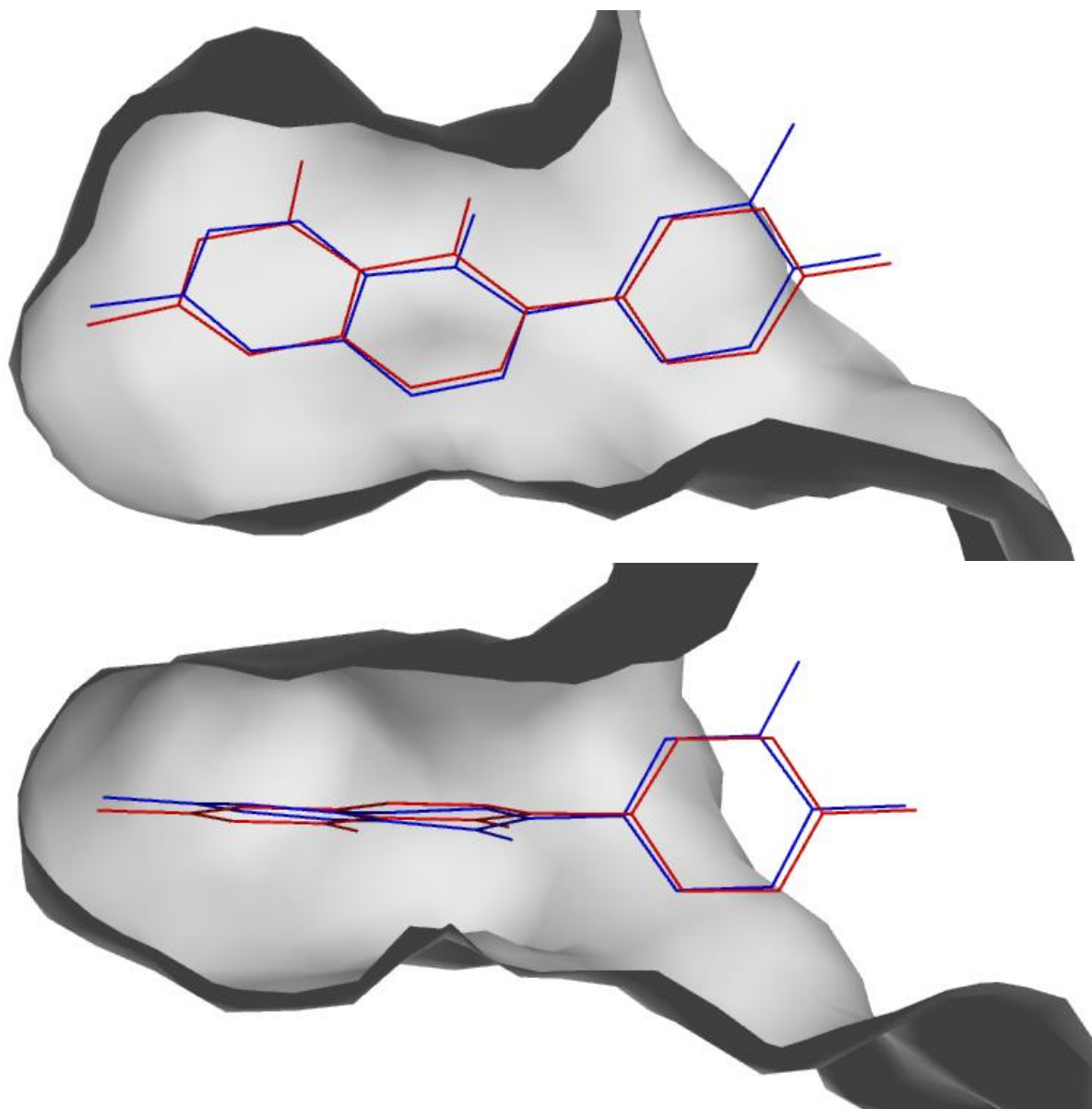


Supporting Information S7



Binding pocket of 47X (blue) on Macrophage migration inhibitory factor (MIF; PDB 3L5R) overlaid with docked Genistein (PDB Hetcode GEN, red). Clearly visible is the high chemical similarity between GEN and 47X. GEN has slightly higher predicted bioavailability in *C. elegans* compared to 47X (GEN: Burns score = 8.75, Bioavailability score = 0.91; 47X: Burns score = 6.47, Bioavailability score = 0.8). However, this is contrasted by the more than 100-fold lower predicted binding affinity (GEN: RF-Score = 4.13, Binding score = 0.3; 47X: RF-Score = 6.67; Binding score = 0.842).