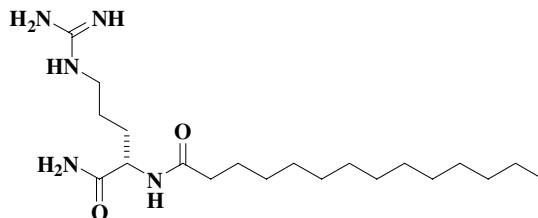


Supplementary Information: CC 049945t

A1

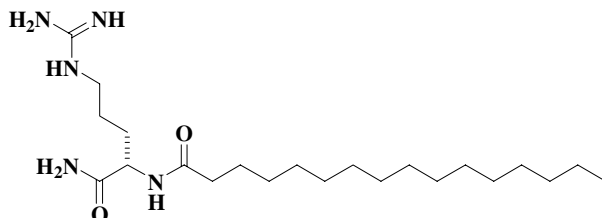


RP-HPLC: 8.80 min (100 %)

MS (ES⁺): m/z (%): 384.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₀H₄₂N₅O₂ [M+H]⁺: 384.3333; found: 384.3326

A2

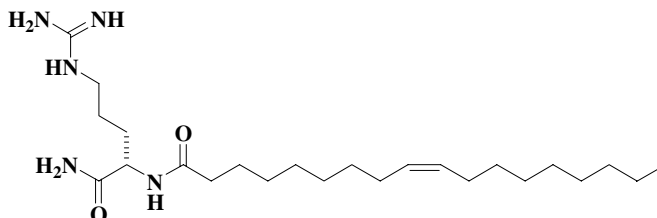


RP-HPLC: 9.99 min (95 %)

MS (ES⁺): m/z (%): 412.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₂H₄₆N₅O₂ [M+H]⁺: 412.3633; found: 412.3645

A3

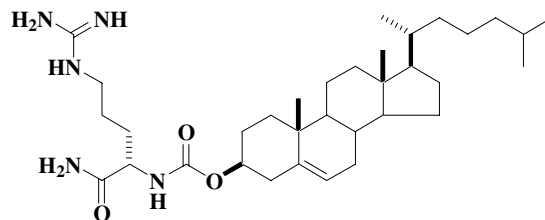


RP-HPLC: 10.37 min (63 %)

MS (ES⁺): m/z (%): 438.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₄H₄₈N₅O₂ [M+H]⁺: 438.3802; found: 438.3802

A4

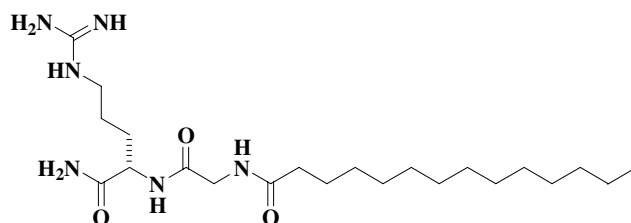


RP-HPLC: 13.79 min (100 %)

MS (ES⁺): m/z (%): 586.5 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₄H₆₀N₅O₃ [M+H]⁺: 586.4691; found: 586.4704

B1

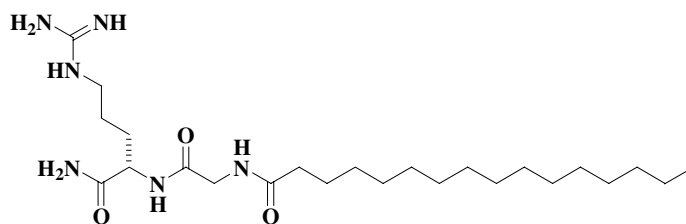


RP-HPLC: 9.25 min (81 %)

MS (ES⁺): m/z (%): 441.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₂H₄₅N₆O₃ [M+H]⁺: 441.3548; found: 441.3557

B2

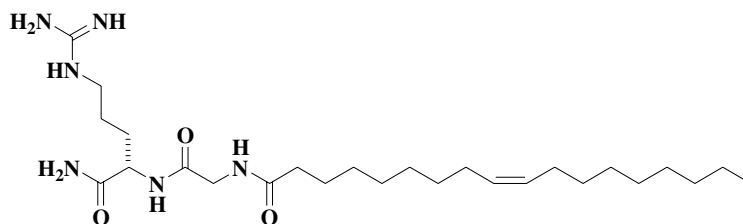


RP-HPLC: 10.18 min (74 %)

MS (ES⁺): m/z (%): 469.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₄H₄₉N₆O₃ [M+H]⁺: 469.3861; found: 469.3859

B3

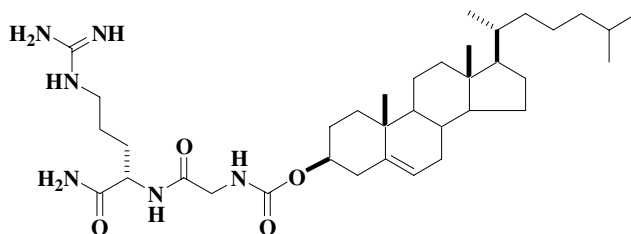


RP-HPLC: 10.18 min (51 %)

MS (ES⁺): m/z (%): 495.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₆H₅₁N₆O₃ [M+H]⁺: 495.4017; found: 495.4016

B4

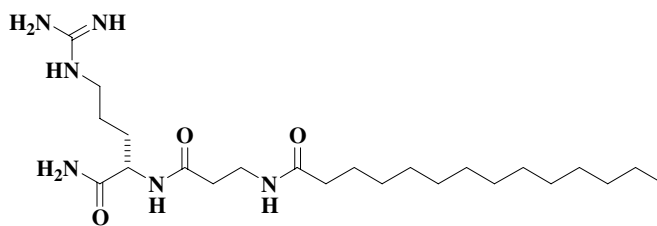


RP-HPLC: 13.48 min (100 %)

MS (ES⁺): m/z (%): 643.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₆H₆₃N₆O₄ [M+H]⁺: 643.4906; found: 643.4939

C1

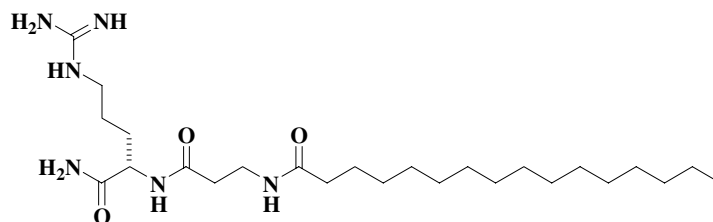


RP-HPLC: 9.22 min (60 %)

MS (ES⁺): m/z (%): 455.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₃H₄₇N₆O₃ [M+H]⁺: 455.3704; found: 455.3708

C2

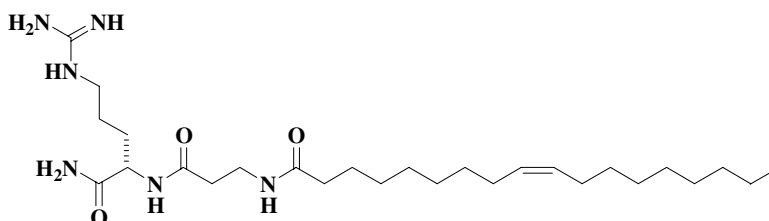


RP-HPLC: 10.13 min (81 %)

MS (ES⁺): m/z (%): 483.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₅H₅₀N₆O₃ [M+H]⁺: 483.4017; found: 483.4017

C3

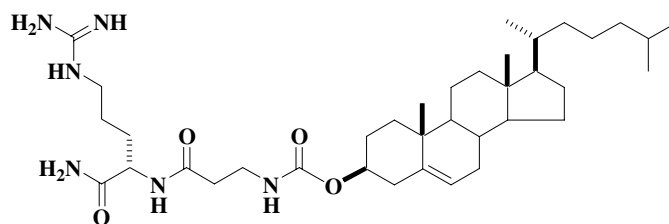


RP-HPLC: 10.46 min (92 %)

MS (ES⁺): m/z (%): 509.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₇H₅₂N₆O₃ [M+H]⁺: 509.4174; found: 509.4184

C4

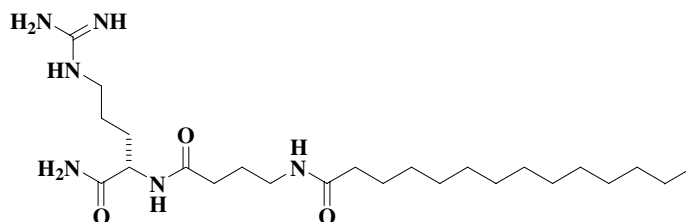


RP-HPLC: 13.66 min (100 %)

MS (ES⁺): m/z (%): 657.6 (60) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₄H₆₅N₆O₃ [M+H]⁺: 657.5062; found: 657.5080

D1

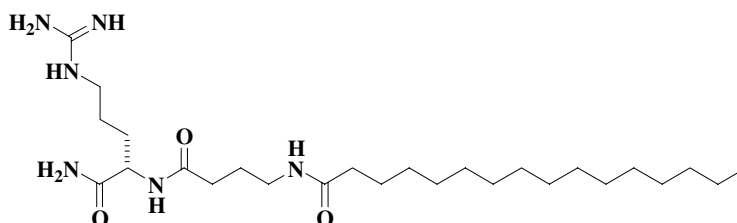


RP-HPLC: 9.32 min (50 %)

MS (ES⁺): m/z (%): 469.5 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₄H₄₉N₆O₃ [M+H]⁺: 469.3861; found: 469.3859

D2

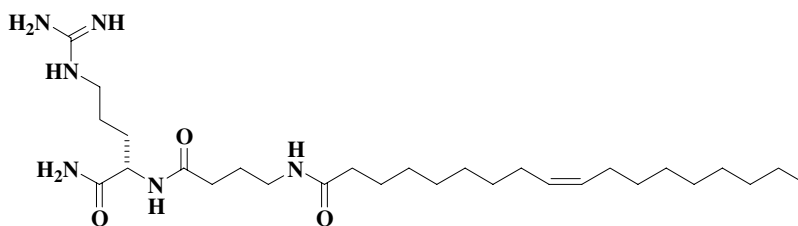


RP-HPLC: 10.24 min (65 %)

MS (ES⁺): m/z (%): 497.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₆H₅₂N₆O₃ [M+H]⁺: 497.4174; found: 497.4173

D3

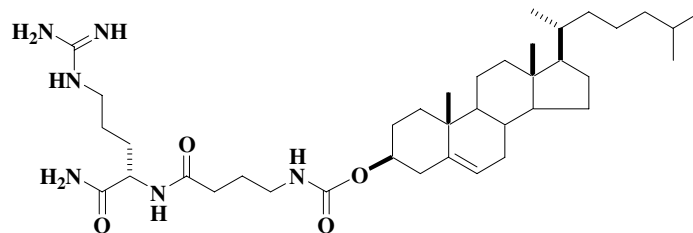


RP-HPLC: 10.42 min (100 %)

MS (ES⁺): m/z (%): 523.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₈H₅₄N₆O₃ [M+H]⁺: 523.4330; found: 523.4347

D4

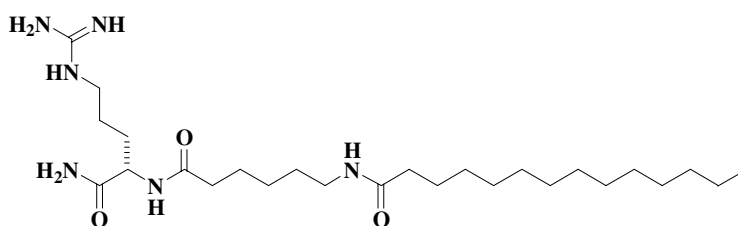


RP-HPLC: 13.87 min (100 %)

MS (ES⁺): m/z (%): 671.5 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₈H₆₇N₆O₄ [M+H]⁺: 671.5219; found: 671.5250

E1

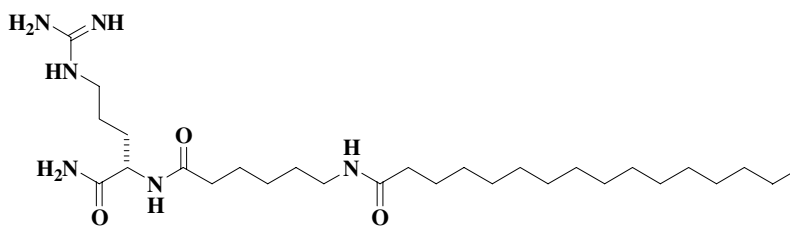


RP-HPLC: 9.26 min (91 %)

MS (ES⁺): m/z (%): 497.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₆H₅₃N₆O₃ [M+H]⁺: 497.4174; found: 497.4175

E2

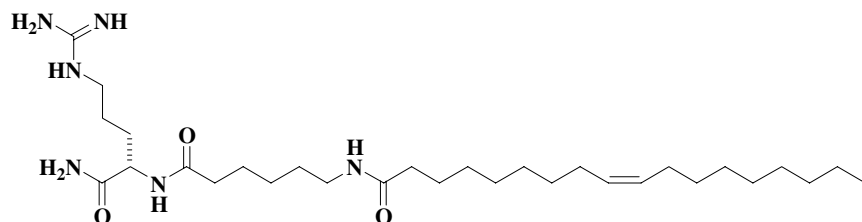


RP-HPLC: 10.21 min (89 %)

MS (ES⁺): m/z (%): 525.4 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₈H₅₆N₆O₃ [M+H]⁺: 525.4487; found: 525.4504

E3

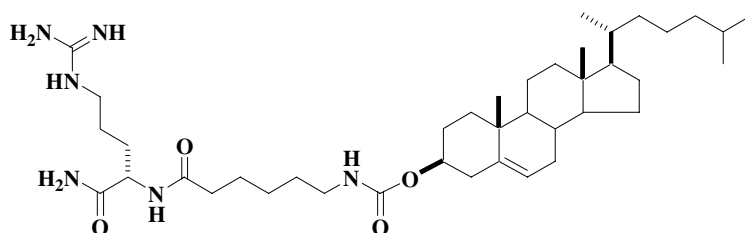


RP-HPLC: 1.05 (25 %), 10.53 min (75 %)

MS (ES⁺): m/z (%): 551.3 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₀H₅₈N₆O₃ [M+H]⁺: 551.4643; found: 551.4648

E4

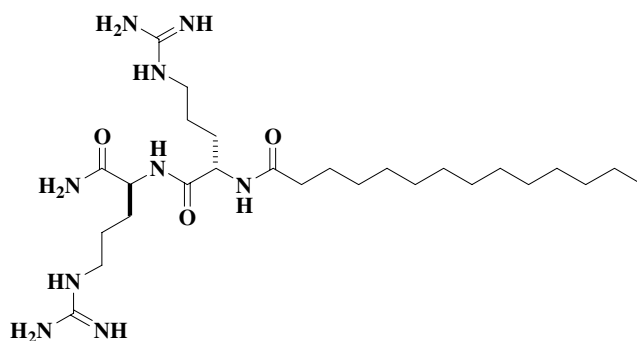


RP-HPLC: 14.46 min (100 %)

MS (ES⁺): m/z (%): 699.2 (100) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₀H₇₁N₆O₄ [M+H]⁺: 699.5562; found: 699.5546

F1

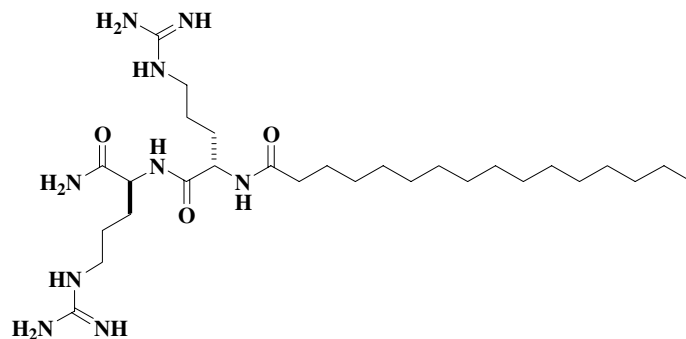


RP-HPLC: 7.73 min (100 %)

MS (ES⁺): m/z (%): 270.8 (100) [M+2H]²⁺, 540.3 (28) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₆H₅₄N₉O₃ [M+H]⁺: 540.4344; found: 540.4367

F2

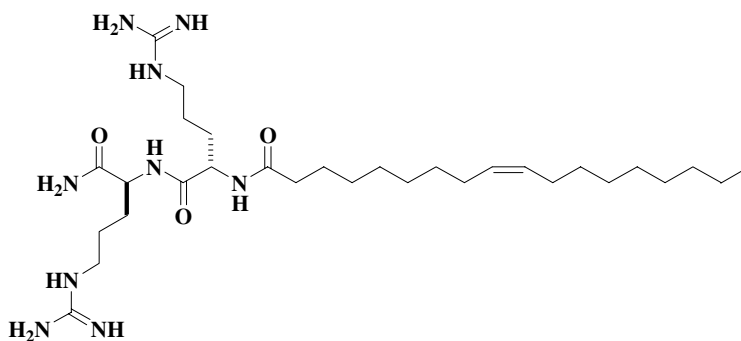


RP-HPLC: 8.42 min (98 %)

MS (ES⁺): m/z (%): 284.8 (100) [M+2H]²⁺, 568.3 (25) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₈H₅₈N₉O₃ [M+H]⁺: 568.4657; found: 568.4667

F3

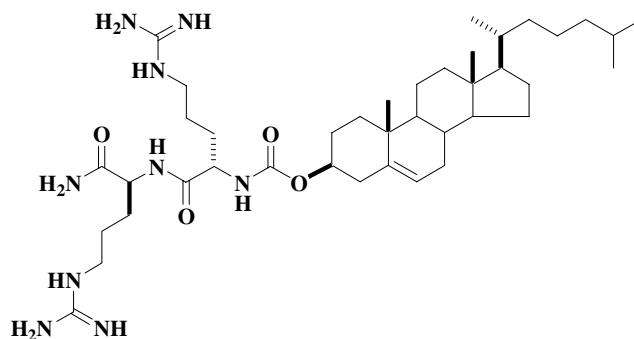


RP-HPLC: 8.71 min (87 %)

MS (ES⁺): m/z (%): 297.9 (100) [M+2H]²⁺, 594.3 (20) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₀H₆₀N₉O₃ [M+H]⁺: 594.4814; found: 594.4835

F4

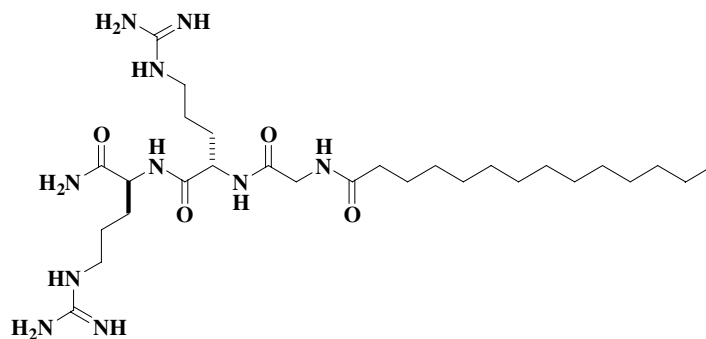


RP-HPLC: 1.00 min (90 %), 11.11 min (10 %)

MS (ES⁺): m/z (%): 371.9 (100) [M+2H]²⁺, 742.2 (35) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₀H₇₂N₉O₄ [M+H]⁺: 742.5702; found: 742.5732

G1

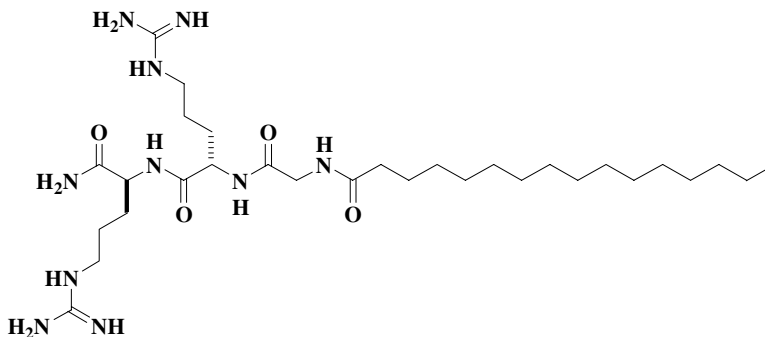


RP-HPLC: 7.97 min (99 %)

MS (ES⁺): m/z (%): 299.4 (100) [M+2H]²⁺, 597.4 (20) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₈H₅₇N₁₀O₄ [M+H]⁺: 597.4559; found: 597.4573

G2

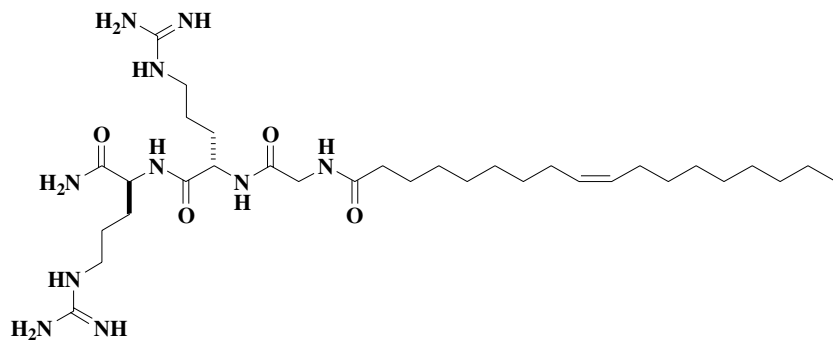


RP-HPLC: 8.62 min (88 %)

MS (ES⁺): m/z (%): 313.4 (100) [M+2H]²⁺, 625.2 (20) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₀H₆₁N₁₀O₄ [M+H]⁺: 625.4872; found: 625.4881

G3

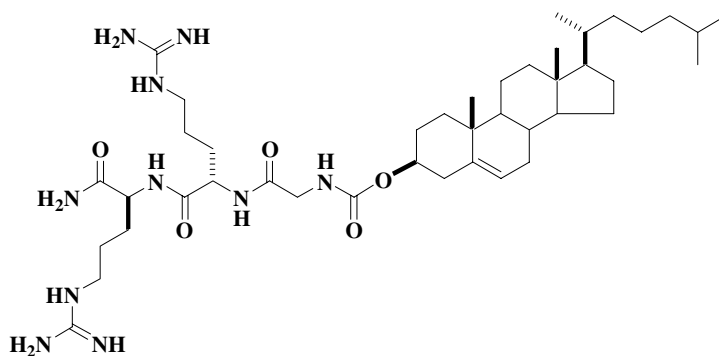


RP-HPLC: 8.83 min (97 %)

MS (ES⁺): m/z (%): 326.4 (100) [M+2H]²⁺, 651.2 (20) [M+H]⁺

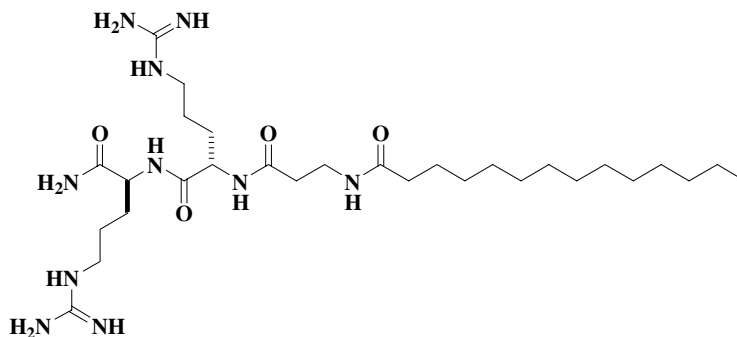
HRMS (ES⁺): m/z calc. for C₃₂H₆₃N₁₀O₄ [M+H]⁺: 651.5029; found: 651.5050

G4



RP-HPLC: 11.27 min (100 %)

H1

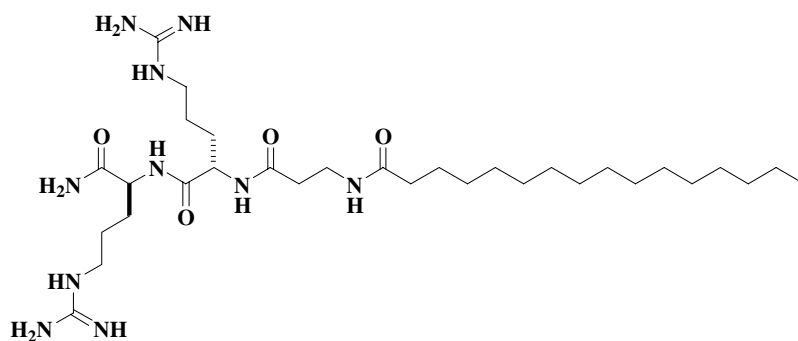


RP-HPLC: 8.35 min (79 %)

MS (ES⁺): m/z (%): 306.3 (100) [M+2H]²⁺, 611.2 (15) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₂₉H₅₉N₁₀O₄ [M+H]⁺: 611.4716; found: 611.4729

H2

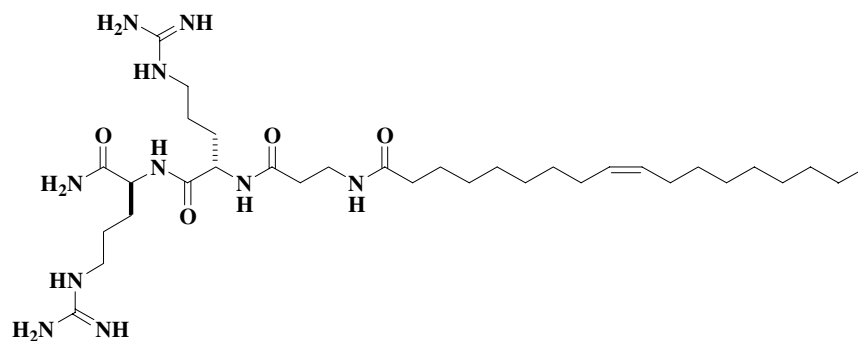


RP-HPLC: 9.01 min (100 %)

MS (ES⁺): m/z (%): 320.3 (100) [M+2H]²⁺, 639.2 (10) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₁H₆₃N₁₀O₄ [M+H]⁺: 639.5029; found: 639.5044

H3

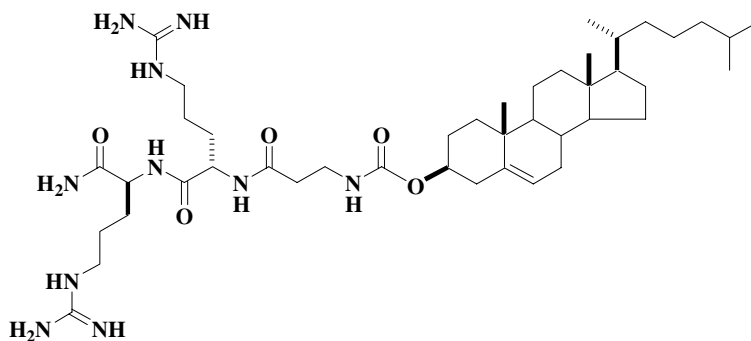


RP-HPLC: 9.23 min (92 %)

MS (ES⁺): m/z (%): 333.4 (100) [M+2H]²⁺, 665.2 (10) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₃H₆₅N₁₀O₄ [M+H]⁺: 665.5185; found: 665.5192

H4

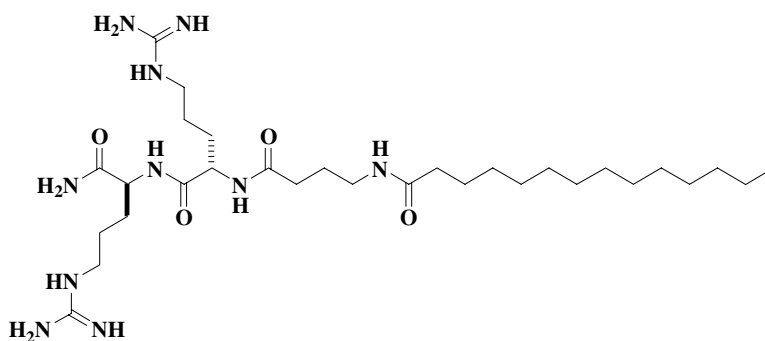


RP-HPLC: 11.44 min (97 %)

MS (ES⁺): m/z (%): 407.3 (95) [M+2H]²⁺, 813.1 (10) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₃H₇₇N₁₀O₅ [M+H]⁺: 813.6073; found: 813.6108

A5

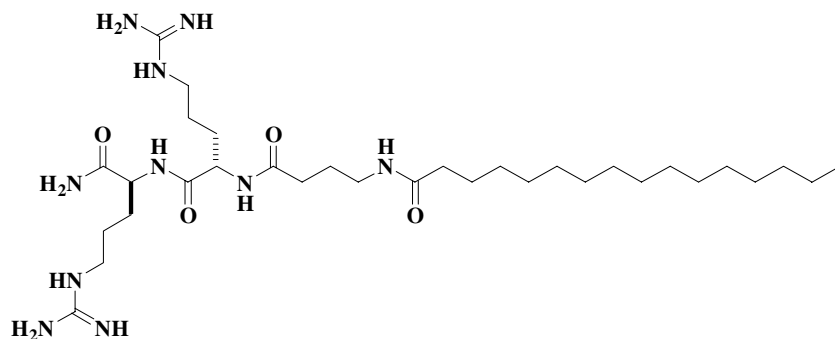


RP-HPLC: 8.09 min (92 %)

MS (ES⁺): m/z (%): 313.4 (100) [M+2H]²⁺, 625.2 (15) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₀H₆₁N₁₀O₄ [M+H]⁺: 625.4872; found: 625.4877

A6

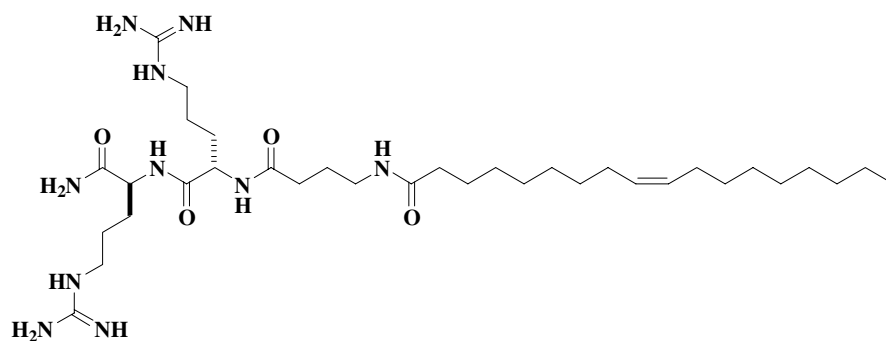


RP-HPLC: 8.76 min (64 %)

MS (ES⁺): m/z (%): 327.4 (100) [M+2H]²⁺, 653.3 (12) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₂H₆₅N₁₀O₄ [M+H]⁺: 653.5185; found: 653.5197

A7

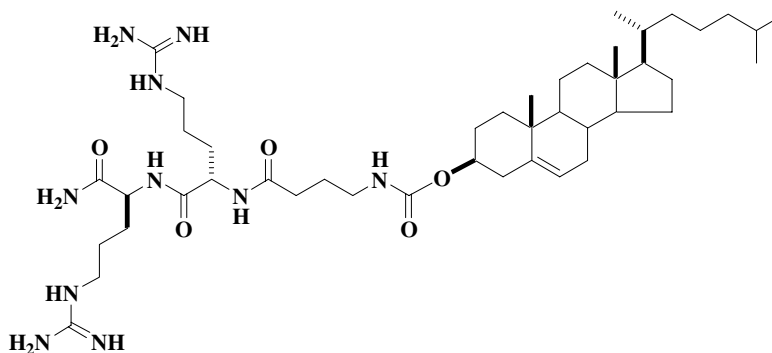


RP-HPLC: 9.10 min (38 %)

MS (ES⁺): m/z (%): 340.4 (100) [M+2H]²⁺, 679.2 (10) [M+H]⁺

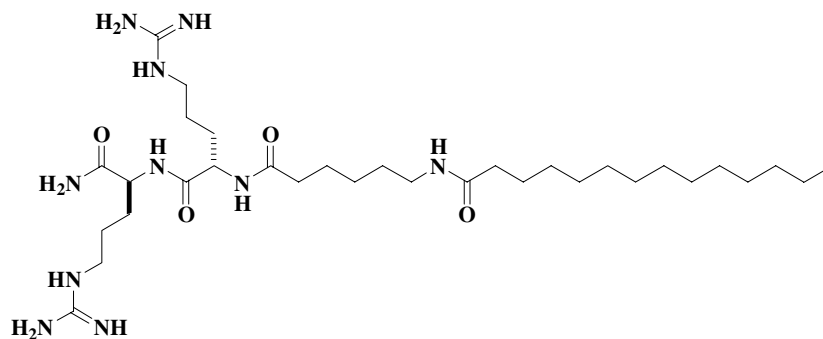
HRMS (ES⁺): m/z calc. for C₃₄H₆₇N₁₀O₄ [M+H]⁺: 679.5342; found: 679.5380

A8



RP-HPLC: 11.79 min (78 %)

B5

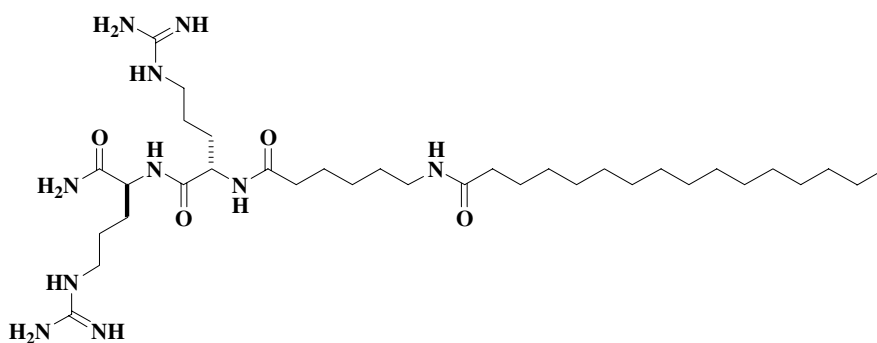


RP-HPLC: 8.35 min (98 %)

MS (ES⁺): m/z (%): 327.4 (100) [M+2H]²⁺, 653.3 (10) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₂H₆₅N₁₀O₄ [M+H]⁺: 653.5185; found: 653.5198

B6

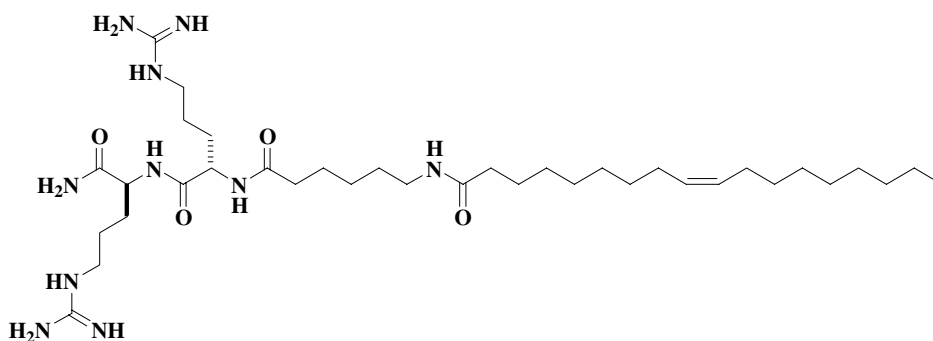


RP-HPLC: 9.03 min (97 %)

MS (ES⁺): m/z (%): 341.4 (100) [M+2H]²⁺, 681.2 (10) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₄H₆₉N₁₀O₄ [M+H]⁺: 681.5498; found: 681.5528

B7

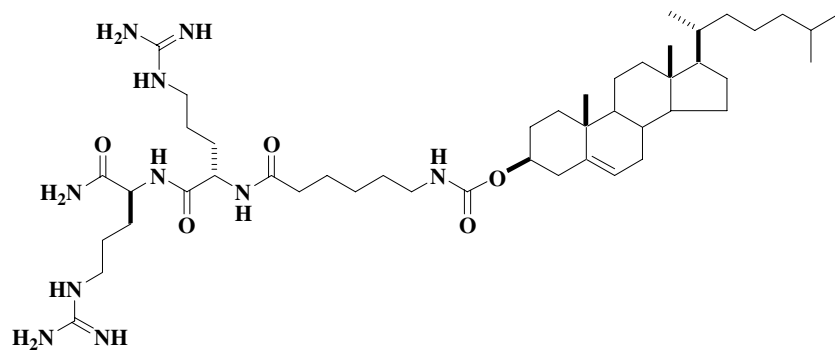


RP-HPLC: 9.38 min (37 %)

MS (ES⁺): m/z (%): 354.3 (100) [M+2H]²⁺, 707.2 (12) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₆H₇₁N₁₀O₄ [M+H]⁺: 707.5655; found: 707.5689

B8

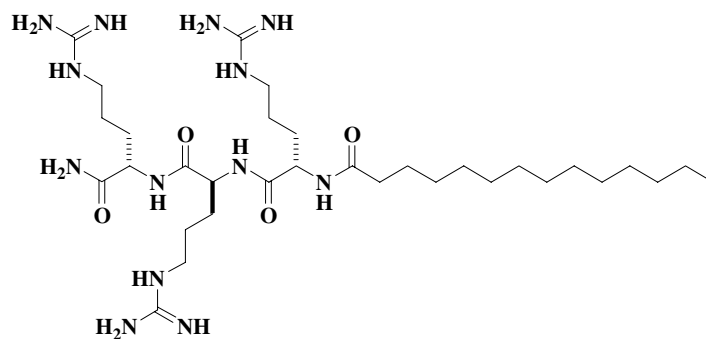


RP-HPLC: 12.36 min (91 %)

MS (ES⁺): m/z (%): 428.3 (100) [M+2H]²⁺, 855.2 (12) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₆H₈₃N₁₀O₅ [M+H]⁺: 855.6542; found: 855.6551

C5

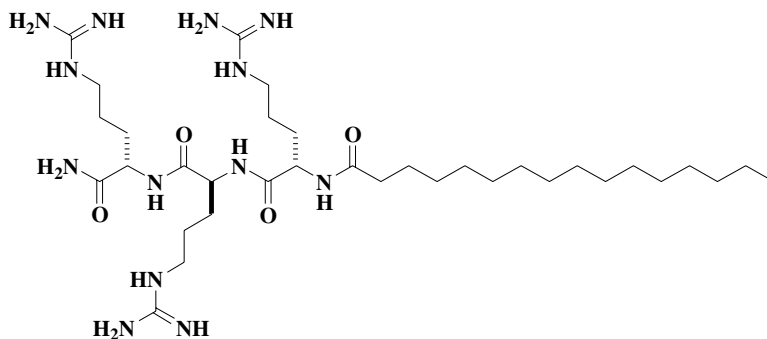


RP-HPLC: 7.78 min (91 %)

MS (ES⁺): m/z (%): 348.8 (100) [M+2H]²⁺, 696.2 (8) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₂H₆₆N₁₃O₄ [M+H]⁺: 696.5355; found: 696.5373

C6

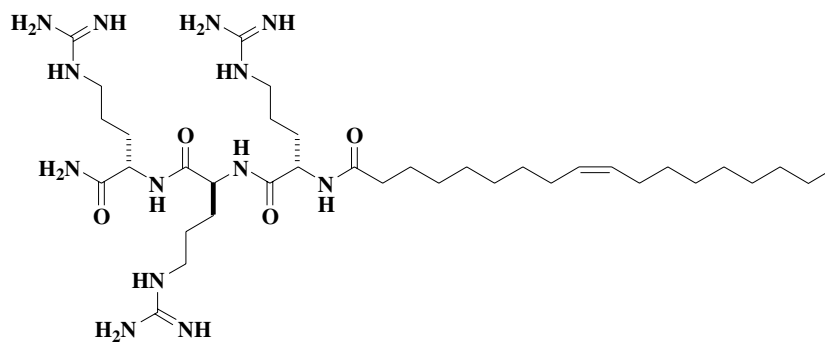


RP-HPLC: 8.40 min (91 %)

MS (ES⁺): m/z (%): 362.9 (100) [M+2H]²⁺, 724.2 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₄H₇₀N₁₃O₄ [M+2H]²⁺: 362.7870; found: 362.7874

C7

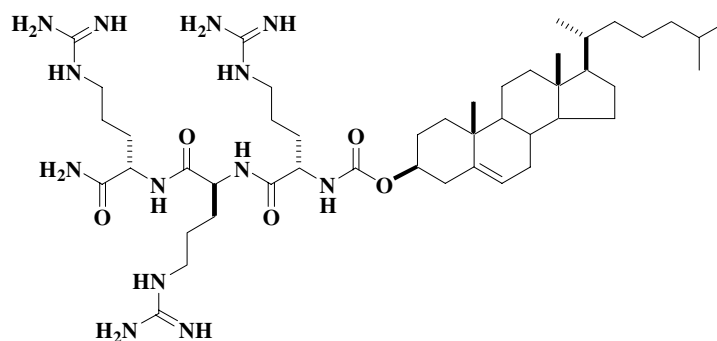


RP-HPLC: 8.57 min (52 %)

MS (ES⁺): m/z (%): 375.9 (100) [M+2H]²⁺, 750.2 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₆H₇₂N₁₃O₄ [M+2H]²⁺: 375.7951; found: 375.7952

C8

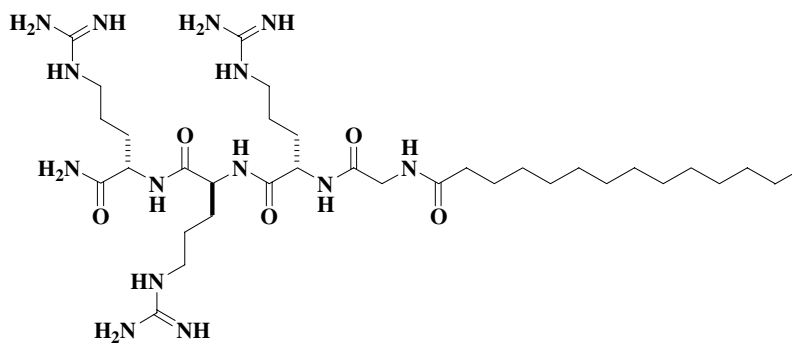


RP-HPLC: 10.26 min (59 %)

MS (ES⁺): m/z (%): 449.8 (100) [M+2H]²⁺, 898.1 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₆H₈₄N₁₃O₅ [M+H]⁺: 898.6713; found: 898.6737

D5

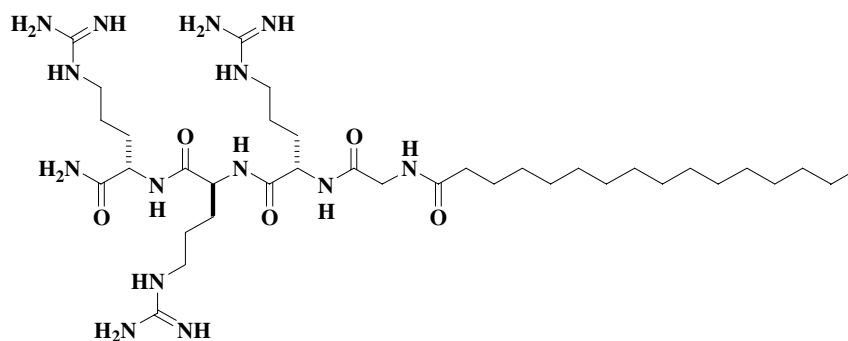


RP-HPLC: 7.97 min (89 %)

MS (ES⁺): m/z (%): 377.3 (100) [M+2H]²⁺, 753.1 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₄H₆₉N₁₄O₅ [M+2H]²⁺: 377.2818; found: 377.2818

D6

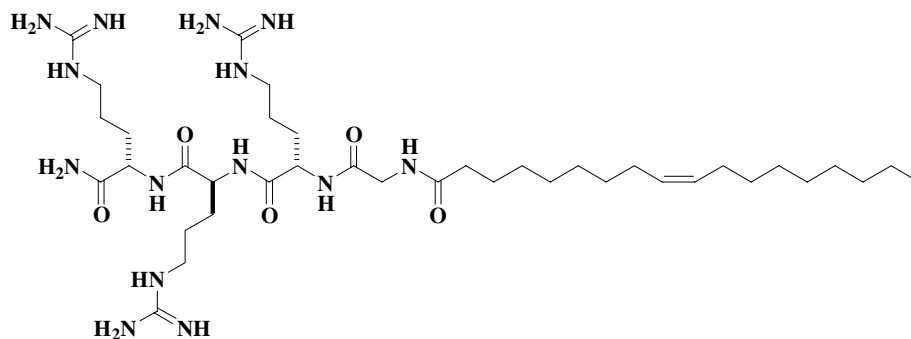


RP-HPLC: 8.50 min (68 %)

MS (ES⁺): m/z (%): 391.4 (100) [M+2H]²⁺, 780.9 (4) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₆H₇₁N₁₄O₅ [M+2H]²⁺: 391.2977; found: 391.2977

D7

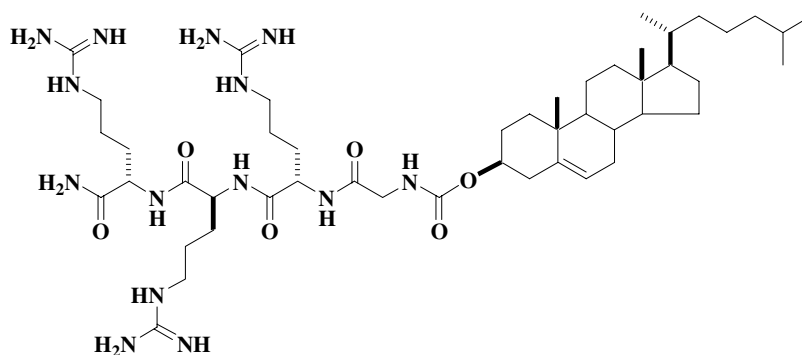


RP-HPLC: 8.72 min (92 %)

MS (ES⁺): m/z (%): 404.3 (100) [M+2H]²⁺, 807.1 (4) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₈H₇₅N₁₄O₅ [M+2H]²⁺: 404.3056; found: 404.3067

D8

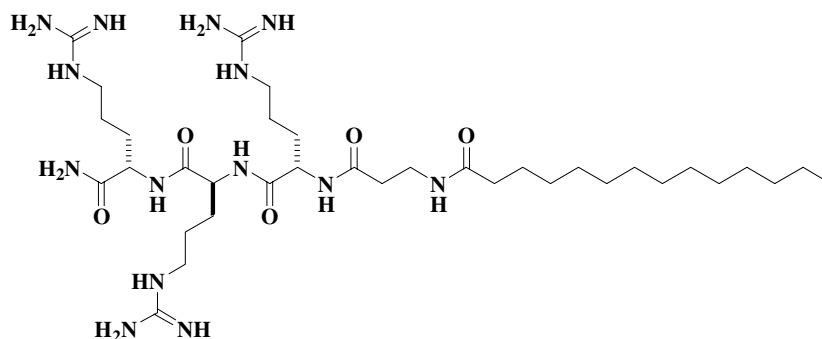


RP-HPLC: 1.07 min (88 %)

MS (ES⁺): m/z (%): 478.3 (95) [M+2H]²⁺, 955.2 (4) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₈H₈₈N₁₄O₆ [M+H]⁺: 955.6928; found: 955.6952

E5

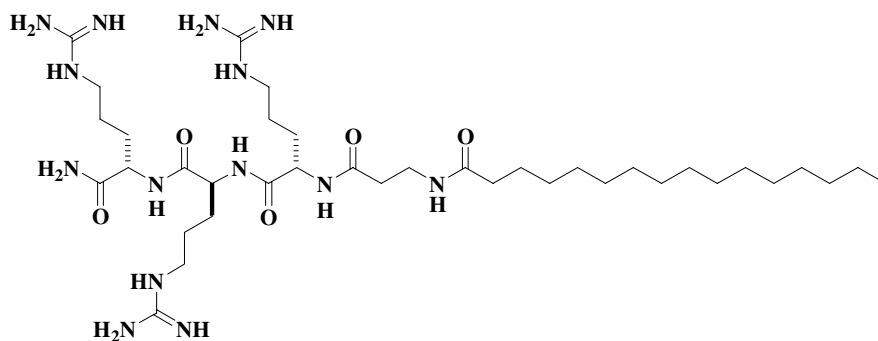


RP-HPLC: 7.69 min (97 %)

MS (ES⁺): m/z (%): 384.3 (100) [M+2H]²⁺, 767.2 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₅H₇₁N₁₄O₅ [M+H]⁺: 767.5727; found: 767.5767

E6

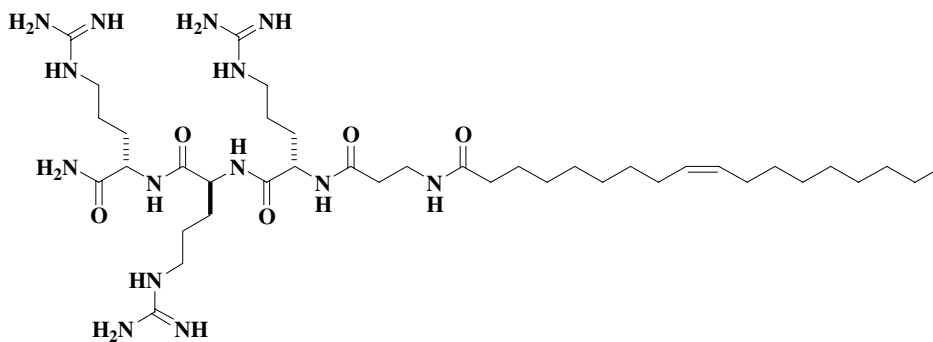


RP-HPLC: 8.24 min (100 %)

MS (ES⁺): m/z (%): 398.3 (100)[M+2H]²⁺, 795.1 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₇H₇₅N₁₄O₅ [M+H]⁺: 795.4060; found: 795.6085

E7

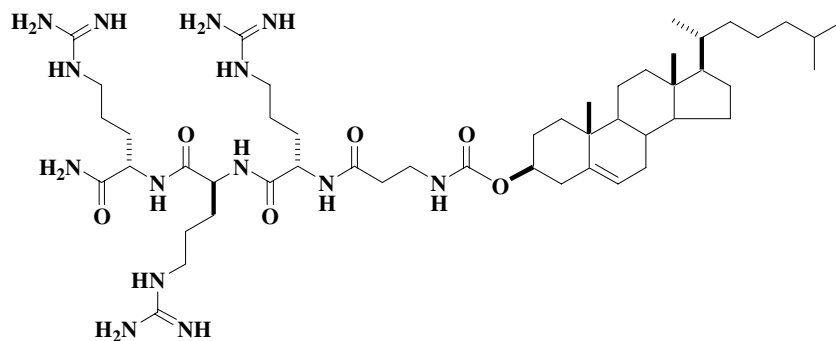


RP-HPLC: 1.12 min (33 %), 8.42 min (57 %)

MS (ES⁺): m/z (%): 411.3 (100) [M+2H]²⁺, 821.2 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₉H₇₇N₁₄O₅ [M+H]⁺: 821.6196; found: 821.6232

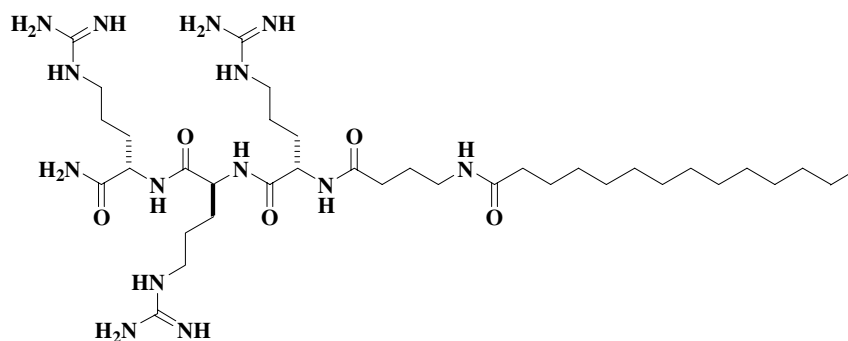
E8



RP-HPLC: 10.36 min (77 %)

MS (ES⁺): m/z (%): 485.4 (100) [M+2H]²⁺

F5

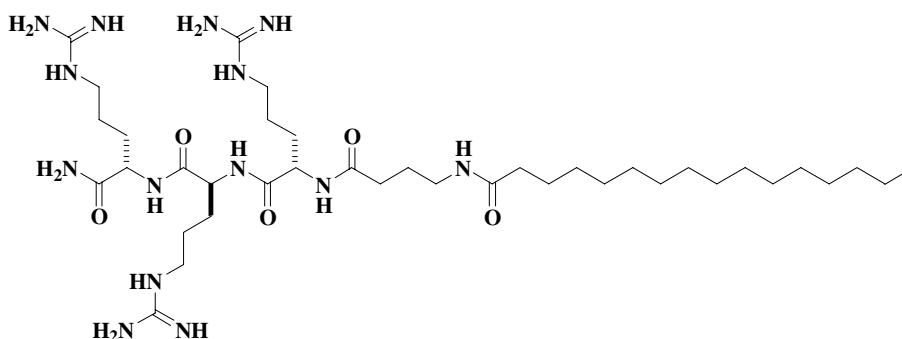


RP-HPLC: 7.70 min (86 %)

MS (ES⁺): m/z (%): 391.3 (100) [M+2H]²⁺, 781.2 (8) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₆H₇₃N₁₄O₅ [M+H]⁺: 781.5883; found: 781.5924

F6

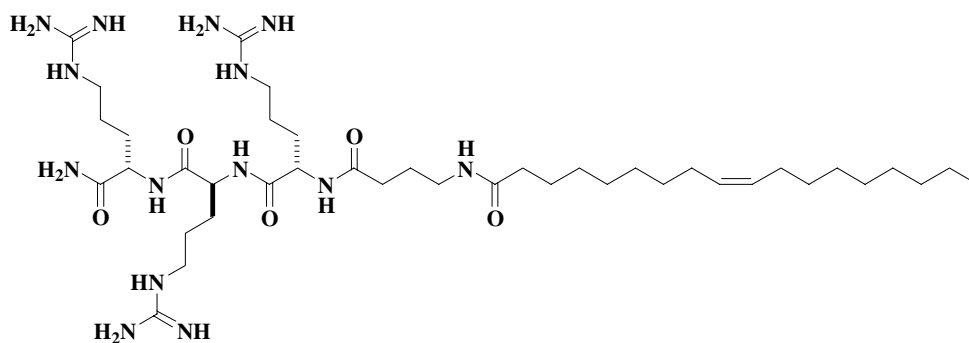


RP-HPLC: 1.09 min (29 %), 8.33 min (66 %)

MS (ES⁺): m/z (%): 405.4 (100) [M+2H]²⁺, 809.2 (8) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₈H₇₈N₁₄O₅ [M+2H]²⁺: 405.3163; found: 405.3140

F7

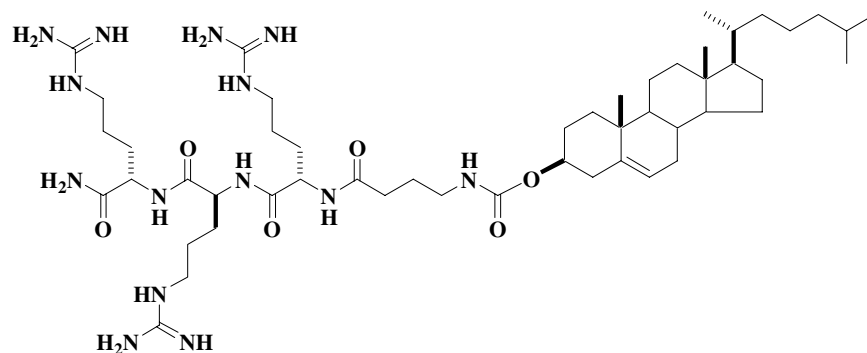


RP-HPLC: 1.09 min (27 %), 8.50 min (64 %)

MS (ES⁺): m/z (%): 418.4 (100) [M+2H]²⁺, 835.1 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₀H₇₉N₁₄O₅ [M+H]⁺: 835.6353; found: 835.6387

F8

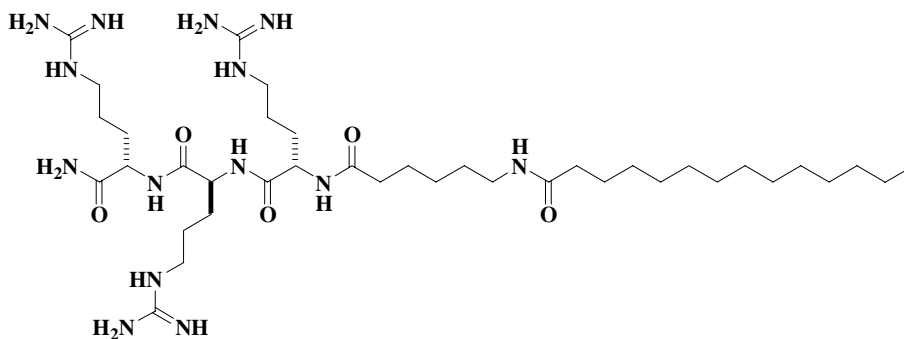


RP-HPLC: 10.59 min (93 %)

MS (ES⁺): m/z (%): 492.4 (100) [M+2H]²⁺, 983.1 (4) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₅₀H₉₁N₁₄O₆ [M+H]⁺: 983.7241; found: 983.7279

G5

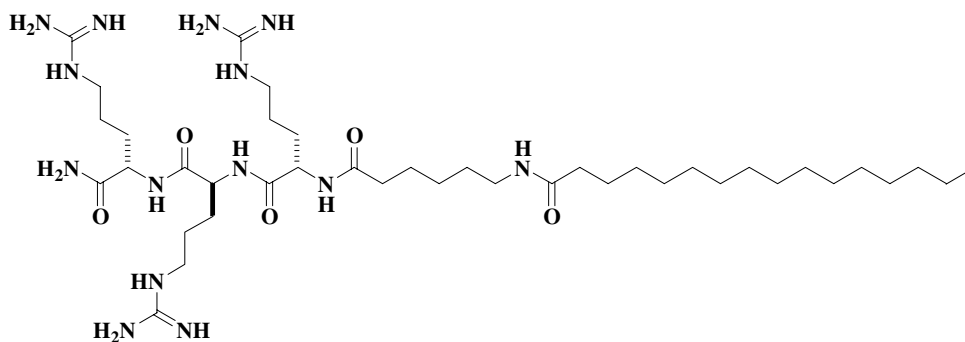


RP-HPLC: 1.09 min (30 %), 7.93 min (66 %)

MS (ES⁺): m/z (%): 405.3 (100) [M+2H]²⁺, 809.1 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₃₈H₇₈N₁₄O₅ [M+2H]²⁺: 405.3134; found: 405.3140

G6

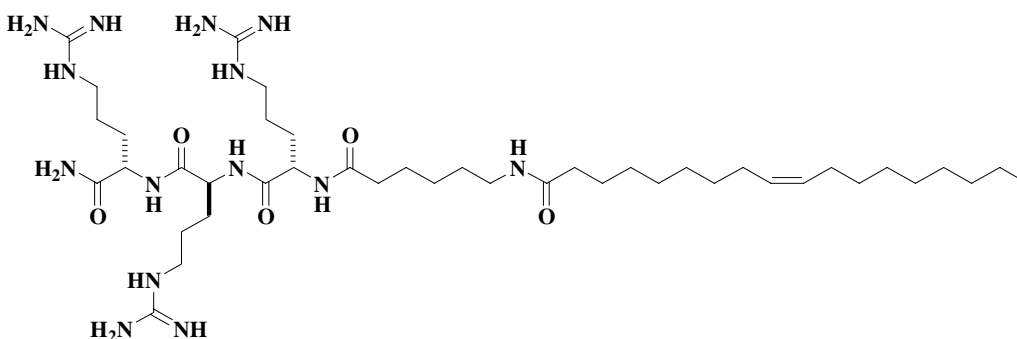


RP-HPLC: 8.57 min (97 %)

MS (ES⁺): m/z (%): 419.4 (100) [M+2H]²⁺, 837.2 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₀H₈₁N₁₄O₅ [M+H]⁺: 837.6509; found: 837.6546

G7

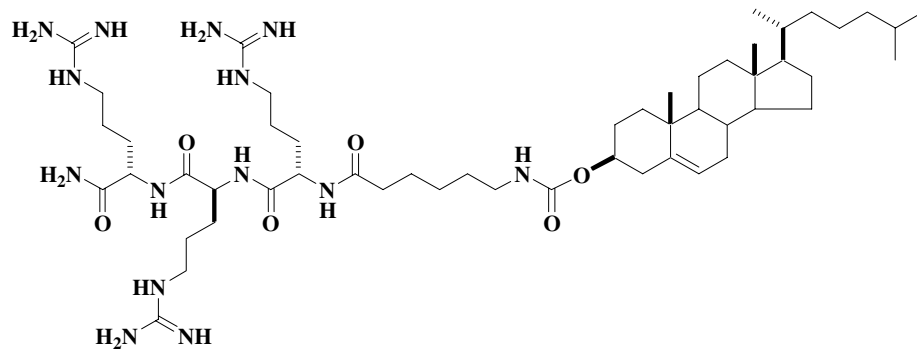


RP-HPLC: 8.75 min (96 %)

MS (ES⁺): m/z (%): 432.4 (85) [M+2H]²⁺, 863.1 (5) [M+H]⁺

HRMS (ES⁺): m/z calc. for C₄₂H₈₄N₁₄O₅ [M+2H]²⁺: 432.3369; found: 432.3378

G8



RP-HPLC: 11.13 min (86 %)

MS (ES⁺): m/z (%): 506.5 (100) [M+2H]²⁺