Motivation

Why did you sign up for this class? Possibly the reason is that later in your studies or career you may be using the methods taught here. Imagine that you have already got a job as a chemist or scientist in a laboratory, where you are the most qualified person to answer any chemistry/science relevant questions. Your task in this scenario would be to find a suitable method and analyze chemical(s) within the sample material (matrix) relevant to your work.

How do you approach this issue? What will be your first step to address this task?

Most people will be hesitant to say that what comes first to their mind is a “google search.”

Is this correct?

Yes, but only in part. The Google search currently offers a Google Scholar search option and there are often many application notes provided by commercial companies, as well as by Wikipedia. All of these tools are appropriate, however the rigor of science requires us to verify the obtained information with a peer reviewed literature search through science related search engines, such as SciFinder and Scopus.

Assignment

Your task will be to perform a search of peer reviewed literature on the chromatographic and/or mass spectrometric characterization of one analyte/sample of your choice. You will need to select from the list of topics (listed below) during the 1st week of classes. If you would rather pursue another topic you will have to have it approved by the instructor.

You will report the peer reviewed literature search results in a form of a paper (2-3 pages double-spaced) written in a similar style as an Introduction section of a mock article to be published in a peer reviewed journal. Use a minimum of 6 recent references from peer reviewed journals. You may supplement those by references from books, but you should not use books as the main reference source. While you may refer to certain websites, you should try to access the original source (that is, even Wikipedia list their sources – use those original credible (i.e., peer-reviewed) articles as your primary source).

Paper

In this assignment, your paper (written in style of an introduction to a research article) should include the following sections:

a) A description of the targeted analyte(s) within a specific matrix, analyte’s use, description of the analyte chemical structure and how the chemistry of this chemical(s)/matrix may affect the analysis. This part of the text should make it clear why this analyte within the particular matrix needs to be analyzed.

b) The Method(s) section (which may consist of several paragraphs) should cover the methods used for the analysis of this chemical within the particular matrix. The methods may include non-chromatographic approaches/protocols, but a justification should be provided why the chromatography or mass spectrometry (or their combination) is the method of choice. In general, methods should not be just listed, instead they need to be evaluated and compared based on their limits of detection, applicability to a particular analyte and matrix, costs, etc.

c) The last section should propose the method of choice for further work (the text prior to this section should make it clear why this method is the optimal starting point).

DOs

• add a reference(s) whenever you refer to any work reported by others
• ensure that the references are up-to-date (covering the latest findings) and are presented in an ACS format
Support any statements describing the quality of the work by quantitative data. For example, support the following statement “the method provided high yields” by adding in parenthesis the actual numerical values, e.g., “(65%)”

Keep your paper logical, straightforward, specific and concise

**DO NOTs**

- use unnecessary idioms. Rather than saying “The work was carried out,” state “the work was performed”
- use contractions, e.g., “don’t” instead of “do not”
- colloquial terms, such as “so” or “exciting science” or “this is fun science”
- use subjective phrases, such as “the analysis was highly sensitive,” instead it is sufficient to say “the analysis was sensitive” or provide a comparison, e.g., “was more sensitive than...”
- use unspecific statements, e.g., instead of saying “the method was great” you may say “the method was highly sensitive with the limits of detection below 1 mg”
- add personal opinions, as all facts should be supported by references

**List of Optional Topics**

- Phthalates introduced to plastic (plastic toys) as plasticizers, regulated by EPA due to the toxicity.
- Caffeine, theobromine, theophylline, active components in tea or coffee
- Fungicides (e.g., tebuconazole, propiconazole) used as preservatives in window frames and wooden products
- Essential oils (e.g., thymol, menthol, eucalyptol, carvone, carvacrol), in peppermint or savory.
- BTEX in gasoline, BTEX concentrations are sometimes used to aid in assessing the relative risk or seriousness of the contamination by gas stations
- Alkanes (C₆-C₁₄) in arson samples
- Polycyclic aromatic hydrocarbons (PAHs), promutagenes found in charred meat products
- Major constituents in liquid bandages

**Grading**

Each paper will be first reviewed by classmates and then graduate students providing their feedback on the 1st and 2nd versions of paper (based on the specified timeline below) each for 5 pt, respectively. The final version will be graded by the instructor (40 pt). The grade will include effort put forward on each version of the paper (1st 5pt, 2nd 5 pt, and 40 pt). Within 40 points in the final version, you will be evaluated for effectiveness of literature search, addressing the three main topics described above, i.e., scientific language, correct formatting of both the text and references.

**Tentative Timeline**

The exact times are posted within the syllabus. The deadlines will be always the evening of the day prior to the class.

- 3rd week of the course, a selection of the topic for 1st assignment
- 4th week of the course, Blackboard submission of the 1st draft of the 1st assignment to your evaluating group
- 4th week of the course, Blackboard submission of the 2nd draft of the 1st assignment to your evaluating group
- 6th week of the course, the final Blackboard submission of the final version of the 1st assignment

**Vocabulary**

Analyte is a compound being analyzed.

Introduction is a section of a typical science oriented article providing the essential background to the problem. The focus of Introduction should be on explaining the reasons why any particular approaches employed earlier for the
analyte determination among other methods are then selected for your work described in experimental and results’ sections.

**Matrix** is a material, which the majority of the sample is made of. The matrix (or interferences from it) may affect the analysis of the sample.

**Peer Reviewed Article:** These are the articles, which are published in a reputable peer reviewed journal, subject to an anonymous review by several experts in fields, who provide critical comments. These experts may suggest rejection of the manuscript if the work quality is questionable (including both science and presentation) or if the topic is not relevant to the theme of the journal. The peer review process ensures a suitable rigor and quality of the works published. Still when reading published papers, one has to think critically whether the reported results or method are accurate and/or make sense.

**Sample:** consists of the matrix and analyte.

**Standard** is a pure chemical being analyzed applied in a defined concentration.

**Scifinder, Scopus:** Chemistry relevant electronic databases of journal articles available on the Chester Fritz library website. Note that these databases cover only a certain scope of journals, which is never comprehensive. Thus searches should always be performed on several search engines.