

Supplementary Table S1. Different categories and types of compounds found in milk thistle seeds or different herbal formulations, their confirmed activities by different references.

| Category | Compounds | Activity/[references] |
|---------------------------------------|--|---|
| Flavonolignans (Silymarin complex) | Silyhermin | Liver protection and regeneration, antioxidant, anti-inflammatory, antitumor/[8,9,16,18, 83, 106, 47] |
| | Dehydrosilybin | |
| | Silybin A / B (Silybinin) | |
| | Silychristin | |
| | Silydianin | |
| Phenolic acids | Gallic acid | Antioxidant/[18,23,65] |
| | Coumaric acid | |
| | Ferulic acid | |
| Terpenoids | Coniferyl alcohol | Antibacterial, antifungal, suppression of NO release/[65] |
| | Carnosic acid | |
| | Secoisolariciresinol | |
| Flavonoids | Apigenin | Antioxidant (radical scavenging) /[8 ,9, 18, 23, 65,] |
| | Naringenin | |
| | Luteolin | |
| | Kaempferol | |
| | Quercetin | |
| | Taxifolin | |
| | (Epi)catechin gallate & Epigallocatechin, Epigallocatechin gallate, Catechin 5-glucoside | |
| | Myricetin | |
| | Campesterol andbeta-Sitosterol | |
| | Apigenin 7-glucuronide | |
| | Luteolin 5-glucoside | |
| | Rutin | |
| Fatty acids and lipids | Myristic acid C12:0 | Components of cell membranes structure and energetic metabolism in mitochondria/[47] |
| | Palmitoleic acid C16:1 | |
| | Palmitic acid C16:0 | |
| | Linolenic acid C18:3 | |
| | Linoleic acid C18:2 | |
| | Oleic acid C18:1 | |
| | Stearic acid C18:0 | |
| | Eicosaenoic acids 20:1, 20:2, C20:3 | |
| | Arachidic acid C20:0 | |
| | Mycolipanolic acid (C24:0) | |
| | Myristyl linolenate | |
| | Palmitoylcholines | |
| | Monoglycerides | |
| | Sphingosine 1-phosphate | |
| | Lysophosphatydylchlines 18:2, 20:3 | |
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