
Subject: Re: thresholds and weights of toxicity risk
Posted by [thomas](#) on Thu, 24 Aug 2023 12:58:04 GMT

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

Dear Norwid,

I admit that fitness criteria are not covered by the manual, because originally they were very simple.

The calculated combined toxicity risk of a compound is simply the sum of risk contributions from the 4 toxicity classes (mutagenic, tumorigenic, irritant, and reproductive effective. A low risk contributes 1, a high risk contributes 2 to the combined score. Thus, a non-existing combined risk would be 0 and the very unlikely theoretical maximum is 8.

Threshold may be fractional numbers, because they describe the sigmoid curve that translate the risk (0..8) into a fitness (1..0)

The determination, whether a compound is assigned a no, low or high risk is based on a statistical approach based on whether and which fragments are present from a predefined fragment list, which are frequently found in toxic compound of the particular toxicity class.

Hope, this explains it somewhat...
