# Aminoacyl-anthraquinone conjugates as telomerase inhibitors: synthesis, biophysical and biological evaluation

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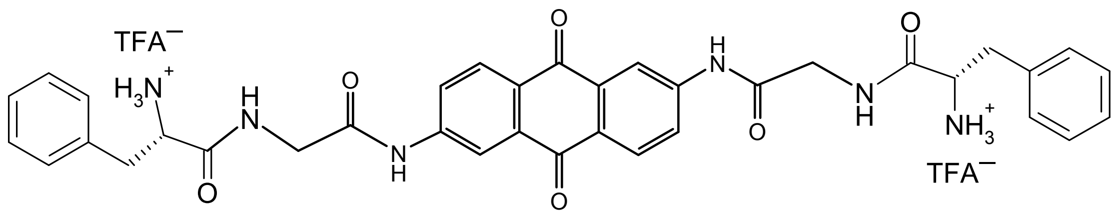
## Supporting Information

1. Structural properties, synthetic procedures and analytical data (NMR, HRMS) for new compounds. The different substances are listed in the same order as in Table 1.
Methods A, B and C are described in the paper.

2. Combustion data of new compounds

# 1. Structural information, synthetic procedure and analytical data for new compounds

**2,6-AQ-Gly-Phe-$NH_3^+$ $TFA^-$**



Method A

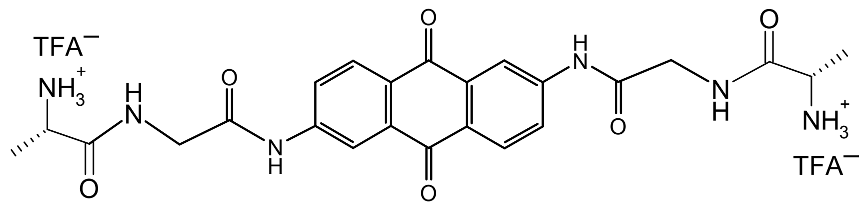
Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Phe-OSu (218 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (80 mg, overall yield 91 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.65 (bs, 2H), 8.81 (t, J=5.4 Hz, 2H), 8.33 (d, J=2.3 Hz, 2H), 8.06 (d, J=8.6 Hz, 2H), 7.98 (bs, 6H), 7.90 (dd, J=8.8 and 2.3 Hz, 2H), 7.21-7.09 (m, 10H), 3.99 (m, 2H), 3.93 (d, J= 5.5 Hz, 4H), 3.03 (m, 2H), 2.84 (m, 2H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.66, 169.11, 168.42, 144.65, 135.28, 134.75, 129.91, 128.96, 128.88, 128.56, 127.51, 123.90, 116.27, 53.78, 43.28, 37.44.

HRMS, *m*/*z*: 324.1397, ($C_{36}H_{34}N_6O_6$ M + 2H requires 324.1343).

**2,6- AQ-Gly-Ala-$NH_3^+$ $TFA^-$**



Method A.

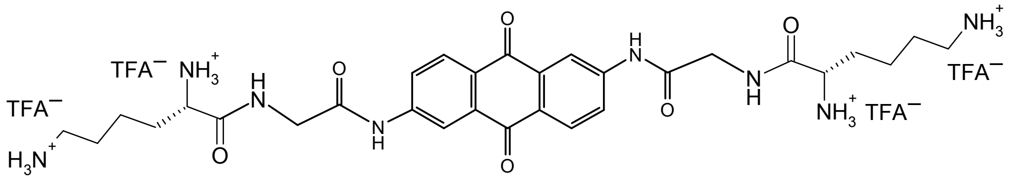
Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Ala-OSu (172 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (69 mg, overall yield 96 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.76 (s, 2H), 8.79 (t, J=5.8 Hz, 2H), 8.44 (d, J=2.3 Hz, 2H), 8.16 (d, J=8.6 Hz, 2H), 8.08 (bs, 6H), 8.01 (dd, J=8.6 and 2.3 Hz, 2H), 1.39 (d, J=6.7 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.24, 170.13, 168.12, 144.28, 134.33, 128.53, 128.10, 123.43, 115.80, 48.08, 42.78, 17.15.

HRMS, *m*/*z*: 248.1061, ($C_{24}H_{26}N_6O_6$ M + 2H requires 248.1030).

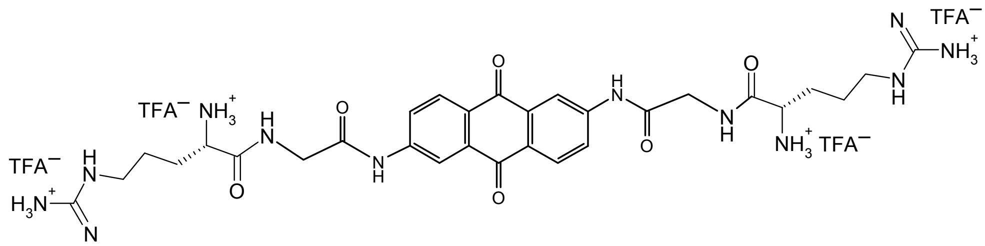
**2,6-AQ-Gly-Lys-$NH_3^+$ TFA$^-$**



Method A.

Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Lys(Boc)-OSu (266 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (94 mg, overall yield 88 %).
$^1$N-NMR (DMSO-$d_6$): δ 10.82 (s, 2H), 8.90 (t, J=5.6 Hz, 2H), 8.44 (d, J=2.3 Hz, 2H), 8.19 (bs, 6H), 8.17 (d, J=8.6 Hz, 2H), 8.02 (dd, J=8.6 and 2.1 Hz, 2H), 7.78 (bs, 6H), 4.16-3.99 (m, 4H), 3.90-3.79 (m, 2H), 2.82-2.69 (m, 4H), 1.82-1.69 (m, 4H), 1.60-1.47 (m, 4H), 1.46-1.32 (m, 4H).
$^{13}$C-NMR (DMSO-$d_6$): δ 181.29, 169.14, 144.31, 134.37, 128.57, 128.15, 123.49, 115.58, 51.90, 42.79, 38.45, 30.44, 26.44, 21.00.
HRMS, *m*/*z*: 315.1622, ($C_{30}H_{40}N_8O_6$ M + 2H requires 315.1608).

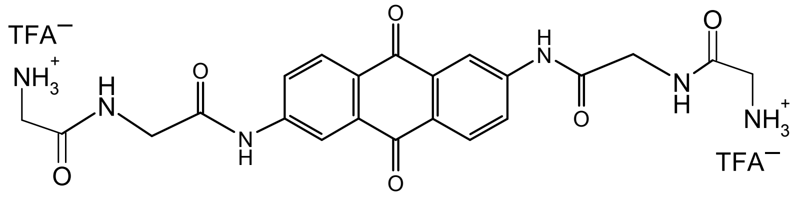
**2,6-AQ-Gly-Arg-$NH_3^+$ TFA$^-$**



Method C.

Reagents used: 2,6-AQ-Gly TFA (58 mg, 0.10 mmol), Fmoc-Arg(Mtr)-OH (152 mg, 0.25 mmol). The product was obtained as slightly yellow powder (88 mg, overall yield 79 %).
$^1$N-NMR (DMSO-$d_6$): δ 10.84 (s, 2H), 8.97 (bs, 2H), 8.46 (s, 2H), 8.17 (d, J=8.2 Hz, 2H), 8.03 (d, J=8.9 Hz, 2H), 7.73 (bs, 4H), 7.21 (bs, 6H), 4.15-3.99 (m, 4H), 3.94-3.86 (m, 2H), 3.21-3.03 (m, 4H), 1.86-1.71 (m, 4H), 1.65-1.49 (m, 4H),
$^{13}$C-NMR (DMSO-$d_6$): δ 181.31, 168.00, 168.03, 156.63, 144.25, 134.38, 128.64, 128.15, 123.47, 115.79, 51.78, 42.77, 28.30, 23.96.
HRMS, *m*/*z*: 333.1786, ($C_{30}H_{40}N_{12}O_6$ M + 2H requires 333.1670).

**2,6-AQ-Gly-Gly-$NH_3^+$ $TFA^-$**



Method A.

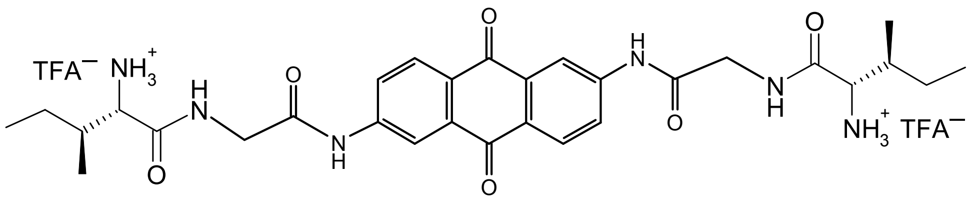
Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Gly-OSu (164 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (64 mg, overall yield 92 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.77 (s, 2H), 8.82 (t, J=5.7 Hz, 2H), 8.47 (d, J= 2.3 Hz, 2H), 8.19 (d, J=8.6 Hz, 2H), 8.07 (bs, 6H), 8.05 (dd, J=8.4 and 2.1 Hz, 2H), 4.09 (d, J=5.7 Hz, 4H), 3.68 (s, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.23, 168.17, 166.59, 144.23, 134.31, 128.52, 128.13, 123.48, 115.88, 42.87, 40.06.

HRMS, *m*/*z*: 353.1298, ($C_{18}H_{16}N_4O_4$ M + 1H requires 353.1244).

**2,6- AQ-Gly-Ile-$NH_3^+$ $TFA^-$**



Method A.

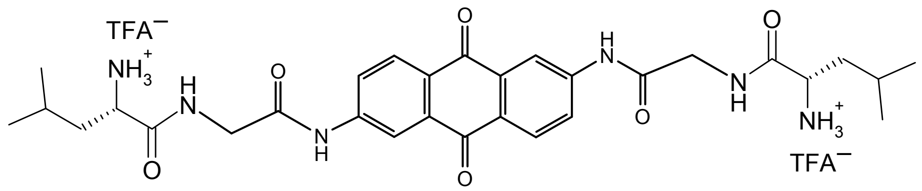
Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Ile-OSu (196 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (76 mg, overall yield 94 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.68 (s, 2H), 8.70 (t, J=5.7 Hz, 2H), 8.31 (d, J=2.1 Hz, 2H), 8.04 (d, J=8.4, 2H), 8.02 (bs, 6H), 7.90 (dd, J=8.6 and 2.1 Hz, 2H), 4.03 (dd, J=16.8 and 5.7 Hz, 2H), 3.87 (dd, J=16.8 and 5.3 Hz, 2H), 3.6 (bs, 2H), 1.78-1.64 (m, 2H), 1.48-1.33 (m, 2H), 1.13-0.99 (m, 2H), 0.83 (d, J=6.9 Hz, 6H), 0.75 (t, J=7.2 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.25, 168.36, 168.06, 144.31, 134.34, 128.56, 128.09, 123.43, 115.78, 56.48, 42.80, 36.18, 24.02, 14.35, 11.15.

HRMS, *m*/*z*: 290.1484, ($C_{30}H_{38}N_6O_6$ M + 2H requires 290.1499).

**2,6-AQ-Gly-Leu-$NH_3^+$ $TFA^-$**



Method A.

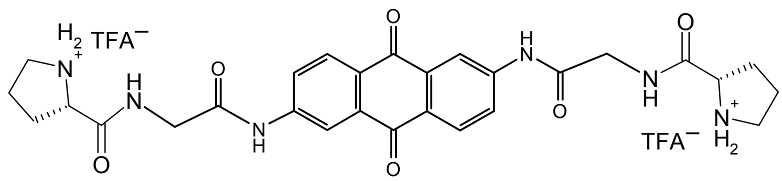
Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Leu-OSu (196 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (74 mg, overall yield 92 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.80 (s, 2H), 8.95 (t, J=5.6 Hz, 2H), 8.47 (d, J=2.1 Hz, 2H), 8.19 (d, J=8.6 Hz, 2H), 8.17 (bs, 6H), 8.05 (dd, J=8.8 and 2.1 Hz, 2H), 4.18-3.98 (m, 4H), 3.92-3.81 (m, 2H), 1.81-1.52 (m, 6H), 0.97-0.89 (m, 12H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.25, 169.61, 168.03, 144.28, 134.37, 128.57, 128.12, 123.45, 115.80, 50.77, 42.79, 30.61, 23.45, 22.56, 21.86.

HRMS, *m*/*z*: 290.1512, ($C_{30}H_{38}N_6O_6$ M + 2H requires 290.1499).

**2,6-AQ-Gly-Pro-$NH_3^+$ $TFA^-$**



Method A.

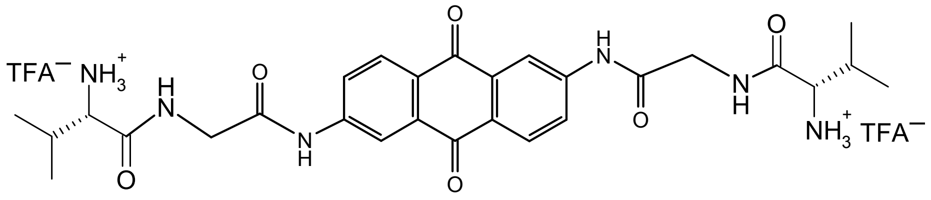
Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Pro-OSu (187 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (74 mg, overall yield 95 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.80 (s, 2H), 9.52-9.15 (bs, 4H), 8.94 (t, J=5.6 Hz, 2H), 8.52 (d, J=1.9 Hz, 2H), 8.19 (d, J=8.6 Hz, 2H), 8.04 (dd, J=8.6 and 1.9 Hz, 2H), 4.27 (t, J=5.6 Hz, 2H), 4.17-4.01 (m, 4H), 3.28-3.16 (m, 4H), 2.42-3.25 (m, 2H), 2.01-1.85 (m, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.25, 168.87, 168.01, 161.99, 144.27, 134.34, 128.56, 128.13, 123.47, 117.36, 115.82, 58.92, 45.64, 42.94, 29.52, 23.48.

HRMS, *m*/*z*: 274.1185, ($C_{28}H_{30}N_6O_6$ M + 2H requires 274.1186).

**2,6-AQ-Gly-Val-$NH_3^+$ $TFA^-$**



Method A.

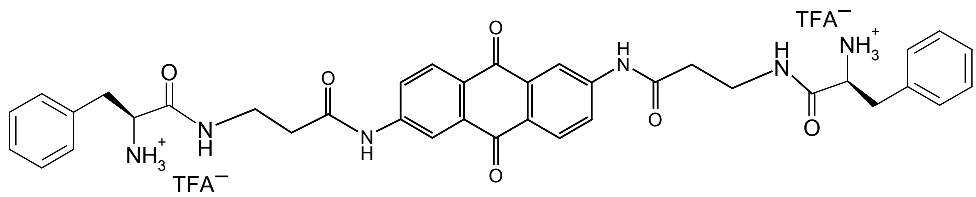
Reagents used: 2,6-AQ-Gly TFA (58 mg, 0,10 mmol), Boc-Val-OSu (188 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (69 mg, overall yield 89 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.81 (s, 2H), 8.84 (t, J=5.8 Hz, 2H), 8.46 (d, J=2.3 Hz, 2H, 8.19 (d, J=8.6 Hz, 2H), 8.11 (bs, 6H), 8.05 (dd, J=8.6 and 2.7 Hz, 2H), 4.23-4.13 (d, J=5.8 Hz, 2H), 4.07-3.96 (m, 2H), 3.70 (d, 5.7 Hz, 2H), 2.19-2.07 (m, 2H), 1.03-0.97 (m, 12H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.27, 168.41, 168.07, 161.05, 144.29, 134.35, 128.59, 128.11, 123.44, 117.32, 115.77, 57.37, 42.75, 29.78, 18.19, 17.65.

HRMS, *m*/*z*: 276.1354, ($C_{28}H_{34}N_6O_6$ M + 2H requires 276.1343).

**2,6-AQ-βAla-Phe-$NH_3^+$ $TFA^-$**



Method B.

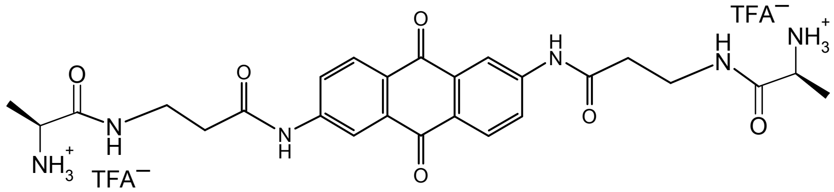
Reagents used: 2,6-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Phe-OH (66 mg, 0.25 mmol). The product was obtained as slightly yellow powder (85 mg, overall yield 95 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.65 (s, 2H, disappears with $D_2O$), 8.53-8.47 (m, 2H, disappears with $D_2O$), 8.48 (d, J=2.3 Hz, 2H), 8.14 (d, J=8.8 Hz, 2H), 8.13 (bs, 6H, disappears with $D_2O$), 7.94 (dd, J=8.6 and 2.3, 2H), 7.32-7.15 (m, 10H), 3.96 (t, J=7.0 Hz, 2H), 3.51-3.40 (m, 2H), 3.33-3.21 (m, 2H), 3.03-2.90 (m, 4H), 3.62-2.50 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.91, 170.80, 168.27, 161.56, 144.84, 134.97, 134.68, 129.82, 129.06, 128.92, 128.44, 127.70, 123.95, 116.33, 53.80, 37.36, 36.17, 35.09.

HRMS, *m*/*z*: 338.1492, ($C_{38}H_{38}N_6O_6$ M + 2H requires 338.1499).

**2,6-AQ-βAla-Ala-$NH_3^+$ TFA$^-$**



Method B.

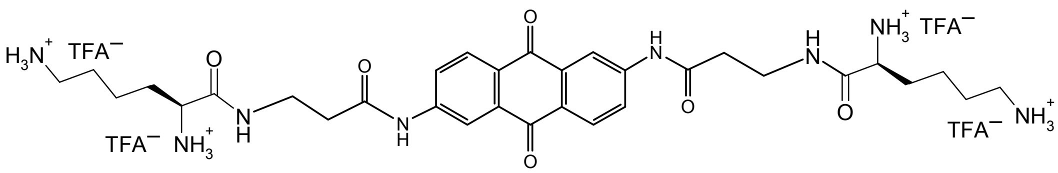
Reagents used: 2,6-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Ala-OH (45 mg, 0.25 mmol). The product was obtained as slightly yellow powder (68 mg, overall yield 90 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.67 (s, 2H, disappears with $D_2O$), 8.51 (t, J= 5.5 Hz, 2H, disappears with $D_2O$), 8.41 (d, J=1.9 Hz, 2H), 8.09 (d, J=8.6 Hz, 2H), 8.06 (bs, 6H, disappears with $D_2O$), 7.85 (dd, J=8.6 and 2.0 Hz, 2H), 3.80-3.69 (m, 2H), 3.55-3.43 (m, 2H), 3.42-3.31 (m, 2H), 2.59 (t, J=5.5 Hz, 4H), 1.29 (d, J=.1 Hz).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.50, 171.73, 170.42, 145.01, 134.98, 129.43, 128.93, 124.69, 116.93, 49.08, 36.78, 35.97, 17.75.

HRMS, *m*/*z*: 262.1181, ($C_{26}H_{30}N_6O_6$ M + 2H requires 262.1186).

**2,6-AQ-βAla-Lys-$NH_3^+$ TFA$^-$**



Method A.

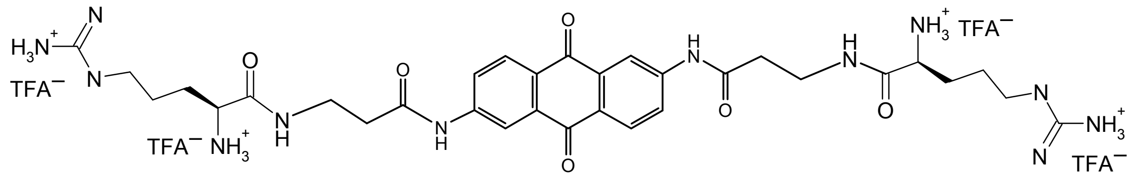
Reagents used: 2,6-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Lys(Boc)-OSu (266 mg, 0.60 mmol). The product was obtained as slightly yellow powder (94 mg, overall yield 86 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.72 (s, 2 H, disappears with $D_2O$), 8.63 (t, J= 5.0 Hz, 2H), 8.50 (d, J=2.1 Hz, 2H), 8.18 (d, J=8.8 Hz, 2H), 8.14 (bs, 6H, disappears with $D_2O$), 8.04 (dd, J=8.6 and 2.1 Hz, 2H), 7.74 (bs, 6H, disappears with $D_2O$), 3.76-3.65 (m, 4H), 3.56-3.39 (m, 4H), 2.77.2.61 (m, 8H), 1.73-1.62 (m, 4H), 1.55-1.43 (m, 4H), 1.36-1.23 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.38, 170.30, 168.43, 144.59, 134.37, 128.55, 128.52, 128.02, 115.81, 51.97, 38.44, 35.99, 34.93, 30.47, 26.52, 21.11.

HRMS, *m*/*z*: 319.1793, ($C_{32}H_{44}N_8O_6$ M + 2H requires 319.1765).

**2,6-AQ-βAla-Arg-$NH_3^+$ $TFA^-$**



Method C.

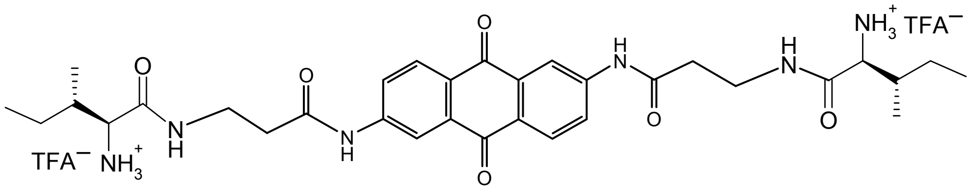
Reagents used: 2,6-AQ-βAla TFA (61 mg, 0.10 mmol), Fmoc-Arg(Mtr)-OH (152 mg, 0.25 mmol). The product was obtained as slightly yellow powder (93 mg, overall yield 81 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.78 (s, 2H, disappears with $D_2O$), 8.67 (bs, 2H, disappears with $D_2O$), 8.46 (s, 2H), 8.14 (d, J=8.4 Hz, 2H), 7.91 (d, J=8.4 Hz, 2H), 7.76 (bs, 2H, disappears with $D_2O$), 7.39 (bs, 2H, disappears with $D_2O$), 7.20 (bs, 6H, disappears with $D_2O$), 3.75-3.63 (m, 2H), 3.51-3.33 (m, 4H), 3.08-2.95 (m, 4H), 2.68-2.57 (m, 4H), 1.73-1.59 (m, 4H), 1.51-1.39 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.46, 171.36, 157.69, 135.44, 129.63, 129.59, 129.11, 124.54, 116.93, 52.97, 37.09, 34.39, 29.33, 25.11.

HRMS, *m*/*z*: 347.1916, ($C_{32}H_{44}N_{12}O_6$ M + 2H requires 347.6840).

**2,6-AQ-βAla-Ile-$NH_3^+$ $TFA^-$**



Method A.

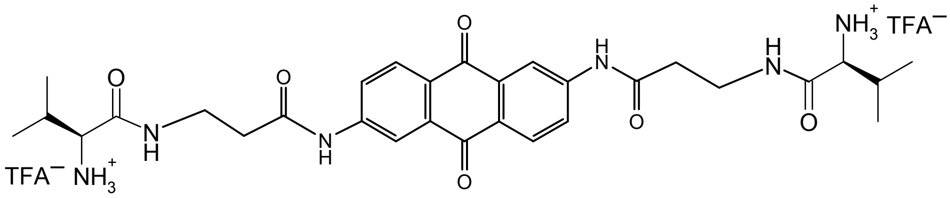
Reagents used: 2,6-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Ile-OSu (196 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (79 mg, overall yield 94 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.60 (s, 2H), 8.51 (bs, 2H), 8.31 (d, J=2.1 Hz, 2H), 8.04 (d, J=8.6, 2H), 7.78 (m, 6H), 7.90 (dd, J=8.6 and 2.1 Hz, 2H), 3.58 (m, 4H), 2.64 (m, 4H), 1.73 (m, 2H), 1.43 (m, 2H), 1.06 (m, 4H), 0.86 (d, J=7.4 Hz, 6H), 0.76 (t, J=7.4 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.25, 168.36, 168.06, 144.31, 134.34, 128.56, 128.09, 123.43, 115.78, 56.48, 42.80, 36.18, 24.02, 14.35, 11.15.

HRMS, *m*/*z*: 304.3743, ($C_{32}H_{44}N_6O_6$ M + 2H requires 304.3720).

**2,6-AQ-βAla-Val-$NH_3^+$ $TFA^-$**




Method A.

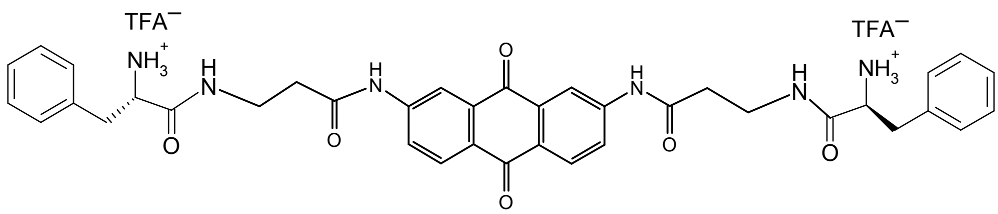
Reagents used: 2,6-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Val-OSu (188 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (53 mg, overall yield 66 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.56 (s, 2H), 8.50 (t, J=5.8 Hz, 2H), 8.46 (d, J=2.3 Hz, 2H), 8.19 (d, J=8.6 Hz, 2H), 8.11 (bs, 6H), 8.05 (dd, J=8.6 and 2.3 Hz, 2H), 3.72 (m, 2H), 3.40 (m, 4H), 3.70 (d, 5.8 Hz, 4H), 1.90 (m, 2H), 0.98-0.95 (m, 12H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.27, 168.41, 168.07, 144.29, 134.35, 128.59, 128.11, 123.44, 115.77, 57.37, 42.75, 29.78, 18.19, 17.65.

HRMS, *m*/*z*: 290.3467, ($C_{30}H_{40}N_6O_6$ M + 2H requires 290.3450).

**2,7- AQ-βAla-Phe-$NH_3^+$ $TFA^-$**




Method B.

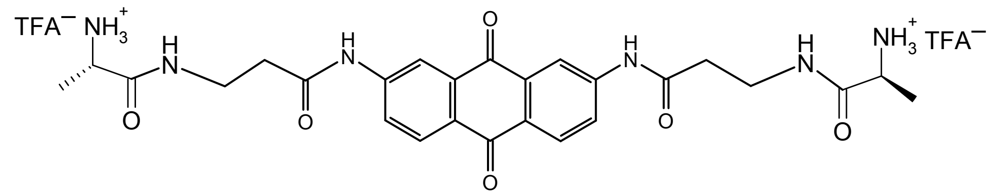
Reagents used: 2,7-AQ-βAla- TFA (61 mg, 0.10 mmol), Boc-Phe-OH (66 mg, 0.25 mmol). The product was obtained as slightly yellow powder (80 mg, overall yield 89 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.63 (s, 2H), 8.54 (d, J=2.1 Hz, 2H), 8.52 (t, J=5.9 Hz, 2H), 8.18 (d, J=8.6 Hz, 2H), 8.16 (bs, 6H), 8.02 (dd, J=8.6 and 2.1 Hz, 2 H), 7.32-7.16 (m, 10 H), 4.00-3.91 (m, 2H), 3.54-3.39 8m, 4H), 3.05-2.88 (m, 4H), 2.64-2.51 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182. 49, 180.34, 170.12, 167.89, 144.25, 134.81, 134.17, 129.33, 128.41, 128.29, 127.98, 127.01, 123,.73, 115.85, 53.36, 37.03, 35.78, 34.63.

HRMS, *m*/*z*: 338.3857, ($C_{38}H_{38}N_6O_6$ M + 2H requires 338.3896).

**2,7-AQ-βAla-Ala-$NH_3^+$ $TFA^-$**



Method B.

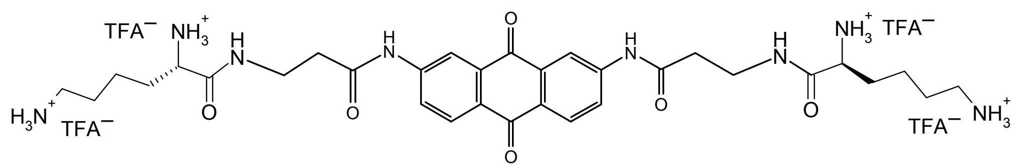
Reagents used: 2,7-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Ala-OH (45 mg, 0.25 mmol). The product was obtained as slightly yellow powder (71 mg, overall yield 94 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.67 (s, 2H, disappears with $D_2O$), 8.43, (bs, 2H), 8.32 (s, 2H), 8.05 (bs, 6H, disappears with $D_2O$), 7.99 (d, J=8.4 HZ, 2H), 7.81 (d, J=9.0 Hz, 2H), 3.81-3.70 m, 2H), 3.56-3.28 (m, 4 H), 2.64-2.51 (m, 4H), 1.30 (d, J=6.9 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.45, 180.31, 170.20, 169.44, 144.25, 134.16, 128.27, 127.98, 123.72, 115.83, 48.07, 36.05, 34.91, 17.17.

HRMS, *m*/*z*: 262.2898, ($C_{26}H_{30}N_6O_6$ M + 2H requires 262.2908).

**2,7-AQ-βAla-Lys-$NH_3^+$ $TFA^-$**



Method A.

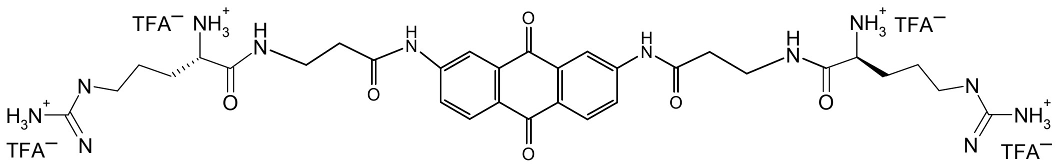
Reagents used: 2,7-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Lys(Boc)-OSu (266 mg, 0.60 mmol). The product was obtained as slightly yellow powder (96 mg, overall yield 88 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.72 (s, 2H, disappears with $D_2O$), 8.50 (t, J=5.1 Hz, 2H, disappears with $D_2O$), 8.35 8s, 2H), 8.05 (d, J=8.2 Hz, 2 H), 7.82 (d, J=8.5 Hz, 2H), 8.16 (bs, 6 H, disappears with $D_2O$), 7.76 (bs, 6H, disappears with $D_2O$), 3.68 (t, J=6.5 Hz, sH), 3.55-3.32 (m, 4H), 2.70 8t, J=7.4 Hz, 4H), 2.64-2.53 (m, 4H), 1.76-1.58 (m, 4H), 1.54-1.39 (m, 4H), 1.32-1.17 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.51, 180.37, 170.27, 168.43, 144.25, 134.21, 128.32, 128.04, 123.75, 115.85, 51.91, 38.36, 36.00, 34.94, 30.44, 26.47, 21.08.

HRMS, *m*/*z*: 320.3968, ($C_{32}H_{44}N_8O_6$ M + 2H requires 320.3947).

**2,7-AQ-βAla-Arg-$NH_3^+$ $TFA^-$**




Method C.

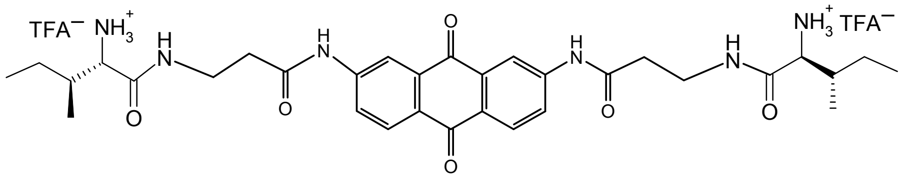
Reagents used: 2,7-AQ-βAla TFA (61 mg, 0.10 mmol), Fmoc-Arg(Mtr)-OH (152 mg, 0.25 mmol). The product was obtained as slightly yellow powder (94 mg, overall yield 82 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.73 (s, 2H, disappears with $D_2O$), 8.58 (bs, 2H, disappears with $D_2O$), 8.46 (s, 2H), 8.14 (d, J=8.4 Hz, 2H), 7.91 (d, J=8.4 Hz, 2H), 7.76 (bs, 2H, disappears with $D_2O$), 7.39 (bs, 2H, disappears with $D_2O$), 7.20 (bs, 6H, disappears with $D_2O$), 3.75-3.63 (m, 2H), 3.51-3.33 (m, 4H), 3.09-2.96 (m, 4H), 2.67-2.56 (m, 4H), 1.73-1.59 (m, 4H), 1.51-1.39 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.46, 180.36, 156.69, 135.44, 129.63, 129.59, 129.11, 125.54, 116.93, 55.01, 37.09, 34.39, 29.33, 25.11.

HRMS, *m*/*z*: 348.3316, ($C_{32}H_{44}N_{12}O_6$ M + 2H requires 348.4081).

**2,7-AQ-βAla-Ile-$NH_3^+$ $TFA^-$**




Method A.

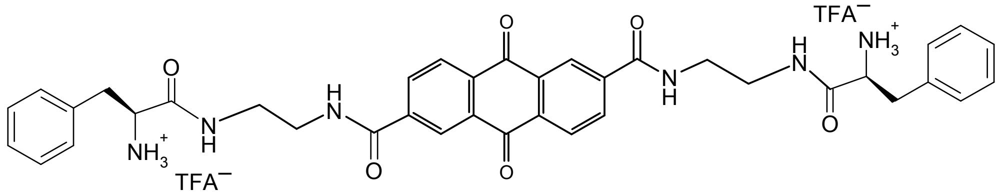
Reagents used: 2,7-AQ-βAla TFA (61 mg, 0.10 mmol), Boc-Ile-OSu (196 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (77 mg, overall yield 93 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.60 (s, 2H), 8.51 (bs, 2H), 8.31 (d, J=2.1 Hz, 2H), 8.04 (d, J=8.6, 2H), 7.78 (m, 6H), 7.90 (dd, J=8.6 and 2.1 Hz, 2H), 3.58 (m, 4H), 2.64 (m, 4H), 1.73 (m, 2H), 1.43 (m, 2H), 1.06 (m, 4H), 0.86 (d, J=7.4 Hz, 6H), 0.76 (t, J=7.4 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.25, 180.41, 168.06, 144.31, 134.34, 128.56, 128.09, 123.43, 115.78, 56.48, 42.80, 36.18, 24.02, 14.35, 11.15.

HRMS, *m*/*z*: 304.3367, ($C_{32}H_{44}N_6O_6$ M + 2H requires 304.3721).

**2,6-AQ-ED-Phe-$NH_3^+$ TFA$^-$**



Method B.

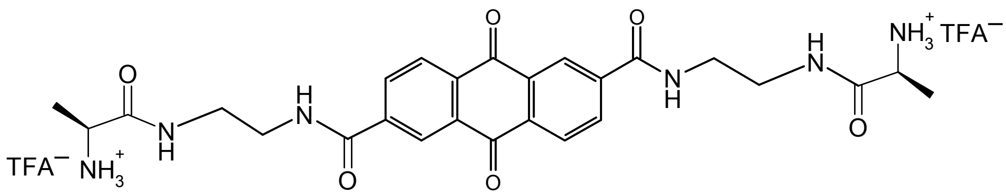
Reagents used: 2,6-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Phe-OH (66 mg, 0.25 mmol). The product was obtained as slightly yellow powder (82 mg, overall yield 91 %).

$^1$N-NMR (DMSO-$d_6$): δ 8.99 (s, 2H), 8.66 (d, J=2.1 Hz, 2H), 8.61 (t, J=5.7 Hz, 2H), 8.37-8.31 (m, 4H), 8.20 (bs, 6H), 7.35-7.23 (m, 10H), 3.95 (t, J=7.1 Hz, 2H), 3.41-3.16 (m, 8H), 3.11-2.91 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 186.37, 182.19, 165.60, 161.42, 139.61, 139.57, 135.04, 135.00, 133.44, 133.33, 129.77, 129.00, 127.69, 126.05, 117.60, 53.94, 38.50, 38.46, 37.16.

HRMS, *m*/*z*: 338.1501, ($C_{38}H_{38}N_6O_6$ M + 2H requires 338.1499).

**2,6-AQ-ED-Ala-$NH_3^+$ TFA$^-$**



Method B.

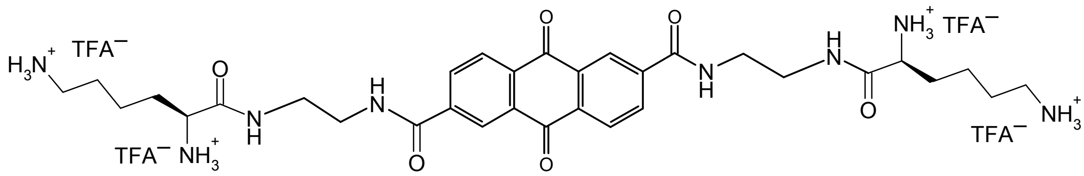
Reagents used: 2,6-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Ala-OH (45 mg, 0.25 mmol). The product was obtained as slightly yellow powder (67 mg, overall yield 89 %).

$^1$N-NMR (DMSO-$d_6$): δ 9.04 (t, J=5.3 Hz, 2H), 8.67 (s, 2H), 8.53 (t, J=5.9 Hz, 2H, disappears with $D_2O$), 8.35 (bs, 2H), 8.08 (bs, 6H, disappears with $D_2O$), 3.75 (q, J=7.1 Hz, 2H), 3.74-3.36 (m, 6H), 3.32-3.23 (m, 2H), 1.32 (d, J=7.1 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.74, 170.49, 166.74, 140.06, 135.39, 133.83, 133.76, 128.30, 126.52, 49.11, 17.58.

HRMS, *m*/*z*: 262.1198, ($C_{26}H_{30}N_6O_6$ M + 2H requires 262.1186).

**2,6-AQ-ED-Lys-$NH_3^+$ TFA$^-$**



Method A.

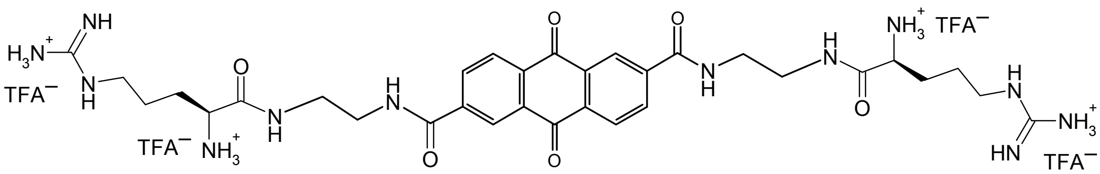
Reagents used: 2,6-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Lys(Boc)-OSu (266 mg, 0.60 mmol). The product was obtained as slightly yellow powder (98 mg, overall yield 90 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 9.07 (s, 2H, disappears with $D_2O$), 8.53 (d, J=1.3 Hz, 2H), 8.67 (bs, 2H, disappears with $D_2O$), 8.27 (d, J=8.2 Hz, 2H), 8.20 (dd, J= 8.1 and 1.5 Hz, 2 H), 7.98 (bs, 12 H, disappears with $D_2O$), 3.69 (t, J=6.5 Hz, 2H), 3.53-3.23 (m, 8 H), 2.78-2.65 (m, 4H), 1.78-1.58 (m, 4H), 1.55-1.40 (m, 4H), 1.33-1.16 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.80, 168.61, 164.82, 139.28, 134.68, 133.15, 132.89, 127.18, 125.55, 52.11, 38.37, 38.23, 30.32, 26.48, 21.15.

HRMS, *m*/*z*: 319.1842, ($C_{32}H_{44}N_8O_6$ M + 2H requires 319.1765).

**2,6-AQ-ED-Arg-$NH_3^+$ TFA$^-$**



Method C.

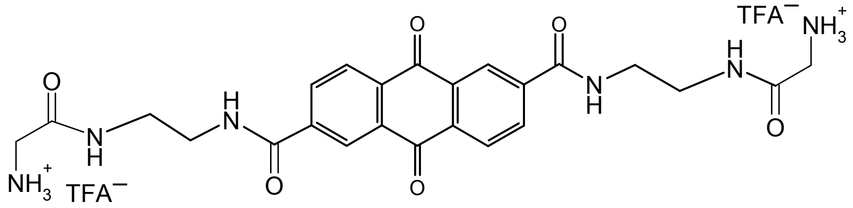
Reagents used: 2,6-AQ-ED TFA (61 mg, 0.10 mmol), Fmoc-Arg(Mtr)-OH (152 mg, 0.25 mmol). The product was obtained as slightly yellow powder (96 mg, overall yield 84 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 9.09, (t, J=5.5 Hz, 2H, disappears with $D_2O$), 8.67 (d, J=1.5 Hz, 2H), 8.66 (bs, 2H, disappears with $D_2O$), 8.38 (dd, J=8.1 and 1.5, 2H), 8.33 (bs, 2H, disappears with $D_2O$), 8.32 (d, J=8.1, 2H), 7.17 (bs, 6H, disappears with $D_2O$),3.71 (t, J=6.2 Hz, 2H), 3.51-3.20 (m, 8H), 3.00 (t, J=7.0 Hz, 4H), 1.76-1.61 (m, 4H), 1.52-1.38 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.74, 168.53, 164.80, 156.69, 139.17, 134.59, 133.06, 132.87, 127.14, 125.60, 51.89, 38.21, 27.99, 23.83.

HRMS, *m*/*z*: 347.1926, ($C_{32}H_{44}N_{12}O_6$ M + 2H requires 347.6840).

**2,6-AQ-ED-Gly-$NH_3^+$ TFA$^-$**



Method B.

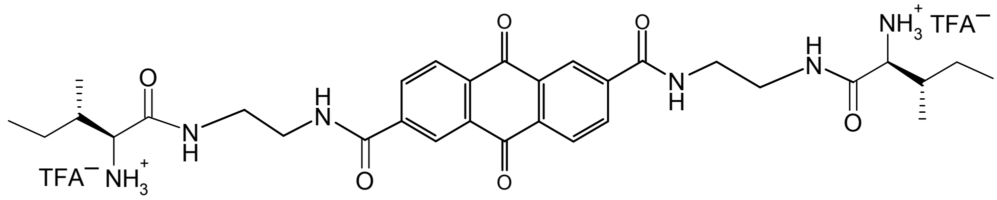
Reagents used: 2,6-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Gly-OSu (164 mg, 0.60 mmol). The product was obtained as slightly yellow powder (64 mg, overall yield 89 %).

$^1$N-NMR (DMSO-$d_6$): δ 8.98 (bt, 2H), 8.53 (t, J=5.9 Hz, 2H, disappears with $D_2O$), 8.35 (s, 2H), 8.08 (bs, 6H, disappears with $D_2O$), 7.94 (d, J=7.1, 2H), 3.75 (t, J=7.1 Hz, 2H), 3.74-3.52 (d, J=5.9 Hz , 4H), 3.36-3.30 (m, 4H), 3.18-3.15 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.74, 170.49, 166.74, 140.06, 135.39, 133.83, 133.76, 128.30, 126.52, 49.11, 17.58.

HRMS, *m*/*z*: 248.2598, ($C_{24}H_{26}N_6O_6$ M + 2H requires 248.2637).

**2,6-AQ-ED-Ile-$NH_3^+$ TFA$^-$**



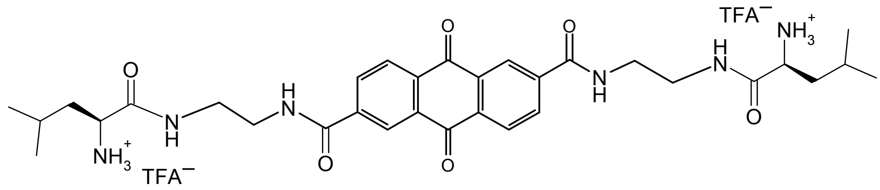
Reagents used: 2,6-AQ-ED TFA (52 mg, 0.086 mmol), Boc-Ile-OSu (281 mg, 0.859 mmol). The product was obtained as a slightly yellow powder (51 mg, overall yield 71%).

$^1$N-NMR (DMSO-$d_6$): δ 10.60 (s, 2H), 8.51 (bs, 2H), 8.31 (d, J=2.1 Hz, 2H), 8.04 (d, J=8.6, 2H), 7.78 (m, 6H), 7.90 (dd, J=8.6 and 2.1 Hz, 2H), 3.45 (m, 4H), 3.24 (m, 4H), 1.43 (m, 2H), 1.06 (m, 4H), 0.86 (d, J=7.4 Hz, 6H), 0.76 (t, J=7.4 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.25, 168.36, 168.06, 144.31, 134.34, 128.56, 128.09, 123.43, 115.78, 56.48, 42.80, 36.18, 24.02, 14.35, 11.15.

HRMS, *m*/*z*: 304.3659, ($C_{32}H_{44}N_6O_6$ M + 2H requires 304.3721).

**2,6-AQ-ED-Leu-$NH_3^+$ $TFA^-$**



Method A.

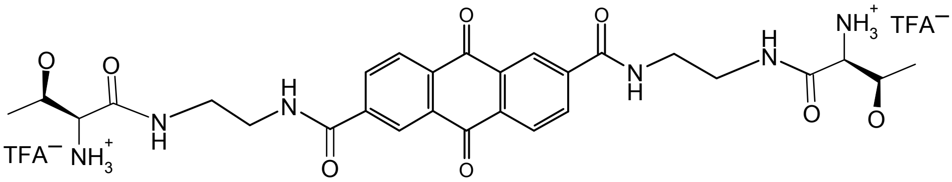
Reagents used: 2,6-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Leu-OSu (196 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (73 mg, overall yield 87 %).

$^1$N-NMR (DMSO-$d_6$): δ 10.82 (s, 2H), 8.91 (t, J=5.5 Hz, 2H), 8.46 (d, J=2.1 Hz, 2H), 8.19 (d, J=8.6 Hz, 2H), 8.17 (bs, 6H), 8.05 (dd, J=8.8 and 2.1 Hz, 2H), 4.14-3.96 (m, 4H), 3.91-3.83 (m, 2H), 1.72-1.51 (m, 4H), 1.39 (m, 2H), 0.81-0.85 (m, 12H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.25, 169.61, 168.03, 144.28, 134.37, 132.27, 128.57, 128.12, 123.45, 115.80, 50.77, 42.79, 30.61, 23.45, 22.56, 21.86.

HRMS, *m*/*z*: 304.3805, ($C_{32}H_{44}N_6O_6$ M + 2H requires 304.3720).

**2,6-AQ-ED-Thr-$NH_3^+$ $TFA^-$**



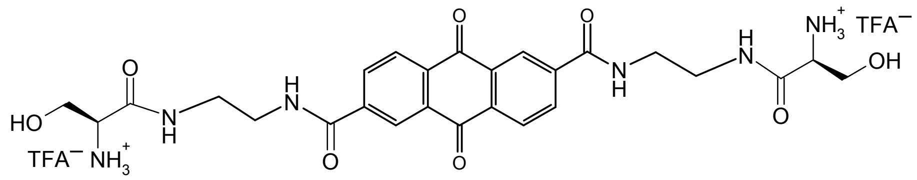
Method A.

Reagents used: 2,6-AQ-ED TFA (52 mg, 0.086 mmol), Boc-Thr(O-Bzl)-OSu (363 mg, 0.859 mmol). The product was obtained as a slightly yellow powder (53 mg, overall yield 62%).

$^1$N-NMR (DMSO-$d_6$): δ 10.79 (s, 2H), 8.90 (t, J=5.7 Hz, 2H), 8.72 (d, J=2.2 Hz, 2H), 8.28 (d, J=8.9 Hz, 2H), 8.22 (bs, 6H), 8.15 (dd, J=8.9 and 2.2 Hz, 2H), 3.85 (m, 1H), 3.56-3.62 (m, 4H), 3.13-3.08 (m, 4H), 3.39-3.28 (m, 4H), 1.72-1.51 (m, 4H), 1.39 (m, 2H), 1.10 (d, J=6.1 Hz, 6H).

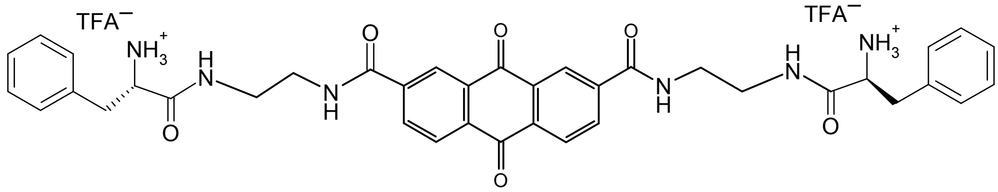
$^{13}$C-NMR (DMSO-$d_6$): δ 181.35, 168.98, 166.67, 145.27, 135.02, 131.99, 128.23, 127.32, 124.52, 117.01, 51.58, 43.75, 33.58, 25.77, 23.86, 23.02.
HRMS, *m*/*z*: 292.3255, ($C_{28}H_{34}N_6O_8$ M + 2H requires 292.3172).

**2,6-AQ-ED-Ser-$NH_3^+$ TFA$^-$**




Method A.
Reagents used: 2,6-AQ-ED TFA (52 mg, 0.086 mmol), Boc-Ser(O-Bzl)-OSu (336 mg, 0.859 mmol). The product was obtained as slightly yellow powder (68 mg, overall yield 82 %).
$^{1}$N-NMR (DMSO-$d_6$): δ 10.81 (s, 2H), 8.95 (t, J=5.5 Hz, 2H), 8.65 (d, J=2.1 Hz, 2H), 8.30 (d, J=8.7 Hz, 2H), 8.17 (bs, 6H), 8.11 (dd, J=8.7 and 2.1 Hz, 2H), 4.14-3.96 (m, 4H), 3.91-3.83 (m, 4H), 1.72-1.51 (m, 4H), 1.39 (m, 2H), 1.10 (d, J=6.1 Hz, 6H).
$^{13}$C-NMR (DMSO-$d_6$): δ 181.44, 169.66, 168.03, 144.28, 134.37, 132.31, 128.59, 127.32, 124.56, 115.77, 50.78, 42.79, 31.63, 23.45, 23.57, 22.76.
HRMS, *m*/*z*: 278.3033, ($C_{28}H_{36}N_6O_8$ M + 2H requires 278.2902).

**2,7-AQ-ED-Phe-$NH_3^+$ TFA$^-$**

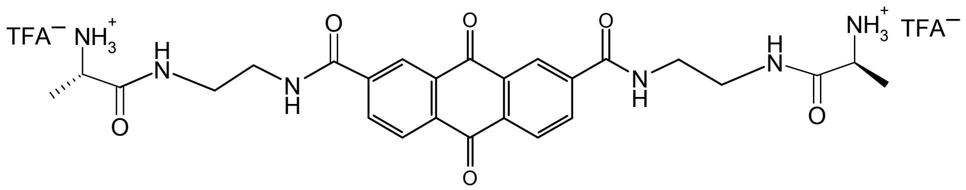



Method B.
Reagents used: 2,7-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Phe-OH (66 mg, 0.25 mmol). The product was obtained as slightly yellow powder (84 mg, overall yield 94 %).
$^{1}$N-NMR (DMSO-$d_6$): δ 8.99 (t, J=4.8 Hz, 2H), 8.67 (d, J=2.1 Hz, 2H), 8.60 (t, J=5.1 Hz, 2H), 8.37-8.29 (m, 4H), 8.20 (bs, 6H), 7.34-7.22 (m, 10H), 3.94 (t, J=6.9 Hz, 2H), 3.40-3.17 (m, 8H), 3.10-2.91 (m, 4H).

$^{13}C$-NMR (DMSO-$d_6$): δ 182.19, 182.17, 170.23, 169.01, 161,34, 139.54, 135.01, 134.99, 133.47, 133.30, 129.73, 128.95, 127.67, 127.65, 126.03, 123.87, 117.45, 38.42, 37.13, 31.00.

HRMS, *m*/*z*: 338.1474, ($C_{38}H_{38}N_6O_6$ M + 2H requires 338.1499).

**2,7-AQ-ED-Ala-$NH_3^+$ TFA$^-$**



Method B.

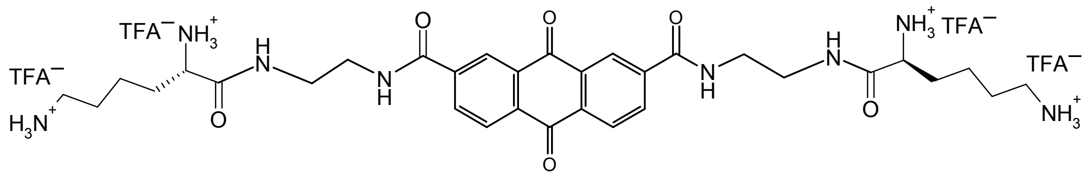
Reagents used: 2,7-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Ala-OH (45 mg, 0.25 mmol). The product was obtained as slightly yellow powder (70 mg, overall yield 93 %).

$^{1}N$-NMR (DMSO-$d_6$): δ 9.20-9.09 (m, 2H), 8.53 (d, J=1.5 Hz, 2H), 8.54 (t, J=5.5 Hz, 2H, disappears with $D_2O$), 8.37-8.33 (m, 2H, disappears with $D_2O$), 8.27 (d, J=8.0 Hz, 2H), 8.19 (dd, J=8.0 and 1.4 Hz, 2H), 8.09 (bs, 6H, disappears with $D_2O$), 3.81-3.71 (m, 2H), 3.49-3.20 (m, 8 H), 132 (d, J=7.1 Hz, 6H).

$^{13}C$-NMR (DMSO-$d_6$): δ 182.99, 182.88, 170.68, 167.12, 140.15, 135.51, 133.98, 133.85, 128.50, 126.70, 49.22, 17.65.

HRMS, *m*/*z*: 262.1191, ($C_{26}H_{30}N_6O_6$ M + 2H requires 262.1186).

**2,7-AQ-ED-Lys-$NH_3^+$ TFA$^-$**



Method A.

Reagents used: 2,7-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Lys(Boc)-OSu (266 mg, 0.60 mmol). The product was obtained as slightly yellow powder (96 mg, overall yield 88 %).

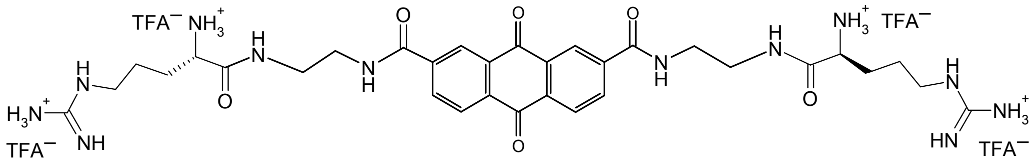
$^{1}N$-NMR (DMSO-$d_6$): δ 9.08 (t, 2H, J=5.1 Hz, 2H, disappears with $D_2O$), 8.72-8.65 (m, 2H, disappears with $D_2O$), 8.54 (d, J=1.3 Hz, 2H), 8.27 (d, J=8.2 Hz, 2H), 8.20 (dd, J=8.0 and

1.5 Hz, 2H), 8.00 (bs, 12 H, disappears with $D_2O$), 3.69 (t, J=6.5 Hz, 2H), 3.51-3.22 (m, 8H), 2.77-2.66 (m, 4H), 1.75-1.59 (m, 4H), 1.53-1.41 (m, 4H), 1.33-1.18 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.89, 181.88, 168.68, 164.98, 139.35, 134.71, 133.25, 132.96, 127.25, 125.68, 52.20, 38.1, 38.46, 30.38, 26.53, 21.21.

HRMS, *m*/*z*: 319.1781, ($C_{32}H_{44}N_8O_6$ M + 2H requires 319.1765).

**2,7-AQ-ED-Arg-$NH_3^+$ $TFA^-$**



Method C.

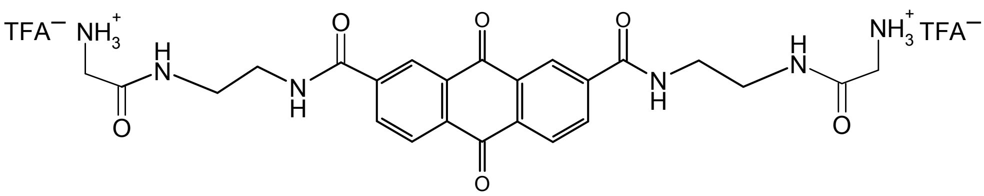
Reagents used: 2,7-AQ-ED TFA (61 mg, 0.10 mmol), Fmoc-Arg(Mtr)-OH (152 mg, 0.25 mmol). The product was obtained as slightly yellow powder (98 mg, overall yield 85 %).

$^1$N-NMR (DMSO-$d_6$): δ 9.19 (bs, 2H, disappears with $D_2O$), 8.79 (bs, 2H, disappears with $D_2O$), 8.67 (s, 2H), 8.49-8.23 (m, 4H, disappears with $D_2O$), 8.42-8.27 (m, 4H), 7.99-7.70 (m, 2H, disappears with $D_2O$), 7.42-7.6.93 (m, 6H, disappears with $D_2O$), 4.05 (s, 2H), 3.81-3.65 (m, 2H), 3.51-3.20 (m, 8H), 3.09-2.94 (m, 4H), 1.76-1.61 (m, 4H), 1.52-1.35 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.78, 168.58, 164.91, 156.66, 156.62, 139.21, 139.17, 134.60, 133.14, 127.16, 64.85, 51.93, 28.00, 23.79, 15.09.

HRMS, *m*/*z*: 347.1936, ($C_{32}H_{44}N_{12}O_6$ M + 2H requires 347.6840).

**2,7-AQ-ED-Gly-$NH_3^+$ $TFA^-$**



Method B.

Reagents used: 2,7-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Gly-OSu (164 mg, 0.60 mmol). The product was obtained as slightly yellow powder (64 mg, overall yield 89 %).

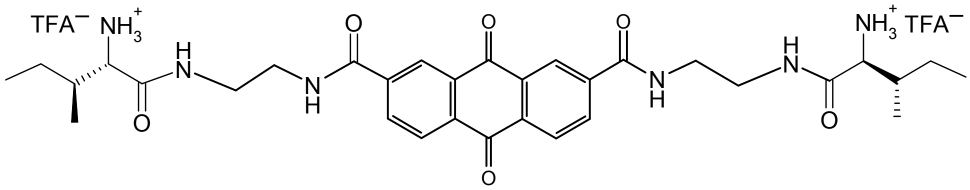
$^1$N-NMR (DMSO-$d_6$): δ 8.53 (d, J=1.5 Hz, 2H), 8.54 (t, J=5.5 Hz, 2H, disappears with $D_2O$), 8.37-8.33 (m, 2H, disappears with $D_2O$), 8.27 (d, J=8.0 Hz, 2H), 8.19 (dd, J=8.0 and 1.5

Hz, 2H), 8.09 (bs, 6H, disappears with $D_2O$), 3.75 (t, J=7.1 Hz, 2H), 3.74-3.52 (d, J=5.9 Hz , 4H), 3.36-3.30 (m, 4H), 3.18-3.15 (m, 4H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.74, 169.09, 166.74, 140.06, 135.39, 133.83, 133.76, 128.30, 126.52, 49.11, 17.58.

HRMS, *m*/*z*: 248.2598, ($C_{24}H_{26}N_6O_6$ M + 2H requires 248.2637).

**2,7-AQ-ED-Ile-$NH_3^+$ TFA$^-$**



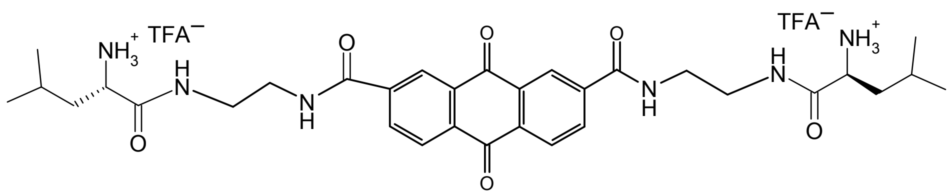
Reagents used: 2,7-AQ-ED TFA (52 mg, 0.086 mmol), Boc-Ile-OSu (281 mg, 0.859 mmol). The product was obtained as a slightly yellow powder (51 mg, overall yield 71%).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.53 (s, 2H), 8.54 (bs, 2H), 8.42 (d, J=2.1 Hz, 2H), 8.04 (d, J=8.6, 2H), 7.78 (m, 6H), 7.90 (dd, J=8.6 and 2.1 Hz, 2H), 3.49 (m, 4H), 3.34 (m, 4H), 1.41 (m, 2H), 1.06 (m, 4H), 0.95 (d, J=7.4 Hz, 6H), 0.82 (t, J=7.4 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 182.76, 170.69, 167.12, 140.15, 135.48, 133.98, 133.85, 128.50, 126.70, 115.78, 56.48, 42.80, 36.18, 24.02, 14.35, 11.21.

HRMS, *m*/*z*: 304.3659, ($C_{32}H_{44}N_6O_6$ M + 2H requires 304.3721).

**2,7-AQ-ED-Leu-$NH_3^+$ TFA$^-$**

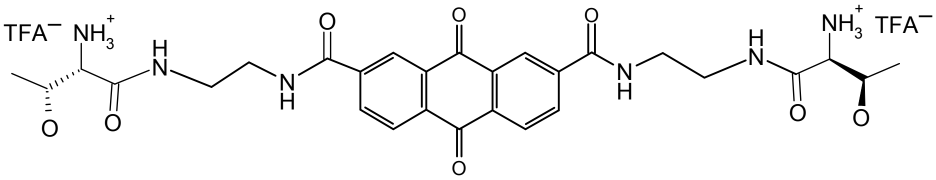


Method A.

Reagents used: 2,7-AQ-ED TFA (61 mg, 0.10 mmol), Boc-Leu-OSu (196 mg, 0.60 mmol). The product was obtained as a slightly yellow powder (73 mg, overall yield 87 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.82 (s, 2H), 8.91 (t, J=5.5 Hz, 2H), 8.46 (d, J=2.1 Hz, 2H), 8.19 (d, J=8.6 Hz, 2H), 8.17 (bs, 6H), 8.05 (dd, J=8.8 and 2.1 Hz, 2H), 4.14-3.96 (m, 4H), 3.91-3.83 (m, 2H), 1.72-1.51 (m, 4H), 1.39 (m, 2H), 0.81-0.85 (m, 12H).
$^{13}$C-NMR (DMSO-$d_6$): δ 181.25, 169.61, 168.03, 144.28, 134.37, 132.27, 128.57, 128.12, 123.45, 115.80, 50.77, 42.79, 30.61, 23.45, 22.56, 21.86.
HRMS, *m*/*z*: 304.3805, ($C_{32}H_{44}N_6O_6$ M + 2H requires 304.3720).

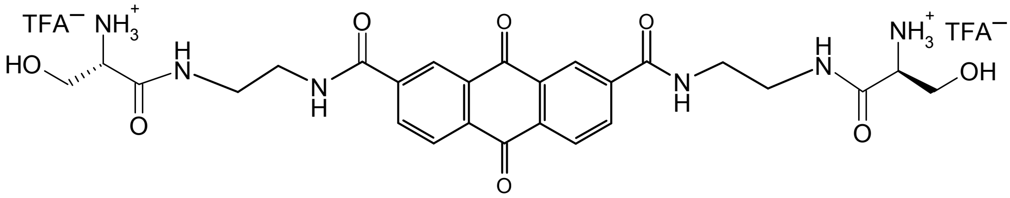
**2,7-AQ-ED-Thr-$NH_3^+$ TFA$^-$**



Method A.

Reagents used: 2,7-AQ-ED TFA (52 mg, 0.086 mmol), Boc-Thr(O-Bzl)-OSu (363 mg, 0.859 mmol). The product was obtained as a slightly yellow powder (53 mg, overall yield 62%).
$^{1}$N-NMR (DMSO-$d_6$): δ 10.79 (s, 2H), 8.90 (t, J=5.7 Hz, 2H), 8.72 (d, J=2.2 Hz, 2H), 8.28 (d, J=8.9 Hz, 2H), 8.22 (bs, 6H), 8.15 (dd, J=8.9 and 2.2 Hz, 2H), 3.85 (m, 1H), 3.56-3.62 (m, 4H), 3.13-3.08 (m, 4H), 3.39-3.28 (m, 4H), 1.72-1.51 (m, 4H), 1.39 (m, 2H), 1.10 (d, J=6.1 Hz, 6H).
$^{13}$C-NMR (DMSO-$d_6$): δ 181.35, 168.98, 166.67, 145.27, 135.02, 131.99, 128.23, 127.32, 124.52, 117.01, 51.58, 43.75, 33.58, 25.77, 23.86, 23.02.
HRMS, *m*/*z*: 292.3255, ($C_{28}H_{34}N_6O_8$ M + 2H requires 292.3172).

**2,7-AQ-ED-Ser-$NH_3^+$ TFA$^-$**



Method A.

Reagents used: 2,7-AQ-ED TFA (52 mg, 0.086 mmol), Boc-Ser(O-Bzl)-OSu (336 mg, 0.859 mmol). The product was obtained as slightly yellow powder (68 mg, overall yield 82 %).

$^{1}$N-NMR (DMSO-$d_6$): δ 10.81 (s, 2H), 8.95 (t, J=5.5 Hz, 2H), 8.65 (d, J=2.1 Hz, 2H), 8.30 (d, J=8.7 Hz, 2H), 8.17 (bs, 6H), 8.11 (dd, J=8.7 and 2.1 Hz, 2H), 4.14-3.96 (m, 4H), 3.91-3.83 (m, 4H), 1.72-1.51 (m, 4H), 1.39 (m, 2H), 1.10 (d, J=6.1 Hz, 6H).

$^{13}$C-NMR (DMSO-$d_6$): δ 181.44, 169.66, 168.03, 144.28, 134.37, 132.31, 128.59, 127.32, 124.56, 115.77, 50.78, 42.79, 31.63, 23.45, 23.57, 22.76.

HRMS, *m*/*z*: 278.3033, ($C_{26}H_{30}N_6O_8$ M + 2H requires 278.2902).

## 2. Combustion data of new compounds

| Compound (see Table 1) | Molecular formula | $C_{calc.}$ | $H_{calc.}$ | $N_{calc.}$ | $C_{found}$ | $H_{found}$ | $N_{found}$ |
|---|---|---|---|---|---|---|---|
| 2,6-AQ-Gly-$NH_3^+$ $TFA^-$ | $C_{18}H_{18}N_4O_4$.2 $C_2F_3O_2$ | 45.53% | 3.13% | 9.65% | 45.30% | 3.12% | 9.67% |
| 2,7-AQ-Gly-$NH_3^+$ $TFA^-$ | $C_{18}H_{18}N_4O_4$.2 $C_2F_3O_2$ | 45.53% | 3.13% | 9.65% | 45.65% | 3.14% | 9.69% |
| 2,6-AQ-βAla-NH3+ TFA- | $C_{20}H_{22}N_4O_4$.2 $C_2F_3O_2$ | 47.38% | 3.64% | 9.21% | 47.25% | 3.65% | 9.18% |
| 2,7-AQ-βAla-NH3+ TFA- | $C_{20}H_{22}N_4O_4$.2 $C_2F_3O_2$ | 47.38% | 3.64% | 9.21% | 47.32% | 3.63% | 9.24% |
| 2,6-AQ-ED-$NH_3^+$ $TFA^-$ | $C_{20}H_{22}N_4O_4$.2 $C_2F_3O_2$ | 47.38% | 3.64% | 9.21% | 47.46% | 3.64% | 9.22% |
| 2,7-AQ-ED-$NH_3^+$ $TFA^-$ | $C_{20}H_{22}N_4O_4$.2 $C_2F_3O_2$ | 47.38% | 3.64% | 9.21% | 47.29% | 3.64% | 9.18% |
| 2,6-AQ-Gly-Phe-$NH_3^+$ $TFA^-$ | $C_{36}H_{36}N_6O_6$.2 $C_2F_3O_2$ | 54.92% | 4.15% | 9.61% | 54.92% | 4.15% | 9.61% |
| 2,6- AQ-Gly-Ala-$NH_3^+$ $TFA^-$ | $C_{24}H_{28}N_6O_6$.2 $C_2F_3O_2$ | 46.54% | 3.91% | 11.63% | 46.51% | 3.92% | 11.57% |
| 2,6-AQ-Gly-Lys-NH3+ TFA- | $C_{30}H_{44}N_8O_6$.4 $C_2F_3O_2$ | 42.86% | 4.17% | 10.52% | 42.96% | 4.18% | 10.54% |
| 2,6-AQ-Gly-Arg-NH3+ TFA- | $C_{30}H_{44}N_{12}O_6$.4 $C_2F_3O_2$ | 40.72% | 3.96% | 15.00% | 40.64% | 3.98% | 14.96% |
| 2,6-AQ-Gly-Gly-$NH_3^+$ $TFA^-$ | $C_{22}H_{24}N_6O_6$.2 $C_2F_3O_2$ | 44.97% | 3.48% | 12.10% | 45.10% | 3.48% | 12.08% |
| 2,6- AQ-Gly-Ile-NH3+ TFA- | $C_{30}H_{4}0N_6O_6$.2 $C_2F_3O_2$ | 50.62% | 5.00% | 10.42% | 50.60% | 4.98% | 10.45% |
| 2,6-AQ-Gly-Leu-NH3+ TFA- | $C_{30}H_{4}0N_6O_6$.2 $C_2F_3O_2$ | 50.62% | 5.00% | 10.42% | 50.79% | 5.01% | 10.42% |
| 2,6-AQ-Gly-Pro-NH3+ TFA- | $C_{28}H_{32}N_6O_6$.2 $C_2F_3O_2$ | 49.62% | 4.16% | 10.85% | 49.56% | 4.15% | 10.89% |
| 2,6-AQ-Gly-Val-NH3+ TFA- | $C_{28}H_{36}N_6O_6$.2 $C_2F_3O_2$ | 49.36% | 4.66% | 10.79% | 49.38% | 4.68% | 10.79% |
| 2,6-AQ-βAla-Phe-NH3+ TFA- | $C_{38}H_{4}0N_6O_6$.2 $C_2F_3O_2$ | 55.88% | 4.47% | 9.31% | 55.68% | 4.45% | 9.34% |
| 2,6-AQ-βAla-Ala-NH3+ TFA- | $C_{26}H_{32}N_6O_6$.2 $C_2F_3O_2$ | 48.01% | 4.30% | 11.20% | 47.92% | 4.29% | 11.21% |
| 2,6-AQ-βAla-Lys-NH3+ TFA- | $C_{32}H_{48}N_8O_6$.4 $C_2F_3O_2$ | 43.96% | 4.43% | 10.25% | 43.78% | 4.43% | 10.22% |
| 2,6-AQ-βAla-Arg-NH3+ TFA- | $C_{32}H_{48}N_{12}O_6$.4 $C_2F_3O_2$ | 41.82% | 4.21% | 14.63% | 41.89% | 4.20% | 14.58% |
| 2,6-AQ-βAla-Ile-NH3+ TFA- | $C_{32}H_{44}N_6O_6$.2 $C_2F_3O_2$ | 51.80% | 5.31% | 10.07% | 52.00% | 5.31% | 10.09% |

| | | | | | | |
|---|---|---|---|---|---|---|
| 2,6-AQ-βAla-Val-$NH_3^+$ $TFA^-$ | $C_{30}H_{4}0N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 50.62% | 5.00% | 10.42% | 50.55% | 4.99% | 10.45% |
| 2,7- AQ-βAla-Phe-NH3+ TFA- | $C_{38}H_{4}0N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 55.88% | 4.47% | 9.31% | 56.05% | 4.48% | 9.28% |
| 2,7-AQ-βAla-Ala-NH3+ TFA- | $C_{26}H_{32}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 48.01% | 4.30% | 11.20% | 47.95% | 4.31% | 11.17% |
| 2,7-AQ-βAla-Lys-NH3+ TFA- | $C_{32}H_{48}N_{8}O_{6}.4\ C_{2}F_{3}O_{2}$ | 43.96% | 4.43% | 10.25% | 43.85% | 4.42% | 10.25% |
| 2,7-AQ-βAla-Arg-$NH_3^+$ $TFA^-$ | $C_{32}H_{48}N_{12}O_{6}.4\ C_{2}F_{3}O_{2}$ | 41.82% | 4.21% | 14.63% | 41.71% | 4.21% | 14.59% |
| 2,7-AQ-βAla-Ile-$NH_3^+$ $TFA^-$ | $C_{32}H_{44}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 51.80% | 5.31% | 10.07% | 51.98% | 5.32% | 10.04% |
| 2,6-AQ-ED-Phe-$NH_3^+$ $TFA^-$ | $C_{38}H_{4}0N_{6}O_{6}\ .\ 2\ C_{2}F_{3}O_{2}$ | 55.88% | 4.47% | 9.31% | 55.72% | 4.48% | 9.28% |
| 2,6-AQ-ED-Ala-$NH_3^+$ $TFA^-$ | $C_{26}H_{32}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 48.01% | 4.30% | 11.20% | 49.92% | 4.32% | 11.20% |
| 2,6-AQ-ED-Lys-$NH_3^+$ $TFA^-$ | $C_{32}H_{48}N_{8}O_{6}.4\ C_{2}F_{3}O_{2}$ | 43.96% | 4.43% | 10.25% | 43.88% | 4.42% | 10.26% |
| 2,6-AQ-ED-Arg-$NH_3^+$ $TFA^-$ | $C_{32}H_{48}N_{12}O_{6}.4\ C_{2}F_{3}O_{2}$ | 41.82% | 4.21% | 14.63% | 41.89% | 4.22% | 14.58% |
| 2,6-AQ-ED-Gly-$NH_3^+$ $TFA^-$ | $C_{24}H_{28}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 46.54% | 3.91% | 11.63% | 46.54% | 3.91% | 11.62% |
| 2,6-AQ-ED-Ile-$NH_3^+$ $TFA^-$ | $C_{32}H_{44}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 51.80% | 5.31% | 10.07% | 51.61% | 5.31% | 10.04% |
| 2,6-AQ-ED-Leu-$NH_3^+$ $TFA^-$ | $C_{32}H_{44}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 51.80% | 5.31% | 10.07% | 51.89% | 5.29% | 10.05% |
| 2,6-AQ-ED-Thr-$NH_3^+$ $TFA^-$ | $C_{28}H_{36}N_{6}O_{8}.2\ C_{2}F_{3}O_{2}$ | 47.41% | 4.48% | 10.37% | 47.41% | 4.47% | 10.35% |
| 2,6-AQ-ED-Ser-$NH_3^+$ $TFA^-$ | $C_{26}H_{32}N_{6}O_{8}\ .\ 2\ C_{2}F_{3}O_{2}$ | 46.04% | 4.12% | 10.74% | 46.00% | 4.13% | 10.74% |
| 2,7-AQ-ED-Phe-$NH_3^+$ $TFA^-$ | $C_{38}H_{4}0N_{6}O_{6}\ .\ 2\ C_{2}F_{3}O_{2}$ | 55.88% | 4.47% | 9.31% | 55.75% | 4.46% | 9.29% |
| 2,7-AQ-ED-Ala-$NH_3^+$ $TFA^-$ | $C_{26}H_{32}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 48.01% | 4.30% | 11.20% | 47.93% | 4.30% | 11.19% |
| 2,7-AQ-ED-Lys-$NH_3^+$ $TFA^-$ | $C_{32}H_{48}N_{8}O_{6}.4\ C_{2}F_{3}O_{2}$ | 43.96% | 4.43% | 10.25% | 43.92% | 4.44% | 10.22% |
| 2,7-AQ-ED-Arg-$NH_3^+$ $TFA^-$ | $C_{32}H_{48}N_{12}O_{6}.4\ C_{2}F_{3}O_{2}$ | 41.82% | 4.21% | 14.63% | 41.82% | 4.23% | 14.59% |
| 2,7-AQ-ED-Gly-$NH_3^+$ $TFA^-$ | $C_{24}H_{28}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 46.54% | 3.91% | 11.63% | 46.56% | 3.91% | 11.63% |
| 2,7-AQ-ED-Ile-$NH_3^+$ $TFA^-$ | $C_{32}H_{44}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 51.80% | 5.31% | 10.07% | 51.69% | 5.31% | 10.04% |
| 2,7-AQ-ED-Leu-$NH_3^+$ $TFA^-$ | $C_{32}H_{44}N_{6}O_{6}.2\ C_{2}F_{3}O_{2}$ | 51.80% | 5.31% | 10.07% | 51.80% | 5.30% | 10.10% |
| 2,7-AQ-ED-Thr-$NH_3^+$ $TFA^-$ | $C_{28}H_{36}N_{6}O_{8}.2\ C_{2}F_{3}O_{2}$ | 47.41% | 4.48% | 10.37% | 47.39% | 4.48% | 10.34% |
| 2,7-AQ-ED-Ser-$NH_3^+$ $TFA^-$ | $C_{26}H_{32}N_{6}O_{8}\ .\ 2\ C_{2}F_{3}O_{2}$ | 46.04% | 4.12% | 10.74% | 46.00% | 4.11% | 10.73% |