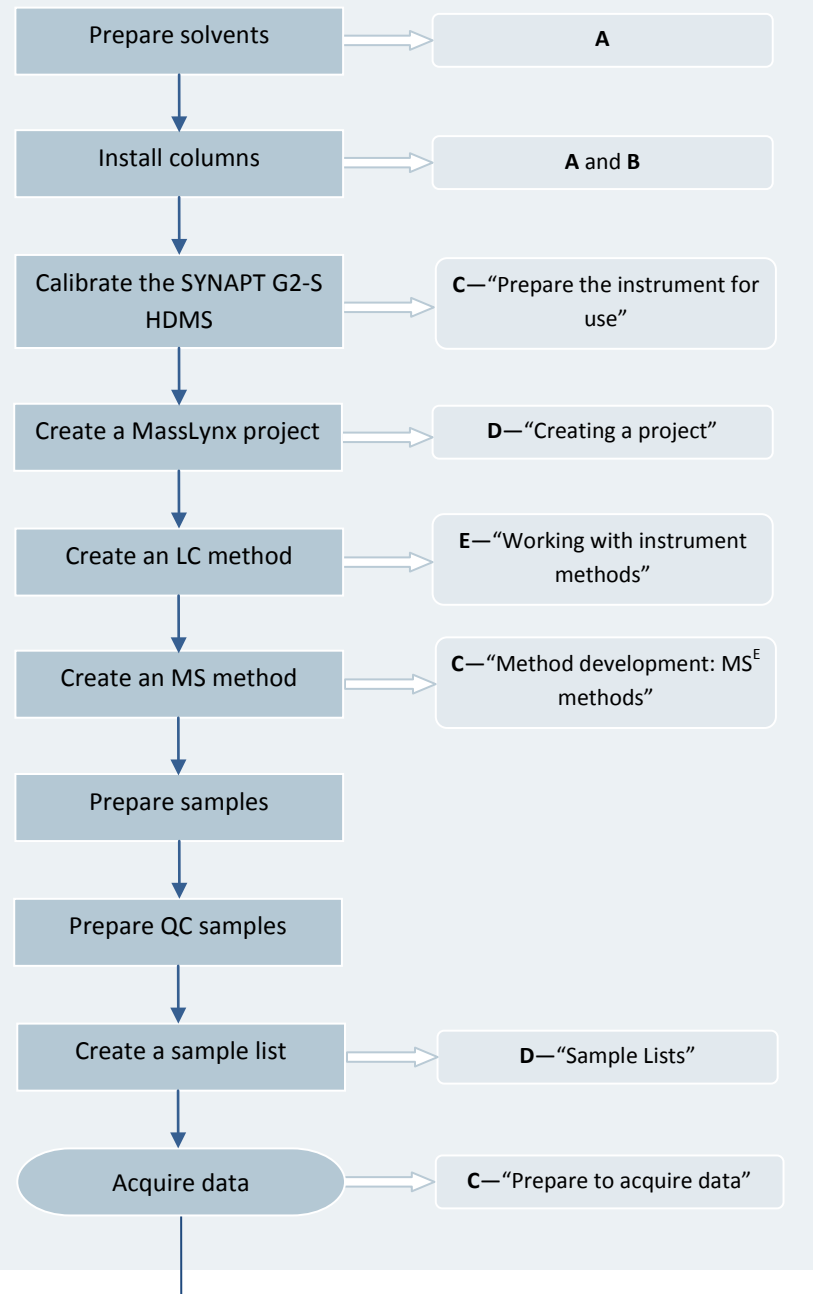


[WATERS OMICS RESEARCH PLATFORM SOLUTION METABOLOMICS AND LIPIDOMICS WORKFLOW (SYNAPT)]

Waters designed the OMICS Research Platform Solution (WORPS), with TransOmics™ Informatics powered by NonLinear Dynamics, as a research tool for performing discovery and for quantifying metabolites in complex mixtures.

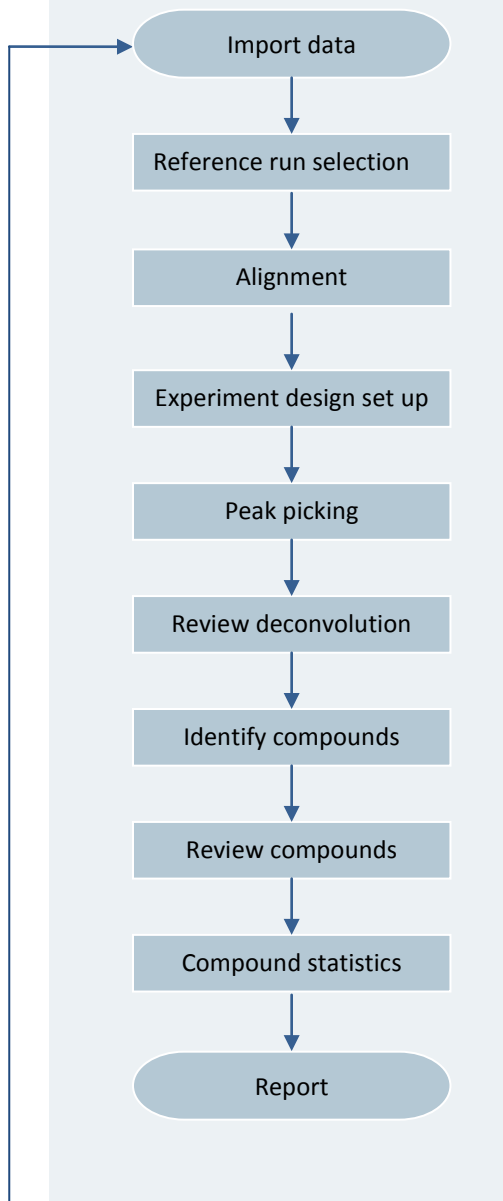
WORKFLOW FOR SETTING UP THE SYSTEM

See additional information over the page for references.



WORKFLOW FOR ANALYZING RESULTS

See Reference F, with additional information over the page, for further details on TransOmics Informatics.



[WATERS OMICS RESEARCH PLATFORM SOLUTION METABOLOMICS AND LIPIDOMICS WORKFLOW (SYNAPT)]

EXAMPLE PARAMETERS FOR ANALYSIS OF METABOLITES IN URINE

UPLC Conditions		Gradient			
Column:	ACQUITY UPLC 1.8 µm HSS T3	Time (min)	%A	%B	Curve
Column temperature:	40°C				
Sample temperature:	6 °C	0.0	99	1	Initial
Flow rate:	500 µL/min	1.0	99	1	6
Injection volume:	1 µL urine, 2 µL System Evaluation Matrix #1, 6s post-injection strong wash	3.0	85	15	6
Run time:	12 mins	6.0	50	50	6
Solvent A:	water/0.1% formic acid	9.0	5	95	6
Solvent B:	acetonitrile/0.1% formic acid	10.0	5	95	6
Wash:	water/0.1% formic acid	10.1	99	1	6
Seal wash:	50:50 water/methanol				

Source Parameters		MS Method Parameters	
Capillary:	Tune for maximum sensitivity 3.5 kV	Ionization mode:	ESI+
Sampling cone:	25 V	TOF acquisition mode:	Resolution
Source temperature:	120 °C	Acquisition method:	Continuum MS ^E
Desolvation temperature:	500 °C	TOF mass range:	50-1200 Da
Desolvation/Nebulizer/Cone gas:	1000/6/50 L/hr	Scan time:	0.1 s
Source offset:	80 V	Collision energy function 2:	Trap CE ramp 20 to 40 V
LockSpray Solution:	0.2 ng/µL leucine enkephalin in 50% methanol/50% water + 0.1% formic acid (556.2771 Da)		

CONSUMABLES

Columns 2.1 mm x 100 mm		Solutions
ACQUITY UPLC 1.8 µm HSS T3:	Medium-polar and nonpolar metabolites	System Evaluation Matrix #1
ACQUITY UPLC 1.7 µm BEH HILIC:	Highly polar metabolites	Analgesic Mix Standard: Acetaminophen, Acetanilide, Caffeine, Phenacetin,
ACQUITY UPLC 1.7 µm CSH C18:	Lipids	

ADDITIONAL INFORMATION

- ACQUITY I-Class UPLC Documentation CD (715003160)
- Symmetry Columns Care and Use Manual* (WAT047278)
- SYNAPT G2-S HDMS online Help (access from the Waters MassLynx software)
- MassLynx online Help (access from the Waters MassLynx software)
- ACQUITY I-Class UPLC System online Help (access from the Waters MassLynx software)
- TransOmics Informatics for Metabolomics and Lipidomics User Guide*

For additional, detailed information, refer to the *Waters Omics Research Platform Solution for Metabolomics and Lipidomics System Guide (SYNAPT)* (715003815). You can also consult the Waters Web site, www.waters.com/omics.