Supplementary Information for: Molecular Simulation-Driven Fragment Screening for the Discovery of New CXCL12 Inhibitors

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SI1: Fragments used for the screening

File: *fragments.mol*

SI2: Results of the screening

File: *fragments.xlsx*

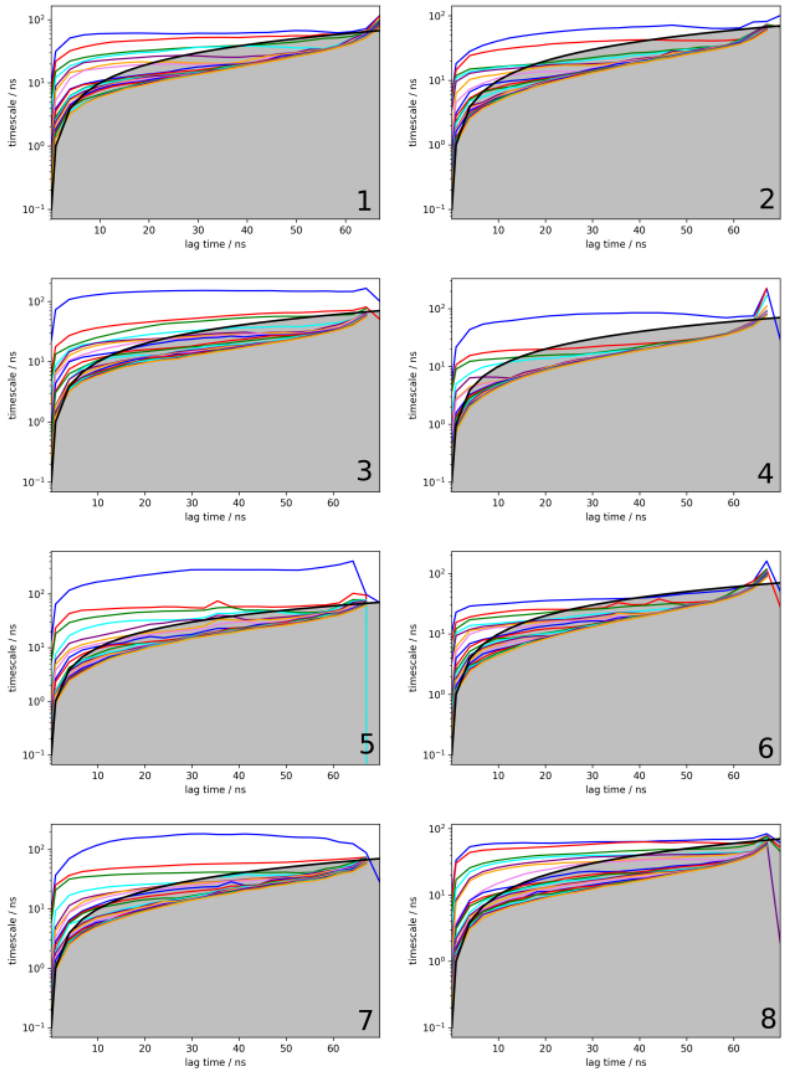

Figure S1: Implied timescales plot for the selected fragments with high ligand efficiency. Numeration corresponds with the main paper.

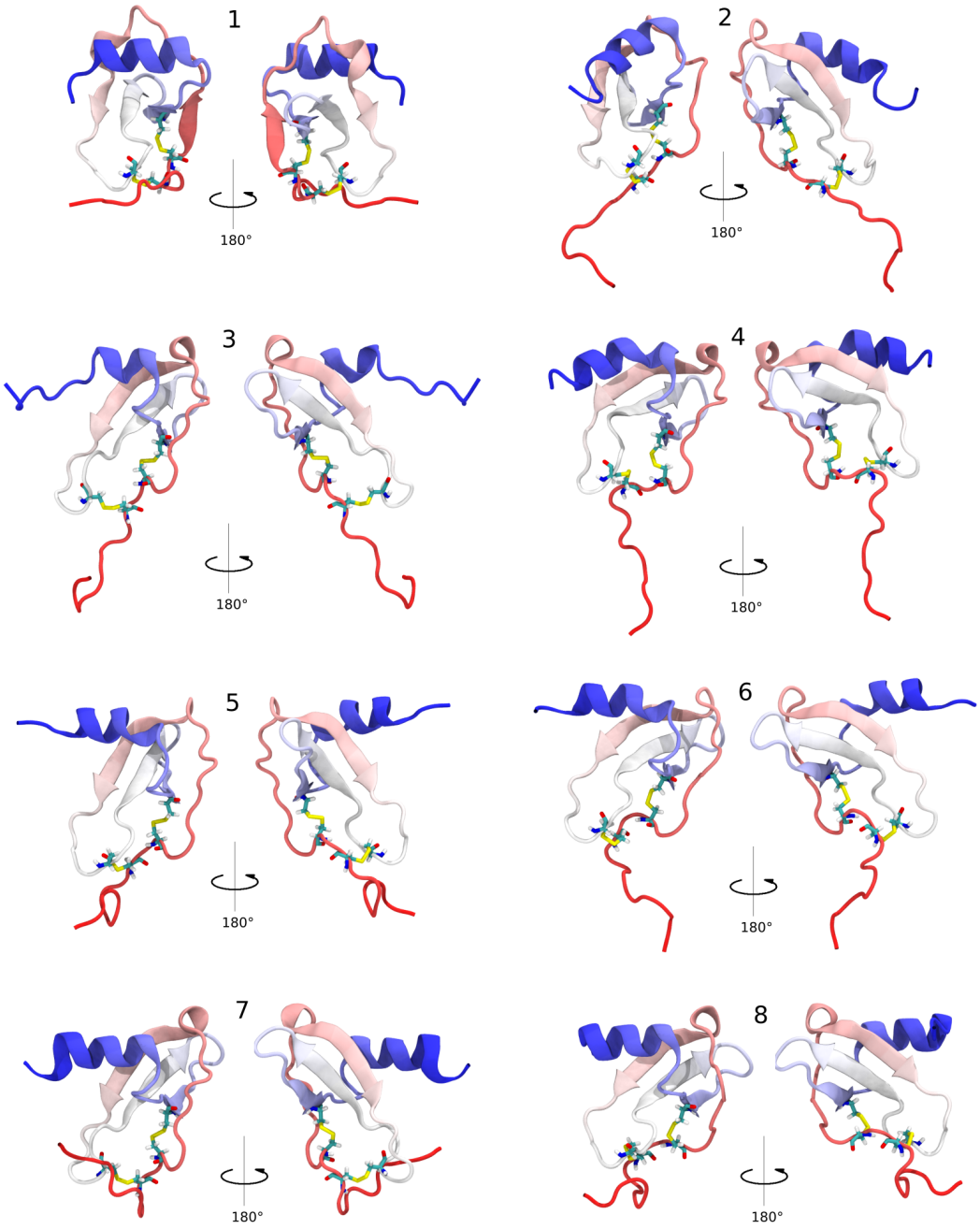

Figure S2: Protein conformations used for docking. One representative was extracted from each macrostate of a MSM built on backbone dihedrals data.

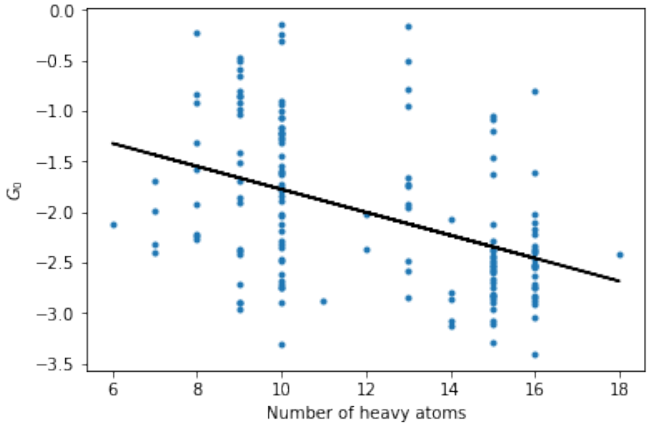

Figure S3: Correlation between fragment binding free energy and number of heavy atoms.