

Supplementary Material: Positional Embeddings and Zero-shot Learning using BERT for Molecular-Property Prediction

FIGURES

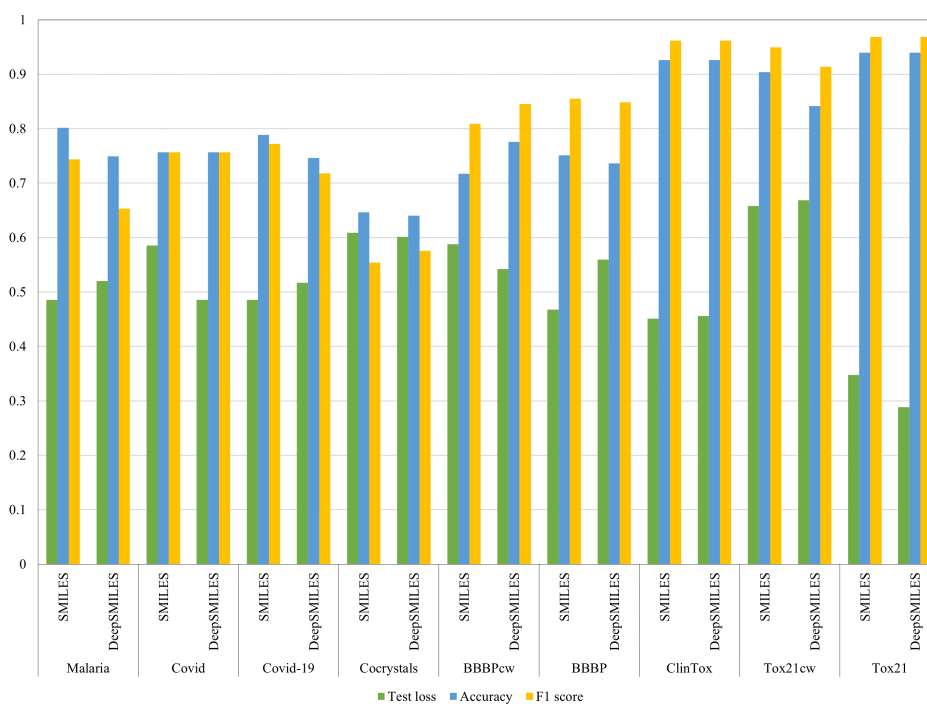


Fig. S1. BERT with the PE "Relative key query": Loss, Accuracy, and F1-score for Classification Tasks.

(BERT = Bidirectional Encoders Representations from Transformers; PE = positional embedding)

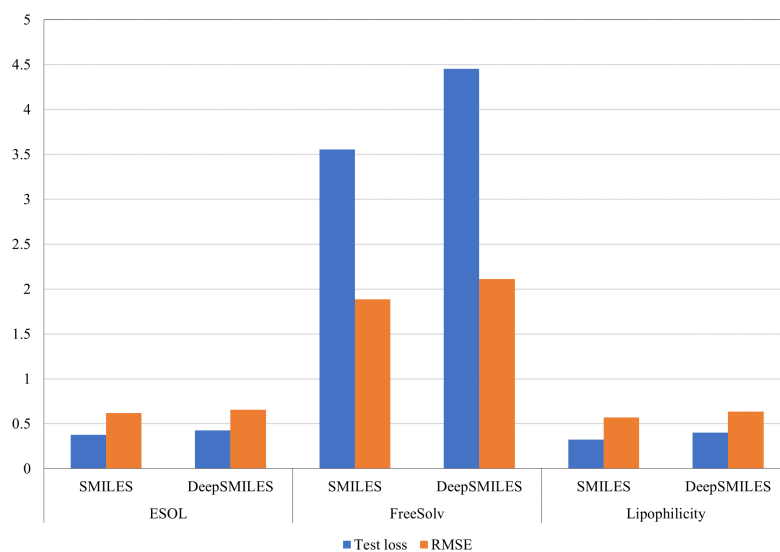


Fig. S2. BERT with Relative key query PE: Loss and RMSE for Regression Tasks.
(RMSE = Root Mean Squared Error)

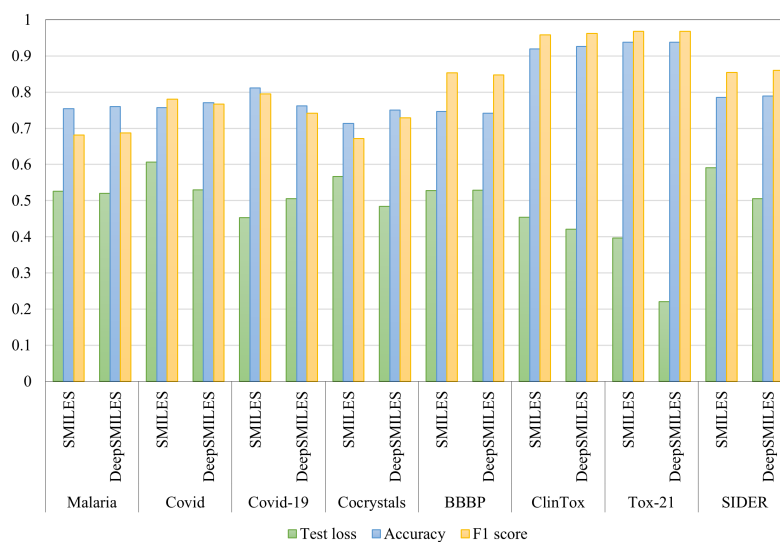


Fig. S3. BERT with Sinusoidal PE: Loss, Accuracy, and F1-score for Classification Tasks.

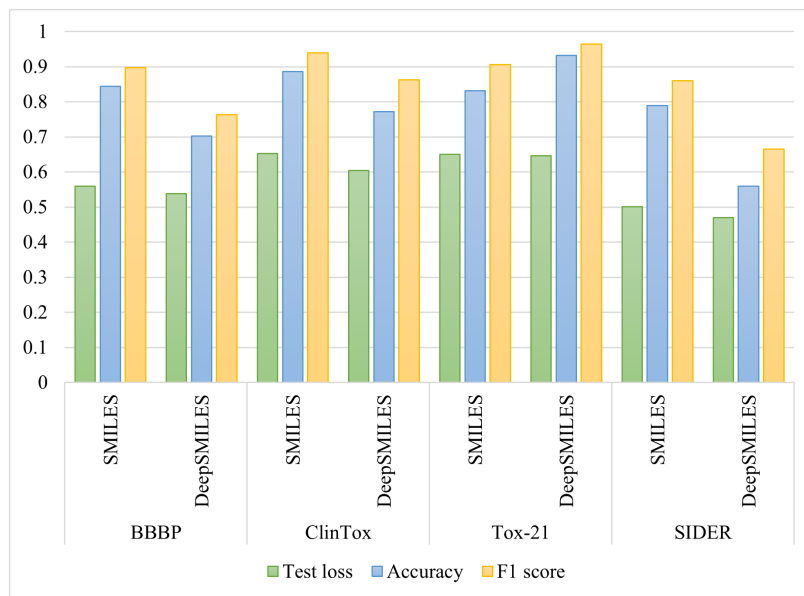


Fig. S4. BERT with Sinusoidal PE: Loss, Accuracy, and F1-score for Classification Tasks with Class Weight.

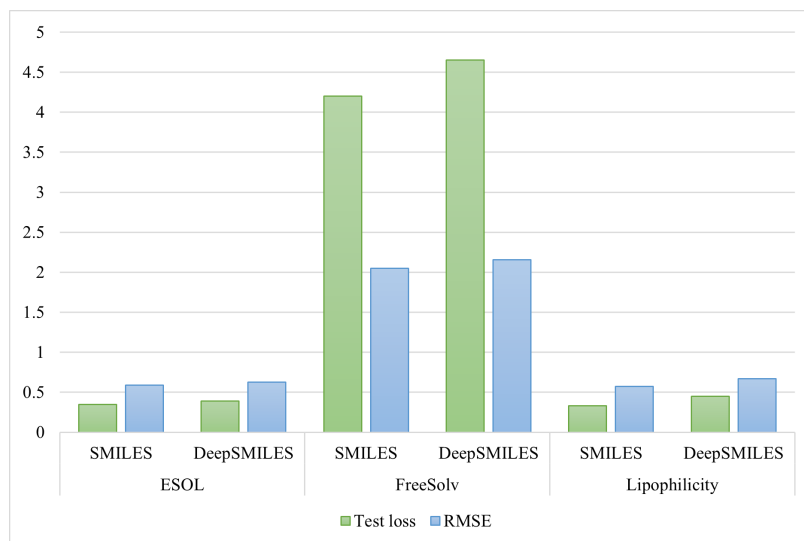


Fig. S5. BERT with Sinusoidal PE: Loss and RMSE for Regression Tasks.

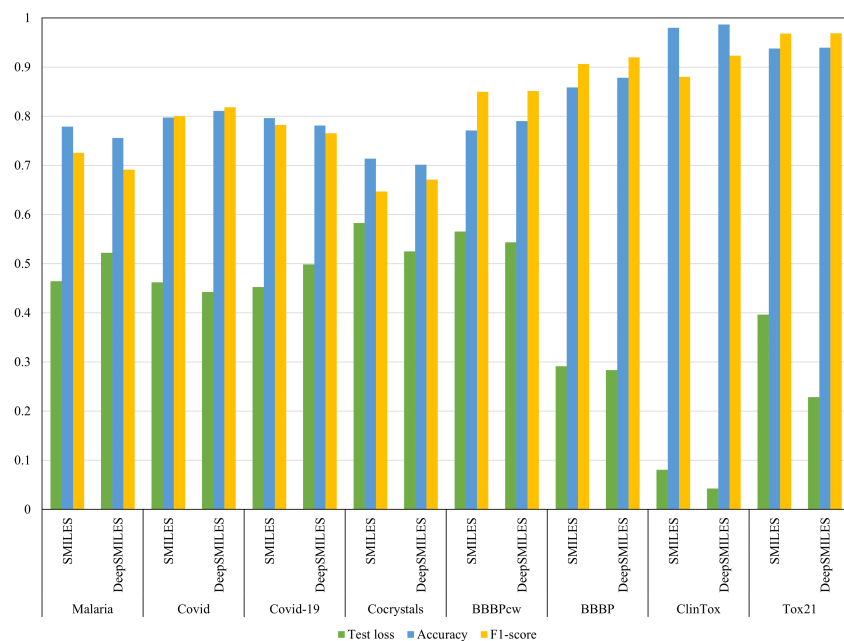


Fig. S6. BERT with the PE "relative_key": Loss, Accuracy, and F1-score for Classification Tasks.

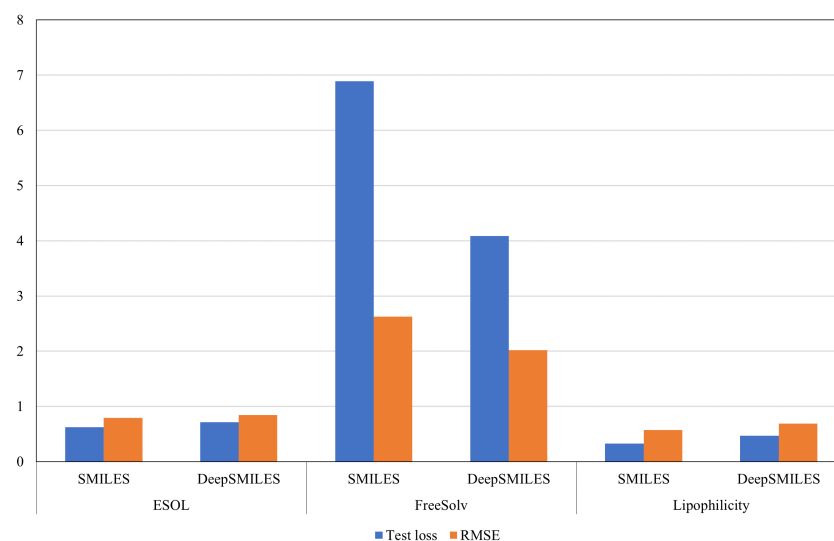


Fig. S7. BERT with the PE "relative_key": Loss and RMSE for Regression Tasks.