🎶 Molecule DJ

Turn molecules into music!
This project takes a chemical structure (in SMILES format) and creates a unique melody for it. Every molecule gets its own musical “fingerprint.”

What is this?

- Molecule DJ is a web app and AI model that transforms any molecule into a melody.
- You can enter a SMILES string (a text way of describing molecules), and the app will:
    - Analyze the molecule’s structure and properties,
    - Turn it into a sequence of musical notes,
    - Let you listen, download, and visualize the melody.

How does it work?

1. You give a molecule (as a SMILES string, like `cco` for ethanol).
2. The backend:
    - Calculates features from the molecule (like weight, atom count, etc.).
    - Picks a musical scale and key based on those features.
    - Maps the SMILES string and molecular fingerprint to a melody, ensuring each molecule sounds different.
    - Uses a trained AI model (LSTM) to generate a musical sequence.
3. You get:
    - A melody you can play in your browser,
    - A MIDI file you can download,
    - A visualization (“DJ beats”) of the tune.

What’s in each file?

File	**What it does**

`train_model.py`	Trains the AI model on molecules and saves it
`utils.py`	Functions for feature extraction and music mapping
`app.py`	The backend web server (Flask)
`index.html`	The main web page (frontend)
`main.js`	Handles user input, playback, and visualization
`style.css`	Makes it look cool
`molecules.csv`	The list of molecules (SMILES) for training
`molecule_dj_model_full.keras`	The trained AI model
`scaler_full.pkl`	Data scaler for features

How do I use it?

1. Install requirements (Python libraries: `rdkit`, `tensorflow`, `flask`, `flask_cors`, `midiutil`, `scikit-learn`, `numpy`, `pandas`).
2. Train the model:
3. `cmd`

```
python train_model.py
```

4. *(You can skip this if you have the model files.)*
5. Start the web app:
6. `Cmd- python app.py`
7. Open your browser:
   Go to http://localhost:5000
8. Enter or select a molecule, hit “Generate,” and enjoy your molecule’s music!

Why do some molecules sound similar?

- The app tries hard to make even similar molecules (like isomers) sound different, by using lots of features, fingerprint bits, and SMILES position.
- All melodies are kept in an audible, pleasant range (no super-low or super-high notes).

Who made this?

- Built with Python, RDKit, TensorFlow, Flask, and Tone.js.