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

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

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; Contraheuma Retard; Coricidin; Coricidin D; Crystar; Darvon Compound; Dolean pH 8; Dominal; Doril; Duramax; ECM; Easprin; Ecosprin; Ecorin; Empirin; Endosprin; Endydol; Entericin; Enterophen; Enterosarine; Entrophen; Ewin; Extren; Gelprin; Globentyl; Globoid; Helicon; Idragin; Istopirin; Kapsazal; Lysooprin (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; Temporal; 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.

### Glossary of Organic Class Names

- Hantzsch-Widman Nomenclature for Heteromonocyclic Rings
- Fused Ring Nomenclature

### Glossary of Terms in Physical Organic Chemistry

- Non-standard Valence States (Lambda Convention)
- Phane Nomenclature

### 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

- IUPAC Atomic Weights and Periodic Table
- Radicals, Ions & Radical Ion Nomenclature

### Fullerenes 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 §§ 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 §§ 3. Get Information


2. Search using “initial keywords” (We will learn later about “searching”.)
Rough §§ 3. Study Information


-- 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

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!

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

-- 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 bromoacetyl salicylic acid as obtained by Loll and co-workers. 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.
Ref. B.
-- Aspirin is a non-steroidal anti-inflammatory drug (NSAID).
-- Aspirin inhibits both isoforms of cyclooxygenase.
-- Bromoacetylsalicylic 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).
Aspirin is a non-steroidal anti-inflammatory drug (NSAID). Aspirin inhibits both isoforms of cyclooxygenase. Bromoacetylsalicylic acid covalently modifies COX-1 and COX-2 by acylation of Ser530. (Transesterification!)

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

Aspirin is made by acetylation of salicylic acid (2-hydroxybenzoic acid).
-- Aspirin is a non-steroidal anti-inflammatory drug (NSAID) [Ref. B]
-- Aspirin inhibits both isoforms of cyclooxygenase. [Ref. B]
-- Bromoacetylsalicylic 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


-- 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)

--- 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

Place cursor here!

- 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!

Then press "Options..."

- 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

Note that the reference citation appears.

Endnote section appears.
SRI-2: Move Source to Endnote

--- 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

Aspirin is an NSAID, non-steroidal anti-inflammatory drug. Aspirin inhibits COX-1 and COX-2. Aspirin covalently modifies COX.

-- 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

aspirin is an NSAID, non-steroidal anti-inflammatory drug (NSAID). It is a cyclooxygenase (COX) inhibitor. Aspirin inhibits COX-1 and COX-2.

Acylation of Ser530 of COX is a key step in the mechanism of aspirin's action. Aspirin covalently modifies COX.

**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

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

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

1,10-Phenanthroline

<table>
<thead>
<tr>
<th>Indicator</th>
<th>$E^0$ (V)</th>
<th>Color of Ox form</th>
<th>Color of Red form</th>
</tr>
</thead>
<tbody>
<tr>
<td>2,2'-Bipyridine (Ru complex)</td>
<td>+1.33 V</td>
<td>colorless</td>
<td>yellow</td>
</tr>
<tr>
<td>Nitrophenanthroline (Fe complex)</td>
<td>+1.25 V</td>
<td>cyan</td>
<td>red</td>
</tr>
<tr>
<td>N-Phenylanlanilic acid</td>
<td>+1.08 V</td>
<td>violet-red</td>
<td>colorless</td>
</tr>
<tr>
<td>1,10-Phenanthroline (Fe complex)</td>
<td>+1.06 V</td>
<td>cyan</td>
<td>red</td>
</tr>
<tr>
<td>N-Ethoxychrysoidine</td>
<td>+1.00 V</td>
<td>red</td>
<td>yellow</td>
</tr>
<tr>
<td>2,2'-Bipyridine (Fe complex)</td>
<td>+0.97 V</td>
<td>cyan</td>
<td>red</td>
</tr>
<tr>
<td>5,6-Dimethylphenanthroline (Fe complex)</td>
<td>+0.97 V</td>
<td>yellow-green</td>
<td>red</td>
</tr>
<tr>
<td>0-Dianisidine</td>
<td>+0.85 V</td>
<td>red</td>
<td>colorless</td>
</tr>
<tr>
<td>Sodium diphenylamine sulfonate</td>
<td>+0.84 V</td>
<td>red-violet</td>
<td>colorless</td>
</tr>
<tr>
<td>Diphenylbenzidine</td>
<td>+0.76 V</td>
<td>violet</td>
<td>colorless</td>
</tr>
<tr>
<td>Diphenylamine</td>
<td>+0.76 V</td>
<td>violet</td>
<td>colorless</td>
</tr>
<tr>
<td>Viologen</td>
<td>-0.43 V</td>
<td>colorless</td>
<td>blue</td>
</tr>
</tbody>
</table>
Complexometric Indicator

Eriochrome Black T Indicator

Titration with EDTA

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 may contain a cationic moiety (i.e., an ammonium salt), or it may be 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 facilitate “wetting”, “emulsification” and “solubilization” of substrates.
SP13: Solar Energy and Solar Cells

Major Modes of Application of Solar Power

Main Types of Solar Cells
Semiconductor SC, sensitized inorganic SC, organic dye sensitized SC, and organic polymer SC.