

AbsoluteIDQ® p180 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	Thermo Scientific	Waters
Mass spectrometer			
6470 Triple Quadrupole	SCIEX 4000, 4500, 5500, 5500+, 6500 or 6500+ series (QTRAP or Triple Quad) with TurboV™ ion source	Thermo Scientific TSQ Vantage with HESI-II ion source	Waters Xevo TQ-XS, TQ-S or TQ-S micro with ESI source
LC and autosampler			
<ul style="list-style-type: none"> – Agilent 1290 Infinity I/II UHPLC system with column oven. NanoLC and microLC are not supported! – Agilent Infinity II: Inline Filter Kit <u>required</u> (p/n 5067-6189) – 96-well plate autosampler with temperature control (10 °C) – Injection volume range: 2 – 20 µL 	<ul style="list-style-type: none"> – Standard flow HPLC or UHPLC system with column oven. NanoLC and microLC are not supported! – 96-well plate autosampler with temperature control (10 °C) – Injection volume range: 2 – 20 µL – Special sample rack for deep-well plates required for the following autosamplers: <ul style="list-style-type: none"> – Shimadzu: part no. 228-37546-92 (Deep-well MTP Rack, DWP-96) – UltiMate 3000: Thermo part no. 6820.4083 (30 – 36 mm height) 	<ul style="list-style-type: none"> – Waters ACQUITY UPLC® system with sample manager, solvent manager, and column oven: <ul style="list-style-type: none"> – Classic (loop-based) – I-Class (FTN) – H-Class (FTN) – Injection volume: <ul style="list-style-type: none"> – loop: 20 µL – FTN: 10 µL 	

LC-MS instrument status

Condition
<ul style="list-style-type: none"> – 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 columns

UHPLC* – Option 1

Analytical column	AbsoluteIDQ® p180 kit UHPLC column: biocrates product number 9120052121193 (Precolumn not required)
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UHPLC* – Option 2

Analytical column	Waters ACQUITY UPLC BEH C18 1.7µm, 2.1 x 75mm (186005604)
Precolumn	Waters ACQUITY BEH C18 1.7µm VANGUARD (186003975)
Precolumn holder	Already included in the Waters VANGUARD precolumn package

* UHPLC not compatible with SCIEX 4000 series

HPLC

Analytical column	Agilent Zorbax Eclipse XDB C18 3.5µm, 3.0 x 100mm (961967-302)
Precolumn	Phenomenex SecurityGuard, C18, 4 x 3mm (AJO-4287)
Precolumn holder	Phenomenex SecurityGuard Cartridge (KJO-4282)

Solvents and chemicals

Solvents and chemicals	Purity
Ethanol, methanol, water, acetonitrile, isopropanol	LC-MS grade
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 >99.5% 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* <u>or</u> 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	– Repeater, e.g. Eppendorf Multipette® E3 (with 1.0, 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.

Software

Agilent	SCIEX	Thermo Scientific	Waters
MS software			
MassHunter version B.09 or later	Analyst® version 1.7 or later	Xcalibur™ version 2.2 or later	MassLynx® 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 10th 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 10th 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®, 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.