

---

Subject: Re: SMARTS searching

Posted by [thomas](#) on Tue, 16 Jan 2018 22:50:52 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

Hi Angus, reading SMARTS and converting them into DataWarrior format (idcodes) is on the list of things to be done, but not available yet. For a small set of substructures one could always draw them by hand, e.g. within a 'substructure list filter', but for the PAINS collection it would be a pain. An issue for the SMARTS to DataWarrior-idcodes conversion will be that SMARTS's and idcode's query features don't map 1-to-1 and that DataWarrior substructure searches don't allow recursive features. Thus, recursive SMARTS would need to be represented by multiple substructure fragments, which will be difficult to implement and also would have its limits. Thomas

---