# Quo Vaditis, Scientia et Educatio?

**Kiralj, Rudolf**

*Source / Izvornik:* **Radovi Zavoda za znanstvenoistraživački i umjetnički rad u Bjelovaru, 2023, 55 - 103**

**Journal article, Published version**
**Rad u časopisu, Objavljena verzija rada (izdavačev PDF)**

https://doi.org/10.21857/y6zolb45lm

RUDOLF KIRALJ

UDK: 021.4:001.81(075.8)
*Izvorni znanstveni članak / Original Scientific Paper*
Rukopis prihvaćen za tisak: 28. 6. 2023.
DOI: https://dx.doi.org/10.21857/y6zolb45lm

# Quo Vaditis, Scientia et Educatio?

## Summary

Exponential growth of human knowledge *i.e.* of science and technology, becomes uncontrollable and more and more is in disagreement with linear biological development of humans. This work makes assessment of the impact of the exponential growth to education in terms of bibliometric analyses of university textbooks and case studies of visual nature in chemistry. Various bibliometric descriptors (number of pages, number of editions with years, font size, and maximum number of characters) were determined for books studied from 12 diverse areas of knowledge, and from 14 branches of chemistry. Case studies in chemistry (spherical harmonics, nucleophilic substitution reactions, and nucleic acid bases) were illustrated using modern calculation and visualization software and chemical databases. All textbooks studied exhibit the increase in the quantity of matter. There are several increase types, linear, parabolic, oscillating and others, visible when analyzing No. pages *versus* time scatterplots. Other descriptors show that some increase is always present. Increased rates from the first to the last edition of textbooks are higher in chemistry than in general knowledge. Converting them into additional time to study textbooks, they range from about 10 minutes to 100 minutes per day. This means students have to spend in general over 2 hours more, and in chemistry 2 – 4 hours per day more than their colleagues who had the first edition textbooks. The three case studies in chemistry indicate that many outdated misconceptions are not erased using modern computer technology, what makes studying textbooks more difficult. Textbooks systematically omit high-quality computer-generated plots of various functions and molecular structures and instead, prefer using inaccurate schematic and artistic presentations. Such situation, in spite of the exponential growth of science and technology, persists for decades, coexisting with good calculation and plotting software and chemical databases. Remedies for this situation are not simple and they include radical changes of textbooks for a whole course.

**Keywords:** exponential growth of knowledge, university textbooks, chemistry textbooks, bibliometric analysis, spherical harmonics, molecular structures, misinterpretations

> ”The heart of the intelligent acquires learning,
> the ears of the wise search for knowledge.”
> (The Proverbs 18:15)

## 1. Introduction

Latin verb *vadere* means to go, to advance, to rush, to hurry, to walk (Waldert, Mossböck, 2022). It is used in numerous English phrases addressing persons or things in singular form „*Quo vadis*?”, meaning „Where are you going?” or „Where are you marching?” (English Grammar, 2022). Much less common are analogous phrases for persons or things in plural form *vaditis* (Waldert, Mossböck, 2022), *i.e.* saying „*Quo vaditis*?”. Searching literature, one finds some interesting examples for „*Quo vadis*, something?”: „*Quo vadis*, electrochemistry?” (Holze, 2020) in a discussion on the nature of electrochemistry, which is becoming extremely interdisciplinary and thus, disappearing as a science; „*Quo vadis*, hydrology?” (Kundzewicz, 2018) in a similar view on interdisciplinarization and modernization of this science; „*Quo vadis*, Tekstil?” (Jokić, 2019) in a review about Tekstil, a Croatian journal dedicated to textile technology, in attempt to internationalize it and make prestigious. Similarly, there are rare examples for „*Quo vaditis*, somethings?”, such as: „*Quo vaditis*, consultants?” (Poór *et al.*, 2022) in a prediction of future of the consulting profession. In all the cited examples of „*Quo vadis/vaditis* something(s)?” one finds uncertainty, doubts, alternatives and even multiple options of future events, *i.e.* future predictions that are not straightforward.

Speaking generally about the evolution of human knowledge (*i.e.*, science and technology) and of humans, Leonhard (Leonhard, 2022) emphasizes that technology is exponential, humans are linear, while nature is cyclical. He stresses that humans are not exponential like technology (Espindola, 2020), and that „the more we connect with technology, the more we must protect what makes us human” (Leonhard, 2022). Furthermore, he advices that „we need to transcend technology, not humanity” (Leonhard, 2022). In other words, human knowledge and technological development must not govern humans but instead, humans must control their knowledge and development. Otherwise, how can we deal with the constant increase of the gap between the human linear and the scientific exponential developments? Instead of changing and adapting human nature to technology, the opposite is needed. Leonhards’ views, if neglected, naturally lead to a question about science, „*Quo vadis, scientia*?” – what is the final purpose of science and technology?

The growth of human knowledge was linear from 100 BC to about 1700 AD, and later became exponential up to present days (Bornmann *et al*., 2021; Pllana, 2019). The exponential growth is observed in specific fields too, such as information technology (Nagy *et al*., 2011), chemometrics (Kiralj, Ferreira, 2006), invention of chemicals (Schummer, 1997), and so on. Even chemical databases the Cambridge Structural Database (CCDC, 2021) and the Protein Databank (RCSB PDB, 2022) increase exponentially. Some authors suggest that the exponential growth will reach saturation in far future, *i.e*. that the growth curve is sigmoidal (Wagner, Kim, 2014; Shestakova, 2018). The current growth of modern science and technology does not show signs of retardation: in the period from 1640 to 2018 the doubling time was in average 17.3 years (Bornmann *et al*., 2021). A natural question that comes to one's mind is how these trends affect education, especially higher education from which more and more future scientists and engineers are recruted. Then, question „*Quo vaditis, scientia et educatio*?" indeed has sense.

Unfortunatelly, both older and novel disciplines that deal with science and education are not much worried about the increasing gap between the human linear and the scientific exponential growths and its consequences for students and young scientists and engineers. They are more concerned with the human progress, how to explain, quantify, intensify and accelerate it, without noticing its eventually negative side effects. Let's name the disciplines: Science of Science (Fortunato *et al*., 2018), Scientonomy or Theory of Scientific Change (Sebastien, 2016), Scientometrics (Kinouchi, 2014; Mingers, Leydesdorff, 2015), Science Criticism (Trench *et al.*, 2016), Philosophy of Science (Rosenberg, 2005), and even Science of Education (Kalantzis, 2005) and Philosophy of Education (Winch, Gingell, 2008; Chazan, 2022).

English word *textbook* (Harper, 2022) and Portuguese *livro-texto* (Dicionário in-Formal, 2022) (both meaning textual book), Croatian *udžbenik* (Hrvatska enciklopedija, 2021) (from verb *učiti*, to learn, to teach), and so on in other languages, have the following meaning: the basic didactic material, used by students and also teachers, to acquire knowledge in specific matter. A good textbook must have several characteristics (Sutradhar, 2021; Wiggins, 2013), among which are appropriate language (simple, clear, lucid, scientific and precise), usefulness (accurately written textbook, presenting subject matter, not being an encyclopedia or a dictionary), good presentation (interesting and attractive, with charts, maps and diagrams), and acceptable size (handy, not bulky size, students should carry the textbook properly), among others. In general, writing good textbooks is hard for academics, regardless of their academic writing skills (Sternberg, 2017). Taking into account this fact, together with research and teaching obligations academics have, and also considering the exponential explosion of human knowledge, it is not hard to understand why there are many inadequate university textbooks.

There are only a few articles which criticize modern university textbooks, showing examples of textbooks increasing in size and not in quality, but increasing in the quantity of additional materials over time (Hamilton, 2006; Lamoureux, Ogilvie, 2021 c), frequently containing un-updated and misleading stuff (Lee *et al*., 2019). Such situation encourages a more extensive inspection of university textbooks, as is done in this work. The basic assumption of this research is that the exponential increase of human knowledge greatly affects education with some negative side effects (Kiralj, 2022). First, didactic materials also increase in size uncontrollably, making the knowledge not well absorbable for students and young scientists and engineers. Second, the increasing gap between the human linear and the scientific exponential growth is another cause of difficulties in learning and teaching at university level. What are the consequences of these trends? Students are trying to overcome these difficulties by learning harder, spending more time in learning, buying expensive textbooks etc. All this produces more stress and anxiety, reduces the time students must have for other needs and thus, decreases the quality of students' life. Some students will be encouraged to practice academic dishonesty to achieve their final goal, by cheating at exams and making plagiarism in student works (Kiralj, 2022). It should be emphasized that two phenomena are increasing with time – human development and student dishonesty (Kiralj, 2020). Other students will give up of any study, thinking that studying is too hard, so that they cannot achieve their academic or non-academic purposes. A significant fraction of potential students will avoid hard studies. For example, it is known that the STEM (science, technology, engineering and mathematics) areas are significantly deficient in students for years, because STEM is considered to be too hard to study and not sufficiently interesting by many young people (UNESCO, 2022; Kennedy *et al*., 2018; Green, Rothschild, 2022).

This work deals with bibliometric analysis of selected university textbooks in various areas, with the purpose to observe common trends over time and their connection with the exponential growth of human knowledge. In addition, chemistry is taken as a case study: all main branches of chemistry (general, inorganic, organic, physical, analytical chemistry and biochemistry) and other selected branches are bibliometrically analyzed in terms of selected textbooks. Examples of un-updated and imprecise didactic elements in some chemistry textbooks, as a common consequence of uncontrolled and rapid increase of textbook size, are illustrated: spherical harmonics, mechanisms of nucleophilic substitution reactions, and structures and properties of nucleic acid bases. These three case studies are based on the lack of good chemical visualization, what is today a cornerstone of modern chemistry (Wu, Shah, 2004; Habraken, 1996; Patron, 2022). A special attention given to chemistry is indeed reasonable, because chemistry has gained the title of „the central science"

(Bertozzi, 2015; Brown *et al.*, 2020) due to its bridging the physical, life and applied sciences, and also because modern chemistry is „the most visual of sciences" (Habraken, 1996).

## 2. Methods

### 2.1. Bibliometric study for selected areas of knowledge

In order to assess the increase of knowledge in university textbooks, several areas of knowledge *i.e.*, areas of science, technology and arts, were selected (Table 1), as well as representative university textbooks and similar literature forms (manual, atlas) with at least five US editions in English. Data on the number of pages, ordinal number of edition and other bibliographic data, were acquired mainly online from various book publishers, booksellers and resellers, antiquarian booksellers, libraries, and from book reviews, and in certain cases determined using printed or pdf books. This way, a dataset was generated for each book studied. In some cases, when a book had more than one issue within an edition in the same year, data introducing minimum variation to the dataset were selected. Bibliometric descriptors were: number of pages, ordinal number of edition, font size, and the maximum number of characters in book (estimated from a page containing the maximum amount of text, including figure captions).

**Table 1.** Selected areas of knowledge with representative books published in multiple editions

| AREA | UDC[a] | *BOOK TITLE* (AUTHORS) | TYPE | EDS[b] | YEAR RANGE |
|---|---|---|---|---|---|
| Computer science | 0 | *Invitation to Computer Science* (Schneider, Gersting) | textbook | 8 | 1995-2018 |
| Statistics | 3 | *Introductory Statistics* (Mann)<br>*Introductory Statistics* (Weiss) | textbook<br>textbook | 11<br>11 | 1991-2021<br>1982-2015 |
| Sociology | 3 | *Sociology* (Macionis) | textbook | 17 | 1987-2018 |
| Law | 3 | *Borkowski's Textbook on Roman Law* (Borkowski, du Plessis) | textbook | 6 | 1994-2020 |
| Physics | 5 | *Fundamentals of Physics* (Halliday, Resnick) | textbook | 12 | 1960-2021 |
| Biochemistry | 5 | *Lehninger Principles of Biochemistry* (Lehninger *et al.*) | textbook | 8 | 1970-2021 |
| Medicine | 6 | *Guyton and Hall Textbook on Medical Physiology* (Guyton, Hall) | textbook | 14 | 1956-2020 |
| Mechanical engin. | 6 | *Mechanics of Materials* (Hibbeler) | textbook | 10 | 1985-2016 |

| | | | | | |
|---|---|---|---|---|---|
| Veterinary scien. | 6 | *The Merck Veterinary Manual* (several authors) | manual | 11 | 1955-2016 |
| Art history | 7 | *Gardner's Art Through Ages* (Gardner, Kleiner *et al.*) | textbook | 16 | 1926-2019 |
| Linguistics | 8 | *Linguistics: An Introduction to Language and Communication* (Akmajian *et al.*) | textbook | 7 | 1979-2017 |
| History | 9 | *The Times Complete History of the World* (Overy) | atlas | 9 | 1978-2015 |

[a]UDC – basic branch of the Universal Decimal Classification. [b]Eds – total number of editions.

Statistical analysis was concerned with visual and numerical identification, quantification and statistical testing of time-dependent trends, *i.e.* dependence of bibliometric descriptors, primarily of the number of pages, on the time variable. The correlation of the number of pages to the time variable was quantified by calculating the Pearson correlation coefficient and testing it by two-tailed $t$-test using online statistical tools *Pearson Correlation Coefficient Calculator* (Stangroom, J. Social Science Statistics; Toronto, ON, 2023: https://www.socscistatistics.com/tests/pearson/default2.aspx), *Value from Pearson (R) Calculator* (Stangroom, J. Social Science Statistics; Toronto, ON, 2023: https://www.socscistatistics.com/pvalues/pearsondistribution.aspx) and *Linear Correlation and Regression* at VassarStats (Lowry, R. Vassar College, Poughkeepsie, NY, 2022: http://vassarstats.net/corr_big.html). Corresponding scatterplots with linear regression line and the second-order polynomial (parabolic) regression curve were visually inspected using the *Polynomial Regression Data Fit* online software (Lutus, P. Beaverton, OR, 2022: https://arachnoid.com/polysolve/). Visual inspection of all the data and detailed regression analyses for aforementioned linear and parabolic regressions, as well as plotting scatterplots with the best regression models, was performed by using the *Scilab 5.5.2* software (Scilab Enterprises, S. A. S.; Versailles, 2015). $F$-test for both types of regression models was carried out using the *P-Value from F-Ratio Calculator (ANOVA)* online software (Stangroom, J. Social Science Statistics; Toronto, ON, 2023: https://www.socscistatistics.com/pvalues/fdistribution.aspx), and two-tailed $t$-test for statistical significance of all regression coefficients was made by means of the *P Value Calculator* at GraphPad online software (GraphPad Software, Inc.; La Jolla, CA, 2023: https://www.graphpad.com/quickcalcs/pValue1/). The significance level in all analyses was $\alpha = 0.05$. Additional simple parameters were calculated for the number of pages: range, the range divided by the number of pages (expressed as percentage), the range divided by the range of years, and the percentage divided by the range of years. These are quite simple indicators suitable to illustrate the increase of materials in the studied books.

## 2.2. Bibliometric analysis for various branches of chemistry

Bibliometric data for selected areas of chemistry were acquired online and sometimes determined from pdf and printed textbooks, in the very same way as the data for selected areas of knowledge. The areas of chemistry were (Table 2): the six main branches of chemistry (general, inorganic, organic, analytical, and physical chemistry and biochemistry) and eight selected minor areas (quantum, medicinal, solid state, organometallic, and structural chemistry, crystallography, spectroscopy and heterocyclic chemistry). Generation and analysis of bibliometric descriptors had the same steps and was carried out using the same set of software as for books from section 2.1.

Table 2. The major and some selected branches of chemistry with representative textbooks published in multiple editions

| BRANCH OF CHEMISTRY | *BOOK TITLE* (AUTHORS) | EDS[a] | YEAR RANGE |
|---|---|---|---|
| General chemistry | *Chemistry: The Central Science* (Brown *et al.*) | 15 | 1977-2021 |
| Inorganic chemistry | *Inorganic Chemistry* (Housecroft, Sharpe) | 5 | 2001-2018 |
| Organic chemistry | *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (March, Smith) | 8 | 1968-2020 |
| Analytical chemistry | *Fundamentals of Analytical Chemistry* (Skoog *et al.*) | 10 | 1963-2021 |
| Physical chemistry | *Atkins' Physical Chemistry* (Atkins *et al.*)<br>*Physical Chemistry* (Levine) | 12<br>6 | 1978-2022<br>1978-2017 |
| Biochemistry | *Biochemistry* (Stryer *et al.*) | 9 | 1975-2019 |
| Quantum chemistry | *Quantum Chemistry* (Levine) | 7 | 1970-2014 |
| Medicinal chemistry | *Introduction to Medicinal Chemistry* (Patrick) | 6 | 1995-2017 |
| Solid state chemistry | *Solid State Chemistry: An Introduction* (Smart, Moore) | 5 | 1992-2020 |
| Organometallic chem. | *The Organometallic Chemistry of the Transition Metals* (Crabtree) | 7 | 1988-2019 |
| Structural chemistry | *Structural Inorganic Chemistry* (Wells) | 5 | 1945-2012 |
| Crystallography | *Structure Determination by X-ray Crystallography* (Ladd, Palmer) | 5 | 1977-2013 |
| Spectroscopy | *Introduction to Spectroscopy* (Pavia *et al.*) | 5 | 1978-2015 |
| Heterocyclic chemist. | *Heterocyclic Chemistry* (Joule, Mills) | 5 | 1972-2013 |

[a]Eds – total number of editions.

## 2.3. Case studies in un-updated concepts in chemistry

Some negative side effects of exponentially grown knowledge, when incorporated into university textbooks, are growth of useless matter, matter of minor importance, and un-updated matter that does not employ modern computer-based tools. In chemistry, outdated concepts are noticeable as omission in using three-dimensional molecular graphics and other chemical visualization techniques, neglection of true molecular structures, *i.e.* experimentally determined or computationally modeled structures, and lack of accuracy in visualization and calculation. Three examples of un-updated concepts in chemistry are presented: real spherical harmonics as angular parts of atomic orbitals, molecular structures as a tool for understanding three-dimensional mechanisms of organic reactions, and three-dimensional molecular structures as means to illustrate structures and properties of nucleic acids.

### 2.3.1. Case study 1: spherical harmonics

Atomic orbitals or atomic wavefunctions are complex mathematical functions of three spatial variables, and their visualization is not straightforward. A natural way to present students atomic orbitals is to illustrate first the angular parts (surface spherical harmonics called simply spherical harmonics) and the radial parts (radial functions) of atomic orbitals (Kiralj, 1998). Then, three-dimensional examples of atomic orbitals are shown, usually in the form of cross-sections or boundary surfaces. For chemists, real spherical harmonics are useful, not imaginary or absolute spherical harmonics, and this is due to the fact that real spherical harmonics have spatial directions which explain well chemical bonding in molecules and crystals and intermolecular forces. In many textbooks, the concept of spherical harmonics (real, imaginary, absolute) is frequently unclear or mixed with atomic orbitals, or it is simply omitted. Why textbooks avoid the use of accurate computer-generated plots of real spherical harmonics for decades? It is hard to understand such a phenomenon in the computer age.

It is not hard making three-dimensional plots of real spherical harmonics for the most common *s*, *p* and *d* orbitals. Three plotting methods were employed in this work. Plots of real spherical harmonics as opaque surfaces were easily generated using the online software *Wolfram Mathematica in Wolfram Cloud* (Wolfram Research, Inc.; Champaign, IL, 2023: https://www.wolframcloud.com/), by selecting quantum numbers and plotting options. In a similar way, real spherical harmonics were plotted as transparent surfaces by means of the online *Desmos Graphing Calculator* (Desmos Studio, PBC, Beaverton, OR, 2023: https://www.desmos.com/calculator/le5w sdgfi6).

The third way of plotting spherical harmonics was a combination of simple calculations and hand-made technology of drawing curves on a sheet of paper. These plots of real spherical harmonics were made in the mid of 1990's by the author and have never been published, because at that time there already was no more interest in hand drawings. The procedure consisted of three steps. First, simple *FORTRAN* routines were written to calculate coordinates of points in spherical coordinate system (two angles varied by 10° increment, and the radius was the function value) and transform the coordinates for a specific normal projection to obtain new coordinates in a plane. Then, mechanical drawing techniques were employed in drawing curves through the points on a sheet of paper. Finally, using the same drawing techniques, the final plots of spherical harmonics were copied into a semi-transparent piece of paper. Although outdated and slow, this method of plotting spherical harmonics is sufficiently accurate, and it could have been used in chemistry textbooks for several decades, even before the appearance of the first modern computers.

### 2.3.2. Case study 2: mechanisms of nucleophilic substitution reactions

Molecular structures, absolute configuration, molecular conformations, intermolecular interactions, structures of crystals, molecular rearrangements and various chemical reactions in organic chemistry, are hard to understand and visualize in mind using only structural formulas. Such formulas mimic three-dimensional structures, but they are essentially two-dimensional objects with only certain three-dimensional information (Kiralj, Ferreira, 2003 a). It should be emphasized that plots of molecular structures made by means of molecular graphics methods are not only reliable molecular representations, but also a source of quantitative information about the molecules and even intermolecular interactions present (Kiralj *et al.*, 1999; Kiralj, Ferreira, 2003 b).

Detailed three-dimensional mechanisms of organic reactions, in which two or more species mutually react through transition structures and an intermediate, are very difficult to be absorbed by students. All becomes easier when three-dimensional molecular structures are used together with two-dimensional formulas along the chemical reaction mechanism. An example of unimolecular nucleophilic substitution reaction ($S_N1$), between a tertiary alcohol and hydrogen chloride in acidic medium was taken from Hornback's textbook *Organic Chemistry* (Hornback, 2006, p. 280), and was compared to bimolecular nucleophilic substitution reaction ($S_N2$). The textbook had an associated movie what was certainly helpful. The problem about movies is that they are usually not made using accurate molecular structures and they simplify reactions too much. Molecular structures of participants of the aforementioned chemical reactions were directly taken from chemical databases *PubChem*

(National Institutes of Health, Bethesda, MD, 2023: https://pubchem.ncbi.nlm.nih.gov/) and the *Cambridge Structural Database CSD* (The Cambridge Crystallographic Data Centre, Cambridge, 2023: https://www.ccdc.cam.ac.uk/structures/), or were obtained by simple molecular modeling of other structures retrieved from the databases. *PubChem* contains modeled molecular structures, *i.e.* the most stable conformers geometry-optimized at molecular mechanics level (PubChem$^3$D, 2019), and the *CSD* database has experimentally determined structures in crystalline state. Simple molecular modeling and molecular graphics was carried out by means of software *ViewerLite 4.2* (Accelrys, Inc., San Diego, CA, 2001). Molecular structures of tert-butyl alcohol and its chlorinated analogue were from the *PubChem* database (PubChem codes 517695 and 10486, respectively), whilst the protonated alcohol was modeled by adding a proton to the C-OH group. The chloride ion was extracted from the crystal structure of *L*-glutamic acid hydrochloride from the *CSD* database (CSD code LGLUTA03). The carbocation intermediate was modeled from the planar structure of a triphenylene derivative (CSD code APOLIB02). Wire and space filling or CPK *i.e.* Corey-Pauling-Koltun (Corey, Pauling, 1953; Koltun, 1965) molecular models were employed to illustrate $S_N1$ and $S_N2$ reaction mechanisms.

### 2.3.3. Case study 3: structures and properties of nucleic acid bases

Modern biochemistry, molecular biology and genetics are heavily based on the structure and properties of nucleic acids, in particular of deoxyribonucleic acid (DNA). However, modern biochemistry textbooks frequently neglect the importance of structures and properties of small molecules in biochemical processes. Three-dimensional illustration of small molecule structures, are scarce in biochemistry textbooks. Nucleic acid bases are usually presented by their two-dimensional formulas (structural formulas), and the same happens to hydrogen-bonded base pairs in DNA. There is no adequate set of molecular graphics plots for bases, base pair and smaller DNA oligomers in textbooks. That is why the structure of double-stranded DNA helix and its semi-flexibility is sometimes hard to be understood by students.

In this work, the five common nucleic acid bases adenine, guanine, thymine, cytosine and uracil, and their parent compounds purine and pyrimidine, were easily drawn using program *Biovia Draw 16.1* (Dassault Systèmes, Vélizy-Villacoublay, 2016), and then partially optimized at molecular mechanics level in *ACD/ChemSketch Freeware 2.5* (Advanced Chemistry Development, Inc., Toronto, ON, 2015). CPK models of the bases were generated by *ViewerLite 4.2* (Accelrys, Inc., San Diego, CA, 2001) to show spatial properties of the molecules. In addition, a structure of a DNA decamer, resolved by nuclear magnetic resonance, was retrieved from the *Protein Databank PDB* (Research Collaboratory for Structural Bioinformatics Protein Data Bank, Piscataway, NJ: https://www.rcsb.org/) (PDB code 1BUT). Illustrative examples of adenine-thymine and cytosine-guanine base pairs, as well as eight stacked base pairs, were extracted from the oligomer structure (structure model 1) and represented with ball-and-stick and CPK models, generated using *ViewerLite 4.2* (Accelrys, Inc., San Diego, CA, 2001). In the same way, a structure of a nucleosome was retrieved (PDB code 7D69), and 125 stacked base pairs were extracted and represented by a multicolored CPK model.

It is easy to find adequate molecular structures from chemical databases, and even to generate them by modern molecular modeling techniques, and then incorporate them into modern chemistry textbooks. Structural databases *Pubchem*, *CSD* and *PDB* were simply searched for molecular structures of the five nucleic acid bases and their parent compounds in various forms: modeled isolated molecules, as ligands in protein structures, and in various forms (neutral form, cationic, derivative, molecular complex, and other forms) in crystal structures of small molecules. Biochemistry textbooks could have been used such structures already some decades ago.

## 3. Results and discussion

### 3.1. Bibliometric study of university textbooks of selected areas of knowledge

Results of bibliometric analysis for 13 selected university textbooks of diverse areas of knowledge (Table 1) are presented in Tables 3 and 4, as well as on Figures 1 – 14. Exploration of No. pages *versus* time scatterplots, and inspection of the best regression models enabled classification of the textbook size increase into several types (type I – type VI), as is quoted in Tables 3 and 4.

**Table 3.** Statistics (*F*-test$^{a}$ and *t*-tests$^{b}$) for books with well visible time-dependent increase of the amount of material

| *BOOK TITLE*<br>[THE BEST MODEL$^{c}$]<br>[TIME DEPENDENCY$^{d}$] | $N^{e}$ | $R^{f}$ | $F$ | $p$ | $t_a$ | $p_a$ | $t_b$ | $p_b$ | $t_c$ | $p_c$ |
|---|---|---|---|---|---|---|---|---|---|---|
| ***Invitation to Computer Science*** [linear] [type I] | 8 | 0.8671<br>0.8784 | 18<br>8.4 | 0.0053<br>0.0249 | 4.114<br>0.645 | 0.0063<br>0.5471 | 4.263<br>0.652 | 0.0053<br>0.5433 | <br>0.659 | <br>0.5392 |
| ***Fundamentals of Physics*** [linear] [type I] | 16 | 0.7345<br>0.8042 | 16<br>12 | 0.0012<br>0.0012 | -3.699<br>1.952 | 0.0024<br>0.0728 | 4.050<br>-1.967 | 0.0012<br>0.0709 | <br>1.985 | <br>0.0686 |
| ***Lehninger Principles of Biochemistry*** [linear] [type I] | 12 | 0.8234<br>0.8400 | 21<br>11 | 0.0010<br>0.0041 | -4.162<br>-0.945 | 0.0019<br>0.3694 | 4.589<br>0.933 | 0.0010<br>0.3754 | <br>-0.918 | <br>0.3827 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| *Gardner's Art Through Ages* [linear] [type I] | 16 | 0.9405<br>0.9412 | 107<br>50 | <0.0001<br><0.0001 | 9.612<br>0.511 | <0.0001<br>0.6179 | 10.357<br>0.453 | <0.0001<br>0.6578 | 0.387 | 0.7053 |
| *The Merck Veterinary Manual* [parabolic] [type II] | 12 | 0.9162<br>0.9846 | 52<br>142 | <0.0001<br><0.0001 | -6.969<br>6.051 | <0.0001<br><0.0001 | 7.230<br>-6.113 | <0.0001<br><0.0001 | 6.180 | <0.0001 |
| *The Times Complete History of the World* [parabolic] [type II] | 29 | 0.8937<br>0.9340 | 107<br>89 | <0.0001<br><0.0001 | 9.535<br>3.818 | <0.0001<br>0.0007 | 10.349<br>3.844 | <0.0001<br>0.0007 | 3.874 | 0.0006 |

[a]*F*-test for linear and parabolic models: *F* - *F*-ratio, *p* - probability with respect to $\alpha = 0.05$; *F* and *p* are typed bold for statistically significant models. [b]*t*-tests for regression coefficients *a*, *b*, and *c* of linear ($y = a + bx$) and parabolic ($y = a + bx + cx^2$) regression models: $t_a$, $t_b$, and $t_c$ are *t*-parameters for *a*, *b*, and *c*, respectively; $p_a$, $p_b$, and $p_c$ are corresponding probabilities with respect to $\alpha = 0.05$; *t*-parameters and probabilities are typed bold for statistically significant models. [c]The best regression model proposed is linear or parabolic. [d]Type of time dependency (type I - type VII). [e]*N* - Number of data points. [f]*R* - Pearson correlation coefficient of *N* (observed *y*) and the time variable (*x*) for linear models, or of the observed and predicted *y* for parabolic models.

Table 4. Statistics (*F*-test[a] and *t*-tests[b]) for books with not so visible or even non-existing time-dependent increase of the amount of material

| BOOK TITLE [PROPOSED MODEL[c]] [TIME DEPENDENCY[d]] | *N*[e] | *R*[f] | *F* | *p* | $t_a$ | $p_a$ | $t_b$ | $p_b$ | $t_c$ | $p_c$ |
|---|---|---|---|---|---|---|---|---|---|---|
| *Borkowski's Textbook on Roman Law* [none] [type III] | 6 | 0.7049<br>0.8776 | 4.0<br>5.0 | 0.1410<br>0.1660 | -1.751<br>-1.896 | 0.1783<br>0.1984 | 1.988<br>1.893 | 0.1410<br>0.1989 | -1.888 | 0.1996 |
| *Linguistics: An Introduction to Language and Communication* [none] [type III] | 7 | 0.7540<br>0.9046 | *6.6*<br>**9.0** | *0.0502*<br>**0.0330** | 2.430<br>2.364 | 0.0594<br>0.0773 | 2.567<br>2.355 | 0.0502<br>0.0781 | 2.346 | 0.0789 |
| *Sociology* [none] [type IV] | 17 | 0.5366<br>0.5366 | **6.0**<br>2.8 | **0.0264**<br>0.0927 | -1.974<br>-0.025 | 0.0671<br>0.9801 | 2.463<br>0.022 | 0.0264<br>0.9825 | -0.017 | 0.9865 |
| *Guyton and Hall Textbook on Medical Physiology* [none] [type IV] | 14 | -0.1328<br>0.2404 | 0.2<br>0.3 | 0.6515<br>0.7214 | 1.015<br>-0.676 | 0.3319<br>0.5144 | -0.464<br>0.683 | 0.6515<br>0.5102 | -0.685 | 0.5090 |
| *Introductory Statistics* (Weiss) [none] [type IV] | 10 | 0.3934<br>0.6647 | 1.5<br>2.8 | 0.2607<br>0.1299 | -1.093<br>-1.904 | 0.3062<br>0.0987 | 1.210<br>1.901 | 0.2607<br>0.0991 | -1.898 | 0.0996 |
| *Introductory Statistics* (Mann) [linear] [type VI] | 12 | -0.6423<br>0.6740 | **7.0**<br>3.7 | **0.0243**<br>0.0656 | 2.882<br>0.841 | **0.0163**<br>0.4221 | **-2.650**<br>-0.835 | **0.0243**<br>0.4255 | 0.829 | 0.4285 |
| *Mechanics of Materials* [parabolic] [type V] | 10 | 0.7462<br>0.9575 | **10**<br>**39** | **0.0132**<br>**0.0002** | -3.063<br>**-5.539** | **0.0155**<br>**0.0009** | **3.171**<br>**5.524** | **0.0132**<br>**0.0009** | **-5.507** | **0.0009** |

[a]*F*-test for linear and parabolic models: *F* - *F*-ratio, *p* - probability with respect to $\alpha = 0.05$; *F* and *p* are typed bold for statistically significant models, and are typed italics for a model

with borderline statistical significance. [b]*t*-tests for regression coefficients *a*, *b*, and *c* of linear ($y = a + bx$) and parabolic ($y = a + bx + cx^2$) regression models: $t_a$, $t_b$, and $t_c$ are *t*-parameters for *a*, *b*, and *c*, respectively; $p_a$, $p_b$, and $p_c$ are corresponding probabilities with respect to $\alpha = 0.05$; *t*-parameters and probabilities are typed bold for statistically significant models. [c]The proposed regression model proposed is linear or parabolic, or no model is proposed. [d]Type of time dependency (type I - type VII). [e]*N* - Number of data points. [f]*R* - Pearson correlation coefficient of *N* (observed *y*) and the time variable (*x*) for linear models, or of the observed and predicted *y* for parabolic models.

The first four textbooks in Table 3 have type I increase (Figures 1 – 4): *Invitation to Computer Science*, *Fundamentals of Physics*, *Lehninger Principles of Biochemistry*, and *Gardner's Art Through Ages*. Type I increase is characterized by well visible situation of constant statistically significant linear increase, with no signs of retardation or eventual stabilization of the number of pages over time. Applying both *F*-test and *t*-test for all regression coefficients, one may notice that parabolic curve is in fact, not statistically significant (Table 3). Textbook *Invitation to Computer Science* has grown for 318 pages in 24 years, meaning a large increase of 54% with respect to the first edition. In other words, the textbook was gradually enlarging by 13.3 pages per year. It is understandable that computer science is a rapid growing area, but it does not show signs of stabilization in near future. Textbook *Fundamental of Physics* has grown for 452 pages or 42% in 62 years, meaning the annual growth of 7.3 pages. This growth is also significant and somewhat surprising, because physics is not a new science but it has a rich history of several centuries and though, should show some stabilization trends. *Lehninger Principles of Biochemistry* is a textbook from an area which experiences rapid and extensive growth together with genetics and other biosciences: in 52 years, the textbook has grown for 402 pages or 48%, what means 6.4 pages per year. *Gardner's Art Through Ages* exhibits a significant growth of 756 pages in 94 years, and this is an increase of 150% or 8.0 pages per year. Why this happens to the art's history textbook? One may guess that there is a rapid exchange of art styles in the 20th and 21st centuries, faster than in previous epochs. Due to the increase of at least 40% of the material, all the four textbooks are harder to be absorbed by students today than in the time of their first edition.

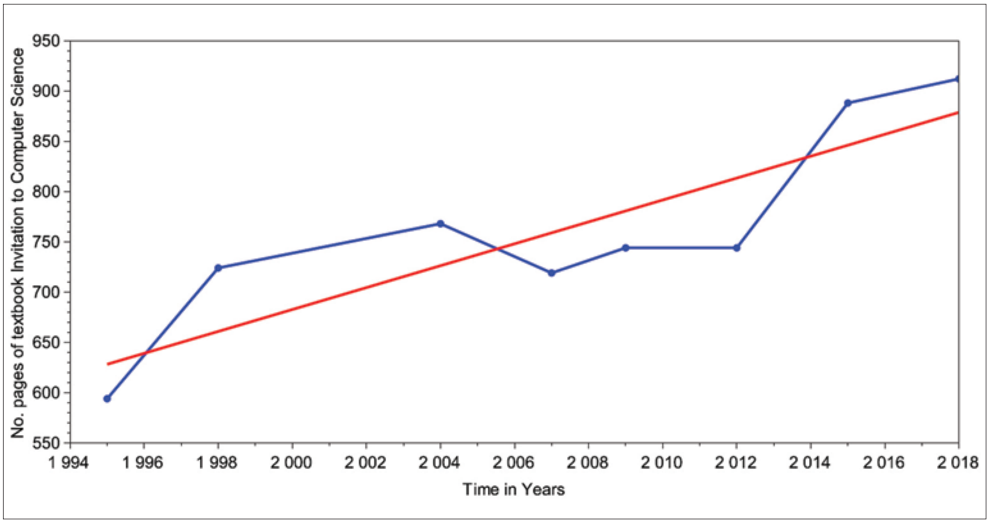


Figure 1. Increasing time dependency type I of the number of pages for textbook *Invitation to Computer Science* (blue) with statistically significant regression line (red, $y = 10.889(2.554) x - 21095(5127)$, $F = 18$, $R = 0.8671$, $p = 0.0053$).

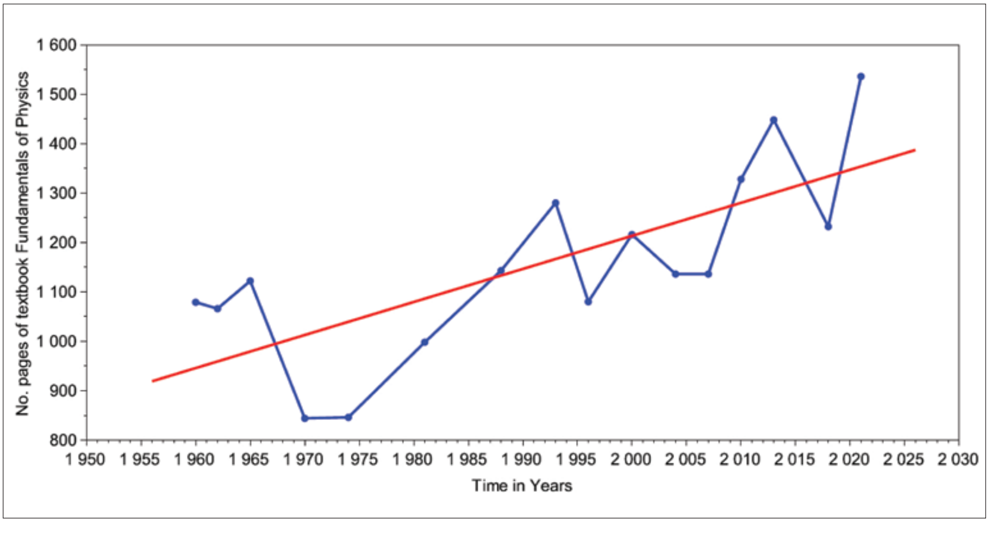


Figure 2. Increasing time dependency type I of the number of pages for textbook *Fundamentals of Physics* (blue) with statistically significant regression line (red, $y = 6.688(1.651) x - 12164(3289)$, $F = 16$, $R = 0.7345$, $p = 0.0012$).

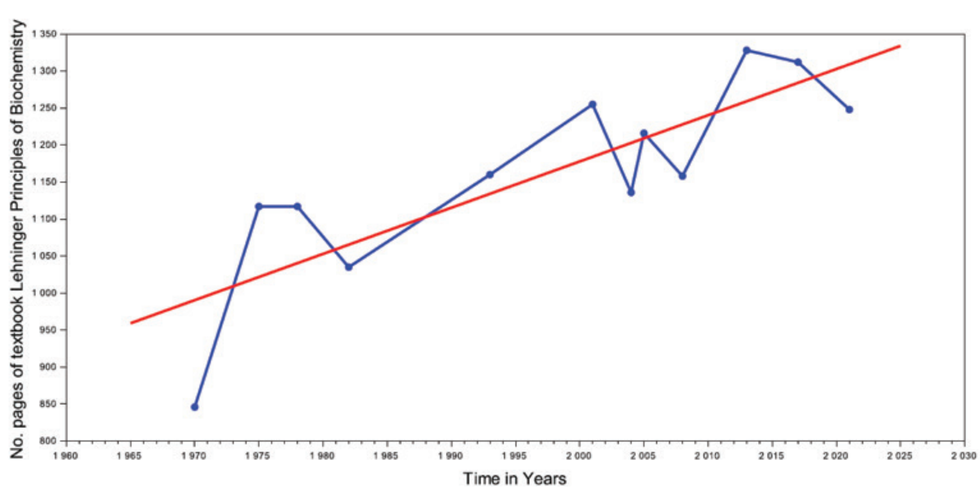


Figure 3. Increasing time dependency type I of the number of pages for textbook *Lehninger Principles of Biochemistry* (blue) with statistically significant regression line (red, $y = 6.247(1.361)\,x - 11316(2719)$, $F = 21$, $R = 0.8234$, $p = 0.0010$).

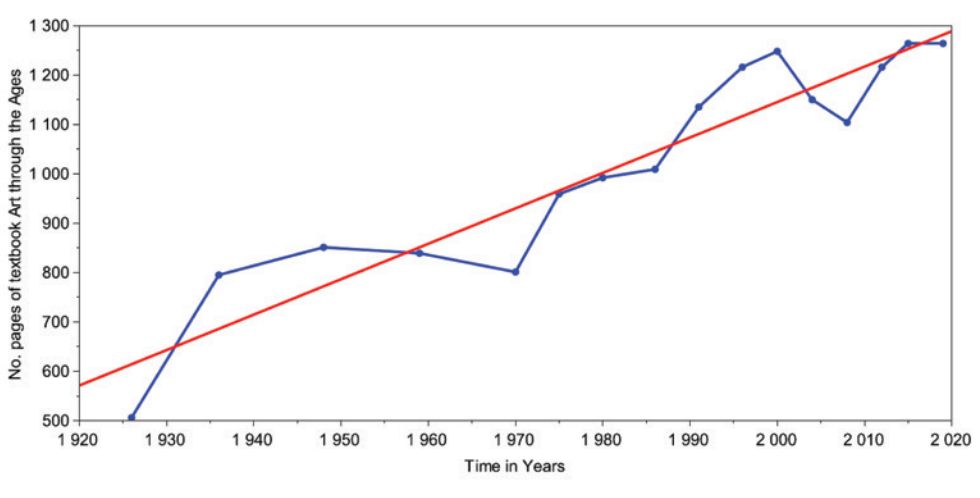


Figure 4. Increasing time dependency type I of the number of pages for arts textbook *Gardner's Art Through Ages – A Global History* (blue) with statistically significant regression line (red, $y = 7.177(0.693)\,x - 13208(1374)$, $F = 107$, $R = 0.9405$, $p < 0.0001$).

*The Merck Veterinary Manual* and atlas *The Times Complete History of the World* have type II increase (Figures 5 and 6): the most statistically significant model is the parabolic model (Table 3), which mimics a rapid, exponential growth. Linear regression is not a good model for the type II. Naturally, both books do not show signs of retardation or stabilization. The veterinary manual has grown for 1931 pages in 62 years, meaning the increase of 139% or 31 pages per year. Veterinary science belongs to a broad spectrum of life sciences still in rapid growth. The historical atlas on the other side, records numerous events of the latest history, what means more events per decade than in previous centuries. That is why the atlas has grown for 72 pages in 38 years, what means the increase of 20% or 1.9 pages per year.

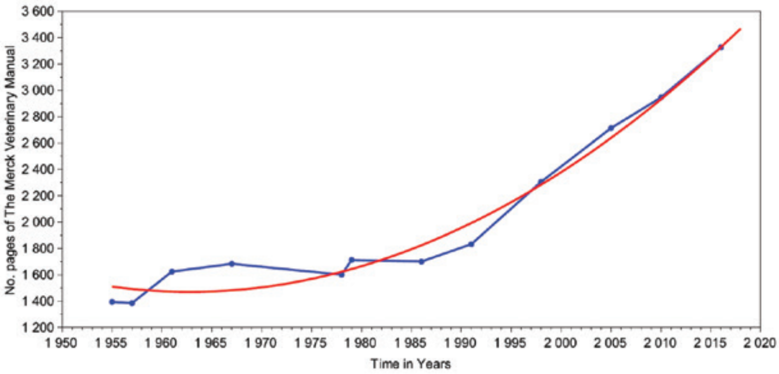


Figure 5. Increasing time dependency type II of the number of pages for textbook *The Merck Veterinary Manual* (blue) with statistically significant regression curve (red, $y = 2524833(417267) - 2571.2(420.6)\,x + 0.6550(0.1060)\,x^2$, $F = 142$, $R = 0.9846$, $p < 0.0001$).

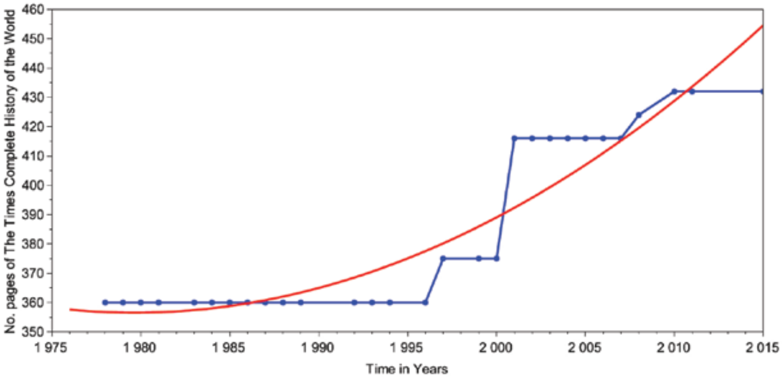


Figure 6. Increasing time dependency type II of the number of pages for historical atlas *The Times Complete History of the World* (blue) with statistically significant regression curve (red, $y = 307522(80541) - 310.3(80.7)\,x + 0.07838(0.02023)\,x^2$, $F = 89$, $R = 0.9340$, $p < 0.0001$).

*Borkowski's Textbook on Roman Law* and *Linguistics: An Introduction to Language and Communication* are two textbooks belonging to the type III increase. This type cannot be described by neither linear nor parabolic regression (Table 4). It can be better understood from scatterplots (Figures 7 and 8): there is a short initial increase, followed by longer retardation and saturation, and at the end there is a short decrease. Number of pages is not the best bibliometric measure, as it will be shown later in this work. In reality, probably there is a slow increase or a saturation area, but no decrease at all. In total, even observed data for the two textbooks show overall increase. The Borkowski's textbook has grown for 58 pages in 27 years or 15%, what accounts for 2.1 more pages every year. The linguistics textbook has grown for 251 pages in 39 years or by 70%, meaning 6.4 pages per year. Both textbooks belong to areas which, by their nature, have no rapid growth in modern times and so, a modest increase is to be expected.

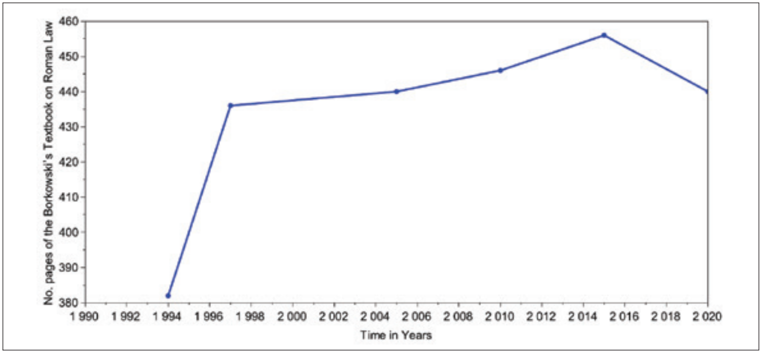


**Figure 7.** Irregular increasing time dependency type III of the number of pages for textbook *Borkowski's Textbook on Roman Law* (blue), without statistically significant regression line or curve.

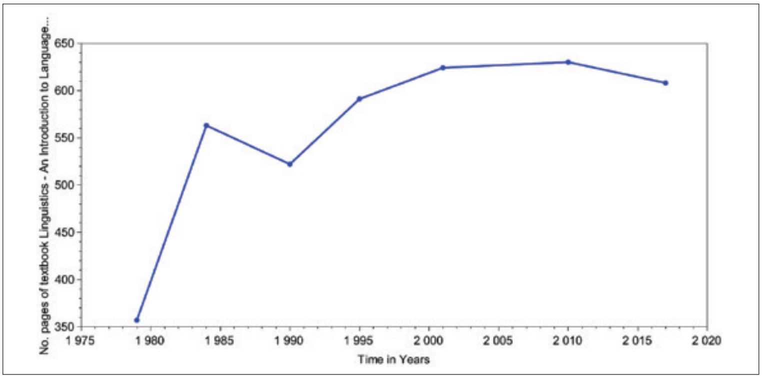


**Figure 8.** Irregular increasing time dependency type III of the number of pages for textbook *Linguistics: An Introduction to Language and Communication* (blue), without statistically significant regression line or curve.

Three textbooks belong to the type IV increase (Table 4): *Sociology*, *Guyton and Hall Textbook on Medical Physiology*, and Weiss' *Introductory Statistics* (Figures 9 – 11). Type IV increase is even more misleading than type III: no regression model can characterize it, and scatterplots show large oscillating tendencies– there is no increasing or decreasing tendency at all. In reality, a slow increase or stabilization tendencies exist, but the number of pages cannot show them. In overall, the textbook of sociology has grown by 15 pages in 32 years or only by 2%, or by 0.5 pages per year. The textbook of physiology has apparently decreased by 16 pages in 65 years or by 2%, meaning the reduction of 0.2 pages per year. The Weiss' textbook has grown for 197 pages in 34 years or by 30%, what means 5.8 pages per year. The three textbooks are from well established areas with long history and therefore, one would expect at least a modest increase or stabilization tendency for all of them.

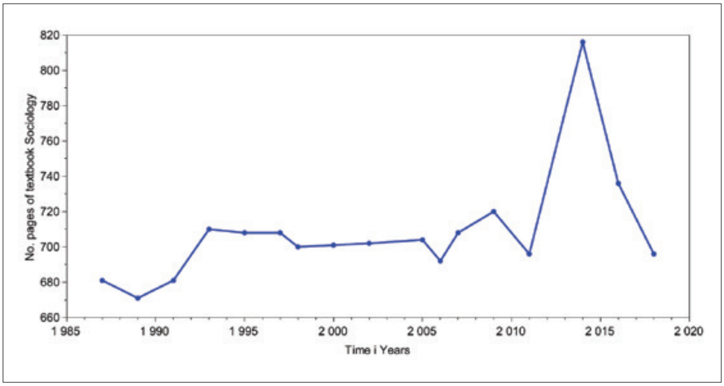


Figure 9. Irregular time dependency type IV of the number of pages for textbook *Sociology* (blue), without statistically significant regression line or curve.

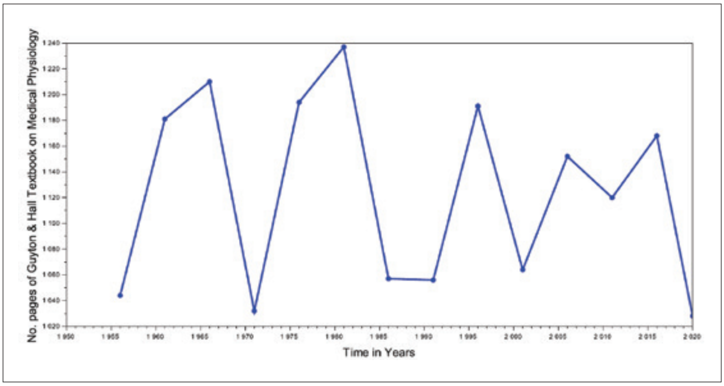


Figure 10. Irregular time dependency type IV of the number of pages for the *Guyton and Hall Textbook on Medical Physiology* (blue), without statistically significant regression line or curve.

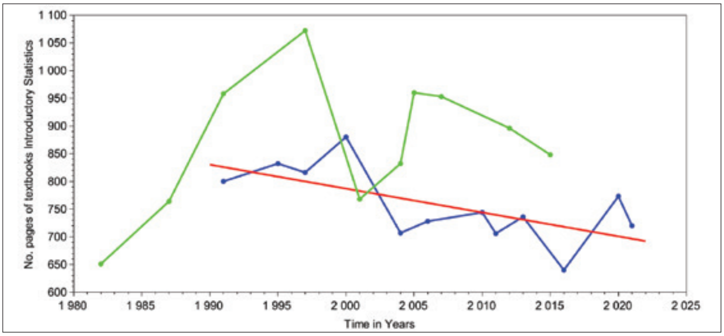


**Figure 11.** Time dependency of the number of pages for textbooks with the same title *Introductory statistics*: Mann's textbook (blue, type VI) with statistically significant regression line (red, $y = -4.308(1.626)\ x + 9402(3263)$, $F = 7$, $R = -0.6423$, $p < 0.03$), and Weiss' book (green, type IV) without statistically significant regression line or curve.

Two more increase types were observed, type V and VI (Table 4) as non-typical kinds of textbook increase in terms of the number of pages (Figures 11 and 12). The textbook *Mechanics of Materials* is an example of the type V non-linear increase: after rapid initial increase, there is a retardation and then stabilization tendency (Figure 12). Parabolic curve with its visible maximum is a statistically significant model, although it is not the best description because of a small fall after the maximum. The textbook has increased by 503 pages in 32 years or by 128%, what means 15.7 pages per year. Type VI increase means in fact negative increase or decrease (Figure 11). Mann's *Introductory Statistics* belong to this increase type: the falling regression line is statistically significant. This textbook shows the fall in the number of pages by 80 in 31 years, meaning the fall of 10% or 2.6 pages per year. In reality, there should be a small increase or stabilization, but not decrease in the quantity of material during time. Probably both textbooks *Introductory Statistics* and *Mechanics of Materials* came to the region of stabilization, as it happens in their respective scientific areas.

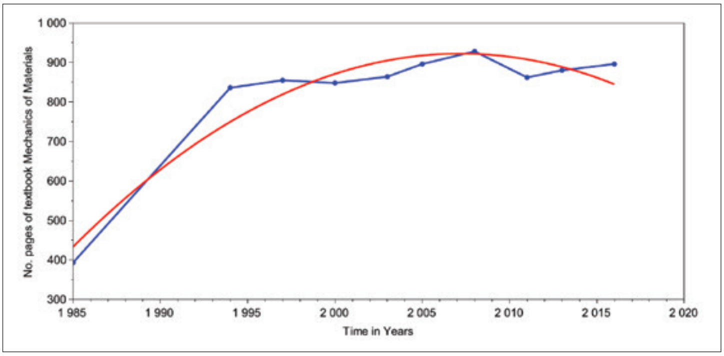


**Figure 12.** Increasing time dependency type V of the number of pages for textbook *Mechanics of Materials* (blue) with statistically significant regression curve (red, $y = -4003933(722805) + 3990.5(722.4)\ x - 0.99406(0.18051)\ x^2$, $F = 39$, $R = 0.9575$, $p = 0.002$).

More reliable statistics would be obtained if some other quantities were measured for all editions and issues of the 13 analyzed books, what is practically an impossible task. Instead of that, limited estimations can be made. In this sense, four electronic (pdf) editions of *Guyton and Hall Texytbook of Medical Physiology* were inspected in terms of the number of pages, font size and the maximum number of characters. While the number of pages undoubtedly decreases with time (Figure 13 left), the number of characters has different trend, irregular increasing – decreasing trend with posterior stabilization (Figure 13 right). What is the reason for such differences in behavior of the two parameters? Obviously, text density gradually increased from the 11th to the 14th edition (Figure 14): font size decreased after the 11th edition, spaces within the text gradually decreased, and there were some changes in margins.

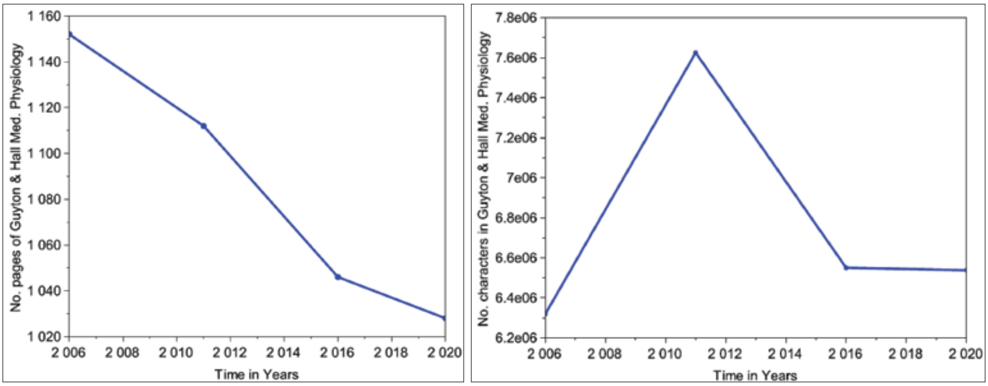


Figure 13. Example of comparing two bibliographic parameters for the 11th, 12th, 13th and 14th editions of the textbook *Guyton and Hall Textbook on Medical Physiology*. While the number of pages decreases by time (left), the maximal number of characters does not have a general decreasing tendency (right).

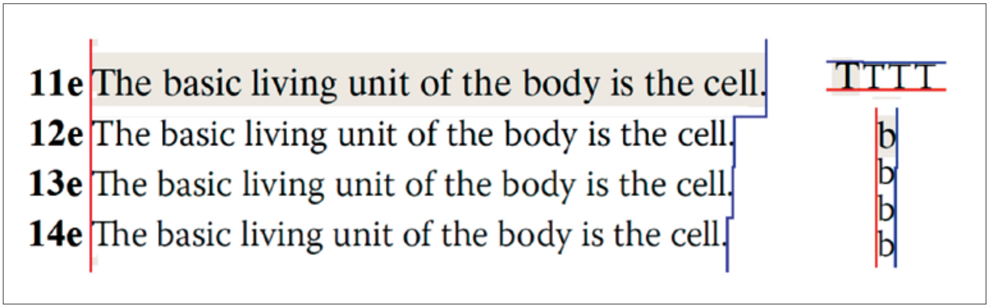

**11e** The basic living unit of the body is the cell.
**12e** The basic living unit of the body is the cell.
**13e** The basic living unit of the body is the cell.
**14e** The basic living unit of the body is the cell.

Figure 14. Example of condensing the text in the 11th, 12th, 13th and 14th editions of the textbook *Guyton and Hall Textbook on Medical Physiology* in pdf format. Font size was reduced in the 12th edition and then kept unchanged (see examples of letter T and b). The total space between letters was gradually reduced after the 12th edition.

Number of pages, although not being the best bibliometric descriptor, is the one for which data can be acquired for all textbooks studied. This descriptor may be converted into time required for regular study of a textbook in question. The number of pages of a standard size textbook written in English, read in an hour (at reading rate about 100 words per minute), is a useful parameter in estimating the total time for reading a particular textbook or its part. Based on students' self-reported values (Quora, 2020 a; Quora, 2020 b; Reddit, 2015) and estimated values (Klatt, Klatt, 2011; Cornell College, 2023) of this parameter, one can use the following data: 4 pages per hour for physics; 6 pages per hour for statistics; 8 pages per hour for computer science and technical sciences; 10 pages per hour for biochemistry; 12 pages per hour for arts, humanities, social sciences, and medical sciences. It is interesting to estimate the time students have to spend additionally, with respect to the first issue of a textbook. Therefore, the difference in the number of pages between the last and the first edition may be converted into the number of additional hours to read the book, what, when divided by 15 (number of weeks per semester) and by 7, yields the number of minutes per day. For books from Table 1, the following extension times per day were obtained. There is no increase or is less than 10 minutes per day for *Introductory Statistics* (Mann), *Borkowski's Textbook on Roman Law*, *The Times Complete History of the World*, *Guyton and Hall Textbook on Medical Physiology*, and *Sociology*. Textbooks with 10-20 minutes per day are *Introductory Statistics* (Weiss), and *Linguistics: An Introduction to Language and Communication*. A textbook within 21-30 minutes per day is *Invitation to Computer Science*. Two textbooks are within the range of 31-40 minutes per day: *Mechanics of Materials* and *Gardner's Art Through Ages*. *Fundamentals of Physics* falls in the range of 50-70 minutes per day, and *The Merck Veterinary Manual* in the range of 71-100 minutes per day. Reading textbooks with more than 10 minutes of study per day with respect to their first editions, mean significant increase of time spent for study. For example, if a student has four such textbooks per semester, each of which requires 25 minutes study a day longer than its respective first edition, there will be in total 100 minutes, almost two hours dedicated more to regular study. A student will need an extra time for preparing for the exams and so, the effective time difference would exceed two hours per day.

## 3.2. Bibliometric study of university textbooks of chemistry

Results of bibliometric analysis for selected university textbooks of main and some minor branches of chemistry (Table 2) are presented in Tables 5 and 6, and on Figures 15 – 20. Analysis of No. pages *versus* time scatterplots and inspection of regression models revealed a very similar classification of increase types to those from section 3.1: type I – type V and novel type VII were identified, as is quoted in Tables 5 and 6.

**Table 5.** Statistics (*F*-test[a] and *t*-tests[b]) for textbooks of major branches of chemistry

| BOOK TITLE [THE BEST MODEL[c]] [TIME DEPENDENCY[d]] | $N$[e] | $R$[f] | $F$ | $p$ | $t_a$ | $p_a$ | $t_b$ | $p_b$ | $t_c$ | $p_c$ |
|---|---|---|---|---|---|---|---|---|---|---|
| *Chemistry: The Central Science* [linear] [type I] | 17 | 0.8766 | **50** | **<0.0001** | **-6.626** | **<0.0001** | **7.055** | **<0.0001** | | |
| | | 0.8808 | **24** | **<0.0001** | -0.716 | 0.4860 | 0.696 | 0.4978 | -0.674 | 0.5115 |
| *Biochemistry* [linear] [type I] | 9 | 0.9025 | **31** | **0.0009** | **-5.171** | **0.0013** | **5.544** | **0.0009** | | |
| | | 0.9086 | **14** | **0.0053** | 0.585 | 0.5797 | -0.600 | 0.5708 | 0.616 | 0.5606 |
| *Fundamentals of Analytical Chemistry* [linear] [type I] | 11 | 0.9017 | **39** | **0.0001** | **-5.725** | **0.0003** | **6.257** | **0.0001** | | |
| | | 0.9094 | **19** | **0.0009** | 0.750 | 0.4747 | -0.773 | 0.4616 | 0.801 | 0.4460 |
| *Atkins' Physical Chemistry* [none] [type IV] | 18 | 0.3064 | 1.6 | 0.2162 | -0.975 | 0.3439 | 1.288 | 0.2162 | | |
| | | 0.3064 | 0.8 | 0.4773 | -0.019 | 0.9852 | 0.017 | 0.9867 | -0.013 | 0.9896 |
| *Physical Chemistry* (Levine) [linear] [type I] | 10 | 0.8781 | **27** | **0.0008** | **-4.525** | **0.0019** | **5.191** | **0.0008** | | |
| | | 0.9333 | **24** | **0.0008** | *-2.364* | *0.0500* | *2.350* | *0.0511* | *-2.331* | *0.0526* |
| *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* [linear] [type I] | 8 | 0.9116 | **29** | **0.0016** | **-5.234** | **0.0020** | **5.430** | **0.0016** | | |
| | | 0.9185 | **13** | **0.0097** | -0.672 | 0.5314 | 0.654 | 0.5418 | -0.635 | 0.5532 |
| *Inorganic Chemistry* [linear] [type I] | 5 | 0.9522 | **29** | **0.0125** | **-5.298** | **0.0131** | **5.400** | **0.0124** | | |
| | | 0.9853 | **33** | **0.0291** | -2.119 | 0.1682 | 2.110 | 0.1694 | -2.100 | 0.1706 |

[a] *F*-test for linear and parabolic models: *F* – *F*-ratio, *p* – probability with respect to $\alpha = 0.05$; *F* and *p* are typed bold for statistically significant models. [b] *t*-tests for regression coefficients *a*, *b*, and *c* of linear ($y = a + bx$) and parabolic ($y = a + bx + cx^2$) regression models: $t_a$, $t_b$, and $t_c$ are *t*-parameters for *a*, *b*, and *c*, respectively; $p_a$, $p_b$, and $p_c$ are corresponding probabilities with respect to $\alpha = 0.05$; *t*-parameters and probabilities are typed bold for statistically significant models. [c] The best regression model proposed is linear or parabolic. [d] Type of time dependency (type I – type VII). [e] *N* – Number of data points. [f] *R* – Pearson correlation coefficient of *N* (observed *y*) and the time variable (*x*) for linear models, or of the observed and predicted *y* for parabolic models.

**Table 6.** Statistics (*F*-test[a] and *t*-tests[b]) for textbooks of selected branches of chemistry

| BOOK TITLE [THE BEST MODEL[c]] [TIME DEPENDENCY[d]] | $N$[e] | $R$[f] | $F$ | $p$ | $t_a$ | $p_a$ | $t_b$ | $p_b$ | $t_c$ | $p_c$ |
|---|---|---|---|---|---|---|---|---|---|---|
| *Structural Inorganic Chemistry* [parabolic] [type V] | 16 | 0.9442 | **115** | **<0.0001** | **10.353** | **<0.0001** | **10.745** | **<0.0001** | | |
| | | 0.9828 | **184** | **<0.0001** | **-5.475** | **0.0001** | **5.394** | **0.0001** | **-5.305** | **0.0001** |
| *Quantum Chemistry* [linear] [type I] | 9 | 0.8740 | **23** | **0.0021** | **-4.438** | **0.0030** | **4.759** | **0.0021** | | |
| | | 0.8768 | **10** | **0.0124** | 0.328 | 0.7539 | -0.340 | 0.7454 | 0.354 | 0.7356 |
| *Introduction to Medicinal Chemistry* [parabolic] [type V] | 6 | 0.8955 | **16** | **0.0158** | **-3.959** | **0.0167** | **4.025** | **0.0158** | | |
| | | 0.9821 | **41** | **0.0067** | **-3.737** | **0.0334** | **3.723** | **0.0337** | **-3.709** | **0.0341** |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| ***Introduction to Spectroscopy*** **[none] [type III]** | 7 | 0.7794 | **7.7** | **0.0388** | *-2.647* | *0.0456* | *2.781* | *0.0388* | | |
| | | 0.9159 | **10** | **0.0260** | 2.374 | 0.0765 | -2.385 | 0.0756 | 2.397 | 0.0746 |
| ***Heterocyclic Chemistry*** **[parabolic] [type II]** | 15 | 0.9165 | **68** | **<0.0001** | **-8.036** | **<0.0001** | **8.263** | **<0.0001** | | |
| | | 0.9472 | **52** | **<0.0001** | **2.523** | **0.0268** | **-2.551** | **0.0254** | **2.581** | **0.0241** |
| ***The Organometallic Chemistry of the Transition Metals*** **[parabolic] [type VII]** | 8 | 0.2611 | 0.4 | 0.5322 | -0.513 | 0.6260 | 0.663 | 0.5322 | | |
| | | 0.9528 | **25** | **0.0026** | **-5.475** | **0.0028** | **5.394** | **0.0030** | **-5.305** | **0.0032** |
| ***Solid State Chemistry: An Introduction*** **[none] [type III]** | 6 | 0.7429 | 4.9 | 0.0907 | -2.122 | 0.1012 | 2.219 | 0.0907 | | |
| | | 0.9384 | 11 | 0.0413 | -2.887 | 0.0632 | 2.881 | 0.0635 | -2.874 | 0.0639 |
| ***Structure Determination by X-ray Crystallography*** **[linear] [type I]** | 5 | 0.9292 | **19** | **0.0224** | **-4.242** | **0.0240** | **4.355** | **0.0224** | | |
| | | 0.9496 | 9.2 | 0.0983 | -0.904 | 0.4615 | 0.893 | 0.4660 | -0.882 | 0.4708 |

[a]$F$-test for linear and parabolic models: $F$ – $F$-ratio, $p$ – probability with respect to $\alpha = 0.05$; $F$ and $p$ are typed bold for statistically significant models. [b]$t$-tests for regression coefficients $a$, $b$, and $c$ of linear ($y = a + bx$) and parabolic ($y = a + bx + cx^2$) regression models: $t_a$, $t_b$, and $t_c$ are $t$-parameters for $a$, $b$, and $c$, respectively; $p_a$, $p_b$, and $p_c$ are corresponding probabilities with respect to $\alpha = 0.05$; $t$-parameters and probabilities are typed bold for statistically significant models. [c]The best regression model proposed is linear or parabolic. [d]Type of time dependency (type I – type VII). [e]$N$ – Number of data points. [f]$R$ – Pearson correlation coefficient of $N$ (observed $y$) and the time variable ($x$) for linear models, or of the observed and predicted $y$ for parabolic models.

Statistically significant linear increasing trends of the type I for three chemistry textbooks are presented in Figure 15 and Table 5: *Chemistry: The Central Science*, *Biochemistry* (Stryer), and *Fundamentals of Analytical Chemistry*. Parabolic curve is not statistically significant (Table 5). Textbook *Chemistry: The Central Science* has grown for 505 pages in 45 years, meaning a large increase of 62% with respect to the first edition. It was gradually enlarging, by 11.2 pages per year. Hamilton has criticized the first thirty-five years of this textbook (Hamilton, 2006), which was already increasing in size and costs, and was sold with supplementary materials: „Who has time to utilize all of these extra materials? Is the general chemistry textbook market driven by actual need or by profit?" One may raise the same questions for other chemistry textbooks. Stryer's *Biochemistry* has grown for 419 pages or 48% in 45 years, meaning the annual growth of 9.3 pages. *Fundamentals of Analytical Chemistry* has grown for 286 pages or 36%, what means 4.8 pages per year.

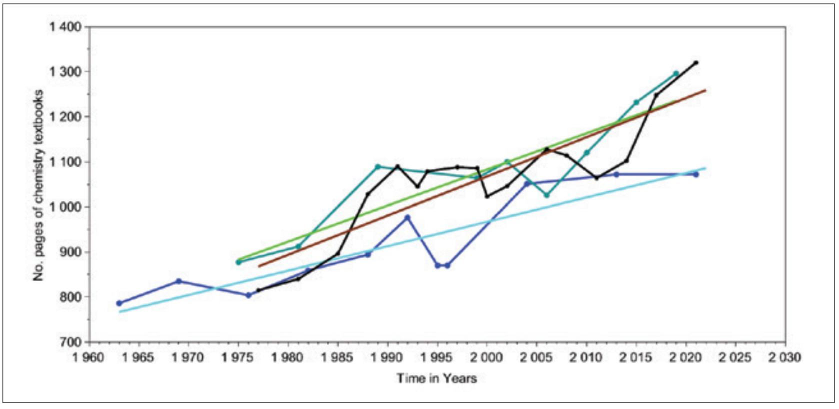


**Figure 15.** Time dependency type I of the number of pages for three chemistry textbooks with statistically significant regression lines: for *Chemistry: The Central Science* (blue and cyan, $y = 8.698(1.233)\ x - 16329(2464)$, $F = 60$, $R = 0.8766$, $p < 0.0001$); for *Biochemistry* (dark and light green, $y = 8.013(1.445)\ x - 14944(2890)$, $F = 31$, $R = 0.9025$, $p = 0.0009$); for *Fundamentals of Analytical Chemistry* (black and dark brown, $y = 5.412(0.865)\ x - 9856(1722)$, $F = 39$, $R = 0.9017$, $p = 0.0001$).

Figure 16 illustrates increasing types for two physical chemistry textbooks: *Atkins' Physical Chemistry* with oscillating type IV increase, and Levin's *Physical Chemistry* with linear type I increase, which is statistically significant (Table 5). The Atkin's textbook shows apparent decrease of 42 pages in 45 years or 4%, or the reduction in the number of pages by 0.9 pages per year. But Levin's textbook shows the opposite trend: the increase of 132 pages in 40 years or 15% increase, what means 3.3 pages more every year. How to explain such different trends for the same main branch chemistry? As it was said already in this work, number of pages is a very rough measure of textbook increase. There is always some increase in the quantity of matter, even a small one, but is not easily detected. Two bibliographic measures for six editions of the Atkin's textbook show almost opposite trends: the number of pages is initially growing and then it is constantly falling (Figure 17 left), but the total number of characters has a constant increasing tendency (Figure 17 right).

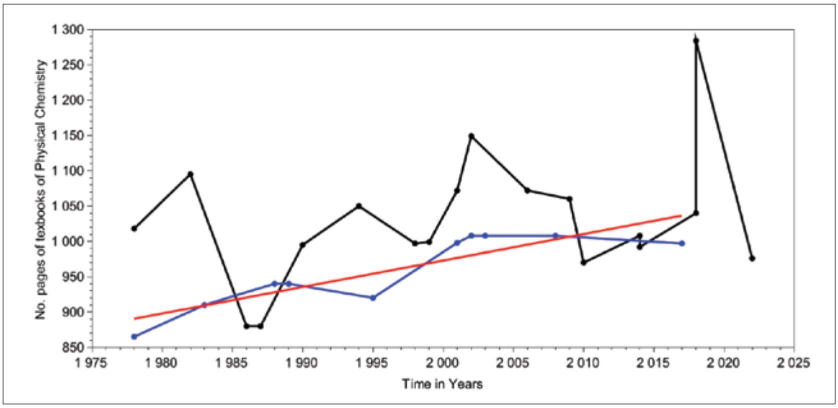


**Figure 16**. Time dependency of the number of pages for two physical chemistry textbooks: for Levin's *Physical Chemistry* (blue and red, type I, $y = -3.745(0.721)\ x - 6516(1440)$, $F = 27$, $R = 0.8781$, $p = 0.0008$); for *Atkins' Physical Chemistry* (black, type IV, no statistically significant regression line or curve).

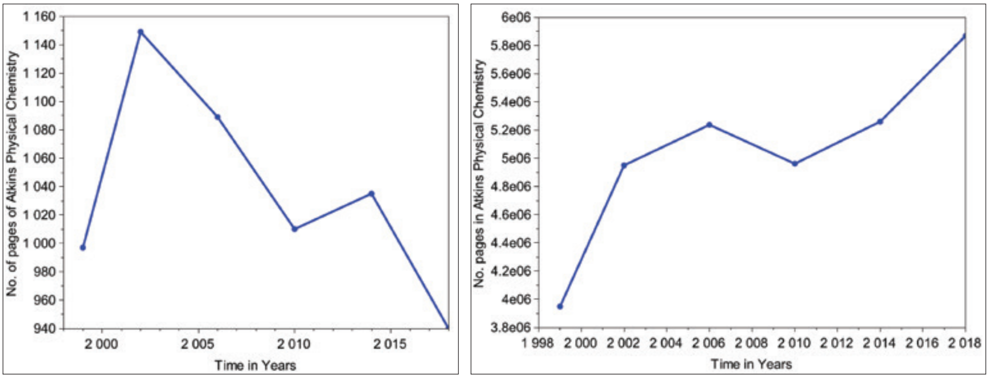


**Figure 17.** Example of comparing two bibliographic parameters for the 6th, 7th, 8th, 9th, 10th and 11th editions of the textbook *Atkins' Physical Chemistry*. While the number of pages mainly decreases by time (left), the maximal number of characters has an irregular increasing tendency (right).

Figure 18 shows increasing tendencies for three chemistry textbooks: *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* with type I increase, *Inorganic Chemistry* also with type I increase, and *Structural Inorganic Chemistry* with parabolic type V increase. The corresponding lines and the curve are statistically significant (Table 5 and Table 6). The two lines are almost parallel due to similar values of the respective regression coefficients. However, *Structural Inorganic Chemistry* experiences stabilization since the mid of 1980's (the book was reprinted several times). The textbook of organic chemistry has grown by 1046 pages or by 95% in 53 years, with the rate of 19.7 pages per year. The textbook of inorganic chemistry has grown less, by 464 pages or by 56% in 18 years, meaning the growth of 25.8 pages per year. The textbook of inorganic structural chemistry has grown by 816 pages or by 136%, what means the increase of 12.0 pages per year. All three textbooks have large increase in the amount of matter.

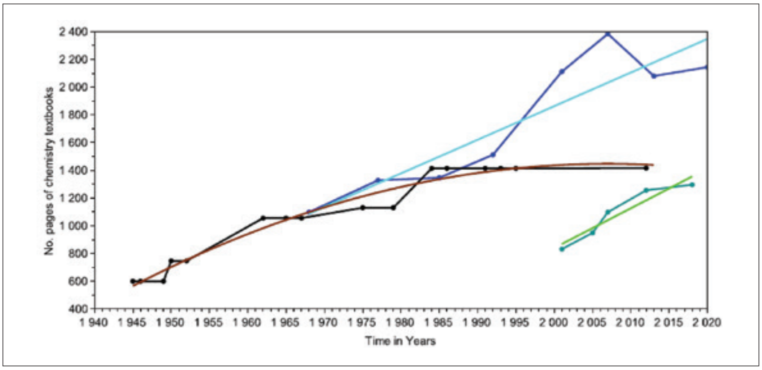


**Figure 18**. Time dependency of the number of pages for three chemistry textbooks with statistically significant regression lines or curves: for *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (blue and cyan, type I, $y = 24.247(4.465)\,x - 46631(8910)$, $F = 28$, $R = 0.9116$, $p < 0.0016$); for *Inorganic Chemistry* (dark and light green, type I, $y = 28.013(5.300)\,x - 56393(10644)$, $F = 29$, $R = 0.9522$, $p = 0.0125$); for *Structural Inorganic Chemistry* (black and dark brown, type V, $y = -913927(166917) + 912.1(169.1)\,x - 0.22721(0.04283)\,x^2$, $F = 184$, $R = 0.9828$, $p < 0.0001$).

Diverse increasing tendencies for four chemistry textbooks are shown in Figure 19: *Quantum Chemistry* (linear type I), *Heterocyclic Chemistry* (increasing parabolic type II), *Introduction to Spectroscopy* (irregular type III), and *Introduction to Medicinal Chemistry* (increasing parabolic with stabilization, type V). Presented lines or parabolas are statistically the most significant regression models (Table 6). The textbook of quantum chemistry has increased by 129 pages or 22% in 45 years, what means the rate of 2.9 pages per year. *Heterocyclic Chemistry* has grown by 348 pages or 94% in 42 years, with high rate of 8.3 pages per year. The textbook of spectroscopy has grown by 184 pages or 31%, meaning 4.8 pages per year. Textbook *Introduction to Medicinal Chemistry* has grown by 496 pages or by 148%, meaning 21.6 pages per year. This group of textbooks have large increase of matter too.

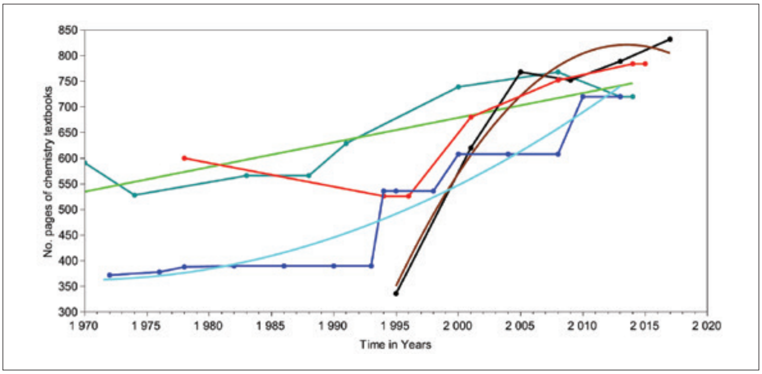


**Figure 19**. Time dependency of the number of pages for four chemistry textbooks with or without statistically significant regression line or curve: for *Heterocyclic Chemistry* (blue and cyan, type II, $y = 782961(310321) - 794.62(311.48)\ x + 0.20171(0.07816)\ x^2$, $F = 68$, $R = 0.9165$, $p < 0.0001$); for *Quantum Chemistry* tones (dark and light, type I, $y = 4.807(1.010)\ x - 8936(2014)$, $F = 23$, $R = 0.8740$, $p = 0.0021$); for *Introduction to Medicinal Chemistry* (black and dark brown, type V, $y = -5559330(1487798) + 5522.8(1483.3)\ x - 1.37143(0.36972)\ x^2$, $F = 41$, $R = 0.9821$, $p = 0.0067$); for *Introduction to Spectroscopy* (red, type III, no regression line or curve).

The increase of the last group of three chemistry textbooks is illustrated on Figure 20 and in Table 6: *Structure Determination by X-ray Crystallography* (linear type I increase), *Solid State Chemistry: An Introduction* (type III), and *The Organometallic Chemistry of the Transition Metals* (novel parabolic type VII). The regression line for the type I and the regression curve (parabola) for the type VII increase are statistically significant models. The type VII (Figure 20) is similar to the type V (Figure 12), but the maximum and the posterior decrease are more pronounced in the type VII. In reality, there is no decrease of the amount of matter, but the text must be denser as the number of pages is decreasing. The crystallography textbook has grown by 381 pages or 95% in 37 years, what corresponds to the rate of 10.3 pages per year. The textbook of solid state chemistry has grown by 150 pages or 51% in 29 years, meaning 5.2 pages per year. *The Organometallic Chemistry of the Transition Metals* has grown by only 42 pages or 10%, meaning only 1.3 pages per year.

When analyzing the increasing statistics for all 16 selected chemistry textbooks (Table 2) and *Lehninger Principles of Biochemistry* (from Table 1), the increase ranges from 10% to 148%, and the increasing rate from 1.3 to 21.6 pages per year. Only *Atkins's Physical Chemistry* was excluded due to its highly irregular trend (Figure 16). In fact, all branches of chemistry exhibit the increase in the amount of matter in textbooks, although at different levels. Branches dealing with diversity of novel organic and inorganic compounds have the largest increase (medicinal chemistry, organic che-

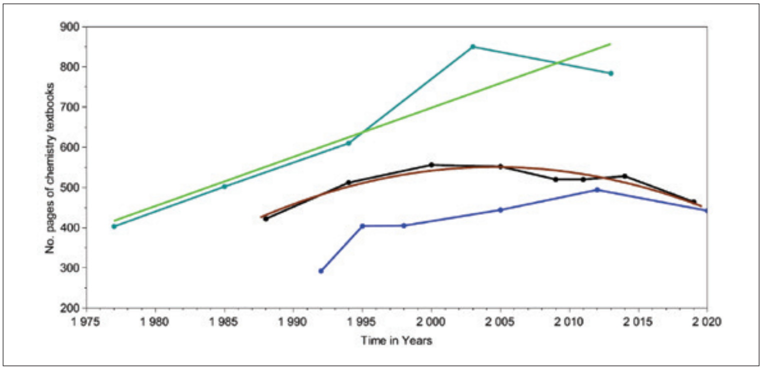


Figure 20. Time dependency of the number of pages for three chemistry textbooks with or without statistically significant regression line or curve: for *Solid State Chemistry: An Introduction* (blue, type III, no regression line or curve); for *Structure Determination by X-ray Crystallography* (dark and light green, type I, $y = 12.226(2.808)\, x - 23753(5600)$, $F = 19$, $R = 0.9292$, $p = 0.0224$); for *The Organometallic Chemistry of the Transition Metals* (black and dark brown, type VII, $y = -1745912(258543) + 1742.5(258.1)\, x - 0.43462\ (0.06442)\, x^2$, $F = 25$, $R = 0.9528$, $p = 0.0026$).

mistry, heterocyclic chemistry, structural chemistry, and crystallography). Branches more interested in properties and processes involving matter, have the smallest increase (physical chemistry, quantum chemistry, and spectroscopy). Organometallic chemistry of the transition metals is an exception; it seems that the branch is already in stabilization of its textbooks. Other branches have significant increase in size of textbooks. It is reasonable that the increase of textbooks is noticeable in all branches of chemistry, because chemistry is a STEM area, still in pronounced progress.

Using the data on students' self-reported values (Quora, 2020 a; Quora, 2020 b; Reddit, 2015) and estimated values (Klatt, Klatt, 2011; Cornell College, 2023) of the number of pages read in one hour, one can set up the following values for chemistry branches: 6 pages per hour for physical chemistry, spectroscopy, crystallography, solid state chemistry and structural chemistry; 10 pages per hour for biochemistry and medicinal chemistry; and 8 pages per hour for all other branches of chemistry. Then, the increase in the number of pages of the last edition with respect to the first edition may be converted in additional time student has to spend per day when reading it. Less than 10 minutes per day are necessary for *The Organometallic Chemistry of the Transition Metals* and apparently for *Atkins's Physical Chemistry*. Between 10 and 20 minutes per day one must spend for Levin's *Physical Chemistry*, *Fundamentals of Analytical Chemistry*, *Quantum Chemistry*, *Introduction to Spectroscopy*, and *Solid State Chemistry: An Introduction*. The time of 21-30 minutes is required for: *Lehninger Principles of Biochemistry, Introduction to Medicinal Chemistry*, and *Heterocyclic Chemistry*. About 31-40 minutes one needs for *Chemistry: The Central Science*, *Structure*

*Determination by X-ray Crystallography*, and *Inorganic Chemistry*. Stryer's *Biochemistry* falls into range 50-70 minutes per day, and *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* and *Structural Inorganic Chemistry* into 71-100 minutes per day. The average value for chemistry textbooks is 33 minutes per day. Supposing that a student has four chemistry textbooks in a semester, reading them will take 132 minutes longer than their first issues, what is more than two hours per day. This time may double when taking into account more intensive preparations for exams and studying additional electronic, online and eventual printed supplementary materials to the textbooks (for example, problem solutions). One should not forget that the number of pages is a bibliometric descriptor which underestimates the real increase of the amount of matter. Finally, any significant reduction of students' free time may cause a decrease in the quality of student's life; it can generate stressful situations and temptations to make various academic misconducts to achieve wanted academic and non-academic goals.

### 3.3. Case study 1: plotting spherical harmonics as angular parts of atomic orbitals

One of the most intriguing concepts in main branches of chemistry that deal with atomic orbitals (general, physical, organic and inorganic chemistry) and also in some minor branches (quantum chemistry, computational chemistry, molecular modeling), are spherical harmonics, angular parts of atomic orbitals. While physicists and mathematicians deal with spherical harmonics as complex surfaces mainly presented by formulas, chemists need to deal with real spherical harmonics, accurately presented in three-dimensional plots. Spherical harmonics give a rather good idea of spatial distribution of atomic orbitals (Kiralj, 1998). Furthermore, atomic orbitals combine into hybrid orbitals, molecular orbitals, orbital interactions and hence, spherical harmonics are indispensable in understanding, interpreting and quantification of atomic orbital interactions of any kind.

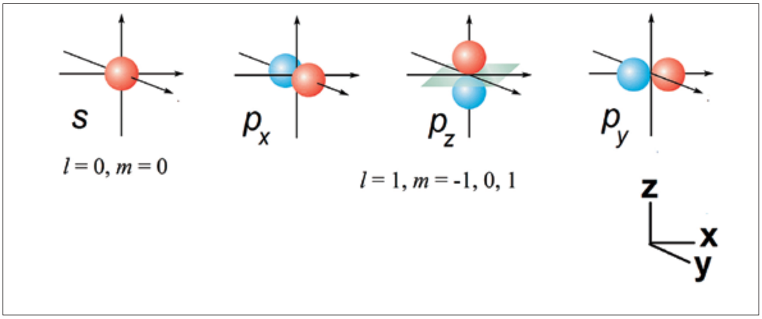


Figure 21. Angular parts (spherical harmonics) of *s* and *p* atomic orbitals. Adapted from textbook *Inorganic Chemistry* (Housecroft, Sharpe, 2018, p. 14).

Accurate plots of spherical harmonics are omitted in textbooks. When one finds a figure of spherical harmonics, it is an artistic interpretation or a symbolic representation (Lee *et al*, 2019), in modern times usually computer-generated. Such an example (Figure 21) may be found in textbook *Inorganic Chemistry* (Housecroft, Sharpe, 2018, p. 14).

McDermott and Henderson were the first ones to make computer-generated three-dimensional plots of spherical harmonics as angular parts of atomic orbitals (McDermott, Henderson, 1990, p. 916), writing *FORTRAN* codes to generate coordinates for a specific plotter. A few years later, spherical harmonics were already built-in functions in the *Mathematica* software (Ferreira, Porto, 1993). Since then, accurate plots of spherical harmonics as angular parts of atomic wavefunctions were occasionally published in educational or research articles published in journals or at various internet sites, by using various computer programs: *Mathematica* (Ferreira, Porto, 1993, p. 593; Tokura, Nagaosa, 2000, p. 463; Supriadi et al., 2019, pp. 6-11), *Winplot* (Chung, 2013, p. 1091; Tania et al., 2017, p. 122), and *Excel* (Lee et al., 2019). Several other programs available online, that were used for plotting spherical harmonics are: *Matlab* (Wikimedia Commons, 2020; MTEX, 2023), *Mathcad* (Mathcad Tutorial 5, 2010), *Scilab* (File Exchange, 2011), *Maple* (Roussel, 2002; Dujany, 2012), *LabVIEW Environment* tools (Broklová, Koupil, 2006), *JavaScript* tools (Vinequai, 2023; Zhang et al., 2012), *Gnuplot* (Kawano, 2004), *GSL* with *libQGLViewer* (Paris, 2017), *R software* (Stack Overflow, 2018), *Python* (Hill, 2020; Zheng, 2022), *Path Tracer* in *Go* (Fogleman, 2016), and *ChimeraX* with *Python* (Goddard, 2020), among others.

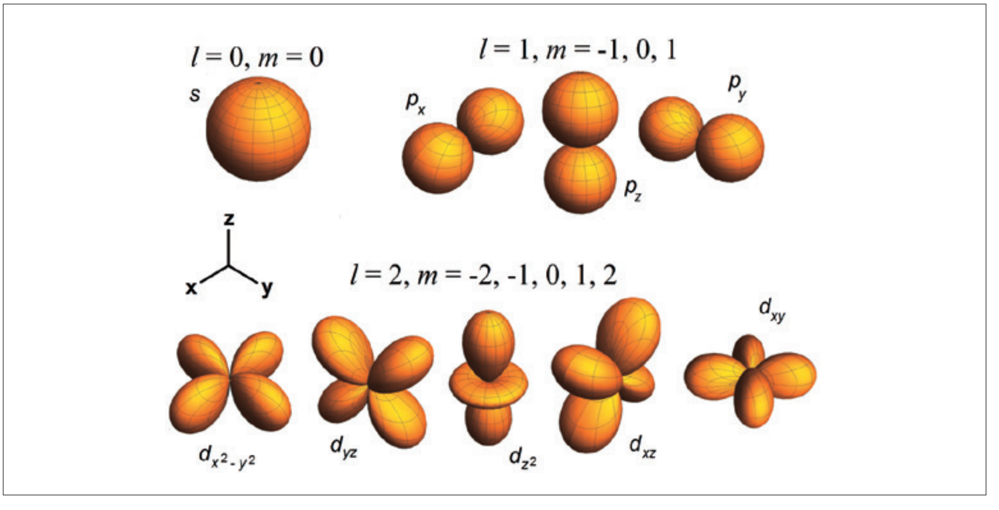


Figure 22. Angular parts (spherical harmonics) of *s*, *p* and *d* atomic orbitals. Drawings were made by using online *Mathematica* software in *Wolfram Cloud*.

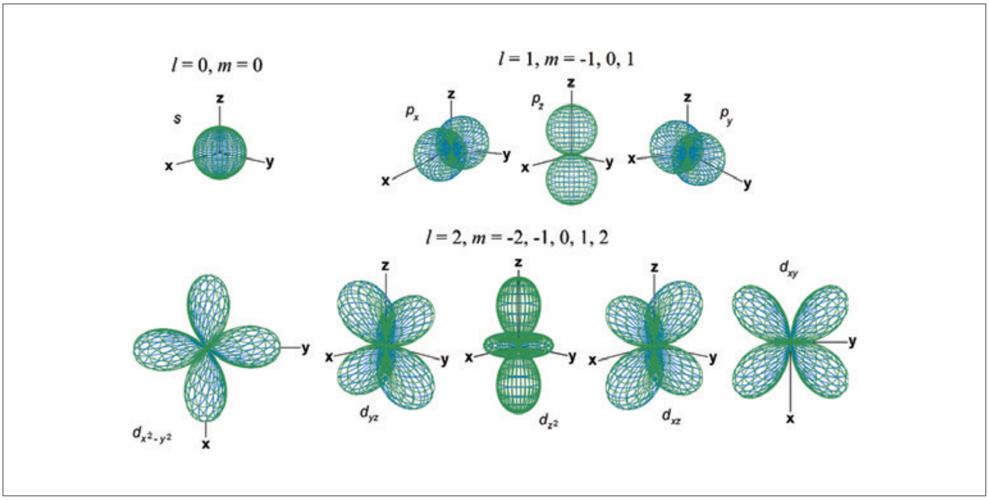


**Figure 23.** Angular parts (spherical harmonics) of *s*, *p* and *d* atomic orbitals. Drawings were made by using online *Desmos* software.

The 21 $^{st}$ century is rich in software about spherical harmonics and so, today it is easy to make three-dimensional plots of these functions. One may use simple plotting options, like built-in functions, or setting plotting parameters, or eventually use plotting scripts for adequate software/module, and fast obtain high-quality plots. Figure 22 was obtained by generating a free user account at *Wofram Cloud* and then using built-in functions for spherical harmonics in *Wolfram Mathematica*, consulting some online examples for plotting these functions. Figure 23 was generated by using online *Desmos Graphing Calculator*, without any registration and example study, because the use of plotting options was self-explanatory. Figure 24 corresponds very well to the plots on the two previous figures. The method of mixed manual-computer-generated plots in this Figure was inspired by the work of McDermott and Henderson, published some time ago (McDermott, Henderson, 1990). Interestingly, there is a free software *PlotYlm* (Matzdorf, R. Quantum Analogues: Spherical Harmonics; Universität Kassel, Kassel, 2023: https://www.uni-kassel.de/fb10/institute/physik/forschungsgruppen/oberflaechenphysik/quantum-analogs/spherical-harmonics) for making black-and-white plots of spherical harmonics, and it works as a desktop program. Based on all the evidences on tools for making plots of spherical harmonics for *s*, *p* and *d* orbitals, one cannot find a reasonable justification why chemistry textbooks have been always avoiding plots or accurate drawings of spherical harmonics, or giving misleading artistic/schematic representations of these complicated functions.

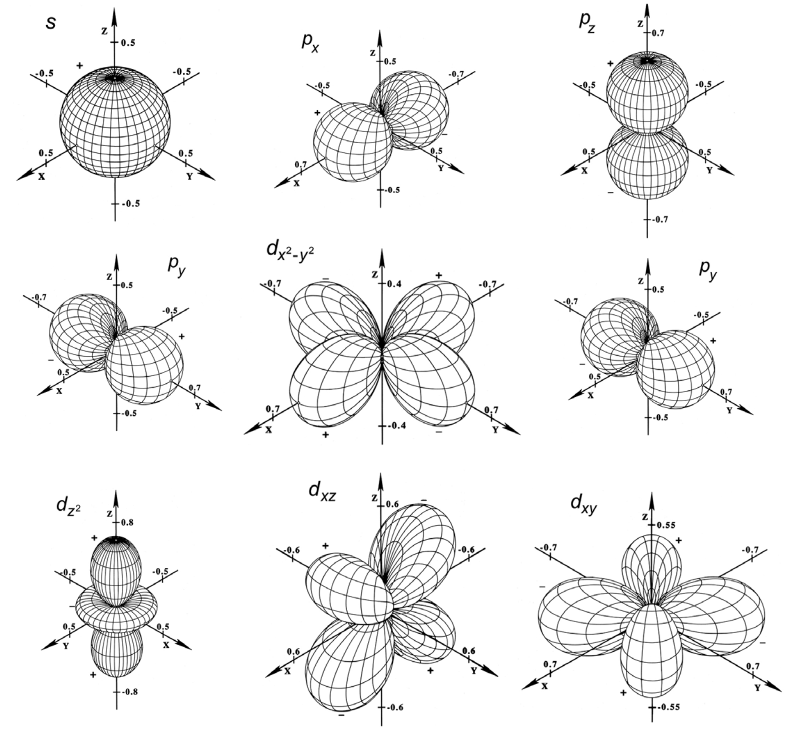


Figure 24. Angular parts (spherical harmonics) of *s*, *p* and *d* atomic orbitals. Drawings were handmade by using calculated coordinates of three-dimensional surfaces in normal projection.

## 3.4. Case study 2: spatial mechanisms of nucleophilic substitution reactions

Textbooks of organic chemistry usually start with nucleophilic substitution reactions. Unimolecular nucleophilic substitution reaction $S_N1$ at a tetrahedral, saturated carbon consists of three steps: 1) leaving a weaker nucleophile (the leaving group); 2) formation of the carbocation; and 3) attack of a stronger nucleophile to form the final product. Bimolecular nucleophilic substitution reaction $S_N2$ at a tetrahedral, saturated carbon consists of only one step: simultaneous leaving a weaker nucleophile and attack of a stronger nucleophile, without formation of a carbocation. How to understand spatial relationships of reaction participants from illustrations in a textbook, without a need to consult simulations, online and other supplementary materials? How to distinguish $S_N1$ from $S_N2$, and to know when $S_N1$ or $S_N2$ occur? Structural formulas are not sufficient for complete understanding of the phenomena, as well as are not artistic interpretations. Good molecular graphics based on real molecular structures (experimentally determined or modelled) are still scarce in textbooks of organic chemistry.

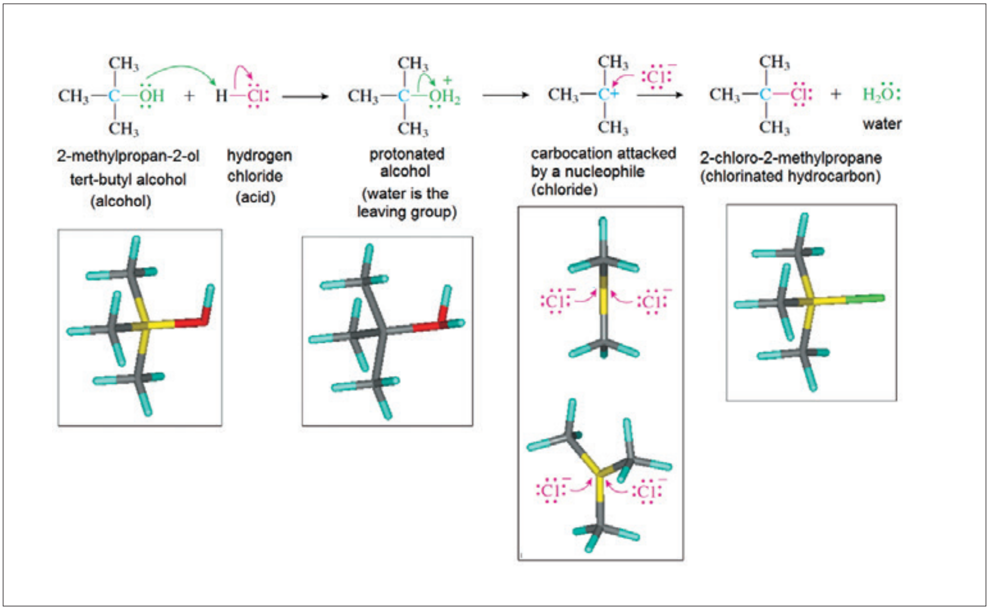


Figure 25. An example of $S_N1$ reaction between a tertiary alcohol and an acid. Reaction presentation with two-dimensional structural formulas of species is from literature (Hornback, 2006, p. 280). Three-dimensional wire models of organic species are modeled in this work, using experimentally determined crystal structures and geometry-optimized structures available in databases CSD and PubChem, respectively.

Figure 25 shows the mechanism of the $S_N1$ reaction between *tert*-butyl alcohol with hydrogen chloride in aqueous medium, with species represented by means of simple structural formulas (Hornback, 2006, p. 280). The hydroxyl group is protonated, then a water molecule is the leaving group, a planar carbocation is formed, and then it is attacked by chloride ion from one side, and the final product – *tert*-butyl chloride is formed. When molecular structures are used as wire models, the mechanism becomes more understandable. The reactant and the product have similar structures, because only a small group replaces another small group. The protonated hydroxyl group looks like a water molecule bound to the central carbon and so, it is easier to imagine that water is the leaving group. Finally, the *tert*-butyl carbocation has a planar, triangular structure, because of which the chloride ion may attack the central carbon from one or the other side of the carbocation's plane. Why the $S_N1$ reaction is possible? Figure 26 gives the answer. The carbocation may be represented with the space-filling (CPK) model that takes into account the true size of atoms, which may be colored differently. The CPK model of the carbocation shows the exposed surface of the central carbon in the form of a triangle from both sides of the molecule. Now, when the chloride anion is shown at its real size, superimposed

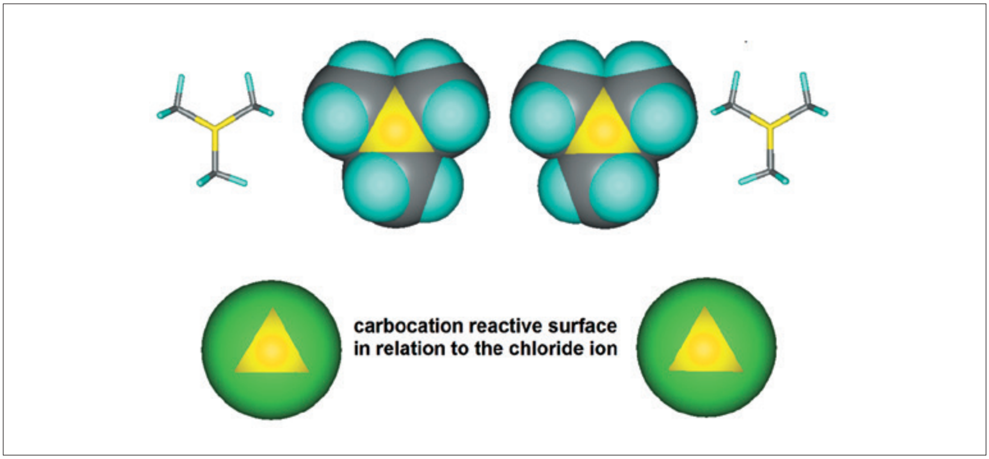


Figure 26. Two views of the wire and space-filling models of the carbocation from the previous figure (up) and the superimposition of the reactive carbon surface (yellow) with the chloride surface (green). Sufficiently large interacting surfaces (yellow and green) and the absence of steric hindrance are reasons why the $S_N1$ reaction occurs between the tertiary alcohol and hydrogen chloride.

with the yellow carbon triangle, three observations can be made. First, the exposed yellow part of the central carbon is sufficiently large to interact with the chloride anion and so, a new covalent C – Cl bond may be established. Second, the carbocation is obviously planar and may react with the chloride from its both sides. Third, there is no sterical hindrance to the central carbon atom, *i.e.* the methyl groups do not prevent the C … Cl contact before the covalent bond is formed.

Is the $S_N2$ reaction possible between the *tert*-butyl alcohol and hydrogen chloride? It may be a question at exam. This reaction is not possible, and the answer cannot be found only by looking at the structural formulas of the reactants (Figure 27). The wire model of the reactant, when looking along the C – O bond and against the -OH group, shows this is the direction in which the chloride anion should attack the central carbon atom. When the CPK model is made in the same orientation, two observations can be made. First, the interacting surface of the central carbon is too small (small yellow triangle), compared to the size of the chloride anion and so, the chemical bond cannot be formed. Second, the central carbon atom is practically covered by the three methyl groups, *i.e.* there is a pronounced steric hindrance by which these groups prevent the mechanism of the $S_N2$ reaction.

The present case study of the $S_N1$ and $S_N2$ reaction mechanisms raises the following questions. Why organic chemistry textbooks do not employ real structures, represented by adequate high-quality molecular graphics? Databases of experimentally determined structures of small molecules exist for decades. There are also

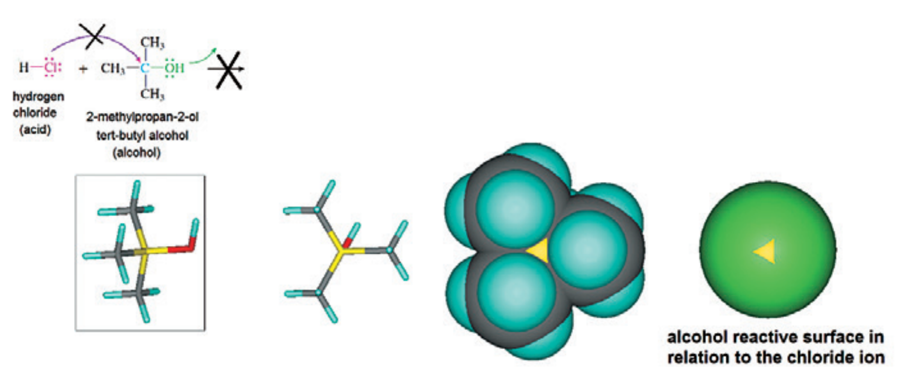


Figure 27. The wire and space-filling models of the reacting tertiary alcohol from Figure 25 and the superimposition of the reactive carbon surface (yellow) with the chloride surface (green). There is no sufficiently large interacting surface (yellow) in relation to the chloride surface (green) due to the steric hindrance. This is the reason why the $S_N2$ reaction does not occur between the tertiary alcohol and hydrogen chloride.

databases of modeled structures for several decades. Literature is full of molecular structures as supplementary data to published articles. There are molecular modeling programs, quantum chemistry software, molecular graphic software, molecular drawing programs and even online applets for drawing molecular structures. Relatively fast and good modeling of small molecules was possible even in the 1990's. There is no real justification why teaching students using outdated methodologies in the computer age.

### 3.5. Case study 3: structures and properties of nucleic acid bases as building blocks of DNA and chromatin

In the case study 1, it has been shown that textbooks lack accurate computer-generated plots and correct interpretation of spherical harmonics as angular parts of atomic orbitals. In the case study 2, a similar kind of textbook errors was assessed: the lack of accurate molecular graphics *i.e.* three-dimensional molecular plots, based on real molecular structures (experimentally determined or modeled). In general, such plots would aid in understanding molecular structure, properties and chemical reactivity of various classes of organic compounds, as well as reaction mechanisms. In this case study, the same trouble occurs with small molecules in biochemistry textbooks, and it is illustrated *via* nucleic acid bases.

Table 7. Examples of experimentally determined and modeled structures of nucleic acid bases and of their parent compounds purine and pyrimidine

| Base | CSD[a] [form] | PubChem[b] | PDB[c] [form] |
|---|---|---|---|
| **Adenine** | ADALEW [molecular crystal] | 190 | 5YW5 [ADE] |
| | ADENCH02 [cation in salt] | | 1BUT [DA] |
| | KEYCUN [derivative in molecular crystal] | | 2KOC [A] |
| **Guanine** | GUANCD01 [cation in salt] | 135398634 | 1IT7 [GUN] |
| | GUANMH10 [hydrate] | | 1BUT [DG] |
| | KEMDOW [molecular crystal] | | 2KOC [A] |
| **Purine** | PURINE [pure compound] | 1044 | 4RHY |
| | LUQBEE [derivative in molecular crystal] | | [3QG, derivative] |
| | CLPURB [derivative] | | |
| **Cytosine** | CYTSIN [pure compound] | 597 | 7QOA [CYT] |
| | ADALAS [molecular crystal] | | 1BUT [DC] |
| | AMCYTS [derivative] | | 2KOC [C] |
| **Pyrimidine** | PRMDIN22 [pure compound] | 9260 | 2GTI [P1R] |
| | BURBOF [molecular crystal] | | |
| | DUKGEW [derivative in molecular crystal] | | |
| **Thymine** | THYMIN03 [pure compound] | 1135 | 5C3Q [TDR] |
| | OGIYOU [molecular crystal] | | 1BUT [DT] |
| | KECYUN [derivative in molecular crystal] | | |
| **Uracil** | URACIL [pure compound] | 1174 | 1UDH [URA] |
| | BIHKIN10 [molecular crystal] | | 2KOC [U] |
| | CENSAP [derivative] | | |

[a] Crystal structures from the Cambridge Structural Database containing bases in various forms. [b] Modeled structures of bases from the PubChem database. [c] NMR solved structures from the Protein Data Bank containing bases as ligands of proteins or bases in a DNA or RNA fragment, with PDB ligand/base codes in the brackets. Only purine was not found as a pure compound but as a derivative.

How to acquire molecular structures of nucleic acid bases, or some relevant structures that can be modified to obtain structures of pure bases? Table 7 shows results of quick search for structures of the common nucleic acid bases, purine and pyrimidine, in the databases *CSD* and *PDB* with experimentally determined structures, and in the database *PubChem* with modeled structures. The three databases, with eventual structures published in article supplements and at various reliable internet sites, represent a plethora of available structures for molecular graphics of the bases. Furthermore, the bases may be easily modelled, as illustrated in Figure 28. Molecular graphics of the bases, shown in two orientations, one in accordance to their structural formula (ball-and-stick and CPK models), and the other one in the perpendicular direction (CPK models), exhibits essential propeties of the bases. These molecules are aromatic (more correctly, heteroaromatic) compounds with high degree of π-electron delocalization, rigid, planar and flat, whose properties like planarity change insignificantly due to hydrogen bonding, covalent bonding to pentose units, and intermolecular interactions (Kiralj, Ferreira, 2003 c). DNA intercalators, which are inserted between two neighboring bases of the same strand, must have the same properties (Kiralj, *et al.*, 1999; Ferreira, Kiralj, 2008). In other words, the bases act as hard, solid bricks, what contributes to relative rigidity of a DNA molecule. This fact is not emphasized in biochemistry textbooks.

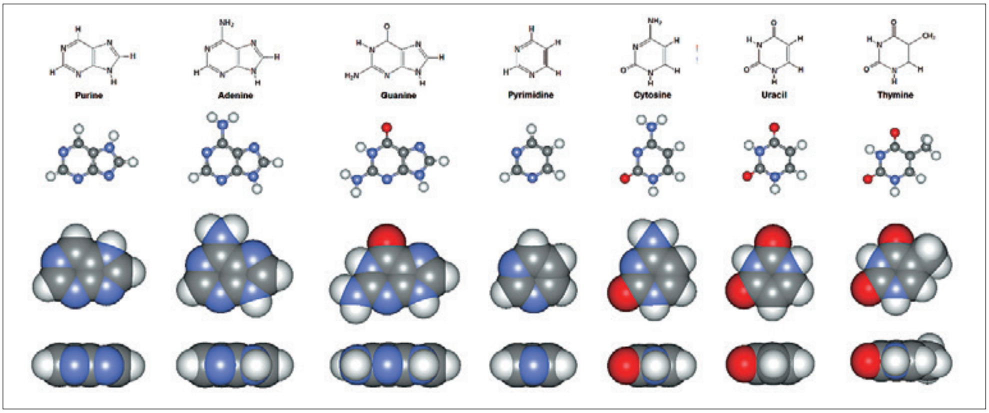
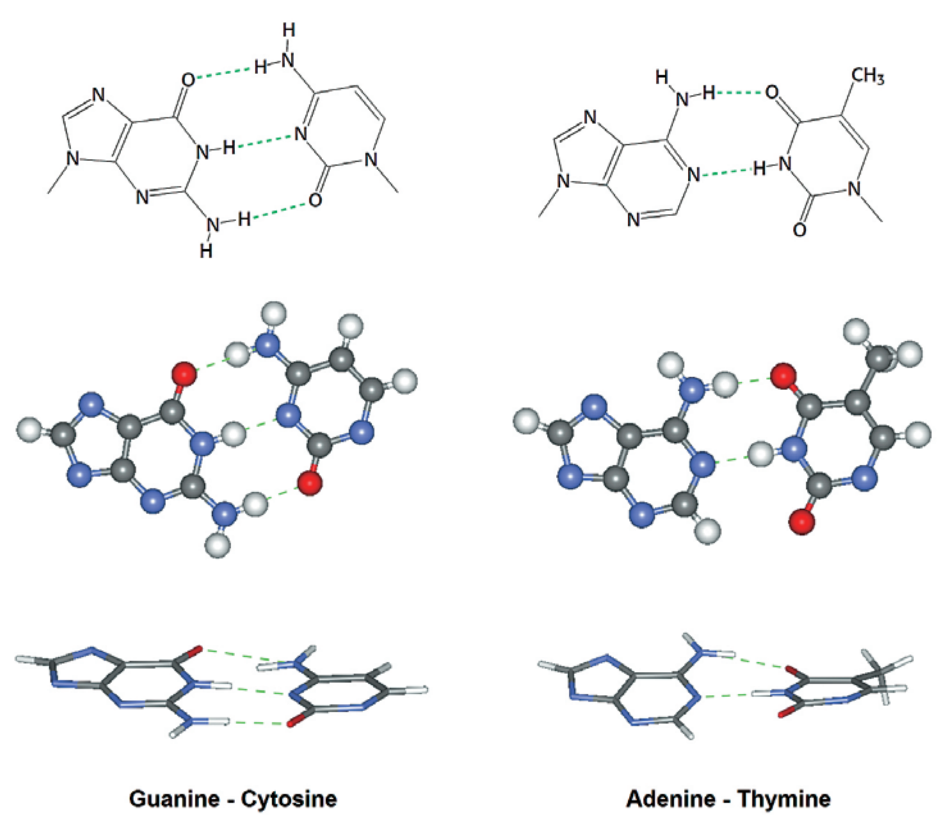


**Figure 28.** Nucleic acid bases and their parent compounds purine and pyrimidine: two dimensional structural formulas (first row) adapted from textbook *Biochemistry* (Stryer *et al.*, 2015, p. 107), three-dimensional ball-and-stick model (second row) and space filling model (two lower rows) for molecules made by drawing their formulas and then modeling them in a three-dimensional space.



**Guanine - Cytosine** **Adenine - Thymine**

**Figure 29.** Hydrogen-bonded base pairs: two dimensional formulas (up) adapted from Stryer's textbook *Biochemistry* (Berg *et al.*, 2015, p. 110), and three-dimensional ball-and-stick (middle) and stick models (down) extracted from the structure of a DNA duplex decamer (PDB: 1BUT), resolved by solution NMR (Dornberger *et al.*, 1998). Carbon-depleted nitrogen atoms are shown because of simplicity of the three-dimensional models. Stick model better illustrates the base-pair nonplanarity and the real hydrogen bond geometry.

Usually in biochemistry textbooks, common hydrogen-bonded base pairs adenine – thymine and guanine – cytosine are represented by structural formulas and hydrogen bonds with inaccurate geometry (Figure 29). A misinterpretation coming from such an approach is that the bases in a base pair are coplanar, *i.e.* the hydrogen-bonded bimolecular association is a planar and rigid structure. That is why a double-stranded DNA is schematically or artistically depicted as a large set of parallel ribbons (each ribbon means a planar base pair) connected with two helically twisted stripes (phosphate – pentose chains). If base pairs were so planar and rigid, DNA would not be able to pack densely in chromatin. If a base pair is isolated from a good structure from the PDB, for example from a high-quality structure of decamer d(CATGGCCATG)$_2$ (Dornberger *et al.*, 1998), and suitable base-pair orientations are selected, then a true geometry is presented (Figure 29). Base pairs are nearly coplanar, meaning that their planes are a bit tilted with respect to each other (Figure 29). This is well visible when a considerable set of stacked bases is extracted from a real structure of DNA oligomer, for example from the aforementioned decamer (Figure 30 left).

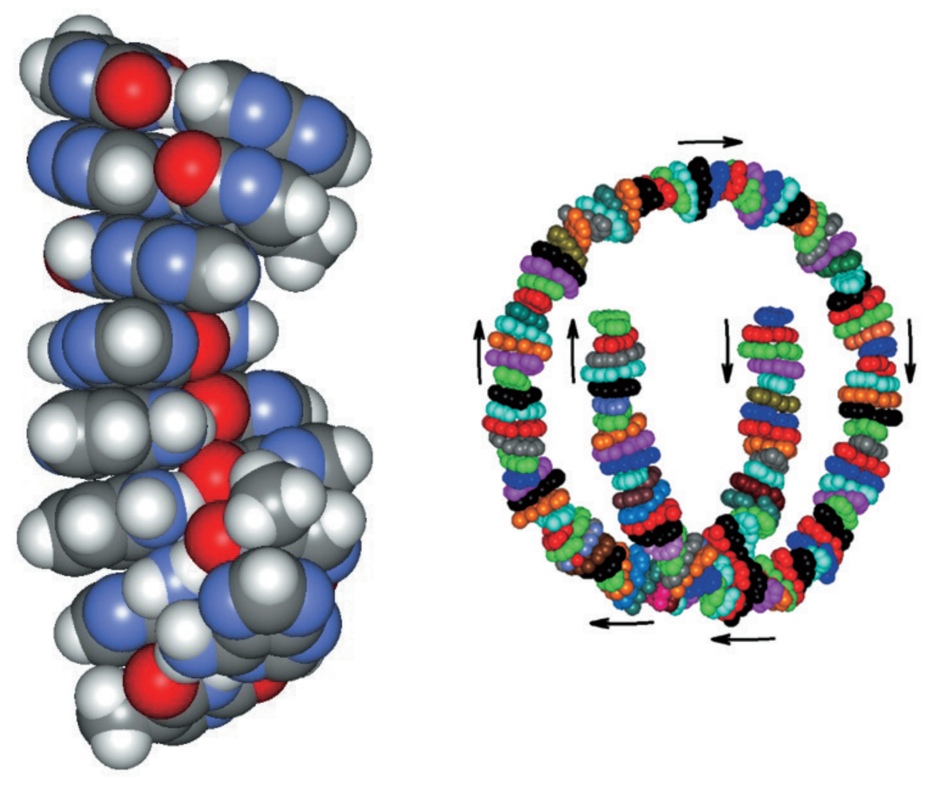


Figure 30. Space filling models of multiple stacked base pairs. Left: eight stacked base pairs extracted from a structure of a DNA duplex decamer (PDB: 1BUT), resolved by solution NMR (Dornberger *et al.*, 1998). Right: left-coiled 125 stacked base pairs extracted from a structure of a nucleosome (PDB: 7D69), determined by electron microscopy (Sato *et al.*, 2021). Phosphate - pentose backbones were removed because of clarity.

In Stryer's textbook *Biochemistry* (Berg *et al.*, 2015, pp. 110-111), the stacking of base pairs is said to be essential for stabilization of the double-stranded DNA structure. In fact, one can talk about base pair stacks, as well as about base stacks within each DNA chain. Aromatic and heteroaromatic molecules have always tendency to form parallel or nearly parallel stacks, in crystalline state as well as in solution (Kiralj, Ferreira, 1997; Kiralj *et al.*, 1999; Kiralj, Ferreira, 2002; Ferreira, Kiralj, 2008). Knowing that base pairs are nearly and not absolutely coplanar, it is reasonable to expect their stacks do not consist of parallel but of nearly parallel base pairs. The structure of the mentioned oligomer (Figure 30 left) nicely shows the near coplanarity of base pairs as well as near parallelism of base pair stacks, and the resulting curvature of the oligomer. Concluding, base pairs are not tightly sticked to each other, the stacks are not rigid structures and they can bend. All interactions between the bases from the same strand and the bases from the two strands form a semi-flexible structure of the double-stranded DNA helix.

Preferrable tendencies to use artistic interpretations, schematic presentations and structural formulas over molecular graphics, may lead to misleading concepts of the DNA molecule. Thus, textbooks should always use real structures (experimentally determined or modelled) whenever appropriate, even together with simple schemes and formulas. Knowing that base stacks, as well as phosphate – pentose chains are semi-flexible, one can understand why a DNA molecule is wound around core histones in a nucleosome (Figure 30 right). The DNA semi-flexibility is responsible for all structural levels of chromatin organization. Currently, nucleosomes are the largest DNA-containing structures which are experimentally determined and deposited in the *PDB* database. It is not reasonable that textbooks avoid using real structures of small molecules and even of larger molecules as DNA oligomers.

### 3.6. Recommendations

The first step to overcome difficulties about contemporary university textbooks is fixing errors reported in this study: selecting and reducing the matter for a specific level (beginner, intermediate or advanced – even excluding too complicated stuff for a certain level), making clear distinction of essential from facultative matter, enabling accurate computer-generated presentations (formulas, tables, graphs, figures), using real cases, providing special appendices or short monographs when necessary. However, changing textbooks within a course independently of one another is not sufficient to deal with optimizing textbook materials. That is why the second step is necessary: textbooks within the same course should be mutually adapted, avoiding unnecessary overlaps and repetitions, and respecting the common sequence of disciplines during the course.

Chemistry course begins with general chemistry, which includes complicated concepts of orbitals and molecular geometry. They are taught in details only later, in physical chemistry and organic/inorganic chemistry. On the other side, mathematics for chemists usually does not provide sufficient foundation for mathematical concepts in chemistry. How to solve these problems in general, and also in particular for the three case studies presented (spherical harmonics, nucleophilic substitution reactions, DNA structure)? First, a mathematics discipline should additionally include visualization of functions of three and four variables, some special functions (Laguerre and Legendre polynomials as the basis for spherical harmonics), and essential geometry elements (stereometry of Platon bodies such as tetrahedron and octahedron, then basic principles of geometrical projections and body presentation). Then, a discipline dealing with computers in chemistry or a specialized discipline should include some molecular graphics (use of databases, simple molecular modeling, and molecular presentations) at the first year of a chemistry course. This course would help in understanding molecular stucture of small molecules as well as of proteins and DNA. With respect to complicated quantum chemical concepts of spherical harmonics, orbitals and electronic structure in general chemistry, there are two types of opinion (Lamoureux, Ogilvie, 2021 a; Lamoureux, Ogilvie, 2021 b; Lamoureux, Ogilvie, 2021 c). According to one, these concepts should be replaced by electrostatic potential, which is easier to be understood and absorbed. Quantum chemical stuff is then left for higher years of a chemistry course. The other opinion is that quantum chemical elements should remain in general chemistry teaching, with additional explanations and specialized monographs (McCaw, 2015). Hovewer, each way has its advantages and disadvantages, there is no ideal solution.

## 4. Conclusion

The basic assumption of this work is that the exponential increase of human knowledge significantly affects education, bringing some negative side effects, visible in size and quality of university textbooks, as well as in increased time required to read them.

Bibliometric analysis of textbooks with multiple editions from 12 diverse areas shows expected results. Increase in the quantity of matter over time indeed exists for all the textbooks studied. Depending on the area in question, the increase rate from the first to the last edition may be small as for Macionis' *Sociology* (2% increase or 0.5 pages per year), up to high as for Halliday and Resnick's *Fundamentals of Physics* (42% increase or 7.3 pages per year). Converting to additional time student has to spend reading the last edition of the textbook with respect to its first edition, *Sociology* requires up to 10 additional minutes per day, while the value for the physics textbook is almost 70 minutes per day. Due to the increase in the quantity of matter of the last editions of textbooks with respect to their first editions, students have to spend more than two hours per day when studying the new textbooks. Although the variable number of pages underestimates the real increase of textbooks, its temporal trends distinguish various increase types, such as linear, parabolic with minimum and maximum, oscillating, and other types.

Bibliometric analysis of textbooks from six major and eight minor branches of chemistry shows similar results to those for general knowledge. The increase of the size of matter is noticeable in all the textbooks studied, and is more pronounced than for general knowledge. With respect to the first editions, the last editions of the textbooks studied vary in increase rate from small rate for *The Organometallic Chemistry of the Transition Metals* (10% increase or 1.3 pages per year) to high for *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* (95% increase or 19.7 pages per year). The additional time spent to read the books is up to 10 and 100 minutes per day, respectively. Today, chemistry students have to spend reading textbooks some 2 – 4 hours longer than their colleagues who used the first editions of the same textbooks.

Three case studies of un-updated concepts in chemistry were described: spherical harmonics, mechanisms of nucleophilic substitution reactions, and structures and properties of nucleic acid bases. Most textbooks treating them suffer from the lack of high-quality computer-generated three-dimensional plots of functions (spherical harmonics) or molecular graphics (molecular structures of small organic molecules). The use of modern software for calculation and plotting, as well as molecular structures from available databases or easy molecular modeling, is simply omitted for decades, and thus, the interpretation of treated issues is incorrect or incomplete. Such textbook errors are numerous, and they multiply as textbooks increase in size.

Based on all the observations made in this work, one cannot conclude that human progress, *i.e.* exponential increase of science and technology, automatically improves education, makes students smarter and more professional, and improves their quality of life. Instead of that, more insight into the STEM crisis is given in terms of problems in modern chemistry education. The question „*Quo vaditis, scientia et educatio*?" indeed has sense, because the future of human knowledge and education is in fact, very uncertain and unpredictable. Possible solutions about university textbooks are not straightforward and they musst include changes in textbooks of a whole course.

## Literature

1. Berg, J. M.; Tymoczko, J. L.; Gatto, G. J. Jr.; Stryer, L. (2015), *Biochemistry, 8th ed.* New York: Freeman.
2. Bertozzi, C. R. (2015), *The Centrality of Chemistry*. ACS Central Science, 1(1), pp. 1-2.
3. Bornmann, L.; Haunschild, R.; Mutze, R. (2021), *Growth rates of modern science: a latent piecewise growth curve approach to model publication numbers from established and new literature databases.* Humanities & Social Sciences Communications, 8, 224 (15 pages)
4. Broklová, Z.; Koupil, J. (2006), *Spherical harmonics.* Available at Internet site: http://kdf.mff.cuni.cz/~koupilova/orbitals/tasks/sphericalharmonics.php?lang=EN (Accessed on: 7 February 2023)
5. Brown, T. L.; LeMay, Jr., H. E.; Bursten, B. E.; Murphy, C. J.; Woodward, P. M.; Stoltzfus, M. W.; Lufaso, M. W. (2020), *Chemistry: The Central Science, 14th edition*. London: Pearson.
6. CCDC – The Cambridge Crystallographic Data Centre (2021), *Celebrating the 1.1 millionth structure (Cambridge Structural Database, CSD)*. Available at Internet site: https://www.ccdc.cam.ac.uk/Community/blog/1.1-millionth-structure/ (Accessed on: 27 December 2022)
7. Chazan, B. (2022), *Principles and Pedagogies in Jewish Education*. Cham: Palgrave Macmillan, pp. 5-12.
8. Chung, W. C. (2013), *Three-Dimensional Atomic Orbital Plots in the Classroom Using Winplot*. Journal of Chemical Education, 90(8), pp. 1090-1092.
9. Corey, R. B.; Pauling, L. (1953), *Molecular Models of Amino Acids, Peptides, and Proteins.* Review of Scientific Instruments, 24(8), pp. 621-627.
10. Cornell College (2023), *Reading a Textbook for True Understanding*. Available at Internet site: https://www.cornellcollege.edu/student-success-center/academic-support/study-tips/reading-textbooks.shtml (Accessed on: 5 February 2023)
11. Dicionário inFormal (2022), *Livro-texto*. Available at Internet site: https://www.dicionarioinformal.com.br/livro-texto/ (Accessed on: 25 December 2022)
12. Dornberger, U.; Flemming, J.; Fritzsche, H. (1998), *Structure determination and analysis of helix parameters in the DNA decamer d(CATGGCCATG)$_2$ comparison of results from NMR and crystallography*. Journal of Molecular Biology, 284(5), pp. 1453-1463.
13. Dujany, G. (2012), *The Hydrogen Atom Orbitals.* Available at Internet site: https://www.maplesoft.com/applications/preview.aspx?id=134917 (Accessed on: 7 February 2023)
14. English Grammar Lessons.com (2022), *Quo Vadis – Meaning, Origin and Usage*. Available at Internet site: https://english-grammar-lessons.com/quo-vadis-meaning/ (Accessed on: 25 December 2022)
15. Espindola D. (2020), *Technology is Exponential But Humans Are Linear*. Available at Internet site: https://www.interceptinghorizons.com/post/technology-is-exponential-but-humans-are-linear (Accessed on: 25 December 2022)

16. Ferreira, M. M. C.; Kiralj, R. (2008), *Exploratory analysis of structural properties of DNA-intercalator complexes in crystalline state*. In: Book of Abstracts of the 11th International Conference on Chemometrics in Analytical Chemistry, Vol. 3. Montpellier: Cemagref, pp. 275-279.
17. Ferreira, M. M. C.; Porto, E. G. (1993), *Uma Química Quântica Visual: Unindo o Útil ao Agradável*. Quimica Nova, 16(6), pp. 589-595.
18. File Exchange (2011), *Spherical harmonics that employ the Condon-Shortley phase*. Available at Internet site: https://fileexchange.scilab.org/toolboxes/129000 (Accessed on: 7 February 2023)
19. Fogleman, M. (2016), *Spherical Harmonics*. Available at Internet site: https://www.michaelfogleman.com/static/spherical-harmonics/ (Accessed on: 7 February 2023)
20. Fortunato S.; Bergstrom, C. T.; Börner, K.; Evans, J. A.; Helbing, D.; Milojević, S.; Petersen, A. M.; Radicchi, F.; Sinatra, R.; Uzzi, B.; Vespignani, A.; Waltman, L.; Wang, D.; Barabási, A.-L. (2018), *Science of Science*. Science, 359(6379), eaao0185 (7 pages)
21. Goddard, T. (2020), *ChimeraX Recipes: Making a Spherical Harmonic Surface*. Available at Internet site: https://rbvi.github.io/chimerax-recipes/spherical_harmonics/spherical_harmonics.html (Accessed on: 7 February 2023)
22. Green, K.; Rothschild, R. (2022), Staying in STEM? Available at Internet site: https://prime.dailybruin.com/stemretention (Accessed on: 28 December 2022)
23. Habraken, C. L. (1996), *Perceptions of Chemistry: Why is the Common Perception of Chemistry, the Most Visual of Sciences, So Distorted?* Journal of Science Education and Technology, 5(3), pp. 193-201.
24. Hamilton, T. D. (2006), *Textbook inflation: thirty-five years of Brown's general chemistry textbook*. Chemistry Education Research and Practice, 7(1), pp. 46-48.
25. Harper D. (2022), *Textbook*. Available at Internet site: https://www.etymonline.com/word/textbook (Accessed on: 25 December 2022)
26. Hill, C. (2020), *Visualizing the real forms of the spherical harmonics*. Available at Internet site: https://scipython.com/blog/visualizing-the-real-forms-of-the-spherical-harmonics/ (Accessed on: 7 February 2022)
27. Holze, R. (2020), *Electrochemistry: quo vadis or where should we head to*? Journal of Solid State Electrochemistry, 24(9), pp. 2087-2088.
28. Hornback, J. M. (2006), *Organic Chemistry, 2nd ed*. Belmont, CA: Thomson Brooks/Cole, p. 280.
29. Hrvatska enciklopedija (2021), *Udžbenik*. Available at Internet site: https://www.enciklopedija.hr/natuknica.aspx?id=62968 (Accessed on: 25 December 2022)
30. Jokić, D. (2019), *Quo vadis, Tekstil? Croatian Journal for Textile and Clothing Technology*. Industria textila˘, 70(2), pp. 170-181.
31. Kalantzis, M. (2005), *The Radford Lecture, AARE, 2005: Elements of a Science of Education*. Australian Educational Researcher, 33(2), pp. 15-42.
32. Kawano, T. (2004), *Spherical Harmonics*. Available at Internet site: http://lowrank.net/gnuplot/spherical_harmonics/index-e.html (Accessed on: 7 February 2023)
33. Kennedy, B.; Hefferon, M.; Funk, C. (2018), *Half of Americans think young people don't pursue STEM because it is too hard*. Available at Internet site: https://www.pewresearch.org/fact-tank/2018/01/17/half-of-americans-think-young-people-dont-pursue-stem-because-it-is-too-hard/ (Accessed on: 28 December 2022)

**34.** Kinouchi, R. R. (2014), *Scientometrics: the project for a science of science transformed into an industry of measurements*. Scientiae Studia (São Paulo), 12(spe), pp. 147-159.

**35.** Kiralj, R. (1998), *Three-Dimensional Representation of Surface Spherical Harmonics and Their Squares Using Normal Projections: Some Comments on the Functions: Preparing for an Undergraduate Exercise*. Journal of Chemical Education, 75(3), pp. 332-338.

**36.** Kiralj, R. (2020), *Students' Academic Honesty – a Prerequisite for the Economic Development*. Radovi Zavoda za znanstvenoistraživački i umjetnički rad u Bjelovaru, 14, pp. 148-182.

**37.** Kiralj, R. (2022), *Presentation at conference „Koliko nas brine akademsko (ne)poštenje studenata?"* [*"How much are we worried about students' (dis)honesty?"*], *Zagreb, 25.11.2022.: Studentsko nepoštenje – pojam, oblici, trendovi, čimbenici, rješenja* [*Students' dishonesty – concept, forms, trends, factors, solutions*]. Available at Internet site: https://www.azvo.hr/hr/azvo-vijesti/2789- odrzana-konferencija-o-akademskom-ne-postenju-studenata (Accessed on: 28 December 2022)

**38.** Kiralj, R.; Ferreira, M. M. C. (1997), *A Simple Prediction of Crystal Density and Related Properties of Condensed Polynuclear Aromatic Hydrocarbons*. In: Resumos – XIV Reunião da Sociedade Brasileira de Cristalografia. São Carlos, SP: Sociedade Brasileira de Cristalografia, p. 6.

**39.** Kiralj, R.; Ferreira, M. M. C. (2002), *(Quantitative) Structure-Spectroscopic Property Relationships (Q)SSPR for 4,9-Diazapyrenium-Nucleotide Binding in Aqueous Media*. In: Turrell, S. (Ed.), Abstracts of the XXVIth European Congress on Molecular Spectroscopy, Villeneuve d'Ascq. Lille: University of Lille, p. 371.

**40.** Kiralj, R.; Ferreira, M. M. C. (2003 a), *A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors I. The chemometric approach*. Journal of Molecular Graphics and Modelling, 21(5), pp. 435-448.

**41.** Kiralj, R.; Ferreira, M. M. C. (2003 b), *A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors II. Molecular graphics and modeling*. Journal of Molecular Graphics and Modelling, 21(6), pp. 499-515.

**42.** Kiralj, R.; Ferreira, M. M. C. (2003 c), *On heteroaromaticity of Nucleobases. Bond Lengths as Multidimensional Phenomena*. Journal of Chemical Information and Computer Science, 43(3), pp. 787-809.

**43.** Kiralj, R.; Ferreira M. M. C. (2006), *The past, present, and future of chemometrics worldwide: some etymological, linguistic, and bibliometric investigations*. Journal of Chemometrics, 20(6-7), pp. 247-272.

**44.** Kiralj, R.; Kojić-Prodić, B.; Piantanida, I.; Žinić, M. (1999), *Crystal and molecular structures of diazapyrenes and a study of* $\pi \ldots \pi$ *interactions*. Acta Crystallographica B, 55(1), pp. 55-69.

**45.** Klatt, E. C.; Klatt, C. A. (2011), *How Much Is Too Much Reading for Medical Students? Assigned Reading and Reading Rates at One Medical School*. Academic Medicine, 86(9), pp. 1079-1083.

**46.** Koltun, W. L. (1965), *Precision Space-Filling Atomic Models*. Biopolymers, 3(6), pp. 665-679.

**47.** Kundzewicz, Z. W. (2018), *Quo vadis, hydrology*? Hydrology Sciences Journal, 63(8), pp. 1118-1132.

**48.** Lamoureux, G.; Ogilvie, J. F. (2021 b), *Orbitals in General Chemistry, Part I: The Great Debate*. Química Nova, 44(2), pp. 224-228.

**49.** Lamoureux, G.; Ogilvie, J. F. (2021 b), *Orbitals in General Chemistry, Part II: Mathematicl Realities*. Química Nova, 44(3), pp. 348-354.

**50.** Lamoureux, G.; Ogilvie, J. F. (2021 c), *Orbitals in General Chemistry, Part III: Consequences for Teaching*. Química Nova, 44(3), pp. 355-360.

**51.** Lee, G.-G.; Park, J.; Lee, S.-K.; Hong, H.-G.; Su Shim, H. S.; Shin, M.-K. (2019), *Three Dimensional Visualization of Hydrogen Atomic Orbitals Using Excel for School Science Education.* Journal of the Korean Chemical Society, 63(3), pp. 220-225.

**52.** Leonhard, G. (2022), *Technology is Exponential, But Humanity is Linear.* Available at Internet site: https://www.futuristgerd.com/2021/01/technology-is-exponential-but-humans-are-linear-kecks-law-and-moores-law-versus-gerds-law/ (Accessed on: 25 December 2022)

**53.** Mathcad Tuorial 5 (2010), *Mathcad ~ Spherical Harmonics in Mathcad ~ tutorial 5.* Available at Internet site: https://www.youtube.com/watch?v=ofQlaNMTTSM (Accessed on: 7 February 2023)

**54.** McCaw, C. S. (2015), *Orbitals With Applications in Atomic Spectra.* London: Imperial College Press.

**55.** McDermott, T.; Henderson, G. (1990), *Spherical Harmonics in a Cartesian Frame.* Journal of Chemical Education, 67(11), pp. 915-917.

**56.** Mingers, J.; Leydesdorff, L. (2015), *A review of theory and practice in scientometrics.* European Journal of Operational Research, 246(1), pp. 1-19.

**57.** MTEX (2023), *Harmonic Representation of Spherical Functions*. Available at Internet site: https://mtex-toolbox.github.io/S2F unHarmonicRepresentation.html (Accessed on: 7 February 2023)

**58.** Nagy B.; Farmer J. D.; Trancik, J. E.; Gonzales, J. P. (2011), *Superexponential long-term trends in information technology*. Technological Forecasting & Social Change, 78(8), pp. 1356-1364.

**59.** Paris, S. (2017), *Spherical Harmonics.* Available at Internet site: https://people.csail.mit.edu/sparis/sh/index.php?img=64 (Accessed on: 7 February 2023)

**60.** Patron, E. (2022), *Exploring the role that visual representations play when teaching and learning chemical bonding: An approach built on social semiotics and phenomenography*. Doctoral Dissertation. Kalmar: Linnaeus University.

**61.** Pllana, D. (2019), *Expanding Entire Volume of Knowledge Influences on Incrementing Individual Knowledge.* Global Journal of Human Social Science, 19(8), pp. 33-42.

**62.** Poór, J.; Csanádi, P.; Németh, G.; Tokár-Szadai, Á.; Szretykó, Gy.; Milovecz, Á.; Szügyi, Gy. (2022), *13. Future of Consulting – Quo Vaditis Consultants?* In: Poór, J.; Sanders; J. E. Németh, G.; Varga, E. (Eds.), Management Consultancy in Central and Eastern Europe. Budapest: Akadémiai Kiadó, pp. 162-185.

**63.** PubChem3D (2019), *PubChem3D Release Note*. Available at Internet site: https://pubchem.ncbi.nlm.nih.gov/docs/pubchem3d (Accessed on: 29 January 2023)

**64.** Quora (2020 a), *How long does it take for you to fully read a standard physics textbook on theoretical physics (about 500-600 pages)?* Available at Internet site: https://www.quora.com/How-long-does-it-take-for-you-to-fully-read-a-standard-physics-textbook-on-theoretical-physics-about-500-600- pages (Accessed on: 5 February 2023)

65. Quora (2020 b), *How many pages an hour can you read from a university textbook?* Available at Internet site: https://www.quora.com/How-many-pages-an-hour-can-you-read-from-a-university-textbook (Accessed on: 5 February 2023)
66. RCSB PDB (2022), *PDB Statistics: Overall Growth of Released Structures Per Year*. Available at Internet site: https://www.rcsb.org/stats/growth/growth-released-structures (Accessed on: 27 December 2022)
67. Reddit (2015), *Is it normal to take 4 hours to read 30 pages*? Available at Internet site: https://www.reddit.com/r/GetStudying/comments/3m jivf/is_it_normal_to_take_4_hours_to_read_30_ pages/ (Accessed on: 5 February 2023)
68. Rosenberg, A. (Ed.) (2005), *Philosophy of Science: A contemporary introduction, 2nd ed*. New York: Routledge.
69. Roussel, M. R. (2002), *Spherical Harmonics.* Available at Internet site: https://people.uleth.ca/~roussel/C3730/notes/spher_harmonics.html (Accessed on: 7 Februry 2023)
70. Sato, S.; Takizawa, Y.; Hoshikawa, F.; Dacher, M.; Tanaka, H.; Tachiwana, H.; Kujirai, T.; Iikura, Y.; Ho, C. H.; Adachi, N.; Patwal, I.; Flaus, A.; Kurumizaka, H. (2021), *Cryo-EM structure of the nucleosome core particle containing Giardia lamblia histones*. Nucleic Acids Research, 49(15), pp. 8934-8946.
71. Schummer, J. (1997), *Scientometric studies on chemistry I: The exponential growth of chemical substances, 1800-1995*. Scientometrics, 39(1), pp. 107-123.
72. Sebastien, Z. (2016), *The Status of Normative Propositions in the Theory of Scientific Change*. Scientonomy, 1, pp. 1-9.
73. Shestakova, I. G. (2018), *To the question of the limits of progress: is singularity possible?* Vestnik of St Petersburg University – Philosophy and Conflict Studies, 34(3), pp. 391-401.
74. Stack Overflow (2018), *R Software plot 3D Quantum orbital (spherical harmonics)*. Available at Internet site: https://stackoverflow.com/questions/51697361/r-software-plot-3d-quantum-orbital-spherical-harmonics (Accessed on: 7 Februry 2023)
75. Sternberg, R. J. (2017), *Why it is so hard for academics to write textbooks*. Psychology Teaching Review, 23(1), pp. 79-84.
76. Supriadi, B.; Ridlo, Z. R.; Fuadah, F.; Halim, M. A.; Maulana, M.; Santoso, Y. R. (2019), *Solution of spherical equation in 3 dimensions for hydrogen atom with quantum numbers* $4 \leq n \leq 5$. Journal of Physics: Conference Series, 1211, 012054 (12 pages).
77. Sutradhar, D. (2021), *Essentials of a Good Textbook*. Available at Internet site: https://yoursmartclass.com/essentials-of-a-good-textbook/ (Accessed on: 27 December 2022)
78. Tania, L.; Saputra, A.; Fadiawati, N.; Muntari, I.; Yolanda, N. (2017), *A student-generated less-familiar atomic orbitals (l = 4–10) representation using simple and real-time visualization software.* Journal of Science Education, 18(2), pp. 121-122.
79. Tokura, Y.; Nagaosa, N. (2000), *Orbital Physics in Transition-Metal Oxides*. Science 288(5465), pp. 462-468.
80. Trench, B.; Fahy, D.; Irwin, A.; Riedlinger, M. (2016), *Science criticism – what is it, and why do we need it? Panel report.* In: Repository of the 14th International Conference on Public Communication of Science and Technology (PCST), Istanbul, 2016. Campbell, ACT: PCST Network (7 pages). Available at Internet site: https://www.pcst.network/conferences/past-conferences/pcst-2016/ (Accessed on: 27 December 2022)

81. UNESCO (2022), *New UNESCO and IEA brief: Missing out on half of the world's potential in mathematics and science*. Available at Internet site: https://www.unesco.org/en/articles/new-unesco-and-iea-brief-missing-out-half-worlds-potential-mathematics-and-science (Accessed on: 28 December 2022)
82. Vinequai (2023), *Spherical Harmonics and Rotations*. Available at Internet site: https://vinequai.com/sphericalharmonics (Accessed on: 7 February 2023)
83. Wagner, S. C.; Kim, D. J. (2014), *The Price of Big Science: Saturation or Abundance in Scientific Publishing?* Policy and Complex Systems, 1(1), pp. 108-127.
84. Waldert, P. J.; Mossböck, M. (2022), *Vocabulary – verb: vado, vadis, vadere C, vasi*. Available at Internet site: https://www.latin-is-simple.com/en/vocabulary/verb/6860/ (Accessed on: 25 December 2022)
85. Wiggins, G. (2013), *Granted, and… ~ thoughts on education: What is a Course*? Available at Internet site: https://grantwiggins.wordpress.com/2013/08/23/what-is-a-course/ (Accessed on: 27 December 2022)
86. Wikimedia Commons (2020), *File: Representative-spherical harmonics.png*. Available at Internet site: https://commons.wikimedia.org/wiki/File: Representative-spherical_harmonics.png (Accessed on: 7 February 2023)
87. Winch, C.; Gingell, J. (Eds.) (2008), *Philosophy of Education: The Key Concepts, 2nd ed*. London: Routledge.
88. Wu, H.-Ka.; Shah, P. (2004), *Exploring Visuospatial Thinking in Chemistry Learning*. Science Education, 88(3), pp. 465-492.
89. Zhang, Q.; Ghanem, K.; Koch, E. (2012), *Spherical Harmonics, Cubic Harmonics*. Available at Internet site: https://www.cond-mat.de/teaching/QM/JSim/spherharm.html (Accessed on: 7 February 2023)
90. Zheng, Q. (2022), *Plotly: Spherical Harmonics*. Available at Internet site: http://staff.ustc.edu.cn/~zqj/posts/Plotly-Spherical-Harmonics/ (Accessed on: 7 February 2023)

# Quo Vaditis, Scientia et Educatio?

## Sažetak

Eksponencijalni razvoj ljudskog znanja tj. znanosti i tehnologije, sve je više izvan kontrole i sve više je u raskoraku s linearnim razvojem ljudskog bića. Ovaj rad procjenjuje utjecaj tog eksponencijalnog razvoja na edukaciju uz pomoć bibliometrijske analize sveučilišnih udžbenika i prikaza slučaja vizualne prirode u kemiji. Razni bibliometrijski opisivači (broj stranica, broj izdanja s godinama, veličina fonta, maksimalan broj znakova) određeni su za proučavane knjige iz 12 različitih područja znanja i iz 14 grana kemije. Prikazi slučajeva u kemiji (sferni harmonici, nukleofilne supstitucijske reakcije i baze nukleinskih kiselina) ilustrirani su upotrebom modernih programa za računanje i vizualizaciju te pomoću kemijskih baza podataka. Svi proučavani udžbenici iskazuju porast količine materije. Postoji nekoliko tipova tog porasta, linearni, parabolični, oscilirajući te drugi, vidljivi iz analiza dijagrama raspršenja broj stranica *vs.* vrijeme. I drugi deskriptori pokazuju da postoji porast. Brzine porasta od prvog do zadnjeg izdanja udžbenika su veće u kemiji nego u općem znanju. Kada se pretvore u dodatno vrijeme za učenje iz udžbenika, studenti su dobili 10 do 100 minuta po danu. To znači da studenti općenito provode iznad 2 sata, a u kemiji 2 – 4 sata po danu više učenja nego njihovi kolege koji su imali prva izdanja udžbenika. Tri prikaza slučaja u kemiji ukazuju da mnogi zastarjeli i krivi koncepti nisu nestali upotrebom moderne kompjutorske tehnologije, što otežava učenje iz takvih udžbenika. Udžbenici sustavno zaobilaze uporabu visokokvalitetnih slika načinjenih računalom, nego umjesto toga, preferiraju netočne shematske prikaze i umjetničke prezentacije. Ovakva situacija, unatoč eksponencijalnom razvoju znanja i tehnologije, postoji desetljećima istovremeno s dobrim programima za računanje i crtanje te kemijskim bazama podataka. Rješenja za takvu situaciju nisu jednostavna i ona uključuju radikalne promjene u udžbenicima cijelog studija.

**Ključne riječi:** eksponencijalni porast znanja, sveučilišni udžbenici, udžbenici kemije, bibliometrijska analiza, sferni harmonici, molekulske strukture, pogrešne interpretacije

Dr. sc. Rudolf Kiralj
Bjelovar University of Applied Sciences
Department of Nursing
Trg Eugena Kvaternika 4, HR – 43000 Bjelovar
Croatia
rkiralj@vub.hr