PES Analysis Tool – Research Lab Edition-

Made by –

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A Professional Web Application for Rapid Potential Energy Surface Analysis

Overview & Purpose

The PES Analysis Tool is a modern, full-stack web application developed for computational chemists to instantly analyze relaxed dihedral scans (potential energy surfaces) without Excel, Origin, or one-off scripts. From a single Gaussian/ORCA output file (or manual data), users obtain in seconds:

- Interactive publication-quality plots
- Global/local minima & transition states
- Accurate rotational barriers (kJ/mol & kcal/mol)
- Full Boltzmann conformational populations at 298.15 K
- Fourier series parameters
- Annotated Matplotlib figures and comprehensive text reports

All with zero installation beyond standard Python packages.

Key Features

1. **Universal File Parsing**
   - Gaussian .log/.out (automatic detection of "Scan" summaries)
   - ORCA relaxed surface scan .out
   - CSV and space/tab-separated text files
2. **Interactive Web Interface**
   - Clean, responsive dark-blue design
   - Real-time Chart.js plot with cubic-spline smoothing
   - Live data table with point deletion
3. **One-Click Scientific Analysis**
   - Automatic detection of minima and transition states (SciPy argrelextrema)
   - Energy barriers relative to global minimum
   - Fourier series fitting ($V_0 + \Sigma V_n(1-\cos(n\theta))$) up to n=3
   - Precise Boltzmann distribution (298.15 K) with percentage populations
   - Conformational entropy contribution and number of significant conformers (>1%)
4. **Publication-Ready Output**
   - Annotated Matplotlib PNG (300 dpi) with labeled minima (▲), transition states (▼), global minimum (★)
   - Energy distribution histogram subplot
   - Downloadable CSV, PNG plot, and detailed text report (ready for Supporting Information)

How to Run (30 seconds)

Bash

```
pip install flask pandas numpy matplotlib scipy
python app.py
```

Open http://localhost:5000 → drag & drop your scan file → analyze instantly.

Technical Implementation

- Backend: Flask (Python 3)
- Data processing: pandas, NumPy, SciPy (CubicSpline, curve_fit, argrelextrema)
- Visualization: Chart.js (interactive) + Matplotlib (static annotated plots)
- Frontend: Pure HTML/CSS/JS (no React/Vue) → single index.html file
- Storage: In-memory + temporary uploads folder (no database required)

Ideal Applications

- Rotational barrier determination (amides, biphenyls, atropisomers)
- Conformational analysis of drug-like molecules
- Teaching computational chemistry laboratories
- Rapid validation of scan convergence and symmetry

Distribution & License

- Two files only: app.py + templates/index.html
- MIT License – freely modifiable and redistributable
- Fully offline, works on Windows/macOS/Linux

This tool has been used in real 2024–2025 research projects on atropisomeric catalysts, ferrocene derivatives, and pharmaceutically relevant scaffolds, routinely saving hours of manual data handling