frontiers

Supplementary Material

Inhibition of tryptophan hydroxylases and monoamino oxidase-A by the proton pump inhibitor, omeprazole - *in vitro* and *in vivo* investigations

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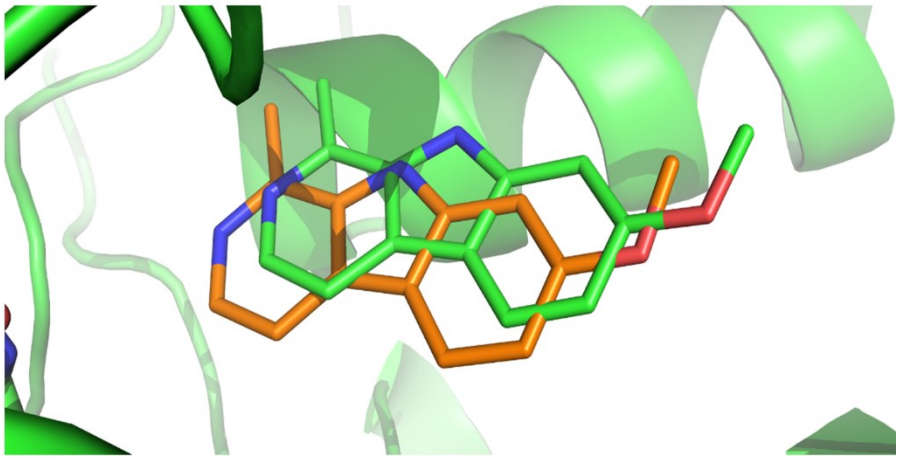
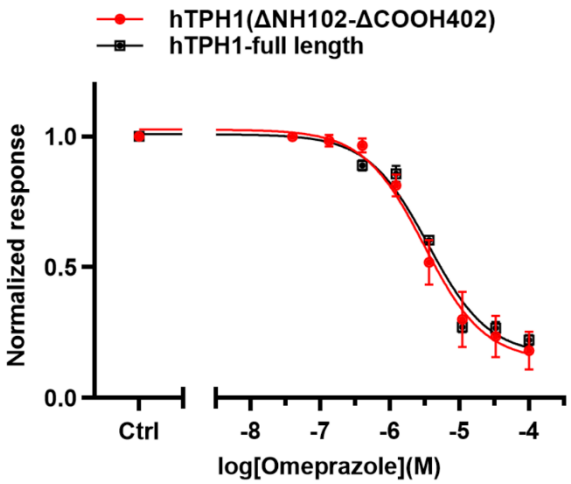
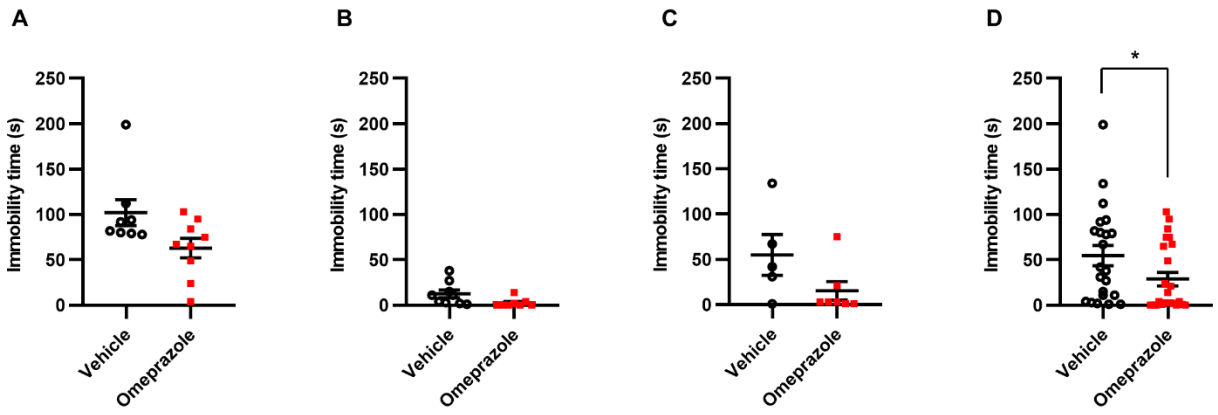
1.1 Supplementary Figures



Supplementary Figure S1. Docking of harmine to MOA-A. Docking pose of harmine (green carbons) superimposed with the conformation of harmine from the x-ray structure (orange carbons). The main reason for the slight shift in position of harmine in the docked vs experimentally determined complex is likely due to the removal of water molecules prior to docking. Inclusion of water molecules resulted in docking poses even closer to the experimental binding pose. However, water molecules were removed prior to the docking procedure to better explore the binding pocket of the receptors.



Supplementary Figure S2. Comparing the potency of omeprazole in inhibiting full-length and doubly truncated tryptophan hydroxylase 1. Omeprazole demonstrated similar inhibitory activity at full-length TPH1 IC_{50} = 3.55 (95% confidence interval; 2.31 to 5.49) µM and at doubly truncated hTPH1(ΔNH102-ΔCOOH402) IC_{50} = 3.09 (95% confidence interval; 2.53 to 3.77) µM.



Supplementary Figure 3. In vivo effects of 100 mg/kg omeprazole on immobility time in the tail suspension test. Immobility time in the tail suspension test, performed on three different groups of animals. Statistical significance was evaluated using the Mann-Whitney test; A) Group 1, $p = 0.059$ B) Group 2; $p = 0.014$ C) Group3; $p = 0.193$ D) Pooled data from all three groups; *, $p = 0.028$.