

## 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.yob** file) 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**.