**Supplementary Table 1. Basic information about SFJD active ingredients**

| Herbs | Mol ID | Molecule name | OB (%) | DL |
| --- | --- | --- | --- | --- |
| HZ | MOL013281 | 6,8-Dihydroxy-7-methoxyxanthone | 35.83 | 0.21 |
|  | MOL013287 | Physovenine | 106.21 | 0.19 |
|  | MOL013288 | Picralinal | 58.01 | 0.75 |
|  | MOL002259 | Physciondiglucoside | 41.65 | 0.63 |
|  | MOL002268 | rhein | 47.07 | 0.28 |
|  | MOL000358 | beta-sitosterol | 36.91 | 0.75 |
|  | MOL000492 | (+)-catechin | 54.83 | 0.24 |
|  | MOL000006 | luteolin | 36.16 | 0.25 |
|  | MOL000098 | quercetin | 46.43 | 0.28 |
| LQ | MOL000173 | wogonin | 30.68 | 0.23 |
|  | MOL003283 | (2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol | 66.51 | 0.39 |
|  | MOL003290 | (3R,4R)-3,4-bis[(3,4-dimethoxyphenyl)methyl]oxolan-2-one | 52.30 | 0.48 |
|  | MOL003295 | (+)-pinoresinol monomethyl ether | 53.08 | 0.57 |
|  | MOL003305 | PHILLYRIN | 36.40 | 0.86 |
|  | MOL003306 | ACon1\_001697 | 85.12 | 0.57 |
|  | MOL003308 | (+)-pinoresinol monomethyl ether-4-D-beta-glucoside\_qt | 61.20 | 0.57 |
|  | MOL003315 | 3beta-Acetyl-20,25-epoxydammarane-24alpha-ol | 33.07 | 0.79 |
|  | MOL000211 | Mairin | 55.38 | 0.78 |
|  | MOL003322 | FORSYTHINOL | 81.25 | 0.57 |
|  | MOL003330 | (-)-Phillygenin | 95.04 | 0.57 |
|  | MOL003347 | hyperforin | 44.03 | 0.60 |
|  | MOL003348 | adhyperforin | 44.03 | 0.61 |
|  | MOL003370 | Onjixanthone I | 79.16 | 0.30 |
|  | MOL000358 | beta-sitosterol | 36.91 | 0.75 |
|  | MOL000422 | kaempferol | 41.88 | 0.24 |
|  | MOL000522 | arctiin | 34.45 | 0.84 |
|  | MOL000006 | luteolin | 36.16 | 0.25 |
|  | MOL000791 | bicuculline | 69.67 | 0.88 |
|  | MOL000098 | quercetin | 46.43 | 0.28 |
| BLG | MOL001689 | acacetin | 34.97 | 0.24 |
|  | MOL002322 | isovitexin | 31.29 | 0.72 |
|  | MOL001721 | Isaindigodione | 60.12 | 0.41 |
|  | MOL001722 | 2-O-beta-D-glucopyranosyl-2H-1,4-benzoxazin-3(4H)-one | 43.62 | 0.31 |
|  | MOL001733 | EUPATORIN | 30.23 | 0.37 |
|  | MOL001734 | 3-[[(2R,3R,5R,6S)-3,5-dihydroxy-6-(1H-indol-3-yloxy)-4-oxooxan-2-yl]methoxy]-3-oxopropanoic acid | 85.87 | 0.47 |
|  | MOL001735 | Dinatin | 30.97 | 0.27 |
|  | MOL001736 | (-)-taxifolin | 60.51 | 0.27 |
|  | MOL001749 | ZINC03860434 | 43.59 | 0.35 |
|  | MOL001755 | 24-Ethylcholest-4-en-3-one | 36.08 | 0.76 |
|  | MOL001756 | quindoline | 33.17 | 0.22 |
|  | MOL001767 | hydroxyindirubin | 63.37 | 0.30 |
|  | MOL001771 | poriferast-5-en-3beta-ol | 36.91 | 0.75 |
|  | MOL001774 | Ineketone | 37.14 | 0.30 |
|  | MOL001779 | Sinoacutine | 49.11 | 0.46 |
|  | MOL001781 | Indigo | 38.20 | 0.26 |
|  | MOL001782 | (2Z)-2-(2-oxoindolin-3-ylidene)indolin-3-one | 48.40 | 0.26 |
|  | MOL001783 | 2-(9-((3-methyl-2-oxopent-3-en-1-yl)oxy)-2-oxo-1,2,8,9-tetrahydrofuro[2,3-h]quinolin-8-yl)propan-2-yl acetate | 64.00 | 0.57 |
|  | MOL001790 | Linarin | 39.84 | 0.71 |
|  | MOL001792 | DFV | 32.76 | 0.18 |
|  | MOL001793 | (E)-2-[(3-indole)cyanomethylene-]-3-indolinone | 54.59 | 0.32 |
|  | MOL001798 | neohesperidin\_qt | 71.17 | 0.27 |
|  | MOL001803 | Sinensetin | 50.56 | 0.45 |
|  | MOL001804 | Stigmasta-5,22-diene-3beta,7alpha-diol | 43.04 | 0.82 |
|  | MOL001806 | Stigmasta-5,22-diene-3beta,7beta-diol | 42.56 | 0.83 |
|  | MOL001810 | 6-(3-oxoindolin-2-ylidene)indolo[2,1-b]quinazolin-12-one | 45.28 | 0.89 |
|  | MOL001814 | (E)-3-(3,5-dimethoxy-4-hydroxy-benzylidene)-2-indolinone | 57.18 | 0.25 |
|  | MOL001820 | (E)-3-(3,5-dimethoxy-4-hydroxyb-enzylidene)-2-indolinone | 65.17 | 0.25 |
|  | MOL001828 | 3-[(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)methyl]-2,4-dihydro-1H-pyrrolo[2,1-b]quinazolin-9-one | 51.84 | 0.56 |
|  | MOL001833 | Glucobrassicin-1-Sulfonate\_qt | 42.52 | 0.24 |
|  | MOL000358 | beta-sitosterol | 36.91 | 0.75 |
|  | MOL000359 | sitosterol | 36.91 | 0.75 |
|  | MOL000449 | Stigmasterol | 43.83 | 0.76 |
|  | MOL000953 | CLR | 37.87 | 0.68 |
| CH | MOL001645 | Linoleyl acetate | 42.10 | 0.20 |
|  | MOL002776 | Baicalin | 40.12 | 0.75 |
|  | MOL000449 | Stigmasterol | 43.83 | 0.76 |
|  | MOL000354 | isorhamnetin | 49.60 | 0.31 |
|  | MOL000422 | kaempferol | 41.88 | 0.24 |
|  | MOL004598 | 3,5,6,7-tetramethoxy-2-(3,4,5-trimethoxyphenyl)chromone | 31.97 | 0.59 |
|  | MOL004609 | Areapillin | 48.96 | 0.41 |
|  | MOL013187 | Cubebin | 57.13 | 0.64 |
|  | MOL004624 | Longikaurin A | 47.72 | 0.53 |
|  | MOL004628 | Octalupine | 47.82 | 0.28 |
|  | MOL004644 | Sainfuran | 79.91 | 0.23 |
|  | MOL004648 | Troxerutin | 31.60 | 0.28 |
|  | MOL004653 | (+)-Anomalin | 46.06 | 0.66 |
|  | MOL004718 | α-spinasterol | 42.98 | 0.76 |
|  | MOL000490 | petunidin | 30.05 | 0.31 |
|  | MOL000098 | quercetin | 46.43 | 0.28 |
| BJC | MOL001676 | Vilmorrianine C | 33.96 | 0.22 |
|  | MOL001677 | asperglaucide | 58.02 | 0.52 |
|  | MOL001678 | bolusanthol B | 39.94 | 0.41 |
|  | MOL001790 | Linarin | 39.84 | 0.71 |
|  | MOL001689 | acacetin | 34.97 | 0.24 |
|  | MOL002322 | isovitexin | 31.29 | 0.72 |
|  | MOL001697 | Sinoacutine | 63.39 | 0.53 |
|  | MOL000358 | beta-sitosterol | 36.91 | 0.75 |
|  | MOL000359 | sitosterol | 36.91 | 0.75 |
|  | MOL000422 | kaempferol | 41.88 | 0.24 |
|  | MOL000449 | Stigmasterol | 43.83 | 0.76 |
|  | MOL000006 | luteolin | 36.16 | 0.25 |
|  | MOL000098 | quercetin | 46.43 | 0.28 |
| MBC | MOL001663 | (4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydropicene-4a-carboxylic acid | 32.03 | 0.76 |
|  | MOL002881 | Diosmetin | 31.14 | 0.27 |
|  | MOL002933 | 5,7,4'-Trihydroxy-8-methoxyflavone | 36.56 | 0.27 |
|  | MOL000358 | beta-sitosterol | 36.91 | 0.75 |
|  | MOL000422 | kaempferol | 41.88 | 0.24 |
|  | MOL000449 | Stigmasterol | 43.83 | 0.76 |
|  | MOL005229 | Artemetin | 49.55 | 0.48 |
|  | MOL005503 | Cornudentanone | 39.66 | 0.33 |
|  | MOL000006 | luteolin | 36.16 | 0.25 |
|  | MOL008752 | Dihydroverticillatine | 42.69 | 0.84 |
|  | MOL002773 | beta-carotene | 37.18 | 0.58 |
|  | MOL000098 | quercetin | 46.43 | 0.28 |
| LG | MOL000449 | Stigmasterol | 43.83 | 0.76 |
| GC | MOL005007 | Glyasperins M | 72.67 | 0.59 |
|  | MOL004806 | euchrenone | 30.29 | 0.57 |
|  | MOL004820 | kanzonols W | 50.48 | 0.52 |
|  | MOL004849 | 3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin | 59.62 | 0.43 |
|  | MOL004913 | 1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone | 48.14 | 0.43 |
|  | MOL004866 | 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone | 44.15 | 0.41 |
|  | MOL004863 | 3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone | 66.37 | 0.41 |
|  | MOL004989 | 6-prenylated eriodictyol | 39.22 | 0.41 |
|  | MOL004864 | 5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone | 30.49 | 0.41 |
|  | MOL004993 | 8-prenylated eriodictyol | 53.79 | 0.40 |
|  | MOL004838 | 8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol | 58.44 | 0.38 |
|  | MOL005020 | dehydroglyasperins C | 53.82 | 0.37 |
|  | MOL004815 | (E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one | 39.62 | 0.35 |
|  | MOL004961 | Quercetin der. | 46.45 | 0.33 |
|  | MOL004980 | Inflacoumarin A | 39.71 | 0.33 |
|  | MOL004945 | (2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one | 36.57 | 0.32 |
|  | MOL004898 | (E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one | 46.27 | 0.31 |
|  | MOL004957 | HMO | 38.37 | 0.21 |
|  | MOL003896 | 7-Methoxy-2-methyl isoflavone | 42.56 | 0.20 |
|  | MOL004941 | (2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one | 71.12 | 0.18 |
|  | MOL004924 | (-)-Medicocarpin | 40.99 | 0.95 |
|  | MOL004988 | Kanzonol F | 32.47 | 0.89 |
|  | MOL005018 | Xambioona | 54.85 | 0.87 |
|  | MOL004948 | Isoglycyrol | 44.70 | 0.84 |
|  | MOL004917 | glycyroside | 37.25 | 0.79 |
|  | MOL005001 | Gancaonin H | 50.10 | 0.78 |
|  | MOL000211 | Mairin | 55.38 | 0.78 |
|  | MOL000359 | sitosterol | 36.91 | 0.75 |
|  | MOL004903 | liquiritin | 65.69 | 0.74 |
|  | MOL004891 | shinpterocarpin | 80.30 | 0.73 |
|  | MOL004805 | (2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyrano[2,3-f]chromen-4-one | 31.79 | 0.72 |
|  | MOL002311 | Glycyrol | 90.78 | 0.67 |
|  | MOL004904 | licopyranocoumarin | 80.36 | 0.65 |
|  | MOL004959 | 1-Methoxyphaseollidin | 69.98 | 0.64 |
|  | MOL004824 | (2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one | 60.25 | 0.63 |
|  | MOL005008 | Glycyrrhiza flavonol A | 41.28 | 0.60 |
|  | MOL005003 | Licoagrocarpin | 58.81 | 0.58 |
|  | MOL005017 | Phaseol | 78.77 | 0.58 |
|  | MOL004966 | 3'-Hydroxy-4'-O-Methylglabridin | 43.71 | 0.57 |
|  | MOL004974 | 3'-Methoxyglabridin | 46.16 | 0.57 |
|  | MOL004827 | Semilicoisoflavone B | 48.78 | 0.55 |
|  | MOL004905 | 3,22-Dihydroxy-11-oxo-delta(12)-oleanene-27-alpha-methoxycarbonyl-29-oic acid | 34.32 | 0.55 |
|  | MOL004884 | Licoisoflavone B | 38.93 | 0.55 |
|  | MOL004885 | licoisoflavanone | 52.47 | 0.54 |
|  | MOL001484 | Inermine | 75.18 | 0.54 |
|  | MOL004810 | glyasperin F | 75.84 | 0.54 |
|  | MOL004912 | Glabrone | 52.51 | 0.50 |
|  | MOL005012 | Licoagroisoflavone | 57.28 | 0.49 |
|  | MOL004879 | Glycyrin | 52.61 | 0.47 |
|  | MOL004855 | Licoricone | 63.58 | 0.47 |
|  | MOL004908 | Glabridin | 53.25 | 0.47 |
|  | MOL004857 | Gancaonin B | 48.79 | 0.45 |
|  | MOL004833 | Phaseolinisoflavan | 32.01 | 0.45 |
|  | MOL004911 | Glabrene | 46.27 | 0.44 |
|  | MOL004808 | glyasperin B | 65.22 | 0.44 |
|  | MOL004814 | Isotrifoliol | 31.94 | 0.42 |
|  | MOL004949 | Isolicoflavonol | 45.17 | 0.42 |
|  | MOL004883 | Licoisoflavone | 41.61 | 0.42 |
|  | MOL004935 | Sigmoidin-B | 34.88 | 0.41 |
|  | MOL004856 | Gancaonin A | 51.08 | 0.40 |
|  | MOL004811 | Glyasperin C | 45.56 | 0.40 |
|  | MOL005000 | Gancaonin G | 60.44 | 0.39 |
|  | MOL004915 | Eurycarpin A | 43.28 | 0.37 |
|  | MOL003656 | Lupiwighteone | 51.64 | 0.37 |
|  | MOL004882 | Licocoumarone | 33.21 | 0.36 |
|  | MOL004907 | Glyzaglabrin | 61.07 | 0.35 |
|  | MOL004828 | Glepidotin A | 44.72 | 0.35 |
|  | MOL002565 | Medicarpin | 49.22 | 0.34 |
|  | MOL004848 | licochalcone G | 49.25 | 0.32 |
|  | MOL004910 | Glabranin | 52.90 | 0.31 |
|  | MOL000354 | isorhamnetin | 49.60 | 0.31 |
|  | MOL005016 | Odoratin | 49.95 | 0.30 |
|  | MOL000239 | Jaranol | 50.83 | 0.29 |
|  | MOL000497 | licochalcone a | 40.79 | 0.29 |
|  | MOL000098 | quercetin | 46.43 | 0.28 |
|  | MOL004860 | licorice glycoside E | 32.89 | 0.27 |
|  | MOL004990 | 7,2',4'-trihydroxy－5-methoxy-3－arylcoumarin | 83.71 | 0.27 |
|  | MOL004991 | 7-Acetoxy-2-methylisoflavone | 38.92 | 0.26 |
|  | MOL000417 | Calycosin | 47.75 | 0.24 |
|  | MOL000422 | kaempferol | 41.88 | 0.24 |
|  | MOL000392 | formononetin | 69.67 | 0.21 |
|  | MOL004328 | naringenin | 59.29 | 0.21 |
|  | MOL000500 | Vestitol | 74.66 | 0.21 |
|  | MOL004985 | icos-5-enoic acid | 30.70 | 0.20 |
|  | MOL004996 | gadelaidic acid | 30.70 | 0.20 |
|  | MOL004841 | Licochalcone B | 76.76 | 0.19 |
|  | MOL004835 | Glypallichalcone | 61.60 | 0.19 |
|  | MOL001792 | DFV | 32.76 | 0.18 |

BJC, Bai Jiang Cao; BLG, Ban Lan Gen; CH, Chai Hu; DL, drug-like index; GC, Gan Cao; HZ, Hu Zhang; LQ, Lian Qiao; LG, Lu Gen; MBC, Ma Bian Cao; OB, oral bioavailability; SFJD, Shufeng Jiedu Capsules.