Subject: Re: PAINS patterns
Posted by evehom on Thu, 23 Jan 2025 19:23:18 GMT
View Forum Message <> Reply to Message

Hi,

Attached is a list with the 480 PAINS in SMARTS format as originally published by Baell et al. These have been curated by Greg Landrum. I presume DW uses the same definitions. If a structure hits any of these it is considered a PAIN.

BW/Evert

File Attachments
1) PAINS.txt, downloaded 230 times