Ratiometric Fluorescent and Colorimetric Dual-Modal Sensing Strategy for Discrimination and Detection of D₂O from H₂O

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Experimental Procedures

1. General Information

All reagents and solvents were obtained commercially and used without further purification unless otherwise noted. Analytical thin-layer chromatography (TLC) was performed on a silica gel plate and analyzed by UV light or by potassium permanganate stains followed by heating. Flash chromatography was carried out utilizing silica gel (200-300 mesh). $^1$H NMR and $^{13}$C NMR spectra were recorded in DMSO-$d_6$ at room temperature on a Bruker AM-400 spectrometer (400 MHz $^1$H, 100 MHz $^{13}$C) unless other noted. Data for $^1$H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, dd = doublet doublet), coupling constants (Hz), integration. Data for $^{13}$C NMR are reported as chemical shifts. HRMS were performed on a Bruker Apex II mass instrument (ESI).

All UV-visible spectra and fluorescence spectra were recorded using a Hitachi UV-2910 spectrophotometer and Hitachi F-7100 luminescence spectrometer, respectively. All fluorescence lifetime measurements were recorded by using the FLIM equipment consisting of the confocal optical microscope (Nanofinder FLEX2, Tokyo Instruments, Inc.) and a time-correlated single-photon counting (TCSPC) module (Becker & Hickl, SPC-150). Fluorescent quantum yields were determined to be 0.04% for HTI in H$_2$O, and 1.56% in D$_2$O, respectively by an absolute method using an integrating sphere on FLS920 of Edinburgh Instrument.

2. General Procedure for Preparation of Compound HTI and MTI

Scheme S1. Synthesis of HTI.

2-[(E)-2-(4-hydroxyphenyl)ethenyl]-1,3,3-trimethyl-3H-indol-1-ium iodide (HTI)

1,2,3,3-tetramethyl-3H-indoleiodide (903.5 mg, 3.0 mmol) and $p$-hydroxybenz-aldehyde (439.6 mg, 3.6 mmol) were added into 40 mL ethanol in a 100 mL Schlenk flask. The mixture was stirred and refluxed for 12h under an argon atmosphere. The process of the reaction was monitored by thin-layer chromatography (TLC). After cooling to room temperature, the reaction mixture was filtered, washed
with petroleum ether, and dried to afford an orange-red solid, no further purification was needed (968.8 mg, 79.7%). The NMR data is agreed with that in the previously reported literature.¹

**Scheme S2. Synthesis of MTI.**

![Scheme S2](image)

(E)-2-(4-methoxystyryl)-1,3,3-trimethyl-3H-indol-1-ium (MTI)

The synthesis of MTI was performed according to the reported literature by using 1,2,3,3-tetramethyl-3H-indoleiodide (903.5 mg, 3.0 mmol) and 4-methoxybenzaldehyde (489.6 mg, 3.6 mmol) with a yield of 72.6%.²

### 3. Experimental Section

#### 3.1 General Procedure for Sensing Studies

Stock solutions of HTI and MTI (10 mM) were prepared in DMSO. Freshly prepared HTI or MTI (4 μL) was diluted to 20 μM to collect the spectrum at room temperature. Solutions of NaCl, KCl, CaCl₂, Mg(ClO₄)₂, Zn(ClO₄)₂, Cu(ClO₄)₂, and Na₂SO₄ were prepared by dissolving their salts into distilled water.

D₂O and distilled H₂O samples were commercially available and stored in either glass or plastic bottles. Before the discrimination experiment and quantitative analysis measurement, freshly opened D₂O and H₂O were distilled and subsequently treated with degas and protection with N₂ atmosphere and stored in glass vessels.

#### 3.2 Detailed Protocols for pH Effects

Different pH values of Britton–Robinson (B–R) buffer (pH 3.00 – 11.00) were prepared. The solution for spectroscopic determination was obtained by diluting 4 μL of the stock solution to get a 20 μM solution in different pH of B–R buffer.

#### 3.3 ¹H NMR Titration

¹H NMR spectrum was sequentially recorded for HTI (15 mg, 0.037 mmol) dissolved in DMSO-<d₆> (0.6 mL), followed by the addition of 10 eq Et₃N (0.37 mmol, 51.3 μL) to adjust the pH value of the above solution, and further treated with 20 eq HCl (0.74 mmol, 64.5 μL) to reinstall the pH value.

#### 3.4 ¹H NMR of HTI in D₂O and H₂O
1H NMR of HTI (0.2 mM) was conducted in degassed pure H2O and D2O (0.5 mL, containing 1% DMSO as cosolvent) with D2O as an external standard.

3.5 NaOH, DCl, and HCl Titration Experiment

Freshly prepared NaOH (0.1 M in H2O, 0 – 6 μL) was added to a solution of HTI in H2O (20 μM). Both absorption and fluorescence spectra were collected after each addition. Similar experiments were conducted by titrating freshly prepared DCl (0.1 M, 0 – 5 μL) or HCl (0.1 M, 0 – 5 μL) into the D2O solution of HTI (20 μM), respectively.

4. Determination of the pKₐ of Sensor HTI

The pKa value of HTI was determined by the Henderson-Hasselbalch equation:

\[
\log\left(\frac{R_{\text{max}} - R}{R - R_{\text{min}}}\right) = pK_a - \text{pH}
\]

Where R is the fluorescence intensity ratio between 558 and 540 nm, R_{\text{max}} (or R_{\text{min}}) is the corresponding maximum (or minimum) limiting values of R. R represents the observed value. The pKₐ value was then calculated based on the plots of \(\log(\frac{R_{\text{max}} - R}{R - R_{\text{min}}})\) vs. pH as shown in Fig. 2e.

Based on the experiment on the pH effect on emission, the pKₐ value of HTI was calculated to be 7.11 in the B–R buffer (containing 0.2 % DMSO) system.

5. Determination of the Detection Limit

The detection limit was calculated based on the fluorescence and absorption titration, respectively. Fluorescence emission spectrum or absorption of sensor HTI in D2O solution was measured by thirty times and the standard deviation (σ) of this blank measurement was achieved. The slope (k) was derived from the calibration curve for quantitative analysis of H2O. The detection limit was determined with the following equation:

\[
\text{Detection limit} = 3\sigma/k
\]

Based on the absorption titration experiment shown in Fig. 5a and 5b, the detection limit value of H2O was calculated to be 0.196% in D2O (containing 0.2% DMSO).

\[
\text{Detection limit of H}_2\text{O} = 3 \times 0.000778/1.19258 = 0.001958 = 0.196\% \ (v/v)
\]

Based on the fluorescence titration experiment shown in Fig. 5c and 5d, the detection limit value of H2O was calculated to be 0.738% in D2O (containing 0.2% DMSO).

\[
\text{Detection limit of H}_2\text{O} = 3 \times 0.002373/0.97188 = 0.00732 = 0.732\% \ (v/v)
\]

A similar method was performed to determine the detection limit of D2O in H2O according to the data in Fig. 5 of the main article.
Based on the absorption titration experiment shown in Fig. 5a and 5b, the detection limit value of D$_2$O was calculated to be 0.597% in H$_2$O (containing 0.2% DMSO).

Detection limit of D$_2$O = 3*0.002373/1.19258 = 0.005969 = 0.597% (v/v)

Based on the fluorescence titration experiment shown in Fig. 5c and 5d, the detection limit value of D$_2$O was calculated to be 1.604% in H$_2$O (containing 0.2% DMSO).

Detection limit of D$_2$O = 3*0.00516/0.97188 = 0.01593 = 1.593% (v/v)

6. Spiked Recovery Experiments

Spiked recovery experiments were carried out based on the absorption method. Firstly, freshly prepared D$_2$O and H$_2$O were degassed and protected with N$_2$, which were mixed to obtain different fractions of H$_2$O in 2 mL of D$_2$O-H$_2$O solution in total, labeled as samples 1 – 8, and the content was labeled as “spiked%”, as shown in Table S1.

HTI (4 μL) was added to 2 mL of the above samples (1-8) to collect the absorption spectrum at room temperature. The absorption ratio ($A_{520\,\text{nm}}/A_{452\,\text{nm}}$) was determined to be the value y for each sample, which could be used to calculate the value x based on the linear relationship from Fig. 5b:

$$y = 1.19258 \times x + 1.05082$$

Data list in Table 1 in the main manuscript was calculated using the following equation:

For sample 1-4,

$$\text{Measured}\% = x \times 100;$$

For sample 5-8,

$$\text{Measured}\% = (1 - x) \times 100.$$

Recovery% = (Measured%/Spiked%) * 100

7. Additional Discussion

Our mechanism for distinguishing D$_2$O from H$_2$O was based on their alkaline difference, and therefore the pH/pD values should be consistent for the used samples. As known, CO$_2$ can be easily adsorbed in either H$_2$O or D$_2$O, which is assumed as the major interference to the pH/pD values of pure H$_2$O or D$_2$O. In our sensing strategy, each H$_2$O and/or D$_2$O sample was degassed and measured under an N$_2$ atmosphere, which fully eliminated the artefacts induced by H$_2$CO$_3$. We would like to make some additional discussion as follows:

7.1 Evaluating the pH/pD Control of Used Samples

Firstly, we compared the HTI spectroscopy in a freshly opened D$_2$O solution with that in a pretreated sample. Two parallel experiments were studied by using different branding D$_2$O samples. For freshly opened D$_2$O samples, different spectroscopies of HTI were noticed between different brands (Fig. S9a and S9c), while the spectra became consistent after these
samples were treated with the degas technique (Fig. S9b and S9d). These results suggested that the pH(pD) values of D₂O were almost consistent in the samples used in our measurements.

Furthermore, we carried out three sets of parallel experiments: Measuring the spectra of HTI in three different batches of H₂O and D₂O samples which were stored in vessels of different brands. The very consistent absorption and emission spectra of HTI in either H₂O or D₂O were noticed in all three parallel experiments (Fig. S10), further confirming the consistent pH(pD) values of H₂O or D₂O samples could be obtained.

Even though all the above D₂O and H₂O samples were stored in different bottles, pretreated in different vessels, and measured separately, consistent results were obtained for either H₂O or D₂O. The results further demonstrated the reliability of our strategy.

7.2 D₂O and H₂O Samples at Different pH

Since the mechanism for distinguishing D₂O from H₂O is based on the alkaline difference between these two pure samples, these probes including our probe HTI and other previously reported probes 3-5 might not be suitable for the discrimination of D₂O from H₂O at different pH/pD values.

7.3 Buffered H₂O and D₂O Samples

HTI was studied in buffered H₂O and D₂O by using the same portion of buffer components of Na₂HPO₄-KH₂PO₄ (10 mM, 1:1). As shown in Fig. S11, HTI displayed almost similar spectral properties in either buffered H₂O or D₂O.⁶ This is because, unlike neat H₂O and D₂O that possess different pH/pD values, buffered D₂O and H₂O in Na₂HPO₄-KH₂PO₄ displayed almost the same pH/pD value (ΔpH (D) = 0.05, pH = 7.0) according to previous work from Rubinson’s group. In this case, the buffered D₂O and H₂O in Na₂HPO₄-KH₂PO₄ would not be suitable for our study on the discrimination of D₂O from H₂O.

Advantages of this work:

In this work, H₂O and D₂O samples were degassed and protected with an N₂ atmosphere to fully eliminate the pH/pD variation induced by CO₂-adsorption, which has been proven to provide consistent pH/pD values of each used sample. We believe this work could provide a more reliable method for discrimination and detection of D₂O and H₂O compared with previously reported probes (Angew. Chem. Int., Ed. 2019, 58, 6280–6284; Chem. Commun., 2020, 56, 1191–1194; Microchem. J. 2022, 176, 107244.).
Supplementary Figures and Tables

**Table S1.** Preparation of samples 1-8 for spiked recovery experiments.

<table>
<thead>
<tr>
<th>Sample (Total 2 mL)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{\text{H}_2\text{O}}$ (mL)</td>
<td>0.06</td>
<td>0.10</td>
<td>0.14</td>
<td>0.20</td>
<td>1.94</td>
<td>1.90</td>
<td>1.86</td>
<td>1.80</td>
</tr>
<tr>
<td>$V_{\text{D}_2\text{O}}$ (mL)</td>
<td>1.94</td>
<td>1.90</td>
<td>1.86</td>
<td>1.80</td>
<td>0.06</td>
<td>0.10</td>
<td>0.14</td>
<td>0.20</td>
</tr>
<tr>
<td>Spiked%</td>
<td>97.0&lt;sup&gt;a&lt;/sup&gt;</td>
<td>95.0&lt;sup&gt;a&lt;/sup&gt;</td>
<td>93.0&lt;sup&gt;a&lt;/sup&gt;</td>
<td>90.0&lt;sup&gt;a&lt;/sup&gt;</td>
<td>97.0&lt;sup&gt;b&lt;/sup&gt;</td>
<td>95.0&lt;sup&gt;b&lt;/sup&gt;</td>
<td>93.0&lt;sup&gt;b&lt;/sup&gt;</td>
<td>90.0&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

<sup>a</sup>$V_{\text{D}_2\text{O}}/V_{\text{D}_2\text{O}+\text{H}_2\text{O}}$; <sup>b</sup>$V_{\text{H}_2\text{O}}/V_{\text{D}_2\text{O}+\text{H}_2\text{O}}$. 
Table S2. Comparison of reported organic optical sensors for D$_2$O/H$_2$O discrimination.

<table>
<thead>
<tr>
<th>Sensor</th>
<th>LR  $^a$ (vol%)</th>
<th>LOD  $^b$ (vol%)</th>
<th>Solvent</th>
<th>Sensing response</th>
<th>Detection interferenced by CO$_2$-induced pH changes</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trace H$_2$O in D$_2$O</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NIM-2F</td>
<td>0 – 50.0</td>
<td>0.24</td>
<td>DMSO/D$_2$O (20:3, v/v)</td>
<td>Single-modal</td>
<td>Colorimetric changes</td>
<td>Yes</td>
</tr>
<tr>
<td>AF</td>
<td>0 – 47.1</td>
<td>0.080</td>
<td>DMSO/D$_2$O (20:1.8, v/v)</td>
<td>Dual-modal</td>
<td>Ratiometric fluorescent/colorimetric changes</td>
<td>Yes</td>
</tr>
<tr>
<td>CF-D$_2$O</td>
<td>0 – 100</td>
<td>0.165 (I$_{450}$)</td>
<td>0.33%</td>
<td>Single-modal</td>
<td>Yes</td>
<td>[4]</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.05 (I$_{550}$)</td>
<td>DMSO</td>
<td>Turn on response at I$<em>{450}$ nm and I$</em>{550}$ nm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>ES</td>
<td>Only trace D$_2$O or H$_2$O was determined in DMSO and CH$_3$CN, respectively. The LOD of H$_2$O in D$_2$O was not determined.</td>
<td></td>
<td></td>
<td>Yes</td>
<td>[5]</td>
<td></td>
</tr>
<tr>
<td>HTI</td>
<td>0 – 100</td>
<td>0.19</td>
<td>0.2% DMSO</td>
<td>Dual-modal</td>
<td>Ratiometric fluorescent/colorimetric changes</td>
<td>No</td>
</tr>
</tbody>
</table>

$^a$ LR: linear range; LOD: $^b$ Limit of detection.
Table S3. Photophysical properties of HTI and MTI in different solvents.

<table>
<thead>
<tr>
<th>Solution</th>
<th>HTI</th>
<th></th>
<th></th>
<th>MTI</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\lambda_{\text{abs}}$ (nm)</td>
<td>$\lambda_{\text{em}}$ (nm)</td>
<td>$\varepsilon$ (cm$^{-1}$ M$^{-1}$)</td>
<td>$\lambda_{\text{abs}}$ (nm)</td>
<td>$\lambda_{\text{em}}$ (nm)</td>
<td>$\varepsilon$ (cm$^{-1}$ M$^{-1}$)</td>
</tr>
<tr>
<td>H$_2$O $^a$</td>
<td>420/520</td>
<td>515/552</td>
<td>33,700/30,400</td>
<td>416</td>
<td>515</td>
<td>22,800</td>
</tr>
<tr>
<td>D$_2$O $^a$</td>
<td>520</td>
<td>558</td>
<td>61,300</td>
<td>416</td>
<td>515</td>
<td>26,700</td>
</tr>
<tr>
<td>pH = 3.00 $^b$</td>
<td>420</td>
<td>515</td>
<td>38,700</td>
<td>n.d. $^c$</td>
<td>n.d. $^c$</td>
<td>n.d. $^c$</td>
</tr>
<tr>
<td>pH = 10.00 $^b$</td>
<td>520</td>
<td>558</td>
<td>68,100</td>
<td>n.d. $^c$</td>
<td>n.d. $^c$</td>
<td>n.d. $^c$</td>
</tr>
</tbody>
</table>

$^a$ Measured in degassed pure H$_2$O or D$_2$O; $^b$ Measured in B-R buffer; $^c$ Data are not detected.

Table S4. Fluorescence lifetimes of HTI (20 $\mu$M) in D$_2$O or H$_2$O (containing 0.2% DMSO) at 298 K using a bi-exponential function.

<table>
<thead>
<tr>
<th>Em</th>
<th>$\tau_1$/ps</th>
<th>Content%</th>
<th>$\tau_2$/ps</th>
<th>Content%</th>
<th>$\chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>D$_2$O $^a$</td>
<td>515 nm</td>
<td>53.87</td>
<td>90.87</td>
<td>710.5</td>
<td>9.13</td>
</tr>
<tr>
<td></td>
<td>560 nm</td>
<td>51.74</td>
<td>92.63</td>
<td>375.6</td>
<td>7.37</td>
</tr>
<tr>
<td>H$_2$O</td>
<td>515 nm</td>
<td>42.75</td>
<td>91.81</td>
<td>233.9</td>
<td>8.19</td>
</tr>
<tr>
<td></td>
<td>560 nm</td>
<td>43.72</td>
<td>91.39</td>
<td>274.9</td>
<td>8.61</td>
</tr>
</tbody>
</table>

$^a$ Excited at $\lambda_{\text{ex}} = 400$ nm and observed at $\lambda_{\text{em}} = 515$ nm and $\lambda_{\text{em}} = 560$ nm, respectively.
**Table S5.** Analysis of trace D$_2$O and H$_2$O based on fluorescent method.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Spiked%</th>
<th>Measured%</th>
<th>Recovery%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trace H$<em>2$O in D$<em>2$O ($V</em>{D2O}/V</em>{D2O+H2O}$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>97.0$^b$</td>
<td>97.2±0.3224$^b$</td>
<td>100.22±0.36</td>
</tr>
<tr>
<td>2</td>
<td>95.0$^b$</td>
<td>94.3±0.1780$^b$</td>
<td>99.27±0.20</td>
</tr>
<tr>
<td>3</td>
<td>93.0$^b$</td>
<td>92.6±0.1048$^b$</td>
<td>99.52±0.12</td>
</tr>
<tr>
<td>4</td>
<td>90.0$^b$</td>
<td>89.7±0.5456$^b$</td>
<td>99.68±0.61</td>
</tr>
<tr>
<td>Trace D$<em>2$O in H$<em>2$O ($V</em>{H2O}/V</em>{D2O+H2O}$)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>97.0$^c$</td>
<td>97.2±0.3224$^c$</td>
<td>100.22±0.36</td>
</tr>
<tr>
<td>6</td>
<td>95.0$^c$</td>
<td>94.3±0.1780$^c$</td>
<td>99.27±0.20</td>
</tr>
<tr>
<td>7</td>
<td>93.0$^c$</td>
<td>92.6±0.1048$^c$</td>
<td>99.52±0.12</td>
</tr>
<tr>
<td>8</td>
<td>90.0$^c$</td>
<td>89.7±0.5456$^c$</td>
<td>99.68±0.61</td>
</tr>
</tbody>
</table>

$^a$Measured in degassed H$_2$O or D$_2$O and each sample was measured three times; $^b V_{D2O}/V_{D2O+H2O}$; $^c V_{H2O}/V_{D2O+H2O}$. 
Figure S1. The relationship of (a) absorption ratio ($A_{520\text{ nm}}/A_{452\text{ nm}}$) and (b) fluorescence ratio ($I_{558\text{ nm}}/I_{540\text{ nm}}$) versus pH values.

Figure S2. (a) Fluorescence spectra of HTI (20 µM) in B–R buffer (0.2% DMSO) at various pH values (6.0–8.0); (b) Linear relationship between $\lg[(R_{\text{max}}-R)/(R-R_{\text{min}})]$ and pH values in the range of 6.0 – 8.0; $R = I_{558\text{ nm}}/I_{540\text{ nm}}$.

Figure S3. Fluorescence decay curves of HTI (20 µM) in D$_2$O or H$_2$O (containing 0.2% DMSO) at 298 K ($\lambda_{\text{ex}} = 400$ nm).
Figure S4. (a) Absorption and (b) fluorescence spectra of HTI (20 µM) in H₂O (0.2% DMSO) with addition of 0.1 M NaOH (0 – 6 µL), Slit: 10 nm/10 nm; (c) Absorption spectra and (d) fluorescence spectra of HTI (20 µM) in D₂O (0.2% DMSO) with addition of 0.1 M DCI (0 – 5 µL), Slit: 5 nm/5 nm; (e) UV-vis absorption spectra and (f) fluorescence spectra of sensor HTI (20 µM) in D₂O (0.2% DMSO) with addition of 0.1 M HCl (0 – 5 µL), Slit: 5 nm/5 nm; (g) Diagram of related structure transformation.

Figure S5. ¹H NMR spectra of HTI (0.037 mmol) was conducted in (a) DMSO-d₆, (b) HTI with 10 eq. Et₃N (0.37 mmol, 51.3 µL) in DMSO-d₆, and (c) introduce 20 eq. HCl (0.74 mmol, 64.5 µL) into sample b.
Figure S6. (a) UV-vis absorption spectra and (b) emission spectra of sensor HTI (20 µM) in H$_2$O (0.2% DMSO) and 9% glycerol (0.2% DMSO).

Figure S7. (a) Absorption and (b) fluorescence spectra of HTI (20 µM) in the absence and presence of the other common species (10 eq., 200 µM) in H$_2$O (0.2% DMSO). (c) Fluorescence responses of sensor HTI (20 µM) to common species in H$_2$O (0.2% DMSO). Bars represent the ratio of the fluorescence intensity in the presence ($I$) and absence ($I_0$) of analytes. From 1 to 11: H$_2$O, MeOH, EtOH, PhMe, NaCl, Na$_2$SO$_4$, KCl, CaCl$_2$, Mg(ClO$_4$)$_2$, Cu(ClO$_4$)$_2$, Zn(ClO$_4$)$_2$. Ex = 452 nm.
Figure S8. Fluorescence stability of HTI (20 µM) in degassed H₂O (containing 0.2% DMSO). Ex = 452 nm.
**Figure S9:** Normalized absorption (a, b) and fluorescence spectra (c, d) of HTI (20 µM) in D$_2$O (0.2% DMSO) sample 1 (from Energy, China) and sample 2 (from Adamas, China). (a) and (c) represented the sample without pre-treatment and (b) and (d) represented the distilled samples with degas and protection with N$_2$.

**Figure S10.** Consistent absorption (a, c) and emission (b, d) spectra of HTI (20 µM) from different batches of degassed H$_2$O and D$_2$O, containing 0.2% DMSO. Ex = 452 nm.
Figure S11. (a) Absorption and (b) fluorescence spectra of HTI (20 μM) in Na$_2$HPO$_4$-KH$_2$PO$_4$ (10 mM, Na$_2$HPO$_4$ : KH$_2$PO$_4$ = 1:1) buffer solution in H$_2$O (black line) and D$_2$O (red line).
Figure S12. ESI-MS spectra of HTI.
References


