Raw spectra lightred white red Signal intensity 4e+05 2e+05 0e+00 1.80 1.75 1.70 1.75 1.70 1.80 1.75 1.70 1.80 ppm Peak detection and AUC quantification lightred white red 1e+06 AUC 5e+05 0e+00 1.75 1.80 1.75 1.70 1.80 1.80 1.75 1.70 1.70 ppm Peak grouping lightred red white 1e+06 AUC 5e+05 0e+00 -1.75 1.70 1.75 1.75 1.70 1.80 1.80 1.70 1.80

ppm