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Potential of bile acids and their derivatives as drug delivery systems

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Introduction: In this work were compared several calculation methods to evaluate the lipophilicity of thirteen different bile acids in two solvent systems conditions. Lipophilicity is very important physicochemical parameter for describing ADME properties and future perspectives of molecule application. In the recent literature information about ADME properties of examined bile acids do not exist, although the interest for bile acids and their implementation as drug delivery systems is increasing.

Materials & Methods: Retention parameters are acquired by normal-phase TLC. The correlations between calculated logP values were obtained using five different softwares and experimentally determined hydrophobicity parameters (R_m^0 , $b_{(tol/but)}$, $b_{(tol/eth)}$ and $b_{(tol/but)}$) were established with good correlation.

Results: Excellent predictive ability of the established mathematical model of studied compounds represents significant tool in development of relations between chromatographic behavior and ADME properties. Examined correlation analysis confirmed significant dependence between R_m^0 and penetration in jejunum, MDCK epithelial cells, skin permeability, ion channel modulations (ICM) and binding affinity to nuclear receptor (NRL) and G protein-coupled receptors (GPCR).

Conclusion: Investigated bile acids showed good pharmacokinetic properties and affinity for GPCR, NRL and ICM. Authors would suggest compounds 5 and 6 for further research. Beside that, derivatives 3 and 4 have a slightly higher hemolytic potential but better ligand properties.

Biography

Jovana Trifunović has completed her PhD in Pharmacy from University of Novi Sad and currently, she is Post-doctoral student at Department of Pharmacology, Toxicology and Clinical Pharmacology at Medical Faculty, University of Novi Sad, Serbia. She was visiting student at Department of Chemistry, University of Graz and at Department of Organic Chemistry at Graz University of Technology, Austria during 2012/2013 and 2014.

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