

Supporting Information for

## “Two-channel image analysis method for the screening of OBOC libraries”

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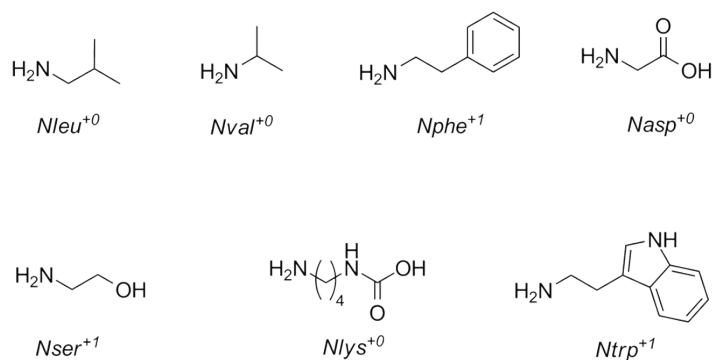


Figure S1 Submonomers for peptoid library synthesis. *Nasp<sup>+0</sup>* was used as a tertbutyl ester, *Nser<sup>+1</sup>* was reacted as triisopropylsilylether, *Nlys<sup>+0</sup>* and *Ntrp<sup>+1</sup>* were Boc-protected.

Table T1 Highly hydrophobic peptoid sequences discovered in the screen. The peptoids were not investigated any further due to their low solubility and bioavailability that renders them unattractive for application as CXCL8 inhibitors.

Peptoid	Sequence
30	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nval <sup>+1</sup> -H
31	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nleu <sup>+0</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nval <sup>+0</sup> -H
32	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> -H
33	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nval <sup>+0</sup> Ntrp <sup>+1</sup> Nval <sup>+0</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> -H
34	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nleu <sup>+0</sup> Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> -H
35	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nval <sup>+0</sup> -H
36	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nval <sup>+0</sup> Nval <sup>+0</sup> -H
37	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> Nphe <sup>+1</sup> Nval <sup>+0</sup> -H
38	H <sub>2</sub> N-Ahx-Nval <sup>+0</sup> Nleu <sup>+0</sup> Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Ntrp <sup>+1</sup> Nval <sup>+0</sup> -H
39	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nval <sup>+0</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> Nphe <sup>+1</sup> Nval <sup>+0</sup> -H
40	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nval <sup>+0</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> -H
41	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Ntrp <sup>+1</sup> Nleu <sup>+0</sup> Nleu <sup>+0</sup> Nser <sup>+1</sup> Nval <sup>+0</sup> -H
42	H <sub>2</sub> N-Ahx-Nleu <sup>+0</sup> Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nleu <sup>+0</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> -H
43	H <sub>2</sub> N-Ahx-Ntrp <sup>+1</sup> Nphe <sup>+1</sup> Nphe <sup>+1</sup> Nleu <sup>+0</sup> Nleu <sup>+0</sup> Nval <sup>+0</sup> -H

Fluorescence Anisotropy Data of peptoids 1-17 and 29

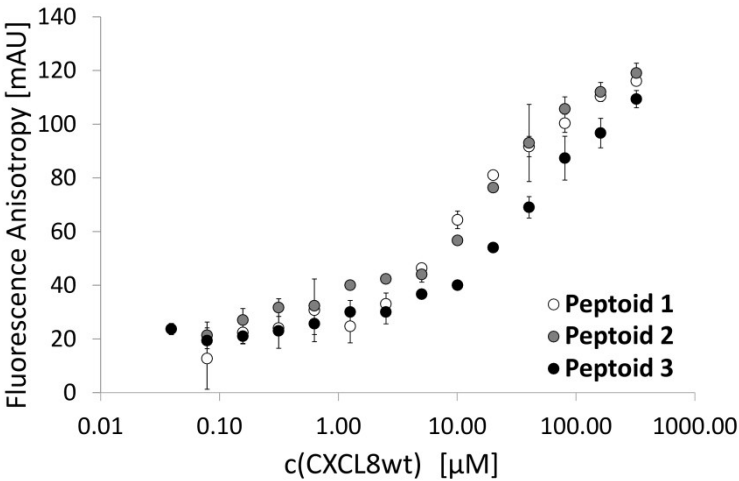


Figure S2 Fluorescence Anisotropy measurements with fluorescently labelled peptoids 1-3 (20 nM respectively in low-salt PBS).

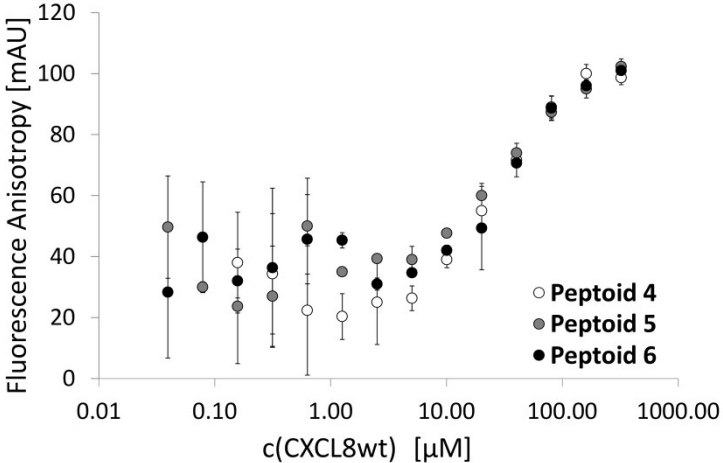


Figure S3 Fluorescence anisotropy measurements with fluorescently labelled peptoids 4-6 (50 nM respectively in low-salt PBS).

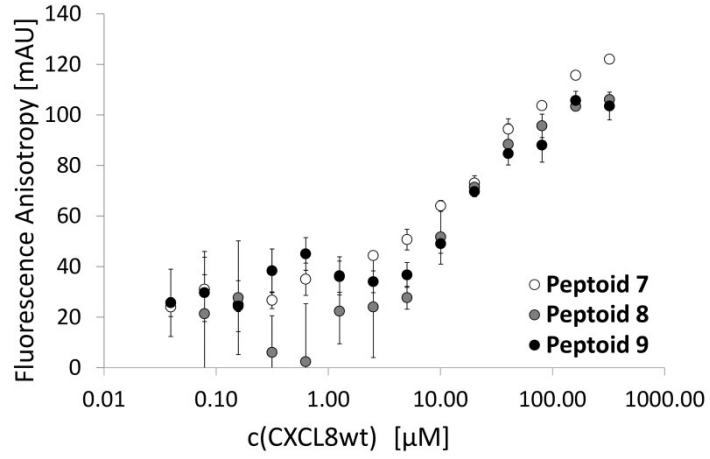


Figure S4 Fluorescence anisotropy measurements with fluorescently labelled peptoids 7 (20 nM), peptoid 8 (50 nM) and peptoid 9 (20 nM) in low-salt PBS.

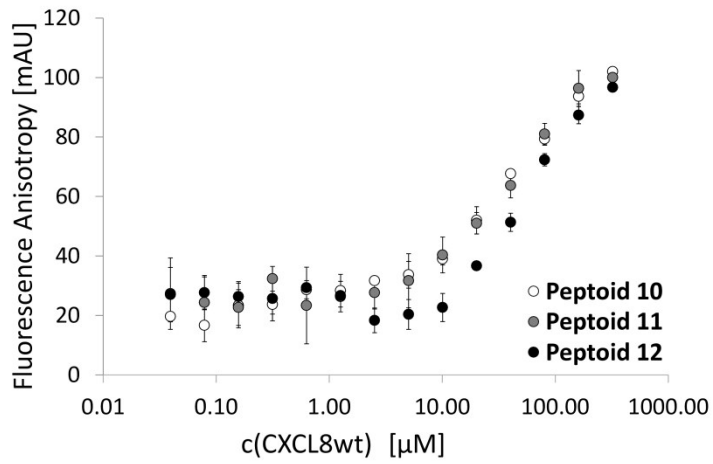


Figure S5 Fluorescence anisotropy measurements with fluorescently labelled peptoids 10-12 (50 nM respectively in low-salt PBS).

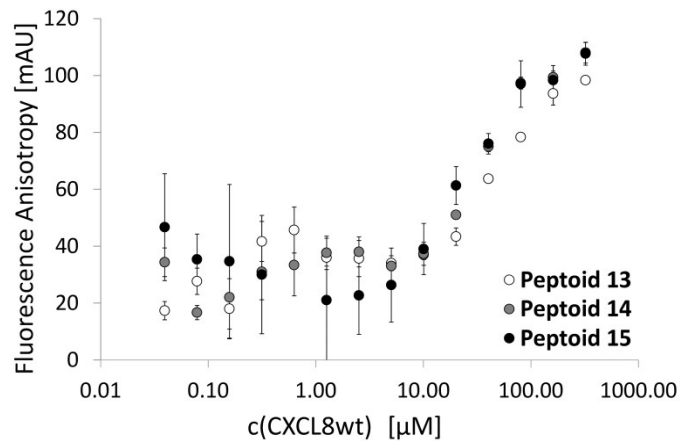


Figure S6 Fluorescence anisotropy measurements with fluorescently labelled peptoids 13-15 (50 nM respectively in low-salt PBS).

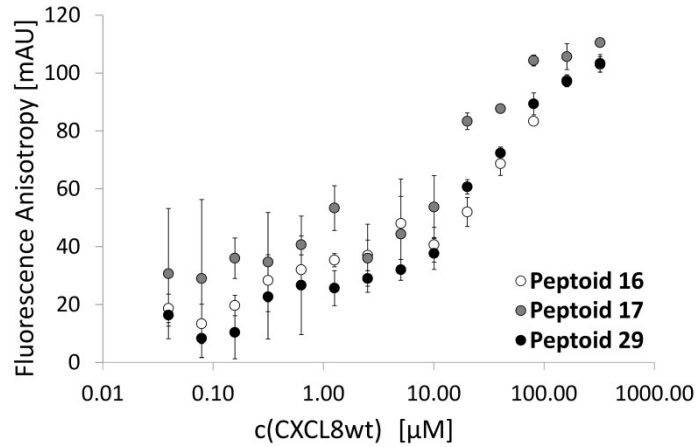


Figure S7 Fluorescence anisotropy measurements with fluorescently labelled peptoids 16 (20 nM), peptoid 17 (50 nM) and peptoid 29 (50 nM) in low-salt PBS.

## MALDI TOF/TOF MS Data of Peptoids 1-17 and 29

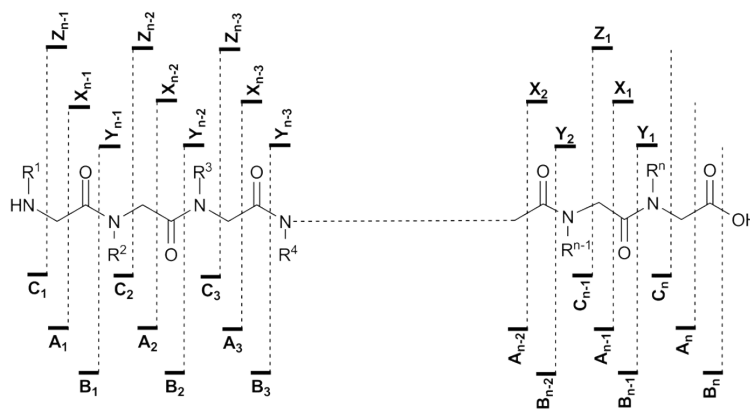
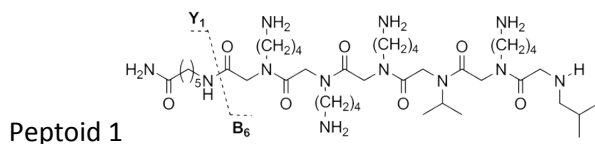
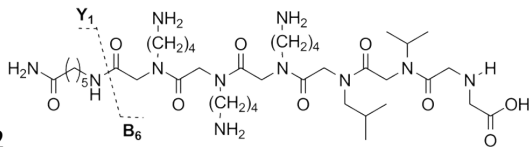


Figure S8 Peptoid fragmentation pattern and fragment names, adapted from Heerma et al.<sup>1</sup>



MALDI-TOF (matrix: CHCA),  $m/z$ : 855.82 (100)[M+H]<sup>+</sup>, 877.81 (92).

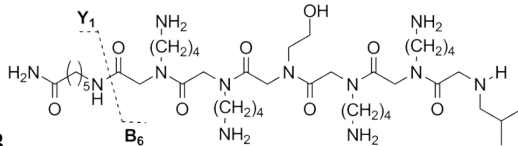
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 742.55 (16)[Y<sub>6</sub>+2 H]<sup>+</sup>, 614.48 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 597.45 (6)[B<sub>5</sub>]<sup>+</sup>, 515.42 (40)[Y<sub>4</sub>+2 H]<sup>+</sup>, 469.36 (13)[B<sub>4</sub>]<sup>+</sup>, 387.29 (7)[Y<sub>3</sub>+2 H]<sup>+</sup>, 341.27 (17)[B<sub>3</sub>]<sup>+</sup>, 242.19 (47)[B<sub>2</sub>]<sup>+</sup>.



Peptoid 2

MALDI-TOF (matrix: CHCA),  $m/z$ : 842.71 (100)[M+H]<sup>+</sup>, 1396.25 (45).

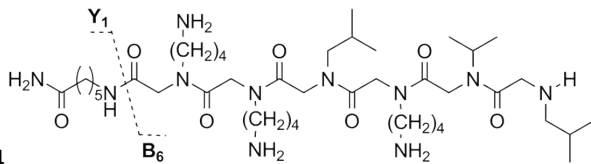
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 727.51 (36)[Y<sub>6</sub>+2 H]<sup>+</sup>, 628.47 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 584.38 (8)[B<sub>5</sub>]<sup>+</sup>, 515.38 (28)[Y<sub>4</sub>+2 H]<sup>+</sup>, 456.28 (10)[B<sub>4</sub>]<sup>+</sup>, 387.30 (14)[Y<sub>3</sub>+2 H]<sup>+</sup>, 328.18 (8)[B<sub>3</sub>]<sup>+</sup>, 215.10 (4)[B<sub>2</sub>]<sup>+</sup>.



Peptoid 3

MALDI-TOF (matrix: CHCA),  $m/z$ : 879.80 (100), 857.82 (87)[M+H]<sup>+</sup>, 656.21 (38)

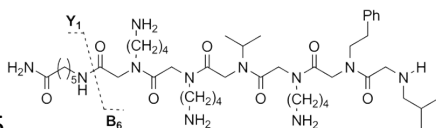
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 744.53 (18)[Y<sub>6</sub>+2 H]<sup>+</sup>, 616.46 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 599.44 (6)[B<sub>5</sub>]<sup>+</sup>, 488.38 (21)[Y<sub>4</sub>+2 H]<sup>+</sup>, 471.33 (9)[B<sub>4</sub>]<sup>+</sup>, 387.31 (6)[Y<sub>3</sub>+2 H]<sup>+</sup>, 370.28 (27)[B<sub>3</sub>]<sup>+</sup>, 257.21 (2)[Y<sub>2</sub>+2 H]<sup>+</sup>, 242.20 (34) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 4

MALDI-TOF (matrix: CHCA),  $m/z$ : 862.82 (100), 840.82 (86) [M+H]<sup>+</sup>.

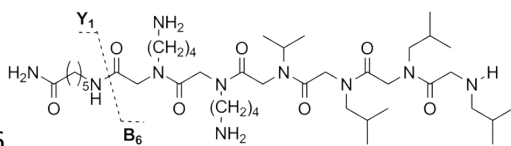
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 727.58 (28)[Y<sub>6</sub>+2 H]<sup>+</sup>, 628.51 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 582.42 (2)[B<sub>5</sub>]<sup>+</sup>, 500.41 (12)[Y<sub>4</sub>+2 H]<sup>+</sup>, 454.35 (6)[B<sub>4</sub>]<sup>+</sup>, 387.31 (4)[Y<sub>3</sub>+2 H]<sup>+</sup>, 341.26 (9)[B<sub>3</sub>]<sup>+</sup>, 213.18 (5)[B<sub>2</sub>]<sup>+</sup>.



Peptoid 5

MALDI-TOF (matrix: CHCA),  $m/z$ : 888.85 (100)[M+H]<sup>+</sup>, 760.72 (20), 1302.24 (20).

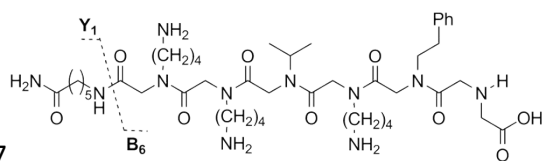
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 775.57 (14)[Y<sub>6</sub>+2 H]<sup>+</sup>, 630.47 (4) [B<sub>5</sub>]<sup>+</sup>, 614.50 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 502.35 (18)[B<sub>4</sub>]<sup>+</sup>, 486.40 (33)[Y<sub>4</sub>+2 H]<sup>+</sup>, 403.29 (19)[B<sub>3</sub>]<sup>+</sup>, 387.32 (7)[Y<sub>3</sub>+2 H]<sup>+</sup>, 275.18 (4)[B<sub>2</sub>]<sup>+</sup>.



Peptoid 6

MALDI-TOF (matrix: CHCA),  $m/z$ : 825.83 (100)[M+H]<sup>+</sup>, 847.79 (35).

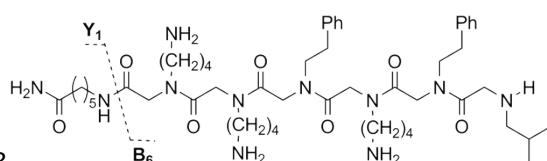
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 712.52 (20)[Y<sub>6</sub>+2 H]<sup>+</sup>, 599.45 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 567.43 (4)[B<sub>5</sub>]<sup>+</sup>, 486.37 (28)[Y<sub>4</sub>+2 H]<sup>+</sup>, 439.31 (22)[B<sub>4</sub>]<sup>+</sup>, 387.30 (7)[Y<sub>3</sub>+2 H]<sup>+</sup>, 340.26 (20)[B<sub>3</sub>]<sup>+</sup>, 227.18 (4)[B<sub>2</sub>]<sup>+</sup>.



Peptoid 7

MALDI-TOF (matrix: CHCA), m/z: 890.72 (100)[M+H]<sup>+</sup>, 762.59 (23), 962.75 (21).

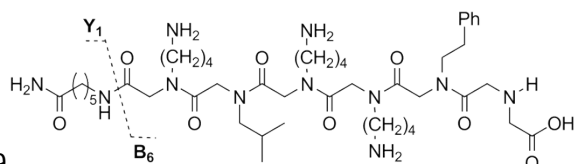
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 775.52 (25)[Y<sub>6</sub>+2 H]<sup>+</sup>, 632.36 (7)[B<sub>5</sub>]<sup>+</sup>, 614.44 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 504.28 (7)[B<sub>4</sub>]<sup>+</sup>, 486.36 (50) [Y<sub>4</sub>+2 H]<sup>+</sup>, 405.19 (13) [B<sub>3</sub>]<sup>+</sup>, 387.28 (18) [Y<sub>3</sub>+2 H]<sup>+</sup>, 277.11 (13)[B<sub>2</sub>]<sup>+</sup>.



Peptoid 8

MALDI-TOF (matrix: CHCA), m/z: 950.85 (100)[M+H]<sup>+</sup>, 972.79 (31), 1554.38 (21).

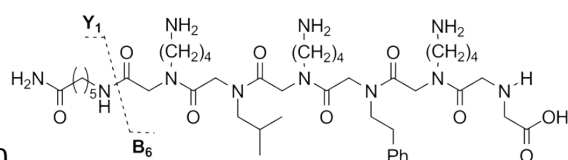
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 837.54 (17)[Y<sub>6</sub>+2 H]<sup>+</sup>, 692.46 (5) [B<sub>5</sub>]<sup>+</sup>, 676.49 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 564.40 (23)[Y<sub>4</sub>+2 H]<sup>+</sup>, 403.27 (13)[B<sub>3</sub>]<sup>+</sup>, 387.30 (4)[Y<sub>3</sub>+2 H]<sup>+</sup>, 275.17 (3) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 9

MALDI-TOF (matrix: CHCA), m/z: 904.70 (100)[M+H]<sup>+</sup>, 976.74 (36), 1734.38 (15).

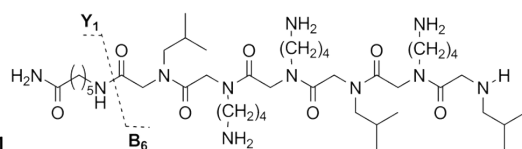
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 789.52 (23)[Y<sub>6</sub>+2 H]<sup>+</sup>, 646.37 (4) [B<sub>5</sub>]<sup>+</sup>, 628.47 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 533.29 (20)[B<sub>4</sub>]<sup>+</sup>, 500.37 (50) [Y<sub>4</sub>+2 H]<sup>+</sup>, 405.19 (8)[B<sub>3</sub>]<sup>+</sup>, 372.29 (4) [Y<sub>3</sub>+2 H]<sup>+</sup>, 277.10 (6) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 10

MALDI-TOF (matrix: CHCA), m/z: 904.71 (100)[M+H]<sup>+</sup>, 671.56 (60), 1201.99 (15).

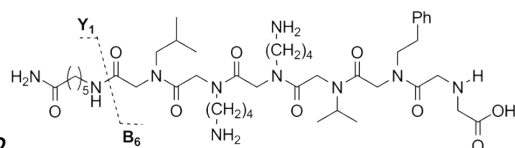
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 789.56 (23)[Y<sub>6</sub>+2 H]<sup>+</sup>, 661.48 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 646.37 (8) [B<sub>5</sub>]<sup>+</sup>, 533.29 (16)[B<sub>4</sub>]<sup>+</sup>, 500.39 (45) [Y<sub>4</sub>+2 H]<sup>+</sup>, 405.21 (2) [B<sub>3</sub>]<sup>+</sup>, 372.29 (6) [Y<sub>3</sub>+2 H]<sup>+</sup>, 244.14 (11) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 11

MALDI-TOF (matrix: CHCA),  $m/z$ : 854.85 (100)[M+H]<sup>+</sup>, 656.62 (62), 876.81 (56).

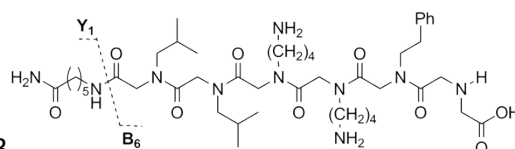
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 741.58 (26)[Y<sub>6</sub>+2 H]<sup>+</sup>, 613.50 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 500.41 (50)[Y<sub>4</sub>+2 H]<sup>+</sup>, 372.32 (8) [Y<sub>3</sub>+2 H]<sup>+</sup>, 355.29 (17) [B<sub>3</sub>]<sup>+</sup>, 242.19 (55) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 12

MALDI-TOF (matrix: CHCA),  $m/z$ : 875.68 (100)[M+H]<sup>+</sup>, 1400.18 (33).

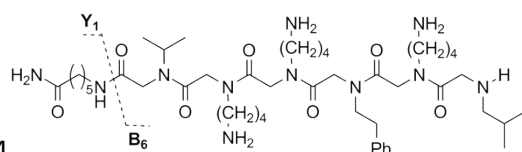
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 760.49 (18)[Y<sub>6</sub>+2 H]<sup>+</sup>, 632.34 (6) [B<sub>5</sub>]<sup>+</sup>, 599.43 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 504.25 (11)[B<sub>4</sub>]<sup>+</sup>, 500.37 (55) [Y<sub>4</sub>+2 H]<sup>+</sup>, 376.18 (16) [B<sub>3</sub>]<sup>+</sup>, 372.28 (14) [Y<sub>3</sub>+2 H]<sup>+</sup>, 277.10 (4) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 13

MALDI-TOF (matrix: CHCA),  $m/z$ : 889.72 (100) [M+H]<sup>+</sup>, 1428.23 (90), 1095.94 (75).

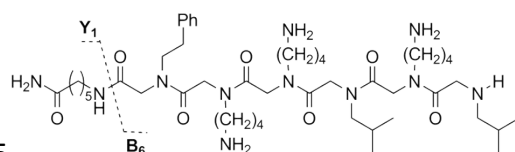
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 774.53 (21)[Y<sub>6</sub>+2 H]<sup>+</sup>, 646.38 (4) [B<sub>5</sub>]<sup>+</sup>, 613.46 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 533.30 (23)[B<sub>4</sub>]<sup>+</sup>, 485.37 (50) [Y<sub>4</sub>+2 H]<sup>+</sup>, 405.21 (9) [B<sub>3</sub>]<sup>+</sup>, 357.27 (4) [Y<sub>3</sub>+2 H]<sup>+</sup>, 277.10 (4) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 14

MALDI-TOF (matrix: CHCA),  $m/z$ : 888.82 (100) [M+H]<sup>+</sup>, 1174.04 (55), 1130.99 (36).

MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 775.54 (24)[Y<sub>6</sub>+2 H]<sup>+</sup>, 659.45 (6) [B<sub>5</sub>]<sup>+</sup>, 647.46 (100)[Y<sub>5</sub>+2 H]<sup>+</sup>, 531.36 (22)[B<sub>4</sub>]<sup>+</sup>, 486.37 (42) [Y<sub>4</sub>+2 H]<sup>+</sup>, 403.27 (17) [B<sub>3</sub>]<sup>+</sup>, 358.28 (12) [Y<sub>3</sub>+2 H]<sup>+</sup>, 242.20 (54) [B<sub>2</sub>]<sup>+</sup>.

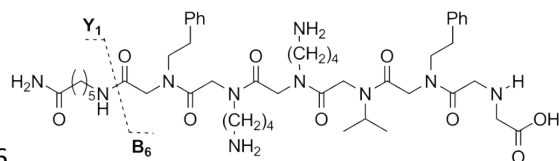


Peptoid 15

MALDI-TOF (matrix: CHCA),  $m/z$ : 902.85 (100) [M+H]<sup>+</sup>, 752.64 (85).



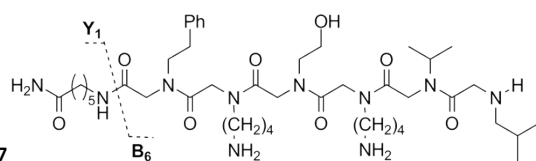
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 789.56 (26)[Y<sub>6</sub>+2 H]<sup>+</sup>, 661.48 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 611.48 (4) [B<sub>5</sub>]<sup>+</sup>, 483.37 (19)[B<sub>4</sub>]<sup>+</sup>, 420.30 (8) [Y<sub>3</sub>+2 H]<sup>+</sup>, 355.27 (17) [B<sub>3</sub>]<sup>+</sup>, 242.19 (67) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 16

MALDI-TOF (matrix: CHCA), m/z: 923.70 (100) [M+H]<sup>+</sup>, 1093.86 (14), 1236.00 (12).

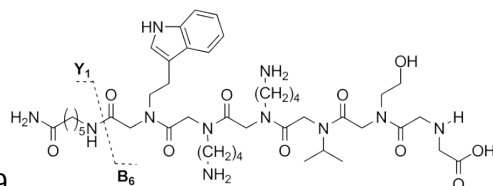
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 808.52 (18)[Y<sub>6</sub>+2 H]<sup>+</sup>, 647.46 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 632.36 (7) [B<sub>5</sub>]<sup>+</sup>, 548.39 (50)[Y<sub>4</sub>+2 H]<sup>+</sup>, 504.28 (10)[B<sub>4</sub>]<sup>+</sup>, 420.30 (12) [Y<sub>3</sub>+2 H]<sup>+</sup>, 376.19 (15) [B<sub>3</sub>]<sup>+</sup>, 277.11 (3) [B<sub>2</sub>]<sup>+</sup>.



Peptoid 17

MALDI-TOF (matrix: CHCA), m/z: 752.63 (100), 837.71 (72), 861.78 (56)[M+H]<sup>+</sup>.

MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 748.52 (24)[Y<sub>6</sub>+2 H]<sup>+</sup>, 649.46 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 570.39 (2) [B<sub>5</sub>]<sup>+</sup>, 521.35 (13)[Y<sub>4</sub>+2 H]<sup>+</sup>, 442.31 (5)[B<sub>4</sub>]<sup>+</sup>, 420.31 (4) [Y<sub>3</sub>+2 H]<sup>+</sup>, 341.27 (10) [B<sub>3</sub>]<sup>+</sup>, 213.16 (4) [B<sub>2</sub>]<sup>+</sup>.

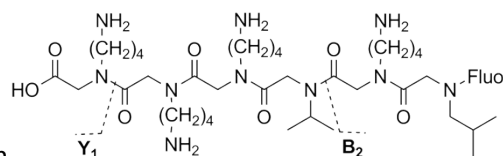


Peptoid 29

MALDI-TOF (matrix: CHCA), m/z: 931.69 (100), 916.69 (76), 902.71 (49)[M+H]<sup>+</sup>.

MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 787.52 (19)[Y<sub>6</sub>+2 H]<sup>+</sup>, 686.46 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 587.41 (67)[Y<sub>4</sub>+2 H]<sup>+</sup>, 572.32 (26) [B<sub>5</sub>]<sup>+</sup>, 459.31 (25) [Y<sub>3</sub>+2 H]<sup>+</sup>, 444.21 (27)[B<sub>4</sub>]<sup>+</sup>, 316.17 (30) [B<sub>3</sub>]<sup>+</sup>.

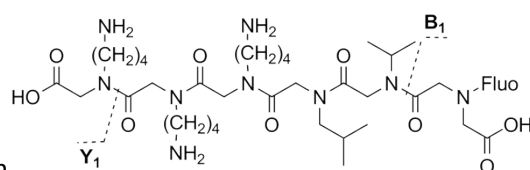
## MALDI TOF/TOF MS Data of fluorescently labelled peptoids 1-17 and 29



Peptoid1-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1101.96 (100) [M+H]<sup>+</sup>, 743.79 (9).

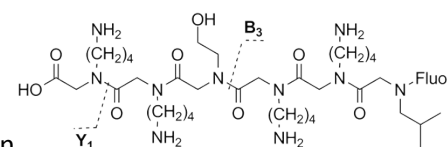
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 955.56 (17) [B<sub>5</sub>]<sup>+</sup>, 827.46 (21)[B<sub>4</sub>]<sup>+</sup>, 699.34 (19) [B<sub>3</sub>]<sup>+</sup>, 630.51 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 600.25 (10) [B<sub>2</sub>]<sup>+</sup>, 502.41 (70) [Y<sub>4</sub>+2 H]<sup>+</sup>, 473.19 (8) [B<sub>1</sub>]<sup>+</sup>, 403.32 (41) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid2-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1088.91 (100) [M+H]<sup>+</sup>.

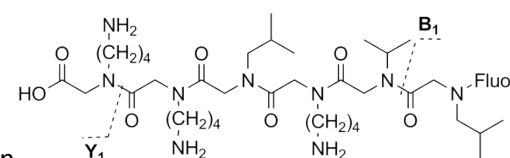
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 942.53 (31) [B<sub>5</sub>]<sup>+</sup>, 814.40 (39)[B<sub>4</sub>]<sup>+</sup>, 686.31 (25) [B<sub>3</sub>]<sup>+</sup>, 615.51 (98) [Y<sub>5</sub>+2 H]<sup>+</sup>, 574.18 (4) [B<sub>2</sub>]<sup>+</sup>, 516.43 (100) [Y<sub>4</sub>+2 H]<sup>+</sup>, 403.35 (64) [Y<sub>3</sub>+2 H]<sup>+</sup>, 275.22 (7) [Y<sub>2</sub>+2 H]<sup>+</sup>.



Peptoid 3-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1103.98 (100) [M+H]<sup>+</sup>.

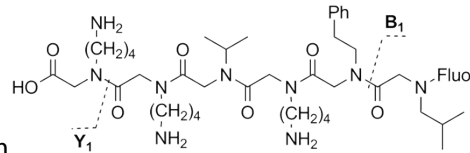
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 958.54 (15) [B<sub>5</sub>]<sup>+</sup>, 829.44 (7)[B<sub>4</sub>]<sup>+</sup>, 728.38 (31) [B<sub>3</sub>]<sup>+</sup>, 632.50 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 600.28 (7) [B<sub>2</sub>]<sup>+</sup>, 504.38 (49) [Y<sub>4</sub>+2 H]<sup>+</sup>, 473.20 (5) [B<sub>1</sub>]<sup>+</sup>, 376.25 (5) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid 4-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1086.97 (100) [M+H]<sup>+</sup>.

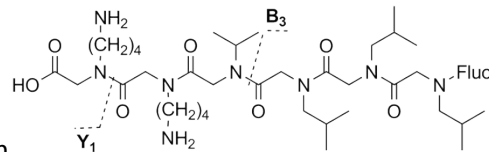
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 940.59 (10) [B<sub>5</sub>]<sup>+</sup>, 812.50 (5)[B<sub>4</sub>]<sup>+</sup>, 699.39 (20) [B<sub>3</sub>]<sup>+</sup>, 615.52 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 571.26 (13) [B<sub>2</sub>]<sup>+</sup>, 516.44 (57) [Y<sub>4</sub>+2 H]<sup>+</sup>, 472.18 (9) [B<sub>1</sub>]<sup>+</sup>, 388.32 (8) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid 5-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1134.98 (100) [M+H]<sup>+</sup>, 1156.98 (6).

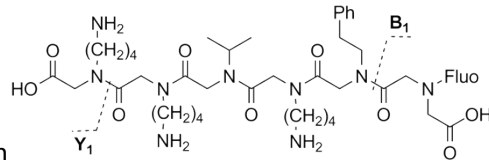
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 988.56 (23) [B<sub>5</sub>]<sup>+</sup>, 860.45 (11)[B<sub>4</sub>]<sup>+</sup>, 761.41 (43) [B<sub>3</sub>]<sup>+</sup>, 663.53 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 633.28 (8) [B<sub>2</sub>]<sup>+</sup>, 502.42 (73) [Y<sub>4</sub>+2 H]<sup>+</sup>, 472.20 (13) [B<sub>1</sub>]<sup>+</sup>, 374.32 (16) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid 6-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1071.95 (100) [M+H]<sup>+</sup>, 1093.94 (18).

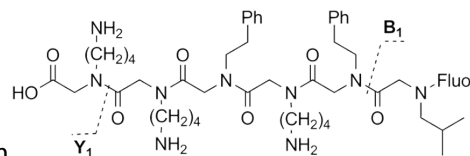
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 925.53 (12) [B<sub>5</sub>]<sup>+</sup>, 797.44 (33)[B<sub>4</sub>]<sup>+</sup>, 698.36 (54) [B<sub>3</sub>]<sup>+</sup>, 600.48 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 585.26 (10) [B<sub>2</sub>]<sup>+</sup>, 487.37 (54) [Y<sub>4</sub>+2 H]<sup>+</sup>, 572.17 (5) [B<sub>1</sub>]<sup>+</sup>, 374.30 (21) [Y<sub>3</sub>+2 H]<sup>+</sup>, 275.21 (4) [Y<sub>2</sub>+2 H]<sup>+</sup>.



Peptoid 7-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1136.92 (100) [M+H]<sup>+</sup>.

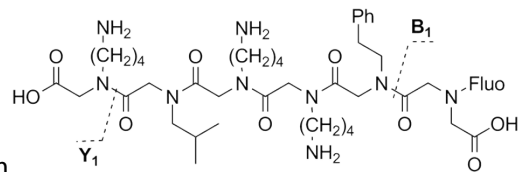
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 990.54 (34) [B<sub>5</sub>]<sup>+</sup>, 862.43 (36)[B<sub>4</sub>]<sup>+</sup>, 763.34 (80) [B<sub>3</sub>]<sup>+</sup>, 663.52 (73) [Y<sub>5</sub>+2 H]<sup>+</sup>, 636.23 (3) [B<sub>2</sub>]<sup>+</sup>, 502.42 (100) [Y<sub>4</sub>+2 H]<sup>+</sup>, 374.30 (41) [Y<sub>3</sub>+2 H]<sup>+</sup>, 275.25 (6) [Y<sub>2</sub>+2 H]<sup>+</sup>.



Peptoid 8-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1197.01 (100) [M+H]<sup>+</sup>, 1219.00 (33).

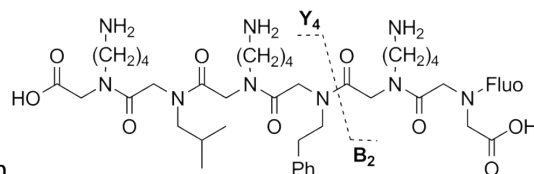
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 1050.57 (23) [B<sub>5</sub>]<sup>+</sup>, 922.49 (7)[B<sub>4</sub>]<sup>+</sup>, 761.40 (34) [B<sub>3</sub>]<sup>+</sup>, 725.52 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 633.30 (8) [B<sub>2</sub>]<sup>+</sup>, 564.43 (66) [Y<sub>4</sub>+2 H]<sup>+</sup>, 472.18 (13) [B<sub>1</sub>]<sup>+</sup>, 436.35 (15) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid 9-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1150.94 (100) [M+H]<sup>+</sup>, 1035.87 (18), 1172.92 (6).

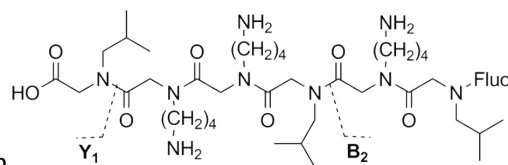
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 1004.50 (28) [B<sub>5</sub>]<sup>+</sup>, 891.44 (40)[B<sub>4</sub>]<sup>+</sup>, 763.34 (43) [B<sub>3</sub>]<sup>+</sup>, 677.53 (72) [Y<sub>5</sub>+2 H]<sup>+</sup>, 516.42 (100) [Y<sub>4</sub>+2 H]<sup>+</sup>, 388.32 (92) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid 10-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1150.93 (100) [M+H]<sup>+</sup>, 1035.86 (13).

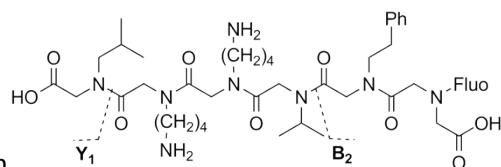
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 1004.50 (32) [B<sub>5</sub>]<sup>+</sup>, 891.41 (43)[B<sub>4</sub>]<sup>+</sup>, 763.32 (36) [B<sub>3</sub>]<sup>+</sup>, 677.53 (92) [Y<sub>5</sub>+2 H]<sup>+</sup>, 602.24 (8) [B<sub>2</sub>]<sup>+</sup>, 549.42 (100) [Y<sub>4</sub>+2 H]<sup>+</sup>, 388.32 (82) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid 11-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1100.96 (100) [M+H]<sup>+</sup>.

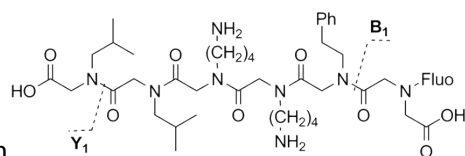
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 969.61 (10) [B<sub>5</sub>]<sup>+</sup>, 841.49 (20)[B<sub>4</sub>]<sup>+</sup>, 713.39 (17) [B<sub>3</sub>]<sup>+</sup>, 629.52 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 600.32 (10) [B<sub>2</sub>]<sup>+</sup>, 501.42 (40) [Y<sub>4</sub>+2 H]<sup>+</sup>, 473.16 (8) [B<sub>1</sub>]<sup>+</sup>, 388.34 (31) [Y<sub>3</sub>+2 H]<sup>+</sup>, 260.22 (3) [Y<sub>2</sub>+2 H]<sup>+</sup>.



Peptoid 12-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1121.87 (100) [M+H]<sup>+</sup>, 1006.80 (23), 1451.36 (9).

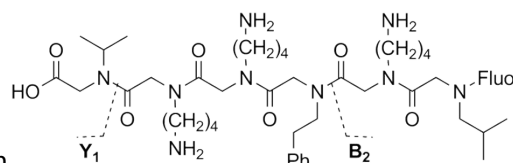
MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 990.51 (17) [B<sub>5</sub>]<sup>+</sup>, 862.41 (49)[B<sub>4</sub>]<sup>+</sup>, 734.31 (54) [B<sub>3</sub>]<sup>+</sup>, 648.53 (57) [Y<sub>5</sub>+2 H]<sup>+</sup>, 635.20 (4) [B<sub>2</sub>]<sup>+</sup>, 487.41 (83) [Y<sub>4</sub>+2 H]<sup>+</sup>, 388.34 (100) [Y<sub>3</sub>+2 H]<sup>+</sup>, 260.23 (7) [Y<sub>2</sub>+2 H]<sup>+</sup>.



Peptoid 13-fluorescein

MALDI-TOF (matrix: CHCA),  $m/z$ : 1135.87 (100)  $[M+H]^+$ , 657.64 (19), 1479.36 (9).

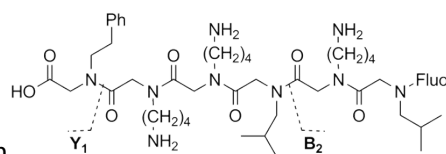
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 1004.55 (23)  $[B_5]^+$ , 891.46 (33)  $[B_4]^+$ , 763.35 (48)  $[B_3]^+$ , 662.52 (58)  $[Y_5+2 H]^+$ , 501.43 (100)  $[Y_4+2 H]^+$ , 373.31 (75)  $[Y_3+2 H]^+$ .



Peptoid 14-fluorescein

MALDI-TOF (matrix: CHCA),  $m/z$ : 1134.93 (100)  $[M+H]^+$ .

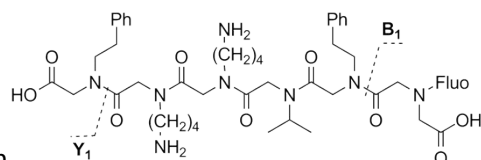
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 1017.61 (27)  $[B_5]^+$ , 889.51 (23)  $[B_4]^+$ , 761.41 (15)  $[B_3]^+$ , 663.53 (100)  $[Y_5+2 H]^+$ , 600.30 (10)  $[B_2]^+$ , 535.41 (42)  $[Y_4+2 H]^+$ , 473.18 (7)  $[B_1]^+$ , 374.32 (30)  $[Y_3+2 H]^+$ .



Peptoid 15-fluorescein

MALDI-TOF (matrix: CHCA),  $m/z$ : 1148.98 (100)  $[M+H]^+$ .

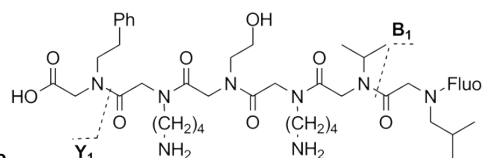
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 841.51 (9)  $[B_4]^+$ , 713.38 (15)  $[B_3]^+$ , 677.54 (100)  $[Y_5+2 H]^+$ , 600.28 (12)  $[B_2]^+$ , 549.43 (44)  $[Y_4+2 H]^+$ , 473.16 (7)  $[B_4]^+$ , 436.32 (30)  $[Y_3+2 H]^+$ , 308.20 (3)  $[Y_2+2 H]^+$ .



Peptoid 16-fluorescein

MALDI-TOF (matrix: CHCA),  $m/z$ : 1169.89 (100)  $[M+H]^+$ , 1547.42 (65), 919.88 (11).

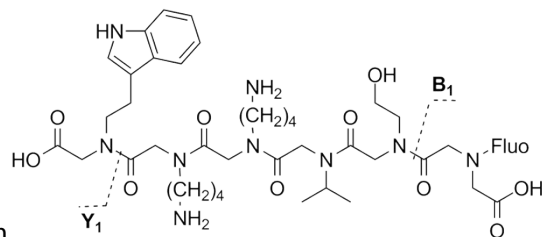
MALDI-TOF/TOF (matrix: CHCA),  $m/z$  (%) [fragment]: 990.54 (18)  $[B_5]^+$ , 862.46 (55)  $[B_4]^+$ , 734.35 (80)  $[B_3]^+$ , 696.57 (60)  $[Y_5+2 H]^+$ , 636.24 (7)  $[B_2]^+$ , 535.45 (100)  $[Y_4+2 H]^+$ , 436.37 (98)  $[Y_3+2 H]^+$ , 308.25 (8)  $[Y_2+2 H]^+$ .



Peptoid 17-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1107.89 (100) [M+H]<sup>+</sup>, 1129.90 (6).

MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 928.55 (8) [B<sub>5</sub>]<sup>+</sup>, 800.44 (8) [B<sub>4</sub>]<sup>+</sup>, 699.38 (27) [B<sub>3</sub>]<sup>+</sup>, 363.47 (100) [Y<sub>5</sub>+2 H]<sup>+</sup>, 571.26 (11) [B<sub>2</sub>]<sup>+</sup>, 537.40 (63) [Y<sub>4</sub>+2 H]<sup>+</sup>, 472.20 (8) [B<sub>1</sub>]<sup>+</sup>, 409.26 (3) [Y<sub>3</sub>+2 H]<sup>+</sup>.



Peptoid 29-fluorescein

MALDI-TOF (matrix: CHCA), m/z: 1148.87 (100) [M+H]<sup>+</sup>, 948.71 (17), 1047.79 (13).

MALDI-TOF/TOF (matrix: CHCA), m/z (%) [fragment]: 930.48 (22) [B<sub>5</sub>]<sup>+</sup>, 802.38 (46) [B<sub>4</sub>]<sup>+</sup>, 675.51 (47) [Y<sub>5</sub>+2 H]<sup>+</sup> and [B<sub>3</sub>]<sup>+</sup>, 574.43 (58) [Y<sub>4</sub>+2 H]<sup>+</sup> and [B<sub>2</sub>]<sup>+</sup>, 475.35 (100) [Y<sub>3</sub>+2 H]<sup>+</sup> and [B<sub>1</sub>]<sup>+</sup>, 347.25 (8) [Y<sub>2</sub>+2 H]<sup>+</sup>.

## ESI MS Data of peptide sequences S1-S6

### Peptide S1

ESI MS (acetonitrile/water 0,1% TFA), m/z: 586.57 (50) [M+3H]<sup>3+</sup>, 879.36 (25) [M+2H]<sup>2+</sup>

### Peptide S2

ESI MS (acetonitrile/water 0,1% TFA), m/z: 528.05 (100) [M+2H]<sup>2+</sup>, 1054.67 (50) [M+H]<sup>+</sup>

### Peptide S3

ESI MS (acetonitrile/water 0,1% TFA), m/z: 430.35 (100) [M+2H]<sup>2+</sup>, 859.56 (24) [M+H]<sup>+</sup>

1. W. Heerma, C. Versluis, C. G. deKoster, J. A. W. Kruijtzter, I. Zigrovic and R. M. J. Liskamp, *Rapid Communications in Mass Spectrometry*, 1996, **10**, 459-464.