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 6 : Figure S5A

File name : Supplementary Figure S5A
Title of data : Bioactively similar reactions
File format : Standard Latex figure, formatted as PNG.
Description of data : Depictions of ten bioactively similar reactant candidates (1-5)

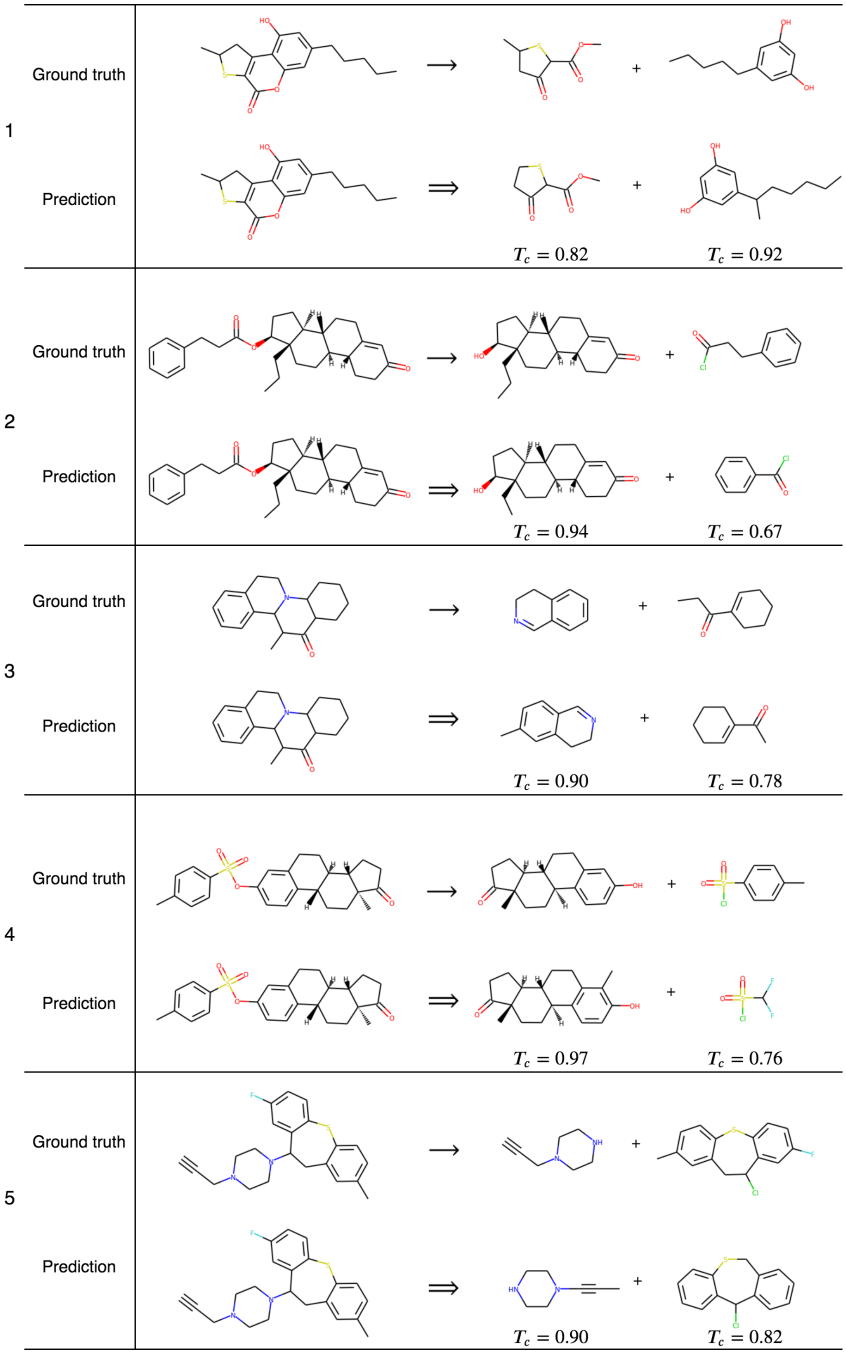

Figure S5A: Ten reactions lie in the bioactively similar region used to assess the quality of retrosynthesis (1-5).