Preparing Quality Control Test Sample

Purpose This procedure provides information on how to prepare a quality control test sample to verify the quality of NMR analysis

Materials

Reagents	Supplies	Equipment
• Quality Control (QC1) Solution • Chenomx ISTD (IS2) Solution (or any other ISTD solution e.g. TSP)	• Eppendorf tubes	• Vortex

Procedure

- The quality control (QC1) solution consists **5.00 mM** each of sodium acetate, valine, glycine and sodium formate.
- The concentration of these compounds in the quality control test sample ready for NMR analysis is **4.50 mM** since the QC1 solution and IS2 are mixed in 9:1 ratio.

Step	Details
1.	Review the Material Safety Data Sheets for all the reagents.
2.	Add 70 µL of Chenomx ISTD to 630 µL of QC1 solution or an ISTD volume equivalent to 10% of the total quality control test sample volume.
3.	Vortex the sample for 30 seconds for uniform mixing.
4.	Read the pH of the samples by using a pH meter. Rinse the pH meter probe thoroughly with distilled water and blot dry with Kimwipes, before moving on to the next sample. Record all pH values in your laboratory notebook.
5.	Transfer the sample containing Chenomx ISTD into an NMR tube. (See L001 Transferring samples to NMR tubes)
6.	(Optional) Repeat Step 2-5 twice to have three replicates in total.
7.	Acquire an NMR spectrum of the QC samples using the parameters compatible with Chenomx software.
8.	Analyze four compounds in the standard solution by Chenomx software. Apply the dilution factor of 1.111 to the results obtained by Chenomx. The expected concentration before applying dilution factor is 4.50 mM and after dilution factor is 5.00 mM The difference between the calculated and known (actual) values for each metabolite should be less than 5%. If the difference it higher, consider the following possibilities: - Errors in the concentration of the internal standard that is being used - Failure to use the Chenomx recommendations for the NMR data acquisition parameters - Measurement errors during sample preparation.

References Not applicable

Related Documents
L001 - Transferring NMR Samples into NMR Tubes
S001 - Preparing Internal Standard Solution
S002 – Preparing Quality Control (QC1) Solution

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