

## The synthesis, kinetics and reaction mechanism of the potassium salicylate alkylation by allyl bromide

© Anatoly K. Brel,<sup>1\*</sup> Svetlana V. Lisina,<sup>1</sup> Elena A. Vasilkova,<sup>1+</sup>  
Arkady O. Litinsky,<sup>2</sup> and Vitaly V. Kamnev<sup>2</sup>

<sup>1</sup> Department of Chemistry. Volgograd State Medical University. Pavshikh Bortsov St., 1. Volgograd, 400131. Russia. Phone: +7 (8442) 38-43-13. E-mail: VasilkovaEA@gmail.com

<sup>2</sup> Department of Physics. Volgograd State Technical University. Lenin St., 28. Volgograd, 400131. Russia. Phone: +7 (8442) 24-81-07.

\*Supervising author; <sup>+</sup>Corresponding author

**Keywords:** salicylic acid (salicylates), alkylation, quantum chemistry computations, nucleophilic substitution.

### Abstract

The kinetics of the potassium salicylate alkylation by allyl bromide has been studied. The density functional theory (DTF) with method B3LYP / LanL2DZ and full molecular geometry optimization has been used. The analyze of calculations led us to conclusion that the reaction into the gas phase and into the solvent runs on  $S_N2$ -mechanism.