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The new conformational ergosterol specifically inhibited cancer through regulating the estradiol-17β dehydrogenase in A549 and the first reducing the 3β-hydroxysteroid dehydrogenase in HepG2

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Cancer is one of the main diseases threatening human health. Although Traditional Chinese Medicine (TCM) shows prominent applications for difficult and miscellaneous diseases, it still lacks in-depth research on its anticancer mechanism. Therefore, this research aims to find key ingredient and clarify the mechanism of its key target and pathway. Based on the in vitro cells experiments of A549 and HepG2, 31 active compounds were extracted from TCM through the solvent and chromatographic system. The key compound-target-pathway network (contained 28 compounds, 52 targets and 25 pathways) was analyzed. We combined with the mice experiments of Lewis and H22 in vivo and transcriptome SMRT sequencing to screen out some key enzymes. TCM exerts anticancer effects through multi-interactions of components, targets, and pathways. Furthermore, combined with the mice experiments of Lewis and H22 in vivo, we found that 5 compounds had the effect of inhibiting the growth of Lewis cancer, and 3 can inhibit the growth of H22 cancer, precisely, the new conformational ergosterol, (3R,9R,10S,13S,14S,17S)-17-((2S,5R,E)-5,6-dimethylhept-3-en-2-yl)-10,13-dimethyl-2,3,4,9,10,11,12,13,14,15,16,17-dodecahydro-1- H-cyclopenta[α]phenanthren-3-ol), from Cordyceps militaris (HN strain) fruiting body specifically inhibited the growth of cancer cells through regulating the oxidation of estradiol to estrone in A549 and reducing the 3β-hydroxysteroid dehydrogenase in HepG2. Transcriptome SMRT sequencing results confirmed that the estradiol-17β dehydrogenase was mutated in A549 cells (ref. XP_011523034.1), respectively, the identity was 79%, gaps were 49/228(21%). and that the 3β-hydroxysteroid dehydrogenase was mutated in HepG2 cells (ref|NP_079469.2), the identity was 86%, gaps were 52/369(14%). The ergosterol from Cordyceps militaris (HN strain) fruiting body specifically inhibited cancer through regulating the estradiol-17β dehydrogenase in A549 and reducing the 3β-hydroxysteroid dehydrogenase in HepG2. That may provide an important target to treat lung cancer and a new target to treat liver cancer.

Key words: New conformational ergosterol, Cordyceps militaris, lung cancer, liver cancer, Traditional Chinese Medicine, SMRT sequencing, Estradiol-17β dehydrogenase, 3β-hydroxysteroid dehydrogenase

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