Subject: Re: fragments
Posted by thomas on Tue, 16 Apr 2019 14:19:30 GMT

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 1787 times