**Table S1**

93 compounds from WPX and their corresponding predicted OB, DL, Caco-2 scores and structures. 88 compounds that meet the parameters which OB ≥ 30%, DL ≥ 0.18, Caco-2 ≥0 were preserved as active compounds. 5 compounds which not meet the criterion but have been validated with various pharmaceutical activities were also reserved as the active components.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **No.** | **Mol ID** | **Molecule name** | **OB** | **DL** | **Caco-2** | **Structure** | **Herb** |
| 1 | MOL000006 | Luteolin | 36.16 | 0.25 | 0.19 |  | *PR，RS* |
| 2 | MOL000020 | 12-senecioyl-2E,8E,10E-atractylentriol | 62.40 | 0.22 | 0.01 |  | *AMK* |
| 3 | MOL000021 | 14-acetyl-12-senecioyl-2E,8E,10E-atractylentriol | 60.31 | 0.31 | 0.33 |  | *AMK* |
| 4 | MOL000022 | 14-acetyl-12-senecioyl-2E,8Z,10E-atractylentriol | 63.37 | 0.30 | 0.42 |  | *AMK* |
| 5 | MOL000028 | α-Amyrin | 39.51 | 0.76 | 1.42 |  | *AMK* |
| 6 | MOL000033 | (3S,8S,9S,10R,13R,14S,17R)-10,13-dimethyl-17-[(2R,5S)-5-propan-2-yloctan-2-yl]-2,3,4,7,8,9,11,12,14,15,16,17-dodecahydro-1H-cyclopenta[a]phenanthren-3-ol | 36.23 | 0.78 | 1.45 |  | *HMM，AMK* |
| 7 | MOL000043 | AtractylenolideⅠ | 37.37 | 0.15 | 1.30 |  | *AMK* |
| 8 | MOL000049 | 3β-acetoxyatractylone | 54.07 | 0.22 | 1.13 |  | *AMK* |
| 9 | MOL000072 | 8β-ethoxy atractylenolide Ⅲ | 35.95 | 0.21 | 1.08 |  | *AMK* |
| 10 | MOL000098 | Quercetin | 46.43 | 0.28 | 0.05 |  | *HMM，HDH* |
| 11 | MOL000211 | Mairin | 55.38 | 0.78 | 0.73 |  | *HMM* |
| 12 | MOL000239 | Jaranol | 50.83 | 0.29 | 0.61 |  | *HMM* |
| 13 | MOL000263 | Oleanolic acid | 29.02 | 0.76 | 0.59 |  | *RS，HDH* |
| 14 | MOL000296 | Hederagenin | 36.91 | 0.75 | 1.32 |  | *HMM，CR* |
| 15 | MOL000354 | Isorhamnetin | 49.60 | 0.31 | 0.31 |  | *HMM* |
| 16 | MOL000358 | Beta-sitosterol | 36.91 | 0.75 | 1.32 |  | *PR，HDH* |
| 17 | MOL000371 | 3,9-di-O-methylnissolin | 53.74 | 0.48 | 1.18 |  | *HMM* |
| 18 | MOL000378 | 7-O-methylisomucronulatol | 74.69 | 0.30 | 1.08 |  | *HMM* |
| 19 | MOL000380 | (6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol | 64.26 | 0.42 | 0.93 |  | *HMM* |
| 20 | MOL000387 | Bifendate | 31.10 | 0.67 | 0.15 |  | *HMM* |
| 21 | MOL000392 | Formononetin | 69.67 | 0.21 | 0.78 |  | *HMM* |
| 22 | MOL000398 | Isoflavanone | 109.99 | 0.30 | 0.53 |  | *HMM* |
| 23 | MOL000409 | Astragaloside IV | 17.74 | 0.15 | (2.22) |  | *HMM* |
| 24 | MOL000417 | Calycosin | 47.75 | 0.24 | 0.52 |  | *HMM* |
| 25 | MOL000422 | kaempferol | 41.88 | 0.24 | 0.26 |  | *HMM* |
| 26 | MOL000438 | (3R)-3-(2-hydroxy-3,4-dimethoxyphenyl)chroman-7-ol | 67.67 | 0.26 | 0.96 |  | *HMM* |
| 27 | MOL000442 | 1,7-Dihydroxy-3,9-dimethoxy pterocarpene | 39.05 | 0.48 | 0.89 |  | *HMM* |
| 28 | MOL000449 | Stigmasterol | 43.83 | 0.76 | 1.44 |  | *HDH* |
| 29 | MOL000902 | Curcumol | 103.55 | 0.13 | 1.12 |  | *CR* |
| 30 | MOL000906 | Wenjine | 47.93 | 0.27 | 0.30 |  | *CR* |
| 31 | MOL000940 | Bisdemethoxycurcumin | 77.38 | 0.26 | 0.49 |  | *CR* |
| 32 | MOL001506 | Supraene | 33.55 | 0.42 | 2.08 |  | *PR* |
| 33 | MOL001601 | 1,2,5,6-tetrahydrotanshinone | 38.75 | 0.36 | 0.96 |  | *RS* |
| 34 | MOL001646 | 2,3-dimethoxy-6-methyanthraquinone | 34.86 | 0.26 | 0.75 |  | *HDH* |
| 35 | MOL001659 | Poriferasterol | 43.83 | 0.76 | 1.44 |  | *RS，HDH* |
| 36 | MOL001663 | (4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid | 32.03 | 0.76 | 0.61 |  | *HDH* |
| 37 | MOL001670 | 2-methoxy-3-methyl-9,10-anthraquinone | 37.83 | 0.21 | 0.73 |  | *HDH* |
| 38 | MOL001689 | Acacetin | 34.97 | 0.24 | 0.67 |  | *PR* |
| 39 | MOL001771 | Poriferast-5-en-3beta-ol | 36.91 | 0.75 | 1.45 |  | *RS* |
| 40 | MOL001942 | Isoimperatorin | 45.46 | 0.23 | 0.97 |  | *RS* |
| 41 | MOL002222 | Sugiol | 36.11 | 0.28 | 1.14 |  | *RS* |
| 42 | MOL002464 | 1-Monolinolein | 37.18 | 0.30 | 0.32 |  | *PR* |
| 43 | MOL002651 | Dehydrotanshinone II A | 43.76 | 0.40 | 1.02 |  | *RS* |
| 44 | MOL006554 | Taraxerol | 38.40 | 0.77 | 1.37 |  | *PR* |
| 45 | MOL006756 | Schottenol | 37.42 | 0.75 | 1.33 |  | *PR* |
| 46 | MOL006824 | α-amyrin | 39.51 | 0.76 | 1.37 |  | *RS* |
| 47 | MOL007036 | 5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one | 33.77 | 0.29 | 1.19 |  | *RS* |
| 48 | MOL007041 | 2-isopropyl-8-methylphenanthrene-3,4-dione | 40.86 | 0.23 | 1.23 |  | *RS* |
| 49 | MOL007045 | 3α-hydroxytanshinoneⅡA | 44.93 | 0.44 | 0.53 |  | *RS* |
| 50 | MOL007048 | (E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-benzofuran-4-yl]acrylic acid | 48.24 | 0.31 | 0.18 |  | *RS* |
| 51 | MOL007049 | 4-methylenemiltirone | 34.35 | 0.23 | 1.25 |  | *RS* |
| 52 | MOL007050 | 2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde | 62.78 | 0.40 | 0.35 |  | *RS* |
| 53 | MOL007058 | Formyltanshinone | 73.44 | 0.42 | 0.54 |  | *RS* |
| 54 | MOL007059 | 3-beta-Hydroxymethyllenetanshiquinone | 32.16 | 0.41 | 0.38 |  | *RS* |
| 55 | MOL007061 | Methylenetanshinquinone | 37.07 | 0.36 | 1.03 |  | *RS* |
| 56 | MOL007064 | Przewalskin B | 110.32 | 0.44 | 0.34 |  | *RS* |
| 57 | MOL007068 | Przewaquinone B | 62.24 | 0.41 | 0.39 |  | *RS* |
| 58 | MOL007069 | Przewaquinone C | 55.74 | 0.40 | 0.42 |  | *RS* |
| 59 | MOL007077 | Sclareol | 43.67 | 0.21 | 0.84 |  | *RS* |
| 60 | MOL007079 | Tanshinaldehyde | 52.47 | 0.45 | 0.57 |  | *RS* |
| 61 | MOL007081 | Danshenol B | 57.95 | 0.56 | 0.53 |  | *RS* |
| 62 | MOL007082 | Danshenol A | 56.97 | 0.52 | 0.33 |  | *RS* |
| 63 | MOL007085 | Salvilenone | 30.38 | 0.38 | 1.46 |  | *RS* |
| 64 | MOL007088 | Cryptotanshinone | 52.34 | 0.40 | 0.95 |  | *RS* |
| 65 | MOL007093 | Dan-shexinkum d | 38.88 | 0.55 | 0.67 |  | *RS* |
| 66 | MOL007094 | Danshenspiroketallactone | 50.43 | 0.31 | 0.88 |  | *RS* |
| 67 | MOL007098 | Deoxyneocryptotanshinone | 49.40 | 0.29 | 0.85 |  | *RS* |
| 68 | MOL007100 | Dihydrotanshinlactone | 38.68 | 0.32 | 1.26 |  | *RS* |
| 69 | MOL007101 | DihydrotanshinoneⅠ | 45.04 | 0.36 | 0.95 |  | *RS* |
| 70 | MOL007105 | Epidanshenspiroketallactone | 68.27 | 0.31 | 0.90 |  | *RS* |
| 71 | MOL007107 | C09092 | 36.07 | 0.25 | 1.63 |  | *RS* |
| 72 | MOL007108 | Isocryptotanshi-none | 54.98 | 0.39 | 0.93 |  | *RS* |
| 73 | MOL007111 | Isotanshinone II | 49.92 | 0.40 | 1.03 |  | *RS* |
| 74 | MOL007115 | Manool | 45.04 | 0.20 | 1.28 |  | *RS* |
| 75 | MOL007118 | Microstegiol | 39.61 | 0.28 | 1.05 |  | *RS* |
| 76 | MOL007119 | Miltionone Ⅰ | 49.68 | 0.32 | 0.35 |  | *RS* |
| 77 | MOL007120 | Miltionone Ⅱ | 71.03 | 0.44 | 0.62 |  | *RS* |
| 78 | MOL007121 | Miltipolone | 36.56 | 0.37 | 0.50 |  | *RS* |
| 79 | MOL007122 | Miltirone | 38.76 | 0.25 | 1.23 |  | *RS* |
| 80 | MOL007123 | Miltirone Ⅱ | 44.95 | 0.24 | 0.04 |  | *RS* |
| 81 | MOL007124 | Neocryptotanshinone Ⅱ | 39.46 | 0.23 | 0.76 |  | *RS* |
| 82 | MOL007125 | Neocryptotanshinone | 52.49 | 0.32 | 0.35 |  | *RS* |
| 83 | MOL007127 | 1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione | 34.72 | 0.37 | 0.50 |  | *RS* |
| 84 | MOL007130 | Prolithospermic acid | 64.37 | 0.31 | 0.10 |  | *RS* |
| 85 | MOL007134 | Danshensu | 36.91 | 0.06 | -0.27 |  | *RS* |
| 86 | MOL007143 | Salvilenone Ⅰ | 32.43 | 0.23 | 1.13 |  | *RS* |
| 87 | MOL007145 | Salviolone | 31.72 | 0.24 | 1.04 |  | *RS* |
| 88 | MOL007149 | NSC 122421 | 34.49 | 0.28 | 1.08 |  | *RS* |
| 89 | MOL007150 | (6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone | 75.39 | 0.46 | 0.03 |  | *RS* |
| 90 | MOL007151 | Tanshindiol B | 42.67 | 0.45 | 0.05 |  | *RS* |
| 91 | MOL007154 | Tanshinone Ⅱa | 49.89 | 0.40 | 1.05 |  | *RS* |
| 92 | MOL007155 | (6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione | 65.26 | 0.45 | 0.44 |  | *RS* |
| 93 | MOL007156 | Tanshinone Ⅵ | 45.64 | 0.30 | 0.48 |  | *RS* |

**Table S2**

The information of GPL-related targets. By combining the compound targets of WPX and the disease related targets, 146 overlapping ones were selected as the key targets in the treatment of GPL.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ID | UniProt | Protein names | Gene names | Organism |
| T01 | Q9UNQ0 | ATP-binding cassette sub-family G member 2 | ABCG2 | Homo sapiens |
| T02 | P15309 | Prostatic acid phosphatase | ACPP | Homo sapiens |
| T03 | P00326 | Alcohol dehydrogenase 1C | ADH1C | Homo sapiens |
| T04 | P35869 | Aryl hydrocarbon receptor | AHR | Homo sapiens |
| T05 | P15121 | Aldose reductase | AKR1B1 | Homo sapiens |
| T06 | O60218 | Aldo-keto reductase family 1 member B10 | AKR1B10 | Homo sapiens |
| T07 | P31749 | RAC-alpha serine/threonine-protein kinase | AKT1 | Homo sapiens |
| T08 | P18054 | Arachidonate 12-lipoxygenase, 12S-type | ALOX12 | Homo sapiens |
| T09 | P09917 | Arachidonate 5-lipoxygenase | ALOX5 | Homo sapiens |
| T10 | P10275 | Androgen receptor | AR | Homo sapiens |
| T11 | Q07812 | Apoptosis regulator BAX | BAX | Homo sapiens |
| T12 | P10415 | Apoptosis regulator Bcl-2 | BCL2 | Homo sapiens |
| T13 | Q07817 | Bcl-2-like protein 1 | BCL2L1 | Homo sapiens |
| T14 | O15392 | Baculoviral IAP repeat-containing protein 5 | BIRC5 | Homo sapiens |
| T15 | P42574 | Caspase-3 | CASP3 | Homo sapiens |
| T16 | Q14790 | Caspase-8 | CASP8 | Homo sapiens |
| T17 | P55211 | Caspase-9 | CASP9 | Homo sapiens |
| T18 | Q03135 | Caveolin-1 | CAV1 | Homo sapiens |
| T19 | P13500 | C-C motif chemokine 2 | CCL2 | Homo sapiens |
| T20 | P20248 | Cyclin-A2 | CCNA2 | Homo sapiens |
| T21 | P14635 | G2/mitotic-specific cyclin-B1 | CCNB1 | Homo sapiens |
| T22 | P24385 | G1/S-specific cyclin-D1 | CCND1 | Homo sapiens |
| T23 | P06493 | Cell division control protein 2 homolog | CDK1 | Homo sapiens |
| T24 | P24941 | Cell division protein kinase 2 | CDK2 | Homo sapiens |
| T25 | P11802 | Cell division protein kinase 4 | CDK4 | Homo sapiens |
| T26 | P38936 | Cyclin-dependent kinase inhibitor 1 | CDKN1A | Homo sapiens |
| T27 | P42771 | Cyclin-dependent kinase inhibitor 2A, isoforms 1/2/3 | CDKN2A | Homo sapiens |
| T28 | O14757 | Serine/threonine-protein kinase Chk1 | CHEK1 | Homo sapiens |
| T29 | O96017 | Serine/threonine-protein kinase Chk2 | CHEK2 | Homo sapiens |
| T30 | O14493 | Claudin-4 | CLDN4 | Homo sapiens |
| T31 | P02452 | Collagen alpha-1(I) chain | COL1A1 | Homo sapiens |
| T32 | P02741 | C-reactive protein | CRP | Homo sapiens |
| T33 | P07339 | Cathepsin D | CTSD | Homo sapiens |
| T34 | P10145 | Interleukin-8 | CXCL8 | Homo sapiens |
| T35 | P11511 | Cytochrome P450 19A1 | CYP19A1 | Homo sapiens |
| T36 | P04798 | Cytochrome P450 1A1 | CYP1A1 | Homo sapiens |
| T37 | P05177 | Cytochrome P450 1A2 | CYP1A2 | Homo sapiens |
| T38 | Q16678 | Cytochrome P450 1B1 | CYP1B1 | Homo sapiens |
| T39 | P08684 | Cytochrome P450 3A4 | CYP3A4 | Homo sapiens |
| T40 | P27487 | Dipeptidyl peptidase IV | DPP4 | Homo sapiens |
| T41 | Q01094 | Transcription factor E2F2 | E2F1 | Homo sapiens |
| T42 | P01133 | Pro-epidermal growth factor | EGF | Homo sapiens |
| T43 | P00533 | Epidermal growth factor receptor | EGFR | Homo sapiens |
| T44 | P19419 | ETS domain-containing protein Elk-1 | ELK1 | Homo sapiens |
| T45 | P04626 | Receptor tyrosine-protein kinase erbB-2 | ERBB2 | Homo sapiens |
| T46 | P21860 | Receptor tyrosine-protein kinase erbB-3 | ERBB3 | Homo sapiens |
| T47 | P03372 | Estrogen receptor | ESR1 | Homo sapiens |
| T48 | Q92731 | Estrogen receptor beta | ESR2 | Homo sapiens |
| T49 | P13726 | Tissue factor | F3 | Homo sapiens |
| T50 | P48023 | Tumor necrosis factor ligand superfamily member 6 | FASLG | Homo sapiens |
| T51 | P49327 | Fatty acid synthase | FASN | Homo sapiens |
| T52 | P05230 | Fibroblast growth factor 1 | FGF1 | Homo sapiens |
| T53 | P09038 | Fibroblast growth factor 2 | FGF2 | Homo sapiens |
| T54 | P17948 | Vascular endothelial growth factor receptor 1 | FLT1 | Homo sapiens |
| T55 | P35916 | Vascular endothelial growth factor receptor 3 | FLT4 | Homo sapiens |
| T56 | P01100 | Proto-oncogene c-Fos | FOS | Homo sapiens |
| T57 | P17302 | Gap junction alpha-1 protein | GJA1 | Homo sapiens |
| T58 | P49841 | Glycogen synthase kinase-3 beta | GSK3B | Homo sapiens |
| T59 | P09488 | Glutathione S-transferase Mu 1 | GSTM1 | Homo sapiens |
| T60 | P09211 | Glutathione S-transferase P | GSTP1 | Homo sapiens |
| T61 | P14210 | Hepatocyte growth factor receptor | HGF | Homo sapiens |
| T62 | Q16665 | Hypoxia-inducible factor 1-alpha | HIF1A | Homo sapiens |
| T63 | P52789 | Hexokinase-2 | HK2 | Homo sapiens |
| T64 | P04035 | 3-hydroxy-3-methylglutaryl-coenzyme A reductase | HMGCR | Homo sapiens |
| T65 | P09601 | Heme oxygenase 1 | HMOX1 | Homo sapiens |
| T66 | Q9Y251 | Heparanase 8 kDa subunit | HPSE | Homo sapiens |
| T67 | P07900 | Heat shock protein HSP 90 | HSP90AA1 | Homo sapiens |
| T68 | P11021 | 78 kDa glucose-regulated protein | HSPA5 | Homo sapiens |
| T69 | P04792 | Heat shock protein beta-1 | HSPB1 | Homo sapiens |
| T70 | P05362 | Intercellular adhesion molecule 1 | ICAM1 | Homo sapiens |
| T71 | P01579 | Interferon gamma | IFNG | Homo sapiens |
| T72 | P01344 | Insulin-like growth factor II | IGF2 | Homo sapiens |
| T73 | P17936 | Insulin-like growth factor-binding protein 3 | IGFBP3 | Homo sapiens |
| T74 | O14920 | Inhibitor of nuclear factor kappa-B kinase subunit beta | IKBKB | Homo sapiens |
| T75 | P22301 | Interleukin-10 | IL10 | Homo sapiens |
| T76 | P01584 | Interleukin-1 beta | IL1B | Homo sapiens |
| T77 | P60568 | Interleukin-2 | IL2 | Homo sapiens |
| T78 | P05112 | Interleukin-4 | IL4 | Homo sapiens |
| T79 | P05231 | Interleukin-6 | IL6 | Homo sapiens |
| T80 | P06213 | Insulin receptor | INSR | Homo sapiens |
| T81 | P10914 | Interferon regulatory factor 1 | IRF1 | Homo sapiens |
| T82 | P05412 | Transcription factor AP-1 | JUN | Homo sapiens |
| T83 | Q12809 | Potassium voltage-gated channel subfamily H member 2 | KCNH2 | Homo sapiens |
| T84 | P35968 | Vascular endothelial growth factor receptor 2 | KDR | Homo sapiens |
| T85 | P09960 | Leukotriene A-4 hydrolase | LTA4H | Homo sapiens |
| T86 | P28482 | Mitogen-activated protein kinase 1 | MAPK1 | Homo sapiens |
| T87 | Q16539 | Mitogen-activated protein kinase 14 | MAPK14 | Homo sapiens |
| T88 | P45983 | Mitogen-activated protein kinase 8 | MAPK8 | Homo sapiens |
| T89 | Q07820 | Induced myeloid leukemia cell differentiation protein Mcl-1 | MCL1 | Homo sapiens |
| T90 | Q00987 | E3 ubiquitin-protein ligase Mdm2 | MDM2 | Homo sapiens |
| T91 | O43451 | Maltase-glucoamylase, intestinal | MGAM | Homo sapiens |
| T92 | P03956 | Interstitial collagenase | MMP1 | Homo sapiens |
| T93 | P08253 | 72 kDa type IV collagenase | MMP2 | Homo sapiens |
| T94 | P08254 | Stromelysin-1 | MMP3 | Homo sapiens |
| T95 | P14780 | Matrix metalloproteinase-9 | MMP9 | Homo sapiens |
| T96 | P05164 | Myeloperoxidase | MPO | Homo sapiens |
| T97 | P01106 | Myc proto-oncogene protein | MYC | Homo sapiens |
| T98 | P21359 | Neurofibromin | NF1 | Homo sapiens |
| T99 | Q16236 | Nuclear factor erythroid 2-related factor 2 | NFE2L2 | Homo sapiens |
| T100 | Q99801 | Homeobox protein Nkx-3.1 | NKX3-1 | Homo sapiens |
| T101 | P35228 | Nitric oxide synthase, inducible | NOS2 | Homo sapiens |
| T102 | P15559 | NAD(P)H dehydrogenase [quinone] 1 | NQO1 | Homo sapiens |
| T103 | O75469 | Nuclear receptor subfamily 1 group I member 2 | NR1I2 | Homo sapiens |
| T104 | P11926 | Ornithine decarboxylase | ODC1 | Homo sapiens |
| T105 | P09874 | Poly [ADP-ribose] polymerase 1 | PARP1 | Homo sapiens |
| T106 | P12004 | Proliferating cell nuclear antigen | PCNA | Homo sapiens |
| T107 | P06401 | Progesterone receptor | PGR | Homo sapiens |
| T108 | P48736 | Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit, gamma isoform | PIK3CG | Homo sapiens |
| T109 | P11309 | Proto-oncogene serine/threonine-protein kinase Pim-1 | PIM1 | Homo sapiens |
| T110 | P00749 | Urokinase-type plasminogen activator | PLAU | Homo sapiens |
| T111 | Q07869 | Peroxisome proliferator-activated receptor alpha | PPARA | Homo sapiens |
| T112 | Q03181 | Peroxisome proliferator-activated receptor delta | PPARD | Homo sapiens |
| T113 | P37231 | Peroxisome proliferator-activated receptor gamma | PPARG | Homo sapiens |
| T114 | P05771 | Protein kinase C beta type | PRKCB | Homo sapiens |
| T115 | P07477 | Trypsin-1 | PRSS1 | Homo sapiens |
| T116 | P60484 | Phosphatidylinositol-3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN | PTEN | Homo sapiens |
| T117 | P43115 | Prostaglandin E2 receptor EP3 subtype | PTGER3 | Homo sapiens |
| T118 | P23219 | Prostaglandin G/H synthase 1 | PTGS1 | Homo sapiens |
| T119 | P35354 | Prostaglandin G/H synthase 2 | PTGS2 | Homo sapiens |
| T120 | P04049 | RAF proto-oncogene serine/threonine-protein kinase | RAF1 | Homo sapiens |
| T121 | Q9NS23 | Ras association domain-containing protein 1 | RASSF1 | Homo sapiens |
| T122 | P06400 | Retinoblastoma-associated protein | RB1 | Homo sapiens |
| T123 | Q04206 | Transcription factor p65 | RELA | Homo sapiens |
| T124 | Q13950 | Runt-related transcription factor 2 | RUNX2 | Homo sapiens |
| T125 | P19793 | Retinoic acid receptor RXR-alpha | RXRA | Homo sapiens |
| T126 | P28702 | Retinoic acid receptor RXR-beta | RXRB | Homo sapiens |
| T127 | P05121 | Plasminogen activator inhibitor 1 | SERPINE1 | Homo sapiens |
| T128 | Q96EB6 | NAD-dependent deacetylase sirtuin-1 | SIRT1 | Homo sapiens |
| T129 | P03973 | Antileukoproteinase | SLPI | Homo sapiens |
| T130 | P00441 | Superoxide dismutase [Cu-Zn] | SOD1 | Homo sapiens |
| T131 | P10451 | Osteopontin | SPP1 | Homo sapiens |
| T132 | P12931 | Proto-oncogene tyrosine-protein kinase Src | SRC | Homo sapiens |
| T133 | P42224 | Signal transducer and activator of transcription 1-alpha/beta | STAT1 | Homo sapiens |
| T134 | P40763 | Signal transducer and activator of transcription 3 | STAT3 | Homo sapiens |
| T135 | P01137 | Transforming growth factor beta-1 | TGFB1 | Homo sapiens |
| T136 | P07204 | Thrombomodulin | THBD | Homo sapiens |
| T137 | P01033 | Metalloproteinase inhibitor 1 | TIMP1 | Homo sapiens |
| T138 | Q9NR96 | Toll-like receptor 9 | TLR9 | Homo sapiens |
| T139 | P01375 | Tumor necrosis factor | TNF | Homo sapiens |
| T140 | P11387 | DNA topoisomerase 1 | TOP1 | Homo sapiens |
| T141 | P11388 | DNA topoisomerase 2-alpha | TOP2A | Homo sapiens |
| T142 | P04637 | Cellular tumor antigen p53 | TP53 | Homo sapiens |
| T143 | P15692 | Vascular endothelial growth factor A | VEGFA | Homo sapiens |
| T144 | P47989 | Xanthine dehydrogenase/oxidase | XDH | Homo sapiens |
| T145 | P98170 | Baculoviral IAP repeat-containing protein 4 | XIAP | Homo sapiens |
| T146 | P07947 | Tyrosine-protein kinase Yes | YES1 | Homo sapiens |

**Table S3**

The GO terms of therapy target genes and their corresponding Count, *P*Value, FDR. Through the GO enrichment of the key targets, 26 top GO terms were obtained which indicate that large numbers of targets involved in the process of tumorigenesis.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **GO ID** | **Term** | **Count** | ***P*Value** | **FDR** |
| GO:0045944 | positive regulation of transcription from RNA polymerase II promoter | 48 | 4.35E-23 | 7.66E-20 |
| GO:0043066 | negative regulation of apoptotic process | 39 | 5.03E-27 | 8.86E-24 |
| GO:0045893 | positive regulation of transcription, DNA-templated | 39 | 4.54E-25 | 7.99E-22 |
| GO:0008284 | positive regulation of cell proliferation | 35 | 2.99E-22 | 5.27E-19 |
| GO:0007165 | signal transduction | 31 | 4.88E-08 | 8.58E-05 |
| GO:0042493 | response to drug | 30 | 3.01E-22 | 5.30E-19 |
| GO:0010628 | positive regulation of gene expression | 27 | 1.96E-20 | 3.46E-17 |
| GO:0006915 | apoptotic process | 26 | 1.70E-11 | 2.99E-08 |
| GO:0000122 | negative regulation of transcription from RNA polymerase II promoter | 23 | 2.39E-07 | 4.21E-04 |
| GO:0007568 | aging | 20 | 2.28E-16 | 3.89E-13 |
| GO:0043065 | positive regulation of apoptotic process | 20 | 1.28E-11 | 2.25E-08 |
| GO:0008285 | negative regulation of cell proliferation | 20 | 1.44E-09 | 2.53E-06 |
| GO:0045892 | negative regulation of transcription, DNA-templated | 20 | 6.02E-08 | 1.06E-04 |
| GO:0001525 | angiogenesis | 19 | 7.81E-13 | 1.37E-09 |
| GO:0006954 | inflammatory response | 19 | 4.72E-09 | 8.31E-06 |
| GO:0071456 | cellular response to hypoxia | 18 | 5.33E-18 | 9.37E-15 |
| GO:0045766 | positive regulation of angiogenesis | 18 | 1.29E-16 | 2.00E-13 |
| GO:0008283 | cell proliferation | 18 | 1.81E-08 | 3.19E-05 |
| GO:0006468 | protein phosphorylation | 17 | 2.10E-06 | 0.003686 |
| GO:0001934 | positive regulation of protein phosphorylation | 16 | 2.71E-13 | 4.77E-10 |
| GO:0001666 | response to hypoxia | 16 | 2.33E-11 | 4.09E-08 |
| GO:0000165 | MAPK cascade | 16 | 8.27E-09 | 1.45E-05 |
| GO:0032355 | response to estradiol | 15 | 4.10E-14 | 7.21E-11 |
| GO:0071222 | cellular response to lipopolysaccharide | 15 | 8.95E-13 | 1.58E-09 |
| GO:0070374 | positive regulation of ERK1 and ERK2 cascade | 15 | 3.52E-10 | 6.19E-07 |
| GO:0006974 | cellular response to DNA damage stimulus | 15 | 3.38E-09 | 5.95E-06 |

**Table S4**

The KEGG Pathways of therapy target genes and their corresponding Count, *P*Value and FDR. Through the KEGG enrichment of the key targets, 21 remarkably enriched pathways which involved in cell proliferation, apoptosis and inflammation were obtained.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Term** | **Pathways** | **Count** | ***P*value** | **FDR** |
| hsa05200 | Pathways in cancer | 58 | 5.71E-36 | 7.20E-33 |
| hsa04151 | PI3K-Akt signaling pathway | 37 | 3.03E-17 | 3.82E-14 |
| hsa04010 | MAPK signaling pathway | 24 | 7.32E-10 | 9.24E-07 |
| hsa04014 | Ras signaling pathway | 23 | 4.16E-10 | 5.25E-07 |
| hsa04068 | FoxO signaling pathway | 22 | 9.91E-14 | 1.25E-10 |
| hsa04066 | HIF-1 signaling pathway | 21 | 1.99E-15 | 2.52E-12 |
| hsa04668 | TNF signaling pathway | 19 | 1.60E-12 | 2.02E-09 |
| hsa04115 | p53 signaling pathway | 18 | 6.05E-15 | 7.56E-12 |
| hsa04110 | Cell cycle | 18 | 2.38E-10 | 3.00E-07 |
| hsa05202 | Transcriptional misregulation in cancer | 18 | 2.72E-08 | 3.43E-05 |
| hsa04060 | Cytokine-cytokine receptor interaction | 18 | 2.52E-06 | 0.003174625 |
| hsa04620 | Toll-like receptor signaling pathway | 17 | 1.91E-10 | 2.41E-07 |
| hsa04015 | Rap1 signaling pathway | 17 | 3.43E-06 | 0.004325218 |
| hsa04012 | ErbB signaling pathway | 16 | 1.04E-10 | 1.31E-07 |
| hsa04660 | T cell receptor signaling pathway | 16 | 1.23E-09 | 1.55E-06 |
| hsa04210 | Apoptosis | 14 | 1.50E-10 | 1.89E-07 |
| hsa04915 | Estrogen signaling pathway | 13 | 4.83E-07 | 6.09E-04 |
| hsa04621 | NOD-like receptor signaling pathway | 12 | 7.07E-09 | 8.92E-06 |
| hsa04370 | VEGF signaling pathway | 12 | 2.23E-08 | 2.82E-05 |
| hsa05230 | Central carbon metabolism in cancer | 11 | 4.11E-07 | 5.19E-04 |
| hsa04064 | NF-kappa B signaling pathway | 11 | 7.37E-06 | 0.009296675 |