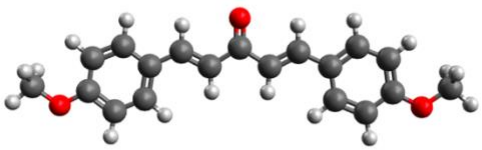
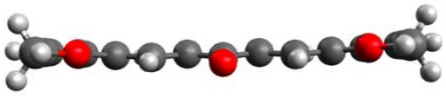
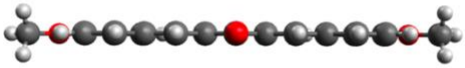
Supplementary Data

- 3D View from the model molecules' equilibrium geometries: optimized at the CAM-B3LYP/6-311++(2d,p) level of theory using Gaussian.

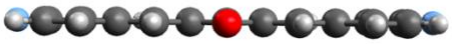


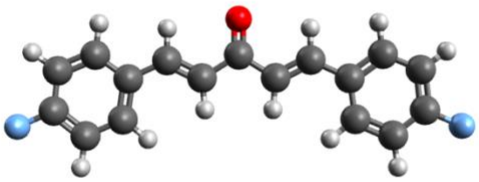
Molecule: 4-DMDBA





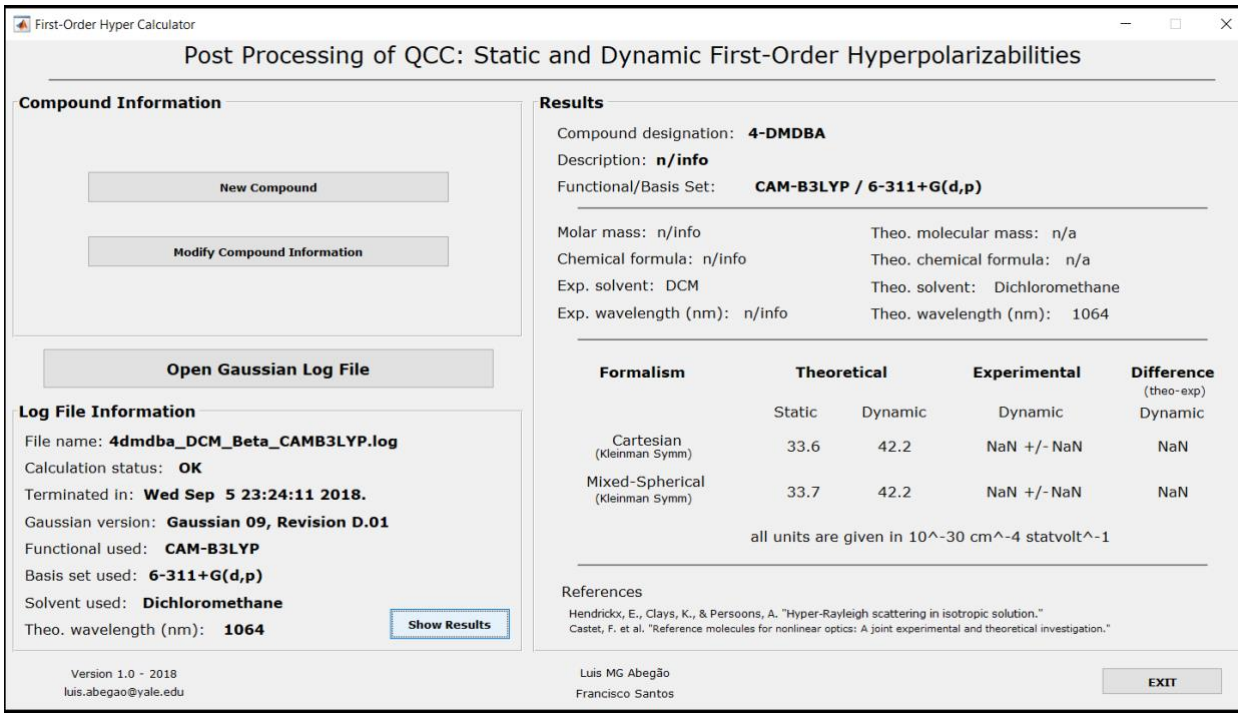
Molecule: 2-DMDBA



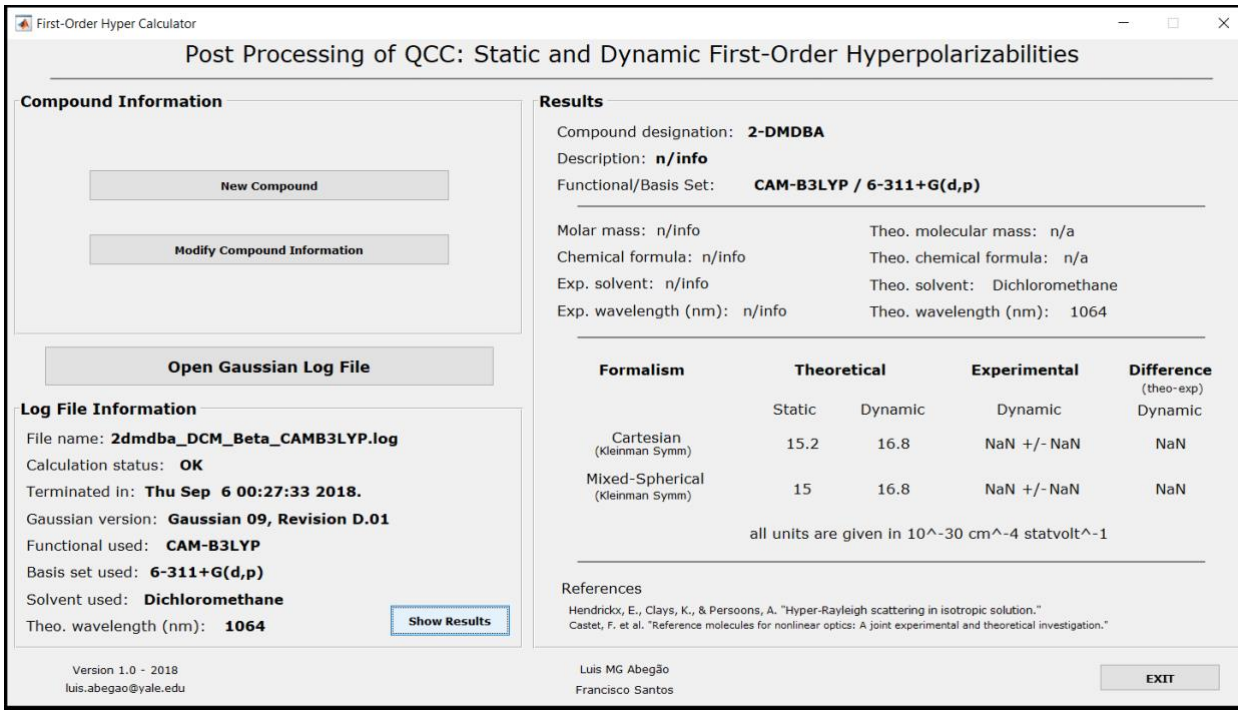


Molecule: 4-DFDBA

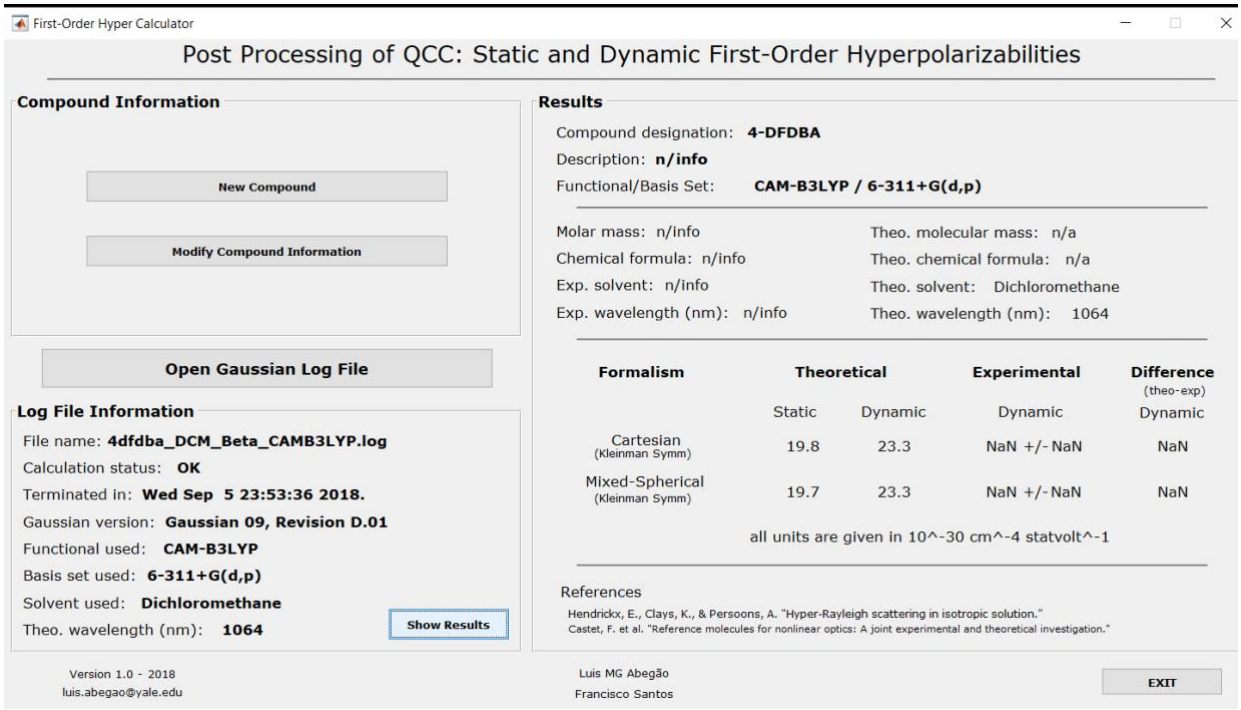
- Print screen from the post-processing software that is used to calculate the first molecular hyperpolarizability, after the geometry optimization process.



Molecule: 4-DMDBA



Molecule: 2-DMDBA



Molecule: 4-DFDBA