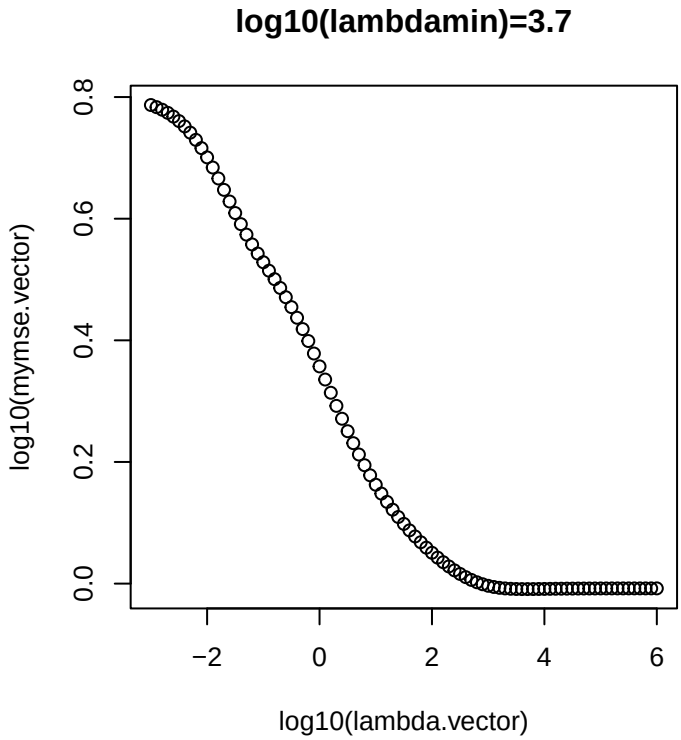
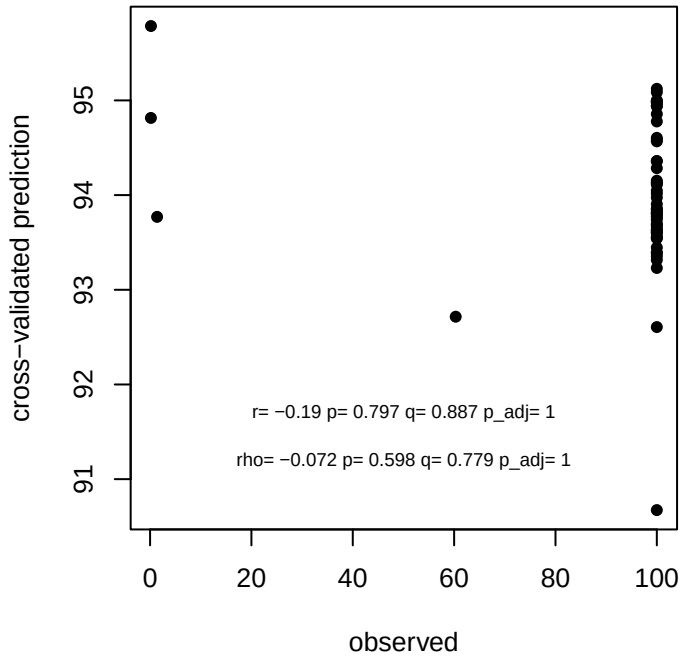
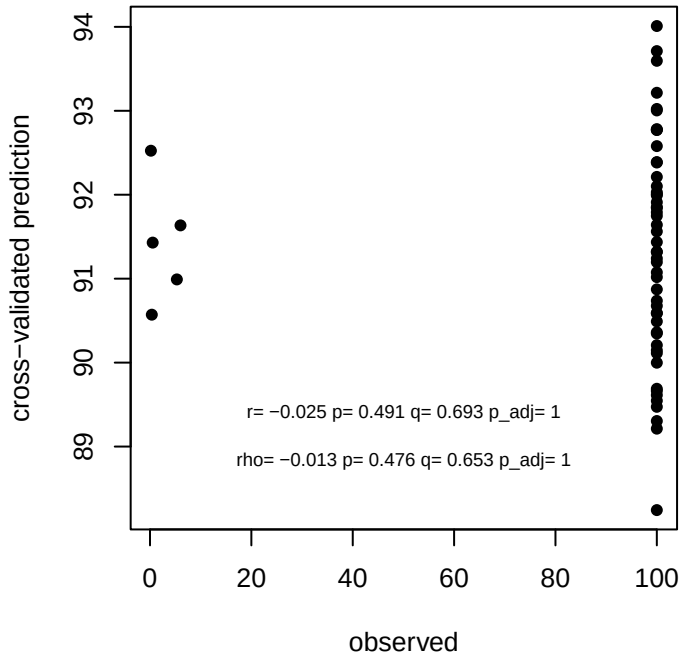
Figure S7: Correlation plots for the predicted bioactivity using Saagar descriptors. Each plot represents a cell-specific phenotype and reports the observed in relation to the cross-validation predictions and the corresponding correlation coefficients.


log10(lambdamin)=3.7
log10(mymse.vector)
0.0
0.2
0.4
0.6
0.8
−2
0
2
4
6
log10(lambda.vector)

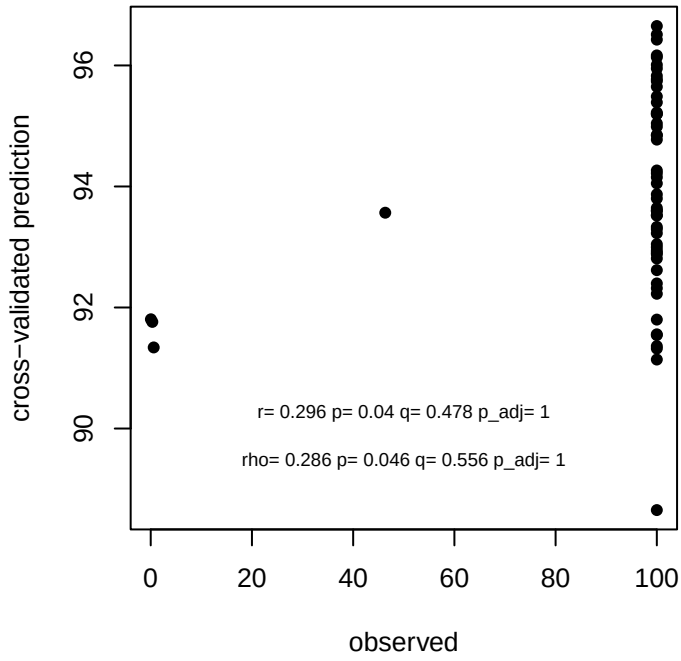
CARDIO_90min_qtprolongation



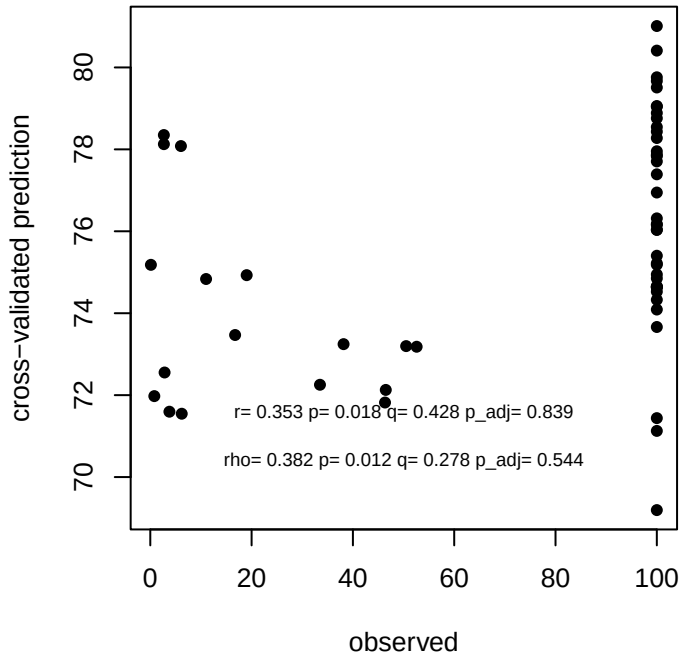
CARDIO_90min_totalcells

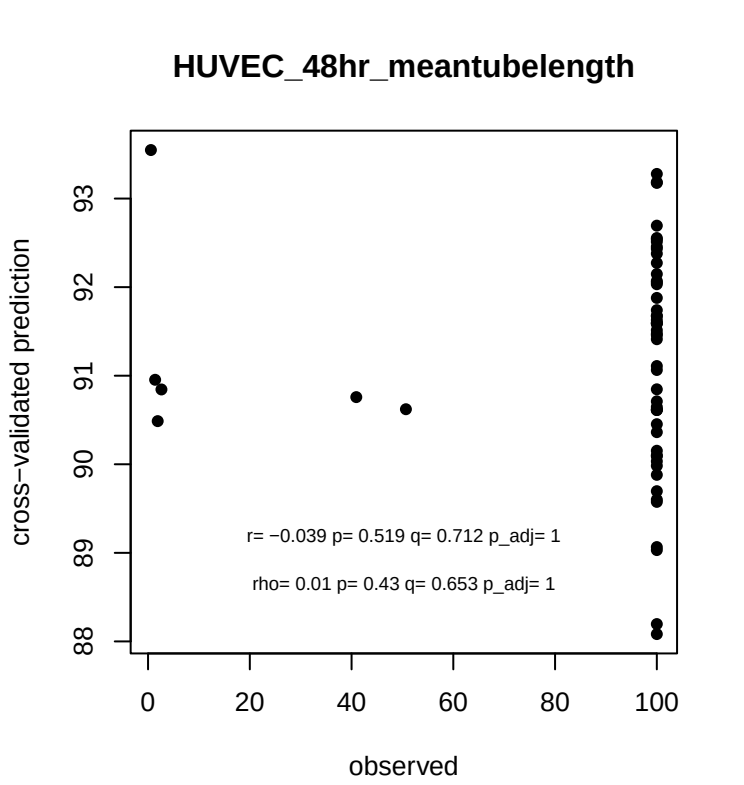


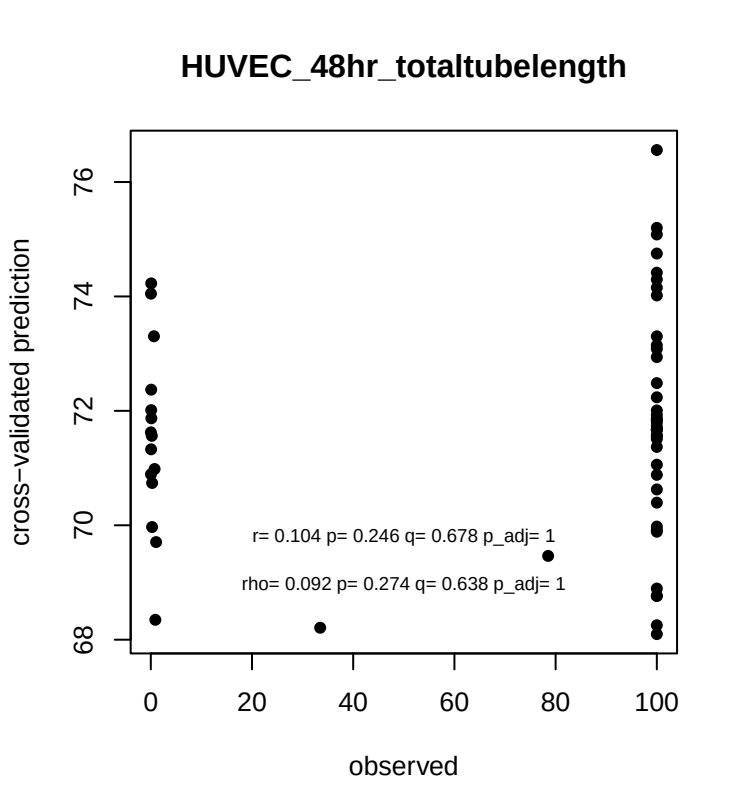
CARDIO_90min_positivechronotrope

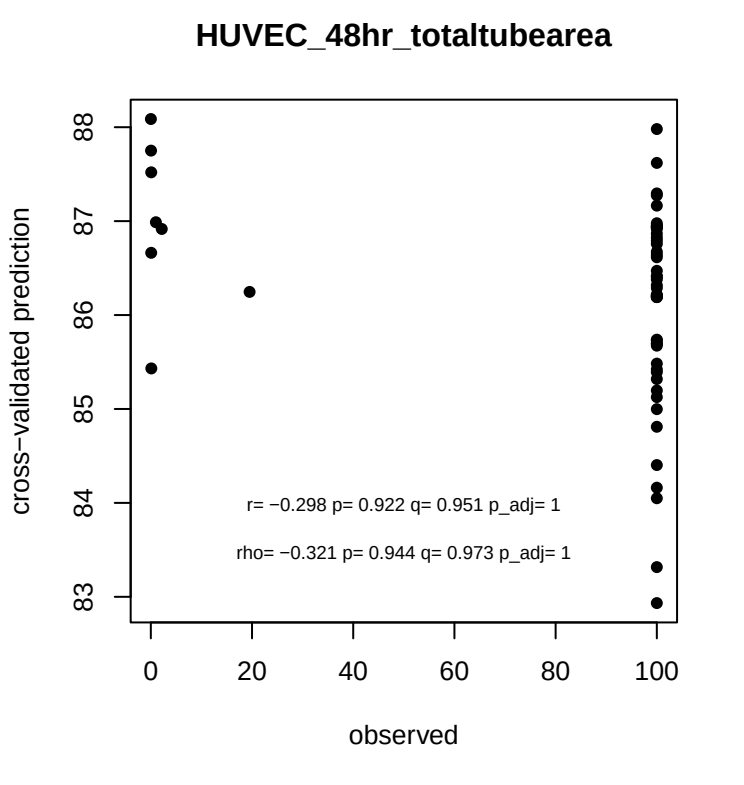


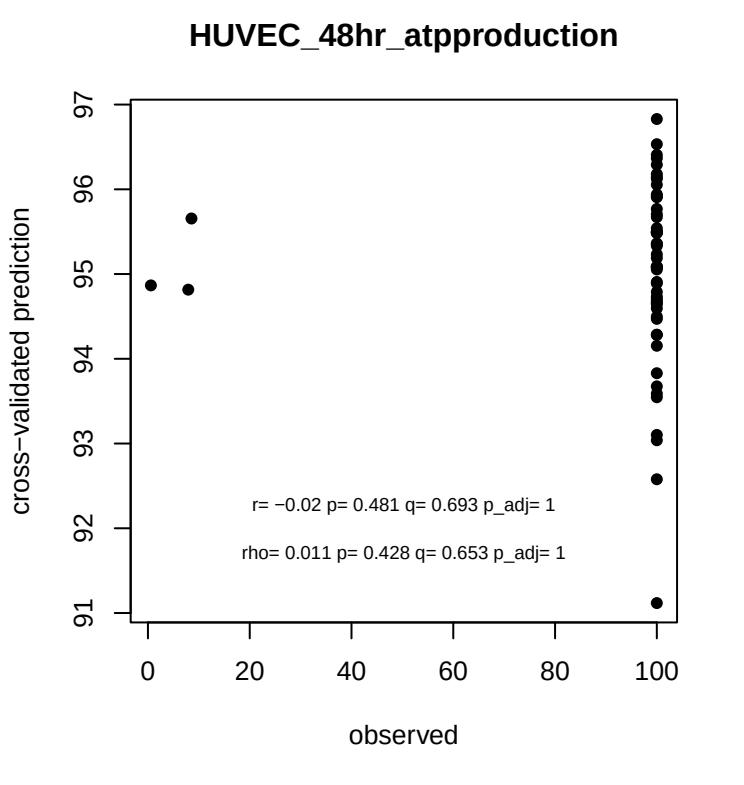
CARDIO_90min_negativechronotrope

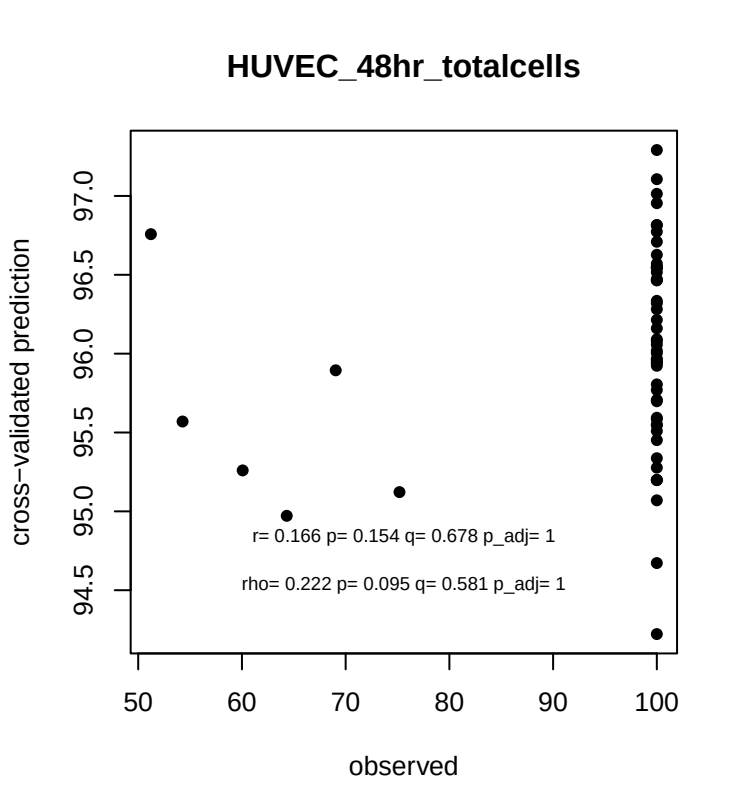


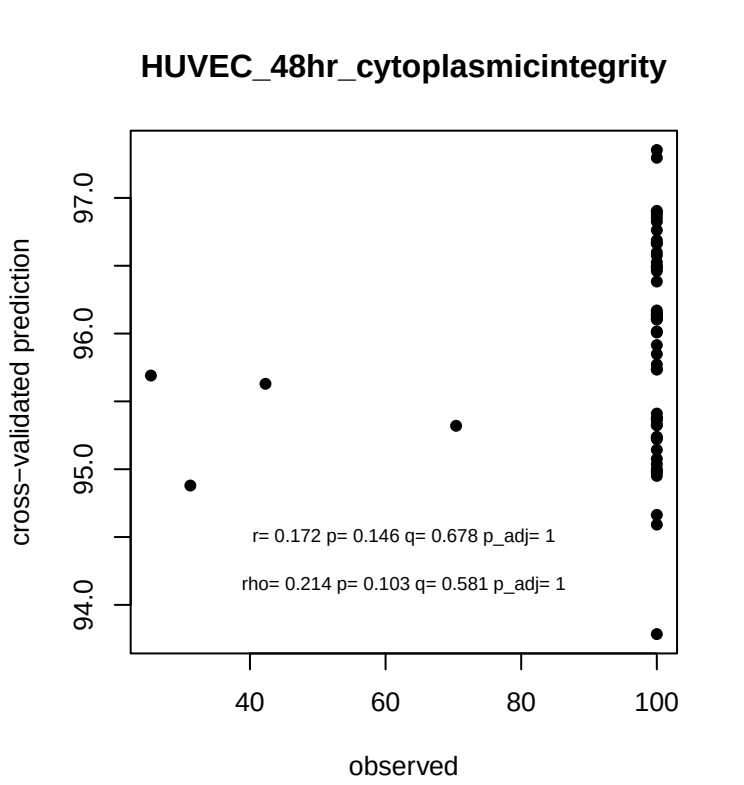

HUVEC_48hr_meantubelength
cross−validated prediction
observed
r= −0.039 p= 0.519 q= 0.712 p_adj= 1
rho= 0.01 p= 0.43 q= 0.653 p_adj= 1

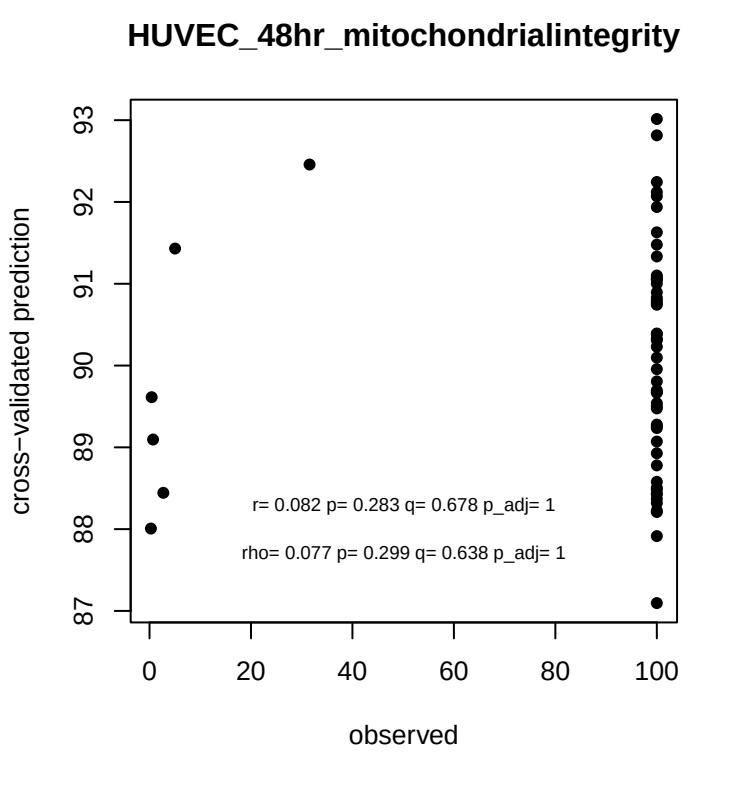

HUVEC_48hr_totaltubelength
cross−validated prediction
observed
r= 0.104 p= 0.246 q= 0.678 p_adj= 1
rho= 0.092 p= 0.274 q= 0.638 p_adj= 1

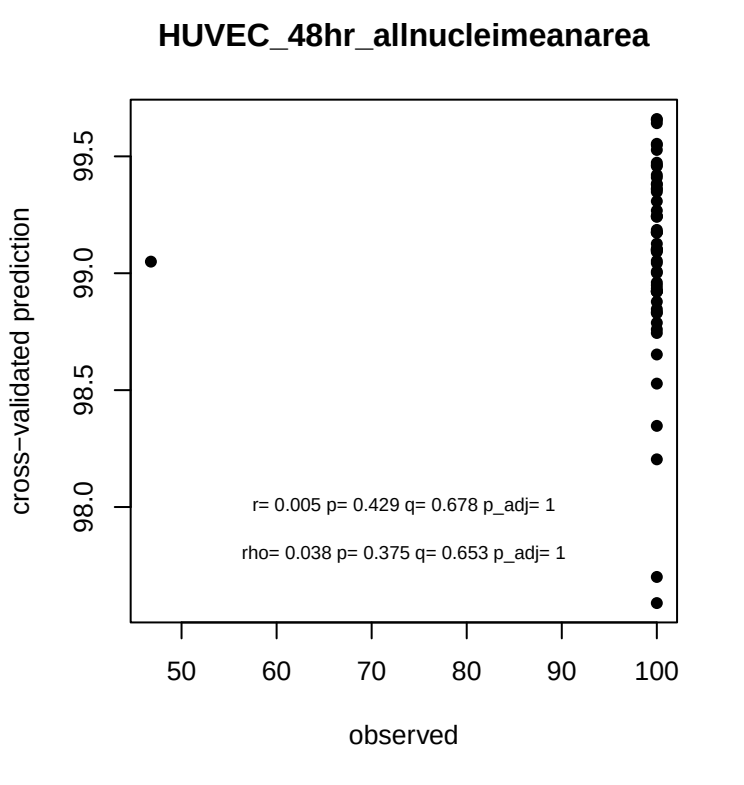

HUVEC_48hr_totaltubearea
cross−validated prediction
observed
r= −0.298 p= 0.922 q= 0.951 p_adj= 1
rho= −0.321 p= 0.944 q= 0.973 p_adj= 1

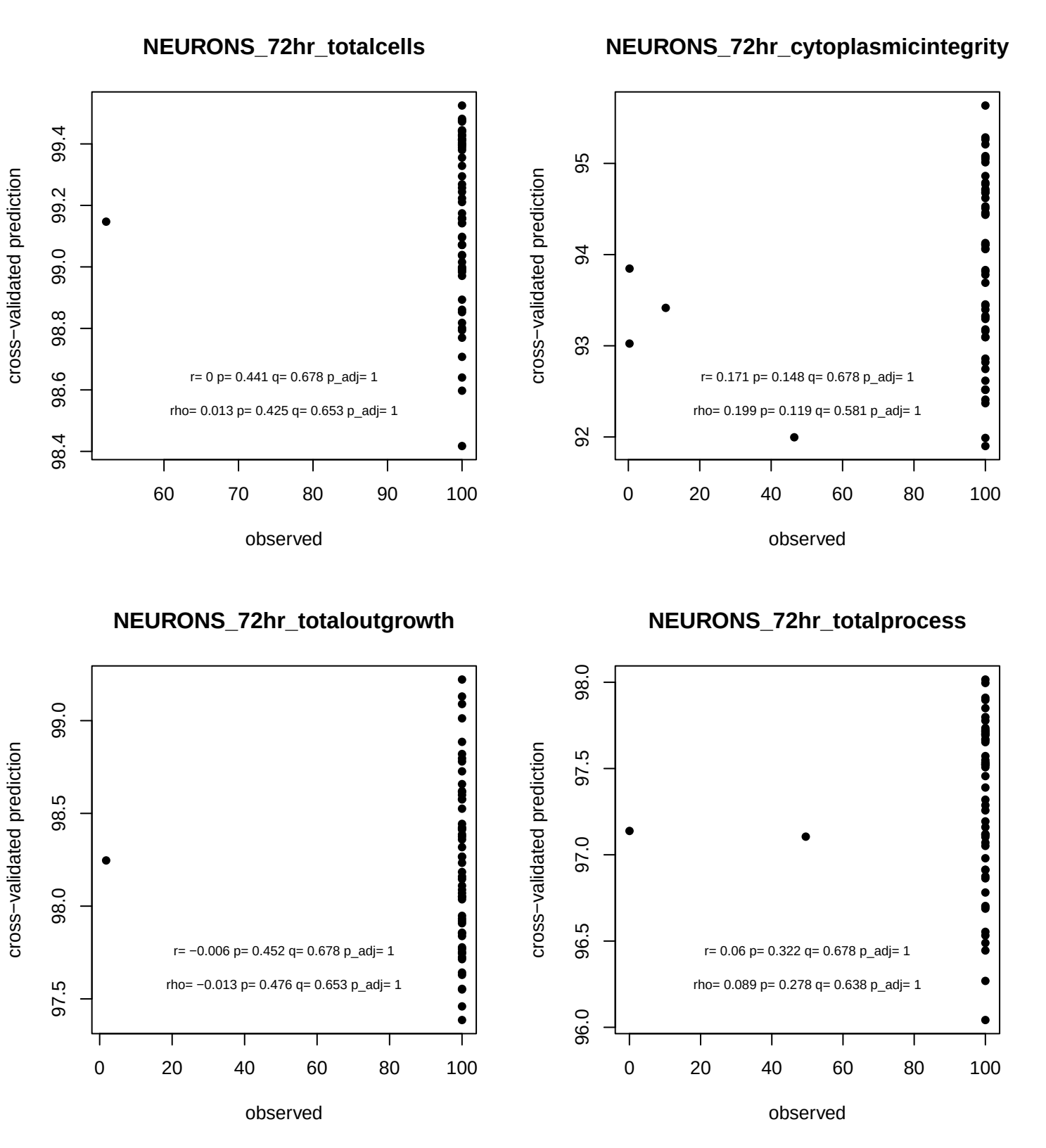

HUVEC_48hr_atpproduction
cross−validated prediction
observed
r= −0.02 p= 0.481 q= 0.693 p_adj= 1
rho= 0.011 p= 0.428 q= 0.653 p_adj= 1


HUVEC_48hr_totalcells
cross−validated prediction
observed
r= 0.166 p= 0.154 q= 0.678 p_adj= 1
rho= 0.222 p= 0.095 q= 0.581 p_adj= 1

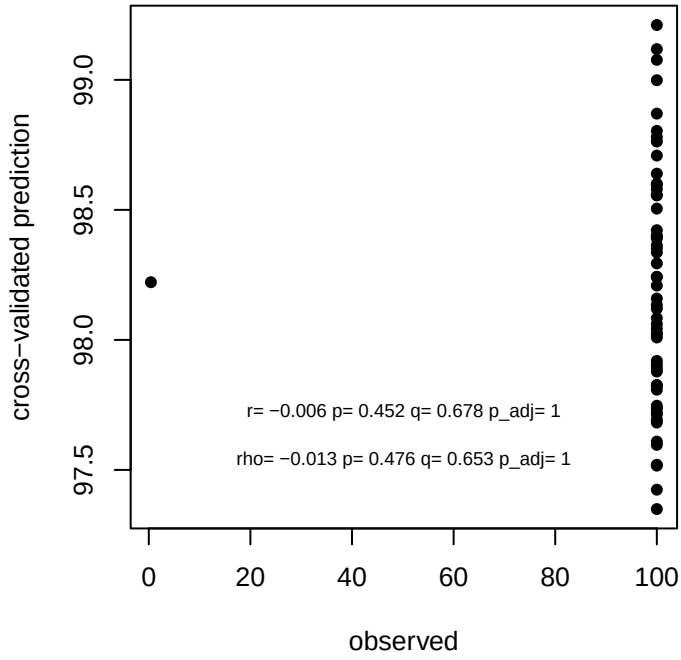

HUVEC_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= 0.172 p= 0.146 q= 0.678 p_adj= 1
rho= 0.214 p= 0.103 q= 0.581 p_adj= 1


HUVEC_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= 0.082 p= 0.283 q= 0.678 p_adj= 1
rho= 0.077 p= 0.299 q= 0.638 p_adj= 1

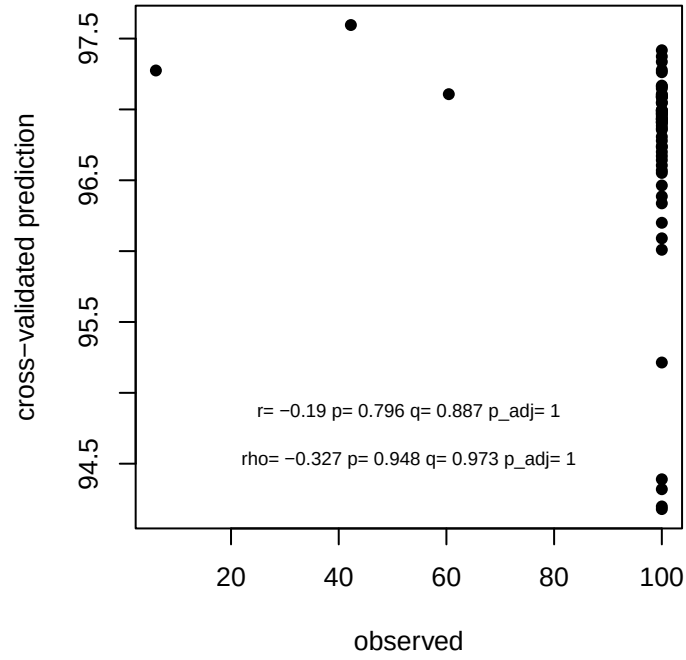

HUVEC_48hr_allnucleimeanarea
cross−validated prediction
observed
r= 0.005 p= 0.429 q= 0.678 p_adj= 1
rho= 0.038 p= 0.375 q= 0.653 p_adj= 1


NEURONS_72hr_totalcells
cross−validated prediction
observed
r= 0 p= 0.441 q= 0.678 p_adj= 1
rho= 0.013 p= 0.425 q= 0.653 p_adj= 1
NEURONS_72hr_cytoplasmicintegrity
cross−validated prediction
observed
r= 0.171 p= 0.148 q= 0.678 p_adj= 1
rho= 0.199 p= 0.119 q= 0.581 p_adj= 1
NEURONS_72hr_totaloutgrowth
cross−validated prediction
observed
r= −0.006 p= 0.452 q= 0.678 p_adj= 1
rho= −0.013 p= 0.476 q= 0.653 p_adj= 1
NEURONS_72hr_totalprocess
cross−validated prediction
observed
r= 0.06 p= 0.322 q= 0.678 p_adj= 1
rho= 0.089 p= 0.278 q= 0.638 p_adj= 1

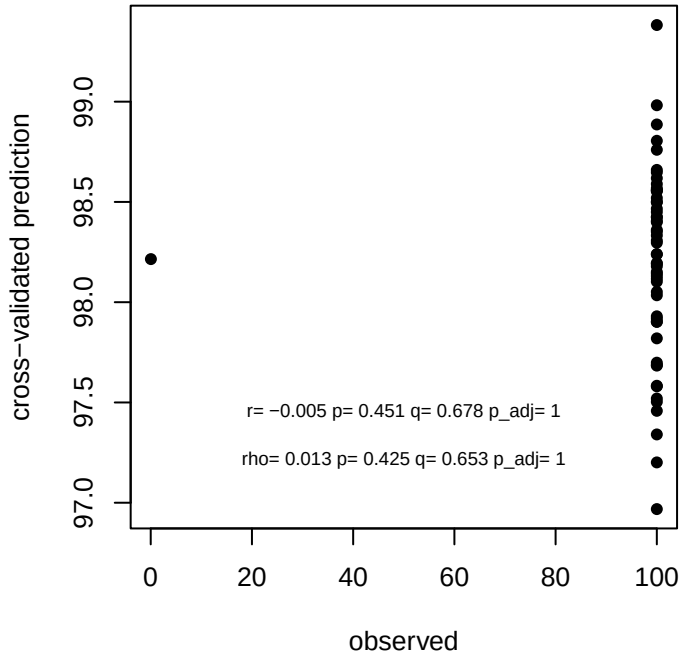
NEURONS_72hr_totalbranches



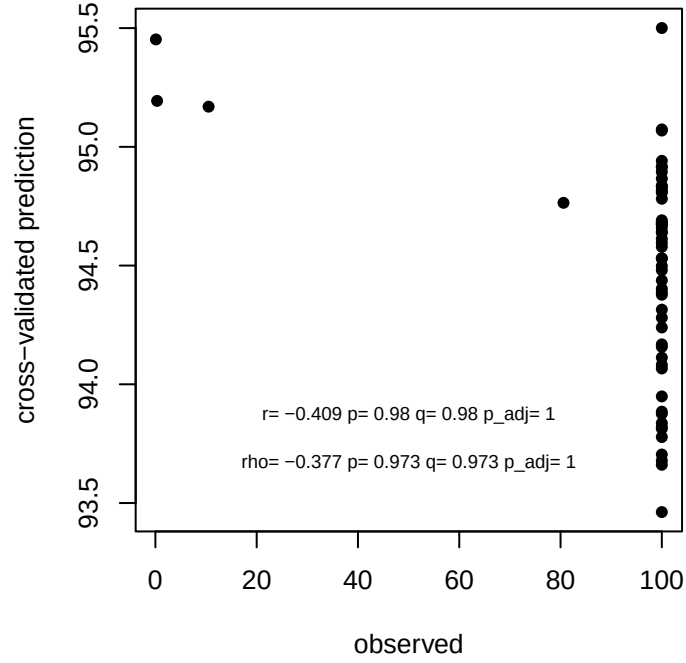
NEURONS_72hr_cellsiwithsignificantgrowth



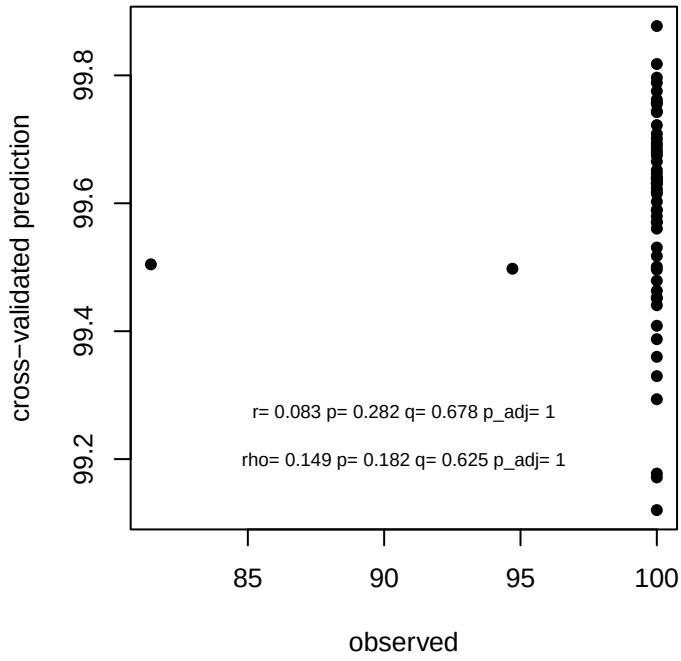
HEPATOCYTES_48hr_totalgranulearea



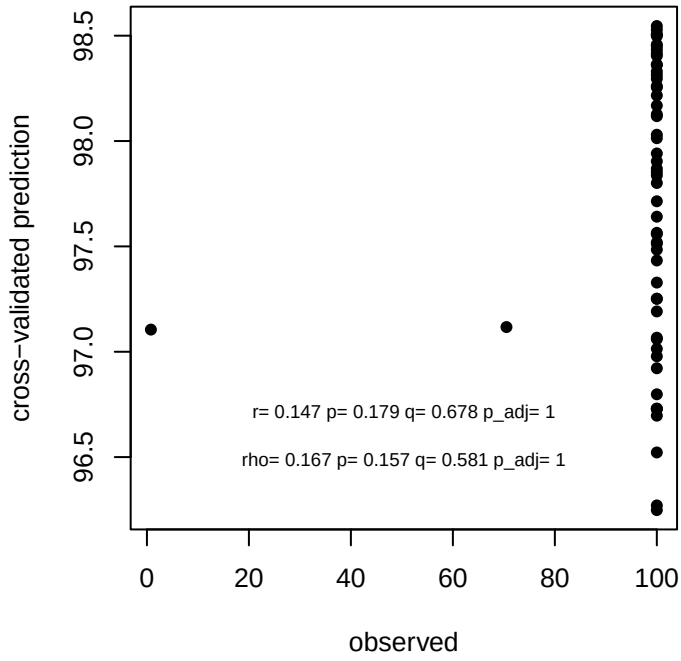
HEPATOCYTES_48hr_granularity



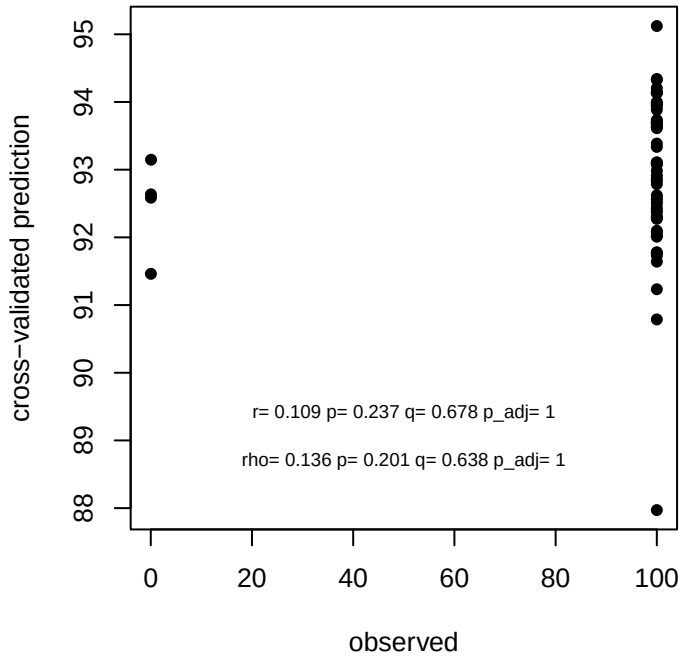
HEPATOCYTES_48hr_totalcells



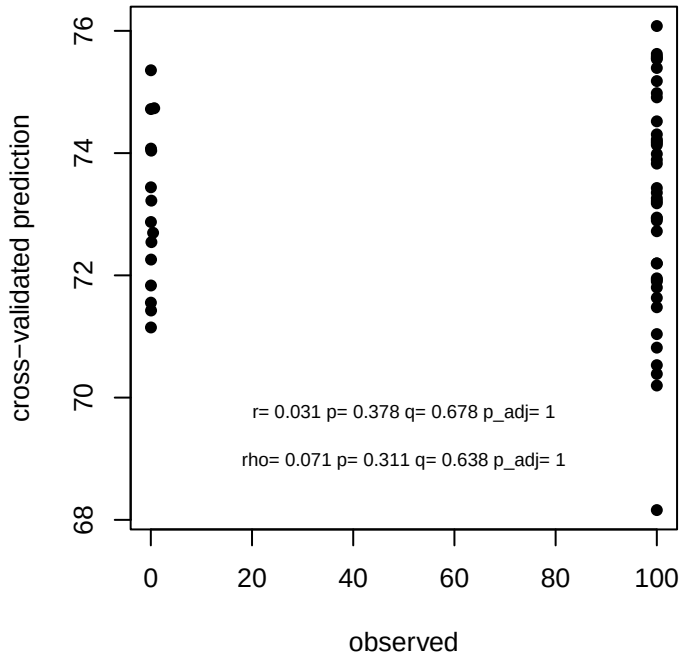
HEPATOCYTES_48hr_allcellsmeanarea



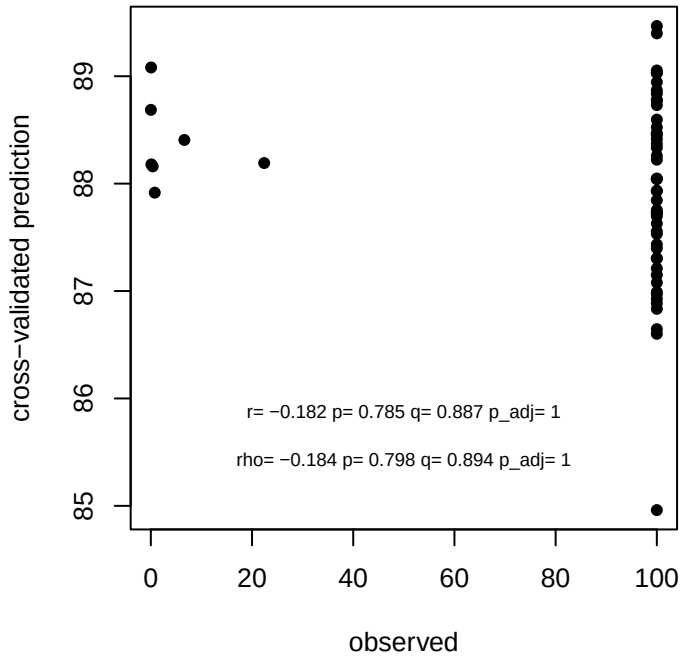
HEPATOCYTES_48hr_cytoplasmicintegrity



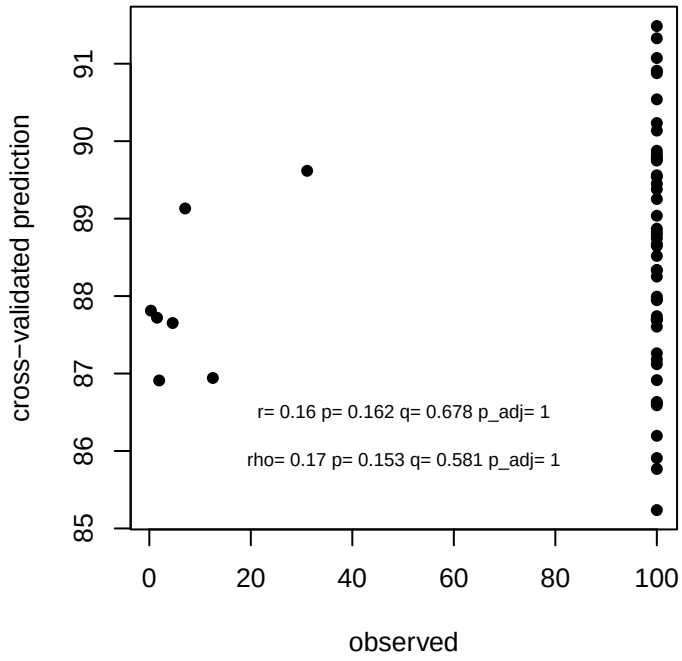
HEPATOCYTES_48hr_mitochondrialintegrity



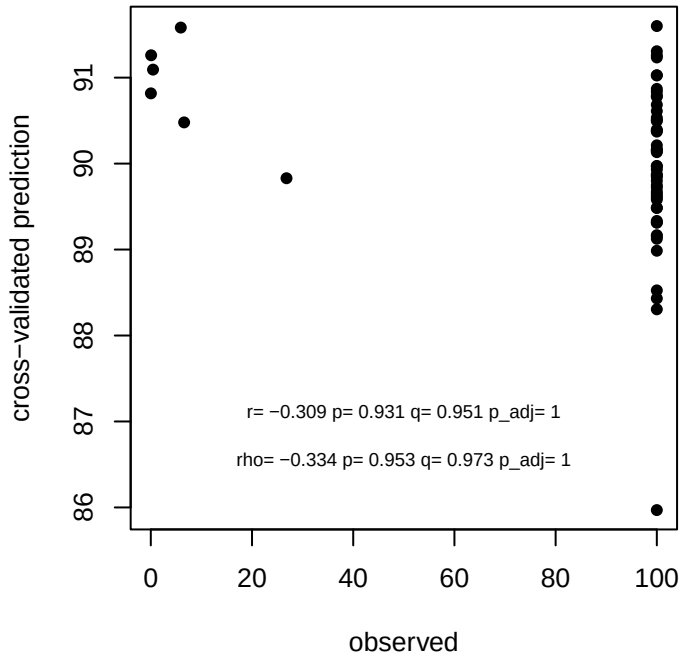
HEPATOCYTES_48hr_mitochondrialintensity



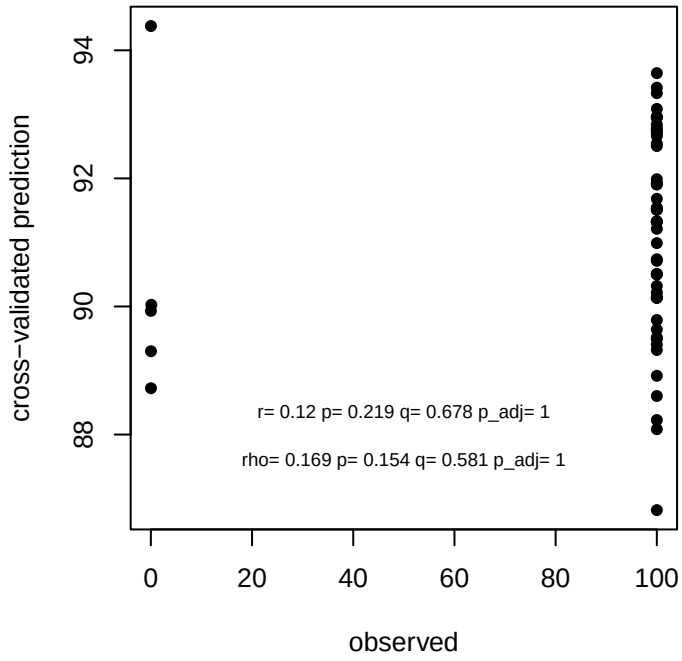
HEPATOCYTES_48hr_nucleiintensity

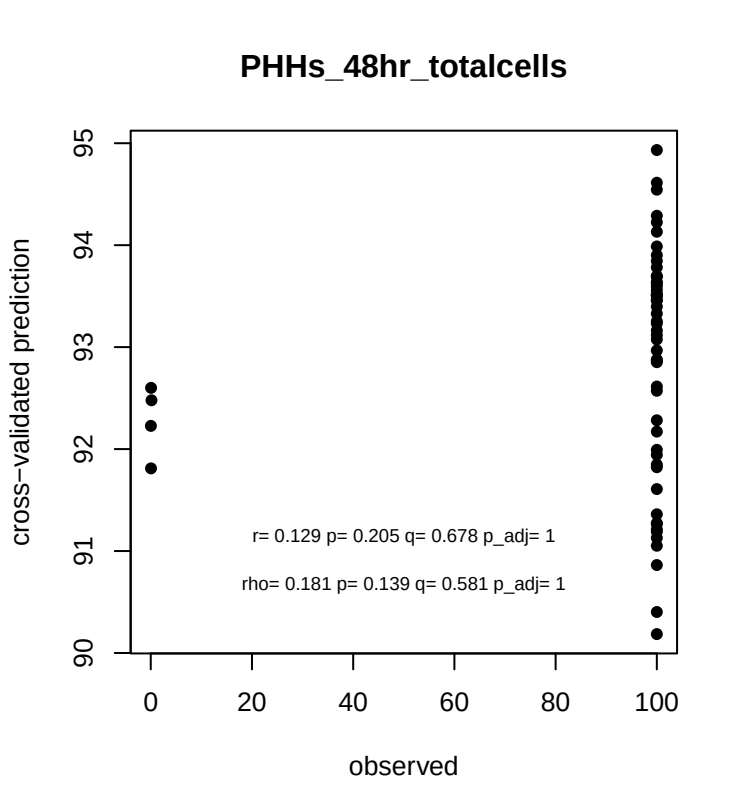


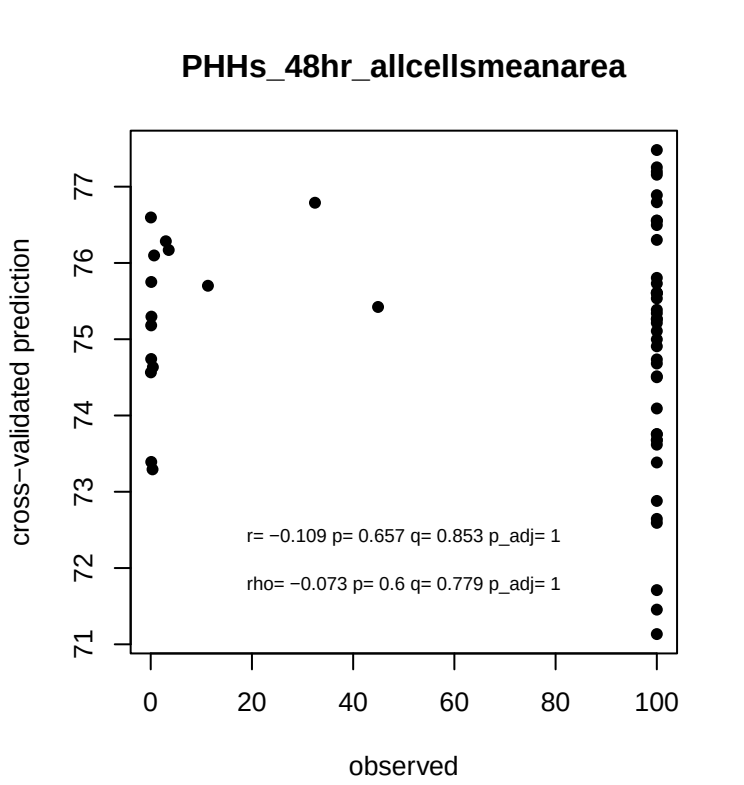
PHHs_48hr_totalgranulearea

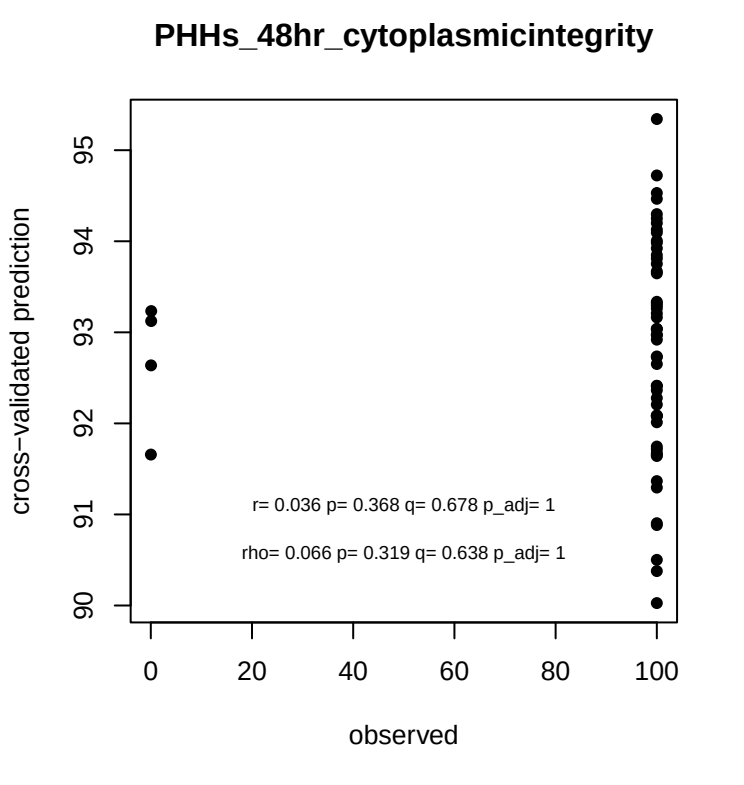


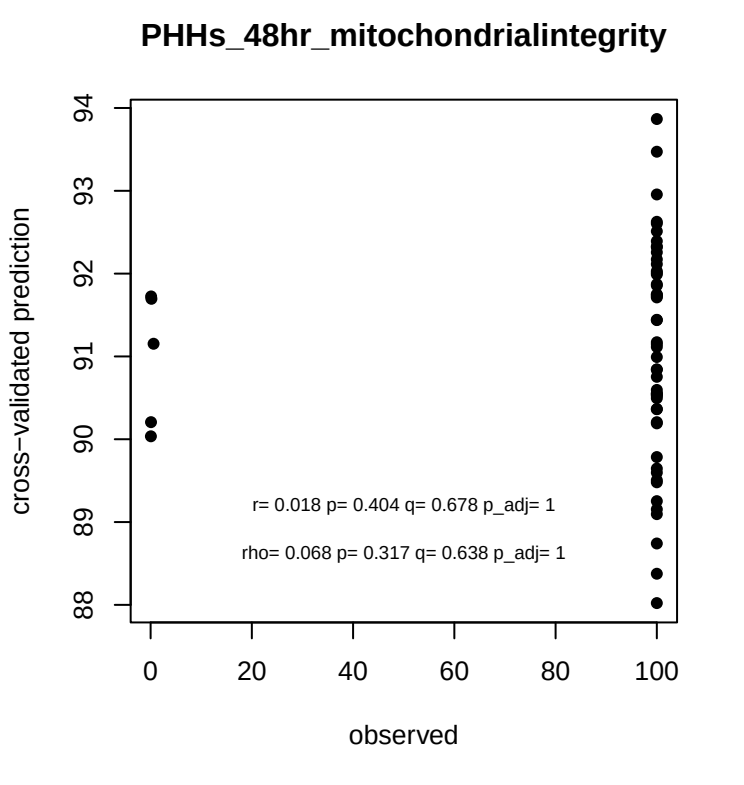
PHHs_48hr_granularity

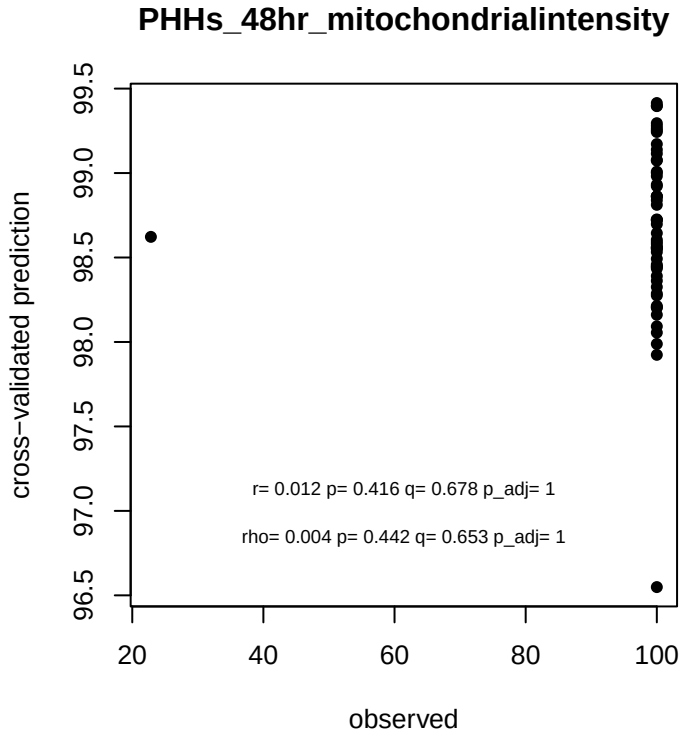


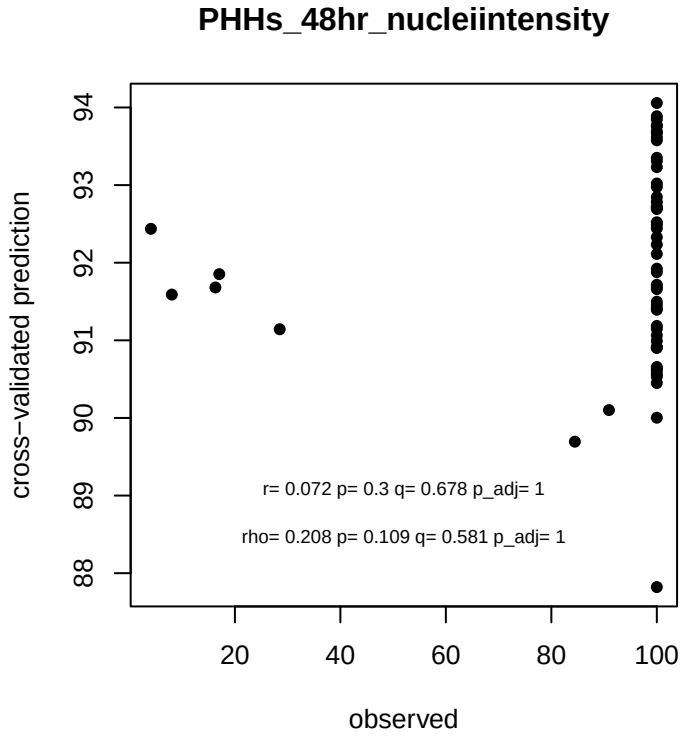

PHHs_48hr_totalcells
cross−validated prediction
observed
r= 0.129 p= 0.205 q= 0.678 p_adj= 1
rho= 0.181 p= 0.139 q= 0.581 p_adj= 1

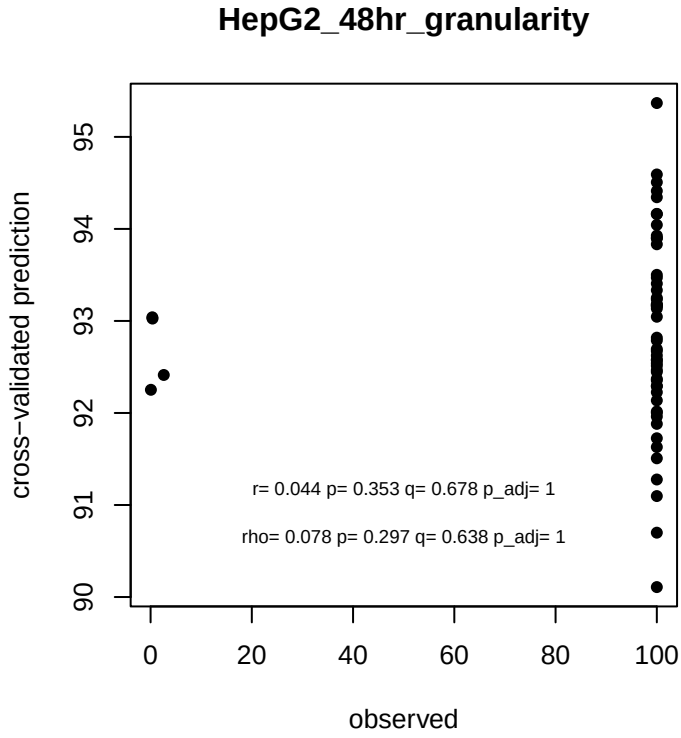

PHHs_48hr_allcellsmeanarea
cross−validated prediction
observed
r= −0.109 p= 0.657 q= 0.853 p_adj= 1
rho= −0.073 p= 0.6 q= 0.779 p_adj= 1

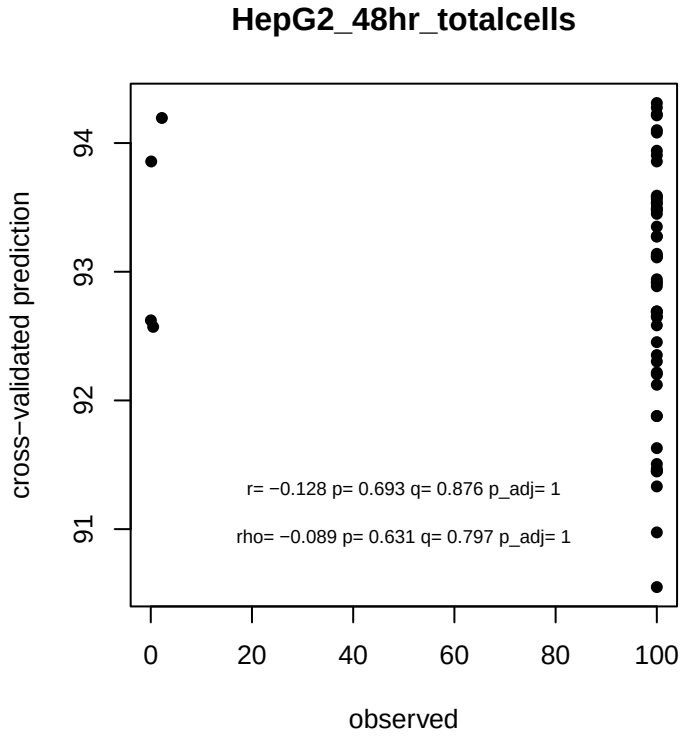

PHHs_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= 0.036 p= 0.368 q= 0.678 p_adj= 1
rho= 0.066 p= 0.319 q= 0.638 p_adj= 1

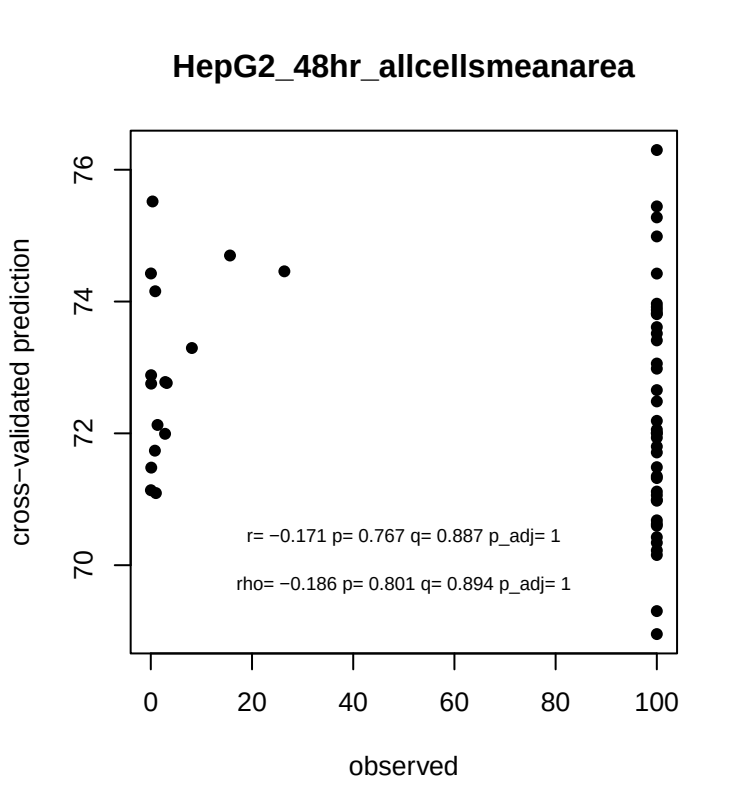

PHHs_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= 0.018 p= 0.404 q= 0.678 p_adj= 1
rho= 0.068 p= 0.317 q= 0.638 p_adj= 1

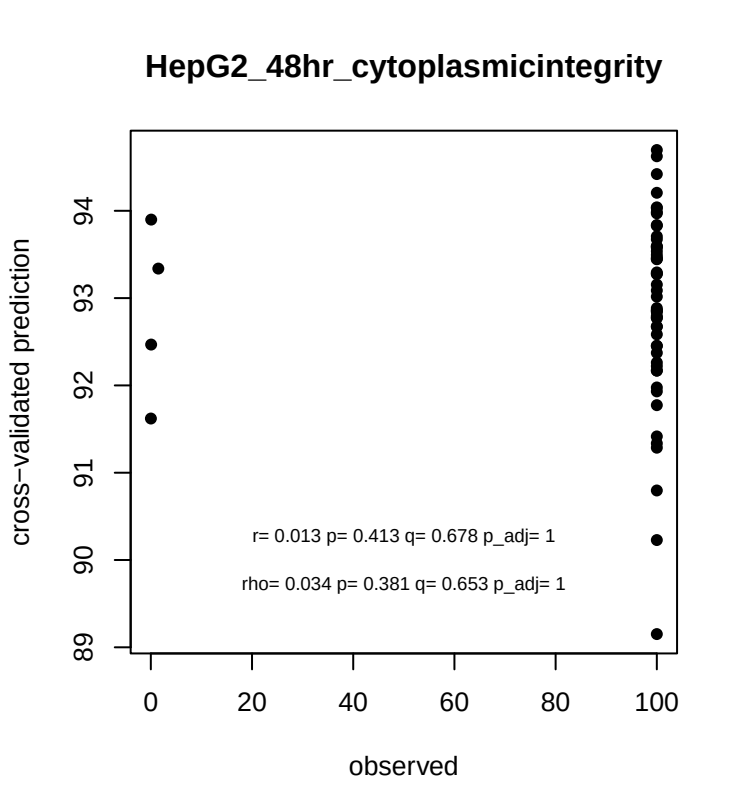

PHHs_48hr_mitochondrialintensity
cross−validated prediction
observed
r= 0.012 p= 0.416 q= 0.678 p_adj= 1
rho= 0.004 p= 0.442 q= 0.653 p_adj= 1

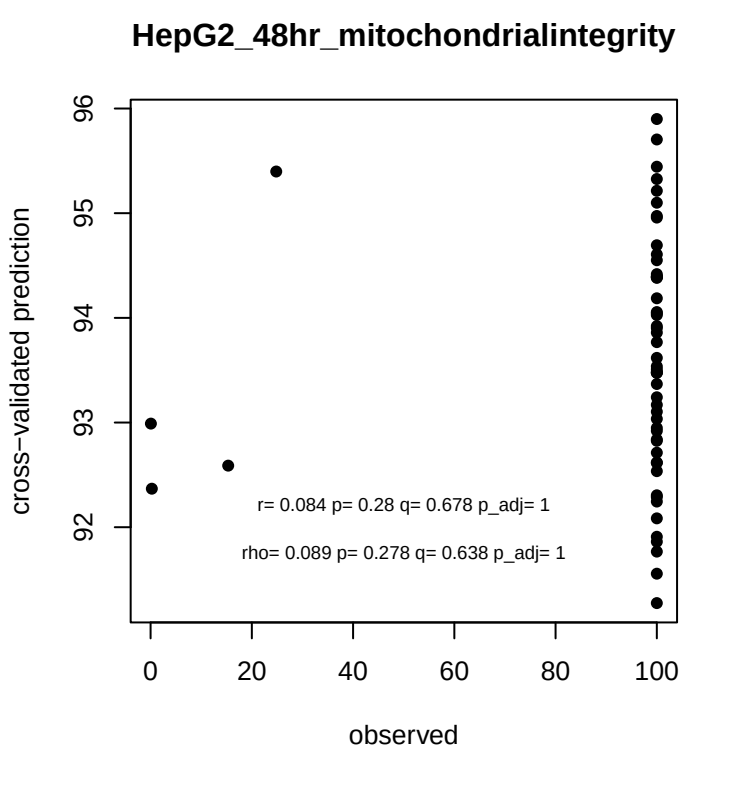

PHHs_48hr_nucleiintensity
cross−validated prediction
observed
r= 0.072 p= 0.3 q= 0.678 p_adj= 1
rho= 0.208 p= 0.109 q= 0.581 p_adj= 1

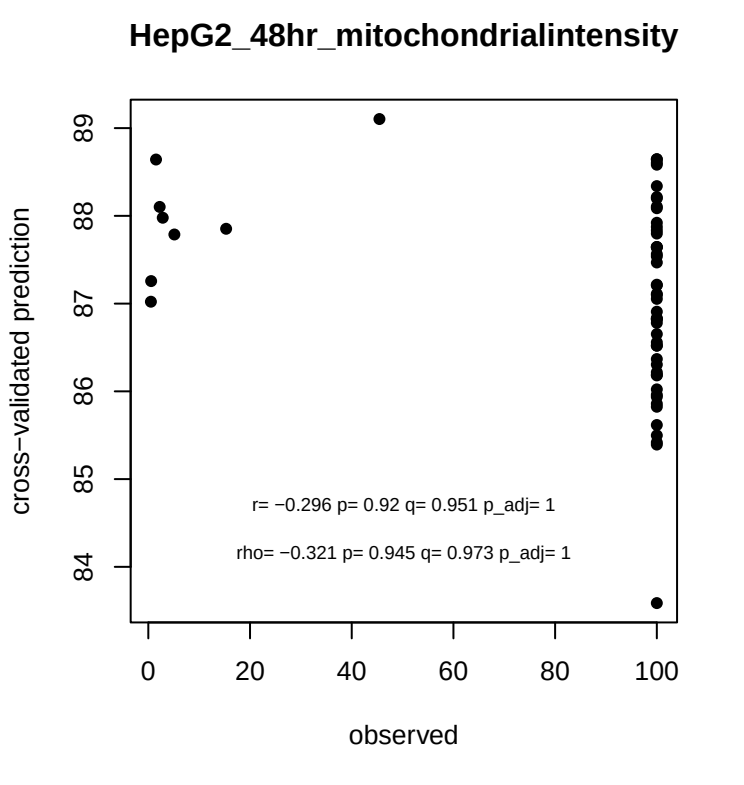

HepG2_48hr_granularity
cross−validated prediction
observed
r= 0.044 p= 0.353 q= 0.678 p_adj= 1
rho= 0.078 p= 0.297 q= 0.638 p_adj= 1

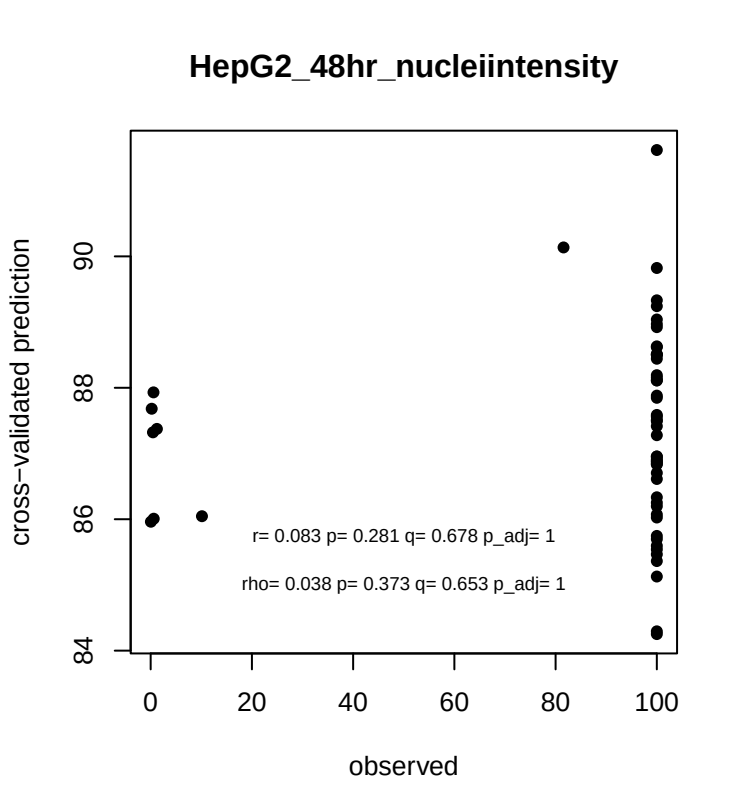

HepG2_48hr_totalcells
cross−validated prediction
observed
r= −0.128 p= 0.693 q= 0.876 p_adj= 1
rho= −0.089 p= 0.631 q= 0.797 p_adj= 1

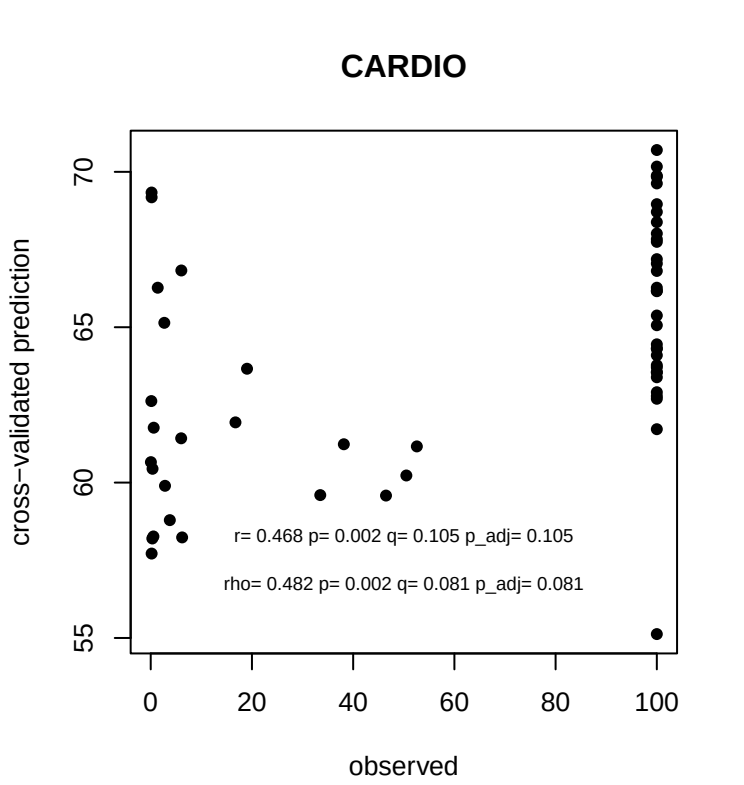

HepG2_48hr_allcellsmeanarea
cross−validated prediction
observed
r= −0.171 p= 0.767 q= 0.887 p_adj= 1
rho= −0.186 p= 0.801 q= 0.894 p_adj= 1

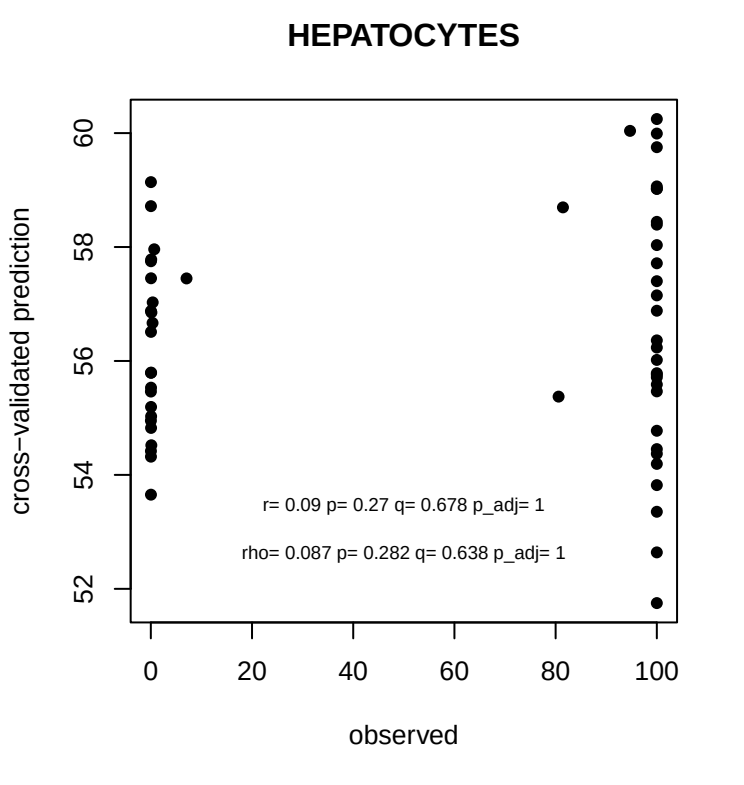

HepG2_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= 0.013 p= 0.413 q= 0.678 p_adj= 1
rho= 0.034 p= 0.381 q= 0.653 p_adj= 1

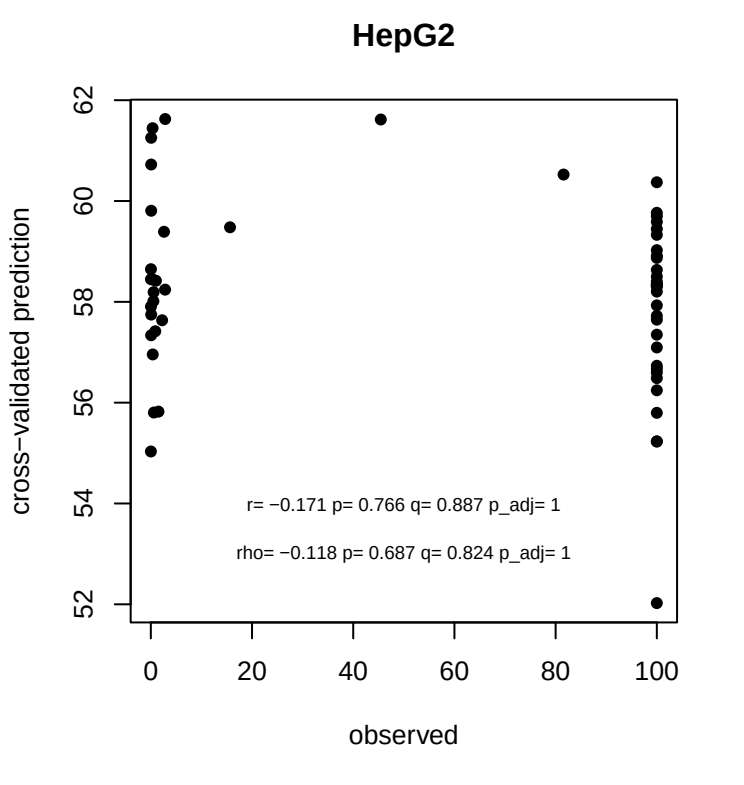

HepG2_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= 0.084 p= 0.28 q= 0.678 p_adj= 1
rho= 0.089 p= 0.278 q= 0.638 p_adj= 1

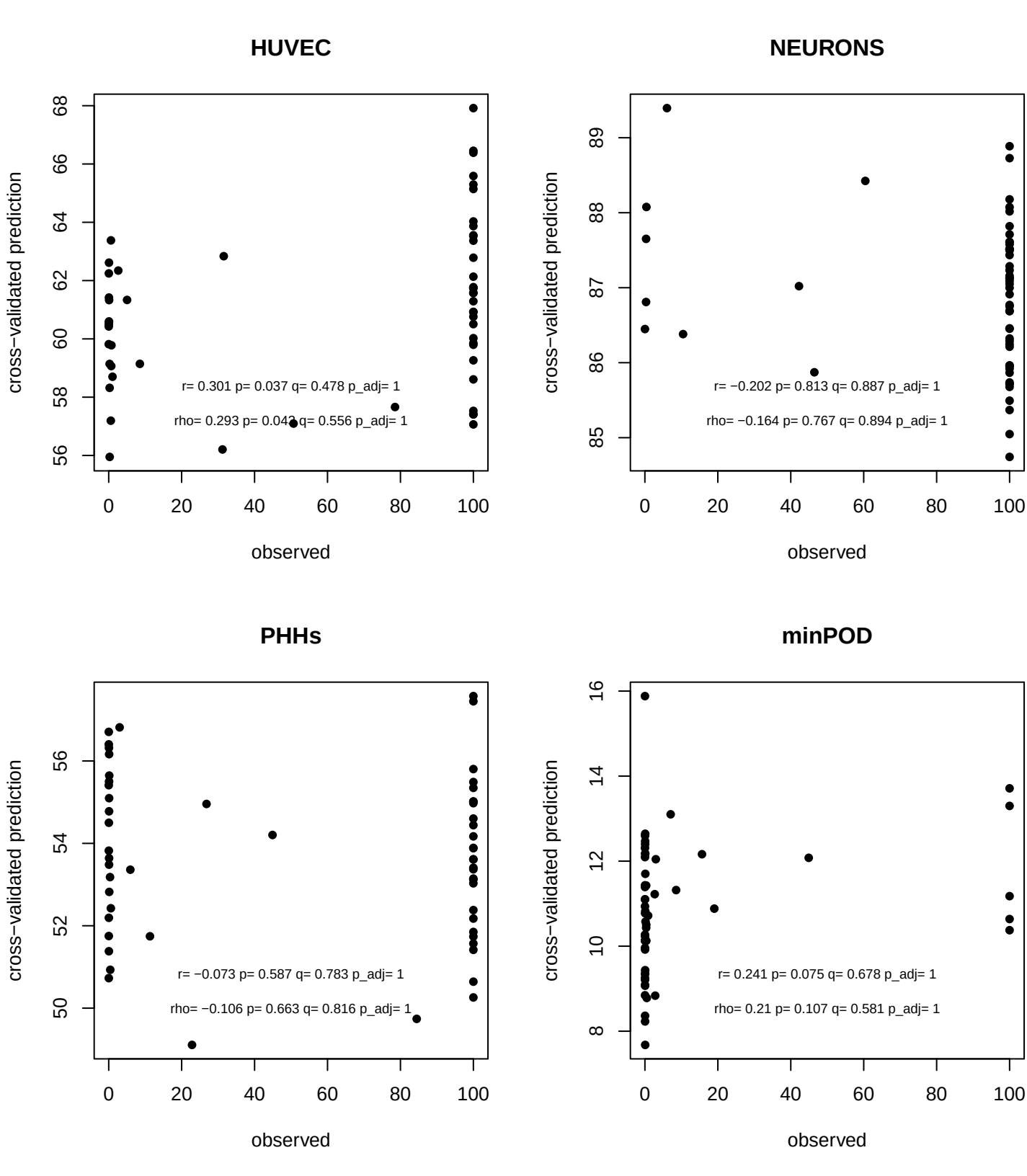

HepG2_48hr_mitochondrialintensity
cross−validated prediction
observed
r= −0.296 p= 0.92 q= 0.951 p_adj= 1
rho= −0.321 p= 0.945 q= 0.973 p_adj= 1


HepG2_48hr_nucleiintensity
cross−validated prediction
observed
r= 0.083 p= 0.281 q= 0.678 p_adj= 1
rho= 0.038 p= 0.373 q= 0.653 p_adj= 1


CARDIO
cross−validated prediction
observed
r= 0.468 p= 0.002 q= 0.105 p_adj= 0.105
rho= 0.482 p= 0.002 q= 0.081 p_adj= 0.081


HEPATOCYTES
cross−validated prediction
observed
r= 0.09 p= 0.27 q= 0.678 p_adj= 1
rho= 0.087 p= 0.282 q= 0.638 p_adj= 1


HepG2
cross−validated prediction
observed
r= −0.171 p= 0.766 q= 0.887 p_adj= 1
rho= −0.118 p= 0.687 q= 0.824 p_adj= 1


HUVEC
cross−validated prediction
observed
r= 0.301 p= 0.037 q= 0.478 p_adj= 1
rho= 0.293 p= 0.042 q= 0.556 p_adj= 1
NEURONS
cross−validated prediction
observed
r= −0.202 p= 0.813 q= 0.887 p_adj= 1
rho= −0.164 p= 0.767 q= 0.894 p_adj= 1
PHHs
cross−validated prediction
observed
r= −0.073 p= 0.587 q= 0.783 p_adj= 1
rho= −0.106 p= 0.663 q= 0.816 p_adj= 1
minPOD
cross−validated prediction
observed
r= 0.241 p= 0.075 q= 0.678 p_adj= 1
rho= 0.21 p= 0.107 q= 0.581 p_adj= 1