# Electron emission and fragmentation of DNA/RNA components induced by proton impact

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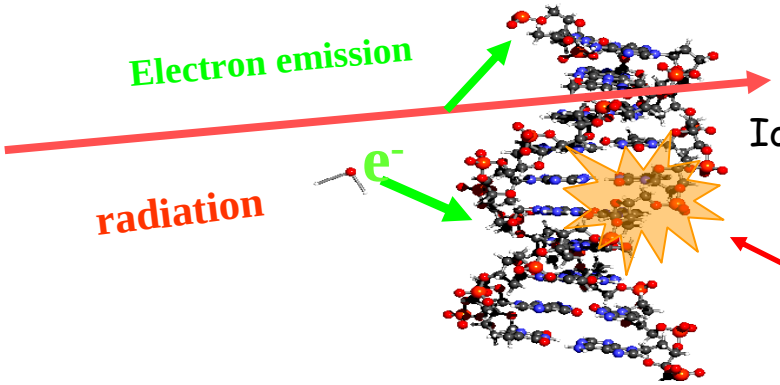
## Damages induced by ionizing radiation  Target: DNA molecule




Ionization, Base damage ≈30%> **Direct effects**

SINGLE, DOUBLE **STRAND BREAK**

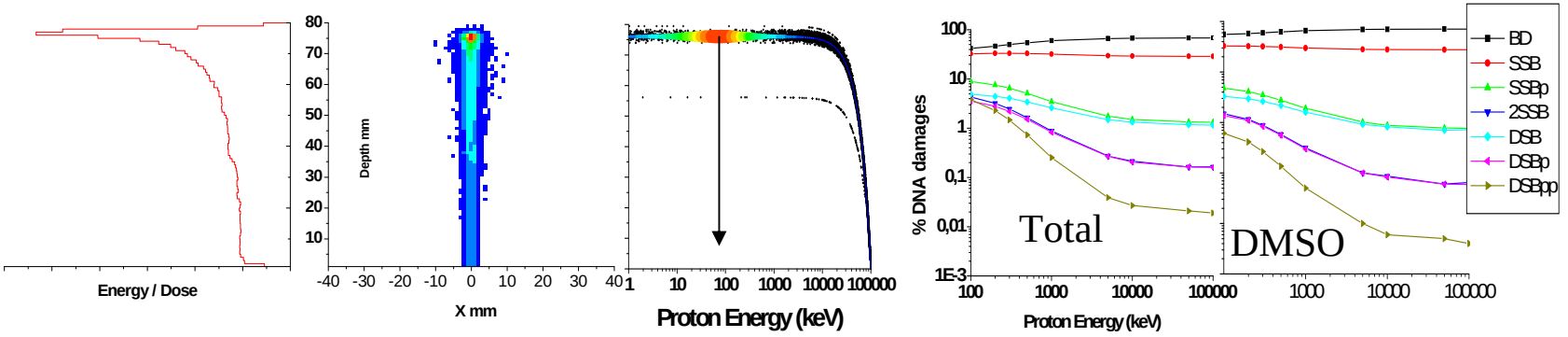
Surroundig water: **radicals ≈70%> Indirect effects**

**Interaction of ions with matter: possibility of strong energy deposition in a well defined region around the Bragg peak**

**100 MeV proton in water:**

*(Semennenko, Steward Rad.Res. (2004) 161)*

Bragg peak  Spatial Dose  Stopping power  DNA damages (MCDS code)

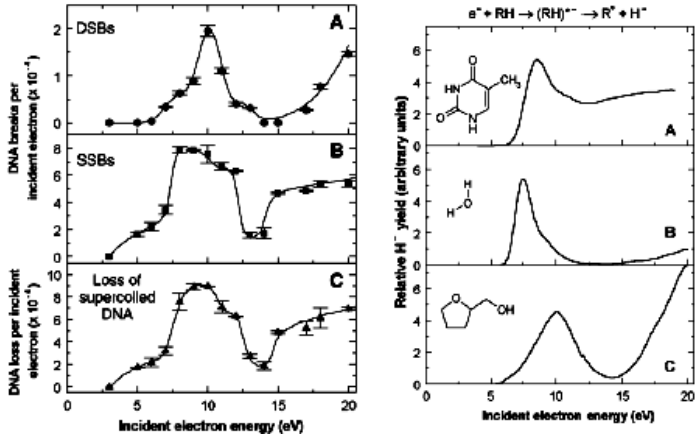



**≈ 100keV**

# Damages induced by electrons ?

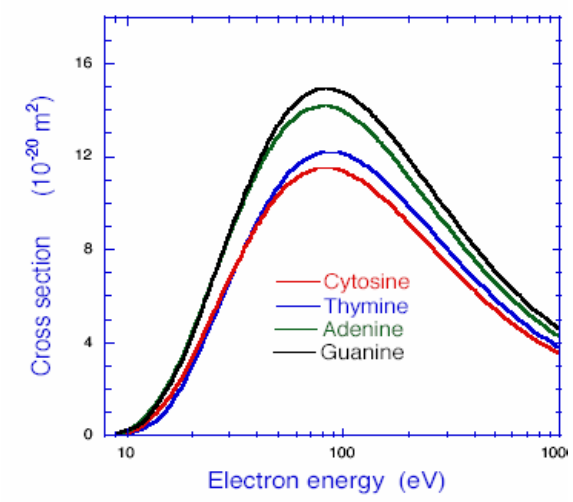
## E<20eV: Dissociative attachement

*(Boudaiffa et al Science **287** (2000))*




## E>20eV: Ionization

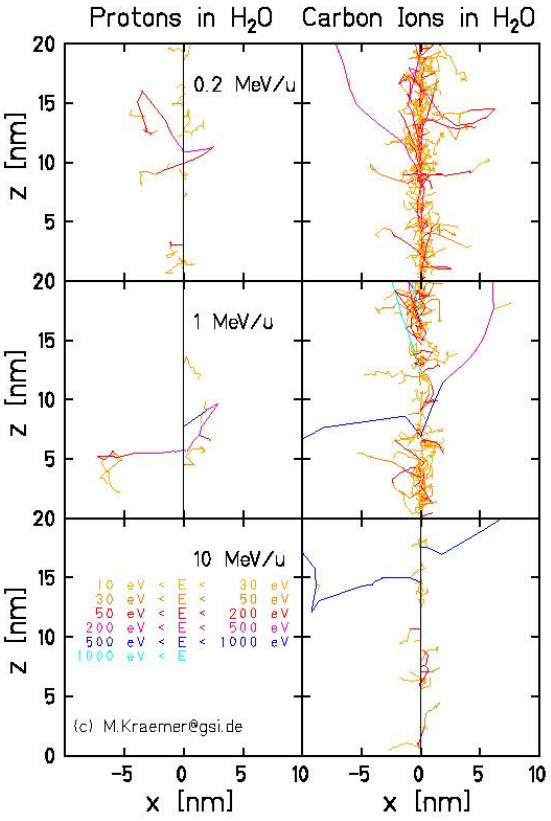
*(Guo et al)*




**Initial electron spectrum??**

## Tracks:

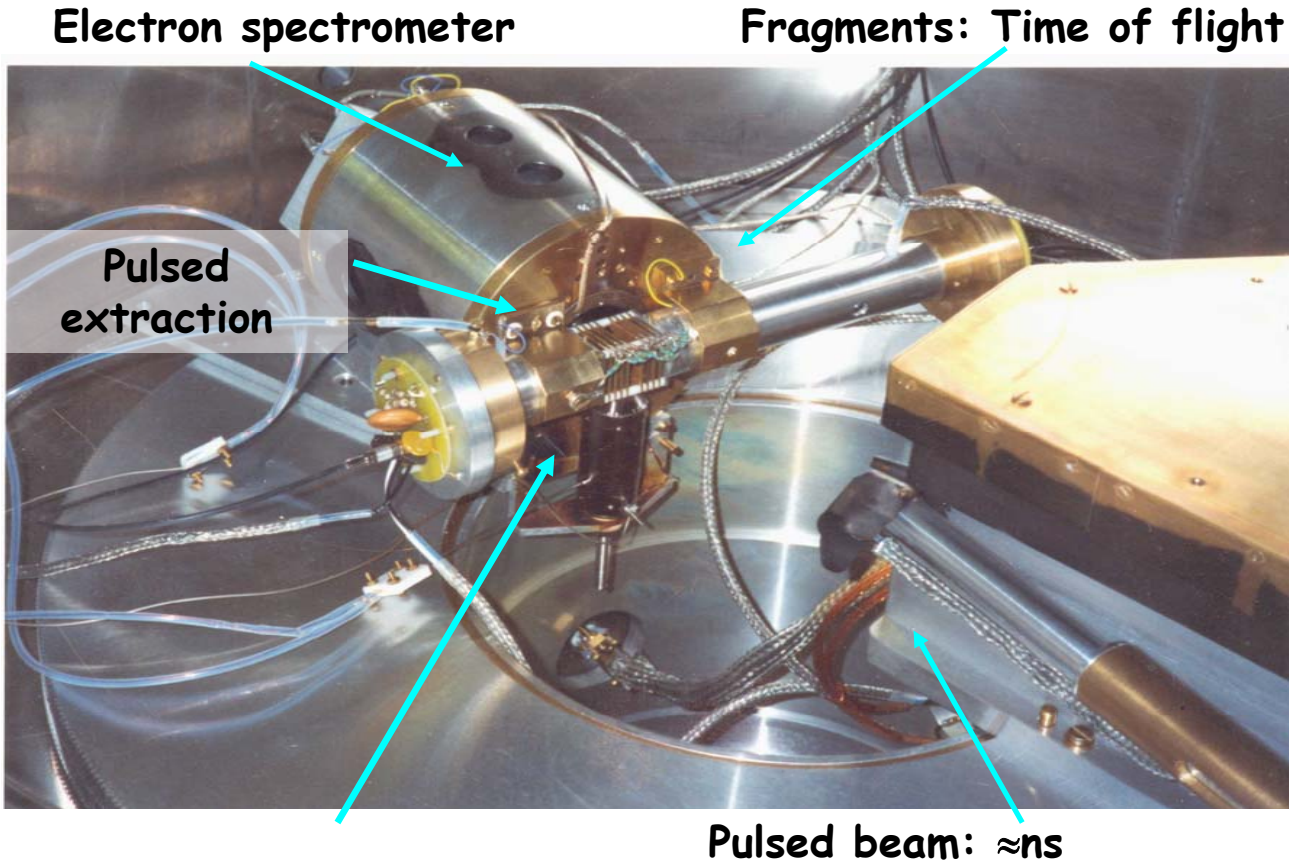
*From GSI*




**Mainly calculations / measurements on water**

**Direct effects: Component of DNA ?**

## Experimental method



Electron emission: Tracks calculations needs **D**ouble **D**ifferential **C**ross **S**ection

Absolute values ?  Difficulty: density of jet !!

IDEA !

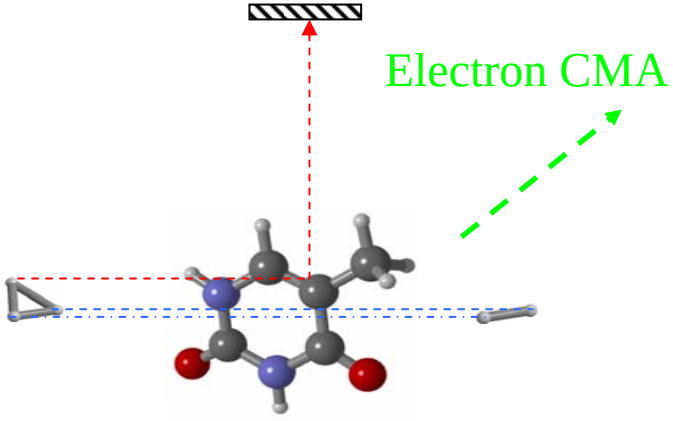
Electron spectroscopy
Given angle and energy (DDCS)

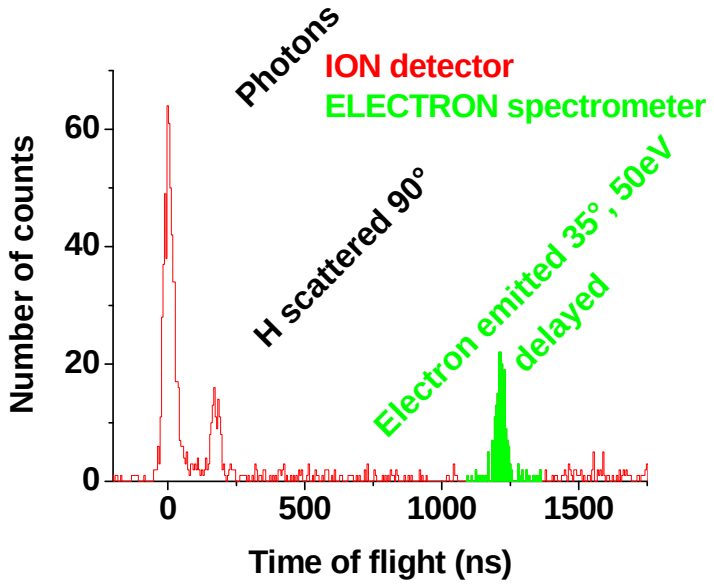
Other 'known' collisionnal process
'Projectile' scattering DCS

*(Meyer et al SPhys Rev.Lett **65** (1990)*

Same experiment

Higher feasibility: molecular beam $H_3^+$_ 25keV≡ 3 $H^+$_ 8.3keV



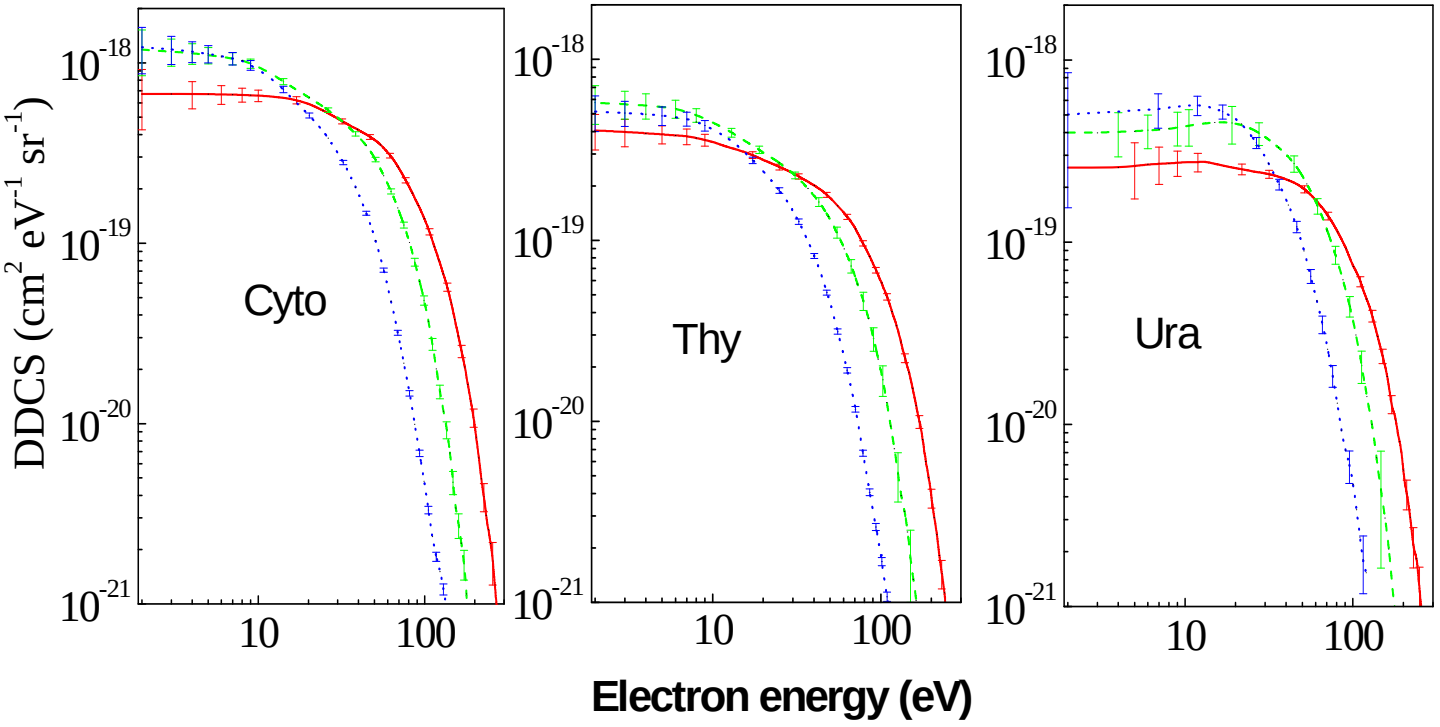

Noise reduction: energy and/or time of flight

Results:

Evaluation of Scattering Cross Section: Use of Moliere, ZBL... potential

Defletion function: low impact parameter b ≈0.01ua << internuclear distances ≈ (2ua)
ATOMIC DESCRIPTION for the scattering process

**Electron spectra**:




☞Low energy electrons

No K shell ionization

# Theoretical description: CTMC Calculations

## Electron: Classical equation of motion

Forces: Proton: $-1/\left|\vec{r}-\vec{R}_p\right|$

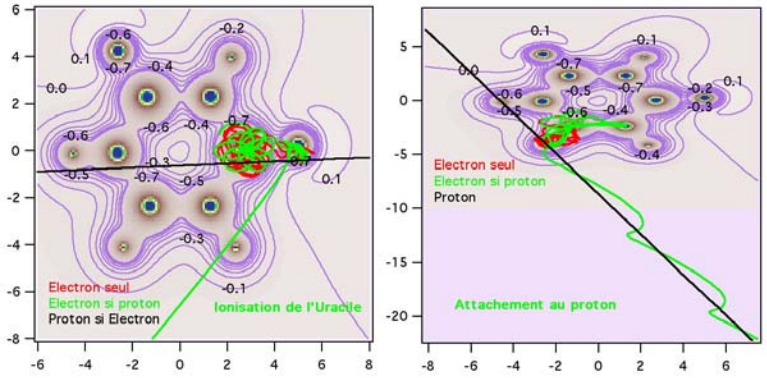
Molecule: $V_e(\vec{r}) = \int \frac{\rho(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|} d^3\vec{r}' - \sum_N \frac{Z_N}{\left|\vec{r}-\vec{R}_N\right|} - \sum_{i=1,n} \Psi_i(\vec{r}) \int \frac{\Psi_i^*(\vec{r}')\Psi_j(\vec{r}')}{\left|\vec{r}-\vec{r}'\right|} d^3\vec{r}'$

MO, MO binding energies, electronic density, electrostatic potential calculated from *ArgusLab* code

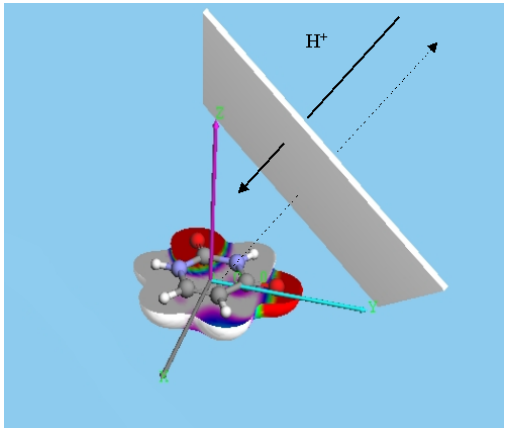
*(Thompson, Planaria Sofware)*

Exchange term is neglected
Potential= electrostatic potential
But bad asymptotic law (SIC)

Example of trajectories (Uracil molecule)




Definition of reference surface for cross section determination

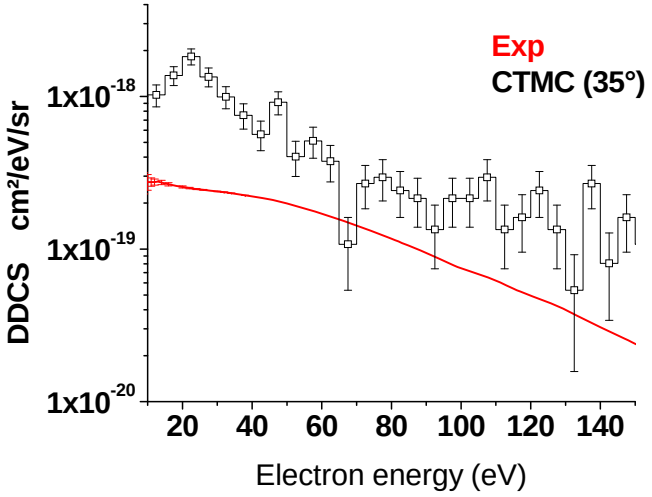


## Results on uracil:

Monoelectronic description !! 42 valence electrons

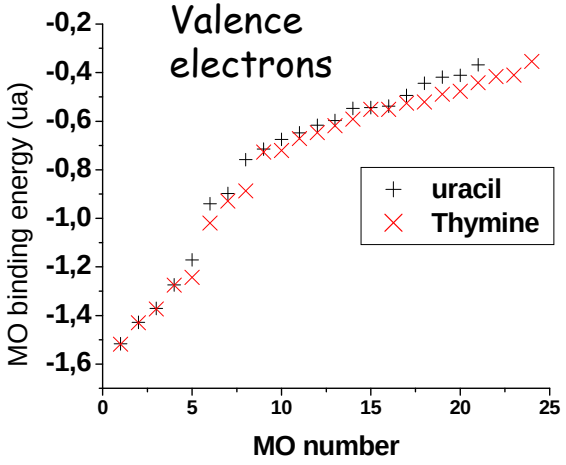
First approximation: all the electrons are equivallent at the lowest binding energy (9.4eV)

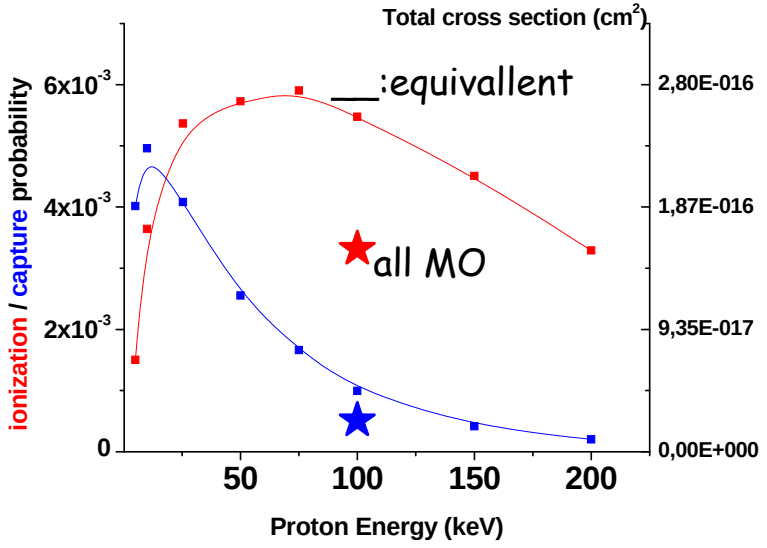
Rather reasonnable agreement: calculation overestimated by (only) a factor 3




**To progress: non equivallent electron**

**☞Binding energy of Molecular Orbitals**




Decreasing of the cross sections

## Conclusion:

☞ Measurment of absolute double differential cross section of electron emission by molecule of biological interest

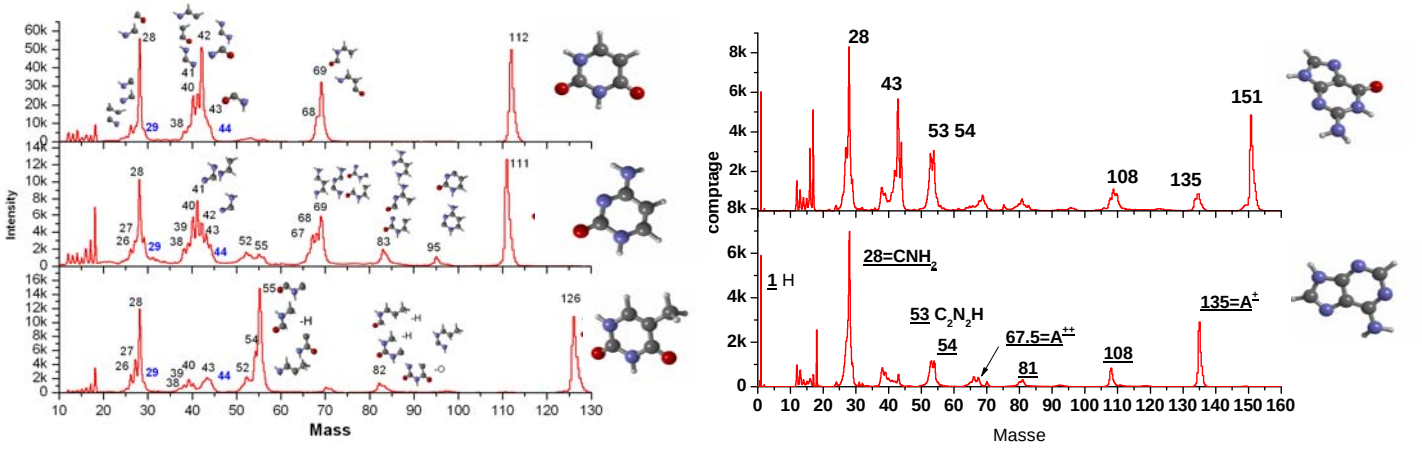
☞ Extension of the experiment: angular distribution

☞ Rather good agreement between CTMC calculation and experiment

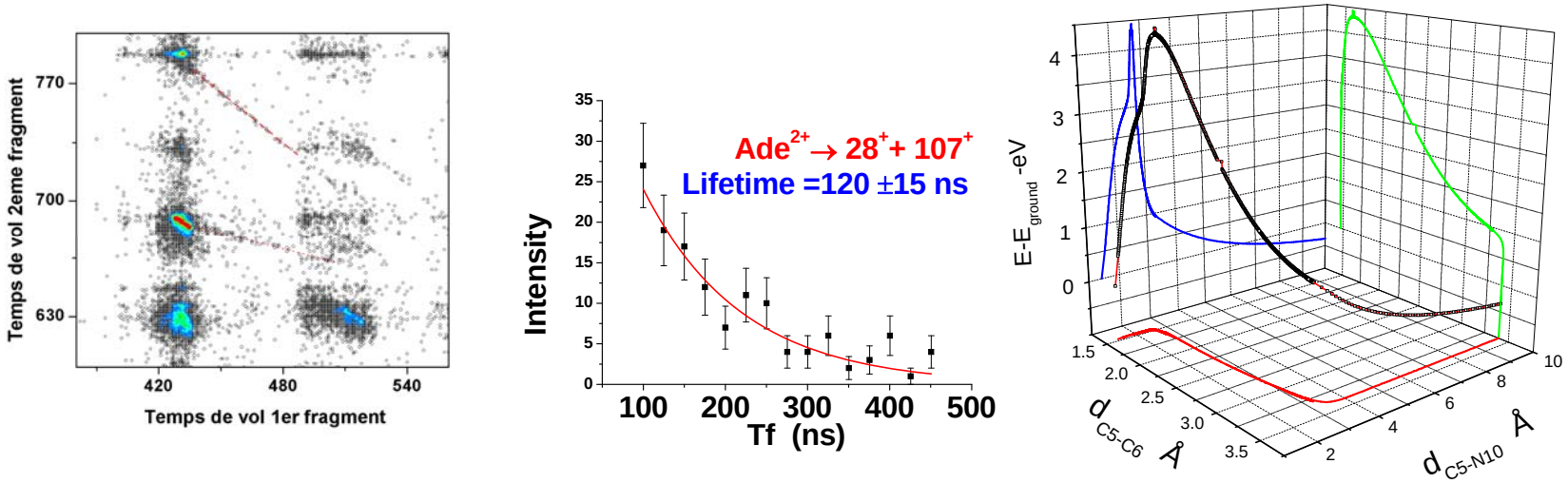
☞ New parametrization of the molecular potential: calculations will be avaiable for all the bases

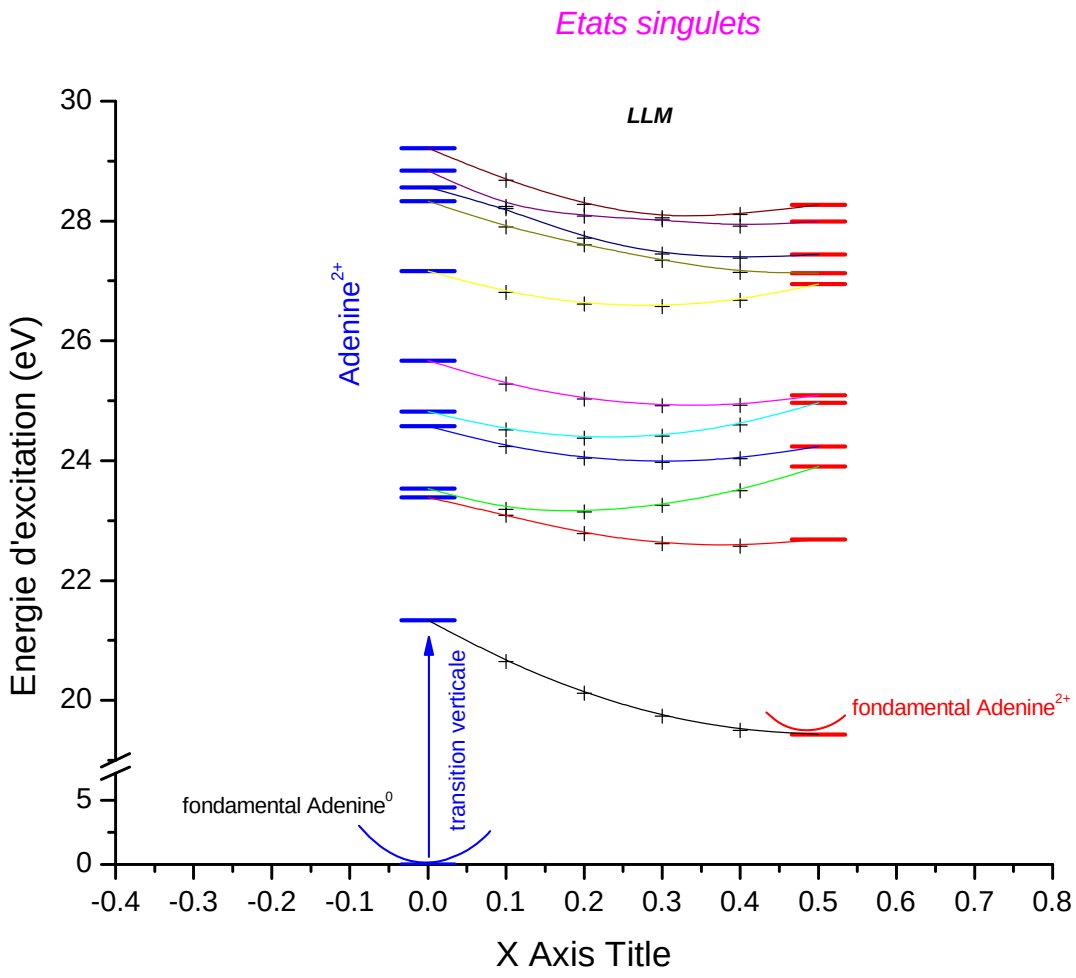
# Ionization of molecule→ fragmentation

## Single ionization




## Double ionization: correlated time of flight spectra, metastability




Etats singulets
LLM
Adenine2+
fondamental Adenine2+
transition verticale
fondamental Adenine0
Energie d'excitation (eV)
X Axis Title
30
28
26
24
22
20
5
0
-0.4
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8