Plan Overview

A Data Management Plan created using DMPTool

Title: Novas estratégias analíticas para determinação de compostos químicos emergentes em amostras ambientais, de alimentos e de fluídos biológicos.

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Funder: São Paulo Research Foundation (fapesp.br)

Funding opportunity number: PI - Auxílio à Pesquisa - Projeto Inicial / Chamada de Propostas (2022)

Grant: PI2022

Template: Digital Curation Centre (português)

Project abstract:

Approximately 2000 new chemicals products are registered and commercialized on a daily basis. However, there are concerns related to the safety and exposure to these products to human health and the environment. To understand the impact of these chemical compounds in the environment and biological systems, the first step is to develop effective methods for their detection and characterization. Therefore, new analytical methods are critical to support the effort of regulatory agencies to identify and quantify the occurrence of emerging compounds in environmental, food and biological samples. There is a public health concern that many of these substances and their metabolites remain in these samples, increasing their potential to impact physiological pathways and cause disease. The advance of bioinformatics, data acquisition and processing allows new analysis concepts: target analysis (target compounds selected to be quantified), suspect screening (known the possible compounds in the sample but lacking method to quantify) and non-target screening (detection of new compounds or markers). The target method is essential to quantify emerging chemical compounds of concern and requires sample preparation procedures that should be in accordance to green chemistry concepts and use designed solvents to extract the analytes based on their physicochemical properties. The MRM-Profiling is a simple and fast tool that can be used for suspect screening of emerging chemicals that requires only a nanoESI source and a triple quadrupole instrument. Thus, this project aims to develop two innovative analytical tools to quantify emerging chemicals in complex samples: 1)MRM-Profiling methods for initial suspect screening of the chemical compounds of concern present in environmental, food and biological samples; and 2) target methods to determine the compounds in the selected samples that uses green chemistry sample preparation procedures incluiding magnetic ionic liquids and natural deep eutectic solvents. The samples will consist of sewage, sludge, seafood, vinegar, soft drinks, cachaça, beer, and urine. The MRM-Profiling will use a direct infusion of small sample volume or sample pool. The experiment presents three steps, the first discovery stage which interrogates

the sample using precursor ion and neutral loss scans in MRM experiments using different collision energies (15, 20, 25, 30, 35, 40 and 45 V) regarding the functional chemical groups. The acquired data is processed using bioinformatics tools and compared to databases such as METLIN. Then, the MRM with signal superior to 30 % of the blank and system artifacts are selected. The second phase, the screening phase applies the selected MRMs to process each sample individually. The last phase is the confirmatory step that uses the product ion scan, or if necessary, tandem mass spectrometry or high-resolution mass spectrometry to further confirm the chemical compounds. All samples will be analyzed through MRM-Profiling, further, the emerging chemical of concern will be confirmed using target methods to determine pharmaceuticals, personal care products, pesticides, plasticizers, flame retardants, and elementary compounds (As, Cd, Cr, Hg, Se, and V). At the end of this project, as result of these two innovative analytical approaches, it is expected not only to determine the major chemicals compounds present in the environmental and biological samples but also to quantify the levels of these compounds using simple and fast methods with reduced environment impact. These results will assist regulatory agencies to better understand the presence and impact of these chemicals in human health and the environment.

Start date: 10-31-2022

End date: 10-30-2027

Last modified: 03-19-2022

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Novas estratégias analíticas para determinação de compostos químicos emergentes em amostras ambientais, de alimentos e de fluídos biológicos.

Os dados referentes as amostras de esgoto, lodo, frutos do mar industrializados, vinagre, refrigerantes, cachaça, cerveja e urina analisadas pelos métodos de MRM-Profiling e métodos target fornecerão informações importantes relativos a presença de compostos químicos emergentes.

As amostras serão coletadas e analisadas por infusão direta no método de MRM-Profiling bem como pelos métodos target usando solventes verdes e moduláveis considerados verdes.

Os resultados obtidos das amostras serão armazenados em software de planilhas como Excel, Libreoffice ou Planilhas Google.

As amostras de urina por serem provenientes de seres humanos, será coletada e analisada com os parceiros internacionais da Purdue University e da Iowa State University, sendo submetida ao comitê de ética da instituição.

Os dados gerados serão propriedade das instituções envolvidas no projeto que serão disponibilizados em bancos públicos das universidades após a conclusão da presente proposta.

Os dados obtidos durante o projeto serão armazenados no Google Drive, Dropbox e pCloud do coordenador do projeto (Prof. Dr. Paulo Clairmont F. de Lima Gomes). Além disso, haverá cópia simultânea desses dados em dois discos rígidos (HDs) diferentes, um sob o cuidado do Prof. Paulo Clairmont e outro sob responsabilidade do Prof. Mario Henrique Gonzalez.

Os dados serão disponibilizados aos interessado que tiverem interesse nas pesquisas desenvolvidas e quando solicitado o seu acesso.

Os dados serão preservados pelo prazo de 5 anos mesmo após o final do projeto e compartilhados conforme solicitação pelos interessados.

Todos os dados obtidos, principalmente, os usados para publicação serão armazenados mesmo após o fim do projeto. Os dados serão preservados pelo prazo de 5 anos mesmo após o final do projeto. Os dados serão compartilhados pelo repositório das instituiçoes envolvidas no desenvolvimento desse projeto, além de publicações em revistas de ampla divulgação internacional.

Os dados serão disponibilizados aos interessado que tiverem interesse nas pesquisas desenvolvidas e quando solicitado o seu acesso.

Poderá haver restrições de dados, caso na etapa de síntese dos novos solventes verdes gerem pedidos de patente. Os demais dados ficaram disponibilizados conforme solicitação.

O Prof. Paulo Clairmont será o responsável pelo gerenciamento dos dados.

O armazenamento na nuvem em plataformas online irá permitir acessos aos documentos e conexão com a comunidade interessada nesses dados.
