Supporting Information

A Simple and Label-free Detection of As^{3+} using 3-nitro-L-tyrosine as a As^{3+} -chelating ligand

Jin-Ho Park 1,2 , Gyuho Yeom 1 , Donggu Hong 1 , Eun-Jung Jo 1 , Chin-Ju Park 1 and Min-Gon Kim 1,*

¹Department of Chemistry, Gwangju Institute of Science and Technology (GIST), 123 Cheomdangwagi-ro, Buk-Gu, Gwangju 61005, Republic of Korea; jhp1223@gist.ac.kr (J.-H.P.); ygh0727@gist.ac.kr (G.Y.); inkohdg@gist.ac.kr (D.H.); jej@gist.ac.kr (E.-J.J.); cjpark@gist.ac.kr (C.-J.P.)

²Center for Systems Biology, Massachusetts General Hospital, Harvard Medical School, Boston, MA 02114, USA; jpark93@mgh.harvard.edu (J.-H.P.)

*Correspondence: mkim@gist.ac.kr (M.-G.K.); Tel.: +82-62-3330; Fax: +82-62-2887

Table S1. Parameter values obtained via ITC measurement

Model	Parameter	Value
Blank (constant)	Blank (μJ)	16.9669
	$K_a (M^{-1})$	2.13E+05
	n	0.640
Independent	∆H (kJ/mol)	5.787
	$K_{d}\left(M\right)$	4.70E-06
	S (J/mol·K)	121.4

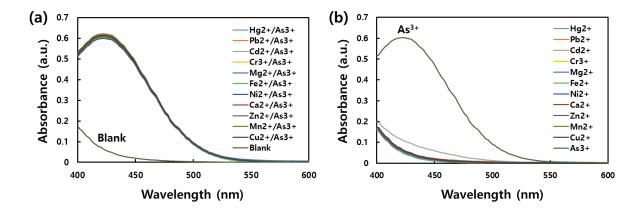


Figure S1. Absorption spectra of mixtures of metal ions and N-Tyr (a) with or (b) without As³⁺.

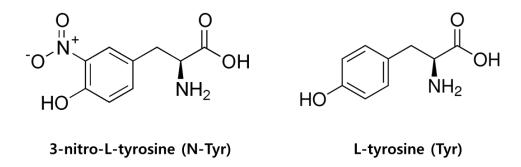


Figure S2. Chemical structure of N-Tyr and Tyr. A NO₂ group exists in chemical structure of N-Tyr.

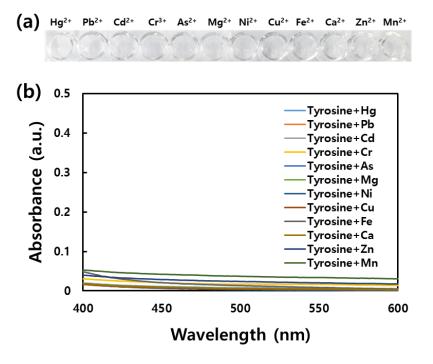


Figure S3. The reaction between various metal ions and Tyr. (a) Images of the mixtures and (b) the corresponding absorption spectra are shown.

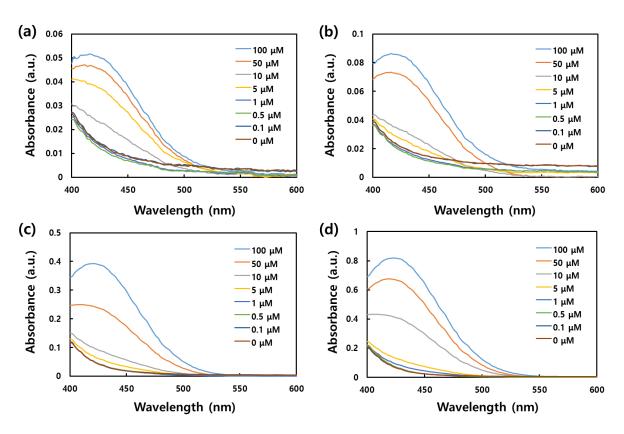


Figure S4. Absorption spectra depending on As^{3+} with different concentrations of N-Tyr, (a) 50 μ M, (b) 100 μ M, (c) 500 μ M and (d) 1,000 μ M.

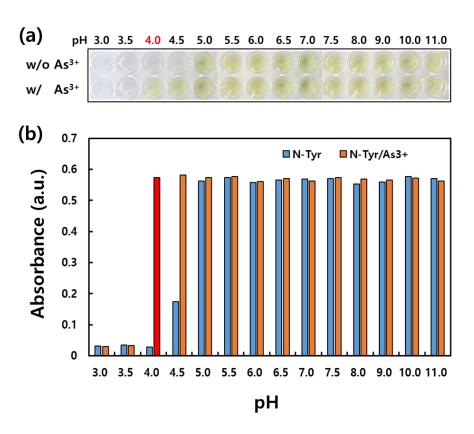


Figure S5. Various pHs were tested with two experimental conditions, N-Tyr alone and As^{3+}/N -Tyr mixture. A selective yellow color with As^{3+} was appeared under pH 4.0. In this test, 0.5 mM N-Tyr and 1 mM As^{3+} were used.

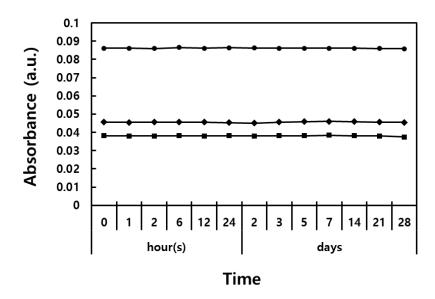


Figure S6. Stability of the As^{3+}/N -Tyr reaction was checked. Three different A^{3+} concentrations, e.g., 0.1 (square), 1 (diamond), and 10 μM (circle), were reacted with 0.5 mM N-Tyr then, stayed at RT condition for 28 days. Almost same absorbance degrees were obtained from each measurement.