Subject: Re: Similarity Search
Posted by thomas on Thu, 31 Oct 2024 09:18:57 GMT
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That should be straight-forward:
- open the file with the 60k compounds
- if you don't see a structure filter, then add a new one from Edit->New Filter
- choose similarity(FragFp) or (Flexophore) in the filter and draw or paste in the query struccture
  (if option "similarity (flexophore)" is missing, you need to calculate flexophores (Chemistry->From Chemical Structure->Calculate Descriptor->Flexophore"

FragFp filtering should be immediate, flexophore filtering may take a few seconds. If the filtering doesn't seem to finish, then the filter process crashed. Then, most likely there is something wrong with the data. You can try then to delete the FragFp or Flexophore column and recreate it. Then try again. Or send me the file (ideally just a few rows that have the same problem) and I check...