

Gamma-Ray Attenuation Characteristics of Some Essential Amino Acids for ^{57}Co , ^{192}Ir , ^{18}F , and $^{116\text{m}}\text{In}$ Sources

Reza Bagheri ¹, Alireza Khorrami Moghaddam ^{2*} 

¹ Northwest Research Complex (Bonab), Radiation Applications Research School, Nuclear Science and Technology Research Institute, Tehran, Iran

² Department of Radiology, Faculty of Allied Medicine, Mazandaran University of Medical Sciences, Sari, Iran

*Corresponding Author: Alireza Khorrami Moghaddam
Email: ar.khorrami@gmail.com

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Abstract

Purpose: In different tissues of the body, proteins are important parts that are made up of building blocks called amino acids. Considering the wide applications of radioactive sources in industry and medicine, the need to study the attenuation characteristics of amino acids is determined.

Materials and Methods: To study the attenuation characteristics of five types of amino acids, MCNPX Monte Carlo code and XMuDat program were used. Linear and mass attenuation coefficients, half and tenth value layers, mean free path, effective atomic and electronic cross-sections, effective atomic numbers and effective electron densities were calculated. ^{57}Co , ^{192}Ir , ^{18}F , and $^{116\text{m}}\text{In}$ gamma sources were considered for this study. To validate the theoretical results, the obtained values were compared with the available experimental data.

Results: The difference between the theoretical and experimental results was less than 11%. The results showed that with increasing photon energy, the linear and mass attenuation coefficients and effective atomic and electronic cross-sections decreased, while the half and tenth value layers and mean free path quantities increased. Furthermore, the linear attenuation coefficients, the effective atomic and electronic cross-sections, as well as the effective atomic number values increased with increasing amino acid density, while the effective electron density behaves independently of the amino acid density.

Conclusion: The presented theoretical methods produced data similar to experimental results with fair accuracy, so by using these methods, attenuation properties of other amino acids can be obtained over a wide range of energies.

Keywords: Amino Acid; Linear Attenuation Coefficient; Effective Electron Density; Monte Carlo N-Particle eXtended Code; XMuDat Program.

1. Introduction

Proteins are large organic matters and one of the largest types of biological molecules made up of subunits called amino acids. Amino acids are molecules that contain functional groups of amino and carboxylic acids. There are about twenty-one types of amino acids that are essential for the human body [1]. Considering the wide applications of X- and gamma rays in fields of medical diagnosis and therapy, industry, agriculture, and so on, the study and estimation of radiation attenuation characteristics by amino acids as the building blocks of living organisms are clearly identified [2,3].

Cobalt-57 source with a half-life of 270 days and a gamma-ray of 122 KeV and a branching ratio of 87% is used in medical tests related to the absorption of vitamin B-12 through the labeling of this type of vitamin [4]. Iridium-192 radioisotope with a half-life of 74.2 days and a gamma-ray of 317 KeV is used in industrial radiography as well as radiotherapy as brachytherapy [5]. Fluorine-18, with a short half-life of 109.7 minutes, which decays through positron emission mode, is one of the first radioisotopes used in Positron Emission Tomography (PET). The positron emitted in the pair production reaction will be converted to two gamma rays of 511 KeV [6]. Indium-116 is also a radioisotope with a half-life of 54 minutes and a gamma-ray emission of 1293 KeV with a branching ratio of 80%, which is used as an indium chloride to bind and label antibodies, proteins, and other molecules [7].

Many experimental and theoretical studies have been done on the interactions and effects of radiation on amino acids. Nair *et al.* [8,9] experimentally measured the total attenuation cross-section of the sixteen amino acids for the gamma rays of cobalt-60, cesium-137, and barium-133 sources under good geometry (very thin beam and absorber). Gowda *et al.* [10] calculated the effective atomic numbers and electron densities of the fifteen amino acids and eleven sugars in the energy range of 30 to 1333 keV using the measured total attenuation cross-section data by Nair *et al.* [8,9]. The effective atomic numbers and electron densities of some biologically important compounds such as cholesterol, fatty acids, sugars and some amino acids containing H, C, N, and O atoms were calculated by Manjunathaguru and Umesh [11] in the energy range of 145–1330 keV using a new matrix method and a semi-empirical relation for Z_{eff} .

Elbashir *et al.* [12] calculated the mass attenuation coefficients, effective atomic numbers, and electron densities of six amino acids using MCNP5 simulations and XCOM program in the energy range of 0.122–1.330 MeV. Lokhande *et al.* [13] experimentally measured the attenuation parameters and energy absorption build-up factor of amine group materials in the energy range of 122 keV to 1330 keV with the gamma-ray count in the narrow beam geometry condition. Photon attenuation coefficient of N-Acetyl-L-tryptophan ($\text{C}_{13}\text{H}_{14}\text{N}_2\text{O}_5$), n-acetyl-L-tyrosine ($\text{C}_{11}\text{H}_{13}\text{NO}_4$), D-tryptophan ($\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}_2$), n-acetyl-L-glutamic acid ($\text{C}_7\text{H}_{11}\text{NO}_5$), D-phenylalanine ($\text{C}_9\text{H}_{11}\text{NO}_2$), and D-threonine amino acids ($\text{C}_4\text{H}_9\text{NO}_3$) were experimentally studied by More *et al.* [14], for ^{57}Co , ^{133}Ba , ^{137}Cs , ^{22}Na , ^{54}Mn , and ^{60}Co radioisotopes.

The effective atomic numbers and the effective electron densities of the eight essential amino acids were calculated by Manohara and Hanagodimath [15], for a wide range of gamma-ray energies (GeV 100-KeV 1) using WinXCOM. The linear and mass attenuation coefficients of glycine amino acid for 360, 662, 1170, and 1330 KeV photons were measured experimentally by Pawar and Mahajan [1]. Pawar and Bichile [16] experimentally measured the mass attenuation coefficient, atomic number, and effective electron density of six amino acids in the energy range of 0.122 to 1.330 MeV using a narrow, collimated gamma-ray beam. Bagheri *et al.* [17] theoretically calculated the gamma-ray attenuation characteristics of 15 types of amino acids against barium-133, cesium-137, and cobalt-60 sources using the MCNP-4C Monte Carlo code and the XCOM program.

In this paper, for the first time, gamma-ray attenuation characteristics of the five essential amino acids of leucine, lysine, phenylalanine, tryptophan, and histidine are calculated for the some widely used radionuclides such as cobalt-57, iridium-192, fluorine-18, and indium-116m sources. Compared to our previously published article [17], in this research, the more up-to-date and advanced version of MCNP Monte Carlo code (MCNPX code version 2.6.0) and more developed computer program (XMuDat) were employed for the study of gamma-ray shielding against new sources. It was tried to tabulate obtained quantities, then interpreted simulated and calculated results in terms of numerical values. Also, in order to confirm and validate the simulated results and theoretical calculations, the obtained values are compared with the other published experimental data.

2. Materials and Methods

2.1. Simulation

In this research, the MCNPX code version 2.6.0 is used to investigate the radiation attenuation properties of selected amino acids. MCNPX code is a special type of nuclear code based on the Monte Carlo method that is able to transport different nuclear particles through materials [18]. Since this code takes into account all the interactions performed within the material, the results of this code will be accurate and reliable. Cylindrical geometry was used to simulate amino acid samples applying macrobody Rectangular Parallelepiped (RPP) card. According to the experimental measurement conditions [8,9], which is subsequently cited and the results are compared with it, the samples with a diameter of one centimeter and thicknesses of about 1 to 2 mm were considered. The source was considered to be a circular disk with a diameter of 1 cm that radiates collimated gamma-rays perpendicular to the surface of the specimens. Only the gamma rays with the highest branching ratio were considered for each source. Photons of 122 (87%), 317 (83%), 511 (97%) and 1293 (80%) KeV energies were assumed for ^{57}Co , ^{192}Ir , ^{18}F and, $^{116\text{m}}\text{In}$, respectively [4-6]. Default energy cut-off values of electrons and photons (1 KeV) were used in simulations [18]. The percentage of elemental composition and density (g cm^{-3}) of amino acids used in the material card of MCNPX code is shown in Table 1.

In accordance with experimental works [8,9], the detector was considered as a cylinder with dimensions of 5 cm (base)×6 cm (height) located inside a lead shield. An ORTEC HPGe detector (model 23210) with 52.5 mm×58.1 mm cylinder crystal was used in experimental works [8,9]. A lead collimator was also placed between the amino acid samples and the detector in order to remove scattered photons. Figure 1 shows the simulated geometry described above. Particle track illustration and 3-D view

of geometry were given in Figure 1, as well. Figure 1b shows that the modeled configuration almost completely eliminates the scattered photons from getting the detector. Also, Figure 1c indicates to well collimation and shielding of source, samples and detector. MCNP/MCNPX Visual Editor computer code of version X_24E was used for plotting of geometry and particles' tracks.

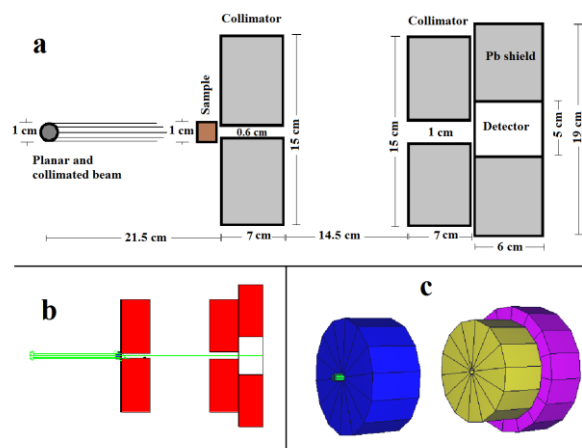


Figure 1. Geometry of modeled configuration. a: sizes are not on scale, b: particle track displaying (2-D view) and c: 3-D view of geometry

In order to calculate the average flux in the detector volume, Tally F4 was applied. This tally calculates the average flux in a cell (detector volume) for one incident photon that originated from the source. About 1 million histories were followed and all simulations were reported with less than 0.5% relative error. In order to variance reduction of tally, the main variance reduction technique of geometry splitting (using imp command) was applied for the transport of particles in the cells with a greater importance. The MCPLIB04 photon transport library was used for the simulations in the MCNPX code.

Furthermore, the theoretical values of mass attenuation coefficients of different elements and compounds have been calculated by Hubbell and Seltzer [19], and Boone and Chavez [20], and they were presented in the form of various computer programs such as WinXCOM [21], and

Table 1. Properties of amino acids used in the material card of MCNPX code [8,9]

Amino acid	Chemical formula	Density (g cm^{-3})	Element			
			H	C	N	O
Leucine	$\text{C}_6\text{H}_{13}\text{NO}_2$	1.035	0.0999	0.5494	0.1068	0.2439
Lysine	$\text{C}_6\text{H}_{14}\text{N}_2\text{O}_2$	1.125	0.0965	0.4930	0.1916	0.2189
Phenyl alanine	$\text{C}_9\text{H}_{11}\text{NO}_2$	1.201	0.0671	0.6544	0.0848	0.1937
Tryptophan	$\text{C}_{11}\text{H}_{12}\text{N}_2\text{O}_2$	1.340	0.0592	0.6469	0.1372	0.1567
Histidine	$\text{C}_6\text{H}_9\text{N}_3\text{O}_2$	1.423	0.0585	0.4645	0.2708	0.2062

XMuDat [22]. The WinXCom program employs the Hubbell and Seltzer [19] database while the XMuDat program can produce mass attenuation coefficient values based on both Hubbell and Seltzer [19] and Boone and Chavez [20] data. In this study, to compare and validate the simulation results, XMuDat computer program was used to calculate the amino acid attenuation properties as well. The Boone and Chavez [20] data source was chosen in the XMuDat program in this research. XMuDat is a program to be used for the calculation of various photon interaction coefficients. Six absorbing materials can be set up individually and simultaneously. Each material can be composed of components chosen from the elements and further from a number of compounds and mixtures of dosimetric interest. This program provides the data for mass attenuation, mass-energy transfer and mass-energy absorption coefficients in a photon energy range of 1 keV to 50 MeV [22].

2.2. Theoretical Calculations

The mass-attenuation coefficient is a fraction of the gamma-ray that disappears during the transition from the unit density thickness of the attenuator. Using this quantity allows us to express the attenuation of the beam as a function of the mass of the environment through which the beam passes, rather than in terms of distance traveled by the beam. Equations 1 and 2 are used to calculate the linear and mass attenuation coefficients in the simulation method with MCNPX code and XMuDat program, respectively [23]. In these relations, μ , μ_m , t , and w_i are the linear and mass attenuation coefficients, thickness and weight fraction of the i th element in the sample, respectively.

$$I = I_0 e^{-\mu t} \quad (1)$$

$$\mu_m = \sum w_i \times \mu_{m,i} \quad (2)$$

The mass attenuation coefficient will be obtained by dividing the linear attenuation coefficient of each amino acid by its density. Furthermore, the Mean Free Path (MFP) is defined as the inverse of the linear attenuation coefficient and the Half and Tenth value Layers (HVL, TVL) are calculated as the division of $\ln 2$ and $\ln 10$ to linear attenuation coefficients of amino acids, respectively.

To define the effective atomic cross-section, it is assumed that all types of elements in the molecules of the absorber are composed of only one type of hypothetical atom or element so that the total molecular cross-section

of the absorber is exactly equal to the total molecular cross-section of the hypothetical substance which all atoms of that substance composed of the hypothetical element. Also, the effective atomic cross-section indicates the interaction probability of an atom from the substituted atoms of the absorber with one of the photons in the beam. The effective electronic cross-section of an electron is also defined as the ratio of the effective atomic cross-section to the number of electrons in the substituted atom. The effective atomic and electronic cross-sections are calculated through the following Equations 3, 4 [24]:

$$\sigma_a = \sum \frac{f_i \times A_i \times \mu_{m,i}}{N_{Av}} \quad (3)$$

$$\sigma_e = \sum \frac{f_i \times A_i \times \mu_{m,i}}{Z_i N_{Av}} \quad (4)$$

In these relations, A_i and Z_i are the atomic mass and atomic number of the i th element in the sample, respectively, and N_{Av} are the Avogadro's number. Also, f_i denotes the fractional abundance of the i th element with respect to the number of atoms such as $f_1 + f_2 + f_3 + \dots + f_i = 1$. The effective atomic number is defined as the ratio of the effective atomic cross section to the effective electron cross-section of the studied material at given photon energy. In other words, the atoms of the absorber are replaced by the atoms with the atomic number of Z_{eff} so that they show the same attenuation properties of the original absorber. The effective electron density is obtained by dividing the mass attenuation coefficient by the effective electronic cross-section and is defined as the ratio of the number of effective electrons present in each gram of the absorber [25].

3. Results

Figure 2 shows the linear attenuation coefficients of the studied essential amino acids at the studied gamma-ray energies. The MCNPX code and the XMuDat program

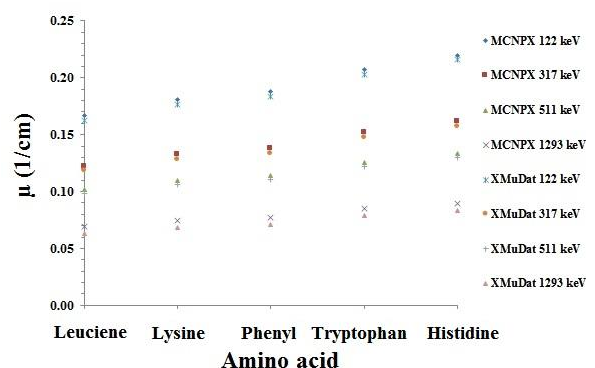


Figure 2. Dependence of linear attenuation coefficient of amino acids on the photon energies

were applied for this purpose. Also, in Table 2, the mass attenuation coefficients of amino acids are given. Equations 1 and 2 have been used to calculate these quantities. The Relative Difference (RD %) between MCNPX code and the XMuDat program is calculated for each amino acid sample in Table 2, as well. In order to confirm and validate the results of simulation and theoretical calculations, the obtained values were compared with the available experimental data [8,9,14,16]. Unfortunately, very limited experimental works were published for the gamma-ray energies studied in this research. Gamma rays of 302.9 and 1332.5 KeV in Nair *et al.* [8,9] work, and 122, 511, and 1275 KeV in More *et al.* [14] and Pawar and Bichile [16] works were selected as the closest gamma-ray energies to

the energies studied in this study. The simulation, computational program, and experimental values along with the RD % values (the difference between theoretical and experimental results) are given in Table 3.

Figure 3 shows the energy dependence of the half and tenth value layers (HVL and TVL) and the mean free path (MFP) quantities for studied amino acids.

The effective atomic cross-sections obtained from the simulation (MCNPX) and computational program (XMuDat) are given in Table 4. Also, the effective electronic cross-sections obtained from the XMuDat computer program are given in Table 5 using Equation 4.

Table 2. Mass attenuation coefficients ($\times 10^{-2} \text{ cm}^{-2} \text{ g}$) of amino acid samples

		Amino acid				
		Leucine	Lysine	Phenyl alanine	Tryptophan	Histidine
Density (g cm^{-3})		1.035	1.125	1.201	1.340	1.423
122 (KeV)	MCNPX	16.10	16.08	15.64	15.48	15.44
	XMuDat	15.73	15.68	15.26	15.15	15.17
	RD %	2.28	2.50	2.43	2.12	1.74
317 (KeV)	MCNPX	11.83	11.75	11.46	11.33	11.33
	XMuDat	11.44	11.41	11.10	11.02	11.02
	RD %	3.29	2.92	3.14	2.77	2.77
511 (Kev)	MCNPX	9.82	9.78	9.48	9.39	9.38
	XMuDat	9.47	9.44	9.19	9.13	9.12
	RD %	3.54	3.44	3.07	2.83	2.76
1293 (KeV)	MCNPX	6.69	6.63	6.44	6.33	6.29
	XMuDat	6.11	6.09	5.93	5.89	5.89
	RD %	8.63	8.04	7.88	6.97	6.37

Table 3. Comparison of theoretical and experimental values of mass attenuation coefficients ($\times 10^{-2} \text{ cm}^{-2} \text{ g}$) for the studied amino acids

		Amino acid						
		Leucine	Lysine	Phenyl alanine	Tryptophan	Histidine		
122 (KeV)	Exp.	16.0 [16]	---	---	---	---		
	MCNPX	16.10	---	---	---	---		
	RD %	0.63	---	---	---	---		
	XMuDat	15.73	---	---	---	---		
	RD %	-1.69	---	---	---	---		
317 (KeV)	Exp.	11.44 [8]	11.54 [8]	11.14 [8]	11.16 [8]	11.15 [8]		
	MCNPX	11.83	11.75	11.33	11.46	11.33		
	RD %	3.43	1.89	1.74	2.72	1.68		
	XMuDat	11.44	11.41	11.02	11.10	11.02		
	RD %	0.03	-1.09	-1.08	-0.5	-1.14		
511 (KeV)	Exp.	9.50 [16]	---	9.39 [14]	---	---		
	MCNPX	9.82	---	9.48	---	---		
	RD %	3.37	---	0.96	---	---		
	XMuDat	9.47	---	9.19	---	---		
	RD %	-0.32	---	-2.13	---	---		
1293 (KeV)	Exp.	6.06 [9]	6.30 [16]	6.06 [9]	5.90 [9]	6.05 [14]	6.05 [9]	5.90 [9]
	MCNPX	6.69	6.69	6.63	6.29	6.29	6.44	6.33
	RD %	10.39	6.19	9.43	6.55	3.97	6.42	7.33
	XMuDat	6.11	6.11	6.09	5.89	5.89	5.93	5.89
	RD %	0.87	-3.02	0.63	-0.24	-2.64	-1.97	-0.15

Also, in Tables 6 and 7, respectively, the values of effective atomic numbers and effective electron densities of the essential amino acids are presented by two methods of simulation (MCNPX) and computational program (XMuDat).

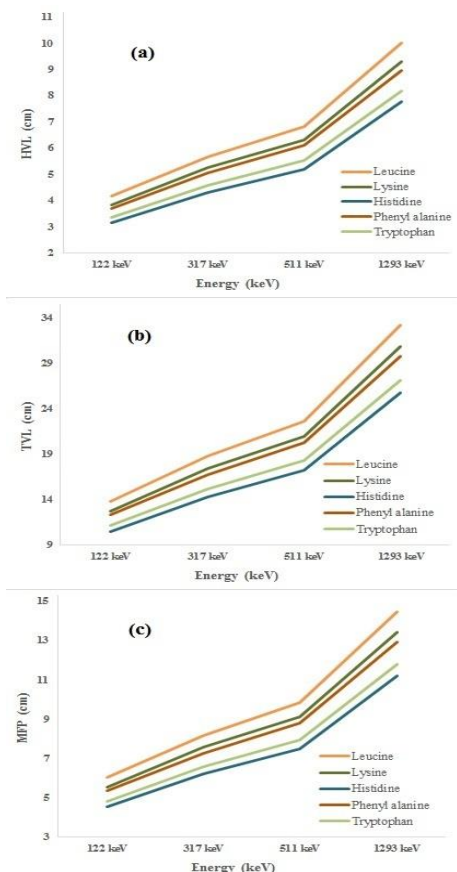


Figure 3. Half (a) and tenth (b) value layers and mean free path (c) of the studied amino acids using MCNPX code

Table 4. Effective atomic cross-sections (barn/atom) of amino acids

Amino acid	Density (g cm ⁻³)	122 (KeV)			317 (KeV)			511 (KeV)			1293 (KeV)		
		MCNPX	XMuDat	RD %	MCNPX	XMuDat	RD %	MCNPX	XMuDat	RD %	MCNPX	XMuDat	RD %
Leucine	1.035	1.59	1.56	2.31	1.17	1.13	3.30	0.97	0.94	3.55	0.66	0.61	8.62
Lysine	1.125	1.63	1.59	2.48	1.19	1.15	2.97	0.99	0.95	3.44	0.67	0.62	8.03
Phenyl alanine	1.201	1.87	1.82	2.41	1.37	1.32	3.12	1.13	1.10	3.07	0.77	0.71	7.88
Tryptophan	1.340	1.94	1.90	2.12	1.42	1.38	2.77	1.18	1.15	2.84	0.80	0.74	6.96
Histidine	1.423	1.99	1.95	1.77	1.46	1.42	2.81	1.21	1.17	2.76	0.81	0.76	6.37

Table 5. Effective electronic cross-sections (× 10⁻² barn/electron) of amino acids using XMuDat program

Amino acid	Density (g cm ⁻³)	122 (KeV)	317 (KeV)	511 (KeV)	1293 (KeV)
		XMuDat	XMuDat	XMuDat	XMuDat
Leucine	1.035	47.191	34.554	28.625	18.485
Lysine	1.125	47.203	34.555	28.625	18.485
Phenyl alanine	1.201	47.262	34.564	28.630	18.486
Tryptophan	1.340	47.284	34.567	28.632	18.487
Histidine	1.423	47.323	34.570	28.633	18.487

4. Discussion

As shown in Figure 2 and Table 2, the linear and mass attenuation coefficients of each of the studied essential amino acids decrease with increasing gamma-ray energy because of the reduction in the probability of interaction through the photoelectric phenomenon. The results also show that there is a good agreement (RD % < 10) between the results of the simulation with MCNPX code and XMuDat calculation program. As the density of amino acids increases, the linear attenuation coefficient of the samples also increases for all four gamma-ray energies. This indicates that the denser the compounds containing the four elements hydrogen, carbon, nitrogen and oxygen, the stronger their attenuation against gamma-rays.

As shown in Table 3, there is a good agreement between the theoretical and experimental results for the studied gamma ray-energies. The difference between the theoretical and experimental results was less than ±11%. It should be noted that the reported error for the experimental results of Nair *et al.* [8,9], was about ±2% and the typical total uncertainty in the measured experimental values of More *et al.* [14] and Pawar and Bichile [16] was estimated to be 2–3%. XMuDat computer program shows less difference with the experimental results than the MCNPX code. The observed differences are related to differences in the type of techniques and the database used. Also, Elbashir *et al.* [12] deduced that the μm values of each amino acid tend to decrease quickly in the low photon energy region and become constant in the medium

Table 6. Effective atomic numbers (Z_{eff}) of studied amino acids

Amino acid	Density (g cm ⁻³)	122 (KeV)			317 (KeV)			511 (KeV)			1293 (KeV)		
		MCNPX	XMudat	RD %	MCNPX	XMudat	RD %	MCNPX	XMudat	RD %	MCNPX	XMudat	RD %
Leucine	1.035	3.38	3.30	2.31	3.39	3.28	3.30	3.40	3.28	3.55	3.58	3.27	8.62
Lysine	1.125	3.45	3.36	2.48	3.44	3.34	2.97	3.45	3.34	3.44	3.63	3.33	8.03
Phenyl alanine	1.201	3.95	3.85	2.41	3.95	3.83	3.12	3.95	3.83	3.07	4.15	3.83	7.88
Tryptophan	1.340	4.11	4.02	2.12	4.12	4.00	2.77	4.12	4.00	2.84	4.30	4.00	6.96
Histidine	1.423	4.20	4.13	1.77	4.22	4.10	2.81	4.22	4.10	2.76	4.38	4.10	6.37

Table 7. Effective electron densities ($\times 10^{-24}$ electron/g) of studied amino acids

Amino acid	Density (g cm ⁻³)	122 (KeV)			317 (KeV)			511 (KeV)			1293 (KeV)		
		MCNPX	XMudat	RD %	MCNPX	XMudat	RD %	MCNPX	XMudat	RD %	MCNPX	XMudat	RD %
Leucine	1.035	0.341	0.333	2.28	0.342	0.331	3.29	0.343	0.331	3.54	0.362	0.331	8.63
Lysine	1.125	0.341	0.332	2.50	0.340	0.330	2.92	0.342	0.330	3.44	0.359	0.330	8.04
Phenyl alanine	1.201	0.331	0.323	2.43	0.332	0.321	3.14	0.331	0.321	3.07	0.348	0.321	7.88
Tryptophan	1.340	0.327	0.320	2.12	0.328	0.319	2.77	0.328	0.319	2.83	0.342	0.318	6.97
Histidine	1.423	0.326	0.321	1.74	0.328	0.319	2.77	0.328	0.319	2.76	0.340	0.319	6.37

photon energy region (Compton Effect territory). This means that if the incident photons energy increase, the smaller attenuation would be obtained and, therefore, more penetration of the gamma-rays in the amino acids will be achieved. The experimental values of More *et al.* [14] for μ_m values agreed with the theoretical values calculated using the XCOM program based on the mixture rule, as well.

Figure 3 also shows that the half and tenth value layers (HVL and TVL) and the mean free path (MFP) quantities increase with increasing gamma-ray energy despite the linear attenuation coefficient quantity (due to the inverse relationship of the mentioned quantities with the linear attenuation coefficient). In other words, as the energy of gamma-rays increases, a thicker half-value layer of amino acids (attenuators) is needed to halve the transmitting gamma-rays. Turşucu *et al.* [26] confirmed that mass attenuation coefficients, effective atomic numbers, and effective electron densities depend on photon energy and chemical content.

Table 4 shows a good agreement between the MCNPX and XMudat values of the effective atomic cross-sections (<8.62%). Tables 4 and 5 show that the values of effective atomic and electronic cross-sections of amino acids decrease with increasing photon energy. The histidine and leucine amino acids have the highest and lowest values of atomic and electron cross-sections, respectively, at all energies. These Tables also show that while increasing the density of amino acids causes a uniform and noticeable increase

in the effective atomic cross-section values, but the effective electronic cross-section acts almost independently of the amino acid type and its density in this range of energy.

Table 6 also indicates that the effective atomic numbers increase significantly with increasing density of amino acids. This is due to the high fraction of higher atomic number elements (oxygen and nitrogen) compared to lower atomic number elements (hydrogen and carbon) in higher density amino acids and implies that the amino acid sample with a higher effective atomic number will absorb the descending photons more intensely. Manohara *et al.* [15,27,28] studied the value of Z_{eff} decreases with increasing energy of three dominant interaction processes (photoelectric, Compton, and pair production) in the wide energy range of 1 keV to 20 MeV. Despite this fact, our result displays approximately no change or variation of Z_{eff} with the selected energy region.

Also, the results of Table 7 show that the effective electron densities of the studied amino acids vary in the range of 0.318×10^{24} - 0.362×10^{24} electron per gram. The effective electron density of the amino acids will operate almost independently of the amino acid type and gamma-ray energy for the studied photon energies. Similar results were also observed by Manjunathaguru and Umesh [11] for H, C, N and O based samples. It is clear that all the amino acids have almost the same behavior, as they consist of approximately similar proportions of hydrogen, carbon, nitrogen and oxygen elements.

The observed differences between the theoretical results (MCNPX code and XMuDat program) and experimental values can be due to differences in the values of variables used in calculations. These variables include different density and elemental composition of samples, energy and intensity of sources, applied databases, etc. The results show that the MCNPX code and the proposed model can accurately estimate the attenuation properties of different amino acids over a wide range of gamma-ray energies.

Even though this study gives the primary data of some essential amino acids in the interested photon energy range for the first time, it is suggested to researchers to do more experimental studies on measurements of the linear and mass attenuation coefficients, half and tenth value layers, mean free path, effective atomic and electronic cross-sections, effective atomic numbers and effective electron densities for studied amino acids and also other biomedically important compounds in order to confirm, understand, and interpret the observed differences between the calculated and measured results.

5. Conclusion

The μ , μ_m , HVL, TVL, mfp, σ_a , σ_e , Z_{eff} , and N_{eff} values of five essential amino acids were simulated and calculated using the MCNPX code and the XMuDat program in the energy range of 122–1293 KeV for ^{57}Co , ^{192}Ir , ^{18}F , and $^{116\text{m}}\text{In}$ gamma-ray sources. The obtained results were compared to available experimental data. This study revealed that MCNPX simulation and XMuDat calculations provide reliable photon interaction parameters for various amino acids within $\pm 11\%$ RD values compared to the previous experimental data. The data calculated using the XMuDat program showed better agreement with experimental data compared to MCNPX simulated results. The theoretical methods produced data close to the experimental values with acceptable approximation, so by using these methods, attenuation properties of other amino acids can be obtained over a wide range of energies.

References

- 1- P.P. Pawar, C.S. Mahajan, "Measurement of mass and linear attenuation coefficients of gamma-rays of glycine for 0.360, 0.662, 1.170 and 1.330 MeV photons.", *Sci Res Rep*, vol. 3, pp. 53–56, (2013).
- 2- M. Donya, M. Radford, A. ElGuindy, D. Firmin, M.H. Yacoub, "Radiation in medicine: origins, risks and aspirations.", *Glob. Cardiol. Sci Pract*, vol. 2014, pp. 437–448, (2014).
- 3- C.F. Huang, J. McConathy, "Fluorine-18 labeled amino acids for oncologic imaging with positron emission tomography.", *Curr Top Med Chem*, vol. 13, pp. 871–891, (2013).
- 4- J.B. Workman, E. Rusche, "Cobalt-57 labeled vitamin B-12 plasma levels for the differential diagnosis of macrocytic anemias.", *J Nucl Med*, vol. 7, pp. 583–588, (1966).
- 5- C.J. Hellier, "Handbook of Nondestructive Evaluation." *McGraw-Hill*. 3rd edition, (2003). ISBN 978-1260441437.
- 6- M. Blau, R. Ganatra, M.A. Bender, " ^{18}F -fluoride for bone imaging.", *Semin Nucl Med*, vol. 2, pp. 31–37, (1972).
- 7- S. Lahiri, M. Maiti, K. Ghosh, "Production and separation of ^{111}In : An important radionuclide in life sciences: A mini review." *J Radioanal Nucl Chem*, vol. 297, pp. 309–318, (2013).
- 8- K.P.G. Nair, C. Gowda, J.S. Kumari, S.J. Anasuya, T.K. Umesh, R. Gowda, "Photon interaction cross sections for some amino acids in the range 30–385 KeV." *Radiat Phys Chem*, vol. 43, pp. 581–584, (1994).
- 9- K.P.G. Nair, T.K. Umesh, R. Gowda, "Total attenuation cross sections of several amino acids at 661.6, 1173 and 1332.5 KeV." *Radiat Phys Chem*, vol. 45, pp. 231–233, (1995).
- 10- S. Gowda, S. Krishnaveni, R. Gowda, "Studies on effective atomic numbers and electron densities in amino acids and sugars in the energy range 30–1333 keV." *Nucl Instr Meth Phys Res B*, vol. 239, pp. 361–369, (2005).
- 11- V. Manjunathaguru, T.K. Umesh, "Effective atomic numbers and electron densities of some biologically important compounds containing H, C, N and O in the energy range 145–1330 keV." *J Phys B: At Mol Opt Phys*, vol. 39, pp. 3969–3981, (2006).
- 12- B.O. Elbashir, M.G. Dong, M.I. Sayyed et al., "Comparison of Monte Carlo simulation of gamma ray attenuation coefficients of amino acids with XCOM program and experimental data." *Results Phys*, vol. 9, pp. 6–11, (2018).
- 13- R.M. Lokhande, C.V. More, B.S. Surun et al., "Determination of attenuation parameters and energy absorption build-up factor of amine group materials." *Radiat Phys Chem*, vol. 141, pp. 292–299, (2017).
- 14- C.V. More, R.M. Lokhande, P.P. Pawar, "Effective atomic number and electron density of amino acids within the energy range of 0.122–1.330 MeV.", *Radiat Phys Chem*, vol. 125, pp. 14–20, (2016).

- 15- S.R. Manohara, S.M. Hanagodimath, "Studies on effective atomic numbers and electron densities of essential amino acids in the energy range 1 KeV–100 GeV.", *Nucl Instrum Methods Phys Res B*, vol. 258, pp. 321–328, (2007).
- 16- P.P. Pawar, G.K. Bichile, "Studies on mass attenuation coefficient, effective atomic number and electron density of some amino acids in the energy range 0.122–1.330 MeV." *Radiat Phys Chem*, vol. 92, pp. 22–27, (2013).
- 17- R. Bagheri, A. Yousefi, S.P. Shirmardi, "Study on gamma-ray attenuation characteristics of some amino acids for ^{133}Ba , ^{137}Cs , and ^{60}Co sources.", *Nucl Sci Tech*, vol. 31, pp. 1-15, (2020).
- 18- D.B. Pelowitz, "MCNPX™ User's Manual." *Version 2.6.0, Report LA-CP-07-1473, Los Alamos, NM: Los Alamos National Laboratory*, (2008).
- 19- J.H. Hubbell, S.M. Seltzer, "Tables of X-Ray Mass Attenuation Coefficients and Mass Energy-Absorption Coefficients 1 KeV–20 MeV for Elements $1 < Z < 92$ and 48 Additional Substances of Dosimetric Interest.", *NISTIR 5632 (Gaithersburg, MD: National Institute of Standards and Physics Laboratory)*, pp. 13–111, (1995).
- 20- J.M. Boone, A.E. Chavez, "Comparison of X-Ray Cross Sections for Diagnostic and Therapeutic Medical Physics.", *Med Phys*, vol. 23, pp. 1997–2005, (1996).
- 21- L. Gerward, N. Guilbert, K.B. Jensen, H. Levring, "WinXCom: a program for calculating X ray attenuation coefficients.", *Radiat Phys Chem*, vol. 71, pp. 653–654, (2004).
- 22- R. Nowotny, "XMuDat: Photon Attenuation Data on PC.", *Tech. Rep. IAEA-NDS-195 (Vienna: International Atomic Energy Agency)*, (1998).
- 23- S. Sharifi, R. Bagheri, S.P. Shirmardi, "Comparison of shielding properties for ordinary, barite, serpentine and steel–magnetite concretes using MCNP-4C code and available experimental results.", *Ann Nucl Energy*, vol. 53, pp. 529–534, (2013).
- 24- K. Kirdsiri, J. Kaewkhao, N. Chanthima, P. Limsuwan, "Comparative study of silicate glasses containing Bi_2O_3 , PbO and BaO : Radiation shielding and optical properties.", *Ann Nucl Energy*, vol. 38, pp. 1438–1441, (2011).
- 25- R. Bagheri, A.K. Moghaddam, S.P. Shirmardi, B. Azadbakht, M. Salehi, "Determination of gamma-ray shielding properties for silicate glasses containing Bi_2O_3 , PbO , and BaO .", *J Non-Cryst Solids*, vol. 479, pp. 62–71, (2018).
- 26- A. Turşucu, P. Önder, D. Demir, T. Öznülüer, "Studies on mass attenuation coefficient, effective atomic number and electron density of some amino acids." *Int J Phys Sci*, vol. 8, pp. 147-156, (2013).
- 27- S. Manohara, S.Hanagodimath, "Effective atomic numbers for photon energy absorption of essential amino acids in the energy range 1 keV to 20 MeV.", *Nucl Instrum Methods Phys Res B*, vol. 264, pp. 9-14, (2007).
- 28- S. Manohara, S. Hanagodimath, K. Thind, L. Gerward, "On the effective atomic number and electron density: A comprehensive set of formulas for all types of materials and energies above 1 keV.", *Nucl Instrum Methods Phys Res B*, vol. 266, pp. 3906-3912, (2008).