Supplementary Information

Docking and QM/MM Studies of NS2B-NS3pro Inhibitors: a Molecular Target against the Dengue Virus

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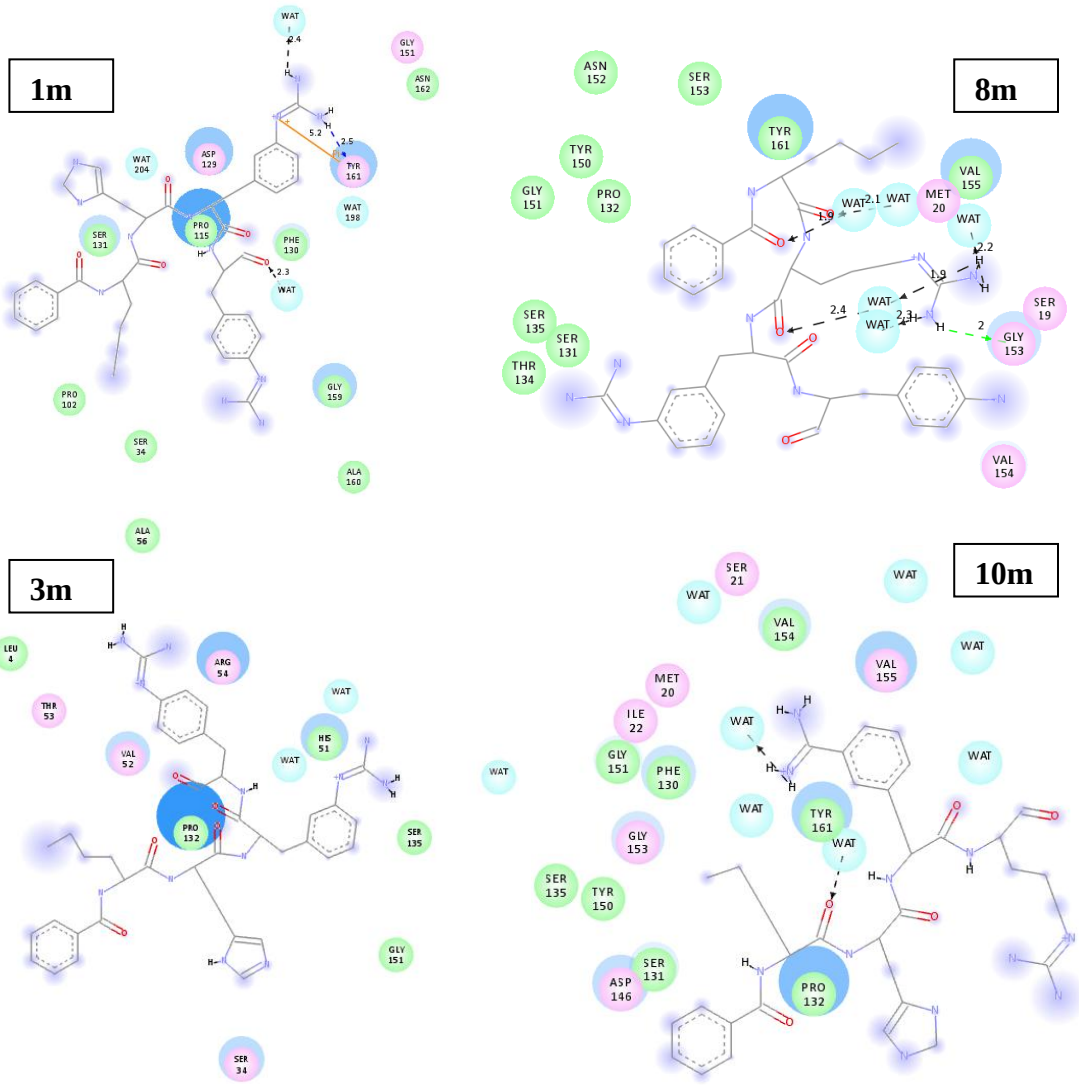

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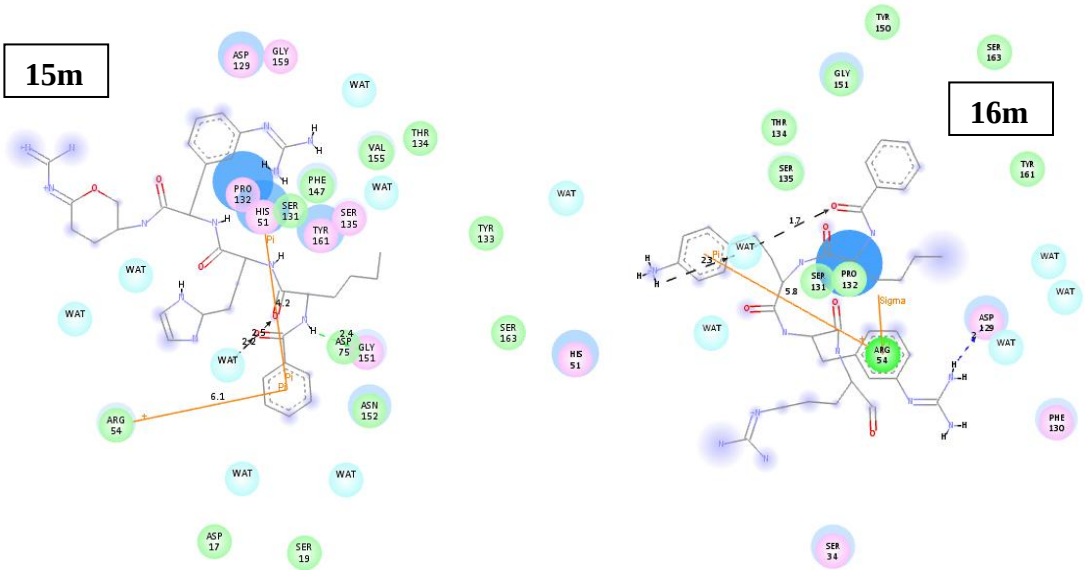

Figure S2. Interactions of compounds **1m**, **3m**, **8m**, **10m**, **15m** and **16m** in the activity site of complex NS2B-NS3pro of DENV-2, showing hydrogen bonds (pink circles with traced line), hydrophobic interactions (green circle), pi-interactions (orange lines), water molecules (blue circles) and close contact residues (pink circles only). The regions of solvent assess are showed for purples circles (in molecule) and for one blue halo (in amino acid residue). This figure was construed utilizing Discovery Studio Visualizer 3.1.[1]

Configuration

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Reference

1. Accelrys Software Solutions Pvt. Ltd.; *Discovery Studio Visualizer Version 3.1,* Accelrys Inc., San Diego, CA, USA, 2011.