**Table S4: Crystal complex molecular docking target protein parameters**

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| **Protein crystal complexes** | **Protein-ligand crystal complex description** | **Protein agonist or antagonist** | **Docking parameters** |
| **ESR1** | | | |
| **3erd** | ESR1 in complex with PDB ligand Diethylstilbestrol | ESR1 antagonist | The center of the active site of protein crystal ESR1-3erd was set as centerx= 5.3, centery= -0.2, centerz= -5.5; the size of the active center was set as sizex= 17.0, sizey= 17.0, sizez= 17.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **2yja** | ESR1 in complex with PDB ligand Estradial | ESR1 agonist | The center of the active site of protein crystal ESR1-2yja was set as centerx= 23.7, centery= 11.1, centerz= 10.2; the size of the active center was set as sizex= 21.0, sizey= 21.0, sizez= 21.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **2jfa** | ESR1 in complex with PDB ligand Raloxifene | ESR1 antagonist | The center of the active site of protein crystal ESR1-2jfa was set as centerx= -44.3, centery= 13.1, centerz= 3.5; the size of the active center was set as sizex= 27.0, sizey= 27.0, sizez= 27.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **KDR** | | | |
| **3vo3** | KDR in complex with PDB ligand N-[3-({2-[(cyclopropylcarbonyl)amino]imidazo[1,2-b]pyridazin-6-yl}oxy)phenyl]-1,3-dimethyl-1H-pyrazole-5-carboxamide | KDR antagonist | The center of the active site of protein crystal KDR-3vo3 was set as centerx= 25.6, centery= -27.7, centerz= -13.2; the size of the active center was set as sizex= 31.5, sizey= 31.5, sizez= 31.5; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **3vhe** | KDR in complex with PDB ligand 1-{2-fluoro-4-[(5-methyl-5H-pyrrolo[3,2-d]pyrimidin-4-yl)oxy]phenyl}-3-[3-(trifluoromethyl)phenyl]urea | KDR antagonist | The center of the active site of protein crystal KDR-3vhe was set as centerx= -24.9, centery= -1.1, centerz= -10.5; the size of the active center was set as sizex= 22.7, sizey= 22.7, sizez= 22.7; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **3cjg** | KDR in complex with PDB ligand N~4~-methyl-N~4~-(3-methyl-1H-indazol-6-yl)-N~2~-(3,4,5-trimethoxyphenyl) pyrimidine-2,4-diamine | KDR antagonist | The center of the active site of protein crystal KDR-3cjg was set as centerx= 8.2, centery= 40.8, centerz= 7.4; the size of the active center was set as sizex= 28.0, sizey= 28.0, sizez= 28.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **3cjf** | KDR in complex with PDB ligand N~4~-(3-methyl-1H-indazol-6-yl)-N~2~-(3,4,5-trimethoxyphenyl)pyrimidine-2,4-diamine | KDR antagonist | The center of the active site of protein crystal KDR-3cjf was set as centerx= 18.4, centery= 17.7, centerz= 18.9; the size of the active center was set as sizex= 18.1, sizey= 18.1, sizez= 18.1; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **LTA4H** | | | |
| **4dpr** | LTA4H in complex with PDB ligand L-Captopril | LTA4H antagonist | The center of the active site of protein crystal LTA4H-4dpr was set as centerx= 4.5, centery= -8.1, centerz= 1.1; the size of the active center was set as sizex= 16.0, sizey= 16.0, sizez= 16.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **3fts** | LTA4H in complex with PDB ligand Resveratrol | LTA4H antagonist | The center of the active site of protein crystal LTA4H-3fts and PDB ligand Resveratrol was set as centerx= -25.2, centery= 0.9, centerz= -2.2; the size of the active center was set as sizex= 21.0, sizey= 21.0, sizez= 21.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **PDE4D** | | | |
| **1xom** | PDE4D in complex with PDB ligand Cilomilast | PDE4D antagonist | The center of the active site of protein crystal PDE4D-1oxm was set as centerx= 14.0, centery= 6.0, centerz= 13.2; the size of the active center was set as sizex= 27.0, sizey= 27.0, sizez= 27.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **1tbb** | PDE4D in complex with PDB ligand Rolipram | PDE4D antagonist | The center of the active site of protein crystal PDE4D-1tbb and PDB ligand Rolipram was set as centerx= 14.2, centery= 6.1, centerz= 11.8; the size of the active center was set as sizex= 28.0, sizey= 28.0, sizez= 28.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **1tb7** | PDE4D in complex with PDB ligand Adenosine monophosphate | PDE4D antagonist | The center of the active site of protein crystal PDE4D-1tb7 was set as centerx= 17.8, centery= 5.7, centerz= 68.2; the size of the active center was set as sizex= 21.0, sizey= 21.0, sizez= 21.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **1zkn** | PDE4D in complex with PDB ligand 3-Isobutyl-1-Methylxanthine | PDE4D antagonist | The center of the active site of protein crystal PDE4D-1zkn was set as centerx= 21.0, centery= -5.1, centerz= 29.7; the size of the active center was set as sizex= 27.0, sizey= 27.0, sizez= 27.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **PPARG** | | | |
| **5lsg** | PPARG in complex with PDB ligand Betulinic acid | PPARG agonist | The center of the active site of protein crystal PPARG-5lsg was set as centerx= 18.2, centery= 17.8, centerz= 14.5; the size of the active center was set as sizex= 21.0, sizey= 21.0, sizez= 21.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **4jaz** | PPARG in complex with PDB ligand Resveratrol | PPARG agonist | The center of the active site of protein crystal PPARG-4jaz was set as centerx= 16.6, centery= 23.2, centerz= 8.2; the size of the active center was set as sizex= 21.0, sizey= 21.0, sizez= 21.0; the parameters were nummodes= 10, exhaustiveness= 50; others were set as default. |
| **3sz1\_MYR** | PPARG in complex with PDB ligand Myristic acid | PPARG agonist | The center of the active site of protein crystal PPARG-3sz1\_MYR was set as centerx= 35.6, centery= -19.9, centerz= 38.4; the size of the active center was set as sizex= 25.5, sizey= 25.5, sizez= 25.5; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **3sz1\_LU** | PPARG in complex with PDB ligand Lutetium | PPARG agonist | The center of the active site of protein crystal PPARG-3sz1\_LU was set as centerx= 39.7, centery= -23.1, centerz= 42.6; the size of the active center was set as sizex= 18.3, sizey= 18.3, sizez= 18.3; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| **3adx** | PPARG in complex with PDB ligand Indomethacin | PPARG agonist | The center of the active site of protein crystal PPARG-3adx was set as centerx= 21.3, centery= 65.9, centerz= 16.1; the size of the active center was set as sizex= 27.0, sizey= 27.0, sizez= 27.0; the parameters were nummodes=10, exhaustiveness=50; others were set as default. |
| Abbreviations: ESR1: Estrogen receptors alpha; KDR: Kinase insert domain receptor; LTA4H: Leukotriene A4 hydrolase; PDB: Protein Databank; PDE4D: cAMP-specific 3',5'-cyclic phosphodiesterase 4D; PPARG: Peroxisome proliferator-activated receptor gamma. | | | |