

**Supplementary Table 3. KEGG pathways identified by GSVA between two CoCu-DEG clusters. ID**

<b>logFC</b>	<b>AveExpr</b>		<b>t</b>	<b>P.Value</b>	<b>adj.P.Val</b>	<b>B</b>
KEGG_PROTEASOME	-0.514214	-0.021759	-15.13745	4.46E-43	8.29E-41	87.1137
KEGG_DNA_REPLICATION	-0.482361	-0.022075	-12.71471	2.13E-32	1.99E-30	62.77938
KEGG_PARKINSONS_DISEASE	-0.378733	-0.019199	-12.24435	1.99E-30	1.23E-28	58.29693
KEGG_OXIDATIVE_PHOSPHORYLATION	-0.382917	-0.018117	-11.78579	1.51E-28	7.02E-27	54.0164
KEGG_CELL_CYCLE	-0.362096	-0.018108	-11.62397	6.81E-28	2.53E-26	52.52797
KEGG_PENTOSE_PHOSPHATE_PATHWAY	-0.315492	-0.018257	-11.55217	1.32E-27	4.10E-26	51.87143
KEGG_HUNTINGTONS_DISEASE	-0.327929	-0.017175	-11.41412	4.72E-27	1.25E-25	50.61573
KEGG_PYRIMIDINE_METABOLISM	-0.317194	-0.019189	-11.22323	2.70E-26	6.27E-25	48.89426
KEGG_ALZHEIMERS_DISEASE	-0.309114	-0.021003	-11.20395	3.21E-26	6.64E-25	48.72142
KEGG_PORPHYRIN_AND_CHLOROPHYLL_METABOLISM	-0.253645	-0.037944	-11.10722	7.71E-26	1.43E-24	47.85664
KEGG_GLUTATHIONE_METABOLISM	-0.268108	-0.026108	-10.93837	3.52E-25	5.95E-24	46.35824
KEGG_MISMATCH_REPAIR	-0.403678	-0.022138	-10.88529	5.65E-25	8.76E-24	45.89016
KEGG_GLYCOLYSIS_GLUONEOGENESIS	-0.224116	-0.02313	-10.73678	2.11E-24	3.02E-23	44.58794
KEGG_GLYOXYLATE_AND_DICARBOXYLATE_METABOLISM	-0.313339	-0.024252	-10.1213	4.43E-22	5.89E-21	39.31444
KEGG_CITRATE_CYCLE_TCA_CYCLE	-0.351093	-0.021677	-10.10571	5.06E-22	6.28E-21	39.18348
KEGG_FOLATE_BIOSYNTHESIS	-0.296017	-0.033599	-10.05187	8.00E-22	9.30E-21	38.73245
KEGG_PROTEIN_EXPORT	-0.371446	-0.017624	-9.932249	2.20E-21	2.40E-20	37.73595
KEGG_RIBOSOME	-0.440127	-0.00877	-9.91832	2.47E-21	2.55E-20	37.62045
KEGG_CYSTEINE_AND_METHIONINE_METABOLISM	-0.221775	-0.031035	-9.547269	5.38E-20	5.27E-19	34.58441
KEGG_PURINE_METABOLISM	-0.214263	-0.02317	-9.482597	9.13E-20	8.49E-19	34.06345
KEGG_BIOSYNTHESIS_OF_UNSATURATED_FATTY_ACIDS	-0.262007	-0.026117	-9.46166	1.08E-19	9.59E-19	33.89533
KEGG_LINOLEIC_ACID_METABOLISM	0.226297	-0.020138	9.438958	1.30E-19	1.10E-18	33.71333
KEGG_PENTOSE_AND_GLUCURONATE_INTERCONVERSIONS	-0.250299	-0.044244	-9.409991	1.65E-19	1.33E-18	33.48155
KEGG_TASTE_TRANSDUCTION	0.148467	-0.013728	9.355618	2.56E-19	1.98E-18	33.04784
KEGG_RNA_POLYMERASE	-0.312704	-0.020275	-9.318326	3.46E-19	2.57E-18	32.75141
KEGG_BASE_EXCISION_REPAIR	-0.306597	-0.014459	-9.254452	5.78E-19	4.14E-18	32.24562

KEGG_ALANINE_ASPARTATE_AND_GLUTAMATE_M ETABOLISM	-0.192363	-0.030697	-9.05376	2.86E-18	1.97E-17	30.67269
KEGG_OOCYTE_MEIOSIS	-0.229943	-0.023443	-9.048804	2.97E-18	1.97E-17	30.63416
KEGG_NUCLEOTIDE_EXCISION_REPAIR	-0.305548	-0.014825	-8.723936	3.74E-17	2.38E-16	28.14226
KEGG_GALACTOSE_METABOLISM	-0.232092	-0.020419	-8.720505	3.84E-17	2.38E-16	28.11631
KEGG_RIBOFLAVIN_METABOLISM	-0.233498	-0.033088	-8.710556	4.15E-17	2.49E-16	28.04107
KEGG_ONE_CARBON_POOL_BY_FOLATE	-0.268353	-0.024557	-8.686701	4.98E-17	2.90E-16	27.86094
KEGG_HOMOLOGOUS_RECOMBINATION	-0.31657	-0.025433	-8.667472	5.78E-17	3.26E-16	27.71601
KEGG_P53_SIGNALING_PATHWAY	-0.208853	-0.022425	-8.521662	1.75E-16	9.59E-16	26.62483
KEGG_PATHOGENIC_ESCHERICHIA_COLI_INFECTI ON	-0.233907	-0.018415	-8.496289	2.12E-16	1.13E-15	26.43637
KEGG_ARGININE_AND_PROLINE_METABOLISM	-0.191944	-0.024934	-8.481079	2.38E-16	1.23E-15	26.32359
KEGG_PYRUVATE_METABOLISM	-0.219296	-0.024872	-8.473244	2.53E-16	1.27E-15	26.26556
KEGG_CARDIAC_MUSCLE_CONTRACTION	-0.164164	-0.027522	-8.34021	6.85E-16	3.35E-15	25.2864
KEGG_REGULATION_OF_AUTOPHAGY	-0.170373	0.02176	-8.335925	7.07E-16	3.37E-15	25.25506
KEGG_BASAL_TRANSCRIPTION_FACTORS	-0.266482	-0.022653	-8.14449	2.90E-15	1.35E-14	23.86735
KEGG_TERPENOID_BACKBONE_BIOSYNTHESIS	-0.281833	-0.025094	-8.133532	3.15E-15	1.43E-14	23.78867
KEGG_AMINOACYL_TRNA_BIOSYNTHESIS	-0.295927	-0.013441	-7.71481	6.34E-14	2.81E-13	20.84393
KEGG_AMINO_SUGAR_AND_NUCLEOTIDE_SUGAR_ METABOLISM	-0.237755	-0.013869	-7.668198	8.78E-14	3.80E-13	20.5237
KEGG_ABC_TRANSPORTERS	0.164451	-0.017364	7.378422	6.47E-13	2.74E-12	18.56771
KEGG_SPLICEOSOME	-0.275831	-0.005334	-7.252119	1.52E-12	6.27E-12	17.73419
KEGG_FRUCTOSE_AND_MANNOSE_METABOLISM	-0.201241	-0.021361	-7.220111	1.88E-12	7.60E-12	17.52481
KEGG_RNA_DEGRADATION	-0.248671	-0.017427	-7.069034	5.11E-12	2.02E-11	16.54678
KEGG_N_GLYCAN_BIOSYNTHESIS	-0.231612	-0.018882	-7.028059	6.69E-12	2.59E-11	16.28445
KEGG_ALPHA_LINOLENIC_ACID_METABOLISM	0.166292	-0.013956	6.916643	1.38E-11	5.23E-11	15.5775
KEGG_STARCH_AND_SUCROSE_METABOLISM	-0.136802	-0.033695	-6.840882	2.24E-11	8.35E-11	15.10213
KEGG_DRUG_METABOLISM_OTHER_ENZYMES	-0.135286	-0.037578	-6.764966	3.64E-11	1.33E-10	14.63017
KEGG_PHENYLALANINE_METABOLISM	-0.171811	-0.031179	-6.645403	7.73E-11	2.76E-10	13.89581
KEGG_ASCORBATE_AND_ALDARATE_METABOLISM	-0.193024	-0.037442	-6.526082	1.62E-10	5.69E-10	13.17391
KEGG_BLADDER_CANCER	-0.165529	-0.019479	-6.375544	4.06E-10	1.40E-09	12.27899
KEGG_GLYCOSPHINGOLIPID_BIOSYNTHESIS_LACT	-0.14748	-0.029269	-6.329583	5.36E-10	1.81E-09	12.0093

## O\_AND\_NEOLACTO\_SERIES

KEGG_PROGESTERONE_MEDIATED_OOCYTE_MATURATION	-0.164358	-0.021829	-6.27533	7.42E-10	2.46E-09	11.69311
KEGG_SYSTEMIC_LUPUS_ERYTHEMATOSUS	-0.142576	-0.020037	-6.236952	9.32E-10	3.04E-09	11.47084
KEGG_VIBRIO_CHOLERAЕ_INFECTION	-0.168031	-0.019696	-6.23434	9.47E-10	3.04E-09	11.45576
KEGG_VALINE_LEUCINE_AND_ISOLEUCINE_BIOSYNTHESIS	-0.227949	-0.023389	-6.160682	1.46E-09	4.61E-09	11.03261
KEGG_NICOTINATE_AND_NICOTINAMIDE_METABOLISM	-0.141007	-0.032357	-6.129131	1.76E-09	5.46E-09	10.85268
KEGG_STEROID_BIOSYNTHESIS	-0.197347	-0.018048	-5.882072	7.30E-09	2.23E-08	9.471481
KEGG_UBIQUITIN_MEDIATED_PROTEOLYSIS	-0.191416	-0.015605	-5.758078	1.46E-08	4.39E-08	8.796979
KEGG_GLYCINE_SERINE_AND_THREONINE_METABOLISM	-0.122122	-0.031326	-5.648679	2.68E-08	7.91E-08	8.212364
KEGG_TAURINE_AND_HYPOTAURINE_METABOLISM	0.14871	-0.019764	5.423848	8.99E-08	2.61E-07	7.042064
KEGG_SELENOAMINO_ACID_METABOLISM	-0.158409	-0.025363	-5.356174	1.28E-07	3.67E-07	6.698091
KEGG_PEROXISOME	-0.15393	-0.015619	-5.250336	2.23E-07	6.27E-07	6.167888
KEGG_CYTOSOLIC_DNA_SENSING_PATHWAY	-0.12486	-0.003506	-5.173037	3.31E-07	9.18E-07	5.786655
KEGG_AMYOTROPHIC_LATERAL_SCLEROSIS_ALS	-0.122543	-0.022299	-5.142284	3.86E-07	1.06E-06	5.636399
KEGG_GLYCOSAMINOGLYCAN_BIOSYNTHESIS_KERATAN_SULFATE	-0.153003	-0.016921	-5.089379	5.05E-07	1.36E-06	5.379803
KEGG_NON_HOMOLOGOUS_END_JOINING	-0.176978	-0.023987	-4.880825	1.41E-06	3.75E-06	4.391728
KEGG_BUTANOATE_METABOLISM	-0.12384	-0.027218	-4.812016	1.97E-06	5.15E-06	4.073984
KEGG_ASTHMA	0.183162	0.010845	4.697147	3.39E-06	8.76E-06	3.552743
KEGG_LYSINE_DEGRADATION	-0.143082	-0.022263	-4.528518	7.39E-06	1.88E-05	2.808519
KEGG_LIMONENE_AND_PINENE_DEGRADATION	-0.158602	-0.027811	-4.435954	1.12E-05	2.82E-05	2.410673
KEGG_EPITHELIAL_CELL_SIGNALING_IN_HELICOBACTER_PYLORI_INFECTION	-0.122232	-0.017631	-4.363857	1.55E-05	3.83E-05	2.106069
KEGG_PANCREATIC_CANCER	-0.130526	-0.018202	-4.340245	1.71E-05	4.20E-05	2.007313
KEGG_HEDGEHOG_SIGNALING_PATHWAY	0.097324	-0.015526	4.203503	3.10E-05	7.49E-05	1.445228
KEGG_ARACHIDONIC_ACID_METABOLISM	0.091883	-0.013796	4.192797	3.24E-05	7.74E-05	1.401926
KEGG_BASAL_CELL_CARCINOMA	0.100029	-0.012722	4.180701	3.42E-05	8.04E-05	1.35313
KEGG_PROPANOATE_METABOLISM	-0.134744	-0.022072	-4.172841	3.53E-05	8.21E-05	1.321494
KEGG_RENAL_CELL_CARCINOMA	-0.123927	-0.017196	-4.037009	6.24E-05	0.000143	0.783544

KEGG_SPHINGOLIPID_METABOLISM	-0.111109	-0.023932	-4.007061	7.06E-05	0.00016	0.667184
KEGG_BETA_ALANINE_METABOLISM	-0.10211	-0.029212	-3.991937	7.51E-05	0.000168	0.608732
KEGG_PRION_DISEASES	-0.105652	-0.015367	-3.965328	8.37E-05	0.000185	0.506394
KEGG_CALCIIUM_SIGNALING_PATHWAY	0.080791	-0.014154	3.875831	0.00012	0.000263	0.166915
KEGG_GLYCOSPHINGOLIPID_BIOSYNTHESIS_GLOB O_SERIES	-0.117674	-0.017605	-3.853944	0.000131	0.000283	0.085006
KEGG_VALINE_LEUCINE_AND_ISOLEUCINE_DEGRA DATION	-0.126087	-0.015296	-3.814449	0.000153	0.000327	-0.061689
KEGG_THYROID_CANCER	-0.111451	-0.019644	-3.742591	0.000203	0.000428	-0.32493
KEGG_VASCULAR_SMOOTH_MUSCLE_CONTRACTI ON	0.088778	-0.014647	3.626011	0.000317	0.000661	-0.741911
KEGG_PROSTATE_CANCER	-0.101859	-0.015892	-3.607693	0.000339	0.000701	-0.806292
KEGG_TRYPTOPHAN_METABOLISM	-0.080124	-0.024739	-3.559881	0.000405	0.00082	-0.972871
KEGG_MELANOMA	-0.081002	-0.02152	-3.559833	0.000406	0.00082	-0.973038
KEGG_DILATED_CARDIOMYOPATHY	0.089625	-0.01128	3.505	0.000496	0.000993	-1.161469
KEGG_REGULATION_OF_ACTIN_CYTOSKELETON	-0.089184	-0.014289	-3.494386	0.000516	0.001021	-1.197622
KEGG_GNRH_SIGNALING_PATHWAY	0.080396	-0.01471	3.474112	0.000556	0.001088	-1.266389
KEGG_GLYCEROLIPID_METABOLISM	-0.073167	-0.02185	-3.360201	0.000837	0.001621	-1.645651
KEGG_CIRCADIAN_RHYTHM_MAMMAL	0.109512	-0.014208	3.317002	0.000974	0.001868	-1.786316
KEGG_GLYCOSYLPHOSPHATIDYLINOSITOL_GPI_AN CHOR_BIOSYNTHESIS	-0.117702	-0.020031	-3.284277	0.001092	0.002073	-1.891716
KEGG_SMALL_CELL_LUNG_CANCER	-0.092642	-0.01771	-3.268762	0.001152	0.002165	-1.941335
KEGG_SNARE_INTERACTIONS_IN_VESICULAR_TRA NSPORT	-0.110064	-0.015749	-3.263336	0.001174	0.002184	-1.958637
KEGG_FC_EPSILON_RI_SIGNALING_PATHWAY	0.080309	-0.012191	3.137232	0.001803	0.003321	-2.352928
KEGG_MATURITY_ONSET_DIABETES_OF_THE_YOU NG	-0.080496	-0.027066	-3.039014	0.002494	0.004548	-2.649669
KEGG_PANTOTHENATE_AND_COA_BIOSYNTHESIS	-0.081088	-0.023307	-3.02088	0.002646	0.004778	-2.70346
KEGG_CHRONIC_MYELOID_LEUKEMIA	-0.094547	-0.013148	-2.991591	0.002908	0.005202	-2.789684
KEGG_PHOSPHATIDYLINOSITOL_SIGNALING_SYST EM	0.08179	-0.015796	2.987537	0.002947	0.00522	-2.801555
KEGG_INTESTINAL_IMMUNE_NETWORK_FOR_IGA_ PRODUCTION	0.111844	0.005086	2.919113	0.003664	0.00643	-2.999566

KEGG_ANTIGEN_PROCESSING_AND_PRESENTATION	-0.087654	-0.003732	-2.87698	0.004182	0.007269	-3.119289
KEGG_GAP_JUNCTION	-0.067521	-0.015589	-2.858762	0.004426	0.007622	-3.170531
KEGG_PATHWAYS_IN_CANCER	-0.06903	-0.01402	-2.822529	0.004949	0.008445	-3.271512
KEGG_INSULIN_SIGNALING_PATHWAY	-0.073665	-0.019116	-2.798877	0.005321	0.008997	-3.336757
KEGG_ADHERENS_JUNCTION	-0.084387	-0.015501	-2.68394	0.007511	0.012585	-3.64622
KEGG_STEROID_HORMONE_BIOSYNTHESIS	-0.061449	-0.025548	-2.666908	0.007896	0.013114	-3.691007
KEGG_MTOR_SIGNALING_PATHWAY	-0.076537	-0.02197	-2.639115	0.008564	0.014097	-3.763492
KEGG_HEMATOPOIETIC_CELL_LINEAGE	0.083917	0.006532	2.616304	0.00915	0.014929	-3.822432
KEGG_NEUROACTIVE_LIGAND_RECEPTOR_INTERACTION	0.050318	-0.017116	2.588367	0.009916	0.016038	-3.893938
KEGG_RIG_I_LIKE_RECEPTOR_SIGNALING_PATHWAY	-0.064953	-0.008088	-2.577236	0.010237	0.016414	-3.92222
KEGG_ALLOGRAFT_REJECTION	0.106854	0.008692	2.467379	0.013935	0.022153	-4.194974
KEGG_HYPERTROPHIC_CARDIOMYOPATHY_HCM	0.059348	-0.01573	2.413485	0.016149	0.025456	-4.32454
KEGG_VASOPRESSIN_REGULATED_WATER_REABSORPTION	-0.072914	-0.0193	-2.349519	0.019175	0.029971	-4.47469
KEGG_ENDOCYTOSIS	-0.06806	-0.013258	-2.329077	0.020242	0.031374	-4.521844
KEGG_TIGHT_JUNCTION	-0.054888	-0.019904	-2.307966	0.021397	0.032891	-4.570113
KEGG_TOLL_LIKE_RECEPTOR_SIGNALING_PATHWAY	-0.064222	-0.00816	-2.283666	0.022798	0.034758	-4.625146
KEGG_TYROSINE_METABOLISM	-0.051171	-0.025545	-2.27135	0.023538	0.035594	-4.65282
KEGG_ETHER_LIPID_METABOLISM	0.050962	-0.019731	2.20885	0.027625	0.041438	-4.790992
KEGG_COLORECTAL_CANCER	-0.067008	-0.016633	-2.177044	0.029931	0.044538	-4.859854
KEGG_CELL_ADHESION_MOLECULES_CAMS	0.065402	3.14E-05	2.162964	0.031004	0.045768	-4.890027
KEGG_GLIOMA	-0.058378	-0.019677	-2.154866	0.031636	0.046333	-4.907292
KEGG_ADIPOCYTOKINE_SIGNALING_PATHWAY	-0.050811	-0.023257	-2.098514	0.036347	0.052817	-5.025679
KEGG_AUTOIMMUNE_THYROID_DISEASE	0.071209	0.02001	2.06734	0.039202	0.056524	-5.089846
KEGG_NOD_LIKE_RECEPTOR_SIGNALING_PATHWAY	-0.062573	-0.012028	-2.064077	0.039511	0.056532	-5.096508
KEGG_OLFACTORY_TRANSDUCTION	-0.044476	0.09938	-2.055628	0.040323	0.057252	-5.113709
KEGG_NOTCH_SIGNALING_PATHWAY	-0.060099	-0.009001	-1.963297	0.05015	0.070666	-5.297163
KEGG_JAK_STAT_SIGNALING_PATHWAY	0.045238	-0.009658	1.93845	0.053115	0.074282	-5.345114

KEGG_METABOLISM_OF_XENOBIOTICS_BY_CYTOCHROME_P450	-0.050642	-0.02922	-1.878295	0.060906	0.084542	-5.45871
KEGG_APOPTOSIS	-0.054734	-0.014625	-1.85402	0.064309	0.088603	-5.503552
KEGG_TYPE_II_DIABETES_MELLITUS	0.040334	-0.018781	1.845925	0.065478	0.08955	-5.518377
KEGG_PRIMARY_BILE_ACID_BIOSYNTHESIS	0.05005	-0.022434	1.842197	0.066022	0.089636	-5.525183
KEGG_FC_GAMMA_R_MEDIATED_PHAGOCYTOSIS	-0.053135	-0.01314	-1.809042	0.071028	0.095734	-5.585113
KEGG_ALDOSTERONE_REGULATED_SODIUM_REABSORPTION	0.043091	-0.015956	1.791273	0.073837	0.098804	-5.616791
KEGG_LYSOSOME	-0.05557	-0.006039	-1.707639	0.088307	0.117322	-5.761737
KEGG_LONG_TERM_DEPRESSION	0.035065	-0.019707	1.632528	0.103181	0.13611	-5.886073
KEGG_TGF_BETA_SIGNALING_PATHWAY	-0.041551	-0.018218	-1.606726	0.108728	0.142419	-5.927508
KEGG_PRIMARY_IMMUNODEFICIENCY	0.062369	-0.002013	1.597753	0.110712	0.144003	-5.941764
KEGG_HISTIDINE_METABOLISM	-0.036857	-0.028017	-1.510267	0.13159	0.16997	-6.076617
KEGG_NON_SMALL_CELL_LUNG_CANCER	-0.0445	-0.020469	-1.502669	0.133538	0.171297	-6.087973
KEGG_COMPLEMENT_AND_COAGULATION_CASCADES	0.036433	-0.006965	1.373747	0.170119	0.216407	-6.272011
KEGG_NEUROTROPHIN_SIGNALING_PATHWAY	-0.040801	-0.013307	-1.370812	0.171032	0.216407	-6.276011
KEGG_GLYCEROPHOSPHOLIPID_METABOLISM	0.030883	-0.018392	1.34768	0.178355	0.224127	-6.307233
KEGG_FATTY_ACID_METABOLISM	-0.040115	-0.022206	-1.343995	0.179543	0.224127	-6.312157
KEGG_O_GLYCAN_BIOSYNTHESIS	-0.034714	-0.020791	-1.314855	0.189145	0.234539	-6.350631
KEGG_SULFUR_METABOLISM	-0.03653	-0.020348	-1.282503	0.200244	0.246658	-6.392365
KEGG_ACUTE_MYELOID_LEUKEMIA	-0.040067	-0.012176	-1.275022	0.202877	0.248258	-6.401869
KEGG_WNT_SIGNALING_PATHWAY	-0.030975	-0.017947	-1.267064	0.205706	0.250074	-6.411917
KEGG_GLYCOSAMINOGLYCAN_DEGRADATION	-0.038493	-0.007653	-1.236695	0.216765	0.261807	-6.449691
KEGG_OTHER_GLYCAN_DEGRADATION	-0.042049	-0.011183	-1.229849	0.219316	0.262538	-6.458079
KEGG_ARRHYTHMOGENIC_RIGHT_VENTRICULAR_CARDIOMYOPATHY_ARVC	0.032139	-0.016561	1.227509	0.220193	0.262538	-6.460936
KEGG_NATURAL_KILLER_CELL_MEDIATED_CYTOTOXICITY	-0.034189	-0.008489	-1.209555	0.227005	0.268936	-6.482676
KEGG_CHEMOKINE_SIGNALING_PATHWAY	-0.033196	-0.008947	-1.184377	0.236811	0.278777	-6.512626
KEGG_ENDOMETRIAL_CANCER	-0.037408	-0.016541	-1.171321	0.242012	0.283109	-6.52791
KEGG_GLYCOSAMINOGLYCAN_BIOSYNTHESIS_CHONDROITIN_SULFATE	-0.035828	-0.008862	-1.130065	0.258976	0.301059	-6.5751

KEGG_ERBB_SIGNALING_PATHWAY	-0.030561	-0.01742	-1.089785	0.276318	0.319225	-6.619547
KEGG_FOCAL_ADHESION	-0.031469	-0.010454	-1.07472	0.283004	0.324931	-6.635759
KEGG_MELANOGENESIS	0.022711	-0.014975	1.042123	0.297844	0.339871	-6.670067
KEGG_ECM_RECEPTOR_INTERACTION	0.031832	-0.007888	0.99585	0.319791	0.36269	-6.716962
KEGG_VIRAL_MYOCARDITIS	0.031135	-0.003898	0.98424	0.32546	0.366164	-6.728395
KEGG_AXON_GUIDANCE	-0.024937	-0.012636	-0.981533	0.326792	0.366164	-6.731042
KEGG_GLYCOSPHINGOLIPID_BIOSYNTHESIS_GANGLIO_SERIES	-0.026971	-0.020059	-0.86752	0.386062	0.429985	-6.835915
KEGG_PROXIMAL_TUBULE_BICARBONATE_RECLAIMATION	-0.017988	-0.027752	-0.762647	0.446024	0.493812	-6.920992
KEGG_T_CELL_RECEPTOR_SIGNALING_PATHWAY	0.021619	-0.012448	0.706841	0.479986	0.528268	-6.961812
KEGG_PPAR_SIGNALING_PATHWAY	-0.013925	-0.022642	-0.672778	0.501391	0.54858	-6.985207
KEGG_LEUKOCYTE_TRANSENDOTHELIAL_MIGRATION	-0.017487	-0.008996	-0.642911	0.520568	0.566232	-7.004771
KEGG_INOSITOL_PHOSPHATE_METABOLISM	0.018332	-0.015631	0.629428	0.529349	0.572435	-7.013313
KEGG_GRAFT_VERSUS_HOST_DISEASE	0.020338	0.000209	0.474316	0.635476	0.680197	-7.098571
KEGG_LEISHMANIA_INFECTION	0.016519	0.004473	0.473141	0.636314	0.680197	-7.099126
KEGG_DORSO_VENTRAL_AXIS_FORMATION	-0.013021	-0.022796	-0.465534	0.641746	0.680331	-7.102682
KEGG_RENIN_ANGIOTENSIN_SYSTEM	0.013426	-0.017151	0.460464	0.645378	0.680331	-7.10502
KEGG_DRUG_METABOLISM_CYTOCHROME_P450	0.011983	-0.026743	0.45763	0.647411	0.680331	-7.106316
KEGG_VEGF_SIGNALING_PATHWAY	0.006718	-0.016058	0.27616	0.782536	0.816138	-7.172651
KEGG_NITROGEN_METABOLISM	0.005951	-0.035188	0.2724	0.785424	0.816138	-7.173678
KEGG_TYPE_I_DIABETES_MELLITUS	0.008905	0.002698	0.236749	0.812946	0.840044	-7.182722
KEGG_GLYCOSAMINOGLYCAN_BIOSYNTHESIS_HEPARAN_SULFATE	-0.005731	-0.021545	-0.211348	0.8327	0.855702	-7.188393
KEGG_MAPK_SIGNALING_PATHWAY	-0.00414	-0.013437	-0.180958	0.856472	0.875295	-7.194334
KEGG_B_CELL_RECEPTOR_SIGNALING_PATHWAY	0.00525	-0.011728	0.166351	0.867946	0.881027	-7.196861
KEGG_RETINOL_METABOLISM	-0.004016	-0.031174	-0.161766	0.871554	0.881027	-7.197611
KEGG_CYTOKINE_CYTOKINE_RECEPTOR_INTERACTION	0.003252	-0.003649	0.12269	0.9024	0.907278	-7.203149
KEGG_LONG_TERM_POTENTIATION	-0.001866	-0.021488	-0.077012	0.938644	0.938644	-7.207695

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**Supplementary Table 8. Lists of drugs in CTRP and PRISM.**

<b>CTRP</b>	<b>PRISM</b>
968	10-deacetylbaaccatin
16-beta-bromoandrosterone	10-hydroxycamptothecin
1S,3R-RSL-3	12-O-tetradecanoylphorbol-13-acetate
3-Cl-AHPC	1-azakenpaullone
5-fluorouracil	1-naphthyl-PP1
A-804598	1-phenylbiguanide
AA-COCF3	2,3-DCPE
abiraterone	2-MeCCPA
ABT-199	2-methoxyestradiol
ABT-737	3-amino-benzamide
AC55649	3-deazaneplanocin-A
afatinib	3-fluorobenzylpiperone
	4-(4-fluorobenzoyl)-1-(4-phenylbutyl)-piperid ine
AGK-2	4-chlorophenylguanidine
alisertib	4E1RCat
alvocidib	4-hydroxy-phenazone
AM-580	4-iodo-6-phenylpyrimidine
apicidin	4-methylgenistein
AT13387	4-methylhistamine
AT-406	4-pyrimidinecarbonitrile
AT7867	5-fluorouracil
austocystin D	5-hydroxymethyl-tolterodine
avicin D	7-aminocephalosporanic-acid
avrainvillamide	7-hydroxystaurosporine
axitinib	7-nitroindazole
AZ-3146	8-bromo-cGMP
azacitidine	8-hydroxy-PIPAT
AZD1480	9-aminoacridine
AZD4547	A61603
AZD6482	A-674563
AZD7545	A-803467
AZD7762	abemaciclib
AZD8055	abiraterone
B02	abiraterone-acetate
bafilomycin A1	ABT-702
barasertib	ABT-737
bardoxolone methyl	ABT-751
Bax channel blocker	AC-264613
BCL-LZH-4	ACDPP
BEC	acesulfame-potassium
belinostat	



bendamustine	acetazolamide
betulinic acid	acetophenazine
bexarotene	acetylcysteine
BI-2536	acetylsalicylsalicylic-acid
BIBR-1532	acipimox
BIRB-796	acivicin
birinapant	ACY-1215
BIX-01294	adapalene
blebbistatin	adaprev
bleomycin A2	adarotene
BMS-195614	adefovir-dipivoxil
BMS-270394	ADL5859
BMS-345541	AEE788
BMS-536924	AEQ3482
BMS-754807	afatinib
bortezomib	afobazole
bosutinib	AG-14361
BRD1812	ajmaline
BRD1835	albendazole
BRD4132	alectinib
BRD6340	alexidine
BRD8899	alfacalcidol
BRD8958	alisertib
BRD9647	almorexant
BRD9876	alogliptin
BRD-A02303741	alpelisib
BRD-A05715709	altretamine
BRD-A71883111	alvespimycin
BRD-A86708339	alvocidib
BRD-A94377914	AM-251
BRD-K01737880	AM-404
BRD-K02251932	AM-580
BRD-K02492147	ambazone
BRD-K04800985	amfenac
BRD-K09344309	AMG-208
BRD-K09587429	AMG-232
BRD-K11533227	AMG458
BRD-K13999467	AMG900
BRD-K14844214	aminoglutethimide
BRD-K16147474	aminopurvalanol-a
BRD-K17060750	amisulpride
BRD-K19103580	ammonium-lactate
BRD-K24690302	amonafide

BRD-K26531177	amoxicillin
BRD-K27224038	amprolium
BRD-K27986637	amsacrine
BRD-K28456706	anagrelide
BRD-K29086754	anastrozole
BRD-K29313308	anguidine
BRD-K30019337	anisomycin
BRD-K30748066	AP1903
BRD-K33199242	AP26113
BRD-K33514849	apatinib
BRD-K34099515	aphidicolin
BRD-K34222889	AR-12
BRD-K34485477	AR-42
BRD-K35604418	arctigenin
BRD-K37390332	arcyriaflavin-a
BRD-K41334119	aripiprazole
BRD-K41597374	ARRY-334543
BRD-K42260513	artemisinin
BRD-K44224150	artesunate
BRD-K45681478	AS-1949490
BRD-K48334597	AS-703026
BRD-K48477130	aspirin
BRD-K49290616	AST-1306
BRD-K50799972	astemizole
BRD-K51490254	asymmetrical-dimethylarginine
BRD-K51831558	AT13387
BRD-K52037352	AT-7519
BRD-K55116708	AT7867
BRD-K61166597	AT-9283
BRD-K63431240	atenolol(-)
BRD-K64610608	atenolol(+/-)
BRD-K66453893	atipamezole
BRD-K66532283	atiprimod
BRD-K70511574	atorvastatin
BRD-K71781559	aurora-a-inhibitor-i
BRD-K71935468	AV-412
BRD-K75293299	avanafil
BRD-K78574327	AVL-292
BRD-K80183349	AVN-944
BRD-K84807411	axitinib
BRD-K85133207	AZ20
BRD-K86535717	AZ3146
BRD-K88742110	AZ-628

BRD-K90370028	AZ960
BRD-K92856060	azacitidine
BRD-K94991378	azalomycin-b
BRD-K96431673	azathioprine
BRD-K96970199	AZD1480
BRD-K97651142	AZD2014
BRD-K99006945	AZD2461
BRD-M00053801	AZD2858
brefeldin A	AZD3463
brivanib	AZD4547
BYL-719	AZD5363
C6-ceramide	AZD5438
cabozantinib	AZD6482
canertinib	AZD7762
CAY10576	AZD8055
CAY10594	AZD8330
CAY10618	AZD8931
CBB-1007	AZD9668
CCT036477	azilsartan
CD-1530	azithromycin
CD-437	azodicarbonamide
cediranib	azomycin-(2-nitroimidazole)
ceranib-2	aztreonam
cerulenin	bafetinib
Ch-55	baicalein
CHIR-99021	baicalin
chlorambucil	balapiravir
CHM-1	BAM7
CI-976	BAN-ORL-24
ciclopirox	barasertib
ciclosporin	barasertib-HQPA
CID-5951923	bardoxolone
CIL41	bardoxolone-methyl
CIL55	baricitinib
CIL55A	batimastat
CIL56	BAY-11-7082
CIL70	BAY-11-7085
cimetidine	BAY-87-2243
clofarabine	BAY-K-8644-(s)-(-)
COL-3	beclomethasone-dipropionate
Compound 1541A	bekanamycin
compound 1B	belinostat
Compound 23 citrate	bendamustine

Compound 7d-cis	bendroflumethiazide
CR-1-31B	benfotiamine
crizotinib	bentazepam
cucurbitacin I	benzethonium
curcumin	benzocaine
cyanquinoline 11	benzylamine
cyclophosphamide	benzyltrimethylhexadecylammonium
cytarabine hydrochloride	bephenium-hydroxynaphthoate
cytochalasin B	berberine
dabrafenib	beta-lapachone
dacarbazine	betamethasone
darinaparsin	betamethasone-dipropionate
dasatinib	beta-naphthol
DBeQ	betulinic-acid
decitabine	bexarotene
dexamethasone	BF2.649
dinaciclib	BGT226
docetaxel	BI-2536
doxorubicin	BI-78D3
ELCPK	BIBR-1532
elocalcitol	BIBU-1361
entinostat	BIBX-1382
epigallocatechin-3-monogallate	bicalutamide
erastin	BI-D1870
erismodegib	bifemelane
erlotinib	BIIB021
etomoxir	bindarit
etoposide	birinapant
ETP-46464	bis(maltolato)oxovanadium(IV)
EX-527	bisacodyl
FGIN-1-27	bisindolylmaleimide-ix
ingolimod	bitopertin
FK-866	BIX-01294
fluvastatin	BIX-02188
foretinib	blebbistatin(-)
FQI-1	BMS-265246
FQI-2	BMS-345541
FSC231	BMS-387032
fulvestrant	BMS-599626
fumonisin B1	BMS-626529
GANT-61	BMS-690514
GDC-0879	BMS-707035
GDC-0941	BMS-754807

gefitinib	BMS-986020
gemcitabine	BNC105
GMX-1778	BNTX
gossypol	bortezomib
GSK1059615	bosentan
GSK2636771	bosutinib
GSK-3 inhibitor IX	brefeldin-a
GSK4112	brequinar
GSK461364	brigatinib
GSK-J4	brilliant-green
GW-405833	brivaracetam
GW-843682X	bromosporine
HBX-41108	broxaldine
HC-067047	broxyquinoline
HLI 373	bruceantin
hyperforin	BTS-54505
I-BET151	bucladesine
I-BET-762	bumetanide
ibrutinib	buparlisib
IC-87114	buphenine
idelalisib	busulfan
ifosfamide	butamben
imatinib	buthionine-sulfoximine
importazole	butylscopolamine-bromide
indisulam	BVD-523
IPR-456	BVT-948
isoevodiamine	BW-180C
isoliquiritigenin	BX-912
isonicotinohydroxamic acid	cabazitaxel
ISOX	cabozantinib
istradefylline	caffeic-acid
itraconazole	caffeic-acid-phenethyl-ester
IU1	calcitriol
JQ-1	camptothecin
JW-480	camylofine-chlorhydrate
JW-55	candesartan
JW-74	canertinib
KH-CB19	canrenone
KHS101	capecitabine
Ki8751	capsaicin
Ko-143	captamine
KPT185	carbachol
KU 0060648	carboplatin

KU-0063794	carboxyamidotriazole
KU-55933	carboxypyridine-disulfide
KU-60019	carfilzomib
KW-2449	cariporide
KX2-391	carmofur
L-685458	carmustine
lapatinib	carvedilol
LBH-589	CB-10-277
LE-135	CCG-50014
lenvatinib	CCMI
leptomycin B	CCT128930
linifanib	CCT129202
linsitinib	CCT137690
lomeguatrib	CD-437
lovastatin	cebranopadol
LRRK2-IN-1	cediranib
LY-2157299	cefdinir
LY-2183240	cefditoren-pivoxil
manumycin A	cefpiramide
marinopyrrole A	CEP-32496
masitinib	CEP-33779
Mdivi-1	CEP-37440
Merck60	cephalomannine
methotrexate	cetrimonium
methylstat	cetylpyridinium
MG-132	CGM097
MGCD-265	CGP-37849
MI-1	CGP-52411
MI-2	CGP-54626
mitomycin-c	CGS-15943
MK-0752	CGS-20625
MK-1775	CH5132799
MK-2206	chicago-sky-blue-6b
ML006	chidamide
ML029	CHIR-124
ML031	CHIR-98014
ML050	CHIR-99021
ML083	chlorambucil
ML162	chloramphenicol-palmitate
ML203	chlorhexidine
ML210	chlorindanol
ML239	chlormidazole
ML258	chlorogenic-acid

ML311	chloropyramine
ML312	chloroxine
ML320	chlorpropamide
ML334 diastereomer	chlorpyrifos
MLN2238	chlorquinaldol
MLN2480	cholecalciferol
momelotinib	chromocarb
MST-312	CI-844
myricetin	cibenzoline
myriocin	ciclesonide
N9-isopropylolomoucine	ciclopirox
nakiterpiosin	CID-5458317
narciclasine	cidofovir
navitoclax	cilostamide
necrostatin-1	cimetidine
necrostatin-7	cinacalcet
necrosulfonamide	cinalukast
nelarabine	cinnarazine
neopeltolide	cinromide
neratinib	ciprofibrate
neuronal differentiation inducer III	cisplatin
niclosamide	CL-218872
nilotinib	cladribine
nintedanib	clebopride
NPC-26	clenbuterol
NSC 74859	clindamycin-phosphate
NSC19630	clobetasol-propionate
NSC23766	clobutinol
NSC30930	clocortolone-pivalate
NSC48300	clofarabine
NSC632839	clofazimine
NSC95397	clofibrate
nutlin-3	clofoctol
NVP-231	clomifene
NVP-ADW742	clonazepam
NVP-BEZ235	clopamide
NVP-BSK805	clotrimazole
NVP-TAE684	CPMD-1
O-6-benzylguanine	CNX-2006
obatoclax	CNX-774
olaparib	cobicistat
oligomycin A	cobimetinib

omacetaxine mepesuccinate	colchicine
OSI-027	colforsin-daproate
OSI-930	colfosceril-palmitate
ouabain	colistin-b-sulfate
PAC-1	combretastatin-A-4
paclitaxel	costunolide
palmostatin B	CP-673451
pandacostat	CP-724714
parbendazole	CP-945,598
parthenolide	CPI-1189
pazopanib	CPP
PD 153035	CR8-(R)
PD318088	creatine
PDMP	crenolanib
pevonedistat	crizotinib
PF-184	crizotinib-(S)
PF-3758309	cromakalim
PF-4800567 hydrochloride	crystal-violet
PF-543	CS-110266
PF-573228	CUDC-101
PF-750	CUDC-907
PHA-793887	curcumin
phloretin	CX-4945
PI-103	CX-5461
pifithrin-alpha	CYC116
pifithrin-mu	cyclocytidine
PIK-93	cycloheximide
piperlongumine	cyclophosphamide
pitstop2	cyclosporin-a
PL-DI	cyclosporine
pluripotin	cyclovalone
PLX-4032	cyclovirobuxin-d
PLX-4720	cyproheptadine
PRIMA-1	cyproterone-acetate
PRIMA-1-Met	cyromazine
PRL-3 inhibitor I	cyt387
procarbazine	CYT-997
prochlorperazine	cytarabine
purmorphamine	cytochalasin-b
PX-12	cytochlor
PYR-41	D-4476
pyrazolanthrone	D-64131
QS-11	D-7193



quizartinib	dabrafenib
QW-BI-011	dacarbazine
R428	dacinostat
RAF265	daclatasvir
regorafenib	dacomitinib
Repligen 136	dalcetrapib
RG-108	danazol
rigosertib	danusertib
RITA	dapivirine
RO4929097	darapladib
ruxolitinib	darifenacin
salermide	dasatinib
saracatinib	daunorubicin
SB-225002	DCEBIO
SB-431542	decitabine
SB-525334	defactinib
SB-743921	deferasirox
SCH-529074	deflazacort
SCH-79797	deforolimus
selumetinib	dehydrocholate-acid
semagacestat	delanzomib
serdemetan	demecarium
SGX-523	deoxycorticosterone-acetate
SID 26681509	dequalinium
sildenafil	desonide
silmitasertib	desoxycortone
simvastatin	dexamethasone-acetate
sirolimus	dexrazoxane
sitagliptin	dianhydrogalactitol
SJ-172550	diaveridine
skepinone-L	diazooxonorleucine
SKI-II	dichlorisone-acetate
SMER-3	dichloroacetate
SN-38	dichlorvos
SNS-032	diclazuril
SNX-2112	dicycloverine
sorafenib	dienogest
sotrastaurin	difluprednate
spautin-1	digitoxigenin
SR1001	digitoxin
SR8278	digoxigenin
SR-II-138A	digoxin
SRT-1720	dihydroartemisinin

staurosporine	dihydroergocristine
StemRegenin 1	dihydromyricetin
STF-31	dimethisoquin
SU11274	dinaciclib
sunitinib	dioscin
SZ4TA2	diphemanil
tacedinaline	diphenyleiodonium
tacrolimus	dirithromycin
tamatinib	disulfiram
tamoxifen	DMH1
tandutinib	docetaxel
tanespimycin	dofetilide
temozolomide	dolastatin-10
temsirolimus	dolutegravir
teniposide	domiphen
TG-100-115	domperidone
TG-101348	dorzolamide
TGX-221	dovitinib
thalidomide	doxercalciferol
tigecycline	doxifluridine
tipifarnib	doxorubicin
tipifarnib-P2	doxycycline
tivantinib	DPI-201106
tivozanib	dronedarone
topotecan	drospirenone
tosedostat	D-Serine
tozasertib	DU-728
TPCA-1	DVD-111
trametinib	E7449
tretinoin	ebastine
triazolothiadiazine	ecamsule-triethanolamine
trifluoperazine	echinomycin
triptolide	efonidipine-monoethanolate
tubastatin A	elacridar
TW-37	elesclomol
UNC0321	eltrombopag
UNC0638	embelin
VAF-347	EMD-53998
valdecoxib	emetine
vandetanib	endo-IWR-1
veliparib	ENMD-2076
VER-155008	enocitabine
vincristine	enoximone

vorapaxar  
vorinostat  
VU0155056  
WAY-362450  
WP1130  
WZ4002  
WZ8040  
XL765  
YK 4-279  
YM-155  
zebularine  
ZSTK-474

entinostat  
enzalutamide  
epiandrosterone  
epinastine  
epinephrine  
epirubicin  
eplerenone  
epothilone-a  
epothilone-b  
epothilone-d  
epinomectin  
eprobemide  
eprosartan  
eptifibatide  
EPZ-5676  
equol  
ER-27319  
erastin  
ercalcitriol  
erdafitinib  
erlotinib  
erteberel  
erythritol  
estradiol  
estradiol-benzoate  
estradiol-cypionate  
estramustine  
estramustine-phosphate  
estrone  
ethacridine-lactate-monohydrate  
ethinyl-estradiol  
etofylline-clofibrate  
etomoxir  
etoposide  
etoposide-phosphate  
ETP-46464  
evacetrapib  
everolimus  
evodiamine  
EVP4593  
exatecan-mesylate  
exemestane  
famciclovir

famotidine  
favipiravir  
fdcyd  
felbamate  
fenaclon  
fenbendazole  
fendiline  
fenofibrate  
fenoprofen  
fenretinide  
FERb-033  
fexinidazole  
FG-4592  
filanesib  
filgotinib  
finafloxacin  
FK-3311  
FK-866  
FK-888  
fleroxacin  
FLI-06  
florfenicol  
floxuridine  
flubendazole  
fludarabine  
fludarabine-phosphate  
fludroxycortide  
flufenamic-acid  
flumatinib  
flumethasone  
flumethasone-pivalate  
fluocinolone-acetonide  
fluorometholone  
fluoromethylcholine  
fluroxene  
flutamide  
fluticasone-propionate  
fluvastatin  
foretinib  
formestane  
forodesine  
forskolin  
fosbretabulin

foscarnet  
FPH1-(BRD-6125)  
FR-122047  
FR-139317  
frentizole  
ftorafur  
fudosteine  
fulvestrant  
G-1  
galeterone  
gambogic-acid  
gamma-aminobutyric-acid  
ganetespib  
gastrodin  
GDC-0068  
GDC-0152  
GDC-0349  
GDC-0879  
GDC-0941  
GDC-0980  
gefitinib  
gemcitabine  
genipin  
genz-644282  
gestrinone  
GGTI-298  
gidazepam  
gilteritinib  
gimeracil  
ginkgolide-a  
givinostat  
golgicide-a  
golvatinib  
gossypol  
GS-39783  
GS-9973  
GSK1070916  
GSK1292263  
GSK1838705A  
GSK1904529A  
GSK2110183  
GSK2126458  
GSK256066

GSK2656157  
GSK2830371  
GSK-3-inhibitor-IX  
GSK429286A  
GSK461364  
GSK650394  
GSK923295  
GSK-J4  
GTP-14564  
guanidine  
GW-3965  
GW-405833  
GW-441756  
GW-501516  
GW-583340  
GW-788388  
GW-842166  
GW-843682X  
GZD824  
HA14-1  
halcinonide  
halobetasol-propionate  
halofantrine  
halofuginone  
harringtonine  
hesperadin  
hexachlorophene  
hexaminolevulinate  
hexylresorcinol  
HMN-214  
homoharringtonine  
homoquinolinic-acid  
homosalate  
hydrocortisone  
hydroxytacrine-maleate-(r,s)  
hydroxyurea  
hyodeoxycholic-acid  
hyoscyamine  
hypericin  
hypoestoxide  
I-BET151  
I-BET-762  
ibrutinib

ibutilide  
ICG-001  
ICI-162846  
icotinib  
idarubicin  
idasanutlin  
idazoxan  
idelalisib  
idoxuridine  
IDRA-21  
idronoxil  
IEM1754  
ifosfamide  
IKK-16  
IKK-2-inhibitor-V  
ilomastat  
imatinib  
imidapril  
imiloxan  
imiquimod  
INC-280  
indibulin  
indiplon  
indirubin  
indisulam  
indoprofen  
ingenol-mebutate  
INH1  
inosine  
iobenguane  
iodipamide  
iododexetimide  
IOWH032  
iproniazid  
ipsapirone  
irinotecan  
isoetharine  
isofloxythepin  
isoflupredone-acetate  
isometheptene-mucate  
isopropyl-myristate  
isoxsuprine  
ispinesib

istradefylline  
itraconazole  
ivermectin  
ixabepilone  
ixazomib  
ixazomib-citrate  
JIB04  
JK-184  
JNJ-16259685  
JNJ-26481585  
JNJ-7706621  
josamycin  
JQ1  
JTC-801  
JTE-607  
JZL-184  
K-858  
KD-023  
KD025  
kenpaullone  
ketoconazole  
ketoprofen  
KF-38789  
KI-16425  
KI-8751  
kifunensine  
KP-1212  
KPT-185  
KPT-276  
K-Ras(G12C)-inhibitor-6  
k-strophanthidin  
ku-0063794  
KW-2449  
KW-2478  
KX2-391  
KY02111  
kynurenic-acid  
L-798,106  
lacitol  
lafutidine  
lanatoside-c  
lanoconazole  
lapatinib



lappaconite  
lasalocid  
latanoprost  
latrepirdine  
LB42708  
LCL-161  
LDN-212854  
LDN-57444  
LE-135  
lenalidomide  
lenvatinib  
lerisetron  
lestaurtinib  
letrozole  
leucovorin  
levobunolol  
levocarnitine  
levocetirizine  
levonorgestrel  
LGX818  
licoalcone-a  
lidamidine  
lidocaine  
linalool  
linifanib  
linsitinib  
litronesib  
lomefloxacin  
lomitapide  
lonafarnib  
lorazepam  
lorlatinib  
lovastatin  
loxistatin-acid  
lucitanib  
lurasidone  
LY2090314  
LY2109761  
LY2183240  
LY2334737  
LY2603618  
LY2606368  
LY2608204

LY2784544  
LY2801653  
LY2874455  
LY3023414  
LY303511  
LY364947  
LY456236  
M-344  
maprotiline  
marimastat  
masitinib  
maxacalcitol  
maytansinol-isobutyrate  
mebendazole  
mechlorethamine  
meclizine  
mefexamide  
meglitinide  
MEK1-2-inhibitor  
MEK162  
melengestrol-acetate  
meloxicam  
melphalan  
menadione  
mephenytoin  
mepivacaine  
mercaptopurine  
mericitabine  
merimepodib  
mesna  
mesoridazine  
metaraminol  
metatinib  
methacycline  
methiazole  
methocarbamol  
methotrexate  
methoxyflurane  
methscopolamine  
methyldopa  
methylphenidate  
methylprednisolone  
metoprolol

metoxibutropate  
metronidazole  
metyrapone  
mevastatin  
mexeneone  
mexiletine  
MG-132  
MGCD-265  
mibampator  
mibefradil  
midodrine  
midostaurin  
mifepristone  
minocycline  
mitomycin-c  
mitoxantrone  
MK-0773  
MK-0812  
MK-1775  
MK-2206  
MK-2461  
MK-3207  
MK-5108  
MK-8245  
MK-8745  
ML133  
MLN0128  
MLN-8054  
MNS-(3,4-Methylenedioxy-nitrostyrene)  
mocetinostat  
monensin  
monobenzene  
morin  
motesanib  
mozavaptan  
MPI-0479605  
MRS-1220  
MTPG  
mubritinib  
mycophenolate-mofetil  
mycophenolic-acid  
N-acetylmannosamine  
nadide

nadifloxacin  
nafcillin  
naftidrofuryl  
naftifine  
naloxone  
naltrexone  
NAN-190  
nanchangmycin  
napabucasin  
naproxen  
narasin  
narlaprevir  
navarixin  
navitoclax  
nefiracetam  
nelarabine  
nemonapride  
nemorubicin  
neratinib  
nexturastat-a  
NH125  
niacin  
niclosamide  
nicorandil  
nicotine  
nilotinib  
nilutamide  
nimorazole  
nintedanib  
niraparib  
niridazole  
nisooxetine  
nitarsone  
nithiamide  
nitisinone  
nitrocaramiphen  
nizatidine  
nizofenone  
NMS-1286937  
NMS-873  
NMS-E973  
nobiletin  
nocodazole

nomegestrol-acetate  
nonoxynol-9  
norepinephrine  
norethindrone  
norethindrone-acetate  
noretynodrel  
norfloxacin  
norgestrel  
novobiocin  
NSC-23766  
NSC-319726  
NSC-3852  
NSC-632839  
NSC-663284  
NSC-697923  
NU6027  
nutlin-3  
NVP-AEW541  
NVP-AUY922  
NVP-BEZ235  
NVP-BHG712  
NVP-BVU972  
NVP-TAE226  
NVP-TAE684  
obatoclax  
obidoxime  
octenidine  
octopamine  
odanacatib  
olaparib  
OLDA  
oleanolic-acid  
oleoylethanolamide  
oligomycin-a  
oltipraz  
omeprazole  
ONC201  
oncrasin-1  
ONX-0914  
oprozomib  
orantinib  
oridonin  
ornithine

orotic-acid  
oseltamivir-phosphate  
OSI-027  
OSI-420  
OSI-930  
osimertinib  
OTS167  
OTX015  
ouabain  
oxaliplatin  
oxazepam  
oxcarbazepine  
oxibendazole  
oxiperomide  
oxiracetam  
oxonic-acid  
oxprenolol  
oxymatrine  
oxymetazoline  
oxyphencyclimine  
oxyquinoline  
P22077  
P276-00  
P5091  
PAC-1  
paclitaxel  
pacritinib  
palbociclib  
paliperidone  
palmatine-chloride  
palmitoylethanolamide  
palomid-529  
panobinostat  
papaverine  
parachlorophenol  
parbendazole  
pardoprunox  
paricalcitol  
parthenolide  
parthenolide-(-)  
pazopanib  
PCI-24781  
PD-0325901

PD-153035  
PD-168393  
PD-173074  
PD-184352  
PD-198306  
PD-318088  
PD-407824  
PD-98059  
pelitinib  
penfluridol  
penicillamine-(D)  
pentagastrin  
pentamidine  
pentostatin  
pepstatin  
peruvoside  
PETCM  
pevonedistat  
PF-03758309  
PF-03814735  
PF-04136309  
PF-04217903  
PF-04457845  
PF-04691502  
PF-05212384  
PF-3845  
PF-477736  
PF-4981517  
PF-562271  
PF-573228  
PFI-1  
PFK-015  
PHA-665752  
PHA-680632  
PHA-767491  
PHA-793887  
PHA-848125  
phenazone  
phenelzine  
pheniramine  
phenylbutazone  
phenylmercuric-acetate  
phlorizin

PI-103  
PI3K-IN-2  
PI-828  
pibenzimol  
picolinic-acid  
PIK-75  
pilaralisib  
pilocarpine  
pindolol  
piperacetazine  
piperazine  
piperine  
pirenperone  
piretanide  
piroxicam  
pitavastatin  
PJ-34  
PKI-179  
plinabulin  
PLX-4720  
podophyllotoxin  
polydatin  
pomalidomide  
ponatinib  
posaconazole  
poziotinib  
PP-1  
PP-121  
PP-2  
PP242  
PPT  
PQ-401  
PR-619  
practolol  
pralatrexate  
pranidipine  
prazosin  
prednisolone  
prednisolone-acetate  
prednisolone-hemisuccinate  
prednisolone-tebutate  
primaquine  
proflavine-hemisulfate



propoxycaïne  
propranolol  
proscillaridin-a  
protirelin  
PRT062070  
PRT062607  
PSB-1115  
PSI-7976  
PTC-209  
pterostilbene  
PU-H71  
puromycin  
pyrimethamine  
pyrithione-zinc  
pyritinol  
pyroxamide  
quinethazone  
quinidine  
quizartinib  
R306465  
R406  
R547  
rabeprazole  
racecadotril  
raclopride  
radezolid  
RAF265  
raloxifene  
raltitrexed  
ramatroban  
ramifenazone  
ranitidine  
refametinib  
regorafenib  
remoxipride  
repaglinide  
repsox  
resatorvid  
resiquimod  
resminostat  
RG108  
RG2833  
RGFP966

rheochrysidin  
RI-1  
ribavirin  
ribitol  
ribociclib  
riboflavin  
rifampin  
rigosertib  
riluzole  
rimexolone  
riociguat  
RITA  
ritodrine  
RKI-1447  
RN-1734  
Ro-04-5595  
Ro-10-5824  
Ro-106-9920  
Ro-4987655  
Ro-90-7501  
Ro-9187  
rociletinib  
romidepsin  
roquinimex  
RS-16566  
RS-17053  
RS-504393  
RS-67506  
RU-58841  
rubitecan  
rucinol  
rutin  
ruxolitinib  
ryuvidine  
S26948  
salidroside  
salinomycin  
salvianolic-acid-B  
salvinorin-a  
sangivamycin  
SAR131675  
saracatinib  
sarafloxacin

satraplatin  
saxagliptin  
SB-200646  
SB-205384  
SB-216641  
SB-218078  
SB-218795  
SB-225002  
SB-228357  
SB-2343  
SB-239063  
SB-242235  
SB-366791  
SB-431542  
SB-505124  
SB-525334  
SB-590885  
SB-657510  
SB-743921  
SB-939  
SC-12267  
SC-144  
SCH-58261  
SCH-900776  
sclareol  
scriptaid  
SCS  
SDZ-WAG-994  
secnidazole  
securinine  
selamectin  
selinexor  
selumetinib  
semaxanib  
se-methylselenocysteine  
serdemetan  
sertindole  
sevelamer  
sevoflurane  
SGI-1027  
SGI-1776  
SIB-1757  
SID-7969543

simvastatin  
sirolimus  
skepinone-I  
SKF-96365  
SKI-II  
S-methylcysteine  
SMI-4a  
SN-38  
SNS-314  
SNX-2112  
SNX-5422  
sobetirome  
sodium-glucoheptonate  
sodium-stibogluconate  
sodium-tanshinone-ii-a-sulfonate  
sonidegib  
sorafenib  
sparfloxacin  
spermidine  
spermine  
spiradoline  
spironolactone  
SR-27897  
SR-33805  
SR-57227A  
SRT1720  
STA-5326  
stattic  
stemregenin-1  
STF-118804  
streptozotocin  
SU014813  
SU3327  
sufentanil  
sulconazole  
sulfabenzamide  
sulfamethazine  
sulfanilamide  
sulfasalazine  
sulmazole  
sunitinib  
suxibuzone  
tacalcitol

tacedinaline  
tacrolimus  
tagatose  
TAK-285  
TAK-632  
TAK-715  
TAK-733  
TAK-901  
talazoparib  
talmapimod  
taltirelin  
taltobulin  
TAME  
tamibarotene  
tamoxifen  
tanaproget  
tandutinib  
tanespimycin  
tanshinone-i  
TAS-103  
taselisib  
tasisulam  
taurine  
tazemetostat  
TC1  
tecastemizole  
tedizolid  
tedizolid-phosphate  
telatinib  
telotristat-ethyl  
temazepam  
temocapril  
temoporfin  
temozolomide  
temsirolimus  
teniposide  
tenovin-6  
tepoxalin  
teprenone  
terbutaline  
terconazole  
terfenadine  
teriflunomide

teroxirone  
tetrahydropapaverine  
tetrahydrouridine  
tetramethylthiuram-monosulfide  
tetrandrine  
tezacaftor  
TG-02  
TG100-115  
TG-100572  
TG-100713  
TG-101209  
TG-101348  
TH-302  
theophylline  
thiamine  
thiocolchicoside  
thioguanine  
thiomersal  
thiopropazine  
thiostrepton  
thiram  
thonzonium  
tiagabine  
tideglusib  
tiletamine  
tilmicosin  
tiludronate  
tioguanine  
tiotidine  
tioxolone  
tipifarnib  
tipiracil  
tipranavir  
tirapazamine  
tivantinib  
tivozanib  
TMC-353121  
TMS  
tofogliflozin  
topotecan  
torasemide  
torcetrapib  
toremifene

torin-1  
torin-2  
tosedostat  
tozasertib  
TPCA-1  
trametinib  
tranilast  
trans-4-Hydroxycrotonic-acid  
trapidil  
tremorine  
trequinsin  
triamcinolone  
triamcinolone-acetonide  
triamterene  
triapine  
trichostatin-a  
tricitabine  
trilabendazole  
trifluridine  
trimebutine  
triptolide  
trolox  
trometamol  
tropisetron  
trovafloxacin  
tryptanthrin  
TU-2100  
tucatinib  
TW-37  
TWS-119  
tyloxapol  
tyrphostin-A9  
tyrphostin-AG-1296  
tyrphostin-AG-1478  
tyrphostin-AG-494  
tyrphostin-AG-99  
U-0126  
U-18666A  
ubenimex  
UH-232-(+)  
UK-383367  
ulipristal  
UNBS-5162

UNC0631  
UNC2250  
uprosertib  
uracil  
uric-acid  
uridine  
usniacin-(+)  
valnemulin  
valrubicin  
vandetanib  
vanoxerine  
vatalanib  
VE-821  
VE-822  
vemurafenib  
venetoclax  
VER-49009  
verubulin  
vidarabine  
vinblastine  
vincamine  
vincristine  
vindesine  
vinflunine  
vinorelbine  
vismodegib  
VLX600  
volasertib  
voreloxin  
vorinostat  
voxtalisib  
VS-4718  
VTP-27999  
VU0238429  
VU0361737  
VU0364770  
VX-702  
VX-765  
warfarin  
WAY-170523  
WAY-600  
WHI-P154  
WP1066



WP1130  
WYE-125132  
WYE-354  
WZ-3146  
WZ-4002  
WZ8040  
xanomeline  
XBD173  
xilobam  
XL388  
XL-647  
XL888  
xylazine  
Y-27632  
Y-320  
Y-39983  
YM-155  
YM-201636  
YM-976  
YO-01027  
zaldaride  
zaleplon  
zardaverine  
ziprasidone  
ZK811752  
ZK-93423  
ZK-93426  
ZLN005  
ZM-306416  
ZM-447439  
zolantidine  
zolmitriptan  
ZSTK-474

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Supplementary Table 9. List of potential therapeutic agents for LUAD patients with high-risk scores.

Drug name	Source	MOA (mechanism of action)	Targets ( <a href="https://pubchem.ncbi.nlm.nih.gov/">https://pubchem.ncbi.nlm.nih.gov/</a> )	Clinical trials in lung cancer ( <a href="https://clinicaltrials.gov/">https://clinicaltrials.gov/</a> )	Experimental evidence in lung cancer ( <a href="https://pubmed.ncbi.nlm.nih.gov/">https://pubmed.ncbi.nlm.nih.gov/</a> )	Drug targets mRNA Log2FC (normal and tumor)	CMap Score	Correlation Coefficient	Correlation P-value	AUC Log2FC	AUC Wilcox FDR
paclitaxel	CTRP	Tubulin inhibitor	PON1, Abcb1a, UGT1A1, UGT1A4, UGT2B10, UGT2B7, UGT1A6, BATF3, CD74, CD83, CYBB, Fcgr1, H2-Aa, H2-DMa, H2-M3, H2-T23, MAP3K14, PSMB9, TNF, TUBB4A, TUBB, TUBA3C, TUBA1B, TUBA4A, TUBB4B, TUBB3, TUBB2A, TUBB8, TUBA3E, TUBA1A, TUBA1C, TUBB6, TUBB2B, TUBB1, NRG1, SRC, NFE2, NULL, EPHA5, TRIM5, MET, CYP1B1, AURKA, CYP3A5, CXCL8, NOTCH1, SLCO1B3, STMN1, BDNF, KRAS, GSTP1, ABCC1, BCL2, PIK3CG, FOS, ABCC2, NR1I2, SOD2, ABCB1, GSTM1, PGP,	Phase 4	PMID: 9473739	1.043919	-71.26	-0.4274251	1.27E-23	0.47697598	2.02E-11

FASN, JAK2, E2F1,  
DSCAM, CDK2,  
ABCG2, ERCC1, ATM,  
GSTT1, NAT2,  
BRCA2, EIF4EBP1,  
MYB, PDCC4, FNTB,  
FGD4, PTEN, MMP2,  
ERBB2, SPATA5,  
TP53, MAD1L1,  
BRCA1, EGFR, LIF,  
ABCC10, CDKN1A,  
AR, SMAD4, TUBA3D,  
PIK3CA, CYP19A1,  
RRM1, TLE3, ERCC2,  
ABCC3, TOP2A,  
DDIT3, CYP3A4,  
SOX10, BIRC5,  
CASP7, CASP3,  
OPRM1, SLC29A1,  
GMNN, CDKN2A,  
PDGFRA, IL2RA,  
EDNRB, SLC01B1,  
SYK, RAF1, AKT1,  
MAP3K1, ACSS2,  
CYP3A7, CYP2C8,  
ABCB11, MAP4,  
MAPT, MAP2, Tlr4

leptomycin B	CTRP	CRM1 inhibitor	AHR, AKT1, APAF1, AR, BACH1, BAX, BCL2, BCL2L1, BIRC2, BIRC3, BIRC5, BRCA1, BTG2, CASP1, GPX1, H2AX,	Preclinical	PMID: 28942004	1.046014	NA	-0.424487	2.73E-23	0.58634325	5.37E-10
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CCL2, CCNB2,  
 CCND1, CCNE2,  
 CDC25A, CDC25C,  
 CDK1, CDKN1A,  
 CHEK1, CHEK2,  
 CXCL10, CXCL8,  
 CYP3A4, DNMT1,  
 E2F1, E2F3, EGFR,  
 EI24, ESR1, FGF1,  
 FOXO1, GADD45A,  
 HAX1, HK2, ID3, IL1B,  
 IL6, MAPK1, MAPK3,  
 MDM2, MDM4, MYH4,  
 NFKB1, NPPA,  
 NR4A1, NR4A2,  
 NUP62, PIDD1, PML,  
 PRC1, PRKCA,  
 PTTG1, RANBP1,  
 RELA, RPS6KB2,  
 RXRA, SESN1,  
 SMAD2, SMAD3,  
 SMAD4, SOD2,  
 STAT4, STK4, TGFA,  
 TGFB2, TNFRSF10B,  
 TNFRSF10D, TP53,  
 TP63, TXNDC5, WTIP,  
 XPO1, XPO4

nakitepiosin	CTRP	Tubulin inhibitor	TUBA4A, TUBB	Preclinical	NA	1.076213	NA	-0.4242508	2.90E-23	0.12312712	8.53E-13
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fluorouracil	CTRP	Thymidylate synthase inhibitor	TYMS, BAX, BBC3, BBS4, BBX, BCAR3, BCAS4, BCAT1, BCKDHA, BCL2, BCL2L1, BCL2L11, BCL2L12, BDH1, BDKRB2, BDNF, BEAN1, BECN1, BGLAP, BHLHE41, BID, BIRC2, BIRC3, BIRC5, BIRC6, BIRC7, BLM, BLVRB, BNIP1, BNIP3, BNIP3L, BOLL, BOP1, BORA, BRCA1, BRIX1, BTG2, BTG3, BTN3A3, BUB1, BUB1B, BUB3, C11orf24, C14orf132, C1orf35, C4BPB, CA12, CA14, CABYR, CAD, CALB2, CANX, CAP2, CASD1, CASP1, CASP10, CASP2, CASP3, CASP4, CASP6, CASP7, CASP8, CASP9, CAT, CAV1, CAV2, CBR3, CBS, CBX1, CCDC186, CCL2, CCN1, CCN2, CCN3, CCNA1, CCNA2, CCNB1, CCNB2, CCNC,	Phase 3	PMID: 32331446	1.045272	NA	-0.3531886	3.90E-16	0.06662838	1.88E-09
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CCND1, CCND2,  
CCND3, CCNE1,  
CCNE2, CCNF,  
CCNG1, CCNG2,  
CCNJL, CD24, CD274,  
CD34, CD38, CD40,  
CD40LG, CD44,  
CD52, CD63, CD8A,  
CD8B, CD9, CDA,  
CDC20, CDC25A,  
CDC25B, CDC25C,  
CDC34, CDC40,  
CDC42EP1, CDC45,  
CDC6, CDC73,  
CDCA5, CDCA7,  
CDCA8, CDH1, CDH5,  
CDH6, CDIPT, CDK1,  
CDK2, CDK5R1,  
CDKN1A, CDKN1B,  
CDKN1C, CDKN2A,  
CDKN2AIP, CDKN2C,  
CDKN3, CDX2,  
CEBPB, CENPQ,  
CENPU, CENPX,  
CEP55, CER1, CES2,  
CFLAR, CHEK1,  
CHEK2, CHI3L1,  
CHRNA4, CHST7,  
CIAO1, CIDEB,  
CITED2, CKB, CKS2,  
CLCN3, CLDN2,  
CLDN4, CLEC11A,  
CLIC1, CLTC, ctk,

COCH, COL12A1,  
COL1A1, COL1A2,  
COL2A1, COL3A1,  
COL4A2, COL5A2,  
COL6A3, COX14,  
COX5B, COX6C,  
COX7C, CP, CPA4,  
CPD, CPE, CPT1A,  
CPXM1, CRABP1,  
CRABP2, CRHBP,  
CRIM1, CRK, CRMP,  
CRYGS, CRYL1,  
CRYZ, CSE1L, CSF1,  
CSF2, CSNK1E,  
CSRP1, CST7, CST8,  
CSTF3, CTBP2,  
CTNND2, CTPS1,  
CTSB, CTSH, CTTN,  
CUL4A, CUL4B,  
CUL5, CUTC, CXCL1,  
CXCL12, CXCL2,  
DAPK1, DARS1,  
CXCL8, CXCR1,  
CXCR4, CYC1, CYCS,  
CYFIP2, CYLD,  
CYP1A1, CYP2A6,  
Cyp2b1, CYP2F1,  
CYP2S1, CYP3A4,  
CYP51A1,  
CYP51A1P2, CYTH3,  
DBF4, DBNDD2, DCC,  
DCK, DCLK1, DCT,  
DCX, DCXR, DDAH2,

DDB2, DDIT3, DDIT4,  
DDX39B, DDX4,  
DENND2C, DEPDC7,  
DES, DFFA, DHFR,  
DHX15, DIABLO,  
DICER1, DIMIT1,  
DKK1, DKK4, DLC1,  
DLG1, DLK1, DNAH2,  
DNER, DNMT3B,  
DPAGT1, DPY19L1,  
DPYD, DPYSL3,  
DRAM1, DRD5, DST,  
DTWD1, DTYMK,  
DUSP1, DUSP14,  
DUSP5, DUSP6, DUT,  
E2F1, E2F2, E2F3,  
E2F4, E2F8, EBP,  
ECHDC3, ECHS1,  
ECT2, EDIL3, EDN1,  
EDNRA, EDNRB,  
EEF1A1, FAM102A,  
EFEMP1, EFHD1,  
EFHD2, EFNB2,  
EGFR, EGR1, EHD2,  
EHF, EIF2AK3,  
EIF2B2, EIF2S1,  
EIF3H, EIF4E,  
EIF4EBP1, EIF4H,  
EIF5, EIPR1, ELMO2,  
ELN, ELOA, ELOVL5,  
EMC1, EML2, EMP3,  
ENAH, ENDOG,  
ENOSF1, ENTPD1,



ENTREP3, EOMES,  
EP300, EP400,  
EPAS1, EPB41L3,  
EPHA2, EPHX1, EPO,  
EPOR, EPPK1,  
EPRS1, EPYC, ERAS,  
ERBB2, ERBB3,  
ERBB4, ERCC1,  
ERCC2, EREG, ERN1,  
ERP29, ESPL1, ETF1,  
ETFB, ETS1, ETV2,  
EXOSC10, F12, F2,  
F3, F8, FABP7, FADD,  
FADS1, FAH,  
FAM107B, FAM114A1,  
FAM171A1, FAM20C,  
FAM234B, FAM76B,  
FANCC, FANCG,  
FANCI, FARS2, FAS,  
FasI, FASTK, FBLN1,  
FBXO5, FKBP11,  
FDXR, FEN1,  
FERMT2, FGD6,  
FGF2, FGF4, FGF5,  
FGF7, FGFR2, FGG,  
FHL2, FHL3, FIBCD1,  
FILIP1L, FKBP1B,  
FKBP5, FKBP1,  
FLRT2, FLT1, FMOD,  
FN1, FNBP1,  
FNDC3B, FOLR1,  
FOS, FOSL1, FOXA2,  
FOXC1, FOXD3,

FOXG1, FOXL2,  
FOXM1, FOXN3,  
FOXO3, FPGS,  
FTLP3, FUT1, FXYD3,  
FYN, FZD2, G0S2,  
GABRB3, GADD45A,  
GADD45B, GADD45G,  
GAL, GALNT3, GAMT,  
GAPDH, GART,  
GAST, GATA2,  
GATA4, GATA6,  
GCLM, GCSH, GDF1,  
GDF15, GDF3, GEM,  
GFAP, GFRA1,  
GINS1, GINS2, GJA1,  
GJC1, GLA, GLI1,  
GLIPR1, GNB2, GNE,  
GOLGA8A, GP1BB,  
GPR132, GPR137C,  
GPR35, GPR87, GPT,  
GPX1, GPX2, GPX4,  
GRAMD4, GRB7,  
GRHL3, GRINA,  
GSPT1, GSR, GSTA4,  
GSTM1, GSTP1,  
GSTT1, GTPBP4,  
GUCY1B1, GYG2,  
H1-3, H10, H2AX,  
H2BC12, H3-7,  
H4C14, H4C2, H4C3,  
HACD1, HAND1,  
HAND2, HAPLN2,  
HBA1, HBB, Hbb-b2,

HBE1, HBZ, HDAC1,  
HDAC2, HDAC3,  
HDAC4, HDAC7,  
HDAC9, HDGFL3,  
HERPUD1, HES1,  
Hexo 1, HGF, HHLA3,  
HIC2, HIF1A, HINT1,  
HK2, HLA-F, HLA-G,  
HM13, HMCES,  
HMG1, HMG20B,  
HMG5, HMMR,  
HMOX1, HNF1A,  
HNF4A, HNRNPA1,  
HNRNPA2B1,  
HNRNPC, HNRNPF,  
HNRNPH1, HNRNPL,  
HOXA1, HOXB3,  
HOXC11, HOXD1,  
HPX, HRAS, HS6ST2,  
HSD17B2, HSPA1B,  
HSPA2, HSPA4,  
HSPA5, HSPA8,  
HSPB1, HSPB2,  
HSPB8, HSPE1,  
HTATIP2, HTR7,  
HTRA1, IAPP, ID1,  
ID2, ID2B, ID3, IDI1,  
IER5, IFI16, IFI27L2,  
IFI35, IFI6, IFIT1,  
IFIT2, IFITM1, IFITM2,  
IFITM4P, IFNA1,  
IFNA2, IFNAR1,  
IFNAR2, IFNB1, IFNG,

IGF1, IGF1R, IGFBP2,  
IGFBP4, IGFBP5,  
IGFBP6, IHH, IKBIP,  
IKBKB, IL10, IL12B,  
IL18, IL1A, IL1B,  
IL1RN, IL27RA, IL3,  
IL6, IL7, IMPA2,  
IMPDH2, INKA2,  
INPP5E, Ins2, INSIG1,  
IQGAP2, IRAK1,  
IREB2, IRF9, Irgm1,  
ISG15, ISL1, ITGAV,  
ITGB2, ITGB4, ITPR1,  
ITSN1, JAG1, JMJD4,  
JUN, JUNB, KANSL1,  
KCNA5, KCNQ2,  
KCTD12, KDM4B,  
KDM5A, KDR, KEAP1,  
KHK, KIAA0040,  
KIF14, KIF15, KIF23,  
KIF26B, KIF2C, KIF3A,  
KIT, KITLG, KLF4,  
KLF5, KLF6, KLHL24,  
KLHL7, KLHL9,  
KLK15, KLK6, KMT2E,  
KNG1, KPNA2,  
KPNA3, KRAS, KRT1,  
KRT16, KRT17,  
KRT18, KRT5, KRT6A,  
KRT86, L1CAM,  
L1TD1, LAMA1,  
LAMB1, LAMC1,  
LARP4B, LASP1,

LCMT2, LDHA, LDHB,  
LEFTY1, LEFTY2,  
LGALS3, LGALS3BP,  
LGALS7, LGALS8,  
LGR4, LGR5, LHX1,  
LIFR, LIG1, LIMK1,  
LIMK2, LIN28A, lin-29,  
LIPH, LMF1, LMNA,  
LMNB1, LMNB2,  
LPAR6, LPO, LPXN,  
LRATD1, LRBA, LRP8,  
LSS, LXN, LY6G6C,  
LY6G6D, LYPLA1,  
M6PR, MACF1,  
MAD2L1, MAD2L2,  
MADD, MAF, MAFF,  
MAGEA12, MAGEA2,  
MAGEA4, MAGEA6,  
MAGEB2, MAGED1,  
MAGED4B, MALAT1,  
MALT1, MAMDC2,  
MAML2, MAN1A1,  
MANEA, MAP1LC3B,  
MAP2, MAP2K1,  
MAP2K2, MAP3K1,  
MAP3K20, MAP4K5,  
MAPK1, MAPK13,  
MAPK3, MAPK7,  
MAPKAP1, MAPT,  
MARCKS, MARS1,  
MAST4, MBD4,  
MBNL1, MBP,  
MCCC2, MCF2, MCL1,

MCM10, MCM2,  
MCM3, MCM4, MCM6,  
MCM7, MCMBP,  
MDFI, MDFIC, MDM2,  
MDM4, MED13L,  
MEF2B, MELK,  
MEOX1, MESP1,  
MESP2, METAP2,  
METRN, MFN1,  
MFN2, MGAT2,  
MGMT, MICA, MICB,  
MIF, MIR577, MKI67,  
MKX, MLF1, MLH1,  
MLLT11, MMP1,  
MMP2, MMP3, MMP9,  
MMS19, MNX1,  
MORF4L2, MPC2,  
MPIG6B, MPO, MPP7,  
MPRIIP, MR1, MRAS,  
MSH2, MSX2, MT1E,  
MT1M, MT1X, MTAP,  
MTHFR, MTOR,  
MTTP, MTUS1, MVP,  
MXI1, MYB, MYBL2,  
MYC, MYCL, MYCN,  
MYD88, MYF5, MYL4,  
MYL9, MYLIP,  
MYO1E, MYO6,  
MYOD1, MYOF,  
NAF1, NAIP, NANOG,  
NASP, NBL1, NBN,  
NBPF10, NCAPG,  
NCL, NCOR1,

NDUFA10, NDUFA4,  
NDUFA6, NDUFAB1,  
NDUFAF1, NDUFAF3,  
NDUFAF4, NDUFB10,  
NDUFB2, NDUFB9,  
NDUFC1, NDUFV1,  
NDUFV3, NEDD4,  
NEK1, NEK2, NEK4,  
NEK6, NEK9, NES,  
NETO2, NEUROD1,  
NEUROG2, NFE2L2,  
NFE2L3, NFIB, NFIC,  
NFKB1, NFKBIA,  
NFYA, AARS1,  
ABCB1, ABCB6,  
ABCC1, ABCC11,  
ABCC2, ABCC5,  
ABCC6, ABCG2,  
ABHD12B, ABI1, ABI2,  
ACAD9, ACADL,  
ACE2, ACKR3,  
ACOT13, ACOT7,  
ACTB, ACTC1,  
ACTG2, ACTL8,  
ACY1, ADAM10,  
ADAM3A, ADAMTS9,  
ADCY9, ADD3,  
ADGRG1, ADGRG6,  
ADGRL2, ADIRF,  
ADM, ADSS2, AFP,  
AGAP3, AGR2,  
AHNAK, AIFM1,  
AKAP12, AKR1B10,

AKR1C1, AKR1C2,  
AKR1C3, AKT1, AKT2,  
ALB, ALCAM,  
ALDH1A1, ALDH1A3,  
ALDH3A2, ALG3,  
ALKBH8, AMFR,  
AMPD2, AMT, ANG,  
ANGPT1, ANGPT2,  
ANGPTL2, ANGPTL3,  
ANGPTL4, ANKRD1,  
ANKRD11, ANKRD36,  
ANKRD36B, ANLN,  
ANP32E, ANXA1,  
ANXA2, ANXA3,  
ANXA4, AP2S1,  
AP3S1, AP4S1,  
APAF1, APBA2,  
APBB2, APEX1,  
APOB, APOBEC3C,  
APOC1, APOC3,  
AQP12B, AQP6,  
AQP9, AREG, ARF1,  
ARF3, ARFGAP1,  
ARHGDIB, ARID5B,  
ARL4C, ARL6IP5,  
ARMCX1, ARPC3,  
ASAH1, ASS1, ATF3,  
ATF4, ATF6, ATG12,  
ATOH8, ATP5F1D,  
ATP5PB, ATP5PF,  
ATP5PO, ATP6,  
ATP7B, ATP9A,  
ATXN10, AURKA,



AVEN, BAD, BAG3,  
BAK1, BARX2, NFYB,  
NINJ1, NIPSNAP2,  
NKAIN1, NKIRAS1,  
NME1, NME4,  
NODAL, NOG, NOM1,  
NOS2, NOS3,  
NOTCH1, NPM1,  
NPM3, NPPA, NQO1,  
NR1D2, NR4A1,  
NR5A2, NR6A1,  
NRG1, NRIP1, NRP1,  
NT5C1A, NT5E,  
NT5M, NTN4, NTRK2,  
NTS, NTSR1,  
NUCKS1, NUPR1,  
OAS2, ODC1,  
OGFRL1, OLFM1,  
OLIG2, OLIG3, OPTN,  
ORC3, ORC6, OTX2,  
OXCT1, P4HB,  
PAFAH1B1, PAICS,  
PAIP1, PANK1,  
PAQR8, PARD3,  
PARP1, PARP14,  
PAX3, PAX6, PBX3,  
PCDHA5, PCLAF,  
PCNA, PCOLCE2,  
PDAP1, PDCD1LG2,  
PDCD4, PDCD6IP,  
PDF, PDIA4, PDLIM5,  
PDXK, PDXP,  
PECAM1, PEG10,

PER1, PER2, PFN2,  
PGLYRP1, PGR,  
PHIP, PHLDA3,  
PHYH, PI4KB, PIR,  
PISD, PLA2G4A,  
PLAT, PLAU, PLCG1,  
PLEKHB1, PLEKHO1,  
PLIN2, PLIN3, plk,  
PLK1, PLK2, PLK3,  
PLOD2, PLP2,  
PLRG1, PLSCR1,  
PMAIP1, PMF1,  
PMS2P4, PNMA2,  
PNP, PNPLA6,  
PNRC1, PODXL,  
POLA1, POLA2,  
POLE2, POLG,  
POSTN, POU5F1,  
PPA2, PPARG,  
PPFIBP1, PPIE,  
PPM1D, PPP1CA,  
PPP1CC, PPP1R15A,  
PPP1R17, PPP1R1B,  
PPP1R2, PPP2CB,  
PPP3CA, PRC1,  
PRDM14, PREPL,  
PRIM1, PRKAG2,  
PRKCI, PRKCZ,  
PRKDC, PRNP,  
PROC, PROCR,  
PRODH2, PROM1,  
PRPF18, PRPS1,  
PRPS2, PRR13,

PRRG1, PRRX1,  
PRSS2, PSG9,  
PSMB10, PSMC3IP,  
PSRC1, PTCH1,  
PTEN, PTGR1, PURA,  
PURG, PTGS2, PTK2,  
PTPRK, PTTG1,  
PTTG3P, PUM1,  
PVT1, PWP2, PXMP2,  
QSOX1, R3HDM2,  
RAB11A, RAB20,  
RAB21, RAB25,  
RAB8A, RAD23B,  
RAD51C, RAD54B,  
RAF1, RAMP1,  
RANBP1, RARRES2,  
RAX2, RB1, RBBP4,  
RBM14, RBM5, RBP1,  
RBPJ, RCBTB2,  
RCC1, RDX, RECQL4,  
REG4, RELA, REPS1,  
REST, REV1, RFC2,  
RFC3, RFC4, RGS1,  
RGS13, RGS16,  
RGS2, RGS4, RGS5,  
RHBDL2, RHOA,  
RIPK1, RIT1,  
RNASE4, RND2,  
RNF34, RNF4,  
RPL10A, RPL21P4,  
RPL23, RPL23AP1,  
RPL24, RPL3, RPL37,  
RPL6, RPRD1B,

RPS26, RPS27L,  
RPS28, RRAS,  
RRBP1, RRM1,  
RRM2, RRM2B,  
RRP15, RSRC2,  
RTKN, RTL8C,  
RUNX2, S100A10,  
S100A11, S100A2,  
S100A3, S100A4,  
S100P, SAA1, sah,  
SAMHD1, SAP30,  
SAT1, SCAMP3,  
SCCPDH, SCD,  
SCG2, SCN2B,  
SCNN1A, SCNN1B,  
SCUBE2, SDCCAG8,  
SDHA, SDHD,  
SEC14L1, SEC23A,  
SEC31A, SEC31B,  
SELENOP, SEMA3A,  
SEPHS1, SEPHS2,  
SEPTIN9, SERF2,  
SERPINA5,  
SERPINA7,  
SERPINB2,  
SERPINB4,  
SERPINB5,  
SERPIND1,  
SERPINE2, SERPINI1,  
SERTAD1, SESN1,  
SESN2, SET, SETD5,  
SEZ6L, SF3B3, SFN,  
SFRP2, SGCE, SHH,

SHISA9, SHMT2,  
SIGLEC1, SIGLEC9,  
SKIC8, SLC13A5,  
SLC15A1, SLC16A1,  
SLC16A6, SLC22A7,  
SLC22A8, SLC25A23,  
SLC25A27, SLC29A1,  
SLC2A1, SLC2A14,  
SLC2A2, SLC2A3,  
SLC35F5, SLC3A2,  
SLC47A1, SLC48A1,  
SLC5A1, SLC9A3,  
SLCO2A1, SMAD4,  
SMARCA1, SMCHD1,  
SMIM10L2A, SMIM14,  
SMN2, SMO, SMOX,  
SMS, SMURF1,  
SNAI2, SNAP29,  
SNAPC1, SNHG15,  
SNORD22, SNRNP48,  
SNRPA1, SNTB1,  
SNX6, SOAT1,  
SOCS1, SOD1, SOD2,  
SOX17, SOX18,  
SOX2, SOX4, SP1,  
SP3, SPAG5,  
SPANXA1, SPANXC,  
SPARC, SPATA25,  
SPINK4, SPN,  
SPOCK1, SPON1,  
SPRR1A, SPRR1B,  
SPRR3, SPRY1,  
SPTAN1, SQLE, SRC,

SREBF1, SREBF2,  
SRI, SRP19, SRP72,  
SRP9, SRRM1,  
SRSF11, SRSF6, SST,  
STARD7, STAT1,  
STAT3, STAU1,  
STBD1, STK38, STK4,  
STOM, STX5,  
STXBP4, SUFU,  
SUPV3L1, su(r),  
SWAP70, SYCP3,  
SYMPK, SYNCRIP,  
SYP, SYTL2, T, TAF3,  
TAF5L, TAGLN,  
TANK, TAOK3, TAP1,  
TAP2, TAT, TAX1BP3,  
TBCD, TBCE, TBRG4,  
TCF15, TCF19, TCF3,  
TCF7L2, TDGF1, TEK,  
TERF2, TERT,  
TFCP2L1, TFDP1,  
TFF1, TFPI, TFRC,  
TGFA, TGFB1,  
TGFB2, TGFB1,  
TGFBR3, TH, THBS1,  
THNSL2, THOC1,  
THSD7A, TIAL1,  
TIGAR, TIMELESS,  
TIMP3, TINF2, TJP3,  
TK1, TK2, TLR3,  
TLR4, TLR9,  
TMEM150C,  
TMEM184B,

TMEM187, TMEM33,  
TMEM40, TMEM74,  
TMEM9B, TMSB10,  
TMSB15A, TMSB4X,  
TMSB4XP6, TNF,  
TNFAIP3,  
TNFRSF10A,  
TNFRSF10B,  
TNFRSF10C,  
TNFRSF10D,  
TNFRSF11B,  
TNFRSF18,  
TNFRSF19,  
TNFRSF1A,  
TNFRSF1B, TNFSF10,  
TNFSF13, TNNI1,  
TNNI3, TNNT1, TNS3,  
TOB1, TOP1, TOP2A,  
TOPBP1, TP53,  
TP53AIP1, TP53I3,  
TP53INP1, TP73,  
TPI1, TPM1, TPMT,  
TPP1, TPP2, TPST2,  
TPT1, TRADD,  
TRAF2, TRAP1,  
TRIAP1, TRIB2,  
TRIB3, TRIM2,  
TRIOBP, TROAP,  
Trp53, TSC2, TSHB,  
TSHZ1, TSPAN8,  
TSPO, TSR1, TST,  
TTYH2, TUBA4B,  
TUBA8, TUBB,

TUBB2A, TUBB3,  
TUBB4B, TUBD1,  
TXNIP, TXNRD1,  
TXNRD3, TYMP,  
TYRP1, U2SURP,  
UBE2C, UBE2S,  
UBE2T, UCHL1,  
UCK2, UCP2, UGDH,  
UGT1A1, UGT8,  
UMPS, UNC13B,  
UNC5B, UNG, ung-1,  
UPP1, UPRT,  
UQCR10, UQCR11,  
UQCRB, UQCRC2,  
UQCRFS1, UQCRH,  
UROD, USH2A,  
USP14, USP9X,  
UTP3, UXT, VANGL2,  
VASP, VAT1, VAV3,  
VCL, VEGFA, VGF,  
VIM, VPREB3, VPS35,  
VPS37A, VPS52,  
WARS1, WBP4,  
WDR4, WEE1, WNT3,  
WNT5A, WNT8A,  
WT1, WTAP, XAF1,  
XAGE1B, XBP1, XIAP,  
XIST, XRCC1,  
XRCC3, XRCC5,  
XRCC6, YARS1,  
YARS2, YBX1, YES1,  
YIF1A, YWHAB,  
YWHAE, YWHAH,



ZBTB18, ZBTB20,  
ZBTB7A, ZC3H3,  
ZCCHC18, ZDHHC9,  
ZFP42, Zfp518a, ZIM2,  
ZKSCAN3, ZMAT3,  
ZMYND8, ZNF263,  
ZNF266, ZNF282,  
ZNF32, ZNF367,  
ZNF408, ZNF473,  
ZNF532, ZNF552,  
ZNF582, ZRSR2,  
ZSCAN18, PARD3B,  
IRS1, MEGF11, IL11,  
ALDH3A1, CYP1B1,  
ITGAL, CHN2, GNAS,  
TMEM167A, XRCC4,  
SLC22A16, CYP19A1,  
CCNK, KLC1, FGFR4,  
MIR27A, PTPRC,  
PON1, CBLB, DLG5,  
IL6R, NOS1, ATM,  
CBR1, PPP2R5D,  
SELE, ABCC4, PERP,  
DPYS, PIK3CA,  
WNT5B, MET,  
SHMT1, FOXO1,  
CYP2C8, INSR,  
SLC19A1, BRAF,  
CYP2C19, MUC2,  
REV3L, RBX1, EXO1,  
ABCG1, IGFBP3,  
APC, PIK3R2, IL2RA,  
CYP2E1, SLCO1B1,

GNL3, GALNT14,  
UPP2, PPAT,  
CYP1A2, CYP2C9,  
ABCC3, ATAD5,  
NR1H4, CDC21

SB-743921	CTRP	KSP inhibitor	KIF11	Preclinical	PMID: 23394180	1.260722	NA	-0.3475159	1.22E-15	0.41608951	3.56E-08
3-CI-AHPC	CTRP	AKT inhibitor	BCL2L1, BIRC2, CHUK, FAS, HSP90AB1, NFKBIA, RALBP1, RELA, TNFRSF10A, TNFRSF10B, XIAP	Preclinical	NA	1.028049	NA	-0.3418504	3.75E-15	0.10593642	1.35E-10

STF-31	CTRP	GLUT1 inhibitor	SLC2A4, CYP19A1, HSD3B1	Preclinical	NA	1.069723	NA	-0.3133482	7.47E-13	0.12603485	2.81E-08
parbendazole	CTRP	Tubulin inhibitor	NR1H4, AR, GMNN, CYP1A2	Preclinical	NA	0.8428409	-91.12	-0.3089235	1.62E-12	0.14344103	1.91E-07
cabazitaxel	PRISM	Microtubule inhibitor	AKT1S1, FOXO3, TUBB4A, TUBB, TUBA3C, TUBA1B, TUBA4A, TUBB4B, TUBB3, TUBB2A, TUBB8, TUBA3E, TUBA1A, TUBA1C, TUBB6, TUBB2B, TUBB1, TUB, IGF2, CYP3A4, NULL, TUBA3D, CYP3A5, CYP2C8, ABCB1, ABCG2, SLCO1B1, SLCO1B3	Phase 2	PMID: 27572899	1.061563	NA	-0.5380321	7.29E-39	0.3482832	2.42E-15
epothilone-b	PRISM	Microtubule inhibitor	CALCA, NGF, TUBB4A, TUBB, TUBA3C, TUBA1B, TUBA4A, TUBB4B, TUBB3, TUBB2A, TUBB8, TUBA3E, TUBA1A, TUBA1C, TUBB6, TUBB2B, TUBB1, CYP3A4, TUBA8	Phase 2	PMID: 21738778	1.103772	-97.63	-0.5094874	2.21E-34	0.3210276	1.92E-14
vincristine	PRISM	Tubulin inhibitor	AR, TYMS, TUBA1A, SRI, TUBB2A, ABL1, CAPG, CXCL12, TUBB4B, NRG1, DROSHA, TUBB3,	Phase 3	PMID: 28988243	1.05251	-38.68	-0.3790285	1.58E-18	0.4474621	1.23E-10

ATRX, PIK3CA,  
 PIK3CG, TUBA1B,  
 TUBA4A, CP, ABCB4,  
 VWF, SMAD3, NTF3,  
 AFP, ABCC3,  
 CYP3A5, NR1I2,  
 LINC00251, TUBB8,  
 BMP7, TUBB, DOK5,  
 TUBB4A, GATA3,  
 TUBB6, FGF2,  
 TUBB1, BDNF,  
 ABCC1, RALBP1,  
 TUBA3E, CDKN1B,  
 GMNN, ODC1,  
 TUBA1C, BCR,  
 MYCN, TUBA3C,  
 PNPLA3, TUBA3D,  
 TOP2A, NULL,  
 ABCC2, CEP72,  
 ABCC10, BCL2,  
 TUBB2B, ACTG1,  
 ABCB1, GSTA1,  
 SLC22A3, ABCB11,  
 ABCG2, SLC01B1,  
 SLC01B3, CYP3A4,  
 CYP3A7

gemcitabine	PRISM	Ribonucleoti de reductase inhibitor	XYLT2, SLC28A1, SMAD4, PTEN, IGF2, SERPINC1, ERBB2, GPX5, DAPK1, DOCK8, NT5C2, CBL, KLC3, TNF, CYP2C8, FANCC, RRM2,	Phase 4	PMID: 29949158	1.057902	-99.12	-0.3522404	4.73E-16	0.5379188	1.35E-10
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RRM1, TENT4A, KDR,  
 PPP1R13L, RRM2B,  
 ERCC2, AKT1, TGM2,  
 DCK, BRCA1, SH2D5,  
 BRCA2, EGFR, SRC,  
 ABCG2, KRAS,  
 ERCC1, MSH5,  
 PPP1R18, IDH1,  
 ATAT1, FHL2, FKBP5,  
 CDA, PRRC2A,  
 POLR1G, SLC29A3,  
 NT5C1A, CDKN2A,  
 HLA-C, POLR2A,  
 NT5C3A, CMPK1,  
 SLC28A3, NRG1,  
 ETS2, CDSN,  
 SLC28A2, ACSS2,  
 HRAS, NT5C, NRAS,  
 CHEK1, MUCL3,  
 PIK3CA, HCP5,  
 SLC29A1, TP53,  
 CIP2A, SERPINA5,  
 ATRX, RAF1,  
 PSORS1C1, WEE1,  
 ESR2, DCTD, ALG10,  
 CASP7, C6orf15,  
 PPCDC, XRCC1,  
 FGFR3, CDC5L,  
 SLC29A2, TK2, TYMS,  
 NME1, ABCB1,  
 ABCC10

SGI-1776	PRISM	PIM Kinase Inhibitor	PIM1, PIM3, PIM2, FLT3, YES1, JAK2,	Preclinical	NA	1.0477	NA	-0.3269775	6.37E-14	0.3311275	1.45E-09
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dolastatin-10	PRISM	Microtubule inhibitor	HASPIN TUBB4A, TUBB, TUBA3C, TUBA1B, TUBA4A, TUBB4B, TUBB3, TUBB2A, TUBB8, TUBA3E, TUBA1A, TUBA1C, TUBB6, TUBB2B, TUBB1, TUB	Preclinical	PMID: 10321512	1.083865	NA	-0.3237382	1.16E-13	0.3295997	1.28E-09
echinomycin	PRISM	HIF1 Inhibitor	HIF1A, VEGFA	Preclinical	PMID: 33572152	1.049149	NA	-0.318722	2.87E-13	0.3816931	1.81E-08
MPI-047960	PRISM	MPS1 inhibitor	TTK	Preclinical	NA	1.372288	NA	-0.3003071	7.02E-12	0.3255934	5.25E-08

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