Electronic Supplementary Information for:

Synthesis of 3-Alkyl Enol Mimics Inhibitors of Type II Dehydroquinase: Factors Influencing Their Inhibition Potency

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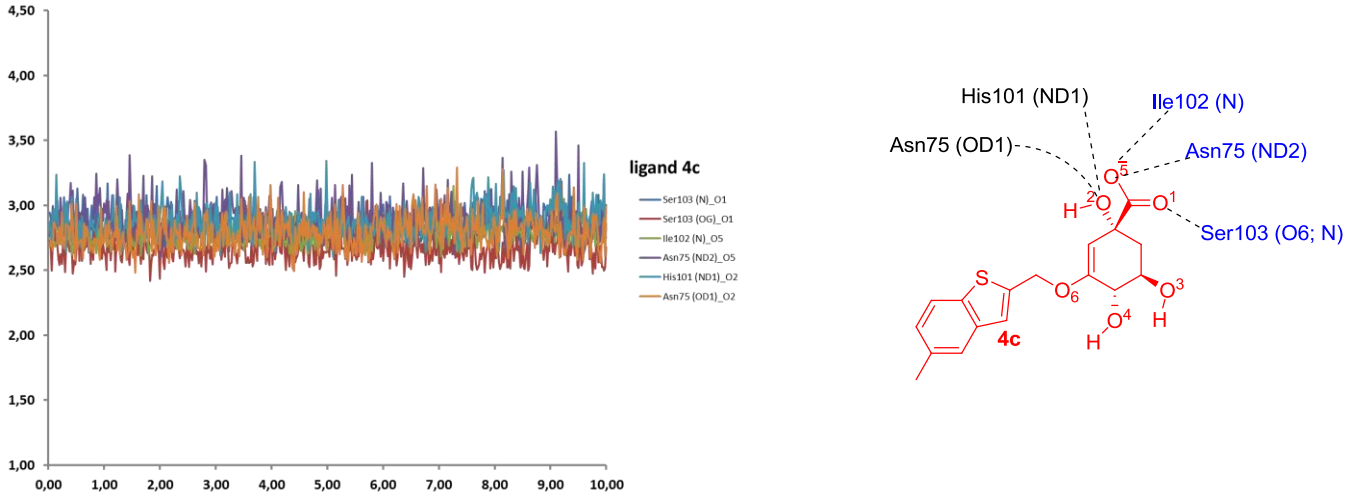
a)



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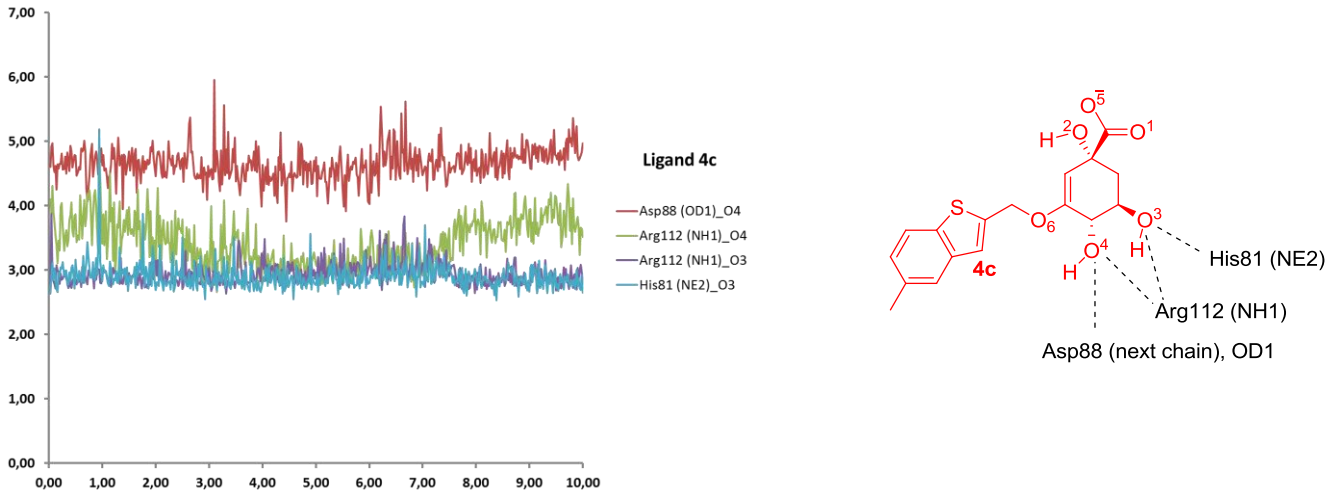
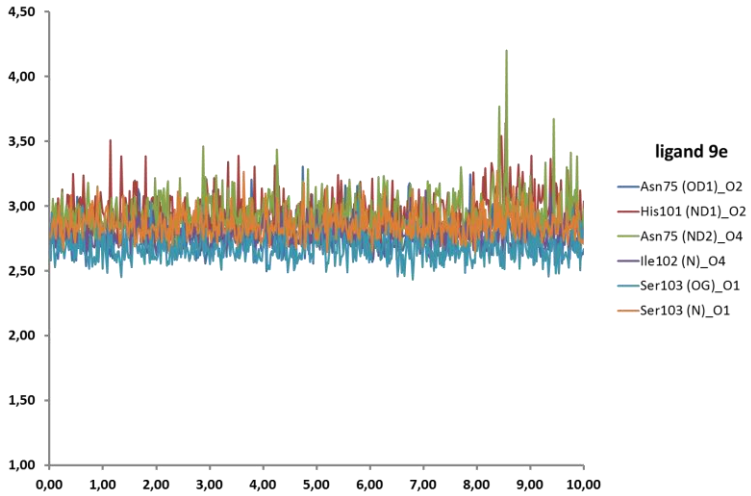
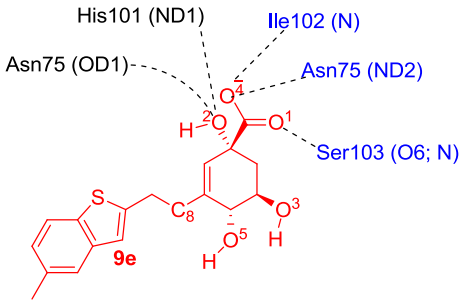


Figure S1. The variation of the distance between polar contacts in the active site with: a) the carboxylate (O5 and O1) and tertiary hydroxyl group (O2) of ligand **4c**; b) the hydroxyl groups (O3 and O4) of ligand **4c** is indicated. Note how no significant changes of these polar contacts of the ligand **4c** with residues Asn75, His101, Ile102, Ser103, His81, Arg112 and Asp88 (neighboring chain) were observed.

a)





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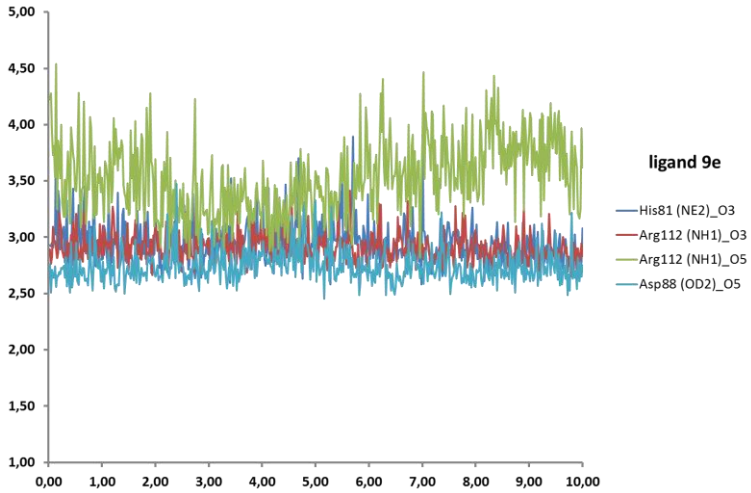


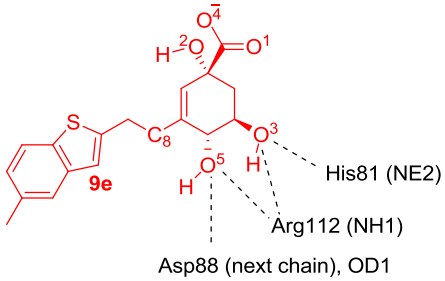
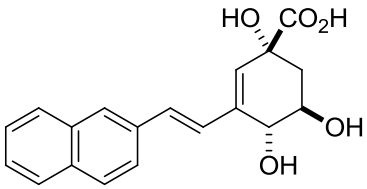
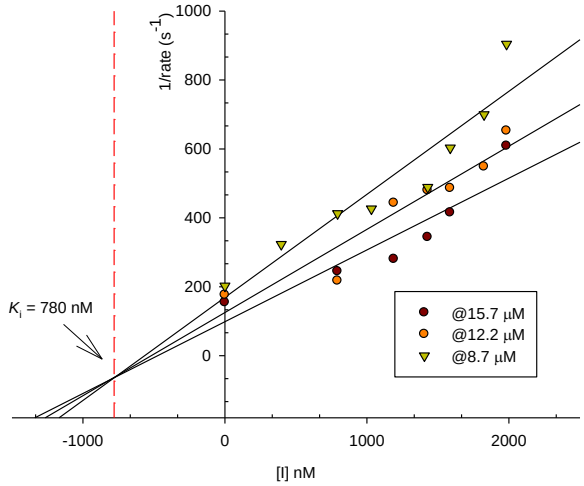


Figure S2. The variation of the distance between polar contacts in the active site with: a) the carboxylate (O1 and O4) and tertiary hydroxyl group (O2) of ligand **6e**; b) the hydroxyl groups (O3 and O4) of ligand **6e** is indicated. Note how no significant changes of these polar contacts of the ligand **6e** with residues Asn75, His101, Ile102, Ser103, His81, Arg112 and Asp88 (neighboring chain) were observed.



5a

M. tuberculosis



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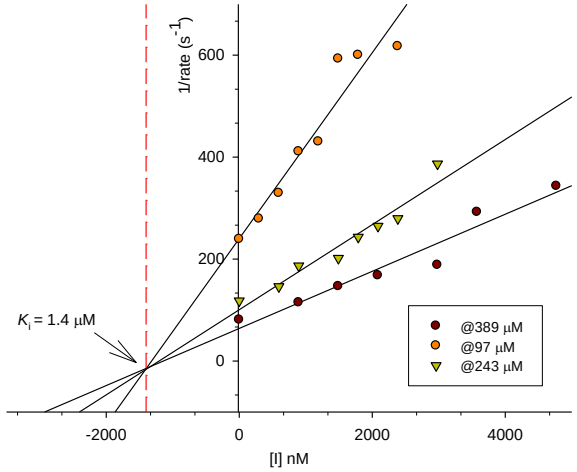

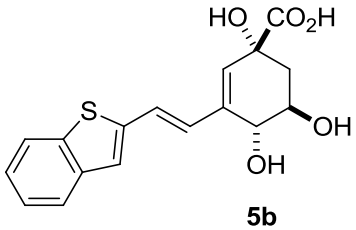

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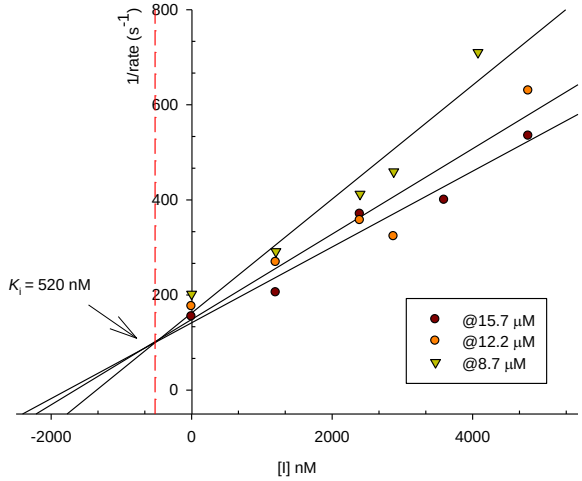

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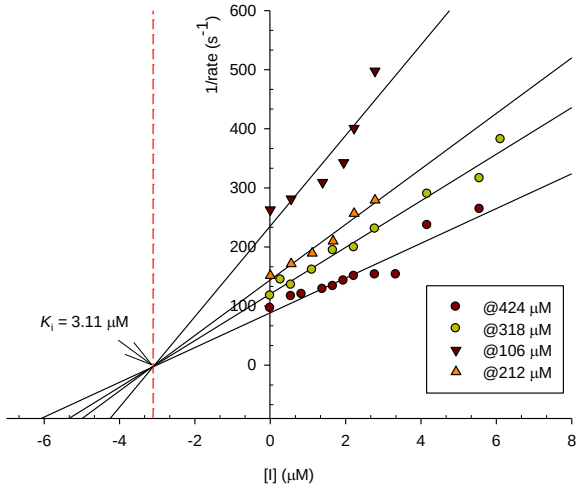

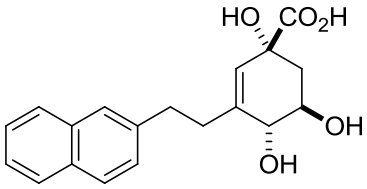

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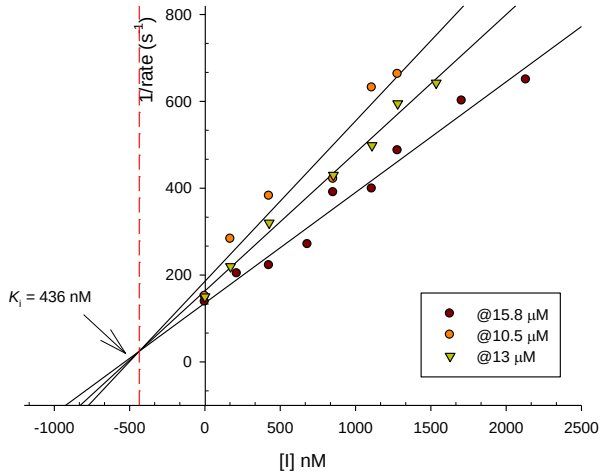
M. tuberculosis



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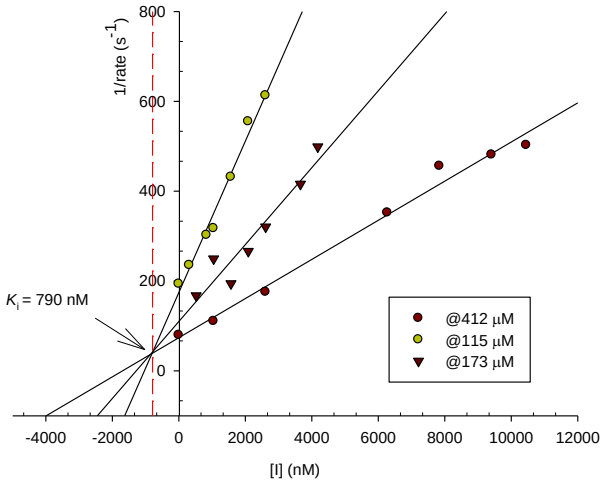
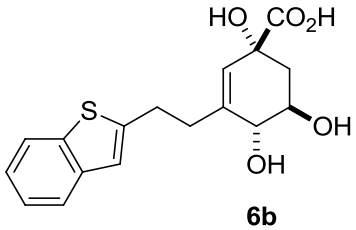
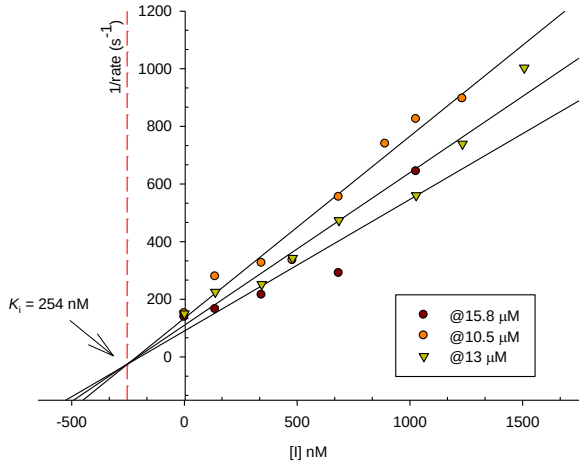




6b

M. tuberculosis



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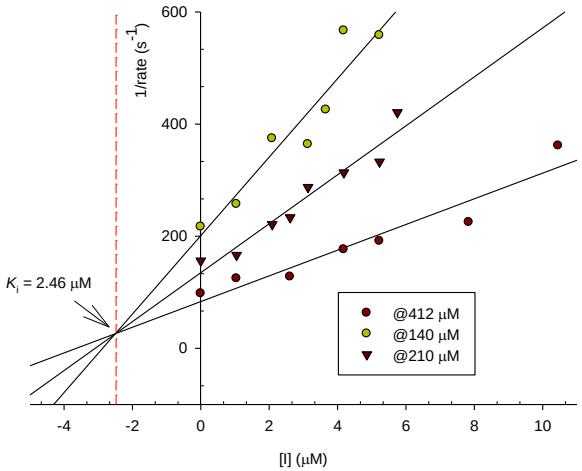
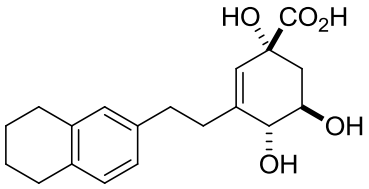
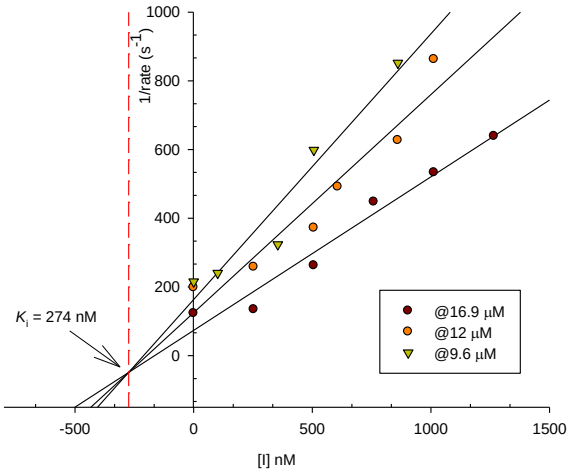




6c

M. tuberculosis



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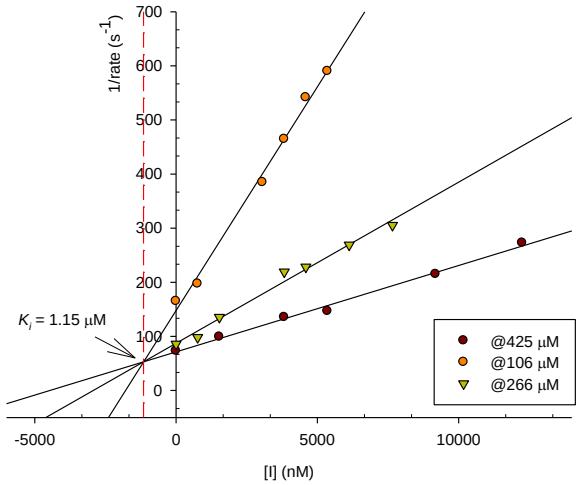
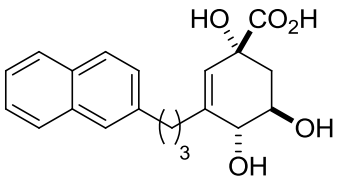
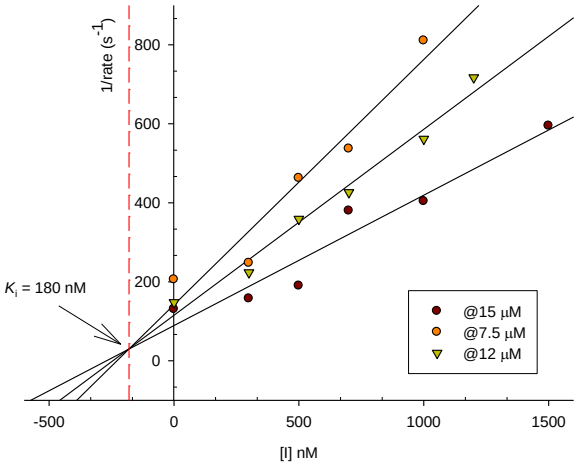


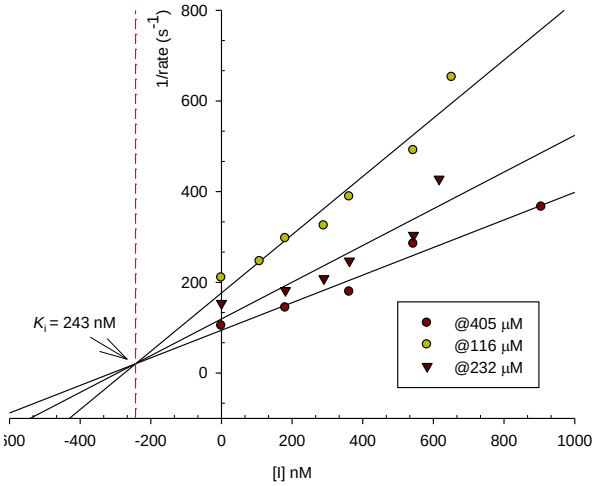


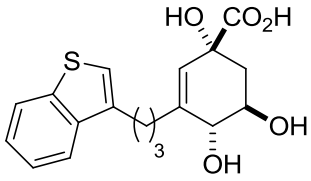
7a

M. tuberculosis



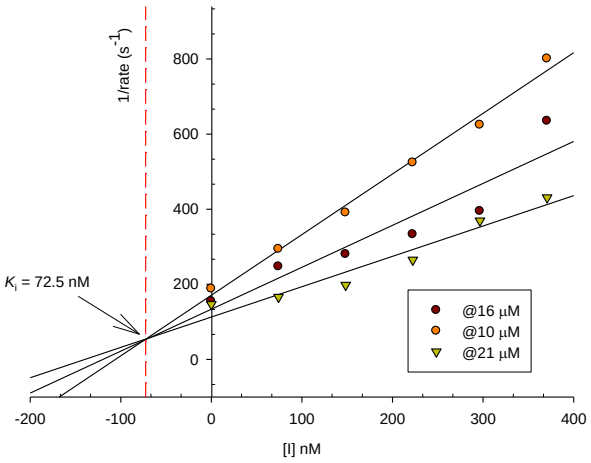
H. pylori





7b

M. tuberculosis



H. pylori