Published in final edited form as:

... *Int Conf Ind Instrum Control*. 2015 May ; 2015: 71–76. doi:10.1109/IIC.2015.7150714.

Evolution of a Structure-Searchable Database into a Prototype for a High-Fidelity SmartPhone App for 62 Common Pesticides Used in Delaware

Malcolm J. D'Souza^{*,1}, Benjamin Barile¹, and Aaron F. Givens¹

¹Department of Chemistry, Wesley College, Dover, DE 19901, USA

Abstract

Synthetic pesticides are widely used in the modern world for human benefit. They are usually classified according to their intended pest target. In Delaware (DE), approximately 42 percent of the arable land is used for agriculture. In order to manage insectivorous and herbaceous pests (such as insects, weeds, nematodes, and rodents), pesticides are used profusely to biologically control the normal pest's life stage. In this undergraduate project, we first created a usable relational database containing 62 agricultural pesticides that are common in Delaware. Chemically pertinent quantitative and qualitative information was first stored in Bio-Rad's KnowItAll® Informatics System. Next, we extracted the data out of the KnowItAll® system and created additional sections on a Microsoft® Excel spreadsheet detailing pesticide use(s) and safety and handling information. Finally, in an effort to promote good agricultural practices, to increase efficiency in business decisions, and to make pesticide data globally accessible, we developed a mobile application for smartphones that displayed the pesticide database using Appery.io™; a cloud-based HyperText Markup Language (HTML5), jQuery Mobile and Hybrid Mobile app builder.

* malcolm.dsouza@wesley.edu (MJD).

Dedicated to Professor Dennis N Kevill, Northern Illinois University, DeKalb, Illinois (IL), on the occasion of his 80th birthday and in recognition of his many contributions to correlation analysis in chemistry and related areas.

Malcolm J. D'Souza is Professor of Chemistry at Wesley College, in Dover, Delaware. He is the Principal Investigator on the Wesley College DE-INBRE, DE-EPSCoR, NSF ARRA, and Cannon Scholar (NSF S-STEM) programs. In 2009, to mark the occasion of its 50th anniversary, the College of Liberal Arts and Sciences, Northern Illinois University (NIU), recognized the accomplishments of Dr. D'Souza as one of its 50 most distinguished alumni of the college. In 2012, he was awarded the American Chemical Society's (ACS) E. Emmett Reid Award, which recognizes high-quality teaching in chemistry at small colleges in the ACS Mid-Atlantic region. In addition to his research in physical organic chemistry, he also has projects, presentations, and publications in the area of chemometrics, STEM education, weight-loss studies, cheminformatics and in the design of commercial databases that assist in the development of new pharmaceutical and agricultural products. Dr. D'Souza also serves as the Associate Dean of Interdisciplinary/Collaborative Sponsored Research.

In 2011, Aaron Givens began research on this database building project as a sophomore in biological chemistry. Aaron's efforts were first recognized in September 2012, with an Undergraduate Education Award from the Delaware Section of the ACS, and in May 2013, Aaron was one of 25 students that received the 2013 ACS National Undergraduate Student Award in Environmental Chemistry. Currently, Aaron is a second year M.S. student at the University of Delaware (UD) in the Plant and Soil Science Department under the direction of Dr. Donald L. Sparks. His research involves the characterization and desorption kinetics of phosphorus in soil sand fractions, with an emphasis on southern Delaware soil.

As a senior in Mathematics, Benjamin Barile developed and built the smartphone app in the Wesley College Directed Research program. Ben's poster (CHED 664) at the 247th National ACS Meeting, March 16-20, Dallas, TX, earned a *Certificate of Merit* in the ACS Division of Environmental Chemistry. Ben is currently enrolled in Towson University's (Towson, MD) graduate school for Applied and Industrial Mathematics, where he is pursuing an M.S. degree with a concentration in Applied Statistics and Mathematical Finance.

Keywords

Wesley College; pesticide database; KnowItAll® Informatics System; Delaware; EPSCoR; IDeA; INBRE; undergraduate research; STEM; smartphone app

I. INTRODUCTION

A pervasive problem of extensive agricultural pesticide use is their widespread harmful impact on the environment, the economy, and on human health [1]. In Delaware (DE), the bioaccumulation of lipophilic contaminants and other chemical residues from pesticide and biocide applications are proven to cause long-lasting ecosystem change [2-9].

To protect human health and to preserve the environment, the United States (US) Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) and the Federal Food, Drug, and Cosmetic Act (FFDCA) provide the Environmental Protection Agency (EPA) broad federal regulation and control of pesticide distribution, sale, and use. Prior to pesticide registration with the EPA [10], laboratory animals are purposefully given acute oral, dermal, and inhalation exposure to pesticides to test for short-term (acute) and long-term (chronic) health effects [11].

A Congressional Research Service (CRS) report prepared for Members and Committees of Congress [12] showed that the honey bee and wild bee populations are negatively affected by the cumulative exposure (at sub-lethal levels) to pesticides, and a very recent long-term study, showed that pesticide exposure is definitively linked to depression in the farming community [13]. Hence, the EPA will only allow growers to use unregistered pesticides if emergency conditions exist.

The United States Department of Agriculture (USDA) operates a Pesticide Data Program (PDP) in cooperation with ten US States: California (CA), Colorado (CO), Florida (FL), Maryland (MD), Michigan (MI), North Carolina (NC), New York (NY), Ohio (OH), Texas (TX), and Washington (WA) [14]. The EPA also provides several pesticide database resources about toxicity, environmental effects, environmental fate, health effects, and regulatory information [15]. Chemical data (including tolerance information and toxicity) and other regulatory information related to pesticide registration, licensing, and pesticide use, is also available at the Pesticide Action Network (PAN) Pesticide Database [16], the Pesticide Data Sheets (PDSs) [17], the Pesticide Properties Database (PPDB) [18], and the Alan Wood website [19].

In addition, the Delaware Department of Agriculture (DDA) provides useful educational resources on pesticides [20]. DE also has an interactive Geographic Information System (GIS) that provides data from the DDA's 104 monitoring wells [21] and an online tool, DriftWatch™, that helps protect pesticide-sensitive crops and commodities from pesticide drift [22].

However, the understanding of the ecological impacts is often lacking as pesticide bio-concentration (bio-accumulation) and bio-magnification (bio-amplification) effects on living

organisms are difficult to quantify. Additionally crucial environmental indicators, such as pesticide water solubility data, vapor pressure, and partition coefficient, are sometimes missing from the manufacturers data summaries.

Over the past decade, in drug discovery and development, molecular modeling simulations and statistical computational approaches [23] have been successfully utilized to estimate missing structural energetics and molecular interaction parameters. Toxicokinetic or ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) and toxicodynamic (molecular interactions) data are accurately estimated using such *in silico* 3-dimensional Computational Molecular Modeling Methods (3D-CAMM) [24].

One commercial interactive platform is the Bio-Rad KnowItAll® Informatics System [25] which combines powerful ADMET tools, data management, database search, and spectral analysis tools for visualizing, processing, and reporting research results [25-27]. In a number of instances, we have demonstrated [28-34] the predictive viability of this KnowItAll® Informatics System for the determination of missing clinical pharmacokinetic drug data.

The first goal of this project is to use the database building capability of the KnowItAll® platform [25] to build a relational database containing 62 pesticides (common to Delaware) in order to facilitate compound screening and functional group identification. We can then use the predictive tools available within the platform and Quantitative Structure Activity Relationship (QSAR) techniques to predict any missing environmental indicators based on structural similarity of pesticides assessed within the database.

The US National Science Foundation (NSF) Experimental Program to Stimulate Competitive Research (EPSCoR) and the National Institutes of Health (NIH) Institutional Development Award (IDeA) programs provide funding to catalyze research and education in science and engineering (STEM) fields [35]. The IDeA Networks of Biomedical Research Excellence (INBRE) is a NIH IDeA program that is managed by the National Institute of General Medical Sciences (NIGMS). In DE, the University of Delaware (UD) is the lead institution on the NSF-EPSCoR (DE-EPSCoR) [36] and the NIH-NIGMS-INBRE (DE-INBRE) [37] cooperative agreements.

The Wesley College (Wesley) Directed Research program in Chemistry [38-41] was initiated to provide a competitive advantage to participating undergraduates by providing information technology training and scientific capacity-building opportunities. This Directed Research program is supported in part, through the DE-EPSCoR program, the DE-INBRE program, and the State of Delaware. One aim of our undergraduate research program is to sponsor and facilitate projects where the State (DE) has a vested interest. Hence, a second project goal is to develop a smartphone app targeted towards Delaware's farmers that can be accessed on all mobile devices and on all personal computers and tablets.

II. MATERIALS AND METHODS

A. Pesticide Data Sources, Retrieval, and Database Implementation

For many generations, the family of Aaron Givens, as resident farmers, have toiled the land in Delaware. Throughout the course of a growing season they administer at least one type of pesticide from eleven distinct structural classes. Working with heuristic information derived from this family and other resident farmers, we developed and populated our database using a decision-analytic model and selecting pesticides whose chemical structure was known. The chemical, environmental and toxicological properties of interest were extracted from several web-accessible sources [14-20].

The manufacturers brand, trade, or product name of the 62 pesticides investigated are: aldicarb, abamectin (B1a), atrazine, azoxystrobin, bifenthrin, bromacil, buprofezin, captan, carbaryl, carboxin, chlorantraniliprole, chlorimuron-ethyl, chlorothalonil, chlorpyrifos, chlorsulfuron, cymoxanil, cyprodinil, cyromazine, dichlorvos, difenoconazole, dimethamid-P, diquat dibromide, diuron, endosulfan, esfenvalerate, ethalfluralin, famoxadone, fenoxycarb, ferbam, fluazifop-P-butyl, flucarbazone-sodium, fludioxonil, flumioxazin, fluroxypyr, glyphosate, glyphosate trimesium, hexazinone, imazapyr, indoxacarb, lambda-cyhalothrin, malathion, maneb, mefenoxam (metalaxyl-M), methomyl, methoxyfenozide, metribuzin, metsulfuron methyl, nicosulfuron, oxamyl, permethrin, primisulfuron-methyl, profenofos, propiconazole, quintozone, quizalofop-p-ethyl, rimsulfuron, metolachlor, spiromesifen, sulfometuron-methyl, abamectin (B1b), glyphosate isopropylamine, and tebuconazole.

The molecular structure, molecular weight, International Union of Pure and Applied Chemistry (IUPAC) name, melting point (°C), water solubility (g/L), vapor pressure (torr), partition coefficient (Log K_{ow}), and trade name for the 62 pesticides were extracted from reliable state or federal government or private sources [14-20]. With the user-friendly KnowItAll® Informatics System's DrawIt™ application [25], 2-D structures of each pesticide were drawn (Fig. 1). Pertinent chemical and physical property data for each of the pesticides were then recorded in the database (Fig. 1). A SearchIt™ application allows users to perform searches and browse by name, structure, sub-structure or properties. A 3D molecular rendering program converts 2D structure drawings to 3D (Fig. 2). The platforms ProfileIt™ predictor application allows the user to generate a comprehensive ADMET profile (Fig. 3)

B. SmartPhone app –Development and Implementation

The diagrammatic representation shown in Fig. 4 depicts the workflow overview of the three-phase life-cycle development of this projects prototype. Due to the commercial and proprietary nature of the KnowItAll® Informatics System [25], the pesticide data was first manually copied and transferred onto a Microsoft® Excel spreadsheet. The Excel spreadsheet was utilized due to it's simplicity, availability, robustness, flexibility, and compatibility in managing generic data. The KnowItAll® 2D molecular structures could not be incorporated directly as the system is not friendly for devices with small-screens and small on-board storage, and the image could not be converted to a specific image file format.

Instead, the Print Screen (PrtScn) computer function was used to paste the images to Microsoft® Paint, where they were cropped and saved in a Portable Network Graphics (PNG) format. Once all of the data was stored in a Microsoft® Excel file, the uses and safety and handling instructions for each of the 62 pesticides were researched [14-20], documented and included. The final phase of the life-cycle was to program the mobile application and make it compatible for all Android, iOS, and Windows smartphones. The browser application interface was Appery.io™; a cloud-based HTML5, jQuery Mobile and Hybrid Mobile app builder, which made it easy to host and export the app's HTML code. Along with the visual user interface design system, Appery.io™ offers a mapping editor to help speed up the app design process.

First, during the design process, we registered an account name, "Pesticide Database," on the Appery.io™ website. The drag and drop Java GUI builder Plugin featuring layout managers was then used to create and arrange the 62 pesticide components in locations intelligently. We used the multicolumn listbox to display more information about each pesticide and the StartScreen (Fig. 5) was designed to replicate the pesticide order that appears in the KnowItAll® database.

On the app, the header bar (swatch) appears as a blue rectangle with white bold font. The pesticide list items are displayed as a white bold font with a blue background. For each pesticide, there are 18 text area components and one image component.

Nine of the text area components display "Melting Point [°C]," "Mol. Weight," "Log K_{ow}," "IUPAC Compound N," "Water Solubility [g/L]," "Vapor Pressure [torr]," "Vapour Pressure Cor," "Safety/ Handling (WASH HANDS AFTER HANDLING ALL PESTICIDES)," and "Uses" in a black bold font. These nine text area titles have nine text area components located directly below to display the related pesticide data in a black font. The nine text area components were populated using data documented on the Microsoft® Excel spread sheet cells and the copy and paste function. The image component was programmed to display the 2D molecular structure of the relevant pesticide (Fig. 6).

Additionally, Move and Fade transition effects were used to animate components as they transitioned between states of an application. Each individual pesticide page also has a "Back" button programmed into the upper left hand corner to transmit the user back to the StartScreen page (Fig. 6).

For example, the instantiate function allows the user to click on "endosulfan" on the StartScreen (Fig. 5) and the app will Fade into the "endosulfan" database page (Fig. 6). The "Back" button function is programmed to redirect the user from the "endosulfan" database page to the initial StartScreen.

This process was tested and retested for all of the 62 pesticides, with the site's web browser tester. The web browser tester was designed to launch the app over a monitor so that the user could check for any errors.

Through the Appery.io™ domain one can access the "Pesticide Database" with any internet connection (<http://pesticidedatabasewesleycollege.app.appery.io>). In order to download the

“Pesticide Database” as an app, the user has to first type in the specific domain through a smartphone web browser and then add the webpage to the users home screen.

III. DISCUSSION AND CONCLUSIONS

Delaware's DuPont™ company is the major manufacturer of sulfometuron-methyl under the brand name Oust®. Sulfometuron-methyl is a sulfonylurea herbicide used for weed control. It is typically applied during the rainy season as it suppresses weed growth through root uptake. Studies have shown [6-8] that in soils with high pH values and/or during extreme climatic conditions, sulfometuron-methyl may leach through the soil profile and enter the ground water.

Fig. 3 illustrates the ADMET profile obtained for sulfometuron-methyl using the KnowItAll® ProfileIT™ application. The water solubility versus pH graph (in Fig. 3) visually demonstrates that solubility increases significantly with an increase in pH (>6). This is due to the hydrophilic nature of sulfometuron-methyl compound and as a result, a greater amount of compound hydrolyzes at higher pH values. Such visual ADMET profiles are important in bioassessments, and in the understanding of the environmental fate and transport of possible stressors present in pesticide formulations.

The specifically designed high-fidelity interactive smartphone app prototype is targeted towards DE farmers. This pilot study integrating existing cloud computing resources and ADMET tools, give us preliminary proof of the concept that such dynamic mobile technology developments can lead to stepwise improvements for the selective use of targeted pesticides.

ACKNOWLEDGEMENTS

The Wesley College Directed Research Program acknowledges support from an IDeA award from NIH-NIGMS (INBRE grant no. P20GM103446, DE-INBRE program); an NSF-EPSCoR award (grant no. IIA-1301765, DE-EPSCoR program); an NSF ARRA grant 0960503; an NSF (DUE) S-STEM grant 1355554 (Cannon Scholar program); and the State of Delaware. The DE-INBRE and DE-EPSCoR grants were obtained through the leadership of the University of Delaware and the authors sincerely appreciate their efforts. Additionally, Aaron Givens acknowledges support from the NASA/Delaware Space Grant (NNG05GO92H) program for an Undergraduate Tuition Scholarship, and Benjamin Barile acknowledges valuable mentoring support from Dr. Frank Fiedler, Associate Professor of Mathematics, Wesley College.

NSF-EPSCoR Award (IIA-1301765, DE-EPSCoR program), NIH-NIGMS IDeA Award (P20 GM103446, DE-INBRE program), NSF ARRA grant 0960503; NSF S-STEM grant 1355554 (Cannon Scholar program) and the State of Delaware.

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Mol Weight (g/mol)	Tradename	LogP	Kow	Water Solubility	Vapor Pressure	Vapor Pressure at 25 Degrees Celsius
291.40	chlorpyrifos	4.4	1.0	0.015	0.0001	0.0001
275.70	disulfoton	NA	NA	NA	NA	NA
344.00	disulfoton	-4.00	9.10	0.0001	0.0001	0.0001
223.00	disulfoton	2.60	2.15	0.0001	0.0001	0.0001
408.00	disulfoton	5.00	5.15	0.0001	0.0001	0.0001
419.00	disulfoton	6.00	6.15	0.0001	0.0001	0.0001
231.70	disulfoton	5.11	5.15	0.0001	0.0001	0.0001
371.30	disulfoton	6.00	6.15	0.0001	0.0001	0.0001
301.30	disulfoton	4.30	4.35	0.0001	0.0001	0.0001

Chemical structure of diazinon: CN(C)COP(=S)(Cl)C1=CC=CC=C1

Name	Value	Unit
Tradename	disulfoton	
Mol Weight	408.00	g/mol
LogP	5.00	
Vapor Pressure	0.0001	mmHg
Vapor Pressure at 25 Degrees Celsius	0.0001	mmHg
Melting Point	100 - 110	°C
Water Solubility	0.0001	g/L
Kow	5.15	

Fig. 1.
A screen-shot of the database containing 62 pesticides that was built using the KnowItAll® Informatics System.

Fig. 2.
A screen-shot of the 3-D structure drawing of endosulfan.

Fig. 3.
A screen-shot of the ProfileIT™ application of sulfometuron-methyl.

Fig. 4.
The three phases in the construction life-cycle of the smartphone app.

Fig. 5.
Screen-shot of the Pesticide Database StartScreen..

Fig. 6.
A Screen-shot of the text area components.