

Supplementary Table 1. Mean collision cross-sections (\AA^2) of Defb14, Defb14-1Cys^V and Defb14-0Cys under buffered and denaturing conditions.

| Charge state | Buffered conditions ^a | | | Denaturing conditions ^b | | |
|----------------------|----------------------------------|--------------------------|---------------|------------------------------------|--------------------------|-------------|
| | Defb14 ^c | Defb14-1Cys ^V | Defb14-0Cys | Defb14 | Defb14-1Cys ^V | Defb14-0Cys |
| [M+3H] ³⁺ | - | <i>d</i> | 659 \pm 3 | <i>d</i> | <i>d</i> | <i>d</i> |
| [M+4H] ⁴⁺ | - | 740 \pm 12 | 798 \pm 9 | 709 | <i>d</i> | <i>d</i> |
| [M+5H] ⁵⁺ | - | 888 \pm 23 | 1008 \pm 7 | 751 | 916 | <i>d</i> |
| [M+6H] ⁶⁺ | - | 986 \pm 19 | 1076 \pm 15 | 881 | 962 | 979 |
| [M+7H] ⁷⁺ | - | 1053 \pm 15 | 1086 \pm 11 | 1008 | 1018 | 1070 |
| [M+8H] ⁸⁺ | - | 1125 \pm 15 | 1116 \pm 7 | <i>d</i> | 1105 | 1170 |
| [M+9H] ⁹⁺ | - | 1216 \pm 9 | 1185 \pm 2 | <i>d</i> | <i>d</i> | <i>d</i> |

^a Errors are quoted as the standard error of the mean

^b Taken from reference (20) in main text: B. J. McCullough, J. Kalapothakis, H. Eastwood, P. Kemper, D. MacMillan, K. Taylor, J. Dorin and P. E. Barran, Anal. Chem., 2008, 80, 6336-6344.

^c Not determined

^d Not observed by IM-MS