Supplementary Material

Luminescence-based Colorimetric Discrimination of Single-nucleotide Transversions by the Combined Use of the Derivatives of DOTA-conjugated Naphthyridine and Its Terbium Complex

Hiroshi Atsumi, [a] Keitaro Yoshimoto, [a, b, c, d] Shingo Saito, [c, e] Moriya Ohkuma, [c] Mizuo Maeda, [c] and Yukio Nagasaki [a, b, d, f, g, *]

[a] *Graduate School of Pure and Applied Science, University of Tsukuba, 1-1-1 Ten-noudai, Tsukuba, Ibaraki 305-8573, Japan*
[b] *Center for Tsukuba Advanced Research Alliance (TARA), University of Tsukuba, 1-1-1 Ten-noudai, Tsukuba, Ibaraki 305-8577, Japan*
[c] *Bioengineering Laboratory, RIKEN, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan*
[d] *Tsukuba Research Center for Interdisciplinary Materials Science (TIMS), University of Tsukuba, 1-1-1 Ten-noudai, Tsukuba, Ibaraki 305-8573, Japan*
[e] *Graduate School of Science and Engineering, Saitama University, 255 Shimo-Okubo, Sakura-ku, Saitama City, Saitama 338-8570, Japan*
[f] *Master's School of Medical Science, Graduate School of Comprehensive Human Sciences, University of Tsukuba, 1-1-1 Ten-noudai, Tsukuba, Ibaraki 305-8573, Japan*
[g] *Satellite Laboratory, International Center for Materials Nanoarchilectonics (MANA), National Institute of Materials Science (NIMS), 1-1-1 Ten-noudai, Tsukuba, Ibaraki 305-8573, Japan*

E-mail: nagasaki@nagalabo.jp

Tel.: 81-029-853-5749

Fax: 81-029-853-5749

Contents

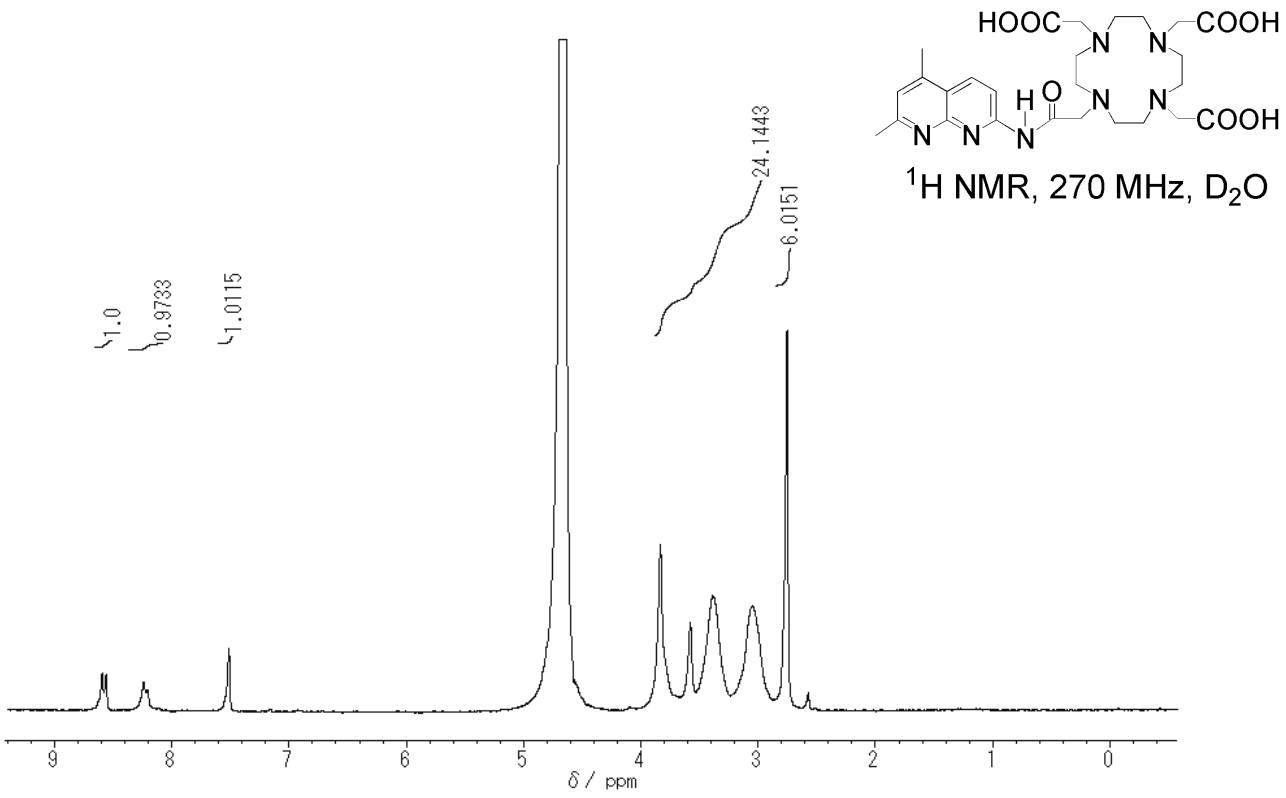
I. Materials and methods

Materials.
1,4,7-tris(*tert*-butoxycarbonylmethyl)-1,4,7,10-tetraazacyclododecane-10-hydroxysuccinimide ester and 2-amino-5,7-dimethyl-1,8-naphthyridine were purchased from Macrocyclics (Texas, USA) and Fluorochem Ltd. (Derbyshire, UK), respectively. The oligonucleotides, which were purified by HPLC, were purchased from Nihon Gene Research Laboratories Inc. (Sendai, Japan). Commercially available chemicals were of the highest quality available. The water used in this study was purified using a Milli-Q system (Nihon Millipore Co., Tokyo, Japan).

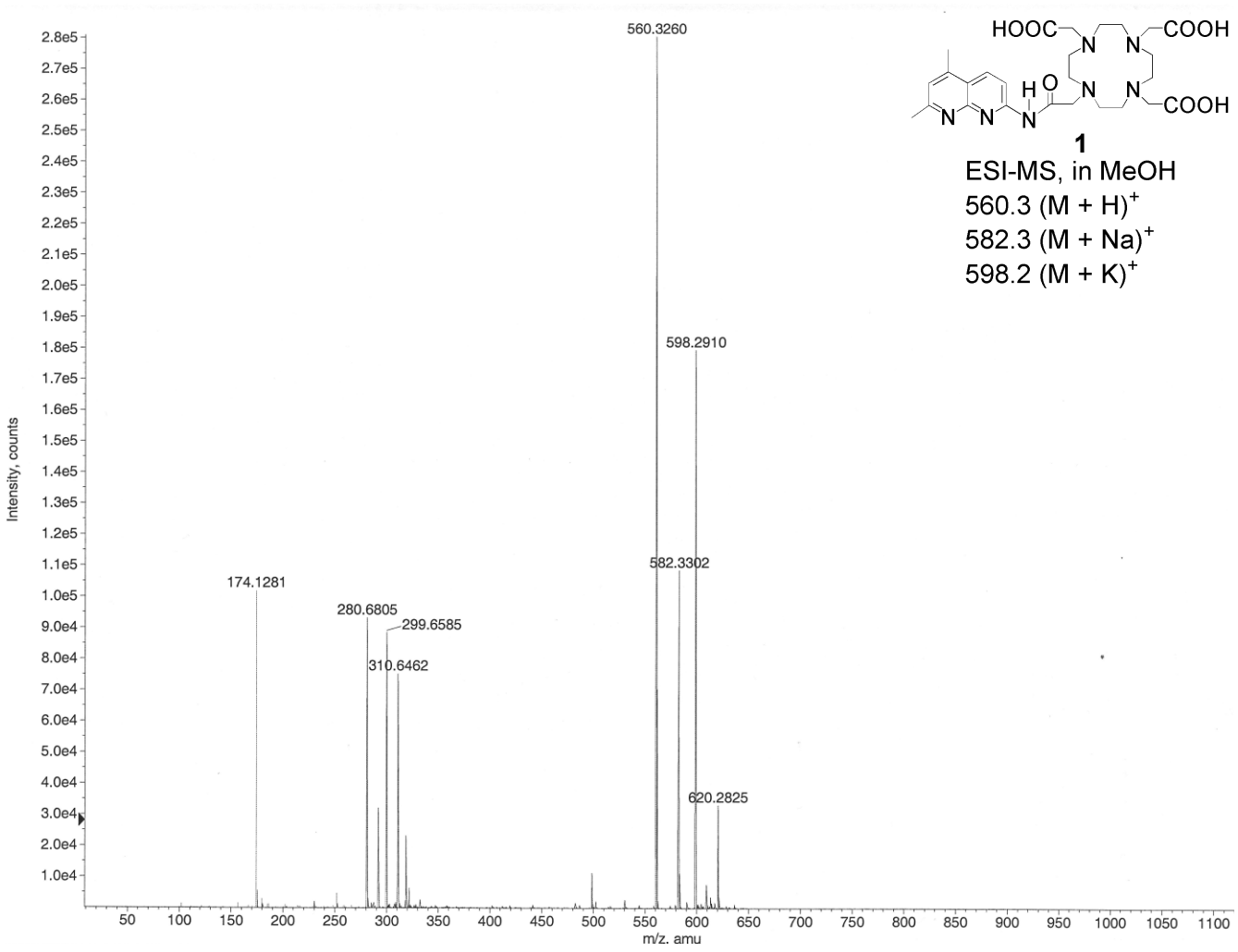
Fluorescence Measurements.
The excitation and emission spectra of the synthesized compounds as shown in Figure 2 were obtained by a HITACHI F-7000 spectrometer (Hitachi High-Technologies Corporation, Tokyo, Japan). For fluorescence titration experiments as shown in Figure 3 and emission lifetime measurement as shown in Figure S1, the emission spectra were obtained by a Varioskan Flash (Thermo Fisher Scientific Inc., Waltham, USA).

UV-visible Absorption Measurements.
The absorption spectra of the synthesized compounds as shown Figure 2 were obtained by a SHIMADZU UV-2500 PC spectrometer (SHIMADZU Co., Kyoto, Japan). For the DNA melting analysis as shown in Table 1, absorbance of DNA in the absence and presence of synthesized compounds was measured at 260 nm as a function temperature using a TMSPC-8 system (SHIMADZU Co., Kyoto, Japan) (8 cells; optical path length = 10 mm). The temperature ranged from 5 to 90 $^{\circ}$C with a heating rate of 1 $^{\circ}$C/ min. The T_m value was determined as the maximum in a plot of $\Delta A_{260}/\Delta T$ versus temperature.

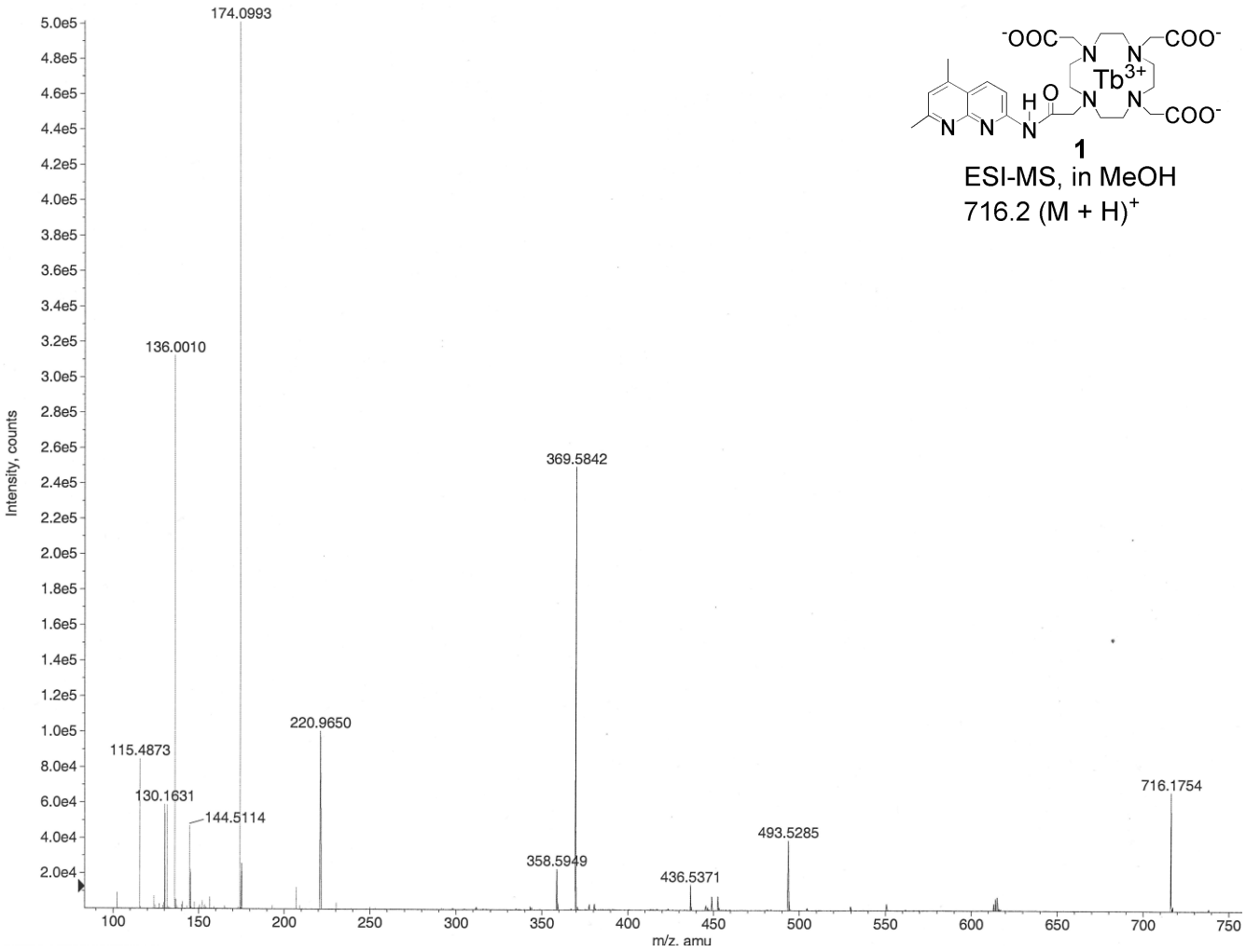
II. ^{1}H NMR spectra of **1**



III. ESI-MS spectra of **1**



IV. ESI-MS spectra of **1-Tb**



V. Emission decay curve

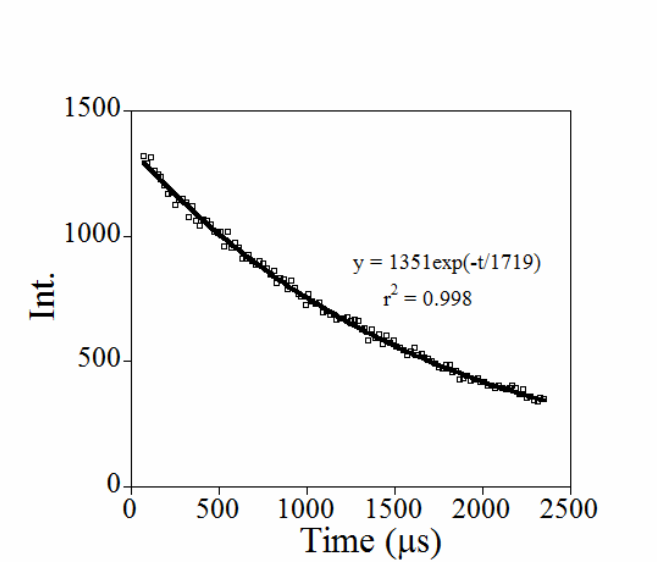


Figure S1. Emission decay curve of **1-Tb** at 545 nm (λ_{ex} = 332 nm) versus time. The data were collected at pH 7.4 (10 mM HEPES buffer) and fitted by an equation of the form $I = I_0 \exp(-t/\tau)$, where I_0 and I are the emission intensities at the t = 0 and time t, respectively, and τ is the emission lifetime. Lifetime of **1-Tb** was 1.7 ms.