Purpose: To assess the impact of adopting a quasi-monochromatic x-ray source for bench-top x-ray fluorescence computed tomography (XFCT) imaging of gold nanoparticle-loaded objects.

Methods: A Monte Carlo (MC) model of an experimental XFCT system was created using the MCNP5 code. This model was used to simulate irradiation of a small animal-sized plastic phantom containing water columns loaded with gold nanoparticles (GNPs) at various concentrations (2% or less by weight) with a Pb-filtered polychromatic x-ray source. MC results were verified with measurements to validate the model. Subsequently, MC simulations were repeated with monochromatic x-ray sources (85, 90, and 95 keV) to determine the most ideal x-ray energy to discriminate between gold K-shell fluorescence peaks and the Compton scatter background. As a practical alternative to monochromatic x-rays, a quasi-monochromatic x-ray spectrum was experimentally created from a polychromatic x-ray spectrum (110 kVp) by using a highly oriented pyrolitic graphite (HOPG) crystal. This spectrum was used for further MC simulations to assess the effect of a quasi-monochromatic x-ray spectrum on the detection of gold K–shell fluorescence x-rays.

Results: Monochromatic x-ray energy needed to exceed 95 keV in order for the gold K-shell fluorescence peaks (67 and 69 keV) to be discernible over the Compton scatter background at the detector position (90 degrees with respect to the beam axis). At the same GNP concentration, there was at least a three-fold increase in the gold fluorescence peak-to-scatter background ratio from using the HOPG-generated quasi-monochromatic source spectrum, compared to that from using the Pb-filtered polychromatic source spectrum.

Conclusions: Since a monochromatic synchrotron x-ray beam, although ideal, is not readily available for a bench-top XFCT system, quasi-monochromatization of a polychromatic x-ray source spectrum to peak at certain energies appears to help dramatically improve the detection efficiency of K-shell fluorescence x-rays from GNPs.