Mary Anne Koda-Kimble Seed Award for Innovation
APPLICATION FORM, 2016-2017

(*See Koda-Kimble Award Description and Criteria for more information)*

1. Provide information for each section below. *Sections will expand with your entry*.
2. When complete, save your application form into a PDF format.
3. Upload your **application as a PDF** via this Web Link:

Koda-Kimble Seed Award for Innovation

If above link does not work, copy and paste this into browser:
https://app.smartsheet.com/b/form?EQBCT=1862fbe391324b8d95d2bd9a5f47d59e

If you have questions please send email to: dean@pharmacy.ucsf.edu

All fields below must be completed:

Proposal title:

Virtual Reality Molecular Playground

Requested award amount:

$18,027 plus indirect costs (if applicable)

Principal applicant (Your last name, first name, title, dept.)

Goddard, Thomas
Computational and Data Science Research Specialist 4
Department of Pharmaceutical Chemistry, UCSF

List additional project collaborators (Last names, first names, titles, depts.)

Iwasa, Janet
Research Assistant Professor
Department of Biochemistry, University of Utah

Johnson, Graham
Director, Animated Cell
Allen Institute for Cell Science

Background: (250 words MAX)

Discovering and investigating the molecular basis of life fascinates research scientists, but K-12 students and much of the public find molecules inscrutable, invisible, and imagined as a world of

lifeless billiard balls. The beautiful dynamics, chemical transformations, and information carrying properties of molecules that choreograph life are seen after years of study that few students undertake. In 2016, the first consumer virtual reality (VR) headsets became available and over 1 million have already been sold for playing immersive games, where the 360 degree visual environment surrounding the participant is a computer generated "synthetic world" that you manipulate and move through. Our lab, the Resource for Biocomputing, Visualization and Informatics (RBVI), has built a prototype software system to show VR worlds of proteins, nucleic acids, and 3D electron and optical microscopy data that included viruses and macrophages to ~30 groups of high school students, college students and scientists, and observed nearly universal engagement and a high level of enthusiasm for these immersive visualizations. The purpose of this project is to expand the RBVI's science outreach capabilities and make the dynamic 3D molecular world that is part of our invisible everyday lives familiar and inviting to potential future scientists by developing a virtual reality experience where key biomolecules of life can be experienced as intuitively as our everyday physical world.

Hypothesis / Problem: (100 words MAX)

Our goal is to inspire and energize K-12 and undergraduate students, and the general public, in science and to demonstrate that understanding the molecular of life is accessible and even beautiful, and to encourage students to pursue work in science and appreciate the work and findings of scientists. We propose to develop a dynamic immersive molecular world involving DNA, RNA and peptides that can be creatively explored using 3D "immersive" visualization to test if virtual reality makes students more comfortable with and curious about modern biology.

Methodology: (500 words MAX)

We will develop a "game," or (in common virtual reality terminology) an "experience" using the readily available "Steam" game distribution platform, which has over 100 million users worldwide and hence is well-accepted by the VR developer community. The 360 degree environment we will create will be a molecular "zoo" that users can explore and interact with. We will enable users to "hold" a single stranded RNA molecule that writhes like a snake, stretches straight by pulling on its ends, and breaks by pulling too hard, all scientifically accurate attributes of RNA. Duplex DNAs, much stiffer and that flex more slowly, can be pulled apart to unzip the DNA and the resulting flexible single DNA strands will then zip themselves back together, also scientifically accurate molecular behavior. Physics-based mass and spring type dynamics will be used to display qualitatively correct molecular dynamics. It will be possible to build RNA from individual nucleotides using a DNA template by finding and positioning the correct complementary bases, and similarly build peptides by finding appropriate tRNAs floating in the environment and "hand placing" them to match an RNA template. The user will stand in for RNA polymerases and ribosomes and directly manipulate the molecular environment, rather than passively observing molecular machines – this is a zoo where you hold and feed the animals, not merely watch them.

The molecular zoo will not be limited to biomolecules. To appreciate chemical reactions you will be able to "shoot" a stream of molecular hydrogen at a cloud of molecular oxygen using a handheld 3D interactive pointer device and have it "ignite," producing water and hydrogen by-products that fly off at speeds related to their masses. A more complex molecule such as TNT can be oxidized to see a more reaction products. The most important aspect of this project is that the VR user will be able to **control, explore and discover** molecular interactions in their personal virtual world, rather than be guided on a fixed path as is currently done in textbooks and videos. We will maximize an individual's engagement with visual and audio effects and the freedom to control their VR environment, e.g., break molecules and create new molecules.

The Principal Applicant of this proposal has developed molecular graphics software for 20+ years at the RBVI using low-level OpenGL programming. This project diverges significantly from that paradigm and will instead use the high-level Unity 3D game platform and physics engine enabling much wider distribution via Steam, and faster development.

The success of this effort will be measured by analytics capture by reviews, criticisms, suggestions, ratings, number of users, and cumulative time used which are standard features of the Steam online distribution platform. We expect dozens of iterations and revisions based on user testing at the RBVI and from online feedback on Steam. Given the limited development time supported by the request budget, this will be a proof of concept implementation, including a limited range of molecular behaviors and user-interactions. Subsequent funding through a STEM (science, technology, engineering and mathematics) education NSF grant or charging a small fee (< $10) for access to the software could enable adding more diverse biomolecules and user interactions.

Budget details: (format as necessary)

10% FTE software development for 1 year (total of 200 hours): $17,127 plus indirect costs (if applicable)

Steam Greenlight subscription for putting software online: $100

Unity 3D physics simulation software: $0

Vive VR headset: $800. (Our Lab currently has one Vive headset; this second headset will enable both a "presenter" and "participant" to view the same 3D scene simultaneously.)

Collaborators consulting by video conference: $0