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## Plan Overview

*A Data Management Plan created using DMPonline*

**Title:** Plataforma metabolomica basada en GC-MS

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**Template:** DMPOnline Template (NWU)

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# Plataforma metabolómica basada en GC-MS

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## Data Collection

### What data will you be collecting ?

Metabolomics data from biological samples. The raw data (vendor-specific files) will be converted into tabulated data in the format of .csv files.

### Who will be involved in your data collection ?

The data associated to this project will be collected by a multidisciplinary team led by Dr. Raúl González-Domínguez (expertise in omics and analytical chemistry), in collaboration with clinicians from Hospital Universitario Puerta del Mar at Cádiz, Spain. Data collection, processing and quality control will be performed by adhering methodologies that have previously been validated and published by the research team and collaborators (DOI: 10.1007/978-1-0716-2699-3\_11; 10.1007/978-1-0716-2699-3\_12; 10.3390/metabo10040135; 10.1021/acs.analchem.3c03660). We will implement a standardized naming of the data generated along the consecution of the research project, according to the format: "acquisition date\_" "project code"\_"experiment"\_"researcher name"\_"versión of the document"; e.g., "20240626\_IFEQ22/00014\_Metabolomics\_RGD". Moreover, the data from the project will have descriptive metadata according the DataCite Metadata scheme 4.0.

The raw data is expected to have a total volume around 50 GB (in vendor-specific format, i.e., .d Agilent files). The data will be converted into the open data format .mzXML and then processed using open access webtools (i.e., MS-DIAL) to generate .csv files, containing tabulated concentrations of each of the analytes under investigation in the study population. These tables are expected to have a volume below 200 MB, thus facilitating their storage and sharing. The storage, preservation and sharing of the data will not imply additional costs.

Along the consecution of the project, the data generated will be uploaded into an online shared folder (Google Drive) to facilitate its finding and use by authorized participating researchers, and the principal investigator (Drs. Raúl González Domínguez) will retain a backup copy in external hard drives. Furthermore, within the context of FAIR principles, the data will be deposited into a specialized and open acces repository (Metabolomics Workbench), which allows the deposition of omics data without expiration dates neither additional costs. This deposition will be performed at the moment of publication of our results in peer-reviewed journals. We will use CC-BY license (<https://creativecommons.org/licenses/by/4.0/>).

Dr. Raúl González Domínguez, with assisstance from personnel from the Research Managment Office at the affiliation entity, will be responsible for developing, implementing, overseeing, and updating this Data Managment Plan during and after the project ending.

## Ethics

### Give a description of your Ethics

The study was performed in accordance with the principles contained in the Declaration of Helsinki. The Ethical Committee of "Hospital Universitario Puerta del Mar" (Cádiz, Spain) approved the study protocol, and all participants and/or legal guardians provided written informed consent.