Supporting information for: Three dimensional cartography of microbiome and metabolome data onto radiological images of the human lung.

Authors: Neha Garg[1], Mingxun Wang[2], Embriette Hyde[3], Ricardo R. da Silva[1], Alexey V. Melnik[1], Ivan Protsyuk[4], Amina Bouslimani[1], Yan Wei Lim[5], Richard Wong[6], Greg Humphrey[3], Gail Ackermann[3], Timothy Spivey[7], Sharon S. Brouha[7], Nuno Bandeira[2], Grace Y. Lin[6], Forest Rohwer[5], Douglas J. Conrad[8,11], Theodore Alexandrov[1,4 ,12], Rob Knight[2,3,9,13], Pieter C. Dorrestein[1,2,3,9,14]

Author Affiliations:

[1.] Collaborative Mass Spectrometry Innovation Center, Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California, San Diego, La Jolla, CA 92093, USA.
[2.] Department of Computer Science & Engineering, University of California, San Diego, La Jolla, CA 92093, USA.
[3.]Department of Pediatrics, University of California, San Diego, La Jolla, CA 92093, USA.
[4.] European Molecular Biology Laboratory, Heidelberg 69117, Germany.
[5.] Biology Department, San Diego State University, San Diego, CA, USA.
[6.] Department of Pathology, University of California San Diego Health, San Diego, CA 92103, USA.
[7] Department of Radiology, University of California, San Diego Health, San Diego, CA 92103, USA.
[8] Department of Medicine, University of California at San Diego, La Jolla, CA 92093, USA.
[9.] Center for Microbiome Innovation, University of California, San Diego, La Jolla, CA 92093, USA.
[10.]Department of Pharmacology, University of California, San Diego, La Jolla,CA 92037, USA.
[11.] To whom correspondence should be addressed regarding the clinical aspects of this study: dconrad@ucsd.edu
[12.] To whom correspondence should be addressed regarding ‘ili: theodore.alexandrov@embl.de
[13.] To whom correspondence should be addressed regarding the sequencing: rknight@ucsd.edu
[14.] Lead contact and to whom correspondence should be addressed regarding the mass spectrometry, 3D visualization, the project and interpretation: pdorrestein@ucsd.edu

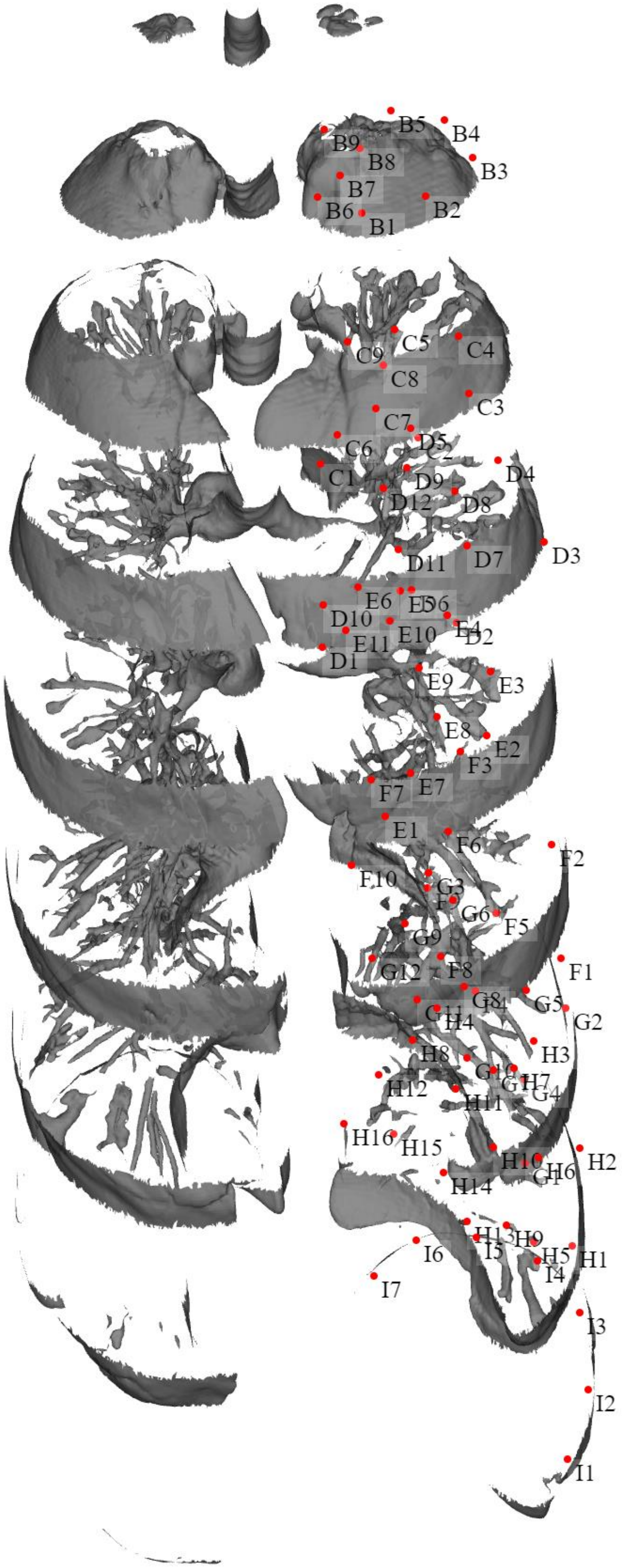

Figure S1. The tissue sections are labelled on to the 3D model of the lung. Related to Figure 1. The physical location of each of the tissue section analyzed in this study is labelled on the 3D model of the lung.

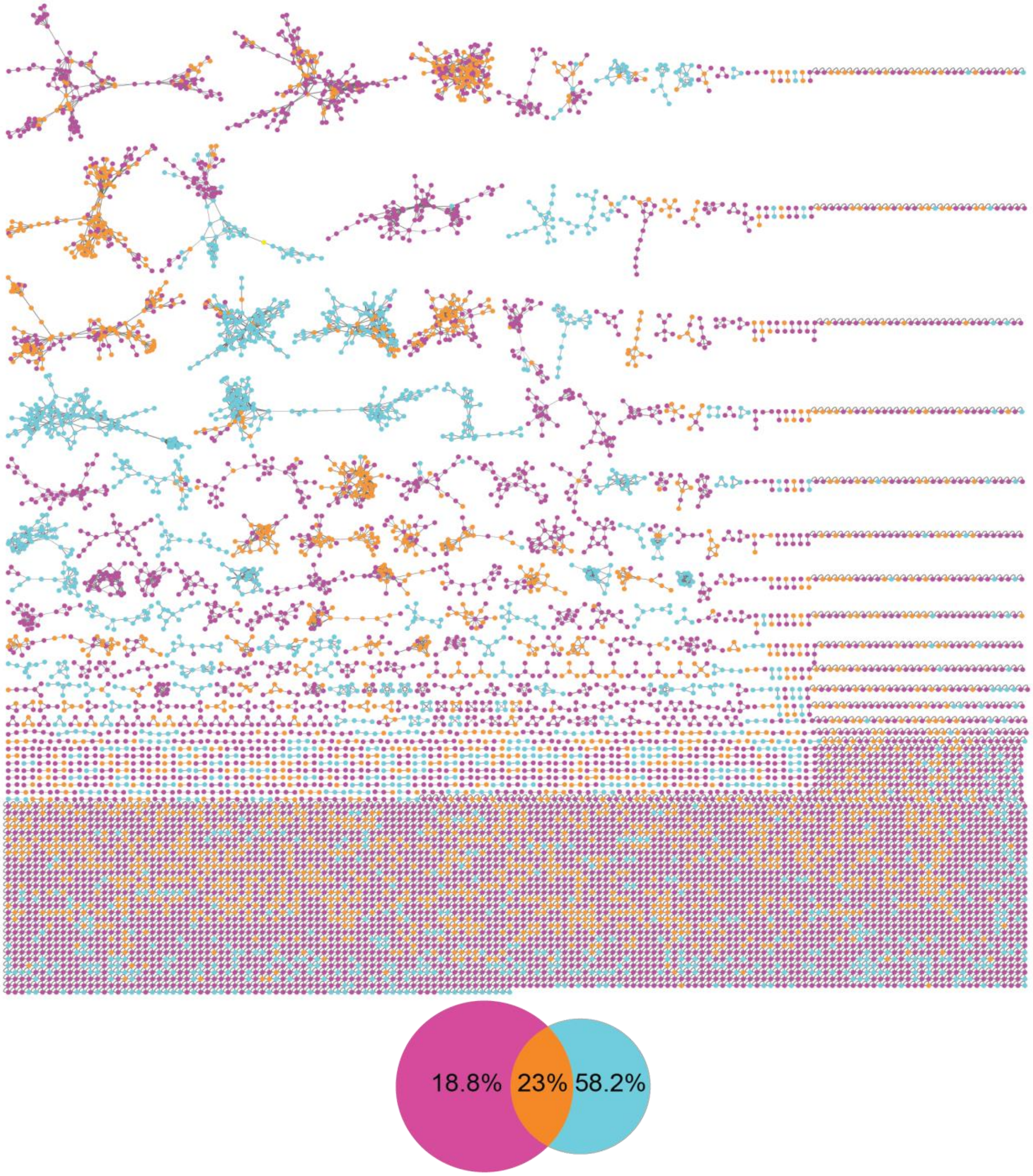

Figure S2. The molecular network of lung tissue and cultured extracts. Related to Figure 2 and 3. The nodes represent the molecular features. The annotations of the underlying spectra are available at GNPS. The orange nodes represents molecules detected in the extracts of both the lung tissue and the cultured microbial isolates, the purple nodes represents molecules detected only in the lung tissue, and the cyan nodes represent molecules detected only in the extracts of cultured microbial isolates.

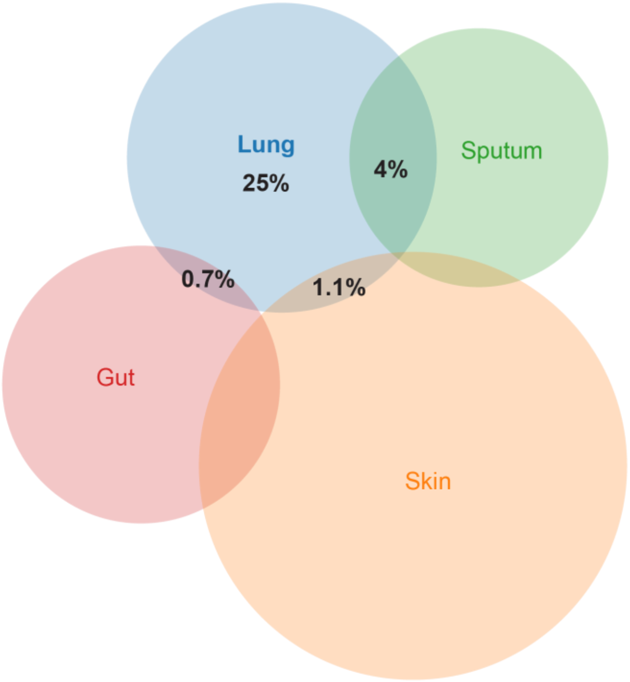

Figure S3. Venn diagram showing overlap of lung metabolome with that of sputum, gut and skin metabolome. Related to STAR method "Molecular networking". The number of unique and shared features in the metabolome is available at http://gnps.ucsd.edu/ProteoSAFe/result.jsp?task=f0488dde74204aac826a305a339c6513&view=network_statistics.

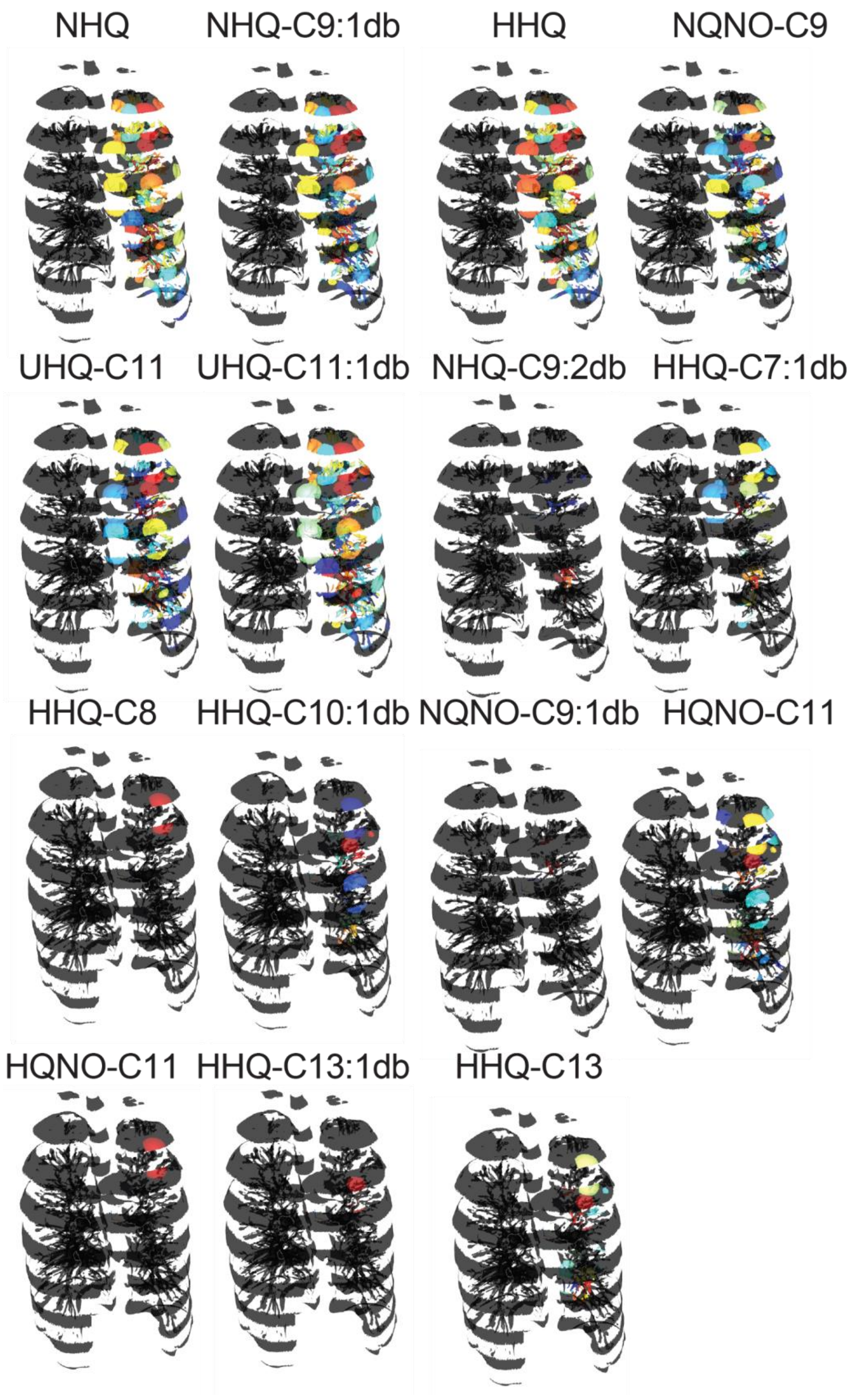

Figure S4. The distributions of various *Pseudomonas* quinolones. Related to Figure 2. The distribution of quinolones detected in this study is shown on the 3D model of the lung.

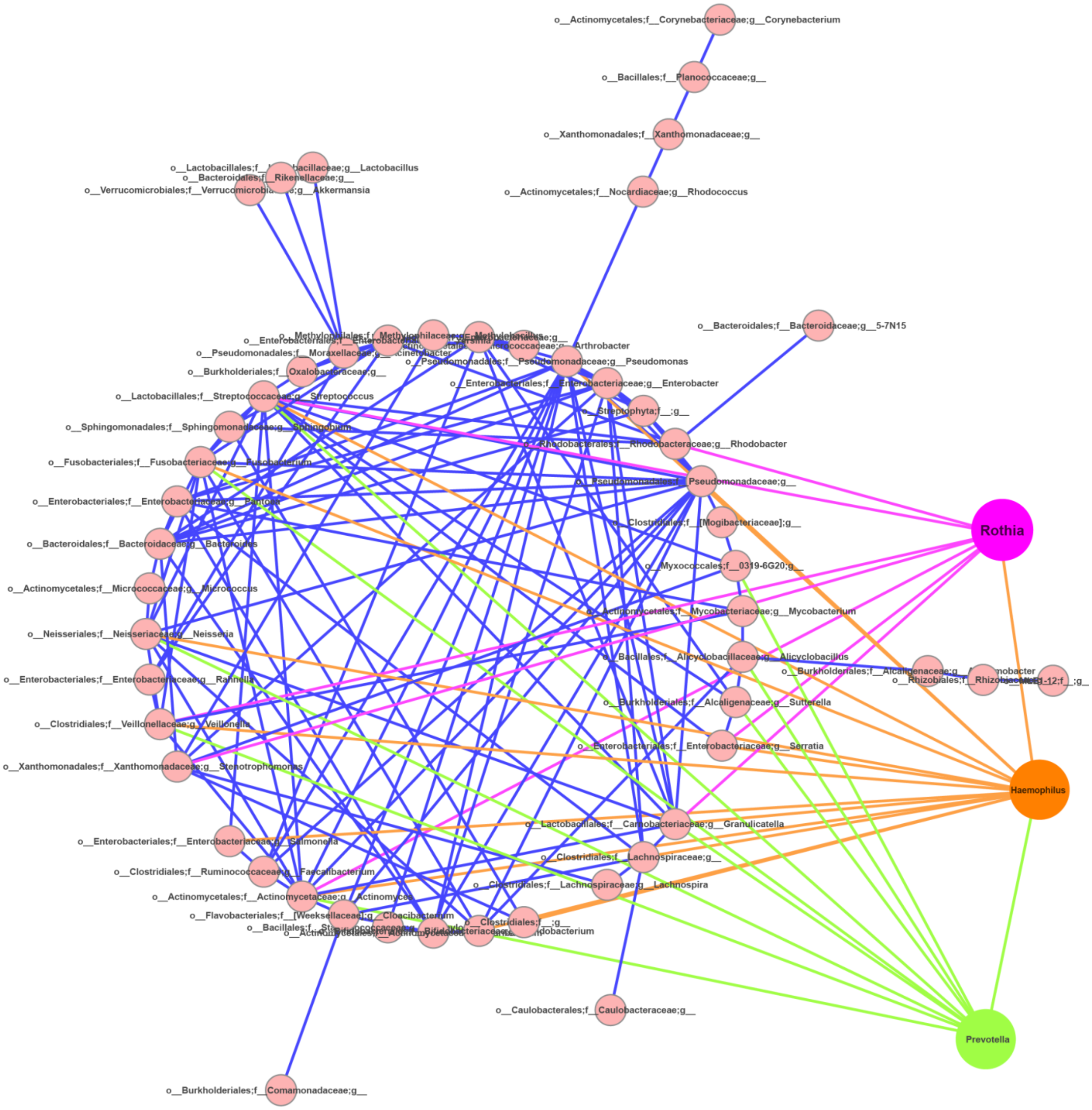

Figure S5. The microbe-microbe correlation network. Related to STAR methods "Quantification and statistical analysis". The connections between *Rothia* (pink node), *Haemophilus* (orange node), and *Prevotella* (green node) are highlighted. Refer to Figure 6 for distribution of these microbes.

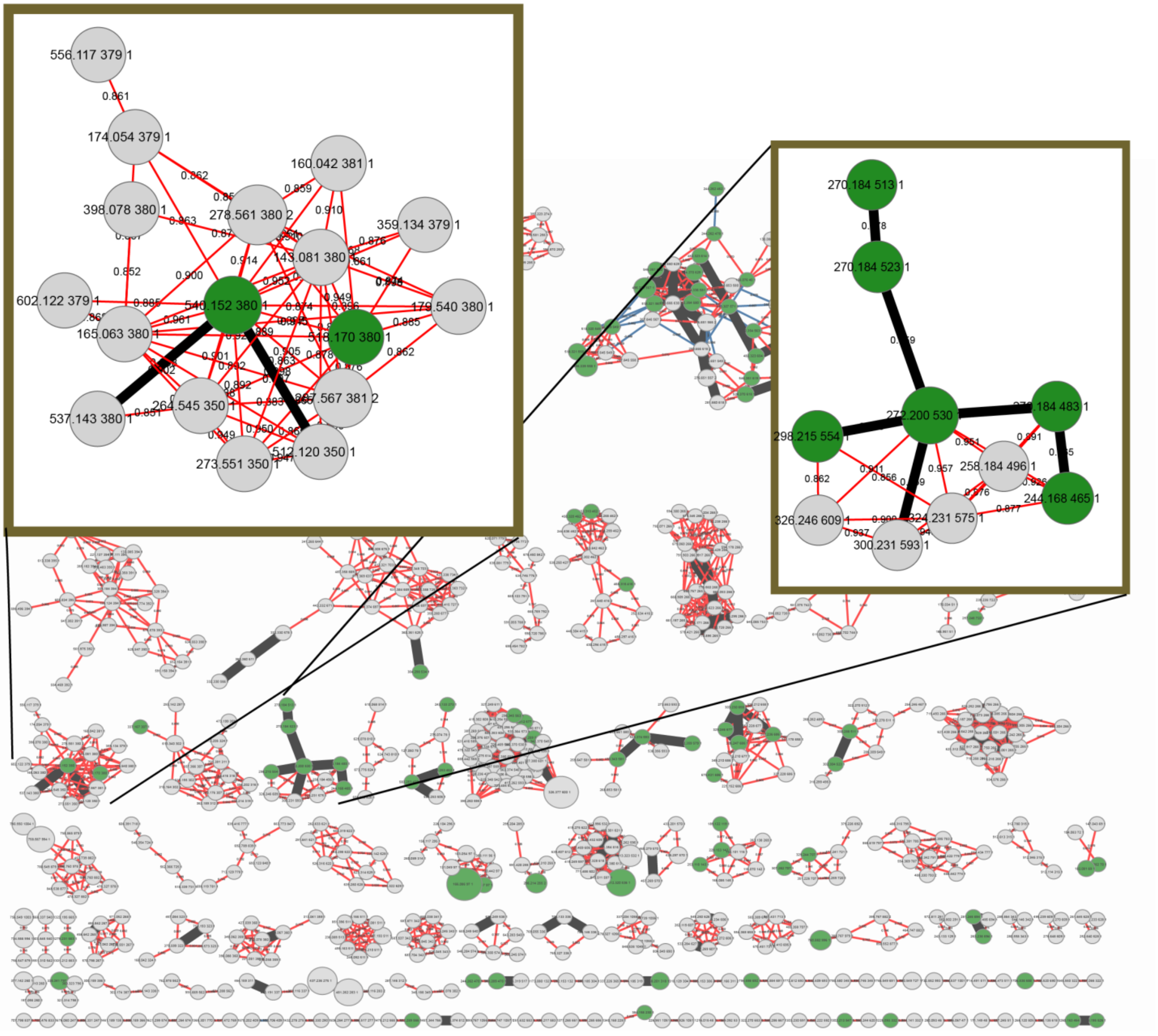

Figure S6. The metabolite-metabolite correlation network. Related to STAR methods "Quantification and statistical analysis". The cluster for Piperacillin (left) and for *Pseudomonas* quinolones (right) are zoomed out. The nodes in green are annotated molecules identified using molecular networking.

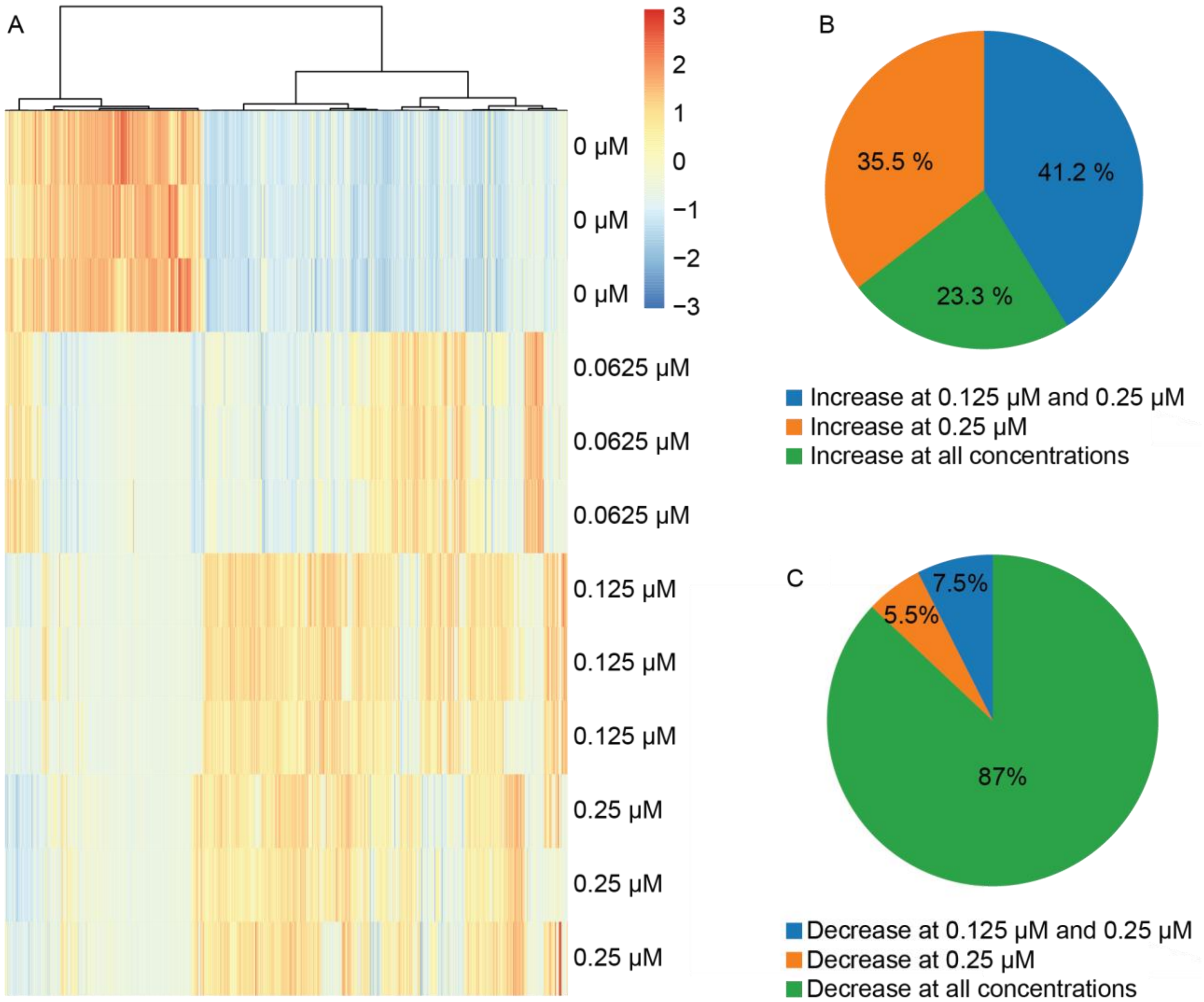

Figure S7. Response to antibiotic exposure. Related to STAR methods "Generation of heat map and pie chart for antibiotic exposure experiment." A) The heat map showing change in abundance of *Achromobacter* metabolome detected by mass spectrometry on exposure to Meropenem. B) The pie chart showing features that showed significant increase on exposure to Meropenem. C) The pie chart showing features that showed significant decrease on exposure to Meropenem.