Supporting Information

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Eupatorione A, an Unusual Sesquiterpenoid from the Aerial Parts of *Eupatorium adenophorum*

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Figure S1: ¹H NMR spectrum of compound 1 in CD₃COCD₃ (600 MHz)
**Figure S2:** Enlarge $^1$H NMR spectrum of compound 1 in CD$_3$COCD$_3$ (600 MHz)

**Figure S3:** $^{13}$C NMR spectrum of compound 1 in CD$_3$COCD$_3$ (150 MHz)
Figure S4: HSQC spectrum of compound 1 in CD$_3$COCD$_3$ (600 MHz)

Figure S5: HMBC spectrum of compound 1 in CD$_3$COCD$_3$ (600 MHz)
Figure S6: $^1$H-$^1$H COSY spectrum of compound 1 in CD$_3$COCD$_3$ (600 MHz)

Figure S7: ROESY spectrum of compound 1 in CD$_3$COCD$_3$ (600 MHz)
Figure S8: MS spectrum of compound 1

Figure S9: HRESIMS spectrum of compound 1

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Figure S10: IR spectrum of compound 1
Scan Analysis Report

Report Time : Sun 07 May 09:44:16 AM 2023
Method:
Beam: Dh\gy\ly\ga-3-3.DDN
Software version: 4.10 (470)
Operator:

Sample Name: ga-3-3
Collection Time: 5/7/2023 9:46:16 AM

Peak Table
Peak Style: Peaks
Peak Threshold: 0.0100
Range: 400.000m to 200.000m

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<tr>
<th>Wavelength (nm)</th>
<th>Abs</th>
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<td>201.200</td>
<td>0.355</td>
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**Figure S11**: UV spectrum of compound 1
Figure S12: The Scifinder similarity report for 1
Table S1: Crystal data for 1

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<tr>
<th>Identification code</th>
<th>cu_2023603_0m</th>
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<tr>
<td>Empirical formula</td>
<td>C_{15}H_{20}O_{3}</td>
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<tr>
<td>Formula weight</td>
<td>248.31</td>
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<tr>
<td>Temperature/K</td>
<td>100</td>
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<tr>
<td>Crystal system</td>
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<tr>
<td>Space group</td>
<td>P2\textsubscript{1}</td>
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<tr>
<td>a/Å</td>
<td>7.0436(5)</td>
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<tr>
<td>b/Å</td>
<td>7.0873(5)</td>
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<td>c/Å</td>
<td>13.7049(10)</td>
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<tr>
<td>α/°</td>
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<tr>
<td>β/°</td>
<td>96.271(4)</td>
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<tr>
<td>γ/°</td>
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</tr>
<tr>
<td>Volume/Å\textsuperscript{3}</td>
<td>680.06(8)</td>
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<tr>
<td>Z</td>
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<tr>
<td>(\rho_{\text{calc}})/g/cm\textsuperscript{3}</td>
<td>1.213</td>
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<tr>
<td>(\mu)/mm\textsuperscript{-1}</td>
<td>0.669</td>
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<td>F(000)</td>
<td>268.0</td>
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<tr>
<td>Crystal size/mm\textsuperscript{3}</td>
<td>0.11 × 0.03 × 0.01</td>
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<tr>
<td>Radiation</td>
<td>CuK(\alpha) ((\lambda = 1.54178))</td>
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<td>2Θ range for data collection/°</td>
<td>6.488 to 148.928</td>
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<td>Index ranges</td>
<td>-7 ≤ h ≤ 8, -8 ≤ k ≤ 8, -16 ≤ l ≤ 17</td>
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<td>Reflections collected</td>
<td>12254</td>
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<td>Independent reflections</td>
<td>2765 [R\textsubscript{int} = 0.1181, R\textsubscript{sigma} = 0.1109]</td>
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<td>Data/restraints/parameters</td>
<td>2765/1/168</td>
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<td>Goodness-of-fit on F\textsuperscript{2}</td>
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<td>Final R indexes [I≥2σ (I)]</td>
<td>R(_1) = 0.0831, wR(_2) = 0.2137</td>
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<tr>
<td>Final R indexes [all data]</td>
<td>R(_1) = 0.0874, wR(_2) = 0.2189</td>
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<tr>
<td>Largest diff. peak/hole / e Å\textsuperscript{-3}</td>
<td>0.56/-0.34</td>
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<tr>
<td>Flack parameter</td>
<td>-0.3(2)</td>
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