Electronic Supplementary Material (ESI) for Analytical Methods.
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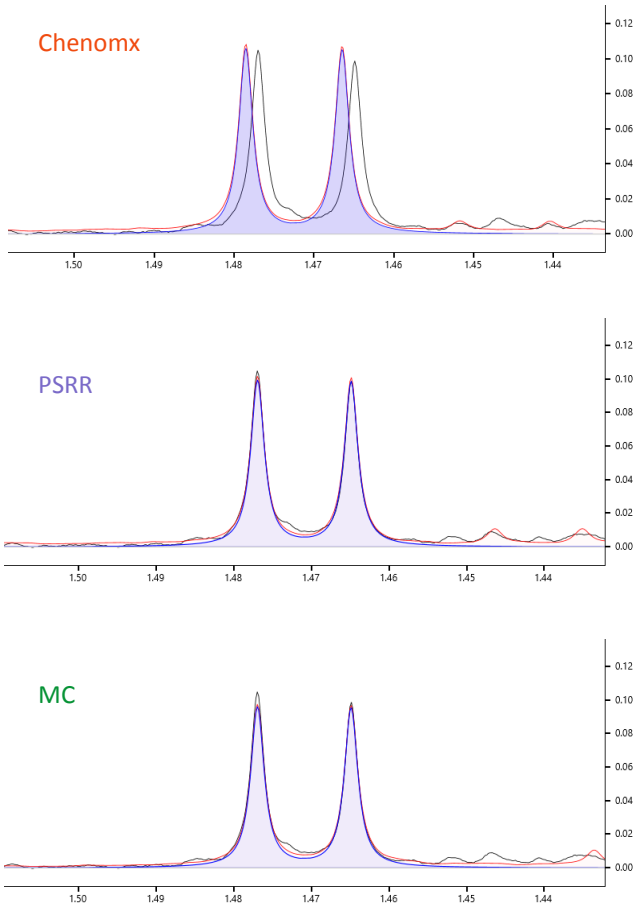
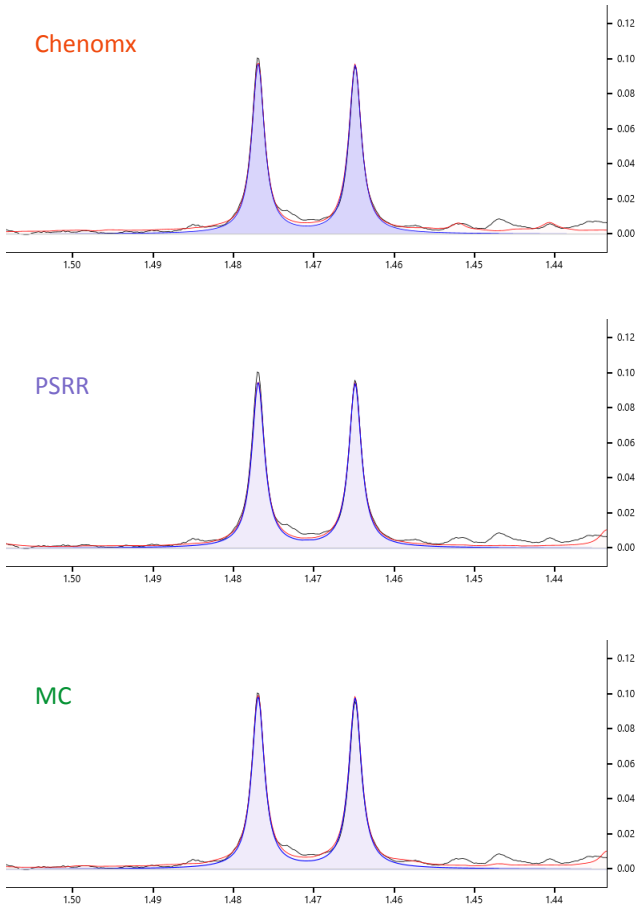
Alanine 1.5 ppm

Replicate sample #7



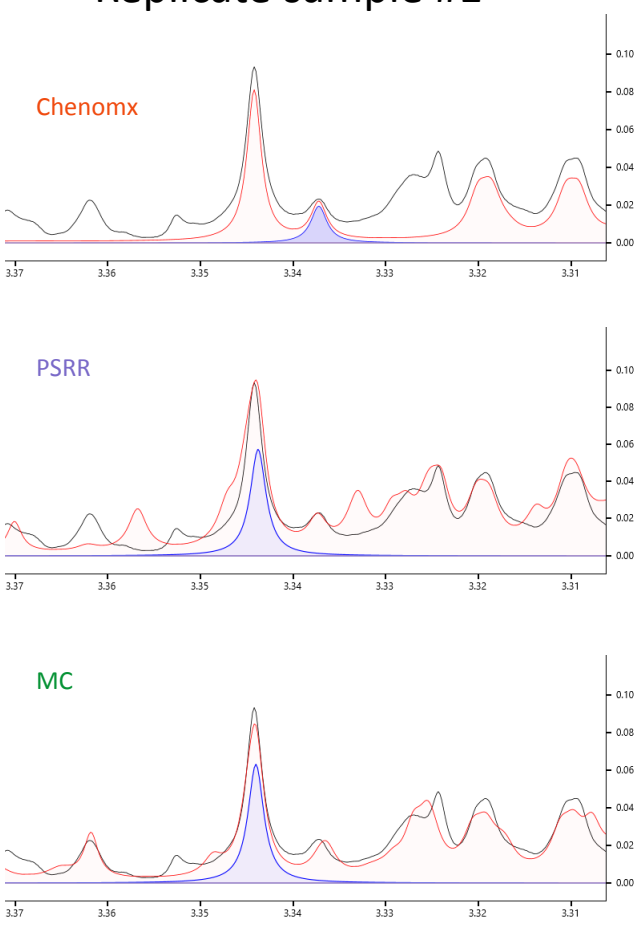
Replicate sample #13



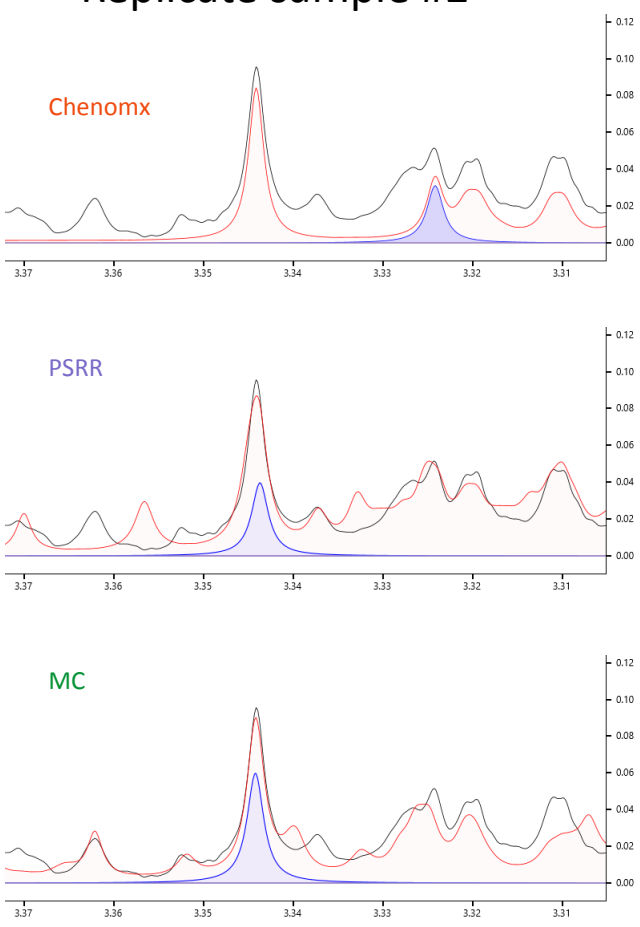
Sample #7 was fitted at different chemical shift position compared with replicates by Chenomx technique while PSRR and MC techniques agreed each other between replicates

Caffeine 3.3 ppm

Replicate sample #1



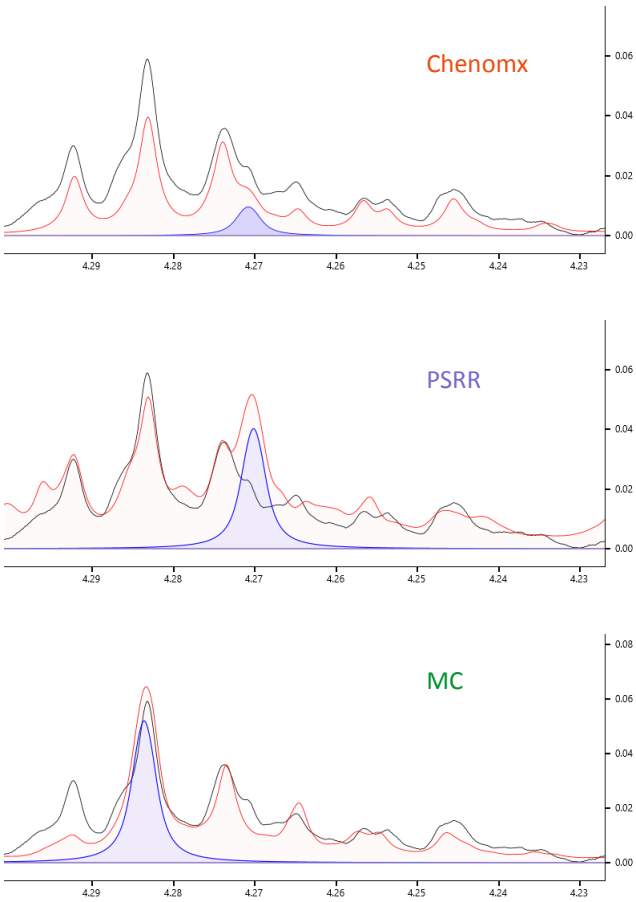
Replicate sample #2



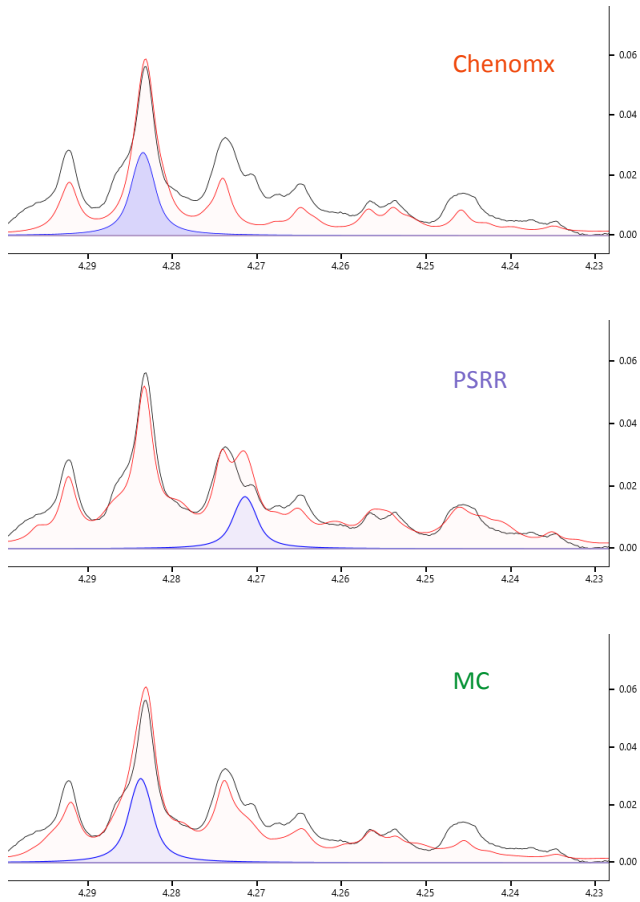
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx technique while a different peak was fitted by PSRR and MC techniques that agreed each other between replicates

Galactarate 4.3 ppm

Replicate sample #1



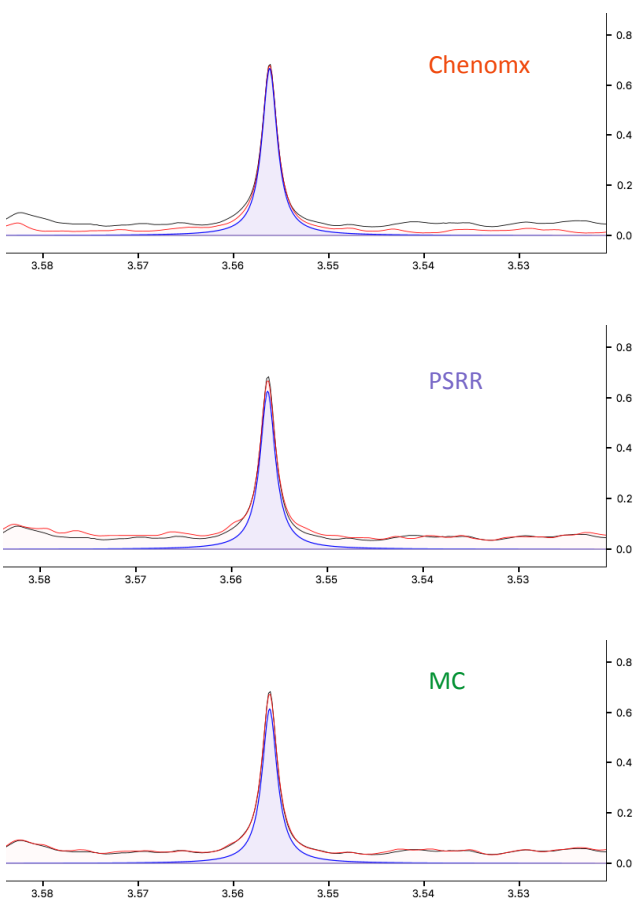
Replicate sample #3



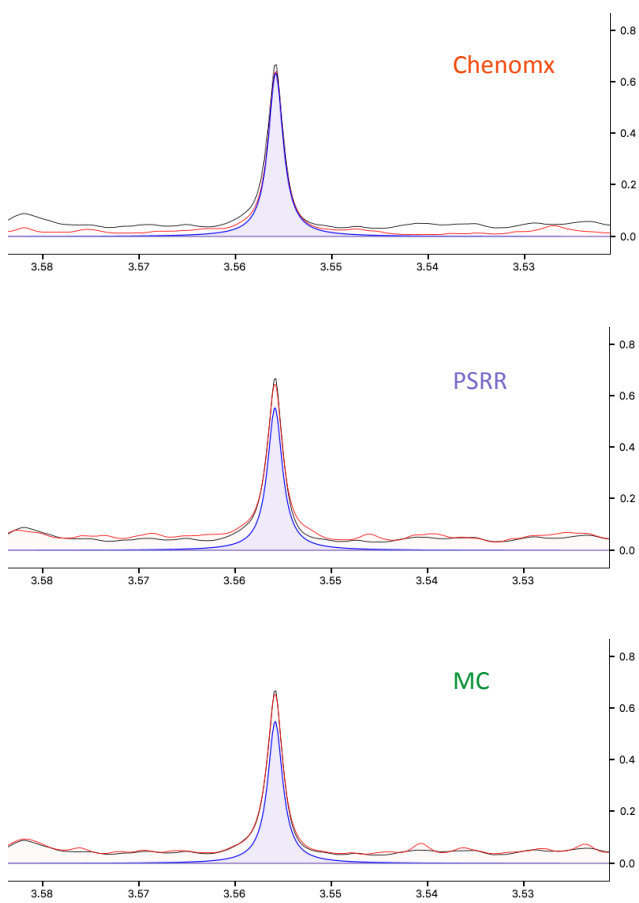
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx technique while different peaks were fitted by PSRR and MC techniques but agreed between replicates

Glycine 3.6 ppm

Replicate sample #1



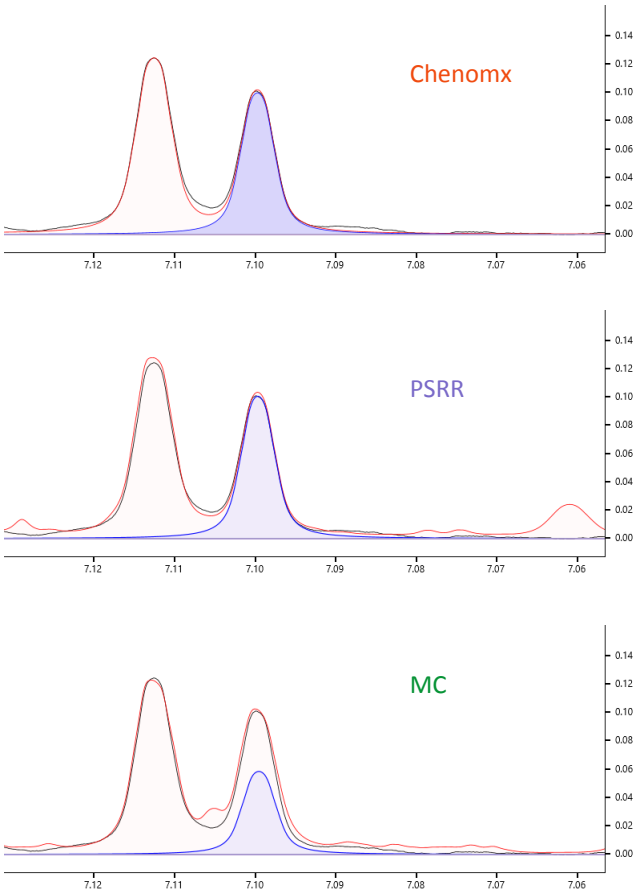
Replicate sample #14



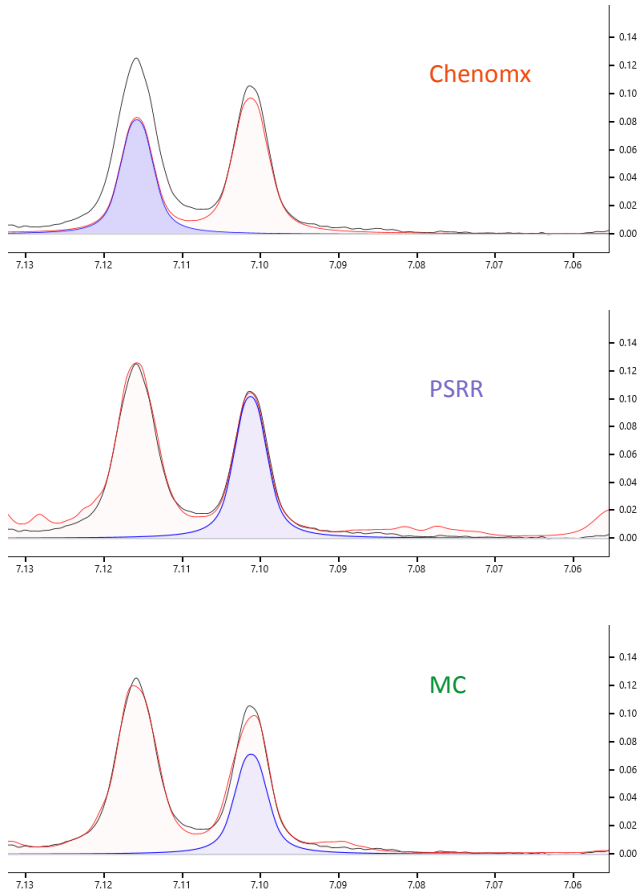
Higher peak height variability between samples for the singlet at 3.6 ppm was observed by using PSRR and MC approaches compared with Chenomx

Histidine 7.1 ppm

Replicate sample #1



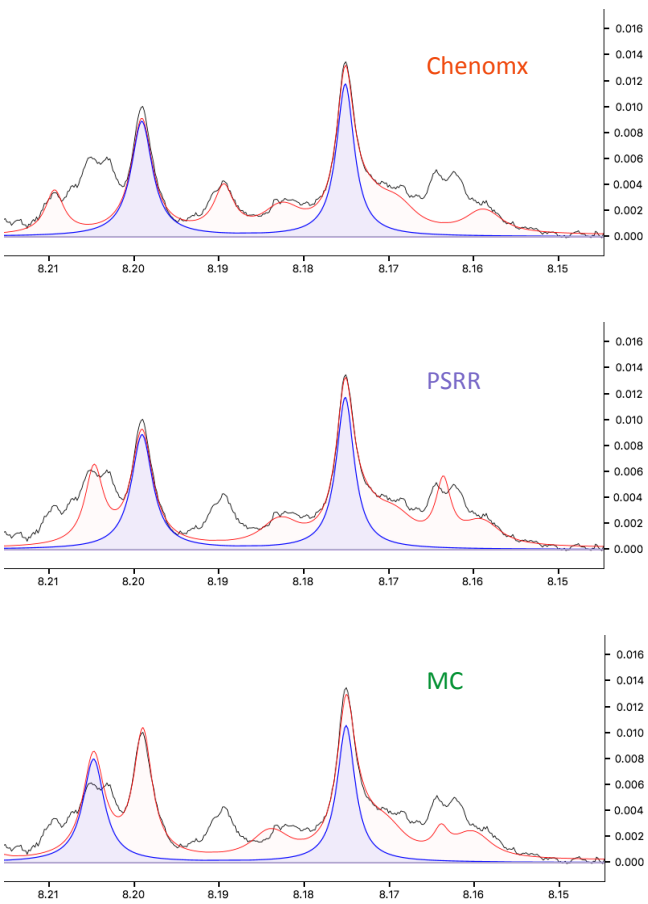
Replicate sample #2



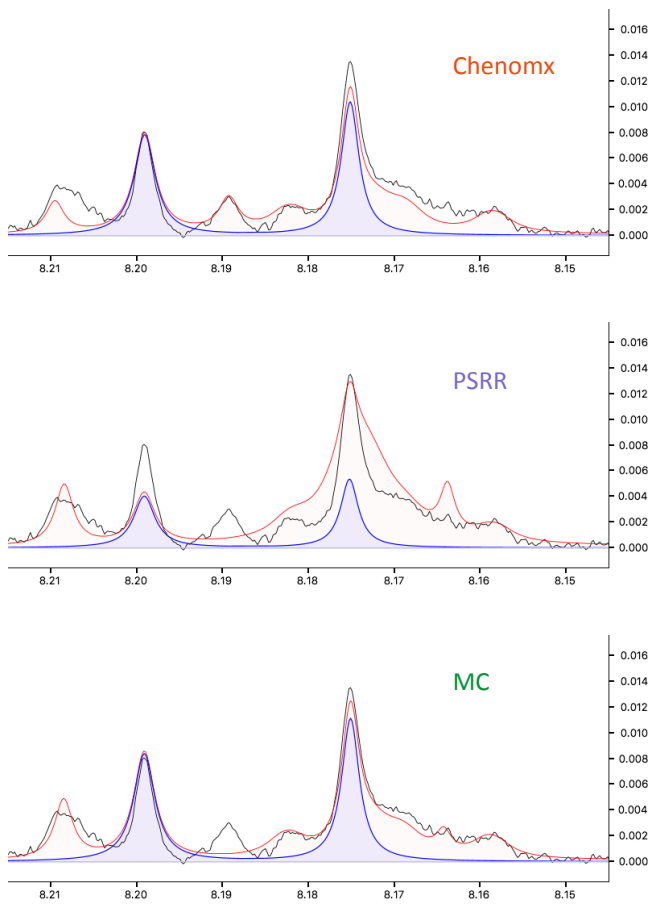
Sample #2 was fitted at different chemical shift position compared with replicates by Chenomx technique while PSRR and MC techniques agreed each other between replicates

Hypoxanthine 8.2 ppm

Replicate sample #1



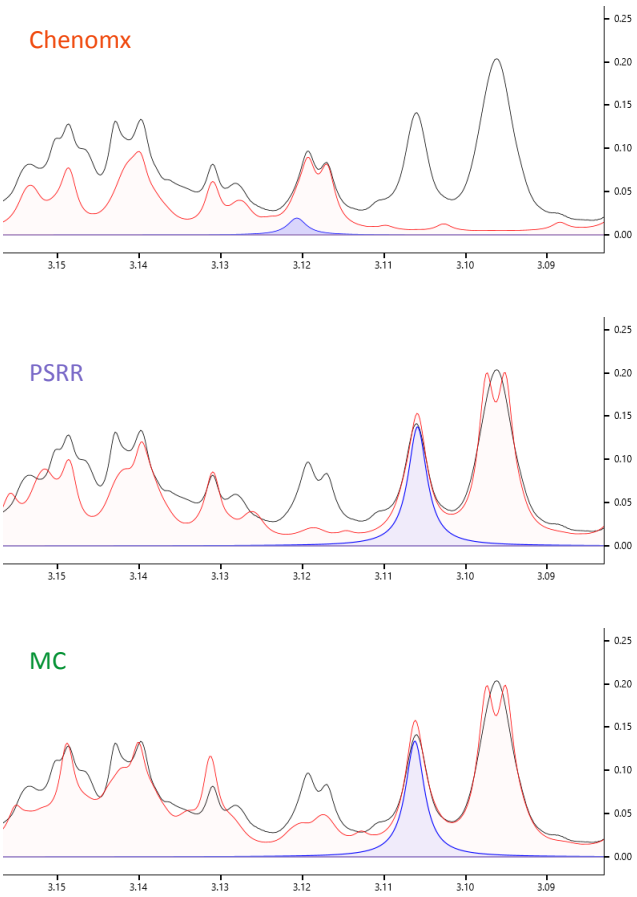
Replicate sample #14



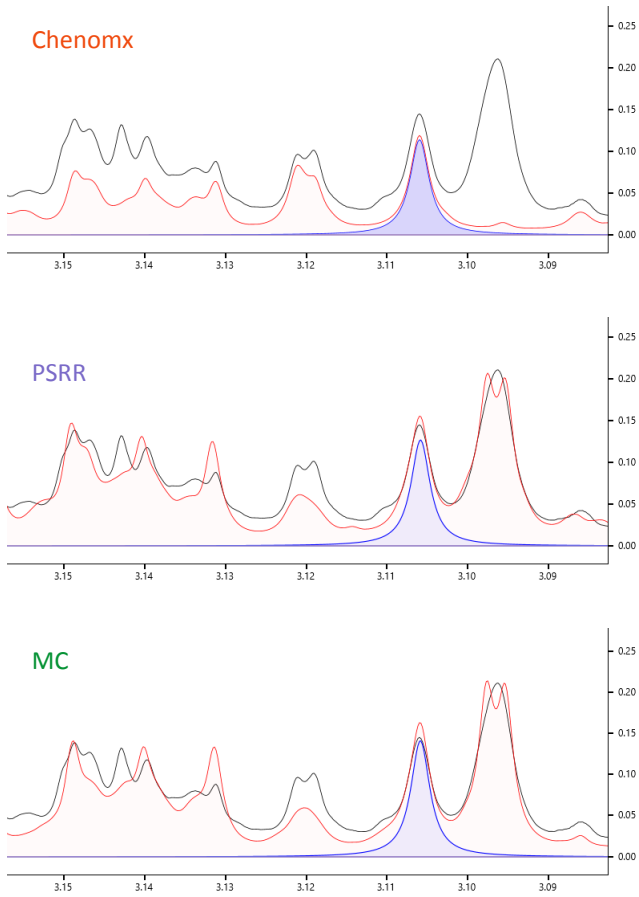
Higher peak height variability between samples for the doublet at 8.2 ppm was observed by using PSRR and MC approaches compared with Chenomx

Malonate 3.1 ppm

Replicate sample #1



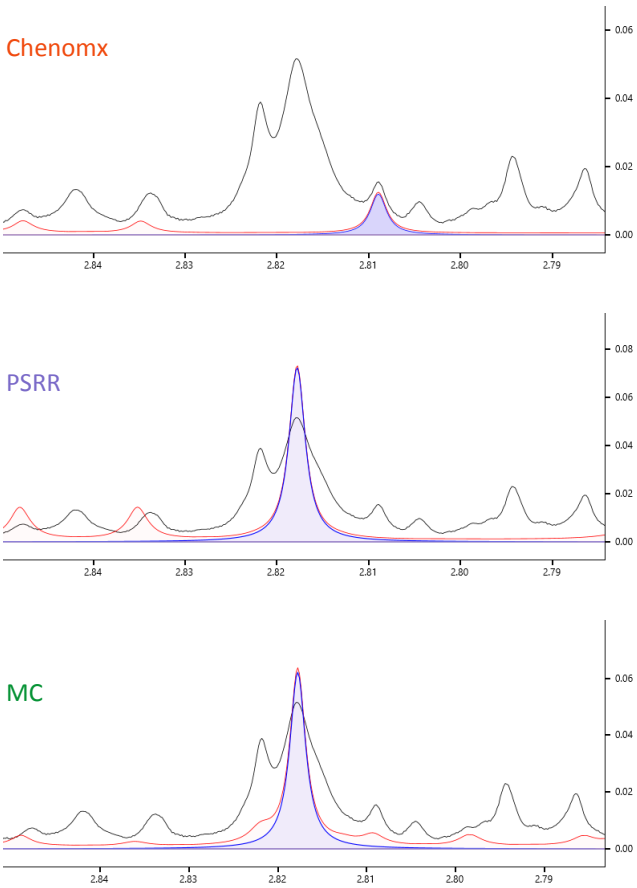
Replicate sample #9



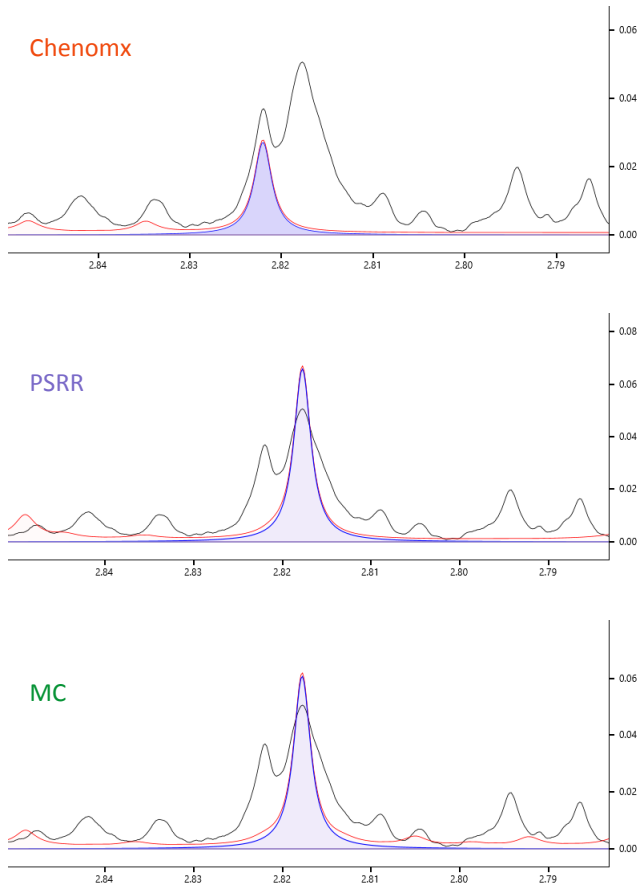
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx technique while PSRR and MC techniques agreed each other between replicates

Methylguanidine 2.8 ppm

Replicate sample #1



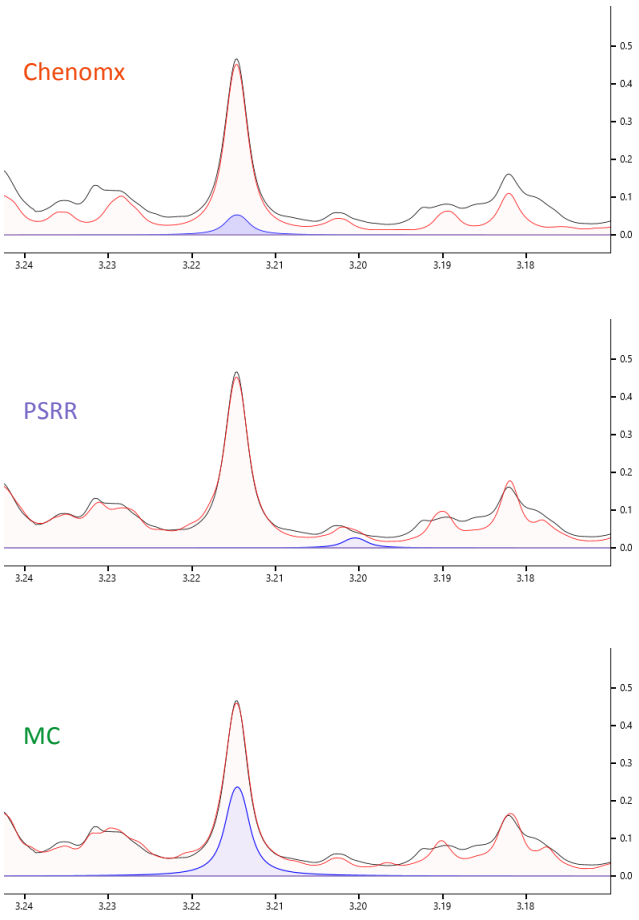
Replicate sample #2



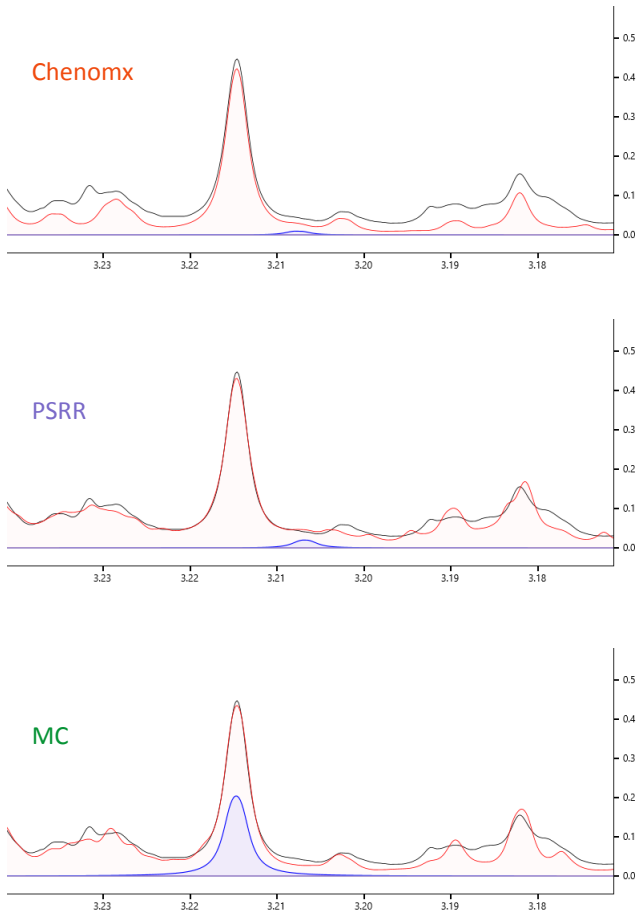
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx technique while a different peak was fitted by PSRR and MC techniques that agreed each other between replicates

O-Phosphocholine 3.2 ppm

Replicate sample #1



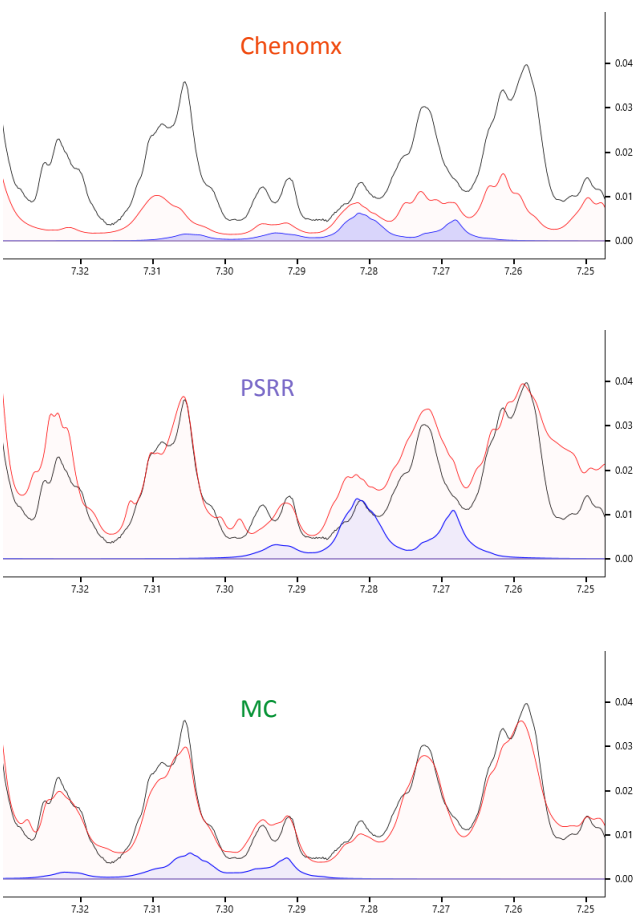
Replicate sample #3



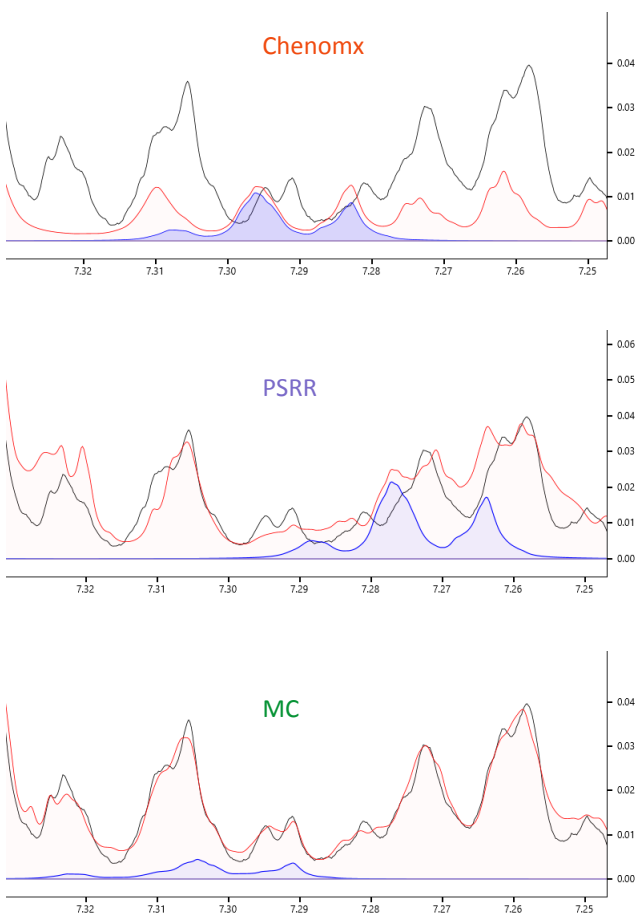
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx technique while different peaks were fitted by PSRR and MC techniques but agreed between replicates

Phenylacetate 7.3 ppm

Replicate sample #1



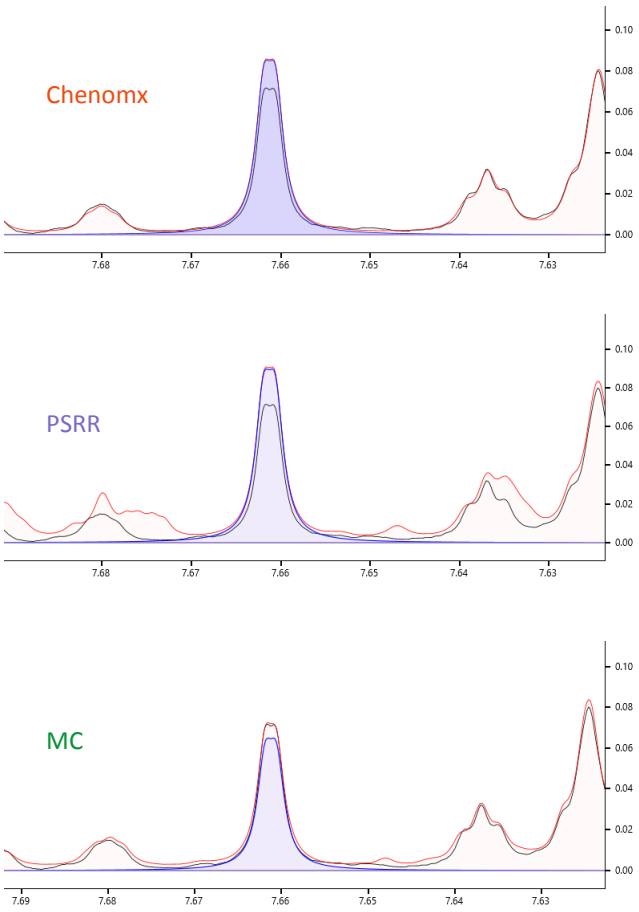
Replicate sample #9



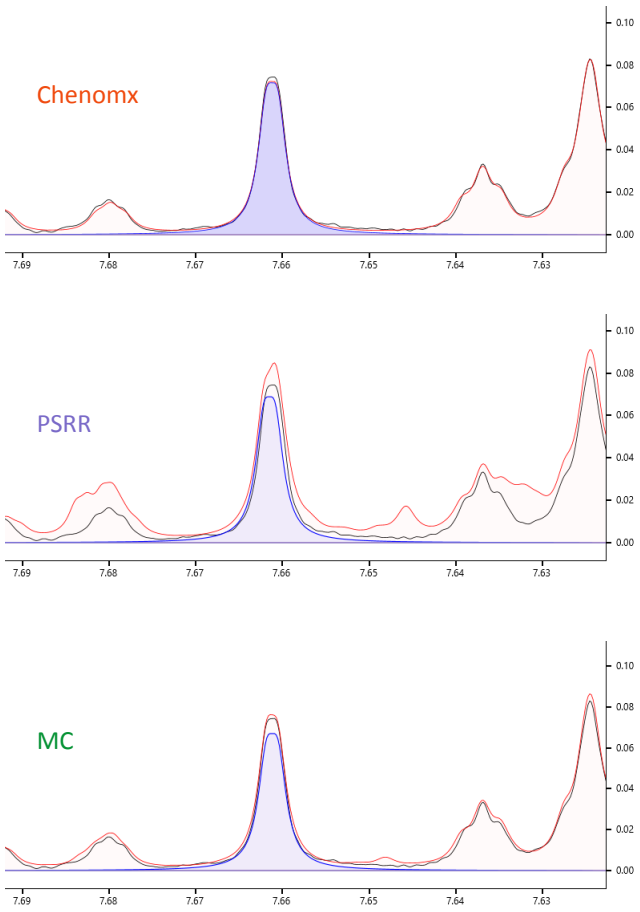
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx technique while different peaks were fitted by PSRR and MC techniques but agreed between replicates

Pseudouridine 7.7 ppm

Replicate sample #1



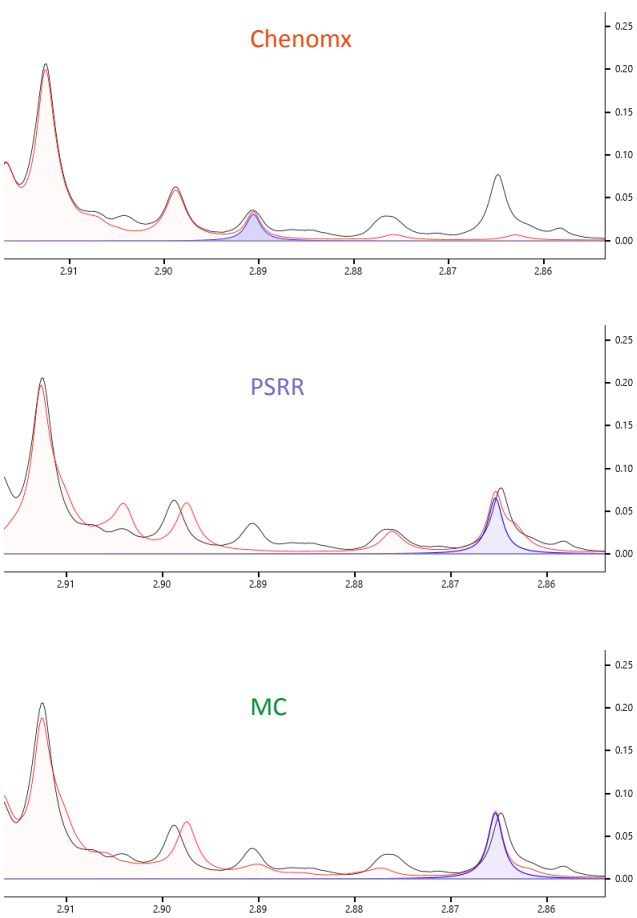
Replicate sample #2



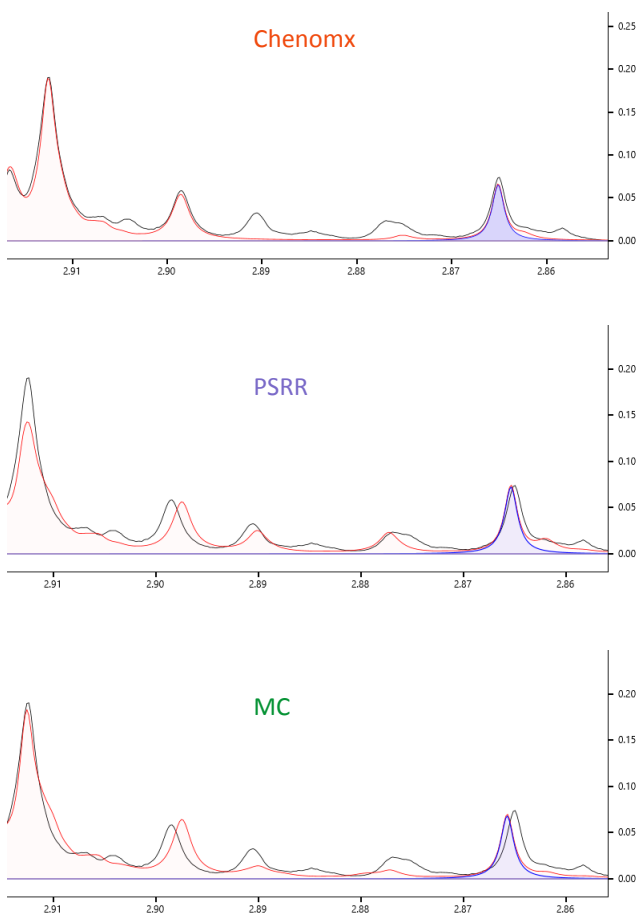
Sample #1 was fitted with the sum line exceeding the spectrum line compared with replicates by Chenomx and PSRR techniques while the sum line matched the spectrum line with the MC technique

Trimethylamine 2.9 ppm

Replicate sample #1



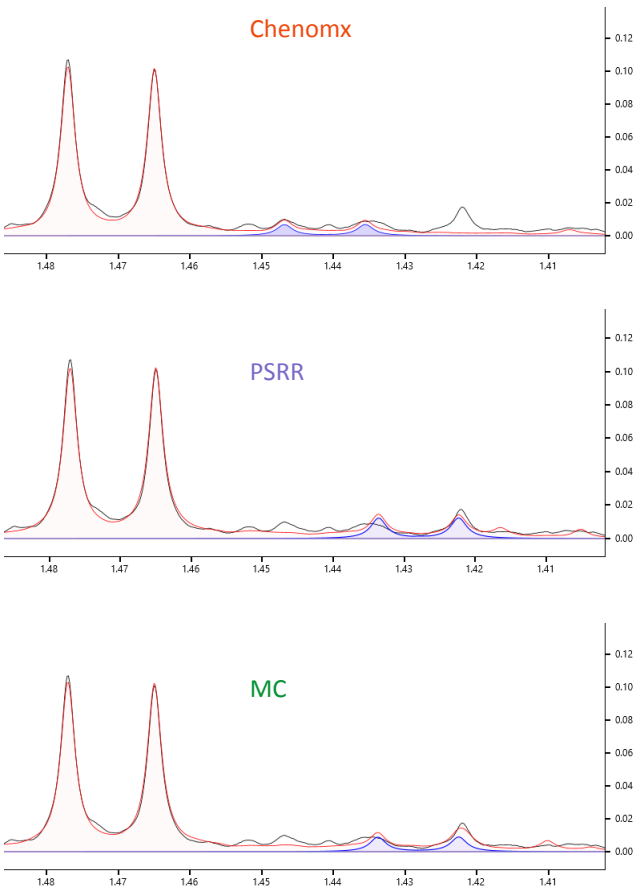
Replicate sample #17



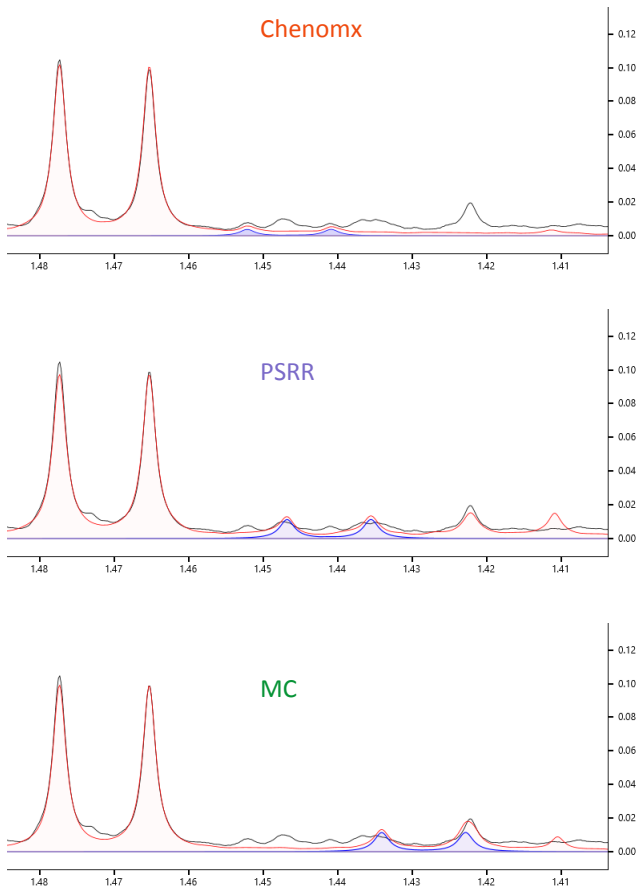
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx technique while PSRR and MC techniques agreed each other between replicates

U144 1.4 ppm

Replicate sample #1



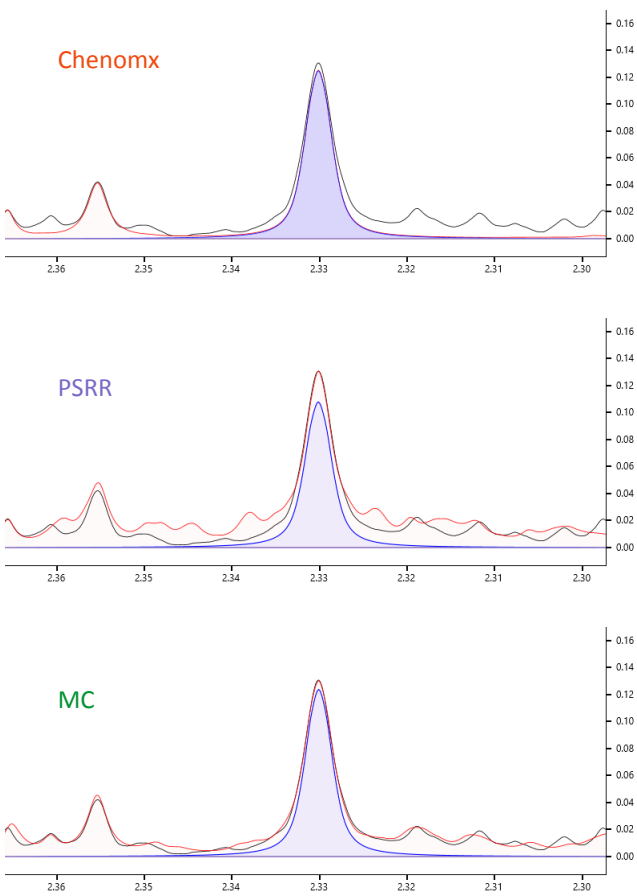
Replicate sample #8



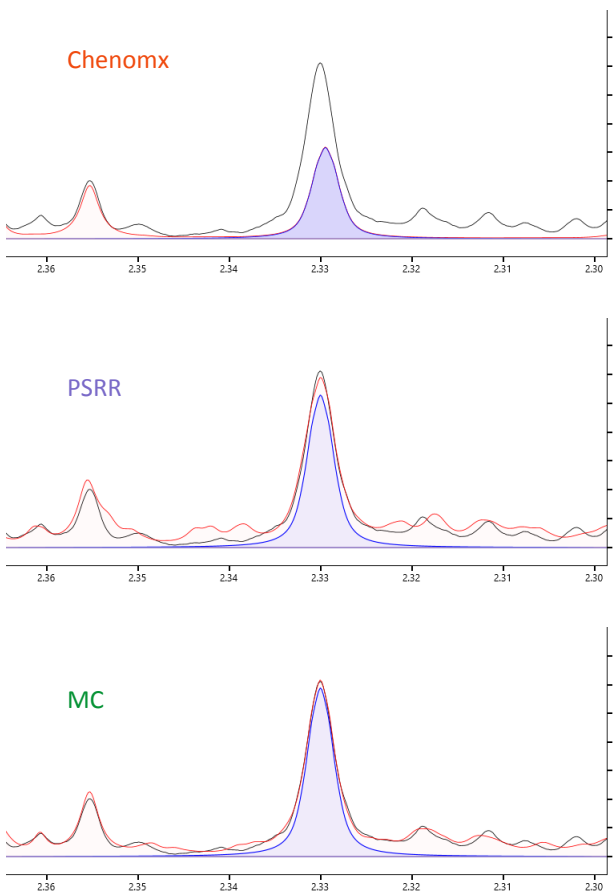
Sample #1 was fitted at different chemical shift position compared with replicates by Chenomx and PSRR techniques while the MC technique agreed between replicates

U233 2.3 ppm

Replicate sample #1



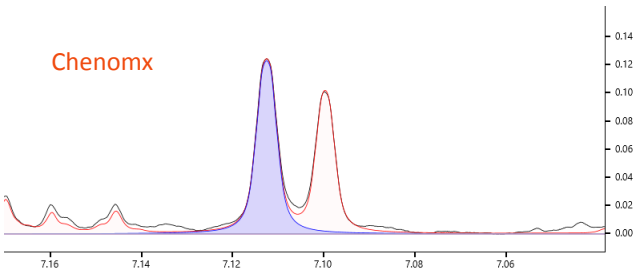
Replicate sample #3

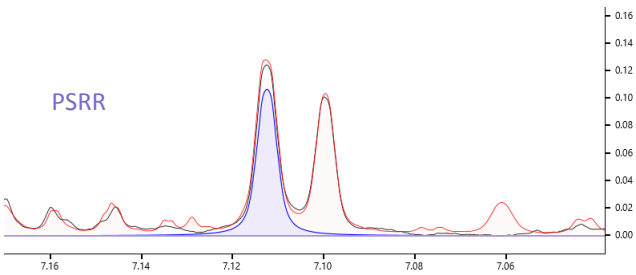


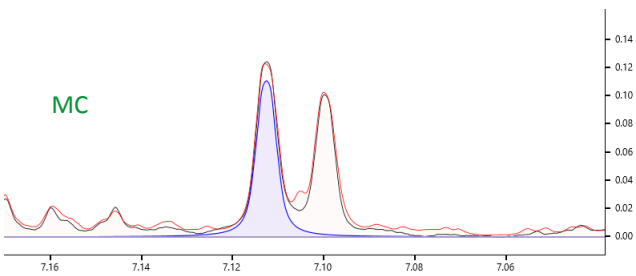
Sample #3 was fitted with a different amplitude compared with replicates by Chenomx technique while the sum line matched the experimental spectrum with PSRR and MC techniques

π -Methylhistidine 7.1 ppm

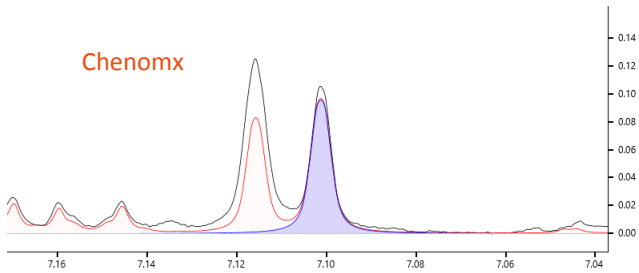
Replicate sample #1

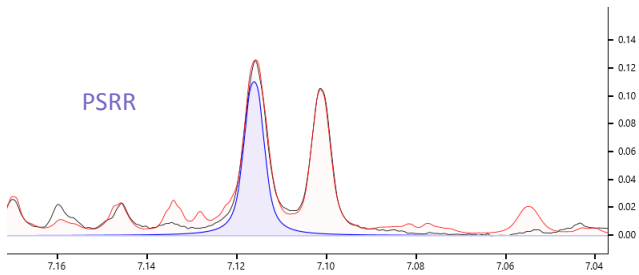


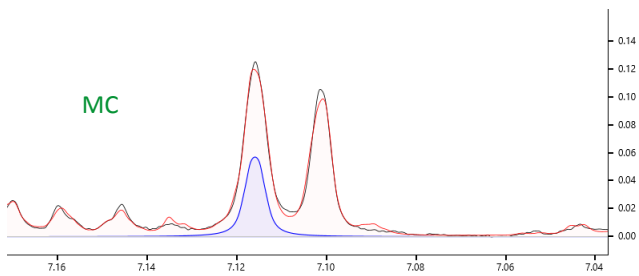




Replicate sample #2







Sample #2 was fitted at different chemical shift position compared with replicates by Chenomx technique while PSRR and MC techniques agreed each other between replicates