Supporting Information

Rec. Nat. Prod. X:X (202X) XX-XX

A New Iridoid Glycoside from Wine-Processed Corni fructus

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Operator Name	(None Entered)	Date of Report	2021/4/16
Department	(None Entered)	Time of Report	23:59:13下午
Organization	(None Entered)		
Information	(None Entered)		

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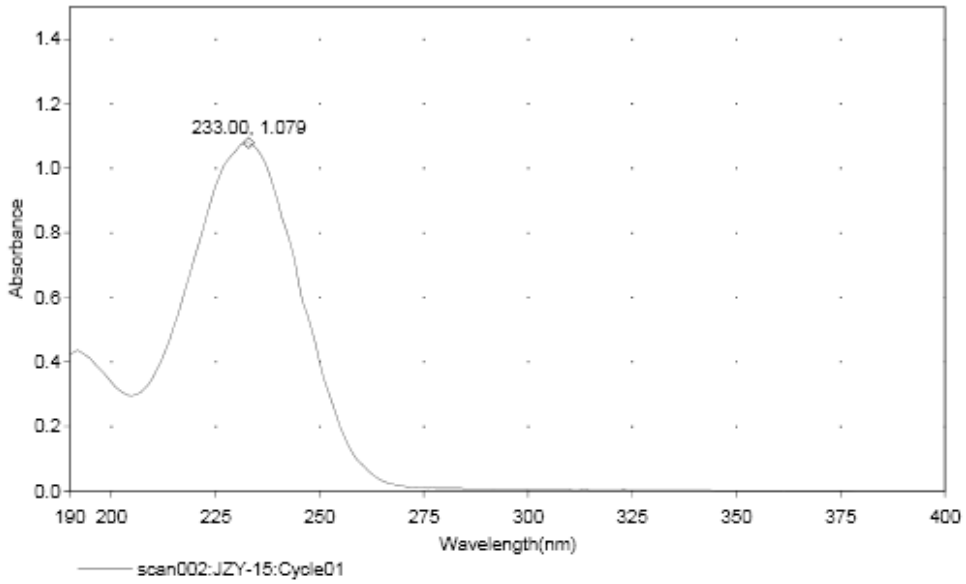

Results Table - scan002,JZY-15,Cycle01

nm	A	**Manual Method**
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		233.00 nm
		Sort By Wavelength

Figure S1: UV spectrum of Spectrum of **1** (cornusglucoside I)

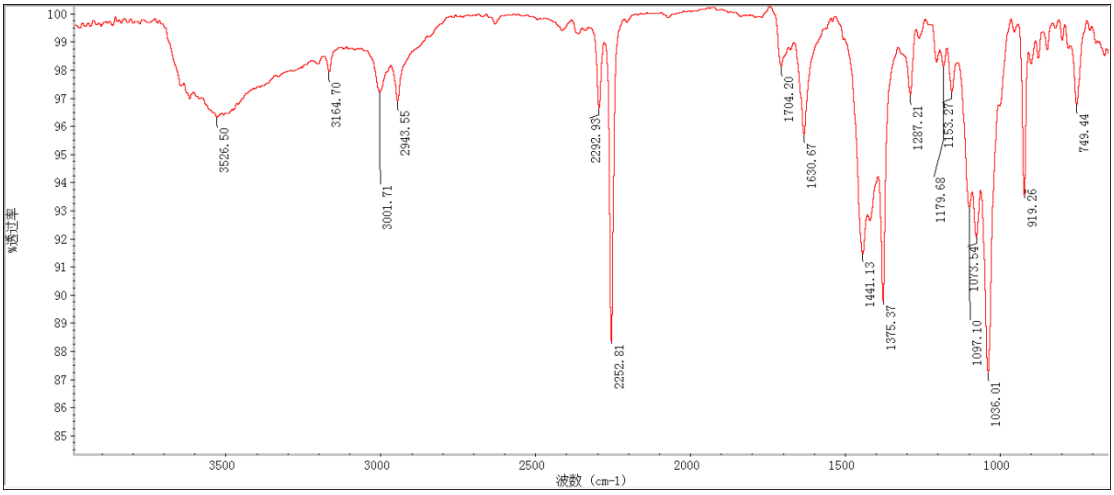

Figure S2: IR spectrum of Spectrum of **1** (cornusglucoside I)

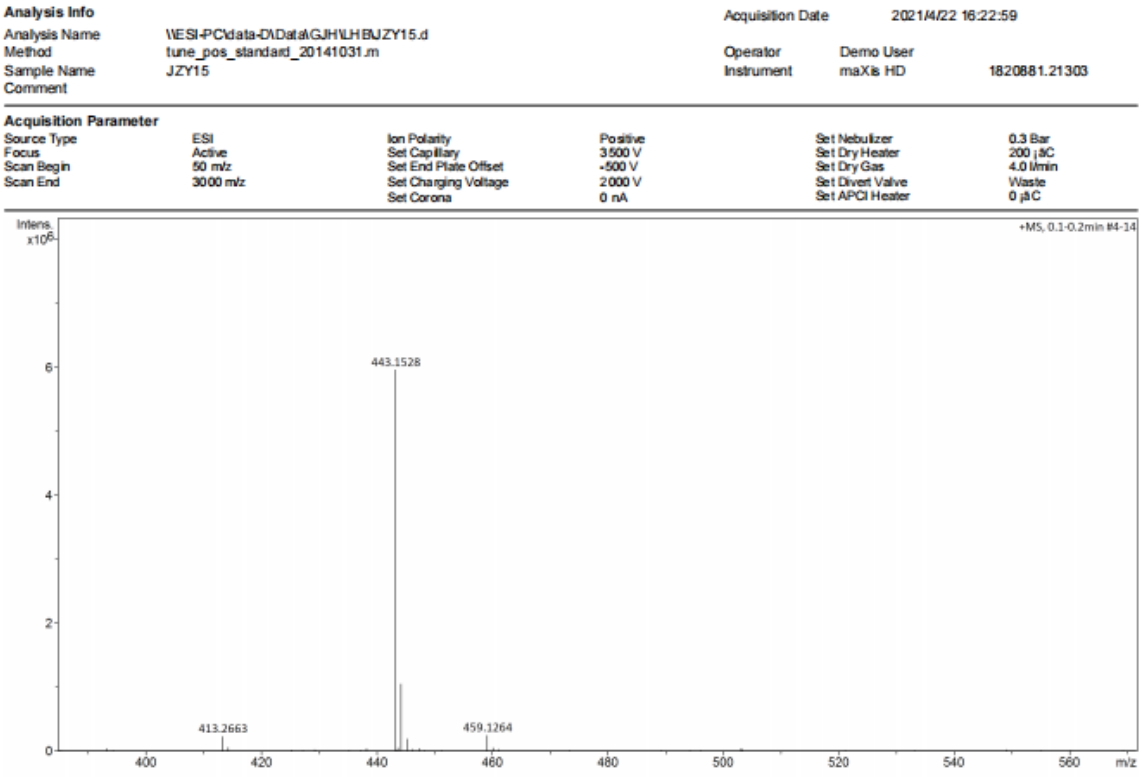

Figure S3: HR-ESI-MS Spectrum of **1** (cornusglucoside I)

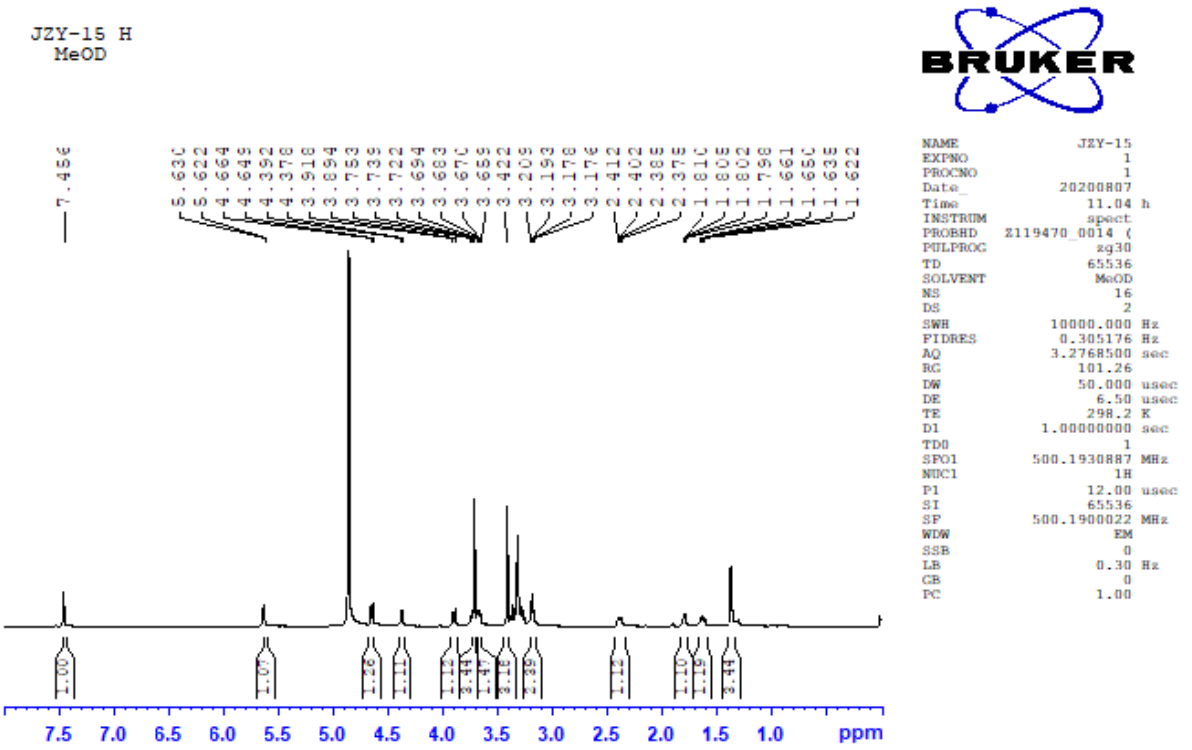

Figure S4: ^{1}H-NMR (500 MHz, methanol-d_4) Spectrum of **1** (cornusglucoside I)

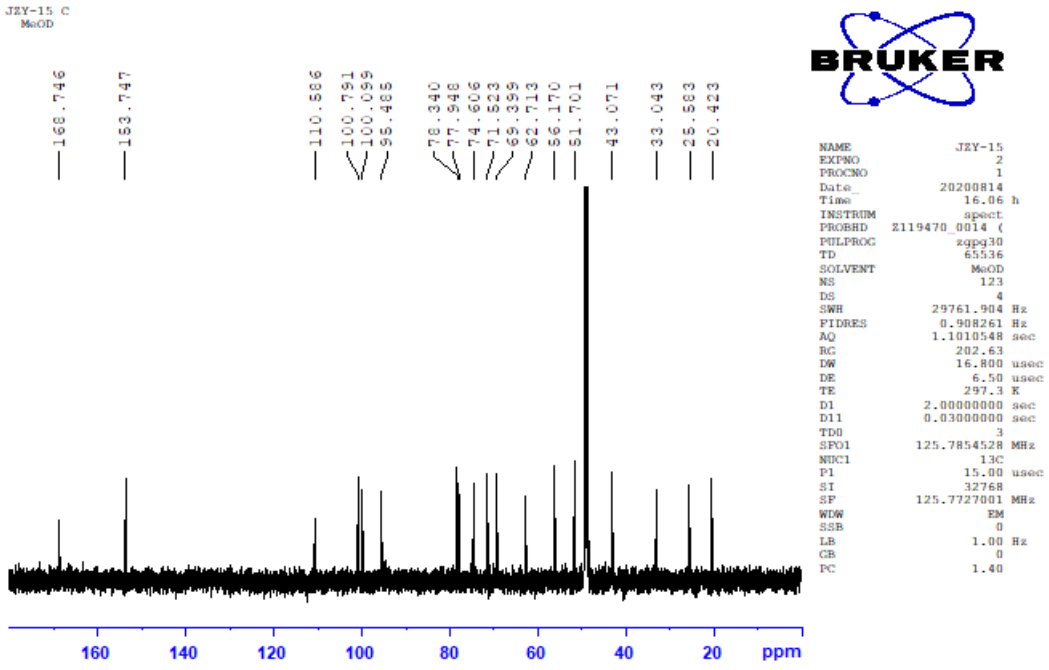

Figure S5: ^{13}C-NMR (125 MHz, methanol-d_4) Spectrum of **1** (cornusglucoside I)

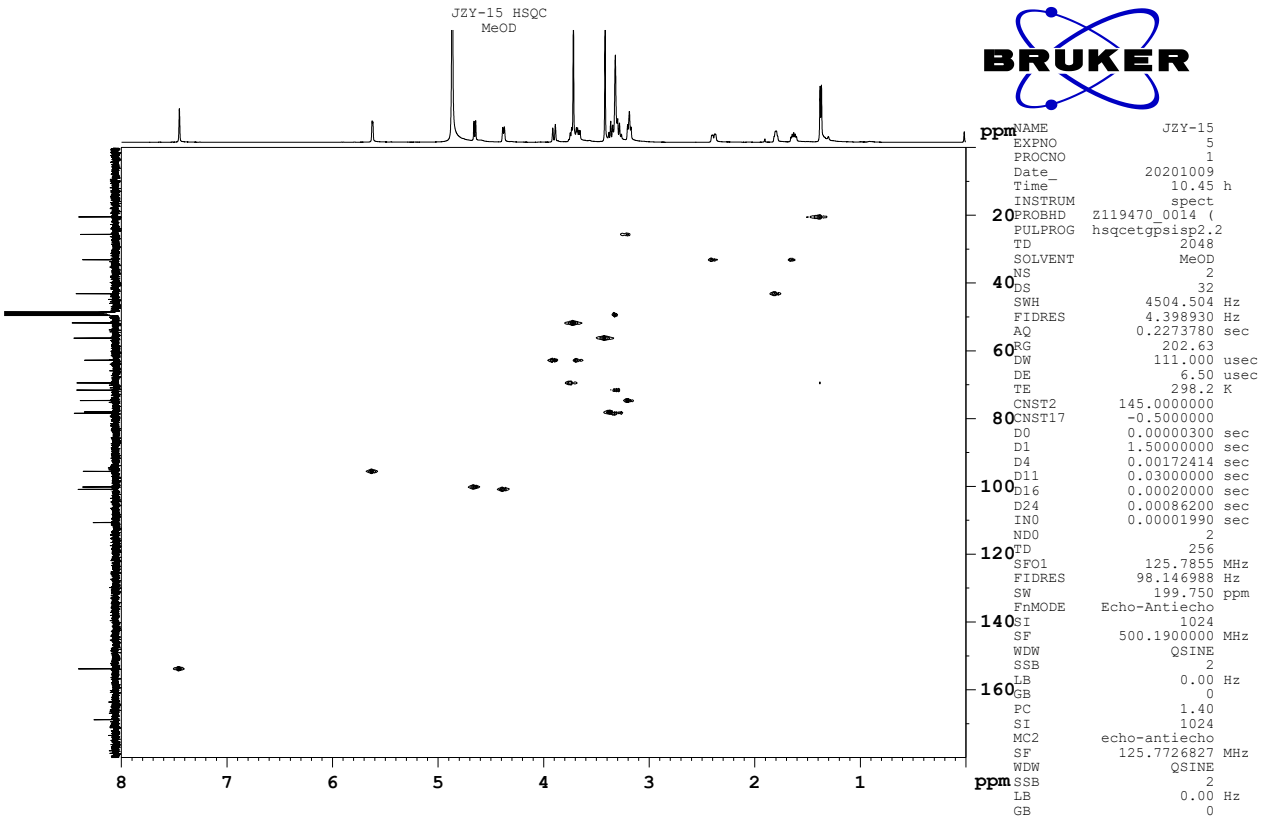

Figure S6: HSQC Spectrum of **1** (cornusglucoside I)

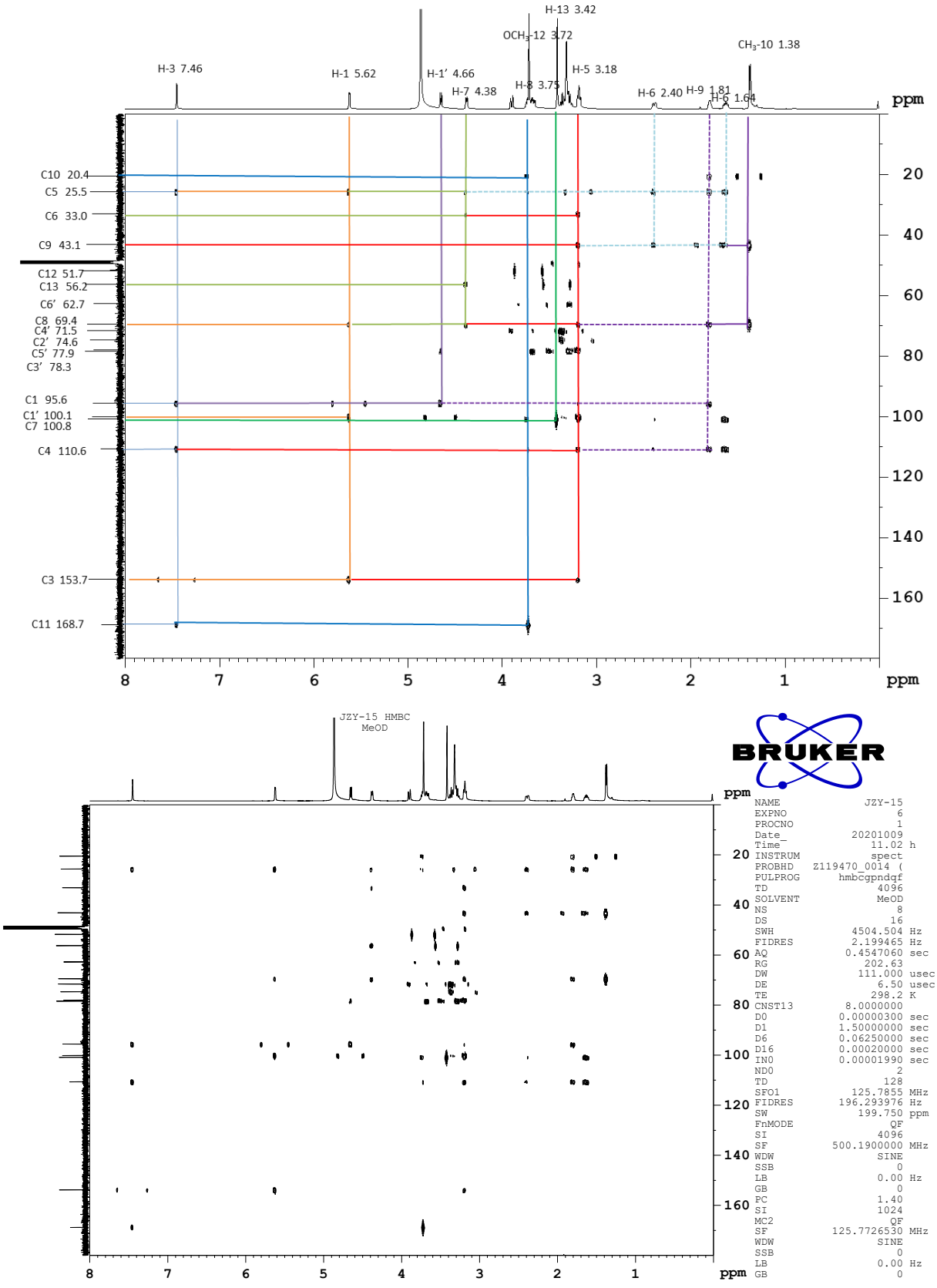

Figure S7: HMBC Spectrum of **1** (cornusglucoside I)

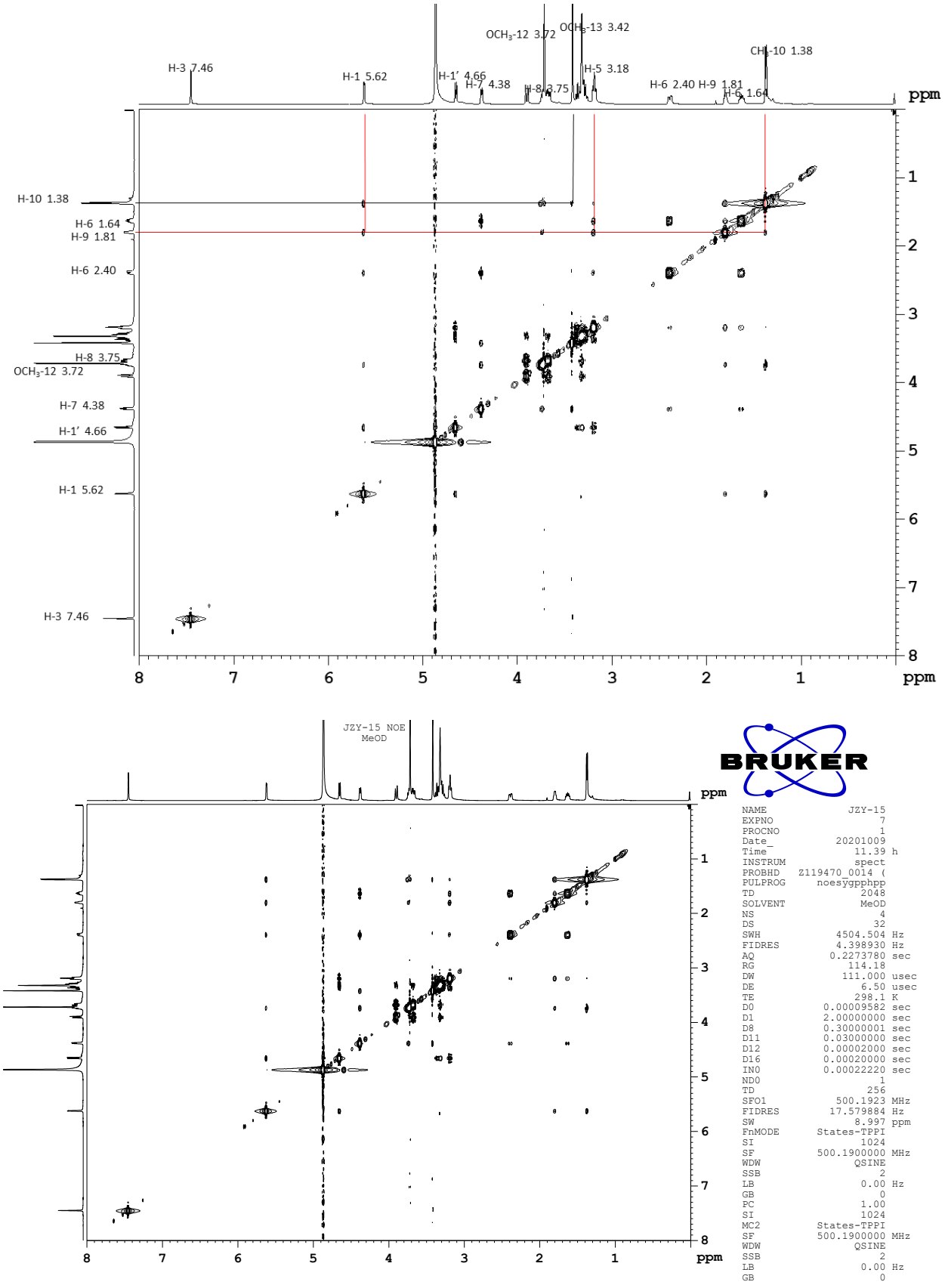

Figure S8: NOESY Spectrum of **1** (cornusglucoside I)

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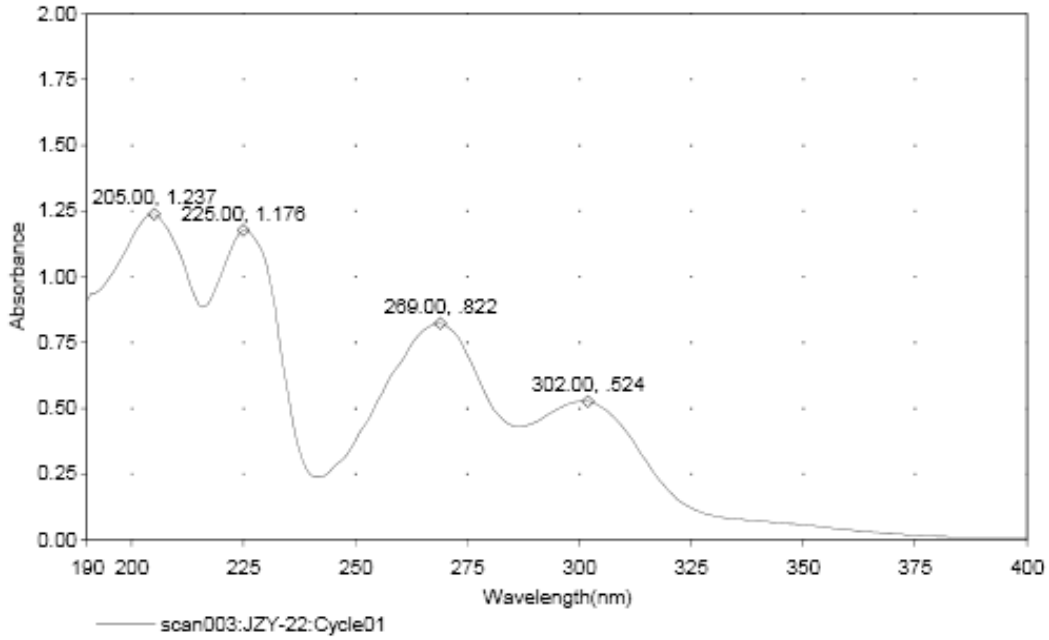
Operator Name	(None Entered)	Date of Report	2021/4/17
Department	(None Entered)	Time of Report	0:09:00上午
Organization	(None Entered)		
Information	(None Entered)		

Scan Graph



Results Table - scan003,JZY-22,Cycle01

nm	A	Manual Method
205.00	1.237	Report Values at 4 Wavelengths
225.00	1.176	205.00 nm 225.00 nm 269.00 nm 302.00 nm
269.00	.822	Sort By Wavelength
302.00	.524	

Figure S9: UV spectrum of Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

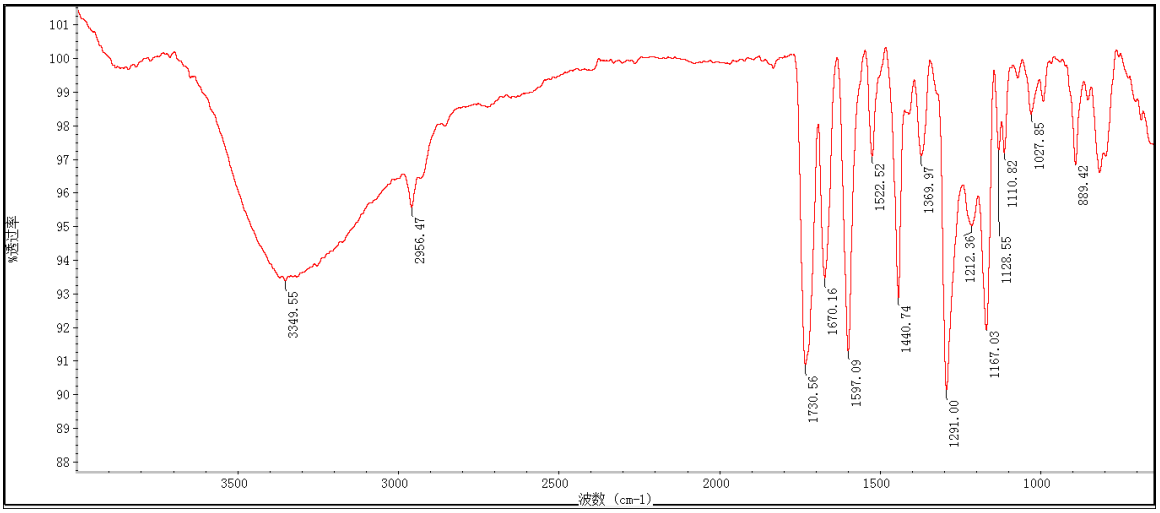


Figure S10: IR spectrum of Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

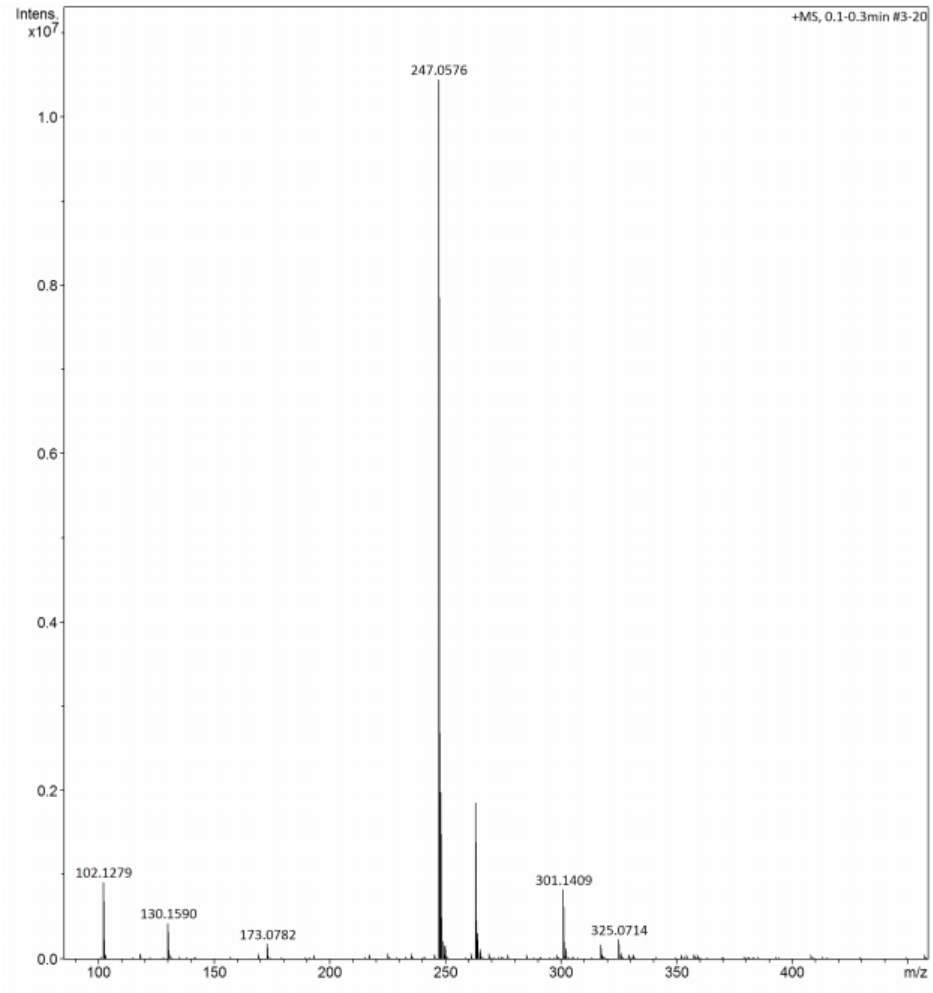


Figure S11: HR-ESI-MS Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

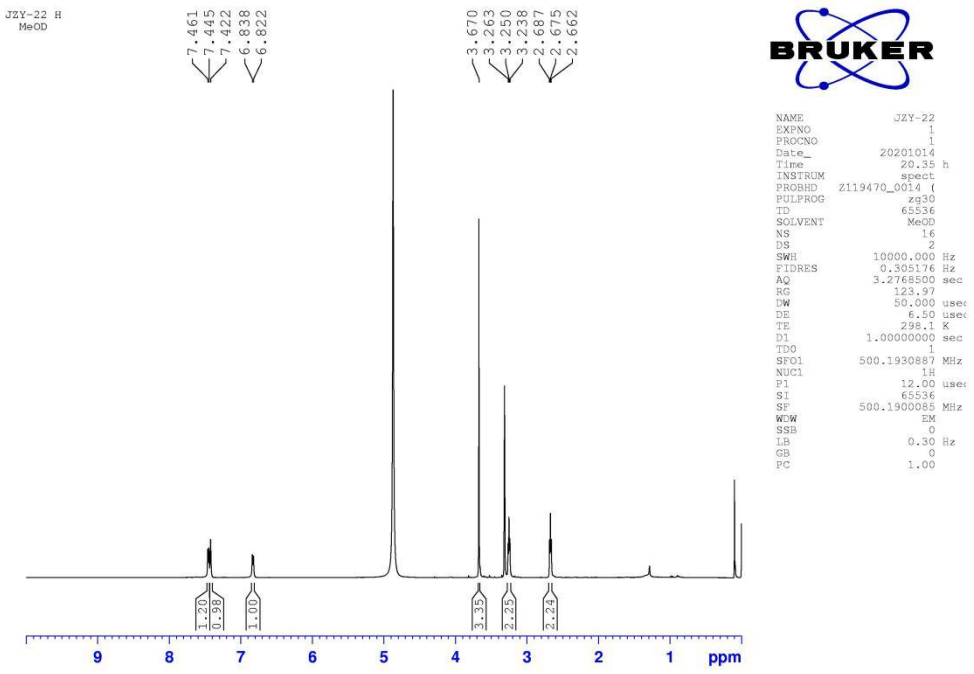


Figure S12: ^{1}H-NMR (500 MHz, methanol-d_4) Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

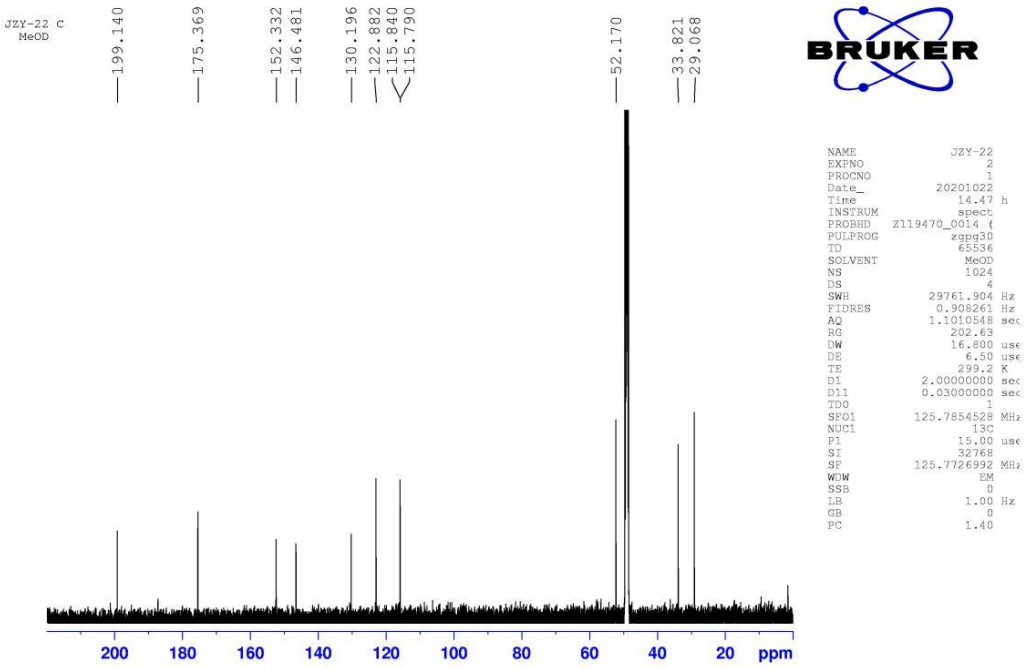


Figure S13: ^{13}C-NMR (125 MHz, methanol-d_4) Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

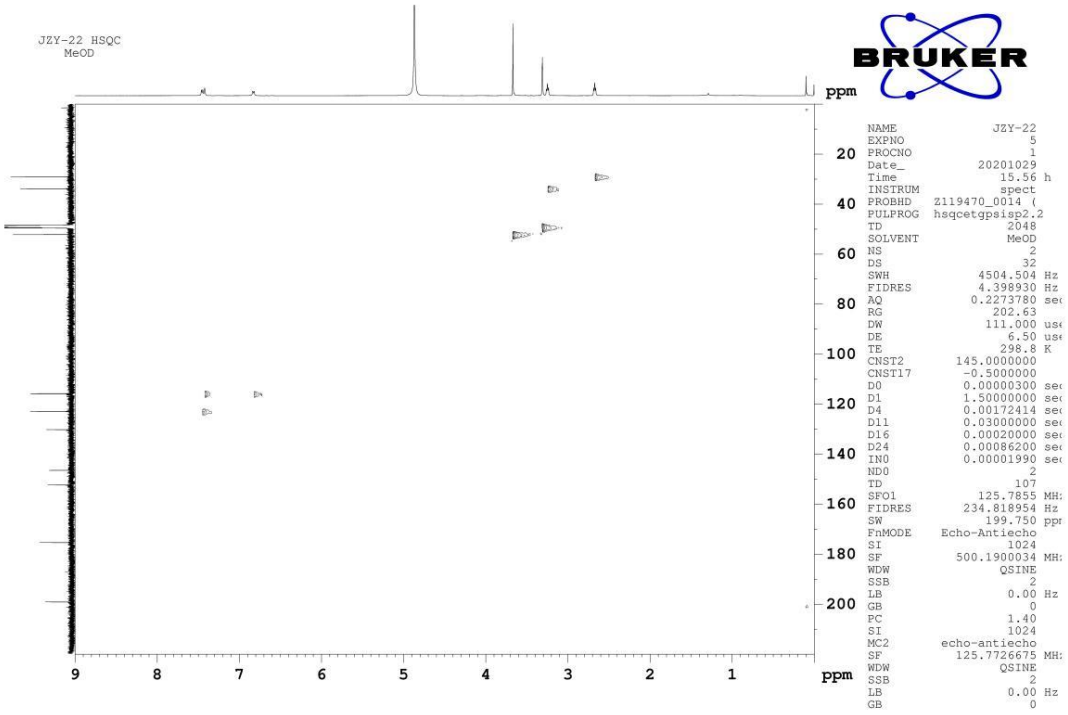


Figure S14: HSQC Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

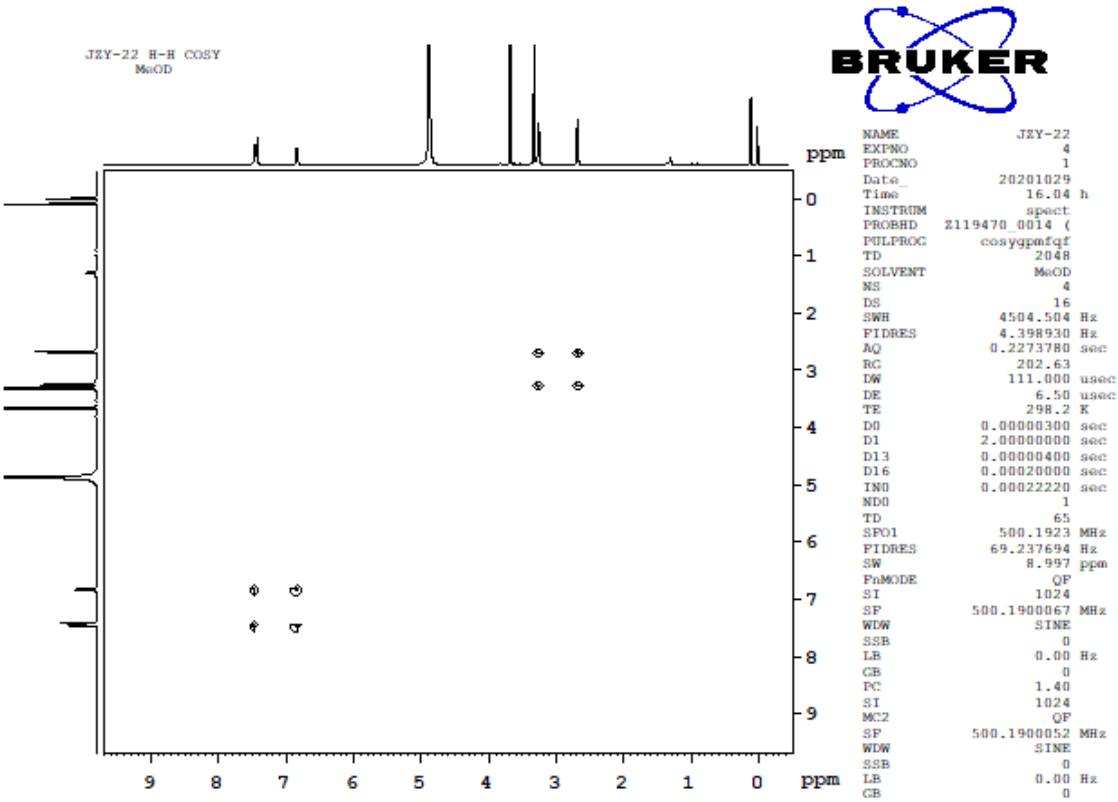


Figure S15: H^1-H^1 COSY Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

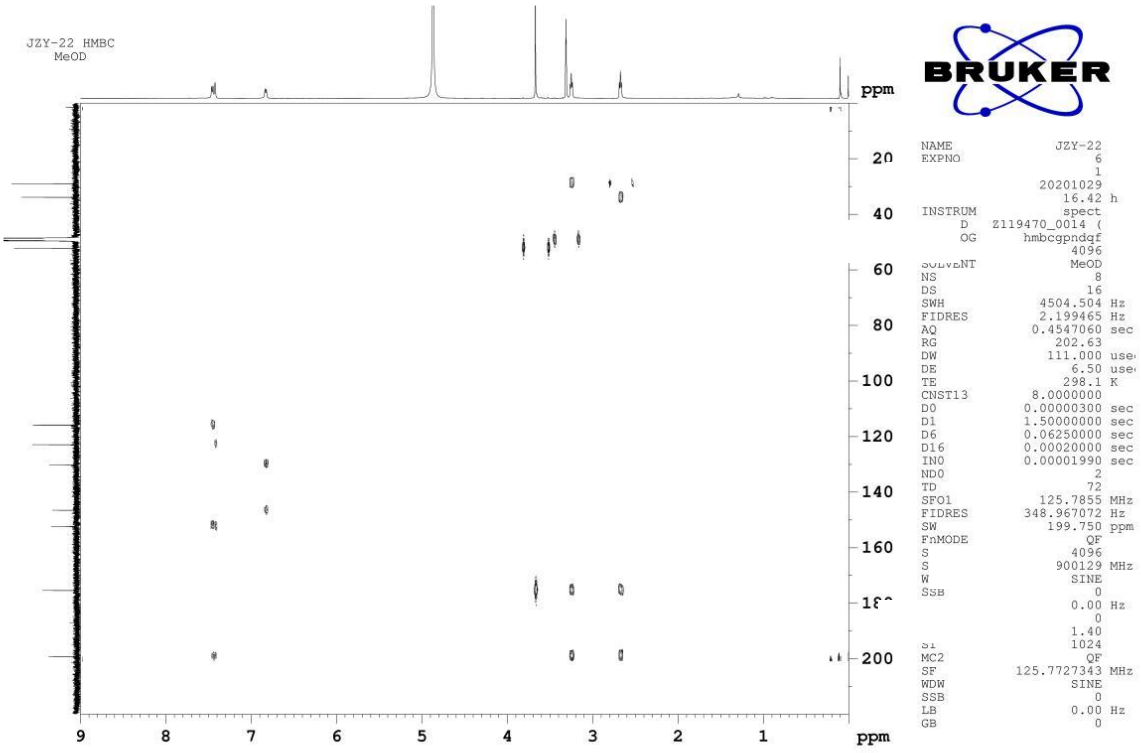


Figure S16: HMBC Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

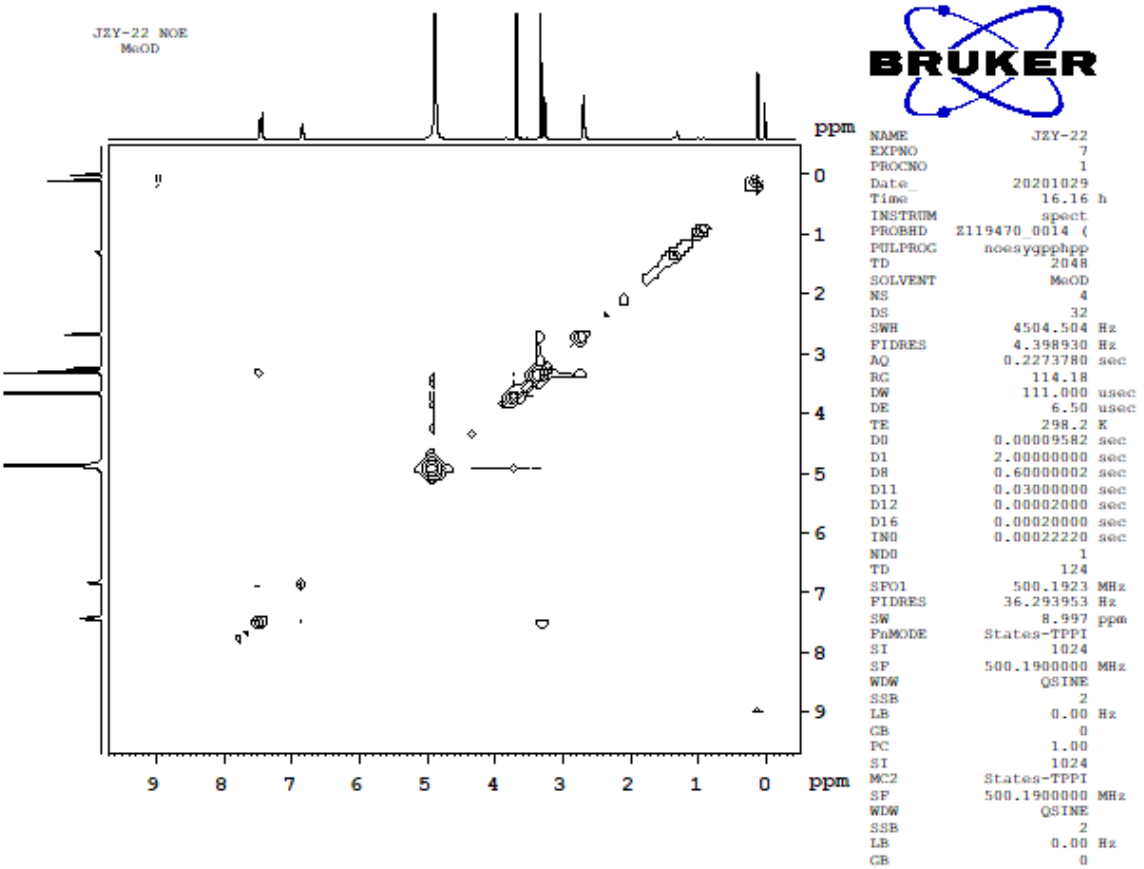


Figure S17: NOESY Spectrum of **2** (methyl 4-(3′,4′-dihydroxyphenyl)-4-oxobutanoate)

Table 1. ^{1}H and ^{13}C NMR spectra data (CD_3OD, 500/125 MHz) for compounds **2** and the ^{1}H NMR in literature .

Position	**2**		
	δ_H	δ_C	LIT δ_H [16]
1		199.1	
2	3.25 (2H, t, 6.2)	33.8	3.25 (2H, t, 6.4)
3	2.67 (2H, t, 6.2)	29.1	2.67 (2H, t, 6.4)
4		175.4	
5	3.67 (3H, s)	52.2	3.67 (3H, s)
1'		130.2	
2'	7.42 (1H, s)	115.8	7.42 (1H, d, 2.1)
3'		146.5	
4'		152.3	
5'	6.83 (1H, d, 8.0)	115.9	6.83 (1H, d, 8.3)
6'	7.45 (1H, d, 8.0)	122.9	7.45 (1H, dd, 8.2, 2.1)

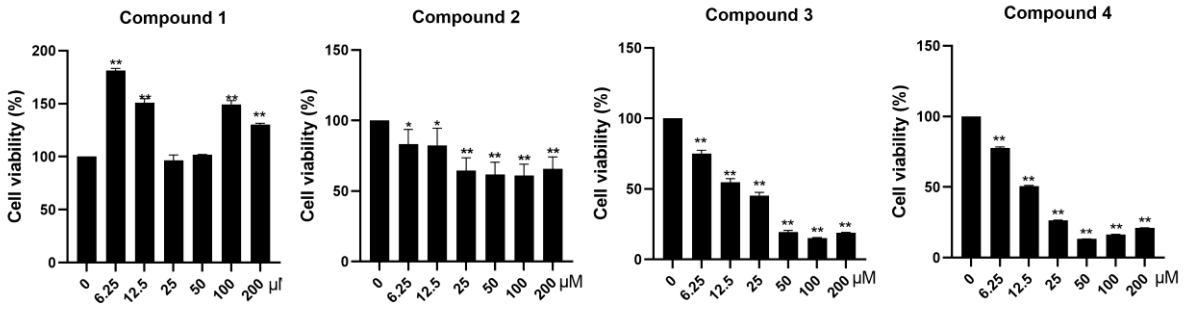


Figure S18: Cell viabilities of RAW 264.7 cells in present of compounds **1–4**. $^{*}P<0.05$, $^{**}P<0.001$, compared with the control group.

S1 : New Compounds Search Eeport of SciFinder

SAVED SEARCHES

Saved Answer Sets

Keep Me Posted

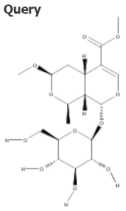
History

Session began October 28, 2021 at 9:55 PM

October 28, 2021 9:55 PM

Explore substances by substructure: structure initiated, resulting in 2 candidates

Query



Explore complete

Candidates Selected
Stereo in answer structure
No stereo in answer structure

Explore results
Answer set 2 created with 53 answers from REGISTRY

October 28, 2021 9:55 PM

Explore substances by exact: structure initiated, resulting in 1 candidate

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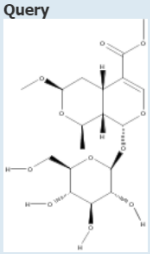

Explore complete

Candidates Selected
Stereo in answer structure

Explore results
Answer set 4 created with 3 answers from REGISTRY

October 28, 2021 9:57 PM

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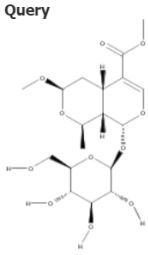
Query



Explore complete

Candidates Selected
≥ 99 (most similar)
95-98

Explore results
Answer set 6 created with 31 answers from REGISTRY

Score: ≥ 99
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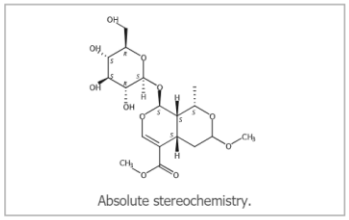
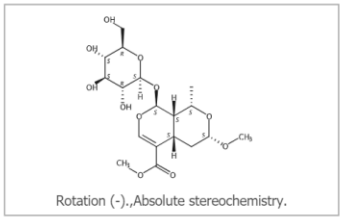


$C_{18}H_{28}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-3-methoxy-1-methyl-, methyl ester, (1*S*,4a*S*,8*S*,8a*S*)-

Key Physical Properties

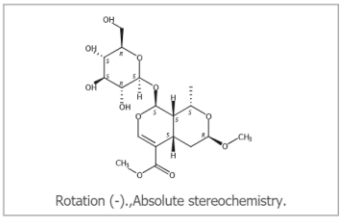
Score: ≥ 99
2. **119943-45-2**



$C_{18}H_{28}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-3-methoxy-1-methyl-, methyl ester, (1*S*,3*S*,4a*S*,8*S*,8a*S*)-

Key Physical Properties

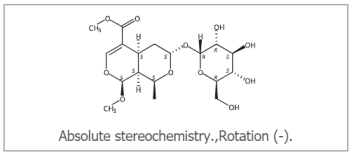
Score: ≥ 99
3. **119943-46-3**



$C_{18}H_{28}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-3-methoxy-1-methyl-, methyl ester, (1*S*,3*R*,4a*S*,8*S*,8a*S*)-

Key Physical Properties

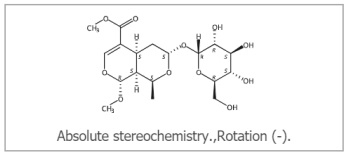
Score: ≥ 99
4. **2172997-11-2**



$C_{18}H_{28}O_{11}$
INDEX NAME NOT YET ASSIGNED

Key Physical Properties

Score: ≥ 99
5. **2172997-12-3**



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Key Physical Properties

Score: 98
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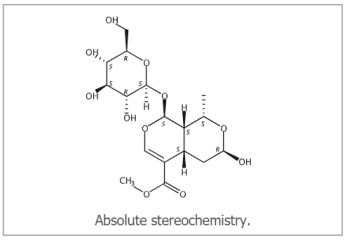
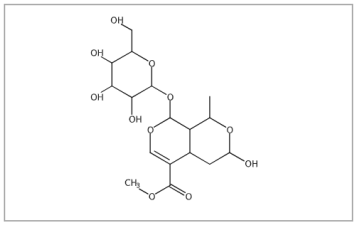


$C_{17}H_{26}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-3-hydroxy-1-methyl-, methyl ester, (1*S*,3*R*,4a*S*,8*S*,8a*S*)-

Key Physical Properties
Regulatory Information
Spectra

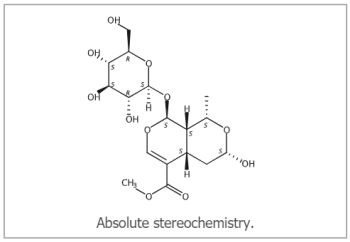
Score: 98
7. **52691-03-9**



$C_{17}H_{26}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 8-(α-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-3-hydroxy-1-methyl-, methyl ester (9CI)

Key Physical Properties
Spectra

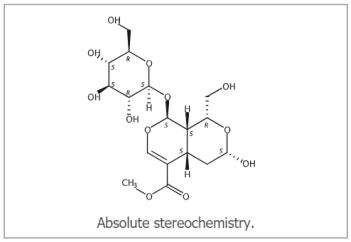
Score: 98
8. **61849-88-5**



$C_{17}H_{26}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-3-hydroxy-1-methyl-, methyl ester, (1*S*,3*S*,4a*S*,8*S*,8a*S*)-

Key Physical Properties
Spectra

Score: 98
9. **94516-24-2**



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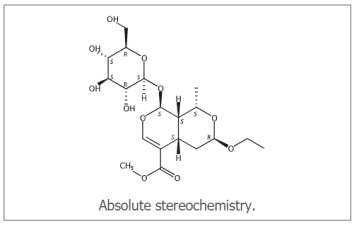
Key Physical Properties

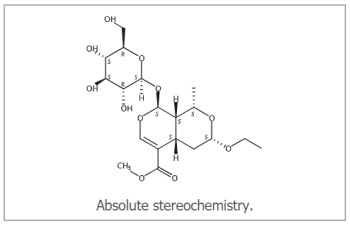
Score: 98
10. **945721-10-8**



$C_{19}H_{30}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 3-ethoxy-8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-1-methyl-, methyl ester, (1*S*,3*R*,4a*S*,8*S*,8a*S*)-

Key Physical Properties

Score: 98
11. **1116650-29-3**



$C_{19}H_{30}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 3-ethoxy-8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-1-methyl-, methyl ester, (1*S*,3*S*,4a*S*,8*S*,8a*S*)-

Key Physical Properties

Score: 98
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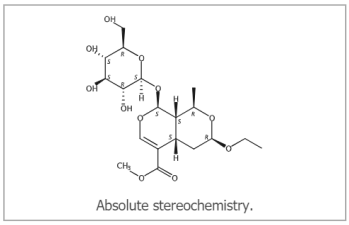

$C_{19}H_{30}O_{11}$
1*H*,3*H*-Pyrano[3,4-*c*]pyran-5-carboxylic acid, 3-ethoxy-8-(β-D-glucopyranosyloxy)-4,4a,8,8a-tetrahydro-1-methyl-, methyl ester, (1*R*,3*R*,4a*S*,8*S*,8a*S*)-

Key Physical Properties