

Supplementary Material

Identification of Absorbed Constituents and their Metabolites Related to Estrogen-Like Activity of Total Glycosides of *Cistanche deserticola* in Rat Serum

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Supplementary Table S1. List of main materials and instruments used in this study.

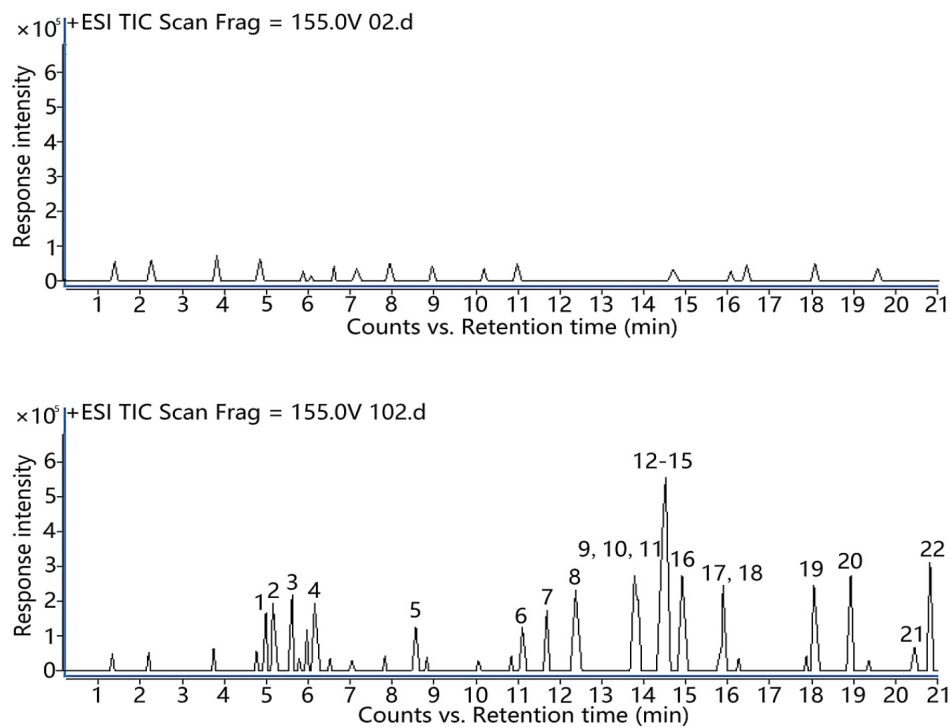
| Materials and instruments | Manufacturers or Sources |
|--|---|
| Diethylstilbestrol (purity: $\geq 98\%$) | Hanpu Pharmaceutical Co., Ltd., Guangzhou, China |
| Mass spectrometry (MS)-grade formic acid, acetonitrile, methanol | Fisher Scientific, Fair Lawn, NJ, USA |
| Phenol red-free RPMI 1640 | HyClone, Logan, UT, USA |
| MTT, DMSO | Sigma-Aldrich, St. Louis, MO, USA |
| Agilent 1290 HPLC system, Agilent 6530 series quadrupole time-of-flight LC/MS system | Agilent Technologies, Inc., Santa Clara, CA, USA |
| ACQUITY UPLC BEH C ₁₈ column (100 mm \times 2.1 mm, 1.7 μ m) | Waters Corp., Jakarta Selatan, Indonesia |
| Genius N118LA nitrogen generator | Peak Scientific, Glasgow, UK |
| Microplate reader | Bio-Rad, Inc., Hercules, CA, USA |
| The electronic analytical balance AR1140 | Ohaus Corporation, Parsippany, NJ, USA |
| XW-80A vortex mixer | Yugong Machinery Technology Co., Ltd., Shanghai, China |
| Raw material of dry <i>Cistanche deserticola</i> | purchased from Sankeshu Medicinal materials market, Harbin, China |
| Wistar rats (weighing 210 \pm 20 g) | from Harbin Medical University, Harbin, China |
| MCF-7 cell line | from Research Center of Pharmaceutical Engineering and Technology, Harbin University of Commerce, Harbin, China |

* Corresponding author: lwdzd@163.com
0030-9923/2023/0003-1301 \$ 9.00/0

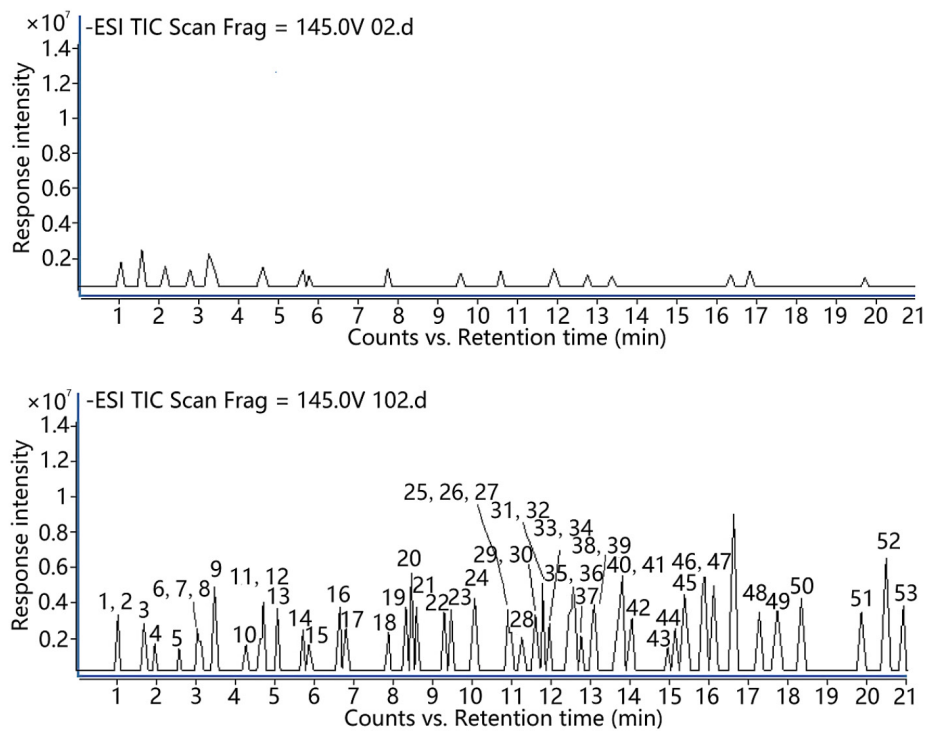


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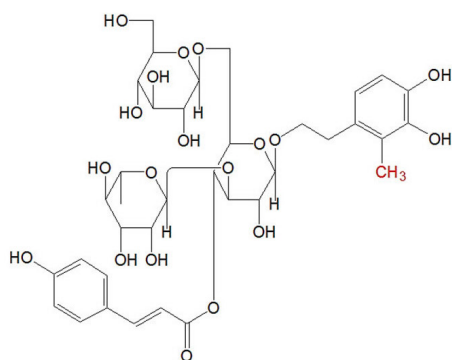
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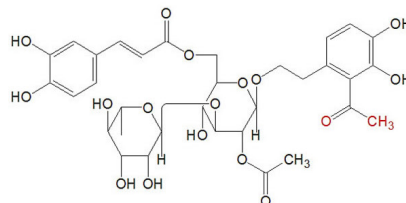
Supplementary Fig. S1. Total ion chromatogram in the positive ion mode. A: blank serum; B: TGs-containing serum.



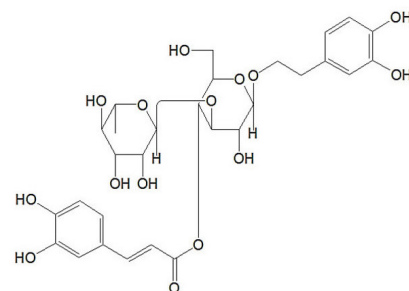
Supplementary Fig. S2. Total ion chromatogram in the negative ion mode. A: blank serum; B: TGs-containing serum.



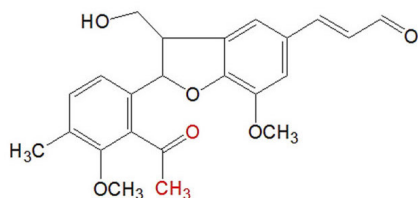
methylated cistantubuloside B



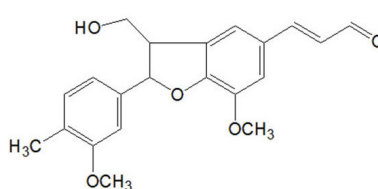
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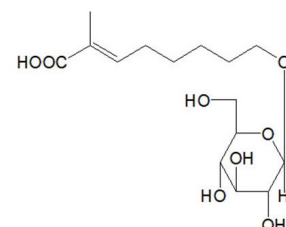
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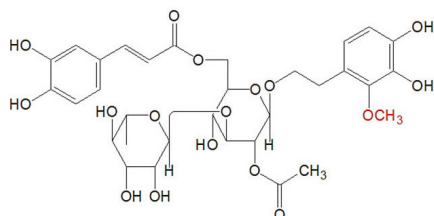
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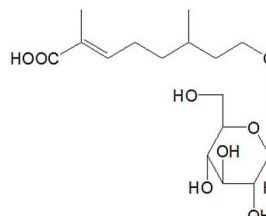
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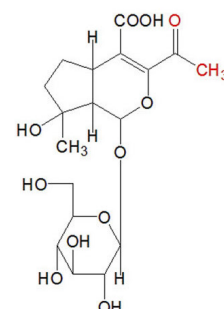
demethylated kankanoside E



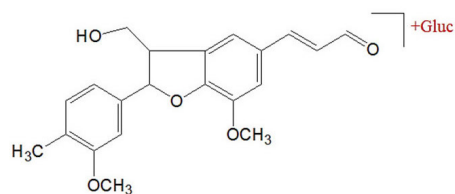
methoxylated tubuloside B



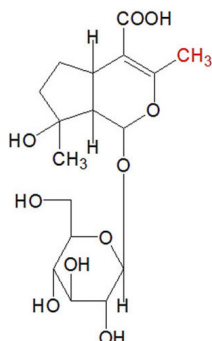
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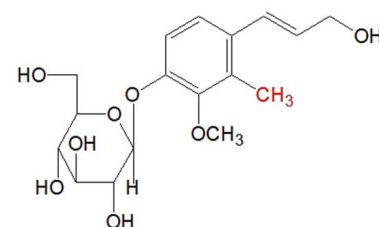
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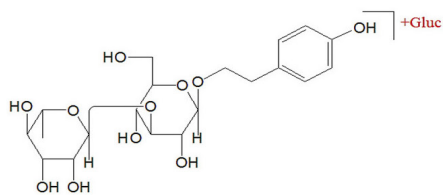
dehydrodiconiferyl alcohol-4-O- β -D-glucoside glucuronidated conjugate



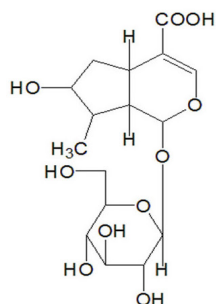
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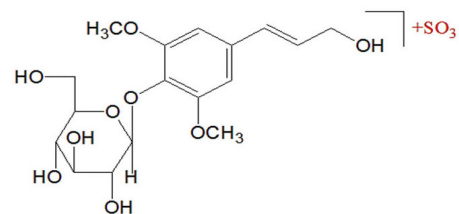
methoxylated coniferin



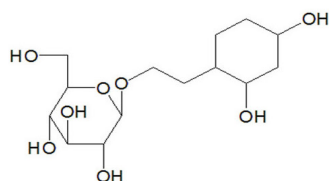
cistanoside G glucuronidated conjugate



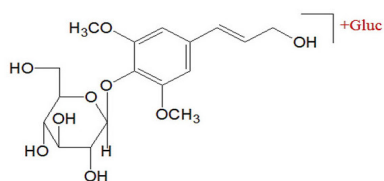
8-epiloganic acid



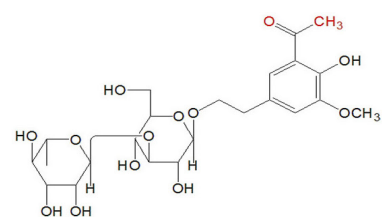
syringin sulfated conjugate



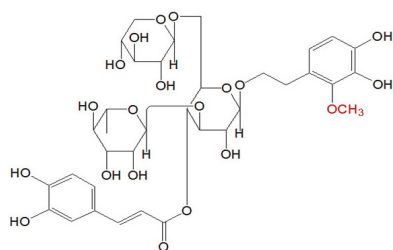
3,4-dihydroxyphenylethanoid glycoside



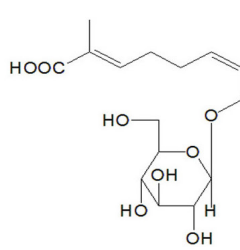
syringin glucuronidated conjugate



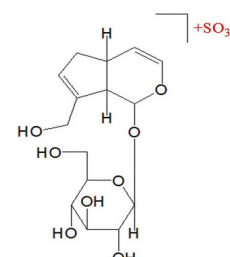
acetylated cistanoside E



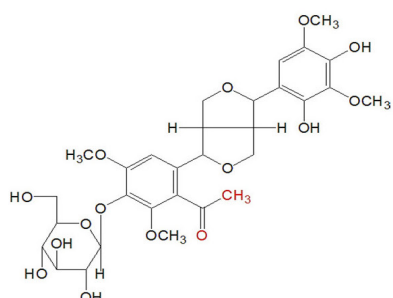
methoxylated arenarioside



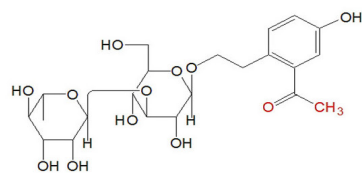
demethylated (2E,6Z)-8-O- β -D-glucopyranosyloxy-2,6-dimethyl-2,6-octadienoic acid



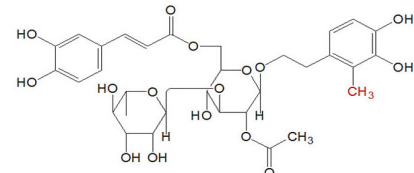
bartsioside sulfated conjugate



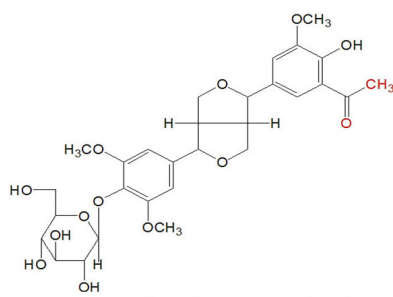
acetylated syringaresinol-O- β -D-glucopyranoside



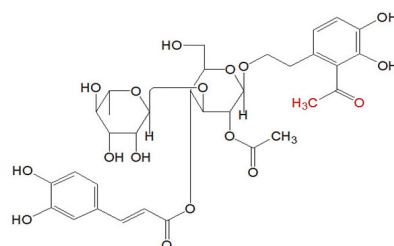
acetylated cistanoside G



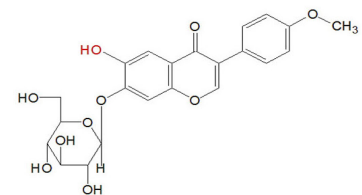
methylated tubuloside B



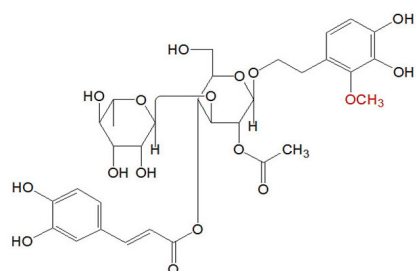
acetylated eucommin A



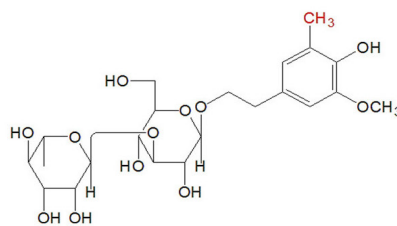
acetylated 2-acetylacteoside



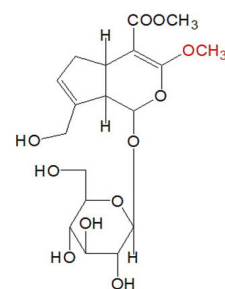
hydroxylated ononin



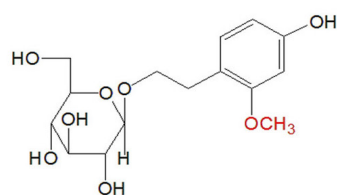
methoxylated 2-acetylacteoside



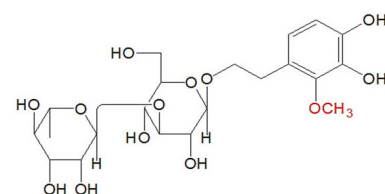
methylated cistanoside E



methoxylated geniposide



methoxylated salidroside



methoxylated decaffeoyl acteoside

Supplementary Fig. S3. *In vivo* active compounds leading to the estrogen-like activity of TGs.