Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary materials

Exploration of stilbenoid trimers as a potential inhibitor of Sirtuin1 enzyme using molecular docking and molecular dynamics simulation approach

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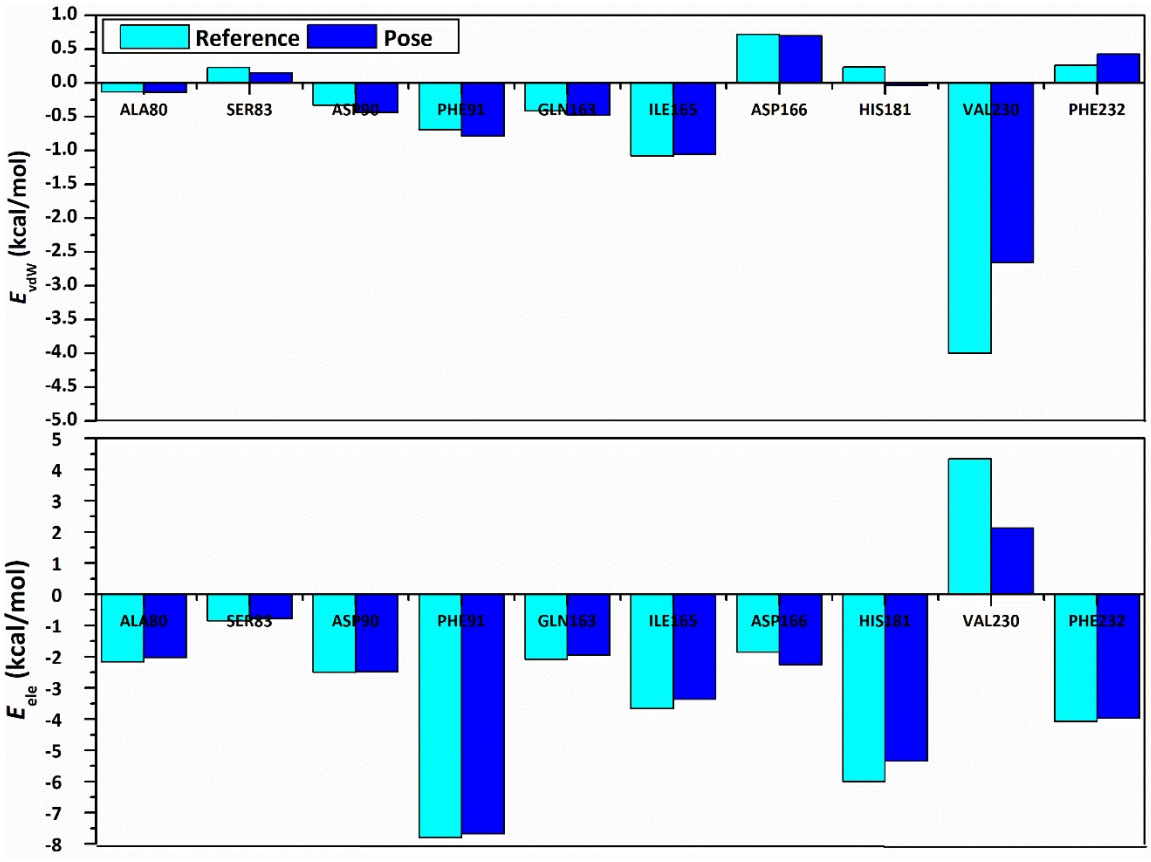

Fig. S1 The footprint similarity: The van der Waals (top) and electrostatic (bottom) energy contribution from each residue on the active site of the SIRT1 enzyme.

Table S1 ADMET prediction of stilbenoid trimers using the pkCSM server

Parameter	TS1	TS2	TS3
Absorption			
Caco-2 Permeability (log Papp in 10^{-6} cm/s)	-0.01	-1.44	-1.15
Intestinal Absorption-Human (% Absorbed)	100	100	92.82
Skin Permeability (Log Kp)	-2.73	-2.73	-2.73
Distribution			
BBB Permeability (log BB)	-1.10	-1.31	-1.74
Metabolism			
CYP1A2 Inhibitor	No	No	No
CYP2C19 Inhibitor	No	No	No
CYP2C9 Inhibitor	No	No	No
CYP2D6 Inhibitor	No	No	No
CYP3A4 Inhibitor	No	No	No
Excretion			
Renal OCT2 Substrate	No	No	No
Toxicity			
AMES Toxicity	No	No	No
Hepatotoxicity	No	No	No
Skin Sensitisation	No	No	No

Hight-Caco-2 Permeability: log Papp > 0.90 and Poor-Caco-2 Permeability: log Papp < 0.90.
Intestinal Absorption-Human (+): HIA > 30% and Intestinal Absorption-Human (-): HIA < 30%.
Hight-Skin Permeability: log Kp > -2.5 and Poor-Skin Permeability: log Kp < -2.5.
BBB Permeability (+): log BB > 0.3 and BBB Permeability (-): log BB < -1.0.

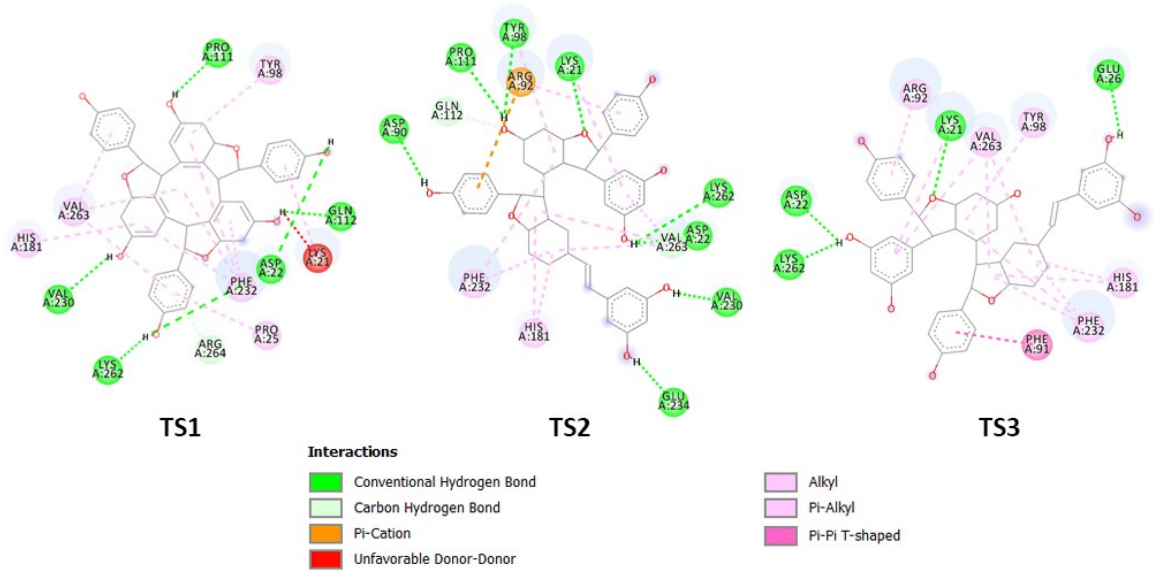

Fig. S2 Interaction types of each complex on active site using flexible conformation

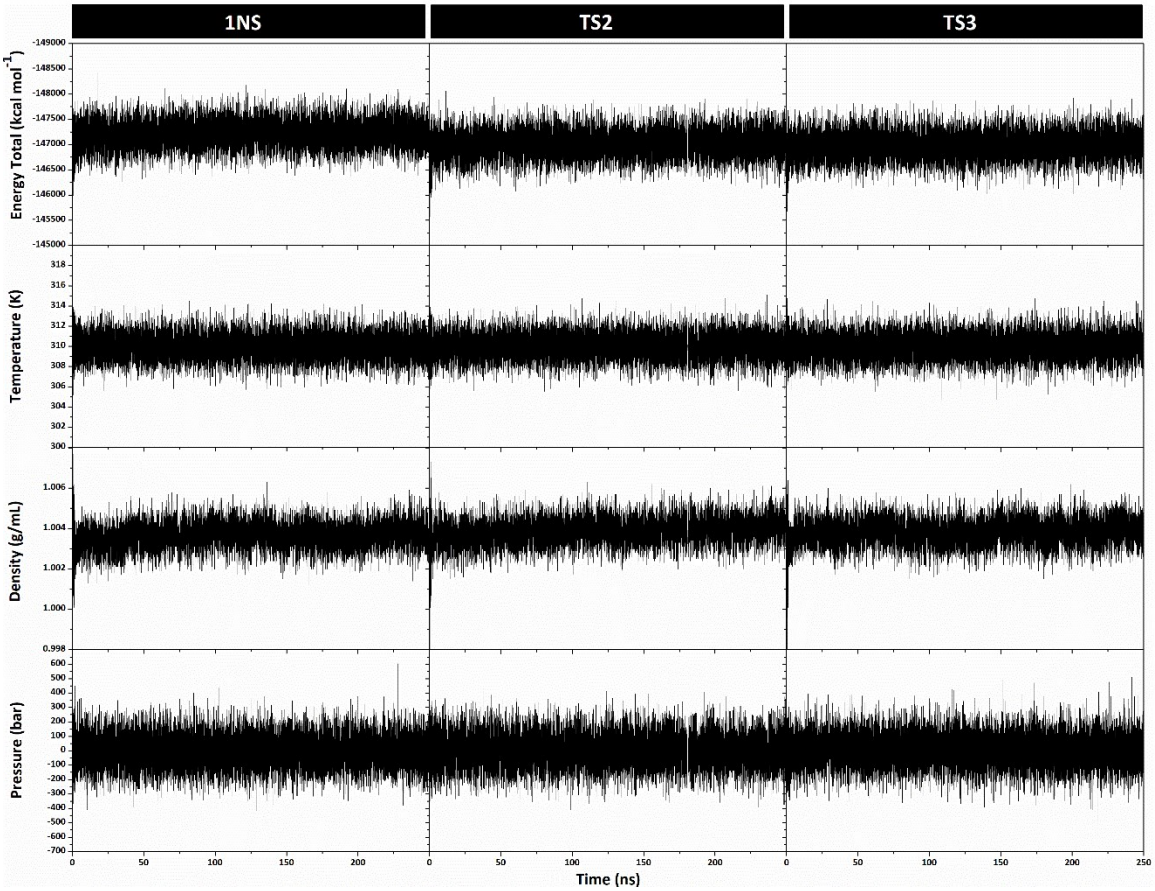

Fig. S3 The *mdout* analysis plotted along 250 ns of MD simulation.

Table S2 The average values of trajectory analysis during the simulation time (200-250 ns)

Parameters	1NS-SIRT1	TS2-SIRT1	TS3-SIRT1	APO Protein
RMSF (nm)	0.61 ± 0.21	0.52 ± 0.18	0.62 ± 0.22	0.62 ± 0.21
B-factor (nm^2)	11.16 ± 7.21	7.98 ± 5.21	11.44 ± 7.99	11.12 ± 7.20
Atom contacts	10.00 ± 2.00	6.00 ± 1.00	6.00 ± 2.00	-
RoG (nm)	2.09 ± 0.01	2.11 ± 0.01	2.11 ± 0.01	2.10 ± 0.00
SASA (nm^2)	10.35 ± 0.98	15.61 ± 1.10	11.94 ± 1.36	9.76 ± 0.93

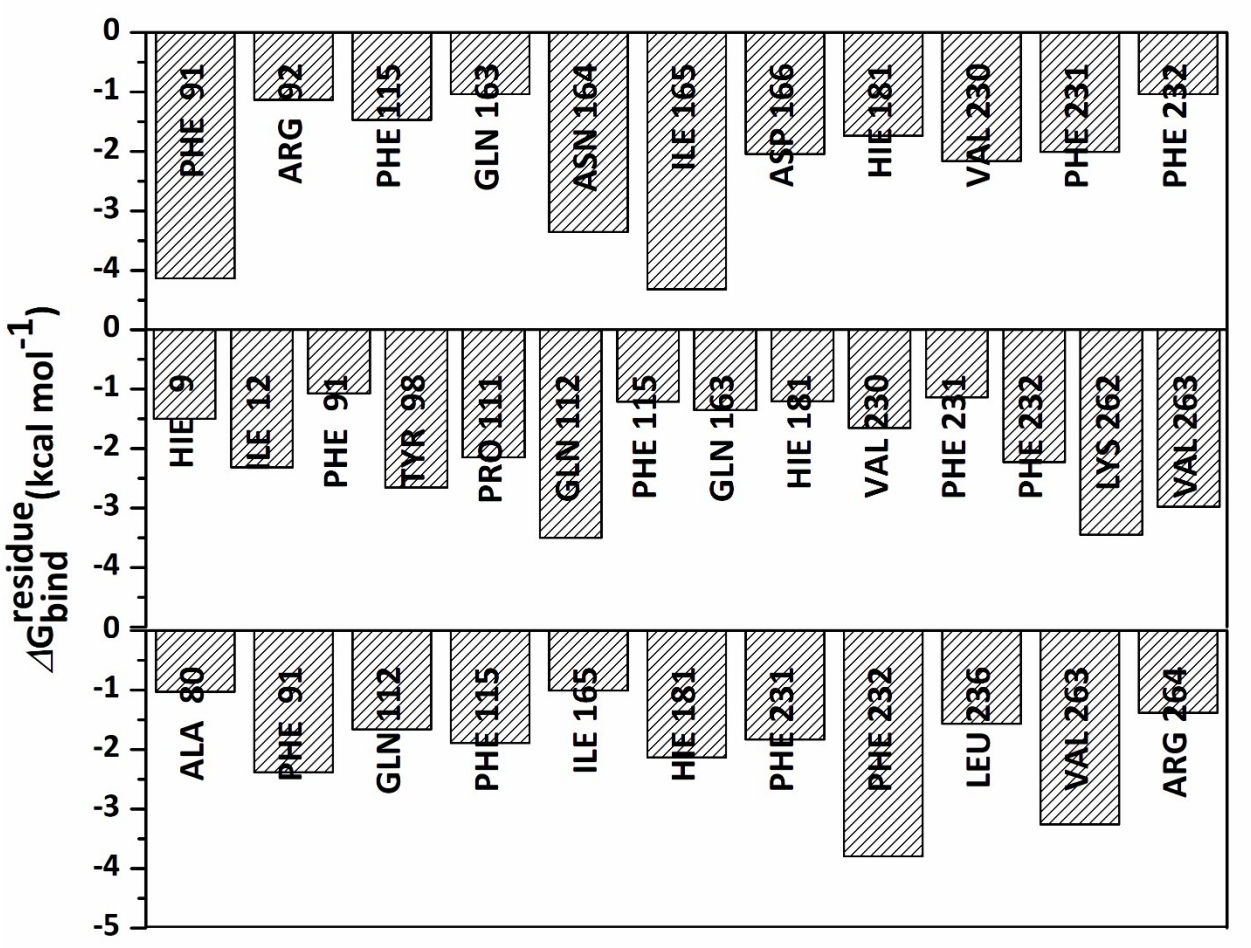

Fig. S4 Per-residue decomposition free energy plotted along the 50 ns of MD simulation using MM-GBSA method: 1NS-SIRT1 (top), TS2-SIRT1 (middle), and TS3-SIRT1 (bottom).

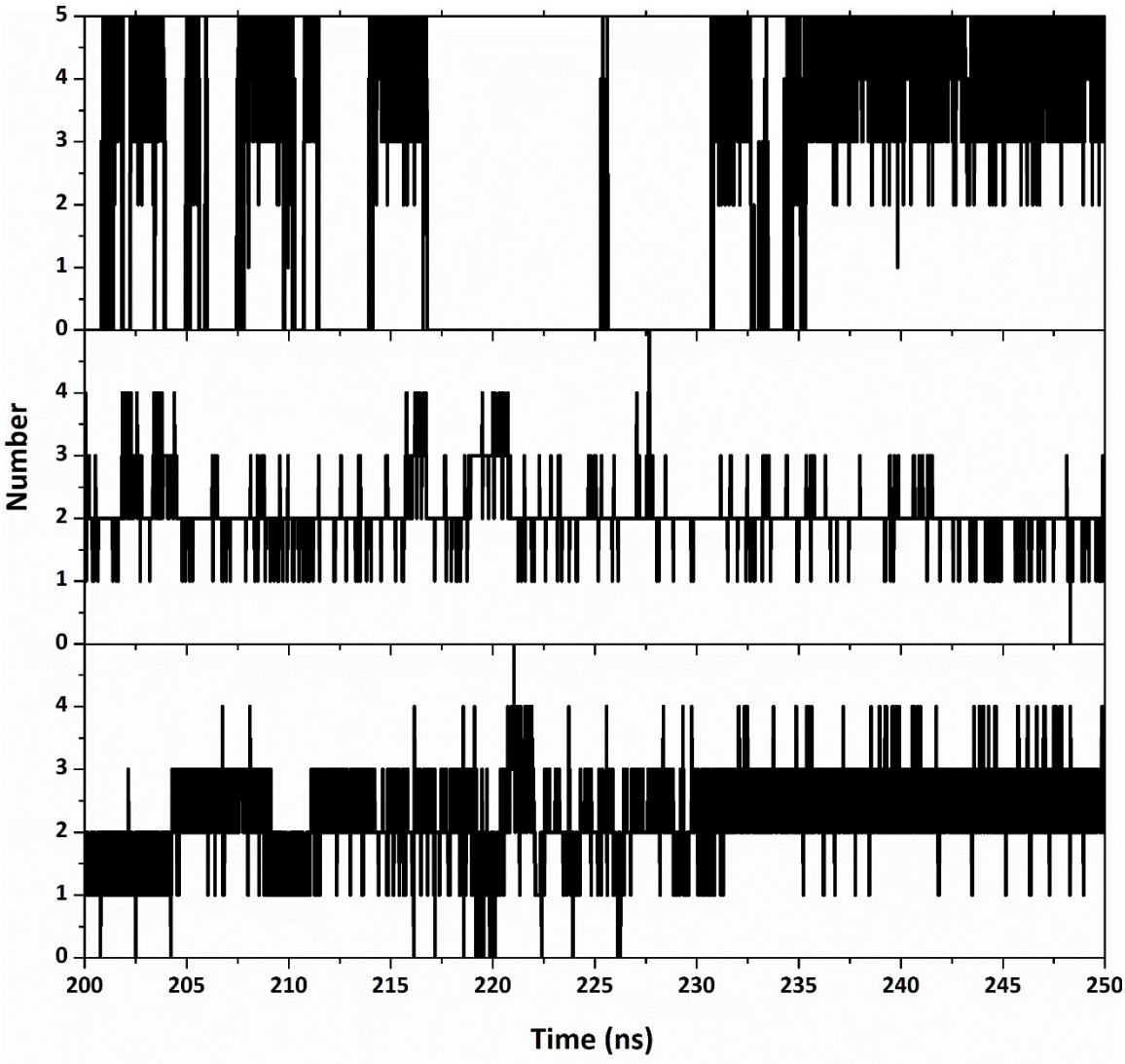

Fig. S5 The number of hydrogen bonds plotted along the 50 ns of MD simulation: 1NS-SIRT1 (top), TS2-SIRT1 (middle), and TS3-SIRT1 (bottom).