

ORGANIC LETTERS – DATA PREPARATION CHECKLIST
(For additional details, refer to the [Organic Letters Guidelines for Authors](#))
NOTE: Additional data may be requested for compounds

Manuscript/Supporting Information (SI) Consistency

- Compounds are labeled consistently between the manuscript and SI:
 - Compound numbers
 - Structures
- Experimental details and spectra in the SI are in the sequence that corresponds to the manuscript

Supporting Information – General

- Manuscript title and all authors are listed on the first page of each SI file
- Pages are numbered in all files for publication
- Table of contents is included
- Files are combined - do not submit a series of files of images/structures
- Introductory Section is present and describes:
 - Standard techniques
 - Instruments (NMR, microwave reactors, etc.)
 - Suppliers for commercial compounds
 - Citations to references for non-commercial known compounds
 - Hazardous reactions or toxic compounds are clearly described

Experimental Details

- Synthetic procedures/data include:
 - Reactant quantities
 - Detailed purification techniques
 - Product quantities
 - Isolated yields
 - Physical state/description of the compounds (i.e., color, solid, etc.)

- Data is reviewed for typos and omissions:
 - Molecular formula
 - HRMS data:
 - HRMS actual values are within the ± 10 ppm error limit
 - HRMS molecular weight matches the structure shown
 - Elemental Analysis:
 - Elemental analysis values are within the $\pm 0.4\%$ error limit
 - Reported formula matches the structure shown
 - Spectral data:
 - ^1H and ^{13}C atoms have been accounted for
 - Reported data corresponds to the spectra provided in the SI

Spectra

- Spectra are labeled with an image of the structure and a compound number
- Spectra are legible and images are not faint or blurry
- Spectra are at least a half page in size
- NMR baseline is displayed with the minimum chemical shift range
 - 1-9 ppm for ^1H spectra
 - 10-190 ppm for ^{13}C spectra
 - Extended range for functional groups that resonate from 9-14 ppm
- Peaks in the ^1H NMR are integrated
- Chemical shift values are included for all peaks in the ^1H and ^{13}C spectra

New Compounds: Essential Data

- ^1H and ^{13}C spectra
- HRMS data or elemental analysis data

Known Compounds - Synthesized by a new/improved method: Essential Data

- A reference in the experimental details section
- Include one or more of the following: ^1H , ^{13}C , elemental analysis, HPLC, GC