

Example of number\_of\_formulas for beech throughfall

	Number of formulas	comments
Registered peaks:	18010	
Unique identified peaks	9878	using the constraints above mentioned in the reply
Multiple identification	2160	These were not further considered, that means, we lose 12% of the peaks, but we exclude false positive ones
Not listed peaks	5972	most of all are $^{13}\text{C}$ isotopic peaks without further scientific information; or not assigned because not within constraints, e.g. CHOP, CHOS <sub>4</sub> , CHOS <sub>2</sub> N <sub>3</sub> , CHOS <sub>3</sub> N <sub>3</sub> ...; or the peaks are so small, that their exactness is smaller than 1 ppm