

**DETECTING THE “UN-NATURAL” IN NATURAL PRODUCTS**

**INTRODUCTION**

There are an increasing number of herbal products being used around the world due to their perceived nature as a safer and cheaper alternative to prescription drugs. However, one major concern is the rising number of reports of adulteration of herbal products containing undeclared synthetic compounds or deliberate substitution of ingredients for economic benefit and pharmacological action. Due to the diversity and complexity of chemical compounds in herbal natural products, it is imperative to develop analytical methods to confirm the natural constitution for proper quality control and authentication. LC-MS based workflows are widely used for the identification of ingredients and potential adulterants because of their high sensitivity and selectivity for samples with complex matrices. However, researchers have a large bottleneck in obtaining results quickly due to the complexity and large scale of LC-MS datasets. In this study, a novel LC-MS-based natural products informatics platform, UNIFI, was used to screen an “all-natural” commercial herbal product used for erectile dysfunction. A streamlined workflow in UNIFI allowed researchers to quickly extract LC-MS results utilizing a traditional medicine (TM) and a synthetic adulterant library (SA) to effectively identify and characterize ingredients in the herbal product. In addition, the embedded structure elucidation tools such as overlay fragmentation also facilitated identification of unreported unknown peaks. In this study, results are shown from comprehensive analysis of the herbal product using a novel informatics platform based on a standard LCMS injection.

**METHODS**

- **Overview of the Waters Natural Product Application Solution with UNIFI**: which combines UPLC® QToF® MS technology with workflow-driven informatics.
- **An easy to use workflow-driven automatic streamlined process incorporating a traditional medicine and a synthetic adulterant library to quickly screen and identify chemical constituents and potential adulterants from commercial herbal supplement workflow.**
- **Significant enhancement in efficiency and productivity with less demand for operators’ technical expertise.**

**RESULTS AND DISCUSSION**

**Streamlined workflow using the Natural Products Application Solution with UNIFI:**

1) A 6.86 mins peak is observed in 5A, which was confirmed using the embedded natural product application solution with UNIFI. The peak was identified as Icariin.

2) Thioaidenafil is observed in LC-MS spectra correlate to what’s on display in 3C, both low energy MS full scan and corresponding high energy fragment ions.

3) The structural isomer determination: Thiosildenafil or Thiosildenafil.

**REFERENCES**

1. Waters Corporations, 34 Maple Street, Millford, MA 01952; Waters Pacific Private Ltd, Singapore; Waters Corporations, Beverly, MA 01915; Waters Corporations, Wilmslow, UK.

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