# HARLEM

# (HAmiltonians for Response properties of LargE Molecules)

HARLEM is a multipurpose interactive Molecular Modeling package. It is designed to combine modern electronic structure, statistical mechanics and Machine Learning techniques controlled by a graphical interface to provide an effective theoretical tool to study complex properties and function of macromolecular systems such as biocatalysis, long-rang electron transfer, ion membrane permeation, ligand binding and protein-protein interactions.

HARLEM provides an interface to popular molecular modeling packages such as GAUSSIAN and AMBER, GROMACS, HARLEM is an open developing platform. HARLEM is currently being developed and maintained by Igor Kurnikov (http://harlemprog.org) and members of Maria Kurnikova’s lab at Carnegie Mellon University (http://crete.chem.cmu.edu).

