

## Supporting Information

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### A New Diterpenoid with Antitumor Cytotoxicity from Millipede

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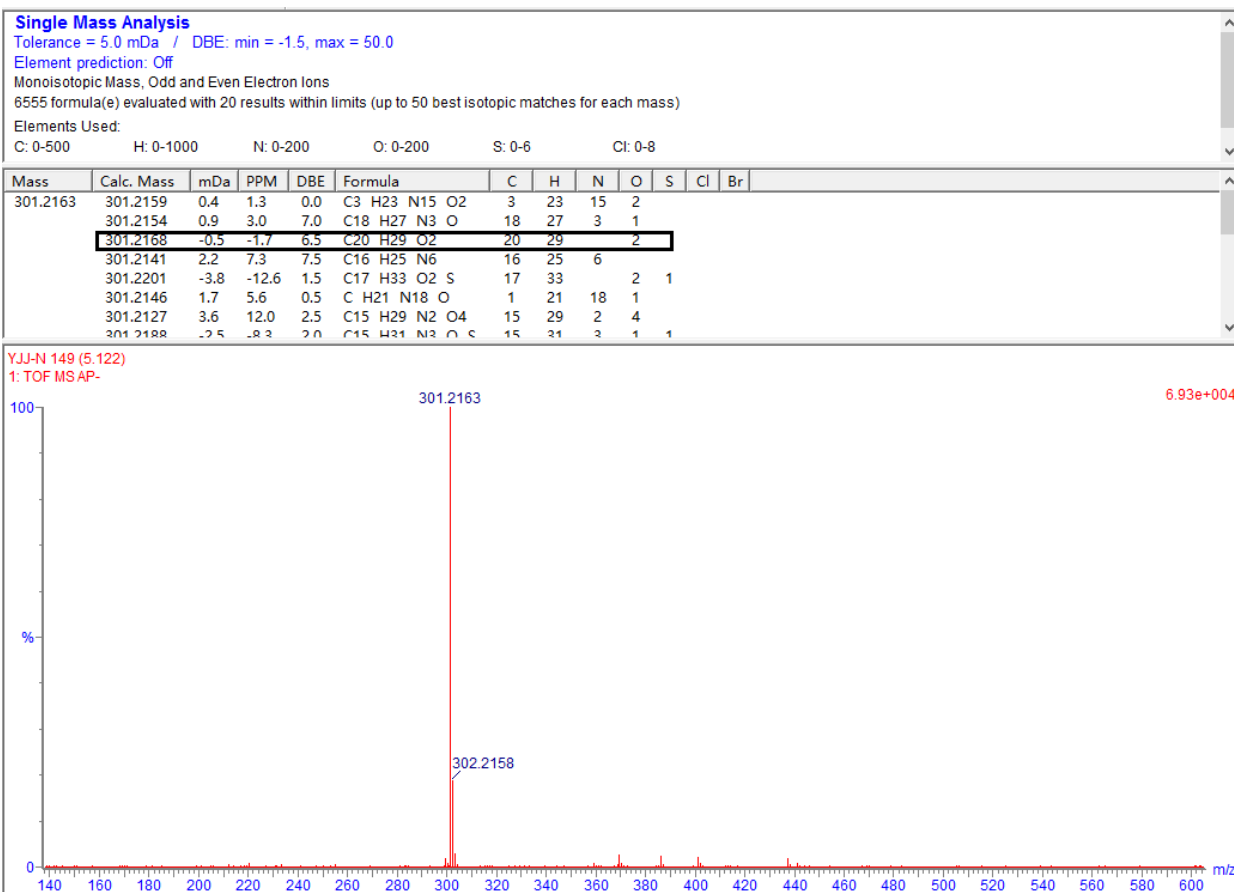
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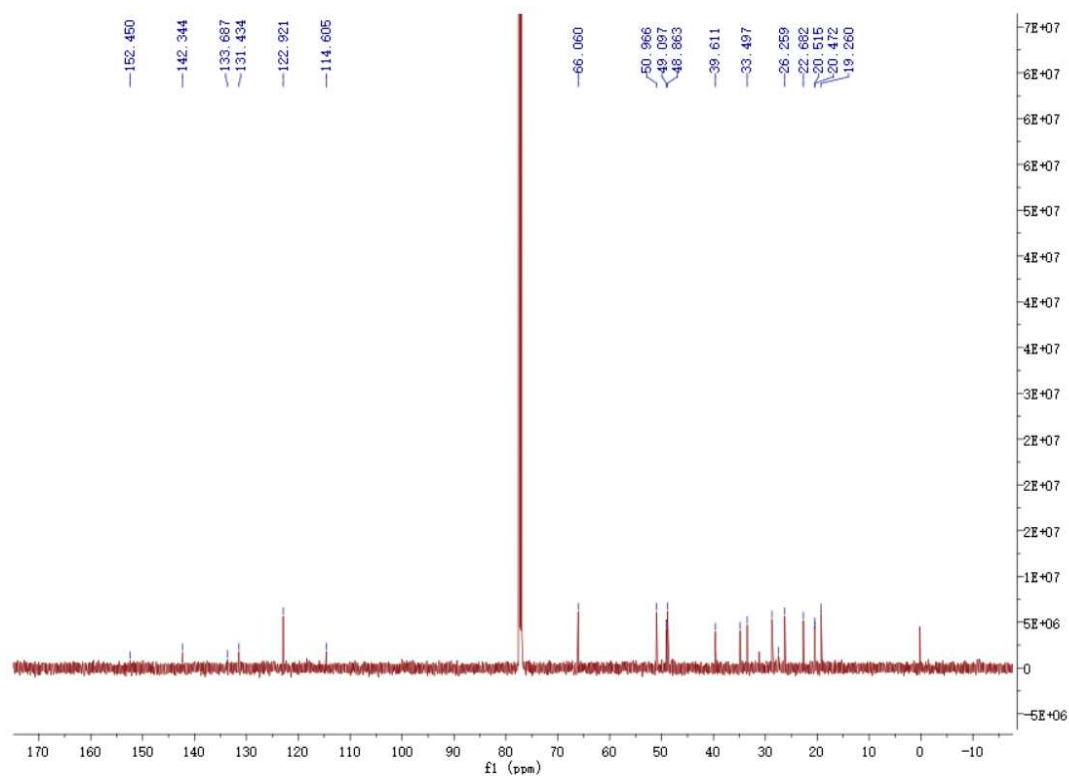
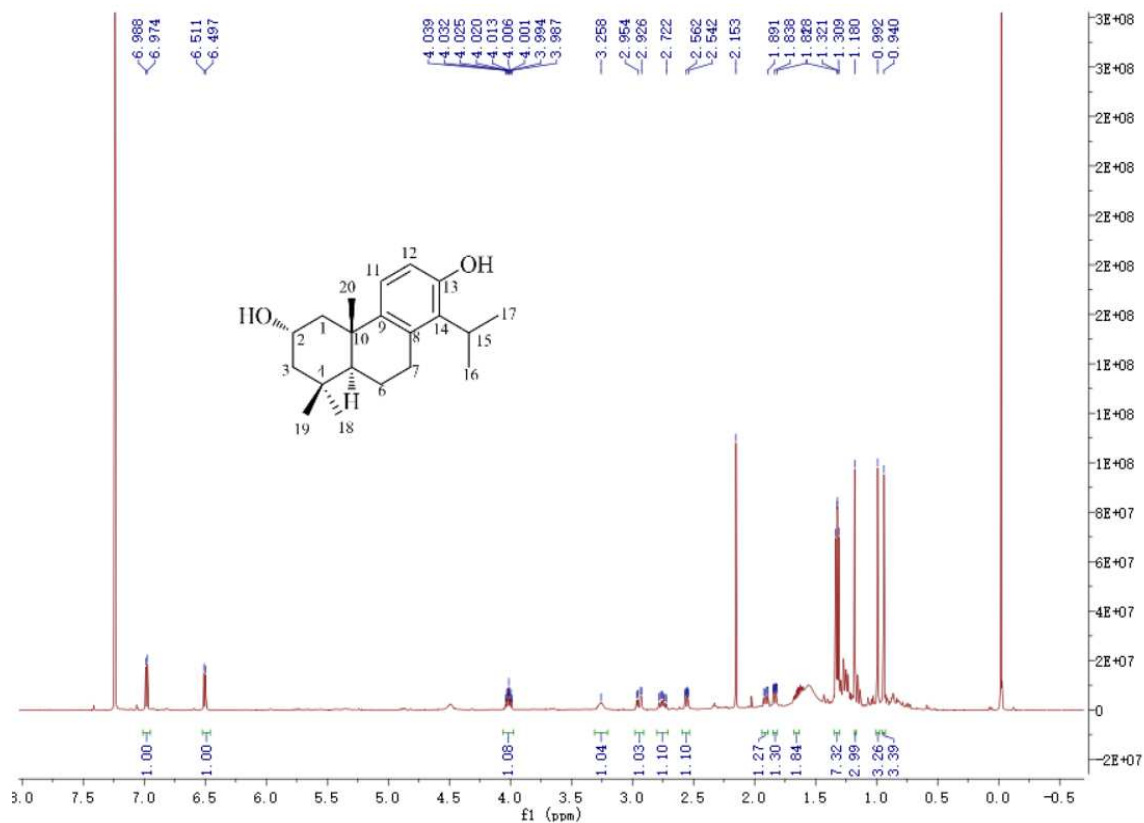
<sup>2</sup>*Key Laboratory of Basic Pharmacology of Ministry of Education and Joint International Research*

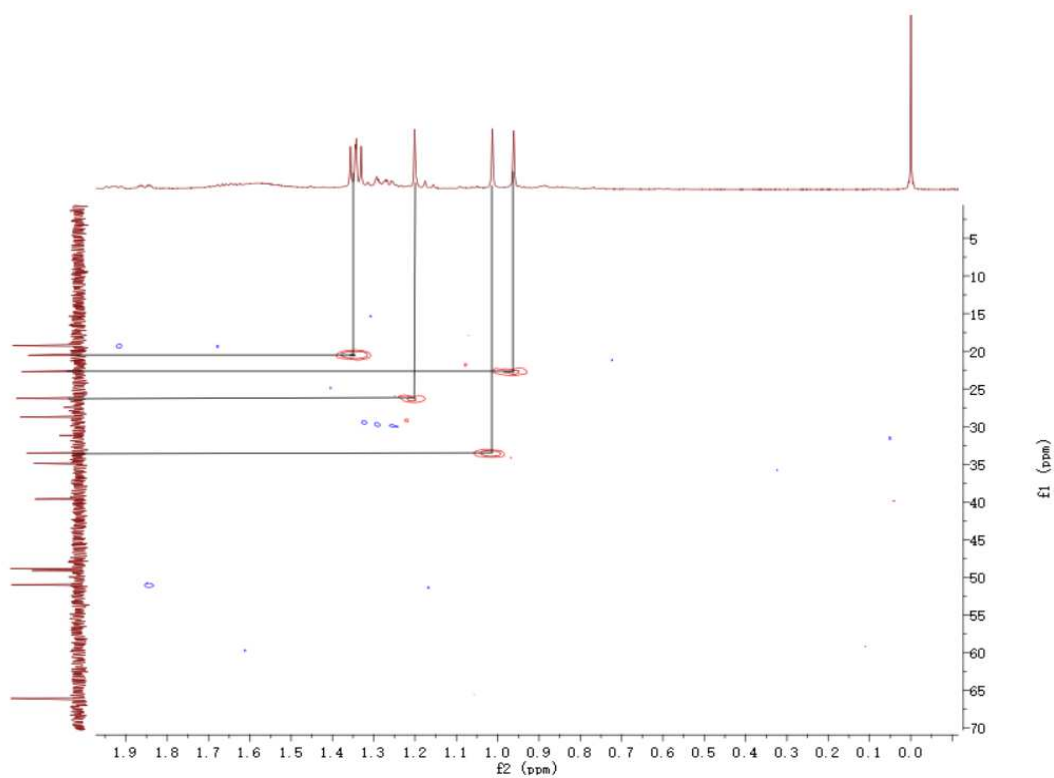
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563006, P. R. China*

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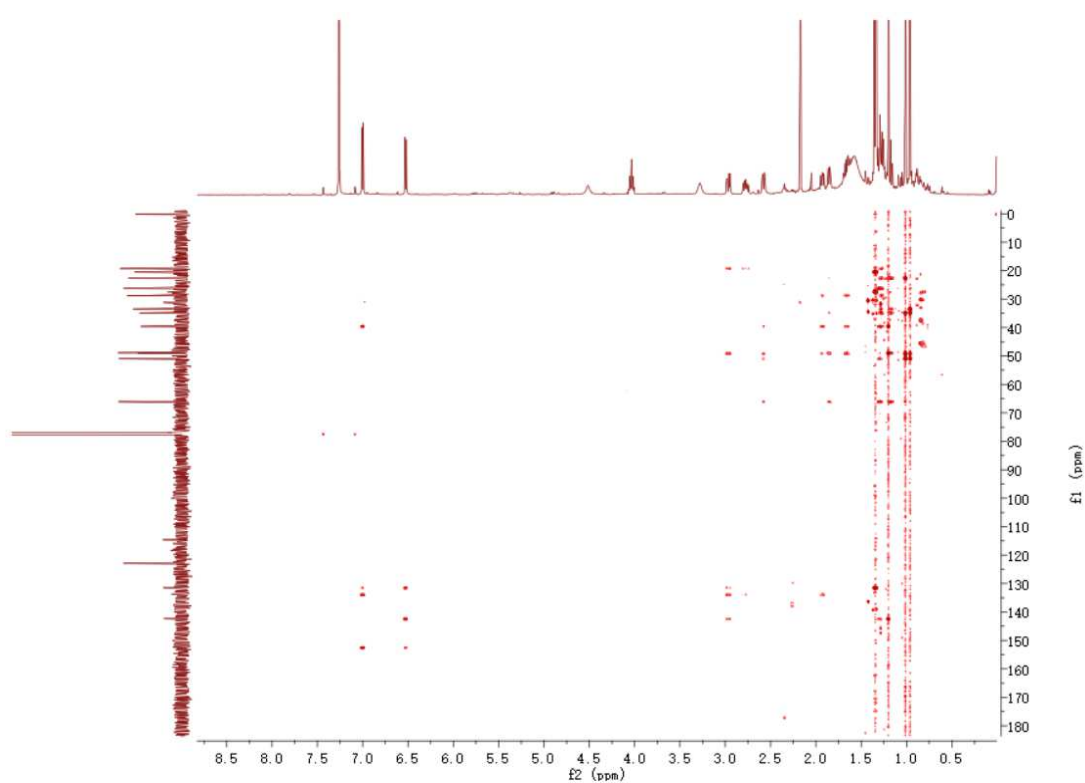


**Figure S1: HR-APCI-MS spectrum of 10**

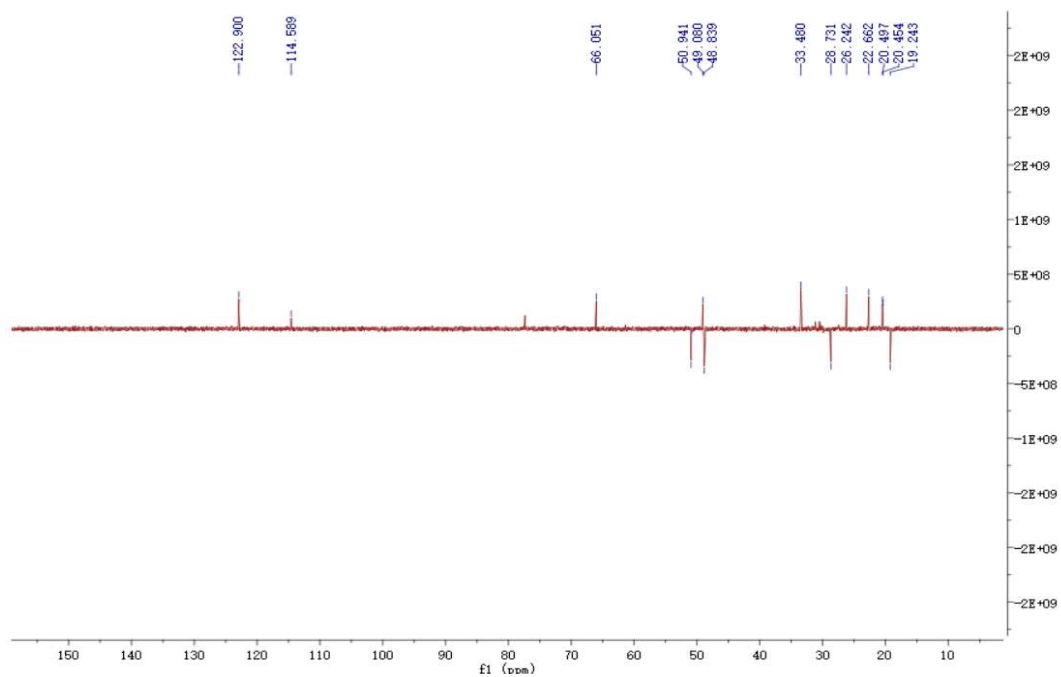




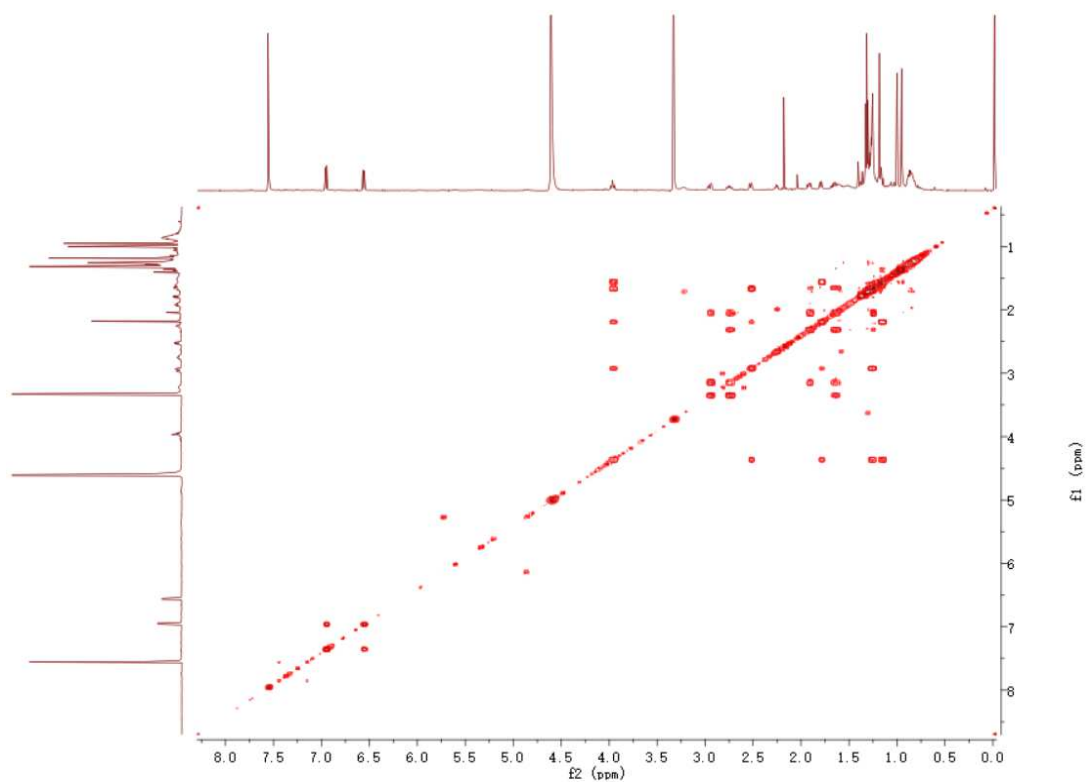
**Figure S4:** HSQC spectrum of **10** (From  $\delta_C$ 10 ppm to  $\delta_C$  70 ppm)



**Figure S5:** HMBC spectrum of **10**



**Figure S6: DEPT spectrum of 10**



**Figure S7:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 10**

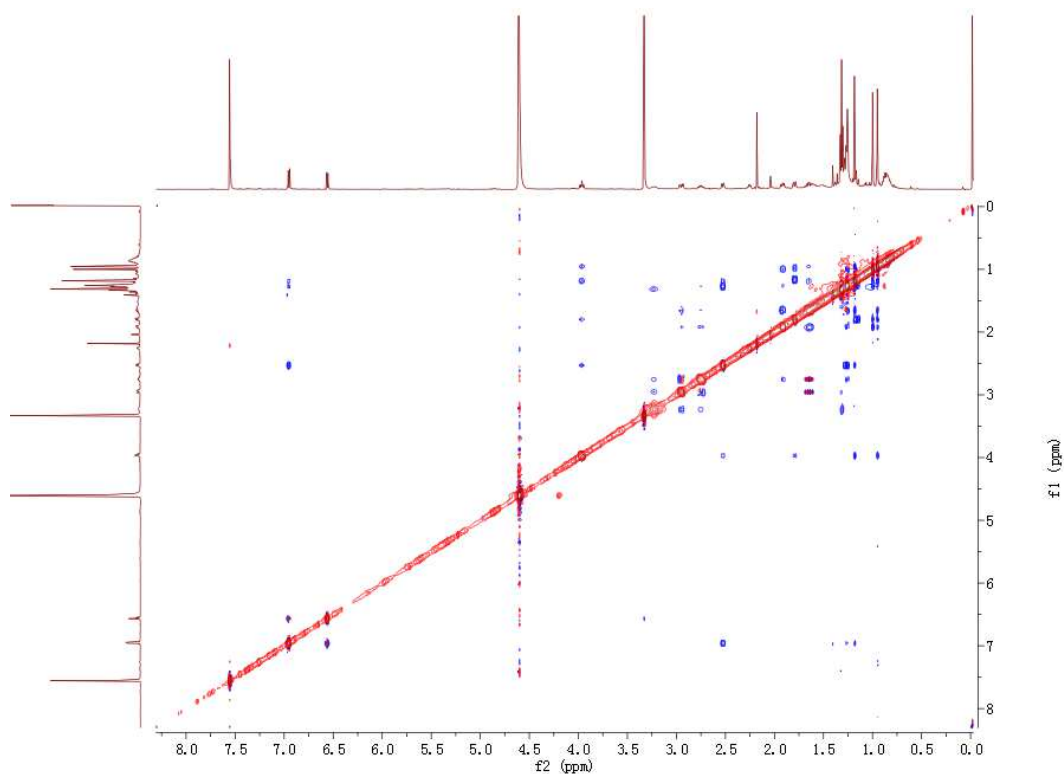


Figure S8: NOESY spectrum of 10

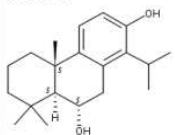
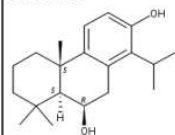
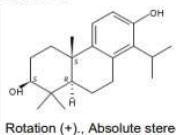
SciFinder®		Page 1
<p>Score: 97 1. <b>1891-80-1</b></p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>20</sub>H<sub>30</sub>O<sub>2</sub></b> 2,9-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS,8aS,9S)-</p> <p><b>Key Physical Properties:</b>  <b>Molecular Weight</b> 302.45  <b>Melting Point (Experimental)</b> Value: 186-187 °C  <b>Boiling Point (Predicted)</b> Value: 407.5±45.0 °C   Condition: Press: 760 Torr  <b>Density (Predicted)</b> Value: 1.054±0.06 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr  <b>pKa (Predicted)</b> Value: 10.80±0.70   Condition: Most Acidic Temp: 25 °C  <b>Related Info:</b>            ~ 3 References            ~ 4 Commercial Sources            Regulatory Information            Experimental Properties</p>	<p>Score: 97 2. <b>297179-13-6</b></p>  <p>Absolute stereochemistry.</p> <p><b>C<sub>20</sub>H<sub>30</sub>O<sub>2</sub></b> 2,9-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS,8aS,9R)-</p> <p><b>Key Physical Properties:</b>  <b>Molecular Weight</b> 302.45  <b>Boiling Point (Predicted)</b> Value: 407.5±45.0 °C   Condition: Press: 760 Torr  <b>Density (Predicted)</b> Value: 1.054±0.06 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr  <b>pKa (Predicted)</b> Value: 10.80±0.70   Condition: Most Acidic Temp: 25 °C  <b>Related Info:</b>            ~ 1 References            ~ 2 Commercial Sources            Regulatory Information</p>	<p>Score: 96 3. <b>3772-56-3</b></p>  <p>Rotation (+), Absolute stereochemistry.</p> <p><b>C<sub>20</sub>H<sub>30</sub>O<sub>2</sub></b> 2,7-Phenanthrenediol, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-8-(1-methylethyl)-, (2S,4aS,10aR)-</p> <p><b>Key Physical Properties:</b>  <b>Molecular Weight</b> 302.45  <b>Melting Point (Experimental)</b> Value: 180.5-181.5 °C  <b>Boiling Point (Predicted)</b> Value: 407.5±45.0 °C   Condition: Press: 760 Torr  <b>Density (Predicted)</b> Value: 1.054±0.06 g/cm<sup>3</sup>   Condition: Temp: 20 °C Press: 760 Torr  <b>pKa (Predicted)</b> Value: 10.86±0.70   Condition: Most Acidic Temp: 25 °C  <b>Related Info:</b>            ~ 25 References            Reactions            ~ 21 Commercial Sources            Spectra            Experimental Properties</p>

Figure S9: Scifinder search results of 10