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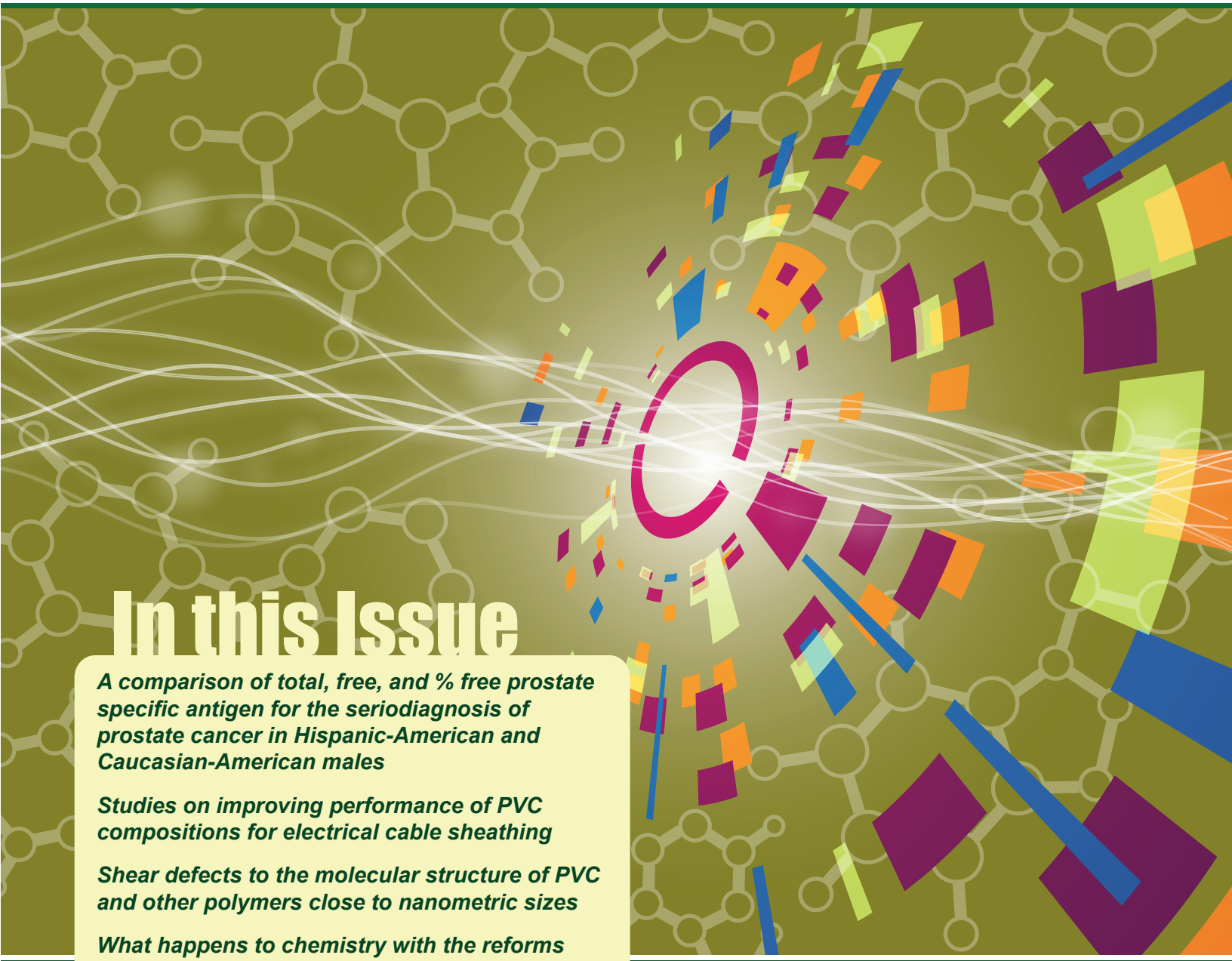

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The Chemist

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Editorial

David Devraj Kumar
Florida Atlantic University

We live in a world heavily influenced by the chemical sciences and their applications in technology. The influence of chemistry is all around us, ranging from food and household products to cell phones and life saving drugs. It is exciting to read about developments in chemistry, and it is similarly exciting to share new ideas and research findings to keep the chemistry community informed of developments in the advancement of chemical sciences. Therefore, it is appropriate that *The Chemist*, the official publication of The American Institute of Chemists, is being relaunched as an online refereed journal. The aim is to provide a scholarly outlet for the widest possible dissemination of research and developments in chemistry. Established in 1923, *The Chemist* has been a respected forum for the dissemination of articles in all aspects of chemical sciences. The peer-reviewed articles include research reports, scholarly discussions, and review articles, as well as book reviews, which are also entertained and encouraged. The newly organized editorial review team of academic and industrial scientists and educators from various parts of the world is pivotal to maintaining the quality of the journal. This first online version of *The Chemist*, volume 85(1 & 2), 2012, contains articles and book reviews that are both informative and thought provoking.

Tori Maywalt and co-authors are reporting a research study comparing the total, free, and % free prostate specific antigen in the serodiagnosis of prostate cancer in Hispanic-American and Caucasian-American males in the United States. Considering the fact that prostate cancer is the leading non-skin-related cancer in men, their study is not only important to improve understanding of prostate cancer in Hispanic-American males in the United States, but also to provide a platform for further research in this area. The study by B. R. Manjunath and co-authors deals with the preparation and testing of polyvinyl chloride compositions containing different amounts of additives for flame-retardant low-smoke electrical cable sheathing applications. David W. Riley is presenting a series of analyses of shear defects to the molecular structure of polyvinyl chloride and other polymers close to nanometric sizes in extrusion engineering. R. E. Yager is challenging people to think about the status of chemistry as an education discipline in the wake of the nanotechnology revolution and the new focus on STEM research and teaching. Finally, the reprinted (with permission) editorial from the *C&E News* "Chemical News Blunder, Powering Up with Cotton" by L. E. Wolf, appearing in the *Public Understanding of Chemistry* section, raises eyebrows about the way chemistry is occasionally, if not often, being portrayed in the media. The variety of articles in this issue should give the readership some impetus to think about the role of chemistry in shaping their thoughts and lives.

Finally, the support of the following individuals and institutions in facilitating the relaunching of *The Chemist* is acknowledged with gratitude. The role of the late Dr. Lila Albin of Purdue University for her leadership in sustaining the journal during a period of neglect should not be overlooked. She also played a significant role in the leadership transition of the journal. She will be missed. The dedication of the reviewers who provided thoughtful reviews and feedback in a timely manner to improve the quality of the manuscripts is very much appreciated. The timely feedback received from Dr. Penelope Fritzer of Florida Atlantic University who served as a guest book review editor and contributed to improving the quality of the book reviews is thankfully acknowledged. The efforts of Mr. Andrew Binder of Florida Atlantic University in recreating The AIC logo are appreciated. The assistance provided by Ms. Deborah Cate in style editing the manuscripts is also appreciated. It is encouraging to note that the Board of Directors and Leadership of The American Institute of Chemists are strongly behind the journal. Finally, it should be noted that the support provided by Florida Atlantic University in establishing a home base for editing *The Chemist* is invaluable in relaunching this important international scholarly periodical.

Thank you

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A Comparison of Total, Free, and % Free Prostate Specific Antigen for the Serodiagnosis of Prostate Cancer in Hispanic-American and Caucasian-American Males

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Abstract: Prostate cancer is the leading non-skin cancer in males in the United States of America. The measurement of prostate specific antigen in serum has been used as a minimally invasive tool for therapeutic monitoring (remission vs. relapse and progression), screening, and, together with other tools, for diagnosis and prognosis of prostate cancer. One objective of this study was to compare two ELISA assays for prostate specific antigen and free prostate specific antigen in serum. The comparison of normal adult PSA reference intervals, predictive values, and probability of prostate cancer based on % free PSA in Hispanic-American and Caucasian-American adult males was a second objective. It was hypothesized that the Diagnostic Automation (manual) assays would be superior to those of the Beckman Access (automated) for detection of prostate cancer and that there would be a genetic bias for PSA results. Tumor marker assays were performed according to the manufacturers' directions. Assays used in this study were Total PSA (Diagnostic Automation, Inc. and Beckman Inc.) and Free PSA (Diagnostic Automation, Inc. and Beckman Inc.). A total of 1,056 samples were tested. We concluded that there was a genetic bias between Hispanic-American and Caucasian-American males. We also concluded that the manual assay was superior to the automated assay for % free PSA, but not for total PSA assays. Our hypothesis about the genetic bias and the superiority of the Diagnostic Automation for % free PSA assays was supported by the study, but our hypothesis that the Diagnostic Automation would be superior for total PSA was not supported by our findings.

Key Words: Prostate specific antigen, prostate cancer, tumor markers.

INTRODUCTION

Cancer is a prominent subject in American culture. Almost everyone in the USA either knows or will know someone who is affected by cancer in some capacity. Cancer, as it is known in our culture, is a group of diseases that are characterized by tumors. Cancer is defined by Merriam-Webster as "a malignant tumor of potentially unlimited growth that expands locally by invasion and systemically by metastasis" or "an abnormal bodily state marked by such tumors" [1]. A tumor is an abnormal growth of tissue that is known as being either malignant or benign. This tumor starts as one transformed or cancerous cell that proliferates. Generally a benign tumor is one that does not pose problems for the patient and a malignant tumor is one that invades neighboring tissues of the host, causes sickness, and at times death [2]. One characteristic growth pattern of a cancerous tumor is known as metastasis, which means to spread throughout other organs or to break off from the original point of growth and begin growing elsewhere in the body.

The word "cancer" dates back to Hippocrates (460-370 B.C.) who used the Greek terms "carcinos" and "carcinoma" to describe ulcer-forming and non-ulcer-forming tumors that he discovered. These terms mean crab and tumors probably were named this due to the finger-like growth projection that they produce. Cancer had been described before this time, but not named. In 1761, Giovanni Morgagni of Padua began performing

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autopsies to find a reason for a person's death. This became the basis for the study of cancer or oncology. The famous Scottish surgeon John Hunter (1728-1793) suggested that surgeons operate on cancers that had not spread and remove tumors that could be removed. This technique flourished with the development of anesthesia a century later and practices like radical mastectomies became commonplace. Many other advances have been made assisted by the discovery of the microscope, the structure of DNA, and the different parts of the cell [3].

Cancer can potentially affect any organ or tissue. More common cancers include those affecting the prostate, breast, stomach, esophagus, pancreas, lung, and colon/rectum. According to the American Cancer Society (ACS), cancer is the second leading cause of death in the United States. An estimated 1,444,920 new cases were diagnosed in 2007 and there are projected to have been 559,650 deaths. According to the National Cancer Institute, in 2002 the prevalence of cancer was 10,146,000 people. The ACS defined cancer prevalence as "a measure of how common a cancer is" and explained that "this number is reflected by cancer incidence, which is the number of people newly diagnosed with cancer in a given time period (usually one year)." Also, cancer prevalence is "affected both by the incidence of a cancer and by how long people normally live with the disease" [4]. Prevalence is the number of all new and old cases of a disease during a particular period of time. It is expressed as a ratio of the number of new cases (numerator) per number of at risk population (denominator). These numbers are for both sexes and do not discriminate among types of cancer. Some of the most prominent cancers are breast, prostate, skin, lung, and colon/rectum. Cancer statistics, as well as the occurrence of different types of cancer vary among geographical locations.

Smoking, sexual activity, alcohol abuse, inappropriate diet, lack of physical activity, and sun exposure are some of the most common lifestyle factors that cause cancer. Other common cancer causing agents are called carcinogens which are electrophylic chemicals or other environmental factors that are responsible for causing cancer. Exposure to certain viruses may cause cancer and the presence of some diseases also contributes to the incidence of cancer within a person. Exposure to radiation can also cause cancer and there are a few hereditary cancers [5].

Some of the unique features of a cancer include cells being able to escape the host's immune system, exponential cell growth, certain biochemical markers, certain morphological properties, and molecular aberrations [5]. Cachexia (weight loss), hemorrhages, pain, palpable tumor masses, nausea, and susceptibility to other diseases are some signs and symptoms of cancer. The symptoms of cancer must be taken into account when making a proper diagnosis. These symptoms are not indicative of just one disease and tumors can be benign. Weight loss can be explained because a cancerous growth utilizes some of the nutrients that an individual ingests. Pain occurs mainly because the tumor is pressing on other tissues or nerves in the body [6].

There is not one definitive test for cancer. Some diagnostic tools that are often used in concert to detect cancer are biopsy, imaging, physical exam, chemical markers, tumor markers, nucleic acid markers, endoscopy, and cancer staging [7]. If a physician orders a blood test or urine test, it is usually to see what else is going on inside the body pertaining to electrolytes or the function of organs. Also, complete blood counts and bone marrow aspirations can be performed to look for abnormal cells. Biopsy is generally used to confirm diagnosis or to determine if a tumor is benign or malignant. Imaging techniques such as x-ray, magnetic resonance imaging (MRI), computed tomography (CT), and ultrasounds can be done to locate and examine a tumor in the body without causing the patient to endure an invasive and painful procedure. Once a cancer is diagnosed, a stage is assigned to it based upon the abnormality of the cells. The TNM system is one of the most commonly used staging systems. This system has been accepted by the International Union Against Cancer (UICC) and the American Joint Committee on Cancer (AJCC). Most medical facilities use the TNM system as their main method for cancer reporting. The TNM system is based on the extent of the tumor (T), the extent of spread to the lymph nodes (N), and the presence of metastasis (M). A number is added to each letter to indicate the size or extent of the tumor and the extent of spread. A stage one cancer has relatively normal cells while a stage five cancer has extremely abnormal cells [8]. Radiation therapy, surgery, chemotherapy, immunotherapy, hormonal therapy, and gene therapy are some forms of treatment for cancer. Cancer prevention generally involves life style changes, and preventative surgery. Life style changes such as cessation of smoking and use of other tobacco products, improved diet and exercise habits, and relief of stress often are most effective preventative measures [8]. The use of a vaccine directed against human papilloma virus (HPV), which is responsible for most of the cervical cancer cases, is an

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exciting new preventative approach [5]. The prostate is an accessory male reproductive organ that is approximately the size and shape of a walnut. This organ is located in front of the rectum and just below the urinary bladder. The main function of the prostate is to store and secrete a clear, slightly alkaline (pH 7.29) fluid that constitutes 10-30% of the seminal fluid, which, along with spermatozoa, constitutes semen [5].

Prostate cancer is the second most common type of cancer seen in American men and skin cancer is the most common. However, prostate cancer causes the most cancer deaths in men [9]. The ACS estimates that during 2006 about 234,460 new cases of prostate cancer were diagnosed in the United States. Approximately 1 in 6 men will be diagnosed with prostate cancer during their lifetime, but only 1 man in 34 will die of this disease. A little over 1.8 million men in the United States are survivors of prostate cancer. While the exact causes of prostate cancer are not yet determined, there are a number of risk factors that greatly increase the chances of an individual developing prostate cancer. The risk factors are: older age, having prostate cancer in male relatives, being African- American or Caucasian, not having a healthy diet, history of gonorrhea, and lack of physical activity [9].

Vasectomy was thought to increase the risk of having prostate cancer, but this theory is not supported by empirical evidence. Symptoms usually present later in the course of the disease and include blood in the urine, burning during urination, weak or interrupted urine flow, the need to urinate frequently (especially at night), impotence, lymphatic obstruction, anemia, weight loss, pulmonary congestion, and pain in the area around the prostate (including the lower back, the pelvis and the upper thighs). Prostate specific antigen testing and digital rectal examination are the two most commonly used diagnostic tools in detecting prostate cancer [9].

It is recommended by the ACS that men begin prostate cancer screening at age 50. However, African-Americans and other men with a history of prostate cancer in the family should get tested by age 45. A biopsy is often done when a tumor is located. It is also important to note that ultrasounds can help physicians to visualize a mass or tumor [9]. Some common treatments of prostate cancer include radiation, hormone therapy, and radical removal of the prostate. Many people who have the prostate removed or the radiation therapy live for up to fifteen years after their treatment.

MATERIALS

Dilutions were prepared using the diluent supplied by the manufacturer. Statistical analysis of the results was performed using SPSS software. All procedures performed in this study were in agreement with ethical standards established by the University of Southern Mississippi (USM). Permission for the study was granted by the USM Human Subjects Protection Review Committee in accordance with Federal Drug Administration regulations (21 CFR 26, 111) and Department of Health and Human Services regulations (45 CFR Part 46).

Test samples were obtained from Memorial Hospital at Gulfport, Singing River Hospital, and Wilford Hall Medical Center (United States Air Force Base, San Antonio). The serum samples were collected using aseptic techniques by hospital employed professionals. The diagnoses of these patients were made by the attending physicians based on pathological examination. Sera were collected, separated, coded, and frozen at -20°C. Later aliquots were thawed at 37°C and assayed in a blind fashion following the manufacturers' test directions in duplicate, sample permitting, for the tumor markers.

Patients were classified as being either: a) with prostate cancer or b) without prostate cancer. Since there was incomplete information about therapeutic/drug regiments, statistical analyses included the entire patient pool (Table 1).

Table 1. Patient Classification

Number of Patients	Cancer Diagnosis
155	With Prostate Cancer
901	Without Prostate Cancer

Eight hundred and nine adult males in good health were selected and tested with no bias in the same manner as the test patients (Table 2).

Table 2. Healthy Control Subjects

Number of Patients	Ethnicity
584	Caucasian-American
184	African-American
41	Hispanic-American

The healthy control subjects consisted of 41 Hispanic-American, 584 Caucasian-American and 184 African-American adult males. These subjects were used

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to generate a healthy adult reference interval/normal reference interval (NRI).

The results for the manual method reactions were read with a Beckman Coulter AD340 plate reader and all washings were done with a Stat Fax 2600 plate washer. Automated assays were performed by the hospitals before the samples were shipped and were performed using a Beckman Coulter Synchron LXi 725/ Beckman Access.

METHODS

The PSA enzyme immunoassay test kit by Diagnostic Automation, Incorporated is intended for the quantitative determination of PSA in human serum. The test is a solid phase two-site immunoassay. Rabbit anti-PSA is coated on the surface of the microtiter wells and another anti-PSA monoclonal antibody labeled with horseradish peroxidase is used as the tracer. The PSA molecules present in the standard solution or serum are "sandwiched" between the two antibodies. Following the formation of the coated antibody-antigen-antibody-enzyme complex, the unbound antibody-enzyme tracers are removed by washing. The horseradish peroxidase activity bound in the wells is then assayed by a colorimetric reaction. The intensity of the color formed is proportional to the concentration of PSA present in the sample [10].

All reagents and samples were allowed to reach room temperature (18-22°C) and were mixed gently before beginning the test. A data sheet with well numbers from the plate was marked with sample identification. All calibrators and controls were tested in duplicate. The assay procedure listed in Figure 1 was followed.

Figure 1. Diagnostic Automation Procedure for Prostate Specific Antigen (PSA) Enzyme Immunoassay Test Kit

1. Secure the desired number of coated wells in the holder.
2. Dispense 50 µl of standards, specimens, and controls into the appropriate wells.
3. Dispense 100µl of zero buffer into each well.
4. Thoroughly mix for 10 seconds. It is very important to have a complete mixing in this setup.
5. Incubate at room temperature (18-22°C) for 60 minutes.
6. Remove the incubation mixture by emptying plate contents into a waste container.
7. Rinse and empty the microtiter wells 5 times with running tap or distilled water.
8. Strike the wells sharply onto absorbent paper or paper towels to remove all residual water droplets.
9. Dispense 100µl of Enzyme Conjugate Reagent into each well. Gently mix for 5 seconds.
10. Incubate at room temperature for 60 minutes.
11. Remove the incubation mixture by emptying plate contents into a waste container.
12. Rinse and empty the microtiter wells 5 times with running tap or distilled water.
13. Strike the wells sharply onto absorbent paper to remove residual water droplets.
14. Dispense 100µl TMB solution into each well. Gently mix for 5 seconds.
15. Incubate at room temperature for 20 minutes.
16. Stop the reaction by adding 100µl of Stop Solution to each well.
17. Gently mix for 30 seconds to make sure that the blue color completely changes to yellow.
18. Using a microtiter plate reader, read the optical density at 450 nm within 20 minutes.

Important note: *The wash procedure is critical. Insufficient washing will result in poor precision and falsely elevated absorbance readings.*

The free-PSA (f-PSA) enzyme immunoassay test kit by Diagnostic Automation, Incorporated is intended for the quantitative determination of f-PSA in human serum. The test is a solid phase two-site immunoassay. An anti-f-PSA monoclonal antibody is coated on the surface of the microtiter wells and another anti-PSA monoclonal antibody labeled with horseradish peroxidase is used as the tracer. The f-PSA molecules present in the standard solution or serum are "sandwiched" between the two antibodies. Following the formation of the coated

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antibody-antigen-antibody-enzyme complex, the unbound antibody-enzyme tracers are removed by washing. The horseradish peroxidase activity bound in the wells is then assayed by a colorimetric reaction. The intensity of the color formed is proportional to the concentration of f-PSA present in the sample [11].

All reagents and samples were allowed to reach room temperature (18-22°C) and were mixed gently before beginning the test. A data sheet with well numbers from the plate was marked with sample identification. All calibrators and controls were tested in duplicate. The assay procedure listed in Figure 2 was followed.

Figure 2. Diagnostic Automation Procedure for Free Prostate Specific Antigen (f-PSA) Enzyme Immunoassay Test Kit

1. Secure the desired number of coated wells in the holder.
2. Dispense 100 µl of standards, specimens, and controls into the appropriate wells.
3. Dispense 100µl of sample diluent into each well.
4. Thoroughly mix for 10 seconds. It is very important to have a complete mixing in this setup.
5. Incubate at 37°C for 60 minutes.
6. Remove the incubation mixture by emptying plate contents into a suitable waste container.
7. Rinse and empty the microtiter wells 5 times with running tap or distilled water.
8. Strike the wells sharply onto absorbent paper or paper towels to remove all residual water droplets.
9. Dispense 200µl of Enzyme Conjugate Reagent into each well. Gently mix for 5 seconds.
10. Incubate at 37°C for 60 minutes.
11. Remove the incubation mixture by emptying plate contents into a suitable waste container.
12. Rinse and empty the microtiter wells 5 times with running tap or distilled water.
13. Strike the wells sharply onto absorbent paper to remove residual water droplets.
14. Dispense 100µl TMB solution into each well. Gently mix for 5 seconds.
15. Incubate at room temperature for 20 minutes in the dark.
16. Stop the reaction by adding 100µl of Stop Solution to each well.
17. Gently mix for 30 seconds to make sure that the blue color completely changes to yellow.
18. Using a microtiter plate reader, read the optical density at 450 nm within 20 minutes.

Important note: *The wash procedure is critical. Insufficient washing will result in poor precision and falsely elevated absorbance readings.*

RESULTS

Quality control samples analyzed over a three month period were used to determine intra- and inter-assay precision (Tables 3-4). The coefficient of variation (%CV) was approximately 5% or less for all but the between-run precision for the Diagnostic Automation, which were higher at 18.30% and 19.23% for Total and %Free PSA, respectively. Serial dilutions of abnormal pool samples were used to determine the linearity of the assays (Table 5 and 6). These results indicate good linearity for the assays with all being at or above 0.9981. The minimum detectable concentration was determined by analyzing approximately 20 replicates of the diluent and establishing the mean +2SD as the cut-off value (Tables 7 and 8). Analytical sensitivities for the assays ranged from 0.000 to 0.008.

The normal reference intervals are given in Tables 9 and 10. They were slightly higher than those cited by the manufacturers' package inserts. There was significant difference between the normal reference intervals of Hispanic-American and Caucasian-American adult males for total PSA, free PSA, and % free PSA by the manual assay and for Total PSA by the automated method.

A comparison of normal adult PSA values by genetic background and by methodology is given in Tables 11-14. A comparison of normal adult PSA, free PSA, and % free PSA by methodology revealed a significant difference for free PSA and % free PSA, but no significant difference for Total PSA.

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Table 3. Comparison of Diagnostic Automation and Beckman Access Assay Precision for Total PSA using Control Sera

Precision	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	CV (%)
Within-Run				
Diagnostic Automation	4	3.89	0.10	2.48
Beckman Access	2	1.00	0.02	2.00
Between-Run				
Diagnostic Automation	52	3.87	0.71	18.30
Beckman Access	40	1.00	0.02	2.20

Table 4. Comparison of Diagnostic Automation and Beckman Access Assay Precision for Free PSA using Control Sera

Precision	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	CV (%)
Within-Run				
Diagnostic Automation	4	2.25	0.09	4.10
Beckman Access	2	1.04	0.02	1.79
Between-Run				
Diagnostic Automation	52	2.08	0.40	19.23
Beckman Access	40	1.04	0.04	3.40

Table 5. Comparison of Diagnostic Automation and Beckman Access Assay Linearity for Total PSA

Assay	R Squared (R^2)
Diagnostic Automation	0.9981
Beckman Access	0.9996

Table 6. Comparison of Diagnostic Automation and Beckman Access Assay Linearity for Free PSA

Assay	R Squared (R^2)
Diagnostic Automation	0.9998
Beckman Access	0.9986

Table 7. Comparison of Diagnostic Automation and Beckman Access Assay Sensitivity (Analytical Sensitivity) for Total PSA

Analytical Sensitivity	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Range (ng/mL)
Assay				
Diagnostic Automation	19	0.00	0.000	0-0.000
Beckman Access	20	0.00	0.004	0-0.008

Table 8. Comparison of Diagnostic Automation and Beckman Access Assay Sensitivity (Analytical Sensitivity) for Free PSA

Analytical Sensitivity	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Range (ng/mL)
Assay				
Diagnostic Automation	20	0.00	0.000	0-0.000
Beckman Access	20	0.00	0.002	0-0.005

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Table 9. Comparison of Diagnostic Automation and Beckman Access Assay Healthy Adult Reference Intervals for Total PSA

Healthy Adults	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Range (ng/mL)
Total Males				
Diagnostic Automation	808	1.67	2.86	0-7.39
Beckman Access	809	1.91	6.59	0-17.07
Hispanic-American Males				
Diagnostic Automation	28	2.56	0.59	1.38-3.74
Beckman Access	28	0.93	1.05	0-3.03
Caucasian-American Males				
Diagnostic Automation	582	1.45	2.34	0-6.13
Beckman Access	584	1.70	3.37	0-8.84

Table 10. Comparison of Diagnostic Automation and Beckman Access Assay Healthy Adult Reference Intervals for Free PSA

Healthy Adults	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Range (ng/mL)
Total Males				
Diagnostic Automation	808	0.07	0.28	0-0.63
Beckman Access	36	0.90	1.26	0-3.42
Hispanic-American Males				
Diagnostic Automation	28	0.09	0.05	0-0.19
Beckman Access	0	-	-	-
Caucasian-American Males				
Diagnostic Automation	582	0.05	0.23	0-1.02
Beckman Access	26	0.65	0.43	0-1.51

Table 11. Comparison of Normal Adult Total PSA Values by Genetic Background

Total PSA	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Probability
Diagnostic Automation				
Hispanic-American Males	28	2.56	0.59	0.000*
Caucasian-American Males	582	1.45	2.34	
Beckman Access				
Hispanic-American Males	28	0.93	1.05	0.003*
Caucasian-American Males	584	1.70	3.37	

*p =< 0.05

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Table 12. Comparison of Normal Adult Free PSA Values by Genetic Background

Free PSA	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Probability
Diagnostic Automation				
Hispanic-American Males	28	0.09	0.05	0.003*
Caucasian-American Males	582	0.05	0.23	
Beckman Access				
Hispanic-American Males	0	-	-	-
Caucasian-American Males	26	0.64	0.43	

*p =< 0.05

Table 13. Comparison of Normal Adult % Free PSA Values by Genetic Background

% Free PSA	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Probability
Diagnostic Automation				
Hispanic-American Males	28	3.52	0.85	0.003*
Caucasian-American Males	582	3.45	3.51	
Beckman Access				
Hispanic-American Males	0	-	-	-
Caucasian-American Males	26	37.6	52.9	

*p =< 0.05

Table 14. Comparison of Normal Adult PSA Values by Methodology (paired t-test)

Assay Method	n	$\bar{X}$ (ng/mL)	SD (ng/mL)	Probability
TOTAL PSA | Assay				
Diagnostic Automation	807	1.67	2.86	0.167
Beckman Access	807	1.91	6.59	
Free PSA | Assay				
Diagnostic Automation	36	0.29	0.87	0.000*
Beckman Access	36	0.90	1.26	
% Free PSA | Assay				
Diagnostic Automation	31	3.55	5.59	0.000*
Beckman Access	31	19.06	9.01	

*p =< 0.05

Table 15. Predictive Values of Total PSA for Prostate Cancer in 1056 Patients

Assay Method	Sensitivity (%)	Specificity (%)	PV (+) (%)	PV (-) (%)	Efficiency (%)	Cut-Off (ng/mL)
TOTAL Males						
Diagnostic Automation	10.32	93.11	20.51	85.77	80.95	4.00
Beckman Access	18.71	87.57	20.57	86.23	77.46	4.00
Hispanic-American						
Diagnostic Automation	-	100.00	-	100.00	-	4.00
Beckman Access	-	86.00	-	100.00	-	4.00
Caucasian-American						
Diagnostic Automation	6.06	93.09	11.76	86.70	81.60	4.00
Beckman Access	14.14	87.60	14.74	87.06	77.93	4.00

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Table 16. Predictive Values of % Free PSA for Prostate Cancer in 1056 Patients

Assay Method	Sensitivity (%)	Specificity (%)	PV (+) (%)	PV (-) (%)	Efficiency (%)	Cut-Off (ng/mL)
TOTAL Males						
Diagnostic Automation	97.25	4.27	13.23	91.18	16.41	25.00
Beckman Access	80.00	33.33	5.13	97.37	35.34	25.00
Hispanic-American						
Diagnostic Automation	-	100.00	-	100.00	-	25.00
Beckman Access	-	-	-	-	-	25.00
Caucasian-American						
Diagnostic Automation	98.15	3.13	11.74	94.12	14.16	25.00
Beckman Access	75.00	33.75	5.36	96.43	35.71	25.00

Cutoffs to determine normal (negative) and abnormal (positive) test results used those cited by the manufacturers (Tables 15 and 16). Using the cut off values established by the manufacturers, we obtained diagnostic sensitivities of <50% by both methods for Total PSA.

Diagnostic sensitivity of a test is the proportion of individuals with the disease who test positively with the test. The diagnostic sensitivities for % free PSA were excellent. Diagnostic sensitivities were not calculated for the Hispanic-American males due to the paucity of positive samples. Diagnostic specificities were, however, excellent for both total and % free assays using the manual method and for total PSA using the automated method. Diagnostic specificity of a test is the proportion of individuals without the disease who test negatively with the test. The other predictive values were as expected. Predictive value (+) is the fraction of positive tests that are true positives. Predictive value (-) is the fraction of negative tests that are true negatives. Diagnostic efficiency is the fraction of all test results that are either true positives or true negatives.

DISCUSSION & CONCLUSION

Based on the results of our study, the hypothesis that there would be a genetic bias between Hispanic-American and Caucasian-American men was accepted. In contrast, the hypothesis that the manual assay would be superior to the automated assay was rejected for total PSA assays, but supported for % free PSA assays. Analytical parameters were acceptable for all the assays. As stated previously, the normal reference intervals we determined were slightly higher than those cited by the manufacturers' package inserts. There was significant difference between the normal reference intervals of Hispanic-American and Caucasian-American adult males for total PSA, free PSA, and % free PSA by the manual assay. This is the first report of a comparison of PSA healthy (normal) adult reference intervals for Hispanic-American males and Caucasian-American males. It is noteworthy that there was a statistically significant difference between the two groups, leading one to believe that one should use a modulated reference interval when diagnosing and monitoring Hispanic-American males. A comparison of normal adult PSA reference intervals by methodology showed significant difference for free PSA and % free PSA, but not total PSA. The Beckman Access results were typically slightly higher than those from the Diagnostic Automation. This would indicate a need for consistent use of one or the other method when diagnosing and performing therapeutic monitoring on individual patients.

Using the cut off values established by the manufacturers, we obtained diagnostic sensitivities of <50% for Total PSA by both methods. While our values were in line with those of other researchers, they were still disappointing. It is speculated that this may be due to inclusion of patients with prostate cancer who may have been diagnosed and were undergoing treatment. Alternatively, the patients may have been diagnosed earlier in the course of the disease.

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Studies on Improving Performance of PVC Compositions for Electrical Cable Sheathing Applications

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Abstract: Flame-retardant Polyvinyl chloride (FR PVC) is by far the most widely used polymer in the wire and cable industry. Studies have been conducted on PVC compositions for use in flame-retardant low-smoke (FRLS) cable sheathing applications in electrical industry. Compositions containing varying amounts of additives were prepared. The compositions that meet the FRLS requirements of Limiting Oxygen Index (LOI) and Smoke Density Rating (SDR) were evaluated for mechanical properties like tensile strength, elongation-at-break and thermal stability. The results are satisfactory as against the required values of Min: 12.5 N/mm^2, Min: 150 % and > 80 minutes. The compositions are to be tested in at least two different laboratories prior to scale-up studies.

Key Words: Polyvinyl chloride, flame-retardancy, DOP, TCP, Tensometer

INTRODUCTION

Despite public safety concerns and controversies relating to environmental impact [1], PVC continues to be among the five major thermoplastic resins [2] and continues to find as widespread use as ever in transport, building, packaging, electrical, electronic and healthcare applications sectors.

PVC, first prepared in 1872 by German chemist Eugen Baumann, and plasticized by B. F. Goodrich in 1926 into the form many of us are familiar with today [2], is unique in that it is used both in its rigid (unplasticized) form as well as flexible (plasticized) form. Flexibility is achieved by incorporating plasticizers or flexibilizers together with the polymer (so that flexible PVC often contains <50% actual PVC) [3]. Rigid PVC and flexible PVC have separately earmarked areas of use. The former is used for pipe, conduit, siding, windows and injection-molded appliance-housings, while the latter find use in wire and cable coatings, wall carvings, floor coverings and upholstery cover fabrics [3].

Rigid PVC contains a high level of chlorine (~56%) and is considered to be flame-retardant with an oxygen index of about 47. Flexible PVC is made by adding generally 25-50 % of a carboxylic acid ester, such as di(ethylhexyl)pthalate (DOP) as a plasticizer to the formulation. The plasticizer is combustible and reduces the flame-retardance of the formulation as measured by the oxygen index. Typical properties of PVC resin would indicate that it is too rigid (Shore D hardness 65-90), has a very high tensile strength that can be decreased without drawbacks (35 to 60 MPa) and is fire-retardant without additives (oxygen index 47). Generally, adding plasticizers, while imparting better flexibility at room temperature and enabling easier processing, simultaneously causes decrease in the tensile strength and lowers the oxygen index [4]. The present work is an attempt to obtain PVC compositions, already found to have acceptable FRLS characteristics in our laboratory, that attain acceptability with respect to mechanical properties as well, by varying the concentrations of additives. Thermal and electrical properties (not reported here) have been recorded and found to be acceptable as per requirements.

EXPERIMENT

The PVC resin (K-70 Grade), procured from M/s IPCL, India, has been used "as received" in the experimental work. Plasticizers DOP and tricresyl

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phosphate (TCP), filler calcium carbonate, mineral flame-retardant additives martinal (commercially available, aluminum hydroxide for the most part) and magnesium hydroxide, a metal-containing flame-retardant zinc borate, a calcium-zinc stabilizer to reduce loss of mechanical and electrical properties, lubricants calcium stearate and stearic acid, a special additive glass and an anti-oxidant bisphenol-A are the components of the polymer matrix.

Compounds of different compositions were prepared using the a Brabender Plasti-Corder (PLE 331) that gives a twin-screw mixing action at 20-30 rpm for about 30 minutes at 180°C and cured using the Hot Press Tester (Labtech Co. Ltd., Seoul, Korea) maintained at a temperature of 175°C and pressure of 90 kg/cm^2. Using the dumbbell cutter, specimens of required dimensions were prepared and the tests carried out under standard laboratory conditions, using Tensometer (Manufacturer: Hounsfield UTM; Model: H50KM) as per ASTM D 412 specifications.

RESULTS & DISCUSSION

Compositions that showed promise, arrived at after long trials, are given in Table 1.

Table 1. Compositions of the PVC systems

Sl. No.	Components (in phr units)												Sample Code
	(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)	(i)	(j)	(k)	(l)	
1	100	30	8	**14**	30	3	1	10	0.2	0.2	**15**	0.6	PM31
2	100	30	**9**	**12**	30	3	1	10	0.2	0.2	**14**	0.6	PM34

(a). PVC, (b).DOP, (c). TCP, (d). $CaCO_3$, (e). Martinal (f). $Mg(OH)_2$, (g). Zinc borate,
(h). Ca/Zn stabilizer, (i). Calcium Stearate, (j). Stearic acid, (k). Glass, (l). Bisphenol-A

The mechanical properties data are recorded in Table 2.

Table 2. Mechanical properties data

Designation	Properties		
	Tensile Strength or T.S(N/sq.mm)	% Elongation at Break	Thermal Stability (minutes)
PM31	14.0 – 15.6	165- 175	75-80
PM34	15.0-15.4	172.5-192.5	95-100

Both the compositions listed in Table 1 show LOI > 30% and SDR < 60%. On considering the evaluation data, the composition PM34 was selected as the final choice and repeat trials (nine times) conducted. The repeatability of this composition has been confirmed.

The results for the sample PM34 are more satisfactory. The values: T.S.:15.2 N/sq.mm, Elongation at Break: 182.5 % and Thermal Stability: 90-95 minutes are satisfactory against the minimum requirements of 12.5 N/sq.mm, 150 % and 80 minutes respectively.

The data demonstrate that small variations in concentrations of plasticizer, filler and FR additives can together bring about significant differences in tensile properties. The synergistic effect is better at 9 phr (parts per hundred resin) TCP, 12 phr $CaCO_3$ and 14 phr glass. The composition is due for verification of reproducibility of the results in two different laboratories.

CONCLUSION

On further confirmation of performance characteristics, the sample PM34 can be considered for extrusion trials and scale-up studies.

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Shear Defects to the Molecular Structure of PVC and Other Polymers Close to Nanometric Sizes

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Abstract: Last fifty years have seen dramatic changes in the understanding of shear and its results on changes in molecular structure, particularly in the field of polymers. Is there a relationship between lubrication and structure that transcends the processes of extrusion, injection molding, and even automotive engines? Yes, they all depend on lubrication for control of the critical molecular structures involved in each process. The key is the rate of shear, studied from 10-3 to 107 reciprocal seconds with all sizes of molecules. The important aspects of these studies are in the change or control of molecular structures associated with shear and the free radicals involved. In addition, the presence of oxygen and other crucial items is a real factor in terms of the life of the equipment and the lubricant. Depending on the type of molecule involved, the structure can be quite stable under shear but in most cases the changes in structure are dramatic. The shear rates vary greatly in extrusion depending not only on the flight clearance, but also on the compression ratio of the screw. Ratios as high as 15 to 1, in contrast to the normal being 3 to 1 have been dealt with. It is also seen the heat of shear exceed 100^{0}C above the extrusion temperature of the melt with the resulting changes in molecular structure. A wide range of polyolefins as well as PVC and the need for controlling additives as well as other factors will be discussed.

Key Words: Shar defects, nanometric size, molecular structure, extrusion, PVC.

INTRODUCTION

All processors have been plagued for half a century by gel particles and imperfections in plastic-molded and extruded materials. Studies on this topic have demonstrated that the causes were inherent in the molecular structure of each polymer. In early days whole shipments (190,000 pounds, for example) to a processor had been rejected and in some cases came close to bankrupting the supplier.

Sometimes these rejected materials were simply an error in judgment. For example, most people knew that ferric chloride was a catalyst for the decomposition of PVC. However, in 1967 a shipment of PVC, colored orange as required by the wire and cable industry, was received at Buffalo by Western Electric from an approved supplier. Within fifteen minutes after the extrusion was started, the material burned up in the extruder. An analysis of the pigment turned out to be ferric oxide; the PVC, though heavily stabilized, still evolved enough HCl to convert the ferric oxide into ferric chloride, and the results were devastating.

A 4 ½ inch extruder used for jacketing large amounts of pairs of cables (25 to be exact) was fitted with a new extruder screw and ran perfectly for a few weeks. Fortunately, I was assigned to monitor that unit and realized that the new screw was changing during the operation and actually wore out completely in five months. The flight clearance went from the new value of 5 mils (the distance between the flight and the barrel) to a value of 30 mils. During this wearing time, I studied the performance of that screw and found that the only way that I could maintain the output was to keep lowering the temperature on the barrel. The conclusion was that as the barrel wore, the degree of shear on the PVC compound increased, and hence, the heat of shear rose dramatically. Thus, the wear on the flights was directly related to some change in the molecular structure of the plastic, causing a possible change in the quality of the polymeric extrudate.

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Initially, it was thought that the only role of the plastic was to convey the filler, calcium carbonate (particle size of 3 mils in diameter), into the space between the flight and the barrel, and hence, causing the wear. However, we studied the rheological effects on the polymer to see if there might be a change in the plastic itself. The tests using infrared spectroscopy [1], solubility [1], as well as all forms of rheology [2], all indicated a gross change in plastic, suggesting that the molecular structure might be altered. Further tests were run or devised to detect any changes in the basic polymer [3]. The plasticizer was extracted using diethyl ether. The evaporated extract was not pure plasticizer, but contained significant amounts of low molecular weight PVC fragments [4].

In addition 200,000 kilograms of jacketing PVC was recycled to find out whether any of it was reusable. Only 10,000 kilograms made acceptable jackets. The rest had so many gel particles on the surface that it had to be rejected. These gel particles were tested and found to be high molecular weight PVC, estimated to be well over a million in weight average molecular weight (Mw) [5]. Furthermore, it was determined that with semi-rigid or even flexible compounds such as those used in jacketing, could only be extruded four times without displaying gels and imperfections in the final product.

To emphasize the active nature of this system, a literature search indicated that this mechano-chemical chain-scission process has been studied extensively by R. J. Ceresa [6]. He indicates that the free radicals are stable enough to be used during mastication for making block and graph copolymers of PVC. This means that not only copolymers can be formed, but also the reactions within PVC itself can be rampant and capable of converting relatively linear PVC into more complex structures and even the precursors of gels [7, 8, 9, 10].

SHEAR MEASUREMENTS

Shear occurs when one surface moves relative to another surface. The speed of this movement converts that operation into a shear rate. This is very important because excessive shearing effect is the primary cause of breaking molecular bonds of polymers.

The relationship between speed and shear rate can be seen in the simple expression Shear rate = □ = 4q/□r3 where q = output in mm3/sec and r = mm. [11] As the output goes up, the shear rate rises directly. Related to this, the heat of shear rises as the square of the shear rate (G = J (dv/dr)2), which is why the shearing function is so effective for melting the polymer in the screw. The shear rates of testing and processing range from a level of 10-3 all the way to 107 reciprocal seconds. The meaning behind all these ranges is as follows:

a. The low range from 10-3 sec-1 to about 10 is very sensitive to changes due to alterations in the molecular structure. This range of testing has been shown to be free of causing any appreciable molecular structural changes during the actual test procedure [1].
b. The next higher range, from 10 to 500—associated with normal channel depths of extrusion— causes a slightly detectable change in the molecular structure [11].
c. The upper range for the screw shear covers 1000 to 5000 sec-1 and begins to account for major levels of fragmentation in the polymer chains [11].
d. Beyond that range, either on the high RPM of the screw (i.e., 80 to 300 RPM) or the shear in the die, shear from both or either can exceed 10,000, 100,000 or one million reciprocal seconds. Here the breaking of the polymer chains becomes rampant and can only be controlled by rapid cooling in the range of 10 microseconds [12] or high levels of stabilization, processing aids, or/and lubricants [13].
e. Higher shears are experienced in the die of wire coating extruders where the polymer coating is in the range of 5 mils (0.125 mm, 125 □m) in thickness. Here the speed of the wire is 1000 meters per minute, giving a shear rate of 4 million sec-1. Actually, these days the wire speeds exceed twice that allowing shear rates to exceed 107 sec-1 [12].

TEST PROCEDURES

The All the useful range of rheological testing has been explored completely. The Rheometric Scientific instruments like the Mechanical Spectrometer are significant for identifying molecular structural changes [14]. However, they have not served our needs for observing fast changes in the process during extrusion or related processes. Capillary rheometry can relate to the higher shear rates and directly to the changes in processing steps such as the melting and shearing in the extruder screw. Here the rheology of the testing relates only to the average viscosity at the particular shear rate and only demonstrates gross viscosity changes as a measure of non-uniformity of density and viscosity and,

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possibly, temperature [15]. Certainly, to define extruder screws and their effective shapes, these capillary viscosities are the best way to attain computer simulation [16]. The molten viscosities are an extension of the unmelted coefficient of friction used so effectively to design complete extruder screws by the process know as Extrud [16].

However, none of these techniques define the manner in which a polymer structure changes effectively as the process alters the material. Furthermore, the analysis requires some judgment of the non-uniformity of the sample through the test procedure. Thus, the real analysis of the sample depends on a long die to attain equilibrium flow, and the ability to get many specimens to show the sensitivity and uniformity of the test data [17]. This has been developed from a modification of the extrusion plastometer [18].

Surprisingly enough, this simple machine has allowed us to detect molecular structural changes in PVC, initially, because the technique runs at such low shear rates and allows equilibrium flow. Then, to a lesser degree, changes can be sensed significantly in polypropylene, polybutylene, and even high-density polyethylene. A complete study of most of the polyolefins is being explored [19].

This technique is widely applicable and is even being applied to polycarbonate and ABS as illustrated effectively in Table 1 [20].

Table 1. Melt Flow for ABS and Polycarbonate by ASTM D 3364 Modified 230°C, 5 Kg Load on Ram

Sample Results	Inidividual Cuts	Average	Flow: mg/min
ABS untested	76 mg/30 seconds 84 77 84 81	80	160 mg/min
ABS Failure	62 mg/15 seconds 65 67 64 64 68 66	65	260
PC failure FL 900	74 mg/30 sec. 68 73 71 74	72	144
PC untested	133 mg/min 134 132 142 147	138	138

Note how the values for each reading vary, but give a good average. Note how much higher the failed sample of ABS is compared with the control. This means that appreciable fragmenting is occurring in the process. (Care is taken to avoid the early and late cuts that are at non-equilibrium conditions.) Note, too, that the temperature of the test is at 230°C. The "normal" melt flow by ASTM D 1238 for polycarbonate is run at 300°C. Lower temperatures enhance the sensitivity of the method for detecting molecular structural changes.

Interestingly enough, the technique has not demonstrated differences in the low-density polyethylene, so far, probably because the molecular

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weight distribution is so broad. This is being looked into with special highly branched side chains.

A complete analytical study was performed on the samples in order to study and define altered flow in the extrusion plastometer. The conclusions arrived at were that the ASTM D 3364 was the best technique for detecting fragmentation and instability in most polymer systems. The analytical systems covered were:

a. Infrared studies of the changes in the polymers with various types of processing
b. Liquid chromatography [1]
c. Solubility studies [1]
d. Other forms of processing such as Brabender testing [1]
e. Comparison between Elongation Rheometry and the Melt Flow technique [21]
f. Gas Chromatography for analyzing the off gases during processing [3]
g. NMR for modified molecular entities [22]

Techniques that will better define the fragments and the more complex molecular structures are being explored.

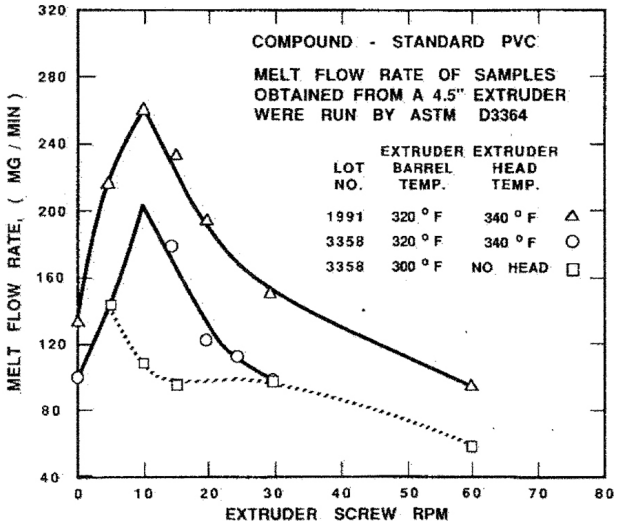
PROCESSING EXAMPLES

Instability Studies Using Extruders

In Figure 1, the instability of melt flow is given as a function of RPM of a 114.3 mm (4 ½") diameter extruder screw vs. Melt Flow Rate. Three lots of flexible PVC were run through the extruder at normal processing temperatures (170°C) and at different screw speeds. The material was sampled coming out of the crosshead for two cases. A third set of samples was taken directly off the tip of the screw. The differences demonstrate what happens for both the effect of the crosshead vs. the screw alone. The barrel settings ranged from 150°C to 160°C, trying to take heat out of the compound. The head was set at 170°C.

The melt flow rates rose from the original. Note that the melt flow values of the pellets rise to a high at 10 RPM, a clear example of the shearing causing the polymer to be fragmented. At higher RPMs, the melt flow falls sharply, indicating a re-assembly of the free radicals into a more complex structure. Note that the flow rates fall far below the original pellet values, indicating that an "incipient crosslinking" is forming. Excessively complex structures will be discussed later.

Figure 1. Melt Flow Rate as a Function of Extruder Screw RPM



The process of shearing and fusing PVC compounds to form pellets for subsequent extrusion can alter the material significantly. If the pellets are prepared in slow speed equipment (or in a low shear mixer), the melt flow of the resulting material is expected to be higher than the starting material. If the pellets are made in high-speed equipment, the flow rates will be lower than that of the dry blend and subsequent processing will need higher energy requirements and, in some cases, not extrudable.

Demonstrating the Change in Molecular Structure in Compounding Operations

Controlled shear can be demonstrated using a fully instrumented 114.3 mm (4 ½") screw 28/1 Length/Diameter fitted with a compact feeder (crammer feeder). By increasing the compactor speed between 50% and 100% (from 0.5 to 1.0), the melt flow by ASTM D 3364 of the resulting pellets increased as the speed increased—totally predictable [1], as indicated in Figure 2. Then, as the compactor went from 1.00 to 1.05, the melt flow decreased slightly indicating that the peak in shear fragmentation had been reached.

This illustrates that in processing, the rheology of molten PVC and other sensitive polymers can be controlled, but not by means normally observed or used in industry. Care must be taken to regulate the rate of shear in the process and to monitor that function, either by means of sensitive instruments associated with the extruder or by carefully controlled design of the extruding equipment.

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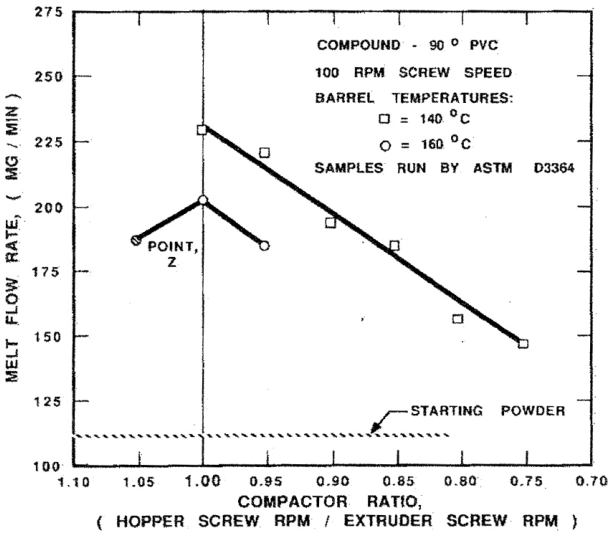
Figure 2. Melt Flow Rate as a Function of Compactor Ratio



Relationship Between Melt Flow and Amperage for Screw of a 150mm Extruder

Having installed a recording amperage meter on a 152.4 mm (6 inch) 20/1 L/D extruder, any appreciable change in the drive motor (440 v.) due to the change in the melt strength of the basic polymer was able to sense. In this case, a uniform pair of samples of flexible jacketing PVC [containing 35 pounds per hundred of resin (phr) of filler—calcium carbonate of 3 micron grind, 60 phr of DOP plasticizer] were used. The PVC Melt Flow by the ASTM Standard gave a value of 300 mg/min and 350 mg/min. The latter sample was loaded into the hopper and the equilibrium amperage of the screw gave a value of 170 amps. This was followed by a hopper load of the 300 melt flow material. The amperage rose to 173, indicating that a difference of 50 mg/min in melt flow is equivalent to 3 amps of difference on the extruder drive motor [1].

Techniques Controlling the Effects of Shear

Despite the fact that rigid PVC is inherently prone to shear damage, the proper use of lubricants has proven to be effective in preventing this shear. A complete study of this factor can be found in the literature [13].

If the plasticizer content is raised toward the 50% level (i.e., 90 to 110 phr) the PVC is protected from change by even levels of shear observed in an extruder screw with a compression ratio as high as 15 to 1. A semi-rigid material was tried in this screw and immediately burned up.

Size Exclusion Chromatography Results

The flow rate increase with fragmentation has been observed also by Pinette [5] in 1990 during processing on a two-roll mill. A series of experiments demonstrated the increase in fragmentation and then, subsequently, a decrease toward crosslinking. To analyze the results, size exclusion chromatography and inherent viscosity measurements were employed on the samples in progressive order of testing. The results are given in Table 2. For details on methods and techniques see references [13] and [14].

Table 2. PVC Melt Flow Correlated with Analytical Structural Methods

Sample Designation*	PVC Melt Flow (MG/MIN)	M_n	M_w	M_W/M_n	Relative Viscosity	Inherent Viscosity
PVC Dry Blend Ref. Material	118	38,000	111,000	2.9	1.140	0.655
350°F/18 MIN.	625	40,000	93,000	2.3	1.133	0.626
390°F /3 MIN.	383	48,000	251,000	5.2	1.132	0.621
390°F /7 MIN.	318	47,000	263,000	5.6	1.132	0.621
390°F/15 MIN.	235	46,000	285,000	6.1	1.133	0.621
390°F/19 MIN.	190	55,000	321,000	5.8	1.134	0.626
390°F/24 MIN.	140	52,000	304,000	5.8	1.135	0.632

*See Reference [13] and [14]

The molecular weights as listed are Number Average Molecular Weight designated as M_n. This molecular weight form is attained by Osmosis and counts the molecular weight based only on the number of end groups of the polymer. The Weight Average Molecular Weight, designated as M_w, is attained by Size Exclusion Chromotograpy. This later term is the most widely used expression and closely and easily related to the

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international term as the K factor and the Inherent Viscosity.

The extrusion process uses the Inherent Viscosity in the range of 0.9 to 1.1 for semi-rigid to flexible PVC and the K factor of 65 to 70.

Note that fragmentation of sample 2 at 18 minutes at 350°F gave a melt flow rate of 625 mg/min (up from 118 mg/min starting material) and was observed to have a 16% decrease in weight average molecular weight (M_w). This represents the high point in the melt flow rate curve observed in the data by D 3364. In contrast, the Mw increases very rapidly at 390°F with increasing time of shear. This appears to be moving in the crosslinking direction.

Further testing substantiates this point. Note how the dispersion (M_w/M_n) increases. Instead of a value of 3 or less, the values now jump to 6, a real measure of the increase in complexity of the structure. Based on the original PVC at 111,000 for an Mw, the final structure is almost three times as large.

New Molecular Structure Detected

The size exclusion chromatography measurements for the material milled by Pinette at 190°C displayed an early elution peak as a well-defined shoulder on the side of the primary PVC elution peak. This peak is not evident at lower temperature work. Based on the analysis, the size of this molecule is near 4 million for its Mw. Figures 3, 4, 5, and 6 show size extrusion chromatography for the original dry blend and milled PVC samples at various temperatures and different time intervals.

Figure 3. Size Extrusion Chromatography for PVC (Original Dry Blend and Milled at 350^{0}F for 18 Minutes)

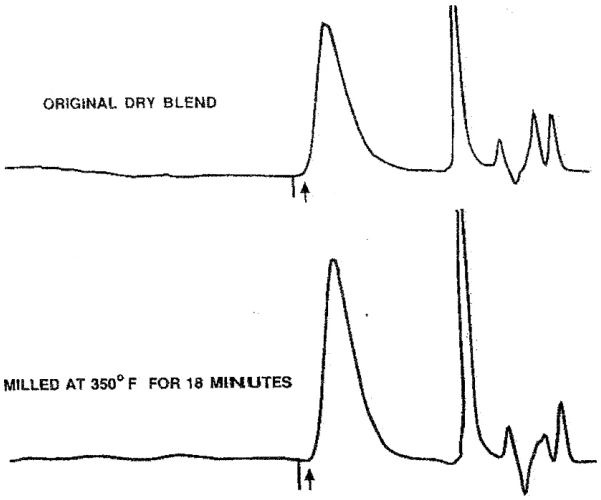


Figure 4. Size Extrusion Chromatography for PVC (Original Dry Blend and Milled at 390^{0}F for 3 Minutes)

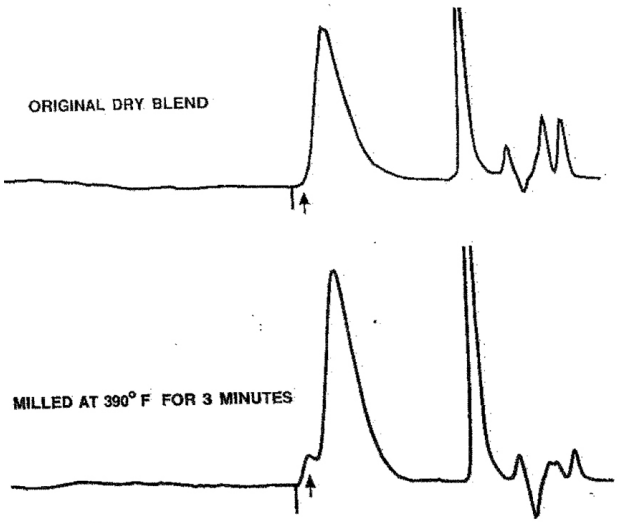
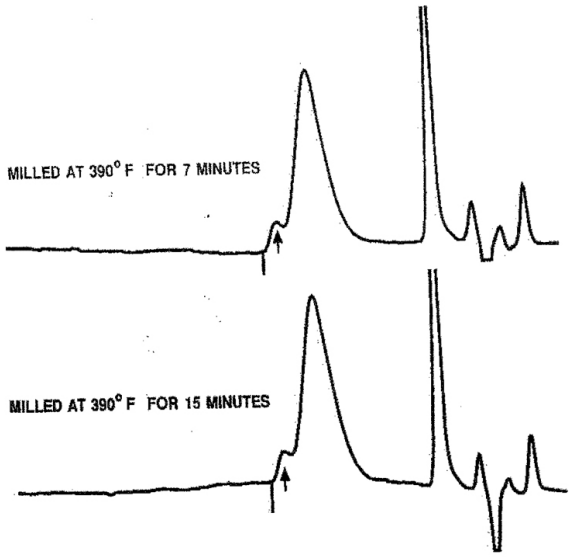


Figure 5. Size Extrusion Chromatography for PVC (Milled at 390^{0}F for 7 & 15 Minutes)



This molecule is a precursor for becoming a gel in the system. From the table of chromatography and inherent viscosity data one can see that the effect of this complex molecule increases the Mw for the entire sample from the original 111,000 to a value close to 300,000. The concentration of this complex molecule is estimated to be in the range of 5% of the total sample.

Interestingly enough, the same size sample was identified from a film of PVC under entirely different processing conditions. Both were exposed to oxygen,

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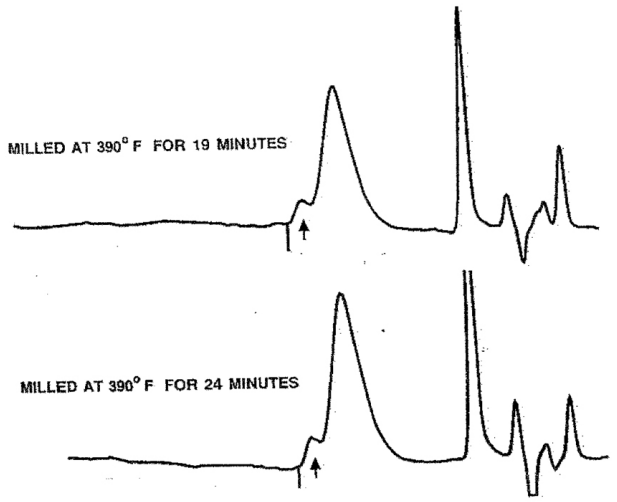
probably intensifying the complexity of the molecular structure in that 5% portion of the system.

Figure 6. Size Extrusion Chromatography for PVC (Milled at 390^{0}F for 19 & 24 Minutes)



SUMMARY

Shearing effects have long been an unrecognized hindrance to proper processing. With the major work in the last fifty years being in the area of heat stabilization, shear changes have now become the major detriment to consistent properties in most polymers. The ranking of shear instability for many polymers has been evaluated and it could be concludet that apparent shear stability ranks in the following order:

Most shear stable	Low density Polyethylene
	Linear low density PE
	High densityPE
	Polybutylene
Almost the least stable	Polypropylene (mostly decreasing in mol. wt.)
Least stable	Poly (vinyl chloride)

The shear effects proceed through a mechanism of fragmentation to a series of re-alignments into a progressively more complex series of structures in PVC. These complex structures are defined as incipient crosslinking. This complex polymeric system has been observed widely in the processing world. However, the results are greatly modified depending on the level of sensitivity to alteration by mechano-chemical chain reactions.

ACKNOWLEDGEMENTS

This paper was presented at the August 2005 meeting of the American Chemical Society. Samples for the analyses reported in figures 3, 4, 5 and 6 were prepared by Roger Pinette.

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The Chemist
Journal of the American Institute of Chemists

What Happens to Chemistry with the Reforms Advocated with STEM?

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Abstract: Few have questioned the appearance of chemistry as a high school course or its place among science offerings in most colleges. The emergence of Nanotechnology and the new focus on STEM research and teaching affect the status of chemistry as a discipline in educational settings. This short "Musing" illustrates the changes and current efforts related to chemistry offerings.

Key Words: Learning structures, centrality of questions, amalgamating science.

MUSINGS

There seems to be hype and dollars supporting education with reference to STEM as a revolutionary change in science education. Funding for STEM reforms is important and exciting! But, what does it really mean? How does it affect chemistry, as typically taught in colleges? And what does it do to chemistry in high schools? Of course, it is easy to interpret STEM as an acronym for educational reform related to Science, Technology, Engineering, and Mathematics. But, is that enough??

Chemistry has long held a special place in the high school curriculum, along with physics. They are commonly 11th and 12th grade offerings labeled "college preparatory." Some now worry that chemistry will disappear with STEM efforts as a focus for education K-16 and for all students.

Physics was first labeled as a course required for entrance to Harvard University in 1896! Ten years later Harvard decided to require chemistry too. Most other universities were quick to follow Harvard! Such "entrance" requirements have identified Chemistry to be but "college preparation" required by universities — now for over a hundred years. It is offered to satisfy college entrance requirements with little concern for why. It is typically taught in high schools similar to the ways it is taught for college undergraduates. The problems will change and intensify if STEM efforts for K-12 curricula succeed. It could well ignore specific reference to the separate science disciplines!

Many chemists were concerned when the 1996 National Science Standards combined physics and chemistry into "physical science," along with biology and earth/space science. Now, STEM also includes Engineering and Technology and reduces Science in general (as the first letter of STEM). The advancement with STEM efforts has made it more difficult to relate school science to terms that designate the separate science disciplines. Physics and chemistry remain unchanged with the actions of the statements contained in the National Science Education Standards (NSES). Is it noteworthy that many chemists were the ones slightly upset because the term "physical science" seemed to emphasize physics more than chemistry?

Chemistry as a high school course has even been controversial with the reforms in science for schools in the early 50s and early 60s. Many linked chemistry to a new focus on the Chemical Bond Approach, marking it as a major reform and change from the typical 11th grade chemistry course defined as "topics" generally used in textbooks. A focus on "Bonding" represented a major change in Chemistry when publicized as an example of reform instruction.

As some curricula are defined as moving toward more student/learner centeredness, the importance of the typical science disciplines classified as school "science"

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become even more of a problem to attain the reforms envisioned. Some actions are being taken to reform college science courses generally, but results with typical standardized testing create more problems, especially in the varying discipline content which STEM no longer uses. With the focus on developing exciting STEM programs, K-12 schools open the question again about specific science discipline content and skills required, similar to the discipline bound departments at most universities.

The excitement in using new learning theories, encouraging more research, and more focus on students personally "doing" science all may decrease interest in Chemistry, per se. Many continue to argue about what information should (must) be included in the reform of high school science courses. The concerns arise again resulting from the negative student attitudes; no focus on individual connections to life as well as no concern for science (chemistry) information or skills for personal use. Most negative student attitudes come from too little focus on the NSES goals which emphasize preparation of students for special citizenship participation and the work to solve 20th century problems. These new contexts are not common for typical Chemistry teaching — at least in any major ways. These changes need to produce more than gaining: 1) college entry; and 2) getting A's by remembering information and skills which are taught and emphasized by Chemistry professors. All these are negative outcomes of typical chemistry teaching which may also suggest failures for current STEM education — unless real changes occur in the teaching and new plans for college curricula!

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Public Understanding of Chemistry

Chemistry and its social-political-economic context 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).

The following article, used with permission from the C & E News, illustrates the necessity of proper representation of chemistry in the media.

Section Editors:
David Devraj Kumar
David M. Manuta
S. E. Baroni

A CHEMICAL NEWS BLUNDER, POWERING UP WITH COTTON

Watchers of the "Tonight Show" -- especially the segment called "Headlines" -- know that there are a lot of unintentionally funny, and sometimes worrisome, mistakes published in print media. Talk-show host Jay Leno encourages viewers and fans to send in error-laden clippings that he then uses to get a few chuckles out of his audience.

Recently, Newscripts received a newspaper clipping from reader David M. Manuta that could elicit both laughs and sad headshakes from our "audience": hawk-eyed chemists who will recognize the molecular mistake immediately.

In its Feb. 27 issue, the Columbus Dispatch ran an article, "Washing Is Rx For Healthy Cars In Winter." The short piece, from the syndicate Content That Works, set out to warn Ohio readers of various hazards that can damage their vehicles' paint jobs', and finishes. In particular, the article says, road deicers are most destructive. "SODIUM MAGNESIUM, used instead of sodium chloride in some locations, can be corrosive ...on a vehicle's undercarriage," the piece reads.

Unsure of what type of fantastical compound "sodium magnesium" might be, Manuta wrote to Content That Works to point out the problem. "Based on the underlying chemistry," he wrote, " 'sodium magnesium' would act as a wonderful deicer, as long as no one is concerned about the ensuing explosion and/or fire!" Manuta, president of Manuta Chemical Consulting, [Inc.] in Ohio, has investigated "too many incidents where reactive metals displace hydrogen from water" and cause explosions, he tells Newscripts.

He postulates that the article probably meant to describe magnesium chloride, a salt that lowers the freezing point of water more than sodium chloride does. This phenomenon was discussed in detail in a 2008 Newscripts column (C&EN, March 31, 2008, page 56). Either way, Manuta says, "there could be potentially devastating consequences for someone tossing pellets containing 'sodium magnesium' on an ice or snow-covered surface." So, readers, don't try this at home.

LAUREN K. WOLF wrote this week's column. Please send comments and suggestions to newscripts@acs.org.

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Book Reviews

Molecular Diagnostics: Fundamentals, Methods, & Clinical Applications (2nd Edition)

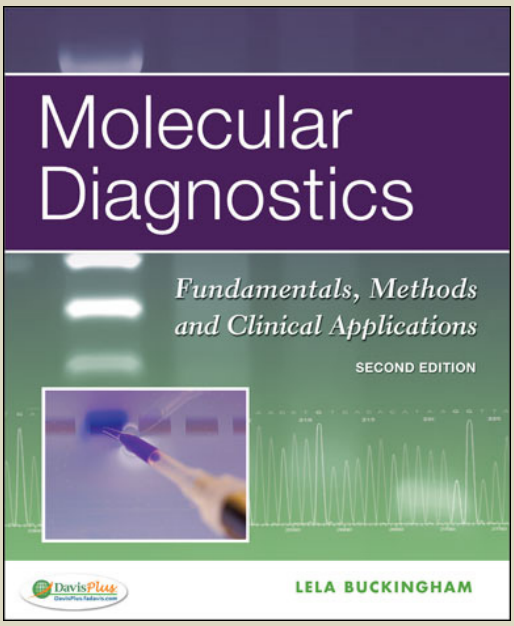
Reviewed by Margot Hall
University of Southern Mississippi, Hattiesburg, MS 39406

This textbook is excellent for an introductory course in clinical molecular biology. The authors have presented an adequate amount of theory and practical applications to support a one semester introductory course without overwhelming a student with endless technical detail. In this fashion, they have written a book that will serve students and professors for some time to come, despite the fact that molecular biology is a continuously evolving discipline.

There are 16 chapters (462 pages) in the soft cover edition of the book. The book is divided into 3 sections:

1) Fundamentals of Nucleic Acid Biochemistry: An Overview,
2) Common Techniques in Molecular Biology, and
3) Techniques in the Clinical Lab.

With approximately 3 to 7 chapters per section, each chapter has a chapter outline, a set of learning objectives, and numerous figures, diagrams, photographs, and tables illustrating the major points. Advanced concepts are placed in separate boxes contained in the chapter. There are also historical highlights that are sectioned off into boxes. Numerous study questions are located at the end of each chapter with answers to these questions located in an appendix at the end of the book.



Authors: Lela Buckingham
Publisher: F.A. Davis Company
ISBN#: 10: 0-8036-26770;
13: 978-0-8036-2677-5
Year: 2011
Price: $69.95

Clinical case studies are located at the end of chapters and are used to reinforce the learning objectives of that chapter. There is a list of references at the end of each chapter and an index at the end of the book. Important terms are bold printed in the text, which is most helpful. However, there is no glossary of terms in the book and that would be my recommended addition for future editions. A list of chapters by section includes the following:

- Section 1 - DNA, RNA, Proteins
- Section 2 - Nucleic Acid Extraction Methods, Resolution and Detection of Nucleic Acids, Analysis and Characterization of Nucleic Acids and Proteins, Nucleic Acid Amplification, Chromosomal Structure and Chromosomal Mutations, Gene Mutations, DNA Sequencing.

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- Section 3 - DNA Polymorphisms and Human Identification, Detection and Identification of Microorganisms, Molecular Detection of Inherited Diseases, Molecular Oncology, DNA-Based Tissue Typing, Quality Assurance and Quality Control in the Molecular Laboratory

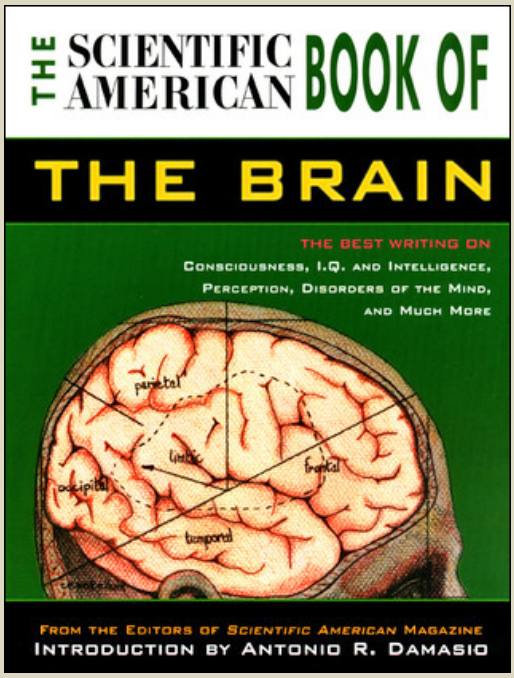
This book is eminently suitable for use by clinical chemists, pathologists, medical technologists, and biochemists. With the increased interest in molecular techniques and their use in the clinical laboratory, the reviewer has been searching for a good textbook. Her students and colleagues agree that this should be the textbook for current and future classes. It should serve as an excellent textbook for an undergraduate or beginning graduate course.

The Scientific American Book of the Brain (1st Edition)

Reviewed by Margot Hall
University of Southern Mississippi, Hattiesburg, MS 39406

This is an intelligently written and very readable little book on the science of the brain. It serves as a wonderful introduction to neuroscience and makes an important contribution to the understanding of such topics as consciousness, I.Q., intelligence, perception, gender ideation, and neurological diseases. It will serve equally well as an introduction to a neuroscience course or a handbook for the lay person with a need to understand the workings of the brain.

This superb text has an introduction written by Dr. Antonio R. Damasio, 32 contributing authors, 340 pages, numerous figures, and photographs including medical imaging studies. In addition to the table of contents and the index, there is one appendix which gives a brief biography of each of the 32 world renowned authors. It is arguably the best little book on one of the most fascinating but hither-to-fore difficult topics, namely the neuroscience behind the workings of the human mind and its diseases.



Publisher:	The Lyons Press/The Globe Pequot Press, Guilford Connecticut
ISBN#:	1-5874-285-6 (pb) or 1-55821-965-X (hc)
Year:	2001
Price:	$19.95

The book is organized into 6 sections, with each of the 26 chapters written as a stand-alone paper. This allows the reader to start with any topic which particularly interests him or her. Section 1 (Mapping the Brain) has four chapters: The Developing Brain, The Visual Image in Mind and Brain, Brain and Language, and Visualizing the Mind. Section 2 (Reasoning and Intelligence) has three chapters: The General Intelligence Factor, The Genetics of Cognitive Abilities and Disabilities, and Uncommon Talents: Gifted Children, Prodigies, and Savants. Section 3 (Memory and Learning) has five chapters: Working Memory and the Mind, Emotion, Memory and the Brain, Creating False Memories, The Split Brain Revisited, and The Biological Basis of Learning and Individuality. Section 4 (Behavior) has five chapters: Sex Differences in the Brain, Evidence for a Biological Influence in Male Homosexuality, The Biological Evidence Challenged, The

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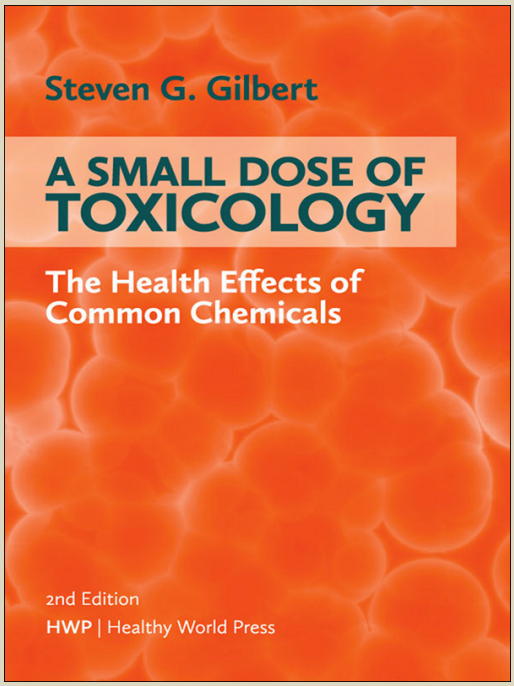
Neurobiology of Fear, and Seeking the Criminal Element. Section 5 (Disease of the Brain and Disorder of the Mind) has six chapters: Attention-Deficit Hyperactivity Disorder, Autism, Understanding Parkinson's Disease, Amyloid Protein and Alzheimer's Disease, The Neurobiology of Depression, and Manic Depressive Illness and Creativity. Section 6 (Consciousness) has three chapters: The Puzzle of Conscious Experience, Can Science Explain Consciousness? and The Problem of Consciousness.

The book gives a brief description of some of the methods used to test the brain, including molecular biology and genetic tests, PET scans, and MRI. This book is highly recommended for any student of biology or biochemistry and for anyone who knows and perhaps loves (which includes most of us) someone who is afflicted with a mental disorder.

A Small Dose of Toxicology: The Health Effects of Common Chemicals

Reviewed by Margot Hall
University of Southern Mississippi, Hattiesburg, MS 39406



Author:	Steven G. Gilbert
Publisher:	CRC Press
ISBN#:	0-415-31168-3
Year:	2004
Price:	$35.95

This book is exactly what it purports to be, namely a small dose of toxicology. Written expressly for those individuals who have no prior scientific background, the book presents in very readable fashion basic facts about common toxic compounds and their effects on people. The book evolved out of a continuing education course which the author taught for the Department of Environmental and Occupational Health Services at the University of Washington.

This book would be excellent for use in an undergraduate safety course or for use in a toxicology course for non-majors (100-200 level). It would serve well as additional material for a high school biology course and a copy of it definitely belongs in every home in America. The book has four especially helpful features: 1) a glossary of terms, 2) equivalent values integrated into the text (e.g., concentration of caffeine equivalent to volume of coffee in mL and in ounces), 3) cases taken from everyday life, and 4) a list of government agencies and non-governmental organizations with their web addresses from which one can obtain further information at the end of each chapter.

This textbook has 1 author, 266 pages, and numerous figures and tables. In addition to the table of contents and the index, there are three appendices: 1) a glossary of terms with definitions and examples, 2) a list of abbreviations used in the text, and 3) and an appendix demonstrating and explaining the principles of dose-response. Each of the 19 chapters has: 1) a website address for a slide presentation, 2) a list of web sites for [a] European, Asian, and international agencies, [b] North American agencies, and [c] non-governmental organizations from which one can obtain further information, and 3) a list of references (approximately 3-10 per chapter).

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The book is organized into four sections. The first section has two chapters on principles of toxicology and toxicology as it affects the reader/citizen. The second section has 12 chapters on toxic agents. These include alcohol, caffeine, nicotine, pesticides, lead, mercury, arsenic, metals, solvents, radiation, animal and plant toxins, and environmental contaminants. The third section has three chapters including: 1) neurotoxicology, 2) cancer and genetic toxicology, and 3) pregnancy and developmental toxicology. The last section has two chapters concerned with applied toxicology: 1) toxins in the home, and 2) risk assessment and risk management. Typical chapter outline uses the following plan: 1) dossier, 2) case studies, 3) introduction and history, 4) biological properties, 5) health effects, 6) reducing exposure, 7) regulatory standards, 8) recommendations and conclusions, and 9) more information and references.

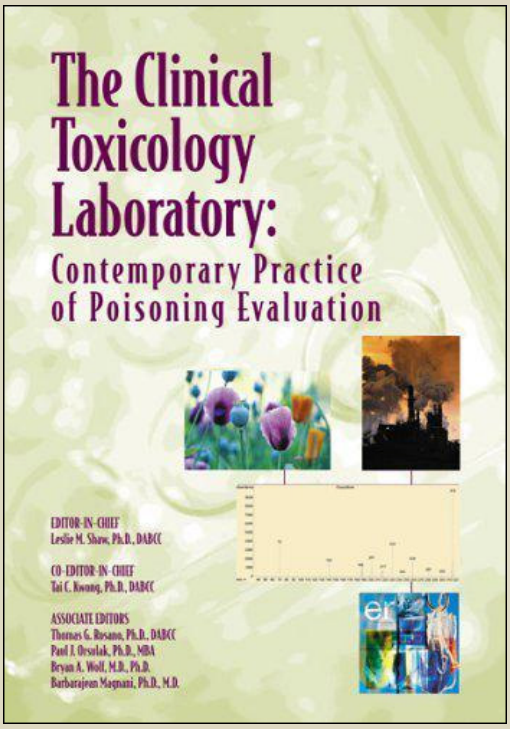
Overall this book is an easy read which will be especially appreciated by those individuals wanting a quick overview of the most salient facts. The book is not recommended for an undergraduate survey course because of the limited scope of the scientific information but is strongly recommended for the non-scientist and non-scientific majors.

The Clinical Toxicology Laboratory: Contemporary Practice of Poisoning Evaluation

Reviewed by Margot Hall
University of Southern Mississippi, Hattiesburg, MS 39406

This excellent textbook is based on a clinical toxicology review course which has been offered in the past by the American Association for Clinical Chemistry (AACC) and which has been extremely well received by the participants. The text focuses on the delivery of real time answers to the clinician dealing with the poisoned patient seen in the hospital emergency room setting. The book targets chemists/toxicologists and physicians involved in the delivery of clinical care to the acutely poisoned and chronically poisoned patient. Forensic toxicology with its attendant crime scene investigation is not a subject of the book. The text has 537 pages, 41 contributing authors, 29 chapters, 7 appendices, and 1 index.

Individual chapters address: 1) the epidemiology of poisoning, 2) toxicokinetics, 3) pharmacokinetics, 4) the clinical presentations and approaches to the diagnosis of the poisoned patient, 5) pharmacogenetics, 6) point-of-care testing methods, 7) samples including urine, blood, plasma, serum and alternative samples (saliva, sweat, hair, meconium), 8) urine adulteration prior to drug and alcohol testing, 9) traditional and advanced analytical techniques,



Editors:	Leslie M. Shaw, and Tai C. Kwong. (Associate Editors: Thomas G. Rosano, Paul J. Orsulak, Bryan A. Wolf, and Barbarajean Magnani)
Publisher:	AACC Press
ISBN#:	1-890883-53-0
Year:	2001
Price:	$99.00

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10) biological monitoring of chemical exposure, 11) a description of the successful toxicology laboratory for different size hospitals, and 12) eighteen chapters on specific toxins.

All of the chapters include learning objectives and a set of self-assessment questions with answers at the back of the book. In addition to these, each chapter on a specific toxin or class of toxins presents the following: a) case studies, b) epidemiology of the toxin, c) chemistry of the toxin, d) nomenclature, e) mechanism of action, f) therapeutic and toxic effects of the toxin, g) pharmacokinetics, h) toxicokinetics, i) methods of analysis with a comparison of their analytical and diagnostic parameters, j) clinical interpretations of concentration data, k) a discussion of current questions and issues relating to the toxin, and l) a list of pertinent references.

There are 7 appendices designed to tabulate in a user-friendly fashion the most important data required in the clinical toxicology setting. Appendix A offers the answers with explanations to the chapter self-assessment questions. Appendix B includes lists of toxins commonly associated with abnormalities of the vital signs (temperature, heart rate, blood pressure, respiratory rate, and papillary responses). Appendix C lists the five most common toxidromes (opioid, sympathomimetic, anticholinergic, cholinergic, sedative hypnotic) and the chemical agents and clinical manifestations associated with them. Appendix D lists the concentrations of drugs and other chemicals that will produce positive results in blood and urine samples for each of the currently commercially available assay methods. Appendix E offers a comparison of test methods for salicylate (aspirin) and acetaminophen (Tylenol®) analysis. Appendix F gives book reviews for 25 selected reference books in the field of toxicology. And Appendix G lists abbreviations used in the book.

This is a superb textbook for both the beginning and advanced student. It should prove useful to clinical chemists, toxicologists, pharmacologists, and clinicians. The learning objectives, case studies, and self-assessment questions add an important dimension to the reader. Of particular note were the efforts to present algorithms by which the physician and the laboratory can use patient history, communication, and clinical presentation to develop a preliminary diagnosis and thus focus the laboratory investigation so as to obtain answers in a timely fashion. Overall, this textbook is an excellent teaching tool for those involved in teaching clinical chemistry, toxicology, and/or clinical medicine. It is highly recommended as the primary text for courses in clinical toxicology.

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The AIC Code of Ethics

Approved by the AIC Board of Directors, April 29, 1983

The profession of chemistry is increasingly important to the progress and the welfare of the community. The Chemist is frequently responsible for decisions affecting the lives and fortunes of others. To protect the public and maintain the honor of the profession, the American Institute of Chemists has established the following rules of conduct. It is the Duty of the Chemist:

1. To uphold the law; not to engage in illegal work nor cooperate with anyone so engaged;

2. To avoid associating or being identified with any enterprise of questionable character;

3. To be diligent in exposing and opposing such errors and frauds as the Chemist's special knowledge brings to light;

4. To sustain the institute and burdens of the community as a responsible citizen;

5. To work and act in a strict spirit of fairness to employers, clients, contractors, employees, and in a spirit of personal helpfulness and fraternity toward other members of the chemical profession;

6. To use only honorable means of competition for professional employment; to advertise only in a dignified and factual manner; to refrain from unfairly injuring, directly or indirectly, the professional reputation, prospects, or business of a fellow Chemist, or attempting to supplant a fellow chemist already selected for employment; to perform services for a client only at rates that fairly reflect costs of equipment, supplies, and overhead expenses as well as fair personal compensation;

7. To accept employment from more than one employer or client only when there is no conflict of interest; to accept commission or compensation in any form from more than one interested party only with the full knowledge and consent of all parties concerned;

8. To perform all professional work in a manner that merits full confidence and trust; to be conservative in estimates, reports, and testimony, especially if these are related to the promotion of a business enterprise or the protection of the public interest, and to state explicitly any known bias embodied therein; to advise client or employer of the probability of success before undertaking a project;

9. To review the professional work of other chemists, when requested, fairly and in confidence, whether they are:
    a. subordinates or employees
    b. authors of proposals for grants or contracts
    c. authors of technical papers, patents, or other publications
    d. involved in litigation;

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10. To advance the profession by exchanging general information and experience with fellow Chemists and by contributing to the work of technical societies and to the technical press when such contribution does not conflict with the interests of a client or employer; to announce inventions and scientific advances first in this way rather than through the public press; to ensure that credit for technical work is given to its actual authors;

11. To work for any client or employer under a clear agreement, preferable in writing, as to the ownership of data, plans, improvements, inventions, designs, or other intellectual property developed or discovered while so employed, understanding that in the absence of a written agreement:
    a. results based on information from the client or employer, not obtainable elsewhere, are the property of the client or employer
    b. results based on knowledge or information belonging to the Chemist, or publicly available, are the property of the Chemist, the client or employer being entitled to their use only in the case or project for which the Chemist was retained
    c. all work and results outside of the field for which the Chemist was retained or employed, and not using time or facilities belonging to a client or employer, are the property of the Chemist;

12. Special data or information provided by a client or employer, or created by the Chemist and belonging to the client or employer, must be treated as confidential, used only in general as a part of the Chemist's professional experience, and published only after release by the client or employer;

13. To report any infractions of these principles of professional conduct to the authorities responsible for enforcement of applicable laws or regulations, or to the Ethics Committee of The American Institute of Chemists, as appropriate.

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The Chemist
Journal of the American Institute of Chemists

Manuscript Style Guide

The Chemist is the official online refereed journal of The American Institute of Chemists (AIC). We accept submissions from all fields of chemistry defined broadly (e.g., scientific, educational, socio-political). *The Chemist* will not consider any paper or part of a paper that has been published or is under consideration for publication anywhere else. The editorial office of *The Chemist* is located at: The American Institute of Chemists, Inc. 315 Chestnut Street Philadelphia, PA 19106-2702, Email: aicoffice@theaic.org.

Categories of Submissions

RESEARCH PAPERS

Research Papers (up to ~5000 words) that are original will only be accepted. Research Papers are peer-reviewed and include an abstract, an introduction, up to 5 figures or tables, sections with brief subheadings and a maximum of approximately 30 references.

REPORTS

Reports (up to ~3000 words) present new research results of broad interest to the chemistry community. Reports are peer- reviewed and include an abstract, an introductory paragraph, up to 3 figures or tables, and a maximum of approximately 15 references.

BRIEF REPORTS

Brief Reports (up to ~1500 words) are short papers that are peer-reviewed and present novel techniques or results of interest to the chemistry community.

REVIEW ARTICLES

Review Articles (up to ~6000 words) describe new or existing areas of interest to the chemistry community. Review Articles are peer-reviewed and include an abstract, an introduction that outlines the main point, brief subheadings for each section and up to 80 references.

LETTERS

Letters (up to ~500 words) discuss material published in The Chemist in the last 8 months or issues of general interest to the chemistry community.

BOOK REVIEWS

Book Reviews (up to ~ 500 words) will be accepted.

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Manuscript Preparation

RESEARCH PAPERS, REPORTS, BRIEF REPORTS & REVIEW ARTICLES

- **The first page** should contain the title, authors and their respective institutions/affiliations and the corresponding author. The general area of chemistry the article represents should also be indicated, i.e. General Chemistry, Organic Chemistry, Physical Chemistry, Chemical Education, etc.

- **Titles** should be 55 characters or less for Research Papers, Reports, and Brief Reports. Review articles should have a title of up to 80 characters.

- **Abstracts** explain to the reader why the research was conducted and why it is important to the field. The abstract should be 100-150 words and convey the main point of the paper along with an outline of the results and conclusions.

- **Text** should start with a brief introduction highlighting the paper's significance and should be understood to readers of all chemistry disciplines. All symbols, abbreviations, and acronyms should be defined the first time they are used. All tables and figures should be cited in numerical order.

- **References and notes** should be numbered in the order in which they are cited, starting with the text and then through the table and figure legends. Each reference should have a unique number and any references to unpublished data should be given a number in the text and referred to in the references. References should follow the standards presented in the AIC Reference Style Guidelines below.

REFERENCE STYLE GUIDELINES

References should be cited as numbers within square brackets [] at the appropriate place in the text. The reference numbers should be cited in the correct order throughout the text (including those in tables and figure captions, numbered according to where the table or figure is designated to appear). The references themselves are listed in numerical order at the end of the final printed text along with any Notes. Journal abbreviations should be consistent with those presented in Chemical Abstracts Service Source Index (CASSI) (http://www.cas.org) guide available at most academic libraries.

- **Names** and initials of all authors should always be given in the reference and must not be replaced by the phrase *et al*. This does not preclude one from referring to them by the first author, et al in the text.

- **Tables** should be in numerical order as they appear in the text and they should not duplicate the text. Tables should be completely understandable without reading the text. Every table should have a title. Table titles should be placed above the respective tables.

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

- **Figure legends** should be in numerical order as they appear in the text. Legends should be limited to 250 words.

  Figure 1. PVC Melt Flow Characterized by Analytical Structural Method

- **Letters and Book Reviews** should be clearly indicated as such when being submitted. They are not peer-reviewed and are published as submitted. Legends should be placed after/under the respective figures.

- **Journals -** The general format for citations should be in the order: **author(s), journal, year, volume, page**. Page number ranges are preferred over single values, but either format is acceptable. Where page numbers are not yet known, articles may be cited by DOI (Digital Object Identifier). For example:

  Booth DE, Isenhour TL. *The Chemist*, 2000, 77(6), 7-14.

- **Books -** For example:

  Turner GK in Chemiluminescence: Applications, ed. Knox Van Dyke, CRC Press, Boca Raton, 1985, vol 1, ch. 3, pp 43-78.

- **Patents** should be indicated in the following form:

  McCapra F, Tutt D, Topping RM, UK Patent Number 1 461 877, 1973.

- **Reports and bulletins, etc. -** For example:

  Smith AB, Jones CD, "Environmental Impact Report for the US", final report to the National Science Foundation on Grant AAA-999999, Any University, Philadelphia, PA, 2006.

- **Material presented at meetings -** For example:

  Smith AB. Presented at the Pittsburgh Conference, Atlantic City, NJ, March 1983, paper 101.

- **Theses -** For example:

  Jones AB, Ph.D. Thesis, Columbia University, 2004.

REFERENCE TO UNPUBLISHED MATERIAL

- For material presented at a meeting, congress or before a Society, etc., but not published, the following form should be used:

  Jones AB, presented in part at the 20th American Institute of Chemists National Meeting, Philadelphia, PA, June, 2004.

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- For material accepted for publication, but not yet published, the following form should be used:

  Smith AB. Anal. Chem., in press

- For material submitted for publication but not yet accepted the following form should be used:

  Jones AB, Anal. Chem. submitted for publication.

- For personal communications the following should be used:

  Smith AB, personal communication.

- If material is to be published but has not yet been submitted the following form should be used:

  Smith AB, unpublished work.

Reference to unpublished work should not be made without the permission of those by whom the work was performed.

Manuscript Selection

The submission and review process is completely electronic. Submitted papers are assigned by the Editors, when appropriate, to at least two external reviewers anonymously. Reviewers will have approximately 10 days to submit their comments. In selected situations the review process can be expedited. Selected papers will be edited for clarity, accuracy, or to shorten, if necessary. The Editor-in-Chief will have final say over the acceptance of submissions. Most papers are published in the next issue after acceptance. Proofs will be sent to the corresponding author for review and approval. Authors will be charged for excessive alterations at the discretion of the Editor-in-Chief.

Conditions of Acceptance

When a paper is accepted by *The Chemist* for publication, it is understood that:

- Any reasonable request for materials to verify the conclusions or experiments will be honored.

- Authors retain copyright but agree to allow *The Chemist* to exclusive license to publish the submission in print or online.

- Authors agree to disclose all affiliations, funding sources, and financial or management relationships that could be perceived as potential conflicts of interest or biases.

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- The submission will remain a privileged document and will not be released to the public or press before publication.
- The authors certify that all information described in their submission is original research reported for the first time within the submission and that the data and conclusions reported are correct and ethically obtained.
- The Chemist, the referees, and the AIC bear no responsibility for accuracy or validity of the submission.

Authorship

By submitting a manuscript, the corresponding author accepts the responsibility that all authors have agreed to be listed and have seen and approved of all aspects of the manuscript including its submission to *The Chemist*.

Submissions

Authors are required to submit their manuscripts, book reviews and letters electronically. They can be submitted via email at aicoffice@theaic.org with "Submission for consideration in *The Chemist*" in the subject line. All submissions should be in Microsoft® Word format.

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Announcements

INVITATION TO AUTHORS

Authors are invited to submit manuscripts for ***The Chemist,*** the official online refereed journal of The American Institute of Chemists (AIC). We accept submissions from all fields of chemistry defined broadly (e.g., scientific, educational, socio-political). *The Chemist* will not consider any paper or part of a paper that has been published or is under consideration for publication anywhere else.

Research Papers (up to ~5000 words) that are original will only be accepted. Research Papers are peer-reviewed and include an abstract, an introduction, up to 5 figures or tables, sections with brief subheadings and a maximum of approximately 30 references.

Reports (up to ~3000 words) present new research results of broad interest to the chemistry community. Reports are peer- reviewed and include an abstract, an introductory paragraph, up to 3 figures or tables, and a maximum of approximately 15 references.

Brief Reports (up to ~1500 words) are short papers that are peer-reviewed and present novel techniques or results of interest to the chemistry community.

Where to Send Manuscripts?

Please submit your manuscripts by email (aicoffice@theaic.org) to the attention of:

The Editor-in-Chief, The Chemist
The American Institute of Chemists, Inc.
315 Chestnut Street,
Philadelphia, PA 19106-2702
Email: aicoffice@theaic.org

Review Articles (up to ~6000 words) describe new or existing areas of interest to the chemistry community. Review Articles are peer-reviewed and include an abstract, an introduction that outlines the main point, brief subheadings for each section and up to 80 references.

Letters (up to ~500 words) discuss material published in *The Chemist* in the last 8 months or issues of general interest to the chemistry community.

Book Reviews (up to ~ 500 words) will be accepted.

NATIONAL CERTIFICATION COMMISSION IN CHEMISTRY AND CHEMICAL ENGINEERING (NCCCCE)

The official credentialing program of the National Certification Commission in Chemistry and Chemical Engineering (NCCCCE) is sponsored by The American Institute of Chemists, Inc. (AIC). Those credentialed will join a select group of professionals who have made the commitment to achieve excellence in their professional development by initial education and experience and by continuing education. Those who fully meet qualifications will be designated as Certified Professional Chemist (CPC) or Certified Chemical Engineer (CChE). They are fully recognized for their accomplishments by their peers. The purpose of the certification program is to recognize chemists and chemical engineers who have a certain basic level of education and/or experience and who have participated in professional career development and continuing education. Please see more at www.theaic.org or contact aicoffice@theaic.org

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CALL FOR NOMINATIONS FOR 2013 THE AIC AWARDS

The Awards Committee of The American Institute of Chemists is inviting nominations for two well established and respected awards in the field of chemical sciences: The AIC Gold Medal and The AIC Chemical Pioneers.

The AIC Gold Medal

Nominations are now being accepted for the 2012 The American Institute of Chemists Gold Medal Award. First presented by the AIC in 1926, the Gold Medal is the AIC's highest award. It recognizes service to the science of chemistry and to the profession of chemistry or chemical engineering in the United States. Previous winners include Nobel laureates Glenn T. Seaborg and Herbert C. Brown, as well as other renowned researchers and scientists representing the many facets of the world of chemistry. Recent medalists include Elizabeth Blackburn, George Whitesides, Roald Hoffman, and Oliver Smithies.

The award winner is expected to deliver a formal lecture on a topic relevant to the basis for winning the award at the award ceremony during the Chemical Heritage Day in April 2012.

Nominations should consist of a nominating letter with the individual's curriculum vita plus two letters of support. All nomination materials are due by **October 5, 2012.**

The AIC Chemical Pioneer Award

First presented by The AIC in 1966, the Chemical Pioneer Award recognizes chemists, chemical engineers, or their associates who have made outstanding contributions that have had a major impact on advances in chemical science and industry and/or the chemical profession. Previous winners include pioneering researchers, educators and executives representing the many facets of the world of chemistry. The AIC Chemical Pioneers include Eugene G. Rochow, Linus C. Pauling, O. A. Battista, Herbert C. Brown, Alan G. Marshall, and George Olah.

The award winner is expected to deliver a formal lecture on a topic relevant to the basis for winning the award at the award ceremony during the 2013 annual meeting of The American Institute of Chemists.

Nominations should consist of a nominating letter with the individual's curriculum vita plus two letters of support. All nomination materials are due by **October 19, 2012.**

For both awards, it is the responsibility of the person making the nomination to collect and submit all the required nomination materials – letter of nomination, two letters of support and the nominees CV. No late nominations will be accepted. Nominations should be mailed to:

Ms. Sarah Reisert
Attn: The AIC Gold Medal Nomination
Chemical Heritage Foundation
315 Chestnut Street
Philadelphia, PA 19106

OR you may email completed nomination materials to SReisert@chemheritage.org

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American Institute of Chemists

www.TheAIC.org

From its earliest days in 1923 to the present, the American Institute of Chemists has fostered the advancement of the chemical profession in the United States.

The Institute has a corresponding dedication "to promote and protect the public welfare; to establish and maintain standards of practice for these professions; and to promote the professional experience through certification as to encourage competent and efficient service."

The AIC engages in a broad range of programs for professional enhancement through the prestigious Fellow membership category, awards program, certification programs, meetings, publications and public relations activities.

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