

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 .



Agent

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:

runtime

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%

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

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

