

# Effective Atomic Number, Electron Density and CT Numbers of Skeletal Muscle Relaxants for Imaging

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**Abstract-** The Effective atomic numbers  $Z_{\text{eff}}$ , Electron density  $N_e$  and CT numbers of skeletal muscle relaxants tubocurarine chloride, gallamine triethiodide, pancuronium bromide, suxamethonium bromide and mephenesin for total and coherent, incoherent, photoelectric absorption, pair production in atomic and nuclear field photon interaction have been calculated in the wide region 1keV to 100GeV. The molecular, atomic, electronic cross sections are calculated using mass attenuation coefficient of relaxants obtained by running WinXCOM programme and finally  $Z_{\text{eff}}$ ,  $N_e$  and CT number of the relaxants have been estimated. The  $Z_{\text{eff}}$ , and  $N_e$  have found to vary with energy and composition of the relaxants and this variation is shown graphically for all photon interaction. Even CT numbers are also not remaining constant with energy. The significance of CT number in visualizing the image of the biological samples is discussed particularly in the low energy region as this region is extensively used in the medical radiology. This helps in cross-sectional image of internal organs in the field of medicine for diagnosing the diseases. The CT number is not only outlining the inhomogeneities of the tissues but also give the direct information of the tissue electron density from which accurate corrections can be made by suitable treatments.

**Keywords;** Effective atomic number, Electron density, CT number, relaxants

## I. INTRODUCTION:

Cross-sectional image of internal organs is prime importance in the field of medicine for diagnosing the diseases. Computed tomography (CT) measures the accurate radiographic density of the small parts of the body which helps in visualizing the image. The CT number is not only outlining the inhomogeneities of the tissues but also give the direct information of the tissue electron density from which accurate corrections can be made by suitable treatments. Even dose calculations are made based on the patient specific information obtained from X-ray computed tomography.

In the present study skeletal muscle relaxants tubocurarine chloride, gallamine triethiodide, pancuronium bromide, suxamethonium bromide and mephenesin have chosen and its composition is given in the table 1 These agents are used as adjuvant to anesthesia to get the relaxation of skeletal muscle during the corrections of dislocations, surgery, radiotherapy etc... and used as relieving painful muscle spasms because of various musculoskeletal and neuromuscular disorders. Hence accurate calculation of photon mass attenuation co-efficient, effective atomic

number  $Z_{\text{eff}}$ , electron density  $N_e$  and CT numbers of above relaxants are important in medical diagnostics. Especially calculation of CT numbers of relaxants is become prime important as it provide the necessary information about relative electron density of relaxants. The contribution of these values will find the application in planning and treatment of the patient in radiotherapy. Hence the above parameters become vital, interesting and exciting field of research for characterization and visualization of matter (biological samples) in medical field.

**Table-1 Composition of skeletal muscle relaxants**

Skeletal muscle relaxants	Composition
Gallamine triethiodide	H:0.067834 C:0.404167 N:0.047132 O:0.053838 I:0.427030
Mephenesin	H: 0.077441 C: 0.659151 O:0.26340
Pancuronium bromide	H:0.082541 C:0.573763 N:0.038234 O:0.087347 Br:

	0.218114
Suxamethonium chloride	H: 0.086249 C: 0.423200 N: 0.070503 O: 0.241598 Cl: 0.178451
Tubocurarine chloride	H:0.067916 C: 0.575857 N: 0.036299 O: 0.228050 Cl: 0.091878

**II. THEORY AND METHODOLOGY:**

When electromagnetic radiation passes through matter, their intensity is attenuated according to the exponential law. If a beam of these radiations having an intensity  $I_0$  passes through a thickness  $x$  of an absorber, the transmitted intensity  $I$  is given as

$$I = I_0 \exp\left(-\frac{\mu}{\rho}x\right)$$

where  $\rho$  is the density of the material.

$(\mu/\rho)$  is the mass attenuation coefficient & is independent of density of the absorber.

When a beam of photons passes through an absorber, the photons interact with the atoms and are either absorbed (photoelectric effect, pair and triplet production, photo nuclear) or scattered away from the beam (Coherent and incoherent scattering). The intensity of the transmitted beam of photons is the sum of the cross-sections, per atom for all the above processes. Hence the total molecular cross section  $\sigma_{mol}$  is determined from the following equation using the values of mass attenuation coefficient of relaxants using  $(\mu/\rho)_{bio}$  obtained by running WinXCOM programme.

$$\sigma_{mol} = \left(\frac{1}{N}\right)\left(\frac{\mu}{\rho}\right)_{bio} \sum_i n_i A_i$$

Where  $N$  is Avogadro number,  $n_i$  is the number of atoms of  $i^{th}$  element and  $A_i$  is its atomic weight in a given molecule.

The effective atomic cross section  $\sigma_{atm}$  are determined by

$$\sigma_{atm} = \frac{\left(\frac{\mu}{\rho}\right)_{bio}}{N \sum_i W_i A_i}$$

$$\sigma_{atm} = \frac{1}{N} \sum_i f_i A_i \left(\frac{\mu}{\rho}\right)_i$$

Where  $f_i$  is the fractional abundance  $(\mu/\rho)_i$  is mass attenuation co-efficient of  $i^{th}$  element.

$$\sigma_{atm} = \frac{\sigma_{mol}}{\sum_i n_i}$$

The effective electronic cross section  $\sigma_{ele}$  are determined by

$$\sigma_{ele} = \left(\frac{1}{N}\right) \sum_i \left\{ \left(\frac{f_i A_i}{Z_i}\right) \left(\frac{\mu}{\rho}\right)_i \right\}$$

Where, and  $Z_i$  is the atomic number of  $i^{th}$  element in a molecule respectively.

Then effective atomic number is calculated using

$$Z_{eff} = \frac{\sigma_{atm}}{\sigma_{eie}}$$

The effective electron density is obtained from

$$N_e = \frac{N}{\sum_i n_i A_i} Z_{eff} \sum_i n_i$$

The CT number is estimated from

$$CT = \frac{(\mu_m - \mu_w)}{\mu_w}$$

**III. RESULTS AND DISCUSSIONS:**

The  $Z_{eff}$  and  $N_e$  and CT numbers of skeletal muscle relaxants tubocurarine chloride, gallamine triethiodide, pancuronium bromide, suxamethonium bromide and mephenesin are determined in the energy region 1keV-100GeV. It is found that  $Z_{eff}$  and  $N_e$  of relaxants vary with energy and composition of them. This variation is shown in the figures1-12 for total and all partial photon interaction (Coherent, Incoherent, Photoelectric absorption, pair production in atomic and nuclear field).

**Total photon interaction:**

The variation of  $Z_{eff}$  with photon energy for total photon interactions is as shown in the figure 1 and this variation is because of dominance of different photon interactions with skeletal muscle relaxants. In lower energy region, photo electric interaction dominates, hence  $Z_{eff}$  varies similar to photo interaction. Except mephenesin, all other relaxants  $Z_{eff}$  increases and becomes maximum and decreases sharply in the energy region 0.002-025MeV. This variation are due to presence of halogens (Cl, Br and I) in their composition and these elemental cross sections varies larger in the energy region 0.002-025MeV. The  $Z_{eff}$  and found to remain constant up to 10MeV which shows that scattering (coherent and Incoherent) processes increases. From 10MeV to100MeV, there is regular increase in the  $Z_{eff}$  with photon energy. This is due to the increase in incoherent and pair production processes. From 100MeV onwards  $Z_{eff}$  remains constant which is due to dominance in pair production processes. The  $Z_{eff}$  values of relaxants vary from the element with lowest  $Z$  to the highest  $Z$  present in their composition.

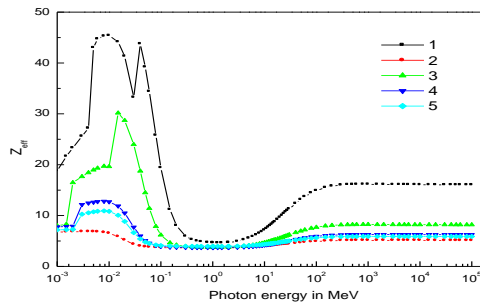


Fig: 1 Variation of  $Z_{eff}$  with Photon energy  $E$  in MeV for total photon interaction (with coherent)  
 (1)Gallamine triiodide (2) Mephnesin  
 (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

The variation of  $N_e$  with photon energy of all relaxants for total photon interaction processes is similar to that of  $Z_{eff}$  and is as shown in the figure 2

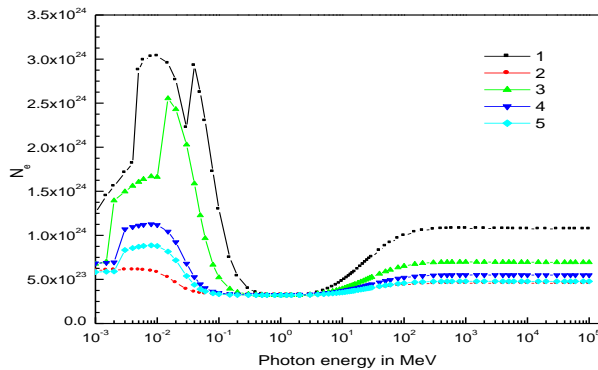


Fig: 2 Variation of  $N_e$  with Photon energy  $E$  in MeV for total photon interaction (with coherent)  
 (1)Gallamine triiodide (2) Mephnesin  
 (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

**Photo electric absorption:**

The variation of  $Z_{eff}$  with photon energy for photo electric absorption interaction is as shown in the figure 3 and this indicates that  $Z_{eff}$  increases up to 0.040MeV for all relaxants except for mephnesin which is independent of photon energy. In case of Gallamine triiodide there is sudden increase in  $Z_{eff}$  at 0.033169MeV which is the K absorption edge of iodine and it remains constant with photon energy. In Pancuronium bromide sudden increase in  $Z_{eff}$  is found at 0.01347MeV which is the K absorption edge of bromine and it remains constant with photon energy. The  $Z_{eff}$  of Suxamethonium chloride and Tubocurarine chloride increases at 0.002822MeV because chlorine (K absorption edge of Cl is 2.8224keV).Thereafter it becomes constant

with increase in photon energy. This is due to the dominance in photoelectric processes in low energy region i.e. less than 1MeV and for the substances of higher atomic number ( $Z$ ) than for low  $Z$  substances.

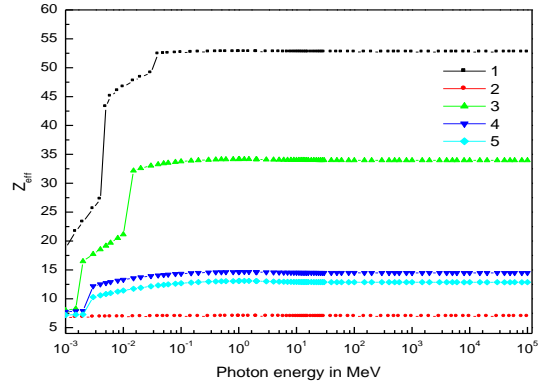


Fig: 3 Variation of  $Z_{eff}$  with Photon energy  $E$  in MeV for photoelectric absorption  
 (1)Gallamine triiodide (2) Mephnesin  
 (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

The variation of  $N_e$  with photon energy of all relaxants for photoelectric absorption processes is similar to that of  $Z_{eff}$  and is as shown in the figure 4

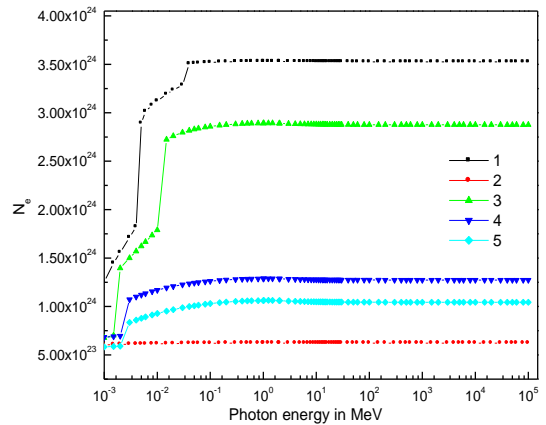


Fig: 4 Variation of  $N_e$  with Photon energy  $E$  in MeV for photoelectric absorption  
 (1)Gallamine triiodide (2) Mephnesin  
 (3) Pancuronium bromide(4) Suxamethonium chloride (5) Tubocurarine chloride

**Incoherent scattering:**

The variation of  $Z_{eff}$  with photon energy for incoherent scattering is as shown in the figure 5 and it indicates that  $Z_{eff}$  increases from 0.001MeV to 0.10MeV shows that it depends on energy. This variation is because of the proportion and the range of atomic numbers of the elements present in

relaxants. Above 0.10MeV  $Z_{eff}$  remains constant and independent of energy for all relaxants.

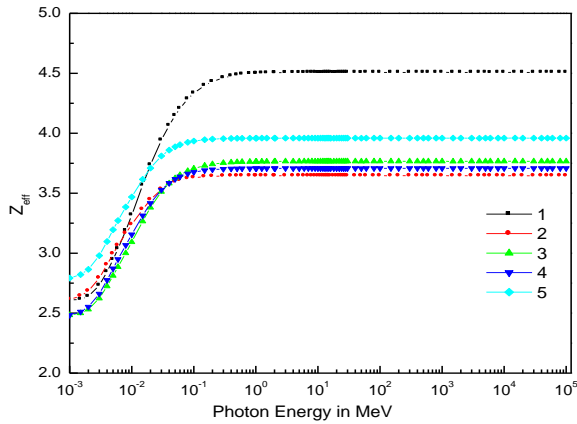


Fig: 5 Variation of  $Z_{eff}$  with Photon energy  $E$  in MeV for incoherent scattering  
(1) Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromide

(4) Suxamethonium chloride (5) Tubocurarine chloride

The variation of  $N_e$  with photon energy of all relaxants for incoherent scattering processes is similar to that of  $Z_{eff}$  and is as shown in the figure 6

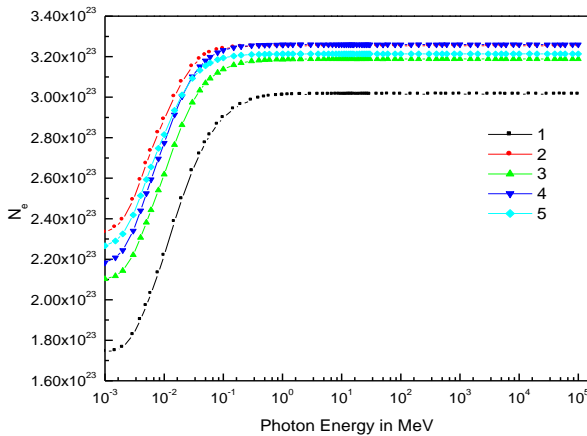


Fig: 6 Variation of  $N_e$  with Photon energy  $E$  in MeV for incoherent scattering

(1) Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromide  
(4) Suxamethonium chloride (5) Tubocurarine chloride

**Coherent scattering:**

The variation of  $Z_{eff}$  with photon energy for coherent scattering is as shown in the figure 7 and it indicates that  $Z_{eff}$  increases for mephenesin up to 0.03MeV and remains constant. All other relaxants shows increment in  $Z_{eff}$  from

0.001MeV to 0.40MeV. Thereafter remains constant i.e. independent of energy. The values of  $Z_{eff}$  for gallamine triethiodide, pancuronium bromide, suxamethonium chloride and tubocurarine chloride have comparatively higher. This is due to the presence of halogens. (42.70% of I in gallamine triethiodide, 21.81% of Br in pancuronium bromide 17.84% of Cl in suxamethonium chloride and 09.87% of Cl in tubocurarine chloride)

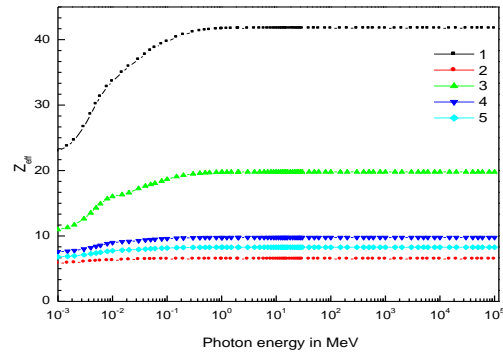


Fig:7 Variation of  $Z_{eff}$  with Photon energy  $E$  in MeV for coherent

(1) Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

The variation of  $N_e$  with photon energy of all relaxants for incoherent scattering process is similar to that of  $Z_{eff}$  and is as shown in the figure 8

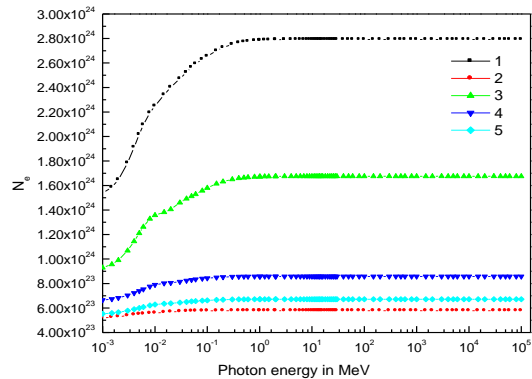


Fig: 8 Variation of  $N_e$  with Photon energy  $E$  in MeV for coherent scattering

(1) Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

**Pair production in electric field:**

The variation of  $Z_{eff}$  with photon energy for Pair production in electric field is as shown in the figure 9. It shows that  $Z_{eff}$  is constant with increase in photon energy from 3MeV to 30MeV i.e. independent of energy. It slightly decreases from

30MeV to 1000MeV and thereafter remains constant for all relaxants. Here also, in case of gallamine triethiodide and pancuronium bromide,  $Z_{eff}$  values are slightly more compared to the other relaxants. This is due to the large range of atomic number of constituent elements in them.

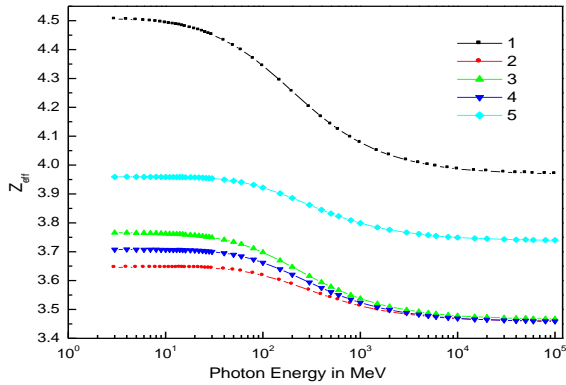


Fig: 9 Variation of  $Z_{eff}$  with Photon energy  $E$  in MeV for pair-production in electricfield  
 (1) Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

The variation of  $N_e$  with photon energy of all relaxants for Pair production in electric field is similar to that of  $Z_{eff}$  and is as shown in the figure 10

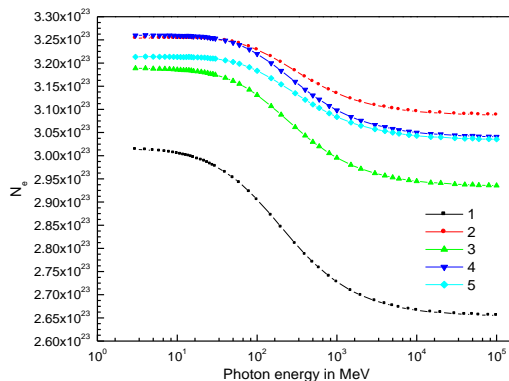


Fig: 10 Variation of  $N_e$  with Photon energy  $E$  in MeV for pair-production in electric fiel  
 (1) Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

**Pair production in nuclear field:**

The variation of  $Z_{eff}$  with photon energy for Pair production in nuclear field is as shown in the figure 11 and it shows that

$Z_{eff}$  slightly decreases with increase in photon energy from 1.25MeV onwards and found to remain constant thereafter. This is because of the fact that pair production in nuclear field is  $Z^2$  dependent. In case gallamine triethiodide and pancuronium bromide the variation of  $Z_{eff}$  values is more compared to the other relaxants This is due to the large range of atomic number of constituent elements in them.

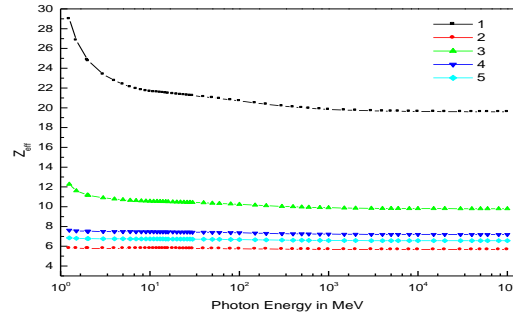


Fig: 11 Variation of  $Z_{eff}$  with Photon energy  $E$  in MeV for pair-production in nuclear field  
 (1)Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromide (4) Suxamethonium chloride (5) Tubocurarine chloride

The variation of  $N_e$  with photon energy of all relaxants for Pair production in nuclear field is similar to that of  $Z_{eff}$  and is as shown in the figure 12

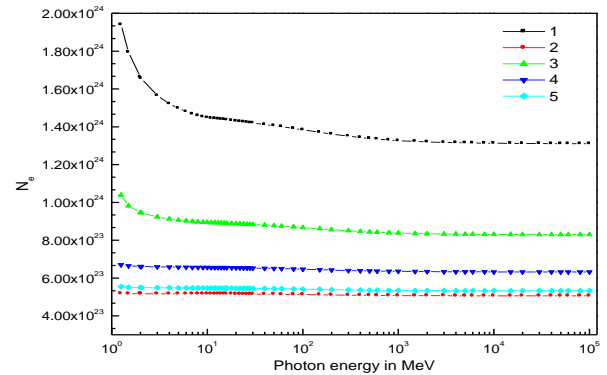


Fig: 12 Variation of  $N_e$  with Photon energy  $E$  in MeV for pair-production in nuclear field  
 (1)Gallamine triethiodide (2) Mephenesin (3) Pancuronium bromie (4) Suxamethonium chloride (5) Tubocurarine chloride

Usually above relaxants may be administered to the patient before treatment. Hence while treating tissue inhomogeneity of the patient, the contribution of CT numbers of relaxants has to be considered, though the values are very small. The CT numbers for total photon interaction is given in the table 2. The CT numbers for coherent, incoherent, and photoelectric absorption region and total photon interaction

helps in visualizing the image of the biological samples and precise accuracy in treating the inhomogeneity of them in medical radiology.

**Table 2. CT numbers of skeletal muscle relaxants**

Energy in MeV	CT Numbers for Total photon interaction				
	1	2	3	4	5
1.00E-03	0.27	-0.35	-0.42	-0.32	-0.34
2.00E-03	0.68	-0.38	0.61	-0.34	-0.37
5.00E-03	7.73	-0.41	1.03	1.15	0.38
1.00E-02	12.31	-0.41	1.40	1.43	0.53
2.00E-02	12.76	-0.32	13.66	1.29	0.49
1.00E-01	4.42	-0.04	0.64	0.02	-0.02
2.00E-01	0.72	-0.03	0.07	-0.02	-0.04
5.00E-01	0.00	-0.03	-0.04	-0.03	-0.04
1.00E+00	-0.07	-0.03	-0.05	-0.03	-0.04
2.00E+00	-0.07	-0.03	-0.04	-0.03	-0.04
5.00E+00	0.07	-0.04	0.00	-0.02	-0.04
1.00E+01	0.32	-0.06	0.07	0.00	-0.04
2.00E+01	0.66	-0.08	0.17	0.02	-0.04
5.00E+01	1.06	-0.10	0.28	0.05	-0.03
1.00E+02	1.23	-0.12	0.33	0.06	-0.03
2.00E+02	1.30	-0.12	0.35	0.06	-0.03
5.00E+02	1.32	-0.12	0.35	0.06	-0.03
1.00E+03	1.32	-0.12	0.35	0.06	-0.03
2.00E+03	1.32	-0.12	0.35	0.06	-0.03
5.00E+03	1.31	-0.12	0.35	0.06	-0.03
2.00E+04	1.31	-0.12	0.35	0.06	-0.03
4.00E+04	1.31	-0.12	0.35	0.06	-0.03
8.00E+04	1.31	-0.12	0.35	0.06	-0.03
1.00E+05	1.31	-0.12	0.35	0.06	-0.03

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