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Dear Dr. Zhen Yang:

Please see enclosed our manuscript "*Weighted Reaction Fingerprints for Visualizing Reactivity Cliffs and Generality*" for consideration in *Tetrahedron Letters*. This work describes the visual analysis of high throughput experimental data. In this study, we analyze multiple campaigns of high throughput synthetic chemistry using weighted reaction fingerprints, which is a method where fingerprints of individual components of the reactions are weighted and summed. We find that by manipulating the weights, the reduced manifold representation of the reaction space can be manipulated. For instance, performing a tSNE on an array of reaction fingerprints, where the catalysts are weighted by 3, creates clusters centered around each catalyst. Through this method, we can identify generalizable conditions for reagents and substrates, as well as reactivity cliffs. As well, the method is utilized to track the progress of high throughput synthetic discovery campaigns, identifying regimes of initial discovery, reaction optimization, and substrate scope evaluation. We believe this work will be of high interest to practicing organic chemists exploring data science methods to study synthetic reactions.

We propose as Reviewers:

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Sincerely,

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