

Broad technology area on which the group is working

#	Name of the group leader	computational engineering and data sciences	molecular biotechnology	mechanical engineering	imaging and optical engineering	Specific technology fields relevant for each group			Life Science fields to which the group applies technologies			What is the group currently working on and what are the plans for the future
1	Julia Mahamid, EMBL Heidelberg	X		X	X	imaging, microscopy	automation	software development	biophysics	structural biology	computational biology	Cellular cryo-electron tomography (cryo-ET) is the only method available for obtaining in situ structural information across scales - from whole cells to individual macromolecules. Fellows in the ARISE program can engage in any of the following developments of innovative technology solutions to advance in-cell cryo-ET to a higher level of robustness: engineering and 3D microprinting of tailored specimen carriers, correlative (super-resolution) light and electron microscopy, automation of cryo-focused ion beam thinning and lamella lift-out, advanced software development for computational analysis. We are engaged in a large number of internal and external collaborations that lend our expertise to a wide range of biological questions, and work with industry partners for instrumentation development.
2	Christoph Müller, EMBL Heidelberg	X		X	X	automation	data management	imaging, microscopy	biophysics	drug design	structural biology	Our group is pioneering the use of single-particle cryo-EM in the drug discovery process. Through the ARISE program we plan to develop a stable workflow for the high-throughput screening of ligand binding to drug targets by single-particle cryo-EM. Critical elements of the workflow comprise sample tracking throughout the workflow, automated EM grid dispensing, automated cryo-EM sample evaluation and HTP processing.
3	Gergely Papp, EMBL Grenoble	X		X	X	automation	image analysis	software development	drug design	structural biology		The EMBL Grenoble Instrumentation team develops methods and instruments for Macromolecular X-ray crystallography and Small Angle X-ray Scattering experiments for more than two decades. Furthermore, motivated by the increasing scientific interest in Cryo-Electron Microscopy in the last decade, a project for automated Cryo-EM sample grid preparation and control (EasyGrid) has been conducted. The team is composed of highly motivated mechanical, electronics and software engineers, and is able to design and manufacture in-house high precision, complex scientific instruments. Scientific projects exploiting these machines and pushing them to their limits are essential to keep the activity of the team at the state of the art.
4	Robert Prevedel, EMBL Heidelberg	X		X	X	automation	imaging, microscopy	software development	biophysics	developmental biology	neurobiology	We are developing advanced optical imaging methods that are based on multi-photon microscopy, active wave-front shaping, photo-acoustics as well as high-resolution spectroscopy. Our aim is to establish our new approaches as disruptive technologies in the life sciences and to further engineer and automate our prototypes for routine service provision.
5	Yannick Schwab, EMBL Heidelberg	X		X	X	automation	imaging, microscopy	software development	cell biology			The Electron Microscopy Core Facility at EMBL is committed to provide access to state of the art methods in cellular electron microscopy to a large user base from EMBL, its member states and beyond. Besides advanced methods for ultrastructural analysis, the EMCF is specialized in CLEM, in volume SEM and has recently developed workflows for high throughput TEM tomography data collection.
6	Alvaro Crevenna, EMBL Rome			X	X	automation	image analysis	imaging, microscopy	epigenetics	tissue biology		As the head of microscopy, I am using my expertise in optics, programming and image analysis for two purposes: a, to further develop imaging technology; and b, to establish complex platforms such as spatial transcriptomics, tissue profiling and correlative X-ray imaging/super-resolution microscopy. I aim at bringing these services for the wider European research community through academic or industry collaborations.
7	Kristina Haase, EMBL Barcelona			X	X	image analysis	imaging, microscopy	microfluidics	biotechnology	translational research	disease modelling	Our group develops human disease models using primary and iPSC-derived cells and by in-house design and fabrication of novel microfluidic chips. Development of these models and associated assays (image-based and biological) are employed for vascular tissue engineering, drug development, and stem cell therapy applications and are at the core of our research. We interface with industrial and clinical partners to develop these models for practical real-world applications.
8	Simone Mattei, EMBL Heidelberg			X	X	automation	image analysis	imaging, microscopy	biophysics	cell biology	structural biology	Our team is part of the EMBL Imaging Centre, a new service unit with the mission to make the cutting-edge electron and light microscopy technologies available to the scientific international user community, including academically developed methods not yet commercially available. We develop methods and software supporting cryogenic correlative light and electron microscopy (cryo-CLEM) and high-throughput fully automated pipelines to tackle the current challenges in cryo-EM sample preparation and screening.
9	Rainer Pepperkok, EMBL Heidelberg			X	X	automation	imaging, microscopy, image analysis	microfluidics	bioinformatics research	biophysics	cell biology	The ALMF and Pepperkok Team at EMBL Heidelberg develop and provide a service in advanced light microscopy and image analysis methods to EMBL scientists and external users from and beyond EMBL member states. Currently we are working on projects developing technology to provide a service in spatial multi-omics/phenomics to integrate automated phenotype recognition in complex biological samples by advanced light microscopy and online image analysis to sort the phenotypes for subsequent (single cell) multi-omics analyses.
10	Eileen Furlong, EMBL Heidelberg	X			X	bioinformatics, software development	data science and big data	image analysis	computational biology	genome biology	tissue biology	The Genomics Technology Development (GenTechDev) Team develops a range of state-of-the-art spatial, multimodal single-cell genomics technologies (e.g. Seq-FISH+) to advance genomic research throughout EMBL, building on our rich expertise in cutting-edge single-cell genomics technology development and imaging. The GenTechDev team work closely with EMBL's core facilities to support users throughout EMBL with their experimental design, technology development and initial data analysis, helping EMBL scientists to stay at the forefront of developments in single-cell (spatial) genomics.
11	Anna Kreshuk, EMBL Heidelberg	X			X	AI and machine learning	image analysis	software development	cell biology	developmental biology	structural biology	Kreshuk Lab develops novel machine learning-based methods for microscopy image analysis, in collaboration with both internal and external scientists. To make such methods accessible to scientists without computational expertise, we also develop and maintain the ilastik software, used by thousands of biologists all over the world.
12	Jonas Ries, EMBL Heidelberg	X			X	image analysis	imaging, microscopy	software development	biophysics	cell biology	structural biology	The Ries group develops superresolution microscopy methods based on single-molecule localization microscopy (SMLM) and MINFLUX. With new optical and computational approaches, we push the resolution of microscopy towards the nanometer scale to enable imaging the structure and dynamics of multi-protein machines in cells.
13	Matthew Hartley, EMBL-EBI Hinxton	X			X	data standards	software development	imaging, microscopy	bioinformatics research	computational biology	cell biology	I have worked at the interface between computational BioImaging technology development and service provision for the last decade. Over that time I have developed novel image analysis algorithms tools and pipelines as well as image data management software. I now lead the BioImage Archive (BIA), which provides services to the global BioImaging community. We work on image archival, visualisation, file formats, data models and data compression as well as AI and machine learning application to large image datasets. We provide services to life sciences researchers wishing to archive their image data across the world. Scientists using the BIA ecosystem number in the hundreds.
14	Timo Zimmermann, EMBL Heidelberg				X	image analysis	imaging, microscopy		biophysics	cell biology		In the new EMBL Imaging Centre the Zimmermann Team will provide a wide range of light microscopy instrumentation that is not yet commonly available to external researchers. We also aim to efficiently connect highest resolution LM approaches (including cryo-fluorescence) to the corresponding EM technology offer of the Imaging Centre.
15	Cornelius Gross, EMBL Rome				X	Image analysis	imaging, microscopy	optical instruments development	neurobiology			We have worked closely with the Prevedel group to apply innovative deep brain imaging technologies for use in behavioral circuit neuroscience applications. Via the ARISE programme we are looking to recruit outstanding postdoctoral fellows who are committed to focusing on technology that can be taken up and used successfully by the wider behavioral neuroscience community. Following the model we have used in the past collaborating with the Prevedel Group to adapt novel three photon microscopy and adaptive optics approaches to in vivo deep brain imaging in mice, we expect the ARISE fellow to push the boundaries of novel deep brain imaging technologies, adapt and establish them for use in living animals, and develop them for distribution to the wider behavioral neuroscience field.

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16	Andrew McCarthy, EMBL Grenoble	X		X		automation	chemistry and chemical biology	data management, software development	biophysics	drug design	structural biology	The McCarthy team is composed of engineers and scientists who provide operational and user support on seven high brilliance X-ray based structural biology beamlines with proven expertise in developing automated data collection instruments and methods in collaboration with our colleagues at the European Synchrotron Radiation Facility (ESRF). We will continue to optimise data collection protocols and analyses methods as well as develop and expand the experimental instruments and techniques currently available in order to realise the scientific potential of the recently completed ESRF-Extremely Brilliant Source upgrade for the European structural biology community.
17	Jan Korbel, EMBL Heidelberg			X		automation	robotics		computational biology	genome biology	translational research	Dr. Korbel has contributed key experimental and computational methods for structural variation characterization to the field some of which have become the standard methodologies used in genetics and disease biology, such as the development of paired-end mapping, which Science Magazine considered as one of the scientific breakthroughs of the year 2007. Recently, we developed the scTRIP method (for single cell tri-channel processing) which – for the first time - enables the scalable and direct detection of SVs including de novo SV formation processes in single cells, and as such can be used to obtain insights into important pathomechanisms acting in human tissues. Currently, we are sharing this technology with collaborators within international research studies, but the amount of collaborative sharing we can pursue in a pure research setting has become a limitation – which in our view will necessitate to provide the technique as a service. We currently see exponential growth of the use of Strand-seq, with 10 laboratories having used the technique this year in collaboration with us (until ~18 months ago all the Strand-seq publications came from only a single lab) and a strong upwards trend with many new expressions of interest, as a number of applications from comprehensive single cell sequencing of genetic variation to single cell multi-omics and haplotype-resolved genomic assemblies (see above) have been described by us and some of our collaborators. In July 2020, Jan Korbel took on the role of Head of Data Science at EMBL Heidelberg, and this position will have both a research and a service remit.
18	Vikas Trivedi, EMBL Barcelona			X		automation	high-precision mechanics	robotics	biotechnology	translational research	Tissue engineering	Trained as an engineer (focus: mechanical engineering and bioengineering), I switched to optics and instrumentation during my PhD where I developed 2-photon light sheet imaging based methods for deep and fast imaging. Current technological focus of my group is development of novel embryonic organoids and high-throughput, long term monitoring of such in vitro systems and therefore demands automated systems for protocol optimization and molecular characterization through staining, all of which can be provided as services to labs both within and outside EMBL as well as in industry.
19	Justin Crocker, EMBL Heidelberg			X		automation	microfluidics	robotics	biotechnology	developmental biology	Planetary biology	Our group builds automation and robotics pipelines for high-throughput developmental biology. We build experimental frameworks that will serve as platforms for future research by allowing a broader community of users to build, execute, and share similar technologies.
20	Maria Garcia, EMBL Hamburg	X	X			bioinformatics	chemistry and chemical biology	computational modelling	bioinformatics research	biophysics	structural biology	The SPC facility supports external and internal researchers carrying out structure determination experiments and has a strong track record in the development and implementation of new technologies and methods to precisely determine the stability, shape and size of different biomolecules and biomolecular assemblies. We develop our own software for the data analysis of biophysical interactions such as Kinetic analysis, Time resolved conformational changes, Analysis of thermal stability data beyond a simple melting temperature analysis, Ligand screening and Processing of spectral data.
21	Josan Marquez, EMBL Grenoble	X	X			AI and machine learning	chemistry and chemical biology	data management, data science and big data	drug design	structural biology	translational research	Our Team has pioneered the development of Online Crystallography; fully automated protein-to structure pipelines integrating crystallization, synchrotron data collection and crystallographic data analysis into continuous workflows operated via the web. These pipelines are currently used by hundreds of scientists worldwide and are based on the CrystalDirect technologies and CRIMS software, which we have contributed to develop. Recently, we have implemented a fully automated pipeline for ligand and fragment screening to support structure guided drug design. EMBL Grenoble is co-located with the European Synchrotron Radiation Facility (ESRF) in Grenoble, which produces some of the world's most brilliant X-ray beams worldwide. EMBL and ESRF jointly operate six crystallography beamlines one of which is the fully automated MASSIF-1 whose operation is highly integrated with the operations at EMBL's HTX Lab. Our interdisciplinary team offers opportunities for scientists, engineers and software developers to work in one of the leading infrastructures for structural biology within the areas of protein crystallography, drug design, automation, and large-scale scientific data management and analysis. Currently, we are particularly interested in profiles in structural biology or computer science orientated towards one or several of the following areas: fragment screening, structure guided drug design, cloud computing, machine learning and artificial intelligence.
22	Michael Zimmermann, EMBL Heidelberg	X	X			chemistry and chemical biology	data science and big data	software development	computational biology			In combination with EMBL's Chemical Biology Core Facility (CBCF) our laboratory combines high-throughput screening and computational approaches to develop tools and pipelines to investigate the mutual interactions between environmental contaminants and biological systems. In this context we are currently establishing a platform available to EMBL and Non-EMBL researchers that involves chemical libraries, screening pipelines together with computational tools, software, and data resources that will enable integrative analyses of the impact of environmental toxins on organisms at the molecular level.
23	Matthias Willmanns, EMBL Hamburg	X	X			Automation	chemistry and chemical biology	data management	biophysics	drug design	structural biology	Our group employs an integrated structural biology approach using X-ray based methods, single particle cryo-electron microscopy, biophysical methods and integrative modelling approaches for large protein complexes. Our structures provide rich opportunities to discover function from structure, where many of them aim to resolve mechanisms relevant for infection processes. In the coming years we aim to generate a multidisciplinary metabolomics/structure service platform for determination of turnover mechanisms of specific drugs or prodrugs by different microorganisms. The platform will include establishment of a pipeline for high resolution structures of selected protein-drug complexes in microorganisms, and in-vitro analysis of the enzymatic processing of specific drugs by microorganisms. The platform will thus integrate technologies in structural biology and metabolomics, complemented by microbial genetics and biochemistry, defining the required skill set of the developer we are looking for. All data generated will be stored in a common data base, as a basis for further improving the integration of procedures. The platform will be useful to both future internal EMBL projects specifically from selected transversal themes (especially microbiome, infection, planetary biology) and for our external user community working on drug discovery in industry and academia. This work will build on our previous and ongoing work with Michael Zimmermann research group (EMBL Heidelberg). Previously we jointly discovered a mycobacterial drug target by a combined structure-based and metabolomics approach to be associated with an unexpected catalytic function, when Michael was working as graduate student at the ETH Zurich (Ehebauer, Zimmermann et al. 2015). In an ongoing pilot project with Michael's research group at EMBL, we have initiated a structure-based functional drug transformation project of selected microbiome targets with evidence for specific drug turnover, but lacking any mechanistic insight into the underlying process. At the present stage, the project connects high-resolution structural biology with biochemical and metabolomic approaches, including in vitro enzymology, as well as ex vivo and in vivo functional assays. In a first step, we determine the high-resolution structures of these targets, coupled by the identification of specific substrates suitable for turnover, including established drugs that are processed by these targets. Part of this analysis is the quantitative measurement of binding affinities, as a prerequisite for structure-based binding studies. As binding in enzymatic reactions is generally weak this may require, depending on the specific target, intervention with the active site topography to strengthen binding and to avoid rapid turnover, which would prevent structure-based ligand binding studies as well. Subsequent protein target ligand structures provide then the basis for mechanistic investigation of the turnover mechanism for specific drugs or prodrugs. In a future perspective this knowledge could be further exploited either by protein engineering e.g. using directed evolution approaches or by medicinal chemistry approaches for rational modification and improvement of established drugs. In addition, as this concept is not limited to the characterisation of drug transformation it could be similarly applicable to other metabolites susceptible to microbial enzyme catalysis such as nutrients or environmental toxins.

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24	Jim Sawitzke, EMBL Rome		X			Genetic Engineering	Virology	Molecular biology	biotechnology	neurobiology	Genome Engineering	For internal and external clients the Genetic & Viral Engineering Facility design and construct new viral cargos which can be delivered to cells or mice for labelling, gene editing, epigenetic modification or gene therapy. We are also developing new technologies and methodologies using these viral tools to more rapidly, accurately, and at a higher frequency create targeted DNA changes in a way that is more accessible to a wide range of researchers.
25	Mikhail Savitski, EMBL Heidelberg		X			chemistry and chemical biology			molecular biology	biotechnology	biophysics	Savitski group is closely linked to the Proteomics core facility, with Mikhael Savitski leading both the facility and the group. Infrastructure in the Proteomics Core Facility is centered around state-of-the-art mass spectrometry for MS and LC-MS/MS experiments. This is complemented by chromatographic and electrophoretic systems for protein and peptide separation. The research team uses and develops stability proteomics for understanding the phenomenon
26	Alex Bateman, EMBL-EBI, Hinxton	X				AI and machine learning	bioinformatics	data management	bioinformatics research	computational biology	structural biology	My group provides a wide range of world leading resources for protein and non-coding RNA sequence and families (InterPro, Pfam, Rfam, tRNAcentral & Rfam). We are particularly interested in applying modern ML/AI approaches to enhance our resources.
27	Peer Bork, EMBL Heidelberg	X				bioinformatics	data science and big data	AI and machine learning	bioinformatics research	computational biology	Planetary biology	The computational biology group has developed and is maintaining Web services and resources on (meta) genomics and function prediction with more than 400.000 different users per month. The current focus is planetary biology that includes global microbial sampling and analysis, with needs for (meta) data organisation and visualization.
28	Robert Finn, EMBL-EBI, Hinxton	X				data science and big data	software development	bioinformatics	computational biology	genome biology	Planetary biology	My group focuses on the analysis of the microbes found within the environment or associated with a host organism, such as humans or plants. DNA sequencing technologies have revolutionised modern molecular biology, facilitating large-scale sequencing of microbial genomes. However, concomitant with the data deluge, there is an urgent need to develop robust computational frameworks that enable these genomes to be rapidly and continually collated, compared, and functionally annotated. Capturing this biodiversity and presenting quality reference datasets enables biologists to gain a greater understanding of evolutionary biology and the adaptations microbes have made to enable them to survive in diverse environments.
29	Andrew Leach, EMBL-EBI, Hinxton	X				AI and machine learning	software development	Cheminformatics	structural biology	drug design	computational biology	We develop and deliver world-leading data and informatics resources, including ChEMBL, that enable important practical drug discovery questions to be addressed (e.g. "which target is best for this disease?"; "what molecule should I make next?"; "is this compound likely to be toxic?"). Our work involves leading technologies in cheminformatics, data science, software engineering, machine learning, AI and text analytics (among others) and team members develop skills that are in high demand in industry and academia.
30	Maria Martin, EMBL-EBI, Hinxton	X				AI and machine learning	bioinformatics	data management	bioinformatics research	computational biology		Our work focuses on developing technologies for the delivery of scalable and robust data infrastructures for protein data (SQL and NoSQL databases, programming languages, Graph Knowledgebases, Apache Lucene and Solr search engines, clustering algorithms) as well as developing novel data mining methods for protein function prediction and large-scale data analysis. The team use Deep Learning algorithms for extracting knowledge from biological data and recommendation systems.
31	Johanna McEntyre, EMBL-EBI Hinxton	X				AI and machine learning	data management	data science and big data	bioinformatics research	computational biology		Using machine learning to find information buried in the research literature promises to change the way we do literature searching and more specifically at EMBL-EBI, will help curators add key information to data resources such as UniProt, the PDB, InAct, and Reactome. The Europe PMC publications database provides a rich data source for the development of text mining techniques to extract key entities or assertions, rank article results, or article classification, in collaboration with one more curated data resources at the EBI.
32	Thomas Schneider, EMBL Hamburg	X				software development			biophysics	structural biology		EMBL Hamburg is operating synchrotron beamlines for macromolecular crystallography for several decades. Currently, we are using radiation from PETRA III for which an upgrade to the next generation synchrotron technology is in the planning. For making synchrotron radiation usable for scientific user community we are constantly developing software for controlling high-rate and high-volume data acquisition, automated sample handling, data flows and data evaluation. A large part of this work takes place in international consortia.
33	Irene Papatheodorou, EMBL-EBI, Hinxton	X				AI and machine learning	bioinformatics	software development	bioinformatics research	computational biology		Cellular and organismal phenotypes are described via EMBL-EBI's resources: Expression and Single Cell Expression Atlas, for gene expression; PRIDE, for protein expression. Integration in a single platform of gene and protein expression data is quite challenging, requiring novel analysis (including e.g. artificial intelligence approaches) and/or visualisation techniques for biologists to take full advantage to having gene and protein expression side by side and uncover relationships between gene and protein expression within and across different species, in baseline or diseased conditions.
34	Sameer Velankar, EMBL-EBI, Hinxton	X				AI and machine learning	data science and big data	Information retrieval & relevance ranking	bioinformatics research	structural biology	translational research	Our work is focused on developing a scalable, state-of-the-art, integrated data management and delivery infrastructure for structural biology data (SQL databases, programming languages, Graph Knowledgebases, Apache Lucene and Solr search engines, clustering algorithms). We are keen on deploying machine learning and AI approaches for deriving knowledge from our integrated structural biology knowledge base. Our technology development work also involves better information retrieval and ranking systems and multiscale structural data visualisation tools (https://github.com/molstar) to enable scientific research in both academic and industry settings.

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35	Juan Antonio Vizcaino, EMBL-EBI, Hinxton	X				bioinformatics	data science and big data	software development	bioinformatics research	computational biology	Proteomics	Improving PRIDE's functionality as the world-leading proteomics data repository, and the integration of proteomics data with other omics data types are two key aspects for the team in the near future. This offers the possibility for the fellow to work in different topics (e.g. data analysis, data visualisation, infrastructure, data management practices, etc), depending their background. In the context of data integration, this would involve different data types such as gene and protein expression information (together with Expression Atlas), post-translational modifications (UniProt), and (meta)proteomics data and (meta)genomics sequences (Ensembl, MGnify). Additionally, support in PRIDE for additional proteomics data types (e.g. top down proteomics, non-mass spectrometry methods) is also a key aspect in our future work.
36	Paul Flicek, EMBL-EBI, Hinxton	X				AI and machine learning	bioinformatics	data science and big data	bioinformatics research	computational biology	genome biology	The Ensembl/GENCODE gene annotation, the leading reference annotation in the field of human and mouse genomics, is the fruit of 20 years of collaborative research, involving a broad network of biologists, experimentalists and bioinformaticians across the world who study all facets of gene transcription, through the convergence of a wide variety of experimental datasets (ESTs, RNA-Seq, CAGE, ChIP-Seq, etc) and computational analyses (evolution, motif discovery, etc). Our work is foundational to the majority of human and mouse genomic studies, hence our utmost efforts to reach exceptional accuracy in our annotations.
37	Jan Kosinski, EMBL Hamburg	X				ai and machine learning	computational modeling	software development	structural biology	structure modeling	biophysics	We develop software for structural modeling of macromolecular complexes. Our main software is Assemblin, a pipeline for modeling complexes by integrating data from cryo-electron microscopy, tomography, and other techniques such as crosslinking mass spectrometry. Another program, Xlink Analyzer, serves as a graphical interface to Assemblin and a tool for analyzing crosslinks and models. In the future, we aim at developing more efficient modeling algorithms, improving user interfaces, creating modeling web services, and extending our methodology with recently developed modeling algorithms based on deep learning. These developments will enable new types of software solutions and services in structural biology.
38	Ugis Sarkans, EMBL-EBI, Hinxton	X				data management	software development		computational biology	bioinformatics		Our team builds and maintains the BioStudies database - a resource that facilitates transparent, reproducible science by aggregating and publishing all outputs of a scientific study. This can include pointers to components of data in specialised community resources, as well as data that do not belong anywhere else. BioStudies acquires data via a variety of routes, both pre- and post-publication. The main challenge for us is to find the right balance between the generic nature of this infrastructure necessary to support a wide variety of users on one hand, and the ability to adjust the system to the specific needs of a particular user community, project, or data type on the other hand.