

SUPPORTING INFORMATION TO:

Silica Nanoparticle-Generated ROS as a Predictor of Cellular Toxicity: Mechanistic Insights and Safety by Design

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Cell Viability Data for 4 and 24 Hours in RAW 264.7 Macrophage Cell Line

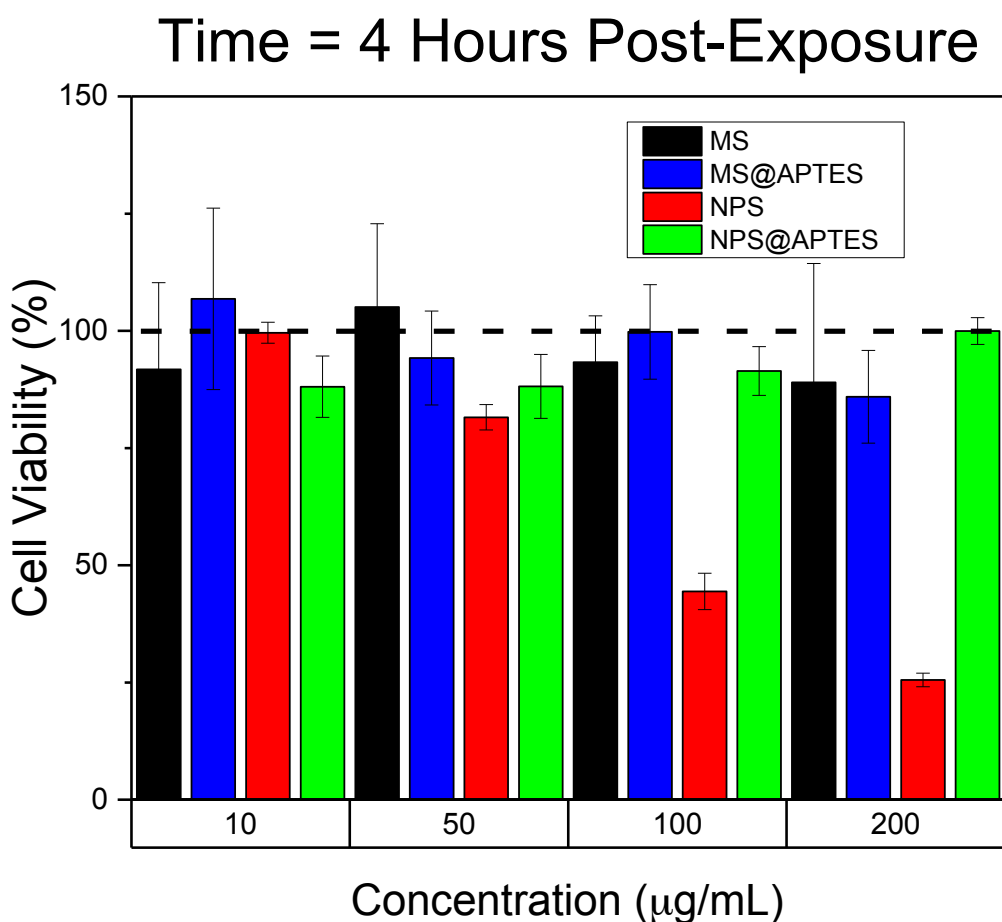


Figure S1. Cell viability data in RAW 264.7 macrophage cell line at 4 hours post-exposure.

Time = 24 Hours Post-Exposure

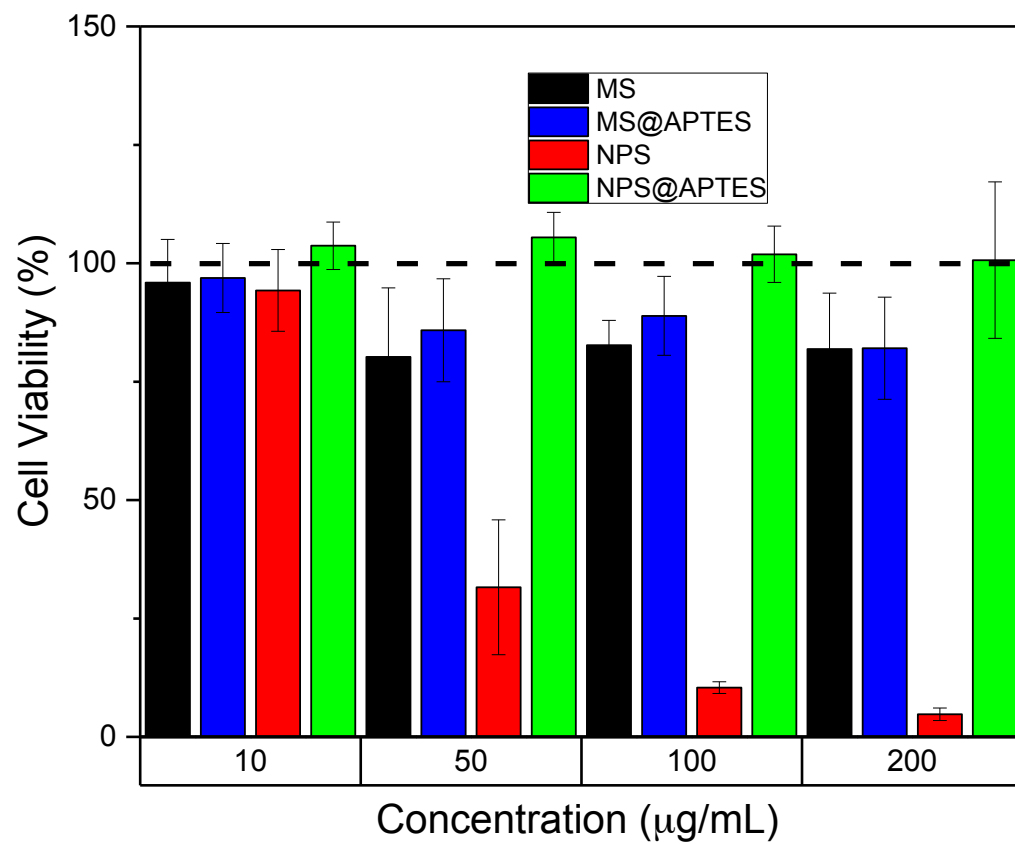


Figure S2. Cell viability in RAW 264.7 macrophage cell line at 24 hours post-exposure.

Cell Viability Time-Dependence of NPS Material

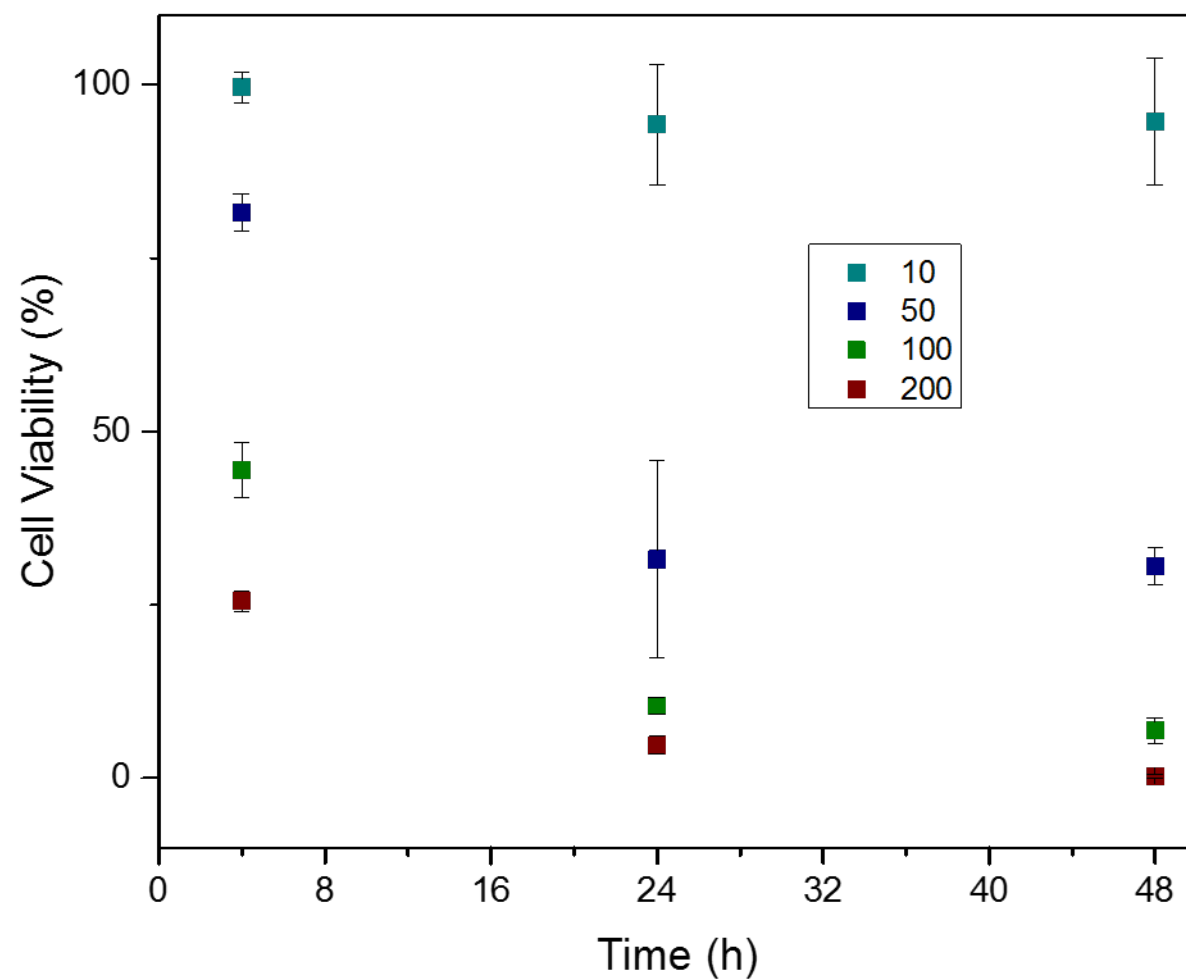


Figure S3. Time-dependent cell viability data in RAW 264.7 macrophage cell line for NPS material as a function of time and concentration (in µg/mL).

Cell Viability Data for Min-U-Sil

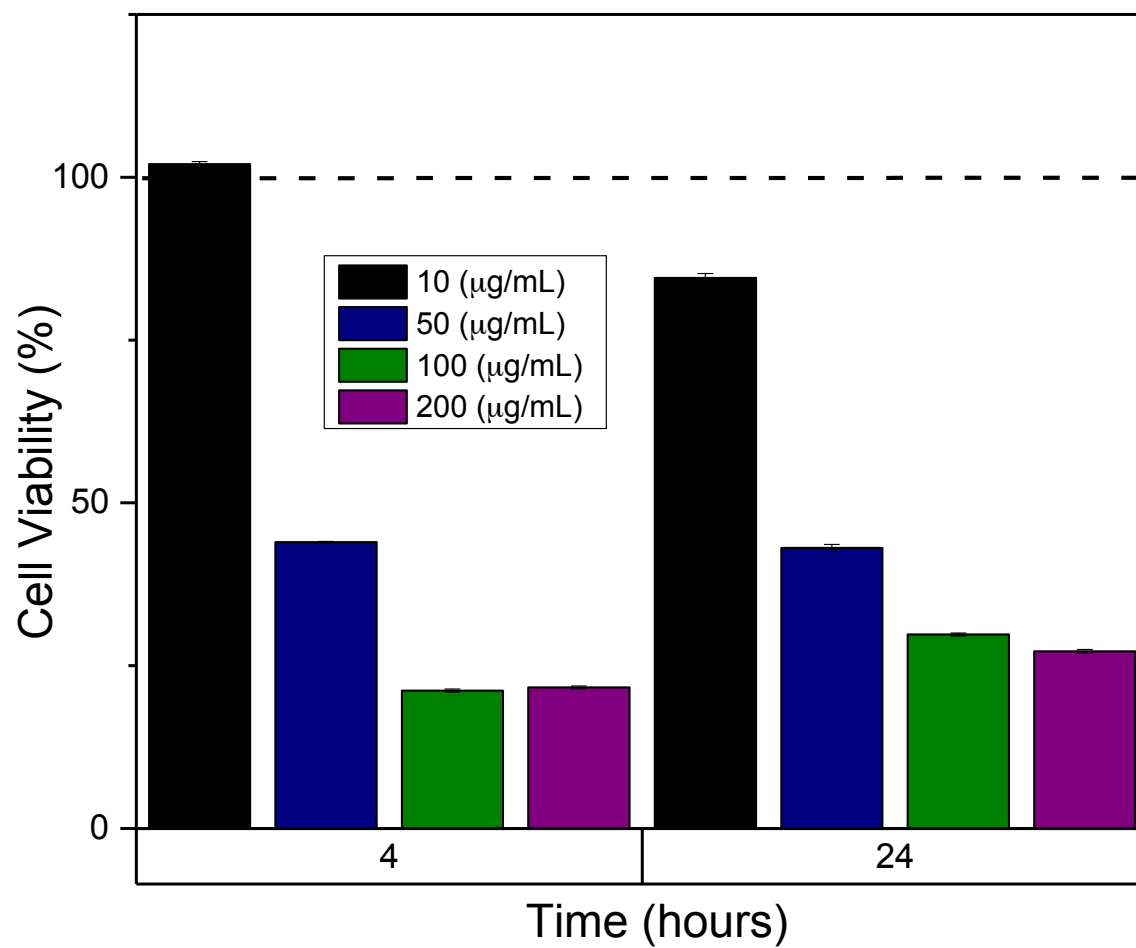


Figure S4. Cell viability data for Min-U-Sil in RAW 264.7 macrophage cell line as a function of time and concentration (µg/mL).

EPR Data Tabulated Values

Sample	Radical Type	Radical Concentration [Absolute] (nM)	Radical Production (pmol/m ²)
MS	OH*	105.52	1.91
MS@APTES	OH*	203.1	5.81
MS@APTES	NO*	104.2	2.98
NPS	OH*	729.8	221.2
NPS@APTES	OH*	284.3	135.4
NPS@APTES	NO*	69.4	33.0
Min-U-Sil	OH*	72.4	188.7

Table ST1. Tabulated data for the EPR spectra, which are displayed graphically in the main text.

EPR Spectrum of Min-U-Sil in Water

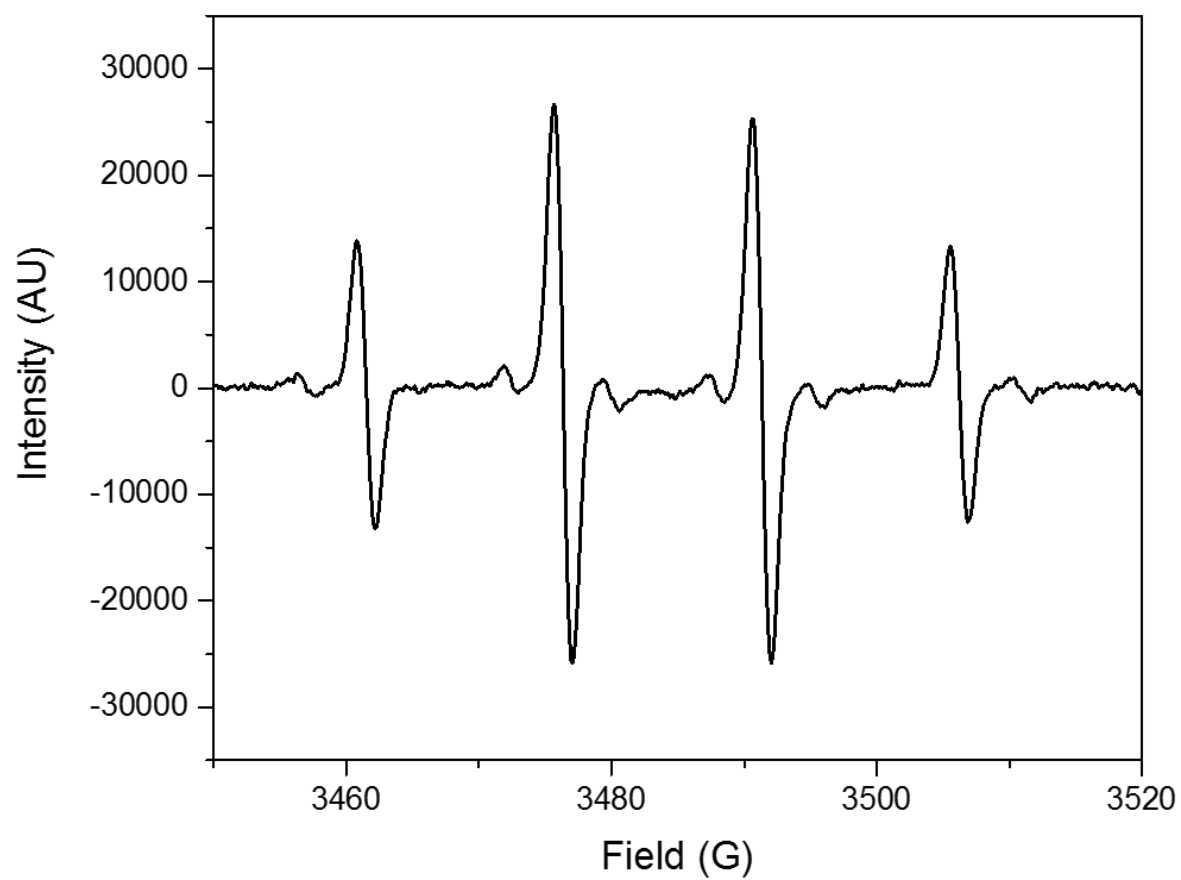
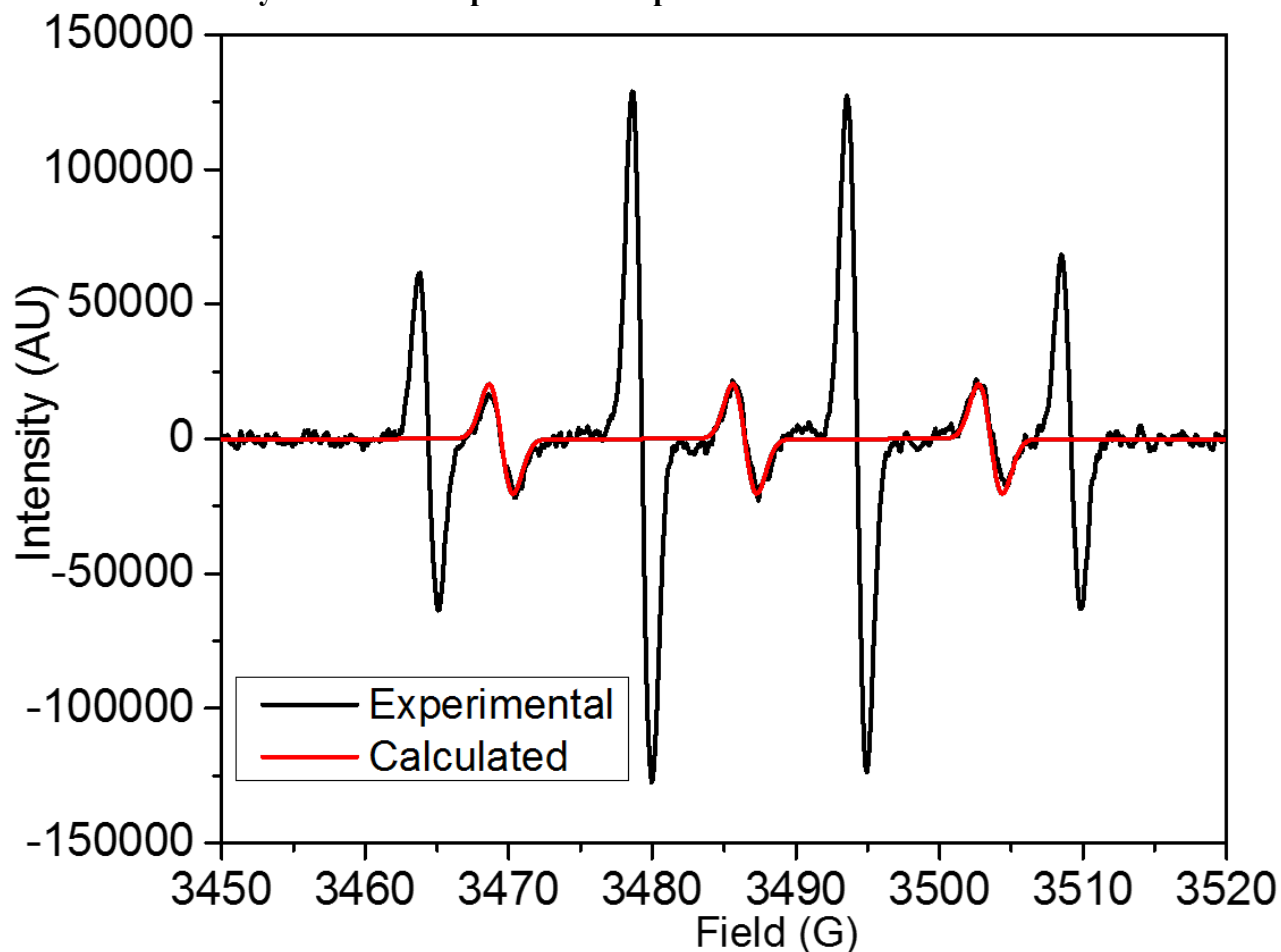


Figure S5. EPR spectrum of Min-U-Sil in water with added peroxide.

Simulated Aminoxy Radical Comparison to Experimental Data



FigureS6. Comparison of experimental MS@APTES EPR spectrum with a calculated EPR spectrum for the proposed aminoxy radical calculated using EasySpin (garlic). The spectral intensity of the calculated spectrum has been matched to that of the experimental spectrum.

***In Vivo* Radical Concentration Calculation**

$$\frac{15,000 \text{ particles}}{\text{cell}} * \frac{\text{g}}{1.90 \times 10^{16} \text{ particles}} * \frac{1102 \text{ m}^2}{\text{g}} = \frac{1.66 \times 10^{-21} \text{ m}^2}{\text{cell}}$$

$$[\text{OH}^*] = \frac{1.91 \text{ pmol}}{\text{m}^2} * \frac{1.66 \times 10^{-21} \text{ m}^2}{\text{cell}} * \frac{\text{cell}}{2 \times 10^{-12} \text{ L}} = 8.31 \times 10^{-10} \text{ (M)} = 0.83 \text{ (nM)}$$

$$\frac{\text{Experimental } [\text{H}_2\text{O}_2]}{\text{In Vivo } [\text{H}_2\text{O}_2]} = \frac{0.200 \text{ M}}{1.0 \times 10^{-7} \text{ M}} = 2 \times 10^6$$

$$\text{Corrected } [\text{OH}^*] = \frac{8.31 \times 10^{-10} \text{ (M)}}{2 \times 10^6} = 4.2 \times 10^{-16} \text{ (M)}$$