

Figure (S1-S2): 2D interaction images of **S1)** Flavumone A with DNAA target protein
S2) Daphnodorin A with DNAA target protein

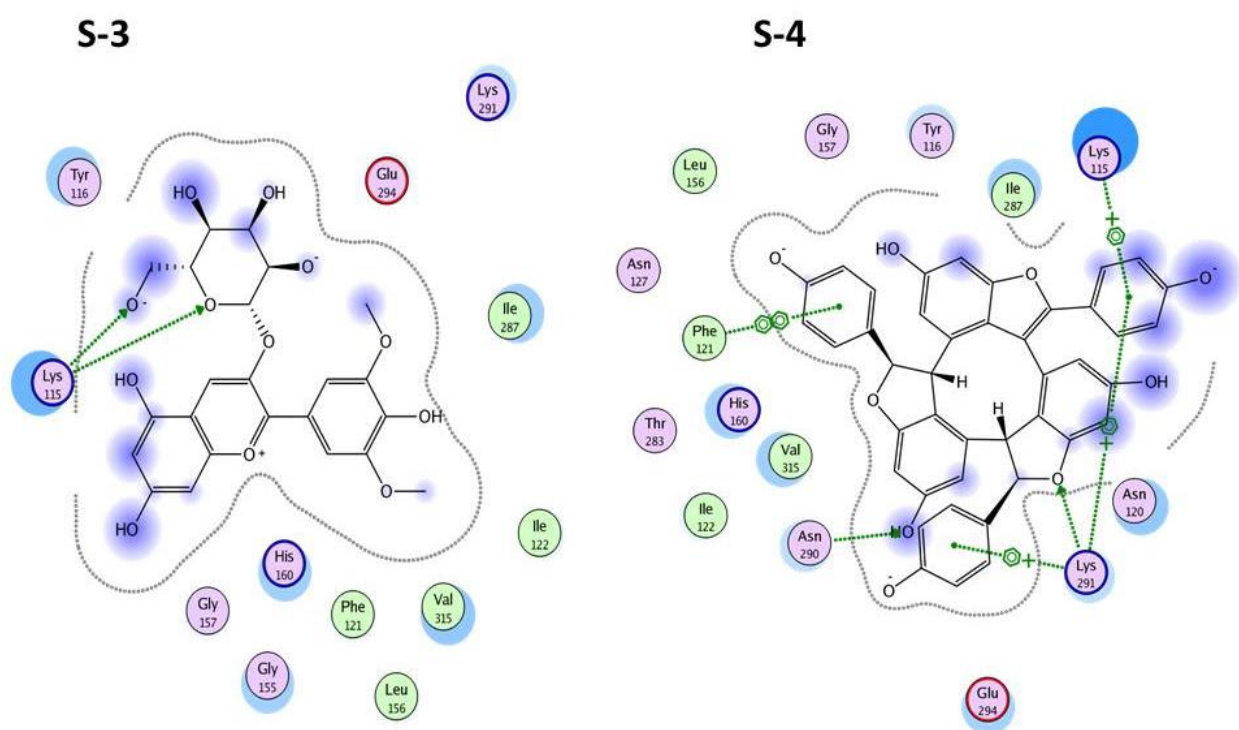


Figure (S3-S4): 2D interaction images of **S3)** Oenin with DNAA target protein **S4)** Sophorastilbene A with DNAA target protein

S-5

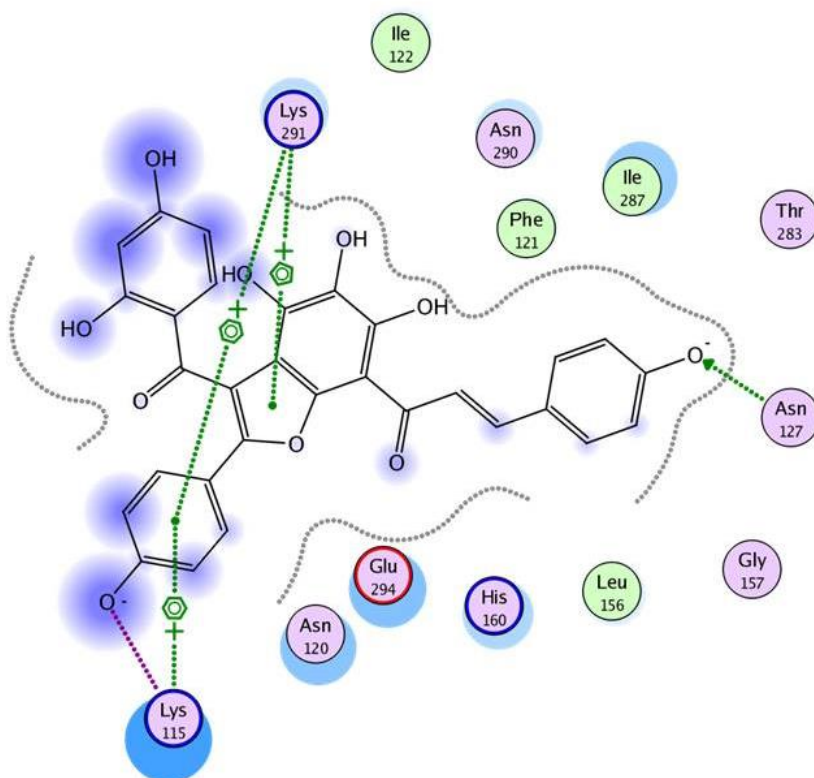
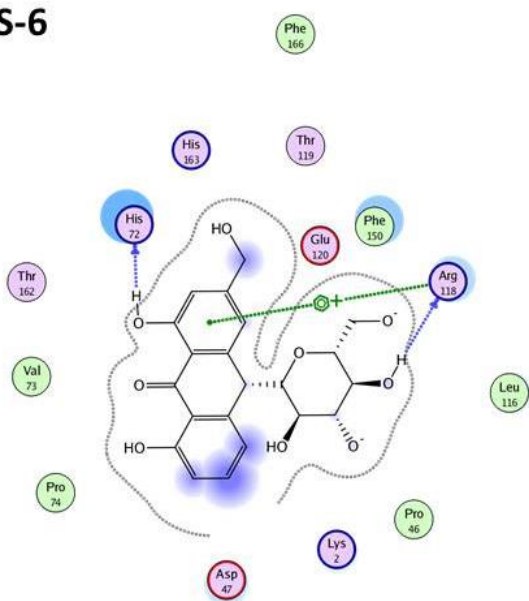


Figure (S5): 2D interaction images of **S5)** Daphnodorin B with DNAA target protein.

S-6



S-7

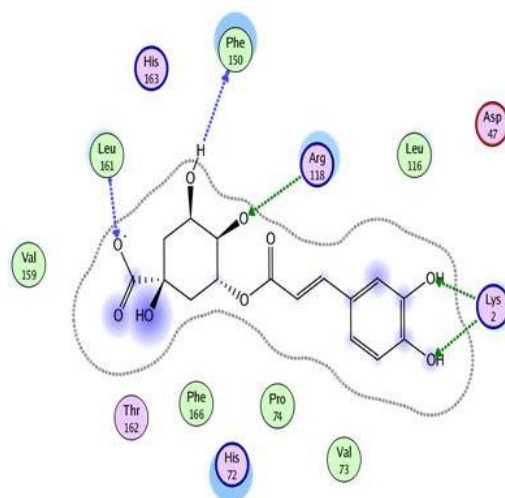
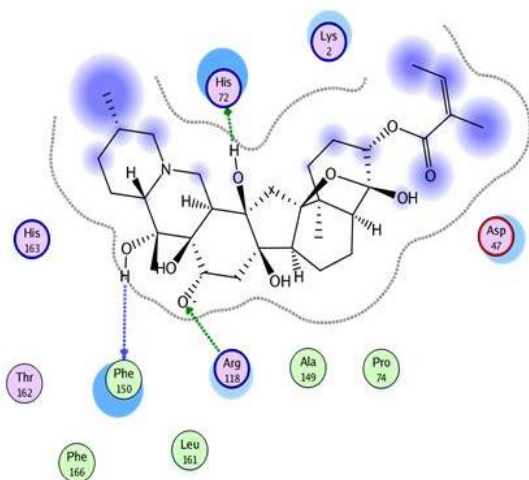


Figure (S6-S7): 2D interaction images of **S6)** Aloin B with TCR target protein and **S7)** Chlorogenic acid with TCR target protein

S-8



S-9

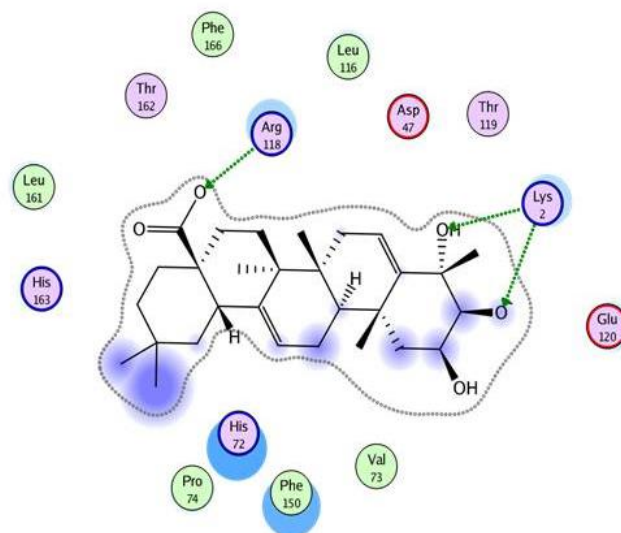


Figure (S8-S9): 2D interaction images of **S8)** Triterpenoids with TCR target protein **S9)** Veratrine with TCR target protein)

S-10

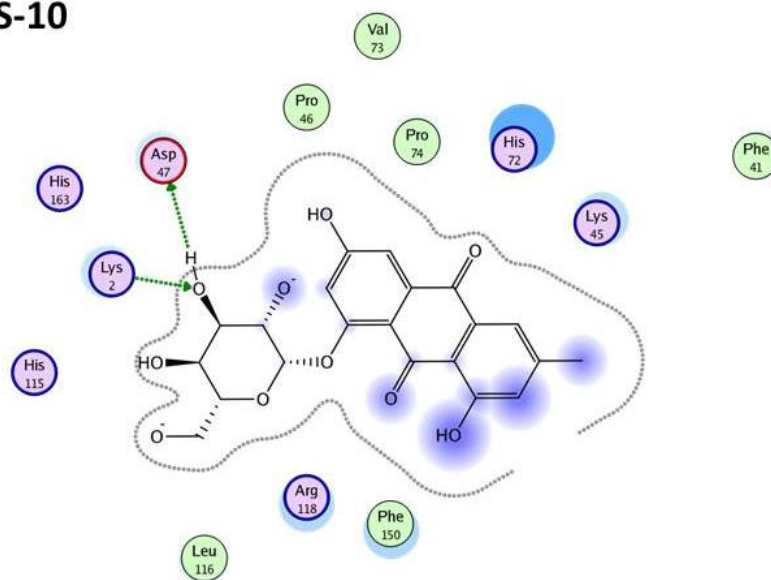


Figure (S10): 2D interaction images of **S10)** 1,6-Dihydroxy-3-methyl-8-[(2S,5S)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxyanthracene-9,10-dione with TCR target protein