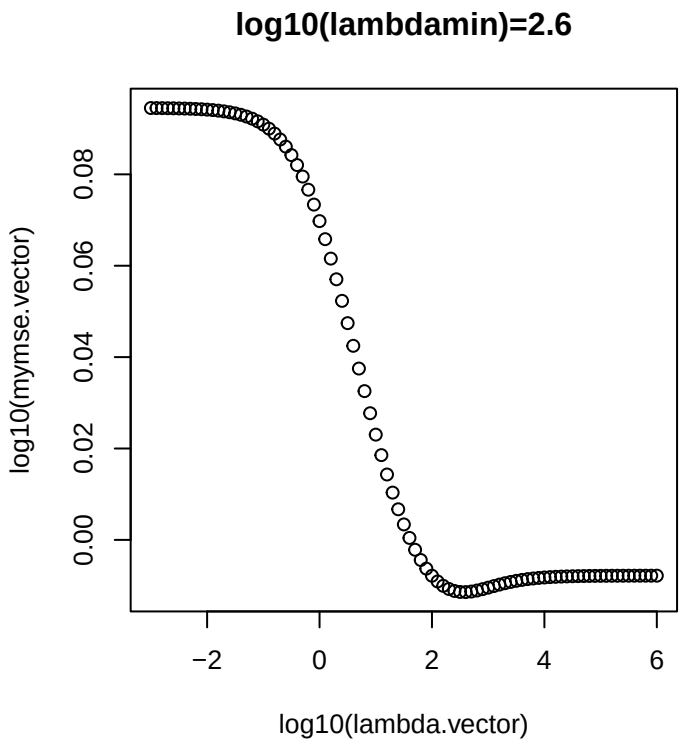
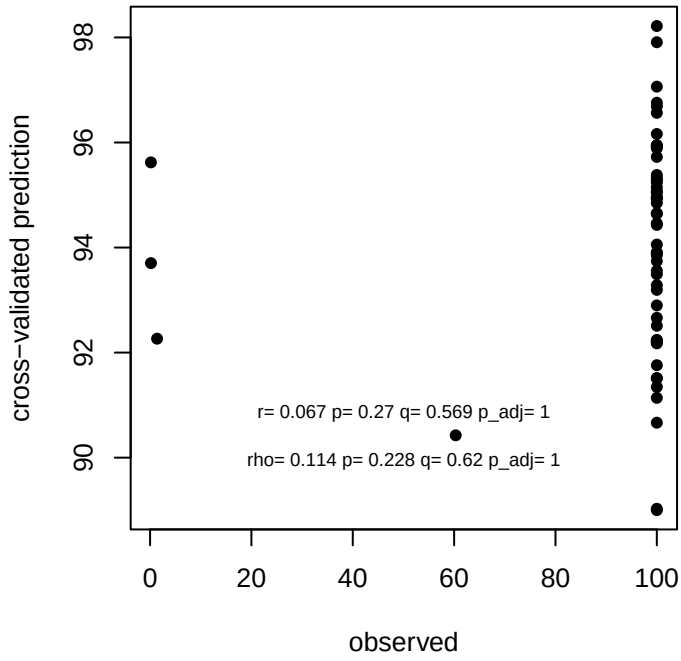
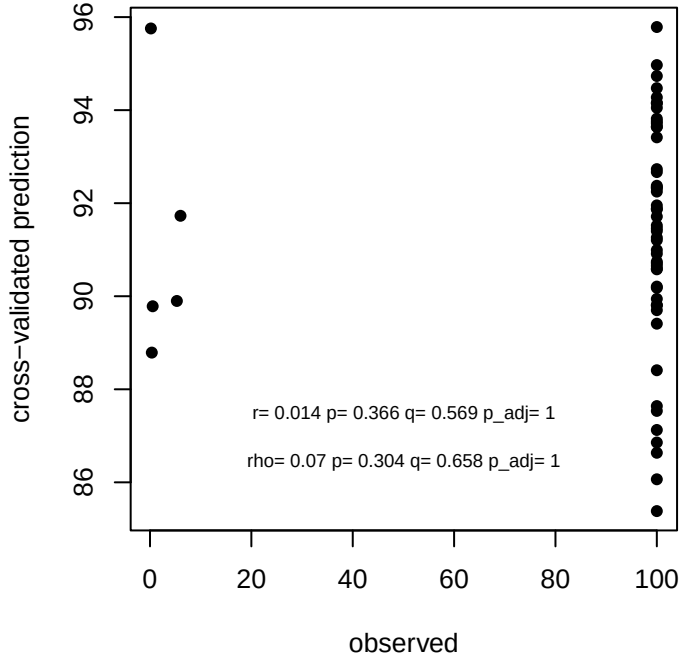
Figure S9: Correlation plots for the predicted bioactivity using the OPERA descriptors. Each plot represents a cell-specific phenotype and reports the observed in relation to the cross-validation predictions and the corresponding correlation coefficients.


log10(lambdamin)=2.6
log10(mymse.vector)
0.00
0.02
0.04
0.06
0.08
−2
0
2
4
6
log10(lambda.vector)

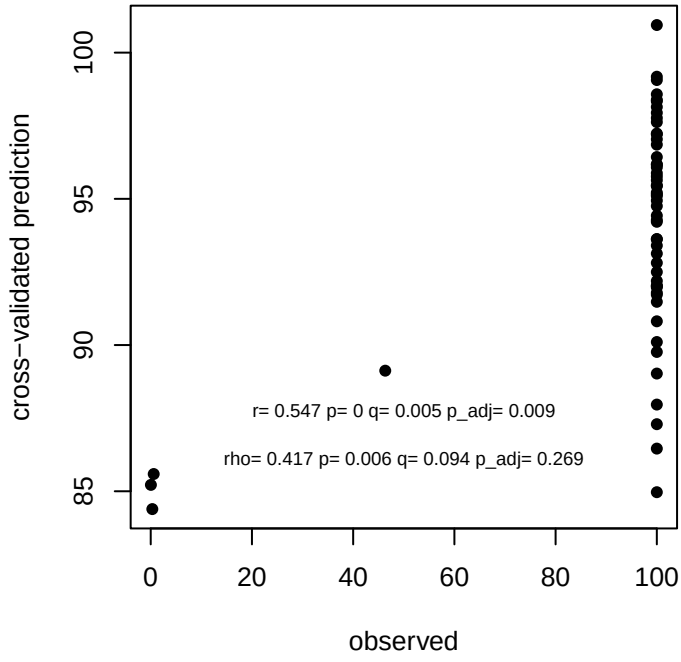
CARDIO_90min_qtprolongation



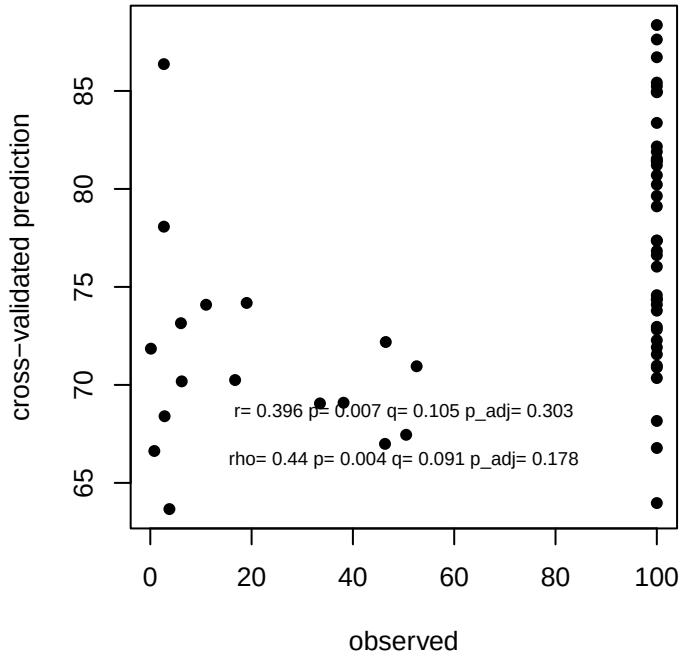
CARDIO_90min_totalcells



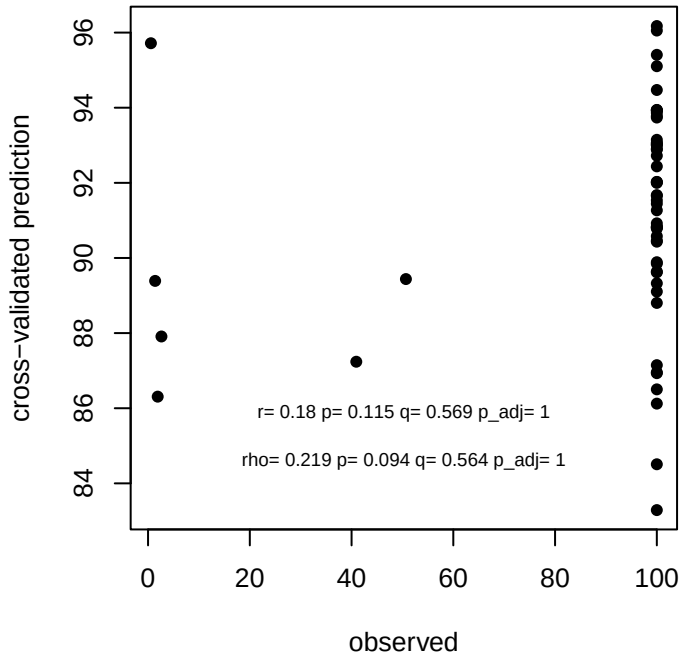
CARDIO_90min_positivechronotrope



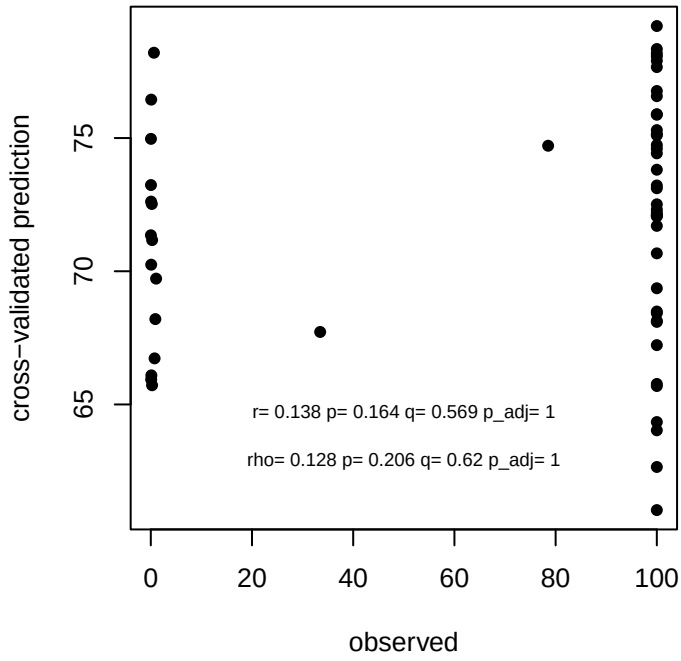
CARDIO_90min_negativechronotrope



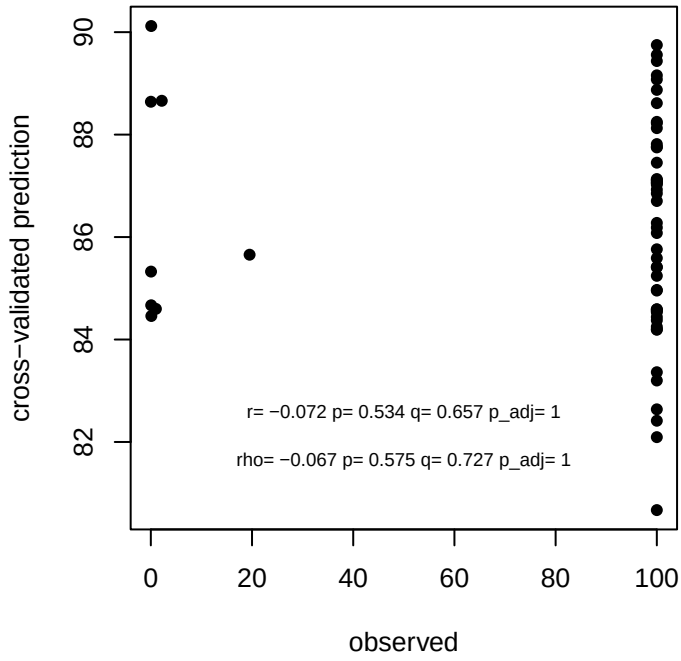
HUVEC_48hr_meantubelength



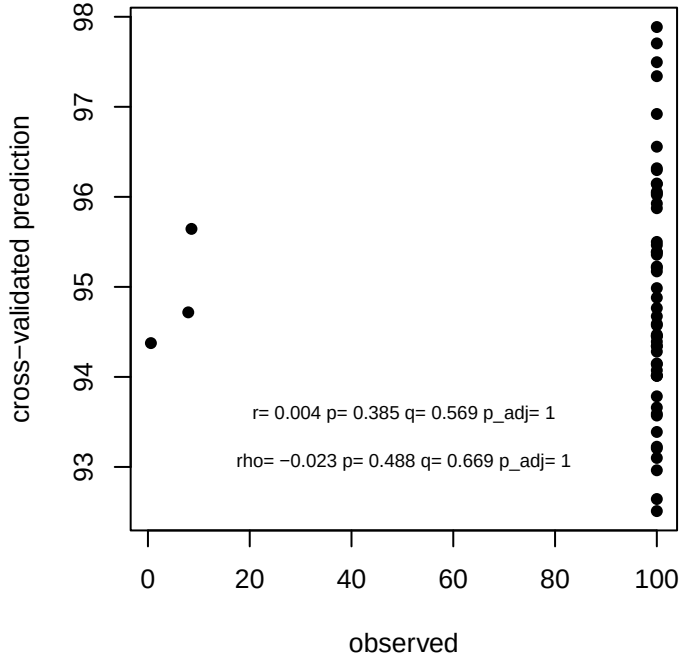
HUVEC_48hr_totaltubelength

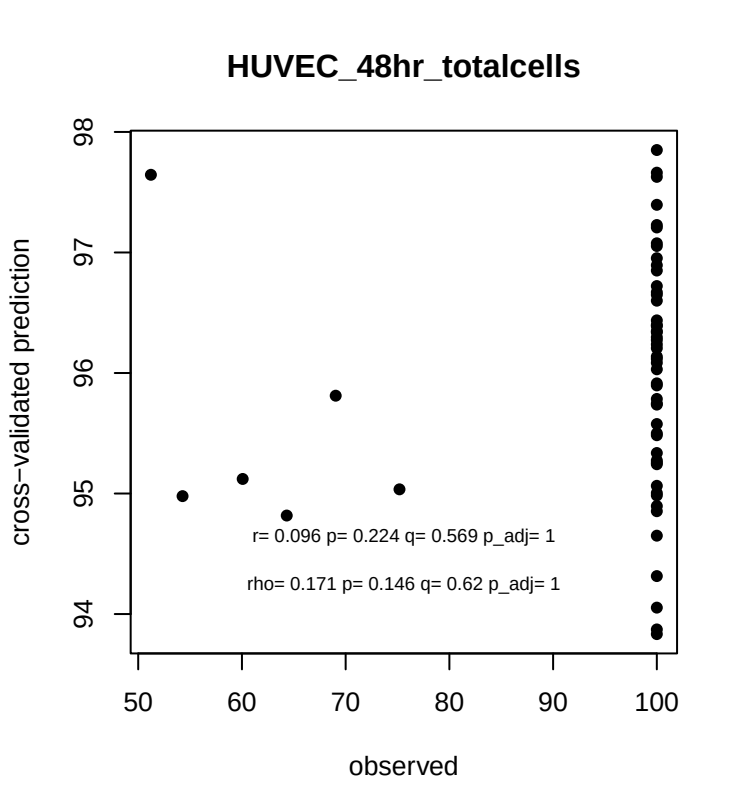


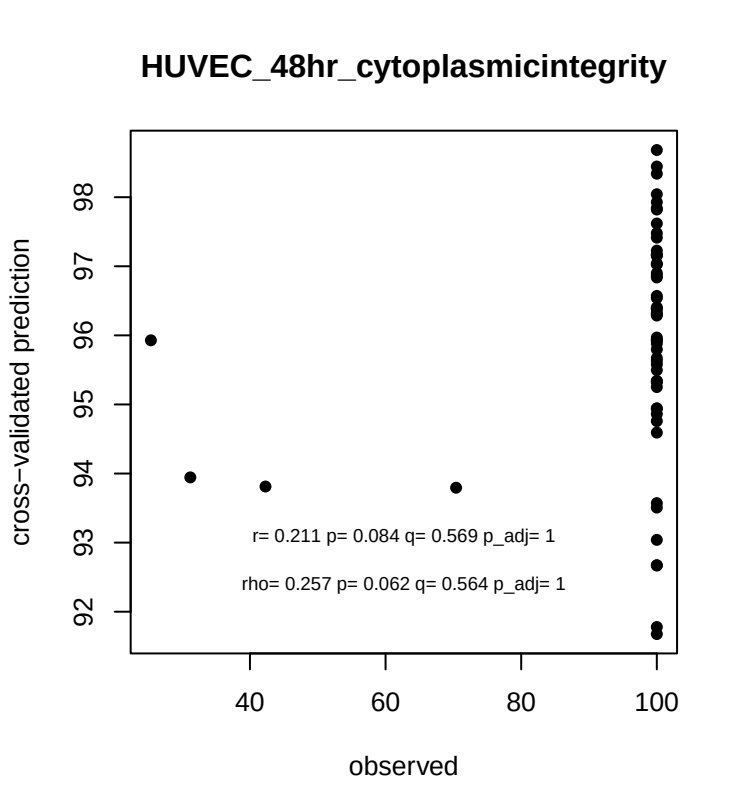
HUVEC_48hr_totaltubearea

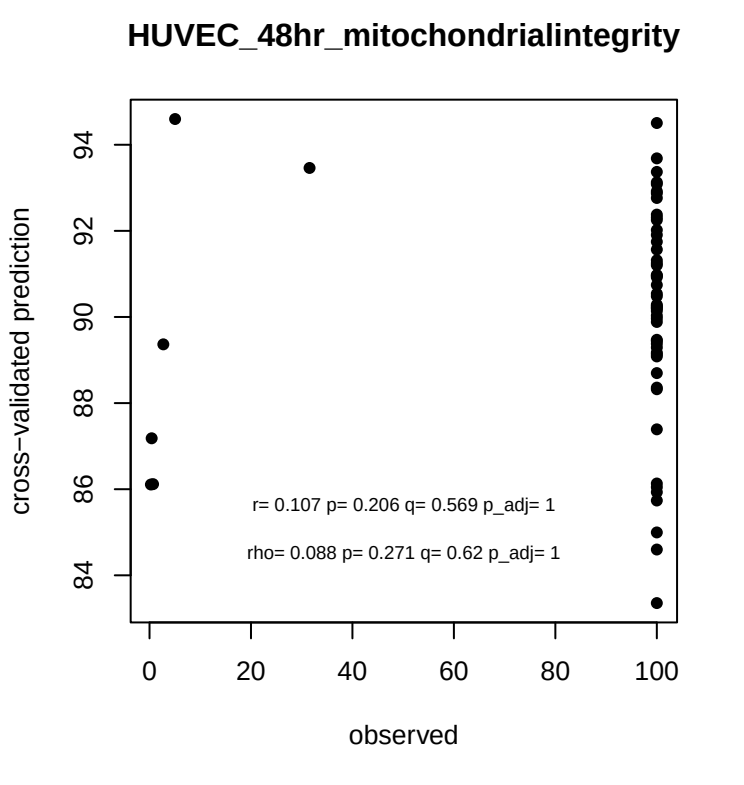


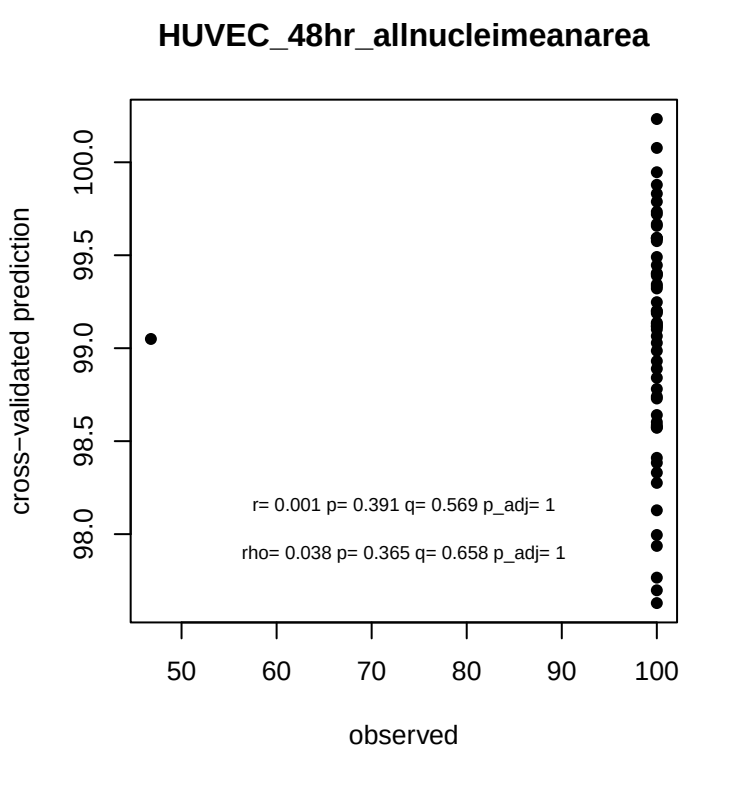
HUVEC_48hr_atpproduction



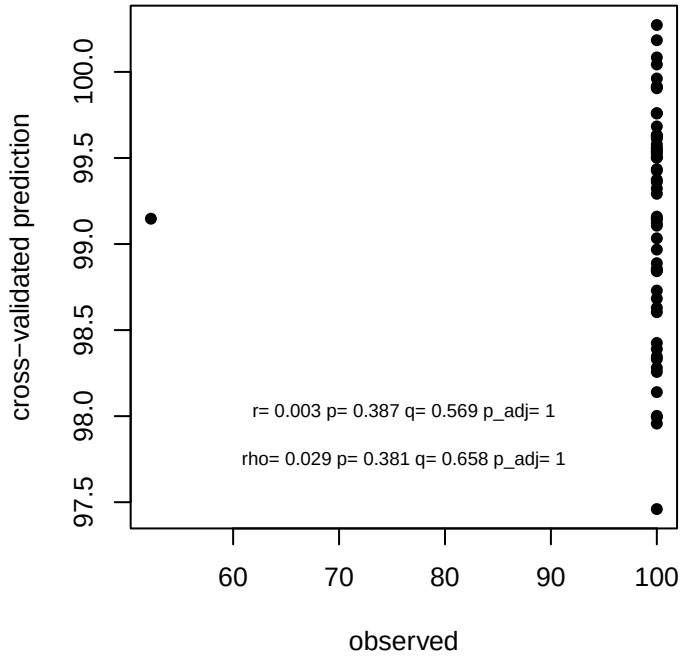

HUVEC_48hr_totalcells
cross−validated prediction
observed
r= 0.096 p= 0.224 q= 0.569 p_adj= 1
rho= 0.171 p= 0.146 q= 0.62 p_adj= 1


HUVEC_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= 0.211 p= 0.084 q= 0.569 p_adj= 1
rho= 0.257 p= 0.062 q= 0.564 p_adj= 1

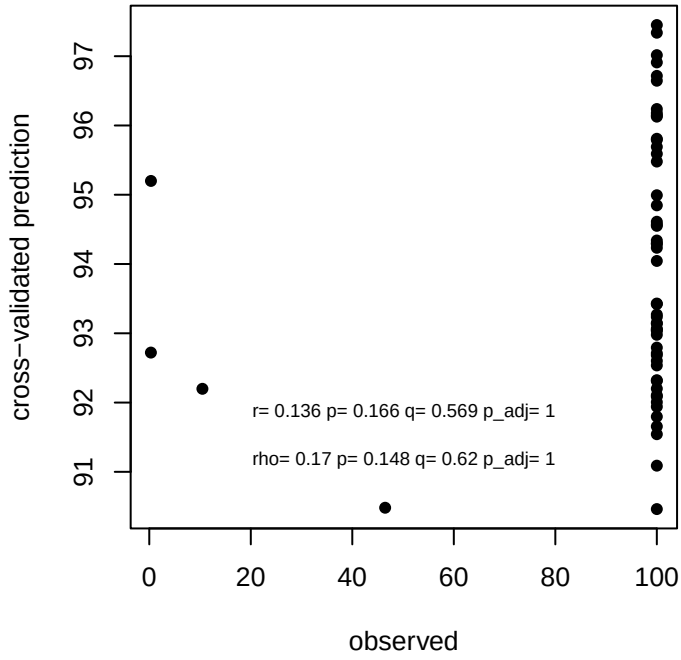

HUVEC_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= 0.107 p= 0.206 q= 0.569 p_adj= 1
rho= 0.088 p= 0.271 q= 0.62 p_adj= 1


HUVEC_48hr_allnucleimeanarea
cross−validated prediction
observed
r= 0.001 p= 0.391 q= 0.569 p_adj= 1
rho= 0.038 p= 0.365 q= 0.658 p_adj= 1

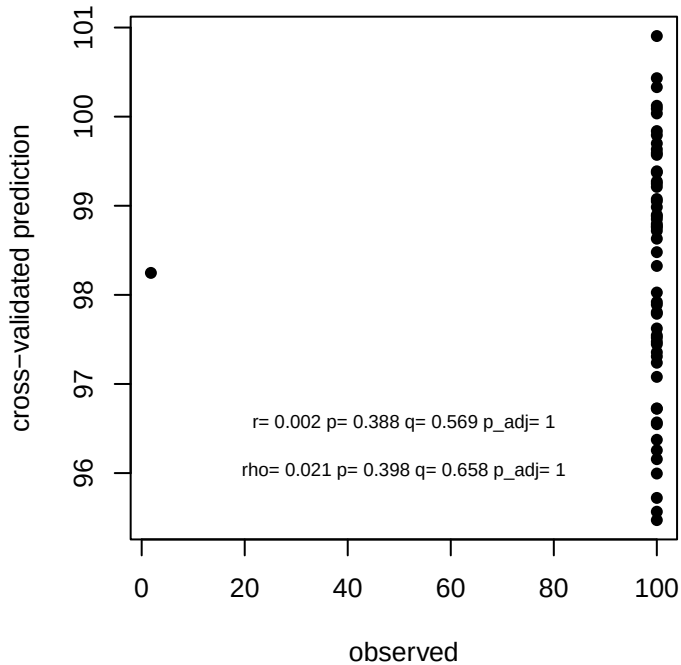
NEURONS_72hr_totalcells



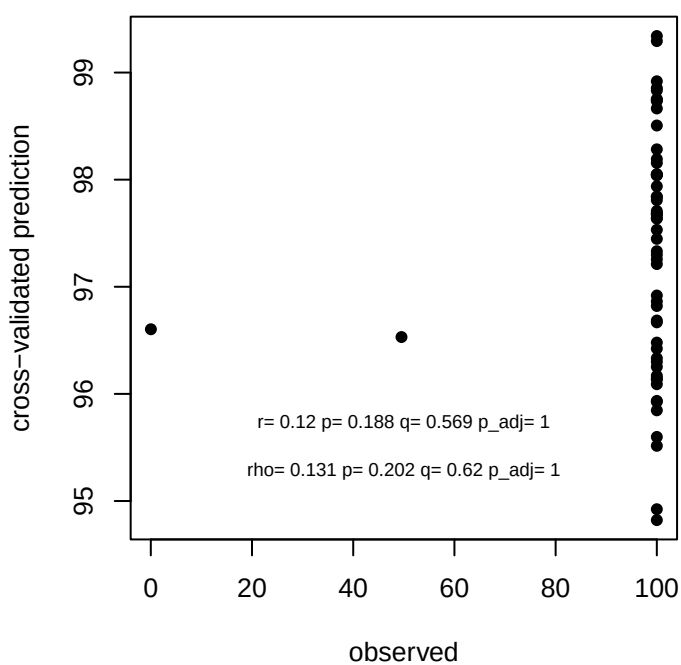
NEURONS_72hr_cytoplasmicintegrity



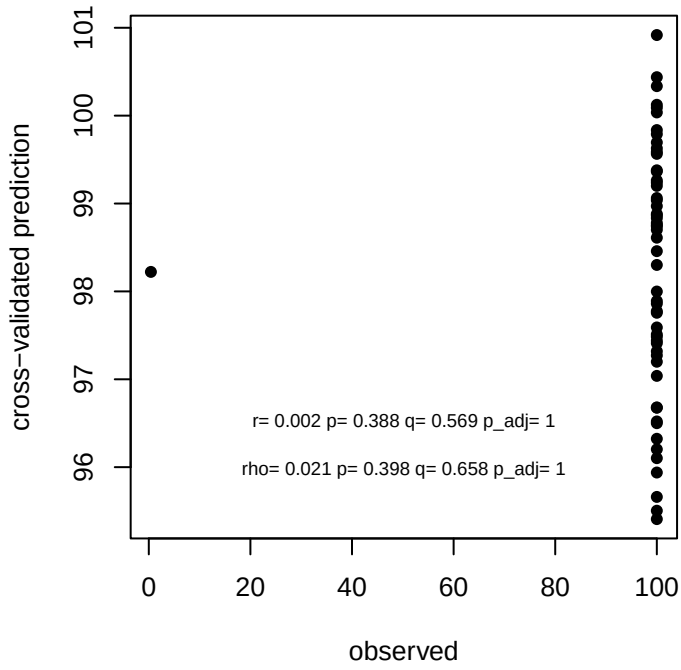
NEURONS_72hr_totaloutgrowth



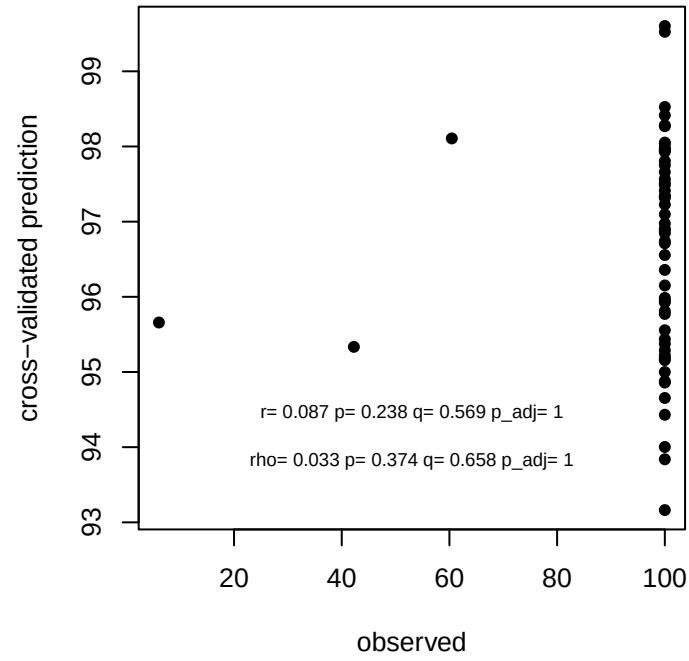
NEURONS_72hr_totalprocess



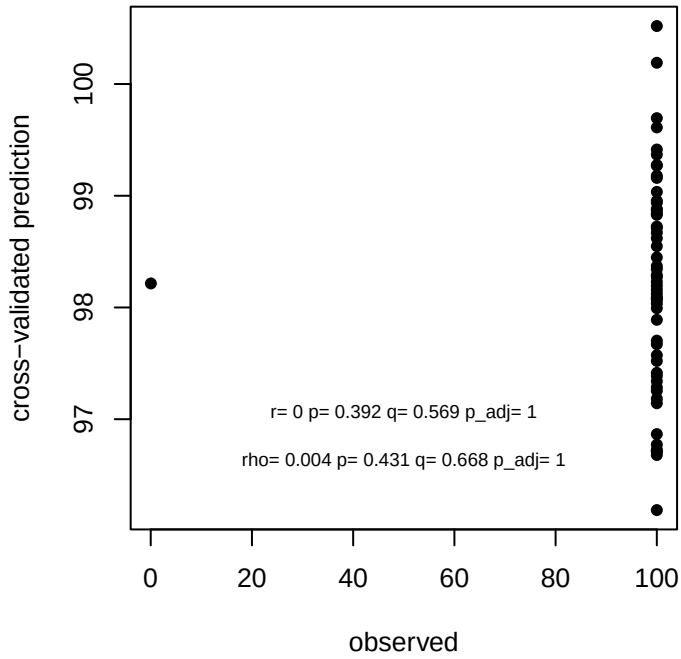
NEURONS_72hr_totalbranches



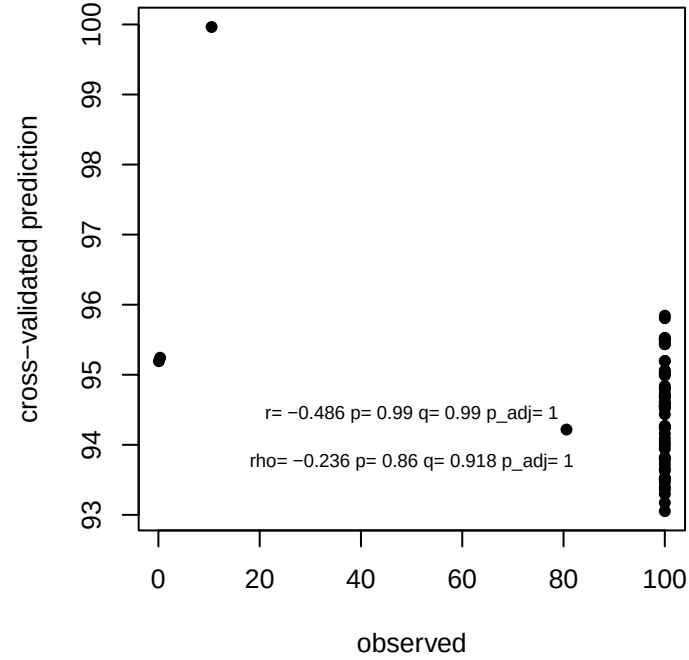
NEURONS_72hr_cellsiwithsignificantgrowth



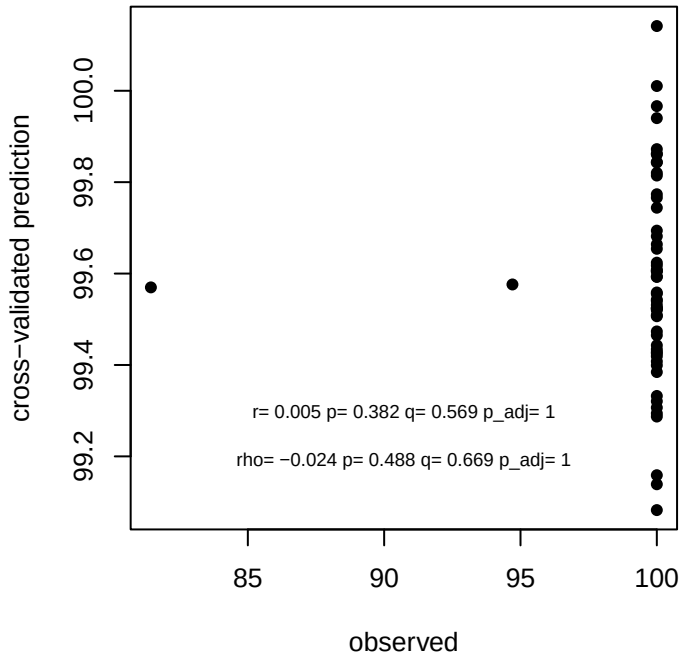
HEPATOCYTES_48hr_totalgranulearea



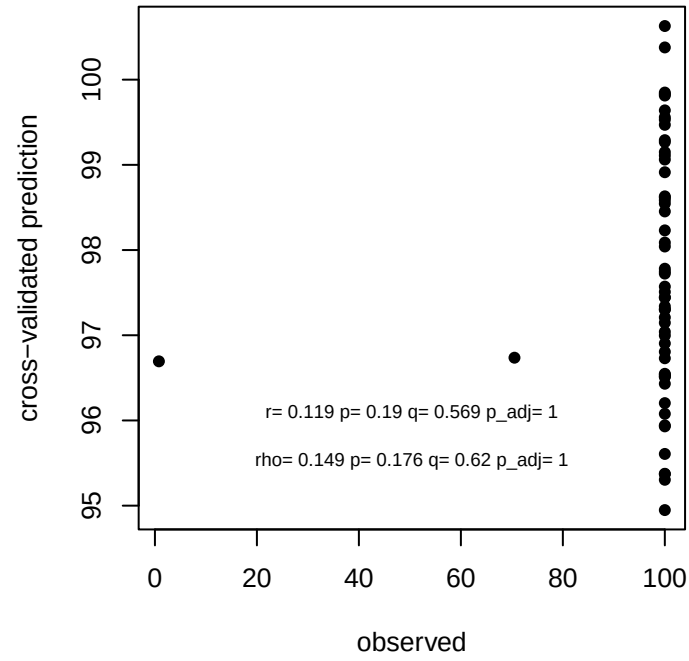
HEPATOCYTES_48hr_granularity



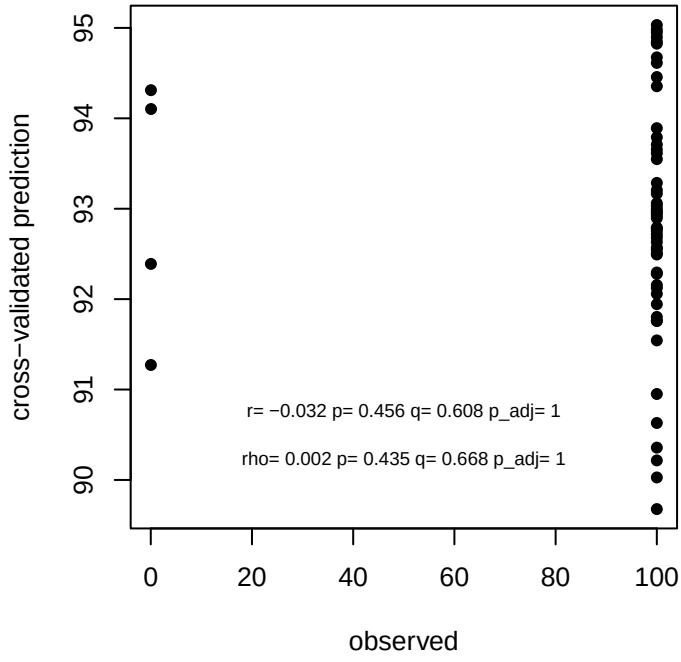
HEPATOCYTES_48hr_totalcells



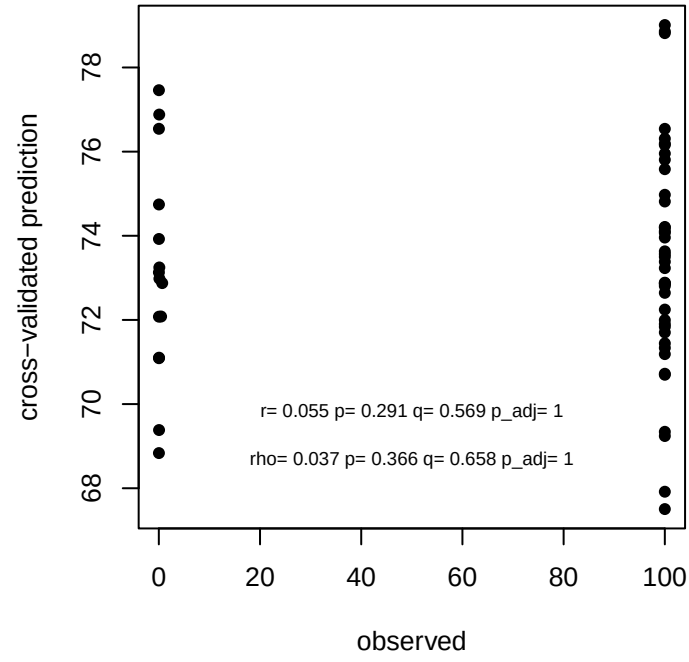
HEPATOCYTES_48hr_allcellsmeanarea



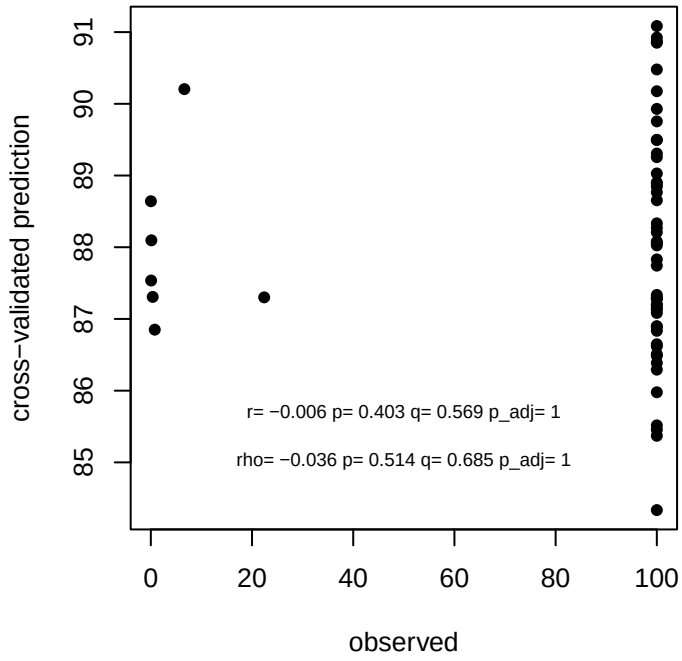
HEPATOCYTES_48hr_cytoplasmicintegrity



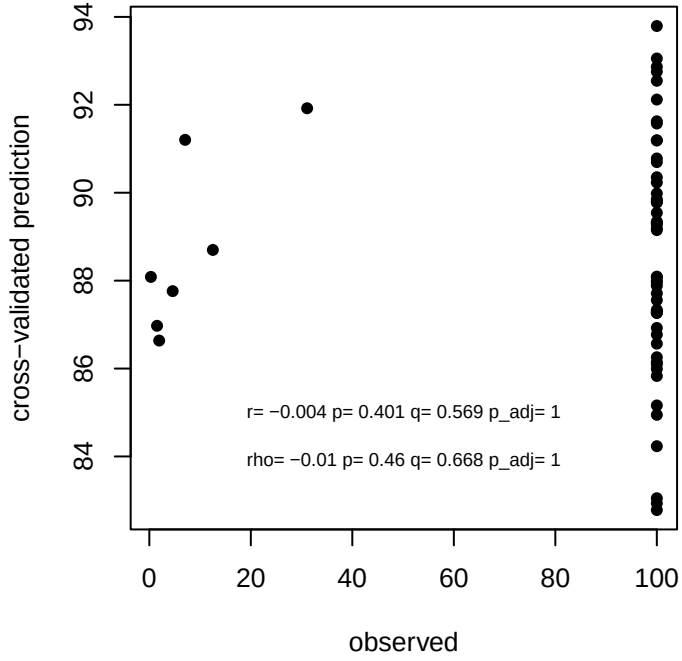
HEPATOCYTES_48hr_mitochondrialintegrity



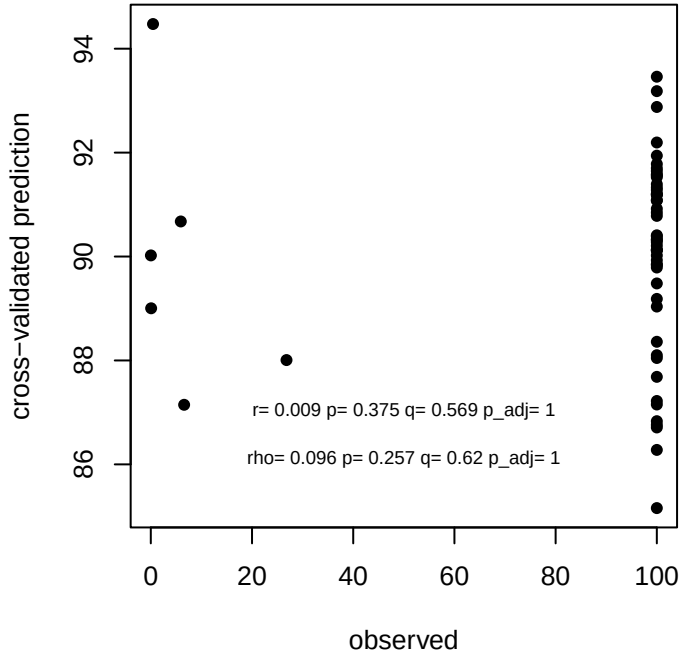
HEPATOCYTES_48hr_mitochondrialintensity



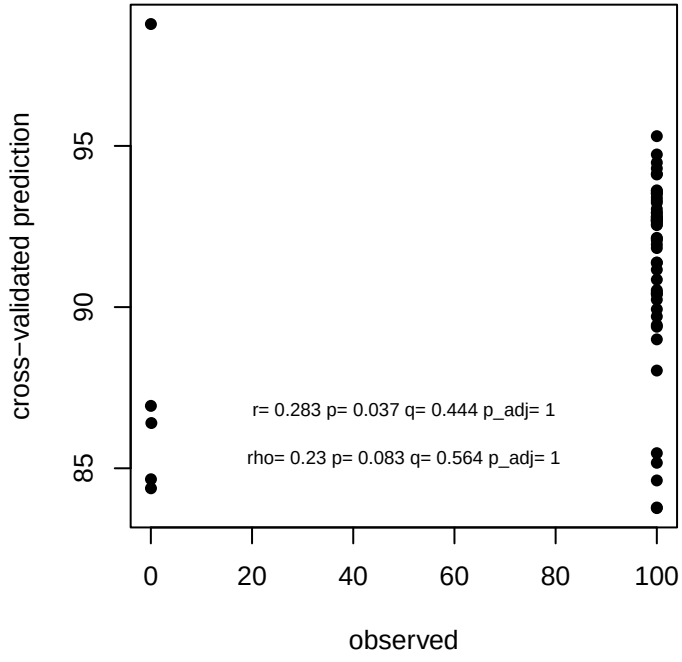
HEPATOCYTES_48hr_nucleiintensity

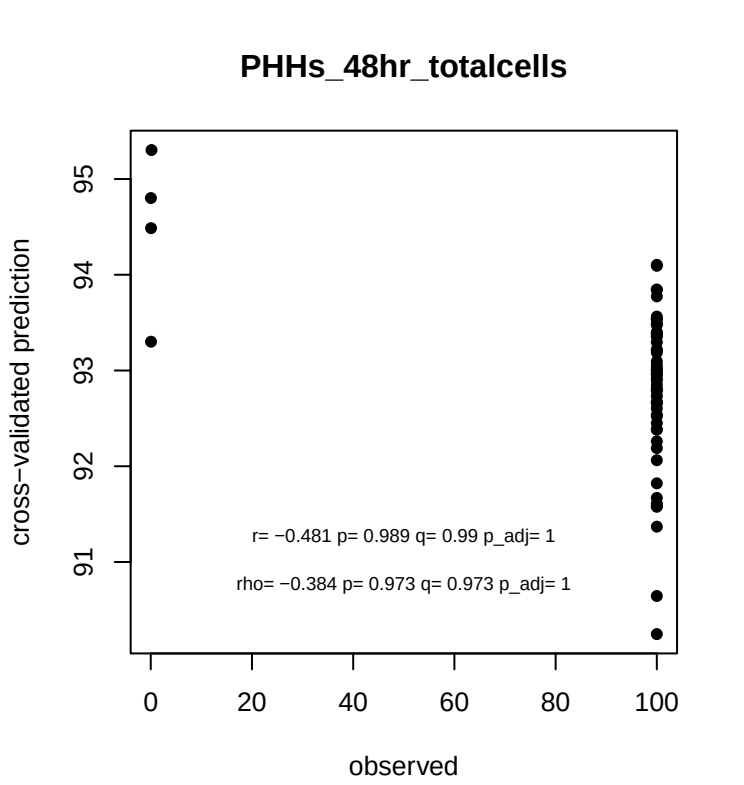


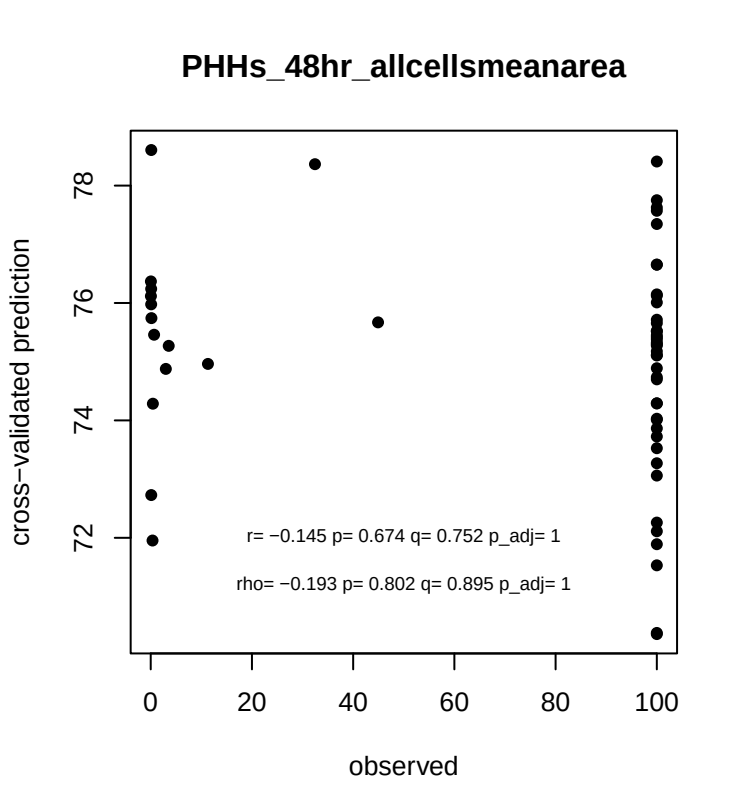
PHHs_48hr_totalgranulearea

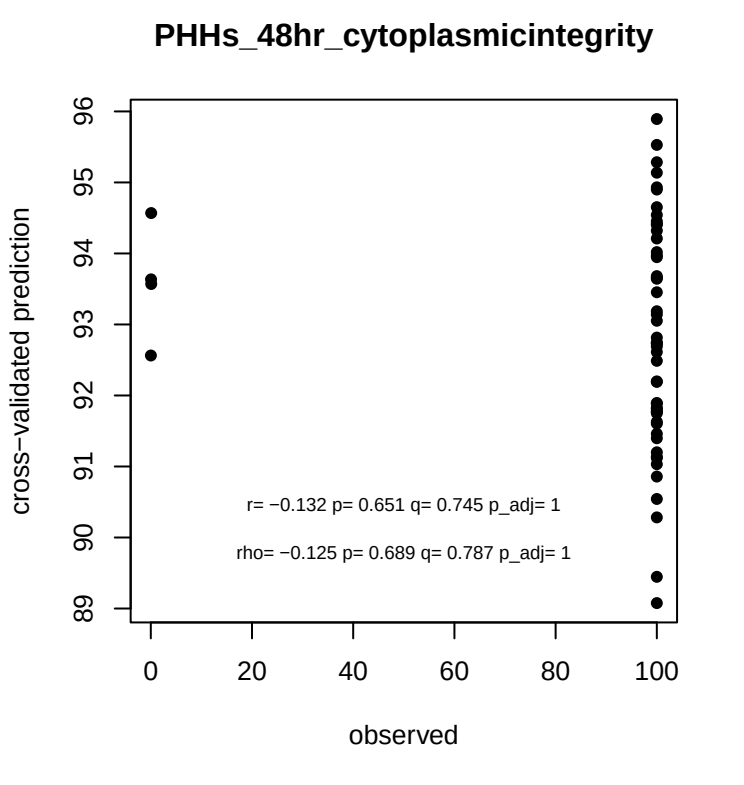


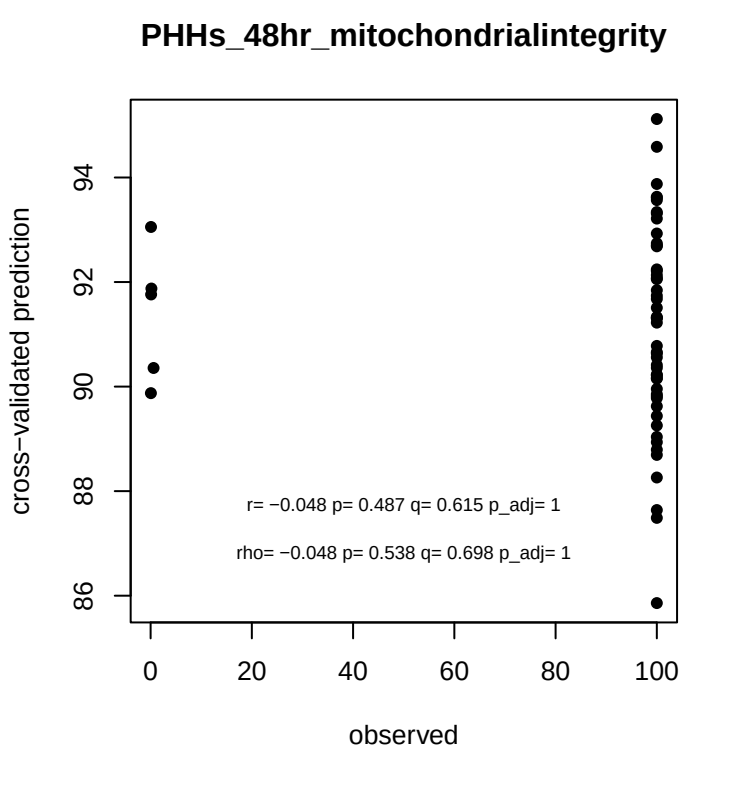
PHHs_48hr_granularity

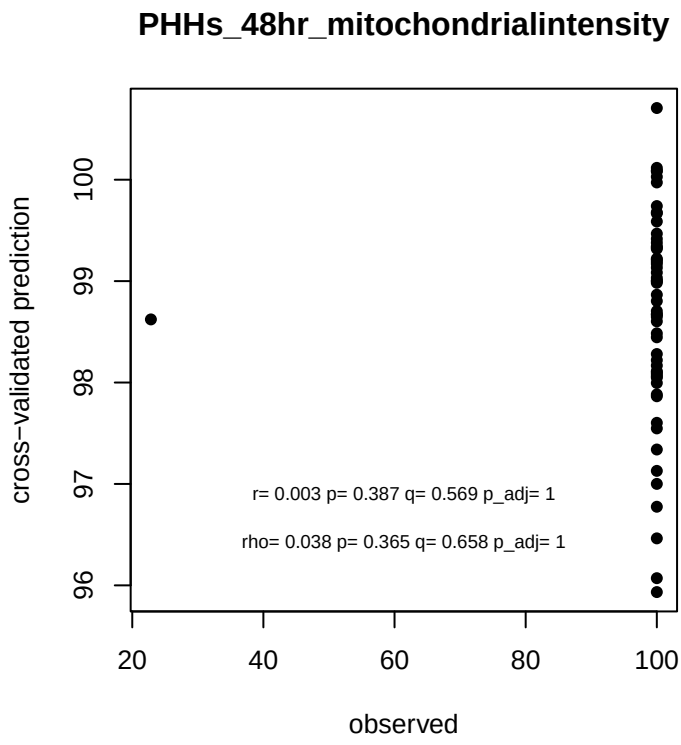


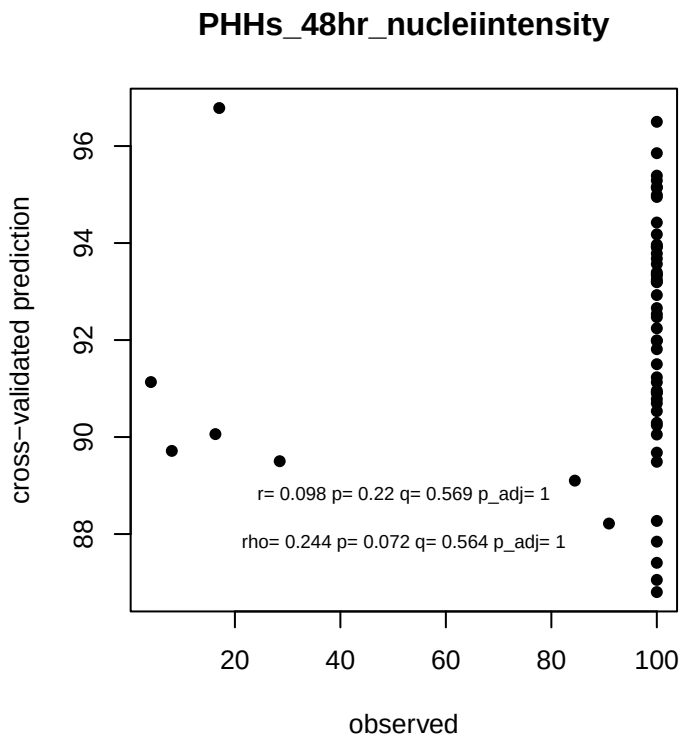

PHHs_48hr_totalcells
cross−validated prediction
observed
r= −0.481 p= 0.989 q= 0.99 p_adj= 1
rho= −0.384 p= 0.973 q= 0.973 p_adj= 1

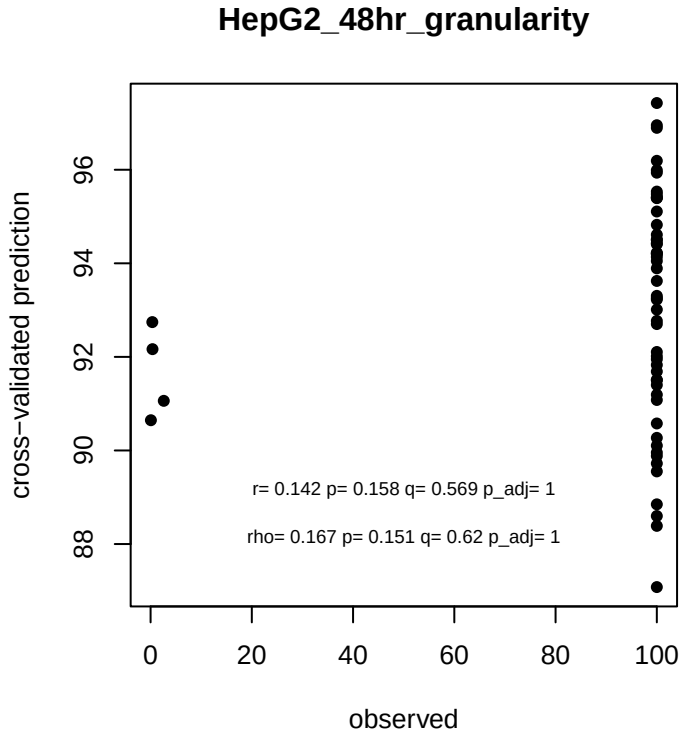

PHHs_48hr_allcellsmeanarea
cross−validated prediction
observed
r= −0.145 p= 0.674 q= 0.752 p_adj= 1
rho= −0.193 p= 0.802 q= 0.895 p_adj= 1

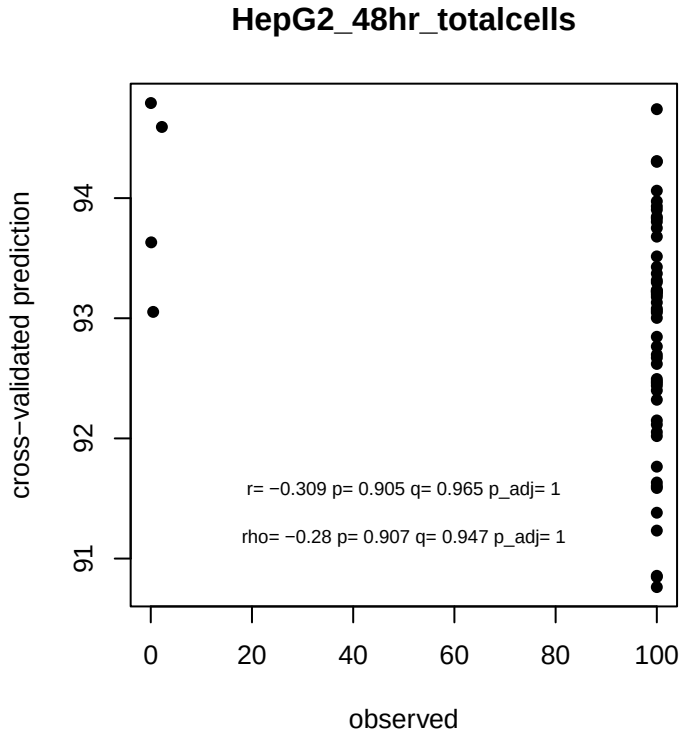

PHHs_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= −0.132 p= 0.651 q= 0.745 p_adj= 1
rho= −0.125 p= 0.689 q= 0.787 p_adj= 1

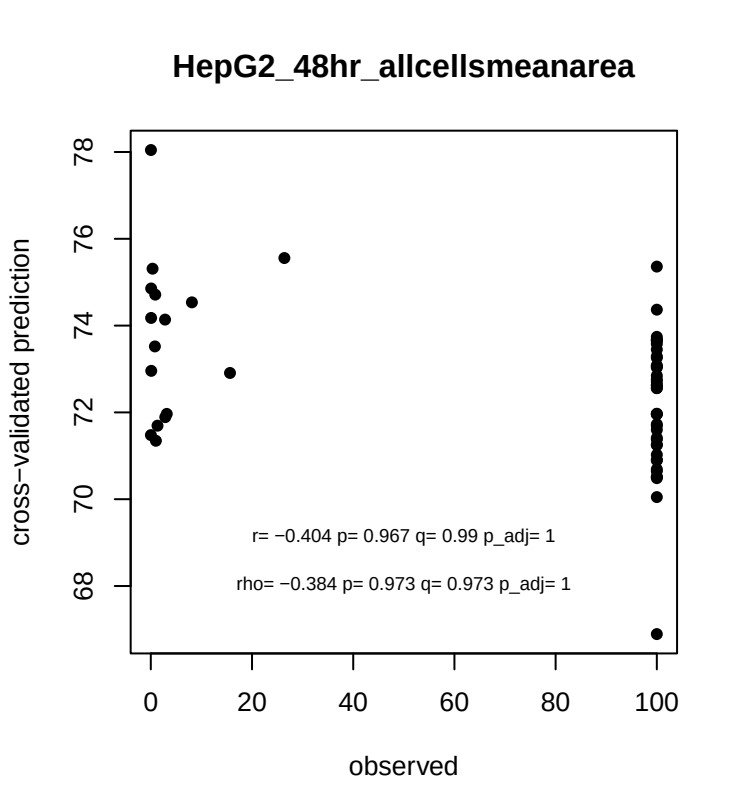

PHHs_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= −0.048 p= 0.487 q= 0.615 p_adj= 1
rho= −0.048 p= 0.538 q= 0.698 p_adj= 1

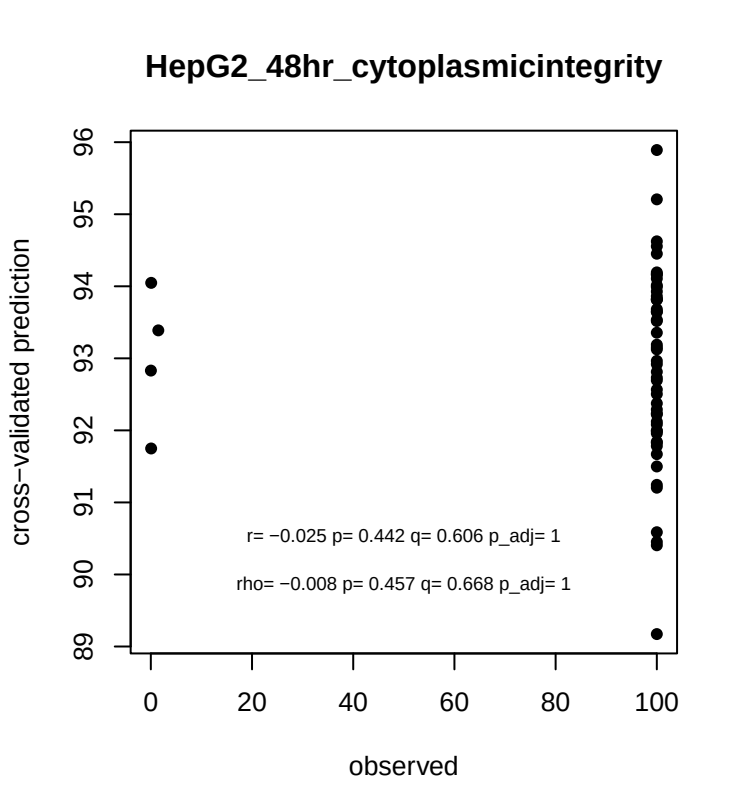

PHHs_48hr_mitochondrialintensity
cross−validated prediction
observed
r= 0.003 p= 0.387 q= 0.569 p_adj= 1
rho= 0.038 p= 0.365 q= 0.658 p_adj= 1

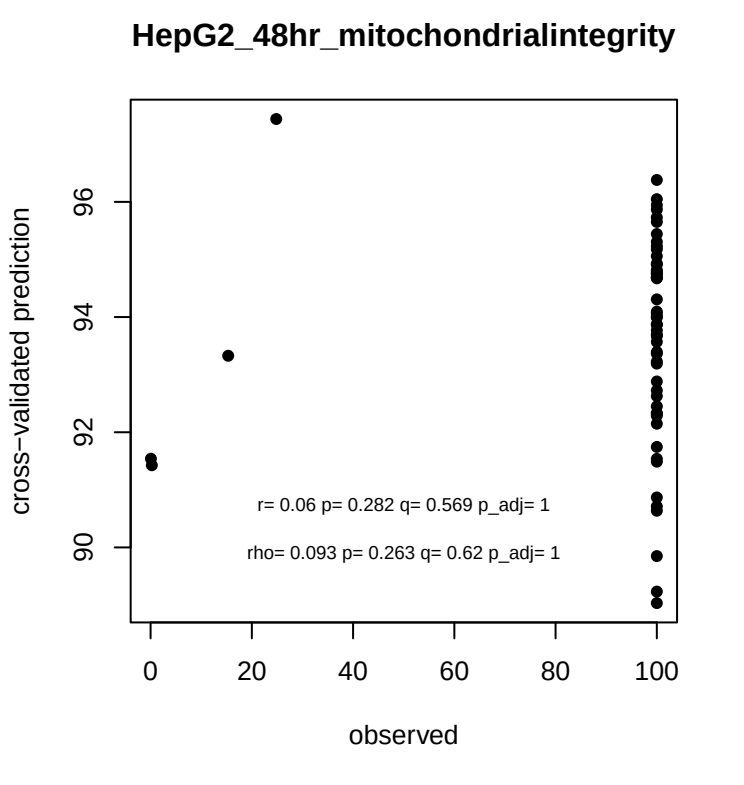

PHHs_48hr_nucleiintensity
cross−validated prediction
observed
r= 0.098 p= 0.22 q= 0.569 p_adj= 1
rho= 0.244 p= 0.072 q= 0.564 p_adj= 1

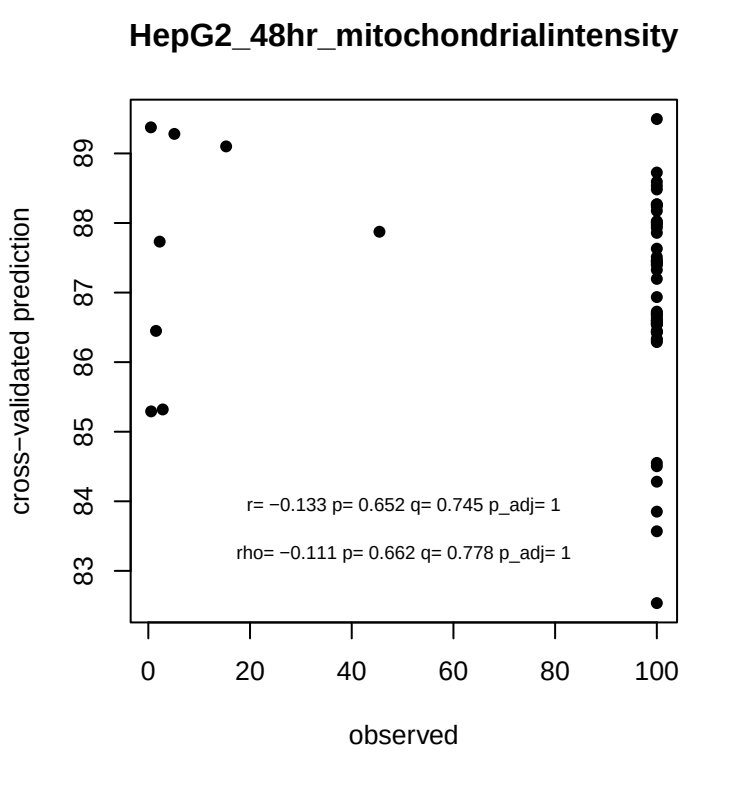

HepG2_48hr_granularity
cross−validated prediction
observed
r= 0.142 p= 0.158 q= 0.569 p_adj= 1
rho= 0.167 p= 0.151 q= 0.62 p_adj= 1

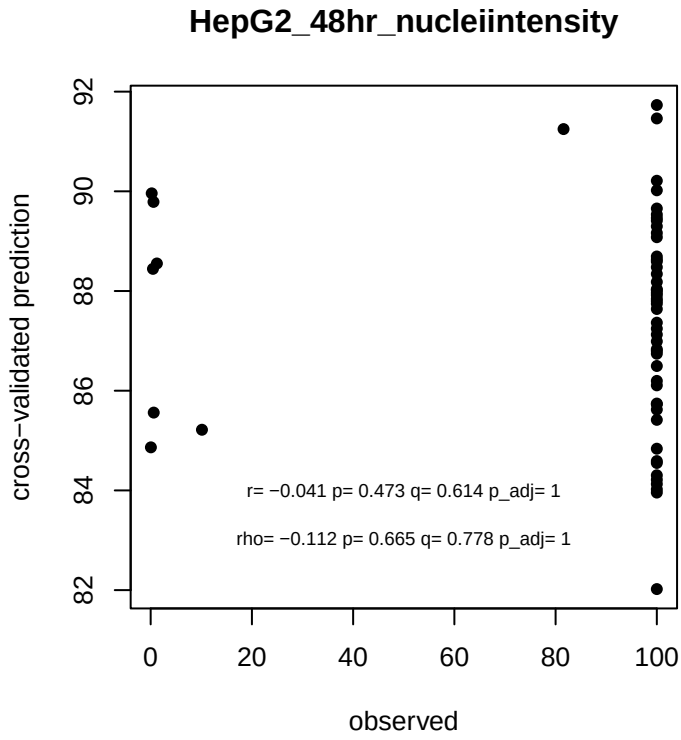

HepG2_48hr_totalcells
cross−validated prediction
observed
r= −0.309 p= 0.905 q= 0.965 p_adj= 1
rho= −0.28 p= 0.907 q= 0.947 p_adj= 1

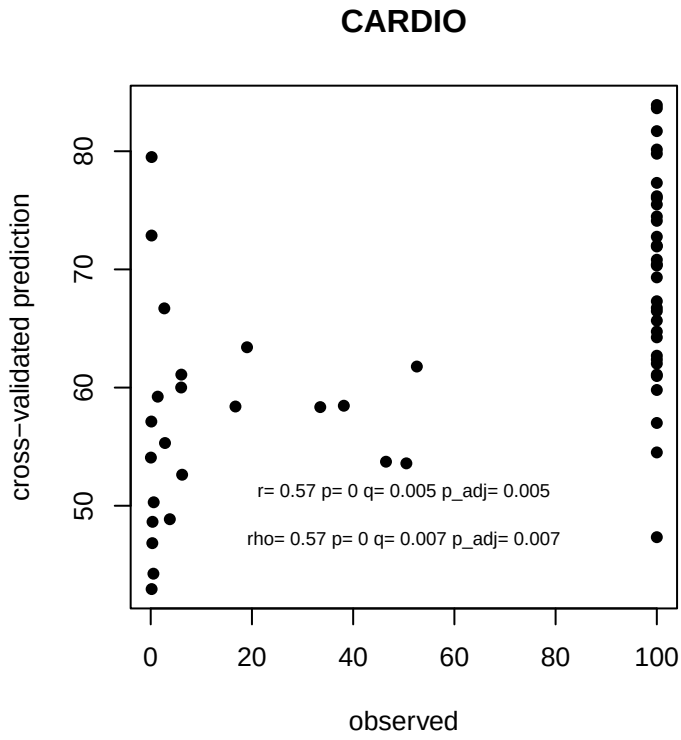

HepG2_48hr_allcellsmeanarea
cross−validated prediction
observed
r= −0.404 p= 0.967 q= 0.99 p_adj= 1
rho= −0.384 p= 0.973 q= 0.973 p_adj= 1

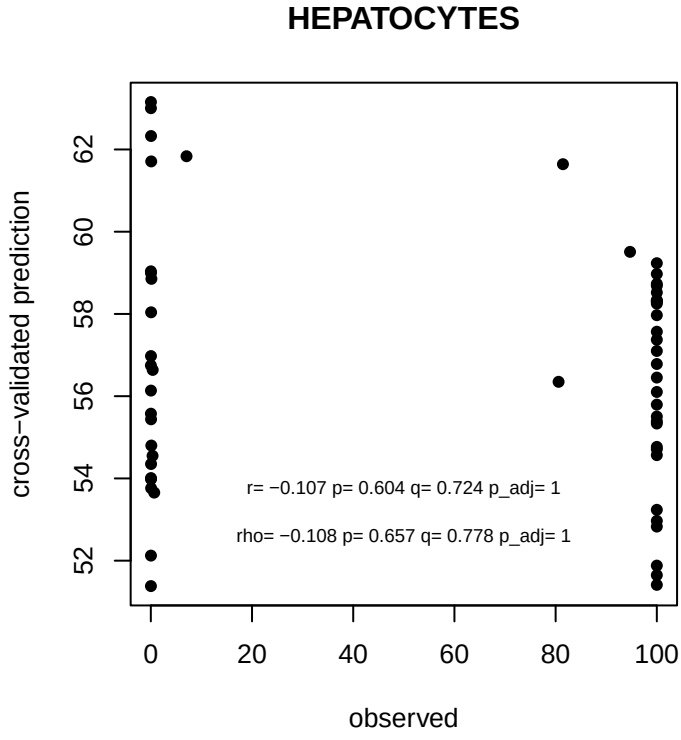

HepG2_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= −0.025 p= 0.442 q= 0.606 p_adj= 1
rho= −0.008 p= 0.457 q= 0.668 p_adj= 1

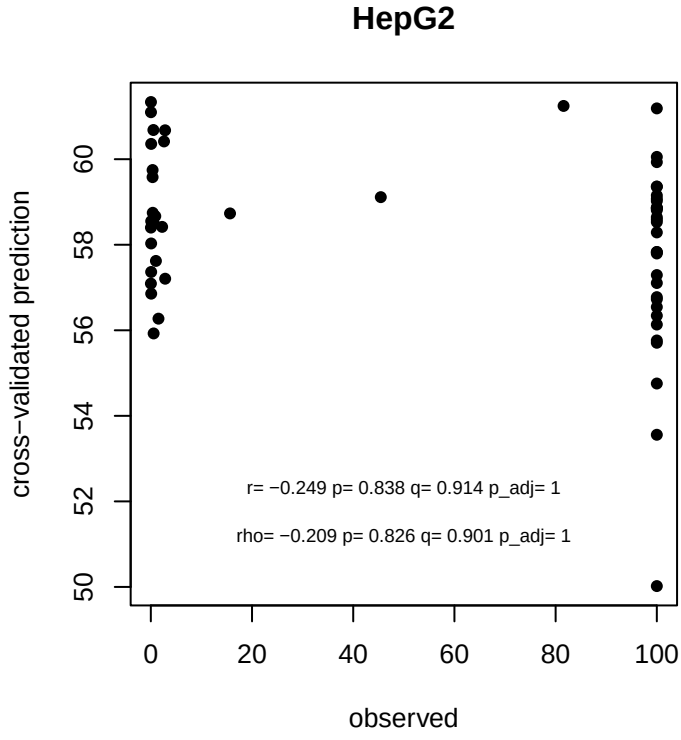

HepG2_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= 0.06 p= 0.282 q= 0.569 p_adj= 1
rho= 0.093 p= 0.263 q= 0.62 p_adj= 1

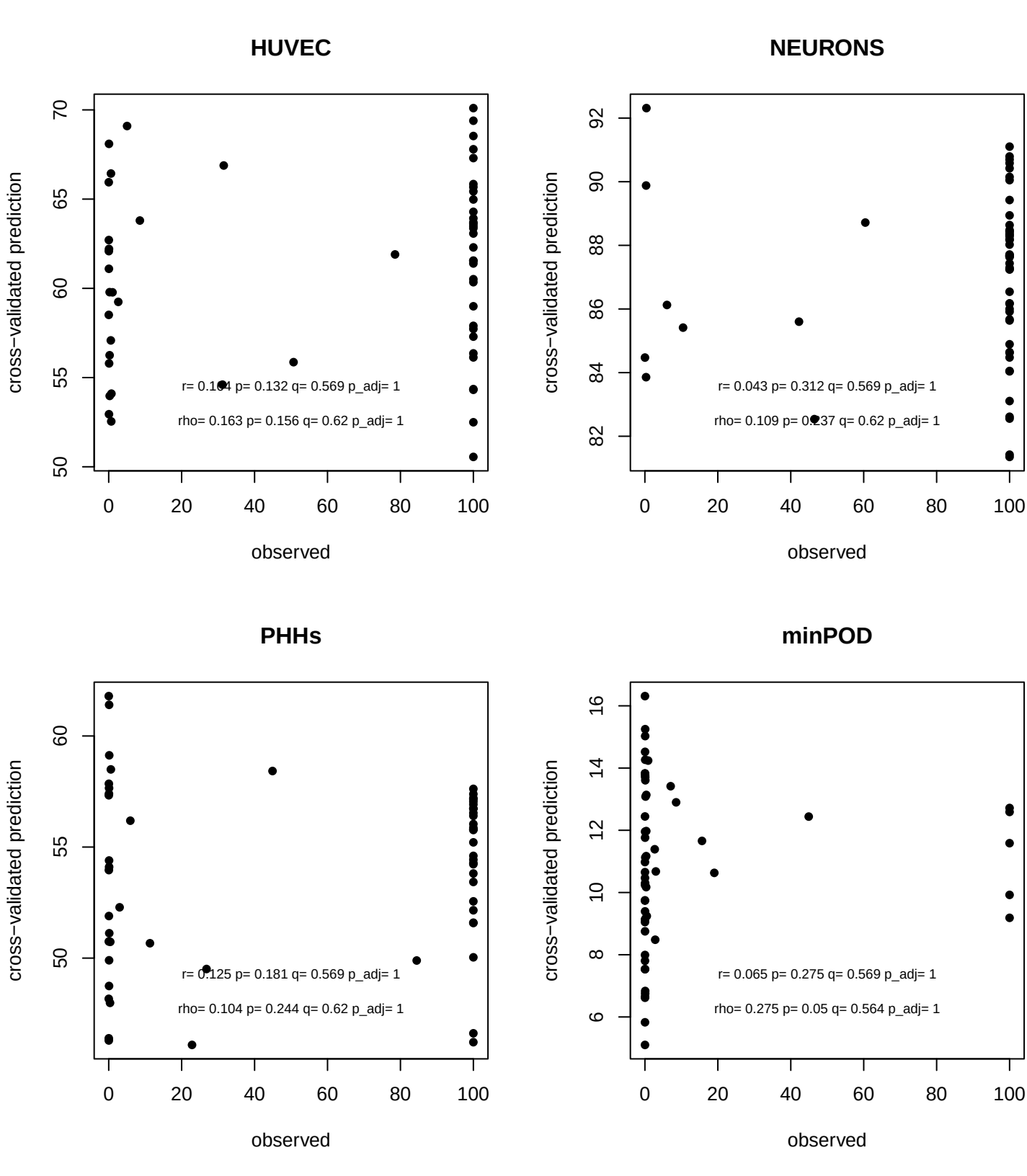

HepG2_48hr_mitochondrialintensity
cross−validated prediction
observed
r= −0.133 p= 0.652 q= 0.745 p_adj= 1
rho= −0.111 p= 0.662 q= 0.778 p_adj= 1


HepG2_48hr_nucleiintensity
cross−validated prediction
observed
r= −0.041 p= 0.473 q= 0.614 p_adj= 1
rho= −0.112 p= 0.665 q= 0.778 p_adj= 1


CARDIO
cross−validated prediction
observed
r= 0.57 p= 0 q= 0.005 p_adj= 0.005
rho= 0.57 p= 0 q= 0.007 p_adj= 0.007


HEPATOCYTES
cross−validated prediction
observed
r= −0.107 p= 0.604 q= 0.724 p_adj= 1
rho= −0.108 p= 0.657 q= 0.778 p_adj= 1


HepG2
cross−validated prediction
observed
r= −0.249 p= 0.838 q= 0.914 p_adj= 1
rho= −0.209 p= 0.826 q= 0.901 p_adj= 1


HUVEC
cross−validated prediction
observed
r= 0.164 p= 0.132 q= 0.569 p_adj= 1
rho= 0.163 p= 0.156 q= 0.62 p_adj= 1
NEURONS
cross−validated prediction
observed
r= 0.043 p= 0.312 q= 0.569 p_adj= 1
rho= 0.109 p= 0.237 q= 0.62 p_adj= 1
PHHs
cross−validated prediction
observed
r= 0.125 p= 0.181 q= 0.569 p_adj= 1
rho= 0.104 p= 0.244 q= 0.62 p_adj= 1
minPOD
cross−validated prediction
observed
r= 0.065 p= 0.275 q= 0.569 p_adj= 1
rho= 0.275 p= 0.05 q= 0.564 p_adj= 1