sciendo

DOI: 10.2478/auoc-2024-0016

Ovidius University Annals of Chemistry Volume 35, Number 2, pp. 118 - 125, 2024

In silico prediction of physicochemical properties and drug-likeness of omega-3 fatty acids

Yordanka STANEVA,[1] Ivelin ILIEV[*],[1] Svetlana GEORGIEVA,[1] and Albena MERDJANOVA[2]

[1] *Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Medical University of Varna, Varna, Bulgaria, 84 Tsar Osvoboditel Blvd.*
[2] *Department of Chemistry, Faculty of Pharmacy, Medical University of Varna, Varna, Bulgaria, 84 Tsar Osvoboditel Blvd.*

Abstract. Omega-3 fatty acids, including alpha-linolenic acid (ALA), eicosapentaenoic acid (EPA), and docosahexaenoic acid (DHA), are recognized for their crucial roles in human health, particularly cardiovascular and cognitive function. In this study, we employed computational methodologies, leveraging the SwissADME platform and ADMETLab 3.0, to predict and cross-validate the physicochemical properties and drug-likeness of these essential fatty acids. SwissADME predictions indicated molecular weights of 278.43 g/mol for ALA, 302.45 g/mol for EPA, and 328.49 g/mol for DHA, with consensus Log $P_{o/w}$ values of 5.09, 5.50, and 5.72 respectively, and varying degrees of water solubility. However, predictions from ADMETLab 3.0 were almost similar: ALA with a molecular weight of 278.22 g/mol, EPA at 302.22 g/mol, and DHA at 328.24 g/mol. Significant discrepancies were observed in lipophilicity, with ADMETLab 3.0 predicting Log $P_{o/w}$ values of 6.461 for ALA, 6.477 for EPA, and 7.006 for DHA, higher than those from SwissADME. Additionally, water solubility predictions from ADMETLab 3.0 showed ALA with a Log S of -5.034, EPA at -4.4, and DHA at -4.638, which differed from SwissADME's estimates. These differences reflect variations in computational approaches and algorithms. Comparison with literature data revealed general alignment in physicochemical properties, such as water solubility and lipophilicity. Furthermore, assessment of drug-likeness according to Lipinski's rule demonstrated compliance for all three fatty acids, albeit with variations in other criteria such as Ghose, Veber, Egan, and Muegge rules. These findings underscore the reliability and applicability of computational approaches in elucidating the physicochemical properties and drug-likeness of omega-3 fatty acids, offering valuable insights for pharmaceutical research and therapeutic applications.

***Keywords*:** alpha-linolenic acid; eicosapentaenoic acid; docosahexaenoic acid; SwissADME.

[*] Corresponding author. *E-mail address:* ivelin.iliev@mu-varna.bg (Ivelin Iliev)