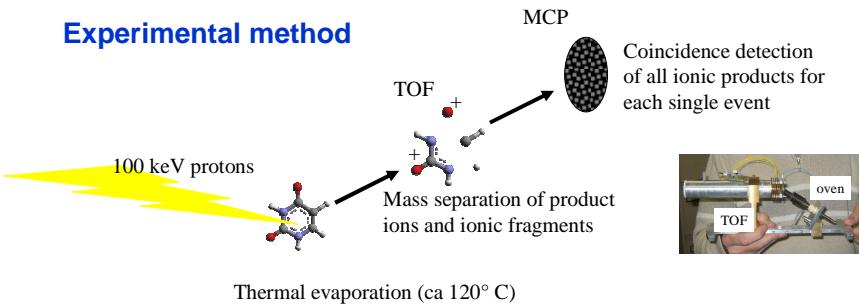


# Ionisation and fragmentation of radiosensitizing molecules upon 100 keV protons collisions: evidence for keto → enol tautomerism for Uracil and halogenated derivatives.

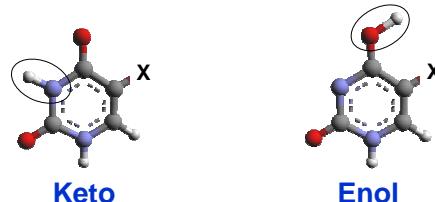
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## Experimental method



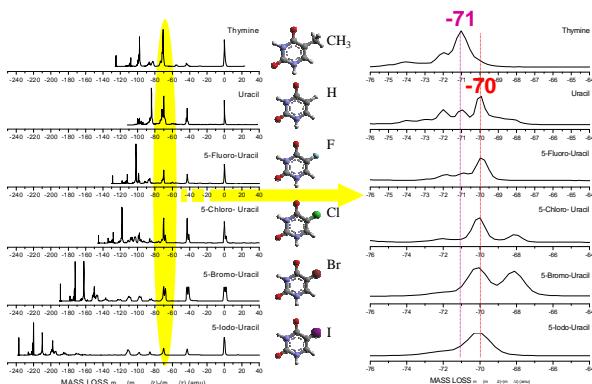
## Keto → Enol tautomerism

Initially, all molecules are in their keto form.  
The enol form is quasi-degenerate but is separated from the keto by a barrier of about 2 eV.

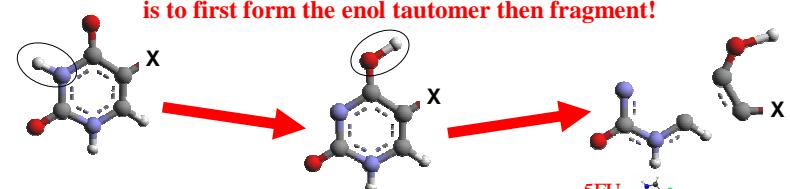


Molecules under investigation  
Thymine: X = CH<sub>3</sub>  
Uracil: X = H  
5-X-Uracil: X = F, Cl, Br, I

## Single ionisation

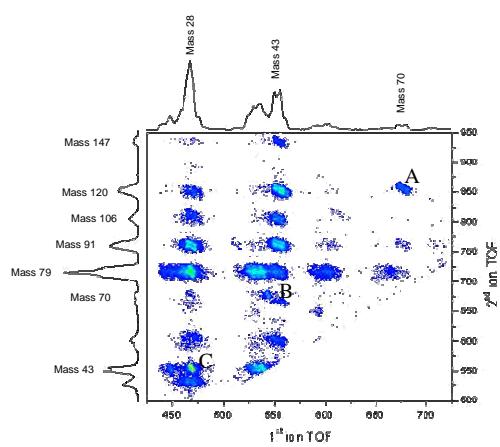


The only way to lose a fragment of mass 70 is to first form the enol tautomer then fragment!



Calculations are underway to establish the reaction path and the associated energetics.

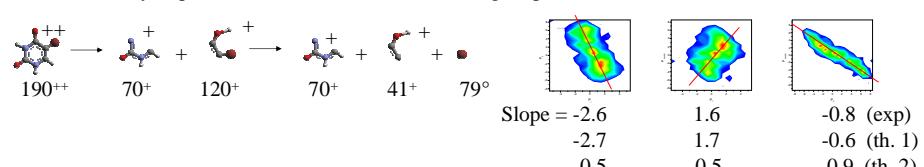
## Double ionisation : the example of 5 – Bromo - Uracil



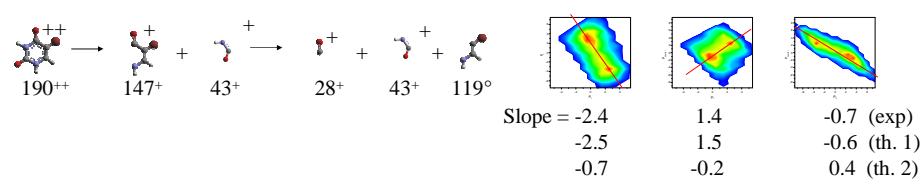
Channel A : two body dissociation with charge separation



Channel B : three body sequential dissociation with initial charge separation



Channel C : three body sequential dissociation with initial charge separation



3 body sequential dissociation: 2 possible sequences  
1- ABC<sup>++</sup> → AC<sup>+</sup> + B<sup>+</sup> → A<sup>+</sup> + B<sup>+</sup> + C<sup>+</sup>  
 $P_B = (-m_B/m_{AC}) P_A$ ;  $P_C = (m_C/m_{AC}) P_A$

2- ABC<sup>++</sup> → A<sup>+</sup> + BC<sup>+</sup> → A<sup>+</sup> + B<sup>+</sup> + C<sup>+</sup>  
 $P_B = (-m_B/m_{BC}) P_A$ ;  $P_C = (m_C/m_B) P_A$