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The Interaction of Neutron and Gamma Radiation With Some Cancer Drug Effect Ingredients: A Simulation Study

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Abstract

In recent years, great advances have been made in cancer treatments with new treatment methods. Radiation therapy has an important place in cancer treatments and approximately 50% of these patients applied radiation therapy. In this investigation, fast neutron and gamma radiation, absorption characteristics were determined of pharmaceutical active ingredients such as Bevacizumab (Avastin), Camptosar (Irinotecan Hydrochloride), Capecitabine, Everolimus, Oxaliplatin, Leucovorin Calcium and Regorafenib which especially used in cancer treatments. GEANT4 Monte Carlo simulation code was used in this calculates. It was found that Everolimus, Leucovorin Calcium has the best neutron attenuation capacity among the investigated drug effect ingredients. In addition to neutron attenuation properties, the gamma-ray attenuation properties of Oxaliplatin is found to good than other drug effect ingredients. According to the results obtained in the present work, we suggest that the Everolimus and Leucovorin Calcium drug effect ingredients by neutron radiotherapy and Oxaliplatin drug effect ingredients by gamma radiothrapy can be used both chemotherapy and radiotherapy. In addition in study examined drug effect ingredients can be used for chemotherapy and radiotherapy combinaison at the same time so, cancer patients to be more effective treatment.

Keywords: Drug, GEANT4, Gamma, Neutron

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1. *Introduction*

Today, radiation is widely used in medicine, research and investigation, industry and electricity generation. In addition, radiation is used in archeology (carbon determination), space exploration, agriculture, military fields, geology, mineral and oil exploration (Wrixon 2013). During these processes, staff or patients can be stay exposed to radiation.

It is always can damage to cells or tissue from being exposed to certain amount of direct ionizing radiation (e.g. gamma rays and X-rays) or indirect ionizing radiation (neutrons).
Over time, exposure to certain dose radiation may cause cancer and other health problems such as acute (ivegen), nausea, vomiting, skin and deep tissue burns, decreased body's ability to fight infections, burning skin flaking (Park et al. 2014). The radiation entering the body not only loses energy, but it is also absorbed and causes the formation of secondary radiation. Various drugs are needed to reduce or eliminate the damage caused by radiation entering the body (Burrıs and Hurtıg 2010).

There are important parameters to be determined in order to examine the interaction of a material with radiation. These are Effective removal cross section, (cm^2/g), Half value thickness (HVL), average free path (λ) and transmission number (TN) for neutrons (Aygün 2019), some gamma radiation shielding paramers, mass attenuation coefficient (MAC), linear attenuation coefficient (LAC) and mean free path (MFP) have been calculated (Carlo et al. 2004), (Kavaz and Yorgun 2018), (Sayyed and Lakshminarayana 2018).

There are three basic ways to prevent radiation from damaging cells and tissues. These are agent protectors given before the radiation effect, the attenuators applied before or after radiation treatment, and repairers given for the purpose of treatment after damage. For this purpose, the most effective way of exposure to radiation is to use drug agents that can absorb radiation (Eaton and Schneider 2014), (Prasanna et al. 2012). Numerous studies have been carried out to determine the radio-protective effect of chemical and biological substances. Radiation shielding properties of six different analgesic and anti-inflammatory drugs were investigated in the range of 1 keV - 100 MeV energy using WinXCom (Sayyed et al. 2017). The gamma radiation interaction parameters were calculated which electron density and effective atomic number of some biological substances (Kurudirek 2016). The mass attenuation coefficients (μ_ρ), molar extinction coefficients (ε), electronic cross-sections (σ_e), total atomic cross-sections (σ_t), effective electron densities (N_{eff}) and effective atomic numbers (Z_{eff}) have been calculated for photons in energy (0.122, 0.356, 0.511, 0.662, 0.884, 1.170, 1.275 and 1.330MeV) of some amino acids such as n-acetyl-l-tryptophan, n-acetyl-l-tyrosine, d-phenylalanine, d tryptophan, n-acetyl-l-glutamic acid, and d-threonine (More et al. 2016).

Fatty acids form the building block of fat in our body and most foods. During the digestion phase, the body breaks down fats into fatty acids, which can then be absorbed by passing into the blood. It has many important functions for the body, especially the energy storage of fatty acids in the body. To know the effect of radiation on living things, it is necessary to know the interaction paramerters of these acids with radiation. The mass attenuation coefficients (μ_ρ) electronic cross-section (σ_e), Z_{eff}, atomic cross-section (σ_t), and effective electron density (Neff) have been measured for gamma radiation of some fatty acids such as the lauric acid ($C_{12}H_{24}O_2$), undecylic acid ($C_{11}H_{22}O_2$), myristic acid ($C_{14}H_{28}O_2$), pentadecylic acid ($C_{15}H_{30}O_2$), tridecylic acid ($C_{13}H_{26}O_2$), and palmitic acid ($C_{16}H_{32}O_2$) (Gaikwad et al. 2016). Vitamins are the simplest organic substances in our body that are absolutely necessary for our body and function as catalysts. A study has shown that many plant antioxidant nutrients such as vitamins A and C have a protective effect against radiation damage (Weiss and Landauer 2003). Nine diffrent quinoline-hydrazone anti-aging was synthesized from biologically active molecules, and absorption parameters were calculated against UVB radiation. As a result, antioxidants with dual inhibitors of quinoline-hydrazone hybrids of enzymes related to skin aging have been found to protect from the effects of UVB radiation (Osorio et al. 2019). In a study, protective properties were investigated of amifostine and palifermin agents to reduce the effect of ionizing radiation on a cell and tissue. It is reported that, amifostine and palifermin have been reduce the toxic effect of radiation in nuclear medicine applications (Patyar and Patyar 2018). In vitro antioxidant activity properties of grape extracts (Flame seedless, Kishmish chorni, Red sphere and Thompson seedless) were determined by ABTS experiment and their protective effect against DNA damage caused by radiation was investigated (Singha et al. 2020). Side effects of hematopoietic and intestinal systems are often seen in this context patients exposed to accidental or medical radiation.
For this, the effects of valeric acid (VA) produced by the intestinal microbiota on the damage caused by radiation were investigated. As a result, it has been determined that VA produced with intestinal microbiota can be used as a therapeutic option to reduce radiation damage in preclinical settings (Li et al. 2020). Many drugs are used in chemotherapy. The interaction parameters of these drugs with radiation have been determined. Thus, the extent of use with radiotherapy was determined (Akman and Kaçal 2018). (Kaçal et al. 2017). Quinoline is an important natural compound made up of various natural compounds in the form of alkaloids from the cinchona plant and used in various biological activities. These compounds are important materials used in the development of new drugs with different properties. For this purpose, six new types of quinoline have been synthesized and shown to be used as an active drug substance. The gamma and neutron radiation absorption parameters of these materials were determined (Aygün et al. 2020).

In this presented study, the neutron and gamma radiation shielding parameters have been determined for seven pharmaceutical active ingredients. Monte Carlo Simulation Geant4 (GEometry ANd Tracking 4) software were used in the theoretical calculations.

2. Materials and Methods

3.1 Theoretical Background

Neutrons are indirect ionizing radiation, and they are interaction with the target material, or energy transfer to heavily charged particles or absorption by the nuclei. They may undergo elastic or inelastic scattering during their passage in target material or initiate nuclear reactions such as fission and neutron capture. This interaction possibility is mostly calculated with removal cross section and total macroscopic cross section values. The total macroscopic cross section ($\sum t$) is determined as follows (Aygün 2019).

$$\sum t = \sum N(\sigma t) \tag{1}$$

N is the number of cores per unit volume in the material. Total microscopic cross-section σt refers to the possibility that certain energy neutrons interact with the material and this is calculated as the sum of microscopic cross sectional scattering (σs) and microscopic cross section attenuation (σa) as follows:

$$\sigma_t = \sigma_s + \sigma_a \tag{2}$$

Effective removal cross section, $\sum R$ (cm^2/g), is a measure of the possibility of fast or fission neutron first collision with a interaction material (Singh and Badiger 2014). The effective removal cross-sections can be determined for alloys, mixtures and combination, according to the mass weight ratio of each element in the mixture. This can be calculated as follows:

$$\sum R = \sum \left(\frac{\sum R}{\rho}\right) i \tag{3}$$

Here $\sum R$; effective removal cross section and ρ; density of the interaction material.
Half value thickness (HVL) is refers to the thickness of the interaction material that reduces the incoming neutron radiation by half. HVL can be calculated by the following equation for neutron radiation: (Zali et al., 2018).

$$HVL = \frac{ln2}{\sum R} \tag{4}$$

The average free path (λ) is the average distance between two consecutive mutual interaction of neutrons, and the neutrons this on the road before a collision. It is expressed as distance within the interaction material and calculated as follows (Lechner 2018).

$$\lambda = 1/\sum R \tag{5}$$

When a gamma ray interacts with a material, the intensity of the beam coming into the material changes according to the Beer-Lambert law (Ekinci et al. 2019).
This is expressed as follows:

$$I = I_0\, e^{-\mu x} \tag{6}$$

I_0 and I are incoming and outgoing gamma-ray intensities, μ (cm^{-1}) is the linear attenuation coefficient and x is the thickness of interaction material.
The mass attenuation coefficient of the volume of a material is a parameter that gives information about how gamma rays that interact with the material can pass through the material. The MAC is defined as

$$\mu_\rho = \mu/\rho \tag{7}$$

ρ ; the sample density
HVL and is calculated for gamma radiation as follows:

$$HVL = \frac{ln2}{\mu} \tag{8}$$

3.2 Monte Carlo Simulation Technique GEANT4 Code:

Due to the confusion and enormous difficulties in conducting modern particle and nuclear physics experiments, robust software was needed. In these experiments, detectors to measure the comprehensive properties of the particle and software to simulate them were necessary. Simulations became needed due to increased particle size, complexity and sensitivity of the detectors to be used. Simulations have been developmented to predict situations that might occur before and after with radiation of target material. Instead of most high dose radiation tests, applying the approvalled radiation transfer codes and softwares is more practical. The most extensive usage of Monte Carlo nuclear interactions is the code Geant4 which simulation is made high accuracy.

GEANT4 (Geometry and Tracking) is a Monte Carlo based tool kit that can simulate events that may occur in the interaction with target material of particles and photon radiaition with a wide range of energy. Geant4 simulation code is used in area such as particle physics, nuclear physics, nuclear medicine, space and laboratory research, agriculture, military. An input file is needed to run the program. This file contains the information about energy and type of the radiation applied, the experiment geometry, the materials used, and the desired parameters as a result of the simulation. After the simulation is done, the results are obtained out in the output files. In this study, GEANT4.10.3 version was used for both gamma ray and neutron 1 to10 MeV energies in simulation calculations. Simulation geometry can be seen in Figure 1. These simulations were completed in five stages using the geometry below.
These,

• Radiation type and properties (Primary Generator Action. cc), experiment geometry using material properties (Detector Construction. cc), and mac files in the src folder are defined in GEANT4 source files.
• The codes required to run the program were entered from the terminal window by going to the folder where the files were prepared.
• System continued with simulation settings / run / initialize command.

• The number and energy of particles to be sent was added with the simulation / run / beamOn command.
• The obtained results were read from the same terminal window.

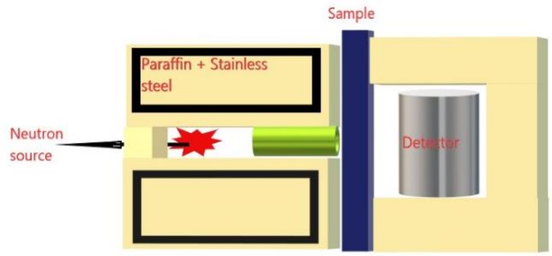

Figure1. GEANT4 simulation geometry

3.3 The Samples Examined and Their Properties

Bevacizumab, commercially known as Avastin, is a drug used to treat both certain types of cancer and some eye diseases. Bevacizumab is different from other cancer drugs because it does not directly affect tumor cells, but destroys the veins that supply them with oxygen and nutrients. Irinotecan is a drug used in the treatment of colon cancer and small size lung cancer. Irinotecan topoisomerase inhibitor comes from the drug group. This drug is blocked the topoisomerase 1, which causes DNA damage and cell death, (Chadwick and Greenaway 2015). Capecitabine, sold under the brand name Xeloda, is a chemotherapy drug used in the treatment of stomach, colorectal and breast cancers (Walko and Lindley 2005). Everolimus is a drug used as an immunosuppressant in infections, tumors and kidney cancer treatments in organ transplants. A lot of research has been done on everolimus and other mTOR (mammalian target of rapamycin) inhibitors to be used in some cancer treatments (Hasskarl 2018). Oxaliplatin is a cancer drug used in the treatment of colorectal cancers sold under the brand name Eloxatin. This drug is often used in combination with fluorouracil and folinic acid (leucovorin) in advanced cancers, and is given by injection into this vein (Shen et al. 2018). Leucovorin Calcium, called Folinic acid is a drug used to reduce the toxic effects of pyrimethamine and methotrexate. It is used in the treatment of cancer together with colorectal 5-fluorouracil, in addition, it can be used in anemia and eliminate folate deficiency caused by methanol poisoning. It can be taken by mouth, intramuscularly or by injection (Boslaugh 2016). Regorafenib is small molecule which has antineoplastic and antiangiogenic activities. Regorafenib is used in metastatic colorectal cancer and advanced gastrointestinal stromal tumors treatments.

3. Results and Discussion

In this study, some parameters that characterize neutron and gamma radiation drug effect ingredients interaction probabilities were calculated with the helping Monte Carlo Simulation program Geant4 code and the calculated results were compared with paraffin and each other. The chemical properties of the studied drug effect ingredients were summarized in Table 1.

3.1 Neutron radiation attenuation properties

In this study, by using the Geant4 code for the simulation of neutron attenuation parameters such as removal cross-section, MFP, half value layer and transmission number were theoretically calculated with the simulation geometry in Figure 1. The obtained results of the fast neutron attenuation parameters with 1-4 MeV energy for the seven types of drug effective ingredients are presented in Table 2 and Figure 2. The effective removal cross section (cm^{-1}) is an important parameters for neutron attenuation in the applications. The higher the effective removal cross section value of a any material, the higher the possibility that the material atoms collision with the neutron particles. These values are desired to be high for materials to be used in neutron absorption studies. This also refers to the absorptive power of the material. It can be easily seen in Figure 2, that the Effective Removal Cross Section values of all samples decrease with increasing energy. This situation is normal. Because when the energy increases, the possibility of neutrons to interact with the material decreases. It can be observed that the Effective Removal Cross Section values of the samples examined according to this figure are quite good compared to the reference paraffin. Especially ED4 and ED6 samples have high values. These results are proof of the ability of these samples to absorb fast neutron.

Sample Code	Sample Name	Molecular Formula	Molecular Weight (g/mol)	Composition (%)	Density (g/cm^3)
P	Paraffin	$C_{22}H_{46}$		C:85.07 H:14.92	0.90±0.1
ED1	Bevacizumab (Avastin)	$C_{6638}H_{10160}N_{1720}O_{2108}S_{44}$	149196.8162	C: 53.43 H: 6.86 N: 16.14 O: 22.60 S: 0.94	1.031±0.1
ED2	Camptosar (Irinotecan Hydrochloride)	$C_{33}H_{39}ClN_4O_6$	586.7	C: 58.52 H: 6.69 N:8.27 O: 21.26 Cl:5.23	1.3±0.1
ED3	Capecitabine	$C_{15}H_{22}FN_3O_6$	359.3501	C: 50.13 H: 6.17 F: 5.28 N: 11.69 O:26.71	1.5±0.1
ED4	Everolimus	$C_{53}H_{83}NO_{14}$	958.240	C: 66.43 H: 8.73 O: 23.37 N: 1.46	1.3±0.1
ED5	Oxaliplatin	$C_8H_{14}N_2O_4Pt$	397.2857	C: 24.18 H: 3.55 N: 7.05 O: 16.10 Pt:49.10	1.01±0.1
ED6	Leucovorin Calcium	$C_{20}H_{23}N_7O_7$	473.4393	C: 50.73 H: 4.89 N: 20.70 O: 23.65	1.7±0.1
ED7	Regorafenib	$C_{21}H_{15}ClF_4N_4O_3$	482.8154	C:52.24 H: 3.13 Cl:7.34 F: 15.73 N: 11.60 O: 9.94	1.491±0.1

Table 1 The chemical formula of drug effect ingredients

Sample code	Dose Energy (MeV)	Half Value Layer (cm)	Mean Free Path λ (mm)	Transmission Number-GEANT4
P	1	15.468	49.7±0.292	95617
	2	23.491	49.4 ±0.292	97086
	3	31.357	49.2 ±0.287	97807
	4	31.5	49.1 ±0.286	97782
ED1	1	20.322	49.0 ±0.289	96647
	2	36.473	49.7 ±0.288	98113
	3	44.709	49.9±0.288	98459
	4	54.140	50.2±0.287	98727
ED2	1	20.748	49.0 ±0.290	96711
	2	36.666	50.0±0.288	98126
	3	45.294	50.1±0.284	98477
	4	46.824	50.3±0.285	98522
ED3	1	14.259	49.8±0.287	95253
	2	26.450	50.0±0.286	97414
	3	31.076	50.2±0.285	97786
	4	33.804	50.3±0.286	97970
ED4	1	13.832	49.2±0.289	95106
	2	24.146	50.1±0.290	97167
	3	29.364	51.2±0.283	97664
	4	31.643	51.9±0.286	97825
ED5	1	34.137	50.2±0.290	97984
	2	59.230	50.3±0.291	98835
	3	75.32	51.9±0.291	99082
	4	88.846	51.9±0.290	99216
ED6	1	15.365	49.86±0.289	95381
	2	26.551	4.903±0.286	97416
	3	30.663	50.403±0.286	97762
	4	34.65	50.107±0.288	98016
ED7	1	24.75	50.334±0.288	97023
	2	35.721	49.602±0.287	98077
	3	39.827	49.700±0.286	98267
	4	47.142	49.700±0.286	98538

Sample Code: P (Paraffin), **ED** (Effect Drug sample)

Table 2 Comparison of quinoline derivatives fast neutron shielding parameters for 1 mm sample thick and 100000 incident neutrons

By looking at the values in Table 2, it can be seen that all samples have both MFP and HVL values close to paraffin. Especially ED4 and ED6 samples have lower MFP and HVL values than those of paraffin. These results show that both examples have better neutron stopping ability than paraffin.

Neutrons are particle type radiation. For this reason, determination of neutron numbers and energies interacting with matter is important in shielding studies. The number of neutron particles coming onto the matter is related to the flux formed per unit volume. This flux depends on the number of elastic, inelastic, scattered and captured neutrons that can be made with the target material. Therefore, the number of neutrons which coming, passing and captured in the material is directly related to the absorption capacity of the material (Schober 2014). Each sample was bombarded with 100000 neutrons to determine the number of neutrons that passed through from all samples. The obtained results are given in Table 2. According to Table 2, it is seen that the number of neutrons passing through all the samples is close to paraffin. A low number of neutrons means that the samples have good absorption power. The ED4 and ED6 samples showed the best performance of all the materials.

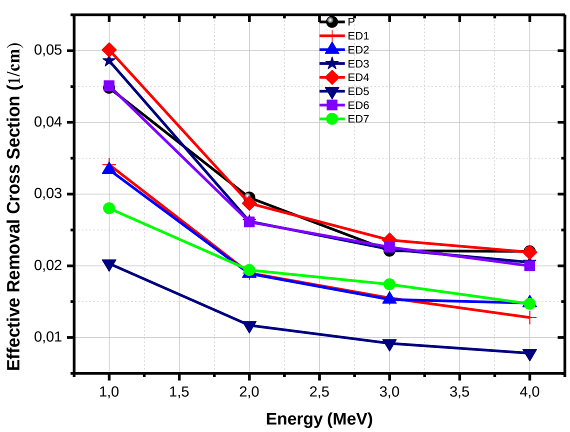

Figure 2. Theoretical 1-4 MeV Neutron Effective Removal Cross Sections

3.2 Gamma Radiation Monte Carlo (Geant4) Simulation Accounts

Gamma radiation attenuation parameters were calculated such as the MFP, MAC, HVL in the energy range from 0.1 to 4.5 MeV by using Geant4 code. The greater the mass attenuation coefficient of a target material, the larger the gamma radiation absorption ability. The all examined samples has a good capacity for gamma radiation shielding as shown in Figure 3.

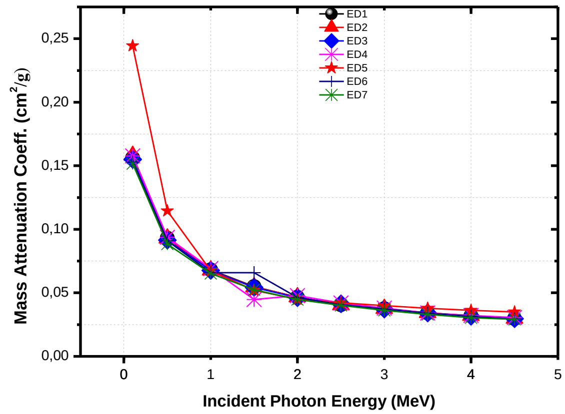

Figure 3. Variation of MAC values for different samples in the energy range of 0.1- 4.5 MeV.

The MAC values dependent on the photon energy of the examined drug effec ingredients are shown in Figure 3. From this graph, we observed that the MAC values of all samples decrease significantly as a function of increasing energy and depends both on the elements in compounds, chemical ratio of the samples and the Compton scattering which predominant region (0.3 - 4 MeV). When the seven drug effect ingredients samples are evaluated together, the ED5 sample containing 49.10% Pt has the highest MAC values. In fact, all samples were determined to absorb gamma radiation. However the obtained results show that the ED5 sample has excellent gamma radiation shielding capacity in the all photon energy region than do other samples. The HVL is indicator as the material thickness value required to halve the interaction photon amount of the target material that interacts with mono-frequency photons, is one of the important attenuation parameters. These parameter is very useful determining the progression characteristic of gamma radiation that interact with any chemical molecules in a tissue or body, especially in medical shielding and radioterapi applications. The thickness of the drug effect ingredients to halve the incoming gamma ray, so the HVL values were also calculated and the changes of these values according to photon energy are given in Figure 4.

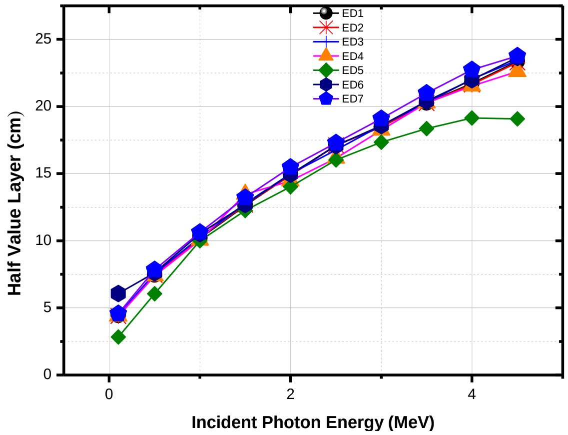

Figure 4. Change of HVL values in the energy range of 0.1-4.5 MeV.

When the figure is examined we can see this HVL values of all drug effect ingredients depending of increasing photon energy have increased as exponentially. Especially the low HVL value of the ED5 sample is proof of its high attenuation power.

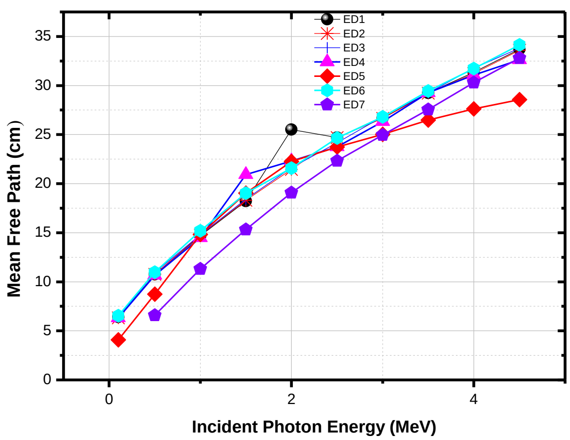

Figure 5. Comparison of mean free path values

The mean free path is the average distance traveled by a photon during two collisions with the target material. It is a very important parameter in radiation shielding studies and low value indicates that collisions are frequent. Thus, materials with low mean free path values have high attenuation capabilities.

When examined Figure 5, it can see that decreasing of mean free path values with increasing photon energy of all samples. As shown in Figure 5, ED5 sample is shown excellent absorption performance among other samples. HVL and MFP values fluctuations are thought to be caused by the elements contained in the materials.

4. Conclusion

In this study for fast neutron and gamma radiation, attenuation characteristics of pharmaceutical active ingredients especially used in cancer treatments such as Bevacizumab (Avastin), Camptosar (Irinotecan Hydrochloride), Capecitabine, Everolimus, Oxaliplatin, Leucovorin Calcium and Regorafenib were determined by using Monte Carlo simulation Geant4 code. It was found that all samples have certain amount absorption capacity neutron radiation. It is reported that, especially Everolimus (ED4) and Leucovorin Calcium (ED6) samples have neutron radiation high absorption performance than another samples. The results analyzed for gamma radiation showed that all samples have gamma radiation absorption ability. It is proved that, in particular the Oxaliplatin (ED5) have high amount absorption ratio gamma from nother samples. These samples are used for cancer in chemotherapy, but in some cases may need to be used with radiotherapy. It is shown that with this studies, these drug effect ingredients can used chemotherapy with in radiotherapy combination.

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