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Abstract

In Silico 3D/4D QSAR Prediction of 5-O-Caffeoylquinic Acid, Cyanidin-3-O-Galactoside Chloride and L-Epicatechin Anti-Inflammatory Activity, Cytotoxicity and Metabolism †

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Abstract: Background and objectives: Sambucus ebulus (SE) fruits are applied in folk medicine for the treatment of inflammatory gastrointestinal disorders and for immune stimulation in the autumn–winter period. LS-MS analysis has revealed that 5-O-Caffeoylquinic acid (Compound **1**, C**1**), Cyanidin-3-O-Galactoside chloride (Compound **2**, C**2**) and L-Epicatechin (Compound **3**, C**3**) are among the most abundant polyphenolic compounds in SE fruit extracts. The aim of the present study was to perform in silico 3D/4D QSAR prediction of their anti-inflammatory properties, metabolism, and cytotoxicity. Methods: Prediction was performed using molecular exterior- and molecular interior-based 3D/4D QSAR analysis with CiS/MC and AlteQ platforms. Calculated probability ranged from 0 (no probability) to 1 (high probability). Results: Anti-inflammatory testing predicted a very high probability to reduce carrageenan-induced paw edema in rats (0.96, 50–60% inhibition of inflammation) for C**3**; intermediate COX2 inhibition for C**2** (0.770, 11–19% inhibition), C**1**, (0.682, 7–10% inhibition) and C**3** (0.500, 2–7% inhibition); low inhibition of COX1 for C**2** (0.370), C**3** (0.355), and C**1** (0.206); low inhibition of LOX-5 for C**2** (0.376) and low anti-peritoneal activity for C**2** (0.345), C**1** (0.339), and C**3** (0.307). Cytotoxicity testing predicted low activity for C**2** (0.122) and C**3** (0.271), and C**1** (0.305). Metabolism modelling revealed high probability of the biotransformation of C**1** (0.904, 4 metabolites) and C**3** (0.817, 3 metabolites) and low probability of the biotransformation of C**2** (0.347) by CYP3A4. It also revealed high probability of biotransformation of C**2** (0.869, 4 metabolites) and low probability of C**3** (0.500) by CYP2D6. Discussion: 3D/4D QSAR in silico modelling appears to be a fast method for screening the possible biological properties of polyphenolic compounds. The method could be of interest in screening for new biologically active compounds for application in different industries, including in nutrition, pharmaceuticals, cosmetics, etc.

Keywords: Sambucus ebulus; polyphenols; in silico; QSAR

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