# Tel-Aviv University
# School of Chemistry
## Laboratory of Mass Spectrometry

**Example: How to report MS results**

**Instruments**

MS: SYNAPT - High Definition Mass Spectrometry. (Waters Inc., USA)
Xevo TXD, (Waters Inc., USA)
Autospec HRMS (Micromass. UK)
LC: Acquity Ultra performance LC. (Waters Inc., USA)

**Conditions:**

LC:

Solvent A1: $H_2O$ (95%) + MeCN (5%)+ Formic Acid(0.1%)
Solvent B2: MeCN (100%) + Formic Acid(0.1%)
flow: 0.3 ml/min column: BEH 2.1/50 1.7 micron

Gradient (Example)

| time | A1 | B1 |
|---|---|---|
| 0 | 100 | 0 |
| 0 | 100 | 1 |
| 100 | 0 | 10 |
| 100 | 0 | 11 |
| 0 | 100 | 11.3 |

**Mass Spectrometry (MS)**

Ionization method: ESI Positive Or Negative
APCI (Atmospheric Pressure Chemical Ionization) Positive
APPI (Atmospheric Pressure Photo Ionization)
MALDI (Matrix assisted Laser Desorption Ionization)

**Liquid Chromatography Mass Spectroscopy (LC-MS)**

The spectra was done using liquid chromatography (LC) (Acquity-UPLC, Waters Inc., USA) coupled with an UV detector (Acquity-TUV detector, Waters Inc., USA) and mass spectrometer (Instrument Name) The stationary phase consisted of a C18 (1.7 µm, 2.1 x 100 mm) column (Waters Inc., USA) and the mobile phase compositions were
A: 95% $H_20$ + 5% MeCN + 0.1 % Formic acid (FA) and
B: Acetonitrile + 0.1 % FA .
The elution gradient was as follows :
linear increase to 50% B over 2 min, ramp to 100% B and hold for 1 min
then return to the starting conditions for additional 2 min .
Samples of 10 µl were injected and the flow rate was 0.5 ml/min .
The temperature in the sample chamber was pre-set to ……°C
and remained stable (±1°C) throughout the measurements .
The UV detector was set to…… nm
Whilst the mass spectrometer was operated both in negative and positive ion modes, the interpretation of the data was conducted only on the latter using/ on both positive and negative ion modes MassLynx software (v4.1, Waters Laboratory Informatics, Waters Inc. USA).