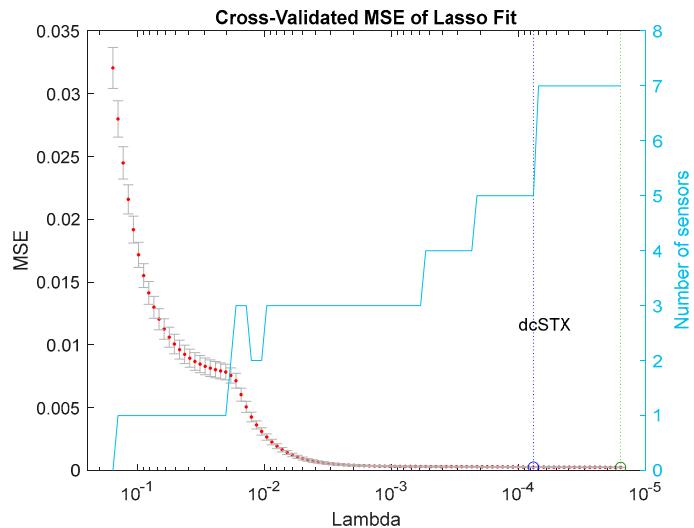
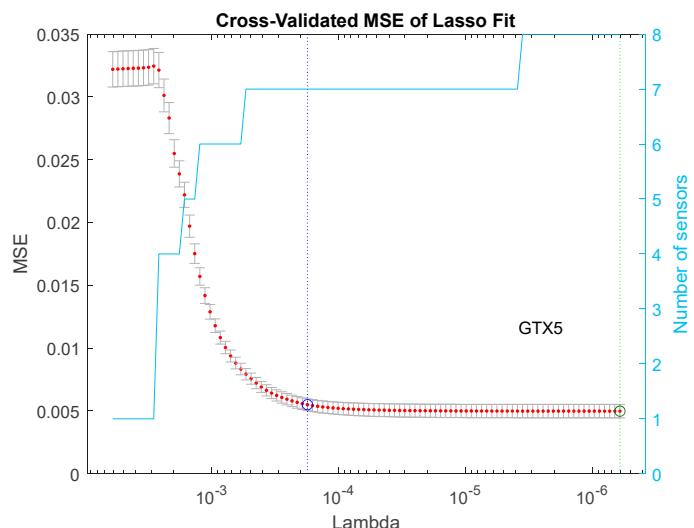


Figure S1. Results of the Lasso regularization for the dcSTX (a), GTX5 (b), C1+2 (c), GTX6 (d) and total toxicity (e) calibration models: cross-validated MSE and number of non-zero regression coefficients in the model vs. Lambda value. The green dot with dashed vertical lines represents the Lambda value with minimal MSE, and the blue dot with dashed vertical line represents Lambda value with minimal MSE plus one standard deviation.

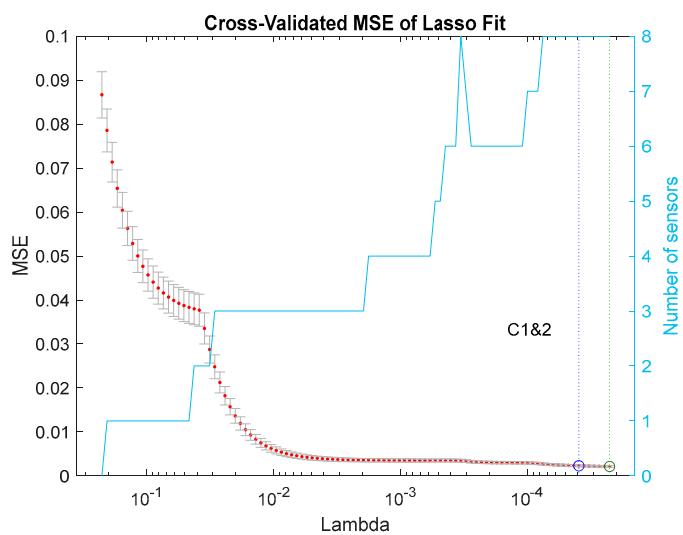
a)



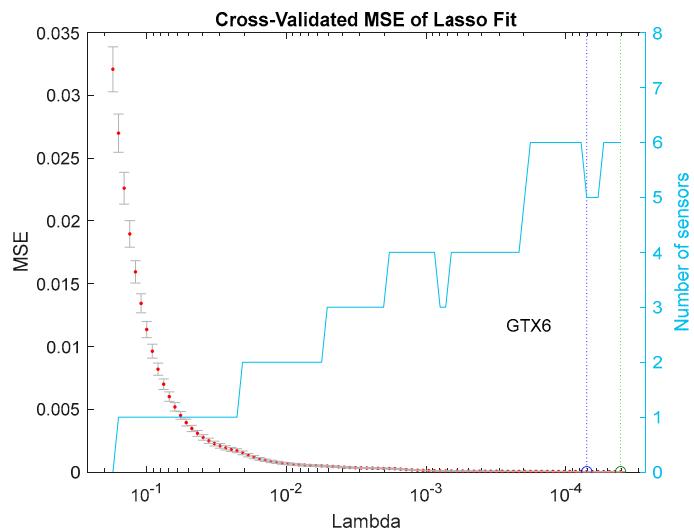
b)



c)



d)



e)

