Why the Sound of Molecules Matters in Al: A New Modality for Molecular Representation and Prediction

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## **Abstract**

We present innovative systems and methods for the analysis and representation of molecular structures and spectral data through sonification, designed explicitly to enrich artificial intelligence (AI) applications. Our approach transforms complex molecular data, including structural representations and various spectral modalities (e.g., IR, NMR, UV), into distinctive audio waveforms. By integrating these sonified molecular representations into multimodal AI frameworks, we create a powerful data moat, substantially enhancing the capabilities of AI-driven discovery and diagnostics across healthcare and educational technologies. The methodologies are underpinned by our recently patented techniques and thoroughly described in our foundational book, \*The Sound of Molecules: A Molecular Encoding for AI\*. Our proposed system demonstrates significant potential for advancing AI applications in pharmaceutical innovation, clinical diagnostics, and interactive STEM education.