Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Golden opportunities in natural product synthesis: first total synthesis of (–)-isocyclocapitelline and (–)-isochrysotricine by gold-catalyzed allene cycloisomerization

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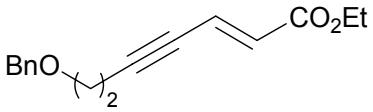
Supporting Information

General remarks: NMR spectra were recorded with a Bruker DRX 400 or DRX 500 spectrometer in $CDCl_3$ as solvent and internal standard (δ = 7.27 for ^1H, δ = 77.0 for ^{13}C). Carbon atoms were assigned with DEPT experiments [symbols used: (+) for CH_3,CH;(–) for CH_2; (×) for $C_{quart.}$]. Peaks for the major isomer of a mixture are marked with an asterisk (*).

Ethyl (*E*)-7-Benzyloxyhept-2-en-4-ynoate (**7**)



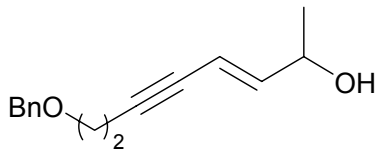
δH (500 MHz, $CDCl_3$): 7.38–7.29 (m, 5 H, ArH), 6.76 (dt, J = 15.9 Hz, J = 2.2 Hz, 1 H, C<u>H</u>=CHC=O), 6.18 (d, J = 15.9 Hz, 1 H, CH=C<u>H</u>C=O), 4.57 (s, 2 H, CH_2Ph), 4.22 (q, J = 7.1 Hz, 2 H, $C\underline{H}_2CH_3$), 3.63 (t, J = 6.9 Hz, 2 H, OCH_2), 2.70 (dt, J = 6.9 Hz, J = 1.9 Hz, 2 H, $OCH_2C\underline{H}_2$), 1.30 (t, J = 7.1 Hz, 3 H, $C\underline{H}_2CH_3$).

δC (125 MHz, $CDCl_3$): 166.0 (x, C=O), 137.9 (x, quaternary ArC), 129.8 (+, <u>C</u>H=CHC=O), 128.4 (+, 2 x *m*–ArC), 127.9 (+, 1 x *p*–ArC), 127.6 (+, 2 x *o*–ArC), 125.6 (+, CH=<u>C</u>H-C=O), 97.0 (x, $CH_2\underline{C}{\equiv}C$), 78.7 (x, $CH_2C{\equiv}\underline{C}$), 73.0 (–, CH_2Ph), 67.8 (–, OCH_2), 60.6 (–, $\underline{C}H_2CH_3$), 21.2 (–,$OCH_2\underline{C}H_2$),14.2 (+, $CH_2\underline{C}H_3$).

FAB–MS: m/z (%) = 259 (50, $[M+H]^+$), 257 (7), 92 (100), 78 (18), 66 (8), 42 (7).

FAB–HRMS: $C_{16}H_{18}O_3$ (258.1256), calcd.: 258.1256 ($[M]^+$), found: 258.1252.

(*E*)-8-Benzyloxyoct-3-en-5-yn-2-ol (**8**)



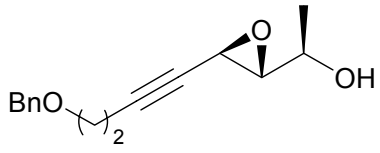
δH (500 MHz, $CDCl_3$): 7.36–7.29 (m, 5 H,ArH), 6.11 (dd, J = 15.9 Hz, J = 6.0 Hz, 1 H, CH=C<u>H</u>C-OH), 5.68 (dd, J = 15.9 Hz, J = 1.5 Hz, 1 H, C<u>H</u>=CHC-OH), 4.57 (s, 2 H, $PhCH_2$), 4.33 (m, 1 H, C<u>H</u>OH), 3.61 (t, J = 7.0 Hz, 2 H, OCH_2), 2.63 (dt, J = 7.0 Hz, J = 2.0 Hz, 2 H, $OCH_2C\underline{H_2}$ 7–H), 1.79 (s, 1 H, OH), 1.29 (d, J = 6.5 Hz, 3 H, CH_3).

δC (125 MHz, $CDCl_3$): 145.7 (+, CHOH), 138.0 (x, quaternary ArC), 128.4 (+, 2 x *m*–ArC), 127.6 (+,2 x *o*–ArC), 127.6 (+,1 x *p*–ArC), 109.4 (+, <u>C</u>H=CHC-OH), 87.5 (x, $CH_2\underline{C}{\equiv}C$), 79.3 (x, $CH_2C{\equiv}\underline{C}$), 72.9 (–, $PhCH_2$), 68.3 (–, $O\underline{C}H_2CH_2$), 68.2 (+, CHOH), 23.0 (+, CH_3), 20.8 (–, $OCH_2\underline{C}H_2$).

FAB–MS: m/z (%) = 229 (10, $[M–H]^+$), 213 (22), 199 (5), 183 (9), 169 (13), 165 (5), 92 (100), 44 (15), 41 (4).

FAB–HRMS: $C_{15}H_{18}O_2$ (230.1307), calcd.: 229.1229 ($[M–H]^+$), found: 215.1243.

(*R*,*R*,*R*)-1-[(4-Benzyloxybut-1-ynyl)oxiran-2-yl]ethanol (**9**)



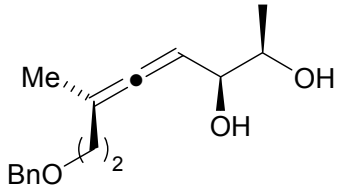
δH (400 MHz, $CDCl_3$) = 7.36–7.29 (m, 5 H, ArH), 4.55 (s, 2 H, $PhCH_2$), 3.96 (dq, J = 6.5 Hz, J = 3.0 Hz, 1 H, C<u>H</u>OH), 3.58 (t, J = 7.0 Hz, 2 H, $OC\underline{H_2}CH_2$), 3.43 (d, J = 1.5 Hz, 1 H, C<u>H</u>(O)CHCHOH), 3.14 (t, J = 2.5 Hz, 1 H, CH(O)C<u>H</u>CHOH), 2.53 (dt, J = 6.5 Hz, J = 1.5 Hz, 2H, $OCH_2C\underline{H_2}$), 2.18 (s, 1H, OH), 1.27 (d, J = 6.5 Hz, 3 H, CH_3).

δC (100 MHz, $CDCl_3$) = 137.8 (x, quaternary ArC), 128.3 (+, 2 x *m*–ArC), 127.7 (+, 1 x *p*–ArC), 127.6 (+, 2 x *o*–ArC), 81.9 (x, $CH_2C{\equiv}\underline{C}$), 77.2 (x, $CH_2\underline{C}{\equiv}C$), 72.9 (–, $PhCH_2$), 67.8 (–, $O\underline{C}H_2CH_2$), 64.0 (+, CH(O)<u>C</u>HCHOH), 63.0 (+, CHOH), 42.1 (+, <u>C</u>H(O)CHCHOH), 20.1 (–, OCH2<u>C</u>H2)), 18.4 (+, CH_3).

FAB–MS: m/z (%) = 245 (3, $[M–H]^+$), 244 (2), 203 (6), 92 (40), 58 (8), 44 (5), 28 (2).

FAB–HRMS: $C_{15}H_{18}O_3$ (246.1256), calcd.: 245.1178 ($[M–H]^+$), found: 245.1141.

(2*R*,3*S*,5*S*)-8-Benzyloxy-6-methylocta-4,5-diene-2,3-diol (**10**)



δH (400 MHz, $CDCl_3$): 7.36–7.28 (m, 5 H, ArH), 5.20 (m, 1 H, C=C=C<u>H</u>), 4.51 (dd, J = 12.0 Hz, 2 H, $PhCH_2$), 4.01 (m, 1 H, C<u>H</u>(OH)CHMe(OH)), 3.77 (m, 1 H, CH(OH)C<u>H</u>Me(OH)), 3.58 (m, 2 H, $OC\underline{H_2}CH_2$), 2.90 (s, 2 H, OH), 2.32/2.22 (m, 2H, $OCH_2C\underline{H_2}$), 1.72 (d, J = 2.8 Hz, 3 H, $C\underline{H_3}C{=}C{=}C$), 1.24 (d, J = 6.3 Hz, 3 H, CH(OH)C<u>H</u>$_3$).

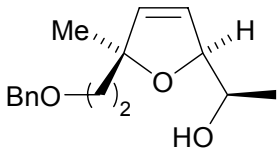
δC (100 MHz, $CDCl_3$): 200.8 (x, C=<u>C</u>=C), 137.7 (x, quaternary ArC), 128.3 (+, 2 x *m*–ArC), 127.8 (+, 2 x *o*–ArC), 127.6 (+, 1 x *p*–ArC), 99.9 (x, <u>C</u>=C=CH), 90.7 (+, C=C=<u>C</u>H), 73.0 (+, <u>C</u>H(OH)CHMe(OH)), 72.7 (–, $PhCH_2$), 70.3 (+, CH(OH)<u>C</u>HMe

(OH), 67.3 (–, O<u>C</u>H_2CH_2), 33.9 (–, OCH$_2$<u>C</u>H$_2$), 18.7 (+,<u>C</u>H_3C=C=C CH), 17.5 (+, <u>C</u>H_3CHOH).

FAB–MS: m/z (%) = 263 (6, $[M+H]^+$), 245 (11, $[M–OH]^+$), 227 (9), 217 (6), 215 (1), 201 (30), 92 (100), 78 (27), 44 (24).

FAB–HRMS: $C_{16}H_{22}O_3$ (262.1569), calcd.: 263.1647 ($[M+H]^+$), found: 263.1652.

(*R*)-1-[(*S*,*S*)-5-(2-Benzyloxyethyl)-2,5-dihydro-5-methylfuran-2-yl]ethanol (**11**)



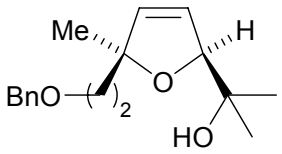
δH (400 MHz, $CDCl_3$ppm): 7.34–7.28 (m, ArH), 5.89 (dd, J = 6.0 Hz, J = 2.1 Hz, 1 H, CH=C<u>H</u>-CH), 5.82 (d, J = 6.0 Hz, 1 H, C<u>H</u>=CH-CH), 4.70 (s, 1 H, CH=CH-C<u>H</u>), 4.51 (dd, J = 12.2 Hz, 2 H, PhCH$_2$), 3.88 (m, 1 H, C<u>H</u>OH), 3.64/3.54 (m, 2 H, OC<u>H</u>$_2$CH$_2$), 2.09/1.85 (m, 2H, OCH$_2$C<u>H</u>$_2$), 1.29 (s, 3 H, furane-CH$_3$), 1.20 (d, J = 6.5 Hz, 3 H, C<u>H</u>$_3$CHOH).

δC (100 MHz, $CDCl_3$): 137.9 (x, quaternary ArC), 136.3 (+, <u>C</u>H=CH-CH), 128.3 (+, 2 x *m*–ArC), 127.8 (+, 2 x *o*–ArC), 127.6 (+, 1 x *p*–ArC), 89.1 (x, quaternary furane-C), 89.0 (+, CH=CH-<u>C</u>H), 72.7 (–, PhCH$_2$), 68.0 (+, <u>C</u>HOH), 66.4 (–, O<u>C</u>H_2CH_2), 39.8 (–, OCH$_2$<u>C</u>H$_2$), 26.6 (+, furane-CH$_3$), 18.1 (+, <u>C</u>H_3CHOH).

FAB–MS: m/z (%) = 263 (55, $[M+H]^+$), 261 (11, $[M–H]^+$), 92 (100), 84 (15), 56 (10).

FAB–HRMS: $C_{16}H_{22}O_3$ (262.1569), calcd.: 263.1647 ($[M+H]^+$),found: 263.1677.

2-[(*S*,*S*)-5-(2-Benzyloxyethyl)-2,5-dihydro-5-methylfuran-2-yl]propan-2-ol (**12**)



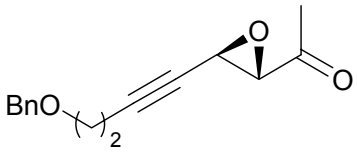
δH (400 MHz, $CDCl_3$): 7.35–7.28 (m, 5 H, ArH), 5.90 (dd, J = 6.0 Hz, J = 2.3 Hz, 1 H, CH=C<u>H</u>-CH), 5.76 (d, J = 6.0 Hz, 1 H, C<u>H</u>=CH-CH), 4.60 (s, 1 H, CH=CH-C<u>H</u>), 4.51 (dd, J = 12.0 Hz, 2 H, $PhCH_2$), 3.62 (m, 2 H, $OC\underline{H}_2CH_2$), 3.00 (s, 1 H, OH), 2.07/1.89 (m, 2H, $OCH_2C\underline{H}_2$), 1.29 (s, 3 H, furane-CH_3), 1.21 (s, 3 H, $(C\underline{H}_3)_2COH$), 1.17 (s, 3 H, $(C\underline{H}_3)_2COH$).

δC (100 MHz, $CDCl_3$): 138.0 (x, quaternary ArC), 136.4 (+, <u>C</u>H=CH-CH), 128.3 (+, 2 x *m*–ArC), 127.7 (+, 2 x *o*–ArC), 127.5 (+, 1 x *p*–ArC), 125.6 (+, CH=<u>C</u>H-CH), 91.6 (+, CH=CH-<u>C</u>H), 89.0 (x, quaternary furane C), 72.7 (–, $PhCH_2$), 71.0 (x, $\underline{C}(CH_3)_2$), 66.5 (–, $O\underline{C}H_2CH_2$), 40.0 (–, $OCH_2\underline{C}H_2$), 26.8 (+, furane-CH_3), 26.2 (+, $(\underline{C}H_3)_2COH$), 25.0 (+, $(\underline{C}H_3)_2COH$).

FAB–MS: m/z (%) = 277 (30, $[M+H]^+$), 259 (11), 92 (73), 60 (13), 40 (7).

FAB–HRMS: $C_{17}H_{24}O_3$ (276.1725), calcd.: 277.1804 ($[M+H]^+$), found: 277.1762.

1-[(2*S*,3*R*)-3-(4-Benzyloxybut-1-ynyl)oxiran-2-yl]ethanone (**13**)



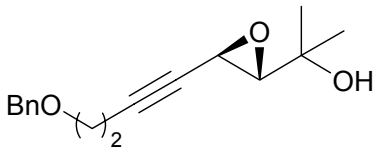
δH (400 MHz, $CDCl_3$): 7.38–7.29 (m, 5 H, ArH), 4.55 (s, 2H, $PhCH_2$), 3.58 (t, J = 6.9 Hz, 2H, OCH_2CH_2), 3.55 (d, J = 1.5 Hz, 1 H, CH(O)CHC=O), 3.49 (d, J = 1.5 Hz, 1 H, CH(O)CHC=O), 2.54 (t, J = 6.8 Hz, 2 H, OCH_2CH_2), 2.09 (s, 3 H, CH_3).

δC (100 MHz, $CDCl_3$): 203.0 (x, C=O), 137.8 (x, quaternary ArC), 128.4 (+, 2 x *m*–ArC), 127.7 (+,1 x *p*–ArC), 127.6 (+, 2 x *o*–ArC), 83.1 (x, $CH_2C{\equiv}C$), 75.6 (x, $CH_2C{\equiv}C$), 72.9 (–, $PhCH_2$), 67.6 (–, OCH_2CH_2), 60.3 (+, CH(O)CHC=O), 45.0 (+, CH(O)CHC=O), 24.8 (+, CH_3), 20.1 (–, OCH_2CH_2).

FAB–MS: m/z (%) = 243 (4, $[M–H]^+$), 242 (2), 226 (1), 225 (1), 222 (1), 92 (30), 52 (8), 44 (11).

FAB–HRMS: $C_{15}H_{16}O_3$ (244.1099), calcd.: 244.1099 ($[M]^+$), found: 244.1075

2-((2*S*,3*R*)-3-(4-Benzyloxybut-1-ynyl)oxiran-2-yl)propan-2-ol (**14**)



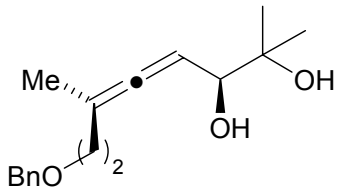
δH (400 MHz, $CDCl_3$): 7.36–7.29 (m, 5 H, ArH), 4.55 (s, 2H, $PhCH_2$), 3.59 (t, J = 7.0 Hz, 2H, OCH_2CH_2), 3.43 (d, J = 1.5 Hz, 1 H, CH(O)CHCOH), 3.07 (d, J = 2.3 Hz, 1 H, CH(O)CHCOH), 2.54 (dt, J = 7.0 Hz, J = 1.0 Hz, 2 H, OCH_2CH_2)), 1.77 (s, 1 H, OH), 1.31 (s, 3 H, CH_3), 1.26 (s, 3 H, CH_3).

δC (100 MHz, $CDCl_3$): 137.9 (x, quaternary ArC), 128.4 (+, 2 x *m*–ArC), 127.7 (+, 1 x *p*–ArC), 127.6 (+, 2 x *o*–ArC), 81.9 (x, $CH_2C{\equiv}C$), 72.9 (–, $PhCH_2$), 67.8 (–, OCH_2CH_2), 67.4 (x, $CH_2C{\equiv}C$), 66.0 (+, CH(O)CHCOH), 42.9 (+, CH(O)CHCOH), 27.5 (+, CH_3), 24.8 (+, CH_3), 20.1 (–, OCH_2CH_2).

FAB–MS: m/z (%) = 261 (4, $[M+H]^+$), 259 (10), 92 (100), 60 (60), 44 (40), 28 (7).

FAB–HRMS: $C_{16}H_{20}O_3$ (260.1412), calcd.: 261.1491 ($[M+H]^+$), found: 261.1463

(*S*,*S*)-8-Benzyloxy-2,6-dimethylocta-4,5-diene-2,3-diol (**15**)



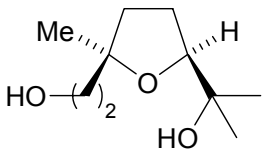
δH (400 MHz, $CDCl_3$): 7.36–7.30 (m, 5 H, ArH), 5.22 (m, 1 H,C=C=C<u>H</u>), 4.53 (dd, J = 11.8 Hz, 2 H, $PhCH_2$), 3.85 (d, J = 3.0 Hz, 1 H, C<u>H</u>OH), 3.60 (m, 2 H, $OC\underline{H}_2CH_2$), 2.91 (s, 2 H, OH), 2.28 (m, 2H, $OCH_2C\underline{H}_2$), 1.74 (d, J = 2.8 Hz, 3 H, $CH_3C=C=C$), 1.18 (s, 3 H, CH_3), 1.11 (s, 3 H, CH_3).

δC (100 MHz, $CDCl_3$): 200.6 (x, C=<u>C</u>=C), 137.7 (x, C–10), 128.4 (+, 2 x *m*–ArC), 128.1 (+, 2 x *o*–ArC), 127.8 (+, 1 x *p*–ArC), 100.8 (x, <u>C</u>=C=CH), 91.3 (+, C=C=<u>C</u>H), 75.7 (+, <u>C</u>HOH), 73.0 (–, $PhCH_2$), 72.9 (x, $\underline{C}(CH_3)_2$), 67.3 (–, $O\underline{C}H_2CH_2$), 34.4 (–, $OCH_2\underline{C}H_2$), 25.4 (+, $\underline{C}H_3C=C=C$), 23.8 (+, CH_3), 18.6 (+, CH_3).

FAB–MS: m/z (%) = 277 (4, $[M+H]^+$), 273 (2), 272 (1), 267 (1), 201 (10), 92 (15), 40 (18).

FAB–HRMS: $C_{17}H_{24}O_3$ (276.1725), calcd.: 277.1804 ($[M+H]^+$), found.: 277.1818.

2-((2S,5*R*)-Tetrahydro-5-(2-hydroxyethyl)-5-methylfuran-2-yl)propan-2-ol (**16**)



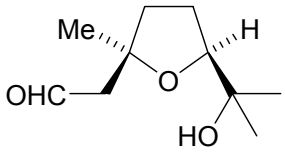
δH (400 MHz, $CDCl_3$): 3.97–3.91 (m, 1 H, C<u>H</u>), 3.86–3.75 (m, 2 H, OC<u>H_2</u>CH_2), 2.54 (s, 1 H, OH), 2.02–1.68 (m, 6 H, C<u>H_2</u>C<u>H_2</u>$C(CH_3)$C<u>H_2</u>), 1.29 (s, 3 H, furane-CH_3), 1.24 (s, 3 H, CH_3), 1.13 (s, 3 H, CH_3).

δC (100 MHz, $CDCl_3$): 85.7 (+, CH), 83.9 (x, CH_2<u>C</u>(CH3)O), 70.9 (x, <u>C</u>$(CH_3)_2$), 59.8 (–, O<u>C</u>H_2CH_2), 41.8 (–, OCH_2<u>C</u>H_2), 38.2 (–, <u>C</u>H_2CH_2CH), 27.7 (+, furane-CH_3), 25.9 (–, CH_2<u>C</u>H_2CH), 25.4 (+, CH_3), 25.0 (+, CH_3).

FAB–MS: m/z (%) = 189 (64, $[M+H]^+$), 171 (100, $[M–OH]^+$), 154 (57), 82 (53).

FAB–HRMS: $C_{10}H_{20}O_3$ (188.1412), calcd.: 171.1351 ($[M–OH]^+$), found: 171.1385

2-((2R,5S)-Tetrahydro-5-(2-hydroxypropan-2-yl)-2-methylfuran-2-yl)acetaldehyde (**3**)



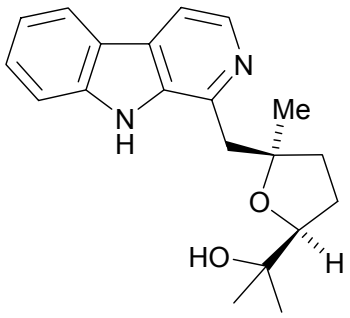
δH (400 MHz, $CDCl_3$): 9.84 (t, J = 2.9 Hz, 1 H, HC=O), 3.83 (m, 1 H, CH), 2.62 (d, J = 2.8 Hz, 2 H, C=OCH_2), 1.95–1.78 (m, 4 H, C<u>H_2</u>C<u>H_2</u>CH), 1.37 (s, 3 H, furane-CH_3), 1.21 (s, 3 H, CH_3), 1.11 (s, 3 H, CH_3).

δC (100 MHz, $CDCl_3$): 202.3 (+, C=O), 85.7 (+, CH), 81.2 (x, CH_2<u>C</u>(CH3)O), 70.9 (x, <u>C</u>$(CH_3)_2$), 54.2 (–, C=O<u>C</u>H_2), 38.2 (–, <u>C</u>H_2CH_2CH), 27.4 (+, furane-CH_3), 26.8 (+, CH_3), 26.0 (–, CH_2<u>C</u>H_2CH), 24.4 (+, CH_3).

FAB–MS: m/z (%) = 187 (12, $[M+H]^+$), 185 (20, $[M–H]^+$), 169 (82, $[M–OH]^+$), 143 (100), 56.0 (35), 42 (20).

FAB–HRMS: $C_{10}H_{18}O_3$ (186.1256), calcd.: 187.1334 ($[M+H]^+$), found: 187.1375.

(–)–Isocyclocapitelline (**2**)



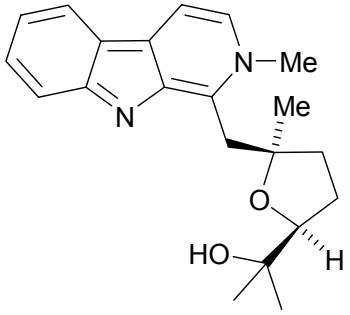
δH (500 MHz, $CDCl_3$): 10.41 (s, 1 H, NH), 8.35 (d, J = 4.7 Hz, 1 H, 8–H), 8.09 (d, J = 7.6 Hz, 1 H, 12–H), 7.83 (d, J = 4.7 Hz, 1 H, 9–H), 7.50 (s, 1 H, 14–H), 7.50 (s, 1 H, 15–H), 7.24 (pt, J = 6.5 Hz, 1 H, 13–H), 3.89 (m, 1 H, 2–H), 3.48/3.21 (dd, J = 13.6 Hz, 2 H, 6–H), 2.08 (m, 2 H, 3–H, 4–H), 1.91 (m, 2 H, 3–H, 4–H), 1.33 (s, 3 H, 1´–H), 1.23 (s, 3 H, 5´–H), 1.21 (s, 3 H, 1´´–H).

δC (125 MHz, $CDCl_3$): 142.8 (x, C–7), 140.8 (x, C–16), 137.4 (+, C–8), 135.9 (x, C–17), 128.7 (x, C–10), 127.9 (+, C–14), 121.6 (x, C–11), 121.6 (+, C–12), 119.4 (+, C–13), 113.2 (+, C–9), 111.8 (+, C–15), 86.4 (+, C–2), 84.0 (x, C–5), 71.2 (x, C–1), 46.6 (–, C–6), 39.0 (–, C–4), 27.9 (+, C–1´), 26.1 (–, C–3), 25.9 (+, C–1´´), 25.8 (+, C–5´).

FAB–MS: m/z (%) = 325 (20, $[M+H]^+$), 165 (4), 52 (6).

FAB–HRMS: $C_{20}H_{24}N_2O_2$ (324.1838), calcd.: 325.1916 ($[M+H]^+$), found: 325.1900.

(–)–Isochrysotricine (**1**)



δH (500 MHz, $CDCl_3$): 8.11 (d, J = 7.7 Hz, 1 H, 10–H), 7.96 (d, J = 8.5 Hz, 1 H, 9–H), 7.93 (d, J = 6.2 Hz, 1 H, 13–H), 7.53 (t, J = 7.6 Hz, 1 H, 15–H), 7.33 (d, J = 6.2 Hz, 1 H, 16–H), 7.13 (t, J = 7.1 Hz, 1 H, 14–H), 4.91 (s, 1H, OH), 4.32/3.19 (dd, J = 14.2 Hz, 2 H, 6–H), 4.12 (s, 3 H, 8´–H), 3.83 (m, 1 H, 2–H), 2.22–1.84 (m, 4 H, 3–H, 4–H), 1.27 (s, 3 H, 1´–H), 1.09 (s, 3 H, 1´´–H), 1.03 (s, 3 H, 5´–H).

δC (125 MHz, $CDCl_3$): 157.3 (x, C–17), 146.2 (x, C–18), 141.8 (x, C–7), 131.0 (x, C–11), 128.2 (+, C–15), 124.6 (+, C–9), 121.8 (+, C–13), 121.6 (x, C–12), 119.3 (+, C–14), 117.6 (+, C–16), 114.0 (+, C–10), 87.4 (+, C–2), 84.2 (+, C–6), 78.1 (x, C–5), 70.1 (x, C–1), 44.4 (+, C–8´), 39.4 (–, C–4), 27.4 (–, C–3), 27.0 (+, C–5´), 25.9 (+, C–1´), 25.5 (+, C–1´´).

FAB–MS: m/z (%) = 339 (2, $[M+H]^+$), 273 (3), 229 (2), 40 (7), 32 (3).

FAB–HRMS: $C_{21}H_{26}N_2O_2$ (338.1994), calcd.: 339.2073 ($[M+H]^+$), found: 339.2103.