TRISKELION

NON-TARGETED ANALYSIS TOOL TO FINGERPRINT BOTANICAL ACTIVE SUBSTANCES

BACKGROUND

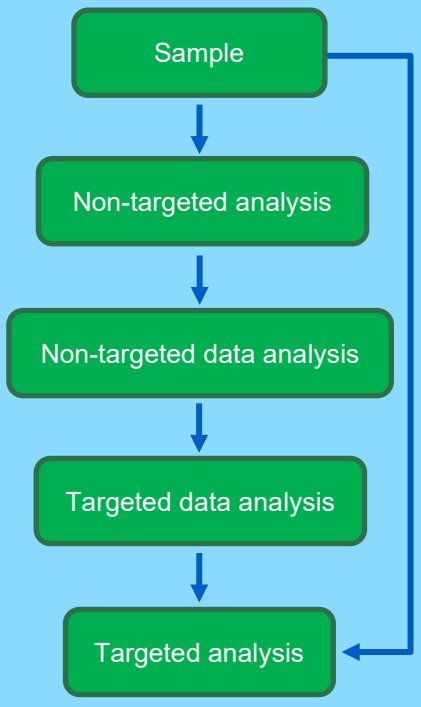
Botanical active substances are natural products that can be extremely difficult to analyse. Identifying the component in the active and performing a conventional five batch analysis is a costly and challenging exercise. To tackle this, the guidance document on botanical active substances used in PPPs (SANCO 11470/2012-rev. 8) includes the possibility to describe a botanical active substance by its chemical fingerprint.

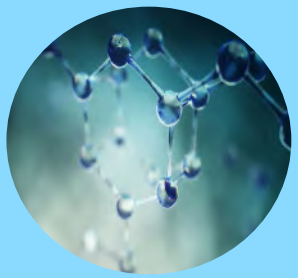
FINGERPRINTING

The fingerprint is defined as a spectroscopic and/or chromatographic profile that is matched against a reference and can be used to assure quality and consistency between samples. Finding a practical fingerprinting methodology capable of comparing complex mixtures has proven difficult, however, Triskelion has developed a methodology to compare UPLC-MS data of complex mixtures without the loss of data.

OUR TECHNIQUE

High resolution non-targeted LC-MS data is integrated to a single MS spectrum. Subsequently, the raw data is exported as intensities per nominal m/z values, equivalent to a barcode or fingerprint. After correction for solvent, the correlation between sample data is calculated to investigate the similarity between (future) batches. Because the underlying data is retained, subsequently targeted data analysis may be performed, to analyse differences and/or similarities between samples in more detail, i.e. on the molecular level.





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