Chapter 1

Tools and Techniques

Writing Text & Paragraphs

Stereotyped Format

Here, that's a good thing!

- Title
- Abstract
- Introduction
- Materials & Methods
- Results
- Discussion
- Conclusion
- References

5. Be thoughtful.
6. Last item.

-- As you progress.

1. Start here!
2. What done? How?
3. Explain, examine.
4. Think hard!

-- As you progress.

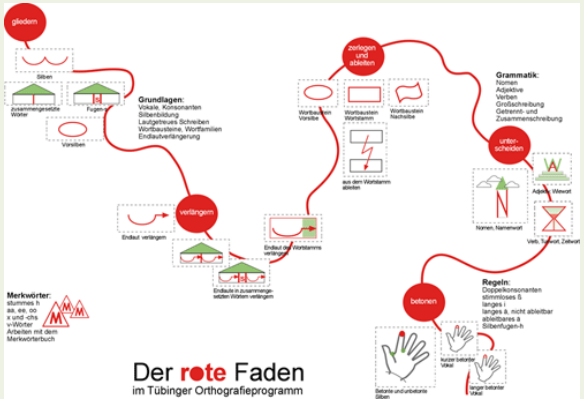
Der Rote Faden

What is this about?

The recurrent theme…

The central theme…

…should be evident in EVERY part of the paper.



Desiderata

Descriptions must be precise.

Try to be objective.

Procedures must be complete.

Data must be exact (or error bars given).

Logic must be transparent.

Conclusions must be clear & concise ("clean").

Do not leave anything to the reader's imagination.

I try to leave out the parts that people skip. Elmore Leonard

Straightforward Message


It may therefore not be unexpected…


These results suggest…


The catalyst probably acts to increase…


The catalyst probably increases…

- Make your statements explicit. Contrast clearly.


In contrast to the hypothesis by X, we conclude…

Avoid Vagueness

- Avoid relative terms such as: a lot, somewhat,…
- Use “very” very rarely.
- Avoid emotional judgments such as: beautiful, disappointing, miraculously,… (BUT some of these terms are fine as rhetorical devices, i.e., certainly, of course, remarkable, obviously,…)
- Avoid “filler words” such as: indeed, in fact, in a sense… (BUT some of these terms are fine as rhetorical devices,
- Avoid casual language such as: bottom line, seat of the pants, cutting edge, …

Write with Precision: Numbers

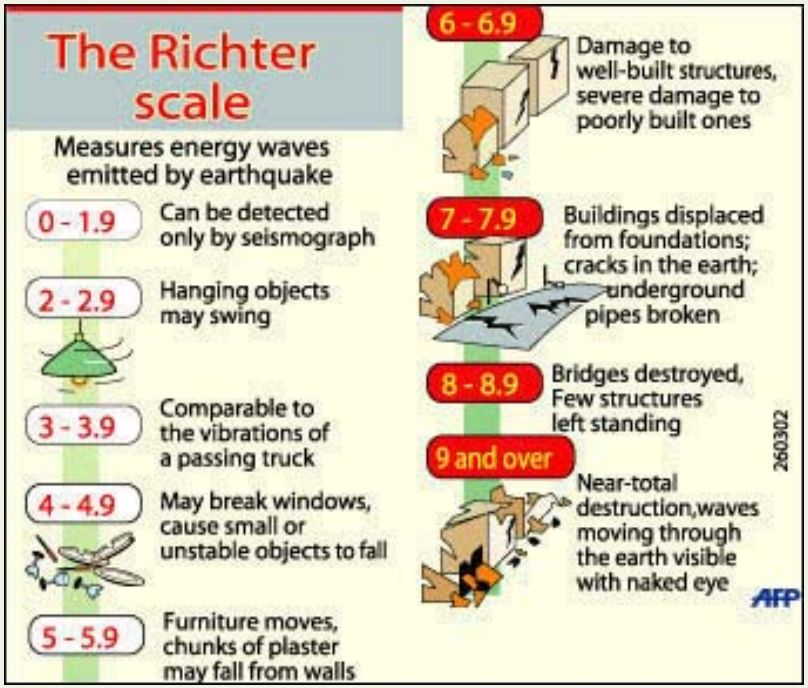
- Use numbers!
  - Not “tall”, but “greater than 2 meters”
  - Not “heavy”, but “greater than 10 kg”
  - Not “brief”, but “less than 1 millisecond”

- Use criteria-based scales.
  - Grade Scale, performance.
  - Richter Scale, earthquakes.
  - Mankoski Scale, pain.

Numbers II: Richter Scale

The Richter magnitude of an earthquake is determined from the logarithm of the amplitude of waves recorded by seismographs.

A measured number with defined consequences.



Numbers III: Mankoski Pain Scale

Andrea Mankoski Pain Scale (1995)
Numbers characterize well-defined and distinguishable consequence of subjective property.

0 - Pain Free
1 - Very minor annoyance - occasional minor twinges. No medication needed.
2 - Minor Annoyance - occasional strong twinges. No medication needed.
3 - Annoying enough to be distracting. Mild painkillers take care of it. (Aspirin, Ibuprofen.)
4 - Can be ignored if you are really involved in your work, but still distracting. Mild painkillers remove pain for 3-4 hours.
5 - Can't be ignored for more than 30 minutes. Mild painkillers ameliorate pain for 3-4 hours.
6 - Can't be ignored for any length of time, but you can still go to work and participate in social activities. Stronger painkillers (Codeine, narcotics) reduce pain for 3-4 hours.
7 - Makes it difficult to concentrate, interferes with sleep. You can still function with effort. Stronger painkillers are only partially effective.
8 - Physical activity severely limited. You can read and converse with effort. Nausea and dizziness set in as factors of pain.
9 - Unable to speak. Crying out or moaning uncontrollably - near delirium.
10 - Unconscious. Pain makes you pass out.

Numbers IV: Wong-Baker Scale

Wong-Baker Faces Pain Rating Scale (1995)

Numbers characterize well-defined and distinguishable consequence of subjective property.

Face 0 is very happy because he or she doesn't hurt at all.
Face 1 hurts just a little bit.
Face 2 hurts a little more.
Face 3 hurts even more.
Face 4 hurts a whole lot.
Face 5 hurts as much as you can imagine, although you don't have to be crying to feel this bad.

Write with Precision: Names I

Use Correct Names

Trivial name. Example: aspirin

Systematic name. Example: acetylsalicylic acid

Be aware of synonyms. Examples: Rhodine (7CI); Salicylic acid acetate (8CI); 2-(Acetyloxy)benzoic acid; 2-Acetoxybenzoic acid; 2-Carboxyphenyl acetate; A.S.A. Empirin; AC 5230; ASA; Acenterine; Acesal; Acesan; Acetard; Aceticyl; Acetilum acidulatum; Acetisal; Acetol; Acetonyl; Acetophen; Acetosal; Acetosalic acid; Acetosalin; Acetylin; Acetylsal; Acetylsalicylic acid; Acetyonyl; Acetysal; Acidum acetylsalicylicum; Acimetten; Acisal; Acylpyrin; Adiro; Albyl E; Asaflow; Asagran; Asatard; Ascoden 30; Ascolong; Ascriptin; Aspalon; Aspergum; Aspirdrops; Aspirin; Aspirin Protect 100; Aspirin Protect 300; Aspirin-Direkt; Aspirina 03; Aspro; Aspro Clear; Aspropharm; Asteric; Astrix; Bayer; Benaspir; Bialpirina; Bialpirinia; Caprin; Cardioaspirin; Cardioaspirina; Claradin; Colfarit; Colsprin; Contrheuma Retard; Coricidin; Coricidin D; Crystar; Darvon Compound; Dolean pH 8; Dominal; Doril; Duramax; ECM; Easprin; Ecosprin; Ecotrin; Empirin; Endosprin; Endydol; Entericin; Enterophen; Enterosarine; Entrophen; Ewin; Extren; Gelprin; Globentyl; Globoid; Helicon; Idragin; Istopirin; Kapsazal; Lysoprin (pharmaceutical); Magnecyl; Measurin; Medisyl; Melhoral; Micristin; Miniasal; Mycropyrin; NSC 27223; NSC 406186; Neuronika; Novid; Nu-seals; O-Acetylsalicylic acid; Persistin; Polopiryna; Rheumintabletten; Rhodine 2312; Rhodine NC RP; Rhonal; SP 189; Salacetin; Salcetogen; Saletin; Salospir; Salycylacetylsalicylic acid; Solpyron; Supac; Temperal; Toldex; Triple-sal; Trombyl; Xaxa; Yasta; Zorprin; o-(Acetyloxy)benzoic acid; o-Acetoxybenzoic acid; o-Carboxyphenyl acetate

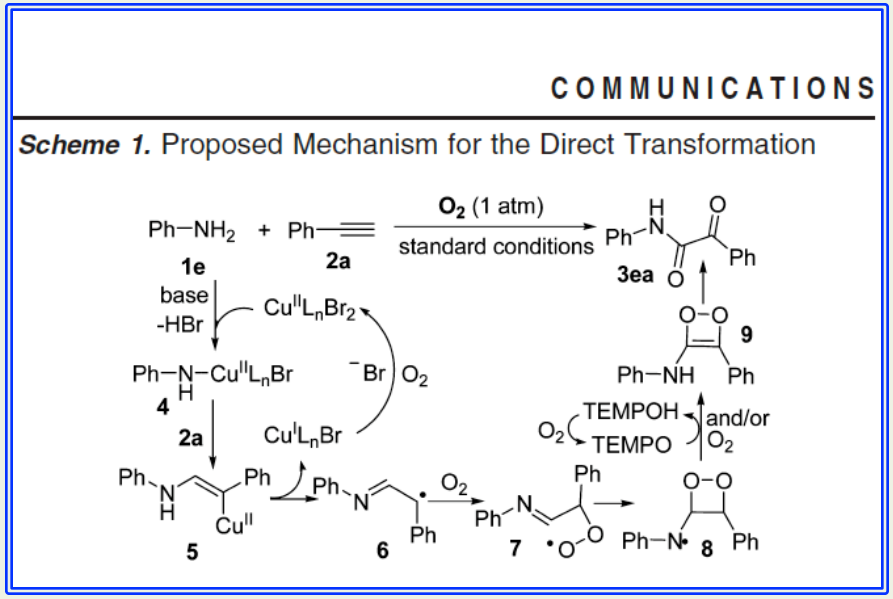
Names II: Abbreviate / Number

Names of chemicals often are long! Often not well-defined either.

Abbreviations, common. Example: DMSO, aspirin.

Abbreviations, defined by you.

Numbers, defined by you.



Dioxygen Activation under Ambient Conditions: Cu-Catalyzed Oxidative Amidation–Diketonization of Terminal Alkynes Leading to α-Ketoamides. Chun Zhang and Ning Jiao *J. Am. Chem. Soc.* **2010**, *132*, 28-29.

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Recommendations on Organic & Biochemical Nomenclature, Symbols & Terminology etc.

If the table below is unusable check this button for an alternative presentation

http://www.chem.qmul.ac.uk/iupac/
World Wide Web material prepared by G. P. Moss
Department of Chemistry, Queen Mary University of London,
Mile End Road, London, E1 4NS, UK
g.p.moss@qmul.ac.uk

To search the database click here.

What's Here and What's New | Changes to Published Documents for World Wide Web Presentation | Main IUPAC Home Page

Full text of IUPAC Recommendations

Glossary of Organic Class Names	Glossary of Terms in Physical Organic Chemistry	Basic Terminology of Stereochemistry
Hantzsch-Widman Nomenclature for Heteromonocyclic Rings	Non-standard Valence States (Lambda Convention)	Cyclic compounds with contiguous formal double bonds (delta Convention)
Fused Ring Nomenclature	Phane Nomenclature	Phane Nomenclature Part II
Glossary of Terms in Bioinorganic Chemistry	Glossary of Medicinal Chemistry Terms	Nomenclature of Isotopically Modified Compounds (Section H)
IUPAC Atomic Weights and Periodic Table (2007 values) New Values	Von Baeyer nomenclature	Spiro nomenclature
Natural product nomenclature (Section F)	Radicals, Ions & Radical Ion Nomenclature	Gold Book IUPAC definitions of terms.
Fullerene nomenclature	Numbering of Fullerenes	Numerical Terms to 9999
Regular single-strand organic polymers nomenclature	Watch this space.	

Past and Present Tense

Use PRESENT TENSE for statements which are true now (and have been true in the past as well):

- Life is good.
- Clouds contain water.
- Everything is made out of atoms.

Use PAST TENSE to describe events that have occurred in the past and are no longer happening:

- The experiment was performed.
- The catalyst was added.

How to Write Text
Examples & Assignment

Lecture Example: Aspirin

Textbook Example: Section 2.2

SP10 Assign. #1 on Aspirin: Handout & online.

SP11 Assign. #1 on Dyes & Indicators: Handout & online.

How to Write Text I: Rough Paragraphs

1. Skeletal Outline
2. Pile in Ideas
3. Collect Information from Outside Resources
4. Form Rough Sentences
5. Arrange Sentences into Themes (Temp. Theme Label)
6. Turn Lists into Rough Paragraphs

Rough §s 1. Skeletal Outline

Working Title: Aspirin Analogs in Medicine

(Heading 1) Introduction
- (Heading 2) A. General History of Painkillers
- (Heading 2) B. General History of Aspirin (we'll work on this!)
- (Heading 2) C. General History of Aspirin Analogs

(Heading 1) Materials & Methods
(Heading 1) Results
(Heading 1) Discussion
(Heading 1) Conclusion
(Heading 1) References

Rough §s 2. Pile in Initial Ideas

Working Title: Aspirin Analogs in Medicine

(Heading 1) Introduction

(Heading 2) A. General History of Painkillers

(Heading 2) B. General History of Aspirin

White Tablets
Made by Bayer
Pain Reliever, Painkiller
Antipyretic (lowers fever)
COX Inhibitor

Write a list of "initial keywords".

"Initial ideas" provide keywords for your search for information.

1. Brainstorm and list "initial keywords"

Rough §s 3. Get Information

Ref. A. *Aspirin and Other Non-Steroidal Anti-Inflammatory Drugs as Cyclooxygenase State of the Art, Barriers and Perspectives.* Avram, S.; Duda-Seiman, D. M.; Svab, I.; Mancas, S.; Duda-Seiman, C.; Mihailescu, D. F. *Current Computer-Aided Drug Design* **2009**, *5*, 1-12.

Ref. B. *Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin.* Tosco, P.; Lazzarato, L. *ChemMedChem* **2009**, *4*, 939-945.

Ref. C. *Aspirin. An ab Initio Quantum-Mechanical Study of Conformational Preferences and of Neighboring Group Interactions*. Glaser, R. *J. Org. Chem.* **2001,** *66,* 771-779.

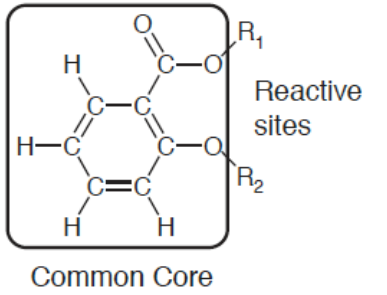
Ref. D. *Synthesis of aspirin : a general chemistry experiment.* Olmsted, John, III *J. Chem. Educ.* **1998**, *75*, 1261-1263.

2. Search using "initial keywords"
(We will learn later about "searching".)

Rough §s 3. Study Information

Ref. D. *Synthesis of aspirin : a general chemistry experiment.* Olmsted, John, III *J. Chem. Educ.* **1998**, *75*, 1261-1263.

-- synthesis of aspirin from "oil of wintergreen"
-- two-step reaction, hydrolysis and condensation
-- "oil of wintergreen" is the methyl ester of 2-hydroxybenzoic acid
-- salicylic acid is a synonym of 2-hydroxybenzoic acid
-- acetylation of salicylic acid with acetic acid anhydride



Compound	R_1	R_2
Oil of Wintergreen	CH_3	H
Salicylic Acid	H	H
Aspirin	H	$C(=O)-CH_3$

Figure 1. The structural core common to oil of wintergreen, salicylic acid, and aspirin.

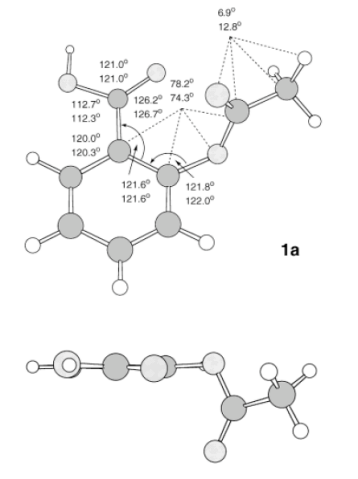
3. Survey & Study!
Make lists.
Look for key ideas.
Look for leading themes.
Make rough schemes.
Learn the vocabulary!

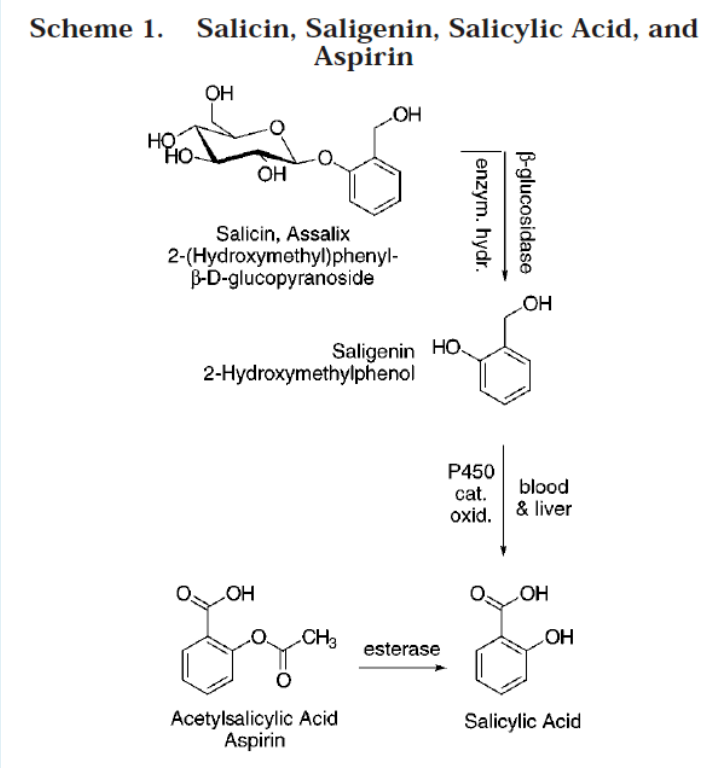
Rough §s 3. Study Information

Ref. C. *Aspirin. An ab Initio Quantum-Mechanical Study of Conformational Preferences and of Neighboring Group Interactions*. Glaser, R. *J. Org. Chem.* **2001,** *66,* 771-779.

-- acetylsalicylic acid is a pro-drug
-- converted into salicylic acid
-- aspirin X-ray structure determined
-- aspirin conformations studied

3. Survey & Study!
Make lists.
Look for key ideas.
Look for leading themes.
Make rough schemes.
Learn the vocabulary!





Rough §s 3. Study Information

Ref. B. *Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin.* Tosco, P.; Lazzarato, L. *ChemMedChem* **2009**, *4*, 939-945.

-- aspirin is an NSAID, non-steroidal anti-inflammatory drug
-- cyclooxygenase (COX) inhibitor
-- aspirin inhibits COX-1 and COX-2
-- acylation of Ser530
-- aspirin covalently modifies COX

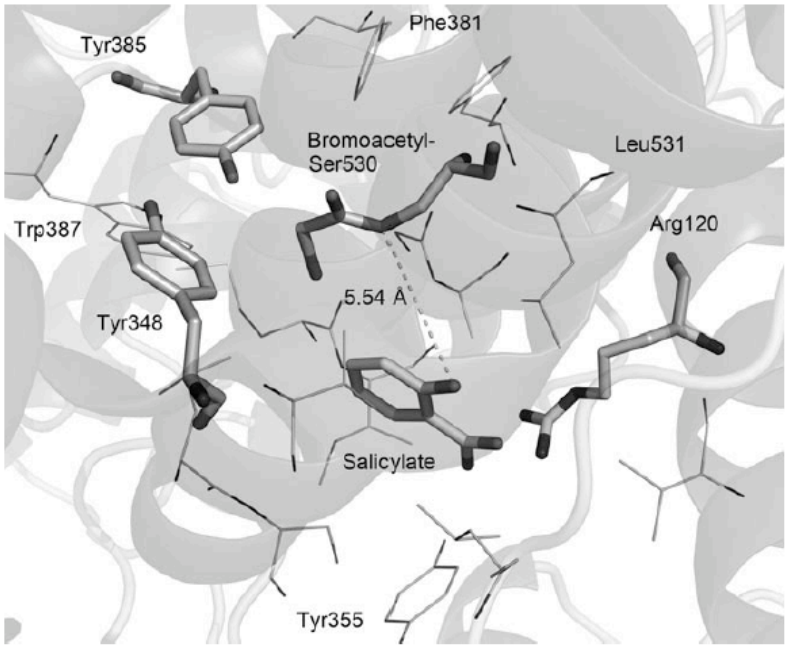


Figure 1. The crystal structure of the COX-2 active site after inactivation by bromoacetylsalicylic acid as obtained by Loll and co-workers.[6] All hydrogens were missing in the original coordinate file. The distance between the phenolic group of salicylate and the Ser 530 oxygen atom is represented as a dotted line.

Rough §s 4. Rough Sentences

4. Collect & Gather.

Ref. B.

-- Aspirin is a non-steroidal anti-inflammatory drug (NSAID).
-- Aspirin inhibits both isoforms of cyclooxygenase.
-- Bromoacetylsalicyclic acid covalently modifies COX-1 and COX-2 by acylation of Ser530.

Ref. C.

-- Acetylsalicylic functions as a pro-drug for salicylic acid.
-- The structure of aspirin has been studied with experimental and theoretical methods.

Ref. D

-- Aspirin is made by acetylation of salicylic acid (2-hydroxybenzoic acid).

Rough §s 5. Create TTL

5. Create TTL = Temporary Theme Label
Think of TTLs as the true keywords!

Ref. B.

Are there steroidal anti-inflammatory drugs?

-- Aspirin is a non-steroidal anti-inflammatory drug (NSAID).
-- Aspirin inhibits both isoforms of cyclooxygenase.
-- Bromoacetylsalicyclic acid covalently modifies COX-1 and COX-2 by acylation of Ser530. *(Transesterification!)*

Ref. C.

What does COX have to do with pain?

-- Acetylsalicylic functions as a pro-drug for salicylic acid.
-- The structure of aspirin has been studied with experimental and theoretical methods.

Ref. D

Why acetylation?

-- Aspirin is made by acetylation of salicylic acid (2-hydroxybenzoic acid).

Rough §s 6. Rough Paragraphs

6. Source-to-Reference Inversion!

-- Aspirin is a non-steroidal anti-inflammatory drug (NSAID) [*Ref. B*]
-- Aspirin inhibits both isoforms of cyclooxygenase. [*Ref. B*]
-- Bromoacetylsalicyclic acid covalently modifies COX-1 and COX-2 by acylation of Ser530. [*Ref. B*]

-- Acetylsalicylic functions as a pro-drug for salicylic acid. [*Ref. C*]
-- The structure of aspirin has been studied with experimental and theoretical methods. [*Ref. C*]

-- Aspirin is made by acetylation of salicylic acid (2-hydroxybenzoic acid). [*Ref. D*]

7. Construct the logical flow and rearrange rough sentences accordingly.

How to Write Text II: Working Draft

- Deconstruct, clean up, reassemble sentences.
- Reexamine the sequential ordering.
- Reassemble paragraphs.
- Smooth transitions.
- Polish.
- Revise. Revise. Revise.

Source-to-Reference Inversion

in three easy steps using Word

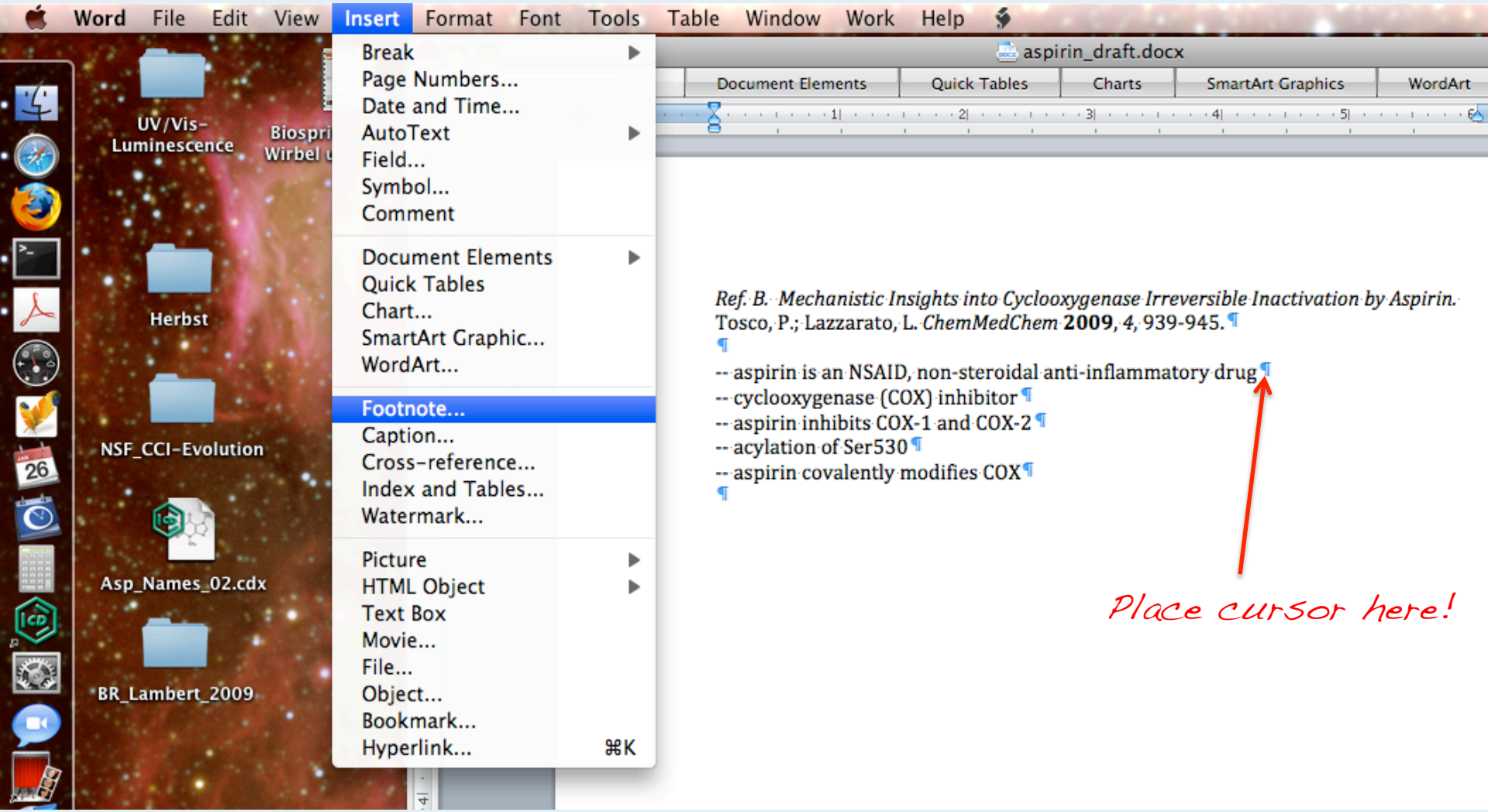
Initially: Type the source in the body of your file

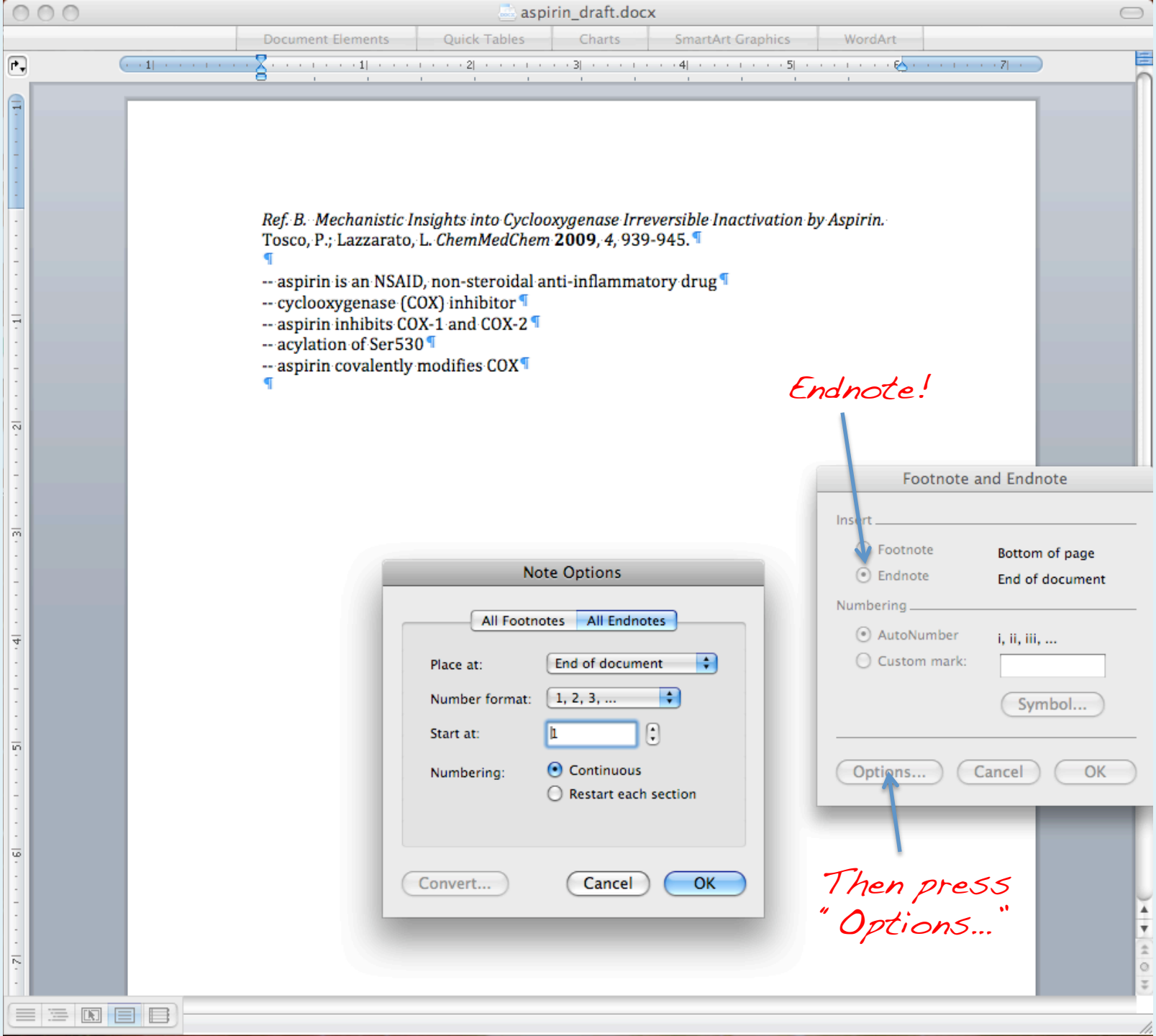
Ref. B. *Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin.* Tosco, P.; Lazzarato, L. *ChemMedChem* **2009**, *4*, 939-945.

-- aspirin is an NSAID, non-steroidal anti-inflammatory drug
-- cyclooxygenase (COX) inhibitor
-- aspirin inhibits COX-1 and COX-2
-- acylation of Ser530
-- aspirin covalently modifies COX

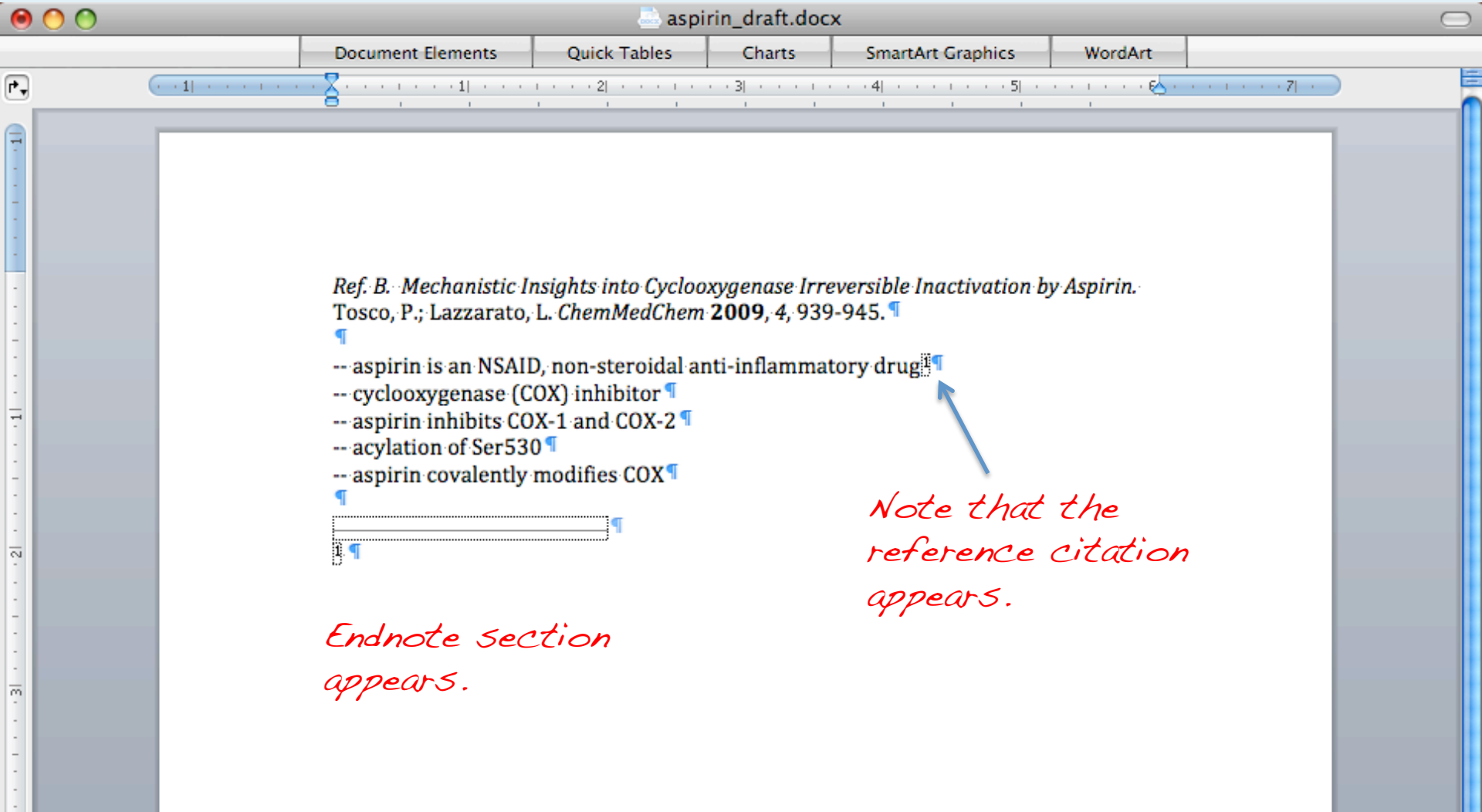
SRI-1: Create an ENDNOTE at the END OF DOCUMENT
SRI-2: Copy the SOURCE to the ENDNOTE (format now or later)
SRI-3: Insert CROSS-REFERENCE CITATIONS MARKS (as needed)

SRI-1: Create Endnote

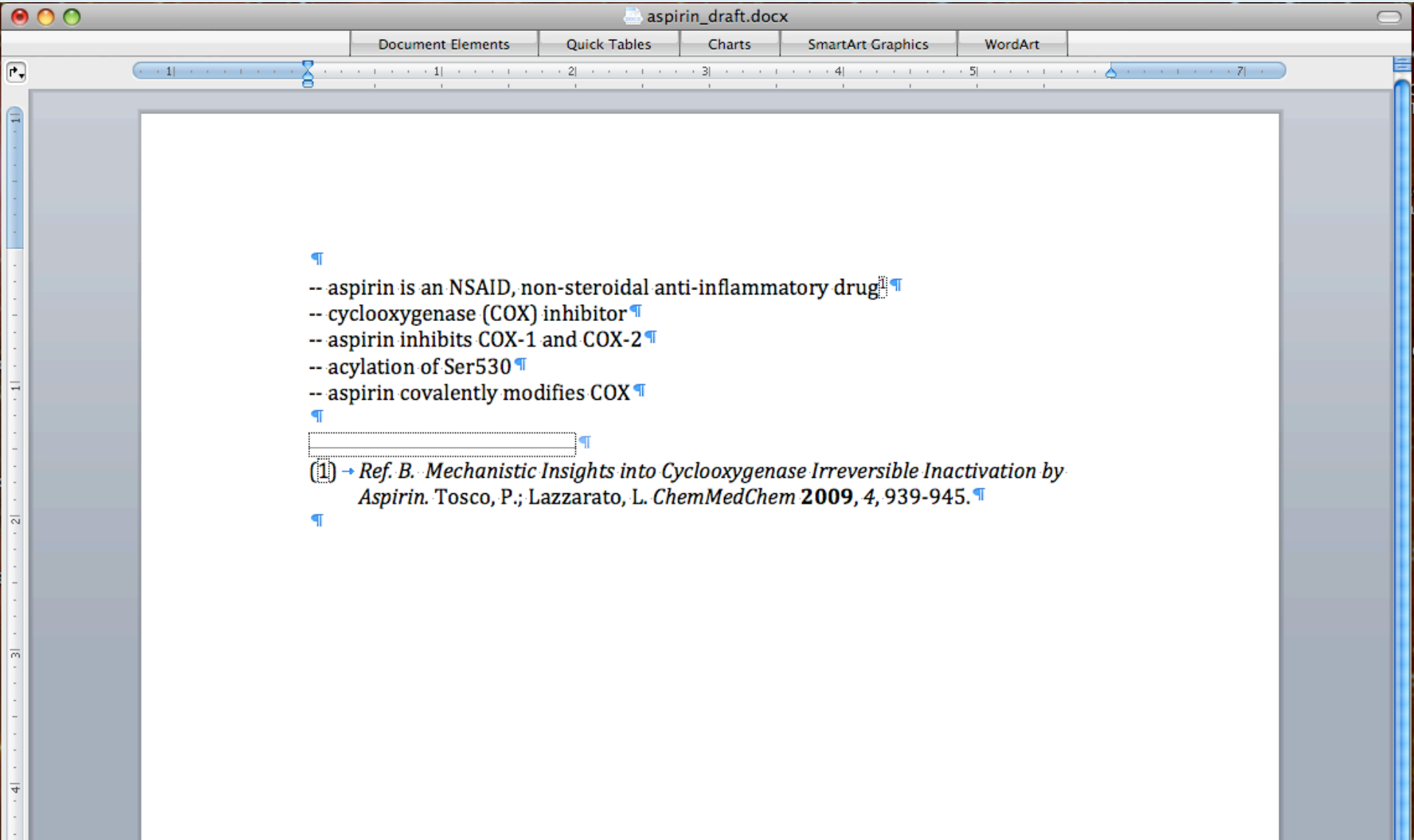



aspirin_draft.docx
Document Elements
Quick Tables
Charts
SmartArt Graphics
WordArt
Ref. B. Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin.
Tosco, P.; Lazzarato, L. ChemMedChem 2009, 4, 939-945.
-- aspirin is an NSAID, non-steroidal anti-inflammatory drug
-- cyclooxygenase (COX) inhibitor
-- aspirin inhibits COX-1 and COX-2
-- acylation of Ser530
-- aspirin covalently modifies COX
Endnote!
Footnote and Endnote
Insert
Footnote
Bottom of page
Endnote
End of document
Numbering
AutoNumber
i, ii, iii, ...
Custom mark:
Symbol...
Options...
Cancel
OK
Note Options
All Footnotes
All Endnotes
Place at:
End of document
Number format:
1, 2, 3, ...
Start at:
1
Numbering:
Continuous
Restart each section
Convert...
Cancel
OK
Then press "Options..."

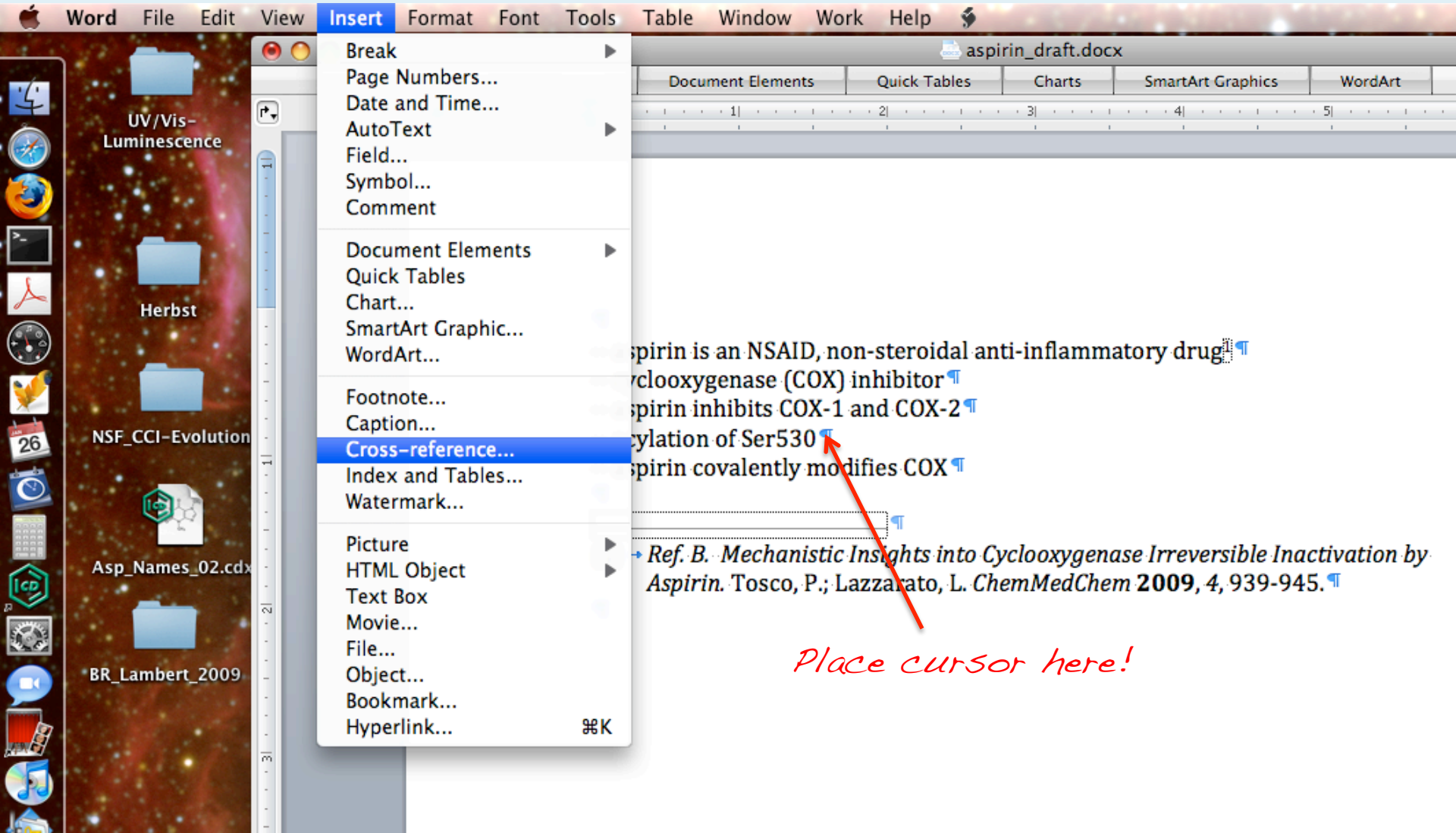
SRI-1: Endnote Mark Inserted



SRI-2: Move Source to Endnote

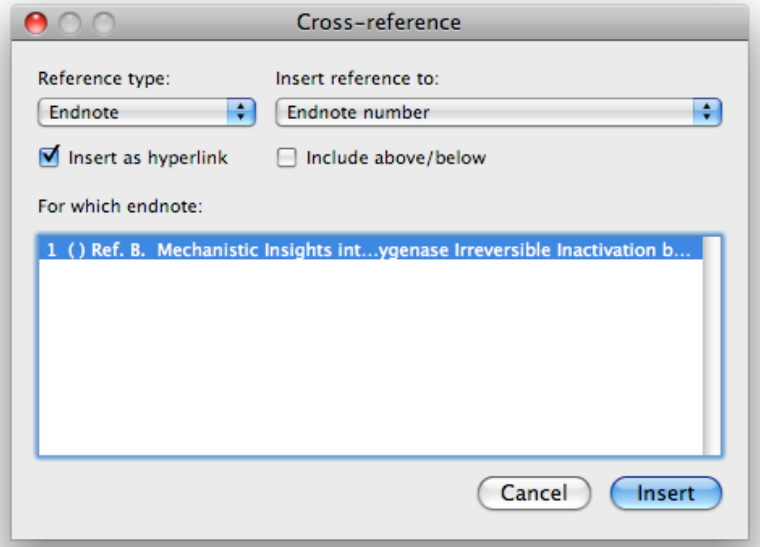


SRI-3: Insert Cross-Reference Mark

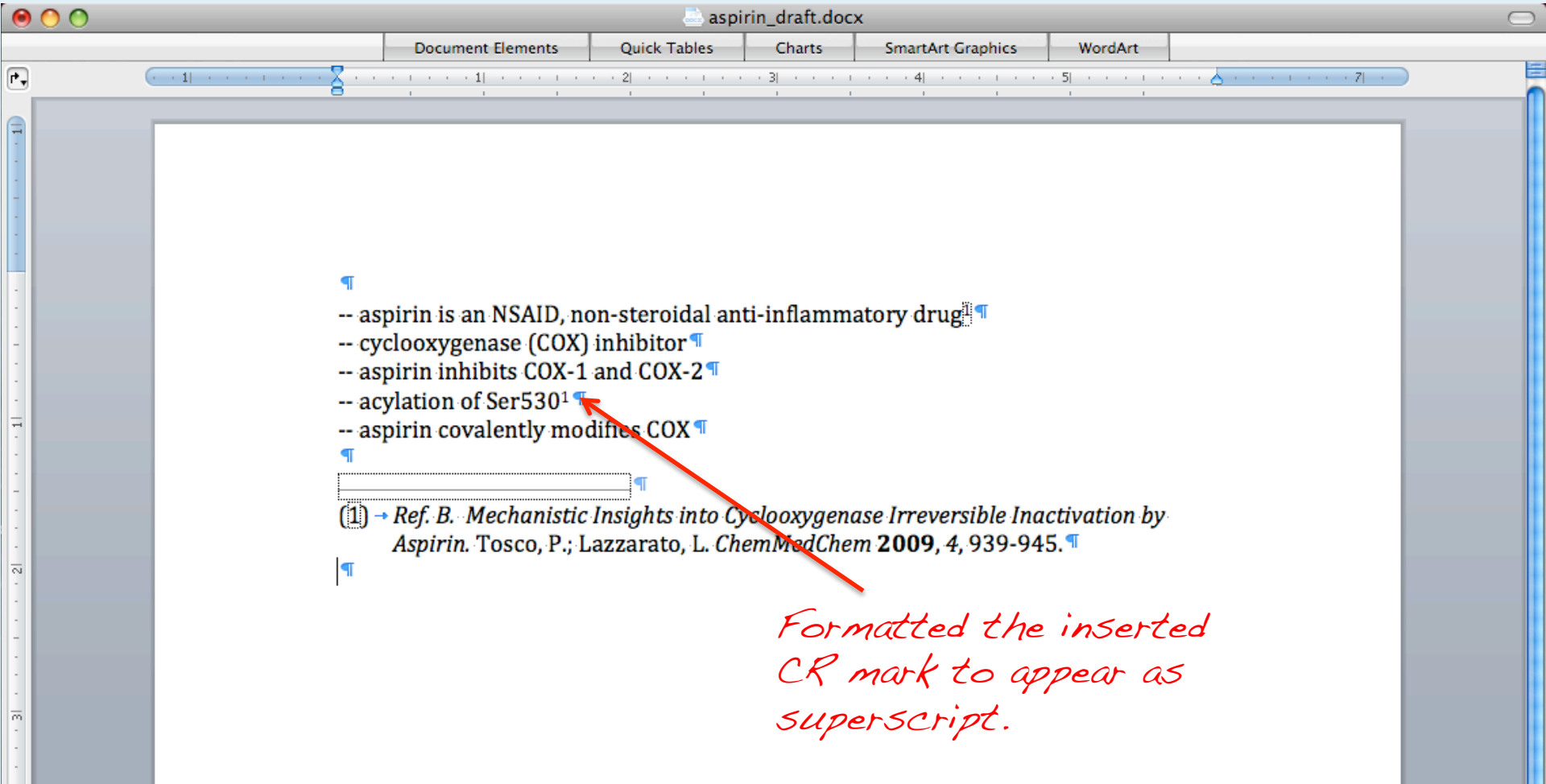


-- aspirin is an NSAID, non-steroidal anti-inflammatory drug[1]
-- cyclooxygenase (COX) inhibitor
-- aspirin inhibits COX-1 and COX-2
-- acylation of Ser530
-- aspirin covalently modifies COX

(1) *Ref. B. Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin.* Tosco, P.; Lazzarato, L. *ChemMedChem* **2009**, *4*, 939-945.



SRI-3: Insert Cross-Reference Mark



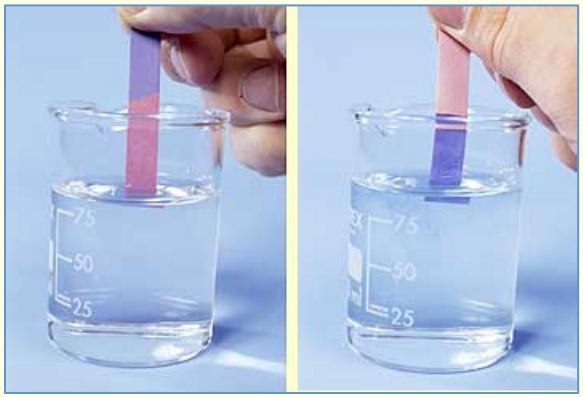
SP11: Colorimetric Chemical Indicators

Colorimetric Titration
A titration in which the end point is marked by a color change. The end point usually is characterized by a huge change of a concentration (several magnitudes).

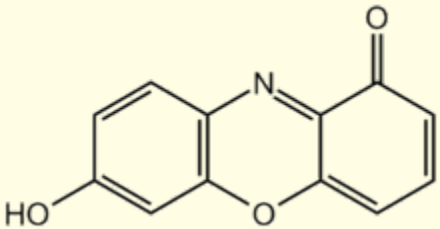
Chemical Indicator (Yes, No)
In chemical analysis, a substance that changes color within a certain definite range of pH, oxidation potential, complex concentration, or in any way renders visible the completion of a chemical reaction.

Chemical Sensor (Yes, No. If yes, how much?)
A chemical system designed to respond to chemical stimuli such as proton concentration, concentration of molecules with a specific functional groups, or concentration of a specific molecule, and to respond in a way that is proportional to the concentration of the chemical stimulus.

pH Indicator



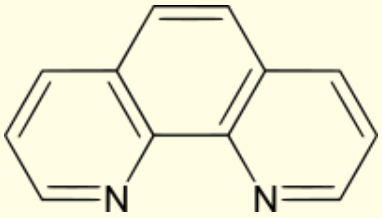
Litmus



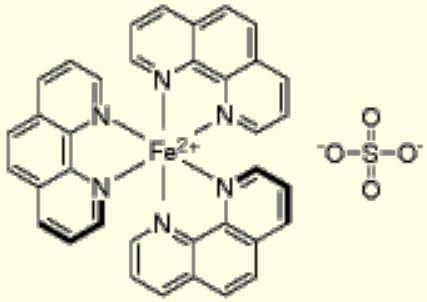
Indicator	Low pH color	Transition pH range	High pH color
Gentian violet (Methyl violet 10B)	yellow	0.0–2.0	blue-violet
Leucomalachite green (first transition)	yellow	0.0–2.0	green
Leucomalachite green (second transition)	green	11.6–14	colorless
Thymol blue (first transition)	red	1.2–2.8	yellow
Thymol blue (second transition)	yellow	8.0–9.6	blue
Methyl yellow	red	2.9–4.0	yellow
Bromophenol blue	yellow	3.0–4.6	purple
Congo red	blue-violet	3.0–5.0	red
Methyl orange	red	3.1–4.4	orange
Bromocresol green	yellow	3.8–5.4	blue
Methyl red	red	4.4–6.2	yellow
Methyl red	red	4.5–5.2	green
Azolitmin	red	4.5–8.3	blue
Bromocresol purple	yellow	5.2–6.8	purple
Bromothymol blue	yellow	6.0–7.6	blue
Phenol red	yellow	6.8–8.4	red
Neutral red	red	6.8–8.0	yellow
Naphtholphthalein	colorless to reddish	7.3–8.7	greenish to blue
Cresol Red	yellow	7.2–8.8	reddish-purple
Phenolphthalein	colorless	8.3–10.0	fuchsia
Thymolphthalein	colorless	9.3–10.5	blue
Alizarine Yellow R	yellow	10.2–12.0	red
Litmus	red	4.5-8.3	blue

Redox Indicator

Ferroin, red, Fe(+II)
Ferrin, blue, Fe(+III)



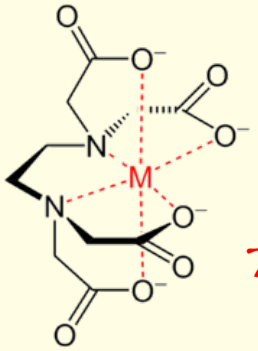
1,10-Phenanthroline



pH independent redox indicators

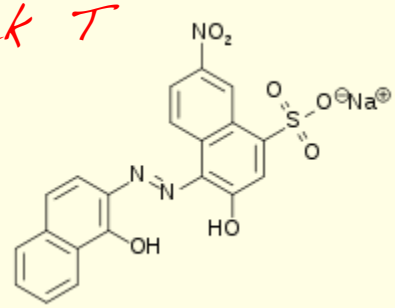
Indicator	E^0, V	Color of Ox form	Color of Red form
2,2'-Bipyridine (Ru complex)	+1.33 V	colorless	yellow
Nitrophenanthroline (Fe complex)	+1.25 V	cyan	red
N-Phenylanthranilic acid	+1.08 V	violet-red	colorless
1,10-Phenanthroline (Fe complex)	+1.06 V	cyan	red
N-Ethoxychrysoidine	+1.00 V	red	yellow
2,2`-Bipyridine (Fe complex)	+0.97 V	cyan	red
5,6-Dimethylphenanthroline (Fe complex)	+0.97 V	yellow-green	red
o-Dianisidine	+0.85 V	red	colorless
Sodium diphenylamine sulfonate	+0.84 V	red-violet	colorless
Diphenylbenzidine	+0.76 V	violet	colorless
Diphenylamine	+0.76 V	violet	colorless
Viologen	-0.43 V	colorless	blue

Complexometric Indicator

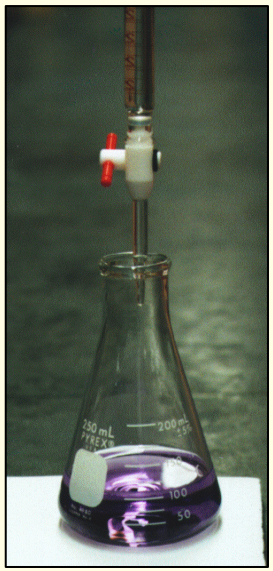


Titration with EDTA

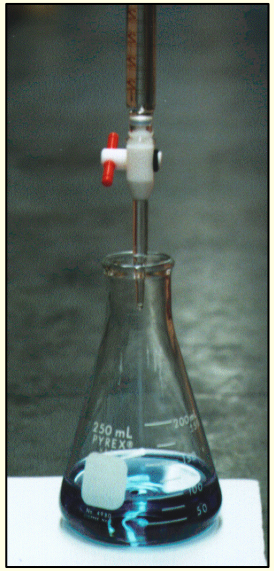
Eriochrome Black T
Indicator



Erio-T is complexed



Erio-T not complexed



SP12: Soap, Detergent, & Ambiphiles

Anionic, Cationic, and Neutral Surfactants

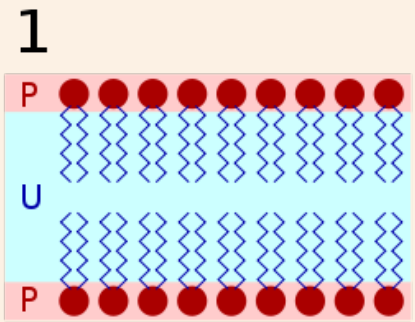
Surfactants are molecules with one hydrophilic and one hydrophobic part (ambiphiles). The hydrophilic part may contain an anionic moiety (i.e., a carboxylate salt), it my contain a cationic moiety (i.e., an ammonium salt), or it may by neutral (i.e., betaine or non-ionic polar headgroup).

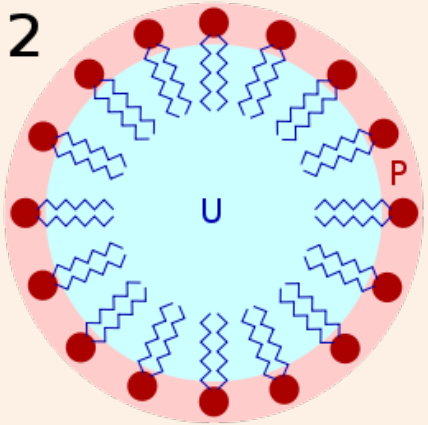
Enzymatic Detergents (protease, amylase, lipase, cellulase)

Proteins that break down peptides, starches, fats and cellulose.

Monolayers, Bilayers and Micelles

Ambiphiles faciliate “wetting”, “emulsification” and “solubilization” of substrates.





SP13: Solar Energy and Solar Cells

Major Modes of Application of Solar Power

Solar Heating – Concentrated Solar Power (heating, turbine, electricity) – Photovoltaic Solar Cells – Photocatalysis (solar power driven fuel production) – Fuel Production from Biomass

Main Types of Solar Cells

Semiconductor SC, sensitized inorganic SC, organic dye sensitized SC, and organic polymer SC.