The crystal structure of Ac-AChBP in complex with α-conotoxin LvIA reveals the mechanism of its selectivity towards different nAChR subtypes

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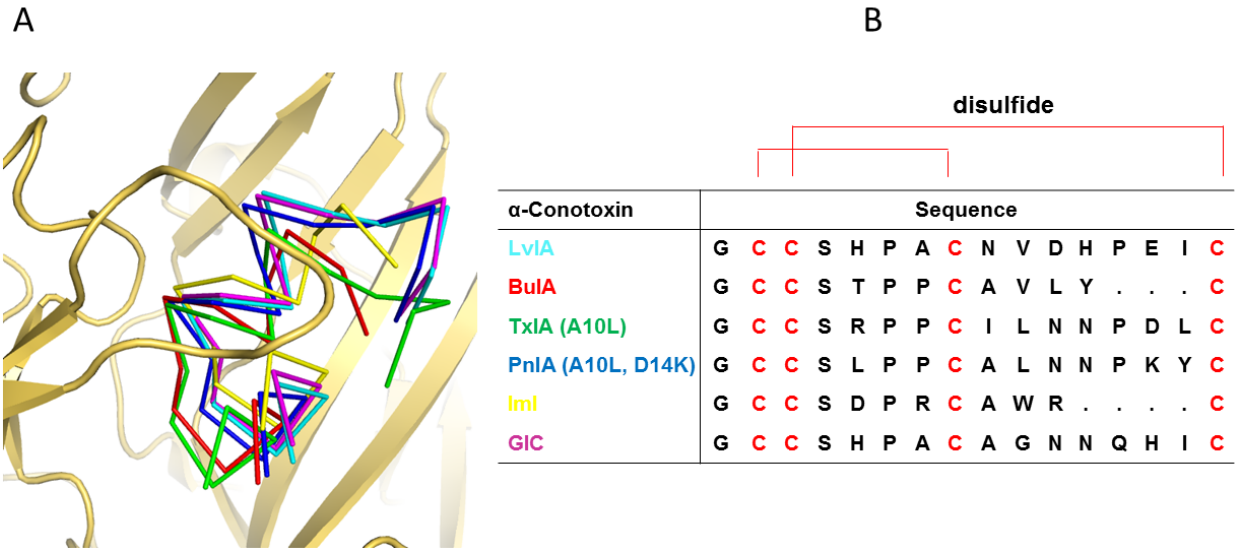
Running Title: Co-crystal structure of α-conotoxin LvIA and acetylcholine binding proteins

Figure S1: **Supplementary Figure 1: Backbone orientations observed in co-crystal structures of Ac-AChBP with five α-conotoxins. (A)** The backbone of LvIA is shown in light blue, BuIA in red, TxIA (A10L) in green, PnIA (A10L, D14K) in blue, ImI in yellow and GIC in magenta. **(B)** Multiple sequence alignment of α-conotoxins LvIA, BuIA, TxIA (A10L), PnIA (A10L, D14K), ImI and GIC. Disulfide bridges between Cys2-Cys8 and Cys3-Cys16 are shown in red.



α-Conotoxin	Sequence
LvIA	G C C S H P A C N V D H P E I C
BuIA	G C C S T P P C A V L Y . . . C
TxIA (A10L)	G C C S R P P C I L N N P D L C
PnIA (A10L, D14K)	G C C S L P P C A L N N P K Y C
ImI	G C C S D P R C A W R C
GIC	G C C S H P A C A G N N Q H I C

Figure S2: Crystal structures of Ac-AChBP in different comformation. (A) Top view of Ac-AChBP/HEPES structure, showing Loop C in close status. **(B)** Top view of Ac-AChBP/LvIA structure, showing Loop C in open status. **(C)** Top view of Ac-AChBP/GIC structure, showing Loop C in close status.