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Subject: Re: Find & Replace or alternative for stereoisomers

Posted by [thomas](#) on Tue, 30 Aug 2022 19:29:16 GMT

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Hi Paul,

this is an unusual request, which you cannot do in DataWarrior directly. However, based on your idea to do text replacements in SMILES, you could run the following macro (copy the macro text below and select 'Macro->Paste Macro' in you open DataWarrior window. The run the macro with 'Macro->Run Macro->Invert Stereo Centers):

```
<macro name="Invert Stereo Centers">
<task name="addSmilesCodes">
structureColumn=Structure
</task>
<task name="findAndReplace">
isStructure=false
column=Smiles
what=@ @
with=##
</task>
<task name="findAndReplace">
isStructure=false
column=Smiles
what=@
with=@ @
</task>
<task name="findAndReplace">
isStructure=false
column=Smiles
what=##
with=@
</task>
<task name="addStructuresFromName">
useServer=false
column=Smiles
isSmarts=false
</task>
</macro>
```