

## 6. Amsterdam Institute for Molecules, Medicine and Systems (AIMMS) – VU University Amsterdam

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Assessments:

	Quality	Relevance	Viability
AIMMS	1	2	1

### 6.1 Introduction and research area

The Amsterdam Institute for Molecules, Medicines and Systems has been founded in 2010 as one of the Interfaculty Research Institutes at VUA. It comprises in total 18 research groups from the Department of Chemistry & Pharmaceutical Sciences (CPS) from the Faculty of Exact Sciences (FEW), the Department of Molecular Cell Biology (MCB) from the Faculty of Earth & Life Sciences), and the Department of Informatics from FEW (BioInf). Formally, AIMMS consists of two departments (Chemistry and Pharmaceutical Sciences (CPS) and Molecular & Cell Biology (MCB)), which are also subject to this evaluation report. In a well elaborated research strategy, AIMMS aims at an integrated understanding of biological processes and systems as a whole. There is strong expertise in basically all areas linked to the discovery of new medicines, ranging from theoretical chemistry, synthetic and medicinal chemistry, molecular toxicology (CPS), to structural biology, microbiology, cell physiology (MCB), up to bioinformatics and neurobiology. With the very recent addition of the Department of Environment & Health (E&H), AIMMS further strengthens its translational approach from molecules to diseases. Furthermore, this will also strengthen the links to the VU Medical Center.

### 6.2 Research quality

#### *AIMMS*

AIMMS demonstrated a very impressive research portfolio exemplified by excellent output statistics and numerous prestigious personal grants. It comprises 18 research groups clustered in 5 major areas (Molecular Sciences, Computational Sciences, Pharmaceutical Sciences, Life Sciences, and Environment & Health), which cover the whole translational chain from molecule to disease. The committee was impressed by the strong collaborative spirit within AIMMS, which is also exemplified in the fact that the self-evaluation report does not assign the numerous achievements to the two individual departments. Over the evaluation period, scientists received 2 Veni, 4 Vidi, 2 Vici, 6 NWO ECHO, and 3 NWO Aspasia grants. Furthermore, there were one ERC starting grant and one ERC consolidator grant awarded. This demonstrates, that scientific excellence is present across all career stages, from young, very talented PIs up to internationally highly recognised senior researches. What is still missing is an ERC advanced grant, which definitely is within reach considering the outstanding research portfolio of most of the senior PIs (of which at least 6 show an H-index > 50).

Both departments publish in a wide range of journal categories with overall high to excellent relative impact, including publications in Science, Nature Commun., Nature Biotechnol., Nature Rev Drug Discov., Angewandte Chemie, and JACS. In order to even further increase the quality of the scientific output, AIMMS set the target of having at least 2 publications per researcher per year in the Q20% journals of his/her scientific domain.

#### *Department of Chemistry and Pharmaceutical Sciences (CPS)*

Traditionally, CPS is known for its world-leading position in GPCR research with focus on histamine receptors. In recent years, the research portfolio has been expanded towards phosphodiesterases and the acetylcholine binding protein. The chemistry groups are heavily engaged in the development of multicomponent reactions, with a focus on green chemistry. The translational value chain is complemented by strong expertise in preclinical toxicology and metabolism. All this is complemented by top level computational approaches. Based on the bibliometric analysis, CPS publishes between 115 to 132 papers per year, with chemistry, physics, and pharmacology & toxicology as top ranked categories. 77% of these publications are in the top quartile of the respective journal ranking. Furthermore, every year between 4% and 6% of the publications belong to the top 1% group in terms of citations. These parameters clearly further demonstrate the outstanding scientific quality of CPS.

#### *Department of Molecular & Cell Biology (MCB)/Bioinformatics group*

Also, MCB shows excellent publication records with 45 to 81 publications per year. According to their discipline, biology & biochemistry, microbiology, and plant & animal science are among the top categories. 70% of the publications are in the top quartile with up to 4% belonging to the top 1% cited publications. Specific strengths of MCB are seen in the field of systems approaches, metabolic models, as well as research on tuberculosis and antibiotic drug resistance. Also, in these fields, there are tight interactions with strong informatics groups.

### **6.3 Relevance to society**

Staff members as well as students of AIMMS actively contribute to dissemination of their research to different target groups. This includes interviews in TV and radio, public courses, lectures at schools, debates with politicians, and of course numerous press releases which are targeted to a broader public. In addition, several groups are also running web services for a more specialised target group, such as the 3D-e-Chem Virtual Machine and a set of KNIME nodes for computer-aided drug discovery, and databases for kinases and phosphodiesterases. Finally, AIMMS also developed a valorisation strategy to target economic target groups such as pharmaceutical companies. This resulted in several spin-offs and patents. Notably, CPS appointed a professor for Science Business & Innovation, who contributes to increasing entrepreneurial thinking of the students and organises collaboration events with e.g. large pharmaceutical companies.

However, considering the huge potential that pharmaceutical and microbiological research offers for society, the activities in the area of societal relevance pursued by AIMMS may be considered as very good, but could be improved. Explaining e.g. the need for research in areas such as antimicrobial resistance to the general public is straight forward and of course generates societal impact. For being world leading in this aspect, opinion leadership in areas

such as openness and ethics in pharmaceutical research, targeting rare diseases, or the whole complex of reducing animal experiments (3Rs) needs to be enlarged.

#### *Department of Chemistry & Pharmaceutical Sciences*

The main contributions of CPS to societal target groups focus on providing cutting edge tools for scientists. These include the eChem toolbox for computer aided drug discovery, data bases for structure-based drug design in the field of kinases and phosphodiesterases, as well as tool compounds for chemical biology approaches. Outreach to the general public is in line with the general policy of VU, but, as outlined above, could be improved

#### *Department of Molecular & Cell Biology/Bioinformatics group*

Members of MCB are very active in communicating the role and importance of microbiologically oriented research to the general public. This is e.g. exemplified by public courses on the microbiome, systems biology, and debates about synthetic biology. Quite some attention was achieved with the work on the microbiology of kisses, which was also announced with a poster at the airport.

## 6.4 Viability

The Amsterdam Institute for Molecules, Medicines and Systems is one of the Interfaculty Research Institutes at VUA. It resulted of a merger of the Departments of Chemistry & Pharmaceutical Sciences (CPS), Molecular & Cell Biology (MCB), and the Bioinformatics Group (IBI-VUA). In 2017, also the Department of Environment & Health joined. AIMMS is headed by a Management Team composed of a Scientific Director, the heads of the three Departments, and the upcoming Scientific Director. From the very beginning on the Management Team followed a clear strategy towards scientific excellence, which is also exemplified by the termination of two groups in CPS which did not get top scores by international chemistry review committee. As all other institutes, also AIMMS was harmed by the non-merger of the Science Faculties of VUA and UvA, mainly with respect to the enormous waste of time spent for preparing the merger. However, due to its very solid strategy and vision towards a translational chain from molecule to disease, there is no need for reorganising AIMMS due to the non-merger. With the new O2 building, AIMMS is excellently equipped for the near future. The groups will come even more closer together, which is already actively facilitated by e.g. O2 lunches and O2 core facility days.

The only risk for maintaining AIMMS as a world-leading top research institution in the field of life sciences is the financial independency of the departments. Legally, the money provided by the university is directly assigned to the three departments. However, the departments expressed their strong intention to fully merge into one department (working title Chemistry & Molecular Life Sciences), which will mitigate this risk and provide a viable and stable organisational structure.

The management group was very coherent across the different departments, which e.g. is shown by joint selection committees for vacant positions, funds for joint PhD students, and a joint valorisation strategy. Also, the number of staff (204 research staff) and funding is provided on an AIMMS level only. Thus, it is difficult to differentiate the viability for the two (yet) individual departments under evaluation (CPS and MCB). Both department heads

expressed the strong will to merge into one organisational unit. Already now all decisions related to funds and positions, as well as the overall strategy are made in the AIMMS Management Team, which is composed of one director and the three department heads.

## 6.5 PhD programs

In 2015, AIMMS established a single Graduate School for all AIMMS PhD students, which includes a Training and Supervision Plan. However, although the regular time for pursuing a PhD is 4 years, more than 50% of the students need more than 6 years to graduate. Comparing to international standards, this is too long and should be reduced. The management team is aware of this and started several activities to overcome this problem: (i) a bonus of €1500 for those who submit their thesis within 4 years and 3 months, (ii) instalment of a PhD committee which regularly participates in the meetings of the management team, (iii) midterm evaluation of the thesis progress, and (iv) re-discussion of the publication requirements for PhD theses (2 accepted and 1 submitted manuscript).

Generally, the PhD students like the true collaborative spirit in AIMMS, as it offers them the possibility to work in interdisciplinary teams. Several of them were funded by AIMMS internal grants for joint PhD positions between different research groups. This is seen as an excellent initiative to foster collaboration and to bring different scientific disciplines close together.

## 6.6 Research integrity

Management, staff, and students are aware of the importance of scientific integrity. Since 2015, every PhD student has to attend a mandatory course on scientific integrity and to sign the code of conduct. In case of conflicts, there are University wide mechanisms in place. In addition, the Director of the Study Program serves as first contact point. With respect to sustainability of data and protocols, several groups are running electronic lab books. The Management Team is also very well aware of the importance of data management and data stewardship and appointed a data manager, who is in charge for development and implementation of an AIMMS wide research data and management plan. This includes concepts for making the data FAIR, testing the viability of new data management technologies, and keeping links to the Amsterdam Data Center.

## 6.7 Diversity

With respect to nationalities, staff and students at AIMMS show impressive diversity with a total of 42 nationalities working at AIMMS. However, with respect to gender diversity, AIMMS unfortunately shows the same misbalance as observed in comparable institutions throughout Europe. While at the level of technicians, 56% are female, this drops to 12% for staff. The management is fully aware of this issue, and made considerable effort to overcome this misbalance, by e.g actively stimulating careers of female scientists by utilising the NOW-Aspasia program. Furthermore, search committees for new professors include at least two female members (VUA policy). It is strongly advised to make the maximum

possible efforts to recruit top level female scientists for the two vacant positions in order to reach the University wide goal of 25% female scientists in 2020.

## 6.8 Conclusion and recommendations

The committee was impressed by the true collaborative spirit at all levels at AIMMS, which, together with several top level individual scientists, definitely contributes to the outstanding scientific excellence of AIMMS. Transition from the retiring Scientific Director Nico Vermeulen to his successor is very smooth as Bas Teusink is already also a member of the management board. With respect to branding, AIMMS still suffers a bit from the fact, that several PIs were previously part of LACDR, the Leiden-Amsterdam Center for Drug Research. In addition, not all publications mention AIMMS as affiliation, as the researches are legally still affiliated to the individual departments. However, when the merger of the three departments has been finished and AIMMS is transformed to one organisational unit, this should no longer be a problem.

### *Recommendations by the committee:*

- Merge the departments into one organizational unit as soon as possible;
- Carefully consider if the name again should be changed (from AIMMS to C&MLS); if yes develop a solid communication strategy for branding the new name;
- Further exploit the chair for science business & innovation to fully capitalize on the huge economic opportunities in the life science area;
- Engage even more in IMI projects; considering the excellence of the institution, it could participate in more IMI and H2020 projects;
- Reduce the duration of PhDs;
- Continue to establish AIMMS internal grants for joint PhD projects, because it is an excellent mean for stimulating collaboration;
- Active search for females for new recruitments on all levels;
- Get more engaged in general societal activities related to pharmaceutical research and its ethical implications;
- Continue to actively work on a coherent data management strategy; maybe establish AIMMS wide electronic lab books, which might also foster further collaborations.