

## Supplementary Information

### Charge and Hydrophobicity Effects of NIR Fluorophores on Bone-Specific Imaging

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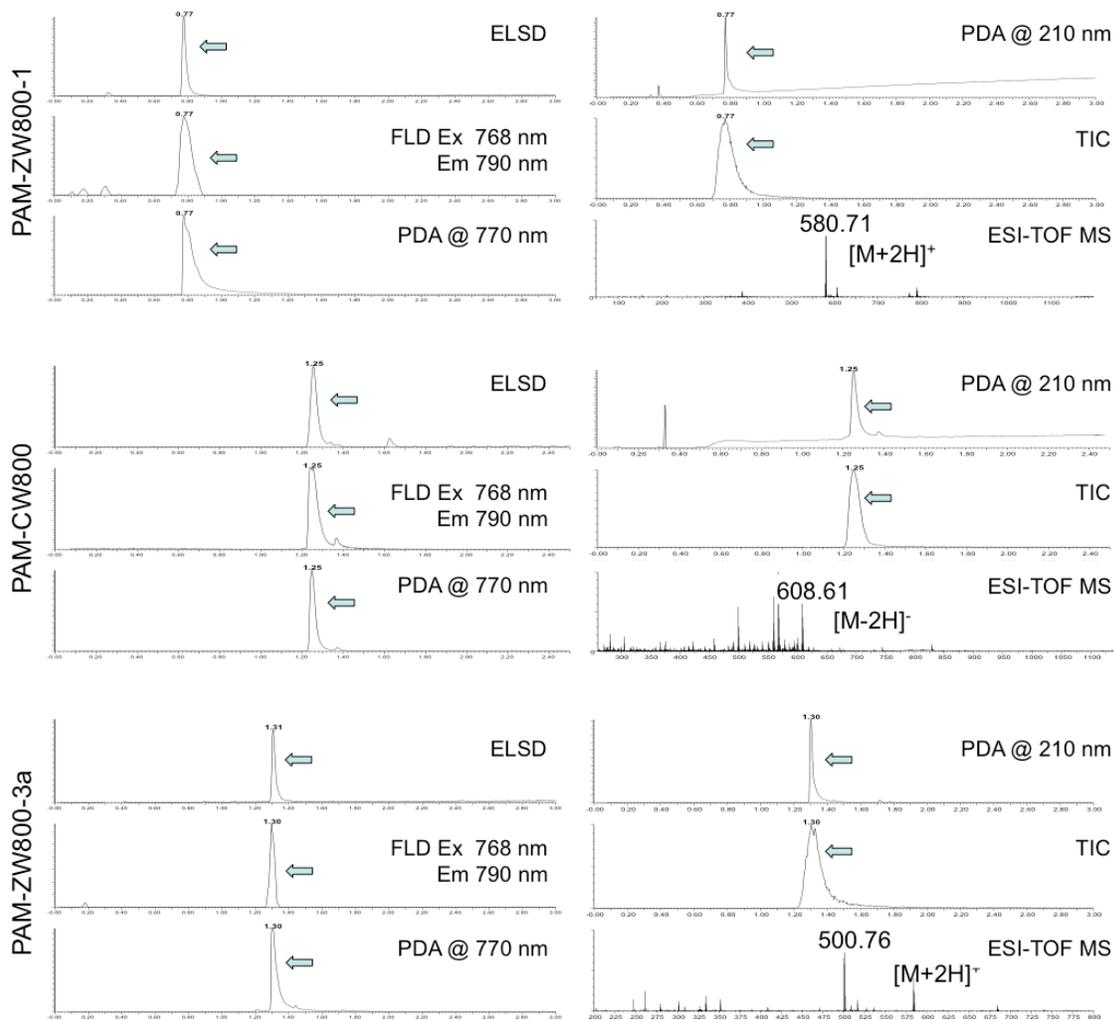
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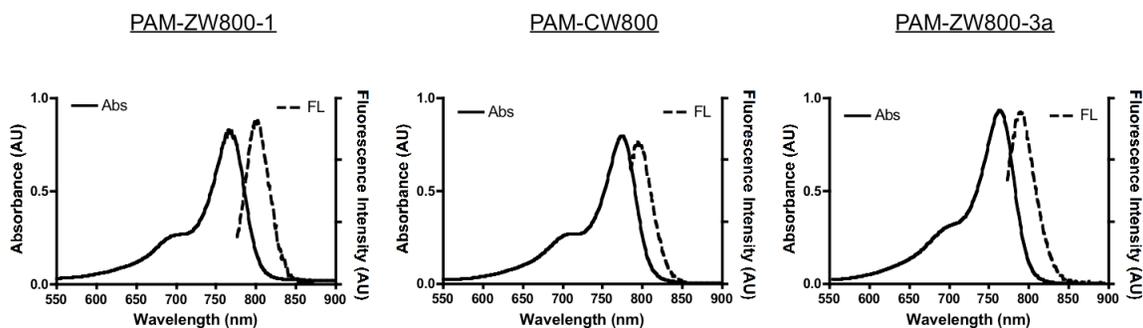
**Figure S1.** LC-MS analysis and purity of the PAM-NIR fluorophore conjugates.

**Figure S2.** Optical properties of NIR fluorophores having systematically varying net charges.

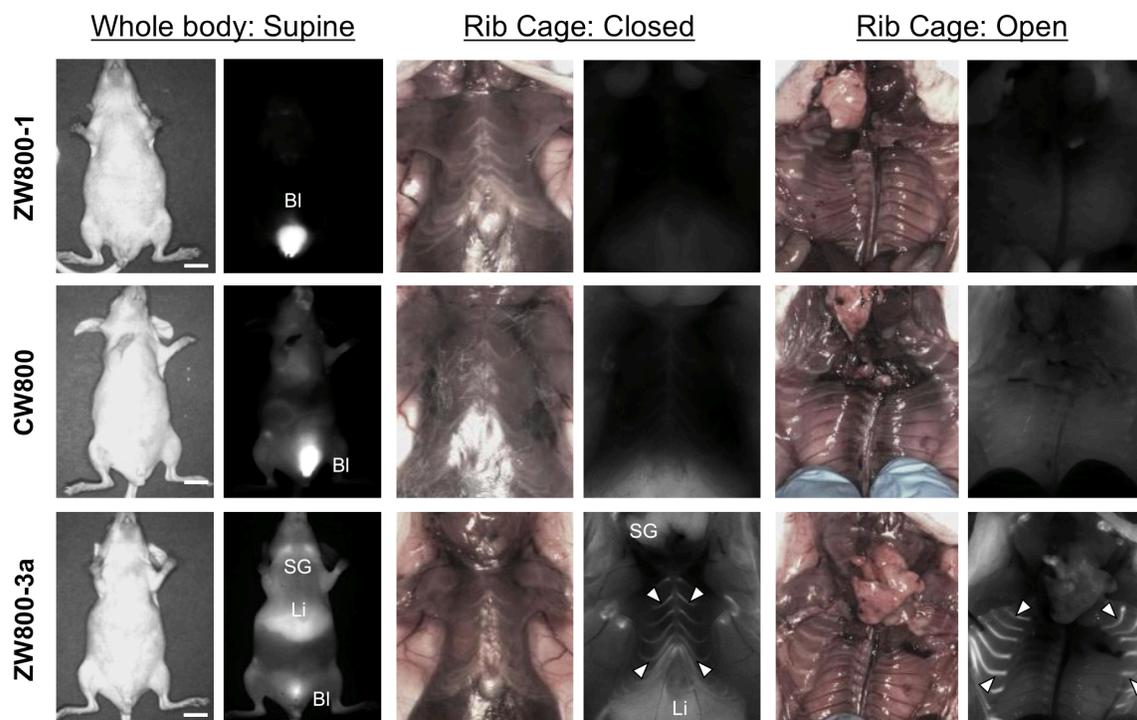
**Figure S3.** *In vivo* biodistribution and bone specific imaging using unconjugated NIR fluorophores in mice.



**Figure S1.** LC-MS analysis and purity of the PAM-NIR fluorophore conjugates: ELSD, fluorescence ( $\lambda_{\text{ex}} = 768 \text{ nm}$ ,  $\lambda_{\text{em}} = 790 \text{ nm}$ ), absorbance (PDA) at 770 nm and 210 nm, total ion chromatogram (TIC), and ESI-TOF mass spectra.



**Figure S2.** Optical properties of NIR fluorophores having systematically varying net charges. All optical measurements were performed at 37°C in 100% fetal bovine serum (FBS), buffered with 50 mM HEPES, pH 7.4. NIR excitation was provided by a 770 nm NIR laser diode light source.



**Figure S3.** *In vivo* biodistribution and bone specific imaging using unconjugated NIR fluorophores in mice. 10 nmol of each NIR fluorophore was injected intravenously into 25 g nude mice 4 h prior to imaging. Arrowheads indicate cartilage tissues. Li = liver, SG = salivary glands, and BI = bladder. Scale bars = 1 cm. All NIR fluorescence images were collected with the same exposure time and are displayed with identical normalization.