Comparative study of lysosome-targetable pH probes based on phenoxazinium attached with aliphatic and aromatic amines

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1. Tables

**Table S1** the possession percentage of each component occupied in frontier molecular orbitals for 1a* at the ground state and the lowest excited state.

<table>
<thead>
<tr>
<th>State</th>
<th>FMOs</th>
<th>E / eV</th>
<th>NEt%</th>
<th>O%</th>
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<tbody>
<tr>
<td>The ground state</td>
<td>LUMO</td>
<td>-3.651</td>
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<td>1</td>
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**Table S2** the possession percentage of each component occupied in frontier molecular orbitals for 1b* at the ground state and the lowest excited state.

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<th>O%</th>
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<td>15</td>
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</table>
2. Figures

![Graphs showing reversible absorption and emission responses of probes 1a-b with changes between basic and acidic conditions.](image)

**Fig. S1** The reversible absorption (top) and emission (bottom) responses of probes **1a-b** with changes between basic and acidic conditions. (a, c) Probe **1a**; (b, d) probe **1b**.
Fig. S2 Absorption and fluorescence responses of probes 1a−b (10 μM) to different analytes in disodium hydrogen phosphate–citric acid buffer, K+ (100 mM), Na+ (100 mM), Ca2+ (0.5 mM), Mg2+ (0.5 mM), Cu2+ (0.3 mM), Mn2+ (0.3 mM), Hg2+ (0.3 mM), Co2+ (0.3 mM), Ni2+ (0.3 mM), Cd2+ (0.3 mM); Cys (0.1 mM), Phe (0.1 mM), Gly (0.1 mM), Glu (0.1 mM), Arg (0.1 mM), Lys (0.1 mM), Pro (0.1 mM), Trp (0.1 mM) and His (0.1 mM) were included. (a–d) Probe 1a; (e–h) probe 1b. (a, b, e, f) Absorption spectra; (c, d, g, h) emission spectra. (a, c, e, g) In pH 7.4 buffer; (b, d) in pH 4.4 buffer; (f, h) in pH 4.2 buffer.
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Fig. S4 $^1$HNMR of compound 4b
Fig. S5 $^1$HNMR of compound 5a.

Fig. S6 $^1$HNMR of compound 5b.
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Fig. S8 $^1$HNMR of compound 1b.
Fig. S9 $^{13}$CNMR of compound 4a.

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**Fig. S12** $^{13}$CNMR of compound 5b.
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Fig. S16 HRMS of compound 4b.
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Fig. S18 HRMS of compound 5b.
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Fig. S20 HRMS of compound 1b.