Supporting Information

# An activatable $T_1$-weighted MR contrast agent: Noninvasive tool for tracking the vicinal thiol motif of thioredoxin in live cells

Jongeun Kang,[1,2,†] Eunha Hwang,[3,†] Hyunseung Lee,[1,†] Mi Young Cho,[1] Sanu Karan,[1,2] Hak Nam Kim,[3] Jong Seung Kim,[4] Jonathan L. Sessler,[5,*] Sankarprasad Bhuniya,[1,6,*] and Kwan Soo Hong[1,2,*]

[1]Research Center for Bioconvergence Analysis, Korea Basic Science Institute, Cheongju 28119, Korea

[2]Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon 34134, Republic of Korea

[3]Center for Research Equipment, Korea Basic Science Institute, Cheongju 28119, Korea

[4]Department of Chemistry, Korea University, Seoul 02841, Korea

[5]Department of Chemistry, University of Texas at Austin, Austin, Texas 78712-1224, United States

[6]Centre for Interdisciplinary sciences, JIS Institute of Advanced Studies and Research, JIS University, Kolkata 700091, India

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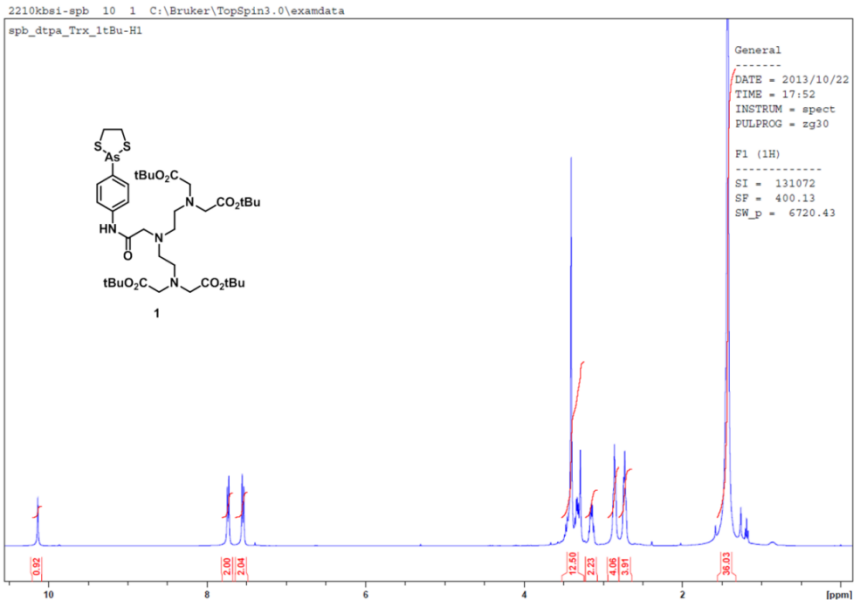



**Figure S1.** $^{1}$H NMR spectrum of **1** in $CDCl_3$.

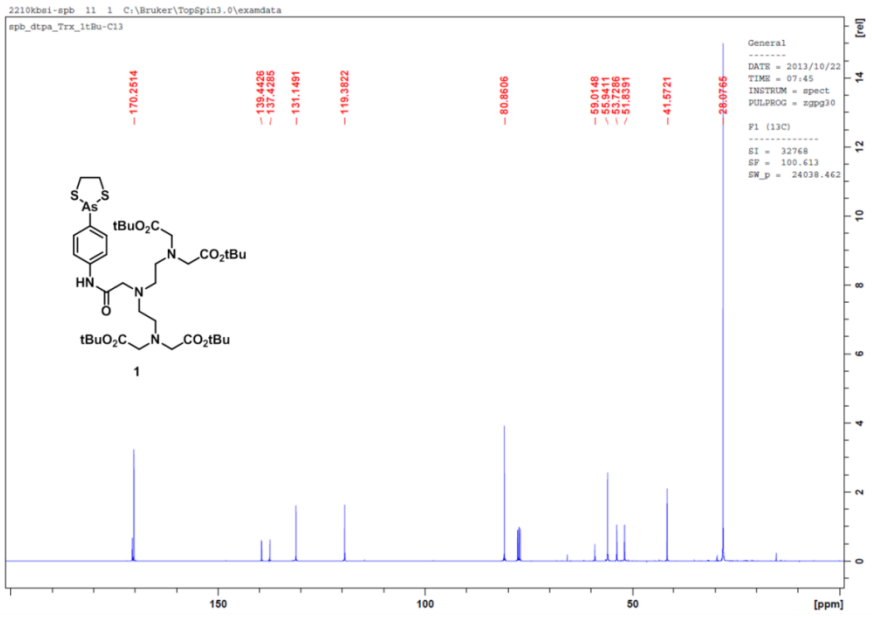



**Figure S2.** $^{13}$C NMR spectrum of **1** in $CDCl_3$.

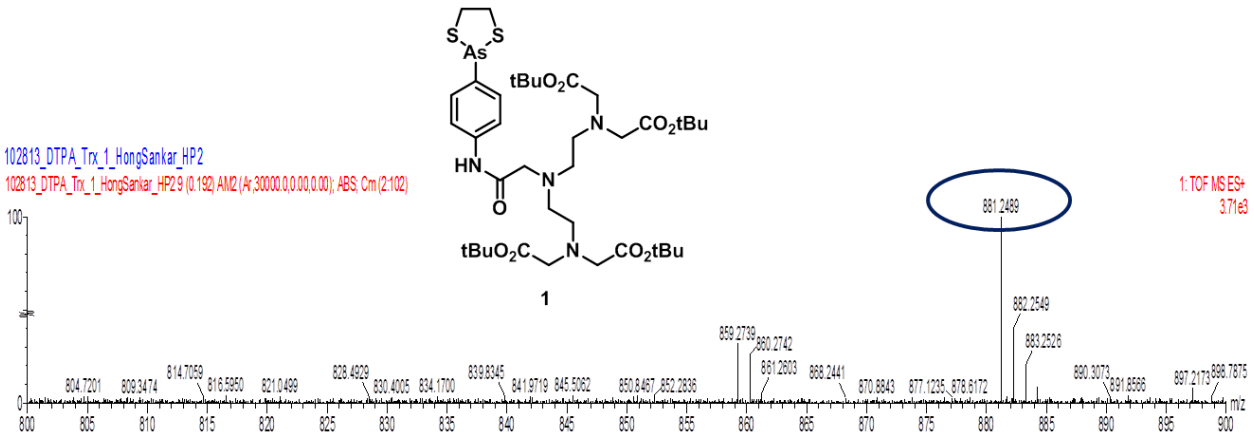



**Figure S3.** MS spectrum of **1**.

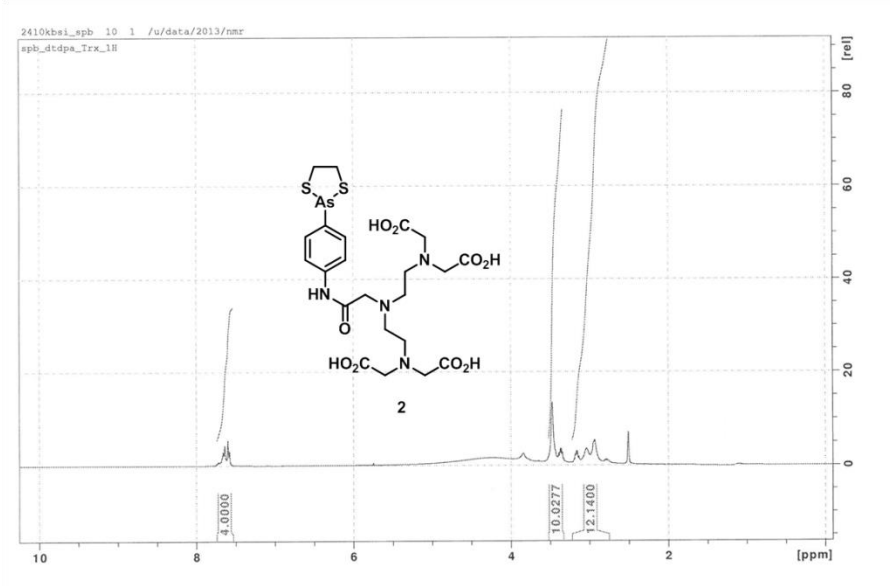



**Figure S4.** $^{1}$H NMR spectrum of **2** in DMSO-$d_6$.

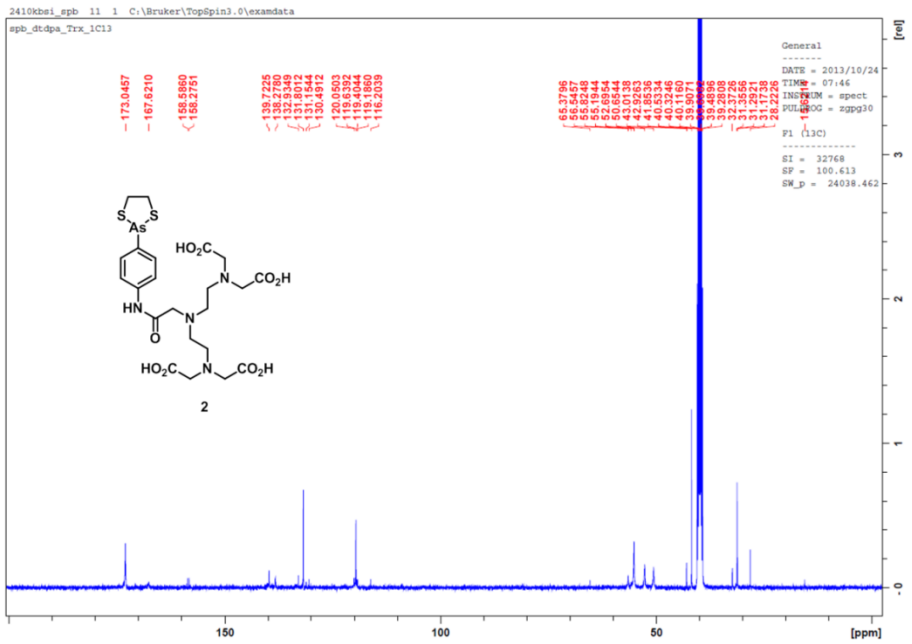



**Figure S5.** $^{13}$C NMR spectrum of **2** in DMSO-$d_6$.

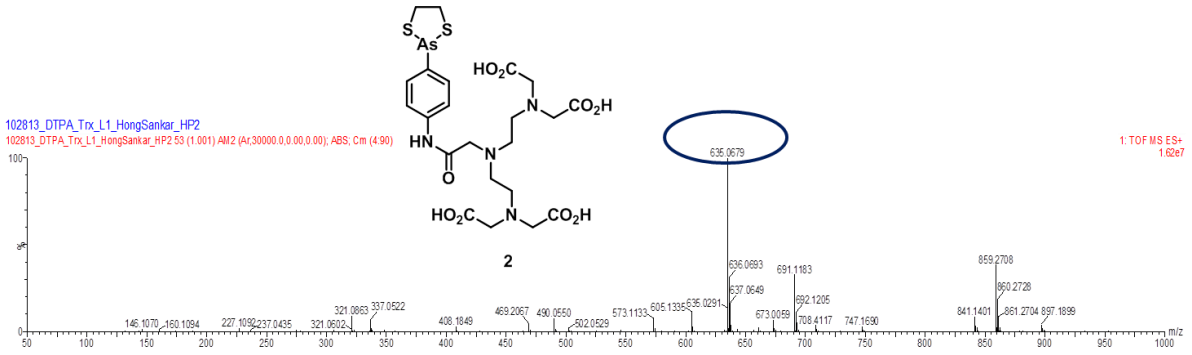



**Figure S6.** MS spectrum of **2**.

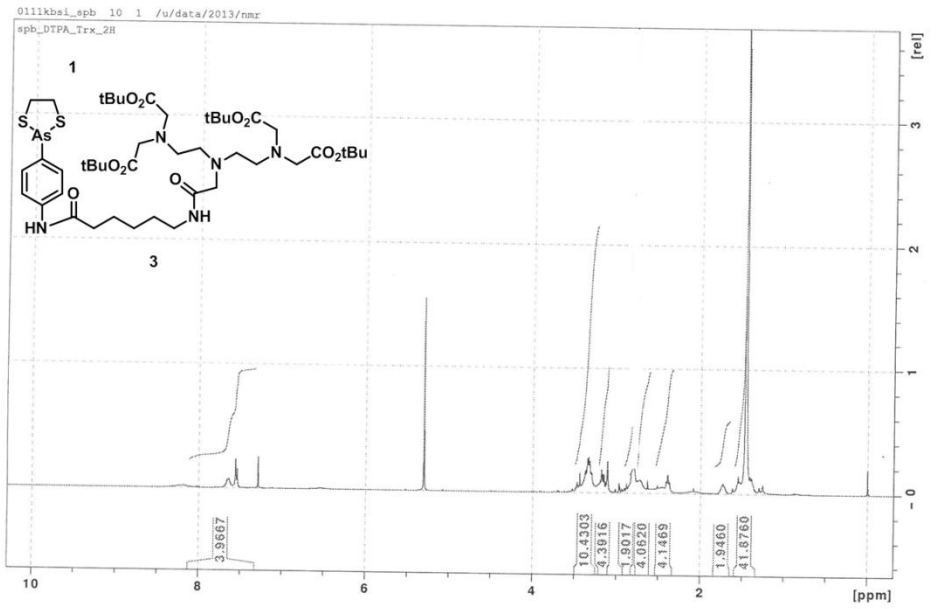



**Figure S7.** $^{1}$H NMR spectrum of **3** in $CDCl_3$.

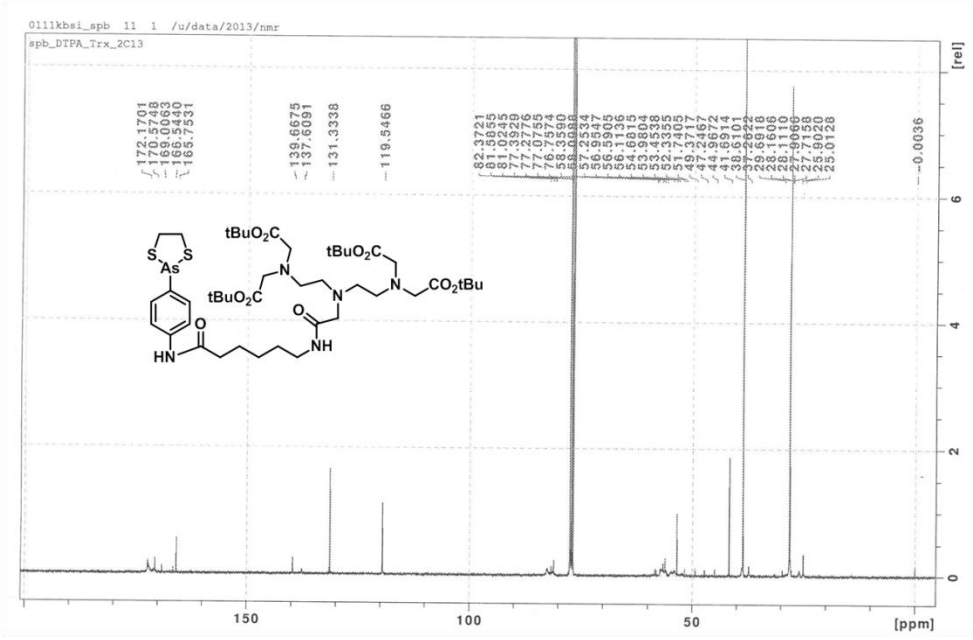



**Figure S8.** $^{13}$C NMR spectrum of **3** in $CDCl_3$.

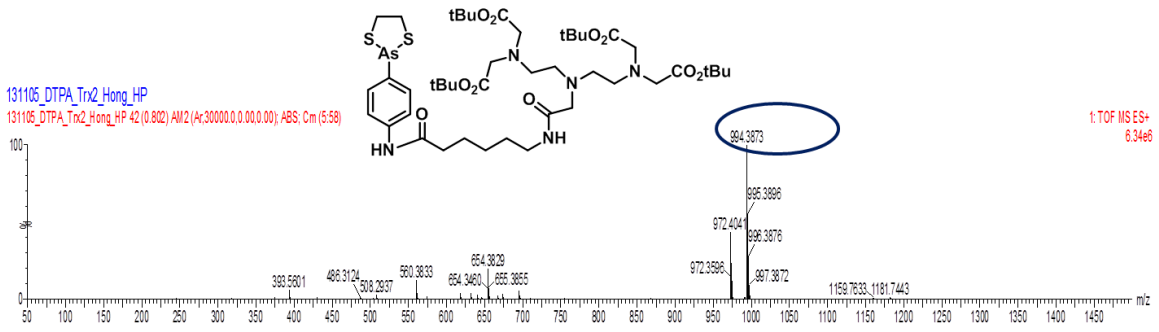



**Figure S9.** MS spectrum of **3**.

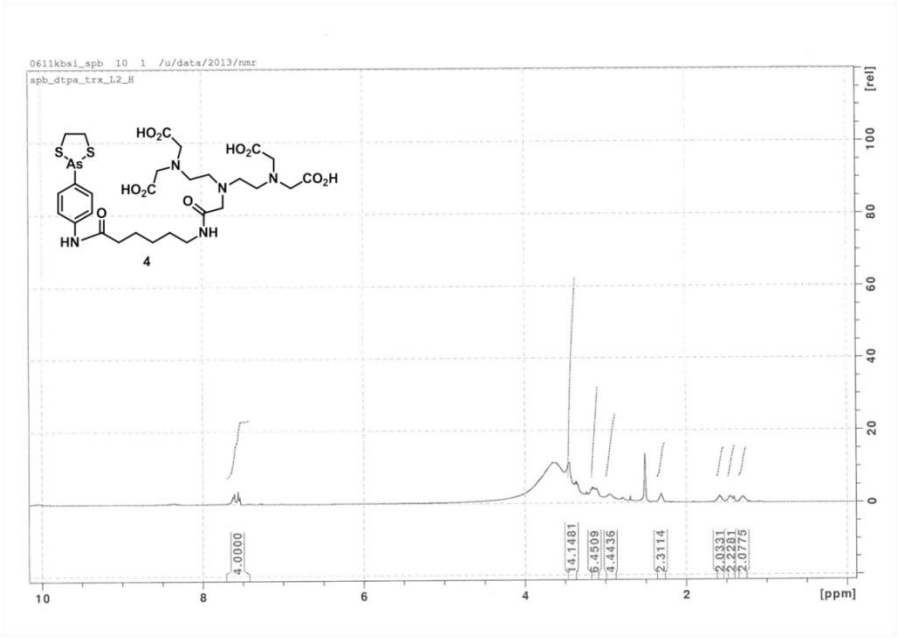



**Figure S10.** $^{1}$H NMR spectrum of **4** in DMSO–$d_6$.

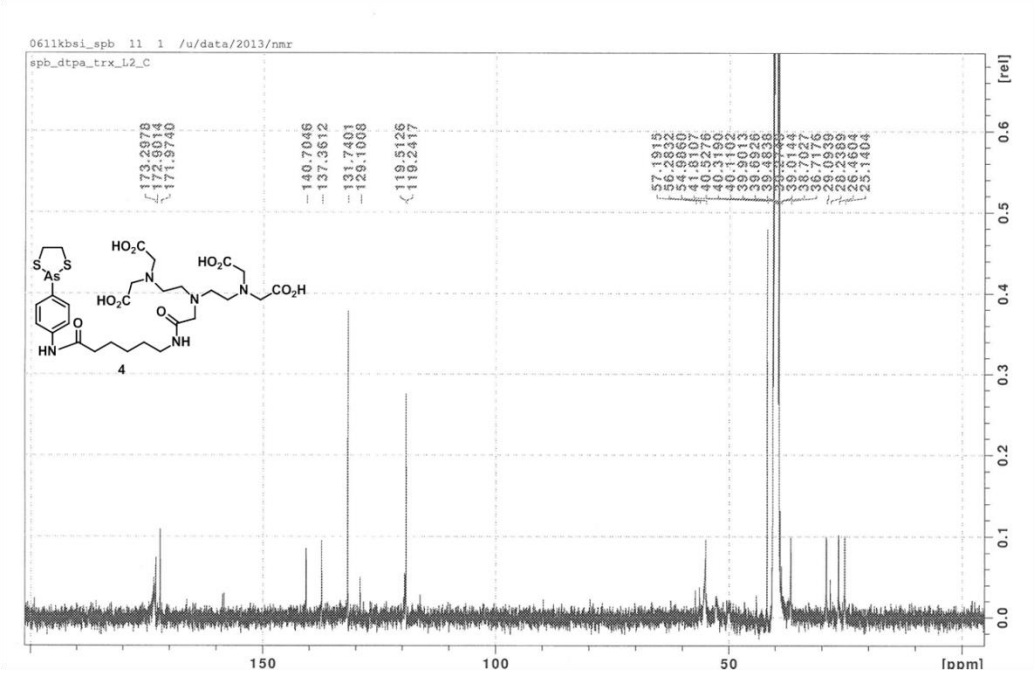



**Figure S11.** $^{13}$C NMR spectrum of **4** in DMSO-$d_6$.

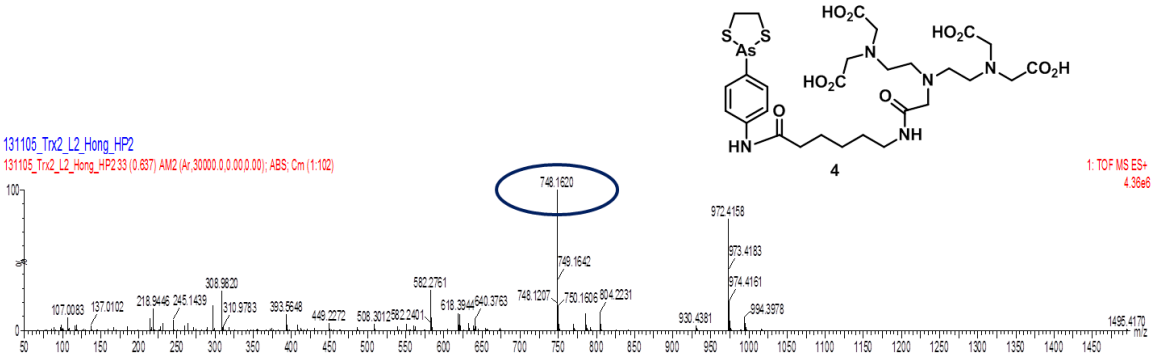



**Figure S12.** MS-spectrum of **4**.

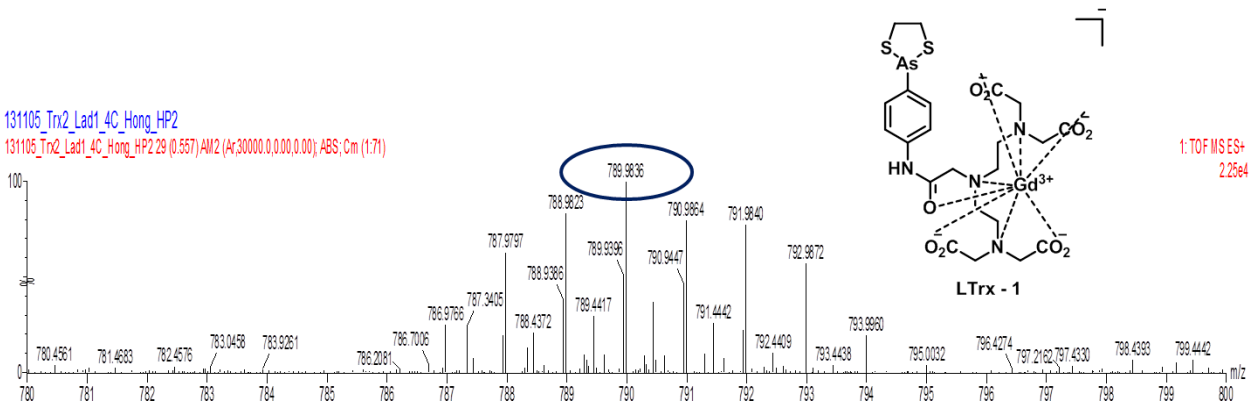
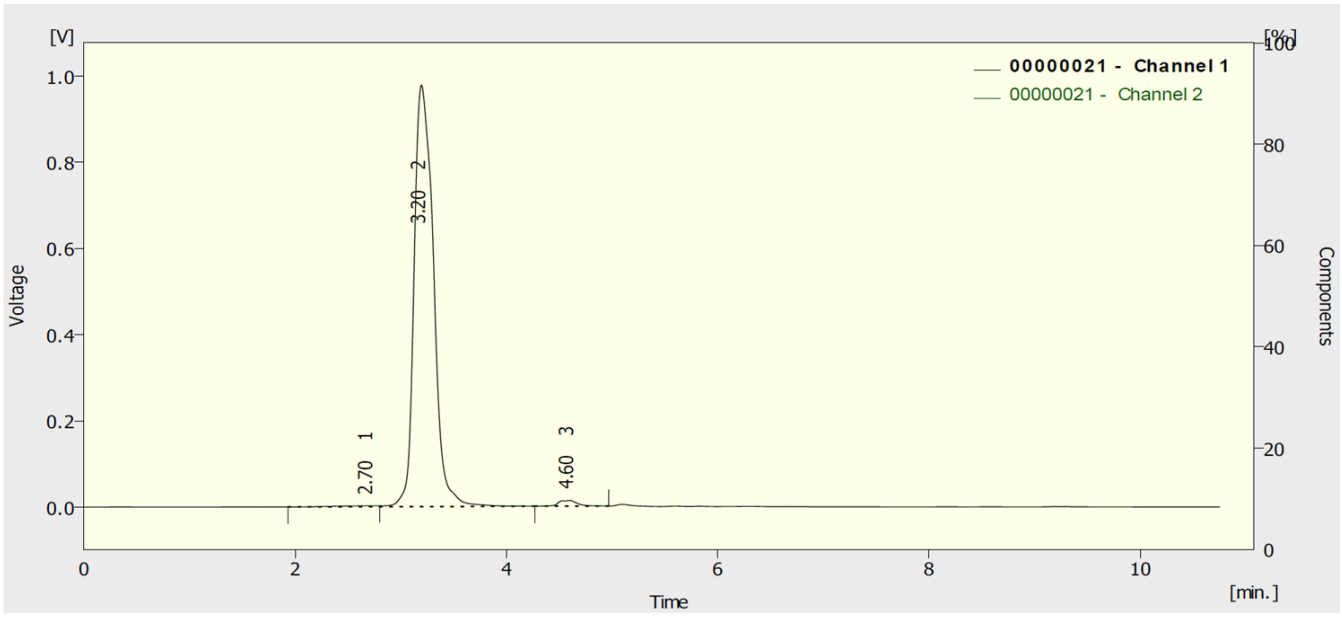



**Figure S13.** MS spectrum of the $Gd^{3+}$ complex, **CA1**.




| | Reten. Time [min] | Area [mV.s] | Height [mV] | Area [%] | Height [%] | W05 [min] | Compound Name |
|---|---|---|---|---|---|---|---|
| 1 | 2.697 | 65.747 | 2.402 | 0.5 | 0.2 | 0.43 | |
| 2 | 3.197 | 12424.976 | 977.861 | 98.2 | 98.4 | 0.20 | |
| 3 | 4.597 | 166.349 | 13.314 | 1.3 | 1.3 | 0.19 | |
| | Total | 12657.072 | 993.578 | 100.0 | 100.0 | | |

**Figure S14.** HPLC (high performance liquid chromatography) spectrum of the $Gd^{3+}$ complex, **CA1**.

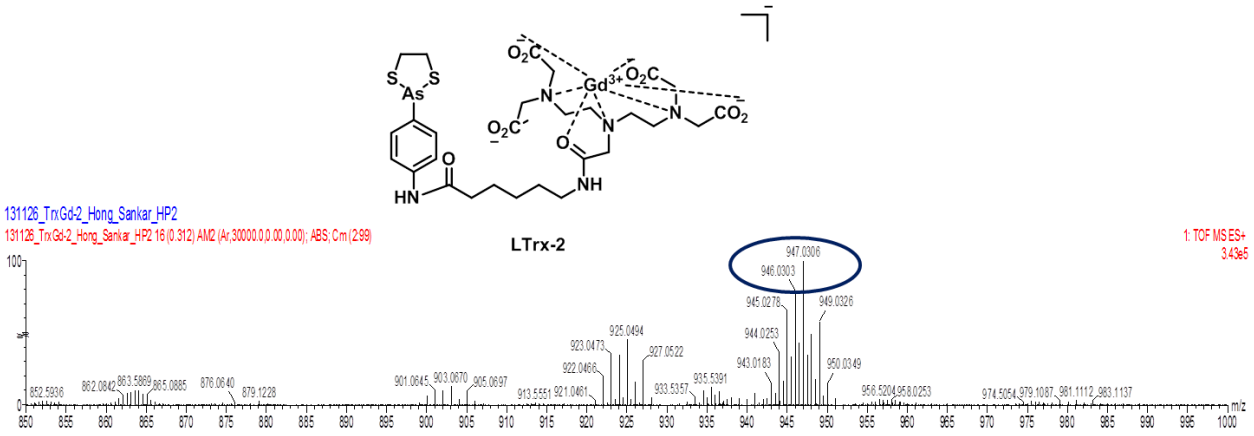



**Figure S15.** MS spectrum of the $Gd^{3+}$ complex, **CA2**.

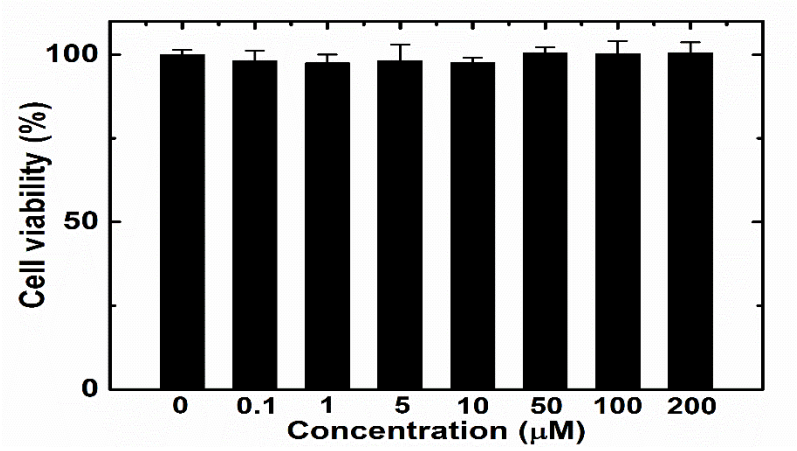



**Figure S16.** Cell viability of MCF-7 cells after incubation for 24 hours with the $T_1$ contrast agent **CA1**. The cells were incubated with different doses of **CA1** and viability was measured by means of an MTT assay as described in the main text.

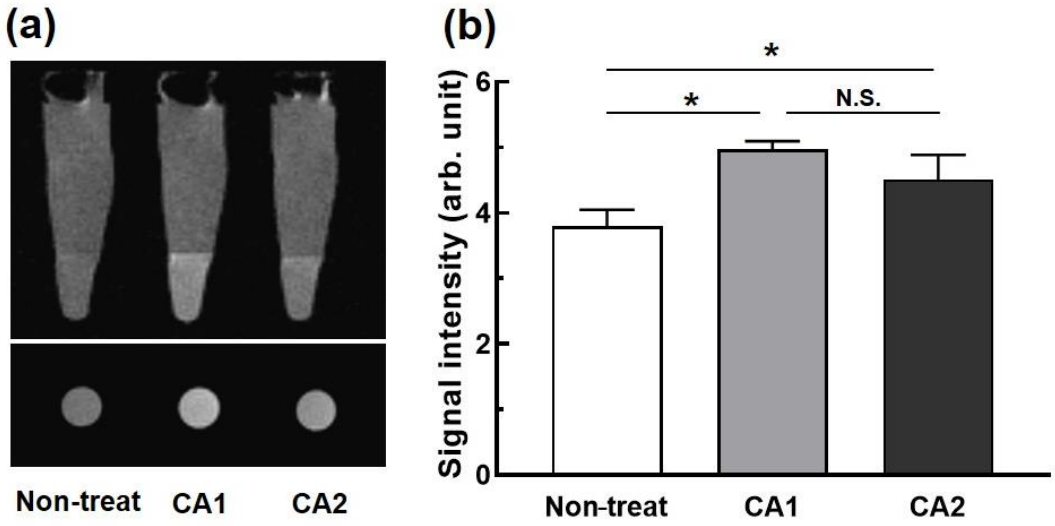



**Figure S17**. **MRI of MCF-7 cells incubated with CA1 and CA2**. (a) $T_1$–weighted MR images at 4.7 T at room temperature were obtained in cell phantom samples of MCF-7 cells incubated without (Non-treat) and with **CA1** or **CA2** (100 μM) and (b) corresponding signal intensities measured from region-of-interests of the MR phantom images (study replicated as 2 independent experiments). *, $p < 0.05$ (Student's t-test).