

JED: Questions Arising

- Does the Acedrg new covalent description allow for automation?
 - I can imagine that creating one description could be applied to a series of similar covalent ligands. Are there any plans to exploit this? I think there should be.
 - Yes, as long as the atom names of the linked part of the structure are the same for your ligands, then you only need make the link once and it can be used for all your covalently linked ligands
- Also, there are only a limited number of covalent warheads that chemists like to use, *e.g.*
 - <http://www.sciencedirect.com/science/article/pii/S1367593117300601>
 - tackling these scenarios would cover 95% of what we (at least in industry) do. *i.e.*, use the same description and apply it to the new ligand in question, just like for sugar links.
 - We hope that it will work that way
- Also, is there anything in the pipeline for non-standard amino acids?
 - Non-standard amino acids can be handled with either modifications or links (as generated by Acedrg's new mode). We don't have anything new to offer for modifications.