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Binding of ciguatera toxins to the voltage-gated Kv1.5 potassium channel in the open state. Docking of gambierol and molecular dynamics simulations of a homology model

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Ciguatera poisoning is a toxinological syndrome from ingestion of seafood contaminated by dinoflagellate toxins which has serious social and economic consequences from the Indo-Pacific to the Caribbean. These polyannealed ethereal-ring toxins, which comprise ciguatoxins, maitotoxin, and gambierol, are known to affect ion channels. Reported here are the first indications at molecular level as to the mode of interaction of these toxins with ion channels. The study concerns gambierol, an eight-ring ladder polyether which is known to affect TRPV1-type of thermal and pain sensation channels, as well as to inhibit voltage-gated currents in K*R* channels of mouse taste cells. Automated docking of gambierol on a homology model of the voltage-gated Kv1.5 potassium ion channel in implicit solvent is followed by molecular dynamics (MD) simulation of the complex in a POPC membrane solvated with water. It is found that gambierol binds to the internal helices of the channel, unequally to the different subunits of the tetramer. Such unequal binding is a novel observation that should stimulate and aid developing a much demanded medical treatment of ciguatera poisoning.

It has come to our attention that this published article contained an error.

The Figures **1A, 1B**, and Figure 2 should have been printed in colour. Please see the Figures in colour below.

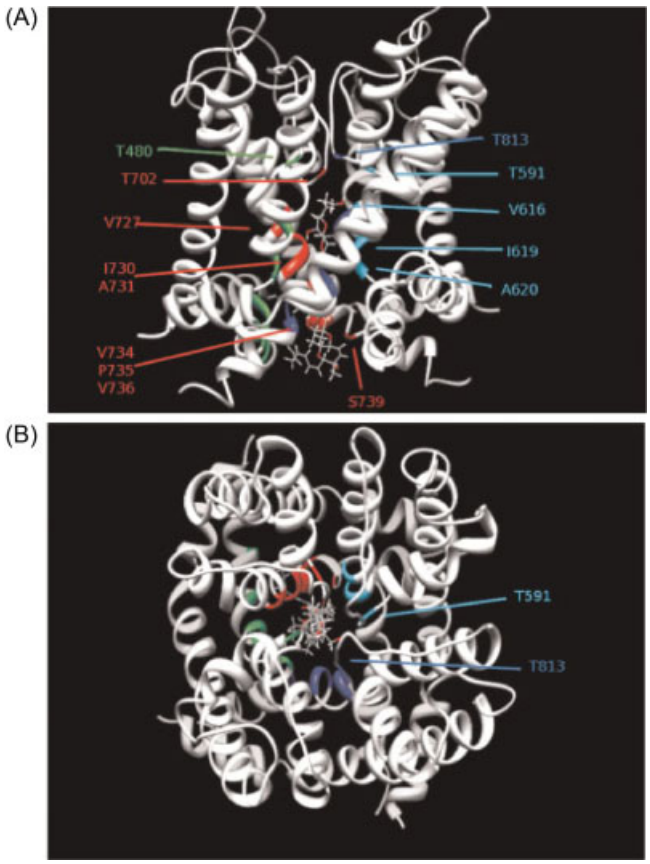

Figure 1A,B

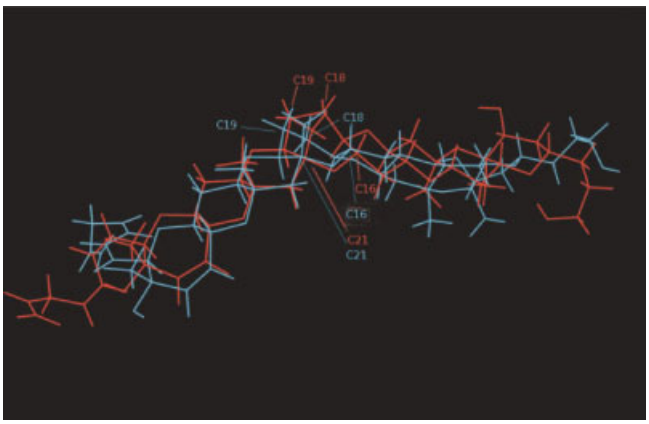

Figure 2

We apologise for any inconvenience caused.