Supplementary Material

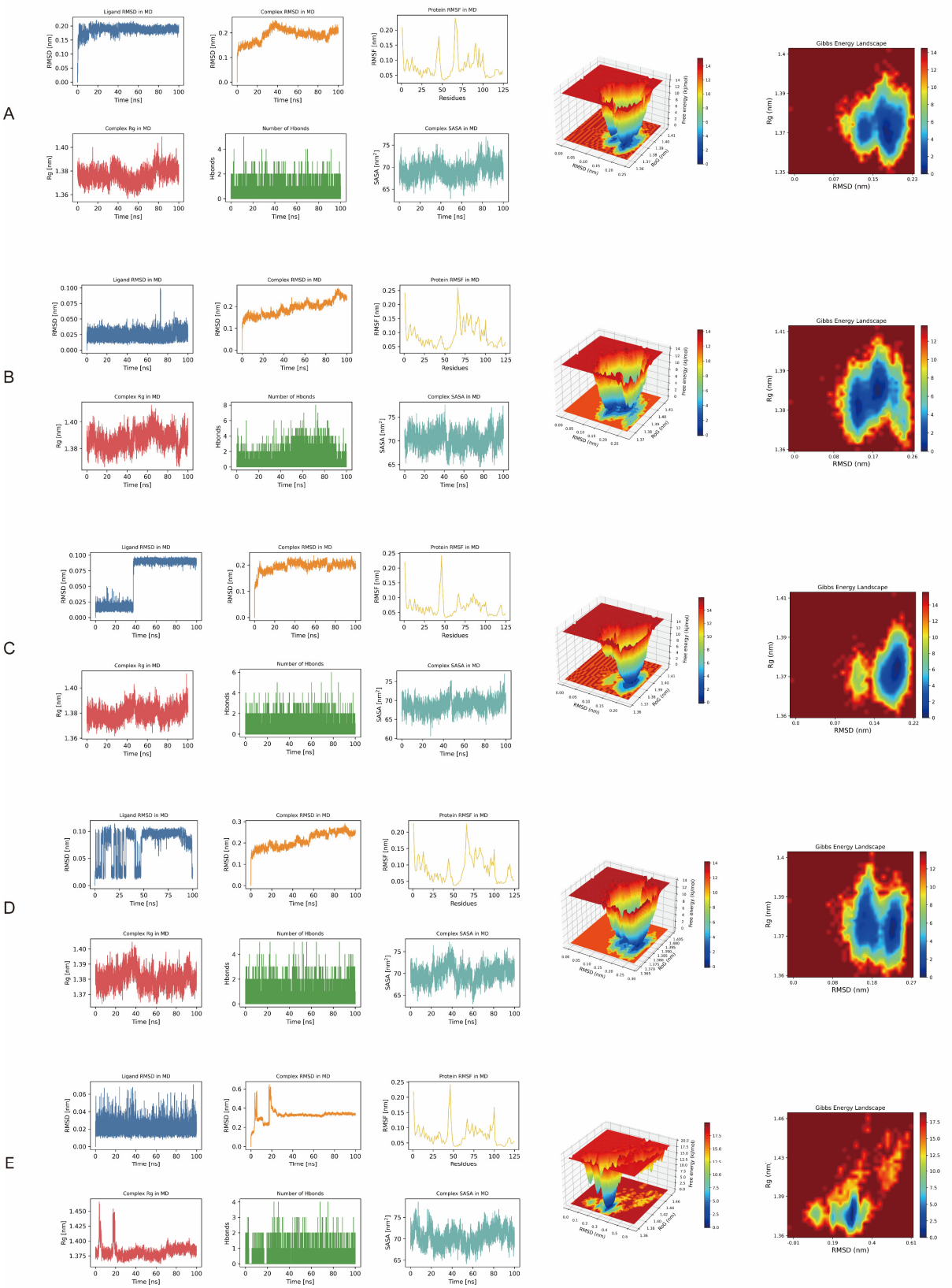


Figure S1. Molecular dynamics (MD) simulation trajectories and 3D free energy landscapes of the five tested compounds complexed with the target protein over 100 ns. (A) DEET, (B) δ-cadinene, (C) α-copaene, (D) α-calacorene, and (E) humulene. For each compound, the subplots show the Ligand RMSD, Complex RMSD,

Protein RMSF, Complex R_g, number of hydrogen bonds, Complex SASA, and the 3D Gibbs free energy landscape (from left to right).

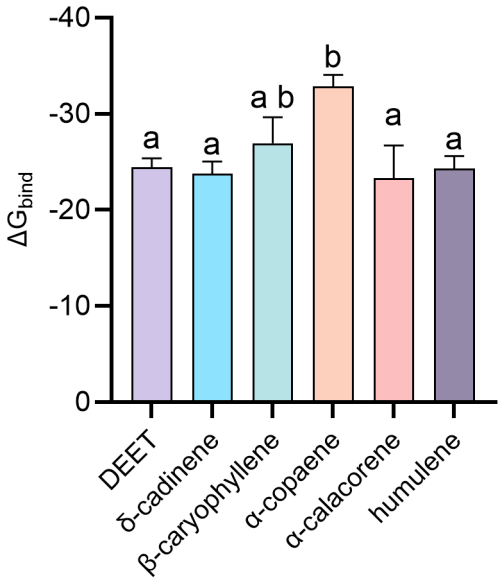


Figure S2. Comparison of the binding free energies (ΔG_{bind}) for DEET and the five candidate compounds complexed with AaegOBP1, calculated using the MM-GBSA method. The binding energy of each complex is presented as the mean ± standard deviation. Different lowercase letters (a, b, ab) above the bars indicate statistically significant differences among the groups ($p < 0.05$), demonstrating distinct binding affinities.

Table S1. Binding free energies and energy components of AaegOBP1-ligand complexes calculated by MM/GBSA (kcal/mol).

Ligand	ΔE_{vdw}	ΔE_{elec}	ΔG_{GB}	ΔG_{SA}	ΔG_{bind}
DEET	-31.48±1.46	-7.82±1.88	18.66±1.94	-3.78±0.14	-24.43±0.95
δ-cadinene	-30.51±1.10	-0.51±0.61	10.90±0.26	-3.67±0.17	-23.79±1.27
β-caryophyllene	-29.56±2.28	-0.75±0.25	7.06±0.89	-3.70±0.21	-26.96±2.69
α-copaene	-36.61±1.74	0.04±0.08	7.67±0.71	-3.95±0.10	-32.84±1.20
α-calacorene	-27.37±2.16	-1.40±0.36	9.07±1.48	-3.62±0.29	-23.32±3.40
humulene	-27.69±1.51	-0.71±0.30	7.33±0.52	-3.25±0.13	-24.32±1.29

Table S2. Primers used for RT-qPCR verification of differentially expressed genes.

Short Name	Full ID	Primer Sequence (5'→3')	Amplicon Size (bp)
LOC-9074	LOC109399074	F: ACAGTGCTTGTGCTGCCCAT R: TACACCTCGCTCAGTTCCGG	96
LOC-3088	LOC109403088	F: TTAATGGACGAAGAATGGGA R: TTTTTGGTTAGGTCAGGGGT	80
LOC-8353	LOC115268353	F: TCTAGCCCTGGCCGTTGTGT R: TCCTGCAGCTCGTCGATGTG	102
LOC-5025	LOC115265025	F: CGATTCACACTAACCCCTCT R: CTGTTGTTCCATATCAGCCA	114
LOC-1575	LOC109401575	F: TTCCATCGCTTCCGTCGTAG R: CATCTCGTTCAGCCCCAGTT	126
LOC-4581	LOC115264581	F: TACGAAAAGGCACACAGGAT R: TGAACGGACAGGAAACAAAT	100
LOC-4219	LOC109424219	F: AACTTCTGCCTGAACTCTCC R: CTCCTTGATTTGAACCTCGT	104
LOC-5824	LOC115255824	F: AAGTTGCTCATCGCCCAAAT R: GATCCTCACTCAAGTCCTCC	88
LOC-9970	LOC115269970	F: GTCAAGACTGCCGAACCTCA R: CCCACAAAACGAACACCAAA	146
LOC-1286	LOC109411286	F: CGACAGACCTAACCGTTCAA R: CTCCCGATACTCCAGAGACA	126
LOC-1045	LOC109411045	F: GGGCTTGAAGGGAGAATACG R: GTGACAATGGCGGTGGACAG	96
LOC-9797	LOC115259797	F: GAAATGGAGTCAACGCAACA R: TCAGATAAGCAGACAACGGG	132
β-Actin	LOC115253654	F: GAAGATGGGACCATCGCAGT R: CTGCGCGTTTCAAGATGAGAG R: CTGCGCGTTTCAAGATGAGAG	194

F: indicates the forward primer; R: indicates the reverse primer. β-Actin was used as the internal reference gene (endogenous control) for normalization.