

Supplementary Materials:

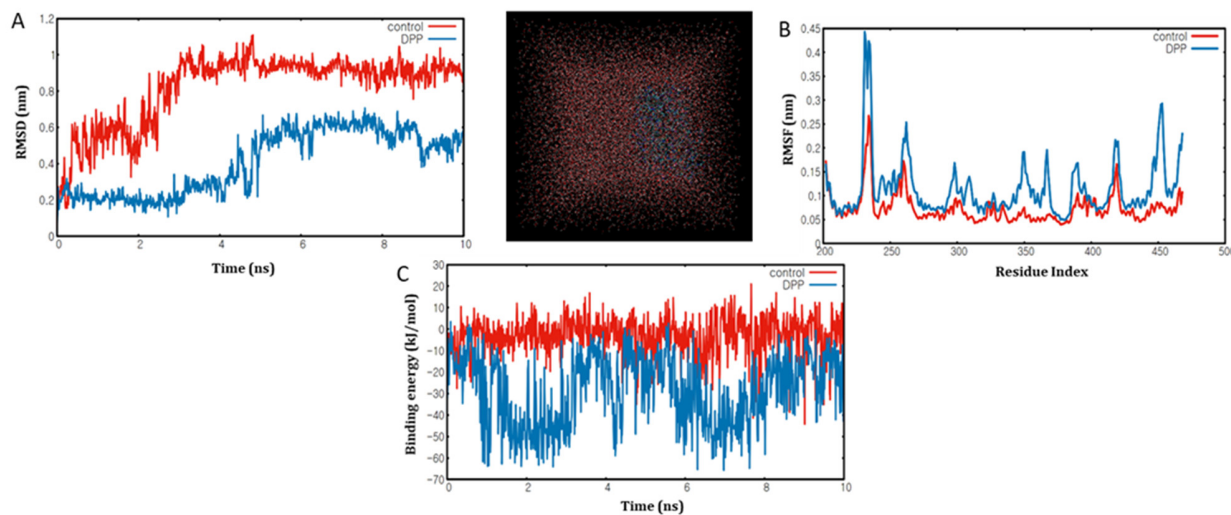


Figure S1. MD simulation analyses (A) Root mean square deviation (RMSD) plot of PPAR γ Rosiglitazone (Red) and 1,3 diphenyl 2 propanone (Blue) complex at 10 ns of molecular dynamic simulation. (B) The RMSF plot of the backbone heavy atoms of the Rosiglitazone (Red) and 1,3 diphenyl 2 propanone (Blue) complex. (C) Binding energy plot of Rosiglitazone (Red) and 1,3 diphenyl 2 propanone (Blue) complex at 10 ns.

Table S1. Hydrogen bond donor and acceptor residues from the molecular dynamic simulation (PPAR γ)

Donor	Hydrogen	Acceptor
ARG288NE	ARG288HE	EQPX478O1
ARG288NH2	ARG288HH21	EQPX478O1
SER289OG	SER289HG1	EQPX478O1