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Fluorinated BPA derivatives enhanced ¹⁰B delivery in tumors

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Figure S1. Synthesis of fluorinated BPA derivatives. (a) 2F-BPA, (b) 3F-BPA, (c) 4F-BPA.



Figure S2. ESI-MS analysis of fluorinated BPA derivatives. (a) 2F-BPA, (b) 3F-BPA, and (c) 4F-BPA.



80 78 76 74 72 7.0 68 66 64 62 60 58 56 5.4 52 5.0 48 46 44 42 4.0 38 36 3.4 32 3.0 28 2.6 2.4 2.2 fl[ppm]

Figure S3. ¹H NMR spectra of f-BPA.



Figure S4. The number change of GL261 and B16-F10 cells after treatment with fructose BPA and fluorinated BPA derivatives.



Figure S5. Hematological analysis of mice intravenously injected with f-BPA and fluorinated BPA derivatives (BPA: 250 mg/kg) at day 3 (n = 3).



Figure S6. Hematological analysis of mice intravenously injected with f-BPA and fluorinated BPA derivatives (BPA: 188 mg/kg) at day 3 (n = 3).



Figure S7. Hematological analysis of mice intravenously injected with f-BPA and fluorinated BPA derivatives (BPA: 375 mg/kg) at day 3 (n = 3).



Figure S8. Body weight growth curves of mice in 3 days after administration of with f-BPA and fluorinated BPA derivatives (n=3). (a) BPA: 188 mg/kg. (b) BPA: 250 mg/kg. (c) BPA: 375 mg/kg.



Figure S9. Hematoxylin & eosin (H&E)-stained slice images of major organs collected from different groups after administration of with f-BPA and fluorinated BPA derivatives. (Scale bar: 100 μm).



Figure S10. The change of boron concentration in the mice blood over time.



Figure S11. The ¹⁰B concentration in GL261 cells after 3h and 24 h incubation with the same ¹⁰B dose (5 ppm) of f-BPA, 2F-BPA, 3F-BPA and 4F-BPA.



Figure S12. The ¹⁰B concentration in B16-F10 cells after 3 h and 24 h incubation with the same ¹⁰B dose (5 ppm) of f-BPA, 2F-BPA, 3F-BPA and 4F-BPA.



Figure S13. The ¹⁰B contents measured by ICP-MS for various organs (including heart, liver, spleen, lung, kidney, tumor and blood) of f-BPA, 2F-BPA, 3F-BPA and 4F-BPA in GL261 tumor-bearing mice.



Figure S14. The ¹⁰B contents measured by ICP-MS for various organs (including heart, liver, spleen, lung, kidney, tumor and blood) of f-BPA, 2F-BPA, 3F-BPA and 4F-BPA in B16-F10 tumor-bearing mice.

Table S1. Serum chemistry of mice intravenously injected with f-BPA and fluorinated BPA derivatives (BPA: 188 mg/kg) at day 3 (n = 3).

	ALT (U/L)	AST (U/L)	BUN (mg/dl)	CREA (µmol/L)	UA (μmol/L)	CK (U/L)	LDH (U/L)
Control	56.00±10.19	185.87±18.01	23.98±3.60	20.68±4.91	73.20±1.40	1541.47±96.75	602.38±32.02
f-BPA	43.42±4.57	172.41±17.26	21.90±5.28	20.34±3.50	52.43±16.73	1562.42±65.95	627.88±46.31
2F-BPA	56.64±16.28	207.75±22.25	25.56±5.39	20.80±5.28	82.71±5.13	1697.36±244.38	837.04±110.03
3F-BPA	46.23±3.80	140.55±31.28	20.99±3.27	16.02±3.41	97.42±34.01	1624.51±494.23	859.72±82.11
4F-BPA	53.12±9.70	146.18±40.36	24.63±7.09	20.66±1.64	60.17±11.74	1446.55±296.24	657.07±85.80

Table S2. Serum chemistry of mice intravenously injected with f-BPA and fluorinated BPAderivatives (BPA: 375 mg/kg) at day 3 (n = 3).

	ALT (U/L)	AST (U/L)	BUN (mg/dl)	CREA (µmol/L)	UA (μmol/L)	CK (U/L)	LDH (U/L)
Control	56.00±10.19	185.87±18.01	23.98±3.60	20.68±4.91	73.20±1.40	1541.47±96.75	602.38±32.02
f-BPA	52.15±12.48	153.87±23.30	22.11±1.44	22.14±0.33	80.87±25.92	1298.54±431.76	679.20±119.06
2F-BPA	45.15±3.69	168.26±16.47	30.70±5.30	21.94±1.55	64.00±19.09	1358.93±320.42	747.72±58.46
3F-BPA	48.83±16.89	102.25±20.70	27.21±5.75	19.71±2.40	71.13±19.68	1398.79±309.34	746.66±93.21
4F-BPA	43.40±5.72	131.85±25.14	21.95±4.62	19.79±4.20	77.04±12.15	1063.47±305.48	610.99±77.60