Subject: Search for "any atom" in structure editor
Posted by TomSilico on Mon, 11 Jul 2022 08:41:03 GMT
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Hi DW,

I've looked through the documentation for this feature and thought it wasn't possible, until I saw a screenshot in another forum post. The title of this post is "How to perform general R group searches in DW". (I can't link it here as this is my first post on this forum).

I'd like to make one atom match "any atom" or e.g. "either carbon or nitrogen" or "not a carbon" in the structure editor. I'd use this both when I apply a structure filter, or when I define the core of a molecule to re-draw molecules of a series so they're oriented the same way (Chemistry > Generate 2D atom coordinates).

It seems like it's possible from the post above when Norwid defines an atom in the structure editor as [C,N] to match both atoms. How can I do this? I've tried using the "?..." button and typing in [C,N] as the atom label. But this seems to only allow specific labels (R, Ala etc...).

In that same post above, it was suggested to replace the two .jar files available for download in the .zip file for improved functionality. I've done this on my machine (Windows, DW5.5.0).

Cheers,

Thomas