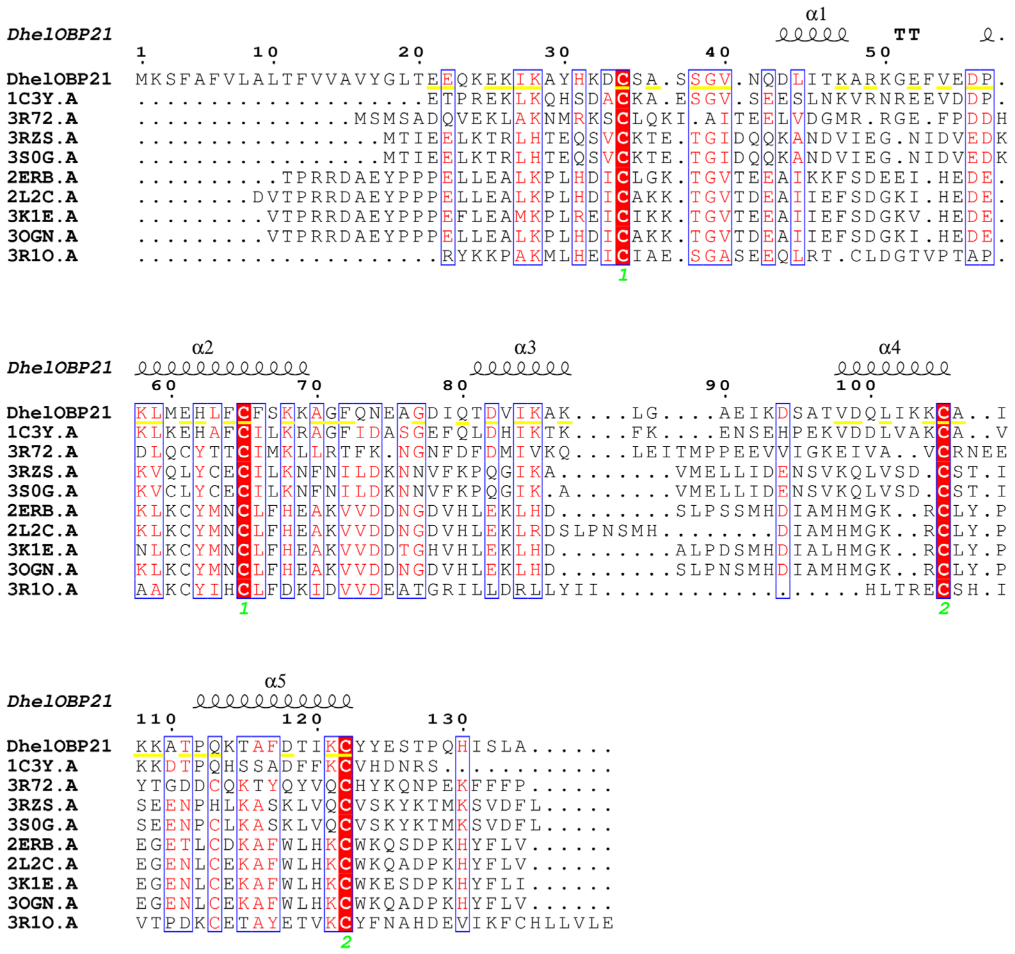
Figure S1. Sequence alignment of DhelOBP21 with homologous proteins. The yellow lines sign the same amino acid residues of DhelOBP21and 1C3Y.

Figure S2. The Ramachandran map of the model of DhelOBP21. The scope of orange dashed line expresses the allowed region. The scope of green dashed line expresses the core region. The yellow square means the amino acid located within the allowed region. The green square means the amino acid located within the core region. The red cross means the amino acid that is outlier.

Figure S3. Comparison of orientations for specific ligands in the binding pocket from the four proteins. The green pockets express the binding sites. The green areas express hydrophobicity and red areas express hydrophilia of binding cavity. The red atom is oxygen atom. The blue atom is nitrogen atom. The gray molecule in the cavity is ligand.

Figure S4. The different protonated states at different pH. (A) There are three residues at N–terminal base shown the transformation of protonated states. The green residue is His31. The blue residue is Ser35 and the yellow residue is His62. (B, C) The different protonated states of His31, Ser35 and His62 at pH 7.4 and 5.0. The red atom is oxygen atom. The blue atom is nitrogen-atoms. The light gray atom is hydrogen atom and the dark grey atom is carbon atom.

Figure S1



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DhelOBP21
              1        10        20        30        40        50
DhelOBP21     MKSFAFVLALTFVVAVYGLTEEQKEKIKAYHKDCSA.SSGV.NQDLITKARKGEFVEDP.
1C3Y.A        ....................ETPREKLKQHSDACKA.ESGV.SEESLNKVRNREEVDDP.
3R72.A        ...............MSMSADQVEKLAKNMRKSCLQKI.AITEELVDGMR.RGE.FPDDH
3RZS.A        .................MTIEELKTRLHTEQSVCKTE.TGIDQQKANDVIEG.NIDVEDK
3S0G.A        .................MTIEELKTRLHTEQSVCKTE.TGIDQQKANDVIEG.NIDVEDK
2ERB.A        ..........TPRRDAEYPPPELLEALKPLHDICLGK.TGVTEEAIKKFSDEEI.HEDE.
2L2C.A        ........DVTPRRDAEYPPPELLEALKPLHDICAKK.TGVTDEAIIEFSDGKI.HEDE.
3K1E.A        .........VTPRRDAEYPPPEFLEAMKPLREICIKK.TGVTEEAIIEFSDGKV.HEDE.
3OGN.A        .........VTPRRDAEYPPPELLEALKPLHDICAKK.TGVTDEAIIEFSDGKI.HEDE.
3R1O.A        .....................RYKKPAKMLHEICIAE.SGASEEQLRT.CLDGTVPTAP.

DhelOBP21
                60        70        80        90        100
DhelOBP21     KLMEHLFCFSKKAGFQNEAGDIQTDVIKAK....LG....AEIKDSATVDQLIKKCA..I
1C3Y.A        KLKEHAFCILKRAGFIDASGEFQLDHIKTK....FK....ENSEHPEKVDDLVAKCA..V
3R72.A        DLQCYTTCIMKLLRTFK.NGNFDFDMIVKQ....LEITMPPEEVVIGKEIVA..VCRNEE
3RZS.A        KVQLYCECILKNFNILDKNNVFKPQGIKA........VMELLIDENSVKQLVSD.CST.I
3S0G.A        KVCLYCECILKNFNILDKNNVFKPQGIK.A.......VMELLIDENSVKQLVSD.CST.I
2ERB.A        KLKCYMNCLFHEAKVVDDNGDVHLEKLHD........SLPSSMHDIAMHMGK..RCLY.P
2L2C.A        KLKCYMNCLFHEAKVVDDNGDVHLEKLRDSLPNSMH........DIAMHMGK..RCLY.P
3K1E.A        NLKCYMNCLFHEAKVVDDTGHVHLEKLHD........ALPDSMHDIALHMGK..RCLY.P
3OGN.A        KLKCYMNCLFHEAKVVDDNGDVHLEKLHD........SLPNSMHDIAMHMGK..RCLY.P
3R1O.A        AAKCYIHCLFDKIDVVDEATGRILLDRLLYII..................HLTRECSH.I

DhelOBP21
              110       120       130
DhelOBP21     KKATPQKTAFDTIKCYYESTPQHISLA......
1C3Y.A        KKDTPQHSSADFFKCVHDNRS............
3R72.A        YTGDDCQKTYQYVQCHYKQNPEKFFFP......
3RZS.A        SEENPHLKASKLVQCVSKYKTMKSVDFL.....
3S0G.A        SEENPCLKASKLVQCVSKYKTMKSVDFL.....
2ERB.A        EGETLCDKAFWLHKCWKQSDPKHYFLV......
2L2C.A        EGENLCEKAFWLHKCWKQADPKHYFLV......
3K1E.A        EGENLCEKAFWLHKCWKESDPKHYFLI......
3OGN.A        EGENLCEKAFWLHKCWKQADPKHYFLV......
3R1O.A        VTPDKCETAYETVKCYFNAHDEVIKFCHLLVLE
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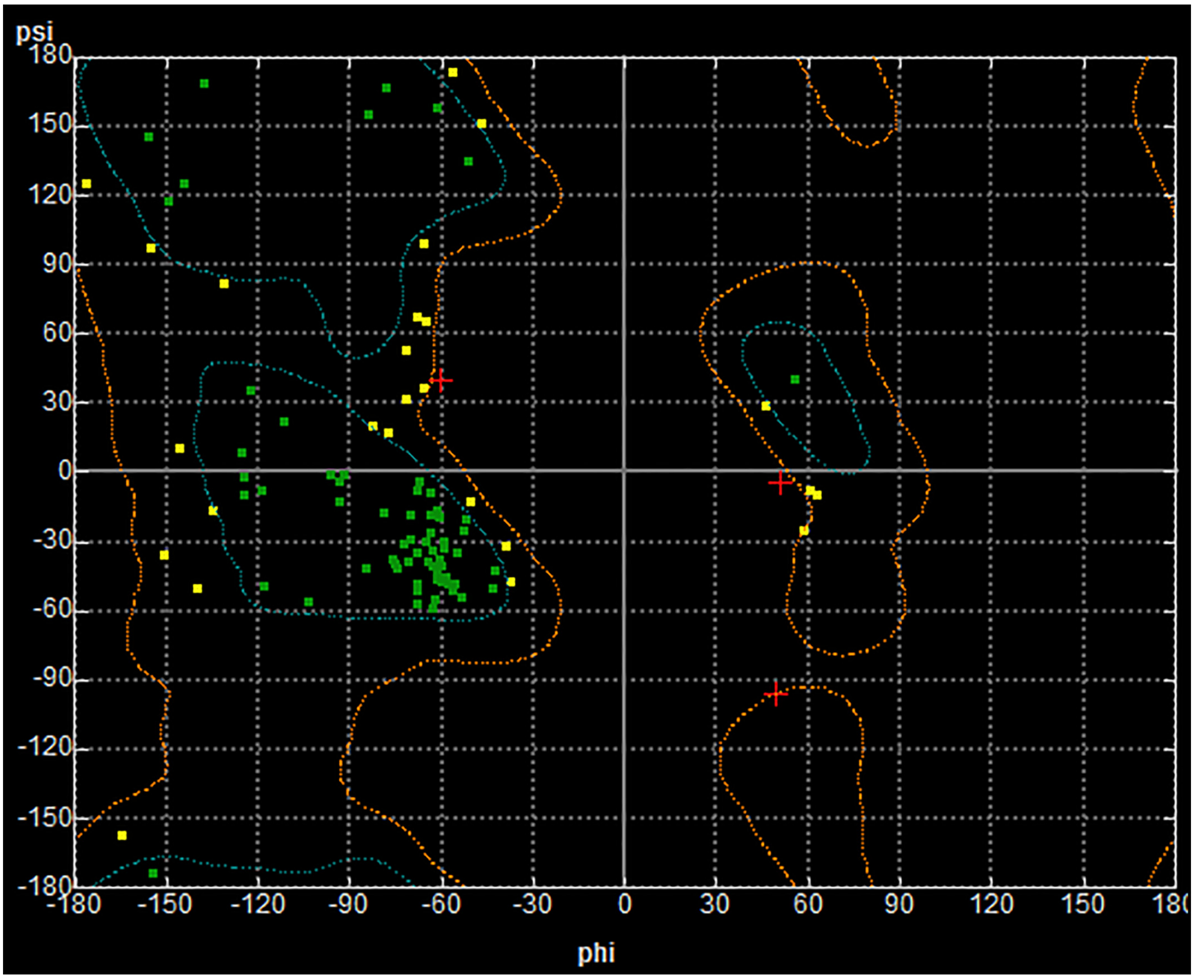
Figure S2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90
60
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0
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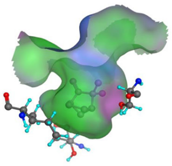
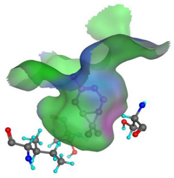
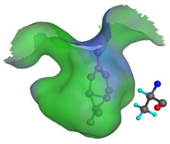
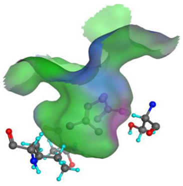
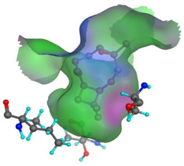
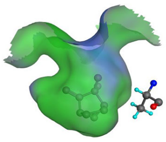
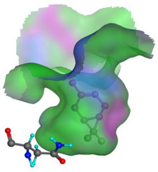
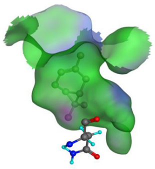
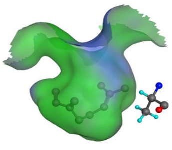
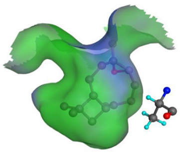
-60
-90
-120
-150
-180
-180
-150
-120
-90
-60
-30
0
30
60
90
120
150
180
phi

Figure S3

Camphene	3-Canene		Myrcene	(-)-Caryophyllene oxide
WT	WT	S67A	WT	WT
				
S67A	I84N	T119N	S67A	S67A
				

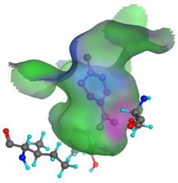
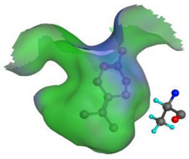
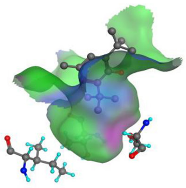
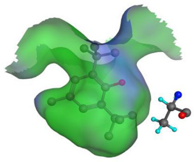
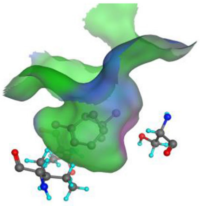
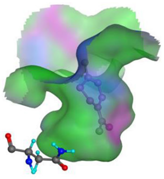
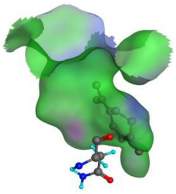
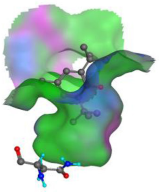
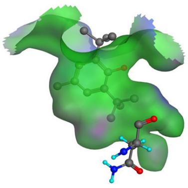
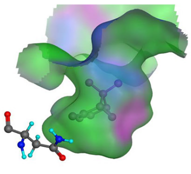
Terpinolene		Butylated hydroxytoluene		(+)-α-Pinene
WT	S67A	WT	S67A	WT
				
I84N	T119N	I84N	T119N	I84N
				

Figure S4