

# Metabolomics Mechanism and Lignin Response to Laxogenin C, a Natural Regulator of Plants Growth

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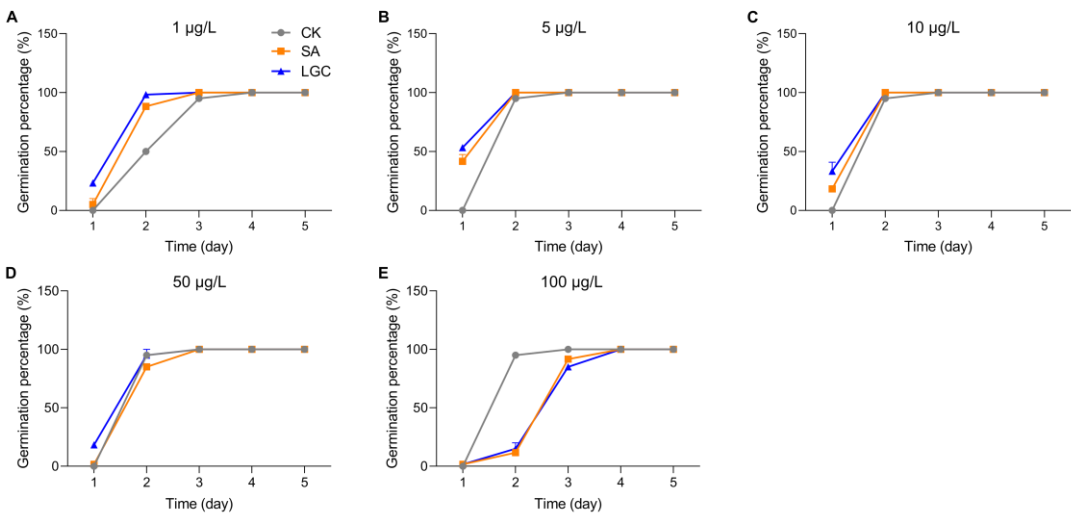
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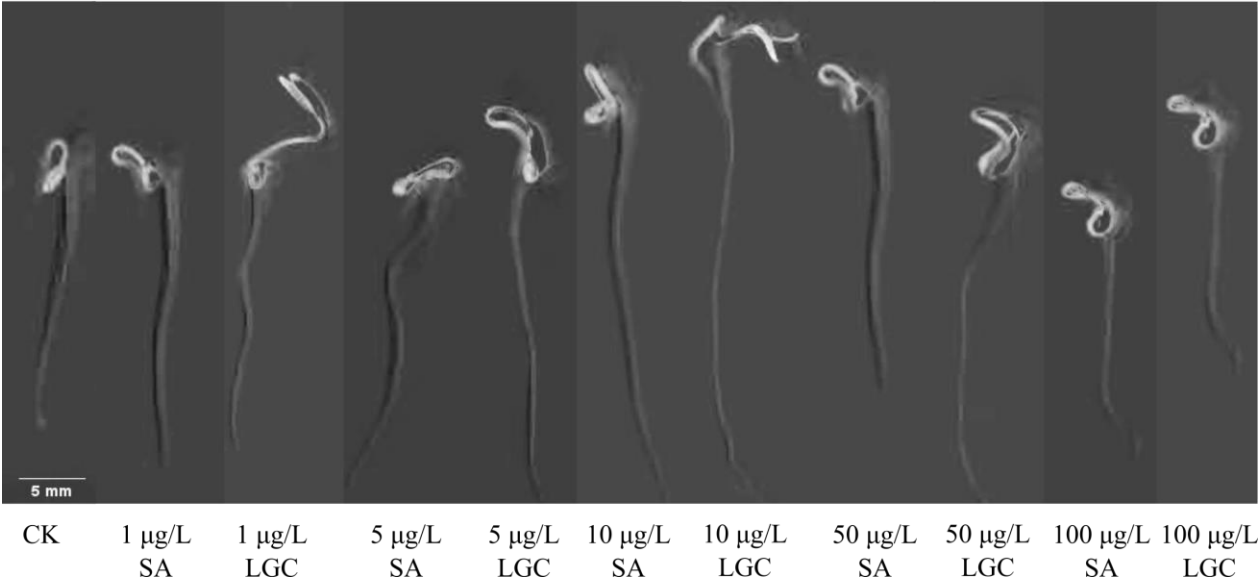
## Contents

Figure S1. Daily germination of seeds treated with LGC and SA .....	2
Figure S2. Tomato seedlings treated with different solutions. ....	3
Figure S3. <sup>1</sup> H NMR spectra of LGC in MeOD .....	4
Figure S4. <sup>13</sup> C NMR spectra of LGC in MeOD .....	5
Figure S5. HR ESI MS of LGC .....	6
Figure S6. <sup>1</sup> H NMR spectra of SA in DMSO- <i>d</i> <sub>6</sub> .....	7
Figure S7. <sup>13</sup> C NMR spectra of SA in DMSO- <i>d</i> <sub>6</sub> .....	8
Figure S8. HR ESI MS of SA .....	9
Figure S9. Measurement and Reference MS/MS Spectra Comparison .....	10
Table S1. Thresholds and Settings in MS-Dial .....	12
Table S2. Hit DMs related to plant growth regulation .....	13

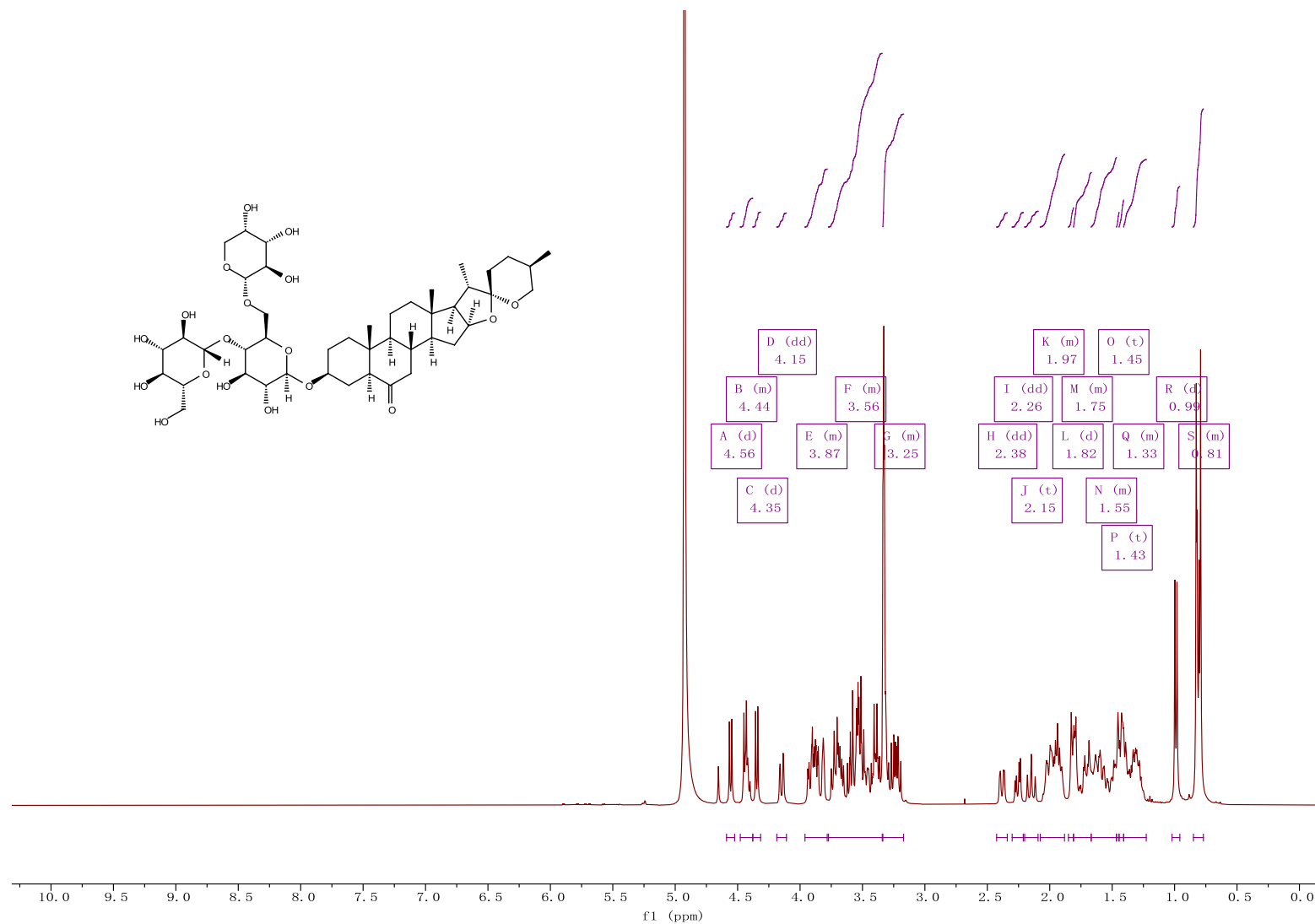
**Figure S1. Daily germination of seeds treated with LGC and SA**



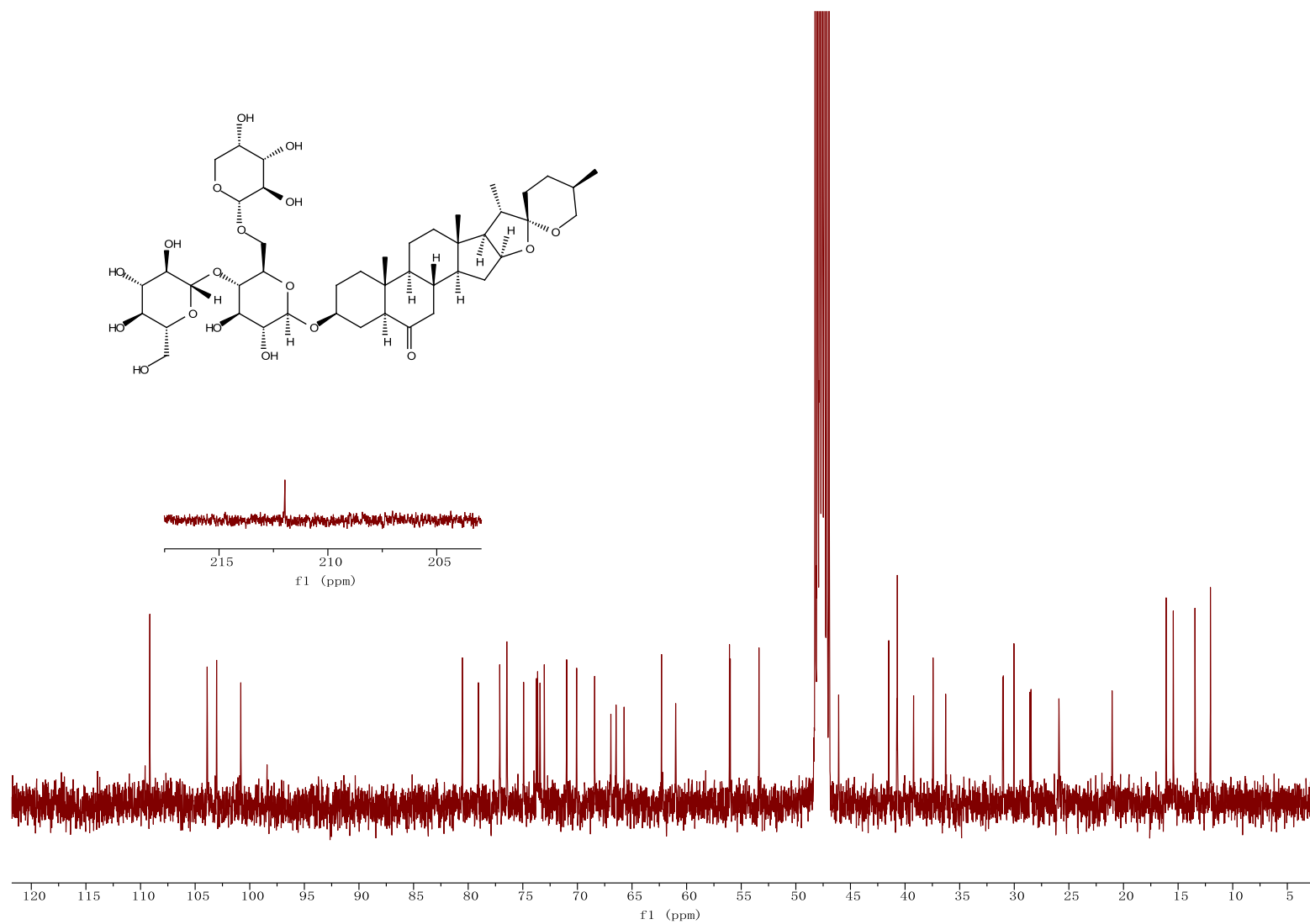
**Figure S2. Tomato seedlings treated with different solutions.**



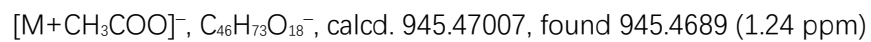
**Figure S3.  $^1\text{H}$  NMR spectra of LGC in MeOD**



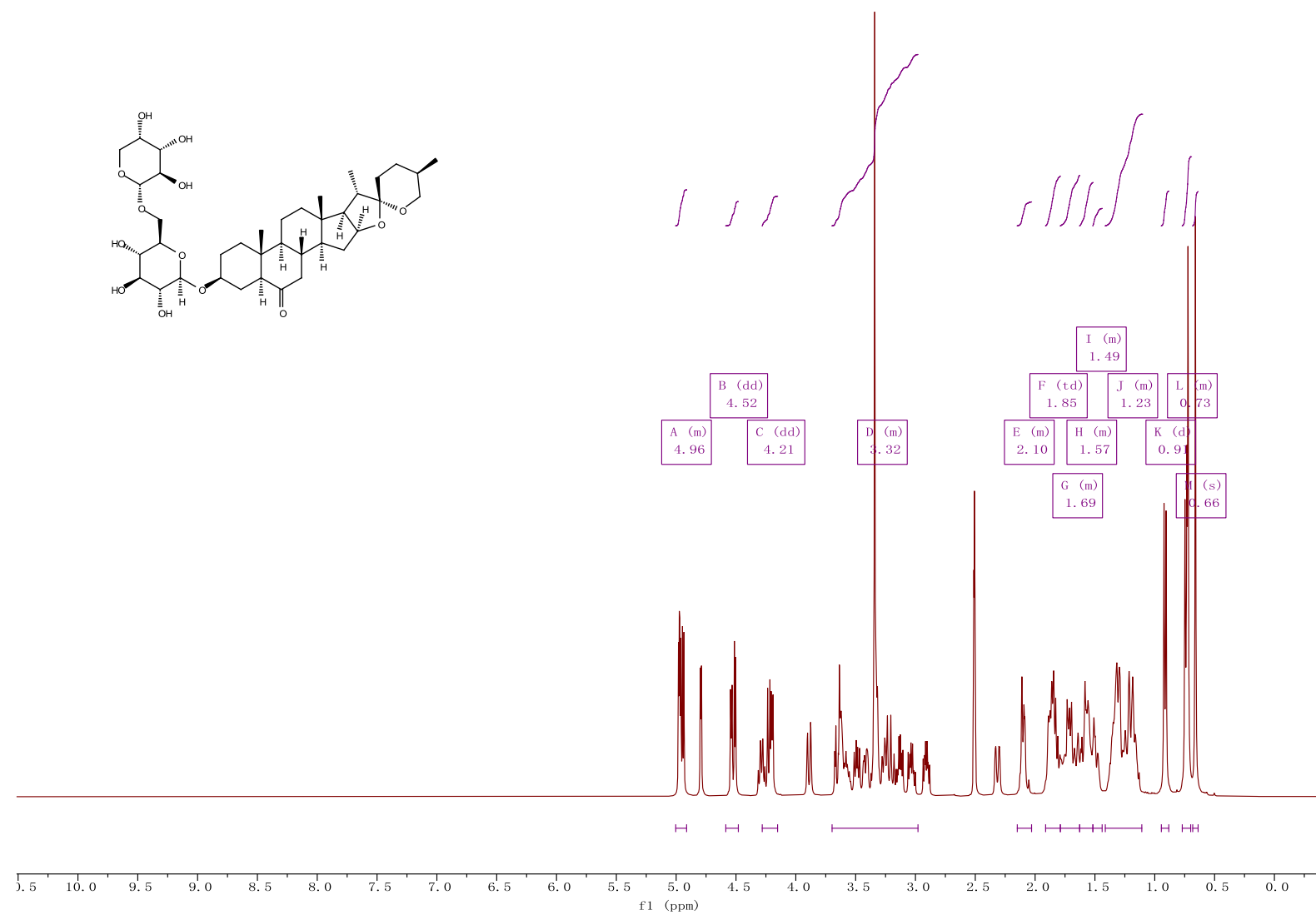
**Figure S4.**  $^{13}\text{C}$  NMR spectra of LGC in MeOD



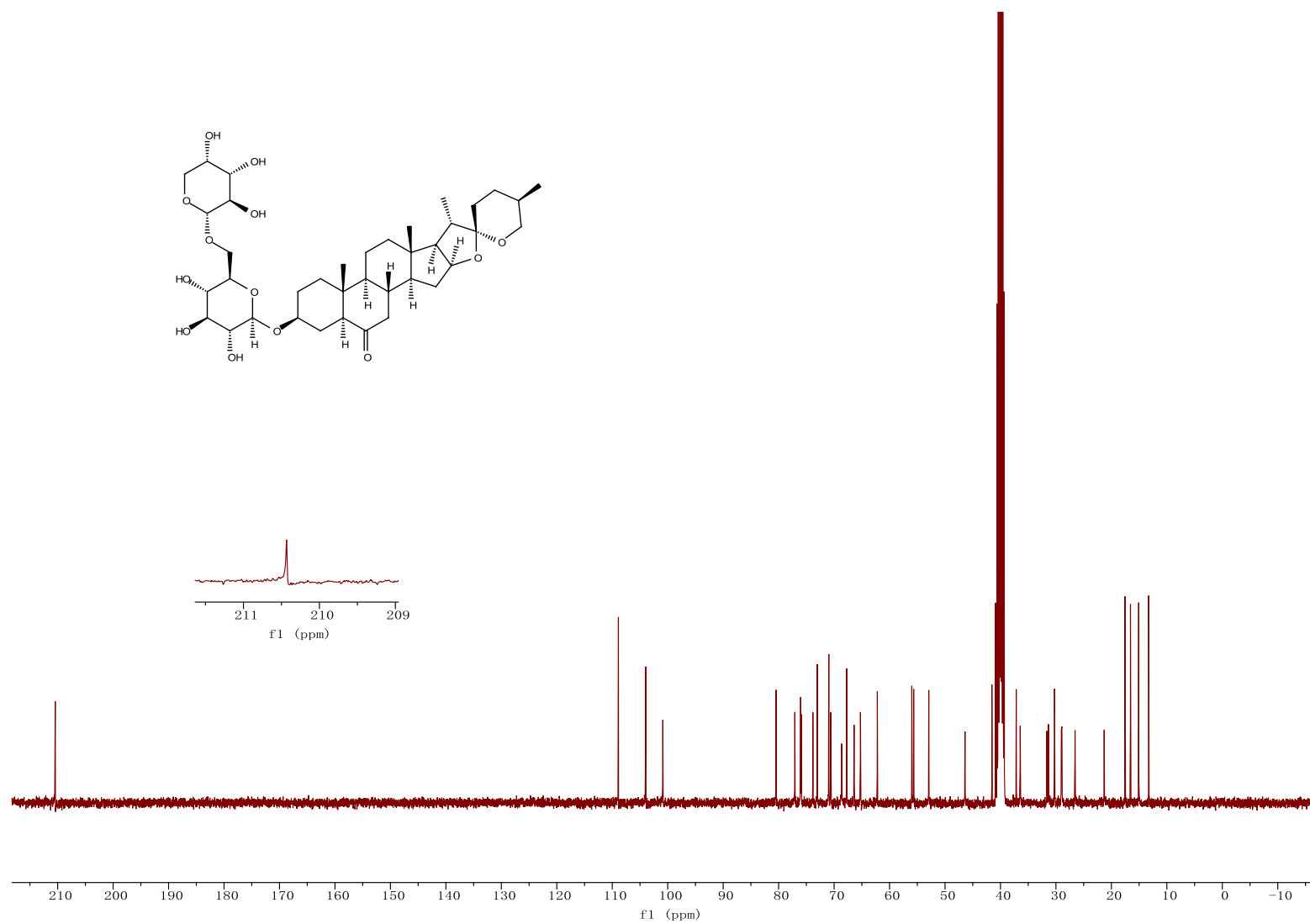
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**Figure S6.  $^1\text{H}$  NMR spectra of SA in  $\text{DMSO}-d_6$**

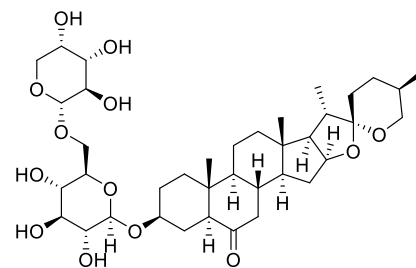


**Figure S7.**  $^{13}\text{C}$  NMR spectra of SA in  $\text{DMSO-}d_6$





**Figure S8. HR ESI MS of SA**



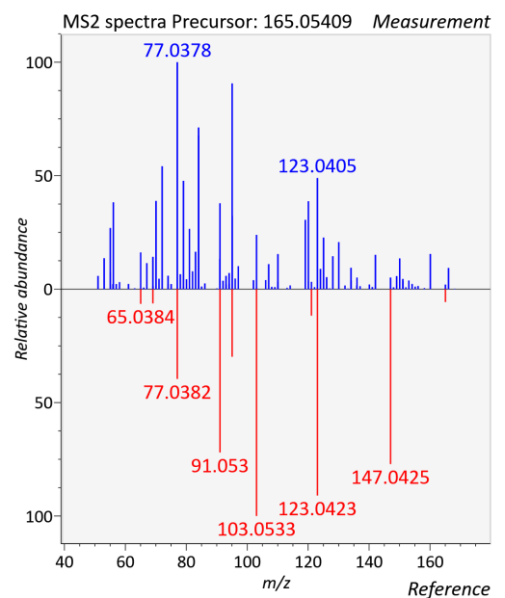
**SA** Chemical Formula:  $C_{38}H_{60}O_{13}$

$[M+CH_3COO]^-$ ,  $C_{40}H_{63}O_{15}^-$ , calcd. 783.41724, found 783.4166 (0.82 ppm)

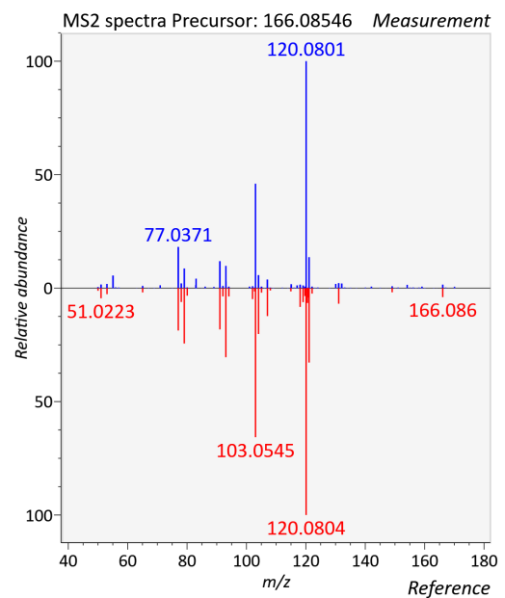
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 1616.4651  
 1617.4684  
 1618.4717  
 1619.4750  
 1620.4783  
 1621.4816  
 1622.4849  
 1623.4882  
 1624.4915  
 1625.4948  
 1626.4981  
 1627.5014  
 1628.5047  
 1629.5080  
 1630.5113  
 1631.5146  
 1632.5179  
 1633.5212  
 1634.5245  
 1635.5278  
 1636.5311  
 1637.5344  
 1638.5377  
 1639.5410  
 1640.5443  
 1641.5476  
 1642.5509  
 1643.5542  
 1644.5575  
 1645.5608  
 1646.5641  
 1647.5674  
 1648.5707  
 1649.5740  
 1650.5773

**Figure S9. Measurement and Reference MS/MS Spectra Comparison**

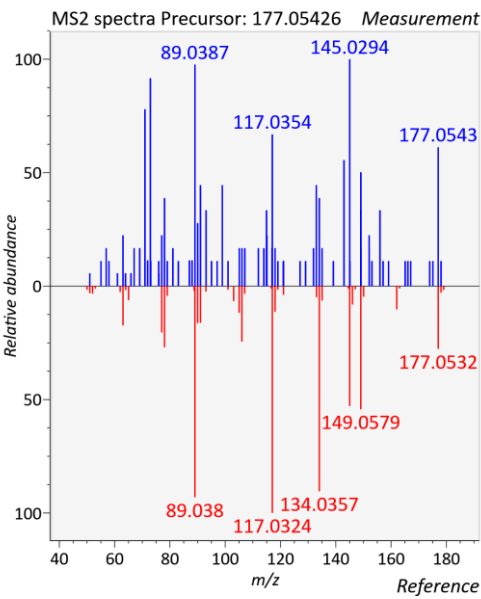
**Alignment ID 181 2-Hydroxycinnamate**



**Alignment ID 184,**



Alignment 220, Ferulate



## Table S1. Thresholds and Settings in MS-Dial

MS-DIAL ver. 4.80

### #Centroid parameters

MS1 tolerance 0.002

MS2 tolerance 0.005

### #Isotope recognition

Maximum charged number 2

### #Peak detection parameters

Smoothing method LinearWeightedMovingAverage

Smoothing level 3

Minimum peak width 5

Minimum peak height 500

### #Peak spotting parameters

Mass slice width 0.05

Exclusion mass list (mass & tolerance)

### #Deconvolution parameters

Sigma window value 0.5

MS2Dec amplitude cut off 0

Exclude after precursor True

Keep isotope until 5

Keep original precursor isotopes False

### #MSP file and MS/MS identification setting

Accurate mass tolerance (MS1) 0.002

Accurate mass tolerance (MS2) 0.005

Identification score cut off 60

### #Adduct ion setting

[M+H]<sup>+</sup>

[M+Na]<sup>+</sup>

[2M+H]<sup>+</sup>

[2M+Na]<sup>+</sup>

### #Alignment parameters setting

Retention time tolerance 0.1

MS1 tolerance 0.01

Retention time factor 0.5

MS1 factor 0.5

**Table S2. Hit DMs related to plant growth regulation**

Alignment ID	KEGG ID	Metabolite name	Formula	Rt(min)	Average M/Z	log2 (G2/G1)	p (G2, G1)	log2 (G3/G2)	P (G3, G2)	log2 (G3/G1)	P (G3, G1)
38	C00183	L-Valine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	1.024	118.08684	/	/	1.00	0.07	/	
49	C00153	Niacinamide	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O	1.024	123.05451	-1.13	0.012	/		-1.10	0.013
63	C01879	L-Pyroglutamic acid	C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub>	1.024	130.04842	-0.88	0.001	/		-0.53	0.017
68	C00407	L-Isoleucine	C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub>	1.081	132.10136	/	/	0.72	0.07	/	
110	C00064	L-Glutamine	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	1.024	147.07642	-0.95	0.001	/		-0.58	0.014
152	C00135	L-Histidine	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	1.024	156.07664	-0.96	0.013	/		/	
181	C01772	trans-2-Hydroxycinnamate	C <sub>9</sub> H <sub>8</sub> O <sub>3</sub>	1.081	165.0546	-1.00	0.015	/		/	
184	C00079	L-Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	1.195	166.08531	-1.20	0.018	1.09	0.12	/	
220	C01494	trans-Ferulic acid	C <sub>10</sub> H <sub>10</sub> O <sub>4</sub>	3.127	177.05426	-0.71	0.002	/		/	
289	C00078	Tryptophan	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	1.195	205.09776	-1.01	0.014	0.86	0.13	/	

Note: /, no significant variation.