21st-Century Tools for a 19th-Century Question: What Is the Molecular Basis of a Scent?

Dr. Richard Gerkin
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2–3 p.m.
Biology (Building 21)
Room 256

How do we know if our computational models of biological systems are any good? Journal articles give us a small piece of the answer, but they tell us more about "how" than "how well." In his lecture, Dr. Richard Gerkin will describe an ongoing initiative, based on the concept of the "unit test" from software development, to formally document the ability of computational models to recapitulate the important features of a biological system as assessed by experimental data.

Performance on a suite of such data-driven tests summarizes the scope and fitness of a model, and across models these test suites can summarize the state of theory and its implementation in a field.

"I use both neuron physiology and human olfaction to demonstrate these concepts," says Dr. Gerkin, "asking how well the best computer models can recapitulate existing experimental observations, and how this informs potential new research directions. I will also describe one of these research directions, in which I aim to construct a high-resolution map of human olfactory perception."

Richard C. (Rick) Gerkin is Assistant Research Professor in the School of Life Sciences at Arizona State University, as well as Affiliated Associate Professor in the School of Mathematical and Statistical Sciences. Dr. Gerkin is the principal investigator, or co-investigator, on two R01 awards from the National Institutes of Health. He holds one patent, and won the DREAM Olfaction Prediction Challenge, an international machine learning competition to predict odor from molecular structure. He is also developing new undergraduate courses in data science for biologists. Dr. Gerkin's work has been featured in *Science*, *The New Yorker*, and *The Atlantic*.

With research interests in neuroscience and neuroinformatics, Dr. Gerkin's main research goals include:

- Developing software infrastructure for data-driven validation of computer models in biology.
- Cracking the olfactory "code" that mediates the transformation from odorant stimulus to odor percept.
- Discovering novel biomarkers for neurodegenerative diseases.

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