**SUPPLEMENTAL FILE 1**

**A picture containing text

Description automatically generated**

“**Insert Not Detected**” – to mark areas that the program mistakenly identified as injections.

“**Delete Name**” – to correct a previous mistake in typing the sample name.

“**Insert Name**” – to correct for an injection being made without typing the sample name.

“**Name Peak**” – to assign a specific name to a specific peak / curve.

“**Delete Peak**” – to remove a specific area from the analysis.

“**Delete Area**” – to disregard a specific area in the analysis, for example in case of areas that are mistakenly analyzed twice by the program.

“**Reintegrate**” – to go back to step 8.2.2 to adjust peak analysis.