Effect of the AD on the VS performance of all combinations of AD, Kernel and Target

1. Kernel Density AD Estimation

1.1 Thrombin

Figure 1: Virtual screening of the Thrombin data set using the Optimal Assignment kernel and the Kernel Density AD Formulation

Figure 2: Virtual screening of the Thrombin data set using the FlexOAK kernel and the Kernel Density AD Formulation
Figure 3: Virtual screening of the Thrombin data set using the Marginalized Graph kernel and the Kernel Density AD Formulation

1.2 Factor Xa

Figure 4: Virtual screening of the Factor Xa data set using the Optimal Assignment kernel and the Kernel Density AD Formulation
Figure 5: Virtual screening of the Factor Xa data set using the FlexOA kernel and the Kernel Density AD Formulation

Figure 6: Virtual screening of the Factor Xa data set using the Marginalized Graph kernel and the Kernel Density AD Formulation
1.3 Platelet Derived Growth Factor Receptor $\beta$

Figure 7: Virtual screening of the PDGFR$\beta$ data set using the Optimal Assignment kernel and the Kernel Density AD Formulation

Figure 8: Virtual screening of the PDGFR$\beta$ data set using the FlexOAK kernel and the Kernel Density AD Formulation
Figure 9: Virtual screening of the PDGFRβ data set using the Marginalized Graph kernel and the Kernel Density AD Formulation

2 Weighted Kernel Density AD Estimation

2.1 Thrombin

Figure 10: Virtual screening of the Thrombin data set using the Optimal Assignment kernel and the Weighted Kernel Density AD Formulation
Figure 11: Virtual screening of the Thrombin data set using the FlexOAK kernel and the Weighted Kernel Density AD Formulation

Figure 12: Virtual screening of the Thrombin data set using the Marginalized Graph kernel and the Weighted Kernel Density AD Formulation
2.2 Factor Xa

Figure 13: Virtual screening of the Factor Xa data set using the Optimal Assignment kernel and the Weighted Kernel Density AD Formulation

Figure 14: Virtual screening of the Factor Xa data set using the FlexOAK kernel and the Weighted Kernel Density AD Formulation
2.3 Platelet Derived Growth Factor Receptor β
Figure 17: Virtual screening of the PDGFRβ data set using the FlexOAK kernel and the Weighted Kernel Density AD Formulation

Figure 18: Virtual screening of the PDGFRβ data set using the Marginalized Graph kernel and the Weighted Kernel Density AD Formulation
3 One Class SVM AD Estimation

3.1 Thrombin

Figure 19: Virtual screening of the Thrombin data set using the Optimal Assignment kernel and the One Class SVM AD Formulation

Figure 20: Virtual screening of the Thrombin data set using the FlexOAK kernel and the One Class SVM AD Formulation
3.2 Factor Xa

Figure 21: Virtual screening of the Thrombin data set using the Marginalized Graph kernel and the One Class SVM AD Formulation

Figure 22: Virtual screening of the Factor Xa data set using the Optimal Assignment kernel and the One Class SVM AD Formulation
Figure 23: Virtual screening of the Factor Xa data set using the FlexOAK kernel and the One Class SVM AD Formulation

Figure 24: Virtual screening of the Factor Xa data set using the Marginalized Graph kernel and the One Class SVM AD Formulation
3.3 Platelet Derived Growth Factor Receptor β

Figure 25: Virtual screening of the PDGFRβ data set using the Optimal Assignment kernel and the One Class SVM AD Formulation

Figure 26: Virtual screening of the PDGFRβ data set using FlexOAK kernel and the One Class SVM AD Formulation
Figure 27: Virtual screening of the PDGFRβ data set using the Marginalized Graph kernel and the One Class SVM AD Formulation