Raw spectra r g W 6e+05 Signal intensity 4e+05 2e+05 0e+00 4.40 4.39 4.38 4.40 4.39 4.37 4.36 4.40 4.37 4.36 4.39 4.38 4.36 ppm Peak detection and AUC quantification r W g 1500000 1000000 -500000 -0 4.37 4.39 4.38 4.40 4.39 4.38 4.40 4.39 4.38 4.36 4.40 4.37 4.36 4.37 4.36 ppm Peak grouping r W g 1500000 1000000 -500000 -0

4.39

4.38

ppm

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