**Supplementary File 3**

Complete results of docking simulation experiments. When more binding energy and predicted Ki values are reported, they refer to alternative binding sites detected.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Protein | Ligand | Mean  Binding energy (kcal/mol) | Lowest  Binding  Energy  (kcal/mol) | Number in cluster | Predicted Ki | Binding  Pocket a |
| TPL-LIKE | β-caryophyllene | -6.16 | -6.20 | 17 | 28.46 μM | groove (3)-chain A |
| -6.02 | -6.04 | 31 | 37.50 μM | groove (3)- chain B |
| isoprene | -3.39 | -3.46 | 46 | 2.92 mM | Near groove (3) –chain A |
| -3.41 | -3.45 | 25 | 2.95mM | Near groove (3) –chain B |
| -2.99 | -3.04 | 16 | 5.94mM | groove (3)- chain A |
| α-pinene | -5.06 | -5.13 | 68 | 173.00 μM | groove (3)- chain B |
| limonene | -4.76 | -4.78 | 25 | 311.41 μM | Near groove (3) –chain A |
| -4.76 | -4.78 | 32 | 356.48 μM | LisH-CRA |
| -4.53 | -4.71 | 33 | 354.67 μM | groove (3)-chain A |
| linalool | -3.94 | -4.35 | 16 | 642.79 μM | groove (3)- chain B |
| -3.76 | -4.13 | 8 | 945.79 μM | groove (3)-chain A |
| -myrcene | -3.95 | -4.19 | 17 | 855.72 μM | groove (3)- chain B |
| -3.76 | -4.00 | 22 | 1.17 mM | LisH-CRA |
| -3.77 | -4.03 | 24 | 1.10 mM | groove (3)- chain B |
| 4DSB\_A  (ABA RECEPTOR) | ABA | -7.26 | -7.72 | 61 | 2.10 μM | Canonical ABA pocket |
| β-caryophyllene | -6.32 | -6.33 | 43 | 22.86 μM | Canonical ABA pocket |
| isoprene | -3.35 | -3.42 | 47 | 3.14 mM | Canonical ABA pocket |
| α-pinene | -4.69 | -4.69 | 86 | 366.90 μM | Canonical ABA pocket |
| limonene | -4.73 | -4.77 | 62 | 319.70 μM | Canonical ABA pocket |
| linalool | -4.12 | -4.56 | 30 | 457.50 μM | Canonical ABA pocket |
| -myrcene | -3.84 | -4.12 | 49 | 957.87 μM | Canonical ABA pocket |
| 3EBL\_A  (GA RECEPTOR) | GA | -9.31 | -9.43 | 50 | 121.92 nM | Canonical GA pocket |
| β-caryophyllene | -6.94 | -7.01 | 83 | 7.30 μM | Canonical GA pocket |
| isoprene | -3.78 | -3.81 | 84 | 1.61 mM | Pocket B |
| α-pinene | -5.5 | -5.54 | 84 | 87.42 μM | Canonical GA pocket |
| limonene | -5.44 | -5.57 | 28 | 82.39 μM | Pocket A |
| -5.34 | -5.43 | 34 | 104.59 μM | Pocket B |
| linalool | -4.69 | -5.16 | 29 | 166.34 μM | Canonical GA pocket |
| -myrcene | -4.10 | -4.30 | 33 | 699.55 μM | Canonical GA pocket |
| -4.92 | -5.19 | 29 | 157.11 μM | Externally to the canonical GA pocket |
| 3AXY (HD3A) | β-caryophyllene | -6.83 | -6.85 | 93 | 9.57 μM | Pocket A |
| isoprene | -3.44 | -3.52 | 86 | 2.64 mM | Pocket B |
| α-pinene | -5.46 | -5.52 | 87 | 90.24 μM | Pocket B |
| limonene | -4.99 | -5.02 | 41 | 209.73 μM | Pocket A |
| -4.9 | -4.93 | 15 | 242.72 μM | Pocket B |
| linalool | -4.96 | -5.23 | 23 | 147.07 μM | Pocket B |
| -4.72 | -4.93 | 36 | 241.47 μM | Pocket A |
| -myrcene | -4.26 | -4.61 | 32 | 415.20 μM | Pocket B |
| -4.29 | -4.52 | 49 | 488.40 μM | Pocket A |
| 1WKP (FLOWERING LOCUS T) | β-caryophyllene | -6.65 | -6.66 | 62 | 13.22 μM | Pocket A |
| -6.19 | -6.20 | 29 | 28.48 μM | Pocket B |
| isoprene | -3.15 | -3.19 | 78 | 4.61 mM | Pocket C |
| α-pinene | -5.14 | -5.26 | 7 | 139.67 μM | Pocket C |
| -5.23 | -5.24 | 77 | 143.49 μM | Pocket B |
| limonene | -5.07 | -5.10 | 47 | 181.16 μM | Pocket A |
| -4.82 | -4.95 | 20 | 234.45μM | Pocket C |
| -4.77 | -4.78 | 17 | 312.82 μM | Pocket B |
| linalool | -4.79 | -4.98 | 27 | 224.96 μM | Pocket A |
| -4.64 | -4.90 | 18 | 256.30 μM | Pocket B |
| -myrcene | -4.26 | -4.54 | 23 | 473.68 μM | Pocket C |
| -4.25 | -4.49 | 22 (+17) | 513.11 μM | Pocket A |
| -4.09 | -4.25 | 21 | 770.36 μM | Pocket B |
| 1WKO (TFL1) | β-caryophyllene | -7.15 | -7.17 | 38 | 5.57 μM | Pocket A |
| -6.91 | -6.91 | 59 | 120.59 μM | Pocket B |
| isoprene | -3.70 | -3.74 | 63 | 1.83 mM | Pocket C |
| α-pinene | -5.30 | -5.35 | 73 | 120.59 μM | Pocket A |
| -4.84 | -4.86 | 14 | 272.98 μM | Pocket B |
| limonene | -5.53 | -5.61 | 44 | 77.40 μM | Pocket C |
| -5.12 | -5.17 | 19 | 161.41 μM | Pocket A |
| -4.88 | -4.91 | 22 | 251.03 μM | Pocket B |
| linalool | -4.98 | -5.46 | 16 (+5+11+4+1) | 99.74 μM | Pocket A |
| -4.68 | -4.91 | 22 (+16) | 251 μM | Pocket B |
| -myrcene | -4.38 | -4.58 | 29 | 442.69 μM | Pocket A |
| -4.00 | -4.15 | 31 | 911.60 μM | Pocket B |
| COI  (partial JA receptor) | JA-Ile | -4.54 | -4.54 | 1 | 65.30 μM | Canonical JA pocket |
| β-caryophyllene | -6.05 | -6.11 | 10 | 33.18 μM | Canonical JA pocket |
| isoprene | -2.78 | -2.80 | 2 | 8.90 mM | Canonical JA pocket |
| α-pinene | -5.23 | -5.30 | 16 | 130.15 μM | Canonical JA pocket |
| -5.00 | -5.03 | 46 | 206.18 μM | Pocket A |
| limonene | -4.79 | -4.97 | 25 (+19) | 228.74 μM | Pocket A |
| -4.68 | -4.74 | 21 | 333.01 μM | Canonical JA pocket |
| linalool | -4.21 | -4.85 | 24 | 278.52 μM | Pocket B |
| -3.91 | -4.15 | 7 | 903.47 μM | Canonical JA pocket |
| -myrcene | -4.16 | -4.42 | 36 | 571.25 μM | Pocket A |
|  | -3.82 | -4.04 | 18 | 1.09 mM | Canonical JA pocket |
| COI & JAZ  (JA receptor complete) | JA-Ile | not available | | | | |
| β-caryophyllene | -6.57 | -6.58 | 9 | 15.04 μM | Canonical JA pocket |
| -6.61 | -6.64 | 38 | 13.50 μM | Pocket A |
| isoprene | -2.82 | -2.84 | 2 | 8.29 mM | Canonical JA pocket |
| α-pinene | -5.92 | -6.02 | 59 | 38.55 μM | Pocket B |
| -5.39 | -5.49 | 14 (+1) | 94.57 μM | Canonical JA pocket |
| -5.11 | -5.12 | 15 | 176.86 μM | Pocket A |
| limonene | -5.11 | -5.25 | 38 | 321.92 μM | Canonical JA pocket |
| linalool | -4.49 | -4.76 | 25 | 142.75 μM | Canonical JA pocket |
| -myrcene | -4.41 | -4.62 | 40 | 321.92 μM | Canonical JA pocket |
| -4.23 | -4.53 | 28 | 408.11 μM | Pocket A |
| SABP2  (SA enzyme) | SA | -5.37 | -5.47 | 34 | 97.25 μM | Canonical SA binding pocket |
| β-caryophyllene | -6.73 | -6.75 | 3 | 11.21 μM | Canonical SA binding pocket |
| -5.71 | -5.71 | 77 | 64.92 μM | Pocket B |
| isoprene | -3.25 | -3.33 | 3 | 3.65 mM | Canonical SA binding pocket |
| -3.24 | -3.26 | 91 | 4.06 mM | Externally to the canonical SA binding Pocket |
| α-pinene | -6.03 | -6.04 | 57 | 37.39 μM | Canonical SA binding pocket |
| -4.82 | -4.82 | 33 | 290.70 μM | Pocket B |
| limonene | -6.12 | -6.14 | 78 | 31.49 μM | Canonical SA binding pocket |
| -4.32 | -4.37 | 16 | 629.66 μM | Pocket B |
| linalool | -4.7 | -5.02 | 17 (+7+2+1) | 208.22 μM | Canonical SA binding pocket |
| -3.86 | -4.17 | 28 | 2.01 mM | Pocket B |
| -myrcene | -5.14 | -5.43 | 57 (+14) | 104.29 μM | Canonical SA binding pocket |
| -3.75 | -4.07 | 27 | 1.04 mM | Pocket B |

a Binding pocket column describes the site where the ligand binds. In most cases, the name of the site is the description of a specific protein region. In some cases, pocket A/B/C refer to different sites where the ligands bind.