

CHEM 4000: Library Seminar

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Objectives

- Overview of the chemical literature
- Searching the bibliographic literature
- Citing sources
- Finding physical and chemical properties of substances
- Introduction to structure/substructure searching

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What's In This Guide

Welcome to the Chemistry research guide. This guide will introduce you to the processes and resources needed to successfully complete your papers and assignments.

Getting Started

[Dictionaries & Encyclopedias](#) | [Books](#)

Finding Articles

[Journal Articles](#) | [Formulating a Search Strategy](#) | [Evaluating Journal Articles](#)

Finding Reference Data

[Physical & Chemical Properties](#) | [Safety and Commercial Availability](#)

Advanced Research

[Substance & Reaction Searching](#) | [Patents](#) | [Theses & Dissertations](#) | [Associations & Organizations](#)

Writing Your Paper

[Compiling a Bibliography](#) | [Bibliographic Management Software](#) | [Writing in Chemistry](#) | [Creating Academic Posters](#)

SciFinder

Related Subject Guides

- [Biochemistry](#) by Jacqueline Kreller-Vanderkooy
- [Physics](#) by Jacqueline Kreller-Vanderkooy
- [Biology](#) by Rajiv Nariani
- [CHEM 3070: Industrial and Green Chemistry](#) by Jacqueline Kreller-Vanderkooy
- [CHEM 3071: Pharmaceutical Discovery](#) by Jacqueline Kreller-Vanderkooy

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Structure of the Chemical Literature

Primary Literature

- Journal Articles
- Patents
- Conference Proceedings
- Dissertations/Theses
- Technical Reports

Secondary Literature

- Bibliographies
- Abstracts and Indexes
- Catalogs

Tertiary Literature

- Handbooks
- Reference Books
- Textbooks/Monographs
- Reviews

Exercise # 1

You want to find some journal articles about fire-resistant paints. How would you do that?

Searching the bibliographic literature

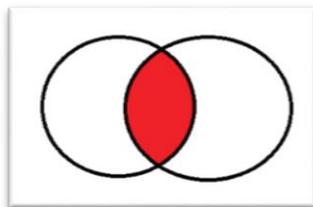
Key bibliographic databases:

- SciFinder (Chemical Abstracts) – most comprehensive index of chemistry literature
- INSPEC – covers physical chemistry and physics
- Web of Science (Science Citation Index) – multidisciplinary science database

Getting a SciFinder Account

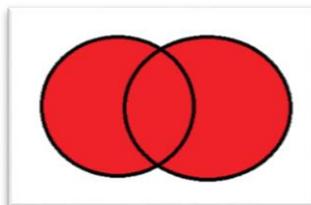
1. [Register for SciFinder to receive access at this link](#). Do this on campus with your York email address to be recognized as a York student.
2. Check your email for a confirmation link. Click it to finish your registration.
3. Log in with the username and password you set up during registration
4. Access SciFinder by searching for it from the main search box on the Library homepage OR from link on [course guide](#).

- Combine concepts using **AND**



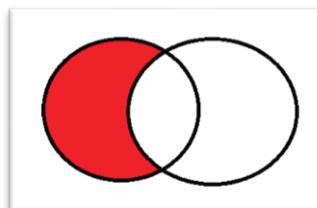
cookies AND cream

- Broaden your search/find alt. spellings & synonyms using **OR**



cookies OR biscuits

- Omit concepts using **NOT**



cookies NOT cake

- Find alt. spellings and pluralizations using **wildcards** *

```
cookie*  
col*r
```

- Find exact phrases using “**phrase searching**”

```
“cookies and cream”
```

- Combine operators:
 - cookie* AND biscuit*
 - “ice cream” (chocolate OR vanilla OR caramel)

Constructing a search string

1. Identify the main concepts of your topic

- Paint Flame-retardant

2. Generate synonyms

- Coating, varnish, colorant, enamel
- Flame-resistant, heat resistant, incombustible, noncombustible, noninflammable, noncandescent, nonflammable

3. Construct your search string using operators

paint* OR
coating* OR
varnish* OR
colorant* OR
enamel*

AND

flame-retardant OR "flame retardant" OR
flame-resistant OR "flame resistant" OR
heat resistant OR "heat resistant" OR
incombustible OR noncombustible OR
noninflammable OR nonflammable OR
noncandescent

Bibliographic searching in SciFinder

- Bibliographic database is known as CAlus or Chemical Abstracts
- Natural language processing
- No need to enter many synonyms or wildcards
- Much less control over the search process
- For more details, see:
 - Wagner, A. B. *J. Chem. Inf. Model.* **2006**, 46, 767-774.

Citing your sources

- [ACS Style Guide](#) (available online)

Chapter 14: References ► 291

Periodicals

RECOMMENDED FORMATS

Author 1; Author 2; Author 3; etc. Title of Article. *Journal Abbreviation* Year, Volume, Inclusive Pagination.

Author 1; Author 2; Author 3; etc. *Journal Abbreviation* Year, Volume, Inclusive Pagination.

- Use the [CAS Source Index \(CASSI\)](#) search tool to find journal abbreviations
- Use [Mendeley](#) or [Zotero](#) to organize your sources

Exercise #2

- Find the melting point and UV/Vis spectrum of chlorophyll a.

Finding physical and chemical properties

Steps

1. Identify the chemical
2. Identify a likely information source
3. Search

Chemical identifiers

- Trivial/common names **ibuprofen**
- Brand names **Advil**
- Systematic names **α -methyl-4-(2-methylpropyl)-benzeneacetic acid**
- Molecular formula **$C_{13}H_{18}O_2$**
- CAS Registry Number **15687-27-1**

CAS Registry Number

- Unique identifier for chemical substances used in the CAS REGISTRY database
- Assigned when a substance first appears in the literature OR when a company asks to have the substance registered
- Proprietary, but CAS numbers are also used in other databases

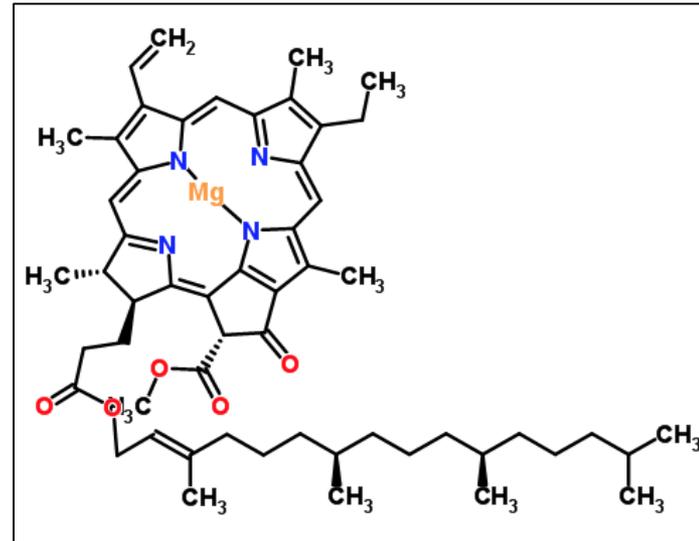
15687-27-1

Determining the CAS number of a substance

- Look the substance up in [SciFinder](#)
- Other places to find CAS numbers:
 - [Wikipedia/Common Chemistry](#)
 - [Sigma-Aldrich catalogue](#)
 - [CRC Handbook of Chemistry and Physics](#)
 - [Combined Chemical Dictionary](#)
 - [ChemSpider](#)

Chlorophyll a

- $C_{55}H_{72}MgN_4O_5$
- CAS Number: 479-61-8
- Systematic Name: [Methyl (3*S*,4*S*,21*R*)-14-ethyl-4,8,13,18-tetramethyl-20-oxo-3-(3-oxo-3-[(2*E*,7*R*,11*R*)-3,7,11,15-tetramethyl-2-hexadecen-1-yl]oxy)propyl)-9-vinyl-21-phorbinecarboxylato(2-)-kappa~2~N,N']magnesium



Sources for physical & chemical properties

Handbooks

- CRC Handbook of Chemistry and Physics
- Combined Chemical Dictionary
- Kaye & Laby
- Lange's Handbook of Chemistry
- NIST Chemistry WebBook

Databases

- SciFinder
- Reaxys
- ChemSpider
- PubChem

Sources for spectra

- NIST Chemistry WebBook
- Spectral Database for Organic Compounds
- ChemSpider
- SciFinder
- Reaxys

Sources for commercial availability

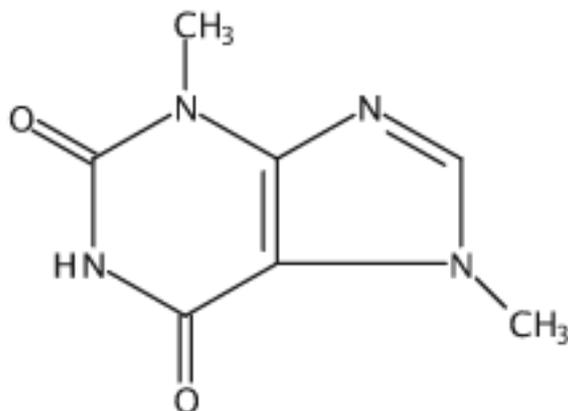
- SciFinder
- Reaxys
- PubChem
- ChemSpider
- Sigma-Aldrich

Sources for safety information

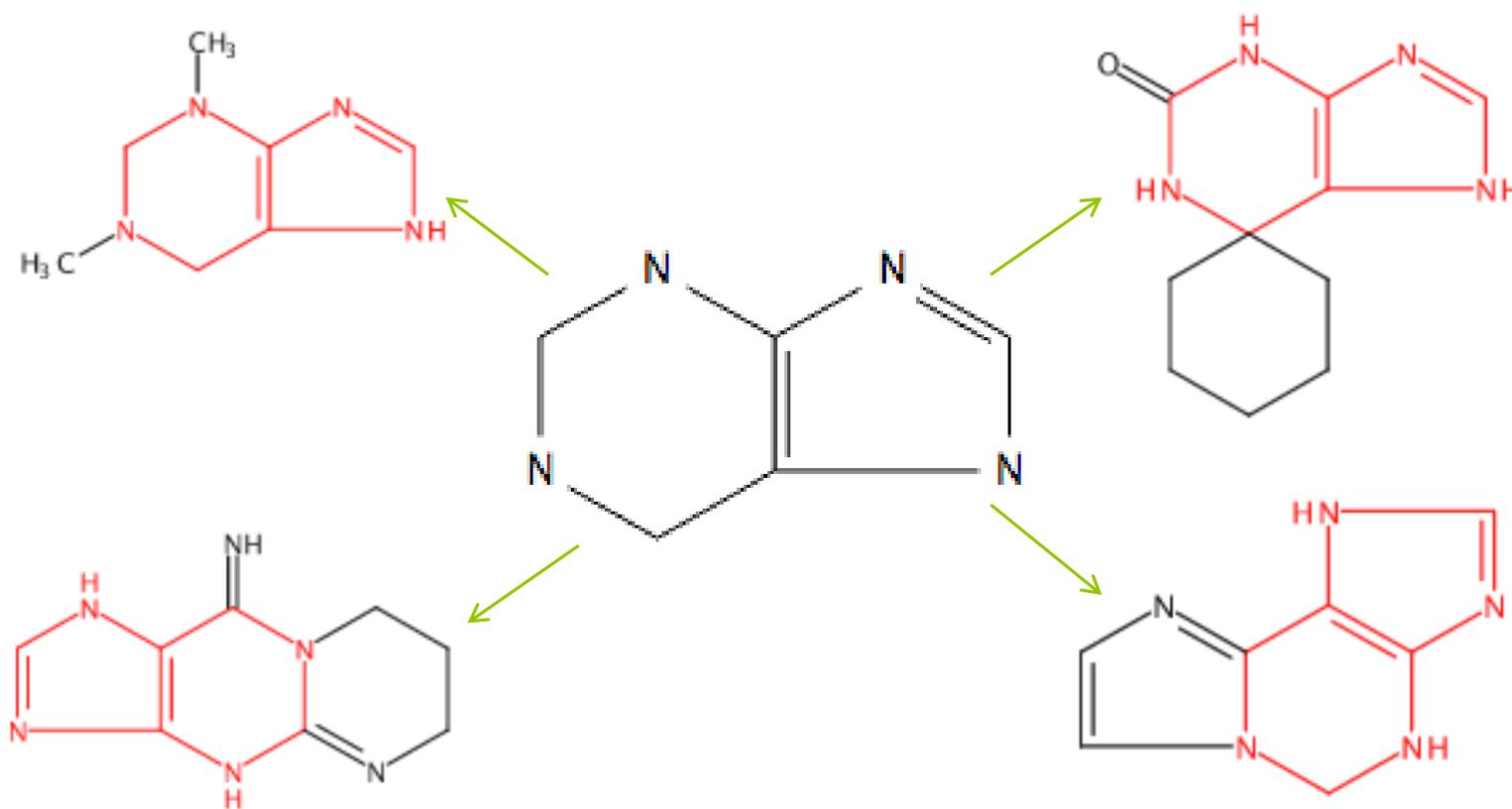
- Sigma-Aldrich (MSDS)
- TOXNET
- ChemSpider

Exercise #3

- Find the name(s) and CAS Registry number of the substance below.



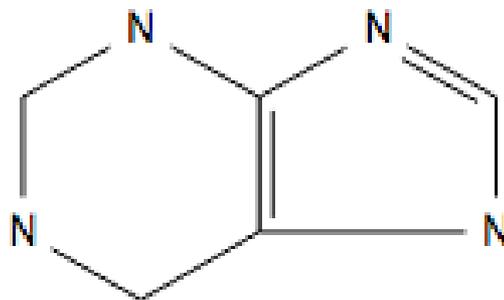
Substructure searching



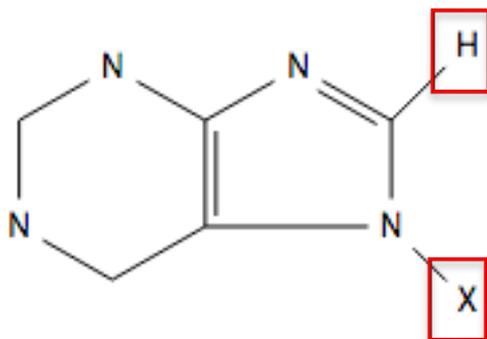
Steps for substructure searching

1. Generate basic substructure
2. Define allowable substitution
3. Define allowable bond order & stereochemistry
4. Define allowable topology

1. Generate basic substructure



2. Define allowable substitution

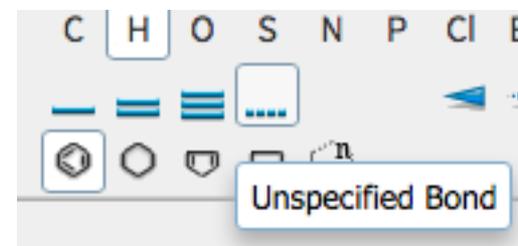
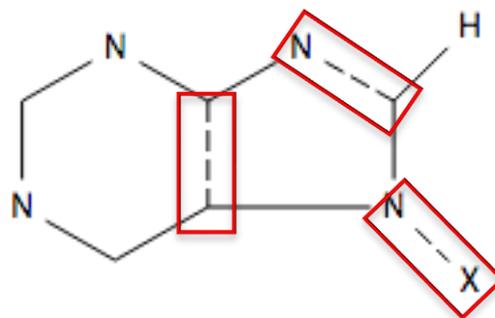


Variables

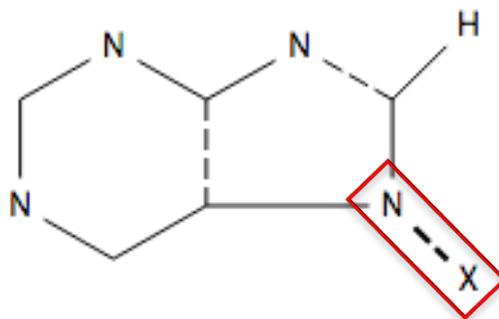
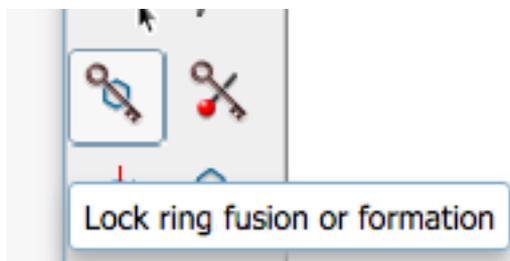
<input type="checkbox"/>	X	Any halogen
<input type="checkbox"/>	M	Any metal
<input type="checkbox"/>	A	Any atom except H
<input type="checkbox"/>	Q	Any atom except C or H
<input type="checkbox"/>	Al	Any alkyl chain
<input type="checkbox"/>	Cy	Any cycle
<input type="checkbox"/>	Cb	Any carbocycle
<input type="checkbox"/>	Hy	Any heterocycle

Close

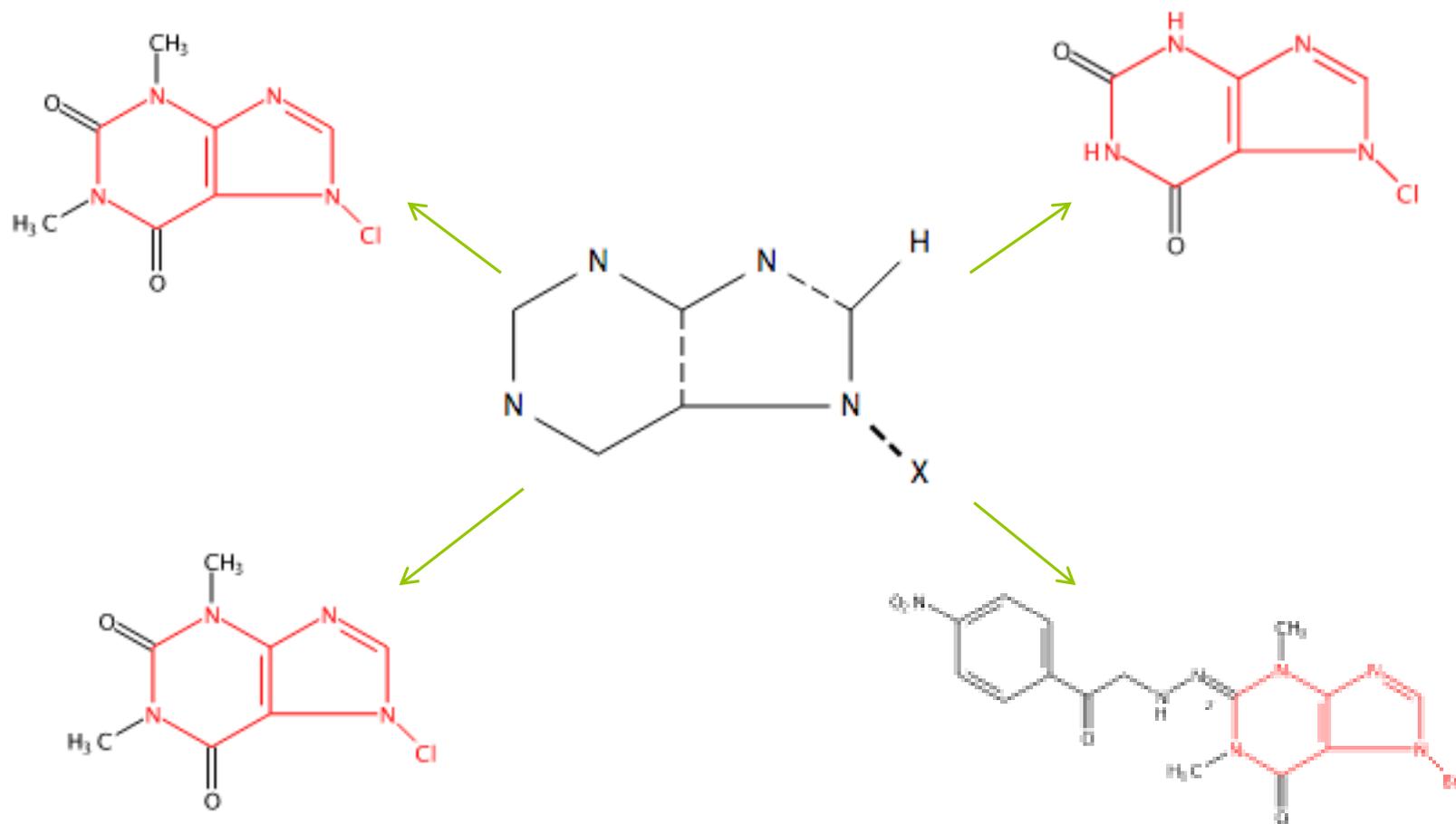
3. Define allowable bond order and stereochemistry



4. Define allowable topology



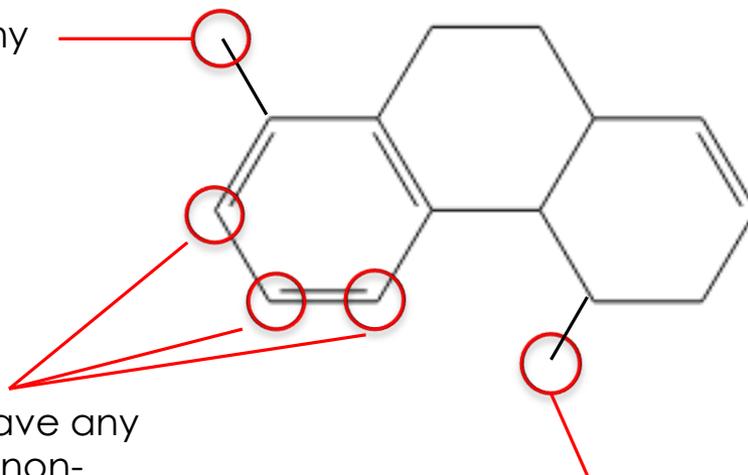
Results



Exercise #4

- Perform a substructure search for the following basic substructure.

Must be any halogen

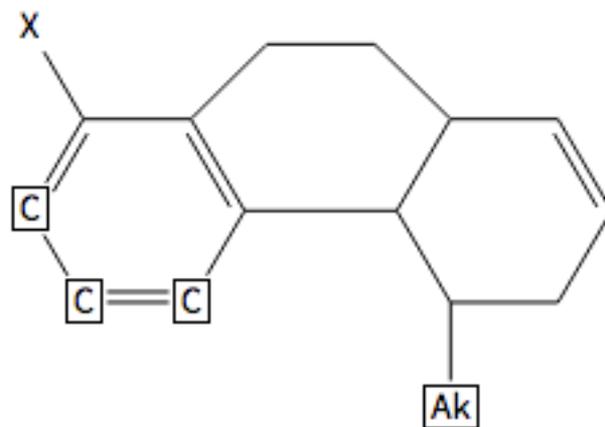


May not have any additional non-hydrogen substituents

Must have an alkyl chain substituent

- Bond order must be as shown
- Unless otherwise stated, any kind of substitution is allowed

Exercise #5 - Solution



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