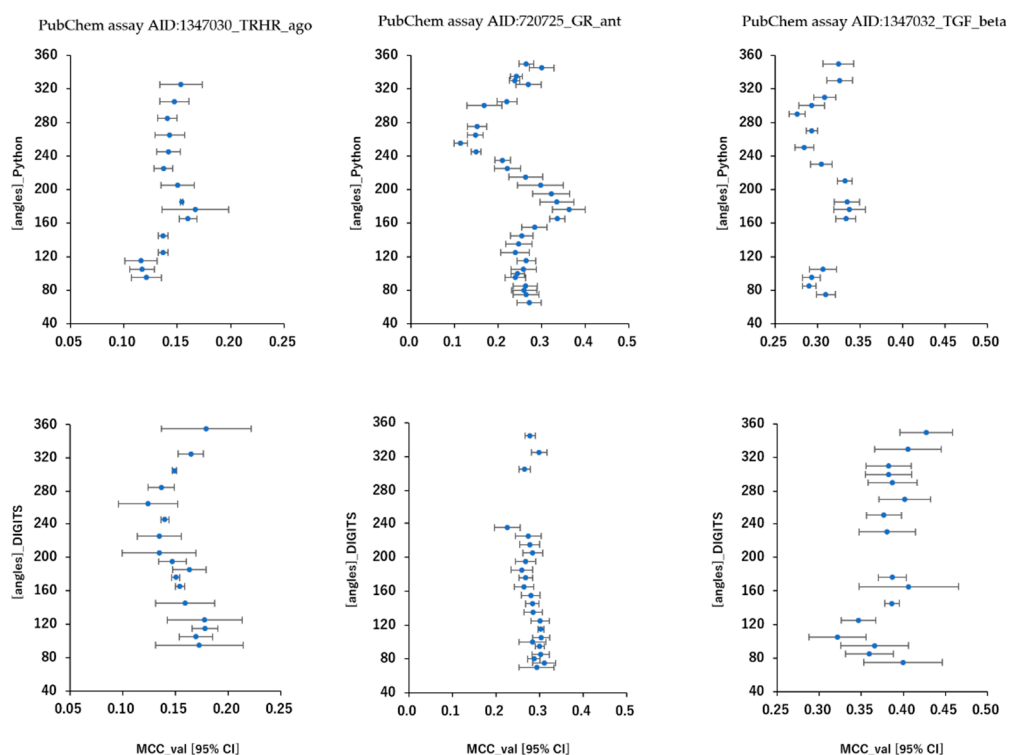Figure S1

Figure S1. MCC with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.
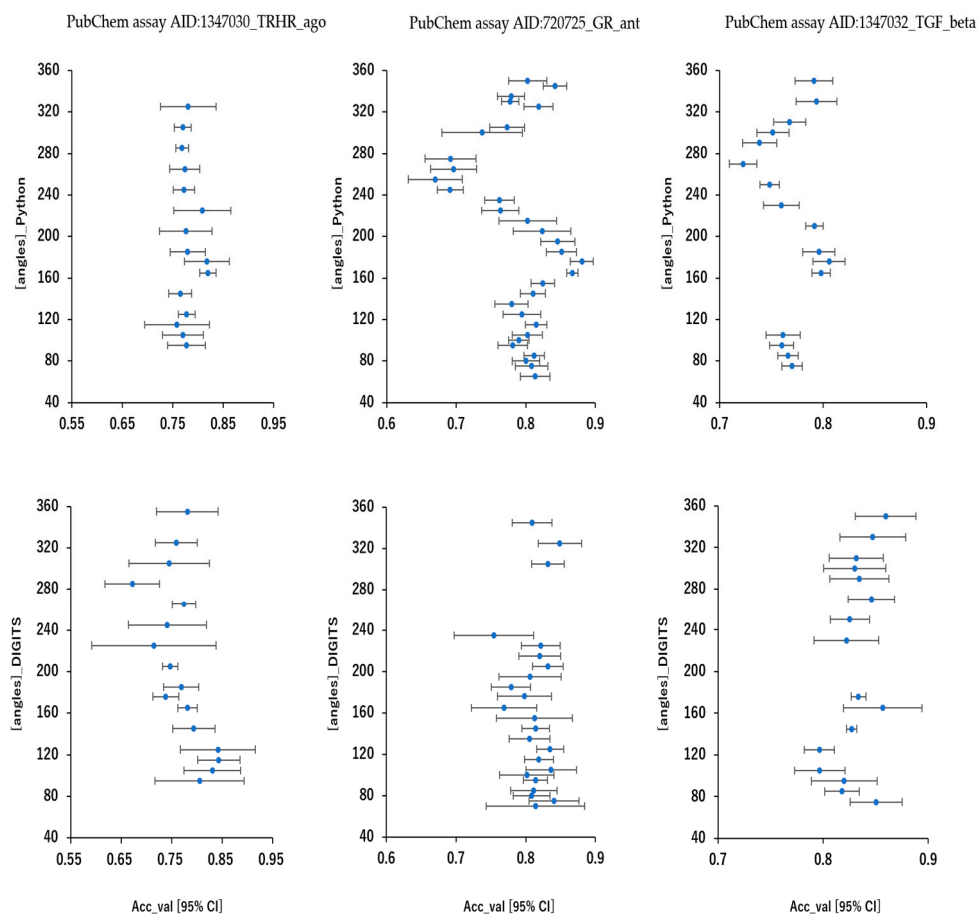
Figure S2

Figure S2. Differences in mean MCC levels shown as dots with 95% confident interval (95% CI) as error bars with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.
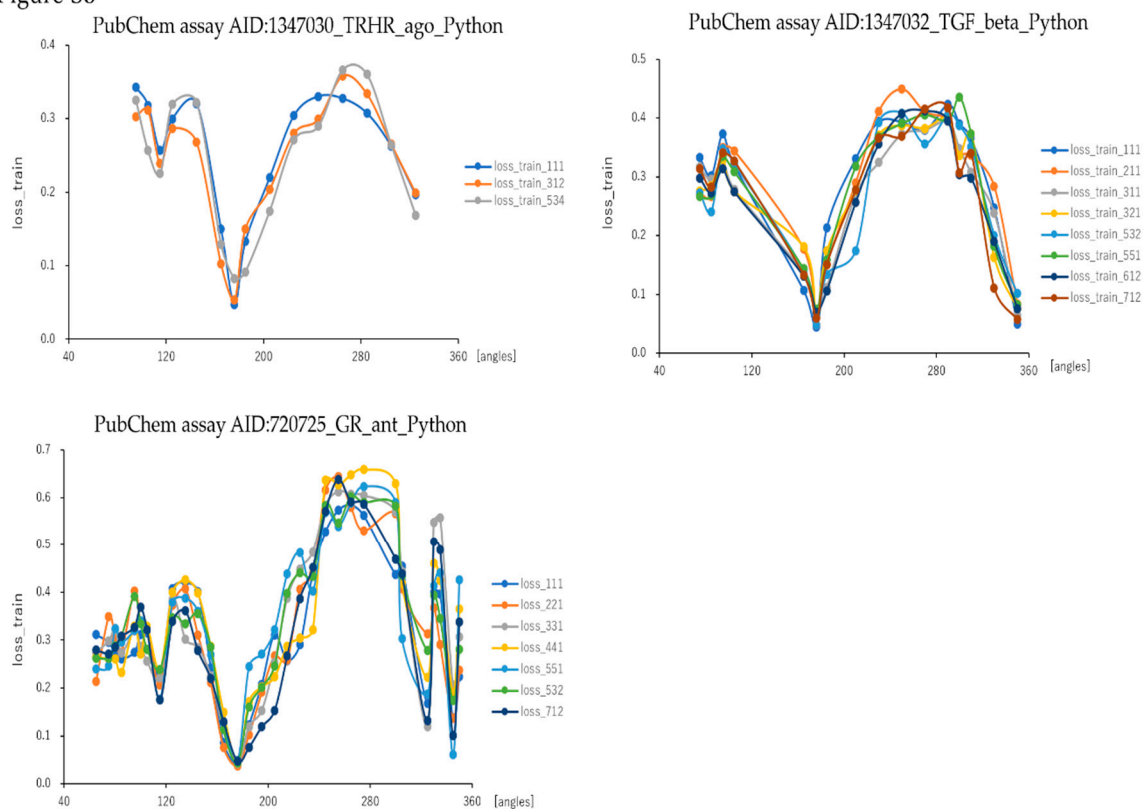
Figure S3

Figure S3. Acc with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n=3.
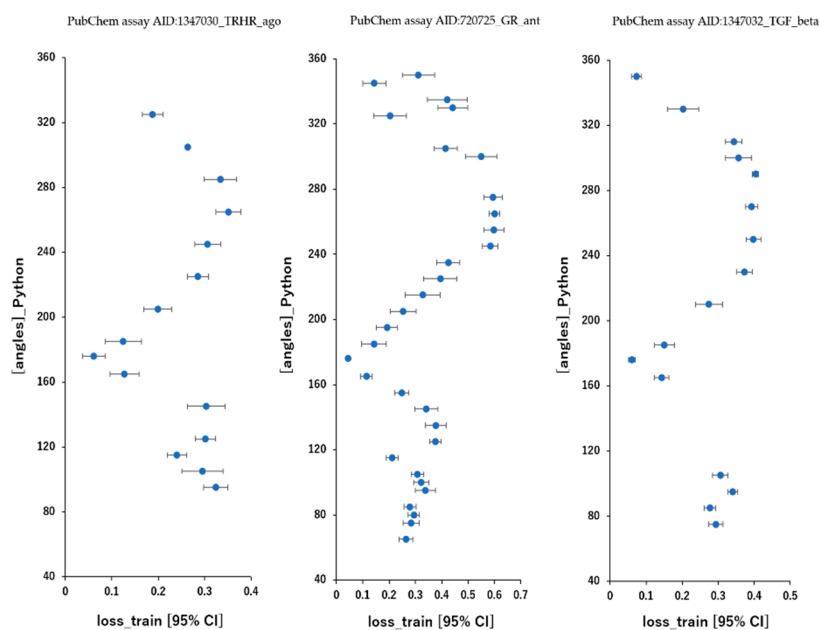
Figure S4

Figure S4. Differences in mean Acc levels shown as dots with 95% confident interval (95% CI) as error bars with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.
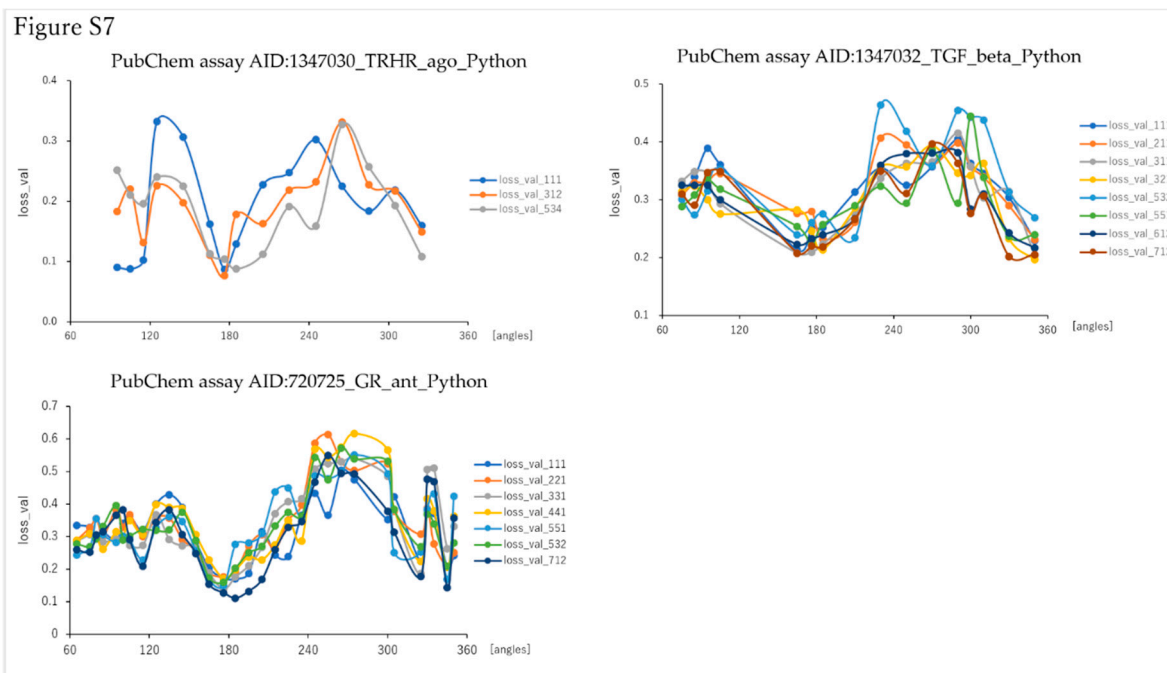
Figure S5

Figure S5. Loss with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the training dataset; n = 3.
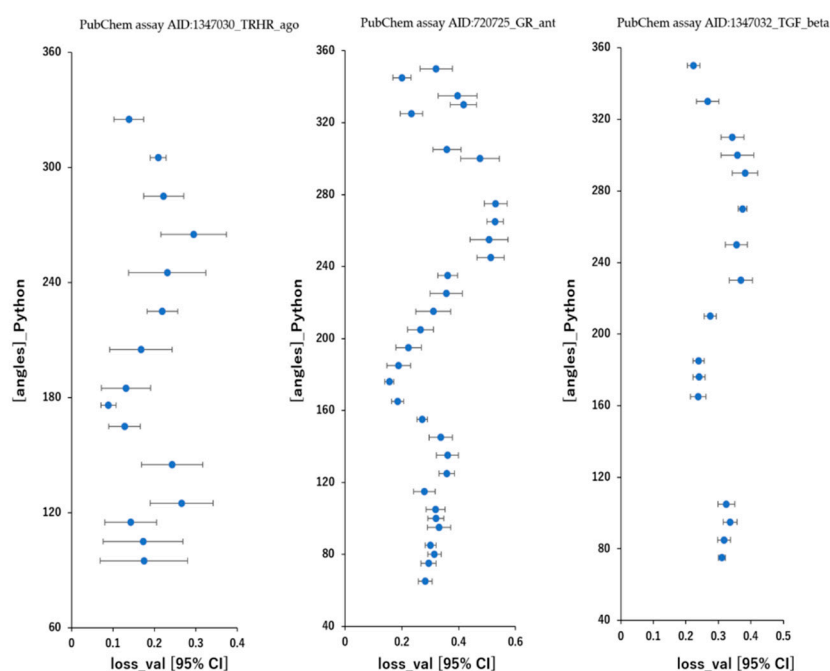
Figure S6

Figure S6. Differences in mean loss levels shown as dots with 95% confident interval (95% CI) as error bars with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the training dataset; n = 3.
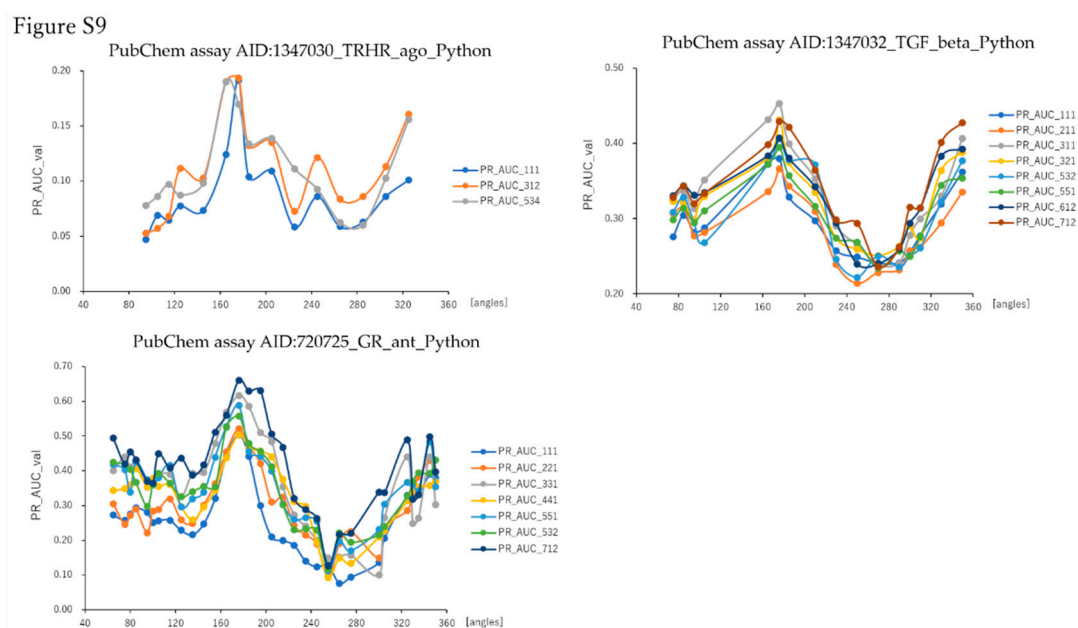
Figure S7

Figure S7. Loss with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.
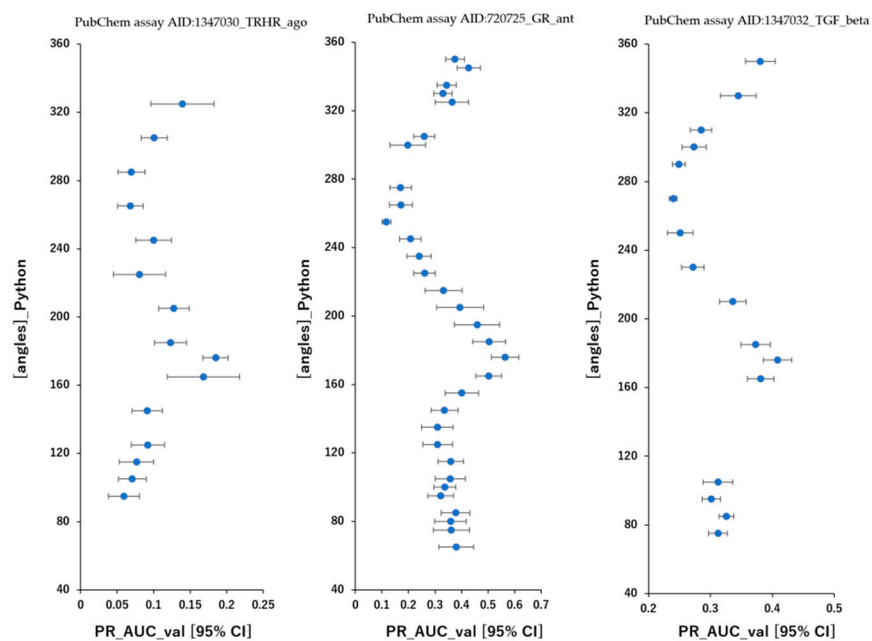
Figure S8

Figure S8. Differences in mean loss levels shown as dots with 95% confident interval (95% CI) as error bars with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.
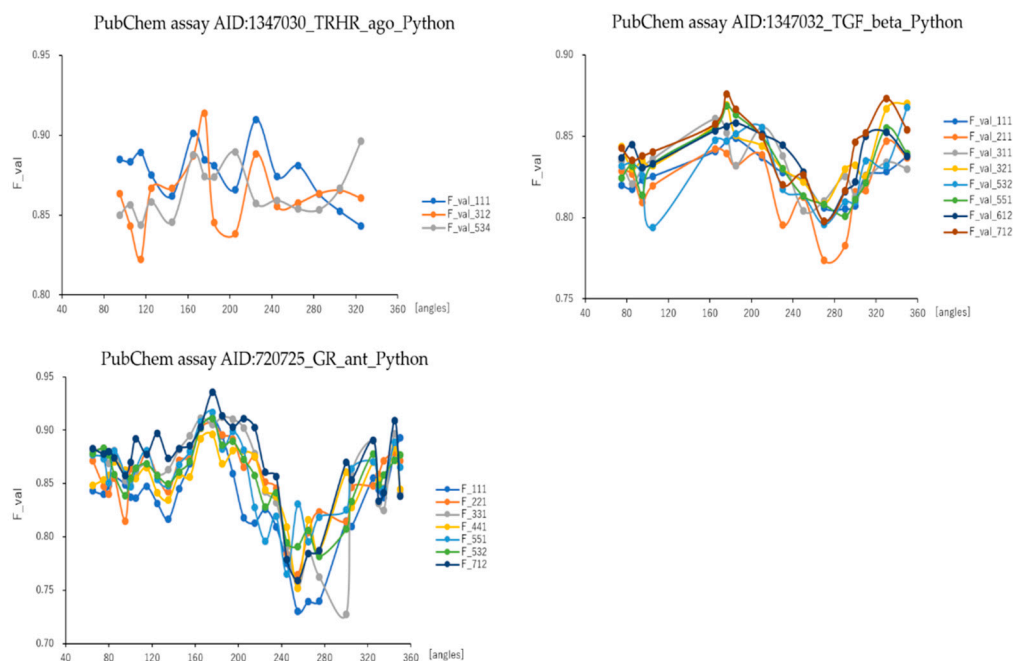
Figure S9

Figure S9. PR_AUC with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.
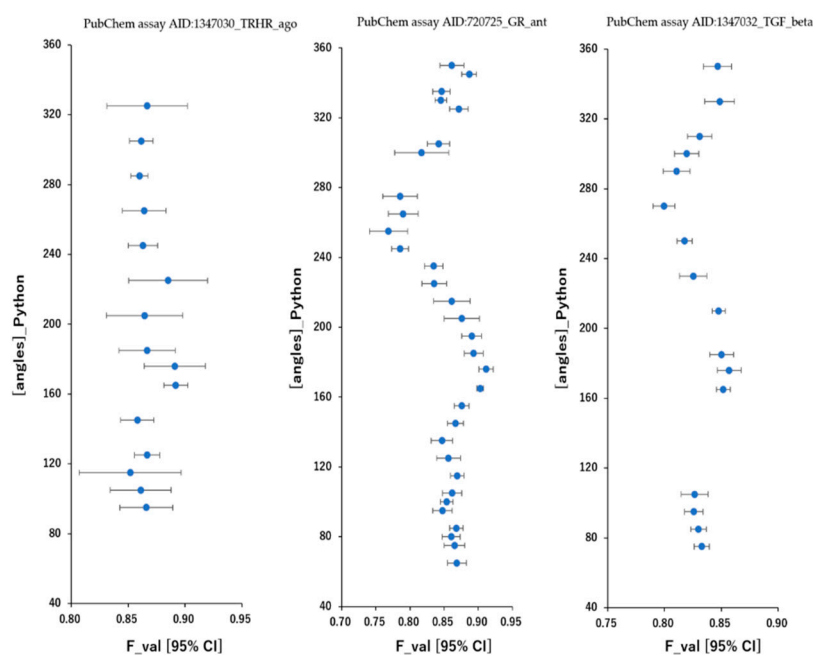
Figure S10

Figure S10. Differences in mean PR_AUC levels shown as dots with 95% confident interval (95% CI) as error bars with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.

Figure S11

Figure S11. F with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.

Figure S12. Differences in mean F levels shown as dots with 95% confident interval (95% CI) as error bars with angles in DeepSnap-DL using TensorFlow and DIGITS of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the validation dataset; n = 3.

Figure S13. Performance with batch size (BSs) in DeepSnap-DL using TensorFlow of prediction models of the glucocorticoid receptor (PubChem assay AID:720725_GR_ant), TGF-beta/Smad (PubChem assay AID:1347032_TGF_beta_ant), and agonist of the thyrotropin-releasing hormone receptor (PubChem assay AID:1347030_TRHR_ago) in the test dataset; n = 2.