Structure Based Docking and Molecular Dynamic Studies of *Plasmodial* Cysteine Proteases against a South African Natural Compound and its Analogs

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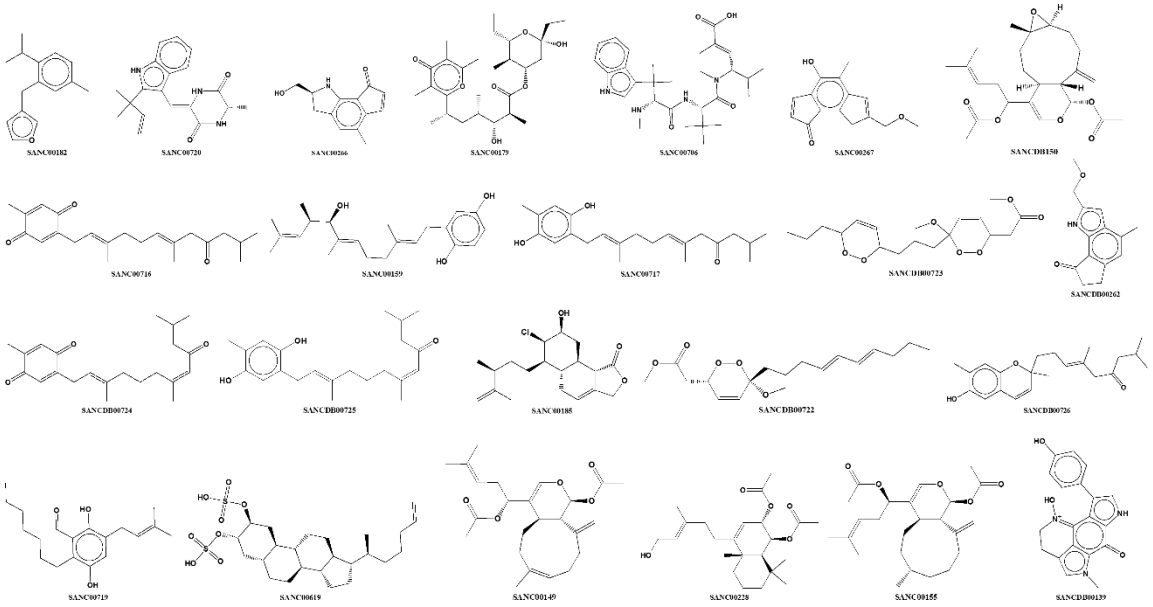
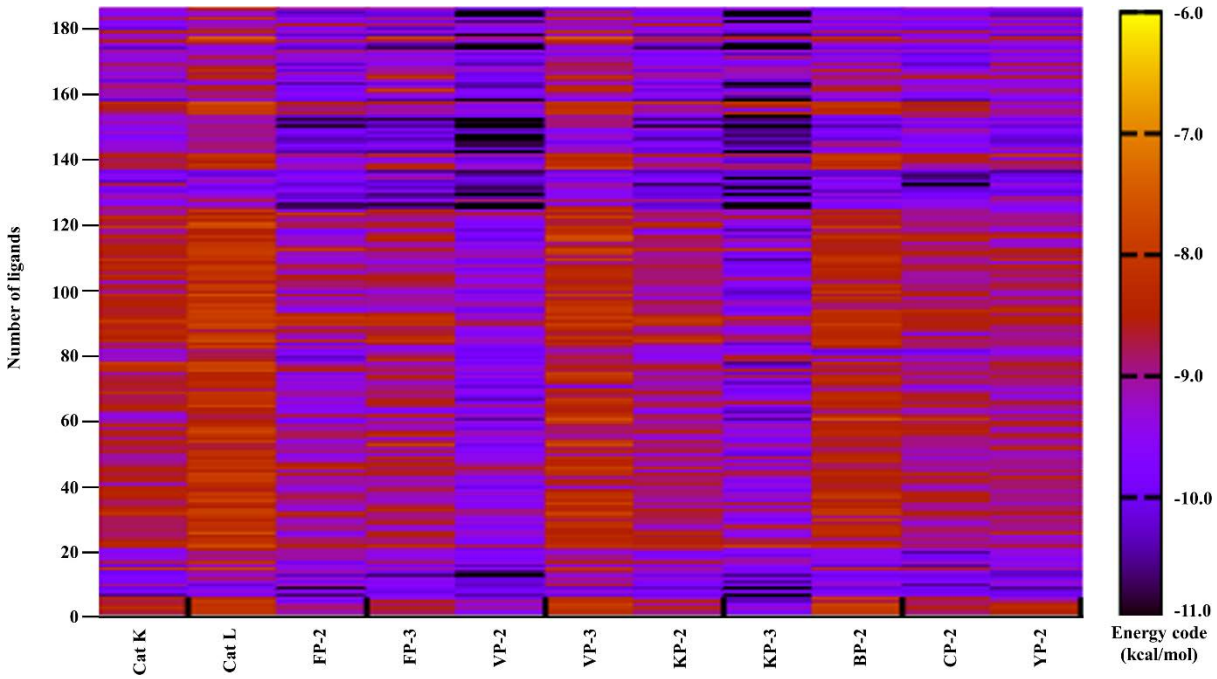
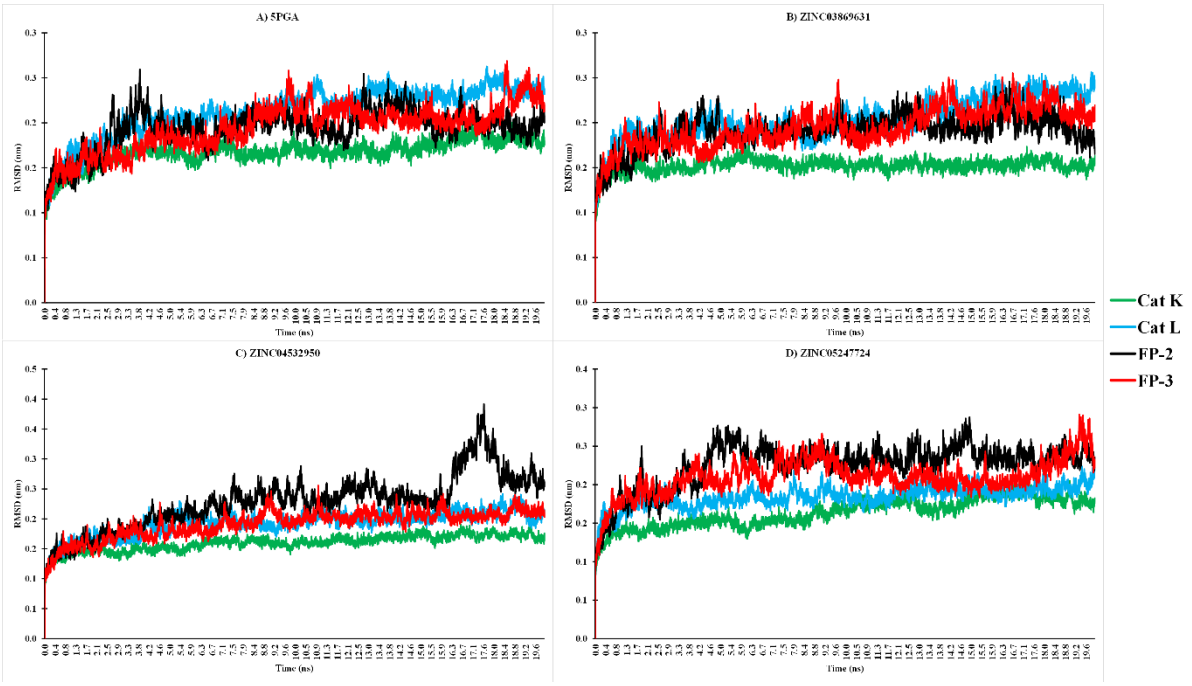


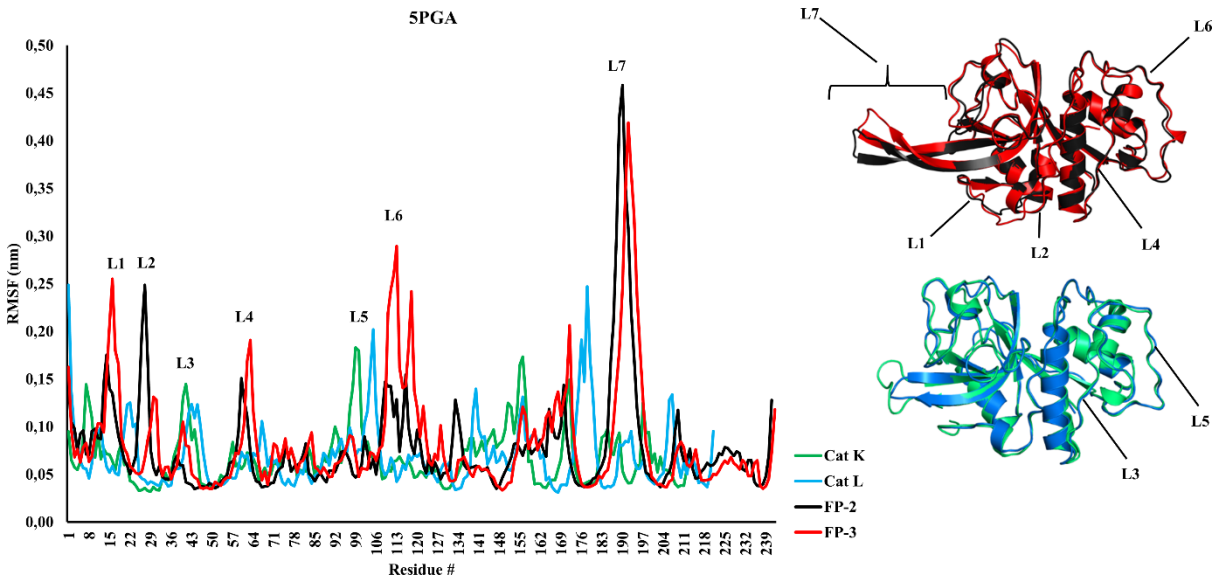
Supplementary Figure S1. 2D of South African non-peptidic compounds with SANCDB identity numbers used for initial docking studies.



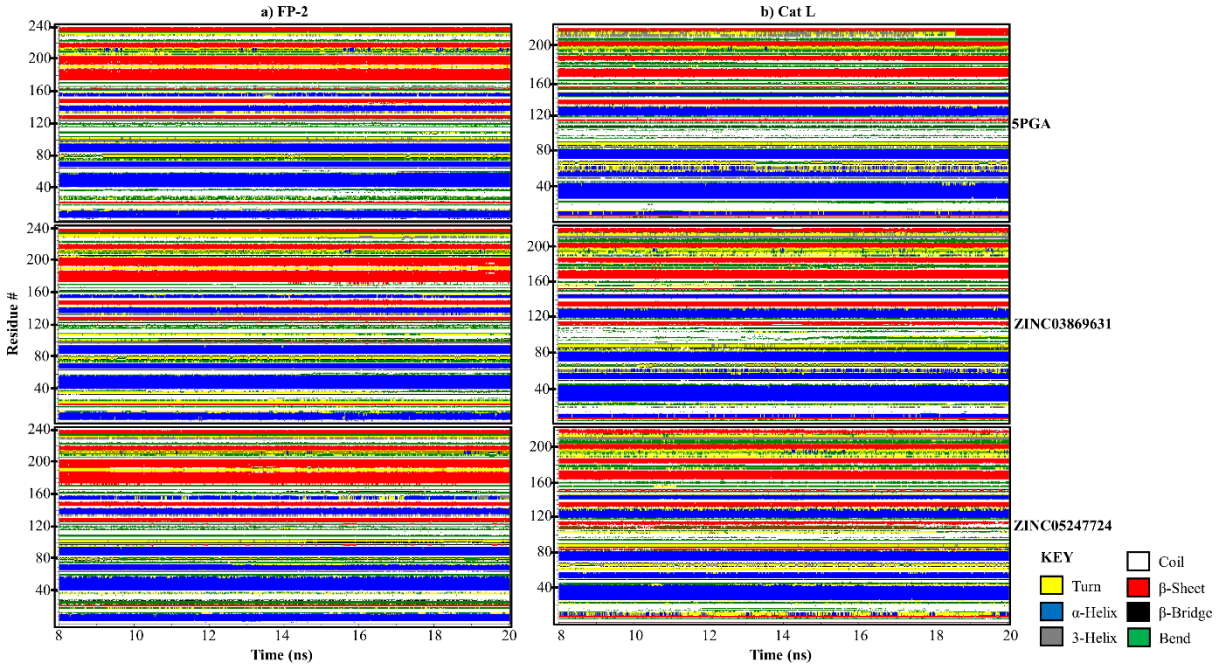
Supplementary Figure S2. Docking results on all proteases using AutoDock4.2 for all 186 ZINC hits obtained via 3D structure similarity search using 5PGA as the query template.



Supplementary Figure S3: RMSD plots of FP-2, FP-3 and Cat L in complex with **a)** 5PGA, **b)** ZINC03869631, **c)** ZINC04532950, and **d)** ZINC05247724.



Supplementary Figure S4: RMSF plot of FP-2, FP-3 and Cat L in complex with 5PGA. The cartoon representation shows the different loop regions (LX) that exhibit highest fluctuations.



Supplementary Figure S5. Conformational evolution of secondary structure elements of a) FP-2 and b) Cat L in complex with 5PGA, ZINC03869631 and ZINC05247724 during the last 12 ns of MD simulation as determined by do_dssp of GROMACS 4.6.5.