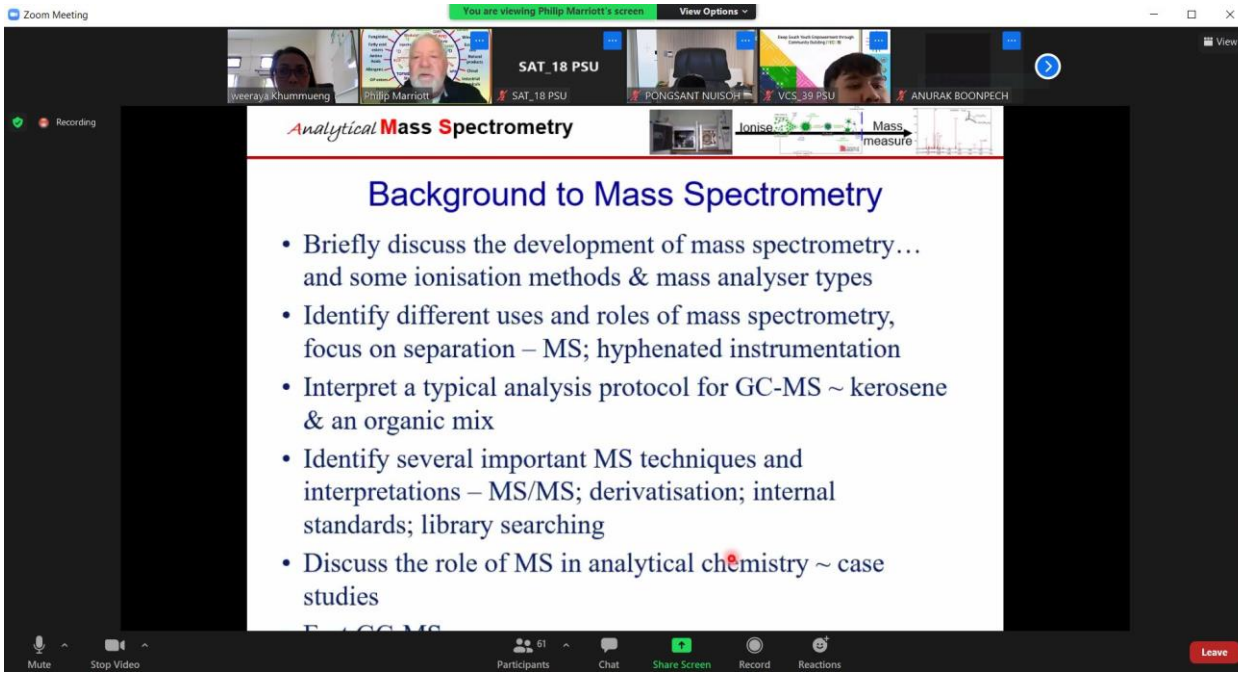

SCIENCE AND TECHNOLOGY
Virtual Visiting Professor
12 Jan 2022
EP 2 : Topic
Gas chromatography, sampling, and applications
19 Jan 2022
EP 3 : Topic
Multidimensional and Comprehensive-two-dimensional gas chromatography and applications
26 Jan 2022
EP 4 : Topic
GC-Mass Spectrometry and applications
2 Feb 2022
EP 5 : Topic
Research group meeting (Research trends in chemistry, energy, food, etc)
Professor Philip Marriott
School of Chemistry, Faculty of Science, Monash University, Melbourne, Australia
Dr. Weeraya Khummueng
Moderator
Meeting ID: 948 4442 6692
zoom


Zoom Meeting
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SAT_18 PSU
Recording
Analytical Mass Spectrometry
Ionise
Mass measure
Background to Mass Spectrometry
• Briefly discuss the development of mass spectrometry… and some ionisation methods & mass analyser types
• Identify different uses and roles of mass spectrometry, focus on separation – MS; hyphenated instrumentation
• Interpret a typical analysis protocol for GC-MS ~ kerosene & an organic mix
• Identify several important MS techniques and interpretations – MS/MS; derivatisation; internal standards; library searching
• Discuss the role of MS in analytical chemistry ~ case studies
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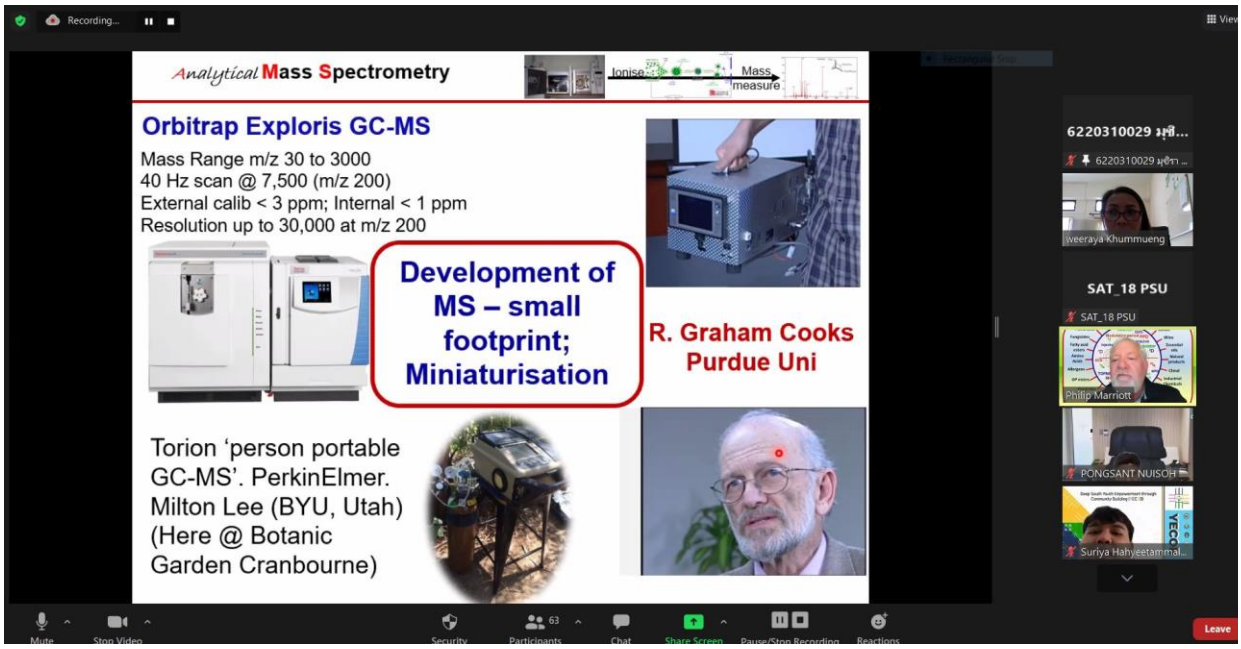
Recording...
Analytical Mass Spectrometry
Ionise
Mass measure
Orbitrap Exploris GC-MS
Mass Range m/z 30 to 3000
40 Hz scan @ 7,500 (m/z 200)
External calib < 3 ppm; Internal < 1 ppm
Resolution up to 30,000 at m/z 200
Development of MS – small footprint; Miniaturisation
R. Graham Cooks
Purdue Uni
Torion 'person portable GC-MS'. PerkinElmer.
Milton Lee (BYU, Utah)
(Here @ Botanic Garden Cranbourne)
6220310029 มุชี...
weeraya Khummueng
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Phillip Marriott
PONGSANT NUISOH
Suriya Hahyeetammal...
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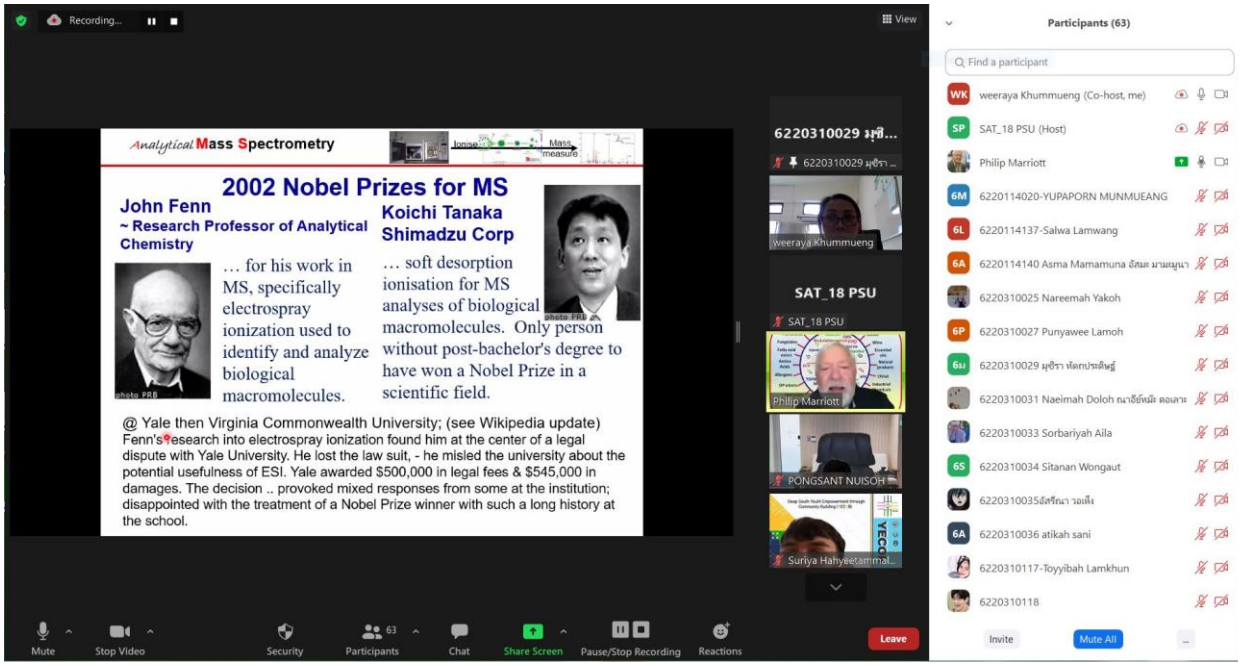
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Analytical Mass Spectrometry
2002 Nobel Prizes for MS
John Fenn
~ Research Professor of Analytical Chemistry
… for his work in MS, specifically electrospray ionization used to identify and analyze biological macromolecules.
Koichi Tanaka
Shimadzu Corp
… soft desorption ionisation for MS analyses of biological macromolecules. Only person without post-bachelor's degree to have won a Nobel Prize in a scientific field.
@ Yale then Virginia Commonwealth University; (see Wikipedia update) Fenn's research into electrospray ionization found him at the center of a legal dispute with Yale University. He lost the law suit, - he misled the university about the potential usefulness of ESI. Yale awarded $500,000 in legal fees & $545,000 in damages. The decision .. provoked mixed responses from some at the institution; disappointed with the treatment of a Nobel Prize winner with such a long history at the school.
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weeraya Khummueng
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Phillip Marriott
PONGSANT NUISOH
Suriya Hahyeetammal...
Participants (63)
Find a participant
weeraya Khummueng (Co-host, me)
SAT_18 PSU (Host)
Philip Marriott
6220114020-YUPAPORN MUNMUEANG
6220114137-Salwa Lamwang
6220114140 Asma Mamamuna
6220310025 Nareemah Yakoh
6220310027 Punyawee Lamoh
6220310029 มุชีรา หัดประดิษฐ์
6220310031 Naeimah Doloh
6220310033 Sorbariyah Aila
6220310034 Sitanan Wongaut
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6220310036 atikah sani
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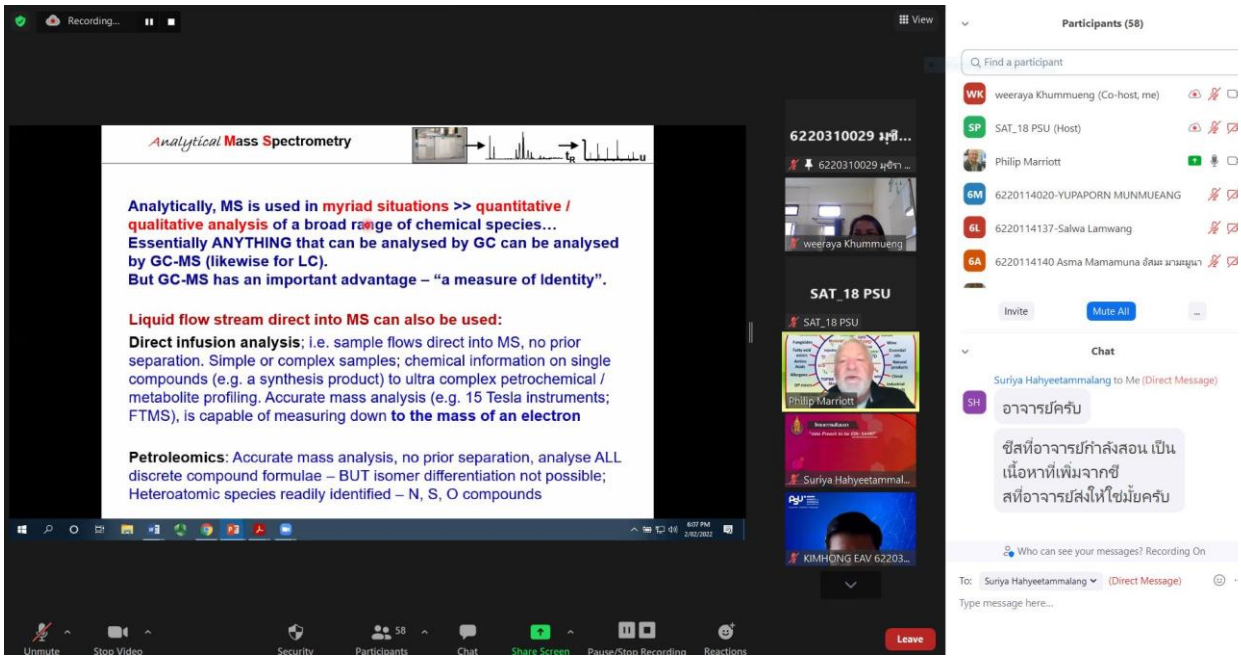
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Analytical Mass Spectrometry
Analytically, MS is used in myriad situations >> quantitative / qualitative analysis of a broad range of chemical species… Essentially ANYTHING that can be analysed by GC can be analysed by GC-MS (likewise for LC).
But GC-MS has an important advantage – "a measure of Identity".
Liquid flow stream direct into MS can also be used:
Direct infusion analysis; i.e. sample flows direct into MS, no prior separation. Simple or complex samples; chemical information on single compounds (e.g. a synthesis product) to ultra complex petrochemical / metabolite profiling. Accurate mass analysis (e.g. 15 Tesla instruments; FTMS), is capable of measuring down to the mass of an electron
Petroleomics: Accurate mass analysis, no prior separation, analyse ALL discrete compound formulae – BUT isomer differentiation not possible; Heteroatomic species readily identified – N, S, O compounds
6220310029 มุฮัร...
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Philip Marriott
Suriya Hahyeetammal...
KIMHONG EAV 62203...
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6220114140 Asma Mamamuna อัสมะ มามะมูนา
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Suriya Hahyeetammalang to Me (Direct Message)
อาจารย์ครับ
ซีสที่อาจารย์กำลังสอน เป็นเนื้อหาที่เพิ่มจากซีสที่อาจารย์สั่งให้ใช่มั้ยครับ
Who can see your messages? Recording On
To: Suriya Hahyeetammalang (Direct Message)
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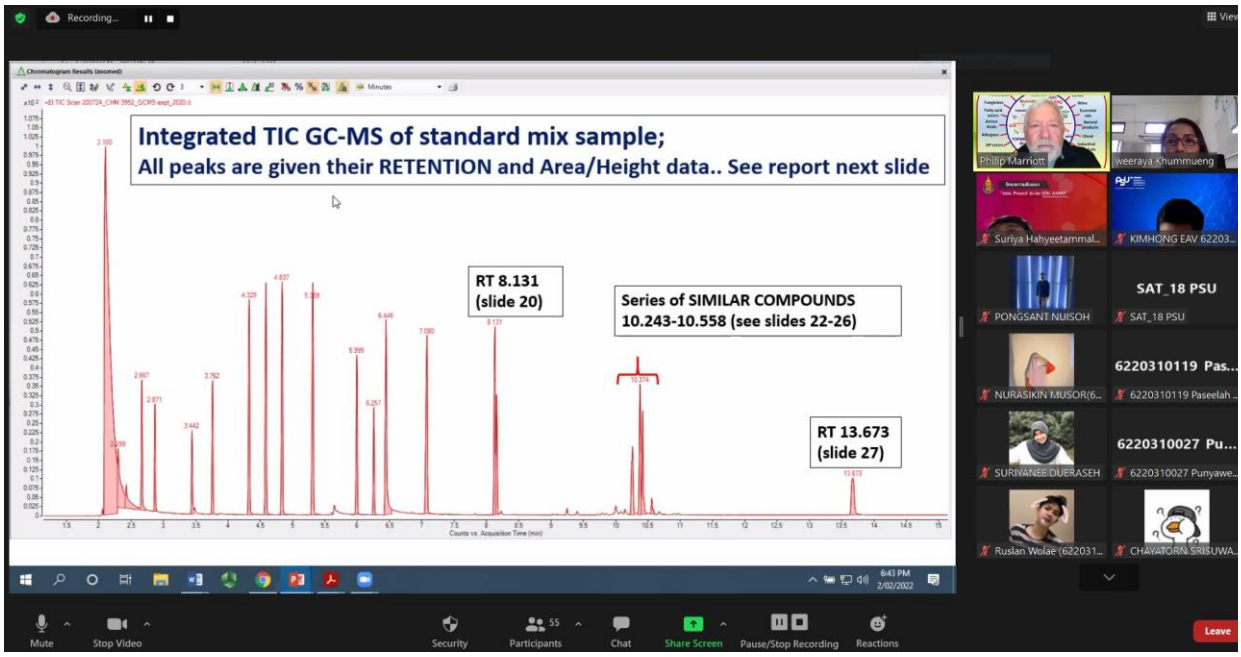
Recording...
Integrated TIC GC-MS of standard mix sample;
All peaks are given their RETENTION and Area/Height data.. See report next slide
RT 8.131
(slide 20)
Series of SIMILAR COMPOUNDS
10.243-10.558 (see slides 22-26)
RT 13.673
(slide 27)
Philip Marriott
weeraya Khummueng
Suriya Hahyeetammal...
KIMHONG EAV 62203...
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Ruslan Wolae (622031...
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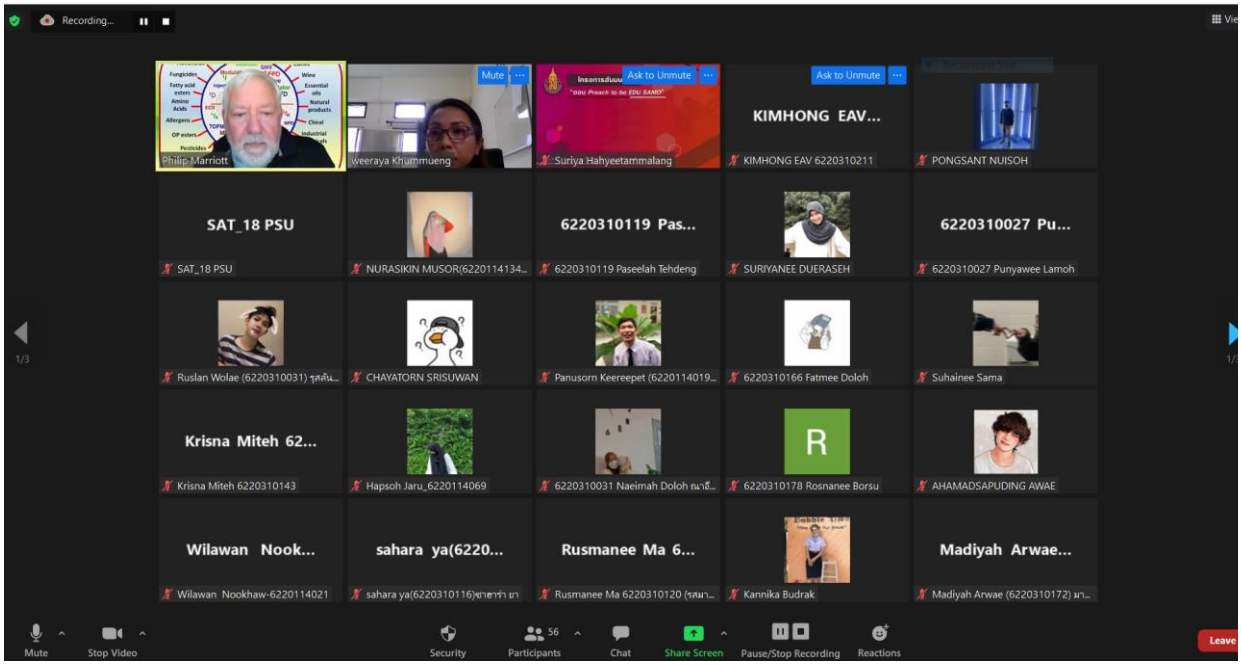
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Suriya Hahyeetammalang
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Suhainee Sama
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Krisna Miteh 6220310143
Hapsoh Jaru_6220114069
6220310031 Naeimah Doloh ณาอี...
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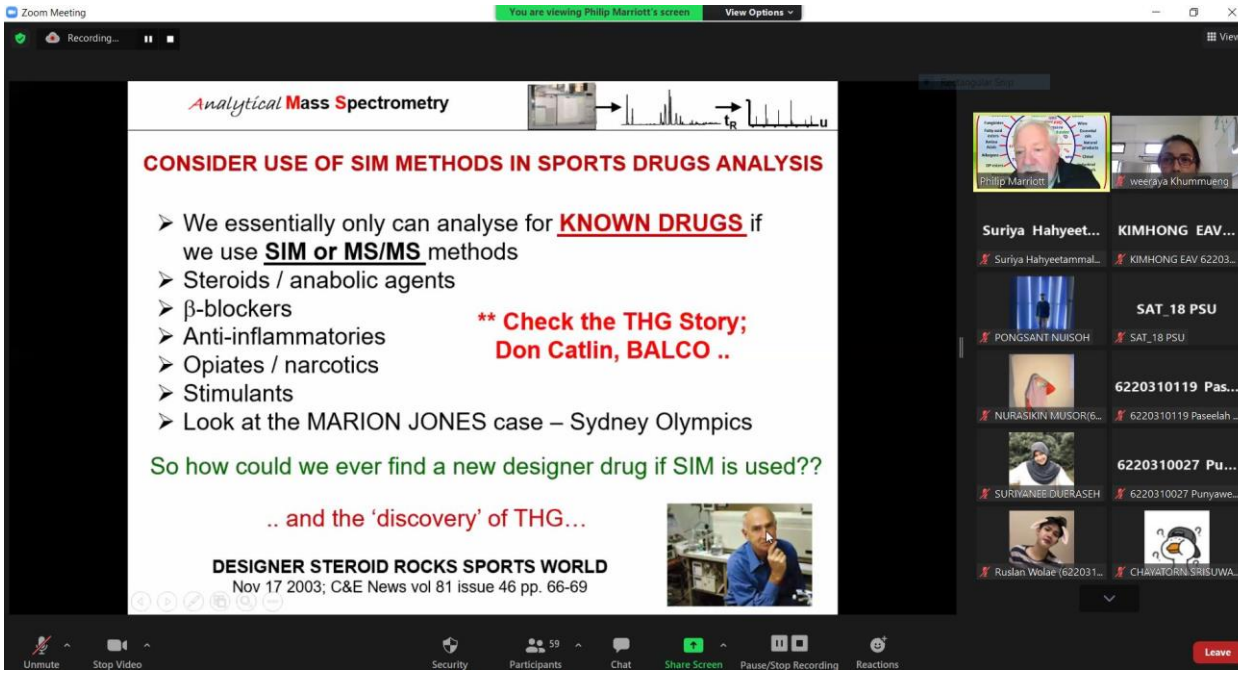
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Analytical Mass Spectrometry
CONSIDER USE OF SIM METHODS IN SPORTS DRUGS ANALYSIS
We essentially only can analyse for KNOWN DRUGS if we use SIM or MS/MS methods
Steroids / anabolic agents
β-blockers
Anti-inflammatories
Opiates / narcotics
Stimulants
Look at the MARION JONES case – Sydney Olympics
** Check the THG Story; Don Catlin, BALCO ..
So how could we ever find a new designer drug if SIM is used??
.. and the 'discovery' of THG…
DESIGNER STEROID ROCKS SPORTS WORLD
Nov 17 2003; C&E News vol 81 issue 46 pp. 66-69
Philip Marriott
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KIMHONG EAV...
Suriya Hahyeetammal...
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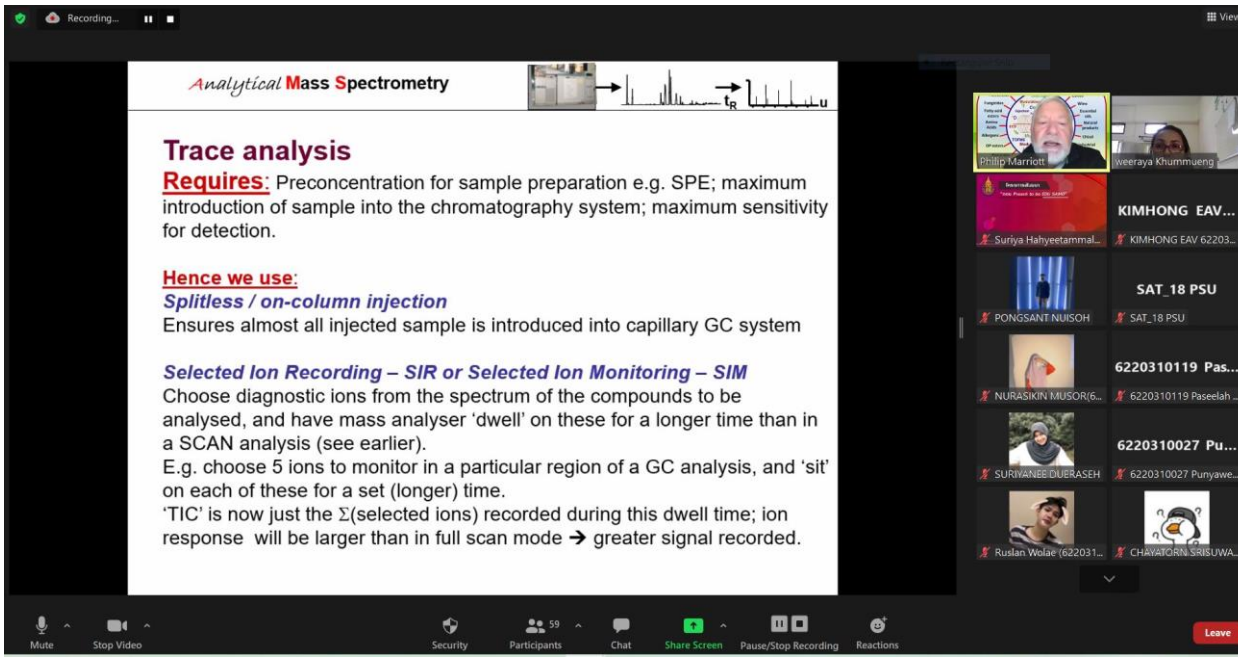
Recording...
Analytical Mass Spectrometry
Trace analysis
Requires: Preconcentration for sample preparation e.g. SPE; maximum introduction of sample into the chromatography system; maximum sensitivity for detection.
Hence we use:
Splitless / on-column injection
Ensures almost all injected sample is introduced into capillary GC system
Selected Ion Recording – SIR or Selected Ion Monitoring – SIM
Choose diagnostic ions from the spectrum of the compounds to be analysed, and have mass analyser 'dwell' on these for a longer time than in a SCAN analysis (see earlier).
E.g. choose 5 ions to monitor in a particular region of a GC analysis, and 'sit' on each of these for a set (longer) time.
'TIC' is now just the Σ(selected ions) recorded during this dwell time; ion response will be larger than in full scan mode → greater signal recorded.
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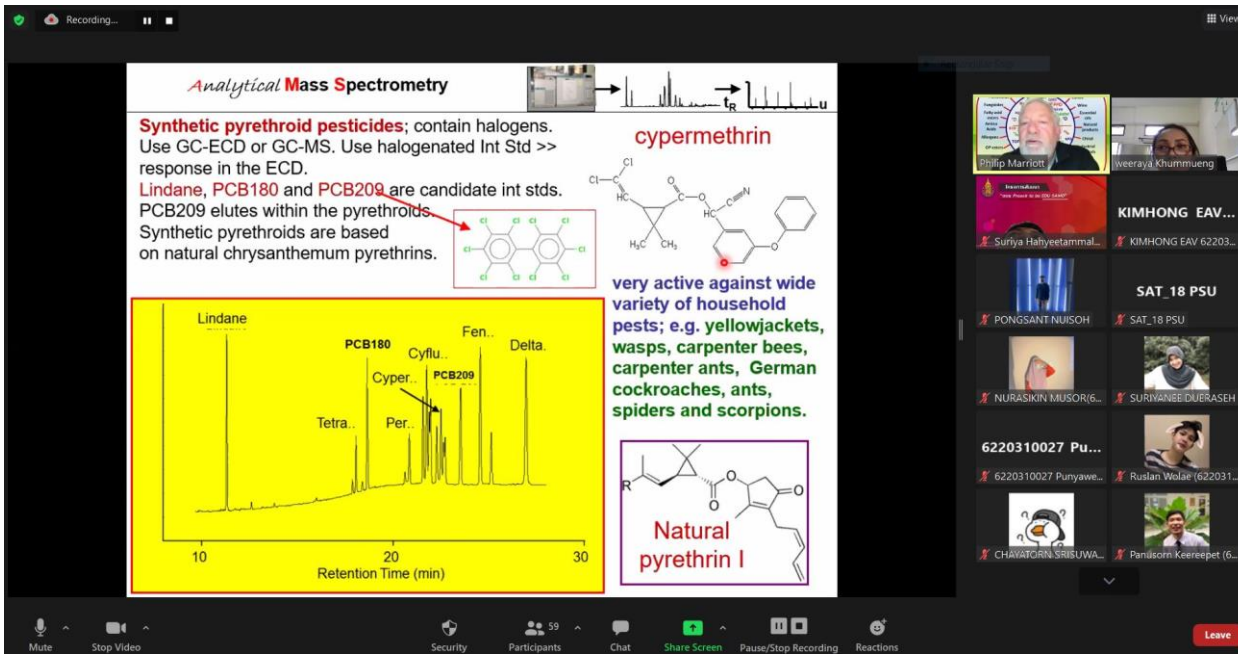
Recording...
Analytical Mass Spectrometry
Synthetic pyrethroid pesticides; contain halogens.
Use GC-ECD or GC-MS. Use halogenated Int Std >> response in the ECD.
Lindane, PCB180 and PCB209 are candidate int stds.
PCB209 elutes within the pyrethroids.
Synthetic pyrethroids are based on natural chrysanthemum pyrethrins.
cypermethrin
very active against wide variety of household pests; e.g. yellowjackets, wasps, carpenter bees, carpenter ants, German cockroaches, ants, spiders and scorpions.
Lindane
PCB180
Cyflu..
Fen..
Delta.
Cyper..
PCB209
Tetra..
Per..
10
20
30
Retention Time (min)
Natural pyrethrin I
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