Low-Level Flow:

1. **User Query:** (Same as before) "Design novel molecules that bind to the main protease of SARS-CoV-2 and inhibit its activity."
2. **Target Identification Agent:**
    - **First:** Parses the user query to identify the target: "main protease of SARS-CoV-2".
    - **Next:** Queries UniProt to retrieve the protein sequence and any available structural information (PDB ID).
3. **Information Enrichment Agent:**
    - **Next:** Using the target name or UniProt ID, this agent queries:
        - **PubChem:** To find any existing small molecules known to interact with or target the main protease (this could include known inhibitors or ligands). This helps in understanding the chemical space and potential starting points.
        - **ChEMBL:** To retrieve bioactivity data, including known inhibitors, their potency (e.g., IC50, Ki), and any associated structural information. This provides valuable context for designing new molecules.
    - **Next:** If a PDB ID was found in Step 2, the agent retrieves the 3D structure of the target protein.
4. **Property Prioritization Agent:**
    - **Next:** Based on the target, the desired outcome (inhibition), and potentially the properties of known inhibitors retrieved from PubChem/ChEMBL, this agent prioritizes key molecular properties (e.g., binding affinity, drug-likeness, specific interactions with the active site).
5. **Molecule Generation/Retrieval Agent:**
    - **Next (Decision Point):**
        - **Option A (De Novo Design):** If the goal is to design entirely new molecules or if existing ligands are not suitable, this agent (incorporating Scaffold Generation and Ligand Design as described before, using RDKit) will generate a library of potential molecules.
        - **Option B (Ligand-Based Design/Optimization):** If known ligands were found in PubChem/ChEMBL, this agent might use these as starting points and employ RDKit for lead optimization (e.g., generating analogs with modified substituents).
6. **3D Structure Generation Agent:**
    - **Next:** For all generated or retrieved 2D molecular structures, this agent uses RDKit or a dedicated tool to generate 3D conformations.

7. **Molecular Docking Agent:**
    - **Next:** This agent uses a docking program to predict the binding affinity of the 3D molecules to the target protein's active site (obtained from the PDB structure).
8. **Property Prediction Agent:**
    - **Next:** This agent uses RDKit and potentially other models to predict relevant molecular properties (e.g., LogP, MW, HBD/HBA, predicted ADMET properties).
9. **Filtering and Ranking Agent:**
    - **Next:** This agent filters the molecules based on the prioritized properties and docking scores, then ranks them according to a defined scoring function.
10. **Result Presentation Agent:**
    - **Finally:** Presents the top-ranked molecules with their structures, predicted binding affinities, properties, and links back to PubChem/ChEMBL if they were derived from existing compounds.
11. **Feedback Loop Agent:** (As before) Allows user feedback for refinement.

Sequence Summary:

1. **User Query**
2. **Target Identification (UniProt)**
3. **Information Enrichment (PubChem, ChEMBL, PDB)**
4. **Property Prioritization**
5. **Molecule Generation/Retrieval (RDKit or database search)**
6. **3D Structure Generation (RDKit or dedicated tool)**
7. **Molecular Docking**
8. **Property Prediction (RDKit and other models)**
9. **Filtering and Ranking**
10. **Result Presentation**
11. **Feedback Loop**