

# **Title: Visible-Light-Promoted Iron-Catalyzed C(sp<sup>2</sup>)–C(sp<sup>3</sup>) Kumada Cross-Coupling in Flow**

Authors: Xiao-Jing Wei, Irini Abdiaj, Carlo Sambiagio, Chenfei Li, Eli Zysman-Colman, Jesus Alcazar,\* and Timothy Noel\*

This dataset is relative to the publication with the above title, published in Angew. Chem. with the following DOI: 10.1002/anie.201906462. The final published version of the manuscript and the corresponding supplementary information are open access. The two files have also been reported here as PDF files. Below are instructions on the nature of the data reported in this dataset

## **GC-MS radical clock experiments**

The “.qgd” files found in this folder (corresponding (original files obtained with a Shimadzu apparatus) represent GC-MS data. These can either be opened with the software provided by Shimadzu, or with the open source software OpenChrom (downloadable here: <https://lablicate.com/platform/openchrom>).

These data represent radical clock experiments, which are discussed in the file “radical clock discussion.docx” found in the folder.

## **Kinetic data**

This folder contains data relative to calibration curves and the reaction profiles with and without light.

### Calibration folder:

The files found in this folder (PDF files) represent the report of GC-FID data relative to the calibration of phenylcyclohexane (PhCy), p-chlorophenylcyclohexane (p-OMePhCy), products of the reaction, and diphenylethylene (diPhethylene), used as radical trap.

The data obtained from the GC-FID chromatograms was processed in MS Excel to give calibration curves. The corresponding MS Excel file is also reported in this folder.

### Reaction profiles:

The files found in this folder (PDF files) represent the report of GC-FID data relative to the kinetic data for the synthesis of phenylcyclohexane (PhCy) and p-chlorophenylcyclohexane with or without irradiation (different runs for each).

The data obtained from the GC-FID chromatograms was processed in MS Excel to give the reaction profiles. The corresponding MS Excel file is also reported in this folder.

## **NMR spectra**

The “.mnova” files reported in this folder contain NMR data. These files can be opened with the software MestrelNova NMR. A free trial version of this software can be downloaded at <https://mestrelab.com/software/mnova/nmr/>.

The structures of the compounds corresponding to each spectrum are included in the file.

The numbering of the compounds corresponds to the numbering found in the final version of the published article, which can be found the main folder (PDF file).

## **UV Vis studies**

The files in these folders represent UV-Vis spectroscopy data. The data are reported in “.opju” files, containing both numerical data and the corresponding 3D graphs absorption/wavelength/time. These files can be opened with the software Origin or OriginPro. A free trial version of this software can be downloaded at <https://www.originlab.com/>.

The graphs, both without and with annotations, have also been reported as pictures (“.jpg” files), which can be more easily opened.

The discussion relative to these data can be found in the supplementary information of the paper, which is reported in the main folder for this publication.