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Corrigendum: DeepCarc: Deep learning-powered carcinogenicity prediction using model-level representation

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A corrigendum on
DeepCarc: Deep learning-powered carcinogenicity prediction using model-level representation

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In the published article, there was an error where the compounds were mismatched with the compound's prediction. A correction has been made to the Section "*DeepCarc Is Employed to Screen DrugBank and Tox21 Compounds*," Paragraphs 1 and 2. The corrected section appears below:

"The DeepCarc was used as a screening tool for identifying the carcinogenicity potential of the compounds from DrugBank (Figure 5A). The predicted probabilistic values ranging from 0 to 1 were split into 10 intervals with a size of 0.1. Of 9,814 compounds, there were 7,555 (i.e., 7,555/9,814 = 76.98%), 920 (9.37%), 442 (4.50%), 277 (2.82%), 186 (1.90%) compounds with their predicted probabilities belong to the intervals of (0, 0.1), (0.1, 0.2), (0.2, 0.3), (0.3, 0.4), and (0.4, 0.5), respectively, indicating low carcinogenicity concern. In total, 434 compounds (4.42%) were predicted with probabilistic values $\geq$0.5, indicating compounds with carcinogenicity risk. Of 434 compounds, there were 26 compounds (0.26%) with the predicted probability $\geq$0.9, indicating high carcinogenicity concern. The predicted probabilistic value of each drug is included in **Supplementary Table 4**.

The DeepCarc further screened the carcinogenicity potential of the compounds from the Tox21 (Figure 5B). Similarly, the predicted probabilistic values were separated into

10 intervals. Of the 7,176 compounds, there were 3,788 (i.e., 3,788/7,176 = 52.79%), 805 (11.22%), 533 (7.43%), 455 (6.34%), 375 (5.23%) compounds with their predicted probabilities belong to the intervals of (0, 0.1), (0.1, 0.2), (0.2, 0.3), (0.3, 0.4), and (0.4, 0.5), respectively, indicating low carcinogenicity concern. The other 1,220 (17.00%) compounds were predicted with probabilistic values ≥0.5, suggesting the compounds possessed carcinogenicity risk. There were 82 (1.14%) compounds with the predicted probabilistic value ≥0.9, suggesting high carcinogenicity concern (**Supplementary Table 5**)."

In the published article, there was also an error in Figure 5 as published. The probability distribution is incorrect due to a mismatched compounds' prediction. The corrected Figure 5 appears below.

In the published article, there was an error in **Supplementary Tables 4, 5** where the compounds were mismatched with the prediction. These files have now been updated in the original article.

The authors apologize for these errors 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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Author disclaimer

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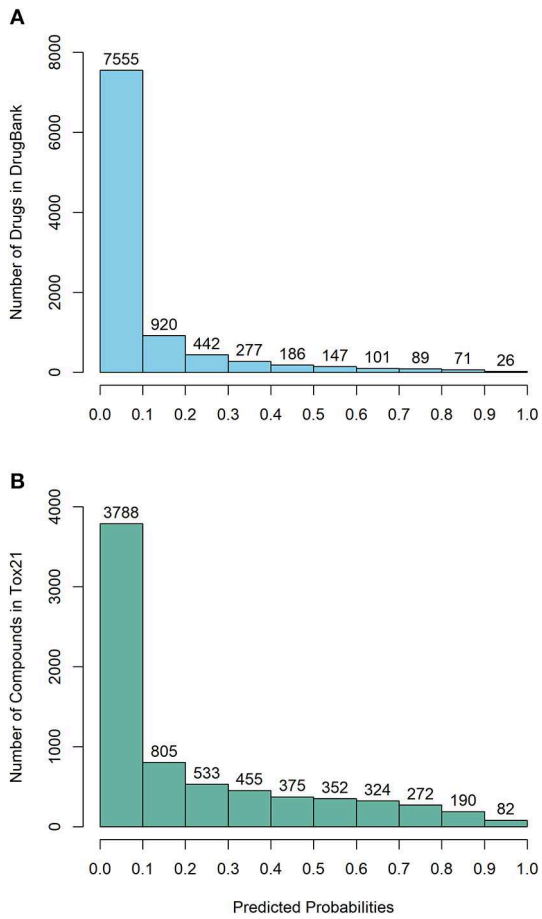

FIGURE 5
The probability distribution of the DeepCarc prediction of the compounds from **(A)** DrugBank; **(B)** Tox21.