

Supporting material

Diffusion Mechanism Modeling of metformin in Human Organic Cationic Amino Acid Transporter one and Functional Impact of S189L, R206C, and G401S Mutation.

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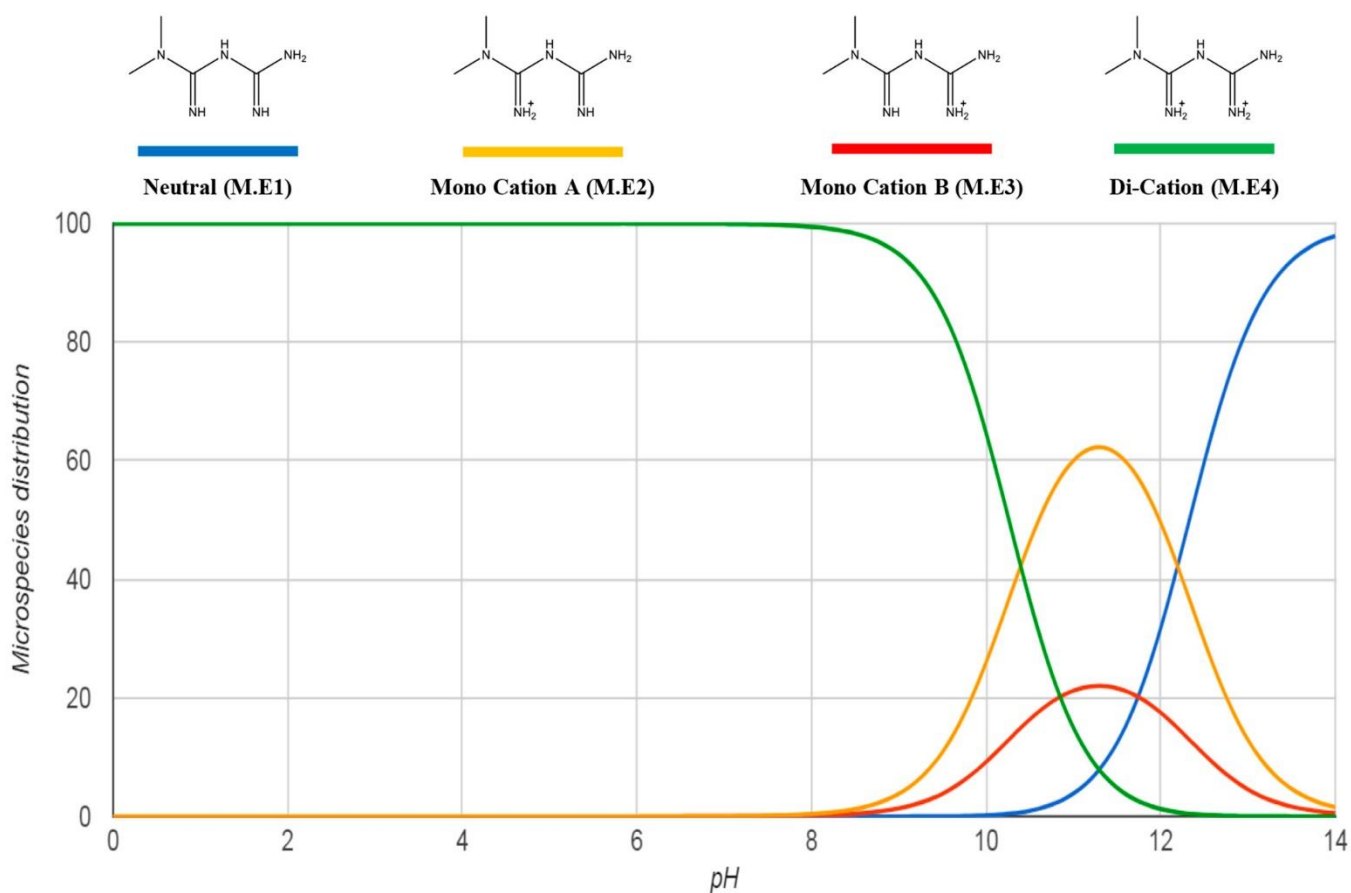


Fig. S1 Metformin characterization for calculation of the α (alpha) fractions

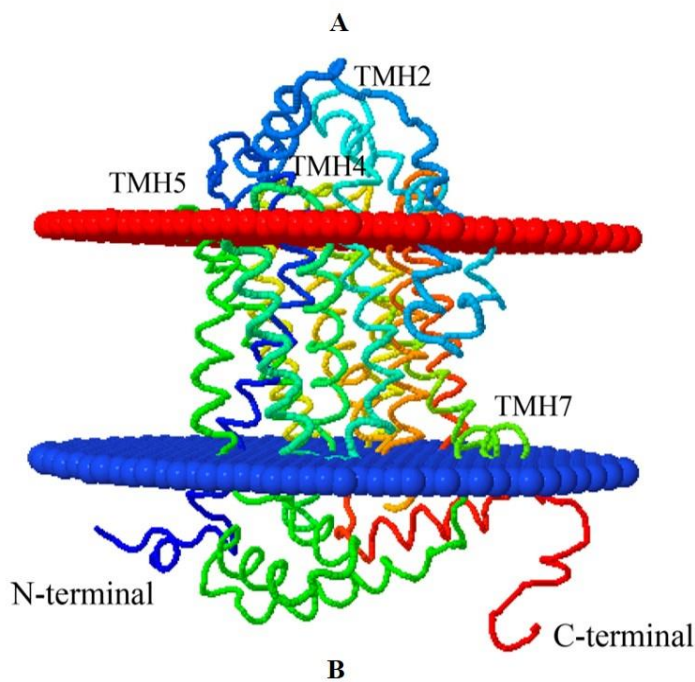
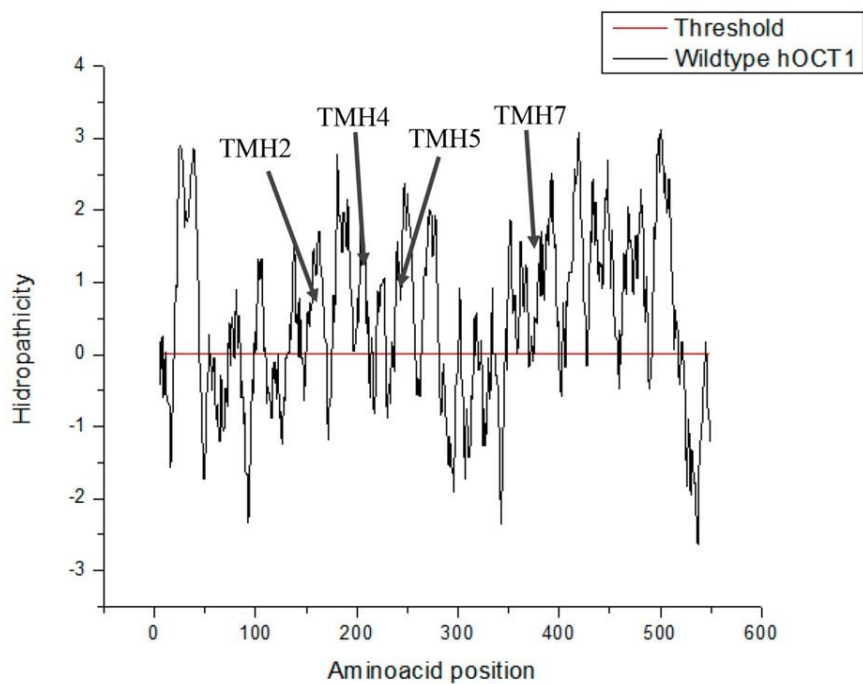


Fig. S2 Characterization of Human Organic Cation Transporter hOCT1: A) Hydropathy index plot for hOCT1; B) Structure of transmembrane α -helices involved in the passive diffusion of the metformin cation

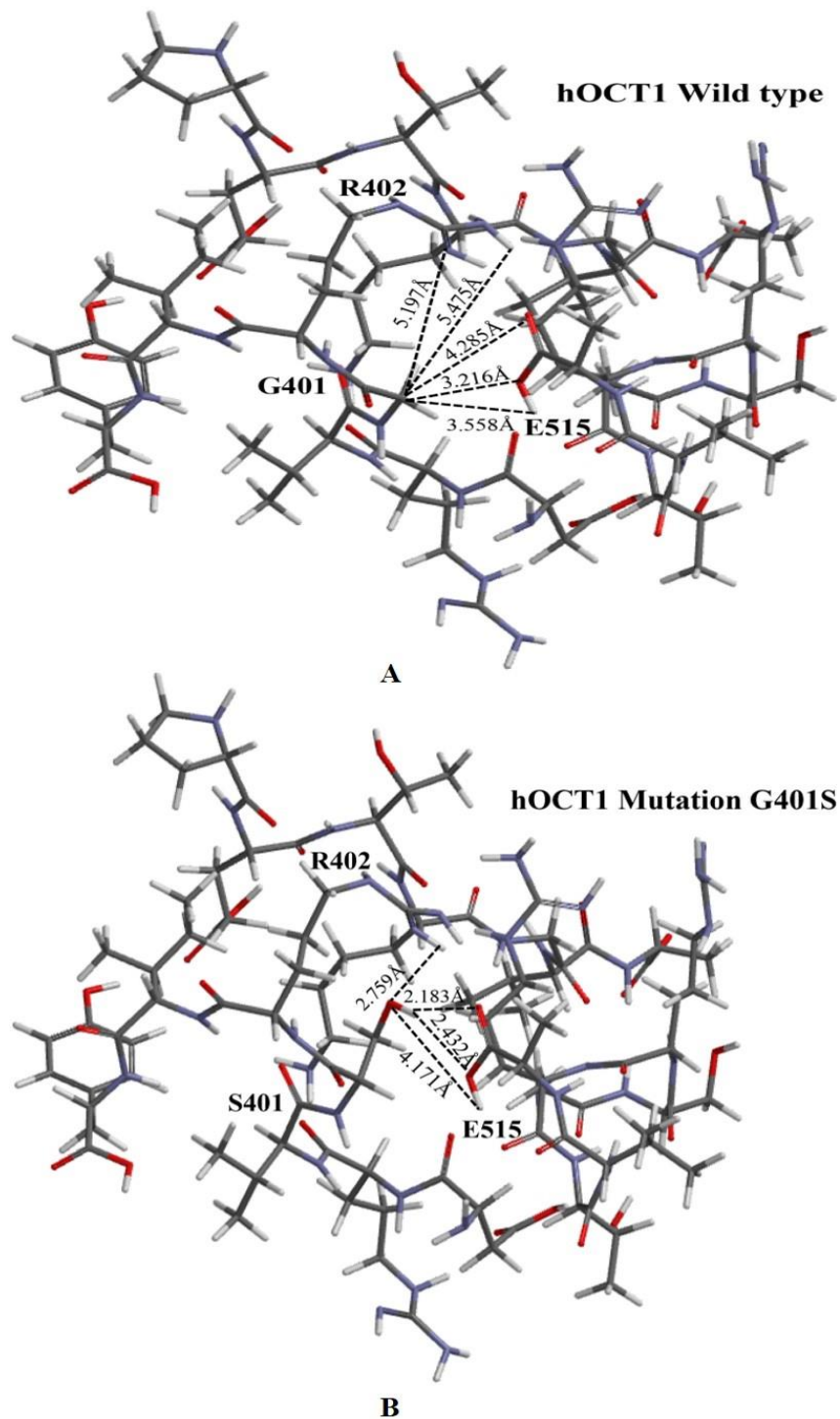


Fig.S3. Stick representation of amino acid structure in the proximity of position 401 in hOCT1: A) Bonding distances for the 401Gly structure; B) Bonding distances for the Ser401 structure

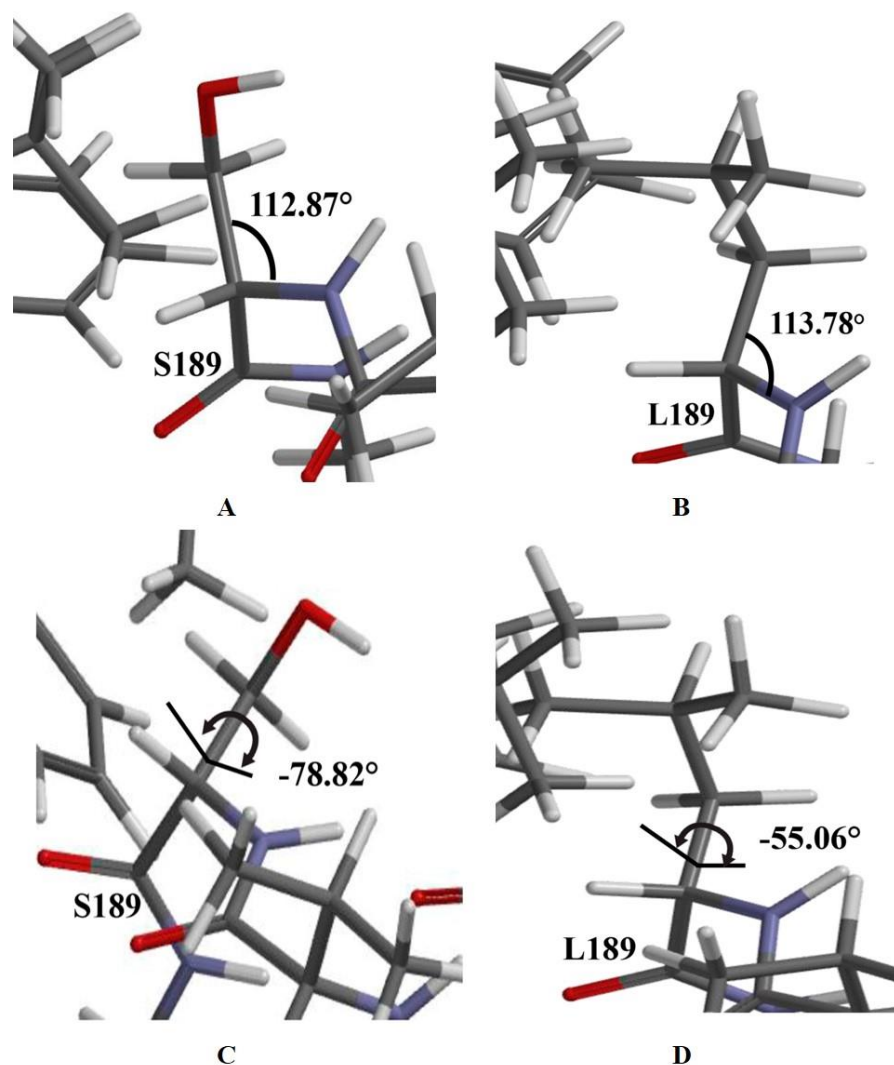


Fig.S4. Structural comparison of the region adjacent to position 189 of the hOCT1 channel: A) 3D visualization of the change in angle of the alpha carbon in the wild type Ser189 channel; B) 3D visualization of the change in angle of the alpha carbon in the wild type Leu189 mutated channel; C) 3D visualization of the change in the dihedral angle between alpha carbon planes in the wild type Ser189 channel; D) 3D visualization of the change in the dihedral angle of the alpha carbon planes Leu189 mutated channel