Supporting Information Available

Asymmetric Synthesis of Fused Bicyclic α -Amino Acids Having a Hexahydro-cyclopenta[c]pyridine Skeleton via Intramolecular

Pauson-Khand Reaction of Chiral

1-Sulfonimidoyl Substituted 5-Azaoct-1-en-7-yne

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General Experimental Details. All reactions were carried out in absolute solvents under argon with syringe and Schlenk techniques in oven-dried glassware. DMF was distilled from CaH_2 , and THF was distilled under nitrogen from sodium-lead/benzophenone. $\text{CITi}(\text{Oi-Pr})_3$ ²¹ of $\geq 96\%$ purity (^1H NMR) was prepared according to the literature. Iminoester **6** was synthesized as described previously.⁹ The γ,δ -unsaturated amino acid derivatives **4a–d** were prepared via allylation of iminoester **6** with bis(allylsulfoximine)titanium complexes according to a previously described procedure.⁹ The allylic sulfoximines **5a–d** of $\geq 98\%$ ee were synthesized from (*S*)-*S*-methyl-*S*-phenylsulfoximine according to the literature.¹³ (*S*)-*S*-methyl-*S*-phenylsulfoximine of $\geq 98\%$ ee, which is also commercially available, was synthesized as described previously.²² All other chemicals were obtained from commercial sources and used without further purification. TLC: silica gel 60 F_{254} plates. Column chromatography: silica gel 60 (0.063–0.200 mm). HPLC: Si 100 column (diameter: 20 mm, flow: 5 mL/min, pressure 17 bar). Optical rotations were measured at approximately 22 °C and are presented in $\text{grad} \times \text{mL/dm} \times \text{g}$, c in g/100 mL. ^1H and ^{13}C NMR: the following abbreviations are used to designate the multiplicity of the peaks in the ^1H NMR spectra: b = broad, s = singlet, d = doublet, t = triplet, q = quartet, sep = septet, m = multiplet, and combinations thereof. Peaks in ^{13}C NMR spectra are denoted as "u" for carbons with zero or two attached protons or "d" for carbons with one or three attached protons, as determined from APT pulse sequence. Assignments in the ^1H NMR spectra were made by GMQCOSY, GNOE, or GTOCSY experiments, and those in the ^{13}C NMR spectra were made by DEPT, HETCOR, or GHSQC experiments. IR spectra: only peaks of $\tilde{\nu} > 800 \text{ cm}^{-1}$ are listed. MS spectra: only peaks of $m/z > 70$ and an intensity $> 10\%$, except decisive ones, are listed.

(+)-(E,S_S,2S,3R)-5-[N-Methyl-S-phenylsulfonimidoyl]-3-isopropyl-2-[(2-methylpropane-2-sulfonyl)-prop-2-ynyl-amino]-pent-4-enoic acid ethyl ester (3b). Following *GPI*, reaction of sulfoximine **4b** (1.0 g, 2.18 mmol) with Cs₂CO₃ (847 mg, 2.40 mmol) and propargyl bromide (0.49 ml, 4.36 mmol, 80% in toluene) afforded the *N*-propargyl amino ester **3b** (1.02 g, 94%) as a light yellow oil. $[\alpha]_D^{+48.1}$ (*c* 0.98, CH₂Cl₂). ¹H NMR (CDCl₃, 400 MHz) δ 0.96 (d, *J* = 6.9 Hz, 3 H), 0.98 (d, *J* = 6.9 Hz, 3 H), 1.12 (t, *J* = 7.2 Hz, 3 H), 1.37 (s, 9 H), 2.30 (t, *J* = 2.5 Hz, 1 H), 2.38 (sepd, *J* = 6.9, *J* = 3.0 Hz, 1 H), 2.74 (s, 3 H), 2.83 (td, *J* = 10.3, *J* = 3.0 Hz, 1 H), 3.58 (dq, *J* = 10.7, *J* = 7.2 Hz, 1 H), 3.87 (dq, *J* = 10.7, *J* = 7.2 Hz, 1 H), 4.16–4.24 (bm, 1 H), 4.42 (bd, *J* = 19.2 Hz, 1 H), 4.50 (d, *J* = 10.3 Hz, 1 H), 6.41 (d, *J* = 14.9 Hz, 1 H), 6.70 (dd, *J* = 14.9, *J* = 10.3 Hz, 1 H), 7.51–7.62 (m, 3 H), 7.84–7.89 (m, 2 H). ¹³C NMR (CDCl₃, 100 MHz) δ 13.9 (d), 16.7 (d), 20.8 (d), 24.5 (d), 27.4 (d), 29.4 (d), 35.4 (u), 48.6 (d), 61.1 (u), 61.2 (d), 62.4 (u), 72.1 (u), 80.5 (u), 128.3 (d), 129.1 (d), 132.6 (d), 133.7 (d), 138.9 (u), 141.5 (d), 170.2 (u). IR (CHCl₃): $\tilde{\nu}$ 3304 (m), 3271 (m), 3061 (w), 2965 (s), 2875 (m), 2805 (w), 2119 (w), 1736 (s), 1627 (w), 1466 (m), 1446 (m), 1395 (w), 1370 (w), 1325 (s), 1249 (s), 1178 (m), 1132 (s), 1109 (m), 1069 (m), 1022 (m), 981 (w), 939 (w), 893 (m), 868 (m), 832 (w), 810 (w) cm⁻¹. MS (EI, 70 eV): *m/z* (relative intensity, %) 497 [M⁺+1] (2), 375 (34), 299 (17), 251 (51), 249 (12), 237 (16), 236 (14), 222 (25), 210 (12), 191 (10), 177 (14), 148 (12), 140 (42), 125 (51), 110 (20), 107 (15), 106 (13), 77 (10), 57 (100). Anal. calcd. for C₂₄H₃₆N₂O₅S₂ (496.69): C, 58.04; H, 7.31; N, 5.64. Found: C, 57.95; H, 7.07; N, 5.62.

(+)-(E,S_S,2S,3R)-5-[N-Methyl-S-phenylsulfonimidoyl]-3-cyclohexyl-2-[(2-methylpropane-2-sulfonyl)-prop-2-ynyl-amino]-pent-4-enoic acid ethyl ester (3c). Following *GPI*, reaction of sulfoximine **4c** (931 mg, 1.87 mmol) with Cs₂CO₃ (790 mg, 2.24 mmol) and propargyl bromide (0.42 ml, 3.73 mmol, 80% in toluene) afforded the *N*-propargyl amino ester **3c** (911 mg, 91%) as a light yellow oil. $[\alpha]_D^{+39.2}$ (*c* 1.02, CH₂Cl₂). ¹H NMR (CDCl₃, 400 MHz) δ 0.94–1.35 (m, 5 H), 1.27 (t, *J* = 7.2 Hz, 3 H), 1.38 (s, 9 H), 1.40–2.03 (m, 6 H), 2.30 (t, *J* = 2.5 Hz, 1 H), 2.75 (s, 3 H), 2.78 (td, *J* = 10.0, *J* = 3.2 Hz, 1 H), 3.57 (dq, *J* = 10.7, *J* = 7.2 Hz, 1 H), 3.87 (dq, *J* = 10.7, *J* = 7.2 Hz, 1 H), 4.17–4.29 (bm, 1 H), 4.39 (bd, *J* = 19.0 Hz, 1 H), 4.53 (d, *J* = 10.0 Hz, 1 H), 6.40 (d, *J* = 14.8 Hz, 1 H), 6.73 (dd, *J* = 10.7, *J* = 14.8 Hz, 1 H), 7.51–7.62 (m, 3 H), 7.85–7.87 (m, 2 H). ¹³C NMR (CDCl₃, 100 MHz) δ 13.9 (d), 24.5 (d), 26.1 (u), 26.2 (u), 26.5 (u), 27.6 (u), 29.4 (d), 31.4 (u), 35.4 (u), 37.4 (d), 48.5 (d), 60.5 (d), 61.0 (u), 62.3 (u), 72.0 (u), 80.4 (u), 128.4 (d), 129.1 (d), 132.5 (d), 133.1 (d), 139.0 (u), 142.5 (d), 170.3 (u). IR (CHCl₃): $\tilde{\nu}$ 3303 (w), 2979 (m), 2854 (s), 2804 (w), 1735 (s), 1626 (w), 1476 (w), 1447 (m), 1369 (w), 1325 (s), 1248 (s), 1175 (m), 1132 (s), 1083 (w), 1022 (w), 982 (w), 890 (m), 867 (m), 817 (w) cm⁻¹. MS (EI, 70 eV): *m/z* (relative intensity, %) 535 [M⁺-1] (3), 415 (44), 339 (11), 291 (68), 289 (14), 176 (14), 250 (12), 217 (13), 188 (15), 156 (12), 150 (23), 140 (46), 125 (60), 107 (19), 79 (11), 57 (100). Anal. calcd. for C₂₇H₄₀N₂O₅S₂ (536.75): C, 60.42; H, 7.51, N, 5.22. Found: C, 60.64, H, 7.34, N, 4.95.

(+)-(E,S_S,2S,3R)-5-[N-Methyl-S-phenylsulfonimidoyl]-3-phenyl-2-[(2-methylpropane-2-sulfonyl)-prop-2-ynyl-amino]-pent-4-enoic acid ethyl ester (3d). Following *GPI*, reaction of sulfoximine **4d** (2.0 g, 4.06 mmol) with Cs₂CO₃ (1.72 g, 4.87 mmol) and propargyl bromide (0.90 ml, 8.12 mmol, 80% in toluene) afforded the *N*-propargyl amino ester **3d** (2.06 g, 96%) as a light yellow oil. $[\alpha]_D^{+31.2}$ (*c* 0.60, CH₂Cl₂). ¹H NMR (CDCl₃, 400 MHz) δ 1.16 (t, *J* = 7.2 Hz, 3 H), 1.27 (s, 9 H), 2.31 (bs, 1 H), 2.69 (s, 3 H), 3.85–4.17 (m, 4 H), 4.32 (t, *J* = 8.8 Hz, 1 H), 4.80 (d, *J* = 8.3 Hz, 1 H), 6.46 (d, *J* = 14.8 Hz, 1 H), 7.15 (dd, *J* = 14.8, *J* = 9.6 Hz, 1 H), 7.21–7.37 (m, 5 H), 7.49–7.60 (m, 3 H), 7.83–7.87 (m, 2 H). ¹³C NMR (CDCl₃, 100 MHz) δ 13.8 (d), 24.4 (d), 29.3 (d), 35.4 (u), 48.7 (d), 61.4 (u), 62.3 (u), 64.4 (d), 73.3 (u), 80.2 (u), 127.8 (d), 128.2 (d), 128.4 (d), 128.5 (d), 128.6 (d), 129.1 (d), 132.6 (d), 132.7 (d), 138.7 (u), 143.3 (d), 149.9 (u), 171.0 (u). IR (CHCl₃): $\tilde{\nu}$ 3274 (m), 3060 (w), 2982 (s), 2937 (m), 2876 (m), 2805 (w), 2120 (w), 1736 (s), 1578 (w), 1477 (m), 1446 (m), 1396 (w), 1367 (w), 1324 (s), 1249 (s), 1131 (s), 1084 (s), 1056 (s), 893 (w), 867 (m), 810 (w) cm⁻¹. MS (EI, 70 eV): *m/z* (relative intensity, %) 530 [M⁺] (2), 409 (12), 285 (27), 271 (35), 256 (43), 182 (59), 140 (52), 125 (45), 115 (53), 77 (12), 57 (100). Anal. calcd. for C₂₇H₃₄N₂O₅S₂ (530.70): C, 61.11; H, 6.46; N, 5.28. Found: C, 61.14; H, 6.50; N, 5.11.

(-)-(E,3*S*,4*R*,4*aR*)-2,3,4,4*a*,5,6-Hexahydro-4-isopropyl-2-(2-methyl-propane-2-sulfonyl)-6-oxo-1*H*-cyclopenta[*c*]pyridine-3-carboxylic acid ethyl ester (**9b**). In THF with NMO: following GP2, reaction of **3b** (117 mg, 0.24 mmol) with Co₂(CO)₈ (90.3 mg, 0.26 mmol) and NMO (169 mg, 1.44 mmol) gave **9b** (45 mg, 51%) as a yellow oil and **8** of ≥ 98% ee as a white solid (25 mg, 68%). [α]_D -62.1 (*c* 1.74, CH₂Cl₂). ¹H NMR (C₆D₆, 500 MHz) δ 0.63 (d, *J* = 7.0 Hz, 3 H), 0.78 (d, *J* = 7.0 Hz, 3 H), 0.91 (t, *J* = 7.3 Hz, 3 H), 1.10 (s, 9 H), 1.40 (m, 1 H), 1.46 (m, 1 H), 1.61 (dd, *J* = 18.0, *J* = 3.4 Hz, 1 H), 2.09 (dd, *J* = 18.0, *J* = 6.4 Hz, 1 H), 2.87 (bm, 1 H), 3.78 (dq, *J* = 11.0, *J* = 7.3 Hz, 1 H), 3.94 (dq, *J* = 11.0, *J* = 7.3 Hz, 1 H), 4.40 (bs, 1 H), 4.52 (bs, 1 H), 4.67 (bs, 1 H), 5.68 (s, 1 H). ¹³C NMR (C₆D₆, 100 MHz) δ 13.8 (d), 18.5 (d), 20.1 (d), 24.1 (d), 28.9 (d), 38.4 (d), 40.7 (u), 45.7 (u), 51.1 (d), 57.3 (d), 60.9 (u), 61.2 (u), 127.7 (d), 170.8 (u), 172.2 (u), 204.6 (u). IR (CHCl₃): $\tilde{\nu}$ 3388 (w), 2976 (w), 2937 (w), 2877 (m), 1716 (s), 1632 (s), 1479 (m), 1465 (m), 1396 (m), 1368 (w), 1322 (s), 1262 (m), 1201 (s), 1180 (s), 1158 (s), 1129 (s), 1097 (w), 1059 (m), 1026 (m), 1008 (m), 954 (m), 902 (m), 857 (w), 810 (m) cm⁻¹. MS (CI, methane): *m/z* (relative intensity, %) 372 [M⁺+1] (18), 298 (10), 280 (11), 252 (100), 75 (10). HRMS (EI, 70 eV, M⁺ - [C₄H₉SO₂]) calcd for C₁₄H₂₀NO₃: 250.144318. Found: 250.144337.

In MeCN without NMO: To a solution of **3b** (297 mg, 0.60 mmol) in CH₂Cl₂ (5 mL) was added Co₂(CO)₈ (225 mg, 0.66 mmol) at room temperature. After 30 min TLC showed the complete consumption of **3b**. Then the solvent was evaporated and the dark red residue was dissolved in dry CH₃CN (10 mL). The mixture was heated to reflux for 1 h and then filtered through a pad of celite and the filtrate concentrated in vacuo. Flash chromatography of the residue gave **9b** and *epi*-**9b** (66 mg, 30%) in a ratio of 66:33. NMR data of the major diastereomer **9b**: ¹H NMR (CDCl₃, 300 MHz) δ 0.95 (d, *J* = 7.2 Hz, 3 H), 1.07 (d, *J* = 7.0 Hz, 3 H), 1.34 (t, *J* = 7.2 Hz, 3 H), 1.36 (s, 9 H), 1.75 (dt, *J* = 5.2, *J* = 12.4 Hz, 1 H), 1.92 (m, 1 H), 2.17 (dd, *J* = 18.3, *J* = 3.2 Hz, 1 H), 2.61 (m, 1 H), 3.31 (bm, 1 H), 4.19 (dq, *J* = 10.9, *J* =

7.2 Hz, 1 H), 4.29 (dq, $J = 10.9$, $J = 7.2$ Hz, 1 H), 4.62 (bs, 3 H), 6.00 (s, 1 H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 14.00 (d), 19.1 (d), 20.3 (d), 24.2 (d), 29.0 (d), 38.6 (d), 41.1 (u), 45.4 (u), 51.3 (d), 57.2 (d), 61.3 (u), 61.8 (u), 127.6 (d), 170.1 (u), 173.7 (u), 206.6 (u). NMR data of the minor diastereomer *epi-9b*: ^1H NMR (CDCl_3 , 300 MHz) δ 1.01 (d, $J = 6.2$ Hz, 3 H), 1.09 (d, $J = 7.0$ Hz, 3 H), 1.34 (t, $J = 7.2$ Hz, 3 H), 1.44 (s, 9 H), 1.77 (m, 1 H), 1.94 (m, 1 H), 2.23 (dd, $J = 9.6$, $J = 3.6$ Hz, 1 H), 2.67 (m, 1 H), 3.41 (bm, 1 H), 3.94 (dq, $J = 10.7$, $J = 7.2$ Hz, 1 H), 4.19 (dq, $J = 10.7$, $J = 7.2$ Hz, 1 H), 4.62 (bs, 3 H), 6.03 (s, 1 H). ^{13}C NMR (CDCl_3 , 100 MHz) δ 14.0 (d), 20.8 (d), 22.0 (d), 24.2 (d), 28.3 (d), 39.7 (d), 40.1 (u), 47.4 (u), 51.3 (d), 58.4 (d), 61.7 (u), 62.7 (u), 131.8 (d), 170.2 (u), 173.7 (u), 206.4 (u).

In CH₂Cl₂ with NMO: To a solution of **3b** (544 mg, 1.10 mmol) in CH_2Cl_2 (5 mL) was added $\text{Co}_2(\text{CO})_8$ (413 mg, 1.21 mmol) at room temperature. After 30 min TLC showed the complete consumption of **3b**. The mixture was cooled to 0 °C, treated with NMO (386 mg, 3.3 mmol) and warmed within 1 h to room temperature. Then mixture was re-cooled to 0 °C, treated with an additional portion of NMO (386 mg, 3.3 mmol) warmed to room temperature within 1 h. The mixture was filtered through a pad of celite which was washed with EtOAc. Concentration of the filtrate in vacuo and purification of the residue by flash chromatography (EtOAc) afforded a mixture of **9b** and *epi-9b* (145 mg, 35%) in a ratio of 85:15.

(-)-(E,3*S*,4*R*,4*aR*)-2,3,4,4*a*,5,6-Hexahydro-4-cyclohexyl-2-(2-methyl-propane-2-sulfonyl)-6-oxo-1*H*-cyclopenta[*c*]pyridine-3-carboxylic acid ethyl ester (**9c**). Following GP2, reaction of **3c** (316 mg, 0.59 mmol) with Co₂(CO)₈ (221 mg, 0.65 mmol) and NMO (414 mg, 3.54 mmol) gave **9c** (134 mg, 55%) as a yellow oil and **8** of ≥ 98% ee as a white solid (60 mg, 66%). [α]_D -40.1 (*c* 1.19, CH₂Cl₂). ¹H NMR (C₆D₆, 400 MHz) δ 0.71–0.81 (m, 1 H), 0.95 (t, *J* = 7.1 Hz, 3 H), 1.12 (s, 9 H), 1.20–1.62 (m, 11 H), 1.71 (dd, *J* = 18.1, *J* = 3.3 Hz, 1 H), 2.15 (dd, *J* = 18.1, *J* = 6.6 Hz, 1 H), 2.90 (m, 1 H), 3.86 (dq, *J* = 11.0, *J* = 7.1 Hz, 1 H), 3.93 (dq, *J* = 11.0, *J* = 7.1 Hz, 1 H), 4.42–4.67 (bm, 3 H), 5.71 (s, 1 H). ¹³C NMR (C₆D₆, 100 MHz) δ 13.9 (d), 24.1 (d), 26.6 (u), 27.0 (u), 27.2 (u), 30.2 (u), 30.6 (u), 37.9 (d), 39.6 (d), 41.1 (u), 45.7 (u), 51.0 (u), 58.0 (d), 60.9 (u), 61.2 (u), 127.7 (d), 170.8 (u), 172.4 (u), 204.7 (u). IR (CHCl₃): $\tilde{\nu}$ 2981 (m), 2929 (s), 2856 (m), 1718 (s), 1632 (m), 1477 (w), 1450 (m), 1399 (m), 1322 (s), 1261 (m), 1185 (s), 1129 (s), 1055 (w), 1025 (m), 1003 (m), 955 (m), 907 (m), 853 (w), 808 (w) cm⁻¹. MS (CI, isobutane): *m/z* (relative intensity, %) 412 [M⁺+1] (100), 292 (38). HRMS (EI, 70 eV, M⁺– [C₄H₉SO₂]) calcd for C₁₇H₂₄NO₃: 290.175619. Found: 290.175609.

(-)-(E,3*S*,4*R*,4*aR*)-2,3,4,4*a*,5,6-Hexahydro-2-(2-Methyl-propane-2-sulfonyl)-6-

oxo-4-phenyl-1*H*-cyclopenta[*c*]pyridine-3-carboxylic acid ethyl ester (9d). Following GP2, reaction of **3d** (340 mg, 0.64 mmol) with Co₂(CO)₈ (240 mg, 0.70 mmol) and NMO (449 mg, 3.84 mmol) gave **9d** (159 mg, 61%) as a white wax and **8** of ≥ 98% ee as a white solid (70 mg, 71%). [α]_D -4.9 (*c* 1.74, CH₂Cl₂). ¹H NMR (C₆D₆, 400 MHz) δ 0.57 (t, *J* = 7.1 Hz, 3 H), 1.15 (s, 9 H), 1.47 (dd, *J* = 18.7, *J* = 2.7 Hz, 1 H), 2.16 (dd, *J* = 18.7, *J* = 6.6 Hz, 1 H), 2.74 (bm, 1 H), 3.32 (bm, 1 H), 3.37 (dq, *J* = 10.7, *J* = 7.1 Hz, 1 H), 3.66 (dq, *J* = 10.7, *J* = 7.1 Hz, 1 H), 4.56-4.80 (bm, 3 H), 5.78 (s, 1 H), 6.85-6.90 (m, 2 H), 7.01-7.08 (m, 3 H). ¹³C NMR (C₆D₆, 100 MHz) δ 13.5 (d), 24.1 (d), 38.0 (d), 40.5 (u), 45.6 (u), 51.8 (d), 60.4 (u), 61.3 (u), 61.7 (d), 127.7 (d), 128.1 (d), 128.5 (d), 128.6 (d), 137.6 (u), 170.1 (u), 171.2 (u), 204.6 (u). IR (CHCl₃): $\tilde{\nu}$ 3403 (w), 3023 (s), 2984 (s), 2934 (s), 2876 (m), 2442 (w), 1715 (s), 1634 (s), 1601 (m), 1478 (s), 1453 (s), 1399 (m), 1383 (m), 1323 (s), 1246 (s), 1210 (s), 1185 (s), 1129 (s), 1060 (s), 1028 (s), 1003 (s), 958 (s), 907 (s), 840 (m), 811 (s) cm⁻¹. MS (CI, isobutane): *m/z* (relative intensity, %) 406 [M⁺+1] (100), 286 (42). HRMS (EI, 70 eV, M⁺-[C₄H₉SO₂]) calcd for C₁₇H₁₈NO₃: 284.128668. Found: 284.128472.

(21) Reetz, M. T.; Westermann, J.; Steinbach, R.; Wenderoth, B.; Peter, R.; Ostarek, R.; Maus, S. *Chem. Ber.* **1985**, *118*, 1421.

(22) (a) Fusco, R.; Terriconi, F. *Chim. Ind. (Milan)* **1965**, *47*, 61. (b) Johnson, C. R.; Schroeck, C. W. *J. Am. Chem. Soc.* **1973**, *95*, 7418. (c) Brandt, J.; Gais, H.-J. *Tetrahedron: Asymmetry* **1997**, *8*, 909.

S10

mercury300

(CDCl₃)

12.6 12.0 11.4 10.8 ppm

S11

S12

unity-500

(C6D6)

12.6 12.0 11.4 10.8 ppm

S13

inova400

(CDCl₃)

APT: C, CH₂

CH, CH₃

DEPT: CH

S14

inova400

(CDCl₃)

12.6 12.0 11.4 10.8 ppm

S15

inova400

(CDCl₃)

S16

inova400

(*C6D6*)

12.6 12.0 11.4 10.8 ppm

S17

inova-400

(CDCl₃)

DEPT: CH

APT: C, CH₂

CH, CH₃

S18

12.6 12.0 11.4 10.8 ppm

inova400

(CDCl₃)