Molecular Optimization by Capturing Chemist's Intuition Using Deep Neural Networks

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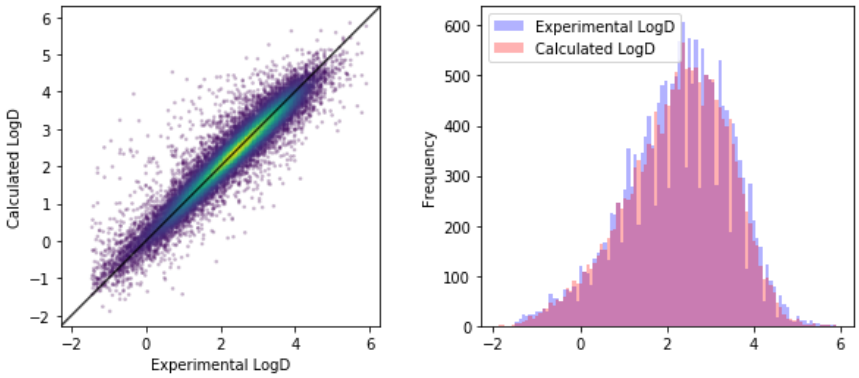
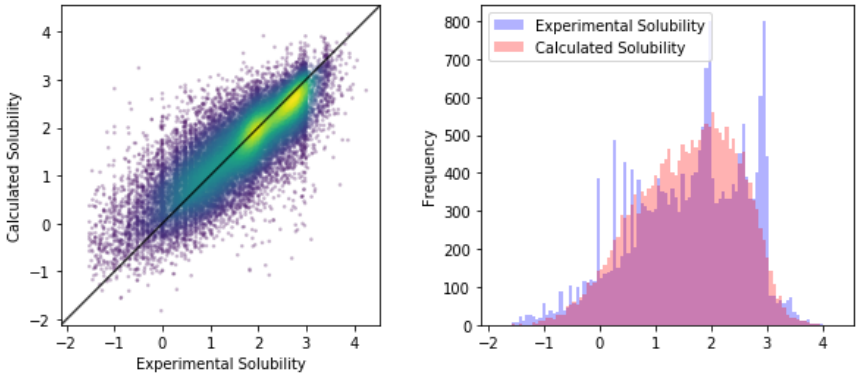
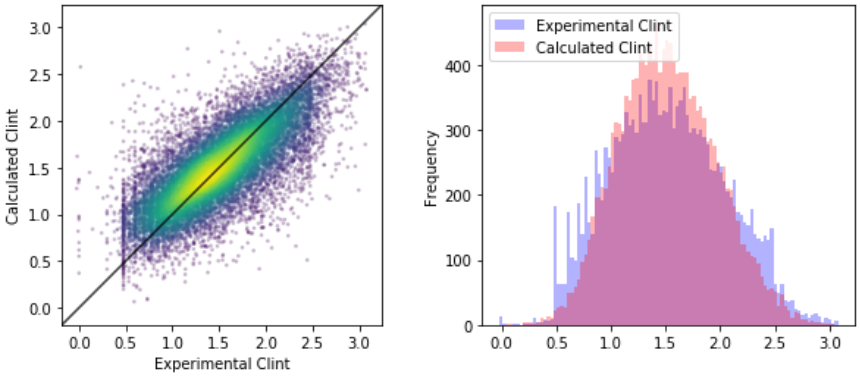
Supplementary material



(a) Experimental LogD vs. predicted LogD and their distributions

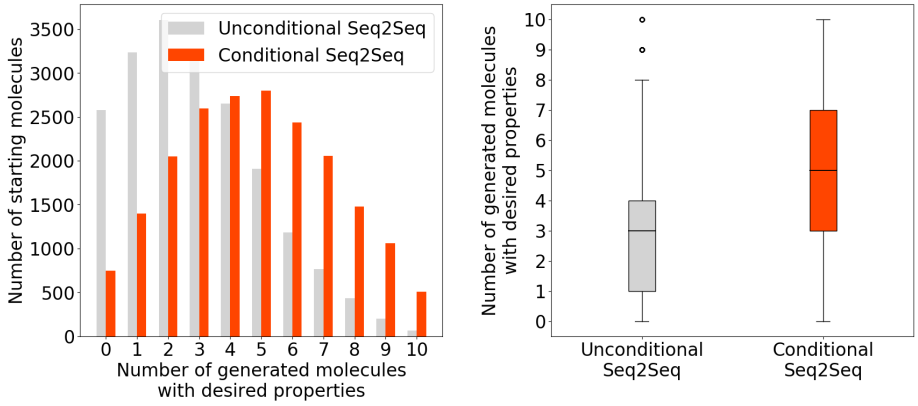


(b) Experimental solubility vs. predicted solubility and their distributions

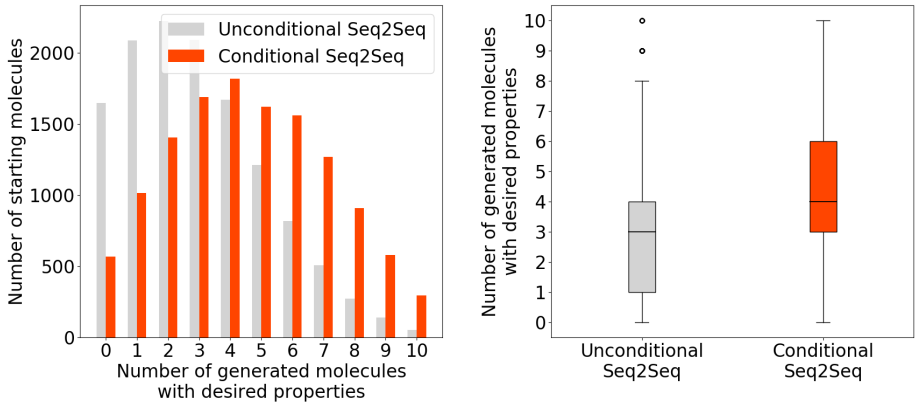


(c) Experimental clint vs. predicted clint and their distributions

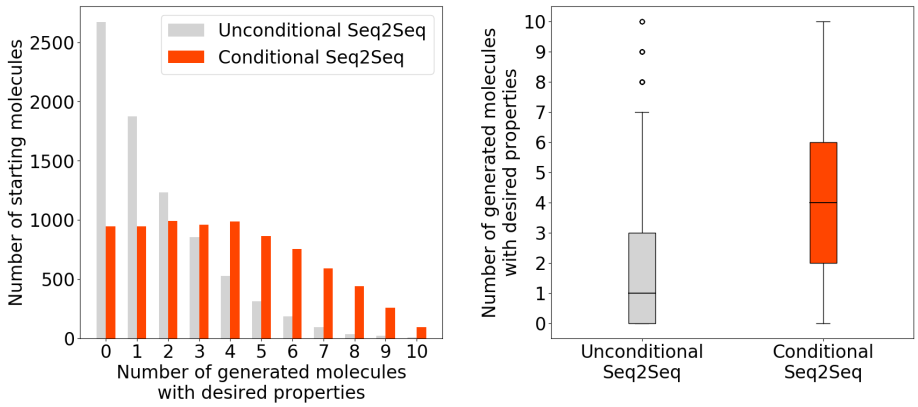
Figure 1 Experimental property values vs. predicted property values and their distributions



(a) Test-Original



(b) Test-Molecule



(c) Test-Property

Figure 2 Number of generated molecules with desirable properties per starting molecule using unconditional Seq2Seq and conditional Seq2Seq on three test sets. Conditional Seq2Seq outperforms unconditional Seq2Seq using K-Sample Anderson–Darling Test at significance level of 0.1%.