**Supplementary Table S5. CDOCKER\_ENERGY between key active compounds**

**and targets (kcal/mol)**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | SX01 | SX02 | SX03 | SX04 | SX11 | SX07 | SX31 | SX27 | SX13 | SX05 |
| FGF1 | -27.07 | 4.92 | 1.97 | 7.00 | -7.74 | -22.06 | -2.59 | -4.11 | -38.21 | 29.62 |
| VEGFA | -21.22 | 9.83 | 15.44 | 18.00 | -0.31 | -18.94 | 7.63 | 6.56 | -29.06 | 39.27 |
| IL2 | -19.90 | 5.95 | 12.44 | 12.97 | 0.23 | -15.25 | 9.47 | 6.04 | -29.85 | 35.67 |
| LGALS3 | -22.81 | 8.38 | 9.63 | 13.04 | -1.82 | -17.71 | 6.53 | -1.70 | -34.94 | 35.61 |
| SLC5A1 | -27.92 | -11.01 | -12.12 | -8.59 | -14.31 | -31.68 | -6.89 | -14.49 | -44.10 | 20.09 |
| F3 | -24.94 | 14.29 | 13.51 | 27.36 | 0.09 | -5.43 | 11.45 | 6.06 | -19.86 | 36.15 |
| ALDH1B1 | -29.62 | 11.79 | 23.49 | 16.61 | -13.51 | -28.87 | 0.99 | 4.60 | -24.23 | 59.96 |
| CES2 | -27.76 | 3.15 | -6.96 | -4.03 | -11.20 | -23.35 | -6.33 | -7.27 | -32.97 | 27.35 |
| IL6 | -26.37 | 12.06 | 10.22 | 15.42 | -3.14 | -17.42 | 6.64 | -1.32 | -30.38 | 32.50 |
| P4HB | -19.07 | 11.81 | 10.37 | 16.90 | 0.30 | -12.82 | 8.62 | 5.80 | -33.19 | 37.54 |
| ESR1 | -35.57 | 7.01 | 7.07 | 20.30 | -6.48 | -24.86 | 16.29 | 12.85 | -3.86 | 42.00 |
| MMP9 | -23.77 | -5.29 | -6.06 | -5.99 | -11.33 | -25.52 | -3.35 | -8.55 | -48.88 | 25.74 |
| HIF1A | -28.66 | -4.02 | -4.20 | 0.83 | -11.41 | -28.22 | -4.41 | -10.90 | -39.94 | 21.41 |
| APP | -25.31 | 2.14 | 5.68 | 8.55 | -7.77 | -21.32 | 2.38 | -4.59 | -32.41 | 35.23 |
| HSPA5 | -33.25 | -2.03 | -3.48 | 0.65 | -30.86 | -43.27 | -10.68 | -2.89 | -53.91 | 16.95 |
| RELA\_NO | -32.32 | -11.75 | -17.25 | -11.50 | -20.56 | -30.32 | -10.19 | -22.30 | -51.73 | 18.35 |
| RELA | -29.08 | 1.33 | 2.31 | ND | -10.61 | -25.92 | -1.37 | -5.31 | -36.45 | 27.97 |
| NFKB1 | -26.29 | 11.39 | 11.31 | 13.55 | -5.21 | -15.02 | -2.30 | 2.06 | -28.96 | 28.88 |