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Case Report

Photon Absorption characteristics of some selected Enzyme Inhibitors used in Cancer Research in the Energy range 1 keV-100 GeV

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Abstract

The absorption parameters such as total mass attenuation coefficients, molecular, atomic, and electronic cross sections, effective atomic numbers and electron densities were calculated for some selected enzyme inhibitors in the photon energy range from 1 keV up to 100 GeV. The changes in the absorption parameters were interpreted with the photoelectric effect, Compton scattering and pair production processes. It is observed that the 2-Imino-1-imidazolidineacetic acid enzyme inhibitor has more radiation shielding feature when compared to other chosen enzyme inhibitors. The present investigation is anticipated to be useful for researchers studying with radiation in several fields and cancer researchers.

Introduction

Enzymes are generally proteins which catalyze chemical reactions and they play essential roles in life processes. Enzyme inhibitors decrease the ratio of an enzyme catalyzed reaction by interfering with the enzyme in some way and this effect may be persistent or transient. Enzyme inhibitors can be used as anti-tumour agents in cancer research. For example, aminoglutethimide restricts the enzyme steroid aromatase, which is related in the biosynthesis of estrogens. It is currently utilized as an effective agent for the treatment of advanced breast cancer in post menopausal women [1]. Camptothecin is an alkaloid that exhibits anti-leukemic and anti-tumour activities [2]. It is naturally obtained and it displays intense blue fluorescence under UV light. Mevinolin, which is a fungal metabolite isolated from fungus Aspergillus sp., is a strong anti-hypercholesterolemic agent. Mevinolin inhibits cell proliferation due to cell cycle arrest in a dose-dependent manner. Mevinolin diminishes the platelet aggregation, macrophage foam cell formation, and LDL oxidation and as a result of that it can significantly attenuate the atherosclerotic process [3].

The radiation are absorbed or scattered by material. The intensity of the radiation is attenuated in the process of the absorption and this process depends on the energy of the radiation and the density, atomic number, thickness and chemical structure of the absorber. The main events during the interaction of the photon with the material ate photoelectric absorption, Compton scattering and pair production. The total mass

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attenuation coefficient for photons of a given energy in a given matter comprises the individual contributions from the photoelectric absorption, Compton scattering and pair production processes. The total mass attenuation coefficient is a measure of probability of interactions of photons with material and it has the dimension cm^2g^{-1}. Since a series of consecutive absorption parameters are calculated from it, the total mass attenuation coefficient is an essential parameter. Using the total mass attenuation coefficient, the molecular, atomic and, electronic cross sections, effective atomic number and electron density parameters can be derived. The probability of interaction is proportional to the cross section. This description can be used for atomic, molecular and electronic cross sections. For example, the probability of interaction with molecule can be called as molecular cross section. An element is characterized by a single atomic number. But, the complex materials such as soil, plastic or biological material cannot be characterized by a single atomic number in a given energy range. The atomic number is represented by the effective atomic number in complex materials. The effective electron density is represented as the electron numbers in the unit mass. The effective atomic number and electron density change depending on photon energy. These parameters have physical significance and allow many characteristic of matter to be visualized with a number. The correct values of these parameters are important in applied science such as calculations of absorbed dose in radiotherapy, medical physics, nuclear industry, radiation physics and shielding. Many researcher and research groups have investigated the total mass attenuation coefficient, effective atomic number and electron density [4-20]. Sayyed et al. [4], calculated the effective atomic numbers and electron densities of six analgesic and anti-inflammatory drugs in the energy range 1 keV to 100 MeV. More et al. [5], determined the mass attenuation coefficients, total atomic cross sections, molar extinction coefficients, electronic cross sections, effective atomic numbers and electron densities for few nylons at 122, 356, 511, 662, 840, 1170, 1275 and 1330 keV energies. The mass attenuation coefficients, atomic and electronic cross sections, effective atomic numbers and electron densities for some enzymes, proteins, amino acids and fatty acids were measured at 122, 356, 511, 662, 1170, 1275 and 1330 keV photon energies by Gaikwad et al. [6]. Isikli and Oto [7], computed the mass attenuation coefficients, effective atomic numbers and electron densities for fourteen anti-oxidants in the energy range 1 keV- 100 GeV using the WinXCOM code. Akman et al. [8], measured the effective atomic numbers and electron densities of some selected lanthanide complexes at 13.92, 17.75, 20.78, 26.34 and 59.54 keV photon energies using a Si(Li) detector. The total mass attenuation coefficients, total molecular, atomic and electronic cross sections, effective atomic numbers and electron densities of selected narcotic drugs were calculated by Akman et al. [9], using the WinXCOM program in the energy range from 1 keV to 100 GeV. Kumar [10], calculated the effective atomic numbers and electron densities of nucleobases DNA in the energy range 1 keV-100 GeV using the WinXCOM. Akman et al. [11], investigated the chemical effect on the total mass attenuation coefficients, molecular, atomic, and electronic cross sections, effective atomic numbers and electron densities for some selected indium complexes at 59.54 keV. The effective atomic numbers and electrons densities of some selected Gd compounds were determined using the total mass attenuation coefficients in the energy range from 39.52 to 57.14 keV by Akman et al. [12]. The effective atomic numbers and electron densities from the measured values of mass attenuation coefficients for some selected samarium compounds near the K edge in the photon energy range from 36.847 up to 57.142 keV were determined by Akman et al. [13]. Kore and Pawar [14], determined the effective atomic numbers and electron densities from mass attenuation coefficients of some amino acids at 122, 356, 511, 622, 1170, 1275 and 1330 keV energies using a NaI(Tl) detector. Manjunatha [15], computed the total mass attenuation coefficients, effective atomic numbers and electron densities of some hormones in the wide energy range 1 keV-100 GeV using the WinXCOM. Manjunatha and Rudraswamy [16], calculated the effective atomic numbers and electrons densities of human organs and tissues in the energy region 1

keV to 100 GeV. Kaçal et al. [17], measured the mass attenuation coefficients of the some elements at 59.5 and 88.0 keV energies using the different three detectors. Manjunatha [18], measured the mass attenuation coefficients, effective atomic numbers, electron densities and electrical conductivities for $YBa_2Cu_3O_7$ in the energy range 0.084 MeV to 1.330 MeV. Seenappa et al. [19], determined the mass attenuation coefficients, linear attenuation coefficients, half value layers and tenth value layers for barium compounds at 32, 74 and 662 keV energies. Manjunatha [20], estimated the gamma attenuation parameters such as mass attenuation coefficient, effective atomic number and electron density of poly methyl methacrylate and Kapton polyimide in the energy ranging from 84 keV to 1330 keV.

In the present work, the total mass attenuation coefficients, molecular, atomic, and electronics cross sections, effective atomic numbers and electron densities of some selected enzyme inhibitors used in cancer research were computed in the photon energy range from 1 keV up to 100 GeV using the WinXCOM program [21]. This program gives the attenuation coefficients of any matter as the sum of the appropriately weighted contributions from the individual elements.

Theoretical calculation process

For a piece of homogeneous material of finite thickness x, the absorption of the monochromatic radiation can be described by the Lambert-Beer law. According to this law, the intensity of the incident photon will be exponentially decreased. The absorption of incident photon depends on the total mass attenuation coefficient μ/ρ, the density of the matter ρ and the thickness of the matter x.

$$I = I_o e^{-(\mu/\rho)x} \tag{1}$$

If this equation is rearranged for μ/ρ;

$$\frac{\mu}{\rho} = \frac{1}{x}\ln\left(\frac{I_O}{I}\right) \tag{2}$$

Where, I_0 and I are primary intensity and transmitted intensity respectively, x is the thickness of the absorber and ρ is the density of the absorber. The total mass attenuation coefficient is the sum of the photoelectric, Compton scattering and pair production cross sections. They are related with average energy of Compton electron per scattered photon, energy reemitted as fluorescent radiation and annihilation radiation, respectively. The total mass attenuation coefficient $(\mu/\rho)_{(M)}$ of a complex material M consisting of a mixture of several chemical elements, can be computed from the total mass attenuation coefficients of the n constituting elements.

$$\left(\frac{\mu}{\rho}\right)_M = \sum_{i=1}^{n} W_i \left(\frac{\mu}{\rho}\right)_i \tag{3}$$

Where, $(\mu/\rho)_i$ is the total mass attenuation coefficient of the ith pure element and W_i its mass fraction in the sample considered. This is called the mixture rule.

The determined values of total mass attenuation coefficients were used to obtain the molecular cross sections (cm^2 $molecule^{-1}$).

$$\sigma_{t,m} = \left(\frac{\mu}{\rho}\right)_{comp} \sum_i (n_i A_i) \tag{4}$$

where, $(\mu/\rho)_{comp}$ is total mass attenuation coefficient of the complex matter, N specifies the Avogadro number, n_i is the number of atom of the ith individual element

and A_i is the atomic weight of the ith constituent element in given complex matter. The simple relationship between the molecular cross section and the atomic cross section is as follows.

$$\sigma_{t,a} = \frac{\sigma_{t,m}}{\sum_i n_i} \tag{5}$$

The atomic cross section has the dimension cm^2 $atom^{-1}$. The electronic cross section can be computed using the following equation.

$$\sigma_{t,e} = \frac{1}{N}\sum_i \frac{f_i A_i}{Z_i}\left(\frac{\mu}{\rho}\right)_i \tag{6}$$

Where, f_i is the fractional abundance of it element in the complex matter and Z_i is the atomic number of ith element in given matter. The electronic cross section has the dimension cm^2 $electrons^{-1}$. The effective atomic number, which is dimensionless magnitude, is calculated from the ratio of the electronic cross section of the atomic cross section, namely.

$$Z_{eff} = \frac{\sigma_{t,a}}{\sigma_{t,e}} \tag{7}$$

With the help of the effective atomic number parameter, the effective electron density can be computed as follows.

$$N_E = \frac{Z_{eff}}{A_{tot}}\left(Nn_{tot}\right) \tag{8}$$

In the equation, A_{tot} is the total atomic weight or molecular weight of complex matter and n_{tot} is the total number of atoms in complex matter. It has the dimension electrons g^{-1}.

Results and Discussion

The chemical formulas and elements weight fraction of the investigated enzyme inhibitors are given in table 1. The total mass attenuation coefficients, molecular, atomic and electronic cross sections, effective atomic numbers and electron densities were obtained for some selected enzyme inhibitors. Firstly, the total mass attenuation coefficient values of selected enzyme inhibitors were obtained in the energy range 1 keV-100 GeV using the WinXCOM program. Later, using the total mass attenuation coefficient values, the molecular, atomic and electronic cross sections values were computed with the aid of the equations (4,5,6), respectively. Thereafter, the effective atomic number values were estimated with the help of the atomic and electronic cross

Table 1: Chemical formulas and elements weight fraction of the investigated enzyme inhibitors.

Enzyme Inhibitor	Chemical formula	Carbon	Hydrogen	Oxygen	Nitrogen
(-)-Deguelin	C23H22O6	0.7004	0.0562	0.2434	
(S)-(+)-Camptathecin	C20H16N2O4	0.6316	0.0424	0.2524	0.0737
2-Imino-1imidazolidineacetic acid	C5H9N3O2	0.4195	0.0634	0.2235	0.2935
2-Propylpentanoic acid	$(CH_3CH_2CH_2)_2CHCO_2H$	0.6663	0.1118	0.2219	
3-3'-Diindolymethane	C17H14N2	0.8290	0.0573		0.1137
7-Ethyl-10hydroxycamtothecin	C22H20N2O5	0.6734	0.0514	0.2039	0.0714
DL-Aminoglutethimide	C13H16N2O2	0.6722	0.0694	0.1378	0.1206
Mevinolin from Aspergillus sp.	C24H36O5	0.7126	0.0897	0.1977	

section values using the equation (7). Finally, the effective electron density values were determined from the effective atomic number values utilizing the equation (8).

The theoretical values of the total mass attenuation coefficients, molecular, atomic, and electronic cross sections, effective atomic numbers and electron densities of the Deguelin enzyme inhibitor are given in table 2. The values of total mass attenuation coefficient, molecular, atomic, and electronic cross sections are shown graphically in figures 1-4. It is clearly seen from table 2 and figures 1-4 that the total mass attenuation coefficients, molecular, atomic, and electronic cross sections depend on the energy and chemical structure of enzyme inhibitor and these parameters decrease with increasing energy. Also, these parameters decrease with increasing element number in the enzyme inhibitors.

Table 2: The selected values of μ/ρ ($cm^2 g^{-1}$), $\sigma_{t,m}$ (cm^2 molecule^{-1}), $\sigma_{t,a}$ (cm^2 atom^{-1}), $\sigma_{t,e}$ (cm^2 electrons^{-1}), Z_{eff} and N_E (electrons g^{-1}) for Deguelin enzyme inhibitor.

Energy (MeV)	μ/ρ	σt,m(x10^{-22})	σt,a(x10^{-22})	σt,e(x10^{-22})	Zeff	NE(x1023)
0.001	2665.850	17459.811	3423.492	5112.446	6.696	70.875
0.002	867.637	5682.534	1114.222	1656.637	6.726	71.187
0.002	381.117	2496.100	489.431	725.850	6.743	71.367
0.003	116.125	760.554	149.128	220.617	6.760	71.544
0.004	49.159	321.962	63.130	93.360	6.762	71.570
0.005	25.071	164.204	32.197	47.675	6.753	71.478
0.006	14.430	94.508	18.531	27.522	6.733	71.266
0.008	6.058	39.675	7.779	11.686	6.657	70.455
0.010	3.133	20.516	4.023	6.161	6.529	69.105
0.015	1.033	6.769	1.327	2.199	6.034	63.868
0.020	0.541	3.543	0.695	1.267	5.481	58.012
0.030	0.291	1.909	0.374	0.789	4.741	50.184
0.040	0.228	1.492	0.293	0.662	4.419	46.774
0.050	0.202	1.322	0.259	0.606	4.276	45.261
0.060	0.188	1.228	0.241	0.573	4.205	44.509
5.000	0.029	0.187	0.037	0.088	4.173	44.171
6.000	0.026	0.171	0.033	0.079	4.207	44.532
7.000	0.024	0.158	0.031	0.073	4.242	44.896
8.000	0.023	0.149	0.029	0.068	4.276	45.257
9.000	0.022	0.141	0.028	0.064	4.310	45.614
10.000	0.021	0.135	0.027	0.061	4.343	45.962
11.000	0.020	0.130	0.026	0.058	4.374	46.298
12.000	0.019	0.126	0.025	0.056	4.405	46.624
13.000	0.019	0.123	0.024	0.054	4.435	46.936
14.000	0.018	0.120	0.023	0.053	4.463	47.242
15.000	0.018	0.117	0.023	0.051	4.491	47.533
16.000	0.018	0.115	0.023	0.050	4.517	47.812
18.000	0.017	0.111	0.022	0.048	4.567	48.338
20.000	0.017	0.108	0.021	0.046	4.613	48.826
22.000	0.016	0.106	0.021	0.045	4.656	49.279
2000.000	0.018	0.119	0.023	0.043	5.399	57.148
3000.000	0.018	0.120	0.024	0.044	5.399	57.140
4000.000	0.018	0.121	0.024	0.044	5.397	57.126
5000.000	0.018	0.121	0.024	0.044	5.397	57.118
6000.000	0.019	0.121	0.024	0.044	5.396	57.110
8000.000	0.019	0.122	0.024	0.044	5.395	57.102
10000.000	0.019	0.122	0.024	0.044	5.394	57.094
15000.000	0.019	0.122	0.024	0.044	5.394	57.086
20000.000	0.019	0.122	0.024	0.044	5.393	57.083
30000.000	0.019	0.123	0.024	0.045	5.393	57.077
40000.000	0.019	0.123	0.024	0.045	5.392	57.071
50000.000	0.019	0.123	0.024	0.045	5.392	57.070
60000.000	0.019	0.123	0.024	0.045	5.392	57.066
80000.000	0.019	0.123	0.024	0.045	5.392	57.065
100000.000	0.019	0.123	0.024	0.045	5.391	57.063

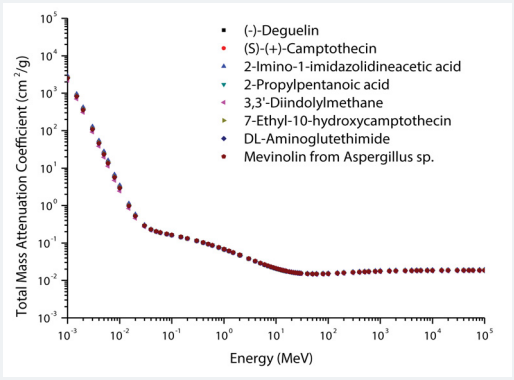

Figure 1: Total mass attenuation coefficients of selected enzyme inhibitors versus photon energy.

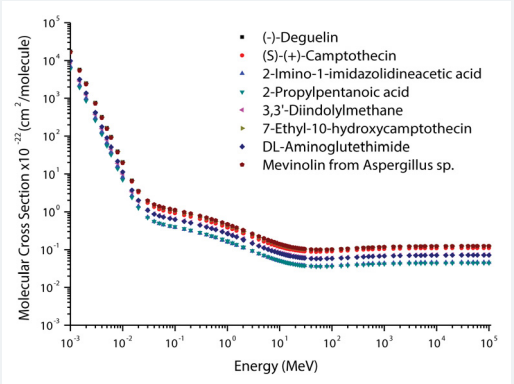

Figure 2: Molecular cross sections of selected enzyme inhibitors versus photon energy.

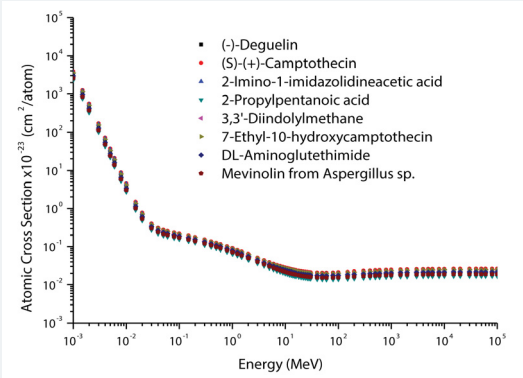

Figure 3: Atomic cross sections of selected enzyme inhibitors versus photon energy.

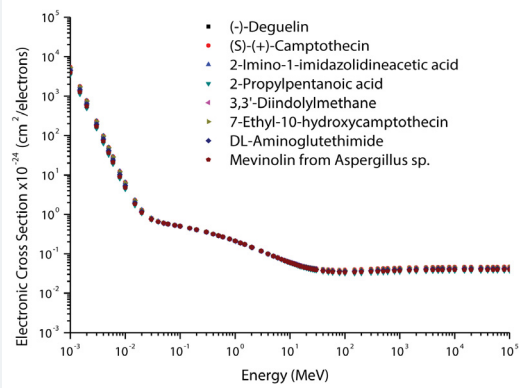

Figure 4: Electronic cross sections of selected enzyme inhibitors versus photon energy.

The variations of effective atomic numbers and electron densities for selected enzyme inhibitors are plotted as a function of photon energy in figures 5-6. As seen from these figures, the effective electron density shows similar behaviour to effective atomic number. It is clearly seen from figures 5-6 that the effective atomic number and electron density values are demonstrated characteristic features with respect to photon energy. According to the figures 5-6, the effective atomic numbers and electron densities decrease almost exponentially with increasing energy at low energy region. The reason for this, the photoelectric interaction dominates in this region. In general, the photoelectric effect varies with atomic number as Z^4 for low energy region and Z^5 for high energy region. Also, this effect changes inversely proportional with energy as $E^{3.5}$. In the medium-energy region, the effective atomic numbers and electron densities take their smallest values due to Compton scattering and these values are almost constant in this region. The reason of this that Compton scattering varies with atomic number as Z, and inversely proportional with energy as E. In the high energy region, the effective atomic numbers and electron densities increase again as a function of the photon energy. The pair production interaction dominates in this region. The pair production changes with atomic number as Z^2 and proportional with energy as E.

The variation of effective atomic numbers as a function of effective electron densities is given in figure 7. According to the figure 7, it is possible to say that the effective atomic number increases linearly with increasing effective electron density.

Conclusion

We studied the changes of the total mass attenuation coefficients, molecular, atomic, and electronic cross sections, effective atomic numbers and electron densities

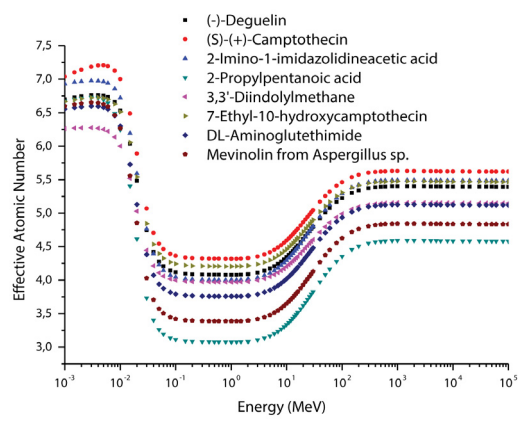

Figure 5: Effective atomic numbers of selected enzyme inhibitors versus photon energy.

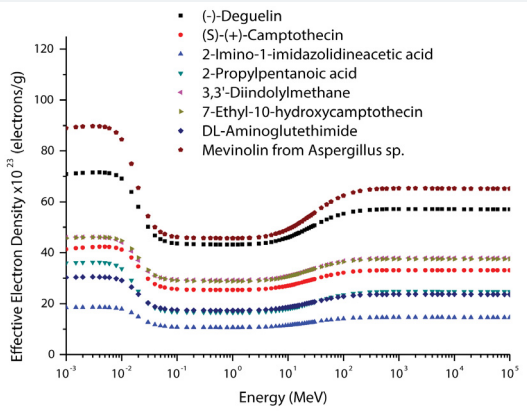

Figure 6: Effective electron densities of selected enzyme inhibitors versus photon energy.

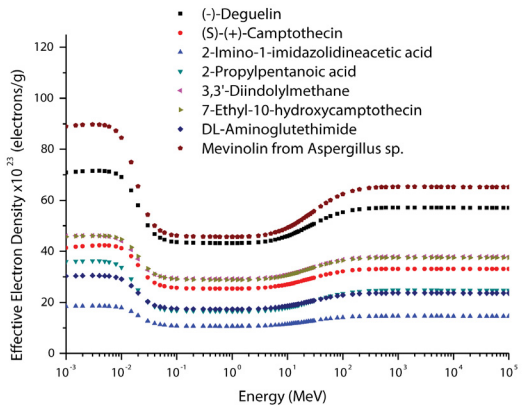

Figure 7: Effective electron densities versus effective atomic numbers of selected enzyme inhibitors.

with photon energy of some selected enzyme inhibitors. The total mass attenuation coefficients, molecular, atomic, and electronic cross sections, effective atomic numbers and electron densities depend on the photon energy, number of elements within enzyme inhibitors and chemical structure of enzyme inhibitors. The variations in the absorption parameters were interpreted with the photoelectric effect, Compton scattering and pair production processes. It can be concluded the present work that the 2-Imino-1-imidazolidineacetic acid enzyme inhibitor has more radiation shielding feature when compared to other chosen enzyme inhibitors. Study of these parameters is clear and reasonable way for evaluating extensive importance in applied areas such as cancer research, calculations of absorbed dose in radiotherapy and radiation shielding. The present investigation is anticipated to be useful for researchers studying with radiation in several fields and cancer researchers.

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