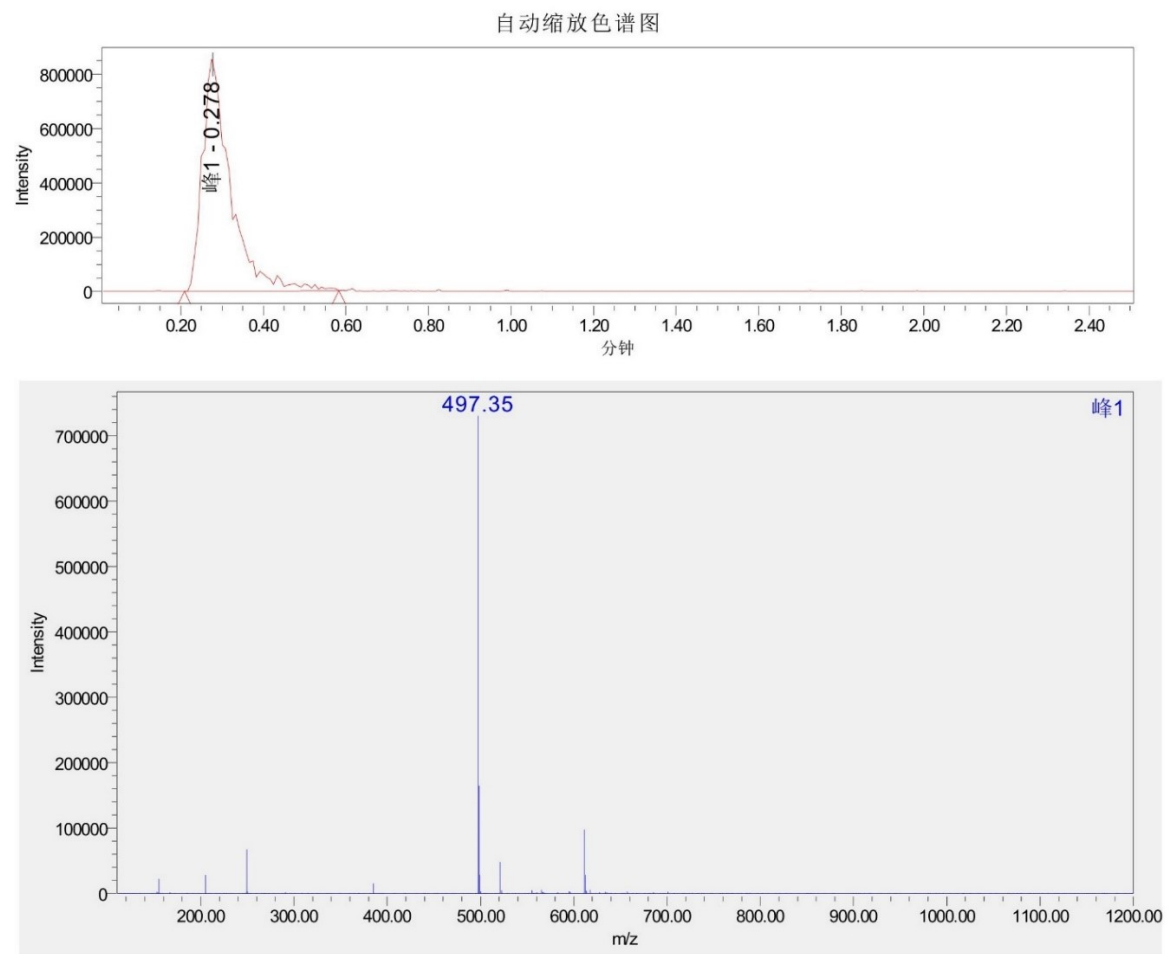


Figure S6. ESI- of Peak Fr3-2 fraction (3,4,5-trimethoxyphenyl-(6'-O-galloyl)-1-O- β -D-glucopyranoside)

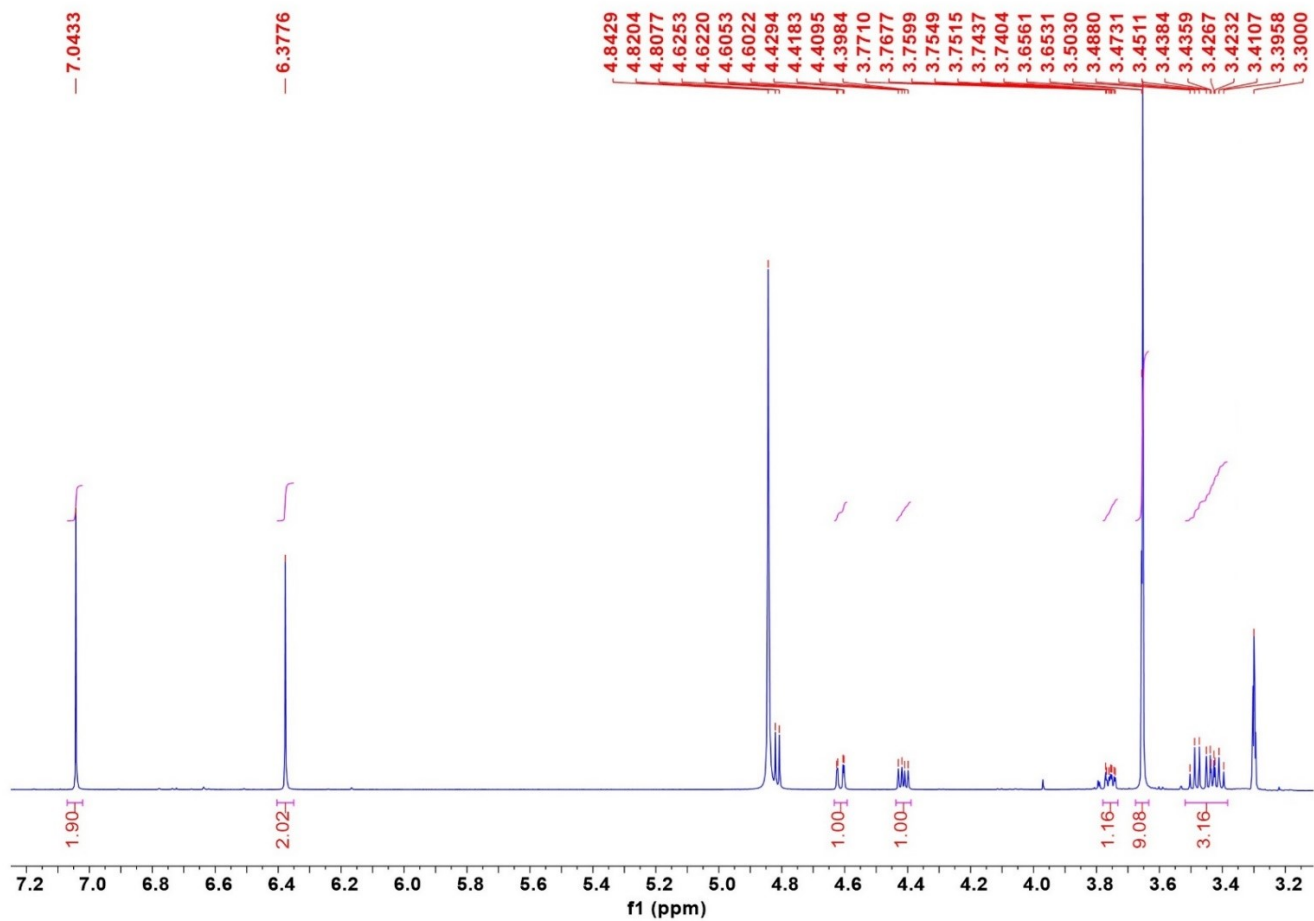


Figure S7. ¹H NMR Spectrum (600 MHz) of Peak Fr3-2 fraction (3,4,5-trimethoxyphenyl-(6'-O-galloyl)-1-O-β-D-glucopyranoside) in MeOH-*d*₄

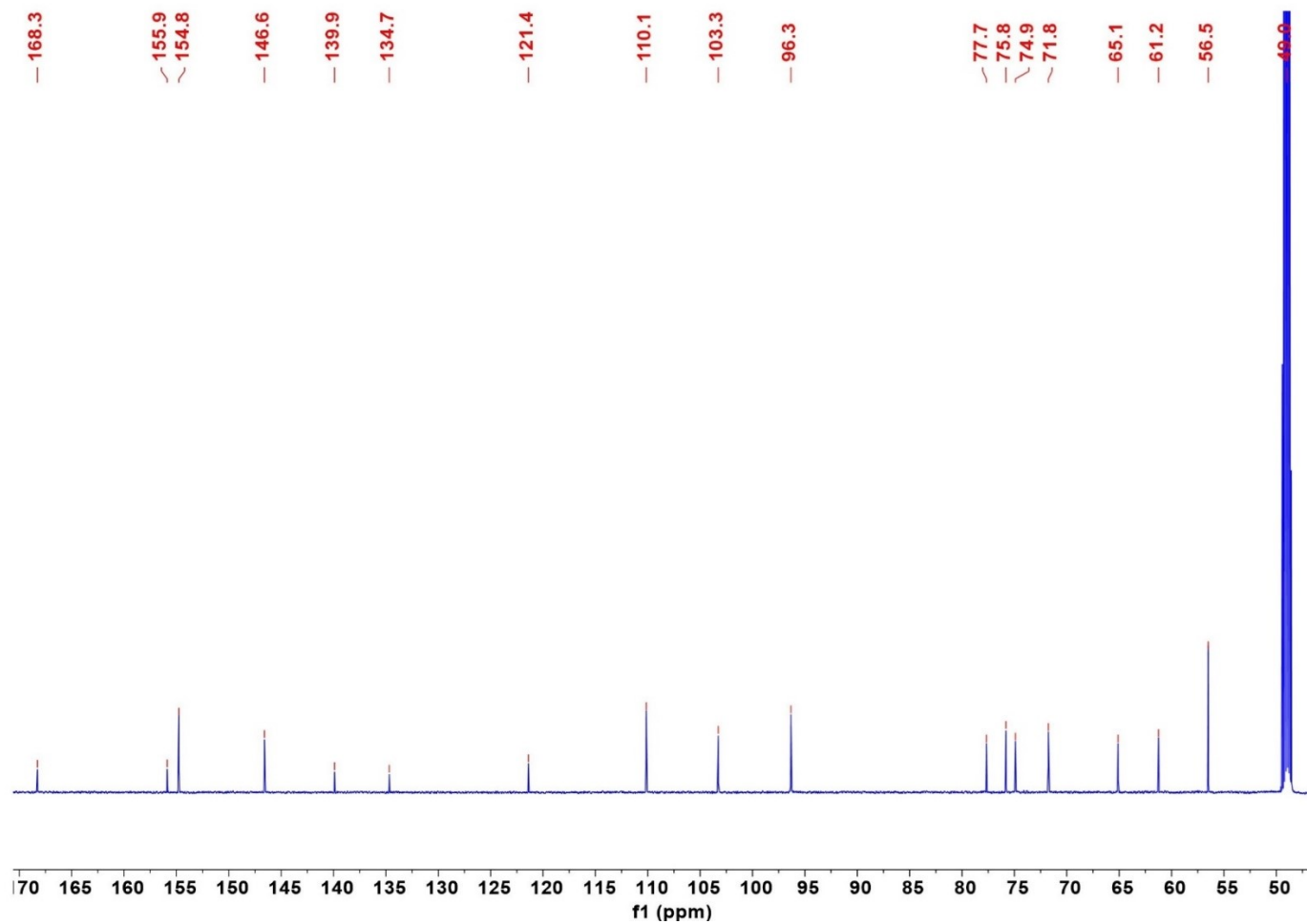
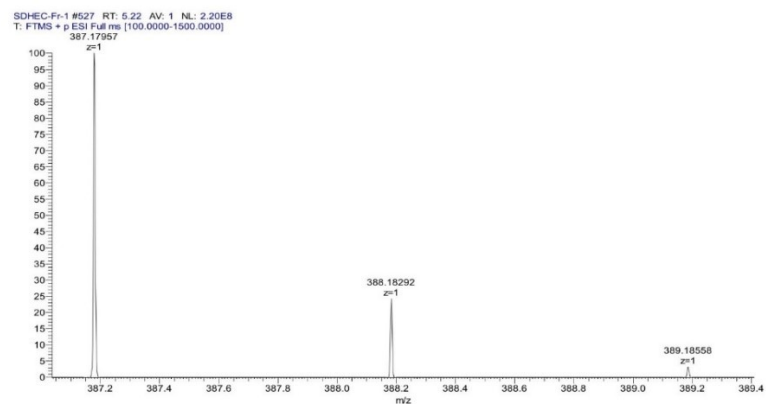
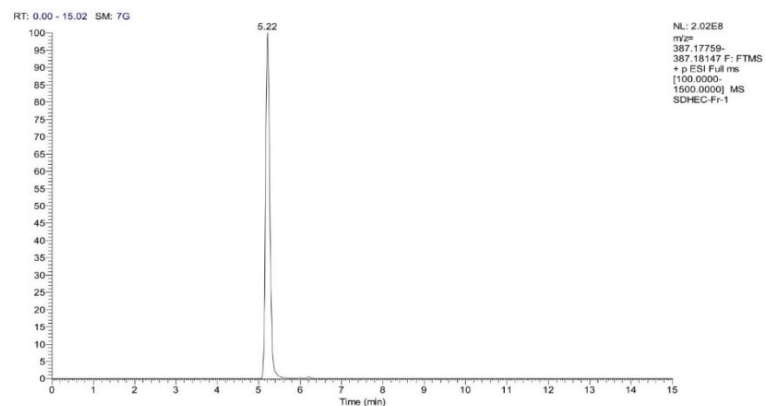


Figure S8. ^{13}C NMR Spectrum (151 MHz) of Peak Fr3-2 fraction (3,4,5-trimethoxyphenyl-(6'-O-galloyl)-1-O- β -D-glucopyranoside) in $\text{MeOH-}d_4$



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
387.17957	387.18022	-1.67	9.5	C22 H27 O6	M+H

Figure S9. HR-ESI-MS of Peak Fr4-1 fraction (saximonsin A)

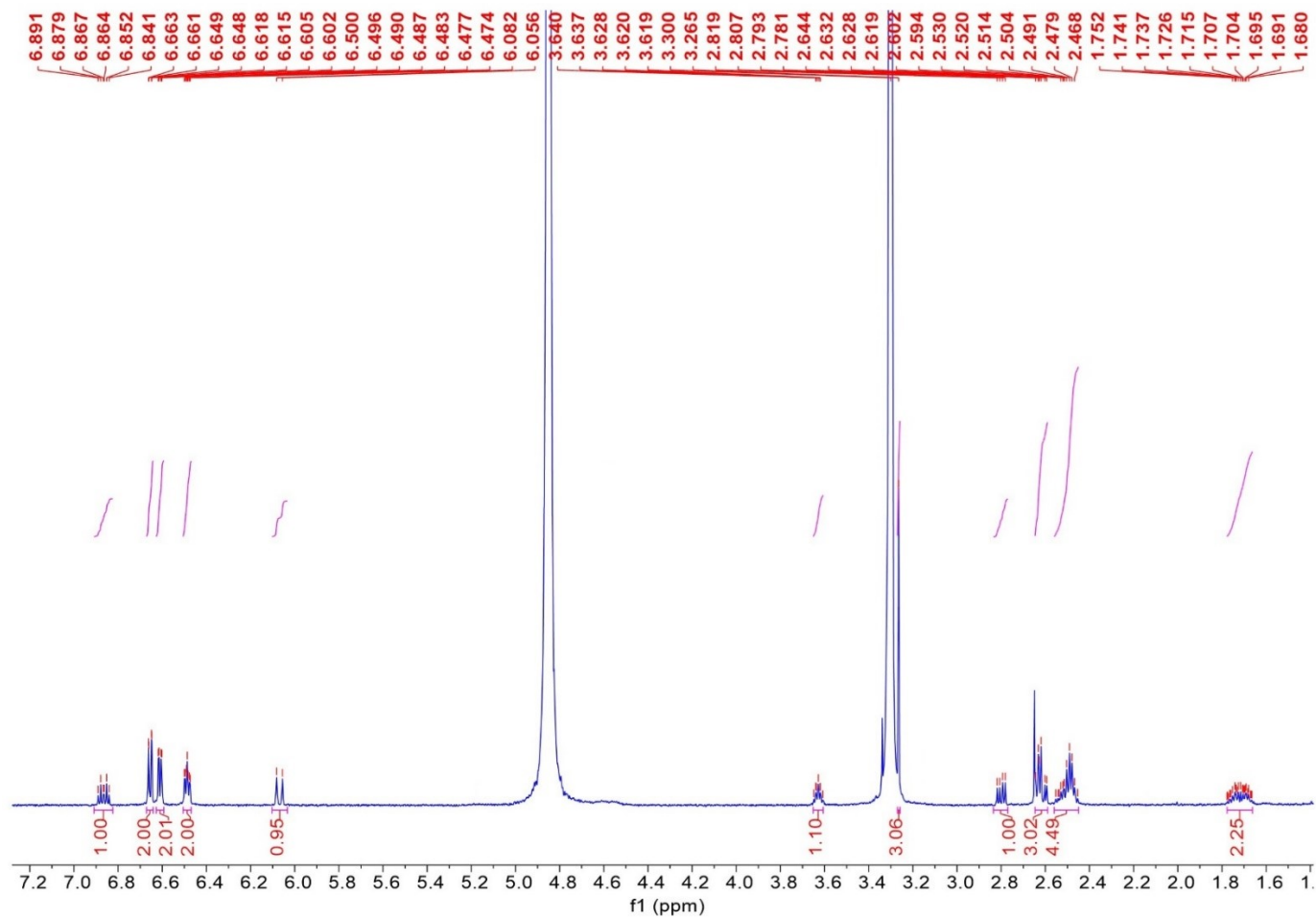


Figure S10. ¹H NMR Spectrum (600 MHz) of Peak Fr4-1 fraction (saximonsin A) in MeOH-*d*₄

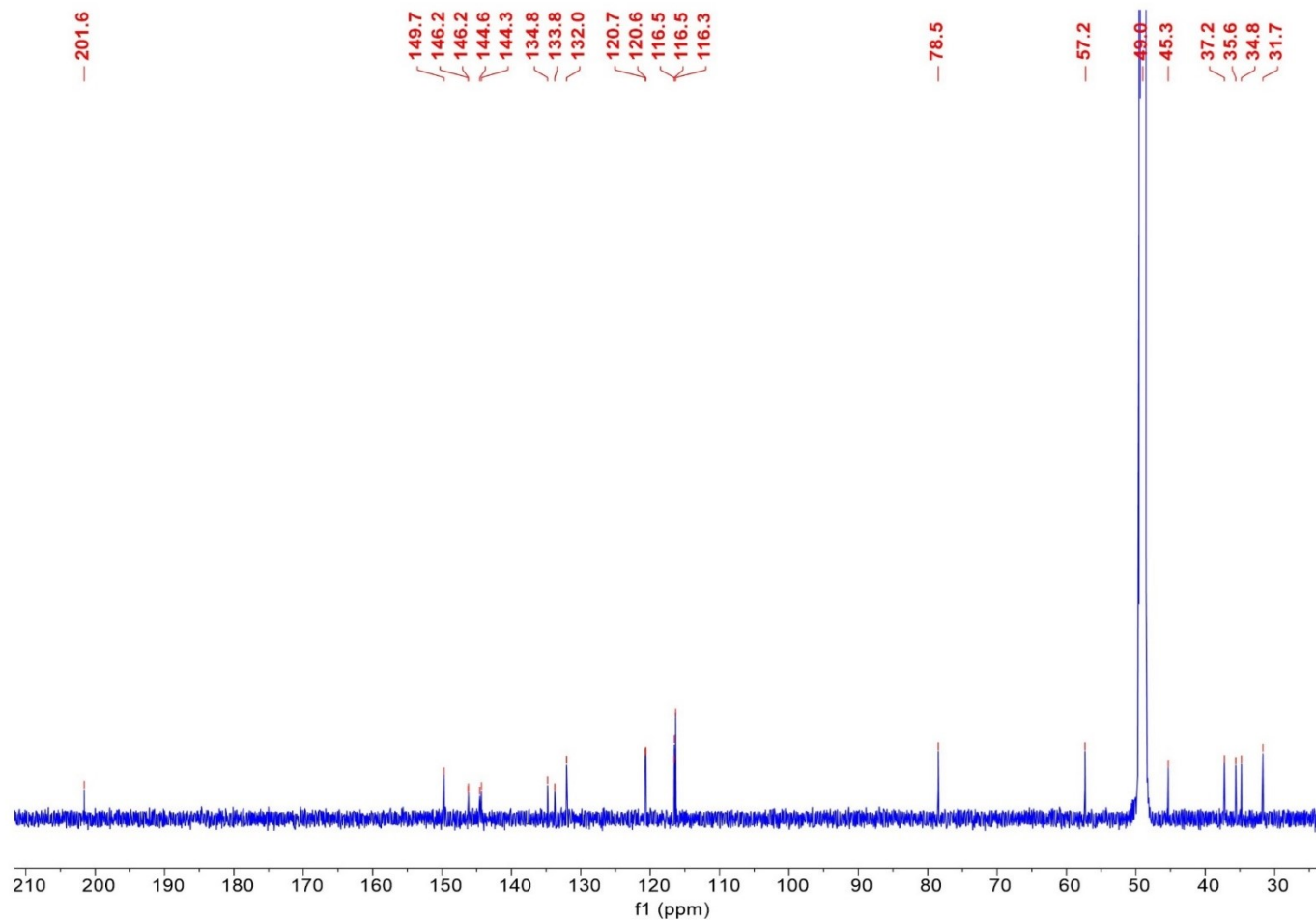


Figure S11. ^{13}C NMR Spectrum (151 MHz) of Peak Fr4-1 fraction (saximonsin A) in $\text{MeOH-}d_4$

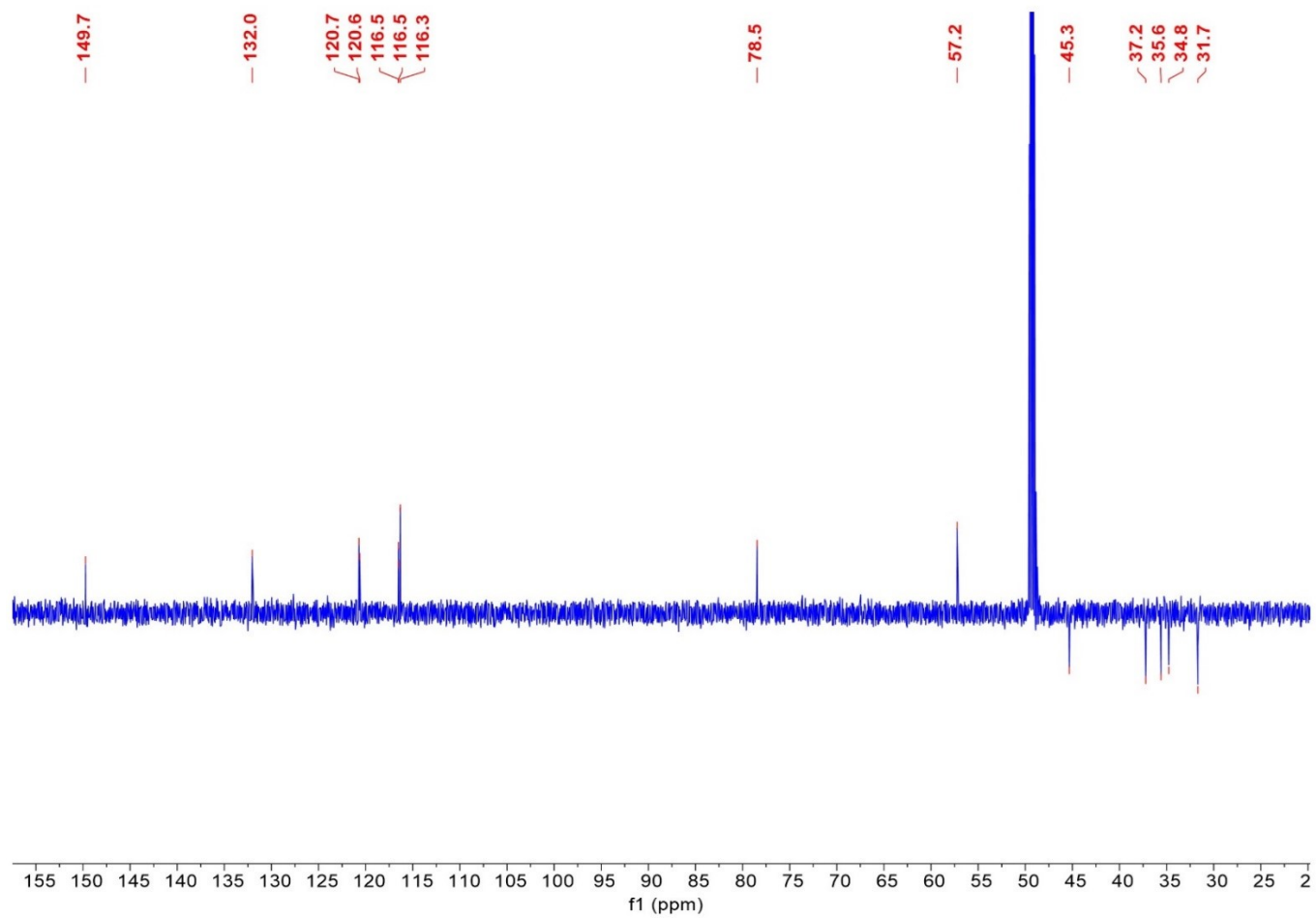


Figure S12. DEPT Spectrum of Peak Fr4-1 fraction (saximonsin A) in MeOH-*d*₄

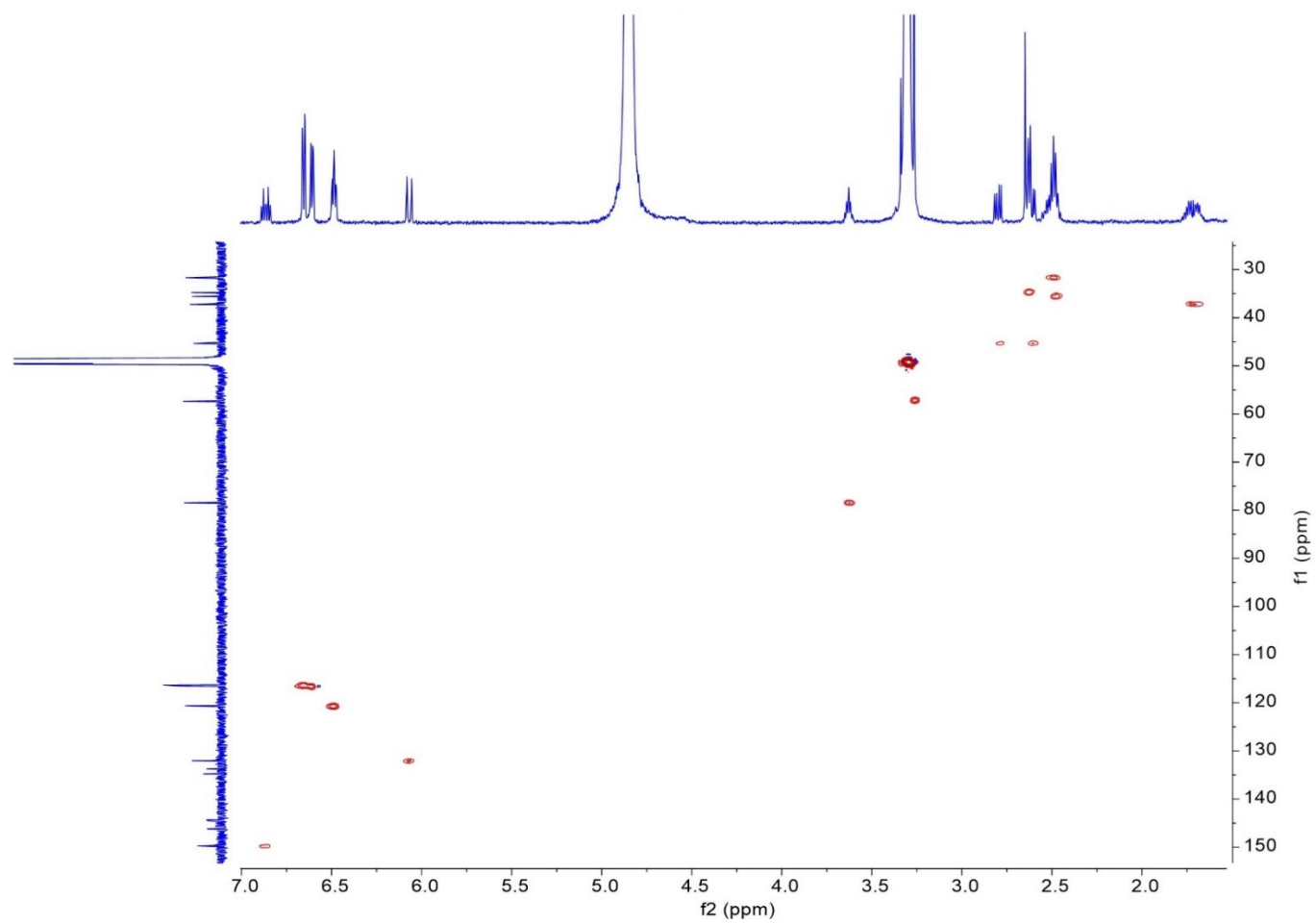


Figure S13. HSQC Spectrum of Peak Fr4-1 fraction (saximonsin A) in MeOH-*d*₄

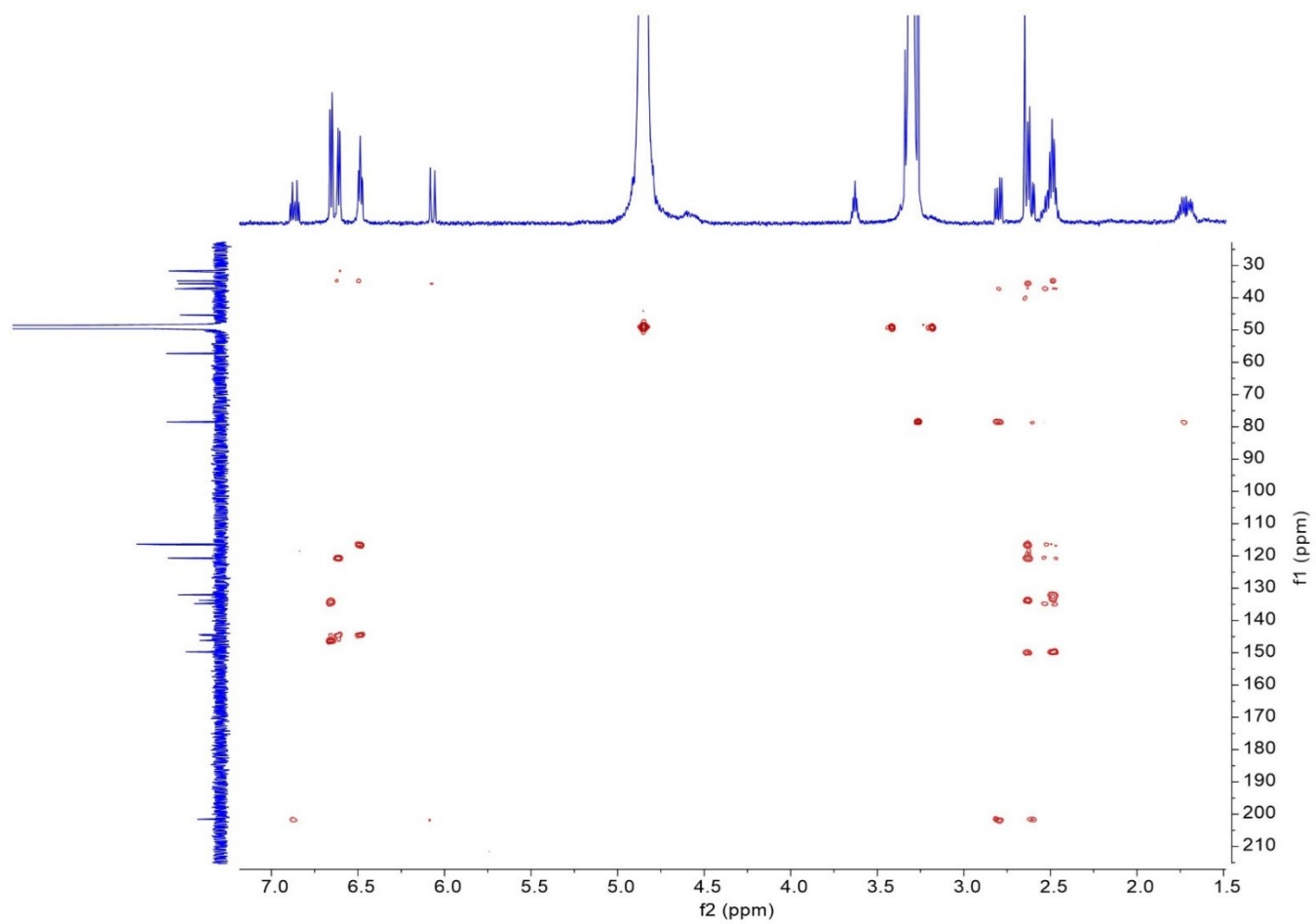


Figure S14. HMBC Spectrum of Peak Fr4-1 fraction (saximonsin A) in MeOH-*d*₄

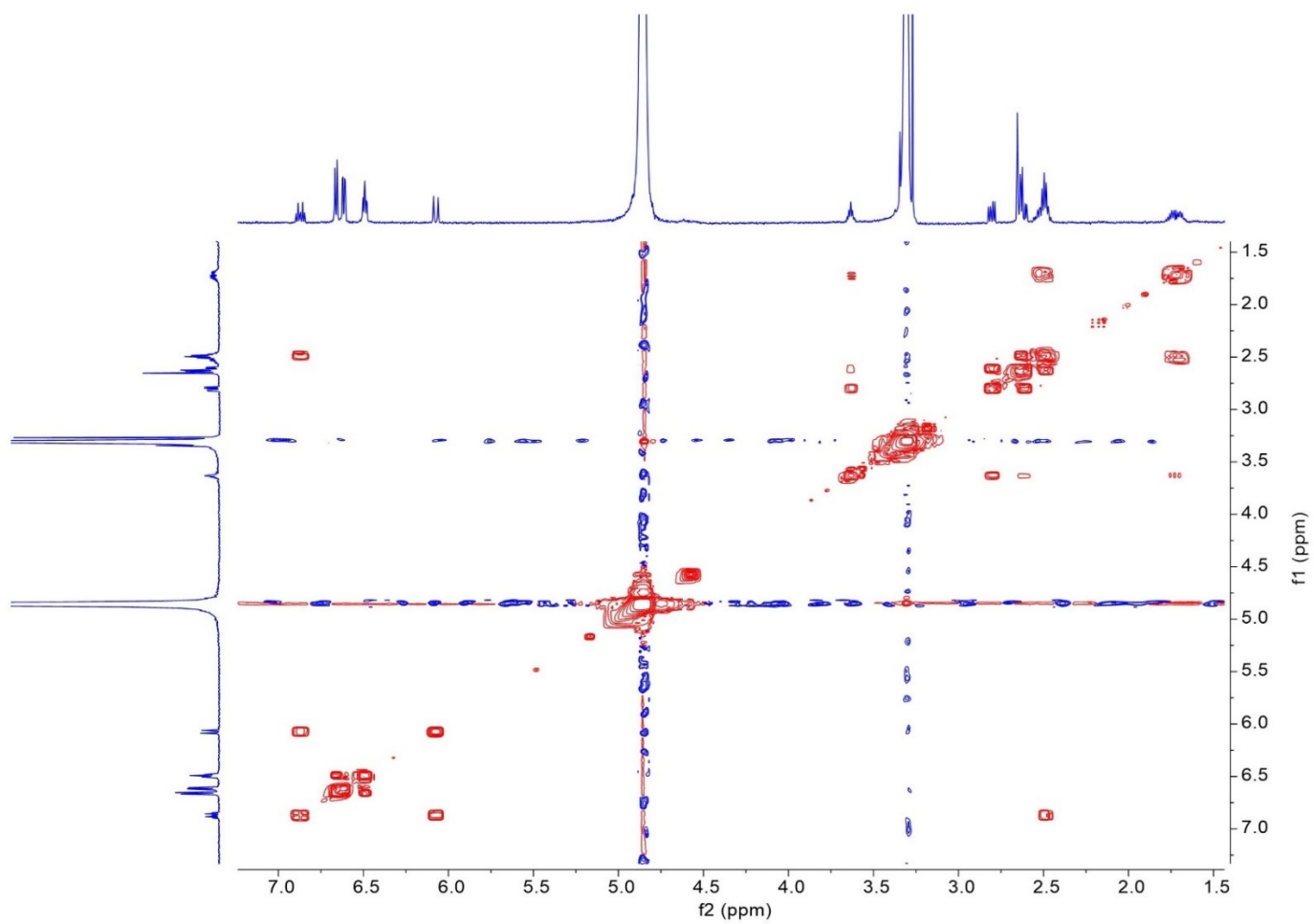


Figure S15. H-H COSY Spectrum of Peak Fr4-1 fraction (saximonsin A) in MeOH-*d*₄

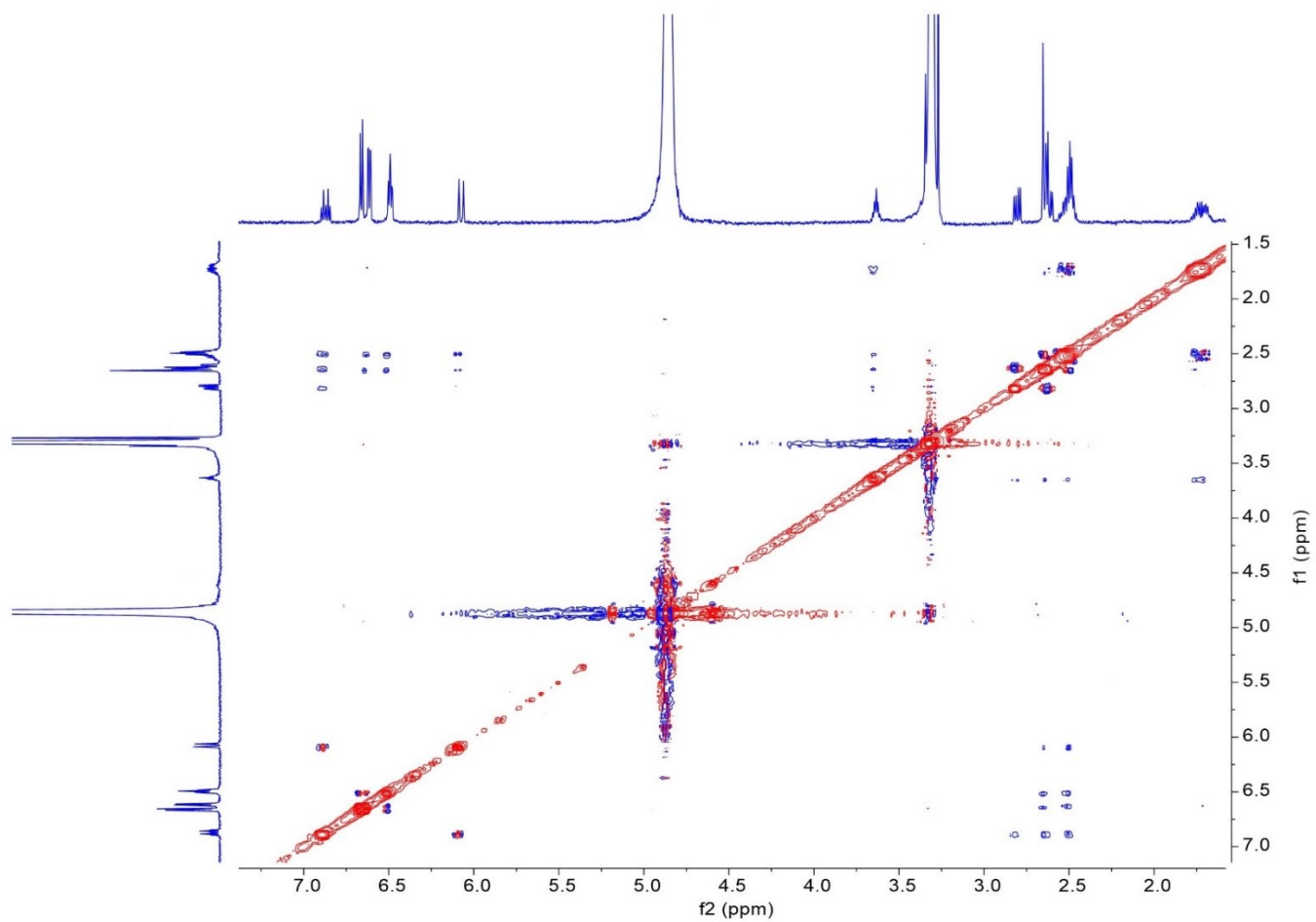
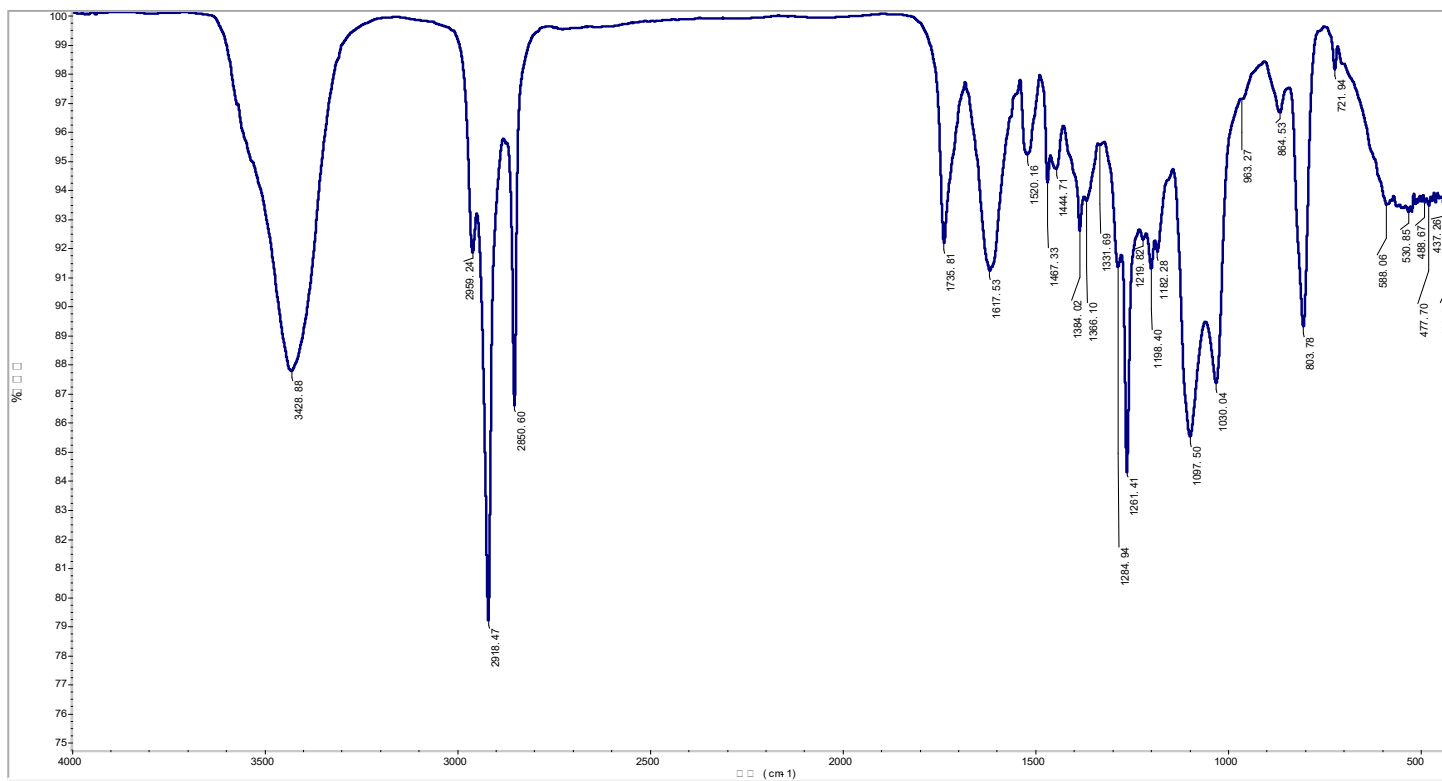


Figure S16. NOESY Spectrum of Peak Fr4-1 fraction (saximonsin A) in MeOH-*d*₄



Sample Name: J DangJ - 1

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: 80. 00

Figure S17. IR spectrum of Peak Fr4-1 fraction (saximonsin A)

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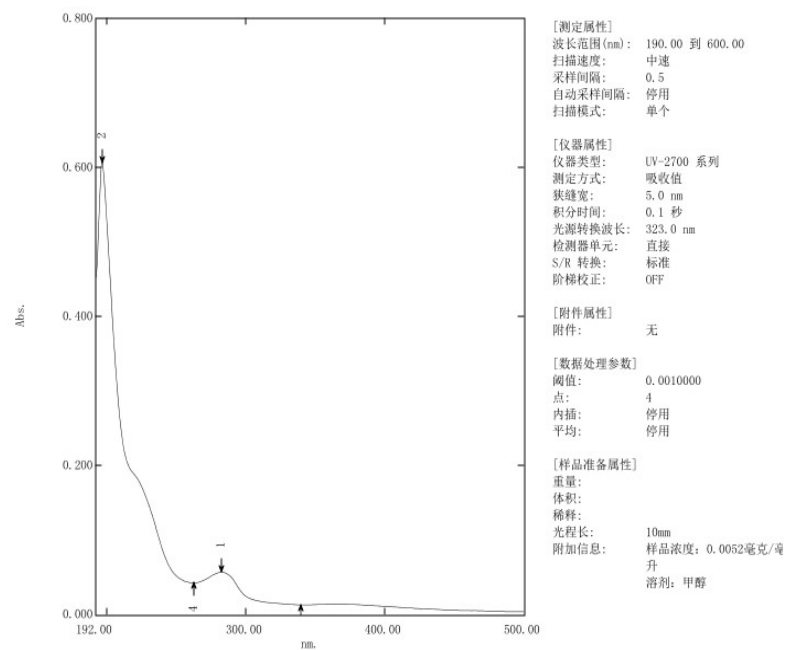


Figure S18. UV spectrum of Peak Fr4-1 fraction (saximonsin A)

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Saturday, 05-SEP-2020

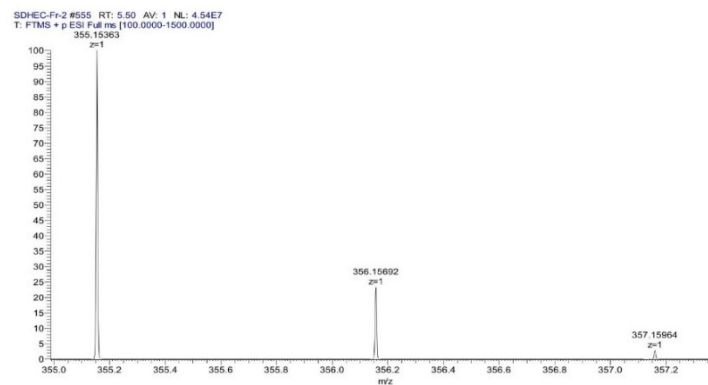
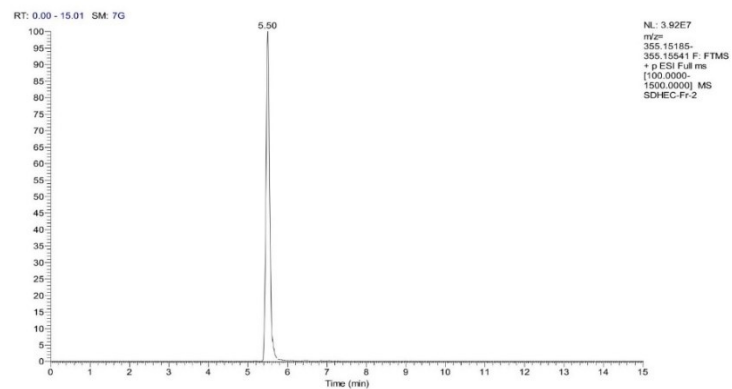
Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>				
5	80.09	4.73	5.90	84.55	72.73				
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lq.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>
1	JDJ-1	10:57:00 AM	72.73	SR	0.0160	589	100.00	0.022	25.2
2	JDJ-1	10:57:08 AM	78.18	SR	0.0172	589	100.00	0.022	25.2
3	JDJ-1	10:57:17 AM	82.73	SR	0.0182	589	100.00	0.022	25.2
4	JDJ-1	10:57:25 AM	82.27	SR	0.0181	589	100.00	0.022	25.3
5	JDJ-1	10:57:33 AM	84.55	SR	0.0186	589	100.00	0.022	25.3

Figure S19. Optical rotation of Peak Fr4-1 fraction (saximonsin A)



m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition	
355.15363	355.15400	-1.04	10.5	C21 H23 O5	M+H

Figure S20. HR-ESI-MS of Peak Fr4-2 fraction (saximonsin B)

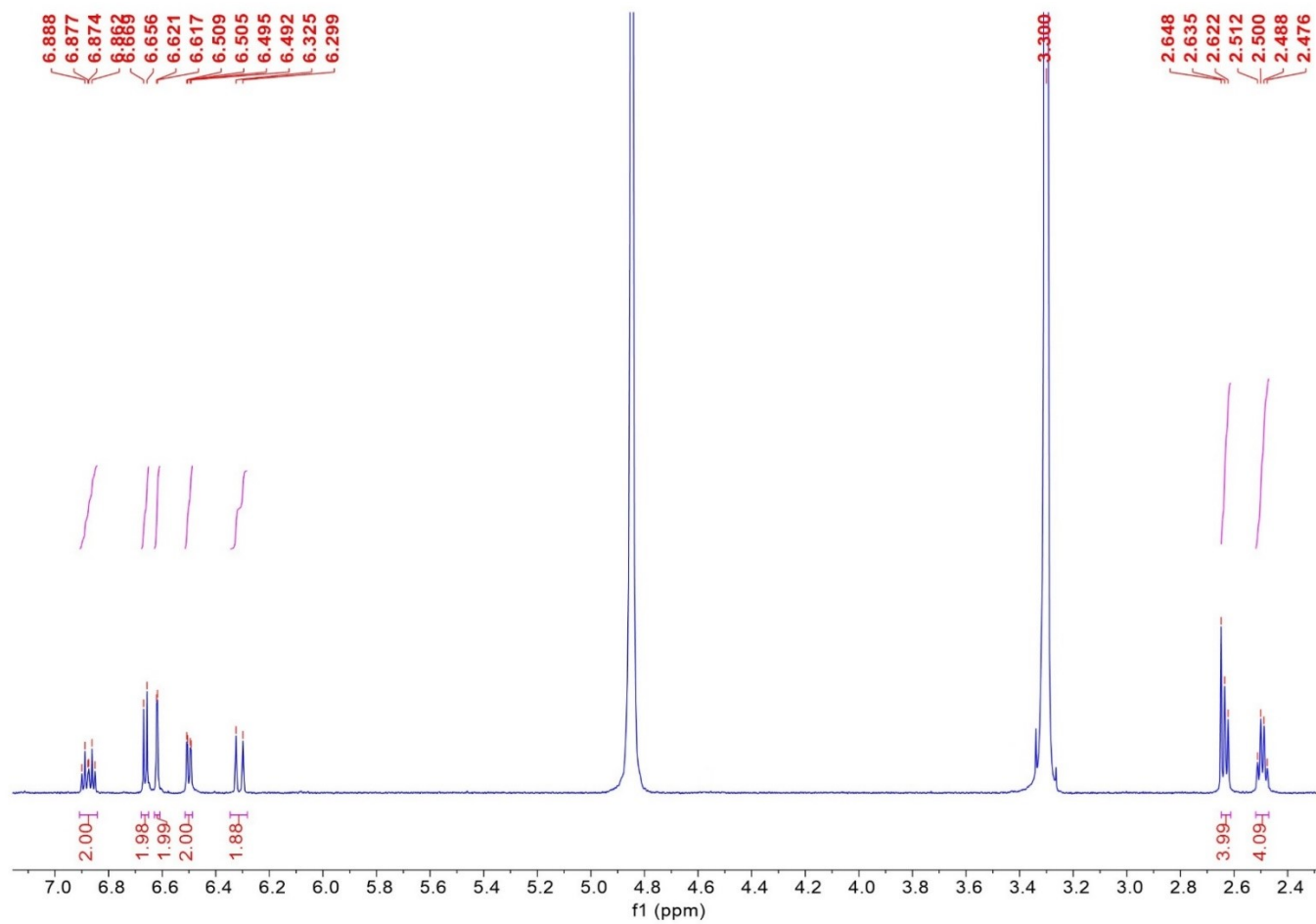


Figure S21. ¹H NMR Spectrum (600 MHz) of Peak Fr4-2 fraction (saximonsin B) in MeOH-*d*₄

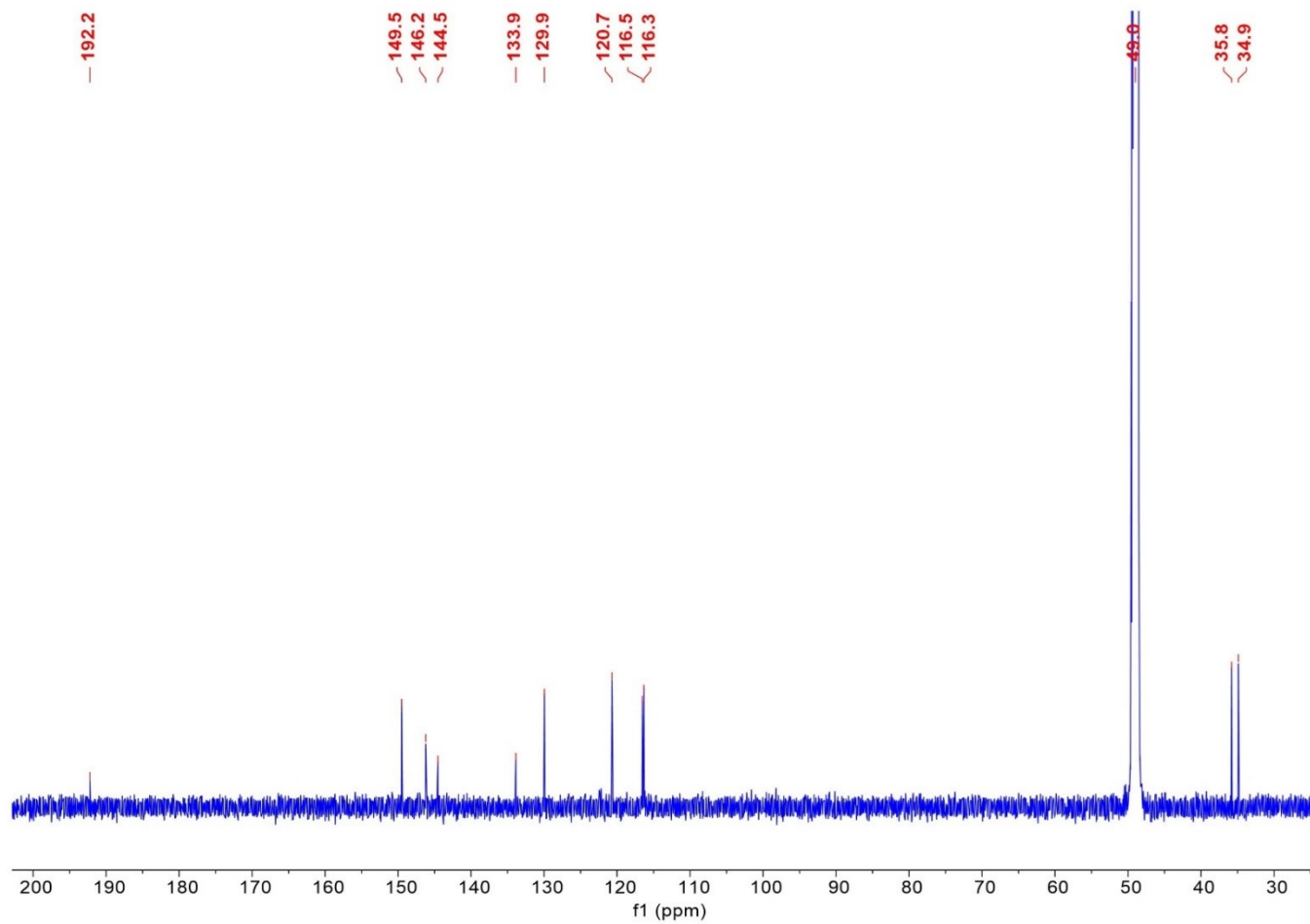


Figure S22. ^{13}C NMR Spectrum (151 MHz) of Peak Fr4-2 fraction (saximonsin B) in $\text{MeOH-}d_4$

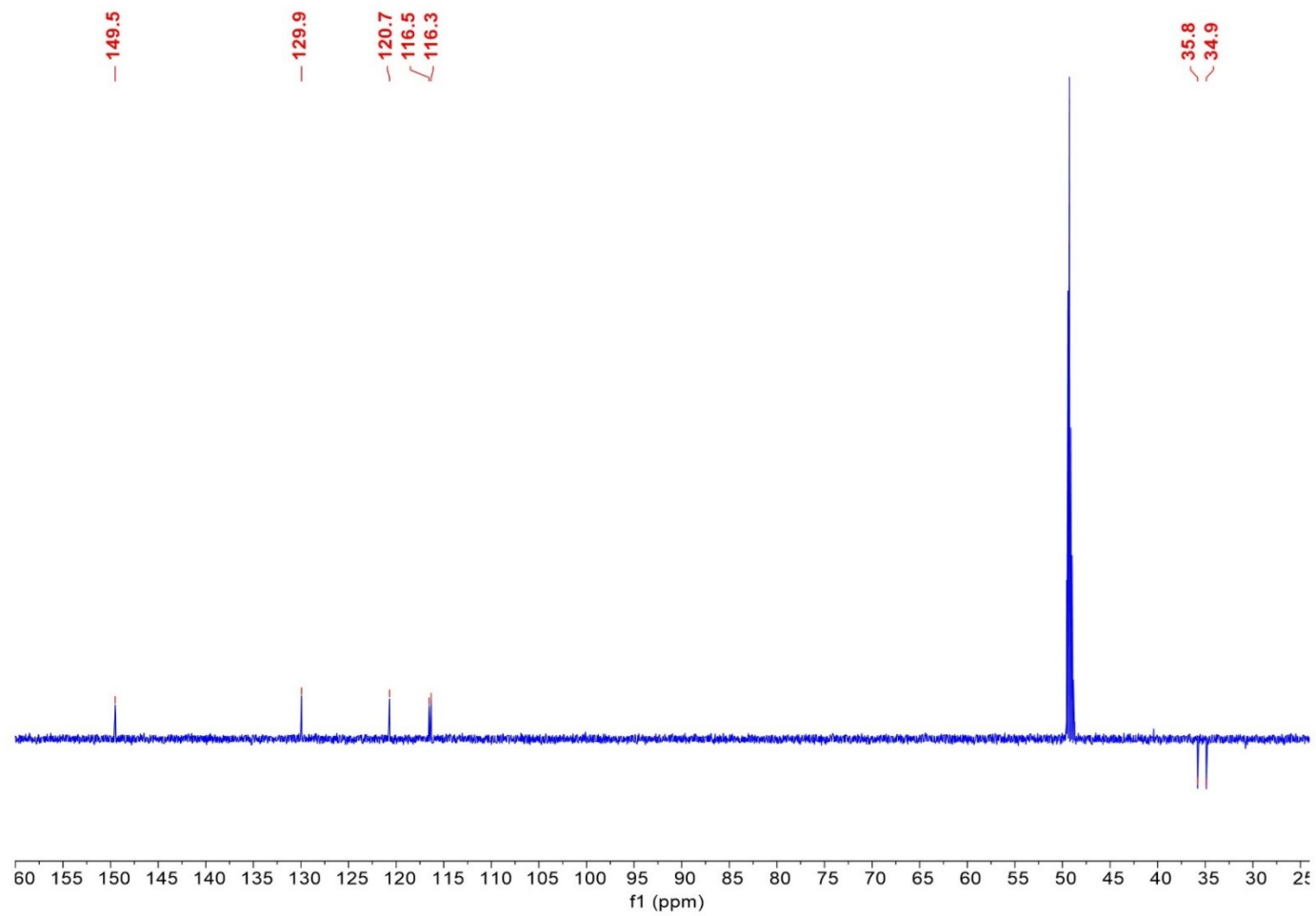


Figure S23. DEPT Spectrum of Peak Fr4-2 fraction (saximonsin B) in MeOH- d_4

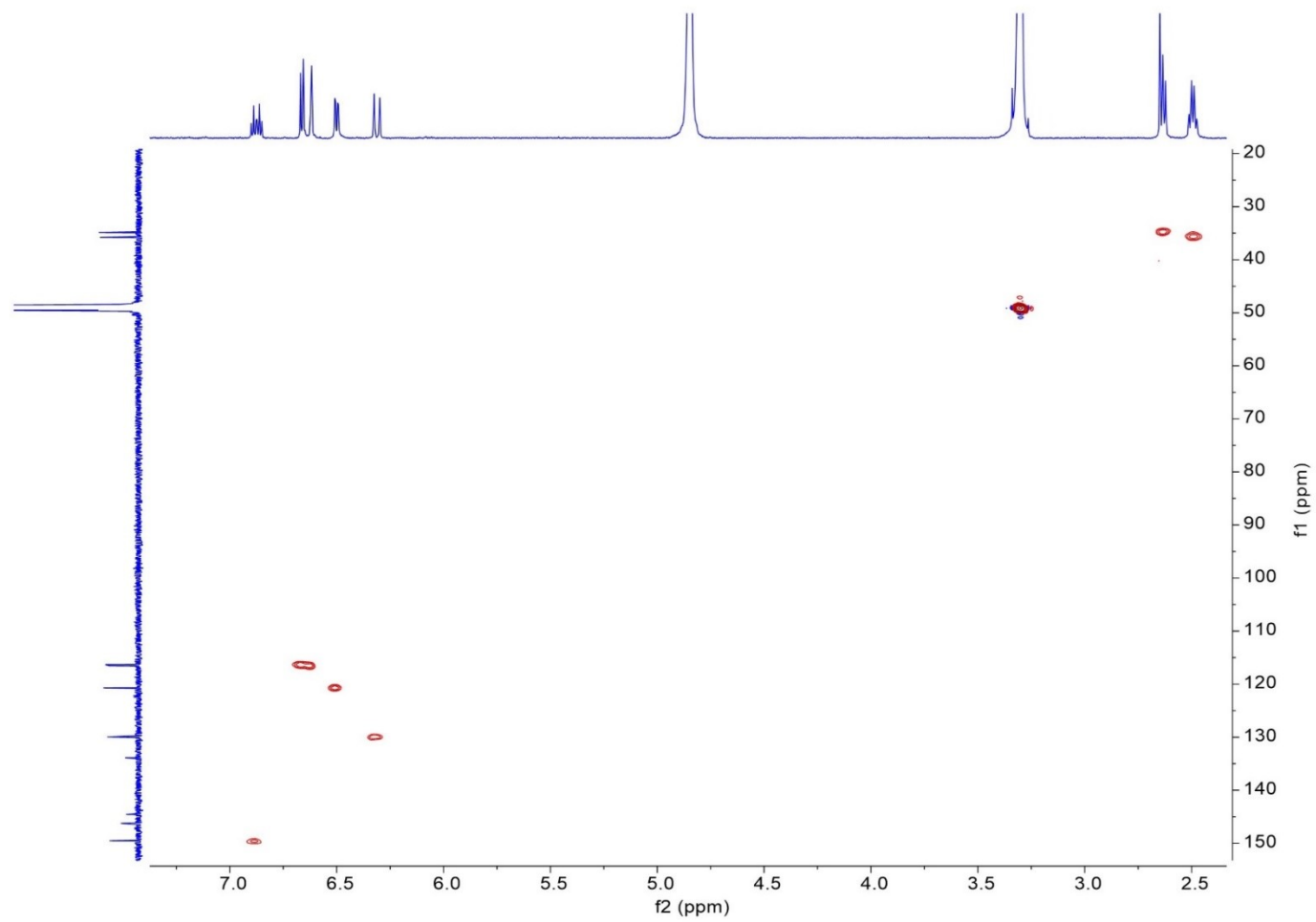


Figure S24. HSQC Spectrum of Peak Fr4-2 fraction (saximonsin B) in $\text{MeOH-}d_4$

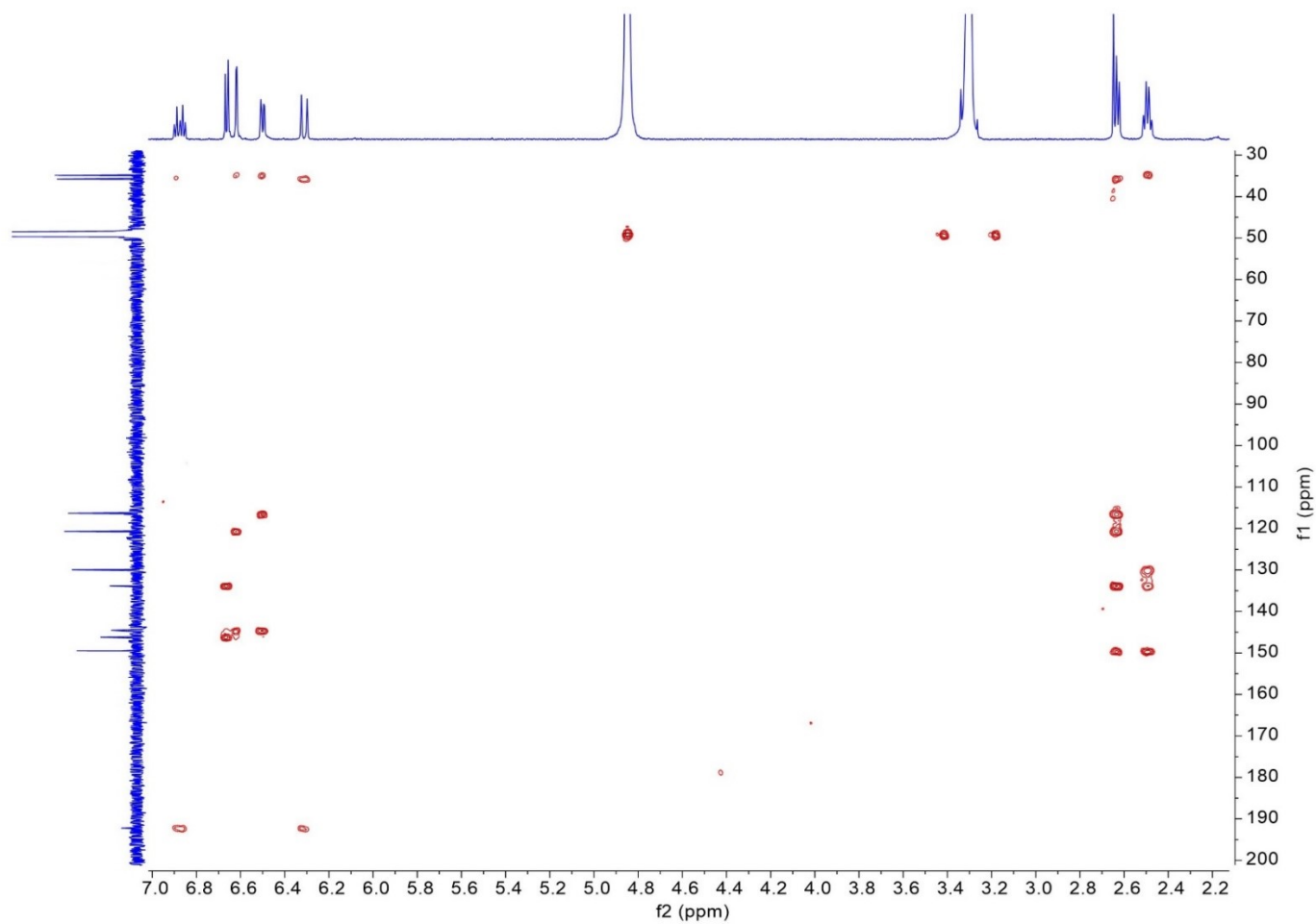


Figure S25. HMBC Spectrum of Peak Fr4-2 fraction (saximonsin B) in MeOH-*d*₄

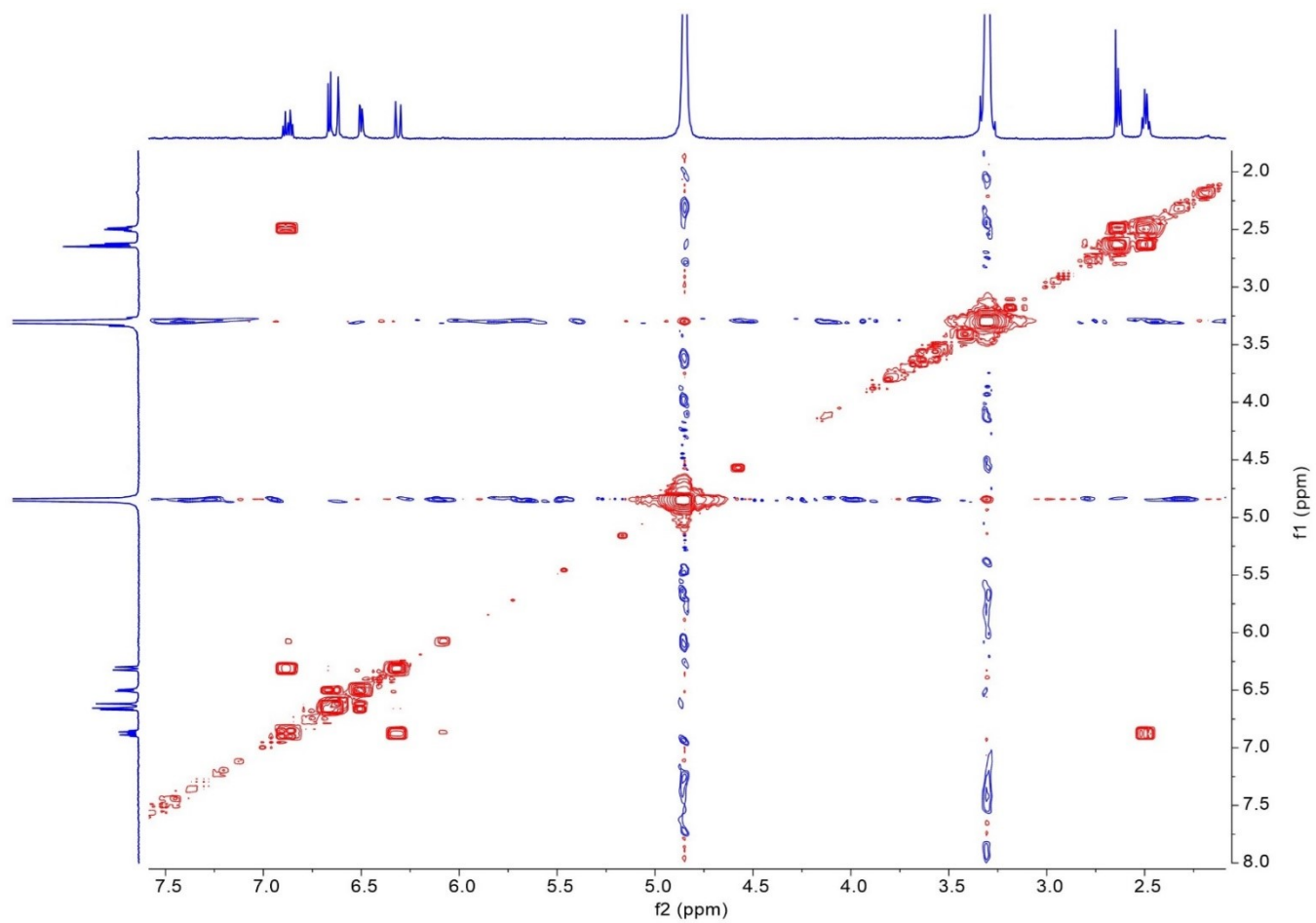


Figure S26. H-H COSY Spectrum of Peak Fr4-2 fraction (saximonsin B) in MeOH- d_4

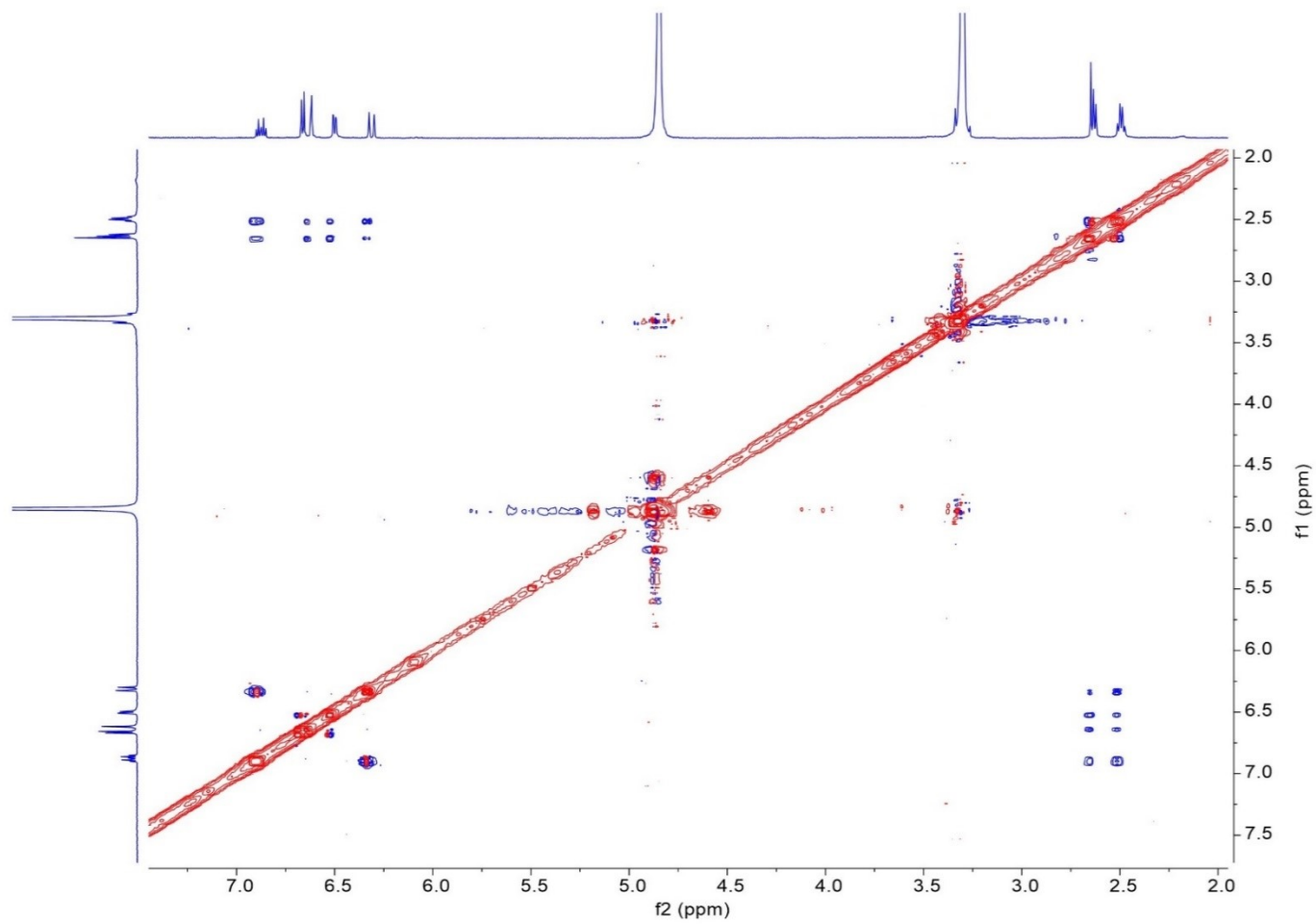
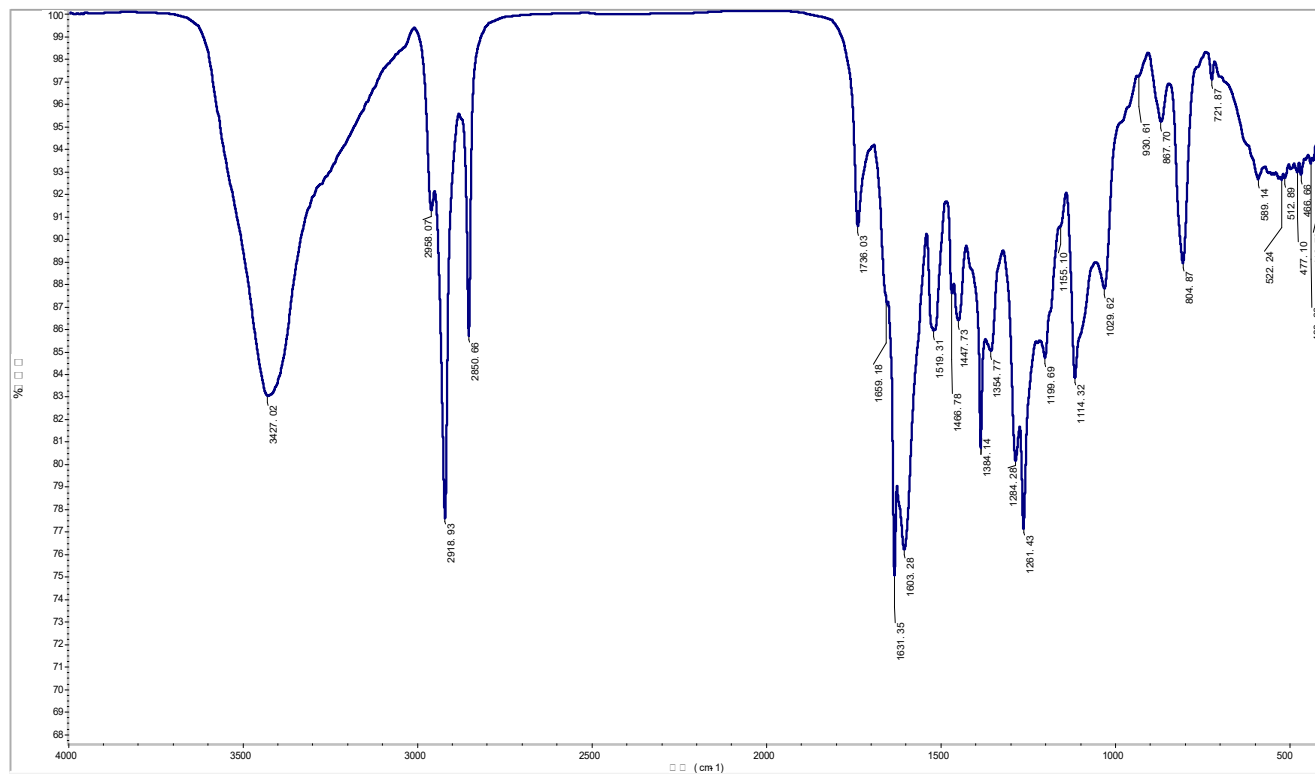


Figure S27. NOESY Spectrum of Peak Fr4-2 fraction (saximonsin B) in MeOH- d_4



Sample Name: J Dangj - 2
 KBr
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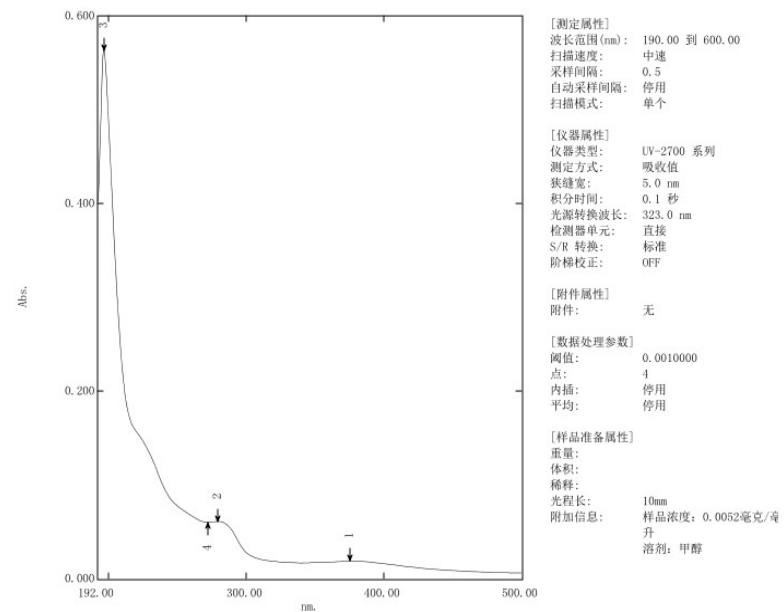
16
 16
 4.000
 1.0
 0.4747
 80.00

Figure S28. IR spectrum of Peak Fr4-2 fraction (saximonsin B)

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数据集: JDJ-2 - RawData



No.	P/V	波长 (nm)	Abs.	描述
1	①	375.00	0.019	
2	②	279.50	0.061	
3	③	196.50	0.563	
4	④	272.50	0.060	

Figure S29. UV spectrum of Peak Fr4-2 fraction (saximonsin B)