Self-assembling α,γ-cyclic peptides that generate cavities with tunable properties.

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Figure 8SI: DFT Optimized structures of bis(methyl picolinate) silver(I) complexes with higher (less stable) energies compared to those presented in the main part of the manuscript. The energies of these conformations are about 11, 5, 13 and 18 kcal/mol (from left to right) less stable than those corresponding to the conformers presented there. The silver ion is in gray whereas the two picolinites are highlighted in orange.
Figure 9SI: Top and lateral views of the DFT optimized structures for the *anti*-eclipsed, clockwise and counter-clockwise alternating dimers, respectively. All the hydrogens, except those from the backbone and those from the pyridines, have been removed for clarity. The side chains were changed to methyl groups to reduce the number of possible conformers.
Materials and Methods:

General:

1-[bis(dimethylamino)methylene]-1H-1,2,3-triazolo-[4,5-b]pyridinium hexafluorophosphate 3-oxide (N-HATU), 1-[bis(dimethylamino)methylene]-1H-benzotriazolium hexafluorophosphate 3-oxide (N-HBTU), 1-[bis(dimethylamino)methylene]-1H-benzotriazolium tetrafluoroborate 3-oxide (N-TBTU), N-(3-dimethylaminopropyl)-N’-ethylcarbodiimide hydrochloride (EDC), hydroxybenzotriazole (HOBt), 4-dimethylaminopyridine (DMAP) and α-aminoacids were purchased from Iris Biotech, Aldrich or from Global Sales Manager, GL Biochem (Shanghai) Ltd, China. All reagents and solvents were used as received unless otherwise noted. CH$_2$Cl$_2$ and DIEA to be used as reaction solvents were distilled from CaH$_2$ over argon immediately prior to use. Analytical thin-layer chromatography was performed on E. Merck silica gel 60 F$_{254}$ plates. Compounds, which were not UV active, were visualized by dipping the plates in a ninhydrin solution and heating. Silica gel flash chromatography was performed using E. Merck silica gel (type 60SDS, 230-400 mesh). Solvent mixtures for chromatography are reported as v/v ratios.

HPLC purification was carried out on a HITACHI D-7000 using a Phenomenex Luna 5μ Silica 100 Angstroms column with CH$_2$Cl$_2$/MeOH gradients between 96:4 and 87:13. $^1$H NMR spectra were recorded on Varian Inova 500 MHz, Varian Mercury 300 MHz or Bruker DPX 250 MHz spectrometers. Chemical shifts (δ) were reported in parts per million (ppm) relative to tetramethylsilane (δ = 0.00 ppm) or by the deuterated solvent. $^1$H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), or quartet (q). All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). $^{13}$C NMR spectra were recorded on Varian Mercury 300 MHz spectrometer. Carbon resonances were assigned using distortionless enhancement by polarization transfer (DEPT) spectra obtained with phase angles of 135. $^1$H NMR Assignments of Cyclic Peptides (CPs). The signals of the $^1$H NMR spectra of the peptides were identified from the corresponding double-quantum-filled 2D COSY, TOCSY and NOESY and/or ROESY spectra acquired at concentration and temperature indicated (Mixing times for NOESY and/or ROESY –between 250 and 1000 ms- were not optimized). Electrospray (ESI) mass spectra were recorded on a Bruker BIOTOF II mass spectrometer. FTIR measurements were made on a JASCO FT/IR-400 spectrophotometer placing the sample on a CaF$_2$ pellet.

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1 L. A. Carpino, et al., *Angew. Chem. Int. Ed.* 2002, 41, 41–445.
Peptide synthesis:

Boc-D-Leu-L-Ahf(Bn)-OMe (3): A solution of N₃-L-Ahf(Bn)-OMe² (271 mg, 0.97 mmol) and Pd/C (208 mg, 10% in wt) in CH₂Cl₂ (10 mL) was stirred at rt for 2 h under hydrogen atmosphere (balloon pressure). The resulting mixture was filtered through a Celite pad, the residue was washed with CH₂Cl₂, and the combined filtrates and washes were concentrated under reduced pressure. The crude was used without further purification.

A solution of the resulting NH₂-L-Ahf(Bn)-OMe in CH₂Cl₂ (15 mL) was successively treated with DIEA (0.71 mL, 3.9 mmol), Boc-D-Leu-OH (225 mg, 1.0 mmol), and N-HBTU (405.0 mg, 1.1 mmol), and the mixture was stirred at rt under Argon for 90 min. The solution was washed with aqueous HCl (5%, 3 x 20 mL) and aqueous saturated NaHCO₃ (2 x 20 mL). The organic layer was dried with anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The resulting crude was purified by flash chromatography (0-2% MeOH/CH₂Cl₂) to give 387 mg of dipeptide 3. [Yellow foam, 86%, Rf = 0.58 (5% MeOH/CH₂Cl₂)].

¹H NMR (CDCl₃, 250 MHz, δ): 7.51-7.24 (m, 6H), 6.63 (d, J = 8.1 Hz, 1H), 4.77 (AB, J = 11.8 Hz, 1H), 4.83-4.49 (m, 2H), 4.66 (AB, J = 11.8 Hz, 1H), 4.47 (d, J = 1.6 Hz, 1H), 4.24-3.91 (m, 3H), 3.77 (s, 3H), 1.86-1.51 (m, 3H), 1.43 (s, 9H), 0.93 (d, J = 5.7 Hz, 6H).

¹³C NMR (CDCl₃, 75.4 MHz, δ): 172.8 (CO), 171.7 (CO), 155.4 (CO), 137.3 (C), 128.3 (CH), 127.8 (CH), 127.7 (CH), 86.6 (CH), 82.1 (CH), 79.8 (C), 72.5 (CH₂), 71.8 (CH₂), 54.7 (CH₃), 53.4 (CH), 52.4 (CH), 41.4 (CH₂), 28.2 (CH₃), 24.7 (CH₃), 24.6 (CH₃), 23.0 (CH). MS (ESI) [m/z(%)]: 487 ([MNa⁺]), 465 ([MH⁺]).

HRMS (ESI) calculated for C₂₄H₃₇N₂O₇: 465.2595, found: 465.2595.

Boc-D-Leu-L-Ahf(Bn)-OH (dp2): A solution of dipeptide 3 (387 mg, 0.83 mmol) in a mixture of MeOH and water (3:1, 20 mL) was treated with LiOH (100 mg, 4.2 mmol). The solution was stirred at rt for 5 h and then the solvent was removed under reduced pressure. The resulting residue was diluted with water (10 mL) and washed with Et₂O (10 mL), and the resulting aqueous solution was acidified to pH 3 with aqueous HCl (5%). The acidic solution was extracted with CH₂Cl₂ (4 x 10 mL), the combined organic extracts were dried with anhydrous Na₂SO₄, filtered and concentrated under reduced pressure to give 365 mg of dipeptide dp2. [Yellow foam, 97%, Rf = 0.20 (5% MeOH/CH₂Cl₂)].

¹H RMN (CDCl₃, 300 MHz, δ): 10.1 (br, 1H), 7.56 (d, J = 6.8 Hz, 1H), 7.49-7.14 (m, 5H), 6.42 (d, J = 7.0 Hz, 1H), 5.35 (d, J = 8.4 Hz, 1H), 4.78 (AB, J = 11.9 Hz, 1H), 4.69 (AB, J = 11.6 Hz, 1H), 4.57-3.91 (m, 5H), 1.74-1.39 (m, 3H), 1.41 and 1.37 (s, 9H), 0.91 (d, J = 6.3 Hz).

² N. Rodríguez-Vázquez, S. Salzinger, L. F. Silva, M. Amorín, J. R. Granja, Eur. J. Org. Chem. 2013, 17, 3477–3493.
Boc-D-Tyr(Me)-L-MeN-Ach-OFm (dp1): A solution of Boc-L-MeN-Ach-OFm (811 mg, 1.86 mmol) in mixture of TFA and CH₂Cl₂ (1:1, 10 mL) was stirred at rt for 10 min. After removal of the solvent under vacuum, the residue was dried under high vacuum for 3 h. The resulting TFA salt was dissolved under Argon in CH₂Cl₂ (10 mL), then DIEA (1.3 mL, 7.5 mmol), Boc-D-Tyr(Me)-OH (550 mg, 1.9 mmol) and N-HATU (778 mg, 2.0 mmol) were successively added. After 1 h stirring at rt, the solution was washed with aqueous HCl (5%, 2 x 10 mL) and aqueous saturated NaHCO₃ (2 x 10 mL). The organic layer was dried with anhydrous Na₂SO₄, filtered and concentrated under reduced pressure, providing a yellow oil that was purified by flash chromatography (0-2% MeOH/CH₂Cl₂) to give 1.0 g of dipeptide dp1. [White foam, 95%, Rf = 0.75 (5% MeOH/CH₂Cl₂)]. ¹H NMR (CDCl₃, 300 MHz, δ): 7.71 (m, 2H), 7.61 (d, J = 7.4 Hz, 1H), 7.54 (m, 2H), 7.43-7.20 (m, 4H), 7.08 (m, 2H), 6.76 (m, 2H), 5.51 (m, 1H), 4.73 (m, 1H), 4.46-4.32 (m, 2H), 4.22-4.04 (m, 1H), 4.14 (AB, J = 6.6 Hz, 1H), 3.95 (AB, J = 6.6 Hz, 1H), 3.73 and 3.60 (s, 3H), 2.89 (m, 1H), 2.70 and 2.46 (s, 3H), 1.96-0.71 (m, 8H), 1.42 and 1.40 (s, 9H). ¹³C NMR (CDCl₃, 75.4 MHz, δ): 174.6 (CO), 171.3 (CO), 158.5 (C), 155.0 (CO), 144.7 (C), 130.4 (CH), 128.4 (C), 127.7 (CH), 127.0 (CH), 124.8 (CH), 119.9 (CH), 113.7 (CH), 79.5 (C), 65.9 (CH₂), 55.1 (CH), 51.5 (CH), 50.3 (CH₂), 46.9 (CH), 42.2 (CH), 39.3 (CH₂), 38.4 (CH₃), 31.3 (CH₃), 29.7 (CH₂), 28.2 (CH₃), 24.2 (CH₂). MS [m/z(%)]: 635.3 ([MNa]+, 62), 613.3 ([MH]+, 38), 557.3 ([MH-Bu]+, 97), 513.3 ([MH-Boc]+, 100). HRMS calculated for C₃₇H₄₅N₂O₆: 613.3272, found: 613.3273.

Boc-D-Leu-L-Ahf(Bn)-D-Tyr(Me)-L-MeN-Ach-OFm (tp1): A solution of dipeptide dp1 (497.0 mg, 0.81 mmol) in mixture of TFA and CH₂Cl₂ (1:1, 10.0 mL) was stirred at rt for 30 min. After removal of the solvent under vacuum, the residue was dried under high vacuum for 3 h. The resulting TFA salt (dp3) was dissolved under Argon in dry CH₂Cl₂ (14 mL), then DIEA (560 µL, 3.2 mmol), dipeptide dp2 (365 mg, 0.81 mmol), and N-HBTU (338 mg, 0.89 mmol) were successively added. After 2 h stirring at rt, the solution was washed with aqueous HCl (5%, 2 x 15 mL) and aqueous saturated NaHCO₃ (2 x 15 mL). The organic layer was dried with anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The resulting
crude was purified by flash chromatography (0-2% MeOH/CH₂Cl₂) to give 645 mg of tetrapeptide tp₁. [White foam, 84%, Rf = 0.42 (5% MeOH/CH₂Cl₂)]. **MS (ESI) [m/z(%)]:** 967.5 ([MNa]+, 30), 945.5 ([MH]+, 12), 748.4 (100). **HRMS (ESI) calculated for C₅₅H₆₉N₄O₁₀:** 945.5008, **found:** 945.5001.

Boc-[D-Leu-L-Ahf(Bn)-D-Tyr(Me)-L-MeN-Ach]₂-OFm (op₁): A solution of tetrapeptide tp₁ (305 mg, 0.32 mmol) in a mixture of piperidine and CH₂Cl₂ (1:4, 6 mL) was stirred at rt for 45 min. The solution was washed with aqueous HCl (5%, 4 x 5 mL), dried with anhydrous Na₂SO₄, filtered and concentrated, to give Boc-D-Leu-L-Ahf(Bn)-D-Leu-L-MeN-Ach-OH (tp₂), which was used without further purification.

A solution of tetrapeptide tp₁ (305 mg, 0.32 mmol) in a mixture of TFA and CH₂Cl₂ (1:1, 8 mL) was stirred at rt for 15 min. After removal of the solvent under vacuum, the residue was dried under high vacuum for 3 h. The resulting TFA salt (tp₃) was dissolved in dry CH₂Cl₂ (12 mL) under Argon, and successively treated with DIEA (222 µL, 1.3 mmol), the previously prepared tp₂ and N-HBTU (134 mg, 0.35 mmol). After 1 h stirring at rt, the solution was washed with aqueous HCl (5%, 2 x 10 mL) and aqueous saturated NaHCO₃ (2 x 10 mL). The organic layer was dried with anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The resulting crude was purified by flash chromatography (0-2% MeOH/CH₂Cl₂) to give 360 mg of octapeptide op₁. [White foam, 70%, Rf = 0.45 (5% MeOH/CH₂Cl₂)]. **MS (ESI) [m/z(%)]:** 1593.8 ([MH]+, 8), 845.4 ([tetrapeptide-Boc]+, 100), 747.9 ([MH-Boc]²⁺, 14). **HRMS (ESI) calculated for C₉₁H₁₁₇N₈O₁₇:** 1593.8531, **found:** 1593.8586.

c-[[L-Ahf(Bn)-D-Tyr(Me)-L-MeN-Ach-D-Leu]₂] (CP₁): The linear octapeptide op₁ (150.0 mg, 94.1 µmol) was dissolved in a mixture of piperidine and CH₂Cl₂ (1:4, 5 mL) and stirred at rt for 45 min. The solution was washed with aqueous HCl (5%, 4 x 5 mL), dried with anhydrous Na₂SO₄, filtered and concentrated to give Boc-[D-Leu-L-Ahf(Bn)-D-Tyr(Me)-L-MeN-Ach]₂-OH, which was used without further purification. The resulting C-unprotected octapeptide was dissolved in a mixture of TFA and CH₂Cl₂ (1:1, 10 mL) and stirred at rt for 30 min. After removal of the solvent under reduced pressure, the residue was dried under high vacuum for 3 h and used without further purification. The
resulting unprotected linear peptide (op2) was dissolved in dry CH$_2$Cl$_2$ (95 mL) and successively treated with DIEA (66 µL, 0.38 mmol) and N-TBTU (39.2 mg, 0.10 mmol). After 12 h, the solvent was removed under reduced pressure, and the residue was dissolved in CH$_2$Cl$_2$ (15 mL), washed with aqueous HCl (10%, 2 x 10 mL), dried with anhydrous Na$_2$SO$_4$, filtered, and concentrated to dryness. The crude was purified by flash chromatography (0-5% MeOH/CH$_2$Cl$_2$) to give 62.5 mg of the desired cyclic peptide. [White solid, 51%, R$_f$ = 0.47 (5% MeOH/CH$_2$Cl$_2$)].

$^1$H NMR (7.5 mM, CDCl$_3$, 300 MHz, δ): 7.29 (m, 12H), 7.09 (d, $J$ = 8.6 Hz, 5H), 6.82 (d, $J$ = 8.5 Hz, 5H), 6.53 (d, $J$ = 8.7 Hz, 1H), 5.59 (d, $J$ = 9.3 Hz, 1H), 4.99-3.82 (m, 18H), 3.80 (s, 6H), 3.44 (m, 2H), 2.53 (m, 2H), 2.24 (s, 6H), 2.11-1.08 (m, 26H), 0.90 (d, $J$ = 7.5 Hz, 6H), 0.87 (d, $J$ = 6.8 Hz, 6H).

$^{13}$C NMR (CDCl$_3$, 75.4 MHz, δ): 175.2 (CO), 174.0 (CO), 172.7 (CO), 172.0 (CO), 170.0 (C), 159.2 (C), 137.7 (C), 130.5 (CH), 128.5 (CH), 127.4 (CH), 114.2 (CH), 87.7 (CH), 84.9 (CH), 72.4 (CH$_2$), 72.1 (CH$_2$), 55.7 (CH), 55.5 (CH$_3$), 51.9 (CH), 45.0 (CH), 42.1 (CH$_2$), 39.6 (CH$_2$), 29.6 (CH$_3$), 28.5 (CH$_2$), 25.2 (CH), 24.9 (CH$_2$), 23.3 (CH$_3$), 21.4 (CH$_2$).

FTIR (298 K, CHCl$_3$): 3297 (amide A), 3006, 2958, 2933, 2869, 1655 (amide II), 1626 (amide I), 1514 cm$^{-1}$ (amide II).

MS (ESI) [m/z (%)]: 1319.7 (M+Na$^+$, 19), 1297.7 (M+H$^+$, 12), 668.3 ([MHK]+$_2^+$, 100), 660.8 ([MH$^+$Na$^+$]$_2^+$, 23). HRMS (ESI) calculated for C$_{72}$H$_{97}$N$_8$O$_{14}$: 1297.7119, found: 1297.7111.

c-{[[L-Ahf-D-Tyr(Me)-L-$^{13}$MeN-Ach-D-Leu-$]_2}$ (CP2): A solution of CP1 (42 mg, 0.032 mmol) in TFA (1 mL) was successively treated with pentamethylbenzene (21 mg, 0.13 mmol), anisole (21 µL, 0.18 mmol) and HBr in AcOH (0.5 mL, 33% in wt). The resulting mixture was stirred at rt for 1h. The solvent was removed under reduced pressure and the crude was purified by HPLC (Phenomenex Luna 5μ silica, 4-8% MeOH/CH$_2$Cl$_2$, 25 min) to give 16.3 mg of the desired cyclic peptide. [White solid, 45%, $t_R$ = 19 min].

$^1$H NMR (20 mM, CDCl$_3$, 300 MHz, δ): 9.27 (d, $J$ = 9.1 Hz, 2H, NH$_{Tyr}$), 8.52 (d, $J$ = 8.9 Hz, 2H, NH$_{Ahf}$), 8.24 (d, $J$ = 8.9 Hz, 2H, NH$_{Leu}$), 7.07 (m, 4H, Ar), 6.79 (m, 4H, Ar), 5.19 (m, 2H, H$_{α_{Tyr}}$), 4.83 (br, 2H, OH), 4.74 (s, 2H, H$_{α_{Ahf}}$), 4.61 (m, 4H, H$_{α_{Leu}}$ + H$_{γ_{Ach}}$), 4.47 (dd, $J_1$ = 9.7 Hz, $J_2$ = 3.8 Hz, 2H, H$_{γ_{Ahf}}$), 4.22 (s, 2H, H$_δ_{Ahf}$), 4.13 (dd, $J_1$ = 9.4 Hz, $J_2$ = 4.2 Hz, 2H, H$_{δ_{Ach}}$), 3.86 (d, $J$ = 8.9 Hz, 2H, H$_{β_{Tyr}}$), 3.79 (s, 6H, OMe$_{Tyr}$), 2.97 (m, 4H, H$_{β_{Tyr}}$), 2.48 (s, 6H, NMe), 1.95 (m, 2H, H$_{α_{Ach}}$), 1.85-1.09 (m, 22H, CH$_2$ ACH + CH$_2$ Leu + CH$_2$ Leu), 0.94 (d, $J$ = 6.4 Hz, 6H, CH$_3$ Leu), 0.91 (d, $J$ = 5.6 Hz, 6H, CH$_3$ Leu). $^{13}$C NMR (CDCl$_3$, 75.4 MHz, δ): 175.0 (CO), 172.2 (CO), 171.4 (CO), 170.4 (CO), 158.9 (C), 130.5 (CH), 128.1 (C), 114.0 (CH), 85.3 (CH), 78.7 (CH), 74.8 (CH$_2$), 57.9
(CH), 55.5 (CH$_3$), 51.6 (CH), 50.3 (CH), 43.8 (CH$_2$), 43.5 (CH), 39.6 (CH$_2$), 32.8 (CH$_2$), 29.9 (CH$_3$), 28.6 (CH$_2$), 28.1 (CH$_2$), 25.2 (CH$_2$), 24.8 (CH$_2$), 22.9 (CH$_3$), 22.8 (CH$_3$). \textbf{FTIR} (298 K, CHCl$_3$): 3399, 3299 (amide A), 3006, 2958, 2933, 2865, 1652 (amide I, II), 1629 (amide I), 1513 cm$^{-1}$ (amide II).

\textbf{MS (ESI)} [m/z (%)]: 1140.6 ([MNa$^+$], 7), 1117.6 ([MH$^+$], 8), 578.3 ([MHK$^+$]$^2^+$, 100), 570.3 ([MHNa$^+$]$^2^+$, 40). \textbf{HRMS (ESI)} calculated for C$_{58}$H$_{85}$N$_8$O$_{14}$: 1117.6180, found: 1117.6227.

Boc-D-Leu-L$^{MeN}$-Ahf(Bn)-OMe (4): A solution of L$^{MeN}$-Ahf(Bn)-OMe$_2$ (600 mg, 2.26 mmol) in dry CH$_2$Cl$_2$ (22 mL) was successively treated with DIEA (1.6 mL, 9.0 mmol), Boc-D-Leu-OH (523 mg, 2.3 mmol) and N-HATU (946 mg, 2.5 mmol). The mixture was stirred at rt under Argon for 90 min. The solution was washed with aqueous HCl (5%, 3 x 20 mL) and aqueous saturated NaHCO$_3$ (2 x 20 mL). The organic layer was dried with anhydrous Na$_2$SO$_4$, filtered and concentrated under reduced pressure. The resulting crude was purified by flash chromatography (0-2% MeOH/CH$_2$Cl$_2$) to give 1.0 g of dipeptide 4. [Yellow foam, 93%, $R_f$ = 0.53 (5% MeOH/CH$_2$Cl$_2$)].

\textbf{H NMR} (CDCl$_3$, 300 MHz, $\delta$): 7.44-7.19 (m, 5H), 5.17 (m, 1H), 5.00 (m, 1H), 4.76 (AB, $J$ = 11.9 Hz, 1H), 4.68-4.31 (m, 1H), 4.59 (AB, $J$ = 12.0 Hz, 1H), 4.38 (d, $J$ = 4.5 Hz, 1H), 4.19-3.98 (m, 3H), 3.72 (s, 3H), 2.79 (s, 3H), 1.80-1.25 (m, 3H), 1.42 (s, 9H), 0.98 (d, $J$ = 6.7 Hz, 3H), 0.93 (d, $J$ = 6.7 Hz, 3H). \textbf{C NMR} (CDCl$_3$, 75.4 MHz, $\delta$): 173.5 (CO), 170.6 (CO), 155.7 (CO), 137.3 (C), 128.3 (CH), 128.0 (CH), 127.8 (CH), 85.5 (CH), 82.4 (CH), 79.5 (C), 71.9 (CH$_2$), 69.3 (CH$_3$), 61.1 (CH), 52.3 (CH$_3$), 49.2 (CH), 42.2 (CH$_2$), 31.5 (CH$_3$), 28.3 (CH$_3$), 24.6 (CH), 23.4 (CH$_3$), 21.6 (CH$_3$). \textbf{MS (ESI)} [m/z (%)]: 501.2 ([MNa$^+$], 100), 423.2 ([MH-$^t$Bu$^+$], 13), 379.2 ([MH-Boc$^+$], 6). \textbf{HRMS (ESI)} calculated for C$_{25}$H$_{38}$N$_2$NaO$_7$: 501.2571, found: 501.2581.

Boc-D-Leu-L$^{MeN}$-Ahf(Bn)-OH (dp5): A solution of dipeptide 4 (700 mg, 1.5 mmol) in a mixture of MeOH and water (3:1, 29 mL) was treated with LiOH (175 mg, 7.3 mmol). The solution was stirred at rt for 2 h and then the solvent was removed under reduced pressure. The resulting residue was diluted with water (15 mL), washed with Et$_2$O (10 mL) and the resulting aqueous solution was acidified to pH 3 with aqueous HCl (5%). The acidic solution was extracted with CH$_2$Cl$_2$ (4 x 10 mL) and the combined organic extracts were dried with anhydrous Na$_2$SO$_4$, filtered and concentrated under reduced pressure to give 670 mg of the desired dipeptide. [White foam, 99%, $R_f$ = 0.32 (5% MeOH/CH$_2$Cl$_2$)]. \textbf{H NMR} (CDCl$_3$, 300 MHz, $\delta$): 9.70 (br, 1H), 7.52-7.10 (m, 5H), 7.10-6.70 (m, 5H), 6.70-6.30 (m, 5H), 6.30-5.90 (m, 5H), 5.90-5.50 (m, 5H), 5.50-5.10 (m, 5H), 5.10-4.70 (m, 5H), 4.70-4.30 (m, 5H), 4.30-3.90 (m, 5H), 3.90-3.50 (m, 5H), 3.50-3.10 (m, 5H), 3.10-2.70 (m, 5H), 2.70-2.30 (m, 5H), 2.30-1.90 (m, 5H), 1.90-1.50 (m, 5H), 1.50-1.10 (m, 5H), 1.10-0.70 (m, 5H), 0.70-0.30 (m, 5H).

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5.61 (m, 1H), 4.90 (m, 1H), 4.75 (AB, \( J = 11.9 \) Hz, 1H), 4.68-4.40 (m, 1H), 4.63 (AB, \( J = 11.6 \) Hz, 1H), 4.43 (dd, \( J_1 = 4.3 \) Hz, \( J_2 = 1.4 \) Hz, 1H), 4.26 (m, 1H), 4.11 (m, 2H), 3.04 (s, 3H), 1.78-1.23 (m, 3H), 1.41 (s, 9H), 0.96 (d, \( J = 6.5 \) Hz, 3H), 0.92 (d, \( J = 6.6 \) Hz, 3H). \( ^{13} \text{C} \) NMR (CDCl\(_3\), 75.4 MHz, \( \delta \)): 174.3 (CO), 172.8 (CO), 156.2 (CO), 137.4 (C), 128.5 (CH), 128.0 (CH), 127.9 (CH), 86.4 (CH), 82.5 (CH), 80.1 (C), 72.2 (CH\(_2\)), 69.4 (CH\(_2\)), 62.3 (CH), 49.6 (CH), 41.9 (CH\(_2\)), 32.3 (CH\(_3\)), 28.4 (CH\(_2\)), 24.7 (CH), 23.5 (CH\(_3\)), 21.7 (CH\(_3\)). MS (ESI) [m/z(%)]: 487.2 ([MNa\(^+\], 100), 409.2 ([MH-Boc\(^+\], 21), 365.2 ([MH-Boc\(^+\], 16). HRMS (ESI) calculated for C\(_{24}\)H\(_{36}\)N\(_2\)O\(_7\): 487.2415, found: 487.2395.

Boc-D-Leu-L-MeN-Ach-OFm (dp4): A solution of Boc-L-MeN-Ach-OFm (700 mg, 1.6 mmol) in a mixture of TFA and CH\(_2\)Cl\(_2\) (1:1, 8 mL) was stirred at rt for 15 min. After removal of the solvent under vacuum, the residue was dissolved under high vacuum for 3 h. The resulting TFA salt was dissolved under Argon in dry CH\(_2\)Cl\(_2\) (16 mL), and DIEA (1.1 mL, 6.4 mmol), Boc-D-Leu-OH (372 mg, 1.6 mmol), and N-HATU (669 mg, 1.8 mmol) were successively added. After 1 h stirring at rt, the solution was washed with aqueous HCl (5%, 2 x 15 mL) and aqueous saturated NaHCO\(_3\) (2 x 15 mL). The organic layer was dried with anhydrous Na\(_2\)SO\(_4\), filtered and concentrated under reduced pressure, providing a yellow oil that was purified by flash chromatography (30% EtAcO/hexanes) to give 755 mg of the dipeptide. [White foam, 86%, \( R_f = 0.65 \) (50% EtAcO/hexanes)]. \( ^1 \text{H} \) NMR (CDCl\(_3\), 300 MHz, \( \delta \)): 7.76 (d, \( J = 7.6 \) Hz, 2H), 7.57 (d, \( J = 7.6 \) Hz, 2H), 7.36 (td, \( J_1 = 25.0 \) Hz, \( J_2 = 7.6 \) Hz, 4H), 5.31 (d, \( J = 9.2 \) Hz, 1H), 4.64 (m, 1H), 4.53-4.35 (m, 3H), 4.19 (t, \( J = 6.7 \) Hz, 1H), 2.90 and 2.79 (s, 3H), 2.08-1.12 (m, 11H), 1.42 (s, 9H), 0.99 (dd, \( J = 6.5 \) Hz, \( J = 1.9 \) Hz, 3H), 0.91 (dd, \( J = 6.7 \) Hz, \( J = 1.4 \) Hz, 3H). \( ^{13} \text{C} \) NMR (CDCl\(_3\), 75.4 MHz, \( \delta \)): 174.9 (CO), 172.8 (CO), 155.7 (CO), 143.8 (C), 141.4 (C), 127.9 (CH), 127.2 (CH), 125.1 (CH), 120.1 (CH), 79.5 (C), 66.2 (CH\(_2\)), 55.1 (CH), 51.7 (CH), 49.2 (CH), 47.1 (CH), 42.9 (CH\(_2\)), 42.6 (CH), 32.8 (CH\(_2\)), 31.6 (CH\(_3\)), 29.3 (CH\(_3\)), 29.0 (CH\(_3\)), 28.5 (CH\(_3\)), 24.8 (CH), 24.5 (CH\(_2\)), 23.6 (CH\(_3\)), 21.8 (CH\(_3\)). MS (ESI) [m/z(%)]: 571.3 ([MNa\(^+\], 24), 549.3 ([MH\(^+\], 11), 493.3 ([MH-\(^t\)Bu\(^+\], 100), 449.3 ([MH-Boc\(^+\], 100). HRMS (ESI) calculated for C\(_{33}\)H\(_{45}\)N\(_2\)O\(_5\): 549.3232, found: 549.3232.

Boc-D-Leu-L-MeN-Ahf(Bn)-D-Leu-L-MeN-Ach-OFm (tp4): A solution of dipeptide dp4 (700 mg, 1.2 mmol) in a mixture of TFA and CH\(_2\)Cl\(_2\) (1:1, 10 mL) was stirred at rt for 30 min. After removal of the solvent under vacuum, the residue was dissolved under high vacuum for 3 h. The resulting TFA salt (dp6) was dissolved in dry CH\(_2\)Cl\(_2\) (12 mL) under Argon, then DIEA (850 \( \mu \)L, 4.8 mmol), dipeptide dp5 (562 mg, 1.2 mmol) and N-HBTU (504 mg, 1.3 mmol) were successively added. After 2 h stirring at rt, the solution was washed with
aqueous HCl (5%, 2 x 10 mL) and aqueous saturated NaHCO₃ (2 x 10 mL). The organic layer was
dried with anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The resulting
crude was purified by flash chromatography (0-2% MeOH/CH₂Cl₂) to give 1.1 g of the
tetrapeptide tp4. [White foam, 99%, Rf = 0.41 (2% MeOH/CH₂Cl₂)]. MS (ESI) [m/z(%)]: 933.4
([MK]+, 3), 917.5 ([MNa]+, 82), 895.5 ([MH]+, 100), 795.5 ([MH-Boc]+, 4). HRMS (ESI) calculated
for C₅₂H₇₁N₄O₉: 895.5216, found: 895.5204.

Boc-[D-Leu-L-MeN-Ahf(Bn)-D-Leu-L-MeN-Ach]-OFm (op3): A solution of tetrapeptide tp4 (515
mg, 0.46 mmol) in a mixture of piperidine and CH₂Cl₂ (1:4, 5 mL) was stirred at rt for 45 min. The solution was washed with aqueous HCl (5%,
4 x 10 mL), dried with anhydrous Na₂SO₄, filtered and concentrated, to give Boc-D-Leu-L-MeN-
Ahf(Bn)-D-Leu-L-MeN-Ach-OH (tp5), which was used without further purification.

A solution of tetrapeptide tp4 (515 mg, 0.46 mmol) in a mixture of TFA and CH₂Cl₂ (1:1, 6 mL)
was stirred at rt for 30 min. After removal of the solvent under vacuum, the residue was dried
under high vacuum for 3 h. The resulting TFA salt (tp6) was dissolved in dry CH₂Cl₂ (5 mL) under
Argon, and successively treated with DIEA (320 µL, 1.9 mmol), the previously prepared tp5 and
N-HBTU (193 mg, 0.51 mmol). After 2 h stirring at rt, the solution was washed with aqueous HCl
(5%, 2 x 10 mL) and aqueous saturated NaHCO₃ (2 x 10 mL). The organic layer was dried with
anhydrous Na₂SO₄, filtered and concentrated under reduced pressure. The resulting crude was
purified by flash chromatography (0-5% MeOH/CH₂Cl₂) to give 683 mg of the desired
octapeptide (op3). [White foam, 98%, Rf = 0.35 (2% MeOH/CH₂Cl₂)]. MS (ESI) [m/z(%)]: 1531.8
([MK]+, 1), 1516.9 ([MNa]+, 24), 1493.9 ([MH]+, 10), 774.7 (100), 769.9 ([MNa]²+, 24), 697.4 ([MH-
Boc]²+, 97). HRMS (ESI) calculated for C₈₅H₁₂₁N₈O₁₅: 1493.8946, found: 1493.8971.

C-[[L-MeN-Ahf(Bn)-D-Leu₁-L-MeN-Ach-D-Leu²]-]₂ (CP3): The
linear octapeptide op3 (400 mg, 0.27 mmol) was dissolved
in a mixture of piperidine and CH₂Cl₂ (1:4, 5 mL) and stirred
at rt for 45 min. The solution was washed with aqueous HCl
(5%, 4 x 10 mL), dried with anhydrous Na₂SO₄, filtered and
consolidated to dryness to give Boc-[D-Leu-L-MeN-Ahf(Bn)-
D-Leu-L-MeN-Ach]-OFm (op3), which was used without further
purification. The resulting octapeptide was dissolved in a
mixture of TFA and CH₂Cl₂ (1:1, 6 mL) and stirred at rt for 20 min. After removal of the solvent
under reduced pressure, the residue was dried under high vacuum for 3 h and used without

further purification. The resulting unprotected linear peptide (op4) was dissolved in dry CH₂Cl₂ (268 mL) and successively treated with DIEA (280 µL, 1.6 mmol) and N-TBTU (112 mg, 0.29 mmol). After 12 h, the solvent was removed under reduced pressure and the residue was dissolved in CH₂Cl₂ (25 mL), washed with aqueous HCl (10%, 2 x 20 mL), dried with anhydrous Na₂SO₄, filtered and concentrated to dryness. The crude was purified by flash chromatography (0-6% MeOH/CH₂Cl₂) to give 200 mg of CP3. [White solid, 62%, Rₓ = 0.37 (5% MeOH/CH₂Cl₂)]. ¹H NMR (16 mM, CDCl₃, 500 MHz, δ): 9.08 (d, J = 9.4 Hz, 1.33H, NH₃eul₁-D₃A₁), 8.79 (d, J = 9.4 Hz, 0.66H, NH₃eul₂-D₃A₁), 8.08 (d, J = 9.2 Hz, 1.33H, NH₃eul₂-D₃A₂), 8.03 (d, J = 9.6 Hz, 0.66H, NH₃eul₂-D₃A₃), 6.96 (br, 4.66H, Bn), 6.68 (br, 4H, Bn), 6.58 (m, 1.33H, Bn), 5.53 (m, 1.33H, ḡnd), 5.45 (m, 0.66H, ḡnd), 5.29 (m, 2H, ḡneul₁), 5.21 (d, J = 5.4 Hz, 0.66H, ḡneul₂-D₃A), 5.13 (m, 2H, ḡneul₂), 4.78 (d, J = 8.3 Hz, 1.33H, ḡneul-D₃B₁), 4.53 (m, 1.33H, ḡneul-D₃B₂), 4.37 (m, 1.33H, ḡneul-D₃B₃), 4.22 (dd, J₁ = 10.2 Hz, J₂ = 8.8 Hz, 1.33H, ḡneul-D₃C₁), 4.06 (m, 2.66H, ḡneul-D₃C₂+ ḡneul-D₃C₃+ ḡneul-D₃C₄), 3.96 (br, 2.66H, ḡneul-D₃C₅), 3.73 (dd, J₁ = 10.7 Hz, J₂ = 9.3 Hz, 1.33H, ḡneul-D₃C₆), 3.66 (AB, J = 9.9 Hz, 0.66H, ḡneul-D₃C₇), 3.60 (AB, J = 9.8 Hz, 0.66H, ḡneul-D₃C₈), 3.33 (s, 2H, NMe₂-D₃A₁), 3.04 (s, 4H, NMe₂-D₃B₁), 2.80 (m, 1.33H, ḡneul-D₃B₁), 2.67 (s, 2H, NMe₂-D₃B₂), 2.62 (s, 4H, NMe₂-D₃B₃), 2.31 (m, 0.66H, ḡneul-D₃B₄), 1.91-1.05 (m, 27.33H, CH₂₃-₃₁ + CH₂₄-₃₂ + CH₂₅-₃₃), 1.04-0.80 (m, 24H, CH₃₁-₃₃), -1.20 (d, J = 11.5 Hz, 0.66H, ḡneul-D₃C₅). ¹³C NMR (CDCl₃, 75.4 MHz, δ): 175.2 (CO), 175.0 (CO), 174.4 (CO), 173.8 (CO), 172.4 (CO), 171.8 (CO), 171.4 (CO), 169.5 (CO), 163.8 (C), 163.6 (C), 128.7 (CH), 128.4 (CH), 128.1 (CH), 127.3 (CH), 127.0 (CH), 82.8 (CH), 82.3 (CH), 79.9 (CH), 77.1 (CH), 72.2 (CH₂), 71.8 (CH₂), 67.9 (CH₃), 66.2 (CH₃), 59.6 (CH), 57.7 (CH), 51.5 (CH), 51.1 (CH), 47.0 (CH), 46.6 (CH), 46.5 (CH), 43.9 (CH₂), 43.5 (CH₂), 31.4 (CH), 30.7 (CH₃), 30.1 (CH₂), 29.8 (CH), 29.3 (CH), 29.0 (CH), 28.7 (CH₂), 25.4 (CH₂), 25.0 (CH₂), 24.7 (CH₂), 24.6 (CH₃), 24.5 (CH₃), 23.7 (CH₃), 23.4 (CH₃), 23.2 (CH₃), 22.5 (CH), 22.1 (CH₃), 21.7 (CH₃). FTIR (298 K, CHCl₃): 3307 (amide A), 3066, 2954, 2925, 2866, 1678 (amide l₁), 1626 (amide l₂), 1526 cm⁻¹ (amide II). MS (ESI) [m/z(%)]: 1219.7 ([MNa]+, 10), 1197.7 ([MH]+, 100), 945.6 (30), 683.6 (60), 599.4 ([MH]⁺, 9). HRMS (ESI) calculated for C₂₆H₃₁N₅O₁₂: 1197.7533, found: 1197.7556.

X-Ray Crystallographic Determination of D₃A
Preparation of single crystals for X-Ray analysis: In a typical experiment, 1.0 mg of pure CP3 was dissolved in 900 µL of CHCl₃, and equilibrated by vapour-phase diffusion against 3.0 mL of hexanes. The corresponding dimer crystallized spontaneously after 7 days.

X-Ray Crystallographic Analysis: Data were collected at 100 K, using Bruker X8 APEXII CCD diffractometer. All calculations were performed on a PC compatible computer using the programs: SORTAV (Blessing, 1995), SHELXT-2014 (Sheldrick, 2014), SHELXL2014/7 (Sheldrick,
ORTEP-3 (Farrugia, 2012), WinGX (Farrugia, 2012). Supplementary crystallographic data for D3a (CIF format) can be obtained free of charge from the journal. The crystal structure was deposited at the Cambridge Crystallographic Data Centre, and the data was assigned to the following deposition number: CCDC 1400134.

c-\{[L-MeN-Ahf-D-Leu^1-L-MeN-Ach-D-Leu^2]_2\} (CP4): A solution of CP3 (50 mg, 0.042 mmol) and Pd/C (36 mg, 10% in wt) in a mixture of MeOH and CH_2Cl_2 (3:1, 20 mL) was stirred at rt for 20 h under hydrogen atmosphere (balloon pressure). The resulting mixture was filtered through a Celite pad, the residue was washed with CH_2Cl_2, and the combined filtrates and washes were concentrated under reduced pressure. The crude was purified by HPLC (Phenomenex Luna 5μ silica, 6-13% MeOH/CH_2Cl_2, 30 min) to give 30 mg of the cyclic peptide CP4. [White solid, 71%, t_R = 22 min].

\[^1^H\] NMR (5 mM, CDCl_3, 298 K, 300 MHz, δ): 7.92 (br, 2H), 5.31 (br, 2H), 5.08 (m, 4H), 4.47 (m, 6H), 4.23 (br, 2H), 3.83 (dd, J_1 = 10.7 Hz, J_2 = 9.0 Hz, 2H), 3.08 (s, 6H), 3.03 (s, 6H), 2.79 (m, 2H), 2.01-1.10 (m, 28H), 1.03-0.80 (m, 24H).

\[^1^H\] NMR (32 mM, CDCl_3, 253 K, 500 MHz, δ): 8.72 (d, J = 9.1 Hz, 0.8H, NH(Leu1)), 8.47 (d, J = 9.1 Hz, 1.2H, NH(Leu1-D4A)), 7.95 (d, J = 8.6 Hz, 0.8H, NH(Leu2)), 7.72 (d, J = 9.4 Hz, 1.2H, NH(Leu2-D4A)), 5.97 (br, 0.8H, OH), 5.48 (br, 1.2H, OH), 5.32 (m, 2H, H_γ AHf), 5.09 (m, 4H, H_α Leu), 4.76 (br, 1H, H_α Ahf-D4A), 4.45 (m, 5H, H_γ Ach + H_β Ahf + H_α Ahf), 3.98 (m, 4H, NMe), 3.07 (s, 6H, NMe_2), 2.98 (s, 4H, NMe_2), 2.62 (m, 2H, H_α Ach), 2.07-1.14 (m, 28H, CH_2 Ach + CH_2 Leu + CH_Leu), 1.07-0.68 (m, 24H, CH_3 Leu).

\[^1^H\] NMR (32 mM, 5% CD_3OH/CDCl_3, 253 K, 500 MHz, δ): 8.83 (d, J = 9.3 Hz, 0.2H, NH(Leu1)), 8.64 (d, J = 8.9 Hz, 1.8H, NH(Leu1-D4A)), 8.15 (d, J = 9.5 Hz, 1.8H, NH(Leu2-D4A)), 7.94 (d, J = 8.0 Hz, 0.2H, NH(Leu2)), 6.11 (s, 1.8H, OH), 5.76 (s, 0.2H, OH), 5.31 (m, 2H, H_β Ahf), 5.13 (m, 4H, H_α Leu), 4.62 (d, J = 7.9 Hz, 2H, H_α Ahf), 4.57 (m, 2H, H_γ Ach), 4.31 (dd, J_1 = 9.7 Hz, J_2 = 8.7 Hz, 2H, H_β Ahf), 4.05 (m, 0.2H, H_δ Ahf), 3.96 (d, J = 9.6 Hz, 3.6H, H_δ Ahf-D4A), 3.84 (m, 0.2H, H_δ Ahf), 3.37 (s, 2H, CH_3OH), 3.09 (s, 5.4H, NMe_2), 3.06 (s, 0.6H, NMe_2), 2.93 (s, 6H, NMe_2), 2.78 (m, 2H, H_α Ach), 1.97-1.15 (m, 28H, CH_2 Ach + CH_2 Leu + CH_Leu), 0.98 (d, J = 6.3 Hz, 4H, CH_3 Leu), 0.87 (dd, J_1 = 8.1 Hz, J_2 = 6.8 Hz, 16H, CH_3 Leu), 0.82 (d, J = 6.9 Hz, 4H, CH_3 Leu).

FTIR (298 K, CHCl_3): 3437, 3298 (amide A), 2955, 2931, 2867, 1676 (amide I), 1621 (amide II), 1537 cm\(^{-1}\) (amide II). MS (ESI) [m/z(%)]: 1017.6 ([MH]^+, 16), 536.8 (32), 528.3 ([MK]^2+, 21), 509.3 ([MH]^2+, 9), 381.3 (100). HRMS (ESI) calculated for C_{52}H_{89}N_{8}O_{12}: 1017.6594, found: 1017.6556.
c-[L-MeN-Ahf(pic)-D-Leu¹-L-MeN-Ach¹-D-Leu²-L-MeN-Ahf-D-Leu³-L-MeN-Ach²-D-Leu⁴⁻] [CP5]: A solution of CP4 (5.5 mg, 5.4 µmol) in CH₂Cl₂ (1 mL) was treated with 2-picolinic acid (0.73 mg, 5.9 µmol), EDC·HCl (1.1 mg, 5.9 µmol), HOBT (0.79 mg, 5.9 µmol) and DMAP (0.72 mg, 5.9 µmol). Each 12 h, additional 2-picolinic acid (1.5 mg, 11.8 µmol), EDC (2.2 mg, 11.8 µmol) and DMAP (1.4 mg, 11.8 µmol) was added during 3-4 days. Then, the solution was washed with aqueous saturated NaHCO₃ (2 x 5 mL) and aqueous HCl (5%, 2 x 5 mL). The organic layer was dried with anhydrous Na₂SO₄, filtered and concentrated to dryness. The crude was purified by HPLC (Phenomenex Luna 5µ silica, 7-11% MeOH/CH₂Cl₂, 30 min) to give 3.2 mg of the cyclic peptide CP5. [White solid, 54%, tₖ = 20 min]. 

**1H NMR (CDCl₃, 300 MHz, δ):** 8.80-8.15 (m, 3H), 7.99-7.56 (m, 3H), 7.43 (m, 1H), 7.11 (m, 0.5H), 6.72 (m, 0.5H), 6.06-3.67 (m, 17H), 3.35 (s, 1.5H), 3.21 (s, 1H), 3.20 (s, 2H), 3.17 (s, 1H), 3.13 (s, 1H), 3.01 (s, 4H), 2.84 (s, 1.5H), 2.37 (m, 2H), 2.12-0.54 (m, 52H). 

**FTIR (298 K, CHCl₃):** 3298 (amide A), 3003, 2956, 2929, 2868, 1747 (C=O), 1683 (amide I), 1540 cm⁻¹ (amide II). **MS (ESI) [m/z(%)]:** 1144.7 ([MNa⁺], 23), 1122.7 ([MH⁺], 32), 572.8 ([IMNa⁺⁺], 8), 511.3 (34), 500.3 (100). **HRMS (ESI) calculated for C₅₈H₉₂N₉O₁₃:** 1122.6809, **found:** 1122.6807.

**ADDITION EXPERIMENT OF AgBF₄:**

**CP5** (2.2 mg, 1.9 µmol) was dissolved in CDCl₃ (400 µL) in a NMR tube. In a flask under Ar and protected from light, AgBF₄ (15.8 mg, 0.081 mmol) (dry box) was dissolved in CD₂CN (2.0 mL). Then, different portions (0.1, 0.2, 0.3, 0.4 and 0.5 equiv) of the solution of AgBF₄ (24 µL, 0.95 µmol) were added to the NMR tube to form mainly the complex s-DS₅⇒Ag. 

**1H NMR (4.5 mM, CDCl₃, 500 MHz, δ):** 8.66 (d, J = 9.1 Hz, 0.25H, NHₘ𝑖𝑛𝑜𝑟), 8.55 (d, J = 9.2 Hz, 1H, NHₗₑᵤₙ(maj)⇒m𝑖𝑛𝑜𝑟), 8.43 (d, J = 9.6 Hz, 0.75H, NHₗₑᵤₙ(maj)⇒m𝑖𝑛𝑜𝑟), 7.99 (d, J = 9.1 Hz, 0.75H, NHₗₑᵤₙ(maj)⇒m𝑖𝑛𝑜𝑟), 7.93 (d, J = 9.2 Hz, 0.75H, NHₗₑᵤ₂(maj)⇒m𝑖𝑛𝑜𝑟), 7.87 (d, J = 4.3 Hz, 0.25H, Picₘ𝑖𝑛𝑜𝑟), 7.78 (s, 1H, NHₗₑᵤ₂+H₆-Pic_major), 7.65 (d, J = 9.1 Hz, 0.25H, NHₘ𝑖𝑛𝑜𝑟), 7.51 (m, 1H, H₃-Pic_major+Pic_minor), 7.23 (m, 0.25H, Pic_minor), 7.10 (m, 1.50H, H₄/H₅-Pic_major), 6.93 (m, 0.25H, Pic_minor), 5.82 (m, 1.50H, Hᵥₐᵥₐ(hiv), 5.63 (dd, J₁ = 9.7 Hz, J₂ = 9.2 Hz, 0.75H, Hᵥₐᵥₐ(hiv), 5.41 (m, 1H, Hᵥₐᵥₐ), 5.27 (m, 1.25H, Hᵥₐᵥ₂), 5.19 (m, 1.5H, Hᵥₐᵤ₂+Hᵥₐᵤ₂+(hiv), 5.12 (m, 1.25H, Hᵥₐᵤ₂), 5.07 (m, 1.5H, Hᵥₐᵤ₂), 4.93 (d, J = 9.0 Hz, 0.75H, Hᵥₐᵥₐ(hiv), 4.81 (br, 0.25H), 4.59 (d, J = 8.5 Hz, 1.50H, Hᵥₐᵥ₂), 4.40 (dd, J₁ = 10.6 Hz, J₂ = 8.9 Hz, 0.75H, Hᵥₐᵥ₂(hiv), 4.33 (dd, J₁ = 11.7 Hz, J₂ = 9.6 Hz, 0.75H, Hᵥₐᵤ₂(hiv), 4.27 (m, 0.75H, Hᵥₐᵤ₂(hiv), 4.12 (dd, J₁ = 9.3 Hz, J₂ = 8.8 Hz, 0.75H, Hᵥₐᵤ₂(hiv), 4.02 (dd, J₁ = 9.8 Hz, J₂ = 8.3 Hz, 0.75H, Hᵥₐᵤ₂(hiv)), 3.97 (dd, J₁ = 10.2 Hz, J₂ = 9.7 Hz, 0.75H, Hᵥₐᵤ₂(hiv)), 3.92 (m, 0.75H, Hᵥₐᵤ₂(hiv)), 3.82 (m, 0.5H), 3.28 (s, 2.25H, NMe₅(Ahf(pic))), 3.16 (s,
0.75H, NMe), 3.14 (s, 0.75H, NMe), 3.13 (s, 2.25H, NMeAhf), 3.06 (s, 2.25H, NMeAch2), 2.96 (s, 0.75H), 2.94 (s, 0.75H), 2.82 (s, 2.25H, NMeAch1), 2.57 (m, 0.75H, HαAch2(major)), 2.48 (m, 0.25H, HαAch(minor)), 2.35 (m, 0.75H, HαAch1(major)), 2.26 (m, 0.25H, HαAch(minor)), 2.02-1.17 (m, 27H, CH2Ach + CH2Leu + CHLeu), 1.04-0.77 (m, 24H, CH3Leu), 0.11 (d, J = 9.0 Hz, 0.75H, HβAch1(major)). MS (ESI) [m/z(%)]: 2957.6 (35), 2546.2 (Dimer+Ag+AgBF4, 71), 2352.3 (Dimer+Ag, 100), 2247.2 (Dimer, 28), 2057.3 (28), 1230.6 (CP+Ag, 19), 942.1 (17). HRMS (ESI) calculated for C116H182AgN18O16: 2350.2518, found: 2350.2604.

ADDITION EXPERIMENT OF OXALIC ACID:

CP5 (2.5 mg, 2.3 µmol) was dissolved in CDCl3 (400 µL) in a NMR tube. In another flask, (CO2H)2 ∙ 2H2O (7.9 mg, 0.063 mmol) was dissolved in CD3CN (1.0 mL). Then, different portions (0.1, 0.2, 0.3, 0.4 and 0.5 equiv) of the solution of (CO2H)2 ∙ 2H2O (17.8 µL, 1.15 µmol) were added to the NMR tube to form mainly the complex s-DSeca(CO2H)2. 1H NMR (5mM, CDCl3, 500 MHz, δ): 8.65 (d, J = 9.2 Hz, 1H, NH[Leu3]), 8.47 (d, J = 9.5 Hz, 1H, NH[Leu1]), 8.15 (d, J = 9.4 Hz, 1H, NH[Leu4]), 7.96 (s, 1H, H6-Pic), 7.92 (d, J = 10.0 Hz, 1H, NH[Leu2]), 7.48 (br, 1H, H3-Pic), 7.18 (br, 2H, H4/H5-Pic), 5.82 (m, 1H, HγAhf(pic)), 5.60 (dd, J1 = 10.3 Hz, J2 = 9.4 Hz, 1H, HβAhf(pic)), 5.46 (m, 1H, HγAhf), 5.30 (m, 1H, HαLeu4), 5.23 (m, 1H, HαLeu3), 5.14 (m, 2H, HαLeu2 + OH), 5.08 (m, 1H, HαLeu1), 4.92 (d, J = 9.1 Hz, 1H, HαAhf(pic)), 4.71 (d, J = 8.5 Hz, 1H, HαAhf), 4.49 (dd, J1 = 11.0 Hz, J2 = 8.7 Hz, 1H, HδAhf), 4.32 (m, 2H, HδAhf(pic) + HγAch2), 4.14 (m, J1 = 11.5 Hz, J2 = 9.0 Hz, 1H, HδAhf), 4.02 (dd, J1 = 10.1 Hz, J2 = 8.9 Hz, 1H, HδAhf(pic)), 3.96 (dd, J1 = 11.1 Hz, J2 = 9.6 Hz, 1H, HδAhf), 3.92 (m, 1H, HγAch1), 3.28 (s, 3H, NMeAhf(pic)), 3.12 (s, 3H, NMeAhf), 3.08 (s, 3H, NMeAch2), 2.83 (s, 3H, NMeAch1), 2.65 (m, 1H, HαAch2), 2.40 (m, 1H, HαAch1), 1.88-1.07 (m, 27H, CH2Ach + CH2Leu + CHLeu), 1.06-0.70 (m, 24H, CH3Leu), 0.15 (d, J = 11.8 Hz, 1H, HβAch1).
NMR and FTIR Spectra:

Boc-\textit{D}-Leu-\textit{L}-Ahf(Bn)-OMe (3): $^1$H NMR (CDCl$_3$, 298 K, 250 MHz), DEPT and $^{13}$C NMR (CDCl$_3$, 298 K, 75.4 MHz).
Boc-D-Leu-L-Ahf(Bn)-OH (dp2): $^1$H NMR (CDCl$_3$, 298 K, 300 MHz), DEPT and $^{13}$C NMR (CDCl$_3$, 298 K, 75.4 MHz).
Boc-D-Tyr(Me)-L-Me-N-Ach-OFm (dp1): $^1$H NMR (CDCl$_3$, 298 K, 300 MHz), DEPT and $^{13}$C NMR (CDCl$_3$, 298 K, 75.4 MHz).
c-\{[L-Ahf(Bn)-D-Tyr(Me)-L-\textsuperscript{Me}N-Ach- D-Leu-]\}_\text{2} \text{(CP1)}$: \textsuperscript{1}H NMR (7.5 mM, CDCl\textsubscript{3}, 298 K, 300 MHz) and \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 298 K, 75.4 MHz).
FTIR (298 K, CHCl$_3$):
c-\{[L-Ahf-D-Tyr(Me)-L^{Me}N-Ach-D-Leu-]-2\} (CP2): $^1$H NMR (20 mM, CDCl$_3$, 298 K, 300 MHz), DEPT and $^{13}$C NMR (CDCl$_3$, 298 K, 75.4 MHz).
**COSY** (20 mM, CDCl₃, 298 K, 500 MHz).

**TOCSY** (20 mM, CDCl₃, 298 K, 500 MHz).
**NOESY** (20 mM, CDCl$_3$, 298 K, 500 MHz).

- [Diagram of NOESY spectrum]

**FTIR** (298 K, CHCl$_3$):

- [Diagram of FTIR spectrum]
Boc-D-Leu-L-MeN-Ahf(Bn)-OMe (4): $^1$H NMR (CDCl$_3$, 298 K, 300 MHz), DEPT and $^{13}$C NMR (CDCl$_3$, 298 K, 75.4 MHz).
Boc-D-Leu-L-Me\textsuperscript{N}-Ahf(Bn)-OH (dp5): \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 298 K, 300 MHz), DEPT and \textsuperscript{13}C NMR (CDCl\textsubscript{3}, 298 K, 75.4 MHz).
Boc-D-Leu-L^MeN-Ach-Ofm (dp4): \(^1\text{H} \text{NMR}\) (CDCl\(_3\), 298 K, 300 MHz), DEPT and \(^{13}\text{C} \text{NMR}\) (CDCl\(_3\), 298 K, 75.4 MHz).
c-{[L-MeN-Ahf(Bn)-D-Leu\(^1\)-L-MeN-Ach-D-Leu\(^2\)-]} \( \text{CP3} \): \(^1\)H NMR (16 mM, CDCl\(_3\), 298 K, 500 MHz), DEPT and \(^{13}\)C NMR (CDCl\(_3\), 298 K, 75.4 MHz).
**COSY** (16 mM, CDCl₃, 298 K, 500 MHz).

**TOCSY** (16 mM, CDCl₃, 298 K, 500 MHz).
NOESY (16 mM, CDCl$_3$, 298 K, 500 MHz).

ROESY (16 mM, CDCl$_3$, 298 K, 500 MHz).
**FTIR (298 K, CHCl₃):**

![FTIR spectrum image]
c-[[L-MeN-Ahf-D-Leu\textsuperscript{1}-L-MeN-Ach-D-Leu\textsuperscript{2}]_2] (CP4):

\textsuperscript{1}H NMR (5 mM, CDCl\textsubscript{3}, 298 K, 500 MHz).

\textsuperscript{1}H NMR (32 mM, CDCl\textsubscript{3}, 253 K, 500 MHz).
**COSY** (16 mM, CDCl$_3$, 253 K, 500 MHz).

**TOCSY** (16 mM, CDCl$_3$, 253 K, 500 MHz).
ROESY (16 mM, CDCl₃, 253 K, 500 MHz).

$^1$H NMR (32 mM, 5% CD₃OH/CDCl₃, 253 K, 500 MHz).
**COSY** (32 mM, 5% CD$_3$OH/CDCl$_3$, 253 K, 500 MHz).

**TOCSY** (32 mM, 5% CD$_3$OH/CDCl$_3$, 253 K, 500 MHz).
ROESY (32 mM, 5% CD$_3$OH/CDCl$_3$, 253 K, 500 MHz).

FTIR (298 K, CHCl$_3$):
c-[L-MeN-Ahf(pic)-D-Leu1-L-MeN-Ach1-D-Leu2-L-MeN-Ahf-D-Leu3-L-MeN-Ach2-D-Leu4-] (CP5):

\(^1\)H NMR (CDCl$_3$, 298 K, 300 MHz).

**FTIR (298 K, CHCl$_3$):**
c-[L-\text{Me}N-Ahf(pic)-D-Leu\textsuperscript{1}-L-\text{Me}N-Ach\textsuperscript{1}-D-Leu\textsuperscript{2}-L-\text{Me}N-Ahf-D-Leu\textsuperscript{3}-L-\text{Me}N-Ach\textsuperscript{2}-D-Leu\textsuperscript{4}]- + 0.5 equiv of AgBF\textsubscript{4} ([\text{D-5}E ∵ Ag]): \textsuperscript{1}H NMR (4.5 mM, CDCl\textsubscript{3}, 298 K, 500 MHz).

\textbf{COSY} (4.5 mM, CDCl\textsubscript{3}, 298 K, 500 MHz).
TOCSY (4.5 mM, CDCl₃, 298 K, 500 MHz).

NOESY (4.5 mM, CDCl₃, 298 K, 500 MHz).
ROESY (4.5 mM, CDCl₃, 298 K, 500 MHz).
c-[L-MeN-Ahf(pic)-D-Leu\(^1\)-L-MeN-Ach\(^1\)-D-Leu\(^2\)-L-MeN-Ahf-D-Leu\(^3\)-L-MeN-Ach\(^2\)-D-Leu\(^4\)-] + 0.5 equiv of (CO\(_2\)H)\(_2\) \cdot 2\(\text{H}_2\)O \(\text{s-D5} \supset\) (CO\(_2\)H)\(_2\): \(^1\text{H}\) NMR (5 mM, CDCl\(_3\), 298 K, 500 MHz).

**COSY** (5 mM, CDCl\(_3\), 298 K, 500 MHz).
**TOCSY** (5 mM, CDCl₃, 298 K, 500 MHz).

**NOESY** (5 mM, CDCl₃, 298 K, 500 MHz).
ROESY (5 mM, CDCl₃, 298 K, 500 MHz).
Computational methods:

The starting geometries of the cyclic peptides investigated in this work were constructed from X-ray crystallographic data of related compounds: c-[(D-Phe-L-MeN-γ-Ach)]4[1] and previous simulations carried out with related systems[2]. The silver complex from these dimers was built using the optimized structures of bis(methyl picolinate) silver(I) complexes. All DFT calculations were carried out using the B3LYP[3] functional with the standard 6-31G(d) basis set for C, N, O and H[4] and Lanl2dz pseudopotential basis set for Ag[5], as implemented in the Gaussian 09[6] program package.

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Geometries

Cartesian coordinates (Å) of conformations optimized at the B3LYP/6-31G(d) basis set for C, N, O and H and Lanl2dz pseudopotential basis set for Ag
| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X                      | Y                      | Z                      |
| 1             | 6             | 0           | 4.129494               | -3.235475              | 0.341259               |
| 2             | 6             | 0           | 3.326356               | 3.043674               | -0.277417              |
| 3             | 6             | 0           | 2.106282               | 2.367067               | -0.224799              |
| 4             | 7             | 0           | 2.023797               | 1.035051               | -0.100148              |
| 5             | 6             | 0           | 3.164118               | 0.318997               | -0.020096              |
| 6             | 6             | 0           | 4.423229               | 0.918155               | -0.065254              |
| 7             | 6             | 0           | 4.503849               | 2.305581               | -0.196990              |
| 8             | 6             | 0           | 2.998973               | -1.171098              | 0.123802               |
| 9             | 8             | 0           | 4.169768               | -1.796073              | 0.196482               |
| 10            | 8             | 0           | 1.917643               | -1.736553              | 0.169547               |
| 11            | 6             | 0           | -4.133667              | 3.233334               | 0.341120               |
| 12            | 8             | 0           | -4.172184              | 1.793882               | 0.196269               |
| 13            | 6             | 0           | -3.322343              | -3.044836              | -0.277613              |
| 14            | 6             | 0           | -2.103201              | -2.366545              | -0.224914              |
| 15            | 7             | 0           | -2.022628              | -1.034423              | -0.100252              |
| 16            | 6             | 0           | -3.163919              | -0.319958              | -0.020261              |
| 17            | 6             | 0           | -4.422205              | -0.920830              | -0.065500              |
| 18            | 6             | 0           | -4.500866              | -2.308371              | -0.197258              |
| 19            | 6             | 0           | -3.000653              | 1.170314               | 0.123702               |
| 20            | 8             | 0           | -1.919984              | 1.737045               | 0.169578               |
| 21            | 47            | 0           | -0.000048              | 0.001765               | -0.022877              |
| 22            | 1             | 0           | 3.606483               | -3.502706              | 1.261834               |
| 23            | 1             | 0           | 3.622283               | -3.682319              | -0.516340              |
| 24            | 1             | 0           | 5.171958               | -3.546543              | 0.381762               |
| 25            | 1             | 0           | 3.340425               | 4.123593               | -0.379162              |
| 26            | 1             | 0           | 1.164464               | 2.903538               | -0.282526              |
| 27            | 1             | 0           | 5.313111               | 0.305151               | 0.002105               |
| 28            | 1             | 0           | 5.471180               | 2.796775               | -0.234872              |
| 29            | 1             | 0           | -5.176512              | 3.543130               | 0.381553               |
| 30            | 1             | 0           | -3.611509              | 3.501150               | 1.261746               |
| 31            | 1             | 0           | -3.626926              | 3.680825               | -0.516419              |
| 32            | 1             | 0           | -3.334935              | -4.124773              | -0.379366              |
| 33            | 1             | 0           | -1.160595              | -2.901643              | -0.282567              |
| 34            | 1             | 0           | -5.312946              | -0.309063              | 0.001815               |
| 35            | 1             | 0           | -5.467507              | -2.800917              | -0.235219              |
Perpendicularly oriented bis(methyl picolinate) silver(I) complex

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X                      | Y                      | Z                      |
| 1             | 6             | 0           | 4.129494               | -3.235475               | 0.341259               |
| 2             | 6             | 0           | 3.326356               | 3.043674                | -0.277417              |
| 3             | 6             | 0           | 2.106282               | 2.367067                | -0.224799              |
| 4             | 7             | 0           | 2.023797               | 1.035051                | -0.100148              |
| 5             | 6             | 0           | 3.164118               | 0.318997                | -0.020096              |
| 6             | 6             | 0           | 4.423229               | 0.918155                | -0.065254              |
| 7             | 6             | 0           | 4.503849               | 2.305581                | -0.196996              |
| 8             | 6             | 0           | 2.998973               | -1.171098               | 0.123802               |
| 9             | 8             | 0           | 4.169768               | -1.796073               | 0.196482               |
| 10            | 8             | 0           | 1.917643               | -1.736553               | 0.169547               |
| 11            | 6             | 0           | -4.133667              | 3.233334                | 0.341120               |
| 12            | 8             | 0           | -4.172184              | 1.793882                | 0.196269               |
| 13            | 6             | 0           | -3.322343              | -3.044836               | -0.277613              |
| 14            | 6             | 0           | -2.103201              | -2.366545               | -0.224914              |
| 15            | 7             | 0           | -2.022628              | -1.034423               | -0.100252              |
| 16            | 6             | 0           | -3.163919              | -0.319958               | -0.020261              |
| 17            | 6             | 0           | -4.422205              | -0.928830               | -0.065500              |
| 18            | 6             | 0           | -4.500866              | -2.308371               | -0.197258              |
| 19            | 6             | 0           | -3.006653              | 1.170314                | 0.123702               |
| 20            | 8             | 0           | -1.919984              | 1.737045                | 0.169578               |
| 21            | 47            | 0           | -0.000048              | 0.001765                | -0.022877              |
| 22            | 1             | 0           | 3.606483               | -3.502706               | 1.261834               |
| 23            | 1             | 0           | 3.622283               | -3.682319               | -0.516340              |
| 24            | 1             | 0           | 5.171958               | -3.546543               | 0.381762               |
| 25            | 1             | 0           | 3.340425               | 4.123593                | -0.379162              |
| 26            | 1             | 0           | 1.164464               | 2.903538                | -0.282526              |
| 27            | 1             | 0           | 5.313111               | 0.305151                | 0.002185               |
| 28            | 1             | 0           | 5.471180               | 2.796775                | -0.234872              |
| 29            | 1             | 0           | -5.176512              | 3.543130                | 0.381553               |
| 30            | 1             | 0           | -3.611049              | 3.501150                | 1.261746               |
| 31            | 1             | 0           | -3.626926              | 3.680825                | -0.516419              |
| 32            | 1             | 0           | -3.334935              | -4.124773               | -0.379366              |
| 33            | 1             | 0           | -1.160595              | -2.901643               | -0.282567              |
| 34            | 1             | 0           | -5.312946              | -0.309063               | 0.001815               |
| 35            | 1             | 0           | -5.467507              | -2.800917               | -0.235219              |
Syn-eclipsed dimer

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 47            | 0           | 0.745805   | -0.189113  | 0.018908   |
| 2             | 6             | 0           | -5.781976  | 4.035521   | -2.455178  |
| 3             | 6             | 0           | 0.647979   | -2.253207  | 2.460937   |
| 4             | 6             | 0           | -3.485474  | 4.624260   | -2.630207  |
| 5             | 6             | 0           | -2.272957  | 5.455639   | -2.009179  |
| 6             | 6             | 0           | -0.877064  | 4.831939   | -2.179156  |
| 7             | 6             | 0           | -0.027689  | 6.051546   | -2.563265  |
| 8             | 6             | 0           | 1.329090   | 5.71976    | -2.195236  |
| 9             | 6             | 0           | 2.300218   | 4.890436   | -2.048908  |
| 10            | 6             | 0           | 1.065067   | -0.785365  | 4.478265   |
| 11            | 6             | 0           | 1.468979   | 5.508053   | -4.546469  |
| 12            | 6             | 0           | -1.017468  | 6.816821   | -3.450465  |
| 13            | 6             | 0           | 0.939188   | -0.923988  | 3.096730   |
| 14            | 6             | 0           | 1.319744   | 1.331999   | 2.765445   |
| 15            | 6             | 0           | 1.456522   | 1.558029   | 4.138536   |
| 16            | 6             | 0           | -6.989822  | 4.890436   | -2.048908  |
| 17            | 6             | 0           | -6.009968  | 1.837397   | -4.315361  |
| 18            | 6             | 0           | -6.493472  | 0.237385   | -2.408727  |
| 19            | 6             | 0           | -5.433062  | -0.813506  | -2.782735  |
| 20            | 6             | 0           | -7.896283  | -0.156542  | -2.982799  |
| 21            | 6             | 0           | -8.281680  | -1.546866  | -2.377667  |
| 22            | 6             | 0           | -7.244069  | -2.603020  | -2.77485  |
| 23            | 6             | 0           | -5.821626  | -2.220519  | -2.295758  |
| 24            | 6             | 0           | -4.834493  | -3.267039  | -2.820879  |
| 25            | 6             | 0           | -6.489187  | 5.548111   | 2.166710   |
| 26            | 6             | 0           | -3.941318  | -5.19573   | -2.516439  |
| 27            | 6             | 0           | -4.562574  | -6.863384  | -2.189915  |
| 28            | 6             | 0           | -2.524364  | -5.402980  | -1.928425  |
| 29            | 6             | 0           | -5.431138  | 4.529140   | 2.610385   |
| 30            | 6             | 0           | -5.717505  | 2.109857   | 2.956237   |
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| 32            | 6             | 0           | -0.131209  | -5.589836  | -2.142933  |
| 33            | 6             | 0           | 0.792498   | -4.631379  | 2.903513   |
| 34            | 6             | 0           | -6.324012  | 0.825256   | 2.384819   |
| 35            | 6             | 0           | 0.783948   | -6.817004  | -2.013568  |
| 36            | 6             | 0           | -7.814384  | 0.784817   | 2.880564   |
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| 39            | 6             | 0           | -8.494707  | -0.525145  | 2.393972   |
| 40            | 6             | 0           | -7.743104  | -1.744872  | 2.946925   |
| 41            | 6             | 0           | 5.745795   | -3.923297  | -2.630905  |
| 42            | 6             | 0           | 6.888473   | -4.840898  | -2.182934  |
| 43            | 6             | 0           | 6.083468   | -2.480723  | -2.142935  |
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|     |   |   |                  |                  |                  |
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| 67  | 6 | 0 | 0.592597        | 5.591710         | 2.198575         |
| 68  | 6 | 0 | -0.558892       | 4.620081         | 2.504466         |
| 69  | 6 | 0 | -1.746620       | 5.601758         | 1.903663         |
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| 73  | 6 | 0 | -3.122948       | 4.730823         | 4.004945         |
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| 83  | 6 | 0 | 5.418304        | 0.403584         | 2.698595         |
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| 85  | 6 | 0 | 8.341347        | 0.531730         | 2.171850         |
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| 88  | 6 | 0 | 5.569873        | -2.117947        | 2.732450         |
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| 94  | 7 | 0 | 1.306777        | 5.749712         | -3.104538        |
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|   |   |   |   |   |   |
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| 76 | 6 |  0 | -6.141977 | -1.890669 |  2.225653 |
| 77 | 6 |  0 | -8.395313 | -0.743138 |  2.215300 |
| 78 | 6 |  0 | -7.727632 |  0.583680 |  2.595712 |
| 79 | 6 |  0 | -5.452314 | -0.562817 |  2.591761 |
| 80 | 6 |  0 | -6.261222 |  0.653284 |  2.099765 |
| 81 | 6 |  0 | -5.651778 |  1.958359 |  2.615561 |
| 82 | 6 |  0 | -5.373481 |  4.360606 |  2.211362 |
| 83 | 6 |  0 | -6.242417 |  5.440555 |  1.555726 |
| 84 | 6 |  0 | -3.898038 |  4.563939 |  1.832939 |
| 85 | 6 |  0 |  5.217665 |  6.441457 |  2.044580 |
| 86 | 6 |  0 | -1.580868 |  4.880714 |  2.340787 |
| 87 | 6 |  0 | -1.077131 |  6.305011 |  2.063521 |
| 88 | 6 |  0 |  4.515894 |  5.183408 |  2.566528 |
| 89 | 6 |  0 | -0.429309 |  4.388134 |  3.227812 |
| 90 | 6 |  0 |  2.109639 |  4.867031 |  3.020170 |
| 91 | 6 |  0 |  0.739189 |  4.832179 |  2.335615 |
| 92 | 6 |  0 | -2.158518 |  4.129232 | -0.474399 |
| 93 | 6 |  0 | -2.833591 | -5.686533 |  0.768422 |
| 94 | 1 |  0 | -4.704481 | -4.495545 | -1.335266 |
| 95 | 1 |  0 | -5.944512 |  2.877475 |  0.784105 |
| 96 | 1 |  0 | -4.564199 |  4.947772 | -1.300138 |
| 97 | 1 |  0 |  4.674783 |  4.342891 | -1.088438 |
| 98 | 1 |  0 |  2.904585 |  5.219597 |  1.162384 |
| 99 | 1 |  0 |  6.138009 | -2.968269 |  0.863248 |
|100 | 1 |  0 |  4.615318 | -4.440279 | -1.211254 |
|101 | 1 |  0 |  0.799662 |  4.218590 |  1.431637 |
|102 | 1 |  0 | -0.349611 |  4.936813 |  4.167971 |
|103 | 1 |  0 |  4.508339 |  5.293627 |  3.655716 |
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|108 | 1 |  0 |  6.249515 |  6.485463 |  2.410755 |
|109 | 1 |  0 |  4.688145 |  7.334901 |  2.388017 |
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| 176| 1 | 0 | -1.619389 | -0.484384 | 6.687081 |
| 177| 1 | 0 | -1.078888 | 1.661521 | 5.516482 |
| 178| 1 | 0 | 0.045723 | 6.014389 | -0.679836 |
| 179| 1 | 0 | -0.329035 | 8.059953 | -2.729813 |
| 180| 1 | 0 | -1.157032 | 7.954197 | -1.162983 |
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| 184| 1 | 0 | -1.686312 | -2.612508 | 5.306850 |
| 185| 1 | 0 | -5.410118 | 3.827135 | -4.033903 |
| 186| 1 | 0 | -7.844600 | 4.143134 | -3.460310 |
| 187| 1 | 0 | -7.372840 | 4.746021 | -1.860796 |
| 188| 1 | 0 | -6.923194 | 5.654503 | -3.326296 |
| 189| 1 | 0 | -6.268366 | 0.225336 | -1.565058 |
| 190| 1 | 0 | -8.526974 | 0.433692 | -2.481015 |
| 191| 1 | 0 | -8.047417 | -0.371020 | -3.975966 |
| 192| 1 | 0 | -9.162904 | -2.005732 | -2.498339 |
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| 194| 1 | 0 | -7.291222 | -2.985092 | -3.868677 |
| 195| 1 | 0 | -7.344305 | -3.724183 | -2.307464 |
| 196| 1 | 0 | -5.415507 | -1.053316 | -4.226759 |
| 197| 1 | 0 | -4.370644 | -0.635452 | -2.876436 |
| 198| 1 | 0 | -5.517858 | -2.318792 | -1.441808 |
| 199| 1 | 0 | 6.135463 | -6.597580 | 2.205711 |
| 200| 1 | 0 | 7.443214 | -5.305882 | 2.157032 |
| 201| 1 | 0 | 6.434278 | -5.598370 | 0.718158 |
| 202| 1 | 0 | -3.771250 | -5.547194 | -3.980898 |
| 203| 1 | 0 | -3.874886 | -7.793639 | -2.829845 |
| 204| 1 | 0 | -5.442864 | -6.963297 | -2.747396 |
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| 206| 1 | 0 | -2.329998 | -4.460095 | -4.774298 |
| 207| 1 | 0 | -0.582148 | -4.506379 | -4.957240 |
| 208| 1 | 0 | -1.497356 | -6.014206 | -5.096941 |
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| 210| 1 | 0 | 7.032505 | -2.109729 | -4.975693 |
| 211| 1 | 0 | 6.017741 | -0.665586 | -5.081725 |
| 212| 1 | 0 | 1.595869 | 6.964522 | -4.196911 |
| 213| 1 | 0 | 0.004332 | 6.192245 | -4.255690 |
| 214| 1 | 0 | 1.460930 | 5.209316 | -4.458311 |
| 215| 1 | 0 | 5.471756 | -4.410088 | 3.377509 |
| 216| 1 | 0 | -6.859347 | 2.344608 | -4.988822 |
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| 218| 1 | 0 | -6.408690 | 0.647721 | -5.119148 |
| 219| 1 | 0 | 5.983247 | -3.927580 | -3.795982 |
| 220| 1 | 0 | -4.276166 | -5.350096 | 3.325967 |
| 221| 1 | 0 | -0.664862 | -5.515471 | 0.796621 |
| 222| 1 | 0 | 0.465889 | -3.495551 | 3.390978 |
| 223| 1 | 0 | 1.946570 | -5.598802 | 0.993438 |
| 224| 1 | 0 | 6.396561 | -0.753382 | 1.098526 |
| 225| 1 | 0 | 5.556551 | 0.346965 | 3.810781 |
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| 227| 7 | 0 | 4.743233 | -4.318828 | -2.218405 |
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|   |   |   |   |   |
|---|---|---|---|---|
| 235 | 7 | 0 | 1.032290 | 5.834093 | -2.470169 |
| 236 | 7 | 0 | -2.960573 | 4.748435 | 2.802409 |
| 237 | 7 | 0 | -4.643584 | 4.585221 | -2.310036 |
| 238 | 7 | 0 | -5.784056 | 3.029985 | 1.780304 |
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| 243 | 7 | 0 | 3.068839 | -5.092171 | 2.624833 |
| 244 | 7 | 0 | -0.886642 | -0.428020 | 2.879645 |
| 245 | 8 | 0 | -4.354707 | -3.329133 | -4.306084 |
| 246 | 8 | 0 | -5.086125 | -3.803876 | 0.531472 |
| 247 | 8 | 0 | -1.422809 | 3.954167 | -1.095253 |
| 248 | 8 | 0 | -5.166850 | 2.052577 | 3.746007 |
| 249 | 8 | 0 | 0.620922 | -3.342266 | 1.690348 |
| 250 | 8 | 0 | 3.870563 | -4.720088 | 0.523526 |
| 251 | 8 | 0 | -0.166076 | -6.838320 | 2.322202 |
| 252 | 8 | 0 | -5.905137 | 2.376518 | -1.130490 |
| 253 | 8 | 0 | -3.600038 | 4.542821 | 0.623215 |
| 254 | 8 | 0 | -3.648794 | 5.288412 | -4.248653 |
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| 256 | 8 | 0 | 0.350641 | 6.177563 | 1.978065 |
| 257 | 8 | 0 | 2.106933 | 5.230817 | -0.553289 |
| 258 | 8 | 0 | -0.518025 | 3.024586 | 3.676558 |
| 259 | 8 | 0 | 3.978690 | 3.155850 | -3.952431 |
| 260 | 8 | 0 | 2.239804 | 4.647404 | 4.225204 |
| 261 | 8 | 0 | 6.443018 | -2.280590 | -0.976338 |
| 262 | 8 | 0 | 5.348114 | 3.813224 | 0.783956 |
| 263 | 8 | 0 | 3.677406 | -4.164819 | -4.242329 |
| 264 | 8 | 0 | 0.912960 | -2.866276 | -3.137779 |
| 265 | 8 | 0 | 2.189338 | -6.145726 | -2.148489 |
| 266 | 8 | 0 | -2.120557 | -5.765349 | -1.071716 |
| 267 | 8 | 0 | 5.284806 | -2.130704 | 3.824062 |
| 268 | 8 | 0 | -1.991237 | -4.752890 | 3.690027 |
| 269 | 8 | 0 | 0.361046 | -2.573422 | -0.955897 |
| 270 | 8 | 0 | -0.402850 | 2.037634 | 1.640282 |
| 271 | 47 | 0 | -0.302711 | -0.482973 | 0.691518 |
Clockwise alternating dimer

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|-------------------------|
|               |               |             | X           | Y           | Z           |
| 1             | 47            | 0           | 0.510593    | -1.809849   | -2.080444   |
| 2             | 6             | 0           | 4.279597    | 5.271816    | 2.563575    |
| 3             | 6             | 0           | -2.602003   | -1.373810   | -3.099635   |
| 4             | 6             | 0           | 1.827602    | 5.307668    | 2.532936    |
| 5             | 6             | 0           | 0.616626    | 5.930012    | 1.826648    |
| 6             | 6             | 0           | -0.661736   | 5.071284    | 1.874243    |
| 7             | 6             | 0           | -1.715448   | 6.093595    | 2.341645    |
| 8             | 6             | 0           | -1.586243   | -1.725562   | -6.745955   |
| 9             | 6             | 0           | -3.917427   | 5.187518    | 2.001785    |
| 10            | 6             | 0           | -2.380163   | -1.488472   | -5.623746   |
| 11            | 6             | 0           | -3.034200   | 5.266145    | 3.304110    |
| 12            | 6             | 0           | -0.881451   | 6.991000    | 3.264789    |
| 13            | 6             | 0           | -1.790521   | -1.541231   | -4.359047   |
| 14            | 6             | 0           | 0.270078    | -2.066596   | -5.236524   |
| 15            | 6             | 0           | -0.239173   | -2.026371   | -6.565402   |
| 16            | 6             | 0           | 5.285399    | 6.383582    | 2.220859    |
| 17            | 6             | 0           | 5.060153    | 3.312683    | 4.544868    |
| 18            | 6             | 0           | 6.282239    | 1.987359    | 2.762456    |
| 19            | 6             | 0           | 7.685662    | 2.259188    | 3.331688    |
| 20            | 6             | 0           | 8.670837    | 1.185988    | 2.845125    |
| 21            | 6             | 0           | 8.185675    | -0.242797   | 2.673879    |
| 22            | 6             | 0           | 6.759105    | -0.498718   | 3.000212    |
| 23            | 6             | 0           | 6.323398    | -1.884471   | 3.160156    |
| 24            | 6             | 0           | -7.041655   | 4.497414    | -2.222015   |
| 25            | 6             | 0           | 5.781995    | -4.285023   | 2.457188    |
| 26            | 6             | 0           | 6.789673    | -5.067499   | 1.691870    |
| 27            | 6             | 0           | 4.337246    | -4.591565   | 2.068855    |
| 28            | 6             | 0           | -5.734862   | 3.749051    | -2.520867   |
| 29            | 6             | 0           | -3.532140   | 4.727903    | -3.005708   |
| 30            | 6             | 0           | 3.446678    | -3.629295   | 4.229416    |
| 31            | 6             | 0           | 1.968067    | -4.588928   | 2.446018    |
| 32            | 6             | 0           | 0.829357    | -3.669915   | 2.888254    |
| 33            | 6             | 0           | 1.395248    | -5.934695   | 2.914117    |
| 34            | 6             | 0           | -2.407452   | 5.626814    | -2.491747   |
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| 37            | 6             | 0           | -2.695525   | 7.076110    | -2.960595   |
| 38            | 6             | 0           | -1.573692   | 8.033507    | -2.542667   |
| 39            | 6             | 0           | -3.977514   | -4.468695   | 3.863220    |
| 40            | 6             | 0           | -4.825744   | -5.741779   | 3.989906    |
| 41            | 6             | 0           | -4.762629   | -3.357886   | 3.172443    |
| 42            | 6             | 0           | -0.211876   | 7.556315    | -3.065187   |
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| 44            | 6             | 0           | -5.029573   | -2.72107    | 5.387057    |
| 45            | 6             | 0           | -6.076759   | -1.275135   | 3.300561    |
| 46            | 6             | 0           | -5.459850   | 0.118887    | 3.527288    |
| 47            | 6             | 0           | -7.548461   | -1.330235   | 3.745540    |
| 48            | 6             | 0           | -8.369306   | -0.237470   | 3.045145    |
| 49            | 6             | 0           | -7.772157   | 1.154927    | 2.869992    |
| 50            | 6             | 0           | -6.287966   | 1.230323    | 2.852979    |
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| 52            | 6             | 0           | 0.082706    | 6.116914    | -2.601803   |
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|54 | 6 | 0 | 1.651994 | 5.511002 | -4.505831 |
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|56 | 6 | 0 | -6.308681 | 5.875454 | 1.758749 |
|57 | 6 | 0 | 1.337378 | 2.107938 | 0.252358 |
|58 | 6 | 0 | 1.188524 | 1.126574 | -0.730956 |
|59 | 6 | 0 | 2.448380 | 5.648707 | -2.168189 |
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|62 | 6 | 0 | 1.346244 | 1.714050 | 1.588241 |
|63 | 6 | 0 | 0.989542 | -2.027383 | 1.087336 |
|64 | 6 | 0 | -2.919110 | -6.093947 | -0.711255 |
|65 | 6 | 0 | -4.426893 | -5.957671 | -1.028912 |
|66 | 6 | 0 | -4.717276 | -3.657497 | -1.797556 |
|67 | 6 | 0 | -4.931445 | -2.209230 | -1.364634 |
|68 | 6 | 0 | -4.979065 | -1.196150 | -2.520470 |
|69 | 6 | 0 | -5.447155 | 0.026780 | -1.723200 |
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|88 | 6 | 0 | 5.977354 | -0.140446 | -1.654658 |
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|95 | 7 | 0 | -2.956799 | 5.533529 | 2.896725 |
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|105 | 7 | 0 | -5.708251 | 3.521612 | 2.218186 |
|106 | 7 | 0 | 3.815014 | -4.427402 | -1.930195 |
|107 | 7 | 0 | 1.052933 | -0.175200 | -0.450712 |
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|110 | 7 | 0 | -4.812085 | -4.565859 | -0.803762 |
|111 | 7 | 0 | -5.803251 | 1.232921 | -2.467567 |
|112 | 8 | 0 | -5.521832 | 2.397377 | -0.547376 |
|   |   |   |   |   |   |
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| 113 | 8 | 0 | -6.225059 | -2.019691 | -0.778927 |
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| 115 | 8 | 0 | -2.540753 | -5.826701 | 0.438265 |
| 116 | 8 | 0 | 0.877962 | -2.309733 | 2.388823 |
| 117 | 8 | 0 | 1.998953 | -3.699823 | -3.092842 |
| 118 | 8 | 0 | 5.660211 | -2.690952 | -0.689737 |
| 119 | 8 | 0 | -5.465261 | 2.893882 | 4.398964 |
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| 140 | 8 | 0 | 0.877962 | -2.309733 | 2.388823 |
| 141 | 8 | 0 | 1.998953 | -3.699823 | -3.092842 |
| 142 | 8 | 0 | 5.660211 | -2.690952 | -0.689737 |
| 143 | 8 | 0 | -5.465261 | 2.893882 | 4.398964 |
| 144 | 8 | 0 | 4.669546 | 1.098335 | 0.000954 |
| 145 | 8 | 0 | 2.540753 | 5.826701 | 3.378265 |
| 146 | 8 | 0 | 0.877962 | -2.309733 | 2.388823 |
| 147 | 8 | 0 | 1.998953 | -3.699823 | -3.092842 |
| 148 | 8 | 0 | 5.660211 | -2.690952 | -0.689737 |
| 149 | 8 | 0 | -2.170598 | -1.576167 | -1.980751 |
| 150 | 8 | 0 | -0.559164 | 4.285794 | 2.637599 |
| 151 | 8 | 0 | 2.540753 | 5.826701 | 3.378265 |
| 152 | 8 | 0 | 0.877962 | -2.309733 | 2.388823 |
| 153 | 8 | 0 | 1.998953 | -3.699823 | -3.092842 |
| 154 | 8 | 0 | 5.660211 | -2.690952 | -0.689737 |
| 155 | 8 | 0 | -5.465261 | 2.893882 | 4.398964 |
| 156 | 8 | 0 | 4.669546 | 1.098335 | 0.000954 |
| 157 | 8 | 0 | 2.540753 | 5.826701 | 3.378265 |
| 158 | 8 | 0 | 0.877962 | -2.309733 | 2.388823 |
| 159 | 8 | 0 | 1.998953 | -3.699823 | -3.092842 |
| 160 | 8 | 0 | 5.660211 | -2.690952 | -0.689737 |
| 161 | 8 | 0 | -5.465261 | 2.893882 | 4.398964 |
| 162 | 8 | 0 | 4.669546 | 1.098335 | 0.000954 |
| 163 | 8 | 0 | 2.540753 | 5.826701 | 3.378265 |
| 164 | 8 | 0 | 0.877962 | -2.309733 | 2.388823 |
| 165 | 8 | 0 | 1.998953 | -3.699823 | -3.092842 |
| 166 | 8 | 0 | 5.660211 | -2.690952 | -0.689737 |
| 167 | 8 | 0 | -5.465261 | 2.893882 | 4.398964 |
| 168 | 8 | 0 | 4.669546 | 1.098335 | 0.000954 |
| 169 | 8 | 0 | 2.540753 | 5.826701 | 3.378265 |
| 170 | 8 | 0 | 0.877962 | -2.309733 | 2.388823 |
| 171 | 8 | 0 | 1.998953 | -3.699823 | -3.092842 |
|   |   |   |   |   |
|---|---|---|---|---|
| 231 | 1 | 0 | -6.735051 | 2.035549 |
| 232 | 1 | 0 | -7.542185 | -0.558541 |
| 233 | 1 | 0 | -6.685888 | -0.175908 |
| 234 | 1 | 0 | 6.237811 | 2.761659 |
| 235 | 1 | 0 | -6.305799 | -6.762686 |
| 236 | 1 | 0 | -4.980545 | -7.946692 |
| 237 | 1 | 0 | -5.020802 | -6.720286 |
| 238 | 1 | 0 | 7.609339 | 0.089603 |
| 239 | 1 | 0 | 7.930529 | 0.828866 |
| 240 | 1 | 0 | 4.045683 | 0.828866 |
| 241 | 1 | 0 | 1.587047 | -6.707346 |
| 242 | 1 | 0 | 3.118496 | -5.885818 |
| 243 | 1 | 0 | 2.989760 | -7.661968 |
| 244 | 1 | 0 | 0.590321 | -6.575378 |
| 245 | 1 | 0 | 0.208573 | -4.539549 |
| 246 | 1 | 0 | 0.086441 | -5.446360 |
| 247 | 1 | 0 | -0.172401 | -8.167330 |
| 248 | 1 | 0 | -0.639061 | -8.810302 |
| 249 | 1 | 0 | 1.820537 | -9.085843 |
| 250 | 1 | 0 | 1.531719 | -8.083377 |
| 251 | 1 | 0 | 2.210035 | -7.065483 |
| 252 | 1 | 0 | 3.292941 | -7.073108 |
| 253 | 1 | 0 | 1.833929 | -5.565841 |
| 254 | 1 | 0 | 6.278714 | -0.576085 |
| 255 | 1 | 0 | 5.540040 | -1.524723 |
| 256 | 1 | 0 | 3.899435 | -1.817778 |
| 257 | 1 | 0 | 5.108559 | 0.107299 |
| 258 | 1 | 0 | 4.216267 | -3.274728 |
| 259 | 1 | 0 | 5.598834 | -5.336955 |
| 260 | 1 | 0 | 6.497624 | -4.885344 |
| 261 | 1 | 0 | 6.657402 | -3.909038 |
| 262 | 1 | 0 | -4.431503 | 4.732271 |
| 263 | 1 | 0 | 6.012816 | -2.510504 |
| 264 | 1 | 0 | 4.878315 | 4.526238 |
| 265 | 1 | 0 | -2.848732 | -5.077905 |
| 266 | 1 | 0 | -5.750255 | 3.209767 |
| 267 | 1 | 0 | 4.134271 | -4.874003 |
| 268 | 1 | 0 | 2.999928 | 5.786340 |
| 269 | 1 | 0 | -4.917917 | -4.241795 |
| 270 | 1 | 0 | 4.702916 | 2.035452 |
| 271 | 1 | 0 | -1.902681 | 4.504347 |
Counter-clockwise alternating dimer

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) |
|---------------|---------------|-------------|------------------------|
|               |               |             | X          | Y          | Z          |
| 1             | 47            | 0           | 0.401803   | 0.752274  | 1.247958   |
| 2             | 6             | 0           | 5.743129   | -3.018519 | 2.560316   |
| 3             | 6             | 0           | 7.752657   | -1.564778 | 3.017826   |
| 4             | 6             | 0           | 5.409451   | -0.590945 | 3.144499   |
| 5             | 6             | 0           | 6.011837   | 0.823458  | 3.089755   |
| 6             | 6             | 0           | 7.420446   | 0.866189  | 3.704125   |
| 7             | 6             | 0           | 8.336335   | -0.144540 | 2.992686   |
| 8             | 6             | 0           | 4.665231   | 2.864323  | 2.905375   |
| 9             | 6             | 0           | 3.683901   | 3.885799  | 3.509438   |
| 10            | 6             | 0           | 1.341269   | 4.226080  | 2.863905   |

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72
|   |   |   |   |   |
|---|---|---|---|---|
| 113 | 8 | 0 | 2.686635 | -3.126956 | -4.654920 |
| 114 | 8 | 0 | -5.185475 | 0.939170 | -0.422129 |
| 115 | 8 | 0 | -5.526239 | 4.056316 | -2.650288 |
| 116 | 8 | 0 | -1.794582 | 3.404943 | -3.496437 |
| 117 | 8 | 0 | -7.176850 | -0.624937 | -2.385464 |
| 118 | 8 | 0 | 2.842421 | 5.148839 | -0.242825 |
| 119 | 8 | 0 | 5.272539 | 3.031859 | -3.038372 |
| 120 | 8 | 0 | 4.490236 | -0.125695 | -0.453893 |
| 121 | 8 | 0 | 6.876899 | -3.055472 | -1.522445 |
| 122 | 8 | 0 | 7.319729 | 1.533531 | -1.465055 |
| 123 | 8 | 0 | 0.172055 | -3.379292 | -3.847190 |
| 124 | 8 | 0 | -7.526239 | -0.624837 | -2.385464 |
| 125 | 8 | 0 | -0.918150 | 4.028147 | -3.038372 |
| 126 | 8 | 0 | -5.444439 | 3.031859 | -3.038372 |
| 127 | 8 | 0 | -0.169893 | -1.841914 | -1.404346 |
| 128 | 8 | 0 | 2.778023 | -0.312518 | -0.918291 |
| 129 | 8 | 0 | -3.728605 | 3.211797 | -1.465055 |
| 130 | 8 | 0 | -5.763086 | 2.188465 | -3.496437 |
| 131 | 8 | 0 | -5.928691 | -3.553860 | -2.650288 |
| 132 | 8 | 0 | -2.414328 | -4.857378 | -3.496437 |
| 133 | 8 | 0 | 3.342724 | -4.975003 | -2.914848 |
| 134 | 8 | 0 | 5.461368 | -3.476680 | -3.667556 |
| 135 | 8 | 0 | -0.708119 | -6.006404 | 0.678230 |
| 136 | 8 | 0 | 0.831120 | 5.965780 | 1.791314 |
| 137 | 8 | 0 | -4.718090 | -1.689742 | -3.730422 |
| 138 | 1 | 0 | 7.704358 | -1.936446 | 4.048611 |
| 139 | 1 | 0 | 8.406632 | -2.249749 | 2.463097 |
| 140 | 1 | 0 | 4.422989 | -0.582468 | 2.670853 |
| 141 | 1 | 0 | 5.286182 | -0.930903 | 4.179725 |
| 142 | 1 | 0 | 6.098546 | 1.111798 | 2.042028 |
| 143 | 1 | 0 | 7.377749 | 0.623656 | 4.775474 |
| 144 | 1 | 0 | 7.829754 | 1.879986 | 3.618898 |
| 145 | 1 | 0 | 9.328300 | -0.140316 | 3.459866 |
| 146 | 1 | 0 | 8.481289 | 0.174713 | 1.950472 |
| 147 | 1 | 0 | 3.158264 | 3.490143 | 4.377344 |
| 148 | 1 | 0 | 0.846008 | 4.398748 | 0.748170 |
| 149 | 1 | 0 | -1.033435 | 3.308317 | 2.810405 |
| 150 | 1 | 0 | -2.159312 | 5.101777 | 0.654378 |
| 151 | 1 | 0 | -1.682917 | 7.051430 | 2.046354 |
| 152 | 1 | 0 | -1.241763 | 6.026292 | 3.438168 |
| 153 | 1 | 0 | -5.909480 | 4.363270 | 2.665857 |
| 154 | 1 | 0 | -7.408217 | 0.395603 | 1.655376 |
| 155 | 1 | 0 | -5.572175 | -0.578586 | 3.899590 |
| 156 | 1 | 0 | -5.252227 | -0.690904 | 2.155815 |
| 157 | 1 | 0 | -7.218912 | -2.124887 | 1.822336 |
| 158 | 1 | 0 | -8.879060 | 1.267607 | 3.452451 |
| 159 | 1 | 0 | -7.758894 | 0.608028 | 4.677839 |
| 160 | 1 | 0 | -8.518702 | -3.033457 | 3.719411 |
| 161 | 1 | 0 | -7.687964 | -2.048765 | 4.860820 |
| 162 | 1 | 0 | -9.408730 | -1.008307 | 2.610185 |
| 163 | 1 | 0 | -9.739684 | -0.919786 | 4.336260 |
| 164 | 1 | 0 | -4.664969 | -5.496905 | 3.066335 |
| 165 | 1 | 0 | -1.226242 | -3.973866 | 0.646653 |
| 166 | 1 | 0 | 0.053057 | -3.525704 | 3.050205 |
| 167 | 1 | 0 | 1.289713 | -4.072300 | 0.553371 |
| 168 | 1 | 0 | 0.971667 | -6.242718 | -0.418221 |
| 169 | 1 | 0 | 0.951375 | -7.043934 | 1.170493 |
| 170 | 1 | 0 | 5.157733 | -5.449907 | 2.404668 |
| 171 | 1 | 0 | 5.924955 | -5.552589 | -0.553530 |
|   |   |   | 5.504731 | -6.980984 | 0.417145 |
|---|---|---|---------|-----------|---------|
| 173| 1 | 0 | 6.937367 | -6.014127 | 0.831473 |
| 174| 1 | 0 | 3.629149 | 1.295669 | 5.128937 |
| 175| 1 | 0 | 4.755421 | 2.581687 | 5.638315 |
| 176| 1 | 0 | 5.306725 | 0.914888 | 5.540043 |
| 177| 1 | 0 | 5.200439 | 4.947166 | 4.675338 |
| 178| 1 | 0 | 4.954505 | 5.588998 | 3.039953 |
| 179| 1 | 0 | 3.745662 | 5.981557 | 4.310187 |
| 180| 1 | 0 | 3.751379 | -4.883869 | 3.606532 |
| 181| 1 | 0 | 2.034343 | -4.677994 | 3.837707 |
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| 183| 1 | 0 | -5.183835 | -7.324381 | 1.434799 |
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| 185| 1 | 0 | -6.607654 | -6.511679 | 1.921621 |
| 186| 1 | 0 | -5.365283 | -2.595659 | 4.898220 |
| 187| 1 | 0 | -4.394517 | -3.923402 | 4.268039 |
| 188| 1 | 0 | -6.057710 | -4.224445 | 4.852071 |
| 189| 1 | 0 | -3.963011 | 5.938414 | 3.792625 |
| 190| 1 | 0 | -4.439466 | 4.222102 | 4.026994 |
| 191| 1 | 0 | -2.771523 | 4.710682 | 4.279274 |
| 192| 1 | 0 | -7.364182 | 4.872658 | 0.725151 |
| 193| 1 | 0 | -6.068940 | 4.396975 | -0.408413 |
| 194| 1 | 0 | -5.860791 | 5.810310 | 0.641148 |
| 195| 1 | 0 | 6.255697 | -1.106543 | -5.136230 |
| 196| 1 | 0 | 4.536590 | -1.430170 | -4.776770 |
| 197| 1 | 0 | 5.248928 | 0.138829 | -4.383293 |
| 198| 1 | 0 | 6.622574 | 6.465994 | -0.924363 |
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| 200| 1 | 0 | 5.289327 | 6.539726 | 0.254171 |
| 201| 1 | 0 | 3.868483 | 7.143859 | -3.606379 |
| 202| 1 | 0 | 2.322650 | 6.664882 | -4.306903 |
| 203| 1 | 0 | 3.591530 | 5.451804 | -4.194035 |
| 204| 1 | 0 | -5.869825 | 4.418852 | -6.007705 |
| 205| 1 | 0 | -5.772651 | 5.768581 | -4.798490 |
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| 207| 1 | 0 | -4.718581 | 1.513649 | -5.746983 |
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| 209| 1 | 0 | -3.291376 | 1.599627 | -4.673748 |
| 210| 1 | 0 | -5.086822 | -6.399649 | -3.381101 |
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| 214| 1 | 0 | -3.168090 | -4.986756 | -5.472311 |
| 215| 1 | 0 | -3.143379 | -3.269813 | -4.971132 |
| 216| 1 | 0 | 7.219898 | -4.521267 | -4.172318 |
| 217| 1 | 0 | 6.485530 | -5.358811 | -2.796840 |
| 218| 1 | 0 | 5.897472 | -5.675447 | -4.448229 |
| 219| 1 | 0 | -3.633849 | 3.564485 | -5.287541 |
| 220| 1 | 0 | -7.943317 | 0.866399 | -3.544295 |
| 221| 1 | 0 | -6.638538 | -0.056316 | -4.318584 |
| 222| 1 | 0 | -6.445959 | 2.090463 | -2.162665 |
| 223| 1 | 0 | -4.102623 | 0.311850 | -2.077160 |
| 224| 1 | 0 | -6.899905 | -1.266114 | -0.766497 |
| 225| 1 | 0 | -4.769692 | -4.007999 | -3.963227 |
| 226| 1 | 0 | 0.612094 | -7.420168 | -2.627872 |
| 227| 1 | 0 | 0.693824 | -8.106012 | -4.246231 |
| 228| 1 | 0 | -1.591329 | -7.178079 | -3.736326 |
| 229| 1 | 0 | -0.839662 | -6.369613 | -5.114482 |
| 230| 1 | 0 | -0.921359 | -5.355123 | -2.226065 |
|   |   |   |   |   |
|---|---|---|---|---|
| 321 | 1 | 0 | 0.341088 | -3.922330 | -4.686162 |
| 322 | 1 | 0 | 0.022246 | -3.279552 | -3.052978 |
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| 326 | 1 | 0 | 5.044580 | -3.363520 | -4.627667 |
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| 329 | 1 | 0 | 6.630460 | -0.985956 | -1.247927 |
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| 338 | 1 | 0 | 0.344950 | 5.652308 | -4.021803 |
| 339 | 1 | 0 | 0.508188 | 4.332645 | -2.863745 |
| 340 | 1 | 0 | 0.988040 | 5.967326 | -1.041338 |
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| 345 | 1 | 0 | -0.448702 | 1.067767 | -3.945183 |
| 346 | 1 | 0 | -0.514198 | 1.996415 | -1.649427 |
| 347 | 1 | 0 | -1.016305 | 1.880650 | 7.024381 |
| 348 | 1 | 0 | -0.796979 | -2.717894 | 5.127700 |
| 349 | 1 | 0 | -0.492366 | 1.339987 | 6.570117 |
| 350 | 1 | 0 | 6.375834 | -1.333030 | 1.360182 |
| 351 | 1 | 0 | 0.182894 | 2.014388 | 4.282468 |
| 352 | 1 | 0 | -6.446639 | 2.145739 | 0.797211 |
| 353 | 1 | 0 | -3.439521 | -5.094071 | 0.394147 |
| 354 | 1 | 0 | 2.930876 | 4.400817 | 1.568257 |
| 355 | 1 | 0 | 5.731466 | -3.284042 | 0.580646 |
| 356 | 1 | 0 | 5.272486 | 3.956901 | -0.009062 |
| 357 | 1 | 0 | 3.947701 | -4.762585 | -2.255493 |
| 358 | 1 | 0 | -5.483102 | -3.409841 | -1.162865 |
| 359 | 1 | 0 | -3.581913 | 5.987338 | -3.657560 |
| 360 | 1 | 0 | -4.625371 | 1.739653 | -0.346397 |
| 361 | 1 | 0 | -2.004509 | 2.727344 | 0.576385 |