
Subject: Nasty functions

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

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

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.

Subject: Re: Nasty functions

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

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

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.

File Attachments

1) [nasty_functions.dwar](#), downloaded 536 times
