

# MxP® Quant 500 kit requirements

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

# LC-MS system

Agilent	SCIEX	Waters		
Mass spectrometer				
Agilent 6495B, 6495C Triple Quadrupole LC/MS System	SCIEX 5500, 5500+, 6500, 6500+, or 7500 series (QTRAP or Triple Quad) with TurboV™ ion source or Optiflow Pro (high flow)	Waters Xevo TQ-S or TQ-XS with ESI source		
LC and autosampler				
<ul> <li>Agilent 1290 Infinity I/II UHPLC system with column oven. NanoLC and microLC are not supported!</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 (10 °C)</li> <li>Injection volume range: 2 – 20 μL</li> </ul>	<ul> <li>Standard flow HPLC or UHPLC system with column oven. NanoLC and microLC are not supported!</li> <li>96-well plate autosampler with temperature control (10 °C)</li> <li>Injection volume range: 5 – 20 μL</li> <li>Special sample rack for deep-well plates required for the following autosamplers:</li> <li>Shimadzu: part no. 228-37546-92 (Deep-well MTP Rack, DWP-96)</li> <li>UltiMate 3000: Thermo part no. 6820.4083 (30 – 36 mm height)</li> </ul>	<ul> <li>Waters ACQUITY UPLC® system with sample manager, solvent manager, and column oven:</li> <li>Classic (loop-based)</li> <li>I-Class (FTN)</li> <li>H-Class (FTN)</li> <li>Injection volume range:</li> <li>2 - 20 μL</li> <li>FTN samplers require extension loop of 50 μL or needle size of 30 μL!</li> </ul>		
Tubing				
Recommended between injector and column system: steel capillary				

- Recommended between injector and column system: steel capillary
- Recommended between column system and mass spectrometer: red PEEK Tubing 1/16" OD x 0.005" ID



# LC-MS instrument status

## Condition

- Serviced, calibrated and tuned instruments according to manufacturer's recommendations on a regular basis
- LC-MS system must be free of ion-pair reagent

# Analytical column

HPLC and UHPLC		
Analytical column	MxP® Quant 500 (XL) kit column system: biocrates product number 9120052121117 (HPLC/UHPLC column + pre-column mixer + connector, factory assembled)	



### Software

Agilent	SCIEX	Waters		
MS software				
<b>MassHunter</b> version 10.1 or later	Analyst® version 1.7 or later SCIEX OS (7500 series) version 2.2 or later	<b>MassLynx<sup>®</sup></b> version 4.1 or later		

biocrates WebIDQ workflow management software and computer requirements

### Option 1: WebIDQ cloud subscription (recommended) - biocrates part number 21629.1

# WebIDQ client

- Web browser: Edge or Chrome (latest version)
- 8 GB RAM
- Recommended: 6 cores (Intel i7 10<sup>th</sup> generation, AMD 5000 series or comparable)

### Option 2: WebIDQ on-premises subscription - biocrates part number 21636.1

#### WebIDQ client

- Web browser: Edge or Chrome (latest version)
- 8 GB RAM
- Recommended: 6 cores (Intel i7 10<sup>th</sup> generation, AMD 5000 series or comparable)

#### WebIDQ server

- Windows 10 or later, 64-bit architecture
- 16 GB RAM
- 8 cores (vCPU)
- Microsoft .NET Framework 4.5.2 or later
- Microsoft Visual C++ Redistributable (32 & 64 bit each): 2005, 2008, 2010, 2012, and 2013

#### Database – For hardware requirements please contact your database provider

- PostgreSQL, compatible versions: 12, 14
- Oracle<sup>®</sup>, compatible versions: 19c, 21c
  - Option 1 (recommended): full commercial version, updates and support provided by Oracle. Database administration required.
- Option 2: Oracle® Database Express Edition (Oracle XE), free of charge. No updates and support provided by Oracle®. Limited to 12 GB.



# Solvents and chemicals

Solvents and chemicals	Purity
Ethanol, methanol, water, acetonitrile, isopropanol	LC-MS grade (ethanol: HPLC grade sufficient)
Formic acid	LC-MS grade (e.g. Honeywell Fluka™ 56302-50ML) Fresh! New bottle or opened within past 6 months
Phenyl isothiocyanate (PITC)	99%, for protein sequencing (e.g. Sigma-Aldrich 317861) Fresh! New bottle or opened within past 6 months
Pyridine	Purity >99% (recommended Acros Organics 131780500, 50mL) Fresh! New bottle or opened within past 6 months
Ammonium acetate	LC-MS grade
Phosphate buffered saline (PBS)	p.a. grade (e.g. Sigma-Aldrich P4417)

# Laboratory equipment

Laboratory equipment				
	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	Examples:  - Porvair blowdown evaporator MiniVap®  - Techne (FSC496D)  - Sample concentrator from BenchTop Lab Systems (96 samples, BT1604)  - VLM evaporators  - Organomation MICROVAP microplate evaporator  - Biotage TurboVap® 96	Examples:  - 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	<ul> <li>Repeater, e.g. Eppendorf Multipette® E3         <ul> <li>(with 2.5 and 10 mL tips) or similar electronic model</li> <li>Single channel: volume range 10 μL – 1000 μL</li> <li>8-Channel: 10 μL – 150 μL</li> </ul> </li> </ul>			
Vortexer	Any model			
Balance	Accuracy < 1 mg			
Solvent bottles	50 – 1000 mL			

<sup>\*</sup> See document "Technical guide-Nitrogen evaporators and pressure manifolds" for details.