



<b>Title:</b>	Advanced Spectroscopy & PAT <b>APPROVED</b>
<b>Long Title:</b>	Adv. Spec. & Process Analytical Tech.
<b>Module Code:</b>	CHEA9001
<b>Duration:</b>	1 Semester
<b>Credits:</b>	10
<b>NFQ Level:</b>	Expert
<b>Field of Study:</b>	Analytical Chemistry
<b>Valid From:</b>	Semester 1 - 2021/22 ( September 2021 )
<b>Module Delivered in</b>	<a href="#">2 programme(s)</a>
<b>Module Coordinator:</b>	Donagh OMahony
<b>Module Author:</b>	Grainne Conneely
<b>Module Description:</b>	The module presents a variety of atomic and molecular spectroscopies, it trains the student to analyse, measure and utilise spectral data for structural determination. The PAT element includes the use of spectroscopy in manufacturing settings, chemometrics, validation considerations and data acquisition in real time.
<b>Learning Outcomes</b>	
<i>On successful completion of this module the learner will be able to:</i>	
LO1	Describe in detail the principles of quantum mechanics
LO2	Critique various atomic and molecular spectroscopies.
LO3	Interpret spectral data, starting from the physical principles that underpin the corresponding techniques.
LO4	Perform structural determination based on spectral data.
LO5	Solve calculations related to atomic and molecular spectroscopies.
LO6	Compare spectroscopy-based techniques for real time monitoring of manufacturing processes.
LO7	Critique the approach to validation of instrumentation associated with PAT.
LO8	Explain the principles and application of Chemometrics in PAT.
<b>Pre-requisite learning</b>	
<b>Module Recommendations</b>	
<i>This is prior learning (or a practical skill) that is strongly recommended before enrolment in this module. You may enrol in this module if you have not acquired the recommended learning but you will have considerable difficulty in passing (i.e. achieving the learning outcomes of) the module. While the prior learning is expressed as named CIT module(s) it also allows for learning (in another module or modules) which is equivalent to the learning specified in the named module(s).</i>	
<b>Incompatible Modules</b>	
<i>These are modules which have learning outcomes that are too similar to the learning outcomes of this module. You may not earn additional credit for the same learning and therefore you may not enrol in this module if you have successfully completed any modules in the incompatible list.</i>	
No incompatible modules listed	
<b>Co-requisite Modules</b>	
No Co-requisite modules listed	
<b>Requirements</b>	
<i>This is prior learning (or a practical skill) that is mandatory before enrolment in this module is allowed. You may not enrol on this module if you have not acquired the learning specified in this section.</i>	
No requirements listed	

**Module Content & Assessment**
**Indicative Content**
**Introduction to Spectroscopy**

Principles of quantum mechanics; interaction of electromagnetic radiation with atoms and molecules; instrumentation.

**Atomic Spectroscopy**

Principles of Spin orbit coupling; determination of term symbols for main group elements, transition metals, ions; spin only magnetic moment and total spin.

**Molecular Spectroscopy**

Rotational spectroscopy, vibrational (infrared and Raman) spectroscopy, nuclear magnetic resonance spectroscopy; Fourier transform methods.

**Additional Methods**

A selection of the following methods and techniques may be presented: electron spin resonance and nuclear quadrupole resonance spectroscopy, Mossbauer spectroscopy, laser spectroscopic analyses.

**Structural Determination from Spectral Data**

Use of various types of spectral data (IR, UV, MS, NMR) interactively for devising solutions to structural problems, baseline / scatter correction and the use of derivatives.

**Introduction to Process Analytical Technologies (PAT)**

Historical perspective, regulatory framework, application to a simple manufacturing process, data collection and analysis.

**Chemometrics**

Physiochemical data processing and analysis. Techniques studied include principal component analysis (PCA) and partial least squares regression (PLS), classification methods such as Soft Independent Modelling of Class Analogies (SIMCA).

**Measurement Technology**

Spectroscopic techniques, on-line versus off-line applications, process control and future trends.

**Validation of PAT instrumentation**

Validation considerations of instrumentation associated with PAT

**PAT Applications**

Review of Case Studies

**Assessment Breakdown**

	%
Course Work	100.00%

**Course Work**

Assessment Type	Assessment Description	Outcome addressed	% of total	Assessment Date
Short Answer Questions	Multiple Choice Questions / Short Answer Questions	1,2,3,4,5	40.0	Week 7
Presentation	Evaluation of case studies, data evaluation, and problem solving.	3,4,6,7,8	20.0	Week 9
Practical/Skills Evaluation	Produce a report and a presentation on the application of PAT to a process using a number of selected spectroscopic techniques	3,6,7,8	40.0	Sem End

No End of Module Formal Examination

**Reassessment Requirement**
**Coursework Only**

*This module is reassessed solely on the basis of re-submitted coursework. There is no repeat written examination.*

**The institute reserves the right to alter the nature and timings of assessment**

**Module Workload**

<b>Workload: Full Time</b>				
<i>Workload Type</i>	<i>Workload Description</i>	<i>Hours</i>	<i>Frequency</i>	<i>Average Weekly Learner Workload</i>
Lecture	Lecture on course material	2.0	Every Week	2.00
Tutorial	Tutorial on course material	2.0	Every Week	2.00
Independent & Directed Learning (Non-contact)	Self Directed Learning	10.0	Every Week	10.00
Total Hours				14.00
Total Weekly Learner Workload				14.00
Total Weekly Contact Hours				4.00

<b>Workload: Part Time</b>				
<i>Workload Type</i>	<i>Workload Description</i>	<i>Hours</i>	<i>Frequency</i>	<i>Average Weekly Learner Workload</i>
Lecture	Lecture on Course Material	2.0	Every Week	2.00
Tutorial	Tutorial on Course Material	2.0	Every Week	2.00
Independent & Directed Learning (Non-contact)	Self Directed Learning	10.0	Every Week	10.00
Total Hours				14.00
Total Weekly Learner Workload				14.00
Total Weekly Contact Hours				4.00

## Module Resources

### Recommended Book Resources

- K. Bakeev 2010, *Process analytical technology: spectroscopic tools and implementation strategies for the chemical and pharmaceutical industries* [ISBN: 9781405121033]
- P. Larkin 2017, *Infrared and Raman Spectroscopy : Principles and Spectral Interpretation* [ISBN: 9780123870186]
- V. P. Gupta 2017, *Molecular and Laser Spectroscopy : Advances and Applications* [ISBN: 9780128498828]

### Supplementary Book Resources

- H. Gunsler and H.U. Gremlich 2002, *IR Spectroscopy: An Introduction* [ISBN: ISBN: 3527288]
- J. Kauppinen and J. Partanen 2001, *Fourier Transforms in Spectroscopy* [ISBN: 3527402896]

### Recommended Article/Paper Resources

- Vargas, Jenny M; Nielsen, Sarah; Cárdenas, Vanessa; et al. 2018, *Process analytical technology in continuous manufacturing of a commercial pharmaceutical product*, *International Journal of Pharmaceutics*, 538(1-2):167-178
- K.A. Esmonde-White, M. Cuellar, C. Uerpmann, B. Lenain & I.R. Lewis 2017, *Raman spectroscopy as a process analytical technology for pharmaceutical manufacturing and bioprocessing*, 409:637–649
- L. Zhong, L. Gao, L. Li, and H. Zang 2020, *Trends-process analytical technology in solid oral dosage manufacturing*, *European Journal of Pharmaceutics and Biopharmaceutics*, 153:187-199

### Other Resources

- Website: *Food and Drug Administration*  
<http://www.fda.gov>
- Website: *Food and Drug Administration Guidance for Industry PAT — A Framework for Innovative Pharmaceutical Development, Manufacturing, and Quality Assurance*  
<https://www.fda.gov/media/71012/download>
- Website: *Health Products Regulatory Authority*  
<http://www.hpra.ie>
- Website: *European Medicines Agency*  
<http://www.emea.europa.eu>
- Website: *International Council for Harmonization*  
<http://www.ich.org>
- Website: *International Organization for Standardization*  
<http://www.iso.org>

**Module Delivered in**

<b>Programme Code</b>	<b>Programme</b>	<b>Semester</b>	<b>Delivery</b>
CR_SASIV_9	<a href="#"><u>MSc in Analytical Sciences with Instrument Validation</u></a>	1	Mandatory
CR_SANIV_9	<a href="#"><u>Postgraduate Diploma in Analytical Sciences with Instrument Validation</u></a>	1	Mandatory