

**SAKARYA UNIVERSITY
INSTITUTE OF SCIENCE AND TECHNOLOGY**

**INVESTIGATION OF RADIATION INTERACTION
PARAMETERS FOR SOME ESSENTIAL
BIOMOLECULES**

PhD THESIS

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Department : PHYSICS

Supervisor : Prof. Dr. Barış TONGUÇ

Co-Supervisor : Assist. Prof. Dr. Halil ARSLAN

July 2020

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DECLARATION

I declare that all the data in this thesis was obtained by myself in academic rules, all visual and written information and results were presented in accordance with academic and ethical rules, there is no distortion in the presented data, in case of utilizing other people's works they were refereed properly to scientific norms, the data presented in this thesis has not been used in any other thesis in this university or in any other university.

M.S. Al-Buriah

13.09.2020

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LIST OF SYMBOLS AND ABBREVIATIONS

LAC	: Linear attenuation coefficient
MAC	: Mass attenuation coefficient
HVL	: Half value layer
MFP	: Mean free path
PEBF	: Photon exposure buildup factor
PEABF	: Photon energy-absorption buildup factor
MC	: Monte Carlo
G-P	: Geometric-progression

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INVESTIGATION OF RADIATION INTERACTION PARAMETERS FOR SOME ESSENTIAL BIOMOLECULES

SUMMARY

Keywords: Radiation, Geant4, Biomolecules

A biomolecule is a building block not only for humans but also for all the living organisms including animals and plants. In this dissertation, the radiation interaction properties of some essential biomolecules such as creatinine hydrochloride (creatinine H), methionine, glycoprotein, glycine, proline, margaric acid, tyrosine, inosine, and lactose were investigated by using the Geant4 simulations and some theoretical approaches. The photon interactions are studied by evaluating different important parameters such as linear attenuation coefficients (μ), mass attenuation coefficients (μ_m), effective atomic number (Z_{eff}), and effective electron density (N_{eff}) over a wide range of energy varying from 1 keV to 1000 MeV. The μ_m values were compared with the theoretical calculations performed via the XCOM program. In addition, the photon energy-absorption processes, which are influential mechanisms for the photon – biomolecule interactions, were investigated. Furthermore, the G-P method was applied to evaluate the photon exposure build-up factor (PEBF/EBF) and photon energy-absorption build-up factor (PEABF/EABF) which are related to the exposure in the air and medium, respectively. Additionally, the charged particle interactions with the selected biomolecules were studied by determining the electron stopping power, and the effective atomic number for electron, proton, alpha particle, and carbon ion for kinetic energies in the range of 0.015 – 15 MeV. The present work gives a full understanding, rich information, and important data for the radiation interactions with the biomolecules involved. Such data are expected to be used in dose calculations for both X / gamma rays and charged particle radiations.

BAZI TEMEL BİYOMOLEKÜLLER İÇİN RADYASYON ETKİLEŞİM PARAMETRELERİNİN İNCELENMESİ

ÖZET

Anahtar kelimeler: Radyasyon, Geant4, Biyomoleküller.

Biyomolekül, sadece insanlar için değil, hayvanlar ve bitkiler de dahil olmak üzere tüm canlı organizmalar için bir yapı taşıdır. Bu tez çalışmasında, kreatinin hidroklorür (kreatinin H), metiyonin, glikoprotein, glisin, prolin, margarik asit, tirozin, inosin ve laktoz gibi bazı temel biyomoleküllerin radyasyon etkileşim özellikleri Geant4 simülasyon programı ve bazı teorik yaklaşımlar kullanılarak araştırılmıştır. Foton etkileşimlerinin incelenmesi amacıyla, bu biyomoleküllere ait doğrusal zayıflatma katsayısı (μ), kütle zayıflatma katsayısı (μ_m), etkin atom numarası (Z_{eff}) ve etkin elektron yoğunluğu (N_{eff}) gibi önemli parametreler 1 keV - 1000 MeV enerji aralığında belirlenmiştir. Simülasyonlardan elde edilen μ_m değerleri, XCOM programı ile yapılan teorik hesaplamaların sonuçları ile karşılaştırılarak test edilmiştir. Bunlara ek olarak, foton - biyomolekül etkileşimleri için oldukça büyük öneme sahip olan foton enerjisi soğurma süreçleri de araştırılmıştır. Ayrıca, havadaki ve ortamdaki maruziyetle ilgili parametreler olan doz yığılma faktörü (PEBF / EBF) ve foton enerji soğurma yığılma faktörü (PEABF / EABF) söz konusu biyomoleküller için G-P metodu kullanılarak hesaplanmıştır. Foton etkileşimlerinin yanı sıra, yüklü parçacıkların biyomoleküllerle etkileşimleri de incelenmiş olup bu bağlamda; elektron durdurma gücü ve 0,015 - 15 MeV aralığındaki kinetik enerjiler için elektron, proton, alfa parçacığı ve karbon iyonu için etkin atom numaraları belirlenmiştir. Bu çalışma, radyasyon ile bazı temel biyomoleküllerin etkileşimlerinin tam olarak anlaşılabilmesi için oldukça zengin ve önemli veriler sağlamaktadır. Bu verilerin, hem X / gama ışınları hem de yüklü parçacık radyasyonları için doz hesaplamalarında kullanılması beklenmektedir.

CHAPTER 1. INTRODUCTION

Radiation is widely used in medicine and its sectors, such as radiology. It is used to scan and take images of the inside of a patient's body to observe bones. The images provide valuable information that is vital in determining the severity and location of bone fractures anywhere around the body. In addition, radiation used in mammograms to test for breast cancer, dental offices to observe teeth, as well as many more applications including the use of photon and/or charged particles for cancer treatment.

One of the most important fields of radiation research focuses on studying the radiation interactions with matter. This field is well known as radiation transmission, radiation transport, or radiative transfer. The transmission of radiation through a medium can be described by absorption, excitation, emission, and scattering processes. Such processes that depend mainly on the energy and type of radiation, are the basic to develop the medical diagnosis and radiation therapy.

Biomolecules such as proteins, lipids, carbohydrates, and nucleic acids are the responsible part in the human body for driving the machinery of life. Therefore, proper understanding of their behaviour with radiation helps to reveal the fundamentals of physics processes taking place in living cells.

The experimental works are appropriate to study the radiation propagation through matter and to test the radiation attenuation properties of different materials. However, the dealing with very tiny materials (like biomolecules) makes the experiment very difficult to implement. Therefore, Monte Carlo simulation method and the theoretical approaches are reliable way that can provide us many advantages such using a wide range of projectile energy.

In this dissertation, radiation interaction properties of essential biomolecules are investigated by using the Geant4 simulations and some theoretical approaches. This radiation study of the essential biomolecules investigates mainly the photon (X/gamma rays) interactions as well as the interactions of charged particles (electron, proton, and alpha) are briefly discussed. The photon interactions are studied by evaluating different important parameters that give a full understanding for the X/gamma rays interactions with the biomolecules involved. Firstly, the linear attenuation coefficients (μ) are estimated by using Geant4 Monte Carlo simulations. The μ values are then converted to their corresponding values of the mass attenuation coefficients (μ_m). The μ_m values are compared with the theoretical calculations performed via XCOM program. The μ_m values are used to obtain effective atomic number (Z_{eff}) and effective electron density (N_{eff}) for the investigated biomolecules. Moreover, we investigate the photon energy-absorption for the chosen biomolecules. Furthermore, the G-P method is applied to evaluate photon exposure buildup factor (PEBF/EBF) and photon energy-absorption buildup factor (PEABF/EABF). The previous photon interaction parameters are used for the photon dose calculations. On the other hand, the charged particle interactions are studied by determining the electron stopping power, and the effective atomic number for electron, proton, alpha particle, and carbon ion. The contents of each chapter are briefly given below.

Chapter 2 deals with theoretical background about the radiation interactions with matter. Chapter 3 discusses the Monte Carlo method focusing on the Geant4 simulations. Chapter 4 gives a general information about biomolecules and their importance in different applications. Chapter 5 presents the obtained results in this work. Finally, conclusions of this study are summarized in Chapter 6.

CHAPTER 2. RADIATION INTERACTION WITH MATTER

Radiation is the word that was discovered in 1896 by Henri Becquerel when he discovered that uranium could fog a piece of film [1]. Later on, the definition of radiation was completed to be that radiation is the emission of energy by a matter. There are lots kinds of radiation such as electromagnetic radiation and nuclear radiation. Electromagnetic radiation encompasses radio waves, microwaves, infrared, visible light, ultraviolet light, and photons (x-rays and gamma-rays). Nuclear radiation is occurred when subatomic particles are emitted from the nucleus of atoms. It is should noting that nuclear radiation is sometimes called ionizing radiation that has enough energy to knock electrons off atoms. There are at least four different kinds of nuclear radiation namely; alpha radiation, beta radiation, gamma radiation, and neutron radiation. Each of these types of radiation have different characteristics and mechanisms to interact with matter [2-10].

2.1. Photon Interaction With Matter

A photon is a quanta of energy that can be considered as a wave and as a particle. For example, photon has a wavelength and frequency like a wave, as well as it has a momentum and energy like a particle. The photon can interact with matter in six different ways namely; coherent scattering, photoelectric effect, incoherent scattering (Compton effect), pair production, triplet production, and photodisintegration effect [11, 12]. We shall discuss briefly all these interactions but we will focus on the three main photon interactions (photoelectric effect, incoherent (Compton) scattering and pair production).

2.1.1. Photoelectric absorption

It is also called photoelectric absorption [13-15]. This type of photon interaction happens when the photon energy (E_p) is close to the binding energy (E_B) of atomic electrons. In this case, a photon gives all its energy to an atomic electron that is ejected from the atom with kinetic energy given by; $(E_p - E_B)$. The likelihood of this interaction is proportional to $(E_p)^{-3}$ and Z^3 , here Z is the atomic number. Moreover, this interaction ceases to become likely for photon energies of 100-200 keV in water, however remains significant process for attenuation in lead for photon energies up to 1 MeV.

2.1.2. Compton scattering

Incoherent effect (or Compton scattering) can be observed at photon energy higher than the binding energy of the atomic electron, so this scattering can be described as a collision with a free electron. In this case, the photon gives a partial part of its energy to an electron and then both the photon and electron are scattered in different directions. It is worth mentioning that Compton effect is not related directly to atomic number but related to the electron density of the matter.

Also, there is another interaction namely; Rayleigh scattering that occurs when the photon energy is very low (less than 10 keV) [16, 17]. In this case, a photon collides with the atomic electron and then it is scattered or deflected at very small angles. The likelihood of this interaction increases as the photon energy decreases and the atomic number increases. In medical applications, this interaction cause loss of contrast in x-rays images and it has no significant effect on attenuation.

Compton, coherent, and photoelectric interactions with different absorbers such as water, compact bone, and sodium iodine for photon energy between 20 and 100 keV is shown in Figure 2.1.. These absorbers are a very appropriate choose to discuss the projectile with low-Z medium (water), medium-Z (compact bone), and high-Z medium (sodium iodine). Compton scattering dominates above 20–30 keV in water

and tissue. Photoelectric effect is important in bone and sodium iodine at low energies and high-Z absorbers. Coherent effect is clearly a small contributor for all of the photon energies.

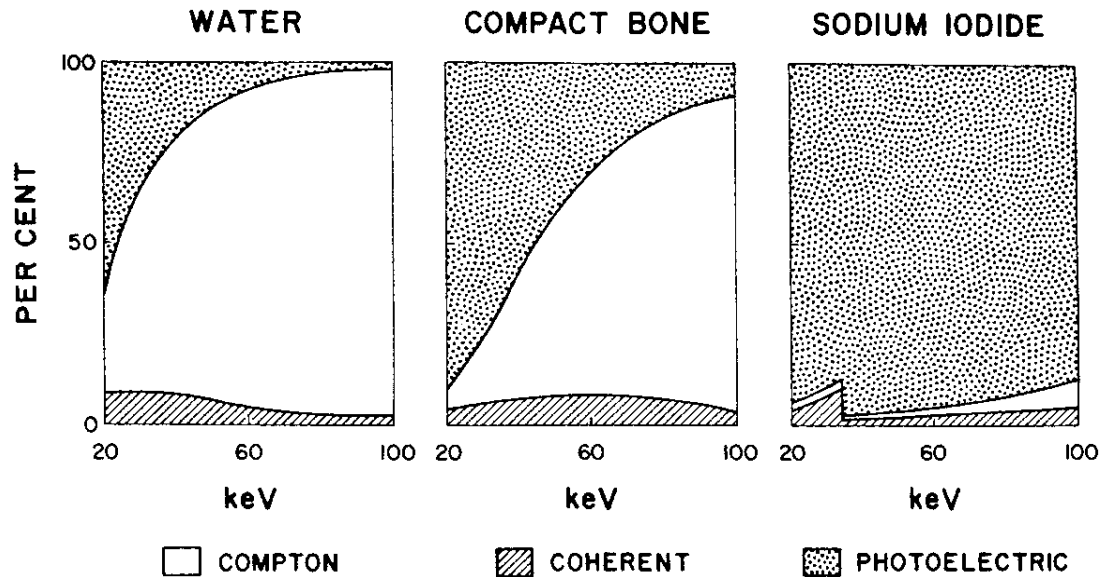


Figure 2.1. Compton, coherent, and photoelectric interactions with different absorbers such as water, compact bone, and sodium iodine [18].

2.1.3. Pair production

It is a process in which photon or energy is converted into matter [19]. When photons (x-rays or gamma-rays) have enough energy (greater than 1.022 MeV), then the photon can create an electron and positron [20]. Triplet production is a special case of the pair production process which happens in the vicinity of electrons. The threshold energy of this interaction is 2.044 MeV.

Finally, we have to mention that there is another photon interaction namely; photodisintegration effect or it is also called phototransduction [21, 22]. The threshold energy of this interaction is above 10 MeV for most nuclei (just for beryllium and deuterium, the threshold energy of this interaction is 2 MeV). In this case, a photon is absorbed by the nucleus of an atom resulting to the emission of proton or neutron.

The pair production, the photoelectric effect and Compton scattering are the main interactions of photon with matter. These processes with their occurrence probabilities as a function with the atomic number and the photon energy is shown in Figure 2.2. Clearly, the occurrence probabilities of these three processes increase as atomic number increases. Moreover, the photoelectric effect dominates the attenuation processes at low photon energies up to 150-400 keV. Therefore, this is a reason why the photon energy range of 15-150 keV is the energy used in diagnostic tests. On the other words, the photoelectric effect has a good influence to improve the medical images.

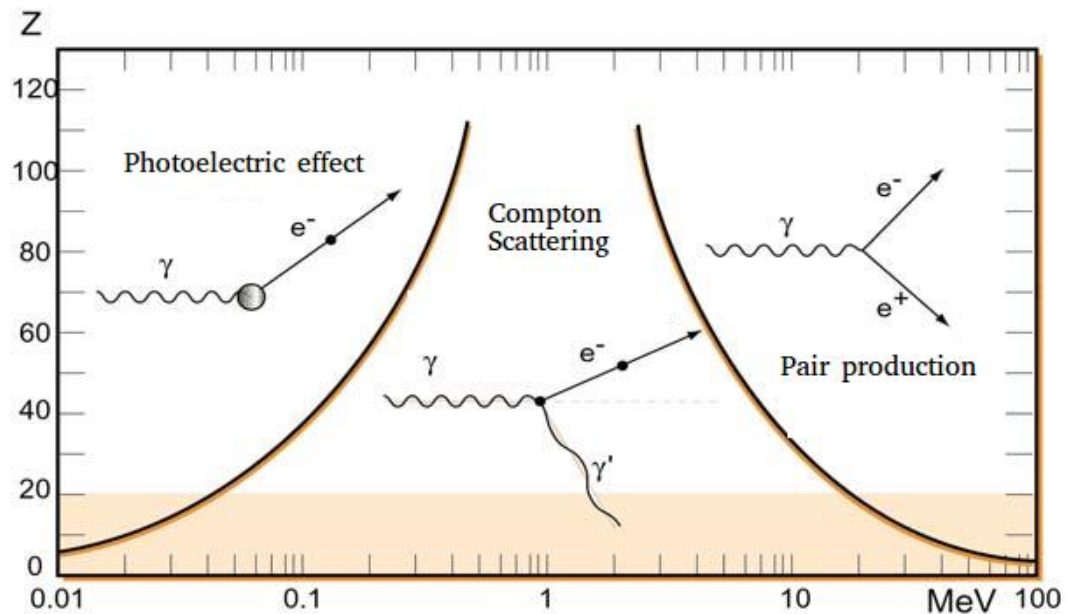


Figure 2.2. Relative importance of the three major types of photon interactions with the photon energy and the atomic number of the attenuating material as parameters.

At the intermediate photon energies, the Compton effect dominates the photon attenuation processes. Such effect is not preferable in medical applications due to the scattered photons from this effect have random directions leading to reduce the contrast of medical images. Finally, when the photon energy is greater than 1.022 MeV then a pair production mechanism may occur. However, this mechanism dominates the photon attenuation processes around 10 MeV (see Figure 2.2.).

2.2. Exponential Attenuation

The exponential attenuation (or the law of Beer- Lambert) is the basic concept to study the interaction of photon and neutron (e.g. uncharged ionizing radiations) that lose their energy in large interactions due to absorption or scattering [23-30].

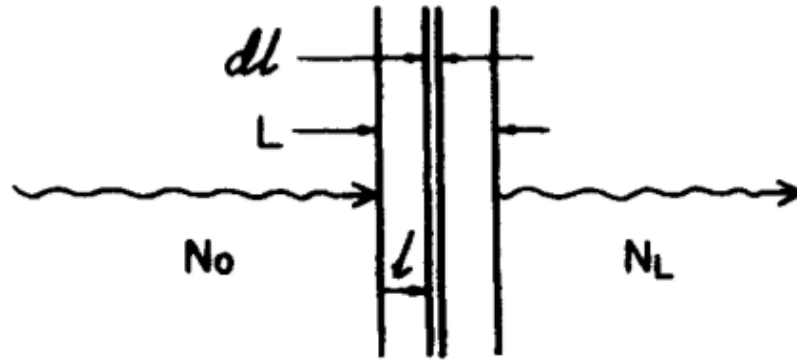


Figure 2.3. Simple exponential attenuation for a number of photons (N_0) passing a material of l thickness [18].

To apply the law of Beer- Lambert, a monoenergetic beam has to consider. This beam may consist of a huge number of photons denoted by N_0 (or by I_0) that incident on material with thickness of L as shown in Figure 2.3. In this case, we consider that the incident photons are totally absorbed without any production of secondaries.

Now if μ is the probability of the photon interaction, then for N incident photons on the thickness of dl we can write the following relation:

$$dN = -\mu N dl \quad (2.1)$$

Then by using a simple mathematic, the last equation can be written as:

$$dN = -\mu N dl \quad (2.2)$$

Moreover, by using the initial and final photon intensities (I_0 and I , respectively). Then, the Lambert–Beer law is well-known as [23-30]:

$$I = I_0 e^{-\mu x} \quad (2.3)$$

Where μ (in unit of cm^{-1}) is the linear attenuation coefficient, which can be expressed as a sum of the contributions from the main photon effects [31, 32]:

$$\mu = \sum_i \mu_i = \tau + \sigma_R + \sigma_C + \kappa \quad (2.4)$$

Here, τ refers to the contribution of photoelectric effect, σ_R refers to the contribution Rayleigh scattering, σ_C refers to the contribution Compton effect, and κ refers to the contribution of pair production process.

If we divide μ by the density of the material (absorber), we can obtain the mass attenuation coefficient (μ/ρ or μ_m). Then the mass attenuation coefficient can be given by the following equation [31, 32]:

$$\mu_m = \frac{\mu}{\rho} = \sum_i \left(\frac{\mu_i}{\rho} \right) = \frac{\tau}{\rho} + \frac{\sigma_R}{\rho} + \frac{\sigma_C}{\rho} + \frac{\kappa}{\rho} \quad (2.5)$$

The atomic cross section (atomic attenuation coefficient) μ_a can be calculated by the following equation [33]:

$$\mu_a = \frac{1}{\rho} \frac{A}{N_A} \mu = \frac{1}{\rho} \frac{A}{N_A} \sum_i (\mu_i) = \frac{1}{\rho} \frac{A}{N_A} (\tau + \sigma_R + \sigma_C + \kappa) \quad (2.6)$$

The electronic cross section (atomic attenuation coefficient) μ_e can be calculated by the following equation [31- 33]:

$$\mu_e = \frac{1}{\rho} \frac{A}{Z N_A} \mu = \frac{1}{\rho} \frac{A}{Z N_A} \sum_i (\mu_i) = \frac{1}{\rho} \frac{A}{Z N_A} (\tau + \sigma_R + \sigma_C + \kappa) \quad (2.7)$$

Here, Z is the atomic number, A mass number, and N_A is Avogadro's number. It is also worth mentioning that the mass attenuation coefficient is strongly related to the atomic cross section and then this parameter (μ/ρ) is more essential than the linear

attenuation coefficient. The reason is that the μ/ρ factor is independent of the density of the absorbing material.

In Figure 2.4., I shall demonstrate the total μ/ρ for two elements namely: carbon in subfigure of (a) and lead in subfigure of (b), these two subfigures give the most important examples to understand the μ/ρ (or partial photon interactions) for low-Z absorbing material and for high-Z absorbing material, here Z refers to the atomic number. From these figures, we can conclude that for low photon energies the photoelectric absorption is the dominant process. By increasing the photon energy and also when the Z is low, the Compton scattering is the dominant process that contribute largely in the attenuation factors. For high photon energies and high Z, the pair production is the dominant process. the Rayleigh scattering plays a secondary role in comparison with the other processes.

2.2.1. Energy transfer

The fraction photon energy that may transfer to kinetic energy for the charged particles released in the absorbing material, can be defined as the total energy transfer fraction (f_{tr}) [34]. Actually, this term can be given as a sum of the main particle photon processes that are mentioned above except the Rayleigh effect. The reason is that the Rayleigh effect does not transfer any energy, unlike the other processes that produce vacancies in the atoms of the absorbing material. Therefore, there are energy transfer fraction for the photoelectric effect (f_{PE}), energy transfer fraction for the Compton scattering (f_C), and energy transfer fraction for the pair production (f_{PP}). All these three fractions increase as the photon energy increases, while they have different relationships as a function of Z (atomic number of the absorbing material). Such that the f_{PP} does not relate to Z of the absorbing material, while the f_C has a slight relation with Z of the absorbing material.

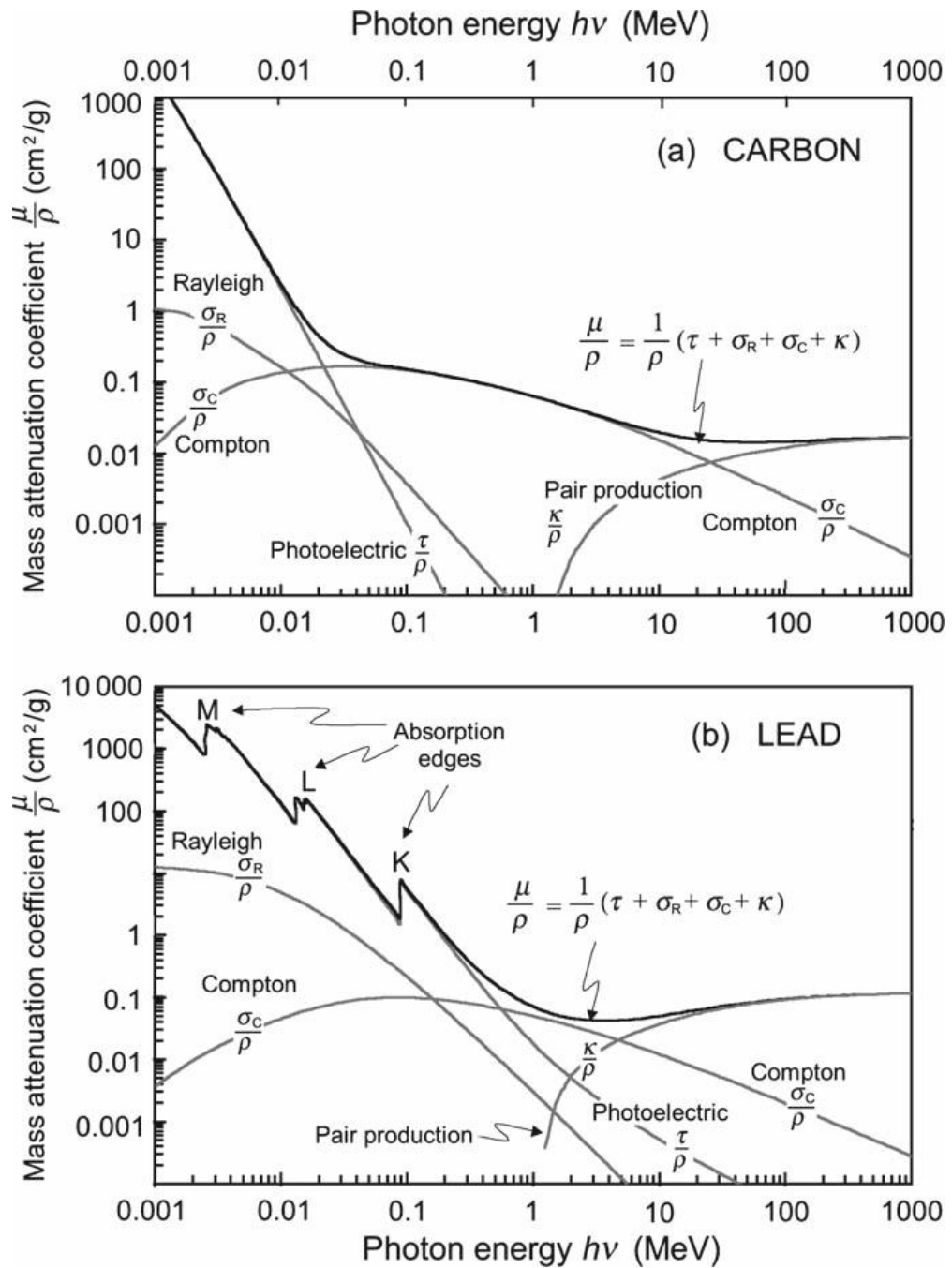


Figure 2.4. Total mass attenuation coefficients as a function of photon energy along with the partial photon interactions for (a) a carbon and (b) a lead [34].

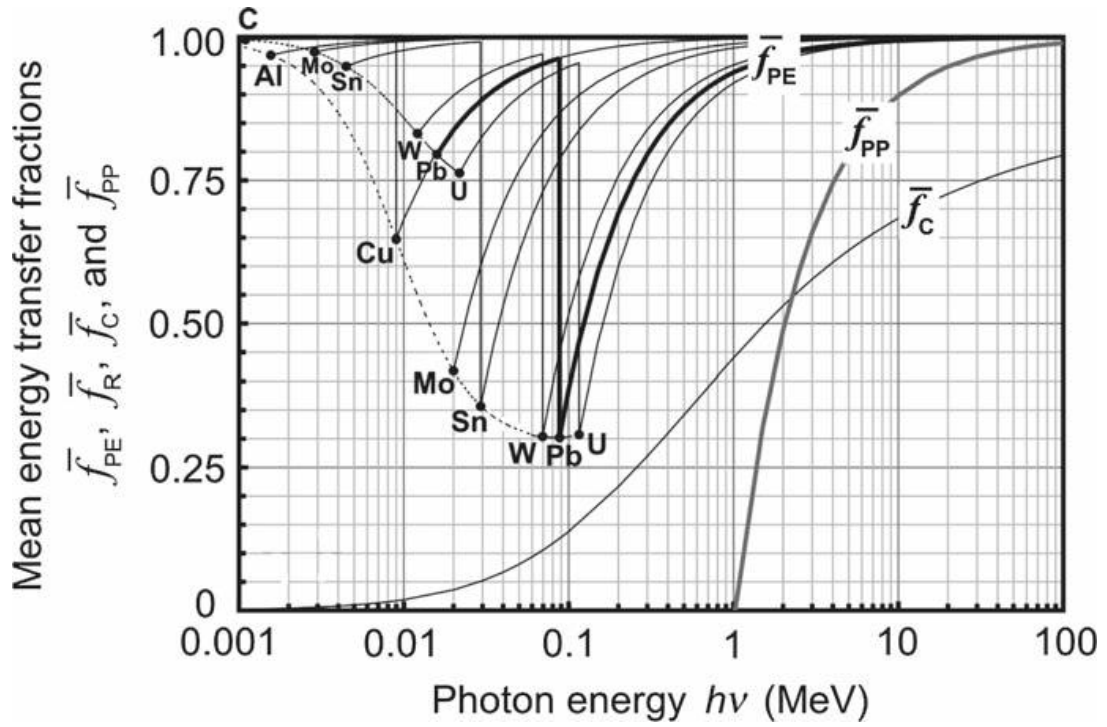


Figure 2.5. Mean energy transfer fractions as a function of photon energy for the photoelectric effect (f_{PE}), the Compton scattering (f_C), and the pair production (f_{PP}) [34].

In contrast, the f_{PE} has a strong relation with the Z of the absorbing material, for example the f_{PE} will be very small when the absorbing material has a high Z . This relation between the energy transfer fractions and both of photon energy and atomic number can be summarized in the following Figure 2.5. When we know the total energy transfer fraction, then by using the mass attenuation coefficients the linear energy transfer coefficient (μ_{tr}) with the help of the following equation [34, 35]:

$$\mu_{tr} = \mu \frac{E_{tr}}{h\nu} = \mu f_{tr} \quad (2.8)$$

2.2.2. Energy absorption

Similar to the discussion of the total energy transfer fraction, we can find the following relation between the linear energy absorption coefficient (μ_{ab} or μ_{en}) and the linear attenuation coefficient [36, 37]:

$$(2.9)$$

$$\mu_{ab} = \mu \frac{E_{ab}}{h\nu} = \mu f_{ab}$$

Here, $h\nu$ is the photon energy. Now, by using the values of μ_{tr} and μ_{ab} , one can easily calculate the mass coefficient that are related to these factors; mass energy transfer coefficient (μ_{tr}/ρ) and mass energy absorption coefficient (μ_{ab}/ρ). Here, we can introduce very important parameter namely; mean radiation fraction (g) that is given by the following relation [38-40]:

$$g = 1 - \frac{\mu_{ab}/\rho}{\mu_{tr}/\rho} \quad (2.10)$$

Figure 2.6. shows the mean radiation fraction g as a function of photon energy for eight selected absorbers ranging from carbon to uranium for (a) total mean radiation fraction g and its bremsstrahlung component g_B and (b) the total mean radiation fraction g and its annihilation component g_A . This data was obtained by utilizing the $g/EGSncMP$ code. Clearly, part (a) shows a linear scale for g and g_B with heavy solid curves the total g and with light solid curves its bremsstrahlung component g_B for the various absorbers. Part (b) shows a logarithmic scale for g and g_A with the total g and its annihilation component g_A .

Finally, all the mentioned coefficients can be expressed in the case of compounds or mixtures by applying the mixture rule that is given by (such an example in the case of linear coefficients) [36-38] :

$$\mu = \sum_i \omega_i \mu_i \quad (2.11)$$

$$\mu_{ab} = \sum_i \omega_i (\mu_{ab})_i \quad (2.12)$$

$$\mu_{tr} = \sum_i \omega_i (\mu_{tr})_i \quad (2.13)$$

Also, the same rule (mixture rule) can be applied for the other attenuation coefficients such as mass, atomic, and electronic attenuation coefficients.

2.3. Buildup Factors

ANSI (American National Standards Institute)-or as known as ANS standards-provided a huge database to derive the buildup factors (BUFs) (as well as different factors such as attenuation coefficients) for some chosen engineering materials and elements for use in radiation studies [41]. The BUFs that are provided by ANS standards were collected from the database of two decades ago. The BUFs was firstly introduced by White in 1950 to study and describe the penetration of gamma ray (emitted from ^{60}Co) in water [42]. Later on, the BUFs of concrete were obtained for a point isotropic gamma ray [43]. Nowadays, many Monte Carlo codes and computer programs can be used to perform complex computationally demanding for calculating BUFs more accurately and in very short time [44-46].

2.3.1. Definition of buildup factor

Photon attenuation is a very complex mechanism that can be described by the attenuation exponential law (the law of Beer- Lambert) only under three conditions, which are [47-50]:

- 1- The source of the photons (X/gamma rays) should emit monoenergetic beam.
- 2- The setup of experimental has to be narrow beam geometry.
- 3- The slab of the studied sample should to be thin.

In the case of one of these conditions is missing, then a correction factor namely; BUF should to be considered to study, describe, and understand the attenuation process. Consequently, the BUF is a correction term that includes the effect of the scattered photons and any produced secondaries in the studied material [47, 48]. In the other word, the BUF is a multiplicative factor that explains the effect of the

uncollided photons. Therefore, the BUF may describe a ratio of the total dose to the response for uncollided dose [49, 50].

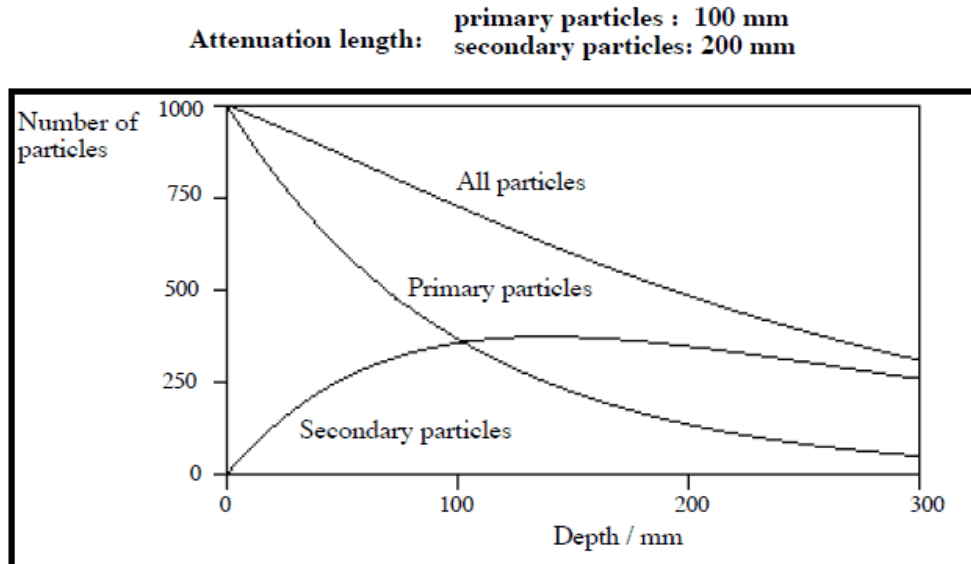


Figure 2.6. Buildup factor of scattered radiation and secondary particles [52].

Generally, there are two types of buildup factors namely; exposure buildup factor (EBF) and energy absorption buildup factor (EABF) [51]. The EBF is related to the exposure of gamma-rays and is defined as the measured value of the dose absorbed in the air by a detector [51]. On the other hand, the EABF is related to the absorbed or deposited energy in the shielding material, and can be defined as the ratio of a particular energy absorbed by per unit volume in the medium to that of non-scattered radiation in the same medium [51]. Figure 2.6. shows the buildup factor that considers the influence of the scattered radiation plus any secondary particles during the dose/dosimetry calculations [52].

2.3.2. Calculation of buildup factor

Calculation work of the buildup factors can be summarized in three steps as [53-55]:

- 1) Calculation of equivalent atomic numbers (Z_{eq}),
- 2) Calculation of G-P fitting parameters,
- 3) Calculation of buildup factors.

The following interpolation formula was used for Z_{eq} values where C corresponds to the ratio of Compton attenuation to the total attenuation $((\mu/\rho)_{Comp}/(\mu/\rho))$, and Z_1 and Z_2 are the elemental atomic numbers related to the ratios C_1 and C_2 , respectively [52-55].

$$Z_{eq} = \frac{Z_1 (\log C_2 - \log C) + Z_2 (\log C - \log C_1)}{\log C_2 - \log C_1} \quad (2.14)$$

The total and partial μ/ρ values for the glass systems were obtained from XCOM photon cross section library as mentioned before. Following this step, Z_{eq} values were then used to compute the G-P fitting parameters by a similar interpolation method developed by ANSI/ANS-6.4.3-1991 [41]. Finally, the fitting parameters were applied to evaluate the values of related buildup factors for the present glasses using the following set of formulae given by [55-60]:

$$B(E, x) = 1 + \frac{(b-1)(K^x - 1)}{K - 1} \quad \text{for } K \neq 1 \quad (2.15)$$

$$B(E, x) = 1 + (b - 1)x \quad \text{for } K = 1 \quad (2.16)$$

$$K(E, x) = cx^a + d \frac{\tanh\left(\frac{x}{X_k} - 2\right) - \tanh(-2)}{1 - \tanh(-2)}, \quad x \leq 40 \text{ MFP} \quad (2.17)$$

In this set of equations, x is the distance of the detector to source in MFP, b is the exposure buildup value at 1 MFP and $K(E, X)$ term is named the dose multiplication factor [60, 61].

2.4. Radiation Dose

For all the types of radiation (directly or indirectly ionizing radiation), there is a relevant term namely; absorbed dose [62, 63]. However, I shall discuss the absorbed dose that is mainly related to the radiation of photons (X/gamma rays) [64-66].

2.4.1. Concepts and units

The concept of radiation dose (or shortly well-known as dose) is related to two important terms [67, 68]:

- 1) The deposited energy in the studied material.
- 2) The damaging effects of the radiation type.

Therefore, the amount of energy deposited per unit mass is called absorbed dose that is measured by the unit of rad (radiation absorbed dose), where 1 rad equals to 100 erg/g of material. In fact, Gray (Gy) is the SI unit of the absorbed dose, where:

$$1\text{Gy} = 1\text{J/Kg} = 100\text{rads} \quad (2.18)$$

Consequently, the Gy/s can be used for indicating the dose rate. Another important concept is the equivalent dose that is commonly known as HT or H. It should mentioning that the absorbed dose is more essential than the equivalent dose that is more biologically important. The unit of HT is sievert (Sv), where 1 Sv equals to 100 rem.

Furthermore, the equivalent dose (HT) is related to the absorbed dose (D) by the following equation [69, 70]:

$$HT = D \times Q \quad (2.19)$$

Here, Q is the quality factor that describes the the damage associated with each kind of radiation, for example, Q equals to 1.0 for photons and electrons, Q equals to 20 for alpha particles, and Q is between 2 and 10 for neutrons. Then, rem equals to rad times Q.

2.4.2. Radiation exposure

When X/gamma rays interact in the air, some atoms are ionized (emission of electric charge) by such radiation. A measure of this ionization is called radiation exposure that is defined by the unit of roentgen (R), and then the exposure rate can be expressed as R/s [71]. Therefore, it can be written as follows

$$1R = \frac{1esu \times 3.336 \times 10^{-10} C/esu}{0.001293g} \times 10^3 g/Kg \quad (2.20)$$

By using a simple mathematic, then we can get the following relation

$$1R = 2.58 \times 10^{-4} C/Kg \text{ of air} \quad (2.21)$$

It should noting that Exposure and exposure rate can be applied only to X/gamma rays and only in air. Not to describe the deposited energy in the body and not for any other type of radiation such as proton, electron or alpha particles. Finally, the fluence rate or flux (number/cm² s) is governed by the inverse square law that is given by the following relation:

$$\phi(\text{number}/\text{cm}^2 \text{ s}) = \frac{S(t/s) f_i}{4\pi r^2} \quad (2.22)$$

Here, S (t/s) is the activity of the point source, f_i is the fractional yield for each emitted radiation, r is the distance between the point source and the matter. For example, the photon (or gamma) flux of a 1 mCi point source of ¹³⁷Cs can be estimated at a given distance (e.g. 100 cm) to be $\phi = 2.5 \times 10^2$ gamma/cm² s. In this example, S = 1 mCi = 3.7×10^7 t/s. Moreover, I used $f_i = 0.85$ gamma/t due to ¹³⁷Cs has half time of 30.07 y and it emits 0.662 MeV gamma rays in 85% of its transformations.

Table 2.1. Different types of radiation with their properties.

Radiation	Charge	Energy	Range in air	Range in H ₂ O
Alpha particles	+2	3-10 MeV	2-10 cm	20 – 125 μ m
Beta particles	+1, -1	0-3 MeV	0-10 m	< 1 cm
Neutrons	0	0-10 MeV	0-100 m	0-1 m
X-rays	0	0.1-100 keV	m-10 m	mm -cm
Gamma-rays	0	0.01-10 MeV	cm-100 m	mm-10 cm

This example is done for gamma rays and the flux can be calculated for any type of radiation by the same way. Generally, charged particles lose their main energy by ionization, while the photons (as well as the neutrons) lose their main energy by the absorption and scattering events. Table shows some features of the major types of radiation.

In the case of photons, the mechanisms of energy transfer and energy absorption can be occurred in two processes as given in Figure 2.7. In the first process, a photon interacts with the matter and gives its energy to an electron (a photon gives its all energy to an electron by the photoelectric effect, while the photon gives a part of its energy by Compton effect) [72]. This process is well-known as kerma (kinetic energy released in matter) that is related to the transferred energy (E_{tr}) [73-79]. In the second process, the ejected electrons may deposit their energy to the matter by ionization and excitation.

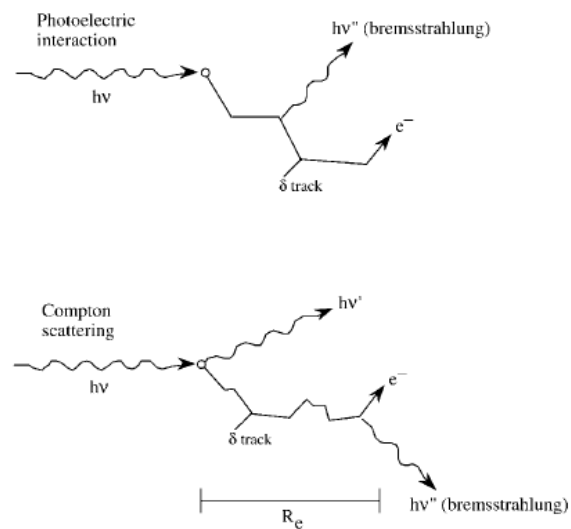


Figure 2.7. The mechanisms of energy transfer and energy absorption occurred in two processes [75].

This process is well-known as absorbed dose that is related to the deposited energy over the entire range (R_e) in the matter. Therefore, there is a direct relation between the kerma and flux of the photons as [75-79]:

$$K_{med} = \phi \left(\frac{\mu}{\rho} \right)_{med} E_{tr}(h\nu) \times 1.6022 \times 10^{-6} \text{ erg/MeV} \quad (2.23)$$

Here, the subscript of med refers to the studied medium. The μ/ρ is the mass attenuation coefficient. Finally, the flux is in unit of photons/cm².

2.4.3. Dose calculation

Dose (or exposure) calculation of the photons beam is a simple task when a fluence rate of the photons or the flux (photons/cm² s) can be obtained. Another important parameter for the dose calculation is the energy fluence (MeV/cm²) that can be utilized to calculate the exposure in air (e.g. EBF) or energy deposited in a matter (e.g. EABF) [80-82].

The relation between the exposure rate and photon flux is given in Figure 2.1. Clearly, there is a direct proportion between the exposure rate and photon flux. In the range between 70 keV and 2 MeV, it can be seen that the curve is a quite linear. Such relation is helpful in dose calculation, e.g. the inverse square law of the exposure rate for point sources depends on source strength and gamma constant for each emitted energy. I shall discuss the last sentence in more details in the coming paragraph.

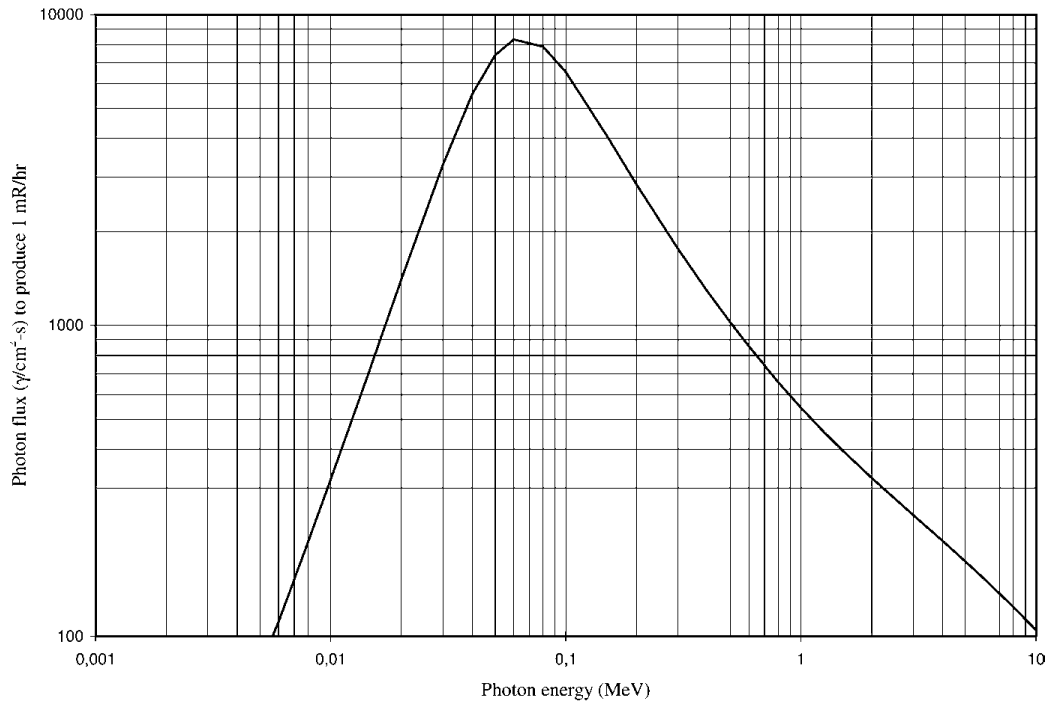


Figure 2.8. Photon flux (Gamma/cm² s) to produce an exposure rate of 1 mR/h [72].

The inverse square law of the exposure (in unit of R/h) at a distance of $r = 1\text{m}$ and per one curie is given by [83]:

Exposure =

$$\frac{Ci \times 3.7 \times 10^{10} \text{ t/s} \times f \times E(\text{MeV}) \times 1.6022 \times 10^{-6} \text{ erg/MeV} \times 0.0275 \text{ cm}^2/\text{g} \times 3600 \text{ s/h}}{4\pi r^2 (100 \text{ cm/m})^2 \times 87.64 \text{ erg/gR}} \quad (2.24)$$

By using a simple mathematic, then we can get the following relation [83]:

$$\text{Exposure} = \frac{0.533 \times Ci \times f E}{r^2} \text{ R/h} \quad (2.25)$$

Here, E is the photon energy in the range of 0.07-3 MeV and the f is the number of emitted photons (see previous example, how $f = 0.85$ is chosen).

Now, it is very interesting to say that exposure rate in the unit of R/h can be expressed as a gamma ray constant (Γ) for a distance of 1 m and for activity of one Ci.

2.5. Charged Particle Interactions with Matter

Photons and neutrons (e.g. uncharged particles) have a probability of passing a thick layer of matter without losing any energy, but electrons and protons (e.g. charged particles) have to lose some or all their energies as they pass through a matter. Moreover, Photons have no limiting “range” through matter, while the electrons and protons have a limiting range [83, 84].

Charged particles are inclosed by its Coulomb electric field. Such field may interact all things (electrons, nucleus, or atoms) that it encounters, as it passes through an absorbing medium. The transferred energy from the charged particles to the absorbing material is a very small, therefore the charged particles undergo a huge number of collisions before their energy is lost. To understand the interactions of charged particles with matter, some important parameters such as stopping power, range, radiation yield, effective atomic number, and mean ionization potential are used. It is also worth mentioning that there are two types of stopping power namely; collision stopping power (it refers to the interaction of charged particle with electrons of absorbing material) and radiation stopping power (it refers to the interaction of charged particle with nuclei of the absorbing material) [85-87]. As the charged particles pass a matter, they experience the Coulomb force (from the positive nuclei and the negative atomic electrons). Therefore, according to the classical atomic radius (a) and the classical impact parameter (b) of the charged particles, one can distinguish three categories of effects between the charged particle and matter (absorbing medium):

- 1) Soft collision, when $b \gg a$.
- 2) Radiation collision (bremsstrahlung production), when $b < a$.
- 3) Hard collision, when $b = a$.

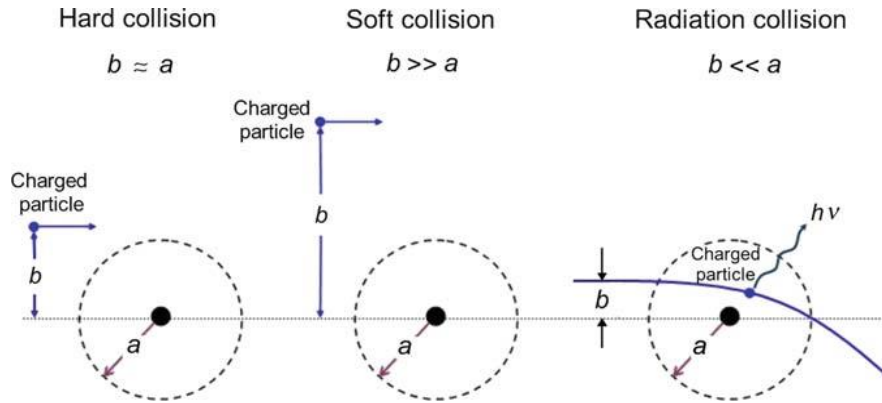


Figure 2.9. Three different types of collision of a charged particle with matter [34].

Figure 2.9. shows these different types of collision of a charged particle with matter. In the soft collision (distant collision), the size of the charged particle is bigger than the size of atom and then the charged particle interacts with the whole atom. The number of interactions will be large and a small amount of energy will be transferred from the charged particle to the atomic electrons. In the radiation collision, the size of the charged particle is smaller than the size of atom and then the charged particle may interact with the nucleus in terms of elastic and inelastic interactions. Generally, the elastic interactions will be more than the inelastic interactions. A small amount of energy will be lost (from the charged particle) in the case of elastic interaction, while a large amount of energy will be lost in the case of inelastic interaction, for example, x-rays production. Finally, in the case of hard interaction, the size of the charged particle is in the order of the size of atom and then a direct Coulomb impact interaction will be occurred and a large amount of energy will be lost [86-88].

2.5.1. Stopping power

The motion of the charged particle within a matter is associated with a huge number of interactions. Such interactions effect the path of the charged particle, according to the type of interaction (soft, hard, or radiation), resulting to lose some energy that may transfer to matter (collision lose) or to photons (radiation lose). Generally, the rate of energy loss (in unit of MeV) per unit of path (in unit of cm) is named the linear stopping power ($-dE/dx$). From this quantity, we can derive an important parameter namely; mass stopping power (S), in unit of $\text{MeV} \cdot \text{cm}^2/\text{g}$, that is given as

a ratio between the $-dE/dx$ and the density of the absorbing medium [88, 89]. According to the interaction type of the charged particle, there are two types of the stopping power namely; radiation (or nuclear) stopping power (S_{rad}) and collision (ionization or electronic) stopping power (S_{col}). Therefore, the total stopping power can be given as the sum of them [88-91].

2.5.2. Range of charged particles

The range (denoted by R) of the charged particle refers to the thickness that can be penetrated by the particle as it passes through a matter. In fact, the R is an experimental notion that depends on mass, charge, and energy of the particle (e.g. electron, proton, or alpha, ...etc), as well as on the chemical components of the absorbing material [90, 91]. Figure 2.10. shows the penetration into matter for heavy charged particles (proton, α particle, heavy ion, etc) and light charged particles (electron or positron).

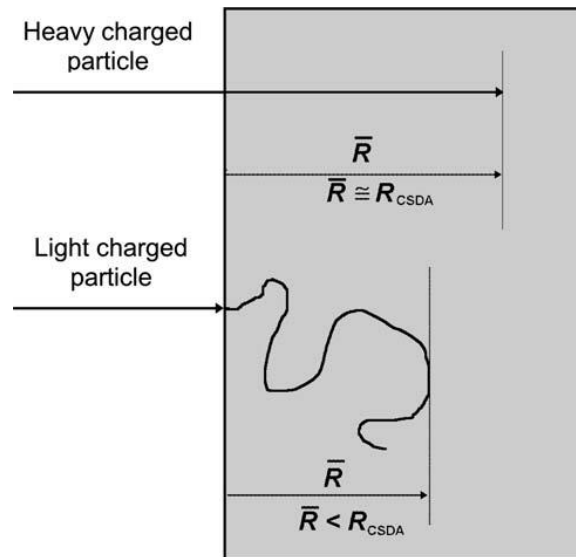


Figure 2.10. Schematic diagram of the penetration into matter for heavy charged particles and light charged particles [34].

As it can be seen from the figure, heavy charged particles have linear paths within a matter. Therefore, they do not show a large amount of energy losses. However, the

light charged particles have a tortuous path within a matter. Therefore, they will experience a large amount of energy losses [90, 91].

CHAPTER 3. MONTE CARLO METHOD

Monte Carlo (MC) method is called referring to the city of Monaco which is the gambling hot spot. This is due to the chance and random results of this method are much like dice, and slot machines. The MC method was first developed by a mathematician of Stanislaw Ulam. This chapter gives fundamental principles of Monte Carlo method, describes Geant4 toolkit, and reports the using of this method in radiation transport studies.

3.1. Fundamental Principles

The Monte Carlo method is a technique that depends on inferential statistical approaches to solve, describe, and understand any problem by using the generation of random events. This generation is not totally random but it is governed by some conditions, rules, and limitations. For example, one needs to know the scientific rules of the studied problem, the boundary limitations of the considered system, and the selection rules [92].

To understand the Monte Carlo method, I will give you an example for solving a simple problem by using this method. Suppose that we need to estimate the value of Pi ($\pi = 3.14$) by using the MC method. For this task, let us draw a circle inside a square as shown in Figure 3.1.

The area of the circle (A_c) is given by $A_c = \pi r^2$, and the area of the square (A_s) is given by $A_s = 4r^2$. By dividing A_c by A_s , we can write that:

$$\frac{A_c}{A_s} = \frac{\pi}{4} \quad (3.1)$$

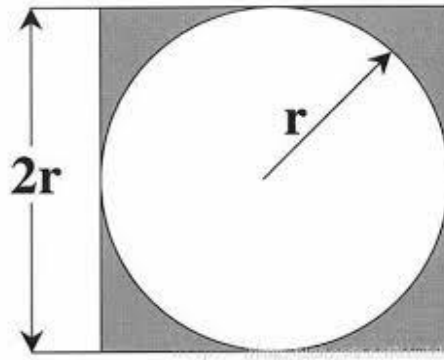


Figure 3.1. A circle with radius of r , inside a square with length side of r .

Here where the MC method comes in. Such that equation 1 can be written as: $\pi = 4 \times$ (number of points in the circle / total number of points). Now, if we assume the radius of circle is 1, then we can generate random events (x, y) and then check the following rule $x^2 + y^2 \leq 1$!

I mean that all the points of $x^2 + y^2 \leq 1$ are inside the circle. So, by using equation 2 we can get the value of π . In fact, this is a simple example (Try it by using Excel) to show how we can imagine the problem with its conditions, boundaries and rules. However, in the physical problems the solution will be complicated and the using of computer is required.

Nowadays, MC methods is a basic part in several fields including medicine, industry, and space. It acts as a bridge between the experimental results and the theoretical predictions. Therefore, a number of general-purpose MC codes were developed to save a time and effort for solving the complicated problems. ETRAN Monte Carlo code was early introduced by Seltzer [93]. This code gives solutions of coupled electron-photon transport problems including the cross sections of multiple-scattering for energies reaching to 1 GeV. Waters developed new Monte Carlo platform namely: MCNPX that can track almost 50 types of particles [94]. It is worth mentioning that MCNPX is derived from MCNP [95]. PENELOPE is a simulation code that was developed for radiation transport in matter by Issy et al., [96]. EGS and EGS4 are also simulation platforms that were developed respectively as mentioned in Refs [97, 98]. GEANT3 is all-particles Monte Carlo code developed

for carrying out the high energy physics [99]. Geant4 is a new version of Geant3 implemented by C++ software language using object-oriented method [100].

3.2. Geant4 Toolkit

Geant4 toolkit is developed as an object-oriented Monte Carlo simulation code system to study the propagation and interaction of a large set of particles with matter in a wide energy range by the help of different electromagnetic, nuclear and hadronic models. Usage of Geant4 started with simulating the interactions of elementary particles at high energies for exploring the standard model (SM) and beyond standard model (BSM). The scope of the code was extended for years and several nuclear and electromagnetic models were included into the code, hence, it is now capable of working over a wide range of particle energies from keV to PeV scale. Today, Geant4 as a simulation toolkit takes an important place in various study fields including medical physics, radiation physics, and space. Geant4 deals with almost 2000 classes containing 1 million lines coded by C++ language [100].

Geant4 simulations were extensively benchmarked with different experiments in various fields as well as were also benchmarked with different theoretical approaches and other Monte Carlo codes. For example, Geant4 models were benchmarked with the experimental results of the hadron therapy [101]. Al-Buriahi et al., studied the photon attenuation properties of some human tissues by using Geant4 toolkit, theoretical calculations and experimental data [102]. Especially in our scope of study, there are many successful researches to show the powerful of Geant4 simulations comparing with other simulations codes and comparing with the theoretical calculations [103-108]. Among these studies, Amako et al., reported an important comparison between the electromagnetic models of Geant4 against NIST database [103]. This study proved the applicable and strengths of the Geant4 models to deal with radiation attenuation investigations on materials. Yoriyaz et al., studied the absorbed fractions of different radiations (proton, electron and photon) by using various simulation codes [108].

3.2.1. Geometry

Geant4 package contains the geometry subroutines to provide the construction of the geometrical model even if the geometry is complicated. This can be achieved by the help of parts namely; LOGICAL and PHYSICAL volumes. The LOGICAL part contains the definition of a detector along with its properties such as its size, shape, and material. The PHYSICAL part has information of the spatial position of the LOGICAL part (or volume). The logical volume, in Geant4 toolkit, can be refined by specifying the shape like a separate entity namely; a solid. Such these shapes like spherical, rectilinear boxes, trapezoids, or cylindrical sections or shells. In Figure 3.2. we show the quadric surfaces used in Geant4 simulations [109]. The physical and chemical properties of these shapes can be defined in the class of Constructed Solid Geometry (CSG).

3.2.2. Particles

The particles category in Geant4 toolkit can implement all facilities that are needful and helpful to mimic the chemical and physical features of particles such as photon, electron, proton, and neutron (as well as muon, neutrino, ..etc), to simulate the electromagnetic and the nuclear interactions. These particles can be defined by using the G4ParticleDefinition class, that can be useful to characterize the fundamental features of particles in terms of charge, mass, and .. etc [110, 111]. Moreover, this class can be used to describe all the sensitive processes that the particle may undergo. For example, all the processes of photon-matter interactions that are denoted by (photoelectric effect, Compton scattering, and ..etc). Additionally, the class of G4ParticleDefinition includes the cuts information such as energy cut, range cut.

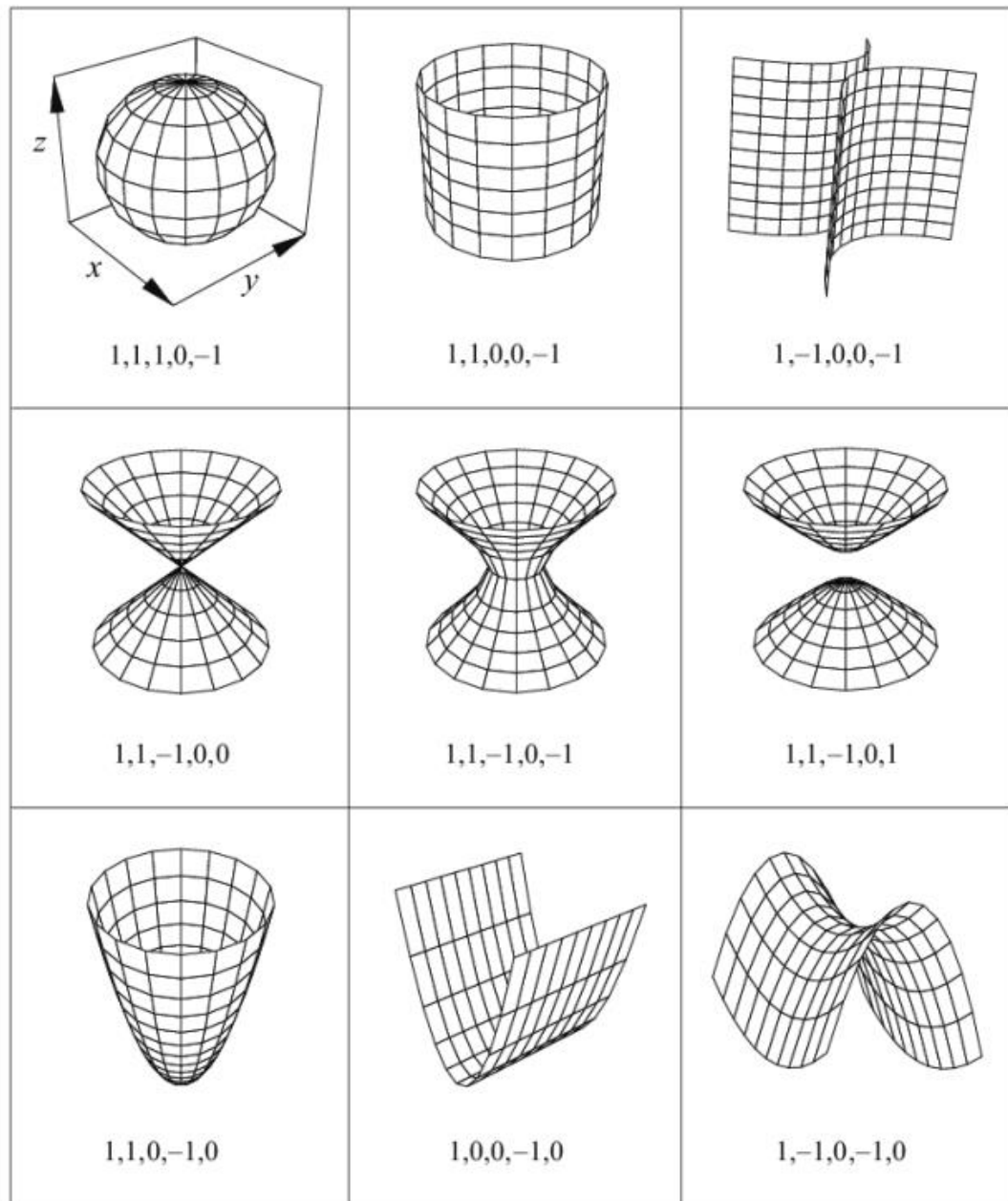


Figure 3.2. Different geometrical shapes that can be defined by using Geant4 simulation toolkit [110].

3.2.3. Materials

In Geant4 toolkit, there is a wide set of materials that are about 280 materials ranging from the fundamental elements such as lithium (Li), lead (Pb), and sodium (Na) to the complex compounds and mixtures such as water (H₂O), lanthanum oxysulfide, or

tissues like lung, bone, and breast. The material description is based on three main classes namely: G4Isotope, G4Element, and G4Material. The first class (G4Isotope) is utilized to describe the isotopes in terms of their atomic number (Z), mass, molar mass, isomer state, and number of protons and neutrons (nucleons number). This class is very simple and has not any computation or physical models. The data in this class is taken from NIST database. The second class (G4Element) is utilized to describe, by the help of relative abundance, the elements as isotopes composition. This class includes the G4AtomicShells utility class that has the information of the shell structure of the atomic electrons. The third class (G4Material) is utilized to describe a material as a compound or mixture along with all its physical features such as temperature, density, pressure, and state [111, 112]. Furthermore, a material owns some ionisation features that can be extracted from G4IonisParamMat object.

3.2.4. Physical models

Geant4 toolkit has no a single model to describe the physical interactions of particles at a wide energy range between 0 and TeV scale, however, Geant4 toolkit offer smart class namely; Physics Lists that can carry out any simulation task. Therefore, the physical models of the particle propagation through any medium can be presented by the following steps; i) Physical Model that includes the final state generator, ii) Physical Processes that includes the cross sections, iii) Physics List that includes the physical processes for every particle involved [110-113].

Physics List manages the physics processes that give a full understanding of the interactions of particle with matter. Geant4 toolkit offers seven main physics processes of the interactions of particle with matter. These seven processes are electromagnetic, hadronic, optical, decay, transportation, parameterisation and photolepton-hadron.

Table 3.1. List of process and model classes for gamma.

EM process	EM model
G4PhotoElectricEffect	G4PEEffectFluoModel
	G4LivemorePhotoElectricModel
	G4LivemorePolarizedPhotElectricModel
	G4PenelopePhotoElectricModel
G4PolarizedPhotoElectricEffect	G4PolarizedPEEffectModel
G4ComptonScattering	G4KleinNishinaCompton
	G4KleinNishinaModel
	G4LivemoreComptonModel
	G4LivemoreComptonModelRC
	G4LivemorePolarizedComptonModel
	G4LowEPComptonModel
G4PolarizedCompton	G4PenelopeComptonModel
	G4PolarizedComptonModel
G4GammaConversion	G4BetheHeitlerModel
	G4PairProductionRelModel
	G4LivemoreGammaConversionModel
	G4BoldyshevTripletModel
	G4LivemoreNuclearGammaModel
	G4LivemorePolarizedGammaModel
G4PolarizedGammaConversion	G4PenelopeGammaConversion
	G4PolarizedGammaConversionModel
	G4LivemoreRayleighModel
G4RayleighScattering	G4LivemorePolarizedRayleighModel
	G4PenelopeRayleighModel
G4GammaConversionToMuons	

3.2.5. Production cuts

Geant4 toolkit has no tracking cuts. This means that the incident projectile is tracked to until its kinetic energy will be equal to zero even if it reaches the border of the simulation geometry. Such that has a negative effect on the accuracy of the results. So, it is very useful to produce some cuts (according to the limitations of study involved) to stop the generation of incident particles and produced secondaries [113].

CHAPTER 4. MATERIALS AND METHODS

In this chapter, we shall illustrate the studied materials in the present thesis. The studied materials are eight essential biomolecules which are the fundamental part of organisms (human, animal, and. etc) to express a life. Therefore, we shall discuss the meaning of these biomolecules, the types of the biomolecules, and some properties of the essential biomolecules involved in the present work. Moreover, the methods used to evaluate the parameters of radiation interaction with these biomolecules are described in detail.

4.1. Materials

4.1.1. Meaning of Biomolecules

A cell is the fundamental part of organisms (human, animal, and. etc) to express a life. It is a warehouse of the most important information that it is responsible for all of bioactivities. The myriads of biomolecules are in living cell. Such biomolecules include disaccharides, monosaccharides, polysaccharides, proteins, amino acids, enzymes, fats and oils, fatty acids, nucleotides, histones, nucleic acids, acidic proteins, haemoglobin, chlorophyll, and a multiple of several other biomolecules. Viruses that include protein and RNA or DNA, are perhaps the simplest of living organisms.

A Biomolecule is a complicated organic molecule. A large number of biomolecules are in living cell that is a fundamental unit of organizations. These include saccharides (monosaccharides and disaccharides), amino acids, fatty acids, nucleotides, haemoglobin, chlorophyll, polysaccharides, proteins, enzymes, fats and oils, nucleic acids, histones, acidic proteins, and a multiple of several other

components. Figure 4.1. shows that the biomolecules are related to the living organisms in the following sequence; Living cells, organs, tissues, cells, organelles, and biomolecules. Moreover, the biomolecules are the building blocks of DNA and RNA, the molecules that are involved in heredity.

The investigations on biomolecules are related to various applications and fields including biochemistry, biology, genetics, medical physics and radiation physics.

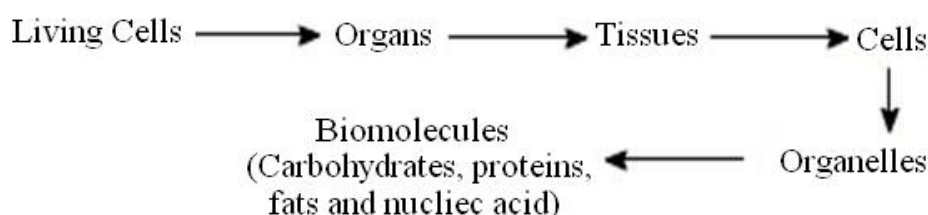


Figure 4.1. Schematic diagram of the relation between the biomolecules and living organisms.

For example, the field of biochemistry is related to the structural and functional properties of the biomolecules in the living organisms. This work gives data and information about the radiation interactions with the biomolecules. These biomolecules are essential to humans, animals, and other organisms due to their important to accelerate the bioactions that may take a long time to sustain life [114-116]. Such work is closely related to the medical physics and radiation physics.

4.1.2. Types of biomolecules

There are many types of biomolecules such as nucleotides, lipids, hormones, carbohydrates, proteins, amino acids, and vitamins. The nucleotides make up DNA and RNA that are included in heredity. The hormones play an important role in the regulation of metabolic processes. The lipids may act as energy providing molecules. The carbohydrates can serve as energy storage molecules. The amino acids provide the preparation of proteins [117]. Therefore, we can divide the types of biomolecules into:

- 1) Small molecules: This type includes lipids, glycolipids, phospholipids, glycolipids, sterols, carbohydrates, sugars, vitamins, hormones, neurotransmitters, and metabolites.
- 2) Monomers: This type includes amino acids, monosaccharides, and nucleotides.
- 3) Polymers: This type includes peptides, polypeptides, oligopeptides, proteins DNA, RNA, nucleic acids, oligosaccharides, polysaccharides (including cellulose), lignin, cellulose, and haemoglobin.

Carbohydrates consist of many groups of glucose units joined together by glycosidic bonds. Figure 4.2. shows the structural chemical formula of glucose. The carbohydrates are named indicating to the general chemical form that is given by $(\text{CH}_2\text{O})_n$, here n is an integer. For $n = 6$ we can write $(\text{C}_6\text{H}_{12}\text{O}_6)$. It is worth mentioning that the name of sugar refers to small carbohydrates that include single sugars (monosaccharides), two sugars linked together (disaccharides), and many sugars linked together (polysaccharide).

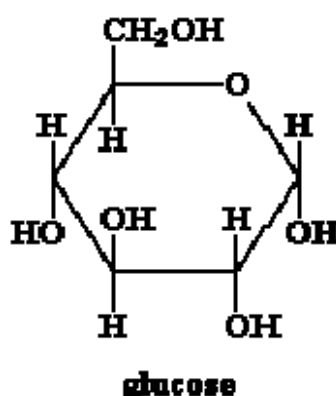


Figure 4.2. Structural chemical formula of glucose [117].

The carbohydrates have many functions such as serving as precursors for building many polymers, providing structural building materials, storing short-term energy, and serving as molecular "tags" to allow recognition of specific cells and molecules.

An amino acid contains both amino (NH_2) and carboxyl (COOH). Figure 4.3. shows the structural chemical formula of amino acid (Alanine as standard amino acid).

Amino acids are critical to life. They have many important functions including the metabolism. Moreover, amino acids are the building blocks of proteins [118].

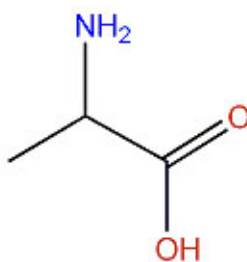


Figure 4.3. Structural chemical formula of amino acid [117].

Figure 4.4. shows twenty-one types of amino acids such as alanine, arginine, asparagine, aspartic acid, cysteine, glutamine, glutamic acid, glycine, histidine, isoleucine, leucine, lysine, methionine, phenylalanine, proline, serine, threonine, tryptophan, tyrosine, and valine.

The proteins can be classified into two categories namely; fibrous and globular. The fibrous proteins are Stringy, generally insoluble in water, physically tough, and most solvents. Moreover, they are elongated, rod- like proteins joined by several types of cross – linkages. The globular proteins are generally spherical or globular, polar groups of the side chains are on the outer side, and tend to be soluble in water and aqueous solutions [119]. Most proteins fold into unique 3-dimensional structures. The shape into which a protein naturally folds is known as its native conformation.

4.1.3. Essential Biomolecules

In this section, some physical and chemical properties of essential biomolecules are summarized. These essential biomolecules were studied in detail in terms of radiation interaction. The selected biomolecules are creatinine hydrochloride (creatinine H), methionine, glycoprotein, glycine, proline, margaric acid, tyrosine, inosine, and lactose. To investigate these biomolecules in terms of photon, electron, and proton

interactions, we need to know some properties of the biomolecules. Such properties are density, mean excitation energy, and mean atomic number for each biomolecule.

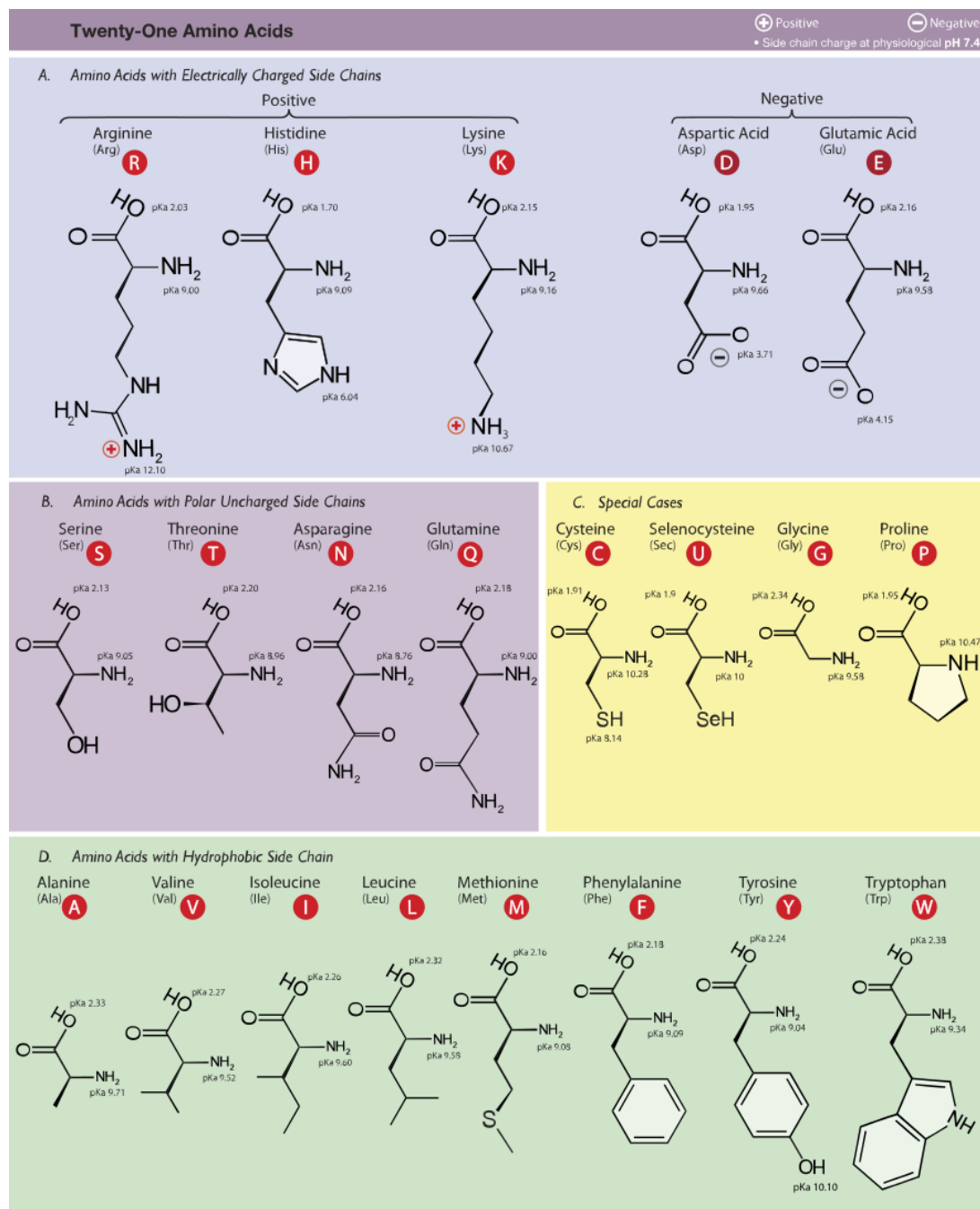


Figure 4.4. Twenty-one types of amino acids [119].

Moreover, the knowing of the properties for the chemical compositions for the studied biomolecules is very important to carry out the radiation investigations in this work. Such properties are atomic number, atomic weight, and fraction weight for

each element in the biomolecules involved. Table 4.1. shows the chemical compositions, mean excitation energy, and density for the investigated biomolecules. Table 4.2. shows the elemental weight fractions for the investigated biomolecules.

Table 4.1 . Chemical composition, density (D), mean excitation energy (E) for the investigated biomolecules.

Biomolecule	Chemical composition	D (g/cm ³)	E (eV)
Creatinine H	C ₄ H ₈ ClN ₃ O	1.09	83.5
Methionine	C ₅ H ₁₁ NO ₂ S	1.34	82.4
Glycoprotein	C ₂₈ H ₄₇ N ₅ O ₁₈	1.55	75.3
Glycine	C ₂ H ₅ NO ₂	1.61	75.5
Proline	C ₅ H ₉ NO ₂	1.38	70.5
Lactose	C ₁₂ H ₂₂ O ₁₁	1.52	77.5

Table 4.2 . Elemental weight fractions for the investigated biomolecules.

Biomolecule	H	C	N	O	Cl	S
Creatinine H	0.053908	0.321193	0.280922	0.106962	0.237015	-
Methionine	0.074305	0.402476	0.09387	0.214449	-	0.2149
Glycoprotein	0.063871	0.453426	0.094423	0.38828	-	-
Glycine	0.067136	0.320006	0.186589	0.426269	-	-
Proline	0.078792	0.521619	0.121658	0.277931	-	-
Lactose	0.064781	0.421069	-	0.514149	-	-

4.2. Methods

4.2.1. Geant4 Monte Carlo Simulation

The Geant4 simulations have been performed on an engine machine equipped with a 32bit Fedora 25 operating system, 8 GB RAM memory and Core i5 processor. To simulate the μ/ρ values of the current bioactive glasses, first μ values have been

evaluated via the geometry conditions as sketched by the following figure. This setup has been adopted from [128] with some modifications to achieve the narrow-beam (or, in other words, good geometry) conditions.

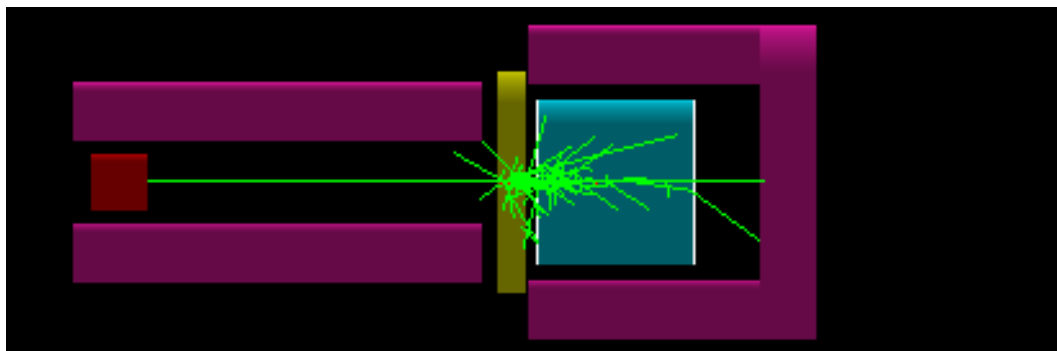


Figure 4.5. The principal geometry to study the radiation transmission in the present work.

Two identical lead collimators have been placed, one after the source and one before the detector region, to avoid as much as possible the scattered gamma-rays to be counted. Construction of the simulation geometry and assignments of the materials to related regions have been made by Geant4 G4Detector Construction class, which is a mandatory class in a simulation. The present biomolecules have been defined in the same class file by entering the weight fractions of the ingredient elements presented in Table 4.2.

The mother volume covering all of the bodies has been filled with vacuum. Elemental data have been obtained by the use of Geant4 material library. The photon energies have been modeled by the implementation of G4 Primary Generator Action class to emit photons in the range of 0.015–10 MeV towards z-axis. The G4 Multifunctional Detector class has been carried out to define a surface current detector that has been attached to a photon filter. By this method, the intensity of the emerging photons on the surface of the detector has been recorded in the units of photons/mm². Hole radius and thicknesses of both collimators have been selected as 0.3 and 6 cm, respectively, and source to detector region distance has been set to 50 cm. To govern the physical processes regarding the photons and electrons, the standard electromagnetic package has been adopted by G4EmPhysicsList class. This package covers the interactions of photons from 1 keV to 100 TeV. The fundamental

photonic interactions have been included such as `G4PhotoElectricEffect`, `G4ComptonScattering`, `G4RayleighScatterin` and `G4GammaConversion`. On the other hand, for simulations of electronic processes, which are bremsstrahlung, ionization, multiple scattering and positron annihilation, the following Geant4 classes have been activated in the code: `G4eBremsstrahlung`, `G4eIonisation`, `G4eMultipleScattering` and `G4eplusAnnihilation`. In simulations, the range cut value, which is the minimum limit for secondary particle creation, has been adjusted to 0.01 cm for all requested particles to assure sufficient precision.

4.2.2. XCOM and ESTAR programs

The XCOM and ESTAR programs are professional platforms to understand the photon and electron interactions with matter, respectively [102]. The XCOM program can generate cross sections on a standard energy grid (spaced approximately logarithmically), or on a grid selected by the user, or for a mix of both grids. Cross sections at energies immediately above and below all absorption edges are automatically included. XCOM provides two forms of output: (a) tables which correspond closely in format to existing tables in the literature; (b) user-selected arrays which are convenient for further computer calculations. The program provides total cross sections and attenuation coefficients as well as partial cross sections for the following processes: incoherent scattering, coherent scattering, photoelectric absorption, and pair production in the field of the atomic nucleus and in the field of the atomic electrons.

The ESTAR program calculates stopping power, density effect parameters, range, and radiation yield tables for electrons in various materials. Select a material and enter the desired energies or use the default energies. Energies are specified in MeV, and must be in the range from 0.001 MeV to 10000 MeV.

4.2.3. SRIM calculations

A heavy charged particle (e.g. proton and alpha) interaction with matter can be studied in terms of stopping power and particle range via the methods and equations described in chapter 2. However, different software platforms were developed to make the calculation procedures more easy and fast. One of the best programs to study the heavy charged particle interaction with matter is called SRIM (Stopping and Range of Ions in Matter) [153]. SRIM is popular in the ion implantation research and technology community and also used widely in other branches of radiation material science.

As the input parameters, it needs the ion type and energy (in the range 10 eV – 2 GeV) and the material of one or several target layers. As the output, it lists or plots the three-dimensional distribution of the ions in the solid and its parameters, such as penetration depth, its spread along the ion beam (called straggle) and perpendicular to it, all target atom cascades in the target are followed in detail; concentration of vacancies, sputtering rate, ionization, and phonon production in the target material; energy partitioning between the nuclear and electron losses, energy deposition rate. The programs are made so they can be interrupted at any time, and then resumed later. They have an easy-to-use user interface and built-in default parameters for all ions and materials. Another part of the software allows calculating the electronic stopping power of any ion in any material (including gaseous targets) based on an averaging parametrization of a vast range of experimental data.

CHAPTER 5. RESULTS AND DISCUSSION

In this chapter, the results of the current thesis are summarized. In the section 5.1., the results of the parameters of photon interaction are presented for each studied biomolecule. Section 5.2 shows the results of the energy absorption parameters. The photon buildup factors (EABF and EBF) are evaluated and discussed in section 5.3. The dose calculation is given in section 5.4. Finally, the interactions of charged particles including electron, proton, alpha, and carbon ion interactions are estimated in section 5.5.

5.1. Photon Interaction With the Biomolecules

5.1.1. Mass attenuation coefficients (μ/ρ)

Variation of μ/ρ for the studied biomolecules was investigated by utilizing Geant4 Monte Carlo simulations over a wide range of photon energies from 1 keV to 1000 MeV as shown in Figure 5.1. As it can be seen from the figure, there are three zones of energies related to the dominating attenuation mechanisms that vary according to the photon energy. At low photon energies, photoelectric effect is the dominating process. By increasing the photon energy, Compton effect dominates the attenuation processes over a wide range of photon energies starting from 150 keV and reaching to 10 MeV. At photon energies above 10 MeV, the attenuation process is governed by the effect of pair production. Although the pair production can be observed at photon energies greater than 1.022 MeV, but it was found to become dominating mechanism around photon energies between 5 and 10 MeV for the biomolecules of interest.

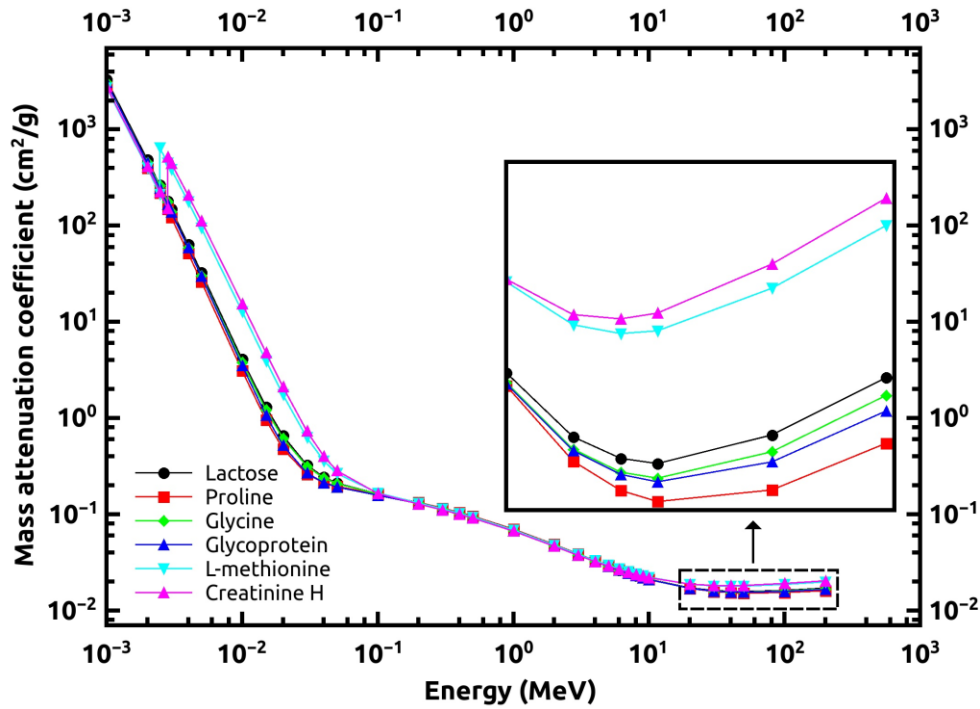


Figure 5.1. Simulation results (via Geant4) for the total mass attenuation coefficients of the essential biomolecules.

In the region of photoelectric effect (low energies), the interaction cross section of the photons with the biomolecule is inversely proportional to E^3 . Therefore, a swift decrease in the μ/ρ values is observed for the photon's energies between 1 keV and 150 keV. In the region of Compton effect (medium energies), the interaction cross section of the photons with the biomolecule is inversely proportional to E . Therefore, the μ/ρ values are observed to be semi-constant for the photon's energies between 150 keV and 10 MeV. Finally, in the region of pair production effect (high energies), the interaction cross section of the photons with the biomolecule is directly proportional to $\log E$. So, above 10 MeV, the μ/ρ values increase as photon energy increases. Also, from Figure 4.1., it is clear that the maximum values of μ/ρ occurred at 1 keV for all of the essential biomolecules. At this photon energy, the μ/ρ values were 2803, 2707, 3098, 3282, 2784, and 3291 for creatinine hydrochloride, methionine, glycoprotein, glycine, proline and lactose, respectively. Moreover, in Figure 5.1., one can see abrupt change (peak) near the K-absorption edges of the high-Z elements like chlorine (Cl) and sulphur (S) in creatinine hydrochloride and methionine, respectively.

In case of methionine, two values can be seen for the μ/ρ values at 2.47 keV which is the sulphur K-absorption edge. First one is $2.13 \times 10^2 \text{ cm}^2/\text{g}$ that is below the absorption edge, and the second one is $6.44 \times 10^2 \text{ cm}^2/\text{g}$ that is immediately above the absorption edge. Similarly, for creatinine hydrochloride, around chlorine K-absorption edge (2.82 keV), the first value of μ/ρ is $1.51 \times 10^2 \text{ cm}^2/\text{g}$ and the second value are $5.21 \times 10^2 \text{ cm}^2/\text{g}$. It should note that for the other biomolecules such as glycoprotein, glycine, proline and lactose, the K-absorption edge is not be observed. The reason is that the K shell binding energy for their atomic electrons is on the order of few hundred electron volts, for example it is 13.6 eV for hydrogen. Therefore, the K-absorption edges of low-Z elements are of course existing but not detectable. In the other words, the weak photons (in eV range) survive about one micron and then they are totally absorbed.

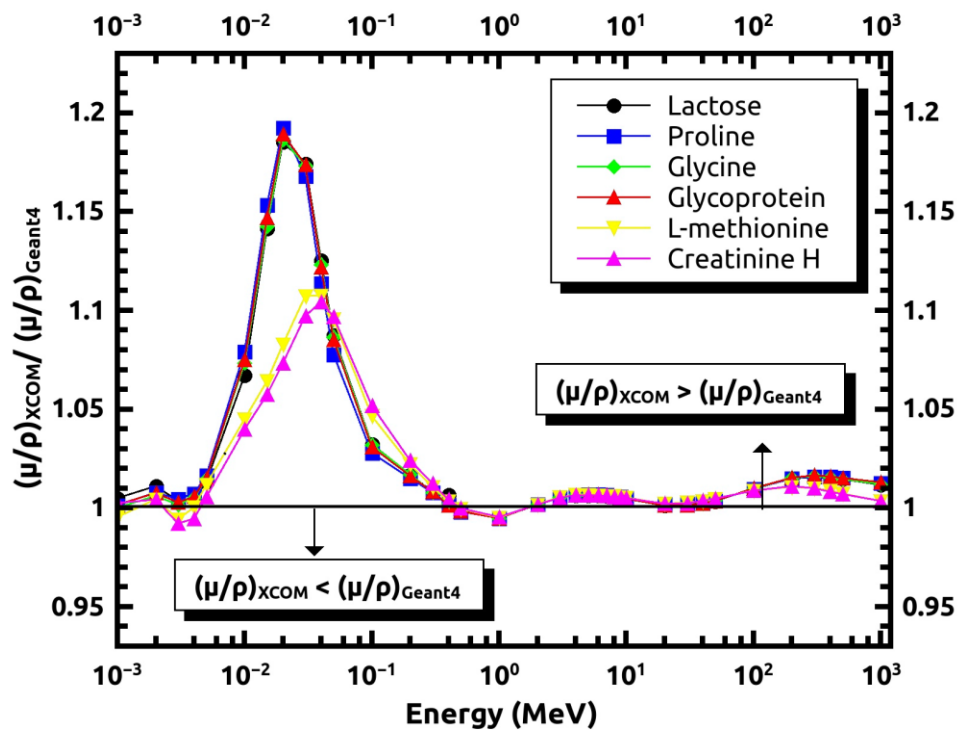


Figure 5.2. Comparison between the theoretical results obtained via XCOM and the simulation results obtained via Geant4 for the total mass attenuation coefficients of the essential biomolecules.

Figure 5.2. shows Comparison between the theoretical results obtained via XCOM and the simulation results obtained via Geant4 for the total mass attenuation coefficients of the essential biomolecules. From this graph, the μ/ρ values obtained

by Geant4 simulation of the essential biomolecules are comparable with those of XCOM (theoretical results). A very good agreement is noted in the intermediate and high photon energies, while a significant difference up to 19 % are found in the low photon energies in the range of 10 -150 keV. Almost all the μ/ρ values obtained by XCOM are higher than those of Geant4 simulation for each studied biomolecule. The higher μ/ρ values of XCOM may be attributed to the effect of chemical composition of studied molecules and mixture rule without neglecting the effects of the atomic wave function of molecular bonding of the compounds/mixtures which can reduce μ/ρ values.

It is worth mentioning that by applying Geant4 simulations one can obtain the initial photon number and the transmitted photon number. Then, by using these numbers the linear attenuation coefficients of the studied sample can be calculated via the Beer–Lambert law as described in chapter 2. After that the mass attenuation coefficients of the samples can be obtained by dividing the linear attenuation coefficients by the density of the studied sample. The Similar findings are reported by several authors who studied and compared the results of Geant4 with the outcomes of XCOM for various materials [120-128]. These successful publications include the radiation attenuation properties by using Geant4 toolkit and XCOM (or WinXCOM) program for different samples (targets) such as biomolecules (contrast agents), polymers, glasses, and scintillation detectors, thermoluminescent dosimetric materials, and various composite materials. Generally, the uncertainties of Geant4 simulation vary from point to point and they are approximately 3 % [103]. On the other hand, the database of XCOM is collected for incoherent and coherent scattering, for photoelectric absorption, and for pair production [129-131]. The authors show that the uncertainties in the values provided are rather difficult to evaluate, depending on the energy range of the photons; they range from 1 % to 5 %, with the lowest and highest energy regions associated with larger uncertainties [132].

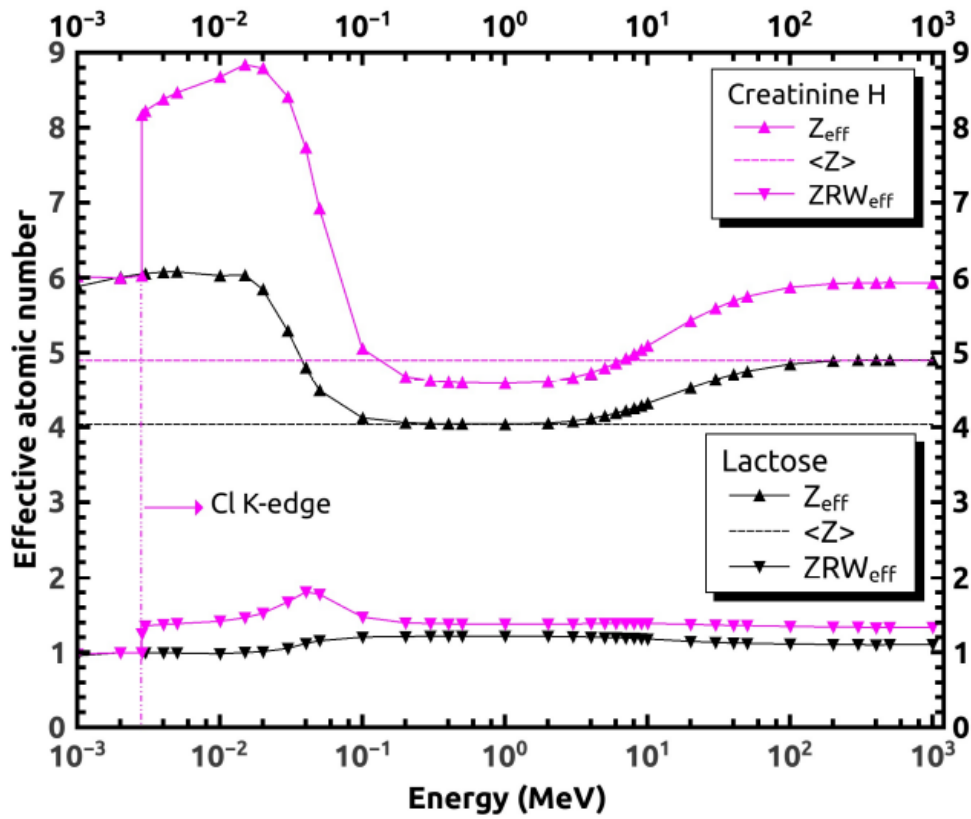


Figure 5.3. Effective atomic numbers (Z_{eff}), effective atomic numbers relative to water ($Z_{\text{RW}_{\text{eff}}}$), mean atomic numbers $\langle Z \rangle$ for the total photon attenuation of two essential biomolecules namely; creatinine H and lactose, for energies from 1 keV to 1000 MeV.

5.1.2. Effective atomic number for photon interaction (Z_{eff})

There are two main notions of effective atomic numbers. One is related to the photon interaction (as shall be discussed in this subsection) and the other is related to the photon energy absorption (as will be shown in the coming section). We mainly refer to the first type by Z_{eff} or $Z_{\text{PI}_{\text{eff}}}$, while the second type is referred by $Z_{\text{PEA}_{\text{eff}}}$. It should be noted that the notion of the effective atomic number is totally different of the well-known notions of atomic number (Z) of the elements or the mean atomic number ($\langle Z \rangle$). Both Z and $\langle Z \rangle$ are constant variables (e.g. do not vary with photon energy), while the effective atomic numbers are energy dependent variables [133]. Such study is very important and standard reference for many works.

Before I shall talk about the effective atomic number for photon interaction in terms of its definition and equations, a short part will be given for Z and $\langle Z \rangle$. The Z is a basic and constant parameter for each element. The values of Z can be found in the periodic table for all of the elements. When we talk about composites materials (mixtures or compounds), then the $\langle Z \rangle$ is the corresponding parameter in this case. The $\langle Z \rangle$ can be calculated by the following equation: $\langle Z \rangle = \sum n_i Z_i / n$. Here, n_i is the number of atoms for i^{th} element and n is the total number of atoms in the studied compound. Moreover, there is another very important parameter namely; a single-valued effective atomic number (Z_{eff}) that is related to the photoelectric effect. This parameter can be obtained directly via XMuDat software [134].

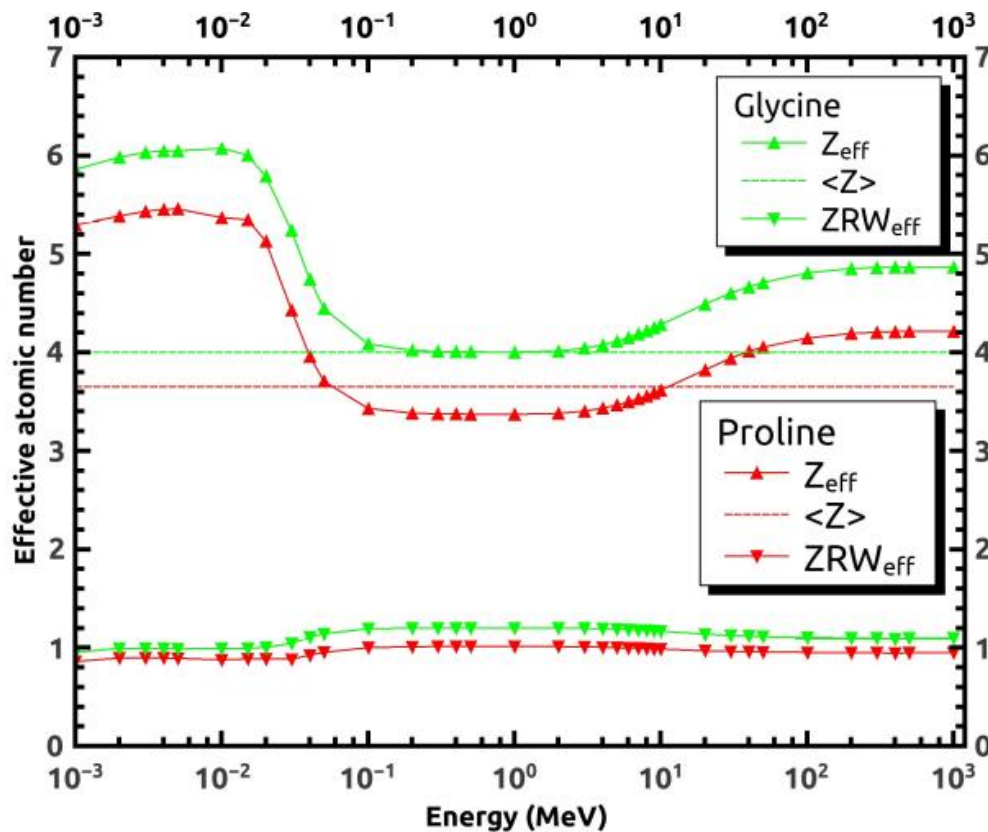


Figure 5.4. Effective atomic numbers (Z_{eff}), effective atomic numbers relative to water ($Z_{\text{RW}_{\text{eff}}}$), mean atomic numbers $\langle Z \rangle$ for the total photon attenuation of two essential biomolecules namely; glycine and proline, for energies from 1 keV to 1000 MeV.

Now, I shall talk about the effective atomic numbers for photon interaction (Z_{eff}). The Z_{eff} is a responsible factor to describe and understand the total and partial photon attenuation processes. For each partial photon interaction process, there is a corresponding effective atomic number (like the case of the mass or linear attenuation coefficients). Figures 5.3., 5.4., and 5.5. show the effective atomic numbers (Z_{eff}), effective atomic numbers relative to water ($Z_{\text{RW}_{\text{eff}}}$), and mean atomic numbers $\langle Z \rangle$ for the total photon attenuation of two essential biomolecules namely; creatinine H, lactose, glycine, proline, methionine and glycoprotein for energies from 1 keV to 1000 MeV. In these figures, one can realize the difference between the notions of effective atomic number and mean atomic numbers. The first notion varies with the photon energy, while the other notion is constant and does not vary with the photon energy.

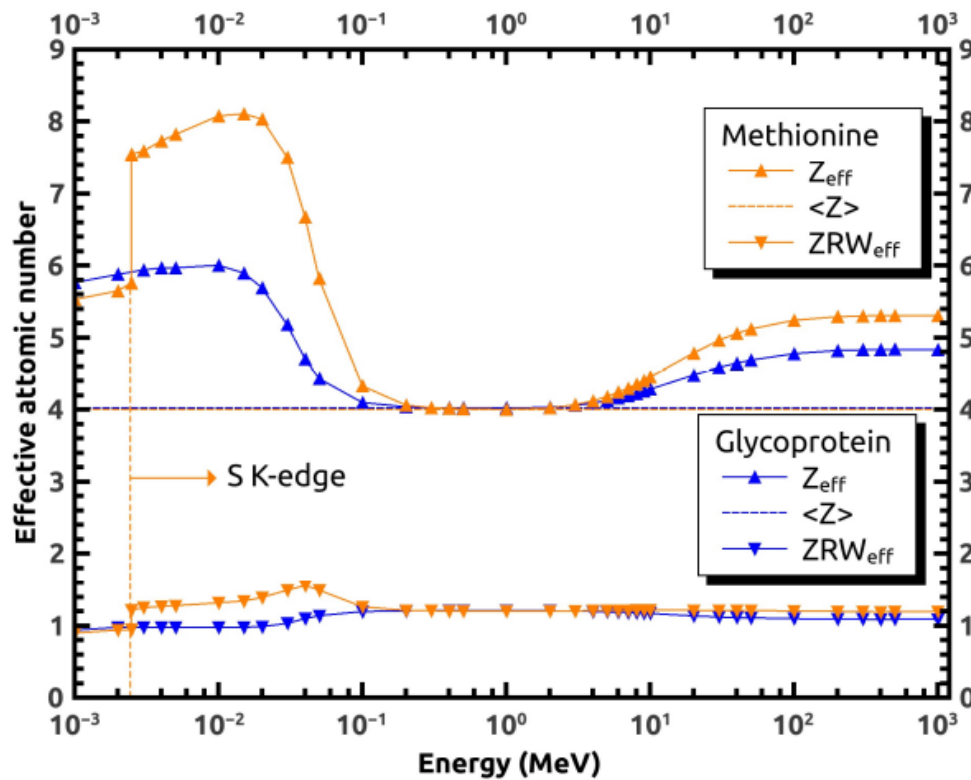


Figure 5.5. Effective atomic numbers (Z_{eff}), effective atomic numbers relative to water ($Z_{\text{RW}_{\text{eff}}}$), mean atomic numbers $\langle Z \rangle$ for the total photon attenuation of two essential biomolecules namely; methionine and glycoprotein, for energies from 1 keV to 1000 MeV.

Moreover, there is an important difference between the effective atomic number (Z_{eff}) and the effective atomic numbers relative to water ($Z_{\text{RW}_{\text{eff}}}$). The Z_{eff} is strongly

dependent on the photon energy, while the Z_{eff} is weakly dependent on the photon energy. In the cases of creatinine H (Figure 5.3.) and methionine (Figure 5.5.), clearly there are peaks around the k- absorption edge of Cl and S, respectively. This phenomenon always occurs when the sample contains of at least one relatively high-Z element due to the photoelectric effect. Except of these differences, the behaviour of Z_{eff} is similar in terms of their variation with photon energy for all the studied biomolecules. Such that, the Z_{eff} values started like constant up to the photon energy of about 0.02 MeV due to the coherent scattering that occurs at very low energies. With the photon energy increasing, the Z_{eff} values decreased very fast up to the photon energy of about 0.2 MeV due to the photoelectric effect. After that the Z_{eff} values become constant in the photon energy range of 0.2-2 MeV due to the incoherent scattering. Finally, for the photon energy above 2 MeV, the Z_{eff} increased due to the effects of the pair production. The Z_{eff} values changed from 4.6 to 8.8 for creatinine H, from 4.0 to 6.0 for lactose, from 4.0 to 6.0 for glycine, from 3.3 to 5.4 for proline, from 4.0 to 8.1 for methionine and from 4.0 to 6.0 for glycoprotein. For all the studied biomolecules, the maximum Z_{eff} values occurred at the photon energy around 0.015 MeV. More studies and details about the Z_{eff} and its calculation methods can be found elsewhere [135-140].

Furthermore, the Z_{eff} values were observed to be equal to the mean atomic numbers for all of the studied biomolecules at the photon energies between 0.2-2 MeV. Table 5.1. provides a comparison between the experimental values (labelled by a, b, c), theoretical values (labelled by *), and the simulation outcomes (labelled by s) in the term of mass attenuation coefficients and effective atomic numbers for studied biomolecules. From Table 5.1., it is seen easily that the Geant4 simulations have a very close values to those obtained by either theoretical calculations or experiments. Such evidence is very important to use the Geant4 simulations confidently whereas the experimental setup is hard to be achieved.

Table 5.1. Comparison between the experimental values (labelled by a, b, c), theoretical values (labelled by *), and the simulation outcomes (labelled by s) in the term of mass attenuation coefficients and effective atomic numbers for studied biomolecules.

Biomolecule	Parameter	Photon energy (keV)					
		122	356	511	662	1170	1330
Creatinine H	$(\mu/\rho)^a$	0.147	0.090	0.082	0.073	0.055	0.049
	$(\mu/\rho)^s$	0.156	0.104	0.091	0.080	0.063	0.060
	$(Z_{\text{eff}})^{a*}$	4.588	4.586	4.587	4.591	4.594	4.596
	$(Z_{\text{eff}})^s$	4.970	4.615	4.601	4.599	4.595	4.598
Methionine	$(\mu/\rho)^a$	0.148	0.094	0.085	0.075	0.057	0.051
	$(\mu/\rho)^s$	0.159	0.107	0.093	0.086	0.065	0.062
	$(Z_{\text{eff}})^{a*}$	4.093	4.095	4.092	4.097	4.098	4.094
	$(Z_{\text{eff}})^s$	4.271	4.020	4.009	4.007	4.006	0.057
Glycine	$(\mu/\rho)^a$	0.147	0.090	0.082	0.073	0.055	0.049
	$(\mu/\rho)^s$	0.156	0.104	0.091	0.080	0.063	0.060
	$(Z_{\text{eff}})^{a*}$	4.588	4.586	4.587	4.591	4.594	4.596
	$(Z_{\text{eff}})^s$	4.970	4.615	4.601	4.599	4.595	4.598
Lactose	$(\mu/\rho)^a$	0.148	0.094	0.085	0.075	0.057	0.051
	$(\mu/\rho)^s$	0.159	0.107	0.093	0.086	0.065	0.062
	$(Z_{\text{eff}})^{a*}$	4.093	4.095	4.092	4.097	4.098	4.094
	$(Z_{\text{eff}})^s$	4.271	4.020	4.009	4.007	4.006	0.057

This part of study (about the photon interaction parameters in term of μ/ρ , Z_{eff} , and N_{eff}) was published in [141]. In this paper, it is seen that there are significant discrepancies between Geant4 simulations and XCOM program up to 20 % in energy region 10–150 keV.

5.1.3. Effective electron density for photon interaction (N_{eff})

We shall also discuss the radiation (photon) interaction with the studied biomolecules in terms of a significant parameter namely: effective electron density (N_{eff}).

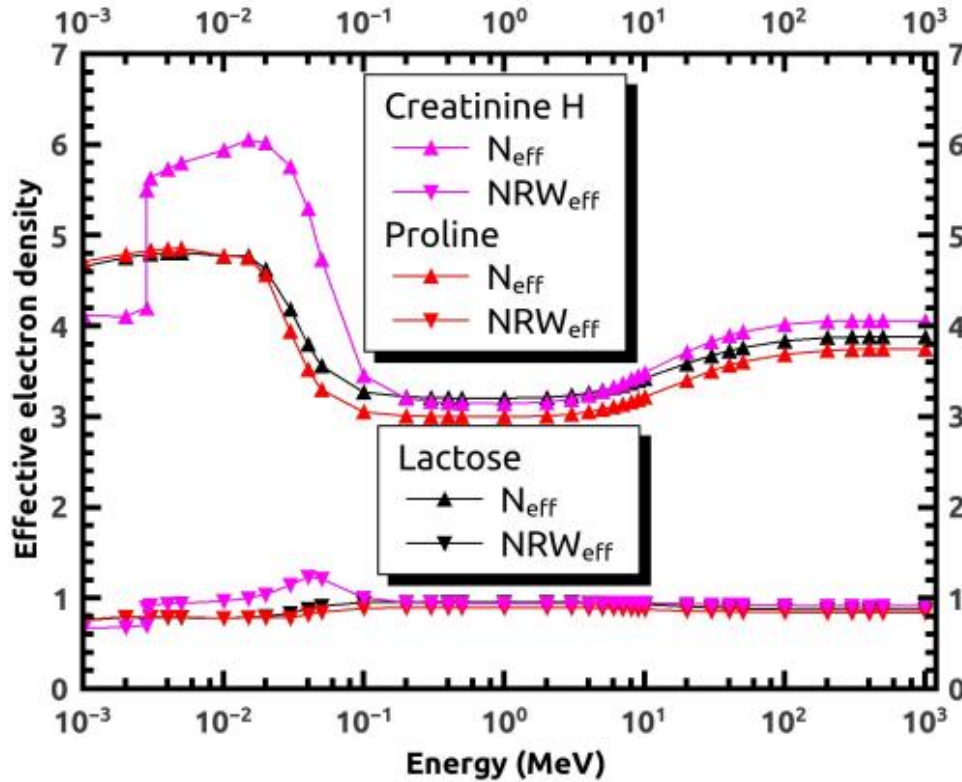


Figure 5.6. Effective electron density (N_{eff}) and effective electron density relative to water (NRW_{eff}) for the total photon attenuation of three essential biomolecules namely; creatinine H, proline, and lactose for energies from 1 keV to 1000 MeV.

We calculated both N_{eff} and their corresponding parameter that relative to water (NRW_{eff}) for all the studied biomolecules, as shown in Figures 5.6. and 5.7. Figure 5.6. shows the N_{eff} and NRW_{eff} for total photon interaction of three essential biomolecules namely; creatinine H, proline, and lactose, over a wide range of energy from 1 keV to 1000 MeV. Like the case of Z_{eff} , there is a clear peak for the creatinine H around the k- absorption edge of Cl element. Figure 5.7. shows the N_{eff} and NRW_{eff} for total photon interaction of three essential biomolecules namely; methionine, glycoprotein, and glycine over a wide range of energy from 1 keV to 1000 MeV. Like the case of Z_{eff} , there is a clear peak for the creatinine H around the

k- absorption edge of S element. Generally, the behaviour of the effective electron density is similar to that of effective atomic number. The reason of this observation is that there is a smooth and direct relation between Z_{eff} and N_{eff} . This relation will be discussed and plotted in Figure 5.14.

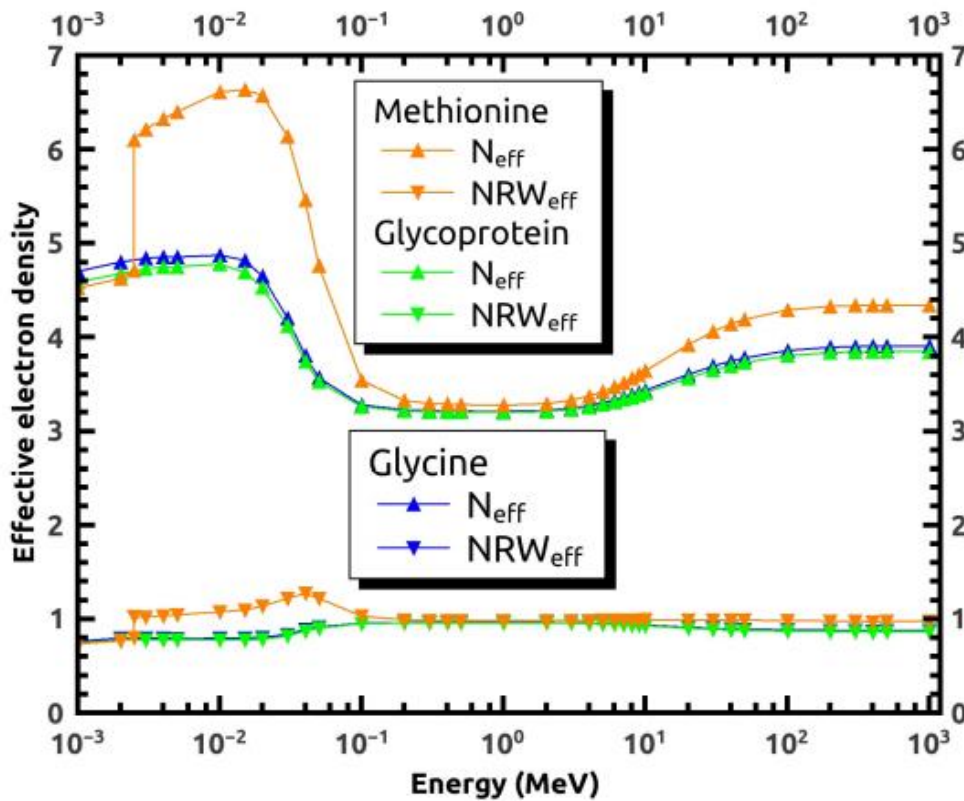


Figure 5.7. Effective electron density (N_{eff}) and effective electron density relative to water (NRW_{eff}) for the total photon attenuation of three essential biomolecules namely; methionine, glycoprotein, and glycine for energies from 1 keV to 1000 MeV.

5.2. Photon Energy Absorption for the Biomolecules

In previous section, the total photon interaction of the studied biomolecules was discussed in detail. In this section, we shall discuss the photon energy absorption for all of these biomolecules.

5.2.1. Mass energy-absorption coefficients (μ_{en}/ρ)

The photon energy absorption like the photon interaction has some parameters that can describe this process. All of these parameters will be investigated below.

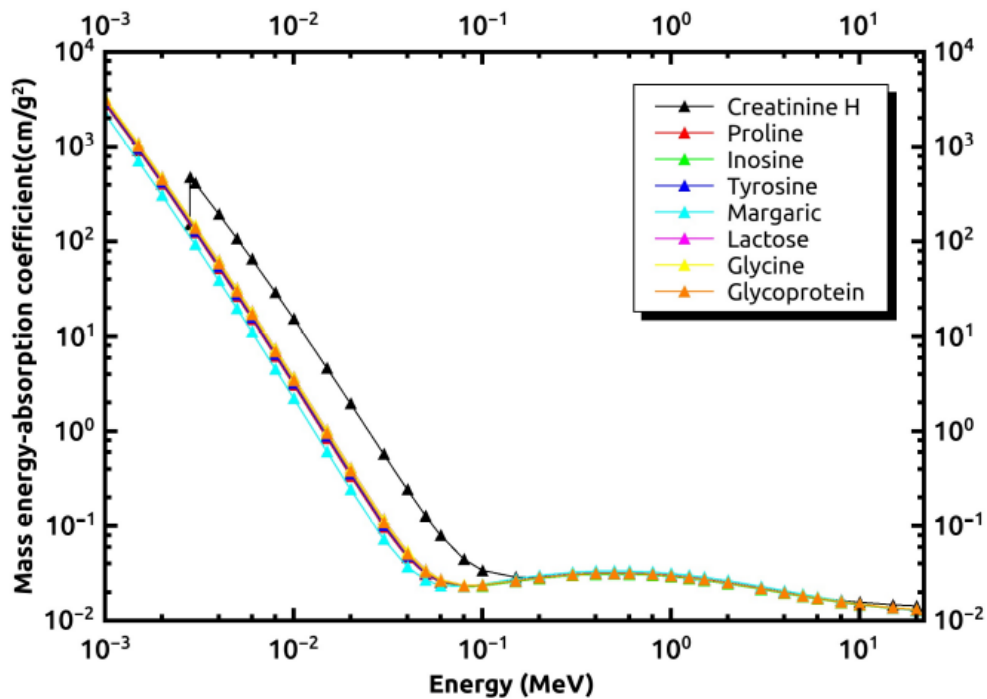


Figure 5.8. Mass energy-absorption of the studied biomolecules for energies from 1 keV to 1000 MeV.

Similar to the mass attenuation coefficient which is the basic term to understand the interaction of photons, the mass energy-absorption coefficient (μ_{en}/ρ) is an essential term to describe the energy-absorption of photons. Moreover, there is an important relation between μ/ρ and μ_{en}/ρ that is given by: $\mu/\rho = \mu_{en}/\rho + \mu_s/\rho$, where μ_s/ρ is the scatter absorption coefficient. Figure 5.8. demonstrates the behaviour of μ_{en}/ρ for all the studied biomolecules for photon energy from 1 keV to 1000 MeV. Obviously, the μ_{en}/ρ values vary with the photon energy.

Such that the μ_{en}/ρ values have different behaviours at three zones that reflect the three main partial photon interaction. In the case of creatinine H, the μ_{en}/ρ parameter has two different values at the same photon energy (2.47 keV) which is the Cl K-absorption edge. These two values were $1.5 \times 10^2 \text{ cm}^2/\text{g}$ and $4.9 \times 10^2 \text{ cm}^2/\text{g}$.

5.2.2. Effective atomic number for energy-absorption (Z_{PEAeff})

By using the μ_{en}/ρ values, one can obtain the effective atomic number for energy-absorption (Z_{PEAeff}) as described in chapter 3. Figures 5.9., 5.10., 5.11., and 5.12. show the Z_{PEAeff} , Z_{PIeff} , and Z_{RWeff} values for creatinine H, lactose, margarinic, glycoprotein, proline, inosine, tyrosine, and glycine for photon energy over a wide range up to 1000 MeV.

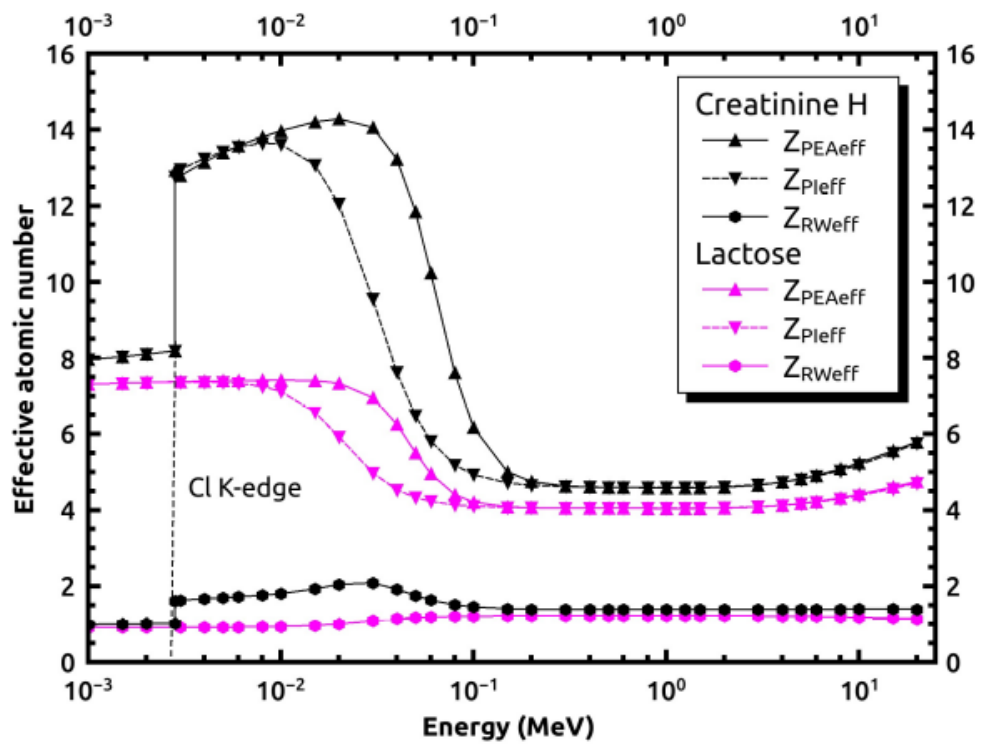


Figure 5.9. Effective atomic number of photon interaction (Z_{PIeff}), effective atomic number of photon energy absorption (Z_{PEAeff}), and effective atomic number relative to water (Z_{RWeff}) of two essential biomolecules namely; creatinine H and lactose for energies from 1 keV to 1000 MeV.

Here, Z_{PIeff} refers to the effective atomic number that is related to the total photon interaction (this parameter was calculated and discussed in previous section and coded as $Z_{\text{PIeff}} = Z_{\text{eff}}$). In these figures, one can realize the difference between the notions of Z_{PEAeff} and Z_{PIeff} . It is seen clearly that both Z_{PEAeff} and Z_{PIeff} have the same behaviour (almost the same values) at low and high photon energies where the absorption processes (photoelectric effect and pair production) are dominants mechanisms. However, there are significant differences between Z_{PEAeff} and Z_{PIeff} at the middle photon energy where the Compton scattering is the dominant process. Moreover, there is an important difference between the Z_{PEAeff} , Z_{PIeff} , and the effective atomic numbers relative to water (Z_{RWeff}).

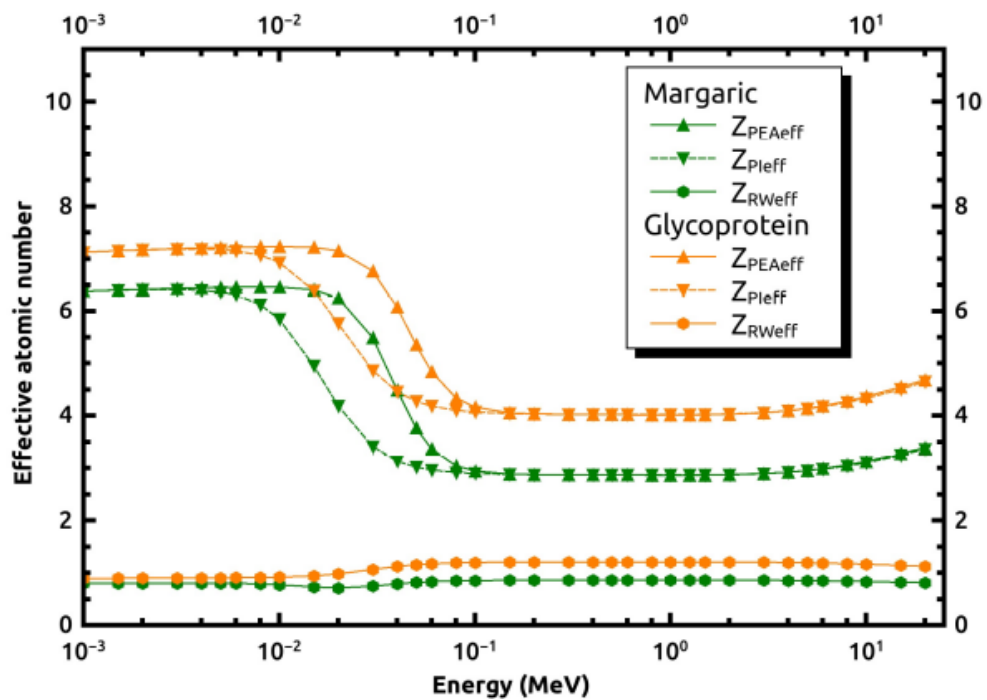


Figure 5.10. Effective atomic number of photon interaction (Z_{PIeff}), effective atomic number of photon energy absorption (Z_{PEAeff}), and effective atomic number relative to water (Z_{RWeff}) of two essential biomolecules namely; margarin and glycoprotein for energies from 1 keV to 1000 MeV.

The values of Z_{PEAeff} and Z_{PIeff} are strongly dependent on the photon energy, while the values of Z_{RWeff} are weakly dependent on the photon energy. In the cases of creatinine H (Figure 5.9.), clearly there is a peak around the k- absorption edge of Cl.

This phenomenon always occurs when the sample contains of at least one relatively high-Z element due to the photoelectric effect. As shown in Figure 5.9., there are two values of the effective atomic number (both Z_{PEAeff} and Z_{PIeff}) at the same photon energy (2.47 keV) which is the Cl K- absorption edge. Furthermore, from Figure 5.9. one can see that the maximum values of the effective atomic numbers for creatinine H occurred at 8 keV and were 13.643 for Z_{PIeff} and 13.806 for Z_{PEAeff} , while the maximum values of the effective atomic numbers occurred at 4 keV in the case of lactose and were 7.364 for Z_{PIeff} and 7.385 for Z_{PEAeff} .

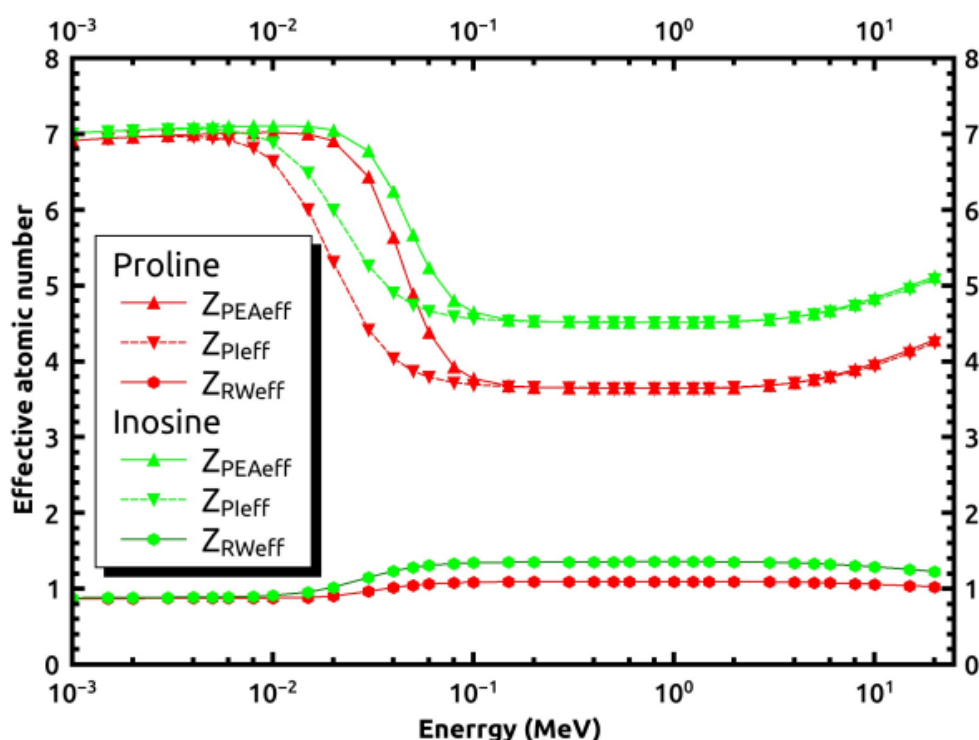


Figure 5.11. Effective atomic number of photon interaction (Z_{PIeff}), effective atomic number of photon energy absorption (Z_{PEAeff}), and effective atomic number relative to water (Z_{RWeff}) of two essential biomolecules namely; proline and inosine for energies from 1 keV to 1000 MeV.

From Figure 5.10., the maximum values of the effective atomic numbers are 6.399 for Z_{PIeff} occurred at 4 keV and 6.456 Z_{PEAeff} occurred at 6 keV for margaric biomolecule, and 7.181 for Z_{PIeff} occurred at 3 keV and 7.189 for Z_{PEAeff} occurred at 6 keV for glycoprotein biomolecule.

From Figure 5.11., the maximum values of the effective atomic numbers are 6.950 for Z_{PIeff} occurred at 5 keV and 7.007 Z_{PEAeff} occurred also at 5 keV for proline biomolecule, and 7.051 for Z_{PIeff} occurred at 5 keV and 7.115 for Z_{PEAeff} occurred at 8 keV for inosinen biomolecule. Finally, from Figure 5.11., the maximum values of the effective atomic numbers are 6.950 for Z_{PIeff} occurred at 5 keV and 7.007 Z_{PEAeff} occurred also at 5 keV for tyrosine biomolecule, and 7.051 for Z_{PIeff} occurred at 5 keV and 7.115 for Z_{PEAeff} occurred at 8 keV for glycine biomolecule.

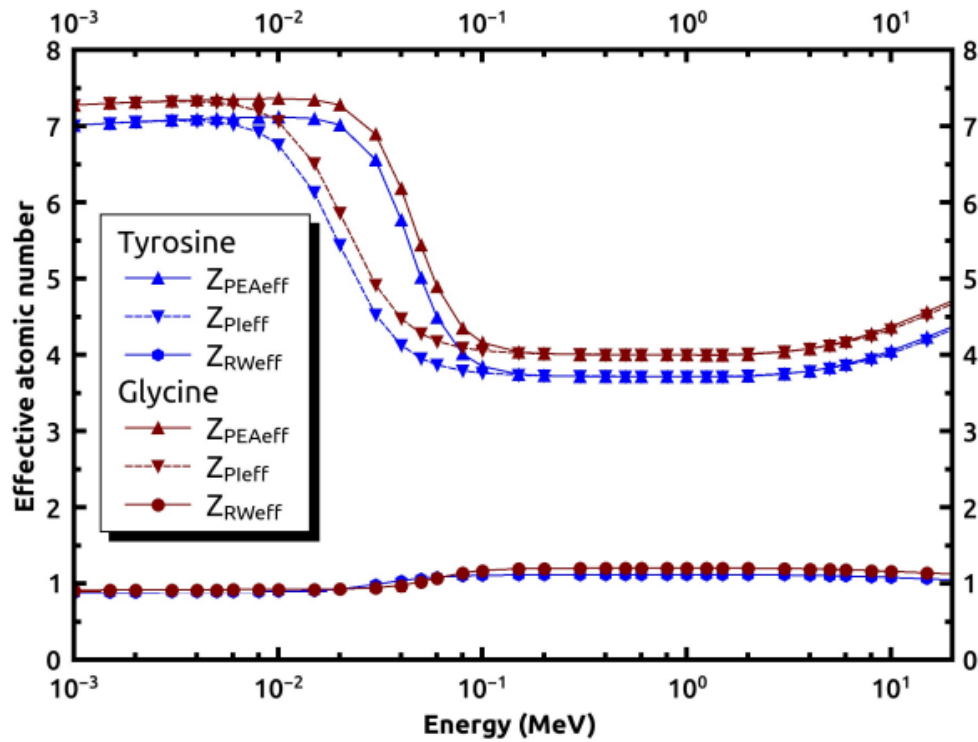


Figure 5.12. Effective atomic number of photon interaction (Z_{PIeff}), effective atomic number of photon energy absorption (Z_{PEAeff}), and effective atomic number relative to water (Z_{RWeff}) of two essential biomolecules namely; tyrosine and glycine for energies from 1 keV to 1000 MeV.

It is also worth noting that the minimum values of the effective atomic numbers (both Z_{PEAeff} and Z_{PIeff}) occurred at 20 MeV for all the studied biomolecules. On the other hand, the effective atomic numbers relative to water (Z_{RWeff}) have approximately a constant value (around 1) for all the studied biomolecules.

These results are very important because of the human body consists of $> 70\%$ water, so the dosimetry tests of radiation are performed usually in water. The differences between Z_{PEAeff} and Z_{PIeff} are very important to give a clear understand for the absorption and scattering processes that occurred during the photon interaction with the studied biomolecules. Therefore, the relative differences between Z_{PEAeff} and Z_{PIeff} were calculated for eight different biomolecules namely; creatinine H, glycoprotein, proline, inosine, tyrosine, margaric, lactose, and glycine. The results of the relative differences between Z_{PEAeff} and Z_{PIeff} of the studied biomolecules were plotted in Figure 5.13. It is clear that the values of Z_{PEAeff} and Z_{PIeff} are equal in the low and high photon energies. Therefore, In these energy regions either Z_{PEAeff} or Z_{PIeff} can be used in radiation dose calculations (or any related calculations).

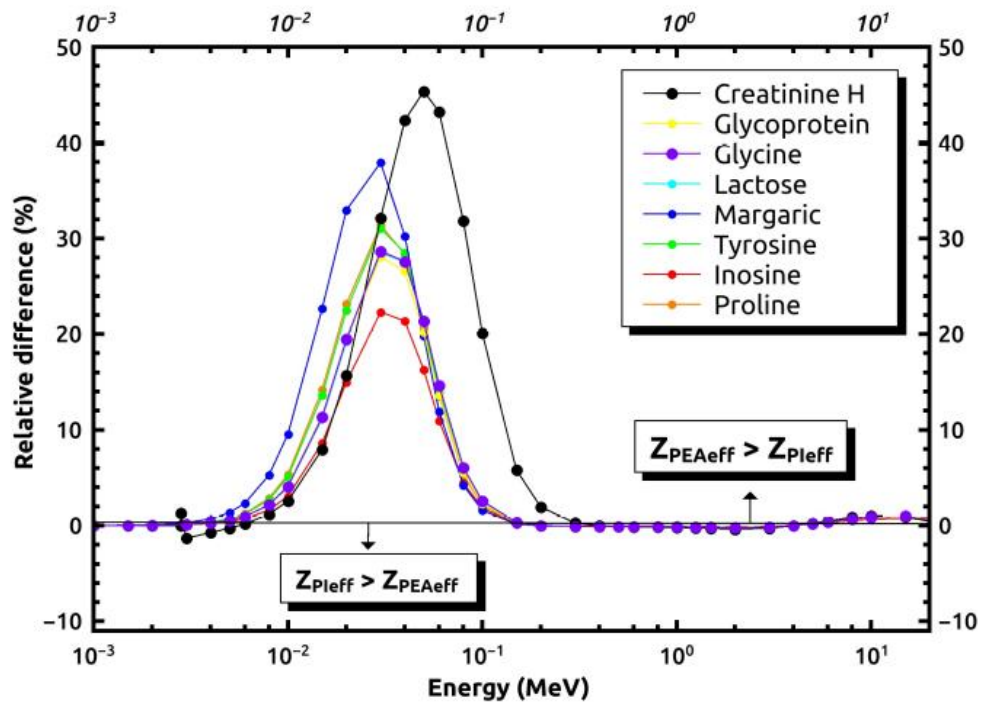


Figure 5.13. Relative differences between Z_{PIeff} and Z_{PEAeff} of the studied biomolecules for energies from 1 keV to 1000 MeV.

Because, they (Z_{PEAeff} or Z_{PIeff}) have the same values in the low and high photon energies.

On the other hand, significant differences between Z_{PEAeff} and Z_{PIeff} were observed in the middle photon energies. This energy region is governed by Compton scattering that varies with Z of the absorbing material. Consequently, the differences between Z_{PEAeff} and Z_{PIeff} have the highest values in the case of creatinine H biomolecule. Moreover, it is clear that the Z_{PEAeff} is less than Z_{PIeff} in the photon energy regions between 15 keV and 60 keV and this is a strong indication to the occurrence of scattering processes more than the absorption processes.

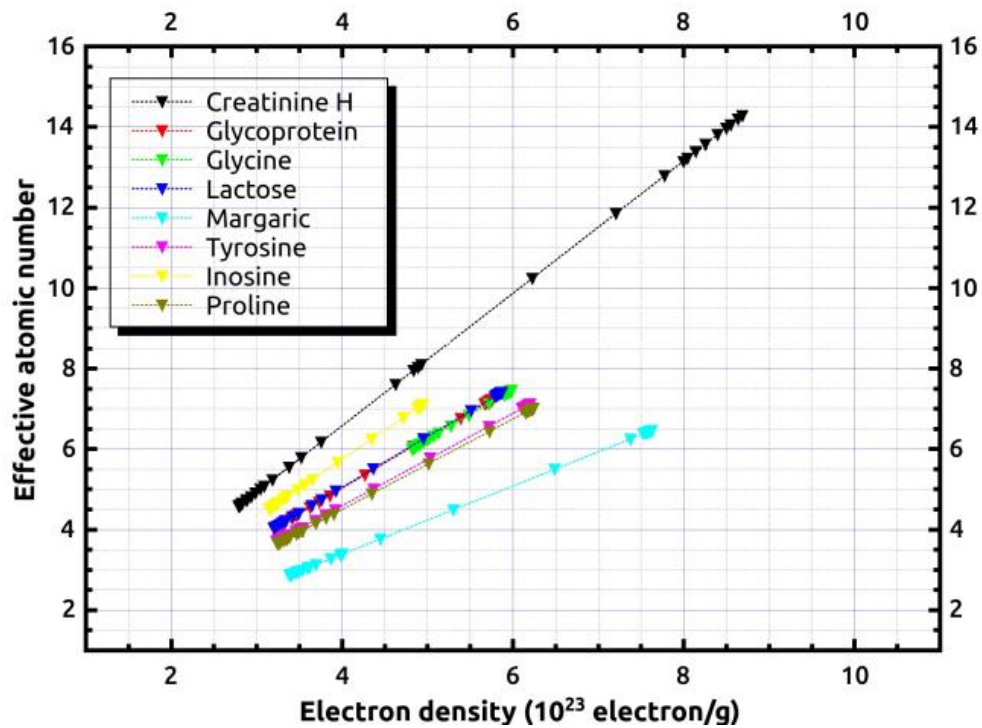


Figure 5.14. The relation between effective electron density (N_{eff}) and effective atomic number for all of the studied biomolecules at energies from 1 keV to 1000 MeV.

Figure 5.14. shows the relation between effective electron density (N_{eff}) and effective atomic number for all of the studied biomolecules at energies from 1 keV to 1000 MeV. Evidently, there is a linear and smooth relation between N_{eff} and Z_{eff} for all the studied biomolecules. This part of study (photon energy-absorption parameters) was published in [142]. Also, the obtained results were compared with those of photon interaction published in [141].

5.3. Buildup Factors of The Biomolecules

5.3.1. Standardization of the procedure

In order to test the validity of our calculation method, we have standardized EBF of water calculated by the present work with those obtained by American National Standards ANSI/ANS-6.4.3 (1991). This Standardization was done for photon energies between 0.015 MeV and 15 MeV. The photon penetration depths were chosen to be 5, 15, 25, and 35 mfp. The obtained results of both the present method and American National Standards are plotted in Figure 5.15. It is seen clearly that the EBF values of the both methods are almost overlapping. Consequently, this comparative approach reveal that the obtained results of present work have negligible errors.

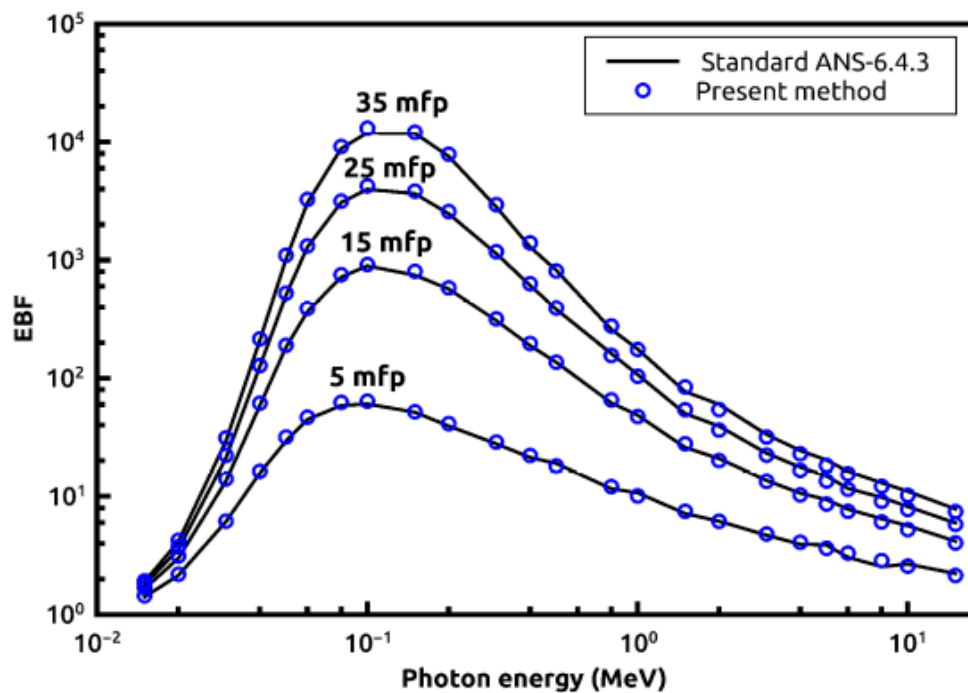


Figure 5.15. EBF of water as a comparison between the present method and the standard ANSI-6.4.3 at some penetration depths of 5, 15, 25, and 35 mfp for photon energies from 1 keV to 15 MeV.

Table 5.2. Equivalent atomic number (Z_{eq}) and G-P fitting parameters for exposure buildup factors (EBF) for creatinine hydrochloride.

E (MeV)	Z_{eq}	a	b	c	d	X_k
0.015	10.76	0.221	1.059	0.383	-0.113	11.880
0.02	10.91	0.211	1.128	0.401	-0.113	13.570
0.03	11.09	0.177	1.379	0.477	-0.093	14.580
0.04	11.20	0.108	1.745	0.640	-0.054	16.149
0.05	11.28	0.098	2.309	0.709	-0.058	14.264
0.06	11.33	0.049	2.711	0.871	-0.042	13.827
0.08	11.40	-0.014	3.156	1.124	-0.010	13.624
0.1	11.45	-0.050	3.256	1.304	0.004	13.400
0.15	11.53	-0.084	3.105	1.510	0.019	14.908
0.2	11.57	-0.094	2.903	1.575	0.023	15.417
0.3	11.62	-0.098	2.621	1.590	0.025	15.276
0.4	11.64	-0.096	2.452	1.557	0.025	15.325
0.5	11.66	-0.092	2.327	1.519	0.026	15.619
0.6	11.66	-0.087	2.231	1.481	0.025	15.326
0.8	11.67	-0.077	2.105	1.407	0.024	15.494
1	11.67	-0.069	2.010	1.352	0.023	15.693
1.5	8.91	-0.054	1.912	1.254	0.021	14.708
2	8.50	-0.036	1.829	1.162	0.013	15.216
3	8.40	-0.011	1.707	1.053	0.002	12.508
4	8.38	0.004	1.621	0.990	-0.007	19.392
5	8.36	0.016	1.551	0.948	-0.012	14.529
6	8.35	0.026	1.504	0.917	-0.023	15.060
8	8.35	0.033	1.416	0.892	-0.020	12.464
10	8.34	0.040	1.357	0.873	-0.026	13.884
15	8.34	0.052	1.265	0.840	-0.041	14.942

Now, we can use the present method (geometric progression method, denoted by G-P method) to estimate both EABF and EBF for all the studied biomolecules namely; methionine, creatinine hydrochloride, glycoprotein, lactose, glycine, and proline.

Table 5.3. Equivalent atomic number (Z_{eq}) and G-P fitting parameters for exposure buildup factors (EBF) for creatinine hydrochloride.

E (MeV)	Z_{eq}	a	b	c	d	X_k
0.015	10.76	0.221	1.059	0.383	-0.113	11.880
0.02	10.91	0.211	1.128	0.401	-0.113	13.570
0.03	11.09	0.177	1.379	0.477	-0.093	14.580
0.04	11.20	0.108	1.745	0.640	-0.054	16.149
0.05	11.28	0.098	2.309	0.709	-0.058	14.264
0.06	11.33	0.049	2.711	0.871	-0.042	13.827
0.08	11.40	-0.014	3.156	1.124	-0.010	13.624
0.1	11.45	-0.050	3.256	1.304	0.004	13.400
0.15	11.53	-0.084	3.105	1.510	0.019	14.908
0.2	11.57	-0.094	2.903	1.575	0.023	15.417
0.3	11.62	-0.098	2.621	1.590	0.025	15.276
0.4	11.64	-0.096	2.452	1.557	0.025	15.325
0.5	11.66	-0.092	2.327	1.519	0.026	15.619
0.6	11.66	-0.087	2.231	1.481	0.025	15.326
0.8	11.67	-0.077	2.105	1.407	0.024	15.494
1	11.67	-0.069	2.010	1.352	0.023	15.693
1.5	8.91	-0.054	1.912	1.254	0.021	14.708
2	8.50	-0.036	1.829	1.162	0.013	15.216
3	8.40	-0.011	1.707	1.053	0.002	12.508
4	8.38	0.004	1.621	0.990	-0.007	19.392
5	8.36	0.016	1.551	0.948	-0.012	14.529
6	8.35	0.026	1.504	0.917	-0.023	15.060
8	8.35	0.033	1.416	0.892	-0.020	12.464
10	8.34	0.040	1.357	0.873	-0.026	13.884
15	8.34	0.052	1.265	0.840	-0.041	14.942

As mentioned in chapter 2, to apply this method one needs firstly to calculate the equivalent atomic number (Z_{eq}) and the five fitting parameters. Tables 5.1., 5.2., 5.3., 5.4., 5.5., and 5.6. summarize the equivalent atomic number and the five fitting parameters of both EABF and EBF for all the studied biomolecules namely; methionine, creatinine hydrochloride, glycoprotein, lactose, glycine, and proline.

Table 5.4. Equivalent atomic number (Z_{eq}) and G-P fitting parameters for exposure buildup factors (EBF) for creatinine hydrochloride.

E (MeV)	Z_{eq}	a	b	c	d	X_k
0.015	10.76	0.221	1.059	0.383	-0.113	11.880
0.02	10.91	0.211	1.128	0.401	-0.113	13.570
0.03	11.09	0.177	1.379	0.477	-0.093	14.580
0.04	11.20	0.108	1.745	0.640	-0.054	16.149
0.05	11.28	0.098	2.309	0.709	-0.058	14.264
0.06	11.33	0.049	2.711	0.871	-0.042	13.827
0.08	11.40	-0.014	3.156	1.124	-0.010	13.624
0.1	11.45	-0.050	3.256	1.304	0.004	13.400
0.15	11.53	-0.084	3.105	1.510	0.019	14.908
0.2	11.57	-0.094	2.903	1.575	0.023	15.417
0.3	11.62	-0.098	2.621	1.590	0.025	15.276
0.4	11.64	-0.096	2.452	1.557	0.025	15.325
0.5	11.66	-0.092	2.327	1.519	0.026	15.619
0.6	11.66	-0.087	2.231	1.481	0.025	15.326
0.8	11.67	-0.077	2.105	1.407	0.024	15.494
1	11.67	-0.069	2.010	1.352	0.023	15.693
1.5	8.91	-0.054	1.912	1.254	0.021	14.708
2	8.50	-0.036	1.829	1.162	0.013	15.216
3	8.40	-0.011	1.707	1.053	0.002	12.508
4	8.38	0.004	1.621	0.990	-0.007	19.392
5	8.36	0.016	1.551	0.948	-0.012	14.529
6	8.35	0.026	1.504	0.917	-0.023	15.060
8	8.35	0.033	1.416	0.892	-0.020	12.464
10	8.34	0.040	1.357	0.873	-0.026	13.884
15	8.34	0.052	1.265	0.840	-0.041	14.942

In the case of creatinine hydrochloride (Table 5.1.), it is clear that the Z_{eq} values vary from 8.34 to 11.66. The maximum Z_{eq} values were noted at intermediate energies such as 500 keV and 600 keV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV. In the case of methionine (Table 5.2.), it is clear that the Z_{eq} values vary from 7.78 to 10.87. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV.

In the case of glycoprotein (Table 5.3.), it is clear that the Z_{eq} values vary from 6.22 to 6.86. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV. In the case of glycine (Table 5.4.), it is clear that the Z_{eq} values vary from 6.35 to 7.02. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV.

Table 5.5. Equivalent atomic number (Z_{eq}) and G-P fitting parameters for exposure buildup factors (EBF) for creatinine hydrochloride.

E (MeV)	Z_{eq}	a	b	c	d	X_k
0.015	10.76	0.221	1.059	0.383	-0.113	11.880
0.02	10.91	0.211	1.128	0.401	-0.113	13.570
0.03	11.09	0.177	1.379	0.477	-0.093	14.580
0.04	11.20	0.108	1.745	0.640	-0.054	16.149
0.05	11.28	0.098	2.309	0.709	-0.058	14.264
0.06	11.33	0.049	2.711	0.871	-0.042	13.827
0.08	11.40	-0.014	3.156	1.124	-0.010	13.624
0.1	11.45	-0.050	3.256	1.304	0.004	13.400
0.15	11.53	-0.084	3.105	1.510	0.019	14.908
0.2	11.57	-0.094	2.903	1.575	0.023	15.417
0.3	11.62	-0.098	2.621	1.590	0.025	15.276
0.4	11.64	-0.096	2.452	1.557	0.025	15.325

Table 5.5.Continue

0.5	11.66	-0.092	2.327	1.519	0.026	15.619
0.6	11.66	-0.087	2.231	1.481	0.025	15.326
0.8	11.67	-0.077	2.105	1.407	0.024	15.494
1	11.67	-0.069	2.010	1.352	0.023	15.693
1.5	8.91	-0.054	1.912	1.254	0.021	14.708
2	8.50	-0.036	1.829	1.162	0.013	15.216
3	8.40	-0.011	1.707	1.053	0.002	12.508
4	8.38	0.004	1.621	0.990	-0.007	19.392
5	8.36	0.016	1.551	0.948	-0.012	14.529
6	8.35	0.026	1.504	0.917	-0.023	15.060
8	8.35	0.033	1.416	0.892	-0.020	12.464
10	8.34	0.040	1.357	0.873	-0.026	13.884
15	8.34	0.052	1.265	0.840	-0.041	14.942

In the case of proline (Table 5.5.), it is clear that the Z_{eq} values vary from 6.35 to 7.02. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV. Finally, in the case of lactose (Table 5.6.), it is clear that the Z_{eq} values vary from 6.35 to 7.02. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV.

Table 5.6. Equivalent atomic number (Z_{eq}) and G-P fitting parameters for exposure buildup factors (EBF) for creatinine hydrochloride.

E (MeV)	Z_{eq}	a	b	c	d	X_k
0.015	10.76	0.221	1.059	0.383	-0.113	11.880
0.02	10.91	0.211	1.128	0.401	-0.113	13.570
0.03	11.09	0.177	1.379	0.477	-0.093	14.580
0.04	11.20	0.108	1.745	0.640	-0.054	16.149
0.05	11.28	0.098	2.309	0.709	-0.058	14.264
0.06	11.33	0.049	2.711	0.871	-0.042	13.827
0.08	11.40	-0.014	3.156	1.124	-0.010	13.624
0.1	11.45	-0.050	3.256	1.304	0.004	13.400
0.15	11.53	-0.084	3.105	1.510	0.019	14.908
0.2	11.57	-0.094	2.903	1.575	0.023	15.417
0.3	11.62	-0.098	2.621	1.590	0.025	15.276
0.4	11.64	-0.096	2.452	1.557	0.025	15.325
0.5	11.66	-0.092	2.327	1.519	0.026	15.619
0.6	11.66	-0.087	2.231	1.481	0.025	15.326
0.8	11.67	-0.077	2.105	1.407	0.024	15.494
1	11.67	-0.069	2.010	1.352	0.023	15.693
1.5	8.91	-0.054	1.912	1.254	0.021	14.708
2	8.50	-0.036	1.829	1.162	0.013	15.216
3	8.40	-0.011	1.707	1.053	0.002	12.508
4	8.38	0.004	1.621	0.990	-0.007	19.392
5	8.36	0.016	1.551	0.948	-0.012	14.529
6	8.35	0.026	1.504	0.917	-0.023	15.060
8	8.35	0.033	1.416	0.892	-0.020	12.464
10	8.34	0.040	1.357	0.873	-0.026	13.884
15	8.34	0.052	1.265	0.840	-0.041	14.942

Table 5.7. Equivalent atomic number (Z_{eq}) and G-P fitting parameters for exposure buildup factors (EBF) for creatinine hydrochloride.

E (MeV)	Z_{eq}	a	b	c	d	X_k
0.015	10.76	0.221	1.059	0.383	-0.113	11.880
0.02	10.91	0.211	1.128	0.401	-0.113	13.570
0.03	11.09	0.177	1.379	0.477	-0.093	14.580
0.04	11.20	0.108	1.745	0.640	-0.054	16.149
0.05	11.28	0.098	2.309	0.709	-0.058	14.264
0.06	11.33	0.049	2.711	0.871	-0.042	13.827
0.08	11.40	-0.014	3.156	1.124	-0.010	13.624
0.1	11.45	-0.050	3.256	1.304	0.004	13.400
0.15	11.53	-0.084	3.105	1.510	0.019	14.908
0.2	11.57	-0.094	2.903	1.575	0.023	15.417
0.3	11.62	-0.098	2.621	1.590	0.025	15.276
0.4	11.64	-0.096	2.452	1.557	0.025	15.325
0.5	11.66	-0.092	2.327	1.519	0.026	15.619
0.6	11.66	-0.087	2.231	1.481	0.025	15.326
0.8	11.67	-0.077	2.105	1.407	0.024	15.494
1	11.67	-0.069	2.010	1.352	0.023	15.693
1.5	8.91	-0.054	1.912	1.254	0.021	14.708
2	8.50	-0.036	1.829	1.162	0.013	15.216
3	8.40	-0.011	1.707	1.053	0.002	12.508
4	8.38	0.004	1.621	0.990	-0.007	19.392
5	8.36	0.016	1.551	0.948	-0.012	14.529
6	8.35	0.026	1.504	0.917	-0.023	15.060
8	8.35	0.033	1.416	0.892	-0.020	12.464
10	8.34	0.040	1.357	0.873	-0.026	13.884
15	8.34	0.052	1.265	0.840	-0.041	14.942

In the case of proline (Table 5.5.), it is clear that the Z_{eq} values vary from 6.35 to 7.02. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV. Finally, in the case of lactose (Table 5.6.), it is clear that the Z_{eq} values vary from 6.35 to 7.02. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV.

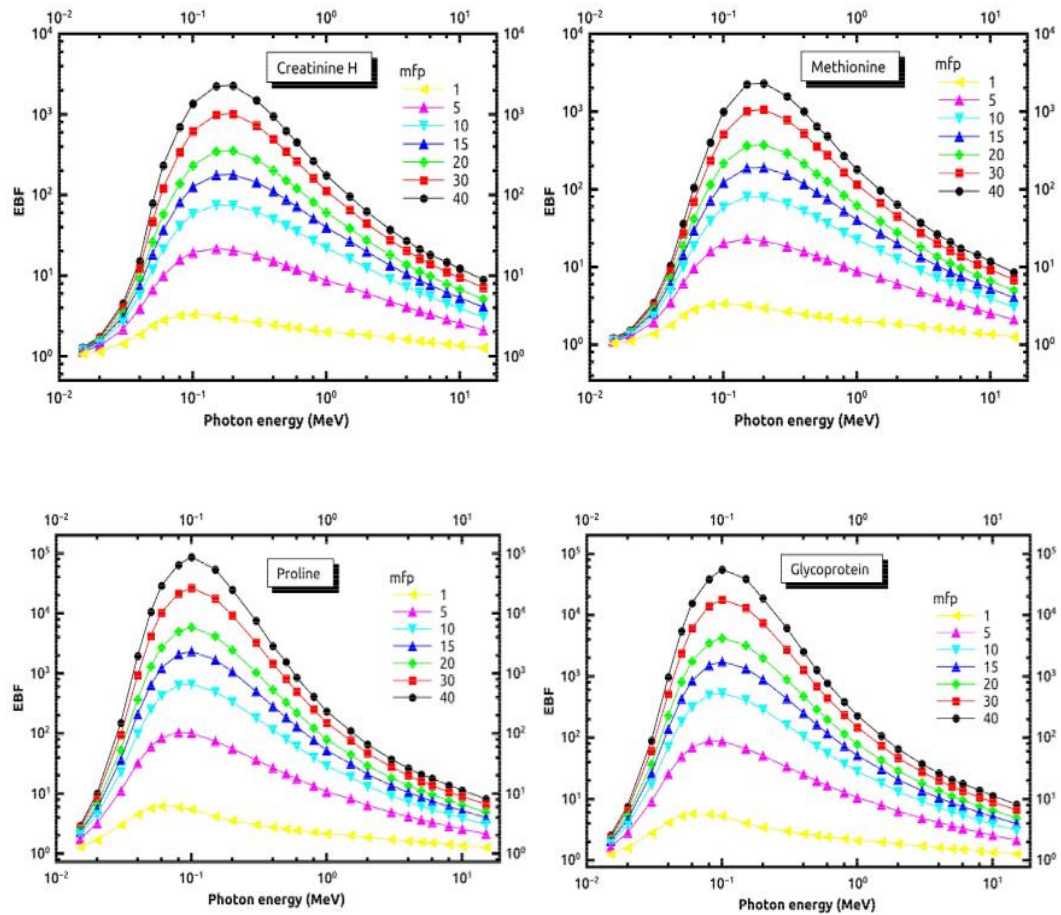


Figure 5.16. EABF as a function of photon energy and at different penetration depths for each biomolecule.

From these tables, one can see that the highest values of Z_{eq} were observed for creatinine H due to it contains the chlorine with $Z = 17$ which is the highest atomic number among all the elements of the biomolecules under this study. Also, methionine has high values of Z_{eq} due to it contains of sulphur ($Z = 16$) as another relatively high- Z element. The rest biomolecules consist of low- Z elements (H, C, N,

O), in this case we found that the lowest values of Z_{eq} were observed for proline which contains the highest amount of oxygen (O = 8, weight fraction = 0.4263).

By using these tables (Table 5.1. – Table 5.6.), both EABF and EBF were calculated for all the studied biomolecules, and then the results were plotted in Figures 5.16. and 5.17.

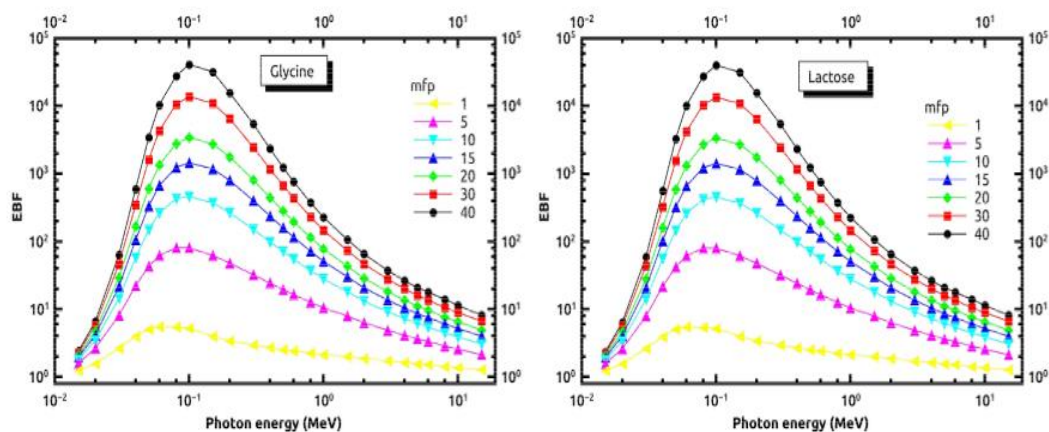


Figure 5.17. EABF as a function of photon energy and at different penetration depths for each biomolecule.

Figure 5.16. shows the EBF of the biomolecules involved for photon energies from 15 keV and 15 MeV at various penetration depths such as 1, 5, 10, 15, 20, 30, and 40 mfp. Figure 5.17. shows the EABF of the biomolecules involved for photon energies from 15 keV and 15 MeV at various penetration depths such as 1, 5, 10, 15, 20, 30, and 40 mfp. It is clear that EABF and EBF increase gradually as the photon energy raises in the low-energy level. Then, the maximum of EABF and EBF was observed for all the studied biomolecules in the intermediate – energy level almost around 0.1 MeV. Thereafter, there is a clear decrease in the values of EABF and EBF with increasing the photon energy for all the biomolecules. Such variation of both EABF and EBF with the photon energy can be explained based on the partial photon interaction mechanism with matter. There are three basic photon interactions viz photoelectric effect, Compton scattering and finally pair production. At the low energy level which can be defined by from 0.03 MeV until 0.1 MeV, a dramatic rising occurred in the values of EABF and EBF due to the dominance of the photoelectric effect. Next, both of EABF and EBF reached their maximum values in the mid-energy region due to the multiple scattering of Compton Effect. Then, in the

high energy region the values of EABF and EBF decrease very fast due to the pair production process. The effect of the chemical composition on the EABF and EBF for all the biomolecules at defined penetration depths of 1 mfp are shown in Figures 5.18. and 5.19., respectively. Clearly, both of EABF and EBF rely on the chemical composition of the studied biomolecule. Such that creatinine H which possesses a maximum Z_{eq} has the smallest values of EABF and EBF among the studied biomolecules. On the other hand, proline which possesses a minimum Z_{eq} has the highest values of EABF and EBF among the studied biomolecules. This is due to that a photon undergoes more interactions with high- Z_{eq} materials leading to reduce the photon buildup processes.

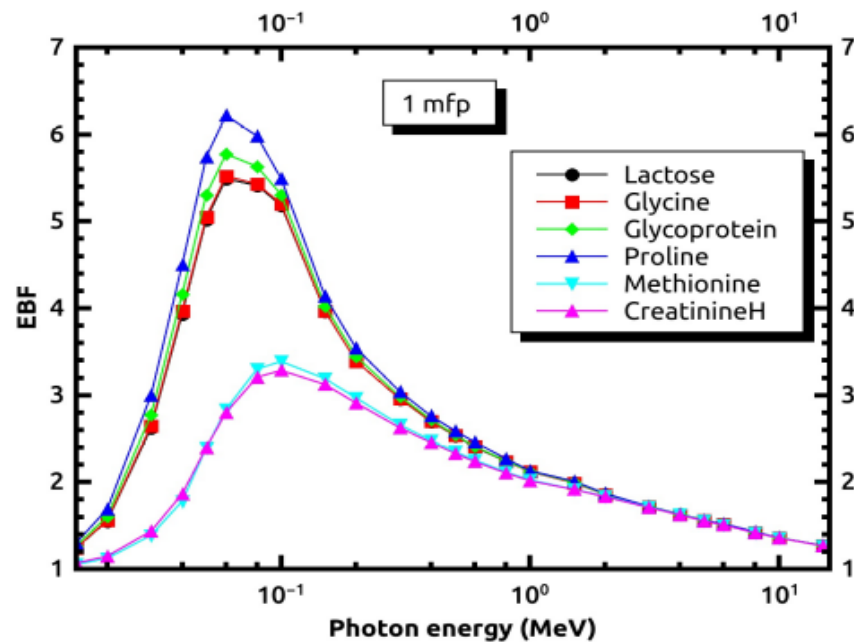


Figure 5.19. EBF of the studied biomolecules at a specific penetration depth of 1 mfp for energies from 1 keV to 15 MeV.

Moreover, it is should mention that the highest values of EABF and EBF were recorded at 40 mfp for all the studied biomolecules. This may be attributed to the secondary photons that come from the pair annihilation processes in the large penetration depths regions. The relation between the buildup factors and the penetration depth up to 40 mfp, at 0.015, 0.15, 1, 8 MeV photon energies, is represented in Figs 5.20. and 5.21. Such figures are of importance in dosimetry to know the dose distribution in the biomolecule (or human tissue).

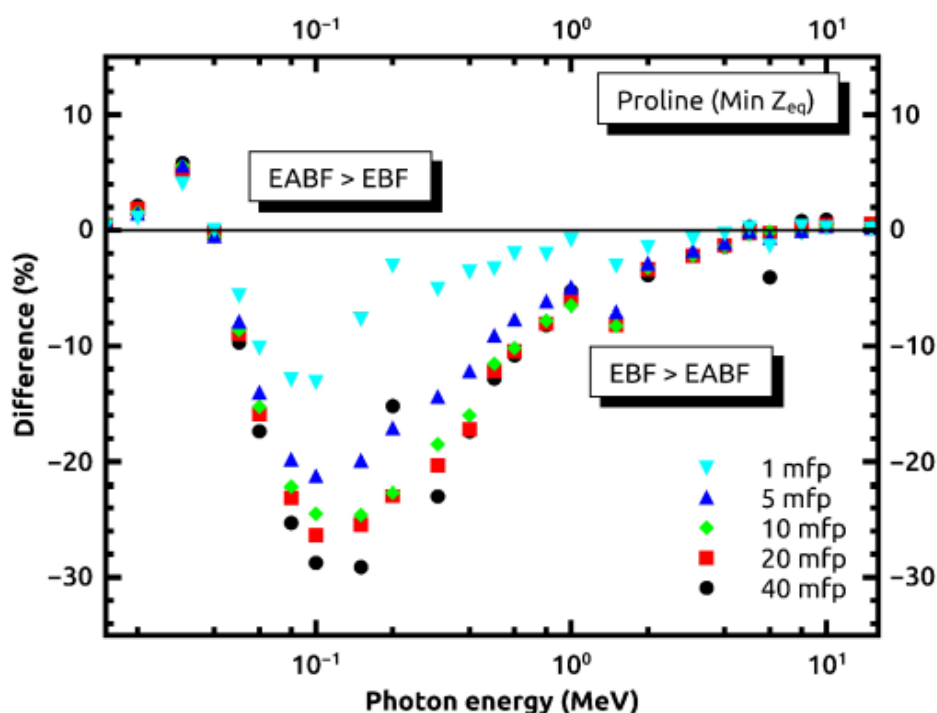


Figure 5.20. Differences between EBF and EABF in the case of proline (Min of Z_{eq}) at penetration depths of 1, 5, 10, 20, and 40 mfp and for energies from 1 keV to 15 MeV.

It is obvious that both of EABF and EBF of the studied biomolecules show strong chemical composition dependence in the low photon energy region (e.g. at 0.015 MeV and 0.15 MeV). In contrast, the EABF and EBF of the studied biomolecules seem to be independent of the chemical composition (or Z_{eq}) in the high photon energy region (e.g. 1 MeV and 8 MeV). Furthermore, from these figures, one can see that all the selected biomolecules possess the maximum values of EABF and EBF at 0.15 MeV among the selected photon energies. Figures 5.22. and 5.23. shows a comparison between EABF and EBF in two cases; i) In the case of Z_{eq} is minimum (e.g. proline) and ii) In the case of Z_{eq} is maximum (e.g. creatinine H). This comparison is achieved in the photon energy range of 0.015–15 MeV up to 40 mfp. In the first case, the difference between EABF and EBF is negative which mean that the values of EBF are larger than those of EABF. This is due to that the Z_{eq} values of the air are in the range of 7 – 8, while we found that the Z_{eq} values of proline are in the range of 5.9 – 6.9. So, the Z_{eq} values of proline are close to those of the air which refers to that many photons will be absorbed in the air leading to increase EBF instead of the EABF. In the other case, the difference between EABF and EBF is

positive which mean that the values of EABF are larger than those of EBF. This due to that the Z_{eq} values of the creatinine H (see Table 2.1.) are larger than those of the air. Therefore, many photons will be absorbed in the biomolecule sample leading to increase EABF instead of EBF.

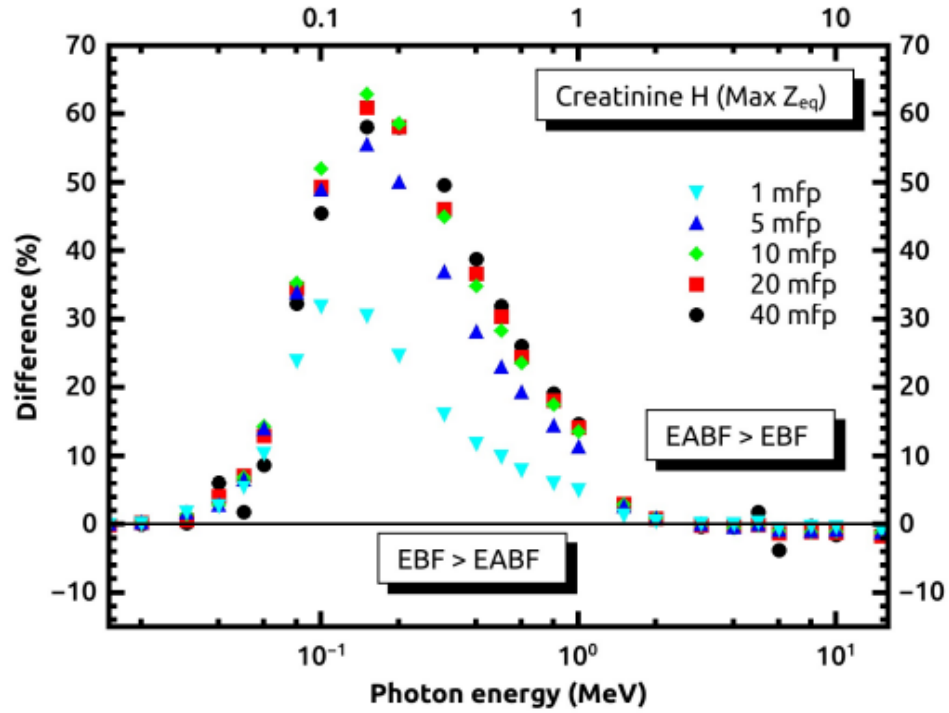


Figure 5.21. Differences between EBF and EABF in the case of creatinine H (Max of Z_{eq}) at penetration depths of 1, 5, 10, 20, and 40 mfp and for energies from 1 keV to 15 MeV.

The buildup factors (PEABF and PEBF) were obtained to understand and describe the photon interaction and photon attenuation as it passes through different elements, compounds, mixtures, and materials such as polymers, glasses, rocks, and ...ect [143-148]. Furthermore, it is worth mentioning that there are some programs to obtain PEABF and PEBF for energies up to 15 MeV and penetration depths between 1 and 40 mfp. One of these programs is BXCOM [149]. Phy-X/PSD is also another program to carry out the radiation attenuation studies [150].

5.4. Dose Calculation

The dose distribution (for photons beam) at a distance r from the source is mainly related to the linear attenuation coefficient (μ) and the exposure buildup factor

(denoted by EBF, here to simplify we will use B), according to the following equation:

$$\frac{D_r}{D_0} = \exp(-\mu \times r) \frac{B}{r} \quad (5.1)$$

Here, D_r is the relative dose and D_0 is the initial dose produced by gamma source. R is the distance from the gamma source. Therefore, the relative dose distribution for different penetration depths (in unit of mfp) can be calculated in aid of the evaluated EBF. Moreover, to perform these calculations we selected different values of r such as $r = 0.001$ cm, 0.01 cm, ...etc.

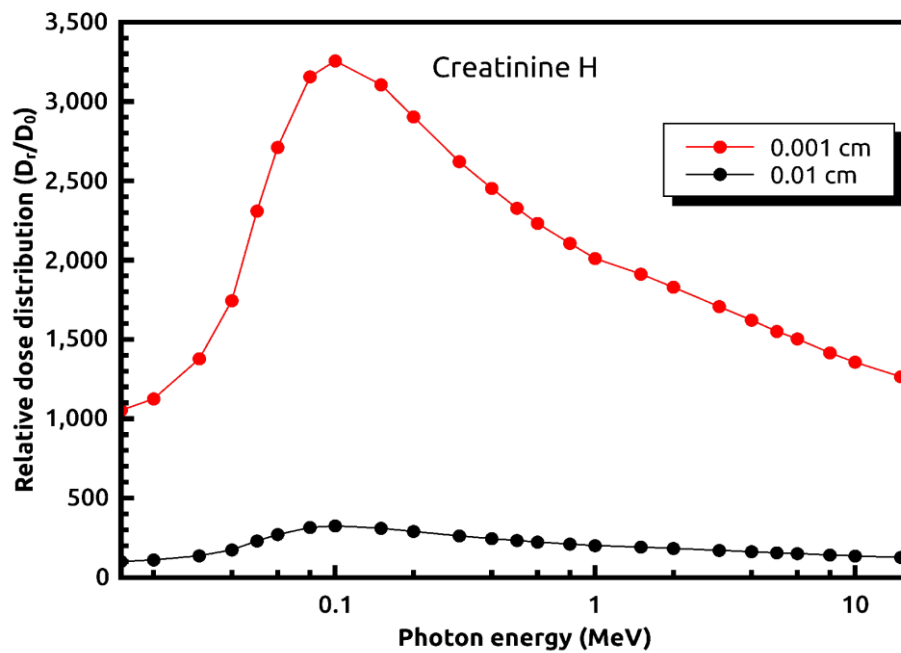


Figure 5.22. Relative dose distribution of gamma ray for the studied biomolecule at different energy levels from 1 keV to 15 MeV and at 1 mfp.

Figure 5.24. shows the relative dose distribution for the creatinine H biomolecule at different energy levels from 1 keV to 15 MeV and at two values of r . It is seen clearly that the relative dose of the biomolecule varies with photon energy and the distance r at the specific penetration depth (in this work the penetration depth was 1 mfp). At a certain $r=0.001$ cm, the relative dose increase as the photon energy increases up to

0.1 MeV, and then there is a swift decrease as the photon energy increases up to 15 MeV.

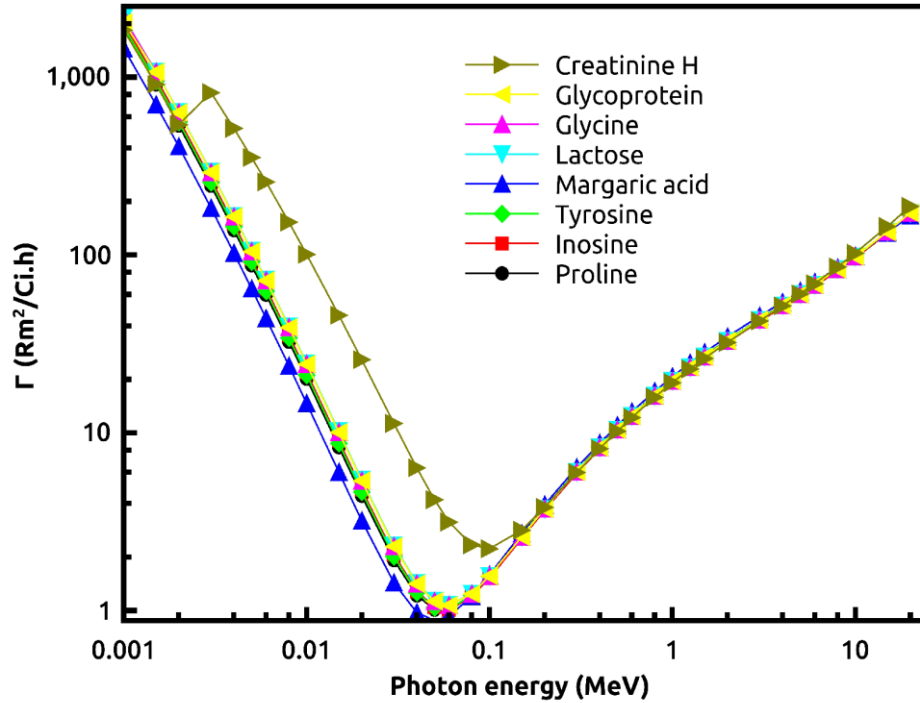


Figure 5.23. Variations of specific gamma ray constant for the studied biomolecule at different energy levels from 1 keV to 15 MeV.

Figure 5.25. shows the variations of specific gamma ray constant for the creatinine H biomolecule at different energy levels from 1 keV to 15 MeV and at one value of r (1 m). It is worth mentioning that the gamma factor or the gamma ray constant (Γ) is the exposure rate (in R/hr) due to photons with the source activity of 1 Ci and at a distance of 1 m from a source. The calculation procedure of this parameter was discussed in chapter 2. distance of 1 m from a source. The calculation procedure of this parameter was discussed in chapter 2.

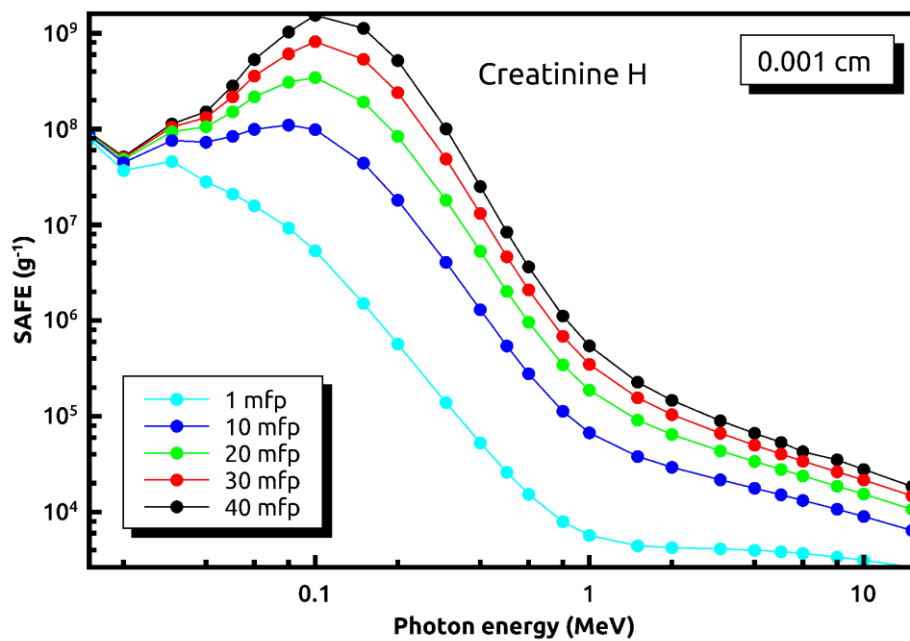


Figure 5.24. Variations of gamma SAFE for the biomolecule namely: lactose at different energy levels from 1 keV to 15 MeV.

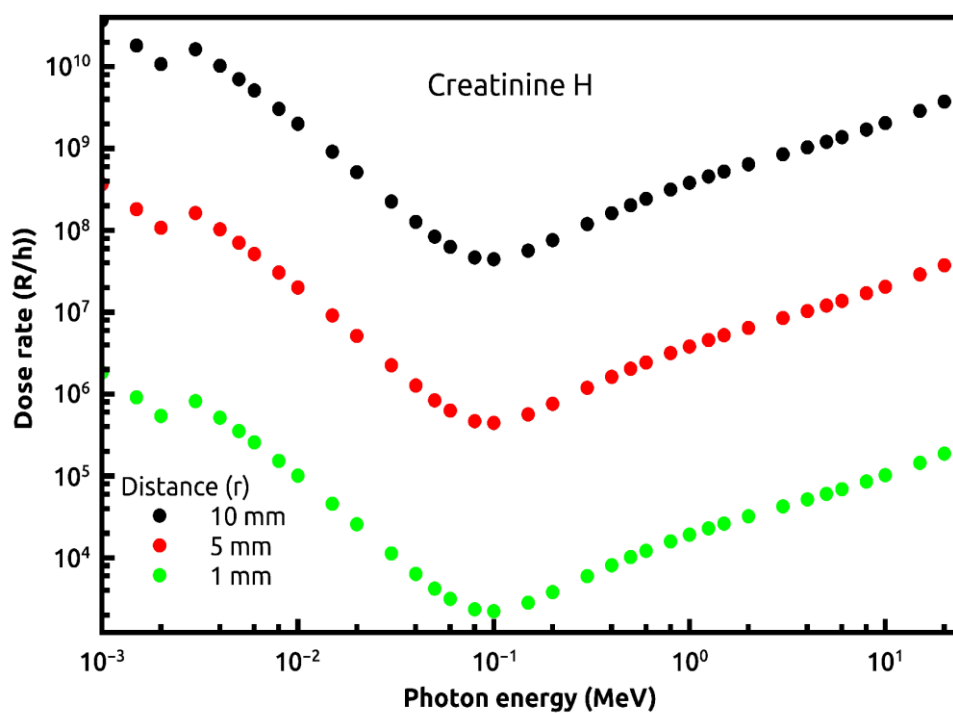


Figure 5.25. Variations of gamma dose rate for the biomolecule namely: creatinine H at different energy levels from 1 keV to 15 MeV.

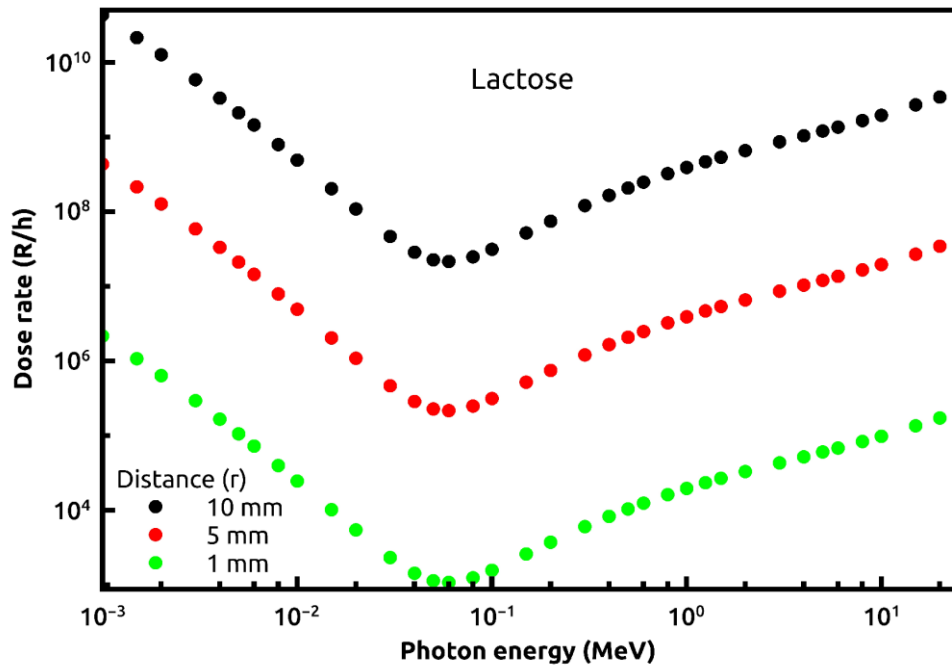


Figure 5.26. Variations of gamma dose rate for the biomolecule namely: lactose at different energy levels from 1 keV to 15 MeV.

From Figure 5.25., one can also see that the variation of the specific gamma ray constant decreased due to the predominant of the absorption processes in the low photon energies between 0.1 and 0.4 MeV. Then, the values of the gamma constant start to increase gradually as the photon energy increases due to the predominant of the scattering processes.

The absorbed dose in a homogenous medium or as well-known by SAFE (specific absorbed fraction of the energy) can be evaluated by using the PEABF values at a certain distance (x) between the gamma source and the absorbing material, via the relation below:

$$SAFE = \frac{\mu_{en} \exp(-\mu x) (PEABF)}{4\pi x^2 \rho} (g^{-1}) \quad (5.2)$$

Here μ_{en} is the linear energy-absorption coefficient.

Figure 5.26. shows the variations of the SAFE values for the creatinine H biomolecule at different energy levels from 1 keV to 15 MeV and at one value of r (0.001 cm) for different penetration depths such as 1, 10, 20, 30, and 40 mfp. In the low photon energies ($E < 0.1$ MeV), the SAFE values increased due to the predominant of the absorption processes. After that (above 0.1 MeV), the SAFE values decreased due to the dominance of the scattering processes.

Finally, the values of gamma constant are used to obtain the dose rate (R/hr) for creatinine H and lactose for photon energies up to 15 MeV at different thicknesses (1, 5, and 10 mm). The results of the dose rate are shown in Figures 5.27. and 5.28. for creatinine H and lactose, respectively. Clearly, the gamma dose rate decreased with increasing thickness. The dose calculations in terms of relative dose distributions, specific gamma ray constant, specific absorbed fraction of the energy (SAFE), and dose rate were reported for bismuth borate glasses [151] and for some alloys [152].

5.5. Interaction of Charged Particles

In this subsection, we shall present the interaction parameters of charged particles such as electron, proton, alpha, and carbon ion with the studied biomolecules (methionine, creatinine hydrochloride, glycoprotein, lactose, glycine, and proline).

5.5.1. Electron Interaction with the Biomolecules

The electron interactions parameters include the stopping power, CSDA range, and effective atomic number. Variation of the total stopping power (TSP) of the electron interaction with the studied biomolecules for energies from 1 keV to 1000 MeV, is shown in Figure 5.27.

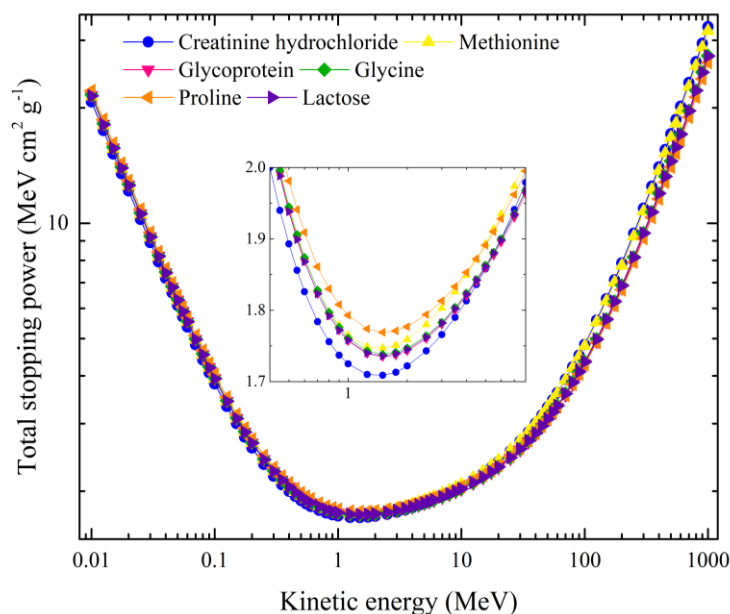


Figure 5.27. Total stopping power of the electron interaction with the studied biomolecules for energies from 1 keV to 1000 MeV.

From this figure, the TSP values decrease as the kinetic energy of the electron increases from 0.01 MeV to 2 MeV. Above 2 MeV, there is a notable increase in the TSP values up to 1000 MeV. Such behaviour may be attributed to the Coulomb force that led to energy lost in terms of collision and radiation interactions.

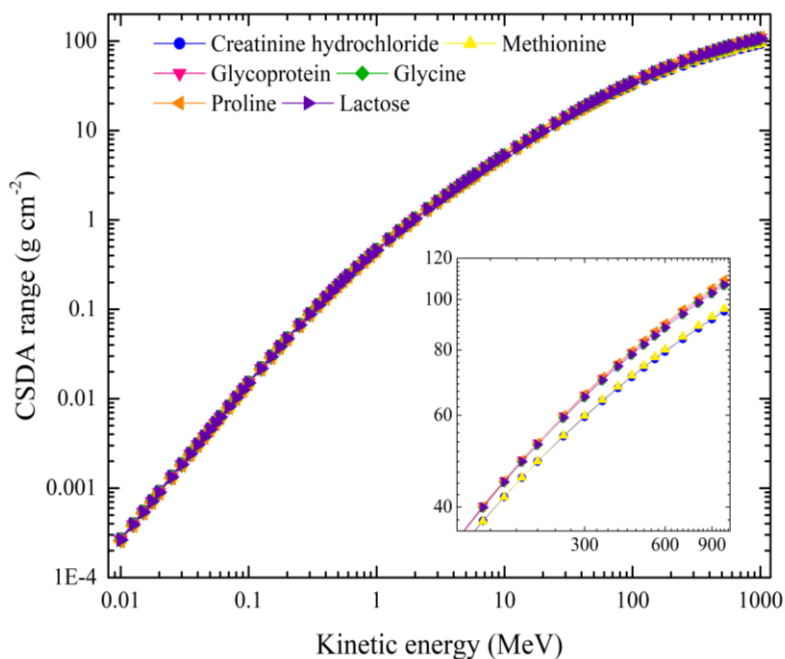


Figure 5.28. CSDA range of the total electron interaction with the studied biomolecules for energies from 1 keV to 1000 MeV.

Moreover, the maximum values of TSP occurred at 1000 MeV for all of the chosen biomolecules, and they were 32.54, 31.74, 26.87, 27.33, 26.25, and 27.3 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively. Therefore, at the high energy (1000 MeV), the creatinine H biomolecule owns the highest TSP values among the studied biomolecules. However, the proline biomolecule owns the highest TSP values among all the studied biomolecules at the low energy (0.01 MeV). Generally, the TSP values come in the following order proline > methionine > glycine > creatinine H > glycoprotein > lactose.

It is also worth to investigate the electron interaction with the biomolecules in terms of CSDA range. Both the stopping power and CSDA range were calculated by using ESRAR program. Variation of the CSDA range of the total electron interaction with the studied biomolecules for energies from 1 keV to 1000 MeV, is shown in Figure 5.28. Clearly, there is a linear relation between the CSDA range and the electron kinetic energy. Furthermore, the maximum values of CSDA range occurred at 1000 MeV for all of the chosen biomolecules, and they were 94.99, 96.03, 108, 106.7, 109.1, and 106.8 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively. Therefore, at the high energy (1000 MeV), the proline biomolecule owns the highest CSDA range values among all the studied biomolecules at the low energy (0.01 MeV). Generally, the CSDA range values come in the following order proline > methionine > glycine > creatinine H > glycoprotein > lactose. Furthermore, by comparing the behaviour of TSP and CSDA range for the studied biomolecules, one can notice that the chemical composition dependence in TSP values is stronger than those in the values of CSDA range for all of the studied biomolecules.

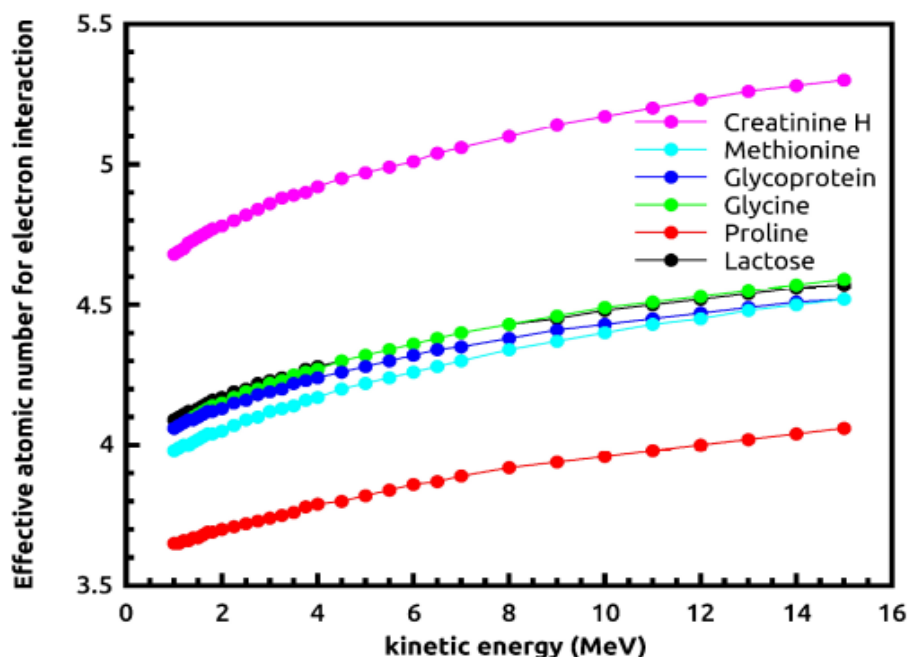


Figure 5.29. Effective atomic number of total electron interaction with the studied biomolecules for energies from 1 keV to 15 MeV.

Figure 5.29. shows the variation of the effective atomic number (Z_{eff}) for the total electron interaction with the studied biomolecules for electron energies from 1 keV to 15 MeV. All of the studied biomolecules have the same variation of Z_{eff} with the electron kinetic energy. Such that the Z_{eff} values increase as the electron kinetic energy increases. Moreover, it is clear that the creatinine H biomolecule owns the highest Z_{eff} values, while the proline biomolecule owns the lowest Z_{eff} values among all the studied biomolecules. The maximum Z_{eff} values that occurred at 15 MeV, were 5.30, 4.52, 4.52, 4.59, 4.06, and 4.57 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively.

5.5.2. Heavy charged particle Interaction with the Biomolecules

For heavy charged particle interaction (proton, alpha particle, and carbon ion) we shall calculate the effective atomic number for each total interaction. Such parameter is sufficient to give the important information for the charged particle interaction with the studied biomolecules. For more detail, one can also calculate other parameters such as stopping power and ranges for each

charged particle. Such calculation can be performed manually or by using SRIM program [153]. This program can provide the values of the stopping power and ranges for all the charged particles such as electron, proton, and alpha particle. Then, the effective atomic number of the total interaction of the charged particle with the absorbing medium can be calculated by applying the interpolation method. On the other hand, there is another important program namely PhyX/ZEXTRA, this program can be used to obtain and study the effective atomic number for the charged particle [154]. Furthermore, the PhyX/ZEXTRA program can be used to calculate the effective atomic number for photon interaction and energy-absorption. Finally, the Auto-Zeff software is also a strong tool to study the effective atomic number for the photon interaction, especially at high photon energies [155].

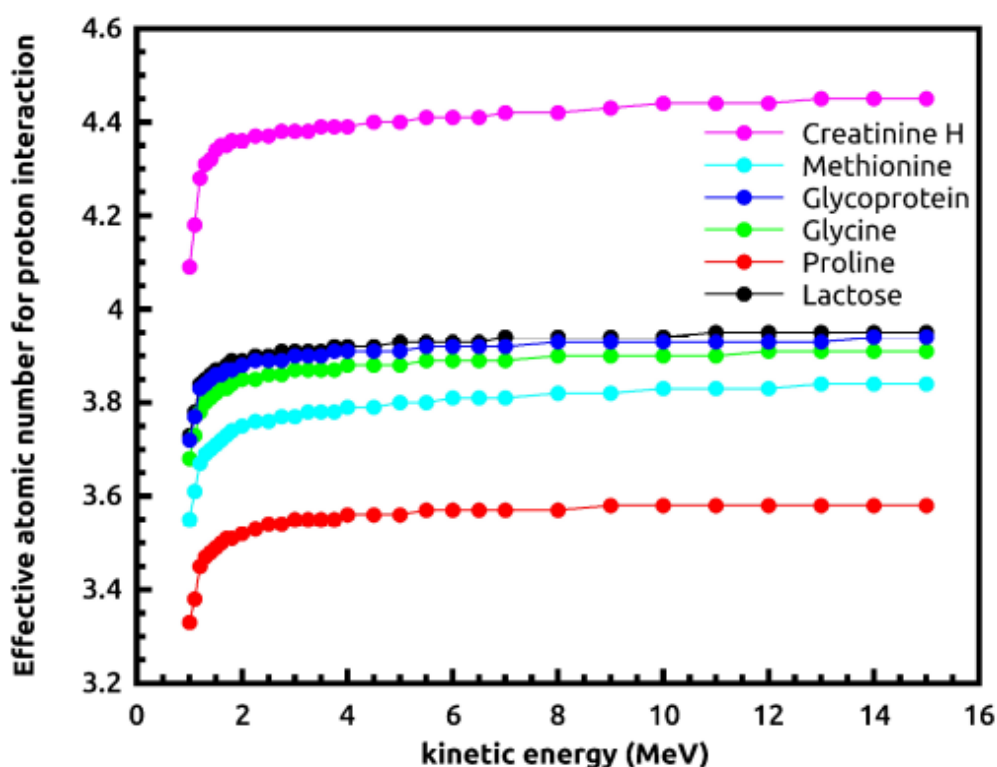
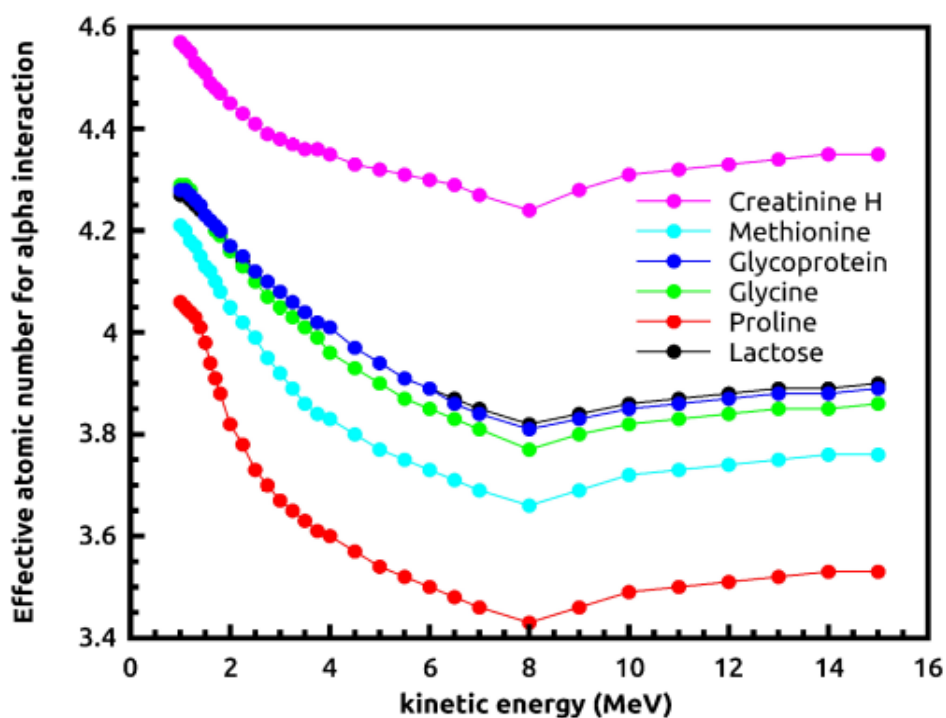


Figure 5.30. Effective atomic number of total proton interaction with the studied biomolecules for energies from 1 keV to 15 MeV.

Figure 5.30. shows the variation of the effective atomic number (Z_{eff}) for the total proton interaction with the studied biomolecules for electron energies from 1 keV to 15 MeV. All of the studied biomolecules have the same variation of Z_{eff} with the electron kinetic energy. Such that the Z_{eff} values increases as the electron kinetic energy increases. Moreover, it is clear that the creatinine H biomolecule owns the highest Z_{eff} values, while the proline biomolecule owns the lowest Z_{eff} values among all the studied biomolecules. The maximum Z_{eff} values that occurred at 15 MeV, were 4.45, 3.84, 3.94, 3.91, 3.58, and 3.95 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively. It is seen clearly that the effective atomic numbers for proton interaction are lower than those of electron interaction. This is normal and can be attributed to the light mass of the electron comparing to the mass of proton



Figure

5.31. Effective atomic number of total alpha interaction with the studied biomolecules for energies from 1 keV to 15 MeV.

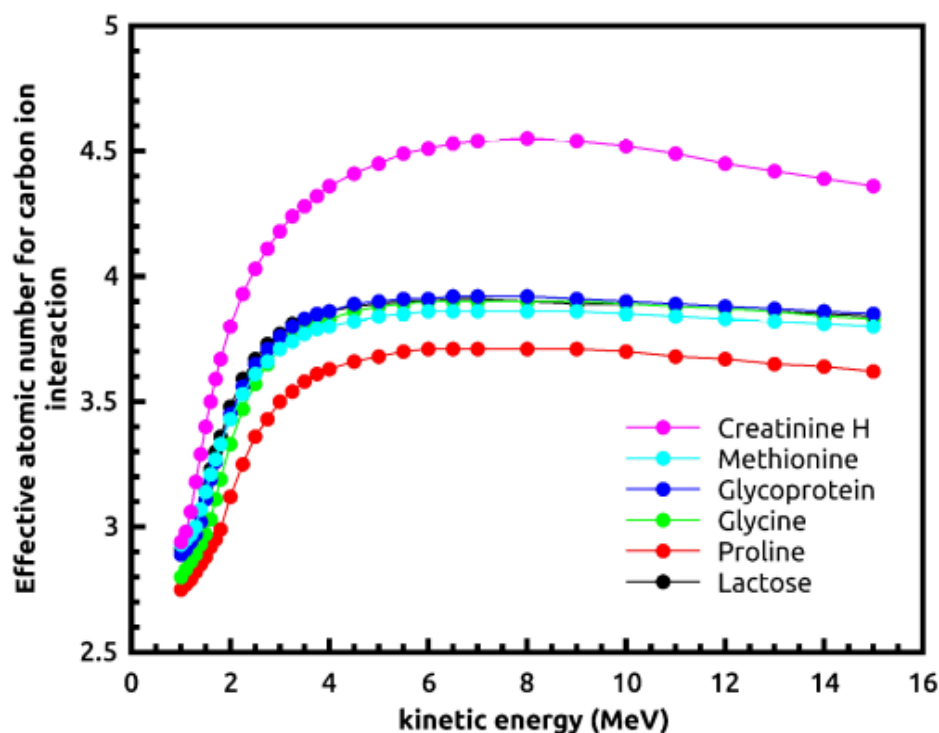


Figure 5.32. Effective atomic number of carbon ion interaction with the studied biomolecules for energies from 1 keV to 15 MeV.

Figure 5.31. shows the variation of the effective atomic number (Z_{eff}) for the total alpha particle interaction with the studied biomolecules for alpha particle energies from 1 keV to 15 MeV. All of the studied biomolecules have the same variation of Z_{eff} with the electron kinetic energy. Such that the Z_{eff} values increases as the alpha particle kinetic energy increases. Moreover, it is clear that the creatinine H biomolecule owns the highest Z_{eff} values, while the proline biomolecule owns the lowest Z_{eff} values among all the studied biomolecules. The maximum Z_{eff} values that occurred at 15 MeV, were 4.35, 3.76, 3.89, 3.86, 3.86, 3.53, and 3.90 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively. It is seen clearly that the effective atomic numbers for alpha particle interaction are lower than those of proton interaction. This is normal and can be attributed to the light mass of the proton comparing to the mass of alpha particle.

Figure 5.32. shows the variation of the effective atomic number (Z_{eff}) for the total carbon ion interaction with the studied biomolecules for carbon ion energies from 1 keV to 15 MeV. All of the studied biomolecules have the same variation of Z_{eff} with the electron kinetic energy. Such that the Z_{eff} values increases as the carbon ion kinetic energy increases. Moreover, it is clear that the creatinine H biomolecule owns the highest Z_{eff} values, while the proline biomolecule owns the lowest Z_{eff} values among all the studied biomolecules. The maximum Z_{eff} values that occurred at 15 MeV, were 4.36, 3.80, 3.85, 3.83, 3.62, and 3.84 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively.

CHAPTER 6. CONCLUSION

In this chapter, the results of the current thesis are summarized. The radiation interaction parameters of essential biomolecules were extracted mainly for photon (X/gamma) interaction. Moreover, the present thesis includes some parameters for charged particles such as electron, proton, alpha, and carbon ion. Furthermore, the dose calculations of photon interaction were presented and discussed in detail. The projectile energy in this study was varying from 1 keV up to 15 MeV. The obtained data in this study was estimated by using Geant4 Monte Carlo simulation, XCOM program, ESTAR program, and different theoretical approaches such as G-P method that is used for evaluating PEABF and PEBF. Finally, an extended comparison was achieved with the experimental values wherever that possible.

The maximum values of μ/ρ occurred at 1 keV for all of the essential biomolecules. At this photon energy, the μ/ρ values were 2803, 2707, 3098, 3282, 2784, and 3291 cm^2/g for creatinine hydrochloride, methionine, glycoprotein, glycine, proline and lactose, respectively. In case of methionine, two values can be seen for the μ/ρ values at 2.47 keV which is the sulphur K-absorption edge. First one is $2.13 \times 10^2 \text{ cm}^2/\text{g}$ that is below the absorption edge, and the second one is $6.44 \times 10^2 \text{ cm}^2/\text{g}$ that is immediately above the absorption edge. Similarly, for creatinine hydrochloride, around chlorine K- absorption edge (2.82 keV), the first value of μ/ρ is $1.51 \times 10^2 \text{ cm}^2/\text{g}$ and the second value is $5.21 \times 10^2 \text{ cm}^2/\text{g}$. The μ/ρ values obtained by Geant4 simulation of the essential biomolecules are comparable with those of XCOM (theoretical results). A very good agreement is noted in the intermediate and high photon energies, while a significant difference up to 19 % are found in the low photon energies in the range of 10 -150 keV.

The Z_{eff} values changed from 4.6 to 8.8 for creatinine H, from 4.0 to 6.0 for lactose, from 4.0 to 6.0 for glycine, from 3.3 to 5.4 for proline, from 4.0 to 8.1 for methionine and from 4.0 to 6.0 for glycoprotein. The Z_{eff} is strongly dependent on the photon energy, while the $Z_{\text{RW}_{\text{eff}}}$ is weakly dependent on the photon energy. Both $Z_{\text{PEA}_{\text{eff}}}$ and $Z_{\text{PI}_{\text{eff}}}$ (or Z_{eff}) have the same behaviour (almost the same values) at low and high photon energies where the absorption processes (photoelectric effect and pair production) are dominant mechanisms. However, there are significant differences between $Z_{\text{PEA}_{\text{eff}}}$ and $Z_{\text{PI}_{\text{eff}}}$ at the middle photon energy where the Compton scattering is the dominant process.

The Z_{eq} values vary from 6.35 to 7.02. The maximum Z_{eq} values were noted at intermediate energies such as 800 keV and 1 MeV, while the minimum values were noted at high energies such as 10 MeV and 15 MeV. The maximum of EABF and EBF was observed for all the studied biomolecules in the intermediate – energy level almost around 0.1 MeV. Thereafter, there is a clear decrease in the values of EABF and EBF with increasing the photon energy for all the biomolecules.

The maximum values of TSP occurred at 1000 MeV for all of the chosen biomolecules, and they were 32.54, 31.74, 26.87, 27.33, 26.25, and 27.3 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively. While the maximum values of CSDA range were 94.99, 96.03, 108, 106.7, 109.1, and 106.8 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively. For electron interaction, the maximum Z_{eff} values that occurred at 15 MeV, were 5.30, 4.52, 4.52, 4.59, 4.06, and 4.57 for creatinine H, methionine, glycoprotein, glycine, proline, and lactose, respectively. The effective atomic numbers for proton interaction are lower than those of electron interaction. This is normal and can be attributed to the light mass of the electron comparing to the mass of proton.

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RESUME

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