

## Description of Additional Supplementary Files

**File Name:** Supplementary Data 1

**Description:** Selection of the available metrics for the modules discussed in the manuscript

**File Name:** Supplementary Data 2

**Description:** Selection of the modules prioritized by our approach.

**File Name:** Supplementary Data 3

**Description:** List of the PFAM domains that are considered important for specialized metabolites.

**File Name:** Supplementary Data 4

**Description:** Annotation of individual genes into five major categories: core biosynthesis, regulator, tailoring, transport, and other.

**File Name:** Supplementary Data 5

**Description:** Exact descriptions of all smCOG annotations.