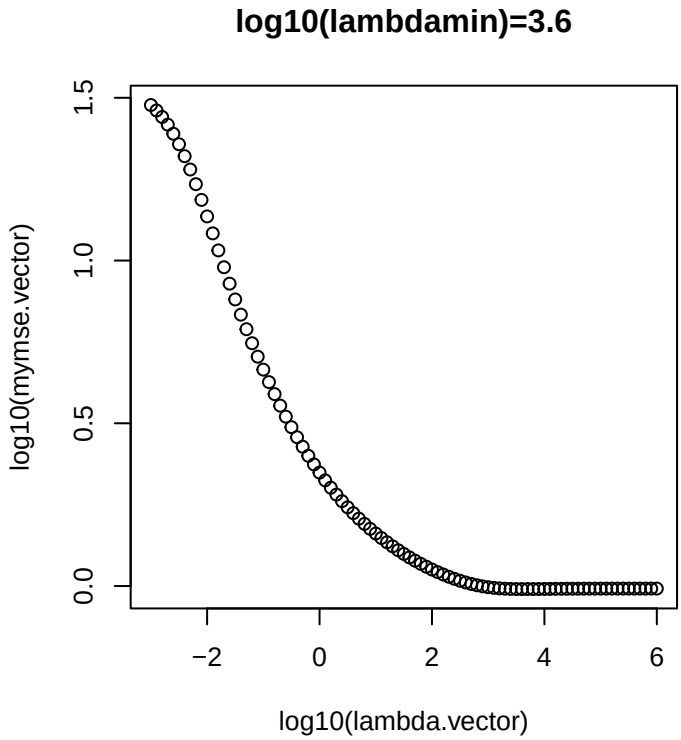
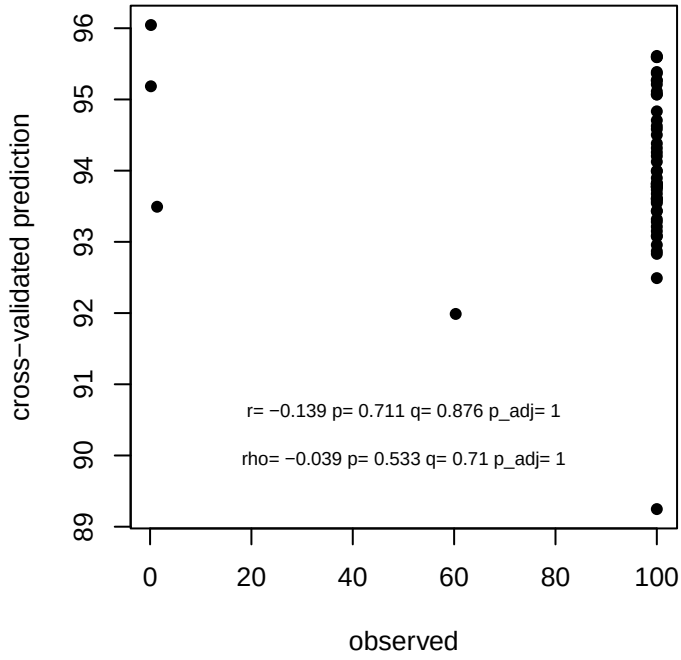
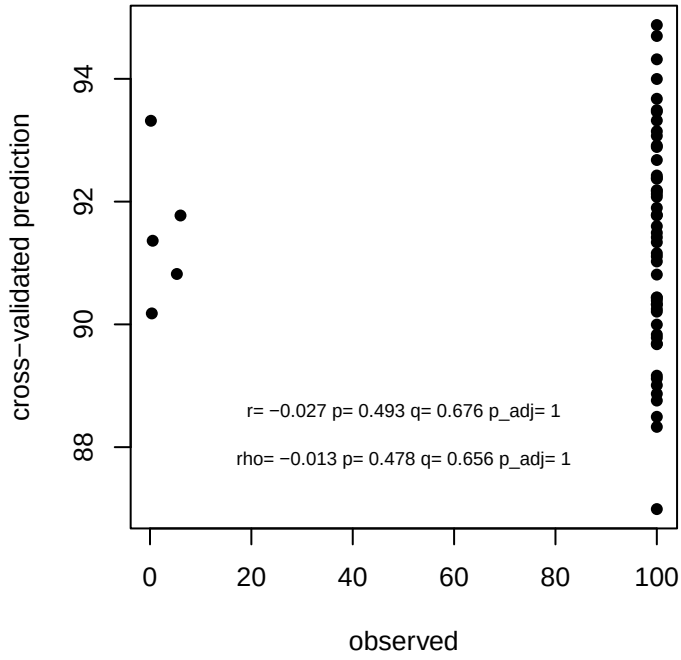
Figure S8: Correlation plots for the predicted bioactivity using the OPERA and Saagar descriptors. Each plot represents a cell-specific phenotype and reports the observed in relation to the cross-validation predictions and the corresponding correlation coefficients.


log10(lambdamin)=3.6
log10(mymse.vector)
0.0
0.5
1.0
1.5
−2
0
2
4
6
log10(lambda.vector)

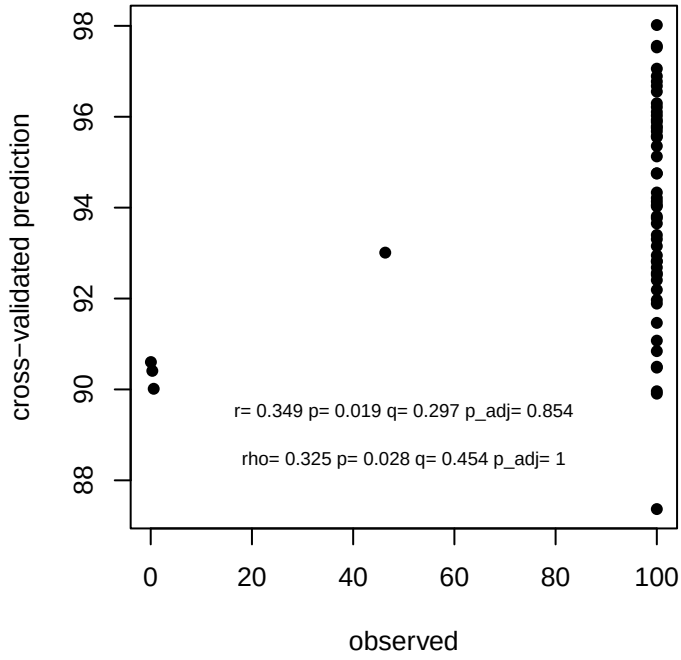
CARDIO_90min_qtprolongation



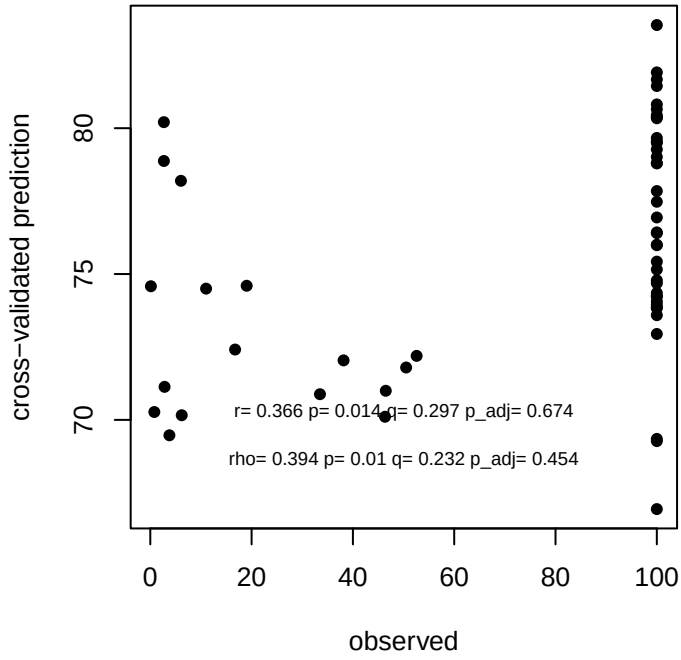
CARDIO_90min_totalcells



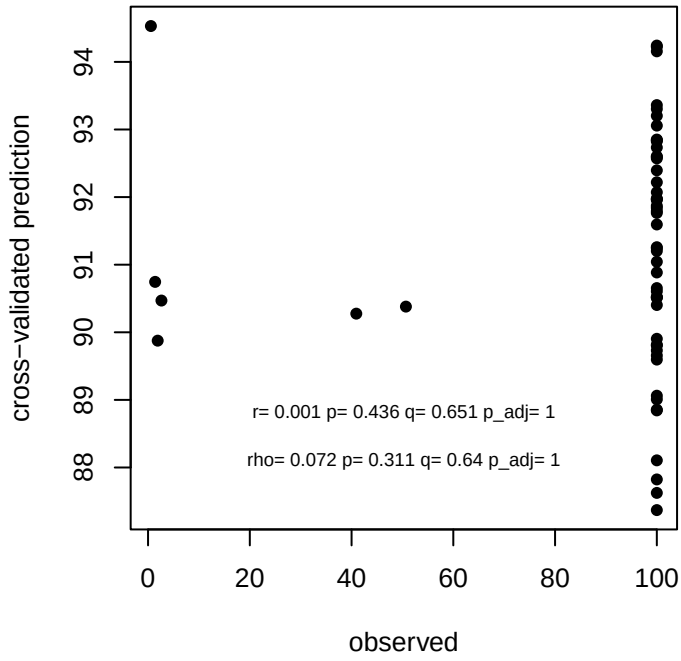
CARDIO_90min_positivechronotrope



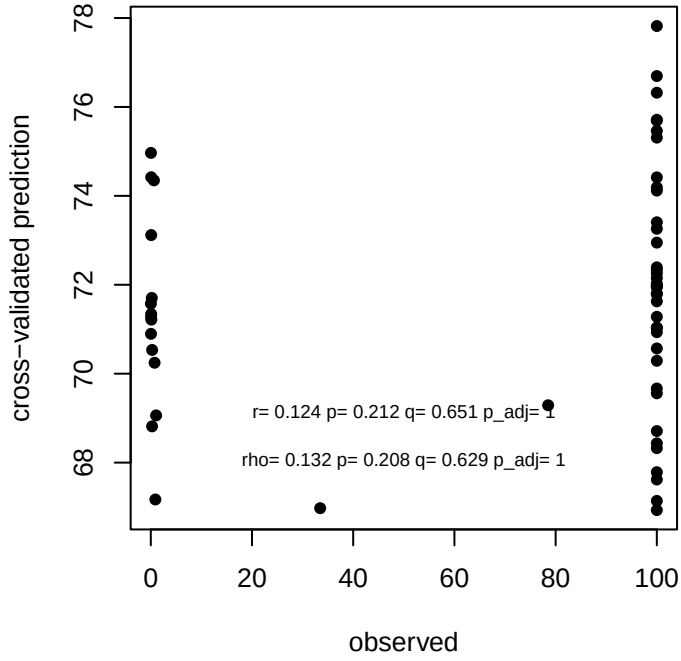
CARDIO_90min_negativechronotrope



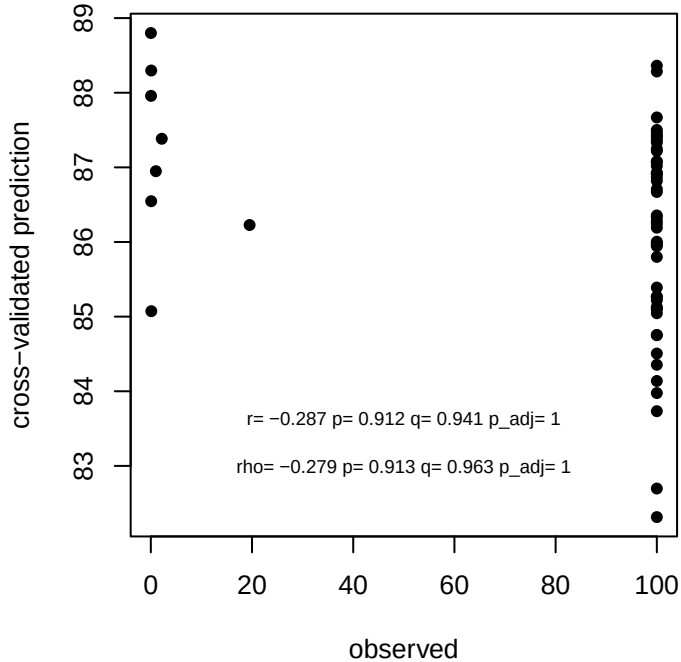
HUVEC_48hr_meantubelength



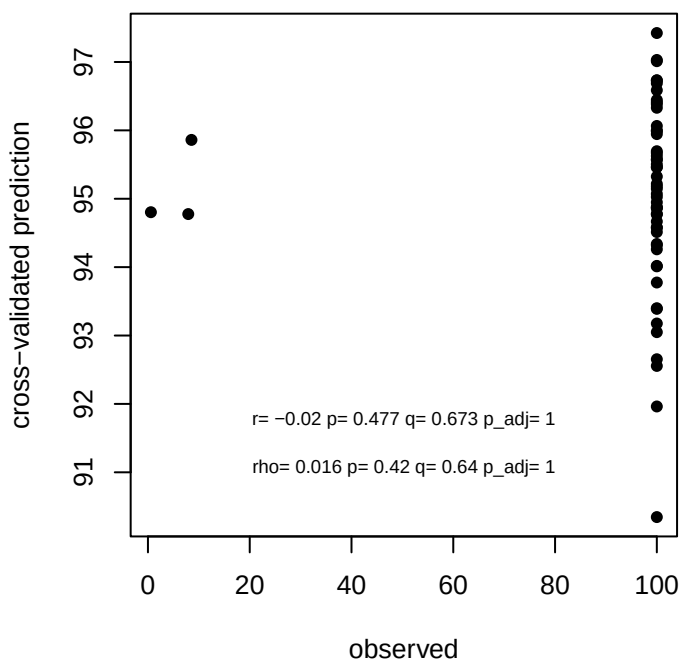
HUVEC_48hr_totaltubelength

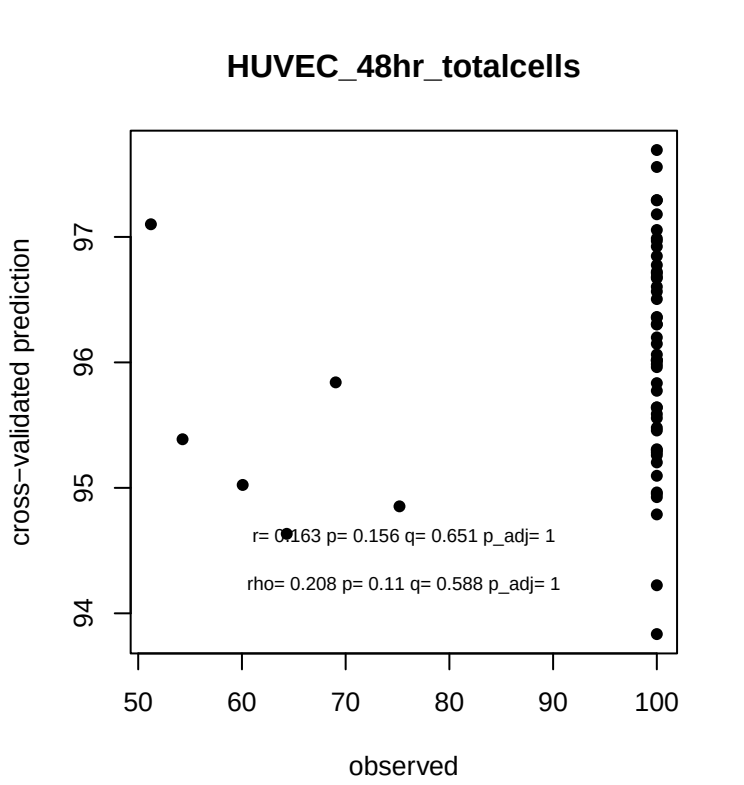


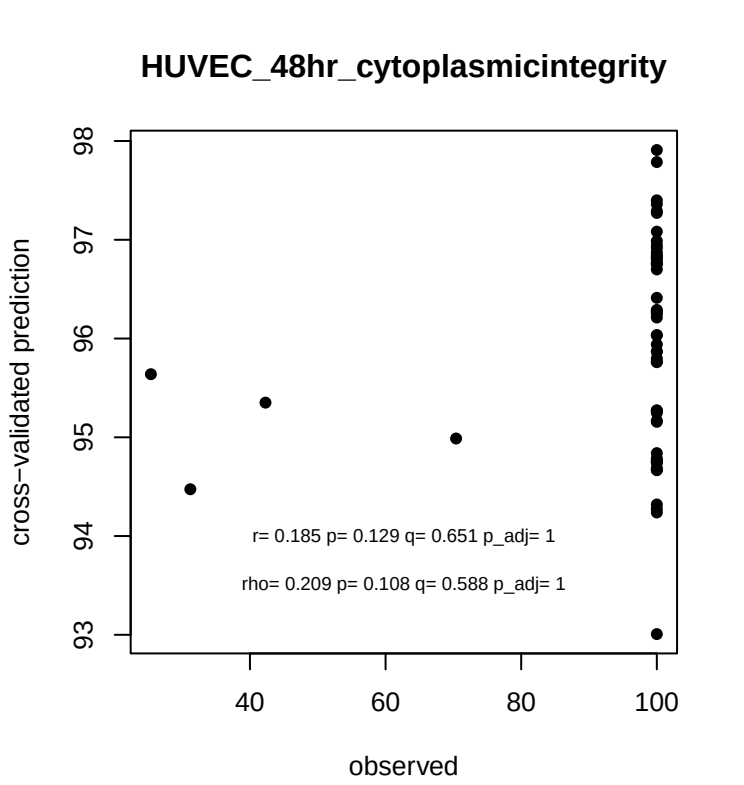
HUVEC_48hr_totaltubearea

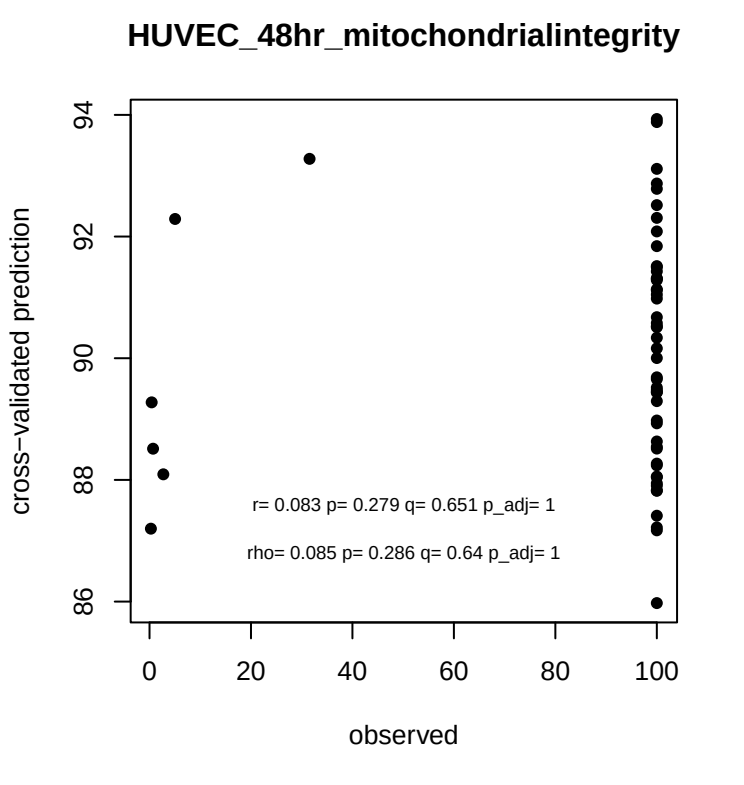


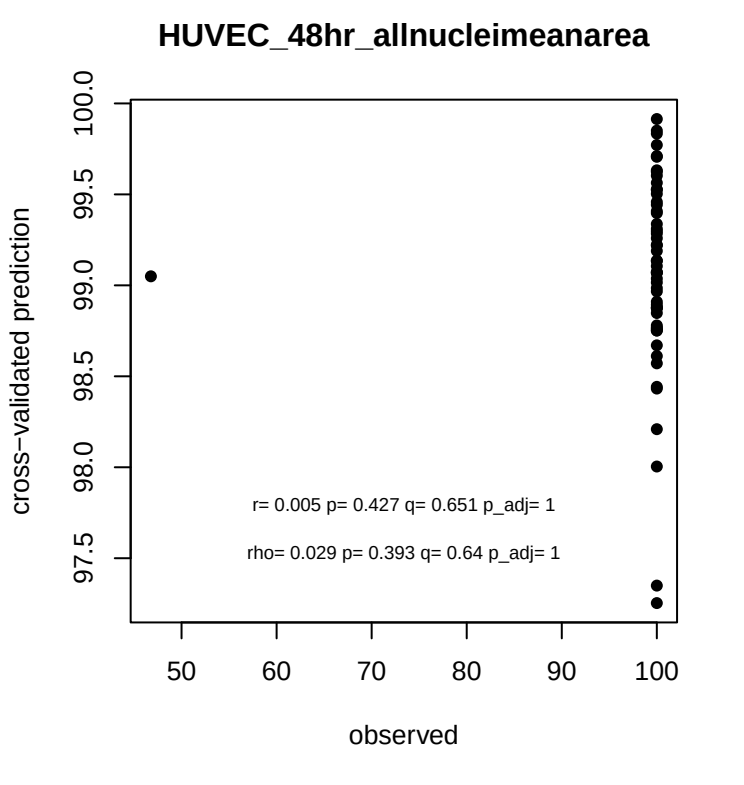
HUVEC_48hr_atpproduction



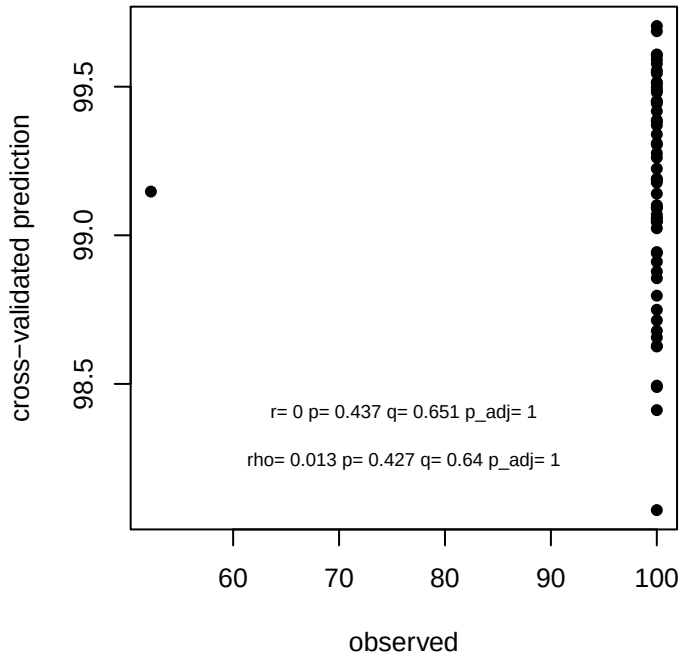

HUVEC_48hr_totalcells
cross−validated prediction
observed
r= 0.163 p= 0.156 q= 0.651 p_adj= 1
rho= 0.208 p= 0.11 q= 0.588 p_adj= 1


HUVEC_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= 0.185 p= 0.129 q= 0.651 p_adj= 1
rho= 0.209 p= 0.108 q= 0.588 p_adj= 1

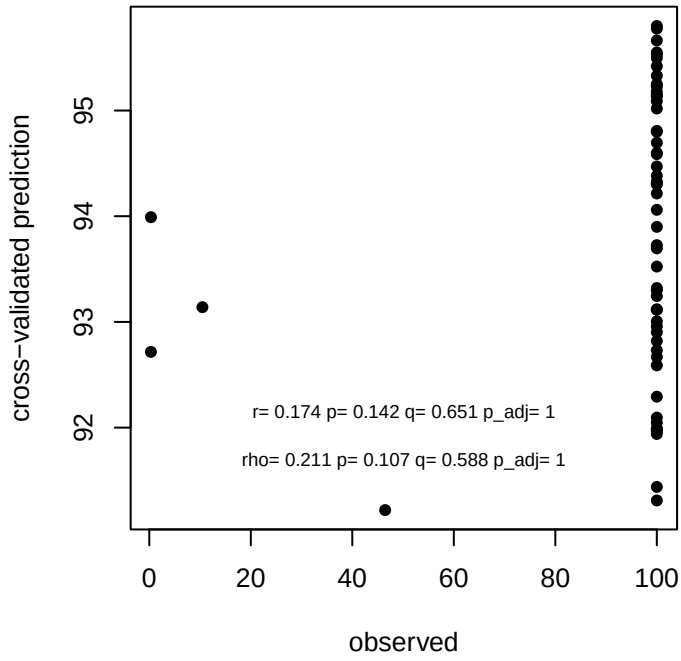

HUVEC_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= 0.083 p= 0.279 q= 0.651 p_adj= 1
rho= 0.085 p= 0.286 q= 0.64 p_adj= 1


HUVEC_48hr_allnucleimeanarea
cross−validated prediction
observed
r= 0.005 p= 0.427 q= 0.651 p_adj= 1
rho= 0.029 p= 0.393 q= 0.64 p_adj= 1

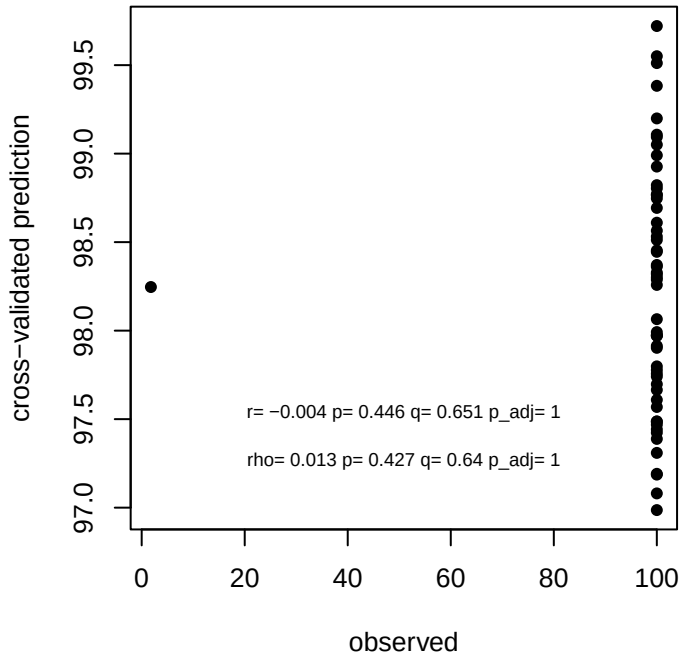
NEURONS_72hr_totalcells



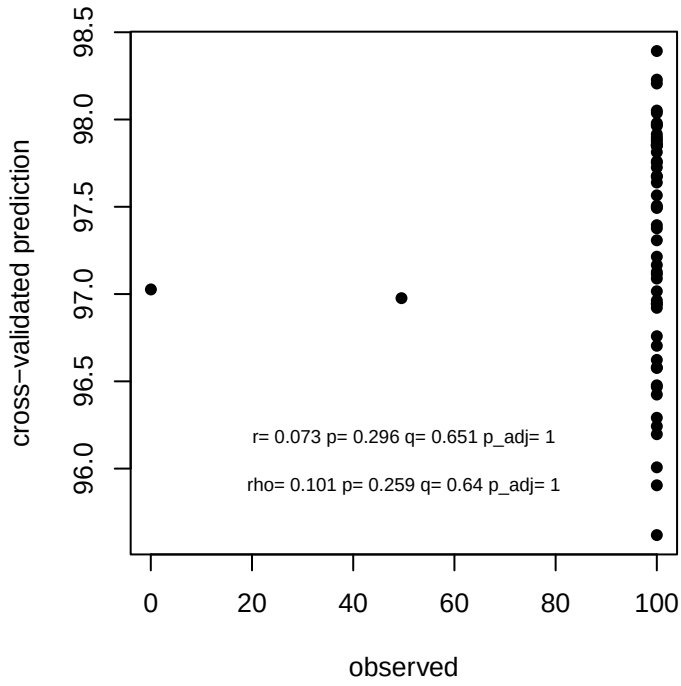
NEURONS_72hr_cytoplasmicintegrity



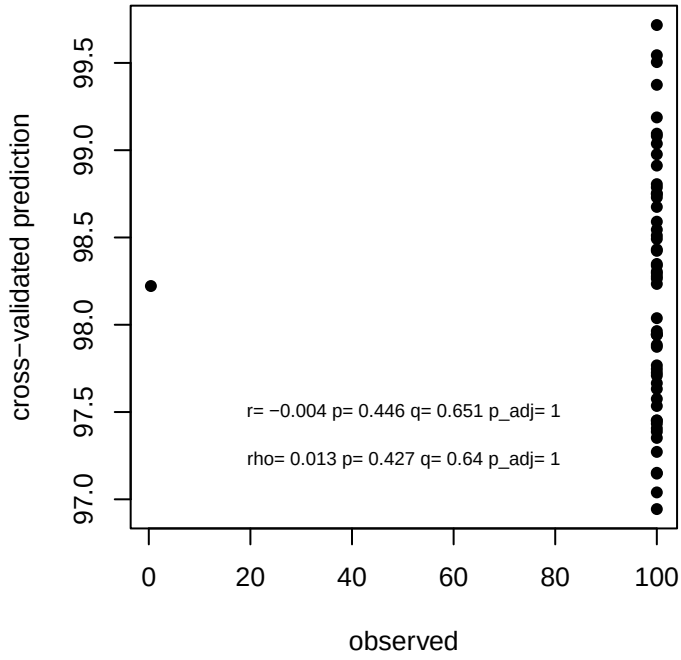
NEURONS_72hr_totaloutgrowth



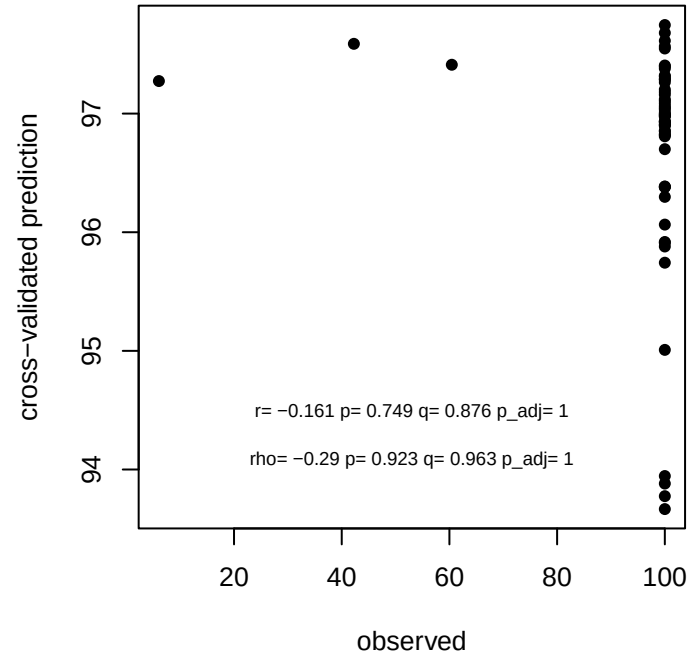
NEURONS_72hr_totalprocess



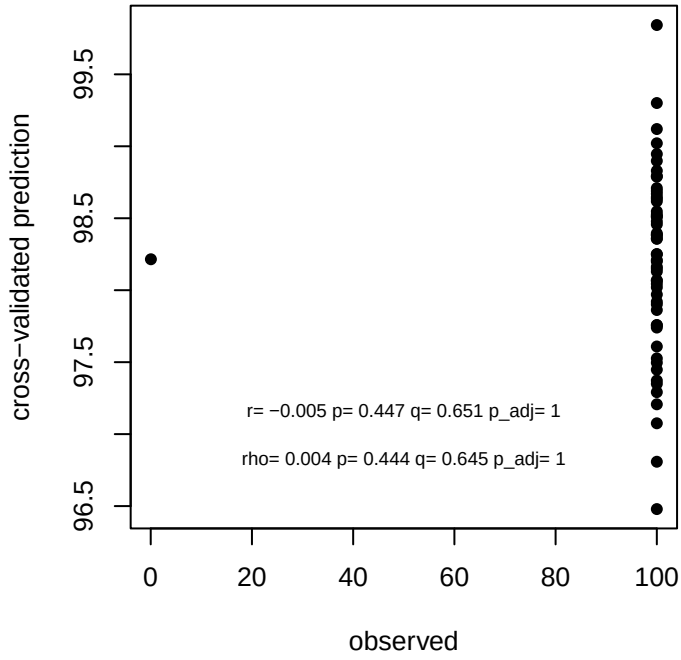
NEURONS_72hr_totalbranches



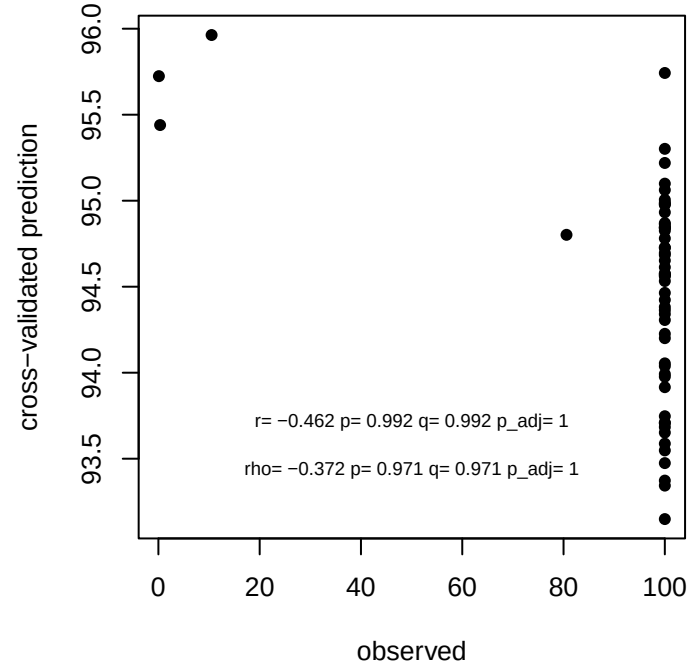
NEURONS_72hr_cellsiwithsignificantgrowth



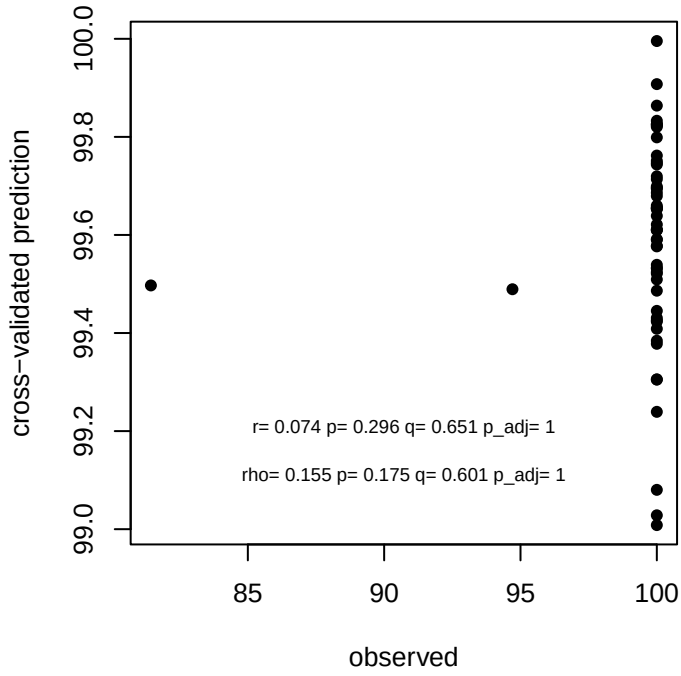
HEPATOCYTES_48hr_totalgranulearea



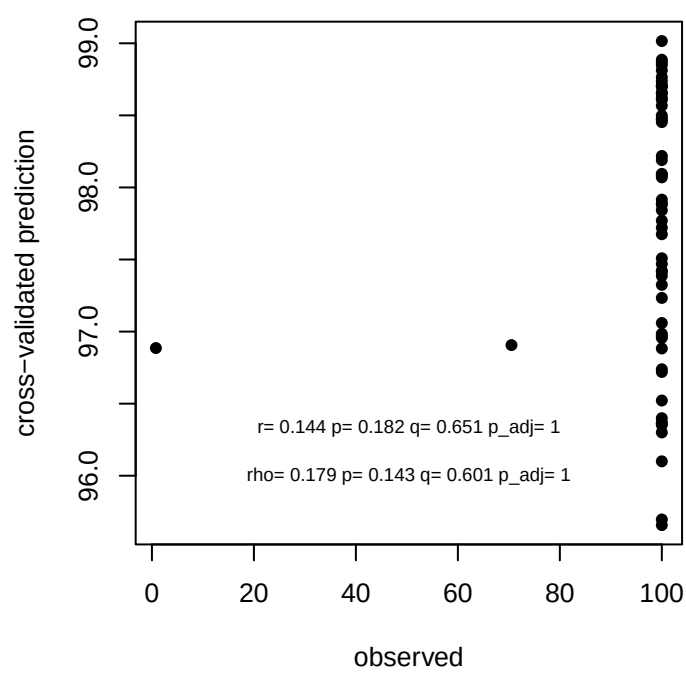
HEPATOCYTES_48hr_granularity



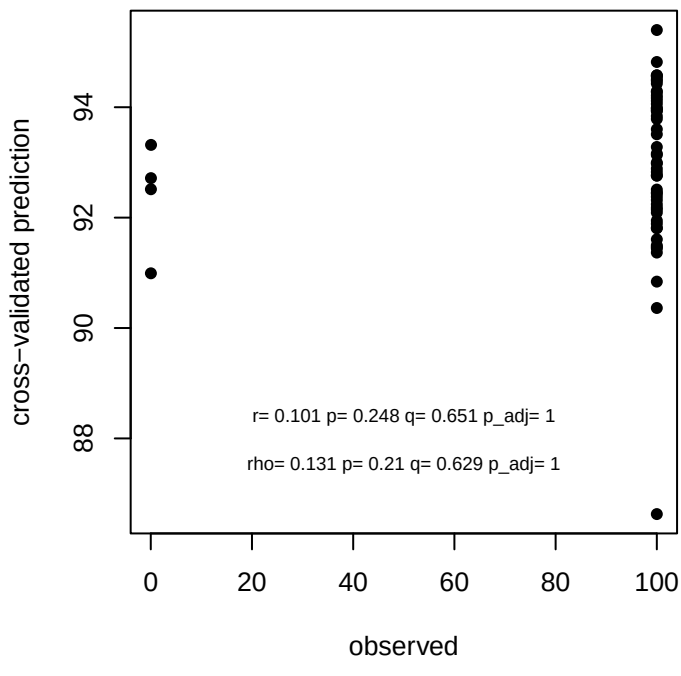
HEPATOCYTES_48hr_totalcells



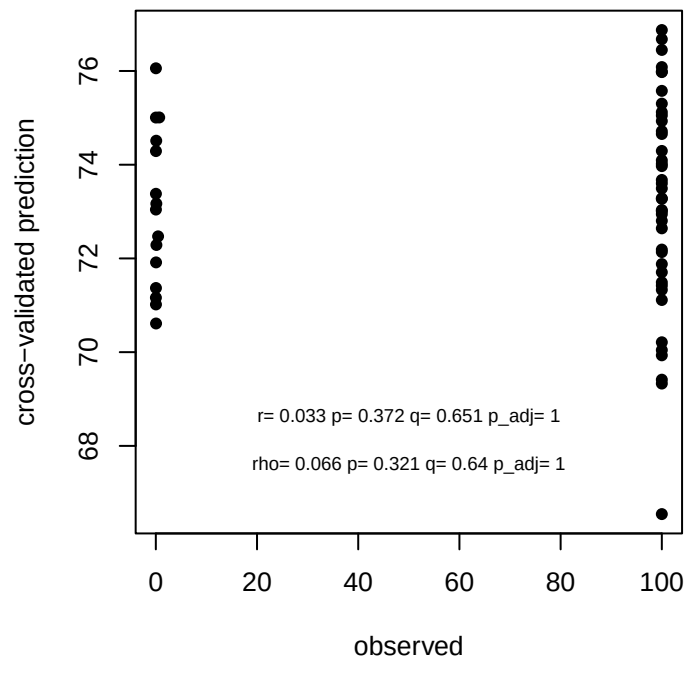
HEPATOCYTES_48hr_allcellsmeanarea



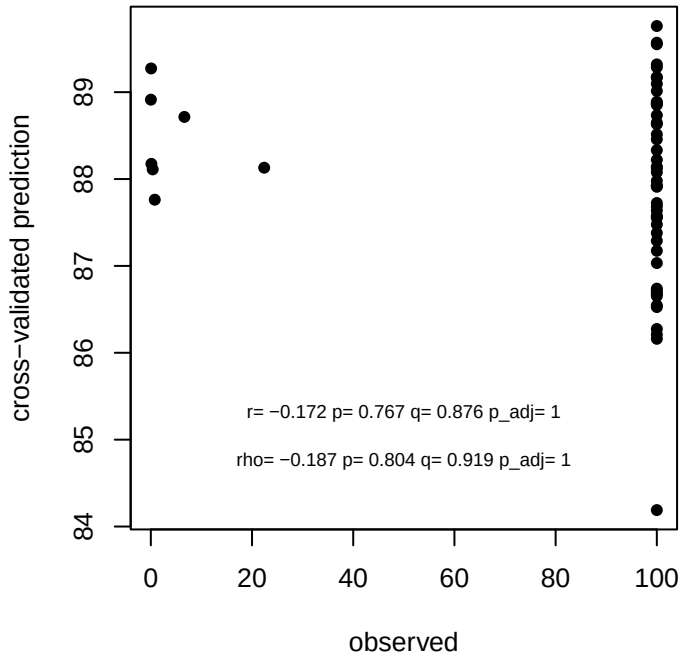
HEPATOCYTES_48hr_cytoplasmicintegrity



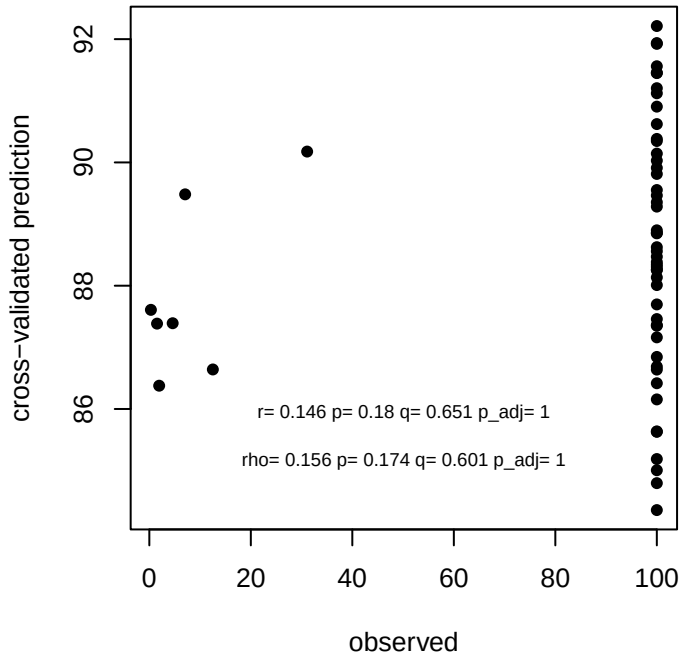
HEPATOCYTES_48hr_mitochondrialintegrity



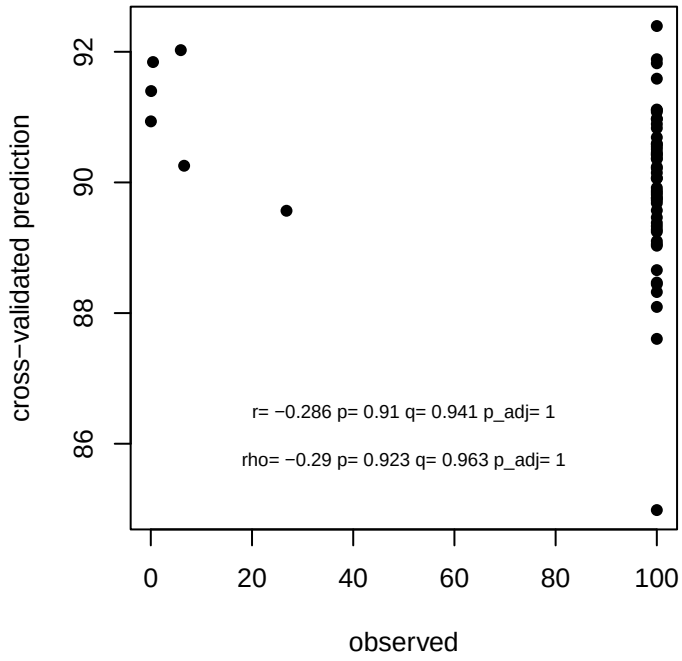
HEPATOCYTES_48hr_mitochondrialintensity



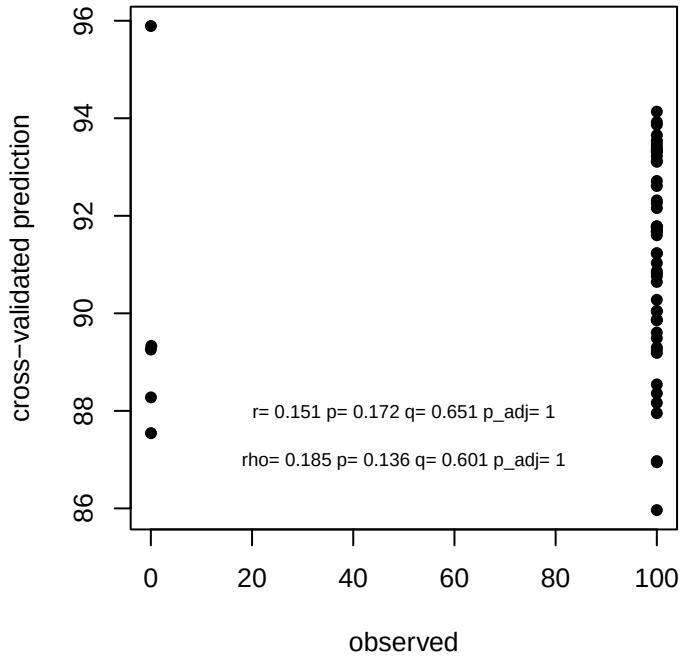
HEPATOCYTES_48hr_nucleiintensity

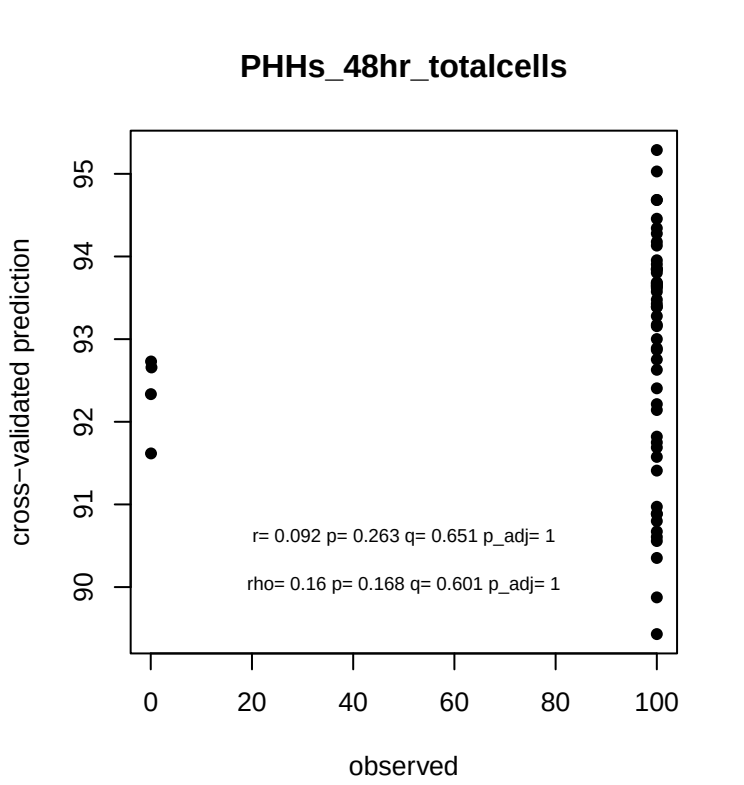


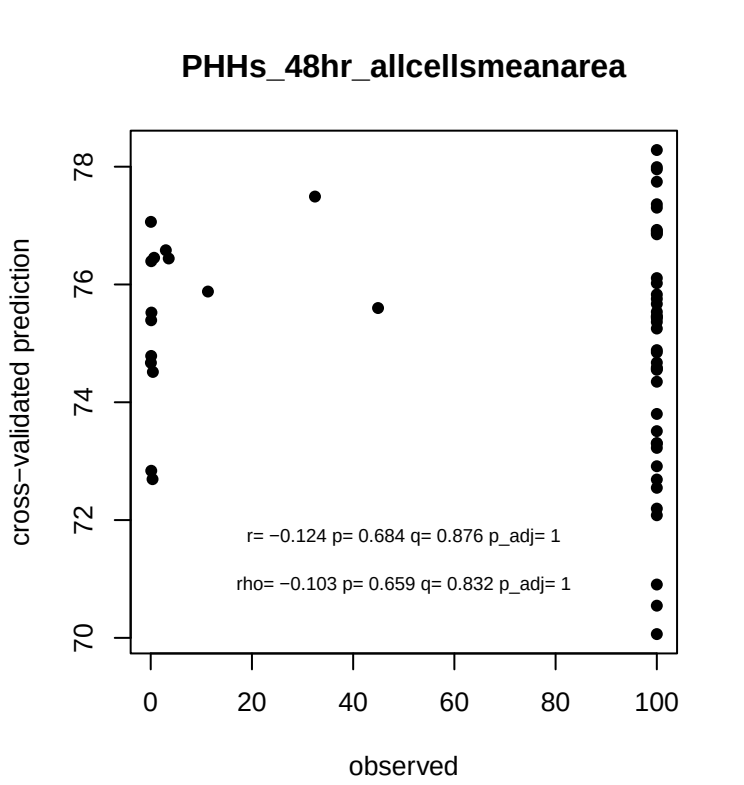
PHHs_48hr_totalgranulearea

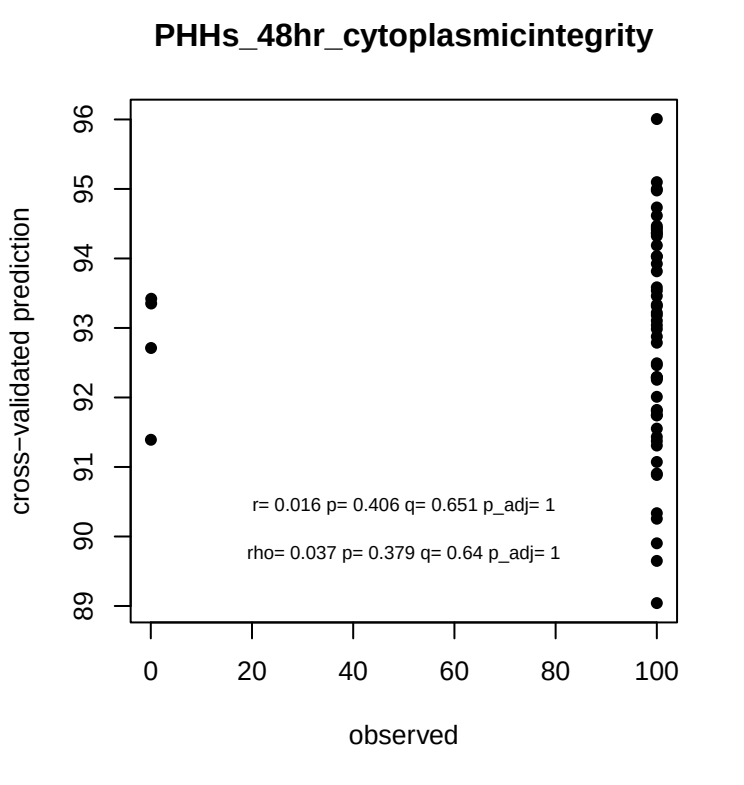


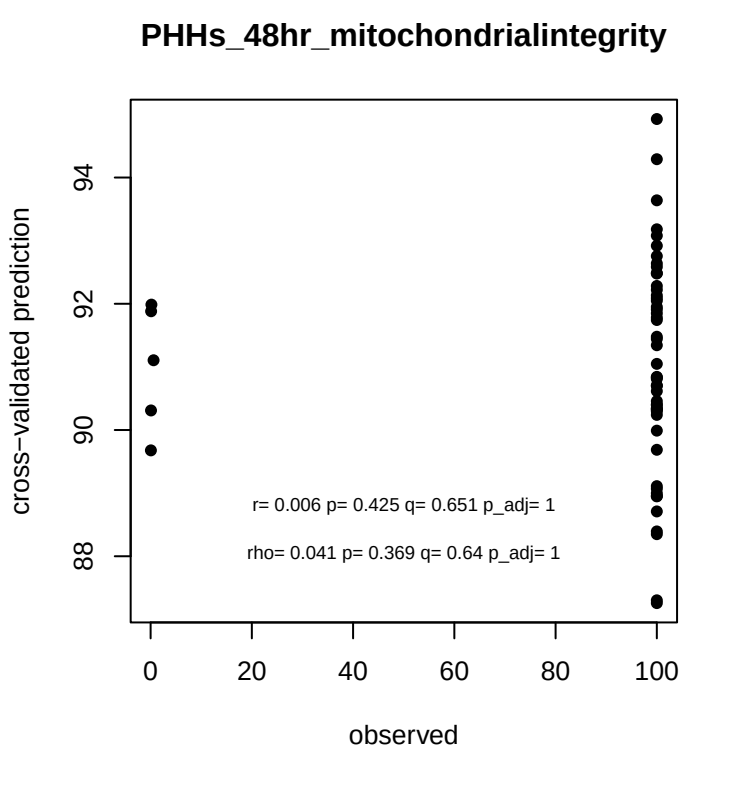
PHHs_48hr_granularity

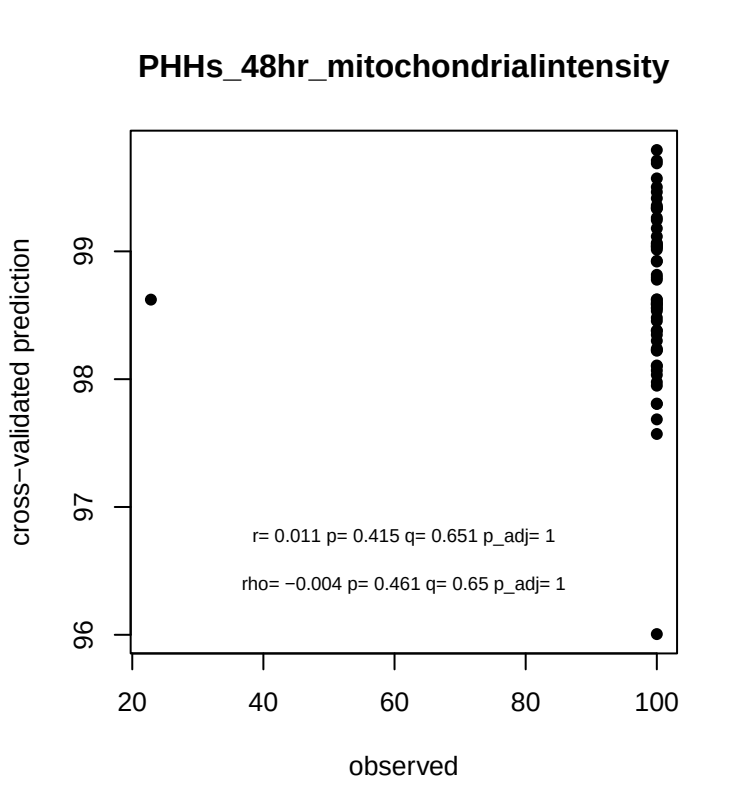


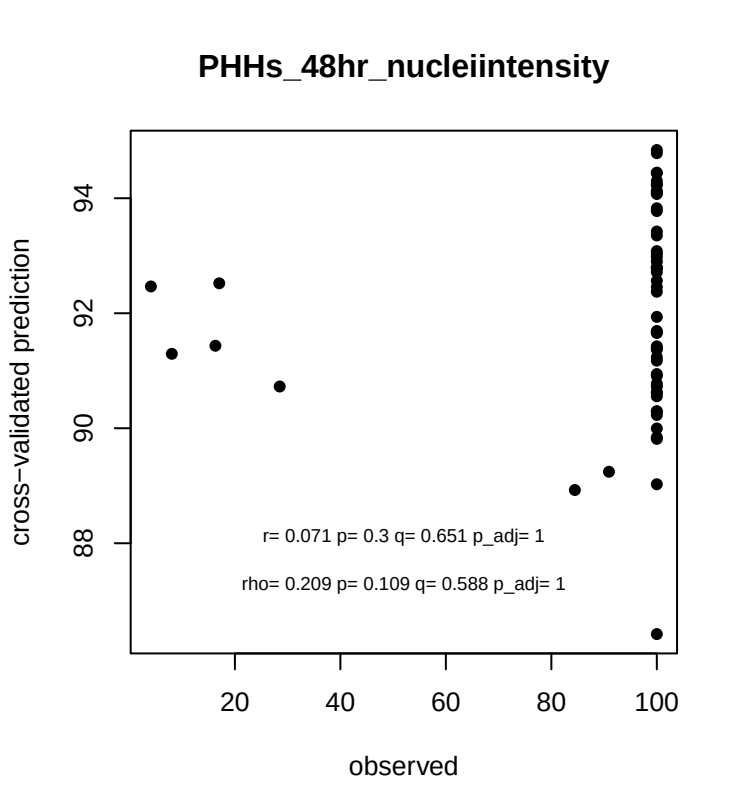

PHHs_48hr_totalcells
cross−validated prediction
observed
r= 0.092 p= 0.263 q= 0.651 p_adj= 1
rho= 0.16 p= 0.168 q= 0.601 p_adj= 1

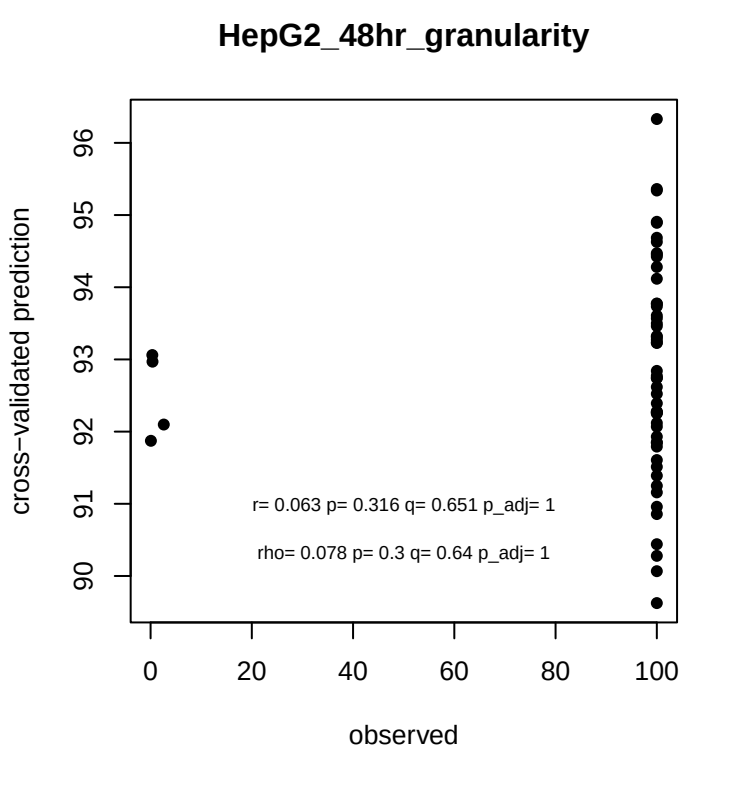

PHHs_48hr_allcellsmeanarea
cross−validated prediction
observed
r= −0.124 p= 0.684 q= 0.876 p_adj= 1
rho= −0.103 p= 0.659 q= 0.832 p_adj= 1

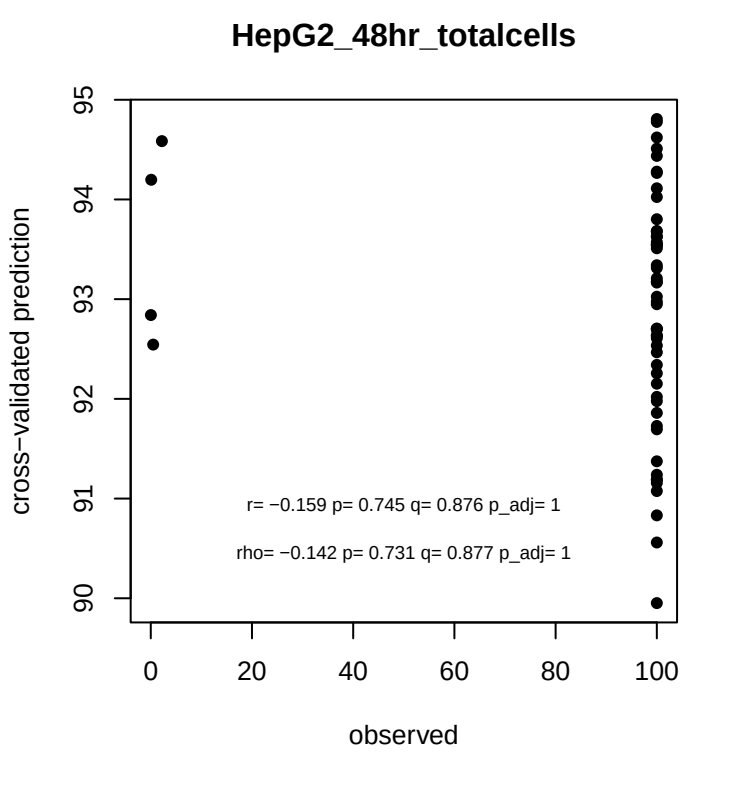

PHHs_48hr_cytoplasmicintegrity
cross−validated prediction
observed
r= 0.016 p= 0.406 q= 0.651 p_adj= 1
rho= 0.037 p= 0.379 q= 0.64 p_adj= 1


PHHs_48hr_mitochondrialintegrity
cross−validated prediction
observed
r= 0.006 p= 0.425 q= 0.651 p_adj= 1
rho= 0.041 p= 0.369 q= 0.64 p_adj= 1

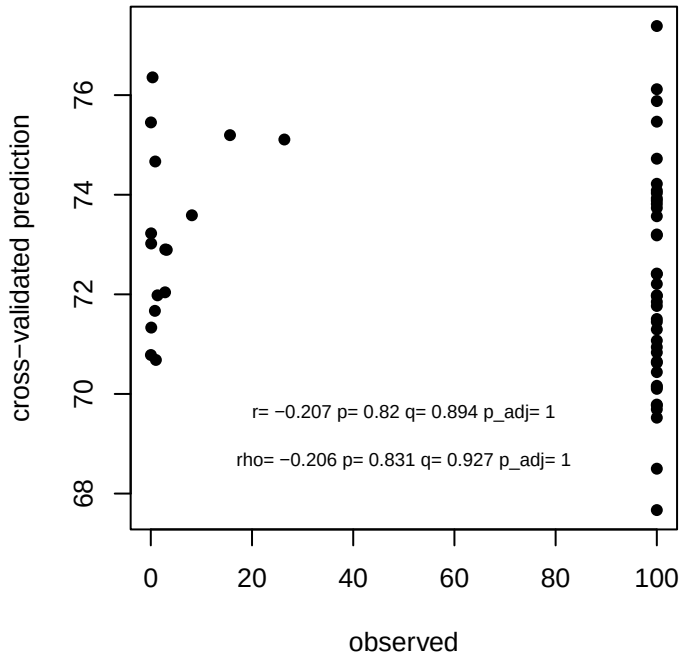

PHHs_48hr_mitochondrialintensity
cross−validated prediction
observed
r= 0.011 p= 0.415 q= 0.651 p_adj= 1
rho= −0.004 p= 0.461 q= 0.65 p_adj= 1


PHHs_48hr_nucleiintensity
cross−validated prediction
observed
r= 0.071 p= 0.3 q= 0.651 p_adj= 1
rho= 0.209 p= 0.109 q= 0.588 p_adj= 1

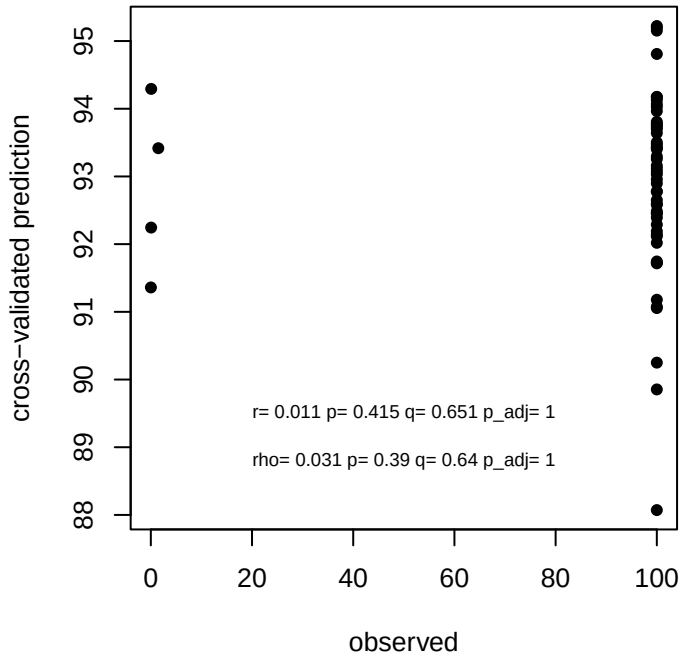

HepG2_48hr_granularity
cross−validated prediction
observed
r= 0.063 p= 0.316 q= 0.651 p_adj= 1
rho= 0.078 p= 0.3 q= 0.64 p_adj= 1


HepG2_48hr_totalcells
cross−validated prediction
observed
r= −0.159 p= 0.745 q= 0.876 p_adj= 1
rho= −0.142 p= 0.731 q= 0.877 p_adj= 1

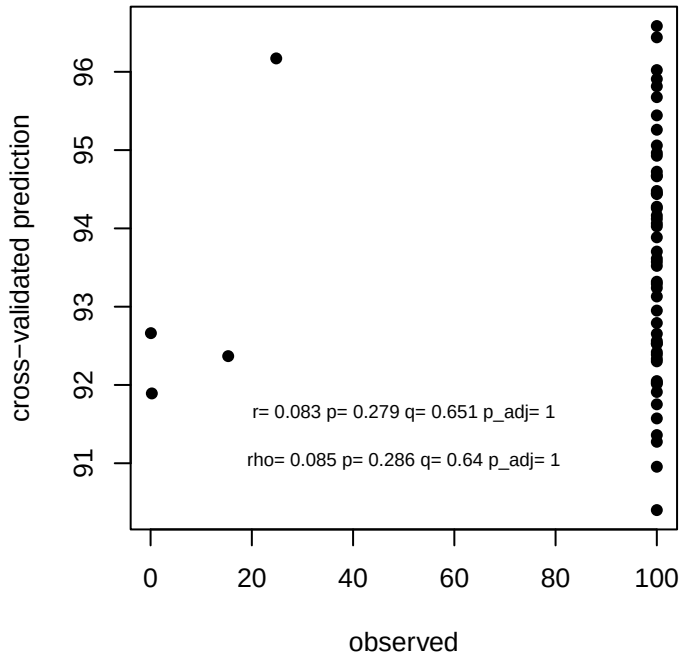
HepG2_48hr_allcellsmeanarea



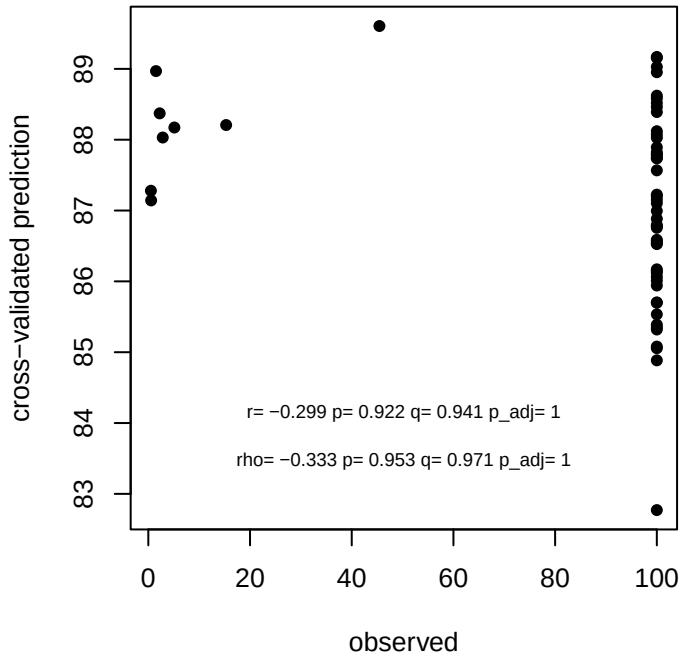
HepG2_48hr_cytoplasmicintegrity

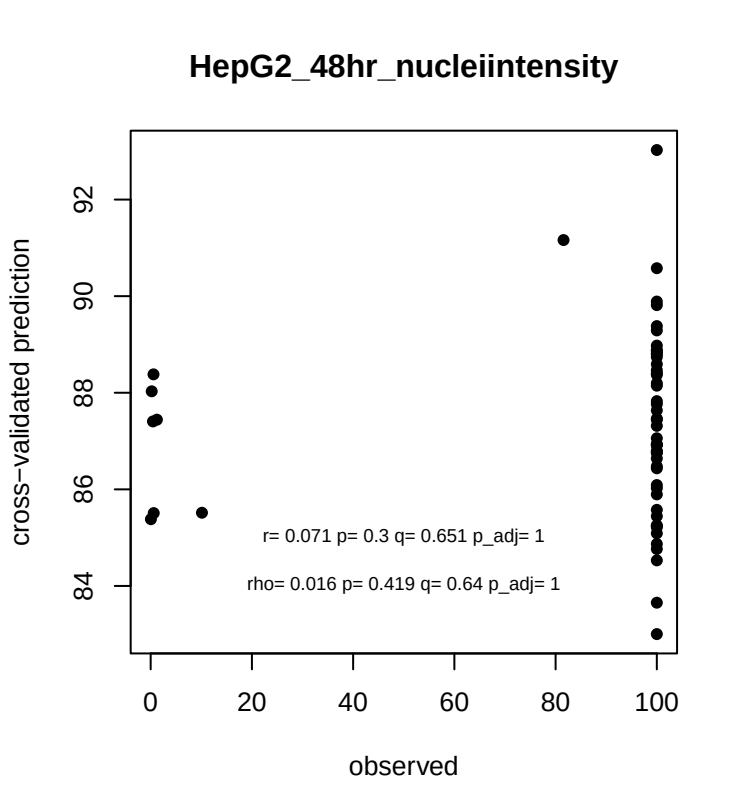


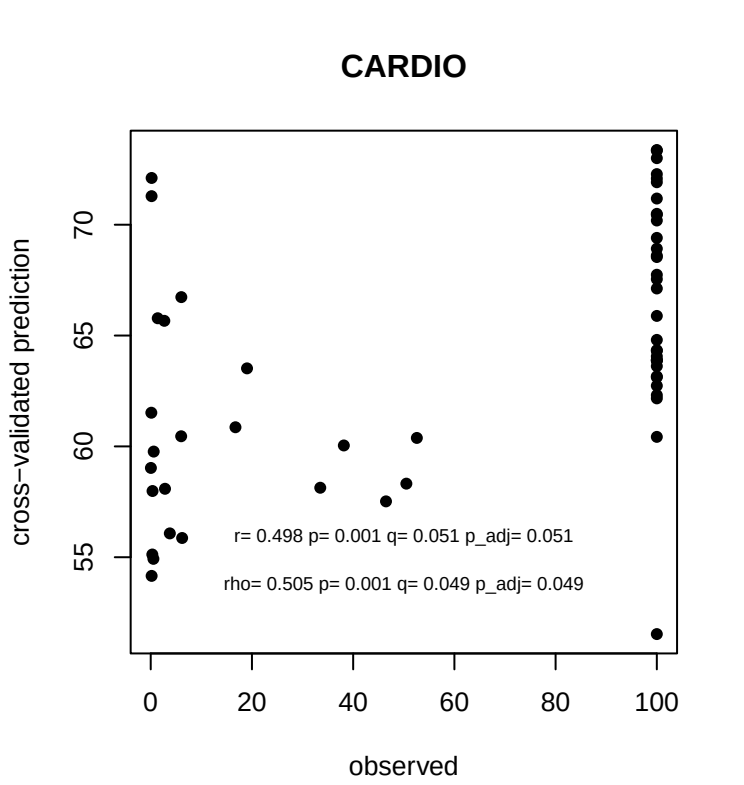
HepG2_48hr_mitochondrialintegrity

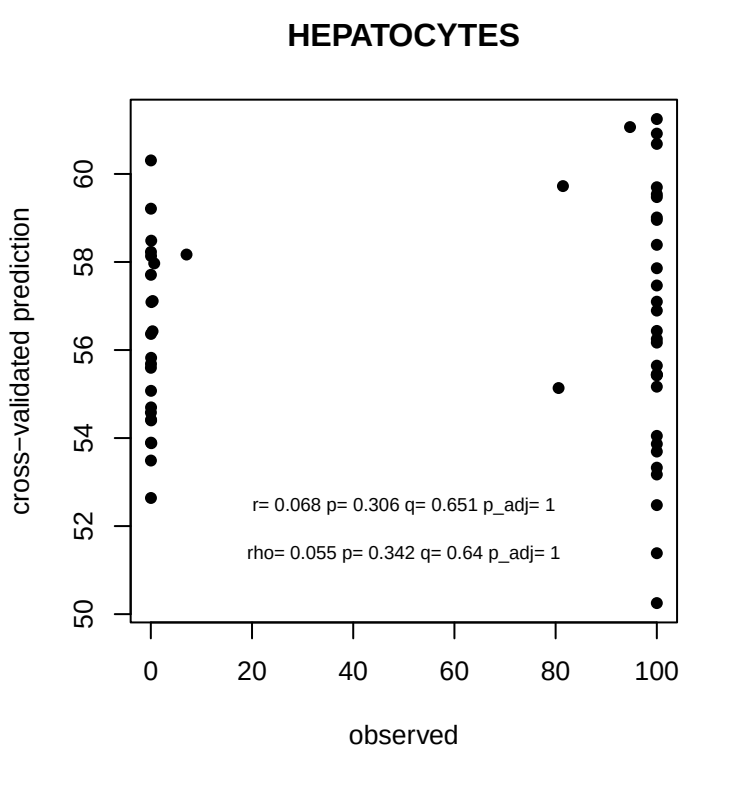


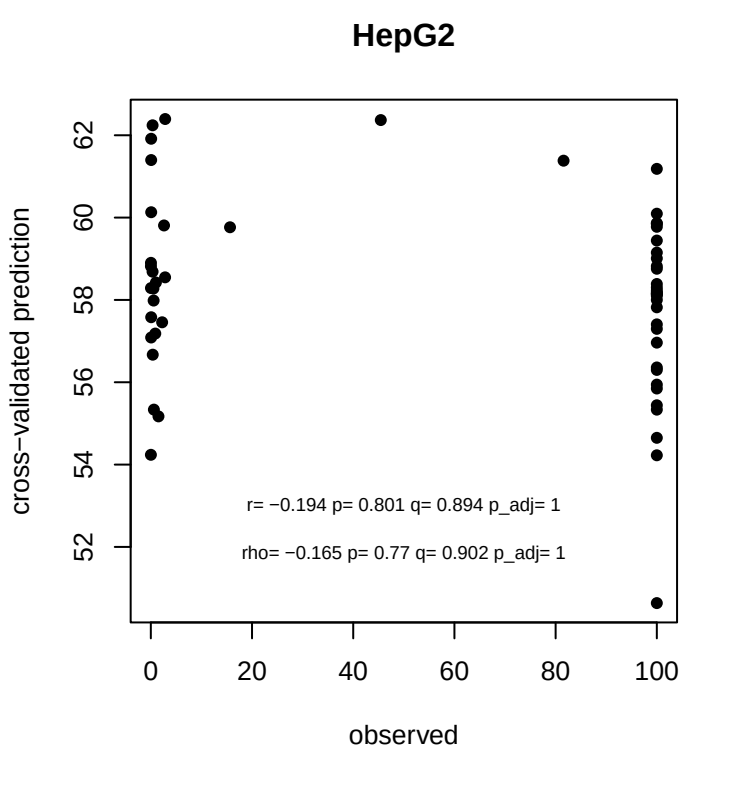
HepG2_48hr_mitochondrialintensity

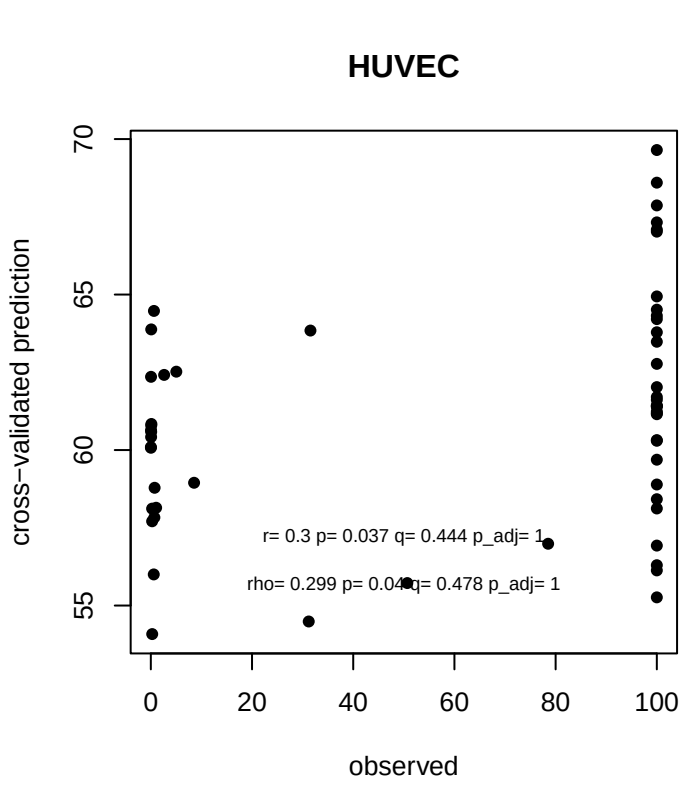


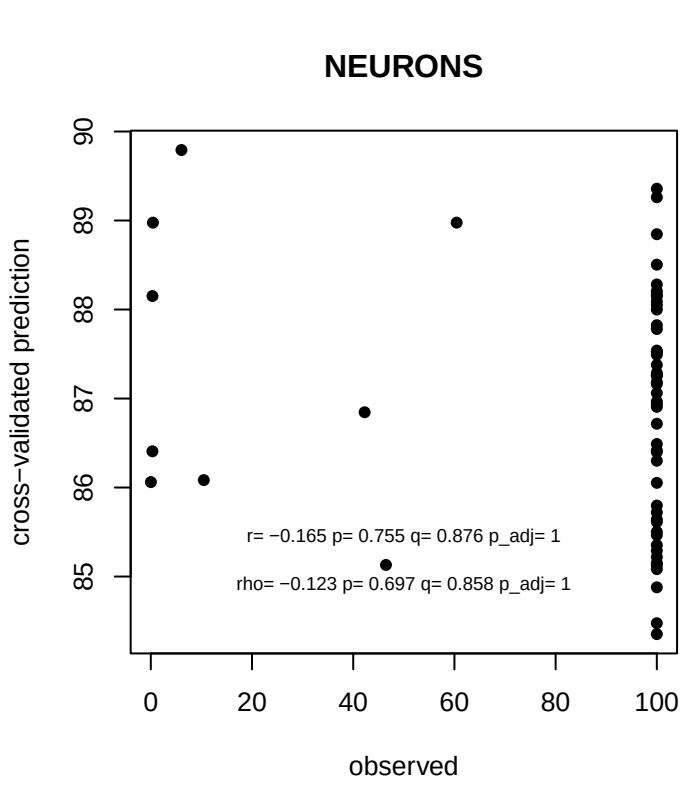

HepG2_48hr_nucleiintensity
cross−validated prediction
observed
r= 0.071 p= 0.3 q= 0.651 p_adj= 1
rho= 0.016 p= 0.419 q= 0.64 p_adj= 1

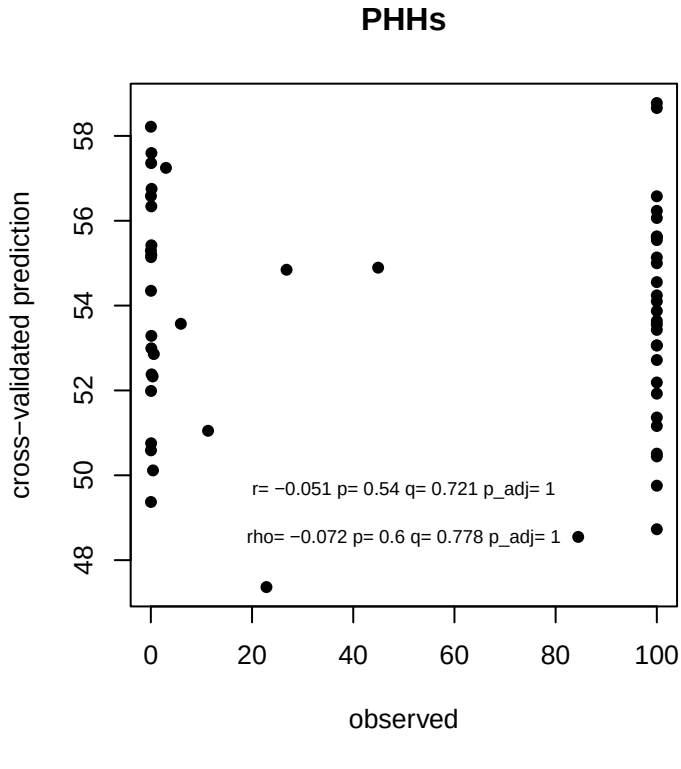

CARDIO
cross−validated prediction
observed
r= 0.498 p= 0.001 q= 0.051 p_adj= 0.051
rho= 0.505 p= 0.001 q= 0.049 p_adj= 0.049

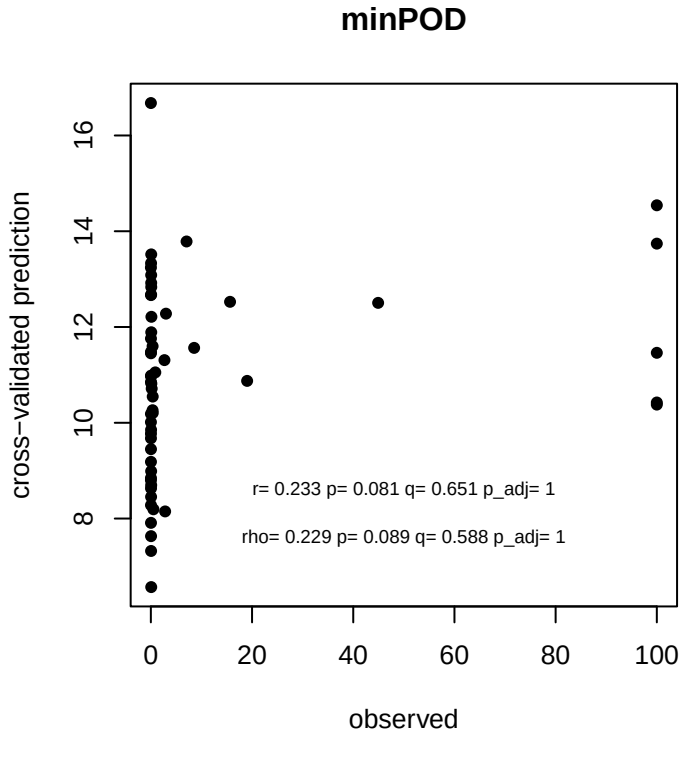

HEPATOCYTES
cross−validated prediction
observed
r= 0.068 p= 0.306 q= 0.651 p_adj= 1
rho= 0.055 p= 0.342 q= 0.64 p_adj= 1


HepG2
cross−validated prediction
observed
r= −0.194 p= 0.801 q= 0.894 p_adj= 1
rho= −0.165 p= 0.77 q= 0.902 p_adj= 1


HUVEC
cross−validated prediction
observed
r= 0.3 p= 0.037 q= 0.444 p_adj= 1
rho= 0.299 p= 0.04 q= 0.478 p_adj= 1


NEURONS
cross−validated prediction
observed
r= −0.165 p= 0.755 q= 0.876 p_adj= 1
rho= −0.123 p= 0.697 q= 0.858 p_adj= 1


PHHs
cross−validated prediction
observed
r= −0.051 p= 0.54 q= 0.721 p_adj= 1
rho= −0.072 p= 0.6 q= 0.778 p_adj= 1


minPOD
cross−validated prediction
observed
r= 0.233 p= 0.081 q= 0.651 p_adj= 1
rho= 0.229 p= 0.089 q= 0.588 p_adj= 1