
Subject: Add reaction from structure

Posted by [yrin0878](#) on Fri, 28 Apr 2023 01:18:52 GMT

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Hi I'm beginner of datawarrior.

It is a good software to analyze chemical data.

But I have a problem.

I have over 100 building blocks, and I want to add a same reaction to all that building blocks.

But when I'm trying to add a reaction, I have to make a reaction column then, draw the reaction to each structures.

This takes too long time :(

Can I apply one reaction to that all structures?

Tell me the way to deal with this problem.

Thank you

File Attachments

1) [datawarrior_Q.png](#), downloaded 620 times

File Edit Data Chemistry Database List Macro Help

Table

#	BB ID	Structure of SMILES	SMILES	Amine protecting group	이름
1	AA0001		<chem>CC(C)(C)OC(=O)NCC(C1=CC=CC=C1)C(=O)O</chem>	Boc	α-[2-[[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]benzeneacetic acid
2	AA0002		<chem>CC(C)(C)OC(=O)NCC(C1=CC=CC=C1)C(=O)O</chem>	Boc	α-[[[(1,1-Dimethylethoxy)carbonyl]amino]methyl]benzeneacetic acid
3	AA0003		<chem>CC(C)(C)OC(=O)NCC(C(C)(C)C)C(=O)O</chem>	Boc	4-[[[(1,1-Dimethylethoxy)carbonyl]amino]-2,2-dimethylbutanoic acid
4	AA0004		<chem>O=C(O)CC1CN(C(=O)OCC2C=CC=CC=C3C=CC=CC=C4C2)C1</chem>	Fmoc	1-[(9H-Fluorenyl)methoxy]carbonyl]-3-pyrrolidineacetic acid
5	AA0005		<chem>C(OC(NCC[C@@H](C(=O)O)O)C1C=CC=C3C=CC=CC=C4)C1</chem>	Fmoc	(2S)-4-[[[(9H-Fluorenyl)ethoxy]carbonyl]amino]-2-hydroxybutanoic acid
6	AA0006		<chem>OC(C(C1CCOCC1)N(C(=O)O)O)C2=CC=CC=C3C=CC=CC=C4C2)C1</chem>	Fmoc	2-(((9H-Fluorenyl)methoxy)carbonyl)amino)-2-(tetrahydro-2H-pyridin-4-yl)acetic acid
7	AA0007		주문 중	Fmoc	2-(1-[[[(9H-fluorenyl)methoxy]carbonyl]piperidin-4-yl]acetic acid
8	AA0008		<chem>CC(C)(C)OC(=O)NCC(C(C)(C)C)C(=O)O</chem>	Boc	3-((tert-butoxy)carbonyl)amino)-2,2-dimethylpropanoic acid
9	AA0009		<chem>O=C(NCC(C)C(=O)O)OCC1C=CC=C3C=CC=CC=C4C1)C3</chem>	Fmoc	3-(((9H-fluorenyl)methoxy)carbonyl)amino)-2-methylpropanoic acid

456 of 563 MB

Selected:1

○ 검색하려면 여기에 키워드를 입력하세요