

# Can one hear properties of the molecule?

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## ABSTRACT

To design a drug, one must identify a small molecule that is complementary in shape and charge to the biomolecular target with which it interacts. Tremendous effort has been expended in the search for small molecules that bind to a biomolecular target, using both experimental and computational approaches. Many recent computational strategies utilize machine-learning algorithms. The main problem faced by machine-learning approaches is that they need to be intelligent and flexible enough to accommodate the inherent uncertainty of in vivo molecular data. We propose a new approach in which important molecules are represented as a sound. Specifically, inspired by Mark Kac's classic paper, "Can One Hear the Shape of a Drum" [1], we compute the acoustic spectrum of a molecule by treating the molecule's surface as a three-dimensional drum, with the density of the drum's membrane determined by key molecular properties/features. Using this idea, together with strategies based on graph-theory, hyperparameter optimization, and spectral theory, allows key molecular features to be represented as sounds. These sounds are shown to be consistent with well-known chemical concepts related to functional groups and molecular similarity. Finally, we compute molecular sounds for a database of molecules and use these as input features for a machine-learning method. Even outside the context of machine learning and drug design, molecular sounds provide a new, effective, and efficient descriptor for computational chemists.

## References

- [1] Kac, M. Can One Hear the Shape of a Drum? *The American Mathematical Monthly* (Apr.) **1966**, Vol. 73, No. 4, Part 2: Papers in Analysis pp. 1-23