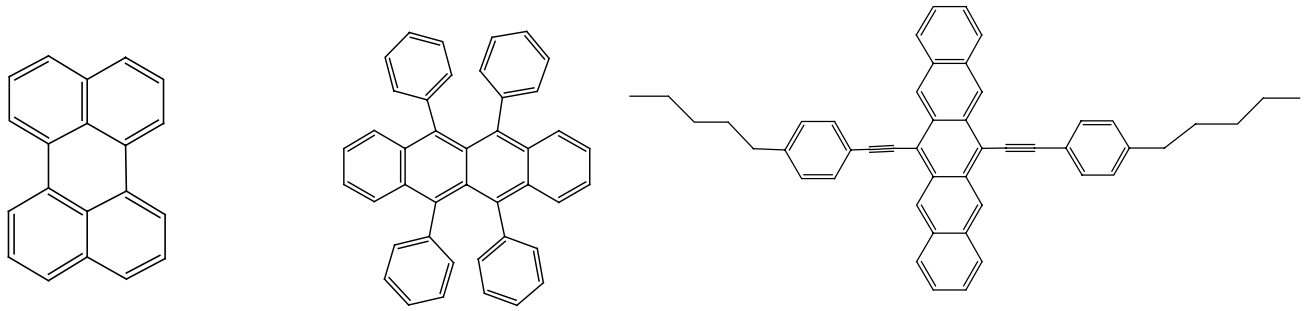
Supplementary information

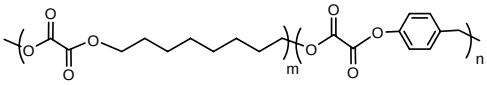
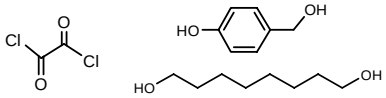
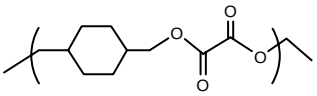
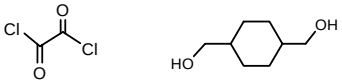
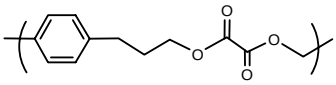
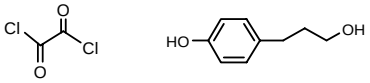
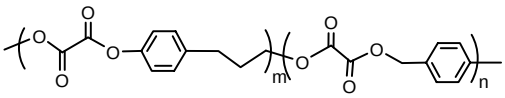
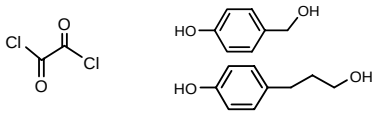
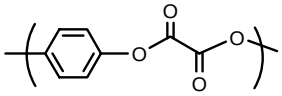
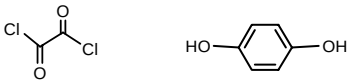
In vivo imaging of hydrogen peroxide with chemiluminescent nanoparticles



Perylene **Rubrene** **6,13-bis (4-pentylphenylethynyl) pentacene**

Figure 1S. Chemical structure of fluorescent dyes used in peroxalate nanoparticles

Table 1S. Properties of peroxalate polymers

No.	Polymer	Monomers	Comments
1			Used in this work
2			Low reactivity to hydrogen peroxide
3			Poor stability in water
4			Poor stability in water
5			No polymerization

Comment on Table 1S.

Peroxalate polymers **2**, **3**, **4** and **5** were synthesized according to the procedure developed for the synthesis of polymer **1**, their chemical structures are shown in Table 1S. Polymers **2**, **3**, **4**, **5** were formulated with rubrene and the their chemiluminescence intensity was evaluated in the presence of hydrogen peroxide. Nanoparticles formulated from polymers **2, 3,** and **4** had a low chemiluminescence intensity in the presence of hydrogen peroxide. Therefore, polymer **1** was chosen for the imaging experiments.

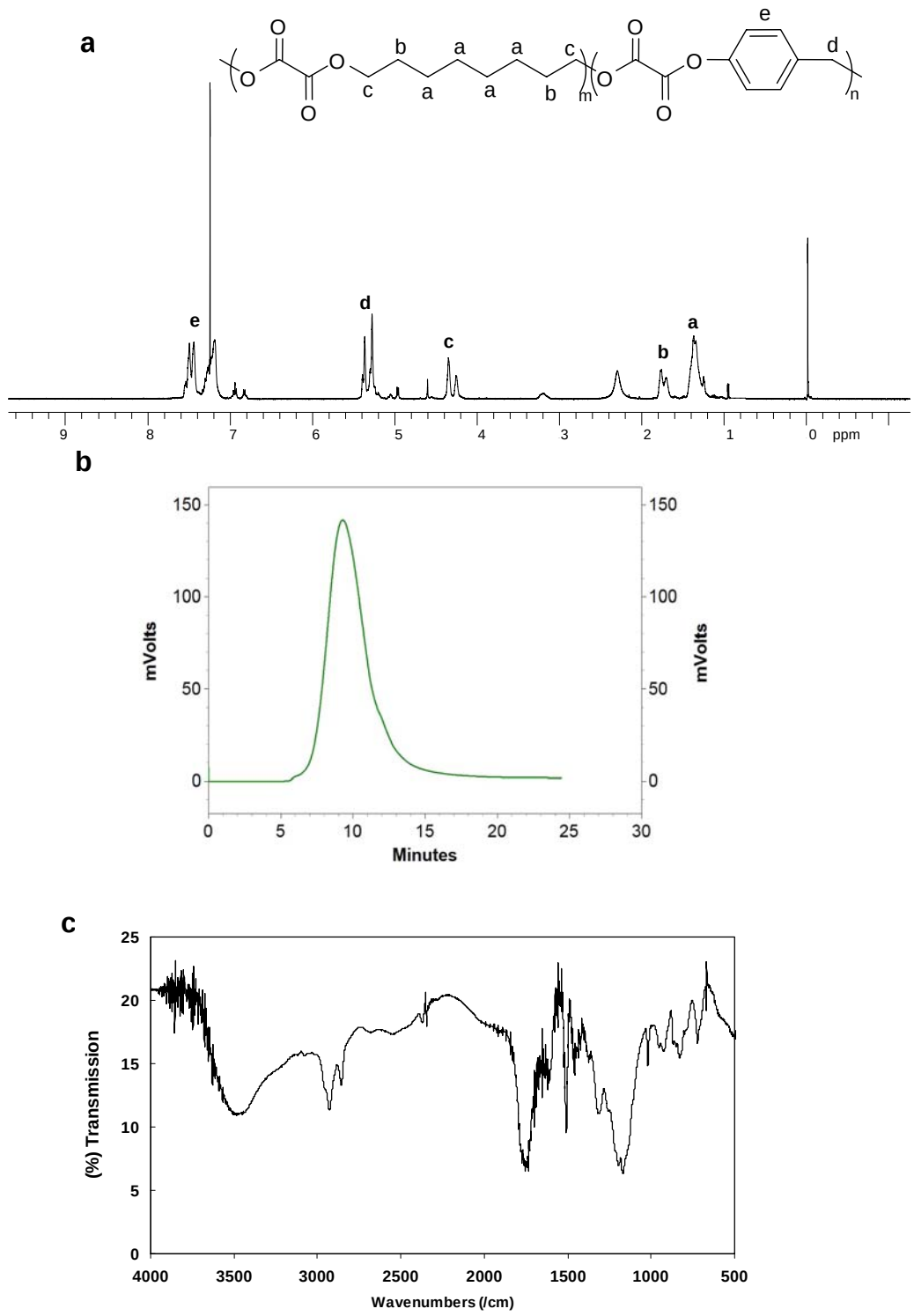


Figure 2S. Characterization of polymer 1. (a) ^{1}H-NMR-spectrum, (b) GPC chromatogram, (c) FT-IR spectrum. The H-NMR spectrum of polymer **1** was measured on a 500MHz spectrometer (Bruker) using deuterated chloroform as the solvent. GPC was measured with a Shimadzu SCL-10A using polystyrene standards. The prominent bands at 1200 and 1750 cm^{-1}, on the FT-IR spectrum, correspond to the C-O and C=O stretches of the peroxalate ester, respectively. The C-H stretch appears at 2900 cm^{-1}.

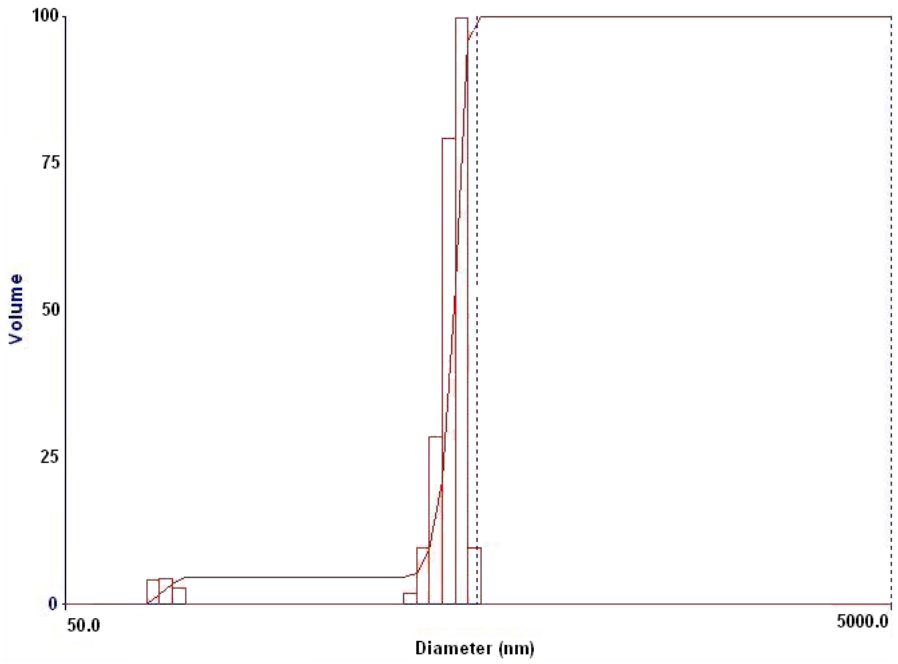


Figure 3S. Dynamic light scattering of rubrene-encapsulated peroxalate nanoparticles. DLS samples were measured at a concentration of 0.25mg/mL in pH 7.4 PBS buffer with a Brookhaven 90Plus particle sizer.

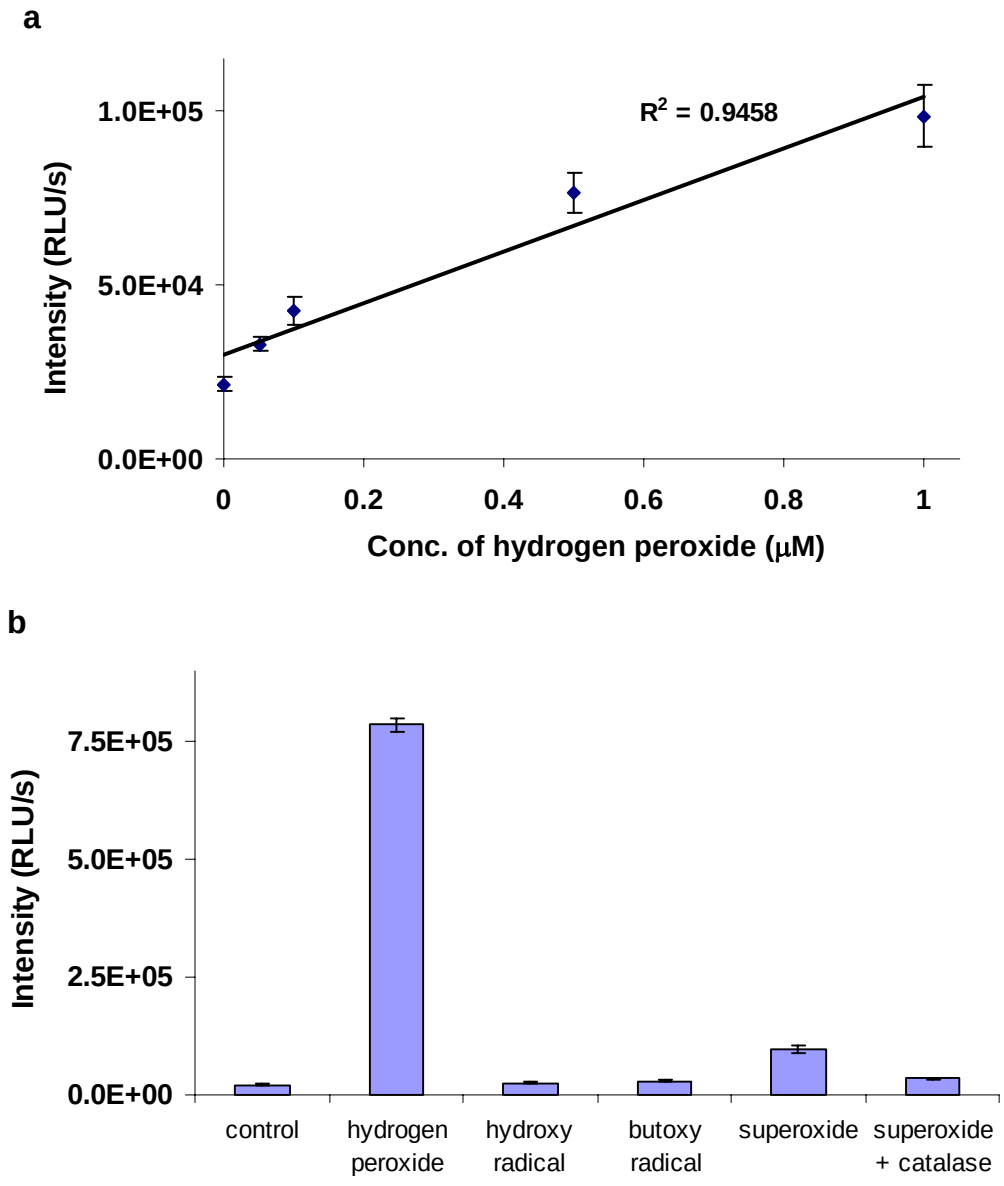


Figure 4S. Sensitivity and selectivity of pentacene containing peroxalate nanoparticles. (a). Chemiluminescence intensity of pentacene containing peroxalate nanoparticles at a concentration of hydrogen peroxide < 1μM. (b) Chemiluminescence response of nanoparticles (1 mg/mL) to various reactive oxygen species. Superoxide was added as solid KO_2. Hydroxyl radical and butoxy radical were generated by the reaction of 10 mM of Fe^{2+} with 1 mM hydrogen peroxide or 1 mM *tert*-butyl hydroperoxide.

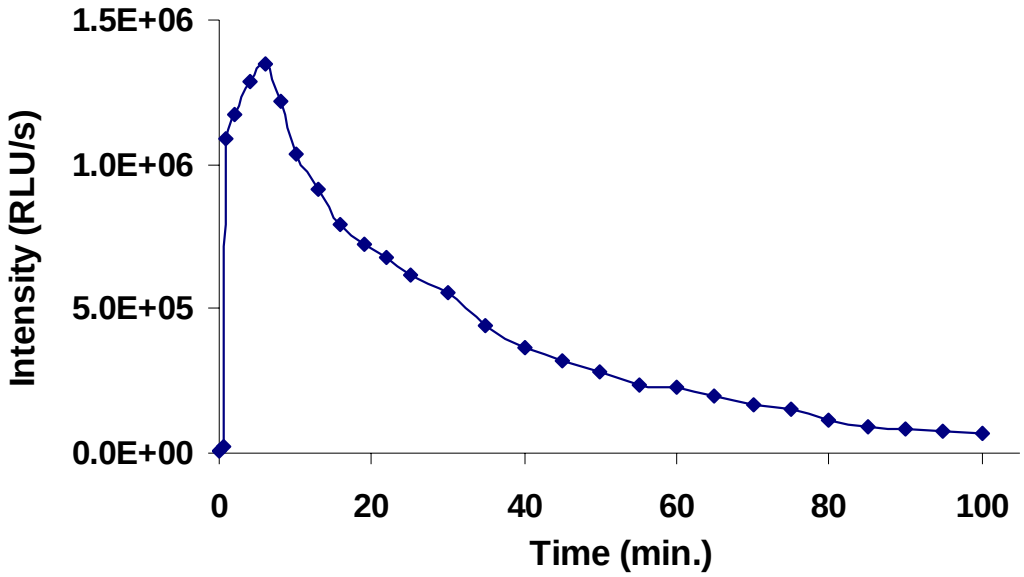


Figure 5S. Kinetics of chemiluminescence from peroxalate nanoparticles containing rubrene in the presence of 10 μM of hydrogen peroxide.