

**Task:** Identify optimal rod-shaped ligand for binding pocket.

**Objective:** Minimize score  $S = (\text{Asphericity} \times 100) + (\text{Eccentricity} \times 10)$ .

**Candidates:** Anthracene, Phenanthrene, Acenaphthylene, Fluorene.

**Action(Tool):**

chemical\_name\_to\_molecular  
parameters: ['Anthracene']



**Environment Feedback:** ✓

**Action(Tool):**

get\_3d\_properties  
parameters:  
{ 'smiles': 'C1=CC=C2C=..' }



**Environment Feedback:** ⚠

**Action(Tool):**

get\_3d\_properties  
parameters:  
{ 'smiles': 'C1=CC=C2C=C3C...',  
'method': 'ETKDGv3' }



**Environment Feedback:** ✓

**Action(Tool):**

geometry\_optimization  
parameters: { 'smiles': ..., 'Energy': }



**Environment Feedback:** ✓

**Environment**



**Setup**



DataBase



Files



Toolkit



Code

**Execution log**

Task	value
Number of Available Tools	53
Actual Tool Utilization	4
Total Steps	6
Total Tool Calls	20
Final Answer	34.9
Expected Answer	34.57
Error	0.95%

Agent

runtime

**OUTPUT :** Optimal Ligand is Acenaphthylene (S=34.9). Molecular structure shown as below:

Molecule	Asphericity×100	Eccentricity×10	S
Acenaphthylene	25.94	8.96	34.9

