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Subject: Criteria for Evolutionary Library

Posted by [evehom](#) on Fri, 07 Mar 2025 14:30:51 GMT

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Hi,

I think the evolutionary library generation in combination with docking is a great tool. However, the list of criteria for driving the score seems to be fixed. Would it be possible to add:

non-hydrogen atom count

nasty functions

PAINS patterns

Many thanks/Evert

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