HIFMB NEWS #01/23

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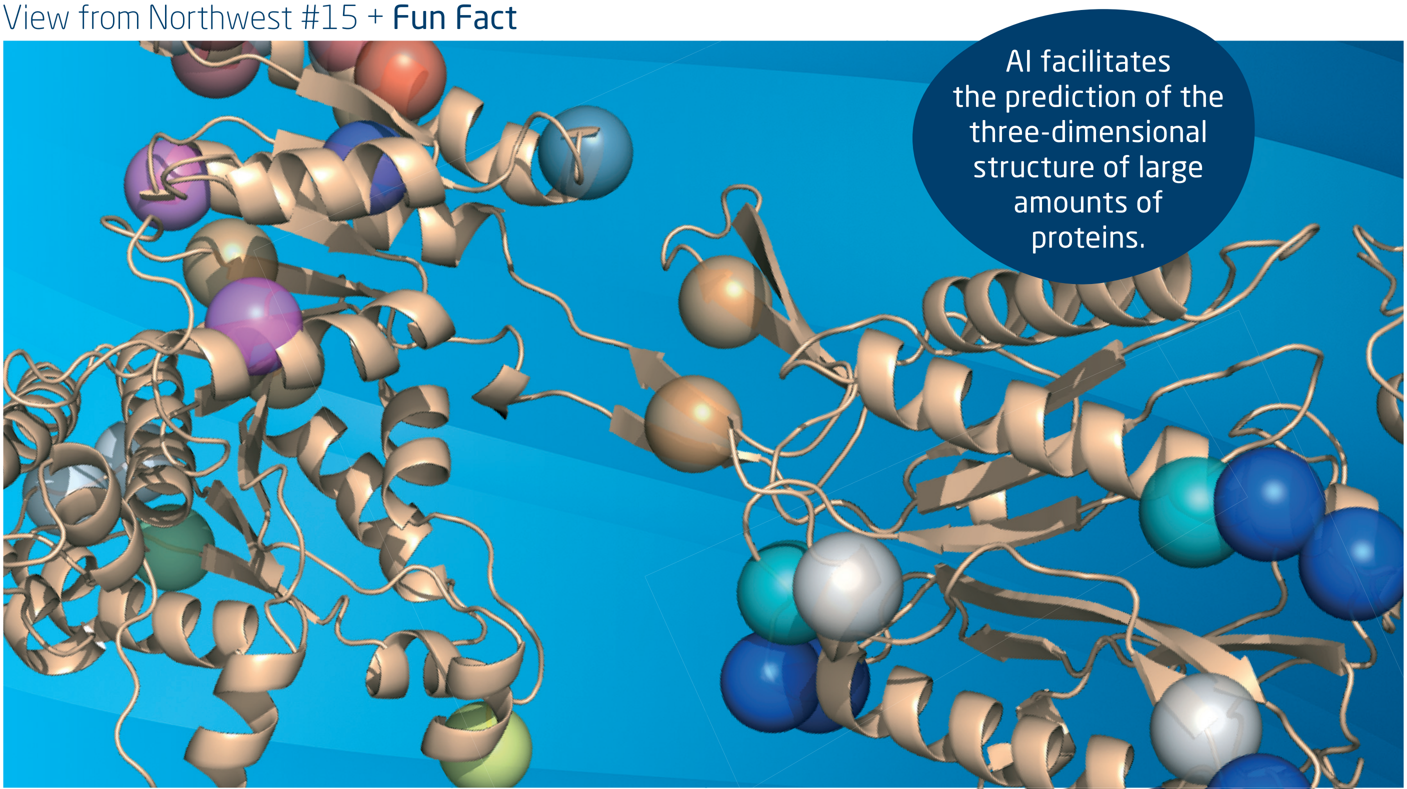


Collage: Mira Antonijevic, © Protein structures: © Delmont & Kiefl et al. (doi:10.7554/eLife.46497).

TOP STORY

Artificial Intelligence and the Evolution of Proteins

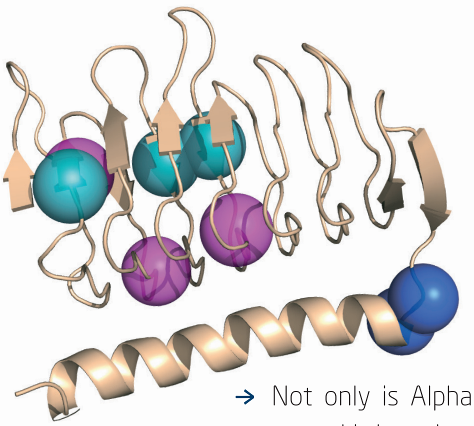
Artificial Intelligence (AI) has become an increasingly significant topic in today's society and science. AI is a computer technology that simulates intelligent human-like behaviour, such as reasoning, learning, and problem-solving. The application of AI has been rapidly advancing, and it has transformed many aspects of our daily lives. From healthcare and finance to transportation and entertainment, AI is being used to streamline and enhance the way we live and work. One question that arises when discussing the role of AI is the extent to which it can be used in the creative arts. The intersection between AI and artistic expression is a complex and fascinating area of study, with many artists exploring the possibilities of AI to create new forms of art. In this context, the importance of AI lies in its potential to revolutionize not only the way we live but also the way we think about and create art.

The paragraph you have just read was not written by a human, but by ChatGPT, a chatbot powered by AI. ChatGPT was asked for an introduction to artificial intelligence and its impact on artists as more AI-generated pictures, paintings, and drawings can be found online, sparking conversations about the role of AI in society.

The use of AI in science is also widespread. For example, it is applied in a program called AlphaFold, which was released in 2021 and was rightfully described as a "transformative" step forward for multiple fields in the biological sciences. AlphaFold is a tool to predict the three-dimensional structure of proteins, a very challenging and computationally-demanding task. →

» With the massive amount of data generated by metagenomic studies, we are able to resolve subtle genetic variations in natural populations. Making sense of these genetic variations is more challenging than it seems. «

Florian Trigodet, microbiologist in the Ecosystem Data Science group



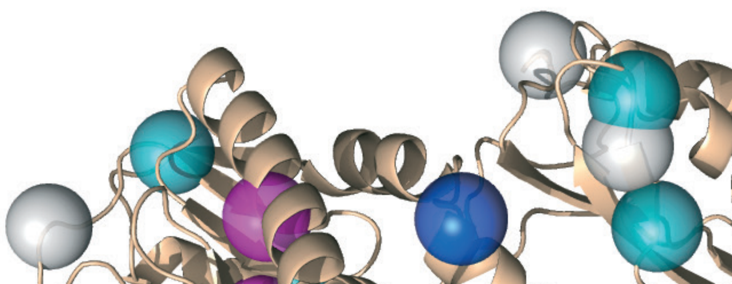
→ Not only is AlphaFold fast, but it is also very accurate, and it has already enabled scientists to study a massive set of proteins for which we had no predicted structures until now: in 2021, there were around 180,000 protein structures validated from lab experiments for hundreds of millions of proteins in publicly available databases. By making so many new protein structures accessible, AlphaFold has become a powerful new tool for scientists studying genomic diversity.

When we study the genomic diversity of microbial populations, we often observe variations within a single population and between samples. And while some variations can be due to random events, others follow selective pressures that we want to study to understand the ecology and evolution of these populations. With the massive amount of data generated by metagenomics studies, we are able to resolve subtle genetic variations in natural populations. Making sense of these genetic variations is more challenging than it seems. Variations at the gene level can sometimes have consequences at the protein level. While proteins can be represented as linear sequences of amino acid residues, they become functional by acquiring their final three-dimensional structure through a process called protein folding. It is important to note that not all amino acids are essential for the final structure and function of a protein. Some amino acid residues will end up in the center of a globular protein and any changes to these residues could be dramatic and prevent the proper folding of the protein. Other amino acid residues are closely associated with the protein function by being physically near or at a ligand binding site.

The Ecosystem Data Science group is also closely following this revolution and in fact we took advantage of AI by leveraging the tool AlphaFold for the study of microbial life. Kiefl et al. have investigated the genetic diversity of the most dominant microbial clade of the surface ocean: SAR11. They analyzed metagenomes from the TARA ocean sequencing project and for each of several important proteins, they reported genetic variations in the context of the protein's predicted 3D structure for a lineage of SAR11 across the world. They found a strong selective pressure against variants occurring at the center of the folded protein and near its ligand binding site, two regions respectively associated with the conservation of stability and function of a protein. With this study, they have shown that microbial ecology does not have to be constrained by sequence only, and demonstrated that we can now investigate genetic variants with structural bioinformatics tools.

Remember the first paragraph written by ChatGPT? The conclusion about AI in art may also apply to the scientific realm: We use AI to create new tools and open new doors, but in the process, it also changes the way we do and think about science.

Reference: Kiefl E, Esen O C, Miller S E, Kroll K L, Willis A D, Rappé M S, Pan T, Eren A M. (2023). Structure-informed microbial population genetics elucidate selective pressures that shape protein evolution. *Science Advances*. 9(8).
doi.org/10.1126/sciadv.abq4632



COLLABORATION

Knowledge Hub on Potential of Nature-based Solutions

In the context of its 'BiodivClim' ERANET COFUND Action supporting research on biodiversity and climate change, Biodiversa+ is establishing a pan-European Knowledge Hub tackling the following topic: "Potential of Nature-based solutions for mitigating and adapting to climate change". The BiodivClim Knowledge Hub, which kick-started its work on the 8th 9th of February is a thematic network consisting of selected researchers with expertise on biodiversity and climate change interlinkages.

Photo © Ute Jacob

COP15: Artist unkown

The knowledge hub will contribute to the integration and sharing of knowledge, research and technological excellence, data and modelling tools, as well as implementation of training and capacity building activities for researchers to increase the capacities of the research community in the field of biodiversity and climate change. It will also improve communication and networking between researchers and stakeholders to enhance research impact and knowledge transfer towards policy and society.

The BiodivClim Knowledge Hub will take the form of a dynamic 'community of practice' and will be composed of two task forces addressing two main objectives:

1. Enhancing research collaborations, knowledge and data sharing and academic outputs and

2. Support science-policy/science-society interfacing to increase the impact of funded research

TRANSFER

New Transfer Office for Marine Biodiversity Change

There is an urgent need to turn scientific data and information into effective action. This requires a dialogue and service-oriented knowledge transfer that responds to stakeholder needs and provides opportunities to bridge the gap between scientific knowledge and action and build bridges across sectors. At HIFMB, we aim to address this challenge by establishing a central point of contact and coordination for stakeholders from science, policy and society to identify transformative pathways to achieve SDG14 and ultimately to effectively conserve marine biodiversity.

Further, the transfer office develops statistical methods for biodiversity analysis and advises on meaningful biodiversity indicators and applies these to a variety of temporal and spatial data from national and international monitoring programmes and projects.

More about the Transfer Office at
hifmb.de/transfer

RESEARCH

Climate Change Disrupts Core Habitats of Marine Species

If climate change continues at the current pace, a majority of marine species will likely lose considerable amounts of their currently suitable habitat ranges by the end of this century. This is the result of a modelling study by an interdisciplinary team of researchers of HIFMB, AWI and GEOMAR.

The researchers based their modelling efforts on occurrence data of more than 33.500 marine species and seven environmental factors such as water depth, water temperature, salinity, and oxygen concentration. Based on this information and assuming three different CO_2 emission scenarios the team estimated whether and where the species, are likely to occur in the future.

The results indicate that species' so-called core habitat ranges – that is the marine area in which chances are higher than 50 percent that a particular species occurs based on its preferred environmental conditions – may not only shift but may also be considerably reduced in case of the high CO_2 emission scenario. In addition to habitat loss, the results give an idea about how the preferred habitat area of many species may be disrupted. Especially along the equator, the model projections reveal areas which are ill-suited for most marine species, for instance because of high temperatures. If such regions developed in the future this would disrupt currently continuous equatorial habitat ranges. Fragmented habitats lead to smaller population sizes which can put species at higher risk to go extinct. However, in the long-run new species could also develop. Another problem is that species can only keep pace with changing environmental conditions to varying degrees. This can lead to a restructuring of food webs and changes in the interactions between habitat-forming species, such as corals, and their inhabitants.

Even though the model does not account for interspecific interactions, the results provide valuable clues on how differently marine environments and communities are likely to change depending on the future CO_2 emission scenarios. Being aware of such a high risk of a fundamental reorganization of marine life will pose further challenges to conservation management.

RESEARCH

Top Recent Publications

Molla N, Delonno J, **Gross T**, Herman J. (2022). Governing change: a dynamical systems approach to understanding the stability of environmental governance. *Earth System Dynamics*. 13(4):1677-1688. doi.org/10.5194/esd-13-1677-2022

Striebel M, Kallajoki L, Kunze C, Wollschläger J, Deininger A, **Hillebrand H**. (2023). Marine primary producers in a darker future: a meta-analysis of light effects on pelagic and benthic autotrophs. *Oikos*. doi.org/10.1111/oik.09501

Hodapp D, **Roca IT**, **Fiorentino D**, Garilao C, Kaschner K, [...] **Brey T**, Froese R. (2023). Climate change disrupts core habitats of marine species. *Global Change Biology*. doi.org/10.1111/gcb.16612

Franke A, **Peters K**, Hinkel J, Hornidge A, Schlüter A, Zielinski O, Wiltshire KH, **Jacob U**, Krause G, **Hillebrand H.** (2022). Making the UN Ocean Decade work? The potential for, and challenges of, transdisciplinary research and real-world laboratories for building towards ocean solutions. *People and Nature*. doi.org/10.1002/pan3.10412

Gutt J, Arndt S, Barnes DKA, Bornemann H, **Brey T**, [...] van **Opzeeland I**, [...] **Teschke K**, et al.(2022). Reviews and syntheses: A framework to observe, understand and project ecosystem response to environmental change in the East Antarctic Southern Ocean. *Biogeosciences*. 19(22):5313-5342. doi.org/10.5194/bg-19-5313-2022

+ More on Google Scholar: scholar.google.de/citations?user=uCoLTyAAAAAJ&hl=en

VIEW FROM NORTHWEST #15

The (Un)happy (Global Change) Ecologist

Most of my current research happens in an explicit context of global change as I aim to understand how humans transform biodiversity and what this transformation means for ecosystems and humans. This is true for much of current ecology, as a quick search across 5 major ecological journals over the last 10 years (>11,000 articles) shows: more than a third explicitly referred to global change pressure in the title or abstract (>4,000). It's a fair guess that even more refer to these pressures in the text. So global change ecology is mainstream – but it does not mean that doing such mainstream global change research leads to being a happy ecologist.

When I started studying biology, I was not doing so because of environmental concerns but because I wanted to understand fundamental rules of life. I quickly fell in love with the breath-taking complexity of ecological systems. Throughout most of my PhD and postdoc I developed an ongoing fascination about how organisms balance their energy and matter requirements, and how they optimize growth over mortality. Biodiversity came into the play as an emergent property arising from these strategies and the way organisms interact. My pet system were benthic microalgae, beautiful but small organisms that are certainly not the mainstream case of "biodiversity". Every new study felt like a treasure box as so little seemed to be known and so much insight emerged.

Neither global change nor humans played a role in this fascination. If possible, I would have worked on pristine systems, the only problem being that there were none. Coastal ecosystems are among the most human-dominated ecosystems on Earth as they are affected by both marine (fisheries, shipping, pollution) and terrestrial (agricultural run-off, tourism, coastal protection) use forms while they experience exceptionally high rates of climate change. So I became more and more part of a community of researchers that tried to understand and predict the consequences of these anthropogenic pressures. But this shift was born out of necessity, not by fascination, and in some darker moments I would like to go back to simple studies of "why does this ecosystem work like this" rather than "how can we prevent that impact". From many conversations, I know that especially early career researchers feel these pressures even more strongly as they experience high levels of urgency. Compared to my naïve beginnings, I do not envy their start into science but hope they find their treasure box to become happy ecologists despite doing global change ecology.

Therefore, I also feel quite strongly about frequent statements that scientists intentionally overblow the dimension of anthropogenic global change to secure funding or positions or earn merits or even money. First, these statements are wrong on many levels: Scientists tend to be rather cautious and balanced in their conclusions, a scientist's wage at least in our system does not depend on what they write, and the best way to secure a position in science is to be unique rather than mainstream. So doing what everyone else does is not a good advice to early career scientists. Second, I am perhaps not alone in stating that I never wanted to be a global change ecologists, it just happened as a consequence of being an ecological scientist in post-pristine times. There is simply no ecology left that can be studied without this context. I wonder how many scientists share this feeling of trading happiness for relevance. If you want to share your thoughts, you find a quick survey (<5 min) here: hifmb.de/un-happy

Sincerely, Helmut Hillebrand
Director – Professor of Pelagic Ecology
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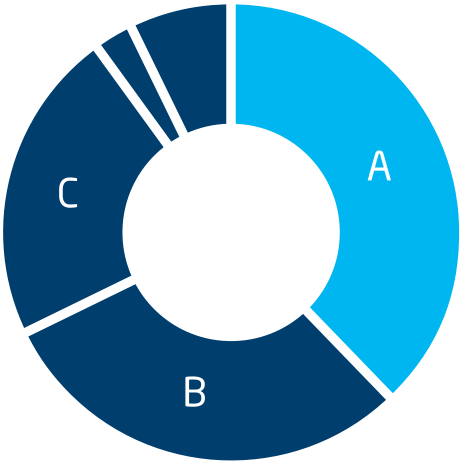
HIFMB TEAM

Fun Fact*

How good are your cooking skills?



A	38 %	With me, full bellies and satisfied faces are guaranteed.
B	30 %	When I do cook, it's always the same dish but it tastes good.
C	22 %	I can tolerate my food.
D	2 %	Fire hazard in the kitchen!
E	8 %	Where is the take-out menu?

* answered by HIFMB employees

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