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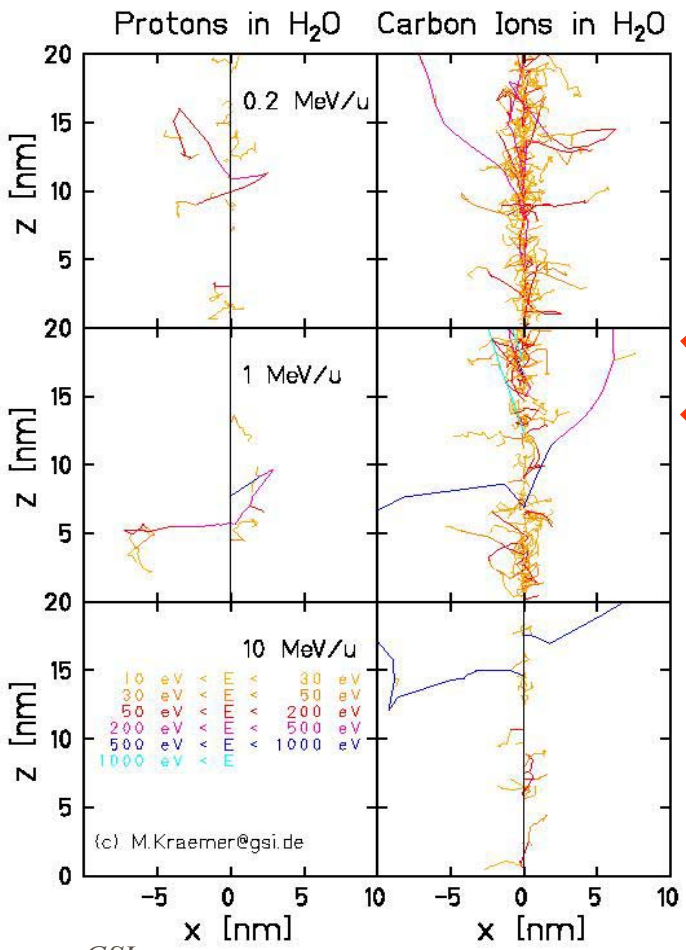
Electron spectroscopy in H^+ to dry DNA, RNA collisions in the 25 – 100 keV energy range

By A Le Padellec, P Moretto-Capelle

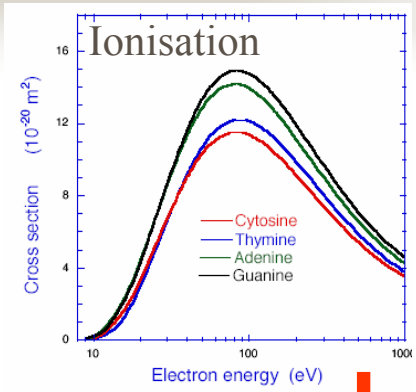
St Malo 15-16 May 06

Ion-matter interaction



Source : GSI

E > 20eV



Huo et al
Space Radiation Research *2004*

ON DNA :

- **Energy spectrum of the secondary electrons ?**
- **Differential cross sections ?**

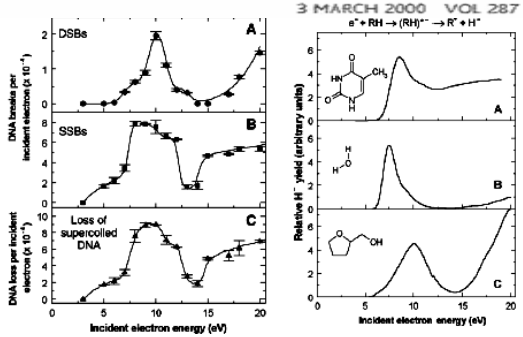
E < 20eV

Resonant Formation of DNA Strand Breaks by Low-Energy (3 to 20 eV) Electrons

Badia Boudaïffa, Pierre Cloutier, Darel Hunting, Michael A. Huels,* Léon Sanche

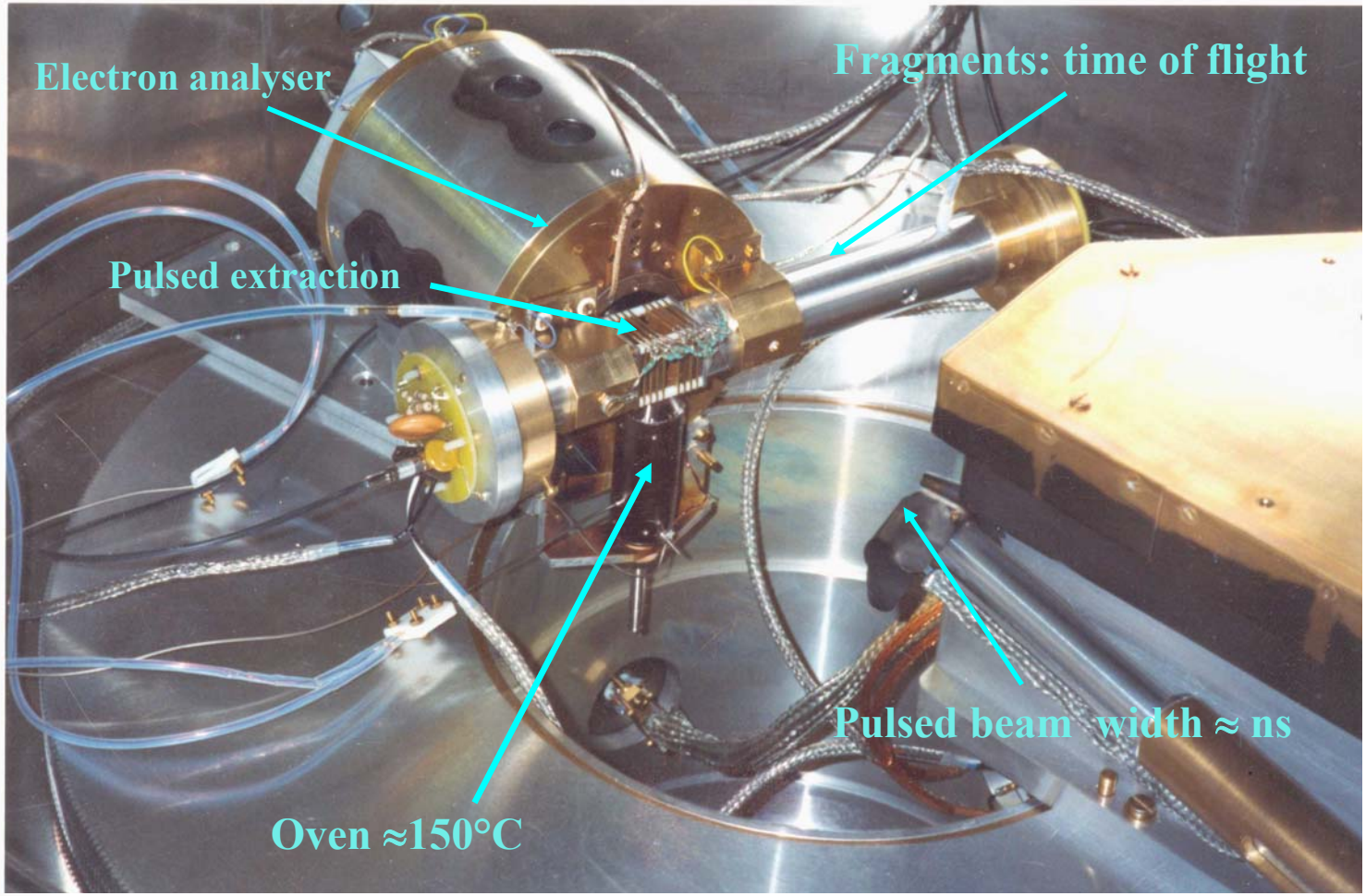
Most of the energy deposited in cells by ionizing radiation is channeled into the production of abundant free secondary electrons with ballistic energies between 1 and 20 electron volts. Here it is shown that reactions of such electrons, even at energies well below ionization thresholds, induce substantial yields of single- and double-strand breaks in DNA, which are caused by rapid decays of transient molecular resonances localized on the DNA's basic components. This finding presents a fundamental challenge to the traditional notion that genotoxic damage by secondary electrons can only occur at energies above the onset of ionization, or upon solvation when they become a slowly reacting chemical species.

1658 3 MARCH 2000 VOL 287 SCIENCE



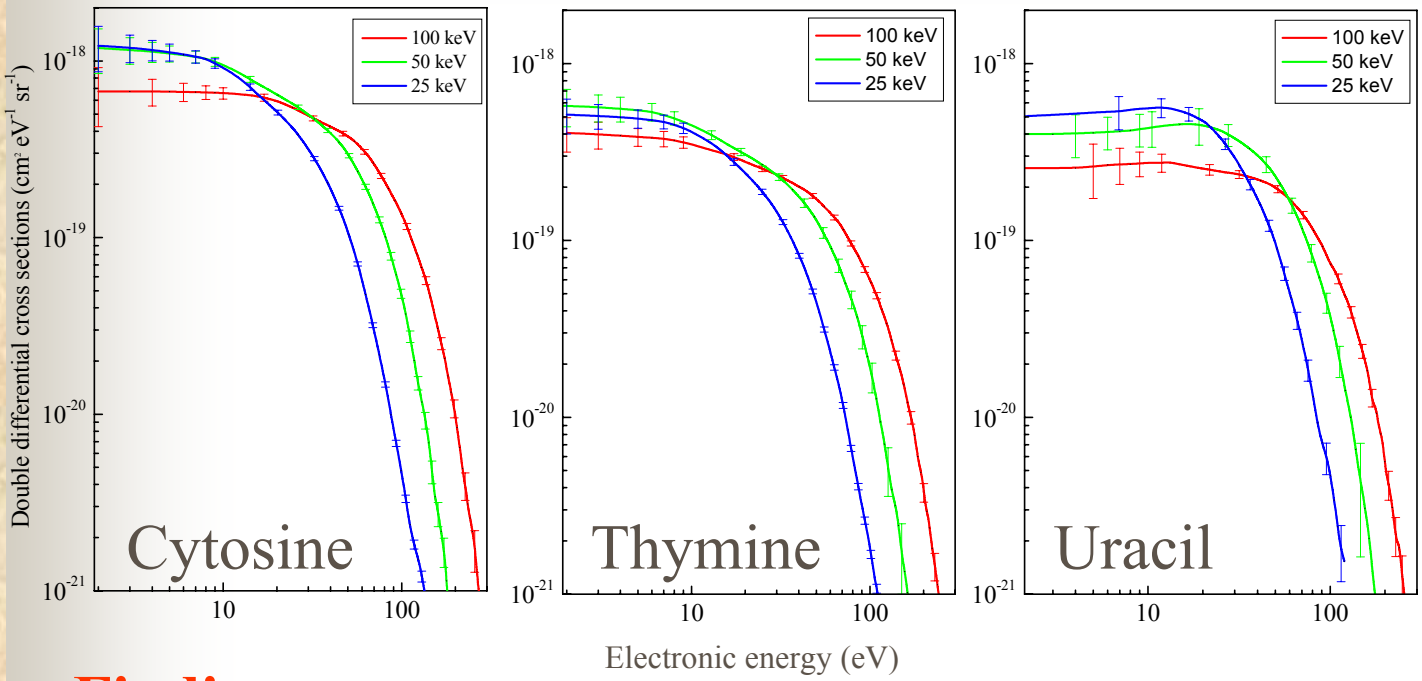
Trace computation ?

Experimental setup



Multicorrelation analysis event by event

RESULTS : double differential cross sections in an absolute scale



Léon Sanche happy !

Findings :

- No low energy peak but instead constant DDCS of sizeable amplitude (no centrifugal barrier as found for C_{60} with its central potential),
- No proton energy dependence,
- At higher energy, exponential decay according to the Bethe-Born formalism – dominance of the dipolar interaction term,
- No line originating from the Auger KLL electrons.

Computation of the electron spectrum H^+ + Uracil at 100keV

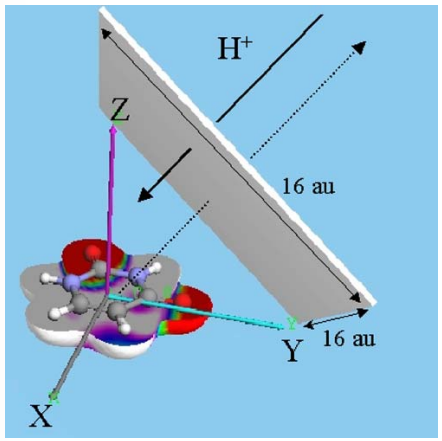
Use of the Classical Trajectory Monte Carlo method

Potentials → **Proton**

Potentials → **Uracil (evaluated from *ArgusLab software*)**

INGREDIENTS :

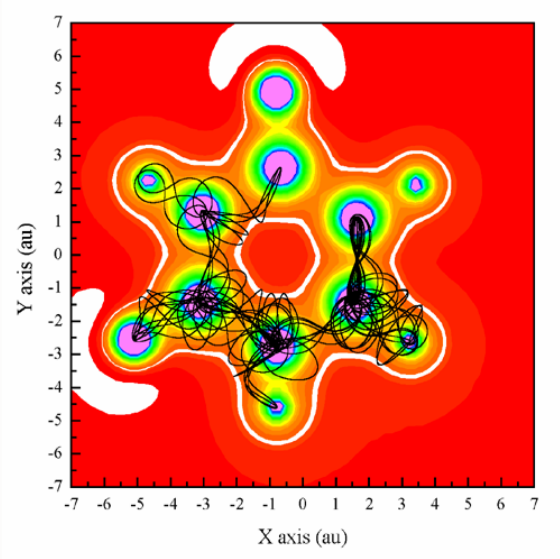
- **Constraint on the binding energy of the ionised electron,**
- **No constraint on the angular momenta,**
- **Fixed molecule and proton in a random direction**



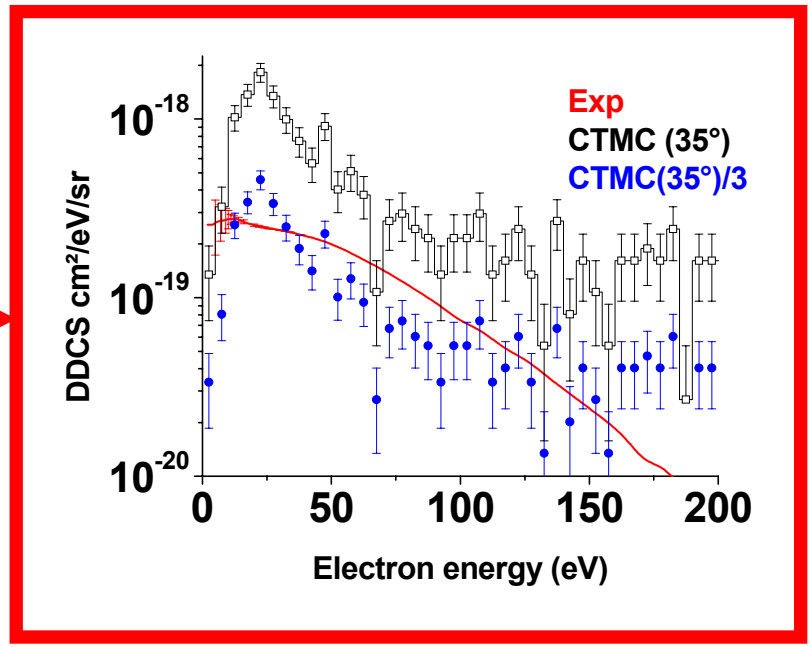
$$\sigma_{(E,\theta)} = \frac{N_v N_{e(E\pm\Delta E/2,\theta\pm\Delta\theta/2)}}{N_{shot}} \frac{S_{ref}}{2\pi \sin\theta \Delta\theta \Delta E}$$

- N_v : number of valence electrons (electrons supposed equivalent),
- $N_{e(E\pm\Delta E/2,\theta\pm\Delta\theta/2)}$: trajectories that led to the emission of an electron $E \pm \Delta E / 2$, $\Theta \pm \Delta\Theta / 2$,
- Θ : emission angle of the electron with respect to the proton beam direction,
- N_{shot} : total number of trajectories

PRELIMINARY RESULTS:

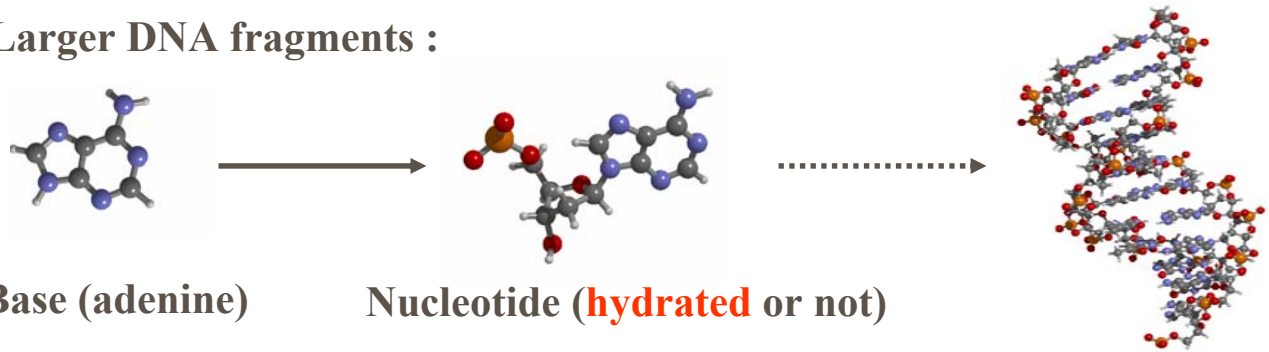


Acceptable and encouraging !



PERSPECTIVES

- **Angular** distribution for the electrons, electron /fragment correlations
- **Solvated** molecules (collaboration with M et B. Farizon IPN, Lyon)
- Larger DNA fragments :



Base (adenine) Nucleotide (**hydrated** or not)

- Radiosensitive molecules (5FU)