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## Checklist for Authors:

1. Is the mandatory supplementary material included? If not, please provide supplementary material (<https://www.mdpi.com/journal/molbank/instructions#mandatorySup>)

### Required:

- $^1\text{H}$  and  $^{13}\text{C}$  NMR 1D and relevant 2D spectra and related spectra used to assign a structure. Note that 1D  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra should be displayed with the normal full range of chemical shifts displayed, 0–10 ppm and 0–200 ppm, respectively, while the y-axis should be expanded to the height of the maximum signal originating from the structure, and not that of the deuterated solvent or an impurity. Spectral expansions of important segments should be included where necessary to clarify details for readers. Deuterated solvents and impurities should be identified and instrument frequency should be identified.
- In the absence of elemental analysis data, GC and/or HPLC chromatograms that demonstrate bulk purity > 95%.
- Where crystallographic data is reported, a CheckCIF report should be included in the supplementary materials together with \*.cif file. Note that all crystallographic data should be submitted to the Cambridge Crystallographic Data Centre (CCDC) <https://www.ccdc.cam.ac.uk>, and be accompanied by a CDCC deposition number.
- For computational studies, the Cartesian coordinates, or z-matrix, number of imaginary frequencies and the total energy must be given.
- A valid 2D MDL molfile (in V2000 format) of the title compound before peer review, which should contain all non-hydrogen atoms of the structure (optionally, explicit hydrogens may be included).

### Not required but welcome:

- Mass spectra, IR, UV-vis and other spectra.
2. Does the manuscript use the template file? If not, please make the revision (check if all manuscript sections are there, including an abstract).
  3. Is the article type appropriate? If not, suggest change (please note that there are only two article types (“Short Note” and “Communication”) for the published paper of Molbank): “Short Notes” must contain only one new compound (exception: characterization data of isolable intermediates may be reported as a note in the “references and notes” section); “Communication” can contain several compounds. Moreover, a Communication should differ from a Short Note not based on the number of compounds, but on the degree of complexity of the manuscript. For example, if someone is presenting the synthesis of  $\text{A+B} \rightarrow \text{C}$  without a significant story behind it then this should be a Short Note, but if

there is significant content in the discussion, such as a tricky structure elucidation, or a correction of the literature or a significant improvement or a new reaction protocol, then these papers should be Communication, even if there is only one compound prepared and reported.

4. Is the format of the Title correct? If not, please make the changes accordingly. "Short Notes" title is only the systematic name of the title compound (note: in the "structure determination" section, we silently accept "Crystal structure of ...", in the "natural products" section, we silently accept "... from <species>" as additional words); "Communications" title can be freely chosen, but should be concise and meaningful.
5. If possible, check CAS (Scifinder) or REAXYS if the title compound is really new. Molbank publishes synthetic papers of known compounds only in very rare, exceptional cases (e.g., if a compound is of particular general interest and its preparation could be significantly improved). If a title compound is claimed to be new, but CAS contains references to this compound, the paper will be rejected immediately.
6. Short Notes or Communications that deal primarily with Structure Determination (e.g. from X-ray, Neutron Diffraction or, less commonly, other definitive structural methods) are acceptable for compounds whose synthesis has been previously reported or are otherwise known compounds in the chemistry literature and databanks. Such papers must clearly cite/acknowledge the prior work and make a case for the significance of the additional information.
7. Check if the Experimental Section is complete. The data must include:
  - A General Methods and Procedures (Note that this should include any reference to the preparation of starting materials or known intermediates that have been prepared according to literature procedures. Authors should not be reproducing experimental procedures of already published materials, unless these have been significantly modified and improved).
  - A clear written and reproducible procedure for the title compound. Note amounts of reactants should be given both in weight units and moles; e.g., "reagent X (X.00, g/mg, Y.50 mol/mmol)".
  - The use of nested parentheses (((()))) should be avoided; instead, a combination of parentheses, square brackets and (if necessary) curly braces ({}()) should be used.
  - Weight and percentage yield; e.g., "xxx mg, yy%".
  - Mp and recrystallization data for solids, including a description of the compound (color and crystal form), and include a comparison to the literature for known compounds; e.g., "colorless needles, m.p. xx.y-xx.z °C (solvent) [lit., [ref] xx.y-xx.z °C (solvent)]" Bp for liquids where possible, and include a comparison to the literature for known compounds; e.g., "yellow oil, b.p. xx.y-xx.z °C (pressure) [lit., [ref] xx.y-xx.z °C (pressure)]" Specific optical rotation, cyclic dichroism or equivalent data should be reported for chiral or enantioenriched products, and include a comparison

to the literature for known compounds; e.g., “[ $\alpha$ ]<sub>D</sub><sup>20</sup> -XY (c a.b, CH<sub>2</sub>Cl<sub>2</sub>) [Lit., [ref] [ $\alpha$ ]<sub>D</sub><sup>20</sup> -XZ (c a.c, CHCl<sub>3</sub>)]”

- R<sub>f</sub> values for compounds isolated by chromatography; e.g. “R<sub>f</sub>0.45(n-Hexane/CH<sub>2</sub>Cl<sub>2</sub>, 75:25)”
  - Elemental analysis (C, H and N) data to within +/- 0.40%; e.g., “Anal. Calcd for C<sub>w</sub>H<sub>x</sub>N<sub>y</sub>O<sub>z</sub>: C, 12.34; H, 5.67; N, 8.90. Found: C, 12.56; H, 6.00; N, 8.88.” In the absence of elemental analysis data, quantitative GC, HPLC, capillary electrophoresis analysis is needed to confirm bulk purity > 95%.
  - IR spectral data including relative intensities as indicated by s (strong), m (medium), w (weak); and or broad (br), sharp (sh) etc. Emphasis should be placed on frequencies related to key functionalities; e.g., “ $\nu_{\max}$  (neat, cm<sup>-1</sup>) 3400 br (O-H), 3100 w (Ar C-H), 2289 s (C $\equiv$ N), 1710 s (C=O)”.
  - UV-vis spectral data, e.g., as “ $\lambda_{\max}$  (solvent) xyz nm (log  $\epsilon$  a.bc), xzz (a.cc), etc.” Please indicate inflections/shoulders as either inf or sh, i.e., xzz inf (a.cc) or xzz sh (a.cc).
  - <sup>1</sup>H NMR, to 2 decimal places unless 3 decimal places are needed to differentiate very similar peaks; multiplets ‘m’ must be listed as ranges rather than by a single value; coupling constants (*J*) should be listed to 1 decimal digit (in Hz); e.g.,  $\delta_{\text{H}}$  (500 MHz, CDCl<sub>3</sub>) x.yz (3H, d, *J* a.b Hz, assignment), x.zz-x.zy (5H, m, assignment) etc. Assignments are acceptable only if there is no ambiguity.
  - <sup>13</sup>C NMR data to 1 decimal place unless 2 decimal places are needed to differentiate very similar peaks. Please indicate multiplicity and coupling constants where possible. Assignments are acceptable only if there is no ambiguity.
  - Relevant 2D NMR.
  - MS/HRMS, for compounds with molecular masses below 1000 amu, found values within 0.003 *m/z* unit of the Calcd value of a parent-derived ion are usually adequate for supporting a compounds molecular formula; e.g., HRMS (ESI) *m/z*: [M + H]<sup>+</sup>, calcd. for C<sub>w</sub>H<sub>x</sub>N<sub>y</sub>O<sub>z</sub> 321.0001; found 321.0004. Note that HRMS data is not evidence of bulk purity but can be used together with or in place of elemental analysis to support the molecular formulae.
8. Please do check language quality carefully (Especially technical science issues, prominent spelling errors, typographical errors, etc. Many can be fixed by simply using a spelling and grammar check available in any word processor. The authors should read through their manuscript and correct these manually as well.

If quality of the language is below an acceptable minimum, please make improvements before submission; you can send your manuscript to a native speaking colleague, or a professional English editing company to check your paper before resubmission. For more details on the MDPI English editing service, please see <https://www.mdpi.com/authors/english>

**Please pay more attention to the following places:**

- Heading capitalization;

- Spaces before units (symbols, fonts);
  - Changing Eqn., Fig. to Equation, Figure;
  - Use of italic/bold;
  - In systematic names, nested parentheses should be avoided; instead, a combination of parentheses, square brackets and (if necessary) curly braces should be used;
  - The format of literature references must follow the guidelines, i.e., the title of the article must be included; journal names must be abbreviated correctly (according to CASSI; authors may be pointed to <http://cassi.cas.org/search.jsp>).
9. Check if a suitable reaction scheme or structure formula of the title compound is included and referenced in the body text.
10. Check if all authors are listed with full (i.e., non-abbreviated) first name (given name) and last name (surname or family name).

**Point-by-Point Response to Reviewers' Comments:** A very thorough point by point response to every review comment must be provided. To the largest extent possible, review comments must be addressed with respect. Where there is disagreement, a clear response on why review comments cannot be addressed must be stated. Such a point-by-point response may be required for multiple rounds of reviews.

**References:** Please ensure that a comprehensive list of all relevant references is provided in numerical order, e.g., relevant papers published in this journal.

**Abstract Graphic:** Authors are required to provide a self-explanatory graphical abstract of the paper to be used along with the abstract in the Journal's Table of Contents and search results. The graphic should not exceed 550 pixels width/height and can be provided as a PDF, JPG, PNG or GIF file. The minimum text size in the graphic should be 12 pt.