

MEDICINAL CHEMISTRY**Manuscript Evaluation Form**

Editor-in-Chief: Dr. Dimitra Hadjipavlou-Litina, Aristotle University of Thessaloniki, Thessaloniki, Greece

PAPER TITLE	Application of ionic liquids for the determination of lipophilicity parameters using TLC method, and QSRR analysis for the antipsychotic drugs
AUTHOR(S) NAME	Dominik Mieszkowski, Marcin Koba, Michał Piotr Marszałł

Sec. A: REFEREE'S ASSESSMENT

(cross as appropriate)

Criterion	Excellent	Good	Fair	Poor					
Originality of the topic	x								
Technical Quality	x								
Importance in its Field	x								
Style & Overall Representation		x							
Readily Understandable	x								
Suitability for the Journal	x								
Adequate Illustrations or Drawings	x								
English language		x							
Description		Yes	No	Comments/ Suggestions					
Does the title represent manuscript's contents?		x							
Is the Abstract accurate and concise?		x							
Are the approach/ methods properly described?		x							
Are the conclusions and interpretations sound?		x							
Are the references properly cited?		x							
Is this a new/ original/ contribution?		x							
Is it within the scope of the journal?		x							
Overall the Paper is Rated:	(Excellent ----- Poor)								
	10	9	8	7	6	5	4	3	2

Sec. B: REFEREE'S RECOMMENDATIONS**OTHER SPECIFIC CRITICISMS**

Accept with minor changes	x	Imperfect style	
Accept with major changes		Too long	
Reject in current form, but may be resubmitted		References incorrectly presented	
Reject, with no resubmission		Typographical and Grammatical errors	x

PAPER TYPE: Research article☐

Review article

☐

Letter article

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Confidential Comments to the Editor (not for Transmission to Authors):

The article is within the scope of the journal and suitable for publication after some revision.

There is one addition that should be made in the title of the article, both chromatographic methods that were used should be mentioned, in order to represent the content of the manuscript completely: using TLC and HPLC methods

Comments for the Authors (continue on another sheet, if necessary):

Review of the article entitled

Application of ionic liquids for the determination of lipophilicity parameters using TLC method, and QSRR analysis for the antipsychotic drugs, by Dominik Mieszkowski, Marcin Koba, Michał Piotr Marszałł

In this article, the retention behavior of antipsychotic drugs was studied in the reversed-phase liquid chromatography (RP-LC) systems, using both planar and column LC, as well as both in the presence and absence of ionic liquids, and the relationships between chromatographic data and selected structural features of analytes were determined using QSRR studies. Significant relationships were found between the retention constants, R_M^0 (with addition of ionic liquids) and \log_{kw} , and the in silico calculated $\log P_s$ indices. Therefore, R_M^0 and \log_{kw} values of the investigated compounds have been recommended for description of their lipophilicity.

The article is within the scope of the journal and suitable for publication after some revision.

In the title of the article mention both chromatographic methods: using TLC and HPLC methods

The English language has to be improved.

For example, in the abstract state: Chromatographic techniques allowed determining R_M^0 and \log_{kw} values of the investigated compounds

In the Introduction, on page 3, line 47, is a useful analytical technique

Line 55, use italic for *n*-octanol-water partition coefficient

Line 60, traditional shake-flask method possesses

On page 4, lines 63 and 64, in the estimation of lipophilicity parameters

Lines 69 and 71, allowing remodeling the stationary/mobile phase system and thus improving lipophilicity assessment process

Page 5, line 91, add comma before, such as

Line 97, the correct spelling is aluminum

On page 6, move subheadings 2.3 and 2.3.1 to the next page

On page 8, line 153, replace models were constructed, instead a models

On page 10, lines 200 and 201: The calculated R_M^0 and \log_{kw} values

On page 11, lines 215-217, state: a significant correlation was also found between R_M^0 indices determined with the addition of [emim][BF₄] and \log_{kw} values (see Figures 3A-B), compared to

Page 12, line 236, the correct spelling is phenomenon

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On pages 13 and 14, lines 270 and 276, the correct spelling is quadruple
 Use molecular formula H₂O for water, with the subscript, instead of H2O, in the entire manuscript, on pages 13 and 14, as well as in Tables 3 and 4 and in the legend of Figure 4.
 Line 286, both TLC and HPLC techniques
 In Conclusion, lines 311 and 312, they may be helpful

State the complete term and the abbreviation at the first place where it appears in the manuscript, in the rest of the text either the abbreviation or full term should be used.

Add or delete spaces between some words or numbers at the adequate places in the manuscript.

Use one space between the numbers and units of measure in the entire manuscript.

Place all the Figures with their legends and Tables with their captions at the first place where they are mentioned in the manuscript.

Figure legends should be placed below figures.

The legends of Figures 2 and 3, should be stated completely in the article:

Figure 2. Correlations between R_M^0 determined in methanol-water vs. R_M^0 determined in acetonitrile-water (with or without addition of ionic liquids).

Figure 3. Correlations between \log_{kw} and R_M^0 determined with (panel A and B) or without (panel C and D) addition of ionic liquids.

Delete the points after the captions of Tables 1-4.

Numbers of issues should be added to references 6, 8, 11, 13-16, 18 and 21, if available.

FIELD OF EXPERTISE OF REFEREE: Materials and chemical technologies, nanotechnologies, biomedical engineering, chemistry, medicinal chemistry

Name & Affiliation of referee: Tamara Jovanovic, Department of Biomedical Engineering, Faculty of Mechanical Engineering, University of Belgrade, Kraljice Marije 16, 11120 Belgrade, Serbia

Dr Tamara Jovanovic / April 3, 2019
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