1. Protein Analysis Examples

Example 1:

- PDB ID: 1AZ5
- Target Description: Beta-secretase 1 (BACE1) is a key enzyme in Alzheimer's disease pathology. Looking for potential binding sites for inhibitor development, particularly focusing on regions that could accommodate small molecules capable of crossing the blood-brain barrier.

Example 2:

- PDB ID: 5KIR
- Target Description: Cyclooxygenase-2 (COX-2) is a key enzyme in inflammation and pain pathways. Interested in identifying selective binding regions distinct from COX-1 to reduce gastrointestinal side effects common in current NSAIDs.

Example 3:

- PDB ID: 6LU7
- Target Description: SARS-CoV-2 main protease (Mpro) which is essential for viral replication. Seeking to identify binding sites for potential antiviral compounds that could inhibit viral processing of polyproteins.

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2. Compound Design & Analysis Examples

Example 1:

- SMILES: `CC(=O)OC1=CC=CC=C1C(=O)O` (Aspirin)
- Optimization Goals: Increase blood-brain barrier penetration, reduce GI toxicity

Example 2:

- SMILES: `CN1C=NC2=C1C(=O)N(C(=O)N2C)C` (Caffeine)
- Optimization Goals: Extend half-life, maintain CNS activity

Example 3:

- SMILES: `COC1=C(C=C(C=C1)OC)CCN(C)CC2=C3C=CC(=O)CC3=CC=C2` (Donepezil - Alzheimer's drug)
- Optimization Goals: Improve BBB penetration, reduce muscarinic side effects

Example 4:

- SMILES: `CC(C)CC1=CC=C(C=C1)C(C)C(=O)O` (Ibuprofen)
- Optimization Goals: Increase COX-2 selectivity, maintain potency

3. Compound Screening Examples

Example 1: General Drug-Like Properties Screening

```
{
   "MW": {"max": 500},
   "LogP": {"min": -0.4, "max": 5.6},
   "TPSA": {"max": 140}
}
```

Compounds (compounds_general.txt):

```
CC(=O)OC1=CC=CC=C1C(=O)O
CN1C=NC2=C1C(=O)N(C(=O)N2C)C
CC(C)CC1=CC=C(C=C1)C(C)C(=O)O
CC(=O)NC1=CC=C(O)C=C1
COC1=C(C=C(C=C1)OC)CCN(C)CC2=C3C=CC(=O)CC3=CC=C2
```

Expected Results: All compounds should pass these general criteria, demonstrating that the platform can handle multiple compounds and basic filtering.

Example 2: CNS Drug Screening

```
{
   "MW": {"max": 400},
   "LogP": {"min": 0, "max": 5},
   "TPSA": {"max": 90},
   "HBD": {"max": 3}
}
```

Compounds (compounds_cns.txt):

```
CN1C=NC2=C1C(=O)N(C(=O)N2C)C
CC(=O)NC1=CC=C(O)C=C1
COC1=C(C=C(C=C1)OC)CCN(C)CC2=C3C=CC(=O)CC3=CC=C2
C1CN(CCC1N2C=NC3=C2NC=N3)C4=CC=C(C=C4)C(F)(F)F
CC(C)CC1=CC=C(C=C1)C(C)C(=O)O
```

Expected Results: This should filter out compounds like donepezil (the long SMILES on line 3) which exceeds 400 MW, and possibly ibuprofen (last compound) based on its properties. Caffeine and paracetamol (first two) should pass, demonstrating selective filtering.

Example 3: Anti-inflammatory Optimization

```
{
   "MW": {"max": 450},
   "LogP": {"max": 4.5},
   "TPSA": {"min": 40, "max": 120},
   "RotBonds": {"max": 8}
}
```

Compounds (compounds_antiinflam.txt):
CC(=O)OC1=CC=CC=C1C(=O)O
CC(C)CC1=CC=C(C=C1)C(C)C(=O)O
CC1=CC=C(C=C1)C(=O)C2=C(C=CC=C2O)O
COC(=O)C1=CC=CC=C1C(=O)OC2=CC=CC=C2C(=O)O
CC(C)C1=CC=CC=C1NC(=O)C(C)OC(=O)C2=CC=CC=C2C(=O)O

Expected Results: This should filter out the last compound (etodolac derivative) for being too large/complex, while allowing aspirin, ibuprofen, and some other anti-inflammatory compounds to pass, demonstrating more complex property filtering.