Photon attenuation parameters of non-essential amino acids using EPICS2017 library interpolations

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Abstract

Mass attenuation coefficients, effective atomic numbers, electron densities and energy absorption and exposure buildup factors for the non-essential and conditionally non-essential amino acids including alanine, arginine, asparagine, aspartic acid, cysteine, glutamic acid, glutamine, glycine, proline, serine, and tyrosine have been acquired using the latest evaluated photoatomic library of EPICS2017. The library was used by constructing an interpolation script that calculates for all photon attenuation parameters. Comparisons were made using alternative Monte Carlo simulation results for 15 energy points from 59.5 to 1333 keV, and in contrast with experimental works in literature. Good agreements for the mass attenuation coefficients were observed between EPICS2017-based values compared with Monte Carlo code and experimental results. Similar trends for the effective atomic numbers and electron densities were observed from EPICS2017 interpolation and from results found in literature. Conversely, buildup factors acquired by Geometric-Progression fitting parameters were reported in this work preliminarily for most of these biomolecules at different penetration depths. Overall, cysteine showed the most significant deviation among the other non-essential amino acids due to the presence of sulfur in its molecular structure.

Keywords Cross section · Endf · Epd197 · Gamma · Mass attenuation coefficient · Phits

1 Introduction

Protein is essential in various biological processes in the human body and plays an important role in the repair, growth, and maintenance of body cells. Proteins can be metabolized and broken down to their building blocks called amino acids (AAs). Each of these AAs can be sub-categorized into essential (EAA) or non-essential (NEAA) based on the ability of the body to synthesize the particular AA [1]. In essence, NEAAs are those which can be produced by the human body, while EAAs are those obtained from diet [2]. With the vast roles of the NEAAs including gene expression, cell signaling, neurological processes, acid-base balance, food digestion and absorption,

breakdown of nutrients, metabolism, fertilization and immunity, allosteric and epigenetic mechanisms, and tumorigenesis, researches have gained interest in targeting NEAAs for cancer therapy and field of oncology [3, 4].

Radiotherapy in the treatment of malignancy uses high doses of radiation in order to target cancer cells and diminish the size of tumors and slow down the growth and proliferation of cells through DNA damage. To calculate the penetration and dose deposition of X-ray and gamma photons in a particular target, the photon mass attenuation coefficient (μ/ρ), effective atomic number, electron density, and buildup factor are important radiological parameters which can be used [5–7]. The former quantities are derived from the μ/ρ or the cross section. These parameters are significant

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in the field of radiology and cancer therapy for estimations and optimizations of doses received by the patient.

Accurate values of μ/ρ are hence important for biomolecules comprising the human body [8, 9]. The widely used XCOM-NIST [10] can conveniently extract μ/ρ for any material for a wide range of photon energies [5, 11–14]. Alternative methods in literature for calculating μ/ρ involve photon transmission experiments and Monte Carlo (MC) simulations [15–22]. A scarcely reported method is by direct interpolations of major libraries other than those available from XCOM-NIST.

This work evaluates for NEAAs the photon attenuation parameters including mass attenuation coefficients, effective atomic numbers, electron densities, and exposure and energy absorption buildup factors, derived using EPICS2017 [23] library for interpolations. The new EPICS2017 library is the official evaluated photon and electron library of the latest ENDF/B-VIII [24]. To compare the mass attenuation coefficients obtained from the EPICS2017, the MC method was used as well as available experimental data found in literature. Exposure and energy absorption buildup factors for the NEAAs were reported in this work at multiple penetration depths using Geometric-Progression (G-P) fitting method.

2 Theory

The mass attenuation coefficient μ/ρ (cm^2g^{-1}) for a medium is described by the Beer–Lambert law or Equation (1), where I_0 and I are beam incident and transmitted intensities, respectively, ρ is the density (g cm^{-3}) of the medium, and x is the thickness or length (cm) [25].

$$I = I_0 e^{-\left(\frac{\mu}{\rho}\right)\rho x} \quad (1)$$

The law of mixtures shown in Equation (2) gives the total mass attenuation coefficients for a multi-element material, which describes it as a linear weighted combination of the $(\mu/\rho)_i$ of its constituent elements, where w_i is weight fraction of the i th element [26].

$$\left(\frac{\mu}{\rho}\right) = \sum w_i \left(\frac{\mu}{\rho}\right)_i \quad (2)$$

The mass attenuation coefficient is subsequently proportional to the total atomic cross section σ_T ($\text{cm}^2 \text{atom}^{-1}$) as shown in Equation (3), where N_A is the Avogadro's number, n_i is the number of atoms in the molecular formula, and A_i is the atomic mass of the i th element.

$$\left(\frac{\mu}{\rho}\right) = \sigma \frac{N_A \sum n_i}{\sum n_i A_i} \quad (3)$$

The total atomic cross section for each element $(\sigma_T)_i$ is the sum of the partial cross sections for photoelectric,

coherent, incoherent, and pair production, described in Equation (4).

$$(\sigma_T)_i = (\sigma_{PE})_i + (\sigma_{coh})_i + (\sigma_{incoh})_i + (\sigma_{PP})_i \quad (4)$$

The electronic cross section is a quantity described by Equation (5), where f_i is the atom fraction of each element and Z_i is the atomic number of each element [27]. It is related to effective atomic number Z_{eff} that is a unitless quantity given by the ratio of total atomic cross section and electronic cross section shown in Equation (6). On the other hand, the electron density N_{eff} (electrons g^{-1}) is related to Z_{eff} by Equation (7). Both the Z_{eff} and N_{eff} are widely used for the calculations of doses in multi-element materials by radiation therapy [28, 29].

$$\sigma_e = \frac{1}{N_A} \sum \frac{f_i A_i}{Z_i} \left(\frac{\mu}{\rho}\right)_i = \sum \frac{f_i}{Z_i} (\sigma_T)_i \quad (5)$$

$$Z_{\text{eff}} = \frac{\sigma_T}{\sigma_e} \quad (6)$$

$$N_{\text{eff}} = N_A \frac{Z_{\text{eff}}}{\sum f_i A_i} = \frac{\left(\frac{\mu}{\rho}\right)}{\sigma_e} \quad (7)$$

The Beer–Lambert law in Equation (1) is only valid for narrow-beam geometry, thin absorbing materials, and monoenergetic photons. In the case of divergences from such conditions, a correction factor called buildup factor $B(E, x)$ accounts for the effects of scattering described in Equation (8). It is a function of both photon energy and penetration depth in terms of the mean free path (mfp) [30]. The mfp is the inverse of the linear attenuation coefficient μ as shown by Equation (9).

$$I = B(E, x) I_0 e^{-\left(\frac{\mu}{\rho}\right)\rho x} \quad (8)$$

$$\text{mfp} = \frac{1}{\mu} \quad (9)$$

Two classifications of the quantity $B(E, x)$ are referred to as the energy absorption buildup factor (EABF) and the exposure buildup factor (EBF), where the quantity of interests are absorbed energy and exposure, respectively [31]. For both classifications of $B(E, x)$, the ANSI/ANS-6.4.3 [32] contains a compilation of G-P fitting parameters (a, b, c, d, X_k) for 23 elements in the photon energy range between 0.015 and 15 MeV, for depth of up to 40 mfp. The use of G-P fitting parameters is an accurate method of estimating buildup factors for different materials at a broad range of energies [33–35].

There are three steps for obtaining the EABF and EBF using the ANSI/ANS-6.4.3 G-P fitting parameters: (1) determination of equivalent atomic number Z_{eq} for the material, (2) evaluation of the G-P fitting parameters for the material, and (3) estimation of EABF and EBF using the parameters [30]. The Z_{eq} represents an equivalent atomic number for multi-element materials. It is obtained by considering the ratio of scattering and total attenuation, which monotonically decreases as a function of atomic number [35]. This is described by Equation (10), where R is the ratio of the μ/ρ of Compton scattering and the total μ/ρ , for the material. The R_1 and R_2 are the ratios of two successive elements with atomic numbers Z_1 and Z_2 . The Z_{eq} is used to obtain the G-P fitting parameters of the material. This is done by considering the tabulated G-P fitting parameters of the elements in ANSI/ANS-6.4.3 as illustrated in Equation (11), where F represents each of the five parameters (a, b, c, d, X_k).

$$Z_{eq} = \frac{Z_1(\log R_2 - \log R) + Z_2(\log R - \log R_1)}{\log R_2 - \log R_1} \quad (10)$$

$$F = \frac{F_1(\log Z_2 - \log Z_{eq}) + F_2(\log Z_{eq} - \log Z_1)}{\log Z_2 - \log Z_1} \quad (11)$$

Afterward, the term $K(E, x)$ is calculated using the solved G-P fitting parameters through Equation (12). This term represents the photon dose multiplication and change in the shape of the spectrum, with penetration from that at 1 mfp [32]. The buildup factors $B(E, x)$ representing EABF or EBF are then estimated using Equations (13) or (14).

$$K(E, x) = cx^a + d \frac{\tanh\left(\frac{x}{X_k} - 2\right) - \tanh(-2)}{1 - \tanh(-2)} \quad \text{for } x \leq 40 \text{ mfp} \quad (12)$$

$$B(E, x) = 1 + \frac{(b-1)(K^x - 1)}{K - 1} \quad \text{for } K \neq 1 \quad (13)$$

$$B(E, x) = 1 + (b-1)x \quad \text{for } K = 1 \quad (14)$$

3 Materials and methods

3.1 Non-essential amino acids

All NEAAs investigated include alanine, arginine, asparagine, aspartic acid, cysteine, glutamic acid, glutamine, glycine, proline, serine, and tyrosine. The chemical constituents of the biomolecules are shown in Table 1. For alanine, arginine, glycine, and proline, experimentally determined mass attenuation coefficients

were previously evaluated by Pawar and Bichile [21]. For asparagine, aspartic acid, glutamine, values were recently evaluated by Kore and Pawar [19], and for serine by Gaikwad et al. [16].

3.2 EPICS2017 interpolation

EPICS2017 [23] holds the most recent photoatomic library and is an official library in the latest ENDF/B-VIII release [24]. EPICS2017 is downloadable from the IAEA NDS website in both the ENDL and ENDF data formats. For this work, the version in the ENDF-6 data format was used. The EPICS2017 library was extracted previously for the development of a simple spreadsheet-based program for photon shielding and dosimetry applications [36]. Our previous program was built using MS Excel spline interpolation extensions and additional features via the VBA language. In this present work, we implement the interpolations using an executable Windows-based program.

It is worth mentioning that the predecessors of EPICS2017 are interpolable using the log-log interpolation law. However, due to several users mis-interpolating by using lin-lin, it was decided to convert the new EPICS2017 into a linearized library. Hence, the interpolation in this work was based on the recommended (lin-lin) law [37] and was applied to all partial cross sections, including coherent scattering, incoherent scattering, pair production, triplet production, and photoelectric separately for each subshell. The total atomic cross section was obtained by summing all relevant partial cross sections. Notably, due to the linearization, it is now possible to interpolate the total atomic cross sections also available from the library [38].

Table 1 Non-essential amino acids

Amino Acids	Molar mass (g mol ⁻¹)	Chemical formula	Mean atomic number, Z
Alanine (Ala)	89.09	C ₃ H ₇ NO ₂	3.69
Arginine (Arg)	174.20	C ₆ H ₁₄ N ₄ O ₂	3.62
Asparagine (Asn)	132.12	C ₄ H ₈ N ₂ O ₃	4.12
Aspartic acid (Asp)	133.10	C ₄ H ₇ NO ₄	4.38
Cysteine (Cys)	121.16	C ₃ H ₇ NO ₂ S	4.57
Glutamic acid (Glu)	147.13	C ₅ H ₉ NO ₄	4.11
Glutamine (Gln)	146.14	C ₅ H ₁₀ N ₂ O ₃	3.90
Glycine (Gly)	75.07	C ₂ H ₅ NO ₂	4.00
Proline (Pro)	115.13	C ₅ H ₉ NO ₂	3.65
Serine (Ser)	105.09	C ₃ H ₇ NO ₃	4.00
Tyrosine (Tyr)	181.19	C ₉ H ₁₁ NO ₃	4.00

3.3 PHITS Monte Carlo method

Comparative MC method to determine mass attenuation coefficients was made using PHITS 3.17 [39]. The default EPDL97 (ENDF/B-VII) [40] photoatomic library was used. The modeled geometry is shown in Fig. 1 comprising of a detector covered with a lead shield. This shield was 5-cm thick and had a beam entry diameter of 4 mm for achieving narrow-beam geometry. Each amino acid sample was modeled as a cylinder of 2-cm diameter. Length of each sample was in the range conforming to Nordfors criteria ($2 \leq \ln(I_0/I) \leq 4$) [41]. The surface-to-surface distance between the lead shield and the amino acid sample was fixed at 10 cm.

Photon source was modeled as a monoenergetic pencil beam with 4-mm diameter. The starting energies simulated were 59.5, 81, 88, 122.1, 136.5, 276.4, 302.9, 356, 383.8, 661.7, 834.8, 1173.2, 1252.9, 1274.5 and 1332.5 keV.

The [T-Track] tally with energy binning was used to obtain uncollided fluences inside the detector cell. Each run was achieved at a total of 10^7 simulated source photons per photon energy for each NEAA sample.

4 Results and discussion

An evaluation of the photon attenuation parameters for the NEAAs was made using the EPICS2017 photoatomic library. The results for the mass attenuation coefficients are shown in Tables 2, 3, 4 and 5, which are from EPICS2017 interpolation, from comparative PHITS simulations, and from available experimental values found in literature [16, 19, 21]. It is seen that the PHITS simulation results agree well with EPICS2017 with only marginally lower values. Nonetheless, the difference is owing to the slight dissimilarity in photoatomic libraries, deviation from narrow

Fig. 1 Narrow beam geometry for PHITS simulations

Table 2 Mass attenuation coefficients (cm^2g^{-1}) of alanine, arginine, and asparagine

Energy (keV)	Alanine (Ala)			Arginine (Arg)			Asparagine (Asn)		
	EPICS2017	PHITS	Pawar and Bichile [21]	EPICS2017	PHITS	Pawar and Bichile [21]	EPICS2017	PHITS	Kore and Pawar [19]
59.5	0.1944	0.1938	–	0.1930	0.1924	–	0.1921	0.1915	–
81.0	0.1749	0.1745	–	0.1745	0.1741	–	0.1724	0.1720	–
88.0	0.1704	0.1700	–	0.1701	0.1697	–	0.1679	0.1675	–
122.1	0.1549	0.1546	0.155	0.1549	0.1546	0.156	0.1524	0.1522	0.141
136.5	0.1497	0.1494	–	0.1498	0.1495	–	0.1474	0.1471	–
276.4	0.1185	0.1183	–	0.1186	0.1184	–	0.1166	0.1163	–
302.9	0.1146	0.1144	–	0.1148	0.1145	–	0.1127	0.1125	–
356.0	0.1077	0.1075	0.107	0.1078	0.1076	0.108	0.1059	0.1057	0.093
383.8	0.1047	0.1044	–	0.1048	0.1045	–	0.1029	0.1027	–
661.7	0.0832	0.0830	0.084	0.0833	0.0831	0.083	0.0818	0.0816	0.075
834.8	0.0747	0.0746	–	0.0748	0.0747	–	0.0735	0.0734	–
1173.2	0.0633	0.0632	0.065	0.0634	0.0633	0.063	0.0622	0.0621	0.058
1252.9	0.0612	0.0611	–	0.0613	0.0612	–	0.0602	0.0601	–
1274.5	0.0607	0.0606	0.060	0.0608	0.0607	0.061	0.0597	0.0596	0.050
1332.5	0.0593	0.0592	0.059	0.0594	0.0593	0.058	0.0583	0.0582	0.048

Table 3 Mass attenuation coefficients (cm^2g^{-1}) of aspartic acid, cysteine, and glutamic acid

Energy (keV)	Aspartic acid (Asp)			Cysteine (Cys)			Glutamic acid (Glu)		
	EPICS2017	PHITS	Kore and Pawar [19]	EPICS2017	PHITS	–	EPICS2017	PHITS	–
59.5	0.1920	0.1915	–	0.2522	0.2512	–	0.1926	0.1920	–
81.0	0.1717	0.1713	–	0.1961	0.1956	–	0.1727	0.1723	–
88.0	0.1671	0.1668	–	0.1864	0.1859	–	0.1681	0.1678	–
122.1	0.1515	0.1512	0.141	0.1593	0.1590	–	0.1526	0.1523	–
136.5	0.1464	0.1461	–	0.1523	0.1519	–	0.1475	0.1472	–
276.4	0.1157	0.1155	–	0.1170	0.1168	–	0.1166	0.1164	–
302.9	0.1119	0.1117	–	0.1130	0.1128	–	0.1128	0.1126	–
356.0	0.1051	0.1049	0.091	0.1060	0.1058	–	0.1060	0.1058	–
383.8	0.1022	0.1019	–	0.1030	0.1027	–	0.1030	0.1027	–
661.7	0.0812	0.0810	0.071	0.0816	0.0815	–	0.0818	0.0817	–
834.8	0.0730	0.0728	–	0.0733	0.0732	–	0.0735	0.0734	–
1173.2	0.0618	0.0617	0.062	0.0621	0.0620	–	0.0623	0.0622	–
1252.9	0.0598	0.0597	–	0.0601	0.0600	–	0.0602	0.0601	–
1274.5	0.0592	0.0591	0.046	0.0595	0.0594	–	0.0597	0.0596	–
1332.5	0.0579	0.0578	0.045	0.0582	0.0581	–	0.0583	0.0582	–

Table 4 Mass attenuation coefficients (cm^2g^{-1}) of glutamine, glycine, and proline

Energy (keV)	Glutamine (Gln)			Glycine (Gly)			Proline (Pro)		
	EPICS2017	PHITS	Kore and Pawar [19]	EPICS2017	PHITS	Pawar and Bichile [21]	EPICS2017	PHITS	Pawar and Bichile [21]
59.5	0.1926	0.1920	–	0.1938	0.1933	–	0.1928	0.1922	–
81.0	0.1733	0.1729	–	0.1737	0.1733	–	0.1742	0.1738	–
88.0	0.1688	0.1685	–	0.1691	0.1687	–	0.1699	0.1695	–
122.1	0.1534	0.1531	0.142	0.1534	0.1531	0.154	0.1546	0.1543	0.155
136.5	0.1483	0.1480	–	0.1483	0.1480	–	0.1495	0.1492	–
276.4	0.1174	0.1172	–	0.1172	0.1170	–	0.1184	0.1182	–
302.9	0.1136	0.1133	–	0.1134	0.1131	–	0.1146	0.1143	–
356.0	0.1067	0.1065	0.092	0.1065	0.1063	0.104	0.1076	0.1074	0.107
383.8	0.1037	0.1034	–	0.1035	0.1033	–	0.1046	0.1043	–
661.7	0.0824	0.0822	0.074	0.0822	0.0821	0.084	0.0831	0.0830	0.083
834.8	0.0740	0.0739	–	0.0739	0.0738	–	0.0747	0.0746	–
1173.2	0.0627	0.0626	0.058	0.0626	0.0625	0.062	0.0633	0.0631	0.065
1252.9	0.0606	0.0606	–	0.0606	0.0605	–	0.0612	0.0611	–
1274.5	0.0601	0.0600	0.048	0.0600	0.0599	0.061	0.0607	0.0605	0.061
1332.5	0.0587	0.0586	0.044	0.0586	0.0585	0.059	0.0592	0.0592	0.059

beam geometry, and relative uncertainties from MC simulation. Importantly, EPICS2017 library has new binding energies translating to new absorption edge energies and cross sections, as compared to the EPDL97 used by the MC method.

On the other hand, experimental results from Pawar and Bichile [21] (alanine, arginine, glycine, and proline) and Gaikwad et al. [16] (serine) showed agreement with the theoretical results. Those obtained by Kore and Pawar [19]

for asparagine, aspartic acid, and glutamine were slightly lower than the theoretical results but were nevertheless found to be in similar trends.

Effective atomic numbers and electron densities obtained using EPICS2017 interpolations are shown in Figs. 2 and 3. In the lower energy region in which photoelectric effect is dominant, the values are highest with a negative slope toward the Compton dominated region. For Compton dominated region, both plots tend

Table 5 Mass attenuation coefficients (cm^2g^{-1}) of serine and tyrosine

Energy (keV)	Serine (Ser)			Tyrosine (Tyr)		
	EPICS2017	PHITS	Gaikwad et al. [16]	EPICS2017	PHITS	–
59.5	0.1940	0.1934	–	0.1897	0.1891	–
81.0	0.1737	0.1733	–	0.1714	0.1710	–
88.0	0.1691	0.1688	–	0.1671	0.1668	–
122.1	0.1534	0.1531	0.152	0.1521	0.1518	–
136.5	0.1483	0.1480	–	0.1471	0.1468	–
276.4	0.1172	0.1170	–	0.1165	0.1163	–
302.9	0.1134	0.1132	–	0.1127	0.1125	–
356.0	0.1065	0.1063	0.119	0.1059	0.1057	–
383.8	0.1035	0.1033	–	0.1029	0.1026	–
661.7	0.0823	0.0821	0.080	0.0818	0.0816	–
834.8	0.0739	0.0738	–	0.0735	0.0734	–
1173.2	0.0626	0.0625	0.063	0.0622	0.0621	–
1252.9	0.0606	0.0605	–	0.0602	0.0601	–
1274.5	0.0600	0.0599	0.057	0.0597	0.0596	–
1332.5	0.0586	0.0585	0.056	0.0583	0.0582	–

Fig. 2 Effective atomic numbers of NEAAs using EPICS2017 **Fig. 3** Electron densities of NEAAs using EPICS2017

to dip toward constants and lowest values. The effective atomic numbers in this constant region are between 3.6 and 4.7. These results were also observed for some EAAs reported by Elbashir et al. [15] using the MCNP5 calculations. Notably the MCNP5 is also based on EPDL97. At the constant region, the effective atomic numbers are found to be in descending order of Cys > Asp > Asn > Glu > Ser > Gly > Tyr > Gln > Ala > Pro > Arg. Electron densities at constant region were found to have a narrow

spread between 3.2 and 3.3 ($\times 10^{23}$ electrons g^{-1}). These values are in descending order of Arg > Ala > Pro > Gln > Ser > Gly > Glu > Asn > Tyr > Cys > Asp. After the constant values at Compton dominated region, rising values are shown due to the increasing probability of pair-production interactions.

EBF and EABF calculated using EPICS2017 and the ANSI/ANS-6.4.3 G-P fitting parameters are shown in

Fig. 4 The buildup factors (EABF and EBF) for NEAAs using EPICS2017

Fig. (4) at multiple penetration depths. It is worth noting that buildup factors account for the contribution of scattered photons toward the quantity of interest (i.e., exposure, absorbed energy). The results showed lower EBF and EABF values at the energy regions where scattering

is relatively low or insignificant. Since photoelectric effect and pair-productions result in the absorption of the primary photons, these interaction events decrease the likelihood that these photons scatter further within the material. Hence, absorption events generally

decrease buildup factors within the medium. EBF and EABF were previously reported for EAAs and some conditional NEAAs [6, 42]. For some EAAs, buildup factors were described with an inverse relation to effective atomic numbers Z_{eff} [6]. In this study, the three highest Z_{eff} and three lowest showed this inverse relationship with EBF and EABF. This was assessed from the NEAAs at 1 to 40 mfps. It is highlighted that all NEAAs are chemically composed of H, C, N, and O atoms with the exception of cysteine that also contains S atoms. This contributes to cysteine's larger effective atomic numbers and electron densities at the lower and higher portions of the energy range considered. Consequently, cysteine also demonstrated the lowest values for both types of buildup factors at a large range of photon energies.

5 Conclusion

Photon attenuation parameters of eleven NEAAs have been determined using interpolation method based on the new EPICS2017 library. The EPICS2017 is the current latest library for electron-photon transport and is officially included in ENDF/B-VIII. The EPICS2017 has been interpolated in this work in the recommended lin-lin law using a Windows-based program. Obtained mass attenuation coefficients of NEAAs were compared with MC method results and experimental values in literatures. An agreement with simulation and experimental values was found. Effective atomic numbers and electron densities were also in agreement with those in literature based on MCNP5 calculations. Buildup factors for energy absorption and exposure quantities have been reported via G-P fitting parameters with the use of the EPICS2017 library. Cysteine was found to have a significantly larger effective atomic number which translates to significantly lower buildup factor values, owing to the S atom comprising its chemical structure. These results can serve in the fields of radiology and medical dosimetry. Furthermore, the interpolation method using EPICS2017 was found to be a useful and recent alternative to the generally used XCOM-NIST.

Declarations

Conflict of interest The authors declare no conflict of interest.

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