Frontiers in Chemistry: Submission Checklist

1. Chemical Structures

Chemical structures should be prepared using ChemDraw or a similar program. If working with ChemDraw please use Frontiers ChemDraw Template, if working with another program please follow the guidelines given below:

Drawing settings: chain angle, 120° bond spacing, 18% of width; fixed length, 14.4 pt; bold width, 2.0 pt; line width, 0.6 pt; margin width 1.6 pt; hash spacing 2.5 pt. Scale 100% Atom Label settings: font, Arial; size, 8 pt.

Assign all chemical compounds a bold, Arabic numeral in the order in which the compounds are presented in the manuscript text. Figures containing chemical structures should be submitted in a size appropriate for incorporation into the manuscript.

2. Data requirements

All necessary data for understanding and verification of results must be provided. This can include:

- Detailed descriptions of any experimental work done. Standard techniques can be stated rather than described, but the solvents used must be clearly defined. The use of non-standard equipment should be detailed, including the name and model number of any commercial instruments. The source and purity of commercial compounds should be given where possible.

- Unedited spectra and graphs either as high resolution images in the SI, or available to download from an appropriate repository with public access.

- Single crystal diffraction data must be accessible from a database (e.g. CCDC) with the reference number clearly provided in the manuscript. An accompanying checkCIF file is required, and any A level alerts must be rationalized in the presented work.

3. Required characterization for compounds

Adequate data is needed to provide evidence for any claimed structures and their homogeneity. In cases where adequate characterisation data cannot be obtained, a justification must be given.

The specific characterization required depends on the nature of the chemical and if it is a new compound (i.e. it has not been either prepared or adequate characterized as part of a previously reported procedure). Relevant characterization techniques may include (but are not limited to):

3.1 Small Molecules

For molecules that are synthesised according to previously reported procedures (wherein the product is unambiguously characterized), strong correlation between experimentally reported data and literature data must be shown to confirm any claimed structures - ideally 1H NMR, 13 C NMR, and mass spectrometry.

For new molecular structures or new procedures to obtain previously reported molecules, additional characterization is needed to verify the proposed structure and sample purity. This should include 1H NMR, 13 C NMR, and other NMR techniques (e.g. 19F, 31 P when appropriate). Elemental analysis should be provided to confirm 95% sample purity and confirm isomeric purity. (error bar: ±0.4% of the calculated value). High-resolution mass spectra are acceptable as proof of the molecular weight providing the purity of the sample has been accurately determined as outlined above. Other desirable forms of characterization may include melting point determination, infrared spectroscopy to corroborate functional group transformations, and UV-Vis spectroscopy for photoactive molecules. For asymmetric reactions, the enantiomeric excess (ee) of the reaction products must be given, and specific rotations are to be given for chiral molecules.

3.2 Extended crystalline materials

In the case of an extended crystalline solids, single crystal diffraction is necessary but not sufficient to determine the bulk structure. A fully indexed powder diffraction pattern can be further used as evidence, and chemical analysis may be performed to corroborate the purity and homogeneous composition.

3.3 Polymeric materials and soft matter

Characterisation should address molecular weight analysis (size exclusion / gel permeation chromatography, MALDI-TOF), rheology, morphology (dynamic light scattering and SEM), composition (Thermogravimetric analysis and NMR).Small molecules on the route to the polymers should be characterised as above and NMR data should be tabulated or presented in spectra.

3.4 Nanomaterials

Characterization must be provided to accurately describe the reported material(s) at both an individual scale (e.g. particle size and morphology) and bulk scale (electrochemical and spectroscopic properties).

3.5 Biomolecules

Sufficient data must be gathered to confirm the identity and purity of biomolecules described. Relevant techniques may include: LC-MS, mass spectrometry, HPLC, gel electrophoresis, NMR spectroscopy, XRD, and sequencing data.

4. Presentation of Data

For examples of how to report some of the most common experimental data, see the following:

4.1 NMR data

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J = 8.3 Hz, 8H), 7.46 (d, J = 8.4 Hz, 8H), 7.33–7.29 (m, 8H), 7.14–7.11 (m, 8H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 150.27, 148.71, 134.78, 131.01, 123.97, 122.99, 112.73.

4.2 Mass spectrometric data

HRMS: m/z = 315.1000 $[M+H]^+$ (calcd. for $C_{18}H_{13}B_2O_4$ $[M+H]^+$ 315.1000)

4.3 Melting point analysis
mp: 145 –147 °C (lit.ref 144–147 °C);

4.4 Elemental Analysis
Analysis (calcd., found for $C_{20}H_{15}Cl_2NO_5$): C (57.16, 57.22), H (3.60, 3.61), Cl (16.87, 16.88), N (3.33, 3.33), O (19.04, 19.09).

4.5 IR Spectroscopy
IR (Nujol): 1761 cm-1 (OC = O), 3559 cm-1 (OH).

4.6 UV Spectroscopy
UV/Vis: λmax = 267 nm.

5. Citation formatting

5.1 References in the main text
In-text references to literature citations provided in the bibliography should be indicated using numbers in square brackets according to the following style: ...**example [1]**. References should be numbered by order of appearance in the main text, and distinction should be made between references to distinct citations by using commas (e.g. [1,2]) or ranges by using dashes (e.g. [1-3]).

5.2 Citations In the bibliography:
Cited papers should be listed using the following format:

1. Lacava C, Ettabib MA, Bucio TD, Sharp G, Khokhar AZ, Jung Y, et al. Intermodal Bragg-Scattering Four Wave Mixing in Silicon Waveguides. *J Lightwave Techn.* (2019) **67**:1680–5. doi: 10.1109/JLT.2019.2901401