Structural characterisation of the catalytic domain of botulinum neurotoxin X - high activity and unique substrate specificity

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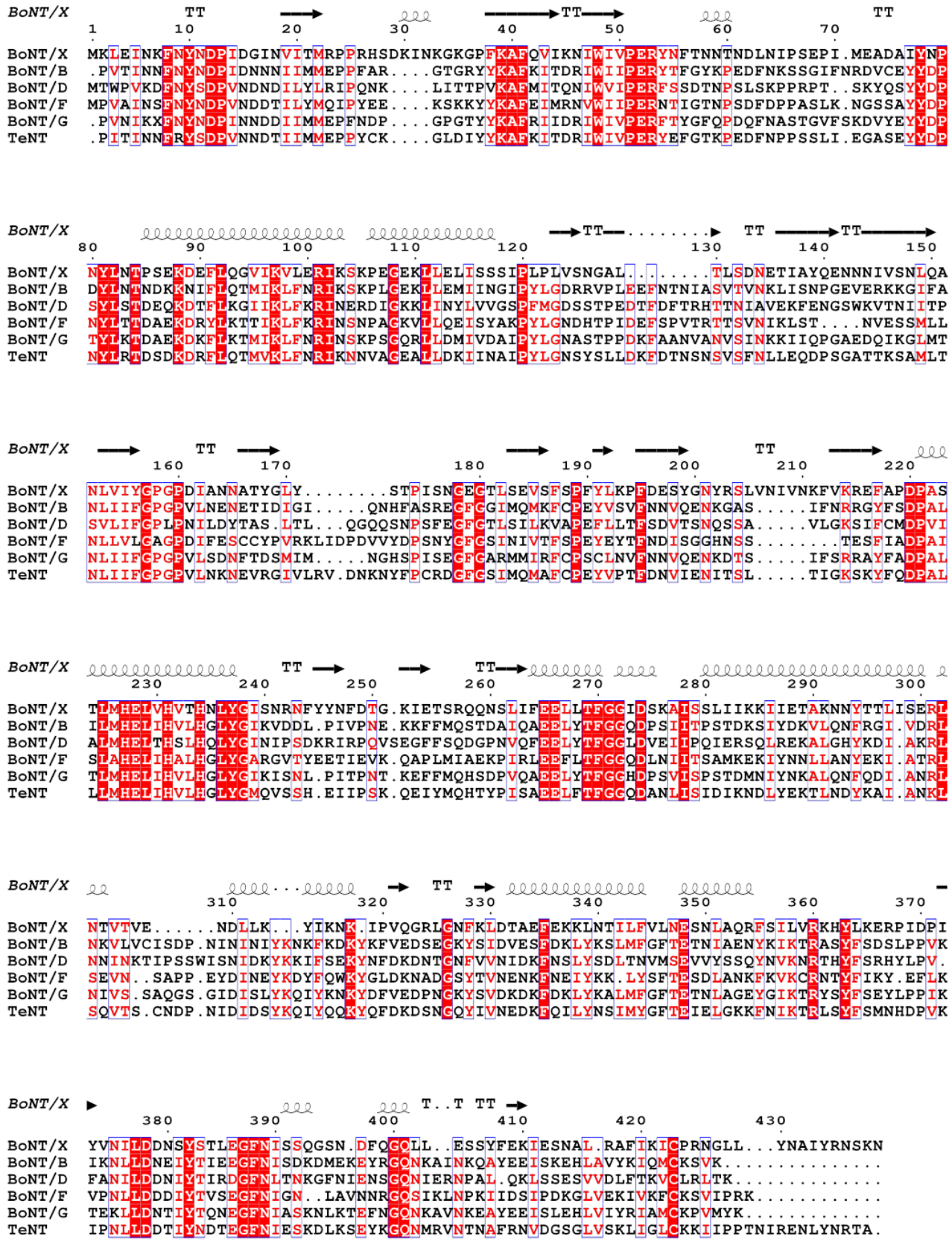
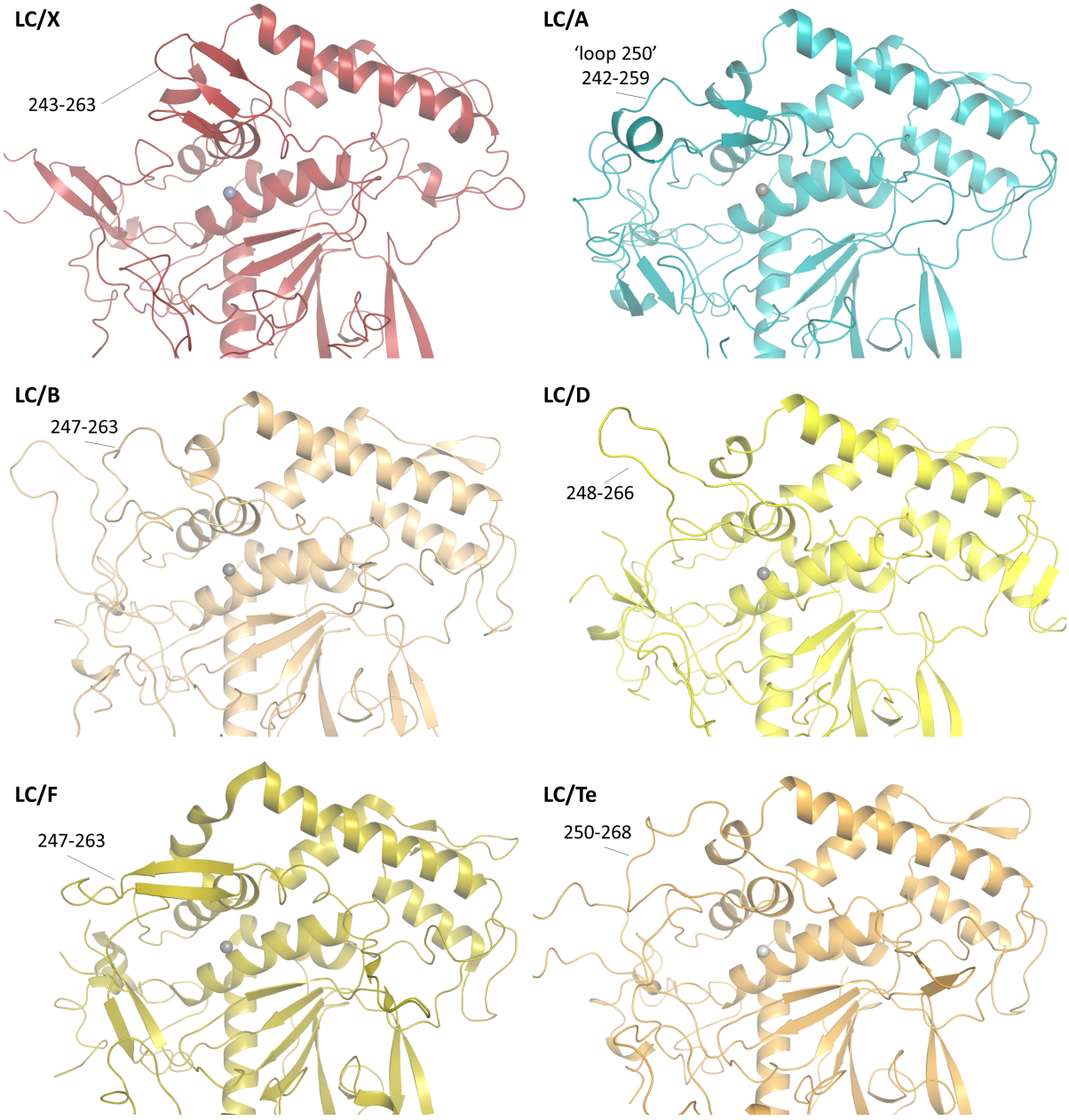
Supplementary information:

Supplementary Figure S1: Sequence alignment of LC/X with other VAMP-cleaving LCs



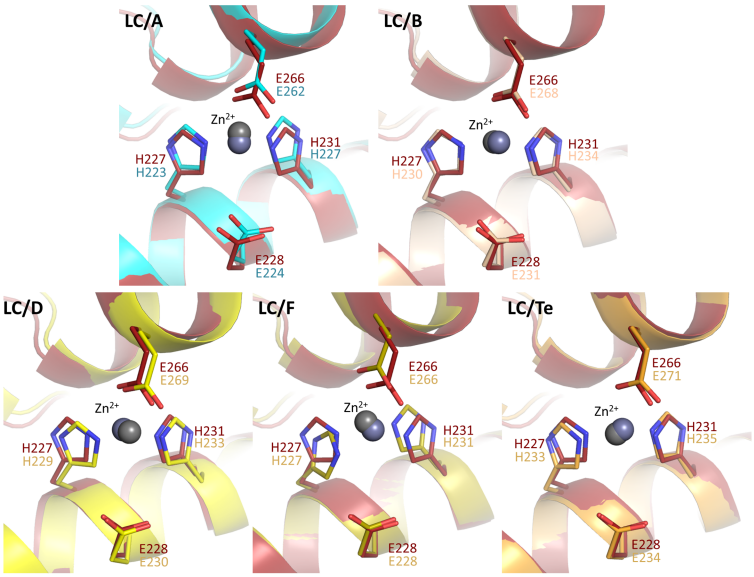
Supplementary Figure S2: Loop 250: Comparison of the loop between LCs

Ribbon representation of LC/X (Red), compared to the LC of serotypes A, (cyan, PDB 3BON), B (sand, PDB 1EPW), D (yellow, PDB 2FPQ), F (gold, PDB 2A97), and Te (light orange, PDB 1Z7H). The zinc ion is shown as a grey sphere.

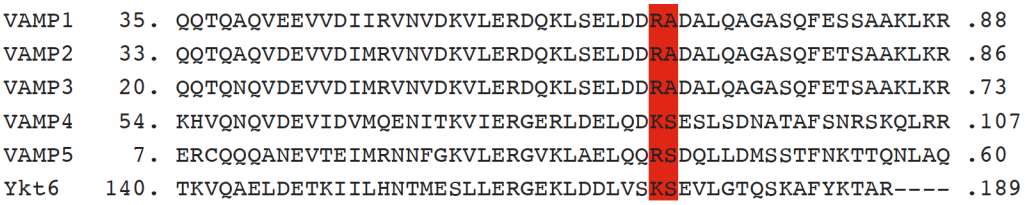


Supplementary Figure S3: Catalytic site: conserved Zn^{2+} coordination

LC/X (Red) was superposed with the LC of serotypes A, (cyan, PDB 3BON), B (sand, PDB 1EPW), D (yellow, PDB 2FPQ), F (gold, PDB 2A97), and Te (light orange, PDB 1Z7H). The zinc ion is shown as a grey sphere and the zinc-coordinating residues as sticks.



Supplementary Figure S4: LC/X cleavage sites on its VAMP substrates.
Cleavage site is highlighted in red.



Supplementary Table S1: Exponential fit parameters (see Fig. 6A)

	A	k (min^{-1})	C	R^2
LC/X	0.19	0.07	0.11	0.95
LC/B	0.15	0.02	0.14	0.94