Determination of Gamma Ray Buildup Factors of Some Enzyme Inhibitors

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Abstract— Gamma ray energy absorption and exposure buildup factors for Sulindac, Sodium valproate, Etoposide and Roscovitine were calculated using the five parameters (G-P) fitting method. In the calculation, the gamma ray energy absorption and exposure buildup factor values were evaluated in the energy range from 0.015 MeV to 15 MeV up to 40 mfp penetration depths. In has been onserved that the buildup factor values change with gamma ray energy values, mean free paths and chemical composition of enzyme inhibitors. As seen from results, Roscovitine has generally the biggest values of the absorption and exposure buildup factors.

Index Terms — Enzyme, inhibitor, gamma, mass and linear, coefficient, absorption

1 INTRODUCTION

Enzyme inhibitor is a molecule decreased an enzyme activity. Enzyme inhibitors used different areas in medicine. Sulindac is used to reducing the level of prostaglandins produced by the body and responsible for pain, fever, inflammation, intestinal polyps in familial adenomatous polyposis and to prevent colon cancer and precancerous lesions [1-3]. Sodium valproate is utilized in treatment of epilepsy, bipolar disorder [4]. Etoposide is utilized in different types of cancer such as lung cancer, testicular cancer, breast cancer, pediatric cancers, and lymphomas [5,6]. Roscovitine is used against lung and breast cancer, biological tool in cell cycle, neurodegenerative diseases, polycystic kidney disease, viral infections and glomerulonephritis,…[7,8].

Investigation of Gamma ray interaction parameters of materials is very important for different areas such as different areas of medicine, agriculture, nuclear physics, atom and molecular physics,… Also, information of the Gamma ray interaction parameters of materials are helps us to understand different futures of materials. The various theoretical and experimental studies related to the interaction parameters such as buildup factors, effective atomic numbers, effective electronic densities, absorption coefficients, mean free paths, half value layers are available in literature for different materials. Energy absorption (EABF) and exposure (EBF) buildup factors for human tissues with endometriosis were determined using geometric progression (G-P) parameters in the energy region 0.015–15

MeV up to a penetration depth of 40 mfp (mean free path) by Kurudirek et al. [9]. Singh et al. [10] computed the mass attenuation coefficients and exposure buildup factors (EBF) for Hollandite ($BaAl_2Ti_6O_{16}$), Perovskite ($CaTiO_3$), Zirconolite ($CaZrTi_2O_7$), Apatite ($Pb_{10}(VO_4)_{4.8}(PO_4)_{1.2}I_2$), and Zircon ($ZrSiO_4$). Oto et al.[11] measured the mass attenuation coefficients, effective atomic numbers (Z_{eff}) and electron densities (N_e) for various ores using the barite, magnetite, limonite, hematite and serpentine ores in the energy range from 81 keV to 778 keV and computed Gamma ray energy absorption buildup factors (EABF) and exposure buildup factors (EBF) in the energy range from 0.015MeV to 15 MeV for penetration depths up to 40 mean free paths. Ekinci et al. [12], Kurudirek [13] and Kavaz et al. [14,15], investigated the equivalent atomic numbers, energy absorption buildup factors and exposure buildup factors for some anti-inflammatory drugs, some dosimetric materials, radioprotective agents and some chemotherapy drugs in the energy range from 0.015 MeV to 15 MeV for penetration depths up to 40 mean free paths. Linear attenuation coefficients, mass attenuation coefficients, half-value layers, tenth-value layers, effective atomic number, electron density, energy absorption and exposure buildup factors for 304 L stainless steel samples, healthy breast tissue, carcinoma breast tissue, equivalent breast tissue, concrete types containing sepiolite mineral, some different ceramics, some selected ternary alloys, different medicinal aromatic plants and different polymers such as Polyamide (Nylon 6) (PA-6), polyacrylonitrile (PAN), polyvinylidenechloride (PVDC), polyaniline (PANI), polyethyleneterephthalate (PET), polyphenylenesulfide (PPS), polypyrrole (PPy), polytetrafluoroethylene (PTFE) were investigated by Büyükyıldız et al. [16}, Büyükyıldız and Kurudirek [17], Sayyed et al. [18,19], Akman et al. [20,21], Kaçal et al. [22].

Although Gamma ray energy absorption buildup factors (EABF) and exposure buildup factors (EBF) for various materials such as compounds, mixture, alloys, etc. are sufficient in the literature, these theoretical parameters are very limited for enzyme inhibitors. In this study, Gamma ray energy absorption buildup factors (EABF) and exposure buildup factors (EBF) were computed using the five-

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parameter geometric progression (G-P) fitting formula for Sulindac, Sodium valproate, Etoposide and Roscovitine in the energy range from 0.015 MeV to 15 MeV for penetration depths up to 40 mfp.

2 THEORETICAL CALCULATION

2.1 Calculation of the Equivalent Atomic Number

The equivalent atomic number (Z_{eq}) of a particular material was computed by matching the $(\mu/\rho)_{Compton}/(\mu/\rho)_{Total}$ of the particular material at a specific energy with the corresponding ratio of an element at the same energy. $(\mu/\rho)_{Compton}$ represents the Compton partial mass attenuation coefficients and $(\mu/\rho)_{Total}$ represents the total mass attenuation coefficients for the elements. The Compton partial mass attenuation coefficient and the total mass attenuation coefficients were obtained for the elements of Z=4-40 and for the chosen materials in the energy region of 0.015–15 MeV using the WinXCom computer program [23].

When the ratio $(\mu/\rho)_{Compton}/(\mu/\rho)_{Total}$ lies between two successive ratios of elements for a chosen material, the interpolation of the equivalent atomic number (Z_{eq}) of a chosen material is determined with the following equation.

$$Z_{eq} = \frac{Z_1(\log R_2 - \log R) + Z_2(\log R - \log R_1)}{\log R_2 - \log R_1} \qquad \text{(Eq-1)}$$

Z_1 and Z_2 represent the atomic numbers of the elements corresponding to the ratios R_1 and R_2, respectively. R represents the ratio for the chosen material at a specific energy.

2.2 Calculation of Geometric Progression Fitting Parameters

Geometric progression (G-P) fitting parameters for buildup factors were calculated by the process of logarithmic interpolation using Z_{eq} values of the enzyme inhibitors. The G-P fitting parameters for elements were taken from the ANSI/ANS-6.4.3 [24] standard reference database, which provides the G-P fitting parameters for elements from beryllium to iron in the energy region 0.015–15 MeV up to a depth of 40 mfp. The Geometrical progression (G-P) fitting parameters for the chosen material are determined with the following equation.

$$C = \frac{C_1(\log Z_2 - \log Z_{eq}) + C_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1} \qquad \text{(Eq-2)}$$

C_1 and C_2 represent the G-P fitting parameters corresponding to the atomic numbers Z_1 and Z_2, respectively, at a given energy. Z_{eq} represents the equivalent atomic number of a chosen material.

2.3 Calculation of Energy Absorption and Exposure Buildup Factors

To calculate the energy absorption and exposure buildup factors, geometric progression (G-P) fitting parameters were used the following formula;

$$B(E,x) = 1 + \frac{b-1}{K-1}(K^x - 1) \qquad \text{for K}\neq 1 \qquad \text{(Eq-3)}$$

$$B(E,x) = 1 + (b-1)x \qquad \text{for K=1} \qquad \text{(Eq-4)}$$

where,

$$K(E,x) = cx^a + d\,\frac{\tanh(x/X_k - 2) - \tanh(-2)}{1 - \tanh(-2)} \qquad \text{for } x \leq 40 \text{ mfp} \qquad \text{(Eq-5)}$$

where, E represents the incident photon energy; x represents the penetration depth in mfp; a, b, c, d and X_k represent the G-P fitting parameters and b represents the value of buildup factor at 1mfp.

3 RESULT AND DISCUSSION

Names and Chemical formula of the enzyme inhibitors are listed in **Table 1**. Also, equivalent atomic numbers of the sulindac ($C_{20}H_{17}FO_3S$), sodium valproate ($C_8H_{15}NaO_2$), etoposide ($C_{29}H_{32}O_{13}$) and roscovitine ($C_{19}H_{26}N_6O$) in the energy range from 0.015 MeV to 15 MeV are given in **Table 2**. **Table 3** provides the G-P energy absorption and exposure buildup factor coefficients for etoposide. The variations of energy absorption buildup factors (EABF) of enzyme inhibiytors with incident photon energy at 1, 5, 10, 20 and 40 mfp are presented in **Figure 1 (a-e)**. Also, exposure buildup factor (EBF) values of the enzyme inhibitors are plotted as a function of the energy at 1, 5, 10, 20 and 40 mfp in **Figure 3 (a-e)**. As seen from **Figure 1(a-e)** and **Figure 3 (a-e)**, it is clearly observed that the energy absorption buildup factors (EABF) and exposure buildup factor (EBF) for sulindac ($C_{20}H_{17}FO_3S$), sodium valproate ($C_8H_{15}NaO_2$), etoposide ($C_{29}H_{32}O_{13}$) and roscovitine ($C_{19}H_{26}N_6O$) change with changing in the studied energy region. As seen from **Figure 1 (a-e)** and **Figure 3 (a-e)**, the energy absorption buildup factors (EABF) and exposure buildup factor (EBF) for enzyme inhibitors display different characteristic futures at different energy regions. Also, the values of the energy absorption buildup factors (EABF) and exposure buildup factor (EBF) of the enzyme inhibitors are small in low and high energy regions. The photoelectric interaction is dominant in low energy region. Also, the proportions between photoelectric absorption and energy, and atomic number are $1/E^{3.5}$ and Z^{4-5}, respectively [25]. Energy absorption and exposure buildup factor values of sulindac are smaller than other enzyme inhibitors in low and intermediate energy regions. EABF and EBF values for sulindac ($C_{20}H_{17}FO_3S$), sodium valproate ($C_8H_{15}NaO_2$), etoposide ($C_{29}H_{32}O_{13}$) and roscovitine ($C_{19}H_{26}N_6O$) have taken maximum values in the intermediate region. EABF and EBF values at 10 mfp show peaks 0.1 MeV for sulindac ($C_{20}H_{17}FO_3S$), sodium valproate ($C_8H_{15}NaO_2$), etoposide ($C_{29}H_{32}O_{13}$) and 0.08 MeV for roscovitine ($C_{19}H_{26}N_6O$). Also, the buildup factor values reach the largest values for 40 mfp. The Compton scattering is dominant in intermediate energy region. The proportions between Compton scattering and energy, and atomic number are 1/E and Z, respectively. In the high energy region, EABF and EBF values decrease with increasing photon energy. In this region, pair production is dominant. The proportions between pair production and energy, and atomic number are E and Z^2, respectively. It can be seen clearly; roscovitine ($C_{19}H_{26}N_6O$) has the maximum EABF and EBF values in the intermediate energy region in all penetration depths. It is seen from **Figure 1 (a-e)** and **Figure 3 (a-e)** that the EABF and EBF buildup factor values are dependent on the chemical composition of the enzyme inhibitors.

TABLE 1
CHEMICAL FORMULA OF ENZYME INHIBITORS

Name	Chemical Formula
Sulindac	$C_{20}H_{17}FO_3S$
Sodium valproate	$C_8H_{15}NaO_2$
Etoposide	$C_{29}H_{32}O_{13}$
Roscovitine	$C_{19}H_{26}N_6O$

TABLE 2
EQUIVALENT ATOMIC NUMBERS OF THE ENZYME INHIBITORS FOR THE ENERGY RANGE 0.015–15 MeV

Energy (MeV)	Sulindac	Sodium valproate	Etoposide	Roscovitine
0.015	8.478	7.230	6.672	6.119
0.02	8.563	7.271	6.681	6.135
0.03	8.678	7.314	6.685	6.143
0.04	8.752	7.336	6.688	6.146
0.05	8.806	7.350	6.691	6.148
0.06	8.849	7.362	6.694	6.150
0.08	8.912	7.378	6.699	6.154
0.1	8.956	7.389	6.703	6.156
0.15	9.018	7.408	6.710	6.159
0.2	9.048	7.417	6.710	6.160
0.3	9.079	7.427	6.715	6.162
0.4	9.096	7.433	6.717	6.162
0.5	9.106	7.437	6.718	6.163
0.6	9.113	7.438	6.718	6.163
0.8	9.119	7.440	6.719	6.164
1	9.119	7.440	6.719	6.164
1.5	6.995	6.209	6.186	5.647
2	6.853	6.155	6.165	5.630
3	6.823	6.142	6.160	5.625
4	6.813	6.136	6.157	5.623
5	6.808	6.135	6.156	5.623
6	6.803	6.132	6.155	5.623
8	6.800	6.129	6.153	5.621
10	6.799	6.126	6.151	5.621
15	6.789	6.123	6.150	5.622

TABLE 3
G-P ENERGY ABSORPTION AND EXPOSURE BUILDUP FACTOR COEFFICIENTS FOR ETOPOSIDE IN THE ENERGY RANGE 0.015–15 MEV

Energy (MeV)	EABF					EBF				
	a	b	c	d	Xk	a	b	c	d	Xk
0.015	0.160	1.286	0.498	-0.078	14.523	0.163	1.281	0.495	-0.081	14.282
0.02	0.116	1.662	0.627	-0.057	15.371	0.115	1.644	0.630	-0.056	15.475
0.03	0.028	3.014	0.936	-0.024	15.011	0.029	2.887	0.935	-0.025	14.847
0.04	-0.073	4.305	1.409	0.028	13.889	-0.075	4.334	1.417	0.030	13.678
0.05	-0.127	5.099	1.758	0.054	14.112	-0.130	5.528	1.777	0.056	13.994

0.06	-0.161	5.225	2.026	0.072	14.028	-0.167	6.003	2.066	0.076	13.927
0.08	-0.191	4.898	2.300	0.083	13.823	-0.203	5.812	2.399	0.092	13.625
0.1	-0.190	4.561	2.332	0.079	14.592	-0.205	5.400	2.455	0.089	14.393
0.15	-0.193	3.687	2.352	0.077	14.561	-0.219	4.083	2.567	0.098	14.118
0.2	-0.184	3.312	2.242	0.076	14.791	-0.215	3.493	2.488	0.094	13.804
0.3	-0.170	2.829	2.076	0.067	14.412	-0.188	3.012	2.215	0.081	14.154
0.4	-0.151	2.622	1.905	0.061	14.379	-0.171	2.738	2.035	0.072	13.895
0.5	-0.138	2.460	1.789	0.057	14.636	-0.153	2.570	1.882	0.066	14.146
0.6	-0.123	2.373	1.675	0.049	14.437	-0.139	2.442	1.767	0.058	13.974
0.8	-0.106	2.201	1.549	0.044	14.171	-0.118	2.260	1.610	0.053	13.969
1	-0.088	2.102	1.437	0.037	14.582	-0.100	2.141	1.493	0.045	13.919
1.5	-0.060	1.939	1.275	0.026	14.308	-0.067	2.002	1.303	0.031	13.912
2	-0.038	1.842	1.169	0.015	14.428	-0.043	1.891	1.189	0.020	13.983
3	-0.011	1.714	1.051	0.003	14.176	-0.014	1.746	1.059	0.006	12.316
4	0.004	1.626	0.988	-0.003	13.071	0.004	1.649	0.987	-0.007	23.969
5	0.015	1.564	0.944	-0.008	14.793	0.017	1.573	0.939	-0.011	14.347
6	0.028	1.515	0.906	-0.018	13.143	0.027	1.524	0.907	-0.016	14.046
8	0.034	1.430	0.882	-0.017	12.099	0.037	1.437	0.871	-0.032	16.198
10	0.040	1.376	0.861	-0.022	14.322	0.041	1.371	0.858	-0.021	12.650
15	0.047	1.281	0.838	-0.033	15.764	0.046	1.275	0.841	-0.030	15.233

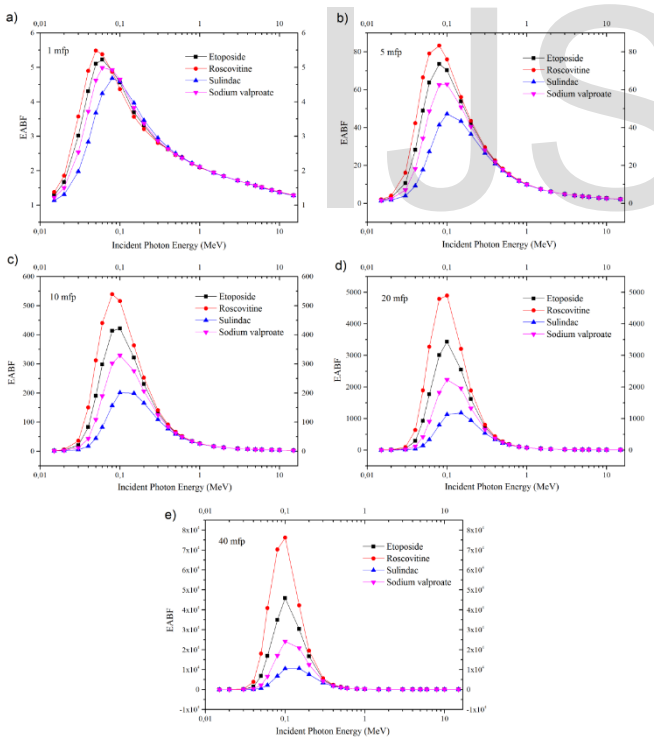

Figure 1. The energy absorption buildup factor for enzyme inhibitors in the energy region 0.015–15 MeV at 1, 5, 10, 20, 40 mfp.

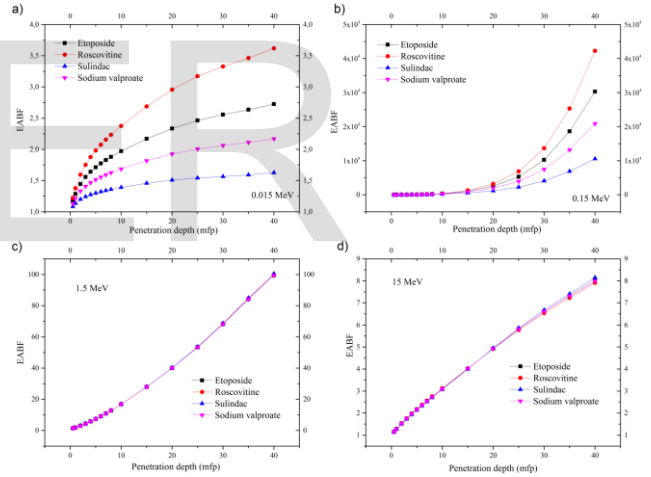

Figure 2. The energy absorption buildup factor for enzyme inhibitors up to 40 mfp at 0.015, 0.15, 1.5, 15 MeV.

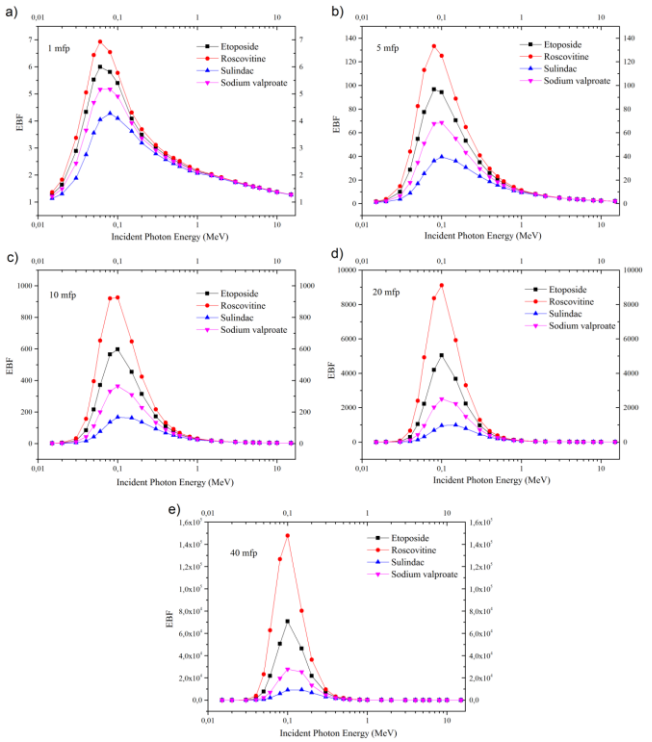

Figure 3. The exposure buildup factor for enzyme inhibitors in the energy region 0.015–15 MeV at 1, 5, 10, 20, 40 mfp.

The variations of energy absorption buildup factors (EABF) of enzyme inhibitors with penetration depth at different incident photon energy (0.015 MeV, 0.15 MeV, 1.5 MeV and 15 MeV) are listed in **Figure 2 (a-d)**. Also, exposure buildup factor (EBF) values of sulindac ($C_{20}H_{17}FO_3S$), sodium valproate ($C_8H_{15}NaO_2$), etoposide ($C_{29}H_{32}O_{13}$) and roscovitine ($C_{19}H_{26}N_6O$) are plotted as a function of the penetration depth at 0.015 MeV, 0.15 MeV, 1.5 MeV and 15 MeV incident photon energy in **Figure 4 (a-d)**. As seen from **Figure 2 (a-d)** and **Figure 4 (a-d)**, there is a significant variation of EABF and EBF for the enzyme inhibitors. EABF and EBF values for sulindac, sodium valproate, etoposide and roscovitine increase with increasing penetration depths. One of the main reasons for this situation could be that the number of scattering photons increases with increasing incident photon energy. The maximum values of EABF and EBF have been obtained at 40 mfp. Also, energy absorption buildup factors (EABF) and exposure buildup factor (EBF) values reach their largest values in the selected penetration range at 0.15 MeV.

The difference between EABF and EBF values for sulindac ($C_{20}H_{17}FO_3S$) and roscovitine ($C_{19}H_{26}N_6O$) for the incident photon energy from 0.015 MeV to 15 MeV are shown **Figure 5-6**. As seen from **Figure 5-6**, the maximum difference occurs in the intermediate energy region. The differences between EABF and EBF values is <18.3% for sulindac. The agreement between energy absorption buildup factors (EABF) and exposure buildup factor (EBF) values is <94.1% for roscovitine.

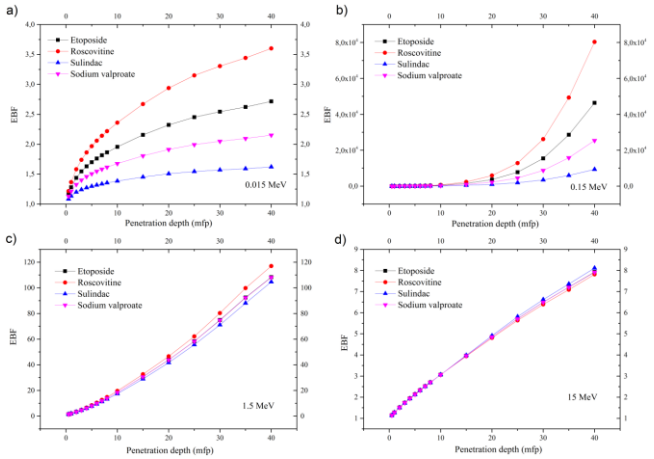

Figure 4. The exposure buildup factor for enzyme inhibitors up to 40 mfp at 0.015, 0.15, 1.5, 15 MeV.

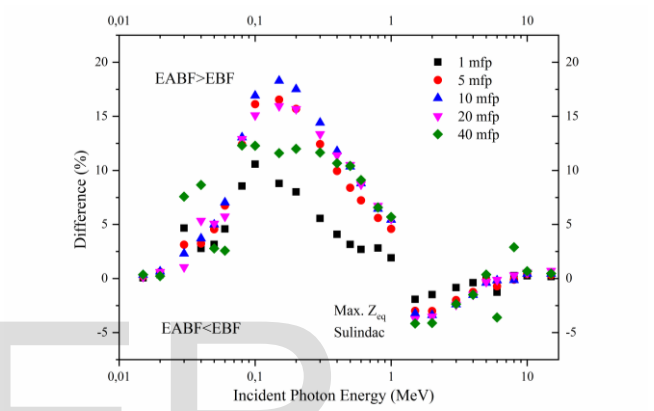

Figure 5. Difference (%) between EABF and EBF for Sulindac in the energy region 0.015–15 MeV up to 40 mfp.

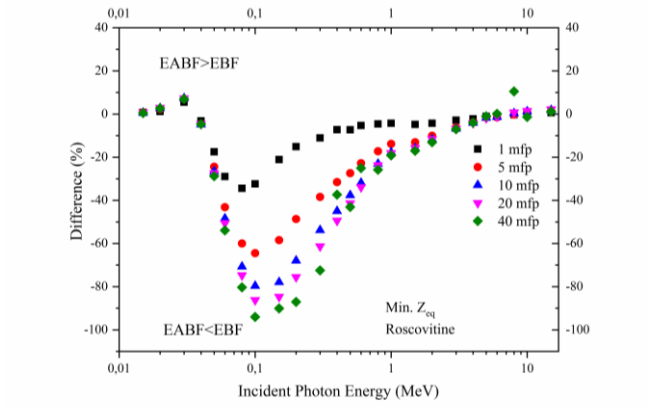

Figure 6. Difference (%) between EABF and EBF for Roscovitine in the energy region 0.015–15 MeV up to 40 mfp.

4 Conclusion

In this study, Gamma ray energy absorption buildup factors (EABF) and exposure buildup factors (EBF) were computed using the five-parameter geometric progression (G-P) fitting formula for sulindac ($C_{20}H_{17}FO_3S$), sodium valproate ($C_8H_{15}NaO_2$), etoposide ($C_{29}H_{32}O_{13}$) and roscovitine ($C_{19}H_{26}N_6O$) in the energy range from 0.015 MeV to 15 MeV for penetration depths up to 40 mfp. Significant differences in EABF and EBF have been

observed for enzyme inhibitors in the intermediate energy region. It is concluded that sulindac is good compound for gamma rays absorption applications among the selected compounds. The presented results in this study are expected to be helpful in radiation dosimetry.

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