pharmaceutics

Supplementary Materials: Gold Nanoparticles Permit in Situ Absorbed Dose Evaluation in Boron Neutron Capture Therapy for Malignant Tumors

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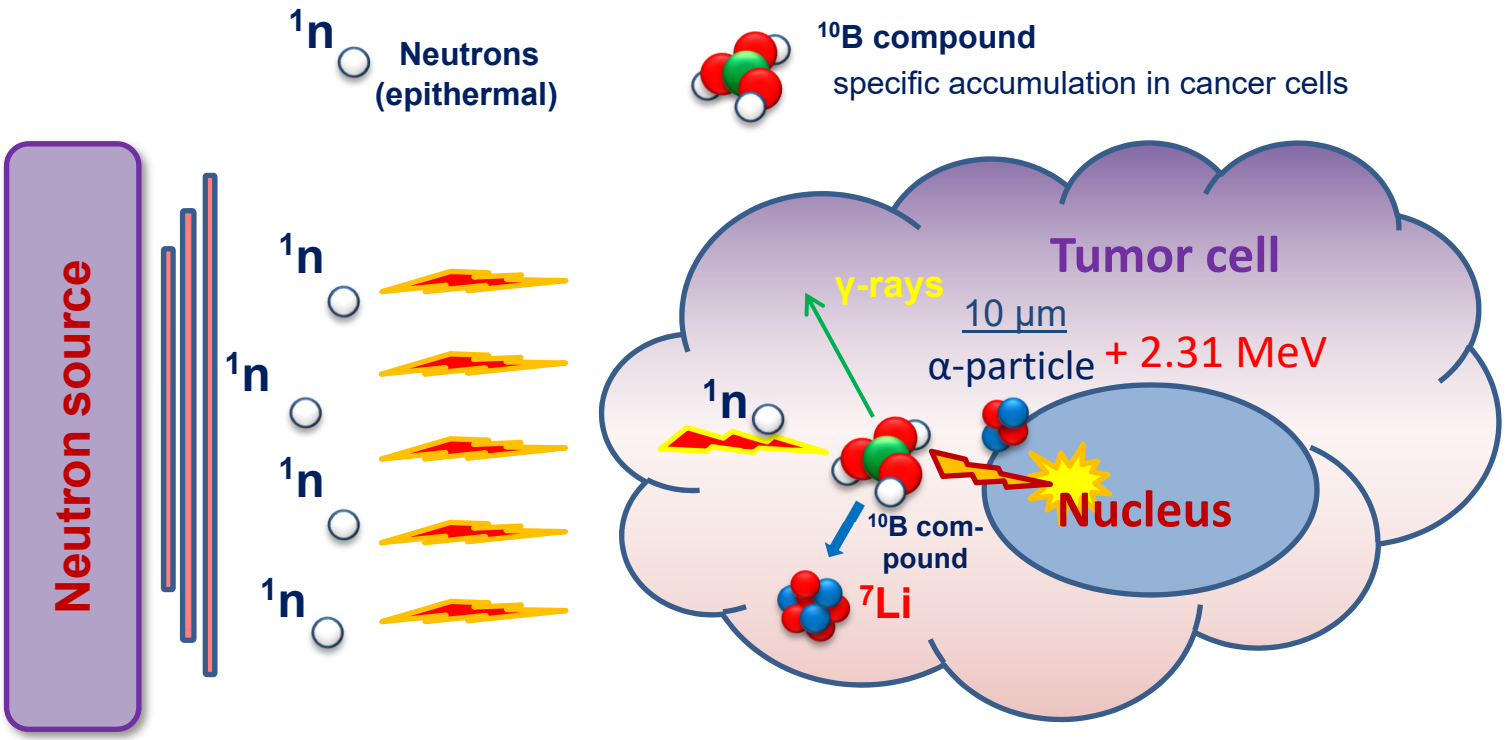

Figure S1. Principle of boron neutron capture therapy (BNCT). BNCT is a binary technology that is realized through boron-10 isotope accumulation in tumor cells and further irradiation of the tumor area with epithermal neutrons, leading to intracellular boron neutron capture reaction ($^{10}B(n,\alpha)^{7}Li$) resulting in the release of high-LET alpha particles and lithium (^{7}Li) ions that damage tumor cell DNA.

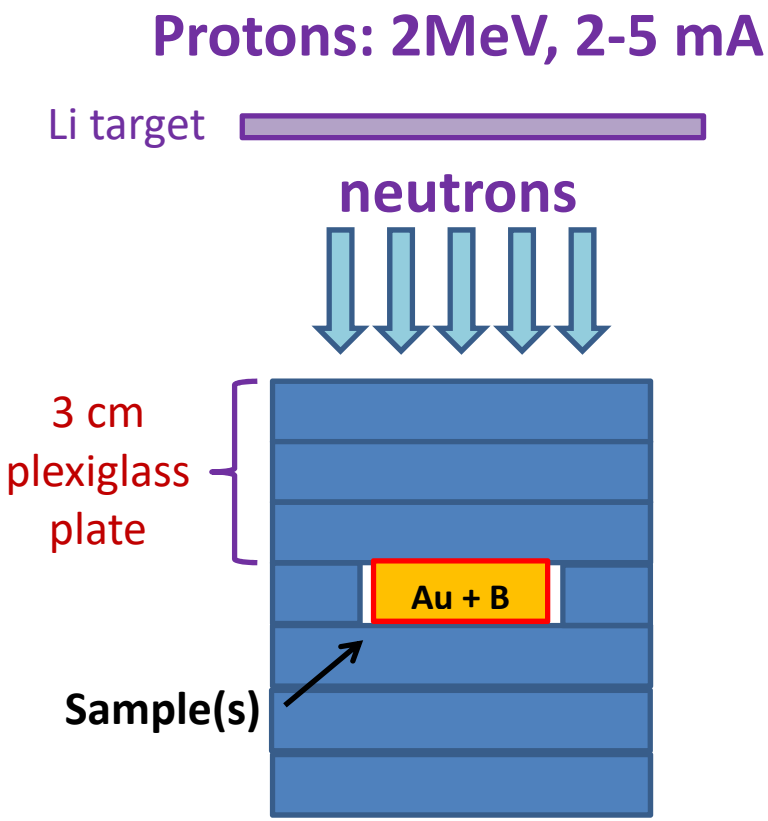

Figure S2. Combined compound irradiation. Cell-containing vials are placed in a plexiglass phantom (20 x 22 cm) at the depth of 3 cm under the neutron-producing target and irradiated with epithermal neutrons.

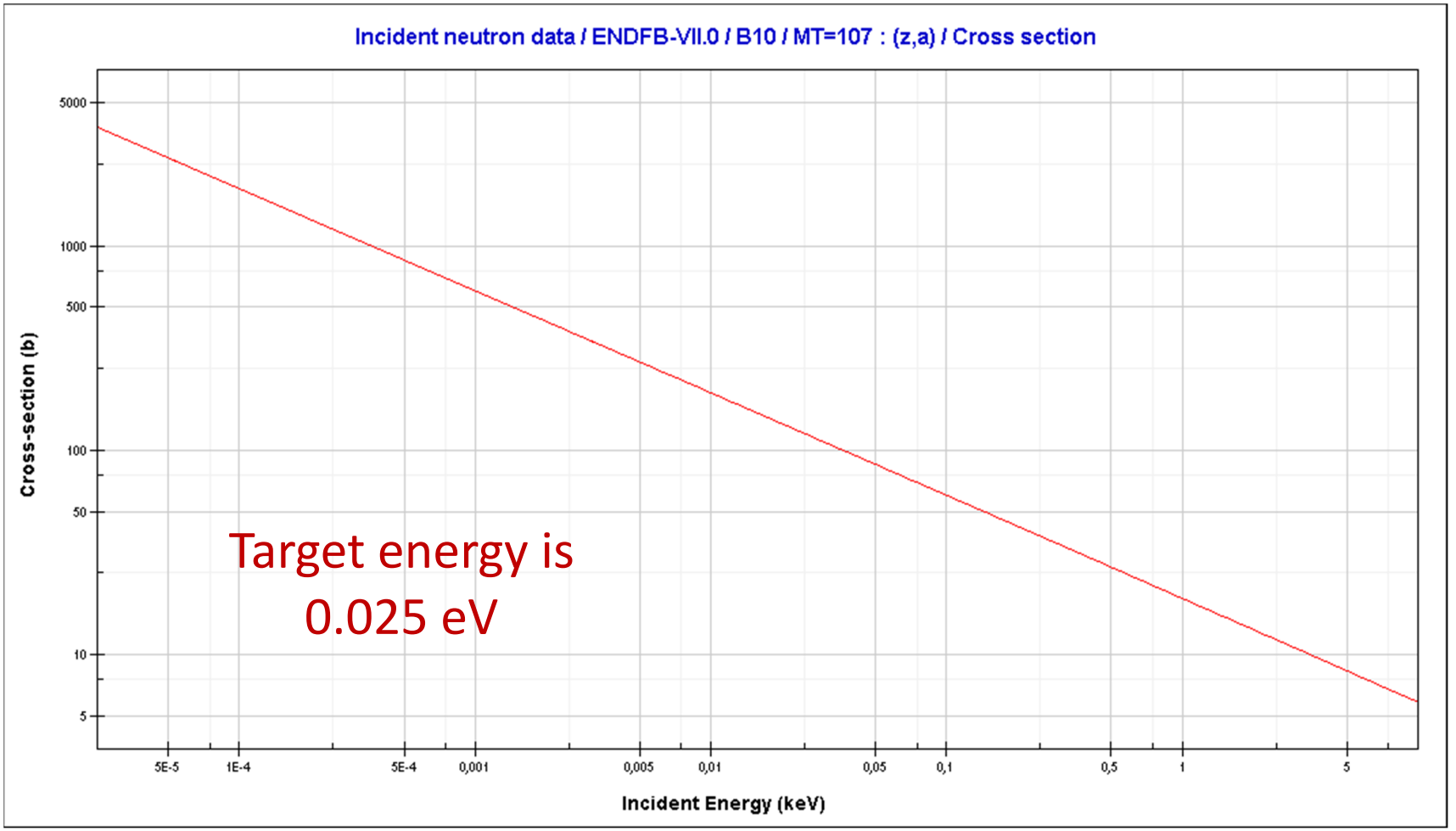

Figure S3. ^{10}B (n,α) ^{7}Li cross section.

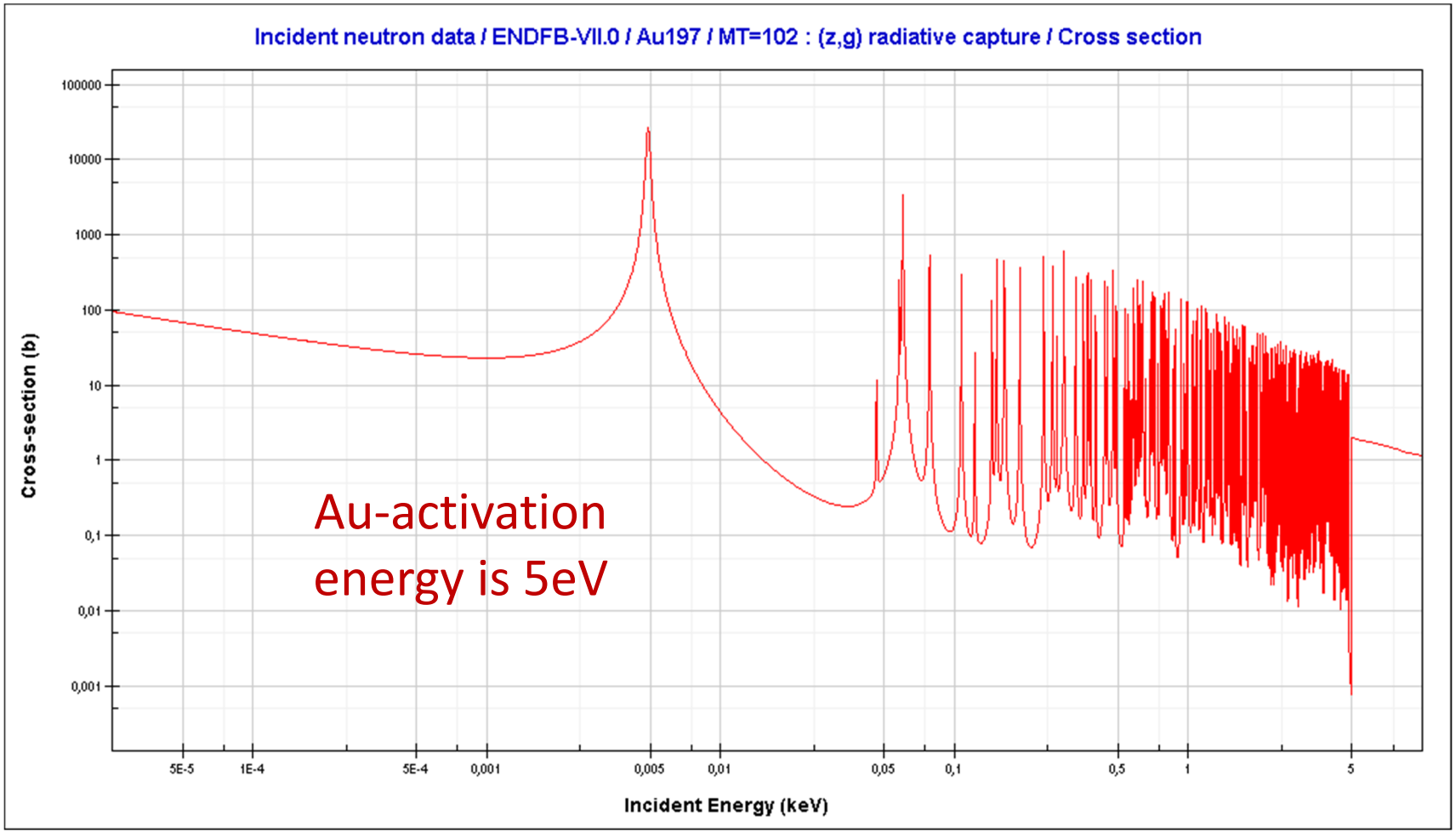

Figure S4. ^{197}Au radioactive capture cross section.

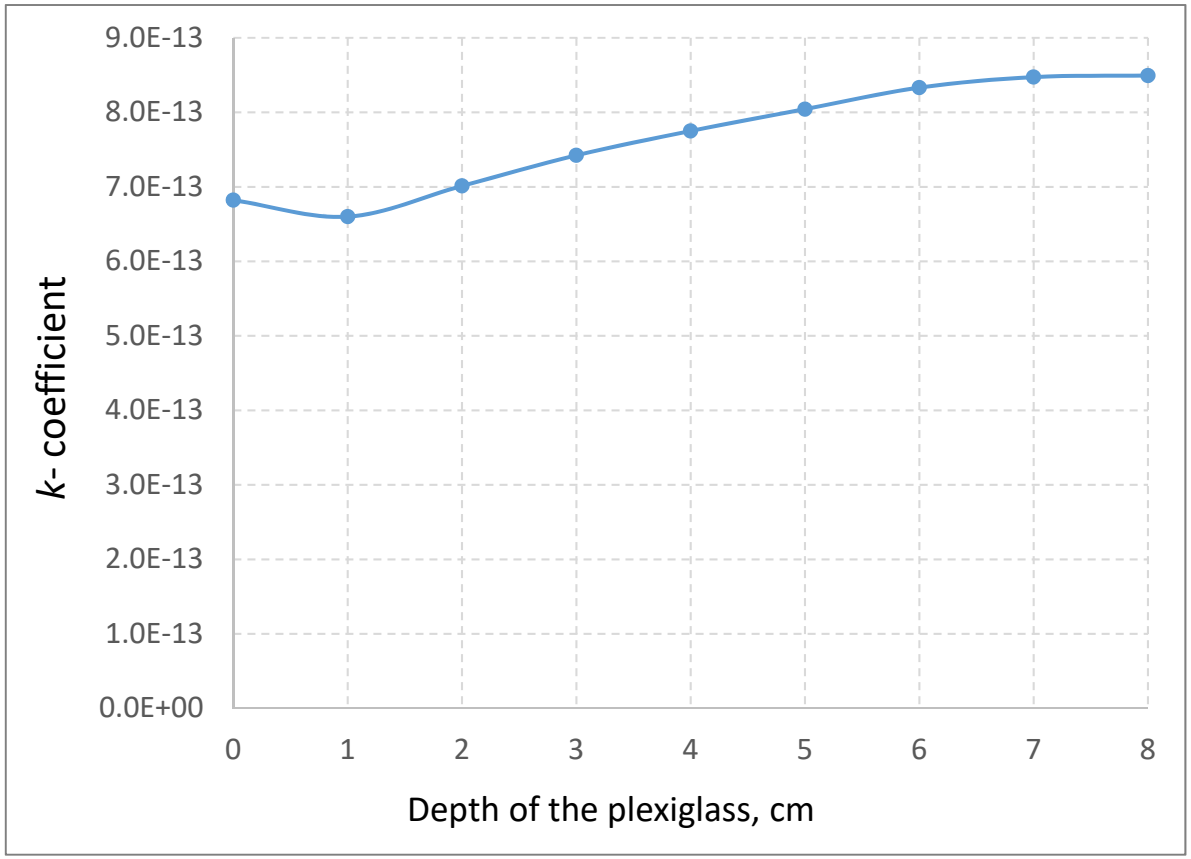

Figure S5. *k* – coefficient values versus depth of the plexiglas. The depth-related irradiation coefficient was calculated by Monte Carlo method calculated using the NMC code with 3D neutron transfer modeling according to ENDF-VII cross-section database.

Depth (cm)	Dose from boron -10 (Gy/min)	Reaction rate in 1g of Au
0,4	2,59841	9,36E+11
0,8	3,34421	9,39E+11
1,2	3,79428	8,65E+11
1,6	4,06395	7,71E+11
2	4,20305	6,75E+11
2,4	4,239	5,82E+11
2,8	4,20214	4,97E+11
3,2	4,0982	4,20E+11
3,6	3,93107	3,51E+11
4	3,72389	2,92E+11
4,4	3,49357	2,39E+11
4,8	3,25098	1,96E+11
5,2	2,98715	1,60E+11
5,6	2,72229	1,28E+11
6	2,4771	1,03E+11

Figure S6. Evaluation of the most suitable depth in plexiglass depending on both boron neutron capture reaction and gold activation.

Table S1. Detailed calculations of estimated boron-related absorbed doses.

Cells	Initial B conc., ppm	Number of cells, $\times 10^6$	Boron concentration, ppm: In 10^6 cells	In all cells	In 1mL MEM	In cells + MEM	Mass of gold: In 10^6 cells, μg	In 1mL MEM, μg	In all cells, μg	In cells+MEM, μg	Convert to g	Count rate in gold line by HPGe	Decays per second	N – number of activated gold atoms	D=(k×N×n)/m Boron dose in samples, GyE
B- Au+	0	2.75	0	0	0	0	47.57	6.39	130.82	137.21	1.37×10^4	10	212.77	71421246	0
B10 Au+	10	3	0.049	0.148	9.95	10.10	46.94	3.06	140.83	143.89	1.44×10^4	12.9	274.47	92133408	4.80
B20 Au+	20	2.15	0.069	0.148	19.95	20.10	43.22	19.03	92.91	111.94	1.12×10^4	13.3	282.98	94990257	12.65
B40 Au+	40	2.9	0.189	0.549	39.82	40.37	48.54	3.07	140.78	143.85	1.44×10^4	12.9	274.47	92133408	19.18
B- Au+	0	1.25	0	0	0	0	47.57	30.18	59.46	89.64	8.96×10^5	12.9	274.47	92133408	0
B10 Au+	10	1.7	0.049	0.084	9.97	10.06	46.94	23.40	79.80	103.20	1.03×10^4	10.3	219.15	73563884	5.32
B20 Au+	20	2.1	0.069	0.145	19.95	20.10	43.22	19.75	90.75	110.50	1.11×10^4	10.3	219.15	73563884	9.93
B40 Au+	40	2	0.189	0.379	39.87	40.25	48.54	17.64	97.09	114.73	1.15×10^4	8.8	187.23	62850697	16.36
B- Au+	0	1.6	0	0	0	0	47.57	24.63	76.11	100.74	1.01×10^4	11.9	253.19	84991283	0
B10 Au+	10	1.4	0.049	0.069	9.98	10.05	46.94	28.09	65.72	93.81	9.38×10^5	11	234.04	78563371	6.24
B20 Au+	20	1.75	0.069	0.120	19.96	20.08	43.22	24.79	75.63	100.42	1.00×10^4	6.9	146.81	49280660	7.31
B40 Au+	40	1.1	0.189	0.208	39.93	40.14	48.54	32.20	53.40	85.60	8.56×10^5	8.1	172.34	57851209	20.13

D – boron dose, GyE

N – number of activated gold atoms

n – boron concentration, ppm

m – mass of gold, g

k – coefficient, which depends on the depth (cm) to the sample in the phantom

Sensetivity HPGe in gold line (411KeV): 0.047

The time of ^{198}Au half-life, s: 232675.2

k= 7.4×10^{-13}

Boron dose in samples, GyE	Cells/Exp	B- Au+	B10 Au+	B20 Au+	B40 Au+
	1	0	4.80	12.65	19.18
	2	0	5.32	9.93	16.36
	3	0	6.24	7.31	20.13
AVERAGE		**0**	**5.45**	**9.96**	**18.56**
SD		0	0.73	2.67	1.96