

Table S2: List of the parameters and their values that are used currently in the KNIME workflows for the map alignment (correcting retention time distortions between maps).

Parameter \ Workflow	Lenient	Default/MS2 Spectral Matching	Strict
max_num_peaks_considered	-1	-1	-1
mz_pair_max_distance	0.005	0.005	0.005
num_used_points	10000	10000	10000
distance_RT → max_difference	30	20	10
distance_MZ → max_difference	20	20	20
distance_MZ → unit	ppm	ppm	ppm