


API Keys

OpenAI API Key

..... 

SerpAPI Key (for patent search) 





Office helper



I need TPSA of aspirin

TPSA accurate



The Topological Polar Surface Area (TPSA) of aspirin is 63.6 Å². TPSA is a property that can provide insights into the drug's ability to permeate cell membranes, which is important in drug design and pharmacokinetics.



Now I need similar molecules and similarity scores

Small World API working well



Here are some molecules similar to aspirin, along with their SMILES representations and similarity scores:

1. **Molecule:** CCOC1=CC=CC=C1C(=O)O

- **Similarity Score:** 0.87
- **Additional Info:** This molecule is an ester similar to aspirin, showing a high degree of structural similarity.

2. **Molecule:** CC(=O)OC1=C(C=CC=C1C(=O)N)C

- **Similarity Score:** 0.72
- **Additional Info:** This compound is an amide derivative, indicating a slight modification in the functional groups compared to aspirin.

3. **Molecule:** COC(=O)OC1=CC=CC=C1C(=O)O

- **Similarity Score:** 0.70
- **Additional Info:** This molecule is another ester variant, with a methoxy group, which slightly alters its chemical properties.

4. **Molecule:** CC(=O)OC1=CC(=CC=C1C(=O)N)C

- **Similarity Score:** 0.68
- **Additional Info:** Similar to the second molecule, this is another amide derivative, reflecting the versatility of aspirin's core structure in forming different derivatives.

5. **Molecule:** CNC(=O)C1=CC=CC=C1OC(=O)C

- **Similarity Score:** 0.67
- **Additional Info:** This compound includes a methylamine group, which introduces basicity into the molecule, differing from the acidic nature of aspirin.

These molecules are structurally similar to aspirin and share some chemical properties, making them interesting for further research in medicinal chemistry.

More details of tool chain planning is shown below.

g about a molecule...



Sample Agent Thinking Process

```
[{'role': 'user', 'content': 'I need TPSA of aspirin'}]
```

user:I need TPSA of aspirin

-----Chat History-----

```
{'chemical': ['aspirin'], 'chemical_identifier_type': ['chemical_name'], 'properties': ['TPSA'],  
'needs_web_search': False, 'needs_patent': False}
```

-----Keyword Selection-----

```
{}
```

-----Raw OpenAI Output-----

```
{}
```

-----Raw OpenAI Output-----

```
{'aspirin': {'chemical_name': 'aspirin'}}
```

-----Recalled Knowledge-----

All know information is extracted to for the tool chain planner to obtain the shortest path.

TPSA ['chemical_name']

-----Initial and Target-----

```
[{'use': 'query_pubchem'}, {'use': 'compute_properties'}]
```

-----Planning...-----

Well designed tool chain path to obtain TPSA from chemical name.

```
[{'aspirin': {'chemical_name': 'aspirin', 'smiles': 'CC(=O)OC1=CC=CC=C1C(=O)O', 'molecular  
formula': 'C9H8O4', '2d structure': {'image':
```

```
'https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/aspirin/record/PNG?image_size=large'  
}}, {'MW': 180.16, 'TPSA': 63.6, 'logP': 1.31, 'logS': 0.41}}]
```

-----API Results-----

```
[{'role': 'user', 'content': 'I need TPSA of aspirin'}, {'role': 'assistant', 'content': [{'aspirin':
```

```
{'chemical_name': 'aspirin', 'smiles': 'CC(=O)OC1=CC=CC=C1C(=O)O', 'molecular formula':  
'C9H8O4', '2d structure': {'image':
```

```
'https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/aspirin/record/PNG?image_size=large'  
}}, {'MW': 180.16, 'TPSA': 63.6, 'logP': 1.31, 'logS': 0.41}}]], {'role': 'assistant', 'content': "The
```

Topological Polar Surface Area (TPSA) of aspirin is 63.6 Å². TPSA is a property that can provide insights into the drug's ability to permeate cell membranes, which is important in drug design and pharmacokinetics."}, {'role': 'user', 'content': 'Now I need similar molecules and similarity scores'}]

user:Now I need similar molecules and similarity scores

-----Chat History-----

```
{'chemical': ['aspirin'], 'chemical_identifier_type': ['chemical_name'], 'properties':  
['similar_molecules'], 'needs_web_search': False, 'needs_patent': False}
```

-----Keyword Selection-----

```
{
```

```
  "chemical_name": "aspirin",
```

```
  "smiles": "CC(=O)OC1=CC=CC=C1C(=O)O",
```

```
  "MW": 180.16,
```

```
  "TPSA": 63.6,
```

```
  "logP": 1.31,
```

```
  "logS": 0.41,
```

```
"2d_structure":  
"https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/aspirin/record/PNG?image_size=large"  
}
```

Raw output can include hallucination, it is processed with proper python functions to identify invalid values and AI checker to remove fabricated information.

size=large

-----Raw OpenAI Output-----

```
{'chemical_name': 'aspirin', 'smiles': 'CC(=O)OC1=CC=CC=C1C(=O)O', 'MW': 180.16, 'TPSA': 63.6, 'logP': 1.31, 'logS': 0.41, '2d_structure':
```

```
'https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/aspirin/record/PNG?image_size=large'  
}
```

-----Raw OpenAI Output-----

```
{'aspirin': {'chemical_name': 'aspirin', 'smiles': 'CC(=O)OC1=CC=CC=C1C(=O)O', 'MW': 180.16, 'TPSA': 63.6, 'logP': 1.31, 'logS': 0.41, '2d_structure':
```

```
'https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/aspirin/record/PNG?image_size=large'  
}}
```

-----Recalled Knowledge-----

All past knowledge extracted to get the shortest path.

```
similar_molecules [{'chemical_name': 'aspirin', 'smiles': 'CC(=O)OC1=CC=CC=C1C(=O)O', 'MW': 180.16, 'TPSA': 63.6, 'logP': 1.31, 'logS': 0.41, '2d_structure':
```

-----Initial and Target-----

```
[{'use': 'query_smallworld'}]
```

Fully used past knowledge and one step API call!

-----Planning...-----

```
{'CCOC1=CC=CC=C1C(=O)O PV-007122236650': 0.8666666666666667,  
'CC(=O)OC1=C(C=CC=C1C(=O)N)C Z3219846910': 0.7162162162162162,  
'COC(=O)OC1=CC=CC=C1C(=O)O Z192948624': 0.6973684210526315,  
'CC(=O)OC1=CC(=CC=C1C(=O)N)C Z638457360': 0.6794871794871795,  
'CNC(=O)C1=CC=CC=C1OC(=O)C Z111504902': 0.6708860759493671} swdict  
[{'aspirin': {'chemical_name': 'aspirin', 'smiles': 'CC(=O)OC1=CC=CC=C1C(=O)O', 'MW': 180.16, 'TPSA': 63.6, 'logP': 1.31, 'logS': 0.41, '2d_structure':  
'https://pubchem.ncbi.nlm.nih.gov/rest/pug/compound/name/aspirin/record/PNG?image_size=large',  
'CCOC1=CC=CC=C1C(=O)O PV-007122236650': 0.8666666666666667,  
'CC(=O)OC1=C(C=CC=C1C(=O)N)C Z3219846910': 0.7162162162162162,  
'COC(=O)OC1=CC=CC=C1C(=O)O Z192948624': 0.6973684210526315,  
'CC(=O)OC1=CC(=CC=C1C(=O)N)C Z638457360': 0.6794871794871795,  
'CNC(=O)C1=CC=CC=C1OC(=O)C Z111504902': 0.6708860759493671}}]
```

-----API Results-----