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7-Amino-2-(*N*,*N*-dimethylamino)quinazoline: A Small, Bright, Easily Synthesized Scaffold for pH Sensors

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1. Experimental procedures

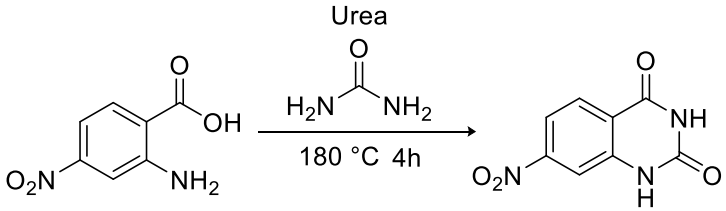
1.1 General information

Chemicals were supplied by WAKO Pure Chemical Industries, Ltd., Kanto Chemical Co., Inc., Tokyo Chemical Industry Co., LTD., or Sigma-Aldrich and were used without purification as commercially available. Most solvents were of the dehydrated or super-dehydrated form. Most reactions were performed under argon and stirring unless otherwise noted. Column chromatography was performed using spherical silica gel (63-219 μm) (Kanto Chemicals). Medium-pressure liquid chromatography was performed using a Yamazen EPCLC W-Prep 2XY system equipped with a Yamazen Ultra Pack B silica column or Yamazen Hi-Flash silica columns. TLC plates were visualized by fluorescence under a UV lamp (254 or 365 nm). Nuclear magnetic resonance (NMR) spectra (1H or 13C) were recorded on a JEOL JNM-ECX500 NMR and JEOL JNM-ECZL500R spectrometer (500 MHz) with tetramethylsilane (TMS) as the internal standard and CDCl3, CD3OD, or DMSO-d6 as solvents. Chemical shifts were recorded in parts per million (ppm,δ), relative to tetramethylsilane (δ 0.00). 1H NMR splitting patterns are reported as singlet (s), doublet (d), triplet (t), doublet of doublets (dd), doublet of triplets (dt), etc. Mass spectra were recorded using a TOF (ESI) analyzer or a magnetic sector (FAB) analyzer. Melting points were measured using an ATM-02, AS ONE melting point apparatus.

UV-visible absorption spectra were recorded at room temperature using a JASCO Co.V750 spectrophotometer (Response: Low, Bandwidth: 0.5 nm, Scan rate: 500 nm min-1). Fluorescence spectra were recorded at room temperature with a JASCO Co. FP-8550 spectrofluorometer (Excitation slit: 5.0 nm, Emission slit: 5.0 nm, Scan rate: 60 nm min-1, PMT voltage: 400 V or 500 V) using a quartz cuvette with a 1-cm path length. Water was doubly distilled and deionized by a Milli-Q water system (WG222, Yamato Sci. Co. Ltd., and Autopure WR-600G, Millipore). pH profile was recorded using LAQUA F-72 pH meter with 9618N-10D Micro ToupH Electrode for Low-Volume Samples.

1.2 Synthetic Procedures

1.2.1 Synthesis of 7-Nitroquinazoline-2,4(1*H*,3*H*)-dione (9)[1]



8 **9**

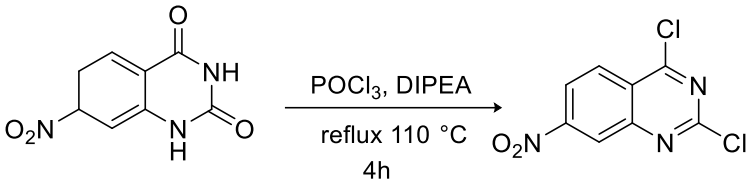
2-Aminobenzoic acid **8** (2.73 g, 15.0 mmol) and urea (40.0 g, 660 mmol) (10 equiv.) were both placed in a flask and then refluxed at 160-180 °C for 4 h with stirring. After cooling, water was added to the mixture, which was then stirred for 10 min to dissolve the unreacted urea. The resulting precipitate was filtered and dried to obtain the desired product.

Orange solid: (2.99 g, 96% Yield).

^{1}H NMR (500 MHz, DMSO-d_6) δ 11.64 (s, 1H), 11.50 (s, 1H), 8.10 (d, J = 8.6 Hz, 1H), 7.90-7.93 (m, 2H)

LRMS (FAB) *m/z* 208 $(M+H)^+$

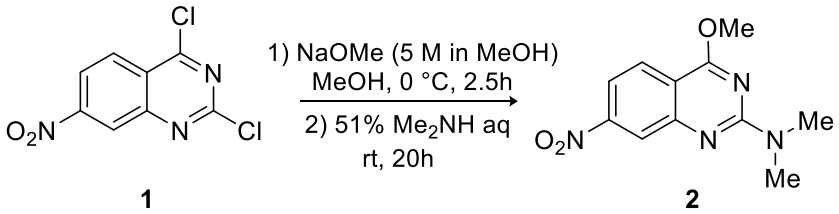
1.2.2 Synthesis of 2,4-Dichloro-7-nitroquinazoline (1)[2]



9 **1**

A mixture of 7-nitroquinazoline-2,4(1*H*,3*H*)-dione (**9**) and *N*,*N*-diisopropylethylamine (2.2 equiv.) in excess of phosphoryl chloride (30 equiv.) was heated under reflux for 4.0 h. The excess phosphoryl chloride was distilled, and the residue was dissolved in chloroform cooled in an ice bath. After neutralization with aqueous 10% ammonia, the product was extracted with chloroform and washed with brine. After being dried over sodium sulfate, the organic layer was concentrated under reduced pressure. The residue was purified by silica gel column chromatography (chloroform) to obtain the desired product.
Colorless solid; (2.71 g, 87% Yield).
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.86 (d, *J* = 1.1 Hz, 1H), 8.48 (d, *J* = 1.1 Hz, 2H)
LRMS (FAB) *m/z* 242 $(M)^-$

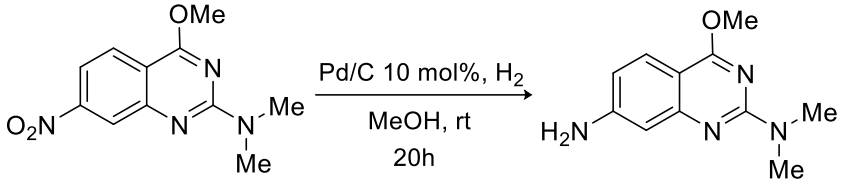
1.2.3 Synthesis of 2-(*N*,*N*-dimethylamino)-4-methoxy-7-nitroquinazoline (2)



1 **2**

Under an argon atmosphere, sodium methoxide in MeOH (5 M) was added to a solution of **1** in dehydrated MeOH, and the mixture was stirred at 0 °C. Then, a 51% dimethylamine aqueous solution was added to the reaction mixture, and the mixture was stirred at room temperature for 20 h. The product was extracted with chloroform and washed with brine. After drying over sodium sulfate, the organic layer was concentrated under reduced pressure. The residue was purified by silica gel column chromatography (4:1 *n*-hexane/ethyl acetate) to obtain the desired product.
Orange solid: (1.49 g, 73% Yield)
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31 (d, *J* = 1.7 Hz, 1H), 8.00 (d, *J* = 9.2 Hz, 1H), 7.80
(dd, *J* = 9.2, 1.7 Hz, 1H), 4.12 (s, 3H), 3.29 (s, 6H)
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.6, 159.9, 153.8, 151.3, 125.4, 120.4, 114.4, 114.3, 54.1, 37.1
HRMS (FAB) *m/z* calcd for $C_{11}H_{13}N_4O_3$ $(M+H)^+$: 249.0982, found: 249.0969
Melting Point 175-176 °C
R*f* = 0.62 (4:1 *n*-hexane /ethyl acetate)

1.2.4 Synthesis of 7-Amino -2-(*N,N*-dimethylamino)-4-methoxyquinazoline (3)



2 **3**

Palladium 10% on carbon was added to a solution of **2** in MeOH. Under a hydrogen atmosphere, the mixture was stirred at room temperature. The product was filtered with Celite. The filtrate was then concentrated under reduced pressure to obtain the desired product.

Colorless solid: (346 mg, 85% Yield)

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.6 Hz, 1H), 6.66 (d, *J* = 2.0 Hz, 1H), 6.48 (dd, *J* = 8.6, 2.0 Hz, 1H), 4.04 (s, 3H), 3.98 (s, 2H), 3.24 (s, 6H)

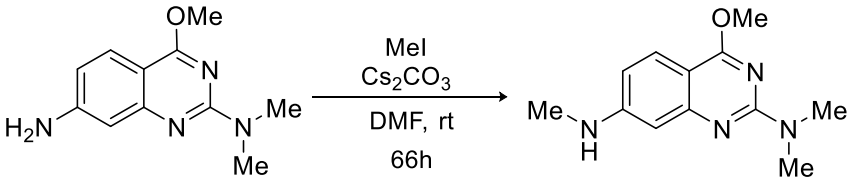
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.5, 159.8, 155.5, 151.1, 125.1, 111.9, 105.7, 103.9, 53.2, 37.0

HRMS (FAB) *m/z* calcd for $C_{11}H_{14}N_4O$ $(M+H)^+$: 219.1240, found: 219.1239

Melting Point 157-158 °C

R*f* = 0.20 (1:1 *n*-hexane /ethyl acetate)

1.2.5 Synthesis of 2-(*N,N*-dimethylamino)-4-methoxy-7-(*N*-methylamino)quinazoline (4a)



3 **4a**

Under an argon atmosphere, a mixture of **3** (437 mg, 2.0 mmol) and cesium carbonate (977 mg, 3.0 mmol) in DMF (7 mL) was stirred at room temperature. After stirring for 1 hour, methyl iodide (128 µL, 2.0 mmol) was added, and the mixture was stirred for 66 hours. The product was extracted with a mixture of *n*-hexane and ethyl acetate (1:4 *n*-hexane/ethyl acetate). The organic layer was washed with water and brine, dried over Na_2SO_4, filtered, and evaporated. The residue was purified by silica gel column chromatography (1:4 *n*-hexane/ethyl acetate) to obtain the desired product.

Colorless solid: (103 mg, 22 % Yield)

^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.6 Hz, 1H), 6.51 (d, *J* = 2.3 Hz, 1H), 6.41 (dd, *J* = 8.6, 2.3 Hz, 1H), 4.06 (s, 1H), 4.03 (s, 3H), 3.24 (s, 6H), 2.91 (s, 3H)

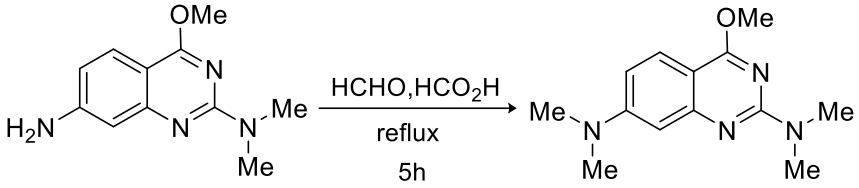
^{13}C-NMR (126 MHz, $CDCl_3$) δ 166.6, 160.0, 156.0, 153.4, 124.6, 111.8, 102.9, 101.3, 53.2, 37.2, 30.4

HRMS (FAB) *m/z* calcd for $C_{12}H_{16}N_4O$ $(M+H)^+$: 232.1324, found: 232.1323.

Melting Point 148-149 °C

R*f* = 0.29 (1:4 *n*-hexane/ethyl acetate)

1.2.6 Synthesis of 2,7-Bis(*N*,*N*-dimethylamino)-4-methoxyquinazoline (4b)



3 **4b**

Compound **3** (873.2 mg, 4.00 mmol) was dissolved in formic acid (50 mL), and 37% formaldehyde (890 μL, 12.0 mmol) solution was added. The mixture was heated under reflux with stirring for 5 h. The reaction mixture was cooled to room temperature and neutralized with aqueous sodium hydroxide, and the product was extracted with chloroform. The organic layer was washed with water and brine and then dried over Na_2SO_4. The organic layer was filtered and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (1:1 *n*-hexane/ethyl acetate) to obtain the desired product.

Colorless solid: (195.4 mg, 20% Yield)

^{1}H-NMR (500 MHz, $CDCl_3$) δ: 7.73 (d, J = 9.2 Hz, 1H), 6.65 (dd, J = 8.9, 2.6 Hz, 1H), 6.61 (d, J = 2.3 Hz, 1H), 4.04 (s, 3H), 3.25 (s, 6H), 3.06 (s, 6H).

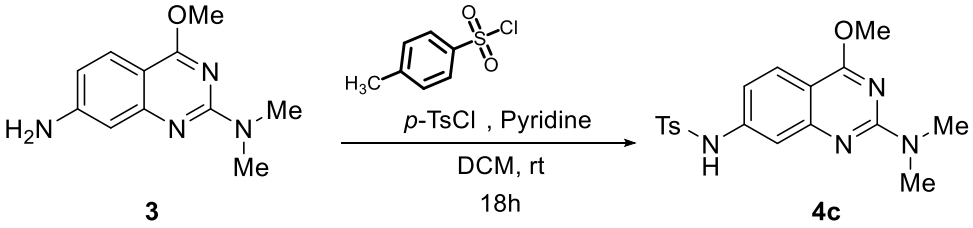
^{13}C-NMR (126 MHz, $CDCl_3$) δ: 166.6, 159.9, 155.3, 154.1, 124.4, 109.6, 103.0, 102.2, 53.1, 40.3, 37.1

HRMS (FAB) *m/z* calcd for $C_{13}H_{19}N_4O$ $(M-H)^-$: 247.1559, found: 247.1562.

Melting Point 141-142 °C

R*f* = 0.28 (1:2 *n*-hexane/ethyl acetate)

1.2.7 Synthesis of 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-4-toluenesulfonylamino)quinazoline (4c)



3 **4c**

Compound **3** (150 mg, 0.60 μmol) was dissolved in pyridine (2 mL) and dichloromethane (DCM) (10 mL) in a round-bottom flask under an argon atmosphere. *p*-TsCl (*p*-toluenesulfonyl chloride, 129 mg, 0.66 μmol) was added to the solution, and the mixture was stirred at room temperature for 18 hours. After the reaction, the mixture was extracted with 0.1 M HCl aqueous solution and DCM to remove pyridine. The organic layer was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (9:1 DCM/methanol) to give a colorless solid. The product was further recrystallized from DCM and *n*-hexane to obtain Colorless crystals.

Colorless crystals: (219 mg, 98% Yield)

^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.74 (d, J = 8.6 Hz, 1H), 7.70 (d, J = 8.2 Hz, 2H), 7.18 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 2.1 Hz, 1H), 6.98 (dd, J = 8.7, 2.1 Hz, 1H), 4.02 (s, 3H), 3.20 (s, 6H), 2.33 (s, 3H).

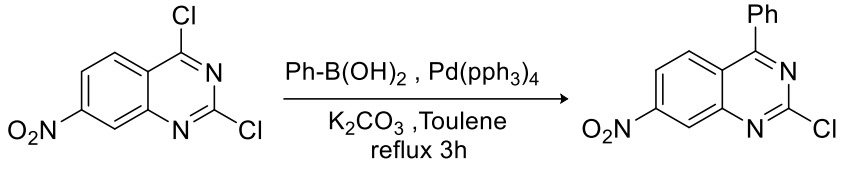
^{13}C NMR (126 MHz, $CDCl_3$) δ 166.7, 159.7, 154.5, 144.1, 141.5, 136.1, 129.8, 127.3, 125.4, 113.9, 113.3, 108.1, 53.6, 37.1, 21.6

HRMS (ESI) *m/z* calcd for $C_{18}H_{21}N_4O_3S$ $(M+H)^+$: 373.1328, found: 373.1332

Melting Point 118-119 °C

R*f* = 0.66 (9:1 DCM/MeOH)

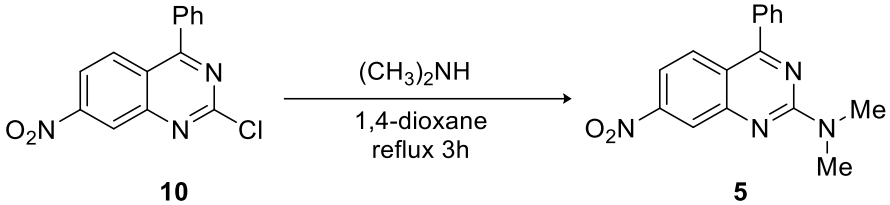
1.2.8 Synthesis of 2-Chloro-7-nitro-4-phenylquinazoline (10)



1 **10**

Under an argon atmosphere, phenylboronic acid (300 mg, 1.2 equiv., 2.4 mmol), $Pd(PPh_3)_4$ (71 mg, 0.061 μmol), and K_2CO_3 (700 mg, 2.5 eq, 5.1 mmol) were added to a solution of 2,4-dichloro-7-nitroquinazoline **1** (0.5g, 2.04 mmol) in toluene (15 mL), and the mixture was heated at reflux (117 °C) for 3 hours. After cooling, the reaction mixture was poured into ice water and extracted with dichloromethane. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (4:1 *n*-hexane/ethyl acetate) to give the desired product.
Yellow solid: (406 mg, 69% Yield)
^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.87 (d, *J* = 2.9 Hz, 1H), 8.34 (d, *J* = 1.9 Hz, 2H), 7.80-7.79 (m, 2H), 7.67-7.60 (m, 3H)
^{13}C NMR (126 MHz, $CDCl_3$) δ 172.3, 159.2, 152.8, 151.3, 135.0, 131.7, 130.3, 129.9, 129.2, 124.1, 121.4
HRMS (FAB) *m/z* calcd for $C_{14}H_9ClN_3O_2$ ($M+H^+$) : 286.0378, found: 286.0358
Melting Point 137-138 °C
R*f* = 0.68 (7:3 *n*-hexane/ethyl acetate)

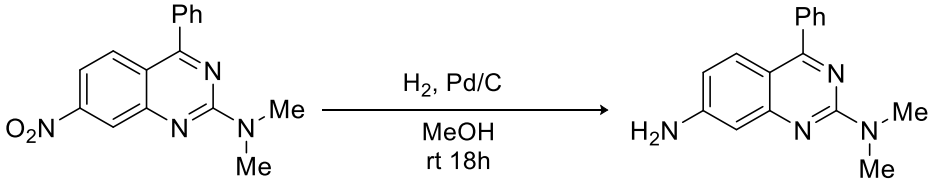
1.2.9 Synthesis of 2-(*N,N*-dimethylamino)-7-nitro-4-phenylquinazoline (5)



10 **5**

Under an argon atmosphere, compound **10** (392 mg, 1.37 mmol) was added to a solution of 50% dimethylamine and 1,4-dioxane. The mixture was heated at reflux (101 °C) for 3 hours. After cooling, the reaction mixture was extracted with chloroform and water. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (4:1 *n*-hexane/ethyl acetate) to give the desired product.
Orange solid: (367 mg, 91% Yield)
^{1}H-NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 2.1 Hz, 1H), 7.94-7.92 (m, 1H), 7.79 (dd, *J* = 9.0, 2.3 Hz, 1H), 7.73-7.71 (m, 2H), 7.57-7.54 (m, 3H), 3.36 (s, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 169.4, 160.0, 153.9, 151.0, 137.2, 130.3, 129.9, 129.3, 128.7, 122.0, 119.9, 114.7, 37.3
HRMS (FAB) *m/z* calcd for $C_{16}H_{14}N_4O_2$ ($M+H^+$) : 294.1119, found: 294.1106
Melting Point 207-208 °C
R*f* = 0.63 (4:1 *n*-hexane/ethyl acetate)

1.2.10 Synthesis of 7-Amino-2-(*N*,*N*-dimethylamino)-4-phenylquinazoline (6)



5 **6**

Compound **5** (330 mg, 1.12 mmol) was dissolved in methanol (25 mL) in a round-bottom flask. Pd/C (10 mol%, 0.11 μmol) was added to the solution, and the flask was placed under a hydrogen atmosphere. The mixture was stirred at room temperature for 18 hours. After completion, the reaction mixture was filtered to remove the Pd/C catalyst, and the filtrate was then concentrated under reduced pressure. The residue was purified by silica gel column chromatography (1:4 *n*-hexane/ethyl acetate) to give a white and red solid. The product was further crystallized from chloroform and diethyl ether to obtain white crystals.
White crystals: (55.2 mg, 18% Yield)
^{1}H-NMR (500 MHz, $CDCl_3$) δ 7.71-7.69 (m, 2H), 7.59 (d, *J* = 8.7 Hz, 1H), 7.50-7.47 (m, 3H), 6.75 (d, *J* = 1.7 Hz, 1H), 6.50 (dd, *J* = 8.7, 2.3 Hz, 1H), 4.09 (s, 2H), 3.30 (s, 6H).
^{13}C NMR (126 MHz, $CDCl_3$) δ 167.6, 159.9, 151.1, 141.2, 138.6, 129.8, 129.3, 129.2, 128.3, 113.4, 111.5, 105.7, 37.2
HRMS (ESI) *m/z* calcd for $C_{16}H_{17}N_4$ $(M+H)^+$: 265.1447, found: 265.1461
Melting Point 244-245 ℃
R*f* = 0.58 (1:4 *n*-hexane/ethyl acetate)

2. UV-vis absorption and photoluminescence spectra in Various Solvents

2.1 7-Amino-2-(*N*,*N*-dimethylamino)-4-methoxyquinazoline (3)

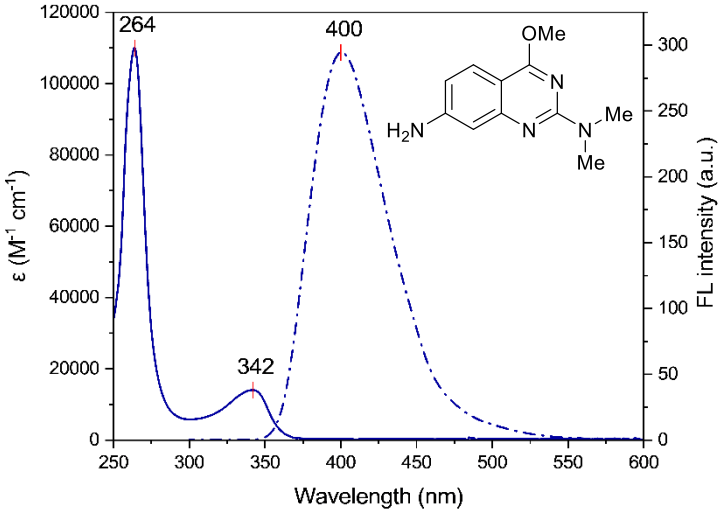


Figure 1S. UV-vis absorption and photoluminescence emission spectra of **3** *(λ_{ex}= 265 nm) in DMSO*

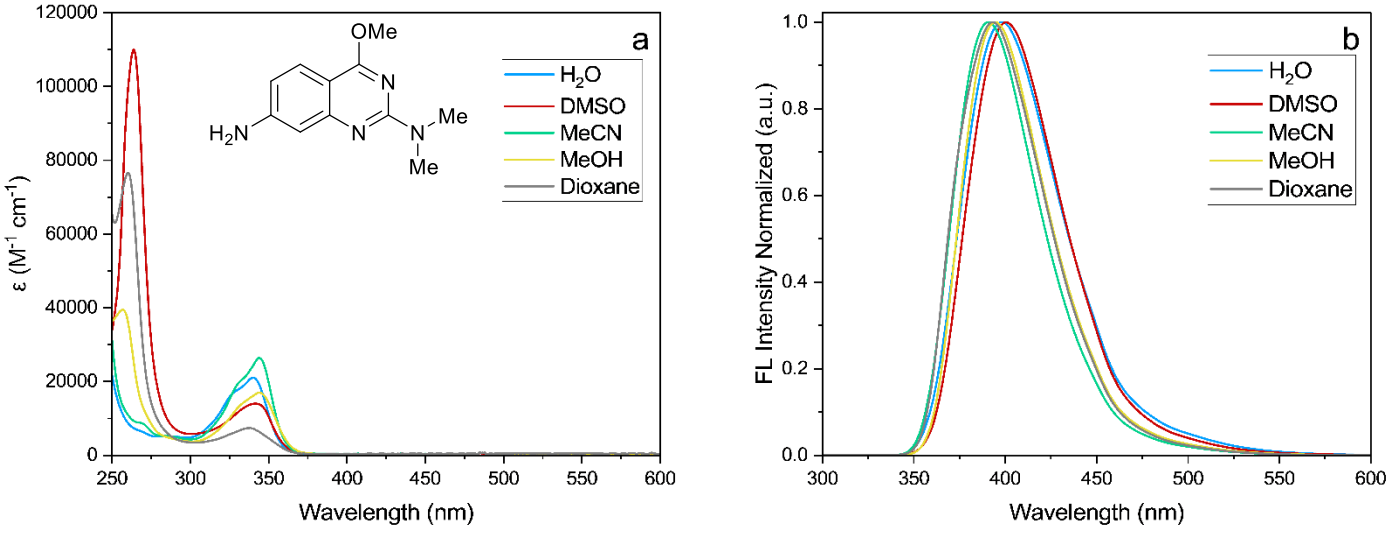


Figure 2S. a) UV-vis absorption b) Photoluminescence emission spectra of **3** *(λ_{ex}= 265 nm) in various solvents*

2.2 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-methylamino)quinazoline (4a)

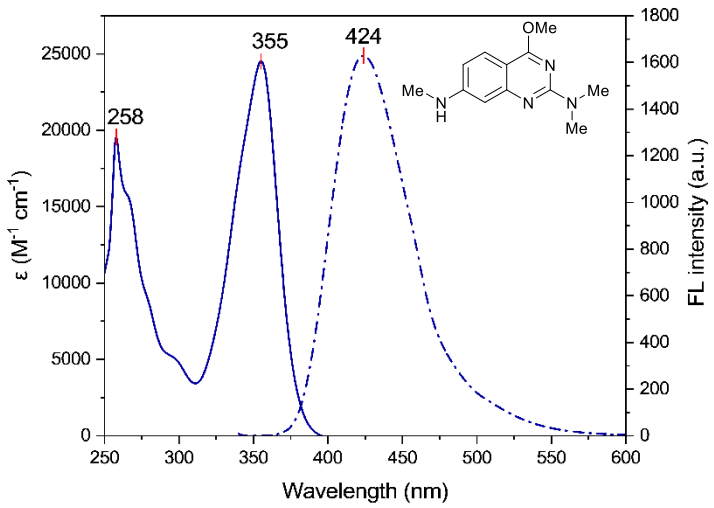


Figure 3S. UV-vis absorption and photoluminescence emission spectra of ***4a*** *(λ_{ex}= 260 nm) in DMSO*

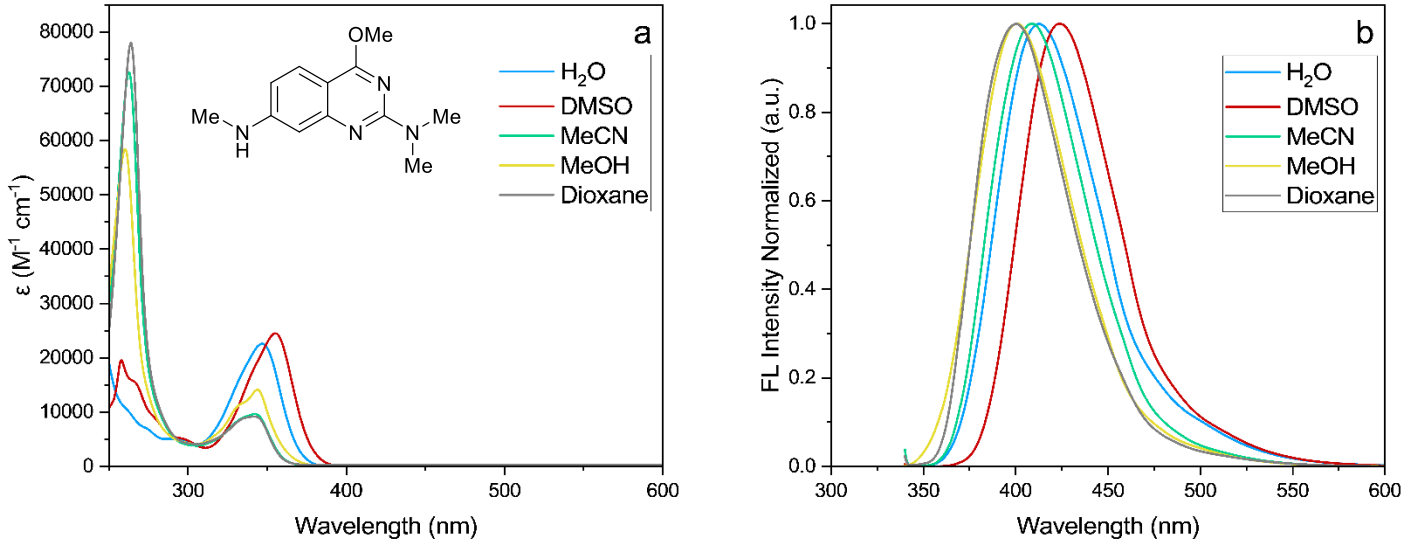


Figure 4S. a) UV-vis absorption b) Photoluminescence emission spectra of ***4a*** *(λ_{ex}= 260 nm) in various solvents*

2.3 2,7-Bis(*N*,*N*-dimethylamino)-4-methoxyquinazoline (4b)

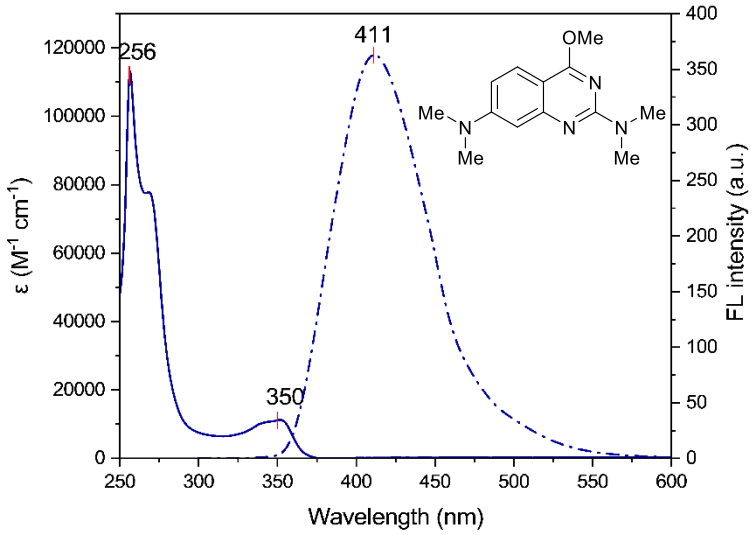


Figure 5S. UV-vis absorption and photoluminescence emission spectra of ***4b*** *(λ_{ex}= 270 nm) in DMSO*

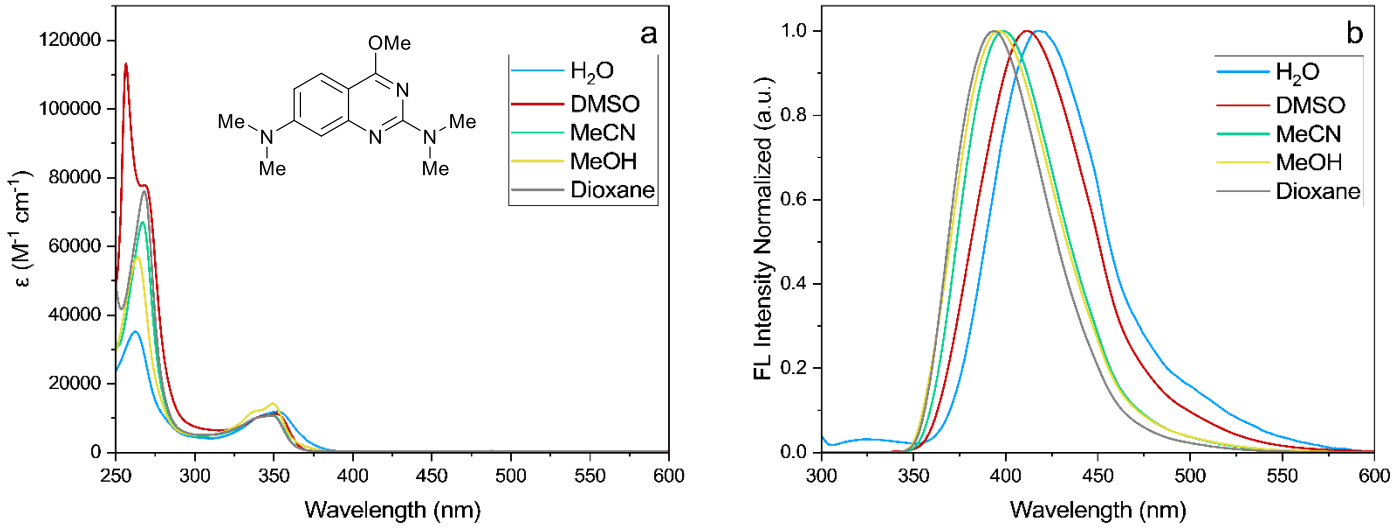


Figure 6S. a) UV-vis absorption b) Photoluminescence emission spectra of ***4b*** *(λ_{ex}= 270 nm) in various solvents*

2.4 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-4-toluenesulfonylamino)quinazoline (4c)

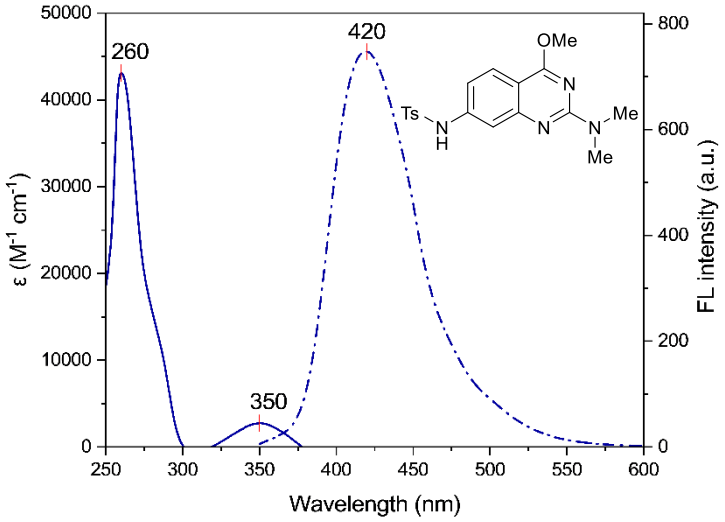


Figure 7S. UV-vis absorption and photoluminescence emission spectra of ***4c*** *(λ_{ex}= 270 nm) in DMSO*

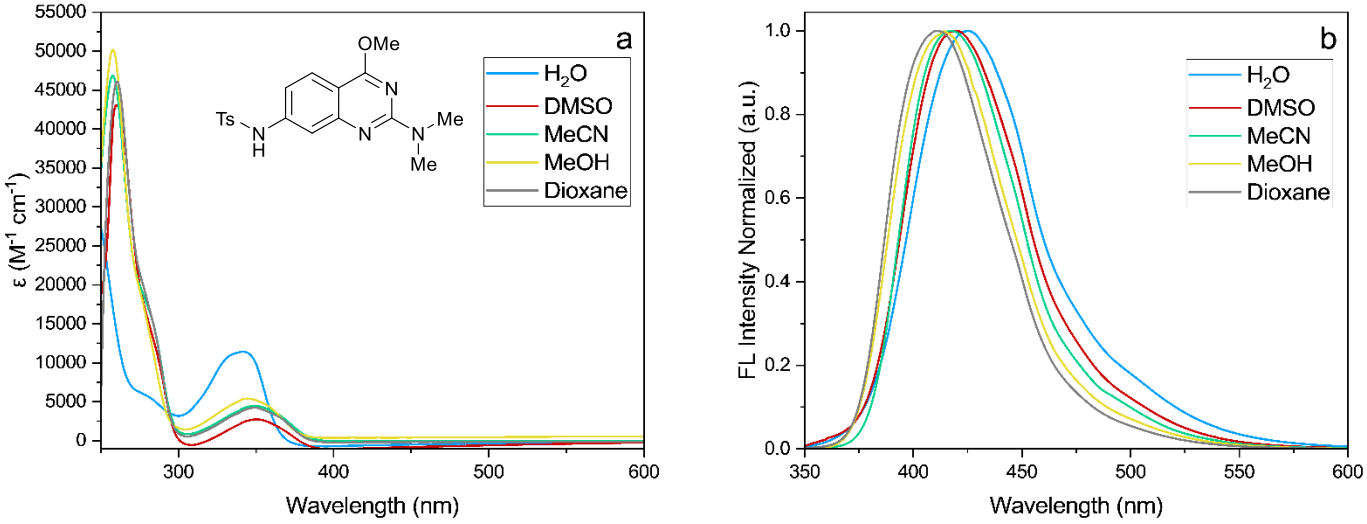


Figure 8S. a) UV-vis absorption b) Photoluminescence emission spectra of ***4c*** *(λ_{ex}= 270 nm) in various solvents*

2.5 7-Amino-2-(*N*,*N*-dimethylamino)-4-phenylquinazoline (6)

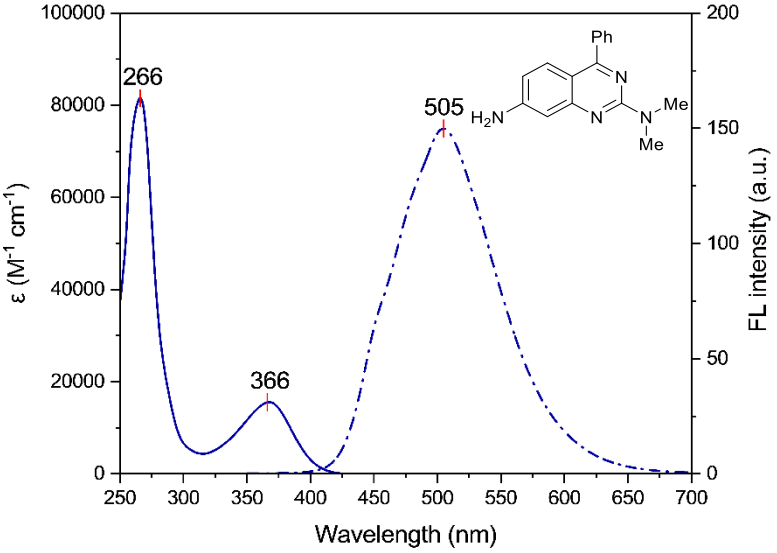


*Figure 9S. UV-vis absorption and photoluminescence emission spectra of **6** (λ_{ex}= 280 nm) in DMSO*

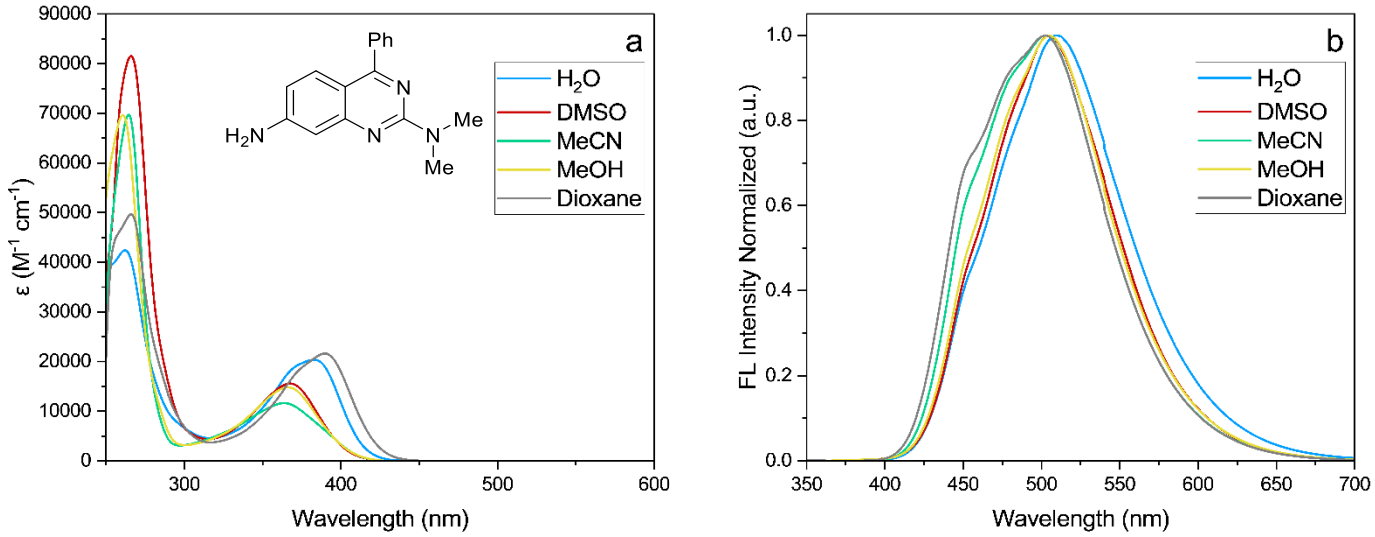


*Figure 10S. a) UV-vis absorption b) Photoluminescence emission spectra of **6** (λ_{ex}= 280 nm) in various solvents*

2.6 2-(*N*,*N*-dimethylamino)-4-methoxyquinazoline (7)

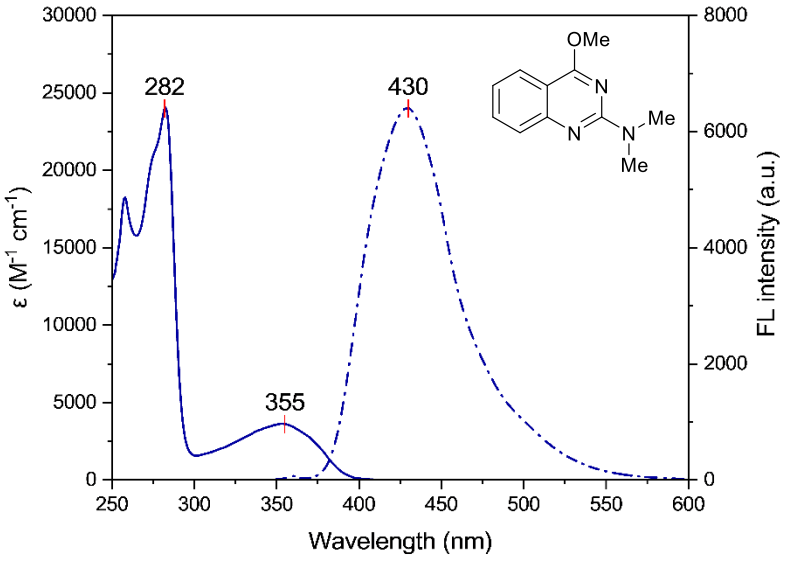


*Figure 11S. UV-vis absorption and photoluminescence emission spectra of **7** (λ_{ex}= 277 nm) in DMSO*

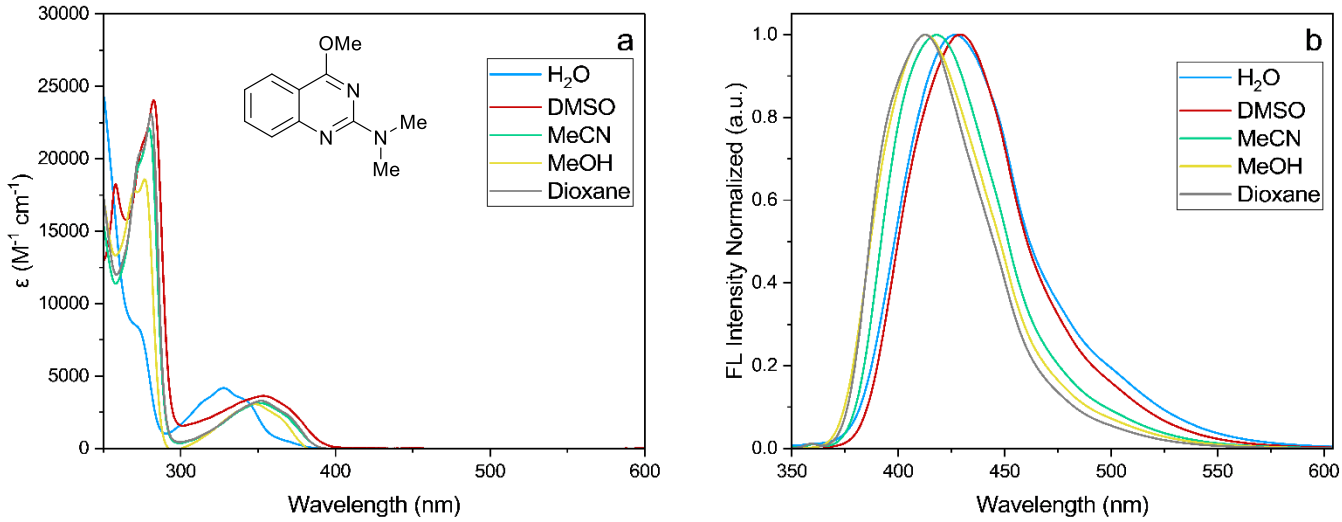


*Figure 12S. a) UV-vis absorption b) Photoluminescence emission spectra of **7** (λ_{ex}= 277 nm) in various solvents*

3. UV-vis absorption and photoluminescence spectra under various pH conditions

3.1 7-Amino-2-(*N*,*N*-dimethylamino)-4-methoxyquinazoline (3)

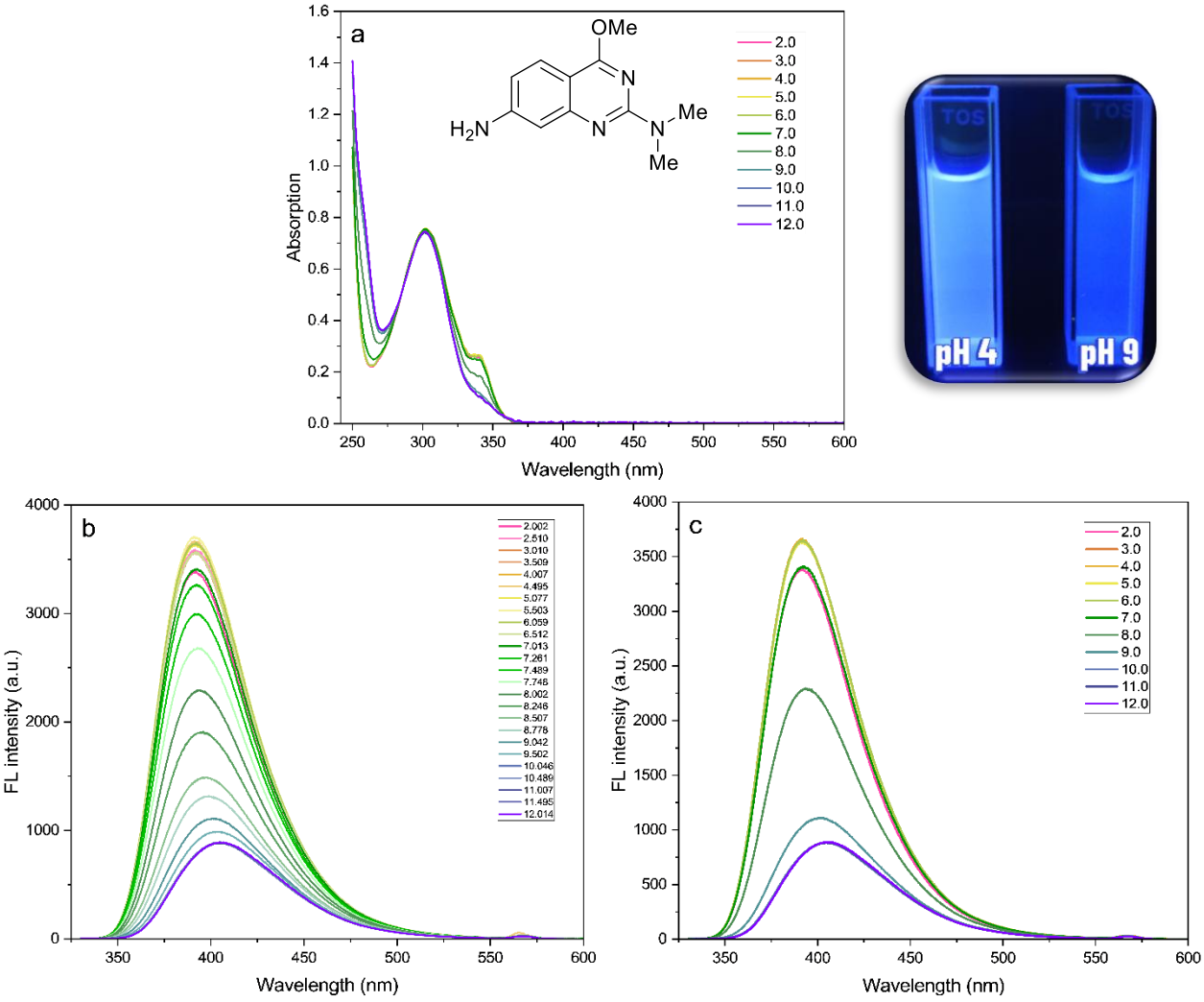


*Figure 13S. a) UV-vis absorption. b and c) Photoluminescence emission spectra of **3** (λ_{ex}= 285 nm) with pH changes*

3.2 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-methylamino)quinazoline (4a)

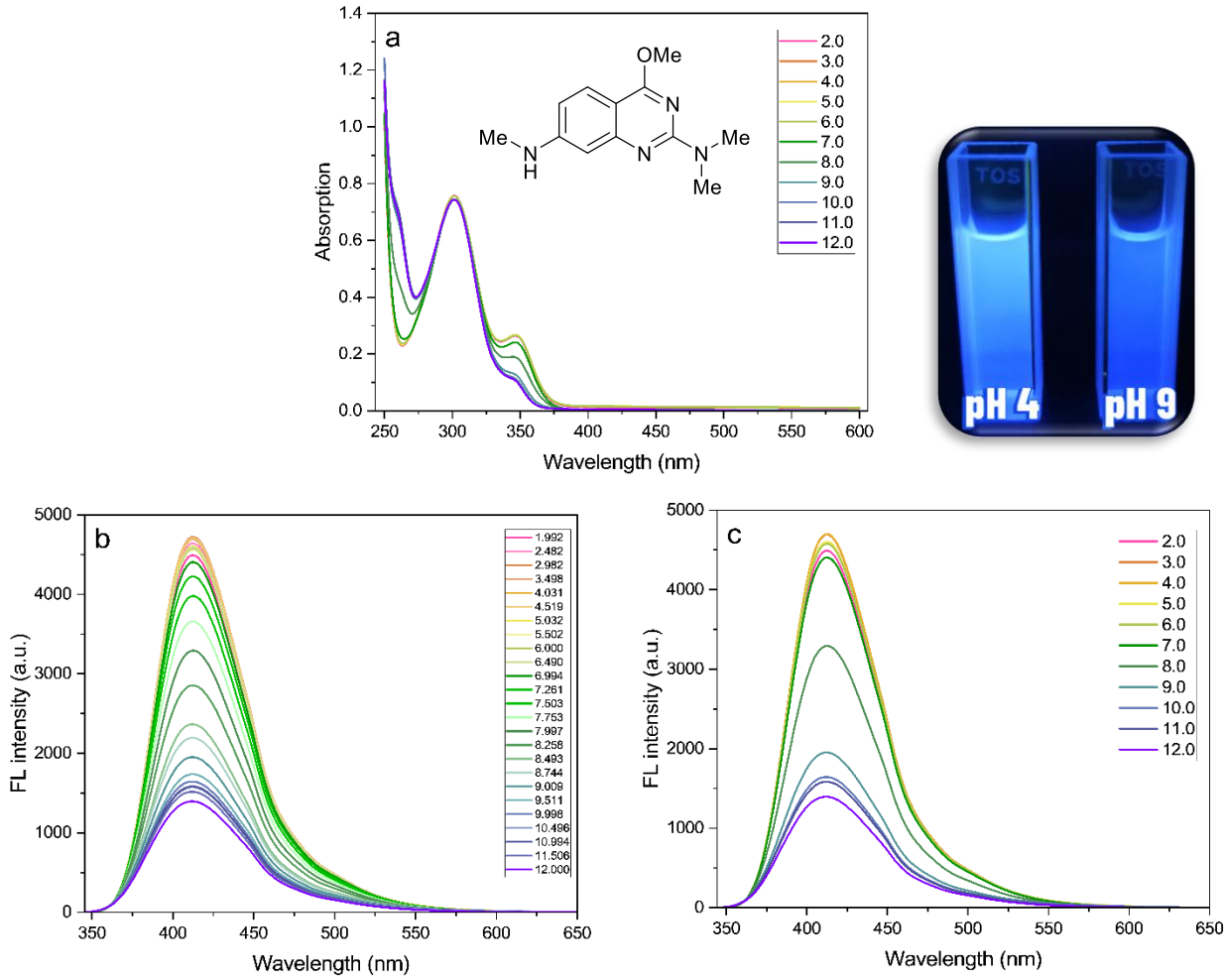


Figure 14S. a) UV-vis absorption. b and c) Photoluminescence emission spectra of ***4a*** *(λ_{ex}= 290 nm) with pH changes*

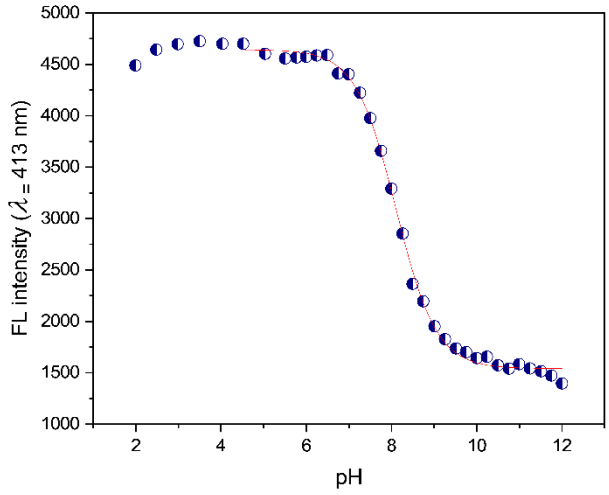


Figure 15S. pH- dependency of ***4a*** *λ_{em}=413 nm (λ_{ex}= 290 nm), pKaH = 8.1*

3.3 2,7-Bis(*N*,*N*-dimethylamino)-4-methoxyquinazoline (4b)

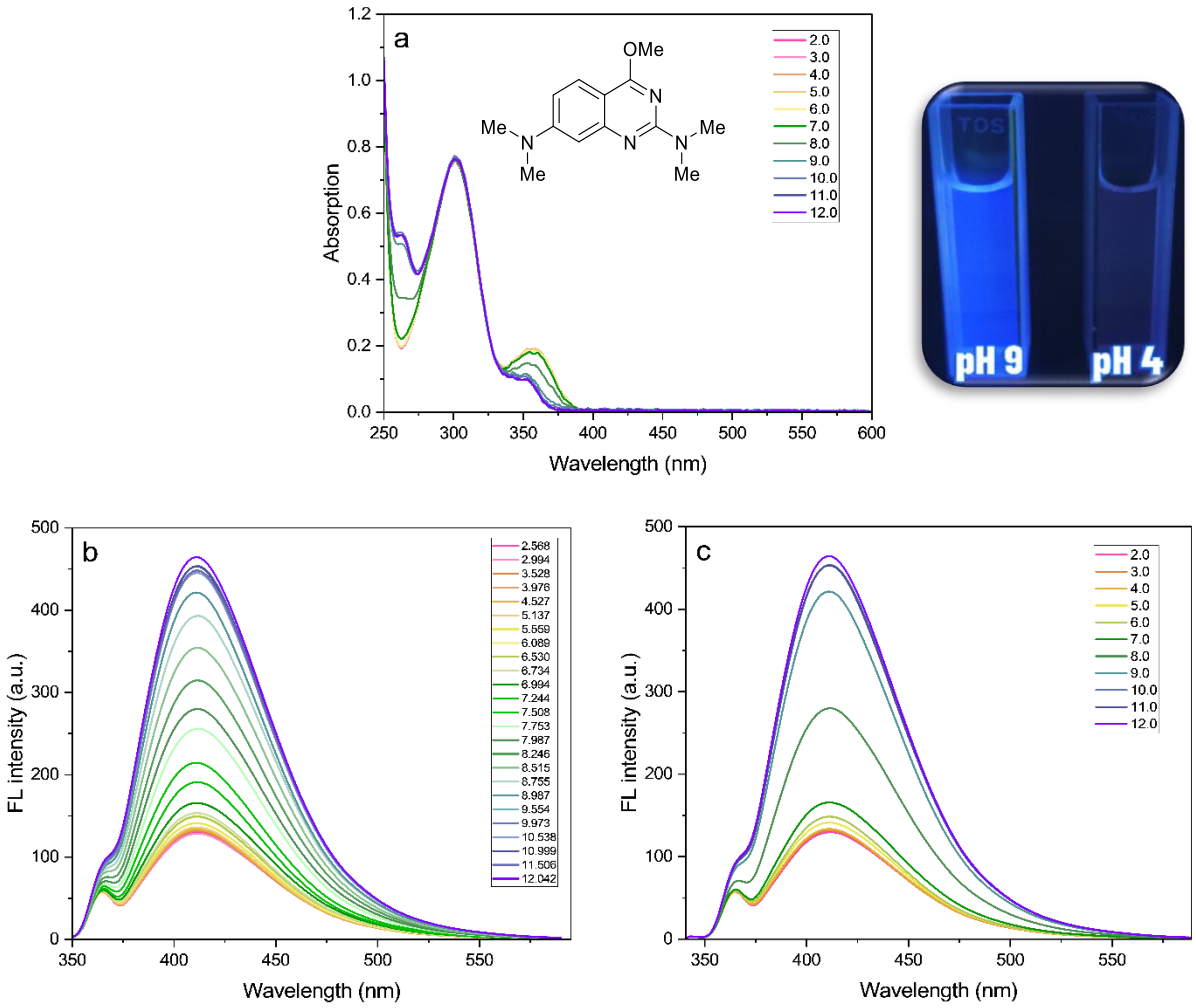


Figure 16S. a) UV-vis absorption. b,c) Photoluminescence emission spectra of ***4b*** *(λ_{ex}= 325 nm) with pH changes*

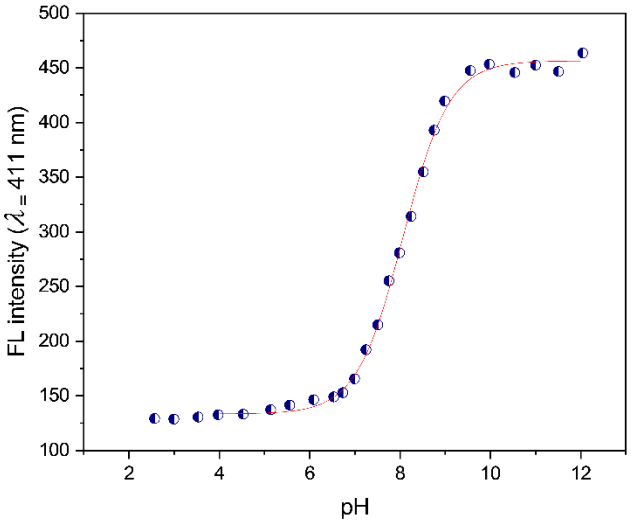


Figure 17S. pH-dependency of ***4b*** *λ_{em}=411 nm (λ_{ex}= 325 nm), pKaH = 8.1*

3.4 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-4-toluenesulfonylamino)quinazoline (4c)

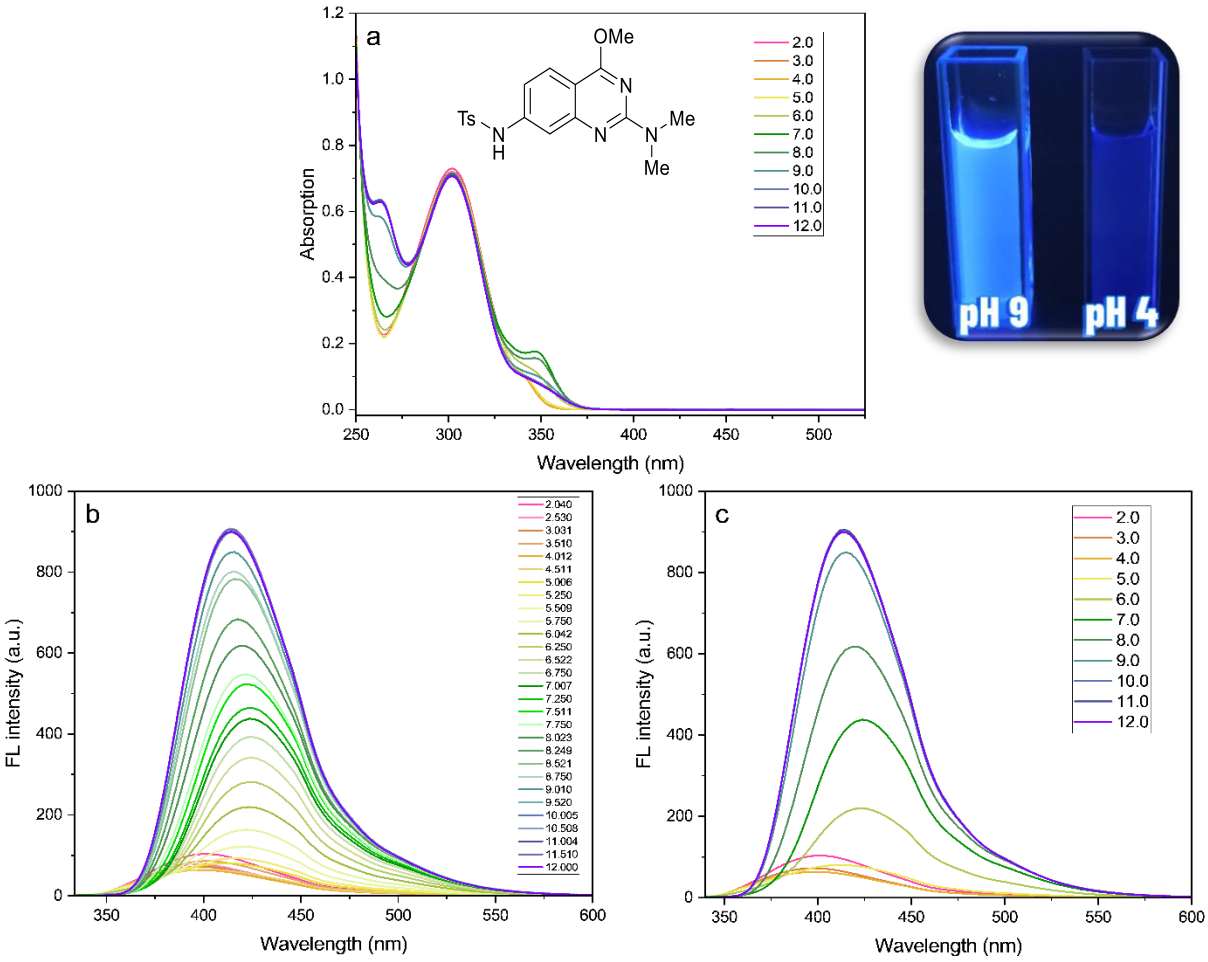


Figure 18S. a) UV-vis absorption. b,c) Photoluminescence emission spectra of ***4c*** *(λ_{ex}= 283 nm) with pH changes*

3.5 7-Amino-2-(*N*,*N*-dimethylamino)-4-phenylquinazoline (6)

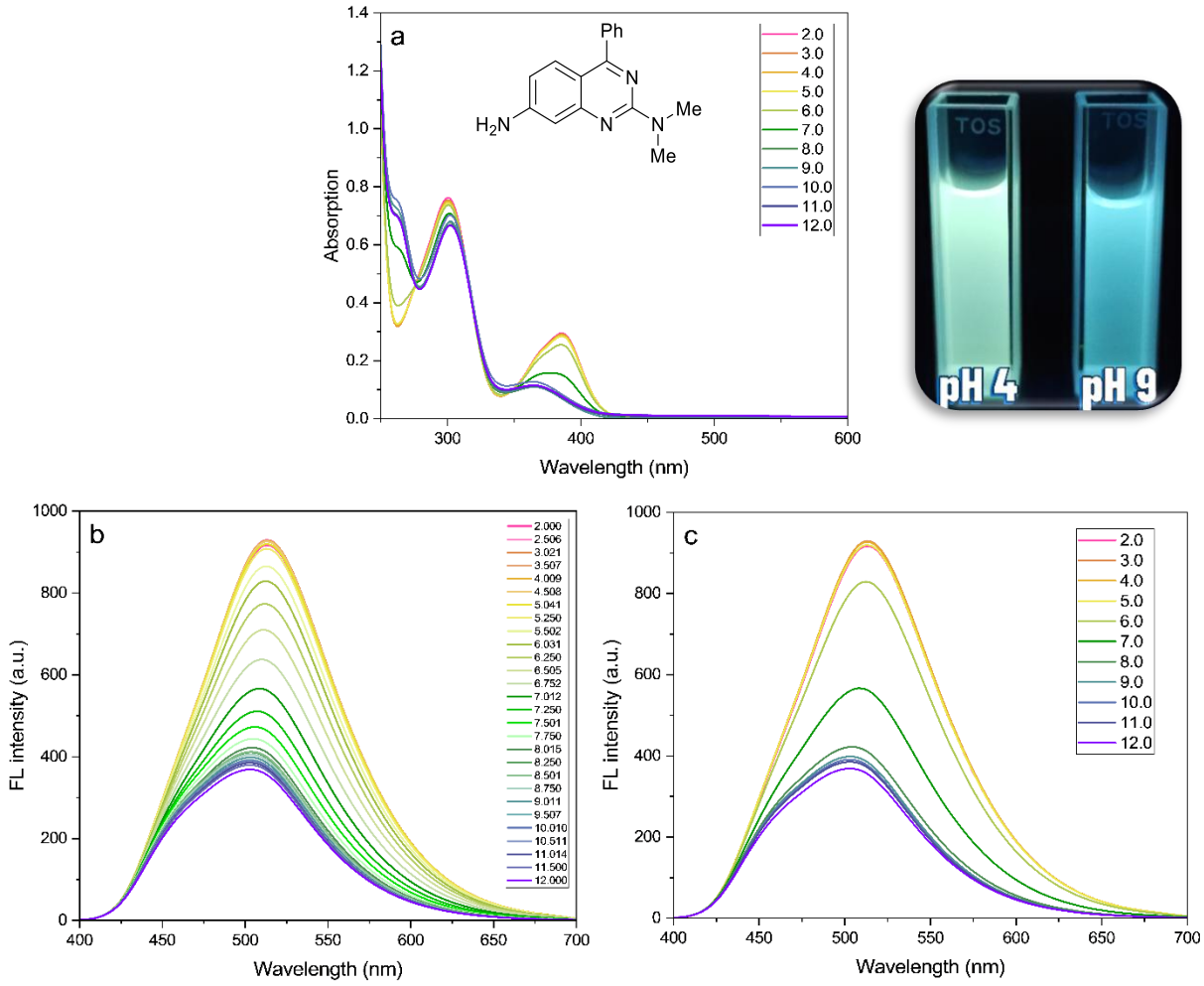


Figure 19S. a) UV-vis absorption. b,c) Photoluminescence emission spectra of ***6*** *(λ_{ex}= 277 nm) with pH changes*

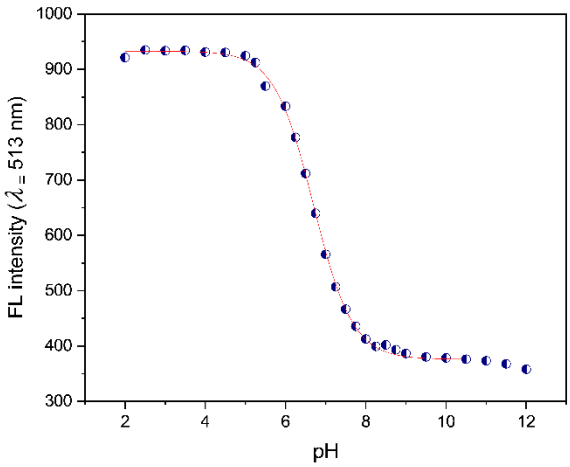


Figure 20S. pH-dependency of ***6*** *λ_{em}=513 nm (λ_{ex}= 277 nm), pKaH = 6.7*

3.6 2-(*N*,*N*-dimethylamino)-4-methoxyquinazoline (7)

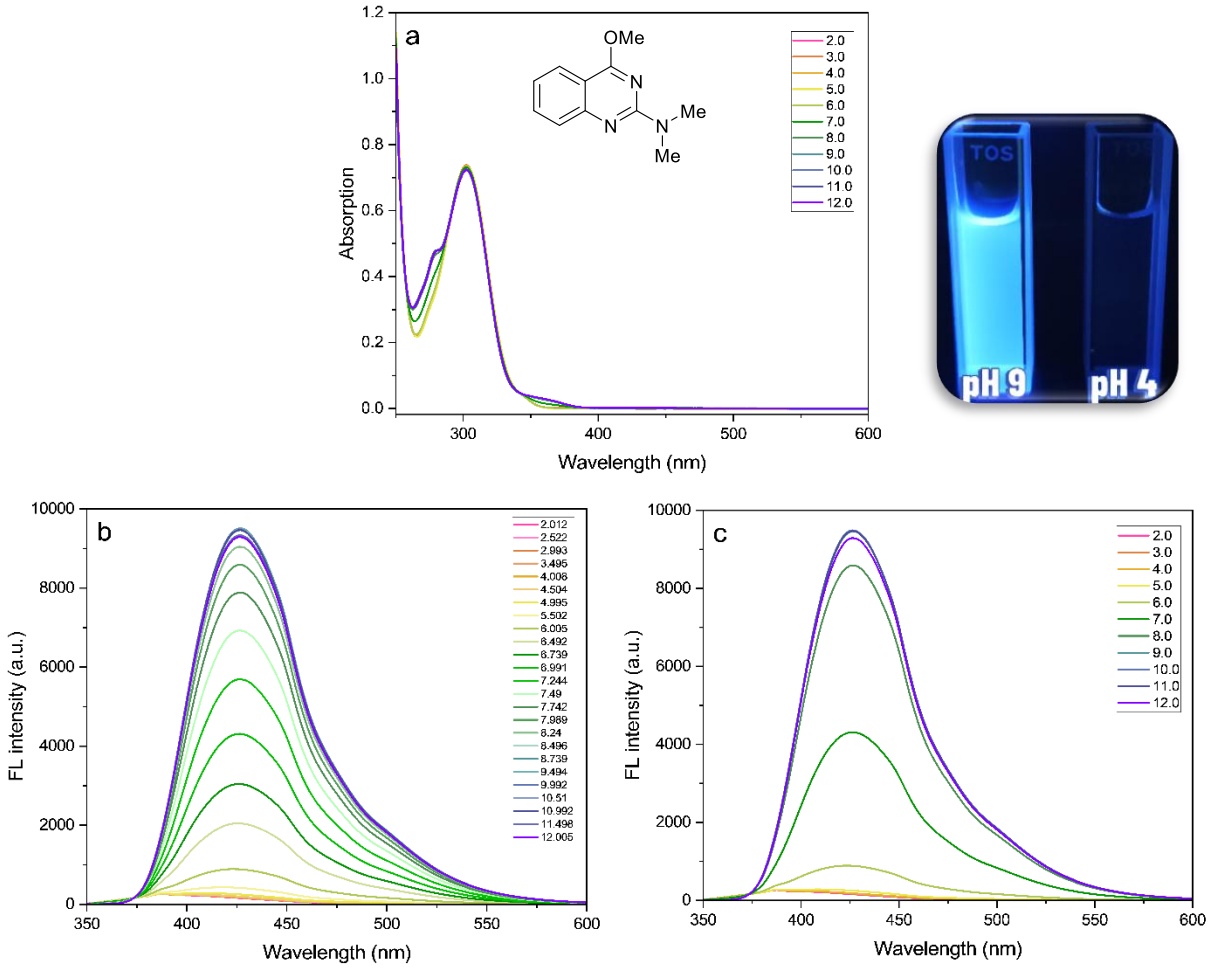


Figure 21S. a) UV-vis absorption. b,c) Photoluminescence emission spectra of ***7*** *(λ_{ex}= 287 nm) with pH changes*

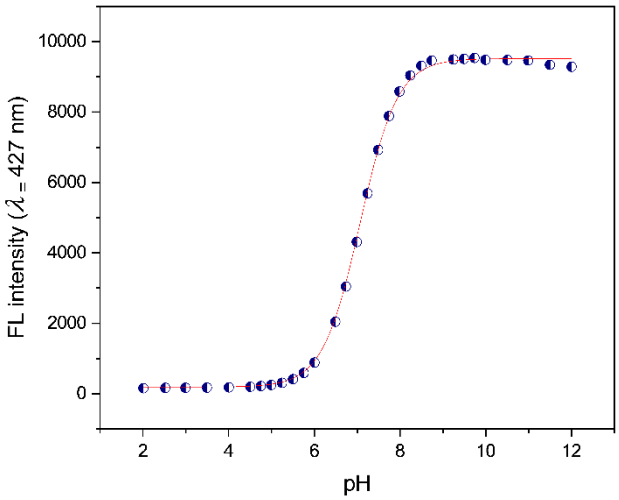
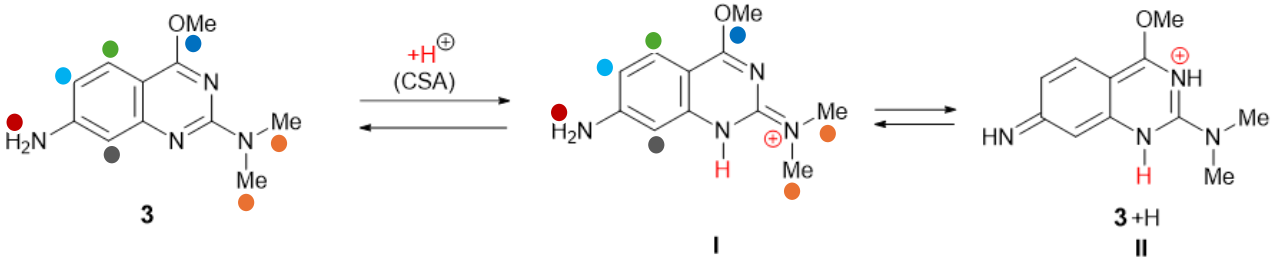


Figure 22S. pH-dependency of ***7*** *λ_{em}=427 nm (λ_{ex}= 287 nm), pKaH = 7.0*

4. ^{1}H NMR Experiments of 3 with and without Camphor Sulfonic Acid



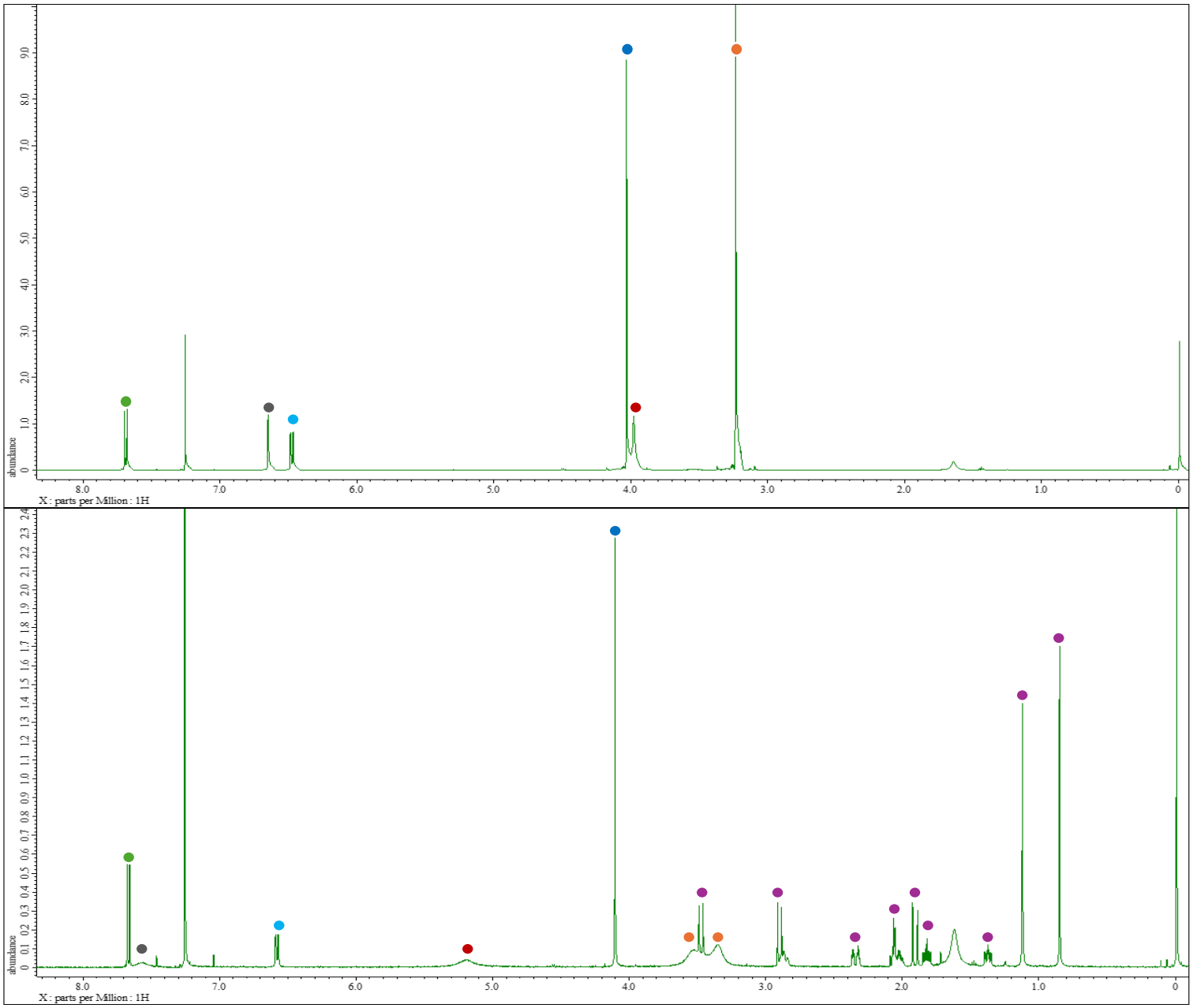
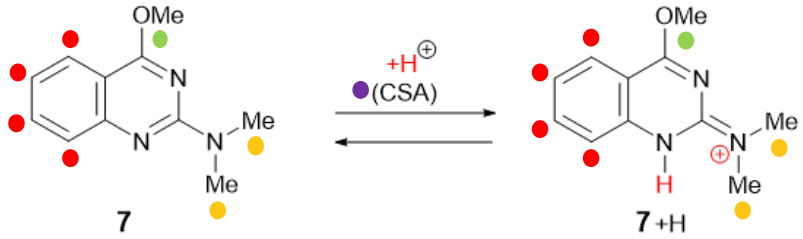


*Figure 23S. ^{1}H-NMR spectra of **3** (top) and **3** with 1 eq. of CSA (bottom) (500 MHz, solvent:$CDCl_3$, scans: 16). [3] = 4mM, [CSA] = 4mM.*

5. ^{1}H NMR Experiments of 7 with and without Camphor Sulfonic Acid



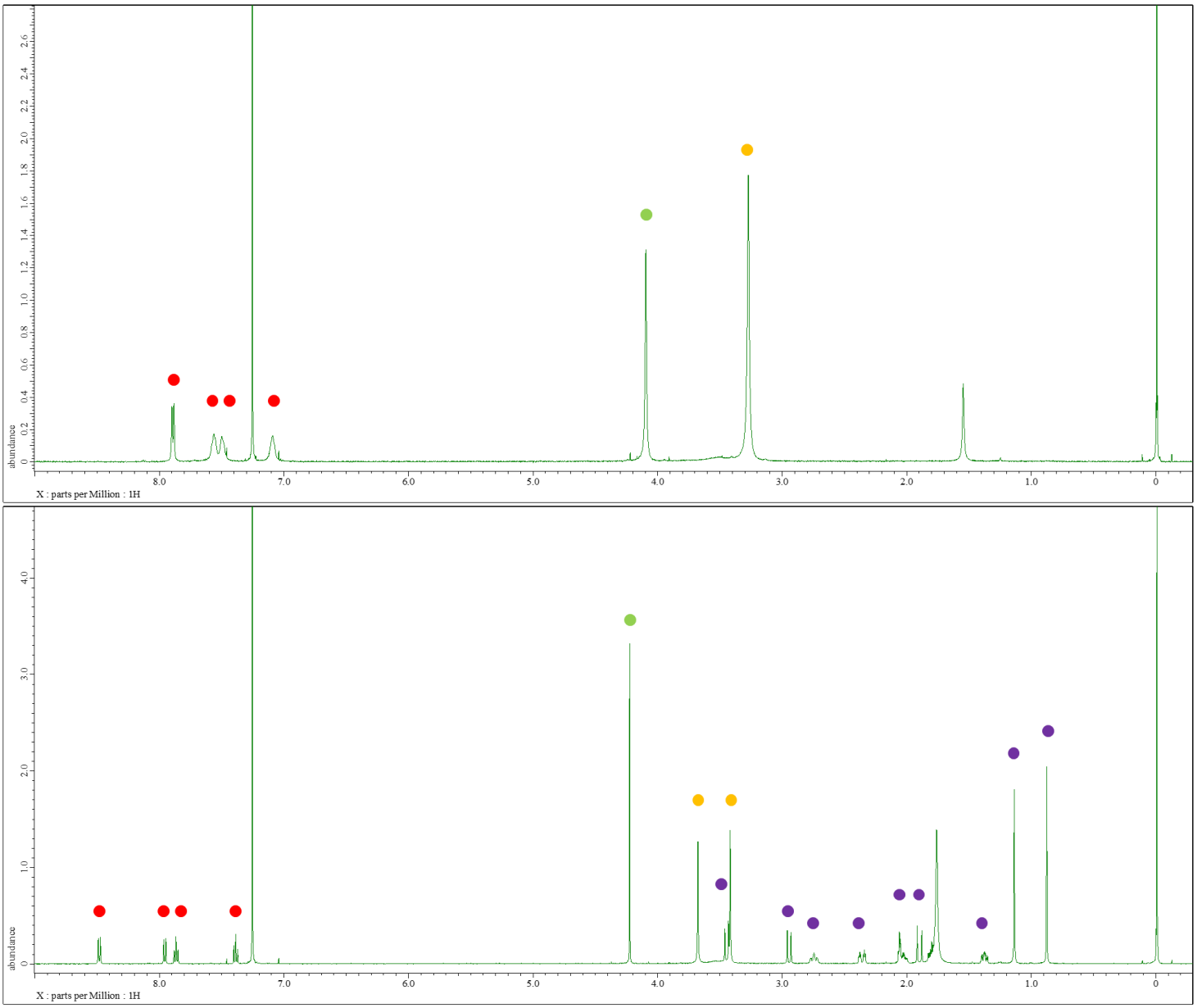


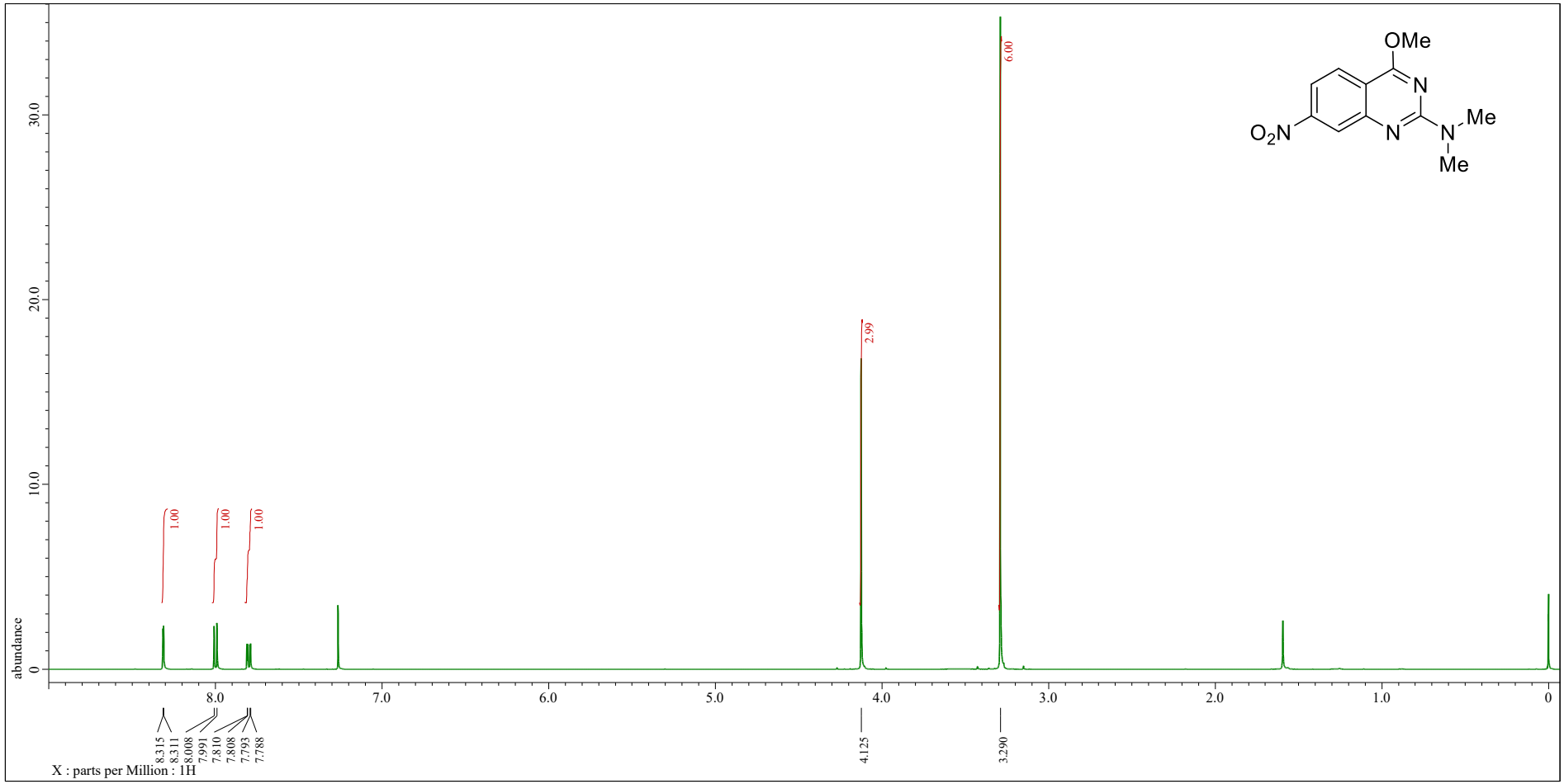
*Figure 24S. ^{1}H-NMR spectra of **7** (top) and **7** with 1 eq. of CSA (bottom) (500 MHz, solvent:$CDCl_3$, scans: 16). [3] = 4mM, [CSA] = 4mM.*

6. References

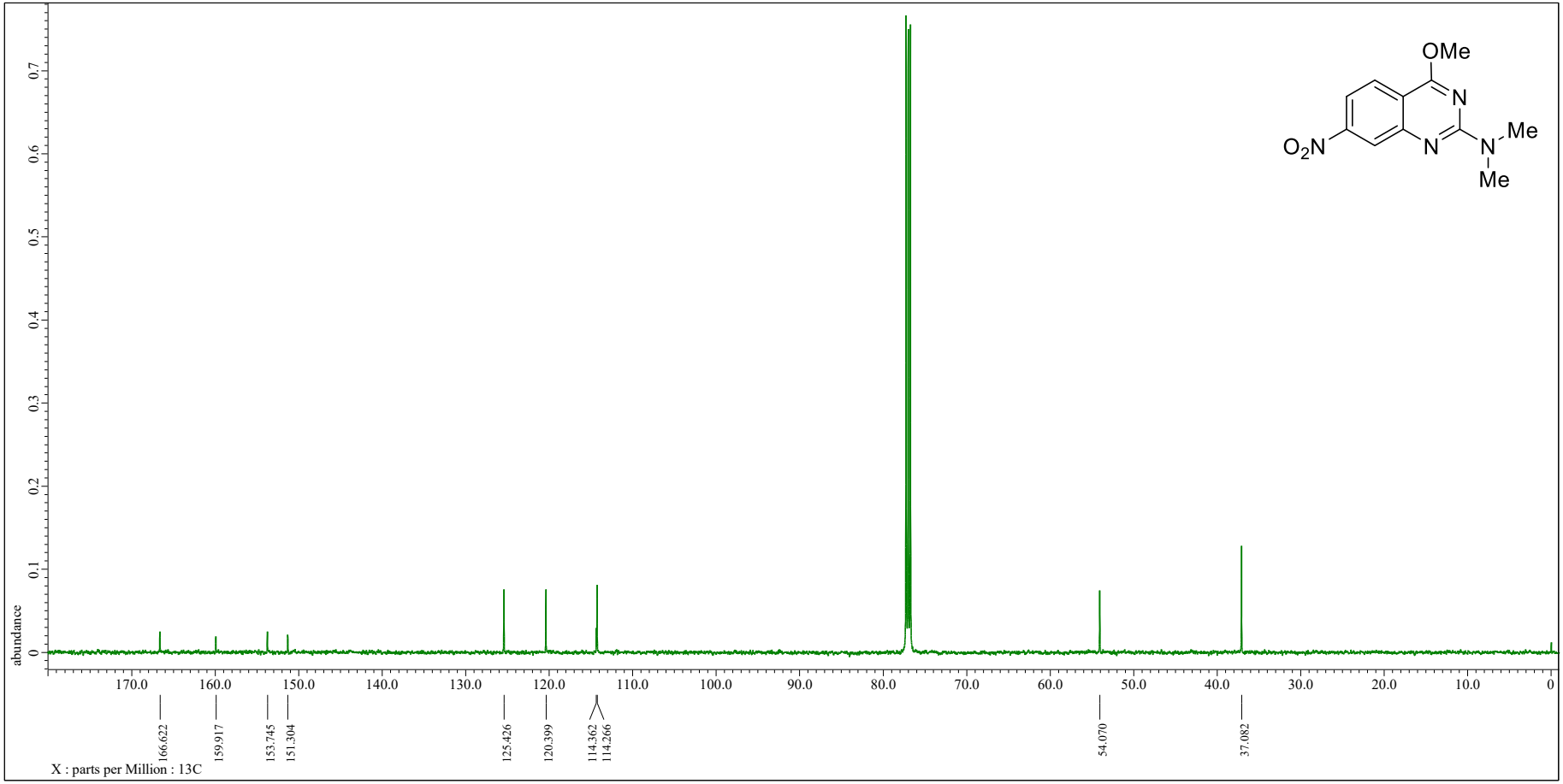
1. E. H. Huntress and J. V. K. Gladding, *J. Am. Chem. Soc.*, 1942, **64**, 2644–2649.
2. W. Peng, Z.-C. Tu, Z.-J. Long, Q. Liu and G. Lu, *Eur. J. Med. Chem.*, 2016, **108**, 644–654.

7. NMR Spectra

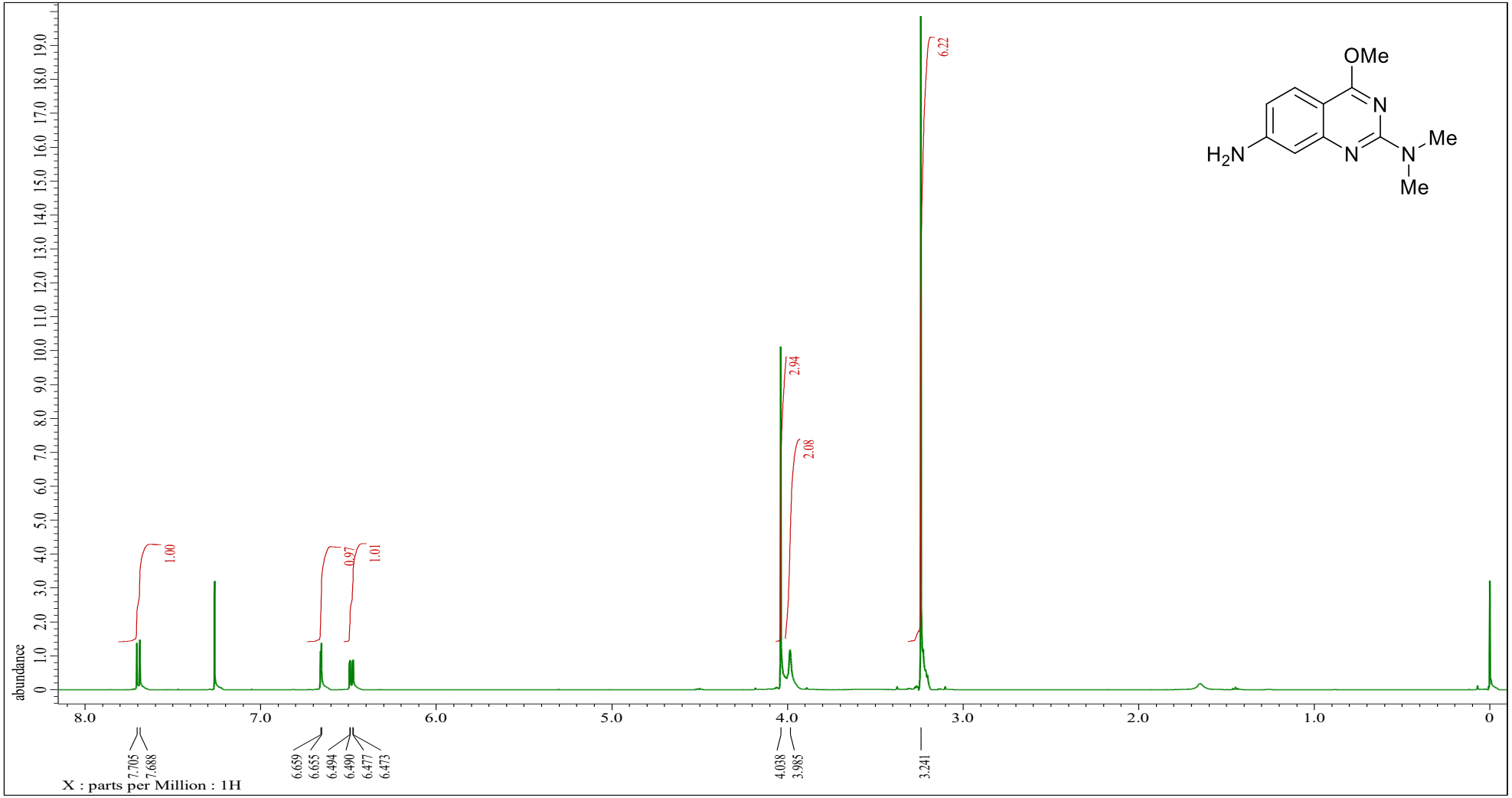
^{1}H NMR for 2-(*N*,*N*-dimethylamino)-4-methoxy-7-nitroquinazoline (2) ($CDCl_3$, 500 MHz)



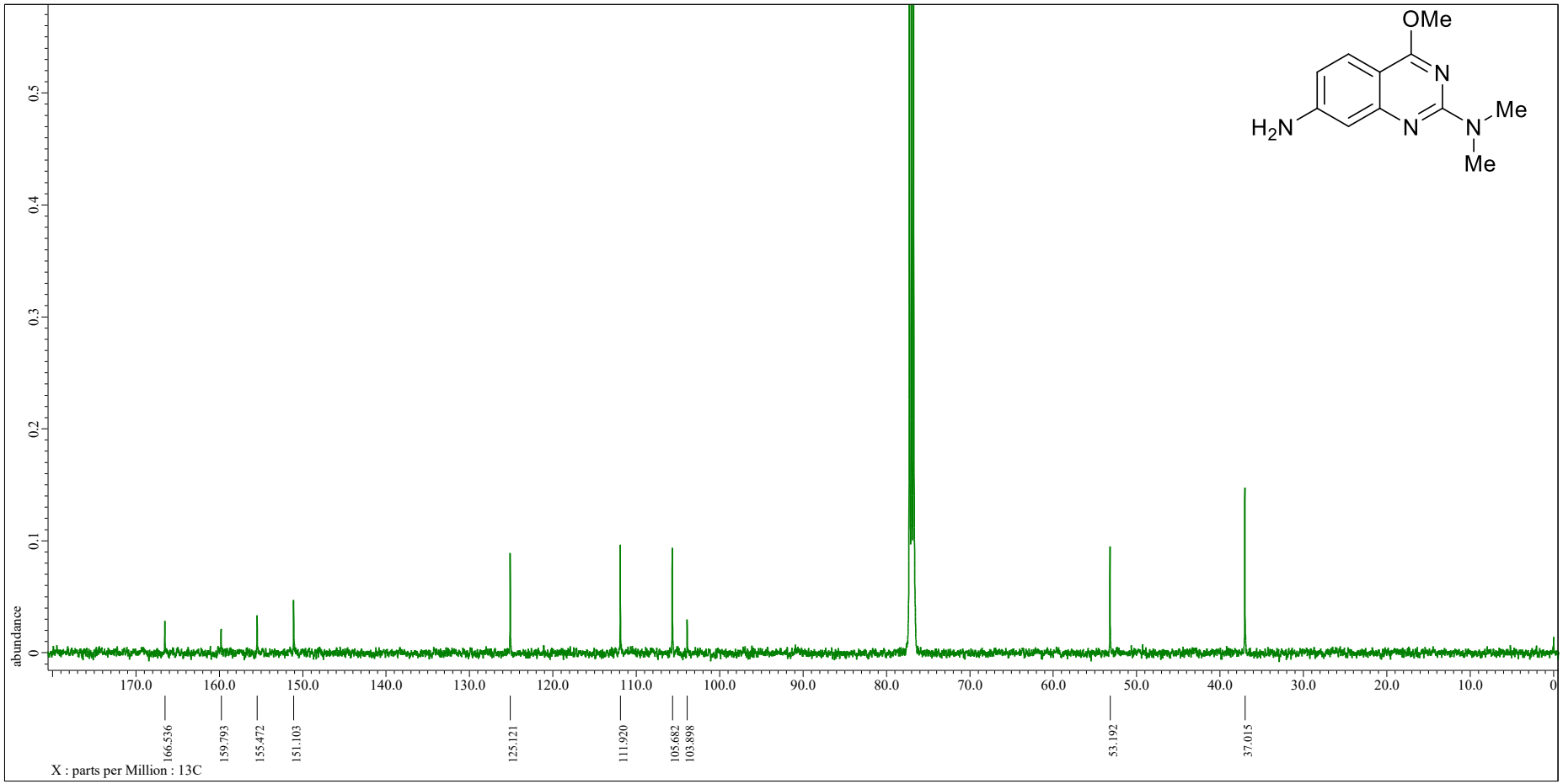
^{13}C NMR for 2-(*N,N*-dimethylamino)-4-methoxy-7-nitroquinazoline (2) ($CDCl_3$, 126 MHz)



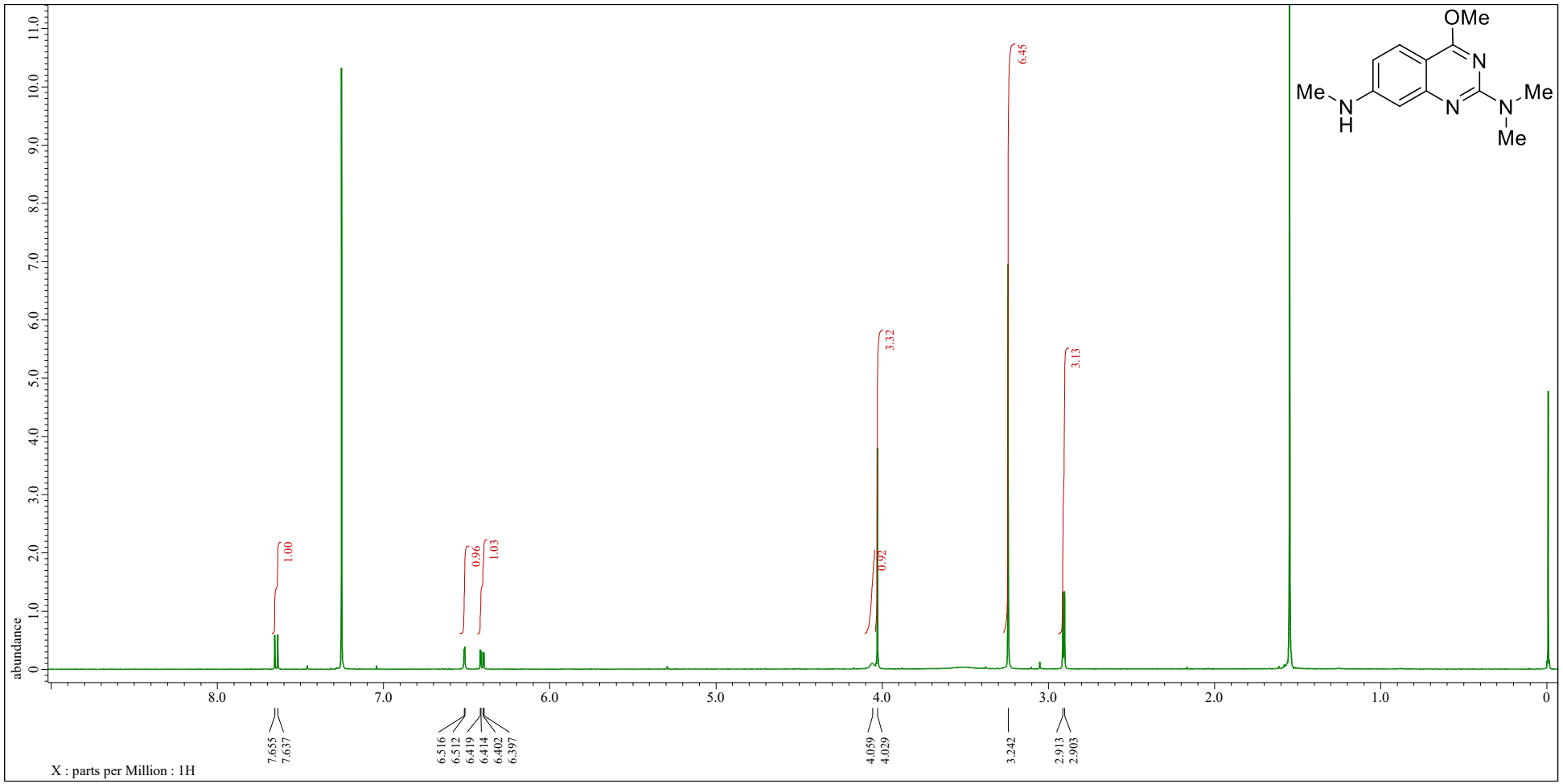
^{1}H NMR for 7-Amino-2-(*N,N*-dimethylamino)-4-methoxyquinazoline (3) ($CDCl_3$, 500 MHz)



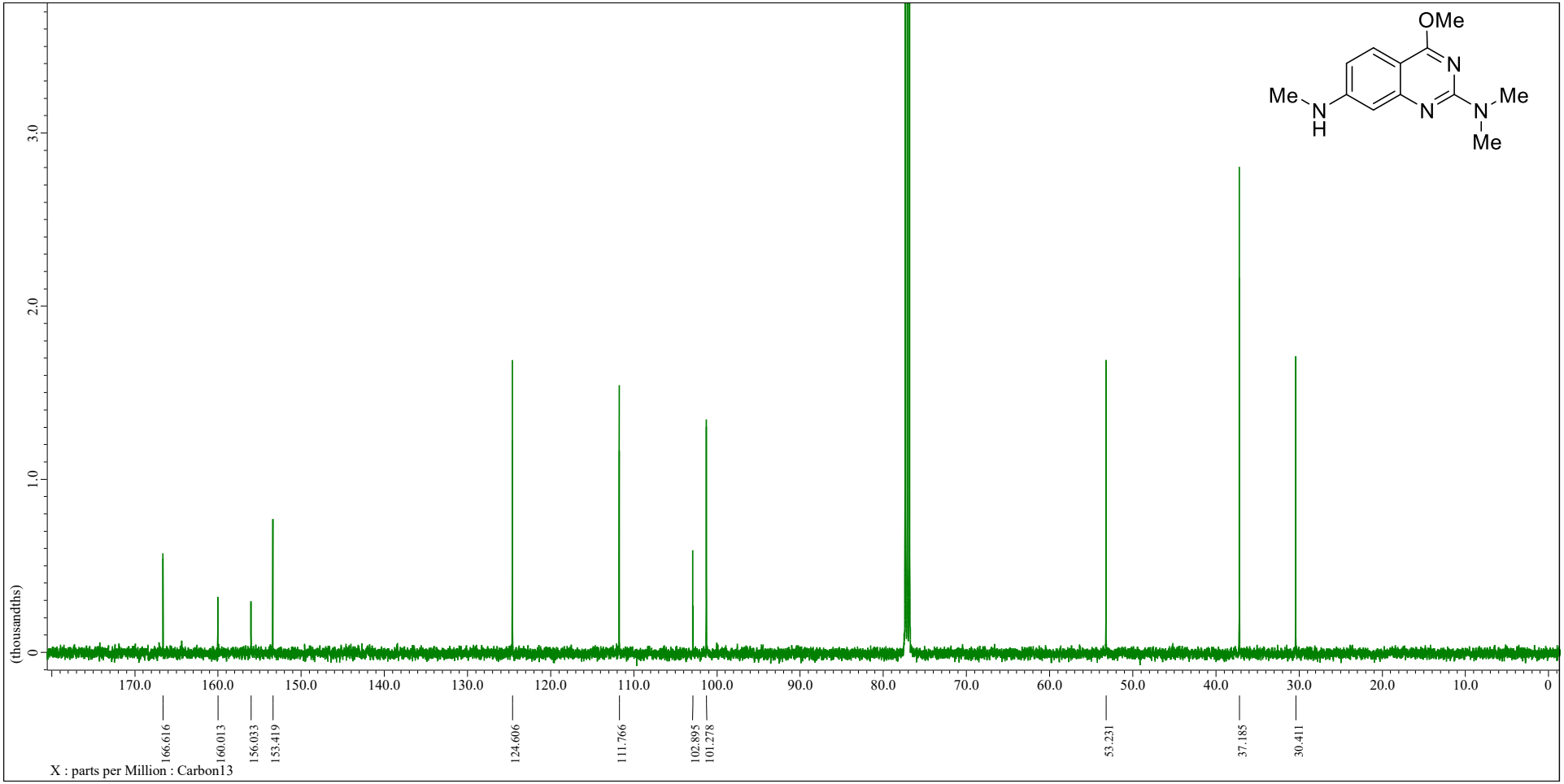
^{13}C NMR for 7-Amino-2-(*N*,*N*-dimethylamino)-4-methoxyquinazoline (3) ($CDCl_3$, 126 MHz)



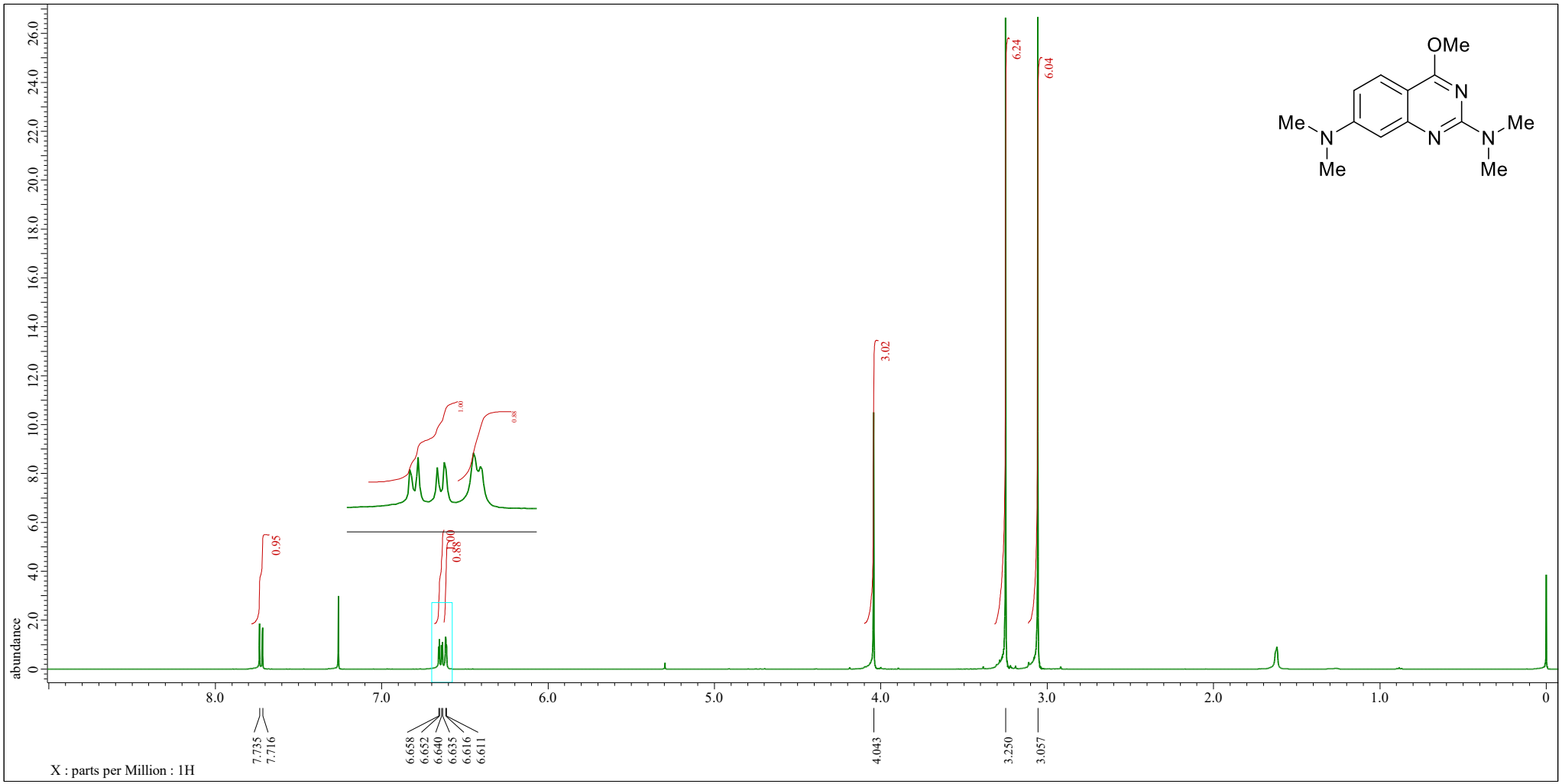
^{1}H NMR for 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-methylamino)quinazoline (4a) ($CDCl_3$, 500 MHz)



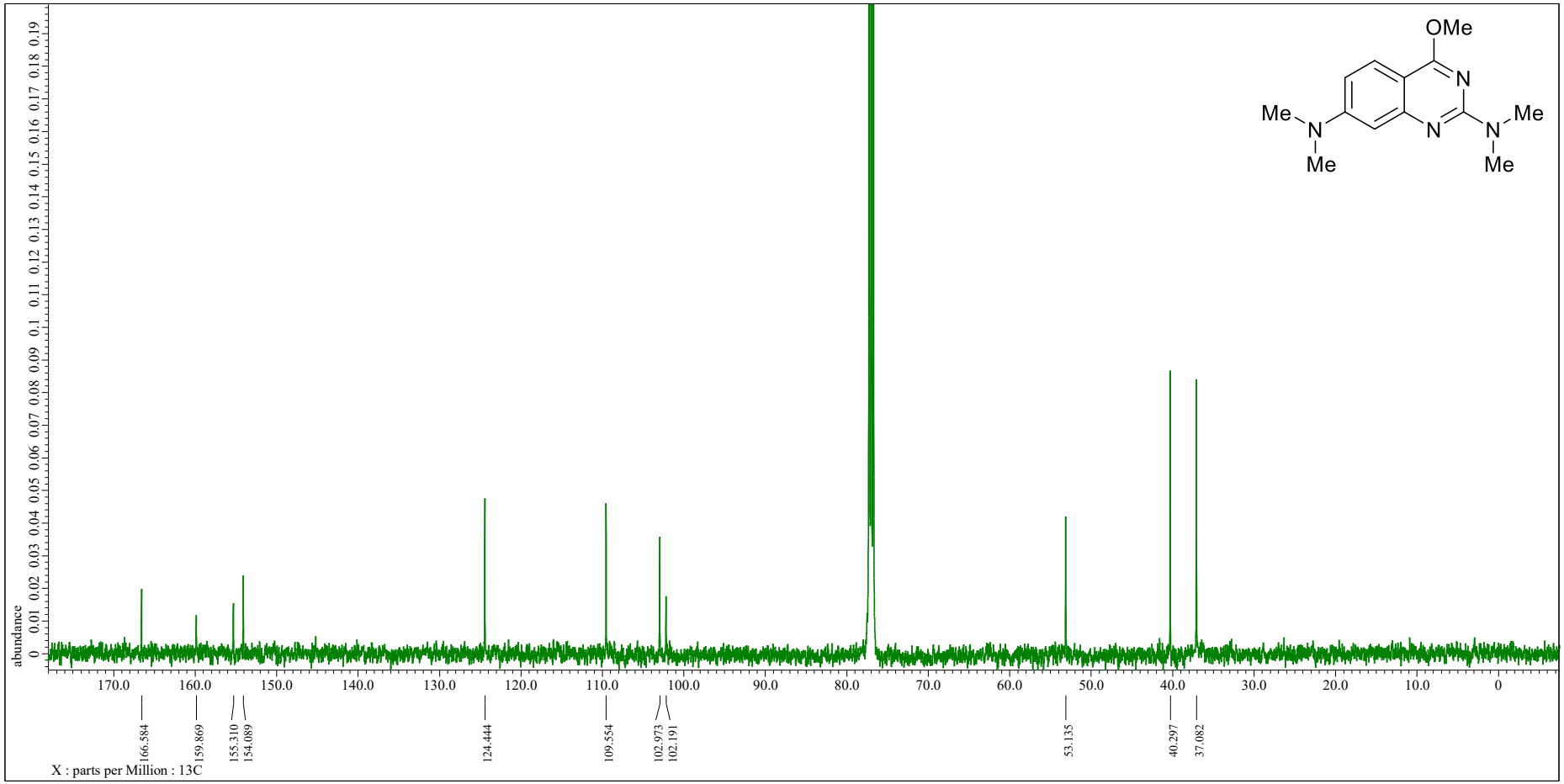
^{13}C NMR for 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-methylamino)quinazoline (4a) ($CDCl_3$, 500MHz)



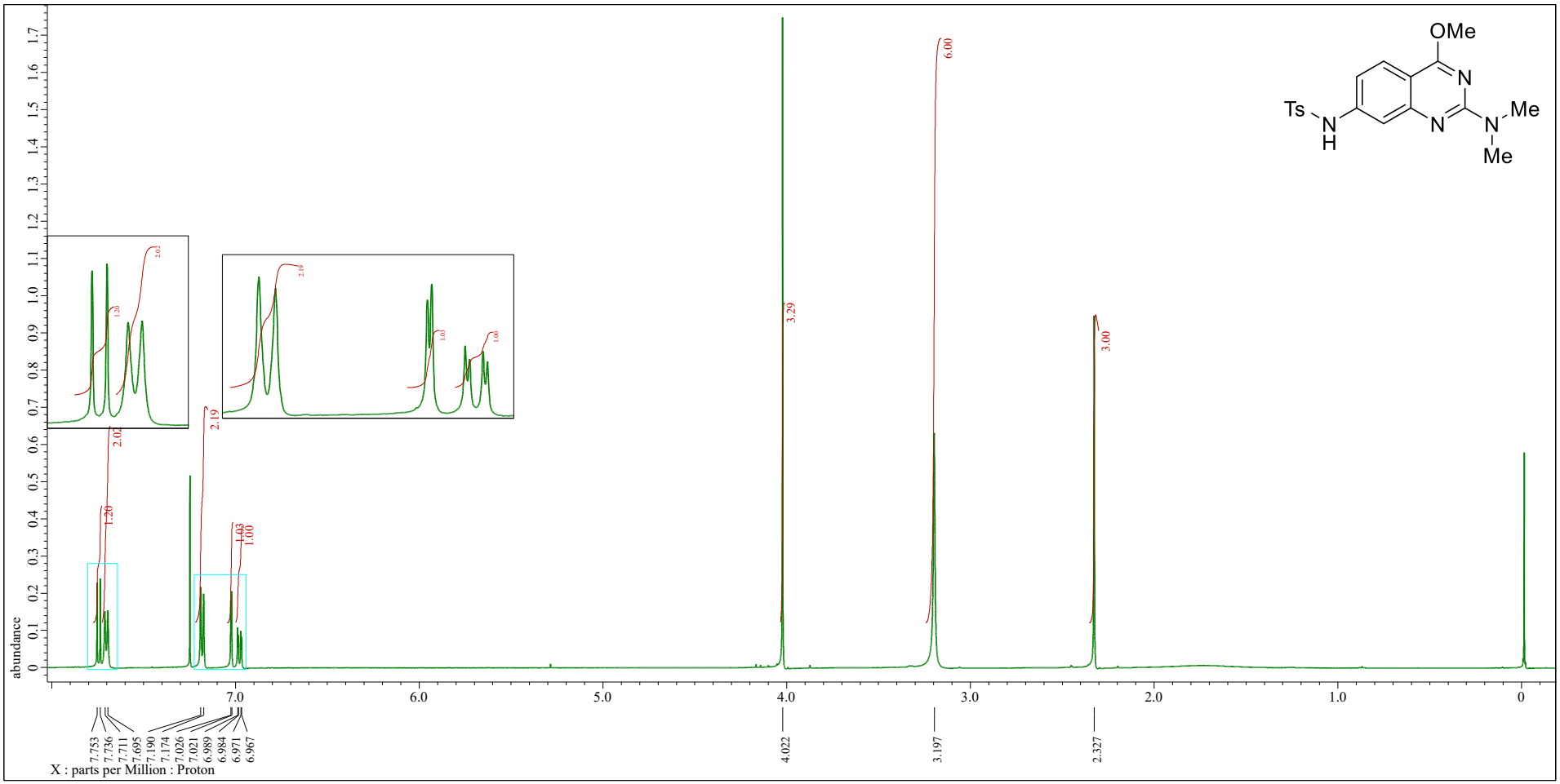
^{1}H NMR for 2,7-Bis(*N*,*N*-dimethylamino)-4-methoxyquinazoline (4b) ($CDCl_3$, 500 MHz)



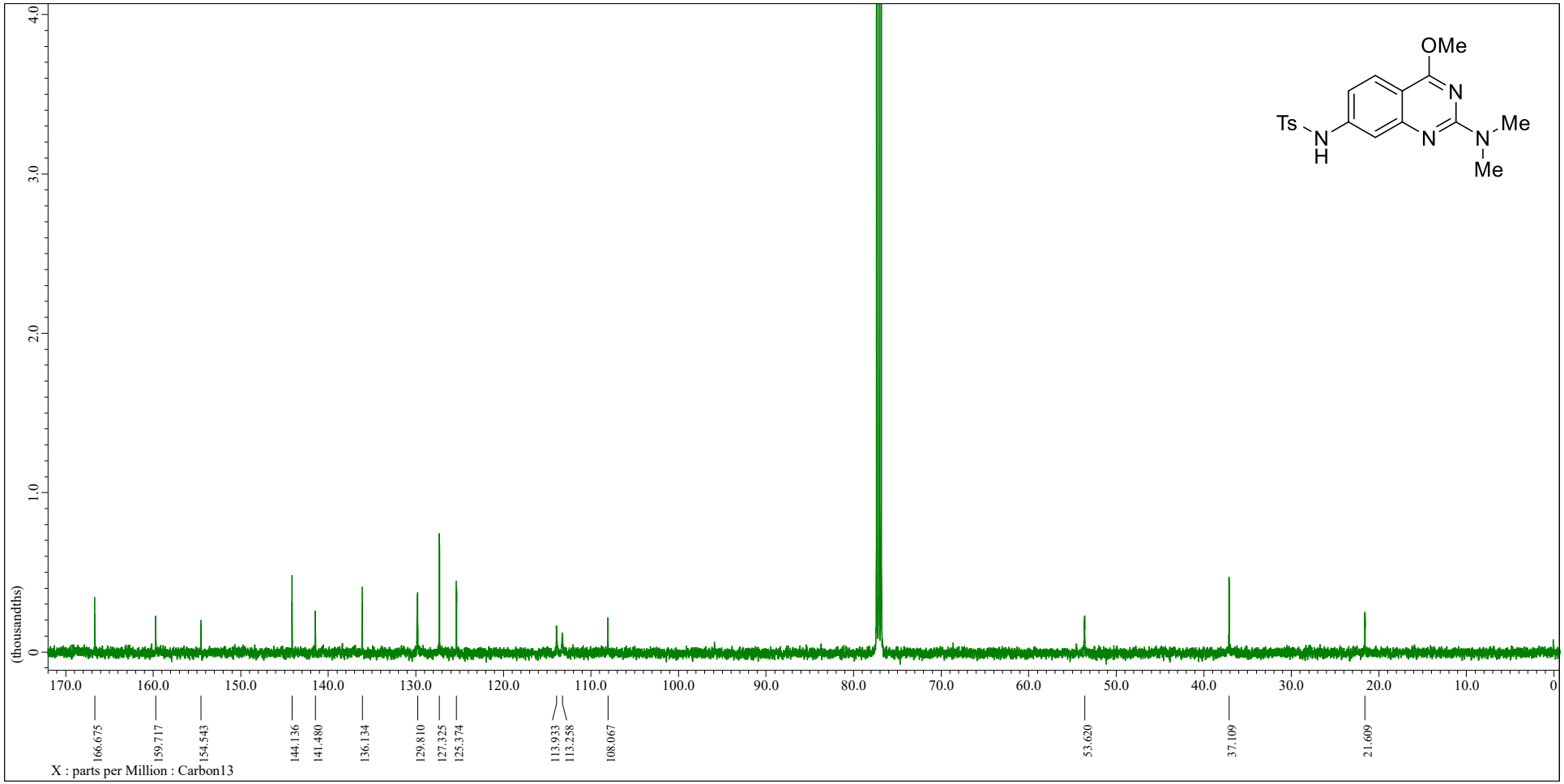
^{13}C NMR for 2,7-Bis(*N*,*N*-dimethylamino)-4-methoxyquinazoline (4b) ($CDCl_3$, 126 MHz)



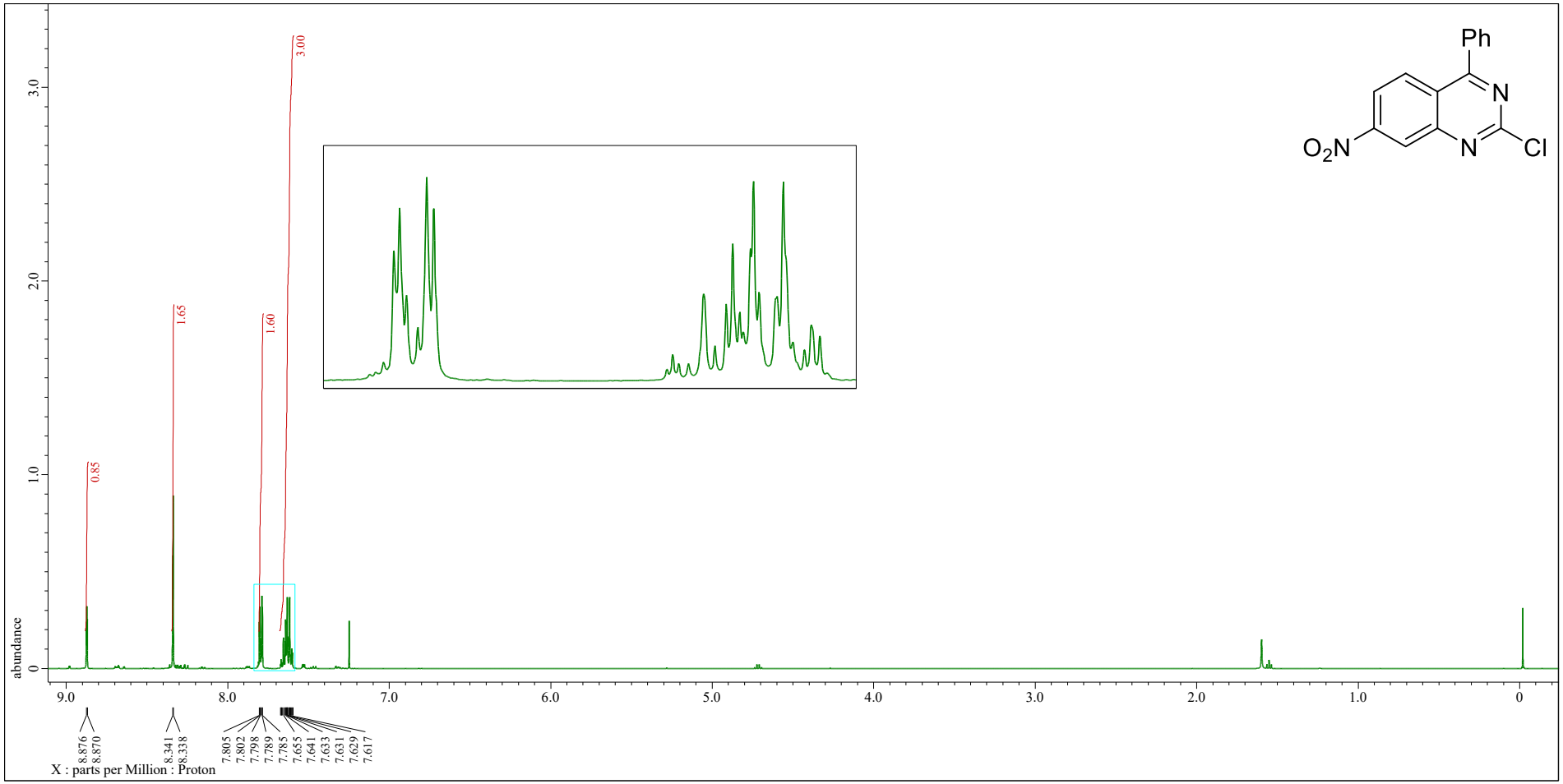
^{1}H NMR for 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-4-toluenesulfonylamino)quinazoline (4c) ($CDCl_3$, 500 MHz)



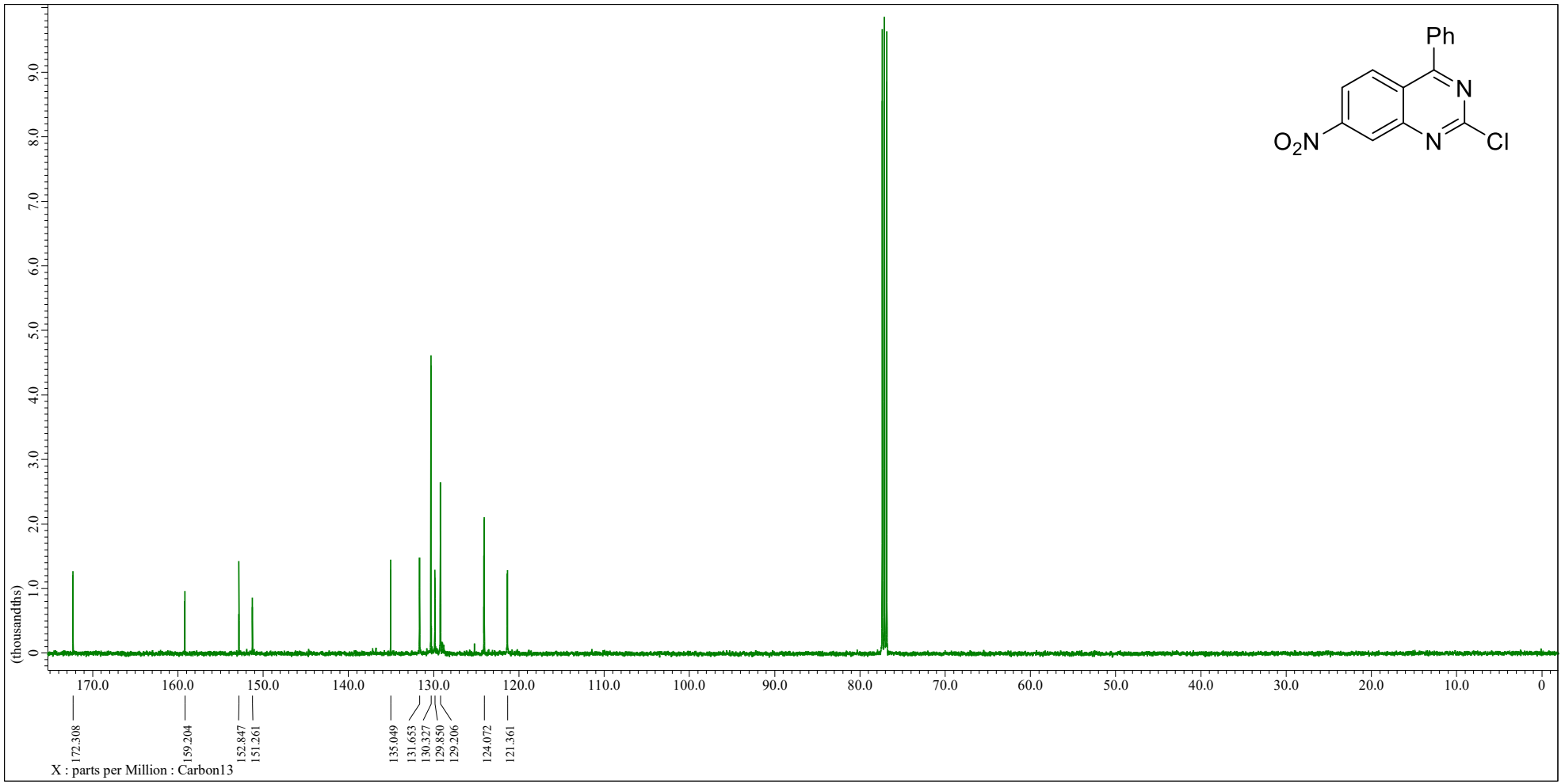
^{13}C NMR for 2-(*N*,*N*-dimethylamino)-4-methoxy-7-(*N*-4-toluenesulfonylamino)quinazoline (4c) ($CDCl_3$, 500 MHz)



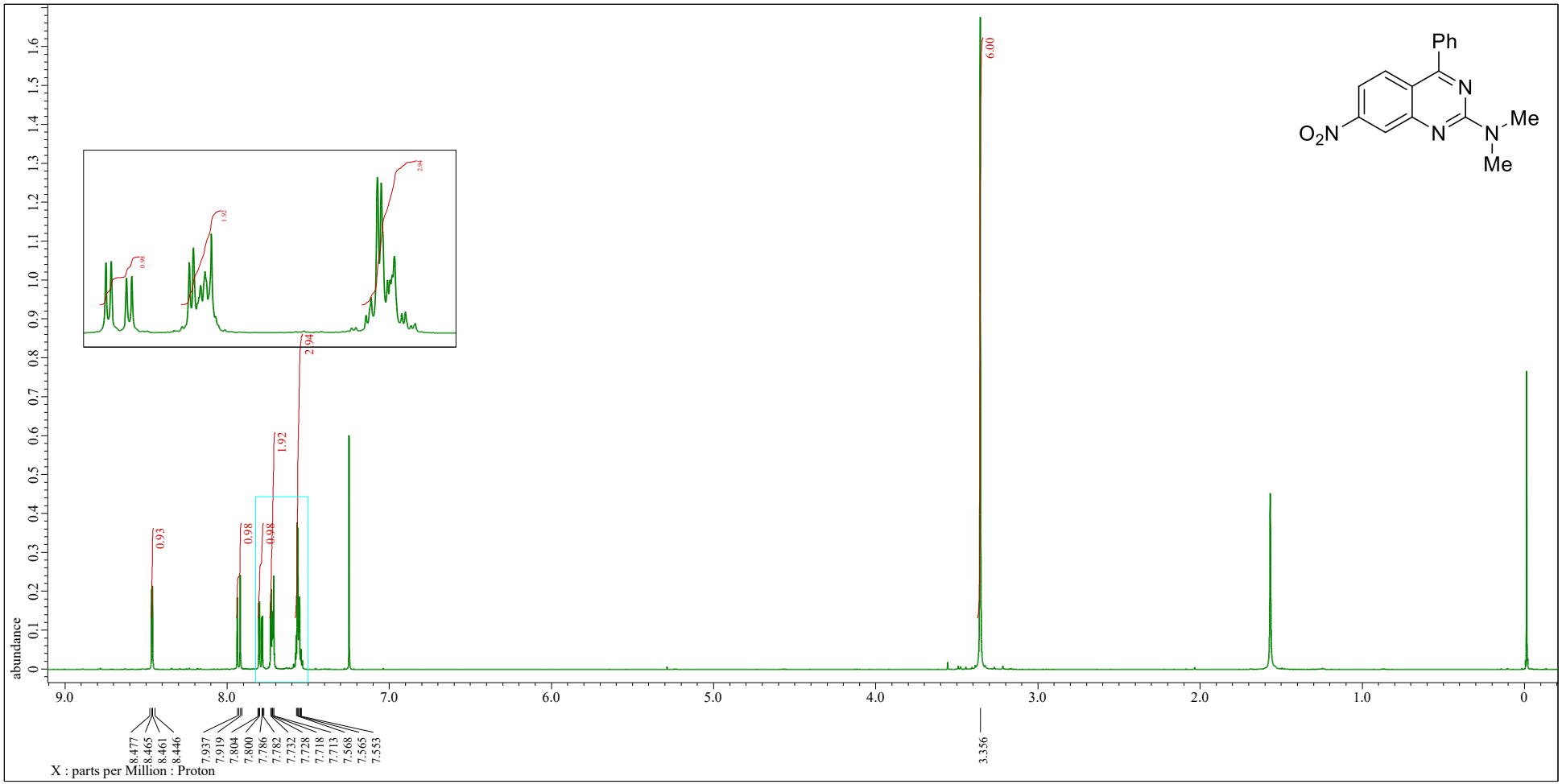
^{1}H NMR for 2-Chloro-7-nitro-4-phenylquinazoline (10) ($CDCl_3$, 500 MHz)



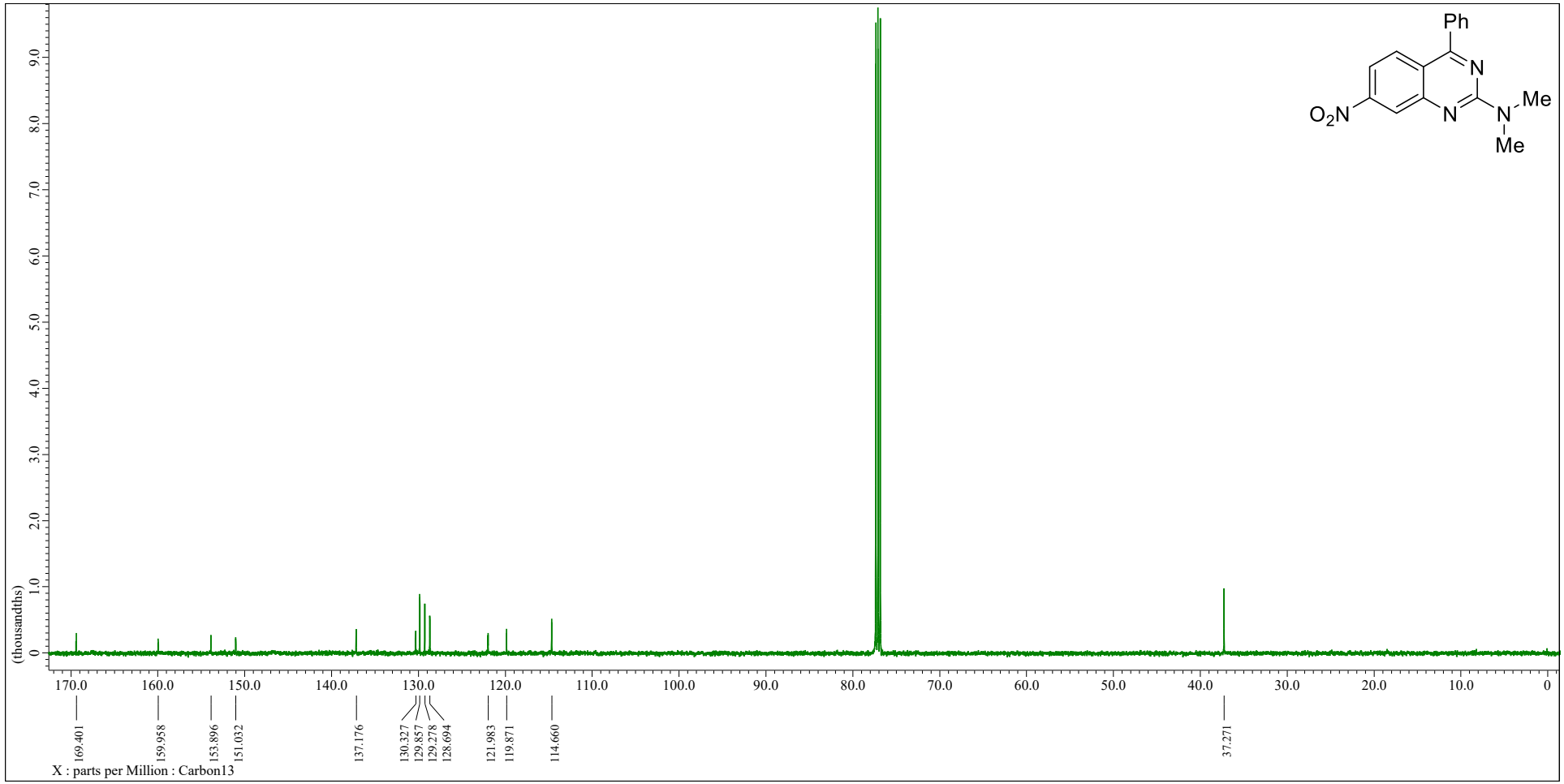
^{13}C NMR for 2-Chloro-7-nitro-4-phenylquinazoline (10) ($CDCl_3$, 500 MHz)



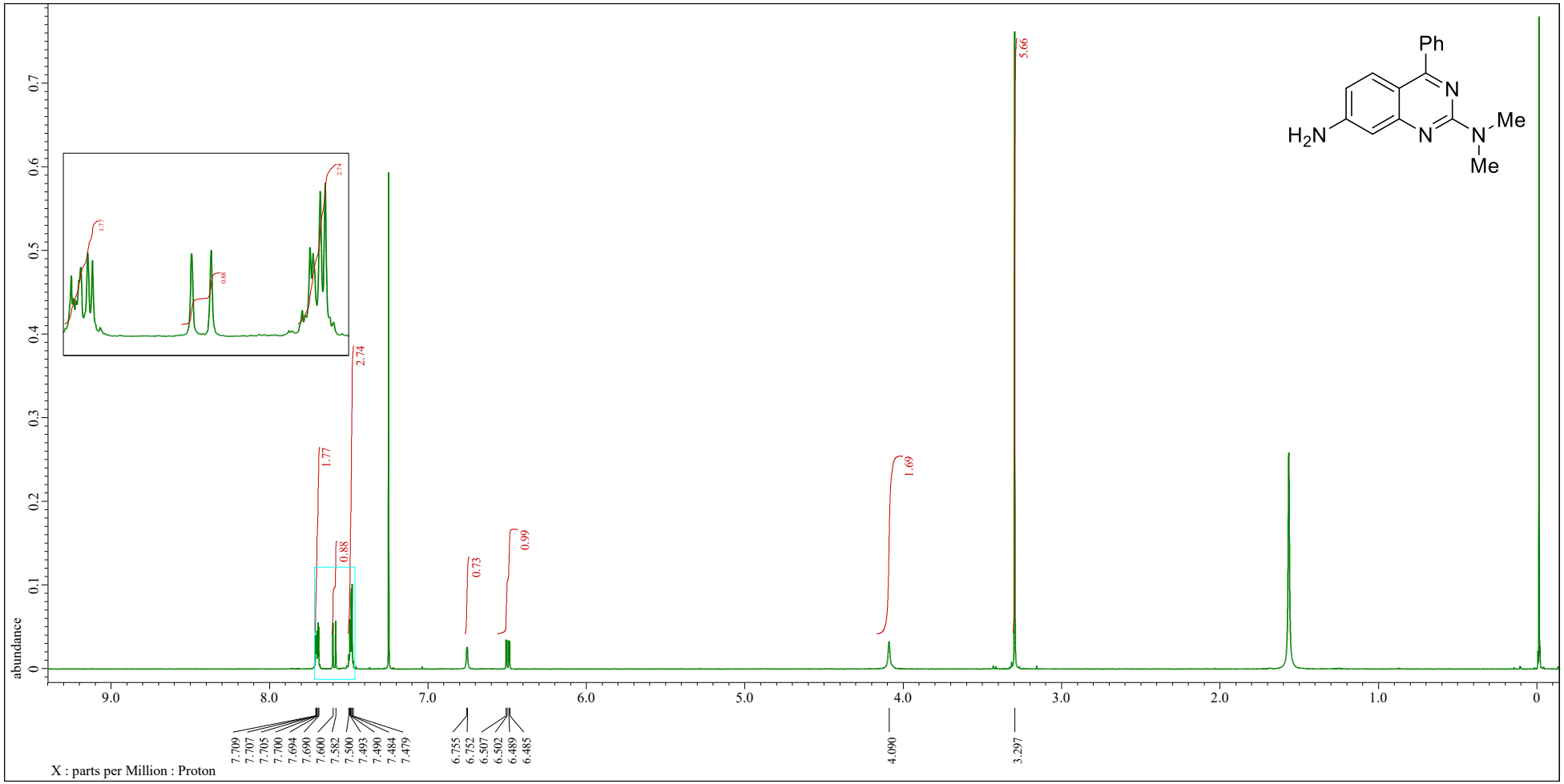
^{1}H NMR for 2-(*N*,*N*-dimethylamino)-7-nitro-4-phenylquinazoline (5) ($CDCl_3$, 500 MHz)



^{13}C NMR for 2-(*N*,*N*-dimethylamino)-7-nitro-4-phenylquinazoline (5) ($CDCl_3$, 500 MHz)



^{1}H NMR for 7-Amino-2-(*N*,*N*-dimethylamino)-4-phenylquinazoline (6) ($CDCl_3$, 500 MHz)



^{13}C NMR for 7-Amino-2-(*N*,*N*-dimethylamino)-4-phenylquinazoline (6) ($CDCl_3$, 500 MHz)