**LCMS Sample Submission Recommendations – February 1st 2021**

**Please submit electronically:**

* **Goal** (one or two keywords)**:** 
  + **Publication** (high res MS for mass confirmation)
  + **PDA** (purity determination with UV/Vis absorption, please specify wavelength (180-800nm, 3D plots available))
  + **Inorganic** (Heavy Metal containing complexes, photochemistry or catalyzation monitoring, oxygen/moisture sensitive species)
  + **Reaction** (tracing of e.g. kinetic data or reaction method optimization)
  + **Batch** (repetitive search for specific molecules in large sample numbers)
  + **Sequencing** (pure and digested proteins for sequence characterization, including MS/MS fragmentation data)
  + **Screening** (targeted and untargeted search in e.g. biological samples, including MS/MS fragmentation data)
  + **Quantification** (determination of absolute values of unknown sample concentrations in comparison to standards (internal or external), Chromatography and Multiple Reaction Monitoring (MRM) based quant.)
  + **Isotope** (confirmation of isotopically labeled species including MS/MS for structural confirmation, H/D exchange for labile X-H (X = N, O, S, (sometimes C) quant., or kinetic isotope effect (KIE) measurements)
* **Sample Identifier** (for reference to vial in rack and to sample name)
* **Sample Name** (all file names will be based on your abbreviated name (if not already included) and the sample name
* **Sum Formula (neutral)**
* **Method** (blank = standard 5min, 12min, 20min or specify)
* **Expected Mass (neutral, protonated or sodiated)**
* **Your Name, PI, email-address**
* **Optional: molecular structure as cdx (not cdxml)**

Please make sure that vials are uniquely labeled, they do not need to show the full sample name as long as proper reference is provided.

**Goal of the Measurement:**

As soon as **a compound** is to be **measured** **more than once** (almost everything except purified samples for publication), it is worth to write a **short description** of the project. **Postprocessing methods** and data reports sheets can be highly **automated** and stepwise **customized** when a project grows. This can save a lot of time in the long run.

**Sample concentrations** should be below **1x10(-4) molar (100 µM), best in the 1x10(-5) molar range** in water / organic solvent mixtures (e.g. MeOH or ACN). Please **specify** if you’re using a **different solvent system**. Protein solutions should be around 30-50µL of 10µM concentration, desalted if possible. As a rule of thumb, **less organic solvents in the sample** leads to **better chromatography** as long as the compound is soluble. Sample injections are normally run on a **50mm** **C18 column** (other columns upon request). Mass spectra are recorded in **positive ion mode**! **Anions** can be measured upon **request**.

Standard solvents are **Acetonitrile** with 0.1% Formic Acid (FA) and **Water** (0.1% FA) for the run. **Short** gradients (5min) are **standard** for small molecule characterization, recommendation for e.g peptides above 600-800 m/z is a **medium** (12min) and for complex mixtures of high mass molecules is a **long** (20min) gradient run.

**Other solvent systems** e.g. Hexane:Ethylacetate can be used upon request.

**Remaining samples** will be **discarded one week after a successful run** or they can be **picked up** (if needed), please specify.