

---

Subject: could DataWarrior "build evolutionary libray" criteria be applied to design minipeptides?

Posted by [juliocoll](#) on Sun, 01 Nov 2026 07:38:00 GMT

[View Forum Message](#) <> [Reply to Message](#)

---

The build evolutionary library of DataWarrior is a powerful tool to design drug-like compounds and selec those with high affinities among many of their possible alternatives. I really appreciated it!

While sucessfully working with the 2-years-old new deep-learning peptide-design programs such as BoltzGen and many others, and if I did not misundertstood their algorithms, I noticed that still they did not employed any affinity-docking evolutionary algorithm to iteratively select for their best peptide designs. Up to now, BoltGen and others generate only structurally fitting peptides.

I wonder if those type of protein-peptide affinity designs could be incorporated into the criteria of the build evolutionary library. In other words, could an affinity minipeptide criteria (6 to 12-mer) be added to the build evolutionary library of DataWarrior? perhaps by restriciting the libraries amino acids during evolution rather than atoms? perhaps by including protein-peptide interaction/affinity predictions by other programs like Prodigy? perhaps other ideas?

---