



# Supplementary Figure S1

## Supplementary Figure S2

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assign (segid " A" and resid  3 and name  HN) (segid " A" and
resid  3 and name HG12) 3.504 1.534 1.534 weight 1.000 !
spec=VJN0...oPep, no=3, id=2, vol=1.033169e-02
assign (segid " A" and resid  6 and name  HN) (segid " A" and
resid  6 and name HB2) 2.507 0.786 0.786 weight 1.000 !
spec=VJN0...oPep, no=6, id=5, vol=6.939026e-02
    or (segid " A" and resid  6 and name  HN) (segid " A" and
resid  6 and name HB1)
    or (segid " A" and resid  6 and name  HN) (segid " A" and
resid  6 and name HB3)
assign (segid " A" and resid  3 and name  HN) (segid " A" and
resid  3 and name HG11) 3.373 1.423 1.423 weight 1.000 !
spec=VJN0...oPep, no=7, id=6, vol=1.320012e-02
assign (segid " A" and resid  3 and name  HN) (segid " A" and
resid  3 and name  HB) 2.775 0.962 0.962 weight 1.000 !
spec=VJN0...oPep, no=9, id=8, vol=4.278010e-02
assign (segid " A" and resid  2 and name  HN) (segid " A" and
resid  2 and name  HB) 3.049 1.162 1.162 weight 1.000 !
spec=VJN0...oPep, no=10, id=9, vol=2.340396e-02
assign (segid " A" and resid  12 and name  HN) (segid " A" and
resid  12 and name HB1) 3.407 1.451 1.451 weight 1.000 !
spec=VJN0...oPep, no=14, id=13, vol=1.229326e-02
assign (segid " A" and resid  10 and name  HN) (segid " A" and
resid  10 and name HB1) 2.245 0.630 0.630 weight 1.000 !
spec=VJN0...oPep, no=16, id=15, vol=1.315039e-01
assign (segid " A" and resid  12 and name  HN) (segid " A" and
resid  12 and name HB2) 2.950 1.088 1.088 weight 1.000 !
spec=VJN0...oPep, no=17, id=16, vol=2.831155e-02
assign (segid " A" and resid  12 and name HD1) (segid " A" and
resid  12 and name HB2) 2.696 0.909 0.909 weight 1.000 !
spec=VJN0...oPep, no=22, id=21, vol=4.948945e-02
    or (segid " A" and resid  12 and name  HD2) (segid " A" and
resid  12 and name HB2)
assign (segid " A" and resid  12 and name HD1) (segid " A" and
resid  12 and name HB1) 2.707 0.916 0.916 weight 1.000 !
spec=VJN0...oPep, no=26, id=25, vol=4.610408e-02
    or (segid " A" and resid  12 and name  HD2) (segid " A" and
resid  12 and name HB1)
assign (segid " A" and resid  5 and name  HN) (segid " A" and
resid  4 and name  HA) 2.909 1.058 1.058 weight 1.000 !
spec=VJN0...oPep, no=29, id=27, vol=2.967369e-02
assign (segid " A" and resid  2 and name  HN) (segid " A" and
resid  1 and name  HA) 2.664 0.887 0.887 weight 1.000 !
spec=VJN0...oPep, no=30, id=28, vol=5.278222e-02
assign (segid " A" and resid  4 and name  HN) (segid " A" and
resid  3 and name  HA) 2.391 0.715 0.715 weight 1.000 !
spec=VJN0...oPep, no=32, id=30, vol=9.453267e-02
assign (segid " A" and resid  2 and name  HN) (segid " A" and
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resid    2 and name   HA) 3.107 1.207 1.207 weight 1.000 !
spec=VJN0...oPep, no=33, id=31, vol=1.611717e-02
assign (segid " A" and resid    3 and name   HN) (segid " A" and
resid    2 and name   HA) 2.221 0.616 0.616 weight 1.000 !
spec=VJN0...oPep, no=34, id=32, vol=1.572275e-01
assign (segid " A" and resid    8 and name   HN) (segid " A" and
resid    7 and name   HA) 2.389 0.714 0.714 weight 1.000 !
spec=VJN0...oPep, no=38, id=36, vol=9.253265e-02
assign (segid " A" and resid   10 and name   HN) (segid " A" and
resid   10 and name   HA) 2.574 0.828 0.828 weight 1.000 !
spec=VJN0...oPep, no=40, id=38, vol=5.693072e-02
assign (segid " A" and resid   11 and name   HN) (segid " A" and
resid   11 and name   HA) 3.060 1.171 1.171 weight 1.000 !
spec=VJN0...oPep, no=41, id=39, vol=2.088676e-02
assign (segid " A" and resid   12 and name   HN) (segid " A" and
resid   11 and name   HA) 2.736 0.935 0.935 weight 1.000 !
spec=VJN0...oPep, no=42, id=40, vol=4.465870e-02
assign (segid " A" and resid   8 and name   HN) (segid " A" and
resid   8 and name   HA) 2.836 1.006 1.006 weight 1.000 !
spec=VJN0...oPep, no=43, id=41, vol=3.252475e-02
assign (segid " A" and resid   9 and name   HN) (segid " A" and
resid   8 and name   HA) 2.527 0.798 0.798 weight 1.000 !
spec=VJN0...oPep, no=44, id=42, vol=7.001019e-02
assign (segid " A" and resid   12 and name   HN) (segid " A" and
resid   12 and name   HA) 3.068 1.177 1.177 weight 1.000 !
spec=VJN0...oPep, no=46, id=44, vol=2.023048e-02
assign (segid " A" and resid   9 and name   HN) (segid " A" and
resid   9 and name   HA) 2.762 0.953 0.953 weight 1.000 !
spec=VJN0...oPep, no=47, id=45, vol=3.840271e-02
assign (segid " A" and resid   10 and name   HN) (segid " A" and
resid   9 and name   HA) 2.389 0.714 0.714 weight 1.000 !
spec=VJN0...oPep, no=48, id=46, vol=9.143525e-02
assign (segid " A" and resid   8 and name   HE3) (segid " A" and
resid   9 and name   HA) 3.141 1.233 1.233 weight 1.000 !
spec=VJN0...oPep, no=49, id=47, vol=1.930137e-02
assign (segid " A" and resid   10 and name   HD1) (segid " A" and
resid   10 and name   HA) 2.507 0.786 0.786 weight 1.000 !
spec=VJN0...oPep, no=53, id=51, vol=7.056875e-02
      or (segid " A" and resid   10 and name   HD2) (segid " A" and
resid   10 and name   HA)
assign (segid " A" and resid   12 and name   HD1) (segid " A" and
resid   12 and name   HA) 2.680 0.898 0.898 weight 1.000 !
spec=VJN0...oPep, no=54, id=52, vol=4.880517e-02
      or (segid " A" and resid   12 and name   HD2) (segid " A" and
resid   12 and name   HA)
assign (segid " A" and resid   8 and name   HN) (segid " A" and
resid   8 and name   HD1) 3.304 1.364 1.364 weight 1.000 !
spec=VJN0...oPep, no=55, id=53, vol=1.313896e-02
assign (segid " A" and resid   10 and name   HN) (segid " A" and
resid   10 and name   HD1) 3.024 1.143 1.143 weight 1.000 !

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spec=VJN0...oPep, no=56, id=54, vol=2.097030e-02
    or (segid " A" and resid 10 and name HN) (segid " A" and
resid 10 and name HD2)
assign (segid " A" and resid 9 and name HN) (segid " A" and
resid 8 and name HE3) 3.722 1.731 1.731 weight 1.000 !
spec=VJN0...oPep, no=69, id=63, vol=6.442704e-03
assign (segid " A" and resid 10 and name HN) (segid " A" and
resid 9 and name HN) 3.412 1.455 1.455 weight 1.000 !
spec=VJN0...oPep, no=77, id=68, vol=1.185256e-02
assign (segid " A" and resid 9 and name HN) (segid " A" and
resid 8 and name HN) 3.524 1.552 1.552 weight 1.000 !
spec=VJN0...oPep, no=78, id=69, vol=8.638570e-03
assign (segid " A" and resid 2 and name HN) (segid " A" and
resid 3 and name HN) 3.378 1.426 1.426 weight 1.000 !
spec=VJN0...oPep, no=82, id=73, vol=1.166580e-02
assign (segid " A" and resid 4 and name HN) (segid " A" and
resid 3 and name HN) 3.581 1.603 1.603 weight 1.000 !
spec=VJN0...oPep, no=84, id=75, vol=8.476181e-03
assign (segid " A" and resid 10 and name HD1) (segid " A" and
resid 8 and name HA) 3.526 1.554 1.554 weight 1.000 !
spec=VJN0...oPep, no=96, id=76, vol=9.068958e-03
    or (segid " A" and resid 10 and name HD2) (segid " A" and
resid 8 and name HA)
assign (segid " A" and resid 3 and name HN) (segid " A" and
resid 2 and name HB) 3.673 1.686 1.686 weight 1.000 !
spec=VJN0...oPep, no=100, id=78, vol=7.676500e-03
assign (segid " A" and resid 4 and name HN) (segid " A" and
resid 3 and name HG22) 3.783 1.789 1.789 weight 1.000 !
spec=VJN0...oPep, no=103, id=81, vol=5.483137e-03
    or (segid " A" and resid 4 and name HN) (segid " A" and
resid 3 and name HG21)
    or (segid " A" and resid 4 and name HN) (segid " A" and
resid 3 and name HG23)
assign (segid " A" and resid 12 and name HE1) (segid " A" and
resid 11 and name HG1) 3.722 1.732 1.732 weight 1.000 !
spec=VJN0...oPep, no=105, id=82, vol=6.300575e-03
    or (segid " A" and resid 12 and name HE2) (segid " A" and
resid 11 and name HG1)
assign (segid " A" and resid 8 and name HD1) (segid " A" and
resid 8 and name HE1) 2.166 0.587 0.587 weight 1.000 !
spec=VJN0...oPep, no=113, id=88, vol=1.429870e-01
assign (segid " A" and resid 8 and name HE1) (segid " A" and
resid 7 and name HA) 3.776 1.782 1.782 weight 1.000 !
spec=VJN0...oPep, no=114, id=89, vol=5.481763e-03
assign (segid " A" and resid 7 and name HN) (segid " A" and
resid 7 and name HB2) 2.715 0.921 0.921 weight 1.000 !
spec=VJN0...oPep, no=116, id=91, vol=4.317954e-02
    or (segid " A" and resid 7 and name HN) (segid " A" and
resid 7 and name HB1)
    or (segid " A" and resid 7 and name HN) (segid " A" and

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resid    7 and name  HB3)
assign (segid "   A" and resid    3 and name  HA) (segid "   A" and
resid    3 and name HG22) 2.700 0.911 0.911 weight 1.000 !
spec=VJN0...oPep, no=118, id=92, vol=4.247479e-02
      or (segid "   A" and resid    3 and name  HA) (segid "   A" and
resid    3 and name HG21)
      or (segid "   A" and resid    3 and name  HA) (segid "   A" and
resid    3 and name HG23)
assign (segid "   A" and resid    3 and name  HA) (segid "   A" and
resid    3 and name HG11) 3.165 1.252 1.252 weight 1.000 !
spec=VJN0...oPep, no=119, id=93, vol=1.759148e-02
assign (segid "   A" and resid    7 and name  HA) (segid "   A" and
resid    7 and name HB2) 2.138 0.572 0.572 weight 1.000 !
spec=VJN0...oPep, no=120, id=94, vol=1.905652e-01
      or (segid "   A" and resid    7 and name  HA) (segid "   A" and
resid    7 and name HB1)
      or (segid "   A" and resid    7 and name  HA) (segid "   A" and
resid    7 and name HB3)
assign (segid "   A" and resid    6 and name  HA) (segid "   A" and
resid    6 and name HB2) 2.176 0.592 0.592 weight 1.000 !
spec=VJN0...oPep, no=121, id=95, vol=1.708650e-01
      or (segid "   A" and resid    6 and name  HA) (segid "   A" and
resid    6 and name HB1)
      or (segid "   A" and resid    6 and name  HA) (segid "   A" and
resid    6 and name HB3)
assign (segid "   A" and resid    3 and name  HA) (segid "   A" and
resid    3 and name  HB) 2.760 0.952 0.952 weight 1.000 !
spec=VJN0...oPep, no=125, id=99, vol=3.883141e-02
assign (segid "   A" and resid    2 and name  HA) (segid "   A" and
resid    2 and name  HB) 3.034 1.151 1.151 weight 1.000 !
spec=VJN0...oPep, no=131, id=100, vol=2.151193e-02
assign (segid "   A" and resid   12 and name  HA) (segid "   A" and
resid   12 and name HB1) 2.585 0.835 0.835 weight 1.000 !
spec=VJN0...oPep, no=133, id=102, vol=6.225432e-02
assign (segid "   A" and resid   12 and name  HA) (segid "   A" and
resid   12 and name HB2) 2.883 1.039 1.039 weight 1.000 !
spec=VJN0...oPep, no=134, id=103, vol=3.120618e-02
assign (segid "   A" and resid    8 and name HD1) (segid "   A" and
resid    7 and name  HA) 3.085 1.190 1.190 weight 1.000 !
spec=VJN0...oPep, no=155, id=123, vol=2.121782e-02
assign (segid "   A" and resid   12 and name  HA) (segid "   A" and
resid   12 and name HE1) 3.590 1.611 1.611 weight 1.000 !
spec=VJN0...oPep, no=157, id=125, vol=8.239377e-03
      or (segid "   A" and resid   12 and name  HA) (segid "   A" and
resid   12 and name HE2)
assign (segid "   A" and resid    8 and name  HA) (segid "   A" and
resid   10 and name HE1) 3.636 1.653 1.653 weight 1.000 !
spec=VJN0...oPep, no=167, id=135, vol=7.649898e-03
      or (segid "   A" and resid    8 and name  HA) (segid "   A" and
resid   10 and name HE2)

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assign (segid " A" and resid 3 and name HB) (segid " A" and
resid 3 and name HG11) 3.006 1.130 1.130 weight 1.000 !
spec=VJN0...oPep, no=169, id=137, vol=2.488300e-02
assign (segid " A" and resid 3 and name HB) (segid " A" and
resid 3 and name HG12) 2.929 1.072 1.072 weight 1.000 !
spec=VJN0...oPep, no=170, id=138, vol=3.032798e-02
assign (segid " A" and resid 3 and name HG11) (segid " A" and
resid 3 and name HG12) 2.185 0.597 0.597 weight 1.000 !
spec=VJN0...oPep, no=173, id=141, vol=1.668313e-01
assign (segid " A" and resid 7 and name HB2) (segid " A" and
resid 8 and name HA) 3.507 1.537 1.537 weight 1.000 !
spec=VJN0...oPep, no=182, id=147, vol=9.864725e-03
    or (segid " A" and resid 7 and name HB1) (segid " A" and
resid 8 and name HA)
    or (segid " A" and resid 7 and name HB3) (segid " A" and
resid 8 and name HA)
assign (segid " A" and resid 9 and name HN) (segid " A" and
resid 9 and name HB1) 3.456 1.493 1.493 weight 1.000 !
spec=VJN0...oPep, no=192, id=154, vol=1.021430e-02
assign (segid " A" and resid 9 and name HN) (segid " A" and
resid 9 and name HB2) 3.535 1.562 1.562 weight 1.000 !
spec=VJN0...oPep, no=193, id=155, vol=9.293246e-03
assign (segid " A" and resid 12 and name HN) (segid " A" and
resid 12 and name HD1) 3.682 1.695 1.695 weight 1.000 !
spec=VJN0...oPep, no=200, id=159, vol=6.752008e-03
    or (segid " A" and resid 12 and name HN) (segid " A" and
resid 12 and name HD2)
assign (segid " A" and resid 12 and name HD1) (segid " A" and
resid 11 and name HG1) 3.936 1.936 1.936 weight 1.000 !
spec=VJN0...oPep, no=205, id=163, vol=4.989948e-03
    or (segid " A" and resid 12 and name HD2) (segid " A" and
resid 11 and name HG1)
assign (segid " A" and resid 12 and name HE1) (segid " A" and
resid 12 and name HB2) 3.819 1.823 1.823 weight 1.000 !
spec=VJN0...oPep, no=210, id=166, vol=5.159995e-03
    or (segid " A" and resid 12 and name HE2) (segid " A" and
resid 12 and name HB2)
assign (segid " A" and resid 8 and name HD1) (segid " A" and
resid 7 and name HB2) 3.613 1.631 1.631 weight 1.000 !
spec=VJN0...oPep, no=215, id=170, vol=6.971925e-03
    or (segid " A" and resid 8 and name HD1) (segid " A" and
resid 7 and name HB1)
    or (segid " A" and resid 8 and name HD1) (segid " A" and
resid 7 and name HB3)
assign (segid " A" and resid 3 and name HB) (segid " A" and
resid 3 and name HG22) 2.251 0.634 0.634 weight 1.000 !
spec=VJN0...oPep, no=225, id=179, vol=1.082322e-01
    or (segid " A" and resid 3 and name HB) (segid " A" and
resid 3 and name HG21)
    or (segid " A" and resid 3 and name HB) (segid " A" and

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resid    3 and name HG23)
assign (segid "   A" and resid    3 and name HG12) (segid "   A" and
resid    3 and name HD12) 2.383 0.710 0.710 weight 1.000 !
spec=VJN0...oPep, no=226, id=180, vol=9.003468e-02
    or (segid "   A" and resid    3 and name HG12) (segid "   A" and
resid    3 and name HD11)
    or (segid "   A" and resid    3 and name HG12) (segid "   A" and
resid    3 and name HD13)
assign (segid "   A" and resid    3 and name HG11) (segid "   A" and
resid    3 and name HD12) 2.260 0.638 0.638 weight 1.000 !
spec=VJN0...oPep, no=227, id=181, vol=1.220956e-01
    or (segid "   A" and resid    3 and name HG11) (segid "   A" and
resid    3 and name HD11)
    or (segid "   A" and resid    3 and name HG11) (segid "   A" and
resid    3 and name HD13)
assign (segid "   A" and resid   11 and name  HG1) (segid "   A" and
resid   11 and name   HA) 3.166 1.253 1.253 weight 1.000 !
spec=VJN0...oPep, no=235, id=186, vol=1.643317e-02
assign (segid "   A" and resid    3 and name   HA) (segid "   A" and
resid    3 and name   HN) 3.061 1.171 1.171 weight 1.000 !
spec=VJN0...oPep, no=237, id=187, vol=2.335292e-02
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Supplementary Table S1

| name   | EC50<br>[μM] | peptide<br>sequence |    |         |         |          |          |     |     |     |           |      |     |   |   |     |     |
|--------|--------------|---------------------|----|---------|---------|----------|----------|-----|-----|-----|-----------|------|-----|---|---|-----|-----|
| B5.11  | 0.05         |                     | Ac | D       | V       | NI*      | D        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B3.15  | 0.13         |                     | Ac | D       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
|        |              | NorLe               |    |         |         |          |          |     |     |     |           |      |     |   |   |     |     |
| B5.6   | 0.2          | Ac                  | u  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
| B2.4   | 0.5          | Ac                  | R  | V       | NorLeuV |          | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
| B2.22  | 0.7          |                     | Ac | L       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
|        |              | NorLe               |    |         |         |          |          |     |     |     |           |      |     |   |   |     |     |
| B2.16  | 1.0          | Ac                  | u  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | R | K | Y   | NH2 |
| B2.18  | 1.0          | Ac                  | R  | V       | L       | V        | W        | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
|        |              | HomoL               |    |         |         |          | HomoL    |     |     |     |           |      |     |   |   |     |     |
| B2.27  | 1.8          | Ac                  | R  | V       | eu      | V        | eu       | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
| B8.1   | 2.2          | Ac                  | D  | V       | NI*     | E        | G        | A   | A   | W   | D         | Y    | K   | Y |   |     |     |
| B2.17  | 4            | Ac                  | R  | V       | L       | V        | NorLeuV  | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B3.19  | 5            |                     | Ac | L       | V       | W        | V        | G   | A   | A   | W         | D    | R   | K | Y | NH2 |     |
| B4.9   | 5            | Ac                  | R  | V       | NorLeuV |          | NI*      | V   | G   | A   | Orn       | W    | D   | Y | K | Y   | NH2 |
| B8.11  | 5.8          | Ac                  | D  | V       | NI*     | D        | G        | P   | A   | W   | D         | Y    | K   | Y |   |     |     |
| B8.7   | 6.8          | Ac                  | D  | V       | NI*     | D        | G        | A   | A   | W   | D         | Y    | R   | Y |   |     |     |
| B3.9   | 8.5          |                     | Ac | L       | V       | NI*      | V        | G   | P   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B2.35  | 10           | K                   | R  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   | E   |
|        |              | NorLe               |    |         |         |          |          |     |     |     |           |      |     |   |   |     |     |
| B2.5   | 11           | Ac                  | u  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | R   | NH2 |
| B2.28  | 11           |                     | R  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   |     |
| B2.21  | 12.7         | Ac                  | R  | V       | F       | V        | F        | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
| B3.11  | 14           |                     |    |         | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   |     |
| B2.12  | 20           | Ac                  | R  | V       | W       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
| B3.4   | 21           |                     | Ac | L       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | R | NH2 |     |
| B3.13  | 21           |                     | Ac | L       | V       | NI*      | C        | G   | A   | C   | W         | D    | Y   | K | Y | NH2 |     |
| B2.26  | 22           | Ac                  | Y  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | K | K | Y   | NH2 |
|        |              |                     |    |         |         |          | HomoL    |     |     |     |           |      |     |   |   |     |     |
| B2.32  | 22           | Ac                  | R  | V       | L       | V        | NI*      | V   | G   | A   | A         | eu   | D   | Y | K | Y   | NH2 |
| B1.1   | 24           | Ac                  | R  | S       | M       | NI*      | S        | Y   | G   | G   | A         | D    | D   | Y | K |     | NH2 |
| B3.7   | 26           |                     | Ac | L       | V       | NI*      | V        | G   | A   | R   | W         | D    | Y   | K | R | NH2 |     |
| B2.1   | 30           | Ac                  | R  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
| PL-120 | 35           | Ac                  | G  | A       | D       | Y        | K        | R   | NI* | T   | V         | K    | V   | N |   |     |     |
|        |              |                     |    |         | HomoL   |          | HomoL    |     |     |     |           |      |     |   |   |     |     |
| B3.3   | 35           |                     | Ac | eu      | V       | eu       | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| CRVL-  |              |                     |    |         |         |          |          |     |     |     |           |      |     |   |   |     |     |
| Cyclic | 35           |                     | C  | R       | V       | L        | V        | NI* | V   | G   | A         | A    | W   | D | Y | K   | Y   |
| B2.30  | 35           | Ac                  | R  | V       | L       | V        | NI*      | V   | G   | A   | A         | A    | L   | D | Y | K   | NH2 |
| B2.7   | 55           | Ac                  | R  | V       | L       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | R   | NH2 |
| B2.11  | 55           | Ac                  | R  | V       | K       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
|        |              |                     |    |         | HomoL   |          | HomoL    |     |     |     |           |      |     |   |   |     |     |
| B3.20  | NI*          |                     | Ac | eu      | V       | eu       | V        | G   | A   | A   | W         | D    | R   | K | Y | NH2 |     |
|        |              |                     |    |         | HomoL   |          |          |     |     |     |           |      |     |   |   |     |     |
| B3.21  | NI*          |                     | Ac | eu      | V       | W        | V        | G   | A   | A   | W         | D    | R   | K | Y | NH2 |     |
| B3.22  | NI*          |                     | Ac | L       | V       | NI*      | V        | G   | A   | Orn | W         | D    | Y   | K | Y | NH2 |     |
|        |              |                     |    |         | HomoL   |          |          |     |     |     |           |      |     |   |   |     |     |
| B3.23  | NI*          |                     | Ac | eu      | V       | W        | V        | G   | A   | Orn | W         | D    | R   | K | Y | NH2 |     |
| B4.1   | NI*          |                     | Ac | NorLeuV |         | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B4.2   | NI*          |                     |    | NorLeuV |         | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B4.3   | NI*          |                     | Ac | NorLeuV |         | NI*      | V        | G   | A   | A   | W         | D    | R   | K | Y | NH2 |     |
| B4.4   | NI*          |                     | R  | V       | NorLeuV |          | W        | V   | G   | A   | A         | W    | D   | Y | K | Y   |     |
| B4.5   | NI*          |                     | R  | V       | NorLeuV |          | NI*      | V   | G   | A   | A         | W    | D   | Y | K |     |     |
| B4.6   | NI*          | Ac                  | R  | V       | NorLeuR |          | NI*      | E   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
| B4.7   | NI*          |                     | R  | V       | NorLeuV |          | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   |     |
| B4.8   | NI*          |                     | R  | V       | NorLeuV |          | NorLeu V | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
|        |              |                     |    |         |         |          | L-4-NH2- |     |     |     |           |      |     |   |   |     |     |
| B4.10  | NI*          | R                   | V  | NorLeuV |         | NI*      | V        | G   | A   | A   | W         | D    | Phe | K | Y |     |     |
| B4.11  | NI*          |                     | Ac | NorLeuV |         | W        | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B4.12  | NI*          |                     | Ac | NorLeuV |         | W        | V        | G   | A   | A   | W         | D    | R   | K | Y |     |     |
| B4.13  | NI*          |                     |    | NorLeuV |         | W        | V        | G   | A   | A   | W         | D    | R   | K | Y |     |     |
| B4.14  | NI*          |                     |    | NorLeuV |         | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | R |     |     |
| B4.15  | NI*          |                     |    | NorLeuV |         | W        | V        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B5.2   | NI*          |                     | Ac | D       | V       | W        | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B5.3   | NI*          |                     | Ac | D       | Leu     | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B5.5   | NI*          | Ac                  | u  | V       | D       | V        | NI*      | V   | G   | A   | A         | W    | D   | Y | K | Y   | NH2 |
|        |              |                     |    |         | NorLe   |          | NorLe    |     |     |     |           |      |     |   |   |     |     |
| B5.7   | NI*          |                     | Ac | D       | u       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B5.8   | NI*          |                     | Ac | D       | V       | NorLeu V | G        | A   | A   | W   | D         | Y    | K   | Y |   |     |     |
| B5.10  | NI*          |                     | Ac | D       | NI*     | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B5.12  | NI*          |                     | Ac | E       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B5.13  | NI*          |                     | Ac | D       | W       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B5.14  | NI*          |                     |    | D       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B6.1   | NI*          |                     | Ac | D       | V       | NI*      | V        | G   | A   | A   | L-1-Nal D | Y    | K   | Y |   |     |     |
| B6.2   | NI*          |                     | Ac | L       | V       | NI*      | V        | G   | A   | A   | W         | pSer | Y   | K | Y | NH2 |     |
|        |              |                     |    |         |         |          | Lys(Me)  |     |     |     |           |      |     |   |   |     |     |
| B6.3   | NI*          |                     | Ac | D       | V       | NI*      | V        | G   | A   | A   | W         | D    | 1)  | K | Y | NH2 |     |
| B7.1   | NI*          |                     | Ac | D       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B7.2   | NI*          |                     | Ac | D       | V       | NI*      | V        | G   | S   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B7.3   | NI*          |                     | Ac | D       | V       | NI*      | V        | G   | A   | S   | W         | D    | Y   | K | Y | NH2 |     |
| B7.4   | NI*          |                     | Ac | D       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B7.5   | NI*          |                     | Ac | D       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B7.6   | NI*          |                     | Ac | D       | D       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B7.7   | NI*          |                     | Ac | N       | V       | NI*      | V        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |
| B7.8   | NI*          |                     | Ac | D       | V       | NI*      | D        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B7.9   | NI*          |                     | Ac | D       | V       | NI*      | D        | G   | A   | A   | W         | D    | Y   | K | Y |     |     |
| B7.10  | NI*          |                     | Ac | D       | V       | NI*      | Y        | G   | A   | A   | W         | D    | Y   | K | Y | NH2 |     |

|       |      |  |    |      |     |        |      |   |      |   |   |   |        |   |      |   |   |     |
|-------|------|--|----|------|-----|--------|------|---|------|---|---|---|--------|---|------|---|---|-----|
| B7.11 | NI*  |  | Ac | D    | V   | NI*    | Y    | G | A    | A | W | D | Y      | K | Y    | L | T | NH2 |
| B8.2  | NI*  |  | Ac | D    | A   | NI*    | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.3  | NI*  |  | Ac | D    | V   | V      | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.4  | NI*  |  | Ac | D    | V   | NI*    | N    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.5  | NI*  |  | Ac | N    | V   | NI*    | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.12 | NI*  |  | Ac | D    | V   | NI*    | D    | P | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.13 | NI*  |  | Ac | D    | V   | L      | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
|       |      |  |    |      |     | Homol  |      |   |      |   |   |   |        |   |      |   |   |     |
| B8.14 | NI*  |  | Ac | D    | V   | eu     | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.15 | NI*  |  | Ac | D    | L   | NI*    | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.16 | NI*  |  | Ac | D    | NI* | NI*    | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.17 | NI*  |  | Ac | E    | V   | NI*    | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
|       |      |  |    |      |     | Homol  |      |   |      |   |   |   |        |   |      |   |   |     |
| B8.18 | NI*  |  | Ac | D    | eu  | NI*    | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.19 | NI*  |  | Ac | D(D) | V   | NI*    | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B8.20 | NI*  |  | Ac | D    | V   | NI*    | D    | G | A    | D | W | D | Y      | K | Y    |   |   | NH2 |
| B8.21 | NI*  |  | Ac | D    | V   | NI*    | D    | G | A    | A | H | D | Y      | K | Y    |   |   | NH2 |
| B8.22 | NI*  |  | Ac | D    | V   | NI*    | D    | G | A    | A | W | D | R      | K | Y    |   |   | NH2 |
| B8.23 | NI*  |  | Ac | D    | V   | NI*    | D    | G | A    | A | W | D | Y      | K | R    |   |   | NH2 |
| B8.24 | NI*  |  | Ac | D    | V   | NI*    | D    | G | A    | A | W | D | Y      | K |      |   |   |     |
| B9.0  | NI*  |  |    |      |     | Ac     | D    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.1  | NI*  |  |    |      |     | Ac     | D    | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.2  | NI*  |  |    |      |     | Ac     | D    | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.3  | NI*  |  |    |      |     | Ac     | D(D) | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.4  | NI*  |  |    |      |     | Ac     | E    | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.5  | NI*  |  |    |      |     | Ac     | E(D) | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.9  | NI*  |  |    |      |     | Ac     | D(D) | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.10 | NI*  |  |    |      |     | D      | G    | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B3.14 | NI*  |  | Ac | L    | V   | NI*    | V    | G | A    | A | W | D | Y      | K |      |   |   | NH2 |
| B9.6  | NI** |  |    |      |     | Ac     | E    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.7  | NI** |  |    |      |     | Ac     | E    | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B9.8  | NI** |  |    |      |     | Ac     | D(D) | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B2.19 | NI** |  |    |      |     | Ac     | A    | A | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B3.1  | NI** |  |    |      |     | Ac     | NI*  | V | G    | A | A | W | D      | Y | K    | Y |   | NH2 |
| B3.8  | NI** |  | Ac | W    | V   | W      | V    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
|       |      |  |    |      |     | (N-Me- |      |   |      |   |   |   | (N-Me- |   |      |   |   |     |
| B3.10 | NI** |  | Ac | L    | V   | NI*    | V    | G | Ala) | A | W | D | Y      | K | TYR) |   |   | NH2 |
| B3.12 | NI** |  |    |      |     | NI*    | V    | G | A    | A | W | D | Y      | K | Y    |   |   |     |
| B3.16 | NI** |  | Ac | L    | V   | D      | V    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |
| B3.17 | NI** |  | Ac | L    | V   | NI*    | V    | G | A    | A | W | D | R      | K | Y    |   |   | NH2 |
| B3.18 | NI** |  | Ac | L    | E   | NI*    | K    | G | A    | E | W | D | Y      | K | Y    |   |   | NH2 |
| B3.2  | NI** |  | Ac | L    | V   | W      | V    | G | A    | A | W | D | Y      | K | Y    |   |   | NH2 |