Supporting Information

Acid Responsiveness of Emissive Morpholinyl Aminoquinolines and Their Use for Cell Fluorescence Imaging

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Table S1. Selected Structural and Refinement Parameters for **1** and **3**.

	1	**3**
Empirical formula	$C_{17}H_{17}F_6N_3O$	$C_{23}H_{28}F_6N_4O_2$
Formula weight	393.33	505.48
Crystal dimensions	0.2 × 0.1 × 0.1 mm	0.2 × 0.1 × 0.1 mm
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$ (#14)	$P2_1/c$ (#14)
a/Å	9.55670(10)	5.5656(2)
b/Å	18.5529(3)	18.4733(5)
c/Å	9.70230(10)	22.5869(7)
α/°	90	90
β/°	91.6470(10)	90.732(3)
γ/°	90	90
Volume/Å	1719.55(4)	2322.08(13)
Z (Z') value	4 (1)	4 (1)
Density (calc.)/g/cm^3	1.512 g/cm^3	1.449 g/cm^3
F (000)	808	1052
Residuals: R_1 ($I > 2.00\sigma(I)$) [a]	0.0385	0.0681
Residuals: wR_2 [b]	0.1074	0.1824
GOF	1.063	1.050
Temperature	93 K	93 K
CCDC no.	2156333	2156336

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = [\sum(w(F_o^2 - F_c^2)^2)/\sum w(F_o^2)^2]^{1/2}$

Table S2. Selected Structural and Refinement Parameters for **5** and **6**.

	5	**6**
Empirical formula	$C_{18}H_{20}F_{12}N_3OP$	$C_{19}H_{22}F_{12}N_3OP$
Formula weight	569.36	567.36
Crystal dimensions	0.1 × 0.1 × 0.1 mm	0.1 × 0.1 × 0.1 mm
Crystal system	orthorhombic	triclinic
Space group	*Pna*2$_1$ (#33)	*P*-1 (#2)
a/Å	55.7279(19)	6.1777(2)
b/Å	8.6632(2)	8.8010(3)
c / Å	9.3599(3)	22.3052(8)
α/°	90	81.551(3)
β/°	90	85.313(3)
γ/°	90	80.624(3)
Volume/Å	4518.79	1181.47(7)
Z (Z') value	8 (2)	2 (1)
Density (calc.)/g/cm^3	1.674 g/cm^3	1.595 g/cm^3
F (000)	2312	576
Residuals: R_1 ($I > 2.00\sigma(I)$) [a]	0.0834	0.0708
Residuals: wR_2 [b]	0.2318	0.1978
GOF	1.036	1.044
Temperature	93 K	93 K
CCDC no.	2156337	2156358

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = [\sum(w(F_o^2 - F_c^2)^2)/\sum w(F_o^2)^2]^{1/2}$

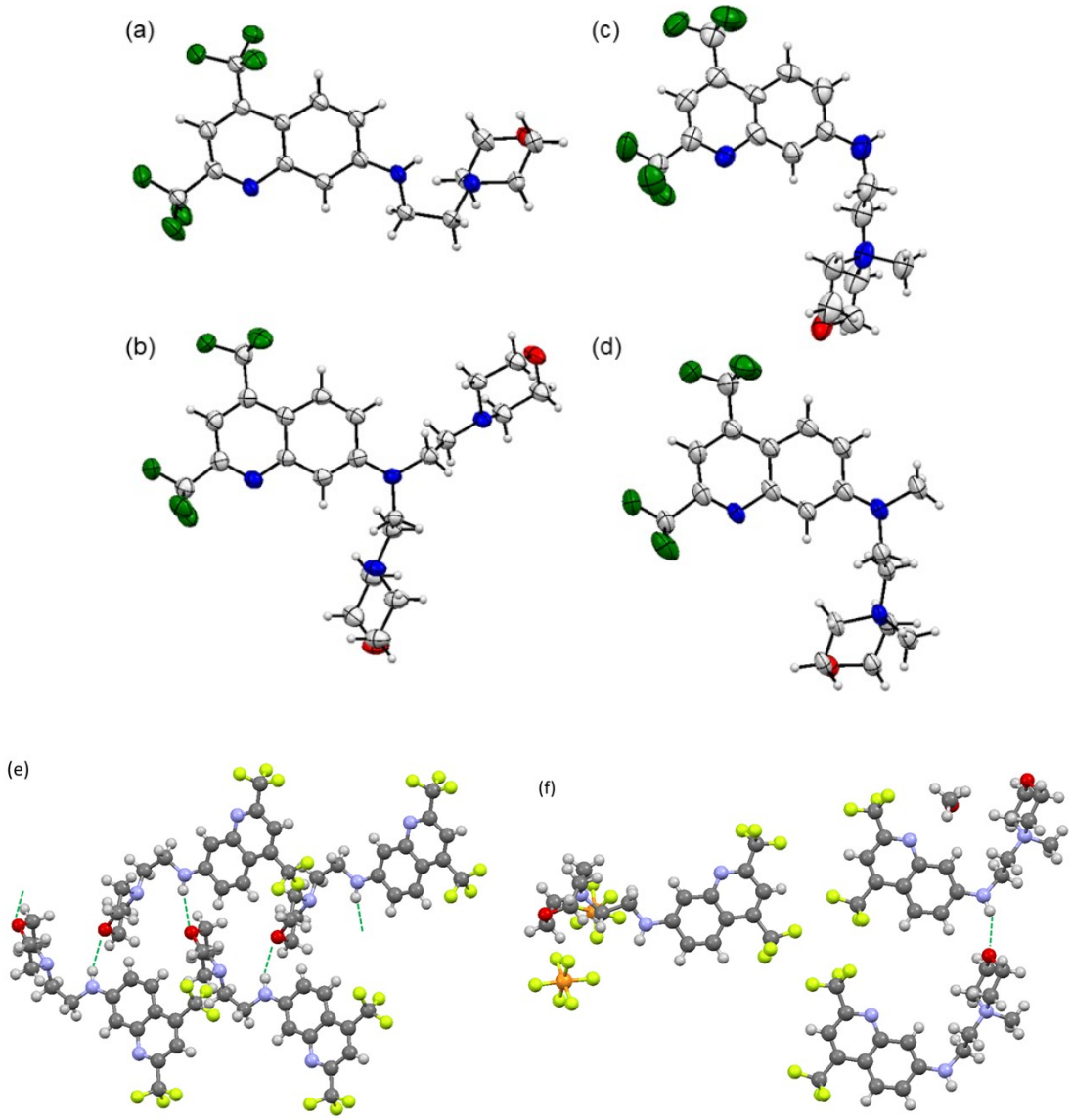


Figure S1. ORTEP-style drawings showing ellipsoids at 50% probability of compounds **1** (a), **3** (b), **5** (c), and **6** (d). Solvent molecules and PF_6^- counter anions are omitted for clarity. Gray, blue, red, and green atoms are C, N, O, and F, respectively. (e) Hydrogen-bonded chains formed between the nitrogen atom in the secondary amine and oxygen atoms in morpholine in compound **1**. Each hydrogen bond is 3.19 Å in length (green dotted lines). (f) Hydrogen bonds between the nitrogen atom in the secondary amine and oxygen atom in morpholine (one of two crystallographically independent molecules) in compound **5**. The hydrogen bond measures 3.13 Å (green dotted lines).

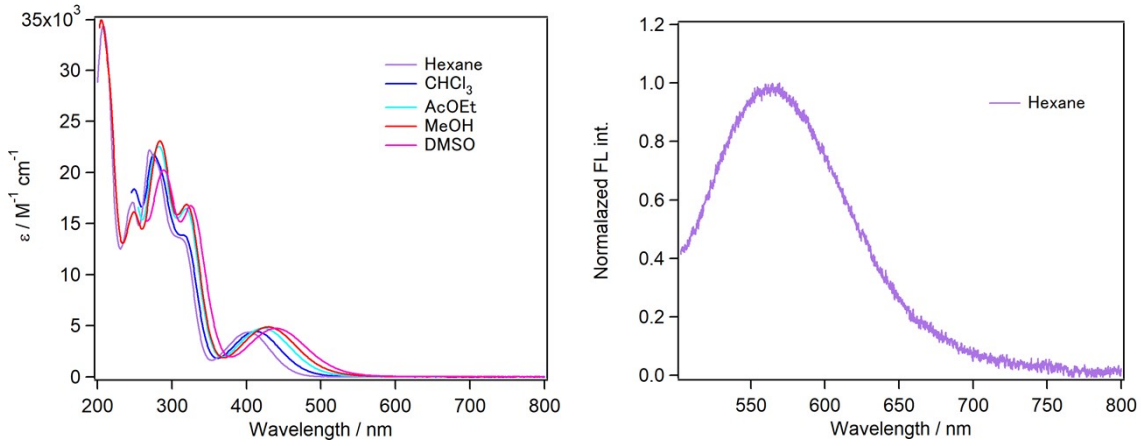
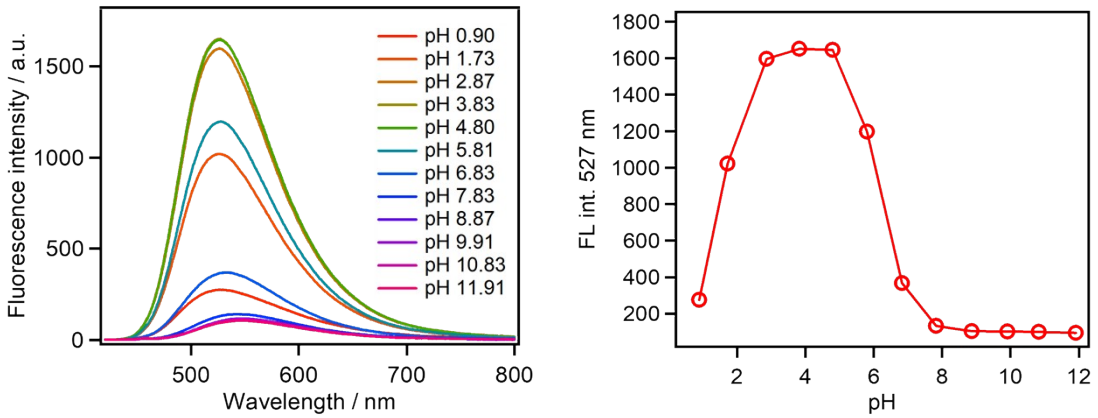
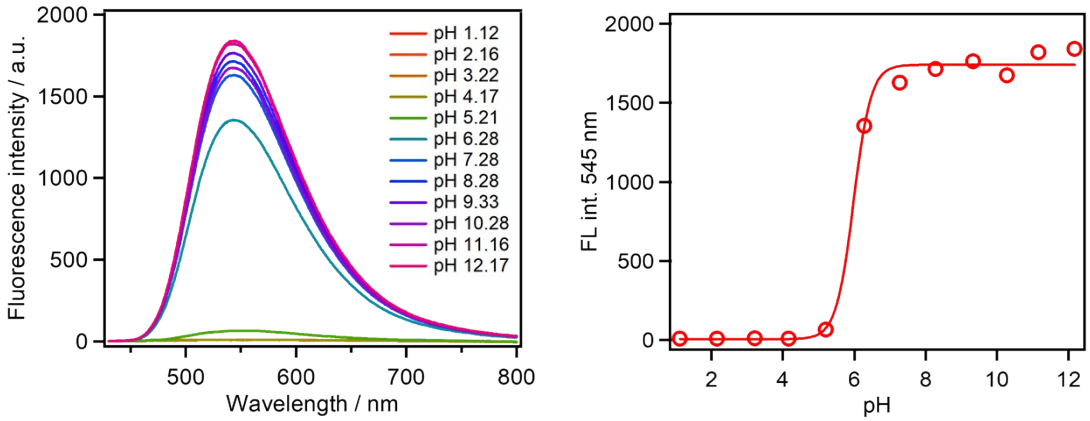


Figure S2. Absorption (left) and fluorescence (right) spectra of compound **4** in the given solvents. No fluorescence (very weak emissions) was observed in $CHCl_3$, AcOEt, MeOH, or dimethylsulfoxide (DMSO) (see Table 2 in the main text).

Compound **1**



Compound **2**



Compound **3**

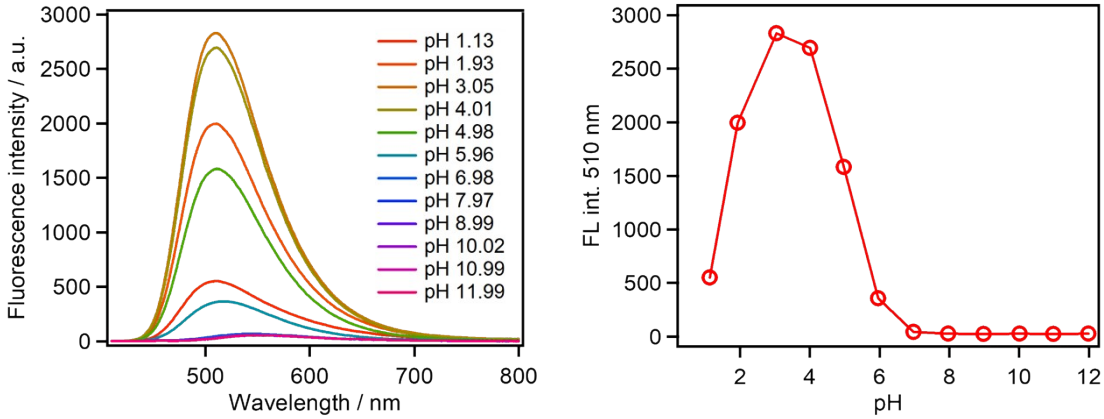
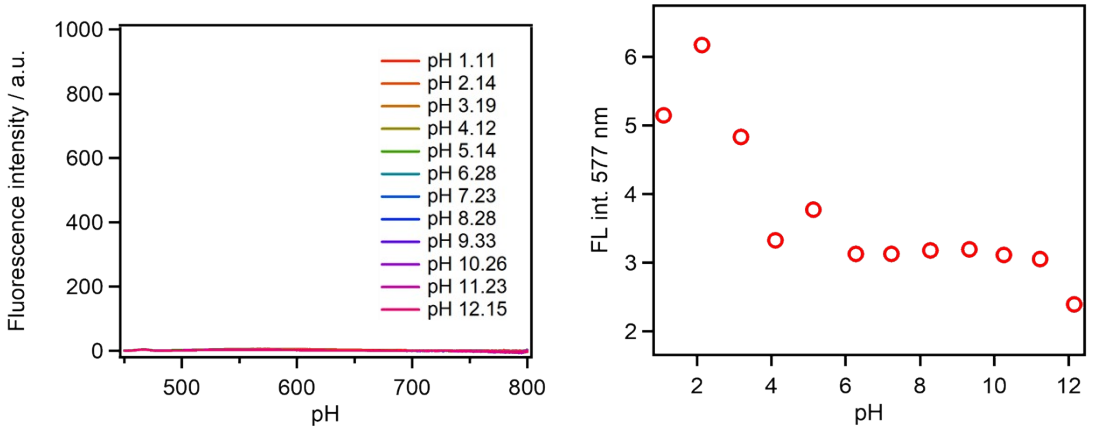


Figure S3-1. Emission spectral changes (left) of compounds **1–3** in 1% DMSO/phosphate buffer conditions (10% DMSO in compound **2**). Right panels represent the emission intensity as a function of pH value.

Compound **4**



Compound **5**

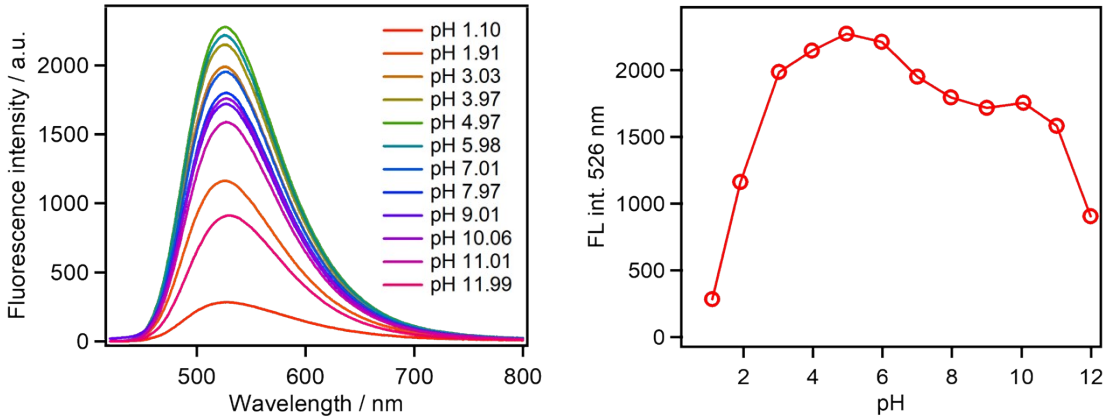


Figure S3-2. Emission spectral changes (left) of compounds **4** and **5** in 1% (compound **5**) or 10% (compound **4**) DMSO/phosphate buffer conditions. Right panels represent the emission intensity as a function of pH value.

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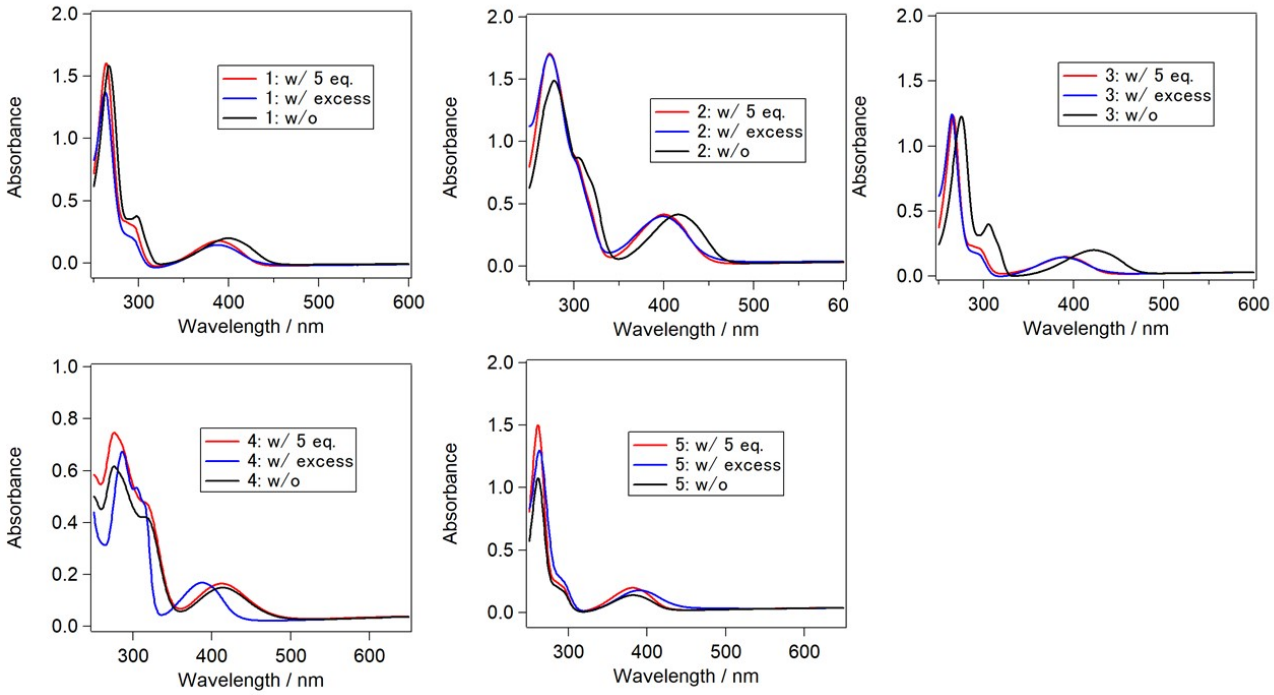


Figure S4-1. Absorption spectral changes of compounds **1–5** (see inset annotations) in $CHCl_3$ without trifluoroacetic acid (TFA) (black lines) and with 5 equiv TFA (red lines) and excess TFA (blue lines).

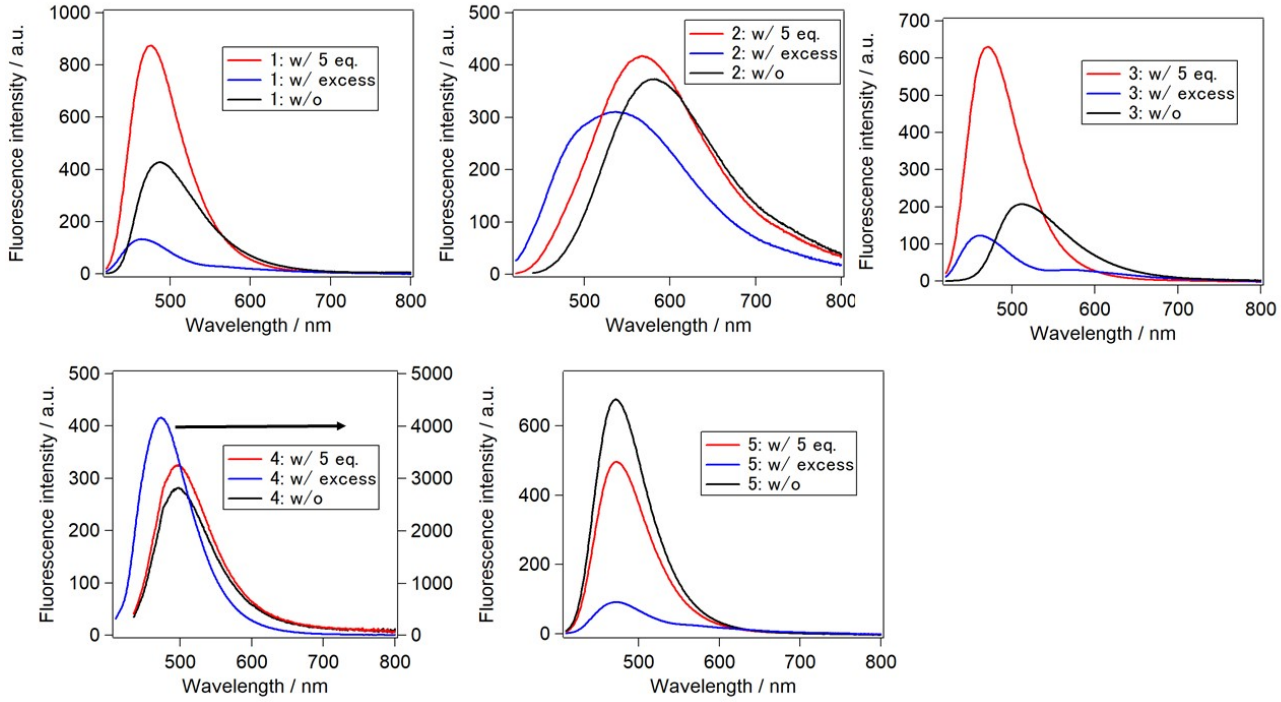


Figure S4-2. Fluorescence spectral changes of compounds **1–5** (see inset annotations) in $CHCl_3$ without TFA (black lines) and with 5 equiv TFA (red lines) and excess TFA (blue lines).

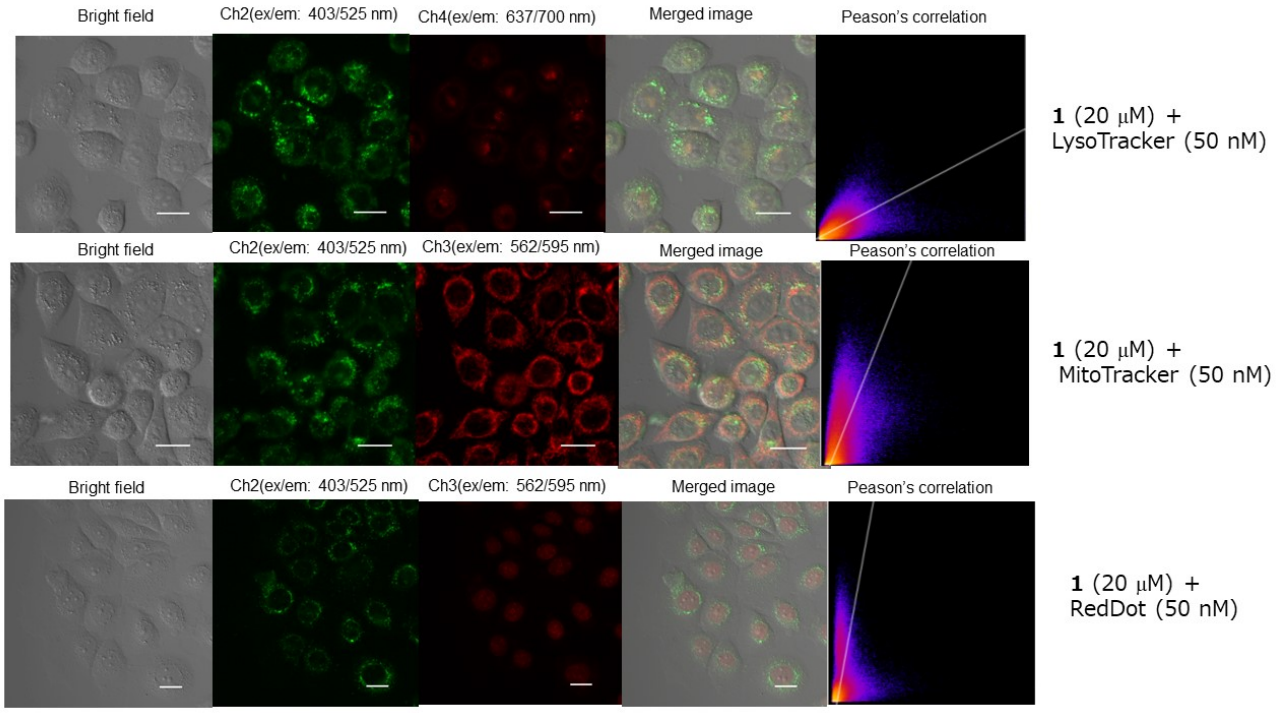


Figure S5. Confocal fluorescent microscopy images. Each panel represents bright field (left), fluorescence images obtained using Ch. 2, 3, or 4 (indicated at the top of the panel), as well as merged bright field and fluorescent images, and Pearson's correlation maps (right). Top, middle, and bottom lines indicate images treated with compound **1** and LysoTracker, MitoTracker, and RedDot, respectively. Scale bars indicate 20 μm.

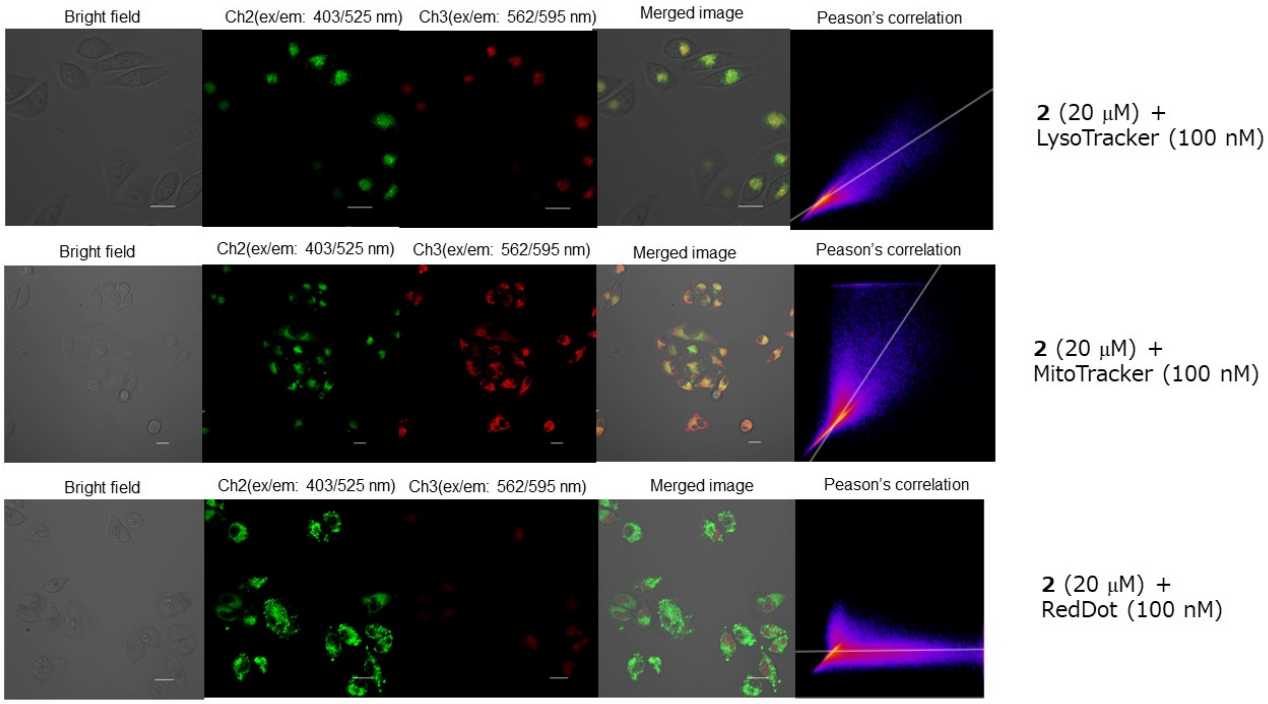


Figure S6. Confocal fluorescent microscopy images. Each panel show bright field (left), fluorescence images obtained using Ch. 2 or 3 (indicated at the top of the panel), as well as merged bright field and fluorescent images, and Pearson's correlation maps (right). Top, middle, and bottom lines indicate images treated with compound **2** and LysoTracker, MitoTracker, and RedDot, respectively. Scale bars indicate 20 μm.

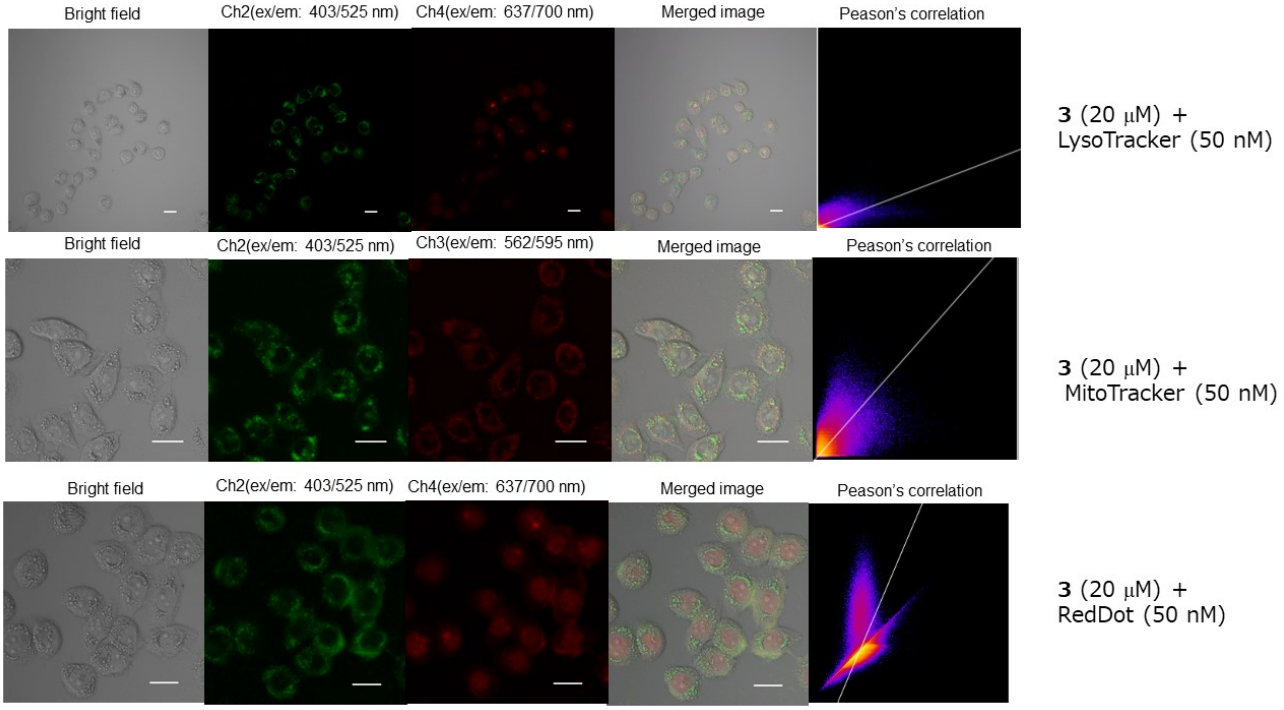


Figure S7. Confocal fluorescent microscopy images. The panels represent bright field (left), fluorescence images obtained using Ch. 2, 3, or 4 (indicated at the top of the panel), as well as merged bright field and fluorescent images, and Pearson's correlation maps (right). Top, middle, and bottom lines indicate images treated with compound **3** and LysoTracker, MitoTracker, and RedDot, respectively. Scale bars indicate 20 μm.

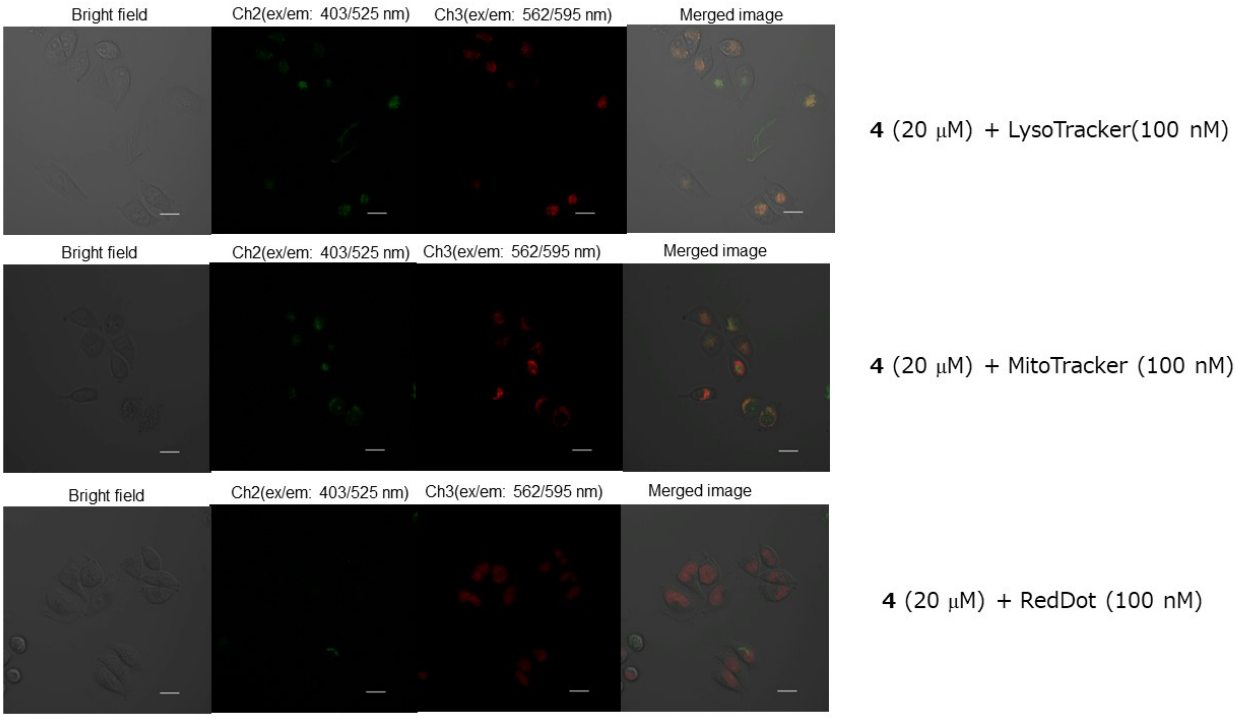


Figure S8. Confocal fluorescent microscopy images. The panels represent bright field (left) and fluorescence images obtained using Ch. 2 or 3 (indicated at the top of the panel), as well as merged bright field and fluorescent images. Top, middle, and bottom lines indicate images treated with compound **4** and LysoTracker, MitoTracker, and RedDot, respectively. Scale bars indicate 20 μm.

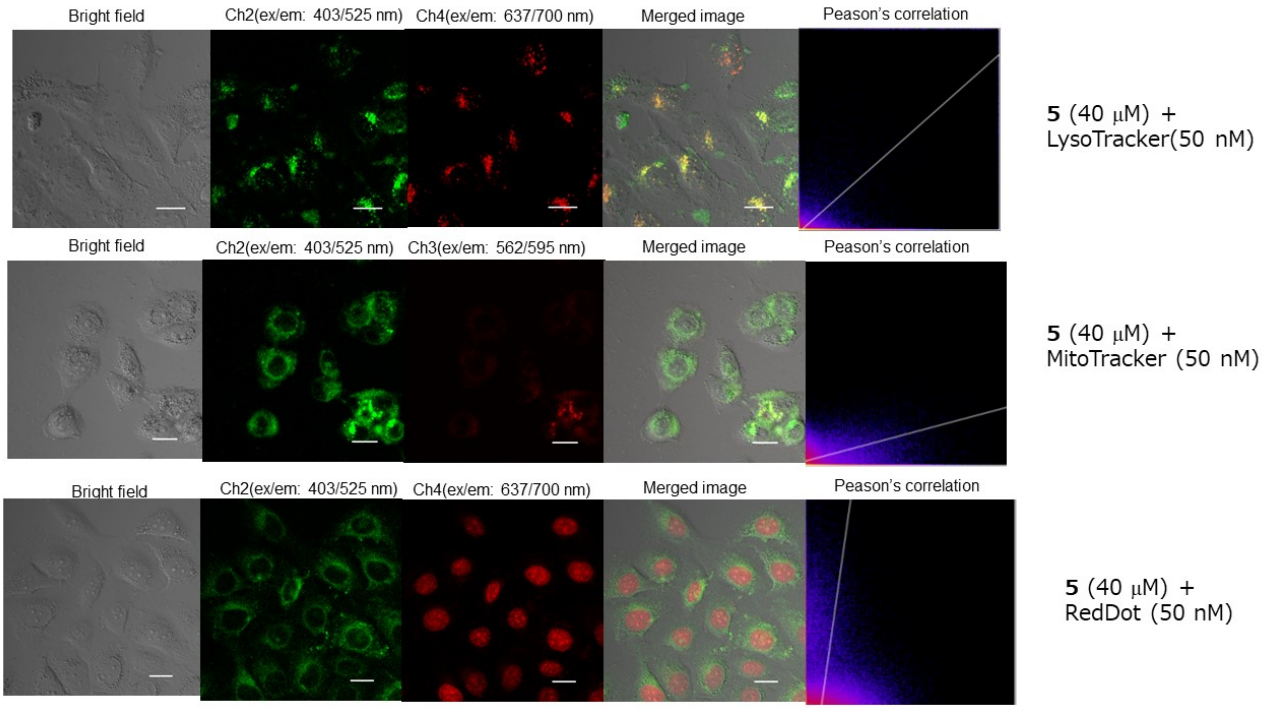


Figure S9. Confocal fluorescent microscopy images. Each panel shows a bright field (left), fluorescence image obtained using Ch. 2, 3, or 4 (indicated at the top of the panel), as well as a merged image of the bright field and fluorescent images, and Pearson's correlation maps (right). Top, middle, and bottom lines indicate images treated with compound **5** and LysoTracker, MitoTracker, and RedDot, respectively. Scale bars indicate 20 μm.

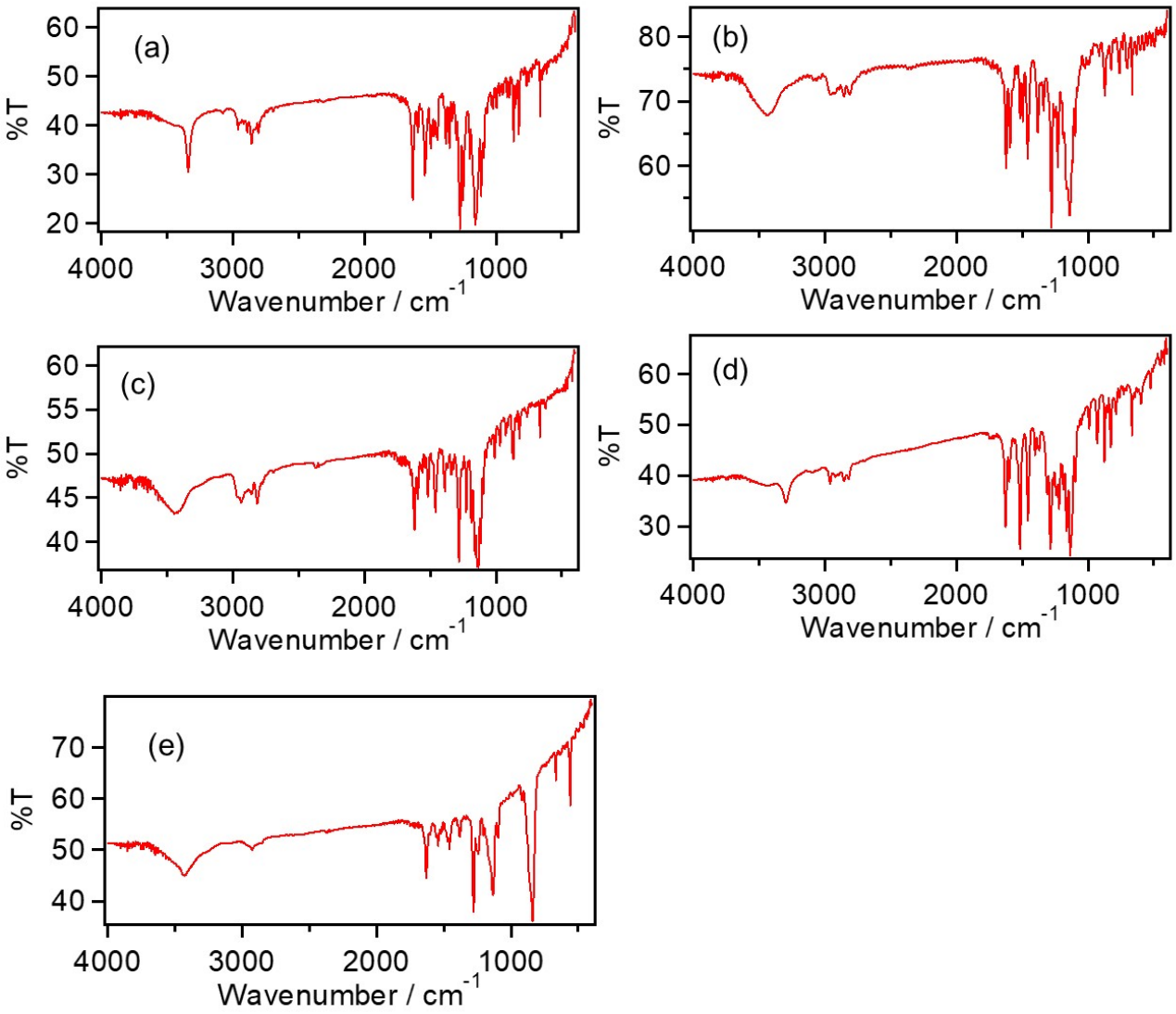
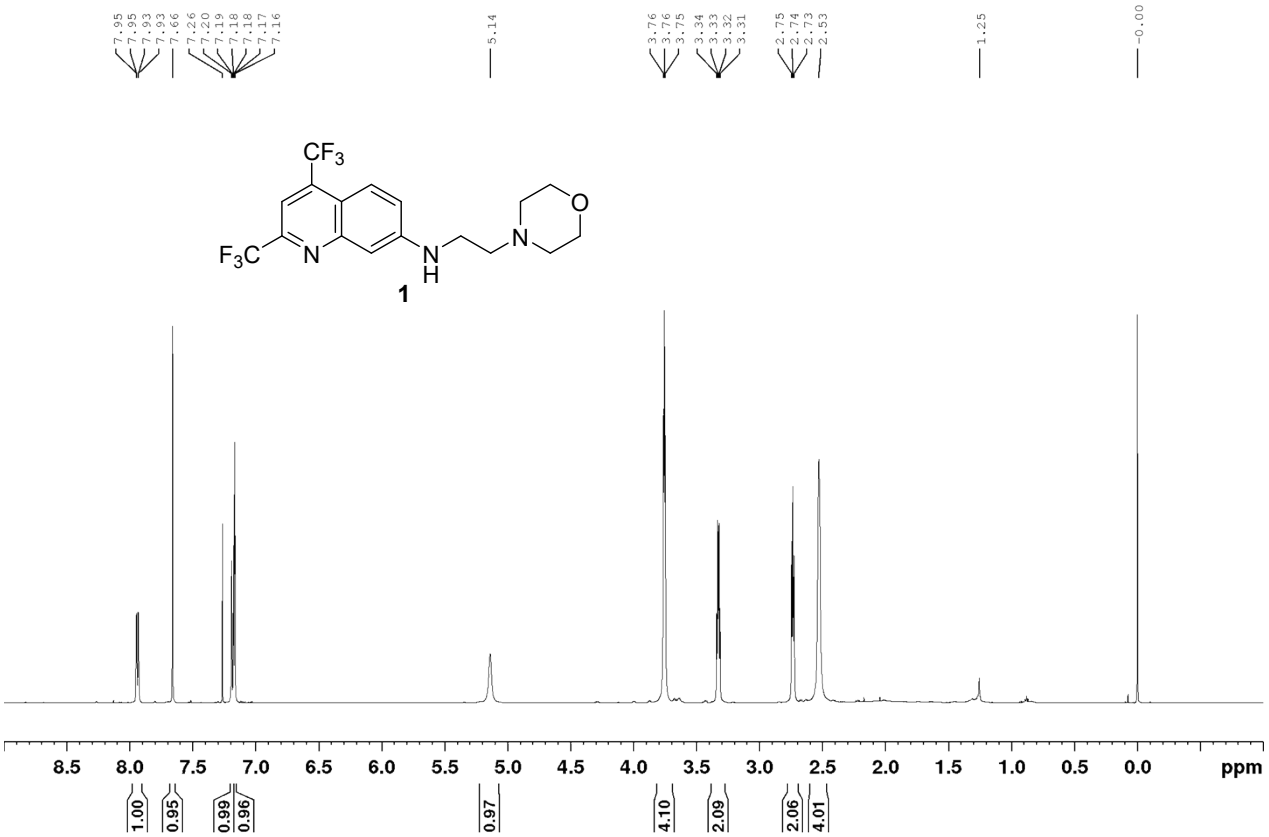
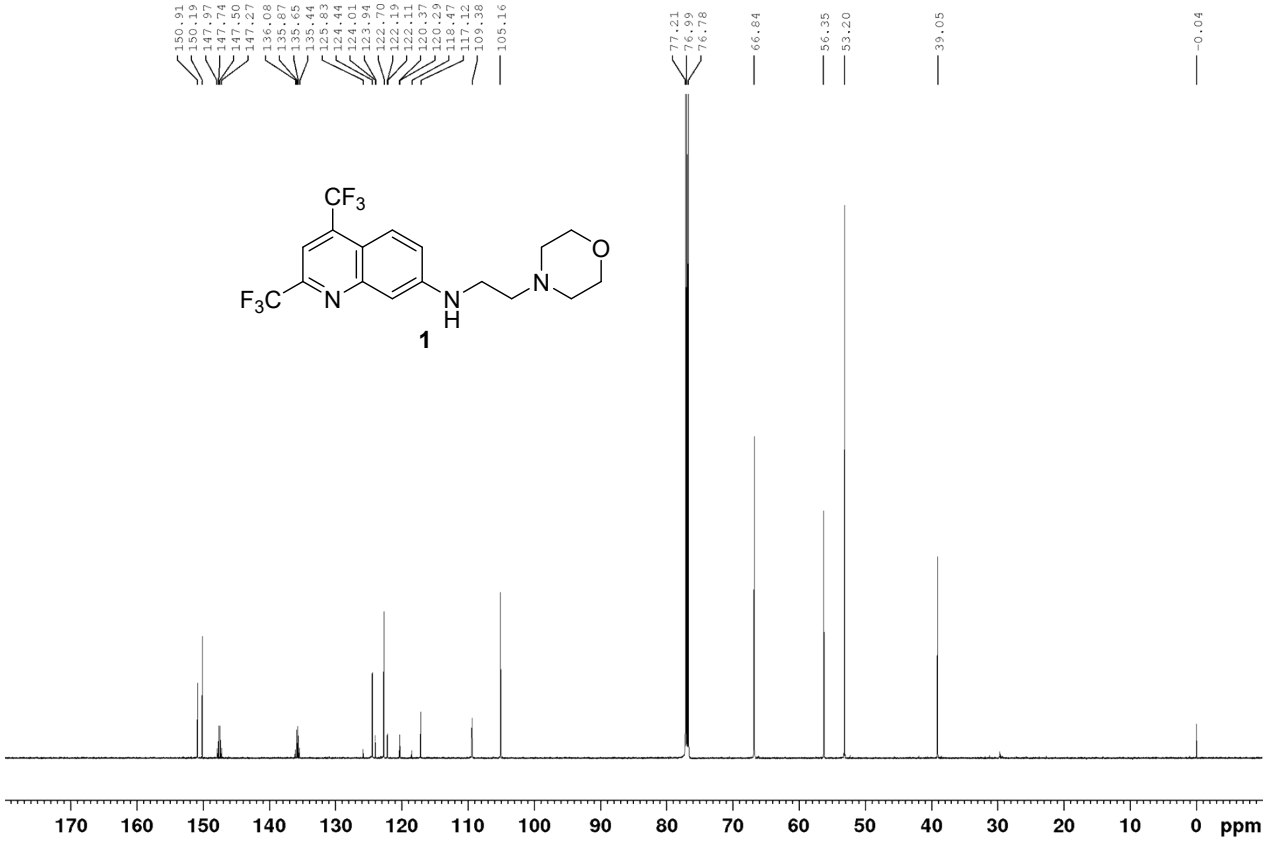


Figure S10. IR spectra of **1** (a), **2** (b), **3** (c), **4** (d), and **5** (e) in KBr.

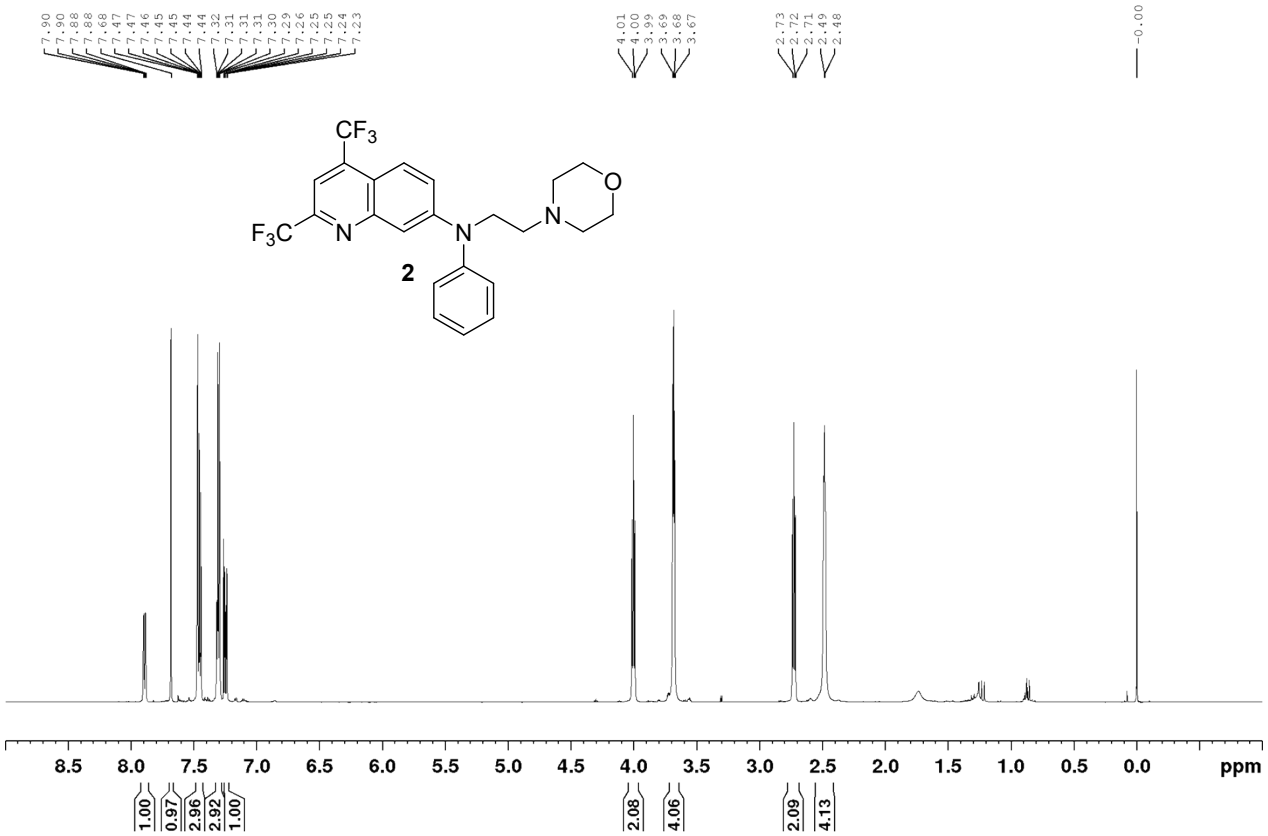
^{1}H-NMR spectrum of **1** (600 MHz, $CDCl_3$)



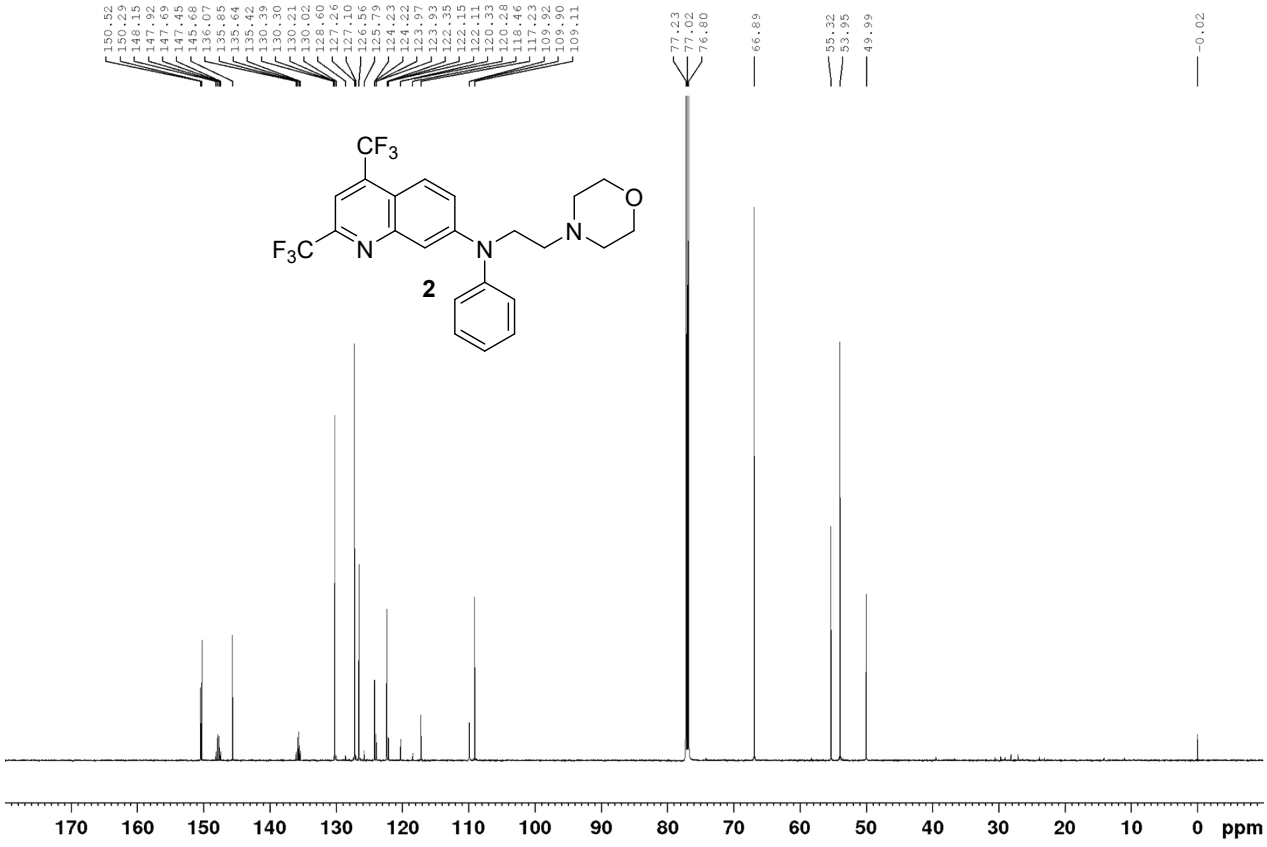
^{13}C-NMR spectrum of **1** (151 MHz, $CDCl_3$)



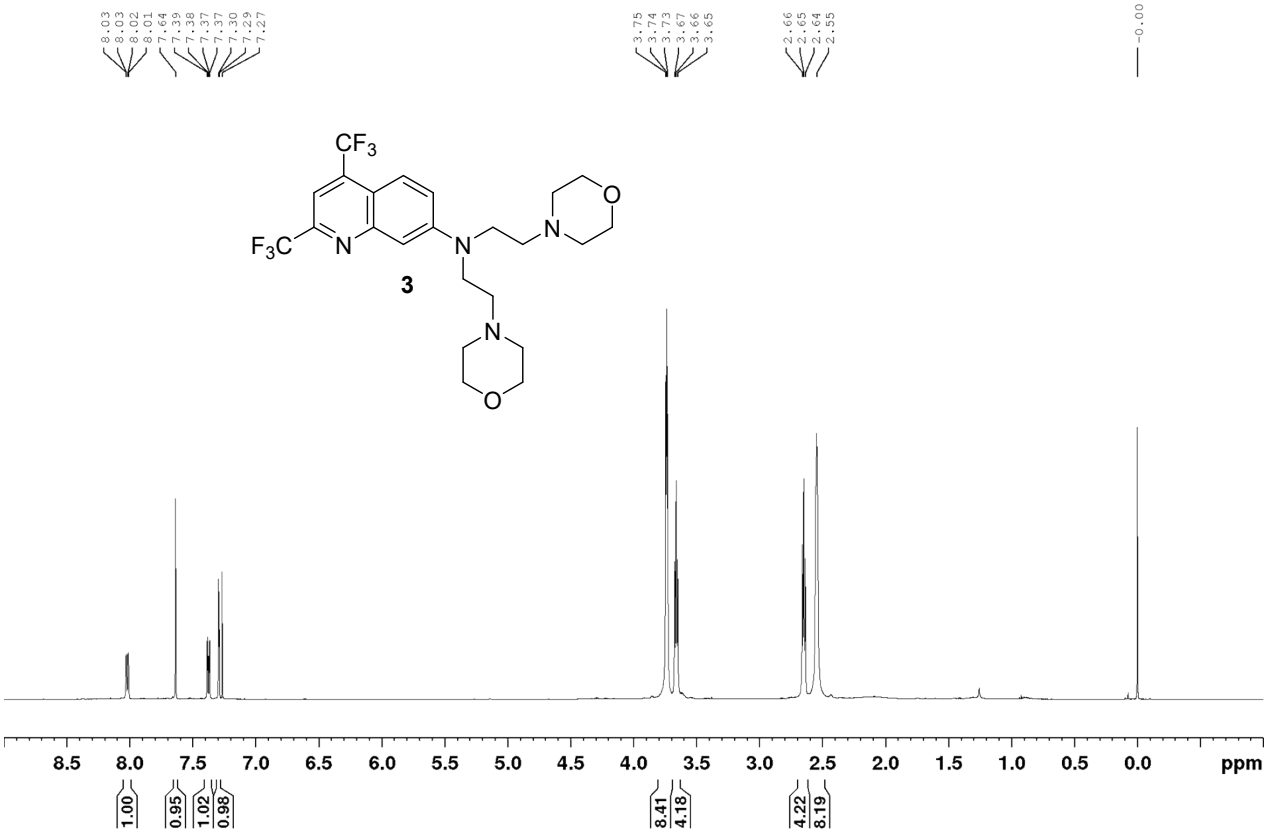
^{1}H-NMR spectrum of **2** (600 MHz, $CDCl_3$)



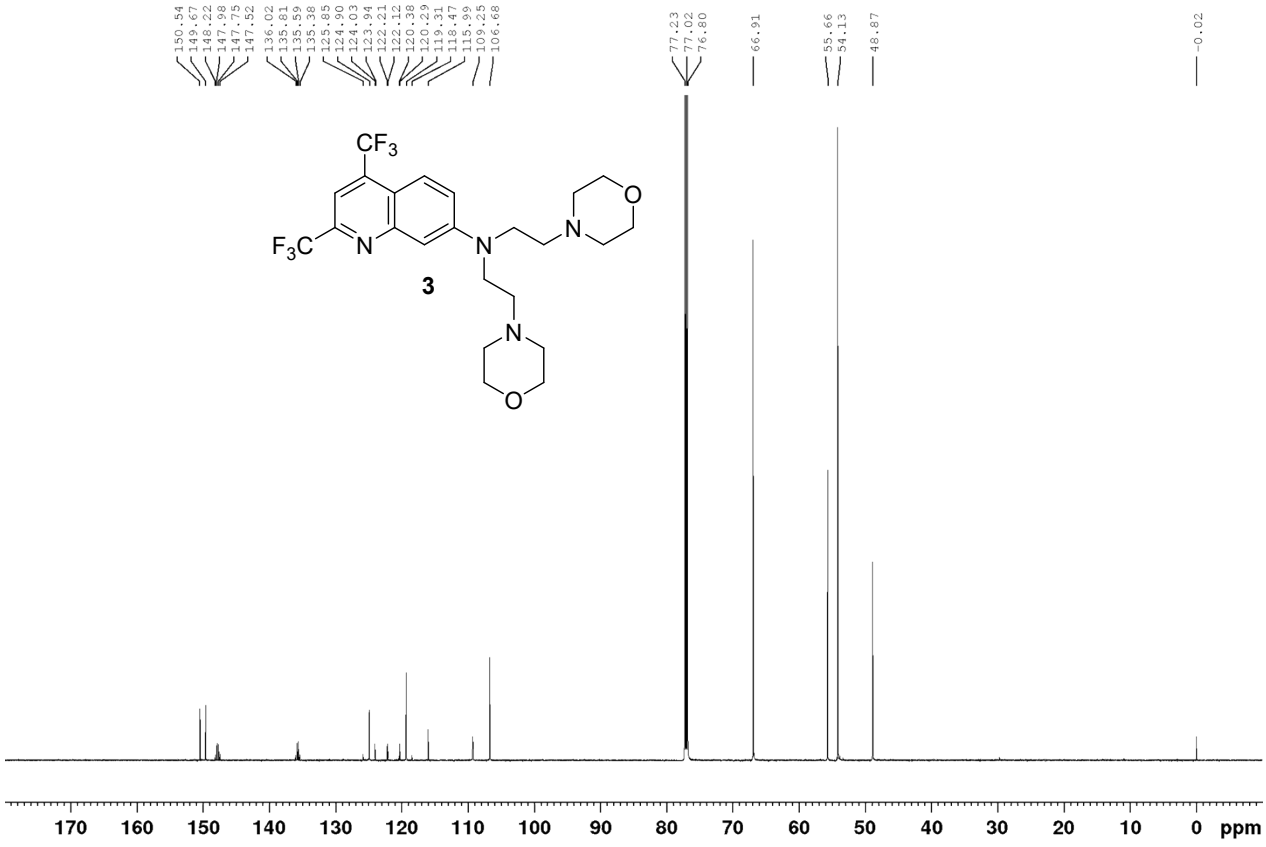
^{13}C-NMR spectrum of **2** (151 MHz, $CDCl_3$)



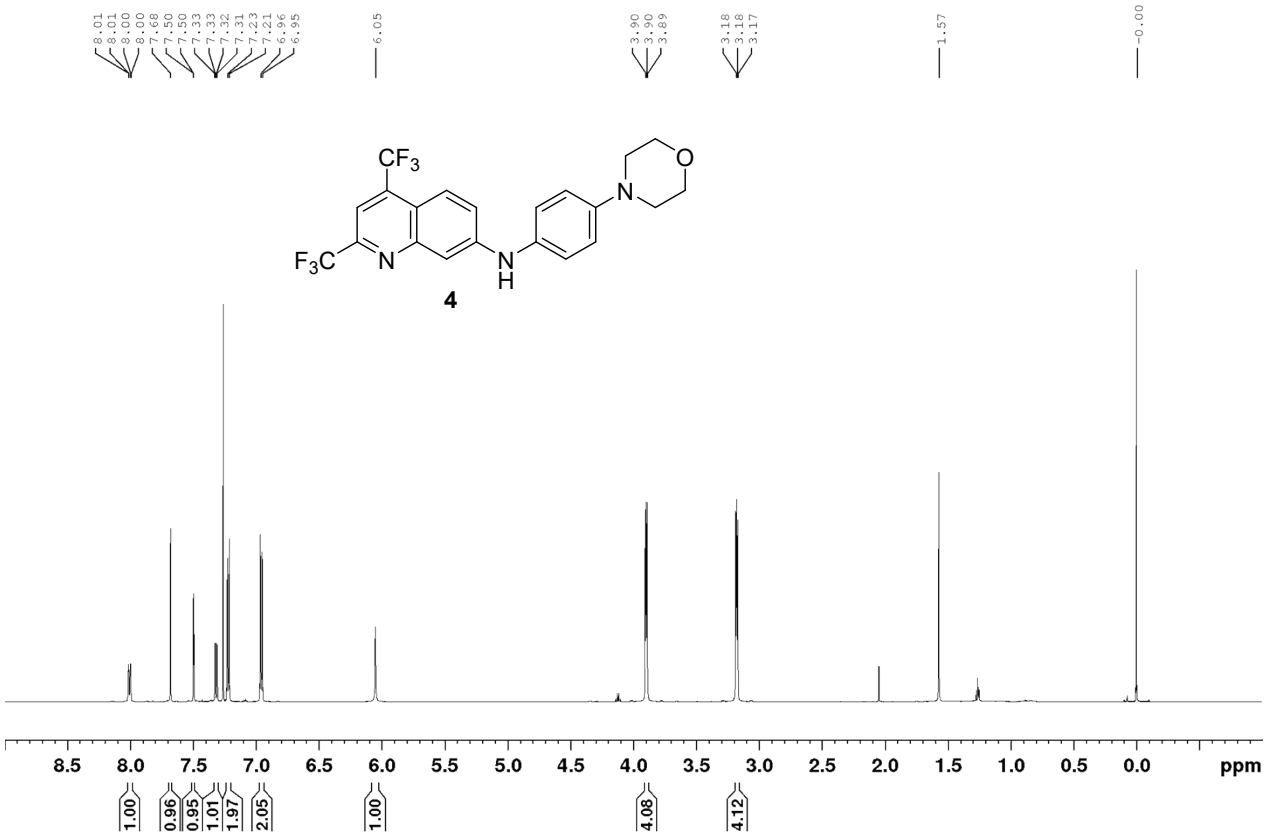
^{1}H-NMR spectrum of **3** (600 MHz, $CDCl_3$)



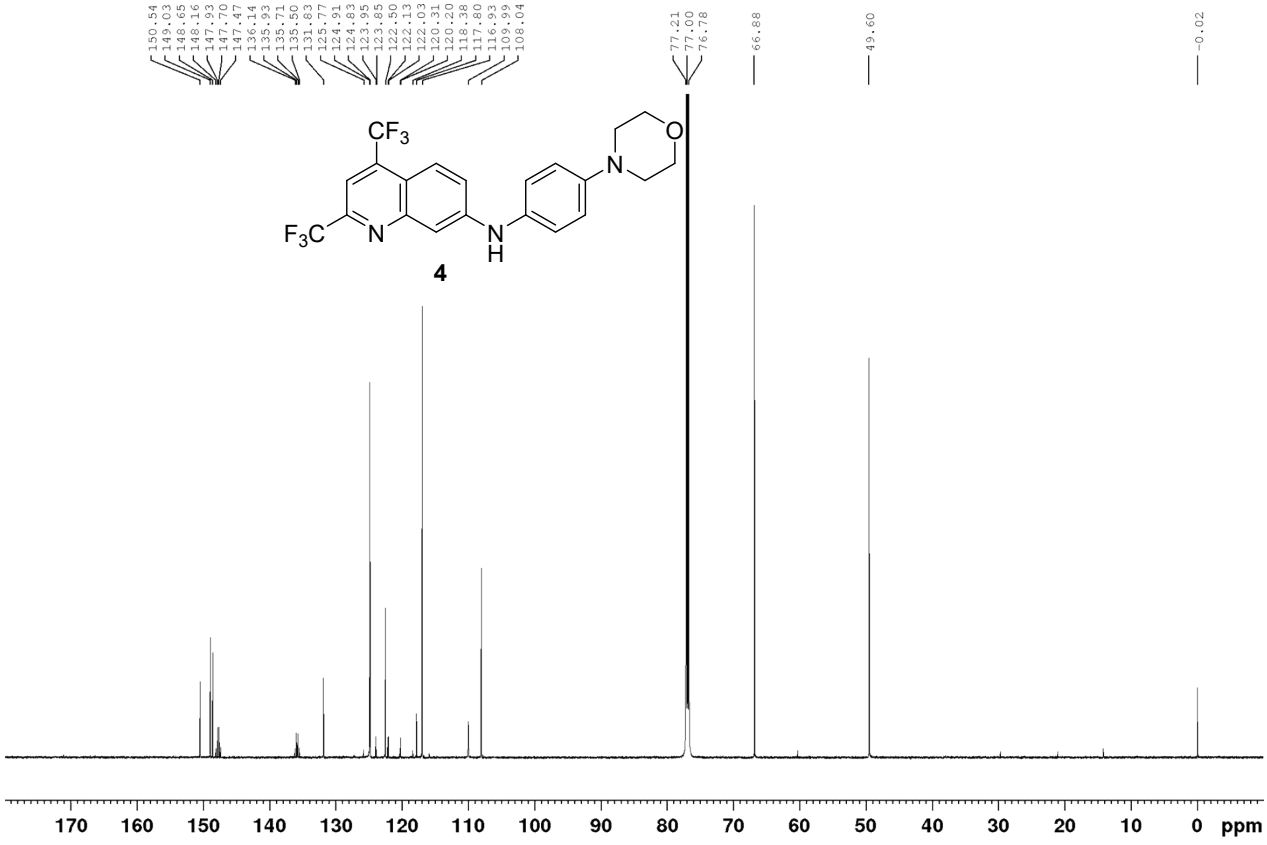
^{13}C-NMR spectrum of **3** (151 MHz, $CDCl_3$)



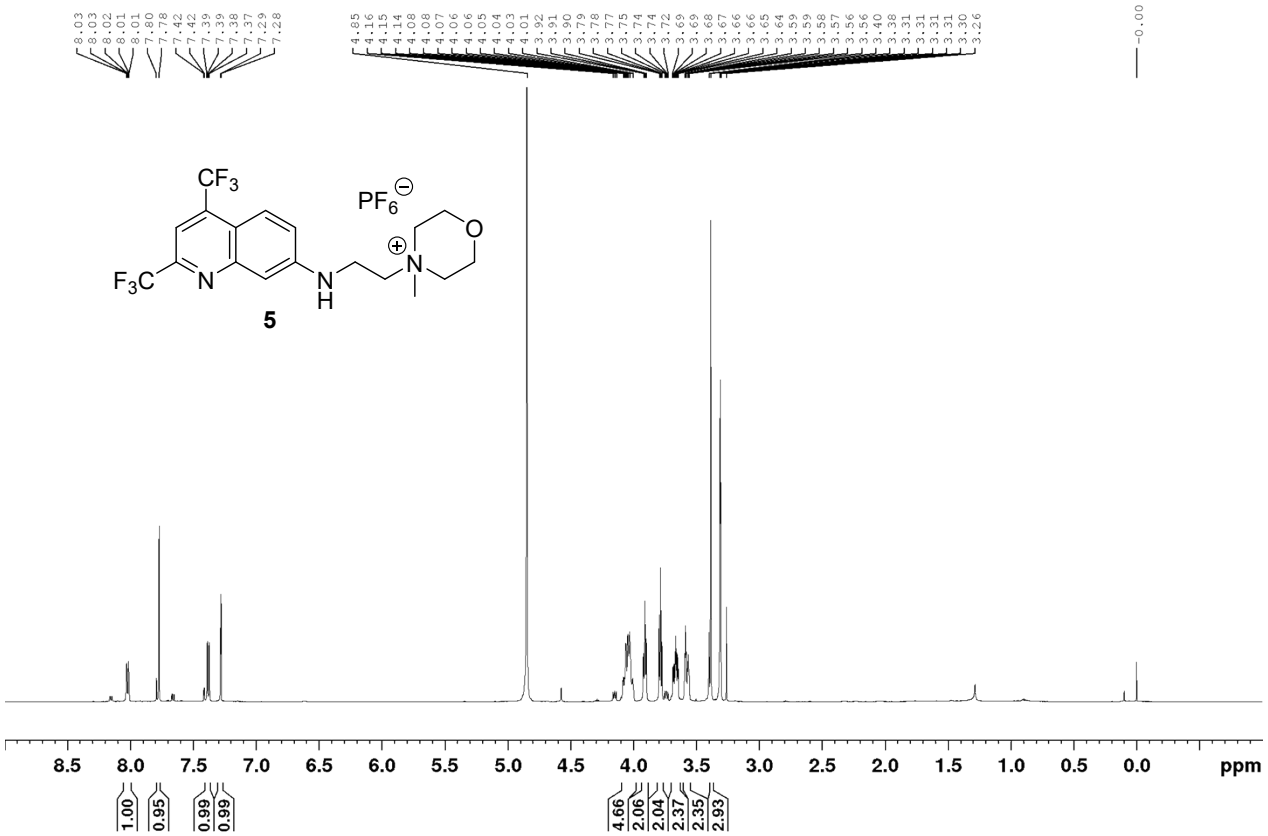
^{1}H-NMR spectrum of **4** (600 MHz, $CDCl_3$)



^{13}C-NMR spectrum of **4** (151 MHz, $CDCl_3$)



^{1}H-NMR spectrum of **5** (600 MHz, MeOD)



^{13}C-NMR spectrum of **5** (151 MHz, MeOD)