Electronic Supplementary Material (ESI) for Molecular Systems Design & Engineering.


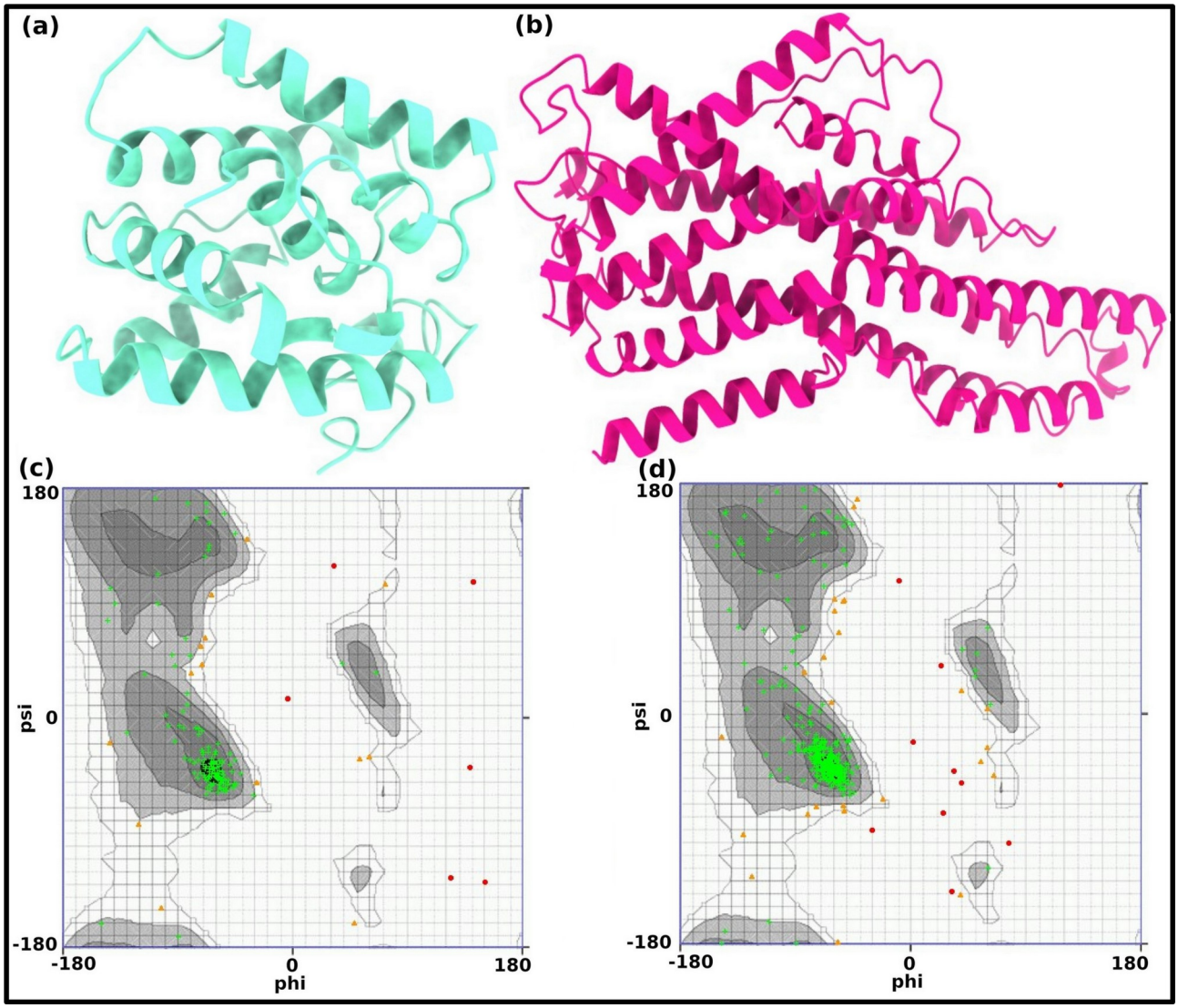


**Figure S1.** 3D structure of modeled proteins with their Ramachandran plots (a, c) OBP1, (b, d) OR1 generated by Zlab server.

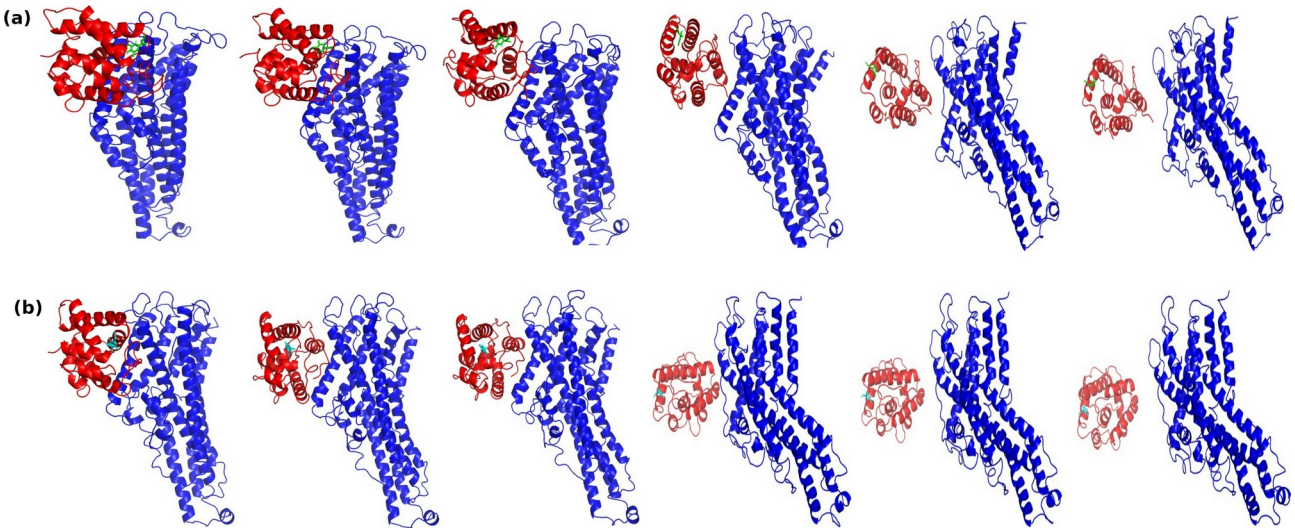


**Figure S2.** Different time interval snapshots from steered molecular dynamics analysis after applying an external pulling force, illustrating the position of the ligand in the active site throughout the simulation. (a) depicts the OBP1-Ethyl gallate (as ligand) and OR1 (receptor) complex, while (b) shows the OBP1-Methyl gallate (as ligand) and OR1 (receptor) complex.

**Table S1.** List of interaction energy generated from molecular docking analysis for the selected molecules.

| S. No. | Protein-ligand complexes | CDOCKER Interaction energy (kcal/mol) |
|---|---|---|
| **1** | **Quercetin** | **-24.7** |
| **2** | Kaempferol | -20.9 |
| **3** | IsoQuercetin | 83.35 |
| **4** | Catechin | -21.88 |
| **5** | Fraxetin | -22.38 |
| **6** | Etyhlbrovioflinecarbo | -14.31 |
| **7** | Ellagic acid | -23.24 |
| **8** | **Ethyl gallate** | **-33.72** |
| **9** | 6-O-galloyl | -23.11 |
| **10** | **Methyl gallate** | **-30.98** |
| **11** | **Gallic acid** | **-27.7** |
| **12** | Blumenol C | 750.9 |
| **13** | Beta-D-glucose | 6.45 |
| **14** | 2-formyl | -23.9 |
| **15** | Shikimic acid | 10.84 |
| **16** | 1-Naphthalenamine | 8.21 |

**Table S2.** The mean and standard deviation of the various structural aspects of MD simulations analysis.

| | Mean | | | | Standard Deviation | | | |
|---|---|---|---|---|---|---|---|---|
| **Complexes** | **H-BOND** | **RMSD** | **RMSF** | **Rg** | **H-BOND** | **RMSD** | **RMSF** | **Rg** |
| **OR1-OBP1** | 7.045 | 0.641 | 0.223 | 2.953 | 2.29 | 0.047 | 0.814 | 0.436 |
| **Ethyl gallate** | 7.781 | 0.951 | 0.182 | 2.878 | 2.419 | 0.142 | 0.634 | 0.278 |
| **Methyl gallate** | 10.333 | 0.686 | 0.170 | 2.885 | 2.744 | 0.051 | 0.674 | 0.272 |
| **Gallic acid** | 9.949 | 0.729 | 0.192 | 2.888 | 2.186 | 0.070 | 0.744 | 0.318 |
| **Quercetin** | 7.062 | 0.724 | 0.177 | 2.937 | 2.178 | 0.747 | 0.814 | 0.233 |

**Table S3.** List of protein-protein binding free energy components computed using MM-PBSA approach during the course of MD simulations.

| Protein-protein complex | ΔE Van der Waal (kJ/mol) | SASA (kJ/ mol) | ΔE Electrostatic (kJ/mol) | ΔE polar solvation (kJ/mol) | ΔE binding (kJ/mol) |
|---|---|---|---|---|---|
| **OR1-OBP1** | -513.521 | -48.850 | -1648.728 | 803.541 | -1407.557 |

**Table S4.** List of protein-ligand binding free energy components calculated using MM-PBSA approach.

| Protein-ligand complexes | ΔE Van der Waal (kJ/mol) | SASA (kJ/mol) | ΔE Electrostatic (kJ/mol) | ΔE polar solvation (kJ/mol) | ΔE binding (kJ/mol) |
|---|---|---|---|---|---|
| **OBP1-ethyl gallate** | -4.564 | -7.315 | -0.760 | 3.491 | -9.148 |
| **OBP1-gallic acid** | -6.201 | 1.073 | 222.392 | -5.199 | 212.066 |
| **OBP1-methyl gallate** | -41.548 | -10.899 | -7.211 | 8.008 | -51.650 |
| **OBP1-Quercetin** | -211.298 | -24.947 | -29.909 | 69.622 | -196.531 |

**Table S5.** List of protein and protein-ligand binding free energy components computed using MM-PBSA technique.

| Protein and Protein-ligand complexes | ΔE Van der Waal (kJ/mol) | SASA (kJ/mol) | ΔE Electrostatic (kJ/mol) | ΔE polar solvation (kJ/mol) | ΔE binding (kJ/mol) |
|---|---|---|---|---|---|
| **OR1-OBP1-ethyl gallate** | -794.872 | -71.779 | -2753.941 | 1341.120 | -2279.473 |
| **OR1-OBP1-methyl gallate** | -722.028 | -66.748 | -2433.139 | 1364.526 | -1857.390 |
| **OR1-OBP1-Quercetin** | -753.777 | -67.388 | -2217.591 | 1109.712 | -1929.045 |

**Table S6.** Antifeedant activities of compounds against *P. xylostella.*

| Feeding deterrence | | | | | |
|---|---|---|---|---|---|
| **Compounds** | **$DC_{50}$ (mg $L^{-1}$)** | **Confidence limits (mg $L^{-1}$)** | **Slope ± SE** | **Chi square** | **p value** |
| **Ethyl gallate** | 865.88 | 663.35 – 1111.86 | 1.06 ± 0.14 | 3.22 | 0.36 |
| **Methyl gallate** | 648.92 | 328.62 – 1020.13 | 0.57 ± 0.13 | 0.65 | 0.88 |
| ***Neembaan (Azadirachtin 0.15% EC)** | 949.17 | 758.78 – 1181.52 | 1.23 ± 0.14 | 1.90 | 0.59 |
| **Growth inhibition** | | | | | |
| | **$IC_{50}$ (mg $L^{-1}$)** | **Confidence limits (mg $L^{-1}$)** | **Slope ± SE** | **Chi square** | **p value** |
| **Ethyl gallate** | 1103.72 | 808.62 – 1535.85 | 0.86 ± 0.14 | 0.79 | 0.85 |
| **Methyl gallate** | 991.29 | 801.43 – 1224.79 | 1.29 ± 0.14 | 0.42 | 0.94 |
| ***Neembaan (Azadirachtin 0.15% EC)** | 901.67 | 722.61 – 1115.05 | 1.27 ± 0.14 | 1.07 | 0.78 |

$DC_{50}$= Deterrence concentration to deter 50% of test population;
$IC_{50}$= Inhibition concentration to inhibit 50% of test population;
* The commercially available botanical insecticide (Neembaan®) in the market for the control of *P. xylostella* on cruciferous crops under field conditions was used as positive control for comparison.