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Subject: Nasty functions

Posted by [sansun](#) on Mon, 21 Nov 2022 05:32:25 GMT

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The datawarrior has option to calculate 'nasty' functions.

Is there a definition for these?

How similar or different are these from PAINS alerts or Eli Lilly Med Chem rules?

Thanks in advance.

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Subject: Re: Nasty functions

Posted by [thomas](#) on Mon, 21 Nov 2022 09:43:30 GMT

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Nasty functions are a list of small substructure fragments (attached to this message), originally defined by medicinal chemists at Actelion, which should be avoided or limited when purchasing screening compounds from providers.

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#### File Attachments

1) [nasty\\_functions.dwar](#), downloaded 536 times

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