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The Chemist

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The Chemist

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The Chemist (Established in 1923)

Editorial

Chemistry the Leading Science

David Devraj Kumar

Florida Atlantic University

Chemistry continues to be the leading science in almost all branches of science and technology. In some areas the role of chemistry is visible, and in other areas it is not so visible. For example in health care, thanks to chemistry, newer and effective pharmaceuticals are synthesized continually paving the way for breakthrough medical treatments. In health care the role of chemistry is overt. In the area of information technology, the quest for smaller size and faster computing power is driven by research and development of materials with semiconducting properties. Chemistry is one of the driving forces behind the ongoing revolution in mechatronics producing technologies for driverless cars and the delivery drones of tomorrow. Without developments in the chemical sciences about the knowledge of how different materials interact with electromagnetic waves, paving the way for high quality materials suitable for optoelectronics and sensing materials, the driverless technology might not have evolved to the level it is now. In mechatronics the role of chemistry is covert. Thus visible or invisible, chemistry is leading science and technology revolution in almost all areas of life.

In this issue of *The Chemist*, Paul Craig and co-authors discuss how to promote hypothesis-driven thinking in undergraduate biochemistry education using protein function prediction. V. Subha and co-authors report green synthesis of copper nanoparticles using *Odina woider* Gum extract and their effect on photo catalytic dye degradation. A retrospective evaluation of the principles, policies, and practices in establishing a post-secondary chemistry department is the focus of the article by John Hill and co-author. Tata Murthy discusses the role of chemistry in oil and gas extraction. And finally, under the public understanding of chemistry section, David Manuta and co-author present a report of false-positive drug test for methamphetamine.

This year *The* Chemist has entered into an agreement to be indexed by EBSCO, the leading research database provider. This is a remarkable milestone in the development of the journal in its current online refereed format since its recent revival in 2012. I would like to acknowledge the members of the Editorial Review Board for their invaluable support reviewing manuscripts for *The Chemist* and enabling to maintain the quality of the journal. The role of the editorial assistants cannot be underestimated either. The journal is attracting manuscripts from around the world and I strongly encourage readers to consider submitting manuscripts for publication in *The Chemist*.

The Chemist
Journal of the American Institute of Chemists

Using Protein Function Prediction to Promote Hypothesis-Driven Thinking in Undergraduate Biochemistry Education

Paul A. Craig,[1] Trevor Anderson,[2] Herbert J. Bernstein,[1] Colette Daubner,[3] Anya Goodman,[4] Stefan M. Irby,[2] Julia Koeppe,[5] Jeffrey L. Mills,[1] Mike Pikaart,[6] Ashley Ringer McDonald,[4] Suzanne O'Handley,[1] Rebecca Roberts,[7] and Robert Stewart.[8]
[1]Rochester Institute of Technology, [2]Purdue University, [3]St. Mary's University, [4]Cal Poly San Luis Obispo, [5]SUNY-Oswego, [6]Hope College, [7]Ursinus College, [8]Oral Roberts University.
([1]E-mail: paul.craig@rit.edu)

Abstract: Students at the Rochester Institute of Technology and Dowling College used bioinformatics software, which they had helped develop, to predict the function of protein structures whose functions had not been assigned or confirmed. Over the course of time, they incorporated other bioinformatics tools and moved the project to the wet lab, where they sought to confirm their *in silico* predictions with *in vitro* assays. In this process, we saw so much personal and professional growth among our students that we chose to implement their approach in an undergraduate biochemistry teaching lab, which we call BASIL, for Biochemistry Authentic Scientific Inquiry Lab. This curriculum has now been implemented by thirteen faculty members on eight campuses, and we look forward to a long-range exploration of BASIL's impact on the students who enroll in courses that use the BASIL curriculum.

Key Words: Biochemistry education, bioinformatics, protein function, structure alignment, course-based undergraduate research experience.

STUDENT INITIATIVE LED TO DRAMATIC CHANGE IN OUR RESEARCH

Early in my career at the Rochester Institute of Technology (RIT),[1] a colleague shared his ideas with me about how to design an undergraduate biochemistry laboratory course that would engage the students in a research endeavor. Starting from his ideas, I created a project-based undergraduate biochemistry laboratory course where students purified and studied a single enzyme using various techniques [1]. I hoped to introduce a basic research component to the course with techniques such as site-directed mutagenesis, but was never able to move the students that far along with the project. At the same time, it was my privilege to direct independent research with a steady stream of inquisitive undergraduate students and found that much more rewarding.

In 2004, Herbert Bernstein and I began collaborating on a project funded by the NSF ATE program that was centered on using 3D visualization across the scientific curriculum, where we focused on molecular visualization. We chose to work with the PyMOL molecular graphics environment because it contained a number of 3D visualization modes. Two of the students on that project, both bioinformatics majors, created a simplified user interface for PyMOL called EZ-Viz, which was designed to help educators use PyMOL without having to learn commands in the Python language [2]. The following year, two additional students built ProMOL, based on the original code of EZ-Viz. ProMOL accesses additional tools in PyMOL to enable the user to create motifs of enzyme

[1] The first-person narrative is from the point of view of Paul Craig.

active sites, then search for those motifs in any protein that has 3D coordinates [3]. Remarkably, these students were biotechnology majors with no background in programming, yet they taught themselves Python as they were developing the code for ProMOL (source code can be found at https://github.com/SBEVSL/sbevsl_migrated/tree/master/promol). These students moved us another step toward our goal of merging the teaching lab with authentic research activities by converting a teaching tool (EZ-Viz) into a research tool (ProMOL).

Students in our research lab then began using ProMOL to predict functions for some of the >3000 proteins in the Protein Data Bank [4,5] that are described as having an "unknown function," many of which resulted from the Protein Structure Initiative [6]. In one of the first cases we studied in depth, an undergraduate student aligned PDB entry 3DS8 [7] against the library of enzyme active sites found in ProMOL and found an excellent alignment with PDB entry 1ORV, a porcine dipeptidyl peptidase which was also a serine hydrolase [8]. He immediately wanted to confirm his findings in the wet lab, so he obtained the plasmid containing the gene for 3DS8, expressed the protein, purified it, and analyzed it by SDS-PAGE to confirm that the protein was pure and had the expected molecular weight. Initial testing with a Quanticleave™ protease assay kit (ThermoFisher Scientific) revealed a low level of proteolytic activity. He decided that this was clearly not a protease, so he began looking for other tools to help him make a better prediction that he could test in the lab. The student then analyzed the sequence of 3DS8 using BLAST [9] and found some of the best sequence alignments were with the esterase/lipase superfamily. Further analysis within ProMOL revealed a very good active site alignment between 3DS8 and PDB entry 1TAH (Figure 1), a lipase with a known and well documented active site [10]. He then shifted his emphasis in the wet lab to test activity with colorimetric esterase substrates. In this process, the student had shifted our research from being strictly *in silico* to becoming *in vitro*. It was clear that his curiosity had been piqued by the computational discoveries, but that it would only be satisfied by moving to the bench to verify his predictions.

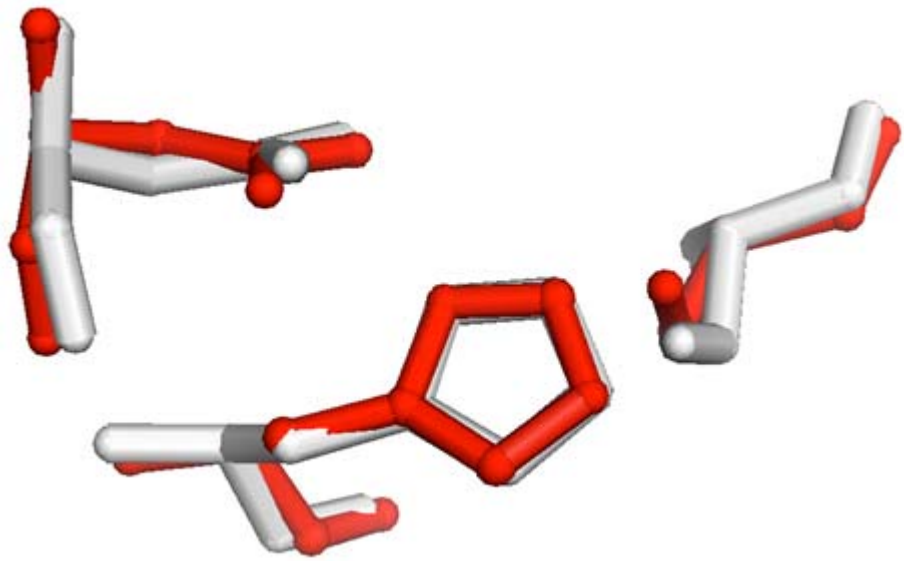

Fig 1. Alignment of PDB entry 3DS8 (red) with triacylglycerol lipase, PDB entry 1TAH (white). The RMSD for the all atom alignment for the three active site residues (aspartate 263 in 1TAH/aspartate 188 in 3DS8; histidine 285/histidine 222; serine 87/serine 102) was 0.42 Å.

After this initial success, the students in our research group realized that they needed to access additional tools to effectively predict protein function based only on the 3D coordinates of protein structures. They subsequently developed the flow chart shown in Figure 2 that integrated results from BLAST [9], Pfam [11], and Dali [12] with our findings with ProMOL. A team of five or six students in our research group then analyzed >3000 protein structures of unknown function from the PDB, which led to >50 promising predictions of protein function [13].

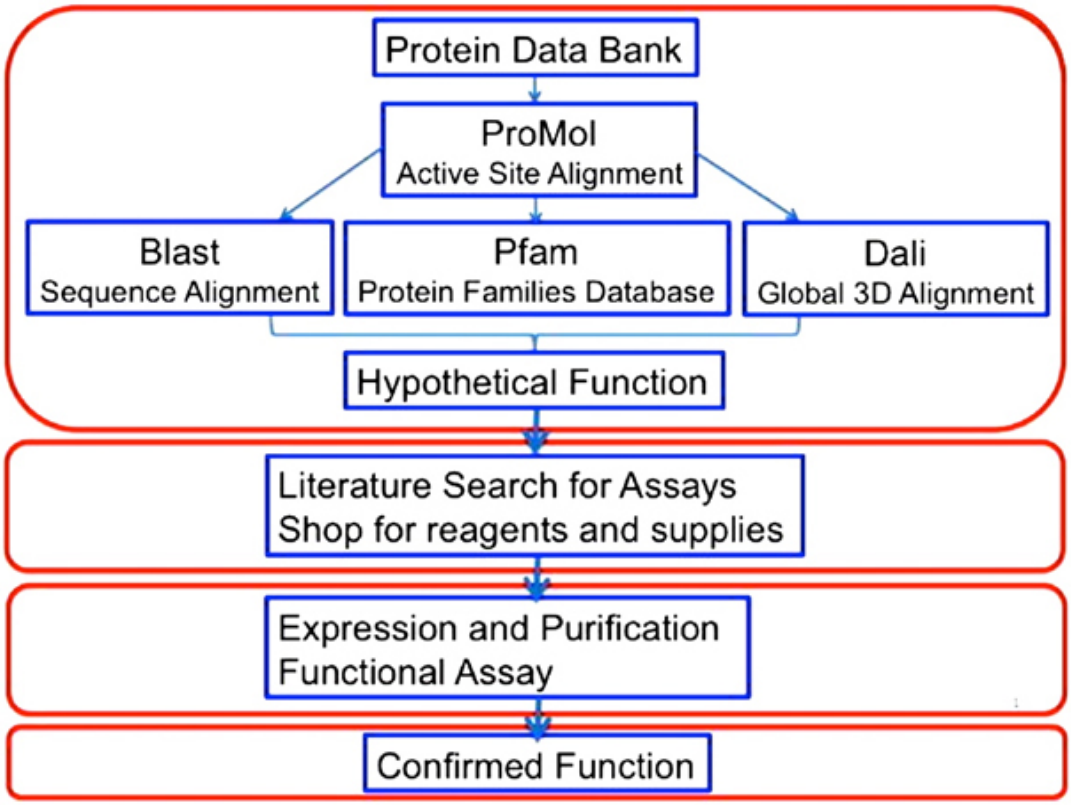

Fig 2. A flowchart for protein function prediction and *in vitro* confirmation of enzyme activity. This figure was published previously [14] and is used with permission.

The faculty members leading this project (Herbert J. Bernstein, Jeffrey L. Mills, and Paul A. Craig) noticed a clear pattern throughout this project over the course of a decade; undergraduate students began with our suggestions, but quickly moved beyond our suggestions to start asking new questions, formulating new hypotheses, and trying new things in the computational lab and in the wet lab. In our research lab, we provided the students with research goals and a set of tools to pursue those goals. In repeated cases, they pushed through the limits of our approach and started asking questions, such as:

"What other things can we do with these tools?"
"What other tools are available that we can use?"
"What tools can we create to better pursue our questions?"

This was reinforced as we watched our students present their findings at conferences. They were thoughtful and effective in their presentations and engaged as peers in dialogue with established scientists; asking and answering questions, discussing shortcomings in their results or their protocols, and seeking and sharing insights into future directions. In one case, a junior undergraduate submitted an abstract to present a poster at the annual meeting of the American Society for Biochemistry & Molecular Biology (ASBMB). Based on her abstract, she was invited to give a talk at the conference. She presented her talk in a session with two established investigators, a post-doc, and a doctoral student. Her presentation was well received and she answered questions accurately and with confidence. Following the session, she asked me why I did not tell her that she would be the only undergraduate presenting a talk in that session. I assured her that I was confident in her knowledge of the project, her understanding of where it fit with the larger scientific questions being addressed in the session, and in her ability to handle herself in a stressful situation. In short, she and the other students engaged in this project were becoming scientists. At that point, we began to consider how we might extend this approach to a larger group of students through an undergraduate biochemistry laboratory course.

CREATION OF A COURSE-BASED UNDERGRADUATE RESEARCH EXPERIENCE

We presented our ideas to our program officer at NIH, who pointed us to the NSF IUSE program. Along with biochemistry colleagues from other universities, we submitted a proposal and received some helpful guidance, mainly that we needed to bring more people on board. Through connections during a poster session at the 2014 ASBMB national conference, we added colleagues with expertise in biochemistry, molecular biology, computational chemistry, and biochemistry education to our team (Table 1), and were able to win funding in the next round.

Table 1. Faculty members and institutions on the project

Institution	Faculty Members
Cal Poly San Luis Obispo	Anya Goodman, Ashley Ringer McDonald
Hope College	Mike Pikaart
Oral Roberts University	Bob Stewart
Purdue University	Trevor Anderson, Stefan Irby
RIT	Herbert Bernstein, Paul Craig, Jeff Mills, Suzanne O'Handley
St. Mary's University	Colette Daubner
SUNY Oswego	Julia Koeppe
Ursinus College	Rebecca Roberts

We are exploring a number of questions as we implement this laboratory experience:

- Can we convert our research lab experience of developing scientists into a Course-based Undergraduate Research Experience (CURE)?
- Can we develop methods to monitor student progress as scientists in a teaching lab?
- How can we, as faculty members, learn to help students grow as scientists?

We faced a number of initial challenges. The first challenge was communication; the team consists of thirteen faculty members on eight campuses in three different time zones. Our solution was to meet weekly in a video chat room hosted by BlueJeans (bluejeans.com), which is licensed on the RIT campus. Our second challenge was the creation of a uniform set of lab/curriculum modules that were sufficiently flexible to be adapted to courses on campuses with different schedules (semesters vs. quarters, length of lab periods, student availability outside of scheduled lab time), varying instrumentation resources, varying levels of expertise, and comfort in both the wet lab and the computer lab. We created a series of ten modules for the computer lab and the wet lab (Table 2). Creating the modules have been an iterative process over a two-year period (a detailed description of these modules will be the subject of a future manuscript). Our third challenge resulted from our varying levels of expertise, particularly with using computational tools in the lab with our students. During the summer of 2015, we held extended online conversations about the software tools for the project; where we discussed how to install the software, how the software works, and how we can teach our students to use it to make *in silico* discoveries about protein function. These conversations led members of our team to create a number of tutorials that focus on testing and practicing these computational techniques (basiliuse.blogspot.com).

During our discussions, it became clear that our project fit the description of a CURE [15]. We are aware of several CUREs that focus on nucleic acids, including SEA-PHAGES [16] and the Genomics Education Partnership [17–19], but few that focus on protein structure and function [20]. At that time, we also adopted the acronym BASIL, for Biochemistry Authentic Scientific Inquiry Lab. Current resources for BASIL, including student modules for the lab and video tutorials, can be accessed from the BASIL blog (basiliuse.blogspot.com).

After the first year of the BASIL project, I conducted a survey of the faculty members that focused on their experience of transitioning to a CURE format to teach an undergraduate biochemistry lab. Survey questions were formed by discussions with Trevor Anderson and Stefan Irby, team members from Purdue who are biochemistry educational researchers, and the educational evaluators for the project. The results of the survey have been reported elsewhere [14]. Here is a brief summary of some of the themes that emerged from the survey:

- It would have been better to firmly establish the modules before implementing them on our campuses.
- It is important to communicate regularly, especially when dealing with challenges, while installing or using the software for the project.
- All participants were eager to share their experiences at national conferences of the American Chemical Society, American Biophysical Society, American Society for Biochemistry & Molecular Biology, and the Biennial Conference on Chemical Education.
- All the team members shared enthusiasm for the project. One stated, "I hope that this research approach will become the norm".
- All agreed that we need to formally evaluate both the attitudes and the learning experiences of the students involved in the project on our campuses.

Our future plans include creating fully annotated instructor resources for each of the modules, formal assessment of student growth as scientists that results from this course, recruitment of additional campuses to implement the BASIL curriculum, and publication of our students' findings in the literature on online protein resources.

Table 2. Online resources for the BASIL curriculum.
These can be downloaded and viewed at basiliuse.blogspot.com.

In vitro modules	*In silico* modules	Tutorials for *in silico* modules
Protein Expression	BLAST	Biochemistry Lab BLAST Tutorial
Protein Purification	Dali	Biochemistry Lab Dali Tutorial
Protein Concentration	Pfam	Biochemistry Lab Pfam Tutorial
SDS-PAGE	ProMOL	Introduction to PyMOL Introduction to ProMOL Motif Finder in ProMOL Structure Query
Enzyme Activity	PyRX	Ligand Docking with PyRX

I was invited to present our project at chemistry and biochemistry departments on several campuses during the past year. On two of the campuses, I shortened my presentation to about 25 minutes, and then engaged the audience in a discussion about becoming scientists. The audiences (25-40 people on each campus) were divided into groups of 4-6 people, including graduate students and faculty members. Each group was asked to discuss, "When did you first start to see yourself as a scientist?" Their answers are summarized in Figure 3.

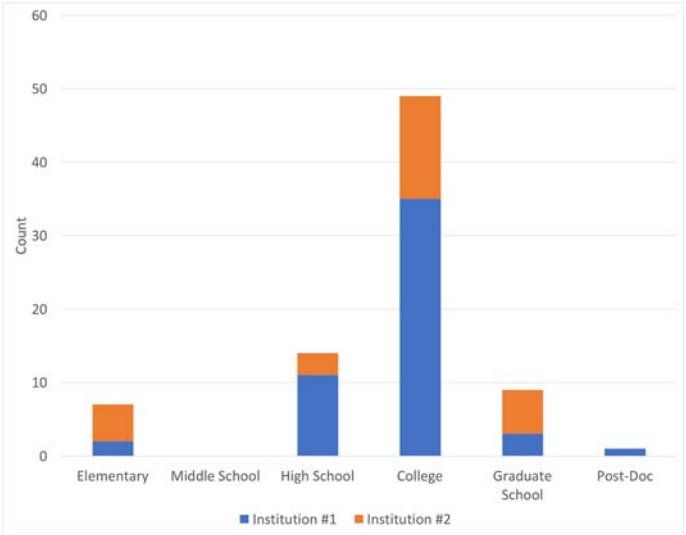

Fig 3. Recollection of seminar participants of their first self-identification as scientists for students and faculty on two major campuses.

The second question for these groups was "How can you tell that students are growing as scientists?". The groups from these two campuses gave the following responses, which will contribute to our future conversations about student growth as scientists in the BASIL project:

- When "what" questions become "why" questions
- When curiosity becomes more important than grades
- When students start designing their own experiments
- When students challenge the instructor
- When students find a better model on their own
- When students begin to engage in "what if" thinking
- When students start teaching each other

CONCLUSION

The BASIL project emerged from the minds and actions of a group of undergraduate research students focused on predicting functions for unannotated protein structures. BASIL is a Course-based Undergraduate Research Experience that is led by faculty members on eight different college campuses that include several undergraduate liberal arts institutions, two large public institutions, one large private institution, and a Hispanic-serving institution. The BASIL modules combine wet bench techniques that are common to most undergraduate biochemistry lab courses with bioinformatics skills for the analysis of protein structures and ligand binding to those structures. As a group, we will continue to refine this curriculum so that it can be readily implemented in a wide variety of campus settings. We are also committed to pursuing larger questions associated with this effort:

- Can our CURE offer benefits of research experience to a larger group of students in a classroom setting?
- How do we define the developmental stages of a scientist?
- What are the observable characteristics that demarcate the transition to becoming a scientist?

The authors welcome public comment on these questions on our blog, basiliuse.blogspot.com.

ACKNOWLEDGMENTS

I would like to thank the many students who have contributed to this project, with particular gratitude to Brett Hanson, Greg Dodge, and Kaitlin Hart; each dynamically shaped the project and carried our whole research group forward to a new level. This material is based upon work supported by the National Science Foundation under Award #1503811, the National Institute of General Medical Sciences under Award #78077, and the campuses represented in the BASIL project. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation, the National Institute of General Medical Sciences, or the campuses represented in the BASIL project.

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Green Synthesis of Copper Nanoparticles Using *Odina wider* Gum Extract and their Effect on Photocatalytic Dye Degradation

V. Subha[1], S. Kirubanandan[2]*, M. Arulmozhi[3] and S. Renganathan[1]*

[1] National Centre for Nanoscience and Nanotechnology, University of Madras, Guindy Campus, Chennai-600025, India.
[2] Dept. of Chemical Engineering, Monash University, Clayton, Melbourne - 3800, Australia
[3] Dept. of Petrochemical Technology, BIT Campus, Anna University, Tiruchirappalli - 620024, India.
*(*E-mails: kirubanandan.shanmugam@monash.edu, mannargudisubha@gmail.com)*

Abstract: The advancement of nanotechnology is empowering researchers in the synthesis of nanoparticles for biological and biomedical applications. Especially, Metal nanoparticles have been used in the field of catalytic reactions for water treatment, magnetic recording, and microelectronics. Copper nanoparticle is used as the key component in the fabrication of future Nanodevices, Nanowires, and Nanoelectronics. In this research work, CuNPs were prepared from *Odina woider* gum plant extract. The bioactive compounds in the extract play as a reducing and a capping agent. The synthesized copper nanoparticles were affirmed by the change of colour after inclusion of *Odina woider* gum into the Copper Sulphate solution. The biosynthesized CuNPs showed 600nm surface Plasmon resonance by UV-Vis Spectra. The CuNPs is characterized by Fourier Transform Infrared examination (FTIR), X-Ray beam diffraction examination (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive X-Ray examination (EDX), and Transmission Electron Microscopy (TEM) investigations. The integrated CuNPs were found to be in a cubical structure with the particle size estimate between 50-100 nm. Synthesized CuNPs have effectively degraded 96% of the acid blue dye in the solution. The biosynthesized copper nanoparticles have potential applications in industrial waste water treatment.

Note: The work reported in this paper was conducted in the Department of Biotechnology at Anna University, Chennai, India.

Key Words: Bioreduction, Nanoparticles, *Odina woider*, Characterization.

INTRODUCTION

Nanotechnology assumes a vital part in present day research [1,2]. Nanotechnology is the most proficient innovation that can be connected to all fields, such as pharmaceutical, gadgets, the health industry, nourishment and bolster, biomedical science, medications, the synthetics industry, vitality science, cosmetic agents, ecological wellbeing, mechanics, and space ventures. Nanotechnology has likewise been used for medicines to fight infection [3], cancer [4], allergy [5], diabetes [6], and inflammation [7]. Green chemistry is an execution, advancement, and foundation of compound preparation.

Materials and procedures for synthesis of nanomaterials are used to minimize the utilization of dangerous chemicals to the environment [8]. There are many methods for the preparation of nanoparticles, such as sol-gel procedure and co-precipitation. Contrasted with those strategies, green synthesis procedures are one of the best techniques to create nanoparticles for cost adequacy, effortlessness, utilization of lower temperatures, and the

use of less dangerous materials, and is perfect for therapeutic and nourishment applications [9,10]. Numerous specialists utilized green blend strategies for various metal nanoparticles because of their developing need of eco-accommodating properties [11]. Green combination procedure has been shown to be the best technique when contrasted with the other procedures; for example, concoction lessening, photochemical decrease, electrochemical diminishment, and warm vanishing [12]. In this study, the plant extract has been utilized as the capping and the reducing agents for the blend of copper nanoparticles due to their lessening properties introduced in the leaf extract [13,14]. In the course of recent years, the metal nanoparticles have been used in investigations for their potential applications in various fields, such as attractive recording media or smaller scale hardware, catalysis [15], nano-sensors, nanoelectronics, optoelectronics, and data stockpiling devices [16]. A few properties such as morphology, size, and appropriation of the particles arise from the nanoparticles [17]. Copper is the most broadly utilized metal due to its electrical, optical, synergist, biomedical, and antifungal/antibacterial applications among different metal particles, compared to gold, silver, palladium, zinc, and quantum dots [18]. Copper results in higher yields and response rate in mellow response conditions when contrasted with other customary catalysts [19]. Copper nanoparticles act as an antimicrobial agent in different fields. The copper is exceptionally toxic to microscopic organisms, such as *E-coli, Staphylococcus aureus, and Pseudomonas aeruginosa*, and non-poisonous to creature cells. Because of this, copper is considered to be a compelling bactericide that is safe for humans in nourishment bundle applications and in water treatment applications [20-22].

Different plants were utilized for the amalgamation of nanoparticles utilizing green synthesis procedure. Nanoparticles were integrated from each part of the plant independently; like the seed, stem, bloom, leaf, and skin of the natural products. The nanoparticles blended from plant concentrate were observed to be secured by the restorative properties of plant concentrate, which could be utilized as a part of meditation that is focused on medication conveyance and corrective applications [23]. In this work, *Odina wodier* gum is used for the synthesis of copper nanoparticles. The plant, *Odina wodier*, is a moderate-sized or large deciduous tree with thick, soft branches belonging to the family *Anacardiaceae*. The *Odina wodier* tree is found in tropical parts of India. *Odina woider* bark decoction is used as astringent in patients with atonic dyspepsia and general debility. *Odina* gum is used as an ointment with coconut milk and as a liniment with brandy for the application of sprains and bruises. *Odina wodier* is also used as a gargle in aphthous conditions of the mouth and for a toothache. Fresh juice of the bark is used on eye sores and obstinate ulcers. Powdered bark mixed with neem oil is an application for chronic ulcers, skin diseases, and is also used as a paste for leprous ulcers. This work explores the biosynthesis of copper nanoparticles using the extract of *Odina woider* gum, and along these lines enhancing the significance of this plant source and of green chemistry in the possible production of different metal nanoparticles in future research [24,25].

MATERIALS & METHODS

Materials

All reagents utilized as a part of this study were procured from Sigma Aldrich Chemicals India. Double distilled water was used for this procedure. Filtration was built up by utilizing Whatman no.1 papers. Dishes and apparatus utilized for the total responses were washed and flushed with double distilled water and dried in a hot air oven.

Arrangement of *Odina woider* Gum

The *Odina wodier* gum was collected from Mannargudi and Tamilnadu, India. The collected gum was cleaned and then soaked in hot water until dissolved. The *Odina wodier* was then centrifuged to remove solid dust. Finally, the supernatant liquid gum was collected and used for the further synthesis of copper nanoparticles. The cleaned gums were dried under sunshade to completely expel dampness, powdered by utilizing the mechanical processor, and put away. A 5 gram portion of the powdered gums were placed into a measuring glass with 100 ml of refined water and permitted to bubble at 60°C for 30 minutes under reflux condition, followed by being cooled off to room temperature.

Preparation of CuNPs

A 25-ml portion of leaf concentrate was slowly added to 100 ml of 1mM (0.001M) solution of copper sulfate with constant stirring [26]. After the total addition of gum concentrate, the blend was kept under incubation for 24 hours. Within a specific time, the solution changed from a shade of green to straw yellow, demonstrating the development of copper nanoparticles. At that point, the solution was centrifuged for 15 minutes at 10,000 rpm and scattered in double distilled water to expel any undesirable natural materials [27,28].

Characterisation

The development of copper nanoparticles was confirmed using UV-Visible spectroscopy, utilizing a Jasco V-550 spectrophotometer instrument. The size of the CuNPs was determined by scans in the range of 300-700 nm. To decide the biomolecules' availability of CuNPs in the extracts, FTIR scans were made between 400 and 4000 cm^{-1}. The specimen was centrifuged at 9500 rpm for 20 min, dried utilizing a hot air stove, and ground with KBr to shape a pellet. At that point, the pellet was examined utilizing a Jusco 5300 model FTIR instrument. The crystalline structure of the copper nanoparticles was clarified using X-Ray diffraction examination utilizing a Rigaku X-Ray diffractometer (Miniflex, UK) instrument working at 40 kV with 2 sec time interim at room temperature (27°C). The mean size of the crystalline Cu and Cu_2O nanoparticles were calculated by the following correlation:

Scherrer formula, $D = K\lambda / \beta \cos\theta$

where D is the average size of crystallite, K is the Scherrer constant with a value from 0.9 to 1, λ is the wavelength of the X-Ray source (0.1541 nm) used in XRD, β is the full width at half maximum of the diffraction peak, and θ is the Bragg's angle.

Morphology and mean molecule size of the CuNPs were evaluated by SEM and TEM examination. The specimens were set up for SEM and TEM examination. The SEM investigation used a Supra Zeiss with 1 nm determination at 30 kV with 20 mm Oxford EDS finder. The basic arrangement in the response blend was dictated by EDX examination. The TEM investigation was completed utilizing a HITACHI H-7650 at a working voltage of 80 kV.

Evaluation of the Photocatalytic Activity of Copper Nanoparticles:

The photocatalytic activity of the green synthesized copper nanoparticles was evaluated by using the aqueous solution of an acid blue dye. It was performed by the addition of CuNPs to 10 ml of the dye solution, and the suspension was subjected to irradiation under sunlight. The aqueous suspension was magnetically stirred throughout the experiment. At different time intervals an aliquot was removed, the absorption spectra was recorded, and the rate of decolourization was determined in terms of change in intensity at λmax of the dyes. The decolourization efficiency % has been calculated as

$$Efficiency\,\% = \frac{Co - C}{Co} * 100$$

where Co=Initial concentration of dye and C=Concentration of dye after photoirradiation.

The initial concentration of dye solution is 100 ppm of acid blue 120.

RESULTS & DISCUSSION

UV-Visible spectroscopy study

The results of the UV-Visible spectroscopy examination of the specimen are shown in Figure 1. It is the best technique for examination to identify CuNPs by the Surface Plasmon Resonance [29,30].

The CuNPs development was affirmed from the crest at 600nm, which is the surface Plasmon resonance band of copper nanoparticles, this outcome agrees with Curtis *et al.* The peak maximum was observed to slowly diminish as size increased. Copper SPR impacts diminish with the time due to the oxidation of the produced copper nanoparticles [39].

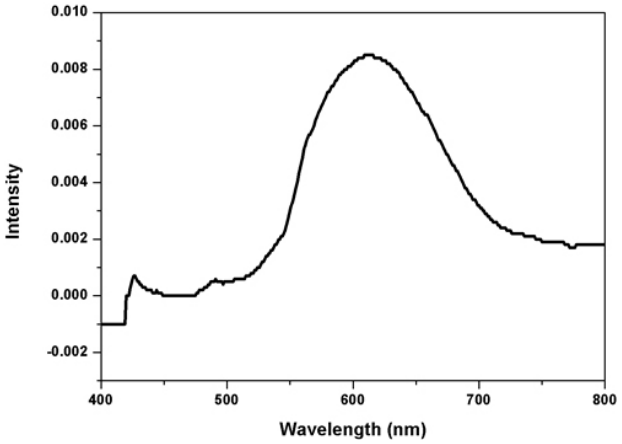

Fig 1: UV-Visible spectra of the green synthesized Cu NPs using UV-Vis Spectroscopy

FTIR Study

The FTIR estimation of plant concentrate and copper nanoparticles are provided in Figure 2, a-Odina Gum extract and b-Odina Gum +CuNPs. The FTIR examination was utilized to distinguish between the *Odina woider* gum and CuNPs. In Figure 2 (a), *Odina woider* gum separation demonstrated top peaks at 3851, 3479 and 1640 cm^{-1}. The top absorbance at 1640 cm^{-1} was expected to agree with C=O stretching [31], the peak of 3479 cm^{-1} for O-H stretching of phenolic compounds [32]. The O-H stretching of hydroxyl groups absorbs at 3851 cm^{-1} [33]. In Figure 2 for copper nanoparticles, absorbance at 3901, 3840, 3852, 3460, and 1636 cm^{-1} were observed. Peaks at 1636 and 3460 cm-1 corresponded to C=O stretching of amides and O-H stretching of a phenolic compound, respectively. Alternate peaks seen in the copper nanoparticle spectra are 3852, 3840, and 3901 cm^{-1} due to O-H stretching alcohols and phenols [1]. The FTIR examination of CuNPs recommended that they might be encompassed by natural particles (e.g., polyphenols, alkaloids, and terpenoids); Kalainila *et al*. reported similar results [37]. The substance constituents display in plant leaves concentrate; for example, flavonoids, alkaloids, and unsaturated fats are in charge of reducing copper particles to copper nanoparticles because of their capping and limit reducing abilities.

Samples	vO–H overlapped with vN–H (cm−1)	vC=O of amide (cm−1)
Odina Woider Gum	3479	1640
CuNPs	3460	1636

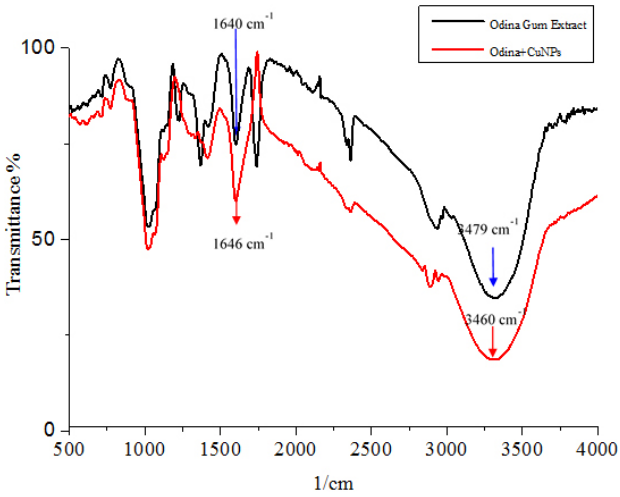

Fig 2. FTIR spectrum of *Odina* extract and of *Odina*-nanoparticles

XRD Examination

Figure 3 shows the XRD examination of the copper nanoparticles. The figure shows the two diverse diffraction tops at 2θ =39.1°, 43°, 68.3°, and 73°. These diffraction crests alluded to the attributes of cubic focused CuNPs. Diffraction crests got to 2θ edge compared to (111) and (113) mill operator index [26]. To decide the normal molecule size of the CuNPs, the Debye-Scherrer equation is utilized.

The crystal structure and size of the nanoparticles are verified by XRD analysis. Peaks observed at 2θ with values of 42.47, 51.73, and 73.42 correspond to (111), (200), and (220) planes of metallic Cu. These three peaks are quite consistent with those of the standard JCPDS Card No. 04-0836 for the standard spectrum of the pure FCC, face centered cubic, metallic Cu. Besides the metallic Cu peaks, several other diffraction peaks appeared at 36.43, 61.58, 73.42, and 77.19 corresponding to (111), (220), (311), and (222) planes of cuprite, respectively, indicating the formation of cubic copper (I) oxide nanocrystals. XRD peaks observed for cuprite is matched well with the standard powder diffraction card of bcc (body centered

cubic) cuprite (JCPDS No. 05-667). The mean size of the crystalline Cu and Cu_2O nanoparticles calculated from the major diffractions peaks using the Scherrer formula is about 28.73 and 25.19 nm, respectively.

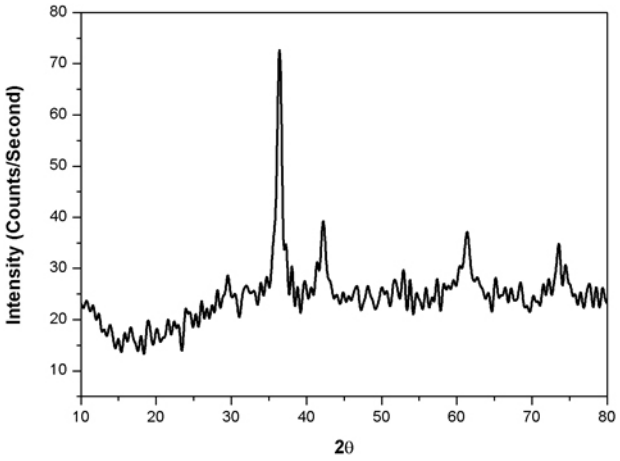

Fig 3. XRD spectrum of nanoparticles

SEM Analysis

The surface morphology and size of the nanoparticles were acquired by Scanning Electron Microscopy (SEM) examination. Figures 4 (a) and 4 (b) show the CuNPs incorporated by the plant concentrate of *Odina wodier*. The electrostatic collaborations and a hydrogen bond between the bio-natural capping atoms bond are in charge of the union of copper nanoparticles utilizing plant extract. It was demonstrated that circular and generally uniform state of the copper nanoparticles was affirmed in the range of 60-100 nm. Due to the Surface Plasmon Resonance, the copper nanoparticle demonstrated the retention peak of higher counts [34]. The quantitative examination of components of CuNPs is investigated by EDAX examination in Figure 4 (c).

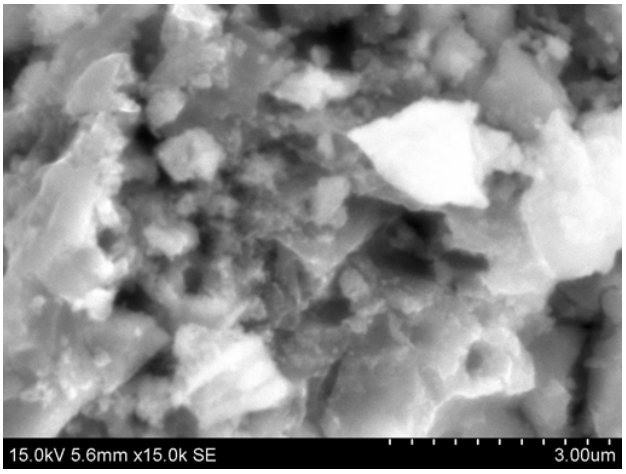

Fig 4 (a). Copper nanoparticles

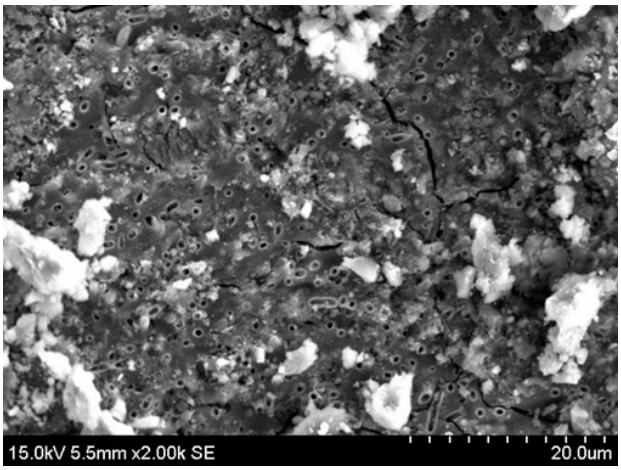

Fig 4 (b). Concentrated copper nanoparticles

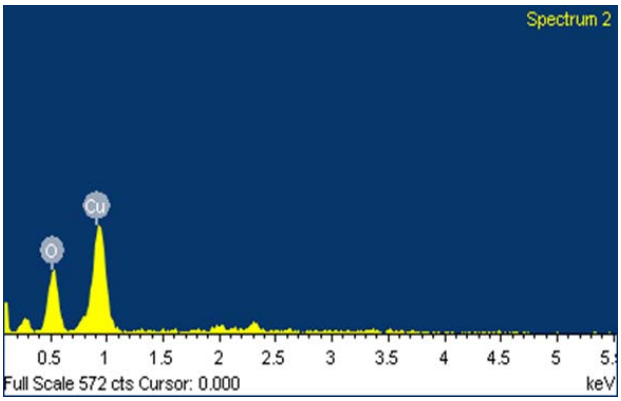

Fig 4 (c). EDX spectrum of copper nanoparticles

The EDX spectrum confirms the formation of biosynthesized copper nanoparticles, while Figure 4 (c) and Table 1 confirm the composition of synthesized copper nanoparticles.

Table 1. Composition of copper nanoparticles

Element	Weight%	Atomic%
O	50.05	79.92
Cu	49.95	20.08
Total	100.00	100.00

TEM Investigation

The shape and size of the developed CuNPs were broke down by TEM examination [35]. Figure 5 demonstrates the TEM representation of biosynthesized CuNPs. The developed CuNPs were cubical fit with particle size estimate in nanoscale. The green synthesized copper nanoparticles' size profoundly relies upon the concentration of *Odina* gum extract. It was affirmed that the concentration of leaf concentrate was observed to increase with the decline in particles size [36,37].

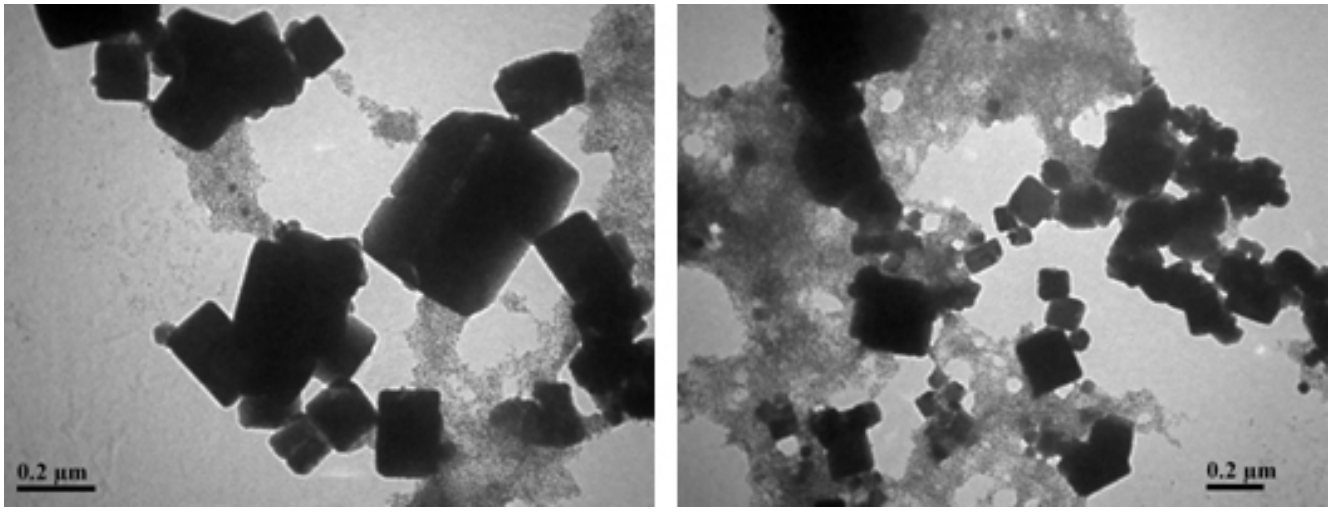

Fig 5. *Odina* gum with copper nanoparticles

Differential Scanning Calorimetry of Copper Nanoparticles

The thermal stability of the copper nanoparticles was explained by differential scanning calorimetry of copper nanoparticles shown in Figure 6. The DSC analysis gives the glass transition temperature which is defined as the peak temperatures in the heating curve. The DSC curve indicates that the copper nanoparticles reach the first exothermic peak at 249.1°C, beginning at 94.3°C; this is due to the oxidation of copper into cuprous oxide.

The DSC thermogram of *Odina* gums show the glass transition temperature at 193.2°C. However, no data for glass transition temperature for *Odina* gum is reported in the literature.

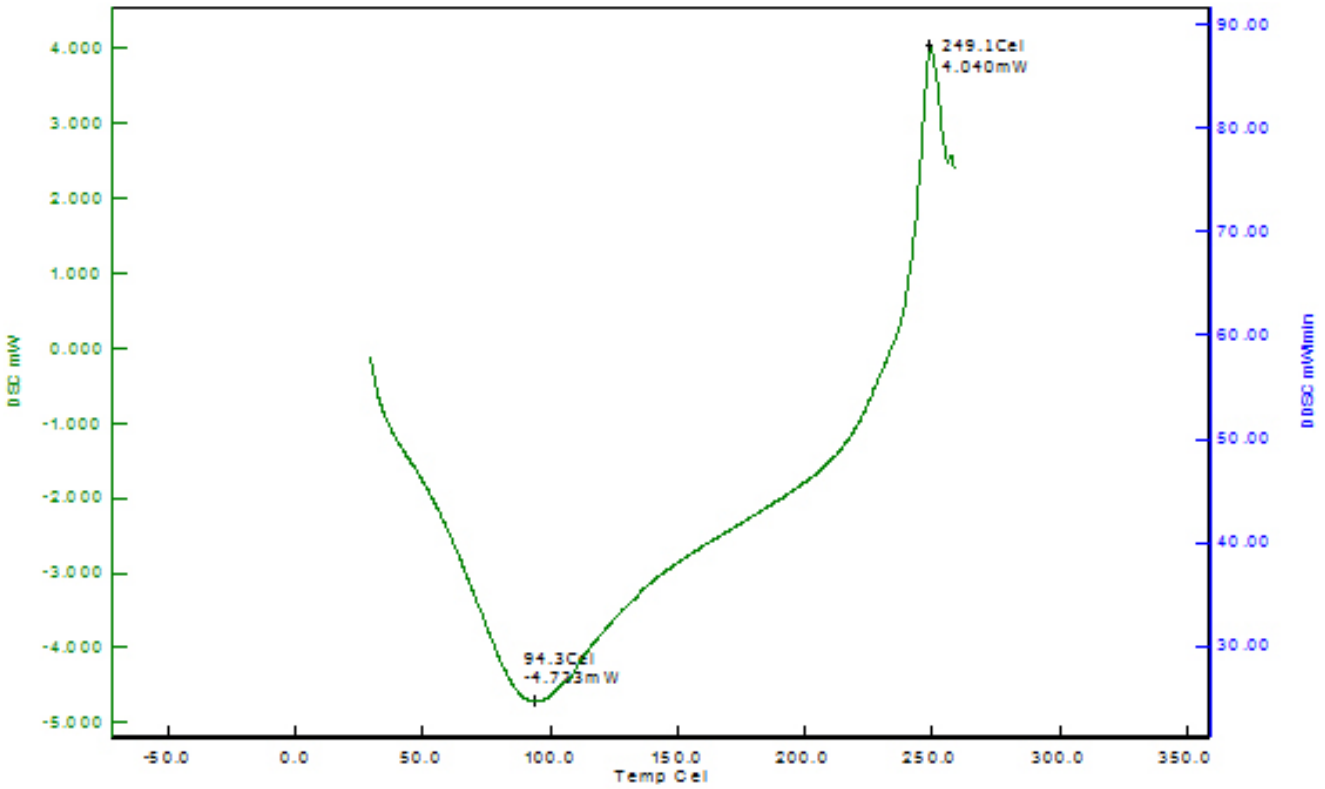

Fig 6 (a). DSC thermogram of copper nanoparticles

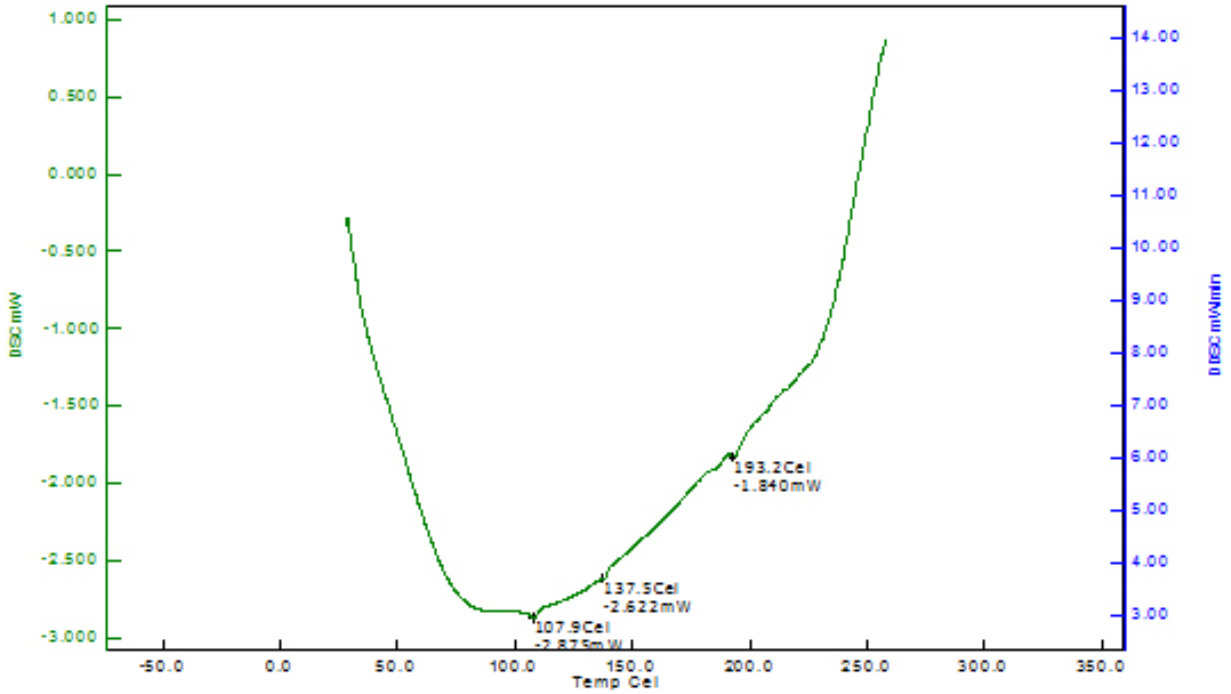

Fig 6 (b). DSC thermogram of *Odina* gums

Dye Degradation by Copper Nanoparticles

Catalysis occurs only on the surface of metals, hence increasing the available surface area of the nanoparticle will greatly enhance the effectiveness of the catalyst. Decreasing the particle size will increase the catalytic activity, but there is a critical size below which further decreases will hinder the catalytic activity [22]. Metal nanoparticles help in the electron transfer from the donor to the acceptor. Nanoparticles possess a large surface area which acts as a substrate for the electron transfer reaction. Just before the electron transfer reaction, both of the reactants are adsorbed into the metal surface. Subsequently, the reactant gains an electron and is reduced.

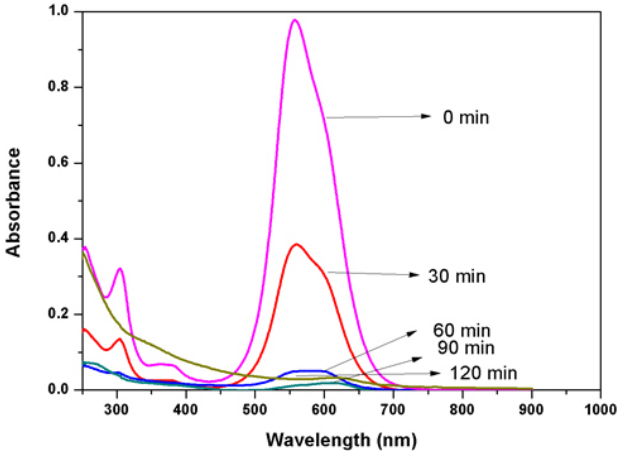

Fig 7. Degradation of dye using copper nanoparticles

Organic-based dyes are one of the major categories of pollutants from the textile and leather industries. These industries produce a large quantity of high content dye effluents, which are highly toxic and very resistant to destruction and degradation in the waste water by a variety of conventional methods. A necessary criterion for the use of these dyes is that they must be highly accumulated in water and stable in light during washing. The accumulation of these dyes in the water causes eutrophication and the reduction of the reoxygenation capacity, and results in severe damage to the aquatic organisms by hindering the infiltration of sunlight [43]. The dye enriched wastewater could be resistant to microbial degradation. Therefore, they are not readily degradable and are typically not removed from water by microbiological treatment systems, biotechnological treatment systems, or conventional methods such as adsorption, ultrafiltration, and chemical and electrochemical methods [44].

Recently, it was reported that metallic nanoparticles were used for the treatment of dye containing wastewater by photo-oxidation. These metallic nanoparticles have low cost, high stability, and act as a photocatalyst for the treatment of dye wastewater. Moreover, metal nanoparticles provide a reduced size, defined shape, large surface area to volume ratio, and mass enhanced reactivity; these properties lead to high photocatalytic activities for degradation of dye wastewater. Currently, green synthesized nanoparticles are used as a catalyst for photo-oxidation for the treatment of dye wastewater. Newly, Copper nanoparticles are considered as a catalyst for photo-oxidation of wastewater and it has several advantages such as low cost, extensive availability, and suitability for numerous applications, including electrical applications, catalysis, sensors, inkjets, and field emission emitters. The bio-synthesised CuNPs act as a photocatalyst for removal of Acid Blue 120, a toxic dye, in the water. Acid Blue 120 is a hazardous substance and a water-soluble heterocyclic aromatic chemical compound used as colourant in the dyeing process of leather, paper, and biological shading. Due to its harmful effect, the complete removal of Acid Blue 120 from the water is necessary.

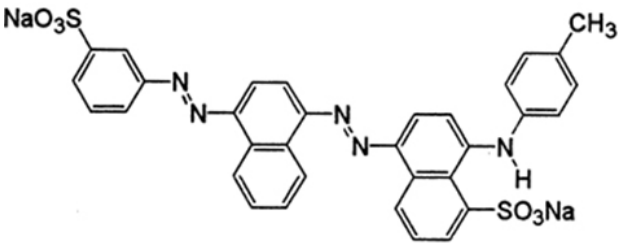

Fig 8. Structure of Acid Blue 120

The structure of Acid Blue 120 is shown in Figure 8. Acid Blue 120 consists of heterocyclic aromatic rings and an azo group. The Acid Blue 120 was used for evaluating photocatalytic activity of CuNPs in an aqueous medium under solar irradiation. The degradation of dye did not immediately occur in the reaction medium. The reaction was monitored by the change in the absorbance observed in the UV spectrum of the reaction mixture after centrifugation to remove the CuNPs. It was observed that as the exposure time increased, the absorption corresponding to Acid Blue 120 depreciated gradually from 0.98 until it reached its minimum value of 0.039. In Figure 6, the absorption peaks at 560 nm, corresponding to Acid Blue, showed rapid degradation and disappeared after 120 minutes. To confirm the photocatalytic activity of the CuNPs, a control experiment was carried out. It was noticed that when the dye solution was kept under sunlight, in the absence of NPs, the dye did not undergo any degradation in the reaction medium. Figure 9 depicts the degradation potential of the synthesized CuNPs for Acid Blue 120, which reached 96%. It was observed that the rate of reaction control, within 60 minutes, reached an equilibrium that followed the first order kinetics for photodegradation of Acid Blue 120.

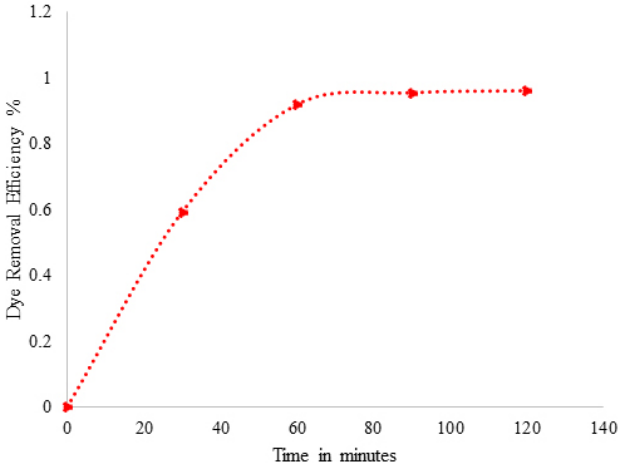

Fig 9. Percentage efficiency of photodegradation using CuNPs

The degradation rate of dyes with metallic nanoparticles obeys first order reaction kinetics and its correlation is given by

$$\ln \frac{Co}{Ct} = kt$$

where Co = Concentration of dyes at the initial time of reaction, Ct = Concentration of dyes at time t after reaction progress, k = first order rate constant of the photochemical reaction, and t = reaction time in minutes.

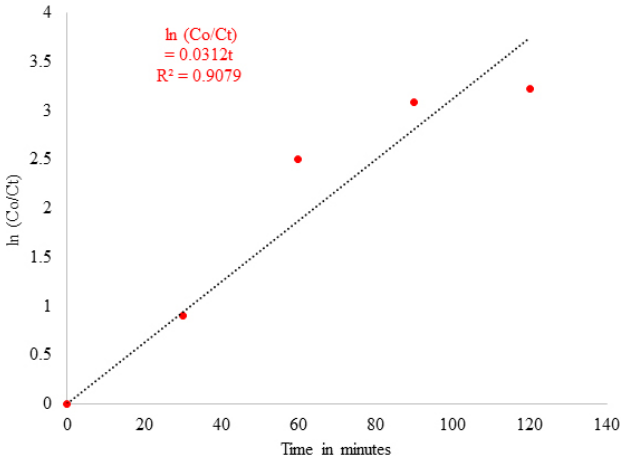

Fig 10. Plot of ln (Co/Ct) versus irradiation time for photodegradation of dyes

Figure 10 confirms a linear relationship between ln (Co/Ct) and irradiation time with a 3.12 x 10^{-2} min^{-1} rate of reaction. Thus, it confirmed that green synthesised CuNPs can be a potential photocatalyst for the effective removal of Acid Blue 120 dyes in the wastewater.

Photocatalytic Mechanism of CuNPs

The photocatalytic mechanism of CuNPs consists of two main parts. The first part of a photochemical reaction is based upon the interaction with light associated with photon absorption, charge creation, dynamics, and surface trapping. The second part of the reaction is controlled by surface reactivity and surface radical formation, such as the formation of H_2O, O_2, and Organic Pollutants [41]. The Photocatalytic mechanism of CuNPs can be summarised as below:

1. Initially, when the CuNPs absorbs solar irradiation, due to the Surface Plasmon Resonance effect, the CuNPs activates photoexcitation and undergoes plasmonic decay [42-44].
2. Secondly, the electron and holes are generated by plasmonic decay which then reacts with O_2 and H_2O molecules to produce active species and anionic superoxide radical (O_2^-) and hydroxyl radical (OH), respectively.

3. Finally, hydroperoxyl radical (HO_2) is generated by the protonation of the superoxide ion (O_2^-). The hydroperoxyl radical then converts to H_2O_2 which ultimately dissociates into highly reactive hydroxyl radicals (OH). Finally, both oxidation and reduction take place on the surface of the photocatalyst.

The complete degradation reaction can be explained by the following chemical reactions:

$$Cu + h\nu \rightarrow h^+(Cu) + e^-(Cu)$$

$$H_2O(ads) + h^+ \rightarrow OH^* + H^+(ads)$$

$$O_2 + e^- \rightarrow O_2^-(ads)$$

$$O_2^-(ads) + H^+ \leftrightarrow HOO^*(ads)$$

$$2HOO^*(ads) \rightarrow H_2O_2(ads) + O_2$$

$$H_2O_2(ads) \rightarrow 2OH^*(ads)$$

CONCLUSION

This investigation indicated a simple method for synthesis of CuNPs and its applications in waste water treatment. Dye degradation in the absence of metallic nanoparticles in biological, chemical, and physical remediation results in dye recycling, poor degradation, and retention of same toxicity. In the case of Photocatalytic degradation, treatment with nanoparticles as a photocatalyst is a novel approach for complete removal of dye from the wastewater. The metal oxide nanoparticles, such as Tin Oxide (SnO_2) and Titanium Oxide (TiO_2), utilized as photocatalysts for the treatment of dyes within wastewater were shown to be highly effective [45]. This study confirmed that Copper nanoparticles provide high surface areas and a large number of active sites without the doping of any semiconducting materials. The present investigation showed a 96% removal of dye with CuNPs, which were synthesized by *Odina* gum extract, showing it to be an effective process.

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Principles, Policies and Practices in establishing a Post-Secondary Chemistry Department: A retrospective evaluation

John Hill[1] and David Devraj Kumar[2]
[1] La Trobe Institute of Molecular Sciences, La Trobe University, Bundoora, Victoria 3086, Australia
[2] STEM Education Laboratory, Florida Atlantic University, Davie, Florida 33314, USA
(E-mails: [1]jce.hill@bigpond.com, [2]david@fau.edu)

Abstract: A brief description of a successful time-tested chemistry department in an Australian university is presented. It is remarkable that the chemistry department in the La Trobe Institute of Molecular Sciences has generated international distinction and survived nearly a half-century as a cohesive, independent academic unit despite several university restructuring efforts [1]. Obviously, this department has shown resilience to many institutional forces of change and financial instabilities and remained committed to academic excellence. Hands-on laboratory based classes in practical and theoretical chemistry continue to generate graduates well-positioned to enter the twenty-first century professional work force in chemistry and its partner sciences.

Key Words: Chemistry Department, University, College, Post-Secondary, Policy, Practice, Evaluation.

INTRODUCTION

Chemistry has always been recognized as an essential discipline in university faculties, schools and colleges of science and is still widely regarded as the 'central science'. The study of organic chemistry dates from the mid-eighteenth century. Inorganic chemistry had its origins in the early twentieth century and analytical and physical chemistry in the early to mid-twentieth century. Hence over the past 150 years, four major branches of chemistry have been recognized (Fig.1). In the late twentieth century, the number of chemistry branches exploded (Table 1) and chemistry enables many other 'sciences' (Fig. 2). Also, two major adjuncts of chemistry, 'Chemical Education' and 'Chemistry in Society', have emerged (Fig. 3) which not only promote and enrich the teaching of chemistry, but also emphasize the 'relevance' of chemistry in the developing world.

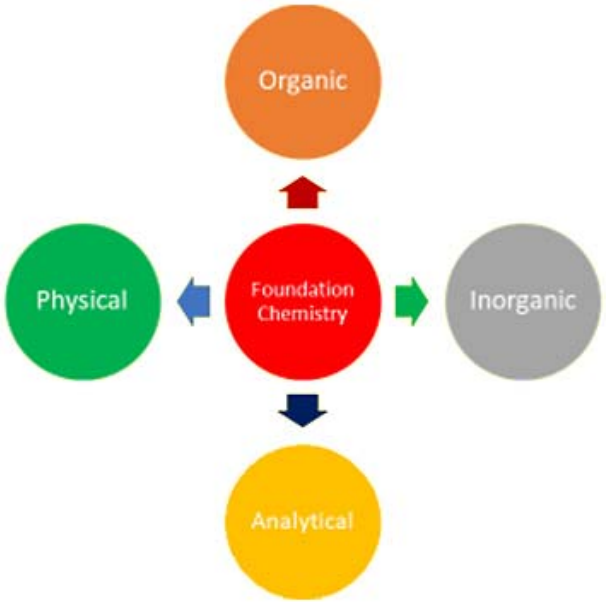

Fig. 1. The four foundation braches of chemistry

Table 1. The New Age Branches of Chemistry

Aquatic Chemistry	Atmospheric Chemistry	Biochemistry
Chemical Kinetics	Chemical Thermodynamics	Computational Chemistry
Coordination Chemistry	Electrochemistry	Environmental Chemistry
Femtochemistry	Food Chemistry	Forensic Chemistry
Geochemistry	Green Chemistry	Industrial Chemistry
Macromolecular Chemistry	Magnetochemistry	Marine Chemistry
Materials Chemistry	Chemical Mathematics	Medicinal Chemistry
Molten Salt Chemistry	Nanochemistry	Natural Product Chemistry
Nuclear Chemistry	Organometallic Chemistry	Pharmaceutical Chemistry
Pollutant Chemistry	Polymer Chemistry	Supramolecular Chemistry
Surface Chemistry	Theoretical Chemistry	Thermochemistry

Fig. 2. Chemistry partner sciences

Most of university foundation chemistry departments around the world have prestigious records in terms of teaching and research and many of these remain as 'stand-alone' entities. It has always been recognized that academic science departments are expensive to establish and to maintain due to setting up teaching and research laboratories and, in particular, purchasing state of the art research instrumentation. Thus, in the late twentieth century, chemistry in many of the newer universities was amalgamated into compatible science departments such as biochemistry, physics, earth, life sciences and others and as a consequence became the minor component of these mega-departments. Although chemistry has always been recognized as the 'central science', financial realities forced these amalgamations coupled with a decline in students electing to study chemistry as their major. Also, many newer universities have not included chemistry as a foundation academic entity.

The factors which lead to the survival of chemistry as a 'stand-alone' department are complex and inter-related. Paramount of these is that 'teaching' is 'informed by research' – meaning that all academic staff in the department should be research active and hence offer topical and challenging research projects which attract higher degree students. The department should be recognized as a world leader and hence a 'center of excellence' in at least one research area and staff must actively apply for external research funding. To support this level of research excellence, the department must have 'state-of-the-art' research instrumentation and support technical staff to support 'cutting edge' research in a variety of areas. Also, academic staff should be appointed not only on their teaching ability, but also on the topicality and relevance of their research interests and how these blend into a cohesive whole. Consistent with this is an assessment of their successful potential for the awarding of external funding. Also of importance is their potential to collaborate with researchers nationally and internationally.

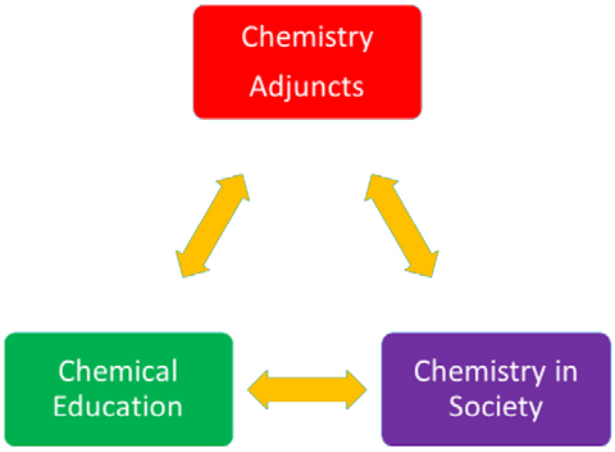

Fig. 3. Chemistry adjuncts

Although not always recognized as of critical importance, instructive teaching and learning strategies also characterize and enhance the 'stand-alone' longevity potential of a chemistry department. In recent times, chemistry departments have established 'learning centers' in which 'state-of-the-art' teaching and learning strategies are implemented with the direct involvement of students on an individual basis. Also, since chemistry is an experimental science, it is essential for students to undertake 'hands-on' laboratory exercises during all 3 years of their course. There are a plethora of ways in which these experiments can be intermeshed with the teaching program and in the final year, it is usual to design experiments which introduce students to the principles and practices of research. In essence, the teaching and learning and research metrics contribute equally to the long-term success of a chemistry department.

As an example of the best principles, practicalities and policies being applied to establish a post-secondary chemistry department, La Trobe University in the State of Victoria, Australia was established in 1967 and was the third University to be established in Melbourne after Melbourne and Monash Universities and La Trobe Chemistry was a foundation department in the School of Physical Sciences. As part of the golden jubilee celebrations of La Trobe University in 2017, the 50-year history of La Trobe Chemistry has been published as an e-book [1] and its 'stand-alone' status throughout this period is testament to the effectiveness of the principles and policies on which it was founded.

Initially, La Trobe Chemistry consisted of three 'divisions', Organic, Physical and Inorganic. The latter was expanded to 'Inorganic and Analytical' in the 1980's. A Professor headed each of these divisions and foundation academic staffs were appointed on the basis of having a higher degree (most had a PhD) and being research active. A further consideration was that appointees would collectively provide a range of research fields in each of these three divisions, which as far as possible would not duplicate those at Melbourne and Monash Departments of Chemistry. Thus, Physical Chemistry concentrated on mass spectrometry, X-Ray crystallography, gas phase kinetics and later, photoelectron spectroscopy. The co-establishment of well-equipped mechanical, glass and electronic workshops enabled some of this equipment to be built 'in-house' since at this time, commercial counterparts were not available. Melbourne and Monash Chemistry Departments were strong in 'natural product synthesis' so La Trobe Organic Chemistry concentrated on 'physical organic chemistry' as its main research theme, with emphasis on the mechanisms of organic reactions. However, there was also research on the synthesis and characterization of heterocyclic compounds and drug design and development. Infrared and UV-Visible spectroscopy and H-1 NMR instrumentation was available in house to support this research. Foundation staff in the Inorganic Division had research interests in both inorganic and analytical areas and included coordination chemistry, solvent extraction, ion-selective electrodes, electrochemistry, gas liquid chromatography, molten salt chemistry and environmental chemistry. Subsequent academic appointments in the 1980's and 1990's added considerably to the range of research fields in all three divisions and included multi-nuclear NMR leading to the establishment of an 'NMR center of excellence', development of new anti-cancer drugs using molecular graphics, organic chemical kinetics and the effect of micelles on catalytic processes, development of flow analytical methods, especially Flow Injection Analysis, use of multi-nuclear NMR, especially Mo-95 to study 'bi-nuclear reaction centers', and the role of molybdenum in biological systems. By the end of the 1980's, La Trobe Chemistry had become a 'stand-alone' department and had several research centers of excellence. In addition to the NMR center, these included mass spectrometry, X-Ray crystallography, bioinorganic chemistry and Center for Scientific Instrumentation. By the end of the twentieth century, most of the first generation of academic staff had left through retirements and hence a next generation of academic staff was appointed which brought 'frontier chemistry' research projects into La Trobe Chemistry. These included medicinal chemistry, supramolecular chemistry, computer design of molecules in conjunction with prediction of their properties, molecular sensing and development of new analytical techniques capable of 'ultra-low' detection limits, nano-structures, polymer inclusion membranes, study of inter-stellar nano-particles using the infra-red beam line of a synchrotron, investigation of nanostructures for applications in electronic devices, gas sensors and batteries and computational chemistry with emphasis on predicting 'new chemistry', modelling reaction mechanisms, and studying metal-containing systems which phosphoresce and luminesce.

Over the 50-year period of its existence, La Trobe Chemistry has a record to be reckoned with in terms of its research output, as measured by the numbers of Honors and Higher Degree graduates, the continuing establishment of internationally recognized research centers of excellence, the successful awarding of external

competitive research funding and the number of peer-reviewed publications produced. The founding principles and strategies for setting up the Department as a research active entity have been endorsed and continue to be implemented.

La Trobe Chemistry also has a distinguished teaching and learning record to be reckoned with based on the 'teaching informed by research' founding ethos of the University established 50 years ago. 'Year 1 Chemistry' has always been subdivided into two streams. In the early decades, these were known as 'Chemistry 1A' and 'Chemistry 1B'. The former was for students who had passed chemistry at the Higher School Certificate (HSC) level and who were likely to study chemistry as their major, whereas the former was for students who were enrolled in other sciences such as biology and agriculture. In later decades, 'Year 1 Chemistry' was restructured into two streams ('Basic Chemistry' and 'General Chemistry') in Semester 1 and 'Applied Chemistry' in Semester 2. The latter course was available for students who had passed 'Chemistry General' in Semester 1. From inception, it was decided that three laboratory sessions per week in Semester 1 in each of the three main branches of chemistry were assessed components of 'Year 1 Chemistry' in order to convince students that 'chemistry' was fundamentally an 'experimental science' and 'theories' had to be confirmed by 'experimentation'. In recent decades, a 'Bridging Chemistry course' was made available to assist students with limited background knowledge of chemistry to prepare for Chemistry 1 courses and a 'Learning Resource Center' was established 'in-house' for enriching and enhancing the student learning experience. From the early 1990's, the Chemistry 1 course was made available online in 'modular' format – thus keeping abreast of ever-advancing teaching and learning strategies and conforming to 'chemical education' philosophies and practicalities of teaching and learning chemistry.

'Chemistry 2' was also initially constructed in two streams which built of the basic concepts of chemistry introduced in 'Chemistry 1' and applied these to expand the chemistry knowledge of students. For example, in organic chemistry, synthesis methodologies and organic reaction kinetics and mechanisms were emphasized in conjunction with the principles of the emerging diagnostic NMR technique. In inorganic chemistry, coordination and 'p-block element' chemistry were introduced together with the principles of the major characterization techniques of infrared and UV-Visible spectroscopy, conductance and magnetometry. For physical chemistry, surface chemistry and the emerging instrumental techniques such as mass spectrometry, molecular spectroscopy and gas phase chemistry were introduced. As for 'Chemistry 1', weekly practical sessions in the three main braches of chemistry were compulsory, which for organic and inorganic chemistry were focused on 'synthesis' in conjunction with 'characterization' using the major spectroscopic techniques. Thus, much emphasis was placed on students having 'hands-on' experience with common and 'emerging' laboratory instrumentation such as 'NMR'.

'Chemistry 3' continued with the two stream format with the B stream having an applied/industrial chemistry emphasis, while the A stream tended to focus on 'emerging chemistry' concepts and introduce the principles and significance of research. 'Chemistry 3' also included weekly laboratory sessions in each branch of chemistry which involved multi-faceted advanced experiments in conjunction with access to 'hands-on' experience with advanced instrumentation such as NMR, HPLC, Thermal Analysis, MS and ESR. The 'Chemistry 3' laboratory program essentially consisted of a series of 'mini-projects' which were undertaken by student pairs. The 'Chemistry 3B' course also included guest lecturers, largely from the chemical industry who gave an insight into their specialist areas and also an overview of career opportunities available to chemistry graduates. This gave students an insight into 'chemistry in the real world'. Recent 'Chemistry 3A' courses of special interest were 'Molecular Design' and 'Fuels, Energy and Environmental Sustainability'. The former was a completely computerized course showing how 'molecules' can be 'designed' to have 'pre-specified' properties and the latter addressed the paradox that the continued combustion of fossil fuels to produce energy is unsustainable if the natural environment is to survive the consequences of global warming.

The 'Chemistry Honors' course (4th year of the conventional BSc degree) continues to be based on a series of lectures on 'specialist and leading edge' chemistry topics plus a minor (research) thesis, the former being assessed by conventional examinations and the latter by the 'supervisor' and by oral defense. Recent honors lecture topics have included 'medicinal chemistry', 'supramolecular chemistry', 'molecular design', 'molecular sensing' and 'computational chemistry' with complementary honors research projects being available in these areas of specialization. Also, in recent decades, honors projects have been designed and co-supervised by personnel from external scientific organizations such as the 'State Forensic Science Laboratory', the 'Environment

Protection Authority' and the CSIRO (various divisions). These collaborations have often led to employment for La Trobe Chemistry honors and higher degree graduates.

'Quality Assurance' has consistently featured prominently in establishing benchmarks and for setting standards for teaching and learning throughout the University and student assessment of teaching has become a routine metric of quality in this domain. La Trobe Chemistry has enthusiastically embraced and implemented these initiatives and the Department as a whole has consistently been acclaimed and rewarded both in the promotion process and more recently by competitive University and State Government citations and awards for its commitment and progressive achievements in the teaching and learning domain. La Trobe Chemistry has a distinguished and sustained record of performance excellence in its cumulative teaching and learning portfolio. In this context, it should be emphasized that steps to maintain quality control have implications for accreditation. In the United States college level chemistry, the American Chemical Society (ACS) accredits programs. The lessons learned from establishing benchmarks and setting standards at the La Trobe Chemistry Department provide insights into the inner workings of a successful time-tested chemistry department which are invaluable to accrediting agencies everywhere.

The viability of an academic chemistry department is dependent on a sustainable annual enrollment of undergraduate and higher degree students and hence it is vital that it continuously strive to attract students to undertake its courses. Furthermore, potential students assess tertiary courses not only on their academic credibility but on their cumulative ability to provide a viable platform for future employment. La Trobe Chemistry has throughout its existence made enthusiastic contributions to annual University Open Days by not only offering 'show and tell' sessions to visitors but also by entertaining them with the ever popular 'Chemistry Magic Show'. Also, interactions with local secondary colleges have been established by inviting Years 10, 11 and 12 'science students' from local schools to be involved in a 'High-School Enrichment Program' in the University chemistry laboratories – using equipment and instrumentation not usually available to them at school level. In recent years, La Trobe Chemistry has introduced 'NMR learning skills' into this program.

In terms of relating its courses to 'career opportunities', La Trobe Chemistry has consistently created and sustained interactions with the chemical industry and Government (scientific) institutions such as the Environment Protection Authority (EPA), CSIRO, National Forensic Science Laboratory and a variety of chemical industries, including the pharmaceutical and the emerging renewable energy industries.

In summary, perhaps the most remarkable achievement of La Trobe Chemistry is that it has survived as a cohesive, independent academic unit for nearly a half-century, when most academic chemistry departments in Australia have either amalgamated with other science departments or closed down. La Trobe Chemistry has continuously demonstrated its sustainability since its foundation despite many university restructuring efforts and continuous financial and infrastructure constraints. Its achievements over the last fifty years, as measured by its quality staff, research publication output, number and financial value of competitive external and internal research grants awarded and the number of higher degree graduates produced, testify to the overall resilience of the department to external and internal forces of change and a determination to survive and develop via passionate commitment to academic excellence. It has re-engineered and restructured its courses strategically and successfully to incorporate the emerging trends in teaching chemistry to meet societal needs [2]. Its history thus far foreshadows it is well placed in terms of moving towards a sustainable and rewarding future and that it is able to retain its leadership status among academic departments of the University in conjunction with continuing recognition of its academic excellence both nationally and internationally.

ACKNOWLEDGMENTS

This paper is an abridged version and a retrospective evaluation of "Brownlee R, Hill J," *La Trobe Chemistry: The first 50 years'* which was a contribution to the La Trobe University 50th Anniversary archive project 2017.

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Role of Chemistry in Oil and Gas Extraction

Tata L. N. Murthy
Gujarat State Petroleum Corporation Ltd. DDW Field, KG Basin, E.G.Dist, Andhra Pradesh, India
(E-mail: lnmurthytata@rediffmail.com)

Abstract: Crude oil and natural gas are both refinery feed stocks; together, they are the main raw materials used for many petrochemical products and fuels, which play a vital role in human life. Crude oil and natural gas can also influence the national economy. We cannot think about present human life without considering the importance of crude oil and natural gas. Day by day, oil and natural gas extraction is becoming a challenge, as oil and gas extraction is moving towards deep sea extraction and ultra-deep sea extraction. Easy oil extraction, such as onshore drilling and shallow water drilling with available technology, has been taken and it is now essential to extract tougher areas with new technology. Chemistry is playing a vital role in realizing the petroleum engineers' dream.

Key Words: Crude Oil, Gas, Extraction, Flow Assurance

DRILLING

It is essential that the borehole pressure, the hydrostatic pressure exerted by the column of "mud" in the wellbore, is a little more than the formation pressure, the pressure in the pore space of formations being drilled. If, for some reason, the formation pressure is greater than the borehole pressure, an influx of fluid flow into the borehole, known as a kick, will occur. If no action is taken to stop the influx of fluid into the borehole, the formation fluids will flow in an uncontrolled manner at the surface. This is known as a blowout. When pressure control over the well is lost, it can cause severe consequences as mentioned below.

1. Loss of human life.
2. Loss of rig and equipment.
3. Loss of reservoir fluids.
4. Damage to the environment.
5. Huge costs to get the well under control again.

The mud is circulated by the drilling crew to remove the drill cuttings and to maintain the hydrostatic pressure of the mud column; this pressure should not be too high, as high pressure can cause formation damage. [1].

The onsite chemist measures mud densities and any ingress of hydrocarbons into the mud. The chemist's observations are highly important, so that early action may be taken to ensure the drilling operations are safe and successful.

STIMULATION (MATRIX ACIDIZING)

Formation damage due to drilling, cementing and completion activities could lead to the reduction of permeability of nearby wellbore areas. Matrix (stimulation) treatments are a common form of well intervention aimed at removing formation damage and restoring the well to its natural, undamaged inflow performance. The majority of the acid stimulations of clastic reservoirs are carried out with "mud acid", a mixture of hydrochloric (HCl) and hydrofluoric (HF) acid. [2]

PVT (PRESSURE, VOLUME, TEMPERATURE) ANALYSIS (INPUTS TO DESIGN SURFACE FACILITIES)

PVT laboratory analysis is vital for many petroleum engineering design calculations. The onsite chemist plays an important role in doing the PVT analysis and giving inputs to the petroleum engineers. Reservoir fluid analysis provides some of the key data for the petroleum engineer. The quality of sampling and testing is important to ensure that correct physical property values are used in various

design procedures. PVT analysis of a reservoir fluid determines:

1. The correlation between pressure and volume at reservoir temperature.
2. Various physical constants that enter into reservoir engineering calculations.
3. The effect of separator pressure and temperature on oil formation volume or gas/oil ratio.
4. Chemical composition of the most volatile components.

Using PVT analysis, chemists carry out downhole (reservoir conditions) sampling and test the sample at downhole conditions. This gives the measurement of the fluid at reservoir conditions. Sampling and testing are carried out with specialized equipment by experienced chemists. [3]

FLOW ASSURANCE

Flow assurance is an important function to ensure the desirable flow of hydrocarbon fluids.

Some crude oils having more wax, ceasing to flow at ambient temperature. In this type of crude oil, a chemical known as pour point depressant (PPD) is used. The PPD decreases the congealing temperature of crude oil, making the crude oil flow freely at ambient temperature. This PPD requirement is critical in cold climates. Chemists test the flow in the laboratory by mixing PPDs in various dosages with the crude oil to determine the required amount of and the dosage rate of PPD, needed for flow to be maintained at field temperature.

Along with crude oil, water is also frequently produced. Sometimes water is injected into the reservoir to maintain reservoir pressure. When it comes to handling produced water and preparing water for injection to the reservoir), it is essential to prevent scale formation, monitor and prevent microbiological corrosion, measure particle sizes, and check corrosion tendencies. The chemist's role is important in testing the water in the laboratory for these tendencies and recommending the chemical treatment (corrosion inhibitors, scale inhibitors, or biocides) along with required dosage rates.

NATURAL GAS DEHYDRATION OPERATIONS

It is essential for natural gas dehydration to be transported. Moisture in natural gas can cause hydrates, physical mixing of moisture with hydrocarbons to form ice-like crystals, which can clog pipelines and cause pipeline corrosion. Trithylene Glycol (TEG) is used in natural gas dehydration to remove the moisture. Anhydrous TEG concentration plays a vital role in gas dehydration. This reaction increases rapidly at higher purities of TEG (i.e., less moisture content). Gas-stripping technology is being used to get a high purity of TEG, for the purpose of optimizing the performance. Testing and reporting the TEG purity is a critical parameter for gas dehydration operations. Chemists use specialized equipment and standard test methods for measuring the water content in TEG.

Similarly, measuring the moisture in dehydrated gas for natural gas transportation is important. Chemists use specialized equipment known as a Bureau of Mines meter, which is employed with standard test methods. The test results are used as inputs for calibration and fine-tuning of online moisture analyzers. Chemists continuously monitor the process chemistry and advise the operations department, preventing huge losses to operations caused by corrosion in the pipelines or completely disturbing the dehydration unit. [4]

OIL FIELD PROCESSING OF CRUDE OIL

Crude oil flows through separators, separated by high pressure, medium pressure, and low pressure. These separators are designed as per the inputs of the PVT chemistry report, and separate water and volatile hydrocarbons. Chemicals, like demulsifiers, are required to break the water and crude oil emulsion, making the crude oil free of water. Chemists test de-emulsifiers in the laboratory for suitability and to confirm the dosage rate. High dosage rates may cause reverse emulsion in the case of some demulsifiers, while low dosage cannot remove water from crude oil. Water is a critical parameter for the sale of crude oil.

CRUDE OIL ANALYSIS

Crude oil is transported to a refinery, mostly by cargo tanker ships. The main parameters to be tested are vapor pressures, water content, density, and salt content. Density of crude oil is the key parameter for calculating the price of crude oil. A sample is collected by an experienced chemist using standard methods, and the density is tested by following standard method. Variation in density, to even the third decimal, can cause great variation to the price of crude oil. Vapor pressure is also an important parameter, particularly if the vapor pressure is higher than 10 psi, which is very dangerous for transportation. It is required to eliminate water and salt content from the tank. Crude oil analysis is critical for crude export and chemists play an important role in this export by providing accurate data.

INTERNAL CORROSION

Oil and gas pipelines are costly and time consuming projects. Ensuring the integrity of these pipelines is essential. Internal corrosion can be understood and prevented only by a chemist. The most suitable corrosion inhibitor should be selected, or tailor-made chemical blends should be prepared by experienced chemists based on the operating and process conditions. The concentration of corrosion inhibitor in the fluid should be checked regularly to ensure the correct dosage rate. This also gives a good idea of the corrosion inhibitor's performance.

Similarly dissolved gases, such as oxygen, hydrogen sulfide, and carbon dioxide, should be tested *in situ* by using field test kits prepared using standard test methods.

Collecting real time data from online monitors, field test kits, and instructing operation teams for proper actions in order to prevent corrosion, is in the hands of chemists only.

CONCLUSION

Chemistry plays a key role in the process of oil and gas extraction. From the designing, drilling, commissioning and operating stage, chemists have valuable inputs in making operations safe, successful, and profitable.

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Public Understanding of Chemistry

Public Understanding of Chemistry: Chemistry and its social-political-economic contexts continue to change. Chemistry and chemistry-based technology that impact our lives make for the complexity and controversy of life and set the stage for thinking about public understanding of chemistry. The Public Understanding of Chemistry section will try to address chemistry in real life context with original contributions (articles/position papers/policy briefs) and/or published articles and columns in reputable sources (used with permission).

FALSE-POSITIVE DRUG TEST FOR METHAMPHETAMINE

Dr. David M. Manuta & Deborah F. Cate

Manuta Chemical Consulting, Inc. (MC^2), 431 Gordon Avenue, Waverly, OH 45690-1208

(Email: mc2@dmanuta.com)

Introduction

On December 22, 2015, a urine sample (UA) was collected from an ex-convict suspected of methamphetamine use. When the test came back positive, he was subsequently charged. With the prospect of a violation of his existing release looming, he reached out to a consulting chemist, Dr. David Manuta at Manuta Chemical Consulting, Inc., to review his case. He claimed to have not previously tested positive for any Drugs of Abuse since he was paroled. A hearing was held by The Colorado Department of Corrections (CDOC) on January 12, 2016.

Abstract: A possible false-positive test result for methamphetamine occurred during the laboratory testing of a parolee's urine. A comparison of the chemical structures of methamphetamine and pseudoephedrine, an ingredient in the over-the-counter medication, Sudafed®, as well as the fallibility of the test itself, makes this conclusion, to a reasonable degree of scientific certainty, not an improbable outcome.

Key Words: immunoassay (IA), methamphetamine, dextroamphetamine, pseudoephedrine, Sudafed®

Background Information

In the document faxed to Dr. Manuta by the Defendant, he described the medications that he was taking at the time, including prescriptions. The defendant also indicated that the test reading for methamphetamine was 377 ng/mL (nanograms per milliliter). A test reading for amphetamine was also reported as 275 ng/mL. The nanogram is a metric mass unit equal to one-billionth of one gram (10^{-9} g), the mass of a typical human cell [1].

The Defendant identified the testing laboratory as Redwood Toxicology Laboratory (RTL). RTL is located in Santa Rosa, CA. With the testing located in California, the urine samples must be collected and preserved in accord with accepted protocols and standards prior to being shipped to the facility. CDOC personnel need to properly package these urine samples, per the accepted methodologies, in order for the test results obtained to be considered meaningful.

In a medical report dated December 14, 2015, it is noted that the Defendant's physician prescribed FLONASE nasal spray, neo-synephrine nasal spray, and Adderall XR. Other medications noted by the Defendant's physician include Albuterol, Advair, and Lisinopril.

The Defendant also noted that he and some of his family members had recently taken Sudafed® for nasal and sinus illnesses. The active ingredient in Sudafed® is the chemical pseudoephedrine.

Discussion

CDOC regulations approve the use of immunoassay (IA) methodologies and gas chromatography-mass spectrometry (GC-MS) for the identification of Drugs of Abuse in urine [2]. According to ImmunoChemistry Technologies, LLC [3], the immunoassay methodologies offer rapid identification of specific molecules. An advantage of ImmunoChemistry Technologies is that many samples can be analyzed in a day via these techniques. False-positive test results can be obtained via the rapid identification techniques such as IA. A check on a positive sample with GC-MS enables one to have greater confidence in the test result [4].

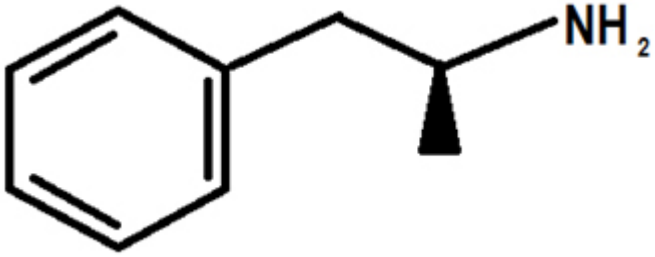

Fig 1. Structure of dextroamphetamine ($C_9H_{13}N$)

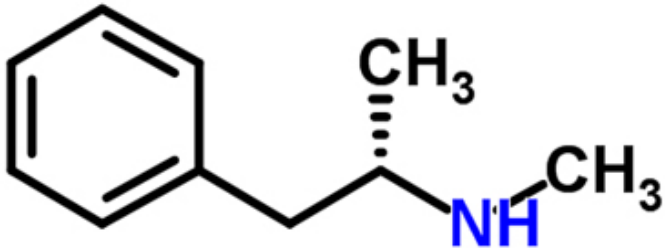

Fig 2. Structure of methamphetamine ($C_{10}H_{15}N$)

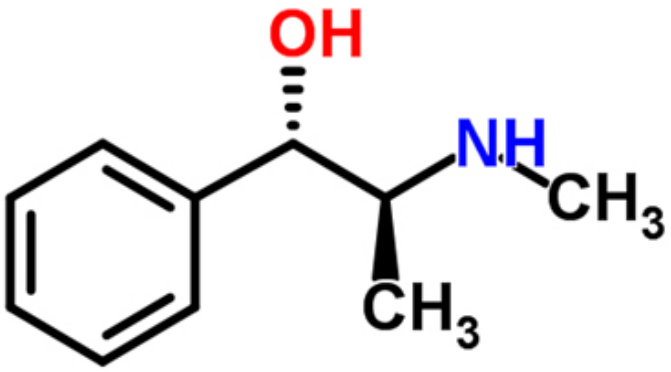

Fig 3. Structure of pseudoephedrine ($C_{10}H_{15}NO$)

Redwood Toxicology Laboratory (RTL), the laboratory used for the urine testing, indicates that approximately 85,000 urinalyses are done each week for Drugs of Abuse. This throughput level suggests that immunoassay methods are used at RTL [5]. This huge throughput corresponds to 12,000 samples per day, 500 samples per hour, and more than 8 samples per minute. Less than 10 seconds per sample appears to be the usual analysis time. Review of the analytical results may not be done prior to sending them to CDOC.

RTL has two methods for determining methamphetamine in urine. The first method has a cut-off limit of 500 ng/mL and the second method has a cut-off limit of 1000 ng/mL [6]. The detection limit for methamphetamine was reported at 250 ng/mL.

A key issue is that the Defendant's apparent level of methamphetamine in his urine was 377 ng/mL. This level is less than the cut-off level that the RTL methods noted in the previous paragraph can detect. There is uncertainty on what was actually measured in the positive test reported by CDOC personnel to the Defendant.

In addition to Sudafed®, the Defendant was known also to be taking Adderall XR. One of the conditions where Adderall XR is prescribed is to control the symptoms of Attention Deficit Hyperactivity Disorder (ADHD) [7]. The Defendant had been previously diagnosed with ADHD. Per his doctor's orders, the Defendant was on a once-a-day 20 mg capsule regimen.

One of the ingredients in Adderall XR is dextroamphetamine ($C_9H_{13}N$) [Fig. 1] [8]. Methamphetamine ($C_{10}H_{15}N$) bears similarities to dextroamphetamine in its chemical structure [Fig. 2] [9], as does pseudoephedrine ($C_{10}H_{15}NO$) [Fig. 3] [10].

The similarities between these three chemical structures are striking. As a result, there is, to a reasonable degree of scientific certainty, some doubt cast regarding whether the immunoassay methodologies used by RTL personnel are sensitive enough to consistently and reliably distinguish between these very similar molecules.

The National Institutes of Health provides data on the biological half-life of pseudoephedrine, an active ingredient in Sudafed®. The half-life of pseudoephedrine is about six (6) hours. Depending on the pH of the urine, it can take up to 16 hours for pseudoephedrine to be eliminated in adults [11]. This means that, to a reasonable degree of scientific certainty, there would be residual pseudoephedrine in the Defendant's urine within the 6-hour biological half-life window.

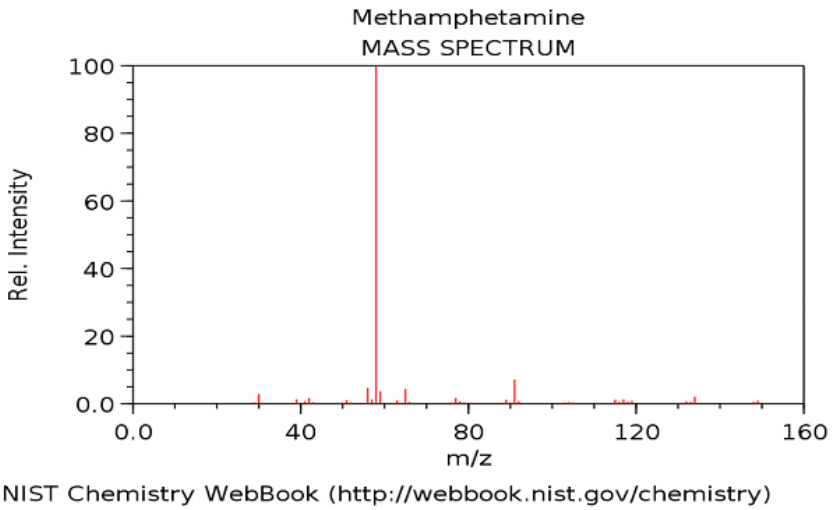

Fig 4. Mass Spectrum of Methamphetamine

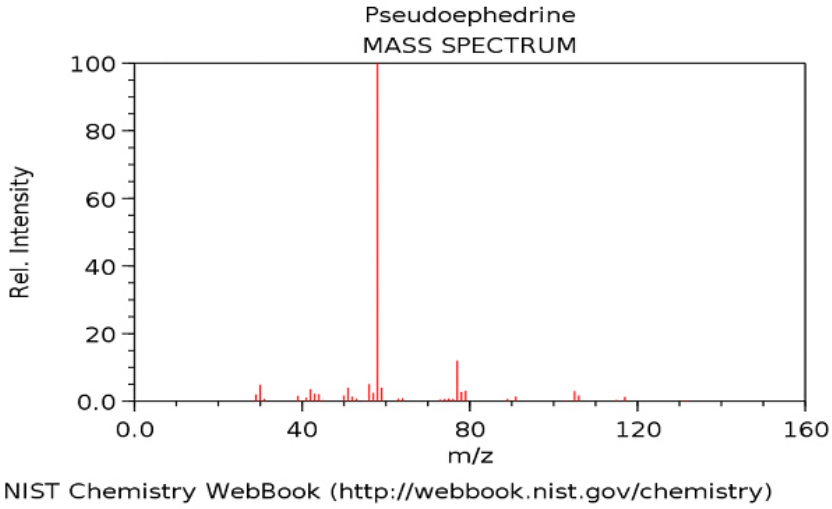

Fig 5. Mass Spectrum of Pseudoephedrine

Given this information, it is certainly possible that had the Defendant been required to submit a urine sample at a time near to when he had last taken Sudafed®, residual pseudoephedrine could be detected. It is reasonable then to consider that residual pseudoephedrine from Sudafed® could have been found, rather than methamphetamine, in the recent positive sample. RTL's comprehensive urine drug test for 22 Drugs of Abuse does not include the detection of pseudoephedrine [12].

Based on the chemical structure similarities between methamphetamine and pseudoephedrine, one would expect their respective mass spectra to look alike. The National Institute of Standards and Technology (NIST) reference mass spectra bear this out as can be seen in Figures 4 and 5 [13]. It would require an experienced chemist to distinguish between these molecules, based on a thorough review of immunoassay test data. Due to the high throughput at the CDOC's contract laboratory, the subtle mass spectral differences between methamphetamine and pseudoephedrine were apparently not examined further.

Concluding Thoughts

CDOC works with RTL on rapid identification of the possibly illegal substances found in urine. The Defendant provided urine samples when requested. This was apparently the first time that one of the Defendant's urine samples was determined to have contained a possibly illegal substance.

Based on the 6-hour biological half-life of pseudoephedrine, it is possible that the Defendant had residual pseudoephedrine in his urine concurrent with producing this test sample. In this instance, the identification of methamphetamine when residual pseudoephedrine is present results in a false-positive.

Likewise, the prescription medication Adderall XR has amphetamine in it. The mass spectrum of amphetamine should be obtained when this urine sample is analyzed. In this instance, the presence of amphetamine is not a true false-positive; rather, it is what one expects to observe from a medication where amphetamine is one of its ingredients.

Given the similar chemical structures of dextroamphetamine (in Adderall XR), methamphetamine, and pseudoephedrine, the immunoassay technique presently in use may not be consistently and reliably sensitive enough to distinguish between the subtle differences in these molecules. As a result, a false-positive for methamphetamine is not an improbable outcome.

With the advent of automated systems containing "the library" of mass spectra, modern instrumentation performs matches of the unknown or sample mass spectrum with a known or reference mass spectrum in "the library." The match of the unknown or sample mass spectrum with a known or reference mass spectrum in "the library" often, but not always, works well. As the mass spectra of methamphetamine and pseudoephedrine are nearly indistinguishable, this would be an example where a false-positive could occur.

Should the mass spectrum of pseudoephedrine not be in "the library", the automated system still tries to find a match. The mass spectrum of methamphetamine is, to reasonable degree of scientific certainty, what can result from this matching process. By relying on "the library" alone without a positive identification by an experienced chemist, this has likely resulted in a false-positive.

RTL's huge throughput has prospective consequences associated with incomplete purging of the system between runs/trials. This can result in cross-contamination based on a residual amount of methamphetamine still present in the system from a previous run/trial.

Also, the standard adult dose for pseudoephedrine is 60 mg. There are six orders of magnitude between mg and ng. As a result, even after multiple biological half-lives, the concentration of pseudoephedrine, detected as methamphetamine, in the parolee's urine would be in the microgram per milliliter (µg/mL) range. Such concentrations would have, to a reasonable degree of scientific certainty, saturated the sensitive detector. Moreover, had the parolee been a habitual user of methamphetamine, he would have, to a reasonable degree of scientific certainty, tested positive for methamphetamine more often than this one time.

When all of the information presented here is read with understanding, it is clear that false-positive results were obtained for methamphetamine and amphetamine in the urine sample collected.

The Defendant was found not guilty at his January 12, 2016 hearing. His curfew ended and his ankle monitoring device was removed at that time. The CDOC appealed the initial exoneration. The parolee was released from custody when the appeal was unsuccessful.

He is now a free man.

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  Table 1. Bond Lengths (Å) of 2-aminophenol

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