Chemo-, Bioinformatics' and Bioengineering Tools in Heritage Science: Repositories and Vocabularies

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Abstract. In recent years nano-, bio-, info-, and cognitive technologies signed significant advances in improvement the beneficial properties of natural biological objects and the creation of entirely new ones that do not exist in nature. This paper examines some of the IT opportunities developed in this process such as databases, vocabularies and linked data, in view of their potential to enable the transition of heritage science to a fundamentally new line — use of renewable supplies and technologies, modelled in respect to the art works' nature, to ecological and to health save norms.

Keywords: Heritage Science, Chemoinformatic, Bioinformatics, Bio-Engineering, Convergent Technologies.

1 Introduction

Heritage science draws on various humanities, sciences and engineering disciplines involved in the field of creation, conservation, and protection of cultural heritage: from archaeology to artificial intelligence, from art history to physics applied to the study of matter. The knowledge on natural substances it continually integrates from various founts goes back far in the history as arts and crafts have prominently used natural compounds to create and utilize diverse materials, including native substances, semi-synthetic derivatives, and synthetic analogues. Natural compounds have, however, two main drawbacks: limited sources that can cause environmental issues and imperfections like side effects, lack of selectivity, insufficient impact, and excessive cost. This is the primary reason for which, since the postcolonial period, fabrication of arts & craft-, of conservation and restoration materials, are oriented exclusively to synthetic products believed, besides, to assure more durable chemo physical properties against the traditionally used of bioorganic origin. Unfortunately, the widespread use of synthetic materials led to diverse unintended consequences regarding both the artefacts as the people operating with them. Nevertheless, recommendations to avoid using synthetic products for treating artifacts typically made of natural substances to the moment have not been widely adopted.

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At the same time, numerous discoveries in recent decades related to chemistry and reactivity of natural organic materials have not yet been integrated in heritage science. As a result, several theories regarding ancient manufacturing practices are more reliant on anecdotal evidence than on rigorous experimental analysis.

Whenever in the EU area lately have been developed some digital tools like EOSC, GBIF or the international research infrastructure called DiSSCo that aggregate scientific data internationally and help manage the exponential increase in research results, the computational facilities to make multidisciplinary and multilingual natural substances data searchable by computers are highly underdeveloped. Drawing on case studies and LIS literature, this paper recommends chemo-& bioinformatics' repositories and vocabularies useful for heritage scientists studying natural materials in artworks or creating restoration & conservation products. It also highlights gaps in existing vocabularies, affecting the discoverability of bioproducts that are mentioned in technical treatises from historically and economically marginalized regions. The scientific method relies on optimizing, integration and building upon previous results.

2 IT Tools Developed by Chemo- and Biotechnologies: The Actual Eurasian Landscape

In contrast to the domain regarding the artistic heritage, in biology and medicine interest in objects from the plant and animal world arose at the earliest stages of the formation of chemical science and did not weaken but only intensified with its development. Though the 1980s saw a decline in this type of research in favor of more readily manipulated synthetic compound libraries, this trend is reversing. Two fundamentally similar approaches have been formed to date in the search for new pharmaceutical substances: i) a diverse chemical modification of a known medicinal substance followed by a structure–activity study; ii) the formation of new hybrid compounds from two or three native natural compounds with known or potential biomedical properties. Over 70% of new chemical substances introduced into medical practice from 1981 to 2006 were derived from natural products. Given the numerous pharmacological targets and the pleiotropic effects of most natural compounds, databases and analytical tools became essential (Lagunin, 2014). Their mass introduction in the investigative process led to the emergence of chemo- and bioinformatics, burgeoning fields dedicated to analyses and systematizing vast amounts of data about wildlife (Gauthier, 2019). These sciences aim to understand the structure of genomes, including those of "simple" microorganisms and humans, relationships among living organisms, evolution, and homologies in key features. Their objectives include predicting the spatial structure of proteins, decoding DNA structures, and managing biological information through storage, search, and annotation. Additionally, they assist in identifying complementary leads and targets. Nowadays bioinformatics is recognized as an interdisciplinary science that leverages advanced computational capabilities to facilitate new scientific discoveries. The field encompasses any application of computers for processing biological data, with research areas including genetics, metagenomics, OMICs, medical informatics, computational biology, proteomics, phenomics, metabolomics, environmental informatics, and structural bioinformatics. Among the most important centers are the National Center for Biotechnology Information (NCBI, United States National Library of Medicine), National Institute of Genetics (DNA Data Bank of Japan), Swiss Institute of Bioinformatics (SIB: Expasy), Australia_Bioinformatics_Resource BIG Data Center (National Genomics Data Center), Beijing Institute of Genomics (Chinese Academy of Sciences).

Research on plant and animal constituents may be conducted through bioactivity-guided fractionation or random screening of extracts. Currently, new drug discovery mainly relies on bioactive principles from traditional activities for known bioactivities using molecular docking. This leaves many plants and animal constituents with unknown biological activity unexplored. Multi-targeted *in silico* approaches can efficiently investigate their potential across various fields, therefore bioinformatics and systems biology are crucial in studying not only medicinal plants' therapeutic potentials but also solving problems in other sectors such as agriculture, industry, technology, food (Newman, 2007), etc.. In fact, information technology, pharmaceuticals, biotechnology, industry and agriculture are already emerging as principal drivers of bioinformatics. Particularly notable developments are in the fields of software (tools, algorithms, and pipelines), use of high computation power (e.g. by Chinese and Russian Supercomputers), and large-scale sequencing projects (the sequencing of 100000 human genomes). Many of these approaches facilitate lead discovery against individual targets using molecular docking (Yadav, 2010) (Sakthivel, 2013), pharmacophores (Rollinger, 2009), quantitative or qualitative “structure–activity” relationships (Q)SAR), machine learning methods (Yadav, 2012) (Prakash, 2013) and combinatorial approaches. The biotechnological sector itself is a driver for development of the pharmaceutical, medical, food, and agricultural industries and has grown by 30% since 2015. As reported by (Nawaz, 2024), the development of bioinformatics in the Eurasian region remains unclear due to a lack of specific data. From 2023 to 2028, the global bioinformatics market is expected to grow to USD 35.5 billion at a CAGR of 13.6%, based on data excluding Russia (BCC Research, 2023; Csermely, 2013). Major omics research companies like Thermo Fisher Scientific, Illumina, and BGI are mostly located outside Russia. The Program for the Development of Biotechnology in the Russian Federation up to 2030 (BIO2030) had set goals that biotechnology production should be 3% of the gross domestic product by 2030. Russia has also created the Bio Tech 2030 platform for cooperation between education research, and industry in the field of biotechnology.

Creating of unified database for storing, sharing, and retrieving biological data becomes an important part of a country’s research independence. Recently, developments in this regard have been observed in China (Nawaz, 2024) and in Russia (Kolesnikov, 2023). On a smaller scale, India has also initiated Indian Biological Data Centre (Nawaz, 2024). These countries, besides generating biological data and establishing indigenous databases and information systems, in some cases are also creating platforms that could bring together scientists from various disciplines (Csermely, 2013) (Zhao, 2010).

3 Bridging between Heritage Science, Chemo- & Bioinformatics' Resources

Regulations in many EU countries mandate the use of synthetic materials for the conservation and restoration of artistic heritage. This restriction, along with the highly interdisciplinary and intersectoral nature of the heritage science domain, limits the benefits from advances in chemo- and bioinformatics that enhance natural biological objects. Challenges present also the lack of interoperable datasets and user-friendly vocabularies to bridge human, historical, and biochemical sciences. Further complexity arises from the variety of scientific methods applicable to numerous materials implied in art & craft works that do not exactly correspond to those adopted by biochemists. Nevertheless, the significant advances signed in recent years by nano-, bio-, info- & cognitive technologies in improving the beneficial properties of natural biological objects and the creation of entirely new ones require fundamental revision of actual EU heritage protection regulation and strategies. On the background of the immerging new knowledge on natural raw materials (NRM), implementing bioinformatics modules results essential for heritage scientists to remain competitive on a global scale.
The vast common interests between chemo-, bioinformatics, and heritage science can be summarized into four main areas for data sharing and interactive development which are, however, far from being exhaustive:

- New knowledge on structure and properties of the main components and tissues during chemical processing of plant & animal raw materials.
- Improvement of existing and creation of new technologies for chemical processing of NRM.
- Ecology and chemical processing of NRM.
- Composition, structure and properties of low molecular weight substancesincluding physiologically active substances extracted from NRM.

3.1 Recommended Repositories

As demonstrated by Lagunin (2014) in his comprehensive analysis of the latest chemo- and bioinformatics resources for *in silico* drug discovery, data on the biological activity of compounds, including herbal medicines, continue to expand. ChEMBLdb features 1.5 million compounds targeting over 9000 targets. Similarly, the Dictionary of Natural Products contains information on over 226,000 natural products and about 210,000 structures. Databases also provide the botanical name, vernacular name, and traditional uses of plants such as ethno-medicinal plant databases and the PFAF database. These are of particular interest to historians of art technology and developers of new products for conservation and restoration as helpful in identifying yet not deciphered substances from plant or animal origin mentioned in ancient technical treatises (Stoyanova, 2008). Repositories like the Dictionary of Natural Products, TradiMed, and SuperNatural offer insights into the phytoconstituents identified in these plants (Lagunin, 2014) providing valuable phytochemical information and important in discovering of new species containing components useful in arts & crafts that integrate the pool of already known ones like natural colorants, alkaloids, tannins, gums, resins, ferments, surfactants, glycosides, essential and technical oils, solvents, fibers, natural preservatives, mordents, pectin-containing complexes particularly chitin and chitosan, etc. For example, these last, thanks to their unique properties, are widely used in a variety of fields because of the high biological activity and compatibility with human, animal and plant tissues, and because they do not pollute the environment, since they are destroyed by microbial enzymes. On the contrary, most of the currently developed synthetic polymers with a regular service life, except for harmless ones, contain special additives that provide photo destruction; they are usually toxic and capable of polluting both during processing of the material and during its operation and disposal (Andrusenko, 2009). Another example illustrating the benefit of screening and mining these databases represents the microcrystalline cellulose (MCC), the main component of the cell wall of higher plants, which, together with its derivatives is widely employed in many industries (textile, pulp and paper, artificial fibers, food, pharmaceutical, etc.) (Kotel'nikova, 2009). MCC, able to absorb toxins and slags and remove them from the body, is used as a matrix for medicinal products but also as filler, binder, stabilizer of emulsions both in medicine as in restoration, Of particular interest are also the silicon-containing compounds (mainly silicon dioxide, or silica (SiO2•pH2O) extracted from plants, especially as regards non-crystalline phases, which are more chemically active and can be largely used in restoration (Zemnuhova, 2009).

As regards the phytochemistry of natural products, deserve to be taken into consideration databases as the BoDD, Cardiovascular Disease Herbal Database (CVDHD), Chemical Abstracts Service (CAS), Dictionary of Natural Products (DNP) Database, Ethnobotany of the Peruvian Amazon, HerbalThink-TCM, Indian–Russian traditional medicine database, IBS natural product library, KNApSAcK Core DB, PubChem substance database, SuperNatural II database, Traditional Chinese Medicine Information Database (TCMID), TIPdb and TradiMed (Lagunin, 2014). The repositories about traditional ethnical plants can significantly integrate existing knowledge on bioproducts historically applied in arts & crafts, particularly on regard of the thematically, historically and economically marginalized regions as the near and far East, North Africa, the Global South. Historical documents indicate that in ancient times, migrations of Eastern peoples introduced advanced material culture to Europe. This included the establishment of industries and technologies previously unknown to the Old Continent, leading to flourishing commercial exchanges and expanded commodity knowledge. The new products influenced European tastes and inspired imitation, promoting innovation in traditional production methods. During the sixteenth and seventeenth centuries, industries such as glassmaking, enameling, goldsmithing, processing of precious stones, silk and leather production, dyeing, and printing of textiles became prosperous thanks to complex production relationships and trade networks, supporting local economies through periods of crisis and competition. However, despite efforts to adopt Eastern technical knowledge, technological advancements in European states remained inconsistent and limited. By the late eighteenth century, Europeans began developing competitive advantages and producing goods like those from the Levant or Asia. Nevertheless, written and material sources show that innovative productions in Europe relied heavily on the participation of skilled Eastern craftsmen. This was due to the lack of extensive knowledge and traditions required for these technologies and the challenges Europeans faced in identifying and obtaining exotic raw materials used in Eastern techniques (Stoyanova, 2009).

Fig. 1a-b: Close ups of gilt leather wall hangings (Venice, Casino, 16th C.): the optical effects are achieved using plant-based lakes and transparent varnishes made from natural resins and dyes.

CVDHD, TCMID, TIPdb and TradiMed are useful resources of data containing information on both phytochemicals and therapeutic effects. Most databases include information about taxonomy (e.g. The Plant List, Tropicos®), traditional medical usage in addition to photographs of the plants. The main database that may be used for active principles discovery based on traditional medicine is the DNP. The SuperNatural II database and the IBS natural products library, which encompass phytoconstituent structures, are valuable resources for predicting the interactions of specific leads with other plant constituents. This data is crucial for re-evaluating existing theories related to the technology of historical artifacts, such as tanning and dyeing. It is noteworthy that in the ancient manufacture of leather (Stoyanova, 2007), in dyeing and printing of textiles, and ink fabrication, tannins and alkaloids played a significant role, but the mechanisms of complex polycentric reactions involving polyfunctional molecules with specific stereochemical selectivity have not been fully understood (Stoyanova, 2016). For example, the tea, *Camellia sinensis L.,* largely used in some painting techniques, has over 45 species, each with around 2000 constituents like tannins, oils, alkaloids, and dyes, some of which are not yet fully identified leads. The tea leaves contain alkaloids such as theobromine, theophylline, and caffeine, in amounts that surpass their content in coffee or cacao, although their effect is milder due to bonding with tannins (Tanaka, 2002). To understand what the efficiency of these active substances depends, it is necessary to conduct mass comparisons of the structures of phytoconstituents while considering data on the properties of the plants as recorded in traditional knowledge therefore, using *in silico* methods to determine the biological activity of medicinal plants is indispensable. Another repository worth mentioning is the EMNPD: a comprehensive database of endophytic microorganism natural products, featuring manually curated data. It includes 6,632 natural products from 1,017 microorganisms, targeting 1,286 entities (94 proteins, 282 cell lines, and 910 species) with 91 bioactivities. The database offers detailed physio-chemical properties, quantitative activity data, and links related to fermentation conditions and taxonomy. As an open-access resource, it supports drug discovery and the study of bioactive substances., EMNPD can be accessed at http:// emnpd. idrbl ab. cn/ without the need for registration, enabling researchers to freely download the data. EMNPD is expected to become a valuable resource in the field of endophytic microorganism natural products and contribute not only to future drug development endeavours but also to creating of conservation and restoration products. For example, great perspectives for the ceramic manufacture and restoration are considered the Unicellular diatoms, the only ones that create beautiful porous symmetrical silicon shells called biominerals. It was found that the shells of some diatoms of the North Sea contain propylamines of N- methyl propylamine fragments capable of rapidly precipitating silicon from solutions with silicic acid. The use of polyamines of the oligo-N-methyl propylamine type makes it possible to create ceramics in natural conditions (Rogoza, 2005) (Rogoza, 2006).

3.2 Controlled Vocabularies and Linked Data

Heritage science faces significant challenge in exploring biotechnological resources due to the lack of data sharing standards that could make interdisciplinary initiatives easier. Like the biotech sector, in the cultural heritage field countries tend to develop own databases that are not always accessible to external clients. These repositories are created based on local criteria and capabilities and particularly as regards historic objects and technical sources, may not always align with international conventions summarized by ICOM and ECCO as CIDOC CRM. These are developed as reference model for cultural heritage data, including archaeology, ancient texts, and buildings, which are used in infrastructures and applications like SSHOC, Ariadne RI, INFN CHN, THESPIAN, and Arches for Science. Among the few open access-controlled vocabularies that encompass chemical and biological terms used in heritage studies are:

- **Getty vocabularies**. Developed and published by The Getty Research Foundation, these are the most used vocabularies in heritage studies.
- **MesH:** Medical Subject Headings (MeSH), created by the US National Library of Medicine, is a vital controlled vocabulary. Although Getty AAT includes many terms for scientific instruments and methods related to Heritage Science, MeSH covers nearly all of them and is updated more frequently. This makes it useful when Getty AAT lacks certain terms or provides mismatched definitions.
- **Gold Book:** The International Union of Pure and Applied Chemistry (IUPAC) offers the Compendium of Chemical Terminology, known as the Gold Book, online. It serves as a valuable complement to Getty AAT and MeSH for standardized chemical terminology and units of measurement.
- **VIAF.** The Virtual International Authority File (VIAF) is a collaborative initiative for libraries, managed by the Online Computer Library Center (OCLC). VIAF consolidates vocabularies from numerous libraries worldwide, mapping and linking authorities back to these sources. Consequently, the content is highly reliable, multilingual, and interoperable. VIAF includes the names of individuals and organizations associated with published works, as well as the titles of those works.

There is a notable lack of vocabularies tailored specifically for the Humanities and Cultural Heritage disciplines. Whenever no scientific analysis of artifacts is possible without deep knowledge on historic (bio) materials and techniques and on the relative written technical sources, with the exceptions of the Slavic speaking countries and Germany, highly significant lacunae are still present in their study. These are dispersed, not or partially translated and not critically assessed by art technologists, hence practically unusable. Instead, the existing vocabularies are of local/national importance and not directly interoperative with information resources regarding the biotech sector because their state-of-art is far not so advanced and the content architecture – not adapted to such exchange (Stoyanova, 2014). Promulgated information and databases often derive from libraries elaborated for external or generic purposes and tracing the provenance of a considerable number of ancient documents written on papyrus, parchment, silk, wood or paper; of oriental dyed and printed textiles or of tanned leather artefacts found *ex loco*, still represents an insuperable problem for archaeometry. In concern to the written or stamped anonymous papers, either textual-linguistic investigations nor palaeographic or watermarks analysis alone can unequivocally answer questions regarding the exact "birthplace". Similarly, attribution of anonymous ancient textiles or leather pieces counts almost entirely on stylistic comparisons.

Several barriers hinder the acquisition of detailed scientific information on this matter. Firstly, the state of relevant databases and libraries is poor. Unlike investigative techniques, the registration, linguistic-philological, and technical analysis of historical sources have been neglected, leading to approximations and errors in laboratory planning and interpretation. For example, for inks used until the 15th century, more than 1000 additives were employed based on written sources, but only two main groups, carbon and gall-tannic, are currently distinguished, which is insufficient for determining their origins. Translations of sources (e.g., Zerdoun Bat-Jehuda, 1983) lacks scientific analysis and contains many enigmatic terms. Thus, the conservation methods proposed by the EU-funded INKCOR project on document corrosion prevention are questionable, especially given that the historical sources on gall-tannic ink fabrication remain unpublished due to "secret know-how." This decision contradicts the objectivity and transparency required in scientific work today, making it unclear why authors assume all ancient inks are exclusively gall tannic. Quite deluding as well the activity of the most recently EU funded ARTECHNE and DURARE projects hosted at the Utrecht university that did not produce more than a bibliographic collection and text normalization of selected works (https://durare.sites.uu.nl/project/ and https://artechne.wp.hum.uu.nl). This severely undermines the reliability of a majority of current peer reviewed scientific analysis on historic artistic goods and strongly prejudices their conservation.

All in all, remarkable gaps still divide the different national schools in their approach to the proper cultural heritage (CH); knowledge of the CH resources scattered worldwide is very fragmentary. The Greek Alchemists Corpus, initiated in an international collaboration without precedents about the end of the 19th c, and intended to collect all these precious documents on a unique platform, has been interrupted by the First World War. Only recently, thanks to the inversion of the tendencies in international relations, in the EU area have been digitalized and became accessible some of these sources: at the web site of the Central German Institute for Conservation (Köln) in the most systematic manner and, single treatises, at the sites of some Russian, Bulgarian, French and Italian libraries & institutions.

4 Conclusions

The complex nature of cultural heritage requires a dedicated interdisciplinary networking effort for to clear artefacts' make-up and to can select the most appropriate strategies for large-scale, long-term damage prevention and preservation. Integrating chemo- and bioinformatics into the heritage sector will help characterization of natural substances implied in artefacts and provide a better basis for their scientific attribution, improve existing theoretical approaches, conservation and restoration treatments, and produce inspiration for new research and applications directions.

Today, world science is recognizing the importance of moving away from narrow specialization towards interdisciplinary research. Nano-, bio-, info-, and cognitive technologies form the basis for future advancements in science and technology, transitioning to fundamentally new, renewable resources and technologies modelled after living nature and utilizing modern technological-scientific achievements. This involves not merely the combination of different technologies but their convergence, interpenetration, and alignment towards a unified goal.

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