RESEARCH

Substructure-based Neural Machine Translation for Retrosynthetic Prediction

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available at the end of the article

Abstract

Keywords: retrosynthesis planning; machine neural translation; seq-to-seq; attention

Additional Files as Figures.

Please find the supporting materials as **figures** within the "Additional Files" section of the BMC article.

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References

Additional Files

Additional File 5 : Figure S4

File name : Supplementary Figure S4

Title of data : Similarity Measure Dependency
File format : Standard Latex figure, formatted as PNG.

Description of data: Effect of similarity metric type on model performance.

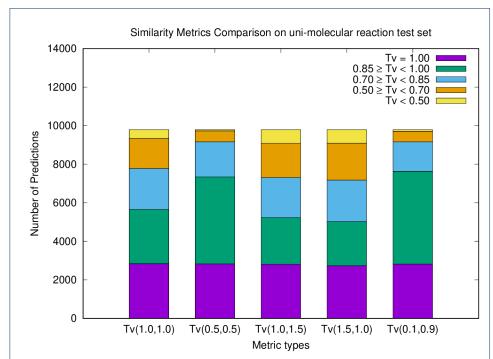


Figure S4: Analysis of different evaluation metrics. Tv(1.0,1.0) and Tv(0.5,0.5) correspond to the Tanimoto and Sörensen–Dice coefficients, respectively. Smaller values of α favoring the contribution of prediction to its similarity to true sequence. Tv(1.5,1.0) and Tv(1.0,1.5) metrics are taken from the work of Jensen et al.(Ref. 63)