**Table 1.**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Peak** | **Name** | **Rt** | **% area** | **DW mg/g** | **Match factor** | **Relation to Apoptosis** | **References** |
| 1 | Pentanoic acid | 10.791 | 0.01 | 0.054207 | 89 | Its derivatives are used to induce apoptosis in cell lines. | {Mukherjee, 2017 #25} |
| 2 | 2,3-Butanediol | 12.863 | 0.05 | 0.286145 | 98 | NA |  |
| 3 | 1,3-Propanediol | 13.57 | 0.01 | 0.05732 | 88 | NA |  |
| 4 | Lactic Acid | 13.819 | 0.14 | 0.891773 | 93 | NA |  |
| 5 | Hexanoic acid | 14.002 | 0.04 | 0.276932 | 96 | Also known as caproic acid. Reported to induce apoptosis in human colorectal, skin, and breast cancer, moreover, it “could potentially be used to prevent and/or treat these cancers”. | {Narayanan, 2015 #26} |
| 6 | Succinimide | 15.525 | 0.01 | 0.060801 | 88 | NA |  |
| 7 | Benzyl alcohol | 16.447 | 0.11 | 0.667908 | 91 | 1% benzyl alcohol was reported to induce high apoptosis and necrosis in human dermal fibroblasts. | {Carvalho, 2012 #27} |
| 8 | 4-Hydroxybutanoic acid | 16.96 | 0.07 | 0.465751 | 86 | NA |  |
| 9 | Glycerol | 17.956 | 6.27 | 39.74729 | 99 | NA |  |
| 10 | 3-Hydroxybutanoic acid | 18.065 | 0.01 | 0.075168 | 92 | NA |  |
| 11 | Dihydroxyacetone | 18.768 | 0.03 | 0.184817 | 78 | Reported to induce G2/M arrest and apoptotic cell death in melanoma A375P cell line. | {Smith, 2018 #28} |
| 12 | Benzoic Acid | 19.244 | 0.19 | 1.22039 | 98 | Sodium benzoate was reported to activate NFκB and induce apoptosis in HCT116 cells. | {Yilmaz, 2018 #29} |
| 13 | Octanoic acid | 19.808 | 0.02 | 0.143862 | 83 | NA |  |
| 14 | phosphoric acid | 20.467 | 3.85 | 24.42644 | 86 | NA |  |
| 15 | 1,2,3-Butanetriol | 20.958 | 0.30 | 1.88296 | 98 | NA |  |
| 16 | Nonanoic acid | 22.371 | 0.11 | 0.679532 | 87 | Reported to induce apoptosis *in vivo* in epidermal Langerhans. | {Forsey, 1998 #30} |
| 17 | Erythrono-1,4-lactone, (E)- | 22.971 | 0.04 | 0.230517 | 89 | NA |  |
| 18 | Pyroglutamic acid | 25.973 | 0.69 | 4.36759 | 94 | NA |  |
| 19 | L-Threitol | 26.515 | 0.09 | 0.581057 | 93 | NA |  |
| 20 | meso-Erythritol | 26.698 | 0.33 | 2.11151 | 95 | NA |  |
| 21 | 3-Hydroxybenzoic acid | 27.584 | 0.11 | 0.674429 | 85 | NA |  |
| 22 | 4-Hydroxybenzoic acid | 29.078 | 0.36 | 2.265056 | 81 | Detected in *Schisandra chinensis* fruit extract, which is known to induce caspase-dependent apoptosis in human ovarian cancer A2780 cells. It was also detected in pinecones of *Pinus koraiensis* extract and exhibited cytotoxic activity, with IC50 value around 1 mg/mL in four human lung cancer cell lines, A549, H1264, H1299, and Calu-6. Similarly, Sitarek and colleagues reported antiproliferative and cell cycle arrest activity on glioma cells for the same compound in the root extract of *Leonurus sibiricus L.* It increased Bax, Bcl-2, p53, Casaspases in glioma and breast cancer cell lines. | {Jeong, 2017 #31;Lee, 2017 #32;Sitarek, 2017 #33;Wang, 2018 #34} |
| 23 | Arabinonic acid, gamma-lactone | 29.429 | 0.06 | 0.402076 | 89 | NA |  |
| 24 | Phloroglucinol | 29.59 | 0.09 | 0.590668 | 92 | Reported to induce apoptosis in distinct cancer cell lines. | {Jin, 2016 #56;Lee, 2018 #55;Park, 2019 #35} |
| 25 | Levoglucosan | 31.084 | 0.66 | 4.189809 | 95 | NA |  |
| 26 | D-(-)-Rhamnose | 31.545 | 0.31 | 1.948759 | 94 | Apoptosis inducer and anti-cancer agent, especially breast cancer. | {Chang, 1998 #36} |
| 28 | Vanillic Acid | 31.962 | 0.71 | 4.500047 | 77 | An anti-oxidant and has some anti-cancer benefits. | {Gong, 2019 #37} |
| 29 | 2-Methoxy-1,3-dioxolane | 32.687 | 2.80 | 17.73789 | 91 | NA |  |
| 30 | Methyl alpha-D-glucofuranoside | 32.951 | 0.52 | 3.281267 | 86 | Close derivates are used for tumor treatment. |  |
| 31 | Protocatechuic acid | 33.068 | 0.25 | 1.559802 | 84 | Known to induce apoptosis in the liver, ovarian human breast, lung, liver, cervix, and prostate cancer cells, as well as others, by modulating FAK, MAPK, c-June, and NF-κB pathways.  It was also reported to lead to cell cycle arrest. | {Kakkar, 2014 #57;Lin, 2015 #42;Tsao, 2014 #40;Xie, 2018 #39;Yip, 2006 #41} |
| 32 | Shikimic acid | 33.068 | 0.46 | 2.892089 | 87 | NA |  |
| 33 | Quininic acid | 33.998 | 13.41 | 85.04314 | 88 | NA |  |
| 34 | D-Fructose | 34.364 | 18.78 | 119.1289 | 91 | NA |  |
| 35 | p-Coumaric acid | 34.679 | 0.24 | 1.521807 | 89 | Reported to induced apoptosis and cell cycle arrest in several cell lines, including colon cancer. | {Kianmehr, 2019 #43;Pei, 2016 #58;Sharma, 2018 #44} |
| 36 | D-Glucose | 34.781 | 3.34 | 21.1588 | 96 | NA |  |
| 37 | D-Sorbitol | 34.972 | 6.79 | 43.05749 | 94 | NA |  |
| 38 | beta-D-Glucopyranose | 35.55 | 2.72 | 17.22668 | 98 | NA |  |
| 39 | 6H-Dibenzo(b,d)pyran-1-ol, 3-hexyl-7,8,9,10-tetrahydro-6,6,9-trimethyl- | 35.887 | 1.07 | 6.810763 | 79 | Also called Synhexyl |  |
| 40 | Palmitic Acid | 35.887 | 1.07 | 6.810763 | 98 | Reported to induce apoptosis in tens of cancer cell lines via MAPK and AMPK/Akt/mTOR, miR-129-3p/Smad3, and estrogen receptor alpha signaling pathways. | {Liang, 2019 #59;Sun, 2019 #45;Zou, 2019 #60} |
| 41 | Myo-Inositol | 36.795 | 18.69 | 118.5457 | 97 | Reported to being involved in apoptosis induction in the Arabidopsis plant. | {Meng, 2009 #47} |
| 42 | Caffeic acid | 37.066 | 0.50 | 3.155426 | 81 | Reported to induce apoptosis and cell cycle arrest in several cell lines including colon, breast, nasopharyngeal carcinoma, melanoma, lung, nasopharyngeal, cancer cells, and others. It altered the mTOR/PI3K/AKT signaling pathway and inactivated NF-κB pathway. | {Liang, 2019 #48;Motawi, 2016 #49;Zeng, 2018 #61} |
| 43 | L-Rhamnose | 37.74 | 0.26 | 1.662177 | 85 | NA |  |
| 44 | Stearic acid | 37.915 | 0.52 | 3.312062 | 91 | Reported to arrest the cell cycle and induce apoptosis in HepG2 and other cancer cell lines. | {Khan, 2013 #51;Liu, 2018 #50} |
| 45 | Glyceryl-glycoside | 38.97 | 0.72 | 4.565657 | 94 | NA |  |
| 46 | D-(+)-Trehalose | 43.451 | 1.31 | 8.317046 | 92 | Induced autophagy | {Rusmini, 2019 #62} |
| 47 | Catechine (2R-E)- | 44.747 | 0.55 | 3.465693 | 86 | NA |  |
| 48 | Catechine, (2R-cis)- | 45.142 | 0.08 | 0.496909 | 84 | NA |  |
| 49 | beta-Sitosterol | 53.782 | 0.19 | 1.17753 | 88 | Also named phytosterol. Reported to induce apoptosis and cell cycle arrest in HCT116, MCF-7, A549, and HeLa cell lines. Altered the PI3K/Akt signaling pathway and AMPK/PTEN/HSP90 | {Alvarez-Sala, 2019 #63;Cao, 2018 #52;Shin, 2018 #64} |
| 50 | stigmasterol | 53.782 | 0.18 | 1.15534 | 90 | Reported to lead to cell cycle arrest, mitochondrial-mediated apoptosis, and inhibition of JAK/STAT signaling pathway. It also inhibited cell migration in human gastric cancer cells. | {Li, 2018 #65} |
| 51 | Sucrose | 55.393 | 10.91285 | 69.21846 | 92 | NA |  |