Journal of the Serbian Chemical Society
JSCS@tmf.bg.ac.rs • www.shd.org.rs/JSCS
J. Serb. Chem. Soc. 79 (6) S58–S59 (2014) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

Diastereoselective addition of alkenylchromium(III) reagents to Garner's aldehyde. The Nozaki–Hiyama–Kishi coupling approach to sphingosines and ceramides

ZORANA FERJANČIĆ[1]*, RADOMIR MATOVIĆ[2] and FILIP BIHELOVIĆ[1]**

[1]*Faculty of Chemistry, University of Belgrade, Studentski trg 16, P. O. Box 158, 11000 Belgrade, Serbia and* [2]*ICTM – Center for Chemistry, Njegoševa 12, 11000 Belgrade, Serbia*

J. Serb. Chem. Soc. 79 (6) (2014) 627–636

PHYSICAL AND SPECTRAL DATA FOR COMPOUNDS **10** AND **12**–**14**

*(S)-2,2-Dimethyl-3-octanoyloxazolidine-4-carboxaldehyde (**10**)*. Yield: 87 %; Colorless oil; IR (film, cm^{-1}): 3399, 2955, 2930, 1826, 1738, 1657, 1409, 1372, 1252, 1216, 1157, 1069; ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 9.61 (1H, *s*), 4.81 (1H, *d*, *J* = 6.5 Hz), 4.32 (1H, *dd*, *J* = 1.0 and 10.0 Hz), 4.07 (1H, *dd*, *J* = 6.5 and 9.5 Hz), 2.21 (1H, *dt*, *J* = 7.5 and 16.0 Hz), 1.95 (1H, *dt*, *J* = 7.5 and 16.0 Hz), 1.48 (3H, *s*), 1.45 (3H, *s*), 1.45–1.41 (2H, *m*), 1.29–1.21 (8H, *m*), 0.86 (3H, *t*, *J* = 7.0 Hz); ^{13}C-NMR (125 MHz, DMSO-d_6, δ / ppm): 200. 04 (C), 169.94 (C), 95.41 (C), 65.54 (CH), 63.47 (CH_2), 35.02 (CH_2), 31.64 (CH_2), 28.99 (2×CH_2), 25.80 (CH_3), 24.68 (CH_2), 23.50 (CH_3), 22.51 (CH_2), 14.37 (CH_3); HRMS (ESI-TOF high acc) Calcd. for $C_{14}H_{26}NO_3$ (MH^+): 256.1907. Found: 256.1906. $[\alpha]_D^{20}$ (*c*=0.64, $CHCl_3$): –38.9.

*(S)-Methyl 3-hydroxy-2-octanamidopropanoate (**12**)*. Yield: 85 %; Colorless, viscous oil; IR (film, cm^{-1}): 3370, 2956, 2930, 2858, 1751, 1655, 1543, 1463, 1440, 1223, 1084; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 6.55 (1H, *d*, *J* = = 7.5 Hz), 4.67 (1H, *dt*, *J* = 4.0 and 7.5 Hz), 3.98–3.96 (1H, *m*), 3.91–3.88 (1H, *m*), 3.79 (3H, *s*), 3.13 (1H, *bs*), 2.26 (2H, *t*, *J* = 7.5 Hz), 1.67–1.61 (2H, *m*), 1.32––1.26 (8H, *m*), 0.88 (3H, *t*, *J* = 7.0 Hz); ^{13}C-NMR (125 MHz, $CDCl_3$, δ / ppm): 173.84 (C), 171.07 (C), 63.35 (CH_2), 54.58 (CH), 52.66 (CH_3), 36.44 (CH_2), 31.61 (CH_2), 29.13 (CH_2), 28.93 (CH_2), 25.51 (CH_2), 22.54 (CH_2), 13.99 (CH_3); HRMS (ESI-TOF high acc): Calcd. for $C_{12}H_{23}NO_4Na$ (MNa^+): 268.1519. Found: 268.1509; $[\alpha]_D^{20}$ (*c*=0.48, $CHCl_3$): +23.9.

*(S)-Methyl 2,2-dimethyl-3-octanoyloxazolidine-4-carboxylate (**13**)*. Yield: 69 %; Colorless oil; IR (film, cm^{-1}): 2956, 2931, 2857, 1755, 1650, 1461, 1411, 1368, 1256, 1210, 1079, 1056; ^{1}H-NMR (500 MHz, DMSO-d_6; 60 °C, δ / ppm):

*,** Corresponding authors. E-mail: (*)zferjan@chem.bg.ac.rs; (**)filip@chem.bg.ac.rs

4.77 (1H, *bt*, *J* = 4.0 Hz), 4.13 (2H, *m*), 3.73 (3H, *s*), 2.25 (1H, *dt*, *J* = 7.5 and 16.0 Hz), 2.00 (1H, *dt*, *J* = 7.0 and 15.5 Hz), 1.55 (3H, *s*), 1.49 (1H, *bt*, *J* = 6.5 Hz), 1.46 (3H, *s*), 1.30-1.25 (8H, *m*), 0.87 (3H, *t*, *J* = 7.0 Hz); ^{13}C-NMR (125 MHz, DMSO-d_6, δ / ppm): 171.01 (C), 169.15 (C), 94.89 (C), 66.20 (CH_2), 58.60 (CH), 55.12 (CH_3), 34.27 (CH_2), 30.80 (CH_2), 28.20 (CH_2), 28.12 (CH_2), 24.85 (CH_3), 23.79 (CH_2), 23.10 (CH_3), 21.66 (CH_2), 13.46 (CH_3); HRMS (ESI-TOF high acc) Calcd. for $C_{15}H_{28}NO_4$ (MH^+): 286.2013. Found: 286.2004; $[\alpha]_D^{20}$ (*c*=1.4, $CHCl_3$): –47.0.

*(*R*)-1-(4-(Hydroxymethyl)-2,2-dimethyloxazolidin-3-yl)-1-octanone* (***14***). Yield: 75 %; Colorless, viscous oil; IR (film, cm^{-1}): 3420, 2956, 2931, 2873, 1627, 1464, 1423, 1372, 1251, 1209, 1079, 1059; ^{1}H-NMR (500 MHz, DMSO-d_6, δ / ppm): 5.05 (1H, *dd*, *J* = 5.0 and 6.5 Hz), 3.92–3.84 (3H, *m*), 3.42–3.39 (1H, *m*), 3.32–3.27 (1H, *m*), 2.38–2.23 (1H, *m*), 2.29–2.23 (1H, *m*), 1.53–1.47 (2H, *m*), 1.47 (3H, *s*), 1.41 (3H, *s*), 1.30–1.21 (8H, *m*), 0.86 (3H, *t*, *J* = 7.0 Hz); ^{13}C-NMR (125 MHz, DMSO-d_6, δ / ppm): 169.31 (C), 93.81 (C), 64.87 (CH_2), 61.44 (CH_2), 58.50 (CH), 34.35 (CH_2), 31.22 (CH_2), 28.65 (CH_2), 28.60 (CH_2), 26.75 (CH_3), 24.71 (CH_2), 22.74 (CH_3), 22.07 (CH_2), 13.94 (CH_3); HRMS (ESI-TOF high acc) Calcd. for $C_{14}H_{28}NO_3$ (MH^+): 258.2064. Found: 258.2053; $[\alpha]_D^{20}$ (*c*=0.6, $CHCl_3$): –9.3.