2-SII for Mutagenicity with 2-layer GIN 10<sup>1</sup>  $10^{-1}$ 10<sup>-3</sup> MSE  $10^{-5}$  $10^{-7}$  $10^{-9}$ GraphSHAP-IQ 8000 2000 6000 4000 **Model Evaluations**