Experimental Procedures

Reactions were carried out using oven-dried glassware under an atmosphere of dry N₂ and magnetically stirred, unless noted otherwise. Air- and moisture-sensitive liquids and solutions were transferred via syringe or stainless steel canula.

Reagents were purchased from commercial suppliers (Acros, Aldrich, Fluka, TCI) and used without further purification, unless noted otherwise.

Solvents (methylene chloride, diethyl ether, tetrahydrofuran, acetonitrile, toluene) for reactions were purified by filtration and dried by passage over activated anhydrous neutral A-2 alumina (MBraun solvent purification system) under an atmosphere of dry nitrogen. Analytical grade solvents were used as received for extractions and chromatographic purifications.

Deuterated solvents were obtained from Armar Chemicals, Switzerland, in the indicated purity grade.

Thin Layer Chromatography were used for monitoring reactions and carried out using Merck silica gel 60 F254 plates, visualized with UV light or developed either with phosphormolybdic acid solution or with potassium permanganate solution followed by heating

Flash Chromatography was performed using Fluka silica gel 60 (230-400 Mesh) at a pressure of ca. 0.3 bar. Eluents and Rf are indicated.

Lyophilizations were performed on a Christ Freeze Dryer Alpha 1-2 LD+.

1H-NMR spectra were recorded on Bruker 400 MHz spectrometers or Bruker 500 MHz spectrometers (equipped with a cryo platform) at 298K in the indicated deuterated solvent. Data are reported as follow: chemical shift (δ, ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet or not resolved signal; br, broad signal), coupling constant(s) (J, Hz), integration. All signals were referenced to the internal solvent signal as standard (CDCl₃, δ 7.26; CD₃OD, δ 3.31; DMSO-d₆, δ 2.50).

13C-NMR spectra were recorded with 1H-decoupling on Bruker 101 MHz or Bruker 125 MHz spectrometers (equipped with a cryo platform) at 298K in the indicated deuterated solvent. All signals were referenced to the internal
solvent signal as standard (CDCl₃, δ 77.0; CD₃OD, δ 49.0; DMSO-d₆, δ 39.5).

³¹P-NMR spectra were recorded with proton coupling and 1H-decoupling on Bruker 162 MHz or Bruker 202 MHz spectrometers (equipped with a cryo platform) at 298K in the indicated deuterated solvent. All signals were referenced to an internal standard (PPP)

IR spectra were recorded on a JASCO FT-IR-4100 spectrometer and data are reported in terms of frequency of absorption (cm⁻¹).

Mass spectra were recorded by the Mass spectroscopy Service of UZH on Finnigan MAT95 MS, Bruker EsquireLC MS, Bruker maXis QToF HR MS and Finnigan TSQ700 MS machines.

Synthesis of 8

The compound 8 was synthesized as described before in two steps starting from myo-inositol 7. Analytical data were identical with the values reported in the literature.¹³


Synthesis of 10

The compound 10 was synthesized as described before in three steps starting from 8. PMB group was introduced by a procedure described in a patent by Postech Foundation WO2005/85159 A1, 2005; Analytical data were identical with the values reported in the literature.⁸e

Synthesis of 11

The compound was synthesized as described before three steps starting from 4-hydroxibenzaldehyde and levulinic acid. Analytical data were identical with the values reported in the literature.\(^\text{10}\)


Synthesis of 12

A) 100 mg (0.263 µmol, 1.0 eq.) 10 and 180 mg (0.315 µmol, 1.2 eq) levulinylbenzyl phosphoramidite (LevB-PA) 11 were dissolved in dry MeCN (5 mL). 40.5 mg (0.342 mmol, 1.3 eq) of DCI was added and mixture was stirred for 10 minutes at room temperature. Progress of the reaction was followed by \(^{31}\)P-NMR. Oxidation was achieved by addition of 0.240 ml (1.32 mmol, 5 eq) \(t\)-BuOOH. Solvent was evaporated and the obtained crude oil 12a was directly used in the next step.

B) The intermediate was dissolved in DCM (10mL) and 5% of TFA (0.5 ml) and stirred for 5 min at room temperature. It was monitored by TLC and \(^{31}\)P-NMR. After completion of reaction, solvent was concentrated in vacuo and
residue was crystalized from Et₂O and purified by column chromatography (Gradient EtOAc to EtOAc: MeOH, 4:1) to get pure final product as brown solid 12 (99.0 mg, 0.150 mmol, 56 % yield)

**TLC** (EtOAc:MeOH, 4:1 v/v): \( R_f = 0.60 \); \(^1\text{H-NMR}\) (500 MHz, DMSO-\(d_6\)): \( \delta \)
- 7.44 (d, \( J = 8.5 \) Hz, 4H),
- 7.09 (d, \( J = 8.5 \) Hz, 4H),
- 5.17 (d, \( J = 3.3 \) Hz, 1H),
- 5.12 (d, \( J = 3.1 \) Hz, 1H),
- 5.11 (d, \( J = 2.3 \) Hz, 1H),
- 4.89 - 4.82 (m, 2H),
- 4.75 - 4.66 (m, 2H),
- 3.45 - 3.37 (m, 3H),
- 2.85 (t, \( J = 6.4 \) Hz, 4H),
- 2.73 (t, \( J = 6.4 \) Hz, 4H),
- 2.15 (s, 6H);

\(^{13}\text{C-NMR}\) (126 MHz, MeOD): \( \delta \)
- 207.91, 171.78, 150.89, 133.94, 128.89, 121.40, 82.05, 74.97, 72.94, 70.39, 68.75, 48.10, 48.02, 47.93, 47.81, 47.76, 47.64, 47.59, 47.47, 47.42, 47.25, 47.08, 37.28, 28.21, 27.64;

\(^{31}\text{P\{1H\}-NMR}\) (203 MHz, MeOD): \( \delta \)
-2.08;

\(^{31}\text{P-NMR}\) (203 MHz, MeOD): \( \delta \)
-1.37 to -3.14 (m);

\(^{31}\text{P-NMR}\) (203 MHz, MeOD): \( \delta \)
-1.37 to -3.14 (m);

\( \text{IR (neat, cm}^{-1}\) 3380.6, 2959.2, 2921.6, 2364.3, 1754.9, 1715.4, 1361.5, 1200.5, 1135.9, 1004.7;

**HRMS** (ESI) \([\text{M+Na}]^+ \text{ calcld}\) 691.1768 for \( \text{C}_{30}\text{H}_{37}\text{NaO}_{15}\text{P} \), found 691.1764

**Synthesis of 14**

![Image](image-url)

50.0 mg (0.075 mmol, 1.0 eq.) of inositol monophosphate 12 and 0.575 g (1.13 mmol, 15.0 eq.) of 9-fluorenylmethyl phosphoramidite (Fm-PA) 13 were coevaporated with dry MeCN (2 mL). The residue was dissolved in dry THF (2 mL). To this solution 177 mg (1.50 mmol, 20.0 eq.) of DCI was added. Progress of the reaction was monitored by \(^{31}\text{P-NMR}\). After completion of the reaction (30-45 min), oxidation was achieved by slow (!) addition of 276.5 mg (1.13 mmol, 15.0 eq.) \( m\text{CPBA (70\% moistened with water) at 0ºC. Mixture was concentrated in vacuo} \) and product was crystalized from MeOH (2 x 3 ml)
yielding 155 mg of 14 as a white sticky solid (0.054 mmol, 73%).

**TLC** (EtOAc:Hexane, 3:2 v/v): \(R_f = 0.33\);

\[ ^1H-NMR \] (500 MHz, CDCl\(_3\)): \(\delta\) 7.65 - 7.51 (m, 24H), 7.44 - 7.34 (m, 9H), 7.34 - 7.29 (m, 6H), 7.27 - 7.20 (m, 12H), 7.21 - 7.13 (m, 8H), 7.12 - 7.06 (m, 5H), 7.05 - 6.98 (m, 21H), 6.85 - 6.81 (m, 3H), 5.66 (d, \(J = 9.0\) Hz, 1H), 5.01 (q, \(J = 9.9\) Hz, 2H), 4.94 (dd, \(J = 11.7, 7.9\) Hz, 2H), 4.73 (dd, \(J = 11.8, 9.7\) Hz, 2H), 4.59 - 4.51 (m, 2H), 4.49 - 4.40 (m, 2H), 4.37 - 4.19 (m, 11H), 4.19 - 4.05 (m, 6H), 4.05 - 4.00 (m, 2H), 3.99 - 3.91 (m, 16H), 3.81 (q, \(J = 6.9\) Hz, 4H), 2.87 - 2.76 (m, 8H), 2.22 (s, 6H);

\[ ^13C-NMR \] (126 MHz, CDCl\(_3\)): \(\delta\) 206.26, 171.04, 150.62, 143.30 - 142.80 (m), 141.39 - 141.11 (m), 133.28, 129.39, 127.71 - 126.83 (m), 125.69 - 125.21 (m), 121.50, 119.89 - 119.64 (m), 77.29, 77.23, 77.03, 76.78, 75.90, 75.63, 74.69, 73.28, 70.05 - 69.10 (m), 47.90, 47.84, 37.89, 29.86, 28.15, 27.35, 21.07, 14.22; 

\[ ^31P{1H}-NMR \] (203 MHz, CDCl\(_3\)) \(\delta\) -0.61, -1.08, -1.42, -2.81; 

\[ ^31P-NMR \] (162 MHz, CDCl\(_3\)): \(\delta\) -0.41 - 0.80 (m), -0.88 - -1.22 (m), -1.26 - -1.62 (m), -2.66 - -2.98 (m); 

\[ IR \] (neat, cm\(^{-1}\)) 2923.6, 2853.2, 2362.4, 2341.2, 1709.6, 1449.2, 1283.4, 1020.2, 983.5; 

\[ HRMS \] (ESI) \([M+2Na]^{2+}\) calcd for C\(_{170}H_{142}Na_2O_{30}P_6\), 1447.3898; found, 1447.3906.

**Synthesis of 14a**

![Diagagram](image)

155 mg (54.4 \(\mu\)mol, 1.0 eq.) of hexaphosphate 14 was dissolved in CH\(_2\)Cl\(_2\) (3.00 mL). TFA (43.6 mL) and mixture of hydrazine acetate 9.75 mg (0.300 mmol, 6.0 eq) in MeOH (0.27 mL) were added. Reaction mixture was stirred overnight at room temperature. It was tracked by \(^31P\)-NMR. After completion it was concentrated in vacuo and precipitated from MeOH, crude material 14a was obtained (115 mg, 0.050 mmol, 87%) and it was used directly in the next step.
TLC (EtOAc): \( R_f = 0.43 \); \(^{31}\text{P\{1 H\}}\text{-NMR}\) (203 MHz, CDCl\(_3\)): \( \delta -0.76\), -0.82, -1.49, -1.75; \(^{31}\text{P-NMR}\) (162 MHz, CDCl\(_3\)): \( \delta -0.79\), -1.50, -1.77; HRMS (ESI) [M]+ calcd for C\(_{146}H_{117}O_{24}P_6\), 2439.6364; found, 2439.6349

Synthesis of 15

The compound was synthesized as described before in three steps starting from myo-inositol. Analytical data were identical with the values reported in the literature.\(^{17a}\)


Synthesis of 16a

57.0 mg (23.3 \( \mu \)mol, 1.0 eq.) of crude hexaphosphate 14a were dissolved in dry CH\(_2\)Cl\(_2\) (2 mL). Coumarine-9-florenylmethyl phosphoramidite (DEACM-Fm PA) 15 26.8 mg (46.6 \( \mu \)mol, 2.0 eq) was added and mixture was coevaporated. Dry mixture was dissolved again in CH\(_2\)Cl\(_2\) (2 mL) and DCl 8.25 mg (69.9 \( \mu \)mol, 3.0 eq.) was added. Reaction was stirred for 10 minutes.
Progress of the reaction was monitored by \(^{31}\text{P-NMR}\). After completion of the reaction, oxidation was achieved by slow (!) addition of 11.4 mg (46.6 µmol, 2.00 eq) mCPBA (70% moistened with water). The reaction mixture was concentrated and MeOH (5 ml) was added. White precipitate was formed and it was centrifugated for 5 min. Solvent was removed and precipitate purified by column chromatography (EtOAc:Hexane 1:1 over EtOAc to EtOAc:MeOH=20:1). Yield: 38 mg 16a as a colorless syrup (15.0 µmol, 55%).

**TLC** (EtOAc): \(R_f = 0.66\); \(^1\text{H-NMR}\) (400 MHz, CDCl\(_3\)): \(\delta 7.77 - 7.33\) (m, 34H), 7.28 - 6.98 (m, 37H), 6.98 - 6.60 (m, 21H), 5.90 - 5.61 (m, 2H), 5.25 - 4.80 (m, 5H), 4.63 - 3.58 (m, 34H), 3.41 - 2.85 (m, 9H); \(^{13}\text{C-NMR}\) (101 MHz, CDCl\(_3\)): \(\delta\) 195.77, 190.49, 187.38, 171.16, 161.41, 155.79, 150.34, 142.85, 141.05, 127.53, 127.16, 126.91, 125.19, 119.69, 119.66, 105.29, 97.19, 77.36, 77.24, 77.04, 76.73, 74.42, 74.15, 73.78, 69.92, 60.42, 50.83, 47.66, 44.37, 29.73, 21.07, 14.22, 12.43; \(^{31}\text{P\{1 H\}-NMR}\) (162 MHz, CDCl\(_3\)): \(\delta 1.06 - 0.34\) (m), -0.54 - -4.26 (m), -11.49 (d, \(J = 32.2\) Hz), -13.11 (d, \(J = 33.8\) Hz); \(^{31}\text{P-NMR}\) (162 MHz, CDCl\(_3\)): \(\delta\) 1.28 - 0.41 (m), -0.36 - 1.94 (m), 1.10 - 5.41 (m), -10.51 - 12.25 (m), -12.56 - 14.24 (m); \textbf{IR}\ (neat, cm\(^{-1}\)) 3122.2, 2931.3, 2362.4, 2239.9, 1639.9, 1653.7, 1600.6, 1422.2, 1240.0, 1009.6, 737.6, 503.3; \textbf{HRMS}\ (ESI) [M]\(^{+}\) calcd for C\(_{174}\)H\(_{143}\)NO\(_{29}\)P\(_{7}\), 2926.7915; found, 2926.7871.

**Synthesis of 6b**

50.0 mg (20.4 µmol, 1.0 eq.) of crude hexaphosphate 14a were dissolved in
dry CH₂Cl₂ (2 mL). 9-fluorenylmethyl phosphoramidite (Fm-PA) 13 21.0 mg (40.9 µmol, 2.00 eq) was added and mixture was coevaporated. Dry mixture was dissolved again in CH₂Cl₂ (2 mL) and DCI 4.83 mg (40.9 µmol, 2.00 eq.) was added. Reaction was stirred for 10 minutes. Progress of the reaction was monitored by ³¹P-NMR. After completion of the reaction, oxidation was achieved by slow (!) addition of 7.10 mg (40.9 µmol, 2.0 eq) mCPBA (70% moistened with water).

The reaction mixture was concentrated and MeOH (5 ml) was added. White precipitate was formed and it was centrifugated for 5 min. Solvent was removed and precipitate purified by column chromatography (DCM:MeOH 5:0.1 to DCM:MeOH=5:0.5). Yield: 40 mg 16b as a colorless syrup (13.9 µmol, 68%).

**TLC** (EtOAc): Rₕ = 0.60; ¹H-NMR (500 MHz, CDCl₃): δ 7.69 - 7.31 (m, 36H), 7.27 - 6.95 (m, 40H), 6.96 - 6.65 (m, 20H), 5.23 - 5.00 (m, 3H), 4.54 - 3.58 (m, 39H), (contains solvents: DCM, MeOH); ¹³C-NMR (126 MHz, CDCl₃): δ 142.89, 141.06, 127.54, 126.92, 125.24, 119.68, 99.98, 77.34, 77.02, 76.75, 76.70, 74.03, 70.65, 69.90, 53.43, 50.84, 47.67, 29.70; ³¹P{¹H}-NMR (203 MHz, CDCl₃): δ -0.17 , -0.07 , -2.68 , -11.20 , -12.15; ³¹P-NMR (203 MHz, CDCl₃): δ -0.73 , -0.95 - -5.31 (m), -12.54 , -14.28; IR (neat, cm⁻¹) 3365.2, 2923.6, 2337.3, 1717.3, 1449.2, 1265.1, 1017.3, 736.7; HRMS (ESI) [M⁺] calcd for C₁₇₄H₁₃₈O₂₇P₇, 2875.7594; found, 2875.7581.

**Synthesis of 17**

20.0 mg (6.83 µmol, 1.0 eq.) of 16a were dissolved in DMF (3 mL) and
piperidine (0.5 ml) was added. The solution was stirred 40 minutes at room temperature. After completion of the deprotection solution was concentrated and product precipitated with Et₂O (10 mL). The precipitate was centrifuged and separated by decantation of solvent. The precipitate was once more dissolved in MeOH and crystallized by addition of Et₂O. Centrifugation process was repeated and yellowish crystals were obtained that were dried in vacuo. Piperidinium counter ions were exchanged to sodium by addition of excess NaI to MeOH solution of 17. After 30 minutes of stirring sodium salt of 17 was precipitated: Yield: 8.02 mg of 17 (8.59 µmol, 95%).

¹H-NMR (500 MHz, D₂O): δ 7.58 (dd, J = 9.9 Hz, 1H), 6.85 (dd, 2H), 6.64 (s, 1H), 6.29 (s, 1H), 5.26 (d, J = 7.8 Hz, 2H), 4.98 (dd, J = 9.2 Hz, 9.2 Hz, 1H), 4.48 (ddd, J = 28.6, 28.6, 28.6 Hz, 2H), 4.17 (ddd, J = 19.1, 19.1, 19.1 Hz, 3H), 3.42 (q, J = 7.0 Hz, 4H), 1.13 (t, J = 7.2 Hz, 6H); ¹³C-NMR (126 MHz, 300 K, D₂O): δ 165.94, 155.61, 154.83, 154.77, 151.27, 125.61, 110.37, 106.13, 103.99, 97.39, 77.55, 76.63, 75.82, 73.23, 63.91, 48.88, 44.51, 22.25, 11.52; ³¹P{¹H}-NMR (203 MHz, D₂O): δ 1.81 , 0.99 (d, J = 21.1 Hz), 0.46 (d, J = 24.1 Hz), -10.74 (d, J = 16.0 Hz), -11.08 (d, J = 16.4 Hz); ³¹P-NMR (203 MHz, 300 K, D₂O): δ 1.81 (d, J = 9.7 Hz), 0.99 (dd, J = 20.8, 9.2 Hz), 0.46 (dd, J = 24.4, 9.7 Hz), -10.76 (dd, J = 15.7, 8.1 Hz), -10.91 to -11.23 (m); IR (neat, cm⁻¹) 3372.9, 2301.4, 1604.5, 1245.8, 1071.3, 948.8; HRMS (ESI) calcd for 483.4617 (M²⁺, C₂₀H₃₂NO₂₉P₇), found 483.4617.

Synthesis of 2

20.0 mg (6.95 µmol, 1.00 eq.) of 16b were dissolved in DMF (3 mL) and piperidine (0.5 ml) was added. The solution was stirred 40 minutes at room
temperature. After completion of the deprotection solution was concentrated and product precipitated with Et₂O (10 mL). The precipitate was centrifugated and separated by decantation of solvent. The precipitate was once more dissolved in MeOH and crystallized by addition of Et₂O. Centrifugation process was repeated and yellowish crystals were obtained that were dried in vacuo. Piperidinium counter ions were exchanged to sodium by addition of excess NaI to MeOH solution of 2. After 30 minutes of stirring sodium salt of 2 was precipitated: Yield: 6.91 mg of 2 (6.98 µmol, 97%).

¹H-NMR (500 MHz, D₂O): δ 5.06 - 5.04 (m, 2H), 4.91 (1H, peak assigned by 1H-31P HSQC correlation spectra (not shown)), 4.55 (dd, J = 18.9 Hz, 18.9, 1H), 4.27 (ddd, J = 15.9 Hz, 15.9 Hz, 15.9 Hz 2H); ¹³C-NMR (126 MHz, D₂O): δ 77.63, 76.06, 73.25; ³¹P{¹H}-NMR (203 MHz, D₂O): δ 1.72 , 1.05 , 0.79 , -8.38 , -11.72 (d, J = 17.2 Hz); ³¹P-NMR (203 MHz, D₂O): δ 1.72 (d, J = 9.2 Hz), 1.04 (d, J = 9.6 Hz), 0.80 , -8.36 , -11.70; IR (neat, cm⁻¹): 3410.5, 2361.4, 1635.3, 1056.8, 918.9; HRMS (ESI) [M]²⁺ calcd for C₆H₆O₂P₇, 368.9066; found, 368.9068

Purity Analysis of 17 by analytical Varian Pro Star HPLC and a C-5 reverse-phase column (Phenomenex C5 3.5 µm, 150 x 4.6 mm) using a 0 – 100 % gradient of CH₃CN in water over 30 minutes run a flow rate of 0.5 ml min⁻¹.
Compound 12, 31P 1H decoupled
Compound 12, $^{31}$P $^1$H coupled
Compound 12, 1H
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Compound 14, 31P 1H decoupled
Compound 14, 31P 1H coupled
Compound 14, 13C
Compound 14a, 31P 1H decoupled (crude)
Compound 14a, 31P 1H coupled (crude)
HR-ESI-MS (Bruker maXis)

Analysis Info
Analysis Name: D:\Data\Service\8035jehres.d
Method: tune_low_neg_Aug2014.m
Sample Name: tP-8-58P1
Comment: Solvent: MeCN
Client: Pavlovic

Acquisition Info
Acquisition Date: 6/19/2015 3:30:21 PM
Operator: ust
Instrument: maXis
Project: 255552.00033

Source Type: ESI
Ion Polarity: Negative
Set Nebulizer: 1.0 Bar
Set Capillary: 4000 V
Set Dry Heater: 180 °C
Scan Begin: 50 m/z
Set End Plate Offset: -500 V
Scan End: 3000 m/z
Set Dry Gas: 4.0 l/min

Intens. x 10^4

Bruker Compass DataAnalysis 4.2
printed: 6/19/2015 3:48:20 PM
by: ust
Page 1 of 2
Compound 16a, 31P 1H decoupled (mixture of diastereomers)
Compound 16a, 31P 1H coupled (mixture of diastereomers)
Compound 16a, 1H (mixture of diastereomers)
Compound 16a, 13C (mixture of diastereomers)
Compound 16b, 31P 1H decoupled
Compound 16b, 31P 1H coupled
Compound 16b, 1H

DCM

MeOH

A (m) 4.10
B (m) 5.12
C (m) 7.47
D (m) 7.11
E (m) 6.87

0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0 8.5
f1 (ppm)
Compound 16b, 13C
Compound 17, 31P 1H decoupled
Compound 17, 31P 1H coupled
Compound 17, 1H

[Chemical structure diagram]

- A (dd) 7.58
- B (dd) 6.85
- C (s) 6.64
- D (s) 6.29
- E (d) 5.26
- F (d) 4.98
- G (dd) 4.48
- H (dd) 4.17
- I (q) 4.9

f1 (ppm): 0.00, 0.50, 1.00, 1.50, 2.00, 2.50, 3.00, 3.50, 4.00, 4.50, 5.00, 5.50, 6.00, 6.50, 7.00, 7.50, 8.00
Compound 17, 13C

\[ \text{Diagram of Compound 17, 13C} \]
Compound 2, 31P 1H decoupled
Compound 2, 31P 1H coupled
 Compound 2, 1H

1H peak at 4.91 discovered by 1H-31P HSQC
Compound 2, 13C