The qualitative analysis and compound report

The Screening Unit provides an analysis report and a compound report of 352 compounds in a preliminary LC-MS evaluation process. For MS analysis compounds are dissolved in DMSO, diluted with acetonitril/water (1:1) to a concentration of 25 µM and filtered before measurement. The qualitative analysis report of each compound consists of six chromatograms whereas the compound report comprises a table of 352 compounds listed with retention time, measured mass and purity according to the UV absorption at 254 nm. If the qualitative analysis does not meet the expected criteria (for example: high deviation between calculated and measured mass or low absorption) the respective compound will be marked with a comment in the compound report and the fourth and sixth chromatogram might be missing in the analysis report. For further and more detailled analytical methods and discussions, please contact Edgar Specker. Phone: +49 30 9406 3064 Mail: specker@fmp-berlin.de

First chromatogram:

TWC: total wavelength chromatogram
Sum of UV absorptions of compounds between the wavelengths 190-950 nm. The first peak is normally assigned to DMSO.

Second chromatogram:

UV absorptions of compounds at 254 nm.

Third chromatogram:

TIC: Total ion current
Entire range of compound masses is being detected.

Fourth chromatogram:

Integration of peaks detected at 254 nm. Integrations are used for the purity calculation of the expected compound. The retention time and the molecular formula of the compound are displayed. Additionally, the retention time is automatically aligned to the retention time in third (TIC) and fifth chromatogram.

Fifth chromatogram:

Extraction of expected mass from TIC according to the molecular formula and calculation of deviation between calculated and measured mass.

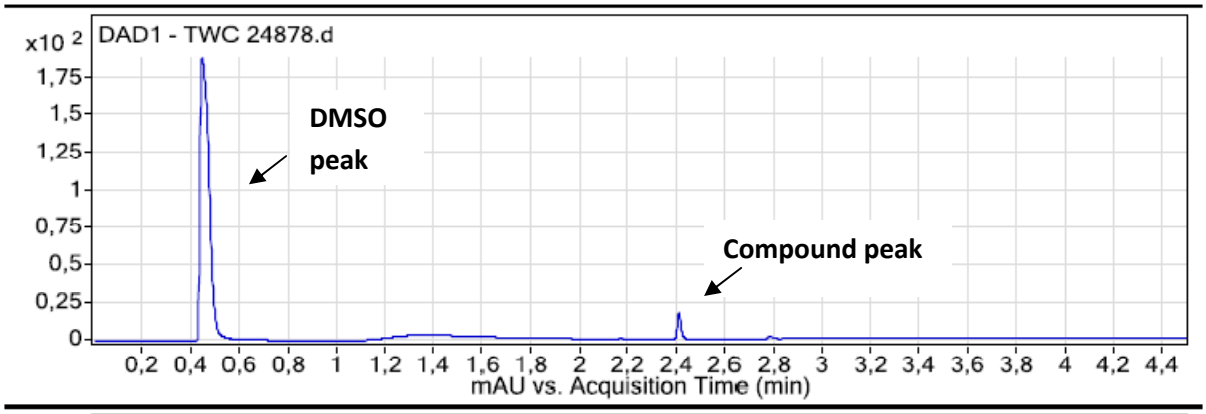
Sixth chromatogram:

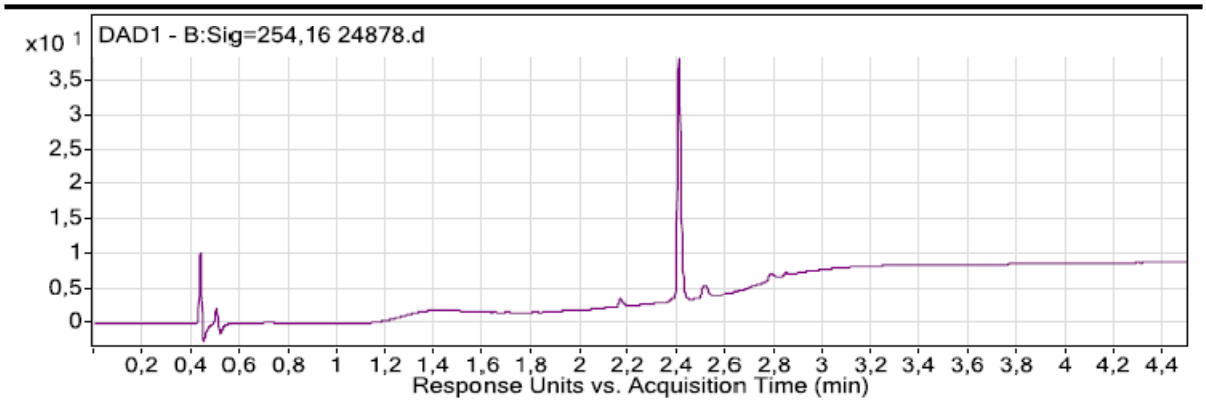
Mass spectra of the compound.

Example of qualitative analysis report:

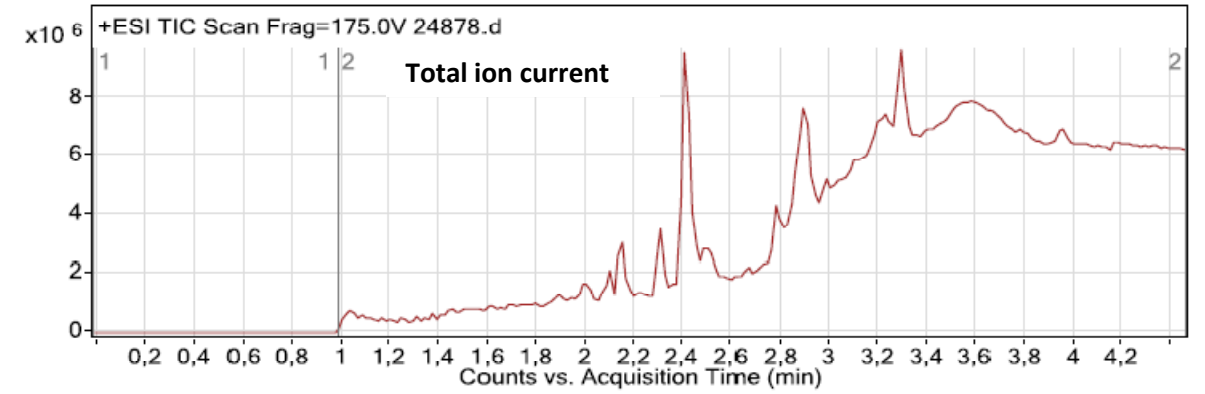
Qualitative Analysis Report

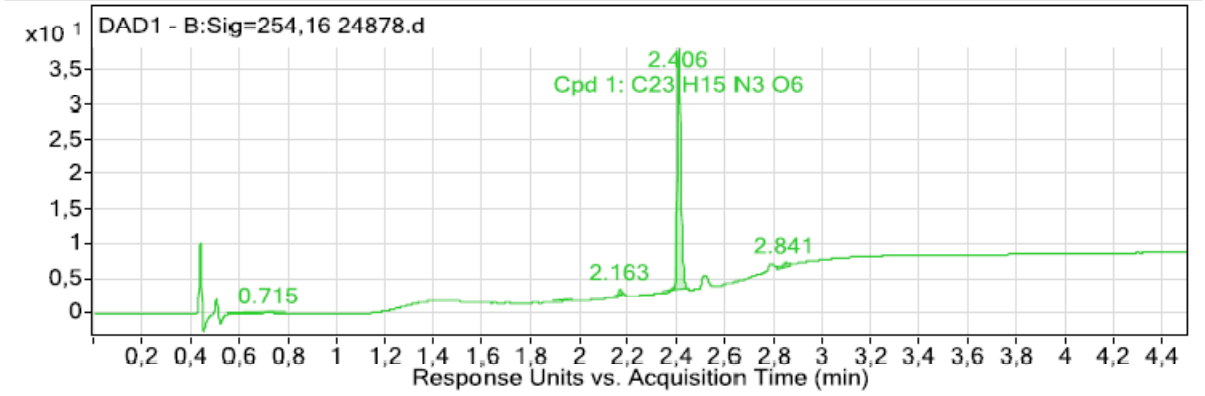
User Chromatograms **Total wavelength chromatogram (190 -950 nm)**





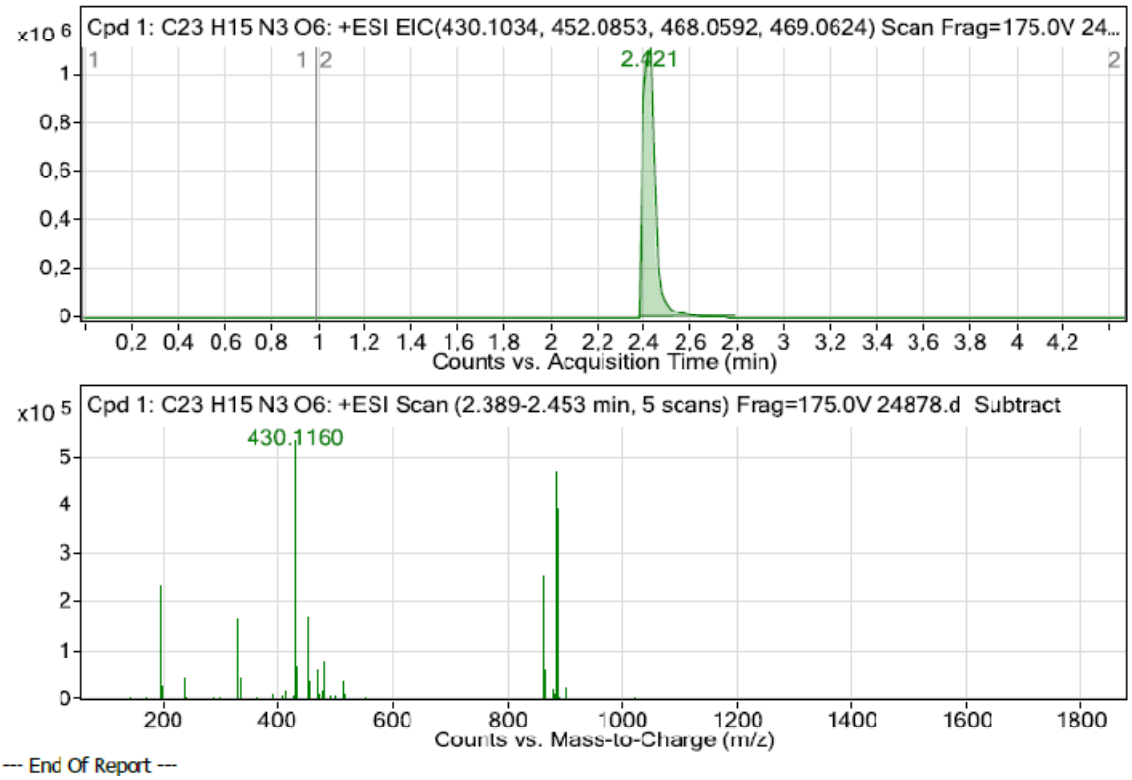
Fragmentor Voltage 175 **Collision Energy** 0 **Ionization Mode** Esi





Qualitative Analysis Report

Compounds



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Example of a compound report:

example_compound_report							
Comp_ID	**RT**	**Mass**	**Formula**	**Tgt Mass**	**Diff (ppm)**	**Purity**	**comments**
102465	1.5610	323.16	C19H21N3O2	323.16	4.4200	100	
102466	1.8790	184.07	C9H12O4	184.07	-19.660		no UV-activity; no ionisation
102467	1.4990	198.08	C12H10N2O	198.08	1.8100	100	
102468	2.5280	238.19	C15H26O2	238.19	2.1500		no UV-activity
102469	2.2960	324.10	C19H16O5	324.10	-0.080000	100	
102470	1.9420	266.07	C15H10N2O3	266.07	9.0200	90.200	
102471	1.7000	411.23	C21H33NO7	411.23	6.9100	100	