Alkaloids and Quinolones as potential MtbTopI inhibitors: An *in-silico* discovery using ADME studies and molecular dynamics simulation

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Supplementary Figures

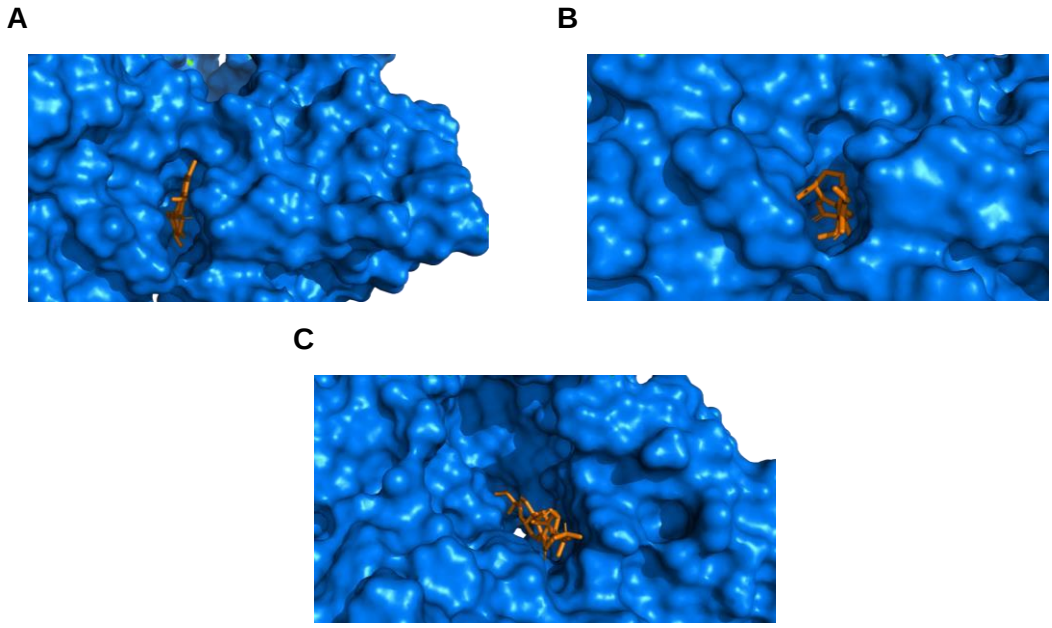

Fig. 1: Redocking results of the best poses of the 3 Alkaloids (orange) selected after drug-likeness prediction A) PubChem CID 10220, B) PubChem CID 23757, C) PubChem CID 23635499

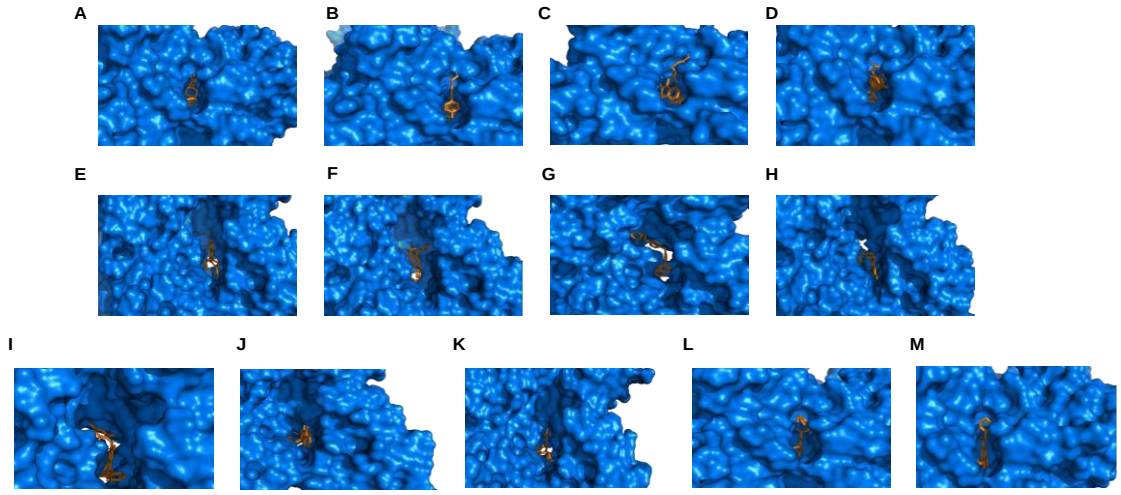

Fig. 2: Redocking results of the best poses of the 13 Quinolones (orange) selected after drug-likeness prediction A) PubChem CID 163839, B) PubChem CID 483150, C) PubChem CID 10096946, D) PubChem CID 12899497, E) PubChem CID 18918418, F) PubChem CID 23646773, G) PubChem CID 54689660, H) PubChem CID 54722219, I) PubChem CID 69306516, J) PubChem CID 85881877, K) PubChem CID 131953858, L) PubChem CID 131953861, M) PubChem CID 131953879.

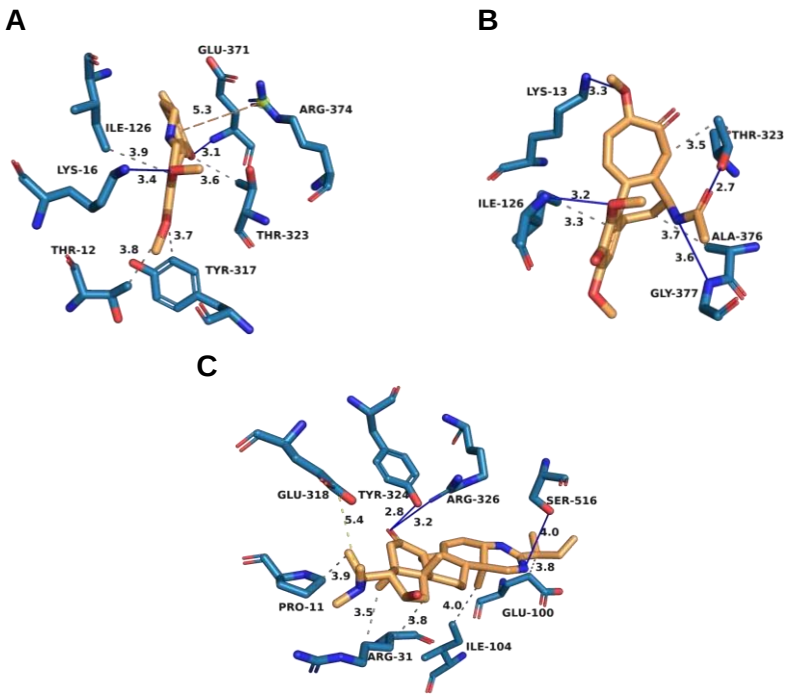

Fig. 3: Interaction analysis of 3 selected Alkaloids (orange) with the receptor (blue) A) PubChem CID 10220, B) PubChem CID 23757, C) PubChem CID 23635499**.**

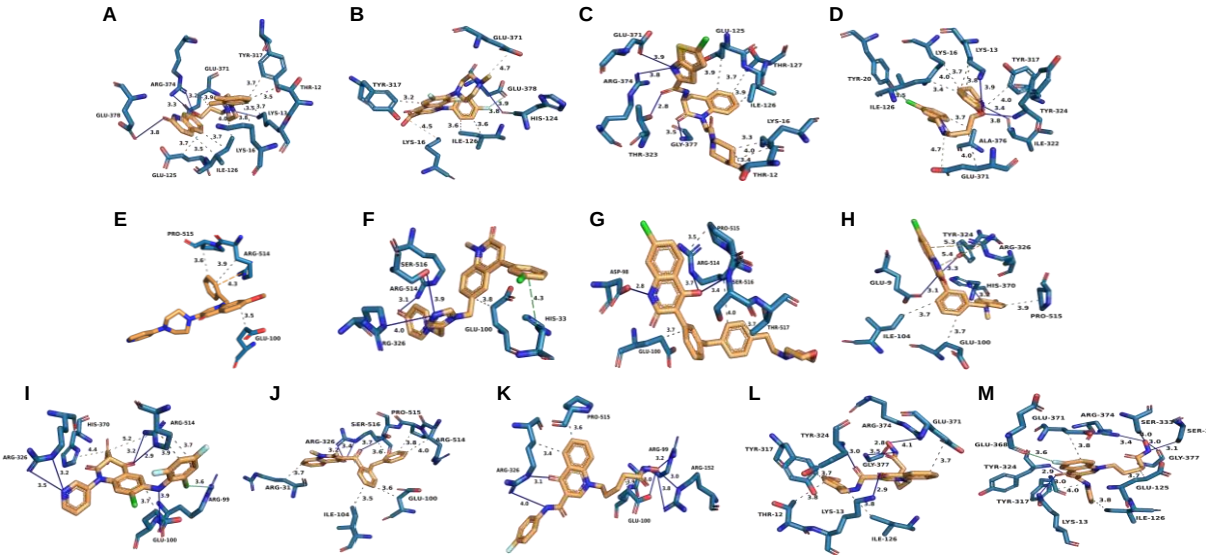

Fig. 4: Interaction analysis of 13 selected Quinolones (orange) with the receptor (blue) A) PubChem CID 163839, B) PubChem CID 483150, C) PubChem CID 10096946, D) PubChem CID 12899497, E) PubChem CID 18918418, F) PubChem CID 23646773, G) PubChem CID 54689660, H) PubChem CID 54722219, I) PubChem CID 69306516, J) PubChem CID 85881877, K) PubChem CID 131953858, L) PubChem CID 131953861, M) PubChem CID 131953879.