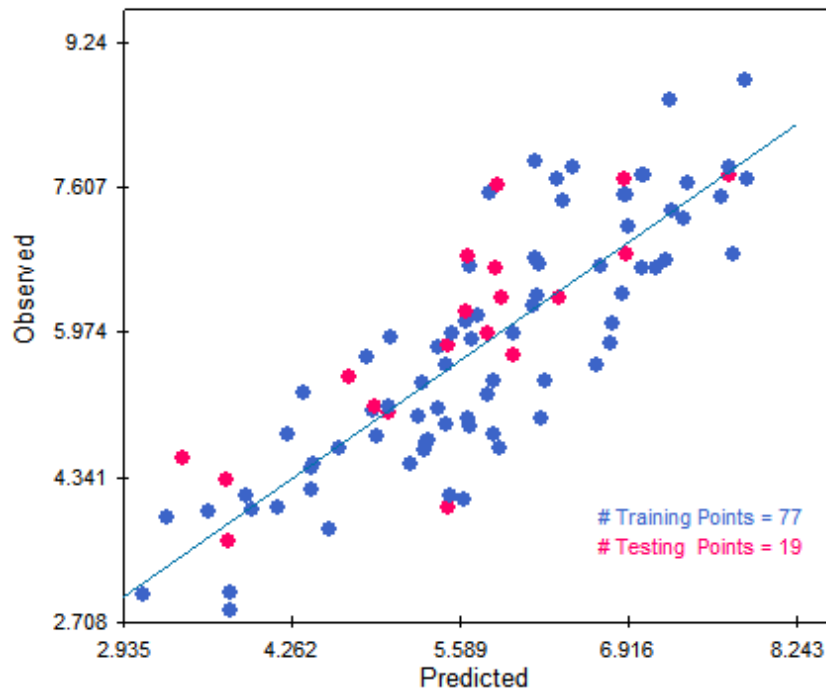


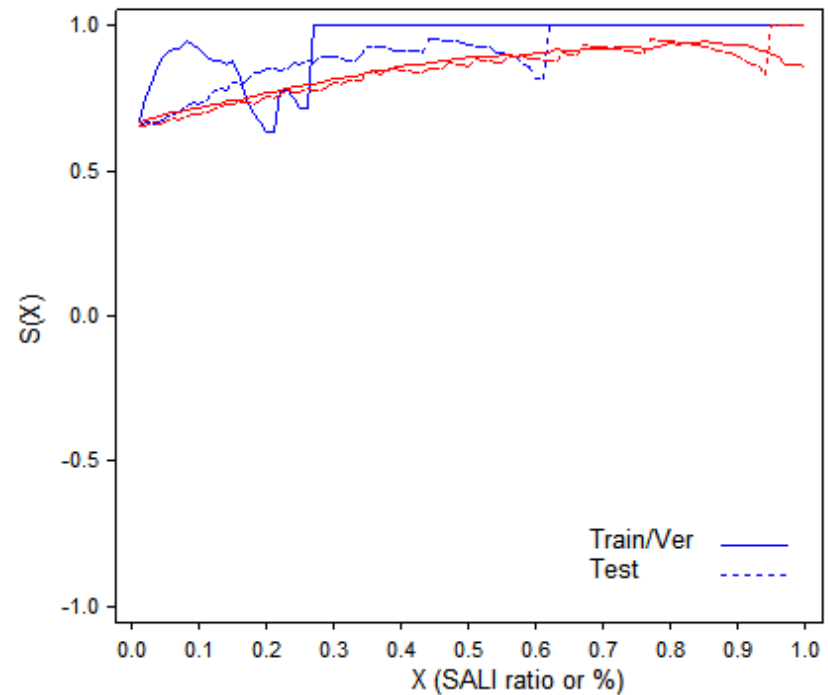
ANNE hERG model 1

- 7 descriptors
- 2 neurons



ALL: Slp=1.004 Int=0.049 QSqd=0.712 RMSE=0.729 MAE=0.575
TEST: Slp=0.921 Int=0.798 QSqd=0.594 RMSE=0.762 MAE=0.569

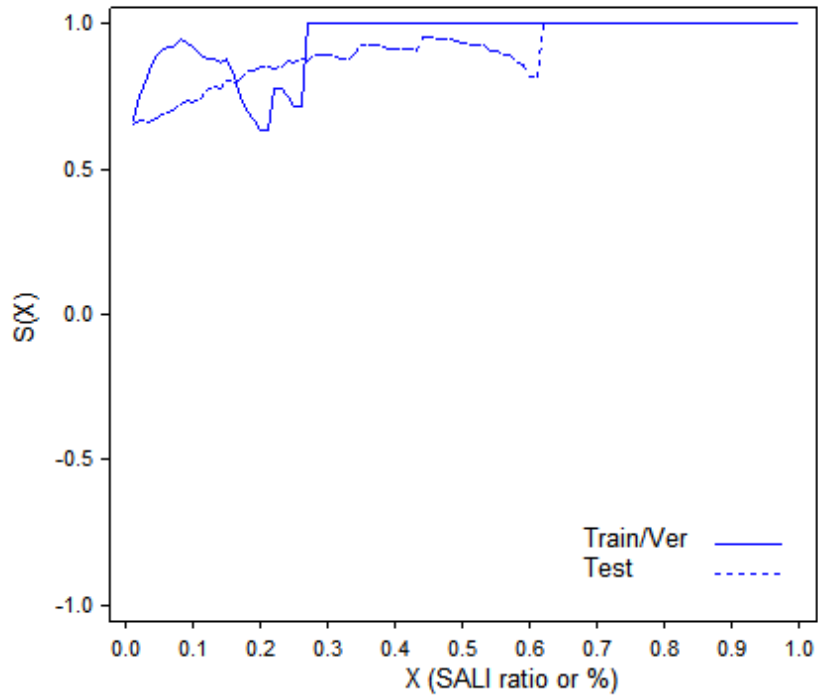
(a) Observed pIC_{50} vs prediction



Train/Ver SCI1=0.95 SCI2=0.852
Test SCI1=0.908 SCI2=0.845

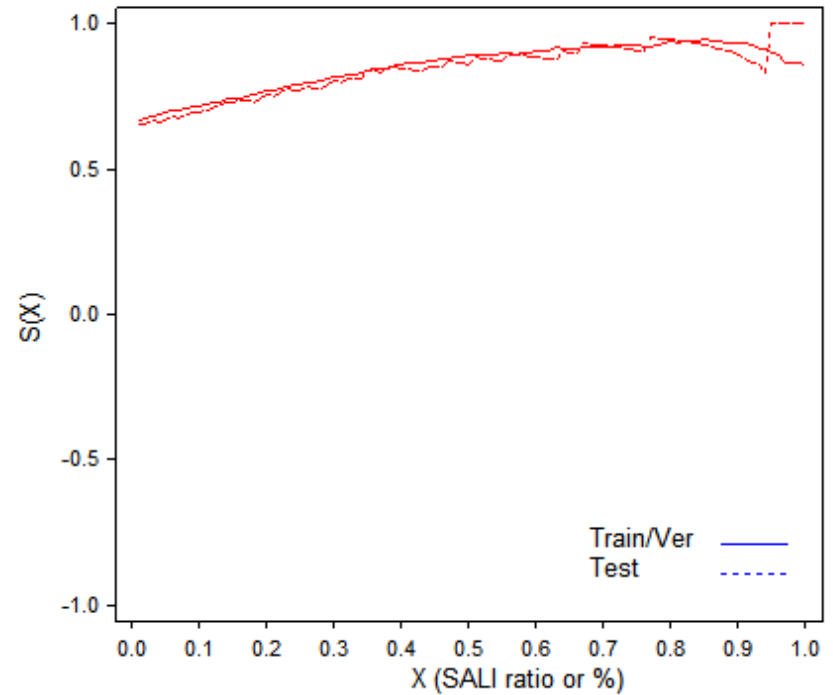
(b) SALI curves of train/Verify set and Test set for SALI ratio (blue) and SALI % (red)

ANNE hERG model 1 (2)



Train/Ver SCI1=0.95
Test SCI1=0.908

(c) SALI curves of train/Verify set and Test set for SALI ratio

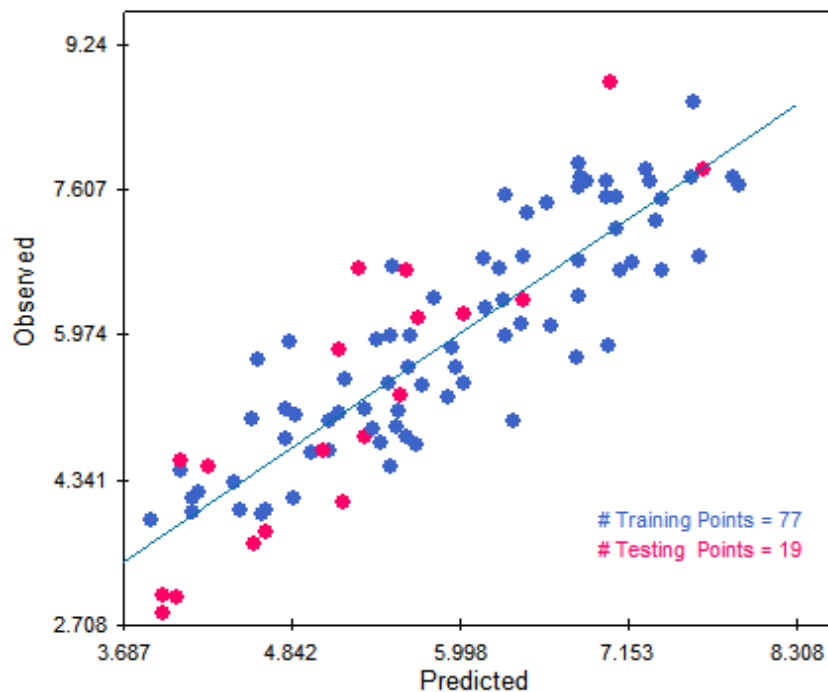


Train/Ver SCI2=0.852
Test SCI2=0.845

(d) SALI curves of train/Verify set and Test set for SALI %

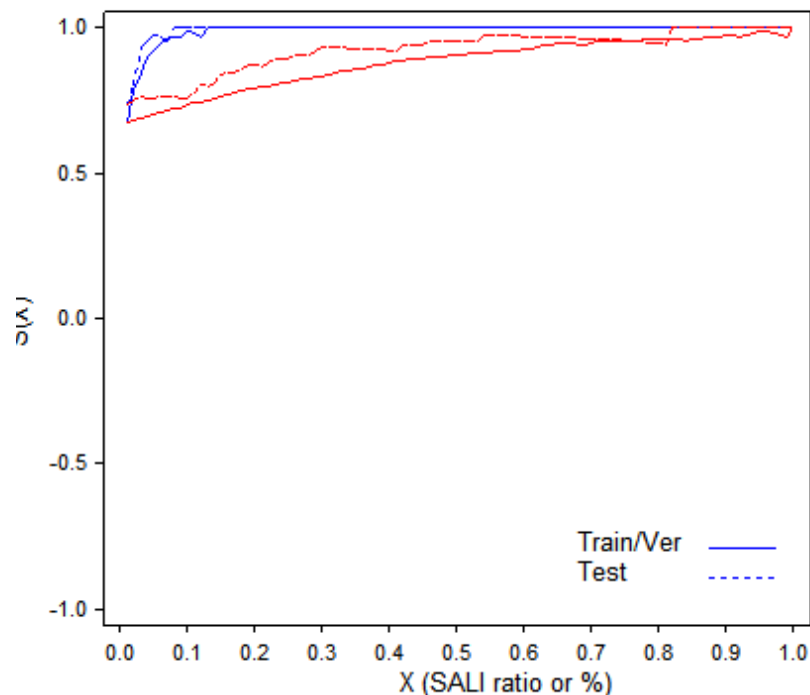
ANNE hERG model 2

- 10 descriptors
- 3 neurons



ALL: Slp=1.113 Int=-0.672 QSqd=0.761 RMSE=0.665 MAE=0.542
TEST: Slp=1.436 Int=-2.344 QSqd=0.723 RMSE=0.855 MAE=0.722

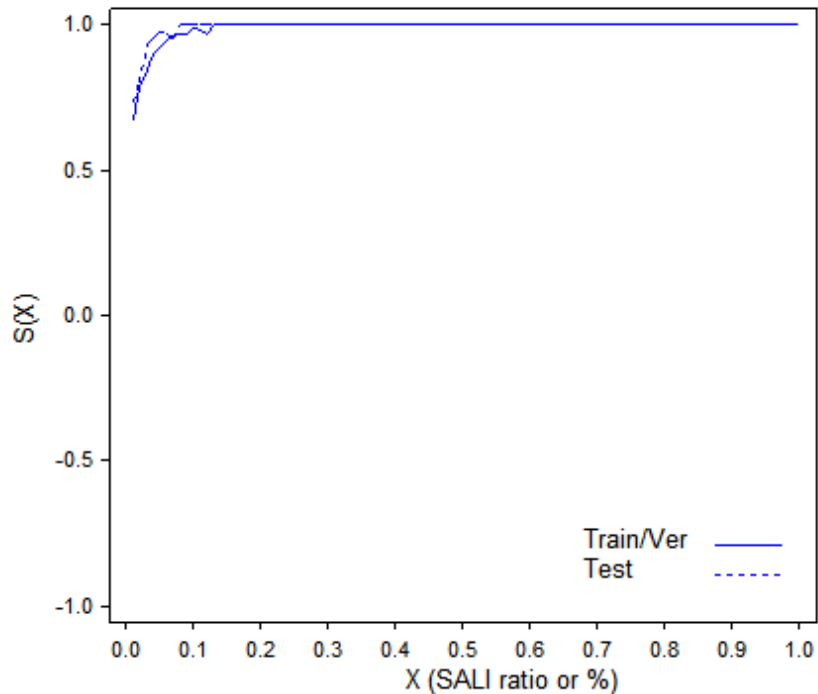
(a) Observed pIC_{50} vs prediction



Train/Ver SCI1=0.989 SCI2=0.88
Test SCI1=0.993 SCI2=0.925

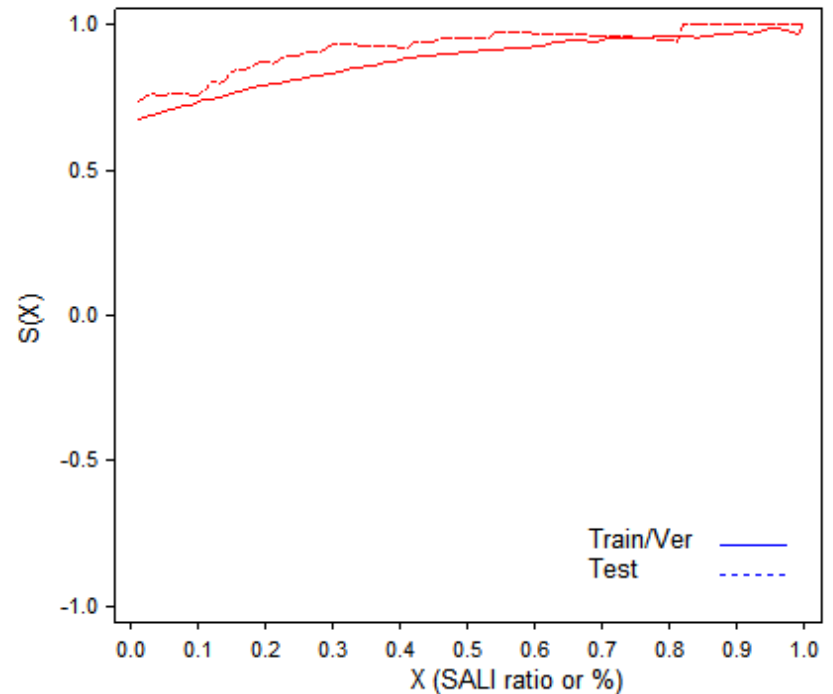
(b) SALI curves of train/Verify set and Test set for SALI ratio (blue) and SALI % (red)

ANNE hERG model 2 (2)



Train/Ver SCI1=0.989
Test SCI1=0.993

(c) SALI curves of train/Verify set and Test set for SALI ratio

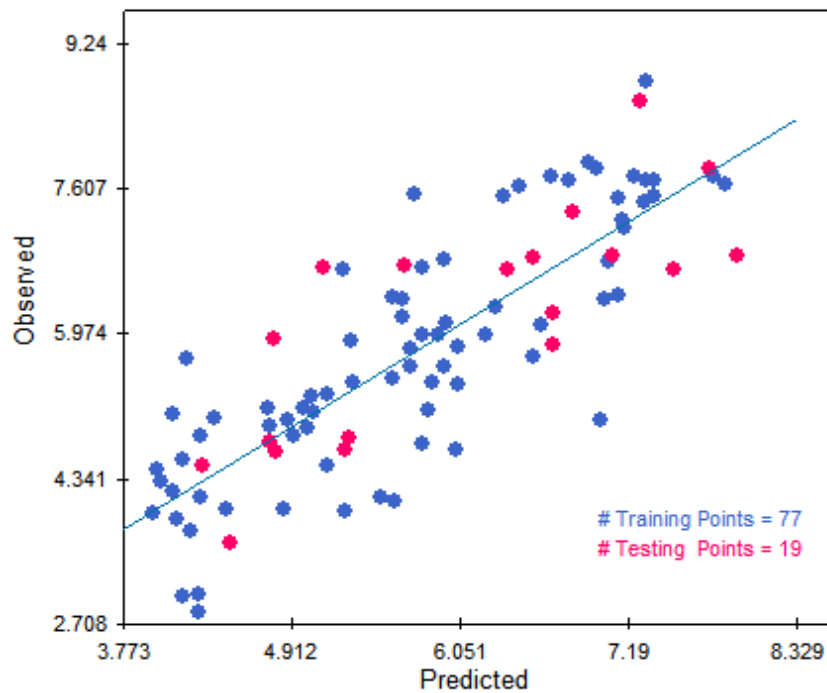


Train/Ver SCI2=0.88
Test SCI2=0.925

(d) SALI curves of train/Verify set and Test set for SALI %

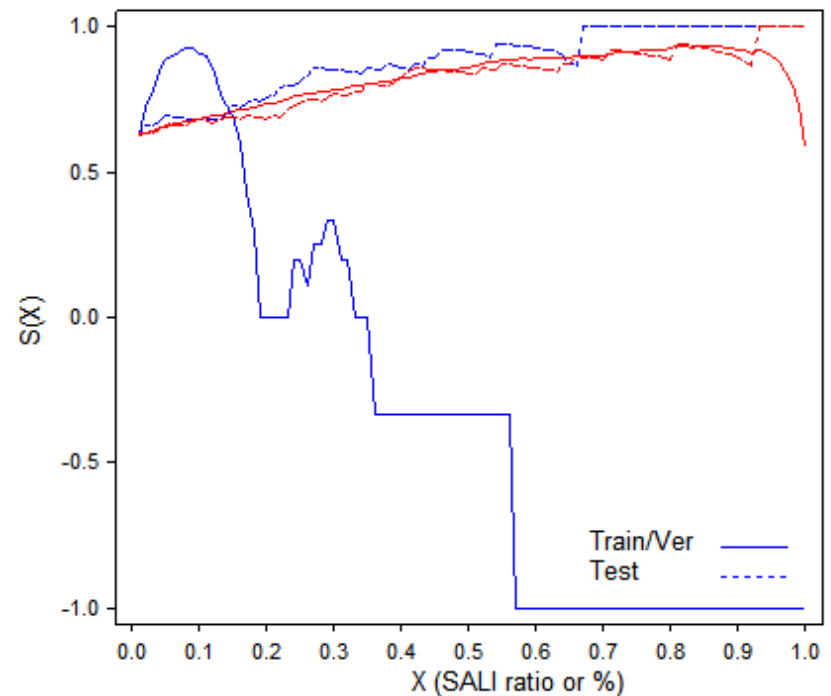
ANNE hERG model 3

- 13 descriptors
- 1 neuron



ALL: Slp=1.013 Int=-0.045 QSqd=0.679 RMSE=0.771 MAE=0.599
TEST: Slp=0.878 Int=0.788 QSqd=0.624 RMSE=0.775 MAE=0.635

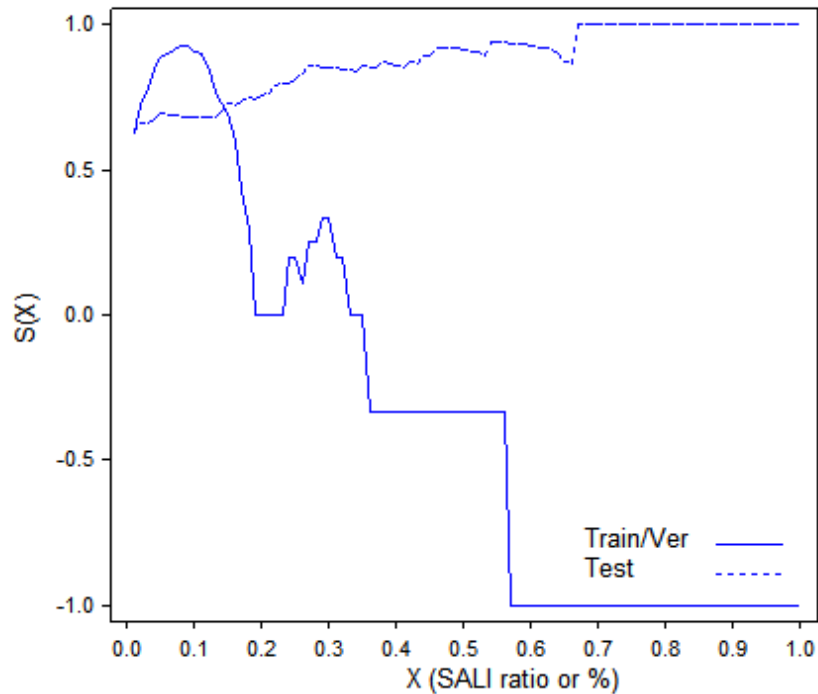
(a) Observed pIC_{50} vs prediction



Train/Ver SCI1=-0.352 SCI2=0.825
Test SCI1=0.883 SCI2=0.825

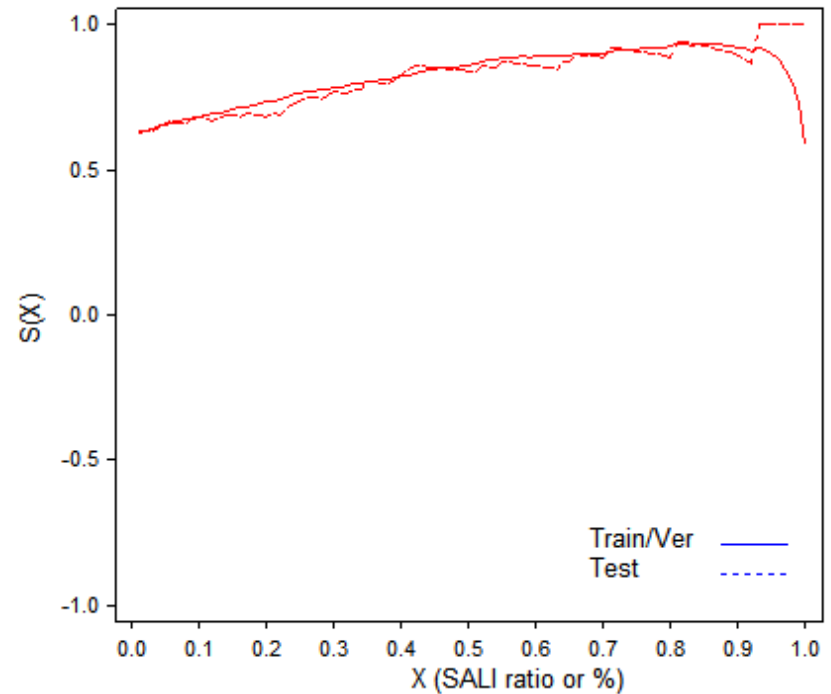
(b) SALI curves of train/Verify set and Test set for SALI ratio (blue) and SALI % (red)

ANNE hERG model 3 (2)



Train/Ver SCI1=-0.352
Test SCI1=0.883

(c) SALI curves of train/Verify set and Test set for SALI ratio

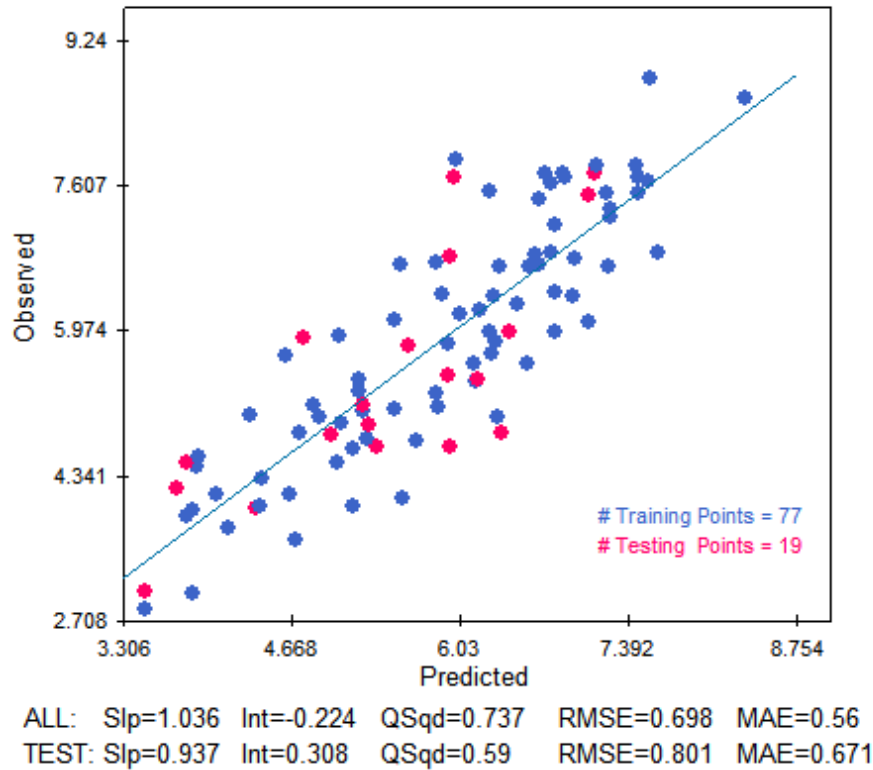


Train/Ver SCI2=0.825
Test SCI2=0.825

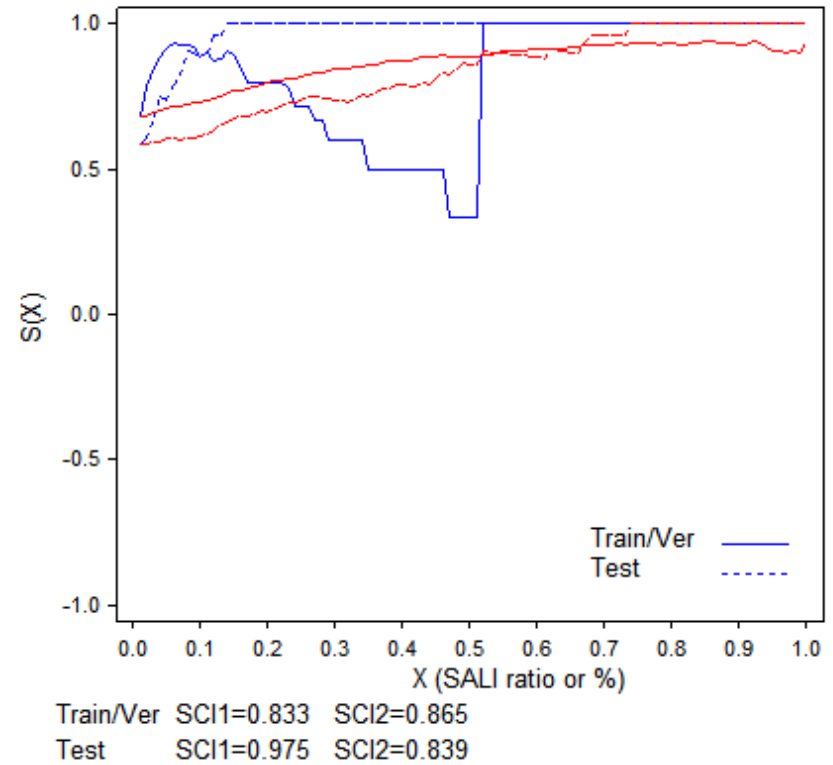
(d) SALI curves of train/Verify set and Test set for SALI %

ANNE hERG model 4

- 13 descriptors
- 2 neuronS

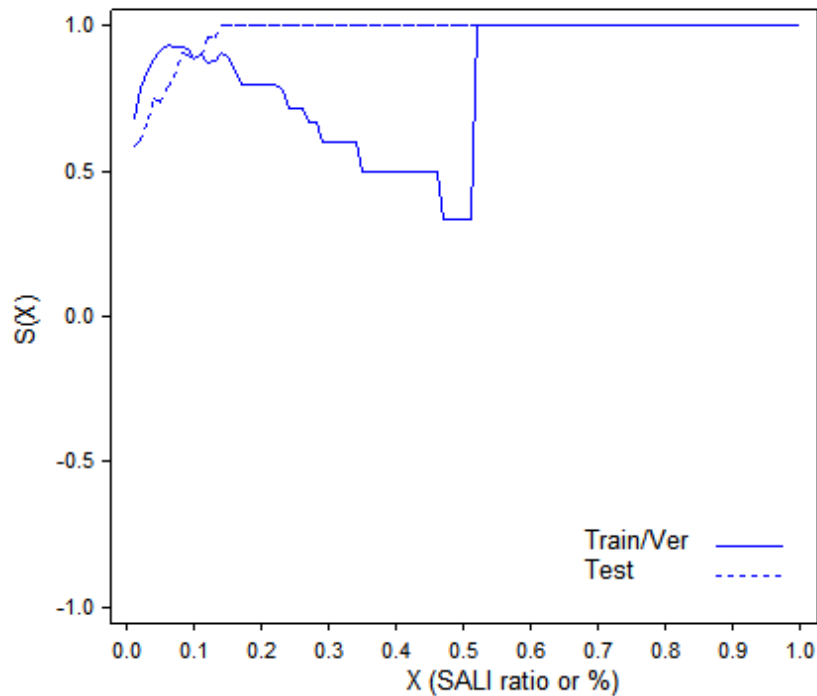


(a) Observed pIC_{50} vs prediction



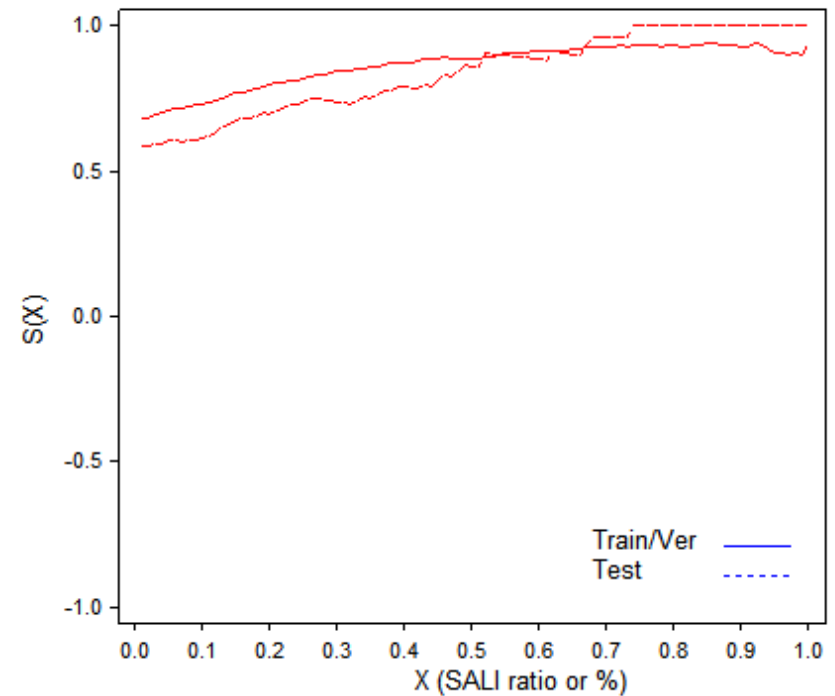
(b) SALI curves of train/Verify set and Test set for SALI ratio (blue) and SALI % (red)

ANNE hERG model 4 (2)



Train/Ver SCI1=0.833
Test SCI1=0.975

(c) SALI curves of train/Verify set and Test set for SALI ratio



Train/Ver SCI2=0.865
Test SCI2=0.839

(d) SALI curves of train/Verify set and Test set for SALI %