Batrachotoxin, Pyrethroids and BTG 502 Share Overlapping Binding Sites On Insect Sodium Channels
Yuzhe Du*, Daniel Garden*, Bhupinder Khambay, Boris S. Zhorov and Ke Dong
Molecular Pharmacology

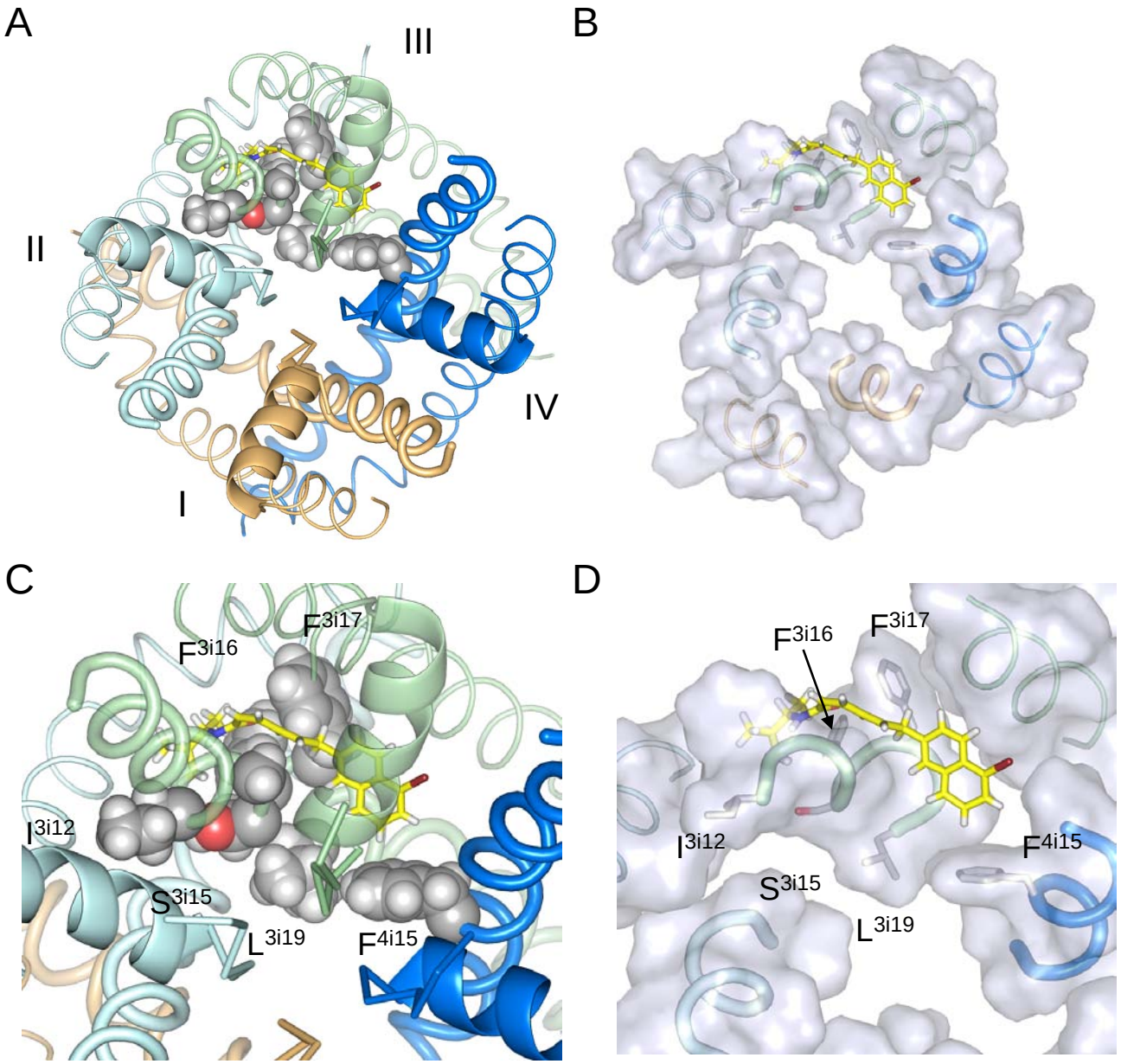

Figure S1. (***A, B***) An alternative binding mode of BTG 502. The toxin wraps around the IIIS6 helix, exposes its linker towards the lipids, and established contacts with all known BTG 502 sensing residues, except S^{3i15}. However, the toxin-channel binding energy in this mode is lower than in the binding mode shown in Fig. 4 where BTG 502 wraps around IIIS6 and exposes its linker to the inner pore. (***C, D***) The zoomed views. The bulky naphthalene ring binds between helices IIIS5 and IIIS6 and the isopropyl group binds between IIS5 and IIIS6.

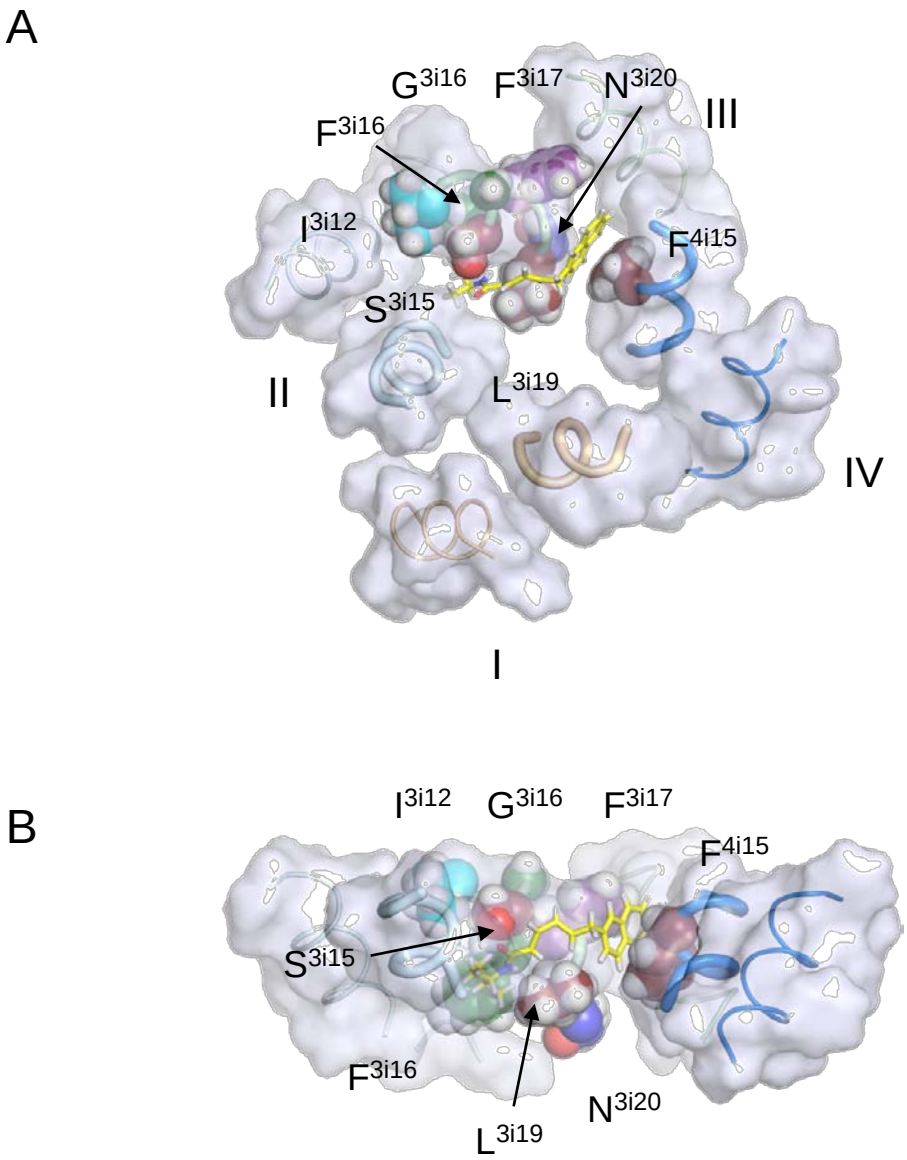

Fig. S2. (***A, B***) BTG 502 sensing residues categorized by their involvement in BTX, BTG 502, deltamethrin binding, as well as BTG 502 antagonism of deltamethrin, summarized in Table 2. Domain I is hidden for clarity. Residues with red carbons affect the binding of BTX and BTG 502, in addition to BTG antagonism of deltamethrin. Residues with purple carbons affect the binding of deltamethrin and BTG 502 binding and also affect BTG 502 antagonism. Residues with green carbons affect binding of all three toxins but not BTG 502 antagonism. Residues with light blue carbons affect binding of deltamethin and BTG 502, but not BTG 502 antagonism. Finally dark blue residues affect binding of delamethrin, but not BTG 502 binding or antagonism.