

Multi-scale Monte Carlo simulations of gold nanoparticle induced DNA damages for kilovoltage x-ray irradiation in a xenograft mouse model using TOPAS-nBio

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Table S1: Simulation results and standard deviations - 100 kVp, front cell, without AuFeNPs

	Overall Value	SD
Total SB	764	$1.08 \cdot 10^{-2}$
Total SB direct	310	$6.879 \cdot 10^{-3}$
Total SB indirect	454	$8.324 \cdot 10^{-3}$
Total SSB	484	$8.595 \cdot 10^{-3}$
Total SSB direct	207	$5.621 \cdot 10^{-3}$
Total SSB indirect	277	$6.502 \cdot 10^{-3}$
Total DSB	140	$4.623 \cdot 10^{-3}$
Total DSB direct	22	$1.833 \cdot 10^{-3}$
Total DSB indirect	59	$3.001 \cdot 10^{-3}$
Total DSB hybrid	59	$3.001 \cdot 10^{-3}$
Dose (Gy)	0.845037	$0.359 \cdot 10^{-3}$
H radicals	28874	$6.624 \cdot 10^{-2}$
OH radicals	62214	$9.699 \cdot 10^{-2}$
H ₂ radicals	12275	$4.325 \cdot 10^{-2}$
H ₂ O ₂ radicals	92414	$1.179 \cdot 10^{-1}$
H ₃ O radicals	7023	$3.272 \cdot 10^{-2}$
e _{aq} radicals	27	$2.03 \cdot 10^{-3}$

Table S2: Simulation results and standard deviations - 100 kVp, front cell, with AuFeNPs

	Overall Value	SD
Total SB	811	$1.113 \cdot 10^{-2}$
Total SB direct	314	$6.923 \cdot 10^{-3}$
Total SB indirect	497	$8.71 \cdot 10^{-3}$
Total SSB	467	$8.443 \cdot 10^{-3}$
Total SSB direct	176	$5.183 \cdot 10^{-3}$
Total SSB indirect	291	$6.665 \cdot 10^{-3}$
Total DSB	172	$5.124 \cdot 10^{-3}$
Total DSB direct	28	$2.067 \cdot 10^{-3}$
Total DSB indirect	62	$3.076 \cdot 10^{-3}$
Total DSB hybrid	82	$3.538 \cdot 10^{-3}$
Dose (Gy)	0.885086	$0.368 \cdot 10^{-3}$
H radicals	46632	$8.407 \cdot 10^{-2}$
OH radicals	134708	$1.419 \cdot 10^{-1}$
H ₂ radicals	34173	$7.204 \cdot 10^{-2}$
H ₂ O ₂ radicals	98057	$1.214 \cdot 10^{-1}$
H ₃ O radicals	2069	$1.777 \cdot 10^{-2}$
e _{aq} radicals	16	$1.563 \cdot 10^{-3}$

Table S3: Simulation results and standard deviations - 100 kVp, center cell, without AuFeNPs

	Overall Value	SD
Total SB	722	$1.066 \cdot 10^{-2}$
Total SB direct	276	$6.594 \cdot 10^{-3}$
Total SB indirect	446	$8.382 \cdot 10^{-3}$
Total SSB	480	$8.695 \cdot 10^{-3}$
Total SSB direct	185	$5.398 \cdot 10^{-3}$
Total SSB indirect	295	$6.817 \cdot 10^{-3}$
Total DSB	121	$4.366 \cdot 10^{-3}$
Total DSB direct	23	$1.903 \cdot 10^{-3}$
Total DSB indirect	53	$2.889 \cdot 10^{-3}$
Total DSB hybrid	45	$2.662 \cdot 10^{-3}$
Dose (Gy)	0.831712	$0.362 \cdot 10^{-3}$
H radicals	28921	$6.734 \cdot 10^{-2}$
OH radicals	62100	$9.842 \cdot 10^{-2}$
H ₂ radicals	12039	$4.351 \cdot 10^{-2}$
H ₂ O ₂ radicals	92726	$1.2 \cdot 10^{-1}$
H ₃ O radicals	7170	$3.359 \cdot 10^{-2}$
e _{aq} radicals	30	$2.174 \cdot 10^{-3}$

Table S4: Simulation results and standard deviations - 100 kVp, center cell, with AuFeNPs

	Overall Value	SD
Total SB	773	$1.103 \cdot 10^{-2}$
Total SB direct	262	$6.424 \cdot 10^{-3}$
Total SB indirect	511	$8.972 \cdot 10^{-3}$
Total SSB	459	$8.503 \cdot 10^{-3}$
Total SSB direct	162	$5.052 \cdot 10^{-3}$
Total SSB indirect	297	$6.84 \cdot 10^{-3}$
Total DSB	157	$4.973 \cdot 10^{-3}$
Total DSB direct	18	$1.684 \cdot 10^{-3}$
Total DSB indirect	75	$3.437 \cdot 10^{-3}$
Total DSB hybrid	64	$3.175 \cdot 10^{-3}$
Dose (Gy)	0.896441	$0.376 \cdot 10^{-3}$
H radicals	47563	$8.623 \cdot 10^{-2}$
OH radicals	138590	$1.461 \cdot 10^{-1}$
H ₂ radicals	35443	$7.451 \cdot 10^{-2}$
H ₂ O ₂ radicals	101424	$1.254 \cdot 10^{-1}$
H ₃ O radicals	1925	$1.741 \cdot 10^{-2}$
e _{aq} radicals	14	$1.485 \cdot 10^{-3}$

Table S5: Simulation results and standard deviations - 100 kVp, back cell, without AuFeNPs

	Overall Value	SD
Total SB	720	$1.079 \cdot 10^{-2}$
Total SB direct	286	$6.798 \cdot 10^{-3}$
Total SB indirect	434	$8.375 \cdot 10^{-3}$
Total SSB	436	$8.394 \cdot 10^{-3}$
Total SSB direct	192	$5.57 \cdot 10^{-3}$
Total SSB indirect	244	$6.28 \cdot 10^{-3}$
Total DSB	142	$4.79 \cdot 10^{-3}$
Total DSB direct	19	$1.752 \cdot 10^{-3}$
Total DSB indirect	67	$3.291 \cdot 10^{-3}$
Total DSB hybrid	56	$3.008 \cdot 10^{-3}$
Dose (Gy)	0.782187	$0.356 \cdot 10^{-3}$
H radicals	28936	$6.822 \cdot 10^{-2}$
OH radicals	61681	$9.934 \cdot 10^{-2}$
H ₂ radicals	11917	$4.384 \cdot 10^{-2}$
H ₂ O ₂ radicals	88797	$1.189 \cdot 10^{-1}$
H ₃ O radicals	7362	$3.447 \cdot 10^{-2}$
e _{aq} radicals	38	$2.478 \cdot 10^{-3}$

Table S6: Simulation results and standard deviations - 100 kVp, back cell, with AuFeNPs

	Overall Value	SD
Total SB	772	$1.117 \cdot 10^{-2}$
Total SB direct	308	$7.055 \cdot 10^{-3}$
Total SB indirect	464	$8.659 \cdot 10^{-3}$
Total SSB	478	$8.789 \cdot 10^{-3}$
Total SSB direct	192	$5.57 \cdot 10^{-3}$
Total SSB indirect	286	$6.798 \cdot 10^{-3}$
Total DSB	147	$4.874 \cdot 10^{-3}$
Total DSB direct	19	$1.752 \cdot 10^{-3}$
Total DSB indirect	50	$2.843 \cdot 10^{-3}$
Total DSB hybrid	78	$3.55 \cdot 10^{-3}$
Dose (Gy)	0.848231	$0.37 \cdot 10^{-3}$
H radicals	46075	$8.597 \cdot 10^{-2}$
OH radicals	135352	$1.463 \cdot 10^{-1}$
H ₂ radicals	34480	$7.444 \cdot 10^{-2}$
H ₂ O ₂ radicals	95191	$1.231 \cdot 10^{-1}$
H ₃ O radicals	2251	$1.907 \cdot 10^{-2}$
e _{aq} radicals	21	$1.842 \cdot 10^{-3}$

Table S7: Simulation results and standard deviations - 200 kVp, front cell, without AuFeNPs

	Overall Value	SD
Total SB	756	$10.801 \cdot 10^{-3}$
Total SB direct	274	$6.503 \cdot 10^{-3}$
Total SB indirect	482	$8.625 \cdot 10^{-3}$
Total SSB	474	$8.553 \cdot 10^{-3}$
Total SSB direct	179	$5.256 \cdot 10^{-3}$
Total SSB indirect	295	$6.747 \cdot 10^{-3}$
Total DSB	141	$4.665 \cdot 10^{-3}$
Total DSB direct	18	$1.667 \cdot 10^{-3}$
Total DSB indirect	64	$3.143 \cdot 10^{-3}$
Total DSB hybrid	59	$3.018 \cdot 10^{-3}$
Dose (Gy)	0.918982	$0.377 \cdot 10^{-3}$
H radicals	40523	$7.883 \cdot 10^{-2}$
OH radicals	85989	$1.144 \cdot 10^{-1}$
H ₂ radicals	16641	$5.061 \cdot 10^{-2}$
H ₂ O ₂ radicals	127663	$1.39 \cdot 10^{-1}$
H ₃ O radicals	9861	$3.898 \cdot 10^{-2}$
e _{aq} radicals	26	$2.003 \cdot 10^{-3}$

Table S8: Simulation results and standard deviations - 200 kVp, front cell, with AuFeNPs

	Overall Value	SD
Total SB	886	$11.693 \cdot 10^{-3}$
Total SB direct	334	$7.179 \cdot 10^{-3}$
Total SB indirect	552	$9.23 \cdot 10^{-3}$
Total SSB	550	$9.213 \cdot 10^{-3}$
Total SSB direct	205	$5.625 \cdot 10^{-3}$
Total SSB indirect	345	$7.297 \cdot 10^{-3}$
Total DSB	168	$5.092 \cdot 10^{-3}$
Total DSB direct	28	$2.079 \cdot 10^{-3}$
Total DSB indirect	67	$3.216 \cdot 10^{-3}$
Total DSB hybrid	73	$3.357 \cdot 10^{-3}$
Dose (Gy)	1.07826	$0.408 \cdot 10^{-3}$
H radicals	61030	$9.659 \cdot 10^{-2}$
OH radicals	176515	$1.628 \cdot 10^{-1}$
H ₂ radicals	44755	$8.282 \cdot 10^{-2}$
H ₂ O ₂ radicals	131031	$1.408 \cdot 10^{-1}$
H ₃ O radicals	2272	$1.872 \cdot 10^{-2}$
e _{aq} radicals	11	$1.303 \cdot 10^{-3}$

Table S9: Simulation results and standard deviations - 200 kVp, center cell, without AuFeNPs

	Overall Value	SD
Total SB	658	$10.159 \cdot 10^{-3}$
Total SB direct	230	$6.007 \cdot 10^{-3}$
Total SB indirect	428	$8.194 \cdot 10^{-3}$
Total SSB	380	$7.721 \cdot 10^{-3}$
Total SSB direct	147	$4.802 \cdot 10^{-3}$
Total SSB indirect	233	$6.046 \cdot 10^{-3}$
Total DSB	139	$4.67 \cdot 10^{-3}$
Total DSB direct	17	$1.633 \cdot 10^{-3}$
Total DSB indirect	73	$3.384 \cdot 10^{-3}$
Total DSB hybrid	49	$2.772 \cdot 10^{-3}$
Dose (Gy)	0.773754	$0.348 \cdot 10^{-3}$
H radicals	32259	$7.096 \cdot 10^{-2}$
OH radicals	68981	$1.035 \cdot 10^{-1}$
H ₂ radicals	13549	$4.605 \cdot 10^{-2}$
H ₂ O ₂ radicals	107197	$1.286 \cdot 10^{-1}$
H ₃ O radicals	7300	$3.382 \cdot 10^{-2}$
e _{aq} radicals	16	$1.584 \cdot 10^{-3}$

Table S10: Simulation results and standard deviations - 200 kVp, center cell, with AuFeNPs

	Overall Value	SD
Total SB	701	$10.486 \cdot 10^{-3}$
Total SB direct	256	$6.337 \cdot 10^{-3}$
Total SB indirect	445	$8.355 \cdot 10^{-3}$
Total SSB	413	$8.049 \cdot 10^{-3}$
Total SSB direct	153	$4.899 \cdot 10^{-3}$
Total SSB indirect	260	$6.386 \cdot 10^{-3}$
Total DSB	144	$4.753 \cdot 10^{-3}$
Total DSB direct	20	$1.771 \cdot 10^{-3}$
Total DSB indirect	61	$3.093 \cdot 10^{-3}$
Total DSB hybrid	63	$3.144 \cdot 10^{-3}$
Dose (Gy)	0.80812	$0.356 \cdot 10^{-3}$
H radicals	51718	$8.971 \cdot 10^{-2}$
OH radicals	150070	$1.516 \cdot 10^{-1}$
H ₂ radicals	38213	$7.719 \cdot 10^{-2}$
H ₂ O ₂ radicals	112756	$1.318 \cdot 10^{-1}$
H ₃ O radicals	2209	$1.861 \cdot 10^{-2}$
e _{aq} radicals	6	$0.97 \cdot 10^{-3}$

Table S11: Simulation results and standard deviations - 200 kVp, back cell, without AuFeNPs

	Overall Value	SD
Total SB	557	$9.478 \cdot 10^{-3}$
Total SB direct	228	$6.064 \cdot 10^{-3}$
Total SB indirect	329	$7.284 \cdot 10^{-3}$
Total SSB	331	$7.306 \cdot 10^{-3}$
Total SSB direct	144	$4.819 \cdot 10^{-3}$
Total SSB indirect	187	$5.492 \cdot 10^{-3}$
Total DSB	113	$4.269 \cdot 10^{-3}$
Total DSB direct	20	$1.796 \cdot 10^{-3}$
Total DSB indirect	49	$2.811 \cdot 10^{-3}$
Total DSB hybrid	44	$2.664 \cdot 10^{-3}$
Dose (Gy)	0.631707	$0.319 \cdot 10^{-3}$
H radicals	27139	$6.601 \cdot 10^{-2}$
OH radicals	58021	$9.628 \cdot 10^{-2}$
H ₂ radicals	11216	$4.249 \cdot 10^{-2}$
H ₂ O ₂ radicals	84361	$1.158 \cdot 10^{-1}$
H ₃ O radicals	6746	$3.297 \cdot 10^{-2}$
e _{aq} radicals	24	$1.967 \cdot 10^{-3}$

Table S12: Simulation results and standard deviations - 200 kVp, back cell, with AuFeNPs

	Overall Value	SD
Total SB	594	$9.787 \cdot 10^{-3}$
Total SB direct	207	$5.778 \cdot 10^{-3}$
Total SB indirect	387	$7.9 \cdot 10^{-3}$
Total SSB	372	$7.746 \cdot 10^{-3}$
Total SSB direct	120	$4.399 \cdot 10^{-3}$
Total SSB indirect	252	$6.375 \cdot 10^{-3}$
Total DSB	111	$4.231 \cdot 10^{-3}$
Total DSB direct	22	$1.884 \cdot 10^{-3}$
Total DSB indirect	46	$2.724 \cdot 10^{-3}$
Total DSB hybrid	43	$2.633 \cdot 10^{-3}$
Dose (Gy)	0.709614	$0.338 \cdot 10^{-3}$
H radicals	43150	$8.313 \cdot 10^{-2}$
OH radicals	122708	$1.393 \cdot 10^{-1}$
H ₂ radicals	30881	$7.04 \cdot 10^{-2}$
H ₂ O ₂ radicals	89501	$1.193 \cdot 10^{-1}$
H ₃ O radicals	2330	$1.938 \cdot 10^{-2}$
e _{aq} radicals	12	$1.391 \cdot 10^{-3}$