

ANALYTICAL CHEMISTRY 256

ROLE - PLAYING LAB

1998-1999 Academic Year
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St. Olaf College
Northfield, MN 55057

Introduction to Role-Playing and Laboratory Computing
Defining the Kinds of Role-Playing Responsibilities
Round-Robin Certification of Laboratory Glassware
Production Quality Control Lead Analysis
Statistical/Chemical Evaluation of Lead Data
Semi-Automated Weak Acid Titration
Graphical Analysis of Weak Acid Titration
Designing a Mock Robot Experiment
Executing the Mock Robot Experiment

The Incredible Edible Easter Egg Grass Advertising Dilemma

The Downsizing Dilemma
The Broken Pill Coating Machine Assembly Line Shutdown Dilemma
The Instrument Purchase Payment Release Dilemma
Closure

ROLES:

Manager: Deciding if the Company should market edible grass
Chemist: Blending solutions to test the validity of edibility
Software: Controlling the spectrophotometer and comparing colors
Hardware: Running the robot spectrophotometer with cell handling

OBJECTIVES:

A competitor claims to have an "edible" Easter egg grass for use in Easter baskets. You have a product that is Food and Drug Administration (FDA) approved to be non-toxic, but have never advertised it as actually edible. It appears the competition may have a marketing edge with its claim to edibility. But, you suspect that their claim is not due to a new green grass dye. Rather, you suspect that all they have done is blend FDA approved blue and yellow dyes and re-marketed them under the edible rubric. If so, you can capitalize on their advertising budget by "copy and improve" management. But, you have to be sure that their green dye is the same as a linear blend of your own FDA approved blue and yellow, or else run the risk of liability and infringement suits. Classic **risk management** depending directly on the quality of your chemistry is involved.

MANAGEMENT INTERVIEW:

Upper Management wants to know whether to copy the competition's advertising without the need of hiring a new chemist to synthesize a new green dye and go through the very expensive FDA new product approval cycle. You are to provide the technical basis, with your own ethical overview, for making the decision. The credibility of your staff and the way they interacted to get the technical information is at issue. The quality of your data will be compared against the losses from making a bad management call. How well you reverse engineered the product is interesting.

The New Product

Manager, and her staff, work for a food packaging company. Among other things that they make is a green dye used to color strips of celluloid to go in children's Easter candy baskets as green "grass" for the Easter bunny to nest in. The dye is water soluble and has had extensive development and testing for potential toxicity (children have been known to eat the entire package, candy, wrapping, artificial grass and all). The green Easter Egg Grass has been part of a successful product line involving Easter sundries for the company for the last five years.

While attending a recent technical trade show, **Chemist** noticed another package of chocolate Easter eggs with light green celluloid "grass" arranged around them. The package was made by her company's largest competitor. When asking about the product, the salesman for the competing company went so far as to say that the grass in the package not only was safe, but, should it be ingested, **actually was edible!** **Chemist** was amazed; to claim something was non-toxic was one thing, but to claim (and probably advertise) that it was actually edible was another thing altogether! The salesman's comments and claims were written down and taken home as potentially dangerous news from the field.

The Group Meeting

Chemist brought this news to **Manager** and the company staff at the next group meeting after returning from the trade show. Frankly, the entire staff was a bit concerned. If the competition was able to make a dyed product that actually was edible, and could advertise it that way, then there was no question that they could take an increased share of the already saturated market. Consumer liability suits were huge at that time, and the people who packaged food products for Easter were especially nervous about the loss in image, as well as money, should they lose a suit during the Easter season due to a child's indigestion.

In the past, the company had simply avoided the issue of toxicity and liability at key consumer market times like Easter by telling potential food company customers that all of its packaging materials were certified by the Food and Drug Administration (FDA) as non-toxic if they were accidentally ingested. The company had never said they were actually edible! If this had to be done as a new marketing approach, then it was going to require re-certification by the FDA, and it looked like a whole lot of new chemistry in the R&D phases as well. This could be seriously expensive.

Manager, however, questioned the truth of the competition's claim. Only a few green consumer oriented food dyes had ever been synthesized, as such, that were non-toxic, and of those on the market today, all were simply **blends of two FDA approved yellow and blue dyes**. That is to say, they were not actually new dye compounds, newly synthesized to be better, and newly tested and approved by the FDA for health protection. Instead, they were blends of previously synthesized and approved dyes, with no new properties of consequence, except their color!

Occasionally, some company would add a little of another FDA approved color to their blue or yellow dyes to give the green a different cast, but **no uniquely green dye** had yet been synthesized as a unique molecule and been reported safe to eat by the FDA. **Hardware**, who had run spectra of most FDA dyes for many years, agreed with **Manager**. The competitor's green dye was probably just the same as the company's; that is, it was probably just a blend of FDA approved blue and yellow.

The Chemistry Problem

Manager decided that it was time to determine for sure from the literature what dyes are in current use, and what the toxicity data on them was. **Chemist**, in response to this, argued that this was a huge job, and balked at doing it. **Manager** decided that **Chemist** could seek help from the **Science Librarian** in doing the necessary literature work to determine what food dyes are in use (as opposed to what general dyes are in use). By doing a literature search like this, **Manager** should learn more or less at the same time what toxicity testing had been done. **Chemist** agreed that food dyes are a narrower area, and agreed to at least explore with **Manager** the possibility of a complete literature search on that topic.

Manager decided it was important, for whatever reasons that might come up in the future, to have the actual chemical structures of the FD&C yellow, blue, green, and red dyes from which this might have been blended if in fact it is just a mix of existing dyes and not a totally new chemical substance. **Chemist** was expected to do this. This is all straight library work. **Software** thought it would be neat to take the structures that **Chemist** found and print them out on a Mac using some kind of structure drawing program. **Upper Management** had "Beaker", and agreed to loan it out.

The Software Problem

Manager also had to admit that she was a little confused about color. What actually is a green green? And, is there such a thing as a "pure" green? What would happen, for example, if more or less of a blue or yellow were mixed together to make a green? She balked at doing all of this in the lab. There has to be a better way. Could this be done on a computer in a spreadsheet, or a color paint program?

Manager also was a little suspicious of "spectrophotometric" methods of color determination. Having heard that consumers are prone to making emotional decisions in response to colors, she wondered how well the data that come back from a spectrophotometer actually will represent what happens in the marketplace. Of special concern is whether colors that look nice can in actual fact be broken down into their components on a numerical or quantitative basis.

For example, if some especially nice green can be made by blending a "smidgen" of yellow with a "dash" of blue, can smidgen and dash actually be represented numerically, or is this all just a waste of company time?

The Ethical Part of the Dilemma

Locks are to keep honest people honest. And patents and copyrights are technical locks. **Manager** has a real problem here.

Suppose that all the competition has done is just mix a little FDA yellow with a little FDA blue to get their green. Suppose they have done no toxicity testing at all, and suppose that it is their marketing people who have come up with the edible gimmick. Suppose that they know that to do this kind of toxicity testing would cost a small fortune if done from "ground zero". But, on the other hand, suppose they have not just mixed dyes. Suppose they actually did the synthesis and research needed to make a whole new dye?

If the competition's green is just a mixture, **Manager** knows she can tell marketing to claim edibility too and run the risk of a law suit as part of the "cost of doing business" in releasing a new product. This cost would probably be less than the cost of hiring a team of synthetic chemists to come up with a new dye and a team of analysts to do the FDA approval work. If the competition is doing it, all she would have to do is wait a few months, watch for liability lawsuits against them, and then rush in with just a little marketing on our own to "ride their coattails" into the marketplace. That's if their "edible green" is really nothing new at all, but just a new mix of the old FDA approved dyes.

But, if they actually have done their homework and synthesized a new dye, **Manager** knows that telling marketing to claim equivalency could lead to a devastating patent infringement lawsuit from the competition! This is just what they have been waiting for; it could tie up the lawyers for months and even lead to an injunction against further marketing of the company's own "non-toxic" Easter egg grass.

The plot is even more convoluted though. What if our company could release a product that was itself just a mixture, but a mixture so subtly blended that the competition could not tell themselves if it was a new product or a mixture of the old ones? Would they be likely to sue then? Can dyes be blended so well that this could be pulled off? What should **Manager** do?

The Plan

While it is true that **Manager** has the responsibility for suggesting what plan is to be followed in attacking the problem, the Company staff have come up with some good ideas. Here are some of their better suggestions.

Software suggested that the spectra of the company's own FDA yellow and blue dyes be run, and a set of working curves made at two or more wavelengths. Then, the competitor's green dye could be analyzed spectrophotometrically, and, assuming that it was indeed just a linear mixture of the same FDA approved yellow and blue, the mixture composition could be determined by the solution of "two equations in two unknowns".

Software claimed to be able to do this, on the spot, with the newest release of the statistical package Minitab, or using the Excel spreadsheet in its "equation solver" mode. **Chemist**, a bit skeptical at the start, looked up the technique of "multicomponent spectrophotometry" in Harris and discovered that **Software was probably right**. The instruction manual for Excel gave some easy instructions for solving matrices of equations, too.

Hardware felt though that more than a **Software** approach would be needed. It would be one thing to determine that the competition's green was just a blend of FDA yellow and blue dyes by deconvoluting a sample extract from their grass product. It would be better to do that, get the calculated proportions, and then actually blend such a green from the company's own FDA yellow and blue, run the spectrum of the blend, and show by comparison that there were no differences between the competition's extract, and the company's blend, at least over the visible spectral regions.

Manager thought these ideas were at least a sensible combination. For example, it made sense that a sample of the competition's green grass could be extracted into hot water to get the water soluble dye from it. This extract would be run on the spectrophotometer by **Hardware**, and the results taken directly into the computer. **Software** then could "deconvolute" the spectrum at the optimum wavelengths to determine what concentrations of FDA yellow and blue dyes could be present (on the assumption that it was just a binary mixture of these two).

But, even this conventional approach, while sensible, did have some worrisome aspects. For example, if it were done this way, **Chemist** would have to make the standards to get the equivalents of molar absorptivities at the wavelengths that **Manager** and **Software** decided were optimum for the deconvolution. But, no absolute dye concentrations were at hand! And, these kind of matrix solution deconvolution techniques assume that Beer's law is obeyed. That could be determined by **Chemist** and **Hardware** in the lab doing progressive dilutions of the stock dyes. Then if it was found that Beer's law was obeyed, it was true that **Software** could do the math literally on the spot as soon as the absorbencies were available.

But, there might be a more direct approach. For example, **Hardware** suggested that **Chemist** could easily make a blend of the FDA yellow and blue to match the competition's green. **Hardware** then could run it on the spectrophotometer, taking the results directly into the lab microcomputer used as the control computer in the mock robot project, and **Software** could then devise a way of numerically subtracting the two spectra in a spreadsheet to determine if they showed essentially the same differences in absorbencies at all wavelengths of concern. If so, **Manager** could see that the competition had just made a mix of known safe dyes, and could tell sales that the company's green grass also was "edible", and all would be eligible for a bonus on their checks as more product was sold on the back of your competition's "edible" advertising.

Software also could use the computer and spreadsheet to electronically blend colors to advise **Hardware** about what kinds of mixtures to look at. Conceivably, it could be faster than mixing solutions. **Software** even had the idea of taking the competitor's green and synthesizing it electronically as a combination of pure or not so pure primary colors. **Manager** had to admit that this was pretty creative.

Manager however did wonder if all these "calculations" were needed. It seemed intuitive to her that molar absorptivities and spreadsheets were overkill. She wondered if just mix-and-match spectrophotometry, or something like that, wouldn't reveal enough information to tell if the competition's green was a new molecule or not.

The Experiment

In the one lab afternoon available, there will not be time for an extraction of the competitor's grass, since this involves an overnight reflux. **Upper Management** will do that, and a ten liter batch of the product dye will be available. In addition, there will be ten liters each of the company's FDA approved red, blue and yellow dyes. Unfortunately, the concentrations of these dyes, as well as the competitor's extract, will be unknown. Absolute assays are singularly difficult and tedious, and there are, obviously, no standards for the competition's product. **Manager** will have to deal with (solve?) this apparent problem!

The spectrophotometer to use will be the Spectral Instruments SI400 CCD parallel instrument. **Hardware** will have to run spectra on this instrument. The company may team up as was done in the "mock robot experiment" to run the instrument directly into the computer using the **LabVIEW** program. It will be up to **Manager** to decide.

Chemist will have to prepare dilutions of all the products. This may be done by volume or by weight. The decision will be up to **Manager**; that is, **Manager** will have to make the interpretations needed to tell **Chemist** what dilutions and blends to make.

As the products are diluted and run, **Software** will have to process the data, mostly on the spot. Excel, can be brought out of **Software's** experience to use in the lab.

In this experiment, **Manager's** biggest job is to understand the method, and to work closely with **Software** and **Chemist** to make sure that the calculations and blends are done right. The theory in our book is fine, and in fact has been proven in practice in the Chem. 382/378 course for the nitrate salts of chromium and cobalt. Basically, it will be up to **Manager** to work up the method directions and recipes needed for the afternoon's work.

The Wrap-up Report

Upper Management wants to know if he can instruct sales to start advertising an edible product. Data will be needed to support the conclusion **Manager** arrives at. **Manager** should summarize the instrumental results, and then tell **Upper Management** if the competitor's product either is, or is not, a mix of FDA yellow and blue dyes. **Manager** should also summarize the ethics of the situation, estimate on the basis of technical results the likelihood that the company will lose a suit if one comes up, and advise **Upper Management** on her feelings as to what would be the right thing to do, both ethically and economically. **Upper Management** will be very interested in the way the staff worked together, since the reliability of the data will be one of the factors influencing his "risk management" decision as to whether to release the "edible" product without FDA testing under new product guidelines. Is the competition real?

What is a "Blue Dye" Color Anyway?

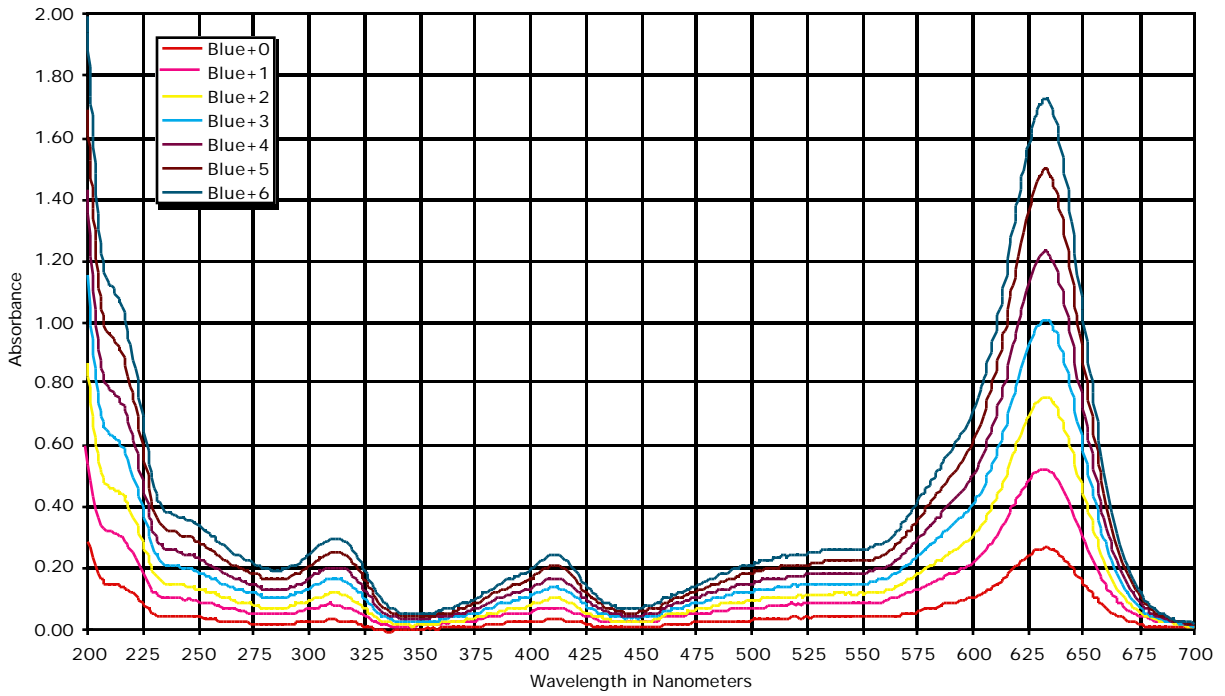
When a solution appears to be colored as you look through it, it is because it has absorbed certain wavelengths of light, and transmitted others. It is the transmitted light that gives it the color. For example, if a solution appears to be red, it is because it has transmitted red light. It will then absorb other colors than red, which usually are at the opposite end of the spectrum (here, blue). Also, if a solution appears to be blue, it is transmitting blue light and absorbing the red region of the spectrum.

Colors Seen and Wavelengths Absorbed in the Visible Spectral Region		
Maximum Absorption Range is:	Absorbed Color is:	Solution Looks to be Colored as:
380-420	Deep Violet	Yellow-Green
420-440	Blue-Violet	Yellow
440-470	Blue	Orange
470-500	Blue-Green	Light Red
500-520	Green	Deep Red
520-550	Yellow-Green	Violet
550-580	Yellow	Blue-Violet
580-620	Orange	Blue
620-680	Light Red	Blue-Green
680-780	Deep Red	Green

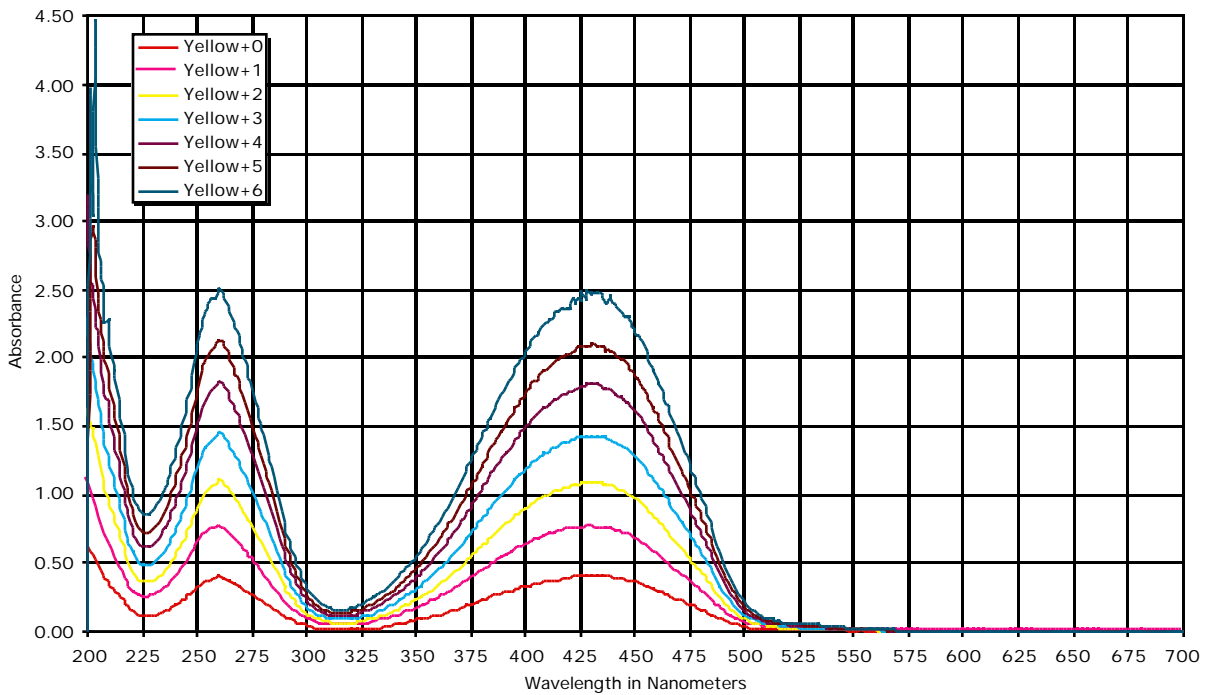
Colors of yellow and green light appear in the middle regions of the spectrum. Thus solutions that are yellow or green absorb the red and the blue regions of the spectrum (or what we call purple). Example spectra of a blue and a yellow FD&C dye follow to help illustrate this.

Following those spectra are the structures of the FD&C Dyes that are FDA approved, and must be considered to be the only choices from which the competition has to blend their so-called edible dye. The label "FD&C" represents approval for use in **F**ood, **D**rugs, and **C**osmetics.

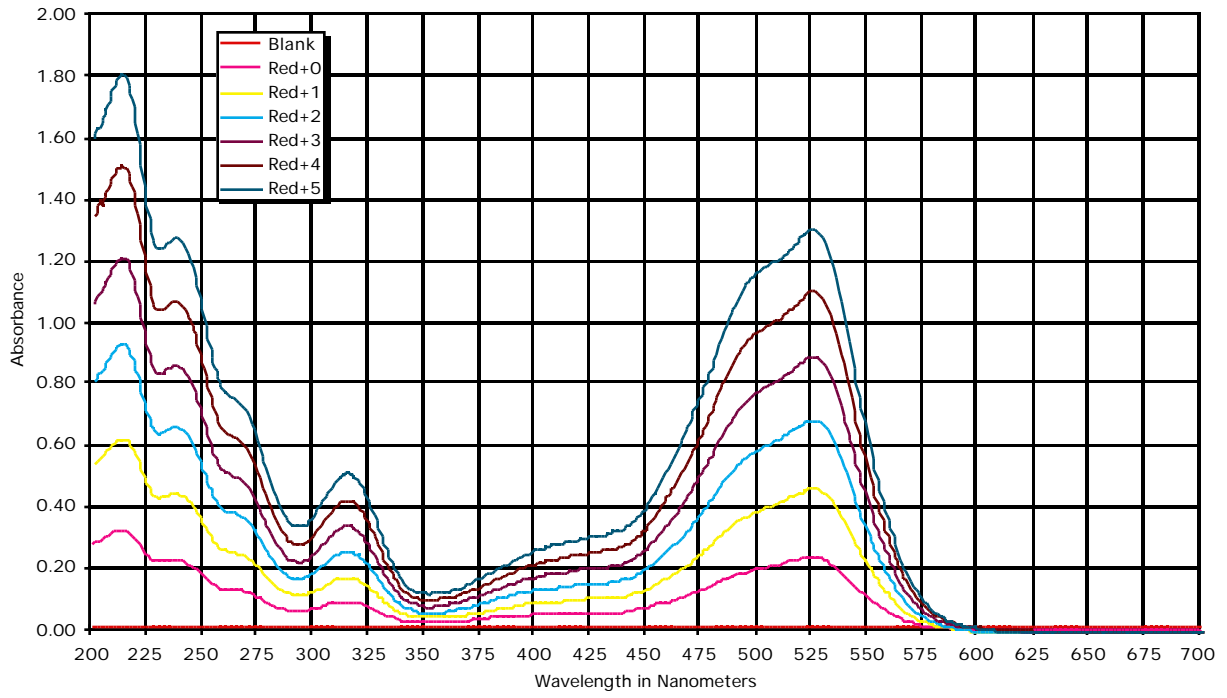
Adding Blue Dye to Water Dropwise
JPW - 9/20/96 - 14:20



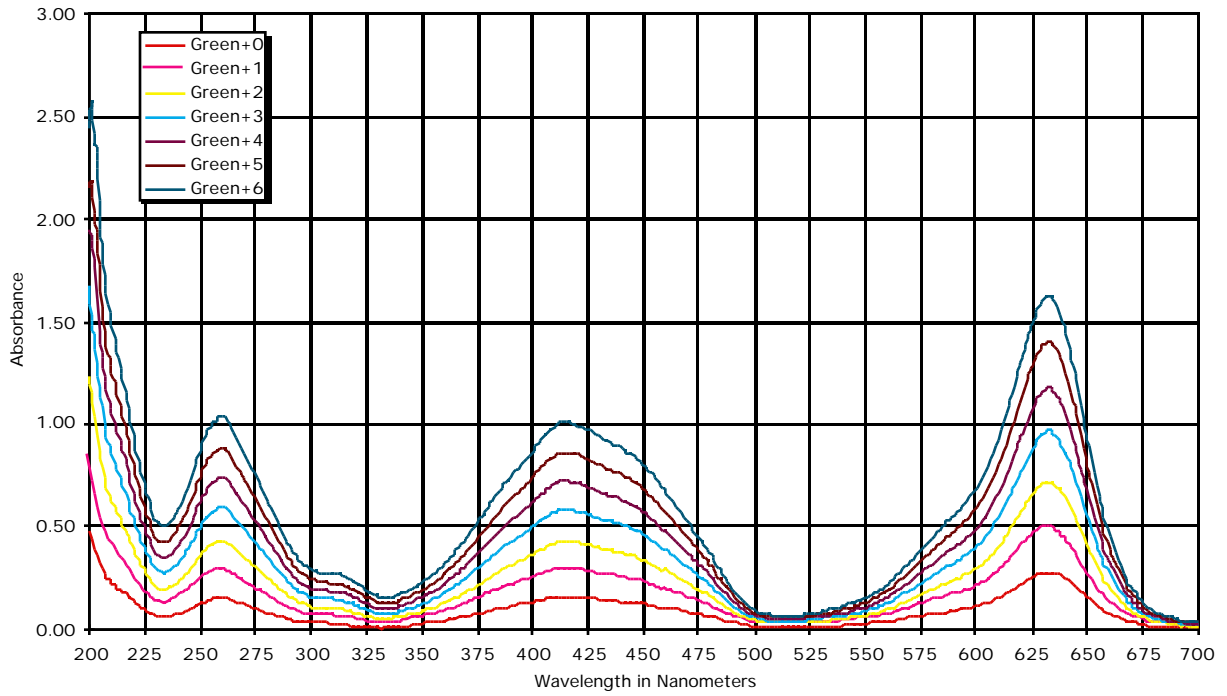
Adding Yellow Dye to Water Dropwise
JPW - 9/20/96 - 13:44



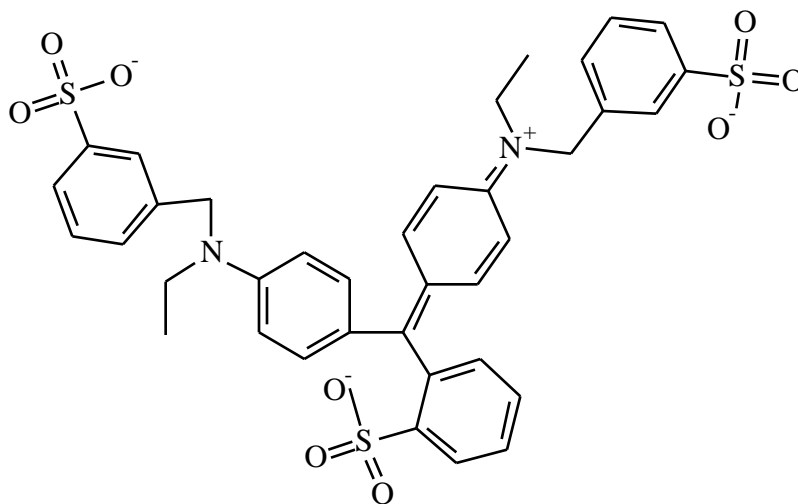
Adding Red Dye to Water Dropwise
JPW - 9/20/96 - 13:10



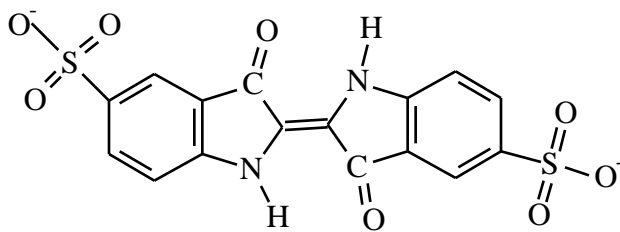
Adding Green Dye to Water Dropwise
JPW - 9/20/96 - 13:24



Brilliant Blue FCF: **FD&C Blue #1**
Triphenylmethane dye - MW = 792.85
max = 630 nm



Indigo carmine:FD&C Blue #2
Sulfonated Indigo Dye
MW = 466.37
max = ?

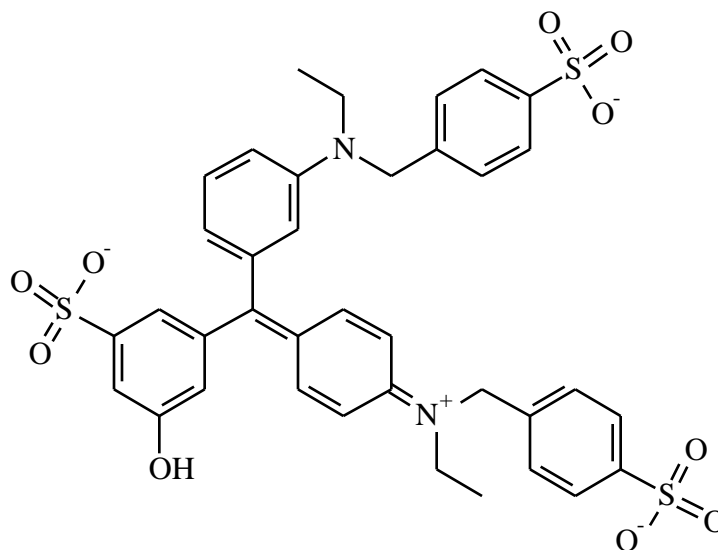


Fast Green FCF: FD&C Green #3

Triphenylmethane Dye

MW = 808.85

max = 628 nm

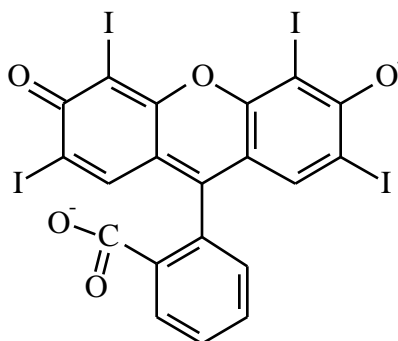


Erythrosine: FD&C Red #3

Fluorescein Type Dye

MW = 879.92

max = 524 nm

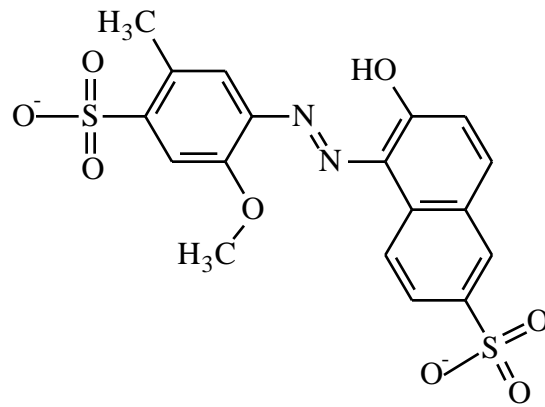


Allura Red AC: **FD&C Red #40**

Azo Dye

MW = 496.42

max = ?

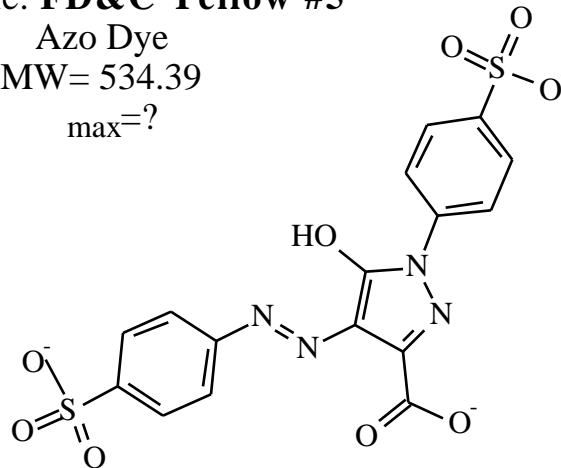


Tartrazine: **FD&C Yellow #5**

Azo Dye

MW = 534.39

max = ?

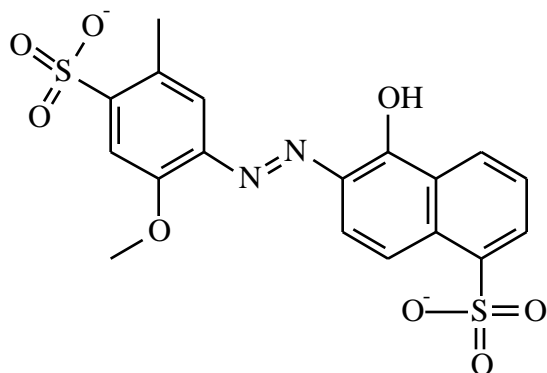


Sunset Yellow FCF: **FD&C Yellow #6**

Azo Dye

MW = 452.37

max = 480 nm



The structures for these dyes were originally collected for Chemistry 256 lab by Paul T. Jackson, spring semester, 1991 from the following sources:

CRC Handbook of Food Additives, 2nd ed.; Furia, T.E., Ed.; Volume 1; CRC Press: Boca Raton, FL, 1972.

The Merck Index, 11th ed.; Budavari, Susan, Ed.; Merck & Company: Rahway, NJ, 1989.

They were transferred to the form shown here by John Walters using the program **Chemintosh**[®] (SoftShell, Int., Grand Junction, CO., Ver. 3.3.1) during the Spring semester, 1994.