

Supplementary information, Video S3 MD simulations of OATP1B1-E_{in}. A representative movie of a 500-*ns* MD simulation of OATP1B1-E_{in}. E3S (green) and functionally crucial residues Y352 (cyan), F356 (blue) and F386 (purple) are shown as sticks. OATP1B1 in the cartoon is colored by its NTD (gold) and CTD (marine).