Supporting Information to:

Phytochemical Investigation of *Perovskia abrotanoides*

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² Ph. D. thesis (University of Freiburg) of SK constitutes a fraction of this investigation

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Physicochemical Data for Compounds 9 – 14

Cirsimaritin (9) (5,4′-dihydroxy-6,7-dimethoxyflavone): Pale yellow crystals from MeOH, C_{17}H_{14}O_{6}, m.p. 258 – 262 °C {255 – 266 °C [10]}; NMR spectral data [10].

Hesperidin (10) {7-[6-O-(6-deoxy-α-L-mannopyranosyl)-β-D-glucopyranosyl)oxy]-2,3-dihydro-5-hydroxy-2-(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one} [13]: White amorphous material, C_{28}H_{34}O_{15}, m.p. 259 – 261 °C {256 – 261 °C [11]}; [α]_{D}^{20} = −70.2° (c 1.0, pyridine) {−68.7 (c 1.0, pyridine) [12]}; NMR spectral data in pyridine-\textit{d}_{5} comparable with those in CD_{3}OD [11].

Rosmarinic acid (11) {3-(3,4-dihydroxyphenyl)-2-[3-(3,4-dihydroxyphenyl)prop-2-enoyloxy]-propionic acid}: Yellow brownish amorphous material, C_{18}H_{16}O_{8}, m.p. 170 – 174 °C {172 °C [14]}; [α]_{D}^{20}: +60.2° (c 1.0, MeOH) {+64.4 (c 1.31, MeOH) [14]}; \textit{1H}- and \textit{13C}-NMR data in CD_{3}OD are comparable with those in D_{2}O [16] and in DMSO-\textit{d}_{6} [17], respectively, under consideration of the solvent shift whereas signal correlations in CD_{3}OD [15] need to be interchanged for C-5′/5′′, C-6′/6′′, C-2′/2′′, and corrections have to be made for C-3′,4′,3′′, and 4′′ as follows: 145.9, 144.8, 146.7, and 149.3 ppm.

24-R-β-Sitosterol (12) (24-R-stigmaster-5-en-3β-ol) [19]: Colorless crystals, C_{29}H_{50}O, m.p. 134 – 138 °C {136 – 138 °C [18]}; [α]_{D}^{20}: −33.1° (c 0.10, CHCl_{3}) {−31.5 (c 0.10, CHCl_{3}) [18]}; NMR spectral data [18].

24-R-Stigmasterol (13) (24-R-stigmaster-5,22-dien-3β-ol): NMR spectral data [20], in mixture with 12 without further attempts for separation.

Stigmast-5-ene-3β,7α-diol (14): Colorless crystals, C_{29}H_{50}O_{2}, m.p. 201 – 204 °C {202 – 204 °C [21]}; [α]_{D}^{20}: −83.5° (c 0.10, CHCl_{3}) {−84.1 (c 0.10, CHCl_{3}) [21]}; NMR spectral data [22].
Table 1Sb $^1$H-NMR chemical shifts (300 MHz) and $^1$H-$^1$H-COSY- and 2D NOE correlations of 7 at 27 °C in CDCl$_3$

<table>
<thead>
<tr>
<th>Proton</th>
<th>δ (ppm)</th>
<th>$^1$H-$^1$H-COSY</th>
<th>NOE at proton</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-CH$_3$α</td>
<td>0.84</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>1-CH$_3$β</td>
<td>0.96</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2α</td>
<td>1.16</td>
<td>2β,3α3β</td>
<td>-</td>
</tr>
<tr>
<td>2β</td>
<td>1.52</td>
<td>2α,3α,3β</td>
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<tr>
<td>3α</td>
<td>1.60</td>
<td>2α2β,3β,4α,4β</td>
<td>-</td>
</tr>
<tr>
<td>3β</td>
<td>1.83</td>
<td>2α,2β,3α,4β</td>
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</tr>
<tr>
<td>4α</td>
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<td>3α,4β</td>
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<td>4β</td>
<td>2.00</td>
<td>3α,3β,4α</td>
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<tr>
<td>5α</td>
<td>2.39</td>
<td>5β</td>
<td>-</td>
</tr>
<tr>
<td>5β</td>
<td>2.73</td>
<td>5α</td>
<td>5α</td>
</tr>
<tr>
<td>6-OH,7-OH</td>
<td>5.00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>8-(CH$_3$)$_2$CH-</td>
<td>3.11</td>
<td>2 × 8-(CH$_3$)$_2$CH-</td>
<td>-</td>
</tr>
<tr>
<td>8-(CH$_3$)$_2$CH-</td>
<td>1.22</td>
<td>2 × 8-(CH$_3$)$_2$CH-</td>
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</tr>
<tr>
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<td>1.24</td>
<td>2 × 8-(CH$_3$)$_2$CH-</td>
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<tr>
<td>9</td>
<td>6.48</td>
<td>-</td>
<td>8-(CH$_3$)$_2$CH-; 10</td>
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<tr>
<td>10</td>
<td>4.80</td>
<td>11β</td>
<td>9,11α,11β</td>
</tr>
<tr>
<td>11α</td>
<td>1.89</td>
<td>11β,11αβ</td>
<td>-</td>
</tr>
<tr>
<td>11β</td>
<td>2.12</td>
<td>10,11αβ,11α</td>
<td>-</td>
</tr>
<tr>
<td>11αβ</td>
<td>1.81</td>
<td>11β</td>
<td>-</td>
</tr>
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</table>
Table 1Sb $^{13}$C NMR chemical shifts (75.4 MHz) and $^1$H-$^{13}$C-correlations of 7 at 27°C in CDCl₃

<table>
<thead>
<tr>
<th>Carbon</th>
<th>δ (ppm)</th>
<th>g-HSQCR with proton</th>
<th>g-HMBCR with proton</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>31.9</td>
<td>-</td>
<td>1-CH₃α,1-CH₃β,3β,11αβ,11β</td>
</tr>
<tr>
<td>1-CH₃α</td>
<td>26.7</td>
<td>1-CH₃α</td>
<td>1-CH₃β</td>
</tr>
<tr>
<td>1-CH₃β</td>
<td>30.6</td>
<td>1-CH₃β</td>
<td>1-CH₃α</td>
</tr>
<tr>
<td>2</td>
<td>32.3</td>
<td>2α,2β</td>
<td>1-CH₃α,1-CH₃β,4α,11αβ</td>
</tr>
<tr>
<td>3</td>
<td>16.2</td>
<td>3α,3β</td>
<td>2β</td>
</tr>
<tr>
<td>4</td>
<td>30.8</td>
<td>4α,4β</td>
<td>2β,5β</td>
</tr>
<tr>
<td>4a</td>
<td>80.0</td>
<td>-</td>
<td>3β,5α,5β,10,11α</td>
</tr>
<tr>
<td>5</td>
<td>38.8</td>
<td>5α,5β</td>
<td>4α,11αβ</td>
</tr>
<tr>
<td>5a</td>
<td>116.5</td>
<td>-</td>
<td>5α,5β,9,10</td>
</tr>
<tr>
<td>6</td>
<td>141.5</td>
<td>-</td>
<td>5α,5β</td>
</tr>
<tr>
<td>7</td>
<td>139.4</td>
<td>-</td>
<td>8-(CH₃)₂CH-9</td>
</tr>
<tr>
<td>8</td>
<td>131.9</td>
<td>-</td>
<td>8-(CH₃)₂CH-,8-(CH₃)₂CH-</td>
</tr>
<tr>
<td>8-(CH₃)₂CH-</td>
<td>27.2</td>
<td>2 × 8-(CH₃)₂CH-</td>
<td>8-(CH₃)₂CH-,9</td>
</tr>
<tr>
<td>8-(CH₃)₂CH-</td>
<td>22.6</td>
<td>2 × 8-(CH₃)₂CH-</td>
<td>8-(CH₃)₂CH-,8-(CH₃)₂CH-</td>
</tr>
<tr>
<td>8-(CH₃)₂CH-</td>
<td>22.8</td>
<td>2 × 8-(CH₃)₂CH-</td>
<td>8-(CH₃)₂CH-,8-(CH₃)₂CH-</td>
</tr>
<tr>
<td>9</td>
<td>112.8</td>
<td>9</td>
<td>8-(CH₃)₂CH-,10</td>
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<tr>
<td>9a</td>
<td>134.4</td>
<td>-</td>
<td>5α,5β,(11α),11β</td>
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<tr>
<td>10</td>
<td>76.1</td>
<td>10</td>
<td>9,11β</td>
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<tr>
<td>11</td>
<td>39.7</td>
<td>11α,11β</td>
<td>11αβ</td>
</tr>
<tr>
<td>11a</td>
<td>51.2</td>
<td>11α</td>
<td>1-CH₃α,1-CH₃β,2α,2β,5α,5β,10,11α,11β</td>
</tr>
</tbody>
</table>
Table 2Sa ¹H-NMR chemical shifts (300 MHz) and ¹H-¹H-COSY- and 2D NOE correlations of 8 at 27 °C in CDCl₃

<table>
<thead>
<tr>
<th>Proton</th>
<th>δ (ppm)</th>
<th>¹H-¹H-COSY</th>
<th>NOE at proton</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-CH₃α</td>
<td>0.85</td>
<td>-</td>
<td>5α</td>
</tr>
<tr>
<td>1-CH₃β</td>
<td>0.95</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>2α</td>
<td>1.13</td>
<td>2β,3α,3β</td>
<td>-</td>
</tr>
<tr>
<td>2β</td>
<td>1.47</td>
<td>2α,3α,3β</td>
<td>-</td>
</tr>
<tr>
<td>3α</td>
<td>1.54</td>
<td>2α,2β,3β</td>
<td>-</td>
</tr>
<tr>
<td>3β</td>
<td>1.72</td>
<td>2β,3α,4β</td>
<td>-</td>
</tr>
<tr>
<td>4α</td>
<td>1.72</td>
<td>3α,4β</td>
<td>-</td>
</tr>
<tr>
<td>4β</td>
<td>1.95</td>
<td>3α,3β,4α</td>
<td>-</td>
</tr>
<tr>
<td>5α</td>
<td>2.16</td>
<td>5β</td>
<td>-</td>
</tr>
<tr>
<td>5β</td>
<td>2.52</td>
<td>5α</td>
<td>5α</td>
</tr>
<tr>
<td>7-OH</td>
<td>6.57</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>8-(CH₃)₂CH-</td>
<td>2.73</td>
<td>8-(CH₃)₂CH-</td>
<td>-</td>
</tr>
<tr>
<td>8-(CH₃)₂CH-</td>
<td>1.32</td>
<td>8-(CH₃)₂CH-</td>
<td>-</td>
</tr>
<tr>
<td>8-(CH₃)₂CH-</td>
<td>1.25</td>
<td>8-(CH₃)₂CH-</td>
<td>-</td>
</tr>
<tr>
<td>9-OCH₃α</td>
<td>3.13</td>
<td>-</td>
<td>8-(CH₃)₂CH-, 10</td>
</tr>
<tr>
<td>9-OCH₃β</td>
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<td>-</td>
<td>8-(CH₃)₂CH-, 10</td>
</tr>
<tr>
<td>10</td>
<td>4.75</td>
<td>11β</td>
<td>-</td>
</tr>
<tr>
<td>11α</td>
<td>1.97</td>
<td>11αβ,11β</td>
<td>-</td>
</tr>
<tr>
<td>11β</td>
<td>2.00</td>
<td>10,11α</td>
<td>-</td>
</tr>
<tr>
<td>11αβ</td>
<td>1.69</td>
<td>11α,11β</td>
<td>-</td>
</tr>
</tbody>
</table>
Table 2Sb $^{13}$C-NMR chemical shifts (75.4 MHz) and $^1H^{13}$-C-correlations of 8 at 27 °C in CDCl$_3$

<table>
<thead>
<tr>
<th>Carbon</th>
<th>$\delta$ (ppm)</th>
<th>g-HSQCR with proton</th>
<th>g-HMBCR with proton</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>32.1</td>
<td>-</td>
<td>11β, 1-CH$_3$α, 1-CH$_3$β</td>
</tr>
<tr>
<td>1-CH$_3$α</td>
<td>26.2</td>
<td>1-CH$_3$α</td>
<td>1-CH$_3$β</td>
</tr>
<tr>
<td>1-CH$_3$β</td>
<td>30.7</td>
<td>1-CH$_3$β</td>
<td>1-CH$_3$α, 2α, 2β, 11αβ</td>
</tr>
<tr>
<td>2</td>
<td>32.8</td>
<td>2α, 2β</td>
<td>1-CH$_3$α, 1-CH$_3$β</td>
</tr>
<tr>
<td>3</td>
<td>16.3</td>
<td>3α, 3β</td>
<td>2α, 4β</td>
</tr>
<tr>
<td>4</td>
<td>30.8</td>
<td>4α, 4β</td>
<td>2α, 2β, 5β, 11αβ</td>
</tr>
<tr>
<td>4a</td>
<td>80.3</td>
<td>-</td>
<td>5β, 10α</td>
</tr>
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<td>5</td>
<td>38.3</td>
<td>5α, 5β</td>
<td>11αβ</td>
</tr>
<tr>
<td>5a</td>
<td>131.3</td>
<td>-</td>
<td>5α, 5β, 10</td>
</tr>
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<td>6</td>
<td>181.3</td>
<td>-</td>
<td>(5β)</td>
</tr>
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<td>7</td>
<td>146.2</td>
<td>-</td>
<td>8-(CH$_3$)$_2$CH-</td>
</tr>
<tr>
<td>8</td>
<td>129.4</td>
<td>-</td>
<td>8-(CH$_3$)$_2$CH-, 8-(CH$_3$)$_2$CH-(2×)</td>
</tr>
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<td>8-(CH$_3$)$_2$CH-</td>
<td>8-(CH$_3$)$_2$CH-</td>
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<tr>
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<td>8-(CH$_3$)$_2$CH-, 8-(CH$_3$)$_2$CH-</td>
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<td>9-OCH$_3$α, 9-OCH$_3$β, 8-(CH$_3$)$_2$CH-</td>
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<td>9-OCH$_3$α</td>
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<td>9-OCH$_3$β</td>
<td>51.9</td>
<td>9-OCH$_3$β</td>
<td>-</td>
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<td>9a</td>
<td>159.3</td>
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<td>5α, 5β, 11β</td>
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<td>11β</td>
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<td>37.0</td>
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<td>1-CH$_3$β</td>
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<tr>
<td>11°</td>
<td>52.3</td>
<td>11αβ</td>
<td>2α, 2β, 5α, 5β, 10, 1-CH$_3$α, 1-CH$_3$β</td>
</tr>
</tbody>
</table>
Table 3Sa \(^1\)H-NMR chemical shifts (500 MHz) and \(^1\)H-\(^1\)H-COSY-, NOESY and TOCSY correlations of 15 at 27°C in CD\(_3\)OD

<table>
<thead>
<tr>
<th>Proton</th>
<th>&amp; (ppm)</th>
<th>(^1)H-(^1)H-COSY with proton</th>
<th>NOESY</th>
<th>TOCSY with proton</th>
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</thead>
<tbody>
<tr>
<td>1(\beta),eq</td>
<td>1.64</td>
<td>1(\alpha),2a,2b</td>
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<td>3;++</td>
</tr>
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<td>1(\beta),2a,2b</td>
<td>3(\alpha),5(\alpha)</td>
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<tr>
<td>2a</td>
<td>1.62</td>
<td>1(\alpha),1(\beta),2b,3</td>
<td>-</td>
<td>3;++</td>
</tr>
<tr>
<td>2b</td>
<td>1.58</td>
<td>1(\alpha),1(\beta),2a,3</td>
<td>24(\beta),25(\beta)</td>
<td>3;++</td>
</tr>
<tr>
<td>3(\alpha),ax</td>
<td>3.20</td>
<td>2a,2b</td>
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<td>5,6(\beta),7(\alpha),7(\beta)</td>
<td>5(\alpha)</td>
<td>5;++</td>
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<td>1.40</td>
<td>5,6(\alpha),7(\alpha),7(\beta)</td>
<td>24(\beta),26(\beta)</td>
<td>5;++</td>
</tr>
<tr>
<td>7(\alpha),ax</td>
<td>1.54</td>
<td>6(\alpha),6(\beta),7(\beta)</td>
<td>5(\alpha),27(\alpha)</td>
<td>5;++</td>
</tr>
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<td>7(\beta),eq</td>
<td>1.35</td>
<td>6(\alpha),6(\beta),7(\beta)</td>
<td>26(\beta)</td>
<td>5;++</td>
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<td>9(\alpha),ax</td>
<td>1.54</td>
<td>11ab,26</td>
<td>5(\alpha),11ab,27(\alpha)</td>
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<td>9,12</td>
</tr>
<tr>
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<td>15(\beta),ax</td>
<td>1.93</td>
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<td>15(\beta),16(\alpha)</td>
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<td>16(\beta),eq</td>
<td>1.62</td>
<td>15(\alpha),15(\beta),16(\alpha),18(\beta)</td>
<td>15(\beta),16(\alpha)</td>
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<td>16(\beta),19(\alpha)</td>
<td>12,20(\beta),29(\beta)</td>
<td>16,19,29,20,21,21,22</td>
</tr>
<tr>
<td>19(\alpha),ax</td>
<td>1.36</td>
<td>18(\beta),20(\beta),29</td>
<td>27(\alpha),29(\beta)</td>
<td>18,20,29</td>
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<td>19(\alpha),21(\alpha),21(\beta),30</td>
<td>18(\beta)</td>
<td>19,18,29,21,21,22,22</td>
</tr>
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<td>21(\beta),eq</td>
<td>1.48</td>
<td>20(\beta),21(\alpha),22(\alpha),22(\beta)</td>
<td>-</td>
<td>++</td>
</tr>
<tr>
<td>21(\alpha),ax</td>
<td>1.34</td>
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<td>16(\alpha)</td>
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</tr>
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<td>21(\alpha),21(\beta),22(\alpha)</td>
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<td>24(\beta)</td>
<td>24(\beta)</td>
</tr>
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<td>23(\alpha)</td>
<td>2(\beta),6(\beta),23(\alpha),25(\beta)</td>
<td>23(\alpha)</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2,6β,11ab,24β,26β</td>
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<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>------------------</td>
<td>-----</td>
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++ Unresolved.
Table 3Sb $^{13}$C-NMR chemical shifts (125.725 MHz) and $^1$H-$^{13}$C-correlations of 15 at 27 °C in CD$_3$OD

<table>
<thead>
<tr>
<th>Carbon</th>
<th>$\delta$ (ppm)</th>
<th>HSQC with proton</th>
<th>HMBC with proton</th>
<th>HMBC with carbon</th>
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<tbody>
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<td>1,23,24</td>
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<tr>
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<td>13,14,16,27</td>
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<td>3,4,5,23</td>
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<td>1,5,9,10</td>
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<td>7,8,9,14</td>
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<tr>
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<td>24.1</td>
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<td>15$\beta$</td>
<td>8,13,14,15</td>
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<td>181.8</td>
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<td>16,16,18</td>
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<td>29</td>
<td>18,19,20</td>
<td>18,19,20</td>
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<td>-</td>
<td>19,20</td>
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Table 4Sa ¹H-NMR chemical shifts (400 MHz) and ¹H-¹H-COSY-NOESY-, and TOCSY correlations of 16 at 27 °C in CDCl₃

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<tr>
<th>Proton</th>
<th>δ (ppm)</th>
<th>¹H-¹H-COSY with proton</th>
<th>NOESY with proton</th>
<th>TOCSY with proton</th>
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</thead>
<tbody>
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<td>1β, eq</td>
<td>1.71</td>
<td>1α,2a,2b</td>
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</tr>
<tr>
<td>1α, ax</td>
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<td>1β,3α,9α</td>
<td>1β,2,2,3</td>
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<tr>
<td>2α</td>
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</tr>
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<td>2β</td>
<td>1.57</td>
<td>1α,1β,2a,3α</td>
<td>24β,25β</td>
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</tr>
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<td>3α, ax</td>
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<td>2a,2b</td>
<td>1α,2a,5α,23α</td>
<td>2a,2b,1α,1β</td>
</tr>
<tr>
<td>5α, ax</td>
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<td>6α,6β</td>
<td>3α,7α,9α,23α</td>
<td>6,6,7,7</td>
</tr>
<tr>
<td>6α, eq</td>
<td>1.53</td>
<td>5α,6β,(7α,7β)</td>
<td>6β,23α</td>
<td>++; see 5α</td>
</tr>
<tr>
<td>6β, ax</td>
<td>1.41</td>
<td>5α,6α,(7α,7β)</td>
<td>6α,24β,25β,26β</td>
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</tr>
<tr>
<td>7α, ax</td>
<td>1.41</td>
<td>6α,6β,7β,26(w)</td>
<td>5α,9α,27α</td>
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</tr>
<tr>
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<td>1.39</td>
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<td>26β</td>
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</tr>
<tr>
<td>9α, ax</td>
<td>1.29</td>
<td>11α</td>
<td>1α,5α,12α,27α</td>
<td>++; see 13β,19β,21β,22β</td>
</tr>
<tr>
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<td>9α,11β,12α</td>
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<tr>
<td>11β, ax</td>
<td>1.29</td>
<td>11α,12α,12β</td>
<td>25β,26β</td>
<td>++; see &quot;9α&quot;</td>
</tr>
<tr>
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<td>11αβ,12α,13β</td>
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<tr>
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<tr>
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<td>12α,12β,18α,27(w)</td>
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</tr>
<tr>
<td>15β, ax</td>
<td>1.56</td>
<td>15α,16α,16β,27(w)</td>
<td>15α,16β,26β</td>
<td>++; see 16β</td>
</tr>
<tr>
<td>15α, eq</td>
<td>1.21</td>
<td>15β,16α,16β</td>
<td>7α,7β,15β,16β</td>
<td>++; see 16β</td>
</tr>
<tr>
<td>16β, eq</td>
<td>2.29</td>
<td>15α,15β,16α</td>
<td>15α,15β,16α,22β</td>
<td>15α,15β,16α</td>
</tr>
<tr>
<td>16α, ax</td>
<td>1.42</td>
<td>15α,15β,16β</td>
<td>15α,16β,27α</td>
<td>++; see 16β</td>
</tr>
<tr>
<td>18α, ax</td>
<td>1.64</td>
<td>13β,19β</td>
<td>27α,29α</td>
<td>++; see 13β,19β,21β,22β</td>
</tr>
<tr>
<td>19β, ax*</td>
<td>3.02</td>
<td>18α,21α,21β</td>
<td>21β,29α,30</td>
<td>18,13,12,11*,9*,21,22</td>
</tr>
<tr>
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<td>19β,21α,22α</td>
<td>19,18,13,12,11,9;21α,22,30,29</td>
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<td>21α, eq*</td>
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<td>21β,22β</td>
<td>++; see 21β/22β</td>
</tr>
<tr>
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<td>21β,22β</td>
<td>++; see 21β/22β</td>
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<tr>
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<td>1.99</td>
<td>21α,21β,22α</td>
<td>21α,22α</td>
<td>see 21β</td>
</tr>
<tr>
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<td>0.99</td>
<td>24β</td>
<td>3α,5α,6α,24β</td>
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</tr>
<tr>
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<td>2β,6β,23α,25β</td>
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<tr>
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</tr>
<tr>
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<td>7α(w)</td>
<td>6β,11β,13β,15β,25β</td>
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</tr>
<tr>
<td>27α,ax</td>
<td>1.00</td>
<td>13β(w),15β(w)</td>
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<tr>
<td>29exoα</td>
<td>4.77</td>
<td>29β,30</td>
<td>18α,19α,29β</td>
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<td>1.71</td>
<td>29α,29β</td>
<td>19α,29β</td>
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</tbody>
</table>

++ unresolved; * mixing time ≥ 0.08 s; (w): LR-w-coupling; °ROESY; ●: pseudo.
Table 4Sb $^{13}$C-NMR chemical shifts (100 MHz) and $^1$H-$^{13}$C-correlations of 16 at 27 °C in CDCl$_3$

<table>
<thead>
<tr>
<th>Carbon</th>
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<th>HSQC with proton</th>
<th>HMBC with proton</th>
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</thead>
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<td>2$a$,23,24</td>
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<td>55.3</td>
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<td>1$\beta$,23,24,25</td>
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<td>15$\beta$,26,27</td>
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</tr>
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</table>

⁺ Just wrong numbering in [30].

* Assignment to be interchanged in [30] on grounds of HMBC.

° Assignment to be interchanged in [30] on grounds of HMBC.