The status of electronic laboratory notebooks for chemistry and biology
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Documenting an experiment in a way that ensures that the record can act as evidence to support a patent claim or to demonstrate compliance with the US Food and Drug Administration’s (FDA’s) predicate rules, puts demands on an electronic laboratory notebook (ELN) that are not trivial. The 1996 General Agreement on Tariffs and Trade (GATT) allowed notebook records that were generated outside of the US to be used to claim precedence in US patent claims. This agreement spurred interest in the development of ELNs in Europe. The pharmaceutical research process became dependent on computer systems during the latter part of the 1990s, and this also led to a wider interest in ELNs. More recently, the FDA began to encourage submissions in an all-electronic form, leading to great interest in the use of ELNs in development and manufacturing. As a result of these influences, the pharmaceutical industry is now actively pursuing ELN evaluations and implementations. This article describes some of the early efforts and the recent drivers for ELN adoption. The state of the ELN market in 2005 is also described.

Keywords: 21 CFR part 11, document management, electronic laboratory notebook, electronic record, electronic signature, ELabJournal, ELN, predicate rules, Scientific Data Management System, SDMS, Semantic Web

Abbreviations
ELN  Electronic laboratory notebook
LIMS  Laboratory information system
SDMS  Scientific data management system

Introduction
Laboratory notebooks represent an important part of the research and development (R&D) workflow. Leonardo Da Vinci kept such notebooks, and used encryption to keep their contents safe [1]. The role of the laboratory notebook is to record work that was done so that research can be repeated, or avoided if the outcome was not the desired outcome, and to allow subsequent research to move forward based on previous results. Traditionally, the laboratory notebook medium is paper and data entries are handwritten. This medium is portable, easy to use, well understood by users, and, with a little care, a durable method of recording.

In the US, laboratory notebooks have evolved a special role in supporting patent claims. To be awarded a patent in the US, an applicant must demonstrate that they were the ‘first-to-invent’ [2], and the date of the invention depends on the applicant using ‘due diligence’ [3] in their ‘reduction to practice’ [4]; that is, the applicant must realize the invention in a timely fashion.

Prior to the 1996 General Agreement on Tariffs and Trade (GATT), the priority date for inventions made outside of the US was the same as the date of filing with the US Patents and Trademarks Office (USPTO). At the conclusion of this agreement, the priority date of applications for foreign inventions was recognized in the US, provided that US practices were followed [5]. The US provides a large market for many products, including pharmaceuticals, and so securing a patent in the US is important; this means that laboratory notebook practices worldwide are determined by US practices.

The need for change
Computers are used extensively in modern R&D, and so much of the data that needs to be recorded in a laboratory notebook is generated electronically. Transcribing data manually into a paper notebook is error-prone, and in many cases, for example, analytical data (spectra, chromatograms, photos, etc), transcription of the data is not possible. The paper-based laboratory notebook is the last non-electronic component of the R&D workflow system, and there is currently much pressure to replace it with an electronic laboratory notebook (ELN).

There are also other influences encouraging the use of ELNs. The incorporation of high-throughput screening (HTS) and high-throughput synthesis into the research process has resulted in an increased volume of electronic data that needs to be transcribed. Furthermore, widespread adoption of US laboratory notebook practices has begun to occur in the rest of the world, particularly in Europe; prior to this, European scientists had not been used to keeping detailed records on paper, and so have demanded an ELN.

During the 1990s, companies began to recognize that the information available in paper notebook records was highly valuable, but was essentially lost to the organization; it was impractical for laboratory notebook users to enter data in the laboratory notebook and then to register the same data separately into one or more databases. Thus, an all-electronic solution was required. A number of ELNs were developed as custom projects in the late 1990s [6], but the R&D market decided that custom ELNs did not provide a competitive advantage, and therefore an off-the-shelf product was needed.

ELNs come of age
Interest in ELNs was subdued until 2004. Prior to 2004, the International Quality and Productivity Center (IQPC) organized conferences on laboratory notebooks in London that attracted a Hardcore of only 30 to 40 participants, but in September 2004, the IQPC conference on ELNs was overwhelmed by 120 delegates [7]; ELNs had become a hot topic.
The book Electronic Laboratory Notebooks, a Foundation for Knowledge Management [8] was published in August 2004 by Michael Elliott of Atrium Research & Consulting, and identified and discussed the merits of 25 ELN products. By the time the second edition was published a year later [9••], some ELN vendors had merged, some had been acquired and some were less visible, but the there were now 29 ELN products on the market and it appeared that ELNs had greatly risen in popularity. Both editions of this publication provide an excellent source of information regarding these products, their supporting technology, the benefits of ELNs, the changes that they drive and the potential for ELNs in knowledge management.

Early successes
The chemistry conducted during drug development is more repetitive than that conducted during drug discovery, and much time is spent duplicating procedures. Transcribing and updating an existing procedure is expensive, time-consuming, tedious and error-prone. Paul van Eikeren of IntelliChem Inc recognized the potential for automating this workflow system, and this ultimately resulted in the release of the IntelliChem intelligent ELN [10]. This product was developed in collaboration with a consortium of pharmaceutical companies and was an early success; by the end of 2005 many major pharmaceutical companies had taken up the use of this ELN. The product proved less attractive in the discovery chemistry field, however, where research is much less repetitive.

As an aid to chemists in the discovery field, researchers at Synthematix Inc developed a product to assist in identifying synthetic routes [11]. Robin Smith (the co-founder of Synthematix) recognized that this product could also be used as an ELN, and promoted it as such. Chemists generally liked the user interface, and the product gained a number of successes, particularly within smaller biotechnology companies that found it to be a cost-effective solution, providing the functions of both synthesis planning and ELN.

Symyx Technologies Inc was founded in 1994 and provides high-throughput technologies to the chemical industry [12]. Symyx’s strength initially lay on the development side, but it recognized that the IntelliChem intelligent ELN product was complementary to the Symyx technology. Consequently, Symyx acquired IntelliChem in November 2004 [13]. In February 2005, Symyx also added Synthematix to its portfolio [14], to allow it to provide ELN coverage across both chemistry discovery and development. Symyx now faces the problem of rationalizing three separate technologies to provide a single, seamless solution.

The company CambridgeSoft Corp exploited the market acceptance and strong brand awareness of its ChemDraw product [15], in producing a personal ELN [16]. CambridgeSoft, similarly to Symyx, was quick to recognize the ELN market momentum and announced the launch of an ‘Enterprise solution’. Chemists were already familiar with ChemDraw, and quickly adopted this ELN product. CambridgeSoft had been successful in working with smaller companies, and was able to extend these early collaborations into the top 20 pharmaceutical companies, including Merck & Co Inc, GlaxoSmithKline plc, NV Organon and, more recently, AstraZeneca plc. However, a product such as the Enterprise solution that was designed as a personal solution may prove difficult to scale up for the pharmaceutical market, and the reliability of this product has apparently not yet been proved.

Consulting products
The consulting organization of Elsevier MDL created the 'ISIS LabJournal' in 1995. Based on the MDL software ISIS, and using MDL ISIS/Base as the user interface, this product served as the starting point for several custom-built ELN solutions that were aimed at synthetic organic chemists, particularly those based in Europe.

The e-solutions company Klee Group developed a custom ELN (Kalabie) [17] for sanofi-aventis, and the European software company Contur [18] developed a custom ELN for Biovitrum AB. Both Klee Group and Contur commercialized their products with some success in 2005. These products are essentially generic ELNs with chemistry capabilities supplied either by Elsevier MDL or Accelrys Software Inc. In 2005, Klee Group joined Elsevier MDL’s Isentris Alliance to strengthen its capabilities in life sciences R&D [19].

Elsevier MDL, Tripos and Waters enter the market
Elsevier MDL and Tripos Inc independently announced the release of ELN products, based on the experience that they had obtained in custom development.

In 2000, Elsevier MDL released Elan, an ELN product with a document-based user interface [20], which was based on a custom solution developed for a large pharmaceutical company. This product had a look and feel that was extremely close to that of the traditional paper notebook, but it was hampered by a dependence on Microsoft Word. In June 2000, Elsevier MDL acquired Afferent Systems Inc [21]. The Afferent product suite was targeted at high-throughput synthesis, included a powerful reaction-based enumerator, and had the capability to convert a graphical protocol into text that could be understood by chemists, and into instructions that could be used to program a robot. Updating these technologies and incorporating them into the MDL Notebook product [22] would produce a powerful ELN for synthesis chemists.

Tripos initially developed an ELN for the Tripos Receptor Research Center, and enjoyed the benefit of having synthesis chemists within the company who could test the product. Schering AG purchased this system as part of a large chemoinformatics project managed by Tripos. In January 2005, Tripos acquired Optive Research [23], and in August 2005 announced the release of Benchware Notebook [24], which is part of the family of products that was developed by Optive.

Waters Corp, a major vendor of scientific instruments and laboratory information systems (LIMSs), had also been acquiring technologies that would enhance the development
of an ELN. In July 2003, Waters acquired Creon Lab Control [25], partly for its ELN technology, and stated an interest in merging the capabilities of LIMSs and ELNs. In January 2004, Waters acquired NuGenesis Technologies Corp [26], and with it the leading scientific data management system (SDMS) NuGenesis SDMS information management platform [27]. The culmination of these acquisitions led Waters to heavily promote the Waters eLab Notebook [28] in 2005. This product exploited the extensive know-how of researchers at Waters in instrument control, LIMSs and SDMSs, but it was weak in its chemistry capabilities, and, in July 2005, Waters announced a collaboration with the German company InfoChem GmbH to fill this chemistry gap [29].

**Biology ELNs**

The initial drive for the development of ELNs came from the field of chemistry, perhaps driven by the early adoption by chemists of computer technologies for drawing chemical structures and for storing and searching them graphically within databases. There was, however, a parallel interest in ELNs in biology, which was initially driven by the volume of data that was being managed in bioinformatics. The use of GenSys Software Inc [30] and Rescentris Inc [31] ELN products began in bioinformatics departments, and may be characterized as generic (ie, blank-page or white-page) notebooks. In principle, a generic notebook can accommodate any workflow, which is initially an attractive feature. Such notebooks, however, have not been as successful as specific notebooks, such as those that serve chemistry. This is possibly because generic notebooks offer little advantage to the user; indeed they are often less convenient than the paper notebooks they replace.

The use of HTS introduced biologists to computer systems, and Microsoft Excel software was readily adopted in this arena. For a long time, biologists did not share the enthusiasm of their chemistry colleagues for ELNs; however, this situation changed during 2005. Prior to 2005, pharmaceutical companies were only marginally interested in the use of biology ELNs to complement chemistry ELNs, but during 2005, biology ELN capabilities gained momentum. While not many pharmaceutical companies were prepared to invest in a biology ELN at this time, they wanted to know that such an entity would be available. Consequently, while the generic ELN vendors were adding chemistry technologies to their products, the chemistry-specific ELN vendors scrambled to substantiate their biology expertise.

IDBS Ltd, whose ActivityBase product [32] has the highest market share in the biology data acquisition market, took a different approach and acquired Deffinity in May 2005, and with it the Deffinity DAT-LAB™ ELN product [33]. IDBS then launched this product as E-WorkBook in June 2005 [34].

**Including database content in the ELN workflow**

The incorporation of information from in-house (ie, proprietary) and commercial databases into laboratory notebooks is an essential part of the R&D workflow. None of the current ELN vendors does this effectively with regard to content integration, but it is anticipated that this situation will change. Infotrieve, a provider of content software technology and information services, acquired GenSys in February 2005 [35], and in May 2005, Infotrieve launched its Life Science Research Center [36], a Web-based information research tool that provides scientists with one-stop search access to critical information that impacts scientific workflow. In June 2005, Infotrieve introduced Infotrieve/ELN [30], which is based on the GenSys ELN product. Infotrieve appears to have identified the lack of content integration in the commercially available ELN products, and hopes to fill the gap.

The current main sources of chemistry data are Chemical Abstracts Services (CAS), the CrossFire Beilstein database and the MDL Available Chemicals Directory (ACD). The CAS data extraction policy makes it difficult to integrate search results from the CAS database into external documents, and this major integration need is unlikely to be resolved in the near future. The other two sources, the CrossFire Beilstein database and MDL ACD, are both available from Elsevier MDL, and the company has announced that integration with these and other data sources is a high priority for their MDL Notebook product.

**Electronic signatures and electronic records**

ELNs provide benefit to the sign-and-witness workflows that are used to support due diligence during reduction to practice. Surrendering a physical laboratory notebook, even temporarily, so that a record can be signed is an inefficient and inconvenient process; consequently, it is often not carried out in the required timely fashion. Records should be signed at or near to the time that the research is conducted, but signing is often carried out 3 to 6 months later at a ‘mass signing party’.

Corporate patent attorneys have been resistant to the idea of becoming ‘fully electronic’ in their work practice, that is, employing electronic signatures, and archiving information as electronic records. This resistance stems from the lack of case law in the area of patents, despite the fact that the Federal Rules of Evidence do not exclude electronic documents [37], and that the decision in a number of high-profile cases has relied on email evidence.

During 2005, however, the attitude toward electronic workflow changed. The reasons for this change are not entirely clear, but perhaps users and companies have now recognized the cost effectiveness of moving to a fully electronic scenario. For this to be effectively achieved, products must incorporate an electronic signature capability, and vendors have begun to promote the capabilities of their products in this area, although it is questionable whether all of the solutions are as robust as they need to be.

Surety, a long-standing vendor of electronic notary services, relaunched its technology as AbsoluteProof® in 2003 [38], and, in September 2005, Surety announced a collaboration with EKM Corp [39] to provide the AbsoluteProof® product as a tightly integrated module within the EKM LABTrack™ product [40].
In February 2005, eight global pharmaceutical organizations, including AstraZeneca, Bristol-Myers Squibb, GlaxoSmithKline, Johnson & Johnson, Merck & Co, Pfizer, Procter & Gamble and sanofi-aventis came together as the founding members of the SAFE-BioPharma Association [41]. The purpose of this organization is to deliver unique electronic identity credentials for legally enforceable and regulatory-compliant digital signatures across the global (bio)pharmaceutical environment.

The hybrid ELN approach
If a company has a manufacturing operation, then the US Food and Drug Administration (FDA) will encourage that company to submit the required regulatory information electronically, and the company will need to introduce an electronic records management system. Such systems are expensive to license and maintain: thus, small companies, and particularly start-ups, are unlikely to become fully electronic. A hybrid approach, in which all data are entered electronically and are searchable, but the legal record constitutes a printout with ‘wet signatures’, will remain popular until electronic record systems become cost-effective.

Amphora Research Systems has developed a suite of products that add extra security to this hybrid model [42]. The product PatentPad® is a documentation system comprising security paper whose appearance can be customized to suit user requirements [43]. The paper contains a latent image that produces copies which can be identified as copies. Amphora controls the release of the paper and details are registered in the SCRIP-SAFE® [44] registry maintained at Amphora.

The discreet business relationship between SCRIP-SAFE® and the customer makes SCRIP-SAFE® a ‘trusted third party’ that can be used to verify the date on which particular PatentPad® paper was manufactured, the authenticity of the paper and the authenticity of the serial numbers. Some companies view the added cost and complexity of this system as a cost-effective way to gain an extra level of confidence should they need to defend a patent.

21 CFR part 11
There are a number of regulatory agencies that influence the way in which the pharmaceutical industry works, with the FDA being the most prominent of these Agencies. The FDA was set up in 1937 under the Code of Federal Regulations Title 21, usually abbreviated to 21 CFR, and sub-regulations in this code are each identified by a numbered part. Good Laboratory Practices (GLP), Good Manufacturing Practices (GMP) and Good Clinical Practices (GCP) are covered by parts 58, 210, 211, 820, 606, 50 and 56. Collectively, these practices are often referred to as cGXP, where the c is an abbreviation of current and X is a wildcard. Often the cGXP regulations are referred to as ‘predicate rules’.

In 1997, part 11 of 21 CFR was added to cover the creation, maintenance and preservation of electronic records and electronic signatures [45•]. 21 CFR part 11 has had a checkered history; it was formulated in response to pharmaceutical industry requests but was originally deemed too severe, delaying the implementation of many ELN systems. Following industry lobbying, however, the FDA relaxed its interpretation of the regulation in 2003, allowing the industry to move forward with ELNs. An updated guidance document was expected in 2005, but has not yet been published.

During 2005, 21 CFR part 11 compliance became a popular requirement for ELNs, even though most ELN installations are not actually covered by this regulation. It is now common to see claims that a product is ‘GMP compliant’ or ‘21 CFR part 11 compliant’. These claims are spurious, however, because only a complete system, including standard operating procedures and all related software at an organization, can be compliant. An ELN that meets certain technical requirements can help an organization become compliant.

VelQuest Corp works closely with the FDA with its SmartLab system [46•], and is currently the leader in the regulated space, although other, more LIMS-oriented companies are also looking at opportunities in this area; for example, Labtrons Inc is currently promoting its NEXXIS qELN product [47] in quality assurance and quality control laboratories.

The future of LIMS
Representing two extremes, an LIMS captures highly structured data through rigid user interfaces (UIs) and uses standard report formats, whereas an ELN contains unstructured data and has flexible UIs and flexible reporting capabilities. An ELN for discovery chemistry tends to have some framework to aid a chemist in setting up a reaction and identifying analytical information, and a development chemistry ELN also has a framework, but both types of ELN are less rigid than an LIMS.

ELNs and LIMSSs will likely merge into a continuum of products, and the introduction of the Waters eLab Notebook and the Labtrons NEXXIS qELN systems represents the start of this merge. Other LIMS and instrument vendors are not as active in combining ELNs and LIMSSs, but there is evidence that they have seen the trend. For example, in July 2005, Agilent Technologies Inc acquired Scientific Software Inc and added its own Enterprise Content Manager (formerly CyberLab) to Scientific Software’s OpenLAB suite [48]. While this is not quite an ELN system, it is closely related. Thermo Electron Corp [49] has been active in building a portfolio of LIMS technologies, but so far has not expressed an interest in ELNs.

The future of ELNs
The ELN will eventually be used by all R&D scientists to record all of their research, and will become their central application. Scientists will expect to be able to extract information from ELNs efficiently and easily. This puts great pressure on the architecture of ELNs; in industrial terms, it must be open, extensible, scaleable and robust. In addition, ELNs must be easy to use, simplify the user’s work process...
and be fast. In the field of pharmaceutical R&D alone, ELNs
must also be able to deal with many different types of data,
for example, chemical structures, chemical reactions,
experiment protocols, digital images, spectra and
chromatograms, and sequences. There are also opportunities
for using ELNs within other industries, for example, in
engineering where computer-aided design images will be
needed.

An ELN that encompasses all of these needs cannot be
supplied by one vendor, as no single vendor has all of the
required expertise. Consequently, a growth in collaborations
may be anticipated, for example, CambridgeSoft already has a
collaboration with Tripos, and Tripos, Symyx and the Klee
Group each have collaborations with Elsevier MDL.

There are also too many vendors in the market; the market is
not sufficient to support the current 29 or more vendors. An
ELN is a mission-critical application, and so purchasing
companies will increasingly look at the financial strengths of
the vendors, which is advantageous to the bigger vendors.
Hence, mergers and acquisitions are likely to continue.

The interest in ELNs has not yet reached academic
researchers, but the Combechem [50] and the SmartTea [51]
projects currently being conducted at the University of
Southampton, UK, are worthy of comment. The Combechem
project focuses on grid-enabled combinatorial chemistry,
involving synthetic, laser and surface chemistry, and
crystallography, for the development of an e-laboratory.
Pervasive computing technology is used to record
information on all aspects of laboratory research and to carry
this information forward through the chain of generation of
chemical knowledge. A Semantic Web approach is used to
provide an end-to-end knowledge sequence in which an
experiment produces data from which results are derived,
and these results are then searched for patterns from which
conclusions are drawn, leading to further experiments [50].

SmartTea provides a highly relevant example of what can be
achieved using this approach [51]. The researchers involved
in this project considered a process that is familiar to many
- that is, the making of a cup of tea - and explored the various
ways in which the process might be achieved using both
normal household equipment and also chemistry equipment.
The experimenters were required to report the
procedures followed in a laboratory notebook style. The obvious conclusion reached during the process was that,
while each experiment resulted in a cup of tea, the reports
recorded for the different processes were not consistent, and
that it would be difficult for experimenters to translate
between the two types of environments, that is, household
and chemistry. Consequently, the research team
deconstructed the data to determine the underlying
workflow and information from each experiment, and
developed a resource description framework map [52] of the
overall process. Perhaps unsurprisingly, it was possible to
distinguish the phases of each experiment as: reaction,
work-up, purification and analysis.

Following on from this research, the team applied the results
to a real chemistry experiment, the synthesis of aspirin. A
similar process was followed as above, and the same four
phases that were found in the SmartTea experiment were
identified. The goal of this project was to develop an
ontology that represented all of the processes, events and
objects that occur in experiments. From this ontology the
researchers should be able to define a standard process and
vocabulary that can be used to capture art experiment, and
then ensure that it can be repeated by different
experimenters, including robotic systems, in different
environments.

Summary

Companies will migrate to all-electronic systems once the
technologies are proven and affordable. The year 2005 was a
period of change in which the ELN market was highly active,
and could even be described as turbulent. Some of the major
changes were as follows:

- The pharmaceutical industry shifted from a position of
  ‘if we get an ELN’ to ‘when we get an ELN’.
- Many companies began evaluations of ELNs, and some
  large-scale implementations of ELNs were announced.
- The number of mergers, acquisitions and collaborations
  between ELN vendors increased.
- E-signatures and e-records began to be considered as an
  inevitable part of the R&D process.
- Biologists became more interested in ELN capabilities.
- Custom solutions were no longer considered a viable
  approach; the market is now demanding off-the-shelf,
  configurable, supported products.
- The difference between LIMSs and ELNs became
  blurred.
- Major companies such as Elsevier MDL, Tripos and
  Waters entered the ELN market.

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Electronic laboratory notebooks for chemistry and biology

   • Provides a good source of information about the technology relevant to ELNs, legal and regulatory matters, the state of the market, and ELN products and vendors.

   • Provides an excellent source of information, superseding the previous edition. This publication contains a prodigious quantity of information.


25. Waters Corporation announces acquisition of Creon Lab Control: Waters Corp, Milford, MA, USA. http://www.waters.com/WatersDivision/content.asp?waterns=LKR-5PWQ59


29. Waters eLab Notebook™ software extends reach to support chemical synthesis work: Waters Corp, Milford, MA, USA. http://www.waters.com/WatersDivision/content.asp?ref=JLEK-6DCQ6


32. idbsActiveBase: http://www.idbs.com/products/abase/


   • Simon Cole, the CEO of Amphora Research Systems, contributes to many ELN conferences and his presentations can be found at this web site, which provides an excellent resource on hybrid ELNs.


42. 21 CFR part 11: US Food and Drug Administration, Rockville, MD, USA. http://www.fda.gov/ohrms/compliance/refpart11/11fbrgndkgj/1f11psdp
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43. VelQuest SmartLab: VelQuest Corp, Hopkinton, MA, USA. http://www.velquest.com/notebooks/overview.asp
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Electronic laboratory notebooks (ELNs) are also transforming the way that the scientific record is captured with a revolutionary transformation from paper notebooks to the digital capture of experiments [6]. ELNs offer significant benefits to researchers by facilitating long-term storage, reproducibility, and enhanced availability of experiment records across multiple devices, ensuring standard operating procedure compliance and providing interfaces to instrumentation, supporting IP protection, collaboration, and open science [4, 21, 24, 43, 49]. More recently, semantic lab notebooks (SLNs) have utilised semantic web technologies to expose research data as formalised metadata [10], and to link between the different data sets collected throughout the experimental process [42]. Taylor, K.: The Status of Electronic Laboratory Notebooks for Chemistry and Biology. Current opinion in Drug Discovery and Development 9(3), 348–353 (2006)Google Scholar. 10. Rethinking Laboratory Notebooks. In: Lewkowicz M., Hassanaly P., Wulf V., Rohde M. (eds) Proceedings of COOP 2010. Springer, London. An electronic laboratory notebook or ELN is, as Harvard defines, a software tool that in its most basic form replicates an interface much like a paper in a paper lab notebook. Despite having been around since the 1990s their use is just beginning to spread throughout the scientific community, according to Nature. Which is why they are rapidly evolving to accommodate the needs of scientists and are becoming a necessary tool in many laboratories around the world. A brief history of electronic laboratory notebooks features. When ELNs first entered the market of scientific software, they were... For chemistry and biology. Free (advanced paid feature). Intellectual property protection, data encryption.