API Keys

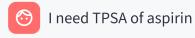
OpenAl API Key

SerpAPI Key (for patent search)

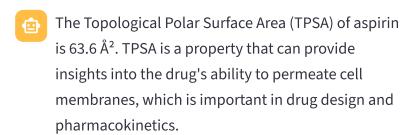
②



Office helper



TPSA accurate





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
 - o 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 gaboutamolecule... below.



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----
                                            All know information is
{}
                                             extracted to for the
----Raw OpenAI Output-----
                                            tool chain planner to
                                            obtain the shortest
----Raw OpenAI Output-----
                                            path.
{'aspirin': {'chemical name': 'aspirin'}}
 ----Recalled Knowledge-----
TPSA ['chemical name']
                                                             Well designed tool chain
----Initial and Target----
                                                             path to obtain TPSA from
                                                             chemical name.
[{'use': 'query_pubchem'}, {'use': 'compute_properties'}]
-----Planning...----
[{'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 Å<sup>2</sup>. 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,
```

```
Raw outputcan include hallucination,
  "2d structure":
                                      it is processed with proper python
"https://pubchem.ncbi.nlm.nih.gov/rest/putfunctions to identify invalid values
                                                                                size=large
                                      and AI checker to remove fabricated
                                      information.
----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'
                                                                All past knowledge
----Recalled Knowledge-----
                                                                extracted to get the
                                                                shortest path.
similar_molecules ['chemical_name', 'smiles', 'MW', 'TPSA', 'logP', 'logS', '2d_structure']
----Initial and Target----
                             Fully used past knowledge
[{'use': 'query_smallworld'}]
                             and one step API call!
----Planning...----
{'CCOC1=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': 0.86666666666666667,
'CC(=O)OC1=C(C=CC=C1C(=O)N)C Z3219846910': 0.7162162162162162,
'COC(=O)OC1=CC=CCCC1C(=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-----
```