UPLC, Sample Manager and QTOF System Performance Check - Proforma

NPC.PRO.MS002 Version 2.1

Effective Date: April 2019

1. Purpose

The purpose of this proforma is to document the Ultra Performance Liquid Chromatography (UPLC) Mass Spectrometer (MS) system instrument checks as outlined in the protocol NPC.SOP.MS002. The required sections of this proforma should be printed on the day of use, completed and then stored with all project specific documentation. This proforma should be used in combination with the SOP.

2. Proforma Approval

Prepared by Dr Verena Horneffer-van der Sluis	Date
Approved by Dr Maria Gomez-Romero	Date
Authorised by Dr Matthew Lewis	Date

UPLC and Q-TOF System Checklist

Please, indicate an action has been performed by ticking the appropriate box (☐)

Assay specifics			
Operator:		**System No.:**	
Project:		**Date:**	
LC system and Sample Manager – Visual inspection			
Non-essential material removed			☐
LC system and Sample Manager have been checked and there are no leaks and/or corrosion			☐
All solvent bottles are in date and topped up where necessary			☐
Comments: n/a ☐			
LC System and Sample Manager – Routine maintenance			
System (line A,B) primed for 4 minutes in methanol			☐
Seal wash primed in parallel			☐
Pressure stable (ΔPSI <20 PSI)			Y/N
Dynamic leak test performed:			☐
Pump A	Accumulator _____nL/min	Primary _____nL/min	Pass/Fail
Pump B	Accumulator _____nL/min	Primary _____nL/min	Pass/Fail
System (line A,B) primed for 4 minutes in fresh isopropanol			☐
Weak and strong needle washes rinsed for 30 seconds			☐
Syringe and sample loop washed			☐
Sample Manager temperature checked and recorded _____**°C**			☐
Comments: n/a ☐			

Table continues

Assay specifics		
Operator:	**System No.:**	
Project:	**Date:**	
MS system – Visual inspection		
System checked for leaks, vapour trap bottle checked and volume of LeuEnk solution at sufficient level		☐
Mass spectrometer in operate mode and correct tune file loaded		☐
Tune file_____		
MS tune page settings correspond to correct NPC standard settings for method		☐
Method (RPOS/RNEG/HPOS/LPOS/LNEG): _____		
Vacuum read back pressure values		
Backing:	**Collision:**	**TOF:**
Vacuum read back values acceptable?		Y/N
Comments: n/a ☐		
MS System – Check of LeuEnk solution		
Check if volume of LeuEnk solution is sufficient (>100 mL) and not expired? *If yes, go to next section. If not, prepare fresh as given in SOP NPC.SOP.MS001*		Y/N
Add 7.5 mL of LCMS grade water to the Waters LeuEnk bottle (3 mg) and mix until dissolved *(400 ng/µL LeuEnk stock solution)* ☐ *n/a if stock already prepared*. Prep date:_____		☐
Prepare 500 mL of 1:1 acetonitrile/H_2O using a measuring cylinder (With/without 0.1% formic acid)		☐
Add respective volume of 400 ng/µL LeuEnk stock solution using an automatic pipette		
Volume of 400 ng/ µL Leu Enk stock solution added:		☐
Mix until the solution is homogenous and sonicate for 5 minutes		☐
Comments: n/a ☐		

Table continues

MS System – Detector and Lockmass *(in assay specific polarity only)*		
Fluidics line B purged with LeuEnk		☐
Detector Set-up (@ $5e^5$ intensity**)**		
	Positive mode	*Negative mode*
Detector Voltage (V)		
Average Ion Area		
Instrument uncalibrated		☐
Nominal m**ass** of LeuEnk model peak acceptable?		Y/N
Veff corrected?		Y/N
Stable LeuEnk signal intensity at $2e^4$ in positive / negative mode		☐
Leu Enk Mass		
	Positive mode (556.2771 m/z)	*Negative mode (554.2614 m/z)*
Lockmass set up		
	Positive mode	*Negative mode*
Flow rate (µL/min)		
LockMass capillary volt (kV)		
DRE %		
Time (s)		
Comments: n/a ☐		

Table continues

MS system –Resolution check *(in assay specific polarity only)*		
Fluidics line A purged twice with SSTM (RPOS/RNEG/HPOS) or line B with LeuEnk (LPOS/LNEG)		☐
Infuse at 15 µL/min and ensure stable signal. Perform acquisition for 2.5 mins. Use ResCal to calculate the resolution		
Positive mode		
Intensity	*$2e^4$*	*$2e^5$*
Flow (µL/min)		
Capillary voltage (kV)		
Res_1		
Res_2		
Res_3		
Res_4		
Res_5		
Res_average		
Res_average value of $2e^4$ entered into Acquisition Settings		☐
Negative mode		
Intensity	*$2e^4$*	*$2e^5$*
Flow (µL/min)		
Capillary voltage (kV)		
Res_1		
Res_2		
Res_3		
Res_4		
Res_5		
Res_average		
Res_average value of $2e^4$ entered into Acquisition Settings		☐
Comments: n/a ☐		

Table continues

MS system – Calibration and last checks *(in assay specific polarity only)*			
Fluidics line C purged twice with sodium formate solution			☐
Calibration			
	Positive mode	*Negative mode*	
RSM (ppm)			
95% Confidence band (ppm)			
Number of peaks acceptable			
Purge lines A and/or C with wash solution twice and flush to remove residual sodium formate and SSTM			☐
Back-up and save system settings			☐
Check MS setting match assays specific values			☐
Save tune file TOF__.ipr			☐
Rest ADC-Results.csv			☐
Comments: n/a ☐			