## **Supporting Information**

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

# Chemical Constituents from the Roots of Rehmannia glutinosa

# Penghua Shu<sup>1</sup>, Shujing Cai<sup>1</sup>, Xiaojian Zhao<sup>1</sup>, Shuo Zang<sup>1</sup>, Ruihua Li<sup>1</sup>, Yabing Ge<sup>1</sup>, Xiaoqing Lu<sup>1</sup>, Xialan Wei<sup>2</sup>, Yuan Yang<sup>1</sup>, Haitang Yang<sup>\*</sup> and

# Na Sun<sup>1\*</sup>

<sup>1</sup> Food and Pharmacy College, Xuchang University, Xuchang, Henan 461000, P. R. China

<sup>2</sup> School of Information Engineering, Xuchang University, Xuchang, Henan 461000, P. R. China

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SciFinder® Page 1 Score: 95 Score: 95 Score: 95 2. 1. 3. 2566620-10-6 2563912-22-9 2563912-27-4 Absolute stereochemistry., Double bond geometry as shown. Absolute stereochemistry., Double bond geometry as shown. Absolute stereochemistry., Double bond geometry as shown. C<sub>15</sub> H<sub>26</sub> O<sub>7</sub> INDEX NAME NOT YET ASSIGNED C16 H28 O7 INDEX NAME NOT YET ASSIGNED C16 H28 O7 INDEX NAME NOT YET ASSIGNED **Key Physical Properties:** Key Physical Properties: **Key Physical Properties:** Molecular Weight Molecular Weight Molecular Weight 318.36 332.39 332.39 **Boiling Point (Predicted)** Boiling Point (Predicted) **Boiling Point (Predicted)** Value: 470.0±45.0 °C | Condition: Press: 760 Value: 475.5±45.0 °C | Condition: Press: 760 Value: 475.5±45.0 °C | Condition: Press: 760 Torr Torr Torr Density (Predicted) Density (Predicted) Density (Predicted) Value: 1.21±0.1 g/cm3 | Condition: Temp: 20 °C Value: 1.19±0.1 g/cm3 | Condition: Temp: 20 °C Value: 1.19±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr Press: 760 Torr Press: 760 Torr pKa (Predicted) Value: 13.04±0.70 | Condition: Most Acidic pKa (Predicted) Value: 13.04±0.70 | Condition: Most Acidic pKa (Predicted) Value: 13.04±0.70 | Condition: Most Acidic Temp: 25 °C Temp: 25 °C Temp: 25 °C Related Info: Related Info: **Related Info:** ~ 2 References ~ 1 References ~ 1 References Reactions Reactions Score: 94 Score: 94 Score: 94 5 6 1186217-51-5 1355684-04-6 1413812-28-8 Double bond geometry as shown., Absolute stereochemistry. Absolute stereochemistry., Rotation (-)., Double bond geometry as shown. Double bond geometry as shown., Rotation (+)., Absolute stereochemistry.  $C_{17} H_{30} O_6$ 2-Decenoic acid, 9-[(3,6-dideoxy- $\alpha$ -L-*arabino*-C16 H28 O6 C<sub>15</sub> H<sub>24</sub> O<sub>7</sub> 2,4-Octadienoic acid, 7-[(6-deoxy-α-L-2-Nonenoic acid, 8-[(3,6-dideoxy-α-L-arabinohexopyranosyl)oxy]-, methyl ester, (2E,9R)hexopyranosyl)oxy]-, methyl ester, (2E,8R)mannopyranosyl)oxy]-, methyl ester, **Key Physical Properties:** Key Physical Properties: (2E,4E,7R)-Molecular Weight **Molecular Weight** Key Physical Properties: 330 42 316.39 **Boiling Point (Predicted)** Molecular Weight **Boiling Point (Predicted)** Value: 474.0±45.0 °C | Condition: Press: 760 316 35 Value: 462.5±45.0 °C | Condition: Press: 760 **Boiling Point (Predicted)** Torr Torr Value: 482.3±45.0 °C | Condition: Press: 760 Density (Predicted) Density (Predicted) Value: 1.11±0.1 g/cm3 | Condition: Temp: 20 °C Torr Value: 1.12±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr Density (Predicted) Press: 760 Torr Value: 1.23±0.1 g/cm3 | Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) pKa (Predicted) Value: 13.56±0.70 | Condition: Most Acidic Value: 13.56±0.70 | Condition: Most Acidic pKa (Predicted) Temp: 25 °C Temp: 25 °C Value: 13.03±0.70 | Condition: Most Acidic Temp: 25 °C Related Info: **Related Info:** ~ 1 References ~ 6 References **Related Info:** Reactions Reactions ~ 1 References Reactions

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Figure S1: SciFinder search report of the new compound with 94-95% similarity

$ \begin{array}{llllllllllllllllllllllllllllllllllll$		SciFinder®	Page 2
7. 158921-24-5 f + f + f + f + f + f + f + f + f + f +	Score: 93	Score: 93	Score: 92
158921-24-52563912-50-374597-40-3 $f + f + f + f + f + f + f + f + f + f +$	7 <u>.</u>	8.	9.
$\begin{aligned} & \downarrow $	158921-24-5	2563912-50-3	74597-40-3
Double bond geometry as shown., Rotation (-), Absolute stereochemistry. C <sub>17</sub> H <sub>39</sub> O <sub>8</sub> C <sub>17</sub> H <sub>39</sub> O <sub>8</sub> C <sub>17</sub> H <sub>39</sub> O <sub>8</sub> C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> NDEX NAME NOT YET ASSIGNED Key Physical Properties: Molecular Weight 362.42 Boiling Point (Predicted) Value: 546.7±50.0 °C   Condition: Press: 760 Tor Density (Predicted) Value: 1.08±0.1 g/cm3   Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 1.08±0.1 g/cm3   Condition: Most Acidic Temp: 25 °C Related Info: ~ 3 References Score: 92 10. Score: 92 10. Score: 92 10. Score: 92 10. Score: 92 10. Absolute stereochemistry. C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> Nonanoic acid, 9-[(6-deoxy-G-L- galactopyranosyl)oxy]-, methyl ester Score: 92 10. Score: 92 10. Score: 92 10. Score: 92 10. Score: 92 10. Score: 92 10. Score: 92 10. Score: 92 11. 143528-33-0 (-, H <sub>30</sub> O <sub>7</sub> Nonanoic acid, 9-[(6-deoxy-G-L- galactopyranosyl)oxy]-, methyl ester Score: 92 11. 143528-33-0 (-, H <sub>30</sub> O <sub>7</sub> Nonanoic acid, 9-[(6-deoxy-G-L- galactopyranosyl)oxy]-, methyl ester Score: 92 12. Score: 92 13. Score: 92 14. 143528-33-0 (-, H <sub>30</sub> O <sub>7</sub> Nonanoic acid, 9-[(6-deoxy-G-L- galactopyranosyl)oxy]-, methyl ester	of a first	and the second s	ar a
$ \begin{array}{c} \mathbf{C}_{17}  \mathbf{H}_{30}  \mathbf{O}_{8} \\ 2\text{-Octenoic acid, 8-(f)-D-glucopyranosyloxy)-2,6-f-} \\ dimetryl-, methyl ester, (2E,6R)-\\ dimetryl-, methyl ester, (2E,6R)-\\ \mathbf{Key Physical Properties:} \\ \mathbf{Molecular Weight} \\ 362.42 \\ \mathbf{Boiling Point (Predicted)} \\ Value: 546.7\pm50.0  ^{\circ}{\rm C} \mid {\rm Condition: Press: 760} \\ Torr \\ \mathbf{Density (Predicted)} \\ Value: 1.24\pm0.1  g/cm3 \mid {\rm Condition: Temp: 20}  ^{\circ}{\rm C} \\ \mathbf{Press: 760  Torr} \\ Press: 760  Torr$	Double bond geometry as shown., Rotation (-)., Absolute stereochemistry.	Absolute stereochemistry., Double bond geometry as shown.	Absolute stereochemistry.
Key Physical Properties: Molecular Weight 362.42Molecular Weight 358.47Key Physical Properties: Molecular Weight 358.47Boiling Point (Predicted) Value: 456.7±50.0 °C   Condition: Press: 760 Torr Density (Predicted) Value: 1.4±0.1 g/cm3   Condition: Temp: 20 °C PKa (Predicted) Value: 1.9±40.70   Condition: Most Acidic Temp: 25 °CKey Physical Properties: Molecular Weight 334.41Boiling Point (Predicted) Value: 456.7±50.0 °C   Condition: Press: 760 TorrDensity (Predicted) Value: 1.0±0.1 g/cm3   Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 1.3.9±0.70   Condition: Most Acidic Temp: 25 °CDensity (Predicted) Value: 1.3.9±0.70   Condition: Most Acidic Temp: 25 °CDensity (Predicted) Value: 1.3.9±0.70   Condition: Most Acidic Temp: 25 °CRelated Info: - 3 References~2 References~2 ReferencesRelated Info: - 10 References Related Info: - 2 ReferencesScore: 92 10. 143528-28-3Score: 92 11. 143528-33-0Score: 92 12. 263759-17.7 - $\phi_{i} - \phi_{i} - \phi_$	\$- <sub>17</sub> H <sub>30</sub> O <sub>8</sub> 2-Octenoic acid, 8-(β-D-glucopyranosyloxy)-2,6- dimethyl-, methyl ester, (2 <i>E</i> ,6 <i>R</i> )-	C <sub>19</sub> H <sub>34</sub> O <sub>6</sub> INDEX NAME NOT YET ASSIGNED Key Physical Properties:	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> Nonanoic acid, 9-[(6-deoxy-α-L- mannopyranosyl)oxy]-, methyl ester
$ \begin{array}{c} \text{Molecular Weight} \\ 362.42 \\ \text{Boiling Point (Predicted)} \\ \text{Value: 454.7t50.0 °C   Condition: Press: 760} \\ \text{Torr} \\ \text{Density (Predicted)} \\ \text{Value: 124±0.1 g/cm3   Condition: Temp: 20 °C} \\ \text{Press: 760 Torr} \\ \text{pKa (Predicted)} \\ \text{Value: 12.94±0.70   Condition: Most Acidic} \\ \text{Temp: 25 °C} \\ \text{Related Info:} \\ \sim 3 \text{ References} \\ \hline \\ \text{Score: 92} \\ 10. \\ 143528-28-3 \\ \hline \\ \hline \\ \hline \\ \text{ch} \\ \hline \\ \text{Absolute stereochemistry.} \\ \hline \\ \text{galactopyranosyl)oxy], methyl ester \\ \hline \\ \end{array} $	Key Physical Properties:	Molecular Weight	Key Physical Properties:
Related Info: ~ 3 ReferencesRelated Info: ~ 10 References ReactionsScore: 92Score: 9210.11.143528-28-3143528-33-0 $a^{+} f^{+} f$	Allocular Weight I62.42 <b>3oiling Point (Predicted)</b> /alue: 546.7±50.0 °C   Condition: Press: 760 Forr <b>Jensity (Predicted)</b> /alue: 1.24±0.1 g/cm3   Condition: Temp: 20 °C <sup>3</sup> ress: 760 Torr SKa (Predicted) /alue: 12.94±0.70   Condition: Most Acidic Femp: 25 °C	Arrowski regime         358.47         Boiling Point (Predicted)         Value: 497.1±45.0 °C   Condition: Press: 760         Torr         Density (Predicted)         Value: 1.08±0.1 g/cm3   Condition: Temp: 20 °C         Press: 760 Torr         pKa (Predicted)         Value: 13.55±0.70   Condition: Most Acidic         Temp: 25 °C         Related Info:	Molecular Weight 334.41 Boiling Point (Predicted) Value: 464.1±45.0 °C   Condition: Press: 760 Torr Density (Predicted) Value: 1.17±0.1 g/cm3   Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.08±0.70   Condition: Most Acidic Temp: 25 °C
Notice intermediation2 References~ 10 References ReactionsScore: 92Score: 9210.143528-28-3143528-33-012. $\alpha - \int_{-10}^{-10} -$	Related Info:	~ 2 References	Related Info:
Score: 92Score: 9210.11.143528-28-3143528-33-0	- 3 References	2 Nelelences	~ 10 References Reactions
10.11.12. <b>143528-28-3143528-33-0</b> $4^{-1}$ $a^{-1}$ <td>Score: 92</td> <td>Score: 92</td> <td>Score: 92</td>	Score: 92	Score: 92	Score: 92
143528-28-3143528-33-0263759-17-7 $a = \int_{a = 1}^{a} \int_{a = 1}$	10.	11.	12.
$ \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c} \begin{array}{c}$	143528-28-3	143528-33-0	263759-17-7
Absolute stereochemistry.       Absolute stereochemistry.       Image: C_{16} H_{30} O_7       Description (C_{16} H_{30} O_7)         C_{16} H_{30} O_7       C_{16} H_{30} O_7       Nonanoic acid, 9-[(6-deoxy- $\alpha$ -L-galactopyranosyl)oxy]-, methyl ester       Double bond geometry as shown., Rotat Absolute stereochemistry.         galactopyranosyl)oxy]-, methyl ester       galactopyranosyl)oxy]-, methyl ester       C_{17} H_{28} O_7	and	and the second s	CH, OL CH
C16 H30 O7     C16 H30 O7       Nonanoic acid, 9-[(6-deoxy-β-L- galactopyranosyl)oxy]-, methyl ester     Double bond geometry as shown., Rotat Absolute stereochemistry.       galactopyranosyl)oxy]-, methyl ester     C17 H28 O7	Absolute stereochemistry.	Absolute stereochemistry.	он
$C_{17} H_{28} O_7$	<b>&gt;<sub>16</sub> H<sub>30</sub> O<sub>7</sub></b> √onanoic acid, 9-[(6-deoxy-β-L- galactopyranosyl)oxy]-, methyl ester	C <sub>16</sub> H <sub>30</sub> O <sub>7</sub> Nonanoic acid, 9-[(6-deoxy-α-L- galactopyranosyl)oxy]-, methyl ester	Double bond geometry as shown., Rotation (+)., Absolute stereochemistry.
Key Physical Properties: Key Physical Properties: 2.7-Octadienoic acid 6-I/6-deoxy-R-D-	Key Physical Properties:	Key Physical Properties:	2.7-Octadienoic acid, 6-[(6-deoxy-ß-D-
Molecular Weight 334.41       Molecular Weight 334.41       Molecular Weight 334.41       Glucopyranosyl)oxyl-2,6-dimethyl-, meth (2E,6R)-         Boiling Point (Predicted) Value: 464.1±45.0 °C   Condition: Press: 760       Torr       Boiling Point (Predicted) Value: 1.17±0.1 g/cm3   Condition: Temp: 20 °C       Key Physical Properties: Molecular Weight 344.40         Value: 1.17±0.1 g/cm3   Condition: Temp: 20 °C       Value: 1.17±0.1 g/cm3   Condition: Temp: 20 °C       Key Physical Properties: Molecular Weight 344.40         Value: 1.17±0.1 g/cm3   Condition: Temp: 20 °C       Value: 1.17±0.1 g/cm3   Condition: Temp: 20 °C       Nale: 1.17±0.1 g/cm3   Condition: Temp: 20 °C         Press: 760 Torr       Pres: 760 Torr       Pres: 760 Torr       Pres: 760 Torr         Value: 13.08±0.70   Condition: Most Acidic       Temp: 25 °C       Density (Predicted)         Value: 13.08±0.70   Condition: Most Acidic       Temp: 25 °C       Density (Predicted)         Value: 13.08±0.70   Condition: Most Acidic       Temp: 25 °C       Press: 760 Torr         PKa (Predicted)       Value: 13.08±0.70   Condition: Most Acidic       Temp: 25 °C         Related Info:       ~ 2 References       ~ 2 References       Value: 13.03±0.70   Condition: Most Acidic	Aloecular Weight 134.41 30iling Point (Predicted) /alue: 464.1±45.0 °C   Condition: Press: 760 Forr Density (Predicted) /alue: 1.17±0.1 g/cm3   Condition: Temp: 20 °C Press: 760 Torr X64 (Predicted) /alue: 13.08±0.70   Condition: Most Acidic Femp: 25 °C Related Info: - 4 References	Molecular Weight 334.41 Boiling Point (Predicted) Value: 464.1±45.0 °C   Condition: Press: 760 Torr Density (Predicted) Value: 1.17±0.1 g/cm3   Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 13.08±0.70   Condition: Most Acidic Temp: 25 °C Related Info: ~ 2 References	<ul> <li>contraction (c) (c) (c) (c) (c) (c) (c) (c) (c) (c)</li></ul>
~ 3 References			~ 3 References

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Figure S2: SciFinder search report of the new compound with 92-93% similarity

### **Elemental Composition Report**

#### **Single Mass Analysis**

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Element prediction: Off Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions 39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass) Elements Used: C: 17-17 H: 31-31 O: 0-10 F: 0-5



Figure S3: HR-ESI-MS spectrum of 1

Page 1



Figure S4: UV spectrum of 1 in CHCl<sub>3</sub>



Figure S5: IR spectrum of 1



Figure S6: <sup>1</sup>H NMR spectrum (400 MHz) of 1 in CDCl<sub>3</sub>





Figure S8: DEPT 135 spectrum of 1 in CDCl<sub>3</sub>





Figure S10: <sup>1</sup>H-<sup>1</sup>H COSY spectrum of 1 in CDCl<sub>3</sub>













Figure S15: <sup>13</sup>C NMR spectrum (100 MHz) of 2 in CDCl<sub>3</sub>



Figure S16: <sup>1</sup>H NMR spectrum (400 MHz) of 3 in CDCl<sub>3</sub>



Figure S17: <sup>13</sup>C NMR spectrum (100 MHz) of 3 in CDCl<sub>3</sub>



Figure S18: <sup>1</sup>H NMR spectrum (400 MHz) of 4 in CDCl<sub>3</sub>



Figure S19: <sup>13</sup>C NMR spectrum (100 MHz) of 4 in CDCl<sub>3</sub>



Figure S20: <sup>1</sup>H NMR spectrum (400 MHz) of 5 in CDCl<sub>3</sub>



Figure S21: <sup>13</sup>C NMR spectrum (100 MHz) of 5 in CDCl<sub>3</sub>



Figure S22: <sup>1</sup>H NMR spectrum (400 MHz) of 6 in CDCl<sub>3</sub>



Figure S23: <sup>13</sup>C NMR spectrum (100 MHz) of 6 in CDCl<sub>3</sub>



Figure S24: <sup>1</sup>H NMR spectrum (400 MHz) of 7 in DMSO-d<sub>6</sub>



Figure S25: <sup>13</sup>C NMR spectrum (100 MHz) of 7 in DMSO- $d_6$ 



Figure S26: <sup>1</sup>H NMR spectrum (400 MHz) of 8 in DMSO-d<sub>6</sub>



Figure S27: <sup>13</sup>C NMR spectrum (100 MHz) of 8 in DMSO- $d_6$ 



Figure S28: <sup>1</sup>H NMR spectrum (400 MHz) of 9 in CD<sub>3</sub>OD



Figure S29: <sup>13</sup>C NMR spectrum (100 MHz) of 9 in CD<sub>3</sub>OD



Figure S30: <sup>1</sup>H NMR spectrum (400 MHz) of 10 in CD<sub>3</sub>OD



Figure S31: <sup>13</sup>C NMR spectrum (100 MHz) of 10 in CD<sub>3</sub>OD