

Supporting Information

Chalcone derivatives binding with human serum albumin and cyclooxygenase-2

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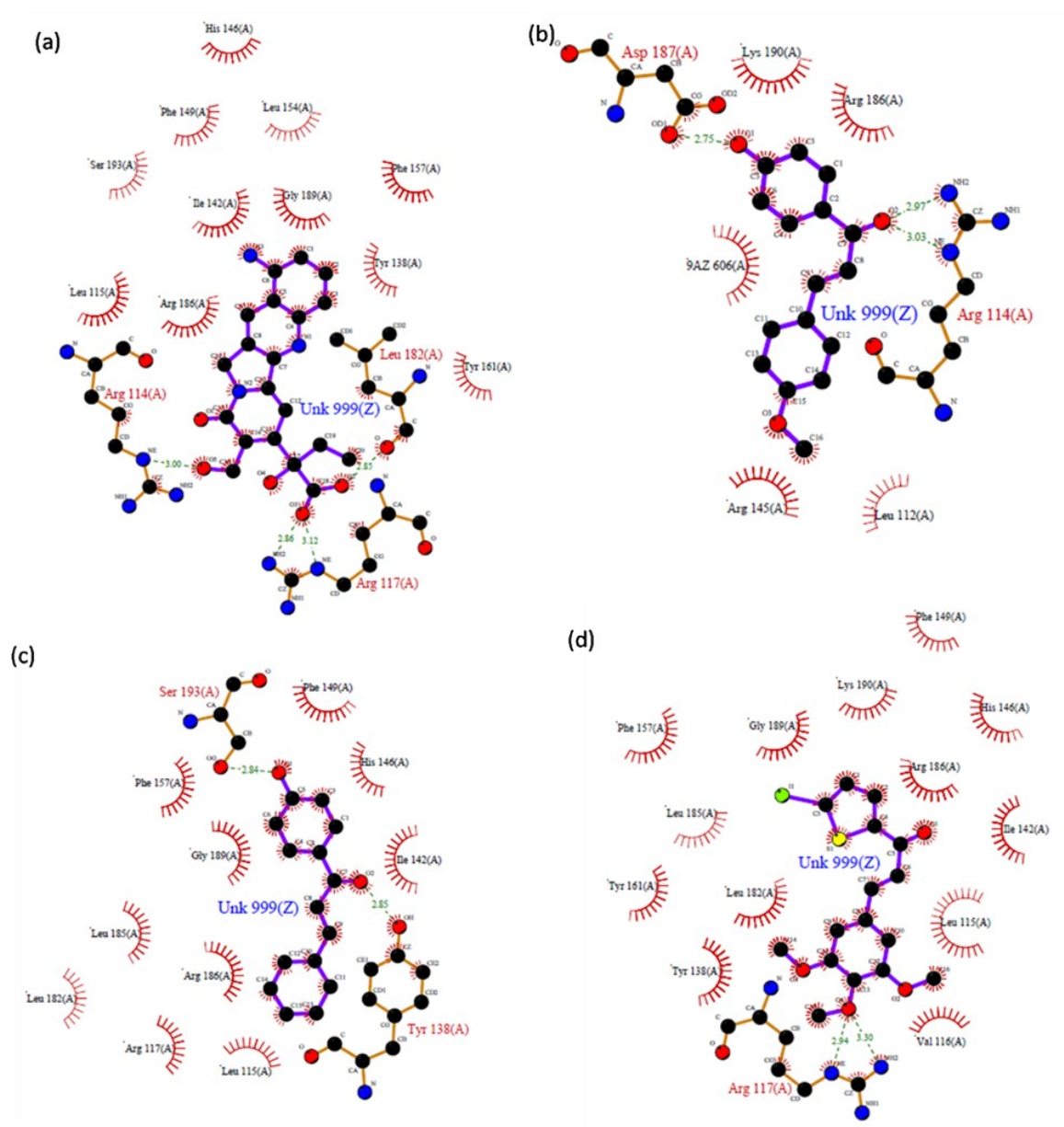


Figure.S1 shows the 2D ligand plot in HSA binding site (a) co-crystal site (b) compound A (c) compound B (d) compound C.

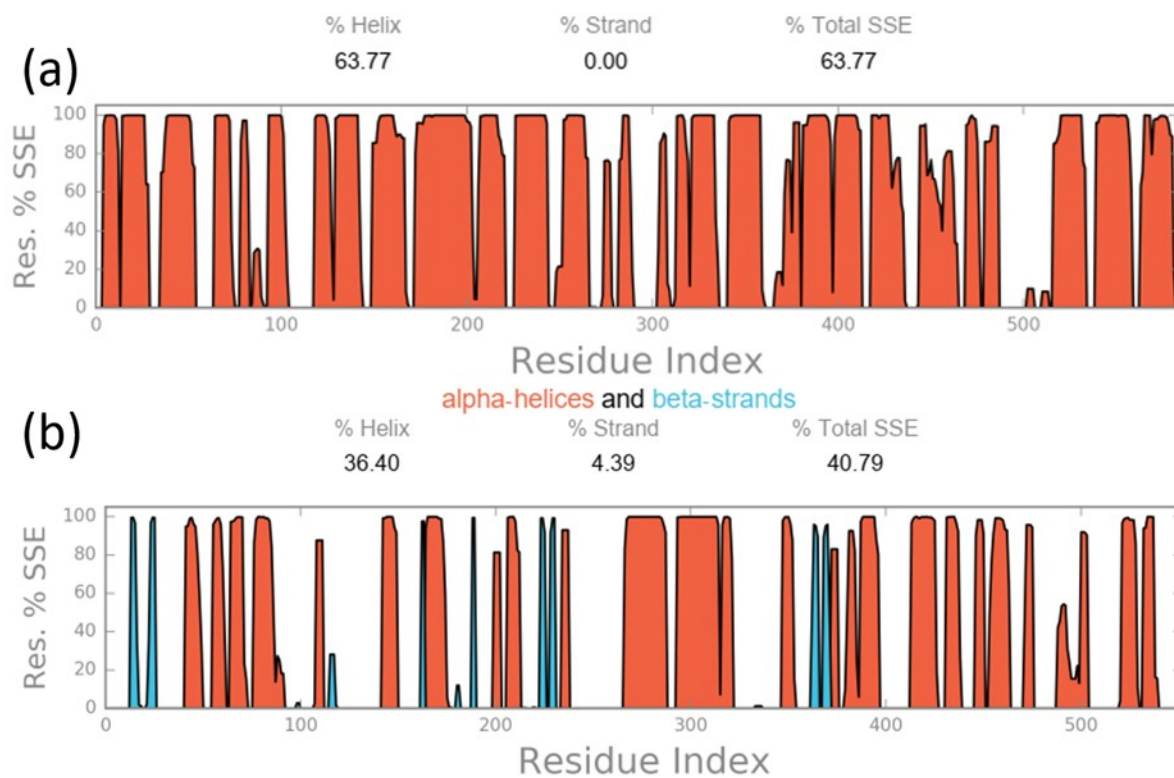


Figure.S3 Protein secondary structure elements analysis plot of compound C in (a) HSA (b) COX-2 complex system.

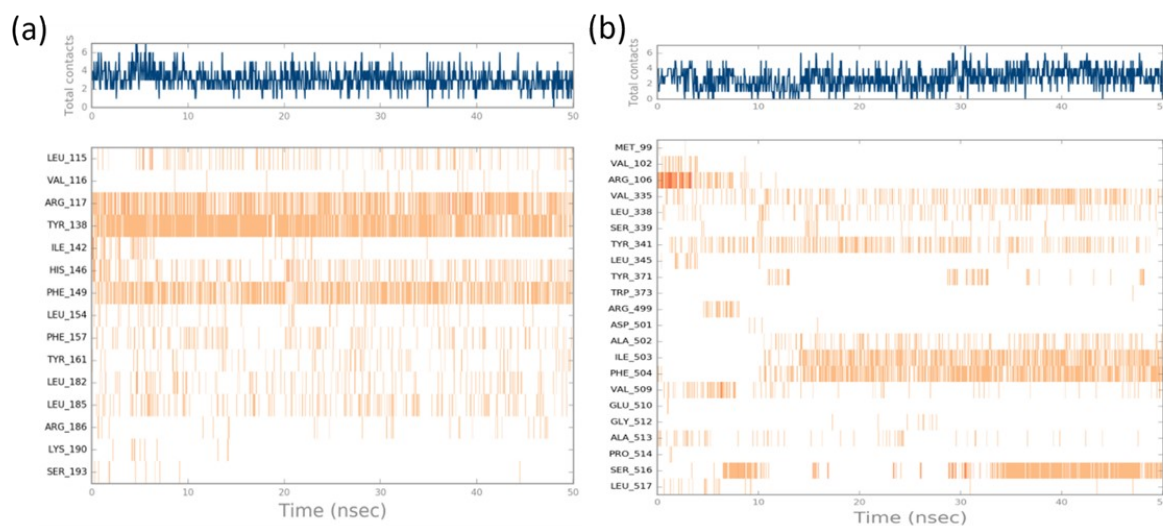


Figure.S4 Total contacts of compound C in (a) HSA (b) COX-2 complex system.

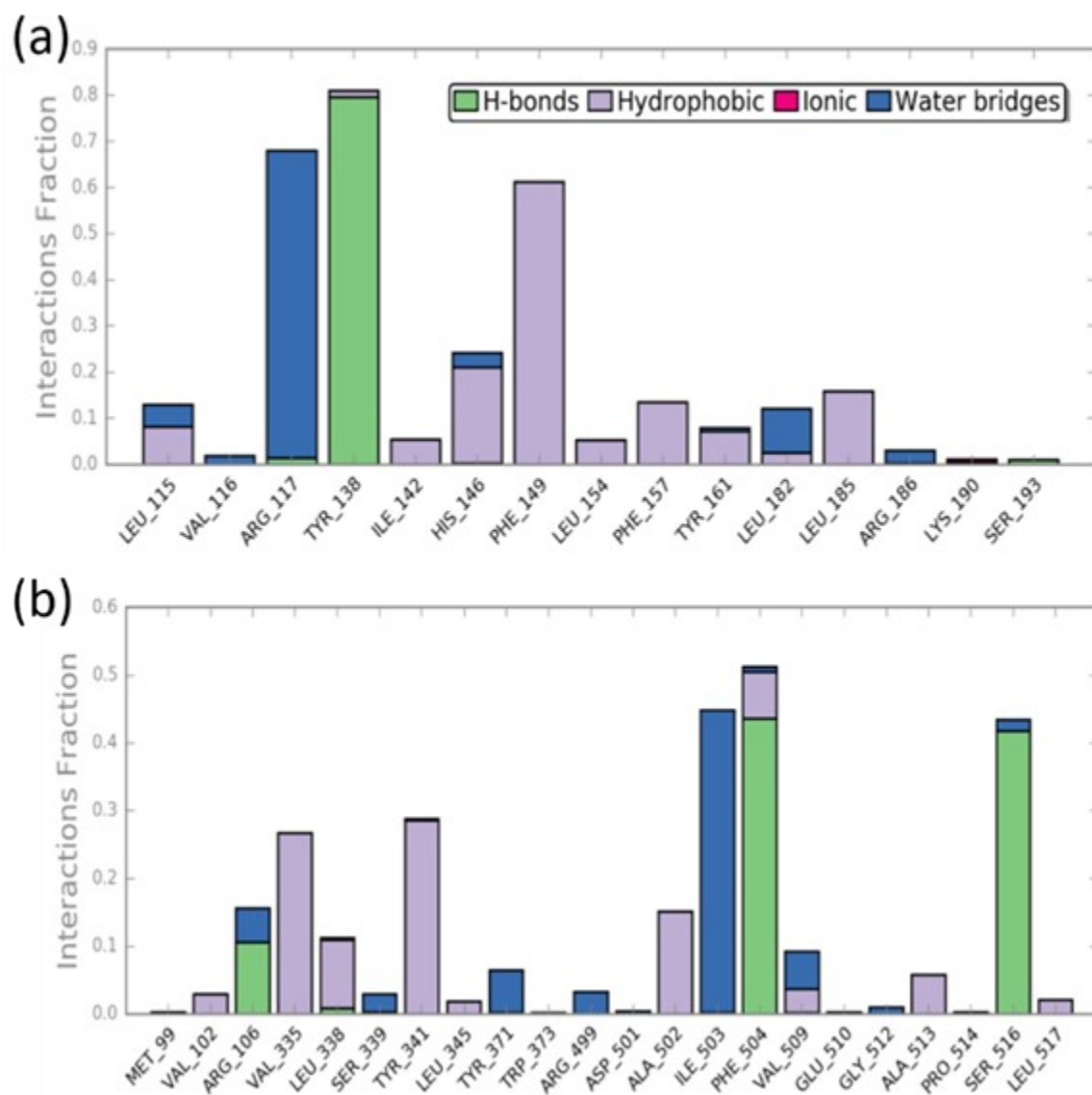


Figure.S5 Protein-ligand interaction fraction plot of compound C in (a) HSA (b) COX-2 complex system.

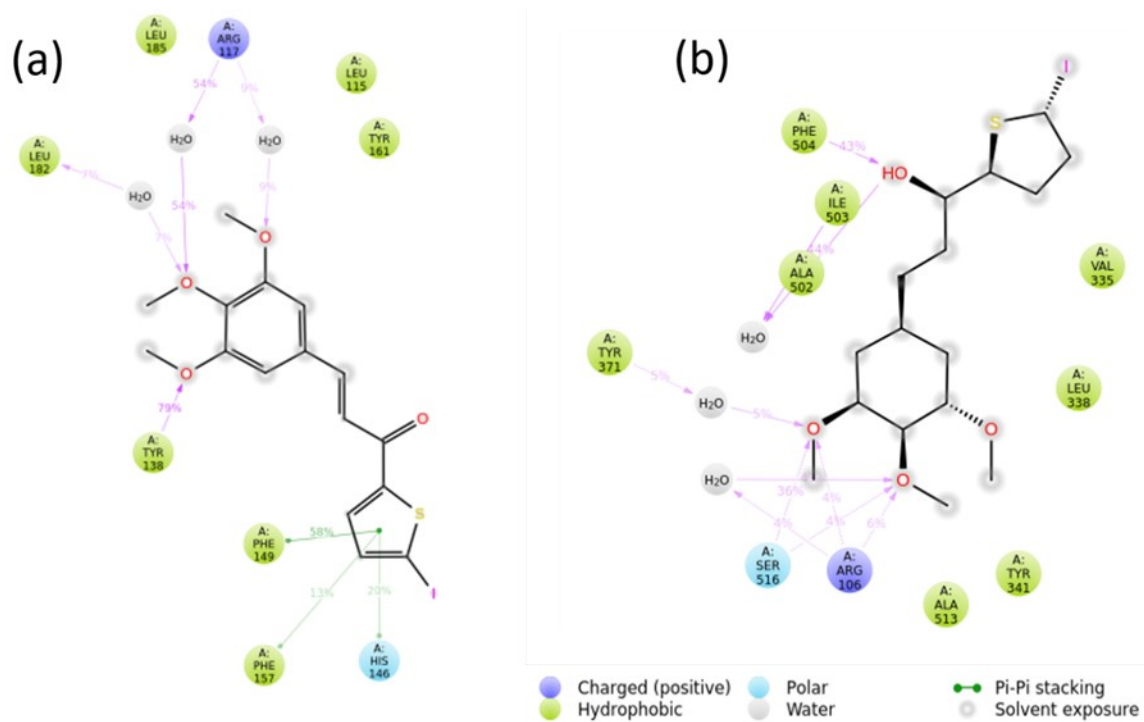


Figure.S6 shows MD ligand plot of compound C in (a) HSA (b) COX-2 complex system.

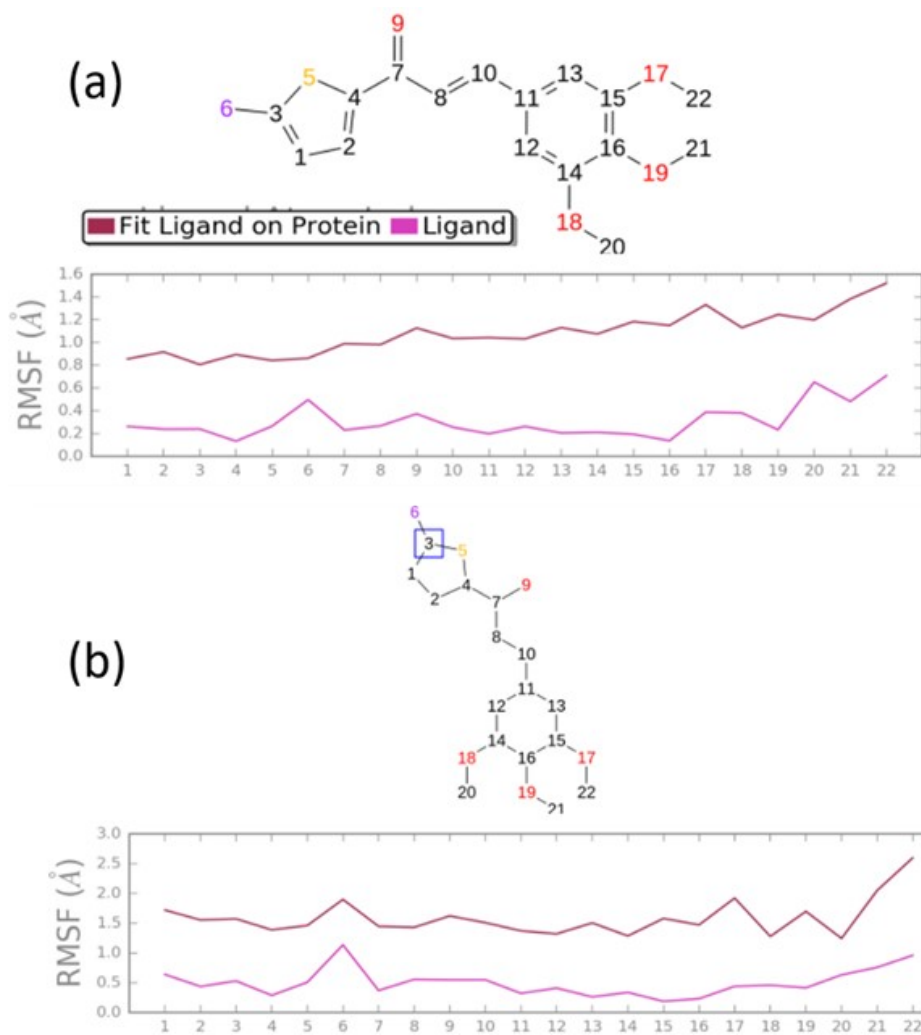


Figure.S7 shows Ligand RMSF plot of compound C in (a) HSA (b) COX-2 complex system.

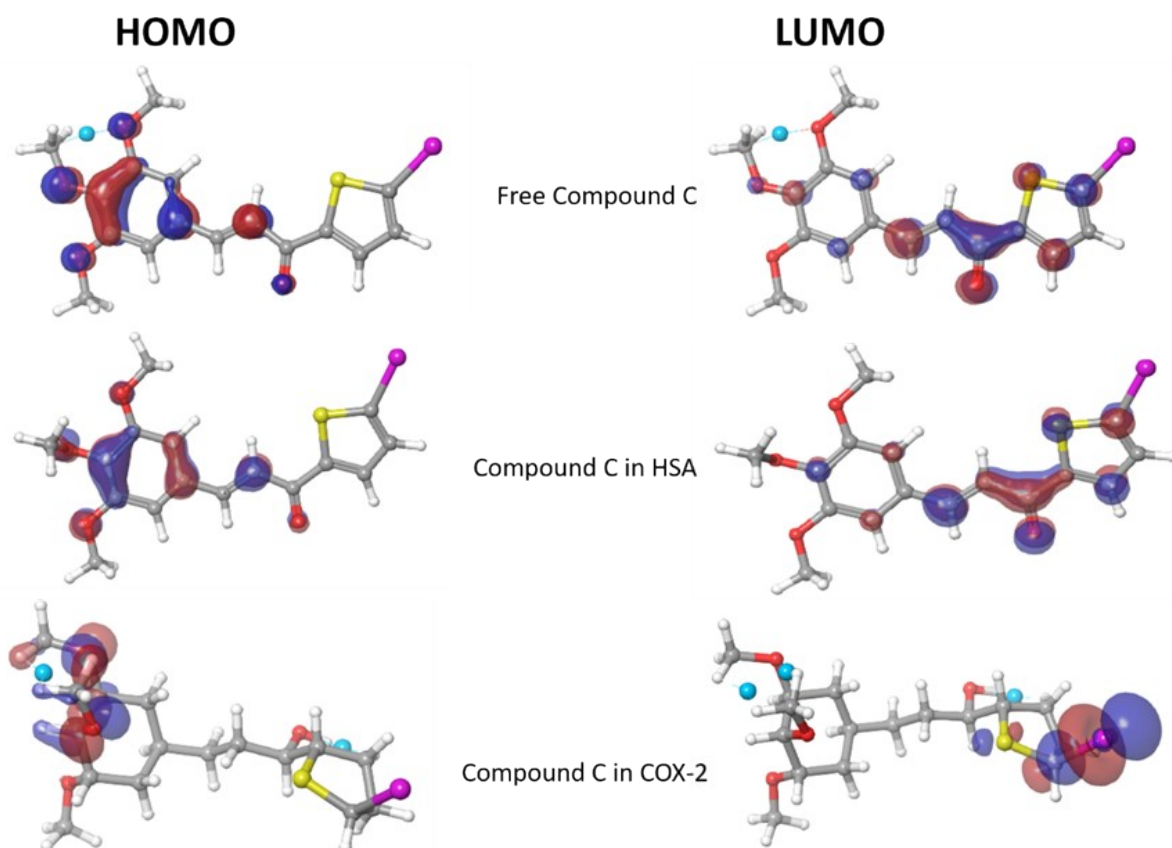


Figure.S8 HOMO-LUMO plot of free compound C and compound C in HSA and COX-2 binding environment.

Table S1. HOMO-LUMO parameters of free compound C and compound C in HSA and COX-2 binding environment.

DFT Globalised Parameter	Compound C	Compound C in HSA	Compound C in COX-2
HOMO (Hartree)	-0.192037	-0.211642	-0.214717
LUMO (Hartree)	-0.073375	-0.078166	-0.037280
ALIE (kcal/mol)	200.77	196.918	182.579
ESP	-32.63	-32.29	-33.42
Interaction Strength (e^-/a_0^{**3})	-0.05	-0.05	-0.05