

Corrigendum: Machine Learning Enables Accurate and Rapid Prediction of Active Molecules Against Breast Cancer Cells

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A Corrigendum on

Machine Learning Enables Accurate and Rapid Prediction of Active Molecules Against Breast Cancer Cells

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In the original article, there was a mistake in **Figures 4** and **5** as published. There are some errors in the figure insertion, **Figure 4** is repeated with **Figure 3**, and **Figure 5** is the result of **Figure 4**. The corrected **Figures 4** and **5** appear below.

The authors apologize for this error and state that this does not change the scientific conclusions of the article in any way. The original article has been updated.

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A _{DNN}	0.801 0.853 0.845 0.653 0.825 0.814 0.853 0.855 0.931 0.864 0.876 0.891 0.860 0.866 0.842	
KNN	0.869 0.863 0.792 0.689 0.791 0.743 0.871 0.886 0.937 0.870 0.795 0.815 0.831 0.841 0.828	
NB	0.756 0.789 0.767 0.623 0.761 0.688 0.599 0.627 0.931 0.720 0.803 0.759 0.724 0.696 0.732 0.815	
RF	0.776 0.860 0.846 0.713 0.831 0.838 0.880 0.886 0.955 0.870 0.888 0.920 0.867 0.887 0.858	
SVM	0.790 0.828 0.852 0.675 0.739 0.803 0.860 0.869 0.958 0.830 0.818 0.860 0.855 0.870 0.829	
XGBoost	0.699 0.877 0.872 0.672 0.812 0.787 0.828 0.864 0.951 0.869 0.872 0.890 0.860 0.867 0.837	
8 B	10000 BT 20 BT 474 BT 549 HB-100 578 MCF-7 B-231 B-361 B435 MB435 B468 BR-3 T 47D AVE MDA-MDA-MBA-MBA-53 B468 SK-BR-3 T 47D AVE	
D	0.924 0.745 0.966 0.742 0.761 0.759 0.920 0.964 0.962 0.922 0.923 0.924 0.952 0.923	
DNN	0.824 0.745 0.866 0.742 0.701 0.758 0.839 0.864 0.962 0.853 0.822 0.873 0.854 0.852 0.822	
NB	0.801 0.806 0.675 0.704 0.724 0.708 0.847 0.872 0.834 0.835 0.818 0.905 0.802 0.747 0.798	
RE	0.849 0.801 0.900 0.707 0.801 0.819 0.866 0.885 0.993 0.873 0.872 0.935 0.850 0.886 0.860	
SVM	0.719 0.501 0.500 0.107 0.501 0.519 0.500 0.505 0.575 0.515 0.515 0.555 0.555 0.500 0	
XGBoost	0.628	
۶ د	200937 BT-20 BT-474 BT-549 HB-100 578 MCF-7 NB-231 B-361 B-435 NB-453 B-468 SK-BR-3 T-47D AVE NDA-NDA-NDA-NDA-NDA-NDA-NBASK-BR-3 T-47D AVE	
DNN	0.682 0.824 0.886 0.696 0.778 0.771 0.875 0.880 0.969 0.815 0.775 0.893 0.847 0.813 0.822	
KNN	0.798 0.733 0.812 0.691 0.784 0.762 0.873 0.894 0.934 0.833 0.775 0.898 0.842 0.865 0.821	
NB	0.719 0.819 0.872 0.680 0.744 0.701 0.682 0.769 0.958 0.811 0.789 0.850 0.801 0.751 0.782 0.846	
RF	0.793 0.838 0.884 0.698 0.823 0.741 0.886 0.904 0.972 0.866 0.851 0.923 0.869 0.885 0.852 -0.781	
SVM	0.682 0.824 0.856 0.697 0.799 0.826 0.872 0.887 0.941 0.863 0.839 0.902 0.868 0.872 0.838 -0.716	
D AGBOOST B	$ = 0.744 \ 0.740 \ 0.827 \ 0.651 \ 0.776 \ 0.735 \ 0.626 \ 0.805 \ 0.976 \ 0.835 \ 0.810 \ 0.896 \ 0.648 \ 0.621 \ 0.615 \ -0.651 \ -0.6$	
DNN	0.781 0.510 0.809 0.682 0.795 0.767 0.851 0.868 0.948 0.816 0.858 0.876 0.878 0.807 0.803	
KNN	0.795 0.691 0.682 0.656 0.848 0.817 0.841 0.851 0.813 0.809 0.750 0.845 0.708 0.837 0.782	
NB	0.804 0.529 0.710 0.668 0.650 0.681 0.600 0.637 0.800 0.643 0.776 0.744 0.672 0.607 0.680 -0.772	
RF	0.813 0.775 0.846 0.708 0.855 0.774 0.861 0.876 0.938 0.864 0.826 0.920 0.834 0.873 0.840	
SVM	0.884 0.721 0.795 0.705 0.859 0.792 0.853 0.849 0.920 0.805 0.809 0.869 0.834 0.830 0.823 -0.596	
XGBoost	0.787 0.819 0.832 0.694 0.829 0.750 0.813 0.855 0.924 0.824 0.811 0.906 0.853 0.850 0.825	
Ø	200937 BT-20 BT-474 BT-549 L-100 S578T MCF-7 NB-231 B-361 B-435 NB-453 B-458 BR-3 T-47D AVE NDA-NDA-NDA-NDA-NDA-NDA-NDA-NDA-NB-5K-BR-3 T-47D AVE	
IGURE 4 Performance on hodels. (C) AUC results of	of fingerprint-based BC prediction models. (A) AUC results of the AtomPairs-based models. (B) AUC results of the MACCS the Morgan-based models. (D) AUC results of the PharmacoPFP-based models.	-based

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FIGURE 5 (A) Summary of the optimal models for each fingerprint-based feature. (B) The best models among various fingerprint-based models for different kind of breast cell lines. The optimal models based on (C) AtomPairs, (D) MACCS, (E) Morgan, and (F) PharmacoPFP for different subtypes of breast cell lines.