**LC-MS Procedural Naming Guide**

**Rationale:** This is a naming guide for LC-MS sample filenames to ensure consistency across analyses and for easy post-processing using our Python script.

**Generic sample filename format: XX\_Y\_Z**

where **XX** is a two-digit number representing the position of the sample in the analysis queue. The number 00 is reserved for calibration standards, after which the numbers starting with 01 (02, 03, etc.) may be used for blanks, controls, samples, sample duplicates, and spiked samples.

where **Y** is a string of text identifying the type of sample:

For a calibration standard, use **Cal**

For a blank, use **Blk**

For a control, use **Ctrl**

For a sample, use **Smp**

For a sample duplicate, use **Dup**

For a spiked sample, use **Spike**

For an extraction blank, use **EB**

For quality control samples, use **QC**

For wash, use **Wash**

where **Z** is a string with identifying information about the sample or its post-processing. Specific guidelines for each type are given below.

**Specific guidelines for calibration standards:** Calibration standards should be placed at the beginning of the sequence, and all begin with 00 in the **XX** position. They should also have **\_Cal** in the \_**Y** position. Next, they should have a two-digit number in the **\_Z** position corresponding to the order of the calibration standards. Lastly, they should have an additional **\_Cppt** at the end of the name, where Cppt is the concentration *C* of the calibration standard in parts-per-trillion by volume.

**Examples:** 00\_Cal\_01\_5ppt, 00\_Cal\_02\_10ppt, 00\_Cal\_03\_25ppt, and so on.

**Specific guidelines for blanks:** Blanks should start with their number in the sequence in the **XX** position. They should then have **\_Blk** in the \_**Y** position. They should then have the ordered number of the blank in the **\_Z** position.

**Examples:** 01\_Blk\_01, 16\_Blk\_02, and so on.

**Specific guidelines for controls:** Controls should start with their number in the sequence in the **XX** position. They should then have **\_Ctrl** in the \_**Y** position. They should then have the ordered number of the control in the **\_Z** position. The user should have the type/origin of the control written down somewhere else as a reference for what is.

**Examples:** 02\_Ctrl\_01, 18\_Ctrl\_02, and so on.

**Specific guidelines for samples:** Samples should start with their number in the sequence in the **XX** position. They should then have **\_Smp** in the \_**Y** position. They should then have the name of the sample in the **\_Z** position, followed by an underscore and a letter representing the replicate, and the extraction blank to be subtracted from it appended at the end. Spaces in sample names should be connected by dashes (-), not underscores. The extraction blank addition should follow the format **\_EB\_##**.

**Examples:** 07\_Smp\_WJ-FGST\_A\_EB\_01, 08\_Smp\_WJ-FGST\_B\_EB\_01,

09\_Smp\_WJ-FGST\_C\_EB\_01, 18\_Smp\_OFS\_A\_EB\_02, 19\_Smp\_OFS\_B\_EB\_02

**Specific guidelines for duplicate samples:** Duplicates should start with their number in the sequence in the **XX** position. They should then have **\_Dup** in the \_**Y** position. They should then have the name of the sample that they are a duplicate of in the **\_Z** position, followed by an underscore and a letter representing the replicate, and the extraction blank to be subtracted from it appended at the end. Spaces in sample names should be connected by dashes (-), not underscores. The extraction blank addition should follow the format **\_EB\_##**.

**Examples:** 08\_Dup\_WJ-FGST\_A\_EB\_01, 20\_Dup\_OFS\_A\_EB\_02

**Specific guidelines for spike samples:** Spiked samples should start with their number in the sequence in the **XX** position. They should then have **\_Spike** in the \_**Y** position. They should then have the name of the sample that was spiked in the **\_Z** position, followed by an underscore and a letter representing the replicate, then the control to be normalized to, and the extraction blank to be subtracted from it appended at the end. Spaces in sample names should be connected by dashes (-), not underscores. The control piece should follow the format **\_Ctrl\_##**. The extraction blank addition should follow the format **\_EB\_##**.

**Examples:** 09\_Spike\_WJ-FGST\_A\_Ctrl\_01\_EB\_01, 20\_Spike\_OFS\_A\_Ctrl\_03\_EB\_02

**Specific guidelines for extraction blanks:** Extraction blanks should start with their number in the sequence in the **XX** position. They should then have **\_EB** in the \_**Y** position. They should then have the ordered number of the extraction blank in the **\_Z** position. The user should have the type/origin of the extraction blank written down somewhere else as a reference for what is.

**Examples:** 15\_EB\_01, 24\_EB\_02, and so on.

**Specific guidelines for quality control (QC) samples:** When being used in the analytical sequence, QC sample names should start with their number in the sequence in the **XX** position. They should then have **\_QC** in the \_**Y** position. Next, they should have the string \_**Cal** in the **\_Z** position, followed by an additional two-digit number **\_##** corresponding to the calibration standard concentration being used for quality control.

**Examples:** 08\_QC\_Cal\_09, 19\_QC\_Cal\_10

**Specific guidelines for washes:** Washes should start with their number in the sequence in the **XX** position. They should then have **\_Wash** in the \_**Y** position. There is no other information about the wash necessary.

**Examples:** 26\_Wash