**Supplementary Table 1. Active components of the Quzhi formula**

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| **No.** | **Mol ID** | **Molecule** | **OB (%)** | **DL** | **Herb** |
| PC1 | MOL013287 | Physovenine | 106.21 | 0.19 | *Polygonumcuspidatum* |
| PC2 | MOL013281 | 6,8-Dihydroxy-7-methoxyxanthone | 35.83 | 0.21 | *Polygonumcuspidatum* |
| PC3 | MOL000492 | (+)-Catechin | 54.83 | 0.24 | *Polygonumcuspidatum* |
| PC4 | MOL000006 | Luteolin | 36.16 | 0.25 | *Polygonumcuspidatum* |
| PC5 | MOL000098 | Quercetin | 46.43 | 0.28 | *Polygonumcuspidatum* |
| PC6 | MOL002259 | Physciondiglucoside | 41.65 | 0.63 | *Polygonumcuspidatum* |
| PC7 | MOL002280 | Torachrysone-8-O-beta-D-(6'-oxayl)-Glucoside | 43.02 | 0.74 | *Polygonumcuspidatum* |
| PC8 | MOL000358 | Beta-sitosterol | 36.91 | 0.75 | *Polygonumcuspidatum* |
| PC9 | MOL013288 | Picralinal | 58.01 | 0.75 | *Polygonumcuspidatum* |
| PC10 | MOL013289 | Polydatin | 21.44 | 0.50 | *Polygonumcuspidatum* |
| PC11 | MOL012744 | Resveratrol | 19.07 | 0.11 | *Polygonumcuspidatum* |
| C | MOL002268 | Rhein | 47.07 | 0.28 | *Cassiaesemen Polygonumcuspidatum* |
| CS1 | MOL006472 | Aurantio-obtusin | 31.55 | 0.37 | *Cassiae semen* |
| CS2 | MOL005043 | Campest-5-en-3beta-ol | 37.58 | 0.71 | *Cassiae semen* |
| CS3 | MOL000953 | CLR | 37.87 | 0.68 | *Cassiae semen* |
| CS4 | MOL006465 | Rubrofusarin-6-beta-gentiobioside | 40.12 | 0.67 | *Cassiae semen* |
| CS5 | MOL006481 | Gluco-obtusifolin | 42.41 | 0.81 | *Cassiae semen* |
| CS6 | MOL000449 | Stigmasterol | 43.83 | 0.76 | *Cassiae semen* |
| CS7 | MOL006466 | Rubrofusarin | 45.55 | 0.24 | *Cassiae semen* |
| CS8 | MOL002281 | Toralactone | 46.46 | 0.24 | *Cassiae semen* |
| CS9 | MOL006489 | Quinizarin | 47.34 | 0.19 | *Cassiae semen* |
| CS10 | MOL006482 | 9,10-dihydroxy-7-methoxy-3-methylene-4H-benzo[g]isochromen-1-one | 63.25 | 0.24 | *Cassiae semen* |
| CS11 | MOL006475 | Obtusin | 81.43 | 0.40 | *Cassiae semen* |
| CS12 | MOL000471 | Aloe-emodin | 83.38 | 0.24 | *Cassiae semen* |
| CS13 | MOL006473 | Cassiaside A | 17.78 | 0.74 | *Cassiae semen* |
| CP1 | MOL005384 | Suchilactone | 57.52 | 0.56 | *Crataegus pinnatifida* |
| CP2 | MOL001645 | Linoleyl acetate | 42.10 | 0.20 | *Crataegus pinnatifida* |
| CP3 | MOL008498 | Ursolic acid | 17.70 | 0.75 | *Crataegus pinnatifida* |