GUIDE FOR AUTHORS

The **UBA** Editorial Board will consider original publications on current topics in bioorganic chemistry, medicinal chemistry, organic chemistry and other related disciplines.

COVER LETTER AND COPYRIGHT

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MANUSCRIPT DESIGN

Please, use the UBA Template to create you manuscripts.

The type of articles

The Editorial Board choose the following publication formats:

Research Article (no more than 40 thousand characters with spaces);
Review and **Digest paper** (up to 60 thousand and 30 thousand characters, respectively);
Short Communications (up to 10 thousand characters, no more than 4 pages template);
Publicistic articles on different topics (are not indexed in scientometric databases);

General design requirements

• Text should be presented in the *MS Word* text editor, chemical formulas and diagrams must be prepared using the *ChemDraw* editor (*ACS Document 1996* style) and inserted into the template as an object.

• Mathematical signs and symbols, Greek letters, units of measurement, as well as initials of authors, volume numbers and pages in literature sources should be separated by the non-breaking space by pressing Ctrl + Shift + Spacebar.

• For chemical compounds first described in the article or which are the main object of study, in addition to the formula, the full name according to the IUPAC nomenclature should be given. To obtain the names, we recommend following the next guidance: 1. *IUPAC Nomenclature of Organic Chemistry*; Rigaudy, J.; Klesney, S. P., Eds; Pergamon: Oxford, 1979. 2. *A Guide to IUPAC Nomenclature of Organic Compounds (Recommendation 1993)*; Blackwell Scientific Publication, 1993; (see

http://www.acdlabs.com). 3. *The ACS Style Guide*; Dodd, J. S., Ed.; American Chemical Society: Washington, DC, 1997.

• Compounds mentioned in the text more than once should be numbered in Arabic numerals (or denoted by a unique code, for example, "protein *CDKN1B*-**A**") and indicated in the text and in diagrams in bold without parentheses. In case of using the full name of the compound, according to the IUPAC system, the number should be given in parentheses. We recommend using only the Latin alphabet for letter indexing.

• The use of abbreviations in the names of compounds should follow well-known rules (see list), in special cases, it is mandatory to provide a decipherment in the text of the article.

• Symbols of physical constants, stereochemical symbols and prefixes that characterize the structural features or positions of the substituent in the molecule should be written next to the formulas in Latin letters and highlighted in italics (for example, *d, J, k, c, m / z, o-, m-, p -, t-, cis-, trans-, de, ee, (R)*-enantiomer).

• The units used to describe measurements of quantities should be expressed as directed in the International System of Units (SI). In the numbers, the whole part should be separated from the fractional by point.

• In molecular formulas, the elements are arranged according to the System of Chemical Abstracts: C, H and then follow the Latin alphabetic sequence.

• If specific organisms (animals, plants, microorganisms) were used in the research, during the first mention of them in the text of the article it is necessary to indicate the full species name of these organisms in Latin (italics) according to modern taxonomy. In case of repeated mention of the genus, a single letter should be used, except when the generic names of different organisms begin with the same letter. Then use abbreviations of several letters, such as *Staph. aureus*, *Str. lactis*.

• When experimenting with laboratory animals, as well as biomaterials from donors or patients, all procedures must be performed in accordance with the bioethical standards of the country where the experiment is performed.

• The editors welcome the authors' submission of supporting materials (file: supporting_materials.pdf), which confirm the authenticity of the results presented in the paper. In their absence, we strongly recommend that you provide the original spectral data for at least one of the basic structures described in the article.

• When using non-commercial self-designed devices, it is advisable to provide photographic images.

Figures and Tables

Color

• The editors welcome the use of color in graphic images. Color images are published at no extra charge. The use of color in tables, captions to images or body of the text is possible only by permission of the editor.

• All images should be readable upon printing on both color and black-and-white printers, so we recommend avoiding pale light blue and yellow lines/colors.

Graphs and Diagrams

• Use serif fonts (Arial, Calibri, Helvetica) for text on graphs and charts. The size of fonts on different graphic objects in the article should be approximately the same. Try not to use letters less than 1.5 mm or more than 7 mm in heigh.

Tables

• Tables must have at least two rows and two columns, a sequential number and a title. Notes to tables are indexed by letters, which are arranged in alphabetical order directly below the tables.

• Tables that require for reading turn of the page clockwise are not allowed.

Illustrations and Photos

• For illustrations, you must provide graphic files in TIFF (or JPG) format with a minimum resolution of 600 dpi and an image width of 8.5 cm for single-column and 17 cm for two-column format. • Illustrations published by other authors are allowed in review publications, but in this case the author of the manuscript is obliged to provide documentary evidence of permission to use these materials from the copyright owner.

The Manuscript Structure:

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• Summary and Keywords
• Introduction
• Results and discussion
• Conclusions
• Experimental section
• Acknowledgments and Data on financial support
• Author’s Contributions (if more than four authors are listed)
• Notification of the presence or absence of Conflict of Interests
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• Foreign language Summary

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The UDC classification index is given as a separate line at the beginning of the manuscript on the left. Abbreviated UDC tables in Ukrainian language can be found on the relevant website: (http://www.udcsummary.info/php/index.php?lang=uk&pr=Y)

The Paper Title

The title page of the manuscript should begin with an informative title (no more than 8-10 significant words), which should accurately reflect the essence of the work. Printed in bold, font size 16.

Authors names and affiliations

Under the title of the article the names of the authors and the name of the institution where the work was performed should be located. The author for correspondence should be identified with an asterisk (*), indicating his/her contact telephone number and e-mail, as well as the ORCID index. Use a superscript (superscript) to index authors from different scientific institutions.

Summary, Foreign language Summary and Keywords

The abstract (summary) should be structured and include relevance, purpose, methods, results and conclusions. The maximum number of keywords is five. The abstract should be repeated at the end of the article in an expanded form (from 1800 characters) in a language other than the language of the main text of the article (Ukrainian or English).

Introduction

The introduction summarizes the history of the subject (with reference to relevant literature sources), indicates the goal of the study.

Results and Discussions

This part presents the main material of the study, with a comprehensive justification of scientific results. The use of common expressions, tautologies, and duplication of results in text, tables, and figures should be avoided.

Conclusions

Should be accompanied by recommendations and suggestions for future research in this area.

Experimental sections

At the beginning of the experimental part, information on materials and reagents, as well as instruments and measurement conditions should be given. The chemical methods should indicate the amount of reagents in molar and mass units (for catalysts - mass and molar percents), the volume of solvents, the yields of the obtained compounds (in both mass units and weight percent). When growing crystals it is necessary to specify the solvent. To characterize the optically active compounds indicate the values of

enantiomeric (*ee*) or diastereomeric (*de*) excesses. Sorbent and eluent should be mentioned to describe thin layer and preparative chromatography.

For all newly synthesized compounds, their physical and spectral characteristics, as well as elemental analysis data or high-resolution mass spectra, must be provided. ***An editor may accept an article that does not contain all the physicochemical parameters of the new compounds if he/she considers that the data provided are sufficient to confirm their structure.***

Physico-chemical characteristics of substances should be given in the following order

• Physical state, melting and boiling point, retention factor, polarization rotation constant

For each crystalline product, indicate the range of melting points together with the solvent used during recrystallization, and for liquid products, the boiling point. Relevant literature data must be provided for the substances described previously. In the case of TLC, the retention factor (R_f), calculated according to the standard method and with a value less than one, as well as the eluent and the imaging method should be indicated. To describe the HPLC / HPLC assay data, the retention time (t_R) and column type should also be indicated. To characterize the optically active substances, give the data of polarimetric analysis (the value of the specific rotation of the plane of polarization α and the concentration of the measured solution).

Examples:

Pale yellow oil; TLC (hexane/EtOAc 4:6, $KMnO_4$-stain) R_f 0.28; $[\alpha]_D^{20}$ -21.7 (*c* 0.60, $CHCl_3$)
White solid; TLC (hexane-ethyl acetate 3:1, UV-vis) R_f 0.55; mp 76-77 °C (Et_2O/hexane)
Yellow oil; bp 85-90 °C/0.1 mmHg
Chiral HPLC: 91:9 *er*, t_R (*R*)-major enantiomer, 17.8 min; t_R (*S*)-minor enantiomer, 23.6 min (Chiralcel OJ-H column; 40% 2-propanol in hexane; 0.5 mL/min).

• NMR Spectra

Indicate the operating frequency of the device, the standard used and the solvent. If TMS is not used as a standard for NMR spectra, the chemical shift of the standard should be indicated on the δ scale.
For describing NMR spectra, please, use the following abbreviations:
s - singlet, br s - extended singlet, d - doublet, t - triplet, q - quartet, dd - doublet of doublets, dt - doublet of triplets, m - multiplet. For signals described as "doublet", "triplet", "doublet of doublets", etc. (and not "singlet" or "multiplet"), it is necessary to provide the corresponding Coupling Constants Spin-Spin Interaction (*J*, Hz). If additional studies have been performed to establish the structure or spatial interactions of the atoms, the two-dimensional methods used should be indicated. To describe the ^{13}C NMR spectra, the ratio of a particular signal to a particular carbon atom is given only when the determination is made on the basis of two-dimensional experiments.

Examples:

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30-7.27 (m, 2H), 7.19-7.17 (m, 3H), 4.44 (dt, *J* 47.4, 6.2 Hz, 2H), 2.61 (t, *J* 7.5 Hz, 2H), 1.74-1.59 (m, 4H), 1.42-1.33 (m, 8H)

^{13}C NMR (125 MHz, $CDCl_3$) δ 142.8, 128.4, 128.2, 125.6, 84.2 (d, $J_{C\text{-}F}$ 162.8 Hz), 35.9, 31.5, 30.4 (d, $J_{C\text{-}F}$ 19.1 Hz), 29.4, 29.2, 29.2, 25.1 (d, $J_{C\text{-}F}$ 5.5 Hz)

^{19}F NMR (282 MHz, $CDCl_3$) δ -218.02 (tt, *J* 48.1, 24.9 Hz)

^{31}P NMR (202 MHz, $CDCl_3$) δ 11.14 (d, *J* 72.0 Hz)

• IR and UV Spectra

For IR and UV spectra, the characteristic band frequencies, wavelengths of absorption maxima, extinction coefficients (or their logarithms) and the conditions under which the spectrum was recorded must be indicated.

Examples:

IR (KBr) ν 3034, 1718, 1627, 1379, 1250, 1046, 835, 754, 728

UV (EtOH) λ (lg ε) 277 (4.70), 323 (4.38)

• Mass-spectra

Indicate the numerical values of *m/z*. It is necessary to indicate the method and energy of ionization, the mass numbers of characteristic ions, their intensity relative to the main ion and, preferably, their genesis. In high-resolution mass spectra, the found and calculated values of *m/z* are given with four decimal places; if the value of m / z found corresponds to a nonmolecular ion, the gross formula and the calculated value of *m/z* are given for it.

Examples:

MS (CI) *m/z* (%) 324 (M^+, 100), 323 (40), 293 (10), 266 (20), 248 (5), 208 (5), 193 (10), 165 (3), 87 (18)

GS/LRMS (EI) *m/z* (%) 392 (M^+, 100), 320 (1.0), 293 (6.1), 292 (29.4), 216 (1.4), 202 (4.5), 163 (12.7), 162 (100), 145 (10.0), 131 (21.4), 105 (22.7), 103 (29.1), 77 (9.5), 70 (1.0)

LC/MS (CI) *m/z* 122 $(M\text{-}OEt)^+$, 168 $(M+H)^+$

High-Resolution Mass-spectra Examples:

HRMS (ESI) *m/z* Calcd. for $C_{22}H_{44}NO_4$ $(M+H)^+$ 386.3270. Found 386.3265

HRMS (ESI) *m/z* Calcd. for $C_{16}H_{16}Cl_2O_2Na^+$ $(M+Na)^+$ 333.0425. Found 333.0419

Elemental Analysis:

Anal. Calcd. for $C_{16}H_{17}NO_6$: C, 60.18; H, 5.37; N, 4.39. Found: C, 60.36; H, 5.57; N, 4.54

• X-ray data

X-ray data should be presented in the form of a drawing of a molecule with numbered atoms (or crystal packaging) and the basic geometric parameters in the form of a table or a caption to the drawing. Complete tables of atomic coordinates, temperature factors, bond lengths, valency and torsion angles are not published in the journal but are deposited with the Cambridge Crystallographic Data Centre (CCDC) (deposit@ccdc.cam.uk). The experimental part provides crystallographic data (unit cell parameters, spatial group, etc.), details of the experiment and refinement of structures, as well as the registration number of the depositor in the Cambridge Bank should be provided.

References

The list of References is compiled in the order of citing sources in the text (indicated by numbers in square brackets) and submitted at the end of the article. It must provide the following information: surnames and initials of all authors in the original transcription, the full title of the article, the title of the journal or book and the following information: 1) for periodicals - year of publication, volume, number of the periodical (except for publications with continuous pagination), numbers of the first and last pages; 2) for non-periodicals - the name of the publisher, place of publication, year of publication. For non-English articles, in the absence of an official translation of the title of the publication, it is submitted in transliterated form (http://litopys.org.ua/links/intrans.htm). The language of the original publication should also be noted. Abbreviations according to ISO 4 (https://paperpile.com/guides/journal-abbreviations-list/) are used to abbreviate the titles of periodicals.

Examples of References

Books:

1. Joule, J. A.; Mills, K. *Heterocyclic Chemistry*, fifth ed., Wiley-Blackwell: New Jersey, 2010.
2. *Fluorine-containing Amino Acids: Synthesis and Properties*, Kukhar V. P., Soloshonok, V. A., Eds., John Wiley & Sons: New York, 1995.
3. Kafarski, P.; Lejczak, B. In *Aminophosphonic and Aminophosphinic Acids: Chemistry and Biological Activity*; Kukhar, V. P., Hudson, H. R., Eds.; John Wiley & Sons: Chichester, UK, 2000; pp 407-442.

Journals:

1. Gerus, I. I.; Balabon, O. A.; Pazenok, S. V.; Lui, N.; Kondratov, I. S.; Tarasenko, K. V.; Shaitanova, E. N.; Ivasyshyn, V. E.; Kukhar, V. P. Synthesis and Properties of Polyfunctional Cyclic *β*-Alkoxy-*α,β*-Unsaturated Ketones Based on 4-Methylene-1,3-dioxolanes. *Eur. J. Org. Chem.* **2018**, *2018*, 3853–3861.
2. Kondratyuk, K. M.; Lukashuk, O. I.; Golovchenko, A. V.; Komarov, I. V.; Brovarets, V. S.; Kukhar, V. P. Synthesis of 5-amino-2-aminoalkyl-1,3-oxazol-4-ylphosphonic acid derivatives

and their use in the preparation of phosphorylated peptidomimetics. *Tetrahedron* **2013**, *69*, 6251–6261.

3. Radchenko, I. V; Kostyuchenko, N. V; Naidenova, I. Yu; Batrak, G. N; Poda, G. I; Mogilevich, S. E; Kibirev, V. K; Luik, A. I. Similarity of the effects of *tosyl-L*-arginine methyl ester, atropine, caffeine and antitumour alkylating agent on some biological functions of thrombin and platelet 2-lipoxygenase. *Ukr. Biokhim. Zh. (1978)* **1993**, *65*, 37-40 (in Ukrainian).

Extended abstract of PhD Dissertations and PhD Theses:

1. Grygorenko, O. O. *Extended abstract of PhD dissertation (Chemistry)*, Kyiv, 1998. (in Ukrainian).
2. Thompson, A. Ph.D. Dissertation, Clemson University, 2007.

Conference thesis:

1. Kukhar, V. P.; Kondratov, I. S.; Gerus, I. I. *A New Synthesis of Fluorocontaining Mevalonic and Mevaldinic Acids*, 18th International Symposium on Fluorine Chemistry, Bremen, Germany, **2006**, 204.

Patents/Chem Abstr:

1. US Patent No 7375249 B2. Process for the synthesis of enantiomeric indanylamine derivatives / Boulton, L. T.; Lennon, I. C; Bahar, E. Patent appl. No 11/358995 21.02.2006. Publ. 20.05.2008.

Websites and Other Online Formats:

1. Triarhou, L. C. Dopamine and Parkinson's Disease. In Madame Curie Bioscience Database [Internet]. (Austin, TX: Landes Bioscience;) 2000-2013. Available from: https://www.ncbi.nlm.nih.gov/books/NBK6271/ (accessed on June 30, 2020).
2. Dopamine, CID=681. In PubChem Database. National Center for Biotechnology Information [Internet]. Available from: https://pubchem.ncbi.nlm.nih.gov/compound/dopamine#section=Use-and-Manufacturing (accessed on June 30, 2020).

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The authors provide brief information on Ukrainian and/or foreign funding of the research project, as well as personal thanks for consultations and interpretation of the results.

Notification of the presence or absence of conflicts of interest

It is desirable to report the absence of conflicts of interest or to declare their existence, especially if it concerns the results of the study, their interpretation and the conclusions of the reviewers.

Author Contributions

If there are more than four authors in the article, you should provide brief information about the personal contribution of each author.

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- ***Accept the article after minor revision.***

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