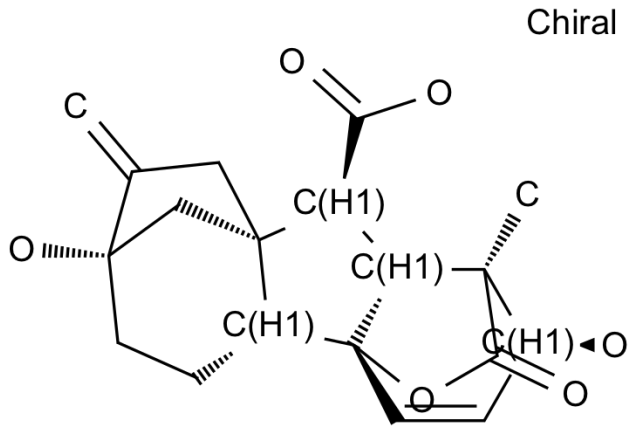
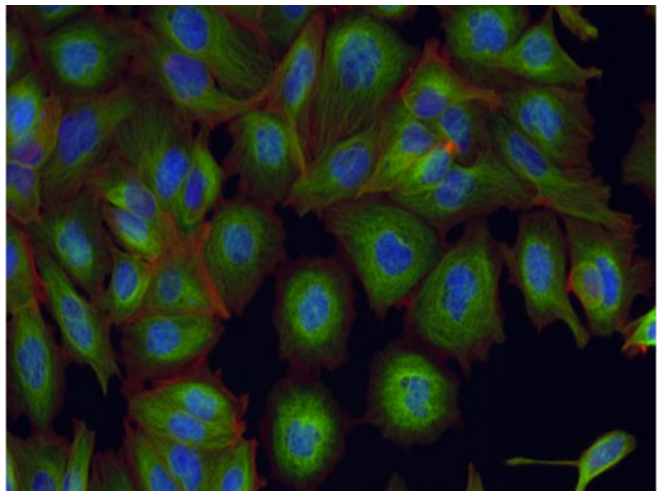
Aspiring to find relations between

Chemical structures and Morphological features

Lakshmi Balasubramanian, Minh Doan, Lassi Paavolainen, David Healey, Juan Caicedo

Are compound structures correlated to morphology features?





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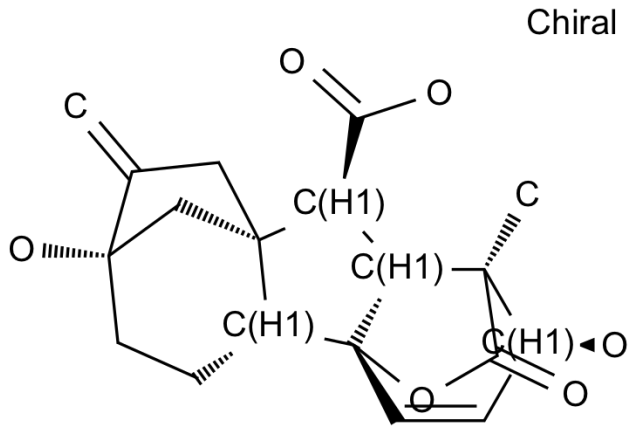

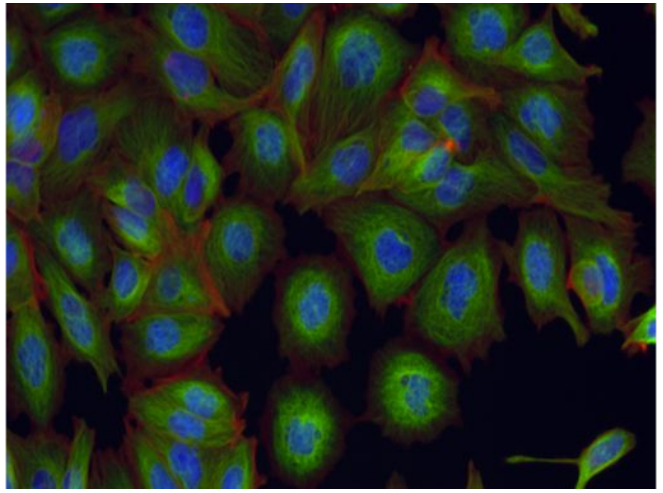

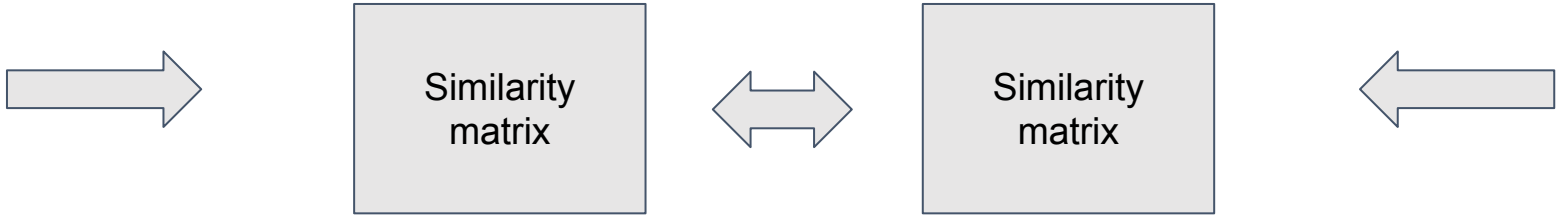

Processing morphology data

1. Normalize features
    a. Remove NaNs
2. Aggregate wells
3. Compute similarity matrix

Processing chemical structures

1. Compute string similarity matrix between SMILES

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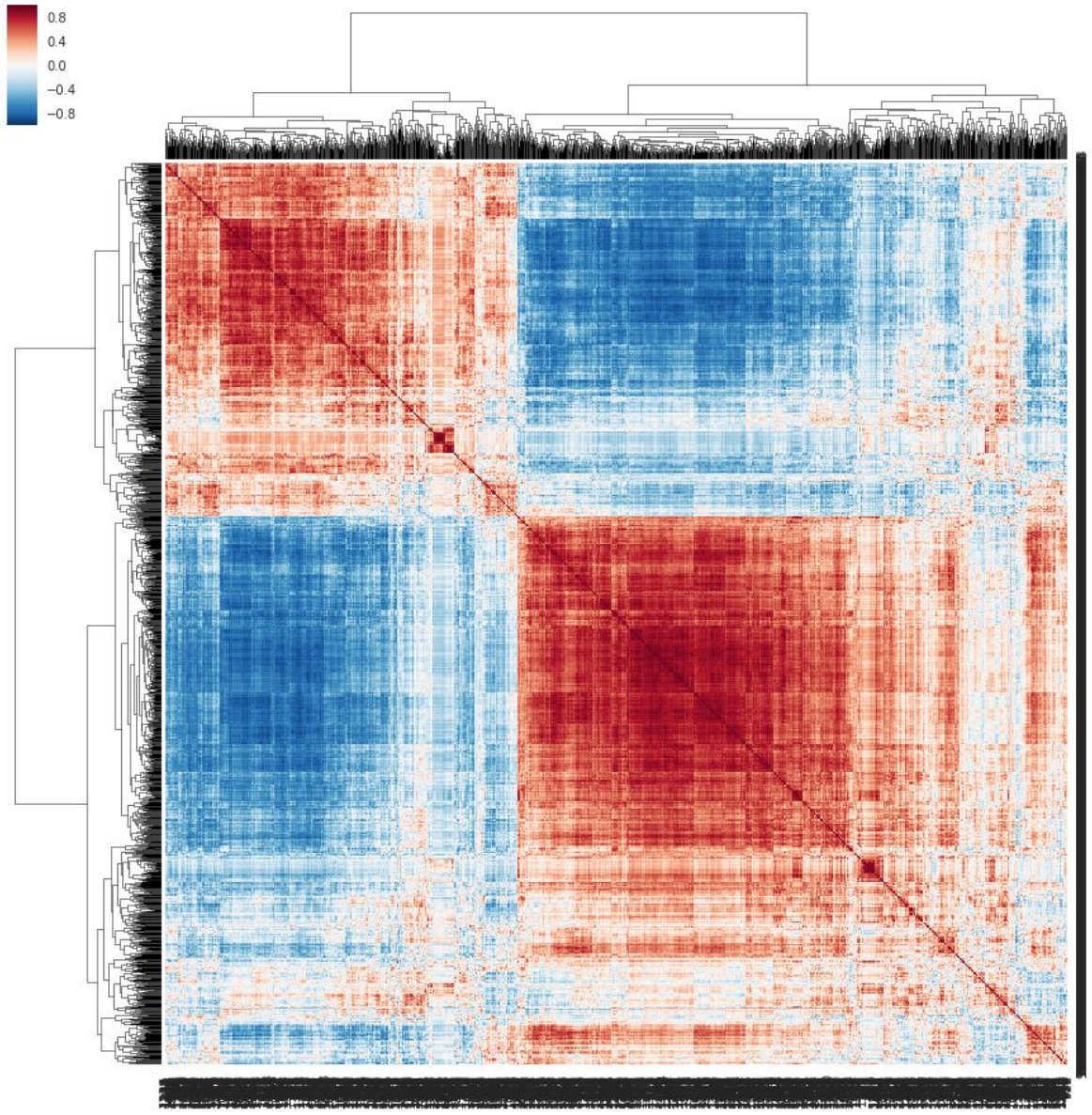
RESEARCH ARTICLE Open Access

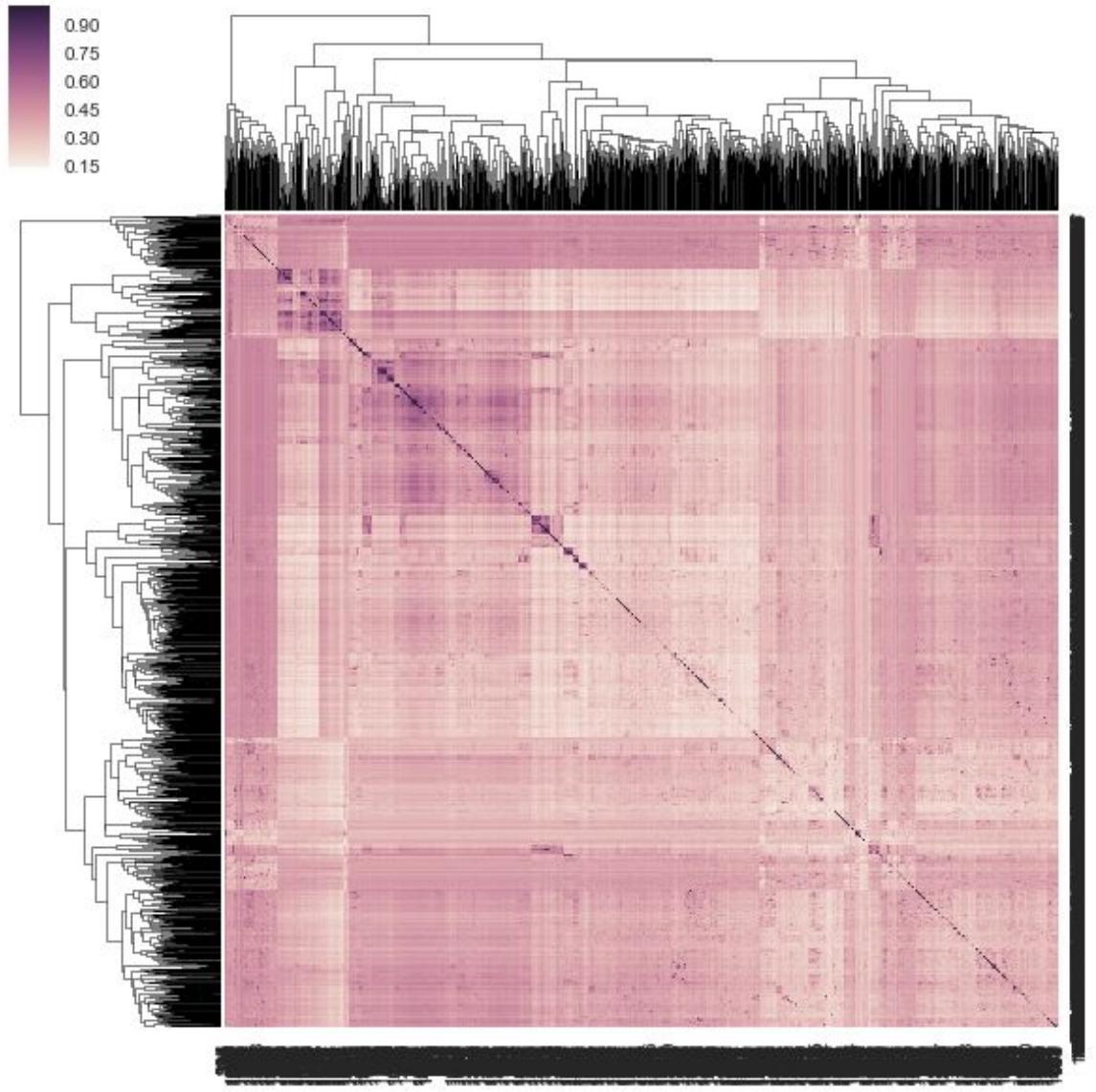
A comparative study of SMILES-based compound similarity functions for drug-target interaction prediction

Hakime Öztürk*, Elif Ozkirimli* and Arzucan Özgür*

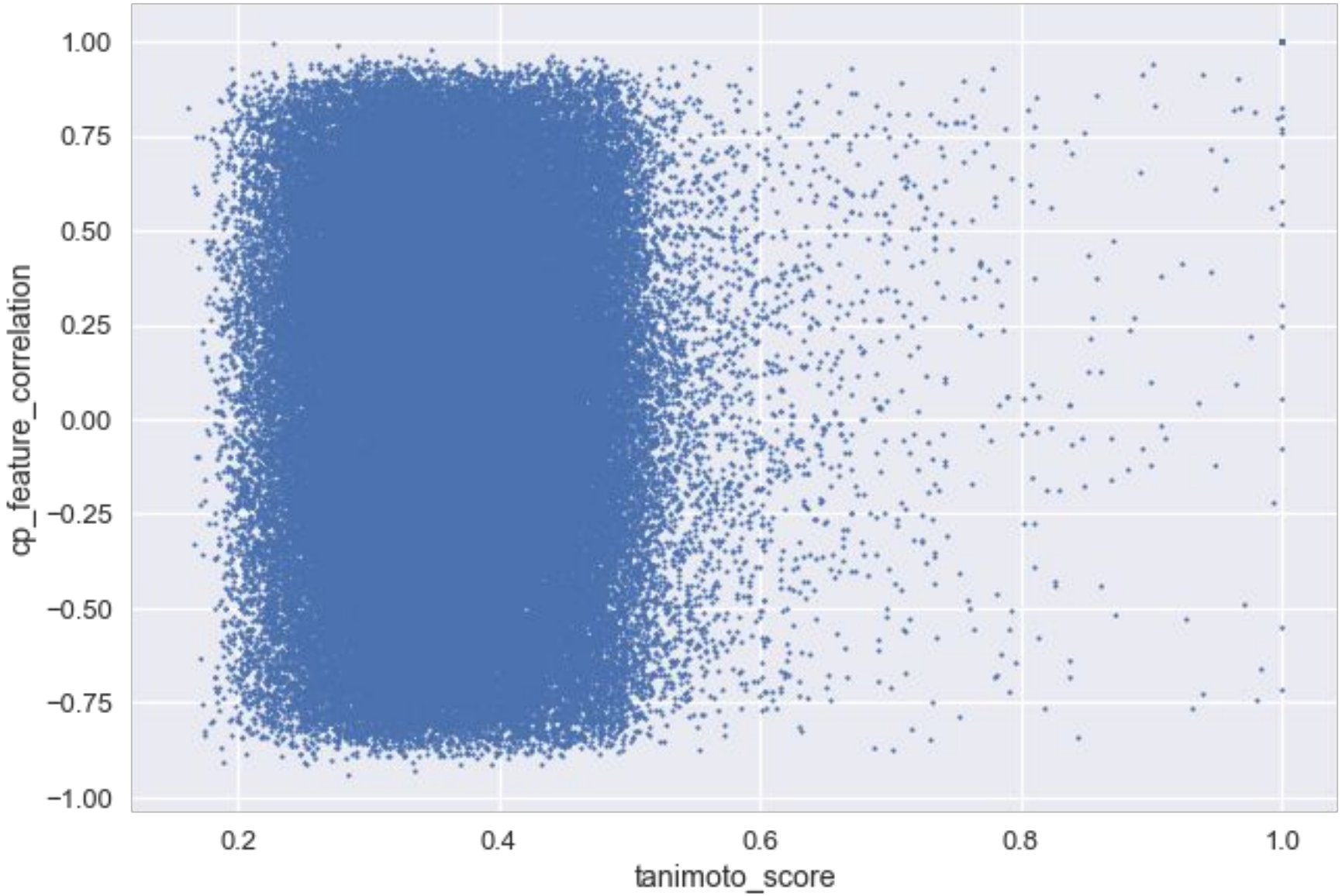
Morphological Features



Chemical structures



Correlation between chemical structures and morphological features



Thank you!