

Supplementary Materials

Self-assembled triphenylphosphonium-conjugated dicyanostilbene nanoparticles and their fluorescence probes for reactive oxygen species

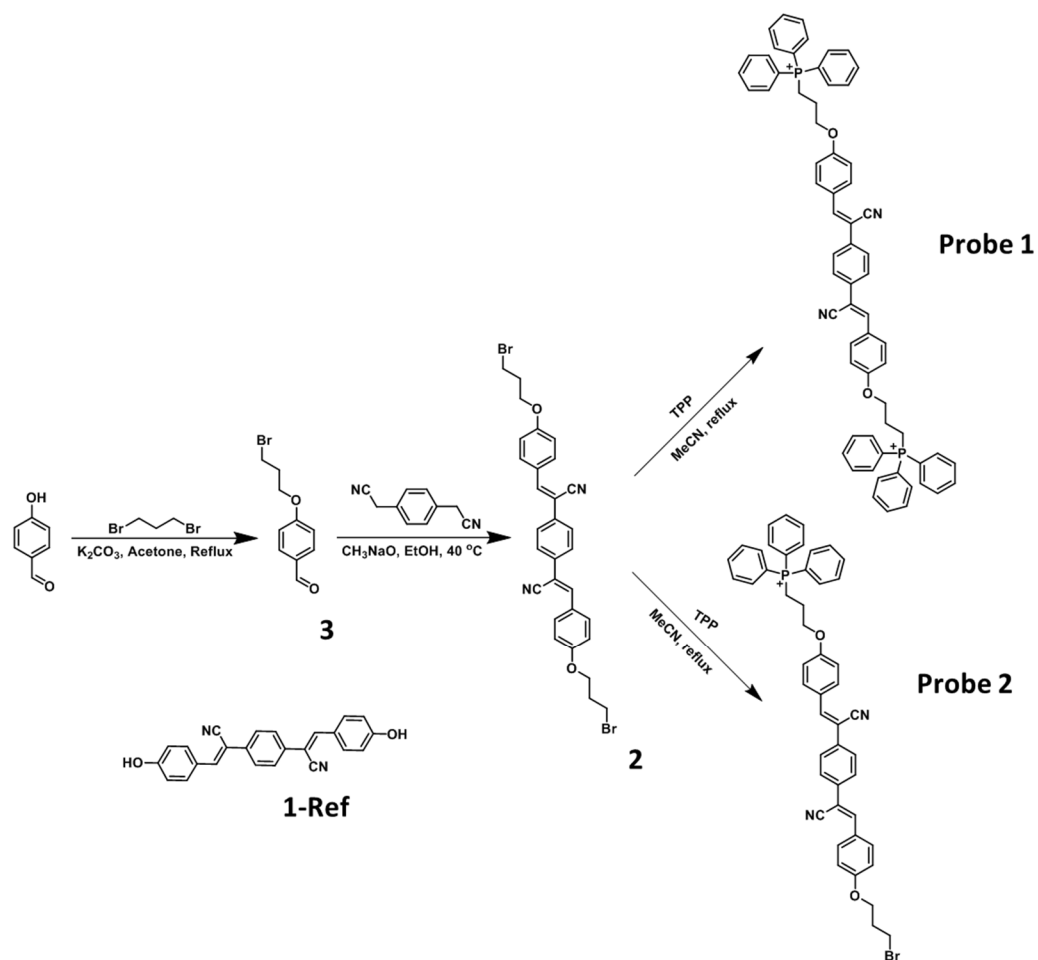
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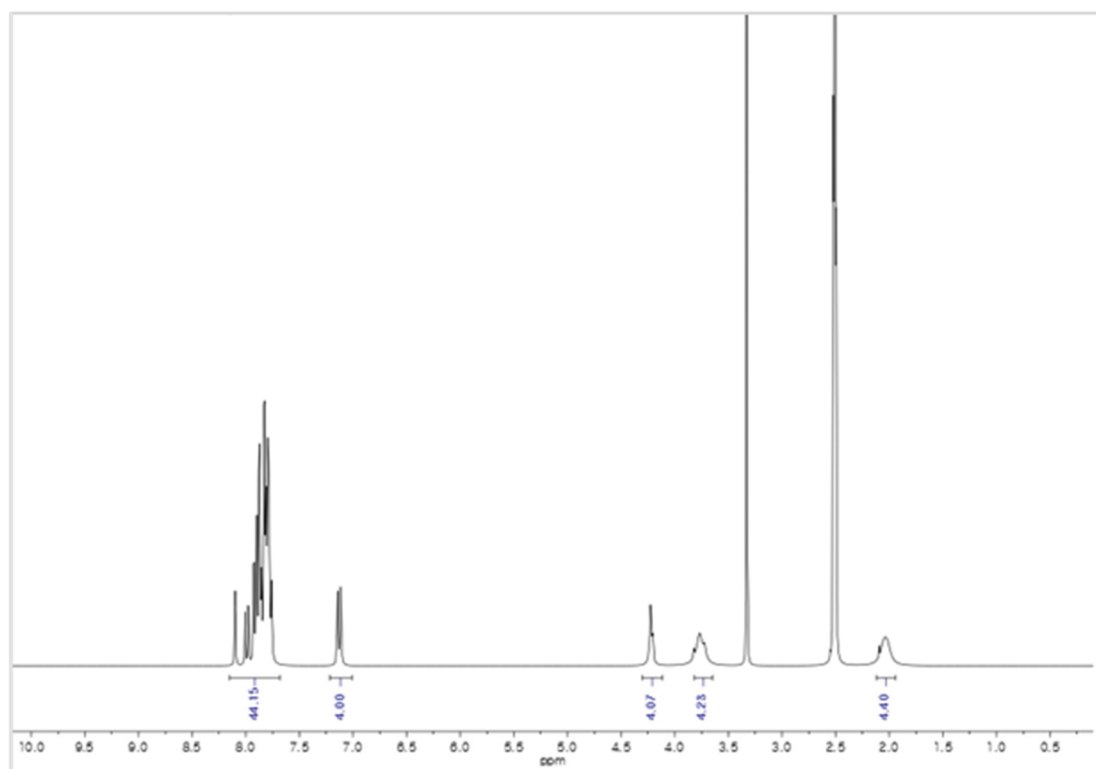
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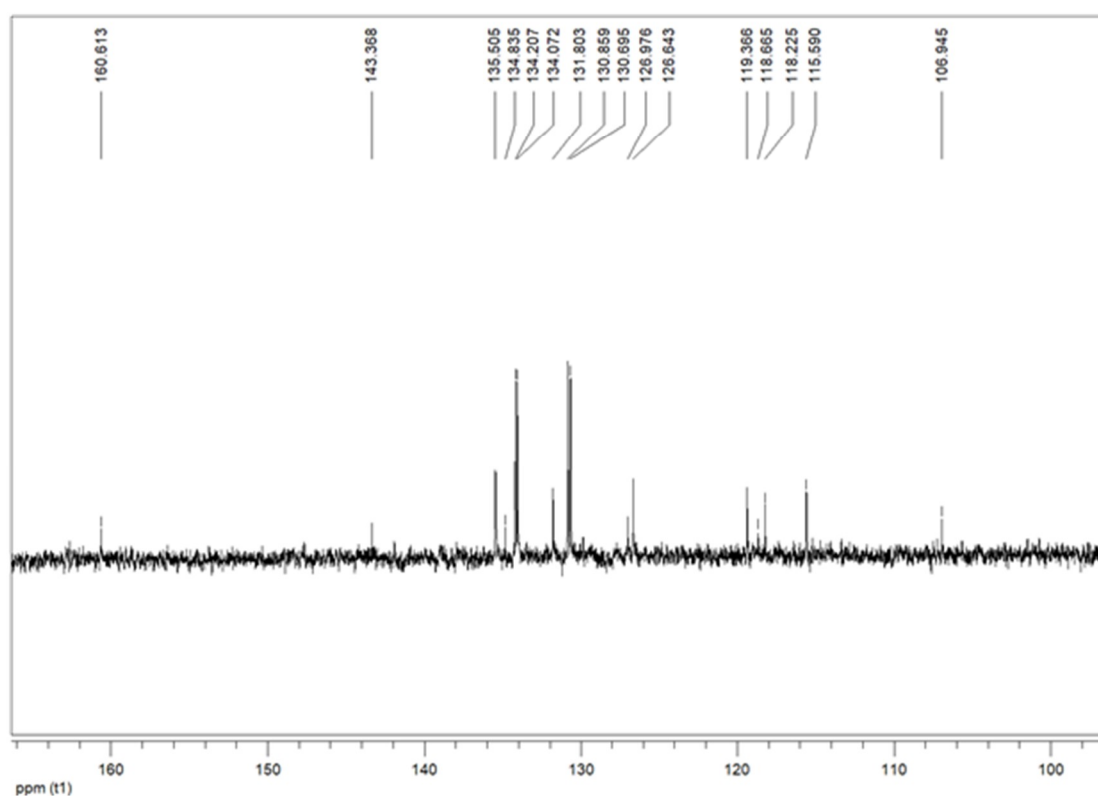


Scheme S1. Synthesis route of probes **1**, **2** and **1-Ref**.

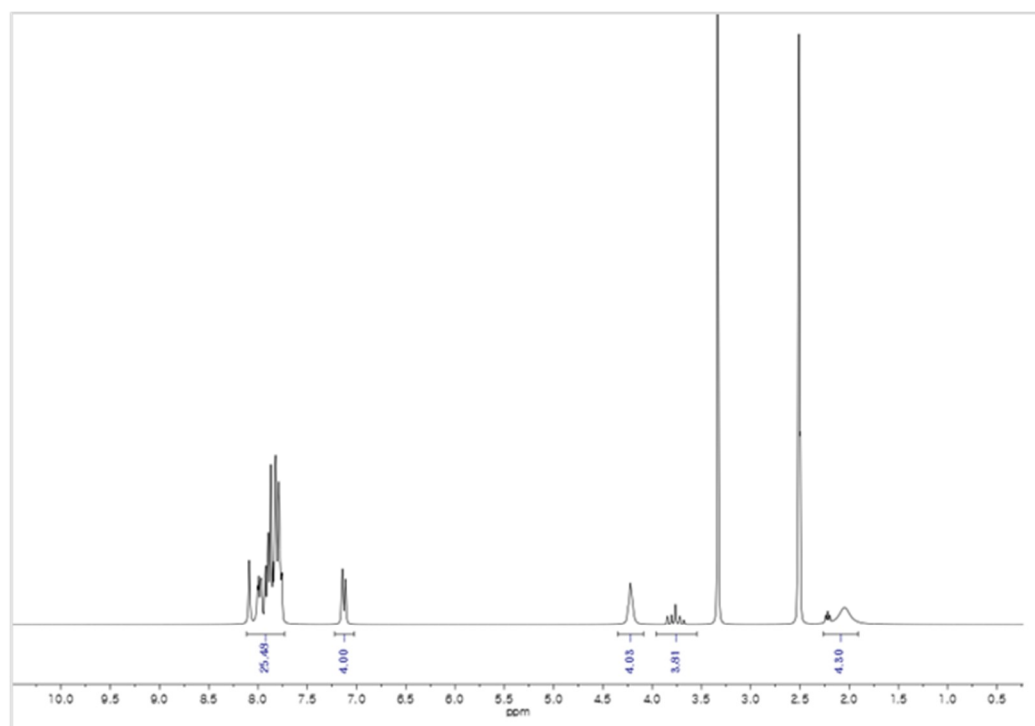
(A)



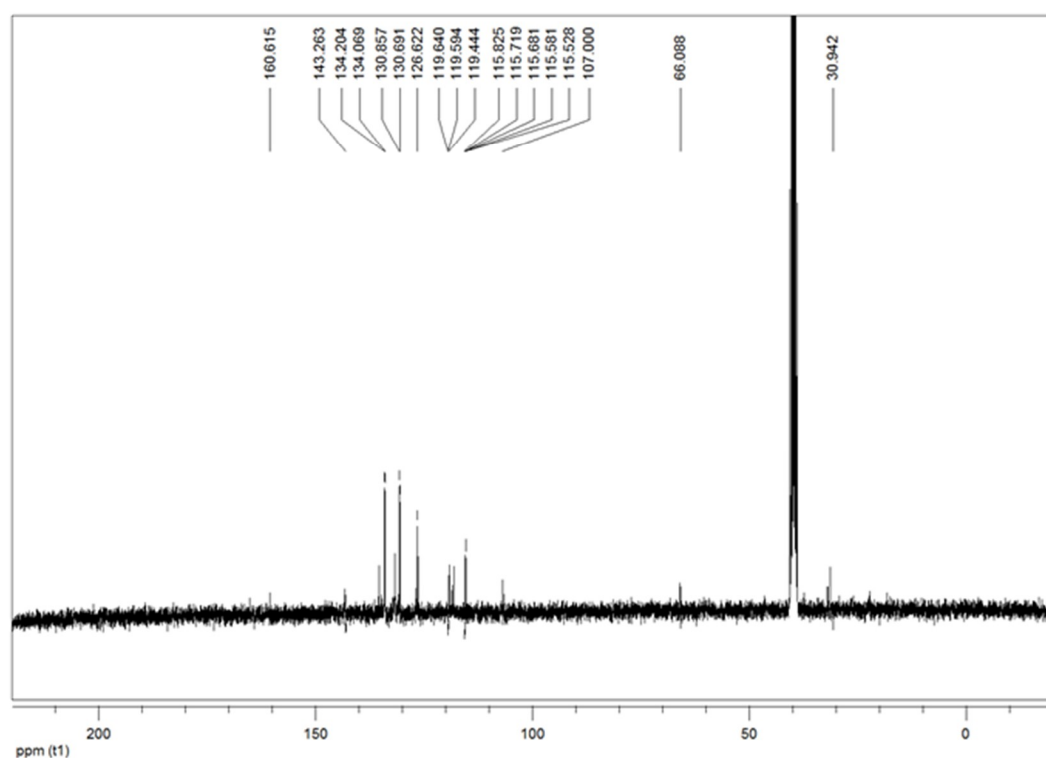
(B)



(C)



(D)



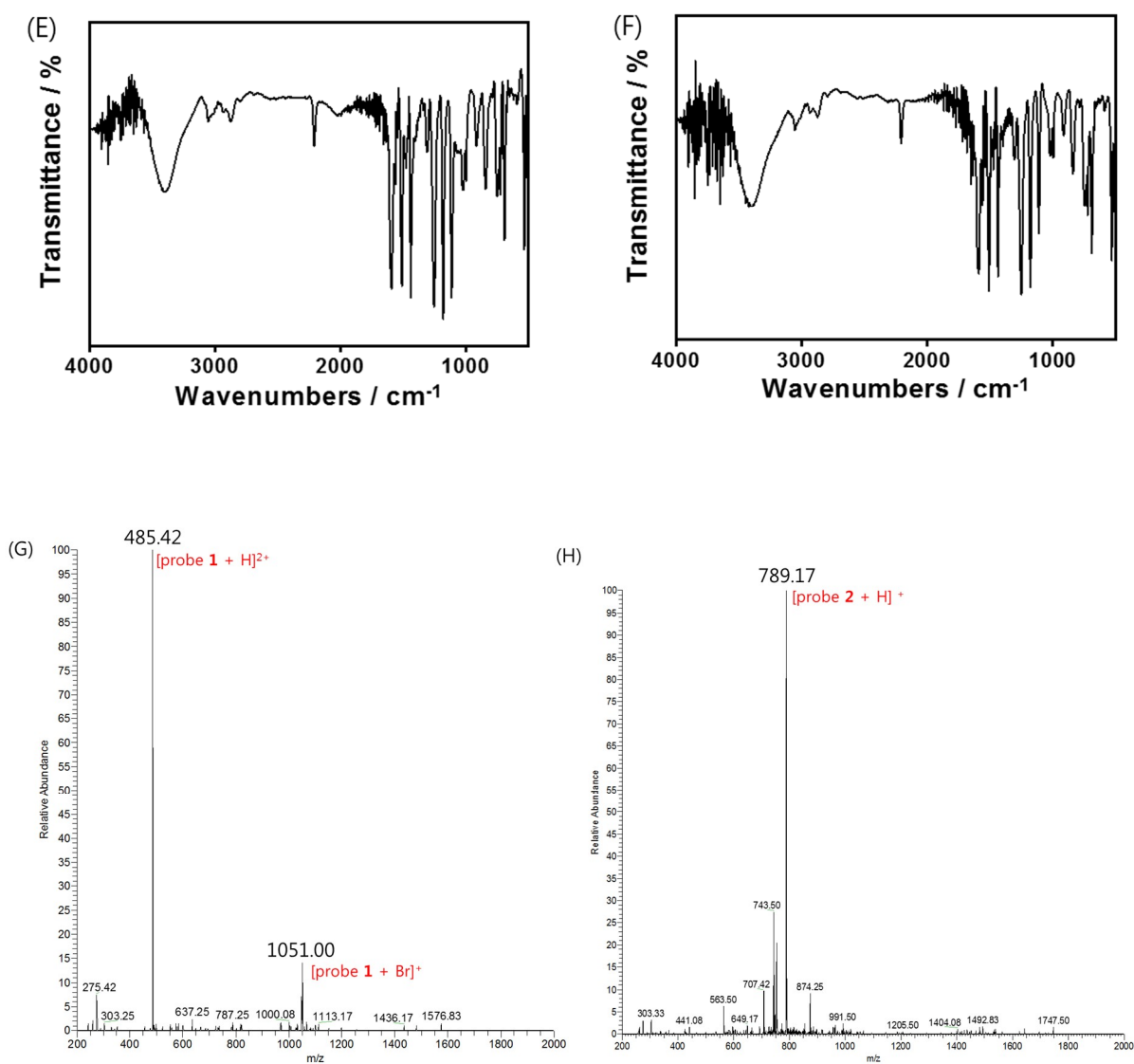


Figure S1. ^1H NMR spectra of probes (A) **1** and (C) **2** in $\text{DMSO}-d_6$. ^{13}C NMR spectra of probes (B) **1** and (D) **2** in $\text{DMSO}-d_6$. FT-IR spectra of probes (E) **1** and (F) **2**. ESI-MS spectra of probes (G) **1** and (H) **2**.

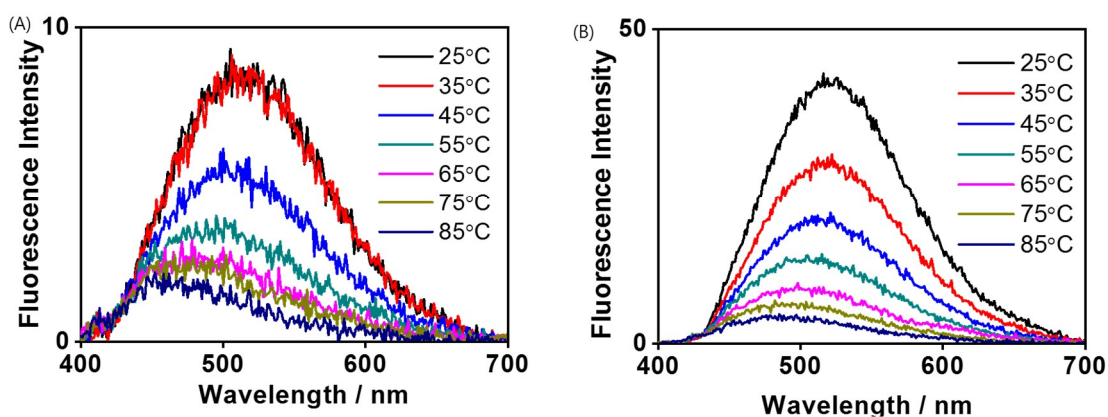


Figure S2. (A) Temperature dependent measurement of Fluorescence spectra of probe 1 (25 μM). (B) Temperature dependent measurement of Fluorescence spectra of probe 2 (6.25 μM).

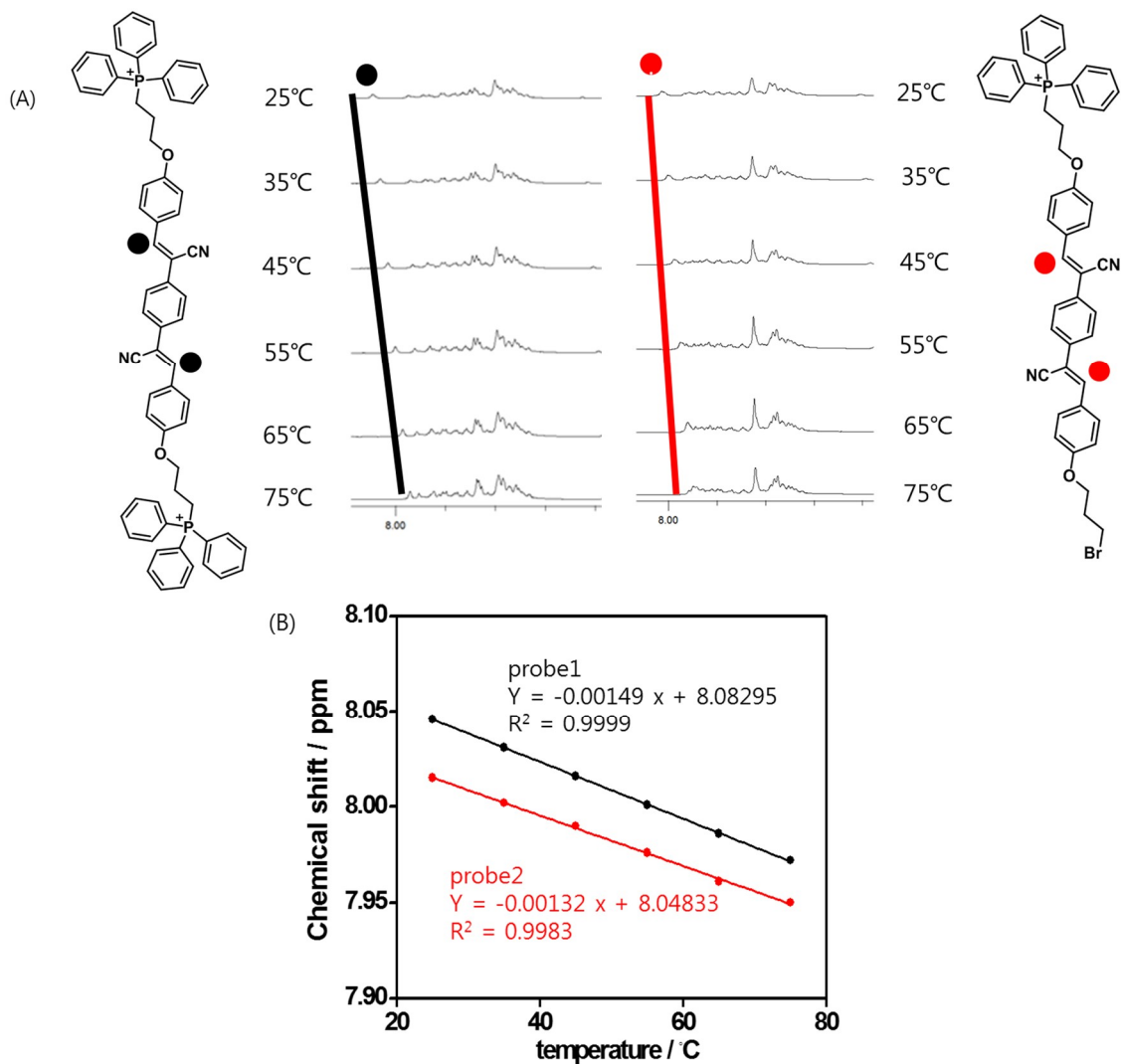


Figure S3. (A) Temperature dependent measurement of ^1H NMR spectra of probes 1 and 2 in $\text{DMSO-}d_6/\text{D}_2\text{O}$ (99:1 v/v%). (B) Linear equation of chemical shift according to temperature.

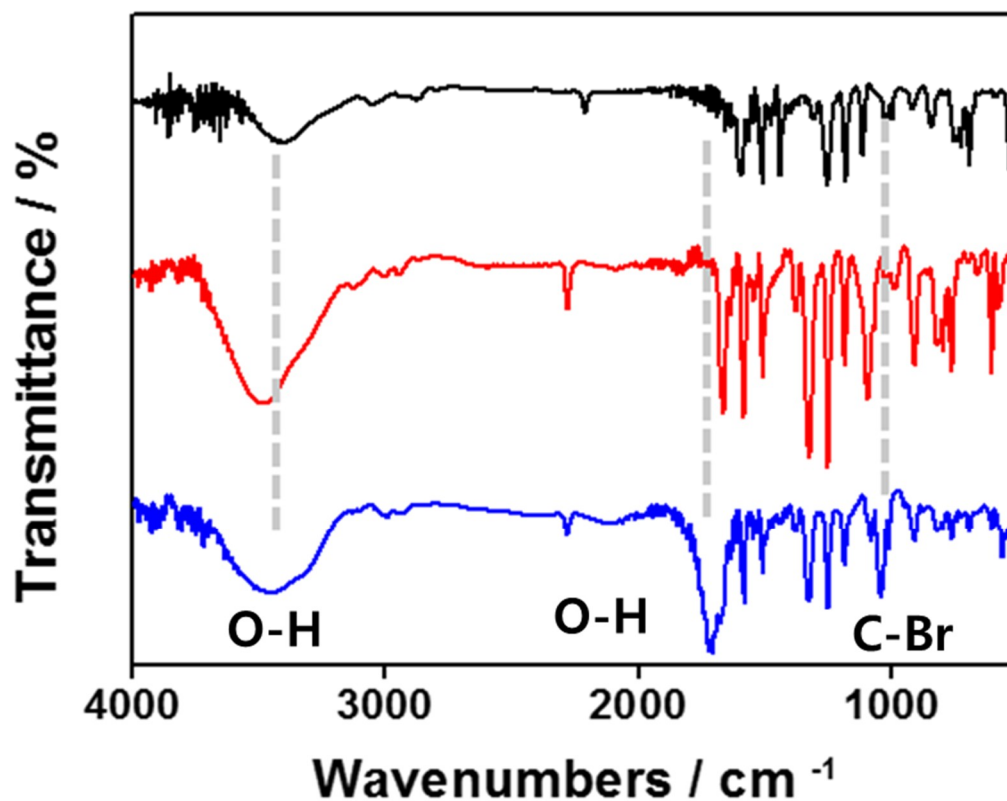


Figure S4. IR spectra of Probe **2** (100 μM) in DMSO/ H_2O (1/99 v/v%). Black line is Probe **2**, Red line is Probe **2** in DMSO/ H_2O (1/99 v/v%) solution, Blue line is Probe **2** with ClO^- (10 equiv.) in DMSO/ H_2O (1/99 v/v%) solution.

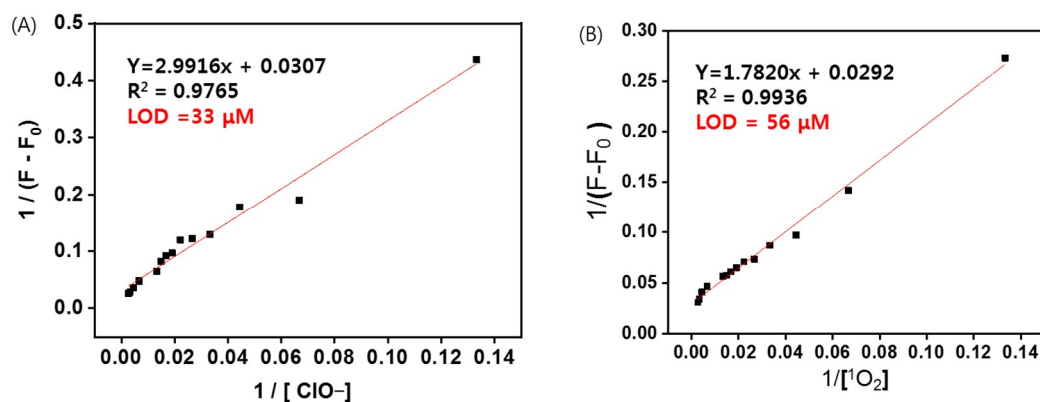


Figure S5. Fit linear equation of fluorescence intensity of probe **1** over (A) ClO^- and (B) $^1\text{O}_2$ to obtain limit of detection.

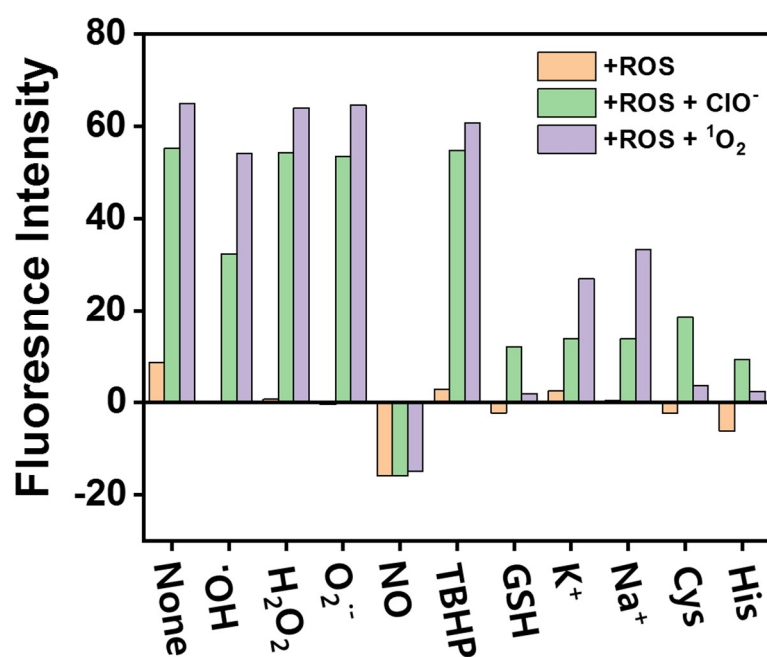


Figure S6. Competition-based fluorescence emission of probe **1** (25 μM) in the presence of various ROS (10 equiv.), Ions (10 equiv.) and Amino acids (10 equiv.) in DMSO/H₂O(1/99 v/v%).

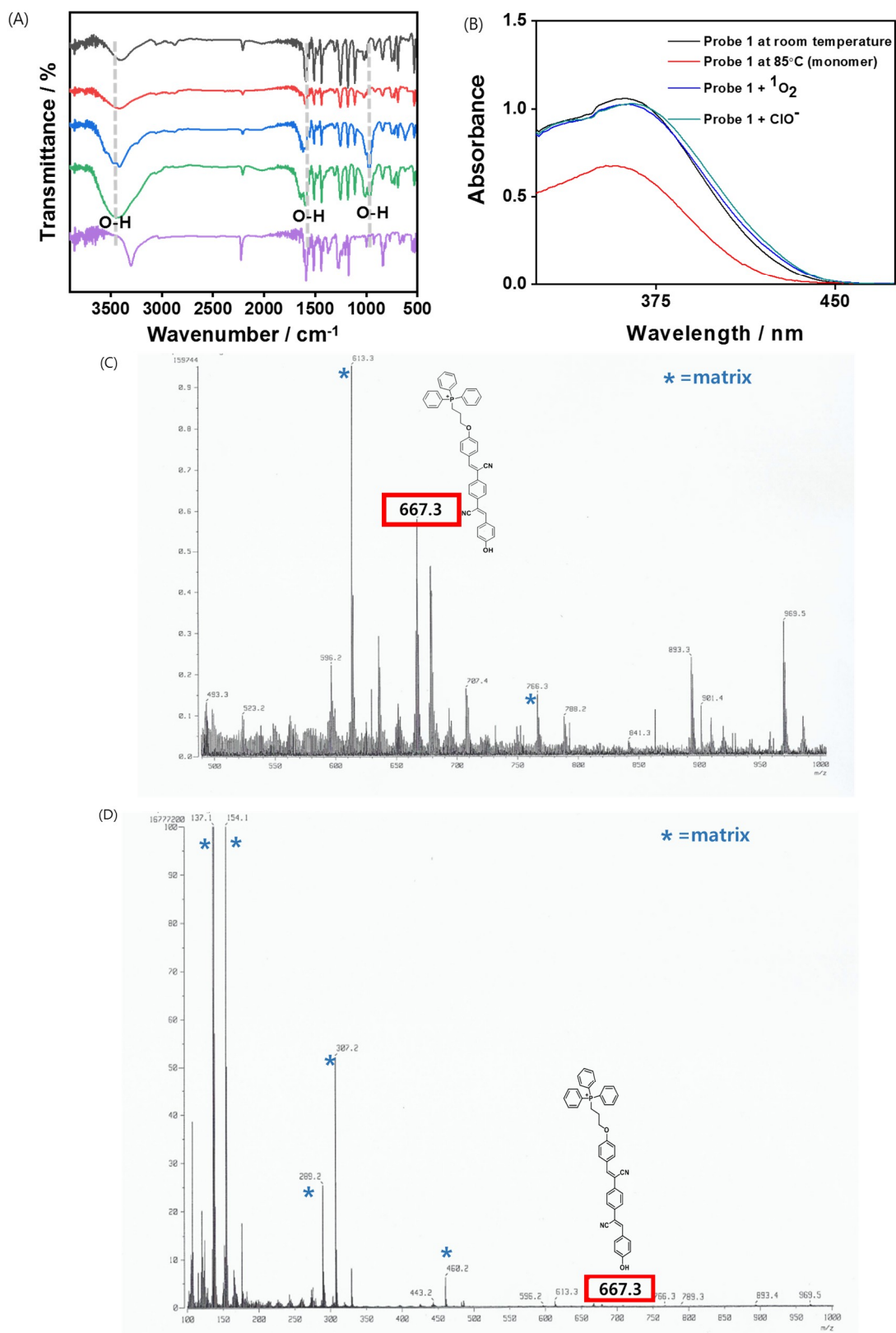


Figure S7. (A) IR spectra of **1** (100 μM) in DMSO/ H_2O (1/99 v/v%). Black line is pristine probe **1**, Red line is freeze-dried self-assembled probe **1** from DMSO/ H_2O (1/99 v/v%) solution, Blue line is self-assembled probe **1** with ClO^- in DMSO/ H_2O (1/99 v/v%) solution, Green line is self-assembled probe **1** with $^1\text{O}_2$ in DMSO/ H_2O (1/99 v/v%) solution and Purple line is dicyanostilbene (**1-Ref**). (B) UV-Vis spectra of probe **1** (100 μM) in DMSO/ H_2O (1/99 v/v%) containing its monomer, self-assembled state, with $^1\text{O}_2$ or ClO^- . FAB-MASS spectra of probe **1** (1mM) after adding (C) ClO^- and (D) $^1\text{O}_2$ at NBA matrix.

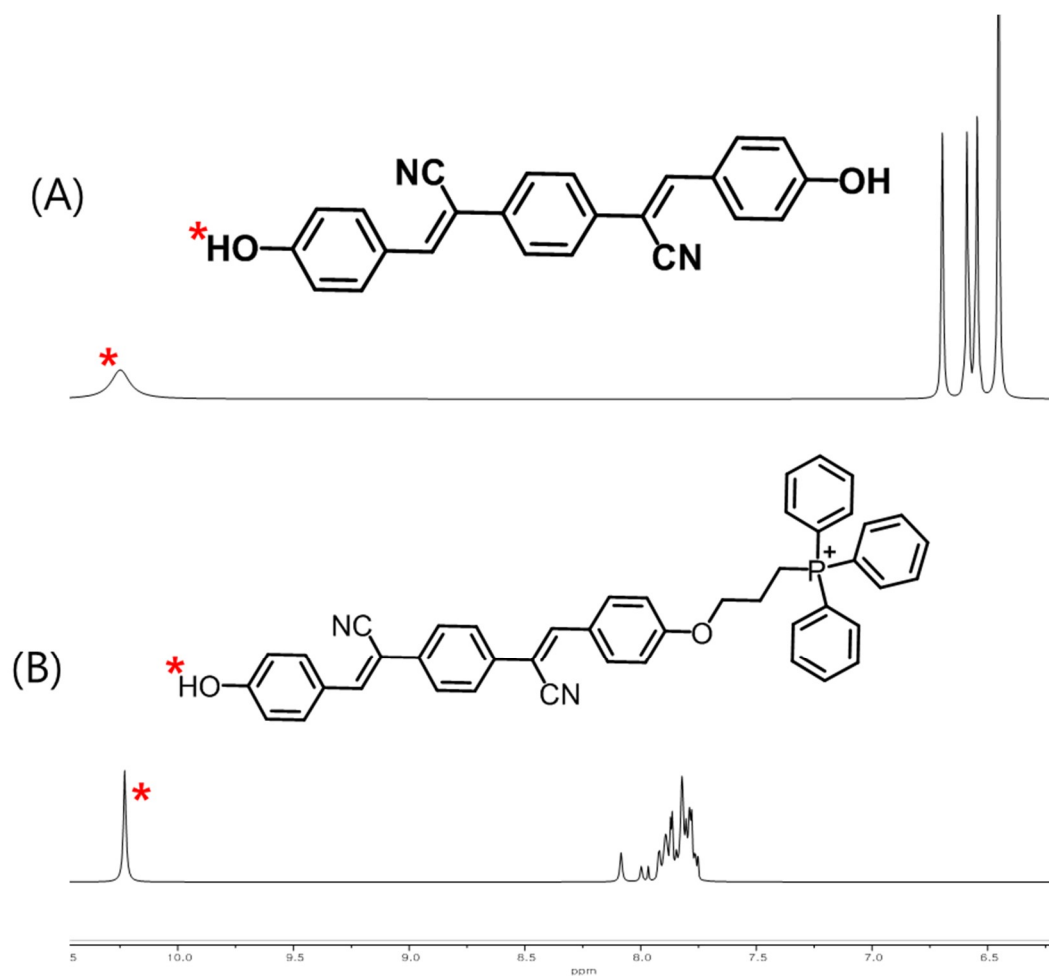


Figure S8. ^1H NMR spectra of (A) dicyanosilbene involving $-\text{OH}$ group (**1-Ref**) and (B) probe **1** after addition of $^1\text{O}_2$.

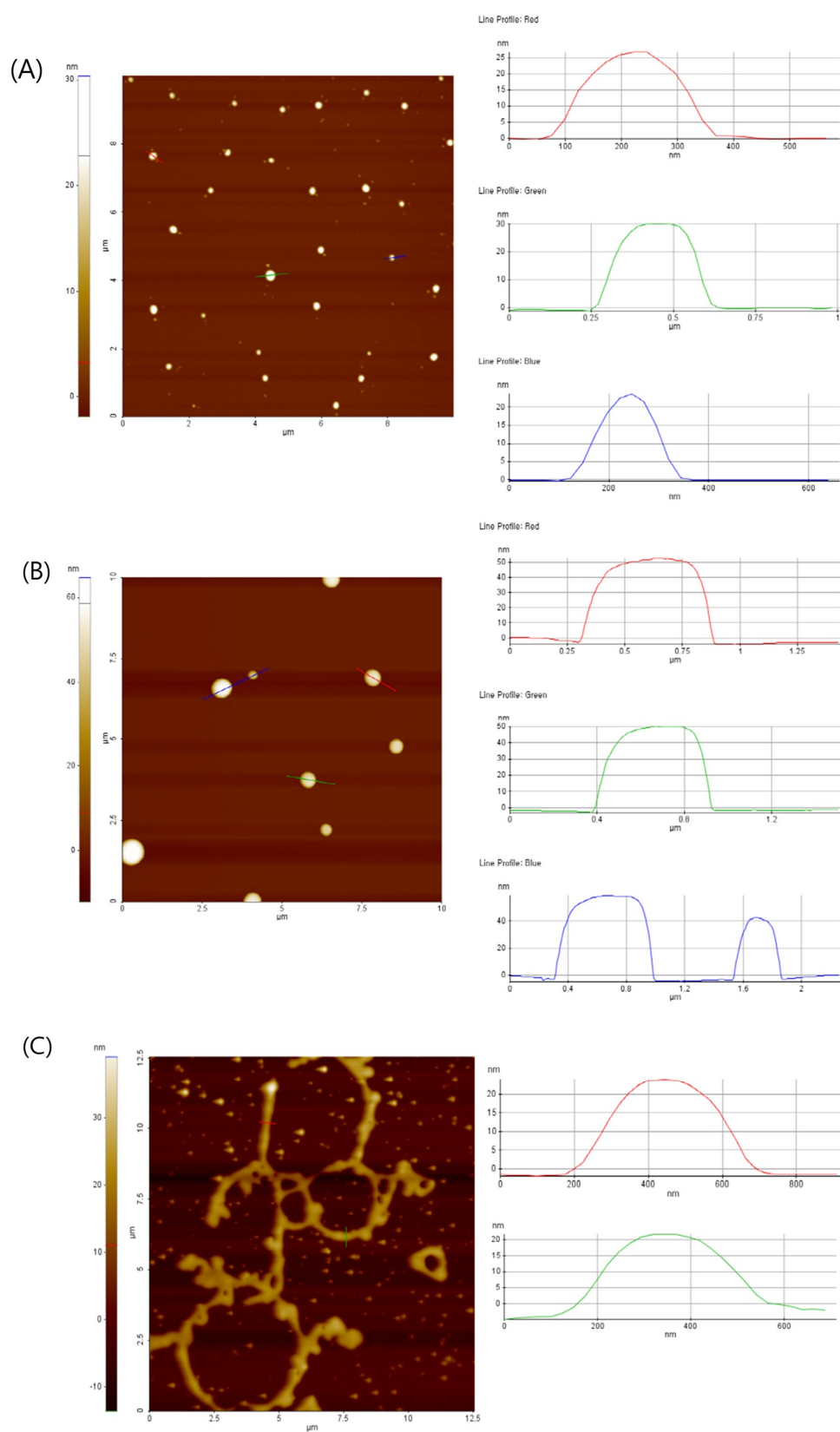


Figure S9. AFM images and height profile of (A) probe **1**, (B) probe **2** and (C) probe **1** + ClO⁻.

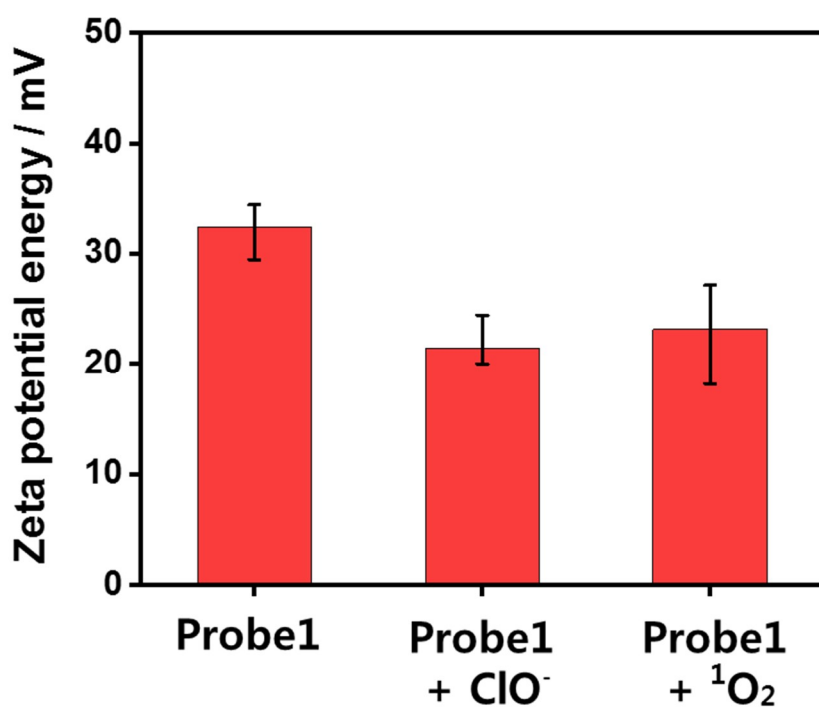


Figure S10. Zeta potential of probe **1** (none, addition of ClO⁻, ¹O₂) at 25 °C.

Table S1. Characterization of probes **1** and **2**.

	Probe 1	Probe 2
Chemical Formula	C ₆₆ H ₅₆ N ₂ O ₂ P ₂ ²⁺	C ₄₉ H ₄₅ BrN ₂ O ₂ P ⁺
Molecular Weight	971.13 g/mol	804.79 g/mol
λ _{max} (monomer)	366nm	367nm
λ _{max} (aggregation)	371nm	372nm
Aggregation type	J-aggregation	J-aggregation
λ _{max} (Fluorecence)	512nm	512nm

References

- S1. Artinez-Abadia, M.; Varghese, S.; Gimenez, R.; Ros, M. B. Multiresponsive luminescent dicyanodistyrylbenzenes and their photochemistry in solution and in bulk. *J. Mater. Chem. C* **2016**, *4*, 2886-2893.
- S2. Niu, J.; Fan, J.; Wang, X.; Xiao, Y.; Xie, X.; Jiao, X.; Sun, C.; Tang, B. Simultaneous fluorescence and chemiluminescence turned on by aggregation-induced emission for real-time monitoring of endogenous superoxide anion in live cells. *Anal. Chem. (Washington, DC, U. S.)* **2017**, *89*, 7210-7215; Long, G. L.; Winefordner, J. D. Limit of detection. A closer look at the IUPAC definition. *Anal. Chem.* **1983**, *55*, 712A-724A.; Mun, G.; Jung, S. H.; Ahn, A.; Lee, S. S.; Choi, M. Y.; Kim, D. H.; Kim, J.-Y.; Jung, J. H. Fluorescence imaging for Fe³⁺ in Arabidopsis by using simple naphthalene-based ligands. *RSC Adv.* **2016**, *6*, 53912-53918.