Kütle spektrometrisi

MassBank norman

High Resolution Mass Spectral Database

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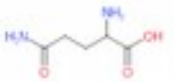
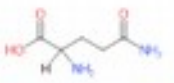
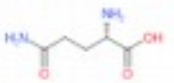
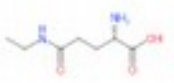
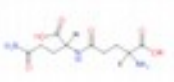
European MassBank (NORMAN MassBank)

Quick Search

Peak Search

Record Index

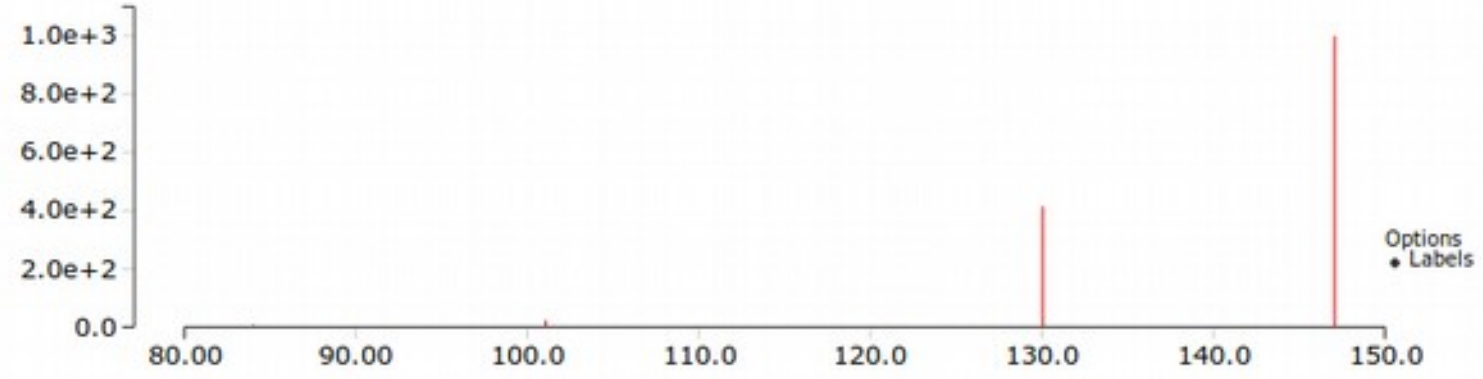
- WEB-API WSDL

	Name	Formula / Structure	ExactMass	ID
☐	⊞ D-Glutamine 5 spectra	C5H10N2O3 	146.06914	
☐	⊞ Glutamine 5 spectra	C5H10N2O3 	146.06914	
☐	⊞ L-Glutamine 19 spectra	C5H10N2O3 	146.06914	
☐	⊞ N-Ethylglutamine 4 spectra	C7H14N2O3 	174.10043	
☐	⊞ gamma-Glutamylglutamine 1 spectrum	C10H17N3O6 	275.11172	

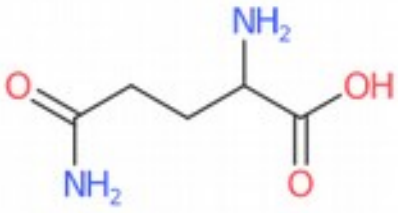
MassBank Record: PB000465

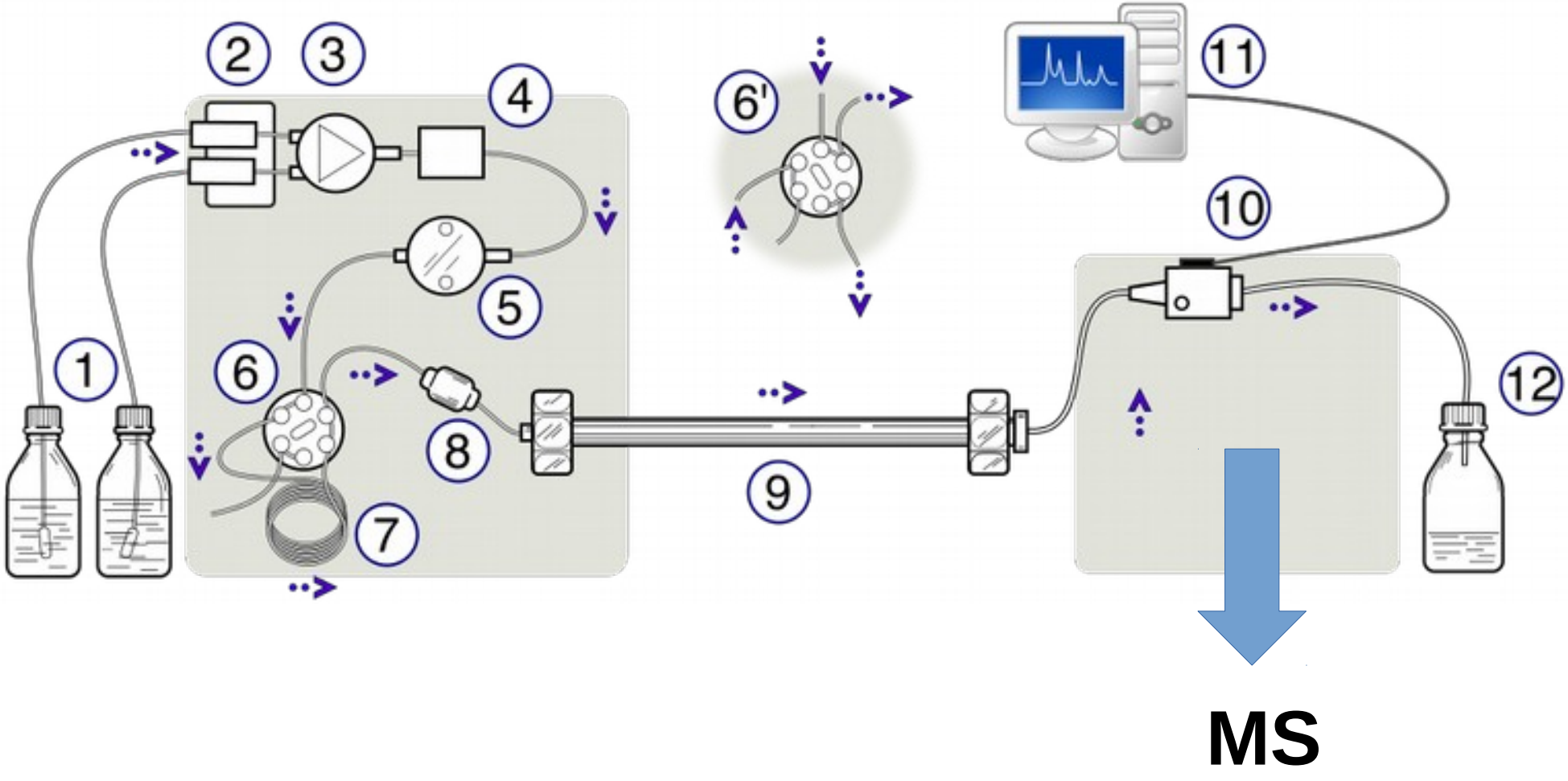
Glutamine; LC-ESI-QTOF; MS2; CE:10 eV; [M+H]+

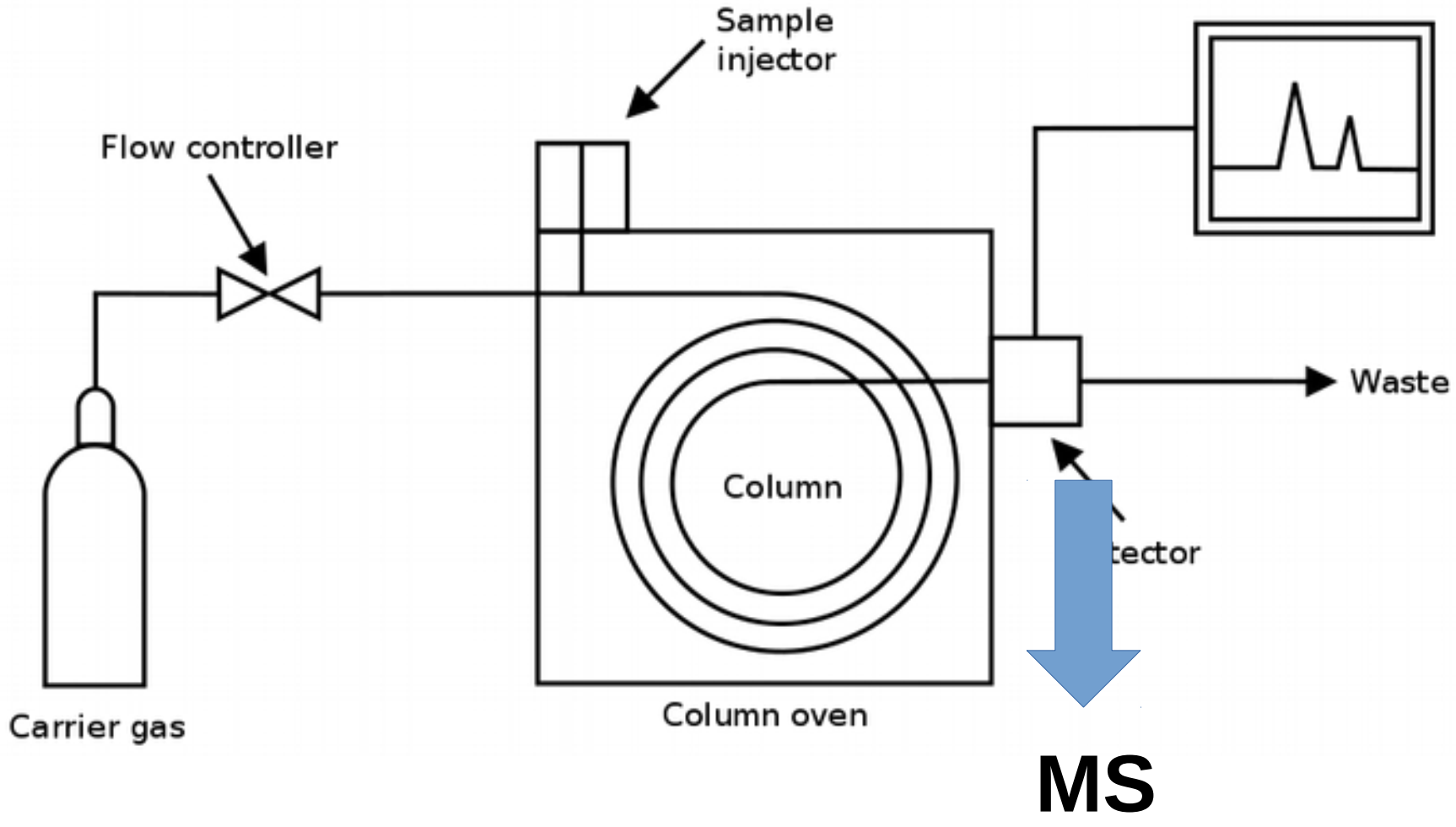
Mass Spectrum



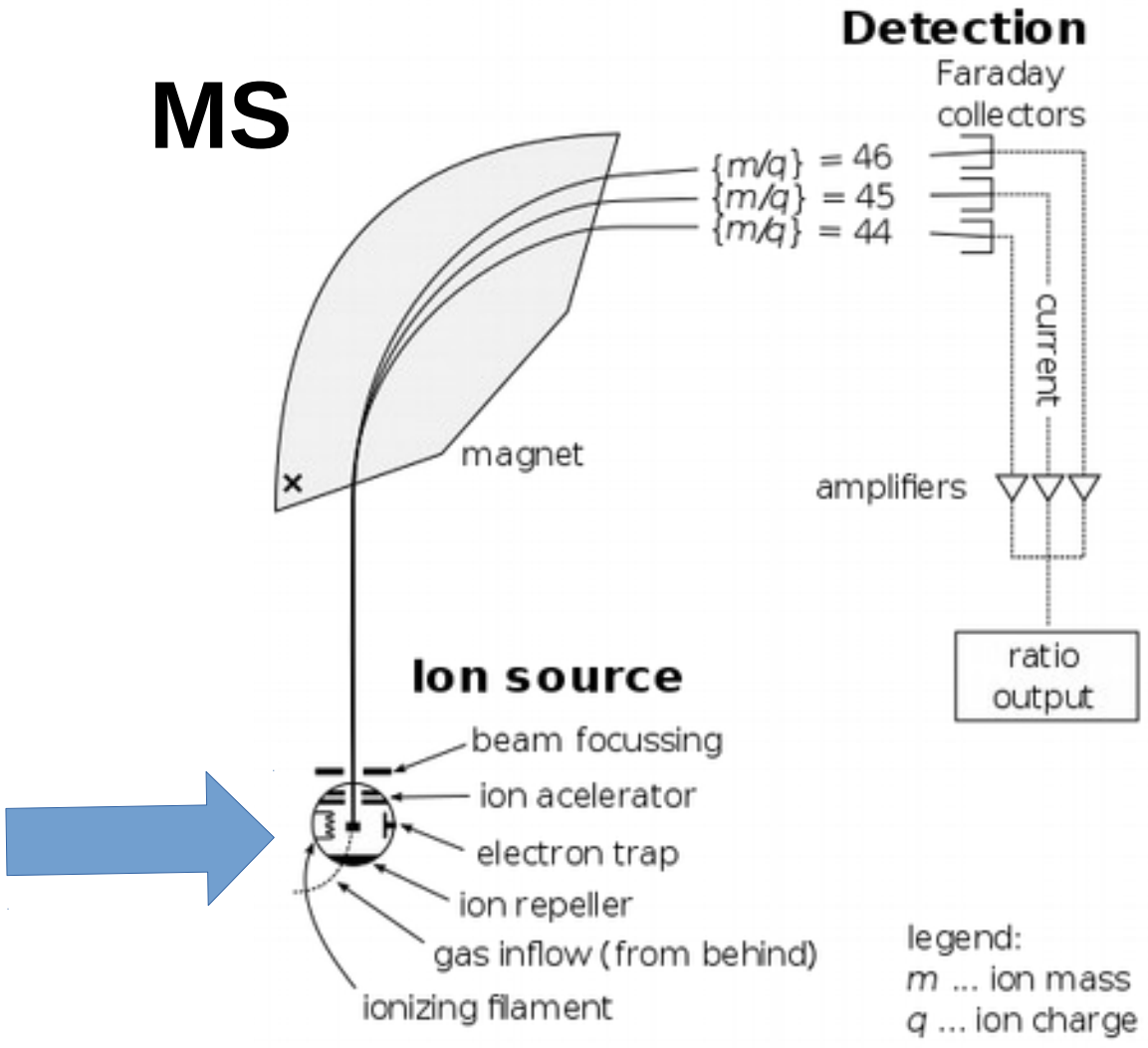
Chemical Structure

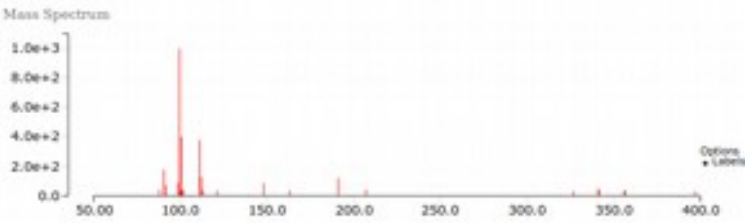



1
2
3
4
5
6
6'
7
8
9
10
11
12
MS

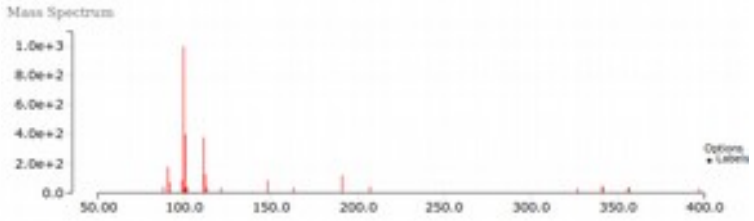

Sample injector
Flow controller
Waste
Column
tector
Carrier gas
Column oven
MS

MS


Detection
Faraday collectors
{m/q} = 46
{m/q} = 45
{m/q} = 44
current
magnet
amplifiers
ratio output
Ion source
beam focussing
ion acelerator
electron trap
ion repeller
gas inflow (from behind)
ionizing filament
legend:
m ... ion mass
q ... ion charge


Mass Spectrum
1.0e+3
8.0e+2
6.0e+2
4.0e+2
2.0e+2
0.0
50.00
100.0
150.0
200.0
250.0
300.0
350.0
400.0

PK$SPLASH: splash10-01ot-9801000000-c10341d61ee2d6369219
PK$NUM_PEAK: 26
PK$PEAK: m/z int. rel.int.
87.9997 1.51 44
90.5064 6.202 179
90.5253 1.296 37
91.5027 2.545 74
98.5079 3.088 89
99.5113 34.59 999
100.0137 1.313 38
100.5083 13.91 402
101.0111 1.123 32
101.5049 1.567 45
111.0200 13.18 381
112.0184 4.504 130
113.0165 1.442 42
121.0656 1.199 35
148.0521 3.063 88
163.0787 1.254 36
191.0712 4.157 120
207.0435 1.081 31
207.0688 1.439 42
326.9312 1.16 34
341.0021 1.72 50
341.8020 1.309 38
356.0340 1.147 33
356.7647 1.391 40
356.8112 1.213 35
397.1271 1.048 30
//



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version="1.1.0">
    <cvList count="2">
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      <fileContent>
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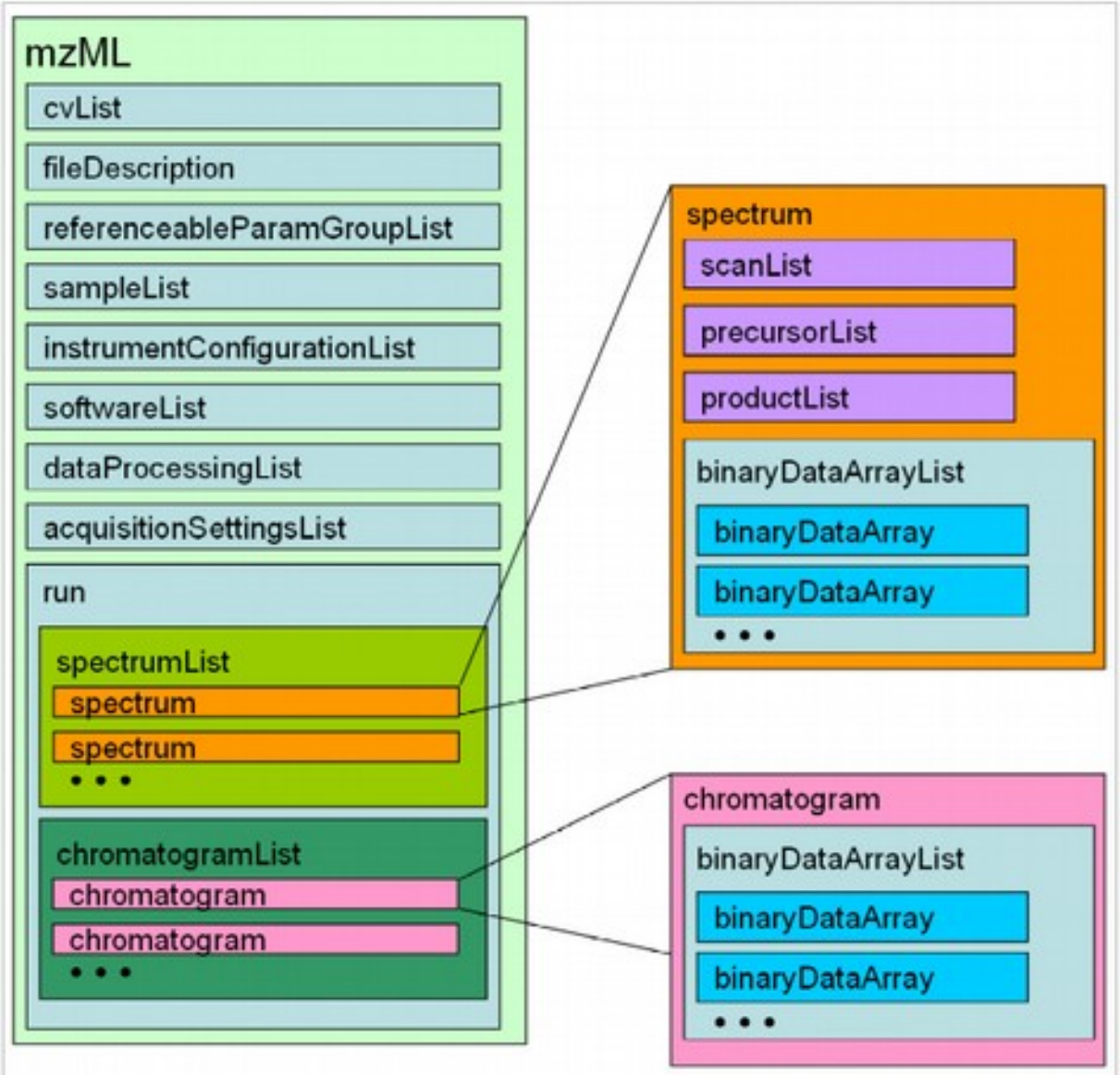
```


mzML
cvList
fileDescription
referenceableParamGroupList
sampleList
instrumentConfigurationList
softwareList
dataProcessingList
acquisitionSettingsList
run
spectrumList
spectrum
spectrum
chromatogramList
chromatogram
chromatogram
spectrum
scanList
precursorList
productList
binaryDataArrayList
binaryDataArray
binaryDataArray
chromatogram
binaryDataArrayList
binaryDataArray
binaryDataArray

```java
package mzreader;

import java.io.File;
import uk.ac.ebi.jmzml.model.mzml.CV;
import uk.ac.ebi.jmzml.model.mzml.CVList;
import uk.ac.ebi.jmzml.model.mzml.Chromatogram;
import uk.ac.ebi.jmzml.model.mzml.MzML;
import uk.ac.ebi.jmzml.model.mzml.Run;
import uk.ac.ebi.jmzml.model.mzml.Spectrum;
import uk.ac.ebi.jmzml.xml.io.MzMLUnmarshaller;
```

```java
public class MzReader {

    /**
     * @param args the command line arguments
     */
    public static void main(String[] args) {
        // TODO code application logic here

        File mzXML = new File("PEG200.mzML");

        MzMLUnmarshaller u = new MzMLUnmarshaller(mzXML);

        MzML completeMz = u.unmarshall();
        CVList cvList = completeMz.getCvList();
        for(CV c : cvList.getCv()) {
            System.out.println(c.getFullName() + "-" + c.getVersion());
            System.out.println(c.toString());
        }
        Run run = completeMz.getRun();
        for(Chromatogram c : run.getChromatogramList().getChromatogram()) {
            System.out.println(c.getId());
        }
        for(Spectrum s : run.getSpectrumList().getSpectrum()) {
            System.out.println(s.getId());

        }
    }
}
```