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Preparation and investigation of ecdysteroid – cinnamic acid hybrid compounds

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During the COVID lock-down, the chemical structures of more than 170 semi-synthetic ecdysteroid derivatives were collected from 21 articles since 2012, when the latest semi-synthetic reviews were published. These ecdysteroids, along with the semi-synthetic ecdysteroid library of our group, were processed into SMILES strings and organized according to their available bioactivities. Altogether, more than 300 ecdysteroids and, where available, their biological data were collected into a database in a way that is appropriate for an in-depth *in silico* evaluation. Further investigations on this database are planned with the ChemGPS-NP [1] software in collaboration.

During the literature survey, some reports on ecdysteroid cinnamic derivatives have been found. These esters were isolated from the fronds of *Microsorium membranifolium* [2]. This inspired us to prepare related new hybrid compounds through semi-synthesis.

20-Hydroxyecdysone (20E) and cinnamic acid were reacted with EDCI.HCl and DMAP in mol. sieve DCM for 4.5 day in room temperature [3]. The crude products were purified via flash chromatography and HPLC. Four ecdysteroid derivatives including two new compounds were obtained, and their structures were confirmed via NMR as the 2-, 2,3-, 2,22, and the 3,22-cinnamates of 20E. The compounds exhibited moderate antioxidant activities on DPPH and ORAC assays. Synthesis of the caffeate and ferulate derivatives of 20E are currently ongoing.

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References:

- [1] Larsson J, et al. *Journal of Natural Products* 2007; 70(5):789–794.
- [2] Ho R, et al. *Molecules* 2012; 17(10):11598–11606.
- [3] Xu S, et al. *Fitoterapia* 2014; 99:300–306.