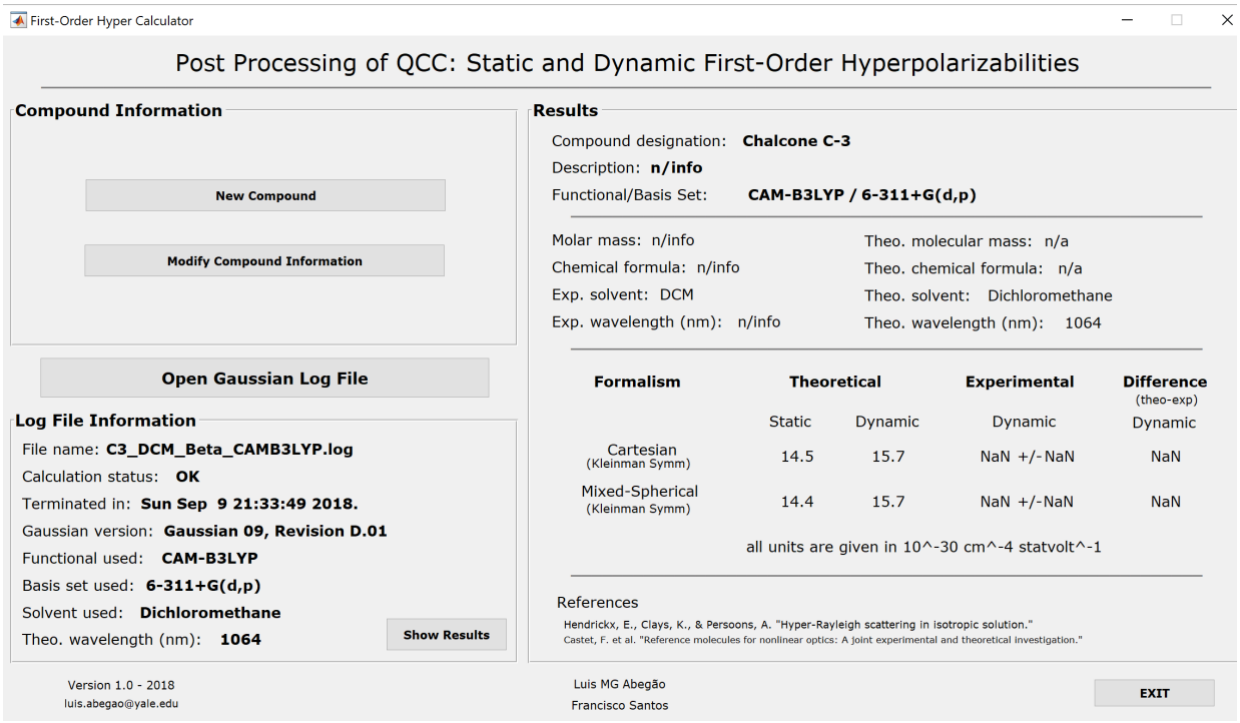
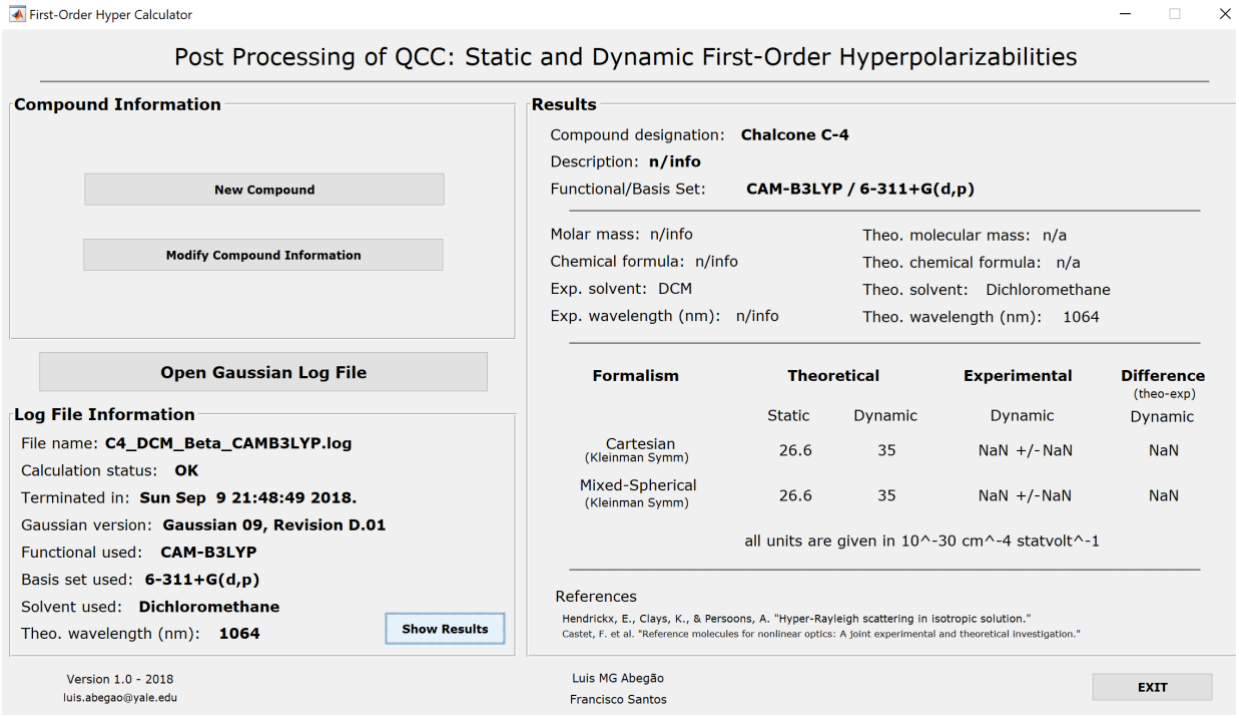
Supplementary Data

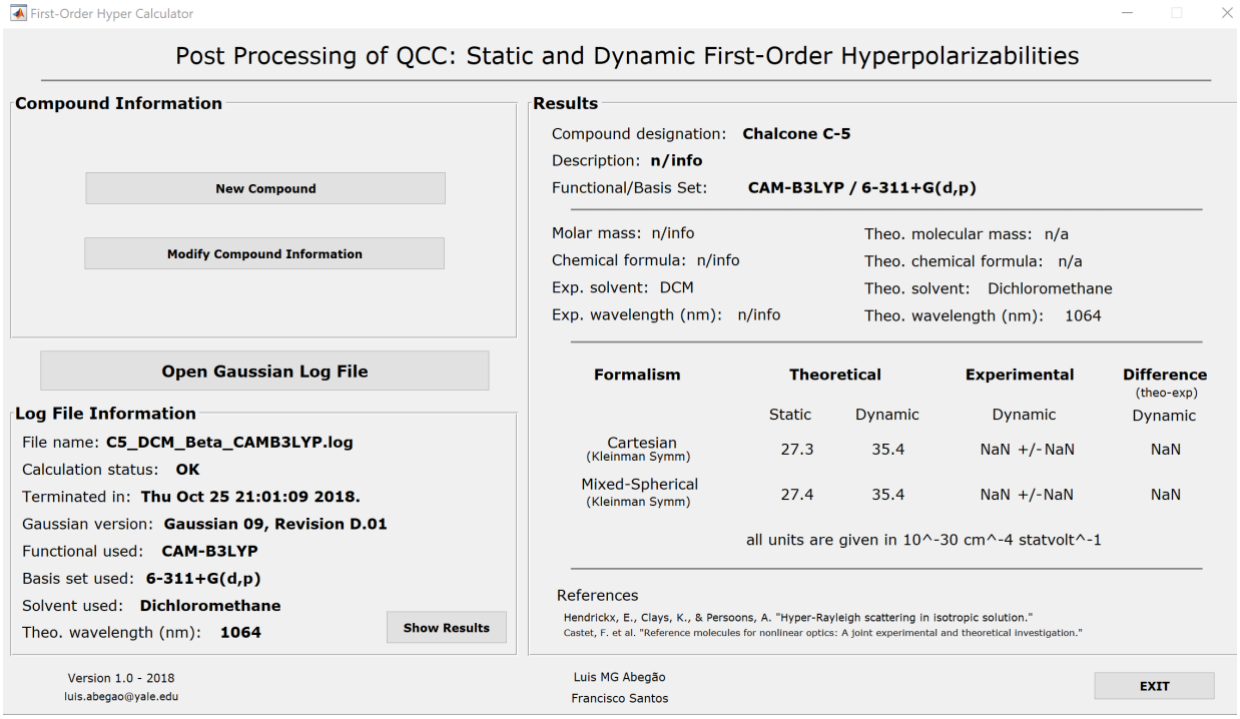
- Print screen from the post-processing software that is used to calculate the first molecular hyperpolarizability, after the geometry optimization process.



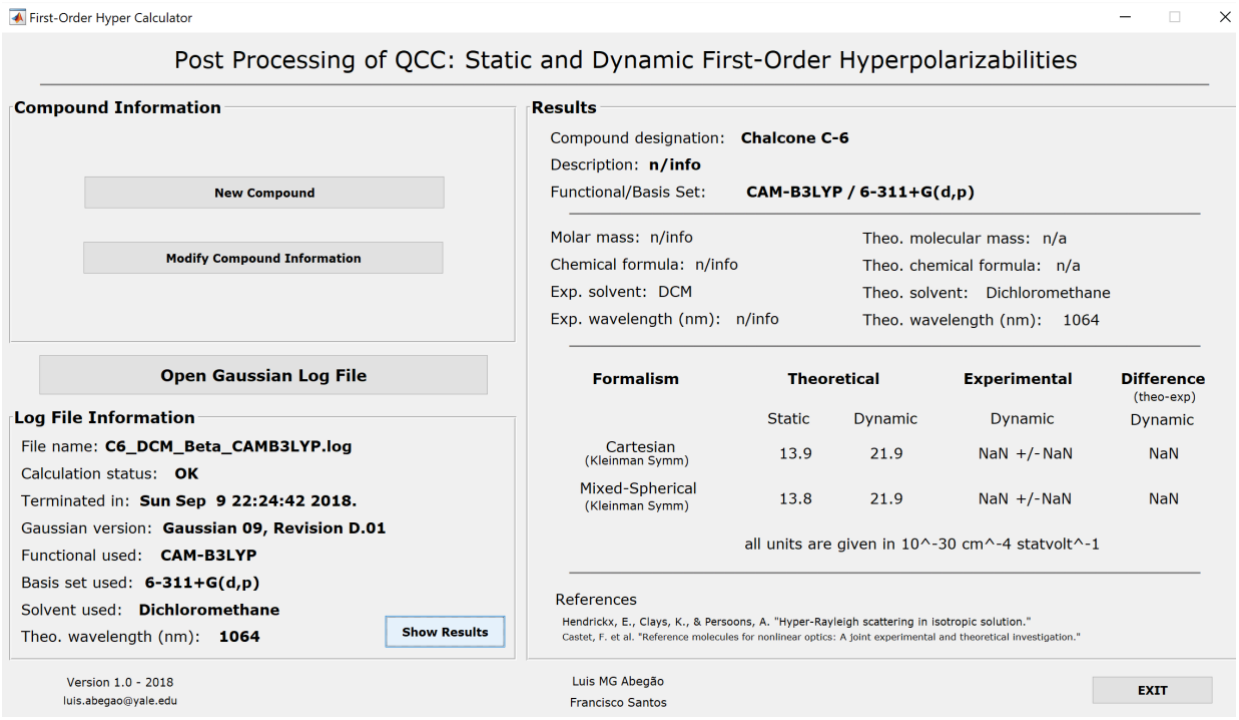
Molecule: C-3



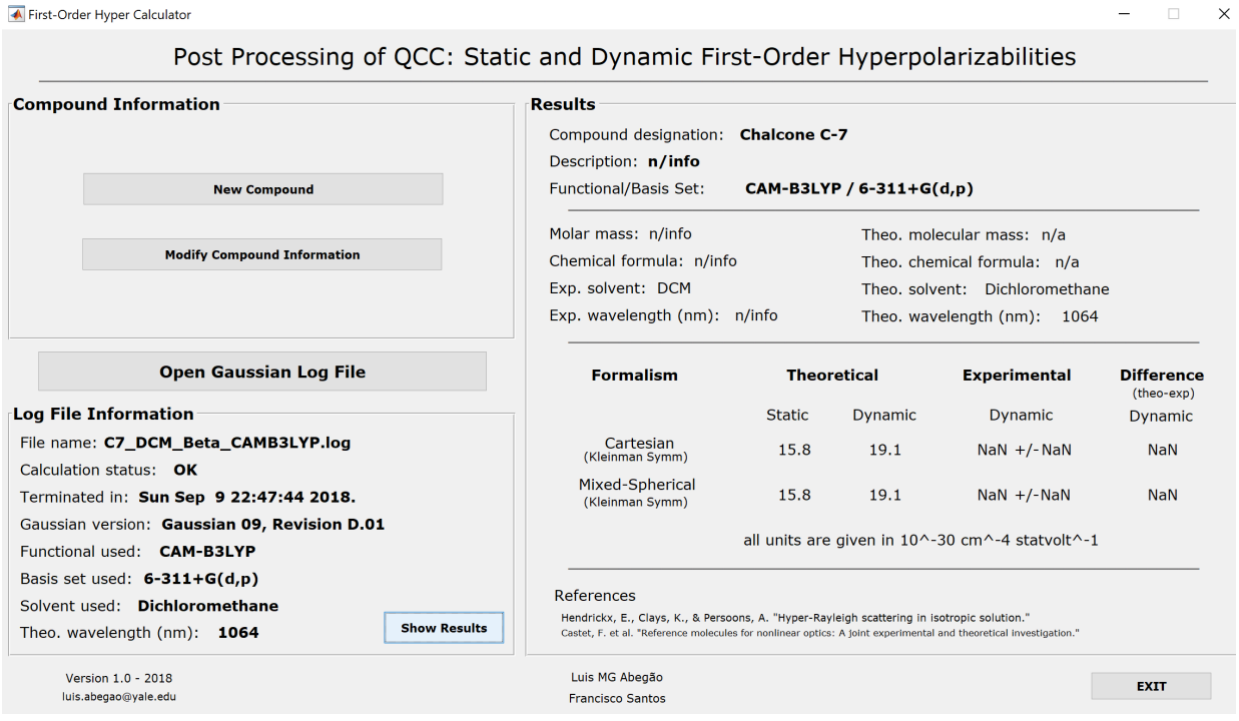
Molecule: C-4



Molecule: C-5



Molecule: C-6



Molecule: C-7