Supporting Information

Sequence Programming with Dynamic Boronic Acid/Catechol Binary Codes

Marco Hebel,[1,2] Andreas Riegger,[2] Maksymilian M. Zegota,[1,2] Gönül Kizilsavas,[1] Jasmina Gačanin,[1,2] Michaela Pieszka,[1,2] Thorsten Lückerath,[1,2] Jaime A. S. Coelho,[3] Manfred Wagner,[1] Pedro M. P. Gois,[3] David Y. W. Ng,[1,*] and Tanja Weil[1,2,*]

[1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

[2]Institute of Inorganic Chemistry I, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany

[3]Research Institute for Medicines (iMed.ULisboa), Faculty of Pharmacy, Universidade de Lisboa, Lisbon, Portugal

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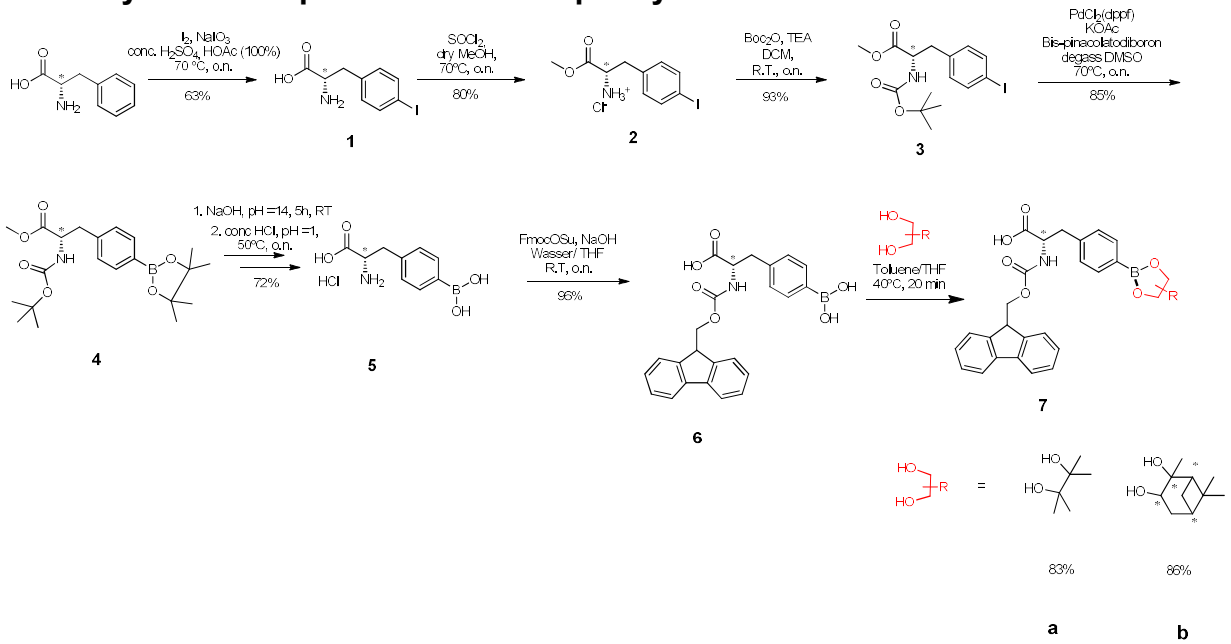
1. Index of Abbreviations

FITC	fluorescein isothiocyanate
Bor- (in peptide sequence)	*para*-borono-phenylalanine
Cat- (in peptide sequence)	L-3,4-dihydroxyphenylalanine
Mal- (in peptide sequence)	6-maleimidohexanoic acid
PEG5000-maleimide	methoxypolyethylene glycol maleimide
TCEP	tris(2-carboxyethyl)phosphine hydrochloride
AEEAc	8-amino-3,6-dioxaoctanoic acid
Fmoc-	Fluorenylmethyloxycarbonyl-
Boc	*tert*-Butyloxycarbonyl-

2. Experimental Procedures

2.1 Synthesis of protected borono-phenylalanine



NMR spectra were recorded on a Bruker 400 or 500 MHz NMR spectrometer. Signals are reported in parts per million (ppm) with respect to residual solvent peak ($CDCl_3$, DMSO-d_6, CD_3OD, D_2O). LC-MS was recorded on or Shimadzu LC-MS 2020. The MALDI-TOF mass spectra were obtained from Bruker Reflex III (MALDI-TOF) and Bruker Solarix (FTICR) spectrometer. All chemical reagents were obtained from commercial suppliers and were used without further purification unless otherwise noted. Thin layer chromatography (TLC, Merck 60 F254) was used to monitor the reactions. TLC plates were stained with $KMnO_4$, ninhydrine, iodine. Acros Organics silica gel was used for column chromatography (0.035 nm – 0.070 nm, 60 Å).

4-Iodo-L-phenylalanine (1)

Phenylalanine (1 equiv.), was dissolved in a mixture of acetic and sulfuric acid (5:1). Then iodine (0.4 equiv.) and sodium periodate (0.23 equiv.) were added. The mixture was heated to 70 °C, stirred overnight and concentrated under vacuum. Water and DCM (4:1) were added to dissolve the solid. The two layers were separated and the aqueous layer was washed with DCM and Et_2O. Subsequently, activated charcoal was added to the aqueous layer, stirred for one hour and filtered. By adjusting the pH of the solution to 4, the white product was precipitated. After filtration the solid was dried under vacuum (Yield: 86%). The NMR data was accordance with the literature.[1] **^{1}H-NMR** (400 MHz, CD_3OD): δ (ppm) = 3.05 (dd, 1H), 3.28 (dd, 1H), 3.91 (dd, 1H), 7.13 (d, 2H), 7.73 (d, 2H). **^{13}C-NMR** (125 MHz, CD_3OD): δ (ppm) = 37.67, 55.74, 95.28,

133.41, 136.03, 140.19, 171.12. **HR-ESI-MS**: m/z = 291.98290 $[M + H]^+$, (calcd. mass: 291.98345 $[M + H]^+$, formula: $C_9H_{10}INO_2$).

4-Iodo-L-phenylalaninemethylester (2)

4-Iodopenylalanine (1 equiv.) was dissolved in dry MeOH. The solution was cooled to 0 °C and thionylchloride (3 equiv.) was added dropwise. The mixture was heated to 70 °C, and stirred overnight. The solvent was partially evaporated to concentrate the solution, which was added to cold Et_2O causing the white product to precipitate. The product was filtered and dried in vacuum (Yield: 94%). The NMR data was in accordance with the literature.[1] **^{1}H-NMR** (400 MHz, CD_3OD): δ (ppm) = 3.10 – 3.22 (m, 2H), 3.81 (s, 3H), 4.33 (dd, 1H), 7.07 (d, 2H), 7.73 (d, 2H). **^{13}C-NMR** (125 MHz, CD_3OD): δ (ppm) = 36.81, 53.63, 54.87, 94.12, 132.55, 135.16, 139.34, 170.26. **HR-ESI-MS**: m/z = 307.00581 $[M + H]^+$, (calcd. mass: 307.00693 $[M + H]^+$, formula: $C_{10}H_{12}INO_2$).

***N*-(*tert*-butyloxycarbonyl)-4-Iodo-L-phenylalaninemethylester (3)**

4-Iodophenylalaninemethylester (1 equiv.) was dissolved in DCM. Then di-*tert*-butyldicarbonat (1.2 equiv.) and TEA (3 equiv.) were added. The solution was stirred overnight and concentrated under vacuum. The crude was purified with column chromatography (*n*-hexane/ethylacetate, 3:1) to afford a clear, highly-viscous oil (Yield: 92%). The NMR was in accordance with the literature.[1] **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 1.42 (s, 9H), 2.92 - 3.10 (m, 2H), 3.71 (s, 3H), 4.56 (dd, 1H), 4.97 (d, 1H), 6.87 (d, 2H), 7.61 (d, 2H). **^{13}C-NMR** (125 MHz, $CDCl_3$): δ (ppm) = 28.41, 52.48, 54.40, 80.23, 92.67, 131.46, 135.85, 137.73, 155.20, 172.28. **LC-MS (ESI)**: m/z = 406 $[M + H]^+$, (calcd. mass: 406 $[M + H]^+$, formula: $C_{15}H_{20}INO_4$).

***N*-(*tert*-butyloxycarbonyl)-4-(pinacolylborono)-L-phenylalaninemethylester (4)**

Potassium acetate (3 equiv.) was placed in a round bottom flask and was dried under vacuum. Then *N*-(*tert*-butyloxycarbonyl)-4-Iodophenylalaninemethylester (1 equiv.), the Pd catalyst ($PdCl_2$dppf, 0.03 equiv.) and bis-pinacolatodiboron (1.3 equiv.) were added, followed by dry DMSO. The clear solution was degassed (4x), heated to 80 °C, and stirred overnight. After removal of the solvent in vacuum, water and DCM were added to the black solid. The aqueous layer was washed with additional DCM (3x). The combined organic layers were dried and concentrated in vacuum. Column chromatography (EA/*n*-hexane, 1:3) was used to isolate the pure product as white solid

(Yield: 87%). The data NMR was in accordance with literature.[2] **^{1}H-NMR** (400 MHz, CD_3OD): δ (ppm) = 1.34 (s, 12H), 1.42 (s, 9H), 2.95 - 3.15 (m, 2H), 3.70 (s, 3H), 4.58 (dd, 1H), 4.95 (d, 1H), 7.12 (d, 2H), 7.73 (d, 2H). **^{13}C-NMR** (125 MHz, CD_3OD): δ (ppm) = 25.00, 28.43, 31.38, 38.53, 52.38, 54.46, 80.08, 83.93, 128.85, 135.15, 139.34, 155.19, 172.36. **LC-MS (ESI)**: m/z = 428 $[M + Na]^+$, (calcd. mass: 428 $[M + Na]^+$, formula: $C_{21}H_{32}BNO_6$).

4-Borono-L-phenylalanine (5)

N-(*tert*-butyloxycarbonyl)-4-(pinacolylborono)-phenylalaninemethylester (1 equiv.) was dissolved in acetone. Concentrated sodium hydroxide solution (10 equiv.) was added and the solution was stirred overnight. The next day, the pH of the solution was adjusted to 0 using concentrated HCl. Then the solution was heated to 50 °C and stirred overnight. The solution was concentrated by partial removal of the solvent and the pH was adjusted to 4 causing the product to precipitate. After filtration the white solid was washed with cold water, Et_2O and dried in vacuum (yield: 81%). The NMR was in accordance with the literature.[3] **^{1}H-NMR** (400 MHz, CD_3OD): δ (ppm) = 2.65 - 2.85 (m, 2H), 3.81 – 3.87 (m, 1H), 6.79 (d, 2H), 7.17 (d, 2H). **^{13}C-NMR** (125 MHz, CD_3OD): δ (ppm) = 44.85, 62.61, 103.19, 141.64, 144.34, 147.03, 179.89.

***N*-(9*H*-Fluorenylmethoxycarbonylamino)-4-borono-L-phenylalanine (6)**

4-Boronophenylalanine (1 equiv.) was suspended in water. Then the pH was adjusted to 11 by adding NaOH. A solution of *N*-(9-Fluorenylmethoxycarbonyloxy)succinimide (1.2 equiv.) was added dropwise to the resulting clear aqueous solution and stirred overnight. The reaction mixture was washed with EA (3x) before the pH was adjusted to 1. Another potion of EA was added (3x) to extract the product. The combined organic layers were dried and concentrated under vacuum to afford a white solid (yield: 69%). **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 3.07 - 3.14 (m, 2H), 4.15 - 4.23 (m, 2H), 4.29 (dd, 1H), 4.44 (dd, 1H), 7.22 - 7.31 (m, 4H), 7.33 - 7.40 (m, 2H), 7.48 - 7.54 (d, 2H), 7.56 - 7.62 (d, 2H), 7.75 - 7.80 (m, 2H). **^{13}C-NMR** (125 MHz, $CDCl_3$): δ (ppm) = 26.29, 38.66, 56.74, 68.00, 120.88, 126.25, 126.36, 128.18, 128.76, 129.62, 135.01, 142.53, 145.22, 158.39, 174.92, 175.28. **LC-MS (ESI)**: m/z = 432 $[M + H]^+$, (calcd. mass: 432 $[M + H]^+$, formula: $C_{24}H_{22}BNO_6$).

General protocol for the protection of the boronic acid

Fmoc-Boronic acid (1 equiv.) was dissolved in a toluene/THF (1:1) mixture. Then (1S,2S,3R,5S)-(+)-pinanediol or pinacol (1 equiv.) was added. The solution was stirred for 15 min before the solvent was completely removed in vacuum. Then another portion of toluene/THF was added, the solution was stirred for another 10 min and solvent again evaporated (repeated 3x). Column chromatography (*n*-hexane/ THF, 4:1 up to 1:2 + 2% FA) was used to isolate the products as white solids.

***N*-(9*H*-Fluorenylmethoxycarbonylamino)-4-(pinacolatoborono)-L-phenylalanine (7a)**

Synthesis was conducted according to the general protocol above. Yield: 83%. The NMR data was in accordance with the literature.[4] **^{1}H-NMR** (400 MHz, MeOH-d_4): δ (ppm) = 1.30 (s, 12H), 2.90 – 3.00 (m, 1H), 3.20 – 3.30 (m, 1H), 4.05 – 4.15 (m, 1H), 4.30 – 4.40 (m, 2H), 7.20- 7.30 (m, 6H), 7.32 – 7.39 (m, 2H), 7.48 - 7.55 (m, 2H), 7.61 – 7.66 (d, 2H), 7.73 – 7.79 (d, 2H). **^{13}C-NMR** (125 MHz, $CDCl_3$): δ (ppm) = 25.17, 36.63, 48.27, 55.20, 67.26, 84.97, 120.82, 126.15, 126.30, 126.36, 128.15, 128.68, 128.70, 129.83, 129.92, 135.86, 142.36, 145.19, 156.20, 174.36. **LC-MS (ESI)**: m/z = 514 $[M+H]^+$, (calcd. mass: 514 $[M+H]^+$, formula: $C_{30}H_{32}BNO_6$).

***N*-(9*H*-Fluorenylmethoxycarbonylamino)-4-(pinandiolborono)-L-phenylalanine (7b)**

Synthesis was conducted according to the general protocol above. Yield: 80% **^{1}H-NMR** (400 MHz, $CDCl_3$): δ (ppm) = 0.85 (s, 3H), 0.98 (d, 1H), 1.26 (s, 3H), 1.39 (s, 3H), 1.73 – 1.75 (m, 1H), 1.83 – 1.89 (m, 1H), 2.05 (t, 1H), 2.09 – 2.17 (m, 1H), 2.30 – 2.40 (m, 1H), 2.79 (t, 1H), 2.85 – 2.95 (m, 1H), 3.10 – 3.18 (m, 1H), 4.14 – 4.17 (m, 1H), 4.17 – 4.25 (m, 2H), 4.47 (dd, 1H), 7.20- 7.40 (m, 6H), 7.59 (d, 2H), 7.60 – 7.62 (m, 2H), 7.75 (d, 2H), 7.89 (d, 2H). **^{13}C-NMR** (125 MHz, $CDCl_3$): δ (ppm) = 23.67, 24.46, 25.17, 26.06, 26.87, 28.43, 35.15, 36.75, 37.79, 39.02, 46.58, 50.90, 55.41, 65.66, 67.06, 77.25, 85.81, 120.09, 120.11, 125.19, 125.36, 127.06, 127.57, 127.62, 128.83, 134.49, 140.68, 140.72, 141.61, 143.76, 155.92, 1732.32. **HR-MS (MALDI-TOF, DHB)**: m/z = 566.27053 $[M+H]^+$, 588.25246 $[M + Na]^+$, (calcd. mass: 566.27085 $[M+H]^+$, 588.25279 $[M+ Na]^+$, formula: $C_{34}H_{36}BNO_6$).

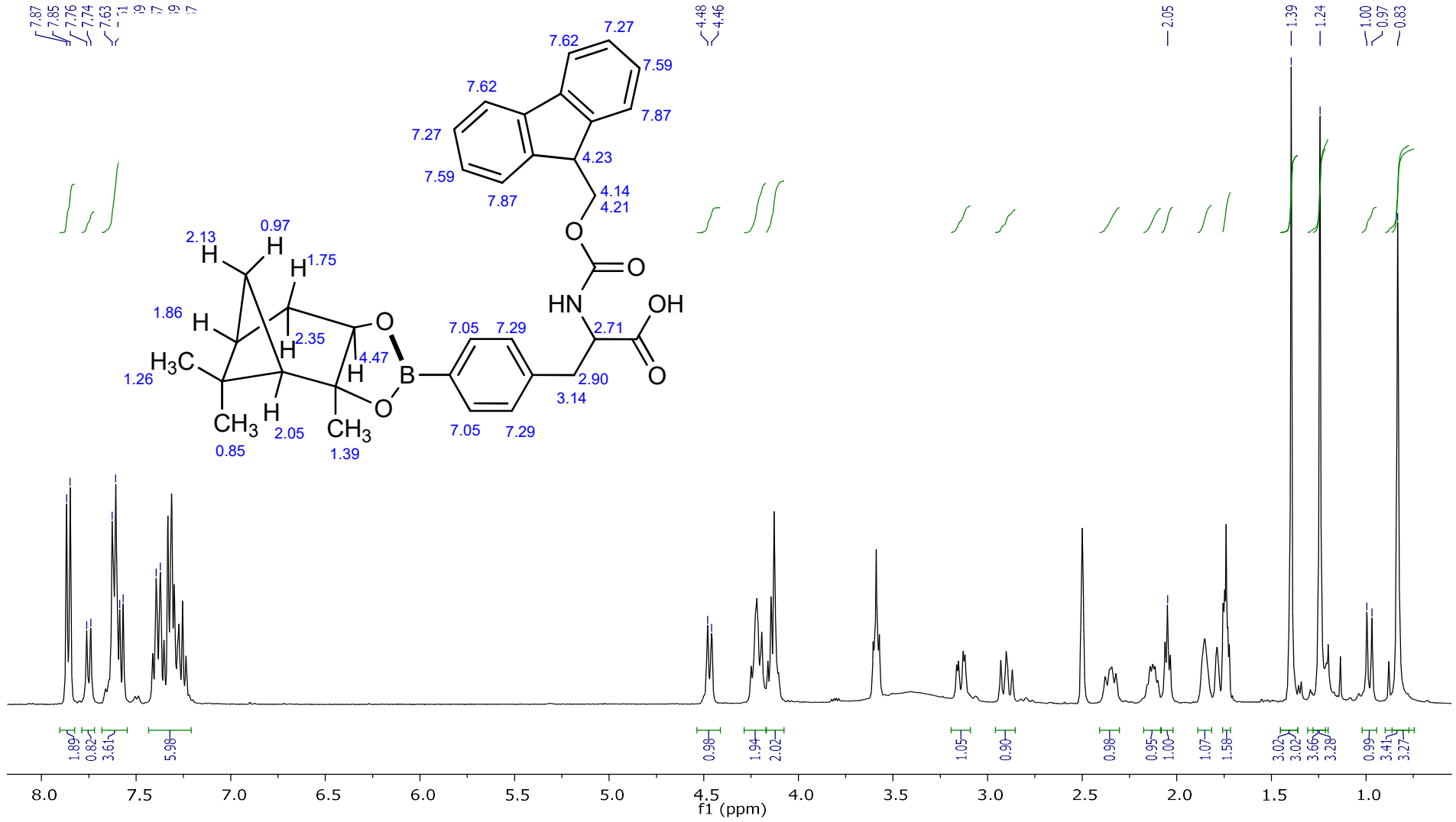


Figure S1. ^{1}H-NMR of *N*-(9*H*-Fluorenylmethoxycarbonylamino)-4-(pinandiolborono)-L-phenylalanine (7b).

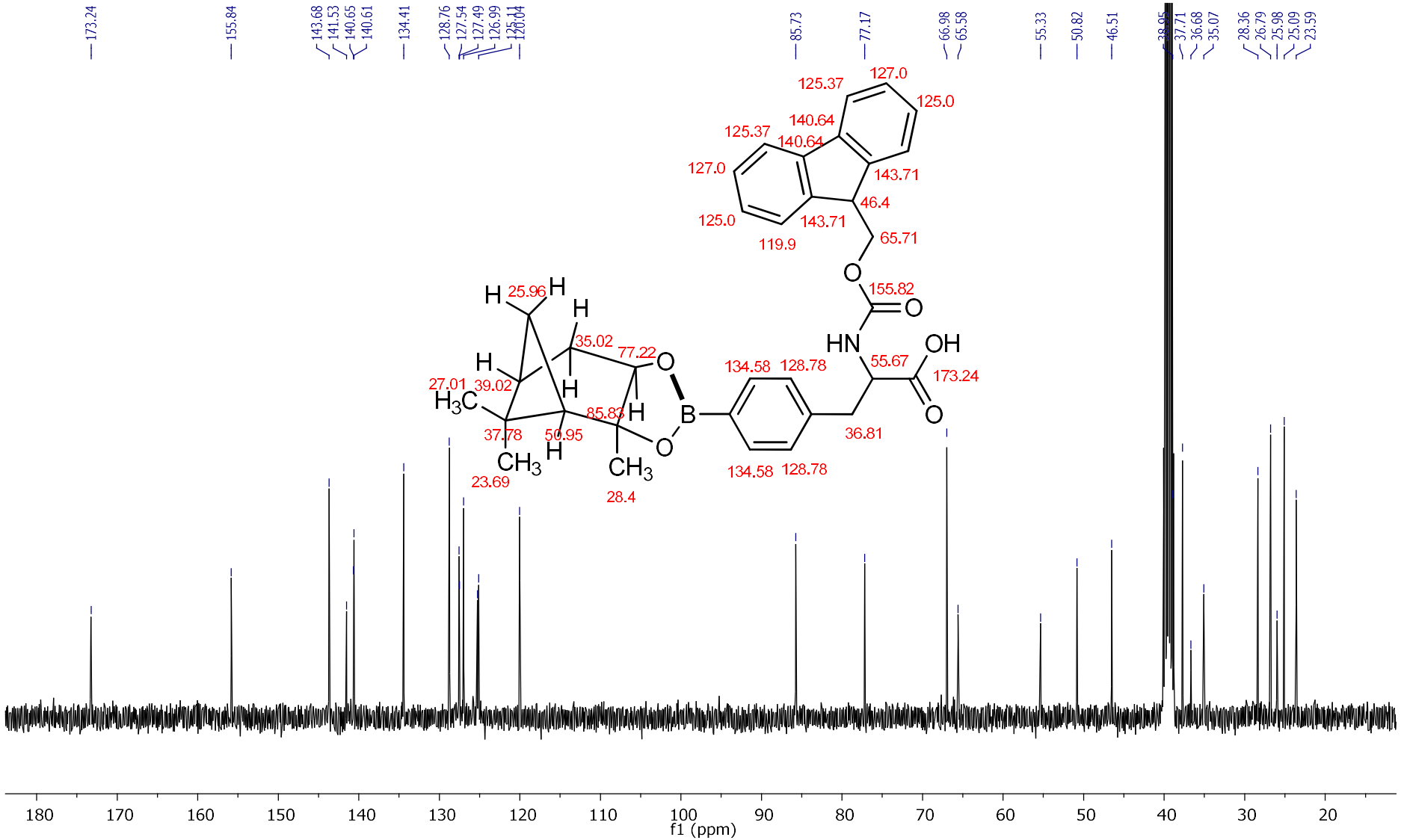


Figure S2. ^{13}C-NMR of *N*-(9*H*-Fluorenylmethoxycarbonylamino)-4-(pinandiolborono)-L-phenylalanine (7b).

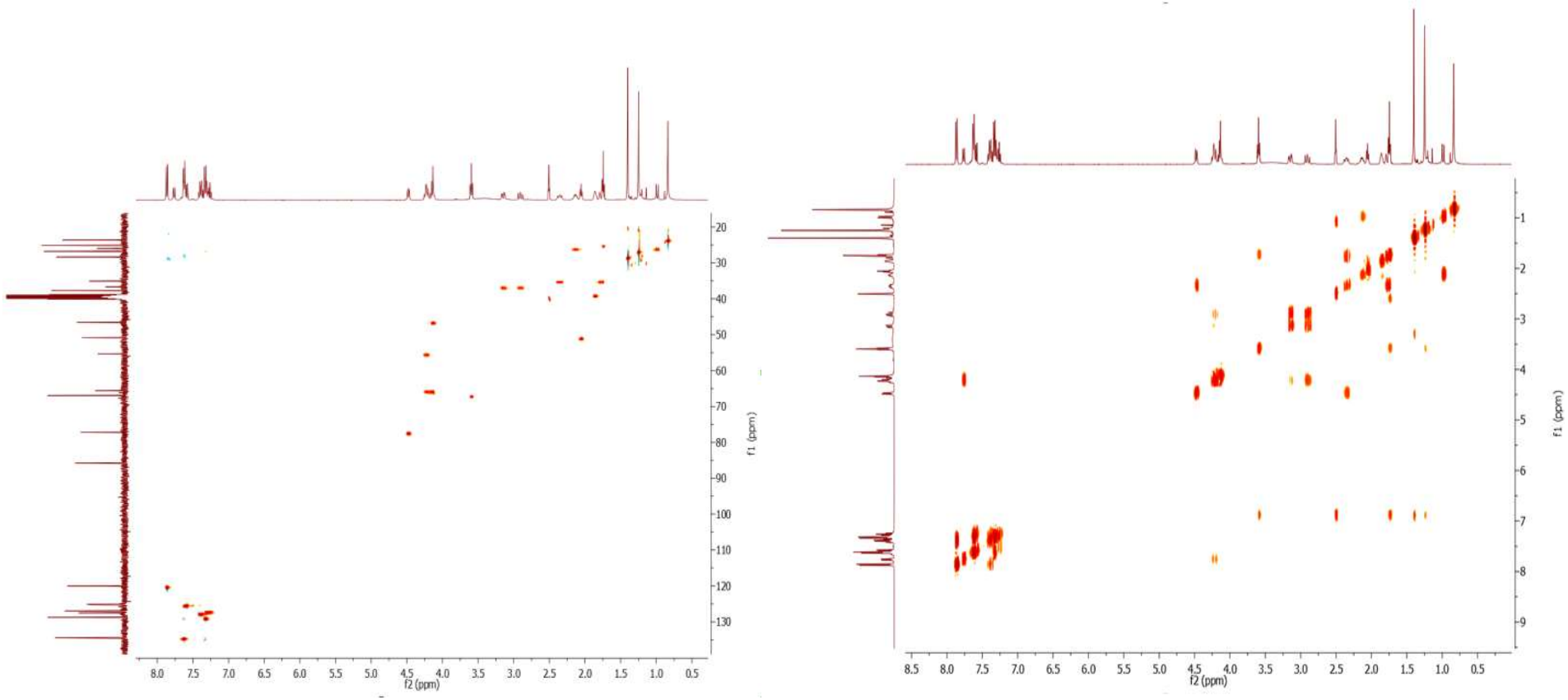
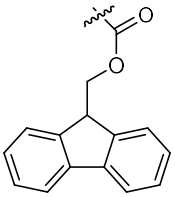


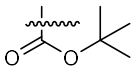
Figure S3. HSQC (left) and H,H COSY (right) of *N*-(9*H*-Fluorenylmethoxycarbonylamino)-4-(pinandiolborono)-L-phenylalanine (7b).

2.2 Solid-phase-peptide-synthesis

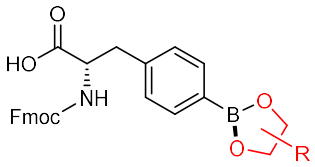
Peptides were synthesized using standard fmoc solid phase peptide synthesis (Fmoc-SPPS). Preloaded resins (catechol containing peptides: Wang Resin, boronic acid containing peptides: tentagel resin) were swelled overnight (DMF, 4°C) and used after 3 washes with fresh DMF (peptide grade):



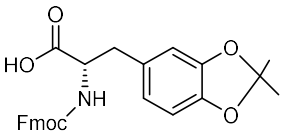
Fmoc



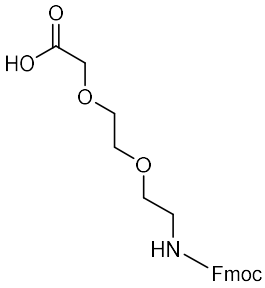
Boc



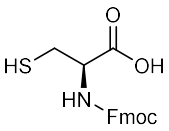
Borono-phenylalanine



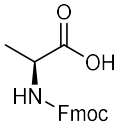
L-DOPA (acetonide protected)



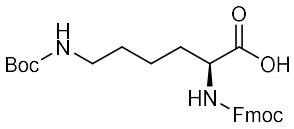
AEEAc



Cysteine



Alanine



Lysine

The deprotection, coupling and final cleavage conditions are given in the protocol listed below.

Deprotection:

- Deprotection #1 (25% Piperidine in DMF, 3 min, R.T.)
- Deprotection #2 (25% Piperidine in DMF, 10 min, R.T.)
- Wash (4x DMF)

Coupling:

- Add reagents (5 equiv. amino acid, 5 equiv. PyBoP, 10 equiv. DIPEA)
- Microwave (5 min, 75°C), for boronic acid containing peptides increase the reaction time subsequently (2 min/boronic acid)

- Wash (4x DMF)

Final cleavage from the solid phase:

For catechol containing peptides: Treat the peptide, which is still bound to the solid phase with 95% TFA, 2.5% TIPS, 2.5% H_2O, 2 h, R.T.
After the final cleavage, the peptides were precipitated by dropping the peptide solution into cold ether. Subsequently, the peptides were purified with HPLC and characterized with mass spectrometry.

For boronic acid containing peptides: Treat the peptide, which is still bound to the solid phase with 95% TFA, 2.5% TIPS, 2.5% H_2O, 2 h, R.T.
After that the peptides were precipitated by dropping the peptide solution into cold ether. In the next steps the following synthesis strategy was used:

1) Excess PBA (5 equiv.) in hydrochloric acid (4 N), add Et_2O (2 Phases), 30 min, exchange the organic phase steadily (3 times), then remove all the solvent.
3) Add conc. hydrochloric acid and stir for 30 min, then remove the hydrochloric acid.

After the final cleavage the peptides were precipitated by dropping the peptide solution into cold ether. Subsequently, the peptides were purified with HPLC and characterized with mass spectrometry.

2.3 Labeling of peptides with fluorescent dyes

DyLight®650-Cys-AEEAc-Cat-Lys-Cat-Lys-Cat-Lys

The catechol peptide with the sequence Cys-AEEAc-Cat-Lys-Cat-Lys-Cat-Lys (0.1926 mg, 0.1634 µmol, 1.1 equiv.) was dissolved in 100 µL degassed phosphate buffer (pH 6.8, 200 mM). TCEP (4.67 mg, 16.34 µmol, 100 equiv.) was added and stirred for 2 h under argon atmosphere. Then DyLight®650-maleimide (0.1621 mg, 0.1485 µmol, 1.0 equiv.) was added as a 10 mg/mL DMF-solution and the mixture was stirred at room temperature overnight under argon atmosphere. The resulting crude solution was purified by HPLC (chapter 5).

Fluorescein-Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys

The boronic acid peptide with the sequence Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys (0.250 mg, 0.2044 µmol, 1.0 equiv.) was dissolved in 500 µL degassed phosphate buffer (pH 7.1, 200 mM). TCEP (2.923 mg, 10.22 µmol, 50 equiv.) was added and stirred for 2 h under argon atmosphere. Then fluorescein-maleimide (2.18 mg, 5.110 µmol, 25 equiv.) was added as a 10 mg/mL DMF-solution and the mixture was stirred at room temperature overnight under argon atmosphere. The resulting crude solution was purified by HPLC (Refer to Section 5).

Fluorescein-Cys-AEEAc-Bor-Lys-Bor-Lys-Ala-Lys-Bor-Lys

The boronic acid peptide with the sequence Cys-AEEAc-Bor-Lys-Bor-Lys-Ala-Lys-Bor-Lys (0.646 mg, 0.4540 µmol, 1.0 equiv.) was dissolved in 1000 µL degassed phosphate buffer (pH 7.1, 200 mM). TCEP (6.492 mg, 22.70 µmol, 50 equiv.) was added and stirred for 2 h under argon atmosphere. Then fluorescein-maleimide (4.850 mg, 11.35 µmol, 25 equiv.) was added as a 10 mg/mL DMF-solution and the mixture was stirred at room temperature overnight under argon atmosphere. The resulting crude solution was purified by HPLC (Refer to Section 5).

2.4 Synthesis of protein/polymer conjugates

Synthesis of Cytochrome-C-Catechol Peptide-Conjugate (CytC-B3)

CytC (3.120 mg, 0.20479 µmol, 1.0 equiv.) was dissolved in 700 µL degassed phosphate buffer (pH 7.4, 200 mM). TCEP (24.79 µg, 0.099 µmol, 0.4 equiv., 19 µL PB-solution) was added and stirred for 2 h under argon atmosphere. Then the maleimide-functionalized catechol peptide (0.317 mg, 0.248 µmol, 1.0 equiv., 156 µL PB-solution) was added and the mixture was stirred at room temperature overnight under argon atmosphere. The resulting crude solution was purified by Vivaspin® 500 Centrifugal Concentrator (Cut-off of 3000 MW) by six-times washing with water.

Synthesis of PEG_{5000}-Boronic Acid Peptide-Conjugate (PEG_{5000}-A3)

The boronic acid peptide with the sequence Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys (0.250 mg, 0.2044 µmol, 1.0 equiv.) was dissolved in 250 µL degassed phosphate buffer (pH 7.1, 200 mM). TCEP (2.713 mg, 9.485 µmol, 50 equiv., 70 µL PB-solution) was added and stirred for 2 h under argon atmosphere. PEG_{5000}-maleimide (9.591mg,

1.900 µmol, 10 equiv.) was dissolved in 1000 µL degassed phosphate buffer (pH 7.4, 200 mM) was added and the mixture was stirred at room temperature overnight under argon atmosphere. The resulting crude solution was purified by HPLC.

2.5 Mass Spectrometry and High-Performance Liquid Chromatography

The catechol containing peptide tags were characterized via LC-MS or MALDI-FTICR using HCCA matrix. Typically, a sample solution (c = 1 mg/mL) was mixed (1:1) with a saturated HCCA matrix solution (50% ACN/ 50% H_2O) and spotted on the steel plate. Then an additional aliquot of the HCCA solution was added to dilute the sample and spotted again (repeat 3x). Spectra can be obtained in positive and negative mode.

Boronic acid containing peptide tags were characterized via MALDI-FTICR measurements. Spectra can be obtained in positive mode.

Preparation A: A sample solution (c = 1 mg/mL) was mixed (1:1) with a saturated DHB matrix solution (50% ACN/ 50% H_2O) and spotted on the steel plate. Then an additional aliquot of the DHB solution was added to dilute the sample and spotted again (repeat 3x).

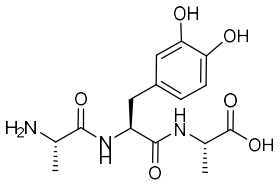
Preparation B: A saturated DHB matrix solution (50% ACN/ 50% H_2O) was spotted on the steel plate. After drying, a droplet of the sample solution (c = 1 mg/mL) was added on top of the DHB crystals. After drying, another droplet of saturated DHB matrix solution was added.

The complexes of boronic acid containing peptides and catechol containing peptides were characterized via MALDI-FTICR using SA matrix in the case of the cytochrome c-PEG5000 complex and using HCCA matrix in the case of the simple peptide tag-complexes. Typically, a sample solution (c = 1 mg/mL) was mixed (1:1) with a saturated matrix solution (50% ACN/ 50% H_2O) and spotted on the steel plate. Then an additional aliquot of the HCCA solution was added to dilute the sample and spotted again (repeat 3x). Spectra can be obtained mainly in negative mode.

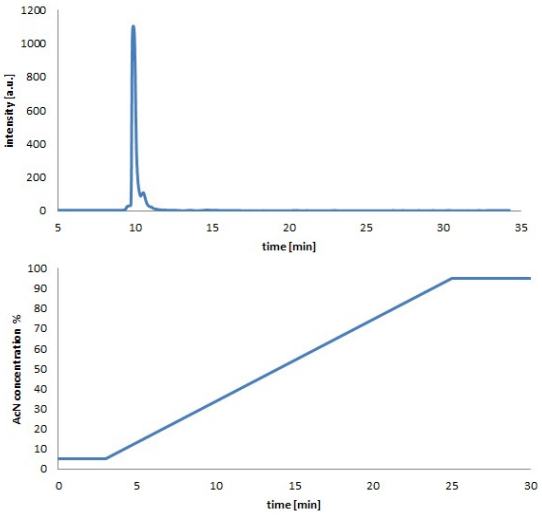
Alanine-based Peptide Tags

Catechol Tags

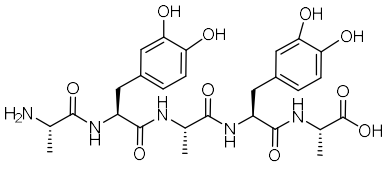
Ala-Cat-Ala



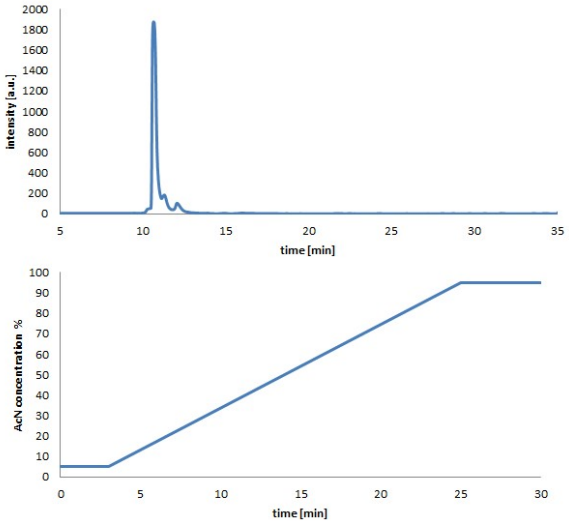
LC-MS: m/z = 340 $[M + H]^+$, (calcd. mass: 340 $[M + H]^+$, formula: $C_{15}H_{21}N_3O_6$).



Ala-Cat-Ala-Cat-Ala



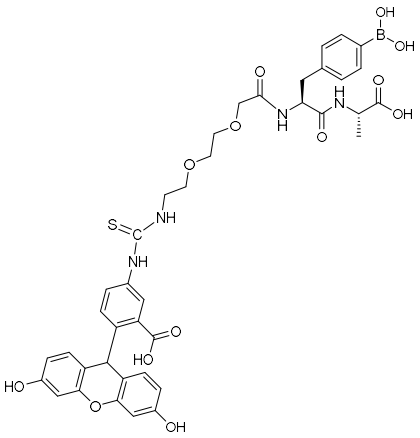
HR-MS (MALDI-TOF, HCCA): m/z = 590.24565 $[M + H]^+$, (calcd. mass: 590.24567 $[M + H]^+$, formula: $C_{27}H_{35}N_5O_{10}$).



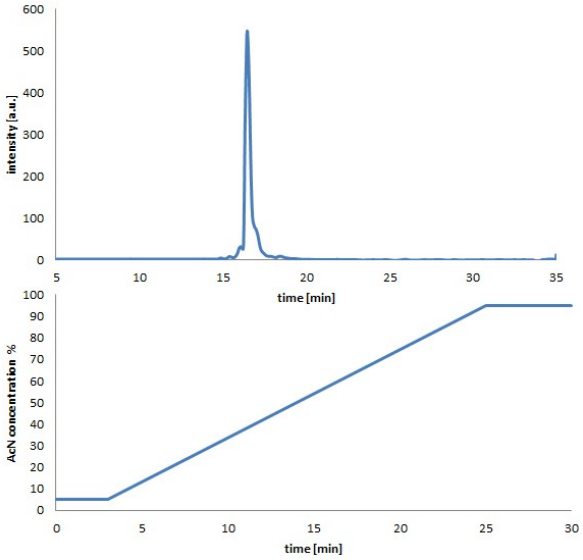
Bor-Tags

Only the main signal of the mass spectra are recorded here. Other detected species resulted from deborylation and water-addition during the measurement with DHB.

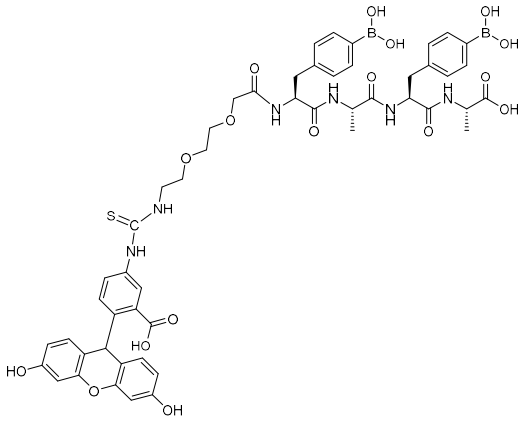
FITC-AEEAc-Bor-Ala



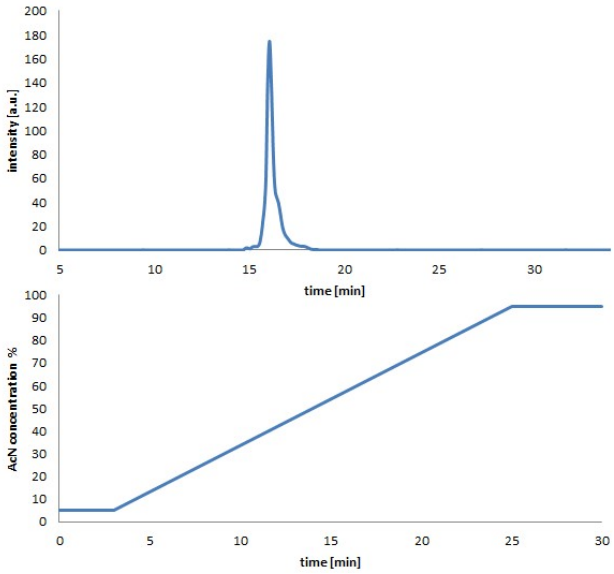
HR-MS (MALDI-TOF, DHB): m/z = 815.23959 $[M + H]^+$, (calcd. mass: 815.24070 $[M + H]^+$, formula: $C_{39}H_{39}BN_4O_{13}S$).



FITC-AEEAc-Bor-Ala-Bor-Ala



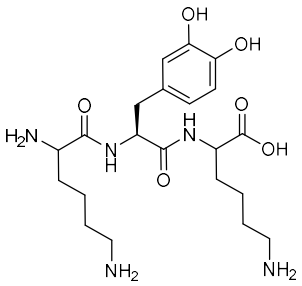
HR-MS (MALDI-TOF, DHB): m/z = 1059.34259 $[M - H_2O + H]^+$, (calcd. mass: 1059.34344 $[M - H_2O + H]^+$, formula: $C_{51}H_{52}B_2N_6O_{16}S$).



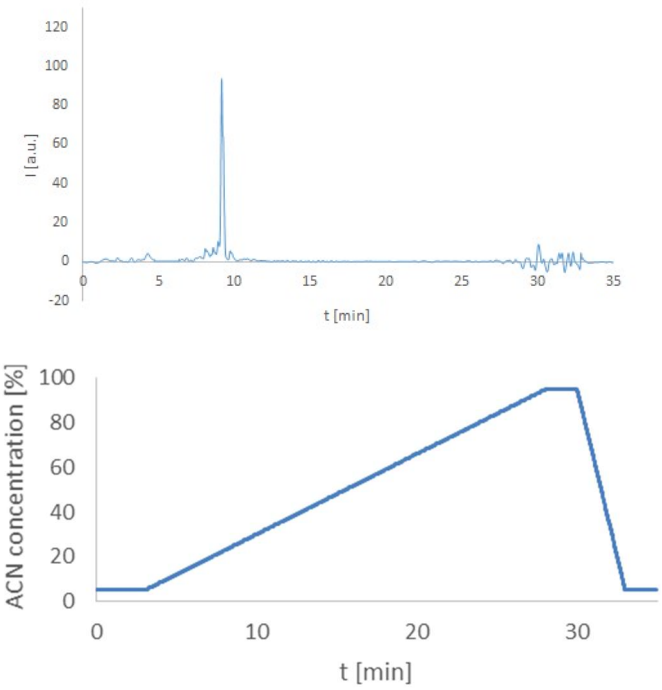
Lysine-based Peptide Tags

Cat-Tags

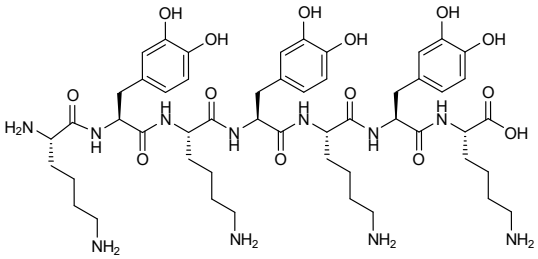
Lys-Cat-Lys



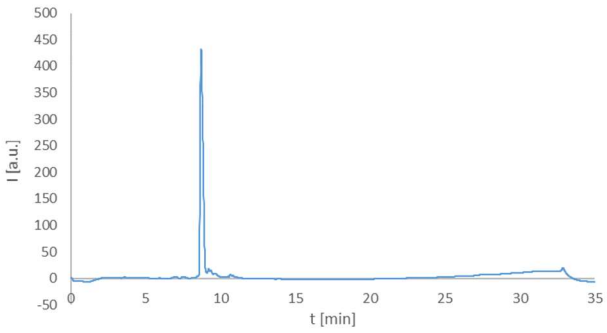
MS (MALDI-TOF, CHCA): m/z = 454.844 $[M + H]^+$, (calcd. mass: 454.2660 $[M + H]^+$, formula: $C_{21}H_{35}N_5O_6$).

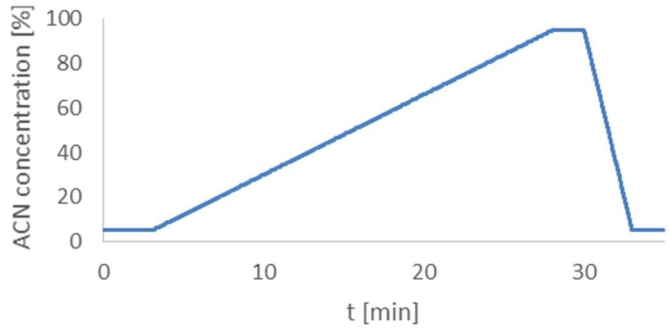


Lys-Cat-Lys-Cat-Lys-Cat-Lys

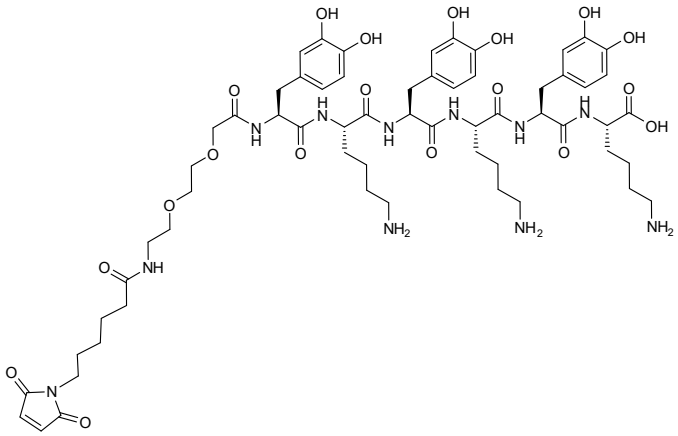


MS (MALDI-TOF, CHCA): m/z = 1066.409 $[M-H]^-$, (calcd. mass: 1066.5579 $[M-H]^-$, formula: $C_{51}H_{77}N_{11}O_{14}$).

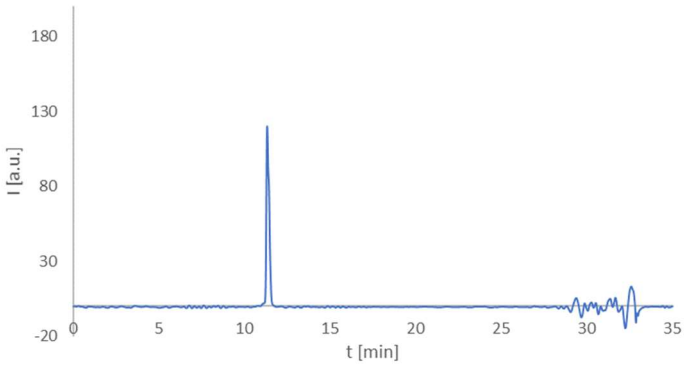


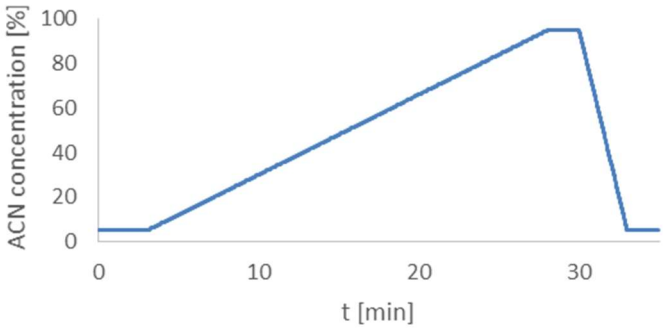


Maleimide-AEEAc-Cat-Lys-Cat-Lys-Cat-Lys

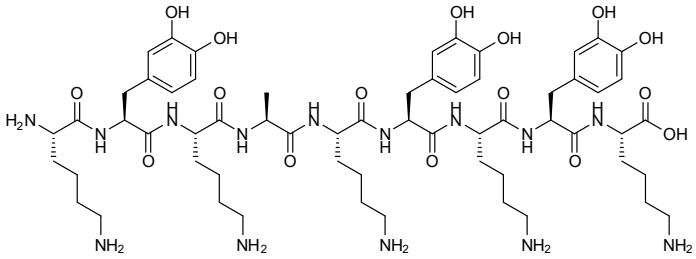


MS (MALDI-TOF, CHCA): m/z = 1276.647 $[M-H]^-$, (calcd. mass: 1276.6107 $[M-H]^-$, formula: $C_{61}H_{87}N_{11}O_{19}$).

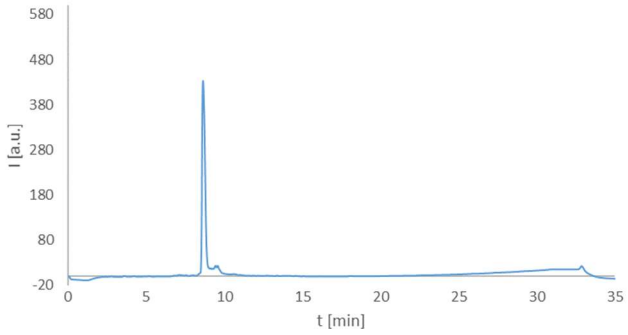


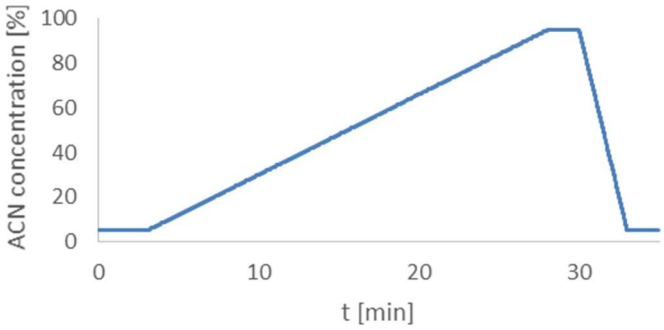


Lys-Cat-Lys-Ala-Lys-Cat-Lys-Cat-Lys

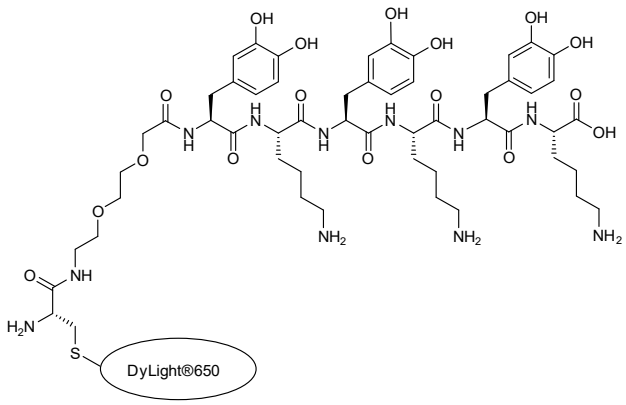


MS (MALDI-TOF, CHCA): m/z = 1265.688 $[M-H]^-$, (calcd. mass: 1265.6899 $[M-H]^-$, formula: $C_{60}H_{94}N_{14}O_{16}$).

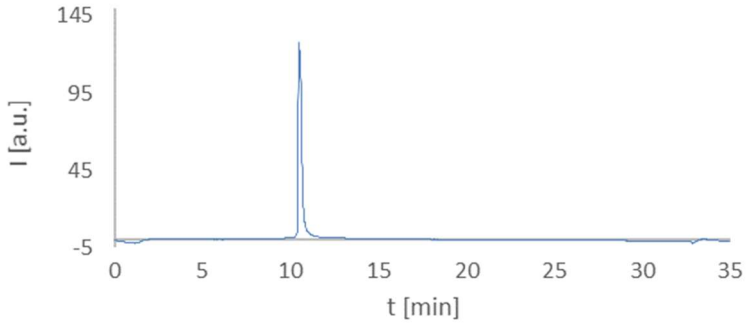


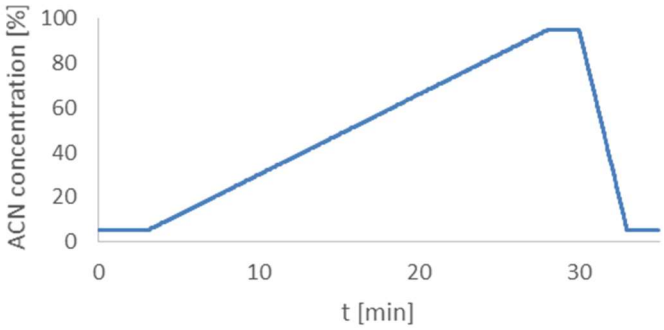


DyLight®650-Cys-AEEAc-Cat-Lys-Cat-Lys-Cat-Lys

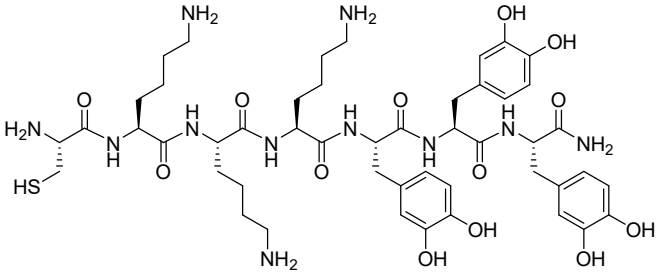


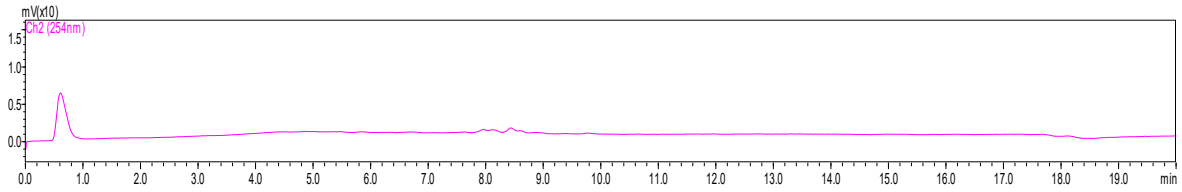
MS (MALDI-TOF, DHB): m/z = 2277.131 $[M-H]^-$, (calcd. mass: 2277.546 $[M-H]^-$, formula: formula cause of DyLight®650 not calculable.





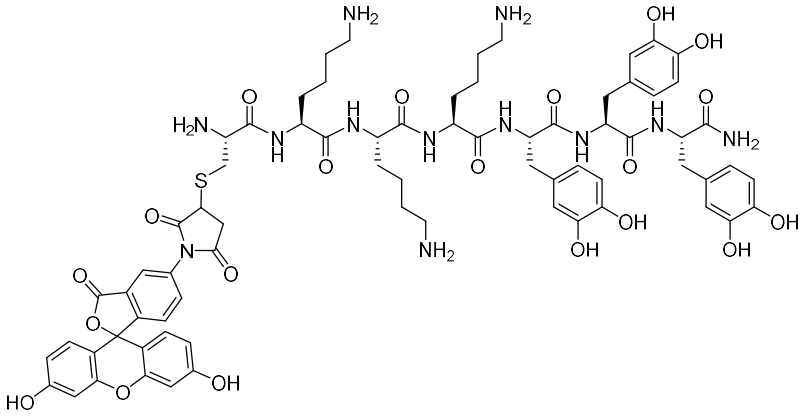
Cys-Lys-Lys-Lys-Cat-Cat-Cat

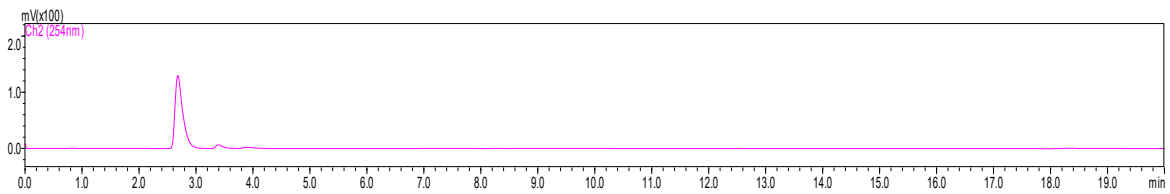




MS (MALDI-TOF, DHB): m/z = 1042.541 $[M+H]^+$ (calcd. mass: 1042.503 $[M-H]^-$ formula: $C_{48}H_{71}N_{11}O_{13}S$)

FITC-Cys-Lys-Lys-Lys-Cat-Cat-Cat



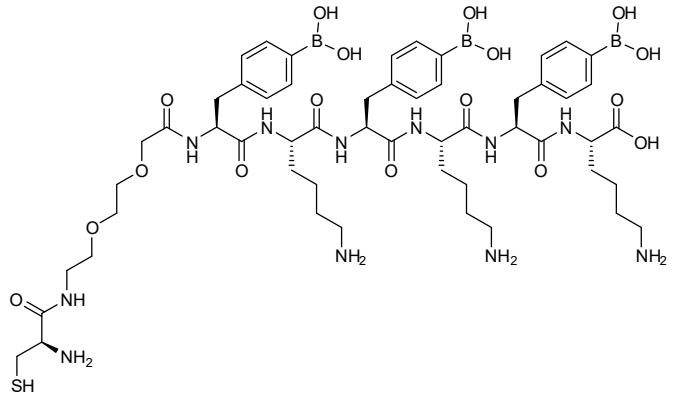


MS (MALDI-TOF, DHB): m/z = 1469.496 $[M+H]^+$ (calcd. mass: 1469.572 $[M+H]^+$ formula: $C_{72}H_{84}N_{12}O_{20}S$)

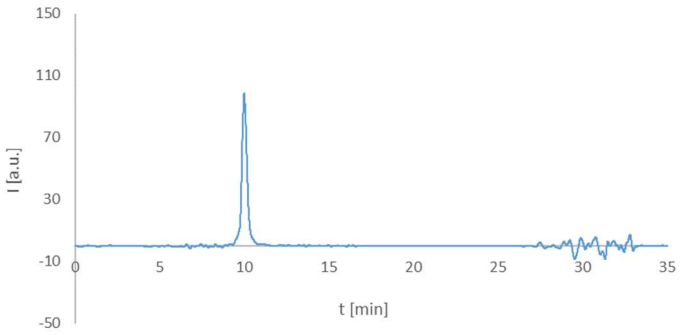
Bor-Tags

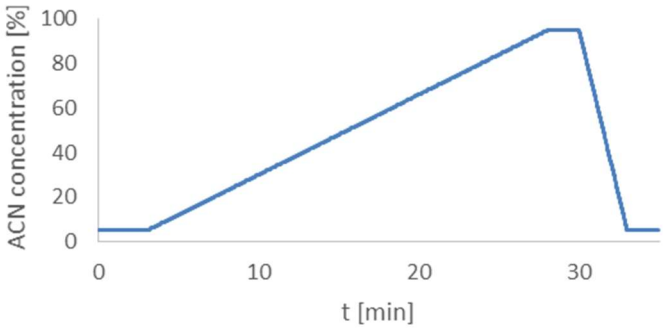
Only the main signal of the mass spectra are recorded here. Other detected species resulted from deborylation and water-addition during the measurement with DHB.

Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys

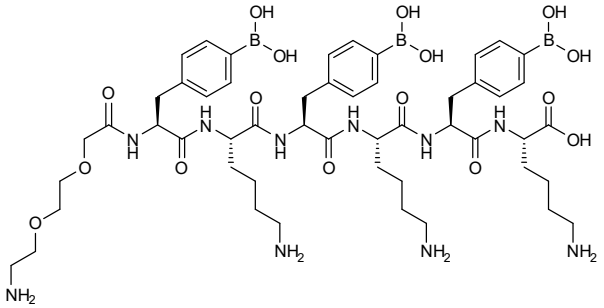


MS (MALDI-TOF, DHB): m/z = 1578.996 [M + 3 DHB – 6 H_2O + H]$^+$, (calcd. mass: 1578.6284 [M + 3 DHB – 6 H_2O + H]$^+$, formula: $C_{54}H_{84}B_3N_{11}O_{17}S$).

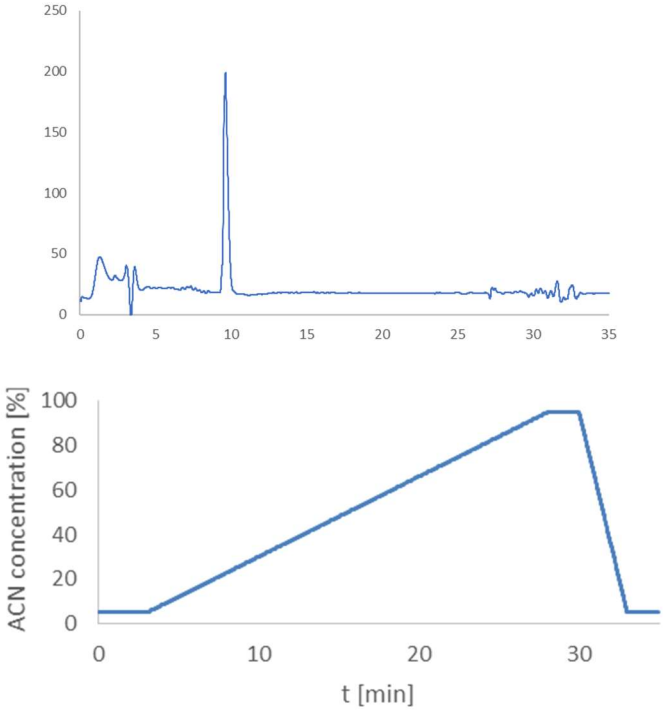




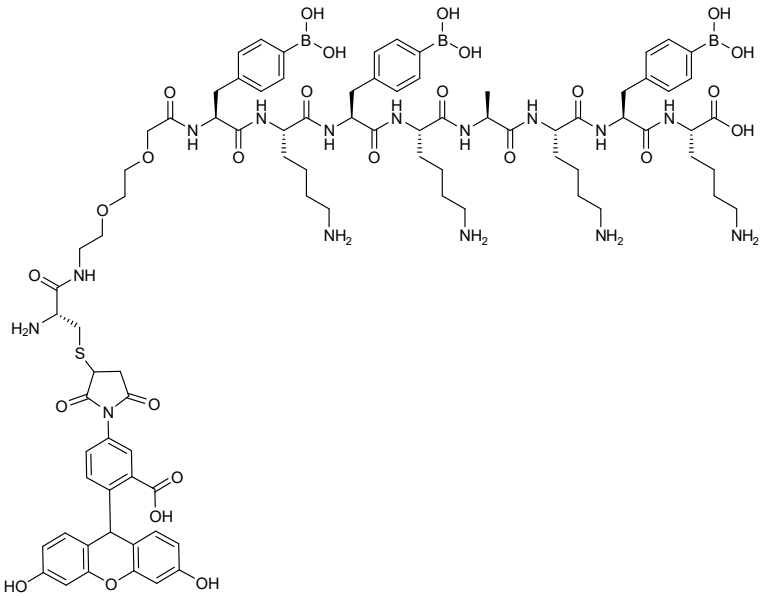
AEEAc-Bor-Lys-Bor-Lys-Bor-Lys



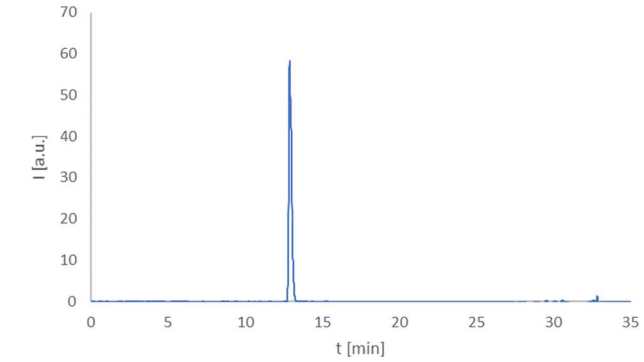
MS (MALDI-TOF, DHB): m/z = 1475.723 [M + 3 DHB – 6 H_2O + H]$^+$, (calcd. mass: 1475.6192 [M + 3 DHB – 6 H_2O + H]$^+$, formula: $C_{51}H_{79}B_3N_{10}O_{16}$).

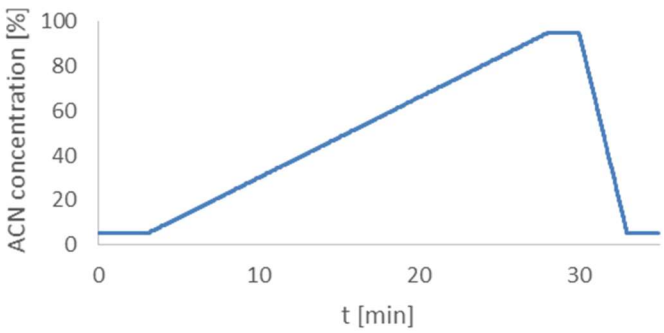


Fluorescein-Cys-AEEAc-Bor-Lys-Ala-Lys-Bor-Lys-Bor-Lys

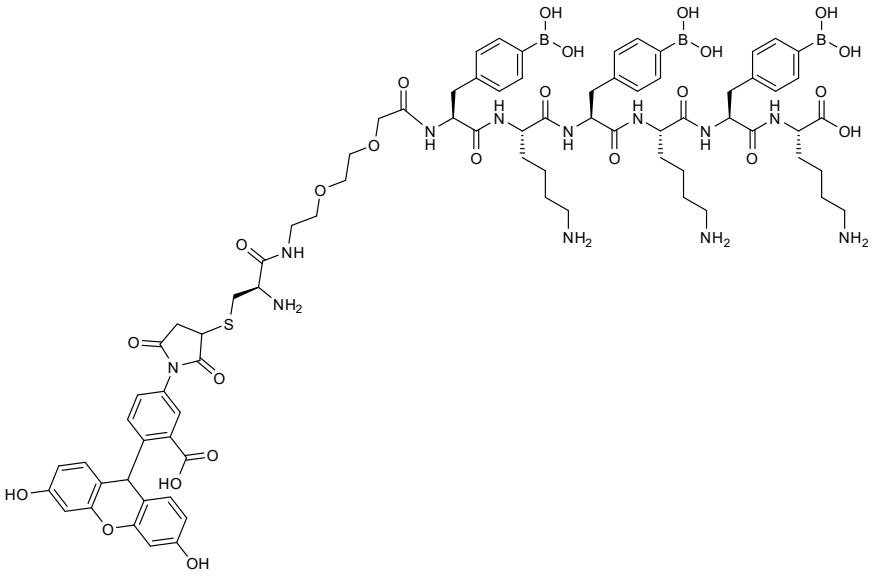


MS (MALDI-TOF, DHB): m/z = 2206.640 [M + 3 DHB – 6 H_2O + H]$^+$, (calcd. mass: 2206.8453 [M + 3 DHB – 6 H_2O + H]$^+$, formula: $C_{87}H_{116}B_3N_{15}O_{26}S$).

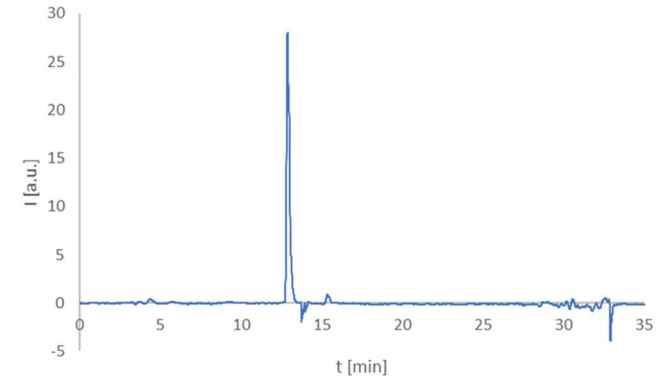


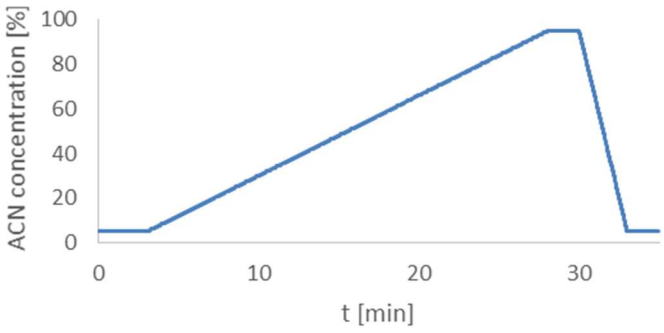


Fluorescein-Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys

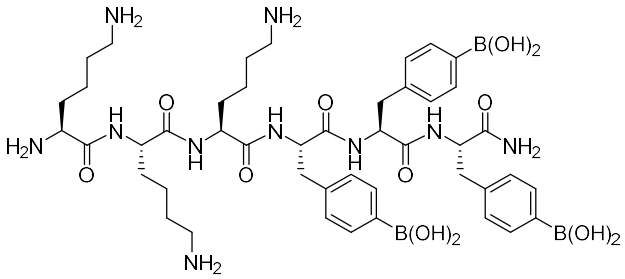


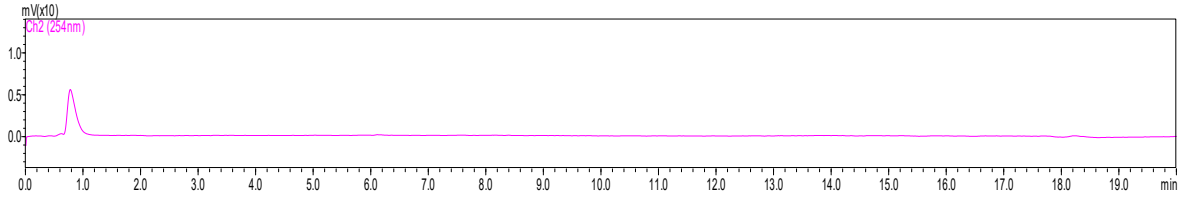
MS (MALDI-TOF, DHB): m/z = 2007.906 [M + 3 DHB – 6 H_2O + H]$^+$, (calcd. mass: 2007.7132 [M + 3 DHB – 6 H_2O + H]$^+$, formula: $C_{78}H_{99}B_3N_{12}O_{24}S$).





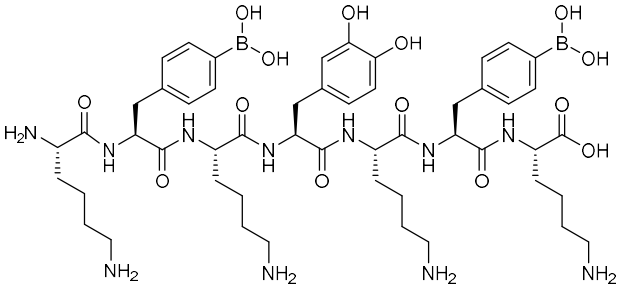
Lys-Lys-Lys-Bor-Bor-Bor



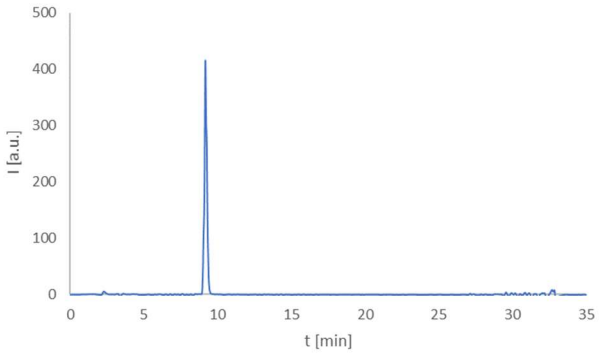


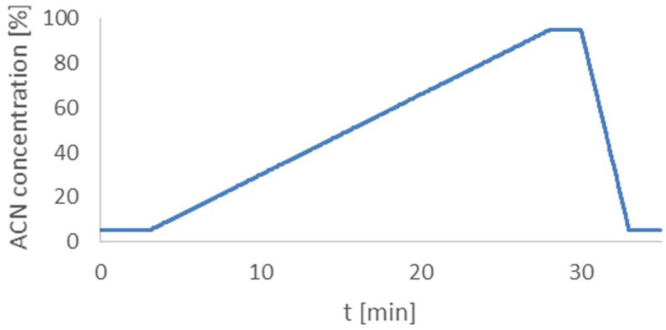
MS (MALDI-TOF, DHB): m/z = 975.563 $[M + H]^+$, (calcd. mass: 975.545 $[M + H]^+$, formula: $C_{45}H_{69}B_3N_{10}O_{12}$).

Lys-Bor-Lys-Cat-Lys-Bor-Lys

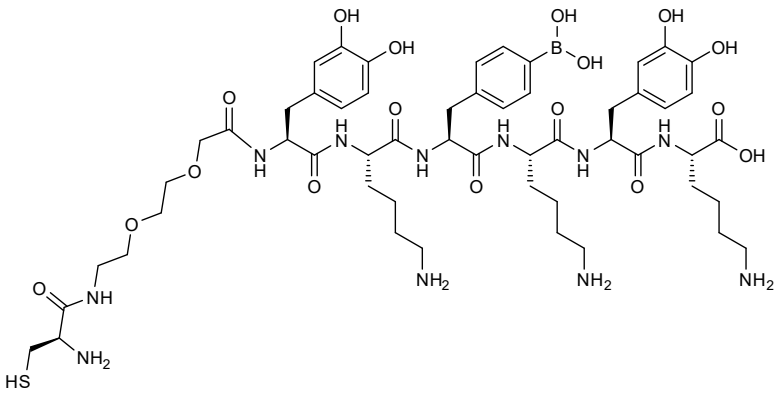


MS (MALDI-TOF, DHB): m/z = 1328.61826 $[M + 3\ DHB - 6\ H_2O + H]^+$, (calcd. mass: 1328.62 $[M + 3\ DHB - 6\ H_2O + H]^+$, formula: $C_{51}H_{79}B_2N_{11}O_{14}$).

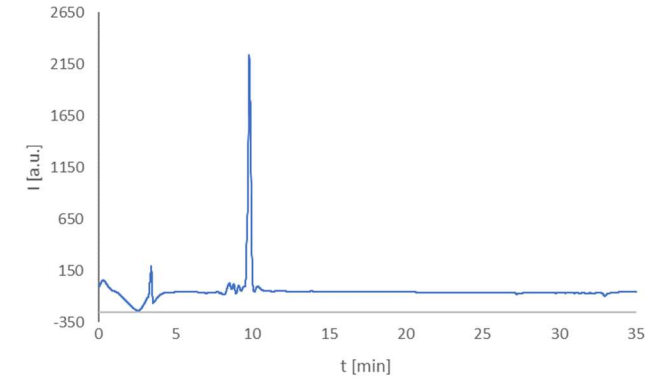


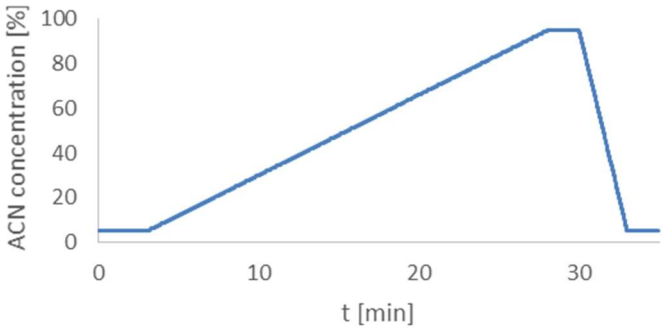


Cys-AEEAc-Cat-Lys-Bor-Lys-Cat-Lys

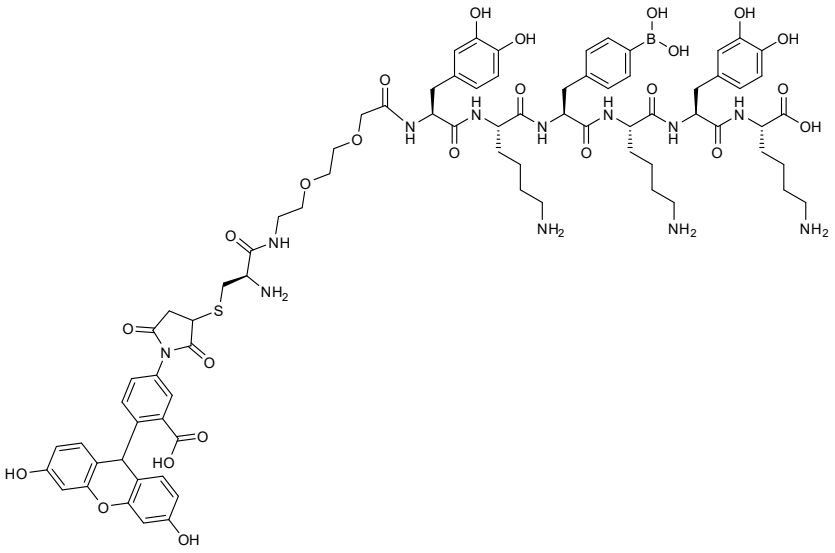


MS (MALDI-TOF, DHB): m/z = 1318.58346 $[M + 1\ DHB - 2\ H_2O + H]^+$, (calcd. mass: 1318.58 $[M + 1\ DHB - 2\ H_2O + H]^+$, formula: $C_{54}H_{82}BN_{11}O_{17}S$).

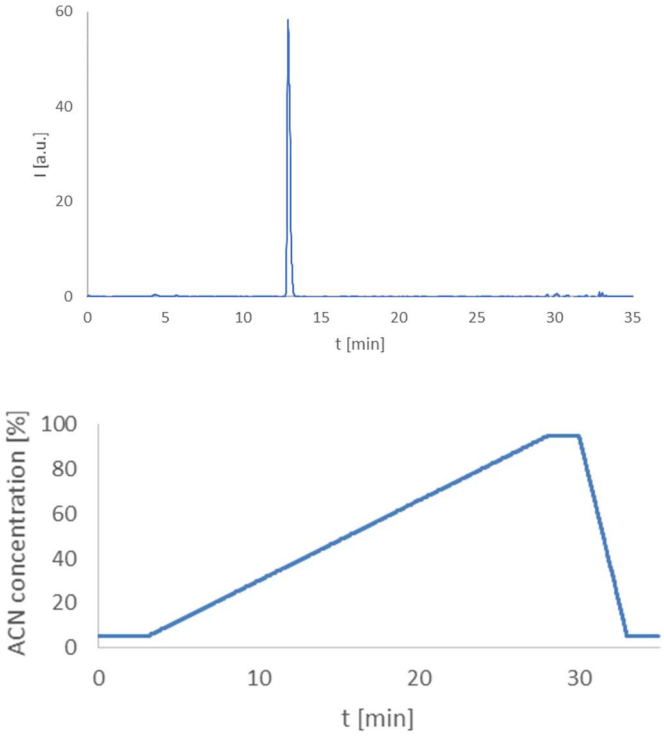




Fluorescein-Cys-AEEAc-Cat-Lys-Bor-Lys-Cat-Lys



MS (MALDI-TOF, DHB): m/z = 1747.65660 $[M + 1\ DHB - 2\ H_2O + H]^+$, (calcd. mass: 1747.67 $[M + 1\ DHB - 2\ H_2O + H]^+$, formula: $C_{78}H_{97}BN_{12}O_{24}S$).



2.6 Binding Affinity Analysis (Fluorescence Quenching Assay)

General procedure:

Fluorescence spectra were recorded on an Infinite® M1000 PRO microplate reader (Tecan®) and on a microscale thermophoresis device (Monolith NT.115 of NanoTemper Technologies GmbH). 20 µL of different concentrations of the non-labeled compound were served (dilutions series with factor of 2 for each step, phosphate buffer 300 mM, pH 7.4). To this a constant amount of the fluorescein-labeled compound (vol. 20 µL, phosphate buffer 300 mM, pH 7.4) below the lowest amount in the dilution series of the non-labeled one was added. After mixing for 2 h at 450 rpm, 35 µL of every mixture was placed in black UV Star® 384 microliter well-plates (Greiner bio-one®) or 10 µL was sucked in a capillary for the microscale thermophoresis device (Monolith NT.115 Capillaries). After 15 min of equilibration time, the fluorescence emission was recorded at 520 nm upon excitation at 488 nm with multiple reads per well (3x3) or with the green/red laser device with a laser power of 20% on the settings of the microscale thermophoresis device.

Exemplary described procedure (of the measurement with Fluorescein-**(AX)$_3$** and **(BX)$_3$**):

At the beginning, the serial dilution of the catechol peptide tag was produced. For that, 8 solutions with a volume of 20 µL each (phosphate buffer 300 mM, pH 7.4) were prepared. Furthermore, one solution with the starting concentration of 0.5 mM of the catechol peptide tag in 40 µL (phosphate buffer 300 mM, pH 7.4) was mixed. 20 µL of the solution was diluted with 20 µL and is iterated for the 8 prepared solutions. At the end the catechol peptide serial dilution has 9 solutions with 20 µL volume each and the following concentrations:

Dilution of catechol peptide	Concentration [mM]
1	0.50000
2	0.25000
3	0.12500
4	0.06250
5	0.03125
6	0.01562
7	0.00781
8	0.00390
9	0.00195

To each of these solutions, 20 µL of a prepared 0.00048 mM fluorescein-boronic acid peptide solution (phosphate buffer 300 mM, pH 7.4) was introduced.

The resulting catechol-boronic acid mixtures (after mixing every solution contained half of the prepared concentrations) were then shaken for 2 h at 450 rpm. In the next step, 35 µL of the solutions were pipetted in the wells/capillaries for fluorescence spectroscopy (general procedure describes settings of the device).

Used peptide sequences:

Fluorescein-Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys	+	Lys-Cat-Lys-Cat-Lys-Cat-Lys
Fluorescein-Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys	+	Lys-Cat-Lys-Ala-Lys-Cat-Lys-Cat-Lys
Fluorescein-Cys-AEEAc-Bor-Lys-Ala-Lys-Bor-Lys-Bor-Lys	+	Lys-Cat-Lys-Ala-Lys-Cat-Lys-Cat-Lys
Fluorescein-Cys-AEEAc-Cat-Lys-Bor-Lys-Cat-Lys	+	Lys-Bor-Lys-Bor-Lys-Bor-Lys
FITC-AEEAc-Bor-Ala-Bor-Ala	+	Ala-Cat-Ala-Cat-Ala
FITC-AEEAc-Bor-Ala	+	Ala-Cat-Ala
Lys-Lys-Lys-Bor-Bor-Bor	+	FITC-Cys-Lys-Lys-Lys-Cat-Cat-Cat

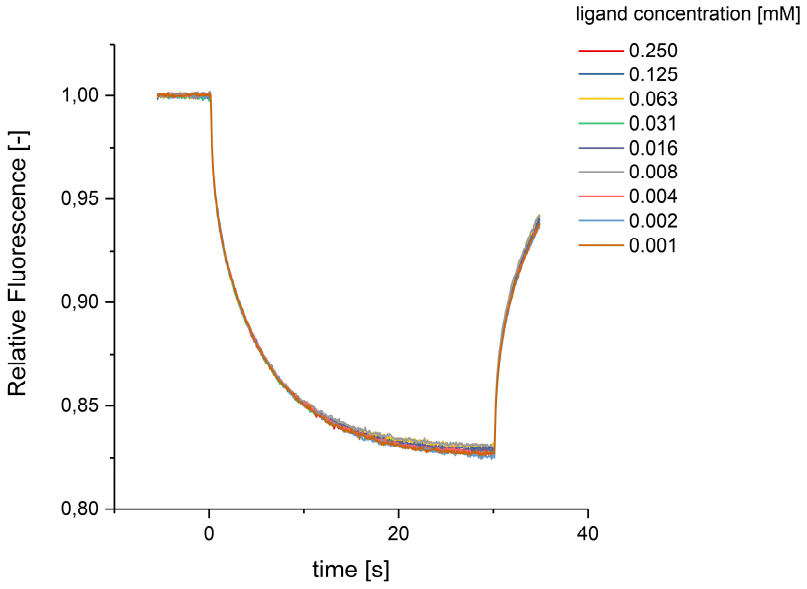


Figure S4. Fluorescence decay as a result of thermophoresis of **(AX)$_3$-(BX)$_3$** binding demonstrating the absence of aggregates and higher ordered structures.

Statistics and reproducibility

The concentration dependent fluorescence data points were plotted in OriginPro 2017G. To compare the binding concentrations (or K_a), the points of inflection were calculated by the OriginPro 2017G software by using sigmoidal fitting according to the Boltzmann function. Each individual experiment was conducted in triplicates with a different batch of synthesized peptides. Three sets of experiments were conducted to obtain the data in Figure 2a of the main manuscript. The point of inflection values of the different experiments were used to determine the arithmetic average binding concentrations (or K_a) and standard deviations. The standard deviation points for **(AX)-(BX)** (blue in Figure 2a) is smaller than the represented square itself and thus not graphically observable.

2.7 Dynamic light scattering

Dynamic light scattering on the **(AX)$_3$-(BX)$_3$** binding complex in 300 mM PB buffer, pH 7.4, was performed using Nano-ZetaSizer (Malvern Instruments). The 173° backscatter was measured using a 633 nm laser at 25 °C. No aggregates were detected.

2.8 FRET experiment

Fluorescence spectra were recorded on an Infinite® M1000 PRO microplate reader (Tecan). 30 µL of the boronic acid peptide tag (Fluorescein-Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys), 30 µL of the catechol peptide tag (Dyelight650®-AEEAc-Cat-Lys-Cat-Lys-Cat-Lys) and 30 µL of the mixture of both (every solution has a concentration of 1 mM of the peptide and was produced with phosphate buffer (300 mM, pH 7.4)) were placed in a black UV Star® 384 microliter well-plate (Greiner bio-one), each. The mixtures were stirred for 2 h at 450 rpm and measured with an excitation wavelength of 488 nm and the emission was recorded 550 nm – 850 nm.

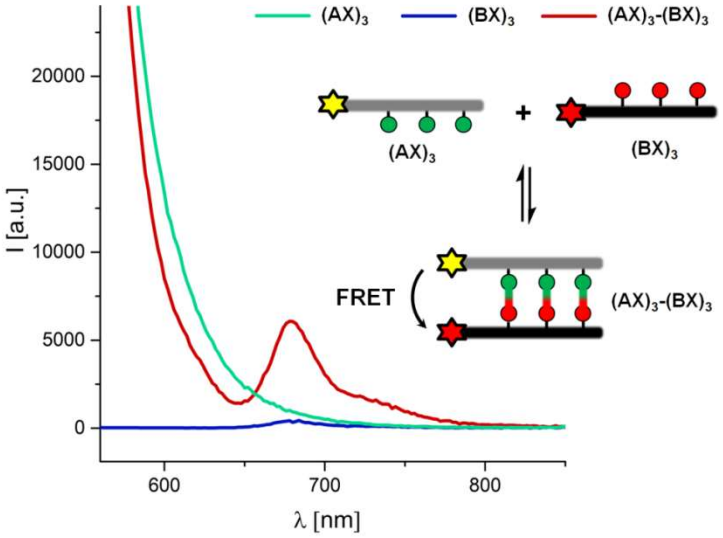


Figure S5. FRET of **$(AX)_3$-$(BX)_3$** binding in phosphate buffer pH 7.4

2.9 ^{1}H NMR Spectroscopy: TOCSY, NOESY, DOSY

The ^{1}H NMR data of **$(AX)_3$**, **$(BX)_3$** and **$(AX)_3$-$(BX)_3$** as well as **BAB** and **BAB-$(BX)_3$** were acquired on a Bruker Avance 850 MHz spectrometer equipped with a 5 mm TXI with a Z gradient. The measurements were performed at 298 K with a sample concentration of 2 mM in 300 mM phosphate buffer, pH 7.4, 9:1 (H_2O:D_2O). Chemical shifts were recorded in parts per million (ppm), using ^{1}H NMR resonance of H_2O to reference the ^{1}H NMR spectrum with the methyl resonance of TMS at 0.0 ppm, according to IUPAC recommended method.[5] Two-dimensional NMR spectra were analyzed using NMRFAM-SPARKY.[6] The proton resonances were assigned manually

with the standard method of using TOCSY (Total Correlations Spectroscopy)[7] fingerprints of the amino acids. Unfortunately, the backbone amide protons were not detectable, thus a sequential assignment was not possible. Additionally, the side chain amine protons of the Lysine groups were also not detectable. The numbering of the assigned groups is to differentiate between the individual amino acids, but shall not indicate the position of this amino acid in the peptide. Additionally, the assigned aromatic protons do not necessarily need to belong to the same numbered group of the H_α and side chain protons, due to the lack of scalar couplings between those two regions in the respective amino acids.

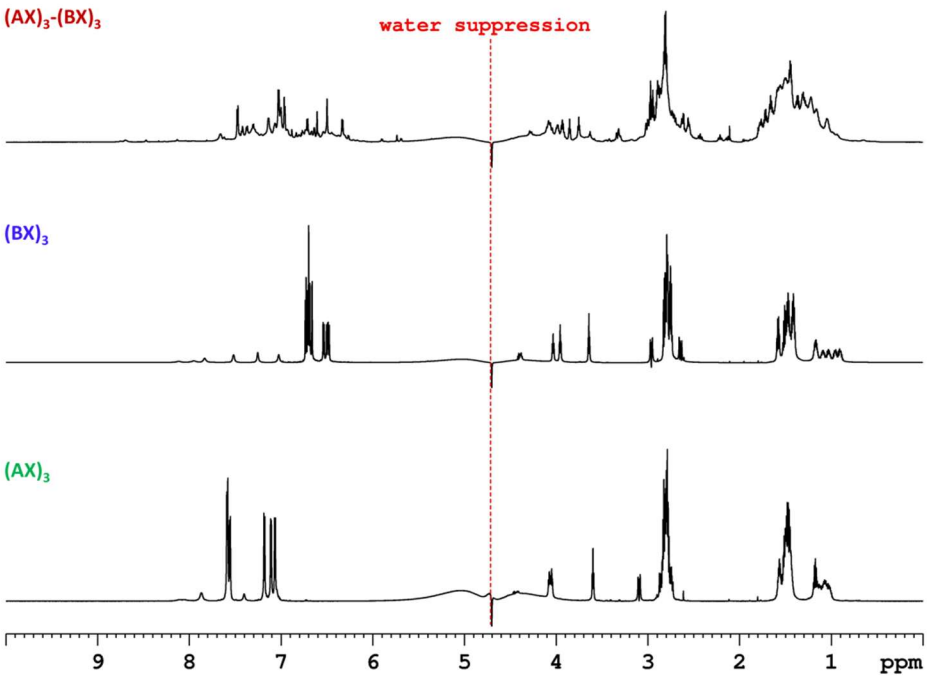


Figure S6. ^{1}H NMR of **$(AX)_3$-$(BX)_3$** and its separate constituents in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

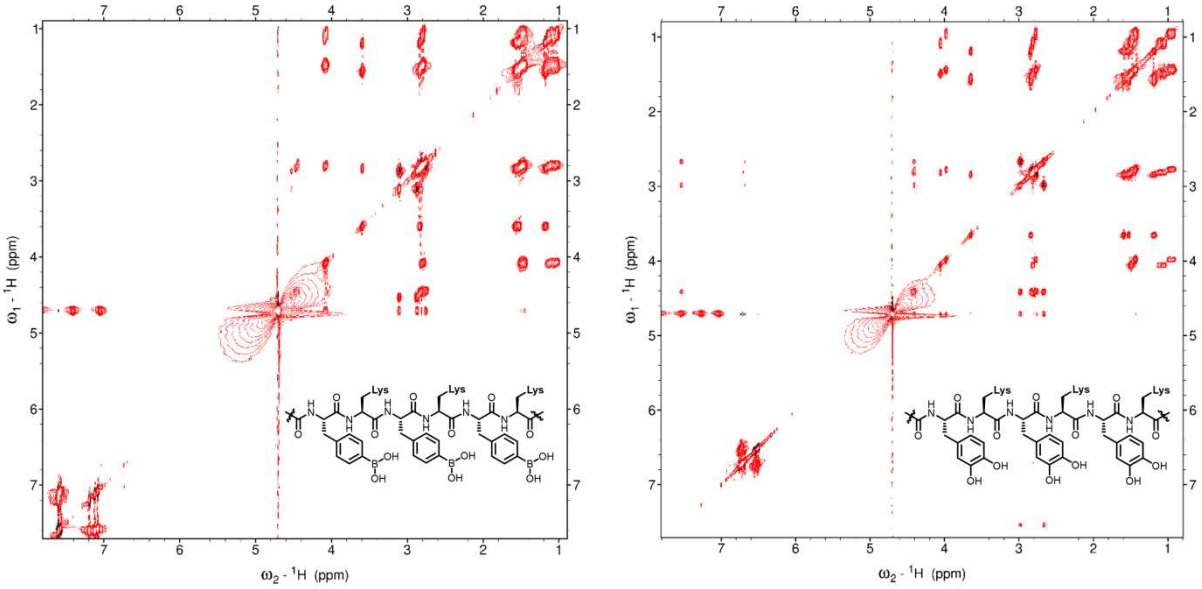


Figure S7. ^{1}H TOCSY NMR of **$(AX)_3$** (left) and **$(BX)_3$** (right) in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

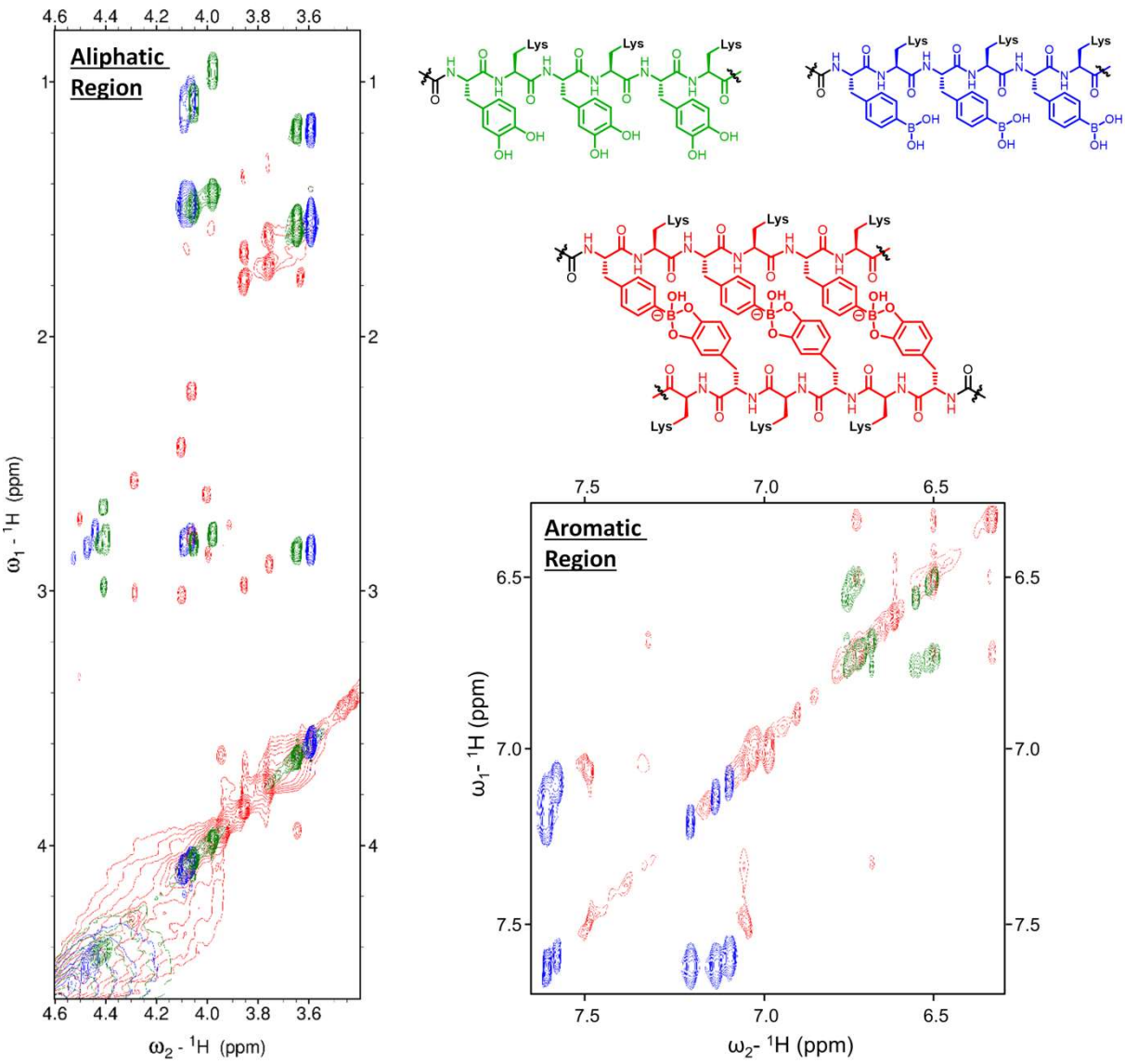


Figure S8. ^{1}H TOCSY NMR of **(AX)$_3$-(BX)$_3$** and its separate constituents in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

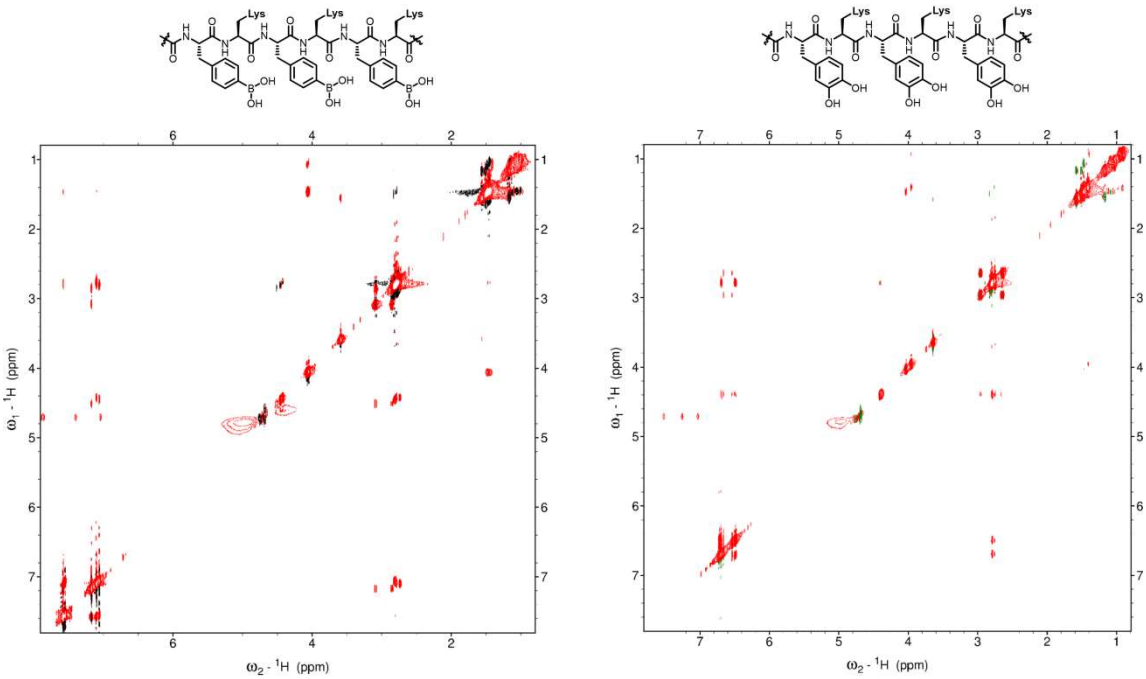


Figure S9. ^{1}H NOESY NMR of **(AX)$_3$** (left) and **(BX)$_3$** (right) in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

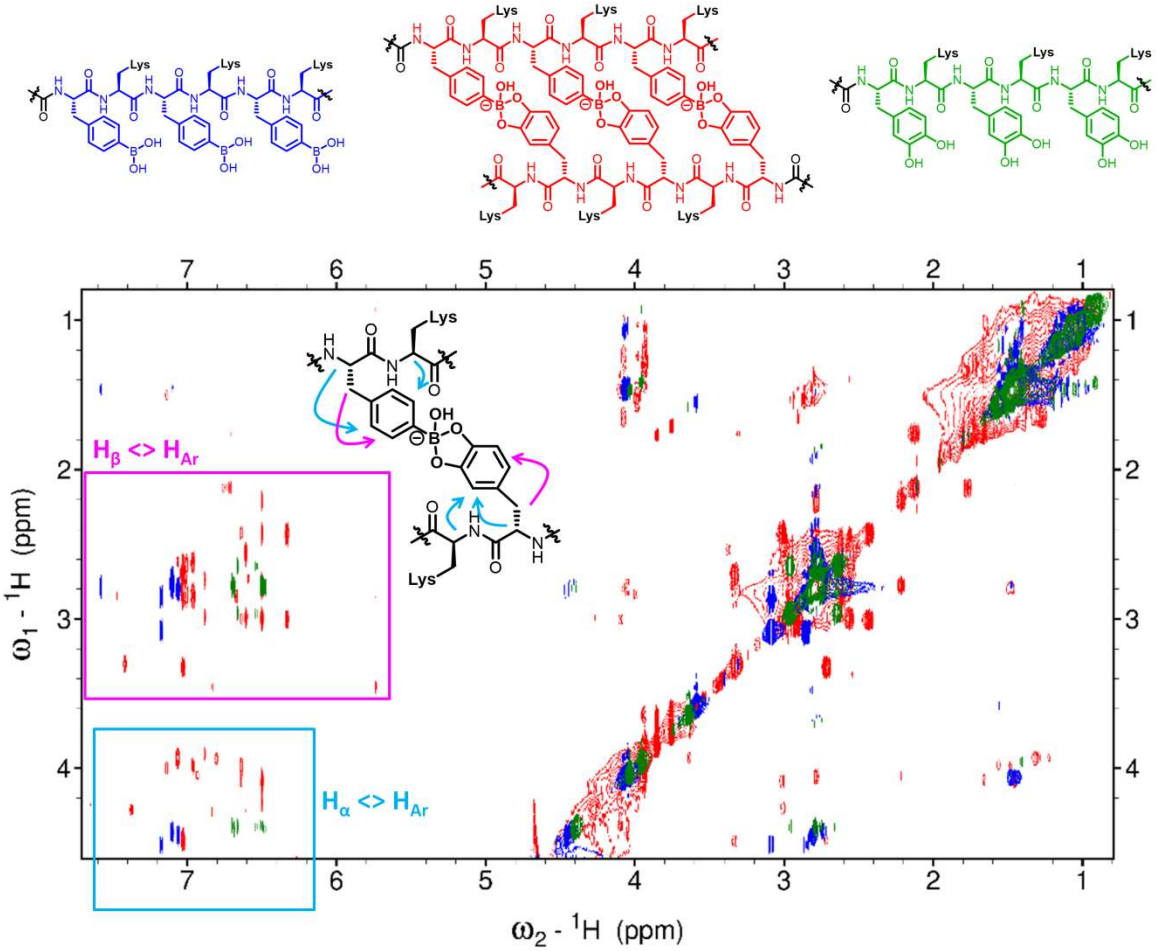


Figure S10. ^{1}H NOESY NMR of **(AX)$_3$-(BX)$_3$** and its separate constituents in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

Proton resonance assignment of $(AX)_3$:

Group	Atom	Nuc	Shift
BA1	HA	1H	4.532
BA1	HB1	1H	3.106
BA1	HB2	1H	2.871
BA1	HD#	1H	7.117
BA1	HE#	1H	7.597
K1	HA	1H	4.092
K1	HB#	1H	1.477
K1	HE#	1H	2.808
K1	HG#	1H	1.085
BA2	HA	1H	4.476
BA2	HB#	1H	2.829
BA2	HD#	1H	7.188
BA2	HE#	1H	7.602
K2	HA	1H	4.067
K2	HB#	1H	1.479
K2	HE#	1H	2.789
K2	HG#	1H	1.056
BA3	HA	1H	4.444
BA3	HB#	1H	2.765
BA3	HD#	1H	7.079
BA3	HE#	1H	7.572
K3	HA	1H	3.594
K3	HB#	1H	1.555
K3	HE#	1H	2.836
K3	HG#	1H	1.181

Proton resonance assignment of $(BX)_3$:

Group	Atom	Nuc	Shift
Cat1	HA	1H	4.428
Cat1	HB1	1H	2.812
Cat1	HB2	1H	2.773
Cat1	HD#	1H	6.557
Cat1	HE	1H	6.746
K1	HA	1H	4.056
K1	HB#	1H	1.493
K1	HD#	1H	1.116
K1	HE#	1H	2.817
K1	HG#	1H	1.053

Cat2	HA	1H	4.408
Cat2	HB1	1H	2.981
Cat2	HB2	1H	2.665
Cat2	HD#	1H	6.52
Cat2	HE	1H	6.72
K2	HA	1H	3.978
K2	HB#	1H	1.436
K2	HD#	1H	0.966
K2	HE#	1H	2.777
K2	HG#	1H	0.938
Cat3	HD#	1H	6.502
Cat3	HE	1H	6.709
K3	HA	1H	3.649
K3	HB1	1H	1.594
K3	HB2	1H	1.532
K3	HD#	1H	1.187
K3	HE#	1H	2.842

Diffusion Ordered NMR (DOSY)

The DOSY experiments with water suppression (stebpgp1s19) were executed with a 5 mm TXI $^{1}H/^{13}C/^{15}N$ z-gradient probe and a gradient strength of 5.516 [G/mm] on the 850 MHz spectrometer. The gradient strength was calibrated the diffusion coefficient of a sample of $^{2}H_2O/^{1}H_2O$ at a defined temperature of 298K and compared with the literature.

The temperature was defined with a standard ^{1}H methanol NMR sample. The control of the temperature was realized with a VTU (variable temperature unit) and an accuracy of +/- 0,1K, which was checked with the standard Bruker Topspin 3.6 software.

In this work, the gradient strength was varied in 32 steps from 2% to 100% and for each gradient 64 number of scans was used. The diffusion time d20 was optimised to 50 ms and the gradient length p30 was kept at 1.4 ms.

The 2D NMR sequences for measuring diffusion coefficient using echoes for convection compensation and longitudinal eddy current delays to store the magnetization in the z-axis, and only be dependent on T_1-relaxation. The calculation of the diffusion value was automatically done with the mono exponential function:

$$\ln\left(\frac{I(G)}{I(0)}\right) = -\gamma^2\delta^2G^2\left(\Delta - \frac{\delta}{3}\right)D,$$

where I(G) and I(0) are the intensities of the signals with and without gradient, γ the gyromagnetic ratio of the nucleus (^{1}H in this measurements), G is the gradient strength, δ the duration of the pulse field gradient (PFG), D the diffusion value in m^2/s and Δ the "diffusion time" between the beginning of the two gradient pulses. The relaxation delay between the scans was 3s.

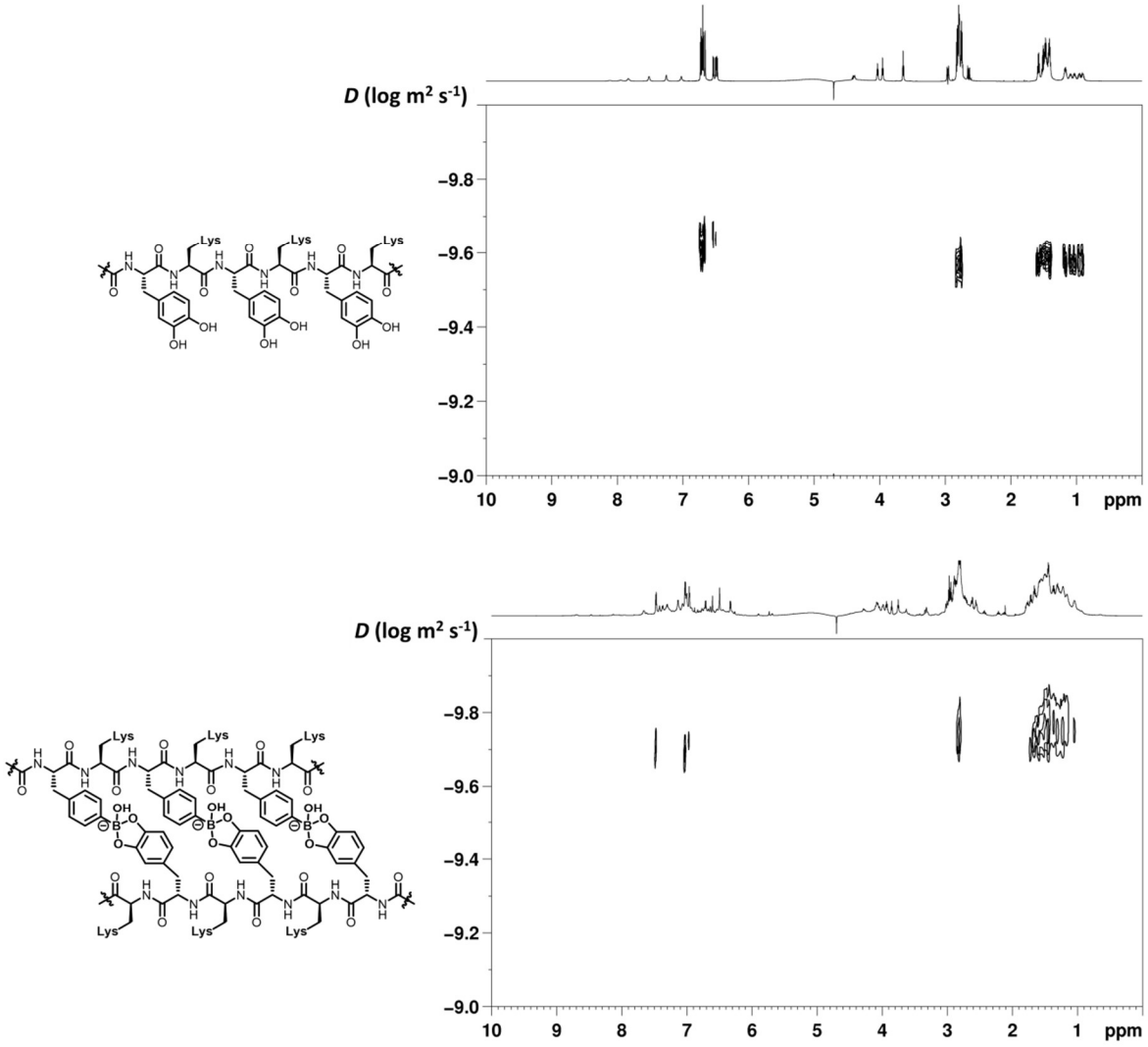


Figure S11. ^{1}H DOSY NMR of **(BX)$_3$ (top)** and **(AX)$_3$-(BX)$_3$** (bottom) in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

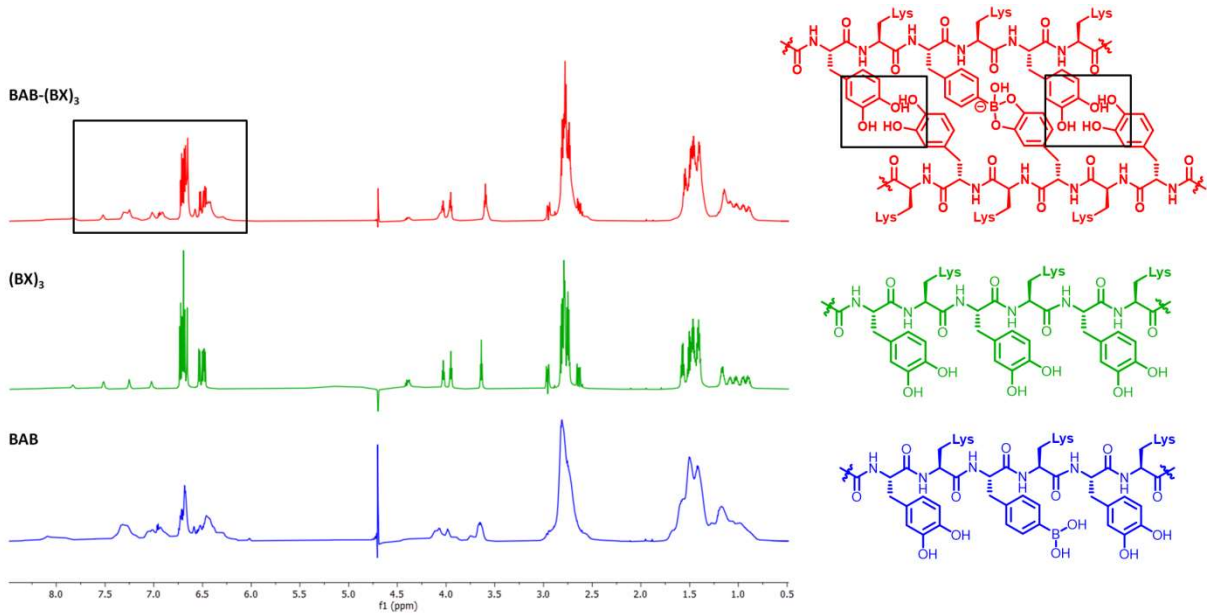


Figure S12. ^{1}H NMR of **BAB**, **(BX)$_3$** and the mismatched **BAB-(BX)$_3$** sequence in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

2.10 ^{11}B NMR Spectroscopy

^{11}B NMR Spectroscopy was conducted using a Bruker 700 MHz NMR Spectrometer at 298K. Samples were prepared at a concentration 25 mM in 300 mM phosphate buffer at pH 2.0, 5.0, 7.4, 10.0 or in DMSO-d_6. Background subtraction of the boro-silicate NMR tube was made using solvents without samples.

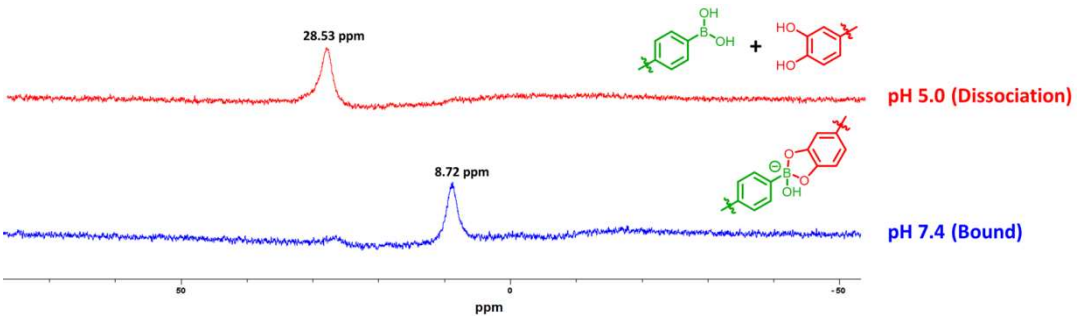


Figure S13. ^{11}B NMR of the pH-responsiveness of the boronic acid/catechol interaction.

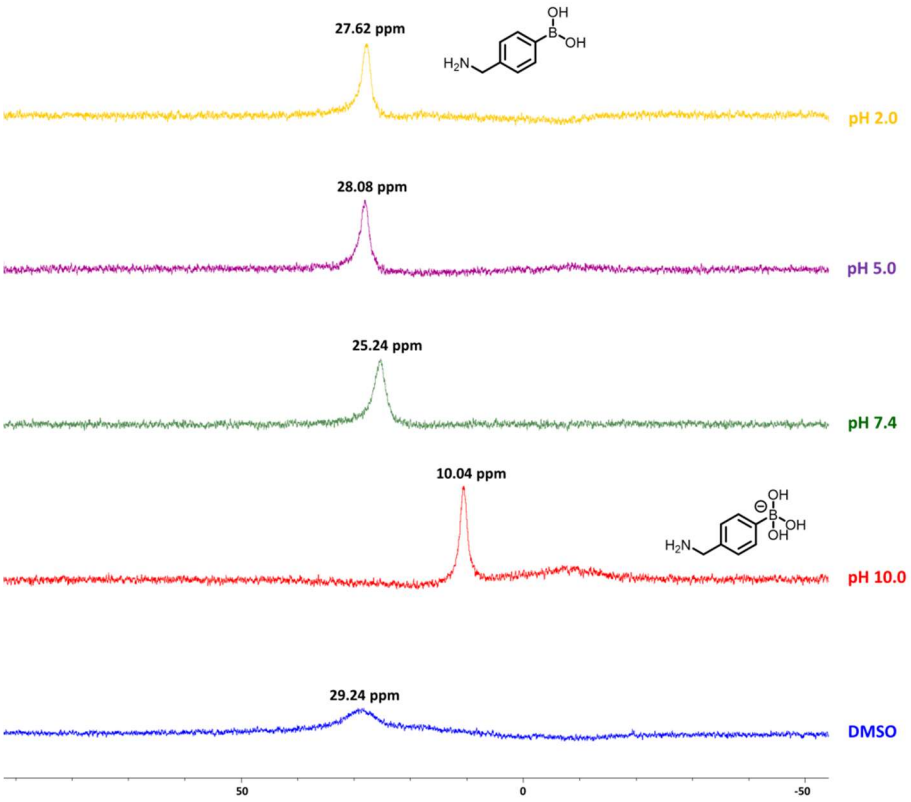


Figure S14. ^{11}B NMR of a water-soluble reference boronic acid (4-aminomethylphenylboronic acid) in different pH and solvents.

2.11 Variable Temperature ^{1}H NMR

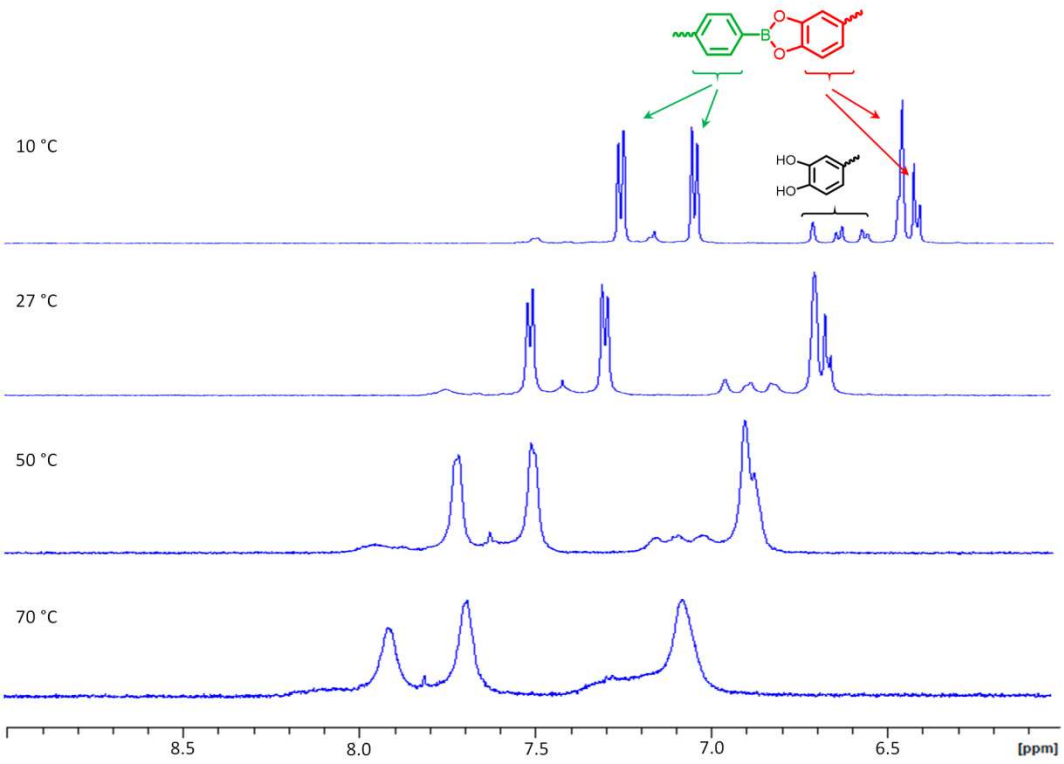


Figure S15. Variable temperature ^{1}H NMR of **(AX)$_1$-(BX)$_1$**.

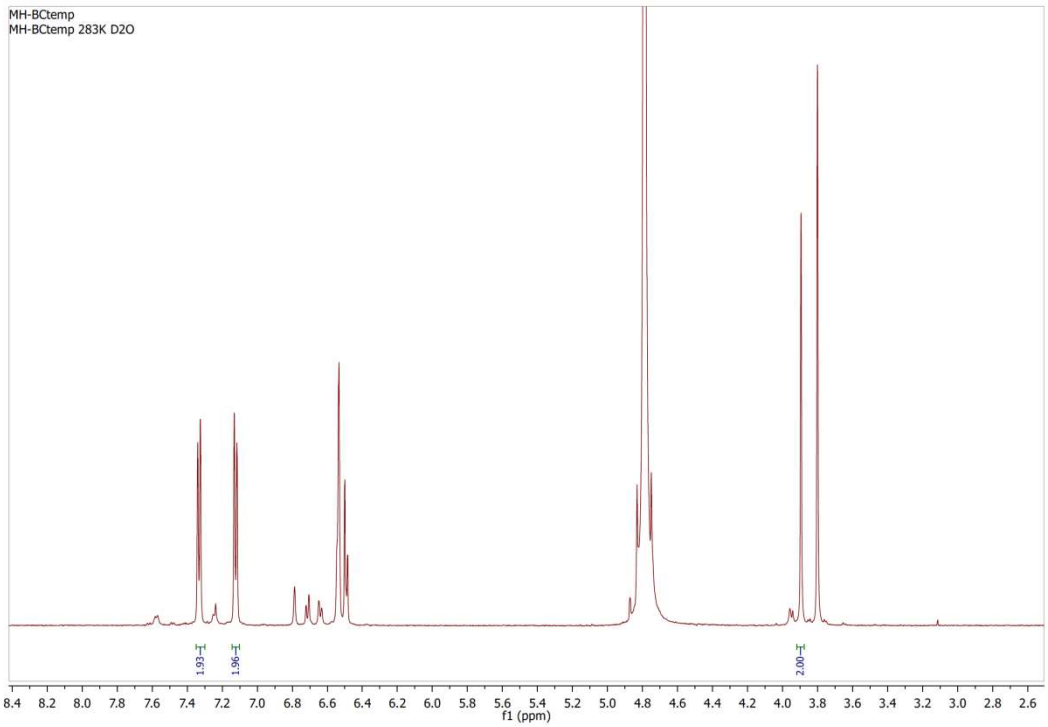


Figure S16. ^{1}H NMR of **(AX)$_1$-(BX)$_1$** at 283 K, 10 °C.

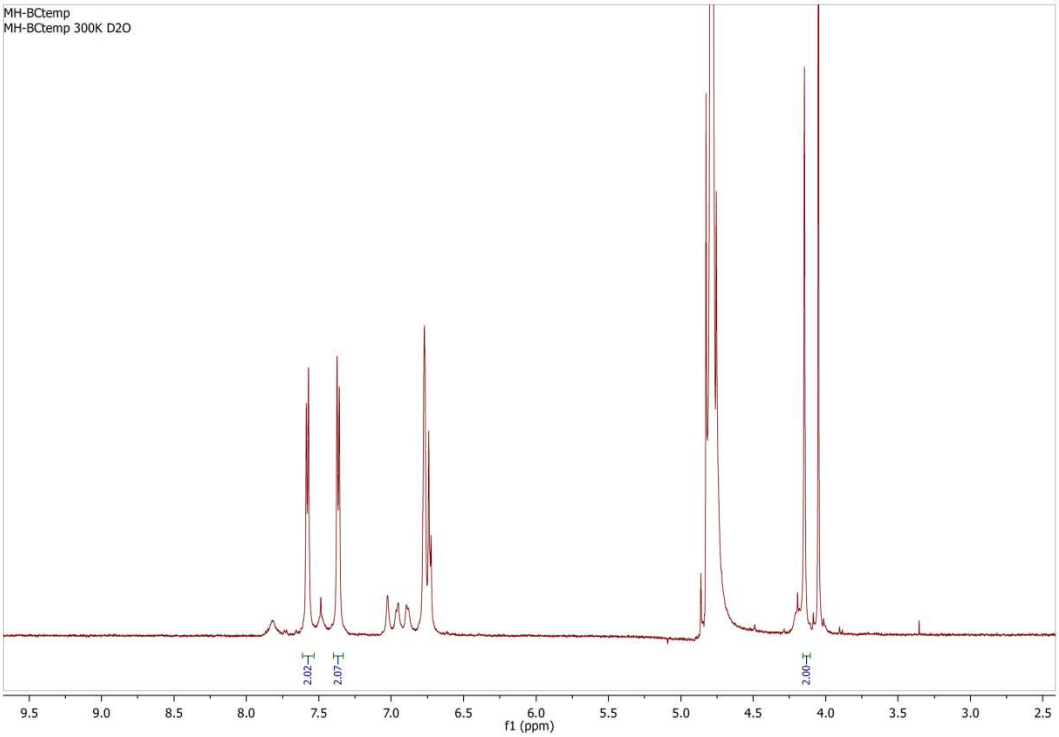


Figure S17. ^{1}H NMR of **(AX)$_1$-(BX)$_1$** at 300 K, 27 °C.

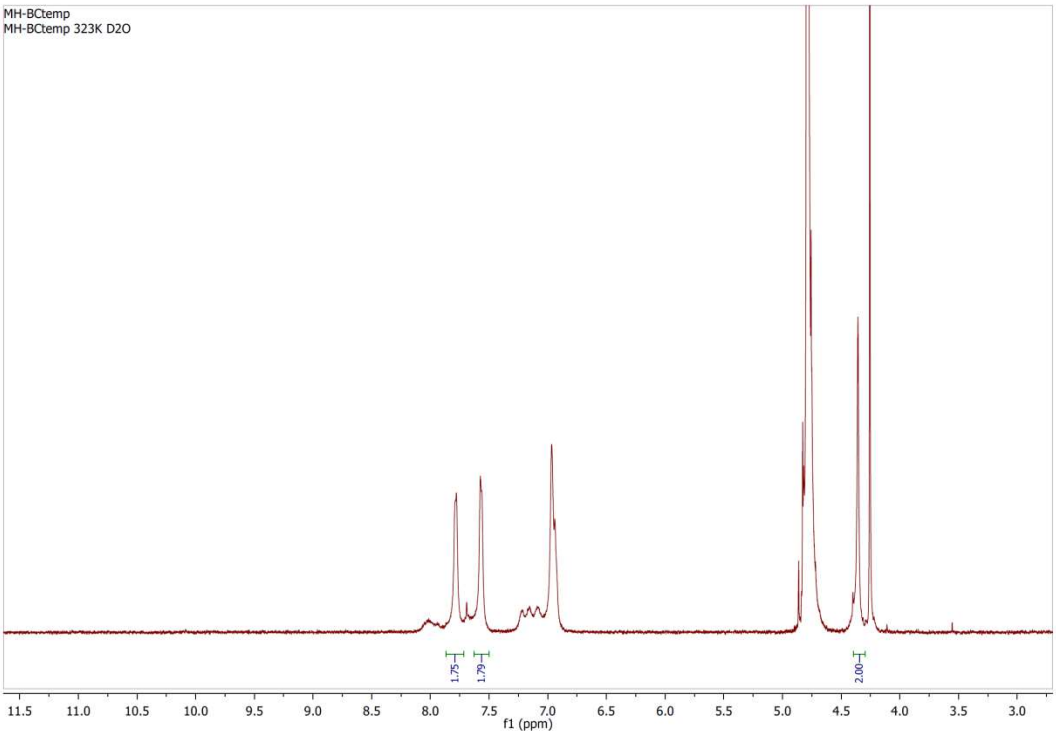


Figure S18. ^{1}H NMR of **(AX)$_1$-(BX)$_1$** at 323 K, 50 °C.

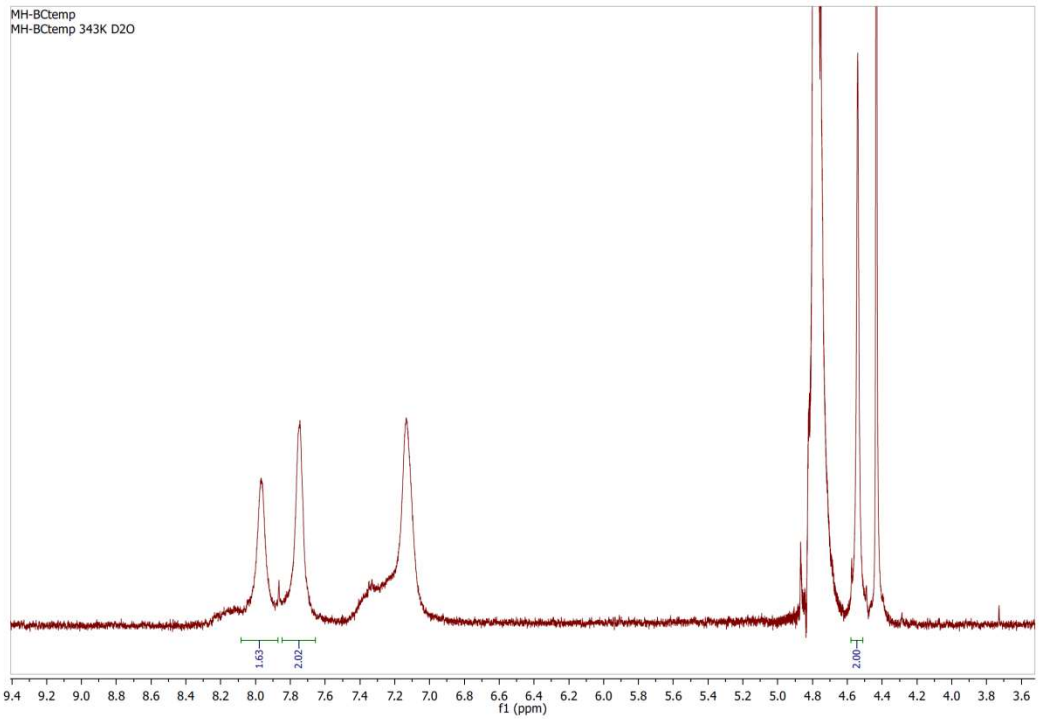
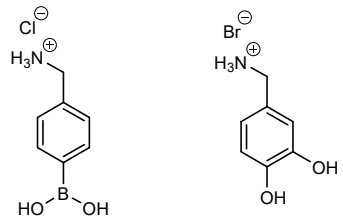


Figure S19. ^{1}H NMR of **(AX)$_1$-(BX)$_1$** at 343 K, 70 °C.

2.12 ATR FT-IR

For analysis of the binding by IR spectroscopy, a mixture of the trivalent peptides Lys-Cat-Lys-Cat-Lys-Cat-Lys and AEEAc-Bor-Lys-Bor-Lys-Bor-Lys (concentration of 0.462 mmol/L for each tag, equiv. 1:1) and a mixture of boronic acid **8** and catechol **9** (concentration of 3.57 mmol/L for each tag, equiv. 1:1) was stirred for 1 h phosphate buffer solution (100 mM, pH 7.4). The same process was done before the measurement of the separate (not mixed) peptides Lys-Cat-Lys-Cat-Lys-Cat-Lys and AEEAc-Bor-Lys-Bor-Lys-Bor-Lys. After the mixing the samples were frozen in liquid nitrogen and lyophilized. The ATR FT-IR spectra of the solid samples were recorded using a Bruker Tensor 27 spectrometer equipped with a diamond crystal as ATR element (PIKE Miracle™) with a spectral resolution of 1 cm^{-1}, each spectrum was an average of 20 scans.



8 **9**

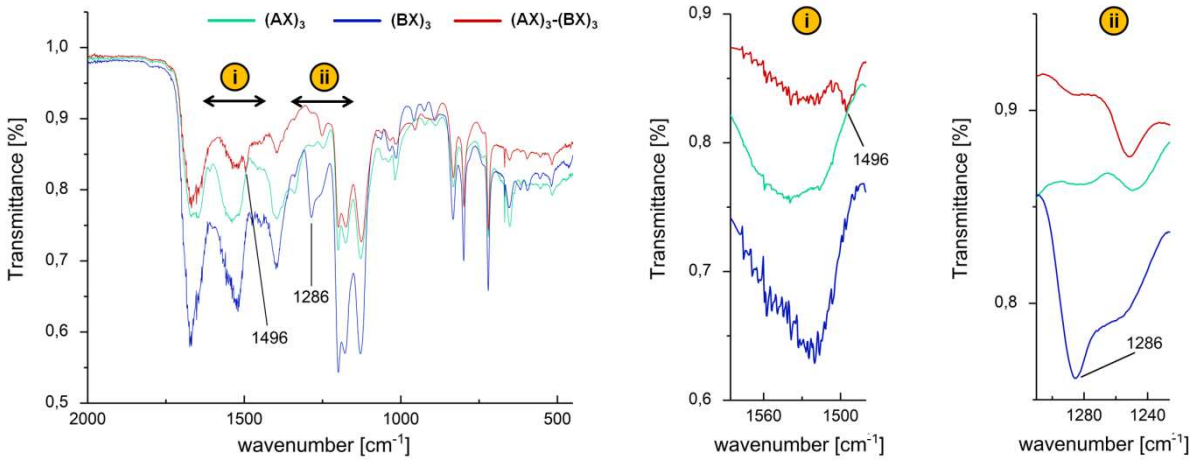


Figure S20. FTIR spectra of **$(AX)_3$-$(BX)_3$** and its separate constituents in phosphate buffer pH 7.4 H_2O/D_2O 9/1 with water suppression.

2.13 Circular Dichroism Spectroscopy

Solutions of **A_3X_3**, **B_3X_3**, **A_3X_3-B_3X_3** as well as **$(AX)_3$**, **$(BX)_3$**, **$(AX)_3$-$(BX)_3$** were each prepared at a concentration of 200 µM in 10 mM phosphate buffer, separately at pH 5.0 and 7.4. The solutions for the binding mixture **A_3X_3-B_3X_3** and **$(AX)_3$-$(BX)_3$** were incubated for at least 1 h at room temperature before measurement to ensure binding is complete. Measurements was conducted using the following parameters on a JASCO-1500 Circular Dichroism Spectrometer.

Path length: 0.1 mm
Scan rate: 5 nm/min
Scan range: 260 nm – 180 nm
Data pitch: 0.2 nm
Data Integration Time: 2 sec

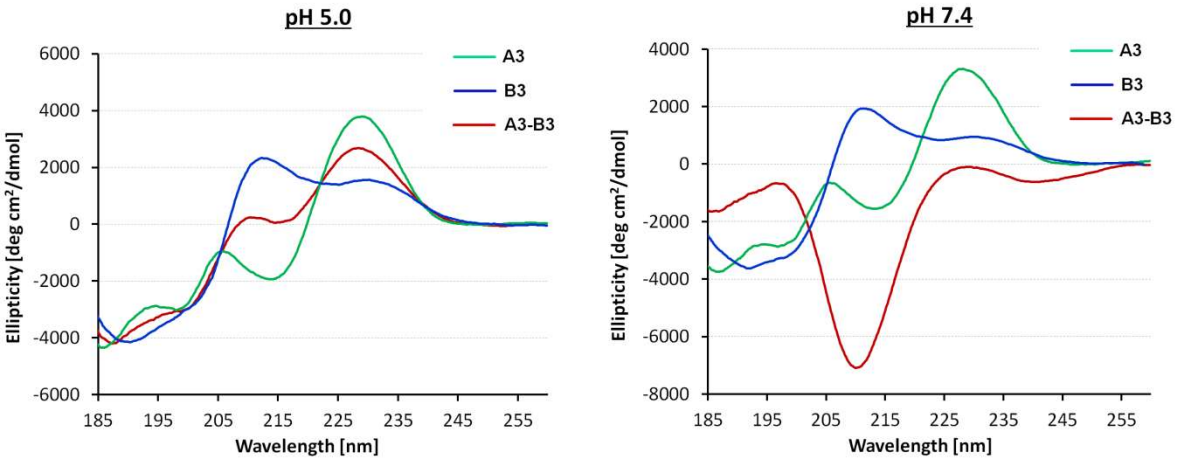


Figure S21. CD spectra of **(AX)$_3$**, **(BX)$_3$** and **(AX)$_3$-(BX)$_3$** at pH 5.0 (left) and pH 7.4 (right).

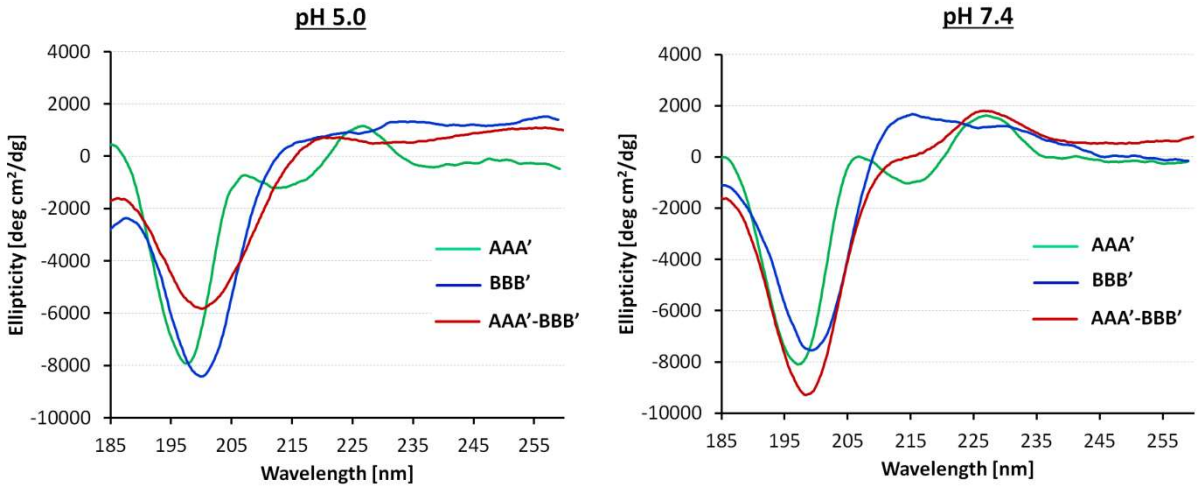


Figure S22. CD Spectra of A_3X_3, B_3X_3 and A_3X_3-B_3X_3 at pH 5.0 (left) and pH 7.4 (right)

2.14 DFT Calculations

DFT calculations were performed using the Gaussian 09 software package[8] and structural representations were generated with *CYLview*[9]. All the geometry optimizations were carried out at the B3LYP/6-31G(d) level of theory. All of the optimized geometries were verified by frequency computations as minima (zero imaginary frequencies) or transition states (a single imaginary frequency corresponding to the desired reaction coordinate). Single-point energy calculations on

the optimized geometries were then evaluated using the functional ωB97X-D[10] and def2-TZVPP basis set, with solvent effects (water) calculated by means of the Polarizable Continuum Model (PCM) initially devised by Tomasi and coworkers,[11] with radii and non-electrostatic terms of the SMD solvation model, developed by Truhler and co-workers.[12]

$(AX)_3$-$(BX)_3$ Structure

	ΔE (H) B3LYP/6-31G(d)	**ΔE (H) ωB97X-D /def2-TZVPP/SMD(water)**
$(AX)_3$-$(BX)_3$-i	-7136.40814413	-7137.69450679 (0.0)
$(AX)_3$-$(BX)_3$-ii	-7136.39862443	-7137.68553871 (5.6)
ABA-BAB-i	-7136.41072008	-7137.68930710 (3.3)

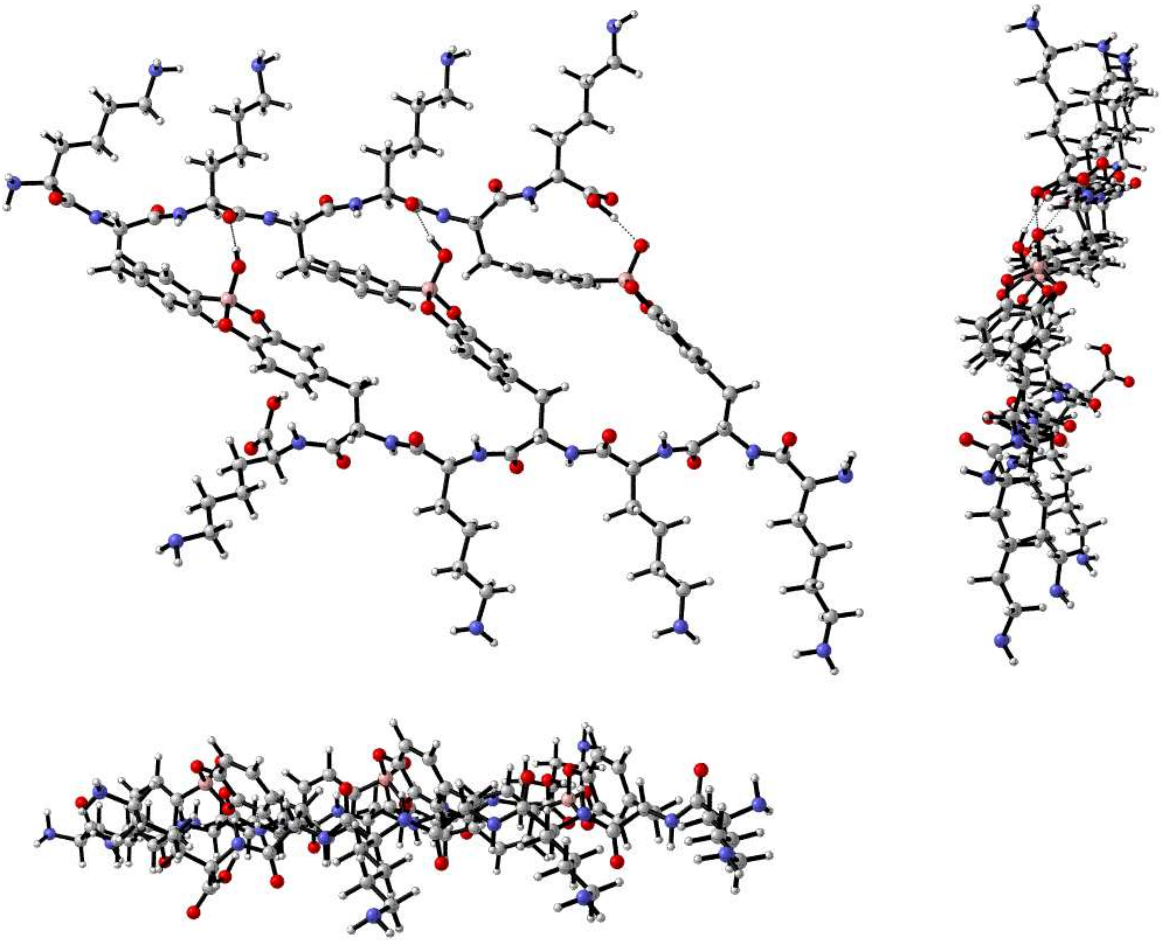


Figure S23. DFT optimized structure of (**$(AX)_3$-$(BX)_3$-i** (B3LYP/6-31G(d), side and bottom views included.

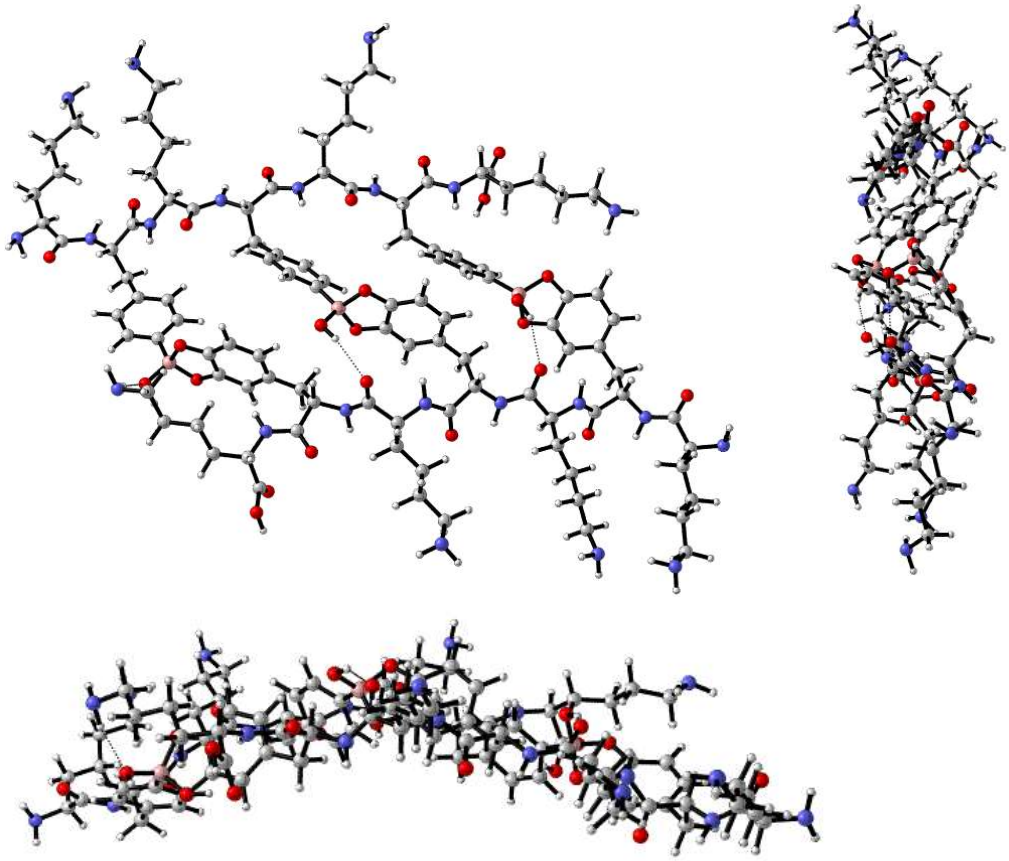


Figure S24. DFT optimized structure of **(AX)$_3$-(BX)$_3$-ii** (B3LYP/6-31G(d), side and bottom views included.

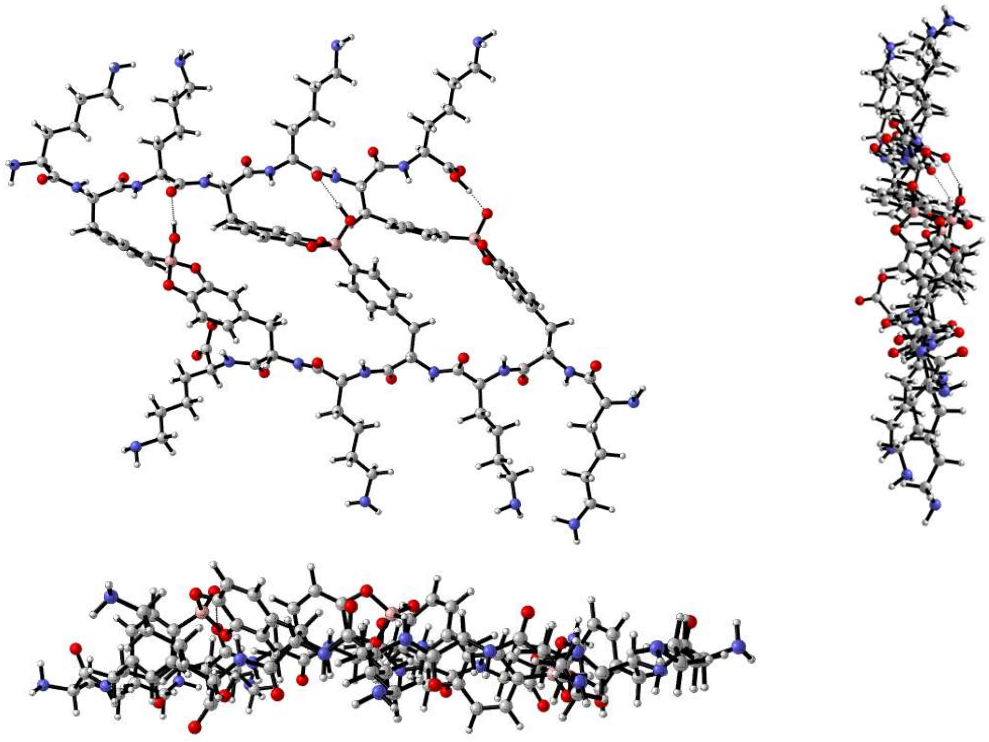
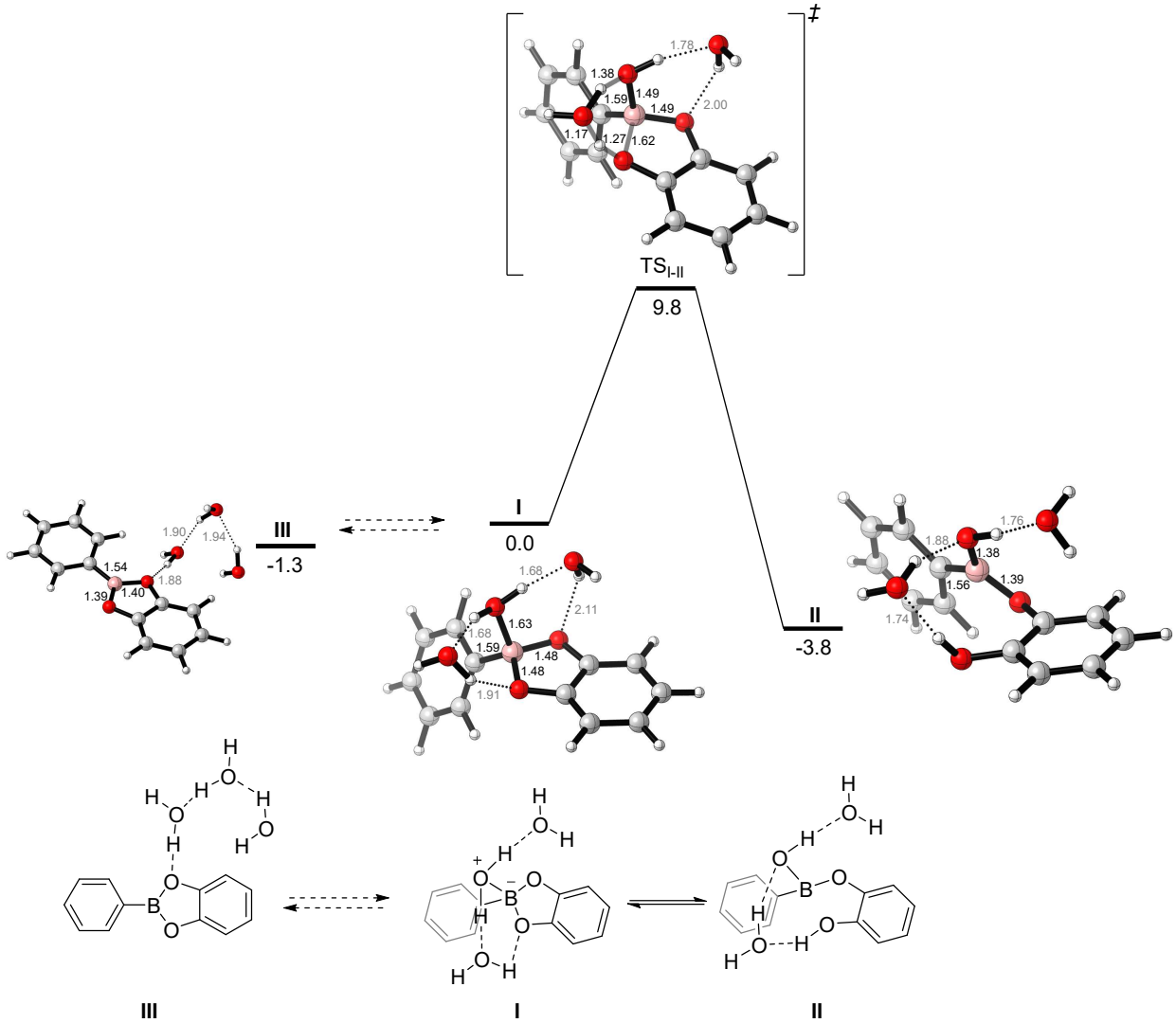


Figure S25. DFT optimized structure of **ABA-BAB-i** (B3LYP/6-31G(d), side and bottom views included.

Study of the dissociation mechanism (model structure)



III I II

Level of Theory		I	TS$_{I-II}$	II	III
B3LYP/6-31G(d)	**ΔE (H)**	-867.3838826	-867.3642104	-867.3827210	-867.3797646
	ΔG (H)	-867.169240	-867.153706	-867.170955	-867.170602
	ΔG rel (kcal mol^{-1})	0.0	9.7	-1.1	-0.9
ωB97X-D/ def2-TZVPP/ SMD(water)	**sp E (H)**	-867.502185137	-867.482401348	-867.505424349	-867.498778601
	ΔG$^{solv, corr}$ (H)	-867.287542565	-867.271896904	-867.293658391	-867.289615986
	ΔG^{solv} rel (kcal mol^{-1})	**0.0**	**9.8**	**-3.8**	**-1.3**

Figure S26. Free energy profile for the dissociation of I**.** DFT calculations were performed at the ωB97X-D /def2-TZVPP/SMD(water)//B3LYP/6-31G(d) level of theory. The distances shown are in Å, and energies are in kcal mol^{-1}.

Optimized Cartesian Coordinates

$(AX)_3$-$(BX)_3$-i

C	9.405461000	-17.658200000	-6.827205000
N	8.152797000	-17.159843000	-6.912273000
C	10.364134000	-16.885510000	-5.892238000
O	9.812786000	-18.632661000	-7.462554000
C	7.091819000	-17.667105000	-7.787678000
C	6.308213000	-16.406434000	-8.193230000
N	6.073347000	-16.234504000	-9.510534000
C	5.344537000	-15.098432000	-10.059129000
C	6.220404000	-18.704430000	-7.037363000
O	6.011871000	-15.575278000	-7.327038000
C	6.263781000	-13.901369000	-10.407615000
C	5.126719000	-19.370975000	-7.849778000
C	5.418894000	-20.048324000	-9.038060000
C	4.419621000	-20.723626000	-9.766763000
C	3.123972000	-20.722814000	-9.271597000
C	2.817356000	-20.055191000	-8.061694000
C	3.799350000	-19.372142000	-7.358615000
O	2.029289000	-21.290885000	-9.801303000
C	4.674627000	-15.596944000	-11.358826000
O	5.183168000	-16.517916000	-12.000595000
N	11.366039000	-17.779365000	-5.296889000
C	11.063616000	-15.773159000	-6.700690000
C	6.970257000	-13.246219000	-9.214649000
C	7.798001000	-12.019885000	-9.622448000
C	8.454711000	-11.325920000	-8.428423000
O	1.512517000	-20.180963000	-7.762057000
C	11.918235000	-14.835459000	-5.841219000
C	12.683856000	-13.797034000	-6.670559000
C	13.446598000	-12.785039000	-5.814721000
N	3.579797000	-14.909513000	-11.736764000
C	2.729468000	-15.263114000	-12.872964000
C	1.850492000	-14.026418000	-13.123102000
N	1.428624000	-13.838904000	-14.395415000
C	0.473332000	-12.797315000	-14.758102000
C	1.896414000	-16.531694000	-12.541295000
O	1.590212000	-13.250573000	-12.195901000
C	1.153121000	-11.462889000	-15.157448000
C	0.880758000	-16.958929000	-13.577289000
C	1.242177000	-17.264866000	-14.894318000
C	0.295530000	-17.752055000	-15.821508000
C	-1.011991000	-17.951189000	-15.397636000
C	-1.383954000	-17.630854000	-14.067202000

C	-0.460514000	-17.125637000	-13.167379000
O	-2.051017000	-18.448978000	-16.080357000
C	-0.313759000	-13.291397000	-15.987825000
O	0.229026000	-13.987620000	-16.843050000
C	1.947314000	-10.764381000	-14.048011000
C	2.497405000	-9.403634000	-14.496361000
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C	-4.124335000	-14.579633000	-18.407772000
C	-3.687559000	-14.576483000	-19.737506000
C	-4.581591000	-14.805163000	-20.812112000
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C	-6.391638000	-10.666539000	-17.989761000
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N	-2.960689000	-8.273236000	-24.236524000
O	-7.672189000	-15.332108000	-19.122987000
O	-6.809694000	-11.895086000	-17.672786000
C	-16.671836000	-16.188703000	-22.536838000
N	-15.996276000	-15.778217000	-21.435112000
C	-18.209079000	-16.286235000	-22.399744000
O	-16.128648000	-16.493841000	-23.600275000
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N	-13.223908000	-17.201122000	-19.618901000
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C	-13.762840000	-19.173480000	-18.248342000
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C	-11.573807000	-15.537820000	-22.253819000
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N	-18.874289000	-15.912327000	-23.656823000
C	-18.609209000	-17.732489000	-22.024040000
C	-13.882273000	-19.790347000	-16.849185000
C	-14.719921000	-21.075564000	-16.870910000
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C	-7.277211000	-17.359103000	-16.247314000
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B	-3.179060000	-18.677883000	-15.074800000
C	-6.794688000	-20.685430000	-13.493208000
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C	-9.741620000	-23.817885000	-12.074155000
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C	-2.551592000	-23.249692000	-8.515843000
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H	1.662633000	-8.762373000	-14.822438000
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H	-18.079558000	-21.664756000	-17.647517000
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H	-14.180421000	-13.853276000	-20.774220000
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H	-19.688174000	-17.822855000	-22.201008000

H	-18.114884000	-18.413812000	-22.731424000
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H	-4.806449000	-30.164685000	-7.008377000
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$(AX)_3$-$(BX)_3$-ii

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O	9.511920000	-18.573525000	-7.151549000
C	6.792721000	-17.555505000	-7.340533000
C	6.164067000	-16.284091000	-7.939979000
N	5.965738000	-16.269563000	-9.275565000
C	5.381125000	-15.138940000	-9.986657000
C	5.799639000	-18.362651000	-6.472550000
O	5.956451000	-15.308619000	-7.208438000
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O	1.616345000	-21.142744000	-9.053862000
C	4.621604000	-15.723116000	-11.196389000
O	4.996265000	-16.772232000	-11.719229000
N	11.408159000	-17.341232000	-5.475468000
C	10.715058000	-15.627534000	-7.113947000
C	7.100179000	-13.281610000	-9.398240000
C	8.179696000	-12.332345000	-9.938958000
C	8.657945000	-11.335732000	-8.881686000
O	1.050796000	-19.691252000	-7.257575000
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O	1.612024000	-13.283109000	-12.143569000
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C	-6.221701000	-17.902613000	-15.550696000
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N	4.328657000	-7.707020000	-14.092409000
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N	9.797827000	-10.532788000	-9.367804000
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N	-4.060167000	-11.549947000	-18.220069000
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C	-3.017347000	-14.345817000	-17.290511000
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C	-5.218561000	-10.011218000	-19.757973000
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O	-6.830527000	-14.936237000	-21.434776000
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H	-3.055693000	-0.615144000	-0.331712000
H	-1.391620000	-0.728371000	1.487488000
H	-2.133869000	-0.721562000	3.861745000
H	-4.560371000	-0.586794000	4.392979000
O	-6.828115000	-3.417457000	-0.239008000
H	-7.311057000	-2.646203000	0.131601000
H	-6.315560000	-3.764698000	0.508893000

H	-5.848418000	-2.354244000	-1.091774000
O	-5.969031000	-0.140848000	-3.556808000
H	-5.682580000	0.600649000	-2.988082000
H	-6.916112000	0.032196000	-3.685440000

TS_{I-II}

C	-5.001298000	0.141950000	2.119884000
C	-4.705766000	-0.525035000	0.917436000
B	-5.721541000	-0.493825000	-0.308121000
C	-8.078739000	-0.000013000	-0.286811000
C	-7.373504000	1.049635000	-0.886298000
O	-6.027407000	0.851528000	-0.869335000
O	-7.195579000	-0.949080000	0.197202000
O	-5.350634000	-1.449389000	-1.384736000
C	-8.051331000	2.137179000	-1.421433000
C	-9.453661000	2.142613000	-1.342205000
C	-10.147859000	1.090173000	-0.745667000
C	-9.458407000	-0.006355000	-0.199719000
C	-3.475781000	-1.197223000	0.837369000
C	-2.577398000	-1.207820000	1.907618000
C	-2.894802000	-0.539292000	3.090261000
C	-4.112717000	0.138536000	3.194468000
H	-5.945952000	0.673325000	2.216901000
H	-5.396549000	-1.021117000	-2.277256000
H	-7.505190000	2.959042000	-1.875018000
H	-10.003180000	2.985270000	-1.752223000
H	-11.232218000	1.116117000	-0.693979000
H	-9.985039000	-0.828155000	0.276158000
H	-3.220176000	-1.715283000	-0.083417000
H	-1.630162000	-1.734836000	1.817407000
H	-2.198779000	-0.544022000	3.925796000
H	-4.366175000	0.663320000	4.112727000
O	-7.017615000	-3.109255000	-0.799501000
H	-7.314858000	-2.150240000	-0.206010000
H	-6.653604000	-3.761799000	-0.175659000
H	-6.172529000	-2.554178000	-1.231617000
O	-5.454233000	0.232011000	-3.539269000
H	-5.452110000	0.852268000	-2.782196000
H	-6.350998000	0.313873000	-3.900280000

II

C	-4.483857000	0.321601000	2.370606000
C	-4.365638000	-0.304516000	1.116924000
B	-5.423483000	-0.070961000	-0.005612000
C	-8.421717000	-0.133709000	-0.274264000
C	-7.560318000	0.971373000	-0.443891000
O	-6.329244000	0.969811000	0.157086000
O	-8.021562000	-1.152174000	0.540976000
O	-5.378773000	-0.844779000	-1.139963000
C	-7.963792000	2.072224000	-1.201783000

C	-9.216696000	2.072162000	-1.825544000
C	-10.063867000	0.969797000	-1.684761000
C	-9.669378000	-0.119879000	-0.904556000
C	-3.262749000	-1.151603000	0.904201000
C	-2.314654000	-1.368374000	1.903607000
C	-2.453467000	-0.736894000	3.142113000
C	-3.540154000	0.109664000	3.375040000
H	-5.330247000	0.977842000	2.553396000
H	-5.917625000	-0.526703000	-1.908756000
H	-7.284492000	2.914862000	-1.295506000
H	-9.526812000	2.932095000	-2.412729000
H	-11.036533000	0.962772000	-2.168269000
H	-10.324732000	-0.975235000	-0.767547000
H	-3.149091000	-1.638490000	-0.061167000
H	-1.467562000	-2.024658000	1.719496000
H	-1.715973000	-0.903635000	3.923569000
H	-3.650007000	0.601008000	4.338565000
O	-6.857563000	-3.201538000	-0.754161000
H	-7.816408000	-1.976830000	0.025256000
H	-6.477043000	-3.724150000	-0.030916000
H	-6.153554000	-2.555098000	-0.981997000
O	-6.735207000	-0.008509000	-3.377284000
H	-6.164422000	0.604541000	-3.865683000
H	-7.482639000	0.538651000	-3.076134000

III

C	-3.908621000	-0.366476000	1.240394000
C	-4.947371000	-1.294574000	1.446565000
B	-6.283948000	-1.191494000	0.684303000
C	-8.296834000	-1.662139000	-0.100004000
C	-7.899645000	-0.449641000	-0.658538000
O	-6.632966000	-0.134660000	-0.168304000
O	-7.302172000	-2.131690000	0.738048000
O	-7.427170000	3.094225000	-2.559934000
C	-8.681108000	0.264916000	-1.548025000
C	-9.923342000	-0.311191000	-1.857151000
C	-10.333302000	-1.528121000	-1.298971000
C	-9.520107000	-2.235323000	-0.401189000
C	-4.734406000	-2.339098000	2.365996000
C	-3.530148000	-2.450320000	3.058346000
C	-2.512421000	-1.518300000	2.840575000
C	-2.702219000	-0.476250000	1.929505000
H	-4.044984000	0.444999000	0.529608000
H	-7.080239000	3.318236000	-1.680935000
H	-8.348701000	1.210826000	-1.978415000
H	-10.580676000	0.205740000	-2.549947000
H	-11.302930000	-1.938065000	-1.566333000
H	-9.825577000	-3.179936000	0.035942000
H	-5.523232000	-3.067197000	2.535298000
H	-3.382526000	-3.262096000	3.765511000

H	-1.571874000	-1.604922000	3.378379000
H	-1.908913000	0.245960000	1.755800000
O	-4.731365000	2.405258000	-3.180861000
H	-4.759695000	1.458449000	-3.385849000
H	-4.704876000	2.436468000	-2.202458000
H	-6.597915000	2.922261000	-3.053712000
O	-5.441272000	2.442772000	-0.453541000
H	-5.913309000	1.597421000	-0.310346000
H	-5.121184000	2.713860000	0.419685000

2.15 Fluorescence Binding of A_3X_3 and B_3X_3

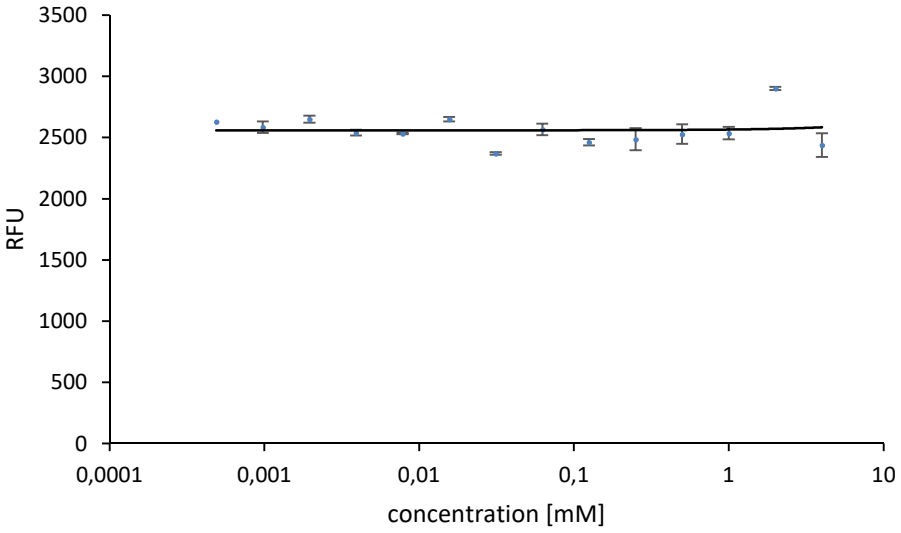

Figure S27. Fluorescence titration of **A_3X_3** against fluorescein labelled **B_3X_3** in 300 mM phosphate buffer, pH 7.4, using the same protocol detailed in Section 7.

2.16 Displacement experiment (Fluorescence Quenching Assay + FRET Assay)

Fluorescence spectra were recorded on an Infinite® M1000 PRO microplate reader (Tecan®). 15 µL of different concentrations of the Lys-Cat-Lys peptide was served (dilutions series with half-to-half concentrations beginning with 5.0 mM, phosphate buffer 300 mM, pH 7.4). To this a constant amount of the Fluorescein-Cys-AEEAc-Bor-Lys-Bor-Lys-Bor-Lys peptide (conc. 110 nM, vol. 15 µL) was added. After mixing for 1 h at 450 rpm, 26 µL of every mixture was placed in black UV Star® 384 microliter well-plates (Greiner bio-one). After 15 min of equilibration time, the fluorescence emission was recorded at 520 nm upon excitation at 488 nm with multiple reads per well (3x3).

After that a dilution series of a trivalent Catechol-tag (Dyelight650®-AEEAc-Cat-Lys-Cat-Lys-Cat-Lys) with 1/3 of the molar amount of the Lys-Cat-Lys peptide was made (26 µL each, phosphate buffer 300 mM, pH 7.4) and dropped into the mixtures. After that the mixtures were stirred for 2 h at 450 rpm and measured with an excitation wavelength of 488 nm and the emission was recorded from 280 nm to 850 nm.

2.17 Alizarin Red S Assay

Fluorescence spectra were recorded on an Infinite® M1000 PRO microplate reader (Tecan®). PEG_{5000}-**$(AX)_3$** (0.104 mM, 1 eq.) and Alizarin Red S (0.313 mM, 1 eq.) was mixed for 90 minutes in a phosphate buffer solution (pH 7.4, 300mM). After that CytC-**$(BX)_3$** was added resulting in a PEG_{5000}-**$(AX)_3$** concentration of 0.09 mM and an Alizarin Red S concentration of 0.27 mM.

The resulting concentrations of CytC-**$(BX)_3$** in the dilution serial is showed in the following table:

Dilution	c [mM]
1	0.09
2	0.045
3	0.0225
4	0.00562
5	0.00281
6	0.00141
7	7.03E-04

The resulting solutions were mixed for 12 h at room temperature. The excitation wavelength was 495 nm and the fluorescence intensity was measured at 556 nm.

2.18 Atomic Force Microscopy

AFM measurements were conducted on a Dimension FastScan Bio™ atomic force microscope from Bruker, which was operated in the PeakForce mode. AFM probes with a nominal spring constant of 0.25 Nm^{-1} were employed (FastScan-D, Bruker) for measurement in liquid. A circular mica disc (15 mm) was used as the substrate. Measurements were performed at scan rates between 0.8 and 2 Hz. Different areas of the mica substrate were scanned in order to ensure the integrity of the shown images. The images were finally processed by the software NanoScope Analysis 1.8.

For sample preparation, the initial sample (conc. **PEG_{5000}-$(AX)_3$**/**CytC-$(BX)_3$** mixture was 1 mM, solvent: phosphate buffer (150 mM, pH 7.4)) was diluted to 25 µM with 40 µL phosphate buffer (75 mM) and subsequently applied onto the freshly cleaved mica substrate. The solution was left to incubate for 15 minutes in order to deposit the desired species on the mica substrate. After successful adsorption, the supernatant was removed and fresh phosphate buffer (250 µL) was added for the measurement.

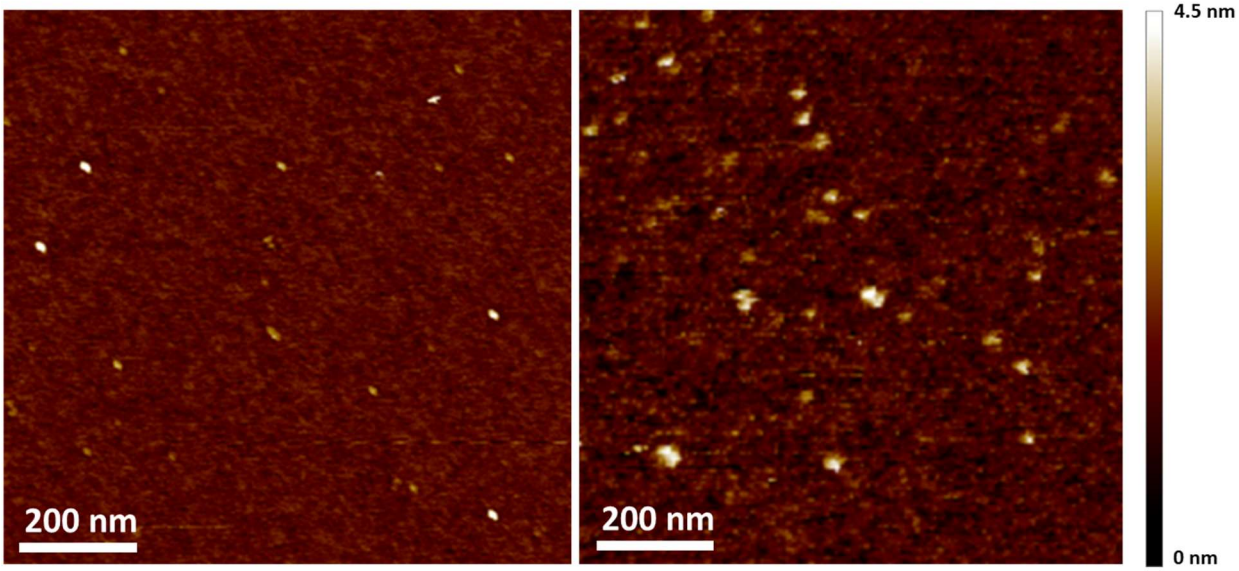

Figure S28. AFM micrograph of **PEG_{5000}-$(AX)_3$** (left) and **PEG_{5000}-$(AX)_3(BX)_3$-CytC** (right).

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