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Integrating Modeling and *In Silico* Techniques in Chemistry Teaching

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Chemistry can be described at three distinct levels; namely, a) the macroscopic level (visible/touchable phenomena), b) the microscopic level (atomic/molecular), and c) the symbolic level (representing matter in terms of formulae and equations) [1]. Students who are studying chemistry are supposed to think at the microscopic levels (in terms of interactions between individual atoms and molecules) and explain phenomena at the macroscopic levels [2-3]. Students are supposed to link 2-dimensional and 3-dimensional structures of chemicals to their physical properties [such as the physical state (gas, liquid, or solid), the appearance of the chemical, boiling & melting points, density, state at room temperature, and color] and chemical properties (enthalpy of formation, flammability, preferred oxidation state, coordination number, etc.). All of these things should be "cooked" in mind.

According to Chandrasegaran [2], students find it difficult to properly bond between the different levels of understanding. It seems that students don't have adequate understanding of the macroscopic/ microscopic representations of molecules and the meaning of the symbols and formulas in chemical equations. These difficulties, along with the difficulties in understanding the 3D structures of molecules, hinder students' ability to solve problems in chemistry. Science educators proposed several solutions to prevail over these difficulties, such as: integrating three dimensional visualization tools, and promoting the switch between different chemical representations [4].

Researchers have found that integrating visual representations such as computerized molecular models, simulations, and animations in teaching may promote students' understanding of unobservable phenomena in science [5], and afford them with the opportunities to make abstract concepts visible. Manipulating chemical structures in 2D/3D representations help students relate the macroscopic, microscopic, and symbolic representation levels of chemicals to each other [5] and enhance students' conceptual understanding and spatial ability [6].

There are many tools that enable students to manipulate chemical structure in either 2D or 3D representations, and build molecular models, Table 1 summarize some of such tools.

Table 1. List of chemical drawing and modeling tools running on Microsoft Windows platform.

Software	Developer	Information
ChemDraw	CambridgeSoft	
Avogadro	Avogadro project team	3D molecule editor and visualize
ChemWindow	Bio-Rad	Freeware for academic research and teaching
KnowItAll	Bio-Rad	Freeware for academic research and teaching
Accelrys Draw	Accelrys	freeware version available; includes name2structure and structure2name
ACD/ChemSketch	ACD/Labs	freeware version available
BALLView	BALL project team	viewer, editor and simulation tool
MedChem Designer	Simulations Plus	freeware - includes calculation of logP, logD(7.4), sigma charges, Hydrogen Bond Donors, Hydrogen Bond Acceptor

Table 1 (continued). List of chemical drawing and modeling tools running on Microsoft Windows platform.

Software	Developer	Information
ICM-Chemist	MolSoft	Easy to use graphical user interface desktop chemistry editor
ChemDoodle	iChemLabs	
ArgusLab		Freeware
Ascalaph	Agile Molecule	Freeware
Amira	Visage Imaging Zuse Institute Berlin	14 day trial version available

It is worth to test, measure, assess, and evaluate how such modeling tools enhance chemistry education and learning processes while incorporated in teaching.

Point of View

We use our five senses to interact with the outside world and collect information from it and according to NLP (Neuro-Linguistic-Programming), we re-present the world to ourselves internally with these five systems called internal representations/ maps. We as individuals make sense of the world through our internal maps and each one of us lives in different reality, based on his filtering systems. Our mental maps are constructed through five representational systems. Actually, we use a combination of the five systems, although one may dominate. The three main dominant ones are visual, auditory and kinaesthetic systems [7]. The olfactory and gustatory systems attribute less. Nowadays we are teaching chemistry mainly through the auditory system. Practicing the modeling tools during chemistry education could work more on the visual and kinaesthetic systems, leading to promotion in students' conceptual understanding of chemistry and mainly for those students with dominant virtual and sensory-based internal maps. The hypothesis that NLP could facilitate knowledge and learning capabilities should be tested in chemistry education era.

Call for contributions in this field

The International Journal of Computational Bioinformatics and In Silico Modeling (IJCBIM) is interested in pushing the field of science education forward and encourage scientists to submit research and review articles related to integrating modeling and *in silico* techniques in science education. We are looking forward to learn how incorporating some of the tools listed in table 1 or any other modeling/ *in silico* tools could affect students' attitude toward learning science in general and chemistry in particular, and students' conceptual understanding of chemicals.

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Short Biography:

Dr. Anwar Rayan Studied Chemistry (degree awarded with distinction) followed by a Ph.D. in Computational Chemistry with Prof. Amiram Goldblum. Postdoctoral Studies on Bioinformatics at the school of pharmacy in Jerusalem. Research fellow in FMP, Berlin, Germany. Dr. Anwar Rayan is currently CEO of GeneArrest LTD company and the head of the Drug Discovery Informatics Lab at the QRC – Al Qasemi Academic College. Founder/ co-founder of 5 companies (IDD therapeutics , Pepticom, Sensotrade, GeneArrest and RAND Biotechnologies). Having more than 39 papers in peer-reviewed journals and 5 patents.

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