

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: Representative LC–MS/MS chromatograms and processed quantification outputs for GABA-d₆, betaine-d₉ and ATPCA uptake assays.

File name: Supplementary Movie 1

Description: Trajectories of free BPDDBA molecules in unbiased MD simulations.

File name: Supplementary Movie 2

Description: Metadynamics trajectory of BPDDBA dissociation from the allosteric pocket.