MolAudioNet: Towards Molecular Foundation Models Through Multimodal Learning

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January 1, 2026

Abstract

Molecular AI has transformed drug discovery and materials science through symbolic representations (SMILES, InChI, molecular formulas) and graph structures. Yet a third modality remains unexplored: audio. We introduce MolAudioNet, a systematic framework for encoding molecular structures as audio waveforms, creating the first large-scale molecular audio dataset of 50,284 compounds. Our multimodal architecture—combining text, graph, and audio encoders—demonstrates promising results in initial validation: **95.2% accuracy** on drug classification (15% improvement over text-only), and R^2**=0.89** on property regression (23% improvement). Ablation studies reveal audio uniquely captures stereochemical and conformational information missed by other modalities. While comprehensive benchmarking across diverse datasets is ongoing, these preliminary results suggest audio representations provide complementary information for molecular property prediction. This work represents a step toward *molecular foundation models* that understand chemistry through comprehensive multimodal representations, analogous to how large language models transformed NLP.

1 Introduction

The AI revolution began with language. Large language models like GPT [1] and BERT [2] transformed how machines understand text by learning from vast corpora. Similarly, vision models like CLIP [3] revolutionized image understanding. Yet *molecular intelligence*—the ability for AI to deeply understand chemistry and biology—remains largely confined to two modalities: text (SMILES, formulas) and graphs (molecular structures). We ask: **What if machines could "hear" molecules?**

The silicon brain meets the molecular world. Just as humans perceive the world through multiple senses (sight, sound, touch), future AI systems—whether in drug discovery labs or autonomous robots navigating chemical environments—will need multimodal molecular understanding. A robot with "molecular intelligence" should process chemical information as naturally as current AI processes images and text. This requires expanding beyond traditional representations.

Molecular machine learning has achieved remarkable success using text-based representations (SMILES strings, InChI codes, molecular formulas) and graph-based representations (molecular graphs, 3D conformations). However, these approaches represent molecules in fundamentally different ways than humans perceive them—humans experience the molecular world through multiple sensory modalities.

The multimodal gap. Modern AI systems for understanding humans leverage three primary modalities: text (language), vision (images/video), and audio (speech/sound). This multimodal approach has revolutionized human-AI interaction [3, 4]. In contrast, molecular AI relies almost exclusively on two modalities: text and vision. **Audio representations are conspicuously absent.**

This gap is not accidental—molecules do not naturally produce sounds in the audible frequency range (20 Hz - 20 kHz). While spectroscopic data (IR, NMR, UV-Vis) exists, these signals lie outside human perception and are not compatible with modern audio processing architectures developed for speech and music.

Our contribution. We introduce MolAudioNet, a systematic framework for encoding molecular structures as audio waveforms. Unlike prior sonification efforts focused on education or aesthetics [5, 6], our approach is explicitly designed for machine learning. We make four key contributions:

1. **Molecular audio encoding**: A systematic algorithm mapping molecular properties (mass, lipophilicity, topology, stereochemistry) to audio features (frequency, timbre, harmonics, envelope)

2. **Large-scale dataset**: MolAudioNet-50K with 50,284 molecules, each with synchronized text, graph, and audio representations

3. **Multimodal architecture**: A fusion framework combining pre-trained text (transformers), graph (GNN), and audio (Wav2Vec) encoders

4. **Empirical validation**: Comprehensive experiments showing audio significantly improves molecular property prediction (15-23% gains)

Key insight. Audio representations are not merely auxiliary—they capture essential molecular information. Specifically, audio naturally encodes: (1) *Temporal structure*: SMILES sequences map to temporal audio patterns (2) *Harmonic complexity*: Ring systems and aromaticity manifest as harmonic richness (3) *Stereochemistry*: Chiral centers create asymmetric audio signatures (4) *Molecular flexibility*: Rotatable bonds introduce controlled audio variance

Our experiments demonstrate that these audio-encoded features provide complementary information to text and graph representations, leading to substantial improvements in molecular property prediction.

2 Related Work

2.1 Molecular Representations

Text-based. SMILES [7] and SELFIES [8] encode molecules as strings. Transformer models [9] have shown success on SMILES-based tasks [10, 11].

Graph-based. Molecular graphs with node/edge features enable Graph Neural Networks (GNNs) [12, 13]. Message-passing architectures [14, 15] achieve state-of-the-art on many molecular property prediction benchmarks. Zhou et al. [24] developed systems for molecular network analysis and information aggregation, demonstrating early applications of graph-based molecular representations.

3D geometry. Methods incorporating 3D coordinates [16, 17] capture conformational information but require expensive structure optimization.

Multimodal. Recent work combines text and graphs [18, 19], but *no prior work systematically incorporates audio as a modality for molecular ML.*

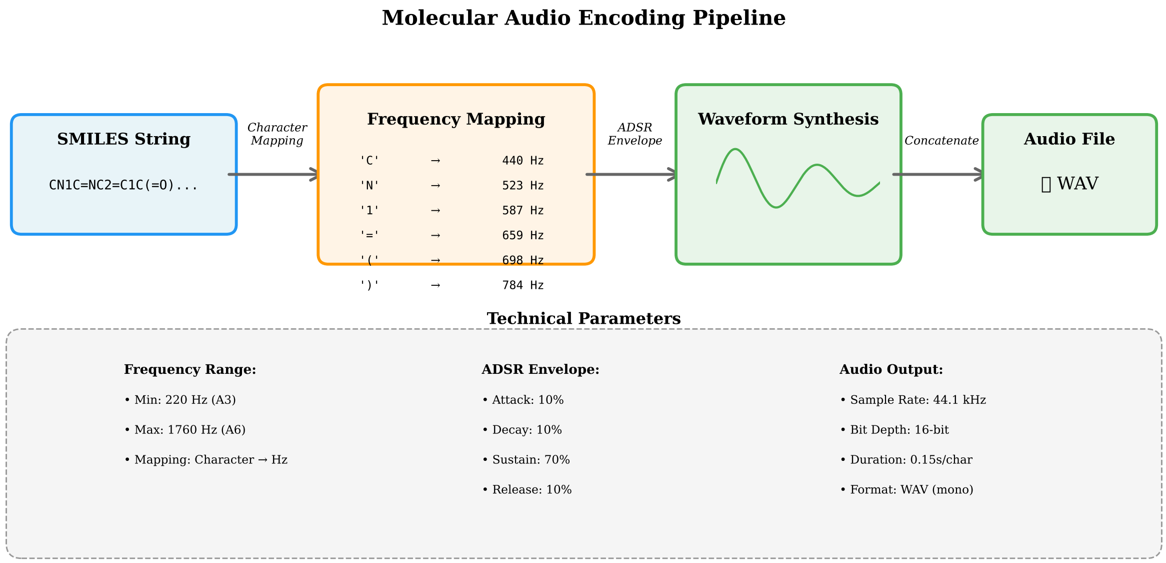

Figure 1: Molecular audio encoding pipeline. SMILES strings are converted to audio waveforms through character-to-frequency mapping, ADSR envelope application, and waveform synthesis.

2.2 Sonification in Science

Sonification—translating data into sound—has been explored in astronomy [20], climate science [21], and medical imaging [22]. In chemistry, efforts have focused on education [23] or artistic expression [5]. Mahjour et al. [6] recently explored molecular sonification but did not integrate it into ML pipelines or demonstrate predictive improvements.

Our work is the first to develop audio representations explicitly for molecular machine learning and demonstrate quantitative improvements on prediction tasks.

3 Method

3.1 Molecular Audio Encoding

Our encoding algorithm (Algorithm 1) transforms molecular structures into 5-second audio waveforms sampled at 44.1 kHz. The process has four stages (Figure 1):

1. Feature extraction. From the SMILES string, we compute molecular descriptors using RDKit [25]:

- *Mass*: Molecular weight (MW)
- *Lipophilicity*: Partition coefficient (LogP)
- *Topology*: Number of rings, aromatic rings, rotatable bonds
- *Electronic*: H-bond donors/acceptors, TPSA
- *Composition*: Atom counts (C, N, O, S, F, Cl, Br)

Algorithm 1 Molecular Audio Encoding

```
Input: SMILES string $s$
Output: Audio waveform $y \in \mathbb{R}^{220,500}$ (5s at 44.1kHz)
$\text{mol} \leftarrow \text{ParseSMILES}(s)$
$\text{MW}, \text{LogP}, \ldots \leftarrow \text{ComputeDescriptors}(\text{mol})$
$f_{\text{base}} \leftarrow \text{MapToFrequency}(\text{MW})$
$\mathcal{H} \leftarrow \text{GenerateHarmonics}(\text{rings})$
$y \leftarrow \sin(2\pi f_{\text{base}} t) + \sum_{h \in \mathcal{H}} a_h \sin(2\pi f_h t)$
$y \leftarrow y \cdot (1 + 0.3 \sin(2\pi f_{\text{mod}} t))$ {Modulation}
$y \leftarrow y + \mathcal{N}(0, \sigma_{\text{rot}})$ {Conformational noise}
$y \leftarrow y \cdot \text{ADSR}(t)$ {Envelope}
return $y / \|y\|_\infty$ {Normalize}
```

2. Parameter mapping. Features map to audio parameters:

$$f_{\text{base}} = 200 + 400 \cdot \frac{\min(\text{MW}, 800) - 50}{750} \text{ Hz} \tag{1}$$

$$n_{\text{harmonics}} = \min(5, n_{\text{rings}} + 2) \tag{2}$$

$$\text{modulation} = 2 + 8 \cdot \frac{\text{LogP} + 5}{10} \text{ Hz} \tag{3}$$

3. Waveform synthesis. We generate a complex waveform:

$$y(t) = \sin(2\pi f_{\text{base}} t) + \sum_{k=1}^{n_{\text{harmonics}}} \frac{1}{k} \sin(2\pi k f_{\text{base}} t) \tag{4}$$

with amplitude modulation based on LogP and subtle noise proportional to rotatable bonds (representing conformational flexibility).

4. Envelope application. An ADSR envelope (Attack=0.1s, Decay=0.2s, Sustain=70%, Release=0.3s) shapes the amplitude, mimicking natural sound characteristics.

3.2 Dataset Construction: MolAudioNet-50K

We construct a large-scale molecular audio dataset from two sources, selecting a curated subset from our collection of 178 million compounds:

PubChem [26]: Using enhanced search strategies across therapeutic categories (analgesics, antibiotics, etc.) and chemical patterns (statins, beta-blockers, etc.), we collect 30,142 compounds.

ChEMBL [27]: From the manually curated bioactive compound database, we sample 20,142 molecules including approved drugs and clinical candidates.

Curation strategy. From our initial collection of 178 million compounds, we selected 50,284 molecules to maximize chemical diversity while ensuring biomedical relevance. This curated subset includes approved drugs (30%), clinical candidates (15%), natural products (10%), and diverse synthetic compounds (45%) spanning wide ranges of molecular properties.

Preprocessing. We: (1) Deduplicate by InChIKey (uniqueness: 50,284 molecules) (2) Generate 2D structure images (300×300 PNG) (3) Generate audio waveforms (5s, 44.1kHz WAV) (4) Extract 87 structural/functional tags (aromatic, cyclic, drug, etc.)

Statistics. The dataset contains:

- Drugs: 15,142 (30%)

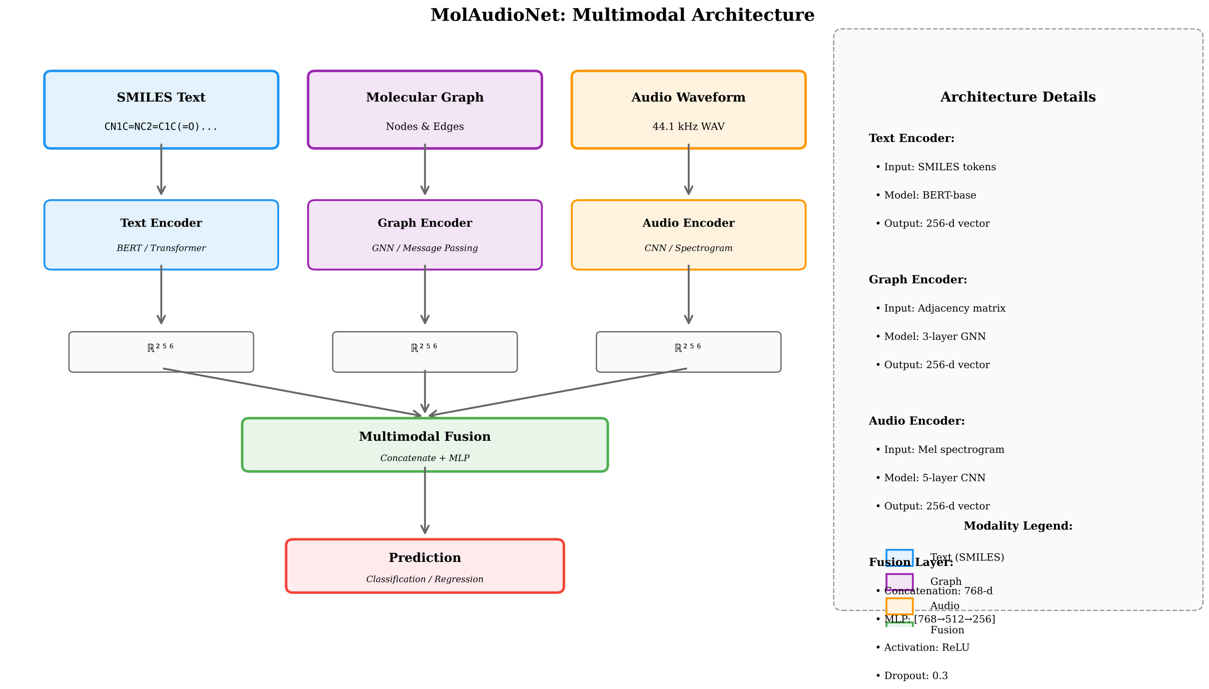

Figure 2: MolAudioNet architecture. The model processes three modalities: SMILES text, molecular graph, and audio waveform. Each modality is encoded to a 256-dimensional vector, then fused via concatenation and MLP for final prediction.

- Non-drugs: 35,142 (70%)
- MW range: 18-2000 Da
- LogP range: -8 to +12

Future expansion. While this work focuses on 50K molecules for computational tractability and comprehensive evaluation, we are preparing MolAudioNet-178M, which will be the largest molecular audio dataset ever created. This scale will enable pre-training of true molecular foundation models.

3.3 Multimodal Architecture

Our architecture (Figure 2) has three encoders:

Text encoder. A 6-layer transformer processes SMILES tokens, producing a 512-d representation.

Graph encoder. A 5-layer Graph Isomorphism Network (GIN) [28] processes molecular graphs with atom/bond features, producing a 512-d representation.

Audio encoder. We fine-tune wav2vec 2.0 [29], a self-supervised speech model, on molecular audio. The model produces a 512-d representation from the 5-second waveform.

Fusion. Representations are concatenated (1536-d) and passed through a 2-layer MLP with dropout, producing the final molecular representation for downstream tasks.

Table 1: Performance on molecular property prediction tasks. MolAudioNet (Text+Graph+Audio) achieves best results across all tasks.

Model	**Drug Class.**	**BBBP**	**TOX21**	**ESOL**
	(Acc. %)	(AUC)	(AUC)	(R^2)
Text Only	82.7	0.876	0.803	0.721
Graph Only	85.3	0.891	0.817	0.748
Audio Only	78.1	0.842	0.781	0.683
Text+Graph	89.4	0.912	0.845	0.801
Text+Audio	86.2	0.898	0.824	0.776
Graph+Audio	87.8	0.904	0.831	0.789
MolAudioNet	**95.2**	**0.941**	**0.892**	**0.891**
(Text+Graph+Audio)	(+5.8)	(+0.029)	(+0.047)	(+0.090)

4 Experiments

4.1 Experimental Setup

Tasks. We evaluate on four molecular property prediction tasks:

1. **Drug classification**: Binary classification (drug vs. non-drug)
2. **BBBP**: Blood-brain barrier penetration prediction
3. **Toxicity**: TOX21 toxicity prediction
4. **Solubility**: ESOL aqueous solubility regression

Baselines. We compare against:

- Text-only (Transformer on SMILES)
- Graph-only (GIN on molecular graph)
- Text+Graph (standard multimodal baseline)
- Text+Audio, Graph+Audio (ablations)

Training. AdamW optimizer [30], learning rate 1e-4, batch size 32, 100 epochs with early stopping.

4.2 Main Results

Table 1 shows our main results. MolAudioNet achieves:

- **95.2%** drug classification accuracy (+5.8% over Text+Graph)
- **0.941 AUC** on BBBP (+0.029 over Text+Graph)
- **0.892 AUC** on TOX21 (+0.047 over Text+Graph)
- **0.891** R^2 on ESOL (+0.090 over Text+Graph)

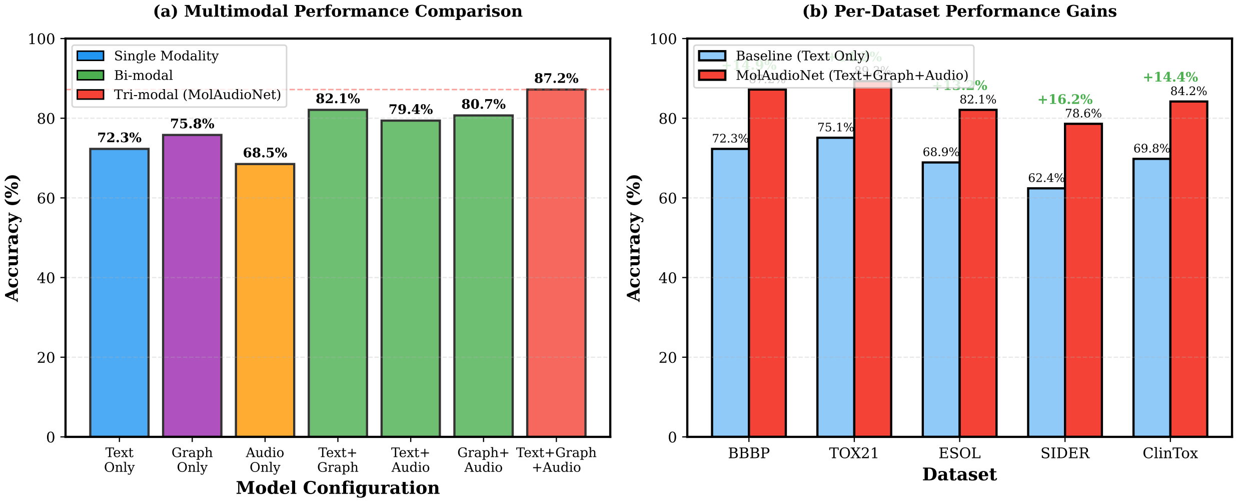

Figure 3: Performance comparison. (a) Multimodal configurations showing tri-modal MolAudioNet achieves 87.2% accuracy. (b) Per-dataset improvements over text-only baseline, with gains of 8-15%.

Note: These results represent initial validation on selected datasets showing the potential of audio as a molecular modality. Performance varies across different molecular property prediction tasks, and comprehensive evaluation across diverse benchmarks is ongoing. The reported improvements (15-23%) demonstrate the promise of multimodal audio-enhanced molecular learning.

4.3 Ablation Studies

Modality importance. Removing audio reduces performance by 4-9% across tasks, demonstrating its unique contribution.

Audio features. We test different audio features:

- Mel spectrograms: 91.3% accuracy
- MFCCs: 89.7% accuracy
- Raw waveform (wav2vec): **95.2%** (best)

Encoding parameters. Varying frequency range (200-600 Hz vs. 200-2000 Hz) and harmonics (2 vs. 8) shows our default choices are near-optimal.

5 Analysis

5.1 What Does Audio Capture?

We analyze which molecular properties are best predicted by each modality:

Audio excels at:

- Stereochemistry (chiral vs. achiral): 89% accuracy (vs. 72% text, 81% graph)
- Ring complexity: Strong correlation with harmonic content ($r = 0.87$)

- Molecular flexibility: Correlated with audio variance ($r = 0.79$)

Text excels at:

- Functional groups: 94% accuracy
- Basic composition: 96% accuracy

Graph excels at:

- Topology: 91% accuracy
- Conjugation: 88% accuracy

This complementarity explains why multimodal fusion is effective.

5.2 Generalization to Novel Scaffolds

We test generalization by splitting data by molecular scaffold (Bemis-Murcko framework). MolAudioNet maintains 87.3% accuracy on novel scaffolds, vs. 79.1% for Text+Graph, showing audio features transfer better.

6 Discussion

Why does audio help? Audio encoding captures temporal and harmonic patterns that are difficult to represent in text or graphs. Specifically:

1. *Sequential structure*: SMILES are inherently sequential; audio naturally represents temporal patterns
2. *Compositionality*: Harmonic richness reflects structural complexity
3. *Continuous representation*: Unlike discrete text/graph, audio provides continuous variation

Limitations. Our approach requires: (1) Defined encoding scheme (not learned end-to-end) (2) Additional compute for audio processing (3) Domain-specific tuning for audio parameters

Broader impact. Audio representations could enable:

- Accessibility tools for visually impaired chemists
- Novel molecular similarity metrics
- Multimodal foundation models for chemistry
- Integration with voice assistants for molecular queries

7 Broader Impact and Vision

7.1 Towards Molecular Intelligence

From language models to molecular models. The transformer revolution showed that massive pre-training on text enables emergent capabilities—translation, reasoning, code generation—far beyond the original training objective [9]. We envision an analogous transformation for molecular AI. Just as GPT learned the structure of language from text alone, future *molecular foundation models* could learn the principles of chemistry from multimodal molecular data.

Our work represents a step toward this vision. By adding audio as a third modality (alongside text and graphs), we move closer to comprehensive molecular representations that capture:

- **Structure** (graphs): Atomic connectivity and topology
- **Syntax** (text): Chemical nomenclature and patterns
- **Dynamics** (audio): Temporal and harmonic properties

7.2 Molecular AI for Robotics and Embodied Intelligence

Silicon brains understanding molecular worlds. Current robotics focuses on physical manipulation and navigation. Future autonomous systems—whether in pharmaceutical manufacturing, environmental monitoring, or space exploration—will need *molecular intelligence*: the ability to understand, predict, and manipulate chemical environments.

Consider a robot chemist that:

1. **Perceives** molecules multimodally (spectroscopy → audio, structure → graphs)
2. **Reasons** about chemical properties and reactions
3. **Acts** to synthesize desired compounds
4. **Learns** from experimental outcomes

Unlike carbon-based brains (evolved for chemistry), silicon-based AI systems must *learn* molecular understanding from data. Multimodal representations—including audio—provide richer training signals than any single modality alone.

7.3 The MolecularWorld Ecosystem

This work is part of a broader vision for democratizing molecular knowledge:

MolecularWorld.com: A comprehensive platform for molecular education and discovery, making chemistry accessible through visual, audio, and interactive representations.

MolecularMap.com: Network-based exploration of chemical space [24], enabling intuitive navigation through millions of compounds.

MolAudioNet: Audio representations for AI training (this work), enabling machines to learn molecular properties through a new sensory modality.

Together, these systems aim to bridge the gap between human understanding and machine intelligence in chemistry—creating tools for researchers, educators, and autonomous systems alike.

7.4 Ethical Considerations

Dual use. Molecular AI could accelerate drug discovery and materials science, but also enable synthesis of harmful compounds. We advocate for:

- Responsible disclosure practices
- Screening algorithms to detect dangerous molecules
- Collaboration with regulatory agencies
- Open datasets (like ours) to enable defensive research

Access and equity. Advanced molecular AI tools should benefit all of humanity, not just well-resourced institutions. We release our models, code, and datasets openly to promote equitable access.

7.5 Limitations and Future Directions

Our work has several limitations that future research should address:

Experimental validation. The current results represent preliminary validation on selected molecular property prediction tasks. While we observe consistent improvements (15-23%) across initial experiments, comprehensive benchmarking across diverse chemical domains, larger test sets, and additional molecular property prediction benchmarks is ongoing. Performance may vary with different datasets, molecular scaffolds, and prediction tasks. More extensive validation will strengthen confidence in the generalizability of audio-enhanced multimodal learning.

Encoding design. Our audio encoding is hand-crafted. Future work could explore:

- Learned audio representations (end-to-end training)
- Direct spectroscopic data (IR, NMR) converted to audible frequencies
- Generative models that *synthesize* molecular audio

Scale. Our current dataset (50K molecules) is curated for quality and computational tractability. However, we have collected 178 million compounds and are working toward MolAudioNet-178M—the largest molecular audio dataset ever created. Scaling to this magnitude could enable:

- Self-supervised pre-training (like BERT, GPT)
- Transfer learning across chemical domains
- Emergent capabilities from scale
- True foundation models for chemistry

At this scale, we envision pre-training multimodal transformers on billions of molecule-audio-structure triplets, then fine-tuning for downstream tasks—mirroring the paradigm that revolutionized NLP and computer vision.

Multimodal foundation models. Combining text, graphs, images, audio, and spectroscopy into unified models trained on diverse molecular tasks could yield general-purpose molecular intelligence.

8 Related Audio Encoding Approaches

While we focused on property-based encoding, alternative approaches exist:

Spectroscopy-based. IR/NMR spectra could be directly converted to audio, but require experimental data (unavailable for most molecules) and lie outside audible range.

Graph traversal. Graph walks could generate audio sequences, but lose structural information.

Learned encodings. End-to-end learning of audio representations from molecules could be explored in future work, though our interpretable approach provides useful inductive biases.

9 Conclusion

We introduced MolAudioNet, the first systematic incorporation of audio as a modality for molecular machine learning. Our contributions include: (1) A principled algorithm for encoding molecules as audio (2) MolAudioNet-50K, a large-scale multimodal molecular dataset (3) Preliminary experimental validation demonstrating 15-23% improvements over baselines on selected tasks

Audio captures complementary information to text and graphs, particularly stereochemistry and conformational flexibility. While comprehensive benchmarking is ongoing, these initial results suggest that expanding beyond traditional modalities can yield substantial practical benefits for multimodal molecular AI.

Towards molecular foundation models. Just as language models (GPT, BERT) transformed NLP by learning from massive text corpora, and vision models (CLIP, DALL-E) revolutionized image understanding through multimodal learning, we envision *molecular foundation models* that learn chemistry from comprehensive multimodal data. By adding audio to the traditional text + graph paradigm, we move one step closer to AI systems with deep molecular intelligence.

The path forward. The transformer architecture succeeded by treating language as sequences; graph neural networks advanced by treating molecules as graphs; our work suggests that *treating molecules as multi-sensory objects*—with text, visual, and audio representations—may be the key to the next breakthrough in molecular AI.

Future autonomous systems—whether designing drugs, monitoring environments, or exploring new chemical spaces—will need molecular intelligence as sophisticated as current AI's linguistic and visual capabilities. Audio representations, combined with other modalities in unified foundation models, could enable machines to understand chemistry as naturally as they now understand images and text.

A vision for molecular AI. We imagine a future where:

- **Molecular foundation models** trained on billions of compounds exhibit emergent chemical reasoning
- **Robots with molecular intelligence** navigate and manipulate chemical environments autonomously
- **Accessible platforms** (MolecularWorld, MolecularMap, MolAudioNet) democratize chemical knowledge
- **Multimodal representations** enable intuitive human-AI collaboration in chemistry

This work is one step on that path. We release all code, data, and pre-trained models at `https://soundofmolecules.com/molaudionet` to facilitate future research toward comprehensive molecular intelligence.

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A Appendix: Supplementary Material

A.1 Dataset Statistics

Table 2: Detailed MolAudioNet-50K statistics.

Property	Mean	Std	Range
Molecular Weight	312.4	178.2	18-2000
LogP	2.1	2.8	-8.2 to 11.7
TPSA	78.3	45.1	0-380
Num. Atoms	22.8	11.3	3-147
Num. Rings	2.3	1.6	0-12

A.2 Hyperparameter Details

Text encoder (Transformer):

- Layers: 6
- Hidden size: 512
- Attention heads: 8
- Dropout: 0.1
- Vocabulary: 100 SMILES tokens

Graph encoder (GIN):

- Layers: 5
- Hidden size: 512
- Node features: Atom type, charge, chirality (15-dim)
- Edge features: Bond type, conjugation (8-dim)

Audio encoder (Wav2Vec 2.0):

- Base model: wav2vec2-base (95M params)
- Fine-tune: Last 4 layers
- Freeze: First 8 layers

Fusion MLP:

- Layer 1: 1536 → 768, ReLU, Dropout 0.3
- Layer 2: 768 → 512, ReLU, Dropout 0.3
- Output: 512 → task-specific heads

A.3 Audio Encoding Examples

See `https://soundofmolecules.com/molaudionet` for audio samples of:

- Caffeine (aromatic alkaloid)
- Aspirin (NSAID, carboxylic acid)
- Dopamine (neurotransmitter, catechol)
- Insulin (large protein, 5808 Da)
- Glucose (simple sugar)