

REPORT

Thermo Scientific™ Compound Discoverer™ software for wide range screening of CECs by UHPLC-HRMS

In accordance to the work plan of TwiNSol-CECs project, “*Thermo Scientific™ Compound Discoverer™*” software was procured for the needs of broadening the range of UHPLC-HRMS analysis towards the wide-range screening of Contaminants of Emerging Concern (CECs). In fact, *Compound Discoverer™* is a small molecule identification application for high-resolution liquid chromatography (LC) – mass spectrometry (MS) and gas chromatography (GC) Orbitrap data. To support the efficient use of the software, a new PC of high performance with two display monitors were purchased following the *Compound Discoverer™* instructions for the optimal hardware support (Figure 1).

UHPLC-HRMS system existing at TFNS is Thermo Scientific™ Accela Exactive instrument with Orbitrap™ mass spectrometers. This system has been used for target analysis and compound mass confirmation, and even though the HRMS unit produces information-rich data without the dedicated software support they cannot be used for wide-range screening. To overcome of this and other challenges of small-molecule analysis a powerful software is required.

With a comprehensive, integrated set of libraries, databases, statistical analysis and visualization tools linked in customizable workflows, the *Compound Discoverer™* software streamlines unknown identification, determination of real differences between samples, and elucidation of biological pathways. Additionally, the software reveals the highest confidence data obtained on LC and mass spectrometry (MS) instrumentation.

For successful data processing appropriate computer configuration (hardware and software) is required according to the recommendations provided in *Compound Discoverer™* User Guide for LC Studies (Software version 3.3, XCALI-98478 Revision A, November 2021), Figure 2. The User Guide specifies hardware (processor, RAM memory, display monitor resolution, DVD-ROM, USB), software (operating program, Microsoft Offices version, etc.), and system settings requirements for processing computer. The purchased computer configuration satisfies the recommended hardware configuration for enhanced performance.



Figure 1. *The box with the provided USB containing all the necessary files for the successful installation of the Compound Discoverer software and the computer (hardware and software) together with display monitors*

The software was successfully installed at the TFNS by Dr. Luka Milovanović, an authorized service engineer of the company (Analysis d.o.o., Belgrade), representative of Thermo Scientific™ instruments and software installation in Serbia (Figure 3).

After the software installation, a detailed introductory training was provided by Dr. Luka Milovanović, who demonstrated the main software tools (Figure 4), including:

- Setting the data processing parameters in the software
- Identification of compounds using MS/MS libraries
- Determination of elemental composition using high-resolution full MS isotopes and MS/MS data
- Search online chemical databases
- Gaining confidence in ID with automated MSⁿ tree search against mzCloud
- Performing the statistics and differential analysis using t-tests, ANOVA, PCA, PLS-DA, volcano plots, box-and-whisker plots, and more
- Viewing trend charts to visualize peak areas, average peak area per group or fractional label incorporation over time, etc.

Table 1. Hardware and software requirements for the processing computer

System	Minimum requirements
Hardware	<ul style="list-style-type: none"> • 3.4 GHz dual-core processor • 16 GB RAM • 500 GB hard drive • DVD-ROM and USB drive • Display monitor resolution of 1920 × 1080
Software	<ul style="list-style-type: none"> • Microsoft Windows 7 SP1 64-bit operating system or Microsoft Windows 10 64-bit operating system • Microsoft .NET Framework 4.7.2 • Microsoft .NET Core Runtime 2.1.19 • Microsoft Office 2013 • PDF reader
System settings	<ul style="list-style-type: none"> • To run processing workflows with online mass spectral database searches, the computer must have unblocked access to the mass spectral databases on the Internet. • The computer must have the correct time and date settings and be synchronized with Internet time. • The Region and Language setting for the operating system must be set to English (United States).

Preface

Table 2 lists the recommended hardware configurations for enhanced performance using the Compound Discoverer application.

Table 2. Recommended hardware configurations for enhanced performance

System	Recommended configurations
Hardware	<ul style="list-style-type: none"> • Dual 8-core processor (for example, 2x Intel™ Xeon™ Gold 6134 CPU @ 3.20 GHz) • 64 GB RAM • 1 TB SSD (solid-state disk) hard drive for OS • 2nd 3 TB (conventional disk) hard drive for data storage • DVD-ROM and USB drive • Two 27 in. UHD monitors: Display monitor resolution of 3840 × 2160 pixels

Figure 2. Specified computer configuration (hardware and software) for software installation

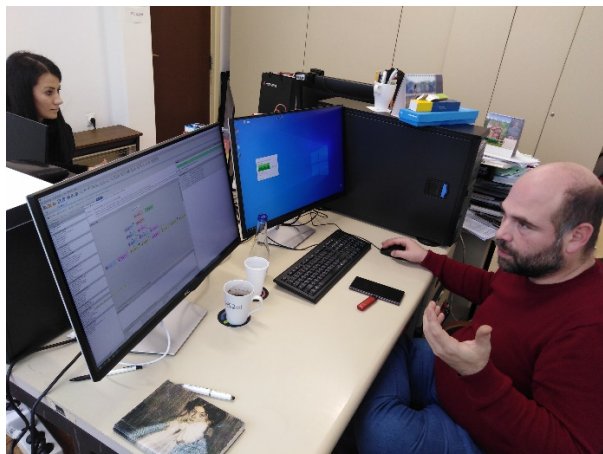


Figure 3. Installation of software by authorized service engineer Dr. Luka Milovanović

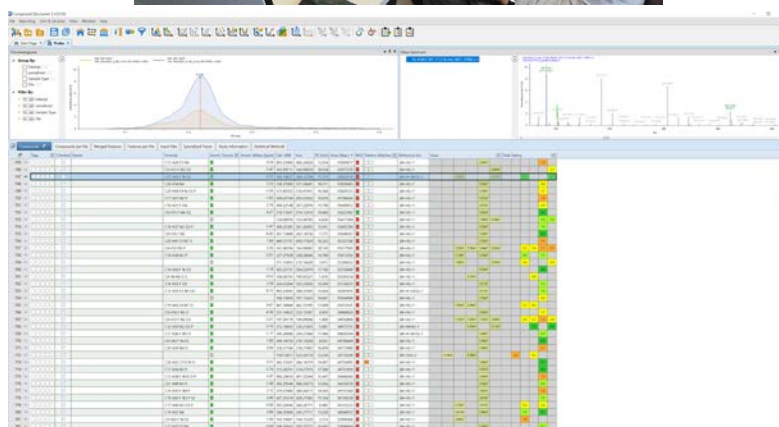
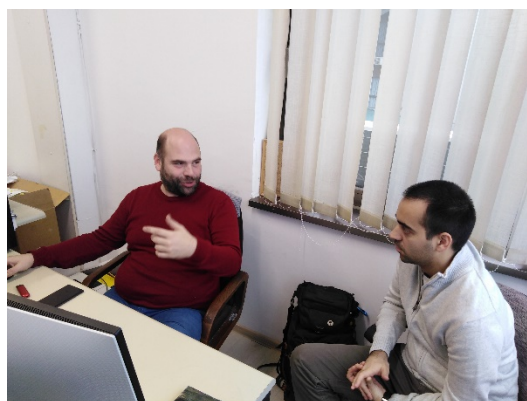


Figure 4. Detailed introductory training on data processing (real sample analysis) on Compound Discoverer software

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