

Supplemental Table-4. Literature mining of 32 candidate compounds

Classification	Compound	CID	Literatures
Flavones	naringenin	932	Li R , Feng Y , Chen J , et al. Naringenin suppresses K562 human leukemia cell proliferation and ameliorates Adriamycin-induced oxidative damage in polymorphonuclear leukocytes[J]. Experimental and Therapeutic Medicine, 2015, 9(3):697---706.
			Liu X , Ye F , Wu J , et al. Signaling Proteins and Pathways Affected by Flavonoids in Leukemia Cells[J]. Nutrition and Cancer, 2015, 67(2):238-249.
			Zhang S J , Sun D , Hao J B , et al. The effect of dietary soyabean isoflavones on photodynamic therapy in K562 leukemia cells[J]. Journal of Photochemistry & Photobiology B Biology, 2012, 110(none):28-33.
	Isoflavon	72304	Zhang D , Zhuang Y , Pan J , et al. Investigation of Effects and Mechanisms of Total Flavonoids of <i>Astragalus</i> , and Calycosin on Human Erythroleukemia Cells[J]. Oxidative Medicine and Cellular Longevity, 2012, 2012:1-5.
			Zhang D , Zhuang Y , Pan J , et al. Investigation of Effects and Mechanisms of Total Flavonoids of <i>Astragalus</i> , and Calycosin on Human Erythroleukemia Cells[J]. Oxidative Medicine and Cellular Longevity, 2012, 2012:1-5.
	4,7-Dihydroxy-5-methoxy-6-methyl-8-formyl-flavan	12939	Ninomiya M , Nishida K , Kaori Tanaka Structure–activity relationship studies of 5,7-dihydroxyflavones as naturally occurring inhibitors of cell proliferation in human leukemia HL-60 cells[J]. Journal of Natural Medicines, 2013, 67(3):460-467.
			Gatouillat, Grégory, Alabdul Magid A , Bertin E , et al. Cytotoxicity and Apoptosis Induced by Alfalfa (<i>Medicago sativa</i>) Leaf Extracts in Sensitive and Multidrug-Resistant Tumor Cells[J]. Nutrition and Cancer, 2014, 66(3):483-491.
	Chryseriol	52806	Marfe G , Tafani M , Indelicato M , et al. Kaempferol induces apoptosis in Two different cell lines Via Akt inactivation, Bax and SIRT3 activation, and mitochondrial dysfunction[J]. Journal of Cellular Biochemistry, 2009, 106(4):643-650.
			Okoye F B C , Sawadogo W R , Sendker J , et al. Flavonoid glycosides from <i>Olax mannii</i> : Structure elucidation and effect on the nuclear factor kappa B pathway[J]. Journal of Ethnopharmacology, 2015, 176(Complete):27-34.
	kaempferol	52808	Roma A , Rota S G , Spagnuolo P A . Diosmetin Induces Apoptosis of Acute Myeloid Leukemia Cells[J]. Molecular Pharmaceutics, 2018:acs.molpharmaceut.7b01151.
			Sghaier M B , Skandrani I , Nasr N , et al. Flavonoids and sesquiterpenes from <i>Tecurium ramosissimum</i> promote antiproliferation of human cancer cells and enhance antioxidant activity: A structure–activity relationship study[J]. Environ Toxicol Pharmacol, 2011, 32(3):0-348.
	Diosmetin	52816	Zahir A , Jossang A , Bodo B , et al. DNA topoisomerase I inhibitors:
	Genkwanin	52816	

			cytotoxic flavones from <i>Lethedon tannaensis</i> [J]. <i>Journal of Natural Products</i> , 1996, 59(7):701-3.
	Kaempferid	52816 66	not founded
	morin	52816 70	Park C , Lee W S , Go S I , et al. Morin, a Flavonoid from Moraceae, Induces Apoptosis by Induction of BAD Protein in Human Leukemic Cells[J]. <i>International Journal of Molecular Sciences</i> , 2014, 16(1):645. Ikegawa T , Ohtani H , Koyabu N , et al. Inhibition of P-glycoprotein by flavonoid derivatives in adriamycin-resistant human myelogenous leukemia (K562/ADM) cells[J]. <i>Cancer Letters</i> , 2002, 177(1):89-93.
	Syringetin	52819 53	Hibasami H , Mitani A , Katsuzaki H , et al. Isolation of five types of flavonol from seabuckthorn (<i>Hippophae rhamnoides</i>) and induction of apoptosis by some of the flavonols in human promyelotic leukemia HL-60 cells[J]. <i>International Journal of Molecular Medicine</i> , 2005, 15(5):805---809.
	6,8-Dihydroxy-7-methoxyxanthone	53167 98	not founded
	isorhamnetin	53186 45	Wu Xunxun,Chen Xiaofei,Dan Jia,Cao Yan,Gao Shouhong,Guo Zhiying,Zerbe Philipp,Chai Yifeng,Diao Yong,Zhang Lei. Characterization of anti-leukemia components from <i>Indigo naturalis</i> using comprehensive two-dimensional K562/cell membrane chromatography and in silico target identification.[J]. <i>Scientific reports</i> ,2016,6. Hibasami H , Mitani A , Katsuzaki H , et al. Isolation of five types of flavonol from seabuckthorn (<i>Hippophae rhamnoides</i>) and induction of apoptosis by some of the flavonols in human promyelotic leukemia HL-60 cells[J]. <i>International Journal of Molecular Medicine</i> , 2005, 15(5):805---809.
	suchilactone	13235 0840	not founded
stilbenes			
	Dihydroresveratrol	18591 4	not founded
	α -Viniferin	19640 2	not founded
	cis-resveratrol	15489 10	Thikrayat A A , Madihally S V . Influence of controlled release of resveratrol from electrospun fibers in combination with siRNA on leukemia cells[J]. <i>European Journal of Pharmaceutical Sciences</i> , 2018, 123:173-183. Wu X P , Xiong M , Xu C S , et al. Resveratrol induces apoptosis of human chronic myelogenous leukemia cells in vitro through p38 and JNK-regulated H2AX phosphorylation[J]. <i>Acta Pharmacologica Sinica</i> , 2015, 36(3):353-361.
	cis-pinosylvin	95488 40	not founded
	4'-methylpinosylvin	44566 996	not founded
Coumarins			
	Majudin	2355	not founded

	Ammidin	10212	not founded
	Cnidilin	82144 9	not founded
	notoptol	53202 28	not founded
	Bergaptin	54713 49	not founded
	8-geranoxy-5-methoxy psoralen	64421 82	not founded
Others			
Biphenyls	Dehydrodieugenol	16522 5	not founded
Lignin	(+)-medioresinol (40957-99-1)	18168 1	Park H J , Lee M S , Lee K T , et al. Studies on Constituents with Cytotoxic Activity from the Stem Bark of Syringa velutina.[J]. CHEMICAL & PHARMACEUTICAL BULLETIN, 1999, 47(7):1029-1031.
benzofuran	Moracin M	18584 8	not founded
Quinones	AIDS214634	21463 4	not founded
Hydroxyhemo globin	Oxysanguinarine	44371 6	not founded
Solanine	Torachrysone	53219 77	not founded