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Study of laws in the a structure of effective 15-lipoxygenase inhibitors using pattern recognition theory and QSAR metods

© **Veronica R. Khayrullina**,[1+] **Anatoliy J. Gerchikov**,[1]
B. Horst,[2] **A. Entzian**,[2] and **Felix S. Zarudiy**[3]
[1] *Department of physical chemistry and chemical ecology. Bashkir state university.*
Z. Validi-Str, 32. Ufa, 420074. Republic Bashkortostan. Russia
Phone: +7 (347) 273-67-27. E-mail: Veronika1979@yandex.ru, gerchikovv@inbox.ru
[2] *Institute of organical chemistry. Martin-Luther university Halle-Wittenberg.*
Kurt-Mothes-Str. 2. Halle. D-06120 Halle/Saale. Germany.
Phone: +7 (0345) 55-25628. E-mail: boegel@chemie.uni-halle.de
[3] *Department of pharmacology №1. Bashkir state medical university.*
Lenin-Str, 3. Ufa. 450000. Republic Bashkortostan. Russia.
Phone: +7 (347) 273-75-81. E-mail: zarudiy@anrb.ru

*Supervising author; [+]Corresponding author

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Abstract

Using the computer system *SARD-21 (Structure Activity Relationship and Design)* and QSAR-methodology for effective 15-lipoxygenase (15-LOX) inhibitors characteristic descriptors have been found. On the basis of this information two models for forecasting the interval inhibitory activity level and two linear regression model for numerical values of IC_{50} for sulphur - nitrogen - and oxygencontaining heterocyclic compounds to enzyme 15-LOX prediction have been constructed. The revealed structural descriptors for the molecular design of [1-(4-chlorbenzol)-5-methoxy-2-methyl-1H-indol-3-yl] acetic acid (operating substance of non-steroidal anti-inflammatory drugs (NSAIDs) – "indometacin") have been applied. As a result 33 potentially highly - and middle efficiency 15-LOX inhibitors have been obtained.