

## Supporting Information

### Multimodal Prussian Blue-type Analogs as Contrast Agents for X-ray Computed Tomography

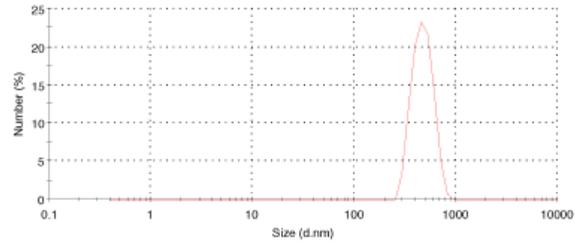
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Khuu<sup>§</sup>, Jose-Ramon Galan-Mascaros<sup>†,‡,\*</sup>, and Karn Sorasaene<sup>§,‡,\*</sup>*

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Institute, Children's Hospital Los Angeles, Keck School of Medicine of USC, Los Angeles, CA  
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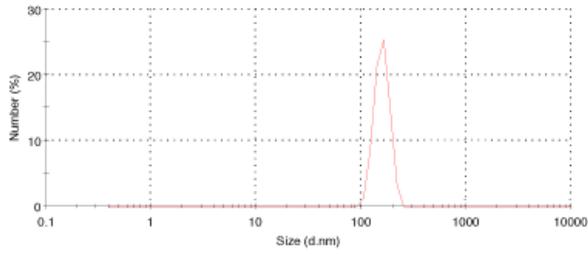
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Spain

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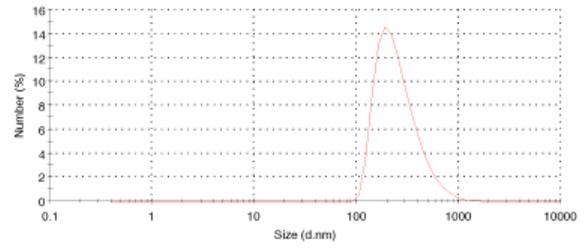
<sup>\*</sup>*Department of Chemistry and Beckman Institute, California Institute of Technology, Pasadena, CA  
91125 USA*



**1**

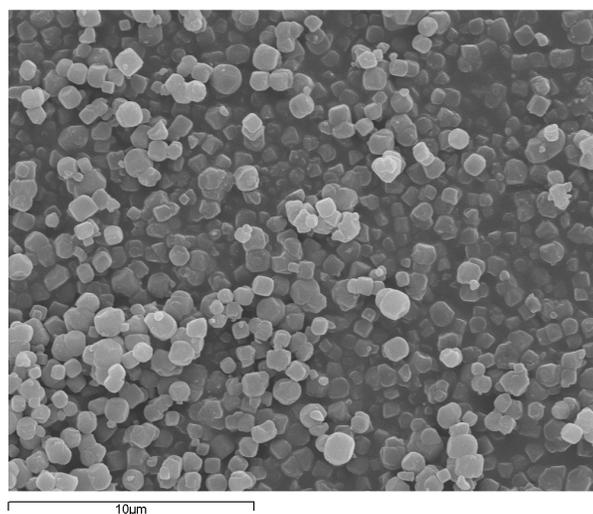


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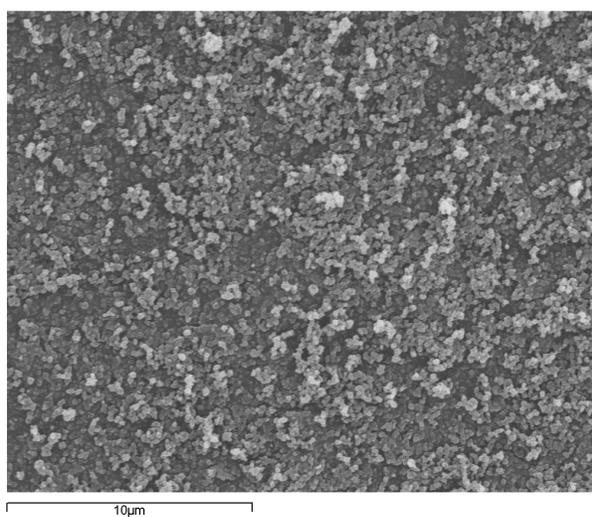


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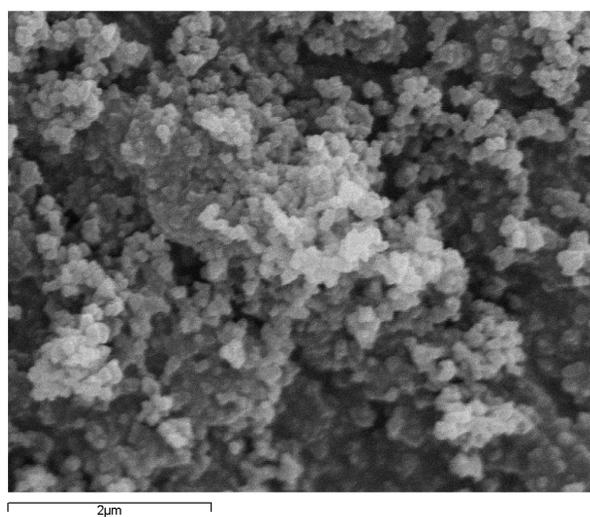
**Figure S1.** Size distribution of PBA 1-3 analyzed by dynamic light scattering (DLS) in aqueous suspensions.



1

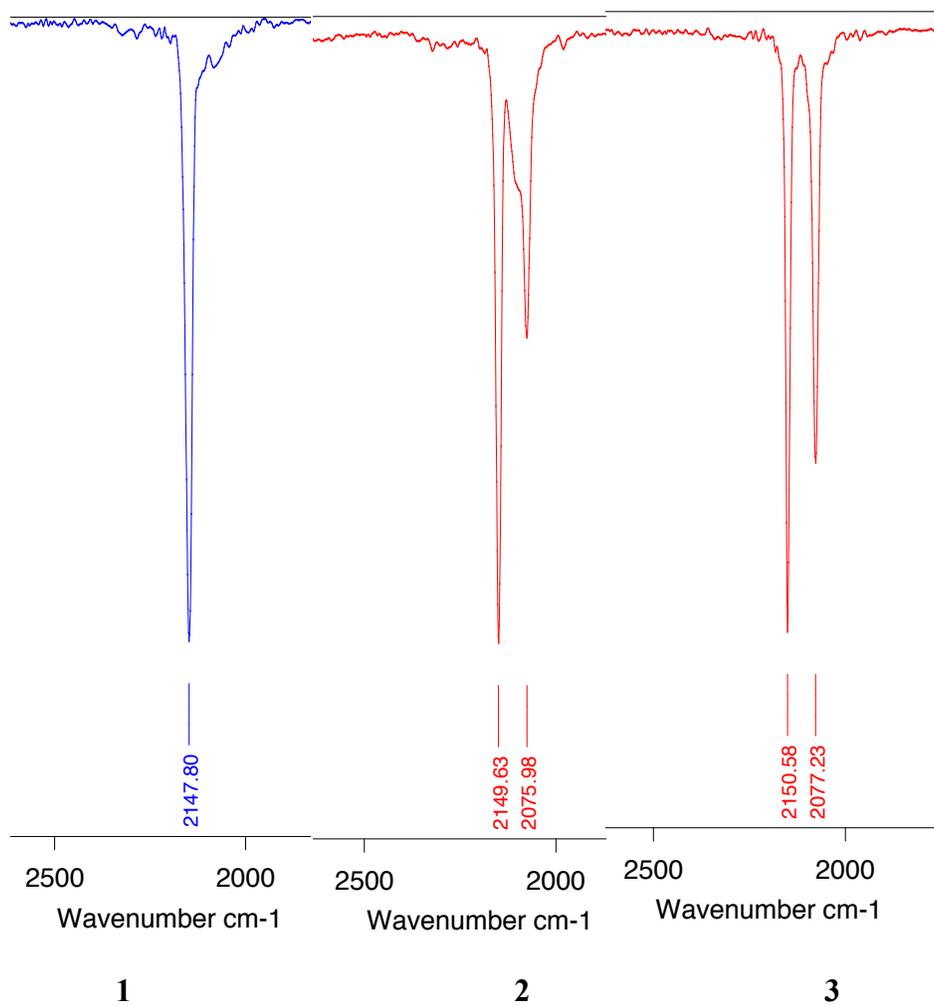


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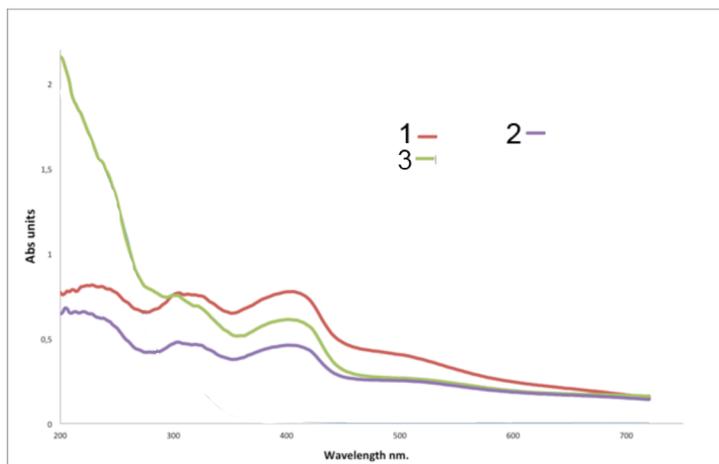


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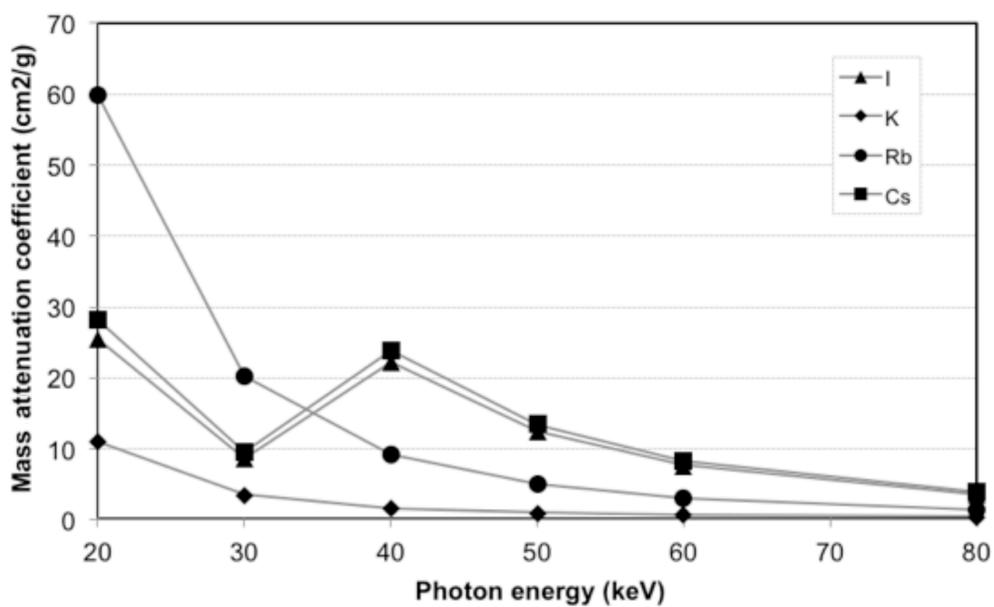
**Figure S2.** Scanning electron microscopic (SEM) images of 1-3.



**Figure S3.** FT-IR spectra of **1-3** highlighting the corresponding CN stretches.

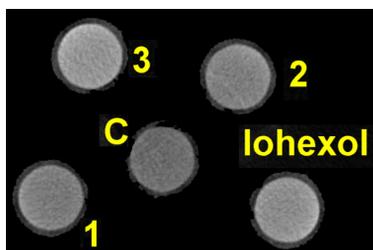


**Figure S4.** UV-vis spectra of **1-3** in water suspension.

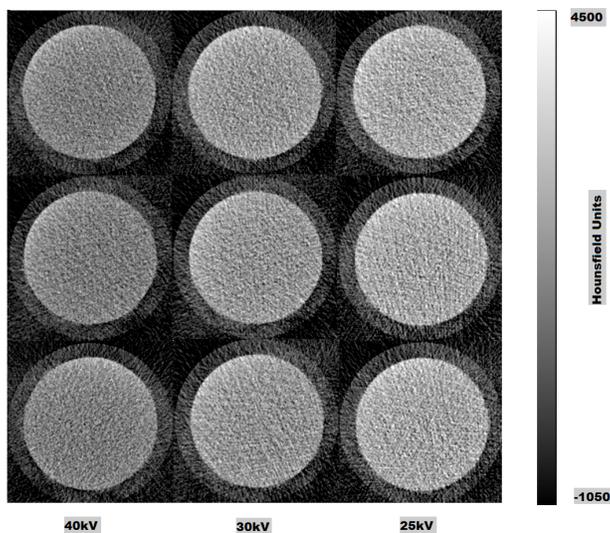


**Figure S5.** Plot of mass attenuation coefficients for the elements I ( $Z = 53$ ), K ( $Z = 19$ ), Rb ( $Z = 37$ ), and Cs ( $Z = 55$ ) as a function of photon energy.

[<http://physics.nist.gov/PhysRefData/XrayMassCoef/tab3.html>].

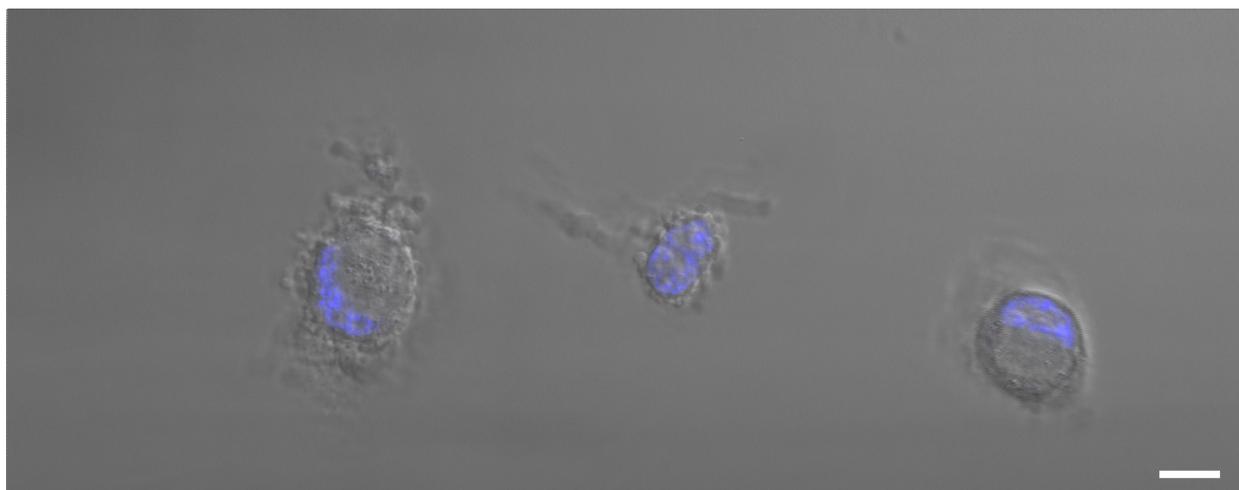


a



b

**Figure S6.** (a) High-resolution X-ray  $\mu$ -CT image of iohexol and PBAs (1-3) suspended in 2.5% agarose. Phantoms scanned at 25 kV; C denotes the control that does not contain any contrast agents. (b) High-resolution X-ray  $\mu$ -CT image of PBA 3 in triplicate scanned at various X-ray tube voltages (25, 30, and 40 kV).



**Figure S7.** Transmitted microscopic image with the 10- $\mu$ m scale bar showing U87-Luc cells not treated with PBAs as a control. The blue areas are nuclei stained with the nuclear dye Hoechst 33342.