



EMBL Structural and Computational Biology Unit Review

The EMBL Structural and Computational Biology Unit was reviewed on 15 to 17 May 2018 by a panel of 16 international experts, including seven members of the Scientific Advisory Committee (SAC). The review was chaired by Jan Löwe, MRC Laboratory of Molecular Biology, Cambridge (UK). The Chair of SAC Paul Nurse and the EMBL Director General Elect Edith Heard attended the review as observers.

Evaluation Summary

EMBL's Structural and Computational Biology Unit currently comprises 11 group leaders, three team leaders and Heads of Unit Peer Bork and Christoph Müller. The Unit is employing an array of integrated structural, biochemical, genomics and computational approaches to investigate the structural and functional organisation of molecular networks. The panel was impressed by the level of integration of the diverse approaches and the unique ability to combine detailed biochemical and structural approaches with large scale genomics and computational approaches.

The overall performance of the Unit, including the quality of research and the training and development of young scientists, greatly impressed the review panel, as did the leadership shown by the Heads of Unit. The Heads of Unit were particularly commended for their open-door policies, their nurturing of young scientists and for generating an environment that encourages excellence. The panel noted that a transition phase was about to begin with five Group Leader departures within the next two years. The panel recommended that the balance between computational approaches and mechanistic/biochemical studies should be maintained and in particular that critical mass in cryo-EM research and training be maintained or increased.

The panel congratulated the Unit members for being highly collaborative, but noted that a few group leaders could benefit from focusing on the most interesting and far-reaching questions raised by their research. The leadership was particularly commended for strategic recruitments and rapid changes that have enabled scientists in the Unit, and within EMBL, to access high resolution and cellular electron microscopy techniques. The Bio-IT programme, coordinated by the Unit, was recognised as a very original and creative approach in both data science training and fostering collaborations across EMBL and partner institutions in the area of IT. Panel members however noted that Bio-IT appeared understaffed.

Several research highlights were identified by the panel as pushing the scientific boundaries of structural and computational biology. These included the work on the potential risk of non-antibiotics promoting antibiotic resistance, a study on the molecular organisation of the inner ring core of the human nuclear pore complex and the structures of RNA polymerase III complexes.

In terms of infrastructure, the panel noted the need for continued investment in the areas of cryo-EM and mass spectrometry. For cryo-EM in particular, more investment is anticipated with the establishment of the new imaging centre and thus the panel recommended a thorough search for experts to run the equipment given the limited number of scientists in the field. Related to the strong cryo-EM activity, the panel members further advised to increase the number of people working on software related to the processing and visualisation of datasets. Spatially resolved mass spectrometry is a promising new area recently recruited to the Unit and EMBL, but will require further investment in equipment and staff to achieve its potential.



Response to the Panel's Recommendations

I would like to thank the panel for their time and effort in reviewing the Structural and Computational Biology Unit. I am pleased with the very positive evaluation of the Unit's performance since the last review and grateful for the constructive feedback. All the group leaders received a detailed evaluation and constructive suggestions from the panel.

The review panel were very positive about the leadership and research performance of the Heads of Unit Peer Bork and Christoph Müller. I take this opportunity to congratulate them for leading by example and creating a highly unusual, creative environment that facilitates original research approaches and collaboration between disciplines.

Some concern was expressed regarding the anticipated departures of five group leaders within the next two years and the potential loss of expertise, especially in mechanistic and biochemical studies, as well as in single molecule microscopy. While I share the panel's concerns, I also agree with their comment that this new phase presents interesting opportunities for shaping the future direction of the Unit. The EMBL model is based on regular turnover and we use such opportunities to explore promising new directions and remain at the cutting edge of quickly-evolving fields. As an example, the last major phase of turnover in the Unit led to the recruitment of three Group Leaders who have turned into leaders in the cryo-EM field.

The panel recommended to maintain this strength in the rapidly growing area of cryo-EM. I agree that cryo-EM is a key technique for structural biology and that it is essential to maintain a critical mass of expertise in this strategic area, in particular with view to the future EMBL Imaging Centre that will provide user access to services in cryo-EM. The recent recruitment of Julia Mahamid shows EMBL's commitment to and ability to attract promising young talent in this field. Cryo-EM remains a high priority for future recruitments on both the research and technical sides.

The reviewers also suggested that the Unit would benefit from providing enhanced cryo-EM training. We have started taking steps in this direction by establishing the cryo-EM service platform and by organising specialised practical courses in cryo-EM and 3D image processing. Finally, the panel recommended to increase the number of people working on software related to the processing and visualisation of imaging datasets. This expertise is crucial for several of EMBL's research units and we have recently recruited two group leaders, in Heidelberg and at EMBL-EBI, that focus their work on developing algorithms and machine learning-based methods at the intersection of biology, computer science and mathematics. Support staff in this area, to train non-experts, remains a priority (but see next paragraph).

The panel noted the successful Bio-IT programme and recommended supporting the programme with additional manpower. The Bio-IT programme in its current shape is a fairly recent addition to the Unit's activities and has proven tremendously valuable for computational scientists across EMBL Heidelberg and in the smaller EMBL sites. The Heads of Unit will consider the panel's recommendation in their continuous effort to evolve and improve the support provided to the Bio-IT community, but finding internal funding for this activity given the current constraints on member state contributions to the Indicative Scheme will be very difficult.

The panel also made recommendations regarding scientific equipment available to the Unit. With regards to the MALDI imaging platform, the panel considered the current platform as adequate for the work performed to date, but recommended to upgrade the instrumentation available to the group as well as to increase staff numbers. These recommendations have been noted.



In summary, I would like to congratulate all Unit members for their performance over the last review period and give credit to Peer Bork and Christoph Müller for providing visionary leadership.

A handwritten signature in blue ink, appearing to read "Iain Mattaj", is written over the typed name and title.

Professor Iain W. Mattaj, FRS, FMedSci
Director General

19 June 2018