

Metabolomics Mass Spectrometry based protocols

	technology	approach	Instrument	mode	Specimen/study	sample prep	data treatment	statistics
1	LC QTOF MS	Untargeted LC-MS polars	UPLC- QTOF-MS Premier/TIMS-TOF-MS	HILIC, ESI, full scan MS	foods, biological fluids, cell culture	LLE, protein precipitation	XCMS, MS dial, Sirius...	PCA, PLS-DA, HCA, AUC ROC
2		Untargeted LC-MS lipophilic		RPLC, ESI, full scan MS	foods, biological fluids, cell culture	LLE, protein precipitation		
3		Targeted - bioactive content/antioxidants	UPLC- QTOF-MS	RPLC, ESI negative, bbCID	olive oil	LLE (MeOH:H2O, 80:20 v/v)	Target screening of 43 antioxidants	quantitative analysis - regression analysis
4		Untargeted bioactive content	UPLC- QTOF-MS	RPLC, ESI, bbCID	olive oil	LLE (MeOH:H2O, 80:20 v/v)	suspect screening of 1600 suspect compounds	PCA, PLS-DA, ACO-RF
5		Untargeted - bioactive content	UPLC- QTOF-MS	RPLC, ESI, bbCID + Auto MS (for identification)	olive oil	LLE (MeOH:H2O, 80:20 v/v)	XCMS, CAMERA, IPO	PCA, PLS-DA, ACO-RF
6		Targeted - bioactive content/antioxidants	UPLC- QTOF-MS	RPLC, ESI negative, bbCID	fruit juices	direct injection	Target screening of 37 antioxidants	quantitative analysis - regression analysis
7		Untargeted - bioactive content	UPLC- QTOF-MS	RPLC, ESI, bbCID + Auto MS (for identification)	fruit juices	direct injection	XCMS, CAMERA, IPO	differential analysis, PCA, PLS-DA
8		lipidomics general	UPLC- QTOF-TIMS-MS	pos/neg ESI untargeted on C8 CSH	various oils, dairy products, meat, tissue, eggs	LLE single or dual extraction	XCMS, MS dial, Sirius...	PCA, PLS-DA, HCA, AUC ROC
9		lipidomics semitargeted	UPLC- QTOF-TIMS-MS	pos/neg ESI untargeted on C8 CSH	specialised sample preparation and focused analysis e.g. in TGs	LLE dual extraction	XCMS, MSdial, bespoke scripts, in house libraries	PCA, PLS-DA, HCA, AUC ROC
10		plastic oligomer analysis	UPLC- QTOF-TIMS-MS	ESI MS-MS	migration from food contact material to foods	LLE	Metaboscape	quantitative analysis
11		polars semitargeted	UPLC- QTOF-TIMS-MS	neg ESI on premier Columns	various specimens/ analysis of ca. 60 organic acids	LLE	Metaboscape	quantitative analysis
12		Untargeted - bioactive content	UPLC- QTOF-MS	RPLC, ESI, bbCID + Auto MS (for	table olives	LLE (MeOH:H2O, 80:20 v/v)	XCMS, CAMERA, IPO	differential analysis, PCA, PLS-
13			Targeted HILIC-MS/MS			Honey/Royal jelly	dilution	

14	LC QqQ MS (MRM)	Targeted HILIC-MS/MS	UPLC-QqQ, Xevo TqD	HILIC Amide, pos/neg ESI	Carobs	LLE	Target Lynx, MRM 120 analytes		
15		Targeted HILIC-MS/MS			Nutrition (blood, urine, feces, tissue liver kidney brain etc)	LLE			
16		Targeted HILIC-MS/MS			various in vitro & Ex-vivo studies (infogest etc)				
17		Targeted HILIC-MS/MS			UPLC-QqQ, Thermo Access				milk
18		HILIC-MS/MS			UPLC-QqQ, Xevo TqD	AminoAcid Panel urine			dilution
19		RPLC-MS/MS	UPLC-QqQ, Sciex 3200	C8 ESI	Bile Acid Panel blood	LLE	MRM 18 analytes		
20		HILIC-MS/MS	UPLC-QqQ, Xevo TqD	HILIC ESI	Carnitines blood	LLE	Target Lynx, MRM 16 analytes		
21		RPLC-MS/MS	UPLC-QqQ, Xevo TqD	C18 ESI MRM	pharmaceuticals in biological samples	LLE	Target Lynx, MRM 84 analytes		regression analysis
22		RPLC-MS/MS	UPLC-QqQ, Sciex 3200	C18 ESI MRM	Ceramides in blood	LLE	MultiQuant, MRM 4 analytes		
23		RPLC-MS/MS		C18 ESI	25OH VitaminD2/D3 blood	LLE/SLE	MultiQuant MRM 4 analytes		
24		HILIC-MS/MS	UPLC-QqQ	ESI MRM	biogenic amines in fish	LLE			regression analysis
25		HILIC-MS/MS	UPLC-QqQ	ESI MRM	aminoacids dried blood spots and dried urine spots	LLE	Target Lynx		
26		HILIC-MS/MS	UPLC-QqQ	ESI MRM	nucleosides in blood/urine	LLE	Target Lynx		
27		HILIC-MS/MS	UPLC-QqQ	ESI MRM	lactose in milk dairy products	LLE			regression analysis
28	HILIC-MS/MS	UPLC-QqQ	ESI MRM	polar metabolites in wine	LLE	Xcalibur, MRM 80 analytes	regression analysis		

29		HILIC-MS/MS	UPLC-QqQ	ESI MRM	coumarin in biscuits, candies	LLE		regression analysis
30	GC MS(MS)	GC-MS	GC-Q Agilent 5973	EI, full scan	small molecules untargeted	MeOX, MSTFA derivatisation	GAVIN, AMDIS, NIST, Fiehn Agilent & Maurer Spectral Databases	PCA, PLS-DA, HCA, AUC ROC
31		GC-MS	GC- EVOQ TQ	EI, full scan	VOCs in biological samples	HS-SMPE, HS		
32		GC-MS		EI, full scan	VOCs in foods (olive oil, spirits)	HS-SMPE, HS		
33		GC-MS/MS		EI MRM MS	small molecules targeted, saliva/blood	MeOX, MSTFA derivatisation	quantitative 12 acids	
34		GC-MS/MS		EI MRM-MS	Organic Acids urine	MeOX, MSTFA derivatisation	quantitative 54 acids C3-C18	
35		GC-MS/MS / GC-FID	EI-MRM-MS	Fatty Acids blood	Methyl esterification	quantitative, 34 acids C12-C24	regression analysis	

