



## Corrigendum



## Corrigendum to “Intercomparison of dose enhancement ratio and secondary electron spectra for gold nanoparticles irradiated by X-rays calculated using multiple Monte Carlo simulation codes” [Phys. Med. 69 (2020) 147–163]

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In our paper [1] we presented the dose enhancement ratios (DERs) and the electron spectra for a single gold nanoparticle (GNP) irradiated by a narrow X-ray beam calculated with multiple Monte Carlo simulation codes. During further analysis of the data for an internal EURADOS report, we identified the following inconsistencies in the simulations, which affect the results presented in the above-mentioned article [1]:

1. PENELOPE#1 and PENELOPE#2: The X-ray spectra in the input files were given as cumulative probabilities. The start points of the X-ray photons were sampled from a square rather than a circular area as PENELOPE main programs do not provide the option of a circular source. The first error was corrected in new simulations of PENELOPE#1 using PENELOPE-2018. The variant source geometry was taken into account for the electron spectra by using a fluence correction factor of  $4/\pi$  (area of the square divided by the area of circle). The impact of the source geometry on the DER is assumed to be small enough to be disregarded for the purpose of this corrigendum. PENELOPE#2 has not performed new simulations and, therefore, data of PENELOPE#2 are not presented in this corrigendum.
2. G4/DNA#1: The electron spectra for a GNP of diameter 50 nm irradiated by 50 kVp X-rays, a GNP of diameter 100 nm irradiated by 50 kVp X-rays and a GNP of diameter 100 nm irradiated by 100 kVp X-rays were not divided by the energy bin width of 5 eV. This error has been corrected in this corrigendum.
3. G4/DNA#2: There was an error in the readout file. The electron spectrum for a GNP of 50 nm diameter irradiated by 50 kVp X-rays was newly simulated and the corrected spectrum is shown in this corrigendum. No new simulations for a GNP of diameter 100 nm irradiated by 50 kVp X-rays have been performed, therefore no data for this spectrum are included in this corrigendum.
4. G4/DNA#3: The electron spectra were not divided by the energy bin width of 5 eV. This error has been corrected in this corrigendum.
5. TOPAS-nBio: The X-rays were sampled from a larger circular source area with a total radius of the radius of the GNP plus 10 nm. Factors of 1.36 and 1.19 (calculated by  $\left(\frac{r_{\text{GNP}}+10}{r_{\text{GNP}}}\right)^2$ ) have been used for correction of the electron spectra of a GNP with diameter of 50 nm and 100 nm, respectively. In this corrigendum, as for PENELOPE#1, the impact of the variant source geometry on the DER is assumed to be small enough to be disregarded.
6. MCNP6: The electron spectra were recorded only for electrons ejected from the GNP in the angular bin 0–15 degree (approximately

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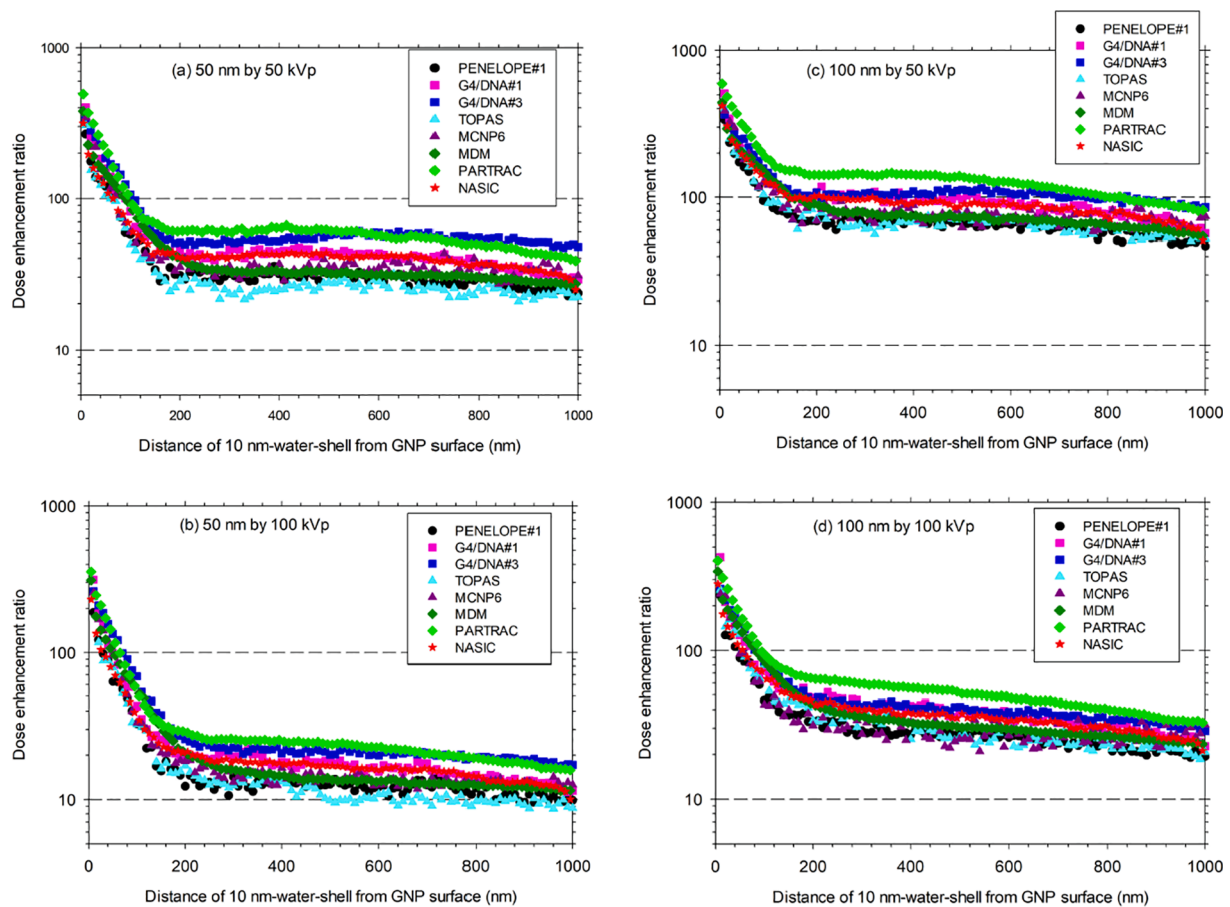
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**Fig. 4.** Dose enhancement ratio in 10 nm-thick shells as a function of distance from the surface of a single GNP irradiated by X-rays: (a) A GNP of 50 nm diameter irradiated by 50 kVp X-rays; (b) A GNP of 50 nm diameter irradiated by 100 kVp X-rays; (c) A GNP of 100 nm diameter irradiated by 50 kVp X-rays; (d) A GNP of 100 nm diameter irradiated by 100 kVp X-rays.

normal direction with respect to the surface of the GNP). The electron spectra were not divided by the energy bin width of 50 eV. In this corrigendum, the electron spectra were multiplied by a factor of 11 (estimated by the participant of MCNP6 from the ratio of the total number of ejected electrons and those ejected in the close-to-normal bin) and divided by the energy bin width of 50 eV in order to reconstruct the total electron spectrum emitted from a GNP.

- MDM: The electron spectra were normalized to a photon fluence of 1 photon per  $\text{cm}^2$  instead of one photon per circular source area. In this corrigendum, the electron spectra for a GNP of diameter 50 nm and a GNP of diameter 100 nm were multiplied by the respective ratio of the two photon fluences of  $7.09 \times 10^7$  and  $2.11 \times 10^7$ , respectively.

For the aforementioned reasons, Figs. 4–8 and Table 2 presented in our paper [1] were replotted and tabulated in the following.

In addition to the above corrected Figs. 4–8 and Table 2, the text regarding to the UF in Sections of “Abstract”, “Results”, “Discussions” and “Conclusion” were correspondingly corrected in the following.

#### Abstract

“Results: The mean dose enhancement ratio of the first 10 nm-thick water shell around a 100 nm GNP ranges from 400 for 100 kVp X-rays to 600 for 50 kVp X-rays with large uncertainty factors up to 1.6.”

#### 3 Results

##### 3.1.2 Uncertainty factor of DER in nanometer ranges

“... It can be seen in Fig. 5(a)–(d) that the UFs of DERs for the results are 1.3–1.6, 1.3–1.5, 1.3–1.5 and 1.2–1.5, respectively, with the maximum UF values occurring at the water shells located at 280 nm, 440 nm, 470 nm and 540 nm, respectively. The UFs at the first 10 nm-thick shells for the four radiation scenarios are relatively small and close

to 1.3.”

##### 3.1.3 DER in micrometer ranges

This sentence “It is noted that, for 100 kVp X-rays, the DER calculated by PENELOPE at 2  $\mu\text{m}$  to 8  $\mu\text{m}$  from the surface of the GNP drops down more steeply than the other results, in contrast to the irradiation scenarios by 50 kVp X-rays.” should be removed.

##### 3.2.2 Uncertainty factor of electron energy spectra

“... Overall, the highest UF, from maximum 8.6 to minimum 1.3 was found for a GNP of diameter 100 nm irradiated by 50 kVp X-rays, and the lowest UF, from maximum 5.6 to minimum 1.1, for a GNP of diameter 100 nm irradiated by 100 kVp X-rays. If the high UF values at the low energy range, say from 50 eV to 200 eV were neglected due to the very high uncertainty of the cross sections of lower electron energies, then the UF of the energy spectra ranges from 2.5 for the scenario of a GNP of diameter 100 nm irradiated by 50 kVp X-rays to 2.2 for the scenario of a GNP of diameter 100 nm irradiated by 50 kVp X-rays. ...

As an example, ... The UF at 100 eV for the four radiation scenarios is very large, expanding from 2.8 to 4.8. The UFs at 1,000 eV and 10,000 eV for these four scenarios is smaller than that at 100 eV, ranging from 1.4 to 1.7 and from 1.3 to 2.9, respectively.”

#### 4 Discussion

##### 4.1 Uncertainty of DER and energy spectra of secondary electrons

“... A quantitative uncertainty analysis revealed a larger uncertainty factor ranging from 1.3 up to 4.8 (see Table 2). A very large uncertainty was found at energy 100 eV for the scenario of a GNP of diameter 50 nm irradiated by 50 kVp X-ray spectra. ...”

“Despite the large variation of electron energy spectra shown in the lower to middle energy ranges in Fig. 7, the DER showed comparably smaller uncertainty factors, from 1.2 up to 1.6 in the whole range from

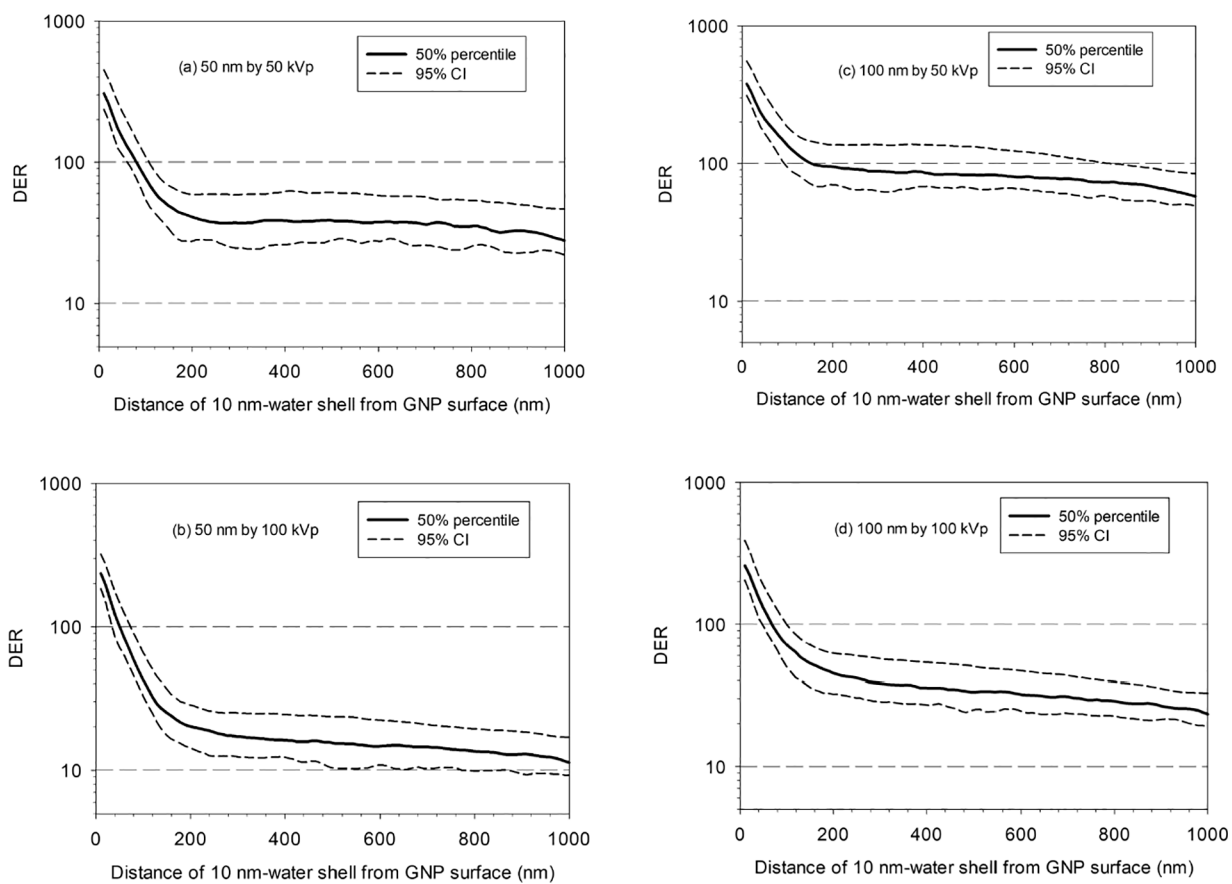
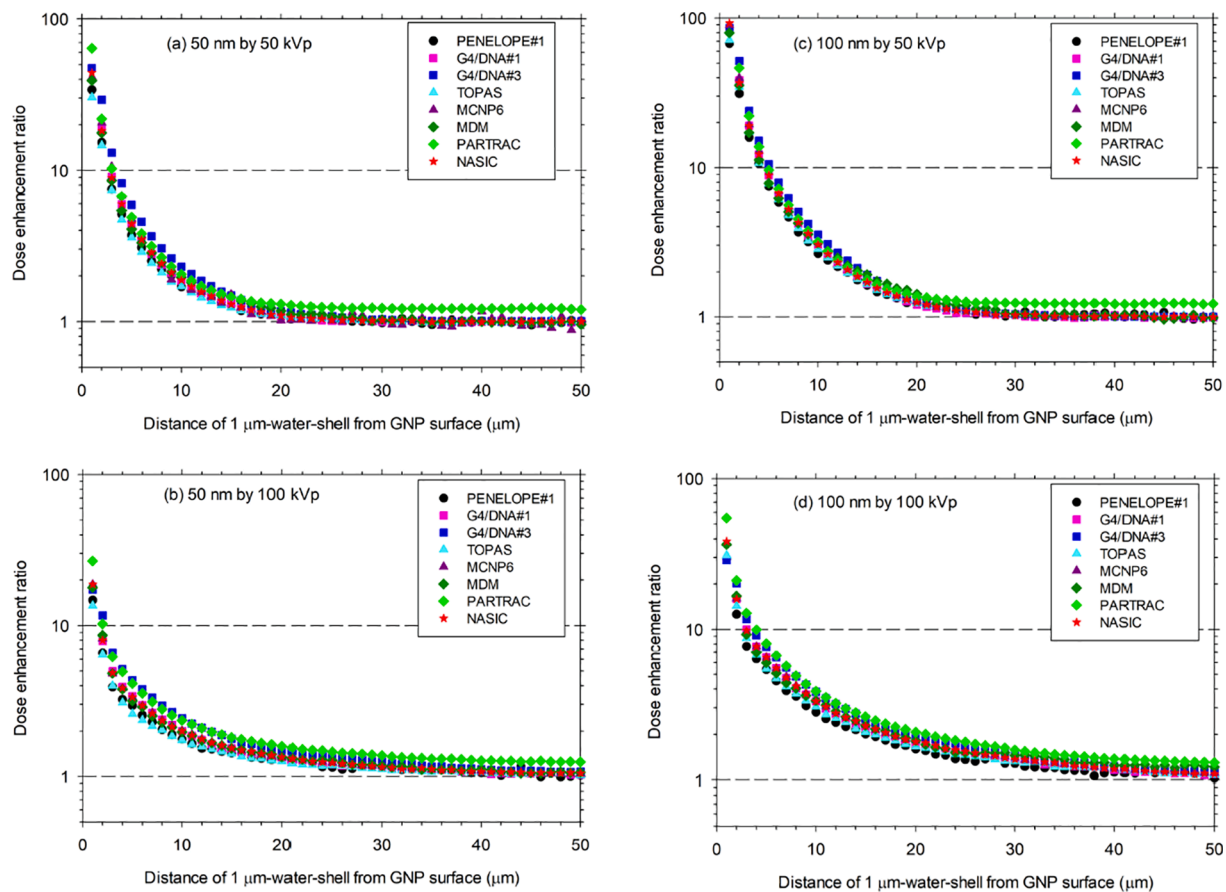
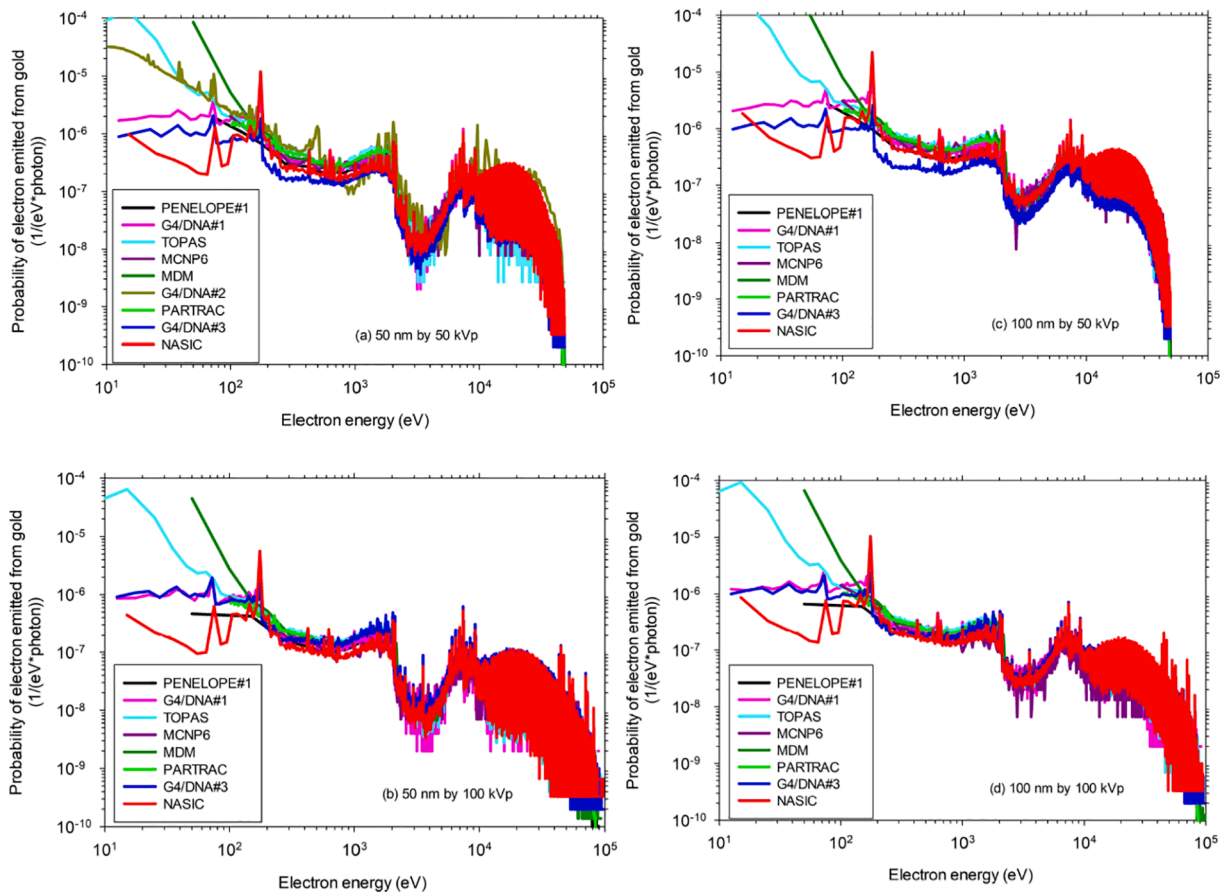


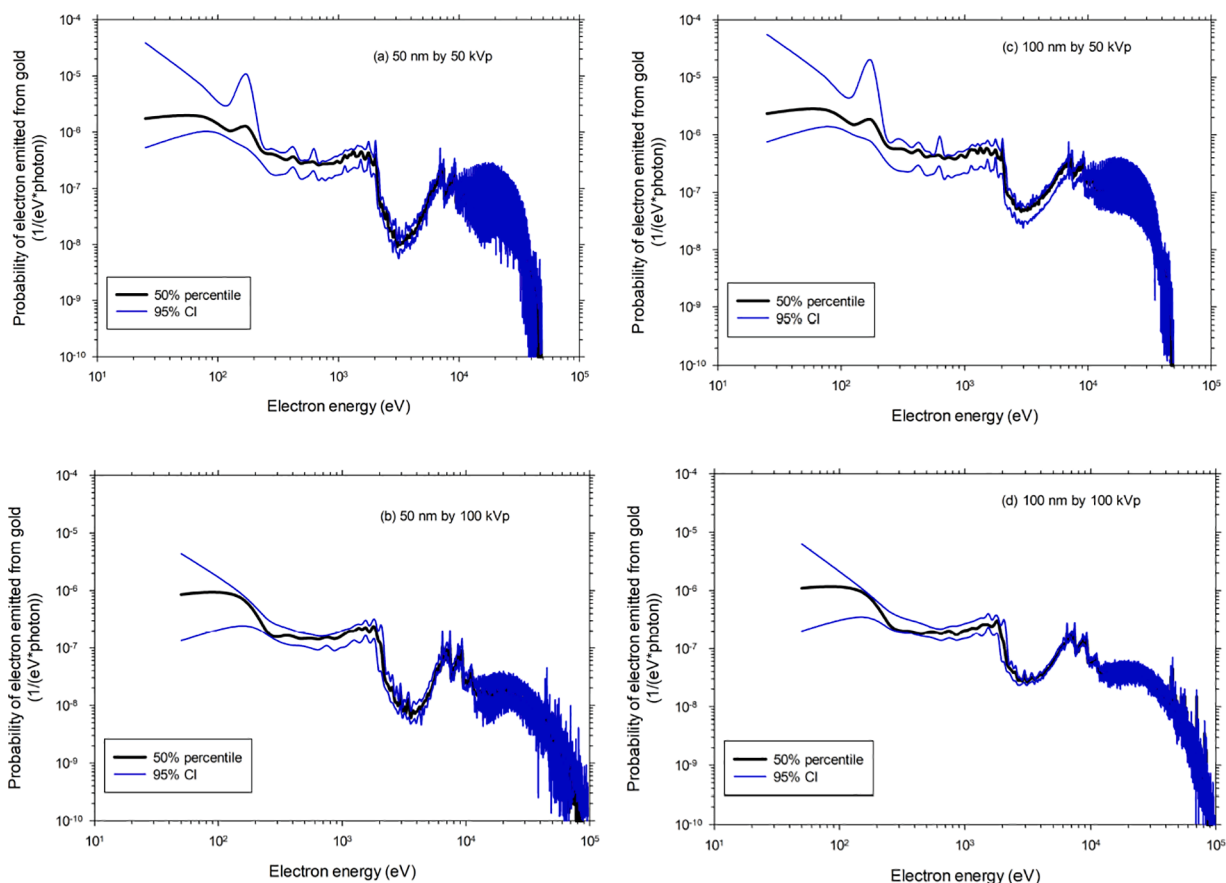
Fig. 5. The 2.5th, 50th and 97.5th percentiles of the different results reported for the DER at different distances from the surface for a GNP of diameter 50 nm and a GNP of diameter 100 nm irradiated by 50 kVp and 100 kVp X-ray spectra.



**Fig. 6.** Dose enhancement ratio (DER) in micrometer ranges of a GNP of 50 nm and 100 nm diameter irradiated by 50 kVp and 100 kVp X-ray spectra. (a) A GNP of 50 nm diameter irradiated by 50 kVp X-rays; (b) A GNP of 50 nm diameter irradiated by 100 kVp X-rays; (c) A GNP of 100 nm diameter irradiated by 50 kVp X-rays; (d) A GNP of diameter 100 nm irradiated by 100 kVp X-rays.



**Fig. 7.** Energy spectra of secondary electrons escaping from the surface of a GNP irradiated by X-ray spectra (a) A GNP of diameter 50 nm irradiated by 50 kVp X-rays; (b) A GNP of diameter 50 nm irradiated by 100 kVp X-rays; (c) A GNP of diameter 100 nm irradiated by 50 kVp X-rays and (d) A GNP of diameter 100 nm irradiated by 100 kVp X-rays for a circular source diameter equal to a GNP diameter plus 10 nm.



**Fig. 8.** The 2.5th, 50th and 97.5th percentiles of energy spectra of secondary electron escaping from the surface of a GNP irradiated by X-ray spectra reported from different exercise participants (a) A GNP of diameter 50 nm irradiated by 50 kVp X-rays; (b) A GNP of diameter 50 nm irradiated by 100 kVp X-rays; (c) A GNP of diameter 100 nm irradiated by 50 kVp X-rays and (d) A GNP of diameter 100 nm irradiated by 100 kVp X-rays. The spectra of MCNP6 were not included in uncertainty analysis because of their bad statistics.

**Table 2**

The 2.5th, 50th and 97.5th percentiles and uncertainty factor (UF) of the reported probabilities for electrons emitted from a single GNP at energies of 100 eV, 1,000 eV and 10,000 eV (normalized in the energy bin width of 1 eV per photon).

GNP size and X-ray	Electron energy (eV)		
	100	1,000	10,000
(nm/kVp)	(2.5th, 50th, 97.5th), UF		
50/50	( $2.0 \times 10^{-7}$ , $1.4 \times 10^{-6}$ , $4.6 \times 10^{-6}$ ), 4.8	( $1.3 \times 10^{-7}$ , $2.6 \times 10^{-7}$ , $3.8 \times 10^{-7}$ ), 1.7	( $1.6 \times 10^{-8}$ , $6.7 \times 10^{-8}$ , $1.3 \times 10^{-7}$ ), 2.9
50/100	( $3.0 \times 10^{-7}$ , $8.5 \times 10^{-7}$ , $2.4 \times 10^{-6}$ ), 2.9	( $1.1 \times 10^{-7}$ , $1.7 \times 10^{-7}$ , $2.1 \times 10^{-7}$ ), 1.4	( $9.8 \times 10^{-9}$ , $2.6 \times 10^{-8}$ , $3.6 \times 10^{-8}$ ), 1.9
100/50	( $8.8 \times 10^{-7}$ , $2.4 \times 10^{-6}$ , $7.1 \times 10^{-6}$ ), 2.8	( $2.6 \times 10^{-7}$ , $4.4 \times 10^{-7}$ , $5.9 \times 10^{-7}$ ), 1.5	( $9.9 \times 10^{-8}$ , $1.6 \times 10^{-7}$ , $1.8 \times 10^{-7}$ ), 1.3
100/100	( $4.3 \times 10^{-7}$ , $9.6 \times 10^{-7}$ , $3.5 \times 10^{-6}$ ), 2.8	( $1.1 \times 10^{-7}$ , $2.3 \times 10^{-7}$ , $2.7 \times 10^{-7}$ ), 1.6	( $4.2 \times 10^{-8}$ , $6.1 \times 10^{-8}$ , $7.0 \times 10^{-8}$ ), 1.3

10 nm to 1000 nm for 10 nm-thick water shells. If the maximum UFs of DERs for each radiation scenario were excluded, the overall UF is smaller than a factor of 1.4. . . .”

The authors would like to apologize for any inconvenience caused.

**5 Conclusion**

“ . . . Despite the larger uncertainty with a maximum UF up to 4.8 for the electron energy spectra, the uncertainty of DER in the 10 nm-thick water shells showed a maximum UF up to 1.6. . . .”

**References**

[1] Li WB, Belchior A, Beuve M, Chen YZ, Di Maria S, Friedland W, Gervais B, Heide B, Hocine N, Ipatov A, Klapproth AP, Li CY, Li JL, Multhoff G, Poignant F, Qiu R, Rabus H, Rudek B, Schuemann J, Stangl S, Testa E, Villagrana C, Xie WZ, Zhang YB. Intercomparison of dose enhancement ratio and secondary electron spectra for gold nanoparticles irradiated by X-rays calculated using multiple Monte Carlo simulation codes. *Physica Med* 2020;69:147–63.