# Molecular Matching with Ion Mobility Spectrometry using Python

## Introduction

The idea of this research is to analyze and identify how useful the Python programming language can be in comparing and identifying substances using Ion Mobility Spectrometry. Ion Mobility Spectrometry is an analytical research method that helps in separating and identifying ionized molecules.

Ion Mobility Spectrometry (IMS) is widely used in identification of molecules in fields like security, military, research etc. and is extensively used in detection of explosives, drugs and chemical weapons.

This research explores the idea of a Python-based workflow for molecular matching with IMS Data with the following steps

1. Data retrieval from an SQLite database:

The SQLite database should have two tables, *measurement* and *library* where the measurement table holds the IMS Data with which we will be working on identifying the relevant data that we need to compare and identify the substance.

1. Calculation of reduced ion mobility:

Reduced ion mobility is an important parameter with which each molecule can be differentiated.

1. Library matching:

Compare the calculated reduced ion mobility values against a reference database (which should be the library table from the SQLite database) and assign the most likely molecular identity.

## Background and Theoretical Framework

### 2.1 What is Ion Mobility Spectrometry

According to James N Dodds and Erin S Baker, Ion Mobility Spectrometry (IMS) is the study of how ions move in gases under the influence of an electric field. The idea is the setup consists of multiple chambers.[[1]](#footnote-1) When we consider a rudimentary setup of an IMS, the first chamber is where the sample gas enters. Then the sample gas is ionized using an external source by exciting the molecules. Then the ionized gas enters another chamber which has an electric field. Each molecule has a different *drift velocity* with which they travel this chamber from start to end. We should know the voltage of this electric field, the temperature, pressure and multiple factors that are required to calculate the reduced ion mobility ion mobility of each molecule in that sample.

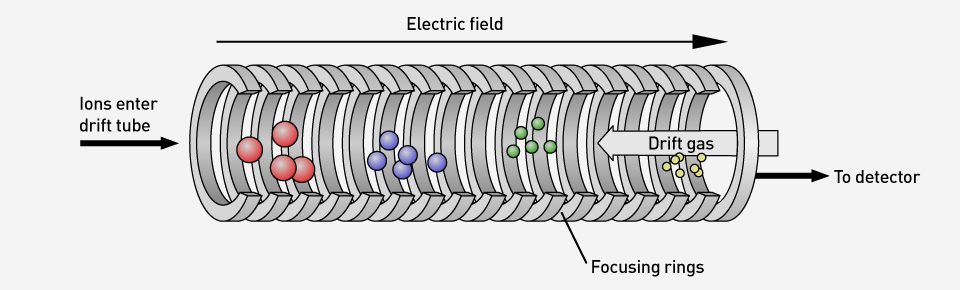


Figure Ion Mobility Spectrometry cross-section [[2]](#footnote-2)

### Principles of Ion Mobility Spectrometry

In IMS, ions that are generated from a sample are introduced in the drift region. In a uniform electric field, each ion’s drift velocity is proportional to the electric field strength . is the proportionality factor between the drift velocity and the electric field strength.[[3]](#footnote-3)

The reduced ion mobility is calculated when other factors such as the temperature and pressure during drift, standard temperature *T*0 = 273 K and standard pressure *p*0 = 1013 hPa are known.

To find the value, we can use the following formula.

Where is the drift length (the length of the chamber or tube where the ionized particles move), is the drift time and is the potential difference in the chamber.

1. Ion Mobility Spectrometry: Fundamental Concepts, Instrumentation, Applications, and the Road Ahead (<https://pmc.ncbi.nlm.nih.gov/articles/PMC6832852/>) [↑](#footnote-ref-1)
2. https://www.analyticon.eu/en/ion-mobility-spectrometry.html [↑](#footnote-ref-2)
3. https://en.wikipedia.org/wiki/Ion\_mobility\_spectrometry#Ion\_mobility [↑](#footnote-ref-3)