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**Graphical Abstract (GA)**

|  |
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**Abstract**

Type here the Abstract in English (maximum 200 words in a single paragraph). Style: Times New Roman 12. Line spacing 2.0 lines. The Abstract should state the scientific problem or purpose of the research and summarize the content of the article. It must be self-consistent and informative, clearly indicating the main findings and their significance. Avoid using abbreviations and references.

**Keywords:** type here 3-6 keywords, in lower case letters, separated by commas, in Times New Roman 12

**Introduction**

Every article should begin with an Introduction, and be organized to contain the following additional sections: Experimental, Results and Discussion, Conclusions, Supplementary Information availability notice, Acknowledgements, References and Supplementary Information data. Use Times NewRoman 12, double line spacing. Number the pages (bottom right).1

The introduction must be clear and concise, and explain to the reader the background and nature of the problem, aided by suitable bibliography.2-5 This section cannot contain sub-items, it needs to be a continuous text. At the end of this section, the authors must state the objective and approach of the research. References should be numbered consecutively in the text, employing Arabic numbers as superscripts, placed immediately after the punctuation marks. Cited references must be collected in the References section, at the end of the manuscript.6

The citations should be typed just after punctuation (without space) as superscripts, see the example:

example 1: …of the environment.1-8 A behavior… {1-8 as superscripts}

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example 2: According to Silva *et al.*,11 … {11 as superscript}

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Experimental

The Experimental section may precede Results and Discussion part (Introduction, Experimental, Results and Discussion, Conclusions, Supplementary Information availability notice, Acknowledgements, References and Supplementary Information data) or follow the Conclusion (Introduction, Results and Discussion, Conclusions, Experimental, Supplementary Information availability notice, Acknowledgements, References and Supplementary Information data), but must be written as a separate section. For specific details regarding the description of equipment, procedures and new chemical structures, authors should consult the Instructions to the Authors. Critical input and output data for chemical computations and spectra used for the identification of any synthesized or identified compound must be included in the Supplementary Information section, at the end of the manuscript. Format for the spectroscopic (NMR, IR, etc.) and other data:

(‒)-(*R*)-2-(1*H*-Benzo[*d*][1,2,3]triazol-1-yl)-1-phenylethanol (**21**)

[α]*D*25 ‒20.5 (*c* 1.20, CHCl3, *ee* > 99%); mp 130-131 °C; UV-Vis (water) λ / nm 600, 1750; IR (KBr) ν / cm-1 3217, 2950, 2902, 2849, 1594, 1492, 1451, 1426, 1275, 1233, 1189, 1158, 1124, 1071, 1029, 883, 749, 746, 699; 1H NMR (400 MHz, CDCl3) *δ* 4.73 (dd, 1H, *J* 12.0, 8.0 Hz, CH2), 4.82 (dd, 1H, *J* 12.0, 4.0, CH2), 5.36 (dd, 1H, *J* 8.0, 4.0 Hz, C*H*OH), 7.28-7.30 (m, 1H, Bt-H), 7.36-7.39 (m, 2H, Ph-H), 7.41-7.45 (m, 3H, 2Ar-H and 1H, Bt-H), 7.50 (dt, 1H, *J* 8.5, 0.9 Hz, Bt-H), 7.91 (dt, 1H, *J* 8.5 Hz, 0.9Bt-H); 13C NMR (100 MHz, CDCl3) *δ* 55.3, 73.1, 109.8, 119.5, 123.8, 125.5, 126.0, 127.3, 128.4, 133.8, 140.5, 145.5; HRMS (ESI) *m/z*, calcd. for C37H28FClN4O3[M + H]+: 631.1906, found: 631.1916, 603.1823 [M + H ‒ N2]+; anal. calcd. for C37H28FClN4O3: C 70.42, H 4.47, N 8.88, found: C 71.48, H 4.52, N 8.92.

*Note:* *J* (in italic, without =), *δ* (delta, in italic, without =) and *m/z* (in italic font).

Results and Discussion

The Results and Discussion section may be organized as a single section or in two separate parts, for the Results and another for their Discussion. Self-consistent Graphics (Figures, Charts, Schemes, etc.), Tables and Equations should be added to allow a more effective, precise and meaningful presentation of the data, and to make more easily understandable the experimental setups and their results. Mere repetition of the information in text and graphics should be avoided. Graphics should use color as much as possible. Color is free of charge in the ONLINE version. Color graphics will be converted into black-and-white in the printed version, except the GA, without loss of information.

In the main documentalso keep tables/figures/schemes/equations and their legends as close as possible of their first citation.

Graphics should be insert in the text and also provided as separate graphic files for manuscript editing. Use slashes in X and Y axes to separate axes names from units [2θ / degrees; Temperature / ºC; Volume / Å3; time / min; Wavenumber / cm-1, etc.]. Use parentheses only to group a set of units [Concentration / (mol L-1); 103 (T/K)-1, etc.]. Use alternated full and open symbols (●, ○, ■, □, ▲, Δ, ♦, ♢) or different types of graphical lines (solid, dashed, dotted, etc.), to distinguish one from the other. Colors are acceptable. Examples of graphics styles:



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Editable files facilitate the correction of details out of *JBCS* standard. Figures from Excel/Origin programs provide pictures with higher quality in the final work (proof, in case of MS accept decision), so the upload of original xls/opj files is desirable since submission.

a)

(a)

(b)

**Figure 2.** Type here the Figure title: (a) …, (b) ….. (adapted from references 21 and 18, respectively).



**Figure 3.** Type here the figure title.Chemical structures should be numbered sequentially, with boldface Arabic numbers. Colors are acceptable to highlight.

**Figure 4.** Mass spectrum of compound **5a**.

**Figure 5.** 13C NMR spectrum (100 MHz, DMSO-*d*6) of compound **4**.

**Figure 6.** FTIR (KBr) spectrum of compound **8j**.

**Figure 7.** A binary phase diagram for eutectic mixture formation (figure from reference 12 with CC-BY attribution).

Equations: use the tool Equation from MS Word, specifying every term (equations should not be added in the main text in an image format).

(1)

Schemes: these graphics contain the major elements of a reaction sequence. For the sake of clarity, the reagents and conditions should be consigned as a footnote to the Scheme.The chemical structures can be drawn in any chemical drawing software, employing ChemDraw (preferred style is ACS 1996) or similar. Original drawings should be no wider than 10.5 cm (22 cm for double-column).

Use the negative symbol (–) instead of the hyphen (-) for negative numbers in tables, text and equations. Only compound numbers must be in bold letter.



**Scheme 1.** (a) Reagents1, conditions1 (yield1%); (b) Reagents2, conditions2 (yield2%); (c) Reagents3, conditions3 (yield3%); d) Reagents4, conditions4 (yield4%). Colors are acceptable to highlight.

Table: specify every acronym/abbreviation/Greek symbol, etc. in the footnote, even that they have been specified in the text.

Table: add units in the header of the table (INSTEAD OF inside the table or the caption).

**Table 1.** Type here the title of the Tablea,b,c



|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| entry No.d | Variable 1e | Variable 2 | Variable 3 | Result |
| **1** | value 11 | value 21 | value 31 | result 1 |
| **2** | value 12 | value 22 | value 32 | result 2 |
| **..** | … | … | … | … |
| **n** | value 1n | value 2n | value 3n | result n |

aStyle for column text: Times New Roman 12, centered, not indented. Use horizontal lines to separate Table sections. Avoid employing vertical rulers; bstyle for Table footnotes: Times New Roman; cstyle for chemical structure graphics of Scheme-Tables: Arial; donly compound numbers must be in bold letter; eobtained from the publication Manjolin *et al*.10

Conclusions

 This section should be inserted just after the Results and Discussion section and be dedicated to briefly summarize the main conclusions of the work.

Supplementary Information

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Acknowledgments

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For manuscript with 6 or more authors, the JBCS requires the specification of the individual contribution of each author in the text. This information, according to the 14 roles from the [CASRAI’s CRediT taxonomy](file:///C%3A%5CUsers%5CBeth%5CDocuments%5CSuzana%5CGN1%5CCredit%5CCRediT%20-%20CASRAI.html), may be added before the Reference, named as Author Contributions.

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References

Authors are responsible for the accuracy and completeness of all references.

🡪 Attention to punctuations “,”, “;”, “.”, and upper and lowercases, and upper and lowercases - they are also important in the format of references.

🡪 Numbering format of the reference list is in arabic followed by dot:

1.

2.

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(*i.a*) There should be a space between author name initials: “… AuthorFamilyName, C. F. D. …” (C. F. D. with space)

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“…Carpenter, M. A.; *Am. Mineral* …" INSTEAD OF “…Carpenter, M. A. ;*Am. Mineral..*.”

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1. Macrino, C. J.; Borges, A. S.; Cunha Neto, A.; Lacerda Jr., V.; Romão, W.; *J. Braz. Chem. Soc.* **2022**, *33*, 173. [[Crossref](https://dx.doi.org/10.21577/0103-5053.20210134)]

2. Sun, Y.; Li, Q.; Wei, S.; Zhao, R.; Han, J.; Ping, G.; *J. Lumin.* **2020**, *225*, 117241. [[Crossref](https://doi.org/10.1016/j.jlumin.2020.117241)]

In case the journal is not easily accessible, the best choice is to quote its Chemical Abstracts number, as follows

3. Provstyanoi, M. V.; Logachev, E. V.; Kochergin, P. M.; Beilis, Y. I.; *Izv. Vyssh. Uchebn. Zadev.; Khim. Khim. Tekhnol.* **1976**, *19*, 708 (*CA 85:78051s).*

Pay attention to the connection words in the names, as for instance: da Silva, M. A. or Silva, M. da, as follows:

4. Guarieiro, A. L. N.; Eiguren-Fernandez, A.; da Rocha, G. O.; de Andrade, J. B.; *J. Braz. Chem. Soc.* **2017**, *8*, 1351. [[Crossref](https://dx.doi.org/10.21577/0103-5053.20210046)]

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→ […; Publisher: City, Country, publication year.]

5. Regitz, M. In *Multiple Bonds and Low Coordination in Phosphorus Chemistry*; Regitz, M.; Scherer, O. J., eds.; Georg Thieme Verlag: Stuttgart, Germany, 1990, ch. 2.

Book with 6. Author*f*amily*n*ame1, C. T.; Author*f*amily*n*ame2, W. In *Infrared Spectroscopy*

editor’s name *(Book title in italic font)*, vol. 2, 3rd ed.; Editor*f*amily*n*ame1, T. V.; Editor*f*amily*n*ame2, C. W., eds.; Elsevier: London, UK, 1992. [in case of electronic address to access the book, the link should be informed]

→ […; Publisher: City, Country, publication year.]

6. Tsutsumi, L. H.; Oishi, D. E. In *Specialty Crops for Pacific Island Agroforestry*; Elevitch, C. R., ed; Permanent Agriculture Resources: Holualoa, USA, 2010. [<https://hilo.hawaii.edu/academics/cafnrm/faculty/documents/Tsutsumi-HoneyBeesProfile.pdf>] accessed in January 2022

(*iv*) **Citing software**

Software/program (employed in the investigation) should be included in the reference list. Cite the developer instead of publication that used the software (although both can be cited, being that the developer citation is mandatory).

7. Rasband, W.; *ImageJ*, 2.0.0-rc-3; National Institutes of Health, USA, 2014.

8. Santa-Cruz, P. A.; Teles, F. S.; *Spectra Lux Software* v.2.0 Beta; Ponto Quântico Nanodispositivos/RENAMI, Brasil, 2003.

9. *Matlab®*, version 7b; The MathWorks Inc.; Natick, MA, USA, 2007.

10. Developer; *Software’s name* (in italic), version; Company/University/etc., Country, year.

(*v*) **Citing web addresses**

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11. Sociedade Brasileira de Química, <http://www.sbq.org.br>, accessed in January 2022.

(*vi*) **Citing Dissertation/Thesis**

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(*vii*) **Composite references**

They should be used whenever possible, rather than a series of individual references, without letters (a), (b), (c), etc. Use only a semi-colon to separate them. The style for composite references is as follows:

13. Knapp, R. R.; Tona, V.; Okada, T.; Sarpong, R.; Garg, N. K.; *Org. Lett.***2020**,*22*, 8430 [[https://doi.org/10.1021/acs.orglett.0c03052](https://doi.org/10.1021/acs.orglett.0c03052%22%20%5Ct%20%22_blank)]; Adamo, C. B.; Junger, A. S.; Jesus, D. P.; *Quim. Nova***2021**, *44*, 1360 [[http://dx.doi.org/10.21577/0100-4042.20170782](http://dx.doi.org/10.21577/0100-4042.20170782%22%20%5Ct%20%22_blank)]; Kefeni, K. K.; Mamba, B. B.; *Sustainable Mater. Technol.* **2020**, *23*, 140 [<https://doi.org/10.1016/j.susmat.2019.e00140>].

(*viii*) **Citing patents**

They should be identified in the following form. Whenever possible, Chemical Abstracts numbers should be quoted in parentheses, check the following example:

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15. Kadin, S. B.; *US pat. 4,730,004* **1988** *(CA 110:P23729y)*.

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16. Neves, B. J.; Moreira-Filho, J. T.; Silva, A. C.; Borba, J. V. V. B.; Mottin, M.; Alves, V. M.; Braga, R. C.; Muratov, E. N.; Andrade, C. H.; *ChemRxiv*, 2020. [https://chemrxiv.org/articles/preprint/Automated\_Framework\_for\_Developing\_Predictive\_Machine\_Learning\_Models\_for\_Data-Driven\_Drug\_Discovery/12250046/1] accessed in July 2020

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17. Valderrama, L.; Demczuk Jr., B; Valderrama, P; Carasek, E.; *J. Braz. Chem. Soc.*, DOI 10.21577/0103-5053.20210153.

**Other examples for specific documents**

18. Conselho Nacional do Meio Ambiente (CONAMA); Resolução No. 491, de 19 de novembro de 2018, Dispõe sobre *Padrões de Qualidade do Ar*; Diário Oficial da União (DOU), Brasília, No. 223, de 21/11/2018, p. 155. [<https://www.in.gov.br/web/guest/materia/-/asset_publisher/Kujrw0TZC2Mb/content/id/51058895/do1-2018-11-21-resolucao-n-491-de-19-de-novembro-de-2018-51058603>] accessed in September 2021

19. Agência Nacional do Petróleo, Gás Natural e Biocombustíveis (ANP); *Anuário Estatístico Brasileiro do Petróleo, Gás Natural e Biocombustíveis*; ANP: Rio de Janeiro, 2018. [<https://www.gov.br/anp/pt-br/centrais-de-conteudo/publicacoes/anuario-estatistico/arquivos-anuario-estatistico-2018/anuario_2018.pdf>] accessed in September 2021

20. Agência Nacional de Vigilância Sanitária (ANVISA); Resolução da Diretoria Colegiada (RDC) No. 239, de 26 de julho de 2018, *Estabelece os Aditivos Alimentares e Coadjuvantes de Tecnologia Autorizados para Uso em Suplementos Alimentares*; Diário Oficial da União (DOU), Brasília, No. 144, de 27/07/2018, p. 90. [[https://www.in.gov.br/materia/-/ asset\_publisher/Kujrw0TZC2Mb/content/id/34380515/do1- 2018-07-27-resolucao-da-diretoria-colegiada-rdc-n-239-de26-de-julho-de-2018-34380387](https://www.in.gov.br/materia/-/%20asset_publisher/Kujrw0TZC2Mb/content/id/34380515/do1-%202018-07-27-resolucao-da-diretoria-colegiada-rdc-n-239-de26-de-julho-de-2018-34380387)] accessed in September 2021

21. Presidência da República Casa Civil; Lei No. 11.097, de 13 de janeiro de 2005, Dispõe sobre a *Introdução do Biodiesel na Matriz Energética Brasileira*; Diário Oficial da União (DOU), Brasília, Brazil, 2005. [[https://www.planalto.gov.br/ccivil\_03/\_ato2004-2006/2005/lei/l11097.htm]](https://www.planalto.gov.br/ccivil_03/_ato2004-2006/2005/lei/l11097.htm%5D%20) accessed in November 2021

22. Commission of the European Communities; *488/2014/ EC: Commission Decision of 12 May 2014*; Official Journal of the European Union, 2014, L 138, p. 75. [[https://eur-lex.europa.eu/legal-content/en/ TXT/?uri=CELEX%3A32014R0488](https://eur-lex.europa.eu/legal-content/en/%20TXT/?uri=CELEX%3A32014R0488)] accessed in September 2021

23. United States Environmental Protection Agency (US EPA); *Method IO-3.4: Determination of Metals in Ambient Particulate Matter Using Inductively Coupled Plasma (ICP) Spectroscopy*; US EPA: Cincinnati, 1999. [<https://www.epa.gov/sites/default/files/2015-07/documents/epa-io-3.4.pdf>] accessed in December 2021

24. World Health Organization (WHO); *Environmental Health Criteria 239, Principles for Modelling Dose-Response for the Risk Assessment of Chemicals*; WHO: Geneva, Switzerland, 2009. [[https://apps.who.int/iris/ handle/10665/43940](https://apps.who.int/iris/%20handle/10665/43940)] accessed in December 2019

25. ISO Guide 35: *Reference Materials: General and Statistical Principles for Certification*, ISO: Geneva, 2006.

26. ASTM D664: *Standard Test Method for Acid Number of Petroleum Products by Potentiometric Titration*, Philadelphia, 2009.

27. EN 14104: *Fat and Oil Derivatives - Fatty Acid Methyl Esters (FAME), Determination of Acid Value*, European Committee for Standardization: Berlin, 2003.

28. Companhia Ambiental do Estado de São Paulo (CETESB); *Guia Nacional de Coleta e Preservação de Amostras*; CETESB: São Paulo, 2011.

29. *The United States Pharmacopoeia (USP)*, USP 37-NF 32, vol. 2, The United States Pharmacopeial Convention, Rockville, 2013, p. 1954-1955.

30. *British Pharmacopoeia 2019*, vol. 1, The Stationery Office, London, 2019, p. I-292-I-293.

31. American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE); *Ventilation for Acceptable Indoor Air Quality*, Standard 62-1999, ASHRAE, Inc.: Atlanta, 1999.

32. *Farmacopeia Brasileira*, 4th ed.; Atheneu: São Paulo, 2002.

33. International Conference on Harmonisation of Technical Requirements for Registration of Pharmaceuticals for Human Use (ICH); *Validation of Analytical Procedures: Text and Methodology Q2(R1)*; ICH: London, 2005.

 **For CRM, NIST, AOCS Official/Standard method, ICSD, JCPDS, PDB, Web of Science, Scopus and PubChem, it is not necessary to include in the reference list.**