Table 1 Molecular docking between ligand and receptor from an LRI predicted by LRI- CellIntTreeB on Dataset 1

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Interface area | Hydrogen bonds | Salt bridges |
| 1 | ENSP00000283147 ENSP00000370542 | BMP6\_SDC1 |  | -33.3 | 2015.9 | 3.9 | 3.83 |
| 2 | ENSP00000363492 ENSP00000370542 | GDF5\_SDC1 |  | -39.3 | 2616.3 | 3.84 | 3.98 |
| 3 | ENSP00000284981 ENSP00000370542 | APP\_SDC1 |  | -7.6 | 629.3 | 3.28 | 2.52 |
| 4 | ENSP00000312999 ENSP00000370542 | GNAI2\_SDC1 |  | -37.9 | 2192.1 | 3.77 | 3.49 |
| 5 | ENSP00000225844 ENSP00000370542 | CCL13\_SDC1 |  | -27.3 | 2414.6 | 3.67 | 3.08 |
| 6 | ENSP00000482232 ENSP00000370542 | CGA\_SDC1 |  | -10.4 | 733.3 | 3.59 |  |
| 7 | ENSP00000469689 ENSP00000370542 | SHANK2\_SDC1 |  | -14.1 | 1877.6 | 3.71 | 3.97 |
| 8 | ENSP00000283147 ENSP00000357097 | BMP6\_FCER1A |  | -24.7 | 1515.8 | 3.85 | 3.91 |
| 9 | ENSP00000363492 ENSP00000357097 | GDF5\_FCER1A |  | -34.0 | 1915.1 | 3.86 |  |
| 10 | ENSP00000312999 ENSP00000357097 | GNAI2\_FCER1A |  | -37.9 | 2192.1 | 3.82 | 3.49 |
| 11 | ENSP00000225844 ENSP00000357097 | CCL13\_FCER1A |  | -16.0 | 1235.6 | 3.81 |  |
| 12 | ENSP00000469689 ENSP00000357097 | SHANK2\_FCER1A |  | -6.6 | 840.6 | 3.61 | 2.61 |
| 13 | ENSP00000398698 ENSP00000357097 | TNF\_FCER1A |  | -17.5 | 800.3 | 3.8 | 3.80 |
| 14 | ENSP00000284523 ENSP00000357097 | WNT3A\_FCER1A |  | -45.7 | 3942.4 | 3.88 | 3.65 |
| 15 | ENSP00000215781 ENSP00000361818 | OSM\_SDC4 |  | -5.7 | 550.2 | 3.78 | 3.92 |
| 16 | ENSP00000276927 ENSP00000361818 | IFNA1\_SDC4 |  | -12 | 1996.3 | 3.78 | 3.92 |
| 17 | ENSP00000369571 ENSP00000361818 | IFNA14\_SDC4 |  | -15.1 | 2094.9 | 3.86 | 3.92 |
| 18 | ENSP00000412897 ENSP00000361818 | IFNA4\_SDC4 |  | -8.2 | 1175.2 | 3.78 | 3.92 |
| 19 | ENSP00000352455 ENSP00000361818 | MFAP5\_SDC4 |  | -14.8 | 1839.4 | 3.84 | 3.92 |
| 20 | ENSP00000378326 ENSP00000361818 | ZP3\_SDC4 |  | -15.7 | 1973.2 | 3.78 | 3.92 |
| 21 | ENSP00000292401 ENSP00000361818 | AZGP1\_SDC4 |  | -14.2 | 1638.6 | 3.78 | 3.92 |
| 22 | ENSP00000266058 ENSP00000361818 | SLIT1\_SDC4 |  | -8.8 | 1569.8 | 3.78 | 3.92 |
| 23 | ENSP00000220809 ENSP00000361818 | PLAT\_SDC4 |  | -15 | 1683.6 | 3.78 | 3.92 |
| 24 | ENSP00000376921 ENSP00000361818 | NTNG2\_SDC4 |  | -10.7 | 1424.1 | 3.78 | 3.92 |
| 25 | ENSP00000321797 ENSP00000361818 | FGF8\_SDC4 |  | -12.1 | 1638.6 | 3.78 | 3.92 |
| 26 | ENSP00000215781 ENSP00000358165 | OSM\_FCGR1A |  | -16.6 | 2243.5 | 3.86 | 3.78 |
| 27 | ENSP00000276927 ENSP00000358165 | IFNA1\_FCGR1A |  | -21.7 | 2959.4 | 3.79 | 3.92 |
| 28 | ENSP00000369571 ENSP00000358165 | IFNA14\_FCGR1A |  | -16.9 | 2240.2 | 3.73 | 3.69 |
| 29 |  |  |  |  |  |  |  |
| 30 |  |  |  |  |  |  |  |

Table 2 Molecular docking between ligand and receptor from an LRI predicted by LRI- CellIntTreeB on Dataset 2

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Ligand receptor | LRI | Molecular docking | Binding energy (kcal/mol) | interface area | Hydrogen bonds | Salt bridges |
| 1 | ENSMUSP00000125697 ENSMUSP00000059270 | Gng2\_Gp1bb |  | -41.1 | 2166.6 | 3.68 | 3.55 |
| 2 | ENSMUSP00000030187 ENSMUSP00000059270 | Tln1\_Gp1bb |  | -13.2 | 732.1 | 3.65 | 3.64 |
| 3 | ENSMUSP00000039600 ENSMUSP00000059270 | Ccl5\_Gp1bb |  | -21.9 | 1224.7 | 3.6 |  |
| 4 | ENSMUSP00000022369 ENSMUSP00000059270 | Vcl\_Gp1bb |  | -38.6 | 1833.4 | 3.74 | 3.68 |
| 5 | ENSMUSP00000074885 ENSMUSP00000059270 | Cxcl2\_Gp1bb |  | -17.8 | 1188.0 | 3.8 |  |
| 6 | ENSMUSP00000032561 ENSMUSP00000059270 | Vasp\_Gp1bb |  | -15.8 | -15.8 | 2.81 |  |
| 7 | ENSMUSP00000040412 ENSMUSP00000059270 | Tnfsf9\_Gp1bb |  | -17.1 | 1152.2 | 3.85 | 3.59 |
| 8 | ENSMUSP00000003274 ENSMUSP00000059270 | Ebi3\_Gp1bb |  | -14.4 | 637.8 | 3.87 | 3.79 |
| 9 | ENSMUSP00000002979 ENSMUSP00000043936 | Lamb1\_Htr2c |  | -0.6 | 427.2 | 3.69 | 3.98 |
| 10 | ENSMUSP00000118318 ENSMUSP00000043936 | Afdn\_Htr2c |  | -35.7 | 2223.0 | 3.84 |  |
| 11 | ENSMUSP00000050716 ENSMUSP00000043936 | Efnb1\_Htr2c |  | -12.1 | 1089.4 | 3.89 | 3.49 |
| 12 | ENSMUSP00000016640 ENSMUSP00000043936 | Cd274\_Htr2c |  | -8.3 | 811.5 | 3.53 | 3.42 |
| 13 | ENSMUSP00000028233 ENSMUSP00000043936 | C5\_Htr2c |  | -12.9 | 1028.4 | 3.86 |  |
| 14 | ENSMUSP00000125697 ENSMUSP00000003469 | Gng2\_Cd79a |  | -73.4 | 3975.9 | 3.82 | 3.96 |
| 15 | ENSMUSP00000030187 ENSMUSP00000003469 | Tln1\_Cd79a |  | -38.4 | 2523.9 | 3.83 | 3.96 |
| 16 | ENSMUSP00000038301 ENSMUSP00000003469 | Gdf7\_Cd79a |  | -37.5 | 2343.7 | 3.83 | 3.96 |
| 17 | ENSMUSP00000058951 ENSMUSP00000003469 | Angptl8\_Cd79a |  | -49.2 | 2795.8 | 3.83 | 3.96 |
| 18 | ENSMUSP00000042705 ENSMUSP00000003469 | Gng10\_Cd79a |  | -39.8 | 2163 | 3.83 | 3.96 |
| 19 | ENSMUSP00000004480 ENSMUSP00000003469 | Sst\_Cd79a |  | -36.5 | 1990.9 | 3.83 | 3.96 |
| 20 | ENSMUSP00000039600 ENSMUSP00000003469 | Ccl5\_Cd79a |  | -46.2 | 2970 | 3.83 | 3.96 |
| 21 | ENSMUSP00000077314 ENSMUSP00000003469 | Gng8\_Cd79a |  | -41.6 | 2152.6 | 3.83 | 3.96 |
| 22 | ENSMUSP00000041047 ENSMUSP00000003469 | Pth2\_Cd79a |  | -54.4 | 2760.3 | 3.83 | 3.96 |
| 23 | ENSMUSP00000049161 ENSMUSP00000003469 | Ctf1\_Cd79a |  | -28.4 | 2244.7 | 3.83 | 3.96 |
| 24 | ENSMUSP00000030384 ENSMUSP00000003469 | Edn2\_Cd79a |  | -17.9 | 2485 | 3.83 | 3.96 |
| 25 | ENSMUSP00000109064 ENSMUSP00000003469 | Ccl20\_Cd79a |  | -33.4 | 1856.1 | 3.83 | 3.96 |
| 26 | ENSMUSP00000035120 ENSMUSP00000003469 | Cck\_Cd79a |  | -21.8 | 1882.6 | 3.83 | 3.96 |
| 27 | ENSMUSP00000031318 ENSMUSP00000003469 | Cxcl5\_Cd79a |  | -42.7 | 2315.4 | 3.83 | 3.96 |
| 28 | ENSMUSP00000067057 ENSMUSP00000003469 | Adcyap1\_Cd79a |  | -23.3 | 2152.7 | 3.83 | 3.96 |
| 29 | ENSMUSP00000002708 ENSMUSP00000003469 | Shh\_Cd79a |  | -18.7 | 1897 | 3.83 | 3.96 |
| 30 | ENSMUSP00000025914 ENSMUSP00000003469 | Vegfb\_Cd79a |  | -27 | 2261.2 | 3.83 | 3.96 |

Table 3 Molecular docking between ligand and receptor from an LRI predicted by LRI- CellIntTreeB on Dataset 3

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Ligand-Receptor | LRI(Gene Names) | Molecular docking | Binding energy (kcal/mol) | Interface area | Hydrogen bonds | Salt bridges |
| 1 | ENSMUSG00000035042 ENSMUSG00000034664 | Ccl5\_Itga6b |  | -17.1 | 1118.6 | 3.76 |  |
| 2 | ENSMUSG00000031302 ENSMUSG00000034664 | Nlgn3\_Itga2b |  | -17.1 | 1036.5 |  | 3.59 |
| 3 | ENSMUSG00000022015 ENSMUSG00000034664 | Tnfsf11\_Itga2b |  | -12.4 | 1979.5 | 3.86 | 3.97 |
| 4 | ENSMUSG00000026697 ENSMUSG00000034664 | Myoc\_Itga2b |  | -14 | 1656.9 | 3.8 | 3.97 |
| 5 | ENSMUSG00000031302 ENSMUSG00000033191 | Nlgn3\_Tie1 |  | -27.1 | 2886.8 | 3.62 | 3.93 |
| 6 | ENSMUSG00000022015 ENSMUSG00000033191 | Tnfsf11\_Tie1 |  | -14.6 | 2065.5 | 3.88 | 3.98 |
| 7 | ENSMUSG00000026697 ENSMUSG00000033191 | Myoc\_Tie1 |  | -7.9 | 1183.7 | 3.8 | 3.79 |
| 8 | ENSMUSG00000035042 ENSMUSG00000033191 | Ccl5\_Tie1 |  | -11.1 | 1352.7 | 3.83 | 3.85 |
| 9 | ENSMUSG00000035042 ENSMUSG00000024913 | Ccl5\_Lrp5 |  | -10.1 | 1424.6 | 3.57 | 3.69 |
| 10 | ENSMUSG00000038300 ENSMUSG00000024620 | Pth2\_Pdgfrb |  | -16.9 | 827.6 | 3.75 |  |
| 11 | ENSMUSG00000035042 ENSMUSG00000024620 | Ccl5\_Pdgfrb |  | -14.6 | 1238.2 | 3.72 |  |
| 12 | ENSMUSG00000042340 ENSMUSG00000024620 | Ctf1\_Pdgfrb |  | -16.9 | 827.6 | 3.75 |  |
| 13 | ENSMUSG00000028635 ENSMUSG00000024620 | Edn2\_Pdgfrb |  | -13.2 | 520.6 | 3.66 | 3.66 |
| 14 | ENSMUSG00000004366 ENSMUSG00000024620 | Sst\_Pdgfrb |  | -13.2 | 520.6 | 3.66 | 3.66 |
| 15 | ENSMUSG00000035042 ENSMUSG00000002897 | Ccl5\_Il17ra |  | -18.5 | 2607.3 | 3.9 | 4 |
| 16 | ENSMUSG00000026166 ENSMUSG00000024620 | Ccl20\_Pdgfrb |  | -13.9 | 607.1 | 3.86 | 3.62 |
| 17 | ENSMUSG00000037660 ENSMUSG00000024620 | Gdf7\_Pdgfrb |  | -15.2 | 734.6 | 3.59 |  |
| 18 | ENSMUSG00000064057 ENSMUSG00000024620 | Scgb3a1\_Pdgfrb |  | -16.5 | 698.3 | 3.58 |  |
| 19 | ENSMUSG00000032532 ENSMUSG00000024620 | Cck\_Pdgfrb |  | -13.9 | 623.3 | 3.73 | 3.32 |
| 20 | ENSMUSG00000039481 ENSMUSG00000024620 | Nrtn\_Pdgfrb |  | -15.8 | 715.8 | 3.75 |  |
| 21 | ENSMUSG00000045232 ENSMUSG00000024620 | Rln3\_Pdgfrb |  | -20.8 | 1496.7 | 3.53 | 2.84 |
| 22 | ENSMUSG00000031302 ENSMUSG00000024913 | Nlgn3\_Lrp5 |  | -29.3 | 2208.3 | 3.86 | 3.86 |
| 23 | ENSMUSG00000022015 ENSMUSG00000024913 | Tnfsf11\_Lrp5 |  | -14.9 | 1882.9 | 3.88 | 3.98 |
| 24 | ENSMUSG00000035042 ENSMUSG00000039115 | Ccl5\_Itga9 |  | -11.5 | 1134.7 | 3.77 |  |
| 25 | ENSMUSG00000027301 ENSMUSG00000024620 | Oxt\_Pdgfrb |  | -13.8 | 611.1 | 3.49 |  |
| 26 | ENSMUSG00000048163 ENSMUSG00000024620 | Selplg\_Pdgfrb |  | -13.5 | 623.0 | 3.75 |  |
| 27 | ENSMUSG00000024659 ENSMUSG00000024620 | Anxa1\_Pdgfrb |  | -13.7 | 629.7 | 3.59 |  |
| 28 | ENSMUSG00000022483 ENSMUSG00000024620 | Col2a1\_Pdgfrb |  | -29.2 | 2223.0 | 3.86 | 3.87 |
| 29 | ENSMUSG00000022015 ENSMUSG00000055471 | Tnfsf11\_Alk |  | -21.7 | 2819.1 | 3.86 | 3.97 |
| 30 | ENSMUSG00000035042 ENSMUSG00000031385 | Ccl5\_Plxnb3 |  | -18.5 | 1237.9 | 3.6 |  |

Table4  Molecular docking between ligand and receptor from an LRI predicted by LRI- CellIntTreeB on Dataset 4

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Ligand-Receptor | LRI(Gene Names) | Molecular docking | Binding energy (kcal/mol) | Interface area | Hydrogen bonds | Salt bridges |
| 1 | P30518 Q14050 | AVPR2\_COL9A3 |  | -27.4 | 1587.1 | 3.7 | 3.76 |
| 2 | P08620 Q14050 | FGF4\_COL9A3 |  | -30 | 1726.1 | 3.70 | 3.76 |
| 3 | P08865 Q14050 | RPSA\_COL9A3 |  | -33.4 | 1954.0 | 3.8 | 3.76 |
| 4 | P06881 Q14050 | CALCA\_COL9A3 |  | -40.4 | 2040.6 | 3.89 | 3.86 |
| 5 | P03971 Q14050 | AMH\_COL9A3 |  | -34.9 | 2768.4 | 3.82 | 3.73 |
| 6 | P0DJI9 Q14050 | SAA2\_COL9A3 |  | -38 | 1875.1 | 3.7 |  |
| 7 | O60391 Q14050 | GRIN3B\_COL9A3 |  | -39.6 | 2474.8 | 3.88 | 3.73 |
| 8 | P22466 Q14050 | GAL\_COL9A3 |  | -30.1 | 1687.3 | 3.7 | 3.76 |
| 9 | O14493 Q14050 | CLDN4\_COL9A3 |  | -43.5 | 2201.4 | 3.86 | 3.94 |
| 10 | P30518 P29400 | AVPR2\_COL4A5 |  | -25.5 | 1566.3 | 3.89 | 3.97 |
| 11 | P08865 P02458-1 | RPSA\_COL2A1 |  | -18.5 | 1606.4 | 3.76 |  |
| 12 | P08620 P02458-1 | FGF4\_COL2A1 |  | -17.3 | 1419.3 | 3.11 |  |
| 13 | P30518 P02458-1 | AVPR2\_COL2A1 |  | -25.5 | 1560.9 | 3.78 |  |
| 14 | P02462 P29400 | COL4A1\_COL4A5 |  | -41 | 3068.5 | 3.86 | 3.76 |
| 15 | P02671-2 P29400 | FGA\_COL4A5 |  | -4.1 | 777.1 | 3.89 | 3.35 |
| 16 | P02708 P29400 | CHRNA1\_COL4A5 |  | -19.9 | 2182.8 | 3.81 | 3.78 |
| 17 | P04264 P29400 | KRT1\_COL4A5 |  | -55.2 | 2464.8 | 2.69 | 3.95 |
| 18 | P05556-2 P29400 | ITGB1\_COL4A5 |  | -32.2 | 1935.6 | 3.7 | 3.94 |
| 19 | P07766 P29400 | CD3E\_COL4A5 |  | -9.6 | 462.3 | 3.86 | 3.64 |
| 20 | C6SUN5 P02458-1 | AgRP\_COL2A1 |  | -18.9 | 1453.1 | 3.7 |  |
| 21 | O14493 P02458-1 | CLDN4\_COL2A1 |  | -29 | 2860.6 | 3.86 | 3.94 |
| 22 | P08174 P02458-1 | CD55\_COL2A1 |  | -11.4 | 1137.3 | 3 |  |
| 23 | P07306 P02458-1 | ASGR1\_COL2A1 |  | -15.1 | 1521.7 | 3.59 |  |
| 24 | B4DIP2 P02458-1 | ERBIN\_COL2A1 |  | -17.1 | 1583.1 | 3.31 |  |
| 25 | P15692 P02458-1 | VEGFA\_COL2A1 |  | -40.1 | 2551.4 | 3.67 | 3.89 |
| 26 | P02462 P02458-1 | COL4A1\_COL2A1 |  | -49.3 | 3683.9 | 3.74 | 3.82 |
| 27 | P07585-4 P02458-1 | DCN\_COL2A1 |  | -17.7 | 1882.1 | 3.7 |  |
| 28 | P02708-2 P02458-1 | CHRNA1\_COL2A1 |  | -22.6 | 2673.7 | 3.84 | 3.6 |
| 29 | O15455 P02458-1 | TLR3\_COL2A1 |  | -13.7 | 1529.9 |  |  |
| 30 | C6SUN5  Q14050 | AgRP\_COL9A3 |  | -32.4 | 1701.3 | 3.81 | 3.73 |