





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 analysed and DNA sequence-dependent flexibility data obtained

**Lead beneficiary**: The University of Nottingham (UNOT)

**Dissemination level: PUBLIC** 

Due date: 01/04/2017

Actual submission date: 31/03/2016



The large set of MD simulation data described in MS29, which represents the most complete available source of information on the sequence-dependent behaviour of B-DNA in solution, has been analysed in terms of DNA flexibility.

This analysis has furthered our understanding of the complex dependence of DNA structure and flexibility on its sequence: the results have been made available in the MuG section of the <a href="BIGNASim">BIGNASim</a> repository as well as in the MuG Interactive <a href="Flexibility Browser">Flexibility Browser</a>, both of which are available through the MuG VRE.

This new data, obtained from simulation using the latest and most refined force field for DNA simulations (parmBSC1), complement the information produced in MS22, providing a significant improvement in accuracy.