## **Supplementary Materials**

Tailoring the Radionuclide Encapsulation and Surface Chemistry of La(<sup>223</sup>Ra)VO<sub>4</sub> Nanoparticles for Targeted Alpha Therapy

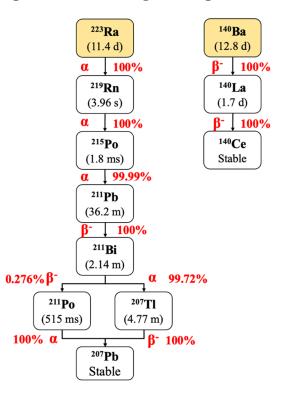
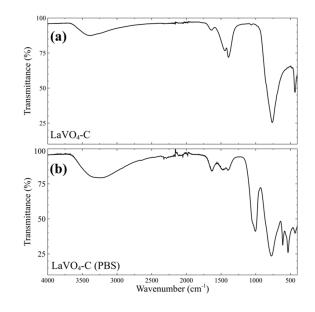


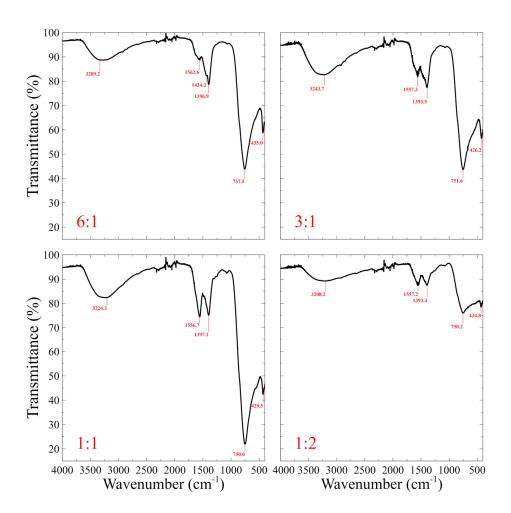
Figure S1. Decay schemes of <sup>223</sup>Ra and <sup>140</sup>Ba.

**Table S1.** Summary of  $\gamma$ -ray energies and intensities used to calculate the activity of each radionuclide [1].

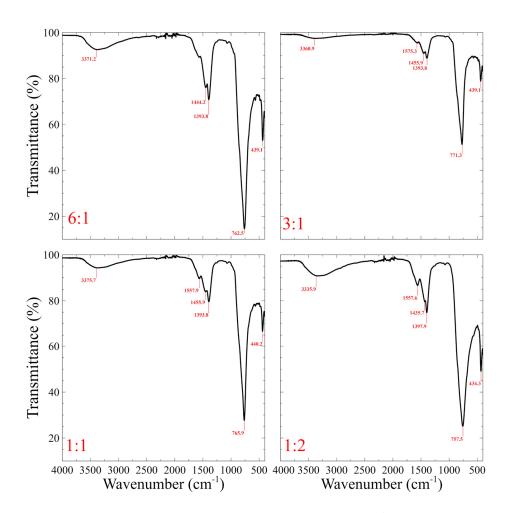
Radionuclide	γ-ray energy (keV)	Intensity (%)
<sup>223</sup> Ra	144.23	3.27
	154.08	5.70
	269.46	13.90
<sup>211</sup> Pb	404.85	3.78
	832.01	3.52
<sup>211</sup> Bi	351.07	13.02
<sup>140</sup> Ba	162.66	6.22
	304.85	4.29
	537.26	24.39
<sup>140</sup> La	328.76	20.30
	487.02	45.50
	815.77	23.28



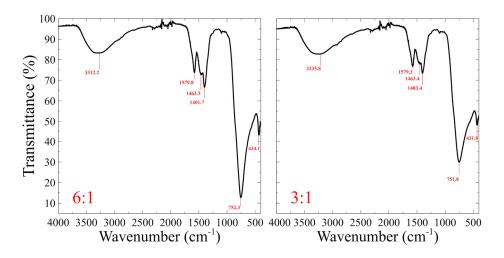
**Figure S2.** Dispersion of LaVO<sub>4</sub> NPs in phosphate-buffered saline (PBS; 1X, pH = 7.4) results in the addition of phosphate groups on the particle surface. FTIR spectra of LaVO<sub>4</sub> NPs synthesized following procedure C (a) before and (b) after dispersion in PBS.



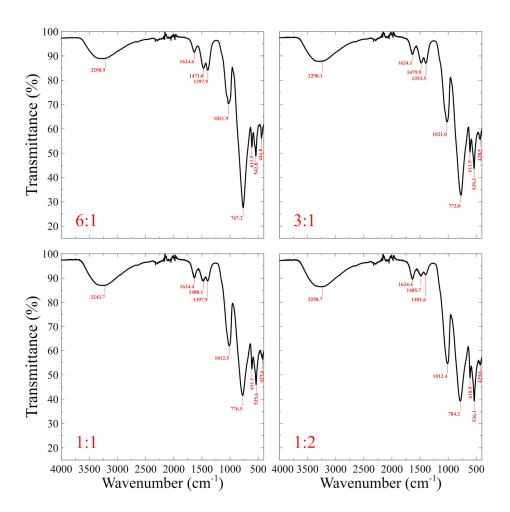
**Figure S3.** Increase molar fraction of NH<sub>4</sub>-Cit results in the appearance of the carboxylate bidentate bond stretching band at  $\sim$ 1,560 cm<sup>-1</sup>, where a 1:1 LaVO<sub>4</sub>:NH<sub>4</sub>-Cit molar ratio exhibits the highest transmittance for the carboxylate bidentate bond stretching band. FTIR spectra of LaVO<sub>4</sub> NPs modified with NH<sub>4</sub>-Cit at different LaVO<sub>4</sub>:NH<sub>4</sub>-Cit molar ratios.



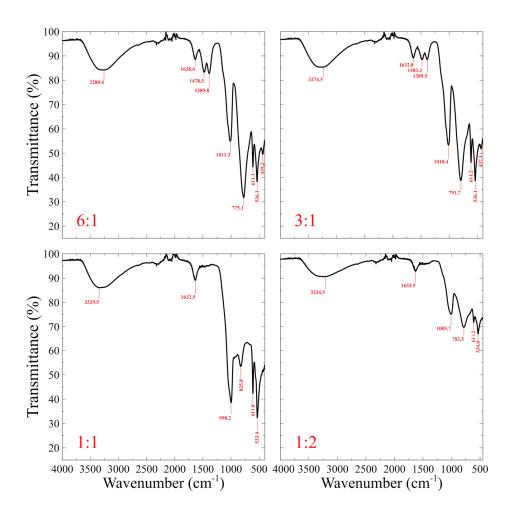
**Figure S4.** Carboxylate bidentate bond stretching band at ~1,560 cm<sup>-1</sup> is evidenced at LaVO4:Na-Cit molar ratios greater than 1:1. FTIR spectra of LaVO4 NPs modified with Na-Cit at different LaVO4:Na-Cit molar ratios.



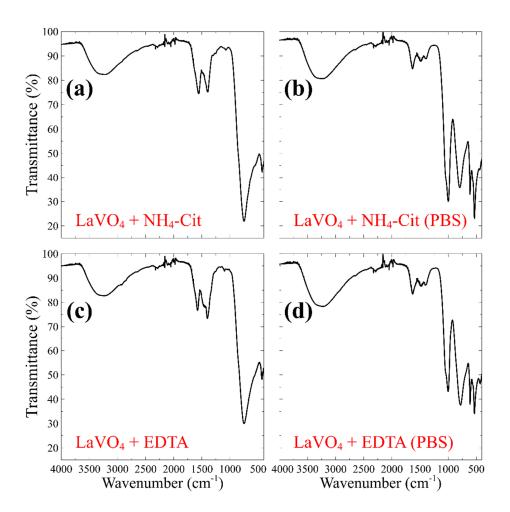
**Figure S5.** Surface modification with EDTA is evidenced by the carboxylate bidentate bond stretching band  $\sim 1,580 \text{ cm}^{-1}$ . A shift of the carboxylate bidentate bond stretching relative to NH<sub>4</sub>-Cit and Na-Cit suggest differences in the coordination of the carboxylate groups around the La cation. FTIR spectra of LaVO<sub>4</sub> NPs modified with EDTA at different LaVO<sub>4</sub>:EDTA molar ratios.



**Figure S6.** LaVO<sub>4</sub> NPs modified with TPP exhibited characteristic phosphate vibration bands at LaVO<sub>4</sub>:TPP molar ratios as low as 1:6. FTIR spectra of LaVO<sub>4</sub> NPs modified with TPP at different LaVO<sub>4</sub>:TPP molar ratios.



**Figure S7.** Characteristic phosphate vibration bands observed in LaVO<sub>4</sub> NPs modified with Hex at LaVO<sub>4</sub>:Hex molar ratios as low as 1:6. LaVO<sub>4</sub>:Hex molar ratios greater than 1:1 removed the vibration bands corresponding to carboxylate groups from precipitation of carbonate species. FTIR spectra of LaVO<sub>4</sub> NPs modified with Hex at different LaVO<sub>4</sub>:Hex molar ratios.



**Figure S8.** Presence of phosphate vibration bands after dispersing  $LaVO_4 + NH_4$ -Cit and  $LaVO_4 + EDTA$  in PBS. FTIR spectra of  $LaVO_4 + NH_4$ -Cit and  $LaVO_4 + EDTA$  NPs (a, c) before and (b, d) after dispersion in PBS (1X, pH = 7.4).

## References

[1] "Nudat 2." https://www.nndc.bnl.gov/nudat2/ (accessed Jun. 12, 2020).