



Supplementary Figure 6. Fundamental operations on model representations of the biomarker chain. The AZD1979 case study considers two fundamental computational operations on model representations of the biomarker chain: traditional forward simulation and input estimation. By complementing these two operations with estimation of an unobserved biomarker causally preceded and followed by observed biomarkers, a set of three fundamental computational operations is established. We believe that user-friendly software tools for these three operations constitute one important factor for improving quality and increasing speed in the data analysis of drug discovery programmes.