| No. | Target  | N0  | Target  | N0  | Target  | N0  | Target  | N0  | Target  |
|-----|---------|-----|---------|-----|---------|-----|---------|-----|---------|
| 1   | ABCG2   | 54  | CHEK1   | 107 | GABRA3  | 160 | METAP1  | 213 | PRKCA   |
| 2   | ACACA   | 55  | CHEK2   | 108 | GABRA5  | 161 | MGAM    | 214 | PRKCB   |
| 3   | ACHE    | 56  | CHRM1   | 109 | GBA     | 162 | MMP1    | 215 | PRSS1   |
| 4   | ACP3    | 57  | CHRM2   | 110 | GC      | 163 | MMP13   | 216 | PSMD3   |
| 5   | ADAM17  | 58  | CHRM3   | 111 | GJA1    | 164 | MMP2    | 217 | PTEN    |
| 6   | ADRA1A  | 59  | CHRM4   | 112 | GRIA2   | 165 | MMP3    | 218 | PTGER3  |
| 7   | ADRA1B  | 60  | CHRNA2  | 113 | GSK3B   | 166 | MMP9    | 219 | PTGS1   |
| 8   | ADRB2   | 61  | CHRNA7  | 114 | GSR     | 167 | MPO     | 220 | PTGS2   |
| 9   | AHR     | 62  | CHUK    | 115 | GSTM1   | 168 | MTAP    | 221 | PTPN1   |
| 10  | AHSA1   | 63  | CLC     | 116 | GSTM2   | 169 | MYC     | 222 | PYGM    |
| 11  | AKR1B1  | 64  | CLDN4   | 117 | GSTP1   | 170 | NCF1    | 223 | QPCT    |
| 12  | AKR1C2  | 65  | CLPP    | 118 | HAS2    | 171 | NCOA1   | 224 | RAF1    |
|   | Gene | Rank |   | Gene | Rank |   | Gene | Rank |   | Gene | Rank |
|---|------|------|---|------|------|---|------|------|---|------|------|
| 13 | AKR1C3 | 66 | CMA1 | 119 | HCK | 172 | NCOA2 | 225 | RASA1 |
| 14 | AKT1 | 67 | COL1A1 | 120 | HERC5 | 173 | NFE2L2 | 226 | RASSF1 |
| 15 | ALB | 68 | COL3A1 | 121 | HIF1A | 174 | NFKBIA | 227 | RB1 |
| 16 | ALOX5 | 69 | CRP | 122 | HK2 | 175 | NKX3-1 | 228 | RELA |
| 17 | AMY1A | 70 | CTSD | 123 | HMOX1 | 176 | NOS2 | 229 | RORA |
| 18 | AMY1B | 71 | CTSS | 124 | HSD11B1 | 177 | NOS3 | 230 | RUNX1T1 |
| 19 | AMY1C | 72 | CXCL10 | 125 | HSD17B1 | 178 | NPEPPS | 231 | RUNX2 |
| 20 | ANXA5 | 73 | CXCL1 | 126 | HSD17B11 | 179 | NQO1 | 232 | RXRA |
| 21 | APOA2 | 74 | CXCL2 | 127 | HSF1 | 180 | NQO2 | 233 | SCN5A |
| 22 | AR | 75 | CXCL8 | 128 | HSP90AA1 | 181 | NR1H2 | 234 | SEC14L2 |
| 23 | AURKA | 76 | CYP19A1 | 129 | HSP90AB1 | 182 | NR1I2 | 235 | SELE |
| 24 | BACE1 | 77 | CYP1A1 | 130 | HSPA5 | 183 | NR1I3 | 236 | SERPINE1 |
| 25 | BAX | 78 | CYP1A2 | 131 | HSPA8 | 184 | NR3C2 | 237 | SLC2A4 |
| 26 | BCHE | 79 | CYP1B1 | 132 | HSPB1 | 185 | NUDT9 | 238 | SLC6A2 |
| 27 | BCL2 | 80 | CYP3A4 | 133 | HTR2A | 186 | ODC1 | 239 | SLC6A4 |
|   | Gene 1 |   | Gene 2 |   | Gene 3 |   | Gene 4 |   | Gene 5 |   | Gene 6 |
|---|--------|---|--------|---|--------|---|--------|---|--------|---|--------|
|28| BCL2L1 | 81| DCAF5 | 134| ICAM1 | 187| OLR1  | 240| SLPI   |   |        |
|29| BIRC5  | 82| DDX6  | 135| IFNG  | 188| OPRM1 | 241| SOD1   |   |        |
|30| BMP2   | 83| DIO1  | 136| IGF2  | 189| PAH   | 242| SPP1   |   |        |
|31| CA1    | 84| DPP4  | 137| IGFBP3| 190| PARP1 | 243| SRC    |   |        |
|32| CA12   | 85| DRD1  | 138| IKBKB | 191| PCOLCE| 244| STAT1  |   |        |
|33| CA2    | 86| DUOX2 | 139| IL10  | 192| PDE3A | 245| STS    |   |        |
|34| CALM1  | 87| E2F1  | 140| IL1A  | 193| PDE4B | 246| SULT1E1|   |        |
|35| CASP3  | 88| E2F2  | 141| IL1B  | 194| PDE4D | 247| SULT2A1|   |        |
|36| CASP7  | 89| EGF   | 142| IL2   | 195| PGR   | 248| TGFBI  |   |        |
|37| CASP8  | 90| EGFR  | 143| IL6   | 196| PIK3CG| 249| TGFBR1 |   |        |
|38| CASP9  | 91| EIF6  | 144| IMPA1 | 197| PIM1  | 250| TGFBR2 |   |        |
|39| CAV1   | 92| ELK1  | 145| INSR  | 198| PLAT  | 251| THBD   |   |        |
|40| CCL2   | 93| EPHB4 | 146| IRF1  | 199| PLAU  | 252| THRBB  |   |        |
|41| CCNA2  | 94| ERBB2 | 147| ITGAL | 200| PLG   | 253| TNF    |   |        |
|42| CCNB1  | 95| ERBB3 | 148| JUN   | 201| PNMT  | 254| TOP2A  |   |        |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 43 | CCND1 | 96 | ESR1 | 149 | KCNH2 | 202 |
| 44 | CD40LG | 97 | ESR2 | 150 | KDR | 203 |
| 45 | CDK1 | 98 | F10 | 151 | KIF11 | 204 |
| 46 | CDK2 | 99 | F2 | 152 | LCN2 | 205 |
| 47 | CDK5R1 | 100 | F3 | 153 | MAOB | 206 |
| 48 | CDK6 | 101 | F7 | 154 | MAP2 | 207 |
| 49 | CDKN1A | 102 | FAP | 155 | MAPK1 | 208 |
| 50 | CDKN2A | 103 | FKBPA1 | 156 | MAPK10 | 209 |
| 51 | CES1 | 104 | FOS | 157 | MAPK14 | 210 |
| 52 | CFB | 105 | GABRA1 | 158 | MAPK8 | 211 |
| 53 | CFD | 106 | GABRA2 | 159 | MAPKAPK2 | 212 |

**Abbreviation:** ALRP-LSDS, Aconiti Lateralis Radix Praeparata and Lepidii Semen Descurainiae Semen
| Compound                  | AKT1 | CASP3 | MAPK1 |
|--------------------------|------|-------|-------|
| Deltoin                  | -9.5 | -6.1  | -7.6  |
| Deoxyandrographolide     | -9.2 | -7.0  | -6.8  |
| Karakoline               | -6.4 | -5.1  | -6.3  |
| Karanjin                 | -10.2| -7.4  | -8.3  |
| Neokadsuranic acid B     | -7.1 | -6.3  | -7.1  |
| Benzoynapelline          | -2.3 | -6.6  | -5.7  |
| Deoxyaconitine           | -5.2 | -4.9  | -4.1  |
| (R)-Norcoclaurine        | -9.1 | -6.4  | -8.3  |
| Ignavine                 | -8.8 | -6.2  | -7.9  |
|                |       |       |       |
|----------------|-------|-------|-------|
| Jesaconitine   | -1.8  | -2.7  | -2.0  |
| Sitosterol     | -9.6  | -5.6  | -8.8  |
| Hypaconitine   | -0.7  | -4.5  | -0.5  |

**Abbreviation:** ALRP, *Aconiti Lateralis Radix Praeparata*
| Compound             | Binding Energy/(kcal·mol) |
|----------------------|---------------------------|
|                      | AKT1 | CASP3 | MAPK1 |
| Isorhamnetin         | -9.7 | -6.7  | -8.0  |
| β-sitosterol         | -10.8| -6.0  | -9.1  |
| Erysimoside          | -6.4 | -2.0  | -3.8  |
| Cynotoxin            | -6.2 | -5.6  | -7.4  |
| Dihomolinolenic acid | -7.0 | -4.6  | -6.3  |
| Kaempferol           | -9.2 | -7.0  | -8.3  |
| Quercetin            | -9.4 | -6.8  | -8.3  |

**Abbreviation:** LSDS, *Lepidii Semen Descurainiae Semen*
