Title: A quantum-based similarity method in virtual screening

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Abstract: One of the most widely-used techniques for ligand-based virtual screening is similarity searching. This study adopted the concepts of quantum mechanics to present as state-of-the-art similarity method of molecules inspired from quantum theory. The representation of molecular compounds in mathematical quantum space plays a vital role in the development of quantum-based similarity approach. One of the key concepts of quantum theory is the use of complex numbers. Hence, this study proposed three various techniques to embed and to re-represent the molecular compounds to correspond with complex numbers format. The quantum-based similarity method that developed in this study depending on complex pure Hilbert space of molecules called Standard Quantum-Based (SQB). The recall of retrieved active molecules were at top 1% and top 5%, and significant test is used to evaluate our proposed methods. The MDL drug data report (MDDR), maximum unbiased validation (MUV) and Directory of Useful Decoys (DUD) data sets were used for experiments and were represented by 2D fingerprints. Simulated virtual screening experiment show that the effectiveness of SQB method was significantly increased due to the role of representational power of molecular compounds in complex numbers forms compared to Tanimoto benchmark similarity measure.