Medicinal Chemistry Program

Graduate Student Handbook

RUTGERS
UNIVERSITY

Graduate Program in Medicinal Chemistry

Department of Medicinal Chemistry
Ernest Mario School of Pharmacy
Rutgers, The State University of New Jersey
160 Frelinghuysen Road
Piscataway, NJ 08854-8020
http://medchem.rutgers.edu/

Phone: (848) 445-5381
Elissa Glinn, Administrative Coordinator
elissa.glinn@pharmacy.rutgers.edu

Updated 08/2022

Foreword

Welcome to the Graduate Program in Medicinal Chemistry.

Over the past few years, it has been noticed that students new to the program are often confused about procedures, curriculum, choosing an advisor, etc. This book is designed as a guide for you in understanding the process of obtaining a graduate degree at Rutgers and to answer many of the questions you may have. We have tried to cover as many topics as we could imagine, but invariably we may have overlooked something. We welcome any suggestions for improving this handbook.

Sincerely,

Graduate Program in Medicinal Chemistry

Dr Jun Wang – Graduate Program Director

Table of Contents

1. Getting Started at Rutgers University

By the time you get this booklet you will probably have already found an apartment or dorm room and are eager to start your career as a graduate student. Before this can happen however, you need to register for classes. If you are a full-time student, you must register for at least 9 credits per semester. You will be able to register for your classes online. If you have been awarded a Teaching Assistantship from the Department of Medicinal Chemistry or any other department you will need to register for Teaching Assistantship (16:663:877) for 6 "E" credits. E-credits count toward full time student status, but do not count toward your degree requirement/graduation or your GPA. Textbooks are available from the Rutgers Bookstore (Barnes & Noble at Rutgers University) located at the Gateway Transit Building, 100 Somerset Street, New Brunswick, NJ 08901-2197 (732) 246-8448. Store hours are typically 10 AM - 6 PM (M-F), 10 AM – 4 PM (Sat.), closed (Sun). You should refer to the graduate program homepage frequently for information and notices (https://pharmacy.rutgers.edu/about/med-chem-graduate-program-2) .

1.1. Course Registration

The number of courses that you should be taking will depend on whether you are a full-time or part-time student. Full-time status requires a minimum of 9 credits and most courses are 3 credits each. You should plan on taking 3 courses during your first semester. If you have been awarded a Teaching Assistantship you will also register for 6 "E-credits" of Teaching Assistantship (16:663:877). These credits count towards your total credits per semester, but do not show on your transcript (they carry no weight). It is a good idea to try to complete your course requirements for your degree during your first two years, especially if you are supported as a Teaching Assistant. As part of your TA package, you are eligible to register for a total of 24 credits each year so you may be able to register for 6 credits of Research in Medicinal Chemistry (16:663:701,702) during the Summer Session following the academic year for which you were a TA. By doing this you can help to minimize the cost to your advisor, should you be awarded a Graduate Assistantship, since the faculty member is responsible for paying your tuition. For online registration please visit: https://sims.rutgers.edu/webreg/. You will need to enter your net id and password which you should have obtained once you were accepted into the program. To activate your net id, go to https://netid.rutgers.edu/index.htm.

Office of the Registrar, New Brunswick
Records Hall
620 George Street, Room 140
College Avenue Campus
New Brunswick, NJ 08901
Office Hours: Monday – Friday, 8:30 AM - 4:30 PM
(848) 445-7000, Press 4, https://nbregistrar.rutgers.edu/

1.2. Expectations

Your decision to study Medicinal Chemistry at Rutgers was most likely a multi-faceted one. You may have wanted to attend a school on the East Coast for proximity to family and friends; you may have wanted to attend a large school for the wealth of resources that are present; perhaps you have already decided to do research for a particular professor in our program. No matter what your reason for coming here was, you have a desire to study Medicinal Chemistry and to graduate with either an M.S. or Ph.D. and then find employment in your field. The faculty members of this program are here to help you achieve your goals, but there are several things that are expected of you as well.

As an undergraduate you wanted to get the best grades so that you would get accepted into the graduate program of your choice. When your application arrived here the Admissions Committee performed a thorough evaluation of your undergraduate record. Since this is a highly selective program, we already know that our students were among the best undergraduates. You will find however, that the emphasis in graduate school is different. While you need to ensure that your GPA stays above 3.00 the most important factors in securing a position upon obtaining your M.S or Ph.D. are the quality of your research and the length of time that it takes to get your degree. The longer it takes, the lower your chances of obtaining the position you want. In our program it takes, on average, 2.5 years to earn a M.S. and 5 years to earn a Ph.D. How can you complete your degree in the shortest possible time? Complete your requirements (courses, seminars, etc.) as soon as possible and get an early start on your research project. Work hard and put in long hours (including weekends) on your research project. It is essential that you keep a complete, accurate, and up-to-date Laboratory Notebook and obtain all the data you need (such as for structural characterization of reaction products) as you go along.

Please note that homework and studying are to be done on YOUR time. If you are in a research group, you are expected to be working on your project during the day. When your lab work is done for the day, then you may make time for completing assignments. Try to find a good balance between research and coursework.

For first year students it is particularly important that you make yourself available by spending as much time as possible in locations where you can be easily found (3rd floor graduate student lounge/office, computer lab, etc.). This is especially true if you have a teaching assistantship. Make yourself known to the faculty and learn about their research groups and interests.

1.3. Academic Integrity

Integrity and honesty are the cornerstones of modern science. At all levels, scientists perform experiments and are expected to report their observations in an honest and unbiased manner. At the doctoral level scientists are routinely placed in positions of trust. For example, Ph.D. level scientists are often asked to review manuscripts and grants for scientific accuracy and relevance before they are released to the public. Scientists, as human beings, are not immune to the many temptations for ethical lapses. Pressure to obtain results that are expected in order to retain funding on a project, to inflate the yields of reactions, to ignore significant by-products of reactions, to not record reactions that did not work as planned, to cheat on an exam, to plagiarize on a term paper, to "borrow" an idea from a grant proposal you are reviewing, etc are all very real. Yet the cost of these breaches in integrity, if revealed, could be the end of your career. Students are encouraged to consult and read through the Chemical Professional's Code of Conduct, which can be found at: https://www.acs.org/content/acs/en/careers/career-services/ethics/the-chemical-professionals-code-of-conduct.html. This document was approved

by the Council Committee on Professional Relations of the American Chemical Society on August 28, 2019 and adopted by the Board of Directors on December 6, 2019.

Rutgers University has a Policy on Academic Integrity for Undergraduate and Graduate Students Rutgers University, New Brunswick Campuses. This can be found online at: http://academicintegrity.rutgers.edu/. Rutgers Graduate School New Brunswick also published a pamphlet on Academic Integrity: Issues for Graduate Students, which can be found at https://gsnb.rutgers.edu/academic-integrity-issues-for-graduate-students. Included within this document are definitions of various violations of academic integrity including cheating, fabrication, facilitating academic dishonesty, plagiarism, and denying others access to information or material. A brief description of these terms is given below. For complete descriptions please refer to the website mentioned above.

Cheating – the use of inappropriate or unacknowledged materials, information, or study aids in an academic exercise.
Fabrication – the falsification or invention of information or data.
Facilitating Academic Dishonesty – Knowingly or negligently allowing your work to be used by others when it is expected that each student is to do his/her own work.
Plagiarism – the representation of the words or ideas of another as one's own. Failing to properly cite a direct quote or paraphrase of another's words.
Denying Others Access to Information or Material – making reference works or materials unavailable to others by stealing or defacing books, journals, reserve materials, or altering or deleting computer files belonging to another.

How can you avoid plagiarism when writing an academic or scientific paper? If you use someone else's words in your paper, you must enclose those words in quotation marks and then provide a footnote or reference number that refers to a reference citation in which the original words are reported. If a quotation is used from a book or paper that itself has quoted those same words, your citation must be to the original report. If you paraphrase another author, you would properly cite that section as "to paraphrase so and so's comment..." and then footnote or reference that statement as before. If you copy material directly from a website, you must properly cite that by referencing the exact web address of the page. If you use someone else's words whether they are enclosed in quotes or not, and do not provide a reference or footnote number immediately following those words, then you have committed plagiarism. It is also plagiarism if you use words or ideas from someone else and list those sources among your references but fail to provide a link between the reference and what it refers to in the text.

What are the penalties for violating academic integrity? Rutgers has categorized the various violations into four levels of severity:

Level One – for minor infractions such as working with another student on a laboratory or homework assignment when such work is prohibited; failure to footnote or properly acknowledge in an extremely limited section of an assignment.

Sanctions may include: an assigned paper or research project on a relevant topic; a make-up assignment at a more difficult level; a grade of zero on the assignment. Records of students convicted of Level One offenses are maintained on file until graduation.

Level Two – dishonesty of a more severe nature or affecting a more significant portion of the coursework. Examples include plagiarism on a more extensive level, using data or materials in a lab experiment without acknowledging the source, e.g. if you use a starting material prepared by

someone else but do not acknowledge that fact, receiving assistance from others on an assignment without acknowledging that fact, cheating on a take-home exam.

Sanctions may include receiving a failing grade for the assignment, a failing grade in the course (for cheating on a take-home exam), and disciplinary probation. Records of students convicted of Level Two offenses are maintained on file until graduation.

Level Three – Dishonesty that affects a major or essential portion of work done to meet course requirements. Included here are the following: copying on an hourly or final exam, plagiarism of major portions of a written assignment, facilitating copying during an exam, using prohibited materials during an exam, altering an exam before submitting for regrading, acquiring or distributing an exam from an unauthorized source prior to the exam, presenting someone else's work as your own, using purchased term papers, denying others access to materials, and fabricating data.

Cases of Level Three and Four dishonesty will be brought before a disciplinary board organized by the Dean of the Graduate School. The minimum sanction will be a one semester suspension from the university. Faculty are ethically bound to report convictions of Level Three and Four offenses on any letters of recommendation they may write for the students.

Level Four - The most serious level of dishonesty. Included here is: any violations of academic dishonesty after returning from a suspension, having someone else take an exam for you, fabrication or falsification of data, plagiarism in a thesis, dissertation, manuscript submitted for publication, **or in other work represented as one's own as a graduate student**, sabotaging another students work, willful violation of the ethical code of the profession for which you are preparing (Medicinal Chemistry).

The sanction for Level Four violations is permanent expulsion from the university and a notation of "academic disciplinary separation" permanently attached to your transcript.

As stated in the Rutgers policy: "violations of academic integrity by graduate students will presumably be penalized more severely than violations by first semester first year students." In other words, graduate students should know better! You are here to learn and become proficient in aspects of medicinal chemistry. This will never happen if you copy work from others.

1.4. The Laboratory Notebook

The most important document that you will write as a graduate student is not your thesis or dissertation, but your Laboratory Notebook. Your lab notebook will serve as a record of everything that you do in the laboratory and will be used for years to come by your advisor and other members of the group as a valuable reference source. It will also contain all the experimental data that you will need to write your thesis or dissertation. As you will find after you graduate, your employers will expect you to maintain an accurate, complete, and up to date lab notebook of your laboratory work. Many companies store completed notebooks in fireproof vaults to protect them in the event of an accident. As the lab notebook represents the results of thousands of dollars of research effort, companies do not have much patience with scientists that fail to keep good lab notebooks. They have strict rules regarding the treatment of lab notebooks. Being caught removing a lab notebook from the company will almost definitely result in your immediate firing. Thus, one of the most important responsibilities you will learn in graduate school is how to keep a good lab notebook.

The first thing that you need to understand is that the lab notebook, which will be provided to you by your advisor, is the **property of your advisor**, it does not belong to you. Lab notebooks must **NEVER** be removed from the building. Keep the book on your desk in the lab, not on the lab bench where something could spill on it. Get in the habit of writing everything down in the lab notebook as you are working. Do not wait for the end of the day to fill in details, which by that time, you might have forgotten and never, write things on scraps of paper that belong in the lab notebook. Every page should be dated with the beginning of the experiment. Amounts of starting materials, reagents, catalysts, solvents should be recorded in units of mass or volume. The number of moles (or millimoles) of starting materials, reagents, and catalysts should be recorded. All details of the experiment from set up, to the reaction itself, to the workup, and final purification of the product(s) should be written down. Results of chromatographic monitoring of the reaction should be drawn (not taped) in the notebook. All spectral data for the products should be tabulated in the notebook as they are collected. A physical description of the product (state, color, etc) as well as the yield in grams (or milligrams) and percent should be included, as should the expected yield. Results from independent laboratories (combustion analysis, high resolution mass spectra) should again be written into the lab notebook and not taped to the page. Hard copies of spectra and other data can be kept in three-ring binders.

Failure to maintain a proper lab notebook will result in delays in publishing or presenting your work (since many experiments will then have to be repeated) and delays in preparing your thesis or dissertation. If experiments need to be repeated, this puts an extra financial burden on your advisor. If you continue to be negligent in maintaining a good lab notebook after having deficiencies explained to you by your advisor it is possible that you could a) lose your financial support, b) be removed from the research group and therefore forced to find another advisor, or in extreme cases, c) removed from the program. Remember, your thesis or dissertation will NOT be approved until you have reported all necessary analytical data for each of your new compounds (see p. 9 or 12 for details on characterizing new compounds).

1.5. Selecting an Advisor

Some students enter the program knowing exactly whom they wish to have as their research advisor. Most students, however, have only a vague idea of the types of research opportunities that exist. It is suggested that students review the web sites of the professors that are part of the program. The student should then contact several faculty members to set up individual meetings at which they can gain greater insight into the types of research projects that are available. **You should make arrangements to work with an advisor by the end of your first semester at Rutgers**. A listing of faculty members who can serve as research advisors (department in parenthesis), arranged according to research interests is shown below.

Synthetic Chemistry
Dr. Longqin Hu (Medicinal Chemistry)
Dr. Matthew Moschitto (Medicinal Chemistry)
Dr. Jun Wang (Medicinal Chemistry)
Dr. Joel Freundlich (Pharmacology, Physiology & Neuroscience – NJMS)
Dr. Leslie Jimenez (Chemistry)
Dr. Lawrence Williams (Chemistry)

Computational Chemistry
Dr. John Kerrigan (CINJ)
Dr. William Welsh (Robert Wood Johnson Medical School)
Dr. Vlad Kholodovych* (RBHS, OIRT/High Perf & Research Comp)

Natural Products Isolation and Structure Elucidation
Dr. James Simon (Cook College)
Dr. Chi-Tang Ho (Cook College)
Dr. Qing-Li Wu* (Cook College)

Antiviral Drugs and Vaccines
Dr. Edward Arnold (Chemistry)

---

* Associate Members – MS students only

2. Seminars

Seminars are usually held in either the department conference room (323A) on the 3rd floor or in another classroom in the Pharmacy building. Most seminars are from 12:00-1:00 on Tuesdays throughout the semester and will be announced in advance. **ALL students are expected to attend ALL seminars.** However, you should **only register** for the course, Seminar in Medicinal Chemistry (16:663:601,602), in the semester in which you plan to **present** your seminar. Students in the M.S. program must present one seminar, while Ph.D. students must present two seminars. Attendance is taken at all seminars. If you have two or more unexcused absences in any semester you will be required to prepare and present an additional seminar during the following semester.

When you decide that you want to present a seminar you will go to the seminar link on the website and review the guidelines posted there and then speak to the Seminar Coordinator, Dr. Matthew Moschitto. He will approve your topic (cannot be directly related to your research project) before you proceed. Consult the guidelines again for preparing your seminar (https://pharmacy.rutgers.edu/med-chem-seminar-schedule). One – two weeks prior to your presentation you must provide a copy of your abstract to the department administrator (Elissa Glinn; elissa.glinn@pharmacy.rutgers.edu) electronically as a Word or pdf file using the appropriate template provided to you. This will be printed and posted around the building. It will also be posted on the web site. Prepare your seminar using PowerPoint. Plan on having your talk last for about 45 minutes, with 15 minutes for questions.

3. The Master of Science Program

Two options are available within the M.S. program:

- **M.S. with thesis**. *For **full-time** students that wish to obtain an entry-level laboratory position within the pharmaceutical industry*. At least 25 course credits are required (including one credit of Seminar in Medicinal Chemistry). A student selects a research adviser and completes an original research project under his or her direction. The student then writes and defends a thesis to complete the degree requirements.
- **M.S. without thesis**. Thirty-one course credits are required (including one credit of Seminar in Medicinal Chemistry and three credits in *Non-Thesis Masters Programmatic Study in Medicinal Chemistry* (16:663:620)). In the *Non-Thesis Masters Programmatic Study in Medicinal Chemistry* (16:663:620), students are required to write a literature review or conduct a small research project that has been approved by an advisor culminating with a final written critical essay. The literature review or the critical essay must be submitted and defended before your committee.

Students in the Ph.D. program do not earn a M.S. degree along the way. The M.S. degree curriculum is outlined below:

Required Core Courses (16 credits)

- Medicinal Chemistry: Research Techniques and Principles (16:663:501) - Fall
- Principles of Drug Design (16:663:502) - Spring
- Heterocycles in Medicinal Chemistry (16:663:506) - Spring
- Interpretation of Organic Spectra (16:160:515) – Spring
- Modern Synthetic Organic Chemistry (16:160:503) – Fall
- Seminar in Medicinal Chemistry (16:663:601 or 602)

Electives: 9 Credits for thesis M.S. and 12 credits for non-thesis M.S. from the approved list.
Research in Medicinal Chemistry (16:663:701,702) (6 credits) – thesis option.
Non-Thesis Masters Programmatic Study in Medicinal Chemistry (16:663:620) (3 credits) – non-thesis option

You must select a research advisor by the end of your first semester of full-time study. It is recommended that you begin your research project as soon as possible. You should plan on working in the lab year-round to minimize the amount of time to earn your degree. Together with your advisor you will select two other faculty members from the medicinal chemistry program to serve on your M.S. Thesis Committee. Your committee is a valuable resource for suggestions relating to your research project. As your research project nears its end you will begin writing your thesis. This is an iterative process between you and your advisor, with your advisor offering corrections and suggestions for improving the written document. The School of Graduate Studies – New Brunswick requires that you strictly adhere to their guidelines when preparing your thesis or dissertation. A style guide can be found online at https://gsnb.rutgers.edu/academics/electronic-thesis-and-dissertation-style-guide. This guide gives detailed information about the order and physical layout of pages in the written document, margins, type of paper required, etc.

While the School of Graduate Studies - New Brunswick does not specify any criteria for the characterization of new compounds, this is central to medicinal chemistry and this program requires that all new compounds be adequately characterized. This means that you should include tabulated ^{1}H and ^{13}C-NMR spectra for all new compounds, IR spectra, where appropriate

(listing all peaks that are diagnostic for specific functional groups). Proof of composition should be included wherever possible. This can be either high-resolution mass spectral or combustion analysis results. Specific rotations should be reported for optically active compounds. Other data can be reported as necessary. In general, criteria for characterization should conform to that specified in the American Chemical Society Guidelines for Authors (http://pubsapp.acs.org/paragonplus/submission/jmcmar/jmcmar_authguide.pdf?). For all compounds the color and physical form (solid, liquid, oil, etc) should be specified and a melting point should be reported for solids. The mass (or volume) and the number of moles (mmol or μmol) of all reactants and reagents and the mass and percent yield of all products should be reported.

When a suitable document has been completed, you will schedule a date for your defense and submit copies to each member of your committee (allow them at least two weeks to read the thesis). During the defense, the members of your committee will ask questions about the work you performed. They may also ask questions relating more to your general background and preparation. Suggestions may also be made for ways to improve the written thesis. It is wise to act on these suggestions and make the necessary corrections or additions to the thesis. When everyone is satisfied that you have met all the requirements for the M.S. degree in Medicinal Chemistry, they will sign the appropriate forms. You will also need to submit those forms as well as a final copy of your thesis to the School of Graduate Studies as per their website requirements (https://gsnb.rutgers.edu/academics/how-apply-degrees). All degrees and diplomas are conferred at the May commencement ceremony, but students who file their application and complete all degree requirements by the announced deadlines in October or January will have their diplomas dated accordingly.

3.1. Suggested Timeline for full-time M.S. (Thesis Option) in Medicinal Chemistry

Year 1			
Fall	**Winter Break**	**Spring**	**Summer**
Courses • Medicinal Chemistry: Research Techniques and Principles • Modern Synthetic Organic Chemistry • Elective – Laboratory Rotation		*Courses* • *Either* Principles of Drug Design [runs in alternate years] *or* Heterocycles in Medicinal Chemistry • Interpretation of Organic Spectra • Elective	
Other • Start thinking about a research advisor	*Other* • **Select Advisor** • Begin research	*Other* • Start thinking about a seminar topic	*Other* • Research

Year 2			
Fall	**Winter Break**	**Spring**	**Summer**
Courses • Elective • Elective		*Courses* • *Either* Principles of Drug Design *or* Heterocycles in Medicinal Chemistry • Seminar in Medicinal Chemistry	
Other • Research • Start preparing your seminar	*Other* • Research	*Other* • Research	*Other* • Research

Year 3			
Fall	**Winter Break**	**Spring**	**Summer**
• Research • Write Thesis	• Defend Thesis		

3.2. Suggested Timeline for full-time M.S. (Non-Thesis Option) in Medicinal Chemistry

Year 1			
Fall	**Winter Break**	**Spring**	**Summer**
Courses • Medicinal Chemistry: Research Techniques and Principles • Modern Synthetic Organic Chemistry • Elective		*Courses* • *Either* Principles of Drug Design [runs in alternate years] *or* Heterocycles in Medicinal Chemistry • Interpretation of Organic Spectra • Elective	
Other • Start thinking about an advisor	*Other* • **Determine an Advisor**	*Other* • Start thinking about a seminar topic	*Other* • Non-Thesis Masters Study in Medicinal Chemistry

Year 2			
Fall	**Winter Break**	**Spring**	
Courses • Elective • Elective		*Courses* • *Either* Principles of Drug Design *or* Heterocycles in Medicinal Chemistry • Seminar in Medicinal Chemistry • Enroll in *Non-Thesis Masters Programmatic Study in Medicinal Chemistry*	
Other • Non-Thesis Masters Study in Medicinal Chemistry • Start preparing your seminar	*Other* • Non-Thesis Masters Study in Medicinal Chemistry	*Other*	

4. The Doctor of Philosophy Program

Most students elect to go directly for their Ph.D. upon entering the program. The curriculum is identical to that for the M.S. degree with the following exceptions:

- Molecular Biology and Biochemistry (16:115:511) is required
- Students must present two seminars instead of one
- 15 Credits of approved electives are required instead of 9 credits
- All Ph.D. candidates must prepare and defend an Independent Research Proposal (16:663:540) to qualify for PhD candidacy

Required Core Courses for Ph.D. (23 credits)

- Medicinal Chemistry: Research Techniques and Principles (16:663:501) – Fall
- Principles of Drug Design (16:663:502) – Spring
- Heterocycles in Medicinal Chemistry (16:663:506) – Spring
- Interpretation of Organic Spectra (16:160:515) – Spring
- Modern Synthetic Organic Chemistry (16:160:503) – Fall
- Molecular Biology and Biochemistry I (16:115:511) - Fall
- Independent Research Proposal (16:663:540)
- Seminar in Medicinal Chemistry, two (16:663:601 or 602)

Electives: 15 Credits from approved list.
Research in Medicinal Chemistry (16:663:701,702) (34 credits).

You must select a research advisor by the end of your first semester of full-time study. It is recommended that you begin your research project as soon as possible. You should plan on working in the lab year-round to minimize the amount of time needed to earn your degree. Together with your advisor you will select two other faculty members from the medicinal chemistry program and one committee member (must be a Ph.D.) from outside the program to serve on your Ph.D. Dissertation Committee. The outside member can be from a different department at Rutgers or from industry (but must not be a member or former member of the research groups of any of the other committee members). Your committee is a valuable resource for suggestions relating to your research project. After all your course work and seminars have been completed you should consider beginning work on your Independent Research Proposal. This must be your own work and not directly related to your research project. It is to be written using the same format used by professors when submitting grants to the National Institutes of Health (NIH), subject to the same page limitations. When complete (your advisor cannot edit it for you), schedule a meeting of the committee and submit copies of the written document to each member (allow at least two weeks for them to read the proposal). At the scheduled meeting, you will present your proposal to the committee (PowerPoint). Members of the committee may ask questions about anything in the proposal or about your general preparation. If you are successful with your proposal, your committee members will then sign paperwork which you will need to submit to the School of Graduate Studies and you will be formally admitted into candidacy for a Ph.D. degree. Thus, the Independent Research Proposal serves as the qualifying examination.

Shortly after being admitted into candidacy for the Ph.D. degree, you must arrange a meeting with your committee to review the scope of the project you are working on, your results up to the present time, and your plans for future experiments. This meeting gives the other members of your committee an opportunity to learn about your project, make sure that it is broad enough in scope for a Ph.D. dissertation, and to offer suggestions for improving the project. It also ensures that there are no unpleasant surprises when you defend your dissertation. As your research

project nears its end, you will begin writing your dissertation. This is an iterative process between you and your advisor, with your advisor offering corrections and suggestions for improving the written document. The School of Graduate Studies – New Brunswick requires that you strictly adhere to their guidelines when preparing your thesis or dissertation. A style guide can be found online at https://gsnb.rutgers.edu/academics/electronic-thesis-and-dissertation-style-guide. This guide gives detailed information about the order and physical layout of pages in the written document, margins, type of paper required, etc.

While the School of Graduate Studies - New Brunswick does not specify any criteria for the characterization of new compounds, this is central to medicinal chemistry and this program requires that all new compounds be adequately characterized. This means that you should include tabulated ^{1}H and ^{13}C-NMR spectra for all new compounds, IR spectra, where appropriate (listing all peaks that are diagnostic for specific functional groups). Proof of composition should be included wherever possible. This can be either high-resolution mass spectral or combustion analysis results. For optically active compounds the specific rotation should be reported. Other data can be reported as necessary. In general, criteria for characterization should conform to that specified in the American Chemical Society Guidelines for Authors (http://pubsapp.acs.org/paragonplus/submission/jmcmar/jmcmar_authguide.pdf?). For all compounds the color and physical form (solid, liquid, oil, etc) should be specified and a melting point should be reported for solids. The mass (or volume) and the number of moles (mmol or μmol) of all reactants and reagents and the mass and percent yield of all products should be reported.

When a suitable document has been completed, you will schedule a date for your defense and submit copies to each member of your committee (allow them at least two weeks to read the dissertation). During the defense, the members of your committee will ask questions about the work you performed. They may also ask questions relating more to your general background and preparation. Suggestions may also be made for ways to improve the written dissertation. It is wise to act on these suggestions and make the necessary corrections or additions to the thesis. When everyone is satisfied that you have met all the requirements for the Ph.D. degree in Medicinal Chemistry, they will sign the appropriate forms. You will then need to submit those forms as well as a final copy of your dissertation to the School of Graduate Studies as per their website requirements (https://gsnb.rutgers.edu/academics/how-apply-degrees). All degrees and diplomas are conferred at the May commencement ceremony, but students who file their application and complete all degree requirements by the announced deadlines in October or January will have their diplomas dated accordingly.

4.1. Recommended Timeline for Ph.D. in Medicinal Chemistry

Year 1			
Fall	**Winter Break**	**Spring**	**Summer**
Courses • Medicinal Chemistry: Research Techniques and Principles • Modern Synthetic Organic Chemistry • Elective – Laboratory Rotation • Elective		*Courses* • *Either* Principles of Drug Design [course runs in alternate years] or Heterocycles in Medicinal Chemistry • Interpretation of Organic Spectra • Elective	*Courses* • Register for up to 6 credits of Research in Medicinal Chemistry if you had a TA during the academic year
Other • Start thinking about a research advisor through laboratory rotations	*Other* • **Determine an Advisor** • Begin Research	*Other* • Research	*Other* • Start thinking about a seminar topic

Year 2			
Fall	**Winter Break**	**Spring**	**Summer**
Courses • Elective • Elective • Molecular Biology and Biochemistry I		*Courses* • *Either* Principles of Drug Design *or* Heterocycles in Medicinal Chemistry • Elective • Seminar in Medicinal Chemistry	*Courses* • Register for up to 6 credits of Research in Medicinal Chemistry if you had a TA during the academic year
Other • Research • Start preparing your first seminar	*Other* • Research	*Other* • Research	*Other* • Research • Start planning your next seminar

Year 3			
Fall	**Winter Break**	**Spring**	**Summer**
Courses • Seminar 2 in Medicinal Chemistry		*Courses* • Independent Research Proposal	
Other • Research • Start thinking about your Ind Research Proposal	*Other* • Research	*Other* • Research • Research Meeting with Committee	*Other* • Research

Year 4			
Fall	**Winter Break**	**Spring**	**Summer**
Other • Research • Start writing your dissertation	*Other* • Research	*Other* • Research	*Other* • Research

Year 5			
Fall	**Winter Break**	**Spring**	**Summer**
• Research • Complete dissertation	• Defend Dissertation		

5. PharmD/PhD dual degree program in Medicinal Chemistry

The Ernest Mario School of Pharmacy has established a joint PharmD/PhD program to meet the needs of interests of highly motivated PharmD students. The program enables students to complete both degrees in approximately nine years by beginning their PhD coursework and research while still enrolled in the PharmD program. Our graduate program joined the dual degree program starting in 2014.

The dual degree PharmD/PhD can arrange to take graduate level courses in their PharmD professional years, and matriculate into the Graduate Program in Medicinal Chemistry at the end of their 2nd professional year in the PharmD program. These students will continue to finish their PharmD degree and graduate with their classmates at the end of their P4 year while their course work during the P3 and P4 year will be tailored to meet the requirements for the Ph.D. degree in Medicinal Chemistry (see the Recommended Timeline for PharmD/PhD in Medicinal Chemistry).

- Students will take two core courses: Medicinal Chemistry: Research Techniques and Principles (30:715:451) and Principles of Drug Design (30:715:452) in their professional years (most likely P1 or P2) to give a total of 6 credits of core courses. These are already offered as electives for PharmD students.

  6 grad cr

- After their admission into dual degree PharmD/PhD in Medicinal Chemistry, they will spend their P2 summer taking Laboratory Rotation in Medicinal Chemistry (16:663:508)

  3 grad cr

- In the 3rd professional year the dual degree students will be advised to take Modern Synthetic Organic Chemistry (16:160:503) in the fall and either Heterocycles in Medicinal Chemistry (16:663:506) or Strategies and Tactics in Synthetic Medicinal Chemistry (16:663:504) in the spring.

  6 grad cr

- In the summer prior to their rotations in the P4 year, the dual degree students will take another 3 credits of research.

  3 grad cr

- In the P4 year, the dual degree students are required to do eight required Advanced Pharmacy Practice Experiences as part of their PharmD. They will take up to 9 credits of graduate course work. Most of the graduate courses are offered early in the morning or late in the evening; Scheduling should not be too difficult.

  6 grad cr

- By now the dual degree students should already have finished about 21 credits of course work and 3 credits of research towards their PhD in Medicinal Chemistry.
- Starting the summer after their graduation with PharmD, the dual degree students will remain in graduate school and work full time with a mentor and an advisory committee for approximately three years predominantly on their dissertation research while finishing a few remaining required/elective courses. Therefore, students can fulfill the requirements of both degrees in six plus three years.

5.1. PhD Curriculum in Medicinal Chemistry for PharmD/PhD Dual Degree Students

GRADUATE PROGRAM IN MEDICINAL CHEMISTRY

Required (20 credits)

16:663:501: **Medicinal Chemistry: Research Techniques and Principles**
16:663:502: **Principles of Drug Design**
16:160:503: **Modern Synthetic Organic Chemistry**
16:160:515: **Interpretation of Organic Spectra**
16:663:506: **Heterocycles in Medicinal Chemistry**
16:663:540: **Independent Research Proposal**
16:663:601 or 602: **Seminar in Medicinal Chemistry**, two

Electives (12 Credits from the following approved list or others with approval of program director)

16:663:508: **Laboratory Rotation in Medicinal Chemistry**
16:160:511: **Advanced Organic Chemistry I**
16:160:512: **Advanced Organic Chemistry II**
16:160:575: **Principles of Organometallic Chemistry**
16:160:602: **Advanced Inorganic Chemistry**
16:115:504**: Biochemistry**
16:115:511: **Molecular Biology and Biochemistry**
16:115:512: **Molecular Biology and Biochemistry II**

Research in Medicinal Chemistry (16:663:701,702) (40 credits).

5.2. Recommended Timeline for PharmD/PhD in Medicinal Chemistry

Year	Courses	Cr	Room	Time	Accrued Credits*	
					Course	Res
P1-P2	• **Medicinal Chemistry: Research Techniques and Principles** (16:663:501) – P1 fall/P2 fall elective • **Principles of Drug Design** (16:663:502) – P2 spring elective	3 3			6	0
Admission to the PharmD/PhD Dual Degree Program and into the Graduate Program in Medicinal Chemistry						
P2 Summer	• **Laboratory Rotation in Medicinal Chemistry** (16:663:508)	3	Various	TBA	9	0
P3 Fall	• **Modern Synthetic Organic Chemistry** (16:160:503)	3			12	0
P3 Spring	• **Heterocycles in Medicinal Chemistry** (16:663:506) or • Elective	3 3			15	0
P3 Summer	• Dissertation Research Credits	3	Various	TBA	15	3
P4 Fall	• **Interpretation of Organic Spectra** (16:160:515)	3			18	3
P4 Spring	• Elective	3			21	3
P4 Summer	• Dissertation Research Credits	3	Various	TBA	21	6
Grad 1 Fall	• Unfinished required courses or electives plus Dissertation Research • **Seminar in Medicinal Chemistry** (16:663:601)	3 7 1			25	13
Grad 1 Spring / summer	• Unfinished required courses or electives plus Dissertation Research • **Independent Research Proposal** (16:663:540)	3 7 3			31	20
Grad 2 Fall	• **Seminar in Medicinal Chemistry** (16:663:602) • Dissertation Research	1 8			32	28
Grad 2 Spring / summer	• Dissertation Research	9			32	37
Grad 3	• Dissertation Research, Writing, and Defense	3			32	40

*Accrued credits shown are course credits and research credits estimated towards PhD in Medicinal Chemistry. Total required number of credits for a PhD at Rutgers is 72. Courses taken during the P3-P4 years should not conflict with the courses and rotations required for the PharmD degree.

6. Academic Requirements

Rutgers University will not confer graduate degrees (either M.S. or Ph.D.) to students having a grade point average (GPA) < 3.00. Rutgers also limits the number of grades of C or C+ work that a graduate student can use to fulfill degree requirements. It is the policy of the Medicinal Chemistry Graduate Program to limit students to a MAXIMUM of two grades of C or C+. Ph.D. students that exceed two C/C+ grades will not be allowed to continue towards a Ph.D. and will instead be reclassified as terminal M.S. students.

7. Departmental Resources

The Department of Medicinal Chemistry is equipped with most of the instrumentation and resources that you will need to complete your research project.

7.1. Instrumentation

- Bruker Avance III 400 Multinuclear NMR Spectrometer (400 MHz)
- Thermo Nicolet Avatar Model 360 FTIR
- Perkin Elmer Model 1600 FTIR
- Hewlett-Packard Model 5972 Gas Chromatograph/Mass Spectrometer System
- Shimadzu Model 2010 Liquid Chromatograph/Mass Spectrometer
- Perkin Elmer Model 241 Multi-Wavelength Polarimeter
- Hewlett-Packard Model 8451A Diode-Array UV/Vis Spectrometer
- Hitachi Model U-2000 UV/Vis Spectrophotometer
- Shimadzu Model PC1200 UV/Vis Spectrophotometer
- BIAcore 3000, surface plasmon resonance biosensor
- Hewlett Packard Model 1090M HPLC Systems – several
- Varex Versa Prep Preparative HPLC System
- Shimadzu HPLC System
- Waters Associates HPLC Systems - several
- Spectra Physics HPLC System
- Hewlett Packard Diode-Array Detectors
- Hewlett Packard Fluorescence Detectors
- Radiomatic Model IC Flow-Thru Beta-Detector
- IN/US Beta-Ram Flow-Thru Detector
- Hewlett Packard Model 5890A GC – several
- Hewlett Packard Model 5890A Series II GC – several
- Perkin Elmer Model 3920B GC

In addition, available equipment used in synthetic chemistry includes:

- Parr Hydrogenation Apparatus
- Polymetrics Model T-408 Ozone Generator
- Parr Autoclave Reactor
- Ace Photochemical Reactors
- Thermolyne Type 21100 Tube Furnace for Flash Vacuum Pyrolysis
- Harrison Research Model 8924 Chromatotrons - several
- Cryocool Model CC-100II Immersion Cooler
- Advanced ChemTech Model 90 Peptide Synthesizer

Other miscellaneous pieces of equipment include:

- Beckman Model L7-55 Ultracentrifuge
- Beckman Model J2-21M Centrifuge
- Beckman GPR Tabletop Centrifuge
- Beckman LS5 Liquid Scintillation Counter
- Leitz Laborlux 11 POL Microscope
- Dubnoff Shaking Incubators
- Harris Low Temperature Freezers
- Nuair Biological Safety Cabinet
- Lab Care America CO_2 Incubator, Model 7101-0

7.2. Computational Laboratory

The Computational Laboratory of the Medicinal Chemistry Department is located on the 3rd floor of the Pharmacy Building, Room 321. The facility has 8 Dell Core 2 Duo workstations. These workstations are all loaded with Windows 10, Microsoft Office, ChemDraw Ultra 17.0, and most run the Spartan06 (Wavefunction, Inc.) software package complete with routines for performing a vast array of molecular mechanics (Tripos Force Field & MMFF94), semi-empirical quantum chemical (MNDO, AM1 & PM3), ab initio (3-21G*, 6-31G*), and density functional (SVWN & BP) calculations. For presentation of graphics and illustration work, the facility is equipped with a 50" plasma display, a Tektronics Phaser 740 color laser printer (1200 x 1200 dpi resolution), HP 2100TN b&w laser printer (1200 x 1200 dpi resolution), and a Hewlett Packard Color Scanner. In addition to these facilities students also have access to the numerous computer centers located throughout the Rutgers Campuses. Students and faculty with an account from the Rutgers University Computer Services can access the UNIX-based mainframe computers, internet 2, and high-performance computing.

7.2.1. Responsibilities of Computer Lab Users

The computer lab is a resource that may be used in certain courses and in your research. Each computer in the lab is equipped with antiviral software that is updated automatically. Despite that, you should not load any questionable files via download or by portable media. These computers are not to be used to view pornography or other questionable content from the internet. If you are working on one of these computers and wish to save your file you must supply your own flash drive. **Files are not to be saved on the hard drives**.

The room and desks should be kept clean. **Eating and drinking in the computer lab is strictly prohibited**. Trash should be properly disposed of in the receptacle. Do not waste paper. Paper, and toner cartridges for the printers, is purchased from the departmental budget. Therefore, **print only what is absolutely necessary**. If there is a problem with any computer or printer, immediately inform one of the faculty members so it can be quickly resolved. Access to the color laser printer is limited. Please see Elissa Glinn if you need color printing for a publication or presentation.

7.3. Conference Room

The Medicinal Chemistry Conference Room (323A) is located on the 3rd floor of the Pharmacy Building. This room is equipped with the latest audio-visual equipment for use in presentations and courses. Included here is a mini TV camera, audio system, DVD recorder, projector, and visualizer/overhead projector. The room is used for small classes, meetings, thesis and dissertation defenses, and seminars. It is not to be used as a lunchroom. Please treat all the furnishings with respect and keep the room clean. If you use it for a meeting, please be sure to return all chairs to their proper locations, erase the whiteboard, raise the screen, and turn off the lights when leaving. Also be sure to lock the door as you leave the room. Please notify Elissa Glinn if you notice any damage to the room or if any of the equipment is not working properly.

8. University Resources

In addition to equipment located within the Medicinal Chemistry Department there is a wealth of other facilities and equipment located in other departments. A sampling of such equipment and services is listed below:

8.1. Instrumentation and Services

- 400, 500, 600, 800 MHz NMR Spectrometers
- A variety of mass spectrometers (MALDI, high resolution, GC/FTIR/MS, MS/MS)
- X-Ray Crystallography facilities
- Peptide Synthesizers
- Glassblowing shop
- Machine Shop
- Electronics Shop
- Rutgers High Performance Computing Facility

8.2. Rutgers University Library System

Rutgers University maintains an excellent library system consisting of 26 libraries scattered among the New Brunswick/Piscataway, Newark, and Camden campuses, plus RU-OnLine, the digital library. Of most importance to the Medicinal Chemistry program are the Library of Science and Medicine (LSM), located adjacent to the Pharmacy Building, and the Chemistry Library, also located on Busch Campus. LSM houses a vast collection of journals and books mainly in the biomedical sciences area, hard-bound copies of Chemical Abstracts, and some chemistry journals and books. The Chemistry Library collection includes books and journals, Chemical Abstracts, Beilstein, and other reference works. RU-Online lists thousands of titles of on-line editions of journals allowing for desktop printing of full-text articles. The collection of chemistry-related journals is impressive. Unlimited access to all American Chemical Society journals back to the first volume of each is allowed. On-line databases are critical for rapidly obtaining information related to your research projects. At Rutgers we have unlimited access to Beilstein CrossFire for structure-based searches of organic chemicals. SciFinder Scholar is the electronic version of Chemical Abstracts that allows for structure and text-based searching. Another database of interest is the Web of Science, the electronic version of the Science Citation Index.

9. Miscellaneous Information

9.1. Special Issues for International Students

Rutgers Global is available to answer all questions relating to policies, laws, and procedures relating to international students. Please visit their web site at: https://global.rutgers.edu/. Students that have been awarded a Teaching Assistantship will be required to take an English Language Examination. Based upon the results of that test you will either be cleared for full duties as a TA, restricted to non-instructional duties, or required to take an English Language course (grade does not affect your GPA). It is important for non-English speaking students that you practice your English language skills as much as possible. You should therefore speak ENGLISH ONLY in the laboratory and avoid speaking with other students in your native language. When you write papers, seminar slides, or your thesis or dissertation you should enlist the help of other English-speaking students to review what you have written for grammar and style. Faculty members have little time for rewriting an entire thesis. Finally, while it is possible to travel to your home country with the necessary documentation, you must realize that with the current state of affairs in the world there might be delays in getting back into the United States. Please take this into account when making travel plans.

9.2. Financial Support

Outside of external fellowships there are two main mechanisms for financial support of graduate students, teaching assistantships and graduate assistantships. There is no separate application process for this support. In some cases, entering students are supported as teaching assistants (TAs). Such support is offered for up to two years to students with Department of Medicinal Chemistry faculty advisors. At that point if their advisor has money from a research grant, the student is typically supported as a graduate assistant (GA). Money for TA positions is given to the department from the university. A TA position includes a stipend, full tuition remission and fees, and health benefits. The Medicinal Chemistry Department has a limited number of TA positions that it can offer. Those positions are awarded on a first come, first serve basis. Other departments, including Life Science and Chemistry, often have unfilled TA positions. In the past several students in the Medicinal Chemistry graduate program have been supported as TAs from these other departments. Since these other departments often do not know until the start of classes whether everyone that was offered a TA position will actually attend Rutgers, those positions often become available at or near the start of the semester. In some cases, students that do not get a TA in the Fall semester, may obtain a position at the start of the Spring semester.

Students are encouraged to make use of the GradFund (Office of Graduate Student External Grants and Fellowships) website (https://gradfund.rutgers.edu). Its mission is to assist graduate students throughout the process of identifying and applying for external fellowships and grants. GradFund offers individual meetings to discuss funding opportunities with graduate students as well as workshops, presentations and mentoring programs. Students may also want to look at the Office of Financial Aid website (https://financialaid.rutgers.edu) as well as the School of Graduate Studies website for additional funding opportunities.

If you obtain a TA in Medicinal Chemistry your duties will typically include helping to proctor examinations, grading exams and quizzes, and conducting small group weekly (usually < 10 students) recitation sessions. If your TA is from Life Science or Chemistry, you will typically be supervising a laboratory session and grading papers. Your TA duties cannot require working

more than 15 hours per week. Students that are supported as GAs are expected to work in the laboratory on their research projects.

If you are supported as a TA or a GA, you are expected to be conscientious about performing your duties. Teaching Assistants who do not show up when expected for recitation sessions or for proctoring exams, or that do not do their share of grading exams and quizzes will not be renewed for a second year. Along the same lines, a GA that spends only minimal time in the lab and does not give good effort will find their advisor less likely to renew their support for subsequent years. We offer no guarantee of support.

9.3. Transferring Credit from another Institution

Students that have taken graduate courses at another U.S. institution may complete an application to have some of those credits transferred to Rutgers. The student must consult with his/her advisor about which courses might be transferred. The student must then obtain the necessary application from Elissa Glinn and get it signed by the Graduate Director (Professor Hu), who must approve the list of courses to be transferred. Only graduate level courses related to the Medicinal Chemistry curriculum completed at a U.S. school with a grade of B or better may be transferred, and then, only at the discretion of the Graduate Director. The student must complete the application and submit a transcript along with the Application for Transfer of Credit to the Office of the Dean of the School of Graduate Studies - New Brunswick, 25 Bishop Place, New Brunswick, NJ. No student may transfer any credits until 12 credits of graduate level course work have been completed at Rutgers with a grade of B or better. For Ph.D. students, no more than 24 credits may be transferred. M.S. students may transfer no more than 12 credits of course work. Credit is not given for courses taken more than six years prior to the application for transfer of credits.

9.4. Food/Meals

The Medicinal Chemistry program is headquartered in the Ernest Mario School of Pharmacy on the Busch Campus of Rutgers University in Piscataway, New Jersey. Busch Campus is separated from the city of New Brunswick by the Raritan River and the John Lynch Memorial Bridge and as such is a little isolated. If you have on-campus housing, you can of course eat at home. There are other locations at which meals can be purchased. Adjacent to the School of Pharmacy is the Robert Wood Johnson Medical School (RWJMS). There is a cafeteria (Woody's) located on the ground floor (a 1-minute walk) that serves a variety of hot and cold food and beverages. About a 10-minute walk in the opposite direction takes you to the Busch Student Center, which has a food court offering several options including deli, pizza, oriental food, and a coffee shop. If you have access to a car you can drive to Stelton Road on which is located several fast food and sit-down restaurants. You can also drive or (better) take the campus bus to the College Avenue Campus in New Brunswick where you will find many places to eat.

9.5. Recreation

There is much to see and do in and around New Brunswick including museums, theaters, movies, and sports. New Brunswick is also located centrally between New York City and Philadelphia. Access to each city is only a train ride away from the New Brunswick station.

9.6. Careers

Rutgers University is located in an area that is surrounded by the highest concentration of pharmaceutical industries in the world. Graduates of our program are in high demand. When companies send notification of employment possibilities, they are forwarded to all faculty members of the program.

APPENDIX

List of Elective Courses – Not all available each semester

(Other courses not listed may be accepted for program credit but require advanced approval from Graduate Director – please submit course syllabus with your request)

- Laboratory Rotation in Medicinal Chemistry (16:663:508) - Fall
- Advanced Organic Chemistry I (16:160:511) - Fall
- Advanced Organic Chemistry II (16:160:512) - Spring
- Principles of Organometallic Chemistry (16:160:575) - Spring
- Advanced Inorganic Chemistry (16:160:571) - Fall
- Biochemistry (16:115:503, 504) - Either Fall or Spring
- Molecular Biology and Biochemistry I (16:115:511) - Fall
- Molecular Biology and Biochemistry II (16:115:512) - Spring