

Supporting Information

Single-Photon-Driven Up-/Downconversion Nanohybrids for *In vivo* Mercury Detection and Real-Time Tracking

Sung Eun Seo,^{†,‡,∇} Chul Soon Park,^{†,∇} Seon Joo Park,[†] Kyung Ho Kim,[†] Jiyeon Lee,[†] Jinhyeong Kim,[†] Sang Hun Lee,[§] Hyun Seok Song,^{||} Tai Hwan Ha,[†] Jae-Hyuk Kim,[⊥] Hee Won Yim,[‡] Hyoung-il Kim,^{‡,*} and Oh Seok Kwon^{†,#,*}

[†]Infectious Disease Research Center, Korea Research Institute of Bioscience and Biotechnology (KRIBB), 125 Gwahak-ro, Yuseong-gu, Daejeon 34141, South Korea

[‡]Department of Civil and Environmental Engineering, Yonsei University, Seoul 03722, South Korea

[§]Department of Bioengineering, University of California Berkeley, CA 94720, USA

^{||}Sensor System Research Center, Korea Institute of Science and Technology, Seoul 02792, Republic of Korea

[⊥]Department of Chemical and Environmental Engineering, Pusan National University, 46241 Busan, Korea

[#]Nanobiotechnology and Bioinformatics (Major), University of Science & Technology (UST), 125 Gwahak-ro, Yuseong-gu, Daejeon, 34141, South Korea

[∇]S.E.S. and C.S.P contributed equally to this work

*To whom correspondence should be addressed:

Dr. O.S. Kwon: Tel: +82-42-860-8284; Fax: +82-42-879-8594; E-mail: oskwon7799@gmail.com

Prof. H.I. Kim: Tel: +82-2-2123-2798; Fax: +82-2-364-5300; E-mail: hi.kim@yonsei.ac.kr

Optimization of the ratio of sensitizer to acceptor (Figure S1)	S3
SEM data of the monodispersed TTA-UC nanocapsules (Figure S2)	S4
Quantum Yield (QY) calculation method (Figure S3)	S5
Photostability test of the TTA-UC nanocapsules (Figure S4)	S6
Schematic diagram of the detection of the TTA-UC nanocapsules (Figure S5)	S7
NMR data of Rho-Hz (Figure S6)	S8
Mass spectrometry data of Rho-Hz (Figure S7)	S9

Optimization of the ratio of sensitizer to acceptor

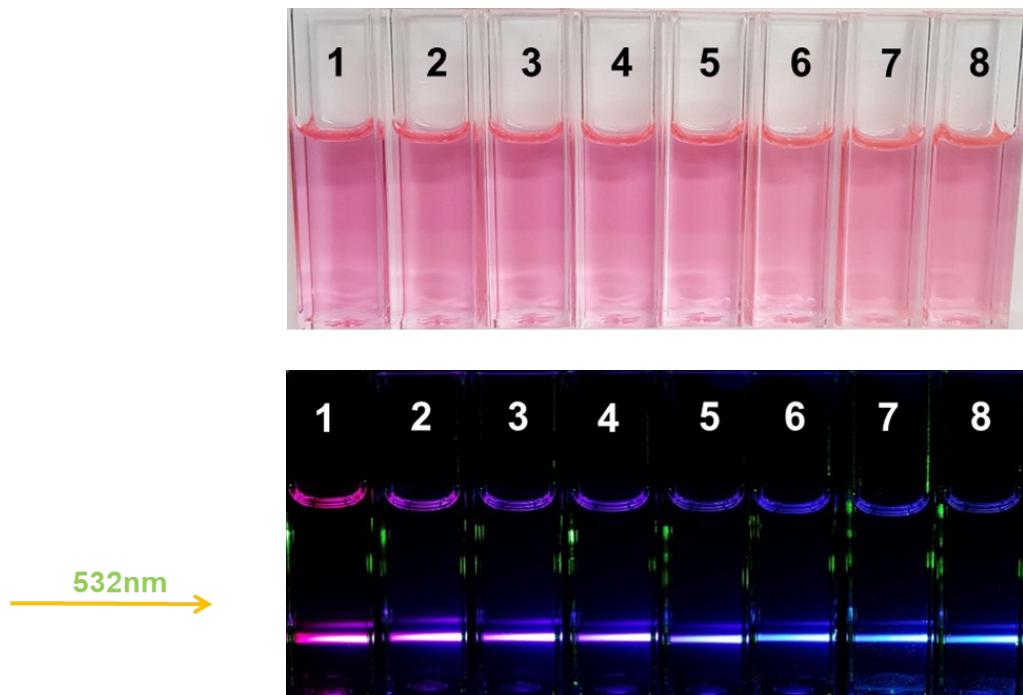


Figure S1. The upconverted emission light dependent on the volume ratio of Sensitizer : Acceptor; Sensitizer(0.0018 M) 100 uL, Acceptor(0.06053M) 50 uL; 100 uL; 200 uL; 300 uL; 500 uL; 1000 uL; 1200 uL; 1400 uL.

SEM data of the monodispersed TTA-UC nanocapsules

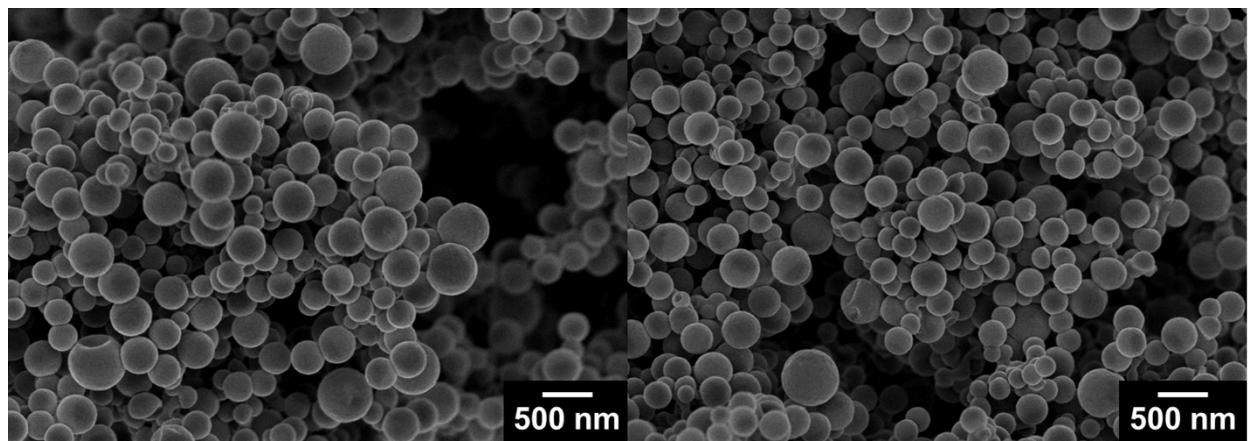


Figure S2. SEM data of the monodispersed TTA-UC nanocapsules.

Quantum Yield (QY) calculation method

$$\Phi_{UC} = 2\Phi_{std} \left(\frac{A_{std}}{A_{UC}} \right) \left(\frac{I_{UC}}{I_{std}} \right) \left(\frac{\eta_{UC}}{\eta_{std}} \right)^2$$

Power	UC QY	I_{UC}/I_{std}
19	0.02811	0.012887
27.16667	0.05648	0.025894
37.66667	0.15094	0.069201
47	0.25367	0.116299
53	0.2969	0.136119
76.33333	0.33006	0.151322
102.66667	0.42484	0.194775
125	0.60571	0.277698
146	0.60865	0.279046
174.33333	0.70599	0.323673
400	1.0243	0.469607
600	1.17025	0.536521
950	1.354	0.620764
1600	1.5232	0.698336
2100	1.62	0.742716
2700	1.6501	0.756516
3010	1.658	0.760138

Figure S3. Quantum Yield (QY) calculation method: where $\Phi_{UC/std}$ (Quantum yield of DPA/PdTPBP dissolved in OA; UC, Rhodamine 6G; std), $A_{UC/std}$ (Absorbance of DPA/PdTPBP dissolved in OA; UC, Rhodamine 6G; std), $I_{UC/std}$ (PL intensity of DPA/PdTPBP dissolved in OA; UC, Rhodamine 6G; std) and $\eta_{UC/std}$ (refractive index of DPA/PdTPBP dissolved OA; UC, Rhodamine 6G; std) denote the quantum yield. And the calculated quantum yield of upconversion is presented in the table.

Photo-stability test of the TTA-UC nanocapsules

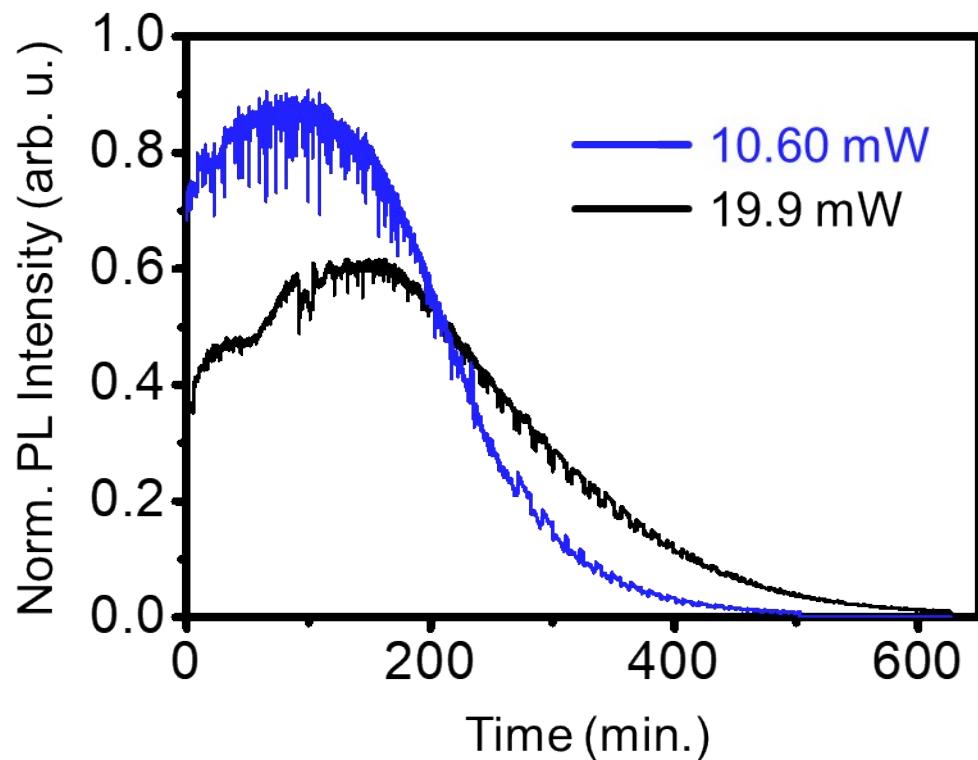


Figure S4. Photo-stability test of the TTA-UC nanocapsules.

Schematic diagram of the detection of the TTA-UC nanocapsules

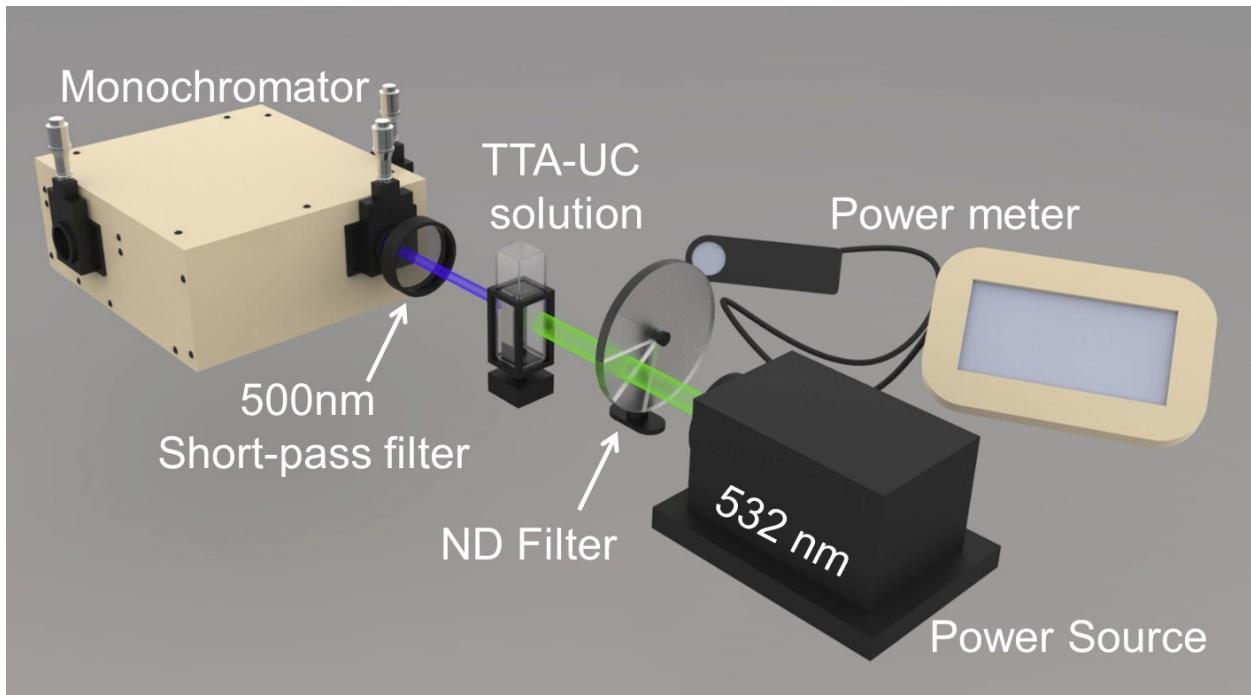


Figure S5. Schematic diagram of the detection of the TTA-UC nanocapsules.

NMR data of Rho-Hz

¹H-NMR(CDCl₃, 400MHz)

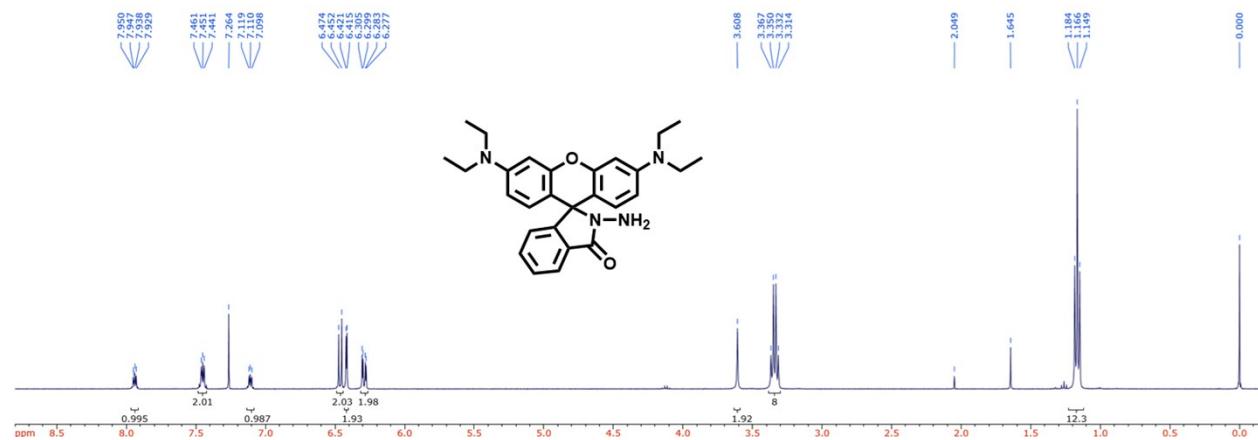


Figure S6. The NMR data and structure (inset) of Rho-Hz; ¹H-NMR (CDCl₃, 400MHz).

Mass spectrometry data of Rho-Hz (Figure S7)

Generic Display Report

Analysis Info

Analysis Name D:\Data\2015\0811\RHO-HZ.d
 Method Tune_low_pos.m
 Sample Name RHO-HZ
 Comment

Operator BDAL@KR
 Instrument micrOTOF-Q

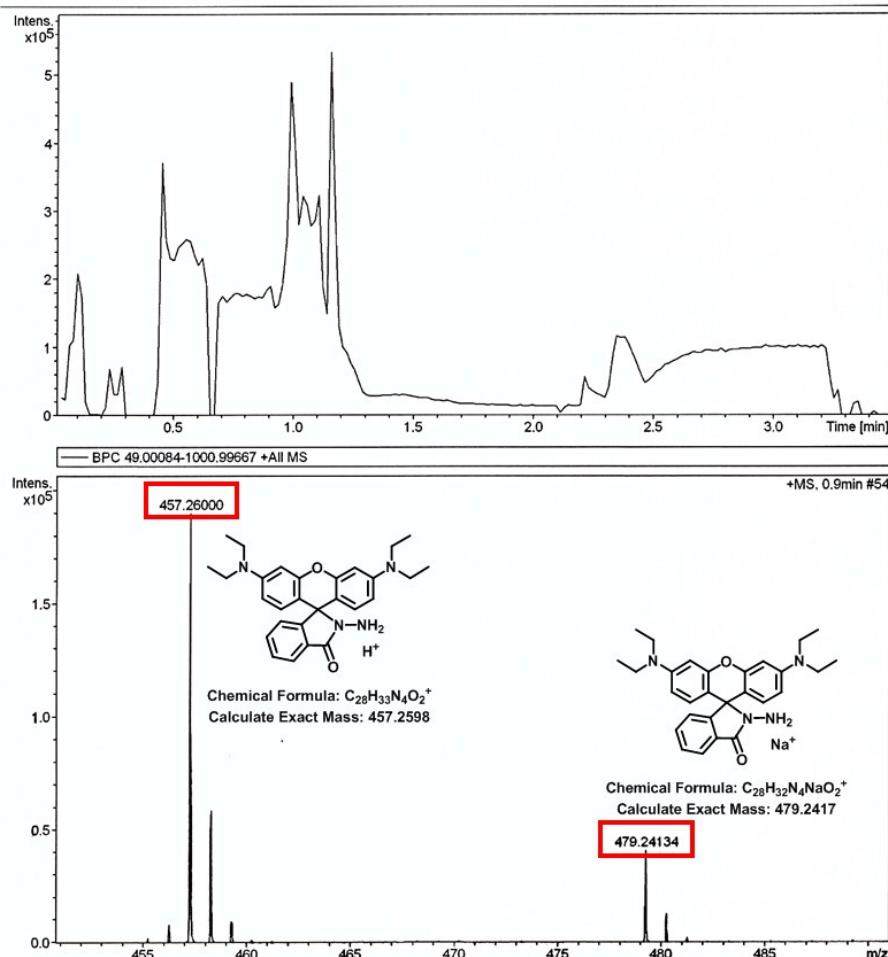


Figure S7. The high resolution mass spectrometry data of Rho-Hz.