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## **MOODLE BASED ELECTRONIC CONTENT FOR STUDENTS IN COMPUTER CHEMISTRY**

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***Abstract.** In this paper we present a Moodle based teaching method in the field of Computer chemistry with focus on Chemoinformatics, QSAR modeling and software programming in chemistry. The main didactic goals are defined. A vast electronic content is created covering various topics in the field of Computer chemistry using the learning platform Moodle. The electronic courses include lessons presented in different formats, exercises, work data files, external links to additional informational resources, open source software and software developed in our department, question database, plenty of grade units and weighted grade scale. The system has been used for more than eight years and a large number of students were approbated in the system.*

**Keywords:** Computer chemistry, Chemoinformatics, Moodle, grading

**Mathematics Subject Classification 2010:** 92E10, 47N60

### **1. INTRODUCTION**

In the last four decades Computer chemistry [1, 2, 3] underwent rapid development and currently is a well established scientific field with cutting age applications in various areas such as pharmaceutical industry and drug discovery, development of new chemical species and nanomaterials, material science, computer simulations, analytical control and chemical registration, ecology and safety etc. In the past computer chemistry education was primary implemented within Ph.D. programs on a more specialized level. Nowadays computer chemistry education becomes popular where Master's and even Bachelor's programs in computer chemistry emerge. In our faculty for more than eight years we teach bachelor's program in the field of computer chemistry. Accordingly a master's degree in computer chemistry was started recently. Since the beginning of the programs we sought efficient ways to use various electronic resources in order to improve the teaching activities. The bachelor's degree in Computer chemistry includes classical chemistry courses and specialized courses in the field of computer chemistry some of which are discussed in the current paper. Computer chemistry requires interdisciplinary knowledge such as chemistry, mathematics, informatics, programming, graph theory, data mining, statistics etc. In this article we describe

the realization of teaching courses for Chemoinformatics, QSAR modelling and Software programming in chemistry. Our main education goal is to deliver a quality knowledge and professional skills in accordance with the modern scientific and industrial standards for the application of computer methods in areas such as design of biologically active compounds and new drugs, theoretical chemical calculations, modelling of physicochemical properties and biological activity, computer-based structure elucidation, processing of information obtained from chemical analyses etc. In order to achieve this we use the learning platform Moodle [4].

## **2. CONTENT AND TEACHING METHODOLOGY**

Computer chemistry curriculum includes various specialized topics: chemical informatics, statistics, QSAR modelling, quantum-chemical calculations, chemical databases and software programming. In principle computer chemistry is characterized by two main areas: Chemoinformatics and Computational chemistry as well as wide range of methodologies developed and applied in these two streams. Students have lectures, seminars and practical classes. The main theory is represented in the lectures where the main goal is not only supplying quality information to the students but an opportunity for the students to get in contact with the expert knowledge of their professors and to have discussions on hot topics in the professional field of the teachers. In order to achieve latter goal, the information representation is not focused only in lectures but a large amount of the activities related to the information transfer are shifted to the electronic content. Students have the opportunity to study some theoretical topic on the Moodle resources and to be more active in the lectures and seminars. Additionally various theoretical and practical problems for homework and self-preparation are communicated via Moodle. In most of the practical classes the students use high-quality software developed by well-known research groups and software companies as well as software developed in our department. The individual assignments of the students cover problems related to the research projects of their teachers.

## **3. LEARNING PLATFORM MOODLE**

Moodle [4] is a widely used open source platform for managing the learning process. Its main advantage such as supporting open standards and flexible design makes Moodle a preferable system for our teaching purposes. In this chapter we focus on some Moodle activities applicable to our teaching goals described in previous section.

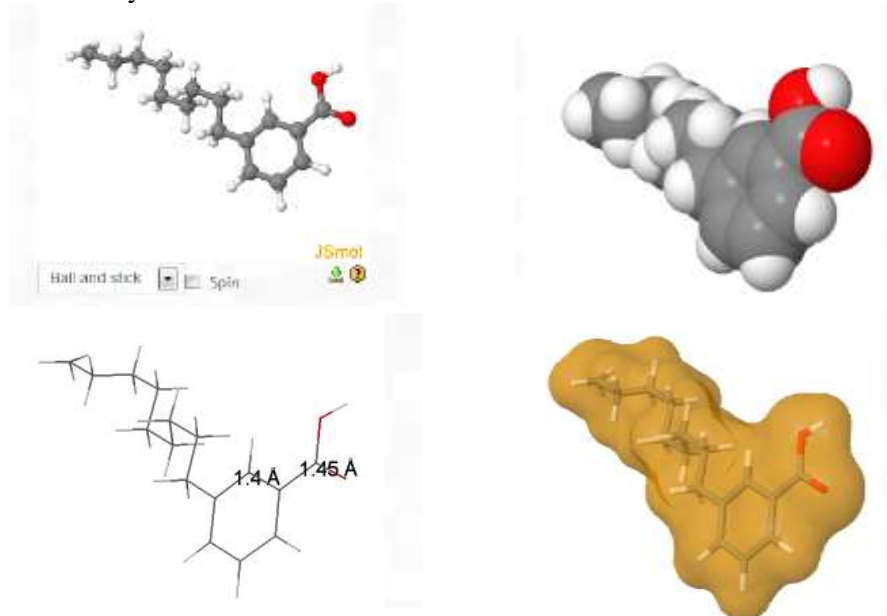
Moodle platform is under the strong Copyleft GPLv3 open source license and it is free of charge. It is scalable software while keeping excellent robustness and reliability thanks to the many years of improvement. Moodle is light, platform

independent and easy to install and maintain, running on the base of standard requirements such as Apache web server [5], MySQL database management system [6] and PHP language for web programming [7]. Moodle supports plenty of built-in functionalities and additional features thanks to the vast user community e.g. third party plugins and gadgets, language packs etc. Lesson presentation in various formats deliver the main knowledge to the students. We use Moodle basic resources such as page and book as well as file resource for additional information represented in \*.pdf, \*.ppt, \*.doc, \*.xls and other formats. Also video tutorials created by the teachers are accessed through the Moodle file resource in different video formats. Presently a variety of chemical databases and resource sites are available for public access worldwide. We provide additional informational resources via related links in any page and activity. Practical exercises were made using the Moodle quiz functionality. Our question base consists of many different question types as multiple choice, matching, calculating, drag and drop type, JME (java molecular editor) [8,9] etc. We have generated self-learning and self-testing quizzes in adaptive mode, which show and explain the mistakes by providing feedback to each choice. The assignment family activities were used for more complex questions as home works, research assignments, diploma thesis etc. The students are given a time slot within which they must submit their work data files. Opensource software packages and software modules developed in our department are attached as additional resources. Typically we supply Java [10] based software modules for solving of practical problems related to the teaching content as well as we use Tcl [11] scripts and R [12] scripts. During the whole learning process the students collect weighted notes from any of the grade items in the course in various grading categories.

#### **4. MOODLE EXAMPLES OF APPLICATION**

There are two basic types of objects studied in chemistry and computer chemistry: chemical compounds and chemical reactions. One of the most important tasks in our teaching activities is the processing of information related to the chemical compounds including: molecule structure, physicochemical properties, biological activities, experimental and analytical data. Chemical structure plays a key role in this information scope. For this purpose we installed and used JSmol [13,14,15] plugin for the visualization of molecule structure in various modes and contexts including the most popular 3D structure models, molecule surfaces etc. (see figure 1). Having the critical structural information embedded in the system, the other types of described information components are handled more or less with typical features of the Moodle platform. The reaction information is handled on the base of the structure manipulation approaches. Additionally for some more complicated cases of information processing we use custom java applications, Tcl or R scripts in order to deliver this type of information to the students. For example, figure 2 illustrates the processing of spectral data by mean of R script. Also supplementary chemical information is stored in the system in various file formats and popular

chemical linear notations as well as structural information is presented to the students by means of embedded links to external chemical and structural databases.



**Figure 1. Visualization of chemical structure and related chemical properties by means of JSmol plugin.**

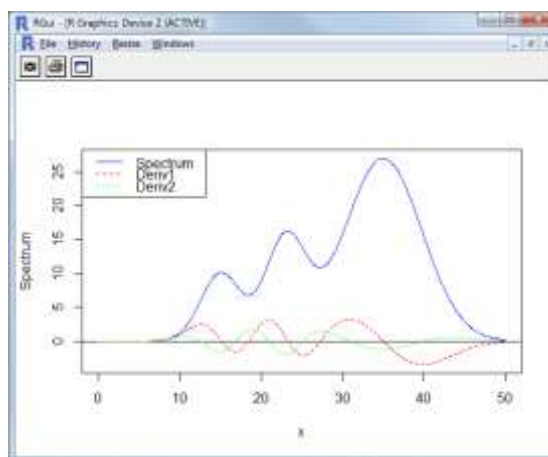
```

...
#Calculation of the first derivative
S1 = Spectrum
for (i in (2:(n-1)))
  S1[i]=(Spectrum[i]-Spectrum[i-1])/dt
S1[1] = S1[2]
S1[n]=S1[n-1]

#Calculation of the second derivative
S2 = S1
for (i in (2:(n-1)))
  S2[i]=(S1[i]-S1[i-1])/dt
S2[1] = S2[2]
S2[n] = S2[n-1]
...
plot(x,Spectrum,type="l",col="blue",ylim=c(m
in,max),lty="solid")
abline(h=0)

lines(x,S1,type="l",col="red",lty="dashed")
lines(x,S2,type="l",col="green",lty="dotted")
...

```



**Figure 2. Processing of UV spectra information by means of R script**

While JSMol is the primary tool for structure visualization there is a need for an instrument for structure information input. For this purpose we use Java Molecular Editor /JME/ developed by Peter Ertl [8]. Figure 3 illustrates the application of

JME which is an additionally installed Moodle plugin providing the functionality for creation of question types in Moodle with structural input.

3 (a)

3 (b)

**Figure 3. Application of JME plugin as 2D chemical structure editor used for structure input**

Figure 3a shows the creation of a JME type of question. The correct answer that is graded (in this example with 100%) is given as a SMILES line notation [16]. For teacher convenience, the SMILES code can be inserted after drawing the structure via the “Insert from editor” button. Additionally feedback can be also provided. Another widely used by us question type is the natively supported by Moodle matching question type.

Figure 3b shows how the JME question is displayed within a student quiz or a test session. The question consists of a question text and the embedded Java Molecular Editor. The students are invited to answer the question by drawing the chemical structure.

Figure 4. Application of matching question type in teaching Chemoinformatics.

With this question type we train students to solve few similar and easy questions. As can be seen from figure 4, chemical structures, matrixes, equations or other objects can be embedded within the question frames. The left hand side questions (Figure 4) require matching between chemical structure and SMILES notation, while the right hand side requires verification of the students' knowledge on different matrix types studied in the Chemoinformatics course.

Multiple choice question type is also supported in Moodle since its early versions. We use it in two major variants: (i) one answer allowed (see figure 5, left): and (ii) multiple answers (Figure 5, right side).

Figure 5. Application of single and multiple choice question type.

The students are expected to select only one answer on the left figure, while on the right side there is more than one option available. The latter question illustrates the SMILES theory and the existence of more than one linear notation for a given structure.

## 5. CONCLUSIONS

The learning platform Moodle is used to implement web based resources for the Bachelor's program in Computer chemistry conducted in the University of Plovdiv. The Moodle software features are efficiently applied to create vast electronic content which plays a central role for the teaching process in various subjects: Chemoinformatics, QSAR modeling, software programming etc. The implemented resources help the program realization and provide a convenient learning infrastructure to prepare professionals for companies and agencies which require efficient processing of chemical information and patents, R&D departments of pharmaceutical companies, chemical and biochemical laboratories.

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