Supporting Information

Experimental Data

Large Scale Preparation of Long Chain ADMET Synthons

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GENERAL INFORMATION

Reagents and Solvents

Unless otherwise specified, all chemical reagents were purchased from common suppliers and were used without further purification. Anhydrous tetrahydrofuran, diethyl ether and dichloromethane were obtained from a solvent purification system.

Instrumentation

All chemical shifts for ^1H NMR and ^{13}C NMR were referenced to the residue signals from CDCl_3 ($^1\text{H} = 7.27$ ppm, $^{13}\text{C} = 77.23$ ppm). Unless otherwise stated, all NMR spectra were recorded at room temperature. High-resolution mass spectrometry (HRMS) were carried out using a Agilent 6220 TOF-MS mass spectrometer in the direct analysis in real-time (DART) mode with the IonSense DART source unless otherwise specified. Elemental analysis data were obtained on a combustion Analyzer. IR/ATR spectra were acquired on a Bruker Vertex 80v. Melting points were recorded on a capillary melting point apparatus. Analytical thin-layer chromatography (TLC) was performed using aluminum supported silica plates with a 254 nm fluorescent indicator and pore size of 60 Å. Column chromatography was performed using ultrapure silica gel (40-63 μm , 230-400 mesh).

EXPERIMENTAL PROCEDURES AND ASSOCIATED DATA

General procedures for the homologation sequence

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((9-Bromononyl)oxy)(tert-butyl)dimethylsilane (2). In a flame-dried 2 L flask equipped with a magnetic stir bar, were introduced in the following order: dry dichloromethane (1.3 L), 9-bromo-1-nonanol (100.0 g, 448 mmol), 1-methylimidazole (110.1 g, 107 mL, 1.34 mol), and iodine (227.5 g, 896 mmol). Once the solids dissolved, *tert*-butyldimethylsilyl chloride (74.3 g, 493 mmol) was slowly added. After 10 minutes, the solvent was removed *in vacuo* and 800 mL of ethyl acetate was added. The iodine was treated with a saturated solution of sodium thiosulfate. After discoloration of both phases, the aqueous phase was extracted with ethyl acetate and the combined organic fractions were washed with brine. The organic contents were dried over magnesium sulfate and the solvent was subsequently removed *in vacuo* affording a thick yellow oil. The crude product was purified by flash column chromatography using hexane/ethyl acetate (98:2) as eluent yielding a colorless oil (148.1 g, 98%); ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 3.60 (t, J = 6.5 Hz, 2H), 3.40 (t, J = 6.9 Hz, 2H), 1.90-1.79 (m, 2H), 1.54 -1.26 (m, 12H), 0.90 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 63.5, 34.2, 33.1, 29.63, 29.53, 28.93, 28.38, 26.20, 25.98, 18.6, -5.0; IR ν_{max} = 2929, 2849, 1472 cm^{-1} ; DART/HRMS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{15}\text{H}_{33}\text{BrOSi}$: 337.1557, found: 337.1562; Elemental analysis: calculated: C 53.40%, H 9.86%, found: C 54.26%, H 10.00%.

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Undec-10-enal (3). In a 1 L flame-dried three-necked flask equipped with magnetic stirrer, were added dry dichloromethane (270 mL), pyridinium chlorochromate (85.44 g, 396.4 mmol), and finely crushed 3 Å molecular sieves (85 g). **10-undecen-1-ol (9spOH)**, available from commercial source) was slowly added to the mixture (45 g, 264.2 mmol). After 2 hours, diethyl ether (270 mL) was added and the resulting heterogeneous mixture was poured in a 4 L beaker equipped with a magnetic stirrer containing diethyl ether (3 L). The remaining tar was triturated 3 times with diethyl ether (100 mL) and the resulting organic solutions were poured in the beaker. After the

precipitated chromium byproduct and molecular sieves settled, the supernatant was purified by passing through a large silica plug. The solvents were removed *in vacuo* and the resulting dark oil was distilled over calcium hydride, affording a sweet-smelling clear liquid (40.1 g, 90%). The ^1H NMR was consistent with the published spectrum.¹

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1-((*tert*-Butyldimethylsilyl)oxy)icos-19-en-10-ol (4). In a flame-dried three necked flask equipped with a 100 mL addition funnel and a condenser, freshly ground magnesium turnings (31.8 g, 1.308 mol) and dry diethyl ether (240 mL) were added. A few drops of 1,2-dibromoethane were added to increase the magnesium surface area and the suspension was allowed to stir for 50 minutes at room temperature. Compound **2** (88.2 g, 261.5 mmol) was subsequently added dropwise at a rate that maintained a slight reflux. After the addition, the solution was refluxed for 5 hours. The Grignard reagent was cooled to room temperature and added dropwise to an undec-10-enal (40.0 g, 237.7 mmol) solution in diethyl ether (400 mL) at 0 °C. The resulting solution was allowed to warm slowly to room temperature and was subsequently heated at 30 °C for 4 hours. The reaction was quenched at 0 °C with a saturated solution of ammonium chloride. The biphasic mixture was extracted with Et₂O. The organic fractions were washed with brine and dried over anhydrous MgSO₄. The solvent was removed *in vacuo* to afford a yellow oil. The crude product was purified by column chromatography using hexanes/ethyl acetate (95:5) as eluent affording 97.2 g of **4** as a white solid (96%). Melting point: 36-37.5 °C; ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.82 (ddt, J = 17.1, 10.3, 6.7 Hz, 1H), 5.05-4.90 (m, 2H), 3.60 (m, 3H), 2.09-1.99 (m, 2H), 1.72-1.20 (m, 30H), 0.90 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 139.4, 114.3, 72.2, 63.6, 37.7, 34.0, 33.1, 29.92, 29.86, 29.80, 29.72, 29.66, 29.34, 29.15, 26.29, 26.24, 26.22, 26.02, 25.88, 18.6, -5.0; IR ν_{max} = 3337, 3082, 2922, 2849, 1647, 1475 cm⁻¹; DART/HRMS: $[\text{M}+\text{H}]^+$ calculated for C₂₆H₅₄O₂Si: 427.3966, found: 427.3976; Elemental analysis: calculated: C 73.17%, H 12.75%, found: C 73.46%, H 13.00%.

¹ Qin, X.; Tzvetkov, T.; Liu, X.; Lee, D.-C.; Yu, L.; Jacobs, D. C. *J. Am. Chem. Soc.* **2004**, *126*, 13232–13233.

O-(1-((*tert*-Butyldimethylsilyl)oxy)icos-19-en-10-yl) S-methyl carbonodithioate (5). In a 1 L flame-dried three-necked round bottom flask, **4** (97.2 g, 227.8 mmol) and THF (300 mL) were added. The solution was cooled to 0 °C and sodium hydride 60% in mineral oil (15.1 g, 378.1 mmol) was carefully added. After 30 min, the mixture was allowed to slowly warm up to room temperature. After 2 hours, the reaction was cooled to 0 °C and carbon disulfide (52.0 g, 683.2 mmol) was added dropwise. After 3 h, the mixture was allowed to slowly warm to room temperature. Eight hours later, the reaction was cooled to 0 °C and methyl iodide (48.4 g, 341.6 mmol) was added dropwise to the reaction. After 1 hour, the reaction was allowed to slowly warm to room temperature, after which the mixture became more viscous. Four hours later, the reaction was cooled to 0 °C and was carefully quenched with a saturated ammonium chloride solution. Diethyl ether was added and aqueous phase was extracted with diethyl ether. The combined organic layers were washed with brine, and dried over sodium sulfate. Removal of the solvents *in vacuo* afforded an impure orange oil (124.3 g).

The following yield and characterization data were obtained on a gram scale: The crude product was purified by column chromatography using hexanes/ethyl acetate (99:1) as eluent affording 1.13 g of **5** as a yellow oil (93%). ¹H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.93-5.65 (m, 1H), 5.05-4.90 (m, 2H), 3.61 (m, 3H), 2.56 (s, 3H), 2.05 (dt, *J* = 8.0, 6.7 Hz, 2H), 1.84-1.22 (m, 30H), 0.91 (s, 9H), 0.06 (s, 6H); ¹³C NMR (75 MHz, Chloroform-*d*) δ (ppm) 216.0, 139.4, 114.3, 85.2, 63.5, 34.01, 33.81, 33.09, 29.73, 29.70, 29.69, 29.61, 29.58, 29.29, 29.12, 26.21, 26.00, 25.3, 18.98, 18.59, -5.0; IR ν_{max} = 3082, 2929, 2849, 1640, 1468, 1100 (C=S) cm⁻¹; DART/HRMS: [M+NH₄]⁺ calculated for C₂₈H₅₆O₂S₂Si: 534.3829, found: 534.3850; Elemental analysis: calculated: C 65.06%, H 10.92%, found: C 65.01%, H 10.88%.

***tert*-Butyl(icos-19-en-1-yloxy)dimethylsilane (6).** To a solution of **5** (crude, 124.3 g) in dioxane (770 mL), were added triethylamine (350 mL, 2.51 mol) and an hypophosphorous acid solution in water (50% w/v, 150.3 g, 588.7 mmol). The mixture was refluxed and an AIBN solution (7.48 g, 45.55 mmol) in dioxane (100 mL) was added continuously over 4 hours. After disappearance of the starting material by TLC analysis, the solvents were removed *in vacuo* and 100 mL of hexanes were added. The resulting mixture was passed through a silica plug using hexanes/ethyl acetate

(98:2) as the mobile phase. The solvents were removed *in vacuo* affording a slightly yellow oil (68.4 g).

The following yield and characterization data were obtained on a gram scale: The crude product was purified by column chromatography using hexanes as eluent affording 613 mg of **6** as a colorless oil (77%). ¹H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.83 (ddt, *J* = 17.0, 10.1, 6.7 Hz, 1H), 5.0-4.90 (m, 2H), 3.61 (t, *J* = 6.6 Hz, 2H), 2.05 (m, 2H), 1.6-1.19 (m, 32H), 0.91 (s, 9H), 0.06 (s, 6H); ¹³C NMR (75 MHz, Chloroform-*d*) δ (ppm) 139.5, 114.3, 63.6, 34.28, 34.06, 33.14, 29.92, 29.89, 29.85, 29.75, 29.69, 29.40, 29.32, 29.19, 26.28, 26.24, 26.22, 26.05, 18.6, -5.0; GC-MS/HRMS: [M+H]⁺ calculated for C₂₆H₅₄OSi: 411.4017, found: 411.4038; Elemental analysis: calculated: C 76.02%, H 13.25%, found: C 75.86%, H 13.20%.

Icos-19-en-1-ol (18spOH). To a solution of **6** (crude, 68.4 g) in acetone (1.6 L), were added water (82 mL) and copper(II) chloride dihydrate (1.94 g, 11.39 mmol). The green mixture was refluxed for 2 hours, after which the solvents were removed *in vacuo*. The resulting solid was dissolved in hexanes and the solution was filtrated over a bed of celite. The solvent was removed *in vacuo*, and the crude solid was recrystallized in pentane affording **18spOH** as pure white flakes (45.3 g, 67% from **4**).

The following yield and characterization data were obtained on a 500 mg scale using pure **6** as starting material: purification by flash column chromatography using hexanes/ethyl acetate (95:5) as mobile phase afforded **18spOH** as pure white flakes (353 mg, 98%). Melting point: 56-56.5 °C; ¹H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.83 (ddt, *J* = 17.0, 10.2, 6.6 Hz, 1H), 5.06-4.89 (m, 2H), 3.65 (t, *J* = 6.6 Hz, 2H), 2.10-1.99 (m, 2H), 1.73-1.18 (m, 32H); ¹³C NMR (75 MHz, Chloroform-*d*) δ (ppm) 139.5, 114.3, 63.2, 33.0, 32.0, 29.90, 29.88, 29.84, 29.82, 29.80, 29.78, 29.76, 29.73, 29.66, 29.38, 29.17, 25.6; IR ν_{max} = 3272, 3079, 2922, 2849, 1647, 1464 cm⁻¹; DART/HRMS: [M+NH₄]⁺ calculated for C₂₀H₄₀O: 314.3417, found: 314.3428; Elemental analysis: calculated: C 81.01%, H 13.60%, found: C 80.99%, H 13.73%.

The following compounds were synthesized according to the procedures described above.

Icos-19-enal (7). After purification by column chromatography using hexanes/ethyl acetate (95:5) as eluent, **7** was afforded as a white solid (22.8 g, 88%). Melting point: 38-40 °C; ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 9.76 (s, 1H), 5.82 (ddt, $J = 17.0, 10.2, 6.6$ Hz, 2H), 5.04-4.87 (m, 2H), 2.42 (t, $J = 7.3$ Hz, 2H), 2.10-1.99 (m, 2H), 1.70-1.19 (m, 30H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 203.1, 139.5, 114.3, 44.1, 33.1, 29.89, 29.86, 29.81, 29.76, 29.74, 29.70, 29.65, 29.58, 29.39, 29.18, 22.3; IR $\nu_{\text{max}} = 3086, 2915, 2849, 2740, 1716$ (C=O) cm^{-1} ; DART/HRMS: $[\text{M}+\text{NH}_4]^+$ calculated for $\text{C}_{20}\text{H}_{38}\text{O}$: 312.3261, found: 312.3267; Elemental analysis: calculated: C 81.56%, H 13.01%, found: C 81.76%, H 12.93%.

1-((tert-Butyldimethylsilyl)oxy)nonacos-28-en-10-ol (8). The crude was purified by column chromatography using hexanes/ethyl acetate (95:5) as eluent. Compound **8** was afforded as a white solid (40.1 g, 94%). Melting point: 57-58 °C; ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.82 (ddt, $J = 17.0, 10.2, 6.7$ Hz, 1H), 5.06-4.89 (m, 2H), 3.60 (m, 3H), 2.04 (m, 2H), 1.67-1.18 (m, 48H), 0.90 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 139.5, 114.3, 72.2, 63.6, 37.7, 34.0, 33.1, 29.95, 29.91, 29.85, 29.80, 29.74, 29.65, 29.39, 29.18, 26.23, 26.21, 26.18, 26.02, 25.89, 18.6, -5.0; IR $\nu_{\text{max}} = 3326, 3079, 2922, 2849, 1647, 1464$ cm^{-1} ; DART/HRMS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{35}\text{H}_{72}\text{O}_2\text{Si}$: 553.5374, found: 553.5381; Elemental analysis: calculated: C 76.01%, H 13.12%, found: C 76.28%, H 13.21%.

Nonacos-28-en-1-ol (27spOH). After 3 steps without purifications, the desired compound was recrystallized with hexanes post-deprotection and isolated as pure white flakes (20.2 g, 66% from **8**). Melting point: 78-79 °C; ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.82 (ddt, $J = 17.0, 10.3, 6.7$ Hz, 1H), 5.06-4.88 (m, 2H), 3.65 (t, $J = 6.6$ Hz, 2H), 2.11-1.98 (m, 2H), 1.18-1.62 (m, 50H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 139.5, 114.3, 63.3, 34.1, 33.0, 29.93, 29.85, 29.74, 29.66, 29.39, 29.18, 26.0; IR $\nu_{\text{max}} = 3326, 3079, 2922, 2846, 1643, 1464$ cm^{-1} ; DART/HRMS: $[\text{M}+\text{NH}_4]^+$ calculated for $\text{C}_{29}\text{H}_{58}\text{O}$: 440.4826, found: 440.4831; Elemental analysis: calculated: C 82.39%, H 13.83%, found: C 82.09%, H 13.70%.

1-((*tert*-Butyldimethylsilyl)oxy)octatriacont-37-en-10-ol (9). After 2 steps, the crude was purified by column chromatography using near boiling hexanes/ethyl acetate (95:5) as eluent. Compound **9** was afforded as a white solid (20.4 g, 79% from **27spOH**). Melting point: 73.5-74.5 °C; ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.82 (ddt, $J = 17.0, 10.2, 6.6$ Hz, 1H), 5.07-4.89 (m, 2H), 3.60 (m, 3H), 2.12-1.99 (m, 2H), 1.62-1.13 (m, 66H), 0.90 (s, 9H), 0.05 (s, 6H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 139.5, 114.3, 72.2, 63.5, 37.7, 34.0, 33.1, 29.94, 29.89, 29.86, 29.81, 29.75, 29.66, 29.39, 29.18, 29.15, 26.21, 26.03, 25.90, 18.6, -5.0; IR $\nu_{\text{max}} = 3348, 3079, 2918, 2846, 1643, 1461$ cm^{-1} ; DART/HRMS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{44}\text{H}_{90}\text{O}_2\text{Si}$: 679.6783, found: 679.6794; Elemental analysis: calculated: C 77.80%, H 13.36%, found: C 77.90%, H 13.37%.

Octatriacont-37-en-1-ol (36spOH). A 0.38 M solution of **9** in THF was used (instead of 0.76 M) for the formation of the xanthate. Similarly the deprotection step was carried out in a dilute environment (factor of 2); additionally 100 mL of heptane was added. **36spOH** precipitated upon cooling of the reaction mixture. The desired product was isolated by vacuum filtration as pure flakes (9.89 g, 60% from **9**). Melting point: 90-92 °C; ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.83 (ddt, $J = 17.0, 10.2, 6.6$ Hz, 1H), 5.05-4.86 (m, 2H), 3.65 (t, $J = 6.6$ Hz, 2H), 2.05 (m, 2H), 1.26-1.62 (m, 68H); ^{13}C NMR (125 MHz, Chloroform-*d*, 50 °C) δ (ppm) 139.5, 114.3, 63.4, 34.0, 33.2, 29.94, 29.91, 29.86, 29.85, 29.76, 29.70, 29.41, 29.25, 26.0; IR $\nu_{\text{max}} = 3323, 3079, 2922, 2849, 1643, 1464$ cm^{-1} ; DART/HRMS: $[\text{M}+\text{NH}_4]^+$ calculated for $\text{C}_{38}\text{H}_{76}\text{O}$: 566.6234, found: 566.6232; Elemental analysis: calculated: C 83.13%, H 13.95%, found: C 83.25%, H 14.05%.

Miscellaneous characterizations:

O-(1-((*tert*-Butyldimethylsilyl)oxy)nonacos-28-en-10-yl) S-methyl. Yellow oil (81%); ^1H NMR

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(300 MHz, Chloroform-*d*) δ (ppm) 5.79 (m, 1H), 5.05-4.89 (m, 2H), 3.60 (m, 3H), 2.55 (s, 3H), 2.10-1.99 (m, 2H), 1.83-1.14 (m, 48H), 0.90 (s, 9H), 0.06 (s, 6H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 216.0, 139.5, 114.3, 85.2, 63.5, 34.1, 33.82, 33.10, 29.91, 29.85, 29.78, 29.74, 29.71, 29.64, 29.62, 29.39, 29.18, 26.22, 26.00, 25.4, 18.98, 18.60, -5.0; IR ν_{max} = 3079, 2929, 2846, 1640, 1461, 1096 (C=S) cm^{-1} ; DART/HRMS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{37}\text{H}_{74}\text{O}_2\text{S}_2\text{Si}$: 643.4972, found: 643.4958; Elemental analysis: calculated: C 69.09%, H 11.60%, found: C 69.21%, H 11.40%.

***tert*-Butyldimethyl(nonacos-28-en-1-yloxy)silane.** White solid (65%); Melting point: 47.5-49 °C; ^1H NMR (300 MHz, Chloroform-*d*) δ (ppm) 5.83 (ddt, J = 17.0, 10.2, 6.7 Hz, 1H), 5.05-4.89 (m, 2H), 3.61 (t, J = 6.6 Hz, 2H), 2.10-1.99 (m, 2H), 1.22-1.56 (m, 50H), 0.9 (s, 9H), 0.06 (s, 6H); ^{13}C NMR (75 MHz, Chloroform-*d*) δ (ppm) 139.5, 114.3, 63.6, 34.1, 33.1, 29.94, 29.89, 29.86, 29.75, 29.69, 26.23, 26.05, 18.6, -5.0; IR ν_{max} = 3079, 2918, 2849, 1640, 1472 cm^{-1} ; DART/HRMS: $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{35}\text{H}_{72}\text{OSi}$: 537.5425, found: 537.5432; Elemental analysis: calculated: C 78.28%, H 13.51%, found: C 78.43%, H 13.49%.

Supporting Information

NMR Spectra

Large Scale Preparation of Long Chain ADMET Synthons

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2

¹H NMR, 300 MHz, CDCl₃

¹³C NMR, 75 MHz, CDCl₃

4

¹H NMR, 300 MHz, CDCl₃

¹³C NMR, 75 MHz, CDCl₃

¹H NMR, 300 MHz, CDCl₃

216.01

¹³C NMR, 75 MHz, CDCl₃

18spOH

¹H NMR, 300 MHz, CDCl₃

¹³C NMR, 75 MHz, CDCl₃

¹H NMR, 300 MHz, CDCl₃

¹³C NMR, 75 MHz, CDCl₃

8

¹H NMR, 300 MHz, CDCl₃

¹³C NMR, 75 MHz, CDCl₃

¹H NMR, 300 MHz, CDCl₃

¹³C NMR, 75 MHz, CDCl₃

9

¹H NMR, 300 MHz, CDCl₃

¹³C NMR, 75 MHz, CDCl₃

C=CCCCCCCCCCCCCCCCCC(=O)SC

¹H NMR, 300 MHz, CDCl₃

Chemical shift (ppm): 7.27, 5.89, 5.87, 5.84, 5.81, 5.78, 5.75, 5.73, 5.71, 5.69, 5.67, 5.03, 4.97, 4.95, 4.92, 3.62, 3.60, 3.58, 2.56, 2.08, 2.06, 2.04, 2.01, 1.76, 1.73, 1.71, 1.69, 1.66, 1.64, 1.55, 1.53, 1.51, 1.49, 1.47, 1.41, 1.38, 1.28, 1.06.

Integration values: 2.00, 1.99, 2.18, 3.12, 2.00, 4.32, 8.25, 4.41.

¹³C NMR, 75 MHz, CDCl₃

Chemical shift (ppm): 216.01, 139.46, 114.29, 85.24, 77.65, 77.23, 76.81, 63.54, 34.05, 33.82, 33.10, 29.91, 29.85, 29.78, 29.74, 29.71, 29.64, 29.62, 29.39, 29.18, 26.22, 26.00, 25.35, 18.98, 18.60, 5.02.