Examples already in MetaboLights Guides

Study ID	Study Title	Authors	Keyword (Ontology)	Measurement Type	Organism (Ontology)	Organism part (Ontology)	Factors (Ontology)	Sample Type	Technique / Acquisition Mode	Chromatography	Mass Spectrometry	Metabolite Annotation	Data Files	Publication
MTBLS3563	Impact of in vitro hormone treatments on the bibenzyl production of Radula complanata (Untargeted metabolomics)	Steffen Neumann; Kristian Peters; Kaitlyn Blatt-Janmaat	Mosses; lichens; liverworts (organism)(SNOMED); Plant Metabolomics(MTBLS); plant hormone(CHEBI); untargeted metabolites(MTBLS); ultra-performance liquid chromatography-mass spectrometry(CHMO); tandem mass spectrometry(CHMO); bibenzyl	Untargeted Metabolomics	Radula complanata (NCBITaxon)	Whole plant (BTO)	Phytohormone treatment: treatment(EFO); Phytohormone concentration: concentration(CHMO)	Experimental Samples (CHMO)	LC-MS/MS; DDA mode; reverse-phase; POS; NEG	Bruker Elite HPLC system; NUCLEODUR X18 C18 Gravity-SB (1.8 µm, 2 mm x 100 mm; Macherey-Nagel) column; 35 °C column oven temperature; binary solvent gradient (0.1% F A: solvent A, MeCN: solvent B); 0.5 mL/min flow rate	Bruker timsTOF Pro; ESI; Q-TOF; scan mass range: 20-1300 m/z	ChEBI ID; Chemical Formula; SMILES; InChI; Metabolite ID; m/z; Modifications; Charge; RT.	.d; .mzML	DOI; DOI
MTBLS4381	Metabolomics to elucidate the effects of novel sustainable feed additives in the feed of farmed salmon (HoloFood Trial A - seaweed-dose response)	Varsha Kale; Jacob Rasmussen; Sandy Rogers	HoloFood; Gut Content; Intestinal Flora(NCIT); untargeted metabolites(MTBLS); nanoflow liquid chromatography-tandem mass spectrometry(CHMO);	Untargeted Metabolomics	Salmo salar (NCBITaxon); blank	Intestinal content(NCIT); solvent(CHEBI)	Animal ID: Animal ID; Treatment: treatment(EFO); Sampling time: timepoint(EFO); Tank code: block(EFO)	Experimental Samples (CHMO); blanks, pooled quality control samples(MTBLS)	LC-MS/MS; DDA mode; reverse-phase; POS	Thermo Scientific Dionex UltiMate 3000 RSLCnano System; Acclaim PepMap RSLC C18 (3 µm, 0.075 mm x 150 mm; Thermo Scientific)	Thermo Scientific Q Exactive HF; nanoESI; Orbitrap; scan mass range: 200-1000 m/z	ChEBI ID; Chemical Formula; SMILES; InChI; Metabolite ID; m/z; Modifications; Charge; RT; taxid; species; search_engine; feat_ID; Compound_Source and	.raw; .mzML	NIAID Data Ecosystem

			intestine(BTO); Atlantic salmon; BioSamples; Host-Microbe Interactions							column; 40 °C column oven temperature; solvent gradient (0.1% FA in 98% H2O: 2% MeCN: solvent A, 0.1% FA in 2% H2O: 98% MeCN: solvent B); 0.3 mL/min flow rate		other 12 extra Compound related classification features; Quantification_values		
MTBLS718	Antiviral metabolite 3'-Deoxy-3',4'-didehydro-cytidine is detectable in serum and identifies acute viral infections including COVID-19	MRC-NIHR National Phenome Centre	untargeted metabolites(MTBLS); COVID-19 (DOID); CMPK2 (OGG); SPATS2L (OGG); IFI27 (OGG); RSAD2(OGG); ultra-performance liquid chromatography-mass spectrometry(CHMO); tandem mass spectrometry(CHMO); biomarker;(CHEBI); Lipidomics(NCIT)	Untargeted Metabolomics; Lipidomics	Homo sapiens (NCBITaxon)	Blood serum (BTO)	Cohort: cohort (EFO); Gender: Gender (NCIT); Age: age (EFO); Condition: Condition(NCIT); ITU admission (COVID only): Patient Admission(OMIT); Mortality (COVID only): mortality(EFO); Sample Collection: Date(NCIT); Delay to freezer storage: timepoint(EFO); Creatinine Concentration: concentration(CHMO); Sample Dilution: Sample Dilution(NCIT);CPMK2: Sequence Read	Experimental Samples (CHMO), pooled quality control samples(MTBLS)	LC-MS/MS; reverse-phase; HILIC; POS; NEG	Waters ACQUITY UPLC system; Waters 2777C Sample Manager; ACQUITY UPLC BEH HILIC (1.7 µm, 2.1 mm x 150 mm; Waters); ACQUITY UPLC BEH C8 (1.7 µm, 2.1 mm x 100 mm; Waters) column; 40 °C (HILIC) and 55 °C (RP) column oven temperature; solvent gradient (0.1% FA in	Waters Xevo G2-S QTof ESI; Q-TOF; scan mass range: 50-1200 m/z (HILIC) and 50-2000 m/z (RP-Lipidomics)	Metabolite ID; m/z; Modifications; Charge; RT; reliability; Quantification_values	.raw.zip; .mzML	DOI

							Count(NCIT); SPATS2L: Sequence Read Count(NCIT); IFI27: Sequence Read Count(NCIT); RSAD2 (viperin): Sequence Read Count(NCIT); unnamed: Sequence Read Count(NCIT)			MeCN: solvent A, 0.1% FA and 20 mM ammonium formate in H2O: solvent B); 0.6 mL/min - 1 mL/min flow rate (HILIC); temperature; solvent gradient (H2O:isopropanol:MeCN (2:1:1, v/v/v), 5 mM ammonium acetate, 0.05% acetic acid, 20 µM phosphoric acid: solvent A,isopropanol:acetonitrile (1:1, v/v), 5 mM ammonium acetate, 0.05% acetic acid: solvent B); 0.6 mL/min - 1 mL/min flow rate (RP-Lipidomics)				
MTBLS1820	Extracellular reef metabolites across the protected	Laura Weber	Coral reef sea water(ENVO); targeted metabolites(MTBLS);	Untargeted Metabolomics; Targeted	Sea water(ENVO)	Exometabolome(MTBLS)	Sea water location: Location(NCIT); Depth: Depth(NCIT);	Experimental Samples (CHMO); pooled	LC-MS/MS; reverse-phase; NEG; Alternating	Thermo Scientific Vanquish UHPLC System	Thermo Scientific Orbitrap Fusion Lumos Tribrid; ESI;	m/z; RT; Quantification_values	.raw; .mzML	DOI

	Jardines de la Reina, Cuba reef-system		untargeted metabolites(MTBLS); Dissolved Organic Matter(MESH); ultra-performance liquid chromatography-mass spectrometry(CHMO); Marine Metabolomics; coral metabolite(CHEBI); tandem mass spectrometry(CHMO)	Metabolomics			Replicate: technical replicate(EFO); Profiling: metabolite profiling assay(OBI)	quality control samples(MTBLS)		(Untargeted); Thermo Scientific Accela 1250 Pump and Thermo Scientific Accela Open Autosampler(Targeted) ACQUITY UPLC HSS T3 (1.8 µm, 2.1 mm x 100 mm; Waters); ACQUITY UPLC HSS T3 VanGuard Pre-column (1.8 µm, 2.1 mm x 5 mm; Waters); 40 °C column oven temperature; (0.1% FA in H2O: solvent A, 0.1% FA in MeCN: solvent B); 0.5 mL/min flow rate (Untargeted and Targeted)	Orbitrap; scan mass range: 100-1000 m/z (Untargeted); Thermo Scientific TSQ Vantage; ESI; Triple Quadrupole; scan mass range: SRM (Targeted)			
MTBLS2289	Overexpression of the vascular brassinosteroid receptor BRL3 confers	Fidel Lozano-Elena	untargeted metabolites(MTBLS); drought tolerance(TO); brassinosteroi	Untargeted Metabolomics	Arabidopsis thaliana(NCBI Taxon); blank	root(BTO); shoot(BTO)	Genotype: genotype(EFO); Timepoint: timepoint(EFO); Drought stress:	Experimental Samples (CHMO); blanks	GC-MS	Agilent 6890N GC; Agilent CTC Analytics Combi PAL	LECO Pegasus III; EI; TOF; scan mass range: 70-600 m/z	ChEBI ID; Chemical Formula; SMILES; InChI;	.peg; .cdf	DOI

	drought resistance without penalizing plant growth		d(CHEBI); Genetic(NCIT); Growth(NCIT); gas chromatography time-of-flight mass spectrometry(CHMO); BRL3 (Arabidopsis thaliana)				treatment(EFO); Replicate: replicate(EFO); Sample weight: Weight(NCIT)			autosampler; DB-35 GC (0.25 µm, 0.32 mm x 30 m; Agilent Technologies) column		Metabolite ID;taxid; species; Quantification_values		

Hands-on session II - MetaboLights Study Semantic Curation - *Part 01*

First part of Session

Group 1

Publication and terms identified in - Hands-on session I

Complete the following table according to the different sections present in a MetaboLights Study

Study ID	Study Title	Authors	Keyword (Ontology)	Measurement Type	Organism (Ontology)	Organism part (Ontology)	Factors (Ontology)	Sample Type	Technique / Acquisition Mode	Chromatography	Mass Spectrometry	Metabolite Annotation	Data Files	Publication

Group 2

Use this preprint to identify terms - https://www.medrxiv.org/content/10.1101/2025.10.16.25338140v1

Complete the following table according to the different sections present in a MetaboLights Study

Study ID	Study Title	Authors	Keyword (Ontology)	Measurement Type	Organism (Ontology)	Organism part (Ontology)	Factors (Ontology)	Sample Type	Technique / Acquisition Mode	Chromatography	Mass Spectrometry	Metabolite Annotation	Data Files	Publication
MTBLS8100	Dietary bioactives increase gut microbiome diversity and alter host and microbial metabolite profiles	Anthony Duncan, Federico Bernuzzi,												

Second part of Session (Time-permitting)

- Compare results with the submissions present in MetaboLights
- Suggest changes/ improvements as required - i.e. missing terms, missing characteristics, alternative ontology terms (Part 02), etc.

Group 1	Group 2