Supporting Information (SI)

αvβ3 Integrin-targeted ICG-derivated theranostic probes for imaging-guided surgery and photothermal therapy of oral cancer

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Scheme S1. The synthetic route of probes Cy-RGD and Cy-2RGD.
Figure S1. $^1$H and $^{13}$C NMR spectra of compound cypate.
Figure S2. MALDI-TOF/MS spectrum of compound cypate.

Figure S3. MALDI-TOF/MS spectrum of compound Cy-RGD.
Figure S4. MALDI-TOF/MS spectrum of compound Cy-2RGD.

Figure S5. NIR fluorescence images of Cy-2RGD with different concentrations at 1000 nm.

Figure S6. Quantitative fluorescence intensity of ICG, Cy-RGD, and Cy-2RGD with various long-pass filters in Fig. 1(d).
Table S1. Quantum yields of Cy-RGD and Cy-2RGD in PBS buffer. ICG was chosen as the reference (Φ = 2.5%). All the measurements were performed at room temperature.

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<th>Cy-RGD</th>
<th>Cy-2RGD</th>
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<td>QY(θ)</td>
<td>2.0%</td>
<td>2.4%</td>
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Figure S7. The stability of Cy-2RGD in PBS buffer at room temperature.

Figure S8. (a) Confocal fluorescence images of CAL-27 cells that were pretreated with or without RGD peptide (5 μg mL⁻¹, 4 h) for 4 h, then followed by incubating with Cy-2RGD (10 μg mL⁻¹) for different time points (1 h, 2 h, and 4 h) at 37 °C, (b) Quantitative fluorescence intensities of (a). Scale bar: 40 μm.
Fig S9. The fitted curve EC50 of Cy-RGD and Cy-2RGD under 808 nm laser irradiation.

Fig S10. Live/dead fluorescence images of oral tumor cells treated with Cy-RGD for 24 h followed by 808 nm laser irradiation (1 W cm⁻², 5 min) or not.
Figure S11. Images and representative mice captured on different days after each treatment.

Figure S12. Survival curve (a) and body weight changes (b) of mice for each treatment group (n=5).
Figure S13. H&E staining graphs of major organs for representative mice with various treatments captured on 21 days. Scale bar: 50 μm.

Supplementary video.mp4