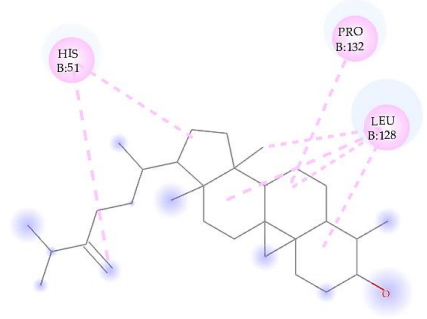
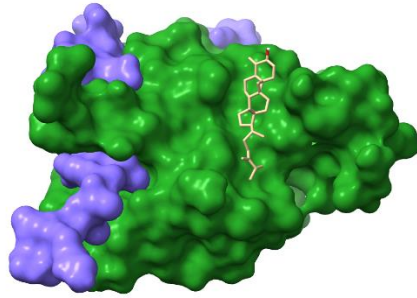


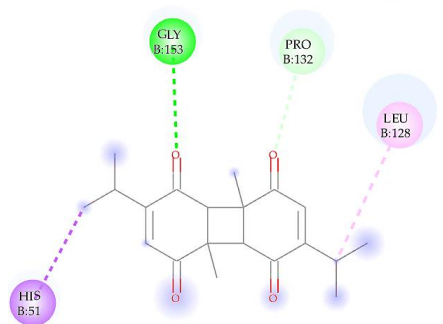
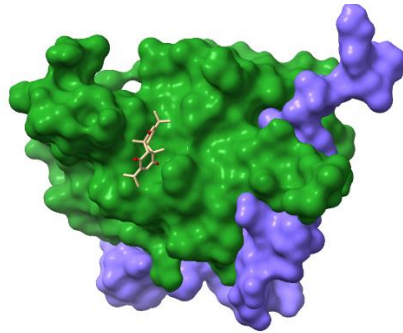
Cycloeucalenol

-8.3



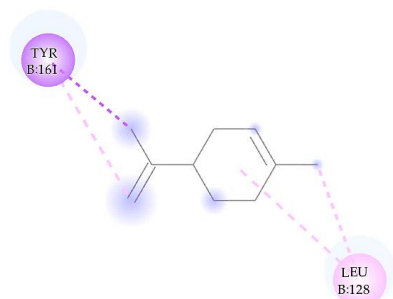
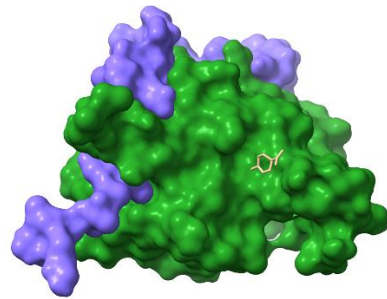
Dithymoquinone

-7.2



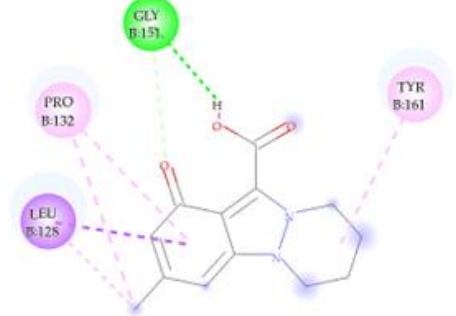
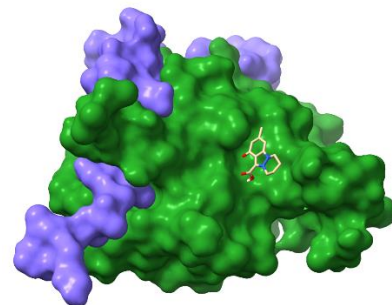
D-Limonene

-5.5



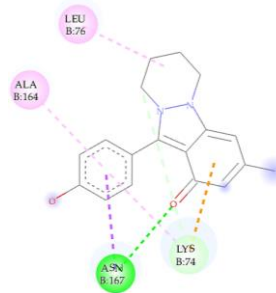
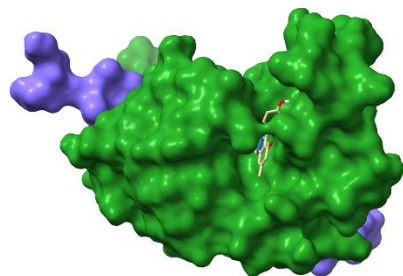
Nigellidine

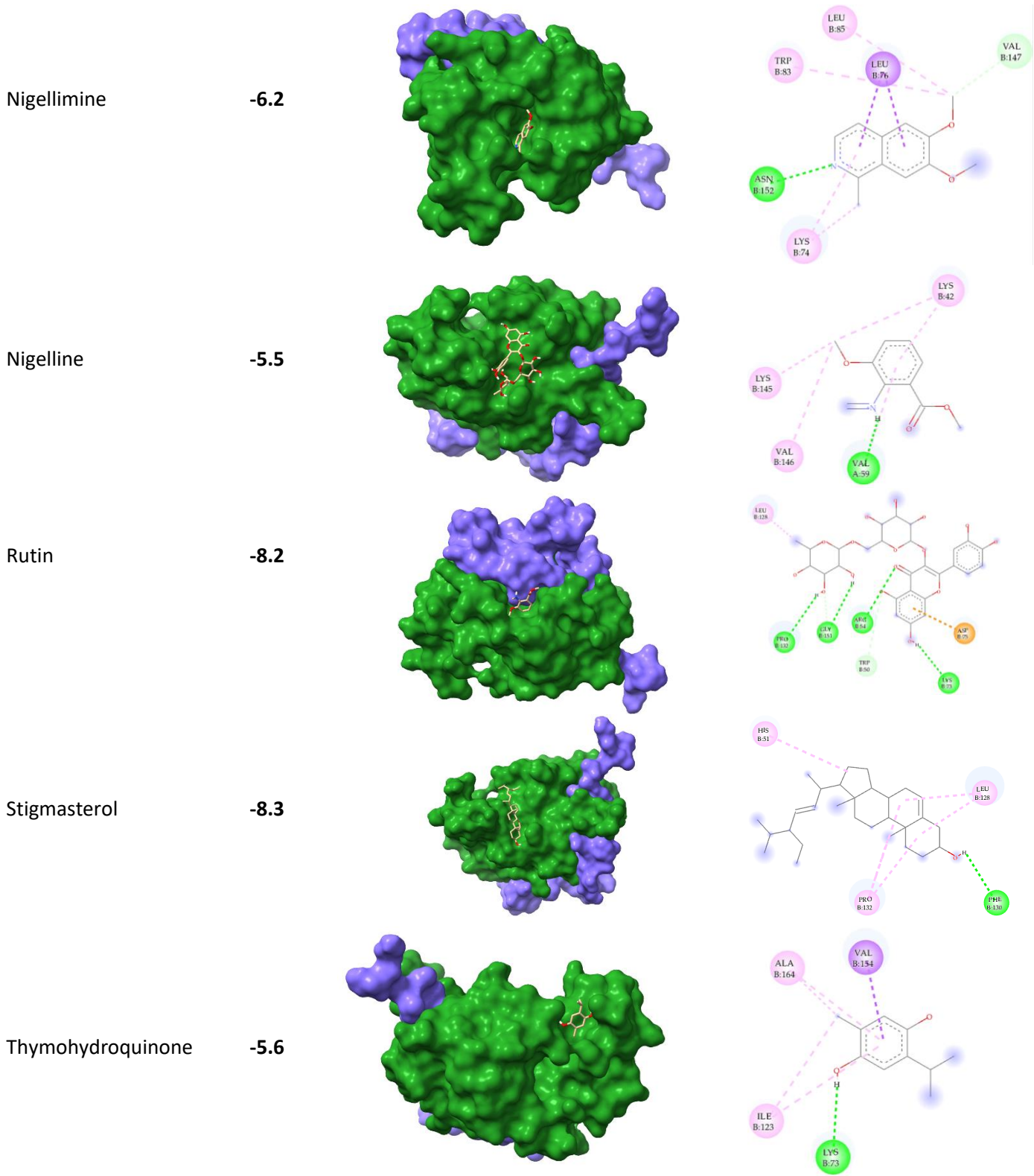
-7.4



Nigellidine

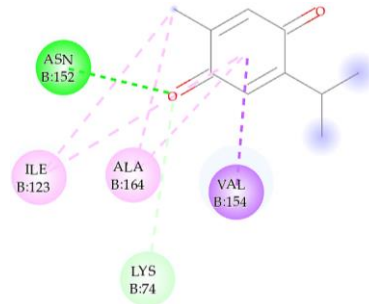
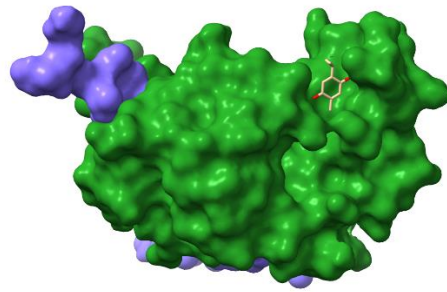
-7.3





Thymoquinone

-5.6



Curcumin (Positive control)

-7.2

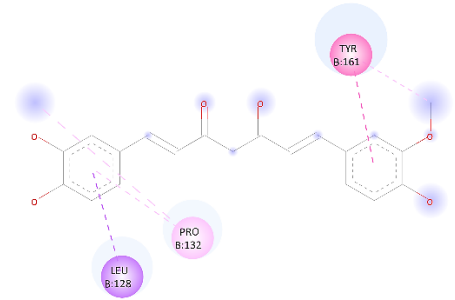
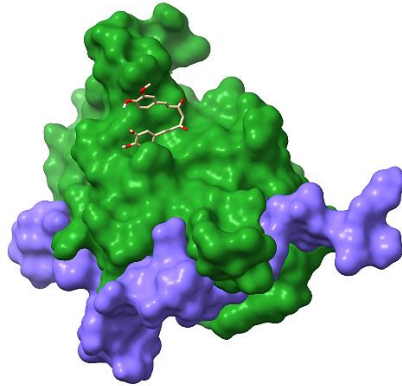
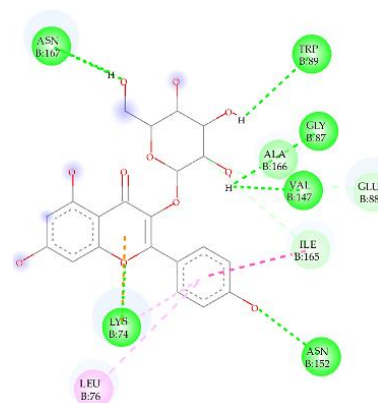


Fig. 1 Docking poses of selected phytochemicals from *N. sativa* with Dengue virus NS2BNS3 protease represented as 3-D models (Left side) and their respective 2-D line models (Right side).

Ligand	Binding Affinity (kcal/mol)	Docking Complex	Interacting amino acid residues
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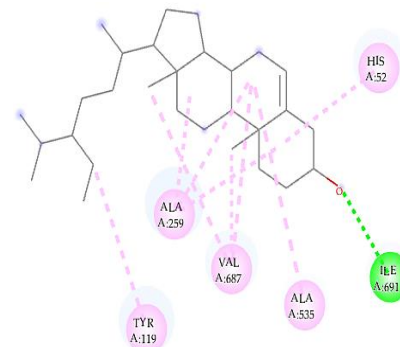
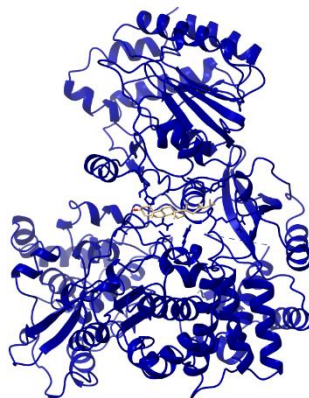
Astragalin

-8.5



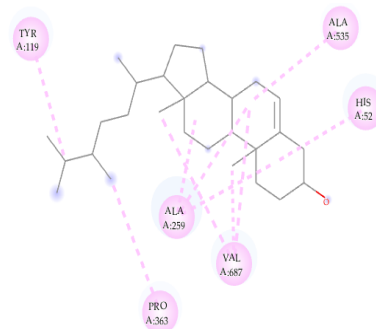
B-Sitosterol

-8.0



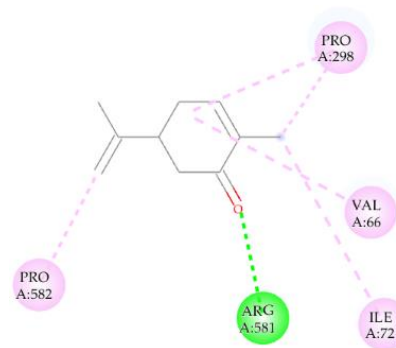
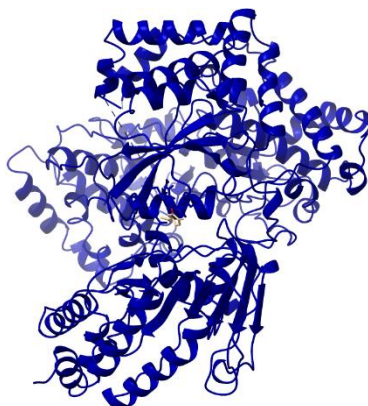
Campesterol

-8.5



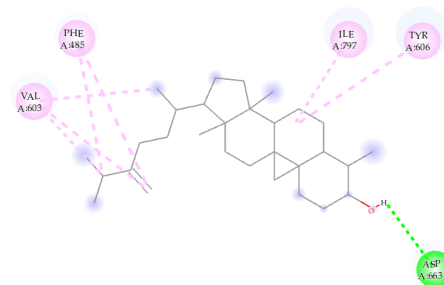
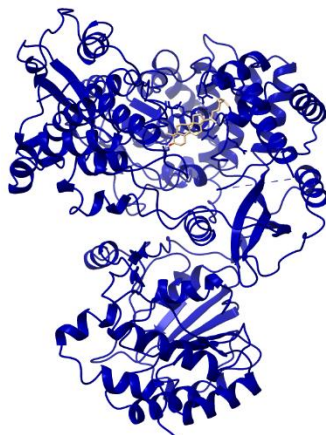
Carvone

-6.4



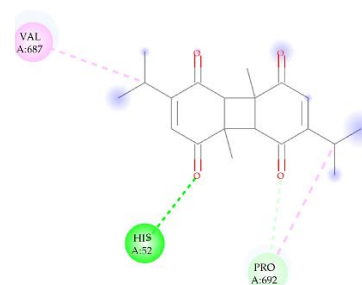
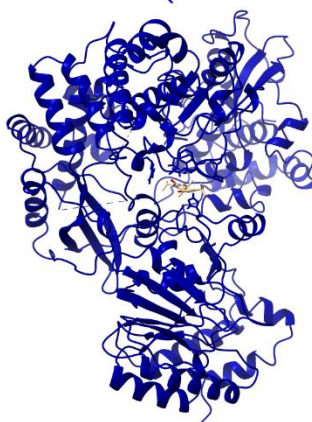
Cycloeucaleanol

-8.0



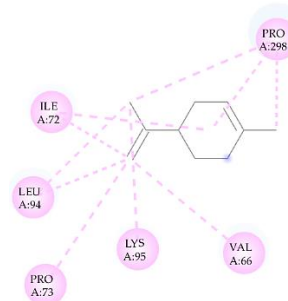
Dithymoquinone

-7.5

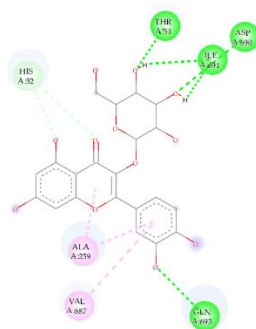
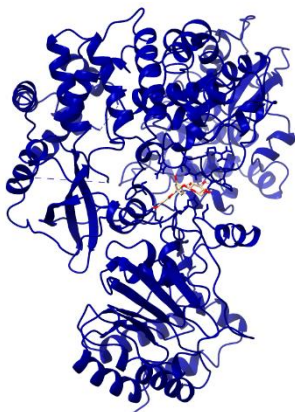


D-Limonene

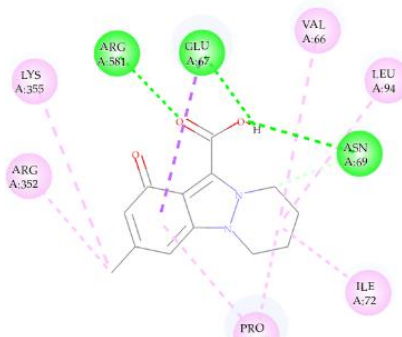
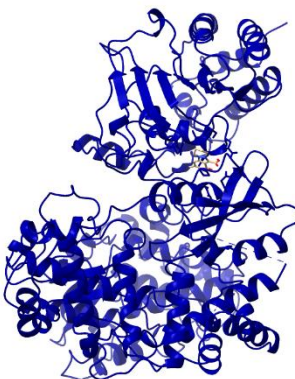
-6.0



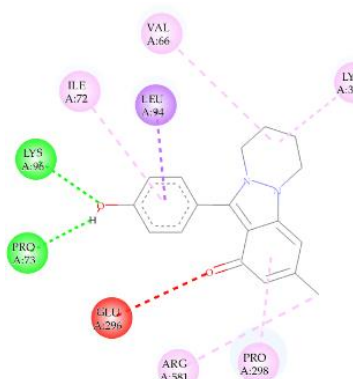
Isoquercetin -8.6



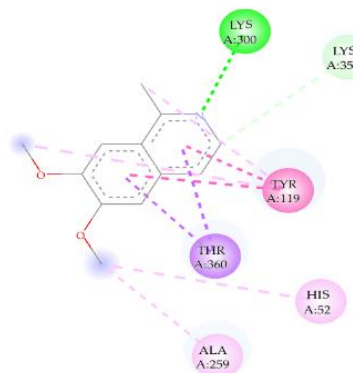
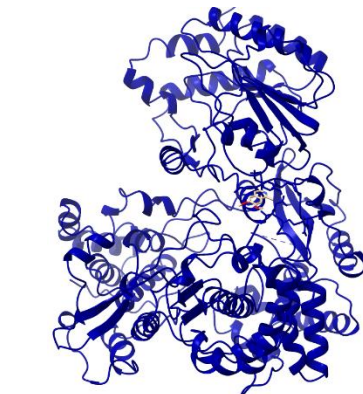
Nigellicine -9.1



Nigellidine -8.4

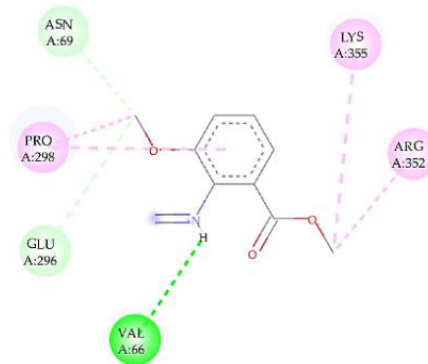
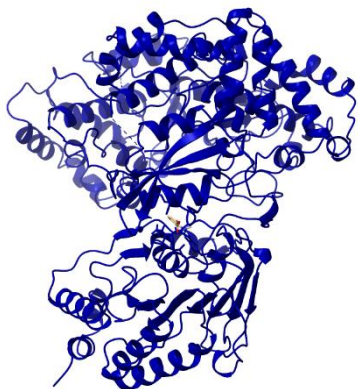


Nigellimine -6.1



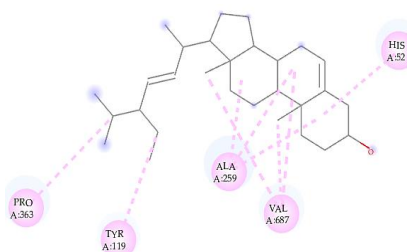
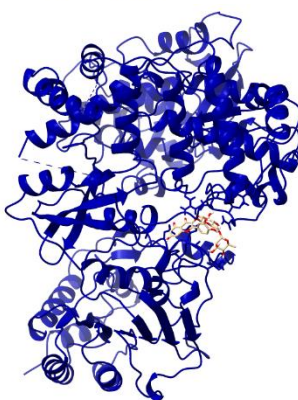
Nigelline

-6.2



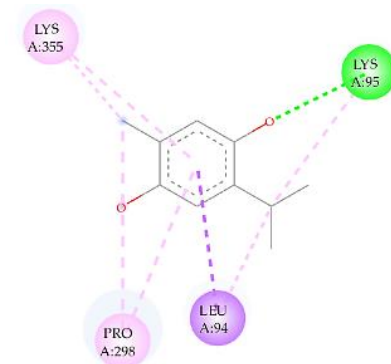
Stigmasterol

-8.8



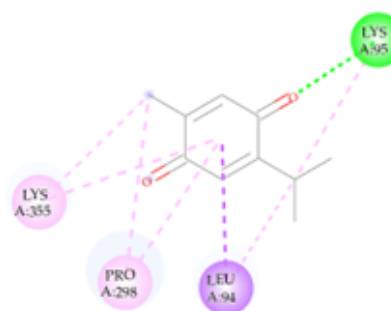
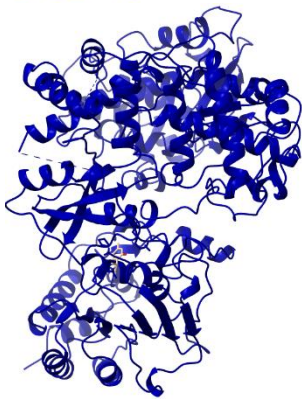
Thymohydroquinone

-6.5



Thymoquinone

-6.7



S-Adenosyl-L-
Homocysteine (SAH)
(Positive control)

-7.2

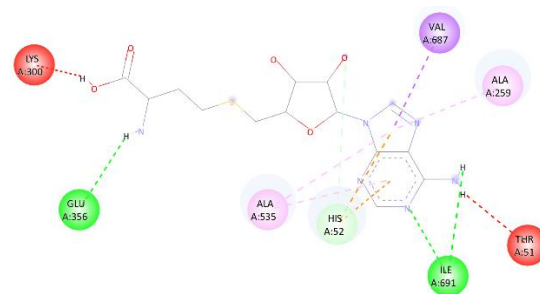
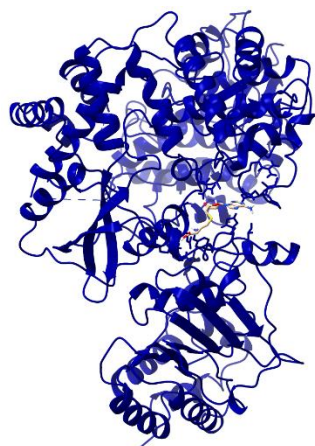


Fig. 2 Docking poses of selected phytochemicals from *N. sativa* with Dengue virus NS5 polymerase represented as 3-D models (Left side) and their respective 2-D line models (Right side).