

Supporting Information

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A New Diterpenoid with Antitumor Cytotoxicity from Millipede

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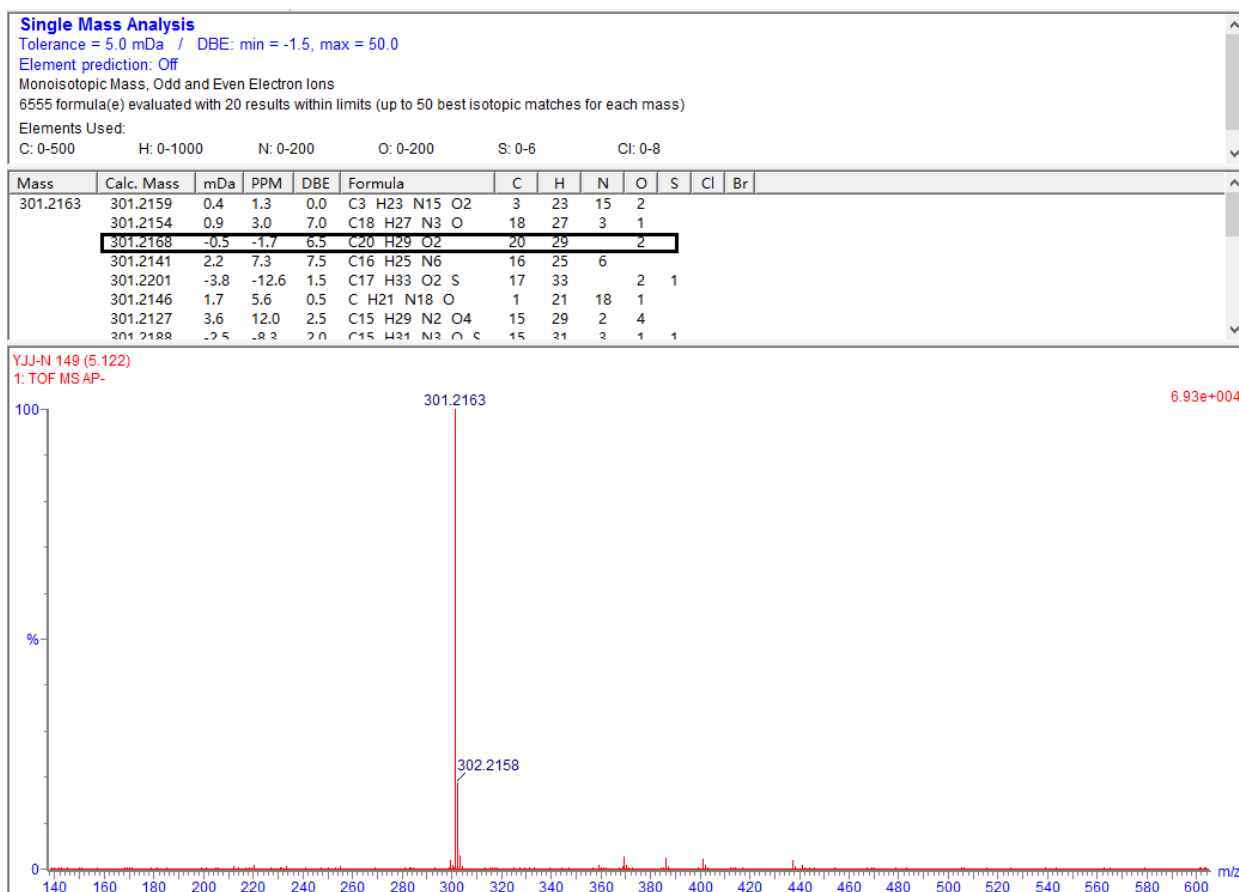


Figure S1: HR-APCI-MS spectrum of 10

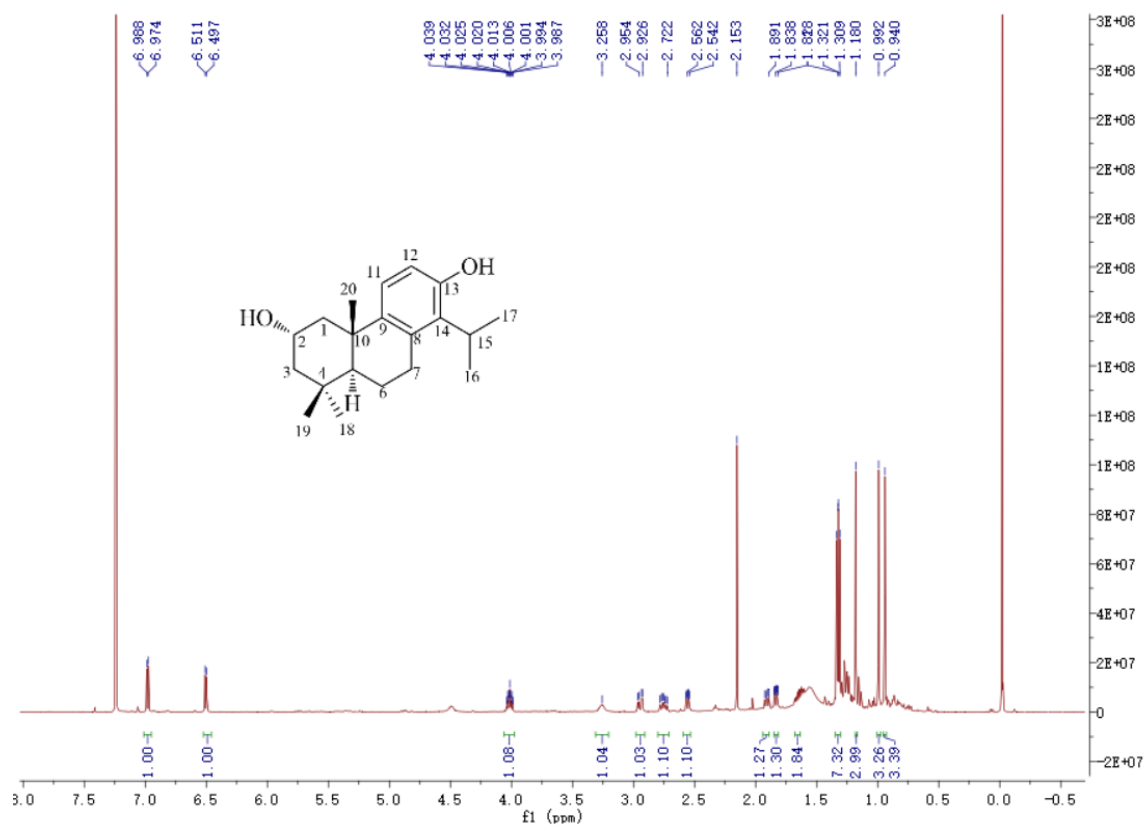


Figure S2: ¹H-NMR (600 MHz, CDCl₃) spectrum of **10**

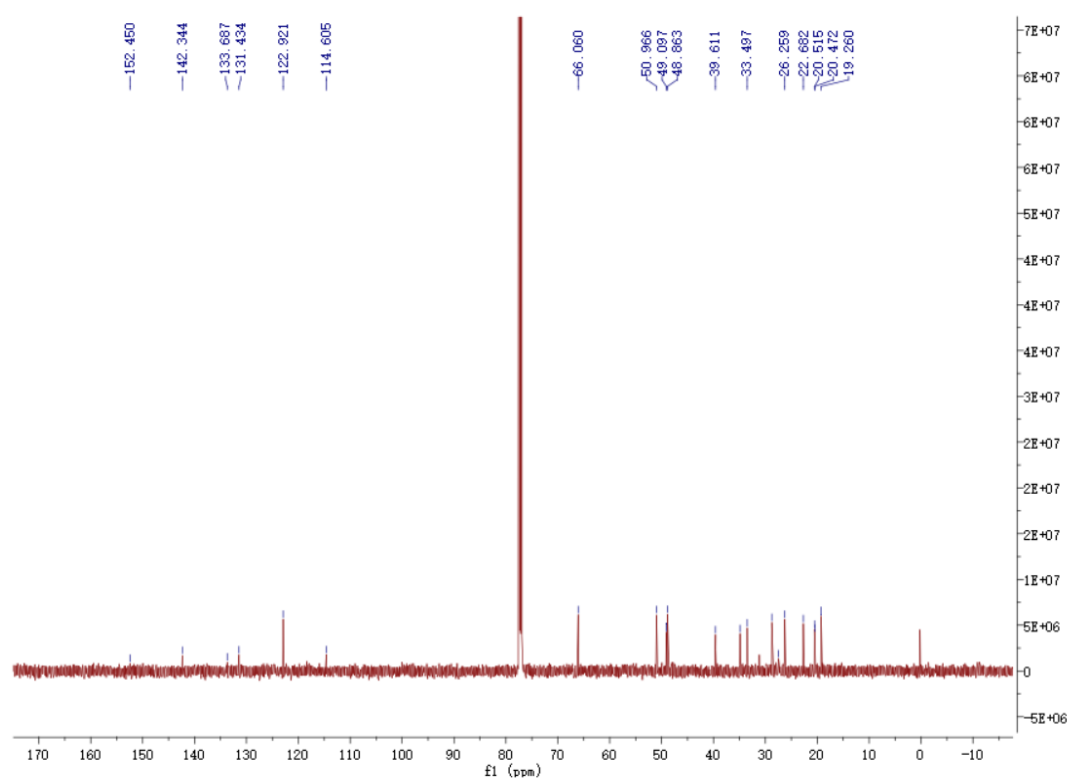


Figure S3: ¹³C-NMR (150 MHz, CDCl₃) spectrum of **10**

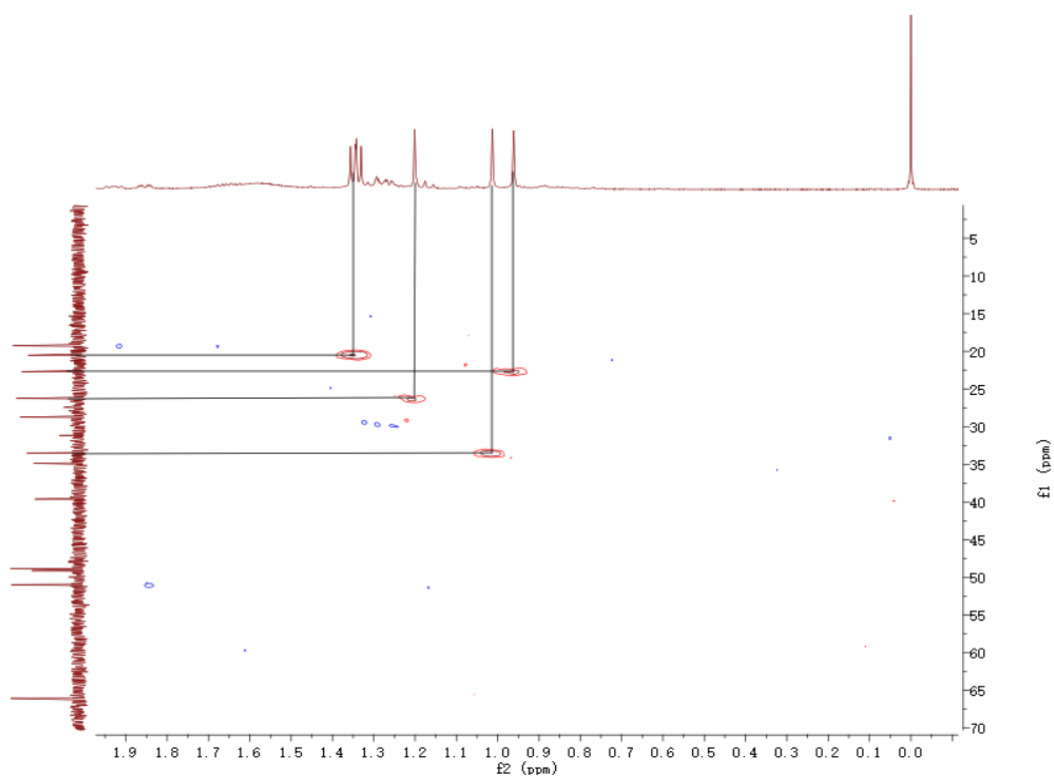


Figure S4: HSQC spectrum of **10** (From δ_C 10 ppm to δ_C 70 ppm)

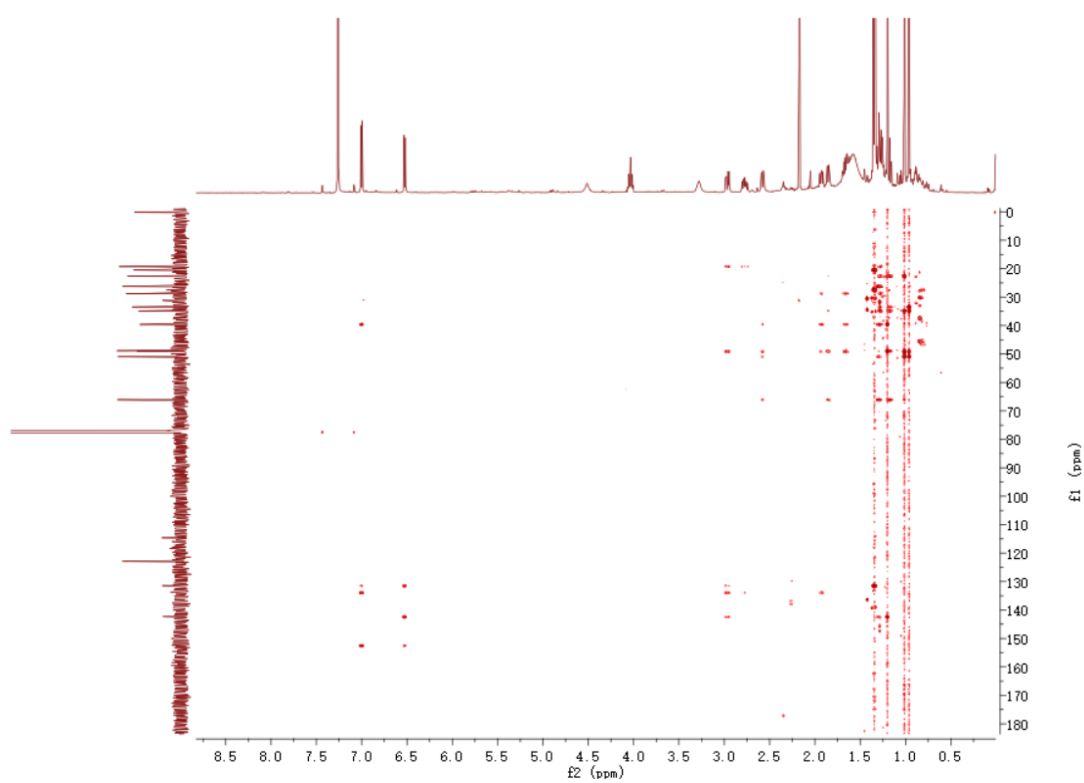


Figure S5: HMBC spectrum of **10**

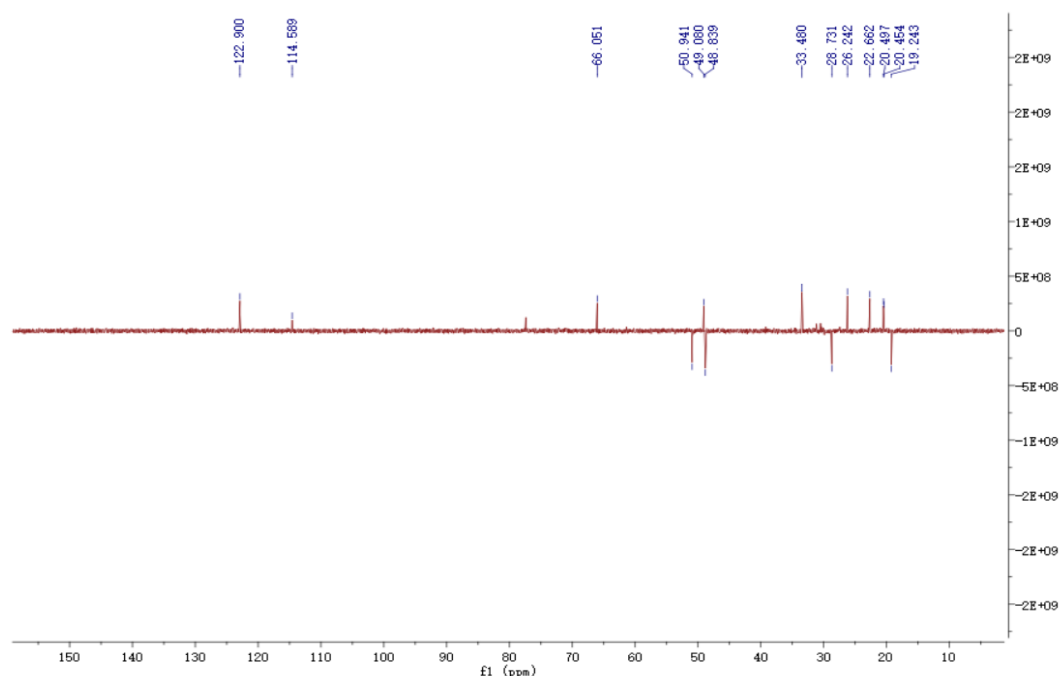


Figure S6: DEPT spectrum of **10**

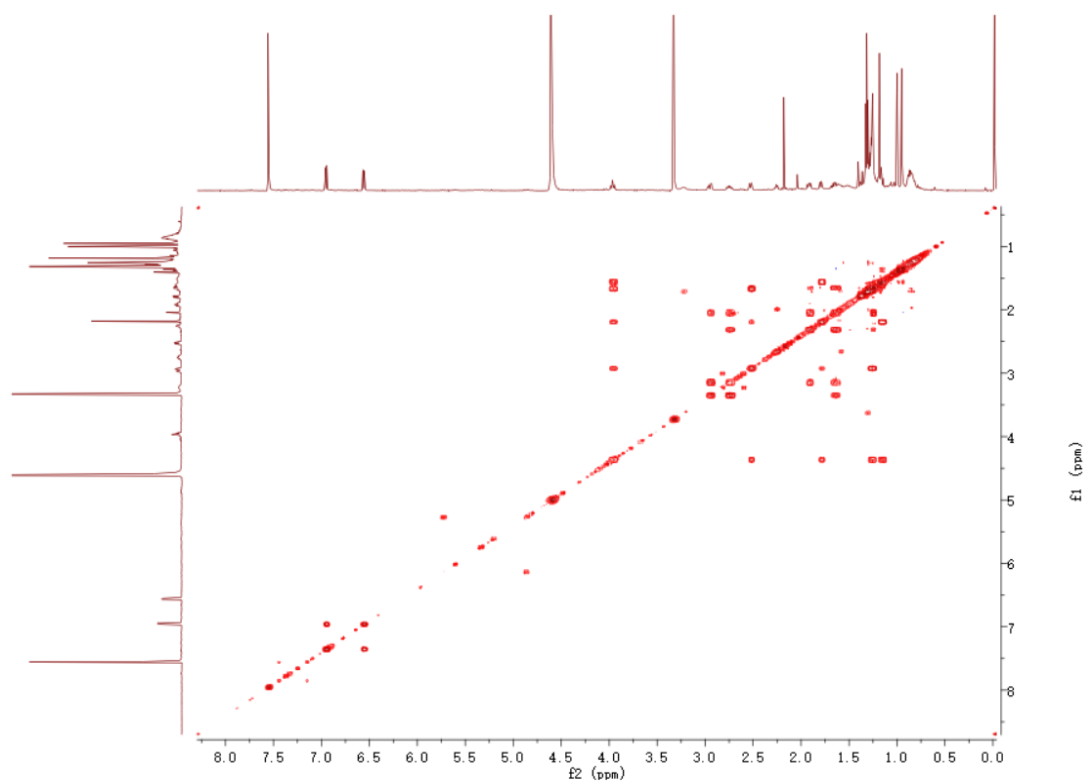


Figure S7: ^1H - ^1H COSY spectrum of **10**

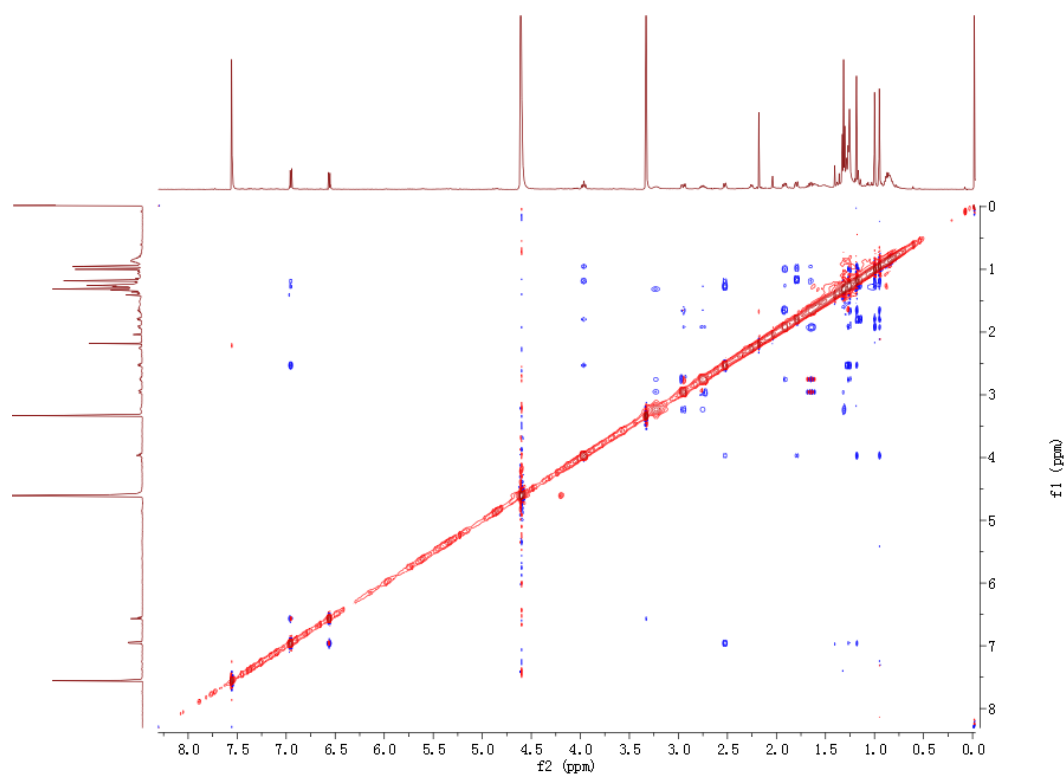


Figure S8: NOESY spectrum of **10**

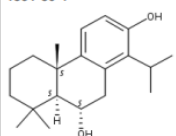
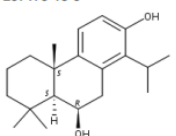
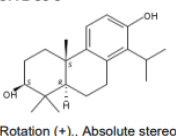
SciFinder®			Page 1
<p>Score: 97</p> <p>1.</p> <p>1891-80-1</p>  <p>Absolute stereochemistry.</p> <p>C₂₀H₃₀O₂ 2,9-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS,8aS,9S)-</p> <p>Key Physical Properties: Molecular Weight 302.45 Melting Point (Experimental) Value: 186-187 °C Boiling Point (Predicted) Value: 407.5±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.054±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 10.80±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 3 References ~ 4 Commercial Sources Regulatory Information Experimental Properties</p>	<p>Score: 97</p> <p>2.</p> <p>297179-13-6</p>  <p>Absolute stereochemistry.</p> <p>C₂₀H₃₀O₂ 2,9-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8,8-trimethyl-1-(1-methylethyl)-, (4bS,8aS,9R)-</p> <p>Key Physical Properties: Molecular Weight 302.45 Boiling Point (Predicted) Value: 407.5±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.054±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 10.80±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References ~ 2 Commercial Sources Regulatory Information</p>	<p>Score: 96</p> <p>3.</p> <p>3772-56-3</p>  <p>Rotation (+), Absolute stereochemistry.</p> <p>C₂₀H₃₀O₂ 2,7-Phenanthrenediol, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-8-(1-methylethyl)-, (2S,4aS,10aR)-</p> <p>Key Physical Properties: Molecular Weight 302.45 Melting Point (Experimental) Value: 180.5-181.5 °C Boiling Point (Predicted) Value: 407.5±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.054±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 10.86±0.70 Condition: Most Acidic Temp: 25 °C Related Info: ~ 25 References Reactions ~ 21 Commercial Sources Spectra Experimental Properties</p>	

Figure S9: Scifinder search results of **10**