
Subject: PAINS patterns

Posted by [benderitter.p](#) on Thu, 23 Jan 2025 14:58:45 GMT

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Dear all,

would there be anywhere the list of SMILES / SD file considered in the assessment of PAINS patterns (in compound properties calculations)?

I checked the documentation, website and forum, but was not able to find it.

Best regards

Subject: Re: PAINS patterns

Posted by [evehom](#) on Thu, 23 Jan 2025 19:23:18 GMT

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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 127 times
