
Subject: Enumeration of Libraries

Posted by [frytz](#) on Fri, 04 Feb 2022 15:16:59 GMT

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I am trying to enumerate a library of compounds. A+B+C.

A+C are predefined while B should be more flexible in length and atomic constitution.

I am using U, Np as indicators to show where the molecules should be joined.

I am not able to define U-X-Y-Np (B) in a flexible manner to join A+C in many different ways. 80

How can I draw fragment B in a way that it will accept many different structures and features?

Thank you for your help.

File Attachments

1) [Screenshot 2022-02-04 161317.png](#), downloaded 656 times

