# Supporting Information\_GC-MS

The product spectrum of mutants of the M5 library were analyzed in triplicate via GC-MS as described in Materials and Methods. Raw data files are provided for download along with analysis parameters for automated extraction of ion intensities via Met-Idea v2.051 and quantification using an in-house MatLab script.

File names and content:

**Collated quantitation results\_OriginalTriplicates.xlsx** – Spreadsheet containing the calculated % terpene products for each enzyme of the M5 library, with a breakdown according to product and retention time. Analysis of three GC-MS replicates is provided as separate tabs.

**Finished tables\_MGA and GC-MS\_M5 library.xlsx** – Spreadsheet containing a list of enzymes in the M5 library with vial number (1-32), mutations present (in the *A. annua* BFS background), kinetics (*kcat* apparent), and products (expressed as % of total).

Directories Rep 1 – 3 contain the following files:

**ionRTlistv2\_R3S1to8.txt** – Tabular summary of mass spec parameters used for automated data processing including ions detected (m/z; major ions of a particular product), retention time (min), MZ tolerance (amu), retention time (RT) tolerance (min) and terpene product. The term in “R3” in R3S1to8 refers to the replicate number (i.e., Rep 1 – 3) while “S1to8” refers to data files 1 through 8. Note, retention time drift occurred in some sample sets, so the retention time was adjusted for automated analysis.

**Rep3\_quantitation report.pdf** – Report generated from automated MatLab analysis of GC-MS samples. “Rep3” refers to the replicate number for the analysis.

**140305-001-3.CDF** – Raw data file from GC-MS run. “001” refers to the vial number (e.g., 001-032) which corresponds to M5 library mutants listed in “Finished tables\_MGA and GC-MS\_M5 library.xlsx.” The last digit “3” refers to the replicate number (Rep3 in this case).

**References**

1. Broeckling, C., Reddy, I., Duran, A., Zhao, P.X. & Sumner, L. MET-IDEA: Data Extraction Tool for Mass Spectrometry-Based Metabolomics. *Analytical chemistry* **78**, 4334-4341 (2006).