



Kick-off meeting of the “AIDD”

26 January 2021

HelmholtzZentrum münchen

German Research Center for Environmental Health

Agenda

Introduction to the AIDD Project

- 10:00-10:15 Administration and financial questions
- 10:15-10:30 Recruitment Process
- 10:30-10:45 Overview of milestones and deliverables for 2021
- 10:45-11:00 Associated partners and SB

Presentation of the Partners (part 1)

- 11:00-11:10 Helmholtz Zentrum Muenchen (GmbH)
- 11:10-11:20 AstraZeneca AB
- 11:20-11:30 Bayer Aktiengesellschaft
- 11:30-11:40 Janssen Pharmaceutica Nv
- 11:40-11:50 Enamine Limited Liability Company
- 11:50-12:00 Technical University of Dortmund
- 12:00-12:10 Freie Universität Berlin
- 12:10-12:20 Katholieke Universiteit Leuven
- 12:20-12:30 Universität Linz

12:30-13:00 Remaining questions on the Contract Agreement

- 13:00-13:10 Vancouver Prostate Center, University of British Columbia (Video Presentation)

13:10-14:00 Lunch break

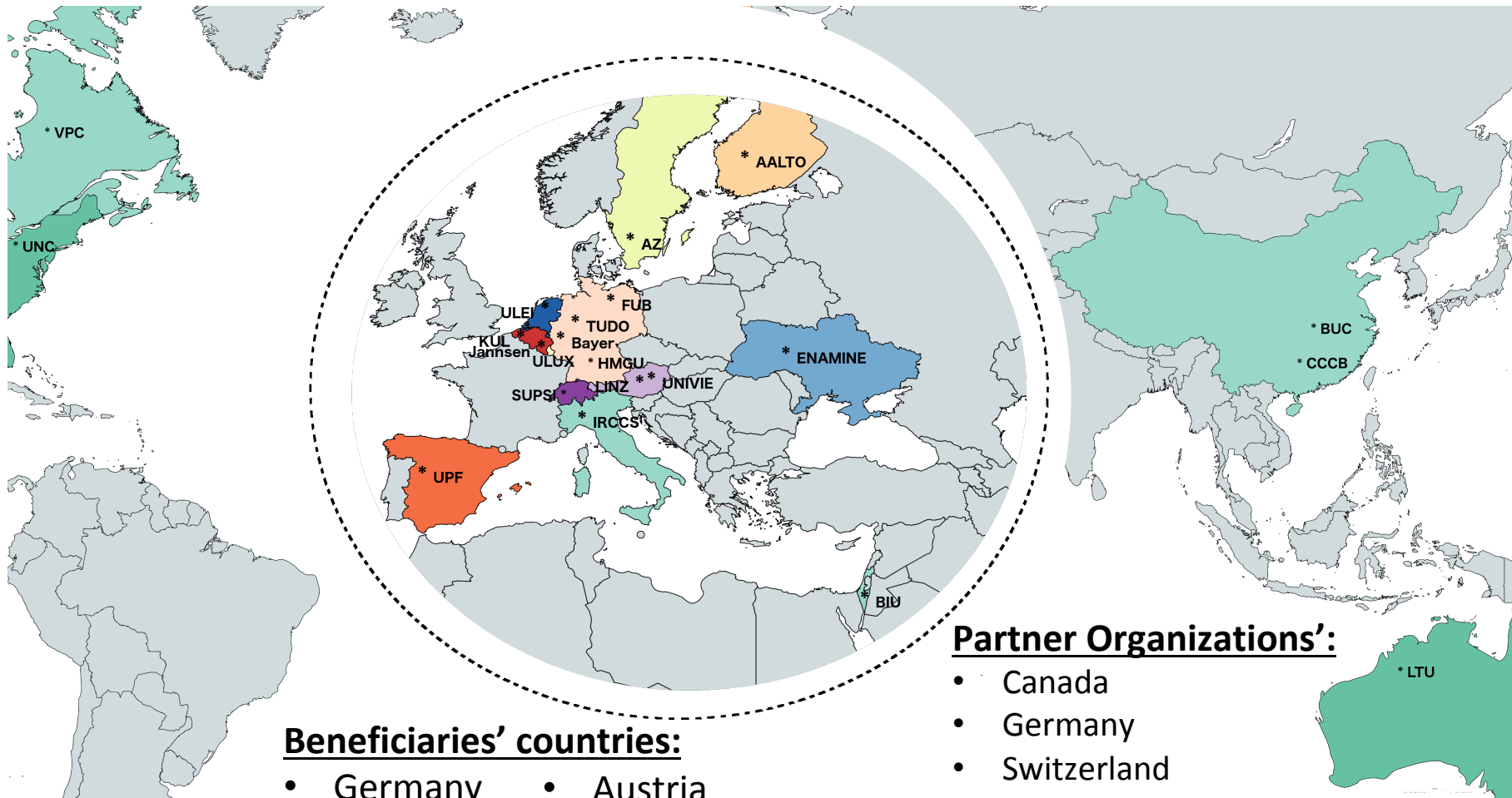
Presentation of the Partners (part 2)

- 14:00-14:10 Scuola Universitaria Professionale della Svizzera Italiana
- 14:10-14:20 Aalto- korkeakoulusäätiö Sr
- 14:20-14:30 Universiteit Leiden
- 14:30-14:40 Université du Luxembourg
- 14:40-14:50 University of Vienna
- 14:50-15:00 Universitat Pompeu Fabra

Miscellaneous

- 15:00-15:30 Miscellaneous and closing remarks

AIDD global map



Beneficiaries' countries:

- Germany
- Sweden
- Belgium
- Ukraine
- Finland
- Austria
- Switzerland
- Netherlands
- Luxemburg
- Spain

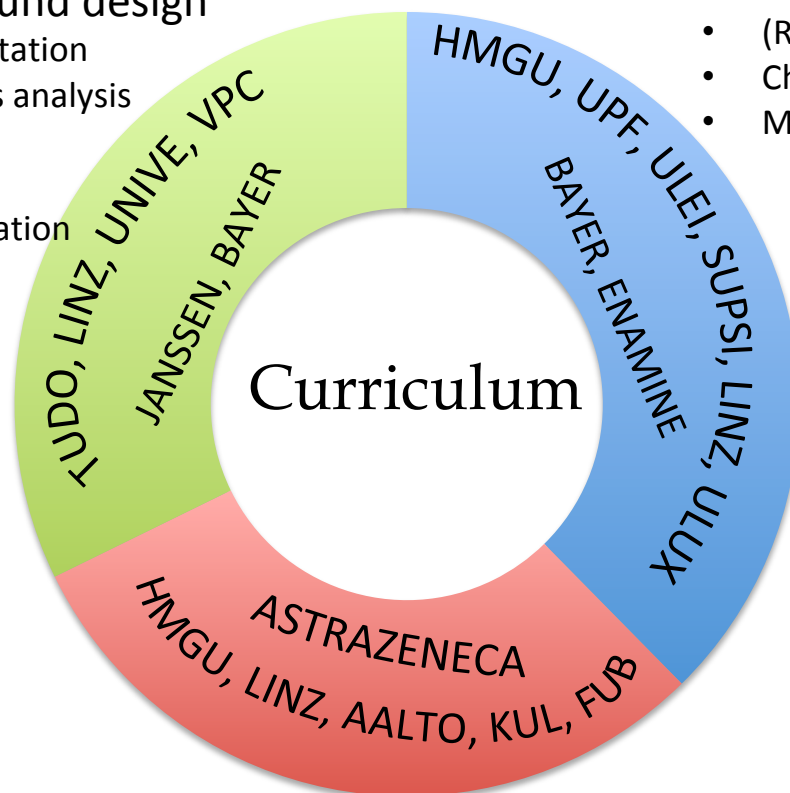
Partner Organizations':

- Canada
- Germany
- Switzerland
- Italy
- Israel
- China
- USA
- Australia

Scientific areas

Intelligent compound design

- Structure representation
- Microscope images analysis
- Toxicity prediction
- Frequent hitters
- Experimental validation



Chemical reactions

- (Retro-)synthesis
- Chemical Reactivity
- Multi-object optimization

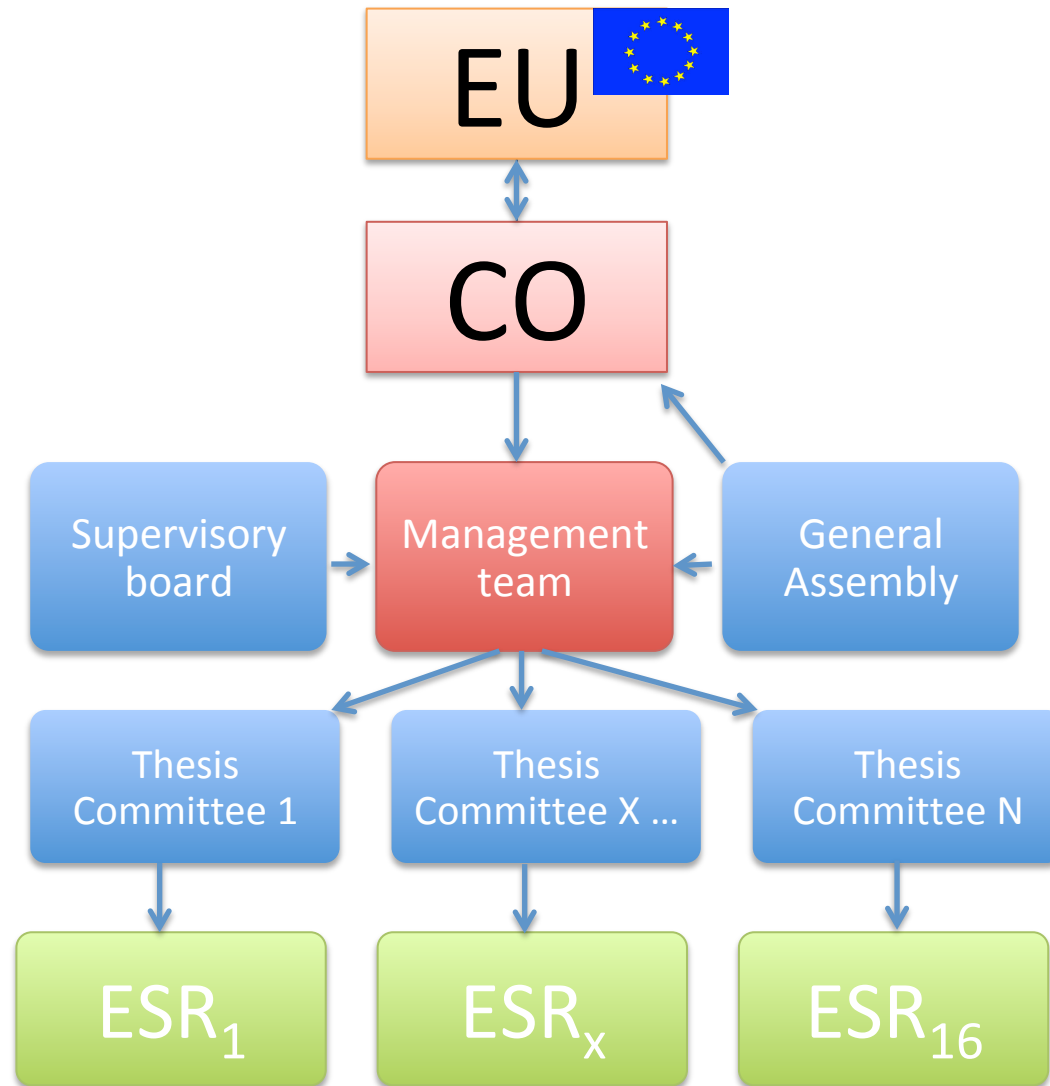
Beyond machine learning

- One Chemistry
- Human in the loop
- Uncertainty modeling
- Boltzmann generators

Management team

- Project Coordinator (Igor Tetko)
- Project Manager (Pavel Karpov)
- WP leader of curriculum (Yves Moreau)
- Organizer of the next meeting (LINZ/HMGU, Günter Klambauer)
- Industrial partner (?)

Project Governance



Payments within the projects

The AIDD project has:

1. Pre-financing payment (EU transfers 80% of the total grant amount to the Coordinator) – to be distributed after Contract Agreement is signed
2. Requests for interim payments:
 1. After the first reporting period (24 month)
 2. After the second reporting period (48 month)
3. Payment of the balance (48 month)

Details are in the GA, pp. 21 – 23.

Recruitment of fellows

15 ESRs + 1 ESR from VPC (Canada)

Eligibility:

1. Early-Stage Researchers (ESRs) shall, at the time of recruitment by the host organization, be **in the first four years** (full-time equivalent research experience) of their research careers and have not been awarded a doctoral degree;
2. At the time of recruitment by the host organization, researchers must not have resided or carried out their main activity (work, studies, etc.) in the country of their host organization for **more than 12 months in the 3 years immediately prior to the reference date**.

For example, if a student from Germany wants to work at Bayer within the AIDD project, he/she has to apply for ESR5, ESR7, or ESR12 because the first hosts in these positions are outside Germany, unless we change the order of employment.

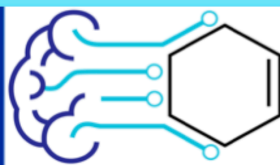
Recruitment of students

All the students must send their documents to

recruit@ai-dd.eu

Details are here: <http://ai-dd.eu/esr-positions#how-to-apply>

- Relevant scientific backgrounds and skills
 - Quality of earned degrees
 - SKYPE interview
 - Recommendation letters
 - Gender equality and minority rights
1. We will check eligibility rules and and group applications by ESRs.
 2. All the PIs will have an access to this mailbox to read applications and to select the best ones.
 3. Use of Code of Conduct for the Recruitment of Researchers (including 40% of female) <https://euraxess.ec.europa.eu/jobs/charter/code>
 4. We will organize a recruitment meeting with the selected students to choose best of the best.



Advanced machine learning for Innovative Drug Discovery (AIDD)

This project is funded by Horizon2020 research and innovation programme under the Marie Skłodowska-Curie actions (negotiation)

[Home](#)[Partners](#)[PhD Positions](#)[News](#)[Contact](#)[Home](#)

PhD Positions

The project offers 15 Ph.D. positions. The positions are expected to start in Summer - early Autumn. Please read the information in the page carefully before applying.

[Eligibility criteria](#)[Common requirements for a candidate](#)[Specific requirements for each position](#)[How to apply](#)

Eligibility and Mobility Rule

Early-Stage Researchers (ESRs) shall, at the time of recruitment by the host organization, **be in the first four years** (full-time equivalent research experience) of their research careers and **have not been awarded a doctoral degree**;

“ **Date of Recruitment** normally means the first day of the employment of the fellow for the purposes of the project (i.e. the starting date indicated in the employment contract or equivalent direct contract).

Full-Time Equivalent Research Experience is measured from the date when a researcher obtained the degree which would formally entitle him/her to embark on a doctorate, either in the country in which the degree was obtained or in the country in which the researcher is recruited or seconded, irrespective of whether or not a doctorate is or was ever envisaged.

”

At the time of recruitment by the host organization, researchers must **not have resided or carried out** their main activity (work, studies, etc.) **in the country of their host organization for more than 12 months in the 3 years immediately prior to the reference date**. Compulsory national service and/or short stays such as holidays are not taken into account. As far as international European interest organizations or international organizations are concerned, this rule does not apply to the hosting of eligible researchers. However, the appointed researcher must not have spent more than 12 months in the 3 years immediately prior to their recruitment at the host organization.

“ **For refugees** under the Geneva Convention (1951 Refugee Convention and the 1967 Protocol), the refugee procedure (i.e. before refugee status is conferred) will not be counted as ‘period of residence/activity in the country of the beneficiary’. ”

More details are available [here](#).

Recruitment of fellows

Offers already published:

- <http://ai-dd.eu/esr-positions>
- <https://euraxess.ec.europa.eu/jobs/594580>
- <https://www.researchgate.net/project/Advanced-machine-learning-for-Innovative-Drug-Discovery-AIDD>
- <https://twitter.com/AiddOne>

To be published once the CA is signed:

- <https://www.nature.com/naturecareers>
- LinkedIn

To provide broader dissemination of the Project, **please join** to AIDD project on ResearchGate, Twitter, and LinkedIn.




Recruitment meeting

- Preliminary date – March-April (by SKYPE)
- Short list 2-3 candidates per position
- On-site/SKYPE/Zoom interview of short-listed candidates before the meeting
- GA will approve the selected candidates
- Use of Code of Conduct for the Recruitment of Researchers (including 40% of female) – responsibility of the GA and industrial partners

Milestones 2021

Month in brackets is the **due date**.


- MS1 Web site available (HMGU, February)
- MS2 Selection of ESR fellows (UPF, June)
- MS3 Launch of the online courses (KUL, August)
- MS4 Schools started (HMGU, September) (changed)
- MS5 Interfaces for software agreed (HMGU, October)
- MS6 All CDPs are prepared (FUB, October)
- MS7 All recruited fellows enrolled in PhD programme (UNIVIE, December)
- MS18 Planned recruitments completed (HMGU, December)




Grant Management


ntetkoig (EXTERNAL) ?


956832 (AIDD) MSCA-ITN..





Call: H2020-MSCA-ITN-2020
Topic: MSCA-ITN-2020 Unit: REA/A/01


Summary for publication 


Deliverables Ethics, DMP, Other Reports 


Milestones 


Publications 

Disseminat... 







Patents (IPR) 

SME Impact 

Gender 

Researchers 


Milestones SAVE

| Number | Name | Lead Beneficiary | Delivery Date (Annex I) ▲ | Achieved | Delivery Date (actual) | Comments |
|--------|------------------------|------------------|---------------------------|--------------------------|------------------------|---|
| 1 | Web site of the proje | HMGU | 28 Feb 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 2 | Selection of ESR fello | UPF | 30 Jun 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 3 | Launch of the online | KUL | 31 Aug 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 4 | Schools started | LINZ | 30 Sep 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 5 | Interfaces for softwai | HMGU | 31 Oct 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 6 | All CDPs are preparec | FUB | 31 Oct 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 7 | All recruited fellows | UNIVIE | 31 Dec 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 18 | Planned recruitments | HMGU | 31 Dec 2021 | <input type="checkbox"/> | <input type="text"/> |  |
| 8 | Data for reaction mor | Enamine | 28 Feb 2022 | <input type="checkbox"/> | <input type="text"/> |  |
| 10 | Project Check | ULEI | 31 Mar 2022 | <input type="checkbox"/> | <input type="text"/> |  |


Deliverables 2021


Month in brackets is the **due date**.


- D5.1 Advertisement of Positions (HMGU, January)
- D5.2 Minutes of the kick-off meeting (ULUX, January)
- D5.3 Web site of the AIDD project (HMGU, January)
- **D5.10 Consortium Agreement (HMGU, February)**
- D5.11 Supervisory Board of the network (HMGU, February)
- D5.4 Recruitment meeting (HMGU, April)
- D5.5 First newsletter (UNIVIE, May)
- D4.1 Preparation of the CDPs (HMGU, November)
- D4.2 WS1 school report (HMGU, November)
- D6.1 HCT Requirement No 1 (HMGU, December)
- D6.2 A – Requirement No 2 (HMG, December)
- D6.3 NEC – Requirement No 3 (HMGU, December)
- D6.4 GEN – Requirement No 4 (HMGU, December)



Grant Management


Project Continuous Report


956832 (AIDD) MSCA-ITN..

HORIZON 2020
Call: H2020-MSCA-ITN-2020
Topic: MSCA-ITN-2020 Unit: REA/A/01


Summary for publication



Deliverables Ethics, DMP, Other Reports



Milestones



Publications



Disseminat...


Patents (IPR)


SME Impact


Gender


Researchers


Training Activities


























Deliverables, Ethics, DMP, Other Reports

 For each Deliverable, a single file (max 52MB) can be uploaded

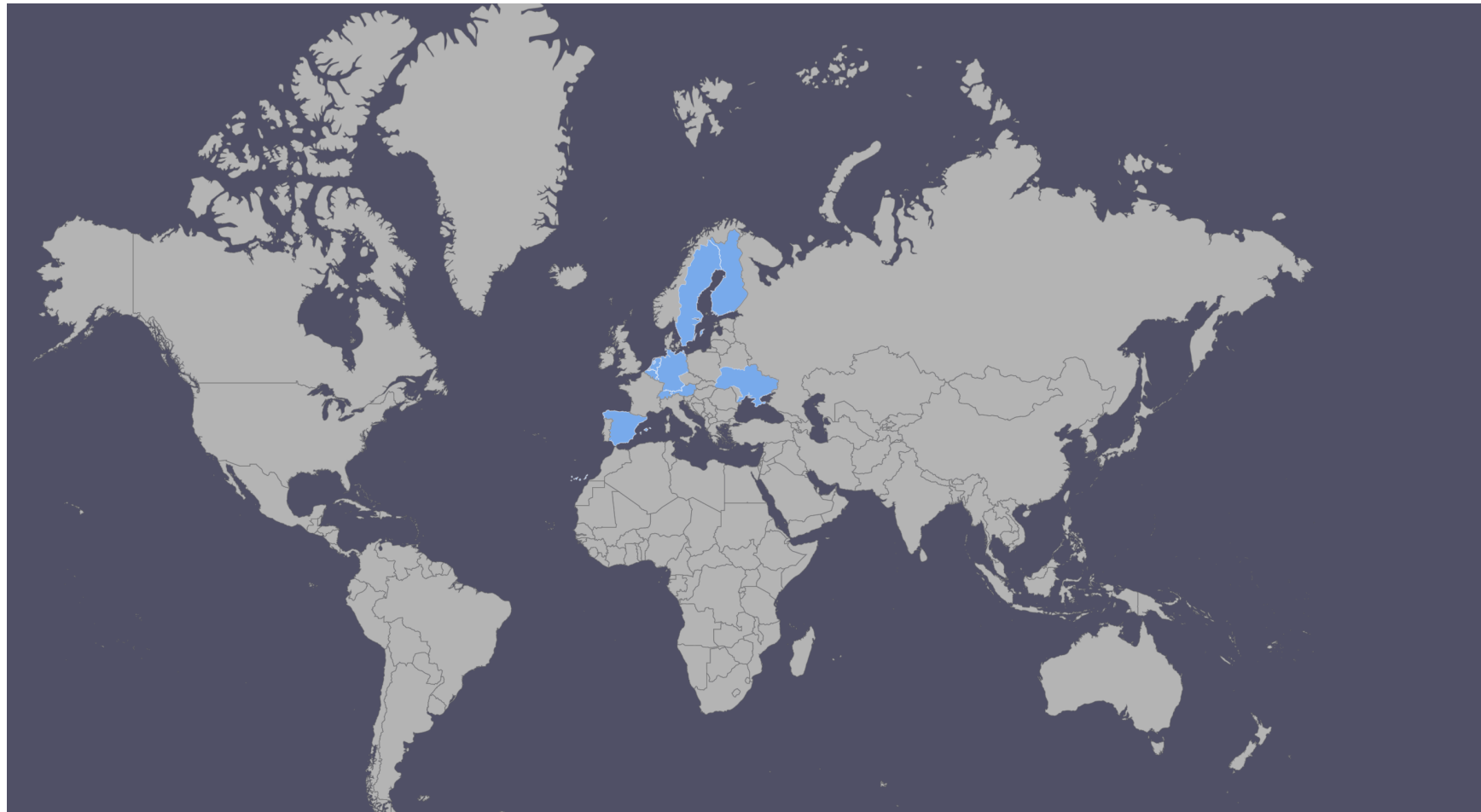
Please download here the template for the Progress Report:  [Download template](#)

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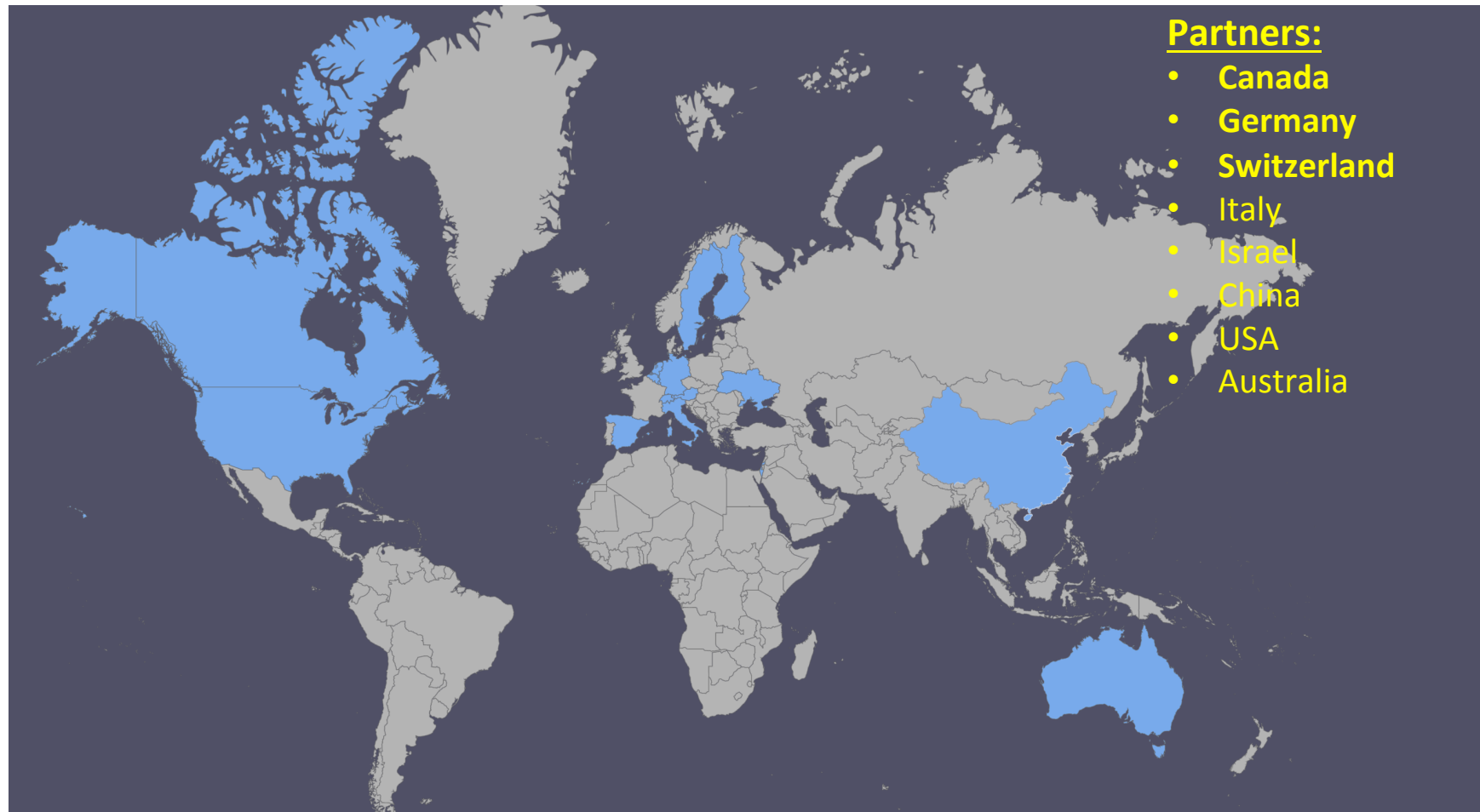
 [Deliverables](#)

| WP No | Del Re | Del N | Title | Description | Lead Beneficiary | Nature | Dissem | Est. | Rev. Du | Receipt | Approval I | Status |
|-------|--------|-------|---------------------|--|------------------|--------|--------|--------|---------|---------|------------|---|
| WP5 | D5.1 | D30 | Advertisement of p | Advertisement of positions  | HMGU | Webs | Publi | 31 Jan | | | | Pending  |
| WP5 | D5.2 | D31 | Minutes of the kick | Minutes of the kick-off meeting  | ULUX | Repo | Publi | 31 Jan | | | | Pending  |
| WP5 | D5.3 | D32 | Web site | The web site and web application system is esta | HMGU | Webs | Publi | 31 Jan | | | | Pending  |
| WP5 | D5.1 | D39 | Consortium Agree | Consortium Agreement  | HMGU | Repo | Confi | 28 Feb | | | | Pending  |
| WP5 | D5.1 | D40 | Supervisory Board | Supervisory Board of the network  | HMGU | Repo | Confi | 28 Feb | | | | Pending  |
| WP5 | D5.4 | D33 | Recruitment meeti | Minutes of the recruitment meeting  | HMGU | Repo | Publi | 30 Apr | | | | Pending  |
| WP5 | D5.5 | D34 | First newsletter | Publication of the first newsletter  | UNIVIE | Othe | Publi | 31 May | | | | Pending  |
| WP4 | D4.1 | D21 | Preparation of the | Preparation of the CDPs by fellows and PIs  | HMGU | Repo | Confi | 30 Nov | | | | Pending  |
| WP4 | D4.2 | D22 | WS1 school report | WS1 school report  | LINZ | Repo | Confi | 30 Nov | | | | Pending  |
| WP6 | D6.1 | D1 | HCT - Requirement | 3.1. In case of use of human cells/tissues avai... | HMGU | Ethic | Confi | 31 Dec | | | | Pending  |
| WP6 | D6.2 | D2 | A - Requirement N | 5.1. Copies of relevant authorisations for anim.. | HMGU | Ethic | Confi | 31 Dec | | | | Pending  |
| WP6 | D6.3 | D3 | NEC - Requirement | 6.1. In case activities undertaken in non-EU co.. | HMGU | Ethic | Confi | 31 Dec | | | | Pending  |
| WP6 | D6.4 | D4 | GEN - Requirement | 12.5. An ethics mentor must be appointed to ad | HMGU | Ethic | Confi | 31 Dec | | | | Pending  |
| WP5 | D5.6 | D35 | Progress Report | Progress Report for the meeting between REA ar | JANSSEN | Repo | Confi | 31 Jan | | | | Pending  |
| WP4 | D4.1 | D21 | Preparation of the | Preparation of the CDPs by fellows and PIs  | ASTRAZENECA | Repo | Confi | 30 Nov | | | | Pending  |

Beneficiaries



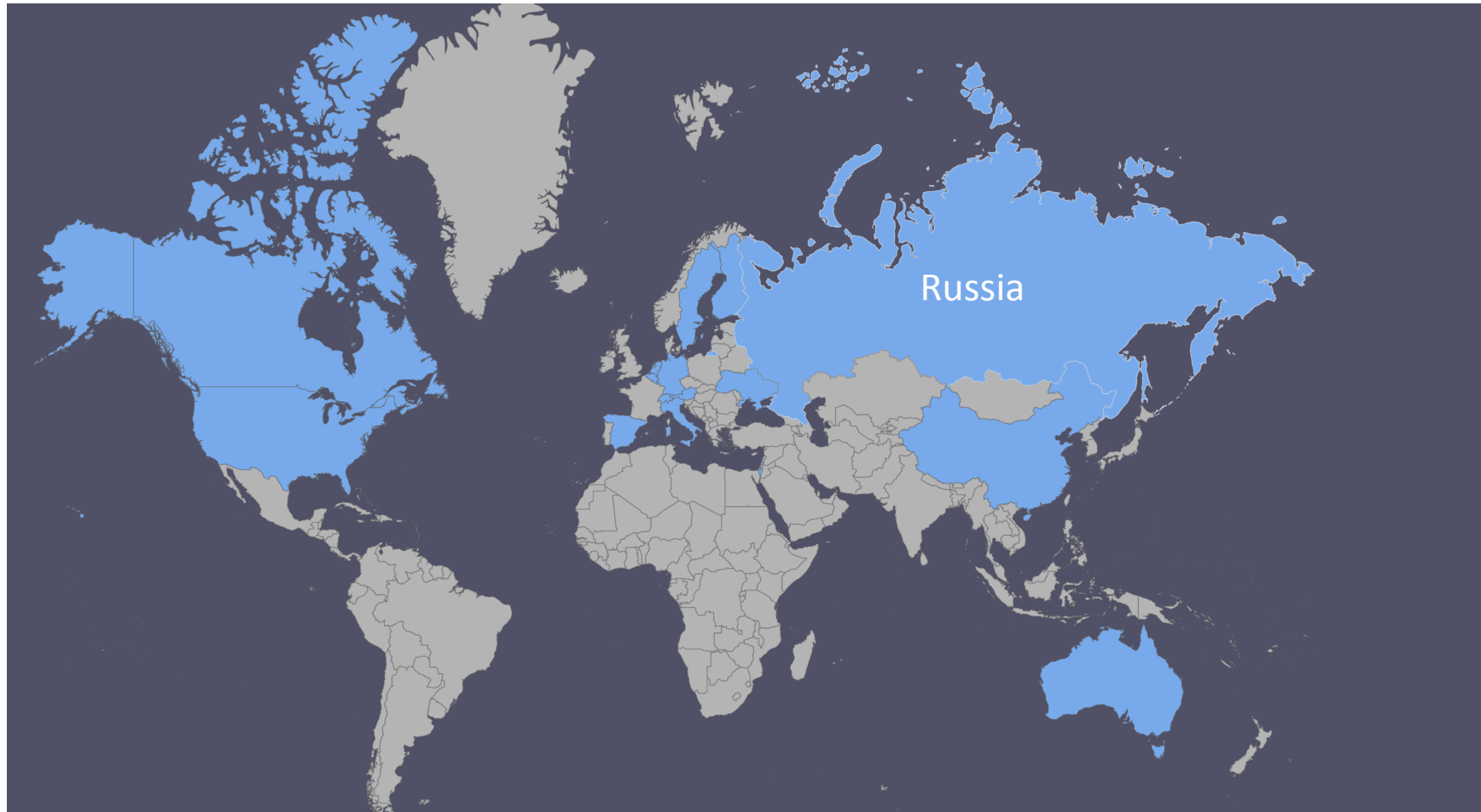
Beneficiaries + Partners



Supervisory board

- Will include beneficiaries and partners
- Need to be formed in February
- Role to be defined in the CA

Beneficiaries + Proposed Partners



Proposed Associated Partner

- Dr. Natalia Bichan
- Senior Scientists, Institute of Solute Chemistry (ISC), Ivanovo, Russia
- Traditional QC, chemical kinetics, ion – molecular interactions, chemical reactions, QSAR/QSPR, antimicrobial activity
- ISC will host project “Computer Synthesis of Chemical Compounds with Desired Properties”

