

MS-Flowinjection



BERGISCHE
UNIVERSITÄT
WUPPERTAL

Analysis Info

Analysis Name D:\Data\210208\ocip test_000001.d
Method POS_MS_flow_low_1min_STAND.m

Sample Name ocip test

Comment ESI: Flowinjection. Zugabe von 10 ul HCOOH.

Acquisition Date 2/8/2021 10:43:31 AM

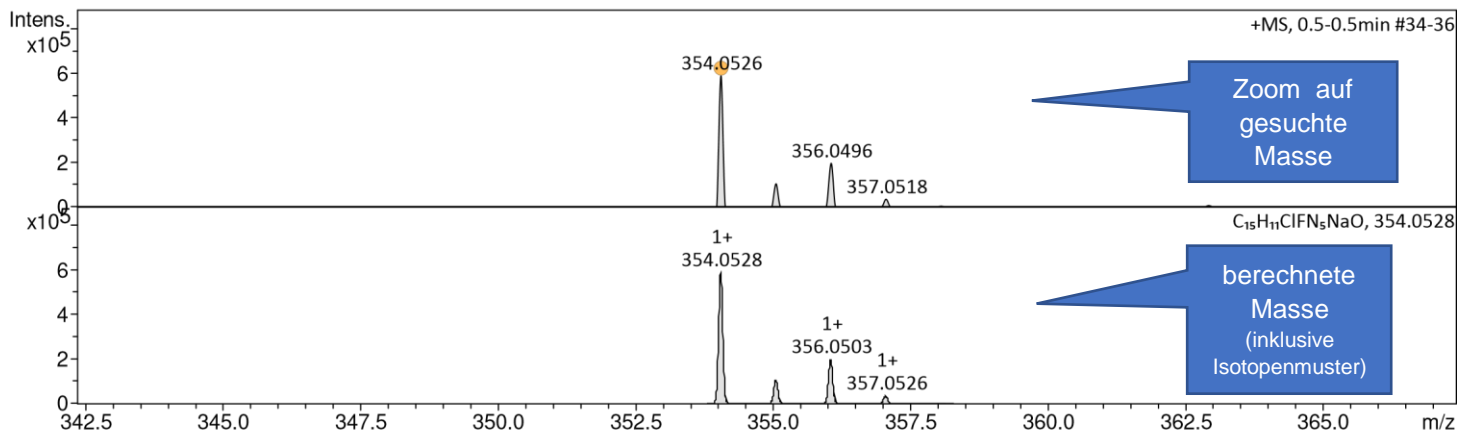
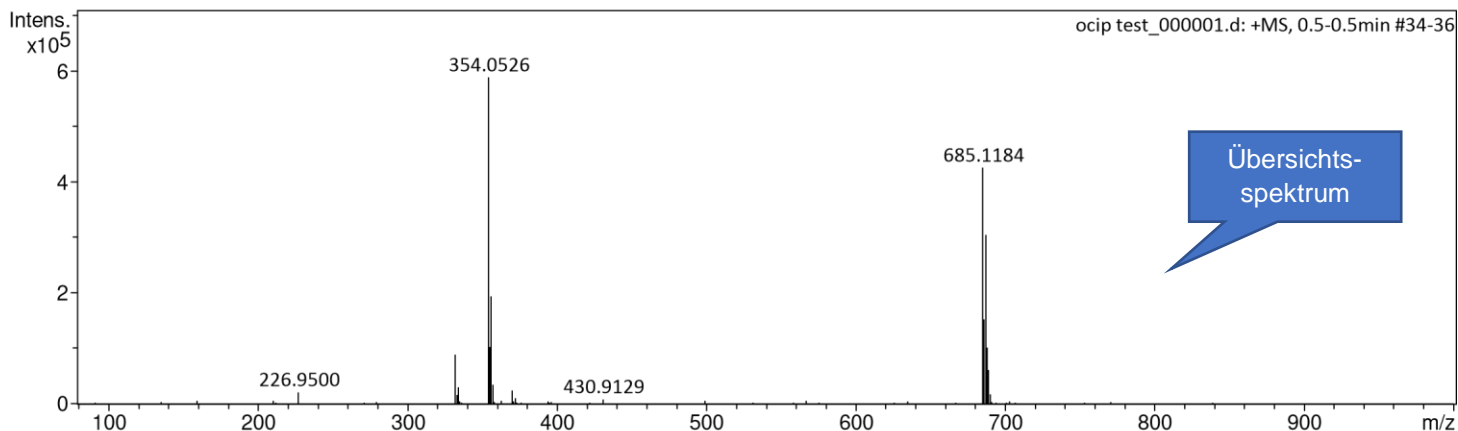
Operator MASSE AK Kirsch

Instrument / Ser# micrOTOF 213750.00

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Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻	Conf	N-Rule
354.0526	1	C15H11ClFN5NaO	354.0528	0.6	5.5	1	100.00	11.5	even		ok

Erklärungen

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Column	Description
Meas. m/z	Measured m/z value.
#	Running number of formula (for each m/z).
Formula	Sum formula.
Score	Score of the formula (a value between 0 and 100%).
m/z	Calculated m/z of the formula.
err [mDa]	Deviation between measured mass and theoretical mass of the selected peak in [mDa].
err [ppm]	Deviation between measured mass and theoretical mass of the selected peak in [ppm].
mSigma	Sigma is a rate for the agreement of the theoretical and measured isotopic pattern of the mass peak of interest. It combines the standard deviation of the masses and intensities for all isotopic peaks. The values are given in [milliSigma] and lower numbers indicate a better fit.
rdb	Number of rings and double bonds in the formula.
e⁻ Conf	Indicates whether the electron configuration is even or odd.
N-Rule	Indicates whether the nitrogen rule is fulfilled.
Adduct	Considered adduct ion.