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RESEARCH ARTICLE

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Investigation of photon ınteraction parameters of some premedication drugs

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Abstract

Premedication, also known as the preparation phase, is the administration of drugs to patients before chemotherapy to reduce the side effects of chemotherapy in oncology patients. Metoclopramide, ranitidine and pheniramine are some of these drugs. Metoclopramide is a routine antiemetic for nausea and vomiting caused by antineoplastic drugs, especially cisplatin, due to its effect on the medulla chemoreceptor trigger zone. Ranitidine, which belongs to the histamine receptor 2 (H2) antagonist family, is a widely used drug clinically to control gastrointestinal symptoms. Pheniramine is an antagonist against allergic symptoms caused by inappropriate histamine release to reduce edema, pruritus and redness. Sometimes patients are given premedication drugs before radiological examination. In this study, photon interaction parameters of some premedication drugs (metoclopramide, ranitidine hydrochloride, and pheniramine) were investigated, namely mass attenuation coefficient (μ_ρ), effective atomic number (Z_{eff}), electron density (N_{el}), exposure and absorption accumulation factors (EBF and EABF). Maximum μ_ρ values for all drugs were found at low gamma energies. It was found that ranitidine hydrochloride has the highest Z_{eff} values in almost the entire energy range due to the presence of S and Cl. In addition, ranitidine hydrochloride showed the lowest EBF and EABF values, indicating that the material does not emit much radiation to the environment.

Keywords: Buildup factors; effective atomic number; mass attenuation coefficients; premedication drugs

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1. Introduction

Premedication, also known as the preparation phase, is the administration of drugs to the patient before chemotherapy to reduce the side effects of chemotherapy in oncology patients. Metoclopramide, ranitidine, and pheniramine are some of these drugs. Metoclopramide is a routine antiemetic for nausea and vomiting caused by antineoplastic drugs, especially cisplatin, due to its effect on the medulla chemoreceptor trigger zone [1-3]. It is also a drug used for stomach and esophageal problems. The chemical formula of metoclopramide is $C_{14}H_{22}ClN_3O_2$ [4].

Ranitidine, belonging to the histamine receptor 2 (H2) antagonist family, is a widely used drug clinically for the control of gastrointestinal symptoms. By blocking histamine receptors, ranitidine reduces the amount of acid produced by the stomach [5,6]. Ranitidine also has the potential to be used as an adjuvant therapy or preventive agent in breast cancer [7]. Its chemical formula is $C_{13}H_{22}N_4O_3S.HCl$ [8].

Pheniramine is an alkylamine derivative antihistamine used in the treatment of allergies and is taken more frequently than other antihistamines [9]. Alkylamine derivatives are among the most potent antihistamines, producing more stimulation and less sleepiness. Pheniramine acts as an antagonist against allergic symptoms resulting from inappropriate histamine release to reduce edema, pruritus, and redness [10, 11]. Its chemical formula is $C_6H_2ON_2$ [12].

Since radiation is used in many fields (medicine, biology, industry, nuclear power plants and radiation dosimetry), it is important to investigate the behavior of radiation in materials. X-rays and Gamma rays are used in diagnosis and treatment in medicine. Therefore, the behavior of radiation within the material must be accurately understood. The interaction of the material with radiation depends on the energy of the photon incident on the material, the density of the material and the atomic number of the elements [13]. There are studies in the literature on the interaction of drugs with radiation. In a study investigating the radiation protective effect of anti-inflammatory drugs, it was stated that radiation can inhibit the cell cycle and disrupt homeostasis. It has been determined that the prodromal, acute, and chronic effects of radiation are accompanied by overproduction of eicosanoids (prostacyclin, leukotrienes, prostaglandins, and thromboxanes), and anti-inflammatory drugs suppress prostaglandin/thromboxane synthesis [14]. In another study, it was reported that natural products such as Apigenin, caffeine, bergenin, coniferyl aldehyde, chlorogenic acid, curcumin, quinic acid and delphinidin are effective radioprotectors due to their low toxicity and quinic acid is the best radioprotector to protect from both thermal and fast neutrons [15]. According to a study on anti-HIV drugs (Kivexa, Combivir, Tenofovir, Lopinavir, and Nelfinavir), it is reported that Combivir, which has a relatively high heavy element content, has the highest radiation attenuation capacity, while Lopinavir has the lowest [16].

These premedication drugs (metoclopramide, ranitidine hydrochloride, pheniramine) are administered to the patient, especially before chemotherapy drugs and these patients may undergo some radiological examinations after taking the drugs. For example, it has been shown that the simultaneous application of chemotherapy and radiotherapy is beneficial in head and neck cancers (chemoradiotherapy) [17]. The spatial cooperation between radiotherapy and chemotherapy has been successfully used in the treatment of various tumors (such as Wilms tumor, acute lymphoblastic leukemia and breast cancer). In radiotherapy applications, when cancer cells are treated, irradiation of normal tissues surrounding the tumor may cause symptomatic damage. Ionizing radiation can interact with cellular macromolecules such as DNA (deoxyribonucleic acid), proteins and lipids (direct effect) or with water molecules in human tissues (indirect effect) and cause the formation of reactive oxygen species. For example, the Hydroxyl radical is highly reactive and damages cellular macromolecules. As a result of these effects, diseases such as organ inflammation, fibrosis, infertility, atrophy, vascular damage and secondary malignancies may occur [15,18].

When a substance is exposed to ionizing radiation, it is necessary to determine some coefficients characterizing the interaction of the radiation with this substance. The first of these parameters is the mass attenuation coefficient (μ_ρ), which characterizes the penetration effect of ionizing radiation. Two other important parameters, the effective atomic number (Z_{eff}) and the electron density (N_{el}), are used in medical radiation dosimetry and these coefficients are obtained using the $\mu\rho$ values. The ‘accumulation factors’, which indicate how radiation interacts with ‘living’ matter,

are divided into two types: the first is the absorption accumulation factor (EABF), where the amount of energy absorbed or deposited in the target is of interest and the detector response function is the absorption in the material (prodrug). The second is the exposure accumulation factor (EBF), where the amount of interest is the exposure and the absorption in air is the detector response function [19]. To the best of our knowledge, there is no detailed study evaluating the EBF and EABF values for commonly used premedication drugs. It is hoped that the current study will bridge this gap and provide insight into possible implications for radiologic practice.

2. Material and methods

This study aimed to calculate μ_ρ, Z_{eff}, N_{el}, EBF and EABF values in metoclopramide ($C_{14}H_{22}ClN_3O_2$), ranitidine hydrochloride ($C_{13}H_{22}N_4O_3S.HCl$) and pheniramine ($C_6H_2ON_2$) drugs. μ_ρ values were calculated theoretically in the wide gamma energy range (1 keV- 100 GeV) by using the WinXCom computer program. WinXCom calculates these values for compounds or mixtures (using the mixture rule). Z_{eff} and N_{el}'s values were obtained using the μρ's.

This study involves calculating various radiation shielding parameters for premedication drugs, using the WinXCom code and several related formulas to assess gamma radiation shielding effectiveness. The mass attenuation coefficient (μ_ρ), which represents how a material attenuates gamma radiation, was computed using the WinXCom software. This software calculates attenuation coefficients and cross sections in the energy range of 1 keV–100 GeV [20, 21]. For a given compound, the μρ value is calculated based on the mass attenuation coefficients of the constituent elements. The mass attenuation coefficient for a mixture is given by the weighted sum of the individual elements using the following formulas:

$$\mu_\rho = \sum_i w_i \left(\mu_\rho\right)_i \tag{1}$$

In Equation (1), w_i represents the weight of the ith element, and $(\mu_\rho)_i$ represents the mass attenuation coefficient. The w_i value for the composite can be calculated by Equation 2:

$$w_i = \frac{a_i A_i}{\sum_j a_j A_j} \tag{2}$$

A_i and a_i in equation (2) represent the atomic weight of the ith element and the number of formula units, respectively. The total molecular cross section is denoted by σ_m (barn/molecule) and is obtained by using the following formulas [22]:

$$\sigma_m = \frac{\left(\mu_\rho\right)}{N_A} M \tag{3}$$

$$M = \sum n_i A_i \tag{4}$$

Where; M is the molecular weight, N_A is the Avogadro number, and ni is the atomic number of the ith element. The total atomic cross section (σ_a (barn/atom)) and electronic cross section (σ_{el} (barn/electron)) values are calculated using equations (5) and (6) [22]:

$$\sigma_a = \frac{\sigma_m}{\sum n_i} \tag{5}$$

$$\sigma_e = \frac{1}{N_A} \sum \frac{A_i}{Z_i} f_i \mu_i \tag{6}$$

Where; f_i is the fractional abundance of the ith element and Z_i is the atomic number. This calculation provides insight into the overall interaction cross-section of the entire molecule, considering the contribution of each atom within the molecular structure. Z_{eff} and N_{el}'s values were derived as follows [22]:

$$Z_{eff} = \frac{\sigma_a}{\sigma_e} \tag{7}$$

$$N_{el} = \frac{(\mu_\rho)}{\sigma_e} \tag{8}$$

In the context of gamma radiation shielding, the concepts of Z_{eff} and N_{el} are used to assess and design materials that can effectively attenuate gamma radiation. These properties indicate how gamma photons interact with materials and how they affect their ability to attenuate radiation. In the context of radiation shielding, EABF and EBF are fundamental parameters for understanding their behavior in materials. Hila et al. [23, 24] introduced significant improvements to their spreadsheet-based program EpiXS, originally developed in their previous work. The updated version significantly improves its usability for photon shielding and shielding analysis by integrating the EPICS2017 and EPDL97 data libraries. These libraries provide detailed cross-section data for elements with atomic numbers 1 to 100 over a wide range of photon energies from 10 eV to 100 GeV. Thanks to these upgrades, EpiXS can reliably calculate theoretical parameters such as EBF and EABF, which are essential for accurate photon interaction modeling in various materials. These parameters play an important role in evaluating the shielding effectiveness of materials against photon radiation. They also provide the basis for the design of efficient and reliable radiation protection systems. These factors measure the rate of absorption or scattering of radiation within a material.

3. Results and discussion

The parameters μ_ρ, Z_{eff}, and N_{el} are concepts used in shielding calculations that determine the probability that a material will interact with gamma photons. Gamma radiation interacts with matter via the photoelectric effect, Compton scattering, and pair production, all of which depend on the Z value of the material. When the μ_ρ for the three examined drugs were evaluated, it was seen that the results were quite close to each other since the chemical contents of these drugs were similar. However, since ranitidine hydrochloride ($C_{13}H_{22}N_4O_3S.HCl$) drug has S and Cl elements, it was observed that mass attenuation values were high with a small difference (Fig. 1).

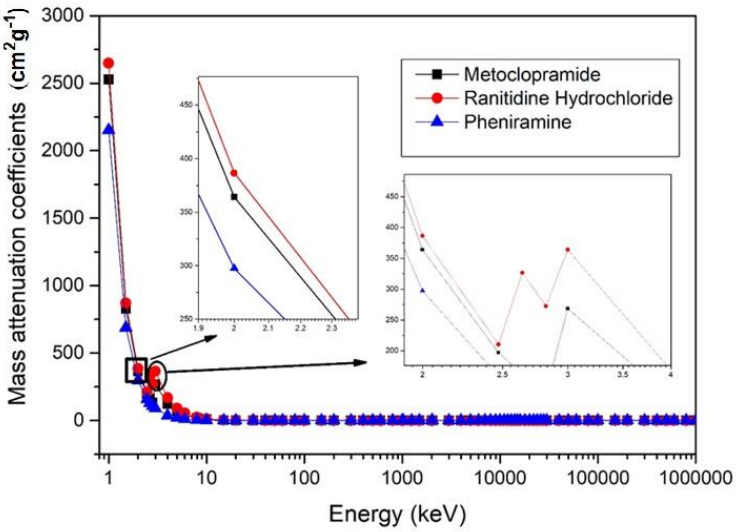

Fig. 1. μ_ρ values of metoclopramide, ranitidine, and pheniramine across 1 keV–100 GeV.

For gamma radiation shielding, the Z_{eff} value of a composite material or compound varies depending on the atomic numbers of the elements constituting that material and the energy of the gamma radiation. For drugs whose Z_{eff} values were examined at the same energy values, as can be seen from Figure 2, the results of the other two drugs, except pheniramine, have a similar tendency and rapid increases are seen in the low energy zone. The main reason for these two results is that these drugs contain elements with higher atomic numbers (S=16, Cl=17). In a study, the EMR (electromagnetic radiation) interaction parameters of some antihypertensive drugs (Fosinopril, Captopril, Losartan Potassium, Irbesartan, Ramipril, Telmisartan) were investigated, and it was found that Losartan Potassium had the largest MAC, Z_{eff} and N_{el} values and the lowest HVL, mfp and buildup factor values [25].

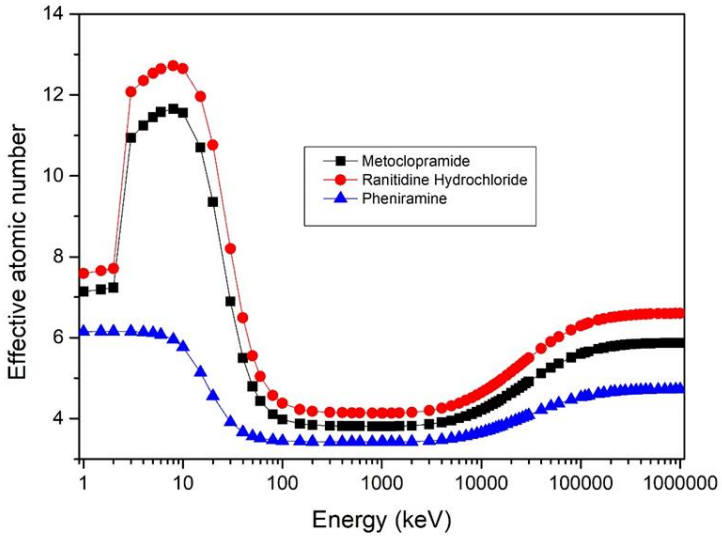

Fig. 2. Z_{eff} values of metoclopramide, ranitidine, and pheniramine across 1 keV–100 GeV.

Similarly, similar interpretations can be made for the N_{el} values. Figure 3 shows that the N_{el} values vary with gamma energy and drug type, and the results for metoclopramide and ranitidine hydrochloride are closer to each other. Cakir conducted a study that included the calculation of various radiation shielding parameters for iodinated contrast agents and the potential benefits of chemoradiotherapy for some tumors. In this study, the radiation interaction parameters (μ_ρ, Z_{eff} and N_{el}) of iodinated contrast agents (such as Iopamidol, Iodixanol, Iohexol, Iopromide, and Ioxagalet) were calculated using computer programs. The Z_{eff} and N_{el} values were found to be highest in the low energy range for all these iodinated contrast agents. The study findings showed that iodinated contrast agents have improved gamma radiation shielding properties, which is important for medical imaging techniques such as CT scans and other radiologic procedures, especially when used in low-energy radiation environments [26].

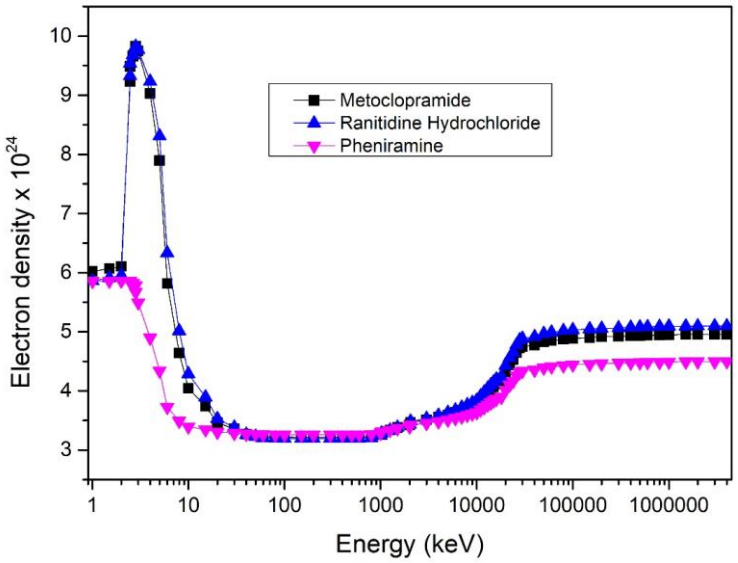

Fig. 3. N_{el} values of metoclopramide, ranitidine, and pheniramine across 1 keV–100 GeV.

In this study, the EpiXS program and the GP-Fitting approach were used together to calculate the equivalent atomic number (Z_{eq}), EABF and EBF parameters, which are the basic shielding parameters. The EBF and EABF parameters of the drugs were compared and discussed in the energy range of 0-15 MeV and penetration depths of 1-40 mfp (mean free path) (Figures 4-5). At low photon energies (typically below 100 keV), the dominant interaction process is the photoelectric effect. In this energy region, the absorption of a photon by an atom in the material results in the ejection of an electron from the inner shell. The probability of the photoelectric effect increases significantly with the Z value of the material and decreases with the energy of the photon (E) (the relationship is approximately proportional to $Z^4/E^{3.5}$).

At intermediate photon energies (100 keV- 10 MeV), the dominant interaction process shifts to Compton scattering. More scattering occurs at these energies, meaning that scattered photons are produced and contribute to both energy absorption and energy exposure. Both EABF and EBF values increase in this energy range because more scattered photons contribute to the total energy stored or exposure. EABF increases because the secondary photons generated by scattering contribute to the total energy absorbed in the material. EBF increases because the scattered photons that don't get absorbed still contribute to the overall exposure (the dose rate in the air or volume surrounding the material). This is where the EBF/EABF ratio tends to peak, as the material's shielding effectiveness is influenced by a combination of absorption and scattering.

At high photon energies (typically above 10 MeV), pair production begins to dominate. Pair production occurs when an incident photon has an energy above 1.022 MeV, the energy required to create an electron-positron pair, and interacts with the electric field of an atomic nucleus. The formation of an electron-positron pair results in the photon effectively being converted into matter. The probability of pair production increases with photon energy and Z, but only becomes significant at very high photon energies. The EABF and EBF decrease when the energy of the photon reaches very high values. The EABF is reduced because the dominant interaction is pair production, which provides a different energy deposition profile than Compton scattering. In pair production, instead of providing scattered gamma photons, a significant number of new particles (electrons and positrons) are produced.

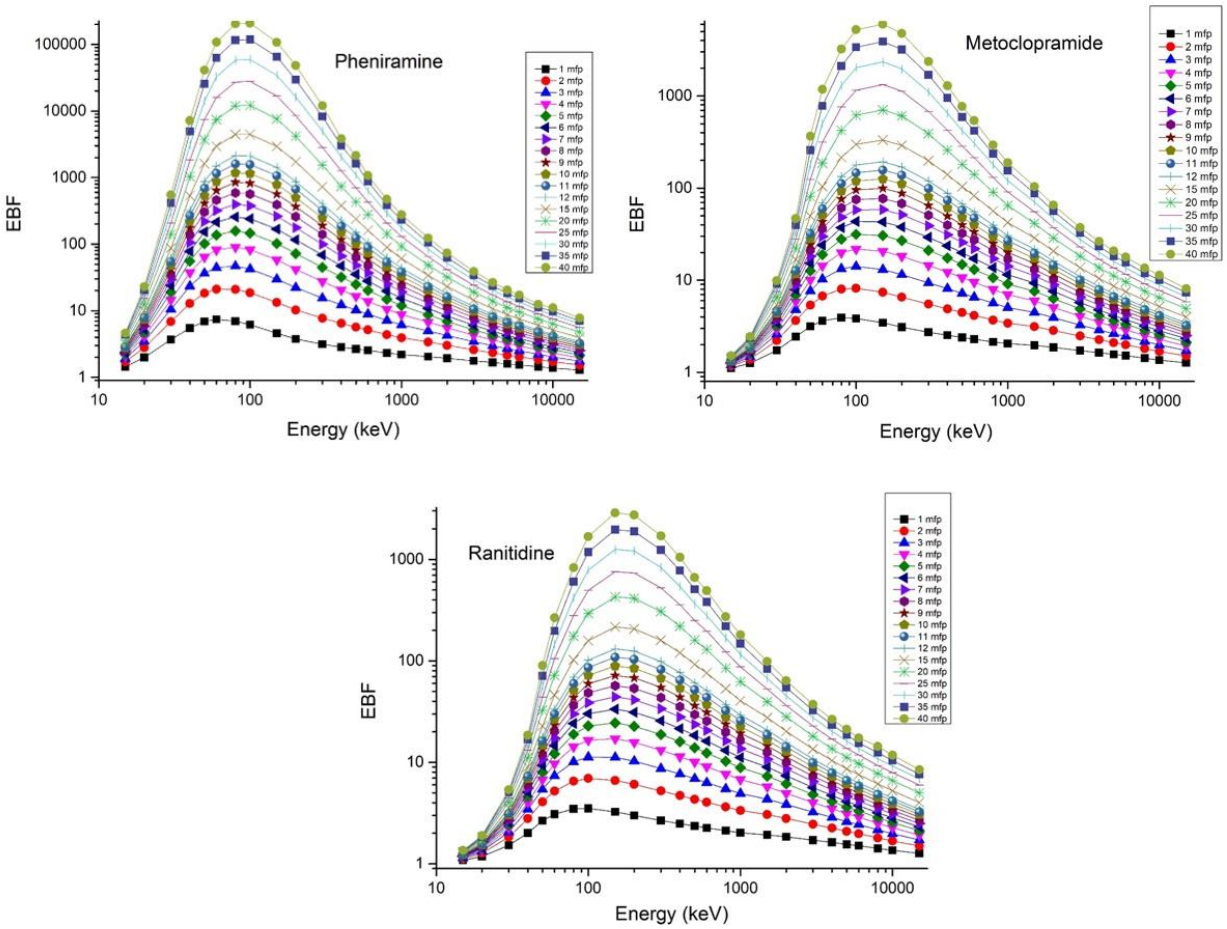

Fig. 4. Change of exposure buildup factors for metoclopramide, ranitidine, and pheniramine with different mfp values depending on photon energy.

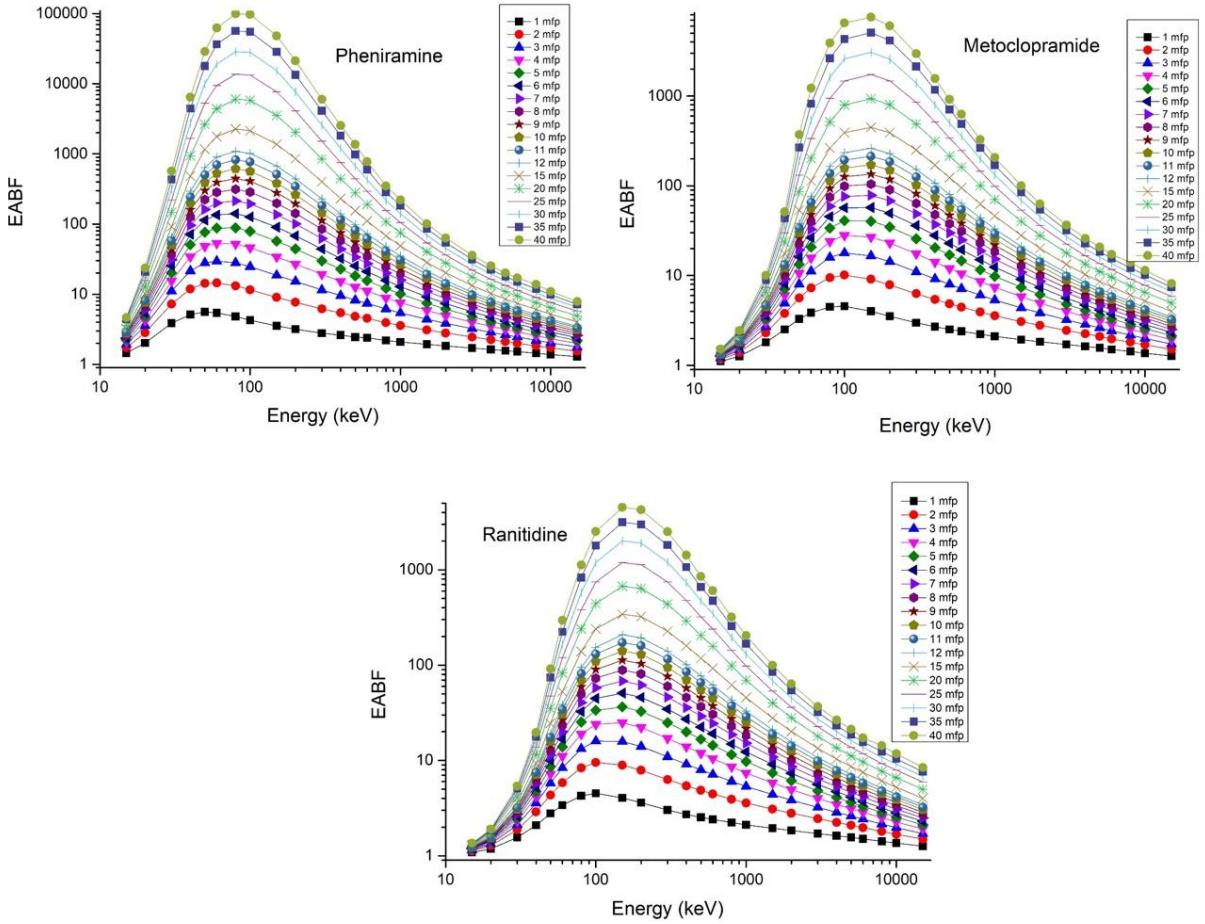

Fig. 5. Variation of absorption factors depending on photon energy for metoclopramide, ranitidine and pheniramine at different MFPs

Furthermore, graphical representations corresponding to a photon energy of 0.15 MeV, as a function of penetration depth, are provided in Figure 6. Ranitidine hydrochloride appears to attenuate gamma radiation more. In a study examining the gamma and neutron interaction parameters of diketone derivatives synthesized as potential anticancer agents (DKD1 (C17H10O5), DKD2 (C27H23NO4), DKD3 (C41H43NO4), DKD4 (C33H48O2), DKD5 (C30H34O2) and DKD6 (C32H35NO2)), it was determined that DKD1 (C17H10O5) showed lower EBF values and had better gamma absorption compared to other selected examples [27]. A similar result is also valid for our study, Ranitidine hydrochloride showed the lowest EBF value. This feature of Ranitidine may be evaluated as radioprotective in chemoradiotherapy.

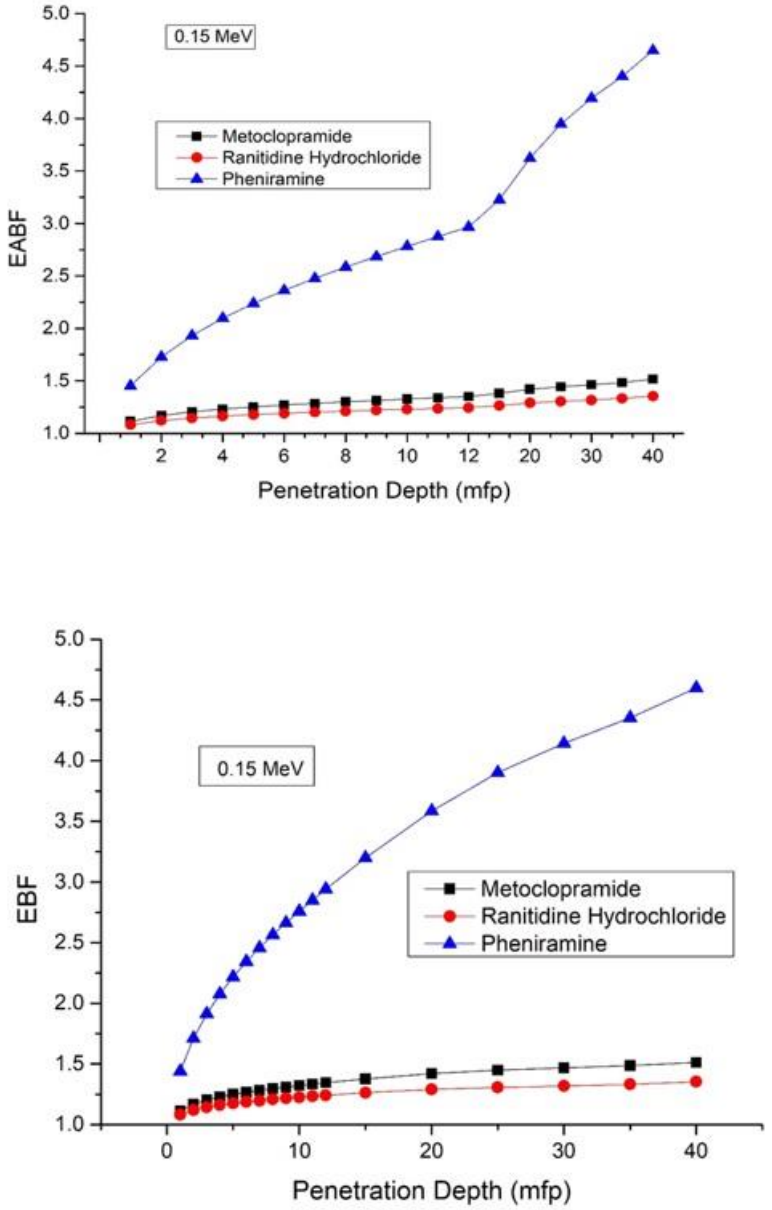

Fig. 6. Energy exposure buildup factor of metoclopramide, ranitidine, and pheniramine up to 40 mfp at 0.15 MeV energy

4. Conclusion

The maximum mass attenuation coefficient was obtained for all drugs at low gamma energies. This is attributed to the dominance of the photoelectric effect due to the probability of interaction with electrons. The μ_ρ parameters depend on the elemental composition of the drugs. At low photon energies, the atomic number of the elements involved strongly influences the photoelectric absorption cross section (the cross section behaves like Z^{4-5}). This

means that heavier elements (higher Z) are more efficient in absorbing low-energy photons. Due to the higher Z dependence, the $\mu\rho$ values are highest for drugs with high atomic number elements. Compton scattering is the dominant interaction mechanism for photons in the intermediate energy range. The attenuation coefficient μ_ρ decreases as the Z value of the material increases, since the Compton scattering cross section is approximately proportional to Z. In other words, for materials with higher atomic numbers, Compton scattering becomes less efficient at intermediate energies and the attenuation due to this mechanism decreases. Therefore, the results have the smallest values in this energy region. As the energy of the photon increases, the relative contribution of Compton scattering decreases. This is because at higher energies, pair production becomes the dominant interaction mechanism (the probability of pair production is proportional to Z^2). The results again appear to increase in this energy range. Ranitidine hydrochloride exhibited the highest effective atomic number (Z_{eff}) in almost the entire energy range due to the S and Cl content. The deposition factors (EBF and EABF) increase due to secondary interactions (scattering and photon production) within the shielding material. Ranitidine hydrochloride showed the lowest EBF and EABF values, indicating that the material does not reflect much radiation to the environment.

Acknowledgements

There is no conflict of interest.

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