

1 **In vitro Screening and MD simulations of thiourea derivatives against SARS-CoV-2 in**
2 **association with multidrug resistance ABCB1 transporter**

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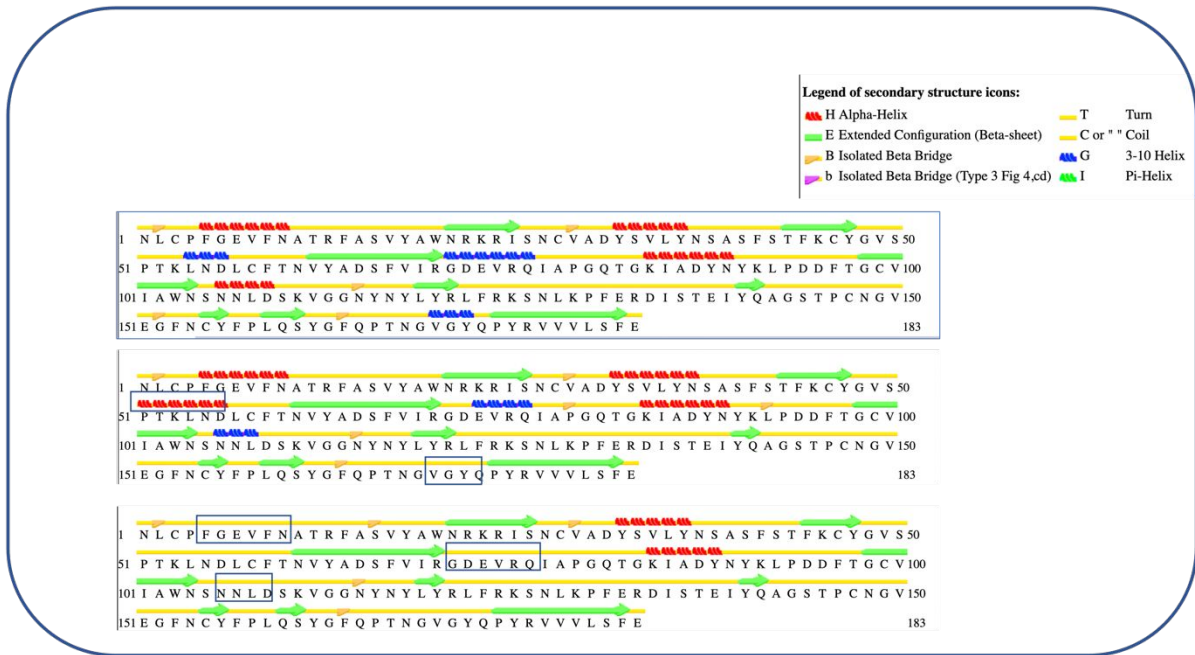
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18 Figure SI- 1. This figure compares the secondary structure changes in the crystal structure
 19 (upper panel), BB-IV-46 (middle panel) and BB-V-19 (lower panel). This analysis done
 20 through STRIDE (ref.¹. STRIDE: a Web server for secondary structure assignment from known
 21 atomic coordinates of proteins. Nucl. Acids Res. , 32, W500-2) shows that there are slight
 22 changes in the secondary structure of RBD as compared to the starting structure. These changes
 23 include the conversion of residues 5-10 from alpha-helix in BB-IV-46 to turns and coils in BB-
 24 V-19, residues 23-26 in BB-IV-46 from 3-10 helix to turns and coils in BB-V-19 and residues
 25 106-108 in BB-IV-46 from 3-10 helix to turns and coils in BB-V-19 as a result of ligand
 26 binding.

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30 (1).Heinig, M.; Frishman, D. J. N. a. r., STRIDE: a web server for secondary structure
 31 assignment from known atomic coordinates of proteins. **2004**, 32 (suppl_2), W500-W502.

32