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|  | Table 1 Molecular docking between ligand and receptor from an LRI predicted by LRI-HDEnHD on Dataset 1 | | | | | |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | ENSP00000002829  ENSP00000317272 | SEMA3F-MET |  | -7.1 | 3.26 | 1096.5 |
| 2 | ENSP00000002829  ENSP00000380948 | SEMA3F-ITGB2 |  | -15.7 | 3.54 | 1281 |
| 3 | ENSP00000002829  ENSP00000410294 | SEMA3F-FGFR2 |  | -28.1 | 3.55 | 2748.7 |
| 4 | ENSP00000002829  ENSP00000263388 | SEMA3F-NOTCH3 |  | -23.9 | 3.53 | 1584.3 |
| 5 | ENSP00000002829  ENSP00000380227 | SEMA3F-ITGA4 |  | -9.2 | 2.75 | 563.9 |
| 6 | ENSP00000002829  ENSP00000379350 | SEMA3F-ITGB1 |  | -43 | 2.45 | 2977.9 |
| 7 | ENSP00000002829  ENSP00000441691 | SEMA3F-ITGAM |  | -12.1 | 3.8 | 1977 |
| 8 | ENSP00000002829  ENSP00000261023 | SEMA3F-ITGAV |  | -22.1 | 2.68 | 1656.9 |
| 9 | ENSP00000002829  ENSP00000386896 | SEMA3F-ITGA6 |  | -31.1 | 2.84 | 2018.5 |
| 10 | ENSP00000002829  ENSP00000296585 | SEMA3F-ITGA2 |  | -13.3 | 2.77 | 2111.3 |
| 11 | ENSP00000002829  ENSP00000293379 | SEMA3F-ITGA5 |  | -43 | 2.45 | 2977.9 |
| 12 | ENSP00000002829  ENSP00000267101 | SEMA3F-ERBB3 |  | -14.3 | 2.49 | 952 |
| 13 | ENSP00000002829  ENSP00000371532 | SEMA3F-VLDLR |  | -58 | 2.74 | 4871.6 |
| 14 | ENSP00000002829  ENSP00000356000 | SEMA3F-PLXNA2 |  | -11.6 | 3.41 | 1117 |
| 15 | ENSP00000002829  ENSP00000447006 | SEMA3F-CNTN1 |  | -21 | 3.34 | 2641.9 |
| 16 | ENSP00000006053  ENSP00000265371 | CX3CL1-NRP1 |  | -5.7 | 2.9 | 679.9 |
| 17 | ENSP00000006053  ENSP00000353582 | CX3CL1-NRP2 |  | -11.6 | 2.9 | 979.3 |
| 18 | ENSP00000006053  ENSP00000280155 | CX3CL1-ADRA2A |  | -6.9 | 3.61 | 1014.6 |
| 19 | ENSP00000006053  ENSP00000302811 | CX3CL1-MTNR1A |  | -10.7 | 3.75 | 963 |
| 20 | ENSP00000006053  ENSP00000350348 | CX3CL1-GRM7 |  | -6.2 | 2.61 | 700.2 |
| 21 | ENSP00000006053  ENSP00000275493 | CX3CL1-EGFR |  | -7.1 | 3.61 | 840.2 |
| 22 | ENSP00000006053  ENSP00000256637 | CX3CL1-SORT1 |  | -7 | 3.61 | 842.2 |
| 23 | ENSP00000006053  ENSP00000380948 | CX3CL1-ITGB2 |  | -6.1 | 2.92 | 703.9 |
| 24 | ENSP00000006053  ENSP00000331736 | CX3CL1-SELE |  | -6 | 3.44 | 701.5 |
| 25 | ENSP00000169298  ENSP00000353582 | ST6GAL1-NRP2 |  | -11 | 3.22 | 1570.4 |
| 26 | ENSP00000169298  ENSP00000317272 | ST6GAL1-MET |  | -8.5 | 3.66 | 1445.7 |
| 27 | ENSP00000169298  ENSP00000410294 | ST6GAL1-FGFR2 |  | -19.6 | 3.41 | 3213 |
| 28 | ENSP00000169298  ENSP00000339824 | ST6GAL1-FGFR3 |  | -20 | 3.22 | 2540 |
| 29 | ENSP00000169298  ENSP00000373700 | ST6GAL1-ALK |  | -19.2 | 3.25 | 2094.6 |
| 30 | ENSP00000169298  ENSP00000398632 | ST6GAL1-CD44 |  | -9.2 | 3.29 | 2371.3 |

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|  | Table 2 Molecular docking between ligand and receptor from an LRI predicted by LRI-HDEnHD on Dataset 2 | | | | | |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | ENSG00000105976  ENSG00000142949 | MET-PTPRF | Docking graph | -40.7 | 3.55 | 3344.6 |
| 2 | ENSG00000150093  ENSG00000122852 | ITGB1-SFTPA1 | Docking graph | 0.0 | 3.56 | 1483.3 |
| 3 | ENSG00000163631  ENSG00000163220 | ALB-S100A9 | Docking graph | -25.7 | 2.94 | 1723.8 |
| 4 | ENSG00000175899  ENSG00000105281 | A2M-SLC1A5 | Docking graph | 1.7 | 2.76 | 576.4 |
| 5 | ENSG00000120885  ENSG00000026508 | CLU-CD44 | Docking graph | -9.2 | 3.22 | 1117.9 |
| 6 | ENSG00000157404  ENSG00000149177 | KIT-PTPRJ | Docking graph | -17.7 | 3.88 | 947.6 |
| 7 | ENSG00000171557  ENSG00000113905 | FGG-HRG | Docking graph | -28.1 | 2.89 | 2177.2 |
| 8 | ENSG00000135414  ENSG00000106799 | GDF11-TGFBR1 | Docking graph | -14.2 | 3.63 | 956.6 |
| 9 | ENSG00000166598  ENSG00000137801 | HSP90B1-THBS1 | Docking graph | 0.5 | 3.84 | 94.6 |
| 10 | ENSG00000175899  ENSG00000136999 | A2M-CCN3 | Docking graph | -7.2 | 2.84 | 1746.5 |
| 11 | ENSG00000138448  ENSG00000120889 | ITGAV-TNFRSF10B | Docking graph | -40.7 | 3.04 | 4000.4 |
| 12 | ENSG00000150093  ENSG00000161634 | ITGB1-DCD | Docking graph | -30.6 | 2.80 | 1964.8 |
| 13 | ENSG00000167768  ENSG00000006606 | KRT1-CCL26 | Docking graph | -54.6 | 3.56 | 2386.3 |
| 14 | ENSG00000085265  ENSG00000198626 | FCN1-RYR2 | Docking graph | -7.8 | 3.48 | 978.0 |
| 15 | ENSG00000163631  ENSG00000048462 | ALB-TNFRSF17 | Docking graph | -6.1 | 2.94 | 1409.8 |
| 16 | ENSG00000150093  ENSG00000080824 | ITGB1-EL52 | Docking graph | -16.3 | 2.83 | 1382.9 |
| 17 | ENSG00000167768  ENSG00000026508 | KRT1-CD44 | Docking graph | -57.1 | 2.32 | 3614.0 |
| 18 | ENSG00000026508  ENSG00000132470 | CD44-ITGB4 | Docking graph | 1.0 | 2.27 | 3092.6 |
| 19 | ENSG00000150093  ENSG00000167768 | ITGB1-KRT1 | Docking graph | -52.7 | 3.56 | 3248.4 |
| 20 | [ENSG00000175899](https://www.veupathdb.org/gene/HostDB:ENSG00000175899" \t "https://www.uniprot.org/uniprotkb/P01023/_blank)  [ENSG00000166482](https://www.veupathdb.org/gene/HostDB:ENSG00000166482" \t "https://www.uniprot.org/uniprotkb/P55083/_blank) | A2M-MFAP4 | Docking graph | 1.7 | 2.76 | 576.4 |
| 21 | P02703  [ENSG00000167768](https://www.veupathdb.org/gene/HostDB:ENSG00000167768" \t "https://www.uniprot.org/uniprotkb/P04264/_blank) | CLPS-KRT1 | Docking graph | -50.7 | 3.04 | 2930.5 |
| 22 | [ENSG00000068078](https://www.veupathdb.org/gene/HostDB:ENSG00000068078" \t "https://www.uniprot.org/uniprotkb/P22607/_blank)  [ENSG00000107831](https://www.veupathdb.org/gene/HostDB:ENSG00000107831" \t "https://www.uniprot.org/uniprotkb/P55075/_blank) | FGFR3-FGF8 | Docking graph | -10.6 | 2.51 | 1758.6 |
| 23 | [ENSG00000163631](https://www.veupathdb.org/gene/HostDB:ENSG00000163631" \t "https://www.uniprot.org/uniprotkb/P02768/_blank)  [ENSG00000157017](https://www.veupathdb.org/gene/HostDB:ENSG00000157017" \t "https://www.uniprot.org/uniprotkb/Q9UBU3/_blank) | ALB-GHRL | Docking graph | -1.3 | 2.94 | 477.6 |
| 24 | [ENSG00000150093](https://www.veupathdb.org/gene/HostDB:ENSG00000150093" \t "https://www.uniprot.org/uniprotkb/P05556/_blank)  [ENSG00000099203](https://www.veupathdb.org/gene/HostDB:ENSG00000099203" \t "https://www.uniprot.org/uniprotkb/Q13445/_blank) | ITGB1-TMED1 | Docking graph | -3.4 | 3.56 | 2177.0 |
| 25 | [ENSG00000150093](https://www.veupathdb.org/gene/HostDB:ENSG00000150093" \t "https://www.uniprot.org/uniprotkb/P05556/_blank)  [ENSG00000189403](https://www.veupathdb.org/gene/HostDB:ENSG00000189403" \t "https://www.uniprot.org/uniprotkb/P09429/_blank) | ITGB1-HMGB1 | Docking graph | -8.3 | 3.56 | 3139.6 |
| 26 | [ENSG00000145192](https://www.veupathdb.org/gene/HostDB:ENSG00000145192" \t "https://www.uniprot.org/uniprotkb/P02765/_blank)  [ENSG00000189403](https://www.veupathdb.org/gene/HostDB:ENSG00000189403" \t "https://www.uniprot.org/uniprotkb/P09429/_blank) | AHSG-HMGB1 | Docking graph | -59.6 | 2.87 | 2893.6 |
| 27 | [ENSG00000150093](https://www.veupathdb.org/gene/HostDB:ENSG00000150093" \t "https://www.uniprot.org/uniprotkb/P05556/_blank)  [ENSG00000146678](https://www.veupathdb.org/gene/HostDB:ENSG00000146678" \t "https://www.uniprot.org/uniprotkb/P08833/_blank) | ITGB1-IGFBP1 | Docking graph | -17.2 | 3.27 | 1287.4 |
| 28 | [ENSG00000189403](https://www.veupathdb.org/gene/HostDB:ENSG00000189403" \t "https://www.uniprot.org/uniprotkb/P09429/_blank)  [ENSG00000067225](https://www.veupathdb.org/gene/HostDB:ENSG00000067225" \t "https://www.uniprot.org/uniprotkb/P14618/_blank) | HMGB1-PKM | Docking graph | -90.2 | 3.25 | 5741.8 |
| 29 | [ENSG00000163631](https://www.veupathdb.org/gene/HostDB:ENSG00000163631" \t "https://www.uniprot.org/uniprotkb/P02768/_blank)  [ENSBTAG00000004777](https://www.veupathdb.org/gene/HostDB:ENSBTAG00000004777" \t "https://www.uniprot.org/uniprotkb/P02638/_blank) | ALB-S100B | Docking graph | -1.3 | 2.94 | 477.6 |
| 30 | [ENSG00000138448](https://www.veupathdb.org/gene/HostDB:ENSG00000138448" \t "https://www.uniprot.org/uniprotkb/P06756/_blank)  [ENSG00000164111](https://www.veupathdb.org/gene/HostDB:ENSG00000164111" \t "https://www.uniprot.org/uniprotkb/P08758/_blank) | ITGAV-ANXA5 | Docking graph | -27.9 | 3.04 | 2880.7 |

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|  | Table 3 Molecular docking between ligand and receptor from an LRI predicted by LRI-HDEnHD on Dataset 3 | | | | | |
|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | ENSMUSG00000054693  ENSMUSG00000025809 | Adam10-Itgb1 |  | -37.1 | 3.16 | 2314.9 |
| 2 | ENSMUSG00000024256  ENSMUSG00000025809 | Adcyap1-Itgb1 |  | -51.7 | 3.64 | 3967.4 |
| 3 | ENSMUSG00000022878  ENSMUSG00000025809 | Adipoq-Itgb1 |  | -50.6 | 3.61 | 4672.8 |
| 4 | ENSMUSG00000041936  ENSMUSG00000025809 | Agrn-Itgb1 |  | -48.1 | 3.82 | 3402.4 |
| 5 | ENSMUSG00000031465  ENSMUSG00000025809 | Angpt2-Itgb1 |  | -36.3 | 2.59 | 2351.4 |
| 6 | ENSMUSG00000033544  ENSMUSG00000025809 | Angptl1-Itgb1 |  | -50.1 | 3.04 | 3645.5 |
| 7 | ENSMUSG00000004105  ENSMUSG00000025809 | Angptl2-Itgb1 |  | -43.6 | 2.17 | 3163.8 |
| 8 | ENSMUSG00000028553  ENSMUSG00000025809 | Angptl3-Itgb1 |  | 49.8 | 3.6 | 3776.3 |
| 9 | ENSMUSG00000024659  ENSMUSG00000025809 | Anxa1-Itgb1 |  | -41.9 | 3.25 | 3807.9 |
| 10 | ENSMUSG00000032081  ENSMUSG00000025809 | Apoc3-Itgb1 |  | -40.5 | 3.16 | 2375.5 |
| 11 | ENSMUSG00000022548  ENSMUSG00000025809 | Apod-Itgb1 |  | -63.2 | 3.16 | 3801.1 |
| 12 | ENSMUSG00000002985  ENSMUSG00000025809 | Apoe-Itgb1 |  | -51.4 | 3.35 | 3459.9 |
| 13 | ENSMUSG00000022892  ENSMUSG00000025809 | App-Itgb1 |  | -67.2 | 2.81 | 4244.5 |
| 14 | ENSMUSG00000022892  ENSMUSG00000027087 | App-Itgav |  | -39.3 | 2.6 | 2951.6 |
| 15 | ENSMUSG00000022892  ENSMUSG00000020122 | App-Egfr |  | -31 | 3.31 | 2629.4 |
| 16 | ENSMUSG00000029378  ENSMUSG00000025809 | Areg-Itgb1 |  | -51.7 | 2.91 | 3969.4 |
| 17 | ENSMUSG00000027596  ENSMUSG00000025809 | Asip-Itgb1 |  | -56.6 | 3.15 | 3223.1 |
| 18 | ENSMUSG00000037053  ENSMUSG00000025809 | Azgp1-Itgb1 |  | -57.1 | 3.58 | 4029 |
| 19 | ENSMUSG00000023279  ENSMUSG00000025809 | Bmp15-Itgb1 |  | -52.5 | 2.16 | 3444.4 |
| 20 | ENSMUSG00000027358  ENSMUSG00000025809 | Bmp2-Itgb1 |  | -36.6 | 2.59 | 2285.5 |
| 21 | ENSMUSG00000029335  ENSMUSG00000025809 | Bmp3-Itgb1 |  | -53.6 | 2.7 | 3952.4 |
| 22 | ENSMUSG00000021835  ENSMUSG00000025809 | Bmp4-Itgb1 |  | -38.8 | 2.59 | 2339.4 |
| 23 | ENSMUSG00000032179  ENSMUSG00000025809 | Bmp5-Itgb1 |  | -52.4 | 3.64 | 3400.1 |
| 24 | ENSMUSG00000039004  ENSMUSG00000025809 | Bmp6-Itgb1 |  | -37.3 | 3.16 | 2331.5 |
| 25 | ENSMUSG00000008999  ENSMUSG00000025809 | Bmp7-Itgb1 |  | -50.2 | 3.55 | 3297.9 |
| 26 | ENSMUSG00000082361  ENSMUSG00000025809 | Btc-Itgb1 |  | -56 | 3.29 | 3513.8 |
| 27 | ENSMUSG00000017446  ENSMUSG00000025809 | C1qtnf1-Itgb1 |  | -56.8 | 3.04 | 3499.9 |
| 28 | ENSMUSG00000024164  ENSMUSG00000025809 | C3-Itgb1 |  | -47.5 | 3.48 | 3796.6 |
| 29 | ENSMUSG00000024164  ENSMUSG00000027087 | C3-Itgav |  | -6.9 | 2.52 | 837.5 |
| 30 | ENSMUSG00000024164  ENSMUSG00000020122 | C3-Egfr |  | -8.7 | 3.42 | 1375.1 |

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|  | Ligand-Receptor | LRI (Gene Names) | Molecular docking | Binding energy (kcal/mol) | Hydrogen bonds | Interface area |
| 1 | ENSMUSP00000000127  ENSMUSP00000087457 | Wnt3-Itgb1 |  | -53.5 | 3.23 | 3497.5 |
| 2 | ENSMUSP00000000127  ENSMUSP00000028288 | Wnt3-Notch1 |  | -21.2 | 3.76 | 1698 |
| 3 | ENSMUSP00000000834  ENSMUSP00000087457 | Faslg-Itgb1 |  | -41.6 | 3.35 | 2644.1 |
| 4 | ENSMUSP00000001008  ENSMUSP00000062677 | Ccl3-Ccr4 |  | -22.7 | 3.89 | 2427.9 |
| 5 | ENSMUSP00000001008  ENSMUSP00000052444 | Ccl3-Cxcr3 |  | -30.8 | 3.89 | 2600.7 |
| 6 | ENSMUSP00000001055  ENSMUSP00000087457 | Icam2-Itgb1 |  | -47.6 | 3.07 | 3400.3 |
| 7 | ENSMUSP00000001055  ENSMUSP00000028288 | Icam2-Notch1 |  | -31.7 | 3.07 | 1729.1 |
| 8 | ENSMUSP00000001319  ENSMUSP00000085122 | Efnb2-Fgfr3 |  | -21.7 | 3.56 | 1020.2 |
| 9 | ENSMUSP00000001319  ENSMUSP00000028499 | Efnb2-Itgav |  | -11.5 | 3.58 | 1139 |
| 10 | ENSMUSP00000001319  ENSMUSP00000087457 | Efnb2-Itgb1 |  | -38 | 2.59 | 2334.4 |
| 11 | ENSMUSP00000001319  ENSMUSP00000067305 | Efnb2-Acvr2a |  | -7.5 | 2.93 | 843.7 |
| 12 | ENSMUSP00000001792  ENSMUSP00000028288 | Il16-Notch1 |  | -36.5 | 2.59 | 2421.4 |
| 13 | ENSMUSP00000002360  ENSMUSP00000087457 | Angptl4-Itgb1 |  | -52.9 | 3.42 | 3290.3 |
| 14 | ENSMUSP00000002708  ENSMUSP00000087457 | Shh-Itgb1 |  | -41 | 3.16 | 2513.3 |
| 15 | ENSMUSP00000002708  ENSMUSP00000126108 | Shh-Acvr2b |  | -11.5 | 3.72 | 1346.7 |
| 16 | ENSMUSP00000002708  ENSMUSP00000029948 | Shh-Bmpr1b |  | -3.5 | 2.46 | 593.1 |
| 17 | ENSMUSP00000002708  ENSMUSP00000067305 | Shh-Acvr2a |  | -3.1 | NULL | 275.8 |
| 18 | ENSMUSP00000002708  ENSMUSP00000028288 | Shh-Notch1 |  | -27.6 | 2.92 | 1844.9 |
| 19 | ENSMUSP00000005406  ENSMUSP00000032207 | App-Klrg1 |  | -27.1 | 2.9 | 2598.7 |
| 20 | ENSMUSP00000005406  ENSMUSP00000028111 | App-Il2ra |  | -39.7 | 2.81 | 2804 |
| 21 | ENSMUSP00000005406  ENSMUSP00000028499 | App-Itgav |  | -39.3 | 2.6 | 2951.6 |
| 22 | ENSMUSP00000005406  ENSMUSP00000029948 | App-Bmpr1b |  | -28.2 | 2.81 | 1821.1 |
| 23 | ENSMUSP00000005406  ENSMUSP00000067305 | App-Acvr2a |  | -30.5 | 3.03 | 2470.2 |
| 24 | ENSMUSP00000005406  ENSMUSP00000035900 | App-Bmpr1a |  | -29.4 | 2.81 | 2234 |
| 25 | ENSMUSP00000005406  ENSMUSP00000022871 | App-Sdc2 |  | -29.8 | 3.44 | 2266.6 |
| 26 | ENSMUSP00000005406  ENSMUSP00000028787 | App-Gfra4 |  | -50.1 | 2.22 | 2705.2 |
| 27 | ENSMUSP00000017841  ENSMUSP00000085122 | Ada-Fgfr3 |  | -18.1 | 2.85 | 1095.2 |
| 28 | ENSMUSP00000017841  ENSMUSP00000028499 | Ada-Itgav |  | -7.7 | 2.06 | 1734.7 |
| 29 | ENSMUSP00000017841  ENSMUSP00000087457 | Ada-Itgb1 |  | -39.4 | 2.85 | 3359.9 |
| 30 | ENSMUSP00000017841  ENSMUSP00000028288 | Ada-Notch1 |  | -18.1 | 2.85 | 1240.9 |