RESEARCH

Substructure-based Neural Machine Translation for Retrosynthetic Prediction

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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 4 : Figure S3

File name : Supplementary Figure S3
Title of data : Fingerprint Dependency
File format : Standard Latex figure, formatted as PNG.
Description of data : Comparison of model accuracy using ECFP and MACCS.

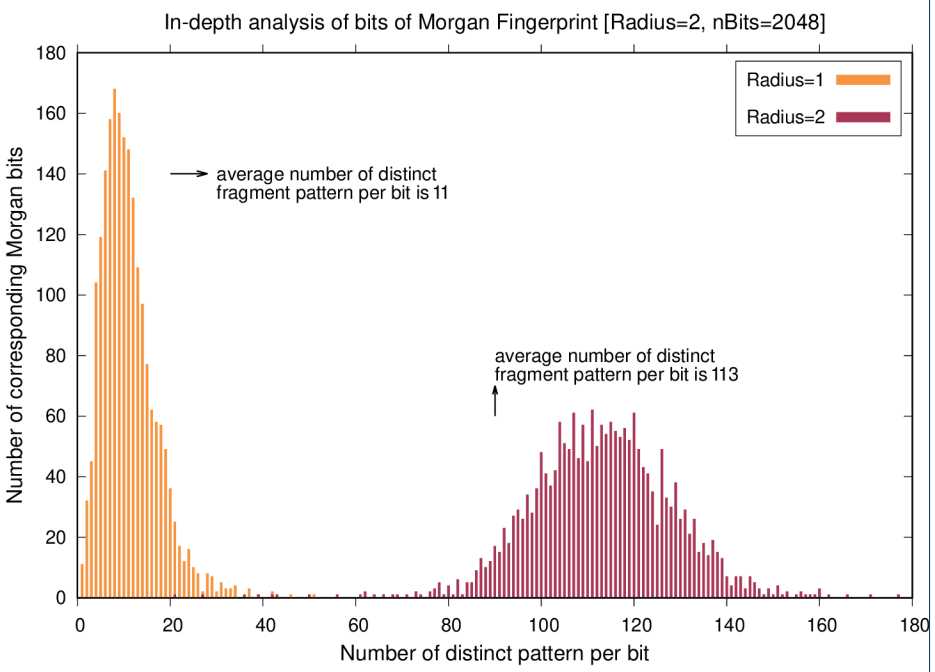

Figure S3: Analysis of ECFP bits on 98K molecules. The radius zero context of each bit is ignored in this analysis.