**Supplementary data**

**Research on the Role and Mechanism of *Aloe vera* (L.) Burm.f. in the Treatment of Burn: Based on Network Pharmacology Analysis and Experimental Verification**

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| **Supplementary Table 1. 313 aloe vera related targets** | | | |
| Gene Symbol | | | |
| NOX4 | ESR2 | HTR2B | SGK1 |
| AVPR2 | MPG | PPARG | AURKA |
| AKR1B1 | SLC22A12 | PRKCG | HDAC4 |
| XDH | CDK5R1 | PRKCD | PLG |
| MAOA | CCNB3 | PRKCB | KDM1A |
| IGF1R | ARG1 | PRKCE | MMP1 |
| FLT3 | CDK6 | PRKCQ | TUBB1 |
| CYP19A1 | CDK2 | PREP | CHRNA7 |
| EGFR | TYR | FABP4 | ADAM17 |
| F2 | HSD17B1 | FFAR1 | SLC5A1 |
| CA2 | AHR | FABP3 | FBP1 |
| PIM1 | ESRRA | CNR1 | MCL1 |
| ALOX5 | APP | FAAH | EPHX2 |
| AURKB | PARP1 | FABP5 | HRAS |
| DRD4 | TTR | FABP1 | PNP |
| ADORA1 | MMP12 | SCD | ADK |
| CA7 | CD38 | CYP26B1 | ADA |
| GLO1 | AKR1B10 | CYP26A1 | MMP7 |
| MPO | TNKS2 | PTGDR2 | CDA |
| PIK3R1 | TNKS | PTPN11 | IGFBP3 |
| ADORA2A | TOP1 | RXRA | LGALS3 |
| DAPK1 | TERT | RARG | LGALS9 |
| PYGL | HSD11B1 | RARB | SLC5A2 |
| CA1 | UGT2B7 | RARA | ADORA2B |
| GSK3B | AR | RXRB | ATIC |
| SRC | PTGS1 | RXRG | TP53 |
| PTK2 | NR1H3 | PTGER4 | PRKCA |
| HSD17B2 | ESR1 | FABP2 | PRKACA |
| KDR | CHRM2 | PTGIR | SLC28A3 |
| MMP13 | SLC6A2 | ENPP2 | SLC5A4 |
| MMP3 | SLC6A4 | PTGES2 | TDP1 |
| CA3 | CYP2C19 | LTB4R | SRD5A1 |
| ALOX15 | NR1I3 | PRKCH | TYMP |
| ABCC1 | CDC25A | GRM2 | HSP90AA1 |
| PLK1 | CDC25B | NR0B2 | SLC29A1 |
| CA6 | SAE1UBA2 | PLA2G4A | KLK1 |
| CDK1 | POLB | FFAR4 | KLK2 |
| MMP9 | PTGES | DAGLA | PSMG3 |
| CA12 | GPBAR1 | TRPA1 | LGALS4 |
| MMP2 | SHH | OXER1 | LGALS8 |
| PKN1 | CNR2 | SLC16A1 | LGALS7 |
| CA14 | PTPN1 | PDE4A | IMPDH1 |
| CA9 | TRPM8 | PSEN2 | IMPDH2 |
| CSNK2A1 | HMGCR | DAGLB | VARS |
| ALOX12 | CYP51A1 | GCG | LARS |
| MET | NPC1L1 | GYS1 | CHIA |
| CA4 | CYP17A1 | ALOX5AP | ERBB2 |
| NEK2 | RORC | RBP4 | FYN |
| CXCR1 | SHBG | MMP8 | CHRM1 |
| CAMK2B | SREBF2 | LDHA | MME |
| ALK | BCHE | ACE | ECE1 |
| AKT1 | RORA | ITGAL | ABL1 |
| ABCB1 | SERPINA6 | AGTR1 | MTOR |
| NEK6 | G6PD | HNF4A | PIK3CD |
| PLA2G1B | VDR | TRPV1 | PRKDC |
| CA5A | CES2 | KDM2A | PIK3CB |
| BACE1 | NR1H2 | KDM5C | HCK |
| CYP1B1 | PTGER1 | PLA2G10 | PI4KB |
| AXL | PTGER2 | PDE4D | PIK3CA |
| ABCG2 | DHCR7 | DHODH | LCK |
| NUAK1 | GLRA1 | EDNRA | MAOB |
| AKR1C2 | PPARD | PDE4B | DRD3 |
| AKR1C1 | SQLE | BMP1 | PHLPP1 |
| AKR1C3 | PTPN6 | CCKBR | ILK |
| AKR1C4 | FDFT1 | MDM2 | PTGS2 |
| CA13 | NOS2 | CMA1 | JAK3 |
| AKR1A1 | NR3C1 | CTSG | JAK1 |
| GPR35 | HSD11B2 | FNTA | PDK1 |
| MAPT | DRD2 | PSEN1 | NPY2R |
| KDM4E | NMUR2 | SOAT1 | CYP27B1 |
| TOP2A | ADRA2A | SOAT2 | CTSK |
| INSR | ADRA2C | F2R | PSENEN |
| ACHE | NQO2 | PTPRF | NCSTN |
| MYLK | RPS6KA3 | HPGDS | APH1A |
| SYK | PPARA | ADORA3 | APH1B |
| PIK3CG | PTPN2 | CHEK1 | FNTB |
| APEX1 | TBXAS1 | WEE1 | ICAM1 |
| PTPRS | CCR1 | HSP90AB1 | ITGB2 |
| SIGMAR1 |  |  |  |

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| --- | --- | --- | --- |
| **Supplementary Table 2. 1115 burn related targets** | | | |
| Gene Symbol | | | |
| TXNL4A | CTLA4 | PROM1 | IDH2 |
| TCTN3 | CYCS | GJB6 | MAP2K1 |
| SCN9A | TRPV3 | MIR22 | CD19 |
| IL6 | MIRLET7C | ATP4A | CDC42 |
| TNF | MIR16-1 | FBN1 | DPP4 |
| POLR1A | CRH | CD34 | ACTB |
| IL1B | VCAM1 | AQP4 | DDC |
| CXCL8 | CXCR4 | NREP | SLC1A2 |
| TTR | PRL | COL17A1 | FOXO1 |
| SCN1A-AS1 | JUN | SCN4A | MAPK3 |
| SCN10A | CCN2 | CST3 | NCAM1 |
| TRPV1 | CCND1 | DRD2 | SQSTM1 |
| MECP2 | PDGFRB | MIR125A | TBP |
| SCN11A | ITGAM | MIR196A1 | CD44 |
| IL2 | VIM | MIR31 | CDK1 |
| IL10 | EZH2 | MIR423 | LOX |
| TLR4 | IL3 | MIR19B1 | MCL1 |
| TP53 | IGFBP1 | MIR486-1 | RAB7A |
| CRP | DEFB103B | CDH5 | SLC5A2 |
| ALB | SH3TC2 | SYP | CASP9 |
| CALCA | LORICRIN | IL18R1 | CD27 |
| INS | ACHE | TLR3 | HTR1A |
| ZFHX2 | VWF | ABCB1 | MOG |
| HFE | SCEL | PDCD1 | ANXA5 |
| PTEN | MMP3 | FGF1 | FXN |
| NLRP3 | DNM1L | GDF15 | PTH |
| CD14 | CP | CCL27 | SOX10 |
| FECH | KRT14 | HOTAIR | ATXN3 |
| TGFB1 | COL1A2 | FCGR3A | BCL2L11 |
| THTPA | NOS3 | LBP | CHI3L1 |
| CPT2 | PLG | CYP3A4 | FUS |
| EGF | ELANE | SCN3A | GAD2 |
| CAPN3 | SERPINA1 | FCGR3B | MAOB |
| FKRP | NAGLU | TGIF1 | NEFH |
| FAS | IVL | PPARG | OPA1 |
| POLG | PLCG2 | ADRB2 | S100B |
| CACNA1A | NDRG1 | MIR122 | SOX2 |
| POMC | SPG7 | BCL2L1 | TSPO |
| FGFR3 | BSCL2 | LRRK2 | ATXN1 |
| MPO | CNTNAP1 | HBG2 | ATXN2 |
| VEGFA | MT-ATP6 | F9 | CD63 |
| TAC1 | IRS1 | F8 | CXCL9 |
| ICAM1 | SLC17A5 | ADRA1A | HCRT |
| CCL2 | F12 | FBXO32 | ATXN7 |
| GJA1 | CTSC | SRC | CNTF |
| TLR2 | IL1A | MIR28 | MFN1 |
| MMP9 | RNASE3 | MIR490 | OXT |
| NGF | HLA-DRB1 | F5 | PPIG |
| IL17A | ITGB1 | ESR2 | SMN1 |
| AR | BGLAP | MAPT | SMN2 |
| IGF1 | MYD88 | GCG | SPAST |
| MIR146A | CNR1 | HRAS | DCAF8 |
| CREBBP | BECN1 | MIR140 | HSPB2 |
| SLC6A4 | THBS1 | MIR143 | FIS1 |
| IL4 | CDKN2A | MIR27A | RAB7B |
| MMP2 | MSR1 | MIR30E | MIR191 |
| CSF3 | AARS1 | MIRLET7D | MIR491 |
| HMGB1 | FIG4 | MIR139 | MIRLET7G |
| SOD1 | GARS1 | MIR141 | APRT |
| ARSA | HARS1 | MIR155 | ALK |
| HSPB1 | HINT1 | MIR23A | HDAC2 |
| PSEN1 | SLC34A1 | MIR29A | SHH |
| FUCA1 | GJB3 | MIR30B | EGR1 |
| SETBP1 | LITAF | MIR193A | PAX6 |
| U2AF1 | BAG3 | MIR30A | CYP2D6 |
| FOXG1 | DARS2 | MIR324 | AFP |
| POMGNT1 | GJB4 | MIR330 | APAF1 |
| GALC | HNRNPUL2-BSCL2 | MIR335 | MAP2 |
| IGFBP3 | SERPINF2 | MIR590 | GAP43 |
| KCNV2 | XDH | MIR9-1 | NES |
| ERCC6 | HIF1A | MIR144 | MIAT |
| GLA | PIK3C2A | MIR151A | PRDM12 |
| PNKP | MAPK8 | MIR455 | SCN5A |
| GAMT | UCHL1 | MIR181A1 | MS4A1 |
| EXOSC3 | FGFR2 | MIR338 | ASIC3 |
| KMT2D | CASP1 | MIR224 | CARD9 |
| TSEN54 | CXCL2 | RELA | SKAP2 |
| IL13 | TMPO | NF1 | PLA2G7 |
| TRPV4 | MAPK1 | NCSTN | F11 |
| CCL3 | C1S | SDHC | PLA2G2A |
| SERPINC1 | KLF4 | MIR195 | RASA1 |
| JAK2 | FOS | MIR29B1 | ALPP |
| THPO | CYBB | CD274 | APEX1 |
| CASP3 | ADCY10 | EPO | GC |
| SMAD3 | MT-ND1 | MIR548D1 | IL3RA |
| TF | GJB2 | FLT1 | AASS |
| IL15 | IL6R | PRNP | SERPINB1 |
| TSC2 | KCNN4 | CASK | TFF3 |
| P2RX3 | BRCA2 | PINK1 | SAA4 |
| CSF2 | ATP2C1 | TNFAIP6 | SERPINB4 |
| F2 | MTX2 | HRH2 | ZNF318 |
| CAMK2B | MMP1 | MTOR | ACO1 |
| VLDLR | CD8A | NOTCH1 | MIR10B |
| PLA2G6 | KDM4C | MME | MIR148A |
| TUBB4A | STAT3 | APOA1 | MIR193B |
| ZEB2 | IL2RB | ACE2 | MIR30C1 |
| AMPD2 | IFNA1 | CAV1 | MIR34C |
| GNAO1 | RHOA | GFAP | MIR370 |
| DCX | THBD | CRYAA | MIR99A |
| POMT1 | FGFR4 | SOCS2 | MIR27B |
| TPP1 | BMP6 | VEGFC | MIR15B |
| MLC1 | FLT3LG | IDH1 | MIR361 |
| SRD5A3 | CHRNA4 | UCP1 | MIR485 |
| ZIC2 | PTGS1 | INSR | MIR542 |
| MICU1 | CCL11 | AGTR1 | CDKN2B |
| AP4B1 | KRT10 | GAPDH | ELAVL4 |
| CEP290 | SERPINA3 | CFHR2 | GRIN2A |
| NALCN | ABCB7 | GBA1 | MERTK |
| TBCK | KDR | MAG | SLC1A3 |
| VPS13B | H2AC18 | FOXP3 | RHO |
| TMEM67 | CREB1 | CD80 | LRP1 |
| AP4M1 | TNFRSF1A | LGALS3 | ABCD1 |
| RNASEH2C | CDKN1A | C9orf72 | CA4 |
| TRAPPC9 | CCR5 | PPARD | ABCA4 |
| ASPM | KIT | NLRC3 | PDE6B |
| CLN6 | TXN | AMY1A | CRB1 |
| WDR62 | MIR223 | GSTT1 | RPE65 |
| RNASEH2B | EP300 | CASP8 | SAG |
| AP4B1-AS1 | TRPM8 | SPP1 | BEST1 |
| HLA-B | NTRK1 | PTPRC | RBP3 |
| DEFB4A | AQP3 | PIK3CA | CRX |
| KRT5 | EPHB2 | STAT5B | ERCC8 |
| HLA-A | IFNGR1 | HTR2A | RPGR |
| LUC7L2 | GABBR2 | SOD3 | VDR |
| GJB1 | CYP2A6 | TNFSF12 | LAMC2 |
| MPZ | NBN | TRIM63 | LAMA3 |
| NEFL | CHD7 | TREML1 | LAMB3 |
| HGF | MAD1L1 | KRT20 | CARMIL2 |
| MUC7 | SGPL1 | UROD | XBP1 |
| RNU4ATAC | TRPM4 | CPOX | PAX5 |
| RNU6ATAC | GNB1 | PPOX | CNR2 |
| MIR21 | WARS1 | UROS | SKI |
| ELN | POFUT1 | VTN | EPX |
| IL18 | PSENEN | MIR204 | GSTA1 |
| CXCL12 | RNASEL | MIR185 | TFF2 |
| IL7 | DNASE1L3 | MIR214 | CPQ |
| FLG | ELAC2 | MIR10A | MCRS1 |
| TP63 | KLF6 | MIR146B | MIR1908 |
| PMP22 | PEX6 | MIR150 | KRT12 |
| NOS2 | SRD5A2 | MIR182 | NTRK2 |
| COL1A1 | CTDP1 | MIR210 | ENG |
| PECAM1 | EXOSC9 | MIR93 | ABCA1 |
| CCL5 | HNF1B | MIRLET7A1 | PPARGC1A |
| ARTN | HOXB13 | MIR101-1 | CANX |
| GPT | IARS2 | MIR186 | PCNA |
| EDN1 | IL36RN | MIR18A | FNDC5 |
| AOC1 | POLK | MIR200A | BIRC5 |
| TRPA1 | ZFHX3 | MIR25 | CACNA1B |
| TET2 | DCTN2 | MIR342 | DHFR |
| PRPF4 | GMPPA | MIR483 | FCGR2A |
| PRPF6 | KDSR | MIR92A1 | KCNB1 |
| COMT | LRSAM1 | MIR124-1 | KCNA2 |
| CDH1 | MCM3AP | MIR183 | PEPD |
| CLPX | MORC2 | MIR424 | SCN1B |
| REN | MSMB | MIR106A | SCN4B |
| STAT1 | MXI1 | MIR130B | CD83 |
| CCL4 | POGLUT1 | MIR296 | GYPC |
| LCN2 | AP1S3 | MIR133A1 | IL17RB |
| CALR | EBF3 | MIR532 | LAP3 |
| NOX4 | RAD51D | TNC | KCNS1 |
| KRT3 | SLC26A1 | ACTA1 | HS3ST4 |
| CD36 | KRT83 | CD3E | HCP5 |
| COMP | DRP2 | F13A1 | KRT13 |
| MFN2 | PTPRQ | INHBA | POGZ |
| SERPINE1 | TAMM41 | KRT6A | MIR192 |
| DCN | MIR203A | TAGLN | HADH |
| F3 | MIR449A | S100A11 | HSD17B10 |
| TERT | MIR521-1 | S100A6 | SND1 |
| IL2RA | GULOP | SFRP2 | TINCR |
| GH1 | ZFHX3-AS1 | CHRFAM7A | UPK3A |
| MIR34A | ASIC4-AS1 | KRT222 | PPARA |
| SLPI | HPC3 | HEXD | AQP1 |
| GDAP1 | LOC109504725 | CD74 | ABCB10 |
| KNG1 | PCAP | IGFBP4 | LDLR |
| HPSE2 | GER | DDT | MET |
| LRIG2 | DDD3 | NUDT6 | CDH2 |
| MB | DUPC1 | CDK4 | CDK5 |
| S100A9 | HPC10 | APP | CDK6 |
| BCL2 | HPC14 | NFE2L2 | CTSB |
| BRCA1 | HPC15 | HDAC1 | DNMT1 |
| MIR145 | HPC4 | SIRT1 | CDK2 |
| MIR127 | HPC5 | AKR1B1 | PCSK9 |
| MIR17 | HPC6 | APOB | XIAP |
| MIR200B | HPC7 | NGFR | PRKCA |
| MIR23B | BDNF | CCR7 | VCP |
| NFKBIA | TMEM216 | NTF3 | CD40 |
| SLC6A3 | CAMP | NQO1 | GAD1 |
| IFNG | MIR24-1 | PRODH | SLC12A2 |
| IL1R1 | ERN1 | UCP2 | ACTG1 |
| SF3B4 | CSF1 | CPB2 | DICER1 |
| EFTUD2 | KRAS | SLC2A4 | EIF2AK3 |
| EIF4A3 | MMP28 | MYLK3 | GATA3 |
| SNRPB | CXCR2 | MATN2 | IGF2 |
| SERPINB8 | S100A4 | TYR | MUSK |
| CWC27 | HSPA5 | NAV1 | RPS6KB1 |
| SNRNP40 | GAST | HTT | BACE1 |
| SNORD118 | RBP4 | KLK3 | CLU |
| MIR106B | SCN8A | MIR574 | GLI1 |
| SELE | C3 | MIR202 | HNRNPA1 |
| NFKB1 | MIR181C | CTSD | MITF |
| MYLK | GSTM1 | MDM2 | MYCN |
| SPTLC1 | FLT3 | TH | NF2 |
| LACTB | APC | KCNQ2 | RB1 |
| DKK1 | SST | SNAP25 | ATRX |
| PTGS2 | ICOSLG | GZMB | CCNB1 |
| IKZF1 | CISH | STAT5A | PRF1 |
| PRX | DST | CYP2C19 | TARDBP |
| MC1R | SMAD2 | AVP | VDAC1 |
| TIMP1 | APOE | CNTNAP2 | ALDH18A1 |
| ALAS2 | BRD4 | LGI1 | CCNA2 |
| TGFA | MIR199A1 | AMPH | DMD |
| USH2A | GDNF | EPRS1 | FOXO3 |
| ACE | SMAD7 | LAMP1 | NTF4 |
| BCHE | AZU1 | GJC2 | SMARCB1 |
| NPY | B2M | HSPD1 | SNAI1 |
| RPL36A-HNRNPH2 | ESR1 | ADM | E2F4 |
| HBEGF | MIR142 | C2CD3 | EWSR1 |
| NPPB | FN1 | CSPP1 | PDYN |
| CAT | TGFB3 | DDX59 | POU5F1 |
| IL5 | LIN28A | TMEM231 | RAB5A |
| SELP | MAOA | DYNC2I2 | CD86 |
| FGFR1 | FMR1 | CPLANE1 | OPTN |
| ATM | NOS1 | SCN7A | TFAM |
| LMNA | SERPINH1 | BNC2 | ADGRG1 |
| CHAT | SLURP1 | MBL2 | CHL1 |
| DYNC1H1 | JAK1 | SPI1 | E2F1 |
| MIR331 | PLAU | AGER | MCOLN1 |
| NPPA | TREM1 | LIF | MYOC |
| MIR205 | MBP | DPP3 | PHOX2B |
| MIR20A | MKI67 | PTPN5 | SLC26A4 |
| MIR221 | BMP2 | DCD | TUSC3 |
| MIR222 | S100A8 | MIR451A | ATL1 |
| MIR15A | GUSB | DPYD | PLP1 |
| VIP | MIRLET7B | IREB2 | CTRL |
| HMOX1 | KLK11 | B3GNT2 | E2F3 |
| PLAT | TFRC | CD68 | CALB2 |
| KRT19 | MIR125B1 | MIR582 | AIF1 |
| EGFR | PRKN | MIR103A1 | HSPB3 |
| IL1RN | HPRT1 | MIR362 | MIA2 |
| HP | ABCG2 | PROX1 | TBC1D24 |
| CCR6 | SERPINA6 | PARK7 | LCOR |
| FGF7 | MIR506 | CCL4L1 | MYO18A |
| HSP90AA1 | PTK2 | GSR | TBL1X |
| ERBB2 | DNMT3A | BMP4 | BLOC1S1 |
| FGF2 | ADIPOQ | NR3C1 | RBFOX3 |
| TGFB2 | SCN1A | SOD2 | TCHP |
| RET | OFD1 | PRKAR1A | MT-CO1 |
| IFNB1 | CDKN1B | TNFRSF1B | CFAP47 |
| MIR126 | IGFBP2 | FGA | MIR26B |
| CFTR | KRT7 | NCF2 | MIR32 |
| CXCL1 | SNCA | TNFAIP3 | MIR132 |
| GHRL | MIR149 | MYLK2 | MIR34B |
| PARP1 | CHRNA7 | NPTN-IT1 | MIR503 |
| IFNA2 | SNAI2 | GGT1 | MIR96 |
| FASLG | AMBP | RASA2 | MIR99B |
| LEP | FOXE1 | MTHFR | MIR181B1 |
| LCN1 | GSN | ITGB4 | MIR301A |
| HSPA4 | MSTN | ITGAV | MIR339 |
| MIR100 | GHR | ADRA1B | MIR345 |
| DEFB1 | LOC110806262 | PRKCB | MIR425 |
| MPL | ATP12A | ADRA1D | MIR218-1 |
| SH2B3 | TGFBR1 | CS | MIR340 |
| CUX2 | PLAUR | PTAFR | MIR409 |
| IGHMBP2 | BDKRB1 | APCS | MIR708 |
| RLS4 | RUNX2 | CXCL5 | H3-7 |
| RLS1 | CHGA | H1-2 | MIR432 |
| RLS2 | KRT1 | TNXA | MIR323A |
| RLS3 | FCER2 | MIR762 | MIR548B |
| RLS5 | UMOD | TRD | MIR7-1 |
| RLS6 | TJP1 | TRG | MIR380 |
| RLS7 | SOCS3 | PF4 | TNFRSF6 |
| RLS8 | SCN2A | TEK | DIM1 |
| LBR | ENO2 | H2BC21 | APT1 |
| CHEK2 | CXCR3 | HPGD | CD95 |
| AKT1 | CTNNB1 | MIR466 | ALPS1A |
| CD4 | DYNC2I1 | IGF1R | BMKS |
| MYC | CD40LG | HDAC6 | ODC1 |
| ADGRE2 | HMBS | PDGFRA | AMD1 |
| CXCL10 |  | SLC2A1 | Bact CM |

|  |  |  |  |
| --- | --- | --- | --- |
| **Receptor** | **Original Ligand** | **Binding Energy (kcal / mol)** | **RMSD** |
| SRC\_2src | ANP | -0.81 | 2.794 |
| TP53\_5aom | FY8 | -8.3 | 1.383 |
| ESR1\_1x7r | GEN | -8.41 | 0 |
| EGFR\_5cas | 4ZQ | -4.86 | 1.94 |
| AR\_3b66 | B66 | -6.3 | 1.098 |
| PTK2\_4i4e | 1BQ | -9.21 | 0.068 |
| HSP90AA1\_3bm9 | BXZ | -7.04 | 0.038 |
| MDM2\_5j7g | 6GG | -7.81 | 1.863 |
| PIK3CA-4jps | 1LT | -4.7 | 1.953 |
| AKT1\_4ejn | 0R4 | -6.41 | 1.401 |
| HRAS\_1clu | DGB | -0.98 | 3.496 |

**Supplementary Table 4.** **Part 1. Binding energy between receptor and original ligand**

**Supplementary Table 4.** **Part 2. Binding energy between receptor and QUE (or AA) ligand**

|  |  |  |
| --- | --- | --- |
| **Receptor** | **QUE (kcal / mol)** | **AA (kcal / mol)** |
| SRC\_2src | -9.1 | -6.8 |
| TP53\_5aom | -7.1 | -5.1 |
| ESR1\_1x7r | -7 | -7.7 |
| EGFR\_5cas | -8.4 | -5.3 |
| AR\_3b66 | -7.4 | -5.9 |
| PTK2\_4i4e | -7.9 | -6.1 |
| HSP90AA1\_3bm9 | -7.5 | -6 |
| MDM2\_5j7g | -7.2 | -6.5 |
| PIK3CA-4jps | -9.3 | -6 |
| AKT1\_4ejn | -9.4 | -6.9 |
| HRAS | -8.2 | -5.8 |
| abe | -8 | -6.2 |

abe=average binding energy, kcal / mol