INDIAN JOURNAL OF HETEROCYCLIC CHEMISTRY

A Quarterly International Refereed Journal – Published since 1991

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1. About the Journal

Indian Journal of Heterocyclic Chemistry - *a Quarterly International Journal*; publishes original research work on heterocyclic compounds pertaining to synthesis, structure, mechanism of the new reactions, spectral studies, biological activities, biochemical studies, physicochemical studies, phytochemistry, etc.

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The Journal is exclusively devoted to publish original research articles including preliminary communications and reviews on heterocyclic chemistry pertaining to structure and synthesis, mechanism of reactions, spectral studies, biologically active compounds, biochemical studies, physicochemical work, phytochemistry, etc. The authors are normally not encouraged to submit the following type of research studies for publications: (i) slight modification in the existing procedures for the synthesis of only reported compounds without any significant achievement in the synthetic protocols (ii) docking studies and biological screening of well-reported compounds. The research developments dealing with only heterocyclic compounds (including carbohydrates) are covered within the scope of the journal.

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All the manuscripts should be written in English language only. Manuscript must be essentially clear, concise and grammatically correct. As the papers are written in English language, it is advised that the authors may take help of the English Checker System online or editing service before submitting the manuscript.

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B. Submission Guidelines

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ii. **Reviews-** Review articles are summaries of recent insights in specific research areas within the scope of Indian Journal of Heterocyclic Chemistry. It should reflect an overview of a field or a comprehensive literature review in the area of heterocyclic chemistry. Key aims of reviews are to provide systematic and substantial coverage of mature subjects, evaluations of progress in specified areas, and/or critical assessments of emerging developments. With only limited space in our journal, we are bit selective. Careful planning of a review is required and text of the review should not be merely summary of the previous work rather arouse the authors' interest.

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Synthesis and solid-state conformations of 6*S*,8a*R/S*-6-alkyl-3,3- dimethyltetrahydrooxazolo[3,4-*a*]pyrazine-5,8-diones (*Pseudo* proline diketopiperazines)

Synthesis and Anticonvulsant Activity of Some New 6,8-*Bis*(aryl)-5-methyl-6,7,8,9-tetrahydro- 5*H*-tetrazolo [1,5-*d*][1,4]diazepines

Hypervalent Iodine(III) Mediated Synthesis of 3-(*β*-Styryl)-2,1-benzisoxazoles and 3-(*β*-Hetaryl)vinyl-2,1-benzisoxazoles

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The name of the author(s) where possible, should be first name, middle initial, and family name for complete identification. Use superscript Arabic numbers to indicate different addresses, which should be as detailed as possible and must include the Department/Division and country name (pin/ZIP code should also be there). The corresponding author should be indicated with an asterisk, and contact details (fax, e-mail etc.) should be placed in a footnote. Information relating to other authors (e.g., present addresses) should be placed in footnotes indicated by the appropriate symbols. For example,

Anne Beauchard[1], Helen F. Dufton[1], Kere Odumah[1], Rhian H. Jaggers[1], Mary F. Mahon[2], Pauline J. Wood[1], Michael D. Threadgill[1*] *[Times New Roman, 10.5, Bold, centered]*

[1]Drug and Target Discovery, Department of Pharmacy and Pharmacology, University of Bath, Claverton Down, Bath BA2 7AY, UK

[2]X-ray Crystallography Unit, Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, UK

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At footnote - [*]Corresponding author: Email: m.d.threadgill@bath.ac.uk *[Times New Roman, 9.5, Normal, Centered]*

g. ABSTRACT *[Times New Roman, 11, Bold, Uppercase]*

The abstract should briefly state the problem and summarize the principal findings. The length of the abstract should not exceed more than 250 words. The abstract should not contain any references. *[Times New Roman, 11, Normal, Justified]*

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Clearly drawn figure of approximately 6x12 cm should be included in the main manuscript file below abstract. All chemical drawings should be drawn in ACS style in ChemDraw (also sent as a CDX file separately). The reaction sequence presented in the graphical abstract should be general and should not include the complete reaction conditions. The graphical abstract is meant as an aid for the rapid viewing of the paper contents and help to capture the readers' attention and may feature a key structure, reaction, equation, etc.

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Provide significant keywords to aid the reader in literature retrieval. Four to seven keywords separated by commas (,) should be listed in alphabetical order after graphical abstract of the title page.

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k. RESULTS AND DISCUSSION *[Times New Roman, 10, Bold, Uppercase]*

In the Results and Discussion section, authors should emphasize on presenting their own research findings. Since page length restrictions are difficult to define for this section, the authors are advised to present this section in a concise and precise manner. This section may be further subdivided into sub-sections as per requirement, e.g., if the manuscript highlights the synthesis, biological evaluation and docking, this part should have three subsections as: (i) Chemistry (ii) Biology/ Pharmacology (iii) Docking.

The inclusion of procedural details in the results and discussion section should be kept to a minimum. The discussion of the routine and well-known characteristics of the compounds should be avoided. However, it is desirable to elaborate (preferably in pictorial form) the characterization data of representative compound(s) for the clear understanding of the readers. *[Times New Roman, 9.5, Normal, Justified]*

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Yields should represent weighed amounts of isolated and purified products, and should be reported as mass and as percentage of the theoretical value. Preferably, integer numbers should be used, e.g., "Yield 93 mg (78%)" instead of "Yield 0.093 g (78%)".

In molecular formulas, elements should be arranged according to the Chemical Abstracts system: C, H, and then all other elements in Latin alphabetical order. Formulas of molecular adducts and onium salts are given with raised dots, e.g. "$C_6H_{12}N_2 \cdot 2HCl$".

When flash or thin layer chromatography is used, both the stationary phase and eluting solvent should be identified.

Melting and boiling point. A melting point range and the appearance should be reported for every crystalline solid product, together with the solvent from which it was recrystallized (and literature data for known compounds), e.g., "yellow needles, mp 76–78°C (EtOH) (mp 77–80°C (*i*-PrOH)[12])". Similarly for liquids the boiling point and the look, e.g., "colorless oil, bp 127–128°C (10 mmHg)".

IR and UV

IR (KBr Pellet, ν, cm^{-1}): 1650 (C=N), 3200–3440 (O–H).

UV (EtOH, λ_{max}, log ε): 242 (4.55), 380 (4.22).

^{1}H and ^{13}C NMR

The solvent, instrument frequency, and the standard should be identified. If a standard other than TMS is used, its chemical shift on the δ scale should be given. To indicate the positions of protons, the designations of the type H-3, H-2,6 (for aromatic protons) and 3-CH, 4,5-CH_2 (for aliphatic protons) should be used. Protons in complex groups, to which a signal relates, should be underlined below, e.g., "3.17–3.55 (4H, m, $N(\underline{CH_2}CH_3)_2$)". Substituents should be indicated as follows: 3-CH_3; the positions of atoms should be indicated as follows: C-3, N-4, etc. If a signal in the spectrum is described as doublet, triplet, etc. (rather than a singlet or a multiplet), it is necessary to present the corresponding value of spin-spin coupling constants. If additional investigations have been made in order to establish

atom connectivities and spatial relationships, the 2D methods used should be identified. The ^{13}C signal assignments to individual atoms are accepted only on the basis of 2D experiments.

NMR

5-Methyl-7-(N-methylpiperazino)benzo[b]furan hydrobromide (1a) [Times New Roman, 9.5, *Italic*, Justified]

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, 1H, J = 2.0 Hz), 7.00 (d, 1H, J = 7.8 Hz), 6.63 (d, 1H, J = 7.8 Hz), 6.77 (d, 1H, J = 2.0 Hz), 3.21 (m, 4H), 2.66 (m, 4H), 2.46 (s, 3H), 2.39 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$): δ 154. 9, 143.3, 125.3, 119.9, 115.7, 109.8, 105.5, 55.4, 514, 46.2, 14.6.

MS

Mass (EI, 70 eV), *m*/*z* (I_{rel}, %): 386 $[M]^+$ (36), 368 $[M–H_2O]^+$ (100), 353 $[M–H_2O–CH_3]^+$ (23).

Mass (CI, 200 eV), *m*/*z* (I_{rel}, %): 387 $[M+H]^+$ (100), 369 $[M+H–H_2O]^+$ (23).

HRMS

Found, *m*/*z*: 292.1684 $[M]^+$. $C_{17}H_{24}O_4$. Calculated, *m*/*z*: 292.1675.

Found, *m*/*z*: 335.0377 $[M+Na]^+$. $C_{13}H_{17}BrN_2NaO_2$. Calculated, *m*/*z*: 335.0371.

Elemental analysis

Found, %: C 55.22; H 4.09; Br 20.42; Cl 9.04; N 7.18. $C_{18}H_{16}BrClN_2O$. Calculated, %: C 55.19; H 4.12; Br 20.40; Cl 9.05; N 7.15.

X-Ray

The data of X-ray structural analysis should be presented as a molecule in figure. Full data should be deposited at the *Cambridge Crystallographic Data Center* (*CCDC*) (the deposit number should be included in the manuscript).

Other analytical data

Other analytical data, if any, may also be added here.

m. **CONCLUSION** *[Times New Roman, 10, Bold, Uppercase]*

This part should have the concentrate of the complete manuscript. However, repetition of the sentences from the previous sections should be avoided. *[Times New Roman, 9.5, Normal, Justified]*

n. **ACKNOWLEDGEMENTS** *[Times New Roman, 10, Bold, Uppercase]*

In this section, authors may duly acknowledge people, places and financial support with grant numbers. *[Times New Roman, 9.5, Normal, Justified]*

o. **REFERENCES** *[Times New Roman, 10, Bold, Uppercase]*

References should be placed at the end of the manuscript and be cited in text in square bracket as superscript in Arabic numeric at appropriate places and vice-versa. All the references should run consecutively throughout the paper. Authors are responsible for the accuracy and completeness of all references and therefore it is advised to check the original source of reference. Preferably, each reference should contain only one literature citation. Journal titles should be abbreviated according to American Chemical Society guidelines. As much as possible, important recent references should be provided. *[Times New Roman, 9.0, Normal, Justified]*

p. **SUPPORTING INFORMATION** *[Times New Roman, 10, Bold, Uppercase]*

Spectral data (IR, NMR, and Mass), Elemental analyses, TGA data and any other types of analytical data should be supplied as supporting information. This material should be ready with the authors for any future correspondence. *[Times New Roman, 9.5, Normal, Justified]*

q. **ABBREVIATIONS AND CONVENTIONS** *[Times New Roman, 10, Bold, Uppercase]*

Standard ACS abbreviations should be used throughout the manuscript and are employed without periods. The preferred forms for some of the more commonly used abbreviations are mp, bp, °C, K, min, h, mL, µL, g, mg, µg, cm, mm, nm, mol, mmol, µmol, M, mM, µM, ppm, HPLC, TLC, GC, ^{1}H NMR, GC-MS, HRMS, FABHRMS, UV, IR, EPR, ESR, DNase, ED50, ID50, IC50, LD50, im, ip, iv, mRNA, RNase, rRNA, tRNA, cpm, Ci, dpm, *V*max, *K*m, *k*, *t*1/2. All non-standard abbreviations should be defined following the first use of the abbreviation. For a detailed listing of standard abbreviations, see The ACS Style Guide; American Chemical Society: Washington, DC, 1997. *[Times New Roman, 9.5, Normal, Justified]*

References to scientific articles:

[1] Ueda, S.; Su, M.; Buchwald, S. L. Highly N^2-selective palladium-catalyzed arylation of 1,2,3-triazoles, *Angew. Chem. Int. Ed*., **2011**, *50*, 8944-8947.

[2] Yan, W.; Wang, Q.; Lin, Q.; Li, M.; Petersen, J. L.; Shi, X. *N*-2-aryl-1,2,3-triazoles: A novel classs of UV/blue-light-emitting fluorophores with tunable optical properties, *Chem. Eur. J.,* **2011**, *17*, 5011-5018.

[3] Beauchard, A.; Dufton, H.F.; Odumah, K.; Jaggers, R.H.; Mahon, M.F.; Wood, P.J.; Threadgill, M.D. Synthesis and solid-state conformations of 6*S*, 8*aR/S*-6-Alkyl-3, 3-dimethyltetrahydrooxazolo [3,4-a] pyrazine-5,8-diones (Pseudoproline Diketopiperazines), *Indian J. Heterocycl. Chem.*, **2018**, *28*, 11-24.

Reference to an edited book:

[4] Busacca, C. A.; Senanayake, C. H. *Transition Metal-Catalyzed Couplings in Process Chemistry: Case Studies from the Pharmaceutical Industry* (Eds.: J. Magano, J. R. Dunetz), Wiley, Weinheim, **2003**.

Reference to a chapter in an edited book:

[5] Almlof, J.; Gropen, O. Relativistic Effects in Chemistry. In *Reviews in Computational Chemistry*; Lipkowitz, K. B., Boyd, D. B., Eds.; VCH: New York, **1996**; Vol. 8, pp 206-210.

r. **Schemes**

Groups of reactions that show action are called schemes. Chemical drawings must be drawn in ChemDraw in ACS style; and CDX files should be sent separately. Schemes may have brief titles *i.e.* caption, describing their contents. The caption should follow the format "**Scheme 1: Synthesis of ……**". *[Times New Roman, 9.0, Bold, Centered]*

All the schemes should be placed at appropriate position in the text and must be cited in text in square bracket e.g. [**Scheme 1**]. All the schemes presented in the text should be Arabic numbered.

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lower-case letters) typed below the table are acceptable. The caption should follow the format "**Table 1: Physical data of …..**". *[Times New Roman, 9.0, Bold, Centered]*

t. Figures (Graphs, Charts, and Illustrations etc.)

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All the nomenclature should be simple, unambiguous and in conformity with the conventions developed by the IUPAC.

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