





Project Acronym: MuG

Project title: Multi-Scale Complex Genomics (MuG)

Call: H2020-EINFRA-2015-1

Topic: EINFRA-9-2015 **Project Number**: 676556

Project Coordinator: Institute for Research in Biomedicine (IRB Barcelona)

Project start date: 1/11/2015

Duration: 36 months

Milestone 29: ABC data entered into the MuG 3D/4D databases

Lead beneficiary: The University of Nottingham (UNOT)

Dissemination level: PUBLIC

Due date: 01/12/2016

Actual submission date: 16/11/2016



Microsecond-scale MD simulations were performed on a set of B-DNA oligomers, whose sequence was specifically designed in order to encompass all of the possible tetranucleotide sequences.

MD simulations were performed in explicit water and physiological salt concentration, using state-of-the-art force fields (parmBSC1) and protocols.

This large set of MD data has been processed and uploaded to the MuG section of the BIGNASim repository, and is available through the MuG VRE:

(http://www.multiscalegenomics.eu/MuGVRE/modules/BigNASimMuG/).