

## Musicians, chemists use sound to better understand science

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A graphic from the journal article illustrates the process of a protein (the chain of spheres at the top) folding, unfolding or misfolding as it moves around. The structural parameters of the protein are coded into sound, producing a variablepitch sound waveform, for example. Timbre, pan, loudness and other parameters can be adjusted based on data input to represent different aspects or qualities of a protein. Credit: Biophysics Sonification Group



Musicians are helping scientists analyze data, teach protein folding and make new discoveries through sound.

A team of researchers at the University of Illinois Urbana-Champaign is using sonification—the use of sound to convey information—to depict biochemical processes and better understand how they happen.

Music professor and composer Stephen Andrew Taylor; chemistry professor and biophysicist Martin Gruebele; and Illinois music and computer science alumna, composer and software designer Carla Scaletti formed the Biophysics Sonification Group, which has been meeting weekly on Zoom since the beginning of the pandemic. The group has experimented with using sonification in Gruebele's research into the physical mechanisms of protein folding, and its work recently allowed Gruebele to make a new discovery about the ways a protein can fold.

Taylor's musical compositions have long been influenced by science, and recent works represent scientific data and biological processes. Gruebele also is a musician who built his own pipe organ that he plays and uses to compose music. The idea of working together on sonification struck a chord with them, and they've been collaborating for several years. Through her company, Symbolic Sound Corp., Scaletti develops a digital audio software and hardware sound design system called Kyma that is used by many musicians and researchers, including Taylor.

Scaletti created an animated visualization paired with sound that illustrated a simplified <u>protein-folding</u> process, and Gruebele and Taylor used it to introduce key concepts of the process to students and gage whether it helped with their understanding. They found that sonification complemented and reinforced the visualizations and that, even for experts, it helped increase intuition for how proteins fold and misfold over time. The Biophysics Sonification Group—which also includes chemistry professor Taras Pogorelov, former chemistry graduate student



(now alumna) Meredith Rickard, composer and pipe organist Franz Danksagmüller of the Lübeck Academy of Music in Germany, and Illinois electrical and computer engineering alumnus Kurt Hebel of Symbolic Sound – described using sonification in teaching in the *Journal of Chemical Education*.

Gruebele and his research team use supercomputers to run simulations of proteins folding into a specific structure, a process that relies on a complex pattern of many interactions. The simulation reveals the multiple pathways the proteins take as they fold, and also shows when they misfold or get stuck in the wrong shape—something thought to be related to a number of diseases such as Alzheimer's and Parkinson's.

The researchers use the simulation data to gain insight into the process. Nearly all data analysis is done visually, Gruebele said, but massive amounts of data generated by the computer simulations—representing hundreds of thousands of variables and millions of moments in time—can be very difficult to visualize.

"In digital audio, everything is a stream of numbers, so actually it's quite natural to take a stream of numbers and listen to it as if it's a digital recording," Scaletti said. "You can hear things that you wouldn't see if you looked at a list of numbers and you also wouldn't see if you looked at an animation. There's so much going on that there could be something that's hidden, but you could bring it out with sound."

For example, when the protein folds, it is surrounded by water molecules that are critical to the process. Gruebele said he wants to know when a water molecule touches and solvates a <u>protein</u>, but "there are 50,000 <u>water molecules</u> moving around, and only one or two are doing a critical thing. It's impossible to see." However, if a splashy sound occurred every time a water molecule touched a specific amino acid, that would be easy to hear.



Taylor and Scaletti use various audio-mapping techniques to link aspects of proteins to sound parameters such as pitch, timbre, loudness and pan position. For example, Taylor's work uses different pitches and instruments to represent each unique amino acid, as well as their hydrophobic or hydrophilic qualities.

"I've been trying to draw on our instinctive responses to sound as much as possible," Taylor said. "Beethoven said, 'The deeper the stream, the deeper the tone.' We expect an elephant to make a low sound because it's big, and we expect a sparrow to make a high sound because it's small. Certain kinds of mappings are built into us. As much as possible, we can take advantage of those and that helps to communicate more effectively."

The highly developed instincts of musicians help in creating the best tool to use sound to convey information, Taylor said.

"It's a new way of showing how music and sound can help us understand the world. Musicians have an important role to play," he said. "It's helped me become a better musician, in thinking about sound in different ways and thinking how <u>sound</u> can link to the world in different ways, even the world of the very small."

**More information:** Carla Scaletti et al, Sonification-Enhanced Lattice Model Animations for Teaching the Protein Folding Reaction, *Journal of Chemical Education* (2022). DOI: 10.1021/acs.jchemed.1c00857

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