Subject: Feature request: Structure does not contain
Posted by smagavi on Thu, 05 Sep 2024 20:15:26 GMT
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I'd like generate a list of all compounds that do not contain a particular element. Is there a way of doing that now? If not, a structure search with "does not maintain" would be great.

Thanks,
Sanjay

Subject: Re: Feature request: Structure does not contain
Posted by thomas on Fri, 06 Sep 2024 07:58:57 GMT
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There are two easy ways to achieve that:
- use a structure filter in 'contains' mode and just draw one atom; then invert the filter
or
- use a structure filter in 'contains' mode and just draw one atom; select the lasso tool, double click the atom and select 'is part of exclude group'

Now you could use 'List->Create Row List From->Visible Rows...'