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|  | Table 1 Molecular docking between ligand and receptor from an LRI predicted by CellConNet on Dataset 1 | | | | | |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | ENSP00000261405  ENSP00000379350 | VWF\_ITGB1 |  | -21.6 | 3.78 | 1812.2 |
| 2 | ENSP00000346839  ENSP00000275493 | FN1\_EGFR |  | -13.4 | 3.63 | 1996.7 |
| 3 | ENSP00000260408  ENSP00000275493 | ADAM10\_EGFR |  | -25.6 | 2.69 | 1908.5 |
| 4 | ENSP00000284981  ENSP00000379350 | APP\_ITGB1 |  | -18 | 2.89 | 1483.6 |
| 5 | ENSP00000398736  ENSP00000379350 | CCN1\_ITGB1 |  | -20 | 3.63 | 1526.4 |
| 6 | ENSP00000272298  ENSP00000355533 | CALM2\_RYR2 |  | -34.4 | 3.81 | 2681.7 |
| 7 | ENSP00000265171  ENSP00000379350 | EGF\_ITGB1 |  | -17.5 | 2.82 | 1262.7 |
| 8 | ENSP00000353654  ENSP00000379350 | COL4A2\_ITGB1 |  | -43 | 3.18 | 3438.6 |
| 9 | ENSP00000272298  ENSP00000483721 | CALM2\_ADCYAP1R1 |  | -13.9 | 2.77 | 811 |
| 10 | ENSP00000291295  ENSP00000483721 | CALM3\_ADCYAP1R1 |  | -17.6 | 3.47 | 1225.8 |
| 11 | ENSP00000272298  ENSP00000327246 | CALM2\_VIPR1 |  | -18.6 | 3.81 | 1883 |
| 12 | ENSP00000291295  ENSP00000327246 | CALM3\_VIPR1 |  | -22.7 | 3.03 | 2190.3 |
| 13 | ENSP00000245907  ENSP00000379350 | C3\_ITGB1 |  | -17.6 | 2.83 | 1278.5 |
| 14 | ENSP00000272298  ENSP00000352561 | CALM2\_CALCR |  | -26.3 | 2.77 | 1850.2 |
| 15 | ENSP00000291295  ENSP00000352561 | CALM3\_CALCR |  | -15.5 | 2.52 | 1736.8 |
| 16 | ENSP00000284981  ENSP00000275493 | APP\_EGFR |  | -7.6 | 2.85 | 1438.3 |
| 17 | ENSP00000478570  ENSP00000243077 | VEGFA\_LRP1 |  | -29.4 | 2.94 | 1897.5 |
| 18 | ENSP00000361405  ENSP00000379350 | MMP9\_ITGB1 |  | -17.5 | 2.83 | 1276.5 |
| 19 | ENSP00000220809  ENSP00000379350 | PLAT\_ITGB1 |  | -17.2 | 2.03 | 1262.8 |
| 20 | ENSP00000260408  ENSP00000379350 | ADAM10\_ITGB1 |  | -23.1 | 2.41 | 2556.8 |
| 21 | ENSP00000260356  ENSP00000261023 | THBS1\_ITGAV |  | -31.4 | 2.19 | 4261.9 |
| 22 | ENSP00000272298  ENSP00000262888 | CALM2\_KCNN4 |  | -11.2 | 3.81 | 1311 |
| 23 | ENSP00000291295  ENSP00000262888 | CALM3\_KCNN4 |  | -13 | 3.03 | 817.4 |
| 24 | ENSP00000305714  ENSP00000379350 | BMP1\_ITGB1 |  | -17.4 | 2.83 | 1273.6 |
| 25 | ENSP00000225964  ENSP00000452786 | COL1A1\_ITGB3 |  | -9 | 2.82 | 1130.6 |
| 26 | ENSP00000284981  ENSP00000380948 | APP\_ITGB2 |  | -12 | 2.85 | 1212.9 |
| 27 | ENSP00000272298  ENSP00000405330 | CALM2\_ESR1 |  | -25.8 | 2.71 | 2220.5 |
| 28 | ENSP00000349467  ENSP00000405330 | CALM1\_ESR1 |  | -22.6 | 3.62 | 2617.4 |
| 29 | ENSP00000002829  ENSP00000317272 | SEMA3F\_MET |  | -7.1 | 3.26 | 1096.5 |
| 30 | ENSP00000006053  ENSP00000350348 | CX3CL1\_GRM7 |  | -6.2 | 2.61 | 700.2 |

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|  | Table 2 Molecular docking between ligand and receptor from an LRI predicted by CellConNet on Dataset 2 | | | | | |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | ENSMUSP00000005406  ENSMUSP00000087457 | App\_Itgb1 |  | -67.2 | 2.81 | 4244.5 |
| 2 | ENSMUSP00000000312  ENSMUSP00000087457 | Cdh1\_Itgb1 |  | -42.1 | 2.75 | 4312.9 |
| 3 | ENSMUSP00000023123  ENSMUSP00000087457 | Col2a1\_Itgb1 |  | -66.8 | 3.82 | 5303.1 |
| 4 | ENSMUSP00000107873  ENSMUSP00000087457 | Vwf\_Itgb1 |  | -62.2 | 2.66 | 4058.2 |
| 5 | ENSMUSP00000024988  ENSMUSP00000087457 | C3\_Itgb1 |  | -47.5 | 3.48 | 3796.6 |
| 6 | ENSMUSP00000043956  ENSMUSP00000026917 | App\_Nrp1 |  | -42.6 | 3.69 | 4017.3 |
| 7 | ENSMUSP00000101049  ENSMUSP00000087457 | Col18a1\_Itgb1 |  | -39.5 | 3.02 | 2847.8 |
| 8 | ENSMUSP00000005406  ENSMUSP00000068468 | App\_Itgam |  | -27.5 | 2.76 | 1758.8 |
| 9 | ENSMUSP00000030683  ENSMUSP00000028288 | Hgf\_Notch1 |  | -19 | 3.62 | 1437.8 |
| 10 | ENSMUSP00000022368  ENSMUSP00000087457 | Plau\_Itgb1 |  | -37.7 | 3.66 | 3698.6 |
| 11 | ENSMUSP00000005406  ENSMUSP00000021028 | App\_Itgb3 |  | -30.5 | 2.81 | 2383.2 |
| 12 | ENSMUSP00000107873  ENSMUSP00000028288 | Vwf\_Notch1 |  | -39.7 | 2.66 | 2747.9 |
| 13 | ENSMUSP00000000312  ENSMUSP00000028499 | Cdh1\_Itgav |  | -4.4 | 2.82 | 982.6 |
| 14 | ENSMUSP00000104314  ENSMUSP00000028288 | Ntn1\_Notch1 |  | -17.7 | 3.87 | 1515 |
| 15 | ENSMUSP00000001319  ENSMUSP00000087457 | Efnb2\_Itgb1 |  | -38 | 2.59 | 2334.4 |
| 16 | ENSMUSP00000002708  ENSMUSP00000028288 | Shh\_Notch1 |  | -15.1 | 3.87 | 1289.6 |
| 17 | ENSMUSP00000015791  ENSMUSP00000087457 | Lama5\_Itgb1 |  | -37.8 | 2.59 | 2341.3 |
| 18 | ENSMUSP00000028233  ENSMUSP00000087457 | Hc\_Itgb1 |  | -42.2 | 3.78 | 3258 |
| 19 | ENSMUSP00000005406  ENSMUSP00000028499 | App\_Itgav |  | -39.3 | 2.6 | 2951.6 |
| 20 | ENSMUSP00000107873  ENSMUSP00000023128 | Vwf\_Itga5 |  | -23 | 2.66 | 1800.2 |
| 21 | ENSMUSP00000005406  ENSMUSP00000045770 | App\_Tlr4 |  | -29.2 | 2.81 | 1904.9 |
| 22 | ENSMUSP00000005406  ENSMUSP00000005218 | App\_Cd44 |  | -28.5 | 2.59 | 2473.6 |
| 23 | ENSMUSP00000130985  ENSMUSP00000087457 | Sema6b\_Itgb1 |  | -34.5 | 3.16 | 2218.1 |
| 24 | ENSMUSP00000104314  ENSMUSP00000087457 | Ntn1\_Itgb1 |  | -45.9 | 2.22 | 3949.7 |
| 25 | ENSMUSP00000074565  ENSMUSP00000087457 | Nlgn1\_Itgb1 |  | -45.4 | 2.59 | 3006.7 |
| 26 | ENSMUSP00000032125  ENSMUSP00000067305 | Bmp10\_Acvr2a |  | -4.7 | 3.18 | 209.3 |
| 27 | ENSMUSP00000043957  ENSMUSP00000028288 | Lama1\_Notch1 |  | -21.2 | 2.19 | 1957.4 |
| 28 | ENSMUSP00000107607  ENSMUSP00000087457 | Cfh\_Itgb1 |  | -44.5 | 2.4 | 3786.2 |
| 29 | ENSMUSP00000022368  ENSMUSP00000028288 | Plau\_Notch1 |  | -20 | 3.4 | 2183.8 |
| 30 | ENSMUSP00000031325  ENSMUSP00000087457 | Areg\_Itgb1 |  | -51.7 | 2.91 | 3969.4 |

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|  | Table 3 Molecular docking between ligand and receptor from an LRI predicted by CellConNet on Dataset 3 | | | | | |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | ENSMUSG00000022483  ENSMUSG00000027087 | Col2a1\_Itgav |  | -33.3 | 3.04 | 2161.8 |
| 2 | ENSMUSG00000017737  ENSMUSG00000025809 | Mmp9\_Itgb1 |  | -53 | 3.1 | 4394.8 |
| 3 | ENSMUSG00000031391  ENSMUSG00000025809 | L1cam\_Itgb1 |  | -39.5 | 3.16 | 2214.8 |
| 4 | ENSMUSG00000024164  ENSMUSG00000025809 | C3\_Itgb1 |  | -47.5 | 3.48 | 3796.6 |
| 5 | ENSMUSG00000019997  ENSMUSG00000025809 | Ctgf\_Itgb1 |  | -39.2 | 3.51 | 2685.3 |
| 6 | ENSMUSG00000053024  ENSMUSG00000025809 | Cntn2\_Itgb1 |  | -42 | 3.25 | 3839.2 |
| 7 | ENSMUSG00000015568  ENSMUSG00000025809 | Lpl\_Itgb1 |  | -44 | 3.17 | 2840.9 |
| 8 | ENSMUSG00000000303  ENSMUSG00000025809 | Cdh1\_Itgb1 |  | -49 | 2.82 | 5010.9 |
| 9 | ENSMUSG00000002603  ENSMUSG00000025809 | Tgfb1\_Itgb1 |  | -44.6 | 3.15 | 2696.3 |
| 10 | ENSMUSG00000028195  ENSMUSG00000025809 | Cyr61\_Itgb1 |  | -43.2 | 2.56 | 3947 |
| 11 | ENSMUSG00000027249  ENSMUSG00000025809 | F2\_Itgb1 |  | -49.9 | 2.05 | 4786.9 |
| 12 | ENSMUSG00000024164  ENSMUSG00000027087 | C3\_Itgav |  | -6.9 | 2.52 | 837.5 |
| 13 | ENSMUSG00000068196  ENSMUSG00000025809 | Col8a1\_Itgb1 |  | -57.6 | 3.58 | 4295.3 |
| 14 | ENSMUSG00000036585  ENSMUSG00000025809 | Fgf1\_Itgb1 |  | -44.8 | 2.28 | 3810.6 |
| 15 | ENSMUSG00000034488  ENSMUSG00000025809 | Edil3\_Itgb1 |  | -44.5 | 3.82 | 3206.1 |
| 16 | ENSMUSG00000056427  ENSMUSG00000025809 | Slit3\_Itgb1 |  | -48.4 | 2.73 | 3392.8 |
| 17 | ENSMUSG00000021822  ENSMUSG00000026923 | Plau\_Notch1 |  | -20 | 3.4 | 2183.8 |
| 18 | ENSMUSG00000003814  ENSMUSG00000025809 | Calr\_Itgb1 |  | -46 | 2.04 | 3486.3 |
| 19 | ENSMUSG00000031538  ENSMUSG00000025809 | Plat\_Itgb1 |  | -44.1 | 2.59 | 3693 |
| 20 | ENSMUSG00000032496  ENSMUSG00000025809 | Ltf\_Itgb1 |  | -36.8 | 2.59 | 3160.6 |
| 21 | ENSMUSG00000001029  ENSMUSG00000025809 | Icam2\_Itgb1 |  | -47.6 | 3.07 | 3400.3 |
| 22 | ENSMUSG00000029103  ENSMUSG00000025809 | Lrpap1\_Itgb1 |  | -37.2 | 2.59 | 2304.1 |
| 23 | ENSMUSG00000022892  ENSMUSG00000025809 | App\_Itgb1 |  | -67.2 | 2.81 | 4244.5 |
| 24 | ENSMUSG00000041936  ENSMUSG00000025809 | Agrn\_Itgb1 |  | -48.1 | 3.82 | 3402.4 |
| 25 | ENSMUSG00000027276  ENSMUSG00000025809 | Jag1\_Itgb1 |  | -39 | 3.8 | 3020.6 |
| 26 | ENSMUSG00000002985  ENSMUSG00000025809 | Apoe\_Itgb1 |  | -51.4 | 3.35 | 3459.9 |
| 27 | ENSMUSG00000001741  ENSMUSG00000026923 | Il16\_Notch1 |  | -36.5 | 2.59 | 2421.4 |
| 28 | ENSMUSG00000022892  ENSMUSG00000021796 | App\_Bmpr1a |  | -29.4 | 2.81 | 2234 |
| 29 | ENSMUSG00000001029  ENSMUSG00000026923 | Icam2\_Notch1 |  | -31.7 | 3.07 | 1729.1 |
| 30 | ENSMUSG00000001300  ENSMUSG00000052155 | Efnb2\_Acvr2a |  | -7.5 | 2.93 | 843.7 |

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|  | Table 4 Molecular docking between ligand and receptor from an LRI predicted by CellConNet on Dataset 4 | | | | | |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | [ENSP00000366109](https://string-db.org/network/9606.ENSP00000366109) [ENSP00000355533](https://string-db.org/network/9606.ENSP00000355533) | ANXA1 \_RYR2 |  | -27.4 | 3.29 | 1269.3 |
| 2 | [ENSP00000295897](https://string-db.org/network/9606.ENSP00000295897) [ENSP00000480150](https://string-db.org/network/9606.ENSP00000480150) | ALB \_HYOU1 |  | -25.2 | 3.19 | 1618.6 |
| 3 | [ENSP00000379350](https://string-db.org/network/9606.ENSP00000379350) [ENSP00000243077](https://string-db.org/network/9606.ENSP00000243077) | ITGB1 \_LRP1 |  | -31.1 | 3.7 | 1831.5 |
| 4 | [ENSP00000366109](https://string-db.org/network/9606.ENSP00000366109) [ENSP00000353094](https://string-db.org/network/9606.ENSP00000353094) | ANXA1 \_SDF4 |  | -13.1 | 2.74 | 556.7 |
| 5 | [ENSP00000323929](https://string-db.org/network/9606.ENSP00000323929) [ENSP00000320866](https://string-db.org/network/9606.ENSP00000320866) | A2M \_CALR |  | -9.4 | 3.55 | 1700.7 |
| 6 | [ENSP00000245907](https://string-db.org/network/9606.ENSP00000245907) [ENSP00000292807](https://string-db.org/network/9606.ENSP00000292807) | C3 \_AP2M1 |  | -18.6 | 2.95 | 2321.2 |
| 7 | [ENSP00000366109](https://string-db.org/network/9606.ENSP00000366109) [ENSP00000262776](https://string-db.org/network/9606.ENSP00000262776) | ANXA1 \_LGALS3BP |  | -11.5 | 2.69 | 435.7 |
| 8 | [ENSP00000379350](https://string-db.org/network/9606.ENSP00000379350) [ENSP00000295897](https://string-db.org/network/9606.ENSP00000295897) | ITGB1 \_ALB |  | -30.1 | 3.7 | 1755.4 |
| 9 | [ENSP00000366109](https://string-db.org/network/9606.ENSP00000366109) [ENSP00000236040](https://string-db.org/network/9606.ENSP00000236040) | ANXA1 \_P3H1 |  | -13.2 | 2.69 | 605.1 |
| 10 | [ENSP00000236040](https://string-db.org/network/9606.ENSP00000236040) | ALB \_P3H1 |  | -11.4 | 3.14 | 1032.4 |
| 11 | [ENSP00000293379](https://string-db.org/network/9606.ENSP00000293379) [ENSP00000320866](https://string-db.org/network/9606.ENSP00000320866) | ITGA5 \_CALR |  | -30.1 | 3.7 | 1755.4 |
| 12 | [ENSP00000379350](https://string-db.org/network/9606.ENSP00000379350) [ENSP00000406773](https://string-db.org/network/9606.ENSP00000406773) | ITGB1 \_DCD |  | -46.3 | 3.7 | 2681.6 |
| 13 | [ENSP00000353224](https://string-db.org/network/9606.ENSP00000353224) [ENSP00000406773](https://string-db.org/network/9606.ENSP00000406773) | TFRC \_DCD |  | -37.9 | 3.54 | 2444.9 |
| 14 | [ENSP00000378669](https://string-db.org/network/9606.ENSP00000378669) [ENSP00000355533](https://string-db.org/network/9606.ENSP00000355533) | ALDOA \_RYR2 |  | -35.6 | 2.81 | 2623.8 |
| 15 | [ENSP00000252244](https://string-db.org/network/9606.ENSP00000252244) [ENSP00000353094](https://string-db.org/network/9606.ENSP00000353094) | KRT1 \_SDF4 |  | -55 | 2.69 | 2458.1 |
| 16 | [ENSP00000346839](https://string-db.org/network/9606.ENSP00000346839) [ENSP00000333769](https://string-db.org/network/9606.ENSP00000333769) | FN1 \_BSG |  | -27.3 | 2.58 | 1977 |
| 17 | [ENSP00000379350](https://string-db.org/network/9606.ENSP00000379350) [ENSP00000480150](https://string-db.org/network/9606.ENSP00000480150) | ITGB1\_HYOU1 |  | -29.5 | 3.7 | 1800.5 |
| 18 | [ENSP00000261023](https://string-db.org/network/9606.ENSP00000261023) [ENSP00000320866](https://string-db.org/network/9606.ENSP00000320866) | ITGAV \_CALR |  | -33.9 | 2.71 | 4015 |
| 19 | [ENSP00000379350](https://string-db.org/network/9606.ENSP00000379350) [ENSP00000325527](https://string-db.org/network/9606.ENSP00000325527) | ITGB1\_FBN1 |  | -30.3 | 3.7 | 1808.9 |
| 20 | [ENSP00000226218](https://string-db.org/network/9606.ENSP00000226218) [ENSP00000406773](https://string-db.org/network/9606.ENSP00000406773) | VTN \_DCD |  | -13.4 | 2.43 | 1555.5 |
| 21 | [ENSP00000366109](https://string-db.org/network/9606.ENSP00000366109) [ENSP00000406773](https://string-db.org/network/9606.ENSP00000406773) | ANXA1 \_DCD |  | -14.3 | 2.69 | 521 |
| 22 | [ENSP00000295897](https://string-db.org/network/9606.ENSP00000295897) [ENSP00000320171](https://string-db.org/network/9606.ENSP00000320171) | ALB \_PKM |  | -40.5 | 3.44 | 3215.7 |
| 23 | [ENSP00000379350](https://string-db.org/network/9606.ENSP00000379350) [ENSP00000243077](https://string-db.org/network/9606.ENSP00000243077) | ITGB1\_LRP1 |  | -31.1 | 3.54 | 1831.5 |
| 24 | [ENSP00000295897](https://string-db.org/network/9606.ENSP00000295897) [ENSP00000353094](https://string-db.org/network/9606.ENSP00000353094) | ALB \_SDF4 |  | -16.7 | 3.19 | 1161.1 |
| 25 | [ENSP00000323929](https://string-db.org/network/9606.ENSP00000323929) [ENSP00000225698](https://string-db.org/network/9606.ENSP00000225698) | A2M \_C1QBP |  | -16.6 | 3.3 | 1981.3 |
| 26 | [ENSP00000295897](https://string-db.org/network/9606.ENSP00000295897) [ENSP00000398632](https://string-db.org/network/9606.ENSP00000398632) | ALB \_CD44 |  | -6.3 | 3.7 | 1377.9 |
| 27 | [ENSP00000236850](https://string-db.org/network/9606.ENSP00000236850) [ENSP00000320171](https://string-db.org/network/9606.ENSP00000320171) | APOA1 \_PKM |  | -38.5 | 2.84 | 3076.5 |
| 28 | [ENSP00000295897](https://string-db.org/network/9606.ENSP00000295897) [ENSP00000333769](https://string-db.org/network/9606.ENSP00000333769) | ALB \_BSG |  | -29.6 | 3.61 | 1895.5 |
| 29 | [ENSP00000261023](https://string-db.org/network/9606.ENSP00000261023) [ENSP00000243077](https://string-db.org/network/9606.ENSP00000243077) | ITGAV \_LRP1 |  | -28.2 | 2.71 | 3426.7 |
| 30 | [ENSP00000261023](https://string-db.org/network/9606.ENSP00000261023) [ENSP00000355533](https://string-db.org/network/9606.ENSP00000355533) | ITGAV \_RYR2 |  | -58.2 | 2.71 | 5097.3 |