

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: HMDB.csv: All of the compounds in HMDB, accessed in 2019-10-02.

File Name: Supplementary Data 2

Description: Keggall.csv: KEGG PMDs annotation database, accessed in 2020-05-04.

File Name: Supplementary Data 3

Description: T3db.csv: All of the compounds in T3DB database, accessed in 2018-10-10.

File Name: Supplementary Data 4

Description: MTBLS28posmzrt.csv: Peaks list from MTBLS28 project.

File Name: Supplementary Data 5

Description: RSI.r: R code to reproduce all of the figures, tables and calculation in this study. The layouts of scatter points and network are relied on a random process, which might produce different figures while the topological properties should be the same.