5th Symposium of Young Researchers on Pharmacognosy

Szeged, 23 July 2024

BOOK OF ABSTRACTS

University of Szeged
Institute of Pharmacognosy

5th Symposium of Young Researchers on Pharmacognosy

BOOK OF ABSTRACTS

(ed. Tivadar Kiss, Judit Hohmann)

Institute of Pharmacognosy, University of Szeged, Szeged, Hungary

23 July 2024

doi: 10.14232/syrpharmacognosy.2024.af

A7

doi: 10.14232/syrpharmacognosy.2024.a7

Preparation and investigation of B-ring modified nitrogen-containing calonysterone derivatives

Glória Papdi, Gábor Girst, Attila Hunyadi, Máté Vágvölgyi

Institute of Pharmacognosy, Faculty of Pharmacy, University of Szeged, 6720, Eötvös utca 6., Szeged, Hungary

Email: papdigloria200128@gmail.com

The non-toxic, bioactive 20-hydroxyecdysone (20E) is the most abundant ecdysteroid derivative in nature, whose base-catalysed autooxidation yields calonysterone, another natural ecdysteroid, possessing a dienone type B-ring [1]. Previously, we identified calonysterone as a potent cytoprotective agent, however, until now, the low reactivity of its B-ring stood as an obstacle to carry out transformations on the pharmacophore site of the molecule [2].
Therefore, in our current work, we set out to perform the oximation of the C-7 carbonyl group on the B-ring of calonysterone. Interestingly, our transformation resulted in a new, C-6 oxime derivative with an intact C-7 carbonyl moiety using hydroxylamine hydrochloride reagent in ethanol. The obtained oxime product was purified by preparative HPLC on a C-18 reversed-phase column. To enhance the chemical diversity towards additional bioactive products, we modified our reaction conditions by replacing ethanol with methanol. As a result, we observed increased by-product formation, and 3 additional compounds were isolated from the reaction by chromatography. Furthermore, we performed experiments to accomplish the Beckmann rearrangement of our new oxime derivative in hand, with the aim to convert the starting material's B-ring into a 7-membered lactam ring. The chromatographic purification and structural elucidation of the products available are currently in progress. All our isolated products are planned to be tested for their cytoprotective properties *in vitro*.

Acknowledgements:
The research was supported by the NKFIH, Hungary (K-134704), and the Ministry of Innovation and Technology of Hungary (TKP2021-EGA-32). M.V. was supported by the New National Excellence Program of the Ministry for Culture and Innovation (ÚNKP-23-4-222).

References

[1] Csábi J et al. *J Nat Prod*, **2015**, 78(10):2339-2345.
[2] Vágvölgyi M et al.*PloS One*, **2024**, 19(2):e0290526