Chemical composition of cold-pressed milk thistle seed flour extract, and its potential health beneficial properties

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Supplemental materials:

Figure Captions

Supplementary Fig. S1 Typical UHPLC chromatogram and UHPLC-Obitrap-MS chromatogram of milk thistle seed extract.

Supplementary Fig. S2 Identification of compound 5, Methyl 5-(6-caffeoyl-glucopyranosyl)-caffeoylquinic acid. (A) MS spectrum; (B) MS² spectrum in negative mode. The high resolution ESI-MS of Methyl 5-(6-caffeoyl-glucopyranosyl)-caffeoylquinic acid showed the 691.1884 of [M-H]⁻ corresponding to the formula of C_{32}H_{36}O_{17} (0 ppm). The detailed analysis of the fragmental ions of Methyl 5-(6-caffeoyl-glucopyranosyl)-caffeoylquinic acid showed peaks of 529.1528 [M-H-caffeoyl]⁻ (C_{23}H_{29}O_{14}) and 367.1031 [M-H-caffeoyl-glucosyl]⁻ (C_{17}H_{19}O_{9}) in negative mode.

Supplementary Fig. S3 Anti-proliferative capacity of milk thistle seed flour extract in LNCaP prostate cancer cells. A final concentration of 0.4 mg flour equivalents/mL milk thistle seed flour extract was treated in LNCaP prostate cancer cells. Relative LNCaP prostate cancer cell numbers were measured every 24 h. Each column represents the mean ± SD (n = 3). Columns marked with different letters indicate significant difference (P ≤ 0.05).
Supplementary Fig. S1 Typical UHPLC chromatogram and UHPLC-Obitrap-MS chromatogram of milk thistle seed extract.
**Supplementary Fig. S2** Identification of compound 5, Methyl 5-(6-caffeoyl-glucopyranosyl)-caffeoylquinic acid. (A) MS spectrum; (B) MS² spectrum in negative mode.
**Supplementary Fig. S3** Anti-proliferative capacity of milk thistle seed flour extract in LNCaP prostate cancer cells.