

Supplementary Materials for

Deep reinforcement learning for de novo drug design

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Fig. S2. Reward functions.

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Fig. S5. Learning curve for generative model.

Fig. S6. Distributions of SMILES's string lengths.

H2: Supplementary Materials

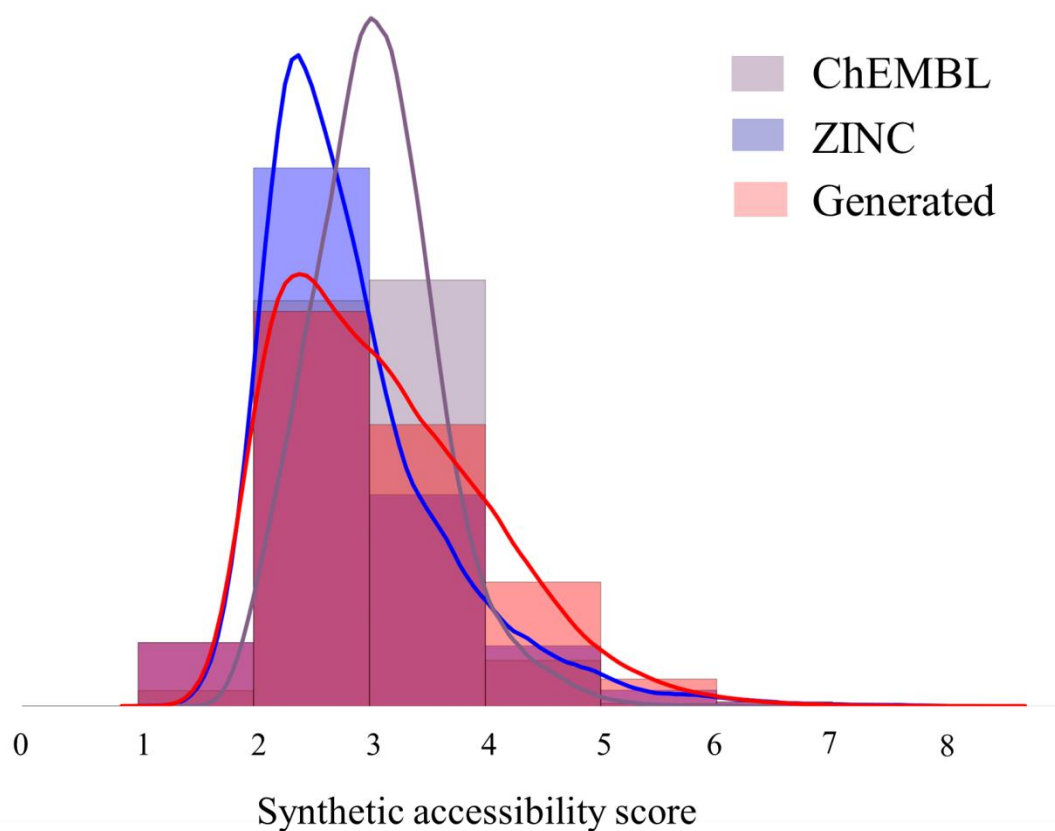


Fig. S1. Distribution of SAS for the full ChEMBL21 database (~1.5 million molecules), random subsample of 1M molecules from ZINC15, and generated data set of 1M molecules with baseline generator model *G*.

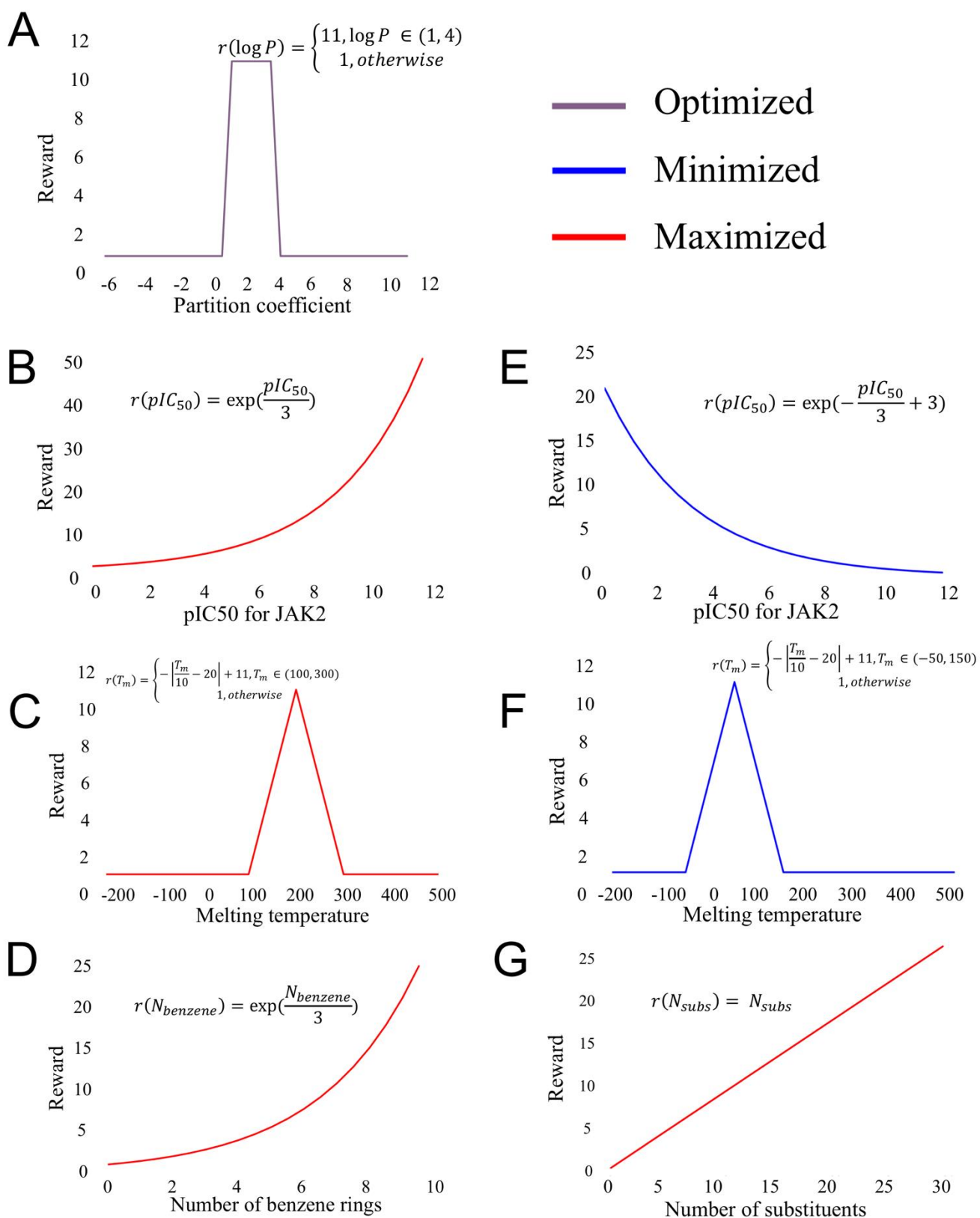


Fig. S2. Reward functions. (A) logP optimization (B) pIC₅₀ for JAK2 maximization (C) Melting temperature maximization (D) Benzene rings maximization (E) pIC₅₀ for JAK2 minimization (F) Melting temperature minimization (G) Substituent maximization.

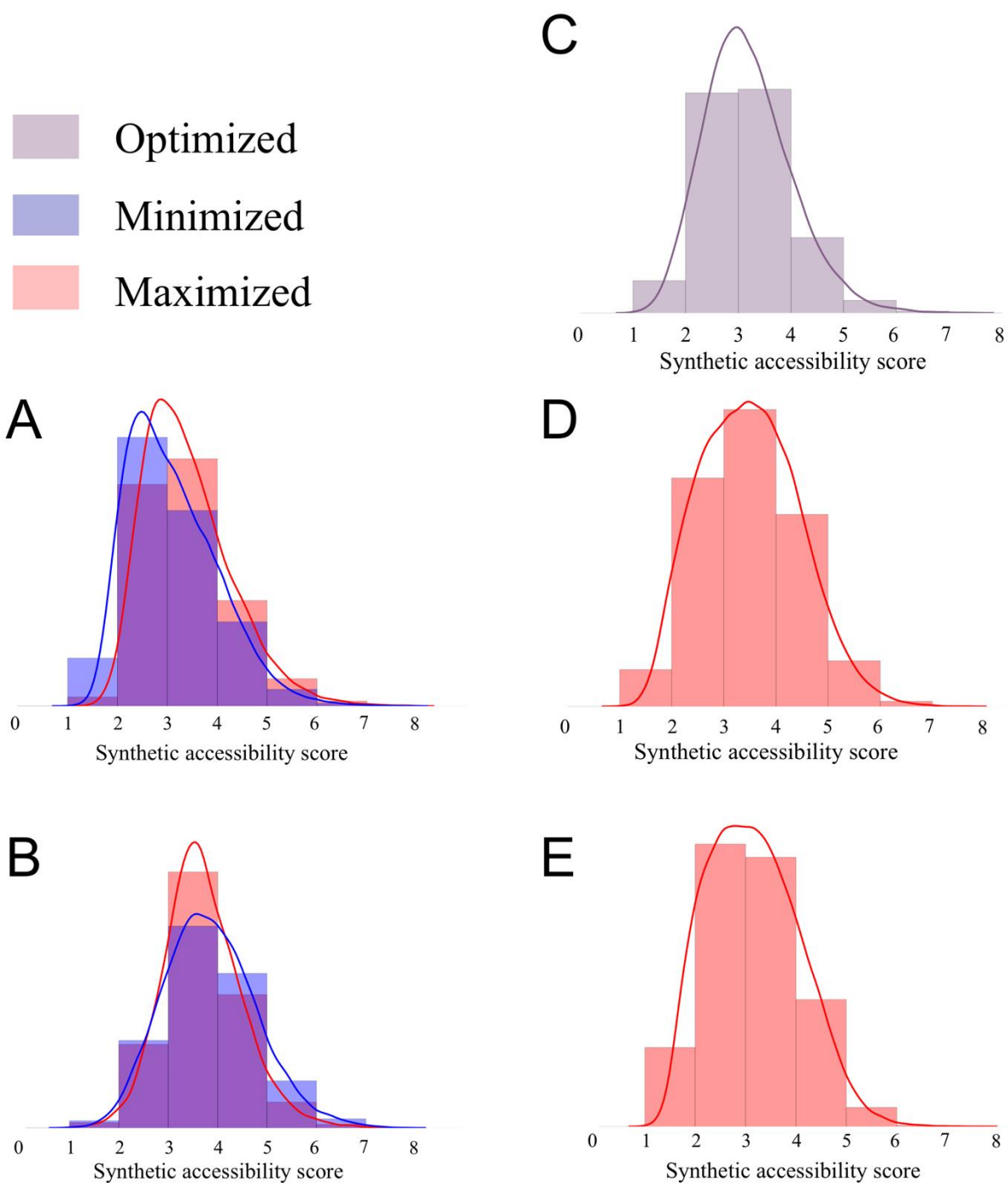


Fig. S3. Distributions of SAS for all RL experiments. (A) Melting temperature (B) JAK2 inhibition (C) Partition coefficient (D) Number of benzene rings (E) Number of substituents.

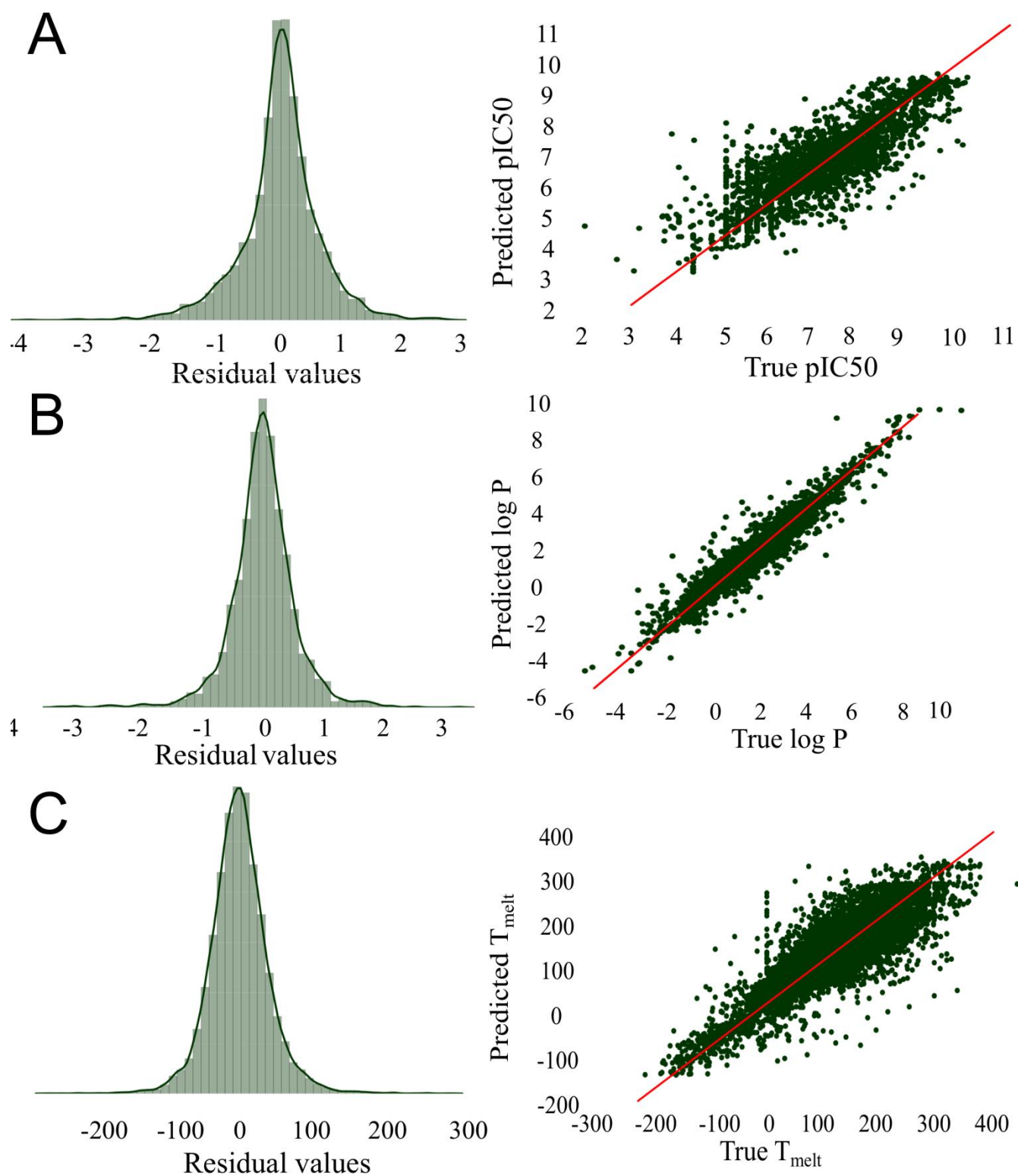


Fig. S4. Distribution of residuals and predicted versus observed plots for predictive models. Results are obtained with external Five-fold Cross-validation. All the values are calculated on hold out test datasets (A) Melting temperature (B) logP (C) pIC₅₀ for JAK2.

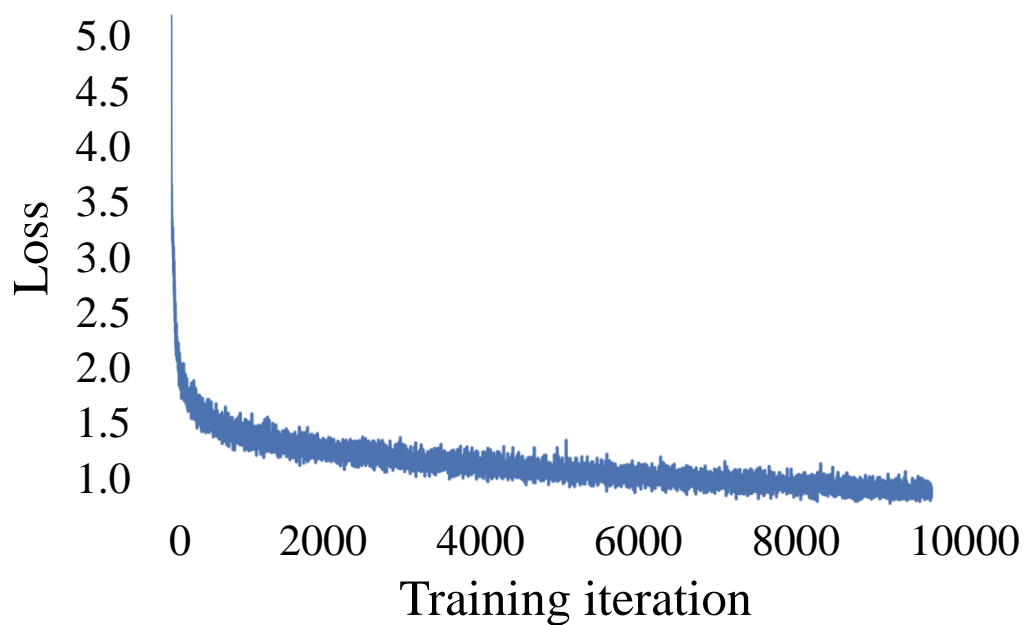


Fig. S5. Learning curve for generative model.

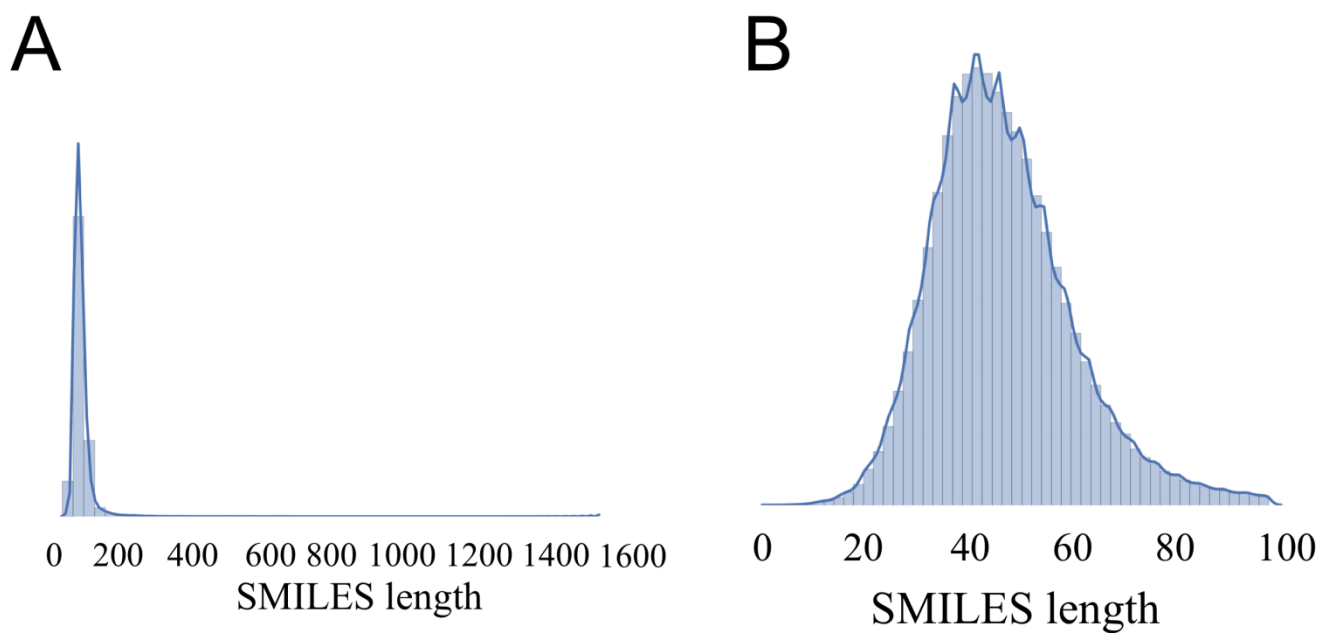


Fig. S6. Distributions of SMILES's string lengths. (A) Initial (B) Truncated.