Table S1: List of the parameters and their values that are used currently in the KNIME workflows for assembling the metabolite features.

Workflow **Parameter**	**Lenient**	**Default/MS2 Spectral Matching**	**Strict**
noise_threshold_int	8	10	12
chrom_peak_snr	2	3	3
chrom_fwhm	10	8	3
trace_termination_criterion	sample_rate	sample_rate	sample_rate
mtd: min_trace_length	2	3	3
mtd: max_trace_length	-1	-1	400
mtd: mass_error	12	10	8
width_filtering	off	off	auto
report_convex_hulls	true	true	true