# Electrospray Ionization Time-of-Flight (ESI-TOF)

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## 1.0 Introduction

Electrospray ionization (ESI) is a "soft" ionization method and is used for exact mass determination. The combination of ESI with a time-of-flight (TOF) mass analyzer allows for the detection of a broad range of molecules (100-3000 *m/z*). Below is an overview and the protocol used by the MSF for ESI-TOF analysis of submitted samples.

### 1.1 Sample Submission Link

The instructions to submit a sample can be found at the link below:

https://www.lsu.edu/science/chemistry/research/mass_spec/procedures/sample_submission_guidelines.pdf

All samples need to be submitted electronically. Submit samples using the following link:

https://www.lsu.edu/science/chemistry/research/mass_spec/submission-forms.php

## 2.0 Solvents

### 2.1 ESI-TOF solvents (HPLC Grade)

Acetonitrile (ACN)

Methanol (MeOH)

Water

Water w/ 0.1% Formic Acid

These solvents are preferred when dissolving submitted compounds to keep consistent with the mobile phase of the instrument (see 3.3).

**Note: if you have solvents that are not HPLC-grade, you are welcome to prepare samples using MSF solvents.*

### 2.2 Non-preferred Solvents

#### 2.2.1 Organic solvents:

This category includes solvents such as (but not limited to) n-hexane, ethyl acetate, N, N-Dimethylformamide (DMF), Dimethyl sulfoxide (DMSO), Dichloromethane (DCM), acetone, etc. In most cases (e.g. DMSO), the problem is the low volatility of the solvent and its capability to dissolve organic matter, which results in damage to the components of the whole system (e.g. tubing, connectors, etc.). If the compound submitted is only soluble in these listed solvents, samples should be diluted with one of the preferred solvents.

#### 2.2.2 Salts such as NaCl and phosphates:

Salts are either non-volatile or hinder the ionization process. If the presence of salts is unavoidable, the concentration should be kept low (µM or lower)

## 2.3 Avoiding particulate matter

Sometimes it happens that a sample is not completely dissolved, especially if the sample is a mixture or a crude organic reaction. If you observe particulate in the solution, transfer an aliquot of the sample (100-200 µL) into a tube and ultracentrifuge the volume at 14,000 g. Afterward, pipette out half of the volume, making sure not to disturb the precipitate at the bottom of the tube.

In general, _____. These devices bleed polymeric material in the sample, which will be present in the spect ( p) (ia)6pe sticulat8ceqTT1 u(s)1 s0 Tc ETBT1 (a

$V_2$ = Final sample volume

Sample calculation using Step 1 concentration…

$M_1$ = 2000 µg/mL

$V_1$ = 2 µL

$M_2$ = 25 µg/mL

$V_2$ = Total Volume (noted as X)

$$\frac{\mu \qquad \mu}{\mu}$$

X= 160 µL Total Volume, therefore the 2000 µg/mL sample will be diluted with the following…

2 µL of sample and 158 µL of solvent

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Link: https://www.lsu.edu/science/chemistry/research/mass_spec/submission-forms.php