Supporting Information

Bioinspired Synthesis of Pentacyclic Onocerane Triterpenoids

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1. General Methods
All reactions sensitive to moisture and/or air were carried out using heat-gun dried (630 °C) glassware under an argon atmosphere. Dry solvents (CH₂Cl₂, Et₂O, THF) were purified by Solvent Purification System M-BRAUN Glovebox Technology SPS-800. Dry DMF was obtained from Acros Organics 99.8%, extra dry over molecular sieves. Dry pyridine was obtained from Sigma Aldrich, anhydrous, 99.8%. Dry MeNO₂ was obtained by distillation over CaH₂. Dry 1,2-dimethoxyethane was obtained by distillation over CaH₂. Dry TMEDA was obtained by distillation over CaH₂. Dry methanol (HiPerSolv CHROMANORM HPLC GRADE) was obtained from VWR Chemicals. Solvents for column chromatography were used after short path distillation using a rotary evaporator. Commercial reagents were used as received unless otherwise stated. All reactions were carried out under magnetic stirring with Teflon coated stirring bars and were monitored by TLC analysis on 0.20 mm silica gel plates (Macherey-Nagel G/UV254). Staining of TLC plates was performed with an acidic vanillin solution (1 g vanillin, 20 mL conc. acetic acid, 10 mL conc. sulfuric acid, 170 mL methanol) and heat. Column chromatography was carried out on silica gel 60 M (0.04–0.063 mm) from Macherey-Nagel and aluminium oxide (basic, Brockmann I, for chromatography, 50-200 μm, 60A) from ACROS Organics. Concentration under reduced pressure was performed by rotary evaporation at 40 °C. ¹H NMR and ¹³C NMR spectra were recorded on Bruker (ECP 400, AC 500, AV 700) or JEOL (ECX 400, Eclipse 500) instruments. Chemical shifts are reported relative to CDCl₃ (¹H: 7.26 ppm; ¹³C: 77.16 ppm) and C₆D₆ (¹H: 7.16 ppm; ¹³C: 128.06 ppm). Chemical shifts are reported in parts per million as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sext = sextet, m = multiplet, br = broad, and combinations thereof), coupling constant and integration. Integrals are in accordance with assignments, coupling constants are given in Hz. For detailed peak assignments, 2D spectra were recorded when necessary (COSY, DEPT, HMQC, HMBC, TOCSY, GOESY, NOESY). IR spectra were measured on a JASCO FT/IR-4100 instrument equipped with an ATR unit. High resolution ESI analyses were performed on a Varian Inc. Ionspec QFT-7. High resolution EI spectra were performed on a Waters Autospec Premier. Optical rotation measurements were performed on a P-2000 polarimeter from Jasco in a 10 cm optical-path length cell with the frequency of the NaD line measured at the temperature and concentration (in g/100 mL) indicated. The enantiomeric excess was determined by chiral HPLC using Agilent Technologies 1200 series with a diode array detector. Melting points were measured with a Stuart melting point apparatus SMP30 and on a Reichert Thermovar Kofler hot-stage-microscope and are uncorrected.
2. Synthesis of Compounds

**Compound 17**

![Chemical Structure](image)

To LiAlH₄ (107 mg, 2.81 mmol, 0.70 eq.) at 0 °C was added a solution of lactone 15 (1.00 g, 4.01 mmol, 1.0 eq.) in THF (6 mL, flask rinsed with 2 x 2 mL) over 5 min. After 40 min of stirring at the same temperature Rochelle salt (1.36 g, 4.81 mmol, 1.2 eq.), DMF (10 mL), freshly ground KOH (900 mg, 16.0 mmol, 4.0 eq.) and 2-Me-C₆H₄CH₂Br (1.10 mL, 1.52 g, 8.22 mmol, 2.1 eq.) were added successively and the reaction mixture was heated to 45 °C for 27 h. Water was added to the reaction and the mixture was diluted with EtOAc. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 10:1) to afford ether 17 (1.43 g, 4.01 mmol, quant.) as a light-yellow oil.

\[ R_f = 0.52 \ (n\text{-pentane/EtOAc} \ 5:1). \]

\[ [\alpha]^{28}_D = -14.2^\circ \ (c = 1.33, \text{CHCl}_3). \]

**¹H-NMR** (500 MHz, CDCl₃): δ [ppm] = 7.30 – 7.28 (m, 1H), 7.22 – 7.14 (m, 3H), 4.58 – 4.48 (m, 2H), 3.64 (ddd, \( J = 8.7, 5.4, 4.1 \) Hz, 1H), 3.38 (ddd, \( J = 10.1, 8.7, 4.5 \) Hz, 1H), 3.24 (s, 1H), 2.34 (s, 3H), 1.90 (dt, \( J = 12.5, 3.2 \) Hz, 1H), 1.77 (ddt, \( J = 15.3, 10.2, 5.2 \) Hz, 1H), 1.68 – 1.53 (m, 4H), 1.46 – 1.34 (m, 3H), 1.30 – 1.20 (m, 2H), 1.18 – 1.10 (m, 4H), 0.93 – 0.82 (m, 5H), 0.79 (s, 6H).

**¹³C-NMR** (126 MHz, CDCl₃): δ [ppm] = 136.7, 135.9, 130.4, 128.7, 128.0, 125.9, 72.4, 72.2, 71.6, 59.4, 56.3, 44.2, 42.1, 39.7, 39.2, 33.6, 33.4, 25.5, 24.5, 21.6, 20.6, 19.0, 18.6, 15.4.

IR (\( \nu/\text{cm}^{-1}, \text{ATR} \)) = 3440, 2926, 2863, 1715, 1460, 1383, 1364, 1288, 1079, 933, 744.

**HRMS (ESI):** \( m/z \) calculated for C₂₄H₃₈O₂Na⁺ [M+Na]⁺: 381.2764, found 381.2762.

Note: On 4.5 g scale 96% yield was obtained.
Compound 13 from 17

To a solution of ether 17 (177 mg, 458 μmol, 1.0 eq.) in THF (5 mL) at −78 °C was added a solution of n-BuLi (0.733 mL, 2.5 M in hexane, 1.83 mmol, 4.0 eq.). After 10 min at that temperature the reaction mixture was warmed to −13 °C (change of cooling baths) and stirred for 90 min. Water was added and the reaction mixture was diluted with EtOAc. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 20:1 to 15:1 to 10:1) to afford alkene 13 (48.2 mg, 204 μmol, 44%) as a white solid.

Crystals suitable for single crystal X-ray diffraction were obtained after slow evaporation from EtOAc/n-hexane.

R_f = 0.50 (n-pentane/EtOAc, 9:1).

[α]_D^28 = −16.4 (c = 2.03, CHCl₃).

¹H-NMR (500 MHz, CDCl₃): δ [ppm] = 5.82 (dt, J = 16.8, 10.2 Hz, 1H), 5.26 (dd, J = 10.2, 2.5 Hz, 1H), 5.15 (dd, J = 16.9, 2.4 Hz, 1H), 1.94 (sbr, 1H), 1.90 (dt, J = 12.6, 3.3 Hz, 1H), 1.75 (d, J = 10.2 Hz, 1H), 1.71 – 1.64 (m, 1H), 1.56 (tt, J = 14.4, 3.7 Hz, 1H), 1.51 – 1.36 (m, 4H), 1.38 – 1.23 (m, 1H), 1.19 (s, 3H), 1.14 (td, J = 13.5, 12.8, 4.3 Hz, 1H), 0.93 – 0.89 (m, 4H), 0.89 – 0.85 (m, 4H), 0.81 (s, 3H).

¹³C-NMR (126 MHz, CDCl₃): δ [ppm] = 135.1, 120.6, 71.5, 67.7, 55.9, 42.2, 42.1, 40.9, 37.2, 33.6, 33.5, 25.2, 21.8, 20.2, 18.6, 15.9.

IR (ν/cm⁻¹, ATR) = 3462, 2993, 2923, 2869, 1462, 1386, 1188, 1128, 935, 911.


Mp = 89 – 90 °C.

Note: For an attempted synthesis of 13, see:¹.
Compound 13 from 17 (gram-scale reaction)

To a solution of ether 17 (4.72 g, 13.2 mmol, 1.0 eq.) in THF (132 mL) at −78 °C was added a solution of n-BuLi (21.1 mL, 2.5 M in hexane, 52.7 mmol, 4.0 eq.). After 10 min at that temperature the reaction mixture was warmed to −13 °C (change of cooling baths) and stirred for 90 min. Water was added and the reaction mixture was diluted with EtOAc. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 20:1 to 15:1 to 10:1) to afford alkene 13 (1.27 g, 5.45 mmol, 41%) as a white solid.
Compound 19

\[
\begin{align*}
\text{Me}_3\text{Si} & \quad \equiv \\
18 & \\
\text{n-BuLi, THF, } -78 \degree C, 2 \text{ h} & \\
\text{then TBAF, } -78 \degree C \text{ to } 23 \degree C, 24 \text{ h} & \\
16 & \quad \longrightarrow \quad 19 \\
\text{C}_{10}\text{H}_{17}\text{Cl} & \quad (172.70) \\
\text{C}_{13}\text{H}_{20} & \quad (176.30)
\end{align*}
\]

To a solution of 1-(trimethylsilyl)propyne (18) (9.52 mL, 7.22 g, 64.3 mmol, 1.2 eq.) in THF (120 mL) at −78 °C was added n-BuLi (25.1 mL, 2.5 M in hexane, 62.7 mmol, 1.2 eq.). The yellow solution was stirred for 2 h at that temperature. Geranyl chloride (16) (9.03 g, 52.3 mmol, 1.0 eq.) in THF (8 mL, flask rinsed with 2 x 1 mL) was added. The reaction mixture was stirred for 2 h at −78 °C. Tetrabutylammonium fluoride (68.0 mL, 1 M in THF, 68.0 mmol, 1.3 eq.) was added to the flask and the reaction mixture was allowed to reach 23 °C over 24 h. Water was added and the reaction mixture was diluted with EtOAc. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/CH₂Cl₂, 0:1 to 1:1) to afford alkyne 19 (7.64 g, 43.4 mmol, 83%) as a slightly yellow oil.

Rₚ = 0.80 (n-pentane).

\(^1\text{H-NMR} \) (700 MHz, CDCl₃): δ [ppm] = 5.19 – 5.16 (m, 1H), 5.12 – 5.07 (m, 1H), 2.26 – 2.18 (m, 4H), 2.10 – 2.05 (m, 2H), 2.03 – 1.98 (m, 2H), 1.94 (t, J = 2.5 Hz, 1H), 1.68 (s, 3H), 1.62 (s, 3H), 1.60 (s, 3H).

\(^{13}\text{C-NMR} \) (176 MHz, CDCl₃): δ [ppm] = 136.9, 131.6, 124.4, 122.6, 84.7, 68.2, 39.8, 27.3, 26.8, 25.8, 19.1, 17.8, 16.3.

\( \text{IR (ν/cm}^{-1}, \text{ATR) = } 3309, 2966, 2921, 2856, 2118, 1445, 1377, 1325, 1242, 1108. \)

\( \text{HRMS (EI)}: m/z \text{ calculated for } \text{C}_{13}\text{H}_{19}^+ \text{[M-H]}^+ \text{ 175.1481, found 175.1488.} \)

The spectral data matched previously obtained data.² ³
To a suspension of Cp$_2$ZrCl$_2$ (3.79 g, 13.0 mmol, 25 mol%) in CH$_2$Cl$_2$ (200 mL) at −30 °C was added AlMe$_3$ (77.8 mL, 2.0 M in toluene, 156 mmol, 3.0 eq.). H$_2$O (935 µL, 51.9 mmol, 1.0 eq.) was added slowly. The reaction mixture was warmed to −23 °C over 1 h. Alkyne 19 (9.14 g 51.9 mmol, 1.0 eq.) in CH$_2$Cl$_2$ (75 mL) was added dropwise to the reaction mixture at that temperature. After 1 h a solution of iodine (15.8 g, 62.2 mmol, 1.2 eq.) in THF (75 mL) was added dropwise at the same temperature. The reaction was allowed to reach 23 °C over 15 h. A saturated aqueous solution of K$_2$CO$_3$ (15 mL) was added dropwise. The reaction mixture was diluted with CH$_2$Cl$_2$. The organic phase was separated and the aqueous phase was extracted with CH$_2$Cl$_2$. The combined organic extracts were washed with brine, dried over MgSO$_4$, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO$_2$, n-pentane) to afford vinyl iodide 20 (11.9 g, 37.2 mmol, 72%) as a colorless oil.

R$_f$ = 0.92 (n-pentane).

$^1$H-NMR (700 MHz, CDCl$_3$): δ [ppm] = 5.87 (sext, $J = 1.1$ Hz, 1H), 5.10 – 5.05 (m, 2H), 2.25 – 2.20 (m, 2H), 2.16 – 2.10 (m, 2H), 2.09 – 2.04 (m, 2H), 2.00 – 1.96 (m, 2H), 1.84 (d, $J = 1.1$ Hz, 3H), 1.69 (d, $J = 1.4$ Hz, 3H), 1.61 (s, 3H), 1.59 (s, 3H).

$^{13}$C-NMR (176 MHz, CDCl$_3$): δ [ppm] = 148.0, 136.2, 131.6, 124.4, 123.1, 74.9, 39.8, 39.7, 26.9, 26.4, 25.9, 24.1, 17.9, 16.2.

IR (v/cm$^{-1}$, ATR) = 2963, 2918, 2850, 1442, 1377, 1267, 1141, 833, 766, 664.

HRMS (EI): m/z calculated C$_{14}$H$_{23}$I $^{[M−I]}$ 191.1794, found 191.1799.

The spectral data matched previously obtained data.$^3$

Note: The use of fresh Cp$_2$ZrCl$_2$ and AlMe$_3$ is necessary for reproducible yield.
Compound S2
Procedure using Corey-Noe-Lin ligand

\[
\begin{align*}
\text{K}_2\text{OsO}_2(\text{OH})_2 (0.30 \text{ mol}) & \quad \text{Corey-Noe-Lin ligand (0.24 mol)} \\
\text{K}_3\text{Fe(CN)}_6, \text{MeSO}_2\text{NH}_2, \text{K}_2\text{CO}_3 & \quad \text{S2} \\
t-\text{BuOH}/\text{H}_2\text{O 1:1, 1 °C, 53 h} & \quad (36\%, 71\% \text{ brsm, 94\% ee})
\end{align*}
\]

K\text{O}_2\text{S(OH)}_2 (3.5 mg, 9.5 µmol, 0.30 mol%), K\text{I}_3\text{Fe(CN)}_6 (3.10 g, 9.43 mmol, 3.0 eq.), Me\text{SO}_2\text{NH}_2 (299 mg, 3.14 mmol, 1.0 eq.), \text{K}_2\text{CO}_3 (1.30 g, 9.43 g, 3.0 eq.) and Corey-Noe-Lin ligand (8.6 mg, 7.5 µmol, 0.24 mol%) were dissolved under stirring in t-BuOH/H\text{O}_2 (32 mL, 1:1) at 23 °C. After solvation the reaction mixture was cooled to 1 °C and stirred for 30 min. Vinyl iodide 20 (1.00 g, 3.14 mmol, 1.0 eq.) was added and the reaction mixture was stirred for 53 h at the same temperature. \text{Na}_2\text{SO}_3 (1.98 g, 15.7 g, 5.0 eq.) and a saturated aqueous solution of \text{Na}_2\text{SO}_3 (5 mL) were added at 1 °C. After 30 min the reaction mixture was allowed to warm to 23 °C and was diluted with EtOAc. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with KOH (2 M) and brine, dried over MgSO_4, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO_2, n-pentane/EtOAc 5:1 to 4:1) to afford diol S2 (399 mg, 1.13 mmol, 36%, 71% brsm, 94% ee) and recovered vinyl iodide 20 (490 mg, 1.54 mmol) as colorless oils.

R_f = 0.11 (n-pentane/EtOAc, 5:1).

[\alpha]_D^{29} = +9.4 (c = 1.38, CHCl_3).
\textbf{\textsuperscript{1}H-NMR} (700 MHz, CDCl\textsubscript{3}): \(\delta\) [ppm] = 5.86 (sext, \(J = 1.1\) Hz, 1H), 5.15 – 5.10 (m, 1H), 3.33 (dd, \(J = 10.6, 2.0\) Hz, 1H), 2.25 – 2.21 (m, 3H), 2.19 (s, 1H), 2.16 – 2.11 (m, 2H), 2.09 – 2.03 (m, 1H), 2.01 (s, 1H), 1.83 (d, \(J = 1.1\) Hz, 3H), 1.61 (q, \(J = 0.9\) Hz, 3H), 1.57 (dddd, \(J = 13.8, 9.1, 7.1, 2.0\) Hz, 1H), 1.40 (dddd, \(J = 14.0, 10.6, 8.8, 5.4\) Hz, 1H), 1.20 (s, 3H), 1.16 (s, 3H).

\textbf{\textsuperscript{13}C-NMR} (176 MHz, CDCl\textsubscript{3}): \(\delta\) [ppm] = 147.8, 136.1, 123.9, 78.3, 75.0, 73.2, 39.5, 36.9, 29.9, 26.7, 26.3, 24.0, 23.4, 16.1.

\textbf{IR} (\(\nu/\text{cm}^{-1}, \text{ATR}\)) = 3407, 3057, 2924, 2853, 1448, 1379, 1268, 1142, 1076, 766.

\textbf{HRMS (ESI)}: \(m/z\) calculated for \(\text{C}_{14}\text{H}_{25}\text{IO}_{2}\text{Na}^+\) [M+Na]\(^+\) 375.0791, found 375.0805.
Procedure using (DHQD)$_2$PHAL

K$_2$OsO$_2$(OH)$_4$ (20.4 mg, 56.0 μmol, 0.50 mol%), K$_3$Fe(CN)$_6$ (11.0 g, 33.5 mmol, 3.0 eq.), MeSO$_2$NH$_2$ (1.05 g, 11.0 mmol, 1.0 eq.), K$_2$CO$_3$ (4.61 g, 33.4 g, 3.0 eq.) and (DHQD)$_2$PHAL (44.9 mg, 58.0 μmol, 0.52 mol%) were dissolved under stirring in t-BuOH/H$_2$O (116 mL, 1:1) at 23 °C. After solvation the reaction mixture was cooled to 1 °C and stirred for 30 min. Vinyl iodide 20 (3.54 g, 11.1 mmol, 1.0 eq.) was added and the reaction mixture was stirred for 71 h at the same temperature. Na$_2$SO$_3$ (7.01 g, 55.6 g, 5.0 eq.) and a saturated aqueous solution of Na$_2$SO$_3$ (5 mL) were added at 1 °C. After 30 min the reaction mixture was allowed to warm to 23 °C and was diluted with EtOAc. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with KOH (2 M) and brine, dried over MgSO$_4$, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO$_2$, n-pentane/EtOAc 5:1 to 4:1) to afford diol S2 (1.28 g, 3.64 mmol, 33%, 44% brsm, 97% ee) and recovered vinyl iodide 20 (896 mg, 2.81 mmol) as colorless oils.
Determination of absolute configuration: Mosher ester analysis of S2

(S)-Mosher ester

\[
\text{S2} \quad \text{C}_{14}\text{H}_{25}\text{IO}_{2} \\ (352.25)
\]

To a solution of diol S2 (8.0 mg, 23 \(\mu\)mol, 1.0 eq.) in \(\text{CH}_2\text{Cl}_2\) (0.5 mL) at 23 \(^\circ\)C was added \(\text{NEt}_3\) (25.2 \(\mu\)L, 182 \(\mu\)mol, 8.0 eq.), (\(R\))-MTPA-Cl (8.50 \(\mu\)L, 45.4 \(\mu\)mol, 2.0 eq.) and DMAP (one crystal) successively. The solution was stirred for 12 h. The solution was directly purified by flash column chromatography (SiO\(_2\), \(n\)-pentane/EtOAc 1:0 to 9:1) to afford ester S3 as a white solid (7.9 mg, 14 \(\mu\)mol, 61%).

\(^1\text{H-NMR}\) (500 MHz, CDCl\(_3\)): \(\delta\) [ppm] = 7.64 – 7.58 (m, 2H), 7.43 – 7.38 (m, 3H), 5.92 – 5.83 (m, 1H), 5.05 – 5.01 (m, 1H), 4.98 (dd, \(J = 9.9, 2.2\) Hz, 1H), 3.58 (s, 3H), 2.24 – 2.20 (m, 2H), 2.16 – 2.09 (m, 2H), 2.00 – 1.92 (m, 2H), 1.83 (s, 3H), 1.82 – 1.75 (m, 1H), 1.65 (dtd, \(J = 14.5, 9.6, 5.4\) Hz, 1H), 1.55 (s, 3H), 1.51 (\(s_{br}\), 1H), 1.18 (s, 3H), 1.14 (s, 3H).

HRMS (ESI): \(m/z\) calculated for \(\text{C}_{24}\text{H}_{32}\text{F}_{3}\text{IO}_{4}\) \([\text{M+Na}]^+\) 591.1190, found 591.1199.

(R)-Mosher ester

\[
\text{S2} \quad \text{C}_{14}\text{H}_{25}\text{IO}_{2} \\ (352.25)
\]

To a solution of diol S2 (7.3 mg, 21 \(\mu\)mol, 1.0 eq.) in \(\text{CH}_2\text{Cl}_2\) (0.5 mL) at 23 \(^\circ\)C was added \(\text{NEt}_3\) (23.0 \(\mu\)L, 166 \(\mu\)mol, 8.0 eq.), (\(S\))-MTPA-Cl (7.76 \(\mu\)L, 41.4 \(\mu\)mol, 2.0 eq.) and DMAP (one crystal) successively. The solution was stirred for 12 h. The solution was directly purified by flash column chromatography (SiO\(_2\), \(n\)-pentane/EtOAc 1:0 to 9:1) to afford ester S4 as a white solid (5.2 mg, 9.1 \(\mu\)mol, 44%).
$^1$H-NMR (500 MHz, CDCl$_3$): $\delta$ [ppm] = 7.65 – 7.61 (m, 2H), 7.43 – 7.39 (m, 3H), 5.88 – 5.86 (m, 1H), 5.01 – 4.98 (m, 1H), 4.97 (dd, $J = 10.2, 2.1$ Hz, 1H), 3.57 (s, 3H), 2.25 – 2.19 (m, 2H), 2.14 – 2.08 (m, 2H), 1.89 – 1.84 (m, 2H), 1.83 (s, 3H), 1.75 – 1.65 (m, 1H), 1.62 – 1.57 (m, 1H), 1.51 (s, 3H), 1.28 (s, 1H), 1.23 (s, 3H), 1.16 (s, 3H).

**HRMS (ESI):** m/z calculated for C$_{24}$H$_{32}$F$_3$IO$_4$Na$^+$ [M+Na]$^+$ 591.1190, found 591.1186.

The assignments were resolved using NMR spectroscopic methods: $^1$H, COSY, HMQC, HMBC. The comparison of both esters shows ($R$)-configuration at C-3.$^4$

$\Delta \delta$ [(S)-MTPA – (R)-MTPA] =

![Diagram of MTPA molecule with delta values]
HPLC-Analysis of \( S_2 \)

HPLC-Analysis was performed using Chiralpak IA, 3% EtOH/hexane, 20 °C, 1 mL/min.

1) Racemic mixture

![Graph](image1)

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Totals: 412.36322 13.58551

2) \( S_2 \) synthesized using CNL-ligand

![Graph](image2)

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Totals: 595.74914 18.01126
3) S2 synthesized using (DHQD)$_2$PHAL-ligand
Compound 14

To a solution of diol S2 (1.52 g, 4.31 mmol, 1.0 eq.) in CH$_2$Cl$_2$ (13 mL) at 0 °C was added pyridine (5.20 mL, 65.0 mmol, 15 eq.) and MsCl (367 µL, 543 mg, 4.74 mmol, 1.1 eq.) sequentially. The reaction mixture was allowed to warm to 23 °C over 15 h. Methanol (60 mL) and K$_2$CO$_3$ (5.95 g, 43.1 mmol, 10 eq.) were added sequentially at 23 °C and the reaction mixture was stirred for 4 h. The reaction mixture was concentrated under reduced pressure. The residue was diluted with CH$_2$Cl$_2$ and water. The organic phase was separated and the aqueous phase was extracted with CH$_2$Cl$_2$. The combined organic extracts were washed with a saturated aqueous solution of CuSO$_4$ and brine, dried over MgSO$_4$, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO$_2$, n-pentane/EtOAc 50:1 to 3:1) to afford epoxide 14 (1.16 g, 3.48 mmol, 81%, 89% brsm.) as a slightly yellow oil and recovered diol S2 (140 mg, 397 µmol) as a colorless oil.

$R_f=0.54$ (n-pentane/EtOAc, 10:1).

$\left[\alpha\right]_{D}^{29} = -2.66$ (c = 0.45, CHCl$_3$).

$^{1}$H-NMR (700 MHz, CDCl$_3$): $\delta$ [ppm] = 5.89 – 5.86 (m, 1H), 5.15 – 5.10 (m, 1H), 2.69 (t, $J = 6.2$ Hz, 1H), 2.25 – 2.21 (m, 2H), 2.19 – 2.11 (m, 3H), 2.08 (dt, $J = 14.4$, 7.5 Hz, 1H), 1.84 (s, 3H), 1.64 – 1.60 (m, 5H), 1.31 (s, 3H), 1.26 (s, 3H).

$^{13}$C-NMR (176 MHz, CDCl$_3$): $\delta$ [ppm] = 147.8, 135.4, 123.7, 74.9, 64.3, 58.5, 39.6, 36.5, 27.6, 26.4, 25.1, 24.1, 18.9, 16.2.

IR (v/cm$^{-1}$, ATR) = 2958, 2923, 2855, 1447, 1377, 1322, 1267, 1139, 1120, 872.

HRMS (ESI): $m/z$ calculated for C$_{14}$H$_{24}$IO$^+$ [M+H]$^+$: 335.0867, found 335.0869.
Alkene 13 (1.18 g, 4.97 mmol, 1.4 eq.) and 9-BBN dimer 5 (1.21 g, 9.94 mmol, 2.8 eq.) were combined and stirred for 5 min, then the reaction flask was heated to 85 °C for 4 h. The reaction flask was allowed to cool to 23 °C and THF (10 mL, degassed by freeze pump thaw 3x) was added. The reaction flask was cooled to 0 °C and NaOH (7.10 mL, 3 M, 21.3 mmol, 6.0 eq., purged with Ar for 20 min) was added dropwise. A solution of epoxide 14 (1.19 g, 3.55 mmol, 1.0 eq.) and AsPh₃ (435 mg, 1.42 mmol, 40 mol%) in THF (6 mL, purged with Ar for 20 min, the flask was rinsed 2x with 1 mL) was added to the reaction mixture. The reaction mixture was purged with Ar for 5 min. Pd(dpdpf)Cl₂ (260 mg, 355 μmol, 10 mol%) was added and the reaction mixture was stirred at 1 °C for 18 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 40:1 to 1:1) to afford epoxy dienol 12 (1.22 g, 2.75 mmol, 77%) as a colorless oil.

Rₛ = 0.64 (n-pentane/EtOAc, 5:1).

[α]ᴰ²⁹ = +0.52 (c = 0.64, CHCl₃).

¹H-NMR (700 MHz, CDCl₃): δ [ppm] = 5.20 – 5.13 (m, 2H), 2.70 (t, J = 6.3 Hz, 1H), 2.19 – 2.11 (m, 1H), 2.11 – 2.03 (m, 5H), 1.99 (t, J = 7.7 Hz, 2H), 1.86 (dt, J = 12.3, 3.2 Hz, 1H), 1.69 – 1.62 (m, 4H), 1.62 – 1.61 (m, 3H), 1.61 – 1.60 (m, 3H), 1.60 – 1.55 (m, 2H), 1.46 – 1.40 (m, 2H), 1.40 – 1.33 (m, 2H), 1.29 (s, 3H), 1.27 – 1.24 (m, 4H), 1.20 (s, 1H), 1.15 (dd, J = 13.6, 4.2
Hz, 1H), 1.12 (s, 3H), 1.03 (t, J = 4.0 Hz, 1H), 0.97 (td, J = 13.0, 3.8 Hz, 1H), 0.91 (dd, J = 12.2, 2.4 Hz, 1H), 0.86 (s, 3H), 0.78 (s, 6H).

$^{13}$C-NMR (176 MHz, CDCl$_3$): $\delta$ [ppm] = 135.1, 134.2, 125.3, 125.1, 74.2, 64.3, 61.7, 58.5, 56.3, 44.7, 42.2, 39.9, 39.8, 39.3, 36.5, 33.6, 33.4, 31.6, 27.6, 26.8, 25.7, 25.1, 24.0, 21.7, 20.7, 18.9, 18.6, 16.4, 16.2, 15.6.

IR (ν/cm$^{-1}$, ATR) = 3479, 2924, 2852, 1458, 1384, 1249, 1158, 1044, 938, 756.

HRMS (ESI): m/z calculated for C$_{30}$H$_{52}$O$_2$Na$^+$ [M+Na]$^+$ 467.3859, found 467.3867.
Compound 10 and compound 21

To a solution of EtAlCl₂ (0.20 mL, 1 M in hexane, 0.20 mmol, 3.0 eq.) in CH₂Cl₂ (33 mL) at −78 °C was added a precooled solution of epoxy dienol 12 (29.3 mg, 66.0 μmol, 1.0 eq.) in CH₂Cl₂ (33 mL) over 1 h (cannula passing through dry ice). The reaction mixture was then stirred for 30 min at the same temperature. NH₃ (aq., 0.2 mL) and MeOH/H₂O (4:1, 0.2 mL) were added successively. The reaction mixture was allowed to reach 23 °C, and then a solution of saturated aqueous Rochelle salt was added. The organic phase was separated and the aqueous phase was extracted with CH₂Cl₂. The combined organic extracts were washed with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 15:1 to 10:1 to 5:1) to afford alcohol 10 (5.9 mg, 13 μmol, 20%) as a white solid and oxane 21 (3.4 mg, 7.6 μmol, 12%) as a colorless oil. Crystals of 10 suitable for single crystal X-ray diffraction were obtained after slow evaporation from CH₂Cl₂/MeCN.

Compound 10

R⁰ = 0.48 (n-pentane/EtOAc, 9:1).

[α]D²⁸ = +6.3 (c = 0.49, CH₂Cl₂).

¹H-NMR (700 MHz, C₆D₆): δ [ppm] = 3.03 – 2.96 (m, 1H), 1.94 (ddt, J = 16.0, 12.8, 3.3 Hz, 2H), 1.82 – 1.65 (m, 4H), 1.64 – 1.48 (m, 3H), 1.47 – 1.39 (m, 6H), 1.37 – 1.32 (m, 3H), 1.36 (s, 3H), 1.35 (s, 3H), 1.22 – 1.15 (m, 4H), 0.95 (s, 3H), 0.91 – 0.89 (m, 1H), 0.87 – 0.82 (m, 3H), 0.85 (s, 3H), 0.79 (s, 3H), 0.75 – 0.73 (m, 1H), 0.74 (s, 3H), 0.74 (s, 3H), 0.68 (s, 3H).

¹³C-NMR (176 MHz, C₆D₆): δ [ppm] = 80.1, 79.9, 78.4, 61.1 (2C), 56.6, 55.5, 45.8, 45.6, 42.3, 40.6, 39.2, 39.1, 38.9, 38.7, 33.7, 33.6, 28.4, 28.1, 25.7, 25.5 (2C), 25.3, 21.8, 21.2, 20.8, 19.3, 16.1 (2C), 15.7.

IR (v/cm⁻¹, ATR) = 3394, 2924, 2855, 1458, 1377, 1283, 1187, 1126, 1084, 1043.
HRMS (ESI): $m/z$ calculated for $C_{30}H_{52}O_2Na^+$ [M+Na]$^+$ 467.3859, found 467.3848. $M_p = 197 – 199$ °C.

Note: The use of fresh EtAlCl$_2$ is necessary for reproducible yield. 10 showed signs of decomposition after treatment with CDCl$_3$ (unpurified) for 12 h.

Compound 21

$R_f = 0.50$ (n-pentane/EtOAc, 9:1).

$[a]_{D}^{28} = -3.9$ ($c = 0.28$, CH$_2$Cl$_2$).

$^1$H-NMR (700 MHz, C$_6$D$_6$): $\delta$ [ppm] = 3.01 (dd, $J = 11.2$, 4.1 Hz, 1H), 1.99 – 1.90 (m, 1H), 1.86 – 1.81 (m, 1H), 1.71 – 1.67 (m, 1H), 1.66 – 1.28 (m, 20H), 1.30 (s, 3H), 1.17 (s, 3H), 1.11 – 1.09 (m, 1H), 1.03 (s, 3H), 1.01 (d, $J = 6.7$ Hz, 3H), 0.91 – 0.89 (m, 1H), 0.86 – 0.84 (m, 2H), 0.85 (s, 3H), 0.81 (s, 3H), 0.78 (s, 3H), 0.68 (s, 3H).

$^{13}$C NMR (176 MHz, C$_6$D$_6$): $\delta$ [ppm] = 80.8, 78.9, 75.0, 57.1, 54.5, 47.5, 45.2, 43.6, 42.4, 40.0, 39.1, 38.3, 37.3, 33.5, 33.4, 32.9, 32.1, 28.8, 28.2, 26.4, 24.3, 21.5 (2C), 21.2, 19.1, 18.0, 17.5, 16.0, 15.5, 15.2.

IR ($\nu$/cm$^{-1}$, ATR) = 3415, 2927, 2867, 1462, 1380, 1322, 1045, 1017, 998, 976.

HRMS (ESI): $m/z$ calculated for $C_{30}H_{52}O_2Na^+$ [M+Na]$^+$ 467.3859, found 467.3850.
Compound 22

To a solution of oxane 21 (3.6 mg, 8.1 \( \mu \)mol, 1.0 eq.) in CH\(_2\)Cl\(_2\) (1 mL) at 23 °C was added \( N,N \)-dimethyl-4-aminopyridine (19.8 mg, 162 \( \mu \)mol, 20 eq.) and 4-bromobenzoyl chloride (9.1 mg, 41 \( \mu \)mol, 5.0 eq.). The reaction mixture was stirred for 3 d at 50 °C in a closed vial. The residue was directly purified by flash column chromatography (SiO\(_2\), n-pentane/EtOAc 1:0 to 20:1 to 5:1) to afford ester 22 (3.7 mg, 5.9 \( \mu \)mol, 73%) as a white solid. Crystals suitable for single crystal X-ray diffraction were obtained after slow evaporation from 1,2-dichloroethane, 2-propanol and benzene.

\( R_f \) = 0.80 (n-pentane/EtOAc, 9:1).

\( [\alpha]^{25}_D \) = −2.4 (c = 0.07, CHCl\(_3\)).

\( ^1H\)-NMR (700 MHz, CDCl\(_3\)): \( \delta \) [ppm] = \( \delta \) 7.91 (d, \( J = 8.5 \) Hz, 2H), 7.58 (d, \( J = 8.5 \) Hz, 2H), 4.69 – 4.62 (m, 1H), 1.94 – 1.86 (m, 1H), 1.85 – 1.79 (m, 1H), 1.79 – 1.69 (m, 3H), 1.68 – 1.58 (m, 6H), 1.49 – 1.35 (m, 6H), 1.27 – 1.24 (m, 6H), 1.22 – 1.16 (m, 2H), 1.14 – 1.08 (m, 2H), 1.04 (s, 3H), 1.01 (s, 3H), 0.92 (d, \( J = 6.6 \) Hz, 3H), 0.89 (s, 3H), 0.89 – 0.86 (m, 2H), 0.85 (s, 3H), 0.78 (s, 3H), 0.73 (s, 3H).

\( ^{13}C\)-NMR (176 MHz, CDCl\(_3\)): \( \delta \) [ppm] = 165.9, 131.8 (2C), 131.2 (2C), 130.0, 128.0, 82.6, 80.7, 75.1, 56.9, 54.0, 47.4, 44.8, 43.3, 42.3, 39.7, 38.2, 38.1, 37.2, 33.5, 33.4, 32.4, 31.7, 28.7, 26.2, 24.2, 24.0, 21.4, 21.2, 21.0, 18.8, 17.6, 17.2, 16.7, 15.9, 15.0.

IR (\( \nu/cm^{-1}\), ATR) = 2925, 2854, 1718, 1591, 1461, 1396, 1377, 1271, 847, 757.

HRMS (EI): \( m/z \) calculated for \( C_{37}H_{55}BrO_3 \) [M]+: 626.3329, found 626.3308.

\( \text{Mp} = 182 – 184 \) °C.
To a solution of alcohol 10 (5.7 mg, 13 μmol, 1.0 eq.) in CH$_2$Cl$_2$ (2.5 mL) at 23 °C was added Dess-Martin periodinan (DMP)$^6$ (10.9 mg, 26 μmol, 2.0 eq.). The reaction mixture was stirred for 4 h. Afterwards, NaOAc (34.9 mg, 256 μmol, 20 eq.) and AcOOH (24.6 μL, 27.8 mg, 128 μmol, 35% in acetic acid, 10 eq.) were added successively. The reaction flask was covered with aluminum foil and stirred for 17 h. Another portion of NaOAc (34.9 mg, 256 μmol, 20 eq.) and AcOOH (24.6 μL, 27.8 mg, 128 μmol, 35% in acetic acid, 10 eq.) were added successively. The reaction mixture was stirred for 5 h. The residue was directly purified by flash column chromatography (SiO$_2$, n-pentane/EtOAc 1:0 to 10:1 to 5:1 and Al$_2$O$_3$, n-pentane/EtOAc 1:0 to 5:1 and SiO$_2$, toluene/Et$_2$O 5:1 to 1:1) to afford cupacinoxepin 4 (3.9 mg, 8.5 μmol, 66%) as a white solid. Crystals suitable for single crystal X-ray diffraction were obtained after slow evaporation from acetone/n-hexane.

$R_f$ = 0.40 (n-pentane/EtOAc, 4:1).

$[\alpha]^{26}_D$ = +49.0 (c = 0.04, CHCl$_3$) [Lit$^7$]$[\alpha]^{22}_D$ = +56.4 (c = 1.3, CHCl$_3$)].

$^1$H-NMR (500 MHz, CDCl$_3$): δ [ppm] = 2.66 (td, $J$ = 13.8, 4.8 Hz, 1H), 2.48 (ddd, $J$ = 14.2, 5.2, 3.5 Hz, 1H), 1.93 – 1.81 (m, 3H), 1.80 – 1.69 (m, 4H), 1.69 – 1.58 (m, 3H), 1.59 – 1.49 (m, 5H), 1.48 (s, 3H), 1.47 – 1.39 (m, 2H), 1.36 (s, 3H), 1.36 – 1.32 (m, 2H), 1.29 (s, 3H), 1.25 (s, 3H), 1.24 – 1.17 (m, 2H), 1.13 (td, $J$ = 13.5, 4.3 Hz, 1H), 1.00 (s, 3H), 0.93 – 0.86 (m, 2H), 0.85 (s, 3H), 0.77 (s, 3H), 0.74 (s, 3H).

$^{13}$C-NMR (176 MHz, CDCl$_3$): δ [ppm] = 175.0, 85.9, 80.5, 78.9, 61.4, 61.0, 56.3, 52.2, 45.3, 43.7, 42.1, 41.2, 40.5, 40.3, 39.0, 33.6 (2C), 32.6, 30.8, 27.4, 26.5, 26.0, 25.5, 25.2, 24.2, 21.6, 20.9, 19.0, 18.4, 16.0.

IR (ν/cm$^{-1}$, ATR) = 2922, 2854, 1719, 1459, 1375, 1286, 1131, 1022, 977, 753.
HRMS (EI): m/z calculated for C\textsubscript{30}H\textsubscript{50}O\textsubscript{3}\textsuperscript{+} [M]\textsuperscript{+}: 458.3754, found 458.3776.

Mp: 204 – 207 °C.
To a solution of alcohol 10 (8.2 mg, 18 µmol, 1.0 eq.) in CH₂Cl₂ (2.5 mL) at 23 °C was added 1,1'-thiocarbonyldiimidazole (69.2 mg, 369 µmol, 20 eq.) and N,N-dimethyl-4-aminopyridine (45.1 mg, 369 µmol, 20 eq.). The reaction mixture was stirred for 13.5 h in a pressure tube at 70 °C. The residue was directly purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 10:1 to 5:1) to afford thiocarbamate S5 (8.5 mg, 15 µmol, 83%) as a white solid.

Rᶠ = 0.32 (n-pentane/EtOAc, 9:1).
[α]D²⁵ = +36.2 (c = 0.71, CH₂Cl₂).

¹H-NMR (700 MHz, C₆D₆): δ [ppm] = 8.41 (s, 1H), 7.52 – 7.48 (m, 1H), 7.02 – 6.95 (m, 1H), 5.12 (dd, J = 12.0, 4.7 Hz, 1H), 1.97 (dt, J = 12.6, 3.2 Hz, 1H), 1.87 (dt, J = 12.8, 3.2 Hz, 1H), 1.84 – 1.73 (m, 4H), 1.68 – 1.55 (m, 4H), 1.51 (dt, J = 13.3, 3.7 Hz, 1H), 1.48 – 1.45 (m, 1H), 1.45 – 1.40 (m, 1H), 1.40 – 1.35 (m, 5H), 1.34 – 1.31 (m, 4H), 1.27 – 1.11 (m, 6H), 1.08 – 1.00 (m, 1H), 0.89 – 0.87 (m, 4H), 0.86 – 0.83 (m, 1H), 0.82 (s, 3H), 0.79 (s, 3H), 0.70 (dd, J = 12.3, 2.3 Hz, 1H), 0.66 (s, 3H), 0.65 (s, 3H), 0.60 (s, 3H).

¹³C-NMR (176 MHz, C₆D₆): δ [ppm] = 184.6, 136.7, 131.6, 118.3, 91.1, 80.3, 79.6, 60.9, 60.7, 56.6, 55.0, 45.5, 45.5, 42.3, 40.7, 39.2, 38.6, 38.4, 38.1, 33.7, 33.6, 28.0, 25.8, 25.6, 25.3, 25.1, 22.6, 21.8, 21.3, 20.3, 19.3, 17.3, 16.2, 15.9.

IR (ν/cm⁻¹, ATR) = 2948, 2865, 1530, 1461, 1385, 1281, 1230, 1127, 1092, 970.

HRMS (ESI): m/z calculated for C₃₄H₅₄N₂O₂S⁺ [M+H⁺]: 555.3979, found 555.3988.
Mp: 199 - 202 °C.
To a solution of thiocarbamate S5 (6.0 mg, 11 μmol, 1.0 eq.) in toluene (4.0 mL, degassed by sparging with Ar for 20 min) at 23 °C was added n-Bu3SnH (8.7 μL, 9.4 mg, 32 μmol, 3.0 eq.) and AIBN (one crystal). The reaction mixture was stirred for 10 min at 160 °C and for 20 min at 120 °C in a pressure tube. Another portion of n-Bu3SnH (8.7 μL, 9.4 mg, 32 μmol, 3.0 eq.) and AIBN (one crystal) were added and the reaction mixture was stirred for 10 min at 160 °C and for 20 min at 120 °C in a pressure tube. The solvent was evaporated and the residue was directly purified by flash column chromatography (SiO2, n-pentane/EtOAc 1:0 to 50:1 to 10:1) to afford onoceranoxide 7 (4.3 mg, 10 μmol, 93%) as a white solid.

\[ \text{R}^2_F = 0.25 \text{ (n-pentane).} \]

\[ [\alpha]^{26}_D = +19.7 \ (c = 0.36, \text{ CHCl}_3) \] [Lit8: [α]D25 = +7.9 ] [Lit9: [α]D25 = +0.02 (c = 0.16, CHCl3).

\(^1H\)-NMR (700 MHz, CDCl3): δ [ppm] = 1.79 – 1.72 (m, 6H), 1.60 – 1.56 (m, 6H), 1.44 – 1.38 (m, 4H), 1.35 – 1.33 (m, 2H), 1.27 – 1.25 (m, 8H), 1.22 – 1.21 (m, 2H), 1.14 – 1.10 (m, 2H), 0.89 – 0.87 (m, 4H), 0.85 (s, 6H), 0.77 (s, 6H), 0.74 (s, 6H).

\(^1H\)-NMR (700 MHz, C6D6): δ [ppm] = 1.97 (dt, J = 12.7, 3.3 Hz, 2H), 1.84 – 1.71 (m, 6H), 1.63 – 1.54 (m, 4H), 1.50 – 1.46 (m, 2H), 1.42 – 1.26 (m, 12H), 1.20 – 1.11 (m, 4H), 0.89 – 0.82 (m, 10H), 0.80 (s, 6H), 0.76 (s, 6H).

\(^13C\)-NMR (176 MHz, CDCl3): δ [ppm] = 80.1 (2C), 60.9 (2C), 56.3 (2C), 45.4 (2C), 42.2 (2C), 40.5 (2C), 39.0 (2C), 33.6 (2C), 33.6 (2C), 25.4 (2C), 25.1 (2C), 21.7 (2C), 20.9 (2C), 19.1 (2C), 15.9 (2C).
$^{13}$C-NMR (176 MHz, C$_6$D$_6$): $\delta$ [ppm] = 80.1 (2C), 61.3 (2C), 56.5 (2C), 45.8 (2C), 42.3 (2C), 40.7 (2C), 39.1 (2C), 33.7 (2C), 33.6 (2C), 25.7 (2C), 25.4 (2C), 21.8 (2C), 21.2 (2C), 19.3 (2C), 16.1 (2C).

IR ($\mu$/cm$^{-1}$, ATR) = 2989, 2927, 2857, 1459, 1371, 1261, 1193, 1086, 1024, 970.

HRMS (ESI): $m/z$ calculated for C$_{30}$H$_{52}$ONa$^+$ [M+Na]$^+$: 451.3910, found 451.3907.

$\textbf{Mp}$: 203 - 205 °C.

Note: For a previous enzymatic synthesis, see:\textsuperscript{9}
8α-hydroxypolypoda-13,17,21 9

Alkene 13 (0.201 g, 850 µmol, 1.0 eq.) and 9-BBN dimer\(^5\) (259 mg, 2.13 mmol, 2.5 eq.) were combined and stirred for 5 min, then the reaction flask was heated to 85 °C for 5 h. The reaction flask was allowed to cool to 23 °C and THF (10 mL, degassed by freeze pump thaw 3x) and NaOH (1.70 mL, 3 M, 5.10 mmol, 6.0 eq., purged with Ar for 20 min) was added. A solution of vinyl iodide 20 (547 mg, 1.72 mmol, 2.0 eq.) and AsPh\(_3\) (117 mg, 0.383 µmol, 45 mol%) in THF (4 mL, purged with Ar for 20 min, the flask was rinsed 2x with 0.5 mL) was added to the reaction mixture. The reaction mixture was purged with Ar for 5 min. Pd(dpdpf)Cl\(_2\) (93.3 mg, 128 µmol, 15 mol%) was added and the reaction mixture was stirred at 23 °C for 17 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with brine, dried over MgSO\(_4\), filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO\(_2\), n-pentane/EtOAc 50:1 to 10:1) to afford triene 9 (229 mg, 534 µmol, 63%) as a slightly yellow oil.

R\(_f\) = 0.54 (n-pentane/EtOAc, 19:1).

\([\alpha]^{25}_D = -0.39 (c = 0.77, \text{CHCl}_3), \quad [\text{Lit}^{10}:\alpha]^{25}_D = -0.9 (c = 0.4, \text{CHCl}_3),\]
\([\text{Lit}^{11}:\alpha]^{24}_D = -0.6 (c = 0.75, \text{CHCl}_3), \quad [\text{Lit}^{12}:\alpha]^{23}_D = -1.8 (c = 0.1, \text{CHCl}_3)\].

\(^1\text{H-NMR}\) (500 MHz, CDCl\(_3\)): δ [ppm] = 5.21 – 5.16 (m, 1H), 5.14 – 5.06 (m, 2H), 2.12 – 2.03 (m, 6H), 2.02 – 1.93 (m, 4H), 1.86 (dt, J = 12.1, 3.1 Hz, 1H), 1.68 (s, 3H), 1.67 – 1.62 (m, 1H), 1.61 (s, 3H), 1.60 (s, 6H), 1.58 – 1.54 (m, 1H), 1.48 – 1.14 (m, 9H), 1.13 (s, 3H), 1.03 (t, J =
4.0 Hz, 1H), 0.98 (td, J = 13.0, 3.7 Hz, 1H), 0.91 (dd, J = 12.1, 2.3 Hz, 1H), 0.87 (s, 3H), 0.79 (s, 6H).

$^{13}$C-NMR (126 MHz, CDCl$_3$): $\delta$ [ppm] = 135.3, 135.1, 131.4, 125.2, 124.6, 124.4, 74.2, 61.7, 56.3, 44.7, 42.2, 39.9 (3C), 39.3, 33.6, 33.4, 31.6, 26.9, 26.8, 25.9, 25.7, 23.9, 21.7, 20.7, 18.6, 17.8, 16.4, 16.2, 15.6.

IR ($\nu$/cm$^{-1}$, ATR) = 3424, 2925, 2860, 1450, 1383, 1157, 1080, 934, 822, 802.

HRMS (ESI): $m/z$ calculated for C$_{30}$H$_{52}$ONa$^+$ [M+Na]$^+$: 451.3910, found 451.3931.

Note: 9 was isolated from fresh rhizomes of Polypodiodes formosana in 1992.$^{10}$ 9 was synthesized in 3 steps in the longest linear synthesis from (+)-sclareolide with an overall yield of 28% and was used as a tricyclization substrate. However, no productive cyclization could be detected under a variety of conditions. For selected conditions see Section 3.

For a previous 13 step racemic synthesis, see:.$^{13}$

For a previous enzymatic synthesis, see:.$^{9,12}$

For a previous 10 step asymmetric synthesis, see:.$^{11}$
Compound S6

To a solution of α-onocerin (20.0 mg, 45.2 μmol, 1.0 eq.) in CH₂Cl₂ (4.0 mL) at 23 °C was added N,N-dimethyl-4-aminopyridine (11.0 mg, 90.4 μmol, 2.0 eq.) and 1,1'-thiocarboxyldiimidazole (16.1 mg, 90.4 μmol, 2.0 eq.). Then the reaction mixture was stirred for 13 h at 60 °C in a closed vial. The residue was directly purified by flash chromatography (SiO₂, n-pentane/EtOAc 30:1 to 4:1 to 2:1) to afford an inseparable mixture (17.5 mg). An aliquot of the obtained material (6.2 mg) was dissolved in toluene (degassed by sparging with Ar for 20 min, 4 mL) in a pressure tube and AIBN (one crystal) and Bu₃SnH (9.10 μL, 33.6 μmol, 0.74 eq.) were added successively. The reaction mixture was stirred at 160 °C for 10 min and at 120 °C for 20 min. The residue was directly purified by flash column chromatography (SiO₂, n-pentane/EtOAc 4:1) to afford alcohol S6 (1.3 mg, 3.05 μmol, 7%) as a white solid.

Rₛ = 0.81 (n-pentane/EtOAc, 4:1).

[α]ᴰ²³ = +11.6 (c = 0.48, CHCl₃) [Lit¹⁴: [α]₁²° = +21° (c = 1.70, CHCl₃)].

¹H-NMR (700 MHz, CDCl₃): δ [ppm] = δ 4.87 – 4.77 (m, 2H), 4.60 – 4.49 (m, 2H), 3.25 (dd, J = 11.8, 4.3 Hz, 1H), 2.40 (dddd, J = 13.0, 11.1, 4.3, 2.4 Hz, 2H), 1.98 (td, J = 12.9, 5.0 Hz, 2H), 1.76 – 1.65 (m, 5H), 1.60 – 1.07 (m, 17H), 0.99 (s, 3H), 0.94 (td, J = 12.9, 3.8 Hz, 1H), 0.87 (s, 3H), 0.79 (s, 3H), 0.76 (s, 3H), 0.64 (s, 3H), 0.63 (s, 3H).

¹³C-NMR (176 MHz, CDCl₃): δ [ppm] = 149.3, 148.6, 106.8, 106.4, 79.1, 58.1, 57.8, 55.8, 54.8, 42.4, 39.7, 39.4, 39.3, 39.2, 38.6, 38.4, 37.2, 33.8 (2C), 28.5, 28.1, 24.7, 24.2, 22.9, 22.7, 21.9, 19.6, 15.5, 14.7 (2C).

IR (ν/cm⁻¹, ATR) = 3350, 3082, 2932, 2846, 1460, 1385, 1227, 1182, 1032, 886.
**HRMS (ESI):** \( m/z \) calculated for \( \text{C}_{30}\text{H}_{50}\text{ONa}^+ \) \([\text{M+Na}]^+\): 449.3754, found 449.3739.

**Mp:** 178 – 180 °C [Lit\(^{14}\): 182 – 184].

Note: This procedure is unoptimized. \( \alpha \)-Onocerin was extracted from spiny restharrow roots.\(^{15}\)

Compound S6 is used as a GC-MS reference to get insight into the structure of the elimination product of the BmeTC catalyzed reaction with 12. See section 6.

![Fig. 1 GC-MS Data for S6.](image)

GC/MS system consisting of a 5977E MSD single-quadrupole mass spectrometer (EI-Mode (70 eV)) with a 7820A GC by Agilent Technologies (Agilent 190915-433UI, 30 m x 250 \( \mu \)m x 0.25 \( \mu \)m). Injection temperature: 300 °C, column temperature: 220-300 °C (increment 3 °C/min).
Optimization of the Wittig-type fragmentation: Synthesis of the Ethers S8 - S21

Compound S7

\[
\begin{align*}
\text{C}_{16}\text{H}_{28}\text{O}_2 & \quad (250.38) \\
\text{C}_{16}\text{H}_{30}\text{O}_2 & \quad (254.41)
\end{align*}
\]

To a stirred suspension of LiAlH\(_4\) (823 mg, 21.7 mmol, 1.0 eq.) in THF (40 mL) at 0°C was added a solution of lactone 15 (5.41 g, 21.6 mmol, 1.0 eq.) in THF (20 mL, flask rinsed with 2 x 20 mL) over 10 min. After stirring for 30 min, KOH (10 mL, 2 M aq.) was added dropwise. The mixture was diluted with CH\(_2\)Cl\(_2\). The organic phase was separated and the aqueous phase was extracted with CH\(_2\)Cl\(_2\). The combined organic extracts were washed with brine, dried over MgSO\(_4\), filtered and concentrated under reduced pressure. Diol S7 (5.49 g, 21.6 mmol, quant.) was obtained as a white solid and was used without further purification.

R\(_f\) = 0.12 (n-pentane/EtOAc 3:1).

[\alpha]^{23}_{\text{D}} = -16.9° (c = 1.05, CHCl\(_3\)).

\(^1\text{H}-\text{NMR}\) (500 MHz, CDCl\(_3\)): δ [ppm] = 3.79 (dt, J = 10.1, 4.3 Hz, 1H), 3.47 (ddd, J = 10.1, 8.2, 5.6 Hz, 1H), 2.75 (s, 2H), 1.90 (dt, J = 12.4, 3.2 Hz, 1H), 1.71 – 1.62 (m, 4H), 1.57 (tt, J = 13.5, 3.5 Hz, 1H), 1.53 – 1.40 (m, 2H), 1.40 – 1.34 (m, 1H), 1.33 – 1.25 (m, 2H), 1.20 (s, 3H), 1.14 (td, J = 13.4, 4.2 Hz, 1H), 0.98 – 0.92 (m, 2H), 0.87 (s, 3H), 0.79 (s, 6H).

\(^{13}\text{C}-\text{NMR}\) (126 MHz, CDCl\(_3\)): δ [ppm] = 73.4, 64.3, 59.3, 56.2, 44.4, 42.1, 39.5, 39.1, 33.6, 33.4, 28.0, 24.8, 21.6, 20.6, 18.6, 15.5.

IR (v/cm\(^{-1}\), ATR) = 3267, 2923, 2867, 1461, 1386, 1189, 1085, 1051, 935, 727.

HRMS (ESI): m/z calculated for C\(_{16}\)H\(_{30}\)O\(_2\)Na\(^+\) [M+Na\(^+\)]: 277.2138, found 277.2147.

Mp = 128 – 130 °C.

The spectral data matched previously obtained data.\(^{16}\)
To a stirred suspension of sodium hydride (60% in mineral oil, 1.13 g, 28.3 mmol, 1.3 eq.) in DMF (30 mL) at 0 °C was added a solution of diol S7 (5.46 g, 21.5 mmol, 1.0 eq.) in DMF (20 mL, flask rinsed with 2 x 5 mL). After 30 min benzyl bromide (3.83 mL, 5.51 g, 32.2 mmol, 1.5 eq.) was added and the mixture was allowed to warm to 23 °C over 13 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 20:1 to 10:1) to afford ether S8 (6.65 g, 19.3 mmol, 90%) as a colorless oil.

Rₑ = 0.88 (n-pentane/EtOAc 3:1).

[α]D²³ = −16.1° (c = 0.88, CHCl₃).

¹H-NMR (700 MHz, CDCl₃): δ [ppm] = 7.38 – 7.30 (m, 4H), 7.30 – 7.25 (m, 1H), 4.53 (d, J = 1.9 Hz, 2H), 3.63 (ddd, J = 9.2, 5.4, 4.1 Hz, 1H), 3.37 (ddd, J = 10.2, 8.8, 4.3 Hz, 1H), 3.32 (s, 1H), 1.90 (dt, J = 12.6, 3.2 Hz, 1H), 1.80 – 1.74 (m, 1H), 1.65 (ddd, J = 13.8, 6.1, 3.7 Hz, 1H), 1.64 – 1.53 (m, 3H), 1.46 – 1.33 (m, 3H), 1.30 – 1.24 (m, 1H), 1.24 – 1.20 (m, 1H), 1.15 – 1.14 (m, 3H), 1.12 (dd, J = 13.5, 4.2 Hz, 1H), 0.91 (dd, J = 12.3, 2.3 Hz, 1H), 0.87 (s, 3H), 0.85 (dd, J = 13.0, 3.7 Hz, 1H), 0.79 (s, 6H).

¹³C-NMR (176 MHz, CDCl₃): δ [ppm] = 138.0, 128.6 (2C), 127.8 (3C), 73.3, 72.4, 72.2, 59.4, 56.2, 44.2, 42.1, 39.6, 39.1, 33.6, 33.4, 25.4, 24.5, 21.6, 20.6, 18.6, 15.4.

IR (ν/cm⁻¹, ATR) = 3438, 2925, 2863, 1457, 1384, 1366, 1076, 930, 910, 732.


The spectral data matched previously obtained data.
To a stirred solution of diol S7 (256 mg, 1.01 mmol, 1.0 eq.) in DMF (4 mL) was added sodium hydride (60% in mineral oil, 60.3 mg, 1.51 mmol, 1.5 eq.) at 0 °C. After 30 min tetrabutylammonium iodide (18.6 mg, 50.3 μmol, 0.05 eq.) and 2-tert-butylbenzyl bromide (341 mg, 1.51 mmol, 1.5 eq.) in DMF (2.0 mL) were added and the mixture was allowed to warm to 23 °C over 20 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 5:1) to afford ether S9 (381 mg, 950 μmol, 94%) as a colorless oil.

**Rf** = 0.39 (n-pentane/EtOAc, 9:1).

$$[\alpha]_{D}^{27} = -3.68 \ (c = 1.34, \ CHCl_3).$$

**1H-NMR** (700 MHz, CDCl₃): δ [ppm] = 7.48 – 7.45 (m, 1H), 7.39 – 7.36 (m, 1H), 7.23 – 7.17 (m, 2H), 4.83 – 4.68 (m, 2H), 3.70 – 3.65 (m, 1H), 3.46 – 3.40 (m, 1H), 3.19 (sbr, 1H), 1.89 (dt, J = 12.6, 3.3 Hz, 1H), 1.82 – 1.76 (m, 1H), 1.67 – 1.56 (m, 4H), 1.43 – 1.40 (m, 10H), 1.39 – 1.36 (m, 1H), 1.29 – 1.22 (m, 2H), 1.18 – 1.15 (m, 1H), 1.14 (s, 3H), 0.94 – 0.90 (m, 2H), 0.88 (s, 3H), 0.83 – 0.80 (m, 1H), 0.80 (s, 6H).

**13C-NMR** (176 MHz, CDCl₃): δ [ppm] = 147.9, 136.3, 131.1, 127.7, 126.3, 126.2, 72.5, 72.5, 71.9, 59.4, 56.3, 44.3, 42.1, 39.7, 39.2, 35.9, 33.6, 33.4, 32.0 (3C), 25.5, 24.5, 21.7, 20.6, 18.6, 15.4.

**IR** (ν/cm⁻¹, ATR) = 3453, 2932, 2867, 1463, 1386, 1363, 1248, 1188, 1074, 934.

**HRMS (ESI):** m/z calculated for C₂₇H₄₄O₂Na⁺ [M+Na]^+: 423.3233, found 423.3240.
Compound S10

To a stirred suspension of sodium hydride (60% in mineral oil, 62.9 mg, 1.57 mmol, 2.0 eq.) in DMF (3 mL) at 0 °C was added a solution of diol S7 (200 mg, 786 μmol, 1.0 eq.) in DMF (3 mL). After 30 min 2-ethylbenzyl bromide (221 mg, 1.11 mmol, 1.4 eq.) in DMF (3 mL) was added and the mixture was allowed to warm to 23 °C over 13 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 20:1 to 5:1) to afford ether S10 (283 mg, 759 μmol, 97%) as a slightly yellow oil.

R_f = 0.61 (n-pentane/EtOAc, 6:1).

[α]_D²⁷ = −16.1 (c = 0.62, CHCl₃).

^1H-NMR (500 MHz, CDCl₃): δ [ppm] = 7.31 (d, J = 7.5 Hz, 1H), 7.25 – 7.14 (m, 3H), 4.65 – 4.48 (m, 2H), 3.66 – 3.60 (m, 1H), 3.38 (td, J = 9.3, 4.5 Hz, 1H), 3.20 (s, 1H), 2.69 (q, J = 7.6 Hz, 2H), 1.89 (dt, J = 12.5, 3.3 Hz, 1H), 1.81 – 1.72 (m, 1H), 1.69 – 1.53 (m, 4H), 1.45 – 1.34 (m, 3H), 1.28 – 1.20 (m, 5H), 1.17 – 1.10 (m, 4H), 0.94 – 0.89 (m, 1H), 0.89 – 0.85 (m, 4H), 0.79 (s, 6H).

^13C-NMR (126 MHz, CDCl₃): δ [ppm] = 142.7, 135.3, 129.1, 128.6, 128.2, 125.9, 72.5, 72.2, 71.2, 59.4, 56.3, 44.2, 42.1, 39.7, 39.2, 33.6, 33.4, 25.5, 25.4, 24.5, 21.6, 20.6, 18.6, 15.4, 15.4.

IR (ν/cm⁻¹, ATR) = 3439, 2930, 2867, 1458, 1384, 1183, 1086, 935, 843, 756.

To a stirred suspension of sodium hydride (60% in mineral oil, 299 mg, 7.48 mmol, 2.0 eq.) in DMF (7 mL) at 0 °C was added a solution of diol S7 (951 mg, 3.74 mmol, 1.0 eq.) in DMF (7 mL). After 30 min 2,4,6-trimethylbenzyl bromide (1.19 g, 5.61 mmol, 1.5 eq.) in DMF (6 mL) was added and the mixture was allowed to warm to 23 °C over 22 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 30:1 to 10:1) to afford ether S11 (1.24 g, 3.20 mmol, 86%) as a slightly yellow oil.

Rf = 0.56 (n-pentane/EtOAc, 6:1).

[α]D²⁷ = −14.9 (c = 3.98, CHCl₃).

¹H-NMR (500 MHz, CDCl₃): δ [ppm] = 6.83 (s, 2H), 4.53 (s, 2H), 3.69 – 3.56 (m, 1H), 3.47 – 3.15 (m, 2H), 2.36 (s, 6H), 2.25 (s, 3H), 1.88 (dt, J = 12.5, 3.2 Hz, 1H), 1.76 – 1.53 (m, 5H), 1.45 – 1.35 (m, 3H), 1.29 – 1.18 (m, 2H), 1.18 – 1.13 (m, 1H), 1.10 (s, 3H), 0.92 (d, J = 2.3 Hz, 1H), 0.89 – 0.85 (m, 4H), 0.79 (s, 3H), 0.78 (s, 3H).

¹³C-NMR (126 MHz, CDCl₃): δ [ppm] = 137.8 (2C), 137.6, 131.0, 129.1 (2C), 72.2, 71.8, 67.2, 59.5, 56.3, 44.2, 42.1, 39.7, 39.1, 33.6, 33.4, 25.6, 24.6, 21.6, 21.1, 20.6, 19.8 (2C), 18.6, 15.4.

IR (ν/cm⁻¹, ATR) = 3439, 2925, 2864, 1613, 1459, 1383, 1235, 1079, 935, 849.

To a stirred suspension of sodium hydride (60% in mineral oil, 281 mg, 7.02 mmol, 2.0 eq.) in DMF (7 mL) at 0 °C was added a solution of diol S7 (893 mg, 3.51 mmol, 1.0 eq.) in DMF (7 mL). After 30 min 2,4,6-triisopropylbenzyl bromide (1.50 g, 5.05 mmol, 1.4 eq.) in DMF (6 mL) was added and the mixture was allowed to warm to 23 °C over 12 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 20:1 to 10:1) to afford ether S12 (1.69 g, 3.60 mmol, quant.) as a slightly yellow oil.

\[ R_f = 0.35 \) (n-pentane/EtOAc, 19:1).

\[ [\alpha]_{D}^{27} = -20.9 \) (c = 1.97, CHCl₃).

\( \text{¹H-NMR} \) (500 MHz, CDCl₃): \( \delta \text{ [ppm]} = 7.00 \) (s, 2H), 4.60 – 4.50 (m, 2H), 3.71 – 3.64 (m, 1H), 3.46 – 3.39 (m, 1H), 3.28 (hept, \( J = 6.8 \) Hz, 2H), 3.06 (sbr, 1H), 2.87 (hept, \( J = 6.9 \) Hz, 1H), 1.86 (dt, \( J = 12.4, 3.1 \) Hz, 1H), 1.80 – 1.70 (m, 1H), 1.69 – 1.57 (m, 4H), 1.47 – 1.33 (m, 4H), 1.29 – 1.23 (m, 1H), 1.19 – 1.13 (m, 1H), 1.10 (s, 3H), 0.97 – 0.90 (m, 2H), 0.89 (s, 3H), 0.80 (s, 6H).

\( \text{¹³C-NMR} \) (126 MHz, CDCl₃): \( \delta \text{ [ppm]} = 148.8, 148.5 \) (2C), 128.7, 121.0 (2C), 72.3, 72.1, 65.5, 59.1, 56.4, 44.3, 42.2, 39.8, 39.2, 34.5, 33.6, 33.4, 29.5 (2C), 25.6, 24.7, 24.6 (2C), 24.5 (2C), 24.1 (2C), 21.6, 20.6, 18.6, 15.4.

\( \text{IR} \) (ν/cm⁻¹, ATR) = 3443, 2957, 2929, 2868, 1607, 1460, 1384, 1074, 877, 753.

\( \text{HRMS (ESI)} \): \( m/z \) calculated for C₃₂H₅₄O₂Na⁺ [M+Na]⁺: 493.4016, found 493.4041.
Compound S13

To a stirred suspension of sodium hydride (60% in mineral oil, 191 mg, 4.77 mmol, 2.0 eq.) in DMF (5 mL) at 0 °C was added a solution of diol S7 (607 mg, 2.38 mmol, 1.0 eq.) in DMF (5 mL). After 30 min tributyl(iodomethyl)stannane (5.52 g, 3.46 mmol, 1.5 eq.) in DMF (5 mL) was added and the mixture was allowed to warm to 23 °C over 24 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 10:1) to afford ether S13 (1.32 g, 2.37 mmol, 99%) as a slightly yellow oil.

Rₐ = 0.61 (n-pentane/EtOAc, 19:1).

[α]²⁷D = −16.8 (c = 1.88, CHCl₃).

¹H-NMR (500 MHz, CDCl₃): δ [ppm] = 3.78 – 3.67 (m, 2H), 3.62 (sbr, 1H), 3.49 (dt, J = 8.6, 4.2 Hz, 1H), 3.24 – 3.16 (m, 1H), 1.89 (dt, J = 12.6, 3.2 Hz, 1H), 1.74 – 1.59 (m, 4H), 1.59 – 1.45 (m, 8H), 1.45 – 1.34 (m, 4H), 1.34 – 1.27 (m, 6H), 1.27 – 1.21 (m, 2H), 1.15 (dd, J = 13.4, 4.0 Hz, 1H), 1.12 (s, 3H), 0.93 – 0.86 (m, 18H), 0.79 (s, 3H), 0.78 (s, 3H).

¹³C-NMR (126 MHz, CDCl₃): δ [ppm] = 77.5, 72.0, 62.4, 59.6, 56.3, 44.1, 42.1, 39.8, 39.1, 33.6, 33.4, 29.3 (3C), 27.5 (3C), 25.4, 24.6, 21.7, 20.6, 18.7, 15.4, 13.9 (3C), 9.1 (3C).

IR (υ/cm⁻¹, ATR) = 3437, 2951, 2923, 2849, 1460, 1381, 1339, 1287, 1073, 934.

To a stirred solution of diol S7 (132 mg, 518 µmol, 1.0 eq.) in DMF (2.5 mL) was added sodium hydride (60% in mineral oil, 26.9 mg, 673 µmol, 1.3 eq.) at 0 °C. After 30 min tetrabutylammonium iodide (9.6 mg, 26 µmol, 0.05 eq.) and 4-(trifluoromethyl)benzyl bromide (173 mg, 725 µmol, 1.4 eq.) in DMF (0.5 mL) were added and the mixture was allowed to warm to 23 °C over 22 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 5:1) to afford ether S14 (192 mg, 466 µmol, 90%) as a colorless oil.

**Rf** = 0.40 (n-pentane/EtOAc, 5:1).

[α]²⁶ D = −18.3 (c = 0.85, CHCl₃).

**¹H-NMR** (700 MHz, CDCl₃): δ [ppm] = 7.60 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 8.0 Hz, 2H), 4.58 (s, 2H), 3.68 – 3.61 (m, 1H), 3.45 – 3.39 (m, 1H), 2.99 (sbr, 1H), 1.90 (dt, J = 12.6, 3.2 Hz, 1H), 1.80 (ddt, J = 15.2, 10.2, 5.3 Hz, 1H), 1.69 – 1.54 (m, 4H), 1.45 – 1.35 (m, 3H), 1.29 – 1.22 (m, 1H), 1.21 (t, J = 4.3 Hz, 1H), 1.17 – 1.14 (m, 3H), 1.12 (dd, J = 13.5, 4.2 Hz, 1H), 0.91 (dd, J = 12.2, 2.3 Hz, 1H), 0.90 – 0.84 (m, 4H), 0.79 (s, 3H), 0.79 (s, 3H).

**¹³C-NMR** (176 MHz, CDCl₃): δ [ppm] = 142.2, 130.0 (q, J = 32.4 Hz), 127.8 (2C), 125.6 (q, J = 3.7 Hz, 2C), 125.1 (q, J = 272.2 Hz), 72.8, 72.7, 72.5, 59.4, 56.3, 44.3, 42.1, 39.7, 39.2, 35.3, 33.4, 25.4, 24.5, 21.6, 20.6, 18.6, 15.4.

**¹⁹F-NMR** (471 MHz, CDCl₃): δ [ppm] = −62.4.

**IR** (ν/cm⁻¹, ATR) = 3455, 2930, 2865, 1622, 1462, 1387, 1325, 1164, 1125, 1070.

**HRMS (ESI):** m/z calculated for C₂₄H₃₅F₃O₂Na⁺ [M+Na⁺]: 435.2481, found 435.2490.
To a stirred solution of diol S7 (301 mg, 1.18 mmol, 1.0 eq.) in DMF (4.0 mL) was added sodium hydride (60% in mineral oil, 70.8 mg, 1.77 mmol, 1.5 eq.) at 0 °C. After 30 min tetrabutylammonium iodide (43.7 mg, 118 μmol, 0.1 eq.) and 2-chlorobenzyl chloride (268 μL, 286 mg, 1.77 mmol, 1.5 eq.) were added and the mixture was allowed to warm to 23 °C over 2 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 5:1) to afford ether S15 (413 mg, 1.09 mmol, 92%) as a colorless oil.

Rf = 0.52 (n-pentane/EtOAc, 5:1).
[α]D²⁷ = −20.6 (c = 1.03, CHCl₃).

¹H-NMR (700 MHz, CDCl₃): δ [ppm] = 7.44 (dd, J = 7.6, 1.6 Hz, 1H), 7.35 – 7.32 (m, 1H), 7.27 – 7.24 (m, 1H), 7.20 (td, J = 7.6, 1.7 Hz, 1H), 4.62 (s, 2H), 3.75 – 3.61 (m, 1H), 3.50 – 3.37 (m, 1H), 3.05 (sbr, 1H), 1.90 (dt, J = 12.6, 3.3 Hz, 1H), 1.80 (ddt, J = 15.2, 10.2, 5.2 Hz, 1H), 1.67 – 1.54 (m, 4H), 1.45 – 1.34 (m, 3H), 1.29 – 1.21 (m, 2H), 1.14 (s, 3H), 1.12 (dd, J = 13.6, 4.1 Hz, 1H), 0.91 (dd, J = 12.2, 2.3 Hz, 1H), 0.90 – 0.84 (m, 4H), 0.79 (s, 3H), 0.79 (s, 3H).

¹³C-NMR (176 MHz, CDCl₃): δ [ppm] = 135.8, 133.0, 129.4, 129.1, 128.8, 127.0, 72.7, 72.6, 70.3, 59.2, 56.2, 44.2, 42.0, 39.7, 39.1, 33.5, 33.4, 25.4, 24.4, 21.6, 20.6, 18.5, 15.4.

IR (ν/cm⁻¹, ATR) = 3448, 2929, 2865, 1446, 1385, 1363, 1102, 1047, 935, 753.

HRMS (ESI): m/z calculated for C₂₃H₃₅ClO₂Na⁺ [M+Na⁺]: 401.2218, found 401.2230.
To a stirred solution of diol S7 (301 mg, 1.18 mmol, 1.0 eq.) in DMF (4.0 mL) was added sodium hydride (60% in mineral oil, 70.9 mg, 1.77 mmol, 1.5 eq.) at 0 °C. After 30 min tetrabutylammonium iodide (43.7 mg, 118 µmol, 0.1 eq.) and 3-methylbenzyl chloride (268 µL, 286 mg, 1.77 mmol, 1.5 eq.) were added and the mixture was allowed to warm to 23 °C over 2 d. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 5:1) to afford ether S16 (317 mg, 837 µmol, 71%) as a colorless oil.

\[ R_f = 0.61 \text{ (n-pentane/EtOAc, 5:1).} \]

\[ [\alpha]^{27}_{D} = -17.7 (c = 1.36, \text{CHCl}_3). \]

\textbf{H-NMR} (700 MHz, CDCl₃): δ [ppm] = 7.23 (t, \( J = 7.6 \text{ Hz, 1H} \)), 7.14 (s, 1H), 7.12 (d, \( J = 7.6 \text{ Hz, 1H} \)), 7.09 (d, \( J = 7.6 \text{ Hz, 1H} \)), 4.49 (s, 2H), 3.66 – 3.59 (m, 1H), 3.38 – 3.32 (m, 1H), 3.30 (br, 1H), 2.35 (s, 3H), 1.90 (dt, \( J = 12.6, 3.3 \text{ Hz, 1H} \)), 1.80 – 1.73 (m, 1H), 1.67 – 1.62 (m, 1H), 1.62 – 1.54 (m, 3H), 1.45 – 1.35 (m, 3H), 1.26 (ddd, \( J = 13.7, 12.2, 3.1 \text{ Hz, 1H} \)), 1.23 (s, 1H), 1.17 – 1.13 (m, 3H), 1.11 (dd, \( J = 13.2, 4.1 \text{ Hz, 1H} \)), 0.90 (dd, \( J = 12.3, 2.3 \text{ Hz, 1H} \)), 0.87 (s, 3H), 0.86 – 0.81 (m, 1H), 0.79 (s, 3H), 0.78 (s, 3H).

\textbf{C-NMR} (176 MHz, CDCl₃): δ [ppm] = 138.1, 138.0, 128.7, 128.6, 128.5, 125.1, 73.3, 72.4, 72.0, 59.3, 56.3, 44.2, 42.1, 39.6, 39.1, 33.6, 33.4, 25.4, 24.5, 21.6, 21.6, 20.6, 18.6, 15.4.

\textbf{IR} (v/cm⁻¹, ATR) = 3444, 2925, 2862, 1610, 1460, 1384, 1246, 1156, 1081, 934.

\textbf{HRMS (ESI)}: \( m/z \) calculated for C₂₄H₃₈O₂Na⁺ [M+Na]⁺: 381.2764, found 381.2780.
Compound S17

To a stirred solution of diol S7 (301 mg, 1.18 mmol, 1.0 eq.) in DMF (4.0 mL) was added sodium hydride (60% in mineral oil, 70.9 mg, 1.77 mmol, 1.5 eq.) at 0 °C. After 30 min tetrabutylammonium iodide (43.7 mg, 118 μmol, 0.1 eq.) and 4-methylbenzyl chloride (269 μL, 286 mg, 1.77 mmol, 1.5 eq.) were added and the mixture was allowed to warm to 23 °C over 2 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 5:1) to afford ether S17 (387 mg, 1.02 mmol, 86%) as a colorless oil.

Rf = 0.50 (n-pentane/EtOAc, 5:1).

$[\alpha]_{D}^{27} = -20.4 \ (c = 1.43, \ CHCl₃)$.

$^1$H-NMR (700 MHz, CDCl₃): δ [ppm] = 7.21 (d, $J = 7.7$ Hz, 2H), 7.15 (d, $J = 7.7$ Hz, 2H), 4.48 (s, 2H), 3.65 – 3.59 (m, 1H), 3.52 – 3.15 (m, 2H), 2.33 (s, 3H), 1.90 (dt, $J = 12.7$, 3.3 Hz, 1H), 1.79 – 1.72 (m, 1H), 1.68 – 1.62 (m, 1H), 1.62 – 1.53 (m, 3H), 1.45 – 1.34 (m, 3H), 1.28 – 1.19 (m, 2H), 1.14 (s, 3H), 1.11 (dd, $J = 13.4$, 4.2 Hz, 1H), 0.90 (dd, $J = 12.4$, 2.3 Hz, 1H), 0.87 (s, 3H), 0.86 – 0.81 (m, 1H), 0.79 (s, 3H), 0.78 (s, 3H).

$^{13}$C-NMR (176 MHz, CDCl₃): δ [ppm] = 137.5, 135.0, 129.2 (2C), 128.0 (2C), 73.2, 72.4, 72.0, 59.4, 56.2, 44.2, 42.1, 39.6, 39.2, 33.6, 33.4, 25.4, 24.6, 21.6, 21.3, 20.6, 18.6, 15.4.

IR (ν/cm⁻¹, ATR) = 3443, 2925, 2861, 1515, 1459, 1384, 1241, 1089, 934, 802.

HRMS (ESI): m/z calculated for C₂₄H₃₈O₂Na⁺ [M+Na]⁺: 381.2764, found 381.2767.
Compound S18

To a stirred solution of diol S7 (300 mg, 1.18 mmol, 1.0 eq.) in DMF (4.0 mL) was added sodium hydride (60% in mineral oil, 70.9 mg, 1.77 mmol, 1.5 eq.) at 0°C. After 30 min tetrabutylammonium iodide (21.8 mg, 59.0 µmol, 0.05 eq.) and 2-(bromomethyl)naphthalene (391 mg, 1.77 mmol, 1.5 eq.) in DMF (0.5 mL) were added and the mixture was allowed to warm to 23°C over 16 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 1:0 to 5:1) to afford ether S18 (375 mg, 950 µmol, 81%) as a colorless oil.

Rᶠ = 0.41 (n-pentane/EtOAc, 5:1).
[α]₂⁷ᵇ = −15.4 (c = 1.36, CHCl₃).

¹H-NMR (700 MHz, CDCl₃): δ [ppm] = 7.85 – 7.81 (m, 3H), 7.77 (s, 1H), 7.51 – 7.43 (m, 3H), 4.74 – 4.66 (m, 2H), 3.69 – 3.64 (m, 1H), 3.44 – 3.38 (m, 1H), 3.30 (s, 1H), 1.91 (dt, J = 12.6, 3.3 Hz, 1H), 1.84 – 1.76 (m, 1H), 1.67 – 1.52 (m, 4H), 1.42 (td, J = 13.2, 4.1 Hz, 1H), 1.39 – 1.31 (m, 2H), 1.28 – 1.23 (m, 1H), 1.21 (t, J = 4.2 Hz, 1H), 1.15 (s, 3H), 1.09 – 1.03 (m, 1H), 0.88 – 0.86 (m, 1H), 0.85 (s, 3H), 0.83 – 0.79 (m, 1H), 0.79 (s, 3H), 0.78 (s, 3H).

¹³C-NMR (176 MHz, CDCl₃): δ [ppm] = 135.5, 133.4, 133.2, 128.4, 128.0, 127.8, 126.8, 126.2, 126.0 (2C), 73.4, 72.5, 72.1, 59.3, 56.2, 44.2, 42.0, 39.6, 39.1, 33.5, 33.4, 25.4, 24.5, 21.6, 20.6, 18.5, 15.4.

IR (ν/cm⁻¹, ATR) = 3444, 3054, 2927, 2862, 1602, 1508, 1461, 1162, 1092, 934.

HRMS (ESI): m/z calculated for C₂₇H₃₈O₂Na⁺ [M+Na⁺]: 417.2764, found 417.2776.
Compound S19

To a stirred solution of diol S7 (105 mg, 413 μmol, 1.0 eq.) in DMF (2.0 mL) was added sodium hydride (60% in mineral oil, 26.1 mg, 652 μmol, 1.6 eq.) at 0 °C. After 30 min 2-methoxybenzyl bromide (151 mg, 731 μmol, 1.8 eq.) in DMF (1.0 mL) was added and the mixture was allowed to warm to 23 °C over 20 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 30:1 to 1:1) to afford ether S19 (112 mg, 300 μmol, 73%) as a colorless oil.

Rᵥ = 0.24 (n-pentane/EtOAc, 10:1).

[α]D²⁴ = −8.14 (c = 0.55, CHCl₃).

¹H-NMR (500 MHz, CDCl₃): δ [ppm] = 7.33 (dd, J = 7.4, 1.7 Hz, 1H), 7.28 – 7.22 (m, 1H), 6.95 (td, J = 7.5, 1.1 Hz, 1H), 6.86 (d, J = 8.2 Hz, 1H), 4.56 (q, J = 12.4 Hz, 2H), 3.83 (s, 3H), 3.72 – 3.63 (m, 1H), 3.43 – 3.34 (m, 1H), 3.09 (s, 1H), 1.90 (dt, J = 12.5, 3.2 Hz, 1H), 1.82 – 1.70 (m, 1H), 1.66 – 1.52 (m, 4H), 1.44 – 1.32 (m, 3H), 1.29 – 1.22 (m, 1H), 1.20 (t, J = 4.3 Hz, 1H), 1.13 (s, 3H), 1.12 – 1.07 (m, 1H), 0.90 – 0.81 (m, 5H), 0.78 (s, 6H).

¹³C-NMR (126 MHz, CDCl₃): δ [ppm] = 157.2, 129.2, 128.8, 126.5, 120.6, 110.3, 72.3, 72.2, 68.2, 59.3, 56.2, 55.4, 44.2, 42.1, 39.6, 39.1, 33.6, 33.4, 25.4, 24.4, 21.6, 20.6, 18.6, 15.4.

IR (ν/cm⁻¹, ATR) = 3378, 2918, 2851, 1599, 1463, 1374, 1241, 1086, 970, 754.

HRMS (ESI): m/z calculated for C₂₄H₃₈O₃Na⁺ [M+Na]⁺: 397.2713, found 397.2713.
Compound S20

To a stirred solution of diol S7 (515 mg, 2.02 mmol, 1.0 eq.) in DMF (10 mL) was added sodium hydride (60% in mineral oil, 123 mg, 3.03 mmol, 1.5 eq.) at 0 °C. After 30 min bromodiphenylmethane (1.03 g, 4.05 mmol, 2.0 eq.) was added and the mixture was allowed to warm to 23 °C over 20 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed repeatedly with brine, dried over MgSO_4_, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO_2_, n-pentane/EtOAc 30:1 to 1:1) to afford ether S20 (765 mg, 1.82 mmol, 90%) as a colorless oil.

R_f = 0.47 (n-pentane/EtOAc, 10:1).

[α]_D^24 = −12.8 (c = 3.15, CHCl_3).

^1^H-NMR (500 MHz, CDCl_3): δ [ppm] = 7.38 – 7.29 (m, 8H), 7.27 – 7.21 (m, 2H), 5.37 (s, 1H), 3.63 (dt, J = 9.1, 4.6 Hz, 1H), 3.42 – 3.32 (m, 1H), 3.03 (s, 1H), 1.91 (dt, J = 12.5, 3.2 Hz, 1H), 1.89 – 1.79 (m, 1H), 1.68 – 1.49 (m, 4H), 1.44 – 1.32 (m, 3H), 1.28 – 1.20 (m, 2H), 1.16 (s, 3H), 1.09 (td, J = 13.4, 12.7, 4.2 Hz, 1H), 0.91 – 0.81 (m, 4H), 0.78 (s, 6H), 0.75 – 0.70 (m, 1H).

^1^3^C-NMR (126 MHz, CDCl_3): δ [ppm] = 142.1, 142.1, 128.6 (2C), 128.6 (2C), 127.7, 127.6, 127.2 (2C), 126.9 (2C), 84.5, 72.6, 70.9, 59.0, 56.2, 44.2, 42.1, 39.5, 39.1, 33.5, 33.4, 25.4, 24.4, 21.6, 20.6, 18.5, 15.4.

IR (ν/cm⁻¹, ATR) = 3401, 2927, 2865, 1600, 1490, 1450, 1182, 1070, 1024, 931.

HRMS (ESI): m/z calculated for C_{29}H_{40}O_{2}Na^+ [M+Na]^+: 443.2920, found 443.2910.
To a stirred solution of caesium carbonate (273 mg, 838 µmol, 2.0 eq.) in THF (2.0 mL) was added diol S7 (107 mg, 419 µmol, 1.0 eq.) at 0 °C. After 10 min 4-nitrobenzyl bromide (181 mg, 838 µmol, 2.0 eq.) in THF (1.0 mL) was added and the mixture was allowed to warm to 23 °C over 3 d then heated to 50 °C for 3 h. Water and EtOAc were added to the reaction mixture sequentially. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 9:1 to 1:1) to afford ether S21 (54.7 mg, 140 µmol, 34%, 42% brsm) as a yellow oil and diol S7 (21.1 mg, 82.9 µmol) as a white solid.

\[ R_f = 0.75 \text{ (n-pentane/EtOAc, 4:1).} \]
\[ [\alpha]_{D}^{23} = -14.9 \text{ (c = 1.10, CHCl₃).} \]

\(^1\text{H-NMR}\) (500 MHz, CDCl₃): \( \delta \) [ppm] = 8.20 (d, \( J = 8.5 \text{ Hz, 2H} \)), 7.49 (d, \( J = 8.5 \text{ Hz, 2H} \)), 4.62 (s, 2H), 3.70 – 3.63 (m, 1H), 3.50 – 3.44 (m, 1H), 2.75 (s, 1H), 1.91 (dt, \( J = 12.5, 3.3 \text{ Hz, 1H} \)), 1.85 – 1.78 (m, 1H), 1.68 – 1.56 (m, 4H), 1.45 – 1.36 (m, 3H), 1.31 – 1.23 (m, 1H), 1.21 (t, \( J = 4.3 \text{ Hz, 1H} \)), 1.16 (s, 3H), 1.15 – 1.10 (m, 1H), 0.92 (dd, \( J = 12.4, 2.3 \text{ Hz, 1H} \)), 0.91 – 0.88 (m, 1H), 0.87 (s, 3H), 0.80 (s, 3H), 0.79 (s, 3H).

\(^{13}\text{C-NMR}\) (126 MHz, CDCl₃): \( \delta \) [ppm] = 147.6, 145.8, 127.9 (2C), 123.9 (2C), 73.2, 72.8, 72.1, 59.3, 56.3, 44.3, 42.1, 39.8, 39.2, 33.6, 33.4, 25.5, 24.5, 21.6, 20.6, 18.6, 15.4.

\( \text{IR (\nu/cm}^{-1}, \text{ATR)} = 3458, 2925, 2862, 1603, 1519, 1460, 1385, 1342, 1098, 1015. \)

\( \text{HRMS (ESI)}: m/z \text{ calculated for C}_{23}\text{H}_{35}\text{NO}_4\text{Na}^+ [M+Na]^+: 412.2458, \text{ found 412.2473.} \)

Note: This procedure is unoptimized.
Compound 13 from S8

\[
\text{S8} \quad \overset{n-\text{BuLi}}{\xrightarrow{\text{THF, } -78 \, ^\circ \text{C to } 0 \, ^\circ \text{C}}} \quad \text{13}
\]

\[
\text{C}_{23}\text{H}_{36}\text{O}_2 \quad (344.53)
\]

To a solution of ether S8 (100 mg, 290 μmol, 1.0 eq.) in THF (4 mL) at −78 °C was added a solution of n-BuLi (396 μL, 2.5 M in hexane, 871 μmol, 3.0 eq.). After stirring for 30 min at that temperature the reaction mixture was warmed to 0 °C and stirred for 12 h while reaching 23 °C. Water was added and the reaction mixture was diluted with EtOAc. The organic phase was separated and the aqueous phase was extracted with EtOAc. The combined organic extracts were washed with brine, dried over MgSO₄, filtered and concentrated under reduced pressure. The residue was purified by flash column chromatography (SiO₂, n-pentane/EtOAc 10:1 to 1:1) to afford alkene 13 (14.2 mg, 60.1 μmol, 21%) as a white solid and S22 (15.2 mg, 44.1 μmol, 15%) as a light-yellow oil and S23 (13.4 mg, 38.9 μmol, 13%) as a light-yellow oil.

S22

Rᵢ = 0.45 (n-pentane/EtOAc, 3:1).

\[ [\alpha]_{D}^{23} = -9.10 \, (c = 1.12, \text{CHCl}_3) \]

\[^{1}H\text{-NMR} \, (500 \text{ MHz, CDCl}_3) : \delta \, [\text{ppm}] = 7.37 \, (d, \, J = 7.2 \text{ Hz, 2H}), 7.33 \, (t, \, J = 7.5 \text{ Hz, 2H}), 7.24 \, (t, \, J = 7.3 \text{ Hz, 1H}), 4.80 \, (dd, \, J = 10.2, \, 3.4 \text{ Hz, 1H}), 3.56 - 2.51 \, (m, \, 1H), \, 1.86 - 1.76 \, (m, \, 2H), \, 1.73 - 1.67 \, (m, \, 1H), \, 1.67 - 1.55 \, (m, \, 4H), \, 1.51 - 1.34 \, (m, \, 4H), \, 1.31 - 1.23 \, (m, \, 3H), \, 1.20 - 1.08 \, (m, \, 4H), \, 0.97 - 0.89 \, (m, \, 2H), \, 0.88 \, (s, \, 3H), \, 0.80 \, (s, \, 3H), \, 0.79 \, (s, \, 3H). \]

\[^{13}C\text{-NMR} \, (126 \text{ MHz, CDCl}_3) : \delta \, [\text{ppm}] = 145.3, \, 128.4 \, (2C), \, 127.2, \, 125.9 \, (2C), \, 74.6, \, 71.8, \, 58.6, \, 56.2, \, 43.9, \, 42.1, \, 41.3, \, 34.0, \, 39.3, \, 33.5, \, 33.3, \, 24.8, \, 21.7, \, 20.6, \, 20.4, \, 18.5, \, 15.4. \]

IR (ν/cm⁻¹, ATR) = 3371, 2991, 2922, 2876, 1456, 1364, 1203, 1157, 1068, 759.

HRMS (ESI): m/z calculated for C_{23}H_{36}O_{2}K⁺ [M+K]⁺: 383.2347, found 383.2362.
S23

$R_f = 0.36$ (n-pentane/EtOAc, 3:1).

$[\alpha]^{23}_D = +20.0$ ($c = 0.76$, CHCl$_3$).

$^1$H-NMR (700 MHz, CDCl$_3$): $\delta$ [ppm] = 7.36 – 7.34 (m, 2H), 7.34 – 7.31 (m, 2H), 7.26 – 7.23 (m, 1H), 4.70 (dd, $J = 9.2$, 4.0 Hz, 1H), 1.89 – 1.77 (m, 3H), 1.70 – 1.62 (m, 3H), 1.59 – 1.53 (m, 1H), 1.53 – 1.49 (m, 1H), 1.49 – 1.43 (m, 1H), 1.43 – 1.32 (m, 4H), 1.29 – 1.22 (m, 2H), 1.17 (s, 3H), 1.15 – 1.11 (m, 1H), 0.98 – 0.93 (m, 2H), 0.86 (s, 3H), 0.78 (s, 3H), 0.76 (s, 3H).

$^{13}$C-NMR (176 MHz, CDCl$_3$): $\delta$ [ppm] = 145.3, 128.5 (2C), 127.4, 125.9 (2C), 76.5, 74.9, 61.6, 56.1, 44.4, 42.5, 42.1, 39.8, 39.3, 33.5, 33.4, 24.5, 22.5, 21.6, 20.7, 18.5, 15.3.

IR ($\nu$/cm$^{-1}$, ATR) = 3352, 2922, 2867, 1737, 1457, 1387, 1126, 1082, 970, 762.

HRMS (ESI): $m/z$ calculated for C$_{23}$H$_{36}$O$_2$K$^+$ [M+K]$^+$: 383.2347, found 383.2363.

Note: No attempt was made to determine the relative configuration of the epimeric alcohols S22/S23
Table 1.: Comparison of the $^1$H-NMR spectra of cupacinoxepin

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Table 2: Comparison of the $^{13}$C-NMR spectra of cupacinoxepin

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$^a$ Signal overlapping
<p>| | | | |</p>
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<td>21.6</td>
<td>0.0</td>
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<tr>
<td>30</td>
<td>33.5</td>
<td>33.6</td>
<td>−0.1</td>
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</table>
Isolated Cupacinoxepin ($^1$H, 600 MHz, CDCl$_3$) $^7$

![Isolated Cupacinoxepin NMR spectrum](image1)

Synthetic Cupacinoxepin ($^1$H, 500 MHz, CDCl$_3$)

![Synthetic Cupacinoxepin NMR spectrum](image2)
Table 3.: Comparison of the $^1$H-NMR spectra of onoceranoxide 7

<table>
<thead>
<tr>
<th>no.</th>
<th>Isolated onoceranoxide$^8$</th>
<th>Synthetic onoceranoxide</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$^1$H mult ($J$, Hz)</td>
<td>$^1$H mult ($J$, Hz)</td>
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<tr>
<td>1, 19</td>
<td>/</td>
<td>1.76 (m), 0.87 (m)</td>
</tr>
<tr>
<td>2, 20</td>
<td>/</td>
<td>1.58 (m), 1.40 (m)</td>
</tr>
<tr>
<td>3, 21</td>
<td>/</td>
<td>1.34 (m), 1.11 (m)</td>
</tr>
<tr>
<td>4, 22</td>
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<td>5, 17</td>
<td>/</td>
<td>0.88 (m)</td>
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<td>6, 16</td>
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<td>1.58 (m), 1.21 (m)</td>
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<td>7, 15</td>
<td>/</td>
<td>1.75 (m), 1.56 (m)</td>
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<td>/</td>
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<td>9, 13</td>
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<td>1.38 (m)</td>
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<tr>
<td>10, 18</td>
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<td>11, 12</td>
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<td>1.77 (m), 1.21 (m)</td>
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<td>0.735</td>
<td>0.74 (s)</td>
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<td>25, 28</td>
<td>0.767</td>
<td>0.77 (s)</td>
</tr>
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<td>26, 27</td>
<td>1.259</td>
<td>1.26 (s)</td>
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Table 4.: Comparison of the $^{13}$C-NMR spectra of onoceranoxide 7

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<th>no.</th>
<th>$^{13}$C-NMR isolated onoceranoxide$^8$</th>
<th>$^{13}$C-NMR synthetic onoceranoxide</th>
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</thead>
<tbody>
<tr>
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<td>$^1$C-NMR 25 MHz, CDCl$_3$</td>
<td>$^1$C-NMR 176 MHz, CDCl$_3$</td>
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<td>1, 19</td>
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<td>40.5</td>
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<td>2, 20</td>
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<tr>
<td>3, 21</td>
<td>42.2</td>
<td>42.2</td>
</tr>
<tr>
<td>4, 22</td>
<td>33.5</td>
<td>33.6</td>
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<td>5, 17</td>
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<td>6, 16</td>
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<td>45.4</td>
<td>45.4</td>
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<td>8, 14</td>
<td>79.9</td>
<td>80.1</td>
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<td>9, 13</td>
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<tr>
<td>10, 18</td>
<td>38.9</td>
<td>39.0</td>
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<td>11, 12</td>
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<td>25.1</td>
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<td>23, 30</td>
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<td>21.7</td>
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<tr>
<td>25, 28</td>
<td>15.8</td>
<td>15.9</td>
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<td>26, 27</td>
<td>25.4</td>
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Table 5.: Comparison of the $^1$H-NMR spectra of 8α-hydroxypolypoda-13,17,21 (9)

<table>
<thead>
<tr>
<th>no.</th>
<th>Isolated $^9$</th>
<th>Synthetic 9 (500 MHz, CDCl$_3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\delta_H$ mult (J, Hz)</td>
<td>$\delta_H$ mult (J, Hz)</td>
</tr>
<tr>
<td>1</td>
<td>/</td>
<td>0.98 td (13.0, 3.7)</td>
</tr>
<tr>
<td>2</td>
<td>/</td>
<td>1.40$^a$</td>
</tr>
<tr>
<td>3</td>
<td>/</td>
<td>1.14$^a$</td>
</tr>
<tr>
<td>4</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>5</td>
<td>/</td>
<td>0.91 dd (12.1, 2.3)</td>
</tr>
<tr>
<td>6</td>
<td>/</td>
<td>1.66$^a$</td>
</tr>
<tr>
<td>7</td>
<td>/</td>
<td>1.86 dt (12.1, 3.1)</td>
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<tr>
<td>8</td>
<td>/</td>
<td>1.36$^a$</td>
</tr>
<tr>
<td>9</td>
<td>/</td>
<td>0.91 dd (12.1, 2.3)</td>
</tr>
<tr>
<td>10</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>11</td>
<td>/</td>
<td>1.44$^a$</td>
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<tr>
<td>12</td>
<td>/</td>
<td>1.26$^a$</td>
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<tr>
<td>13</td>
<td>5.07 – 5.21 bt (6.2)</td>
<td>5.21 – 5.16 m</td>
</tr>
<tr>
<td>14</td>
<td>/</td>
<td>/</td>
</tr>
<tr>
<td>15</td>
<td>/</td>
<td>1.99$^a$</td>
</tr>
<tr>
<td>16</td>
<td>/</td>
<td>1.96 – 2.11 m$^a$</td>
</tr>
<tr>
<td>17</td>
<td>5.07 – 5.21 bt (6.2)</td>
<td>5.14 – 5.06 m$^a$</td>
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<tr>
<td>18</td>
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<td>/</td>
</tr>
<tr>
<td>19</td>
<td>/</td>
<td>1.99 (m)</td>
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<tr>
<td>20</td>
<td>/</td>
<td>1.96 – 2.11 m$^a$</td>
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</table>
21  5.07 – 5.21 bt (6.2)  1.96 – 2.11 m<sup>a</sup>  
22  /  5.14 – 5.06 m<sup>a</sup>  
23  0.869  0.87 s  
24  0.789  0.79 s  
25  0.789  0.79 s  
26  1.130  1.13 s  
27  1.616  1.60 s<sup>a</sup> or 1.61 s  
28  1.602  1.60 s<sup>a</sup> or 1.61 s  
29  1.602  1.68 s  
30  1.681  1.60 s<sup>a</sup>  

<sup>a</sup> Signal overlapping

**Table 6.:** Comparison of the $^{13}$C-NMR spectra of 8α-hydroxypolypoda-13,17,21

<table>
<thead>
<tr>
<th>no.</th>
<th>$^{13}$C Natural 9&lt;sup&gt;10&lt;/sup&gt; (68 MHz, CDCl₃)</th>
<th>$^{13}$C Synthetic 9 (176 MHz, CDCl₃)</th>
<th>Deviation</th>
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<td>−0.3</td>
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<td>4</td>
<td>33.3</td>
<td>33.4</td>
<td>−0.1</td>
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<td>56.3</td>
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<td>0</td>
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<td>−0.1</td>
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<td>−0.1</td>
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<td>74.1</td>
<td>74.2</td>
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<td>−0.1</td>
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<td>39.3</td>
<td>−0.1</td>
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<td>25.6</td>
<td>25.7</td>
<td>−0.1</td>
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<td>31.5</td>
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<td>−0.1</td>
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<td>125.1</td>
<td>125.2</td>
<td>−0.1</td>
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<td>135.0</td>
<td>135.1</td>
<td>−0.1</td>
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<td>15</td>
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<td>124.4</td>
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<td>26.8</td>
<td>26.8 or 26.9</td>
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<td>124.6</td>
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<td>16.2 or 16.4</td>
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55
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<th>Value 2</th>
<th>Value 3</th>
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<td>16.2 or 16.4</td>
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<td>25.7</td>
<td>25.9</td>
<td>-0.2</td>
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<tr>
<td>30</td>
<td>17.7</td>
<td>17.8</td>
<td>-0.1</td>
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3. Screening of Reaction Conditions

Scheme 1.: Selected screening conditions for the formation of alkene 13.

Direct conversion of the primary alcohol into a leaving group, selenide or xanthate ester led to ambroxide formation via intramolecular substitution.

Table 7.: Selected screening conditions for the Wittig-type fragmentation.

<table>
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<tr>
<th>Entry</th>
<th>R&lt;sup&gt;1&lt;/sup&gt;</th>
<th>R&lt;sup&gt;2&lt;/sup&gt;</th>
<th>Conditions</th>
<th>Yield (%)/Observation</th>
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<tbody>
<tr>
<td>1</td>
<td>H</td>
<td>H</td>
<td>n-BuLi (3 eq.), THF, −78 °C, 30 min to 0 °C&lt;sup&gt;18&lt;/sup&gt;</td>
<td>20</td>
</tr>
<tr>
<td>2</td>
<td>H</td>
<td>H</td>
<td>n-BuLi (4 eq.), Et&lt;sub&gt;2&lt;/sub&gt;O, −78 °C, 30 min to 0 °C</td>
<td>&lt;5</td>
</tr>
<tr>
<td>3</td>
<td>H</td>
<td>H</td>
<td>n-BuLi (4 eq.), 1,2-dimethoxyethane, −78 °C, 30 min to 0 °C</td>
<td>16</td>
</tr>
<tr>
<td>4</td>
<td>H</td>
<td>H</td>
<td>LDA (4 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>&lt;5</td>
</tr>
<tr>
<td>5</td>
<td>H</td>
<td>H</td>
<td>s-BuLi (4 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>28</td>
</tr>
<tr>
<td>6</td>
<td>H</td>
<td>H</td>
<td>s-BuLi (5 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>26</td>
</tr>
<tr>
<td>7</td>
<td>H</td>
<td>H</td>
<td>t-BuLi (4 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>20</td>
</tr>
<tr>
<td>8</td>
<td>H</td>
<td>H</td>
<td>n-BuLi (4 eq.), THF, TMEDA (4 eq.), −78 °C, 30 min to 0 °C</td>
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</tr>
<tr>
<td>9</td>
<td>H</td>
<td>SiMe&lt;sub&gt;3&lt;/sub&gt;</td>
<td>n-BuLi (3 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>24&lt;sup&gt;a&lt;/sup&gt;</td>
</tr>
<tr>
<td>10</td>
<td>Me</td>
<td>H</td>
<td>n-BuLi (4 eq.), THF, −78 °C, 30 min to −40 °C</td>
<td>No product formation</td>
</tr>
<tr>
<td>11</td>
<td>Me</td>
<td>H</td>
<td>n-BuLi (4 eq.), THF, −78 °C, 30 min to −28 °C</td>
<td>42</td>
</tr>
<tr>
<td>12</td>
<td>Me</td>
<td>H</td>
<td>n-BuLi (4 eq.), THF, −78 °C, 10 min to −13 °C (0.46 mmol scale)</td>
<td>44</td>
</tr>
<tr>
<td></td>
<td>Me</td>
<td>H</td>
<td>Reagent (4 eq.), THF, °C, min to °C</td>
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<td>---</td>
<td>----</td>
<td>---</td>
<td>-----------------------------------</td>
<td>---</td>
</tr>
<tr>
<td>13</td>
<td>Me</td>
<td>H</td>
<td>n-BuLi (4 eq.), THF, −78 °C, 30 min to −13 °C</td>
<td>41</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>(13.2 mmol scale)</td>
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<tr>
<td>14</td>
<td>Me</td>
<td>H</td>
<td>n-BuLi (4 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>37</td>
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<tr>
<td>15</td>
<td>Me</td>
<td>H</td>
<td>n-BuLi (4 eq.), THF, −78 °C, 30 min to 50 °C</td>
<td>34</td>
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<tr>
<td>16</td>
<td>Me</td>
<td>H</td>
<td>s-BuLi (4 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>35a</td>
</tr>
<tr>
<td>17</td>
<td>Me</td>
<td>H</td>
<td>n-BuLi (8 eq.), THF, −78 °C, 30 min to 0 °C</td>
<td>29</td>
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</table>

*a determined by H-NMR using an internal standard
Table 8.: Screening of ether derivatives for Wittig-type fragmentation

Ether derivatives with alkyl substituents and benzylic hydrogen atoms in the 2-position of the aromatic ring gave higher yields of alkene 13 than ethers with electron withdrawing-, electron donating-, or sterically hindered substituents.
Table 9: Tricyclization attempts of substrate 9 to give pentacyclic derivatives

<table>
<thead>
<tr>
<th>Entry</th>
<th>Conditions</th>
<th>Concentration [mmol/mL]</th>
<th>Observation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Hg(OTFA)$_2$ (1.2 eq.), MeNO$_2$, $-20 ^\circ$C, Work up: NaCl (aq.)</td>
<td>0.004</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>2</td>
<td>Hg(OTf)$_2$ (1.4 eq.), MeNO$_2$, Me$_2$NPh (1.5 eq.), $-20 ^\circ$C, Work up: NaCl (aq.)</td>
<td>0.006</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>3</td>
<td>Hg(OTf)$_2$ (1.2 eq.), MeNO$_2$, tetramethylurea (1.3 eq.), $-20 ^\circ$C, Work up: NaCl (aq.)</td>
<td>0.003</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>4</td>
<td>Hg(OTf)$_2$ (1.2 eq.), CH$_2$Cl$_2$, tetramethylurea (2.4 eq.), $-20 ^\circ$C, Work up: NaCl (aq.)</td>
<td>0.007</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>5</td>
<td>Hg(OTf)$_2$ (1.2 eq.), MeCN, tetramethylurea (2.4 eq.), $-20 ^\circ$C, Work up: NaCl (aq.)</td>
<td>0.005</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>6</td>
<td>SnCl$_4$ (2.0 eq.), rac-BINOL (2.2 eq.), CH$_2$Cl$_2$, $-78 ^\circ$C</td>
<td>0.01</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>7</td>
<td>HFIP, eosin Y, rt, green LED</td>
<td>0.1</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>8</td>
<td>BDSB, MeNO$_2$/CH$_2$Cl$_2$ (3:1), $-20 ^\circ$C</td>
<td>0.003</td>
<td>Complex mixture</td>
</tr>
</tbody>
</table>
Table 10.: Screening conditions 12 to 10:

<table>
<thead>
<tr>
<th>Entry</th>
<th>Conditions</th>
<th>Concentration (mmol/mL)</th>
<th>Observation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>SnCl₄ (1.0 eq.), CH₂Cl₂, −78 °C</td>
<td>0.005</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>2</td>
<td>SnCl₄ (2.0 eq.), rac-BINOL (2.2 eq.), CH₂Cl₂, −78 °C</td>
<td>0.002</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>3</td>
<td>SnCl₄ (2.0 eq.), rac-BINOL (2.2 eq.), CH₂Cl₂, −90 °C</td>
<td>0.001</td>
<td>Incomplete conversion</td>
</tr>
<tr>
<td>4</td>
<td>Picric acid (1.8 eq.), MeNO₂, no stirring, 1 °C</td>
<td>0.01</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>5</td>
<td>CSA (0.1 eq.), MeNO₂, 0 °C</td>
<td>0.005</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>6</td>
<td>HFIP, 1 °C</td>
<td>0.003</td>
<td>Incomplete conversion</td>
</tr>
<tr>
<td>7</td>
<td>HFIP, TFA (0.05 eq.), CH₂Cl₂, 1 °C</td>
<td>0.003</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>8</td>
<td>HFIP, Ph₄PBF₄ (10 eq.), 1 °C</td>
<td>0.001</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>9</td>
<td>HFIP, NaSbF₆ (10 eq.), 1 °C</td>
<td>0.003</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>10</td>
<td>HFIP, AgSbF₆ (10 eq.), 1 °C</td>
<td>0.003</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>11</td>
<td>HFIP, Bu₄NPF₆ (10 eq.), 1 °C</td>
<td>0.003</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>12</td>
<td>BF₃·OEt₂ (2.3 eq.), CH₂Cl₂, −78 °C</td>
<td>0.005</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>13</td>
<td>Cp₂TiCl₂ (2.2 eq.), Mn (100 eq.), THF, rt</td>
<td>0.005</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>14</td>
<td>Cp₂TiCl₂ (0.55 eq.), Mn (24 eq.), TMSCl (8 eq.), 2,4,6-collidine (14 eq.), THF, rt</td>
<td>0.005</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>14</td>
<td>TIPSOTf (5.0 eq.), 2,6-lutidine, CH₂Cl₂, −78 °C to rt</td>
<td>0.0015</td>
<td>Incomplete conversion</td>
</tr>
<tr>
<td>15</td>
<td>InCl₃ (1.0 eq.), CH₂Cl₂, −78 °C</td>
<td>0.005</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>16</td>
<td>Me₂AlCl (3.0 eq.), CH₂Cl₂, −78 °C⁰</td>
<td>0.001</td>
<td>Incomplete conversion</td>
</tr>
<tr>
<td>17</td>
<td>Et₂AlCl (3.0 eq.), CH₂Cl₂, −78 °C⁰</td>
<td>0.001</td>
<td>Incomplete conversion</td>
</tr>
<tr>
<td>18</td>
<td>MeAlCl₂ (3.0 eq.), CH₂Cl₂, Et₂O, −78 °C⁰</td>
<td>0.001</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>19</td>
<td>EtAlCl₂ (2.0 eq.), CH₂Cl₂, −78 °C⁰</td>
<td>0.001</td>
<td>14% 10, 8% 21</td>
</tr>
<tr>
<td>Run</td>
<td>Lewis Acid (eq.), Solvent, Temp</td>
<td>Yield</td>
<td>Notes</td>
</tr>
<tr>
<td>-----</td>
<td>-------------------------------</td>
<td>-------</td>
<td>-------</td>
</tr>
<tr>
<td>20</td>
<td>EtAlCl₂ (3.0 eq.), CH₂Cl₂, −78 °C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.001</td>
<td>20% 10, 12% 21</td>
</tr>
<tr>
<td>21</td>
<td>EtAlCl₂ (3.0 eq.), CH₂Cl₂, −78 °C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.0005</td>
<td>17% 10, 16% 21</td>
</tr>
<tr>
<td>22</td>
<td>EtAlCl₂ (3.0 eq.), CH₂Cl₂, −90 °C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.001</td>
<td>Complex mixture</td>
</tr>
<tr>
<td>23</td>
<td>EtAlCl₂ (5.0 eq.), CH₂Cl₂, −78 °C&lt;sup&gt;a&lt;/sup&gt;</td>
<td>0.001</td>
<td>Complex mixture; trace product formation detected</td>
</tr>
<tr>
<td>24</td>
<td>EtAlCl₂ (3.0 eq.), CH₂Cl₂, −78 °C&lt;sup&gt;c&lt;/sup&gt;</td>
<td>0.001</td>
<td>Complex mixture</td>
</tr>
</tbody>
</table>

<sup>a</sup> Substrate in CH₂Cl₂ (precooled by passing the needle through dry ice) was added to a solution of Lewis acid in CH₂Cl₂ at −78 °C.

<sup>b</sup> No tricyclization product was obtained if the corresponding trimethylsilyl ether (OTMS) was used under the same conditions as starting material instead of the tertiary alcohol.

<sup>c</sup> EtAlCl₂ in CH₂Cl₂ (precooled by passing the needle through dry ice) was added to a solution of substrate in CH₂Cl₂ at −78 °C.

Note: No signals corresponding to S6 were observed in ¹H-NMR analysis of the crude reaction mixture.
4. NMR Spectra

$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
$^1$H-$^1$H-COSY (700 MHz, CDCl$_3$)
$^1$H-$^1$H-COSY (700 MHz, CDCl$_3$)
HMOC (700 MHz, CDCl₃)
HMBC (700 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, C$_{6}$D$_{6}$)

$^{13}$C-NMR (176 MHz, C$_{6}$D$_{6}$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
Zoom in HMQC spectrum
\(^1\)H-NMR (700 MHz, C\(_6\)D\(_6\))

\(^{13}\)C-NMR (176 MHz, C\(_6\)D\(_6\))
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
HMOC (700 MHz, CDCl₃)
Zoom in HMQC spectrum

HMBC (700 MHz, CDCl₃)
\( ^1\text{H-NMR} (700 \text{ MHz, CD}_2\text{D}_2) \)

\( ^{13}\text{C-NMR} (176 \text{ MHz, CD}_2\text{D}_2) \)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^1$H-NMR (500 MHz, CDCl$_3$)

$^{13}$C-NMR (126 MHz, CDCl$_3$)
$^{13}$C-NMR (126 MHz, CDCl$_3$)

$^1$H-NMR (500 MHz, CDCl$_3$)
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
\textsuperscript{13}C-NMR (126 MHz, CDCl\textsubscript{3})
$^1$H-NMR (700 MHz, CDCl$_3$)

$^{13}$C-NMR (176 MHz, CDCl$_3$)
5. Literature Comparison: Polyene Cyclizations terminated by Aliphatic Alcohols

Table 11 Selected examples of ring systems produced via polyene cyclization terminated by aliphatic alcohols.

<table>
<thead>
<tr>
<th>Entry</th>
<th>Number and ring size of carbocycles formed (6 = Cyclohexane, 5 = Cyclopentane)</th>
<th>Oxygen containing ring formed</th>
<th>Nucleophile</th>
<th>Reagents</th>
<th>Yield (ratio of cyclization products)</th>
<th>Lit.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6,6 Tetrahydrofuran</td>
<td>Primary alcohol</td>
<td>1. [Ir(COD)Cl]2 (4 mol%), R1 (16 mol%), Zn(OTf)₂ (20 mol%), DCE; 2. BF₃·OEt₂, CH₂Cl₂ (R)-BINOL-Me·SnCl₄, CH₂Cl₂</td>
<td>79% (2 steps) (10:1, &gt;99% ee)</td>
<td>19</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>6,6 Tetrahydrofuran</td>
<td>Primary alcohol</td>
<td>(dppe)PtI₂ (10 mol%), AgBF₄ (22 mol%), 2.1 Ph₃COMe resin, EtNO₂</td>
<td>54% (56 (42% ee):26:9:9)</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>6,6 Tetrahydrofuran</td>
<td>Primary alcohol</td>
<td>FSO₃H, 2-nitropropane</td>
<td>78% (40:35:2:1)</td>
<td>22</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>6,6 Tetrahydrofuran</td>
<td>Secondary alcohol</td>
<td>picric acid, MeNO₂</td>
<td>75% (1.2:1)</td>
<td>23</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>6,6,5 Tetrahydrofuran</td>
<td>Primary alcohol</td>
<td>CISO₃H</td>
<td>58% (88 (56% ee):12)</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>6,6 Tetrahydrofuran</td>
<td>Tertiary alcohol</td>
<td>(R)-BINOL-Me·SnCl₄, CH₂Cl₂</td>
<td>74% (81:19)</td>
<td>25</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>6 Tetrahydrofuran</td>
<td>Tertiary alcohol</td>
<td>R₂-SnCl₄</td>
<td>70%</td>
<td>26</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>6 Tetrahydrofuran</td>
<td>Tertiary alcohol</td>
<td>FSO₃H, 2-nitropropane</td>
<td>15%</td>
<td>27</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>6,6 Tetrahydrofuran</td>
<td>Primary alcohol</td>
<td>Hg(TFA)₂, C₆H₃N(CH₃)₂, then NaCl</td>
<td>7%</td>
<td>28</td>
<td></td>
</tr>
<tr>
<td>Entry</td>
<td>Oxepane</td>
<td>Alkyl</td>
<td>Reactants</td>
<td>Yield</td>
<td>Remarks</td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>---------</td>
<td>-------</td>
<td>-----------</td>
<td>-------</td>
<td>---------</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>Oxepane</td>
<td>Secondary alcohol</td>
<td>Hg(TFA)$_2$, MeNO$_2$ then KBr, Br$_2$, O$_2$, LiBr, py</td>
<td>30% (1:1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>Oxepane</td>
<td>Secondary alcohol</td>
<td>2,4,4,6-tetrabromo-cyclohexa-2,5-dienone, MeNO$_2$</td>
<td>12% (19:81)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>Oxepane</td>
<td>Secondary alcohol</td>
<td>Hg(TFA)$_2$, MeNO$_2$ then KBr, Br$_2$, O$_2$, LiBr, py</td>
<td>29% (3.1:1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>Oxepane</td>
<td>Tertiary alcohol</td>
<td>squalene cyclase from <em>Alicyclobacillus acidocaldarius</em></td>
<td>19.3%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>Oxepane</td>
<td>Tertiary alcohol</td>
<td>BmeTC</td>
<td>18% (64:36)</td>
<td>This work</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>Oxepane</td>
<td>Tertiary alcohol</td>
<td>EtAlCl$_2$, CH$_2$Cl$_2$</td>
<td>32% (1.7:1)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

These examples highlight the difficult formation of fused ring systems containing oxepane rings with tertiary alcohols in polyene cyclizations, as previously only enzymatic transformations of this kind were known (Entry 15 and 16). Furthermore, the examples indicate that EtAlCl$_2$, while being widely used in polyene cyclizations terminated by allylsilanes and silyl enol ethers, has not been used frequently in alcohol terminated polyene cyclizations and therefore this constitutes an extension of the previously known scope of terminating nucleophiles.
6. Enzymatic Studies

![Diagram showing GC-MS chromatograms](image)

**Fig. 2** Top: GC-MS chromatogram of authentic 12. Second from the top: GC-MS chromatogram of authentic 10 (possible partial degradation due to transportation). Third from the top: GC-MS chromatogram of authentic 21. Bottom: GC-MS chromatogram of the reaction products of 12 with BmeTC. All measurements performed with “GC-MS Niigata”.

The mass spectrometric studies indicated that one of the products formed from the enzymatic reaction of 12 with BmeTC (Fig. 2, Bottom) has a similar GC-MS retention time and comparable GC-MS mass spectrum as authentic 10 (Fig. 2, Second from the top and Fig. 3 respectively). In addition, 21 could not be detected in the enzymatic reaction mixture (within the limits of detection) (Fig. 4).
**Fig. 3** Top: GC-MS mass spectrum of authentic 10 (measured with "GC-MS Niigata"). Bottom: GC-MS mass spectrum of enzymatic reaction product with a similar retention time as authentic 10 (measured with "GC-MS Niigata").

**Fig. 4** Zoom in the GC-MS chromatogram of the reaction of 12 with BmeTC (measured with "GC-MS Niigata").
Fig. 5 Top: GC-MS mass spectrum of compound S6 from the reaction of 12 with BmeTC (measured with "GC-MS Niigata"). Middle: GC-MS mass spectrum of authentic S6 (measured with "GC-MS Berlin"). Bottom: GC-MS mass spectrum of authentic compound 21 (measured with "GC-MS Niigata").
Mass spectrometric studies indicated that the fragmentation pattern of \( S_6 \) synthetized from the enzymatic reaction of \( 12 \) with BmeTC (Fig. 2 Bottom and Fig. 5 Top) shows similarities to the fragmentation pattern of \( S_6 \) synthesized from \( \alpha \)-onocerin \( 6^{15} \) by mono deoxygenation (Fig. 5 Middle; \( S_6 \), for the synthesis see page 29 in the Supporting Information).\(^{34}\) While the relative configuration and the possible hydration level of the elimination product could not be elucidated, its connectivity resembles \( S_6 \). The tetracyclic product results from an epoxypolyene dicyclization followed by elimination.

"GC-MS Niigata":

GC-MS (injection temperature, 300°C; oven temperature, 220–300°C at an increment of 3°C min\(^{-1}\)) was performed on a JMS-T100GCV spectrometer (JEOL) equipped with a DB-1 capillary column (30 m × 0.25 mm × 0.25 μm; J&W Scientific, Inc.), using the EI mode operated at 70 eV. HRMS was performed on a JMS-T100LP spectrometer (JEOL) using ESI mode.

"GC-MS Berlin":

GC/MS system consisting of a 5977E MSD single-quadrupole mass spectrometer (EI-Mode (70 eV)) with a 7820A GC by Agilent Technologies (Agilent 190915-433UI, 30 m × 250 μm x 0.25 μm). Injection temperature: 300 °C, column temperature: 220-300 °C (increment 3 °C/min).

Enzymatic assay for BmeTC

*Escherichia coli* BL21(DE3) harboring pColdTF-BmeTC was grown at 37°C in LB medium (1 L) with 100 μg mL\(^{-1}\) ampicillin. Expression of the recombinant protein was induced by adding 0.1 mM isopropyl \( \beta \)-D-1-thiogalactopyranoside when the OD\(_{600}\) reached ~0.6. Further cultivation of BL21(DE3) recombinants was performed for 24 h at 15°C. *E. coli* cells expressing recombinant BmeTC were harvested by centrifugation and resuspended in 15 mL/5 g *E. coli* cells of buffer A containing 50 mM Tris-HCl (pH 7.5), 2.5 mM dithiothreitol, 1 mM EDTA, and 0.1% Tween80. The cells were disrupted by sonication with UP200s (Hielscher Ultrasonics GmbH, Teltow, Germany) at 4–10°C for 40 min. The resulting suspension was centrifuged at 10,000 × g for 20 min. The pellet was discarded, and the resulting supernatant was used as a cell-free extract. The reaction mixture for analyzing the enzymatic activity of BmeTC contained substrate \( 12 \) (0.1 mg) emulsified with Tween80 (2 mg) in buffer A (1 mL), and 4 mL of cell-free extract containing BmeTC in a total volume of 5 mL. The reaction was carried out at 30°C for 64 h and terminated by using a 15% KOH/MeOH solution (6 mL). The lipophilic enzymatic product was extracted from the incubation mixtures with \( n \)-hexane (5 mL × 3). Tween80 detergent was removed by passing the extract through a short SiO\(_2\) column (\( n \)-hexane: EtOAc = 100:20) and then subjecting the eluent to GC-MS.
# 7. Density Functional Calculations

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<td>Figure S7</td>
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</tbody>
</table>
Methods-QCC analysis

Calculations were performed with GAUSSIAN09.\textsuperscript{35} Geometries were optimized using the B3LYP method with the basis set of 6-31G(d).\textsuperscript{36} All stationary points were characterized as minima or transition state structures using frequency calculations at the same level. All reported energies include zero-point energy corrections (unscaled) from the frequency calculations at the same level. Intrinsic reaction coordinate (IRC) calculations were used for further characterization of transition state structures.\textsuperscript{37} mPW1PW91//6-31+G(d,p)\textsuperscript{38} energies are also shown, since it is known that B3LYP underestimates the relative energies of cyclic structures versus acyclic isomers.\textsuperscript{38} These energies do not include zero-point energy corrections. The validity of this computational approach for examining terpene-forming carbocation rearrangements is well-established.\textsuperscript{39} Structural images were created with \textit{Ball&Stick}.\textsuperscript{40}
Key
Capital letters are used to label carbocations and subsequent numbers to discern different conformers or stereoisomers.
Structures A1, A2 and A3 in the Supporting Information are conformers of the structure 23 in the manuscript.
B1 in the Supporting Information corresponds 10+H\(^+\) in the manuscript.
The structures A4, A5 and A6 in the Supporting Information are conformers of the structure 24 in the manuscript.
D3 in the Supporting Information corresponds 21+H\(^+\) in the manuscript.
Figure S1 | Formation of B1 (10+H⁺). Energies (kcal/mol; B3LYP/6-31G(d)//B3LYP/6-31G(d) in normal texts and mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d) in brackets) are shown.
Figure S2 | Formation of D1. Energies (kcal/mol; B3LYP/6-31G(d)//B3LYP/6-31G(d) in normal texts and mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d) in brackets) are shown. 1,2-Hydride shift step has a barrier of <1kcal/mol.
Figure S3 | Formation of B2. Energies (kcal/mol; B3LYP/6-31G(d)//B3LYP/6-31G(d) in normal texts and mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d) in brackets) are shown.
Figure S4 | Formation of D2. Energies (kcal/mol; B3LYP/6-31G(d)//B3LYP/6-31G(d) in normal texts and mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d) in brackets) are shown. The B3→C2 conversion is a concerted reaction combined with ring opening/1,2-hydride shifting events. See Figure 2 for a different 1,2-hydride shift, which has a significantly smaller energy barrier.
Figure S5 | Formation of B4. Energies (kcal/mol; B3LYP/6-31G(d)//B3LYP/6-31G(d) in normal texts and mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d) in brackets) are shown.
Figure S6 | Formation of D3 (21+H+). Energies (kcal/mol; B3LYP/6-31G(d)//B3LYP/6-31G(d) in normal texts and mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d) in brackets) are shown. Computed energy barrier for 1,2-hydride shift for A5 is small. Overall the highest energy step is conformation change of C for cyclization.
Figure S7 | Formation of B5 and D4. Energies (kcal/mol; B3LYP/6-31G(d)//B3LYP/6-31G(d) in normal texts and mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d) in brackets) are shown. The B5→D4 conversion is a concerted reaction consisting of asynchronously occurring ring opening/1,2-hydride shift/ring closure events, which is formally known as a dyotropic rearrangement.
Table S1 | Reaction energetics (kcal/mol; mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)) for formation of B (6-6-7-6-6) and D (6-6-6-6-6). Isomers B1 (10+H\(^+\)) and D3 (21+H\(^+\)) are observed in experiments.

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Coordinates and Energies

Figure S1

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Imaginary Frequencies: none found

Zero-point correction = 0.789404 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1311583 hartrees (-831533.053144833 kcal/mol)

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Imaginary Frequencies: 1 (-20.2839 1/cm)

Zero-point correction = 0.789355 (Hartree/Particle)

mpW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1303754 hartrees (-831532.561867254 kcal/mol)

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HF = -1325.3116578 hartrees (-831646.318386078 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.792935 (Hartree/Particle)
mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1426158 hartrees (-831540.242840658 kcal/mol)

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Figure S2

A2

B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2962234 hartrees (-831636.633145734 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.787463 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1287411 hartrees (-831531.536327661 kcal/mol)

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Imaginary Frequencies: 1 (-311.9691 1/cm)

Zero-point correction = 0.786609 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

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Imaginary Frequencies: none found

Zero-point correction = 0.789253 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

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Imaginary Frequencies: 1 (-86.5045 1/cm)

Zero-point correction = 0.791042 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)/B3LYP/6-31G(d)

HF = -1325.1200739 hartrees (-831526.097572989 kcal/mol)

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Imaginary Frequencies: none found

Zero-point correction = 0.793255 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

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Figure S3

A3

B3LYP/6-31G(d)//B3LYP/6-31G(d) HF = -1325.2929549 hartrees (-831634.5821299 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.789575 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.124118 hartrees (-831528.63528618 kcal/mol)

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TS (A3-B2)

B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2898625 hartrees (-831632.641617375 kcal/mol)

Imaginary Frequencies: 1 (-47.7848 1/cm)

Zero-point correction = 0.789374 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1203105 hartrees (-831526.246041855 kcal/mol)

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HF = -1325.3020195 hartrees (-831640.270256445 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.793403 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1334742 hartrees (-831534.506395242 kcal/mol)
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Figure S4

**TS (B2-B3)**

B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2907561 hartrees (-831633.202360311 kcal/mol)

Imaginary Frequencies: 1 (-129.4894 1/cm)

Zero-point correction = 0.793808 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1221209 hartrees (-831527.382085959 kcal/mol)

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HF = -1325.3024083 hartrees (-831640.514232333 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.794067 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.134127 hartrees (-831534.91603377 kcal/mol)

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B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2805712 hartrees (-831626.811233712 kcal/mol)

Imaginary Frequencies: 1 (-454.5552 1/cm)

Zero-point correction = 0.787672 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1150602 hartrees (-831522.951426102 kcal/mol)

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**C2**

B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2928466 hartrees (-831634.514169966 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.790064 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1222667 hartrees (-831527.473576917 kcal/mol)

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B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2929496 hartrees (-831634.578803496 kcal/mol)

Imaginary Frequencies: 1 (-41.8966 1/cm)

Zero-point correction = 0.789791 (Hartree/Particle)
mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1220757 hartrees (-831527.353722507 kcal/mol)

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HF = -1325.2999789 hartrees (-831638.989759539 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.792954 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.132435 hartrees (-831533.85428685 kcal/mol)

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Figure S5

A4

B3LYP/6-31G(d)//B3LYP/6-31G(d)

\[ HF = -1325.2928738 \text{ hartrees} \ (\approx -831634.531238238 \text{ kcal/mol}) \]

Imaginary Frequencies: none found

Zero-point correction = 0.789474 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

\[ HF = -1325.1233606 \text{ hartrees} \ (\approx -831528.1600106 \text{ kcal/mol}) \]

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HF = -1325.2923137 hartrees (-831634.179769887 kcal/mol)

Imaginary Frequencies: 1 (-38.2880 1/cm)

Zero-point correction = 0.789995 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

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B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2957415 hartrees (-831636.330748665 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.792784 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1267061 hartrees (-831530.259344811 kcal/mol)

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Figure S6

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HF = -1325.2922916 hartrees (-831634.165901916 kcal/mol)

Imaginary Frequencies: none found
Zero-point correction = 0.788821 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1233298 hartrees (-831528.140682798 kcal/mol)

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B3LYP/6-31G(d)//B3LYP/6-31G(d)

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Imaginary Frequencies: 1 (-223.2825 1/cm)

Zero-point correction = 0.786511 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1250975 hartrees (-831529.249932225 kcal/mol)

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Imaginary Frequencies: none found
Zero-point correction = 0.789460 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -1325.1265879 hartree (-831530.185173129 kcal/mol)

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HF = -1325.2931965 hartrees (-831634.733735715 kcal/mol)

Imaginary Frequencies: 1 (-20.5860 1/cm)

Zero-point correction = 0.789442 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

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c4

B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.2989312 hartrees (-831638.332317312 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.790497 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1293716 hartrees (-831531.931972716 kcal/mol)

Coordinates (from last standard orientation):

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Center   Atomic   Coordinates (Angstroms)
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TS (C4-D3)

B3LYP/6-31G(d)//B3LYP/6-31G(d)

$HF = -1325.2980053$ hartrees ($-831637.751305803$ kcal/mol)
Imaginary Frequencies: 1 (-32.0139 1/cm)

Zero-point correction = 0.790246 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1279553 hartrees (-831531.043230303 kcal/mol)

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D3 (21+H+)

B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -1325.3107582 hartrees (-831645.753878082 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.792668 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1429776 hartrees (-831540.469873776 kcal/mol)

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Figure S7

A6

B3LYP/6-31G(d)\(\rightarrow\)B3LYP/6-31G(d)

\[ \text{HF} = -1325.294389 \text{ hartrees} (-831635.48204139 \text{ kcal/mol}) \]

Imaginary Frequencies: none found

Zero-point correction = 0.789027 (Hartree/Particle)

\[ \text{mpW1PW91/6-31+G(d,p)}\rightarrow\text{B3LYP/6-31G(d)} \]

\[ \text{HF} = -1325.1254244 \text{ hartrees} (-831529.455065244 \text{ kcal/mol}) \]

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HF = -1325.2867663 hartrees (-831630.698720913 kcal/mol)

Imaginary Frequencies: 1 (-45.5886 1/cm)

Zero-point correction = 0.788399 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -1325.1183373 hartrees (-831525.007839123 kcal/mol)

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HF = -1325.2936448 hartrees (-831635.015048445 kcal/mol)

Imaginary Frequencies: none found

Zero-point correction = 0.793242 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

HF = -1325.1247813 hartrees (-831529.051513563 kcal/mol)

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\[ \text{HF} = -1325.2809765 \text{ hartrees} \approx -831627.06563515 \text{ kcal/mol} \]

Imaginary Frequencies: 1 (-370.9670 1/cm)

Zero-point correction = 0.787814 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)

\[ \text{HF} = -1325.1147309 \text{ hartrees} \approx -831522.744787059 \text{ kcal/mol} \]

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Coordinates (from last standard orientation):

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HF = -1325.3103885 hartrees (-831645.521887635 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.792922 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -1325.1424285 hartrees (-831540.125308035 kcal/mol)
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8. Crystallographic Data

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CCDC 1529116 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures

Oxane 22
CCDC 1529117 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures

Oxepane 10
CCDC 1529118 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures
9. References


