

NO-2012

38-UCCh.

FORMAT 2

Submit originals (including syllabus) and one copy and electronic copy to the Faculty Senate Office  
See <http://www.uaf.edu/uafgov/faculty-senate/curriculum/course-degree-procedures/> for a complete description of the rules governing curriculum & course changes.

**CHANGE COURSE (MAJOR) and DROP COURSE PROPOSAL**  
Attach a syllabus, except if dropping a course.

RECEIVED

SEP 21 2012

**SUBMITTED BY:**

Department	Chemistry & Biochemistry	College/School	CNSM
Prepared by	Thomas Green	Phone	474-1559
Email Contact	tkgreen@alaska.edu	Faculty Contact	tkgreen@alaska.edu

Dean's Office  
College of Natural Science & Mathematics

**1. COURSE IDENTIFICATION: As the course now exists.**

Dept  Course #  No. of Credits

COURSE TITLE

**2. ACTION DESIRED: Check the changes to be made to the existing course.**

Change Course  If Change, indicate below what is changing. Drop Course

NUMBER	TITLE	DESCRIPTION	FREQUENCY OF OFFERING
<input type="text"/>	<input type="text"/>	<input checked="" type="checkbox"/>	<input type="text"/>

\*Prerequisites will be required before a student is allowed to enroll in the course.  
Reference the registration implications below due to Banner coding of these terms:  
Prerequisite: Course completed and grade of "C" (2.0) or higher prior to registering for the course that requires it.  
Concurrent: Course may be taken simultaneously (and allows for a course to have been previously completed).  
Co-requisite: Courses MUST be taken simultaneously and does NOT allow for fact that a course was previously completed!

**CREDITS (including credit distribution)**  **COURSE CLASSIFICATION**

**ADD CROSS-LISTING**  Dept.  (Requires approval of both departments and deans involved. Add lines at end of form for additional signatures.)  
**STACKED (400/600)**  Dept.  Course #   
Include syllabi.

Stacked course applications are reviewed by the (Undergraduate) Curricular Review Committee and by the Graduate Academic and Advising Committee. Creating two different syllabi—undergraduate and graduate versions—will help emphasize the different qualities of what are supposed to be two different courses. The committees will determine: 1) whether the two versions are sufficiently different (i.e. is there undergraduate and graduate level content being offered); 2) are undergraduates being overtaxed?; 3) are graduate students being undertaxed? In this context, the committees are looking out for the interests of the students taking the course. Typically, if either committee has qualms, they both do. More info online - see URL at top of this page.

**OTHER (please specify)**

**3. COURSE FORMAT**

NOTE: Course hours may not be compressed into fewer than three days per credit. Any course compressed into fewer than six weeks must be approved by the college or school's curriculum council and the appropriate Faculty Senate curriculum committee. Furthermore, any core course compressed to less than six weeks must be approved by the core review committee.

COURSE FORMAT: (check all that apply)  1  2  3  4  5  6 weeks to full semester

OTHER FORMAT (specify all that apply)  
Mode of delivery (specify lecture, field trips, labs, etc)

Governance  
9/27/12 TLP

4. **COURSE CLASSIFICATIONS:** (undergraduate courses only. Use approved criteria found on Page 10 & 17 of the manual. If justification is needed, attach on separate sheet.)

H = Humanities  S = Social Sciences

Will this course be used to fulfill a requirement for the baccalaureate core?

YES  X  NO  X

IF YES\*, check which core requirements it could be used to fulfill:

O = Oral Intensive,  W = Writing Intensive,  Natural Science,   
\*Format 6 also submitted  \*Format 7 submitted  \*Format 8 submitted

4.A **Is course content related to northern, arctic or circumpolar studies? If yes, a "snowflake" symbol will be added in the printed Catalog, and flagged in Banner.**

YES  NO

5. **COURSE REPEATABILITY:**

Is this course repeatable for credit? YES  NO

Justification: Indicate why the course can be repeated (for example, the course follows a different theme each time).

How many times may the course be repeated for credit?  TIMES

If the course can be repeated with variable credit, what is the maximum number of credit hours that may be earned for this course?  CREDITS

6. **COMPLETE CATALOG DESCRIPTION** including dept., number, title, credits, credit distribution, cross-listings and/or stacking, clearly showing the changes you want made. (Underline new wording ~~strike through old wording~~ and use complete catalog format including dept., number, title, credits and cross-listed and stacked.)

Example of a complete description:

PS F450 Comparative ~~Aberiginal~~ Indigenous Rights and Policies (s)  
3 Credits  
Offered As Demand Warrants  
Case study Comparative approach in ~~assessing Aberiginal~~ analyzing Indigenous rights and policies in different nation-state systems. ~~Seven Aberiginal situations~~ Multiple countries and specific policy developments examined for factors promoting or limiting self-determination. Prerequisites: Upper division standing or permission of instructor. (Cross-listed with ANS F450.) (3+0)

**CHEM F324 W Advanced Organic Chemistry Laboratory (n)**  
4 3 Credits Offered Spring  
A laboratory designed to illustrate modern techniques of isolation, purification, analysis and structure determination of covalent, principally organic, compounds. Emphasis on research techniques including 2D nuclear magnetic resonance spectroscopy. Intended for chemistry majors. Special fees apply. Prerequisites: ENGL 211X or ENGL F213X; CHEM F212 or permission of instructor. Co-requisites: CHEM F322. (2 1 +6)

7. **COMPLETE CATALOG DESCRIPTION AS IT SHOULD APPEAR AFTER ALL CHANGES ARE MADE:**

**CHEM F324 W Advanced Organic Chemistry Laboratory (n)**  
3 Credits Offered Spring  
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8. **IS THIS COURSE CURRENTLY CROSS-LISTED?**

YES/NO  No  If Yes, DEPT  NUMBER

**DROPPING A CROSS-LISTING:**  
YES  DEPT  NUMBER

Changing or dropping requires written notification of each department and

dean involved. Attach a copy of written notification.

9. **GRADING SYSTEM:** Specify only one.

LETTER:  PASS/FAIL:

10. **ESTIMATED IMPACT**

WHAT IMPACT, IF ANY, WILL THIS HAVE ON BUDGET, FACILITIES/SPACE, FACULTY, ETC.

This course will be taken primarily by chemistry majors. We have offered this lab previously as a 4-credit lab. One credit has moved to Chem 321 Organic Chemistry I (see other course change). The department has determined that it can accommodate 2 sections of 10 students in Reichardt 137, which is enough to cover expected enrollments. Reichardt 137 is well-equipped with the necessary glassware and supplies. A lab fee will be assessed. The overall budget will be minimally affected since we are actually shifting some of the second-semester lab exercises to first-semester and reducing credits from 4 to 3.

11. **LIBRARY COLLECTIONS**

Have you contacted the library collection development officer (kljensen@alaska.edu, 474-6695) with regard to the adequacy of library/media collections, equipment, and services available for the proposed course? If so, give date of contact and resolution. If not, explain why not.

No  Yes  We offer the lab already and sufficient library resources are available.

12. **IMPACTS ON PROGRAMS/DEPTS:**

What programs/departments will be affected by this proposed action?  
Include information on the Programs/Departments contacted (e.g., email, memo)

CHEM 324 is a requirement of the BS in Chemistry with Environmental option, but is an elective for the Biochemistry option.

13. **POSITIVE AND NEGATIVE IMPACTS**

Please specify positive and negative impacts on other courses, programs and departments resulting from the proposed action.

There are no apparent negative impacts.

**JUSTIFICATION FOR ACTION REQUESTED**

The purpose of the department and campus-wide curriculum committees is to scrutinize course change and new course applications to make sure that the quality of UAF education is not lowered as a result of the proposed change. Please address this in your response. This section needs to be self-explanatory. If you ask for a change in # of credits, explain why; are you increasing the amount of material covered in the class? If you drop a prerequisite, is it because the material is covered elsewhere? If course is changing to stacked (400/600), explain higher level of effort and performance required on part of students earning graduate credit. Use as much space as needed to fully justify the proposed change and explain what has been done to ensure that the quality of the course is not compromised as a result.

Chem 324 Organic Chemistry Laboratory would change from 4 to 3 credits with this change. One credit is moving to the first semester organic course, as part of Chem 321 Organic Chemistry I.

**APPROVALS:** (Additional signature blocks may be added as necessary.)

 Date 20 Sep 2012

Signature, Chair,  
Program/Department of: Chem + Biochem

 Date 9/26/2012

Signature, Chair, College/School  
Curriculum Council for: CNSM

 Date 9/26/12

Signature, Dean, College/School  
of: CNSM

Offerings above the level of approved programs must be approved in advance by the Provost:

Date

Signature of Provost (if applicable)

**ALL SIGNATURES MUST BE OBTAINED PRIOR TO SUBMISSION TO THE GOVERNANCE OFFICE.**

Date

Signature, Chair  
Faculty Senate Review Committee:  Curriculum Review  GAAC  
 Core Review  SADAC

**ADDITIONAL SIGNATURES:** (As needed for cross-listing and/or stacking; add more blocks as necessary.)

Date

Signature, Chair,  
Program/Department of:

Date

Signature, Chair, College/School  
Curriculum Council for:

Date

Signature, Dean, College/School  
of:

**ATTACH COMPLETE SYLLABUS (as part of this application).**

The guidelines are online:

<http://www.uaf.edu/uafgov/faculty-senate/curriculum/course-degree-procedures-/uaf-syllabus-requirements/>

The Faculty Senate curriculum committees will review the syllabus to ensure that each of the items listed below are included. If items are missing or unclear, the proposed course (or changes to it) may be denied.

**SYLLABUS CHECKLIST FOR ALL UAF COURSES**

During the first week of class, instructors will distribute a course syllabus. Although modifications may be made throughout the semester, this document will contain the following information (as applicable to the discipline):

**1. Course information:**

Title,  number,  credits,  prerequisites,  location,  meeting time (make sure that contact hours are in line with credits).

**2. Instructor (and if applicable, Teaching Assistant) information:**

Name,  office location,  office hours,  telephone,  email address.

**3. Course readings/materials:**

Course textbook title,  author,  edition/publisher.  
 Supplementary readings (indicate whether  required or  recommended) and  
 any supplies required.

**4. Course description:**

Content of the course and how it fits into the broader curriculum;  
 Expected proficiencies required to undertake the course, if applicable.  
 Inclusion of catalog description is *strongly* recommended, and  
 Description in syllabus must be consistent with catalog course description.

**5.  Course Goals (general), and (see #6)**

**6.  Student Learning Outcomes (more specific)**

**7. Instructional methods:**

Describe the teaching techniques (eg: lecture, case study, small group discussion, private instruction, studio instruction, values clarification, games, journal writing, use of Blackboard, audio/video conferencing, etc.).

**8. Course calendar:**

A schedule of class topics and assignments must be included. Be specific so that it is clear that the instructor has thought this through and will not be making it up on the fly (e.g. it is not adequate to say "lab". Instead, give each lab a title that describes its content). You may call the outline Tentative or Work in Progress to allow for modifications during the semester.

**9. Course policies:**

Specify course rules, including your policies on attendance, tardiness, class participation, make-up exams, and plagiarism/academic integrity.

**10. Evaluation:**

Specify how students will be evaluated,  what factors will be included,  their relative value, and  how they will be tabulated into grades (on a curve, absolute scores, etc.)  Publicize UAF regulations with regard to the grades of "C" and below as applicable to this course. (Not required in the syllabus, but may be a convenient way to publicize this.) Faculty Senate Meeting #171:  
<http://www.uaf.edu/uafgov/faculty-senate/meetings/2010-2011-meetings/#171>

**11. Support Services:**

Describe the student support services such as tutoring (local and/or regional) appropriate for the course.

**12. Disabilities Services:** Note that the phone# and location have been **updated**.

The Office of Disability Services implements the Americans with Disabilities Act (ADA), and ensures that UAF students have equal access to the campus and course materials.

State that you will work with the Office of Disabilities Services (208 WHITAKER BLDG, 474-5655) to provide reasonable accommodation to students with disabilities.

8/1/2012

**CHEMISTRY 324W / Spring 2012**  
**ADVANCED ORGANIC LABORATORY**  
**3.0 Credits**

Lecture: .....Monday 1:00-2:00; Reichardt 165  
Labs: .....Tues. and Thurs., 2:45-5:45; Reichardt 137  
Instructor: .....Fenton Heirtzler, Office 161 Nat Sci, 474-5507; [frheirtzler@alaska.edu](mailto:frheirtzler@alaska.edu)  
.....Office hours by appointment, or drop-in.  
Course Website: [http://chem.uaf.edu/heirtzler/Chem\\_324\\_Website.htm](http://chem.uaf.edu/heirtzler/Chem_324_Website.htm)

Teaching Assistant: Jamie McKee [jamckee@alaska.edu](mailto:jamckee@alaska.edu)

**Required Materials:**

- (1) PAVIA et al. , MICROSCALE+MACROSCALE TECH IN ORGAN.LAB , \$112 new at the UAF bookstore, \$84 used. Amazon.com: \$106 new, with free shipping, \$48 used + \$4 shipping
- (2) Laboratory notebook: available free of charge to registered Chem 324 students in Rm. 194
- (3) NEW: a laboratory coat or jacket is REQUIRED (cotton is recommended). Good value ones are available over Amazon.com.

**Recommended Materials:**

USB memory stick for backing up data and text files

**Fees:**

- (1) Material fee for chemicals, glassware breakage, and other supplies \$120
- (2) Chemistry computer lab fee \$45 (charged only once for multiple chem classes)
- (3) Key deposit \$5 cash (Bring it to first lab.)

**Course Goals:** This course emphasizes several aspects of chemistry laboratory practices:

- 1) Synthetic procedures
- 2) Spectroscopic analyses (NMR, MS, and IR)
- 3) Standard work-up procedures
- 4) Scientific writing
- 5) Style in laboratory journals
- 6) Use of relevant computer software
- 7) Chromatographic analysis (gc, tlc)
- 8) Purification techniques (crystallization, distillation, extraction, chromatography...)
- 9) Literature searches
- 10) Chemical calculations including stoichiometry

**Experiment sources:** While the text for this course is an excellent guide to the techniques used by organic chemists, it is not a source of standard organic laboratory experiments. Rather, the

experiments will come from (a) the Chem 324W laboratory manual or directly from the chemical literature (especially for your research project). Consequently, the precise details of the procedure you will follow may differ in terms of the reagents, reaction times, reaction scale, apparatus setup, and scope of the experimental. This approach will provide you with the experience of using procedures from the chemical literature as templates for designing your own synthetic strategies. *Because the details of each experiment will be explained in lecture, it is imperative you attend (and be on time).*

**Laboratory Safety:** Laboratory safety is a major concern of all chemical laboratories but is especially important in organic labs due to the presence of flammable solvents, potentially hazardous fumes, highly reactive reagents, etc. The first lab (Tuesday or Wed) will deal explicitly with these hazards and the appropriate safety measures to follow. Subsequent lectures, besides covering the theory and practicalities of the next week's experiment will also cover specific hazards that you may encounter. Please attend these lectures and be prepared for the lab by doing any assigned readings and having your notebook prepared before coming to lab. If you are not prepared for lab you may be asked to leave.

**Course requirements:**

- I. **Laboratory Report.** A written report is required for each experiment. Some will be shorter, others longer. The report layout is the usual one used in the sciences and *should have the following titles:* Introduction, Results, Discussion, Experimental Section, Acknowledgments and References (see below for details). The final draft of lab reports (and reaction products, if applicable) are generally due as announced in the lecture or lab.
- II. **Laboratory Notebook.** Update your laboratory notebook during the day's experiment, *not* afterwards. Use the passive voice, abbreviations and shorthand, when possible. During the lab period make notes on (i) your actual procedure including mass data, (ii) significant visual observations, (iii) TLC sheets taped in, including solvent info, and (iv) spectra or references to location of spectra in a separate collection. DATE each page or entry.
- III. **Preparation for Laboratory Class.** Independent of the lab notebook and prior to entering the laboratory, you should have planned out (i) a balanced chemical equation, (ii) a procedural outline or flow chart, and (iii) physical and hazardous properties for each chemical (including solvents) you plan to use in the experiment. Obtain this information from the Web – for example, if you look up the compound at the Aldrich Chemical Co web site - <http://www.sigmaaldrich.com/catalog/search/AdvancedSearchPage> then follow the link to MSDS, the Material Safety Data Sheet will provide the appropriate information. (*Please keep in mind that the MSDS info is geared to handling chemicals on the industrial scale.*) We will in some labs also have pre-lab questions that will be due at the beginning of lab.
- IV. **Research Project.** The second half of the laboratory class will be devoted to a "Research Project". This will typically involve devising and/or implementing the synthesis of a target compound over several reaction steps. Your final report will be either a poster or an article in the style of the *Journal of Organic Chemistry*. Project ideas are available from the instructor. Suggestions of projects which realistically fall within the remit of synthetic organic chemistry and student skill levels will also be entertained.

- V. **Lectures.** It is essential that you attend all lectures and arrive on time to the laboratory in order to fully understand the experiment and safety issues. Each lecture will begin by pointing out salient features for the upcoming experiment. Questions regarding 1) the correct use of laboratory apparatus, 2) what the “work-up” is, 3) appropriate stopping points in the experiment, etc., will be addressed. In addition, as time allows, other topics will be covered that are described in the syllabus. Much of the midterm exam will come from these lectures. Some experiments may have to be modified from the description given in the handouts. A discussion of these modifications will be presented in the lecture and possibly at the beginning of the lab itself. *This is why lecture attendance is mandatory. Also, always check the marker board in lab for important announcements.*
- VI. **Writing Intensive designation.** In brief, the W designator means that a majority of your grade is based on your written work; that some of the work will be resubmitted with revisions based on previous comments; and that factors such as content, organization, tone, word choice, grammar, spelling, sentence structure, etc., contribute to the final grade. The prerequisite for all W courses is Engl 211X or 213X. While you may collaborate with classmates in interpreting data and proofreading reports, it is essential that you *write* your reports independently. Each paragraph should portray your own creativity and not simply paraphrase someone else’s writing. It is a common misconception that changing the word choice, sentence structure or organization of an existing document protects against a charge of plagiarism; it does not. You may use another student’s formulas in a report if such a move is (1) approved by the other person, and (2) proper credit is given to the individual who created them in the Acknowledgements section.
- VII. **Reaction Products.** For most experiments, you will also hand in your chemical product. Put the compound in a vial with a piece of foil as a cap-liner (to prevent contamination by the cardboard cap-liner). Always label the vial neatly with your name, compound, mass, and mp or bp. Poorly labeled vials may be disposed of by chemistry personnel during routine cleanups. **NEVER DISPOSE OF YOUR PRODUCT UNTIL YOUR REPORT HAS BEEN GRADED.** Store it in the refrigerator or freezer in 139 Reichardt until it is time to hand it in to prevent evaporation or degradation.

**Breakdown of a full laboratory report (not all lab reports will require this level of detail):**

- Introduction:
  - Describe the chemistry goals for the experiment. Write a balanced chemical equation for the reaction, if any.
- Results & Discussion:
  - The percent yield along with an estimation of product purity by spectroscopic and/or chromatographic analyses should be provided
  - Spectra (usually IR and/or NMR) along with their interpretation, which means writing out descriptions of where the peaks are, and which atoms or groups caused those peaks, and why you assigned those atoms. In particular, evidence for the presence or absence of any possible contaminants should be addressed by a



detailed examination of the spectra, using reference spectra when available. Be sure to include a discussion of the integration analysis of the  $^1\text{H-NMR}$  spectra.

- Gas chromatographic traces, if required, should be included and peak identification should be attempted.
- A detailed mechanism using electron-pushing notation is usually required.
- Please do not refer to or display NMR spectra calculated by ACD software anywhere in the report.
- Experimental Section: Describe the procedure *which you carried out* (as opposed to what you intended to do) using the *passive voice*, third person language. Be succinct, but do not leave out important details. We will learn how to write these by reading some from the original literature.
- Acknowledgment: Acknowledge any student whose data or graphics are used in your report. **Do not** acknowledge the teaching assistant or professor.
- References: Include a reference to the original literature in each formal report. If possible, use the Endnote application available in the Chemistry Computer Lab. Never include a reference without a reference to it (a "callout") appearing somewhere in the text. Standard journal abbreviations may be found at <http://library.caltech.edu/reference/abbreviations/>

#### Technical notes on the general preparation of lab reports:

- Prepare lab report using Microsoft Word, or compatible, software.
- Please use the spelling and grammar checkers before handing anything in!
- Submit reports in electronic form.
- Chemical structures should be drawn using computer software which is available on the PCs in Rm. 172: ChemWindow, ACD ChemSketch or MarvinSketch (available free download from the Internet).
- Chemical structures, reactions, and mechanisms should be inserted directly in the text, near to where they are discussed, and not at the end.
- Portions of spectra which are discussed in the text should be labeled as Figures (1,2,3....) and imbedded within the text to the Results and Discussion Section.
- Complete IR and NMR spectra should be pasted as graphics in a separate section of "Figures" at the end of the report.
- Formatting: Use 12-pt Times Roman font, single space, margins 1.0" all around.

#### Miscellaneous:

- Tardy reports

The policy on handing in late report **final copies** is:

- 10% for delay of 3 - 10 days
- 20% for delay of 11 - 17 days
- 30% for delay of 18 - 24 days

- Absences

Absences from laboratory period will be accommodated by re-scheduling experiments for alternative times. However, it is **standard policy** that for special consideration from illness or other circumstances beyond personal responsibility, a written statement from medical authorities is required.

- Grades

The final letter grade will be based on the total number of points accrued during the semester, apportioned as follows:

A+	98 - 100%	B-	80 - 83%
A:	93 - 98%	C+	78 - 80%
A-	90 - 93%	C	73 - 78%
B+	88-90%	C-	70 - 73%
B	83 - 88%	D+	68 - 70%
		D	63 - 68%

The breakdown of marks for the entire course is as follows

		Max. points
Expt 1	Spectroscopic Identification of Unknown Organic Compounds (1 week)	80
Expt 2	Stereoselectivity in the Reduction of 4-tert-Butylcyclohexanone (1 week)	80
Expt 3	Steam Distillation and GC-MS Analysis of Volatile Fragrances in Spices (1 week)	40
Expt 4	Diastereoselectivity in the Grignard Reaction and Cram's Chelation Rule (2 weeks)	120
	Midterm exam (held in class)	100
Expt 5	Diels-Alder Reaction of Cyclopentadiene and Maleic Anhydride (1 week)	40
Expt 6	A Mixed Aldol Condensation/Michael Addition Experiment (2 weeks)	80
Expt 7	Benzoin Condensation of Pyridine-2-Carboxaldehyde (1 week)	40
Expt 8	Air Oxidation of a Dihydroxyalkene to an $\alpha$ -Diketone (1 week)	40
	Research project (poster or paper)	180
	Final exam (held during examination period)	100
	Laboratory notebook	100
	Total points	1000

**Students with documented disabilities** who may need reasonable academic accommodations should discuss these with the academic staff during the first two weeks of class. You will need to provide documentation of your disability to Disability Services in the Center for Health and Counseling, 474-7043, TTY 474-7045.

### References

The following references may be useful and should be found in (and should not be removed from) the laboratory:

*Aldrich Chemical Catalog* gives physical properties as well as safety issues for most commercially available organic reagents. (You can order your own free.)

*The Merck Index* is an excellent reference book for over 10,000 important organic substances. It has a handy cross index and molecular formula index that you will find useful.

*The CRC Handbook* is another reference book that provides some physical and spectral information on a wealth of substances. (The Merck Index is easier to use and more relevant.)

*Advanced Organic Chemistry: Reactions, Mechanisms, and Structure* by March (McGraw-Hill) is particularly useful because it provides good references to the chemical literature.

*The Chemist Companion: A handbook of practical data, techniques, and references* by A.J. Gordon and Richard A. Ford (John Wiley & Sons) is a good source of information for all chemists (inorganic, organic, analytical...).

*Reagents for Organic Synthesis* by Fieser and Fieser, volumes 1-13 (John Wiley & Sons) has detailed discussions about nearly every organic reagent with references to the chemical literature. At times details about how the reagent is typically used in a given reaction is provided.

*Organic Synthesis*; collective volumes 1-5 (John Wiley & Sons) provides very detailed procedures for specific syntheses. The scale of the reactions, however, is usually large.

*Spectroscopic Identification of Organic Compounds*; 6th Ed., by R.M. Silverstein, G.C. Bassler, and T.C. Morrill (John Wiley & Sons) provides good discussion and extensive tables for the interpretation of standard IR, H NMR, C NMR, and mass spectra. More advanced topics such as 2-D NMR and NMR of other nuclei are also discussed.

WWW.HAZARD.COM is a good on-line source of Material Safety Data Sheets (MSDS). The department also keeps a set of MSDS in NSF 139.

Scifinder Scholar – literature searching

ACD labs NMR software

HyperChem software for molecular calculations

Japan spectral database <http://riodb01.ibase.aist.go.jp/sdbs/>