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.

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.
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.

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

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

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

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

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

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.
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.

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

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.
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.