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Evaluation of Radiation Attenuation Properties of Some Cancer Drugs

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Abstract

The present study was conducted to estimate the radiation attenuation parameters of six different antineoplastic drugs used in the cure of cancer diseases. The effective atomic number and electron density of anastrozole, epirubicin, gemcitabine, ifosfamide, methotrexate and paclitaxel were computed theoretically in the energy region of 1 keV to 100 GeV. The energy absorption buildup factors (EABF) and exposure buildup factors (EBF) for these chemotherapy drugs were also examined by applying Geometric Progression (GP) fitting method. The variation of EABF and EBF values with photon energy and penetration depth were presented graphically and discussed. The results obtained from this study pointed out that buildup factors rely on the chemical combination of the drugs, incident photon energy and penetration thickness. It was observed that ifosfamide had a significantly better radiation absorption effect compared to other drugs. The data obtained from this study are expected to be useful in the fields of radiation biology, radiation dosimetry and radiotherapy.

Keywords: Cancer drugs; Radiation; Effective atomic number; Effective electron density; Buildup factors.

Bazı Kanser İlaçlarının Radyasyon Soğurma Özelliklerinin Değerlendirilmesi

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Öz

Bu çalışma, kanser hastalıklarının tedavisinde kullanılan altı farklı antineoplastik ilacın radyasyon zayıflama parametrelerini değerlendirmek için gerçekleştirilmiştir. Anastrozol, epirubisin, gemsitabin, ifosfamid, metotreksat ve paklitakselin etkin atom numarası ve etkin elektron yoğunluğu 1 keV ile 100 GeV enerji bölgesinde teorik olarak hesaplandı. Bu kemoterapi ilaçları için enerji soğurma yığılma faktörleri (EABF) ve maruz kalma yığılma faktörleri (EBF) de GP fit yöntemi uygulanarak incelenmiştir. EABF ve EBF değerlerinin foton enerjisi ve nüfuz etme derinliği ile değişimi grafiksel olarak sunulmuş ve tartışılmıştır. Bu çalışmadan elde edilen sonuçlar, yığılma faktörlerinin ilaçların kimyasal kombinasyonuna, gelen foton enerjisine ve nüfuz etme kalınlığına bağlı olduğuna işaret etti. İfosfamidin diğer ilaçlara göre önemli ölçüde daha iyi radyasyon soğurma etkisine sahip olduğu gözlemlendi. Bu çalışmadan elde edilen verilerin radyasyon biyolojisi, radyasyon dozimetrisi ve radyoterapi alanlarında faydalı olması beklenmektedir.

Anahtar Kelimeler: Kanser ilaçları; Radyasyon; Etkin atom numarası; Etkin elektron yoğunluğu; Yığılma faktörleri.

1. Introduction

Ionizing radiation (X, gamma rays, etc.) performs a major act in the diagnosis and cure of illness in medical applications such as diagnostic radiology, radiotherapy and like, as it has the ability to acquire images and destroy cells or tumours [1]. Radiotherapy technologies, which are being updated day by day with the use of high energy radiation in cancer treatments, are now being implemented as a priority option for many types of cancer. Today, 60-70% of cancer cases receive radiotherapy at least once in the process after the disease is diagnosed [2]. In some cases, simultaneously chemotherapy and radiotherapy are effectively applied in the treatment of some types of cancer, and this treatment is called chemoradiotherapy. In this way, by increasing the sensitivity of the cells to radiation with chemotherapy, radiation is provided to be more effective on the cells. When ionizing radiation passes through biological tissues, it can cause chemical alterations in tissues, leading to cell damage or cell and tissue death [3]. Therefore, evaluation of the interaction parameters of X or gamma rays with chemotherapy drugs may be beneficial for the estimation of absorbed radiation doses and radiation dose limits in chemoradiotherapy treatments.

The prior knowledge of radiation attenuation parameters such as mass attenuation coefficients (μ_m), effective atomic number (Z_{eff}), effective electron density (N_{el}) and buildup factors are critical in various practices such as medical physics, radiation physics, radiation

dosimetry, radiotherapy, computerized tomography, and radiation biology. The most basic parameter among these parameters is the mass attenuation coefficient, which measures the probability of photon interaction (absorption or scattering) with the drug sample and this parameter and other parameters can be calculated using μ_m [4]. Buildup factor, an important term in radiation dosimetry besides that shield design can be categorized as energy absorption buildup factor (EABF) and exposure buildup factor (EABF). It depends on the atomic number of the absorber medium [5]. EABF is defined as the amount of absorbed or deposited energy in the interacting material and the detector response function is as the absorption in the interacting medium. EBF is defined as the amount of exposure and the detector response function is as the absorption in air [2, 6]. Various methods have been developed in the literature to work out the buildup factors that take into account various parameters such as photon energy, absorbing medium properties and distance [7-10]. The GP fitting method [7, 11] is the most widely used method to calculate buildup factors of various materials. Using the GP fitting method, many researchers have studied buildup factors of various materials such as concretes [12], alloys [13, 14], glasses [15, 16], polymers [17], building materials [18] human organs and tissues [19], teeth [20], bioactive compounds [21], amino acids [22], enzyme inhibitors [23], thermoluminescent dosimetric (TLD) materials [24], solvents [6] and like. In these studies, it was emphasized that GP method is a suitable method for calculating photon buildup factors for various materials.

Antineoplastic drugs used in the cure of cancer illness are drugs conceived to disturb or avoid cellular proliferation by inhibiting deoxyribonucleic acid (DNA) synthesis. Antineoplastic drugs are generally classified as alkylating agents, antimetabolites, antitumor antibiotics, hormone and hormone antagonists, alkaloids and other antineoplastic drugs [25]. Anastrozole ($C_{17}H_{19}N_5$), epirubicin ($C_{27}H_{26}NO_{11}$), gemcitabine ($C_9H_{11}F_2N_3O_4$), ifosfamide ($C_7H_{15}Cl_2N_2O_2P$), methotrexate ($C_{20}H_{22}N_8O_5$) and paclitaxel ($C_{47}H_{51}NO_{14}$) are some of the commonly used antineoplastic drugs in chemotherapy. Anastrozole is an aromatase inhibitor utilized in the handling of second-level breast cancer and avoids the production of the hormone oestrogen, which triggers the formation of breast cancer. Epirubicin is an anthracycline antitumor antibiotic and is used alone or in combination with other chemotherapy drugs to cure certain diseases such as breast and ovarian cancer. Ifosfamide, an alkylating oxazophosphorine agent, is one of the chemotherapy drugs that avoid the reproduction of cancer cell DNA by averting its reproduction. Today, it is used in the treatment of lymphoma, soft tissue sarcoma and advanced breast, testicle, ovarian, stomach and lung cancers. Methotrexate is a type of antimetabolite agent that inhibits DNA replication or causes apoptosis by synthesizing incorrect codes and is extensively used in the cure of various types of cancer diseases such as head and neck cancers, ovarian, bladder, cervix, stomach, large intestine, testicle, breast, bone cancer, choriocarcinoma cancers and etc.

Similar to methotrexate, Gemcitabine is a type of antimetabolite agent. It is a chemotherapy drug used in the treatment of pancreas, lung, bladder and breast cancers as well as other tumours such as ovarian cancer, mesothelioma and head and neck cancers. Paclitaxel is an antitumor agent active against a wide variety of cancers that are generally considered to be resistant to conventional chemotherapy. It is effective in the treatment of metastatic breast or ovarian cancer [25-31].

Radio protective effects of various drugs have been estimated by many researchers. Oto et al. computed gamma ray interaction parameters (i.e. μ_m, Z_{eff}, N_{el}, EABF and EBF) of different drugs used in cholinergic medications using WinXCOM computer program [1]. Sayyed et al. calculated Z_{eff}, N_{el}, EABF and EBF for Nonsteroidal anti-inflammatory drugs (NSAIDs) [32]. Kavaz et al. computed photon buildup factors of some chemotherapy drugs by using the GP fitting method in the energy region 0.015–15 MeV up to penetration depths of 40 mean free paths (mfp) [33]. Akman and Kaçal calculated some essential radiation attenuation parameters such as μ_m, Z_{eff} and N_{el} of some drugs used in Chemotherapy with the help of the WinXCOM program [34]. Ekinci et al. investigated the EABF and EBF of some anti-inflammatory drugs by using the GP fitting method [35]. Yorgun and Kavaz determined μ_m, Z_{eff}, N_{el} of some cancer drugs at 13.81, 17.7, 26.34 and 59.54 keV photon energies. They also computed EABF and EBF of these cancer drugs in the energy region 0.015–15 MeV up to penetration depths of 40 mfp [2].

The aim of this research work is to estimate radiation interaction parameters of six different antineoplastic chemotherapy drugs commonly used for cancer treatment. There is almost no study in the literature on the radiation absorption parameters of these drugs. Therefore, it may be useful to investigate the radiation interaction parameters of these drugs for chemoradiation dose limits and dose calculations. For this purpose, Z_{eff} and N_{el} values of some chemotherapy drugs such as anastrozole, epirubicin, gemcitabine, ifosfamide, methotrexate and paclitaxel were computed in the energy range of 1 keV–100 GeV. Additionally, the energy absorption and exposure buildup factors of these antineoplastic chemotherapy drugs were calculated by means of GP fitting method for the energy range 0.015-15 MeV up to the penetration depth of 40 mfp.

2. Materials and Methods

2.1. Computation of Z_{eff} and N_{el}

The mass attenuation coefficients for investigated drug samples were computed by using mixture rule given in the following equation [36, 37]:

$$\mu_m = \frac{\mu}{\rho} = \sum_i w_i \left(\frac{\mu}{\rho}\right)_i \quad (1)$$

where ρ is the density, w_i and $\left(\frac{\mu}{\rho}\right)_i$ are the weight fraction and mass attenuation coefficient for individual element in drugs, respectively. The theoretical μ_m values for the investigated drugs were determined using WinXCOM software package [38]. For the drug samples, the effective atomic number were computed with the help of the following formula [1, 33]:

$$Z_{eff} = \frac{\sum_i f_i A_i \left(\frac{\mu}{\rho}\right)_i}{\sum_j f_j \frac{A_j}{Z_j}\left(\frac{\mu}{\rho}\right)_j} \quad (2)$$

where f_i, A_i, Z_i and $\left(\frac{\mu}{\rho}\right)_i$ are the molar fraction, atomic weight, atomic number and mass attenuation coefficient of relative element in the drug samples, respectively. In addition, the effective electron density, a parameter closely related to the effective atomic number, can be calculated by following equation [33, 35]:

$$N_{el} = N_a \frac{nZ_{eff}}{\sum_i n_i A_i} = N_A \frac{Z_{eff}}{\langle A \rangle} \ (electrons/g) \quad (3)$$

where N_A represents the Avogadro constant and ⟨A⟩ indicates average atomic mass of the material.

2.2. Computation of EABF and EBF

The energy absorption and exposure buildup of chemotherapy drugs under the study were determined in three steps. In the first step, Compton partial mass attenuation coefficient ($(\mu/\rho)_{Compton}$) and the total mass attenuation coefficient $(\mu/\rho)_{Total}$ values were determined for different elements (Z = 4–30) and also for investigated drug samples using WinXCOM program. Then the interpolation formula given in Eqn. (4) was employed to compute the equivalent atomic number (Z_{eq}) of chosen drug by matching the ratio R ($(\mu_m)_{Compton}/(\mu_m)_{Total}$) at a particular photon energy with the convenient ratio of the pure element at the same energy [7,39];

$$Z_{eq} = \frac{Z_1(\log R_2 - \log R) + Z_2(\log R - \log R_1)}{\log R_2 - \log R_1} \quad (4)$$

where R signifies the ratio for chosen drug samples at particular energy which lies between R_1 and R_2. Z_1 and Z_2 denote atomic numbers of the elements corresponding to the ratios R_1 and R_2, respectively. More details for the calculation procedure can be found in reference [38]. In the

second step, in order to evaluate buildup factors the GP fitting coefficients for elements were acquired from the ANSI/ANS-6.4.3 database [40]. This database provides the GP fitting parameters for 23 elements (Z=4–92), water, air and concrete in the energy region of 0.015-15 MeV up to 40 mfp [39]. The obtained Z_{eq} values were used to determine geometric progression (GP) fitting coefficients (a, b, c, d, and X_k) for the drug samples using the following relation [33, 39, 41];

$$P = \frac{P_1(\log Z_2 - \log Z_{eq}) + P_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1} \tag{5}$$

where P denotes GP fitting parameters of studied drug samples. P_1 and P_2 are the values of GP fitting coefficients corresponding to the Z_1 and Z_2 atomic numbers at a specific energy, respectively. In the last step, the computed GP fitting coefficients were used to generate the energy absorption and exposure build-up for selected antineoplastic drugs at some standard photon energies in the energy range 0.015-15 MeV up to 40 mfp penetration depths. This calculation was accomplished by using the following GP fitting formulas [7, 33, 39, 41];

$$B(E,X) = 1 + \frac{b-1}{K-1}(K^X - 1) \quad for\ K \neq 1 \tag{6}$$

$$B(E.X) = 1 + (b-1) \quad for\ K = 1 \tag{7}$$

$$K(E,X) = \mathrm{cx}^{\mathrm{a}} + d\frac{\tanh\left(\frac{\mathrm{x}}{X_k} - 2\right) - \tanh(-2)}{1 - \tanh(-2)} \qquad for\ \mathrm{x} \leq 40\ mfp \tag{8}$$

where E, x and K (E, X) are the photon energy, penetration depth in mfp and dose multiplicative factor, respectively. a, b, c, d and X_k are the GP fitting parameters and b is the buildup factor at one mfp.

3. Results and Discussion

The chemical formula and elemental composition of the studied antineoplastic chemotherapy drugs are presented in Table 1. The μ_m values of anastrazol, epirubicin, gemcitabine, ifosfamide, methotrexate and paclitaxel drugs were computed using WinXCOM software package [37]. From the computed μ_m values Z_{eff} and N_{el} values of investigated drugs were worked out with the help of the Eqn. (2) and (3) in the energy range from 1 keV to 100 GeV.

Table 1: Chemical formula and elemental composition of investigated drugs

Drug	Chemical Formula	Weight fraction of elements (%)						
		H	C	N	O	F	P	Cl

Anastrozole	$C_{17}H_{19}N_5$	0.065	0.696	0.239	-	-	-	-
Epirubicin	$C_{27}H_{26}NO_{11}$	0.048	0.600	0.026	0.326	-	-	-
Gemcitabine	$C_9H_{11}F_2N_3O_4$	0.042	0.411	0.160	0.243	0.144	-	-
Ifosfamide	$C_7H_{15}Cl_2N_2O_2P$	0.058	0.322	0.107	0.123	-	0.119	0.272
Methotrexate	$C_{20}H_{22}N_8O_5$	0.049	0.529	0.247	0.176	-	-	-
Paclitaxel	$C_{47}H_{51}NO_{14}$	0.060	0.661	0.016	0.262	-	-	-

Figure 1 and 2 show the variation of the computed Z_{eff} and N_{el} values with photon energy for the investigated antineoplastic chemotherapy drugs. Z_{eff} and N_{el} values of ifosfamide have a peak at 1.892 keV photon energy, which correspond to the K absorption edge of chlorine. The computed Z_{eff} values ranged from 3.68-6.30 for Anastrozole, 4.35-6.98 for epirubicin, 4.69-7.47 for gemcitabine, 4.70–12.35 for ifosfamide, 4.32-6.81 for methotrexate and 4.00-6.83 for paclitaxel, respectively. The N_{el} values also ranged from 3.10×10^{23}–4.26×10^{23} electrons/g for Anastrozole, 3.31×10^{23}–4.11×10^{23} electrons/g for epirubicin, 3.30×10^{23}–4.05×10^{23} electrons/g for gemcitabine, 3.15×10^{23}–8.26×10^{23} electrons/g for ifosfamide, 3.30×10^{23}–4.09×10^{23} electrons/g for methotrexate and 3.35×10^{23}-4.28×10^{23} electrons/g for paclitaxel, respectively. The highest Z_{eff} and N_{el} values of the studied drugs were observed in the low energy region (E<0.1 MeV) where photoelectric absorption which is cross section proportional to the Z^{4-5} and $E^{-3.5}$ is the dominant interaction mechanism [23].

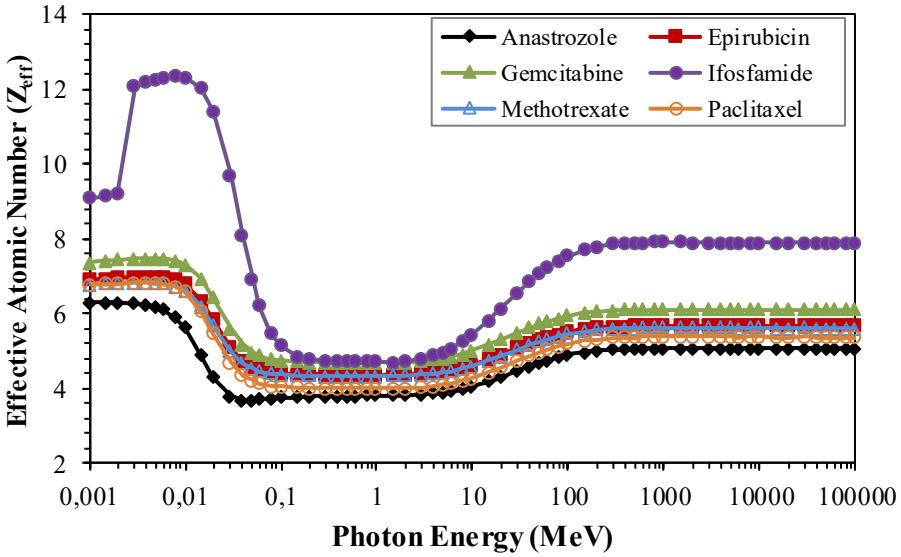

Figure 1: Z_{eff} values of investigated chemotherapy drugs versus photon energy

As seen from Figs. 1 and 2, the lowest Z_{eff} and N_{el} values of the studied drugs were determined in the intermediate energies (0.1 MeV<E 10 MeV). It was seen that in this energy region where Compton scattering is the most important interaction process, Z_{eff} and N_{el} values are almost independent to photon energy. This may be due to the weak dependence of the Compton scattering cross section to atomic number and photon energy (i.e. proportional to Z and E^{-1}) [37].

At energies greater than 10 MeV, Z_{eff} and N_{el} values increase slowly with increasing photon energy and are almost constant at further energies. This change can be clarified by actually that pair production is the dominant interaction process at high energies. Because the pair productions cross section is directly proportional to E and Z^2 [13]. This observed trend in Z_{eff} and N_{el} values is consistent with the results of the study reported by Oto et al. [1] who investigated radiation interaction parameters of some cholinergic drugs. As shown in Figs. 1 and 2, ifosfamide has considerably higher Z_{eff} and N_{el} values than other studied drugs in the low and high energy regions. In the intermediate energy region, the Z_{eff} values of ifosfamide are slightly larger than those of the other drugs, while the N_{el} values are approximately the same. The reason for this apparent difference in the Z_{eff} and N_{el} values of ifosfamide may be that ifosfamide contains phosphate (Z=15, weight fraction= 0.119) and chlorine (Z=17, weight fraction =0.272), unlike other drugs.

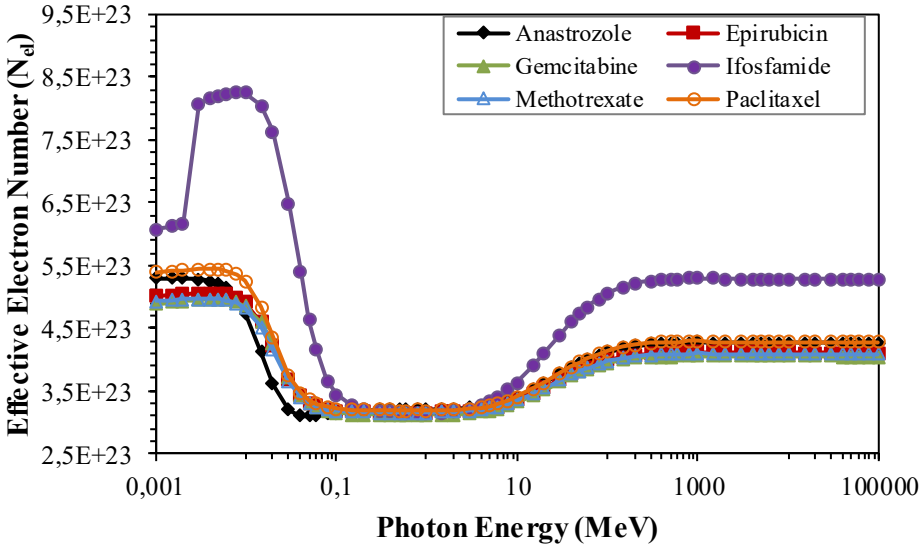

Figure 2: N_{el} values of investigated chemotherapy drugs versus photon energy

The Z_{eq} values calculated using the interpolation formula given in Eqn. (4) in the 0.015-15 MeV energy range for the examined drugs are given in Table 2. It is obviously sighted from Table 2 that ifosfamide has the highest Z_{eq} values among the examined antineoplastic drugs, while anastrozole has the lowest Z_{eq} values. The high Z_{eq} values of ifosfamide are due to the presence of phosphate (Z=15, weight fraction= 0.119) and chlorine (Z=17, weight fraction=0.272) in the chemical structure of ifosfamide, unlike other drugs. Similarly, the reason why anastrozole has low Z_{eq} values is due to the lack of oxygen, fluorine, phosphate and chlorine in the chemical structure of anastrozole. The GP fitting coefficients of the EABF and EBF for investigated radioprotectors are listed in Table 3-8 at the energy region of 0.015-15 MeV.

Table 2: Z_{eq} values of investigated drugs at the energy region of 0.015-15 MeV

Energy (MeV)	Anastrozole	Epirubicin	Gemcitabine	Ifosfamide	Methotrexate	Paclitaxel
0.015	6.009	6.639	7.094	11.85	6.514	6.446
0.02	6.014	6.636	7.099	11.97	6.509	6.443
0.03	6.008	6.618	7.097	12.09	6.489	6.422
0.04	5.989	6.598	7.086	12.13	6.468	6.399
0.05	5.970	6.578	7.072	12.14	6.451	6.378
0.06	5.951	6.562	7.059	12.13	6.436	6.360
0.08	5.922	6.535	7.036	12.08	6.413	6.331
0.1	5.901	6.515	7.017	12.00	6.396	6.309
0.15	5.867	6.483	6.980	11.79	6.368	6.274
0.2	5.850	6.463	6.954	11.62	6.352	6.253
0.3	5.831	6.444	6.929	11.39	6.335	6.232
0.4	5.823	6.435	6.917	11.26	6.327	6.222
0.5	5.819	6.429	6.910	11.18	6.323	6.217
0.6	5.816	6.427	6.906	11.14	6.321	6.214
0.8	5.813	6.424	6.903	11.09	6.319	6.211
1	5.813	6.423	6.902	11.08	6.318	6.210
1.5	5.673	6.262	6.701	10.28	6.177	6.032
2	5.630	6.206	6.637	9.77	6.126	5.968
3	5.620	6.193	6.623	9.60	6.114	5.953
4	5.617	6.190	6.620	9.56	6.111	5.949
5	5.617	6.189	6.620	9.53	6.110	5.948
6	5.617	6.188	6.618	9.53	6.110	5.947
8	5.616	6.186	6.617	9.51	6.108	5.944
10	5.617	6.184	6.617	9.51	6.106	5.942
15	5.618	6.184	6.614	9.50	6.107	5.942

Table 3: GP fitting parameters for anastrozole in the energy range 0.015-15 MeV

Energy (MeV)	**EABF**					**EBF**				
	b	**c**	**a**	**Xk**	**d**	**b**	**c**	**a**	**Xk**	**d**
0.015	1.397	0.526	0.153	14.421	-0.077	1.385	0.538	0.146	14.310	-0.072
0.02	1.895	0.737	0.077	16.436	-0.037	1.872	0.730	0.080	16.546	-0.040
0.03	3,716	1.150	-0.026	12.601	0.008	3.503	1.150	-0.026	12.846	0.008
0.04	5.073	1.740	-0.128	14.102	0.056	5.276	1.750	-0.130	13.917	0.064
0.05	5.598	2.078	-0.165	14.488	0.070	6.749	2.123	-0.171	14.344	0.074
0.06	5.420	2.304	-0.187	14.668	0.079	7.270	2.408	-0.200	14.522	0.089
0.08	4.841	2.510	-0.206	14.823	0.083	6.888	2.725	-0.230	14.456	0.101
0.1	4.280	2.569	-0.210	14.926	0.083	6.107	2.836	-0.239	14.368	0.104
0.15	3.538	2.484	-0.203	15.230	0.076	4.573	2.892	-0.247	14.292	0.107
0.2	3.184	2.360	-0.194	15.211	0.073	3.775	2.771	-0.239	14.949	0.108
0.3	2.785	2.142	-0.176	14.990	0.070	3.148	2.494	-0.219	14.343	0.099
0.4	2.613	1.942	-0.155	14.758	0.063	3.027	2.268	-0.201	13.324	0.085
0.5	2.452	1.811	-0.140	15.794	0.062	2.661	2.072	-0.180	13.936	0.084
0.6	2.392	1.673	-0.121	14.937	0.047	2.544	1.904	-0.159	13.615	0.068
0.8	2.196	1.567	-0.110	14.100	0.047	2.320	1.726	-0.139	13.727	0.068
1	2.087	1.463	-0.094	14.158	0.041	2.203	1.567	-0.114	13.737	0.057
1.5	1.939	1.277	-0.061	14.308	0.027	2.031	1.330	-0.073	13.718	0.037
2	1.840	1.173	-0.039	14.390	0.016	1.918	1.199	-0.046	14.147	0.023
3	1.715	1.051	-0.012	13.942	0.004	1.764	1.062	-0.015	12.253	0.008
4	1.627	0.989	0.003	13.594	-0.003	1.664	0.983	0.005	22.560	-0.007
5	1.567	0.944	0.015	14.609	-0.008	1.584	0.937	0.017	14.663	-0.011
6	1.521	0.901	0.029	12.647	-0.017	1.531	0.907	0.026	14.563	-0.016

8	1.438	0.874	0.037	11.762	-0.018	1.443	0.870	0.037	16.022	-0.030
10	1.382	0.858	0.040	14.389	-0.022	1.377	0.854	0.042	12.741	-0.020
15	1.287	0.837	0.047	15.238	-0.030	1.280	0.837	0.047	14.811	-0.028

Table 4: GP fitting parameters for epirubicin in the energy range 0.015-15 MeV

Energy (MeV)	EABF					EBF				
	b	c	a	Xk	d	b	c	a	Xk	d
0.015	1.292	0.499	0.160	14.518	-0.078	1.286	0.497	0.162	14.284	-0.081
0.02	1.677	0.634	0.114	15.440	-0.056	1.659	0.637	0.112	15.544	-0.055
0.03	3.081	0.956	0.023	14.782	-0.021	2.945	0.955	0.024	14.657	-0.022
0.04	4.400	1.450	-0.080	13.915	0.032	4.450	1.458	-0.082	13.707	0.034
0.05	5.176	1.806	-0.132	14.170	0.056	5.711	1.829	-0.136	14.048	0.059
0.06	5.261	2.073	-0.166	14.143	0.073	6.222	2.124	-0.172	14.036	0.078
0.08	4.890	2.342	-0.194	14.045	0.083	6.040	2.465	-0.209	13.808	0.094
0.1	4.495	2.388	-0.195	14.666	0.080	5.526	2.561	-0.213	14.395	0.093
0.15	3.636	2.395	-0.197	14.684	0.078	4.175	2.659	-0.227	14.125	0.100
0.2	3.266	2.283	-0.188	14.784	0.076	3.579	2.558	-0.221	14.231	0.098
0.3	2.817	2.095	-0.172	14.613	0.068	3.061	2.287	-0.197	14.248	0.086
0.4	2.625	1.913	-0.152	14.554	0.062	2.778	2.097	-0.179	13.733	0.075
0.5	2.459	1.794	-0.138	15.185	0.059	2.604	1.932	-0.160	14.163	0.071
0.6	2.383	1.671	-0.121	14.650	0.048	2.482	1.800	-0.143	13.827	0.059
0.8	2.200	1.555	-0.107	14.139	0.045	2.281	1.642	-0.124	13.902	0.057
1	2.096	1.447	-0.090	14.430	0.038	2.161	1.513	-0.104	13.864	0.049
1.5	1.938	1.276	-0.060	14.315	0.026	1.999	1.300	-0.066	14.001	0.031
2	1.841	1.169	-0.038	14.403	0.015	1.889	1.188	-0.043	13.981	0.020
3	1.714	1.051	-0.011	14.104	0.003	1.745	1.059	-0.014	12.385	0.006
4	1.627	0.988	0.004	13.123	-0.003	1.649	0.987	0.004	23.623	-0.007
5	1.565	0.944	0.015	14.740	-0.008	1.572	0.939	0.017	14.315	-0.011
6	1.514	0.907	0.028	13.308	-0.018	1.523	0.907	0.027	13.980	-0.016
8	1.430	0.881	0.034	12.096	-0.017	1.437	0.872	0.037	16.010	-0.031
10	1.375	0.861	0.040	14.322	-0.022	1.371	0.859	0.041	12.715	-0.021
15	1.281	0.838	0.047	15.732	-0.033	1.275	0.841	0.046	15.225	-0.030

Table 5: GP fitting parameters for gemcitabine in the energy range 0.015-15 MeV

Energy (MeV)	EABF					EBF				
	b	c	a	Xk	d	b	c	a	Xk	d
0.015	1.228	0.479	0.166	14.429	-0.081	1.226	0.471	0.173	14.292	-0.087
0.02	1.538	0.570	0.137	14.855	-0.068	1.523	0.577	0.133	14.963	-0.065
0.03	2.657	0.824	0.059	15.588	-0.038	2.563	0.829	0.056	15.778	-0.040
0.04	3.914	1.246	-0.045	13.748	0.014	3.871	1.253	-0.047	13.568	0.016
0.05	4.838	1.606	-0.107	13.918	0.045	4.964	1.614	-0.109	13.826	0.047
0.06	5.119	1.896	-0.148	13.764	0.069	5.454	1.913	-0.151	13.684	0.070
0.08	4.914	2.213	-0.185	13.441	0.105	5.407	2.268	-0.192	13.316	0.110
0.1	4.660	2.245	-0.183	14.466	0.089	5.195	2.326	-0.191	14.380	0.082
0.15	3.745	2.302	-0.189	14.420	0.077	3.977	2.461	-0.210	14.111	0.095
0.2	3.357	2.202	-0.180	14.799	0.076	3.410	2.420	-0.209	13.395	0.090
0.3	2.838	2.061	-0.168	14.259	0.067	2.974	2.160	-0.182	14.083	0.077
0.4	2.621	1.900	-0.151	14.259	0.060	2.711	1.993	-0.165	14.005	0.070
0.5	2.461	1.786	-0.138	14.283	0.056	2.548	1.850	-0.148	14.135	0.063
0.6	2.366	1.679	-0.124	14.305	0.050	2.418	1.747	-0.135	14.065	0.058
0.8	2.202	1.546	-0.105	14.190	0.044	2.247	1.590	-0.114	14.009	0.050
1	2.106	1.432	-0.087	14.672	0.036	2.129	1.480	-0.097	13.953	0.044
1.5	1.934	1.276	-0.060	14.355	0.026	1.980	1.282	-0.061	14.493	0.027

2	1.838	1.173	-0.039	14.151	0.017	1.872	1.182	-0.041	13.964	0.019
3	1.711	1.054	-0.012	13.224	0.004	1.730	1.060	-0.014	13.243	0.005
4	1.628	0.984	0.006	13.777	-0.005	1.639	0.988	0.004	19.265	-0.006
5	1.566	0.937	0.018	14.068	-0.012	1.567	0.940	0.018	13.913	-0.012
6	1.504	0.922	0.022	15.397	-0.017	1.520	0.904	0.029	13.151	-0.017
8	1.430	0.874	0.037	12.066	-0.021	1.429	0.880	0.035	13.645	-0.023
10	1.369	0.866	0.039	14.326	-0.022	1.365	0.866	0.039	13.530	-0.022
15	1.276	0.839	0.048	15.335	-0.034	1.273	0.841	0.047	15.125	-0.032

Table 6: GP fitting parameters for ifosfamide in the energy range 0.015-15 MeV

Energy (MeV)	**EABF**					**EBF**				
	b	**c**	**a**	**Xk**	**d**	**b**	**c**	**a**	**Xk**	**d**
0.015	1.039	0.402	0.209	13.063	-0.127	1.039	0.398	0.213	13.098	-0.131
0.02	1.087	0.428	0.183	14.507	-0.094	1.086	0.438	0.179	14.318	-0.092
0.03	1.288	0.442	0.192	14.242	-0.102	1.282	0.447	0.190	14.444	-0.102
0.04	1.625	0.548	0.146	15.245	-0.077	1.598	0.550	0.146	15.117	-0.078
0.05	2.175	0.615	0.133	13.753	-0.072	2.050	0.638	0.121	14.471	-0.063
0.06	2.732	0.767	0.081	13.357	-0.056	2.429	0.781	0.075	14.637	-0.057
0.08	3.748	1.048	0.002	14.331	-0.016	2.926	1.030	0.007	13.644	-0.021
0.1	4.267	1.285	-0.049	12.623	0.008	3.101	1.229	-0.035	12.292	-0.004
0.15	4.088	1.619	-0.107	13.330	0.039	3.064	1.478	-0.079	15.006	0.016
0.2	3.636	1.721	-0.122	13.723	0.044	2.897	1.570	-0.094	15.490	0.023
0.3	3.037	1.743	-0.126	13.991	0.046	2.634	1.605	-0.101	15.270	0.026
0.4	2.729	1.688	-0.120	14.211	0.042	2.469	1.575	-0.099	15.188	0.027
0.5	2.541	1.628	-0.113	14.286	0.040	2.343	1.540	-0.096	15.076	0.029
0.6	2.404	1.565	-0.103	14.563	0.036	2.249	1.494	-0.089	15.400	0.026
0.8	2.228	1.467	-0.090	14.856	0.032	2.115	1.419	-0.080	15.223	0.025
1	2.112	1.386	-0.077	14.872	0.028	2.021	1.356	-0.070	15.699	0.023
1.5	1.937	1.255	-0.054	14.286	0.021	1.890	1.241	-0.051	15.049	0.018
2	1.843	1.159	-0.035	14.701	0.013	1.811	1.158	-0.035	14.792	0.013
3	1.708	1.053	-0.010	12.225	0.000	1.696	1.054	-0.011	11.500	0.001
4	1.617	0.984	0.008	13.076	-0.010	1.614	0.991	0.005	16.231	-0.008
5	1.548	0.944	0.019	12.944	-0.014	1.544	0.952	0.002	14.850	-0.016
6	1.491	0.919	0.026	15.568	-0.027	1.499	0.915	0.006	13.305	-0.024
8	1.398	0.900	0.032	12.303	-0.020	1.411	0.897	0.003	12.969	-0.023
10	1.339	0.882	0.038	13.916	-0.028	1.352	0.874	0.005	13.557	-0.030
15	1.241	0.872	0.043	14.734	-0.034	1.264	0.832	0.058	14.664	-0.048

Table 7: GP fitting parameters for methotrexate in the energy range 0.015-15 MeV

Energy (MeV)	**EABF**					**EBF**				
	b	**c**	**a**	**Xk**	**d**	**b**	**c**	**a**	**Xk**	**d**
0.015	1.312	0.504	0.158	14.500	-0.078	1.305	0.505	0.159	14.289	-0.079
0.02	1.720	0.654	0.107	15.635	-0.052	1.700	0.655	0.106	15.740	-0.052
0.03	3.210	0.996	0.013	14.338	-0.015	3.059	0.995	0.014	14.288	-0.016
0.04	4.540	1.509	-0.090	13.954	0.037	4.619	1.518	-0.092	13.749	0.039
0.05	5.265	1.861	-0.139	14.236	0.059	5.923	1.888	-0.143	14.110	0.062
0.06	5.297	2.120	-0.170	14.255	0.074	6.436	2.180	-0.178	14.143	0.080
0.08	4.884	2.375	-0.196	14.214	0.083	6.207	2.515	-0.213	13.948	0.095
0.1	4.452	2.424	-0.198	14.714	0.081	5.608	2.620	-0.219	14.396	0.095
0.15	3.610	2.417	-0.199	14.748	0.078	4.222	2.707	-0.232	14.128	0.102
0.2	3.244	2.302	-0.190	14.781	0.075	3.619	2.591	-0.224	14.430	0.100
0.3	2.813	2.103	-0.173	14.695	0.068	3.082	2.317	-0.200	14.287	0.088
0.4	2.626	1.916	-0.152	14.623	0.062	2.794	2.121	-0.182	13.670	0.077

0.5	2.458	1.796	-0.138	15.394	0.060	2.617	1.951	-0.162	14.170	0.073
0.6	2.387	1.669	-0.121	14.730	0.047	2.497	1.813	-0.145	13.772	0.060
0.8	2.199	1.557	-0.108	14.127	0.045	2.288	1.654	-0.126	13.877	0.059
1	2.094	1.450	-0.091	14.374	0.039	2.169	1.521	-0.105	13.844	0.050
1.5	1.939	1.275	-0.060	14.307	0.027	2.003	1.303	-0.067	13.901	0.032
2	1.842	1.168	-0.037	14.452	0.015	1.893	1.190	-0.043	13.985	0.020
3	1.714	1.051	-0.011	14.272	0.003	1.748	1.058	-0.014	12.222	0.006
4	1.626	0.989	0.003	12.999	-0.003	1.650	0.986	0.004	24.450	-0.008
5	1.564	0.945	0.015	14.868	-0.008	1.573	0.939	0.017	14.391	-0.011
6	1.516	0.904	0.029	12.913	-0.018	1.524	0.907	0.026	14.137	-0.015
8	1.430	0.882	0.034	12.102	-0.017	1.438	0.870	0.037	16.455	-0.033
10	1.376	0.860	0.040	14.321	-0.022	1.372	0.857	0.041	12.562	-0.021
15	1.282	0.838	0.047	15.805	-0.033	1.275	0.841	0.046	15.244	-0.030

Table 8: GP fitting parameters for paclitaxel in the energy range 0.015-15 MeV

Energy (MeV)	**EABF**					**EBF**				
	b	**c**	**a**	**Xk**	**d**	**b**	**c**	**a**	**Xk**	**d**
0.015	1.323	0.507	0.158	14.490	-0.078	1.315	0.509	0.158	14.291	-0.078
0.02	1.742	0.665	0.103	15.739	-0.050	1.723	0.665	0.103	15.844	-0.050
0.03	3.279	1.016	0.008	14.103	-0.012	3.119	1.016	0.008	14.093	-0.013
0.04	4.616	1.542	-0.095	13.975	0.039	4.711	1.551	-0.097	13.772	0.041
0.05	5.317	1.893	-0.143	14.274	0.061	6.046	1.923	-0.147	14.146	0.064
0.06	5.318	2.148	-0.173	14.324	0.075	6.568	2.215	-0.181	14.209	0.082
0.08	4.880	2.396	-0.198	14.330	0.083	6.321	2.549	-0.216	14.043	0.096
0.1	4.421	2.450	-0.201	14.750	0.081	5.668	2.663	-0.223	14.397	0.097
0.15	3.588	2.435	-0.200	14.801	0.079	4.262	2.746	-0.235	14.131	0.103
0.2	3.224	2.319	-0.191	14.778	0.075	3.655	2.620	-0.226	14.608	0.101
0.3	2.808	2.111	-0.173	14.775	0.069	3.101	2.346	-0.203	14.324	0.090
0.4	2.627	1.919	-0.153	14.691	0.062	2.809	2.145	-0.185	13.607	0.078
0.5	2.457	1.797	-0.138	15.606	0.060	2.630	1.971	-0.165	14.176	0.075
0.6	2.391	1.667	-0.120	14.812	0.047	2.512	1.825	-0.147	13.716	0.060
0.8	2.199	1.559	-0.108	14.115	0.045	2.296	1.666	-0.128	13.852	0.061
1	2.092	1.454	-0.091	14.316	0.039	2.177	1.528	-0.107	13.822	0.051
1.5	1.941	1.275	-0.060	14.293	0.027	2.010	1.310	-0.069	13.729	0.033
2	1.843	1.167	-0.037	14.518	0.014	1.900	1.193	-0.044	14.003	0.021
3	1.715	1.050	-0.011	14.451	0.003	1.753	1.058	-0.014	12.013	0.006
4	1.626	0.990	0.003	12.920	-0.002	1.654	0.986	0.004	25.241	-0.008
5	1.564	0.947	0.014	14.992	-0.007	1.576	0.939	0.017	14.521	-0.011
6	1.519	0.900	0.030	12.390	-0.018	1.526	0.908	0.026	14.387	-0.015
8	1.431	0.883	0.034	12.061	-0.016	1.440	0.868	0.038	16.930	-0.034
10	1.379	0.859	0.040	14.330	-0.022	1.374	0.855	0.042	12.407	-0.021
15	1.284	0.838	0.047	15.811	-0.032	1.277	0.840	0.046	15.202	-0.029

The variation of EABF and EBF values with incident photon energy for anastrozole, epirubicin, gemcitabine, ifosfamide, methotrexate and paclitaxel at some chosen penetration depth were plotted in Figs. 3 and 4, respectively. It was monitored that the EABF and EBF values of the studied drugs at 1, 5, 10 and 40 mfp, increased with increasing energy, reached the maximum value in the intermediate energies and then decreased again in the further energies. As can be seen from Figs. 3 and 4, the EABF and

EBF values of ifosfamide are smaller than EABF and EBF values of other drugs. The maximum EABF and EBF values were seen at the 0.3 MeV photon energy for ifosfamide and 0.1 MeV photon energy for anastrozole, epirubicin, gemcitabine, methotrexate and paclitaxel. This trend observed in EABF and EBF values can be explained on the basis that while Compton scattering is the dominant interaction mechanism in the medium energy region, photoelectric absorption and pair production are the dominant interaction mechanisms in the low and high energy region, respectively. On the other hand, this trend is also in line with the observation of Sayyed et al. [32] who estimated photon buildup factors of some anti-inflammatory drugs. It was also seen that the values of EABF and EBF increased with increasing depth of penetration and became very high for the greatest at penetration depth 40 mfp. This increase is a result of multiple scattering events for large penetration depths [17].

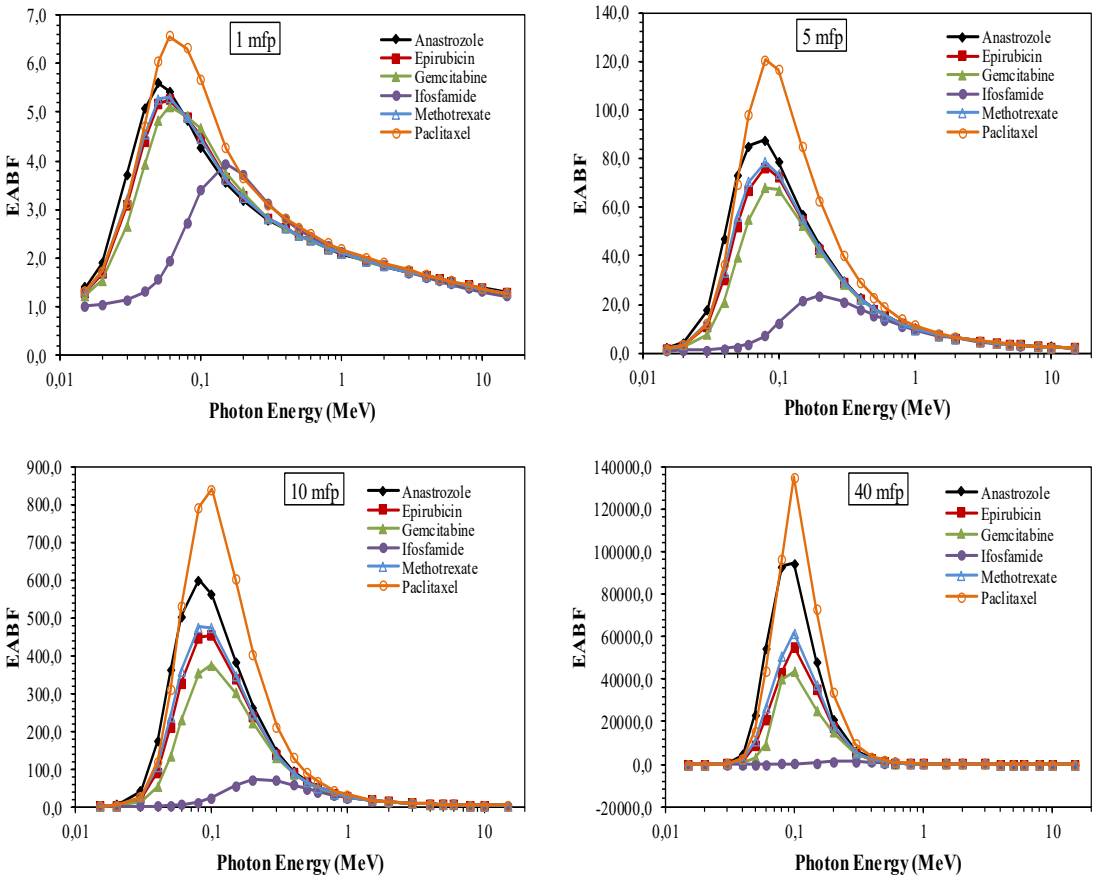

Figure 3: The EABF values of drugs in the energy range of 0.015-15 MeV at 1, 5, 10 and 40 mfp

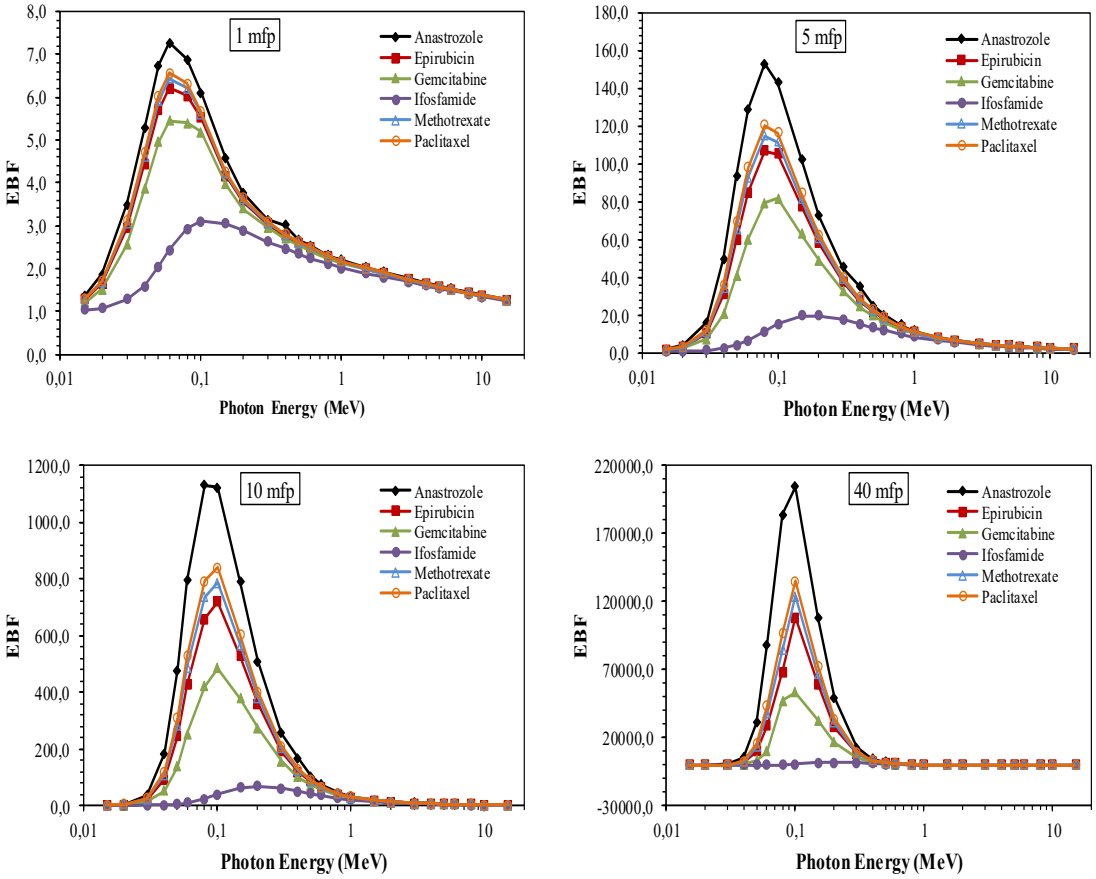

Figure 4: The EBF values of drugs in the energy range of 0.015-15 MeV at 1, 5, 10 and 40 mfp

The EABF and EBF values of the investigated anti neoplastic chemotherapy drugs against the mfp for 0.015, 0.15, 1.5 and 15 MeV photon energies are given in Figs. 5 and 6, respectively. From Figs. 5 and 6, it was observed that the EABF and EBF values of the studied chemotherapy drugs increased with the increase in mfp values. It is clear from these figures that EABF and EBF values of the investigated drugs at 0.15 and 1.5 MeV energies are higher than the others. It was seen that ifosfamide, which has the highest Z_{eq} value, has the smallest EABF and EBF values at low energies (0.015 and 0.15 MeV). On the other hand, Anastrozole has the highest EABF and EBF values at 0.015 and 0.15 MeV photon energies owing to its low Z_{eq} value. Also, the EABF and EBF values of ifosfamide remains nearly constant at 0.015 MeV energy, while the EABF and EBF values of other drugs increase with increasing mpf values. At 0.15 MeV, EABF and EBF values of the studied chemotherapy drugs increased with the rising up in mfp values. The maximum values were observed for anastrozole and paclitaxel and minimum value was observed for ifosfamide in this energy. It was seen that the EABF and EBF values of drug samples

decreased with the increasing Z_{eq} values at lower than the 0.15 MeV, because the cross section of photoelectric absorption, which is the effective interaction process at low energies, is strongly dependent on Z_{eq}^{4-5}. Contrary to others, the EABF and EBF values for 1.5 MeV photon energy are almost independent of the chemical composition (i.e. Z_{eq}) of the drugs as reported by Kavaz et al. [34]. This result can be clarified by the predominance of Compton scattering at 1.5 MeV energy. As can be seen from Figs. 5 and 6, the values of EABF and EBF of the drugs increase with increase in Z_{eq} at 15 MeV between 10 and 40 mfp and ifosfamide showed higher values than other drugs due to the dominance of pair production in this region. This result is agreeing with the findings reported by Kavaz et al. [42] who evaluated EABF and EBF factors of some radio protective agents.

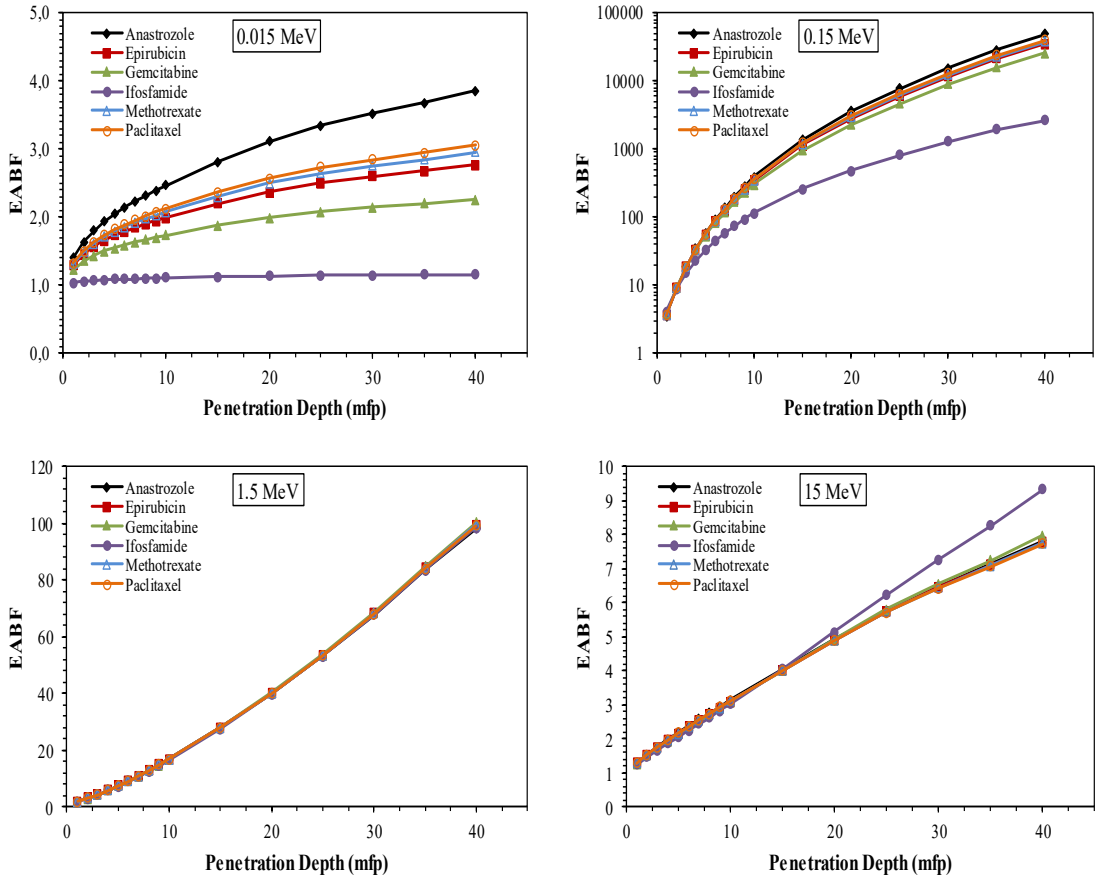

Figure 5: The energy absorption buildup factor for the drugs up to 40 mfp at 0.015, 0.15, 1.5 and 15 MeV

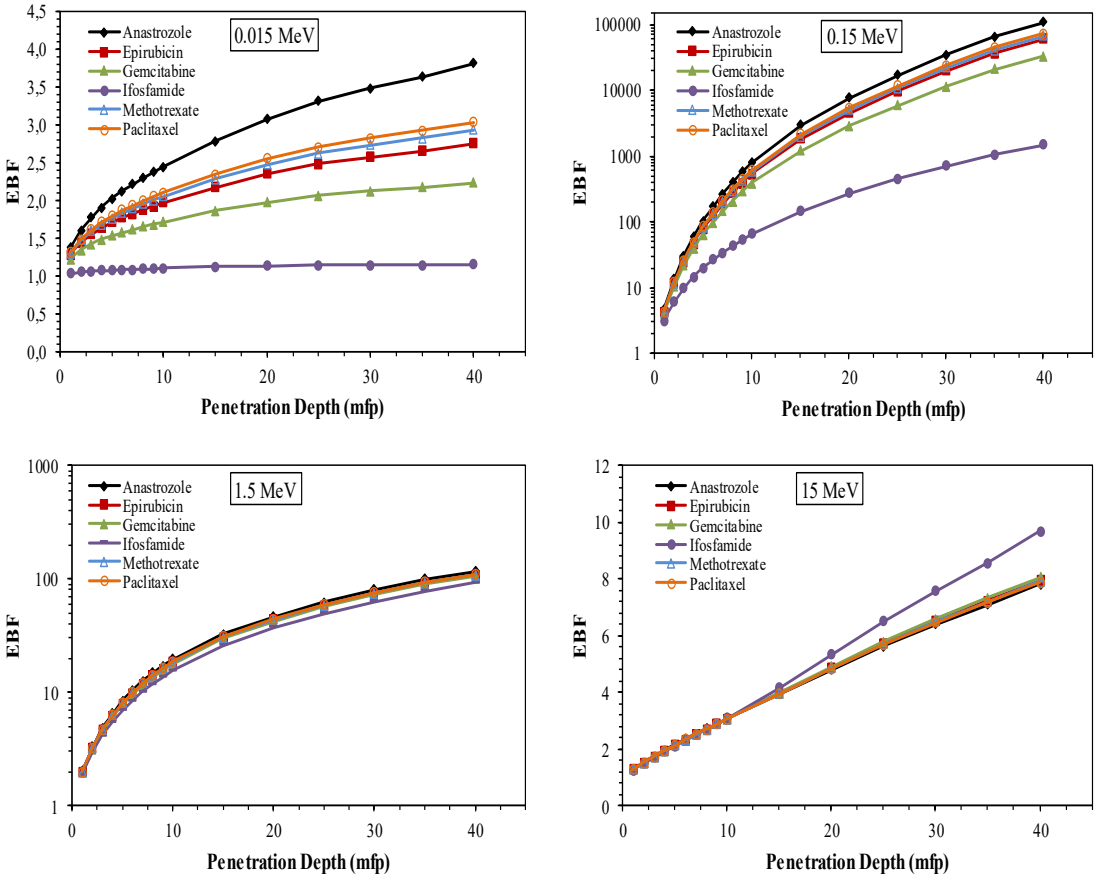

Figure 6: The energy exposure buildup factor for the drugs up to 40 mfp at 0,015, 0.15, 1.5 and 15 MeV

4. Conclusion

The present study was carried out to obtain information on photon interaction parameters of different antineoplastic chemotherapy drugs. The energy absorption buildup factors and exposure buildup factors of anastrozole ($C_{17}H_{19}N_5$), epirubicin ($C_{27}H_{26}NO_{11}$), gemcitabine ($C_9H_{11}F_2N_3O_4$), ifosfamide ($C_7H_{15}Cl_{12}N_2O_2P$), methotrexate ($C_{20}H_{22}N_8O_5$) and paclitaxel ($C_{47}H_{51}NO_{14}$) chemotherapy drugs were computed using GP fitting method. Also, Z_{eff} and N_{el} values were determined with the help of the WinXCOM program for photon energies from 1 keV to 100 GeV. The results obtained in this study showed that Z_{eff} and N_{el} values are dependent on the photon energy. The highest Z_{eff} values were found for ifosfamide and the lowest Z_{eff} values for anastrozole. This study also showed that buildup factors vary depending on the chemical composition (i.e. Z_{eq}) of the drugs, photon energy and mean free path. Among the studied samples, ifosfamide has the largest buildup factor values at 15 MeV photon energy, while it has the smallest values at 0.015, 0.15 and 1.5 MeV photon energies. It was concluded that ifosfamide has

better photon absorption properties since it contains phosphorus and chlorine in its chemical structure, unlike other drugs. It is predictable that the results of this work will be beneficial in areas such as radiation dosimetry and chemoradiotherapy.

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