SERVEI ESPECTROMETRIA DE MASSES

Ionization Technique: MALDI

Instrument: 4800 *Plus* MALDI TOF/TOF (ABSciex – 2010)

General Experimental conditions:

Ionization Source: MALDI (Matrix Assisted Laser Desorption Ionization)
Solid State Laser (Nd:YAG) (355nm, 200Hz, 3-7ns pulse).
Analyzer: TOF/TOF (Time of Flight) in reflector mode or linear mode depending on the m/z
Ion Lecture: positive or negative
Matrix: depends on the sample nature
SA (sinapinic acid)
CHCA (α-cyano-4-hydroxycinnamic acid)
DHB (2,5-dihydroxybenzoic acid)
Dithranol (1,8,9-trihydroxyanthracen)

Ionization methode: Electrospray (ion spray) (ESI-MS) Positive/negative mode

Instrument: LC/MSD-TOF (2006) (Agilent Technologies)

Instrumental conditions:

Capillary: 4 KV (positive), 3.5KV (negative)
Fragmentor: 215V
Gas temperature: 325º C
Nebulizing Gas: N_2 Pressure = 15 psi
Drying Gas: N_2 Flow= 7.0 l/min

Dual Source equipped with a lock spray (for internal reference mass in exact mass measurements). Internal reference masses (+) m/z= 121.050873 (Purine), 922.009798 (HP-0921) Internal reference masses (-) m/z= 112.9856 (TFA Anion), 119.0363 (Purine), 1033.9881 (HP-0921).

Sample introduction:

Sample (microliters) is introduced into the source with an HPLC system (Agilent 1100), using a mixture of H_2O:CH_3CN 1:1 as eluent (200µl/min) (depending on the nature of the sample we add 1% formic acid to the eluent).

Standard deviation for the monoisotopic peak = [(exp. mass monoisotopic peak – calc. mass monoisotopic peak)/calc. mass monoisotopic peak]$\cdot 10^6 \leq 5$ ppm

Ions, radicals or molecules that can be added to the molecular cation peak or fragments of the molecular cation in the ESI-(+) experiment.	Most probable mass
•CN (coming from acetonitrile)	26.0031
MeCN (acetonitrile)	41.0265
CN^- (coming from acetonitrile)	26.0031
H^+	1.0078
HCN (coming from acetonitrile)	27.0109
K^+	38.9637
Na^+	22.9898
$NH4^+$	18.0344