Date:	January 15, 2020
Subject:	**Minutes for NIH U01 program - SITEP meeting, 8 AM, January 15, 2020**
Focus:	**Collagen**
Meeting Location:	MIT

Summary – Scientific Progress – Past month

<u>Collagen</u>
(Jonny, Eesha, Om)

- Jonny/Eesha: Deep Learning Model
    - We eliminate unusable sequences, clear data because some sequence are the same but have different Tm values, or the peptides are very short. The sequence length will affect how the model will work. We eliminate the inconsistencies.
    - We carry out Normalization before neural network and Sequence Embedding
    - We tried several latent space dimensions
    - We tried several neural network setup
    - The results are better: we do not have over feeding and no over training
    - The predictions are better: the variance is 5C
    - We run a new generic algorithm: all the sequences are Gly-X-Y
    - We introduced crossover and mutation
    - New results: Tm value is very high and stable. The objective function is maximizing Tm value using generative algorithm.
    - BLAST analysis of Sequence: we generate more than 10 000 sequences and check them. BLAST shows you if there is a match in sequence.
    - Concerns: BLAST analysis, Target T values (aiming for height T or range of Ts), Training data set integrity.
    - We can evolve our understanding with experiments on the peptides with have (from previous model).
    - We need to investigate whether the method is able to create something new or is only able to create some variation of the data set.
    - With our current model, overall, the generated sequences have not appeared in the data set.
    - Future work: Find the design envelope: how far away can we go but also predict. We should try more random sequences, away from GXY-GXY, and check the results from those sequences. We want to understand where the limits are and find the measure of order, and plot stability to order value.
    - The generative algorithm is very useful when we design proteins.
    - Future applications: We can also design composites: stable+unstable+stable… sequence. Or design gradient: very stable to very unstable. We can also investigate wave propagation analysis.

<u>Administrative Matters</u>

- Model Credibility Plan (MCP) Updates:
    - Eesha will take the lead on the MCP at MIT
    - Eesha will collect the models and communicate with Genin group on a frequent base

- Modeling of SELPs and Fredrick's work
    - Diego has finished previous ones
    - The new results from Fredrick's work in last December was not good so no modeling needed
    - Andrew at MIT is interested in working on modeling of SELPs. He will be taking over Diego's role on modeling

- New IMAG wiki website
    - Last chance to update the website before its release is today at midnight

- o Shengfei will upload publications, figures, medias, and codes that are published or available
- o In the late afternoon Shengfei found out there was an authorization problem or bug on the new IMAG wiki website, which did not allow him to edit/upload materials. Thus, the uploading will be delayed.

Publications – updates

- Martín-Moldes Z, Ebrahimi D, Plowright R, Dinjaski N, Perry CC, Buehler MJ, Kaplan DL, "Osteoconductivity of silk calcified organic-inorganic interfaces." In preparation.
- Martín-Moldes Z, López Barreiro D, Perry CC, Buehler MJ, Kaplan DL, "Osteoconductivity of silk silicified organic-inorganic interfaces." In preparation.
- Guo C, Qin Z, Buehler MJ, Kaplan DL, "Processing Silk with High Pressure and Heat". In preparation
- J. Yeo, Y. Qiu, G.S. Jung, Y. W. Zhang, M. J. Buehler, and D. L. Kaplan. "Adverse effects of Alport syndrome-related missense mutations on collagen IV: unified insights from molecular dynamics simulations and experiments". In submission.
- López Barreiro, D., Martín Moldes, Z., Hawker, M.J., Shen, S., Yeo, J., Martin-Martinez, F.J., Kaplan, D.L., Buehler, M.J., "Conductive Silk-Based Composites Using Biobased Carbon Materials", Advanced Materials, 1904720, 2019.
- J. Yeo, G.S. Jung, F. J. Martín-Martínez, J. Beem, Z. Qin, M. J. Buehler.
  Multiscale Design of Graphene-Based Materials for High-Performance Separation Membranes. Adv. Mater. 2019. https://doi.org/10.1002/adma.201805665
- E. Beniash, C. A. Stifler, C.-Y. Sun, G. S. Jung, Z. Qin, M. J. Buehler, and P. U. P. A. Gilbert, "The hidden structure of human enamel," *Nature Communications*, vol. 10, no. 1, p. 4383, 2019

Logistics & Housekeeping

Next SITEP meeting: February 12, 2020, Tufts.

Current Participants:
- David Kaplan   david.kaplan@tufts.edu
- Markus Buehler   mbuehler@mit.edu
- Isabelle Su   isu@mit.edu
- Chi-Hua Jonny Yu   jonnyyu@mit.edu
- Zaira Martin Moldes   Zaira.Martin_Moldes@tufts.edu
- Rachael Parker   Rachael.parker@tufts.edu
- Chengchen Guo   Chengchen.guo@tufts.edu
- Diego López Barreiro   dlopezb@mit.edu
- Fredrik Backlund   Fredrik.Backlund@tufts.edu
- Laura Chambre   Laura.chambre@tufts.edu
- Om Prakash Narayan   om.narayan@tufts.edu
- Kai Guo   kaiguo@mit.edu
- Eesha Khare   ekhare@mit.edu
- Shengfei Zhou   shengfei@mit.edu
- Mario Milazzo   milazzo@mit.edu
- Constancio Gonzalez Obeso   Constancio.Gonzalez_Obeso@tufts.edu
- Andrew Lew   lewan@mit.edu

Past Participants (position while in SITEP, current position) – Alums of program:
- Sreevidya Krishnaji Tarakkad (PhD student, faculty member, IISER Bhopal India)
- Michelle Kinahan (PhD student, Scientific Writer, Beckman Coulter)
- Seunghwa Ryu (post doc, faculty member, KAIST)
- Greta Gronau (graduate student/M.S., graduate student in Germany)
- Graham Bratzel (graduate student/M.S., Product Engineer, Jet Parts Engineering, Inc.)

- Qin Wang (post doc, Associate Professor, Hubei University China)
- David Li (M.S. student, PhD candidate, Carnegie Mellon University)
- Shangchao Lin (post doc, faculty member, Florida State University)
- Shun Zhou (post doc, supervisor and project manager, GenScript)
- Olena (Rabotyagova) Tokareva (post doc, Scientist, Monsanto, Corp., Cambridge, MA)
- Shu-Wei Chang (post doc, faculty member, National University Taiwan)
- Bo An (post doc, Senior Scientist, CSL Behring, IL)
- Tristan Giesa (post doc, Consultant, Exponent, Inc., CA)
- Nina Dinjaski (post doc, Licensing Associate, Tufts University, MA)
- Shengjie Ling (post doc, Assistant Professor, Shanghaitech University)
- Davoud Ebrahimi (post doc, Consultant, Mott MacDonald)
- Anna Tarakanova (post doc, Assistant Professor, University of Connecticut)
- Wenwen Huang (post doc, Assistant Professor, Zhejiang University)
- Jingjie Yeo (post doc, Assistant Professor, Cornell University)
- Yimin Qiu (post doc)
- Zhao Qin (research scientist, Assistant Professor, Syracuse University)
- Francisco Martin Martinez (research scientist, Lecturer, Swansea University)
- GangSeob Jung (PhD student, Post doc, Oak Ridge National Lab)
- Fredrik Backlund (post doc, research scientist, Sweden)