BioExcel Centre of Excellence for Computational Biomolecular Research

Fact Sheet

Project Information

BioExcel-2
Grant agreement ID: 823830

Funded under
EXCELLENT SCIENCE - Research Infrastructures

Total cost
€ 7,998,833,75

EU contribution
€ 7,998,833,75

Coordinated by
KUNGLIGA TEKNISKA HOEGSKOLAN
Sweden

Closed project

EC signature date
12 November 2018

Start date
1 January 2019
End date
30 June 2022

Objective

Life Sciences have become increasingly digital and this is accelerating. Computational techniques play key roles in processing, analysis and generating new knowledge from experiments, even in replacing them. This has been enabled due to tremendous advances in techniques such as docking and molecular simulations at both atomistic and quantum levels to which world-leading European research and software are contributing. Pushing computational capabilities towards Exascale will
advance the area, enabling researchers to tackle increasingly complex questions related to biomolecules' function, mechanisms, dynamics and interactions. This will impact on our daily life, in health, for the development of new drugs and efficient drug delivery methods, in biotechnology, environment, agriculture, food industry and education. To exploit this great computational power, in academia and industry, significant efforts on software efficiency, scaling, usability and education are needed. This is the mission of the BioExcel Centre of Excellence for Computational Biomolecular Research launched in 2015 with EC support. It has made significant contributions by focusing on highest-impact European codes, workflows and an extensive, international education program. BioExcel-2 will continue and expand this work, with a focus on Exascale impact, improved usability, expanded training and commercial applications, while strengthening its user-driven governance. Specifically it will: * Push performance, efficiency, scalability and usability of the selected software packages towards Exascale in a co-design manner, contributing to the EuroHPC vision * Support convergence of HPC, HTC, and HPDA with workflows combining simulations with data management and analytics * Support and enlarge the user community by providing support, workforce development, continued training, guidance, and best practices * Develop a sustainable and open community centre with user-driven governance and clear KPIs.

**Fields of science**

- **natural sciences** > **computer and information sciences** > **software**
- **social sciences** > **sociology** > **governance**
- **natural sciences** > **biological sciences** > **biochemistry** > **biomolecules**
- **agricultural sciences** > **agriculture, forestry, and fisheries** > **agriculture**
- **social sciences** > **economics and business** > **business and management** > **employment**

**Keywords**

- Biomolecular Life Science
- Drug Discovery
- Biotechnology
- Exascale
- HPC
- HPDA

**Programme(s)**

- **H2020-EU.1.4. - EXCELLENT SCIENCE - Research Infrastructures**
- **H2020-EU.1.4.1.3. - Development, deployment and operation of ICT-based e-infrastructures**
Topic(s)

INFRAEDI-02-2018 - HPC PPP - Centres of Excellence on HPC

Call for proposal

H2020-INFRAEDI-2018-2020

See other projects for this call

Sub call

H2020-INFRAEDI-2018-1

Funding Scheme

RIA - Research and Innovation action

Coordinator

KUNGLIGA TEKNISKA HOEGSKOLAN

Net EU contribution

€ 1 993 750,00

Address

Brinellvagen 8
100 44 Stockholm

Sweden

Region

Östra Sverige > Stockholm > Stockholms län

Activity type

Higher or Secondary Education Establishments

Links

Contact the organisation  Website  Participation in EU R&I programmes  HORIZON collaboration network

Other funding

€ 0,00
UNIVERSITEIT UTRECHT
Netherlands
Net EU contribution
€ 1 046 875,00
Address
Heidelberglaan 8
3584 CS Utrecht
Region
West-Nederland > Utrecht > Utrecht
Activity type
Higher or Secondary Education Establishments
Links
Contact the organisation  
Website  
Participation in EU R&I programmes  
HORIZON collaboration network  
Other funding
€ 0,00

FUNDACIO INSTITUT DE RECERCA BIOMEDICA (IRB BARCELONA)
Spain
Net EU contribution
€ 469 687,50
Address
Carrer baldiri reixac 10-12 parc scientific de barcelona
08028 Barcelona
Region
Este > Cataluña > Barcelona
Activity type
Research Organisations
Links
Contact the organisation  
Website  
Participation in EU R&I programmes  
FORSCHUNGZENTRUM JULICH GMBH

Germany

Net EU contribution

€ 178 442,50

Address

Wilhelm johnen strasse
52428 Julich

Region

Nordrhein-Westfalen > Köln > Düren

Activity type

Research Organisations

Links

Contact the organisation  Website  Participation in EU R&I programmes  HORIZON collaboration network

THE UNIVERSITY OF EDINBURGH

United Kingdom

Net EU contribution

€ 777 301,25

Address

Old college, south bridge
EH8 9YL Edinburgh

Region

Scotland > Eastern Scotland > Edinburgh

Activity type

Higher or Secondary Education Establishments
THE UNIVERSITY OF MANCHESTER

United Kingdom

Net EU contribution

€ 711,937.50

Address

Oxford road
M13 9PL Manchester

Region

North West (England) > Greater Manchester > Manchester

Activity type

Higher or Secondary Education Establishments

JYVÄSKYLÄN YLIOPISTO

Finland

Net EU contribution

€ 314,406.25

Address

Seminaarinkatu 15
40100 Jyväskylä

Region

Manner-Suomi > Länsi-Suomi > Keski-Suomi
EUROPEAN MOLECULAR BIOLOGY LABORATORY

Germany

Net EU contribution

€ 824 683.75

Address

Meyerhofstrasse 1
69117 Heidelberg

Region

Baden-Württemberg > Karlsruhe > Heidelberg, Stadtkreis

Activity type

Research Organisations

Links

Contact the organisation  Website  Participation in EU R&I programmes  HORIZON collaboration network

Other funding

€ 0,00

MAX-PLANCK-GESELLSCHAFT ZUR FORDERUNG DER WISSENSCHAFTEN EV

Germany

Net EU contribution

€ 483 750.00

Address

Hofgartenstrasse 8
80539 Munchen
Region
Bayern > Oberbayern > München, Kreisfreie Stadt

Activity type
Research Organisations

Links
Contact the organisation Website Participation in EU R&I programmes HORIZON collaboration network

Other funding
€ 0,00

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ACROSSLIMITS LTD
Malta
Net EU contribution
€ 197 087,50

Address
Tower business centre 2nd fl tower street swatar BKR 4013 Birkirkara

SME Yes

Region
Malta > Malta

Activity type
Higher or Secondary Education Establishments

Links
Contact the organisation Website Participation in EU R&I programmes HORIZON collaboration network

Other funding
€ 0,00

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BARCELONA SUPERCOMPUTING CENTER CENTRO NACIONAL DE SUPERCOMPUTACION
Spain

8 of 11
Net EU contribution
€ 468 662,50

Address
Calle jordi girona 31
08034 Barcelona

Region
Este > Cataluña > Barcelona

Activity type
Research Organisations

Links
Contact the organisation Website Participation in EU R&I programmes HORIZON collaboration network

Other funding
€ 0,00

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IAN HARROW CONSULTING LTD

Net EU contribution
€ 102 375,00

Address
Kd tower plaza suite 9 cotterells
HP1 1FW Hemel hempstead

SME Yes

Region
East of England > Bedfordshire and Hertfordshire > Hertfordshire

Activity type
Private for-profit entities (excluding Higher or Secondary Education Establishments)

Links
Contact the organisation Participation in EU R&I programmes HORIZON collaboration network

Other funding
€ 0,00
NORMAN RICHARD ALBERT
Norway
Net EU contribution
€ 253 600,00
Address

Links
Contact the organisation
Participation in EU R&I programmes
HORIZON collaboration network

Other funding
€ 0,00

NOSTRUM BIODISCOVERY SL
Spain
Net EU contribution
€ 176 275,00
Address
Avinguda josep tarradellas 8-10 3
08029 Barcelona
SME
Yes
Region
Este > Cataluña > Barcelona
Activity type
Private for-profit entities (excluding Higher or Secondary Education Establishments)

Links
Contact the organisation
Participation in EU R&I programmes
HORIZON collaboration network

Other funding
€ 0,00