Fukui function calculation of arachidonic acid in complex with cyclooxygenase 2 (COX2) enzyme using GUIDE

1. Start **YASARA** and click on the **File** button on the YASARA window taskbar. Load the PDB structure (PDB ID: **1DCX**) from the Protein Data Bank (https://www.rcsb.org/) by navigating to **File > Load > PDB file from local PDB**.
2. Click the **GUIDE** menu on the YASARA window taskbar and select the **QM calculation** option.
3. In the QM calculation window, enter the working directory information and select **ORCA** as the calculation method. Click **OK** to proceed.
4. Another window will appear for selecting the **Type of QM calculation**. Select **Fukui function** and click **OK**.
5. Select the functional and basis set information by choosing **PBE** and **DEF2-SVP** from the functional and basis set lists. Click **OK** to confirm the selection.
6. A message will appear on the YASARA screen prompting you to select your molecule. From the YASARA object list, select the arachidonic acid (ACD) molecule and click the Continue button. This will initiate the Fukui function calculation, and the results will be stored in the working directory in the **fukuifunction_results.txt** file. After the calculation, a YASARA .yob file will be generated, which can be loaded IN YASARA to visualize the results. The calculated arachidonic acid results are provided in the **sample_analysis_protocols** GitHub folder under the name **ACD.yob**.