PhD Thesis proposal

General Information		
PhD Thesis Title	***Extraction and analytical control of bioactive molecules found in pharmaceutical and environmental samples***	
School	Faculty of Medicine and Medical Sciences, Faculty of Sciences.	
Research Unit	NA	
Laboratory	NA	
Axis	Development and validation of analytical procedures for xenobiotic compounds	
PhD Supervisor	Name & Title: Joseph Saab, Professor, HDR Email: josephsaab@usek.edu.lb	University Address: Faculty of Sciences, Holy Spirit University of Kaslik-USEK
Co-supervisor (if applicable)	Name & Title: Souheil Hallit, Pharm.D., M.Sc, MPH, PhD Email: souheilhallit@usek.edu.lb Name & Title: Walid Hleihel, PhD. Email : walidhleihel@usek.edu.lb	University Address : Faculty of Medicine and Medical Sciences, Holy Spirit University of Kaslik-USEK Faculty of Sciences, Holy Spirit University of Kaslik-USEK
Location (s)	Location 1: USEK	Work shift calendar /per year (%): 100%
	Location 2: (if applicable)	Work shift calendar /per year (%):
Funding and scholarship	(Currently in fundraising, in progress)	
Applicant Profile and/or Special Requirements	<u>Applicant profile:</u> Master of Sciences: Masters in Chemistry, Masters in Biochemistry. <u>Special requirements</u>: practical knowledge in GC MS, HPLC-DAD, quantitative liquid-liquid extraction, quantitative solid-liquid extraction.	

Subject's national or worldwide Context, Objectives & Research lines
For around 30 years now, scientific research is focusing on the intense misuse, overuse and exposure to bioactive molecules including drugs, drug metabolites, and environmental pollutants containing in pharmaceutical and environmental samples; since it has been correlated with resistance to multiple pathogenic issues around the globe. This pandemic matter is drawing attention into the analytical study of the bioactive class of drugs. Studies consist of design and optimization of extraction and separation techniques of these bioactive molecules. Therefore, the target is to reach a proper quantification and further identification of these molecules in complex pharmaceutical as well as in environmental matrices. Nevertheless, the main concern is that a wide range of bioactive is non-volatile, moderately or highly polar and water soluble.

These complex matrices can be aqueous or biological liquids or pharmaceutical solids; thus, controlling quantitatively the bioactive substances is challenging from the perspective of analytical chemistry. This is due to the presence of biologically or pharmaceutically active and/or inactive interfering species that might affect the quantification of target molecules, possibly distorting results by excess or by defaults. In order to avoid this issue, pre-treatment methods, such as liquid-liquid or solid-liquid extraction, are applied; validating proper cleaning and proper signal detection. Many techniques will be used in bioactive residue analysis; the adequate method depends on the complexity of the sample, the nature of the matrix/analytes, and the analytical techniques available

The aim of this PhD thesis will help the analyst developing effective and validated analytical strategies for the analysis and quality control of different xenobiotics from different sample types, quickly, accurately and at acceptable cost.

The experimental results are of public health relevance since these analytes are extracted from pharmaceutical and environmental samples, hence the interpretation of these results can be linked to human exposure assessment.

Outcomes (OCs): What do we wish to achieve?	
OC1:	Extraction of bioactive molecules including drugs, drug metabolites.
OC2:	Analysis, validation and quantification of bioactive molecules from different samples
OC3:	Optimization on the molecular level of analytes, using quantitative structure-property relationship (QSPR).

References (R) (5 most recent peer-reviewed publications)	
R1:	Yao, Y., Shao, Y., Zhan, M. et al. (2018), Rapid and Sensitive Determination of Nine Bisphenol Analogues, Three Amphenicol Antibiotics, and Six Phthalate Metabolites in Human Urine Samples Using UHPLC-MS/MS, *Analytical and Bioanalytical Chemistry,* 410(16):3871-3883. doi:10.1007/s00216-018-1062-2. https://www-ncbi-nlm-nihgov.ezproxy.usek.edu.lb/pubmed/29671029
R2:	Cherkashina K., Vakh C., Lebedinets S., Pochivalov A., Moskvin L., Lezov A., Bulatov A. (2018), An Automated Salting-out Assisted Liquid-Liquid Microextraction Approach Using 1-octylamine: On-line Separation of Tetracycline in Urine Samples Followed by HPLC-UV determination, *Talanta*, 184:122-127, doi:10.1016/j.talanta.2018.02.112. https://www-ncbi-nlm-nih-gov.ezproxy.usek.edu.lb/pubmed/29674022
R3 :	Melikian A. A., Djordjevic M. V., Chen S., Richie Jr, J. & Stellman S. D. (2007), Effect of Delivered Dosage of Cigarette Smoke Toxins on the Levels of Urinary Biomarkers of Exposure, *Cancer Epidemiol Biomarkers Prev*, (16)(7) 1408-1415; doi: 10.1158/1055-9965.epi-06-1097, https://www.ncbi.nlm.nih.gov/pubmed/17627005.
R4 :	Lafossas C., Benoit-Marquié F. & Garrigues J.C. (2019), Analysis of the Retention of Tetracyclines on Reversed-Phase Columns: Chemometrics, Design of Experiments and Quantitative Structure-Property Relationship (QSPR) Study for Interpretation and Optimization*, Talanta,* 198:550-559, doi: 10.1016/j.talanta.2019.02.051. https://www-ncbi-nlm-nih-gov.ezproxy.usek.edu.lb/pubmed/30876599
R5 :	Antibiotic Resistance in Lebanon, Antimicrobial Resistance (AMR) Control. http://resistancecontrol.info/2017/antibiotic-resistance-in-lebanon/