Subject: Re: Doubly Substituted Reactants for Combinatorial Library
Posted by nbehrnd on Fri, 25 Jun 2021 18:52:37 GMT
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Dear SN,

you may consider chemical graph generators to generate list of reactants as .sdf files. Two examples:

OMG requires Java 1.8, e.g. openjdk version 1.8.0_242 (one may still find in Xubuntu 18.04 LTS), or java 8.0.292-zulu (however OpenJDK 11.0.11 e.g., in Linux Debian bullseye will (currently) not work). Then, an input like

java -jar OMG.jar -ec C4H12N2 -o out_bisamine.sdf

yields a list of hydrocarbons including those with two amines. Some of the entries (see .sdf below) may be «surprising» from a chemical point of view. However a) you may pre-define non-overlapping fragments which must be present to guide the generator. Remember that you may create an empty structure table, populate this first column with DW structure editor, and eventually export this as .sdf (File -> Save Special) and then run

java -jar OMG.jar -ec C4H12N2 -o out_bisamine.sdf -fr fragments.sdf

to constrain the generation. And b), once the list is imported into DW, use e.g. the entries below Chemistry -> From Chemical Structure -> Calculate Properties to remove suggestions by ring counts / heterocyclic ring count, H-donors / acceptors, etc.

For MOLGEN there is a dedicated test page. Note, here Hill formulae may be provided as range; this may fit e.g., your aim to define diamines with a varying number of methylene groups as spacer. Based on their example 2 about halogenated halogens, the input criterion C1-3N1-2H4-10 yields 468 suggestions with one or two amino groups. The generation may be constrained, e.g. skipping cycles (set cycles = 0), and double bonds (set maximal bond multiplicity = 1) as parameters in addition. Then, there are just 29 entries matching all three criteria. Or, derived from example 4, a sum formula of C[sp2_a]6H4-6N[val=5,d=2]0-2O0-4 altogether with the limit of one cycle only, yields a list of 74 molecules, including benzenes with one or two nitro groups in ortho/meta/para relationship.

The web site offers only a glimpse of the program. The possibility to define fragments required / fragments to skip which the web page not offers is not shown, but present in limited (Windows) versions of the program one may download. Equally, the web site's work stops the molecule generation with entry #1000. Despite their rough conformations, the suggestions displayed are good enough to be exported as .sdf to continue processing in DataWarrior (the filtering mentioned above): just open JSmol's pulldown menu, File -> Save -> Save a copy of genXYZ.sdf to fetch the information.

Below a selection of output .sdf generated by OMG / MOLGEN.

Norwid

File Attachments

1) out_bisamine.sdf, downloaded 554 times
2) gen245_molgen_bisamines.sdf, downloaded 580 times
3) gen259_molgen_PhNO2.sdf, downloaded 563 times
4) gen259_PhNO2.dwar, downloaded 555 times