Abstract Submitted for the MAR15 Meeting of The American Physical Society

Easy GROMACS: A Graphical User Interface for GROMACS Molecular Dynamics Simulation Package AYTEN DIZKIRICI, MUSTAFA TEKPINAR, Yuzuncu Yil University — GROMACS is a widely used molecular dynamics simulation package. Since it is a command driven program, it is difficult to use this program for molecular biologists, biochemists, new graduate students and undergraduate researchers who are interested in molecular dynamics simulations. To alleviate the problem for those researchers, we wrote a graphical user interface that simplifies protein preparation for a classical molecular dynamics simulation. Our program can work with various GROMACS versions and it can perform essential analyses of GROMACS trajectories as well as protein preparation. We named our open source program '*Easy GROMACS*'. *Easy GROMACS* can give researchers more time for scientific research instead of dealing with technical intricacies.

> Mustafa Tekpinar Yuzuncu Yil University

Date submitted: 14 Nov 2014

Electronic form version 1.4