

## AbsoluteIDQ® Stero17 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

SCIEX	Waters
<b>Mass spectrometer</b>	
SCIEX 5500 or 6500+ series (QTRAP or Triple Quad) with TurboV™ ion source	Waters Xevo TQ-XS, TQ-S or TQ-S micro with ESI source
<b>LC and autosampler</b>	
<ul style="list-style-type: none"> <li>– Standard flow HPLC or UHPLC system with column oven.</li> <li><b>NanoLC and microLC are not supported!</b></li> <li>– 96-well plate autosampler with temperature control (10 °C)</li> <li>– Injection volume range: 10 – 20 µL</li> <li>– Special sample rack for deep-well plates required for the following autosamplers:               <ul style="list-style-type: none"> <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> </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 range: 5 – 10 µL</li> </ul>
<b>Tubing</b>	
<ul style="list-style-type: none"> <li>– Recommended between injector and column system: steel capillary</li> <li>– Recommended between column system and mass spectrometer: red PEEK Tubing 1/16" OD x 0.005" ID</li> </ul>	

### LC-MS instrument status

Condition
<ul style="list-style-type: none"> <li>– <b>Serviced, calibrated and tuned instruments</b> according to manufacturer's recommendations on a regular basis</li> <li>– LC-MS system must be <b>free of ion-pair reagent</b></li> </ul>

### Solvents and chemicals

Solvents and chemicals	Purity
Acetonitrile, isopropanol, methanol, water	LC-MS grade
Dichloromethane	p.a. grade or higher

## Analytical column

HPLC	
Analytical column	<b>AbsoluteIDQ® Stero17 kit HPLC column:</b> biocrates product number 9120052120301
Precolumn	<b>AbsoluteIDQ® Stero17 kit HPLC precolumn:</b> biocrates product number 9120052120349
Precolumn holder	<b>AbsoluteIDQ® Stero17 kit HPLC setup box:</b> biocrates product number 9120052120318

UHPLC	
Analytical column	<b>AbsoluteIDQ® Stero17 kit UHPLC column:</b> biocrates product number 9120052120356
Precolumn	<b>AbsoluteIDQ® Stero17 kit UHPLC precolumn:</b> biocrates product number 9120052120363
Precolumn holder	<b>AbsoluteIDQ® Stero17 kit UHPLC setup box:</b> biocrates product number 9120052120370

## Software

SCIEX	Waters
MS software	
Analyst® version 1.5.2 or later	MassLynx® version 4.1 or later
Data processing computer	
<ul style="list-style-type: none"> <li>– Oracle® database:               <ul style="list-style-type: none"> <li>– <b>Option 1 (recommended):</b> full commercial version, updates and support provided by Oracle. Expert required.</li> <li>– <b>Option 2:</b> Oracle Database Express Edition (Oracle XE), free of charge, provided by biocrates. No updates and support provided by Oracle.</li> </ul> </li> <li>– MetIDQ™ software (provided by biocrates)</li> <li>– Windows 7 or later, 64-bit architecture</li> <li>– Microsoft .NET Framework 4.5.2 or later</li> <li>– Microsoft Visual C++ redistributables (32 &amp; 64 bit each): 2005, 2008, 2010, 2012, and 2013</li> </ul>	

## Laboratory equipment

Laboratory equipment	
Shaker	Any model with adjustable speed (450 – 1200 rpm) including a tray for plates and vials. Recommended: Eppendorf MixMate® or ThermoMixer®
Pipettes	<ul style="list-style-type: none"> <li>– Repeater, e.g. Eppendorf Multipipette® E3 (with 1.0 and 10 mL tips) or similar electronic model</li> <li>– Single channel: volume range 10 µL – 1000 µL</li> <li>– 8-Channel: 1000 µL</li> </ul>
Vortexer	Any model
Ultrasonic bath	Any model
Solvent bottles	50 – 1000 mL
Drying and extraction – Option 1	
Nitrogen evaporator for 96-well plates*	Vacuum-based system
<b>Examples:</b> <ul style="list-style-type: none"> <li>– Porvair blowdown evaporator MiniVap®</li> <li>– Techne (FSC496D)</li> <li>– Sample concentrator from BenchTop Lab Systems (96 samples, BT1604)</li> <li>– VLM evaporators</li> <li>– Organomation MICROVAP microplate evaporator</li> <li>– Biotage TurboVap® 96</li> </ul>	<b>Vacuum pump, e.g.:</b> <ul style="list-style-type: none"> <li>– Waters WAT085114, WAT085123 or WAT085115</li> </ul> <b>Vacuum manifold for 96-well SPE plates, e.g.:</b> <ul style="list-style-type: none"> <li>– Extraction plate manifold for Oasis 96 Well Plates, Waters 186001831</li> <li>– PlatePrep 96-well vacuum manifold, starter kit, Sigma-Aldrich 575650-U</li> </ul>
<b>Requires nitrogen supply and installation in fume hood</b>	
Drying and extraction – Option 2	
Pressure manifold for 96-well plates*	Adapter for pressure manifold
<b>Examples:</b> <ul style="list-style-type: none"> <li>– Waters positive pressure-96 processor (186006961)</li> <li>– Biotage® PRESSURE+ 96 manifold (PPM-96)</li> <li>– CEREX® system 96 processor (288-0001)</li> <li>– Agilent positive pressure manifold 96 processor (PPM-96)</li> <li>– TECAN Resolvex® M10 96</li> </ul>	<b>biocrates product number 9120052120981</b>
<b>Requires nitrogen supply and installation in fume hood</b>	

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