### **Description of Additional Supplementary Files**

## File name: Supplementary Data 1

Description: Primers used in this study.

#### File name: Supplementary Data 2

Description: The raw data, mzmL files, and mfql files of the shotgun lipidomic and small-molecule analysis.

#### File name: Supplementary Data 3

Description: The topology files, initial structure files, simulation parameter control files, and result data files of molecular dynamics trajectories.

# File name: Supplementary Movie 1

Description: The lipids binding pathway within MtEfpA.

### File name: Supplementary Movie 2

Description: Conformational transition of *Mt*EfpA between inward-open and outward-open conformation.