Supplementary data

Table S1. Ayurvedic medical plants and their major constituents

Plant species	**Major components**	**References**
Juglans regia L.	Juglone	(Raafa, 2018)
Syzygium aromaticum (L.) Merr. & L.M.Perry	Eugenol, caryophyllene, α-humulene, caryophyllene oxide	(Alma *et al*.,2007)
Eruca sativa Mill.	2-Phenylethylisothiocyanate	(Khoobchandani *et al*., 2010)
Myristica fragrans Houtt	Caryophyllene oxide, palmitic acid , 2-Phenylethylisothiocyanate	(Shafiq et al., 2016)
Punica granatum L.	Gallic acid, apigenin, quercetin, pelargonidin, cyanidin, punicalin, punicalagin, granatin A, granatin B.	(Singh *et al*., 2018)
Azadirachta indica A. Juss	Nimbidine, azadirachtin (azadirachtin A), salannol, salannin	(Biswas *et al*., 2002)

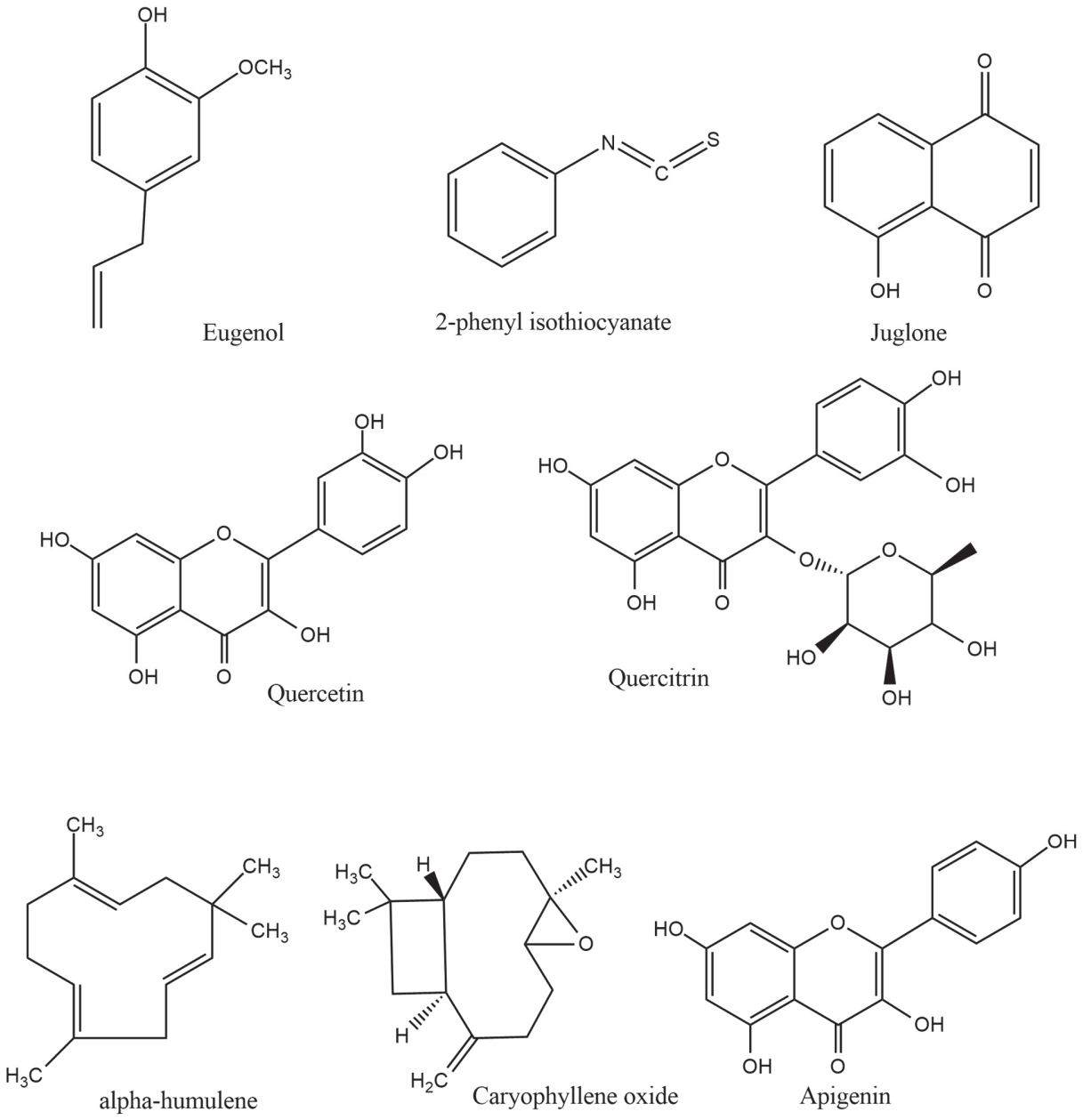

Figure S1. Structure of tested compounds including Eugenol($C_{10}H_{11}O_2$), 2-Phenyl isothiocyanate (C_7H_5NS), Juglone ($C_{10}H_6O_3$), Quercetin($C_{15}H_{10}O7$), Quercitrin ($C_{21}H_{20}O_{11}$), Alpha humulene ($C_{15}H_{22}$), Caryophyllene oxide ($C_{15}H_{24}O$), Apigenin ($C_{15}H_{10}O_6$).

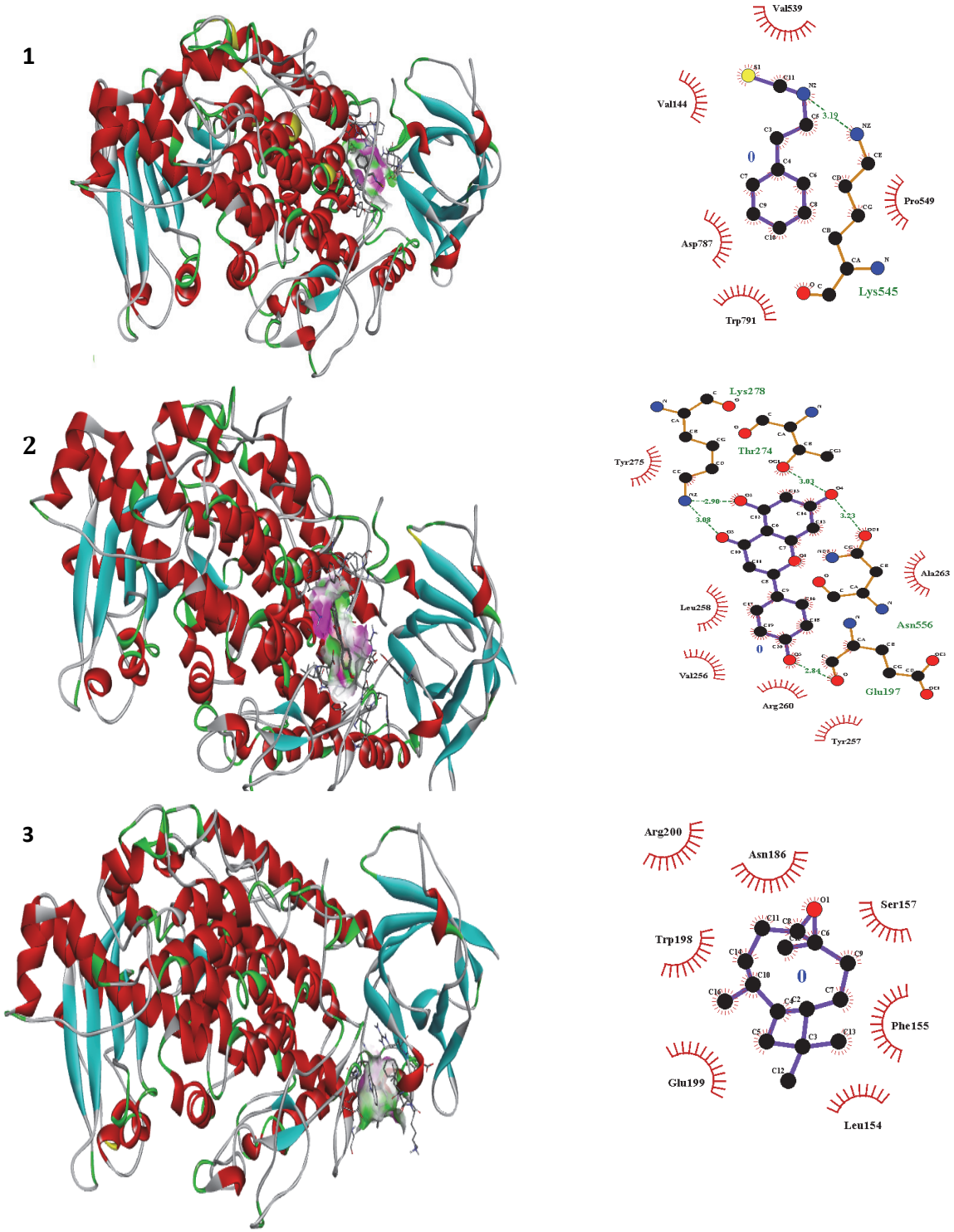

Figure S2. 3D H-bonding interactions of 2-phenyl isothiocyanate pose no. 1 [1], apigenin pose no. 5[2] caryophyllene oxide pose no. 1 [3] with binding sites of transcriptional regulator **1IK3.**

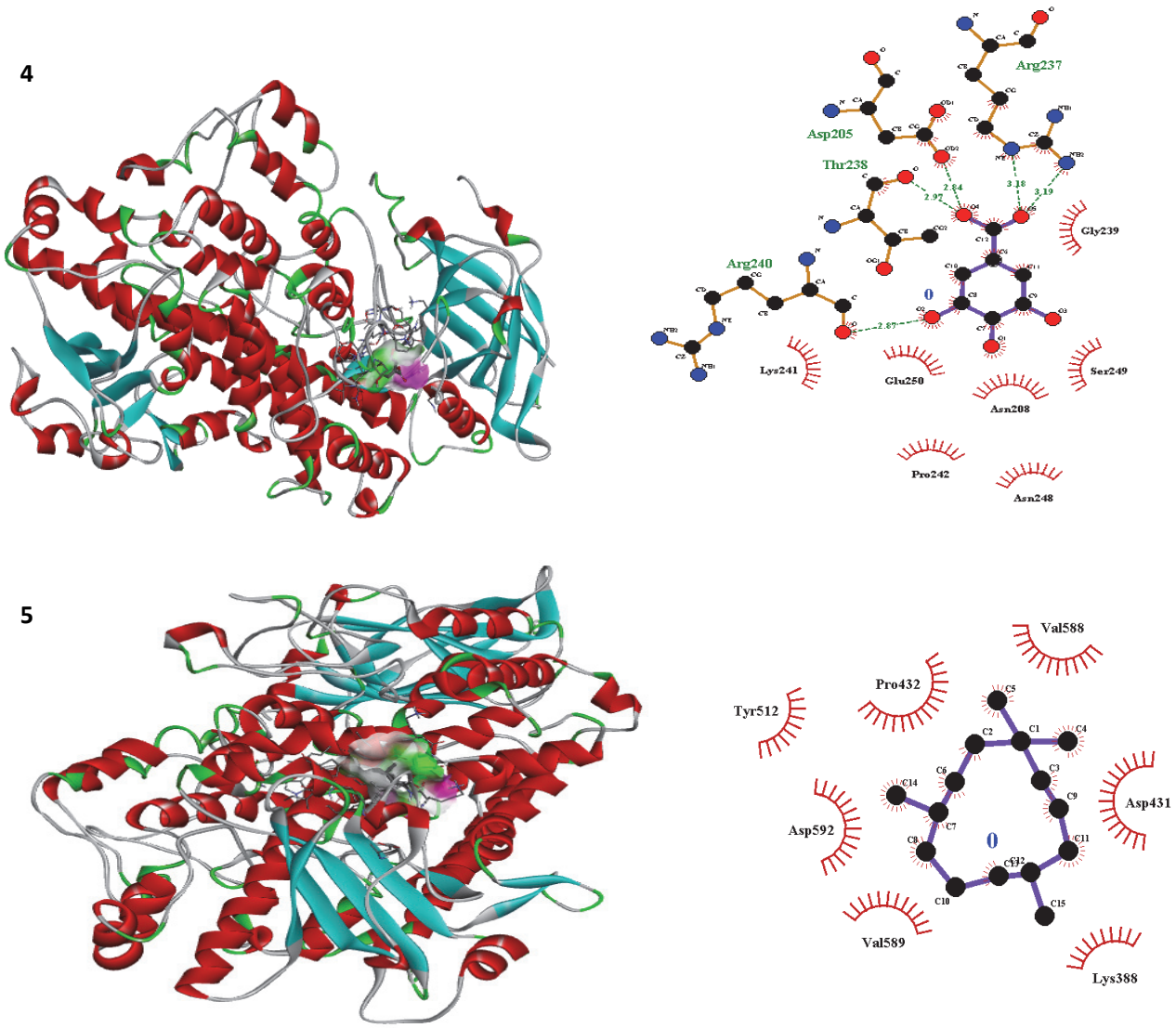

Figure S3. 3D H-bonding interactions of Eugenol pose rank 3 [4], α-humulene pose no. 1 [5] with binding sites of transcriptional regulator **1IK3**

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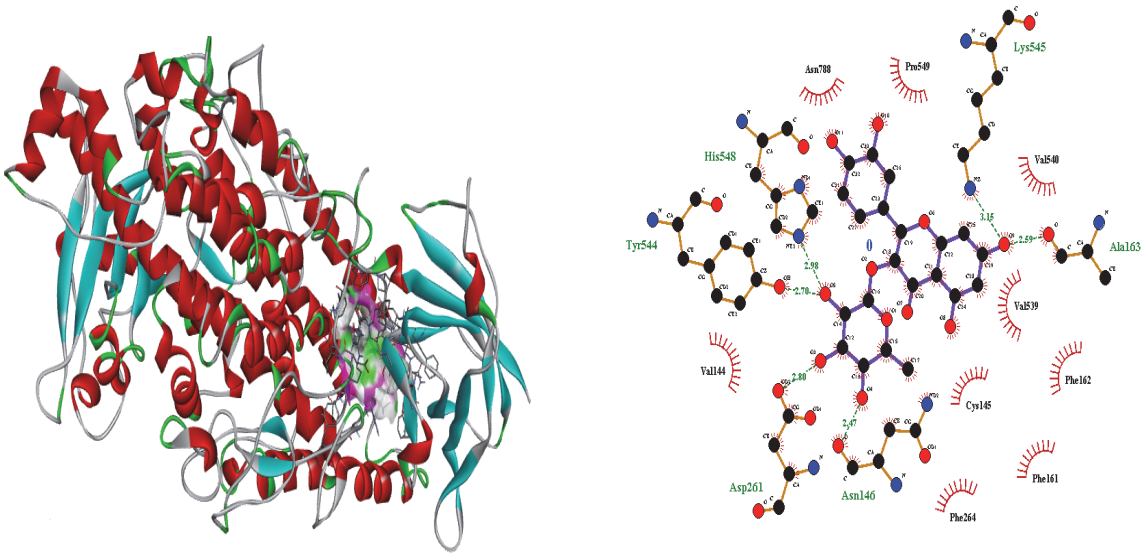

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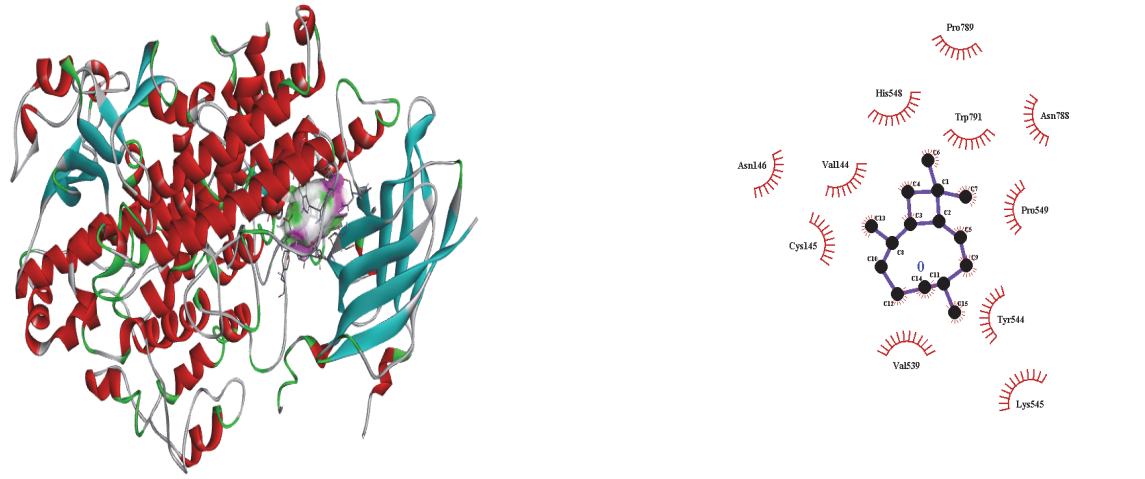

Figure S4. 3D H-bonding interactions of Quercitrin pose no. 4 [6] and transcaryphyllene pose no.1 [7] with binding sites of transcriptional regulator **1IK3.**

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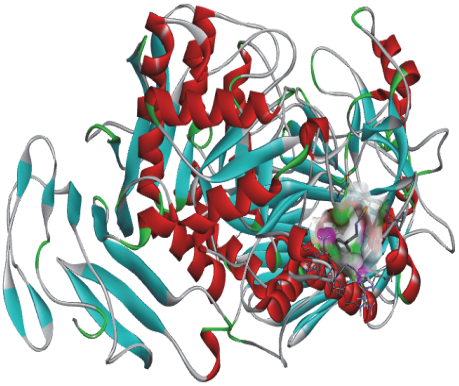
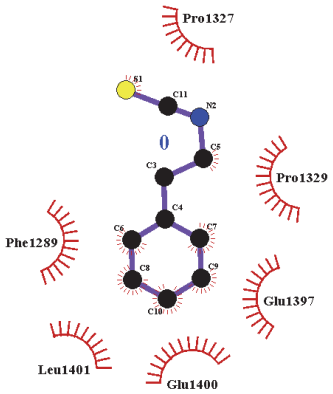
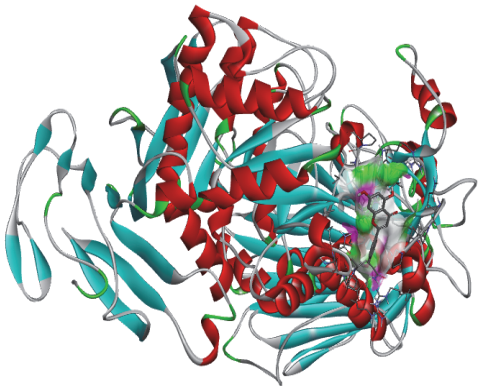
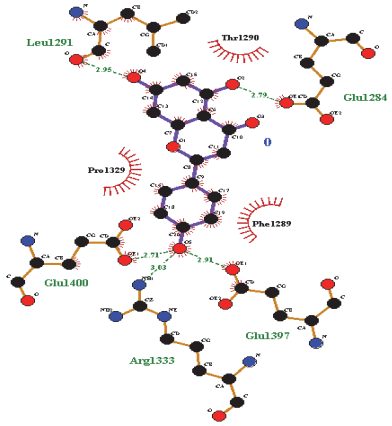


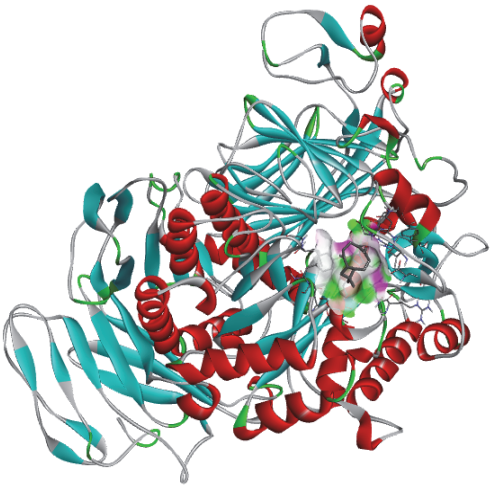

Pro1327
Pro1329
Phe1289
Glu1397
Leu1401
Glu1400

9




Leu1291
Thr1290
Glu1284
Pro1329
Phe1289
Glu1400
Glu1397
Arg1333

10



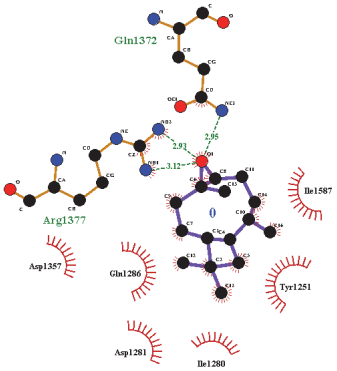

Gln1372
Arg1377
Ile1587
Asp1357
Gln1286
Tyr1251
Asp1281
Ile1280

Figure S5. 3D H-bonding interactions of 2-phenylisothiocyanate pose no. 1 [8], apigenin pose no. 1 [9]; caryophyllene oxide pose no. 1 [10] with binding sites of transcriptional regulator **3TOP**.

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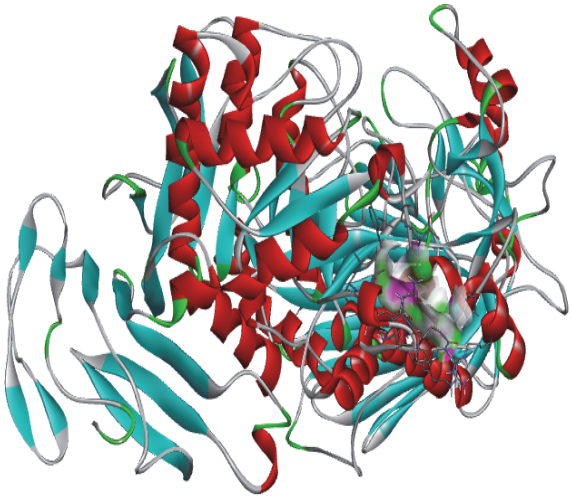

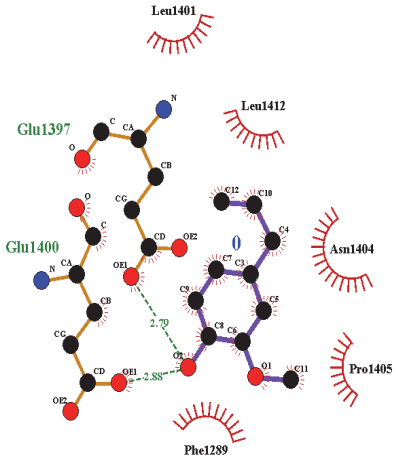

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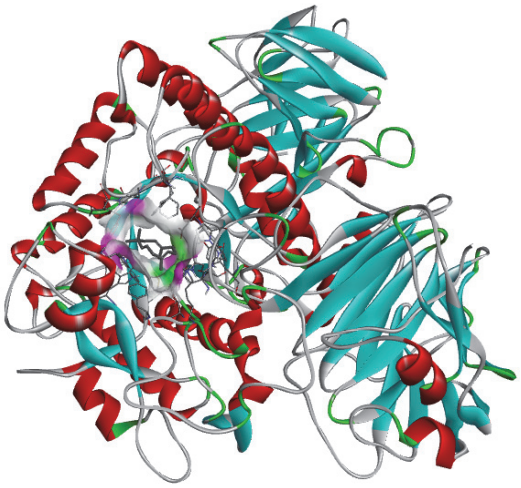

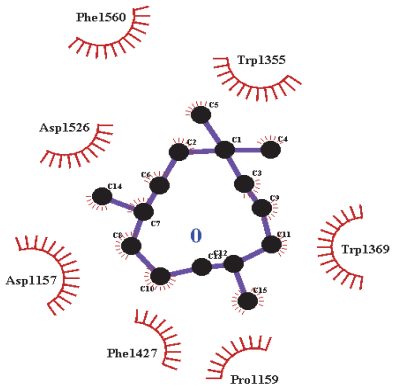

Figure S6. 3D H-bonding interactions of eugenol pose no. 2 [11] and α-humulene pose no. 1 [12] with binding sites of transcriptional regulator **3TOP**.

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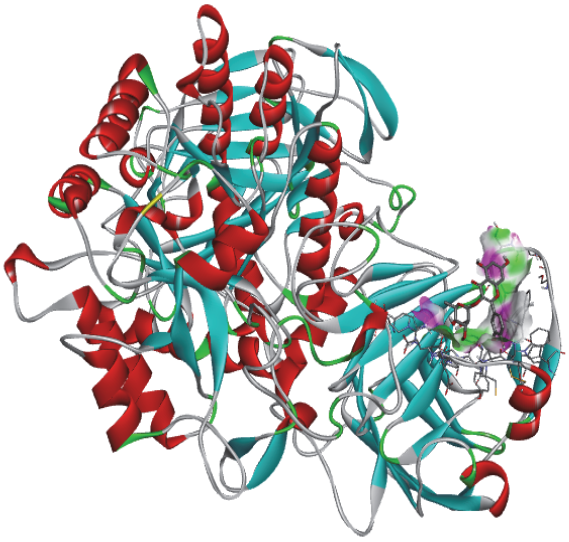

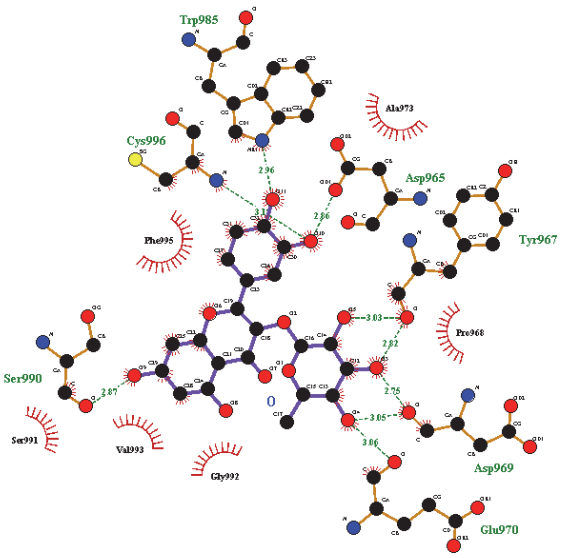

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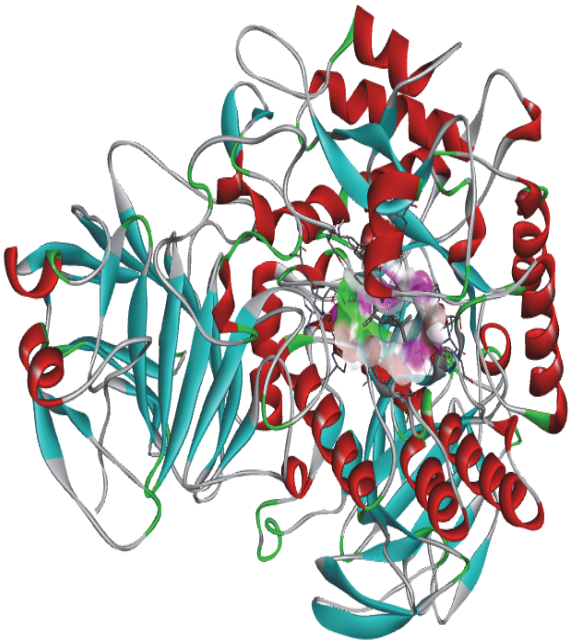

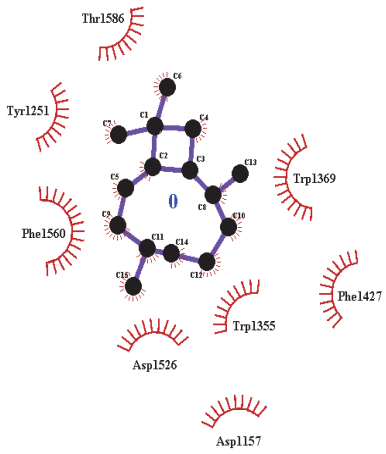

Figure S6. 3D H-bonding interactions of quercitrin pose no. 4 [13] and transcaryphyllene pose no. 1 [14] with binding sites of transcriptional regulator 3TOP.

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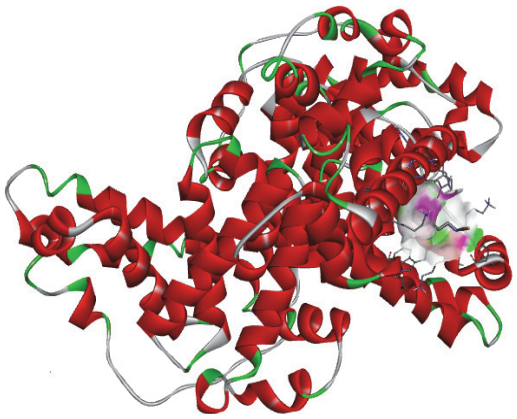

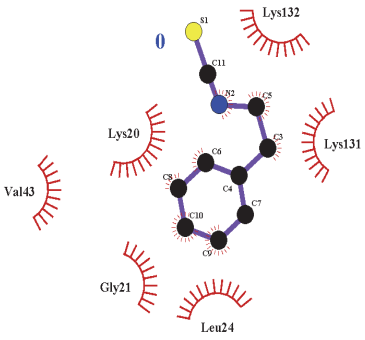

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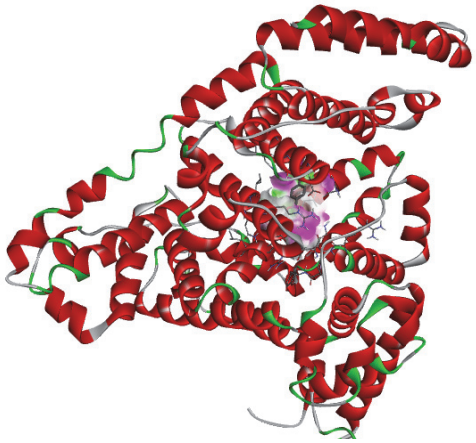

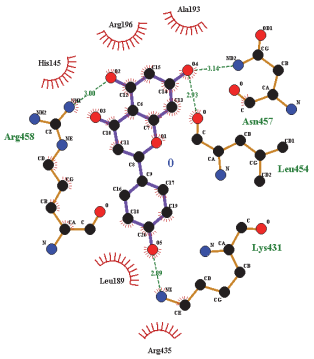

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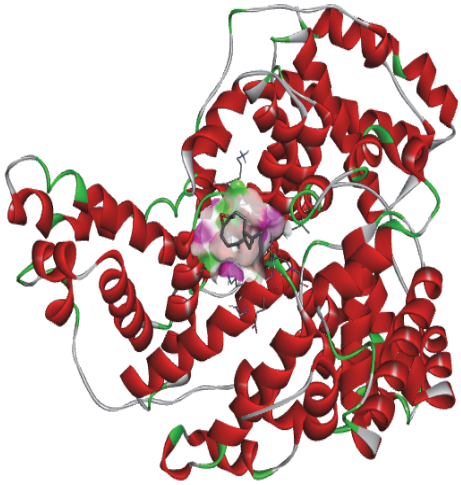


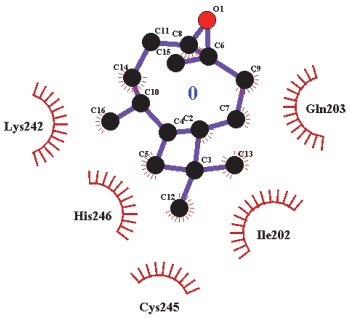
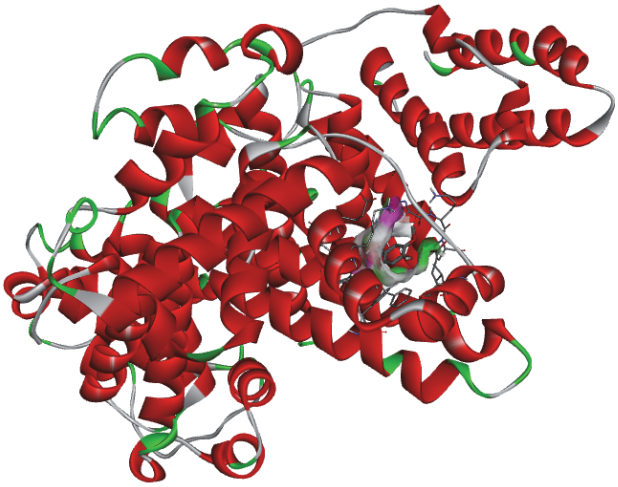
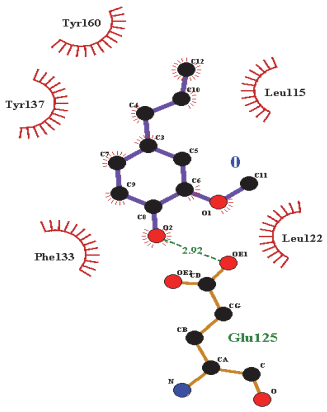


Figure S7. 3D H-bonding interactions of 2-phenylisothiocyanate pose no. 1 [15], apigenin pose no. 3[16] caryophyllene oxide pose no. 1 [17] with binding sites of transcriptional regulator **4F5S.**

18





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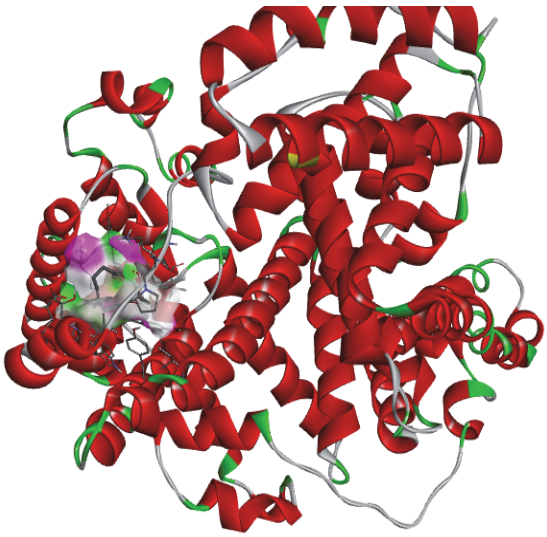

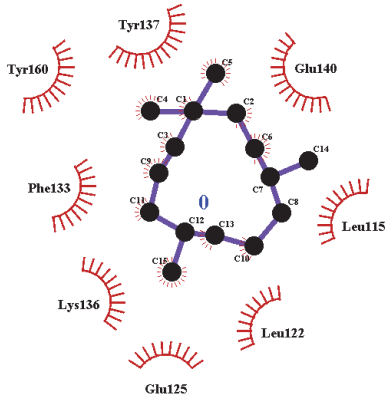

Figure S8. 3D H-bonding interactions of eugenol pose no. 1 [18], α-humulene pose no. 1[19] with binding sites of transcriptional regulator **4F5S**.

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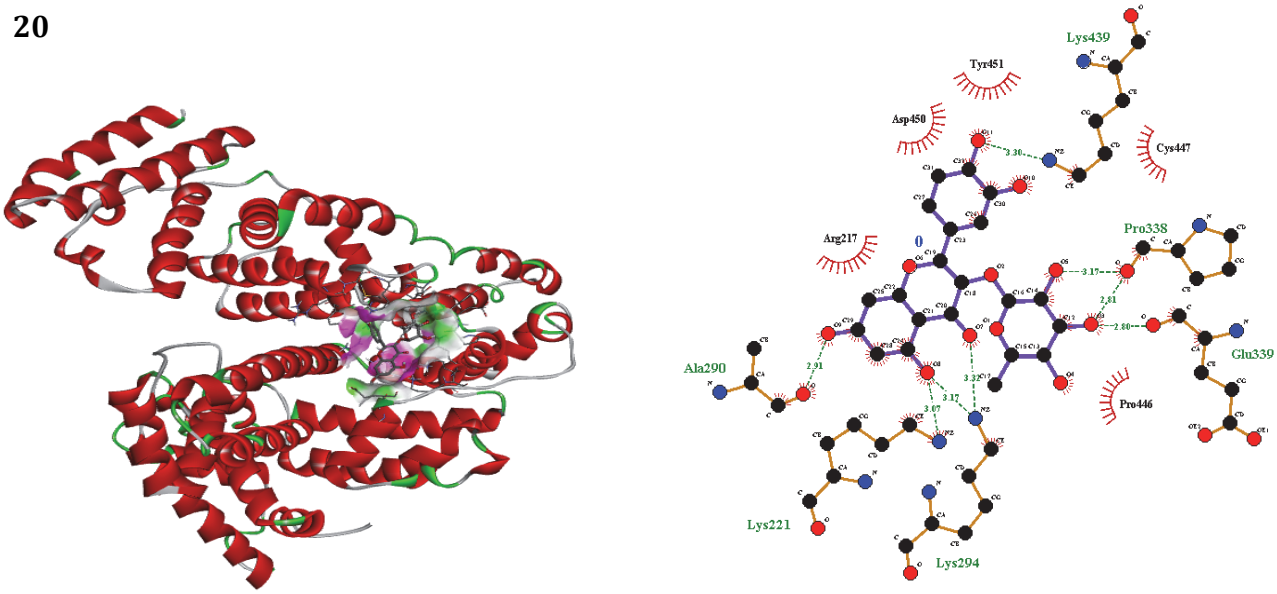

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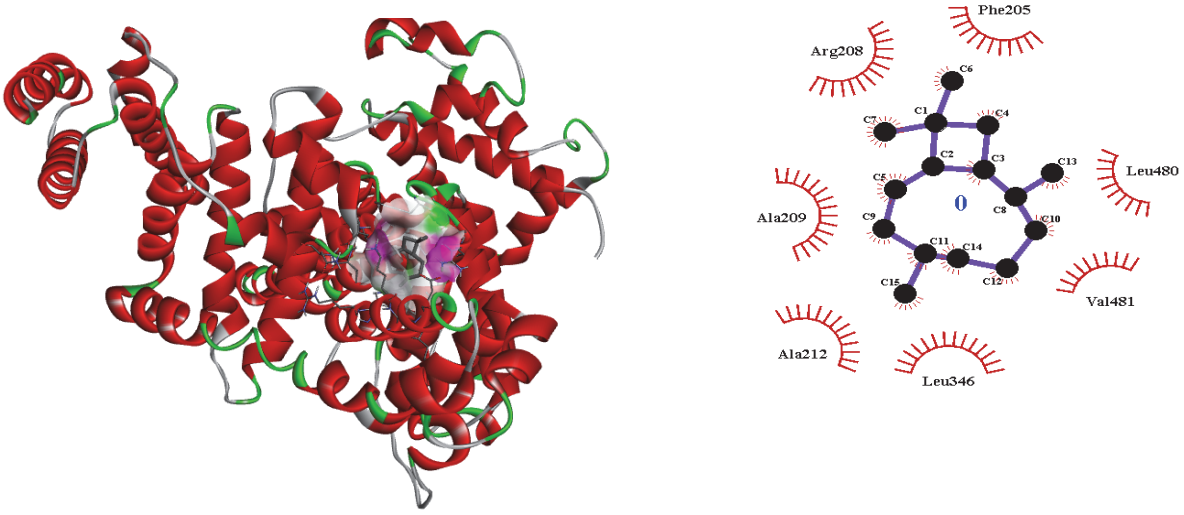

Figure S9. 3D H-bonding interactions of quercitrin pose no. 5 [20] and transcaryphyllene pose no. 1 [21] with binding sites of transcriptional regulator **4F5S**.