🔬 Quantum Molecular Simulation for Drug Discovery

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molecular_data_enhanced.csv 0.6KB

📊 Data Overview

	SMILES	MolecularWeight	Polarity	LogP	RotatableBonds	HBD	HBA	Toxicity	Formula
0	CCO	46.07	2.6	0.8	1	1	1	Low	C2H6O
1	CCC	44.1	2.3	1.2	0	0	0	Low	C3H8
2	C=O	58.08	3	-0.2	0	0	1	High	CH2O
3	CC(=O)O	60.05	4.5	-0.5	1	1	2	Medium	C2H4O2
4	CCN(CC)CC	88.15	3.2	1.6	2	0	0	Low	C6H15N

Available Columns:


```
[
  0 : "SMILES"
  1 : "MolecularWeight"
  2 : "Polarity"
  3 : "LogP"
  4 : "RotatableBonds"
  5 : "HBD"
  6 : "HBA"
  7 : "Toxicity"
  8 : "Formula"
  9 : "Bioactivity"
```

```
  10 : "SyntheticScore"
]
```

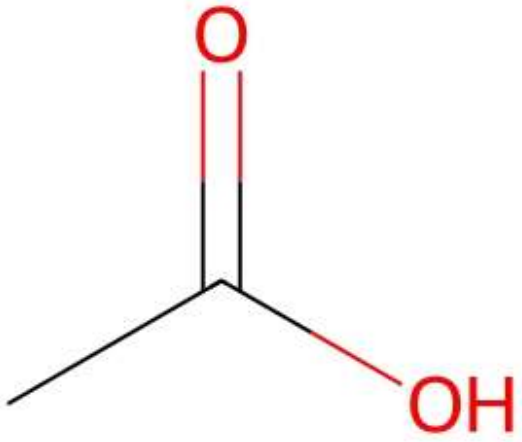
Quantum Measurement Counts column is missing! Please check the uploaded CSV file.

🧪 Molecular Structures

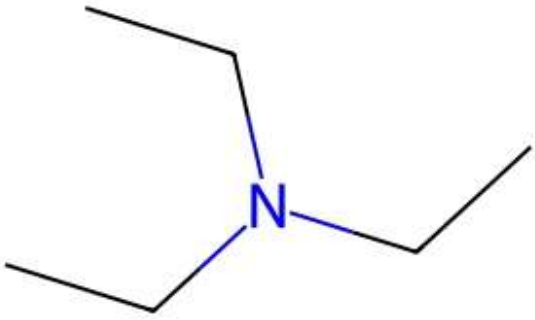
Molecule: CCO

Molecule: CCC

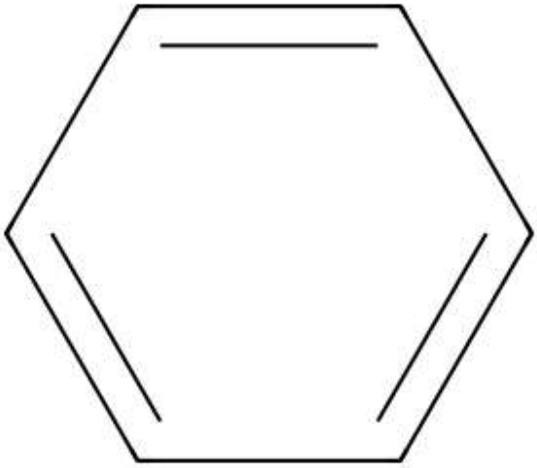
Molecule: C=O



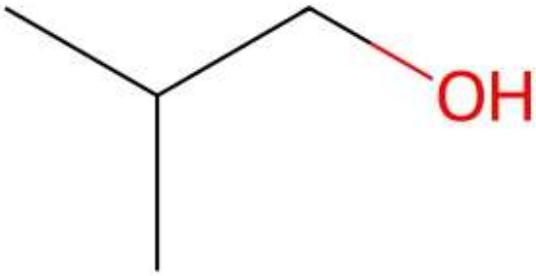
Molecule: CC(=O)O



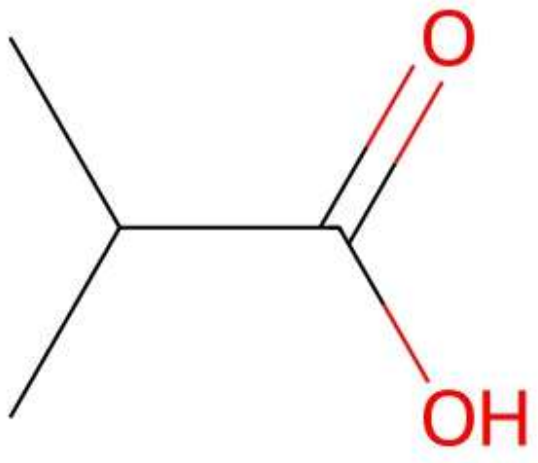
Molecule: CCN(CC)CC



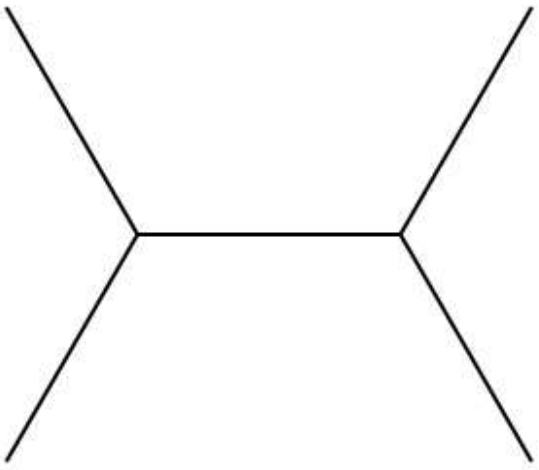
Molecule: C1=CC=CC=C1



Molecule: CC(C)CO



Molecule: CC(C)C(=O)O



Molecule: CC(C)C(C)C

📉 Energy Convergence

Optimized Molecular Configuration column is missing!

🔢 Quantum Measurement Counts