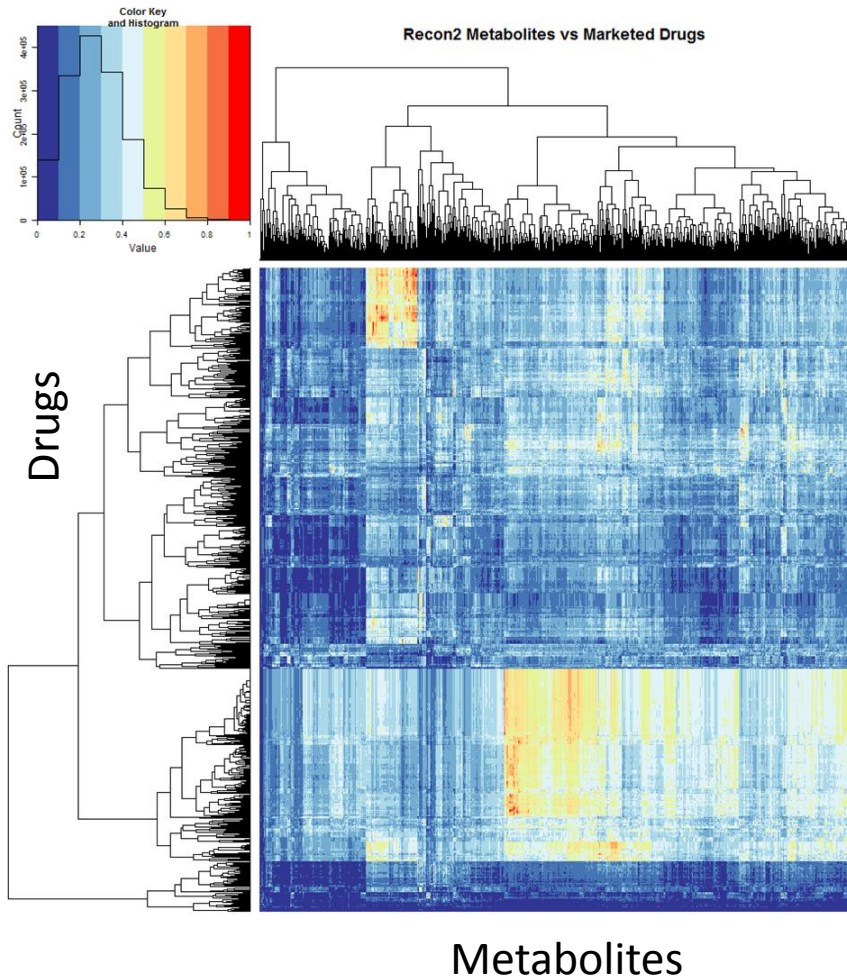
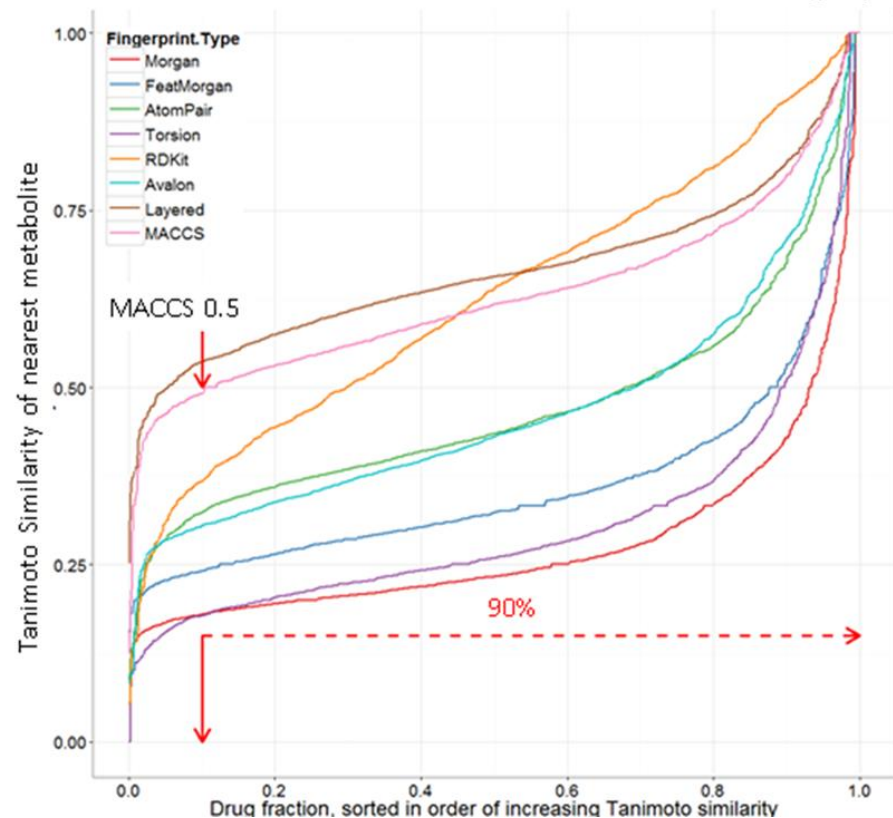


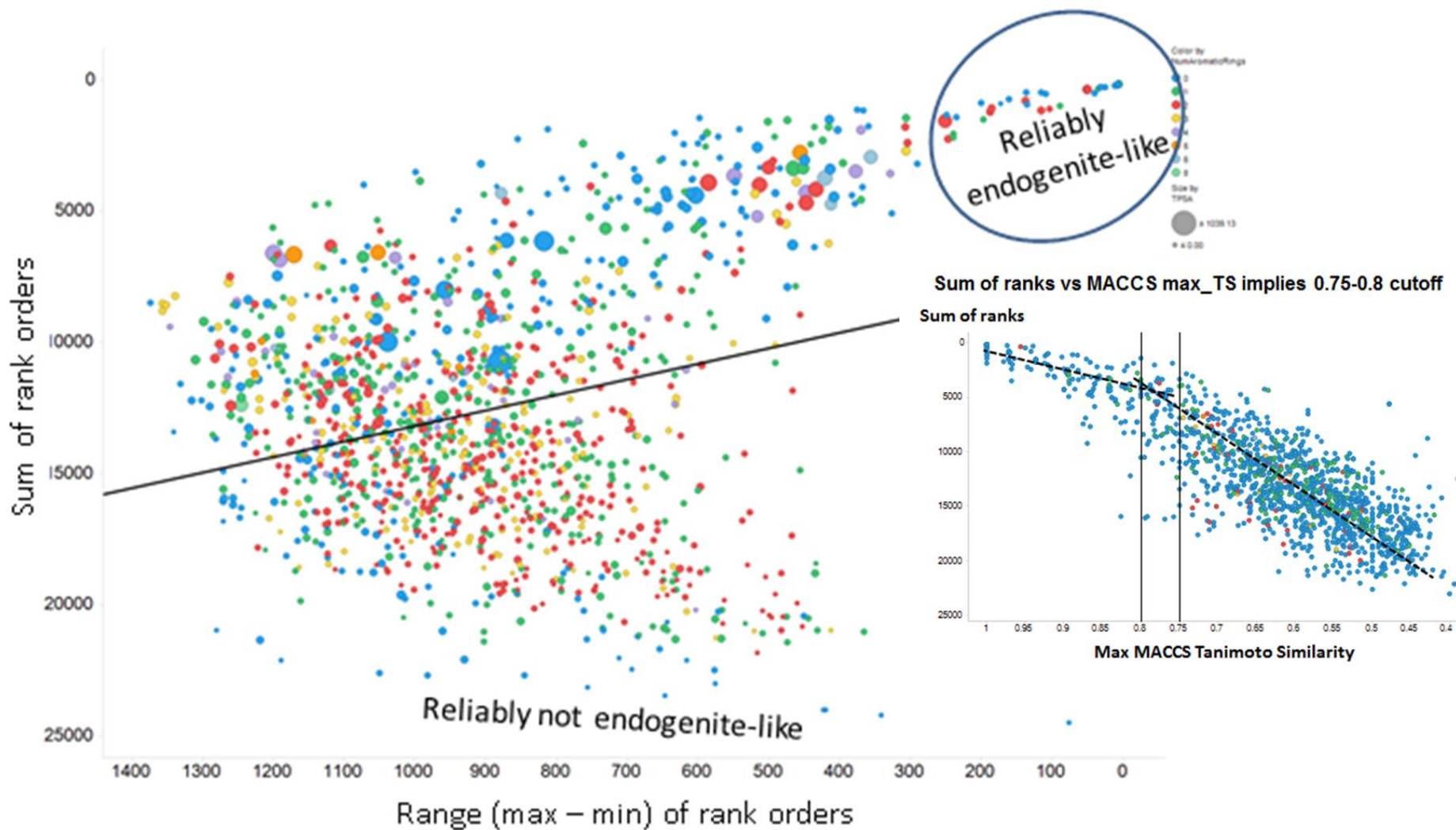
Analyses of drug-metabolite similarities



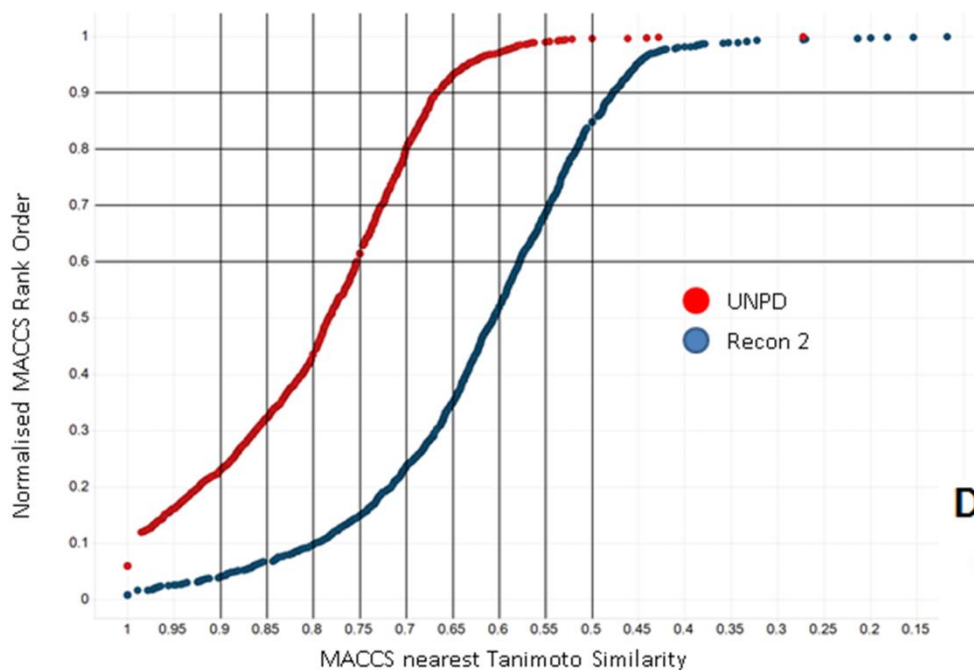
Cumulative Closest Tanimoto distance for different fingerprints



Sum of rank orders vs range



Drugs are much more like natural products



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Original scientific paper

Consensus rank orderings of molecular fingerprints illustrate the 'most genuine' similarities between marketed drugs and small endogenous human metabolites, but highlight exogenous natural products as the most important 'natural' drug transporter substrates

Steve O'Hagan^{1,2}, Douglas B. Kell^{1,2,3,*}

D Maximum rankwith TYPICAL encoding, 196k NPs

Maximum normalised rank

