



## Memorandum of Understanding

between



## CHAIN and WeNMR

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### 1. Background:

#### WeNMR

The WeNMR project, a FP7 European Commission e-Infrastructure project (contract no. 261572, [www.wenmr.eu](http://www.wenmr.eu)), aims to optimize and extend the use of the NMR and SAXS research infrastructures through the implementation of an e-infrastructure in order to provide the user community with a platform integrating and streamlining the computational approaches necessary for NMR and SAXS data analysis and structural modelling. WeNMR builds on the established eNMR e-Infrastructure and its steadily growing virtual organization, which is currently the second largest VO in the area of life sciences.

The main objective of WeNMR is to establish an e-Infrastructure-based global virtual research community for structural biology in the life sciences. To this end six objectives are defined:

- To operate, maintain and further develop a user-friendly science gateway for the NMR and SAXS communities
- To establish a virtual research platform to serve as a digital knowledge repository, data exchange medium, and forum for (interaction with) the user community
- To provide support to software developers, users and other e- Infrastructure projects in an e-Science knowledge and training centre
- To foster the adoption and use of e- Infrastructure on a global scale by supporting a wide range of flanking disciplines within the life sciences
- To operate and consolidate the eNMR Grid infrastructure in line with NGIs and the EGI, and to extend it to interoperate with other worldwide Grid initiatives
- To develop a model to ensure sustainability of the project.

Next to being an EU e-Infrastructure project, WeNMR also acts a recognized Virtual Research Community under the EGI for structural biology.

#### CHAIN

CHAIN project receives funding support from the European Commission in the context of its Seventh Framework Programme.

The objectives of the CHAIN project (Grant Agreement no. 260011, [www.chain-project.eu](http://www.chain-project.eu)) can be divided into three main areas:

- I. Define a strategy and a model for external collaboration, in close collaboration with EGI.eu, which will enable operational and organisation interfacing of EGI and external e-Infrastructures. This strategy will take into account current organisational models, while, regarding operational models, a peering model will be defined between Europe and other continents.
- II. Validate this model, as a proof-of-principle, by supporting the extension and consolidation of worldwide Virtual Research Communities, which work on common

areas (Bioinformatics, Chemistry, etc.) and/or increasingly require distributed facilities (e.g., large instruments, distributed data and databases, digital repositories, etc.) across the regions for trans-continental research. The limited support for such existing communities will be complemented by a coordinated activity of support for the international expansion to other prospective communities that have not exploited yet the full benefits of large intercontinental e-Infrastructures.

- III. Propose and explore concrete steps forward towards the coordination with other projects and initiatives (e.g., EGI-InSPIRE, EUMEDGRID-Support, EU-IndiaGrid2, LinkSCEEM2, PRACE, the Indian National Knowledge Network, GISELA, etc.). The project will act as a worldwide policy-watch and coordination instrument, by exploring and proposing concrete steps for the coordination with other initiatives and studying the evolution of e-Infrastructures towards not only Grids and HPC but also Cloud Computing, Virtualisation, Desktop and Voluntary Computing and other trends that may emerge. This interaction with other e-Infrastructures will also imply a strong commitment to standards' adoption.

## **2. Purpose of this Memorandum of Understanding (MoU)**

The purpose of this MoU is to establish the terms under which the collaboration between the CHAIN and the WeNMR initiatives will be carried out. As a consequence, it is expected that the outcomes and impact of both initiatives will be increased and improved.

The term VRC (Virtual Research Community) is defined as an organisational grouping that represents a community of users with common interests. The EGI VRC model brings together the stakeholders within a standard, flexible, persistent and sustainable structure. A VRC could then be a self-organising group that collects and represents the interests of a focussed collection of researchers across a clear and well-defined field and/or a group of researchers who are common users of a specific e-Science application. Named contacts are agreed upon by the VRC to perform specific roles and these then form the communication channel between the VRC and CHAIN. In this sense WeNMR is not only a project itself, but also a group of users and developers devoted to NMR and SAXS studies who form a VRC. Thus, the actions agreed on in this MoU are linked to WeNMR in a two-fold basis: Project and VRC. Despite of the last, either WeNMR project or WeNMR VRC are only represented by the associated EC funded Project WeNMR (contract no 261572) coordinator.

Both initiatives have a common interest in a close cooperation in order to achieve their respective objectives. This is witnessed by the fact that the two projects have the following partner in common:

- I. Istituto Nazionale di Fisica Nucleare (INFN)

This Memorandum of Understanding (MoU) specifies the way in which such cooperation will be undertaken.

In this MoU, the undersigned are:

- WeNMR, an FP7 funded e-Infrastructure (contract number 261572), coordinated by UTRECHT UNIVERSITY, a legal entity established under the laws of the Netherlands and governed by public law under section 1.8 of the Higher Education and Research Act (*Wet op het hoger onderwijs en wetenschappelijk onderzoek*) and having its registered offices at Heidelberglaan 8, Utrecht, the Netherlands, for the benefit of the Science faculty, in this matter duly represented by Prof. Dr. Alexandre Bonvin, coordinator of the WeNMR project ("WeNMR");
- CHAIN, an FP7 funded Coordination and support action (contract number 260011) coordinated by ISTITUTO NAZIONALE DI FISICA NUCLEARE, a legal entity established under the laws of the Republic of Italy and having its registered offices at Via E. Fermi 40, 00044 Frascati, (Rome), Italy, in this matter duly represented by Prof. Federico Ruggieri, coordinator of the CHAIN project ("CHAIN").

### 3. Common Activities

Activities which will be undertaken in common by the two initiatives are listed in Annex 1 to this MoU. The initiatives may from time to time wish to add other activities to the MoU. In such case the new activities to be added will be agreed in writing by the respective initiatives managements or people in charge, and be defined by an amendment of this MoU, simply adding a new Annex 1.

### 4. Communication

The Project Managers or people in charge of the two initiatives will maintain regular contact to discuss any managerial matters related to the cooperation described in this MoU. Each initiative will appoint one Principal Point of Contact to act as the primary technical channel of communication between the initiatives as is necessary for the promotion of effective cooperation between the projects.

### 5. Administrative Matters

Each initiative will maintain full responsibility for its own activities, including the fulfilment of its obligations under its Grant Agreement with the European Commission or funding agency and provides no warranty, express or implied, in respect of its contribution to any activity agreed by the initiatives under this MoU, including but not limited to those of fitness for a particular purpose and the infringement of third-party proprietary rights.

Any proprietary rights relating to the results of activities undertaken by the initiatives under this MoU shall be jointly held by the projects, and each initiative herewith grants the other initiative a free, irrevocable and perpetual license to use such rights, including the granting of sub-licenses to such rights, for its own purposes, including the right for each project to place the results of such activities in the public domain, in its own name and under its own responsibility.

This Agreement will terminate when either of the initiatives is complete, or when either initiatives gives notice of termination to the other, in which case a minimum notice of three months will be given.

In the event that - for whatever reason - this MoU is terminated the Parties retain the right to use data and results that were shared prior to termination of this MoU, under the provisions detailed herein. Parties are not entitled to use any such information (including knowledge and know how) which has come to their attention pursuant to the termination of this MoU. All Parties are not prevented by this MoU from cooperating with other projects performing similar activities to those described in this MoU, unless explicitly set forth herein.

Duly signed in 2-fold by:

Signed on behalf of CHAIN by:

Signed on behalf of WeNMR by:

Name: Federico Ruggieri (project director)

Name: Alexandre M.J.J. Bonvin (project coordinator)

Signature:   
Date: 21/09/2014

Signature:   
Date: 21 - 09 - 2014

## Annex 1 – Coordinated Activities

### Promotion of Grid Infrastructures and WeNMR and CHAIN objectives and road-map for the future

- Both initiatives will cooperate in supporting the WeNMR community required services in those Grid Infrastructures targeted by CHAIN, either in developed or emerging continents, promoting as much as possible the adoption of standards and best practices.
- CHAIN project will present in its web page the information about the VRCs interacting with. In order to dynamically fill the tables containing the related information, WeNMR will work on setting up automatic sources of information or providing them periodically in order to fill in the tables in a static way at least.
- Both initiatives will work on maximising the impact of both CHAIN and WeNMR, through the efficient coordination of dissemination of their joint or individual. They will collaborate, where relevant, in the organisation of workshops aiming at discussing common issues.
- CHAIN will foster the contacts of the research communities with WeNMR; WeNMR will provide support to enable the discovery of new users and to engage them. In this sense, WeNMR will report to CHAIN about the identification of research groups that are part of WeNMR (i.e. form its associated VRC) and active in CHAIN's regions of interest. CHAIN will encourage and support users associated with the project to make use of the WeNMR support services either directly or through their National or Community gateways.
- CHAIN will exchange with WeNMR the information and know-how related to NGIs and both initiatives will provide feedbacks related to the CHAIN questionnaire.
- Both initiatives will contribute to the definition of the road-maps for the future activities in the common field of interest.
- Both initiatives will contribute to the raising of awareness of both new potential users and decision makers, through the presentation of the results of the grid activities, about the usefulness of e-Infrastructures for e-Science.

CHAIN will fully exploit the collaboration with WeNMR providing complementary actions on those countries and/or institutes which are not participating to WeNMR.

The list of contact people is the following:

CHAIN:

- Prof. Dr. Federico Ruggieri – INFN Roma Tre – Via della Vasca Navale 84, 00146 Roma, Italy. +39 0657337232 – [Federico.Ruggieri@roma3.infn.it](mailto:Federico.Ruggieri@roma3.infn.it)
- Prof. Dr. Roberto Barbera – INFN Catania – Via S. Sofia, 64 - 95123 Catania – Italy - +390953785504 - [roberto.barbera@ct.infn.it](mailto:roberto.barbera@ct.infn.it)
- Dr. Rafael Mayo García – CIEMAT – Avda. Complutense, 22 – 28040 Madrid – Spain - +34-91-346-0000 – [rafael.mayo@ciemat.es](mailto:rafael.mayo@ciemat.es)

WeNMR:

- Prof. Dr. Alexandre Bonvin - Bijvoet Center for Biomolecular Research - Faculty of Science - Utrecht University - Padualaan 8, 3584 CH Utrecht - The Netherlands - +31-30-253-3859 - [a.m.j.bonvin@uu.nl](mailto:a.m.j.bonvin@uu.nl)
- Dr. Reinout Raijmakers - Bijvoet Center for Biomolecular Research - Faculty of Science - Utrecht University - Padualaan 8, 3584 CH Utrecht - The Netherlands - +31-30-253-6804 - [r.raijmakers@uu.nl](mailto:r.raijmakers@uu.nl)