

**Table S1:** Potential targets information of KDZ injection

ID	Target Name	UniPort ID	Name	Related disease
T-01	Phenylalanine-4-hydroxylase	P00439	PAH	tyrosinemia; heart defects congenital; metabolic diseases; enzyme deficiency
T-02	Epidermal growth factor receptor	P00533	EGFR	restenosis; Prothrombin Thrombophilia; stroke, ischemic; acute myocardial infarction; elevated plasma prothrombin levels and an increase; cerebrovascular disease,
T-03	Prothrombin	P00734	F2	ischemic; metabolism disorders; Vascular Disease; thrombotic diseases; restenosis; atherosclerosis, coronary; coronary ischaemic syndrome; heart anomalies, congenita; coronary artery disease
T-04	Coagulation factor X	P00742	F10	
T-05	Complement factor D	P00746	CFD	
T-06	Plasminogen	P00747	PLG	pathologic neovascularization; coronary arteriosclerosis; ischemia; myocardial ischemia; thrombosis; cardiovascular diseases
T-07	Urokinase-type plasminogen activator	P00749	PLAU	atheroma; thrombosis; mitral valve prolapse
T-08	Carbonic anhydrase 2	P00918	CA2	Vascular Disease
T-09	L-lactate dehydrogenase B chain	P07195	LDHB	
T-10	Cathepsin B	P07858	CTSB	
T-11	Insulin-like growth factor 1 receptor	P08069	IGF1R	left ventricular hypertrophy; pathologic neovascularization; cardiac growth; cholesterol, HDL   triglycerides

				cholesterol, total; myocardial infarct; plasma lipid levels; triglycerides   atherosclerosis, coronary   lipoprotein; heart disease, ischemic; atherosclerosis, coronary   diabetes, type 2   lipoprotein; cholesterol   cholesterol, LDL   lipoproteins   fatty acid
T-12	Coagulation factor VII	P08709	F7	
T-13	Glutathione S-transferase P	P09211	GSTP1	
T-14	Androgen receptor	P10275	AR	
T-15	Pyruvate dehydrogenase E1 component subunit beta, mitochondrial	P11177	PDHB	
T-16	Alcohol dehydrogenase class-3	P11766	ADH5	
T-17	Proto-oncogene tyrosine-protein kinase Src	P12931	SRC	
T-18	Macrophage migration inhibitory factor	P14174	MIF	atheroma; restenosis; coronary disease; IL-12 production from monocyte
T-19	Ras-related C3 botulinum toxin substrate 2	P15153	RAC2	
T-20	Bone morphogenetic protein 7	P18075	BMP7	
T-21	Thymidine phosphorylase	P19971	TYMP	mitochondrial diseases; pathologic neovascularization
T-22	Liver carboxylesterase 1	P23141	CES1	
T-23	Chymase	P23946	CMA1	cardiovascular diseases; atheroma; heart failure; HDL Cholesterol; left ventricular hypertrophy
T-24	Cathepsin S	P25774	CTSS	

T-25	Amine oxidase [flavin-containing] B	P27338	MAOB	ischemia; cerebrovascular disorders; effects cardiovascular
T-26	Nitric oxide synthase, endothelial	P29474	NOS3	
T-27	Phosphoenolpyruvate carboxykinase, cytosolic [GTP]	P35558	PCK1	
T-28	Vascular endothelial growth factor receptor 2	P35968	KDR	
T-29	TGF-beta receptor type-1	P36897	TGFR1	
T-30	Caspase-3	P42574	CASP3	cerebral ischemia; ischemic brain injury
T-31	Mitogen-activated protein kinase 8	P45983	MAPK8	
T-32	Glycogen synthase kinase-3 beta	P49841	GSK3B	
T-33	Death-associated protein kinase 1	P53355	DAPK1	ischemia
T-34	Mitogen-activated protein kinase 10	P53779	MAPK10	thrombosis, deep veinlipid metabolism disorder; cardiomegaly; Thrombin activatable fibrinolysis inhibitor; angina; atherosclerosis, coronary; Hyperprothrombinemia; restenosis
T-35	Triosephosphate isomerase	P60174	TPI1	metabolic diseases
T-36	Troponin C, slow skeletal and cardiac muscles	P63316	TNNC1	
T-37	Peroxisome proliferator-activated receptor alpha	Q03181	PPAR	
T-38	Aldo-keto reductase family 1 member C1	Q04828	AKR1C1	
T-39	Hydroxyacyl-coenzyme A dehydrogenase, mitochondrial	Q16836	HADH	

---

**Table S2:** Comparison of molecular docking results in the top 10.

<b>Sybyl-X 1.3</b>			<b>Autodock Vina</b>	
Compound–Target	Total Score	C Score	Compound–Target	Vina Score (kcal/mol)
KDZ-6 – MIF	11.39	4	KDZ-6 – MAOB	-11.2
KDZ-6 – MAOB	10.68	4	KDZ-8 – CA2	-10.9
KDZ-6 – MAPK8	10.32	5	KDZ-3 – MAOB	-10.8
KDZ-7 – SRC	9.95	4	KDZ-8 – AKR1C1	-10.8
KDZ-6 – GSTP1	9.53	4	KDZ-4 – CA2	-10.7
KDZ-6 – PPARD	9.39	5	KDZ-6 – CA2	-10.7
KDZ-6 – RAC2	9.28	4	KDZ-10 – MAOB	-10.7
KDZ-6 – AKR1C1	9.17	4	KDZ-6 – AKR1C1	-10.6
KDZ-6 – LDHB	9.07	4	KDZ-9 – MAOB	-10.5
KDZ-7 – MIF	8.93	5	KDZ-10 – CA2	-10.5