Supporting Information for:

Evaluation of the inhibitory activities of thyme compounds against coronavirus disease-19 (COVID-19) by molecular docking and molecular dynamic simulation

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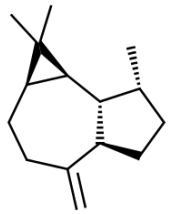
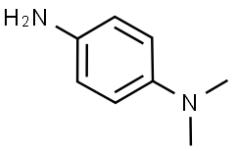
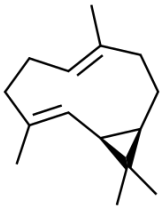


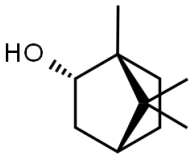
(+)-Aromadendrene



1,4-Benzenediamine N,N-dimethyl



Bicyclogermacrene



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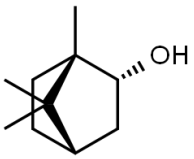

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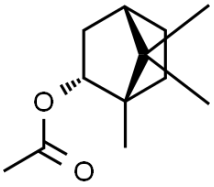

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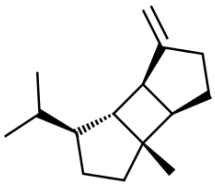
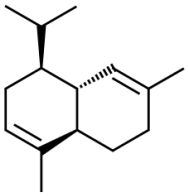
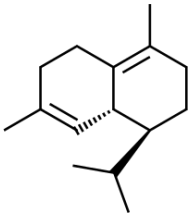


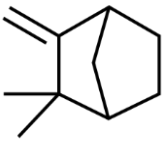
(-)-β-Bourbonene



α-cadinene



(+)-δ-cadinene



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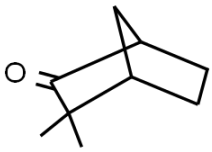
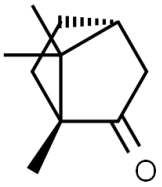
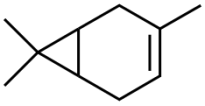


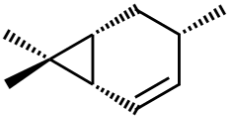
Camphenilone



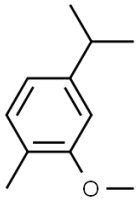
Camphor



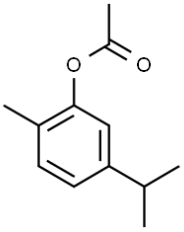
3-Carene



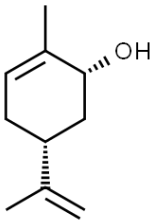
cis-(+)-4-carene



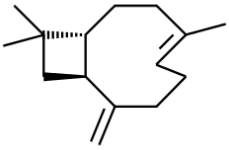
Carvacrol methyl ether



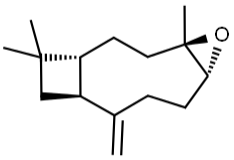
Carvacryl acetate



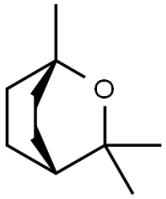
(−)-cis-carveol



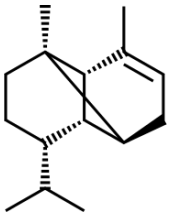
(-)-β-caryophyllene



(-)-β-Caryophyllene oxide



1,8-Cineole



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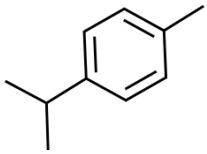
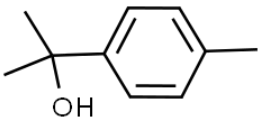
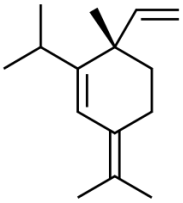


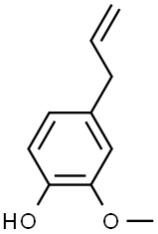
p-cymene



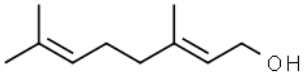
p-cymen-8-ol



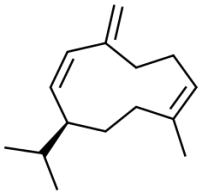
α-Elemene



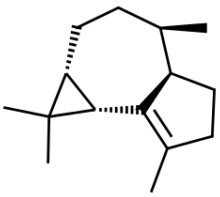
Eugenol



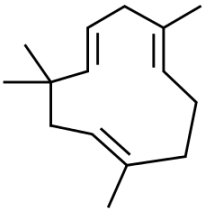
Geraniol



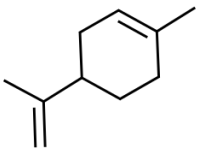
Germacrene D



α-Gurjunene



α-humulene



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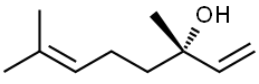
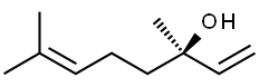
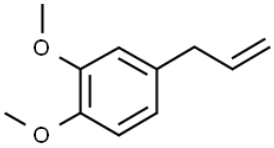


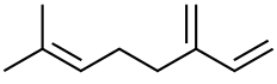
(S)-(+)-Linalool



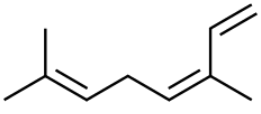
(R)-(–)-Linalool



Methyl eugenol



β-Myrcene



(Z)-β-ocimene

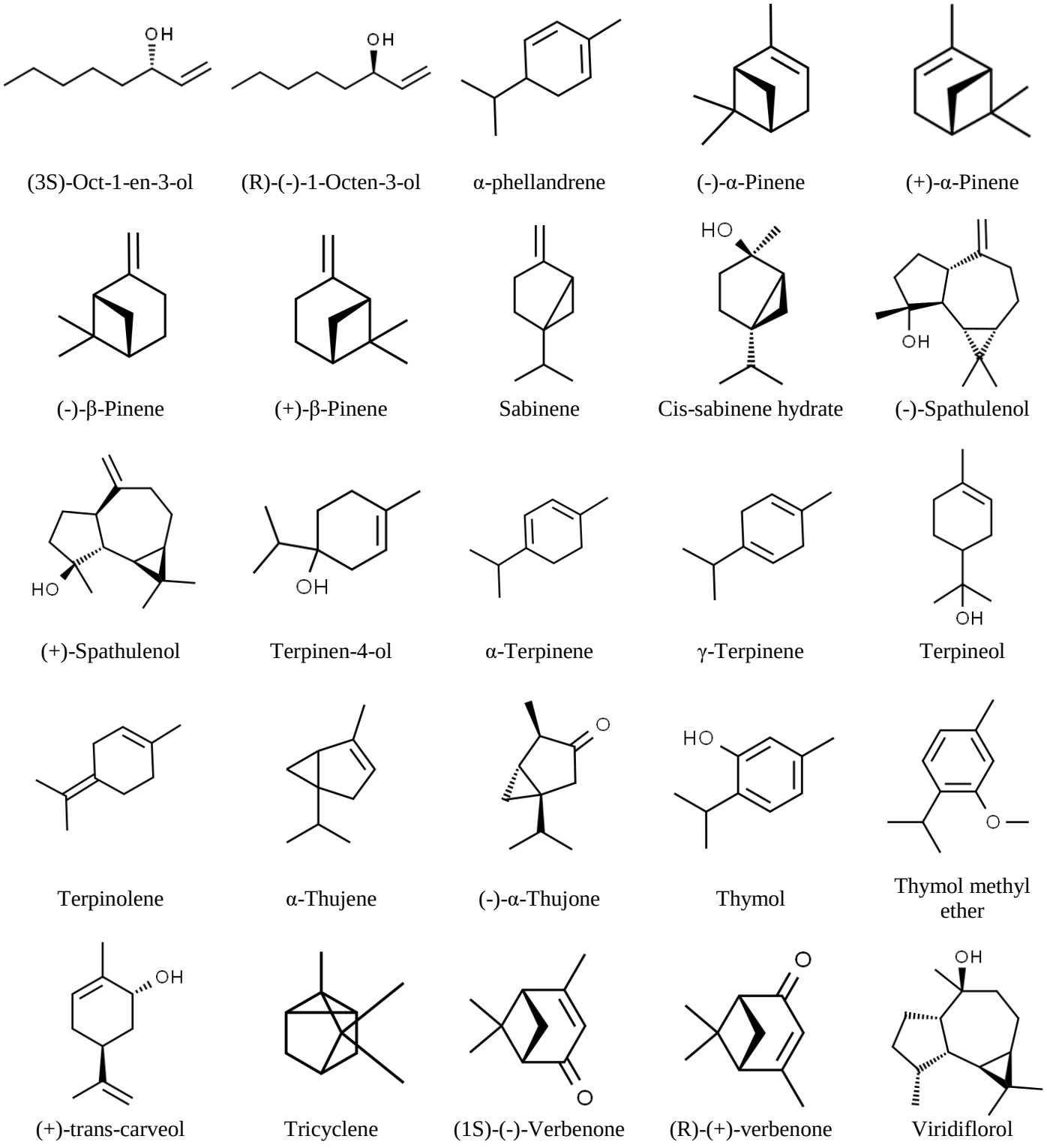


Fig. S1. The chemical structures of 60 thyme compounds used for molecular docking simulation with the target proteins

Table S1. The results obtained from docking of thyme compounds with ACE2 enzyme (PDB ID: 1R42)

No	Compound	Binding affinity (kcal/mol)	Binding pocket	Involved receptor residues (interaction force and distance Å)
1	(R)-(-)-1-Octen-3-ol	-4.2	S2	Phe390 (Pi-alkyl, 4.56, 5.25) , Asp350 (H-bond, 3.25), Arg393 (H-bond, 3.08)
2	(3S)-Oct-1-en-3-ol	-4.5	S1	Ala413 (H-bond, 3.09), Phe438 (Pi-donor, 2.98; Pi-alkyl, 4.44, 5.02)
3	Geraniol	-4.7	S2	Asp350 (Hydrophobic), Phe390 (H-bond, 3.00), Arg393 (H-bond, 3.07)
4	Camphenilone	-5.0	Not located in active site	
5	(−)-Cis-Carveol	-5.0	S2	Arg393 (H-bond, 2.93), Asp350 (Hydrophobic), Asn394 (Hydrophobic), Phe390 (Pi-alkyl, 5.25; Pi-sigma, 3.98)
6	(R)-(–)-Linalool	-5.0	Not located in active site	
7	Methyl eugenol	-5.0	S2	Phe390 (Pi-Pi stacking, 4.35; Pi-alkyl, 4.75), Arg393 (Pi-alkyl, 4.25), Asn394, and Asp350 (Hydrophobic)
8	Camphor	-5.0	Not located in active site	
9	1,8-Cineole	-5.1	Not located in active site	
10	(S)-(+)-Linalool	-5.1	S2	Phe390 (H-bond, 2.81), Arg393 (H-bond, 2.92), Asp350, and Asn394 (Hydrophobic)
11	(-)-α-Pinene	-5.1	Not located in active site	No locate in active site
12	(-)-β-Pinene	-5.1	Not located in active site	No locate in active site
13	Camphene	-5.2	Not located in active site	No locate in active site
14	(+)-Trans-Carveol	-5.2	Not located in active site	No locate in active site
15	Cis-Sabinene hydrate	-5.2	S2	Phe390 (H-bond, 3.20), Arg393 (Pi-alky, 4.78), Asp350 (Hydrophobic)
16	(−)-Borneol	-5.2	Not located in active site	No locate in active site
17	Terpineol	-5.2	Not located in active site	No locate in active site
18	Terpinen-4-ol	-5.2	Not located in active site	No locate in active site
19	Thymol methyl ether	-5.2	S2	Thr347, Ala348, and Asp350 (Hydrophobic)
20	Tricyclene	-5.2	Not located in active site	No locate in active site
21	Carvacrol methyl ether	-5.3	S2	Phe390 (Pi-Pi stacking, 4.19; Pi-alkyl, 4.47), Asn394, and Arg393 (Hydrophobic)
22	l-Bornyl acetate	-5.3	Not located in active site	
23	(+)-α-Pinene	-5.3	Not located in active site	

24	(+)-Borneol	-5.3	Not located in active site	
25	p-Cymen-8-ol	-5.3	Not located in active site	
26	α-Thujene	-5.4	S2	Phe390 (Pi-alkyl, 4.25, 4.27, 5.15; Pi-sigma, 3.86), Asp350, and Arg393 (Hydrophobic)
27	(-)-α-Thujone	-5.4	S2	Phe390 (Pi-alkyl, 4.32, 4.78, 5.17; Pi-sigma, 3.48), Asp350, and Arg393 (Hydrophobic)
28	(+)-β-Pinene	-5.4	Not located in active site	
29	Sabinene	-5.4	S2	Phe390 (Pi-alkyl, 4.24, 4.27, 5.07; Pi-sigma, 3.85), Asp350, Arg393 (Hydrophobic)
30	β-Myrcene	-5.4	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 4.17, 4.41, 5.08, 5.30, 5.32)
٣1	(1S)-(-)-Verbenone	-5.4	Not located in active site	
32	3-Carene	-5.5	Not located in active site	
33	1,4-Benzenediamine N,N-dimethyl	-5.5	S1	Ala413, and Phe438 (Hydrophobic)
34	Cis-(+)-4-Carene	-5.5	Not located in active site	
35	Limonene	-5.5	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 4.67, 4.72, 5.02; Pi-sigma, 3.88)
36	(R)-(+)-Verbenone	-5.6	Not located in active site	
37	(Z)-β-Ocimene	-5.6	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 3.92, 3.99, 4.24, 4.92)
38	Eugenol	-5.9	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 5.08, 5.44; Pi-Pi stacking, 4.09)
39	(-)-Spathulenol	-6.1	S2	Ala348, and Asp350 (Hydrophobic)
40	p-Cymene	-6.2	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 4.79, 4.85; Pi-Pi stacking 4.08)
41	α-Elemene	-6.3	S2	Ala348, Thr347, and Asp350 (Hydrophobic)
42	α-Terpinene	-6.3	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 4.0, 5.07)
43	Carvacryl acetate	-6.3	S1	Phe438 (Pi-alkyl, 4.91, 5.44; Pi-sigma, 3.68; Pi-Pi stacking, 4.28), Ala413 (Hydrophobic)
44	Germacrene D	-6.3	S2	Phe390 (Pi-alkyl, 4.15, 4.69, 5.39), Arg393, Asp350, and Asn394 (Hydrophobic)
45	(-)-β-Bourbonene	-6.3	Not located in active site	
46	α-Cadinene	-6.3	S2	Arg393 (Pi-alkyl, 4.27, 4.30, 5.12), Phe390, and Asp350 (Hydrophobic)
47	(+)-Spathulenol	-6.3	S2	Ala348, and Asp350 (Hydrophobic)
48	α-Phellandrene	-6.4	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 4.11, 4.81, 5.14)
49	γ-Terpinene	-6.4	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 4.97, 5.13, 5.22; Pi-Pi stacking, 4.08)
50	Viridiflorol	-6.4	S2	Phe390 (Pi-alkyl, 3.92, 4.42, 4.58), Asp350 (H-bond, 2.96), Arg393, and Asn394 (Hydrophobic)

51	α-Humulene	-6.5	S2	Phe390 (Pi-alkyl, 4.77; Pi-sigma, 3.82), Arg393, and Asp350 (Hydrophobic)
52	(-)-β-Caryophyllene oxide	-6.5	Not located in active site	
53	(+)-Aromadendrene	-6.5	S2	Ala348, and Asp350 (Hydrophobic)
54	α -Gurjunene	-6.6	S2	Phe390 (Pi-alkyl, 4.06, 4.80, 5.46; Pi-sigma 3.89), Asp350, Arg393, Asn394 (Hydrophobic)
55	(+)-δ-Cadinene	-6.6	Not located in active site	
56	Bicyclogermacrene	-6.7	S2	Phe390 (Pi-alkyl, 4.32, 4.65), Asp350, Asp382, Tyr385, Asn394, and Arg393 (Hydrophobic)
57	Copaene	-6.7	Not located in active site	
58	(-)-β-caryophyllene	-6.7	Not located in active site	
59	Thymol	-6.8	S1	Ala413 (Hydrophobic), Phe438 (Pi-alkyl, 4.75, 5.24; Pi-Pi stacking 4.05)
60	Terpinolene	-7.0	S1	Phe438 (Pi-alkyl, 4.41, 4.86, 5.37; Pi-Pi stacking 3.30)

Table S2. The results obtained from docking of thyme compounds with papain-like protease (PDB ID: 5Y3e)

No	Compound	Binding affinity (kcal/mol)	Involved receptor residues (interaction type and distance Å)
1	(3S)-Oct-1-en-3-ol	-4.5	Asp165 (H-bond, 2.42), Tyr265 (Pi-alkyl, 3.74), Tyr274, and Thr302 (Hydrophobic)
2	(R)-(-)-1-Octen-3-ol	-4.6	Asp165 (H-bond, 2.20), Tyr265 (Pi-alkyl, 4.69), Pro249, Tyr274, and Thr302 (Hydrophobic)
3	(S)-(+)-Linalool	-4.9	Pro249 (Alkyl, 4.32, 4.81), Tyr265 (Pi-alkyl, 4.88, 5.14), Asp165, Tyr274, and Thr302 (Hydrophobic)
4	β-Myrcene	-4.9	Pro248 (Alkyl, 4.53), Pro249 (Alkyl, 4.16, 4.71, 4.87), Tyr265 (Pi-alkyl, 4.07, 4.66, 5.15), Asp165, Tyr269, and Thr302 (Hydrophobic)
5	(+)-Borneol	-5.1	Pro248 (Alkyl, 4.60), Pro249 (Alkyl, 4.68, 5.20), Asp165, and Thr302 (Hydrophobic)
6	(Z)-β-Ocimene	-5.1	Pro249 (Alkyl, 4.49, 4.75, 4.79), Tyr265 (Pi-alkyl, 4.04, 5.18), Asp165, Tyr269, and Thr302 (Hydrophobic)
7	Tricyclene	-5.1	Pro249 (Alkyl, 4.21, 4.55, 4.98, 5.10), Tyr265 (Pi-alkyl, 4.28, 4.61; Pi-sigma, 3.60), Tyr274 (Pi-alkyl, 5.36), Asp165, and Thr302 (Hydrophobic)
8	Camphene	-5.2	Pro249 (Alkyl, 4.15, 4.63, 4.78, 5.41) , Tyr265 (Pi-alkyl, 4.31, 4.62; Pi-sigma, 3.56), Tyr274 (Pi-alkyl, 5.25), Asp165, and Thr302 (Hydrophobic)
9	Camphenilone	-5.2	Pro249 (Alkyl, 4.09, 4.95), Tyr265 (Pi-alkyl, 3.75), Tyr274 (Pi-alkyl, 5.50), Asp165, and Thr302 (Hydrophobic)
10	(R)-(–)-Linalool	-5.2	Not located in active site
11	(+)-α-Pinene	-5.2	Not located in active site
12	(+)-β-Pinene	-5.2	Not located in active site
13	Sabinene	-5.2	Not located in active site
14	1,8-Cineole	-5.3	Pro249 (Alkyl, 4.10, 4.72, 4.78), Tyr265 (Pi-alkyl, 4.59, 4.67) , Asp165, Pro248, Tyr274, and Thr302 (Hydrophobic)
15	1,4-Benzenediamine N,N-dimethyl	-5.3	Asp165 (Pi-anion, 3.89), Pro249 (Alkyl, 4.20; Pi-alkyl, 4.72), Tyr 265 (Pi-alkyl, 4.95, Pi-Pi T-shape, 5.03), Tyr269, Tyr269, and Thr302 (Hydrophobic)
16	Limonene	-5.3	Not located in active site
17	(-)-α-Pinene	-5.3	Pro249 (Alkyl, 4.47, 5.43), Tyr265 (Pi-alkyl, 3.52), Asp165, Pro248, and Thr302 (Hydrophobic)
18	(-)-β-Pinene	-5.3	Pro249 (Alkyl, 4.50, 5.40), Tyr265 (Pi-alkyl, 3.58), Asp165, Pro248, and Thr302 (Hydrophobic)
19	Camphor	-5.3	Pro248 (Alkyl, 4.85), Pro249 (Alkyl, 4.35, 5.22), Tyr265 (Pi-alkyl, 4.85; Pi-sigma, 3.81), Asp165, and Thr302 (Hydrophobic)

20	α-Thujene	-5.4	Pro249 (Alkyl, 4.23, 4.52), Tyr265 (Pi-alkyl, 4.62, 4.66), Asp165, and Pro248 (Hydrophobic)
21	(−)-Borneol	-5.4	Not located in active site
22	Geraniol	-5.5	Not located in active site
23	3-Carene	-5.6	Pro249 (Alkyl, 4.38, 4.68, 4.75), Tyr265 (Pi-alkyl, 4.56, 4.74, 4.98, 5.20), Tyr269, Tyr274, Thr302 Asp165, and Pro248 (Hydrophobic)
24	(−)-Cis-Carveol	-5.6	Asp165 (H-bond, 2.70), Pro249 (Alkyl, 4.49), Tyr265 (Pi-alkyl, 4.75, 5.41), Tyr274 (H-bond, 2.90), Thr302 (Hydrophobic)
25	Cis-(+)-4-Carene	-5.6	Pro249 (Alkyl, 4.48, 466, 4.78), Tyr265 (Pi-alkyl, 4.52, 4.73, 5.0, 5.21), Tyr269, Tyr274, Thr302 Asp165, and Pro248 (Hydrophobic)
26	Eugenol	-5.6	Pro249 (Alky, 4.24; Pi-alkyl, 4.71), Tyr265 (Pi-Pi T-shaped, 4.78), Tyr269, Thr302, and Asp165 (Hydrophobic)
27	(R)-(+)-Verbenone	-5.6	Pro248 (Alkyl, 4.48), Pro249 (Alkyl, 4.85, 4.92), Tyr265 (Pi-alkyl, 4.82), Thr302, and Asp165 (Hydrophobic)
28	Thymol methyl ether	-5.6	Not located in active site
29	(+)-Trans-Carveol	-5.7	Pro249 (Alkyl, 4.32, 5.07), Tyr265 (Pi-alkyl, 4.61, 4.96, 5.18), Tyr269, Thr302, and Asp165 (Hydrophobic)
30	(-)-α-Thujone	-5.7	Pro249 (Alkyl, 4.58, 4.78, 4.82), Tyr265 (Pi-alkyl, 4.32; Pi-sigma, 3.52), Tyr269, Tyr274, Thr302, Asp165, and Pro248 (Hydrophobic)
٣1	Methyl eugenol	-5.7	Not located in active site
32	(1S)-(-)-Verbenone	-5.7	Pro249 (Alkyl, 4.15, 4.40), Tyr265 (Pi-alkyl, 4.61; Pi-sigma, 3.79), Thr302, and Asp165 (Hydrophobic)
33	α-Terpinene	-5.8	Not located in active site
34	Cis-Sabinene hydrate	-5.8	Pro249 (Alkyl, 4.75, 4.85, 5.35), Tyr265 (Pi-alkyl, 4.33, 5.28; Pi-sigma, 3.56), Tyr274 (Pi-alkyl, 5.31), Tyr269, Thr302, Asp165, and Pro248 (Hydrophobic)
35	Terpinolene	-5.8	Not located in active site
36	α-Phellandrene	-5.9	Not located in active site
37	γ-Terpinene	-5.9	Not located in active site
38	p-Cymen-8-ol	-5.9	Not located in active site
39	Terpinen-4-ol	-5.9	Pro249 (Alkyl, 4.16, 4.45), Tyr265 (Pi-alkyl, 4.44; Pi-sigma, 3.74), Thr302, and Pro248 (Hydrophobic)
40	Thymol	-5.9	Not located in active site

41	Carvacrol methyl ether	-6.0	Not located in active site
42	p-Cymene	-6.0	Not located in active site
43	Carvacryl acetate	-6.1	Not located in active site
44	l-Bornyl acetate	-6.1	Pro249 (Alkyl, 4.75, 5.05), Tyr265 (Pi-alkyl, 4.48, 4.70), Tyr269, Tyr274, and Asp165 (Hydrophobic)
45	Terpineol	-6.2	Asp165 (H-bond, 3.01), Pro249 (Alkyl, 4.19, 4.61), Tyr265 (Pi-alkyl, 4.47; Pi-sigma, 3.70), Thr302 (Hydrophobic)
46	Germacrene D	-6.4	Not located in active site
47	α-Cadinene	-6.4	Not located in active site
48	α-Elemene	-6.5	Pro249 (Alkyl, 4.21, 4.43, 5.23), Tyr265 (Pi-alkyl, 4.37; Pi-sigma, 3.54), Tyr274, Thr302, and Asp165 (Hydrophobic)
49	Copaene	-6.5	Pro249 (Alkyl, 3.92), Tyr265 (Pi-alkyl, 4.05, 5.22; Pi-sigma, 3.50), Tyr269, Tyr274, Thr302, and Asp165 (Hydrophobic)
50	Bicyclogermacrene	-6.6	No locate in binding site
51	(-)-Spathulenol	-6.7	Pro249 (Alkyl, 4.70, 5.37), Tyr265 (Pi-alkyl, 5.01, 5.44), Tyr269, Thr302, and Asp165, Pro248 (Hydrophobic)
52	(+)-Aromadendrene	-6.8	Not located in active site
53	(-)-β-Caryophyllene oxide	-6.9	Not located in active site
54	(-)-β-Bourbonene	-6.9	Pro249 (Alkyl, 4.39, 5.37), Tyr265 (Pi-alkyl, 4.75, 5.19; Pi-sigma, 3.69), Tyr269, Tyr274, Thr302, and Asp165 (Hydrophobic)
55	(-)-β-Caryophyllene	-6.9	Not located in active site
56	(+)-δ-Cadinene	-6.9	Not located in active site
57	Viridiflorol	-6.9	Not located in active site
58	(+)-Spathulenol	-7.0	Asp165 (H-bond, 2.99), Pro249 (Alkyl, 4.0, 5.42), Tyr265 (Pi-alkyl, 4.02), Tyr274 (H-bond, 2.45)
59	α-Humulene	-7.1	Pro249 (Alkyl, 4.22, 4.53), Tyr265 (Pi-alkyl, 4.66),Tyr269, Tyr274, Thr302, and Asp165 (Hydrophobic)
60	α-Gurjunene	-7.1	Not located in active site

Table S3. The results obtained from docking of thyme compounds with main protease (PDB ID: 6LU7)

No	Compound	Binding affinity (kcal/mol)	Involved receptor residues (interaction type and distance Å)
1	(R)-(-)-1-Octen-3-ol	-3.7	Cys145 (H-bond, 3.12, 3.26), Leu141 (H-bond, 2.83), Gly143, Asn142, Glu166, Met165, Phe140, and His163 (Hydrophobic)
2	(3S)-Oct-1-en-3-ol	-3.7	Thr190 (H-bond, 2.71, 3.34), Gln192 (H-bond, 3.07), Met165 (Alkyl, 4.77), Pro168 (Alkyl, 4.15), Glu166, and Gln189 (Hydrophobic)
3	Geraniol	-3.9	His163 (H-bond, 3.02), Gln189, Met165 (Alkyl, 4.02, 4.46), Glu166, and Thr190 (Hydrophobic)
4	(−)-Cis-Carveol	-4.1	Cys145 (Alkyl, 4.25), Asn142 (H-bond, 3.02), Leu141, Glu166, Met165, Gly143, and His163 (Hydrophobic)
5	(S)-(+)-Linalool	-4.1	Not located in active site
6	β-Myrcene	-4.1	Not located in active site
7	Tricyclene	-4.1	Not located in active site
8	1,8-Cineole	-4.2	Phe140, His164, Met165, Glu166, Leu141, Gly143, and Asn142 (Hydrophobic), Cys145 (Alkyl, 4.26, 5.42)
9	Camphene	-4.2	Not located in active site
10	(R)-(–)-Linalool	-4.2	Met165 (Alkyl, 4.44), Cys145 (Alkyl, 4.43), Met49 (Alkyl , 3.86, 5.14, 5.26), His41 (Pi-alkyl, 4.12, 4.39, 4.56, 4.64), Asp187, His164, and Gln189 (Hydrophobic)
11	(-)-α-Pinene	-4.2	Not located in active site
12	(+)-Borneol	-4.2	Leu141 (H-bond, 2.96), Gly143 (H-bond, 3.34), Cys145 (Alkyl, 4.34), His163 (Pi-alkyl, 4.28), Asn142, Met165, and Glu166 (Hydrophobic)
13	Cis-(+)-4-Carene	-4.3	Not located in active site
14	(-)-β-Pinene	-4.3	Not located in active site
15	(+)-β-Pinene	-4.3	Not located in active site
16	(−)-Borneol	-4.3	Asn142 (H-bond, 2.70), Cys145 (Alkyl, 4.60, 4.74), His163 (Pi-alkyl, 5.45), Met165, Glu166, Leu141, and His164 (Hydrophobic)
17	α-Thujene	-4.4	Not located in active site
18	Camphenilone	-4.4	Cys145 (Alkyl, 5.19; H-bond, 3.31), Gly143 (H-bond, 2.92), Leu141, His163, His164, Met165, and Asn142 (Hydrophobic)
19	(+)-Trans-Carveol	-4.4	Not located in active site

20	Sabinene	-4.4	Not located in active site
21	(Z)-β-Ocimene	-4.4	Not located in active site
22	3-Carene	-4.5	Met165 (Alkyl, 4.49, 5.44), Met49 (Alkyl, 3.98, 4.80, 5.28), His41 (Pi-alkyl, 4.20, 4.52), His164, Gln189, Asp187, and Tyr54 (Hydrophobic)
23	Limonene	-4.5	Not located in active site
24	(+)-α-Pinene	-4.5	Not located in active site
25	(-)-α-Thujone	-4.5	Phe140, Glu166, His172, Asn142, Leu141, Met165, and His164 (Hydrophobic), His163 (H-bond, 3.04)
26	Camphor	-4.5	Glu166 (H-bond, 2.94), His164, His163, Leu141, Gly143, Asn142, and Met165 (Hydrophobic)
27	p-Cymene	-4.5	His41 (Pi-alkyl, 4.08), Met165 (Alkyl, 4.52, Pi-Alkyl at 4.53), Asp187, His164, Gln189, and Glu166 (Hydrophobic)
28	(R)-(+)-Verbenone	-4.5	His163 (H-bond, 3.09), Asn142, Leu141, Gly143, Met165, Glu166, Cys145, and His164 (Hydrophobic)
29	α-Terpinene	-4.6	Met165 (Alky, 4.39, 4.51), His41 (Pi-alkyl, 4.08), Asp187, His164, Gln189, and Glu166 (Hydrophobic)
30	Carvacrol methyl ether	-4.6	Not located in active site
٣1	γ-Terpinene	-4.6	Not located in active site
32	Methyl eugenol	-4.6	Not located in active site
33	Thymol methyl ether	-4.6	Asp187, His164, and Gln189 (Hydrophobic), Met165 (Alky, 5.22; Pi-alky, 4.88), His41 (Pi-alky, 4.16, 4.42)
34	1,4-Benzenediamine N,N-dimethyl	-4.7	Leu141 (H-bond, 2.80), Met165 (Alkyl, 5.33), Glu166 (H-bond, 3.16), Cys145 (Pi-alky, 4.91), His163, Asn142, and Gly143 (Hydrophobic)
35	α-phellandrene	-4.7	Not located in active site
36	Terpinen-4-ol	-4.7	His172, Glu166, Phe140, Asn142, His164, and Met165 (Hydrophobic), Cys145 (Alky, 4.45, 4.78), Leu141 (H-bond, 3.07), His163 (H-bond, 3.33)
37	α-Elemene	-4.8	Met49 (Alkyl, 4.91), His41 (Pi-alkyl, 4.36, 4.85), Cys145 (Alkyl, 3.89, 4.81), His163 (Pi-alkyl, 4.48), Glu166, Met165, Leu141, Phe140, Asn142, and Gly143 (Hydrophobic)
38	(1S)-(-)-Verbenone	-4.8	Met165 (Alkyl, 3.95, 5.24), Met49 (Alkyl, 3.75, 4.71), His41 (Pi-alkyl, 4.55), His164, Gln189, and Asp187 (Hydrophobic)
39	Terpineol	-4.8	Not located in active site
40	Eugenol	-4.9	Leu141 (H-bond, 2.71), Cys145 (H-bond, 3.21), Met165 (Alkyl, 5.09), Gly143 (H-bond, 3.02), His163 (Pi-alkyl, 4.60; H-bond, 3.04), Asn142, Gln189, His165, and Phe140 (Hydrophobic)
41	Germacrene D	-4.9	His163 (Pi-alkyl, 4.82), Met165 (Alkyl, 4.98), Cys145 (Alkyl, 4.91), Gln189, Met49, His164, Gly143, Asn142, and Leu141 (Hydrophobic)

42	l-Bornyl acetate	-4.9	His41 (H-bond, 3.16), Cys145 (Alkyl, 3.91), His164, Met49, and Gly143 (Hydrophobic)
43	Terpinolene	-4.9	Not located in active site
44	α-Humulene	-5.0	Met49 (Alkyl, 3.50), His41 (Pi-sigma, 3.97), Cys145 (Alkyl, 5.07), Met165 (Alkyl, 4.68), His164, Gln189, Asn142, and Glu166 (Hydrophobic)
45	Cis-Sabinene hydrate	-5.0	Thr190 (H-bond, 2.71, 3.13), Gln192 (H-bond, 3.14), Pro168 (Alkyl, 4.53), Leu167 (Alkyl, 4.87), Met165 (Alkyl, 4.07, 5.06, 5.17), Gln189, and Glu166 (Hydrophobic)
46	(-)-β-Caryophyllene	-5.0	Cys145 (Alkyl, 3.93, 4.33, 4.80, 5.34), Met49 (Alkyl, 4.30), His41 (Pi-alkyl, 4.31, 5.05), Gly143, Leu141, Met165, Asn142, His164, and Gln189 (Hydrophobic)
47	p-Cymen-8-ol	-5.0	Not located in active site
48	Thymol	-5.0	Not located in active site
49	(-)-β-Bourbonene	-5.1	Met165 (Alkyl, 5.08), Cys145 (Alkyl, 4.59, 5.10), Gly143, Phe140, Leu141, Gly166, Met49, His164, Gln189, and Asn142 (Hydrophobic)
50	Carvacryl acetate	-5.2	Met165 (Alkyl, 4.69; Pi-alkyl at 4.59), His164, His41, Asp187, Gln189, and Glu166 (Hydrophobic)
51	α-Cadinene	-5.2	Not located in active site
52	α-Gurjunene	-5.2	Asn142 (Hydrophobic), Leu141 (Alkyl, 4.66, 4.92)
53	(-)-β-Caryophyllene oxide	-5.3	Met49 (Alkyl, 4.34), His41 (Pi-alkyl, 4.17, 5.04), Cys145 (Alkyl, 4.0, 4.36, 4.67, 5.28), Leu141, Asn142, Met165, His164, Gln189, and Gly143 (Hydrophobic)
54	(+)-Aromadendrene	-5.3	Not located in active site
55	Copaene	-5.4	Not located in active site
56	Bicyclogermacrene	-5.5	Leu141, Asn142, Met49, and His41 (Hydrophobic), Cys145 (Alkyl, 3.95, 4.55, 4.83, 5.44)
57	(+)-δ-Cadinene	-5.5	His41 (Pi-alkyl, 4.06), Met49 (Alkyl, 3.68), Met165 (Alkyl, 4.91), His164, Glu166, and Gln189 (Hydrophobic)
58	(+)-Spathulenol	-5.5	Met49 (Alkyl, 4.74, 5.35), Cys145 (Alkyl, 4.25, 5.48, 5.49), His41 (Pi-alkyl, 4.76, 4.82), Met165 (Alkyl, 5.30), Asn142 (H-bond, 2.73), His164, Gln189, Leu141, Glu166, and Gly143 (Hydrophobic)
59	Viridiflorol	-5.5	Cys145 (H-bond, 2.57), Met165 (Alkyl, 5.47), Met49 (Alkyl, 4.78, 5.19), His41 (Pi-alkyl, 4.69), His163 (H-bond, 2.70), Glu166, His164, Gln189, Gly143, Asn142, and Leu141 (Hydrophobic)
60	(-)-Spathulenol	-5.6	Glu166 (H-bond, 2.28), His41 (Pi-alkyl, 4.41, 5.05), Cys145 (Alkyl, 5.06), Gln189, Asn142, and His164(Hydrophobic), Met165 (Alkyl, 4.02), Met49 (Alkyl, 5.44)