
Subject: Re: fragments

Posted by [thomas](#) on Tue, 16 Apr 2019 14:19:30 GMT

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The drug score does not use fragments. It is a mathematical equation combining other properties. The druglikeness, however, uses >5000 substructures. Everyone has an associated druglikeness contribution value, some positiv, some negativ, which were derived from the frequency these fragments occur in commercial drugs or organic chemicals. I attach a text file, which when opened from DataWarrior shows the chemical structures and the contributions of these fragments.

File Attachments

1) [druglikenessFragments.txt](#), downloaded 1667 times
