**Supplementary Table S4. Detailed information of docking parameters**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Gene | Uniprot ID | PDB code | Docking site | Docking coordinate(X, Y, Z) Å |
| IL6 | P05231 | 1ALU | GLU42, ASN61[1] | 5.392, -30.536, 3.504 |
| VEGFA | P15692 | 1BJI | Active cavity | 36.059, -28.890, 0.000 |
| ESR1 | P03372 | 1ERE | ARG394, GLY521[2] | 6.151, 53.525, 131.421 |
| HIF1A | Q16665 | 3KCX | HIS279, ILE281 | -21.331,25.461,9.364 |
| MMP9 | P14780 | 4HMA | TYR179, LEU187, ALA191, PHE192, HIS230, LEU234[3] | 7.967, 13.951, -2.996 |
| APP | P05067 | 5BUO | Active cavity | 13.864, 23.025, 13.986 |
| FGF1 | P05230 | 1AFC | ASN18, LYS112, LYS113, LYS118, ARG122, GLN127 [4] | 20.736, 18.465, 10.283 |
| IL2 | P60568 | 3QB1 | ARG38, VAL69, LYS76[5] | 16.202, 20.076, -9.631 |
| LGALS3 | P17931  | 1KJL | ASN174, GLU184, ARG160, ALA146 [6] | -0.914, -3.938, -2.862 |
| SLC5A1 | P13866 | 2XQ2# | LEU74, SER77, TYR290, ASP294, GLN295[7] | -1.864, -31.824, -52.181 |
| F3 | P13726  | 2HFT | Active cavity | 35.135, 42.671, 41.832 |
| ALDH1B1 | P30837 | 5I13# | Active cavity | 92.116, 43.166, 41.290 |
| CES2 | O00748 | 5A7G# | SER228, GLY347, GLU103[8] | 91.169, 88.498, 24.784 |
| P4HB | P07237 | 4EKZ | TRP396, GLY398 [9] | -11.447, -47.531, 3.629 |
| HSPA5 |

|  |  |
| --- | --- |
|  |  P11021 |

 | 3LDL | ARG367, GLY364, TYR39, ILE61 [10] | 19.150, -7.243, 1.555 |
| RELA | Q04206 | 1NFI | Active cavity | -5.808, 95.005, 90.899 |

#The structure was constructed by homology modeling

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