

**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 identified 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

**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.)
  - ☐ 1 mmol scale detailed method included for one-step transformations

- ☐ Data is reviewed for accuracy, omissions and typos:
  - ☐ Molecular formula
  - ☐ HRMS data:
    - ☐ HRMS actual values are within the  $\pm 10$  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:
    - ☐  $^1\text{H}$  and  $^{13}\text{C}$  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  $^1\text{H}$  spectra
  - ☐ -10-190 ppm for  $^{13}\text{C}$  spectra
  - ☐ Extended range for functional groups that resonate from 9-14 ppm
- ☐ Peaks in the  $^1\text{H}$  NMR are integrated
- ☐ Chemical shift values are included for all peaks in the  $^1\text{H}$  and  $^{13}\text{C}$  spectra

### **New Compounds: Essential Data**

- ☐  $^1\text{H}$  and  $^{13}\text{C}$  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:  $^1\text{H}$  or  $^{13}\text{C}$  NMR spectra, elemental analysis, HPLC, GC