

A FAIR road to a bioAFM databank

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A FAIR road to a bioAFM databank

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30 **The 2020s are characterized by the proliferation of artificial intelligence (AI), a development that,**
31 **while not novel, has been propelled by the recent accessibility of vast quantities of data. To pursue**
32 **this avenue, it is of the utmost importance to create high-quality, open databanks. A number of**
33 **biophysical communities are concurrently engaged in the development of their respective**
34 **databanks and databases. In this commentary, we aim to direct attention toward the initial efforts**
35 **to establish a high-quality databank with atomic force microscopy (AFM) data: bioAFM-DB. There**
36 **are encouraging signs within the community suggesting a shift toward depositing AFM data in**
37 **public repositories. This commentary outlines the current state of this endeavor, its challenges, and**
38 **potential courses of action.**

39

40 Databanks are repositories that gather and store scientific data, thereby enabling the development
41 of databases that facilitate the organization and retrieval of this data. Public repositories have
42 existed for more than 50 years, long before the advent of “Big Data.” One of the oldest repositories in
43 the molecular biology field is the Protein Data Bank (PDB), which emerged from a handful of
44 crystallographers in 1971.¹ Databanks evolve based on available computational infrastructure and
45 changes in the global needs of the research community. Currently, the Registry of Research Data
46 Repositories (re3data.org) contains over 3,300 repository sites^{Suppl. ref 1}, some of which are related to
47 “Microscopy”. For instance, the registry includes extensions of the PDB, such as the Nucleic Acid
48 Knowledgebase;² specialized resources, such as the Yeast Resource Center Public Image Repository³
49 and the Brain Image Library;⁴ and general image repositories, such as the Image Data Resource,⁵ and
50 the BioImage Archive.⁶ Some microscopy-related repositories manage electron microscopy (EM) data,
51 such as the Electron Microscopy Data Bank,⁷ which stores electron density maps, and the Electron
52 Microscopy Public Image Archive,⁸ which provides raw images and 3D cryo-EM maps.

53 Currently, there is no repository for scanning probe microscopy (SPM). SPM is a family of microscopy
54 techniques^{Suppl. ref 2} derived from the scanning tunneling microscope (STM), which was developed in the
55 early 1980s^{Suppl. ref 3}. A prevalent member of the SPM family, atomic force microscopy (AFM)⁹ was
56 developed in 1986 and has become widespread in both material and biological sciences^{Suppl. ref 4}. AFM
57 detects a sample surface with a sharp probe integrated at the end of a flexible cantilever, which allows
58 a spatial topographic map to be obtained at nanoscale resolution and physical properties to be
59 measured^{Suppl. ref 5}. Key benefits of using AFM in life science applications over other types of
60 microscopies include the ability to image biological samples in physiological buffer conditions (i.e., in
61 liquid and at a controlled temperature) and an exceptional signal-to-noise ratio, which enables imaging
62 individual molecules with sub-nanometer resolution in topography^{Suppl. ref 6}. Moreover, AFM allows
63 probing physical properties of biological samples, including active biomolecules, proteins, nucleic acids,
64 biomaterials, living cells and tissues, and obtain stiffness, adhesion or viscosity maps^{Suppl. ref 7}.
65 Development of faster scanning AFM technologies has allowed imaging of biological processes and

biomolecular dynamics down to sub-nanometer spatial and sub-second temporal resolutions^{Suppl. ref 8}. In this commentary, we advocate for establishing a path towards the creation of a bioAFM databank (bioAFM-DB) and the development of its associated databases.

Is now the right time to develop a repository for AFM data? We believe so because AFM has reached a level of maturity and use that was not the case 20 years ago^{Suppl. ref 9}. Specifically, in the last 10 years,

among the average yearly 9000 published articles containing “Atomic Force Microscop*” topics, only 9.2% contained AFM, or its explicit name, in their titles, indicating that it has become a routine biophysical tool. Other signs of maturity include the availability of high-quality, free and open-source software for handling AFM data, such as WsXM^{Suppl. ref 10}, Gwyddion^{Suppl. ref 11}, AtomicJ^{Suppl. ref 12}, FiberApp^{Suppl. ref 13}, SmarTrace^{Suppl. ref 14}, Nanite^{Suppl. ref 15}, Topostats^{Suppl. ref 16}, AutoSmarTrace^{Suppl. ref 17}, dForce2.0^{Suppl. ref 18}, PyFMLab^{Suppl. ref 19}, NanoLocz^{Suppl. ref 20}, CellMAP^{Suppl. ref 21}, and a growing population of AFM analysis scripts at GitHub^{Suppl. ref 22, ref 23}. Furthermore, there is a continuous increase in applications using AFM data in structural biology such as AFM-Assembly^{Suppl. ref 24}, BioAFMViewer^{Suppl. ref 25}, Trace_y^{Suppl. ref 26}, and recently with high-speed AFM films such as tools based on rigid-body fitting^{Suppl. ref 27, ref 28} and flexible fitting^{Suppl. ref 29, ref 30} via normal mode analysis NMFF-AFM^{Suppl. ref 31}, NanoLocz^{Suppl. ref 32}, BioAFMViewer 5.0^{Suppl. ref 33}, and AFMFit^{Suppl. ref 34}. Another incentive for the timing of an AFM data repository is the recent ambition of research institutions and funding agencies to encourage researchers to find, access, interoperate, and reuse scientific data.

Both the USA National Science Foundation (NSF) and the National Institutes of Health (NIH) mandate data sharing as a core expectation of federally funded research. In 2016, the European Commission established the FAIR Data Principles, FAIR being an acronym for Findable, Accessible, Interoperable, and Reusable.¹⁰ These principles establish guidelines that go beyond the common practice of including statements such as “data is available upon request” in publications. The FAIR principles aim at correcting shortcomings in data availability, including missing or incomplete data descriptors, rigid or non-standardized file formats, a lack of data organization and validation, and low persistence of data

91 over time^{Suppl. ref 34}. The FAIR principle acknowledges the effort involved in producing data and the
92 global economy surrounding data access and storage within the research community. The
93 importance of data archiving has been extensively discussed^{10,11,Suppl. ref 35}. Multiple scientific fields
94 are progressing in the FAIR definition of their data such as NMR-based metabolomics data^{Suppl. ref 36},
95 optical tweezers¹² and biomolecular simulations.¹³ The benefits of data archiving include physical
96 access to raw data,¹⁴ which is often different from the processed data found in the supplementary
97 materials of published articles. Data archiving fosters reproducibility in research, conserves
98 taxpayer resources by eliminating redundant research, and maintains public confidence in science.
99 Undoubtedly, the most significant benefit of publicly accessible data is accelerating scientific
100 discoveries by building on available data beyond its original purpose. A paradigmatic example of
101 this is the above mentioned PDB, whose founders may not have anticipated successful reutilization
102 of their data in the prediction tools like AlphaFold2^{Suppl. ref 37} and RoseTTAFold^{Suppl. ref 38} when
103 depositing their experimentally determined X-ray structures. We, as researchers developing and
104 applying AFM to biological and biomolecular systems co-signing this commentary, agree on the
importance of distributing AFM data and support this effort.
105 AFM data sharing would require a certain level of standardization regarding data acquisition, storage
106 and annotation. Several proactive standardization actions should be mentioned. As early as 2010, the
107 issue of AFM data management was raised within a European network on applications of atomic force
108 microscopy to nanomedicine and life sciences (COST Action TD1002). This Action proposed a
109 Standardized Nanomechanical Atomic force microscopy Procedure (SNAP) that improved
110 reproducibility of elasticity measurements^{Suppl. ref 39}. Earlier round-robin experiments pointed towards
111 similar standardized calibration of AFM cantilevers^{Suppl. ref 40}. The SNAP approach was further improved
112 during the Marie Skłodowska-Curie Innovative Training Network Phys2BioMed, by including sample
113 preparation and data analysis standardized routines^{Suppl. ref 41}. Also developed during the Phys2BioMed,
114 effort in standardization continued with a tentative definition of a common text-based AFM universal
115 file format^{Suppl. ref 19, ref 42}. Additional efforts include the establishment of a dataset of simulated-AFM
116 images of small organic molecules^{Suppl. ref 43} or the recent development of a structural biology-

117 compatible file format for AFM^{Suppl. ref 44}. In short, an AFM databank should store the experimental raw
118 AFM data, its accompanying metadata and its related processing steps to improve the reproducibility in
119 this field.

120 Therefore, why does an AFM databank not already exist? The daunting procedural tasks required for
121 developing a strategy to deposit AFM data in a public repository may answer this question. One major
122 hurdle in creating an AFM databank is the wide variety of samples and associated preparation
123 protocols as well as heterogeneity of data types. AFM crosses a range of fields, from physics and
124 chemistry to biology. There is an enormous number of sample types, ranging from mineral materials to
125 biological tissues, from hard to soft specimens, and from conductive to insulating surfaces. This variety
126 of samples correlates with a wide range of measurement modes, from topographic images to force
127 measurements. There is also the possibility of datasets from AFM systems coupled, for example, to
128 optical microscopes^{Suppl. ref 45} or infrared^{Suppl. ref 46} and Raman^{Suppl. ref 47} spectroscopies. Thus, defining the
129 minimum metadata for all these types of samples and information requires a significant effort.
130 Furthermore, there are several AFM instrument manufacturers, including laboratories building their
131 own instruments, each with several models and various levels of historical legacy in their data formats.
132 The FAIR principles cannot be applied to these proprietary formats; therefore, most data from AFM
133 instruments cannot be stored in a database without prior conversion and without a reading tool that
134 ensures interoperability (as found in AFMReader^{Suppl. ref 48}, for instance). Another issue raised by the
135 community concerns data quality, as there are no clear definitions of what constitutes good and bad
136 topographic images or force-distance curves. This issue requires an open discussion among the AFM
137 communities.

138 In retrospect, a possible reluctance to distribute AFM data may originate from a lack of understanding
139 of how and for what "others" who did not produce the data might use it. For instance, a particular
140 group may want to test its developed data processing tools on AFM data from other laboratories. For
141 that, multiple images or force-distance curves of different quality (good, fair, or poor) would be

142 needed. It is, however, unusual that a scientific publication necessitates the deposition of “poor
143 quality” AFM data. A clear advantage of a databank should be the deposition of complete
144 datasets, rather than a couple of images or force curves included in published works.

145 To fulfill the FAIR principle, the bioAFM data repository must adhere to the following constraints:

146 1) A robust infrastructure is required to upload, store and distribute the data (FA).

147 2) A specific ontology should be agreed upon to prepare the minimum informative metadata, both
148 human and computer readable (I).

149 3) Deposited data should contain the minimum information necessary to reproduce and analyze the
150 data; including functional/dedicated open software (IR).

151 4) Data quality must be appropriately annotated (FIR)

152

153 Where do we stand now? Fortunately, the maturity of the AFM field means that this project does not
154 have to start from scratch. A group of volunteers has started working on this AFM metadata. The group
155 officially met before and during the AFM data symposium, which was held alongside the 15th
156 AFMBioMed conference, in Barcelona in April 2025, and advanced in dividing the metadata into
157 subsections: sample, cantilever, experimental conditions, recording parameters and data. The
158 European Bioinformatics Institute (EBI) of EMBL generously oversees these preliminary metadata
159 efforts and is committed to following the development process for the potential integration of the AFM
160 database into the EBI. The EBI's contribution is invaluable to our community because it provides the
161 necessary infrastructure for data deposition, finding, access, dissemination, and visualization. One clear
162 benefit of collaborating with the EBI is its expertise in providing time-based data access through
163 appropriate release.

164 The development of a databank is an ambitious long-term project. While the initial design strategies
165 should be as broad as possible, it is impractical to start the project with every type of AFM data. The

166 project will progress in steps to grow into a full-scale repository. Following the positioning of the EBI in
167 the field of life sciences, the "bio" side of the databank will develop first, and the immediate focus will
168 target three AFM data types: topography, spectroscopy, and nanomechanics. Volunteers are welcome
169 and encouraged to join this initiative by contacting the corresponding authors, and contribution not
170 only from academia but also from the industrial sector will be essential. In addition to the minimal
171 metadata required for deposition, two major topics need further discussion:

172 1) What constitutes a dataset or a databank entry?

173 Several questions arise: which of the experimentally recorded data should be stored in the database?

174 Should the data be linked to a scientific publication? Can large datasets be stored as a single entry?

175 Should all recorded data be deposited or just the relevant data used in the associated publication? Let

176 us take the example of AFM topography. Depending on the experimental imaging mode, several kinds

177 of data are recorded simultaneously, also known as channels (deflection, height, amplitude error,

178 phase signal). Most often with AFM height images, if we ignore the trace and retrace measurements,

179 only a single channel (height) is used. Should it be the only deposited data? Should the accompanying

180 measurements and calibrations be also deposited? How to handle the tip convolution effect in AFM

181 topography? All these details will be discussed and evaluated during the course of establishing this

182 databank and its underlying databases. There is nevertheless a topic of importance for initial

183 deposition in the databank: reference datasets (images, pulling, indenting). These datasets are

184 especially important for standardization efforts in research and in metrology. They should allow for

185 poor-quality, noisy, and diverse AFM measurements of realistic AFM data, which may be valuable for

186 developers of novel AFM data processing tools. In the era of artificial intelligence and machine-

187 learning, the need for extremely large, diverse, and accurately annotated datasets has become even

188 more pressing^{Suppl. ref 9}. Training robust models requires not only raw data but also high-quality ground-

189 truth labels, which are scarce, labor-intensive to generate, and often inconsistent across laboratories.

190 As a starting point, since many journals have policies that require data deposition, the initial data

deposited in the repository could likely be that included in submitted manuscripts. However, there is plenty of room for discussion.

2) Defining the architecture and format of the AFM data files in the repository to allow conversion from a proprietary format to the open repository's format and their import/export tools.

Although any specific data format can be deposited in a databank, a lack of a common format will reduce the effectiveness of AFM data dissemination, both inside and outside the AFM community. It highlights the particular role of file conversion and reading software tools, such as those from Gwyddion^{Suppl. ref 11}, afmformats^{Suppl. ref 15}, Topostats^{Suppl. ref 16}, AFMReader^{Suppl. ref 48}, NanoLocz^{Suppl. ref 20} and PyFMReader^{Suppl. ref 19}. The development of an integrative AFM file format has already begun, as demonstrated by the Universal Spectroscopic and Imaging Data (USID) format developed at the Oak Ridge National Laboratory^{Suppl. ref 49} or the UFF mentioned above^{Suppl. ref 19}. A possible starting point is to deposit raw AFM data and include a tool for exporting and downloading raw data to transform it into manageable data, as AFMReader does. Once again, as a community, it will be important to reach an agreement about a common AFM data exchange file format.

Our ultimate goal is to promote a unified platform, in the spirit of the PDB,¹ to all AFM communities. We will have fulfilled part of our goals if we reach the following three objectives: 1) Disseminate bioAFM data in various biological fields beyond the laboratories that produce it; 2) Improve user education on using bioAFM data, particularly regarding the associated pitfalls; 3) Increase the integration of bioAFM data into other biophysical pipelines, such as integrated structural biology for AFM topography. This platform will include an online AFM data deposition mechanism, appropriate validation of depositions, and a referencing key, such as an entry code or digital object identifier (DOI). In a second stage, improvements will involve interlinking with other databases such as MBDB,¹⁴ MechanoPro-DB^{Suppl. ref 50}, MechanoBase^{Suppl. ref 51}. A possible starting point could be the BioStudies system at EBI.¹⁵ The bioAFM databank will be established through a governance framework that

216 defines usage policies and the ethical implications of using open data. We anticipate reaching a
217 significant milestone in this active development process at a symposium organized alongside the next
218 AFMBioMed conference, in Brno, in 2027.

219 **The development of bioAFM-DB and its related databases is poised to address open questions across**
220 **diverse fields—from single-molecule conformations and molecular binding mechanisms to the**
221 **mechanics of aging, and diseases. By making AFM findings accessible to broader scientific**
222 **communities, bioAFM-DB will enable cross-validation of experimental data with other microscopies**
223 **(such as EM and super-resolution) and biophysical tools (including optical tweezers and**
224 **nanoindenters), as well as with computational models. This integration will further establish bioAFM**
225 **as a standard tool in biophysics and exemplifies the transformative potential of merging biophysics**
226 **and data science, driving knowledge forward through a multidisciplinary approach.**

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