Computer Modeling Of Radiation Biophysics using the Geant4

M. Batmunkh, L. Bayarchimeg

Sector of Mathematical Modeling of Radiation-Induced Effects

Laboratory of Radiation Biology, Joint Institute for Nuclear Research

Group names

1- Shimaa Husien
2- Togtokhtur Tudevdorj
3- Brynkevich Hanna
4- Blagodarova Yana
5- El Moataz Bellah Ahmed
6- Fatma Mohamed Fouad
7- Sommya Mostafa Mousa
8- Ahmed Samir Mohamed

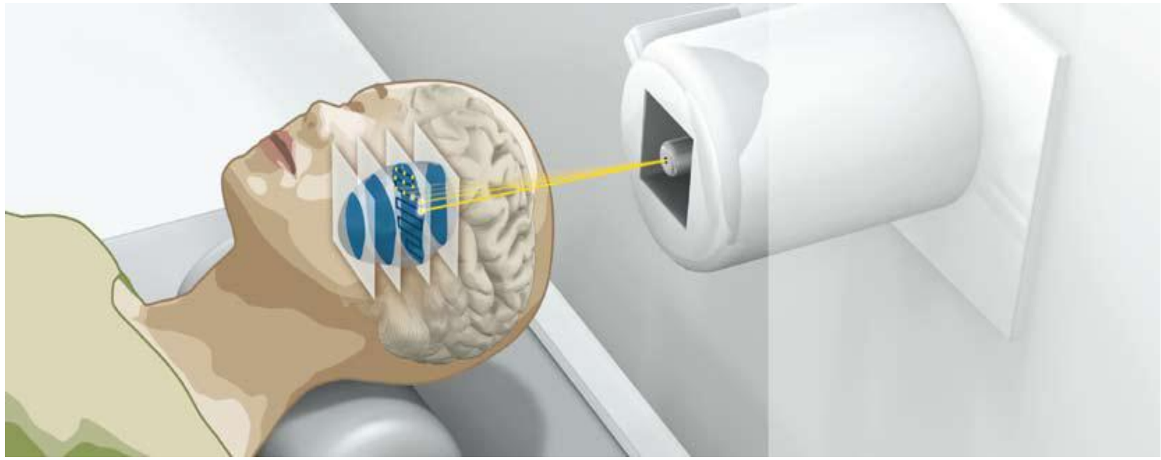
Contents

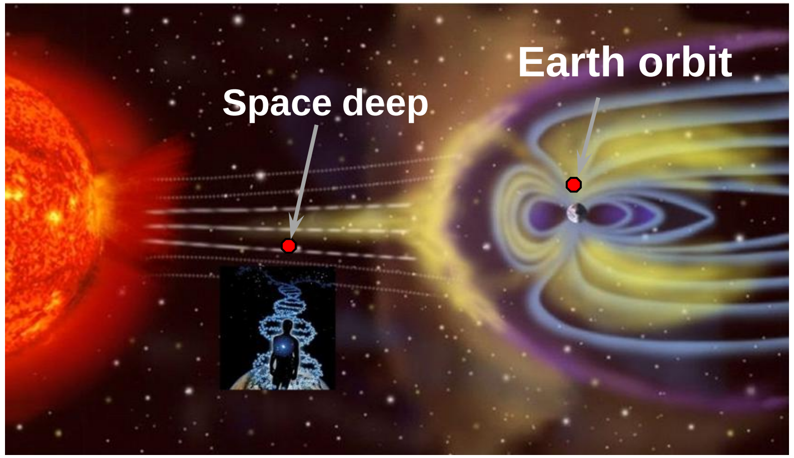
Introduction

- ***Radiation biophysics*** is studying the effect of ionizing radiation upon biomolecules to living organisms (DNA, chromosomes, cells).
- The most sensitive target to radiation is the DNA molecule.
- **Monte Carlo-based computer simulation system “Geant4”** has been used to better understand and predict damage done by charged particles like electrons and protons

Motivation

The prediction of biological effects of ionizing radiation is very useful in the treatment of **cancer cells** and as well as for **radiation protection**, especially for **astronauts in space travel.**





Simulation Method

The Geant4 is a general particle-matter Monte Carlo simulation toolkit, which includes the Gent4-DNA models for microdosimetry simulations of stochastic nature of particle track structure in small targets.

GEANT4 A SIMULATION TOOLKIT GEANT4-DNA A SIMULATION TOOLKIT

Monte Carlo virtual-experiment applications of radiation biophysics developed in the Geant4 toolkit is used in this practice.

Particle energy and physical interaction of particles with biological media:

Particle	**Kinetic energy (keV)**	**Physical processes in liquid water**
Electron	0.1, 0.3, 1, 2, 5, 10, 20, 100, 300.	Elastic scattering, ionization Electronic excitation, Dissociative electron attachment.
Proton	10, 20, 100, 300, 1000, 5000.	Ionization, electronic excitation, charge decrease, Elastic scattering.

Simulation of radiation transport in matter Microdosimetry

By:- Fatma Mohamed Fouad

Biotechnology Department , Cairo university, Egypt.

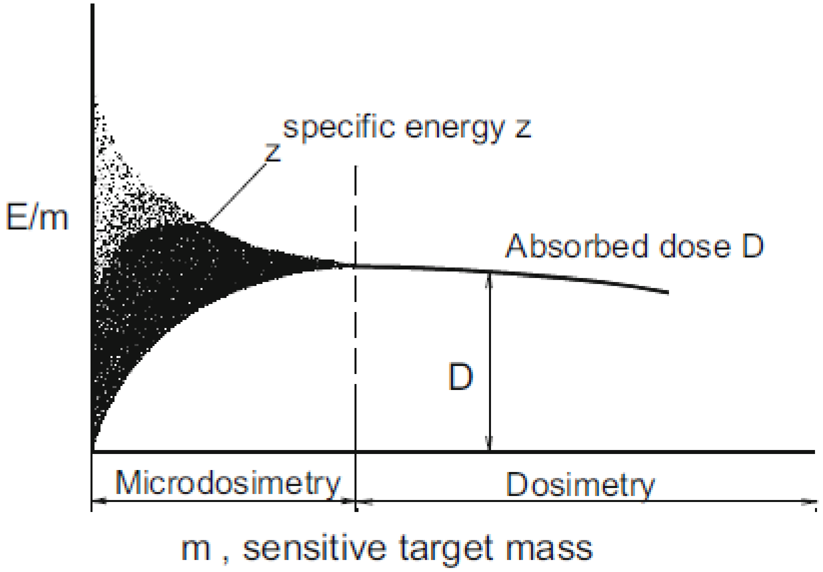
El Moataz Bellah Ahmed

Master student in Applied Radiation Physics,

Helwan University& Children’s Cancer Hospital Egypt.

Microdosimetry

- Microdosimetry is the theoretical and experimental investigation of imparted-energy probability distributions in a “microscopic” volume of matter that is crossed by a single ionization particle.
- Microdosimetry is not a “small” dosimetry or a “microscopic” dosimetry.



Representation of the variation of the specific energy z depending on the mass m sensitive site.

Lineal Energy

- The Idea of Microdosimetry: to Measure the **Lineal Energy** as a Substitute of LET.
- It is the quotient of the energy imparted to the volume, by a single particle or radioactive decay inside it, and the volume mean chord.

$$y = \frac{\varepsilon}{\bar{d}}$$

- y is used to be expressed in **keV/µm**, similarly to LET, where the linear dimension is that one of the tissue-equivalent site size.
- YD:- Dose-mean Lineal Energy (keV/µm)

$$\bar{y}_D = \int y d(y) \mathrm{d}y = \frac{\int y^2 f(y) \mathrm{d}y}{\int y f(y) \mathrm{d}y}$$

- where f(y) and d(y) represent the frequency and dose distributions of lineal energy, respectively.

Specific energy

A **specific energy**, It is the quotient of the energy imparted to the volume, by one particle or a radioactive decay inside it, and the volume mass.

$$z = \frac{\varepsilon}{m}$$

ZD:- Dose mean specific Energy (J/Kg) Gray.

$$\hat{Z}D = \int Zd(Z)\ dZ = \frac{\int Z^2 f(Z)dZ}{\int Zf(Z)dZ}$$

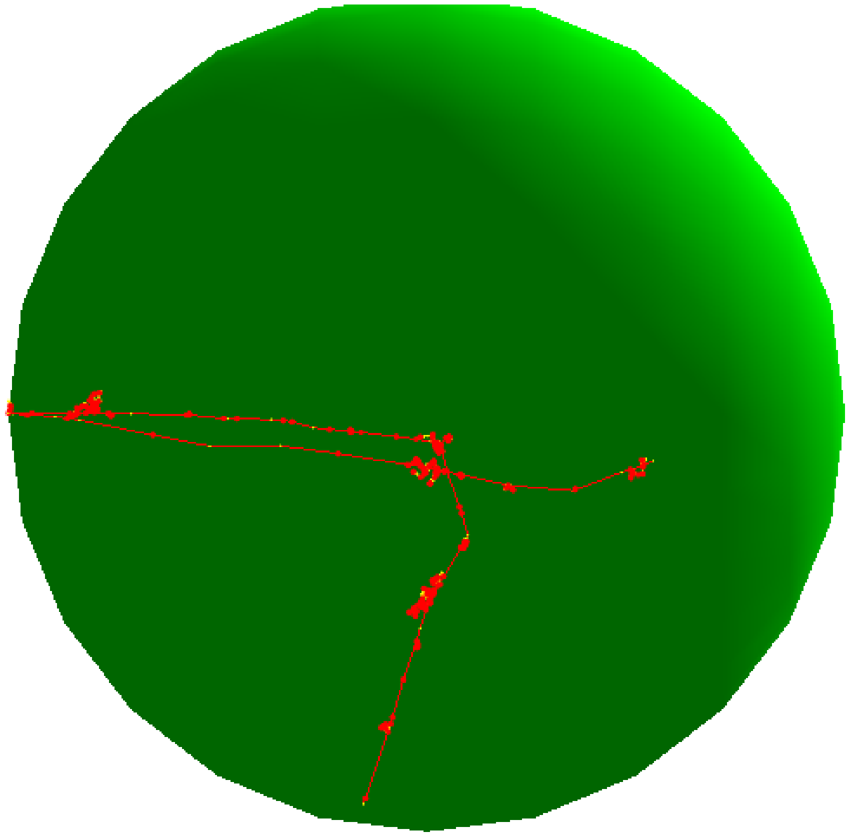
The physical dimension is J/Kg but, similarly to **absorbed dose**, z is used to be expressed in Gray, where the mass m is that one of the site, differently than absorbed dose, z is a stochastic variable.

Aim of this virtual experiment

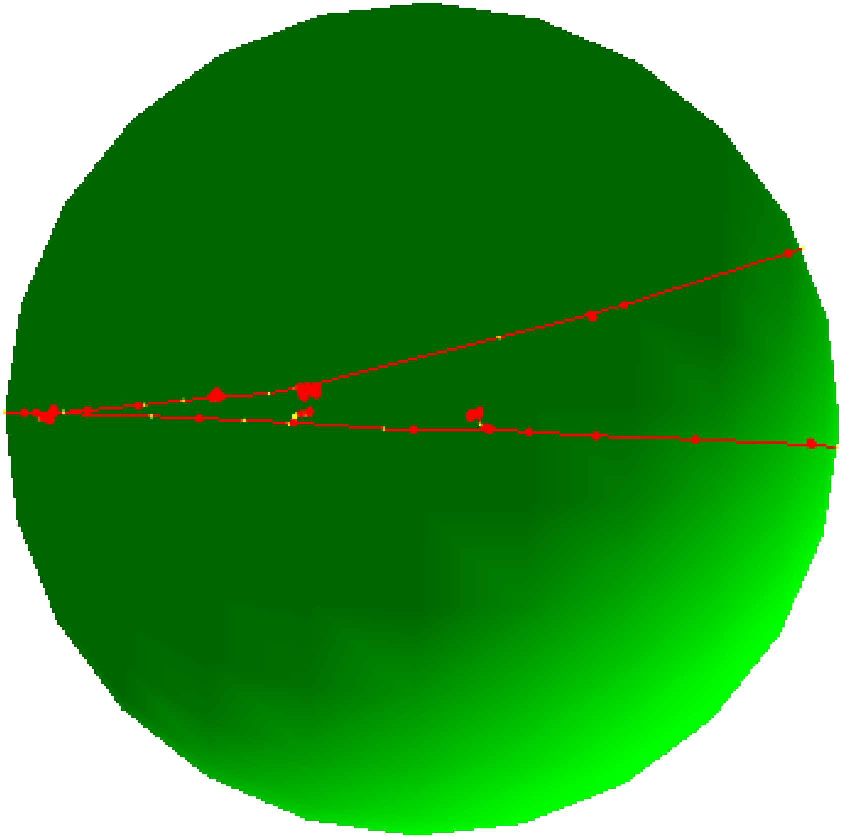
(1) To simulate stochastic nature of particle track structure in small targets (Nano – and Micrometer)

(2) To calculate microdosimetric quantities (yD, zD) in different biological targets following different types of radiation.

Simulation of electron’s track structures in water volume with the diameter of 300 nm



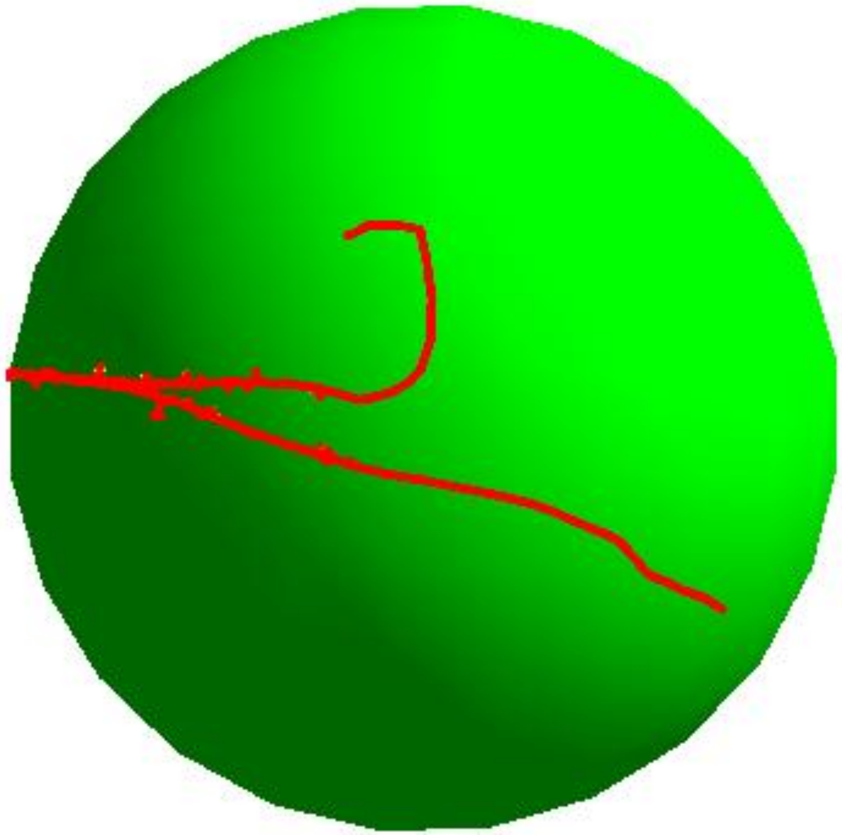
- track structure for **5 keV electron** by 2 particles.



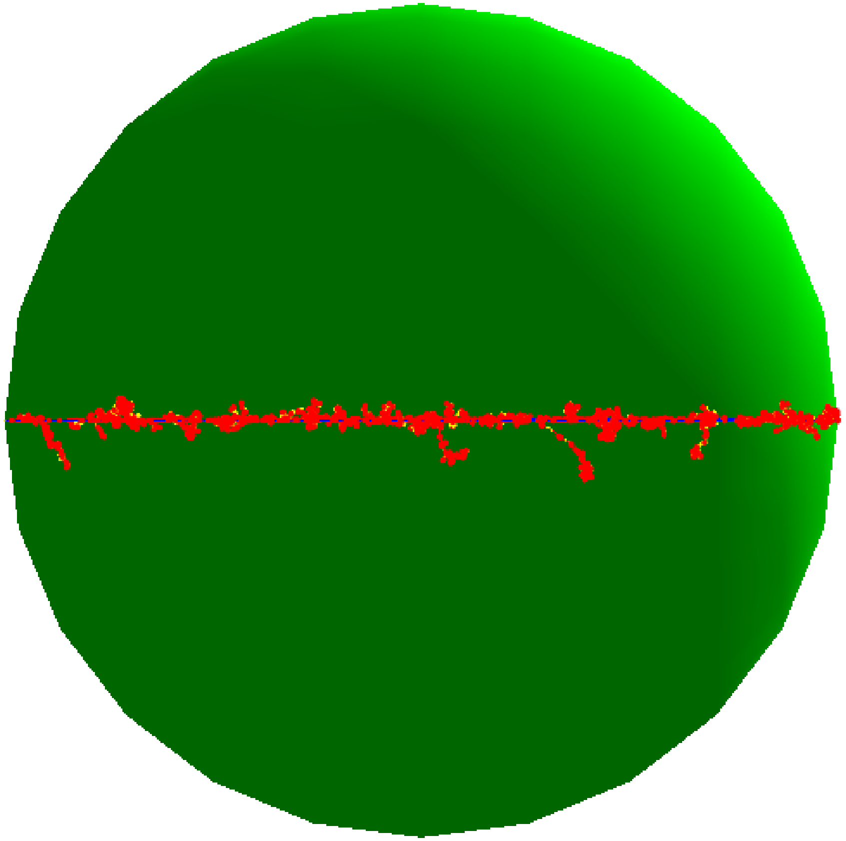
- track structure for **10 keV electron** by 2 particles.

Simulation of proton's track structures in water volume with the diameter of 300 nm

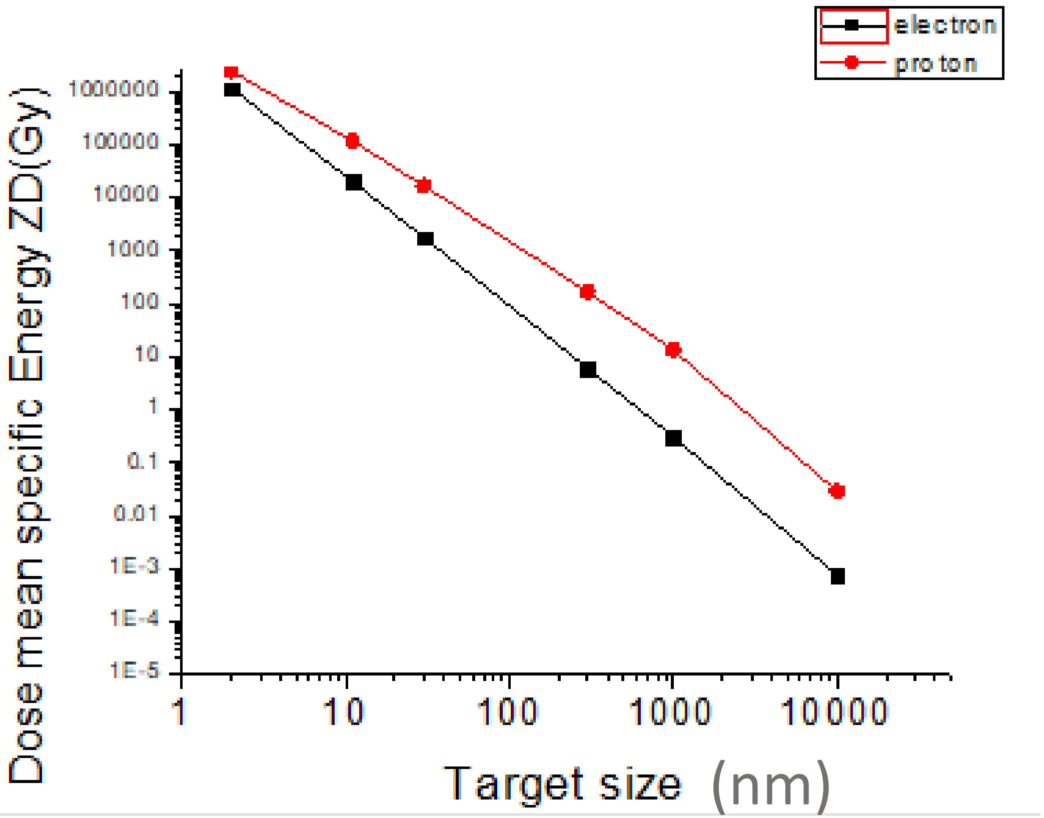
track structure for **10 keV proton** by 2 particles.



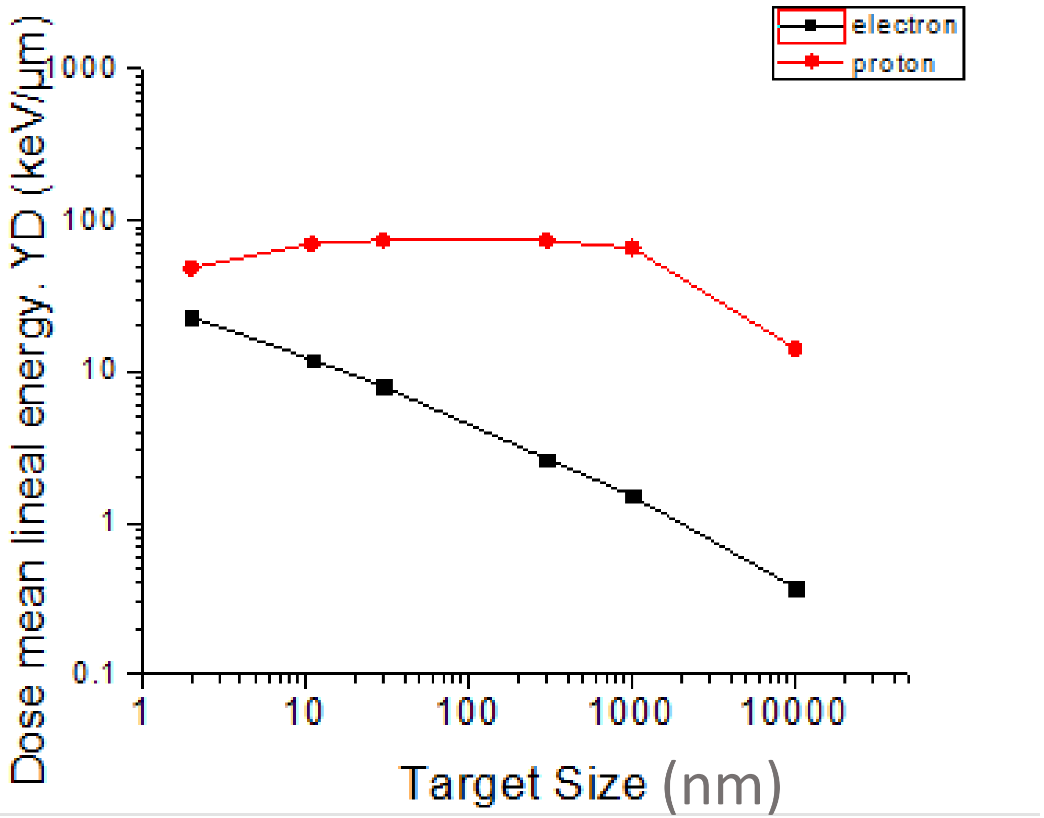
track structure for **5000 keV proton** by 2 particles.



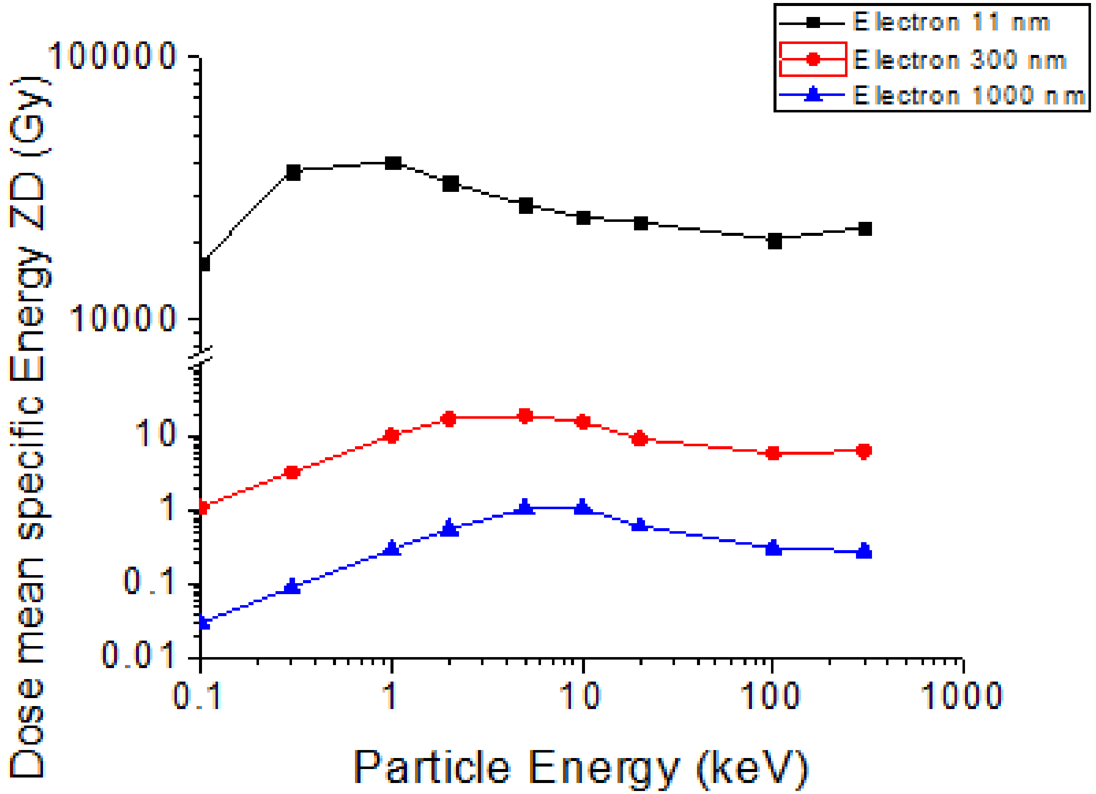
A relationship between Target size and Dose mean specific Energy (ZD) for electron and proton at 100 keV.

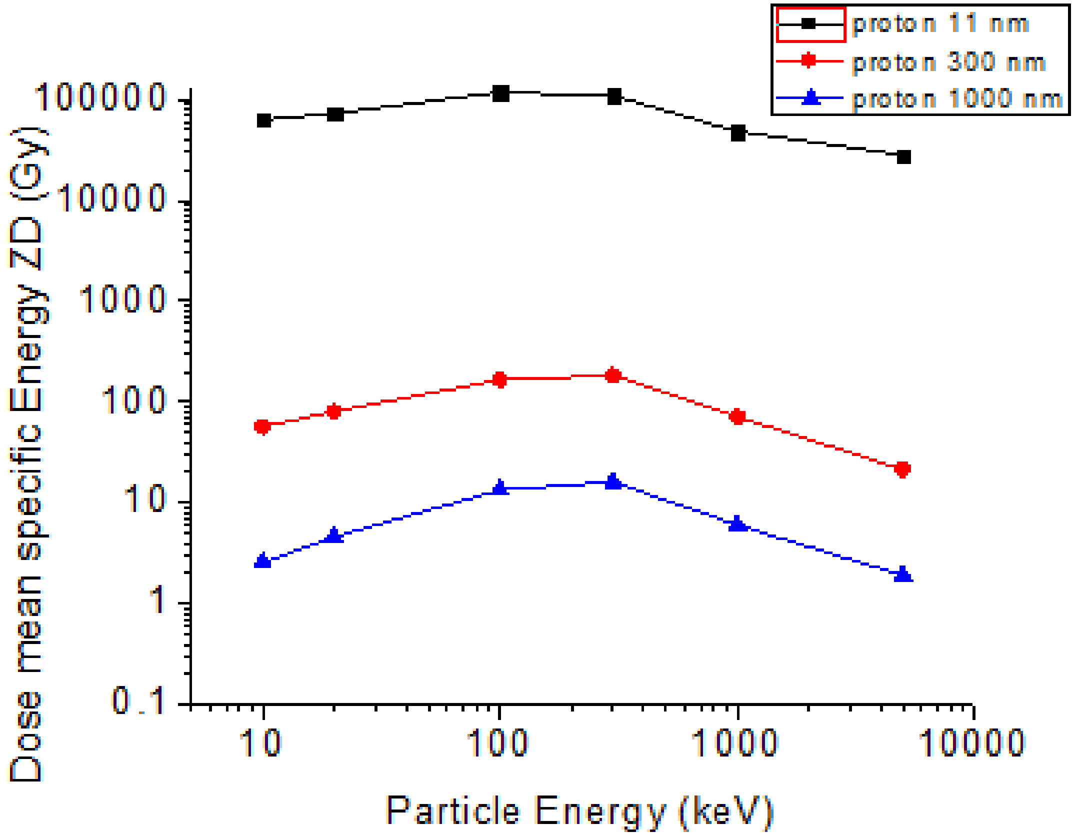


A relationship between Target size and Dose mean Lineal Energy (YD) for electron and proton at 100 keV.

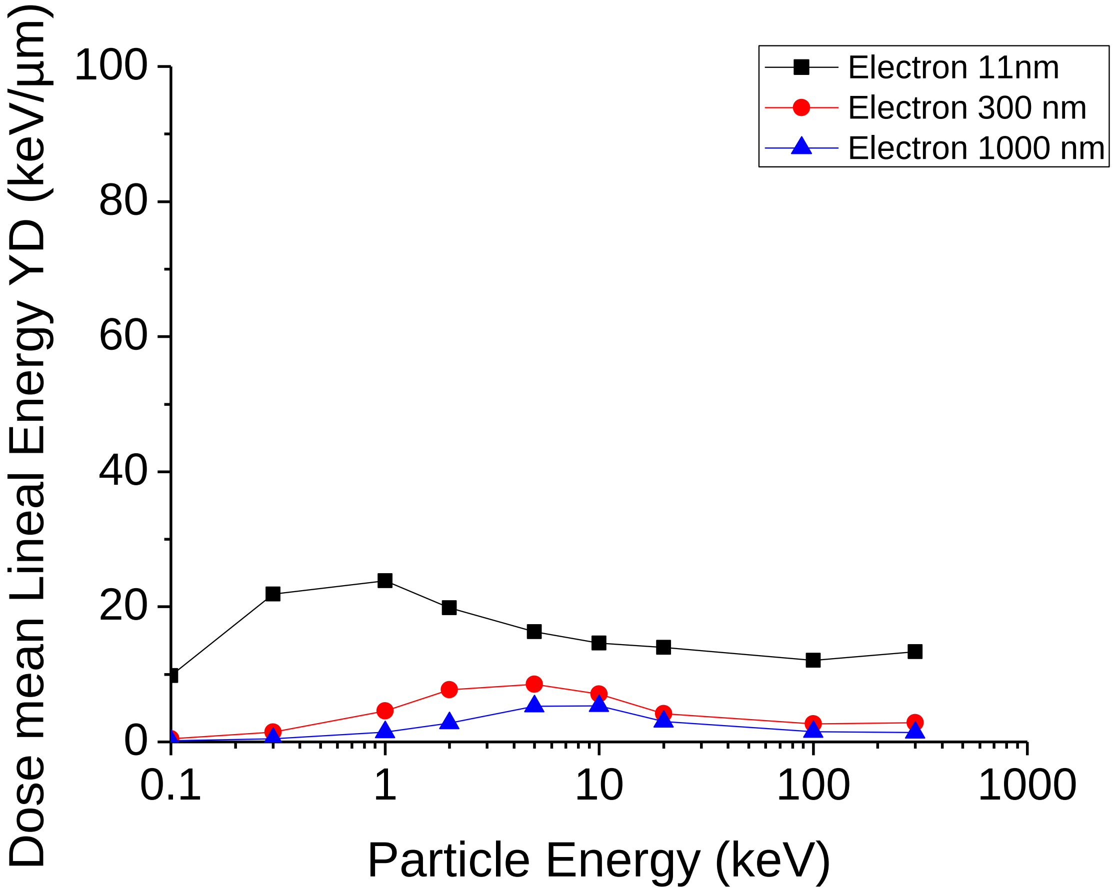


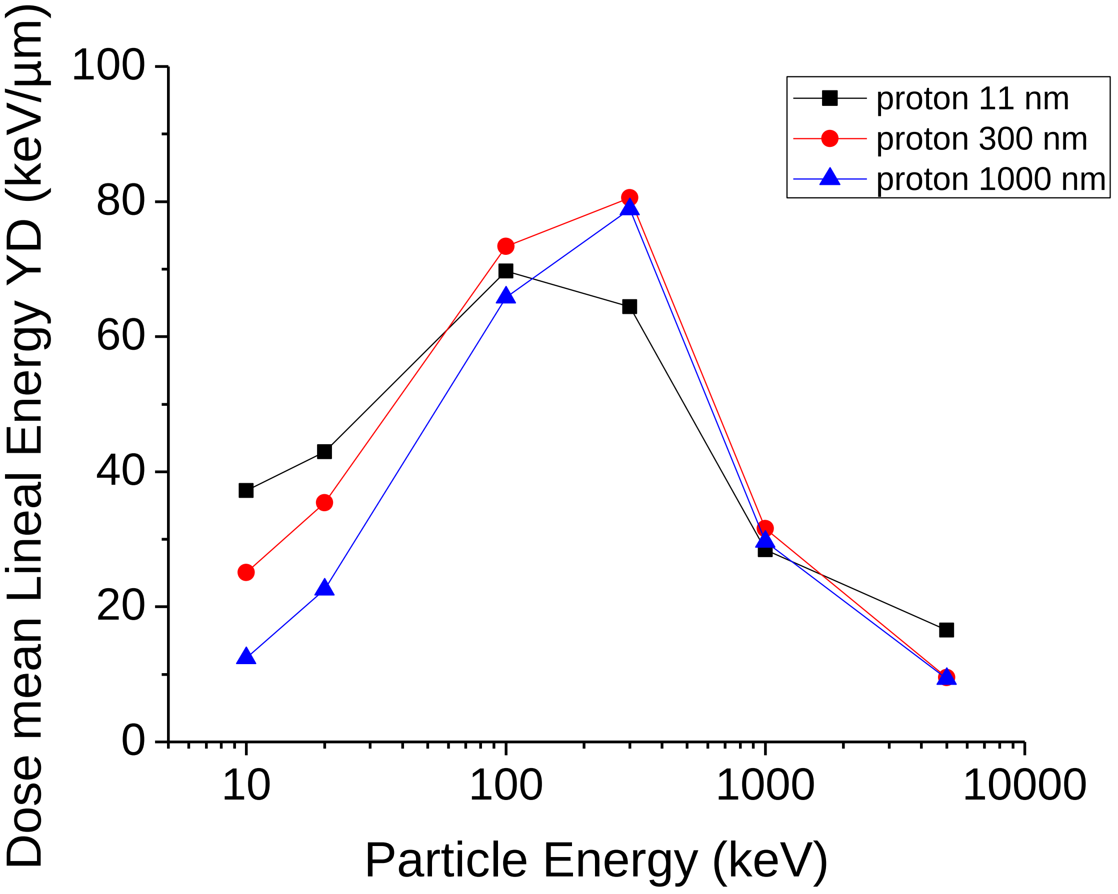
Dose mean specific energy (ZD) for electrons and protons with particle energies from 0.1 keV to 5000 keV in targets with diameters of 11 nm, 300 nm and 1000 nm.



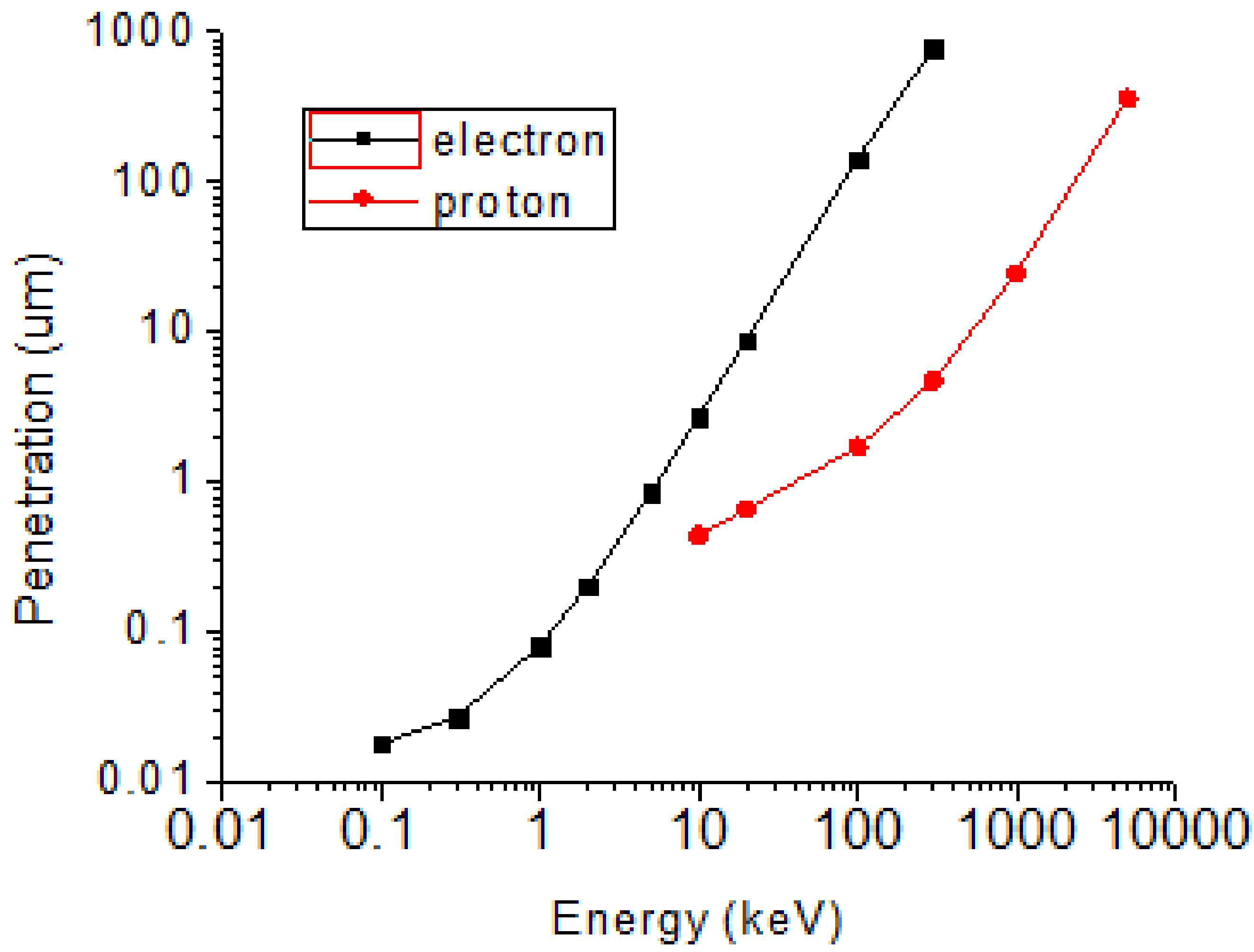


Particle energy with Dose –mean lineal energy YD for electrons & protons





Relationship between depth penetration & particle kinetic energy



This curve shows a relationship between the energy of the particles (electrons and protons) with the penetration depth (um)

Conclusion

1) Electrons and protons track structures have been obtained in water volume with 300 nm diameter.
2) The microdosimetric quantities yD, zD have been calculated against the target sizes at 100 keV electron and proton.
3) The dose-mean specific energy for electrons is less that the dose-mean specific energy for protons.
4) The dose-mean lineal energy for protons is about 3 times more than electrons.
5) yD and zD quantities are very sensitive for target size and particle energy.
6) For the same particle energy against the penetration depth , electrons can penetrate more depth that proton.

Simulation of particle track at chemical stage “Chemistry”

Togtokhtur Tudevdorj

Bachelor Student “Department of Physics, National University of Mongolia, Mongolia”

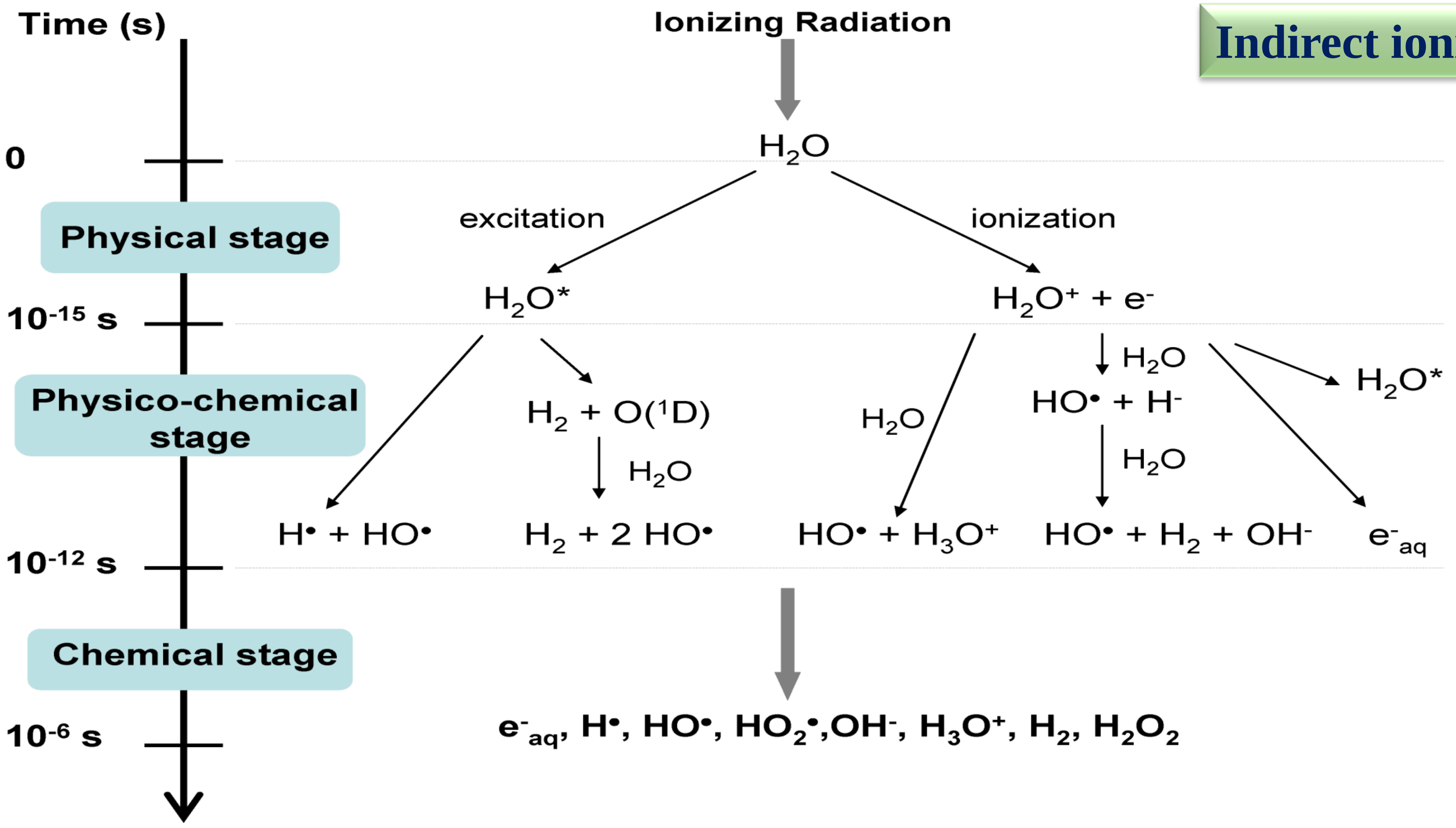
Shimaa Husien

Master Student “Environmental Science and industerial development”,

Faculty of Post graduate of advanced studies, Beni suef University, Egypt.

Scenario of radiation chemistry in liquid water

Indirect ionization

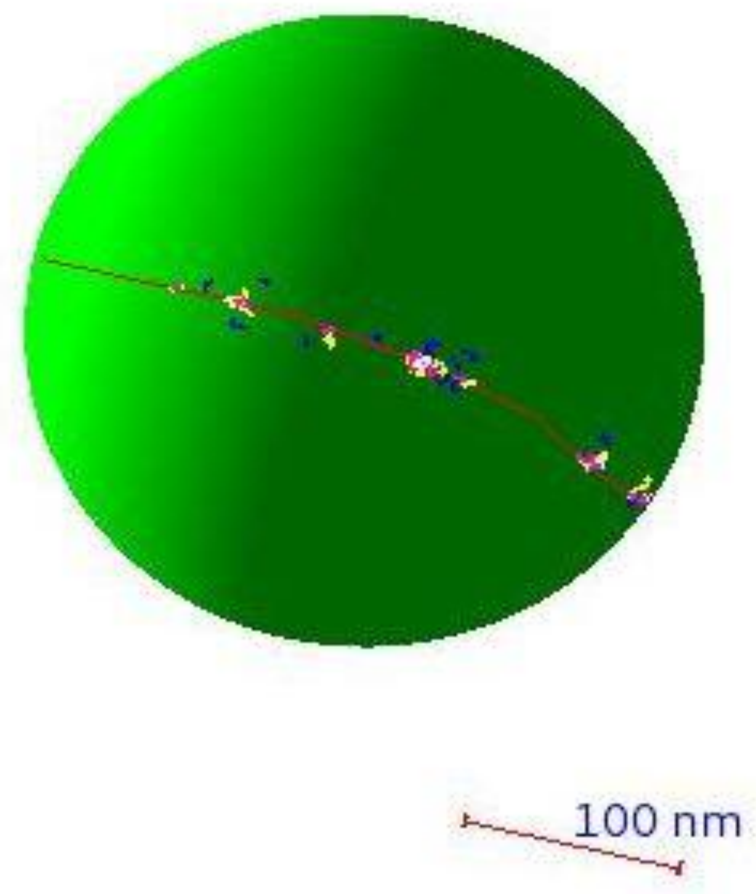


Aim of this work

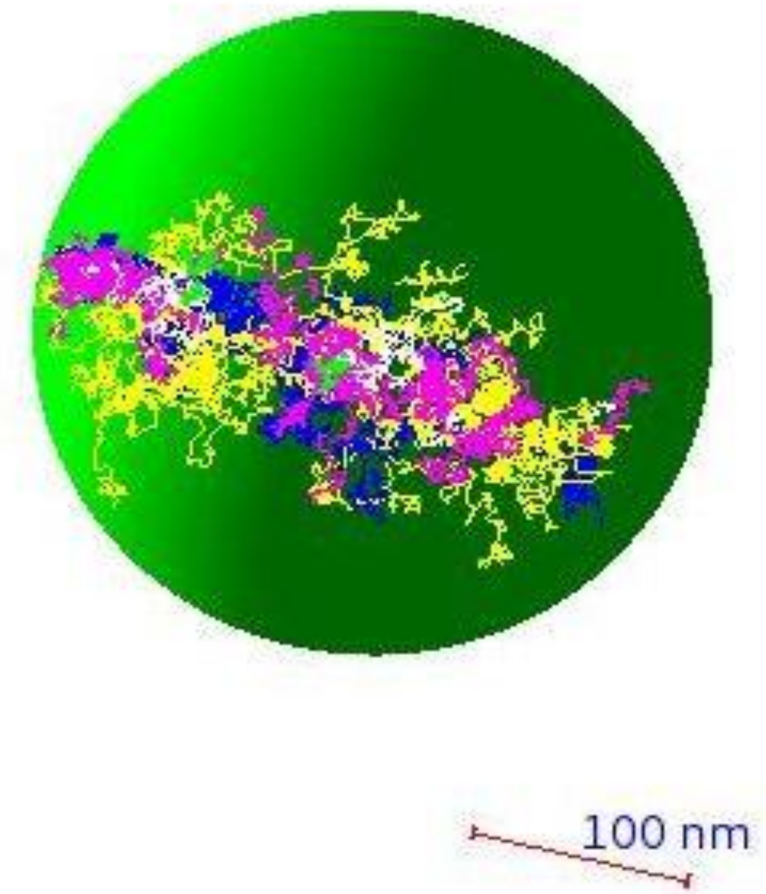
- To simulate formation of free radicals in liquid water after irradiation using Geant4 Monte Carlo simulation toolkit
- To calculate number of free radicals in target volume after electron and proton irradiation.
- To calculate radiochemical yields of free radicals at different time of reactions.

Simulation of 10 keV electron track structure

1 picosecond

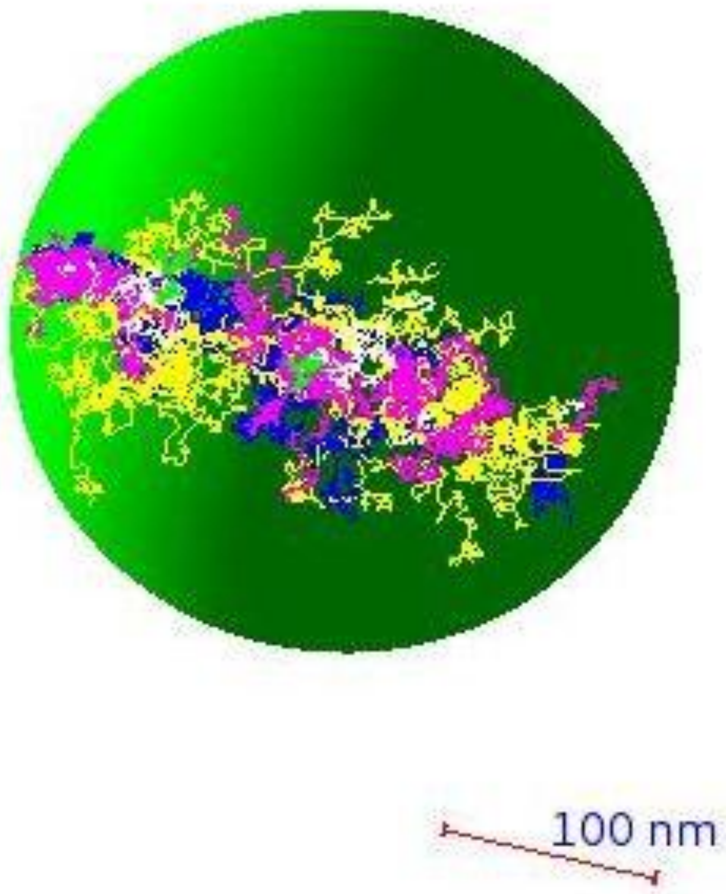


100 nanosecond

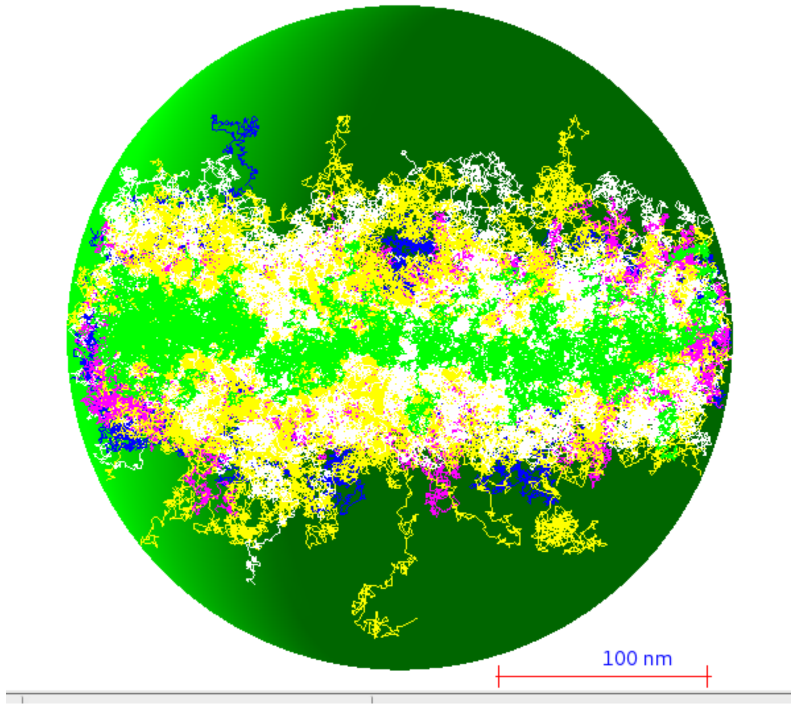


Comparison between track structure for 10 keV electron and proton at 100 nanosecond

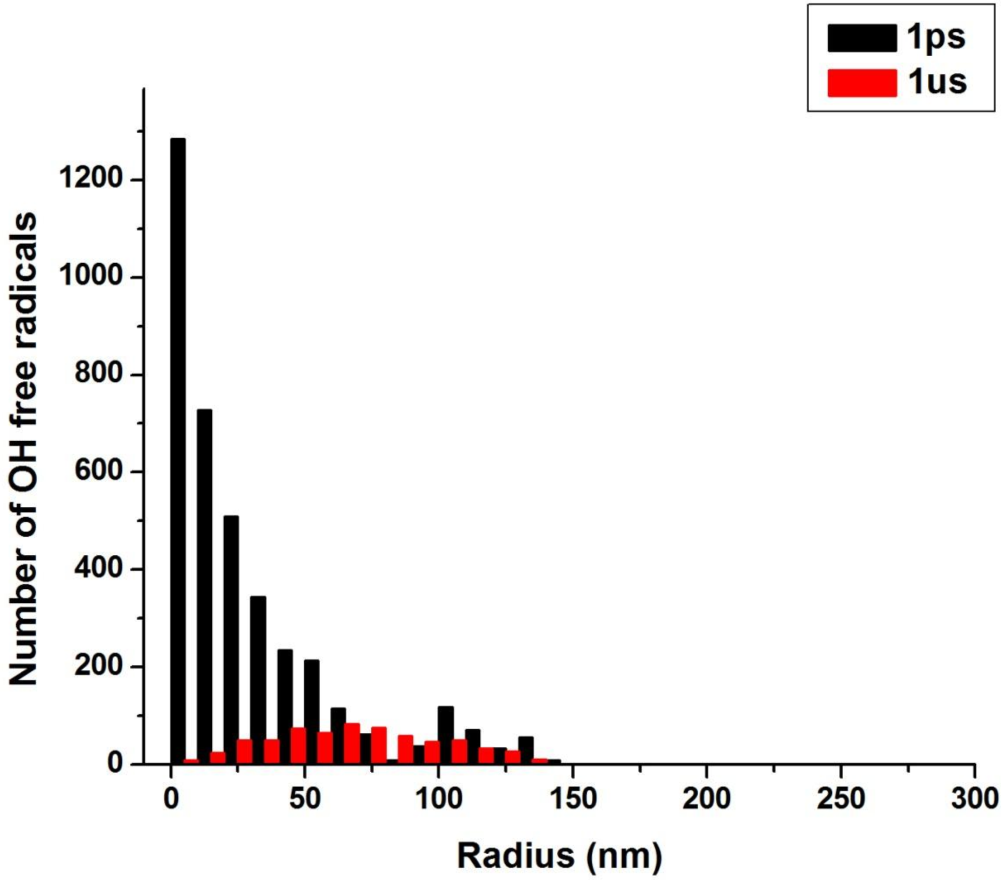
Electron



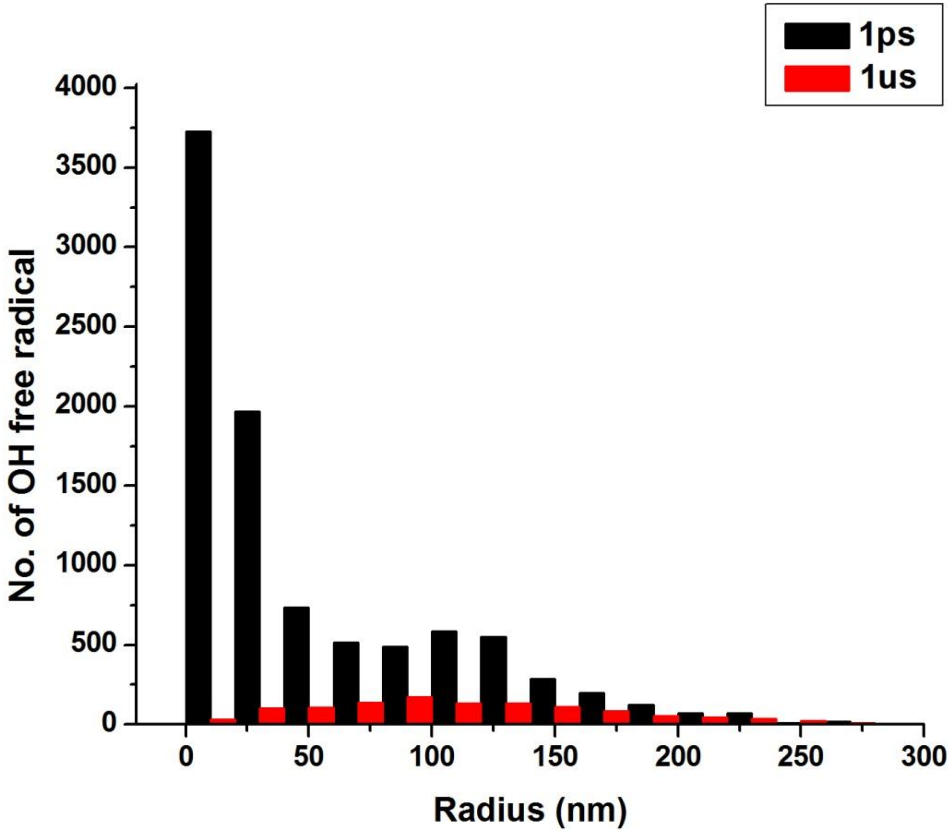
Proton



Radial distribution of OH radicals at 1 picosecond and 1 microsecond.

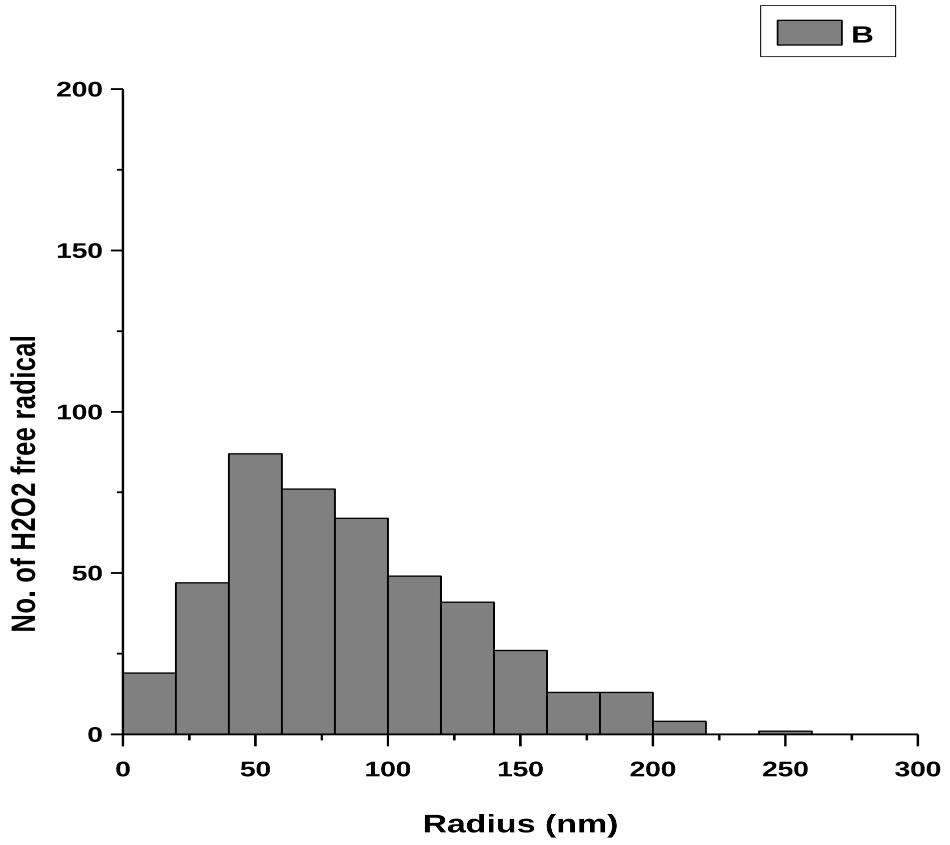


Electron, 10 keV

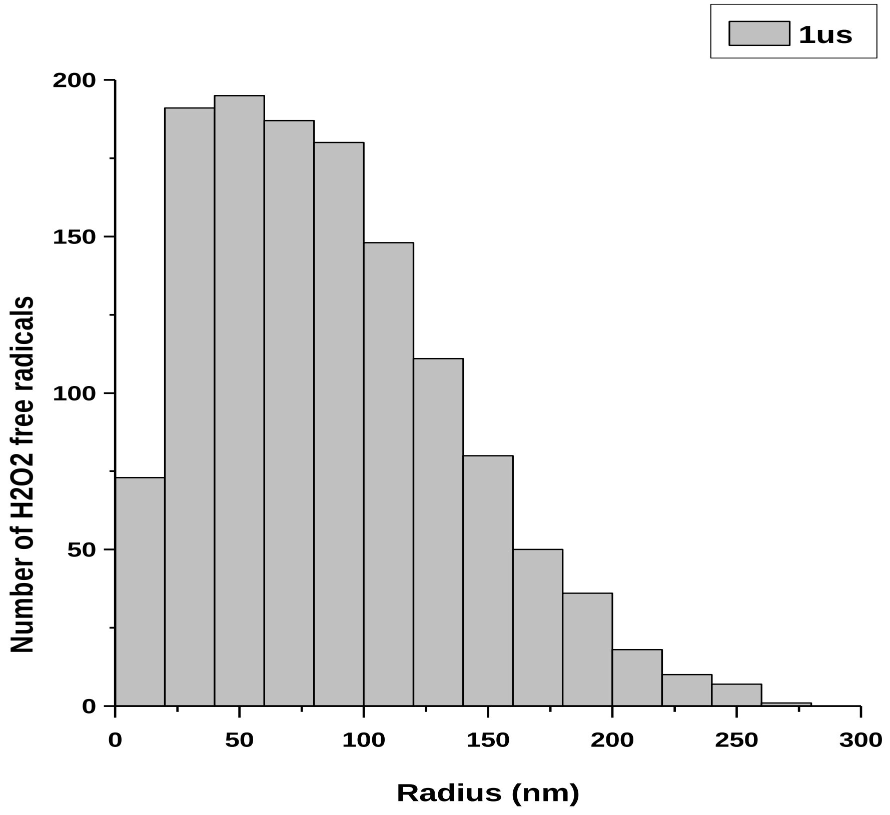


Proton, 10 keV

Radial distribution of H_2O_2 radicals at 1 microsecond



Electron, 10 keV



Proton, 10 keV

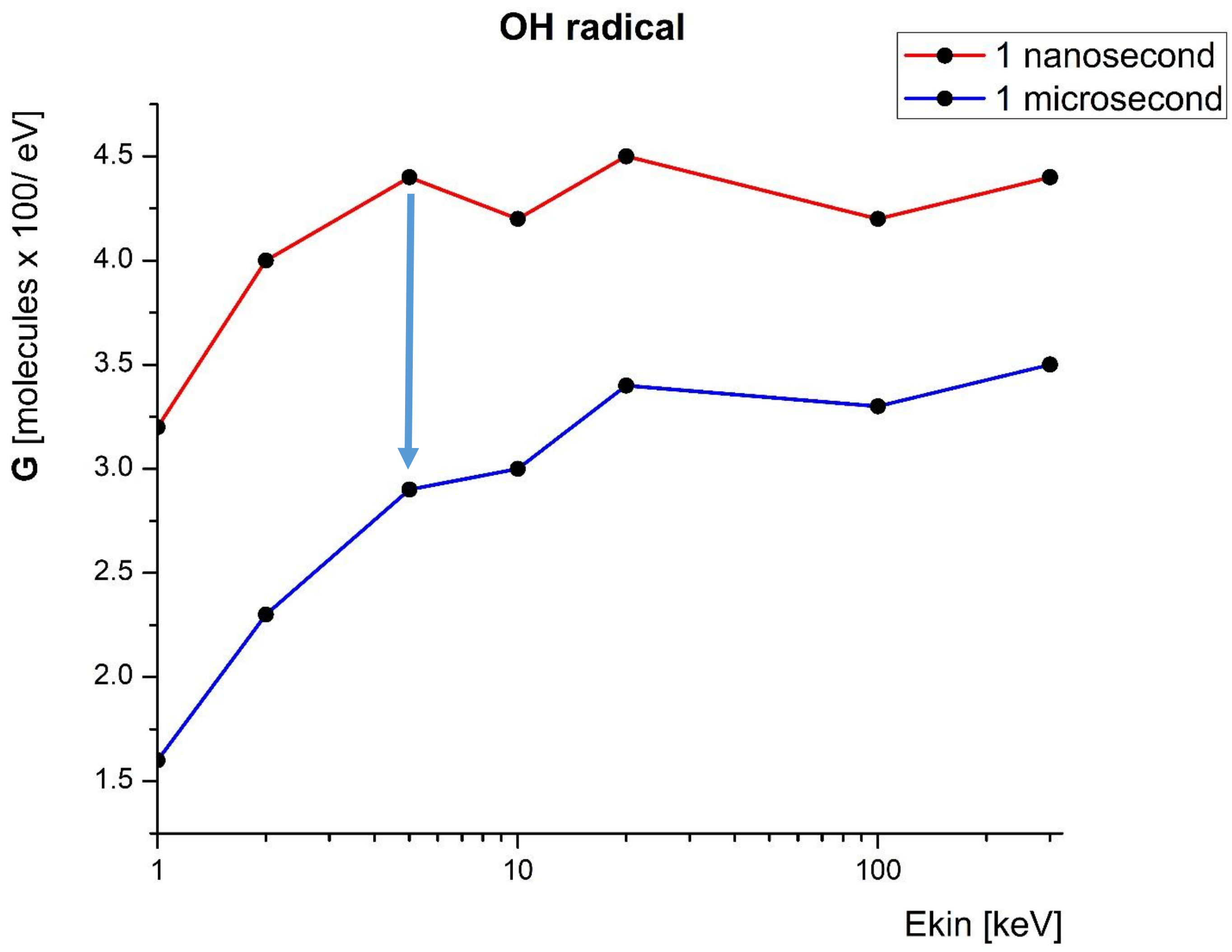
Time dependent radiochemical yield and more efficient some species in water radiolysis

For a given molecular species, the time-dependent radio-chemical yield ***G*** is defined as the number of molecules produced for a total absorbed energy of **100 eV** in the irradiated medium (liquid water) :

$$G_{yield} = \frac{N(t) \times 100}{E\ (eV)}$$

- ***N*(*t*)** is number of molecules
- ***E*** is the total energy deposit by the incident ionizing particle

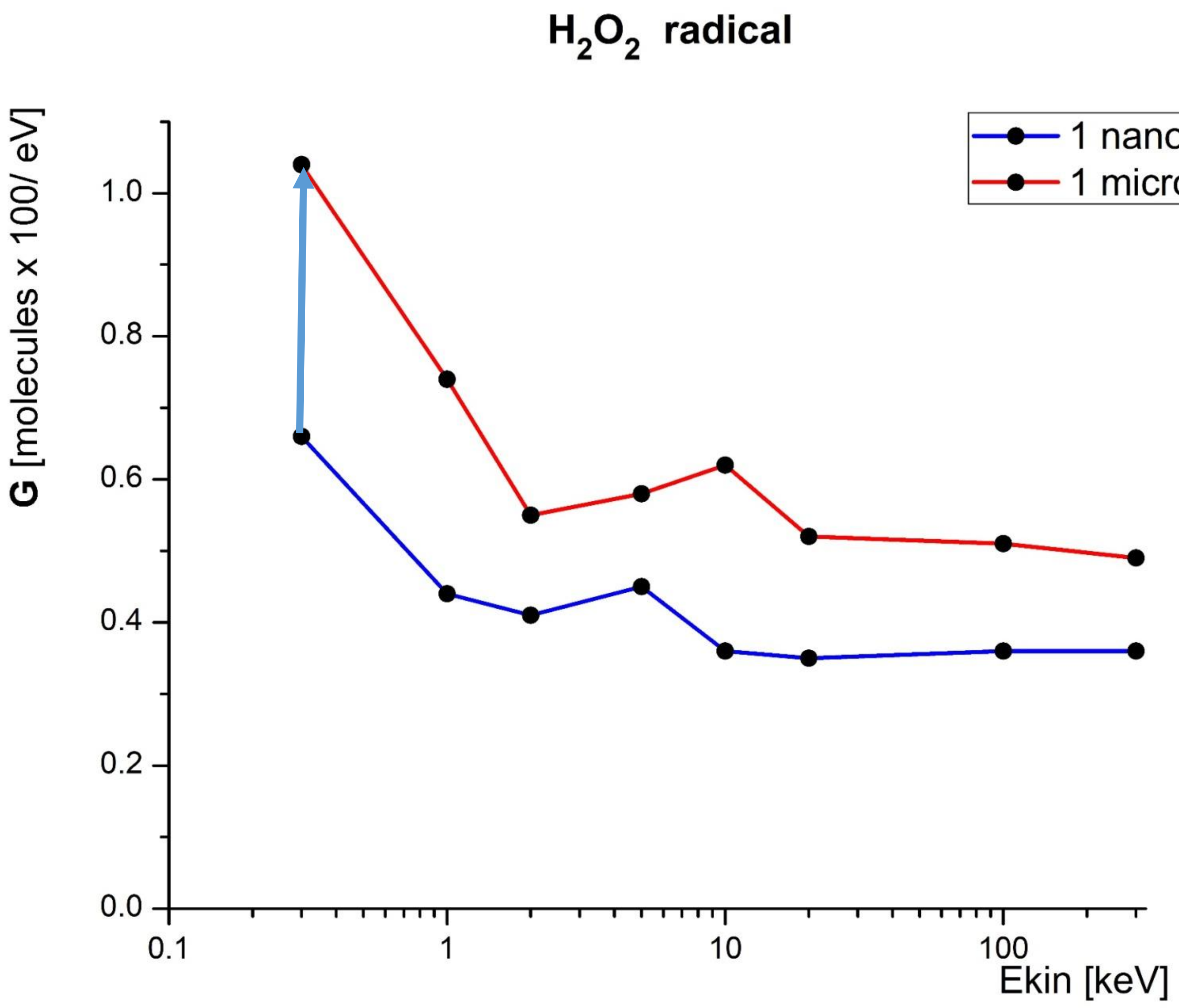
Relationship between radiochemical yield and kinetic energy of electron



Result

Result

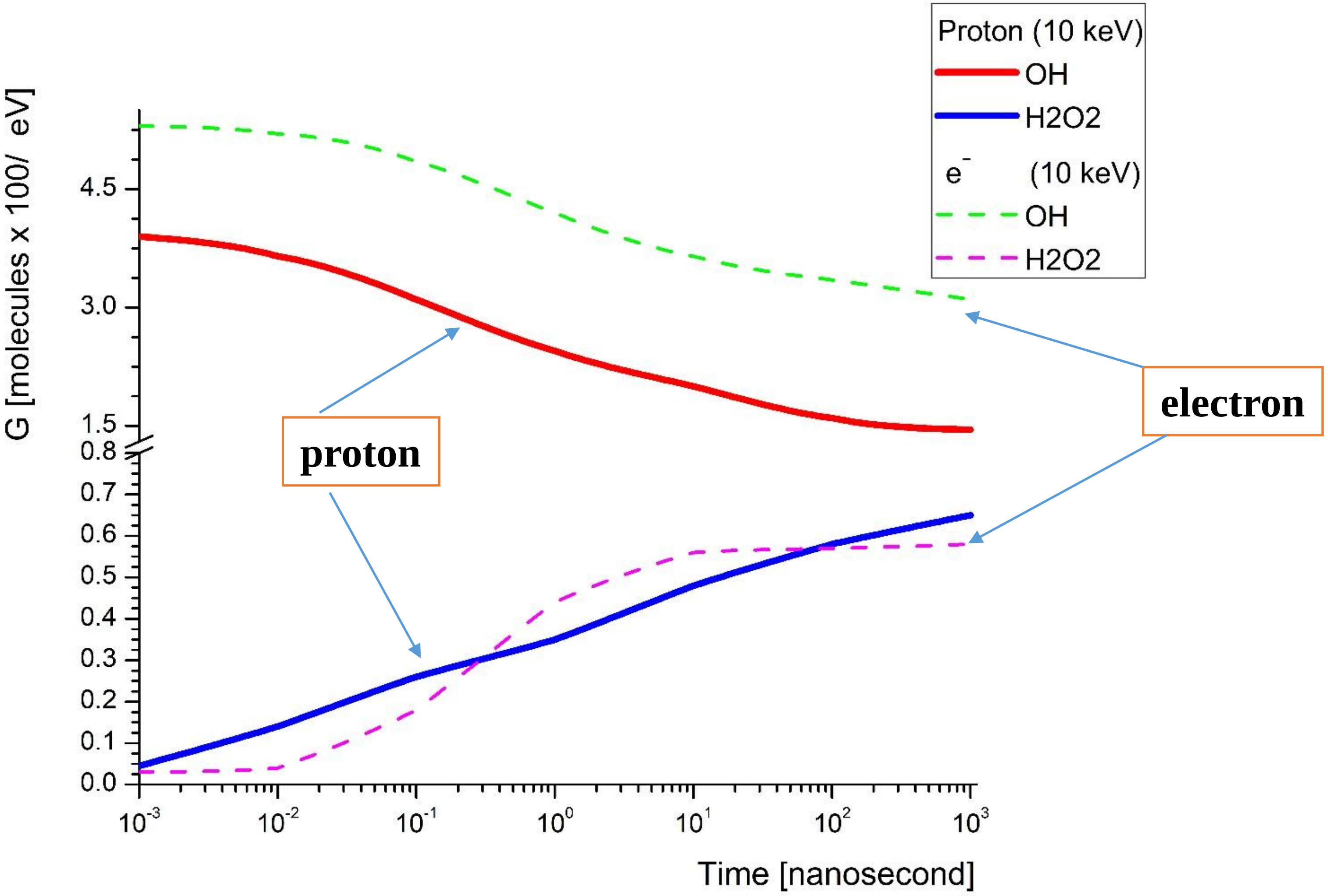
Result



Result

Results

Radiochemical yield of OH and H_2O_2



Conclusion

1. Track structure simulated for electron and proton at the chemical stage from 1 ps to 1 us.
2. We estimated radial distribution of OH and H_2O_2 radicals for 10 keV electron and proton at 1 ps and 1 us.
3. As the results, were obtained number of free radicals for 10 keV proton is three times more than electron.
4. Calculation of radiochemical yield of OH, H_2O_2 which it depends on electron kinetic energy.
5. Radiochemical yield increases for OH and decreases for H_2O_2 when particle energy increases.

A damage Prediction

Biological effect of ionizing radiation

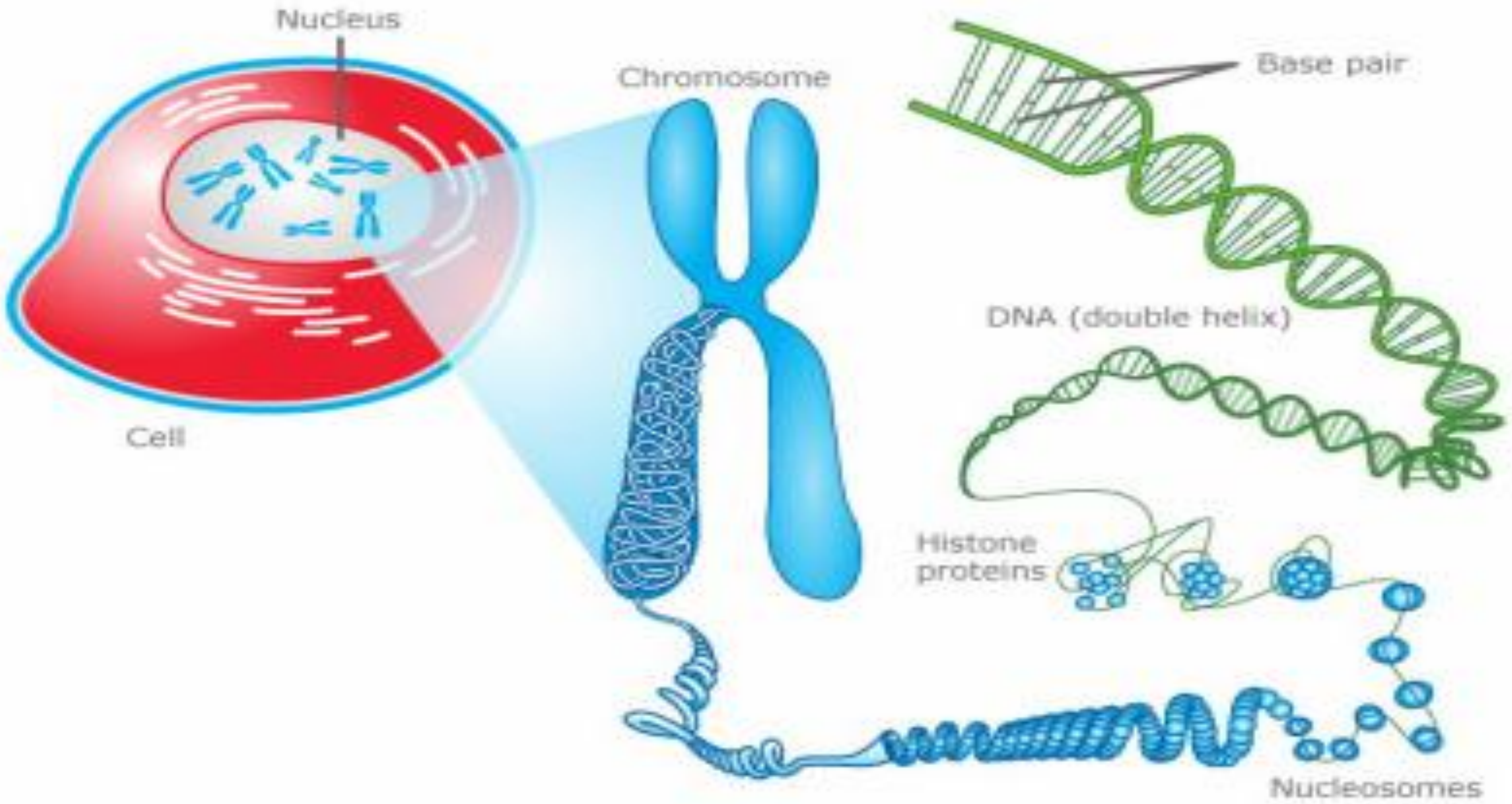
Methods

Motivation

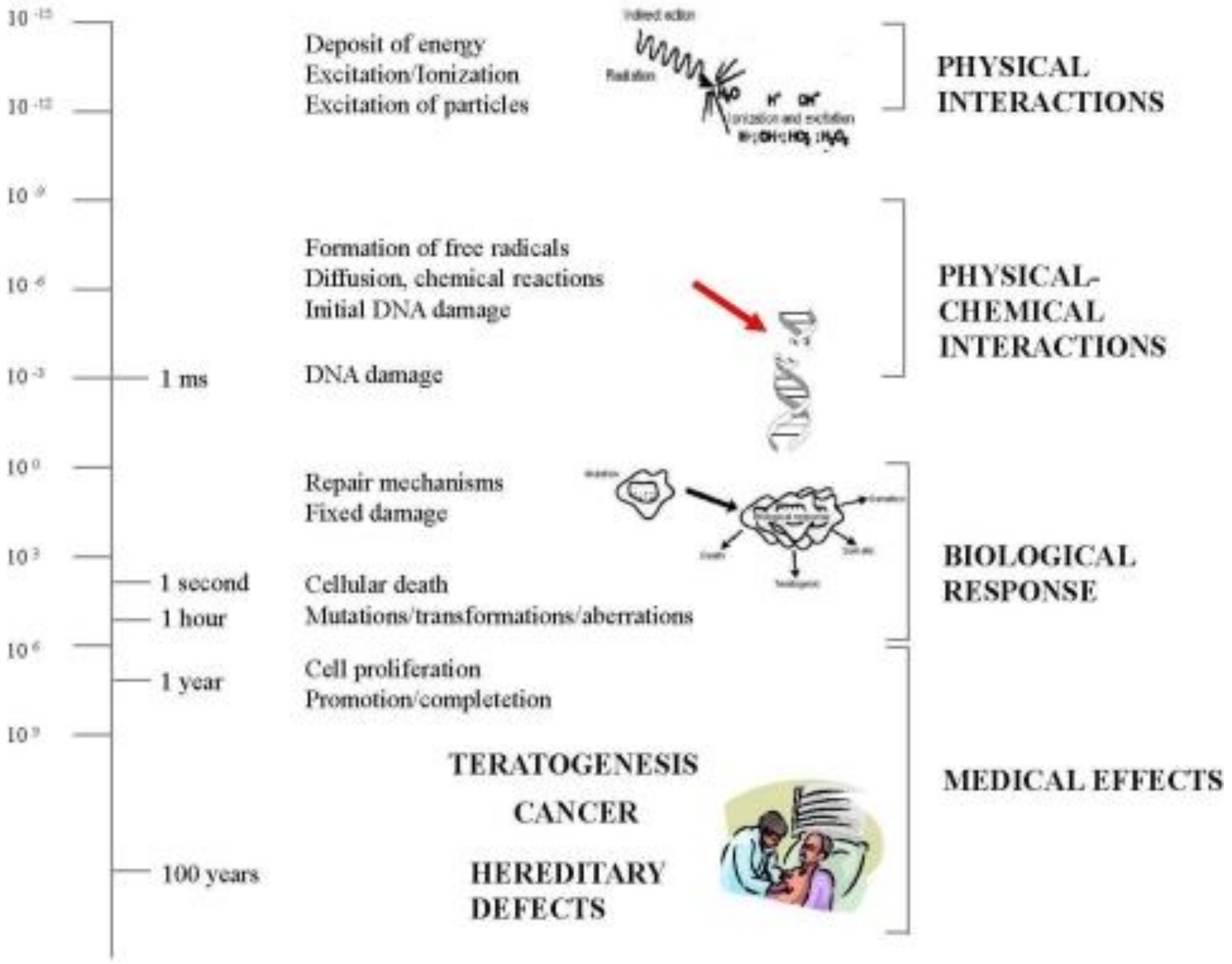
DNA damage

Radiation Biology lab

Task 3 : DNA Damage results


Nucleus
Chromosome
Base pair
Cell
DNA (double helix)
Histone
proteins
Nucleosomes

effects of Ionizing Radiation



Aim of this work

1) Simulating the particle track

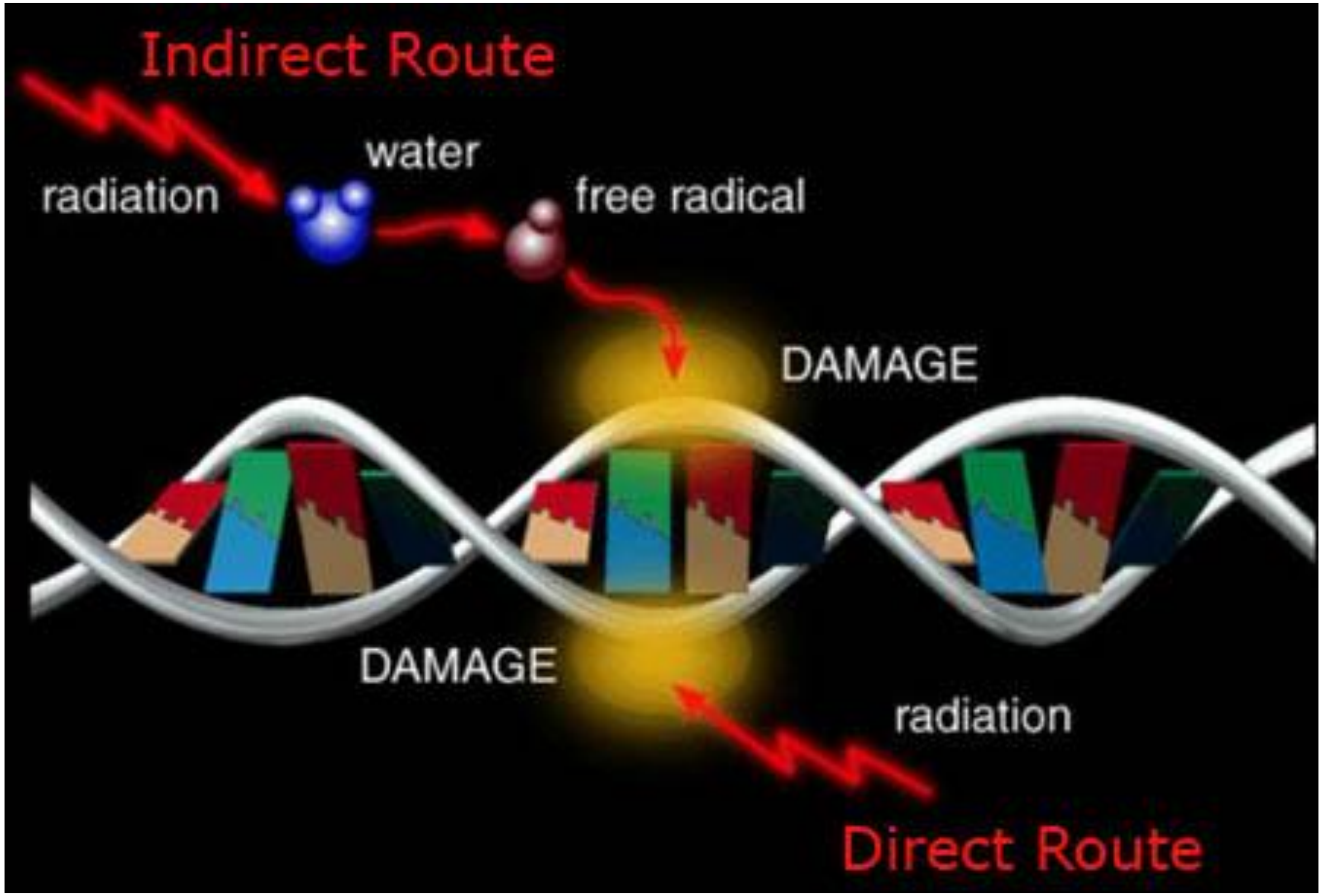
2) Simulating the target

3) Simulating the particle track-DNA interaction

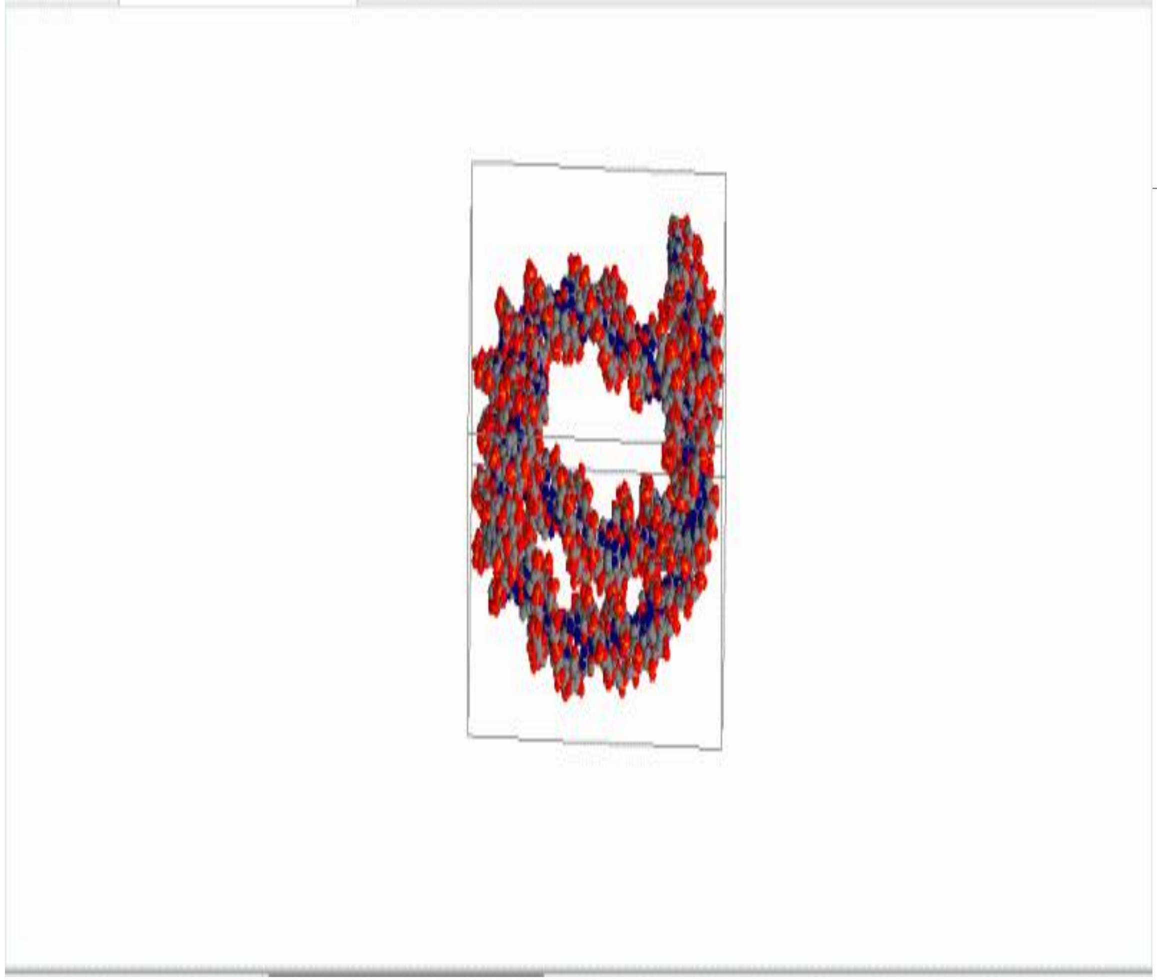
4) Calculating exact number of DNA strand breaks after different radiation

5) To know which particle is more effective e- or protons, and at which energy they deposit more energy in DNA.

DNA damage



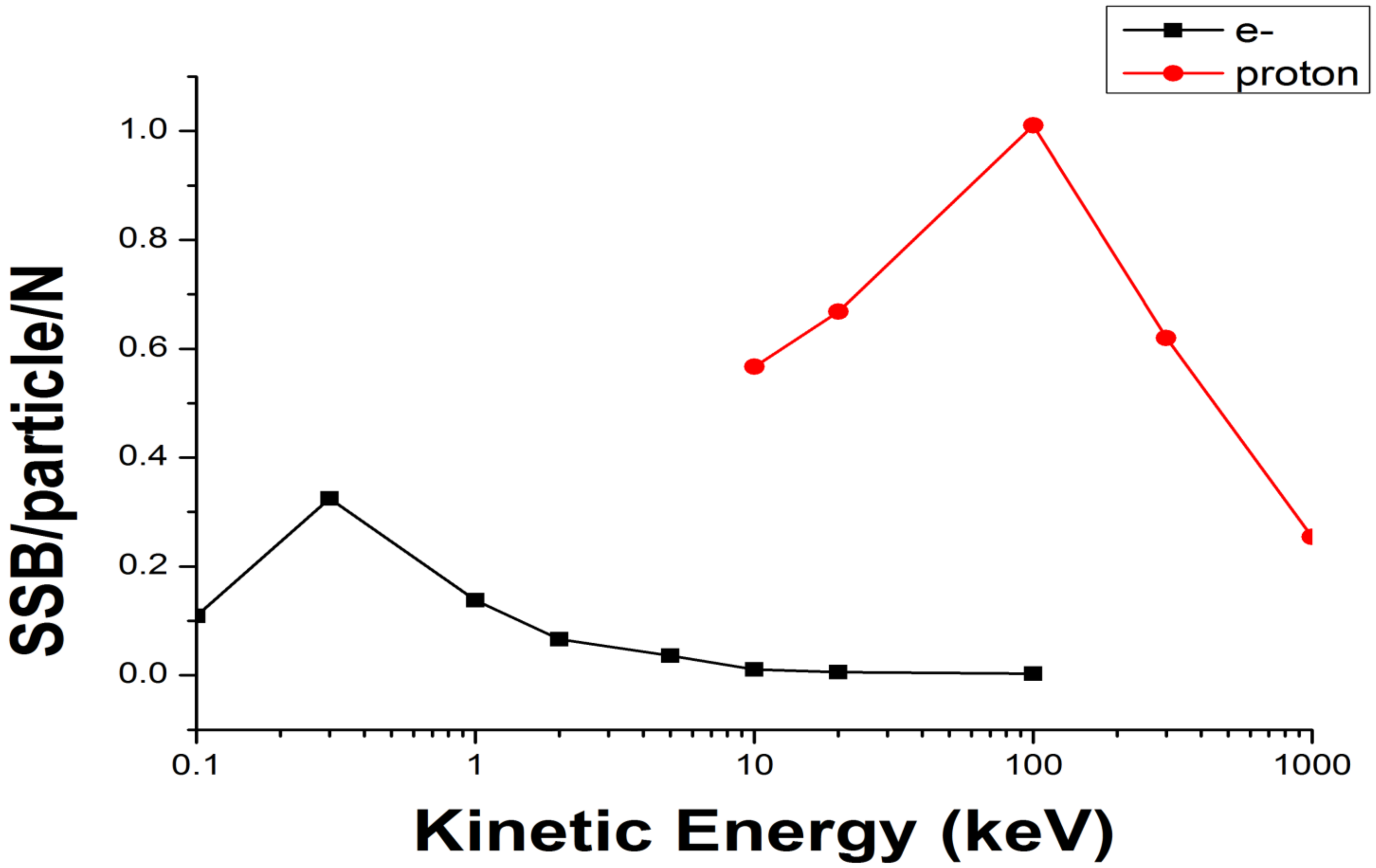
- Direct
- indirect



Results

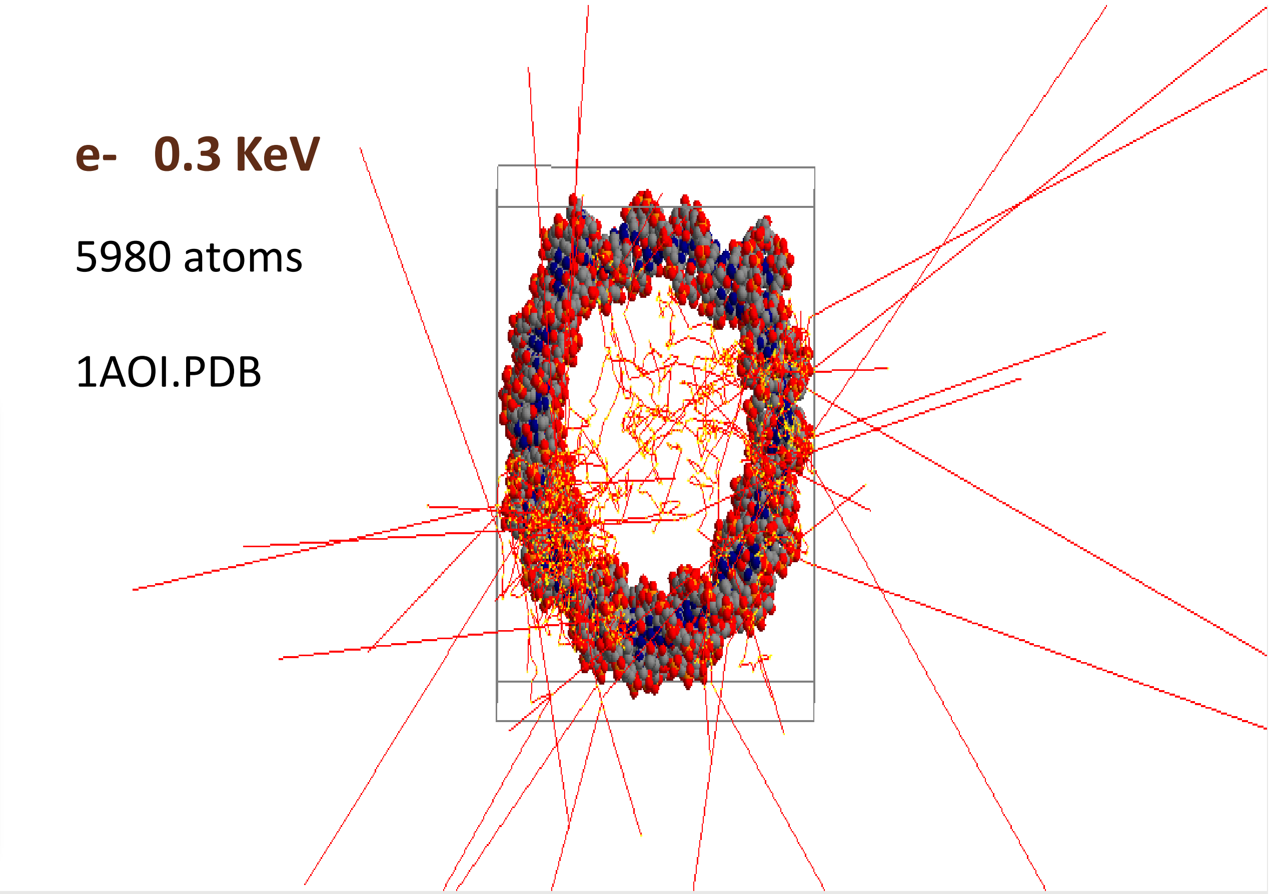
Simulation of DNA-radiation interaction

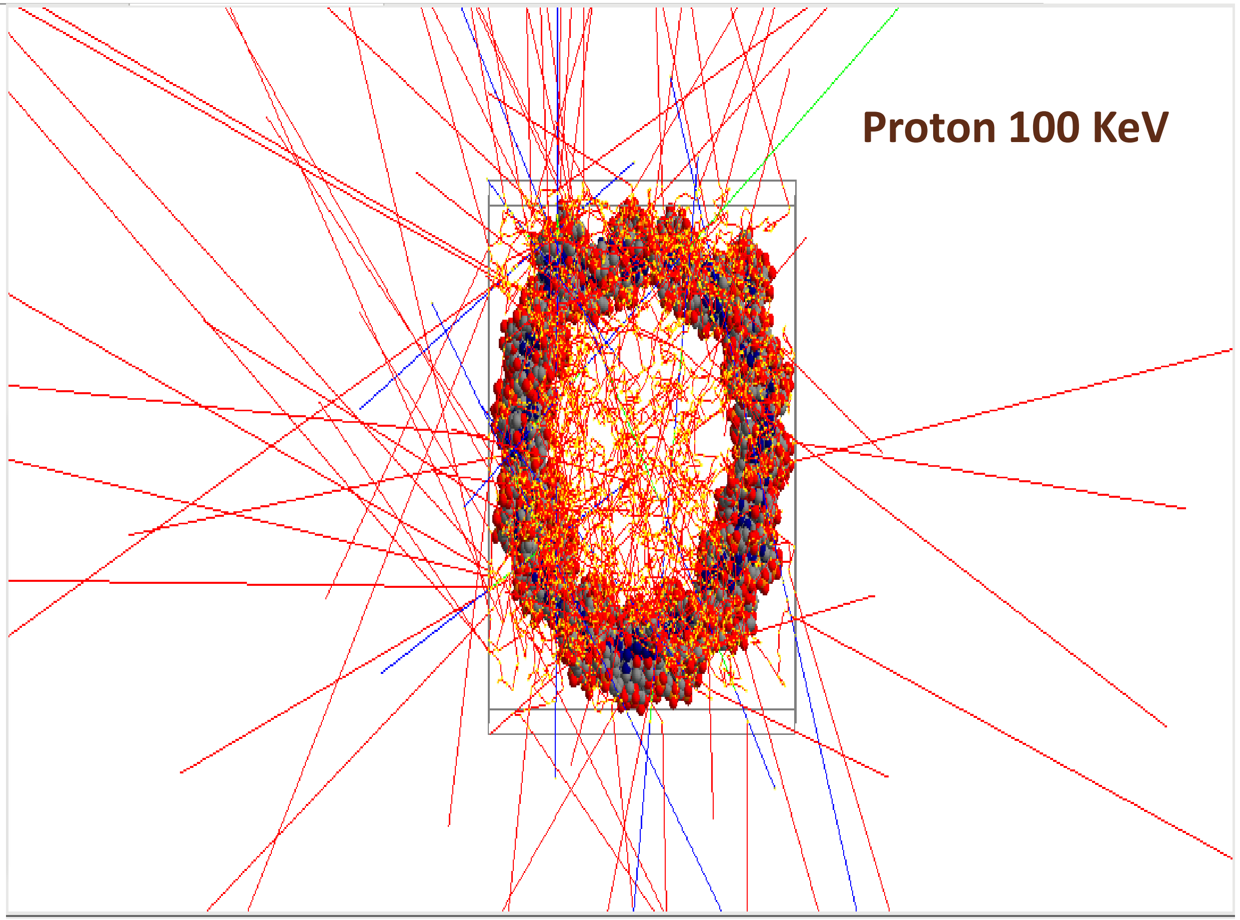
Optimum energy curve in geometry of DNA nucleosome

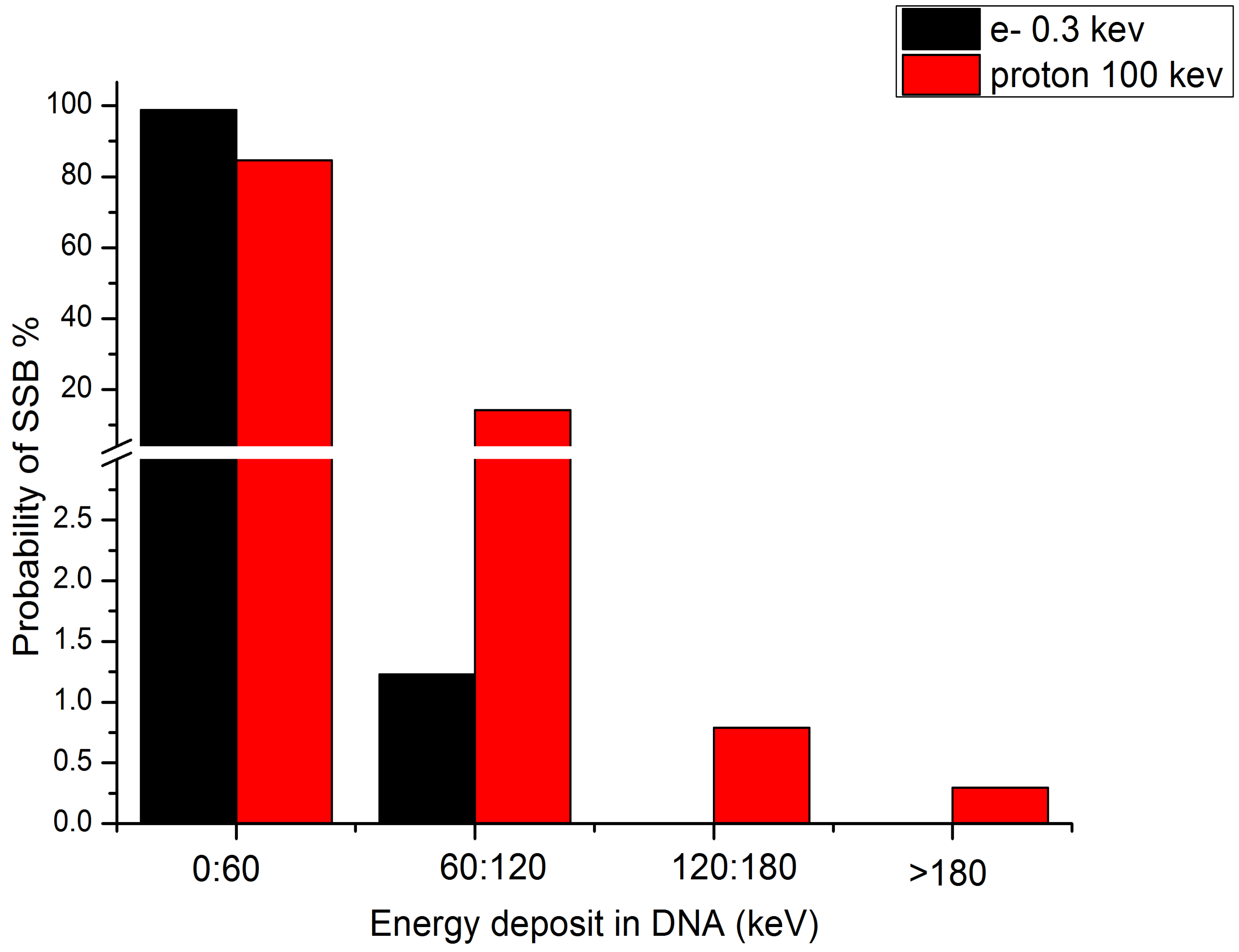


This diagram shows the number of breaks caused per particle with different energies.

Tracking simulation of different particles in DNA nucleosome

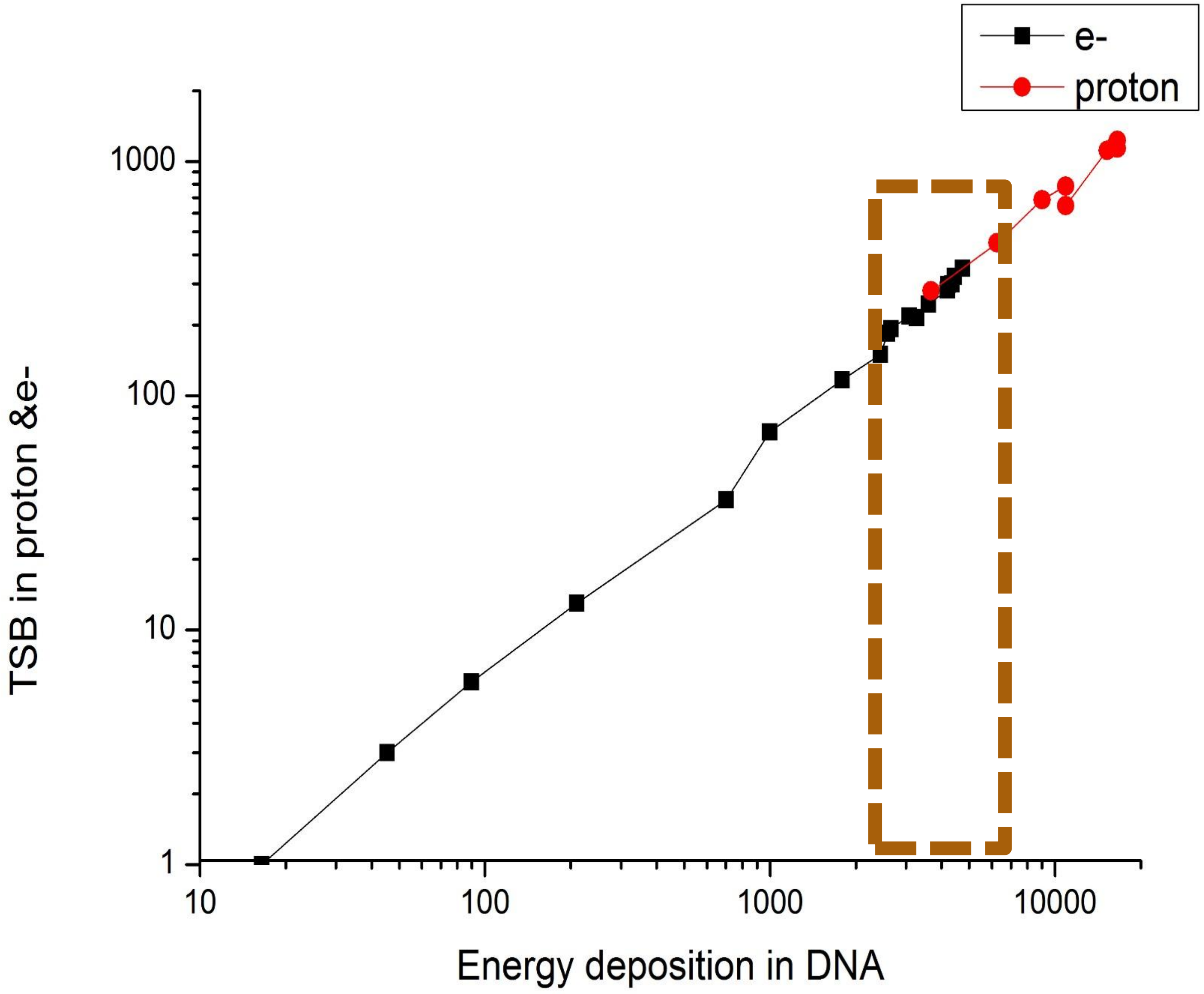






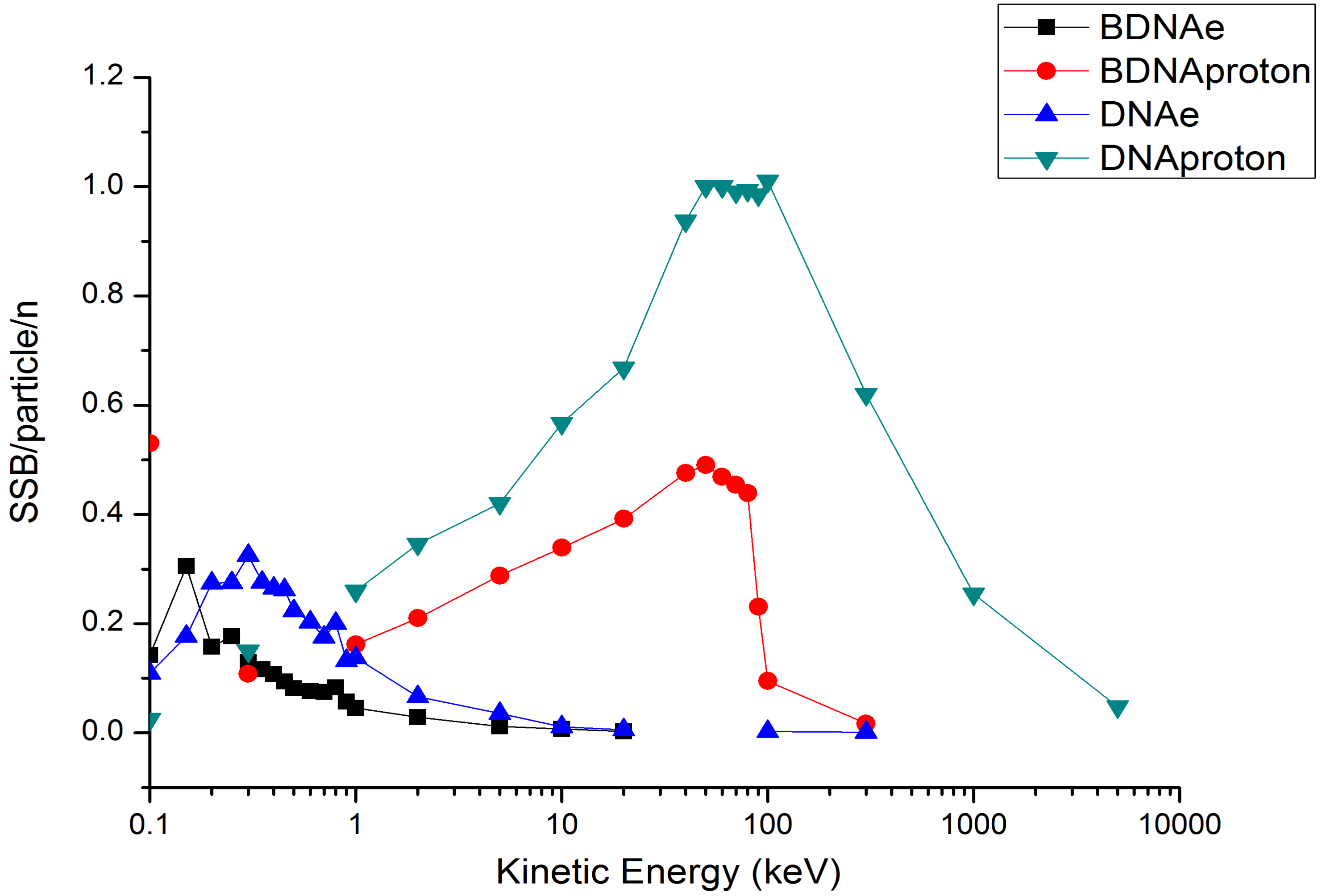
Probability SSB vs ED

This histogram shows the probability of having Single Strand Breaks in DNA vs the amount of energy deposited to cause this break.



TSB vs ED in proton and e-

This curve shows the total strand break produced vs energy deposition after exposure to proton and electron it shows that at energy between (1113:1190) the (TSB) produced are approximately the same.



Comparison between optimum energy of e- & proton in case of nucleosome and DNA segment

Conclusion

The results showed that:

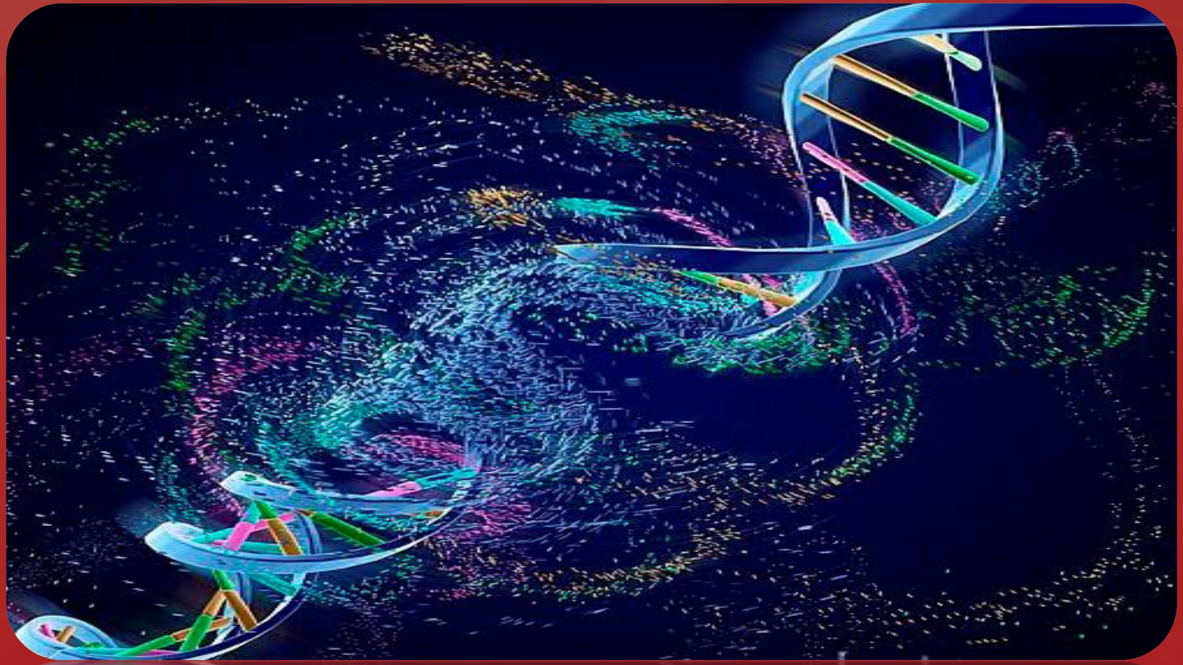
- e- and proton deposit the highest energy in the DNA at these energies 0.3 KeV, 100 KeV respectively that makes them the optimum energies to be used for this aspect.
- This means that more SSB, and DSB are being produced at these energies.
- More than 80% of the DNA damage is produced by the low energy e- and protons, which is <60 ev.
- At similar energy depositions in DNA between (1113:1190 eV), the DNA TSB produced are approximately the same.
- The calculations of optimum energy in case of DNA segment show slight decrease (shift) when compared with that of DNA nucleosome. This can be attributed to the smaller surface area of the segment.

Simulation of radiation therapy using proton and Carbon-12

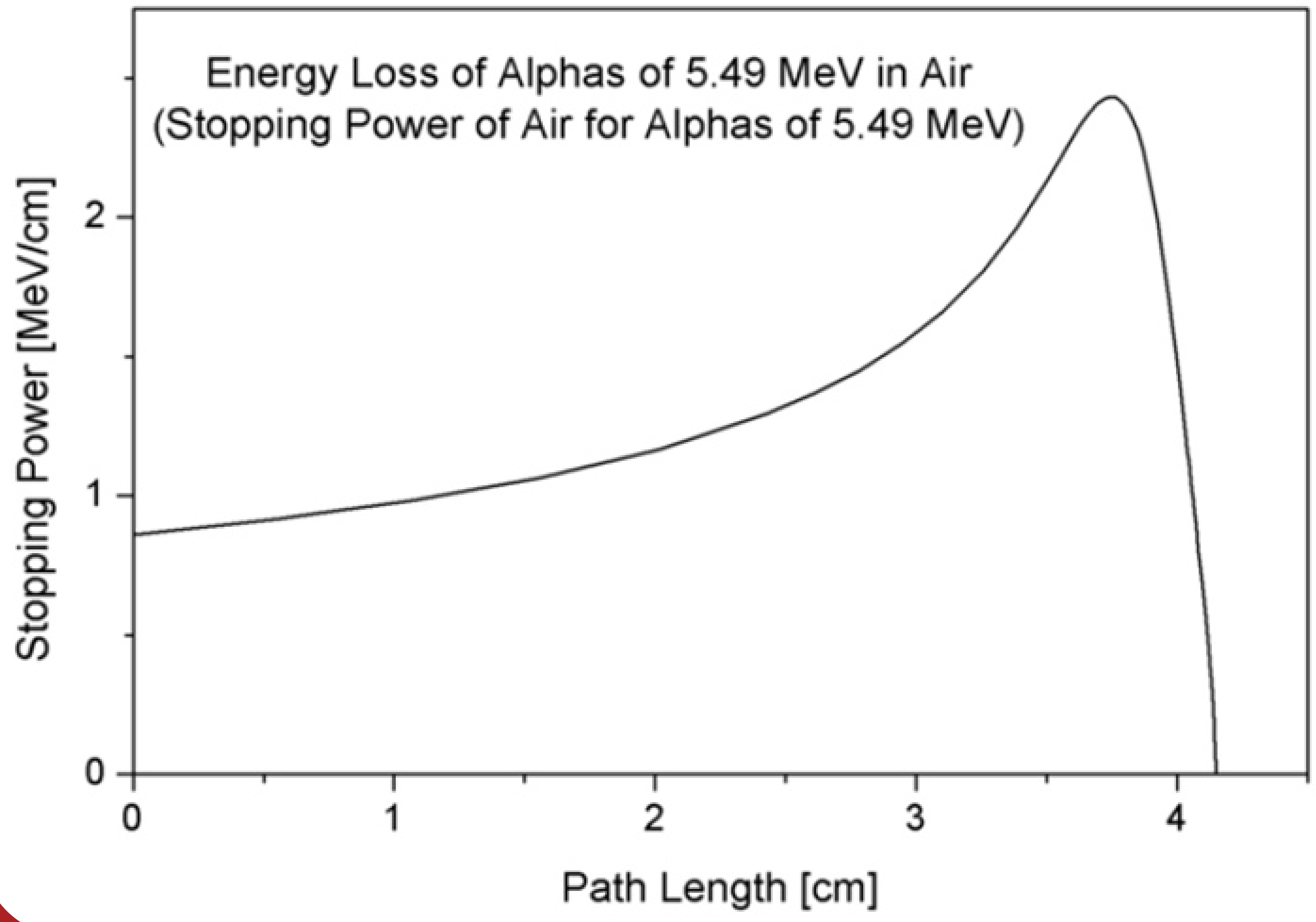
Brynkevich Hanna,
Blagodarova Yana. ISEI BSU, Belarus

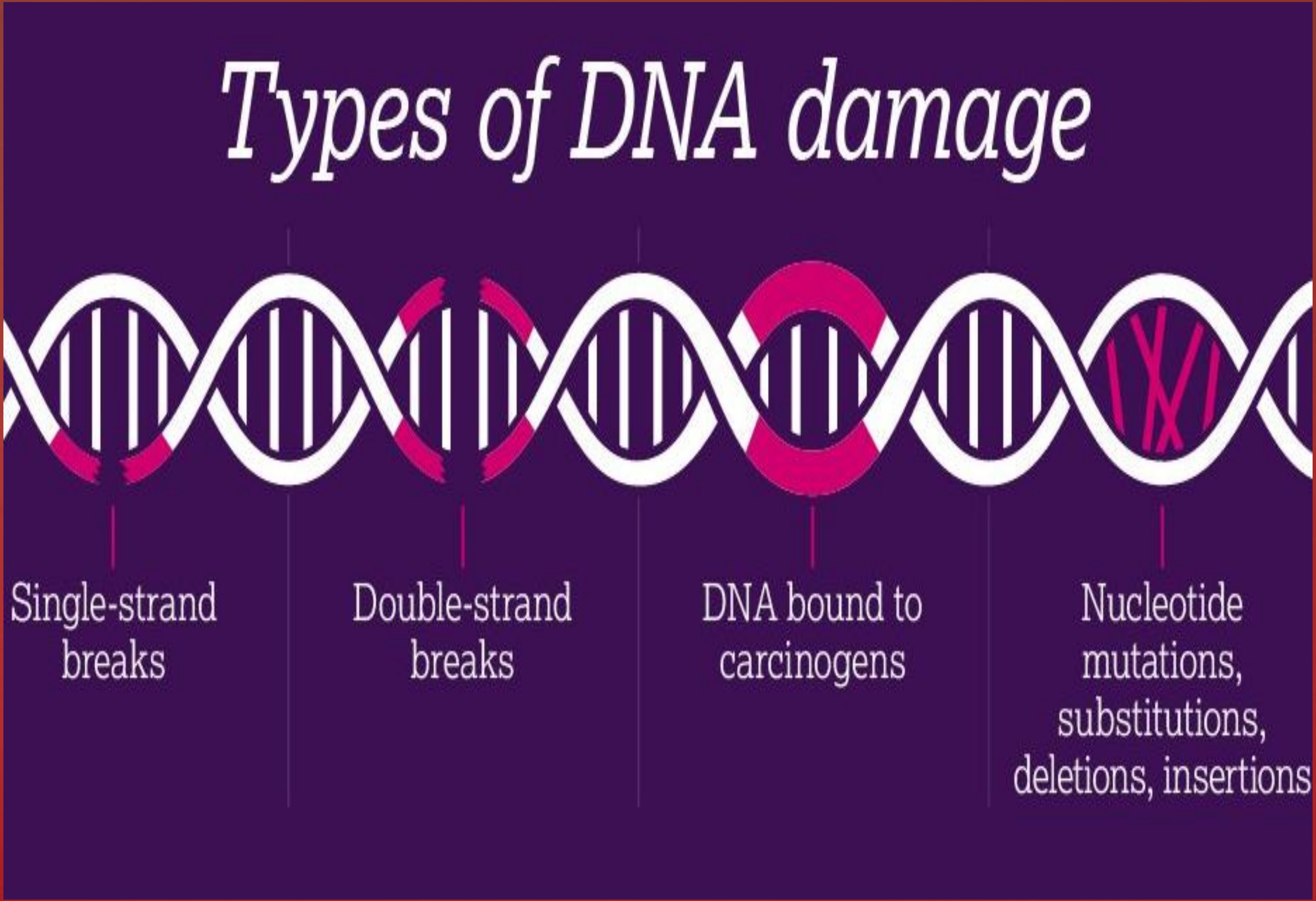
Aim of this practice

Simulate charged particles track structure in the biological media and calculate DNA DSB, which is close to Bragg peak.

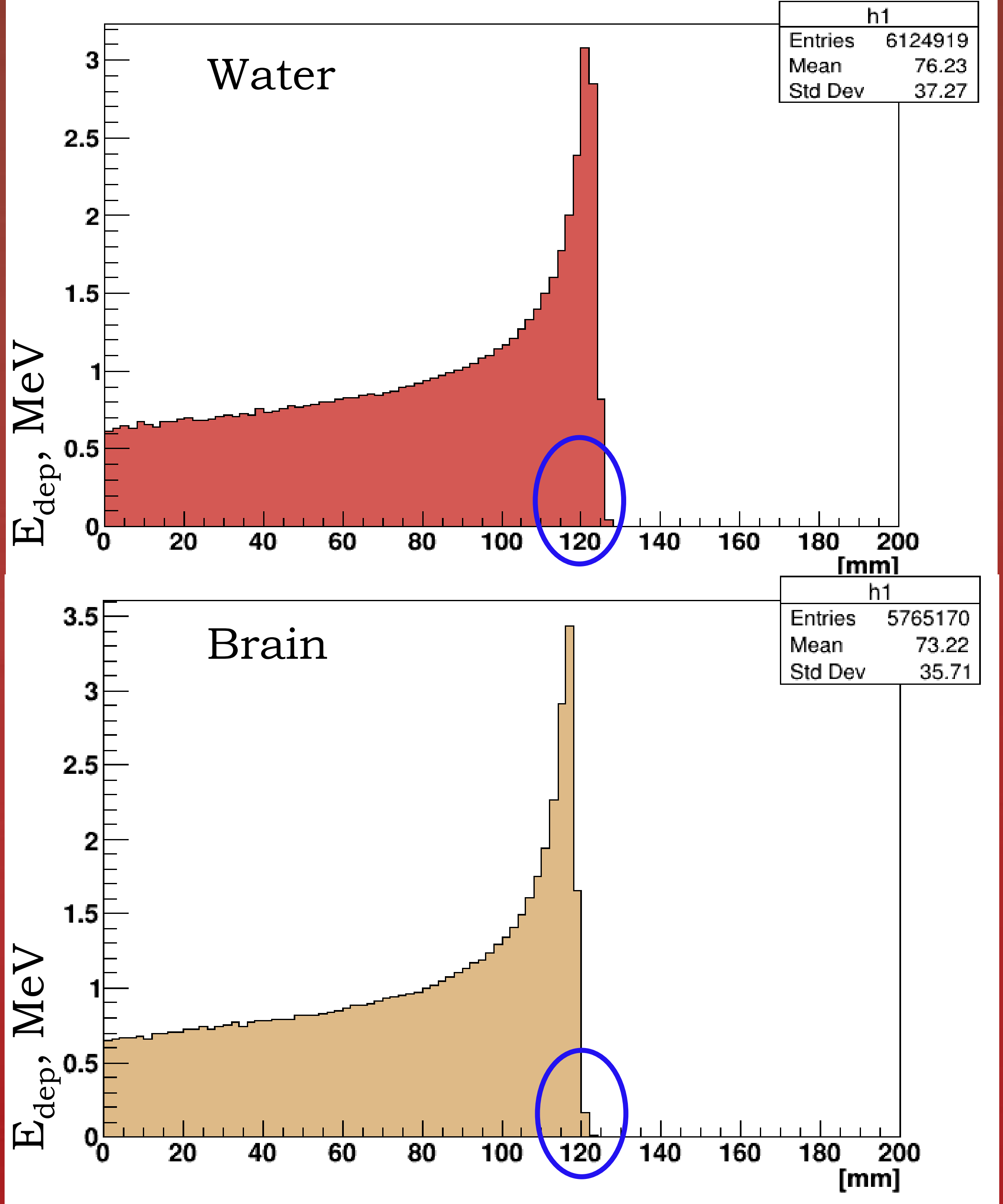


Bragg curve

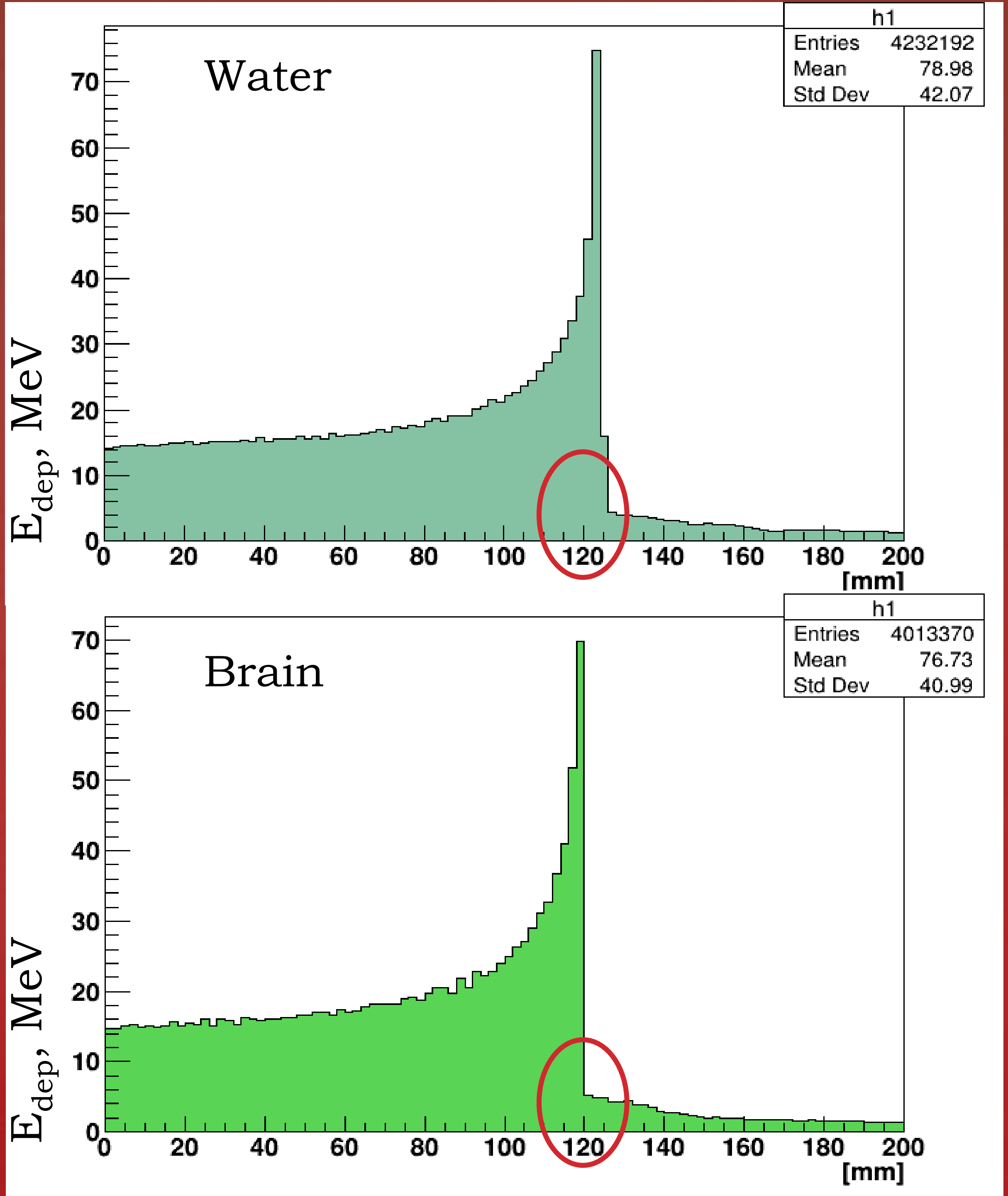

Energy Loss of Alphas of 5.49 MeV in Air
(Stopping Power of Air for Alphas of 5.49 MeV)
Stopping Power [MeV/cm]
0
1
2
0
1
2
3
4
Path Length [cm]


Types of DNA damage
Single-strand breaks
Double-strand breaks
DNA bound to carcinogens
Nucleotide mutations, substitutions, deletions, insertions

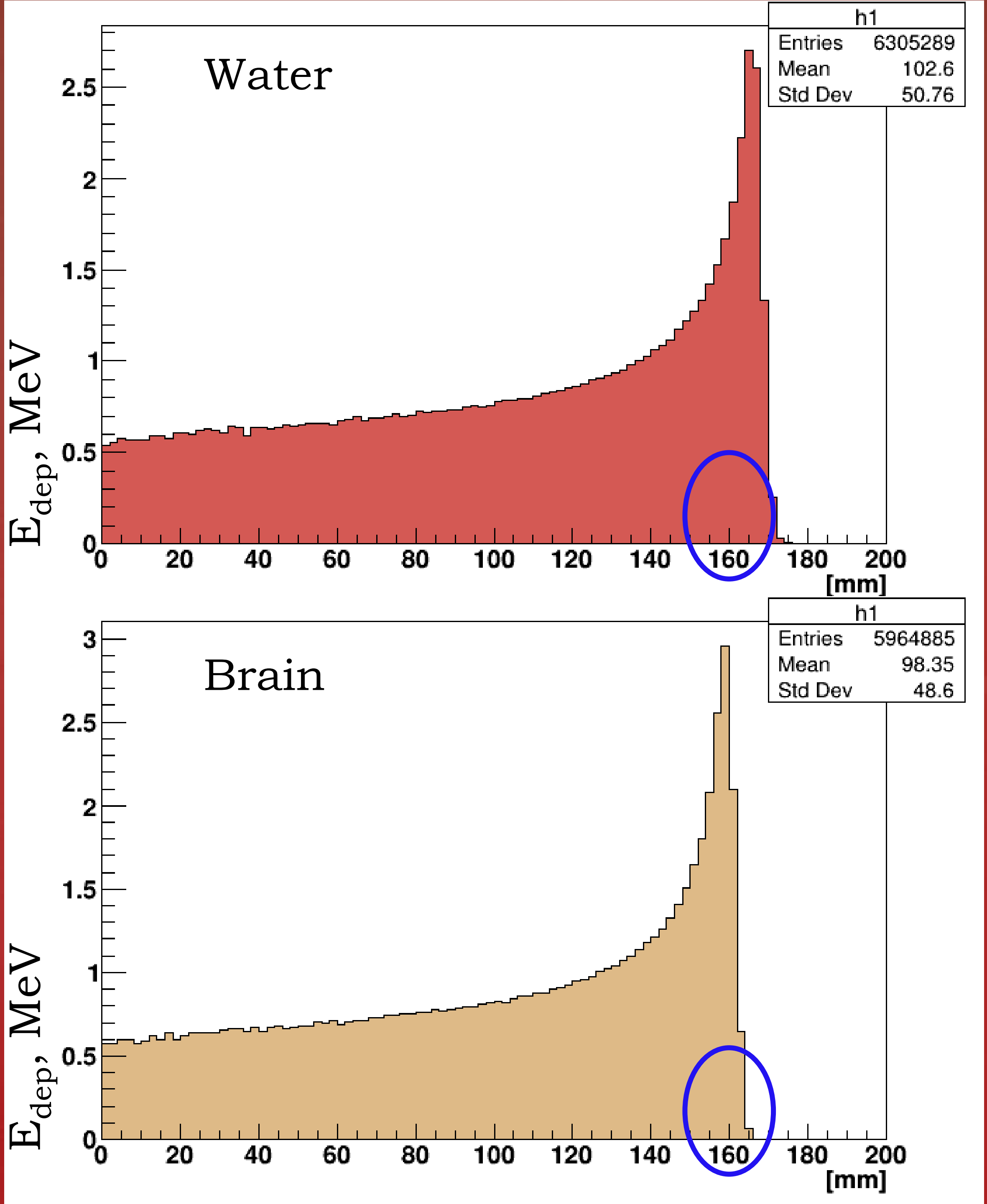
ATOM	WATER, 1 g/cm^3	BRAIN, 1,04 g/cm^3
	%	%
H	**11,19**	**10,7**
C		**14,5**
N		**2,2**
O	**88,81**	**71,2**
Na		**0,2**
P		**0,4**
S		**0,2**
Cl		**0,3**
K		**0,3**



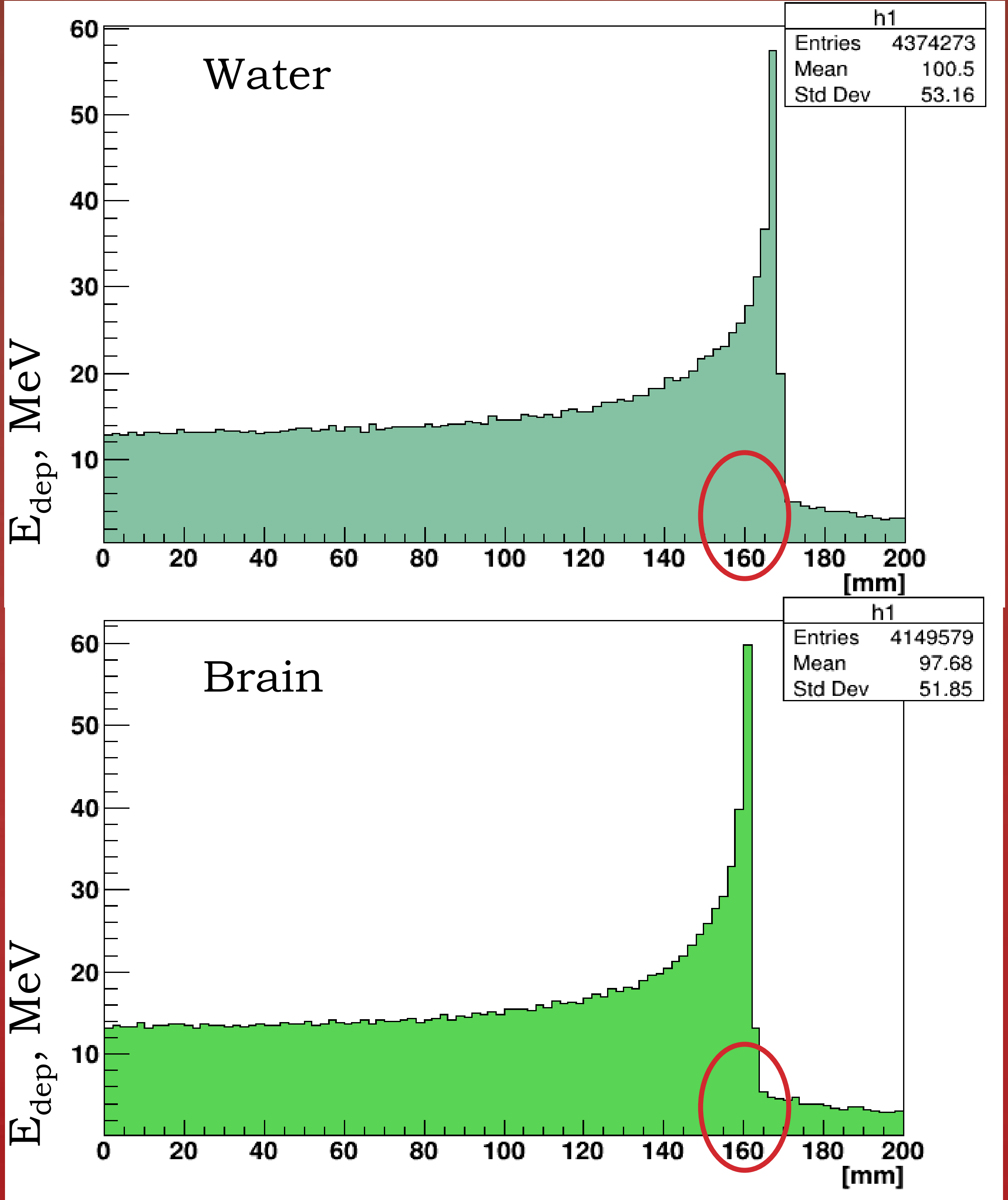
The depth of penetration and energy loss for a **proton with energy of 130 MeV** in water phantom and in the brain phantom



The depth of penetration and energy loss for a **Carbon-12 with energy of 245 MeV/nucleon** in water phantom and in the brain phantom

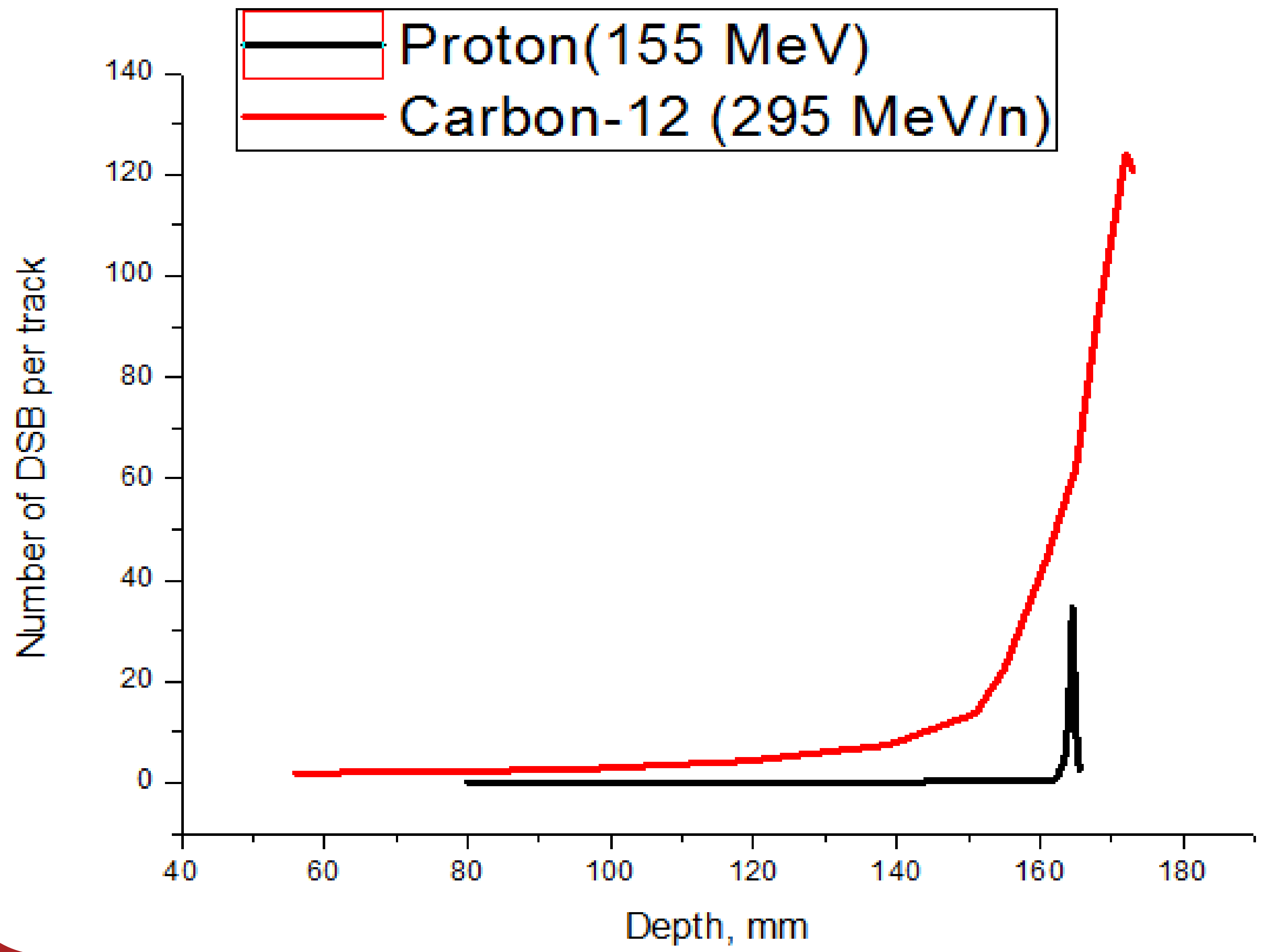


The depth of penetration and energy loss for a **proton with energy of 155 MeV** in water phantom and in the brain phantom



The depth of penetration and energy loss for a **Carbon-12 with energy of 295 MeV/nucleon** in water phantom and in the brain phantom

Number of DNA DSB in Bragg peak region:



Quantities of radiations effects at Bragg peak

	WATER		BRAIN		
	Depth (mm)	Energy deposit (MeV/mm)	Depth (mm)	Energy deposit (MeV/mm)	DSB (/particle/um)
Proton 155 MeV	**165**	2,7	**160**	2,95	**34,5**
Carbon-12 295 MeV/nucleon	**165**	58	**160**	60	**124**

Conclusion:

We gained practicle experience with computational methods to simulate and calculate biological effects of charged particles using Geant4 Monte Carlo simulation toolkit.

We calculated depth-dose distributions and DNA damage in water and brain phantom induced by proton and carbon ions with different energies.

According our research, high energy heavy particles less effective for radiation therapy then low energy particles.

The largest number of DNA DSB in the Bragg peak region was found 35 for protons and 124 for carbon ions.

Any Questions?