

# ECSBM 2019 Conference Programme

## Monday 19 August

	George Moore Lecture Theatre	Lynch Theatre (Th F)
08:00-09:10	Registration	
09:15	Conference Welcome	
09:30 - 11:10	Invited Talks (Chair Marloes Groot)	
09:30 - 10:10 (Plenary)	John Kelly TRANSIENT SPECTROSCOPIC STUDIES OF THE PHOTOPHYSICAL PROPERTIES OF DNA-INTERCALATED MOLECULES	23
10:10 - 10:40 (Invited)	Erik Nibbering ULTRAFAST PROTON TRANSPORT ALONG SOLVENT BRIDGES: HYDRATED EXCESS PROTON AND HYDROXIDE/METHOXIDE TRANSFER MECHANISMS	62
10:40 - 11:10 (Invited)	Maria Paula Marques SYNCHROTRON-BASED FTIR AND QUASI-ELASTIC NEUTRON SCATTERING IN THE SEARCH FOR NEW CHEMOTHERAPEUTIC TARGETS	5
11:10 - 11:40	Coffee Break & Posters	
	<b>Monday 2A (Chair Marina Rubini)</b>	<b>Monday 2B (Chair Steven Bell)</b>
11:40 - 12:00	Mike Towrie ULTRA - A FACILITY FOR ULTRAFAST SPECTROSCOPY OF BIOLOGICAL MOLECULES	79
12:00 - 12:20	Monica Marini DNA/LIGANDS STRUCTURAL STUDY.	41
12:20 - 12:40	Thori Gunnlaugsson OBSERVING, CORRELATING AND TUNING SUPRAMOLECULAR INTERACTIONS AND FUNCTIONS THROUGH IMAGING.	83
12:40 - 13:00	Dermot Brougham 1H NMR STUDIES OF DYNAMICS AND TRANSPORT IN HYDRATED BIOMIMETIC NETWORKS	83
13:00 - 14:30	Lunch Break & Posters	
	<b>Monday 3A (Chair Malgorzata Baranska)</b>	<b>Monday 3B (Chair Andreas Barth)</b>
14:30 - 14:50	Kevin O' Dwyer AUTOMATED CONFOCAL RAMAN SPECTROSCOPY PLATFORM FOR CYTOLOGY	78
		50
		50

14:50 - 15:10	Aidan Meade	PREDICTING RECURRENCE IN LYMPH NODE NEGATIVE BREAST CANCER USING DEEP LEARNING WITH CHEMICAL IMAGING	44	Jurgen Kohler	HOW CAN OPTICAL SINGLE PARTICLE SPECTROSCOPY CONTRIBUTE TO ELUCIDATE THE SECONDARY STRUCTURES IN CHLOROSOMES?	
15:10 - 15:30	Peter Mojzeš	RAMAN MICROSCOPY OF MICROALGAE:NEW CHALLENGES AND OPPORTUNITIES IN THE WORLD OF PHOTOSYNTHETIC MICROORGANISMS	39	Gary Hastings	FOURIER TRANSFORM VISIBLE AND INFRARED DIFFERENCE SPECTROSCOPY AND QUANTUM CHEMICAL VIBRATIONAL FREQUENCY CALCULATIONS FOR THE STUDY OF PIGMENTS IN PHOTOSYNTHETIC PROTEINS	76
15:30 - 16:00	Coffee Break & Posters					
	Invited 2 (Chair Fiona Lyng)					
16:00 - 16:30 (Invited)	Klaus Gerwert (IOS Press Lecture)	LABEL-FREE TISSUE CLASSIFICATION BY QCL BASED IR-IMAGING				
16:30 - 17:00 (Invited)	Ute Neugebauer	RAMAN SPECTROSCOPIC CHARACTERIZATION OF LEUKOCYTE ACTIVATION DURING STIMULATION AND INFECTION				
17:00 -17:30	Flash Presentations (Chair Dermot Brougham)					
17:30 -19:00	Poster Session					

## Tuesday 20 August

	George Moore Lecture Theatre			Lynch Theatre (Th F)		
09:00	Invited 3 (Chair Klaus Gerwert) Aquilant Sponsored Session					
09:00 - 09:40 (Plenary)	Duncan Graham	RAMAN AND SERS SPECTROSCOPY FOR BIOANALYSIS	10			
09:40 - 10:10 (Invited)	Tia Keyes	MICROCAVITY SUPPORTED LIPID BILAYERS: VERSATILE MICROFLUIDIC MODELS FOR BIOPHYSICAL STUDIES OF MEMBRANE PROTEINS AND LIPIDS.	87			

10:10 - 10:40 (Invited)	Donal O'Shea	REAL-TIME NEAR INFRARED FLUORESCENCE IMAGING RESEARCH TOOLS WITH THE POTENTIAL FOR CLINICAL USE	9			
10:40 - 11:10	<b>Coffee Break &amp; Posters</b>					
	<b>Tuesday 2A ( Chair Maria Paula Marques)</b>			<b>Tuesday 2B (Chair Tia Keyes)</b>		
11:10 - 11:30	Tanja Ducic	CORRELATIVE FTIR AND X-RAY FLUORESCENCE IMAGING OF OXIDISED LIPIDS AND COPPER IN SINGLE ASTROCYTE CELLS FROM THE ALS HSOD1 G93A RAT MODEL	26	Marek Prochazka	SURFACE-ENHANCED RAMAN SCATTERING (SERS) OF BIOMOLECULES ON GRADIENT SILVER SURFACES	34
11:30 - 11:50	Nirod Sarangi	UNRAVELING DRUG-BIOMEMBRANE INTERACTION ON MICROCAVITY SUPPORTED BILAYERS	37	Steven Bell	SURFACE-ENHANCED RAMAN SPECTRA OF PLANKTONIC BACTERIA, BIOFILMS AND THE HEADSPACE ABOVE BACTERIAL CULTURES	84
11:50 - 12:10	Sergey Alexandrov	SPECTRAL ENCODING OF SPATIAL FREQUENCY APPROACH FOR LABEL-FREE VISUALIZATION OF STRUCTURE WITH SUB-WAVELENGTH RESOLUTION	40	Arandi Bezerra-jr	PLASMONICS AND SERS ACTIVITY OF METAL NANOPARTICLES: BEYOND GOLD AND SILVER	46
12:10 - 12:25	Isha Behl	EARLY DETECTION OF POTENTIALLY MALIGNANT ORAL LESIONS USING MINIMALLY INVASIVE BRUSH BIOPSY CYTOLOGY AND RAMAN MICROSCOPY	21	Alexandre Verdin	DEVELOPMENT OF SERS NANOPROBES FOR MULTIPLEX RECEPTORS IMAGING IN CANCEROUS TISSUES	52
12:25 - 12:40	Stephen Devereux	SINGLE WALLED CARBON NANOHORNS AS LIGHT ACTIVATED CELLULAR AGENTS	43	Sawsan Almohammed	ENHANCED PHOTOCATALYSIS AND BIOMOLECULAR SENSING WITH FIELD -ACTIVATED NANOTUBE-NANOPARTICLE TEMPLATES	74
12:40 - 14:10	<b>Lunch Break &amp; Posters</b>					
	<b>Tuesday 3A (Chair Vladimir Baumruk)</b>			<b>Tuesday 3B (Tanja Ducic)</b>		
14:10 - 14:30	Erik Goormaghtigh	COMBINING PROTEIN MICROARRAYS AND INFRARED IMAGING ALLOWS HIGH THROUGHPUT STRUCTURAL CHARACTERIZATION OF PROTEINS	6	Nandan Das	POLARIZATION ASSISTED SPECTRAL SPATIAL FREQUENCY ANALYSIS TO VISUALIZE SUB-DIFRACTIONAL TISSUE ANISOTROPY: PROMISES FOR PRE-CANCER DETECTION	49
14:30 - 14:50	Karin Hauser	MOLECULAR MECHANISM OF POLYGLUTAMINE AGGREGATION STUDIED WITH INFRARED SPECTROSCOPY	13	Markus Mangold	MID-INFRARED BIOSPECTROSCOPY APPLICATIONS OF QUANTUM CASCADE LASER FREQUENCY COMBS	29
14:50-15:10	Bryan Hennelly	IMPROVED PERFORMANCE OF NEAR INFRARED EXCITATION RAMAN SPECTROSCOPY USING REFLECTIVE SUBSTRATES FOR CYTOLOGY SAMPLES	81	Laurence Van Gulick	INVESTIGATION OF AGE-INDUCED MECHANICAL AND MOLECULAR REMODELING OF TYPE I COLLAGEN USING STRESS-STRAIN TEST AND RAMAN SPECTROSCOPY	85
15:10-15:25	Jehan Waeytens	HOW TO INVESTIGATE ISOLATED AMYLOID FIBRILS AT THE NANOSCALE: IR NANOSPECTROSCOPY CHALLENGES AND PROSPECTS	18	Aine Muldoon	SPECTROSCOPY AND LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY STUDIES ON THE EFFECT OF HIGH PRESSURE PROCESSING ON POLYPHENOXIDASE INACTIVATION, GLYCAEMIC INDEX AND PHENOLICS OF IRISH POTATO CULTIVARS	22

15:25-16:05	Coffee Break & Posters (Conference Photo)		
	Invited 4 (Chair Erik Goormaghtigh) Horiba Sponsored Session		
16:05 - 16:20	Adam Holland Horiba	A-TEEM™ - A NOVEL FLUORESCENCE-BASED APPROACH TO MOLECULAR FINGERPRINTING	
16:20 - 16:40	Olivier Piot	SCORING OF TUMOUR AGGRESSIVENESS OF SQUAMOUS CELL LUNG CARCINOMAS BY MID-INFRARED IMAGING	48
16:40 - 17:10 (Invited)	Malgorzata Baranska	RAMAN IMAGING IN THE LIFE SCIENCES: PHARMACOLOGY OF ENDOTHELIUM	64
17:10 - 17:40 (Invited)	Catherine Kendall	RAMAN SPECTROSCOPY IN MOLECULAR CANCER DIAGNOSTICS: CURRENT CHALLENGES AND FURTHER PROSPECTS	
17:40 -19:00	Poster Session		

<b>Wednesday 21 August</b>				
	George Moore Lecture Theatre		Lynch Theatre (Th F)	
	Registration			
	Invited 5 (Chair Neil Hunt)			
09:00 - 09:30 (Invited)	Thomas L. C. Jansen	WHAT DO WE LEARN FROM FLUORESCENCE-DETECTED TWO-DIMENSIONAL ELECTRONIC SPECTROSCOPY?	8	
09:30 - 10:00 (Invited)	Jens Bredenbeck	MAPPING VIBRATIONAL ENERGY TRANSFER IN PROTEINS WITH NON-CANONICAL AMINO ACIDS AND ULTRAFAST INFRARED SPECTROSCOPY	57	
10:00 - 10:30 (Invited)	Lauren Webb	USING VIBRATIONAL STARK EFFECT SPECTROSCOPY TO INVESTIGATE CARCINOGENIC MUTANTS OF H-RAS	86	
10:30- 11:00	Coffee Break & Posters			
	Wednesday 2A (Chair Karin Hauser)			Wednesday 2B (Chair Aoife Gowan)
11:00 - 11:20	Neil Hunt	MONITORING BASE SPECIFIC DYNAMICS DURING MELTING OF DNA-LIGAND COMPLEXES USING TEMPERATURE-JUMP TIME-RESOLVED INFRARED SPECTROSCOPY	7	Murali Krishna Chilakapati   SALIVA RAMAN SPECTROSCOPY: EXPLORATIONS OF SAMPLING METHODS   15

11:20 - 11:40	Artur Nenov	PHOTOPHYSICS OF PYRIMIDINE NUCLEOSIDES TRACKED WITH SUB-20-FS UV PULSES AND MIXED QUANTUM-CLASSICAL MOLECULAR DYNAMICS SIMULATIONS AT THE QM(CASPT2)/MM(AMBER) LEVEL	82	Alessandro Ferragina	VIS-NIR SPECTROSCOPY FOR THE PREDICTION OF FATTY ACID CONTENT IN LAMB MEAT	
11:40 - 12:00	Frantisek Sanda	TIME-RESOLVED AND TWO-DIMENSIONAL ELECTRONIC SPECTRA INDICATE ANHARMONIC VIBRATIONS IN LARGE MOLECULES	56	David Perez Guaita	INVESTIGATING DRUG UPTAKE AND MODE OF ACTION IN VITRO USING RAMAN MICROSCOPY AND MCRALS	66
12:00 - 12:20	Till Stensitzki	COMPARISON OF THE INITIAL PHOTOREACTION OF BACTERIORHODOPSIN IN MICROCRYSTALS AND IN SOLUTION BY FS PUMP-PROBE SPECTROSCOPY	55	Eva Kocisova	DROP COATING DEPOSITION RAMAN (DCDR) SPECTROSCOPY USED FOR SENSITIVE DETECTION OF BIOLOGICALLY IMPORTANT MOLECULES	36
12:20 - 12:35	Florian N. Brünig	BARRIER-CROSSING INFRARED SPECTRAL SIGNATURES OF PROTON-TRANSFER DYNAMICS IN THE H5O2+ CATION	20	Damien Traynor	NEW TECHNOLOGY FOR CERVICAL CANCER SCREENING AND HPV TESTING BASED ON RAMAN SPECTROSCOPY	118
12:35 - 12:50	Julian M Schmidt-Engler	ADDING ANOTHER DIMENSION TO OUR UNDERSTANDING OF PROTEINS: 2D-IR SPECTROSCOPY OF THE IR LABEL -SCN	54	Liron Zada	STIMULATED RAMAN SCATTERING MICROSCOPY FOR THE EVALUATION OF SILICONE CONTENT IN BREAST IMPLANT CAPSULES	24
12:50	Lunch/Excursion					

## Thursday 22 August

	George Moore Lecture Theatre			Lynch Theatre (Th F)	
	<b>Invited 6 (Chair Dilip Rai)</b>				
09:30 - 10:00 (Invited)	Andreas Barth	THE INTERNAL STRUCTURE OF AMYLOID-BETA OLIGOMERS STUDIED BY ISOTOPE-EDITED FTIR SPECTROSCOPY	19		
10:00 - 10:20	Fiona Lyng	RAMAN SPECTROSCOPIC SIGNATURES IN MURINE HIPPOCAMPUS FOLLOWING PARTIAL BODY IRRADIATION			
10:20 - 10:40	Mahmoud Huleihel	RAPID DETECTION OF BACTERIAL SUSCEPTIBILITY TO ANTIBIOTICS USING INFRARED SPECTROSCOPY AND MULTIVARIATE ANALYSIS	30		
10:40 - 11:00	Anita P Pax	THE MICROSTRUCTURE OF DAIRY PRODUCTS CHARACTERISED USING RAMAN AND FTIR IMAGING TECHNIQUES	38		

11:00 - 11:30	Coffee Break		
	<b>Thursday 2A (Chair Luis Alberto Batista De Carvalho )</b>		
11:30 - 12:00 (Invited)	Steve Meech	BACTERIAL LIGHT SENSING MECHANISM PROBED BY ULTRAFAST VIBRATIONAL SPECTROSCOPY AND UNNATURAL AMINO ACID SUBSTITUTION	65
12:00 - 12:20	Henrike M. Müller-Werkmeister	TIME-RESOLVED SERIAL SYNCHROTRON CRYSTALLOGRAPHY WITH PHOTOCAGED SUBSTRATES – WATCHING AN ENZYME AT WORK	27
12:20 - 12:40	Alberto Mezzetti	PHOTOPROTECTION MECHANISMS IN CYANOBACTERIA AND DIATOMS INVESTIGATED BY TIME-RESOLVED INFRARED SPECTROSCOPY: FROM ISOLATED PROTEINS TO IN VIVO STUDIES	59
12:40 - 12:55	Sandra Estalayo	SPECTROSCOPIC STUDIES OF THE PHOTOADDUCT FORMED BETWEEN THE COMPLEX [Ru(TAP)3]2+ AND GUANOSINE 5'-MONOPHOSPHATE	
12:55 - 14:00	Lunch Break		
	<b>Thursday 3A (Chair Hugh Byrne)</b>		
14:00 - 14:20	Frederik Großerüschkamp	QCL-BASED IR-IMAGING OF COLORECTAL CANCER TISSUE FOR CLINICAL DIAGNOSTICS	12
14:20 - 14:40	Andras Gorzszas	RACE TO UNDERSTAND PANCREATIC ISLET BIOCHEMISTRY	16
14:40 - 15:10 (Invited)	Marloes Groot (Teledyne Princeton Instruments)	INSTANT PATHOLOGY WITH HIGHER HARMONIC GENERATION	31
15:10 - 15:20	Closing Ceremony		