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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

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#### File Attachments

1) [PAINS.txt](#), downloaded 276 times

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