

University of Florida
College of Public Health & Health Professions Syllabus
PHC 6XXX: Artificial Intelligence in Toxicology and Environmental Health (3 credit hours)

Semester: Spring 2023
Delivery Format: On-Campus
Location: HPNP G-105
Time: 9:35am to 12:35pm

Instructor Name: Zhoumeng Lin, BMed, PhD, DABT, CPH
Room Number: 4156, HPNP Building
Phone Number: 352-273-6160
Email Address: linzhoumeng@ufl.edu
Office Hours: Friday, 2:00 pm to 3:00 pm
Co-Instructor: Wei-Chun Chou, PhD, Building 471, Room 4, w.chou@ufl.edu
Teaching Assistant: to be named
Preferred Course Communications (e.g., email, office phone): Discussion Board on Canvas and Office hours (in-person and/or via Zoom)

Prerequisites: PHC 6304 Environmental Toxicology Applications in Public Health or with permission from the instructor

PURPOSE AND OUTCOME

Course Overview

This course will discuss fundamental principles, methodology and applications of using machine learning and artificial intelligence approaches to study research questions on toxicology and environmental health, including physiologically based pharmacokinetic (PBPK) modeling, quantitative structure-activity relationship (QSAR) modeling for toxicity prediction, quantitative adverse outcome pathway analysis, air pollution, and ecotoxicological assessment.

Relation to Program Outcomes

This course fits to the MS and PhD programs of study in environmental Health, one Health and toxicology because students will benefit from this course by learning quantitative modeling and analysis skills and advanced machine learning and artificial intelligence approaches to study the impact of environmental chemicals on human health, environmental health, and animal health. This course will also be beneficial to students in the graduate certificate program of "Artificial Intelligence in Public Health and Healthcare" because the course content is within the scope of this certificate program. This course is unique relative to other course offerings because the application of machine learning and artificial intelligence approaches in toxicology and environmental health is an emerging field and has not been thoroughly discussed in existing courses.

Course Objectives and/or Goals

Upon successful completion of this course, students will be able to:

1. Describe different toxicology and environmental health research topics that can be studied with machine learning and artificial intelligence approaches

2. Compare and contrast different machine learning and artificial intelligence approaches in studying a specific toxicology and environmental health research question and identify an optimal approach
3. Critically evaluate the strengths and limitations of studies that apply machine learning and artificial intelligence approaches to investigate toxicology and environmental health research problems
4. Design a study that uses appropriate machine learning, artificial intelligence, toxicology, and environmental health approaches to study the exposure, toxicokinetic, toxicity, risk, and impact on human health of environmental chemicals

Instructional Methods

This course is offered weekly, in-person. The instructional methods will include assigned readings, lectures, computational modeling and analysis demo using a recent publication as a case study, student presentations, class discussions, and assignments that include written critique and oral presentation formats.

1. Relevant reading materials will be assigned prior to the start of each week.
2. Each week there will be a lecture to introduce the principles of applying different machine learning and artificial intelligence approaches to different toxicology and environmental health research questions.
3. There will also be a lecture to demo how to perform computational modeling and analysis to reproduce the results of a recent publication as a case study.
4. Each week one student is assigned to present a selected recent publication, including the strengths, limitations, applications of machine learning and artificial intelligence approaches, as well as major findings.
5. Each week the class will be concluded with class discussions to make sure all students are engaged and students' questions are answered by the end of the class.

DESCRIPTION OF COURSE CONTENT

Topical Outline/Course Schedule

Week	Date(s)	Topic(s)	Readings
1	01/09/22-01/15/22	<ul style="list-style-type: none"> • Course Overview and Expectations • Introduction of Machine Learning and Artificial Intelligence in Toxicology and Environmental Health 	Lin and Chou (2022)
2	01/16/22-01/22/22	<ul style="list-style-type: none"> • Intuitive Explanation with Minimal/Simple Math of Artificial Intelligence (AI) Methods 	Chapter 1 in Sean (2018) Chapter 5 in Nicolotti (2018)
3	01/23/22-01/29/22	<ul style="list-style-type: none"> • Hands-on Coding Exercises of AI Methods Using Python 	Chapter 1 in Sean (2018)
4	01/30/22-02/05/22	<ul style="list-style-type: none"> • Hands-on Coding Exercises of AI Methods Using R 	Chapter 1 in Sean (2018)
5	02/06/22-02/12/22	<ul style="list-style-type: none"> • AI in Absorption, Distribution, Metabolism, and Excretion (ADME) 	Chou and Lin (2022) Chapter 8 in Sean (2018)
6	02/13/22-02/19/22	<ul style="list-style-type: none"> • AI in Physiologically Based Pharmacokinetic/Toxicokinetic (PBPK/PBTK) Modeling 	Chou and Lin (2022)
7	02/20/22-02/26/22	<ul style="list-style-type: none"> • AI in Quantitative Structure-Activity Relationship (QSAR) Modeling 	Chapters 1-4 in Nicolotti (2018)

Week	Date(s)	Topic(s)	Readings
8	02/27/22-03/05/22	<ul style="list-style-type: none"> AI in Quantitative Adverse Outcome Pathway (qAOP) Analysis 	Hemmerich and Ecker (2020) Jin et al. (2022)
	03/05/22	<ul style="list-style-type: none"> Mid-Term Exam due 	
9	03/06/22-03/12/22	<ul style="list-style-type: none"> AI in Toxicogenomics 	Lin and Chou (2022) Rahman et al. (2022)
10	03/13/22-03/19/22	Spring Break	
11	03/20/22-03/26/22	<ul style="list-style-type: none"> Big Data in Toxicology and Environmental Health 	Chapter 11 from Sean (2018) Chapter 13 from Sean (2018)
12	03/27/22-04/02/22	<ul style="list-style-type: none"> AI in Air Pollution Assessment 	Liu et al. (2022)
13	04/03/22-04/09/22	<ul style="list-style-type: none"> AI in Predicting Health Outcomes of Air Pollution 	Lee et al. (2022)
14	04/10/22-04/16/22	<ul style="list-style-type: none"> AI in Ecotoxicological Assessment 	Xu et al. (2022)
15	04/17/22-04/23/22	<ul style="list-style-type: none"> AI in Predicting Health Outcomes Based on Human Biomonitoring Data 	Carwile et al. (2022)
16	04/24/22-04/30/22	<ul style="list-style-type: none"> Current Challenges and Future Perspectives of AI in Toxicology and Environmental Health 	Chapter 14 from Sean (2018)
	05/01/22	<ul style="list-style-type: none"> Final Exam due 	

Course Materials and Technology

- Carwile JL, Seshasayee SM, Ahrens KA, Hauser R, Driban JB, Rosen CJ, Gordon CM, Fleisch AF. 2022. Serum PFAS and Urinary Phthalate Biomarker Concentrations and Bone Mineral Density in 12-19 Year Olds: 2011-2016 NHANES. *J Clin Endocrinol Metab.* 107(8):e3343-e3352.
- Chandrasekaran SN, Ceulemans H, Boyd JD, Carpenter AE. Image-based profiling for drug discovery: due for a machine-learning upgrade? *Nat Rev Drug Discov.* 2021 Feb;20(2):145-159.
- Chou WC, Lin Z. Machine learning and artificial intelligence in physiologically based pharmacokinetic modeling. *Toxicological Sciences.* 2022, in press.
- Ekins S. *Computational Toxicology: Risk Assessment for Chemicals. 2nd Edition. Wiley Series on Technologies for the Pharmaceutical Industry Ser. 2018. Pages: 1-425.*
- Hemmerich J, Ecker, GF. In silico toxicology: from structure-activity relationships towards deep learning and adverse outcome pathways. *WIREs Computational Molecular Science.* 2020, 10:e1475.
- Jin Y, Qi G, Shou Y, Li D, Liu Y, Guan H, Zhang Q, Chen S, Luo J, Xu L, Li C, Ma W, Chen N, Zheng Y, Yu D. High throughput data-based, toxicity pathway-oriented development of a quantitative adverse outcome pathway network linking AHR activation to lung damages. *J Hazard Mater.* 2022 Mar 5;425:128041.
- Lee ES, Kim JY, Yoon YH, Kim SB, Kahng H, Park J, Kim J, Lee M, Hwang H, Park SJ. 2022. A Machine Learning-Based Study of the Effects of Air Pollution and Weather in Respiratory Disease Patients Visiting Emergency Departments. *Emergency Medicine International.* 2022, 2022:4462018.
- Lin Z, Chou WC. Machine learning and artificial intelligence in toxicological sciences. *Toxicological Sciences.* 2022, in press.
- Liu X, Lu DW, Zhang AQ, Liu Q, Jiang GB. 2022. Data-Driven Machine Learning in Environmental Pollution: Gains and Problems. *Environmental Science & Technology.* 56(4):2124-2133.
- Nicolotti O. *Computational Toxicology: Methods and Protocols. 1st Edition. Springer Nature. 2018. Pages: 1-587.*
- Rahman SM, Lan J, Kaeli D, Dy J, Alshawabkeh A, Gu AZ. Machine learning-based biomarkers identification from toxicogenomics - Bridging to regulatory relevant phenotypic endpoints. *J Hazard Mater.* 2022 Feb 5;423(Pt B):127141.

Tandon A, Howard B, Ramaiahgari S, Maharana A, Ferguson S, Shah R, Merrick BA. Deep Learning Image Analysis of High-Throughput Toxicology Assay Images. *SLAS Discov.* 2022 Jan;27(1):29-38.
 Xu M, Yang H, Liu G, Tang Y, Li W. 2022. In silico prediction of chemical aquatic toxicity by multiple machine learning and deep learning approaches. *J Appl Toxicol.*, in press.

For technical support for this class, please contact the UF Help Desk at:

- helpdesk@ufl.edu
- (352) 392-HELP - select option 2
- <https://helpdesk.ufl.edu/>

Additional Academic Resources

[Career Connections Center](#): Reitz Union Suite 1300, 352-392-1601. Career assistance and counseling services.

[Library Support](#): Various ways to receive assistance with respect to using the libraries or finding resources.

[Teaching Center](#): Broward Hall, 352-392-2010 or to make an appointment 352- 392-6420. General study skills and tutoring.

[Writing Studio](#): 2215 Turlington Hall, 352-846-1138. Help brainstorming, formatting, and writing papers.

Student Complaints On-Campus: [Visit the Student Honor Code and Student Conduct Code webpage for more information.](#)

On-Line Students Complaints: [View the Distance Learning Student Complaint Process.](#)

ACADEMIC REQUIREMENTS AND GRADING

Learning assessment methods: Students will be graded with the following four learning assessment methods. All assignments should be submitted to Canvas by clicking the "Submit" button of each specific assignment.

1. **Weekly Quizzes (70 points, 14% of total points, due at 11:59 pm EST the Sunday of the week):** Except the first week and the Spring Break week, there will be weekly quizzes to test how well students understand the theoretical aspects of the course contents. Each weekly quiz will consist of 5 single-choice or multiple-choice questions and will account for 5 points. In total, the weekly quizzes will account for 70 points for 14 weeks. The weekly quizzes are due at 11:59 pm EST the Sunday of the week.
2. **Weekly Journal Reviews (140 points, 28% of total points, due at 11:59 pm EST the day before the journal presentation):** Except the first week and the Spring Break week, there will be one or two weekly student-led journal presentations depending on the number of students. The presenters will be assigned by the instructors each week. The instructors will pick up the journal papers and inform students one week before the presentation date. All students need to submit a written critique

before 11:59 pm EST the day before the journal presentation date. Each weekly journal review will account for 10 points. In total, the weekly journal reviews will account for 140 points for 14 weeks.

3. **Journal Presentations (140 points, 28% of total points, due at 11:59 pm EST the day before the journal presentation):** Except the first week and the Spring Break week, there will be one or two weekly student-led journal presentations depending on the number of students. The presenters will be assigned by the instructors each week. The instructors will pick up the journal papers and inform students one week before the presentation date. Depending on the number of students, each student is anticipated to present twice throughout the semester. The presentation material (e.g., the PowerPoint file) should be emailed to the instructors by 11:59 pm EST the day before the journal presentation.

4. **Mid-Term and Final Exams (75 points for the mid-term exam and 75 points for the final exam, 30% of total points, due at 11:59 pm EST on Sunday of 03/05/2022 for the mid-term exam and at 11:59 pm EST on Monday of 05/01/2022 for the final exam):** The mid-term and final exams will be a research problem-based assignment. Specially, the instructors will choose a recent publication related to the use of AI methods to study a specific area of toxicology and environmental health sciences, such as PBPK, QSAR, air pollution, and ecotoxicology assessment. Students will obtain the model code from the supplementary materials of the paper or the instructors will provide the example code. The instructors will design 3-5 specific challenging questions and provide instructions on how to run computational simulations with different AI methods to generate simulation results to answer the challenging questions. The instructors will post the mid-term and final exams one week before the due date to provide sufficient time for the students to complete the exam. The exam should be submitted to Canvas. The mid-term exam is due at 11:59 pm EST on Sunday of 03/05/2022 and the final exam is due at 11:59 pm EST on Monday of 05/01/2022.

Grading

Requirement	Due date	Points or % of final grade (% must sum to 100%)
Weekly Quizzes	11:59 pm EST the Sunday of the week	14%
Weekly Journal Reviews	11:59 pm EST the day before the journal presentation	28%
Journal Presentations	11:59 pm EST the day before the journal presentation	28%
Mid-term Exam	11:59 pm EST on Sunday of 03/05/2022	15%
Final Exam	11:59 pm EST on Monday of 05/01/2022	15%

Note: All grading rubrics, additional assignment instructions and requirements, will be posted on Canvas for each specific assignment.

Point system used (i.e., how do course points translate into letter grades).

Example:

Total Points Earned	Percentage Earned	Letter Grade
≥465	93-100	A
450-464	90-92	A-
435-449	87-89	B+
415-434	83-86	B
400-414	80-82	B-
385-399	77-79	C+
365-384	73-76	C
350-364	70-72	C-
335-349	67-69	D+
315-334	63-66	D
300-314	60-62	D-
<300	Below 60	E

Please be aware that a C- is not an acceptable grade for graduate students. The GPA for graduate students must be 3.0 based on 5000 level courses and above to graduate. A grade of C counts toward a graduate degree only if based on credits in courses numbered 5000 or higher that have been earned with a B+ or higher.

Letter Grade	Grade Points
A	4.0
A-	3.67
B+	3.33
B	3.0
B-	2.67
C+	2.33
C	2.0
C-	1.67
D+	1.33
D	1.0
D-	0.67
E	0.0
WF	0.0
I	0.0
NG	0.0
S-U	0.0

More information on UF grading policy may be found at:

<http://gradcatalog.ufl.edu/content.php?catoid=10&navoid=2020#grades>

Exam Policy: There are not proctored exams.

Policy Related to Late Assignment, Make up Exams or Other Work

Assignments turned into Canvas up to 24 hours late will be discounted by 10% of the total points of the assignment. For example, if an assignment is worth 10 points and the assignment is submitted 12 hours late,

then the grade would be penalized by lowering the score by 1 point. Assignments turned in more than 24 hours late will not be graded and will contribute zero points toward your total points, unless arrangements have been made and approved in advance by the instructor. Missed assignments will contribute zero points toward your final points.

Special Circumstances. In the event of exceptional circumstances that may interfere with your ability to complete an assignment or meet a deadline, please contact the instructor as soon as possible before the deadline. Such special cases will be dealt on an individual basis, provided that you have sufficient documentation.

Please note: Any requests for make-ups due to technical issues MUST be accompanied by the UF Computing help desk (<http://helpdesk.ufl.edu/>) correspondence. You MUST e-mail me within 24 hours of the technical difficulty if you wish to request a make-up.

Policy Related to Required Class Attendance

Please note all faculty are bound by the UF policy for excused absences.

Excused absences must be consistent with university policies in the Graduate Catalog (<https://catalog.ufl.edu/graduate/regulations/#text>). Additional information can be found here: <https://catalog.ufl.edu/ugrad/current/regulations/info/attendance.aspx>

STUDENT EXPECTATIONS, ROLES, AND OPPORTUNITIES FOR INPUT

Expectations Regarding Course Behavior

You are expected to maintain a civil tone and respect the opinions of other students. While class discussion is encouraged, aggressive or patronizing tone and language are unacceptable and may result in the loss of your discussion privileges.

Communication Guidelines

You are encouraged to post questions related to course contents to the Discussion Board on Canvas. The instructors will check the Discussion Board daily and will try to answer questions within 24-48 hours. You are also encouraged to join the weekly office hour in-person or by Zoom to make sure your questions are answered in a timely manner. The office hour will be from 2:00 pm to 3:00 pm EST every Friday.

Academic Integrity

Students are expected to act in accordance with the University of Florida policy on academic integrity. As a student at the University of Florida, you have committed yourself to uphold the Honor Code, which includes the following pledge:

“We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.”

You are expected to exhibit behavior consistent with this commitment to the UF academic community, and on all work submitted for credit at the University of Florida, the following pledge is either required or implied:

“On my honor, I have neither given nor received unauthorized aid in doing this assignment.”

It is your individual responsibility to know and comply with all university policies and procedures regarding academic integrity and the Student Honor Code. Violations of the Honor Code at the University of Florida will not be tolerated. Violations will be reported to the Dean of Students Office for consideration of disciplinary action. For additional information regarding Academic Integrity, please see Student Conduct and Honor Code or the Graduate Student Website for additional details:

<https://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/>
<http://gradschool.ufl.edu/students/introduction.html>

Please remember cheating, lying, misrepresentation, or plagiarism in any form is unacceptable and inexcusable behavior.

Recording Within the Course:

Students are allowed to record video or audio of class lectures. However, the purposes for which these recordings may be used are strictly controlled. The only allowable purposes are (1) for personal educational use, (2) in connection with a complaint to the university, or (3) as evidence in, or in preparation for, a criminal or civil proceeding. All other purposes are prohibited. Specifically, students may not publish recorded lectures without the written consent of the instructor.

A “class lecture” is an educational presentation intended to inform or teach enrolled students about a particular subject, including any instructor-led discussions that form part of the presentation, and delivered by any instructor hired or appointed by the University, or by a guest instructor, as part of a University of Florida course. A class lecture does not include lab sessions, student presentations, clinical presentations such as patient history, academic exercises involving solely student participation, assessments (quizzes, tests, exams), field trips, private conversations between students in the class or between a student and the faculty or lecturer during a class session.

Publication without permission of the instructor is prohibited. To “publish” means to share, transmit, circulate, distribute, or provide access to a recording, regardless of format or medium, to another person (or persons), including but not limited to another student within the same class section. Additionally, a recording, or transcript of a recording, is considered published if it is posted on or uploaded to, in whole or in part, any media platform, including but not limited to social media, book, magazine, newspaper, leaflet, or third party note/tutoring services. A student who publishes a recording without written consent may be subject to a civil cause of action instituted by a person injured by the publication and/or discipline under UF Regulation 4.040 Student Honor Code and Student Conduct Code.

Policy Related to Guests Attending Class:

Only registered students are permitted to attend class. However, we recognize that students who are caretakers may face occasional unexpected challenges creating attendance barriers. Therefore, by exception, a department chair or his or her designee (e.g., instructors) may grant a student permission to bring a guest(s) for a total of two class sessions per semester. This is two sessions total across all courses. No further extensions will be granted. Please note that guests are **not** permitted to attend either cadaver or wet labs. Students are responsible for course material regardless of attendance. For additional information, please review the Classroom Guests of Students policy in its entirety. Link to full policy:

<http://facstaff.php.ufl.edu/services/resourceguide/getstarted.htm>

Online Faculty Course Evaluation Process

Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/students/>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their

Canvas course menu under GatorEvals, or via <https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.

SUPPORT SERVICES

Accommodations for Students with Disabilities

If you require classroom accommodation because of a disability, it is strongly recommended you register with the Dean of Students Office <http://www.dso.ufl.edu> within the first week of class or as soon as you believe you might be eligible for accommodations. The Dean of Students Office will provide documentation of accommodations to you, which you must then give to me as the instructor of the course to receive accommodations. Please do this as soon as possible after you receive the letter. Students with disabilities should follow this procedure as early as possible in the semester. The College is committed to providing reasonable accommodations to assist students in their coursework.

Counseling and Student Health

Students sometimes experience stress from academic expectations and/or personal and interpersonal issues that may interfere with their academic performance. If you find yourself facing issues that have the potential to or are already negatively affecting your coursework, you are encouraged to talk with an instructor and/or seek help through University resources available to you.

- The **Counseling and Wellness Center** 352-392-1575 offers a variety of support services such as psychological assessment and intervention and assistance for math and test anxiety. Visit their web site for more information: <http://www.counseling.ufl.edu>. On line and in person assistance is available.
- **U Matter We Care** website: <http://www.umatter.ufl.edu/>. If you are feeling overwhelmed or stressed, you can reach out for help through the You Matter We Care website, which is staffed by Dean of Students and Counseling Center personnel.
- The **Student Health Care Center** at Shands is a satellite clinic of the main Student Health Care Center located on Fletcher Drive on campus. Student Health at Shands offers a variety of clinical services. The clinic is located on the second floor of the Dental Tower in the Health Science Center. For more information, contact the clinic at 392-0627 or check out the web site at: <https://shcc.ufl.edu/>
- Crisis intervention is always available 24/7 from: Alachua County Crisis Center: (352) 264-6789 <http://www.alachuacounty.us/DEPTS/CSS/CRISISCENTER/Pages/CrisisCenter.aspx>
- **University Police Department:** [Visit UF Police Department website](#) or call 352-392-1111 (or 9-1-1 for emergencies).
- **UF Health Shands Emergency Room / Trauma Center:** For immediate medical care call 352-733-0111 or go to the emergency room at 1515 SW Archer Road, Gainesville, FL 32608; [Visit the UF Health Emergency Room and Trauma Center website.](#)

Do not wait until you reach a crisis to come in and talk with us. We have helped many students through stressful situations impacting their academic performance. You are not alone so do not be afraid to ask for assistance.

Inclusive Learning Environment

Public health and health professions are based on the belief in human dignity and on respect for the individual. As we share our personal beliefs inside or outside of the classroom, it is always with the understanding that we value and respect diversity of background, experience, and opinion, where every individual feels valued. We believe in, and promote, openness and tolerance of differences in ethnicity and culture, and we respect differing personal,

spiritual, religious and political values. We further believe that celebrating such diversity enriches the quality of the educational experiences we provide our students and enhances our own personal and professional relationships. We embrace The University of Florida's Non-Discrimination Policy, which reads, "The University shall actively promote equal opportunity policies and practices conforming to laws against discrimination. The University is committed to non-discrimination with respect to race, creed, color, religion, age, disability, sex, sexual orientation, gender identity and expression, marital status, national origin, political opinions or affiliations, genetic information and veteran status as protected under the Vietnam Era Veterans' Readjustment Assistance Act." If you have questions or concerns about your rights and responsibilities for inclusive learning environment, please see your instructor or refer to the Office of Multicultural & Diversity Affairs website:

www.multicultural.ufl.edu