

## Supplemental Table-4. Literature mining of 32 candidate compounds

| Classification | Compound   | CID         | Literatures  |
|----------------|--|-------------|--|
| Flavones       |  |             |  |
|                | naringenin                                       | 932         | <p>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]. <i>Experimental and Therapeutic Medicine</i>, 2015, 9(3):697---706.</p> <p>Liu X , Ye F , Wu J , et al. Signaling Proteins and Pathways Affected by Flavonoids in Leukemia Cells[J]. <i>Nutrition and Cancer</i>, 2015, 67(2):238-249.</p> <p>Zhang S J , Sun D , Hao J B , et al. The effect of dietary soyabean isoflavones on photodynamic therapy in K562 leukemia cells[J]. <i>Journal of Photochemistry &amp; Photobiology B Biology</i>, 2012, 110(none):28-33.</p> |
|                | Isoflavon  | 72304       | <p>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]. <i>Oxidative Medicine and Cellular Longevity</i>, 2012, 2012:1-5.</p>  |
|                | 4,7-Dihydroxy-5-methoxy-6-methyl-8-formyl-flavan | 12939<br>4  | <p>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]. <i>Oxidative Medicine and Cellular Longevity</i>, 2012, 2012:1-5.</p>  |
|                | Chryseriol                                       | 52806<br>66 | <p>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]. <i>Journal of Natural Medicines</i>, 2013, 67(3):460-467.</p> <p>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]. <i>Nutrition and Cancer</i>, 2014, 66(3):483-491.</p>  |
|                | kaempferol                                       | 52808<br>63 | <p>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]. <i>Journal of Cellular Biochemistry</i>, 2009, 106(4):643-650.</p> <p>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]. <i>Journal of Ethnopharmacology</i>, 2015, 176(Complete):27-34.</p>  |
|                | Diosmetin  | 52816<br>12 | <p>Roma A , Rota S G , Spagnuolo P A . Diosmetin Induces Apoptosis of Acute Myeloid Leukemia Cells[J]. <i>Molecular Pharmaceutics</i>, 2018:acs.molpharmaceut.7b01151.</p>   |
|                | Genkwanin  | 52816<br>17 | <p>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]. <i>Environ Toxicol Pharmacol</i>, 2011, 32(3):0-348.</p> <p>Zahir A , Jossang A , Bodo B , et al. DNA topoisomerase I inhibitors:</p>   |

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|-----------|---------------------------------|---------------|--|
|           |                                 |               | cytotoxic flavones from <i>Lethedon tannaensis</i> [J]. <i>Journal of Natural Products</i> , 1996, 59(7):701-3.  |
|           | Kaempferid                      | 52816<br>66   | not founded  |
|           | morin                           | 52816<br>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.<br>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<br>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<br>98   | not founded  |
|           | isorhamnetin                    | 53186<br>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.<br>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<br>0840 | not founded  |
| stilbenes | Dihydroresveratrol              | 18591<br>4    | not founded  |
|           | $\alpha$ -Viniferin             | 19640<br>2    | not founded  |
|           | cis-resveratrol                 | 15489<br>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.<br>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<br>40   | not founded  |
|           | 4'-methylpinosylvin             | 44566<br>996  | not founded  |
| Coumarins | Majudin                         | 2355          | not founded  |

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

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