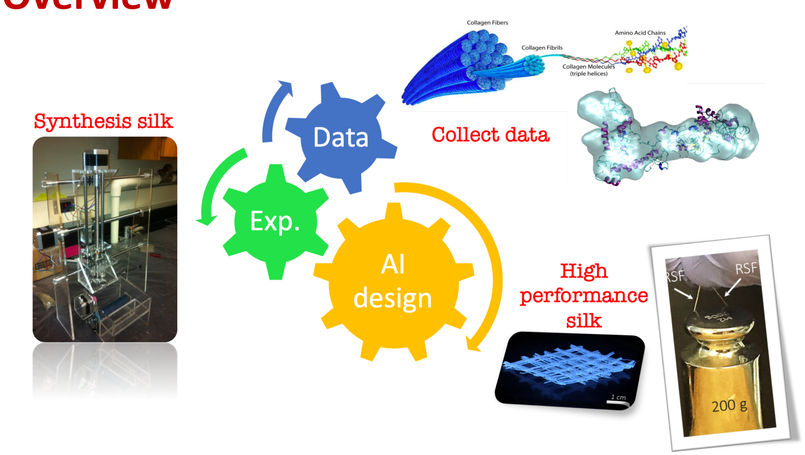
Using Artificial Intelligence to Generate *de novo* Thermally Stable Collagen Sequences

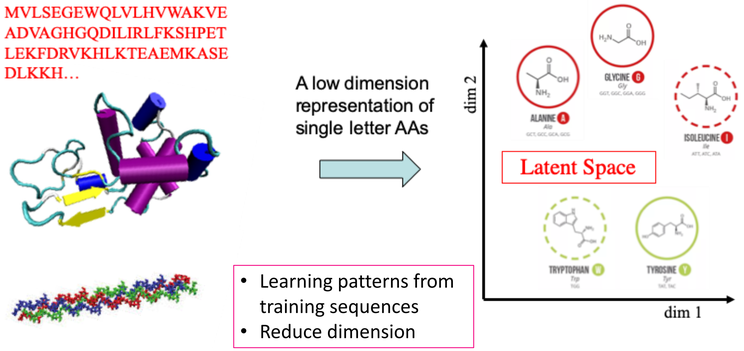
Chi-Hua Yu[1,2], Om Prakash Narayan[3], Rachael Parker[3], David Kaplan[3] and Markus J. Buehler[1*]

[1] Laboratory for Atomistic and Molecular Mechanics, MIT, [2]Department of Engineering Science, NCKU [3]Department of Biomedical Engineering, Tufts University; *mbuehler@MIT.EDU

Overview



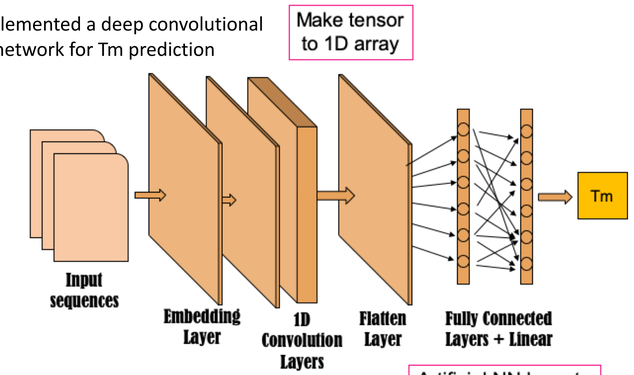
Learning from sequences pattern



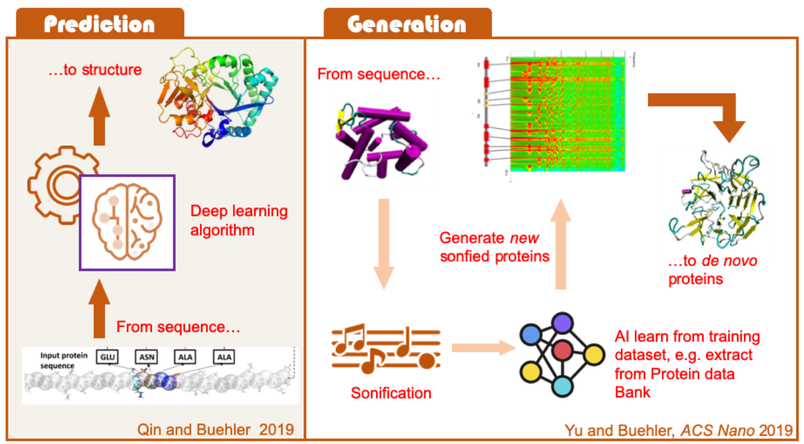
- Learning patterns from training sequences
- Reduce dimension

Silknet – Deep learning model

- We implemented a deep convolutional neural network for Tm prediction

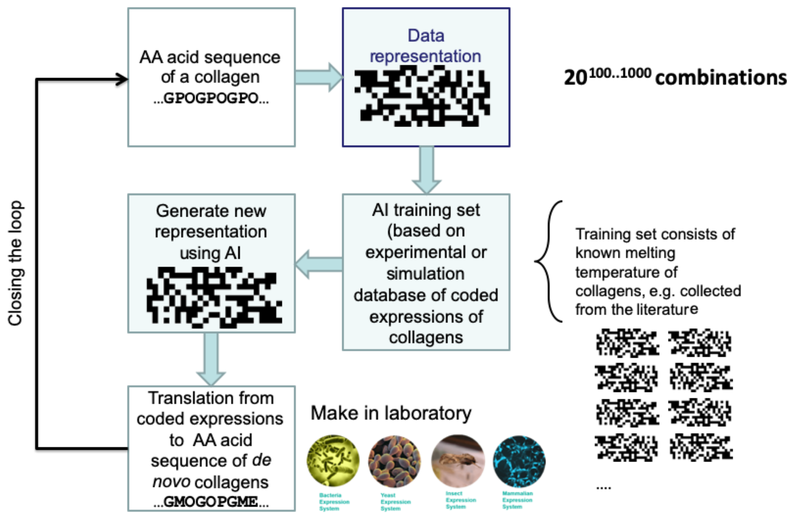


Machine learning (ML) on protein design

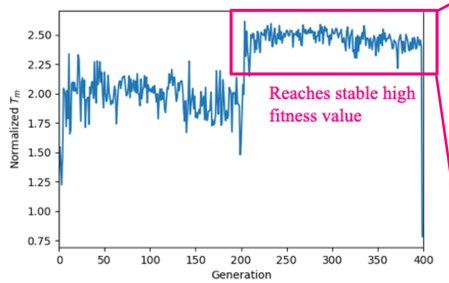


Our research group use ML to predict 2nd structure as well as design de novo proteins.

Self-evolved design approach



Results



Most stable collagens

sequence
GPOGPOGPOGPOGPOOGROGROGROGRO
GPOOGPOGPOGPOGPGPPOGDKGPOPOGPOGO
GPOGPOGPOGPOGPOPPOGDKGPOPOGPOGO
POGPOGPOGPOGPOPOGOPOGPOGGPOOGP
POGPOGPOGPOGPOGPOGDKGPOPOGPOGO
POGPOGPOGPOGPOGPOGDKGPOPOGPOGO
GOGPOOGPOGPOGPOGPOGPOGDKGPOPOGPOGO
OOGPOGPOGPOGPOGPOGDKGPOPOGPOGO

Future work

- Experimental synthesis collagen sequences for verification.
- Apply to function design

References

C.H. Yu and M. J. Buehler, Nano Futures (2019)
C.H. Yu and M. J. Buehler, ACS Nano, (2019)
Z Qin, M. J. Buehler et al; bioRxiv, 660639

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