Supplementary material

Inverse Molecular Docking as a Novel Approach to Study Anticarcinogenic and Anti-Neuroinflammatory Effects of Curcumin

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Table S1. Details for FR-β-curcumin interactions identified by PLIP.

Hydrogen bonds			
Residue	Distance D-H--A (Å)	Angle (°)	H-bond donor?
APS 97	0.88	155.72	No
HIS 151	0.82	145.33	No
ARG 152	0.78	136.90	Yes
ARG 152	0.68	129.84	No
SER 190	0.95	169.07	Yes
π-Stacking interactions			
Residue	Distance (Å)	Angle (°)	Type
TYR 101	4.32	4.35	P
TRP 187	3.96	28.59	P
TRP 187	4.12	27.53	P

*D – donor, A – acceptor, P - parallel.

Table S2. Details for PDE4D-curcumin interactions identified by PLIP.

Hydrogen bonds			
Residue	Distance D-H--A (Å)	Angle (°)	H-bond donor?
HIS 366	0.91	162	No
ASN 375	0.63	120.95	Yes
MET 439	0.81	140.25	Yes
ASN 602	0.73	131.99	Yes
Hydrophobic interactions			
Residue	Distance (Å)	Angle (°)	Type
MET 439	3.61	NA	NA

*D – donor, A – acceptor, NA – not applicable .