

## LxQuant kit requirements

This document specifies additional lab equipment and chemicals that are required but not included with the kit. Before starting with the kit, ensure that all required items are available.

### LC-MS system

Agilent	SCIEX	Waters
Mass spectrometer		
6495C Triple Quadrupole LC/MS System	5500+, 5500 or 6500+ series (QTRAP or Triple Quad) with TurboV™ ion source	Xevo TQ-XS with ESI source
LC system and autosampler		
<ul style="list-style-type: none"> <li>– Agilent 1290 Infinity I/II UHPLC system with column oven.</li> <li>– 800 bar injection valve (Agilent part no. 5067-6698) replaces standard 1300 bar valve</li> <li>– 1290 Infinity II inline filters, 0.3 µm (2 pcs., before and after injection valve, Agilent part no. 5067-6189)</li> <li>– 96-well plate autosampler with temperature control (4 °C)</li> <li>– Injection volume: 20 µL</li> </ul>	<ul style="list-style-type: none"> <li>– Standard flow HPLC or UHPLC system with column oven.</li> <li>– 96-well plate autosampler with temperature control (4 °C)</li> <li>– Injection volume: 20 µL</li> <li>– Shimadzu and ExionLC autosamplers capable of accepting 96 well plates: <a href="#">Plate calibration video</a></li> </ul>	<ul style="list-style-type: none"> <li>– Waters ACQUITY UPLC® system with sample manager, solvent manager, and column oven:               <ul style="list-style-type: none"> <li>– Classic (loop-based)</li> <li>– I-Class (FTN)</li> <li>– H-Class (FTN)</li> </ul> </li> <li>– Injection volume: 20 µL</li> <li><b>FTN samplers require extension loop of 50 µL or needle size of 30 µL!</b></li> </ul>
NanoLC and microLC are not supported!		
Tubing		
<ul style="list-style-type: none"> <li>– Recommended between injector and analytical column: steel capillary</li> <li>– Recommended between analytical column and mass spectrometer: red PEEK Tubing 1/16" OD x 0.005" ID</li> </ul>		
Condition		
<ul style="list-style-type: none"> <li>– <b>Instrument is well maintained and serviced</b> on a regular basis according to manufacturer's recommendations</li> <li>– <b>MS tuned and calibrated in both positive <u>and</u> negative ion modes</b></li> <li>– LC-MS system must be <b>free of ion pairing reagents</b></li> </ul>		

## Laboratory equipment

Equipment	Requirements (may be available from local distributor)	
	Nitrogen evaporator for 96-well plates	Pressure manifold for 96-well plates
Nitrogen evaporator* or pressure manifold* – Requires nitrogen supply – Must be in a fume hood – No heater required	<b>Examples:</b> – Porvair blowdown evaporator MiniVap® – Techne (FSC496D) – Sample concentrator from BenchTop Lab Systems (96 samples, BT1604) – VLM evaporators – Organomation MICROVAP microplate evaporator – Biotage TurboVap® 96	<b>Examples:</b> – Porvair UltraPPM LITE – Waters positive pressure-96 processor (186006961) – Biotage® PRESSURE+ 96 manifold (PPM-96) – CEREX® system 96 processor (288-0001) – Agilent positive pressure manifold 96 processor (PPM-96) – TECAN Resolvex® M10 96
Centrifuge	Must be able to centrifuge 96-well plates of 5 cm height at 500 x g	Not required when a pressure manifold is used.
Shaker	Any model with adjustable speed (450 – 1200 rpm) including a tray for plates and vials. Recommended: Eppendorf MixMate® or ThermoMixer®	
Pipettes	– Repeater, e.g. Eppendorf Multipette® E3 (with 2.5 and 10 mL tips) or similar electronic model – Single channel: volume range 10 µL – 1000 µL – 8-Channel: 10 µL – 150 µL	
Vortexer	Any model	
Balance	Accuracy < 1 mg	
Solvent bottles	50 – 1000 mL	

\* See document “Technical guide-Nitrogen evaporators and pressure manifolds” for details.

## Solvents and chemicals

Solvents and chemicals	Purity
Methanol, water, acetonitrile, isopropanol	LC-MS grade
Ammonium acetate	LC-MS grade
Phosphate buffered saline (PBS)	p.a. grade (e.g. Sigma-Aldrich P4417)

## Software

Agilent	SCIEX	Waters
MS software		
<b>MassHunter</b> version 10.1 or later	<b>Analyst®</b> version 1.7.3 or later <b>SCIEX OS</b> version 3.4 or later	<b>MassLynx®</b> version 4.2 or later
biocrates WebIDQ workflow manager		

Subscriptions available through biocrates webshop or local distributor:

– <b>WebIDQ basic</b> subscription (4 GB storage space)	biocrates part number 22336.1
– <b>WebIDQ core</b> subscription (8 GB storage space)	biocrates part number 21629.3
– <b>WebIDQ core+</b> subscription (50 GB storage space)	biocrates part number 21926.3
– <b>WebIDQ on-premises</b> subscription	biocrates part number 21636.3

For detailed system requirements please visit:

<https://shop.biocrates.com/faq/What-are-the-system-requirements-for-WebIDQ>