Supporting Information

For

Photophysical tuning of shortwave infrared flavylium heptamethine dyes via substituent placement

Monica Pengshung[a], Jingbai Li[b], Fatemah Mukadum[b], Steven A. Lopez[b*], Ellen M. Sletten[a*]

[a] *Department of Chemistry and Biochemistry, University of California, Los Angeles, 607 Charles E. Young Drive East, Los Angeles, California 90095, United States*

[b] *Department of Chemistry and Chemical Biology, Northeastern University, 360 Huntington Avenue, Boston, Massachusetts 02115, United States*

*Prof. Steven A. Lopez: s.lopez@northeastern.edu
*Prof. Ellen M. Sletten: sletten@chem.ucla.edu

Table of Contents

Supporting Figures:

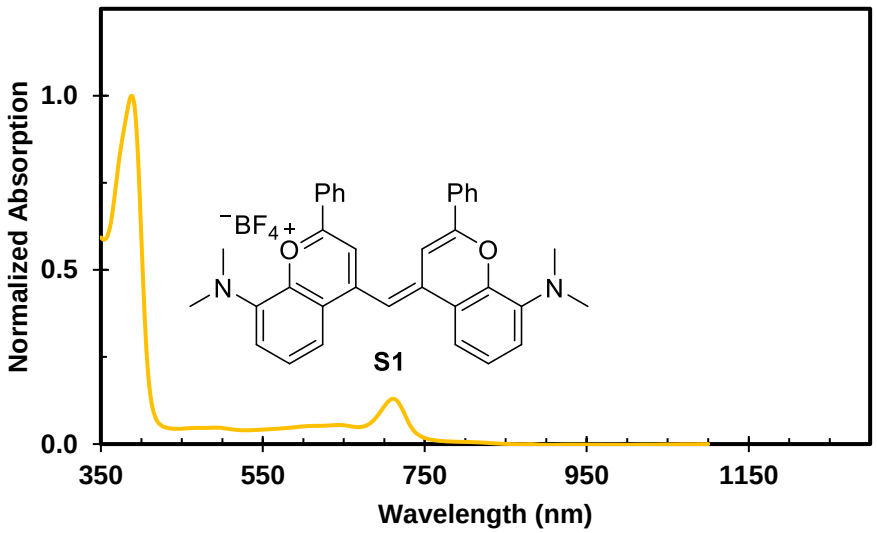


Figure S1. Normalized absorption spectra of **8c** shows the presence of a species that absorbs at 722 nm, which we attribute to monomethine dye (**S1**) impurity.

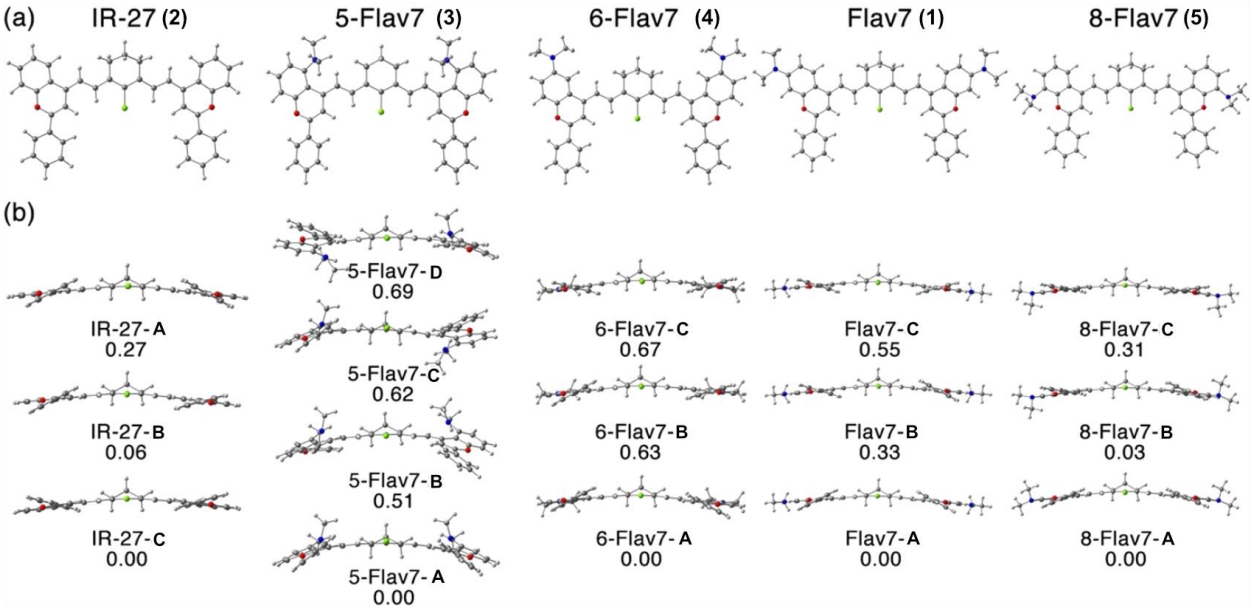


Figure S2. A) The global minimum geometries of **IR-27** (**2**), **5-Flav7** (**3**), **6-Flav7** (**4**), **Flav7** (**1**), and **8-Flav7** (**5**) dyes optimized at M062X/6-31+G(d,p) level of theory. B) The comparison of the optimized local minimum geometries of **IR-27** (**2**), **5-Flav7** (**3**), **6-Flav7** (**4**), **Flav7** (**1**), and **8-Flav7** (**5**) dyes. The relative energies are in kcal·mol^{-1}, corrected with Gibbs free energy at 298.15 K.

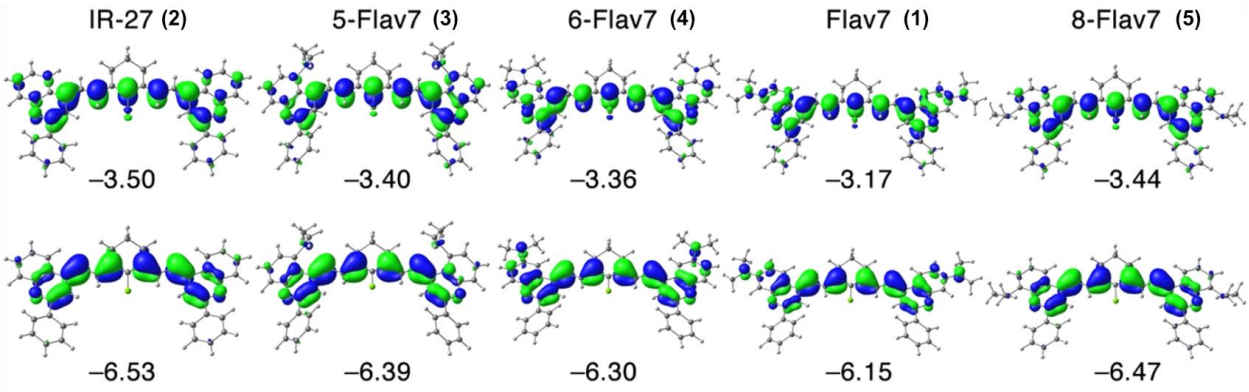
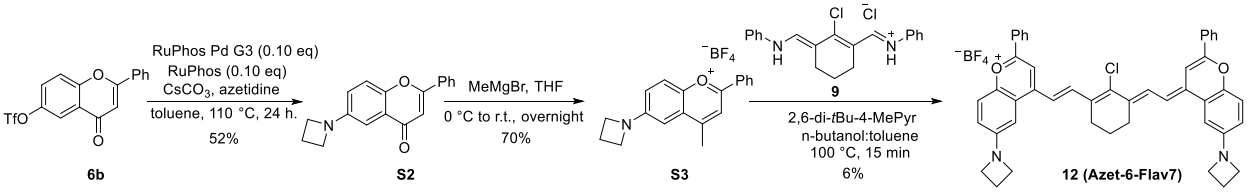


Figure S3. The frontier molecular orbitals (HOMO/top and LUMO/bottom) of **IR-27** (**2**), **5-Flav7** (**3**), **6-Flav7** (**4**), **Flav7** (**1**), and **8-Flav7** (**5**) dyes in their global minimum computed at M062X/6-31+G(d,p). The orbital energies are in eV.



Scheme S1. Synthesis of Azet-6-Flav7 **12**.

Photophysical Procedures:

Absorbance spectra were collected on a JASCO V-770 UV-Visible/NIR spectrophotometer with a 2000 nm/min scan rate after blanking with the appropriate solvent. Photoluminescence spectra were obtained on a Horiba Instruments PTI QuantaMaster Series fluorometer. Quartz cuvettes (1 cm) were used for absorbance and photoluminescence measurements. Absorption coefficients in dichloromethane were calculated with serial dilutions with Hamilton syringes in volumetric glassware. Error was taken as the standard deviation of the triplicate experiments. Relative quantum yields were determined in dichloromethane relative to IR-26.

Fluorescence quantum yield measurements:

The fluorescence quantum yield (Φ_F) of a molecule or material is defined as follows:

$$\Phi_F = \frac{P_E}{P_A} \qquad (1)$$

Where P_E and P_A represent the number of photons emitted and absorbed, respectively. To determine the quantum yield, we used a relative method with IR-26 as a known standard in the same region of the electromagnetic spectrum.

To compare an unknown to a reference with a known quantum yield, the following relationship was used:

$$\Phi_{F,x} = \Phi_{F,r}\,(m_x / m_r)(\eta_x{}^2 / \eta_r{}^2)$$

Where m represents the slope of the line (y = mx + b) obtained from graphing integrated fluorescence intensity versus optical density across a series of samples, η is the refractive index of the solvent and the subscripts *x* and *r* represent values of the unknown and reference, respectively.

The $\Phi_{F,r}$ of IR-26 was taken to be 0.05%, as previously determined.[1]

To obtain a plot of integrated fluorescence intensity versus absorbance for the reference and unknown, five solutions and a solvent blank were prepared with absorbance maxima between 0.01 and 0.1 au. Absorbance and emission spectra (with an excitation wavelength of 885 nm) were acquired for all samples. IR-26 and the unknown dyes were diluted in dichloromethane to concentrations with optical densities less than 0.1 to minimize effects of reabsorption. The baseline corrected (at 1500 nm) fluorescence traces were integrated, and the raw integrals were corrected by subtracting the integral over an identical range from fluorescence traces of the blank solvent. The integrated fluorescence intensities were then plotted against the baseline corrected absorbance values at the relevant wavelength (885 nm), and the slope and error in slope were obtained ($R^2 > 0.99$ for all traces).

Synthetic Procedures:

Materials:

Chemical reagents were purchased from Acros Organics, Alfa Aesar, Fisher Scientific, Sigma-Aldrich, or TCI and used without purification unless noted otherwise. Anhydrous and deoxygenated solvents (THF, toluene) were dispensed from a Grubb's-type Phoenix Solvent Drying System constructed by J.C. Meyer. Oxygen was removed by three consecutive freeze–pump–thaw cycles in air-free glassware directly before use. Thin layer chromatography was performed using Silica Gel 60 F254 (EMD Millipore) plates. Flash chromatography was executed with technical grade silica gel with 60 Å pores and 40 – 63 μm mesh particle size (Sorbtech Technologies).

Instrumentation:

Solvent was removed under reduced pressure with a Büchi Rotovapor with a Welch self-cleaning dry vacuum pump and further dried with a Welch DuoSeal pump. Nuclear magnetic resonance (^{1}H-NMR, ^{13}C-NMR) spectra were taken on Bruker Advance AV-400, AV-500 and processed with MestReNova or TopSpin software. All ^{1}H-NMR and ^{13}C-NMR peaks are reported in ppm in reference to their respective solvent signals. High resolution mass spectra (electrospray ionization (ESI)) were obtained on a Thermo Scientific Q Exactive™ Plus Hybrid Quadrupole-Orbitrap™ with Dionex UltiMate 3000 RSLCnano System.

4-oxo-2-phenyl-4*H*-chromen-5-yl trifluoromethanesulfonate (6a)

Triflic anhydride (0.60 mL, 3.0 mmol, 4 eq) was added slowly dropwise to a solution of 5-hydroxyflavone (200 mg, 0.8 mmol, 1 eq) in anhydrous pyridine (2.5 mL, 30 mmol, 40 eq) at 0 °C. The reaction was warmed to room temperature and left to stir for 1 hr. The solution was quenched with saturated $NaHCO_3$ (15 mL), extracted with ethyl acetate (3 x 20 mL), dried over $NaSO_4$, filtered and evaporated to give a yellow crystalline solid. The crude product was purified via silica gel chromatography with hexane: ethyl acetate (9:1) to afford pure **4-oxo-2-phenyl-4*H*-chromen-5-yl trifluoromethanesulfonate** (260 mg, 3.0 mmol, 85%) as a beige solid. ^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.87 (m, 2H), 7.76 – 7.70 (m, 1H), 7.65 (dd, *J* = 8.6, 1.2 Hz, 1H), 7.58 – 7.51 (m, 3H), 7.23 (s, 1H), 6.81 (s, 1H). NMR matched the literature.[2]

5-(dimethylamino)-2-phenyl-4*H*-chromen-4-one (7a)

Flavone **6a** (200 mg, 0.50 mmol, 1 eq), RuPhos-Pd-G3 (45 mg, 0.10 mmol, 0.1 eq), RuPhos (20 mg, 0.10 mmol, 0.1 eq) and cesium carbonate (240 mg, 0.80 mmol, 1.5 eq) was evacuated and subsequently purged with nitrogen for three cycles. Anhydrous toluene (5 mL) was added to solubilize all solids and then dimethylamine (0.40 mL, 0.80 mmol, 1.5 eq) was added. The solution was heated to 110 °C in a heating block and turned from a cloudy brown to clear orange-yellow. After 24 hours of stirring, the solution was concentrated down to give an orange red solid. The crude product was purified via silica gel chromatography with hexanes: ethyl acetate (9:1→ 4:1) to afford pure **5-(dimethylamino)-2-phenyl-4*H*-chromen-4-one** (110 mg, 0.40 mmol, 83%) as a yellow/green solid. ^{1}H-NMR (400 MHz, Chloroform-*d*): δ 7.84 – 7.75 (m, 2H), 7.45 – 7.30 (m, 4H), 6.92 (dd, *J* = 8.3, 1.0 Hz, 1H), 6.74 (dd, *J* = 8.2, 1.2 Hz, 1H), 6.62 (s, 1H), 2.89 (d, *J* = 1.3 Hz, 6H). ^{13}C-NMR (101 MHz, Chloroform-*d*) δ 177.9, 160.3, 159.1, 152.9, 133.1, 131.6, 131.1, 128.9, 125.9, 115.2, 111.6, 108.6, 108.6, 44.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{16}NO_2^+$ 266.1103; Found 266.1093.

5-(dimethylamino)-4-methyl-2-phenylchromenylium (8a)
5-(dimethylamino)-2-phenyl-4*H*-chromen-4-one **7a** (110 mg, 0.40 mmol, 1 eq) was dissolved in THF (5.3 mL, anhydrous) and cooled to 0 °C. MeMgBr (1.4 M in THF/toluene, 0.60 mL, 0.80 mmol, 2 eq) was added dropwise over 30 min turning the solution from yellow to orange brown. The mixture was warmed to room temperature and left to stir overnight, at which point was quenched with 5% fluoroboric acid solution, turning the solution purple, then extracted with dichloromethane (3 x 15 mL), dried over $NaSO_4$, filtered and evaporated. The crude solid was washed with cold ethyl acetate (50 mL) to afford pure **3a** as a purple solid (96 mg, 0.35 mmol, 98%). ^{1}H-NMR (400 MHz, Acetonitrile-d_3): δ 8.36 (dd, J = 8.5, 1.3 Hz, 2H), 8.14 (s, 1H), 8.07 (t, J = 8.3 Hz, 1H), 7.85 – 7.79 (m, 1H), 7.78 – 7.67 (m, 1H), 7.58 (dd, J = 8.3, 1.0 Hz, 1H), 7.36 (dd, J = 8.4, 1.0 Hz, 1H), 3.15 (s, 3H), 2.99 (s, 6H). ^{13}C-NMR (101 MHz, Acetonitrile-d_3) δ 172.6, 168.3, 157.5, 155.5, 139.8, 135.8, 130.0, 129.0, 128.6, 120.3, 116.5, 116.4, 109.3, 44.6, 23.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}NO$ 265.1383; Found 265.1375.

4-((E)-2-((E)-2-chloro-3-(2-((E)-5-(dimethylamino)-2-phenyl-4*H*-chromen-4-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-5-(dimethylamino)-2-phenylchromenylium tetrafluoroborate (5-Flav7, 3)
A Schlenk flask was charged with flavylium **8a** (80 mg, 0.20 mmol, 1 eq), 2,6-di-*tert*-butyl-4-methylpyridine (240 mg, 1.1 mmol, 5 eq), N-[(3-(anilinomethylene)-2-chloro-1-cyclohexen-1-yl)methylene]aniline hydrochloride **9** (25 mg, 0.1 mmol, 0.3 eq) and acetic anhydride (2.5 mL). The dark magenta solution was freeze pump thawed 3x and then heated to 100 °C in an oil bath for 10 min. The reaction was monitored by UV-Vis for the disappearance of the 500 nm peak and formation of 1004 nm peak. Upon completion, the solution was cooled to r.t and dried immediately onto silica. The product was purified via silica gel chromatography twice with dichloromethane: ethanol (99.5: 0.5 → 99.25: 0.75 → 99:1) to afford pure **5-Flav7** as a dark green-brown solid (4 mg, 0.01 mmol, 8%). ^{1}H-NMR (400 MHz, Methylene Chloride-d_2) δ 7.96 – 7.69 (m, 5H), 7.51 (dd, J = 5.5, 1.9 Hz, 9H), 7.19 (s, 5H), 7.04 (s, 3H), 3.09 (s, 12H), 2.40 (s, 4H), 1.72 (d, J = 7.2 Hz, 2H). HRMS (ESI) m/z: $[M]^+$ Calcd for $C_{44}H_{40}ClN_2O_2^+$: 663.2278; Found 663.2264. Absorbance (dichloromethane, λ_{max}/nm) = 1004 nm. Emission (dichloromethane, λ_{max}/nm) = 1038 nm.

4-oxo-2-phenyl-4*H*-chromen-6-yl trifluoromethanesulfonate (6b)
Triflic anhydride (0.42 mL, 2.5 mmol, 4 eq) was added dropwise to a solution of 6-hydroxyflavone (150 mg, 0.60 mmol, 1 eq) in anhydrous pyridine (2.0 mL, 24 mmol, 60 eq) at 0 °C. The solution was warmed to room temperature and left to stir for 1 hr, at which point it was quenched with saturated $NaHCO_3$ (10 mL), extracted with ethyl acetate (3 x 15 mL), dried over $NaSO_4$, filtered and evaporated to give an orange solid. The crude product was purified via silica gel chromatography with hexane: ethyl acetate (9:1) to afford pure **4-oxo-2-phenyl-4*H*-chromen-6-yl trifluoromethanesulfonate** as a white fluffy solid (185 mg, 0.50 mmol, 83%).^{1}H-NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, J = 3.0 Hz, 1H), 7.91 (dd, J = 8.1, 1.7 Hz, 2H), 7.68 (d, J = 9.1 Hz, 1H), 7.63 – 7.50 (m, 4H), 6.84 (s, 1H). ^{13}C-NMR (101 MHz, Chloroform-*d*) δ 176.7, 164.1, 154.9, 146.2, 132.1, 131.1, 129.2, 127.1, 126.4, 125.1, 120.8, 120.3, 118.3, 117.1, 107.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{10}F_3O_5S^+$ 371.0123; Found 371.0120.

6-(dimethylamino)-2-phenyl-4*H*-chromen-4-one (7b)
Flavone **6b** (200 mg, 0.5 mmol, 1 eq), RuPhos-Pd-G3 (50 mg, 0.05 mmol, 0.1 eq), RuPhos (20 mg, 0.05 mmol, 0.1 eq) and cesium carbonate (260 mg, 0.80 mmol, 1.5 eq) was put on a high vac and subsequently purged with nitrogen for three cycles. Toluene (5.0 mL, anhydrous) was added to solubilize all solids and then dimethylamine (0.4 mL, 0.8 mmol, 1.5 eq) was added. The solution was heated to 110 °C in a heating block, turning the solution a deeper orange color. After 24 hours of stirring, the solution was concentrated down to give an orange yellow solid. The crude product was purified via silica gel chromatography with hexanes: ethyl acetate (9:1 → 4:1) to afford pure **6-(dimethylamino)-2-phenyl-4*H*-chromen-4-one** as a yellow/green solid (122 mg, 0.5 mmol, 85%). ^{1}H-NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.89 (m, 2H), 7.53 – 7.49 (m, 3H), 7.46 (d, *J* = 9.1 Hz, 1H), 7.34 (d, *J* = 3.2 Hz, 1H), 7.15 (dd, *J* = 9.2, 3.2 Hz, 1H), 6.78 (s, 1H), 3.03 (s, 6H). ^{13}C-NMR (101 MHz, Chloroform-*d*) δ 178.8, 162.7, 148.9, 148.2, 132.2, 131.2, 128.9, 126.2, 124.5, 119.8, 118.7, 106.6, 105.0, 40.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}NO^+$ 266.1103; Found 265.1095.

6-(dimethylamino)-4-methyl-2-phenylchromenylium (8b)
6-(dimethylamino)-2-phenyl-4*H*-chromen-4-one **7b** (120 mg, 0.5 mmol, 1 eq) was dissolved in THF (5.7 mL, anhydrous) and cooled to 0 °C. MeMgBr (1.0 M in THF, 1.0 mL, 1.0 mmol, 2 eq) was added dropwise over 30 min turning the solution from yellow to orange brown. The solution was warmed to room temperature and left to stir overnight. The following morning the reaction mixture was quenched with 5% fluoroboric acid solution, turning the solution blue-purple, then extracted with dichloromethane (3 x 5 mL), dried over $NaSO_4$, filtered and evaporated to afford pure **8b** as a blue-purple solid (110 mg, 0.4 mmol, 85%). ^{1}H-NMR (400 MHz, Acetonitrile-d_3) δ 8.43 – 8.22 (m, 3H), 8.08 (d, *J* = 9.6 Hz, 1H), 7.82 – 7.77 (m, 2H), 7.70 (ddd, *J* = 8.3, 6.7, 1.4 Hz, 2H), 6.92 (d, *J* = 3.1 Hz, 1H), 3.15 (s, 6H), 2.97 (s, 3H). ^{13}C-NMR (101 MHz, Acetonitrile-d_3) δ 167.5, 150.5, 149.6, 135.5, 130.1, 129.1, 128.7, 127.1, 126.8, 120.3, 117.9, 100.6, 39.8, 20.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}NO^+$ 265.1383; Found 264.1379.

4-((E)-2-((E)-2-chloro-3-(2-((E)-6-(dimethylamino)-2-phenyl-4*H*-chromen-4-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-6-(dimethylamino)-2-phenylchromenylium tetrafluoroborate (6-Flav7, 4)
A Schlenk flask was charged with **8b** (70 mg, 0.2 mmol, 1 eq), 2,6-di-*tert*-butyl-4-methylpyridine (210 mg, 1.0 mmol, 5 eq), *N*-[(3-(anilinomethylene)-2-chloro-1-cyclohexen-1-yl)methylene]aniline hydrochloride **9** (20 mg, 0.06 mmol, 0.3 eq) and n-butanol:toluene (0.4 mL: 1.6 mL). The dark purple solution was freeze pump thawed 3x and then heated to 100 °C in an oil bath for 10 min. The reaction was monitored by UV-Vis for the disappearance of the 500 nm peak and formation of 1048 nm peak. Upon completion, the solution was cooled to r.t. Excess toluene (30 mL) was added at 0 °C and solid precipitate was collected via vacuum filtration and washed with toluene. The crude product was purified via silica gel chromatography twice with dichloromethane: ethanol (99.5: 0.50 → 99.25: 0.75 → 99:) to afford pure **6-Flav7** as a dark blue-black solid (4 mg, 0.01 mmol, 9%). ^{1}H-NMR (400 MHz, Methylene Chloride-d_2) δ 8.54 (d, *J* = 13.7 Hz, 2H), 8.09 – 8.04 (m, 6H), 7.73 (s, 2H), 7.63 – 7.56 (m, 8H), 7.31 (dd, *J* = 9.3, 2.9 Hz, 2H), 7.08 (d, *J* = 13.8 Hz, 2H), 7.04 (d, *J* = 2.9 Hz, 2H), 3.14 (s, 12H), 2.90 (t, *J* = 6.2 Hz, 4H), 2.32 (t, *J* = 7.5 Hz, 2H). HRMS (ESI) m/z: $[M]^+$ Calcd for

$C_{44}H_{40}ClN_2O_2^+$: 663.2278; Found 663.2265. Absorbance (dichloromethane, λ_{max}/nm) = 1048 nm. Emission (dichloromethane, λ_{max}/nm) = 1080 nm.

8-bromo-2-phenyl-4*H*-chromen-4-one (6c)

3'-bromo-2'-hydroxylacetophenone (300 mg, 1.0 mmol, 1 eq) was dissolved in THF (2.8 mL, anhydrous) to give a pale-yellow solution. LiHMDS (1M in THF, 5.6 mL, 5.6 mmol, 4 eq) was added slowly at -78 °C, turning the solution brown. The reaction was left to warm up to r.t. for two hours then cooled back down to -78 °C. Benzoyl chloride (0.10 mL, 1.4 mmol, 1 eq) was added and the reaction was left stirring at -78 °C for 1hr. The reaction was quenched with 2M HCl (5 mL), then extracted into dichloromethane (3 x 15 mL), dried over $NaSO_4$, filtered and evaporated to give a yellow solid. The solid was dissolved in a solution of conc. H_2SO_4 and AcOH (2.8 mL: 2.8 mL) and heated to reflux in an oil bath. After ten minutes, the reaction was cooled to r.t and water was added. Beige solid **8-bromo-2-phenyl-4*H*-chromen-4-one** (110 mg, 0.80 mmol, 60%) was collected via vacuum filtration. ^{1}H-NMR (300 MHz, Chloroform-*d*) δ 8.23 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.16 (dd, *J* = 8.4, 1.4 Hz, 1H), 8.10 – 8.05 (m, 1H), 7.97 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.69 – 7.57 (m, 2H), 7.52 (dd, *J* = 8.3, 6.7 Hz, 1H), 7.35 (t, *J* = 7.9 Hz, 1H), 6.94 (s, 1H). NMR matched literature.[3]

8-(dimethylamino)-2-phenyl-4*H*-chromen-4-one (7c)

8-bromo-2-phenyl-4*H*-chromen-4-one **6c** (200 mg, 0.7 mmol, 1 eq), SPhos-Pd-G3 (60 mg, 0.07 mmol, 0.1 eq), SPhos (30 mg, 0.07 mmol, 0.1 eq) and cesium carbonate (300 mg, 1.0 mmol, 1.5 eq) was put on a high vac and subsequently purged with nitrogen for three cycles. Toluene (4.0 mL, anhydrous) was added to solubilize all solids and then dimethylamine (1.0 mL, 2.0 mmol, 3 eq) was added. The solution was heated to 110 °C in a heating block, turning the solution a cloudy brown/orange color. After 24 hours of stirring, the solution was concentrated down to give an orange yellow solid. The crude product was purified via silica gel chromatography with hexanes: ethyl acetate (9:1 → 4:1) to afford pure **8-(dimethylamino)-2-phenyl-4*H*-chromen-4-one** as a yellow solid (75 mg, 0.30 mmol, 42%). ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.95 (dd, *J* = 6.7, 3.1 Hz, 2H), 7.79 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.57 – 7.47 (m, 3H), 7.28 (t, J = 7.8 Hz, 1H), 7.21 (d, J = 1.6 Hz, 1H), 6.82 (s, 1H), 2.97 (s, 6H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.9, 162.7, 149.4, 142.9, 132.0, 131.5, 129.1, 126.2, 124.9, 121.5, 117.6, 107.3, 43.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{16}NO_2^+$ 266.1103; Found 266.1094.

8-(dimethylamino)-4-methyl-2-phenylchromenylium (8c)

8-(dimethylamino)-2-phenyl-4*H*-chromen-4-one **7c** (50 mg, 0.2 mmol, 1 eq) was dissolved in THF (2.20 mL, anhydrous) and cooled to 0 °C. MeMgBr (1.0 M in THF, 0.3 mL, 0.4 mmol, 2 eq) was added dropwise over 30 min turning the solution from yellow to orange brown. The mixture was warmed to room temperature and left to stir overnight, at which point it was quenched with 5% fluoroboric acid solution, turning the solution purple, and extracted with dichloromethane (3 x 5 mL), dried over $NaSO_4$, filtered and evaporated to afford **8c** as a brown solid that was pushed forward crude due to instability in air. ^{1}H NMR (400 MHz, Acetonitrile-*d*$_3$) δ 8.81 – 8.71 (m, 1H), 8.53 (dd, *J* = 8.6, 1.3 Hz, 2H), 8.47 (dd, *J* = 20.1, 8.0 Hz, 2H), 8.11 (t, *J* = 8.2 Hz, 1H), 8.04 – 7.97 (m, 1H), 7.84 (dd, *J* = 8.6, 7.4 Hz, 2H), 3.48 (s, 6H), 3.19 (d, *J* = 0.8 Hz, 3H). HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{19}NO_2^+$ 265.1383; Found 265.1379.

4-((E)-2-((E)-2-chloro-3-(2-((E)-8-(dimethylamino)-2-phenyl-4*H*-chromen-4-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-8-(dimethylamino)-2-phenylchromenylium tetrafluoroborate (8-Flav7, 5)

A Schlenk flask was charged with **8c** (30 mg, 0.10 mmol, 1 eq), 2,6-di-*tert*-butyl-4-methylpyridine (100 mg, 0.5 mmol, 3 eq), N-[(3-(anilinomethylene)-2-chloro-1-cyclohexen-1-yl)methylene]aniline hydrochloride **9** (7 mg, 0.02 mmol, 0.3 eq) and acetic anhydride (0.50 mL). The magenta solution was freeze pump thawed 3x and then heated to 100 °C in an oil bath for 10 min. The reaction was monitored by UV-Vis for the disappearance of 500 peak and formation of 990 nm peak. Upon completion of the reaction by UV-Vis, the solution was cooled to r.t. Excess toluene (10 mL) was added and solid precipitate was collected via vacuum filtration and washed with toluene. The crude product was unable to be purified and fully characterized due to instability of the compound. HRMS (ESI) m/z: $[M]^+$ Calcd for $C_{44}H_{40}ClN_2O_2^+$: 663.2278; Found 663.2269. Absorbance (dichloromethane, λ_{max}/nm) = 990 nm. Emission (dichloromethane, λ_{max}/nm) = 1015 nm.

6-(azetidin-1-yl)-2-phenyl-4*H*-chromen-4-one (S2)

Flavone **6b** (25 mg, 0.10 mmol, 1 eq), RuPhos-Pd-G3 (60 mg, 0.01 mmol, 0.1 eq), RuPhos (3 mg, 0.01 mmol, 0.1 eq), cesium carbonate (30 mg, 0.10 mmol, 1.5 eq) and azetidine hydrochloride (10 mg, 0.1 mmol, 1.5 eq) was put on a high vac and subsequently purged with nitrogen for three cycles. Toluene (0.30 mL, anhydrous) was added to solubilize all solids. The solution was heated to 110 °C in a heating block, turning the solution a deep brown color. After 24 hours of stirring, the solution was concentrated down to give a dark black solid. The crude product was purified via silica gel chromatography with hexanes: ethyl acetate (9:1 → 4:1) to afford pure **6-(azetidin-1-yl)-2-phenyl-4*H*-chromen-4-one (S2)** as a yellow solid. (10 mg, 0.04 mmol, 52%).^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.93 – 7.87 (m, 2H), 7.50 (dd, *J* = 5.2, 1.8 Hz, 3H), 7.44 (d, *J* = 8.9 Hz, 1H), 7.10 (d, *J* = 2.9 Hz, 1H), 6.83 (dd, *J* = 8.9, 2.9 Hz, 1H), 6.78 (s, 1H), 3.95 (t, *J* = 7.2 Hz, 4H), 2.58 – 2.24 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 178.7, 162.8, 149.6, 149.4, 132.2, 131.3, 128.9, 126.2, 124.5, 118.7, 118.5, 106.6, 104.1, 52.7, 29.7, 16.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{16}NO_2^+$ 278.1103; Found 278.1090

6-(azetidin-1-yl)-4-methyl-2-phenylchromenylium (S3)

6-(azetidin-1-yl)-2-phenyl-4*H*-chromen-4-one **S2** (30 mg, 0.08 mmol, 1 eq) was dissolved in THF (1.0 mL, anhydrous) and cooled to 0 °C. MeMgBr (1.4 M in THF/toluene, 0.2 mL, 0.3 mmol, 2 eq) was added dropwise over 30 min turning the solution from yellow to orange brown. The reaction was warmed to room temperature and left to stir overnight. The reaction was quenched with 5% fluoroboric acid solution, turning the solution blue-purple, then extracted with dichloromethane (3 x 5 mL), dried over $NaSO_4$, filtered and evaporated to afford pure **S3** as a blue-purple solid (20 mg, 0.06 mmol, 70%).^{1}H NMR (400 MHz, Acetonitrile-d_3) δ 8.41 – 8.30 (m, 4H), 8.09 (d, *J* = 9.3 Hz, 1H), 7.81 (d, *J* = 7.4 Hz, 1H), 7.72 (t, *J* = 7.7 Hz, 2H), 7.44 (dd, *J* = 9.3, 2.8 Hz, 1H), 6.74 (d, *J* = 2.8 Hz, 1H), 4.20 – 4.02 (m, 4H), 2.96 (d, *J* = 0.8 Hz, 3H), 2.48 (p, J = 7.4 Hz, 2H). ^{13}C-NMR (101 MHz, Acetonitrile-d_3) δ 167.8, 167.3, 151.3, 150.0, 135.5, 130.1, 129.2, 128.7, 126.9, 125.7, 120.5, 118.1, 99.3, 51.9, 20.6, 16.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{19}NO^+$ 277.1383; Found 277.1381

6-(azetidin-1-yl)-4-((E)-2-((E)-3-(2-((E)-6-(azetidin-1-yl)-2-phenyl-4*H*-chromen-4-ylidene)ethylidene)-2-chlorocyclohex-1-en-1-yl)vinyl)-2-phenylchromenylium tetrafluoroborate (Azet-6-Flav7, 11)

A Schlenk flask was charged with **S3** (80 mg, 0.2 mmol, 1 eq), 2,6-di-*tert*-butyl-4-methylpyridine (210 mg, 1.0 mmol, 5 eq), *N*-[(3-(anilinomethylene)-2-chloro-1-cyclohexen-1-yl)methylene]aniline hydrochloride **9** (20 mg, 0.07 mmol, 0.3 eq) and n-butanol:toluene (0.4 mL: 1.6 mL). The dark purple solution was freeze pump thawed 3x and then heated to 100 °C in an oil bath for 10 min. The reaction was monitored by UV-Vis for the disappearance of the 500 nm peak and formation of 1039 nm peak. Upon completion, the solution was cooled to r.t. Excess toluene (30 mL) was added at 0 °C and solid precipitate was collected via vacuum filtration and washed with toluene. The crude product was purified via silica gel chromatography twice with dichloromethane: ethanol (99.5: 0.50 → 99.25: 0.75 → 99:1) to afford pure **Azet-6-Flav7** as a dark green-black solid (3 mg, 0.004 mmol, 6%).^{1}H-NMR (400 MHz, Methylene Chloride-d_2) δ 8.49 (d, J = 14.0 Hz, 2H), 8.08 – 8.01 (m, 6H), 7.69 (s, 2H), 7.51 (d, J = 8.8 Hz, 4H), 7.22 – 7.15 (m, 4H), 7.11 (d, J = 13.5 Hz, 4H), 3.76 (t, J = 6.0 Hz, 8H), 2.89 (s, 4H), 2.32 (t, J = 7.5 Hz, 4H), 1.82 (d, J = 6.6 Hz, 2H). HRMS (ESI) m/z: $[M]^+$ Calcd for $C_{46}H_{40}ClN_2O_2^+$: 687.2773; Found 687.2765. Absorbance (dichloromethane, λ_{max}/nm) = 1039 nm. Emission (dichloromethane, λ_{max}/nm) = 1080 nm.

Computational Methods:

Computational Details

The conformations of **Flav7** dyes (**1**, **3–5)** were searched using the OPLS3e force field potential implemented in the Schrödinger release 2019-2 program suite.[4] The conformational search used Mixed torsional/Low-mode sampling method and removed the redundant conformers based on the maximum atom deviation of 1 Å. The probability of a torsion rotation and molecule translation was set to 0.5 and the distance range of the low-mode move was 3.0–12.0. For each rotatable bond, the conformers were further searched in 100 steps. The 10 lowest conformers were found after 10,000 iterations within an energy window of 47.8 kcal mol^{-1} (200 kJ mol^{-1}). The lowest 10 conformers were optimized to the ground-state minimum with M06-2X/6-31+G(d,p). The polarizable continuum model (PCM) was utilized to include the solvent effect of dichloromethane. All stationary points were confirmed by the computations of the Hessian matrix that all vibrational frequencies are positive and real. The conformers were sorted according to the calculated Gibbs free energy at 298.15 K. The geometry optimization and thermochemistry calculations were done by Gaussian16. B01.[5] The global minimum geometries were used for excited-state calculations. The vertical excitation energies were computed using CIS(D)/cc-pVDZ. In order to speed up the calculations, the resolution of identity (RI) approximation RIJCOSX (RI for Coulomb integral and COSX numerical integration for HF-exchange) was used together with the cc-pVDZ/C auxiliary basis sets. The CIS(D) single point calculations were performed by ORCA 4.2.1 program package.[6]

Cartesian coordinates for optimized structures and calculated thermodynamics energies with the first 10 vibrational frequencies.

IR-27-A

C	0.000004	-4.008458	0.965780
C	-1.251704	-3.434080	0.315814
C	1.251658	-3.434065	0.315736
H	-2.135549	-3.793980	0.848997
H	1.335146	-3.792390	-0.719546
C	-1.247269	-1.918994	0.325379
C	1.247191	-1.918989	0.325283
C	-0.000012	-1.261953	0.372243
H	0.000027	-3.759949	2.033555
Cl	-0.000032	0.491933	0.447708
H	-1.335248	-3.792398	-0.719463
H	0.000010	-5.098310	0.882578
H	2.135550	-3.793946	0.848858
C	-2.446041	-1.205811	0.238235
H	-2.375268	-0.125124	0.265503
C	-3.712415	-1.777798	0.092814
H	-3.782504	-2.855941	0.038720
C	2.446005	-1.205806	0.238061
H	2.375222	-0.125119	0.265273
C	3.712311	-1.777823	0.092587
H	3.782374	-2.855960	0.038381
C	-4.900277	-1.042328	-0.003081
C	-4.941615	0.383627	0.033589
C	-6.111854	1.077424	-0.053505

O	-7.292412	0.452487	-0.195704
C	-7.347705	-0.907391	-0.257213
C	-6.194003	-1.701396	-0.161117
C	-6.374288	-3.099777	-0.229791
C	-7.631182	-3.651855	-0.384792
C	-8.762372	-2.824142	-0.477737
C	-8.624576	-1.449954	-0.413917
H	-4.030291	0.959355	0.107276
H	-9.474833	-0.780466	-0.480222
H	-9.747664	-3.260922	-0.599046
H	-7.743274	-4.729096	-0.434341
H	-5.518336	-3.759665	-0.160795
C	4.900242	-1.042364	-0.003282
C	4.941603	0.383568	0.033722
C	6.111864	1.077359	-0.053365
O	7.292361	0.452378	-0.195823
C	7.347621	-0.907460	-0.257585
C	6.193890	-1.701458	-0.161562
C	6.374117	-3.099836	-0.230553
C	7.630976	-3.651922	-0.385762
C	8.762194	-2.824226	-0.478600
C	8.624458	-1.450053	-0.414484
H	4.030294	0.959274	0.107696
H	9.474731	-0.780574	-0.480706
H	9.747465	-3.261008	-0.600065
H	7.743009	-4.729158	-0.435556
H	5.518149	-3.759711	-0.161655
C	-6.240143	2.542485	-0.028082
C	-7.369246	3.153964	-0.590886
C	-5.241380	3.336516	0.553148
C	-7.485279	4.540615	-0.587651
C	-5.365226	4.721552	0.556060
C	-6.484604	5.327026	-0.016984
H	-8.145399	2.543131	-1.038478
H	-4.380476	2.876943	1.027607
H	-8.357722	5.007227	-1.032752
H	-4.591845	5.328314	1.014911
H	-6.578764	6.408056	-0.013048
C	6.240255	2.542395	-0.027595
C	7.369425	3.153928	-0.590216
C	5.241530	3.336359	0.553796
C	7.485556	4.540566	-0.586644
C	5.365485	4.721387	0.557053
C	6.484923	5.326914	-0.015811
H	8.145544	2.543153	-1.037943
H	4.380572	2.876752	1.028115
H	8.358043	5.007220	-1.031612
H	4.592133	5.328089	1.016032
H	6.579167	6.407935	-0.011609

	Energies (Hartree)
E(M06-2X)	-2152.12197769
E(M06-2X)+ZPE	-2151.53294900
E(M06-2X)+U	-2151.49791000
E(M06-2X)+H	-2151.49696500
E(M06-2X)+G	-2151.60589200
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	8.0881
2	12.6565
3	13.1359
4	21.7115
5	27.6595
6	33.7767
7	35.2910
8	47.4242
9	56.4398
10	57.0378

IR-27-B

C	-0.000489	-3.976896	1.039103
C	-1.255931	-3.420309	0.381106
C	1.247446	-3.422313	0.364869
H	-2.136316	-3.759062	0.933680
H	1.320730	-3.805538	-0.662269
C	-1.248387	-1.905641	0.339030
C	1.246047	-1.907449	0.338709
C	-0.001129	-1.248414	0.365482
H	-0.002043	-5.068686	0.987035
Cl	-0.000218	0.506874	0.388180
H	-1.349537	-3.812959	-0.640790
H	0.007059	-3.698196	2.099358
H	2.134657	-3.771955	0.899062
C	-2.447120	-1.195236	0.226359
H	-2.376757	-0.114138	0.213932
C	-3.712293	-1.772663	0.095401
H	-3.780465	-2.851860	0.064607
C	2.445850	-1.197902	0.241743
H	2.376708	-0.116744	0.248522
C	3.712005	-1.774290	0.109148
H	3.779678	-2.853046	0.065316
C	-4.900428	-1.040952	-0.026163
C	-4.947702	0.384188	0.024401
C	-6.115156	1.075833	-0.108421
O	-7.290649	0.447113	-0.273456
C	-7.344529	-0.913649	-0.309419
C	-6.189804	-1.704255	-0.198855

C	-6.366135	-3.103593	-0.258993
C	-7.620650	-3.659661	-0.418551
C	-8.753182	-2.835294	-0.524764
C	-8.619010	-1.460320	-0.471490
H	-4.049380	0.957910	0.201222
H	-9.469999	-0.793343	-0.552129
H	-9.736522	-3.275317	-0.650129
H	-7.729851	-4.737451	-0.462223
H	-5.509032	-3.760913	-0.180108
C	4.901780	-1.042734	0.011406
C	4.947840	0.383179	0.050813
C	6.120252	1.073299	-0.034042
O	7.298897	0.444832	-0.178045
C	7.349604	-0.915088	-0.243274
C	6.193403	-1.705615	-0.148744
C	6.368906	-3.104294	-0.223062
C	7.623878	-3.660087	-0.380591
C	8.757802	-2.835870	-0.470876
C	8.624566	-1.461446	-0.402385
H	4.038543	0.961425	0.129419
H	9.477009	-0.794574	-0.467030
H	9.741582	-3.275481	-0.594230
H	7.732228	-4.737494	-0.434660
H	5.510620	-3.761535	-0.157486
C	-6.251141	2.539889	-0.069825
C	-7.486795	3.117726	0.253972
C	-5.155176	3.366561	-0.355382
C	-7.616032	4.502076	0.308644
C	-5.291877	4.749328	-0.301760
C	-6.520469	5.320350	0.033365
H	-8.337661	2.481880	0.472097
H	-4.202696	2.936111	-0.646340
H	-8.573247	4.941969	0.567855
H	-4.441053	5.381868	-0.531659
H	-6.624407	6.399718	0.073808
C	6.253809	2.537829	-0.002305
C	7.385820	3.147580	-0.561115
C	5.257564	3.333084	0.581589
C	7.507271	4.533747	-0.551249
C	5.386820	4.717601	0.591162
C	6.509151	5.321400	0.022153
H	8.160122	2.535828	-1.010648
H	4.394397	2.874767	1.053124
H	8.382045	4.999011	-0.993179
H	4.615393	5.325174	1.052232
H	6.607635	6.402012	0.031449

	Energies (Hartree)
E(M06-2X)	-2152.12198105
E(M06-2X)+ZPE	-2151.53292500
E(M06-2X)+U	-2151.49787700
E(M06-2X)+H	-2151.49693300
E(M06-2X)+G	-2151.60623400
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	7.2853
2	11.4128
3	13.0340
4	20.4640
5	26.9581
6	32.0415
7	36.5838
8	44.9773
9	55.5552
10	56.2697

IR-27-C (Global Minimum)

C	0.000084	-3.951233	1.100492
C	-1.251816	-3.409879	0.423091
C	1.251625	-3.409961	0.422350
H	-1.335619	-3.819774	-0.592911
H	1.334652	-3.819640	-0.593806
C	-1.247206	-1.896125	0.356285
C	1.247159	-1.896196	0.355908
C	0.000006	-1.237627	0.367704
H	0.000028	-5.043887	1.071473
Cl	0.000037	0.517741	0.350659
H	-2.135534	-3.742049	0.974145
H	0.000420	-3.650284	2.154665
H	2.135654	-3.742410	0.972726
C	-2.446814	-1.188980	0.236859
H	-2.378245	-0.107972	0.211418
C	-3.711582	-1.769760	0.113365
H	-3.777629	-2.849273	0.089211
C	2.446801	-1.189083	0.236480
H	2.378259	-0.108065	0.211364
C	3.711520	-1.769851	0.112639
H	3.777556	-2.849355	0.088141
C	-4.901038	-1.041232	-0.010722
C	-4.952143	0.383908	0.041567
C	-6.121392	1.072553	-0.089978
O	-7.295236	0.440989	-0.256973
C	-7.345238	-0.919883	-0.296488
C	-6.188529	-1.707609	-0.186489
C	-6.360768	-3.107188	-0.251793
C	-7.613523	-3.666341	-0.414667

C	-8.748256	-2.844869	-0.519382
C	-8.617969	-1.469676	-0.461725
H	-4.055717	0.959532	0.221855
H	-9.470721	-0.804845	-0.541489
H	-9.730207	-3.287236	-0.647385
H	-7.719532	-4.744276	-0.462474
H	-5.501740	-3.762283	-0.175141
C	4.900991	-1.041296	-0.011309
C	4.952122	0.383812	0.041586
C	6.121398	1.072493	-0.089580
O	7.295222	0.440945	-0.256796
C	7.345172	-0.919895	-0.297077
C	6.188430	-1.707638	-0.187516
C	6.360594	-3.107189	-0.253668
C	7.613321	-3.666302	-0.416867
C	8.748097	-2.844817	-0.521075
C	8.617880	-1.469655	-0.462622
H	4.055694	0.959353	0.222119
H	9.470669	-0.804825	-0.541996
H	9.730027	-3.287158	-0.649329
H	7.719285	-4.744211	-0.465332
H	5.501526	-3.762284	-0.177460
C	-6.261690	2.536101	-0.046421
C	-7.499184	3.109173	0.278785
C	-5.167922	3.367036	-0.327971
C	-7.632415	4.492934	0.338821
C	-5.308570	4.749188	-0.268922
C	-6.538999	5.315412	0.067612
H	-8.348363	2.470065	0.493930
H	-4.213983	2.940411	-0.619808
H	-8.591050	4.929070	0.599139
H	-4.459350	5.385061	-0.495558
H	-6.646002	6.394309	0.112376
C	6.261777	2.536008	-0.045336
C	7.499338	3.108864	0.280001
C	5.168023	3.367143	-0.326367
C	7.632653	4.492588	0.340672
C	5.308755	4.749258	-0.266682
C	6.539254	5.315257	0.069976
H	8.348509	2.469617	0.494759
H	4.214019	2.940730	-0.618297
H	8.591343	4.928545	0.601084
H	4.459542	5.385282	-0.492917
H	6.646324	6.394126	0.115235

	Energies (Hartree)
E(M06-2X)	-2152.12198024
E(M06-2X)+ZPE	-2151.53288300
E(M06-2X)+U	-2151.49784300
E(M06-2X)+H	-2151.49689900

E(M06-2X)+G	-2151.60632700
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	6.3769
2	10.4480
3	14.1495
4	21.5123
5	25.2992
6	32.7785
7	36.6316
8	43.4580
9	55.3467
10	55.6913

5-Flav7-A (Global Minimum)

C	-1.245789	-1.342661	0.212040
C	-1.257151	-2.831848	-0.069522
C	-0.001401	-3.518219	0.450332
C	1.244942	-2.833884	-0.094914
C	1.249775	-1.348334	0.205592
C	-0.002291	-0.709688	0.372666
Cl	0.003202	1.002599	0.768876
C	-2.451556	-0.624373	0.257589
C	2.448473	-0.637965	0.257440
C	3.712082	-1.195632	0.021671
C	-3.706066	-1.183202	0.035632
C	4.909230	-0.470954	0.008244
C	-4.913124	-0.457481	0.013478
C	-4.926168	0.968053	0.108505
C	-6.044515	1.697354	-0.151708
O	-7.177405	1.100373	-0.552279
C	-7.275813	-0.258068	-0.596236
C	-6.208579	-1.094570	-0.203103
C	6.207916	-1.084527	-0.283102
C	7.254954	-0.218922	-0.661675
O	7.148960	1.136729	-0.553117
C	6.027451	1.700045	-0.068611
C	4.927190	0.951261	0.195215
C	6.497494	-2.492382	-0.316468
C	-6.483288	-2.507114	-0.155595
C	6.132421	3.161530	0.070355
C	5.259565	3.861175	0.915438
C	5.356811	5.243640	1.030439
C	6.325944	5.941571	0.307882
C	7.202699	5.248892	-0.526563
C	7.111989	3.864876	-0.643983
C	-6.151395	3.162952	-0.097578
C	-5.241746	3.914459	0.659823
C	-5.342166	5.300856	0.695847

C	-6.350082	5.949951	-0.019028
C	-7.262773	5.205725	-0.766317
C	-7.169474	3.817807	-0.804493
H	-1.356767	-2.998005	-1.151066
H	-2.138463	-3.279446	0.399145
H	-0.005599	-4.573874	0.166358
H	0.009758	-3.472096	1.545830
H	2.135166	-3.294131	0.342192
H	1.310965	-2.986311	-1.181138
H	2.379966	0.419403	0.482227
H	-3.781774	-2.243779	-0.156945
H	-4.015875	1.510504	0.317664
H	4.029471	1.473560	0.491857
H	4.519631	3.327411	1.503075
H	4.681790	5.775640	1.692512
H	6.400434	7.020210	0.400110
H	7.959218	5.786559	-1.088526
H	7.792208	3.327703	-1.295525
H	-4.470502	3.419786	1.241293
H	-4.638884	5.874651	1.289933
H	-6.426365	7.031965	0.011270
H	-8.048688	5.706351	-1.321936
H	-7.876929	3.239866	-1.388612
C	-8.670125	-2.101313	-1.151214
H	-9.602248	-2.504110	-1.533275
C	8.661041	-2.017587	-1.331773
H	9.589487	-2.390224	-1.751539
C	8.466274	-0.656410	-1.192647
H	9.212050	0.074668	-1.481183
C	-8.492903	-0.732018	-1.077776
H	-9.255051	-0.024770	-1.381967
C	7.697804	-2.925073	-0.884063
H	7.913836	-3.984048	-0.939547
C	-7.688093	-2.977654	-0.682970
H	-7.894910	-4.039858	-0.683570
N	5.585389	-3.412993	0.214024
N	-5.557041	-3.387774	0.405502
C	5.745057	-4.810261	-0.156494
H	4.848290	-5.348628	0.159558
H	5.841983	-4.904596	-1.239661
H	6.614376	-5.282733	0.327184
C	5.288704	-3.270238	1.641451
H	6.053415	-3.780202	2.245408
H	4.314130	-3.717194	1.859620
H	5.259190	-2.220859	1.930905
C	-5.189117	-3.154551	1.804206
H	-5.884557	-3.681515	2.472794
H	-4.176102	-3.526172	1.987619
H	-5.215917	-2.092716	2.043654
C	-5.707719	-4.806078	0.121147
H	-5.828621	-4.965252	-0.951882

H	-4.796858	-5.314405	0.446256
H	-6.559482	-5.257121	0.653178
H	-2.380023	0.434315	0.475955
H	3.784047	-2.251027	-0.198574

	Energies (Hartree)
E(M06-2X)	-2419.94066256
E(M06-2X)+ZPE	-2419.20426100
E(M06-2X)+U	-2419.16115300
E(M06-2X)+H	-2419.16020900
E(M06-2X)+G	-2419.28635900
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	6.7374
2	8.7196
3	14.1953
4	20.4989
5	25.1626
6	27.5456
7	31.6595
8	36.5387
9	39.0069
10	47.7465

5-Flav7-B

C	1.246385	-1.353931	0.176080
C	1.224052	-2.833623	-0.151198
C	-0.000070	-3.522207	0.437775
C	-1.274911	-2.836907	-0.034333
C	-1.249188	-1.344576	0.227941
C	-0.014415	-0.713485	0.366998
Cl	0.003311	0.999328	0.761796
C	2.438477	-0.651435	0.226402
C	-2.464079	-0.620053	0.274896
C	-3.711664	-1.178335	0.076767
C	3.706478	-1.208334	-0.047705
C	-4.924427	-0.441968	0.039704
C	4.896556	-0.491288	-0.040754
C	4.935334	0.910331	0.294178
C	6.005136	1.687882	0.008705
O	7.097884	1.175601	-0.595627
C	7.216979	-0.172975	-0.777498
C	6.191139	-1.071940	-0.425657
C	-6.221937	-1.086515	-0.068655
C	-7.303775	-0.281536	-0.493372
O	-7.198781	1.074363	-0.557389
C	-6.049303	1.695890	-0.269097
C	-4.919100	0.980126	-0.002310
C	-6.492928	-2.491106	0.109326

C	6.489934	-2.469425	-0.561708
C	-6.144862	3.159920	-0.340823
C	-5.187945	3.963827	0.295007
C	-5.278282	5.348898	0.215707
C	-6.322165	5.943510	-0.494765
C	-7.280899	5.147498	-1.121790
C	-7.198414	3.760924	-1.044082
C	6.130686	3.129470	0.285181
C	4.992510	3.925639	0.475062
C	5.125722	5.280772	0.758409
C	6.393181	5.858330	0.848880
C	7.528237	5.073511	0.648613
C	7.400816	3.716567	0.364335
H	2.131436	-3.305394	0.234336
H	1.235776	-2.965689	-1.242145
H	0.051281	-3.478922	1.532223
H	-0.013857	-4.577099	0.151272
H	-2.135599	-3.275926	0.479572
H	-1.425232	-3.015832	-1.107876
H	-2.389189	0.441122	0.481878
H	3.766917	-2.250186	-0.327850
H	4.089698	1.376349	0.779550
H	-3.992397	1.526835	0.092574
H	-4.387255	3.513313	0.872225
H	-4.538703	5.964681	0.716172
H	-6.390416	7.024775	-0.554947
H	-8.094032	5.606791	-1.673722
H	-7.941239	3.142301	-1.535211
H	4.000674	3.496128	0.378907
H	4.238355	5.889311	0.897978
H	6.494099	6.916393	1.067784
H	8.516186	5.517258	0.714945
H	8.284097	3.106098	0.212511
C	8.623388	-1.911474	-1.597105
H	9.543382	-2.246152	-2.064803
C	-8.703891	-2.163523	-0.860499
H	-9.645262	-2.595918	-1.182854
C	-8.532604	-0.790808	-0.898413
H	-9.307474	-0.111906	-1.232896
C	8.416939	-0.564122	-1.368818
H	9.145341	0.192648	-1.635192
C	-7.708967	-3.001926	-0.352984
H	-7.915635	-4.060307	-0.263251
C	7.679989	-2.854818	-1.183009
H	7.901008	-3.906281	-1.313373
N	-5.558455	-3.316311	0.723816
N	5.592601	-3.432221	-0.074780
C	-5.099894	-2.945202	2.064606
H	-4.053465	-3.236798	2.198316
H	-5.708349	-3.456520	2.822786
H	-5.182957	-1.871157	2.222347

C	-5.711170	-4.755608	0.580372
H	-6.544501	-5.153050	1.179369
H	-5.863903	-5.016905	-0.468222
H	-4.788441	-5.228675	0.924112
C	5.750240	-4.797706	-0.549061
H	5.818705	-4.813180	-1.638473
H	6.634790	-5.298451	-0.124422
H	4.865386	-5.364614	-0.249174
C	5.349626	-3.396764	1.369099
H	4.391121	-3.875983	1.590752
H	6.144744	-3.933596	1.907572
H	5.313265	-2.370894	1.732861
H	2.379957	0.403206	0.467749
H	-3.797945	-2.245387	-0.075495

	Energies (Hartree)
E(M06-2X)	-2419.94066842
E(M06-2X)+ZPE	-2419.20399400
E(M06-2X)+U	-2419.16099000
E(M06-2X)+H	-2419.16004600
E(M06-2X)+G	-2419.28555300
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	5.3820
2	12.7412
3	14.7075
4	21.9387
5	24.4691
6	29.2008
7	31.2763
8	36.4881
9	39.1389
10	47.8937

5-Flav7-C

C	1.259006	-1.241783	-0.455679
C	1.249575	-2.750470	-0.599446
C	0.006097	-3.238406	-1.331729
C	-1.252935	-2.749888	-0.628394
C	-1.236676	-1.250424	-0.409640
C	-0.012410	-0.591256	-0.386051
Cl	-0.012438	1.158201	-0.215809
C	2.445163	-0.541125	-0.342380
C	-2.459539	-0.563614	-0.201289
C	-3.686813	-1.182879	-0.091592
C	3.727505	-1.136697	-0.299675
C	-4.918139	-0.493549	0.083589
C	4.912914	-0.429670	-0.157576

C	4.932156	1.012186	-0.101859
C	6.008722	1.700912	0.339661
O	7.130437	1.062716	0.737211
C	7.264238	-0.282586	0.538332
C	6.227567	-1.071365	0.002291
C	-6.164550	-1.181959	0.362793
C	-7.359634	-0.459835	0.136828
O	-7.346019	0.882020	-0.091480
C	-6.197509	1.562413	-0.170568
C	-4.999070	0.910950	-0.117974
C	-6.307559	-2.565313	0.743682
C	6.539782	-2.448332	-0.254341
C	-6.386069	3.003934	-0.377619
C	-5.344100	3.900667	-0.100955
C	-5.524792	5.263366	-0.308655
C	-6.743568	5.742995	-0.791096
C	-7.785491	4.855059	-1.059646
C	-7.612854	3.490530	-0.851225
C	6.114690	3.165747	0.457633
C	7.376822	3.774296	0.483407
C	7.484396	5.159720	0.570785
C	6.337602	5.949828	0.640824
C	5.078506	5.347434	0.628498
C	4.965137	3.963960	0.541022
H	1.298860	-3.212043	0.396801
H	2.143495	-3.069217	-1.141252
H	0.004538	-4.330217	-1.386897
H	0.017776	-2.857015	-2.359608
H	-2.130921	-3.012706	-1.225326
H	-1.363682	-3.258257	0.340135
H	-2.398921	0.510836	-0.070794
H	3.800517	-2.214317	-0.328790
H	4.066814	1.579052	-0.414086
H	-4.107906	1.484913	-0.325769
H	-4.401514	3.541748	0.299071
H	-4.717106	5.952262	-0.085885
H	-6.881825	6.807083	-0.952547
H	-8.734019	5.225314	-1.433821
H	-8.421083	2.799865	-1.064317
H	8.269069	3.160727	0.425081
H	8.466065	5.621883	0.582676
H	6.423234	7.029298	0.711591
H	4.182694	5.955641	0.698391
H	3.980992	3.506936	0.561895
C	8.720899	-2.150777	0.789724
H	9.665144	-2.581879	1.105472
C	-8.702205	-2.408696	0.321521
H	-9.668884	-2.900066	0.288104
C	-8.620286	-1.044605	0.102083
H	-9.488839	-0.429399	-0.098615
C	8.494436	-0.796508	0.945299

H	9.230197	-0.125804	1.373241
C	-7.570162	-3.157457	0.649643
H	-7.691417	-4.204253	0.895385
C	7.762296	-2.964290	0.181257
H	7.994165	-4.008007	0.013049
N	-5.209465	-3.291661	1.185973
N	5.622129	-3.264205	-0.937204
C	-4.455255	-2.767244	2.327073
H	-3.393348	-3.008162	2.217817
H	-4.826790	-3.217066	3.257730
H	-4.559851	-1.686010	2.400928
C	-5.312137	-4.742162	1.222163
H	-4.308351	-5.148145	1.366734
H	-5.704405	-5.117345	0.275328
H	-5.947772	-5.098914	2.046469
C	5.327450	-2.856957	-2.312951
H	4.378047	-3.300302	-2.628263
H	5.243189	-1.773622	-2.388594
H	6.119636	-3.198088	-2.996174
C	5.809494	-4.703392	-0.844388
H	4.914520	-5.188161	-1.242103
H	5.930168	-5.001311	0.198895
H	6.675375	-5.061167	-1.423914
H	2.375514	0.536139	-0.250687
H	-3.742127	-2.263009	-0.116134

	Energies (Hartree)
E(M06-2X)	-2419.94075785
E(M06-2X)+ZPE	-2419.20392300
E(M06-2X)+U	-2419.16096900
E(M06-2X)+H	-2419.16002500
E(M06-2X)+G	-2419.28526600
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	6.8042
2	11.3263
3	14.1169
4	17.2364
5	25.7601
6	30.1513
7	36.8751
8	38.6557
9	41.3806
10	48.4327

5-Flav7-D

C	-1.253209	-1.266180	-0.376234
C	-1.259602	-2.781592	-0.405764
C	0.007811	-3.341248	-1.037803
C	1.241751	-2.794594	-0.332394
C	1.240724	-1.279654	-0.283591
C	0.004241	-0.616858	-0.348196
Cl	0.012931	1.140449	-0.355182
C	-2.449651	-0.551930	-0.327366
C	2.447906	-0.578014	-0.134324
C	3.691048	-1.180587	0.032114
C	-3.720578	-1.139336	-0.273625
C	4.908948	-0.480533	0.142178
C	-4.921197	-0.428087	-0.171958
C	-4.940409	1.002673	-0.069885
C	-6.056371	1.684878	0.290594
O	-7.194101	1.037376	0.601473
C	-7.296279	-0.311805	0.426154
C	-6.227632	-1.084288	-0.073998
C	6.189523	-1.150847	0.347038
C	7.354995	-0.407328	0.058549
O	7.312436	0.934518	-0.174772
C	6.147160	1.599489	-0.167990
C	4.967058	0.935774	-0.038489
C	6.382854	-2.529880	0.713543
C	-6.508444	-2.468190	-0.344509
C	6.306593	3.047295	-0.370299
C	5.280053	3.932440	-0.011749
C	5.433548	5.298972	-0.217662
C	6.610969	5.795866	-0.778931
C	7.638449	4.919957	-1.128638
C	7.492125	3.551429	-0.922996
C	-6.164955	3.144563	0.445357
C	-5.259463	3.998499	-0.200114
C	-5.359914	5.375821	-0.036506
C	-6.364647	5.915639	0.768090
C	-7.273814	5.070760	1.404110
C	-7.179933	3.691391	1.242369
H	-2.132245	-3.129123	-0.965512
H	-1.367596	-3.165642	0.618098
H	0.040834	-3.058045	-2.096497
H	0.001312	-4.433420	-0.990524
H	2.140982	-3.137321	-0.851289
H	1.293940	-3.191534	0.691355
H	2.382946	0.503258	-0.114974
H	-3.796962	-2.217044	-0.278211
H	-4.034220	1.571860	-0.216504
H	4.058883	1.509229	-0.152089
H	4.370714	3.561295	0.449447
H	4.637236	5.977724	0.068681
H	6.728296	6.862847	-0.937998

H	8.555865	5.302178	-1.563672
H	8.289773	2.870661	-1.198590
H	-4.490714	3.593116	-0.849990
H	-4.659135	6.029201	-0.545467
H	-6.441376	6.990796	0.893360
H	-8.058053	5.485590	2.028653
H	-7.885385	3.035192	1.739889
C	-8.716521	-2.207150	0.652062
H	-9.659482	-2.656175	0.945816
C	8.753408	-2.325192	0.187118
H	9.728262	-2.794935	0.109537
C	8.626020	-0.966664	-0.036263
H	9.468081	-0.331750	-0.284020
C	-8.526246	-0.846288	0.802577
H	-9.289614	-0.188805	1.201145
C	7.652677	-3.094356	0.571378
H	7.805503	-4.138084	0.812877
C	-7.729038	-3.005815	0.070414
H	-7.940116	-4.053178	-0.101806
N	5.315652	-3.288029	1.197054
N	-5.568700	-3.261396	-1.012267
C	4.655829	-2.799673	2.410450
H	5.161054	-3.195713	3.302725
H	4.675656	-1.711880	2.454723
H	3.612339	-3.128589	2.420735
C	5.460076	-4.735125	1.212150
H	6.147253	-5.084727	1.998014
H	4.476543	-5.170699	1.403612
H	5.812953	-5.089713	0.242021
C	-5.735234	-4.704677	-0.950403
H	-4.821997	-5.167134	-1.332566
H	-5.878735	-5.024328	0.083413
H	-6.579289	-5.062789	-1.560363
C	-5.191905	-2.823388	-2.358384
H	-5.181520	-1.736693	-2.426489
H	-4.191180	-3.194932	-2.600097
H	-5.902217	-3.214760	-3.100987
H	-2.374384	0.528683	-0.317580
H	3.748265	-2.258440	0.083073

	Energies (Hartree)
E(M06-2X)	-2419.94069164
E(M06-2X)+ZPE	-2419.20412700
E(M06-2X)+U	-2419.16108500
E(M06-2X)+H	-2419.16014100
E(M06-2X)+G	-2419.28537000
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	8.0170
2	12.3712

3	14.0882
4	19.0158
5	26.9956
6	28.2504
7	36.1168
8	38.7086
9	42.8228
10	47.3794

6-Flav7-A (Global Minimum)

C	1.245082	-1.128467	0.438670
C	1.245159	-2.643171	0.475350
C	-0.006800	-3.192978	1.146144
C	-1.258879	-2.637821	0.480256
C	-1.249815	-1.123337	0.431850
C	-0.001148	-0.469856	0.458778
Cl	0.002412	1.287727	0.469585
C	2.448387	-0.422644	0.337082
C	-2.448776	-0.412782	0.310852
C	-3.714056	-0.987705	0.184782
C	3.711262	-1.002249	0.206383
C	-4.904463	-0.257019	0.047773
C	4.907067	-0.275717	0.099742
C	4.957175	1.147537	0.138567
C	6.130529	1.839713	0.040916
O	7.300842	1.210491	-0.116011
C	7.342855	-0.151374	-0.179225
C	6.194314	-0.947064	-0.069710
C	-6.199214	-0.924884	-0.070128
C	-7.341649	-0.126057	-0.214607
O	-7.285966	1.236469	-0.238700
C	-6.108441	1.862799	-0.133227
C	-4.940923	1.166198	-0.001039
C	-6.368404	-2.321241	-0.043420
C	-7.631157	-2.917970	-0.168607
C	7.604644	-2.943190	-0.311849
C	6.348251	-2.343433	-0.144215
C	-6.226141	3.328278	-0.199268
C	-7.357252	3.912252	-0.786607
C	-7.465230	5.297281	-0.867408
C	-6.453301	6.111080	-0.358150
C	-5.330922	5.534107	0.237718
C	-5.215901	4.150528	0.319268
C	6.262751	3.305160	0.071884
C	5.273481	4.099715	0.668030
C	5.402124	5.484558	0.677636
C	6.517295	6.089838	0.096514
C	7.508664	5.302884	-0.489553
C	7.387219	3.916649	-0.499936
H	1.324745	-3.034419	-0.548480

H	2.129291	-2.989332	1.017374
H	-0.003720	-2.908832	2.205042
H	-0.009509	-4.285195	1.099959
H	-2.141910	-2.973861	1.030659
H	-1.348975	-3.035560	-0.540147
H	4.049104	1.726238	0.228587
H	-4.025976	1.739561	0.038403
H	-5.498739	-2.949204	0.079269
H	5.471356	-2.969189	-0.072802
H	-8.142173	3.280139	-1.187020
H	-8.340122	5.741245	-1.330649
H	-6.540718	7.190885	-0.420193
H	-4.547673	6.162484	0.648353
H	-4.351264	3.715681	0.809788
H	4.415698	3.640470	1.148471
H	4.635516	6.091138	1.148085
H	6.615365	7.170504	0.105766
H	8.378017	5.768861	-0.941470
H	8.156066	3.305524	-0.959743
C	8.738222	-2.087314	-0.429032
H	9.726606	-2.504384	-0.573529
C	-8.760522	-2.059039	-0.302670
C	-8.613497	-0.690262	-0.326999
C	8.605500	-0.718647	-0.359924
H	9.468436	-0.067309	-0.445655
N	7.751495	-4.306300	-0.358339
N	-7.786616	-4.281373	-0.167135
C	-9.119738	-4.855581	-0.087809
H	-9.720197	-4.580707	-0.960635
H	-9.652690	-4.538679	0.818624
H	-9.032977	-5.940853	-0.073754
C	-6.639295	-5.122048	0.118649
H	-6.222324	-4.925168	1.116589
H	-6.943743	-6.166153	0.069722
H	-5.848993	-4.967474	-0.623690
C	9.031174	-4.882493	-0.737071
H	9.353681	-4.550519	-1.732838
H	8.936273	-5.967019	-0.750975
H	9.810962	-4.624728	-0.013247
C	6.568264	-5.145510	-0.363836
H	6.874567	-6.189956	-0.388395
H	5.976218	-4.990275	0.544684
H	5.926810	-4.948225	-1.234513
H	-3.784333	-2.067132	0.180161
H	-2.375781	0.668177	0.295678
H	2.381269	0.658797	0.336376
H	3.774409	-2.081430	0.168490
H	-9.757135	-2.473200	-0.386387
H	-9.472954	-0.036572	-0.428226

	Energies (Hartree)
E(M06-2X)	-2419.95380856
E(M06-2X)+ZPE	-2419.21835500
E(M06-2X)+U	-2419.17410400
E(M06-2X)+H	-2419.17316000
E(M06-2X)+G	-2419.30434700
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	4.2165
2	8.2699
3	11.5008
4	18.3992
5	24.7808
6	27.7695
7	29.2701
8	33.0316
9	37.7436
10	42.4027

6-Flav7-B

C	1.246926	-1.117230	0.408394
C	1.248295	-2.631045	0.472874
C	0.000296	-3.169071	1.160523
C	-1.255723	-2.628696	0.489971
C	-1.248064	-1.115535	0.409071
C	-0.001013	-0.460072	0.416788
Cl	-0.000053	1.297338	0.388479
C	2.448700	-0.411670	0.295662
C	-2.449719	-0.409623	0.280806
C	-3.712857	-0.990399	0.166632
C	3.713699	-0.991139	0.179140
C	-4.906856	-0.264512	0.030415
C	4.908310	-0.264713	0.066107
C	4.955375	1.159537	0.070815
C	6.128042	1.851676	-0.032168
O	7.301695	1.221846	-0.160922
C	7.347162	-0.141226	-0.189387
C	6.198888	-0.936640	-0.076021
C	-6.194206	-0.938060	-0.125949
C	-7.342061	-0.143417	-0.249968
O	-7.294501	1.219460	-0.244544
C	-6.124635	1.850921	-0.095980
C	-4.955797	1.158718	0.049659
C	-6.352364	-2.335785	-0.148105
C	-7.610164	-2.937291	-0.298467
C	7.616030	-2.934760	-0.254660
C	6.357619	-2.334097	-0.106215

C	-6.257132	3.316540	-0.087065
C	-5.160315	4.135335	-0.390552
C	-5.294135	5.519463	-0.365249
C	-6.521026	6.100048	-0.040896
C	-7.617611	5.289406	0.252537
C	-7.490779	3.903917	0.226758
C	6.256425	3.317838	-0.036938
C	5.259599	4.124130	0.530111
C	5.384442	5.509149	0.506546
C	6.503398	6.102989	-0.079088
C	7.502263	5.304545	-0.636193
C	7.384542	3.918107	-0.613362
H	2.135457	-2.967086	1.016181
H	1.322167	-3.040889	-0.544099
H	0.008196	-2.864257	2.213625
H	-0.001245	-4.261994	1.135722
H	-2.135602	-2.953017	1.052311
H	-1.351072	-3.048110	-0.521280
H	4.045283	1.738417	0.136123
H	-4.056617	1.735643	0.211745
H	-5.478212	-2.961158	-0.045718
H	5.483040	-2.960141	-0.011821
H	-4.208749	3.696937	-0.672622
H	-4.442032	6.145284	-0.608614
H	-6.622792	7.180246	-0.022469
H	-8.573755	5.736247	0.503977
H	-8.342373	3.274105	0.459379
H	4.398842	3.674233	1.014052
H	4.611891	6.125014	0.954695
H	6.598583	7.183816	-0.095784
H	8.374569	5.761689	-1.091442
H	8.159254	3.297870	-1.050604
C	8.751773	-2.079783	-0.354616
H	9.745035	-2.498016	-0.456126
C	-8.745527	-2.082809	-0.410382
C	-8.608873	-0.712993	-0.389887
C	8.614738	-0.710027	-0.324505
H	9.478937	-0.059133	-0.400391
N	7.761215	-4.298013	-0.307429
N	-7.755346	-4.300366	-0.342689
C	-9.084401	-4.887648	-0.303886
H	-8.988509	-5.972119	-0.317119
H	-9.635525	-4.599947	0.601256
H	-9.672173	-4.593634	-1.179405
C	-6.600812	-5.142557	-0.093533
H	-5.816338	-4.958311	-0.835650
H	-6.898971	-6.186461	-0.174146
H	-6.178427	-4.975463	0.907424
C	9.090029	-4.885018	-0.257116
H	9.631321	-4.602311	0.655604
H	8.994729	-5.969443	-0.277928

H	9.687153	-4.585775	-1.124443
C	6.606058	-5.141049	-0.063979
H	6.182641	-4.979925	0.937610
H	5.822495	-4.951952	-0.805735
H	6.903768	-6.184611	-0.150889
H	-3.778246	-2.070124	0.160856
H	-2.379859	0.670986	0.241613
H	2.379868	0.669481	0.276292
H	3.778746	-2.070717	0.159738
H	-9.738099	-2.501907	-0.515113
H	-9.472336	-0.062720	-0.478239

	Energies (Hartree)
E(M06-2X)	-2419.95383556
E(M06-2X)+ZPE	-2419.21820100
E(M06-2X)+U	-2419.17406400
E(M06-2X)+H	-2419.17312000
E(M06-2X)+G	-2419.30334200
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	4.9248
2	9.5501
3	13.4646
4	19.8613
5	24.8933
6	26.6720
7	29.8016
8	34.1601
9	38.0890
10	41.1018

6-Flav7-C

C	1.247404	-1.091842	0.477145
C	1.253435	-2.601392	0.609256
C	0.005177	-3.113925	1.315384
C	-1.250319	-2.602848	0.621161
C	-1.247360	-1.093281	0.489333
C	-0.000363	-0.436402	0.465814
Cl	-0.001921	1.318558	0.368869
C	2.448323	-0.391444	0.321527
C	-2.450443	-0.394498	0.345019
C	-3.712587	-0.982321	0.247202
C	3.710503	-0.977345	0.215335
C	-4.908376	-0.264056	0.095307
C	4.904609	-0.257930	0.054323
C	4.958614	1.165616	0.052549
C	6.128101	1.851455	-0.114644
O	7.294560	1.213915	-0.266067

C	7.337243	-0.149232	-0.253816
C	6.188145	-0.938005	-0.107122
C	-6.190833	-0.944914	-0.071246
C	-7.340941	-0.156980	-0.214070
O	-7.301296	1.206360	-0.209963
C	-6.136370	1.844556	-0.049048
C	-4.965388	1.159407	0.109736
C	-6.339775	-2.343484	-0.101817
C	-7.593261	-2.952523	-0.256879
C	7.594870	-2.944478	-0.271859
C	6.340984	-2.336434	-0.114980
C	-6.277786	3.309440	-0.041279
C	-5.182391	4.135009	-0.331215
C	-5.324816	5.518309	-0.307014
C	-6.559023	6.091413	0.002575
C	-7.654146	5.274026	0.282400
C	-7.518614	3.889312	0.257815
C	6.265968	3.316630	-0.126972
C	7.505757	3.903506	0.162632
C	7.637987	5.288741	0.168200
C	6.540587	6.099614	-0.121455
C	5.307391	5.519389	-0.421683
C	5.168251	4.135553	-0.426811
H	2.140092	-2.908838	1.170256
H	1.333218	-3.055678	-0.388282
H	0.009934	-2.767259	2.355489
H	0.005894	-4.206964	1.334027
H	-1.338758	-3.057069	-0.375668
H	-2.131309	-2.911450	1.190368
H	4.063335	1.747698	0.217924
H	-4.071651	1.741244	0.284167
H	-5.461189	-2.963538	-0.005454
H	5.465529	-2.957362	0.002419
H	-4.224771	3.702454	-0.601599
H	-4.473545	6.149355	-0.539612
H	-6.667499	7.170975	0.020171
H	-8.615956	5.714968	0.522404
H	-8.369134	3.254307	0.480015
H	8.358100	3.273635	0.392280
H	8.599038	5.735185	0.400969
H	6.646500	7.179573	-0.118804
H	4.454340	6.145160	-0.661854
H	4.211286	3.697105	-0.689904
C	8.732094	-2.095725	-0.405268
H	9.722046	-2.519591	-0.515468
C	-8.728502	-2.104631	-0.410011
C	-8.600348	-0.733950	-0.386337
C	8.600418	-0.725199	-0.399980
H	9.465168	-0.079220	-0.505643
N	7.734174	-4.308638	-0.303174
N	-7.735356	-4.317177	-0.259614

C	-9.010258	-4.909503	-0.629609
H	-9.323012	-4.617045	-1.640872
H	-8.914156	-5.993611	-0.599792
H	-9.797498	-4.625050	0.075775
C	-6.548314	-5.150987	-0.240972
H	-5.957940	-4.968129	0.663428
H	-5.906933	-4.974803	-1.116255
H	-6.849954	-6.197080	-0.237057
C	6.578996	-5.143500	-0.033327
H	6.167587	-4.964529	0.970154
H	5.787546	-4.963845	-0.769156
H	6.872183	-6.189382	-0.106215
C	9.061207	-4.900838	-0.271654
H	8.961028	-5.985017	-0.273862
H	9.641587	-4.617341	-1.155516
H	9.622256	-4.606933	0.625364
H	-3.773905	-2.062199	0.263681
H	-2.384241	0.684804	0.274283
H	2.379637	0.687675	0.250569
H	3.773506	-2.057061	0.234411
H	-9.714463	-2.529294	-0.548745
H	-9.464171	-0.088673	-0.503295

	Energies (Hartree)
E(M06-2X)	-2419.95384087
E(M06-2X)+ZPE	-2419.21813600
E(M06-2X)+U	-2419.17398300
E(M06-2X)+H	-2419.17303900
E(M06-2X)+G	-2419.30327800
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	4.8192
2	8.5956
3	14.3703
4	22.1717
5	25.0460
6	29.2303
7	29.6955
8	34.9430
9	38.3428
10	42.7317

Flav7-A (Global Minimum)

C	-0.000117	-3.479553	1.129915
C	-1.252343	-2.929378	0.459690
C	1.252603	-2.929282	0.460708
H	-1.337806	-3.329083	-0.560504
H	1.339261	-3.329421	-0.559215

C	-1.247782	-1.414875	0.411246
C	1.247738	-1.414795	0.411555
C	0.000045	-0.761281	0.428003
H	-0.000045	-4.572093	1.088190
Cl	-0.000017	0.999040	0.424447
H	-2.135577	-3.268875	1.007652
H	-0.000573	-3.191197	2.187767
H	2.135390	-3.268248	1.009735
C	-2.451653	-0.707844	0.305291
C	-3.716060	-1.282849	0.192144
H	-3.788039	-2.362616	0.176427
C	2.451709	-0.707690	0.305275
H	2.381181	0.373426	0.292530
C	3.715999	-1.282691	0.192512
H	3.788058	-2.362462	0.177526
C	-4.912441	-0.551649	0.084902
C	-4.944680	0.881475	0.076134
C	-6.112270	1.571393	-0.009285
O	-7.301225	0.944791	-0.107406
C	-7.362890	-0.417547	-0.129608
C	-6.194946	-1.201147	-0.032707
C	-6.398536	-2.602439	-0.062645
C	-7.645839	-3.161162	-0.177642
C	-8.815586	-2.343079	-0.272282
C	-8.637926	-0.945625	-0.244887
H	-4.029894	1.455057	0.113899
H	-9.468088	-0.254969	-0.309806
H	-7.734200	-4.239589	-0.193765
H	-5.548264	-3.270492	0.006122
C	4.912482	-0.551459	0.084838
C	4.944561	0.881588	0.074700
C	6.112144	1.571549	-0.011133
O	7.301080	0.944845	-0.108261
C	7.362884	-0.417473	-0.129169
C	6.194925	-1.201046	-0.031889
C	6.398565	-2.602390	-0.060537
C	7.645907	-3.161125	-0.174708
C	8.815675	-2.343055	-0.269721
C	8.637968	-0.945574	-0.243655
H	4.029672	1.455040	0.111662
H	9.468111	-0.254949	-0.309086
H	7.734341	-4.239559	-0.189910
H	5.548300	-3.270415	0.008542
C	-6.240779	3.038196	-0.028521
C	-7.373216	3.633816	-0.600590
C	-5.236800	3.849510	0.518199
C	-7.487666	5.020444	-0.640951
C	-5.357906	5.234436	0.476972
C	-6.481174	5.823663	-0.105285
H	-8.154092	3.009784	-1.021119
H	-4.372877	3.402781	0.999587

H	-8.363641	5.473737	-1.093102
H	-4.579236	5.854088	0.909117
H	-6.573755	6.904434	-0.135434
C	6.240651	3.038319	-0.031849
C	5.235746	3.850292	0.512212
C	7.374047	3.633300	-0.602699
C	5.356946	5.235159	0.469621
C	7.488596	5.019879	-0.644420
C	6.481220	5.823723	-0.111371
H	4.370931	3.404226	0.992595
H	8.155630	3.008820	-1.021228
H	4.577521	5.855296	0.899704
H	8.365351	5.472633	-1.095593
H	6.573868	6.904457	-0.142584
N	-10.048249	-2.896038	-0.382898
C	-11.219528	-2.037574	-0.456601
H	-11.175601	-1.383772	-1.335017
H	-12.109964	-2.658017	-0.533968
H	-11.308539	-1.413693	0.440124
C	-10.209192	-4.342657	-0.407577
H	-9.844181	-4.800351	0.518344
H	-11.267109	-4.575295	-0.510197
H	-9.676522	-4.786737	-1.255207
N	10.048354	-2.896070	-0.379442
C	10.209298	-4.342709	-0.403827
H	9.843933	-4.800206	0.522038
H	9.676955	-4.786940	-1.251585
H	11.267255	-4.575360	-0.505968
C	11.219602	-2.037633	-0.454188
H	11.175939	-1.385255	-1.333689
H	11.308216	-1.412322	0.441559
H	12.110111	-2.658137	-0.530181
H	-2.381218	0.373284	0.293145

		Energies (Hartree)
E(M06-2X)		-2419.96835111
E(M06-2X)+ZPE		-2419.23263800
E(M06-2X)+U		-2419.18847700
E(M06-2X)+H		-2419.18753200
E(M06-2X)+G		-2419.31744800
Number of imaginary frequencies		0
Top 10 frequencies (cm^{-1})		
1		4.1716
2		9.2423
3		12.3633
4		19.6019
5		25.1219
6		28.4616
7		29.3913
8		36.0974

9		44.7574
10		49.9678

Flav7-B

C	-0.000224	-3.445717	1.207913
C	1.255397	-2.912002	0.530942
C	-1.249479	-2.913933	0.517439
H	2.135509	-3.232233	1.095411
H	-2.135361	-3.243175	1.067210
C	1.248337	-1.399548	0.436728
C	-1.247130	-1.400864	0.435579
C	0.000918	-0.746471	0.435050
H	-0.006454	-3.130264	2.257977
Cl	0.000204	1.013108	0.383839
H	1.349678	-3.341788	-0.476197
H	0.000969	-4.538972	1.194278
H	-1.327040	-3.336575	-0.494148
C	2.452631	-0.695747	0.308385
C	3.715452	-1.275316	0.207736
H	3.785279	-2.355341	0.212317
C	-2.451410	-0.697217	0.318222
H	-2.382170	0.383598	0.285941
C	-3.715682	-1.275657	0.215870
H	-3.785679	-2.355671	0.212789
C	4.912567	-0.548506	0.075309
C	4.950732	0.884177	0.082370
C	6.115805	1.570474	-0.054556
O	7.299238	0.939243	-0.183356
C	7.359232	-0.423209	-0.177190
C	6.190389	-1.202783	-0.059841
C	6.389714	-2.604981	-0.080012
C	7.634415	-3.167945	-0.200927
C	8.805522	-2.353863	-0.313378
C	8.631666	-0.955675	-0.300166
H	4.047822	1.459201	0.228295
H	9.462364	-0.268006	-0.386417
H	7.719856	-4.246692	-0.208446
H	5.538344	-3.270040	0.002826
C	-4.913256	-0.548278	0.102019
C	-4.949579	0.884884	0.088846
C	-6.118817	1.571281	-0.000574
O	-7.305980	0.941176	-0.099804
C	-7.363723	-0.421459	-0.118608
C	-6.194033	-1.201593	-0.016572
C	-6.393631	-2.603405	-0.044609
C	-7.639124	-3.165907	-0.161736
C	-8.810816	-2.351316	-0.260982
C	-8.637027	-0.953358	-0.236175
H	-4.036548	1.461052	0.129624
H	-9.468885	-0.265128	-0.305099
H	-7.724352	-4.244607	-0.176423

H	-5.541599	-3.268965	0.026776
C	6.251985	3.036713	-0.059685
C	7.478931	3.626604	0.273665
C	5.163191	3.853407	-0.395606
C	7.606624	5.012556	0.287733
C	5.297441	5.237648	-0.381637
C	6.517673	5.821016	-0.037310
H	8.324915	2.998604	0.530260
H	4.217840	3.411920	-0.693610
H	8.557860	5.461188	0.554359
H	4.451333	5.861348	-0.650223
H	6.620188	6.901288	-0.028635
C	-6.251608	3.037727	-0.022192
C	-7.385246	3.629159	-0.596218
C	-5.250777	3.852910	0.524553
C	-7.503986	5.015387	-0.638439
C	-5.376139	5.237403	0.481470
C	-6.500617	5.822430	-0.102691
H	-8.163789	3.002193	-1.016698
H	-4.385978	3.409575	1.007482
H	-8.380937	5.465363	-1.092015
H	-4.599894	5.859984	0.913774
H	-6.596597	6.902868	-0.134182
N	10.035563	-2.911271	-0.428916
C	10.191728	-4.358554	-0.448595
H	11.248003	-4.594993	-0.558944
H	9.833154	-4.810742	0.482487
H	9.650494	-4.804771	-1.289670
C	11.208286	-2.056852	-0.524434
H	12.096935	-2.680538	-0.596029
H	11.303629	-1.418423	0.361227
H	11.160763	-1.417668	-1.413416
N	-10.041757	-2.907943	-0.373773
C	-11.215130	-2.052885	-0.452954
H	-12.103700	-2.675933	-0.531000
H	-11.308248	-1.426828	0.441834
H	-11.170656	-1.401289	-1.332997
C	-10.198484	-4.355018	-0.396494
H	-11.255485	-4.590889	-0.501155
H	-9.834308	-4.810168	0.531012
H	-9.662564	-4.799004	-1.242148
H	2.382845	0.384535	0.260928

	Energies (Hartree)
E(M06-2X)	-2419.96836422
E(M06-2X)+ZPE	-2419.23255600
E(M06-2X)+U	-2419.18842600
E(M06-2X)+H	-2419.18748200
E(M06-2X)+G	-2419.31692900
Number of imaginary frequencies	0

Top 10 frequencies (cm^{-1})	
1	5.2045
2	8.6358
3	14.0535
4	21.6955
5	24.8694
6	28.3178
7	34.8493
8	35.1887
9	44.6377
10	48.6914

Flav7-C

C	0.000013	-3.414011	1.283592
C	-1.252333	-2.895879	0.588575
C	1.252363	-2.895881	0.588581
H	-1.337896	-3.343254	-0.411711
H	1.337962	-3.343295	-0.411684
C	-1.247666	-1.385235	0.468949
C	1.247672	-1.385243	0.468881
C	0.000020	-0.731630	0.454409
H	0.000015	-4.507305	1.293136
Cl	0.000032	1.026476	0.366586
H	-2.135544	-3.208734	1.152195
H	0.000012	-3.076197	2.326698
H	2.135573	-3.208681	1.152235
C	-2.452226	-0.684836	0.330685
C	-3.714547	-1.267738	0.235811
H	-3.782116	-2.347822	0.249849
C	2.452246	-0.684852	0.330516
H	2.384111	0.394839	0.268529
C	3.714540	-1.267759	0.235622
H	3.782107	-2.347844	0.249665
C	-4.912564	-0.544911	0.095457
C	-4.954904	0.887880	0.098022
C	-6.121248	1.570440	-0.045660
O	-7.302460	0.935506	-0.178332
C	-7.358585	-0.427162	-0.168585
C	-6.188340	-1.203123	-0.043104
C	-6.383611	-2.605802	-0.060876
C	-7.626159	-3.172685	-0.186535
C	-8.798877	-2.362257	-0.306968
C	-8.628930	-0.963577	-0.296677
H	-4.054383	1.465660	0.247926
H	-9.461072	-0.278463	-0.389280
H	-7.708450	-4.251684	-0.192009
H	-5.530722	-3.268249	0.027347
C	4.912572	-0.544925	0.095279
C	4.954904	0.887858	0.097999

C	6.121268	1.570431	-0.045505
O	7.302487	0.935521	-0.178112
C	7.358600	-0.427154	-0.168613
C	6.188328	-1.203122	-0.043374
C	6.383588	-2.605806	-0.061448
C	7.626136	-3.172673	-0.187135
C	8.798878	-2.362233	-0.307299
C	8.628948	-0.963551	-0.296703
H	4.054383	1.465636	0.247911
H	9.461102	-0.278423	-0.389081
H	7.708419	-4.251673	-0.192822
H	5.530683	-3.268265	0.026547
C	-6.261908	3.036285	-0.053844
C	-7.492701	3.622873	0.271050
C	-5.173551	3.855999	-0.383828
C	-7.624723	5.008457	0.282705
C	-5.312079	5.239835	-0.372220
C	-6.536223	5.819906	-0.036287
H	-8.338376	2.992609	0.523036
H	-4.224917	3.417107	-0.675147
H	-8.579007	5.454440	0.542817
H	-4.466126	5.865825	-0.635943
H	-6.642049	6.899873	-0.029374
C	6.261903	3.036279	-0.053505
C	7.492598	3.622855	0.271778
C	5.173618	3.855994	-0.383716
C	7.624588	5.008441	0.283595
C	5.312116	5.239832	-0.371945
C	6.536157	5.819894	-0.035623
H	8.338214	2.992581	0.523940
H	4.225080	3.417097	-0.675342
H	8.578790	5.454424	0.544008
H	4.466227	5.865833	-0.635848
H	6.641960	6.899862	-0.028582
N	-10.026860	-2.923484	-0.427323
C	-10.178571	-4.371210	-0.445265
H	-11.233608	-4.611067	-0.560011
H	-9.632116	-4.817348	-1.283046
H	-9.822931	-4.820722	0.488242
C	-11.201302	-2.072657	-0.532451
H	-11.303134	-1.431067	0.350192
H	-12.087930	-2.698978	-0.606291
H	-11.150782	-1.436724	-1.423624
N	10.026850	-2.923454	-0.427691
C	11.201354	-2.072639	-0.532262
H	12.087971	-2.698979	-0.606056
H	11.302974	-1.431315	0.350598
H	11.151097	-1.436443	-1.423263
C	10.178534	-4.371183	-0.445896
H	11.233543	-4.611034	-0.560914
H	9.631900	-4.817146	-1.283646

H	9.823070	-4.820858	0.487603
H	-2.384099	0.394857	0.268766

		Energies (Hartree)
E(M06-2X)		-2419.96837486
E(M06-2X)+ZPE		-2419.23245300
E(M06-2X)+U		-2419.18835300
E(M06-2X)+H		-2419.18740900
E(M06-2X)+G		-2419.31657500
Number of imaginary frequencies		0
Top 10 frequencies (cm^{-1})		
1		5.9731
2		7.8644
3		14.9789
4		23.6640
5		24.2216
6		33.2668
7		34.0750
8		35.7069
9		44.2020
10		47.8972

8-Flav7-A (Global Minimum)

C	1.247281	-1.808789	0.419757
C	1.251768	-3.322111	0.496613
C	0.000025	-3.858866	1.177915
C	-1.251783	-3.322091	0.496749
C	-1.247268	-1.808771	0.419885
C	-0.000008	-1.150884	0.427792
Cl	0.000007	0.605103	0.397817
C	2.447558	-1.102758	0.295490
C	-2.447570	-1.102719	0.295716
C	-3.711394	-1.685174	0.176771
C	3.711392	-1.685226	0.176390
C	-4.905013	-0.961050	0.053092
C	4.904982	-0.961104	0.052746
C	4.953321	0.463869	0.072467
C	6.129647	1.143761	-0.033197
O	7.297357	0.498131	-0.166819
C	7.349792	-0.859462	-0.200599
C	6.189140	-1.640061	-0.112540
C	-6.189207	-1.640051	-0.111679
C	-7.349837	-0.859451	-0.200067
O	-7.297343	0.498147	-0.166932
C	-6.129619	1.143803	-0.033679
C	-4.953294	0.463918	0.072193
C	-6.330660	-3.040487	-0.221896
C	-7.577833	-3.596328	-0.411979
C	-8.647040	-1.408807	-0.358594
C	8.646964	-1.408802	-0.359441

C	7.577643	-3.596240	-0.414027
C	6.330506	-3.040435	-0.223574
C	-6.292808	2.605918	-0.031711
C	-7.485187	3.171800	-0.506442
C	-7.644161	4.554154	-0.518746
C	-6.622955	5.382398	-0.053449
C	-5.439324	4.822760	0.430073
C	-5.272789	3.442343	0.443455
C	6.292883	2.605875	-0.030582
C	7.485368	3.171925	-0.504847
C	7.644390	4.554281	-0.516547
C	6.623124	5.382368	-0.051105
C	5.439382	4.822560	0.431951
C	5.272802	3.442144	0.444728
H	2.135472	-3.650833	1.049822
H	1.335513	-3.739075	-0.516550
H	0.000017	-4.951737	1.156384
H	0.000084	-3.550802	2.230084
H	-1.335660	-3.739062	-0.516399
H	-2.135429	-3.650789	1.050064
H	2.378203	-0.021999	0.264570
H	3.775469	-2.764761	0.165476
H	4.045965	1.043970	0.156786
H	-4.045913	1.044045	0.156053
H	-5.464072	-3.686663	-0.172648
H	-7.679463	-4.672134	-0.504899
H	7.679201	-4.671998	-0.507592
H	5.463866	-3.686570	-0.174706
H	-8.278118	2.527905	-0.872222
H	-8.566481	4.984684	-0.894210
H	-6.750047	6.460023	-0.062415
H	-4.647308	5.461935	0.805581
H	-4.357162	3.022256	0.845941
H	8.278357	2.528165	-0.870738
H	8.566801	4.984930	-0.891651
H	6.750249	6.459993	-0.059596
H	4.647305	5.461600	0.807562
H	4.357070	3.021936	0.846847
C	8.727002	-2.793411	-0.475964
H	9.692589	-3.265290	-0.612965
C	-8.727153	-2.793469	-0.474351
H	-9.692766	-3.265378	-0.611072
N	9.752971	-0.548400	-0.457260
N	-9.753000	-0.548385	-0.456868
C	-10.046996	0.241419	0.744021
H	-10.762819	1.023945	0.481404
H	-9.146284	0.714701	1.131055
H	-10.487208	-0.388377	1.532207
C	-10.966731	-1.144008	-0.997220
H	-11.680222	-0.341861	-1.197087
H	-10.747853	-1.655948	-1.936684

H	-11.439164	-1.855693	-0.301065
C	10.966685	-1.143799	-0.997886
H	11.439061	-1.855869	-0.302085
H	11.680223	-0.341582	-1.197312
H	10.747815	-1.655239	-1.937624
C	10.046982	0.240837	0.743994
H	10.762745	1.023536	0.481728
H	10.487272	-0.389319	1.531849
H	9.146265	0.713874	1.131318
H	-2.378185	-0.021962	0.264763
H	-3.775482	-2.764706	0.165981

	Energies (Hartree)
E(M06-2X)	-2419.94681906
E(M06-2X)+ZPE	-2419.21032300
E(M06-2X)+U	-2419.16704300
E(M06-2X)+H	-2419.16609900
E(M06-2X)+G	-2419.29310300
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	5.3456
2	8.8636
3	12.2326
4	19.8724
5	19.9335
6	30.5383
7	33.2592
8	39.8454
9	40.5785
10	46.4734

8-Flav7-B

C	1.248444	-1.817999	0.452494
C	1.252284	-3.332128	0.510809
C	-0.006144	-3.877119	1.172947
C	-1.251147	-3.332025	0.485905
C	-1.246006	-1.817876	0.427632
C	0.001149	-1.160205	0.455579
Cl	0.001506	0.596029	0.447492
C	2.450001	-1.110761	0.349316
C	-2.444970	-1.110027	0.301266
C	-3.708360	-1.690071	0.166718
C	3.714800	-1.692094	0.235153
C	-4.900340	-0.963403	0.042353
C	4.908200	-0.965765	0.123820
C	4.955701	0.458686	0.170217
C	6.127941	1.142459	0.044886
O	7.293253	0.500373	-0.122914

C	7.348203	-0.856842	-0.166535
C	6.194969	-1.641731	-0.032655
C	-6.184694	-1.639309	-0.133638
C	-7.343961	-0.856486	-0.220417
O	-7.289794	0.500777	-0.176925
C	-6.121700	1.143775	-0.034320
C	-4.946810	0.461479	0.071683
C	-6.327525	-3.038632	-0.255354
C	-7.574689	-3.591339	-0.454538
C	-8.641299	-1.402915	-0.387659
C	8.646654	-1.402638	-0.326532
C	7.610232	-3.598828	-0.144478
C	6.353411	-3.044683	-0.026644
C	-6.282683	2.606099	-0.022950
C	-7.472405	3.177107	-0.498212
C	-7.629127	4.559775	-0.501744
C	-6.608310	5.383214	-0.027151
C	-5.427340	4.818406	0.456865
C	-5.263050	3.437669	0.461509
C	6.292979	2.603832	0.087394
C	7.566792	3.152441	0.297355
C	7.731614	4.533203	0.348212
C	6.633753	5.377742	0.185105
C	5.366141	4.836120	-0.033867
C	5.193905	3.457302	-0.084421
H	2.130543	-3.667491	1.068690
H	1.346154	-3.736703	-0.506453
H	-0.016627	-3.581819	2.228702
H	-0.005873	-4.969644	1.138145
H	-2.140205	-3.667508	1.026312
H	-1.324909	-3.736539	-0.533071
H	2.381627	-0.029608	0.331022
H	3.778448	-2.771277	0.204483
H	4.056117	1.032798	0.337535
H	-4.039041	1.039815	0.163282
H	-5.461946	-3.686280	-0.207816
H	-7.677313	-4.666255	-0.556282
H	7.726917	-4.677034	-0.130051
H	5.495238	-3.694767	0.082173
H	-8.265059	2.536995	-0.871172
H	-8.549404	4.994311	-0.877600
H	-6.733685	6.461076	-0.029208
H	-4.635693	5.453739	0.839612
H	-4.349585	3.013406	0.864520
H	8.420394	2.495861	0.428744
H	8.718994	4.949619	0.517688
H	6.764984	6.454211	0.223607
H	4.510954	5.488676	-0.174048
H	4.206274	3.053304	-0.279618
C	8.747053	-2.790473	-0.298389
H	9.717834	-3.260305	-0.401923

C	-8.722757	-2.786534	-0.514636
H	-9.688499	-3.256080	-0.658392
N	9.748727	-0.538519	-0.434995
N	-9.745847	-0.540351	-0.482752
C	-10.042470	0.240740	0.723196
H	-9.142440	0.710260	1.116356
H	-10.756780	1.025901	0.464381
H	-10.485546	-0.394495	1.505380
C	-10.958709	-1.130258	-1.031244
H	-11.434148	-1.846557	-0.341894
H	-11.670572	-0.325691	-1.227170
H	-10.737675	-1.635385	-1.973883
C	11.050479	-1.146908	-0.200915
H	11.358152	-1.823153	-1.014667
H	11.791332	-0.348132	-0.126348
H	11.042035	-1.701665	0.739700
C	9.772613	0.305542	-1.634539
H	10.527574	1.083818	-1.499827
H	10.031005	-0.284764	-2.527024
H	8.808300	0.784908	-1.794404
H	-2.374744	-0.029047	0.283066
H	-3.773493	-2.769385	0.145593

	Energies (Hartree)
E(M06-2X)	-2419.94683115
E(M06-2X)+ZPE	-2419.21031400
E(M06-2X)+U	-2419.16704000
E(M06-2X)+H	-2419.16609600
E(M06-2X)+G	-2419.29305800
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	5.0190
2	8.8976
3	12.9208
4	19.7627
5	20.7120
6	30.1376
7	35.2200
8	37.9451
9	41.3123
10	46.3612

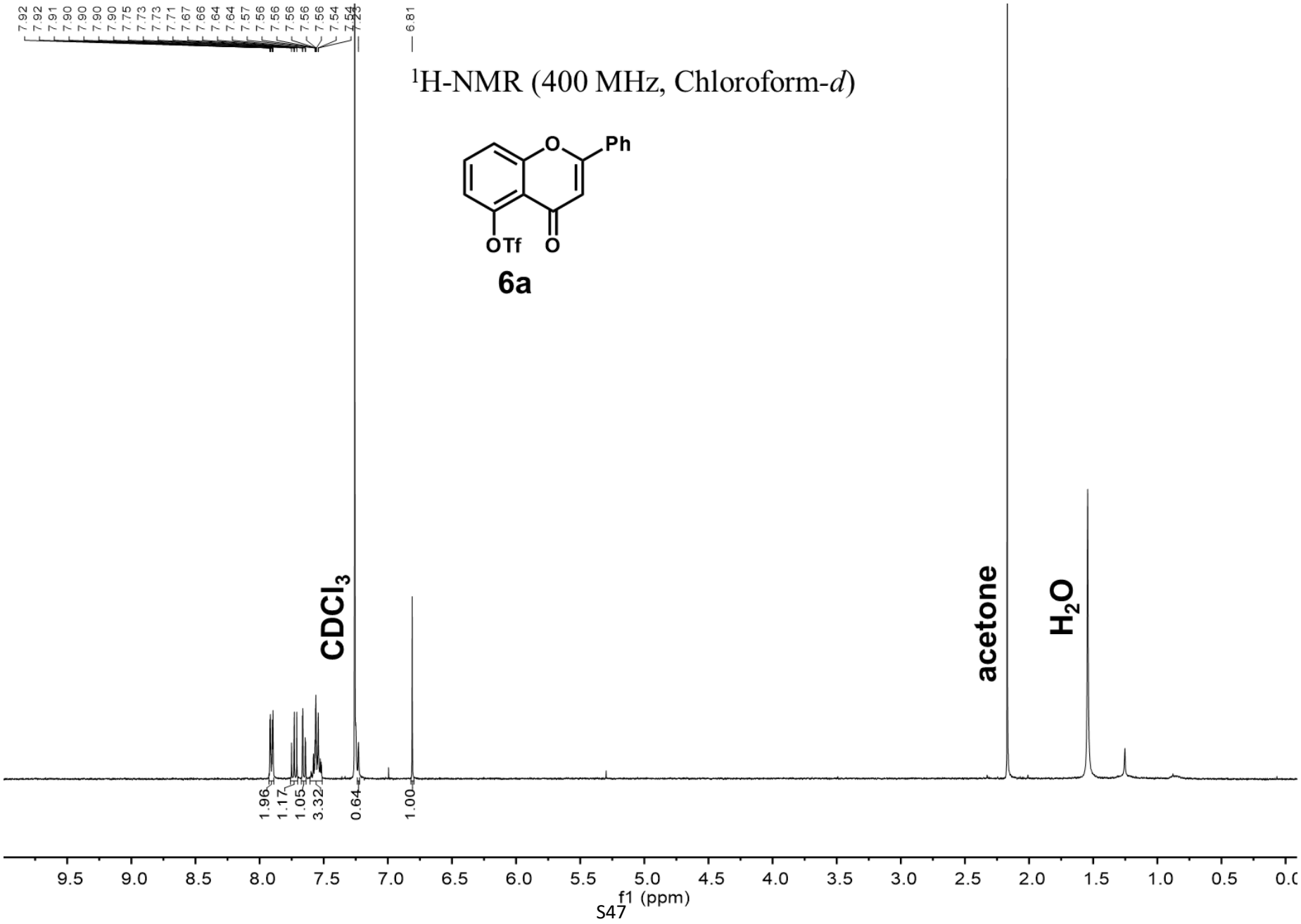
8-Flav7-C

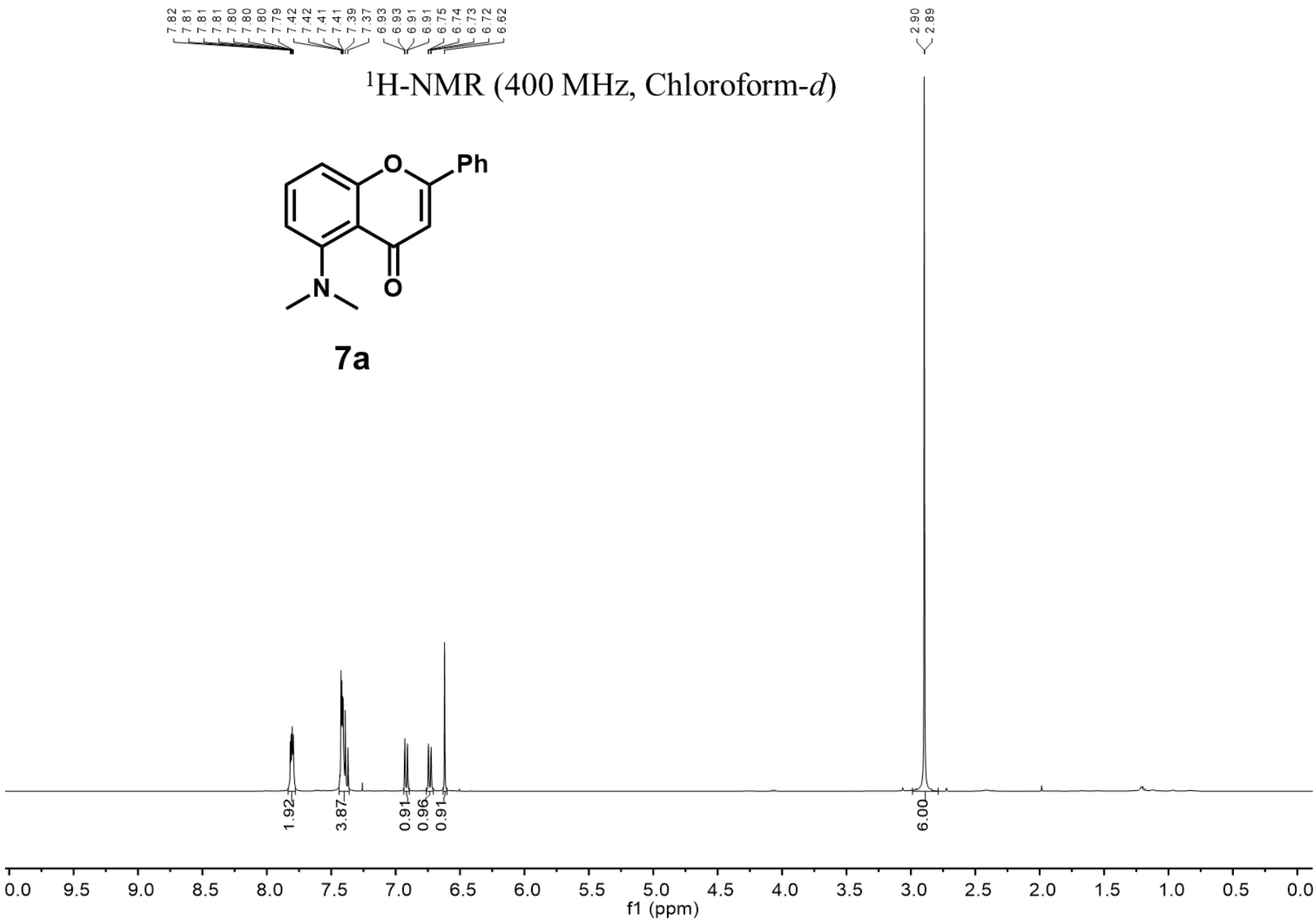
C	1.247289	-1.824348	0.471830
C	1.251739	-3.339024	0.513677
C	0.000018	-3.891300	1.182495
C	-1.251782	-3.338993	0.513866
C	-1.247275	-1.824322	0.471898
C	-0.000004	-1.166801	0.494342
Cl	-0.000004	0.589392	0.506056
C	2.447648	-1.115738	0.364544

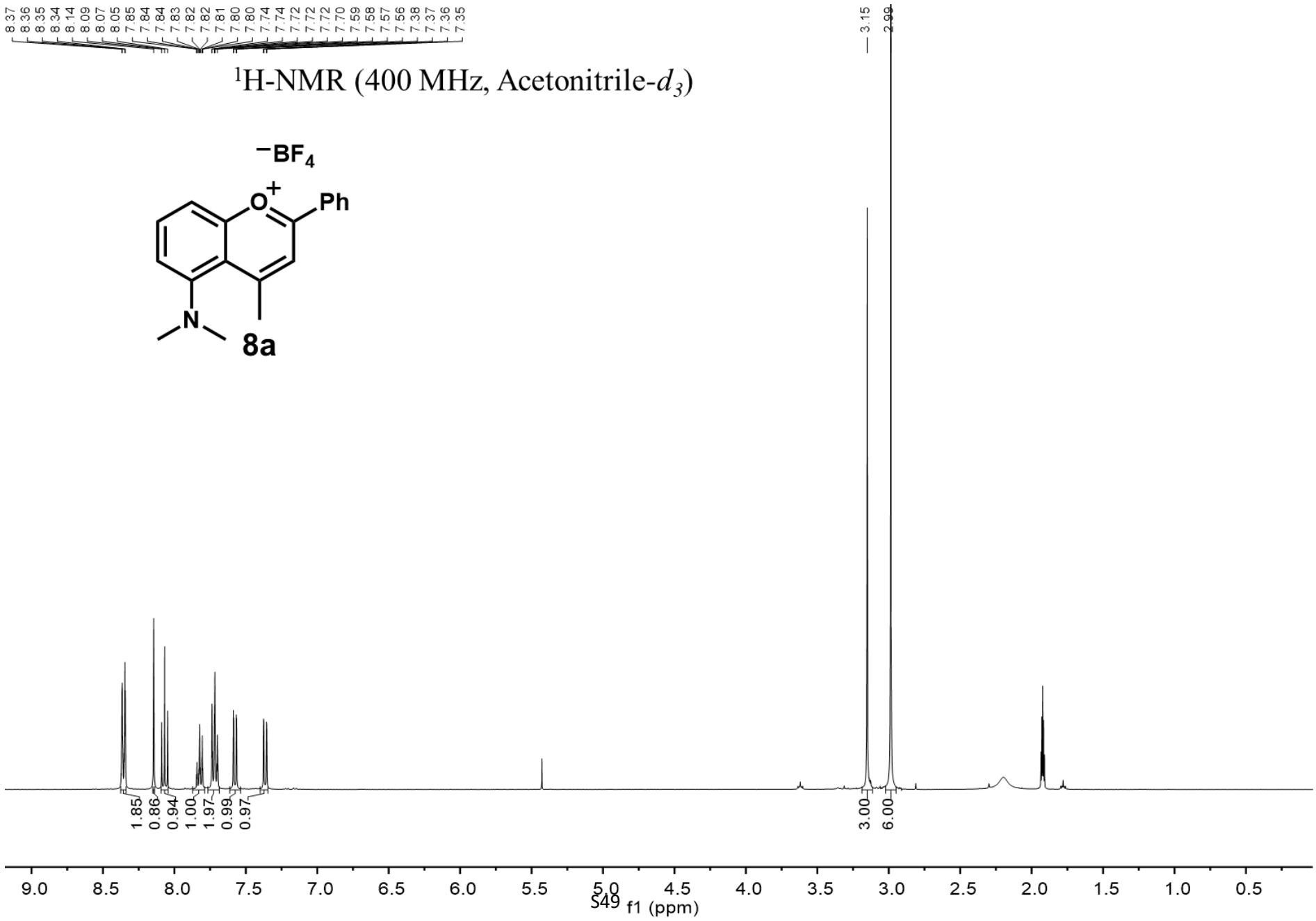
C	-2.447646	-1.115696	0.364541
C	-3.711620	-1.695315	0.233735
C	3.711657	-1.695339	0.233768
C	-4.903759	-0.967468	0.118836
C	4.903774	-0.967484	0.118980
C	4.950988	0.456623	0.176228
C	6.121708	1.141982	0.045660
O	7.285903	0.501876	-0.136869
C	7.341322	-0.854973	-0.190385
C	6.189616	-1.641504	-0.052869
C	-6.189538	-1.641516	-0.053289
C	-7.341291	-0.855008	-0.190604
O	-7.285956	0.501826	-0.136631
C	-6.121780	1.141950	0.045899
C	-4.951010	0.456614	0.176261
C	-6.348716	-3.044366	-0.058947
C	-7.604796	-3.596951	-0.191216
C	-8.638680	-1.398879	-0.364998
C	8.638759	-1.398813	-0.364542
C	7.605029	-3.596889	-0.190057
C	6.348909	-3.044351	-0.058002
C	-6.286355	2.603076	0.097458
C	-5.185544	3.457003	-0.060312
C	-5.357361	4.835548	-0.001527
C	-6.626272	5.376424	0.211668
C	-7.725810	4.531473	0.360712
C	-7.561404	3.150992	0.301586
C	6.286254	2.603130	0.096914
C	5.185417	3.457018	-0.060871
C	5.357226	4.835578	-0.002363
C	6.626156	5.376500	0.210576
C	7.725722	4.531587	0.359639
C	7.561327	3.151095	0.300784
H	2.135527	-3.680329	1.059073
H	1.335483	-3.732541	-0.508809
H	0.000117	-3.607251	2.241369
H	-0.000011	-4.983385	1.135997
H	-2.135499	-3.680209	1.059434
H	-1.335722	-3.732581	-0.508577
H	2.378696	-0.034487	0.357440
H	3.775532	-2.774172	0.193096
H	4.052626	1.029000	0.355667
H	-4.052668	1.029000	0.355792
H	-5.491787	-3.695701	0.052159
H	-7.722091	-4.675175	-0.185797
H	7.722412	-4.675101	-0.184231
H	5.492038	-3.695711	0.053399
H	-4.196790	3.053620	-0.251074
H	-4.500785	5.488536	-0.130764
H	-6.757172	6.452681	0.256606
H	-8.714185	4.947335	0.525667

H	-8.416335	2.494049	0.422036
H	4.196644	3.053580	-0.251427
H	4.500625	5.488532	-0.131610
H	6.757063	6.452767	0.255301
H	8.714109	4.947500	0.524394
H	8.416273	2.494173	0.421242
C	8.740121	-2.786765	-0.347334
H	9.710287	-3.255263	-0.462064
C	-8.739937	-2.786854	-0.348229
H	-9.710073	-3.255365	-0.463153
N	9.739531	-0.533293	-0.475249
N	-9.739520	-0.533426	-0.475438
C	-11.043305	-1.142876	-0.255842
H	-11.042268	-1.704767	0.680570
H	-11.345157	-1.812755	-1.077013
H	-11.784295	-0.344268	-0.180788
C	-9.753893	0.319777	-1.668621
H	-8.788245	0.800004	-1.817431
H	-10.005653	-0.263558	-2.567561
H	-10.509610	1.097297	-1.533769
C	9.753819	0.319414	-1.668798
H	10.509519	1.097007	-1.534283
H	10.005554	-0.264284	-2.567504
H	8.788144	0.799560	-1.817754
C	11.043350	-1.142623	-0.255467
H	11.042346	-1.704184	0.681143
H	11.784314	-0.343967	-0.180709
H	11.345208	-1.812784	-1.076405
H	-2.378689	-0.034444	0.357351
H	-3.775482	-2.774152	0.193117

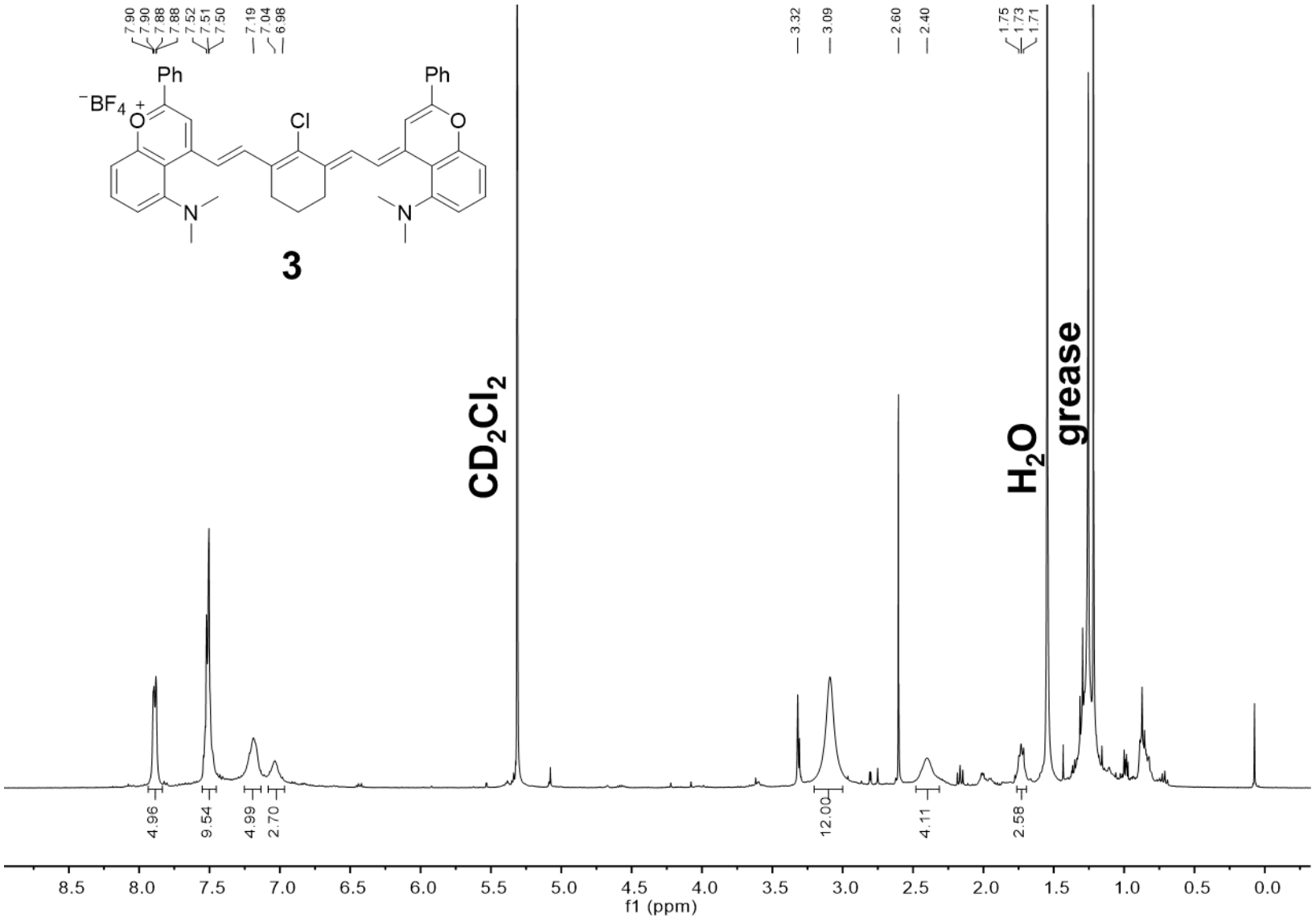
	Energies (Hartree)
E(M06-2X)	-2419.94682576
E(M06-2X)+ZPE	-2419.21025300
E(M06-2X)+U	-2419.16700600
E(M06-2X)+H	-2419.16606200
E(M06-2X)+G	-2419.29261000
Number of imaginary frequencies	0
Top 10 frequencies (cm^{-1})	
1	6.7184
2	8.3922
3	13.7188
4	19.6240
5	20.9459
6	31.3400
7	36.3008
8	39.5887
9	40.9120
10	46.5358

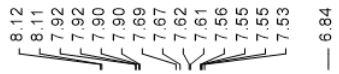

7.92
7.92
7.91
7.90
7.90
7.90
7.90
7.75
7.73
7.73
7.71
7.67
7.66
7.64
7.64
7.57
7.56
7.56
7.56
7.56
7.56
7.54
7.23
6.81
1H-NMR (400 MHz, Chloroform-d)
O
Ph
OTf
O
6a
CDCl3
acetone
H2O
1.96
1.17
1.05
3.32
0.64
1.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


7.82
7.81
7.81
7.81
7.80
7.80
7.80
7.79
7.42
7.42
7.41
7.41
7.39
7.37
6.93
6.93
6.91
6.91
6.75
6.74
6.73
6.72
6.62
2.90
2.89
1H-NMR (400 MHz, Chloroform-d)
O
Ph
N
O
7a
1.92
3.87
0.91
0.96
0.91
6.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

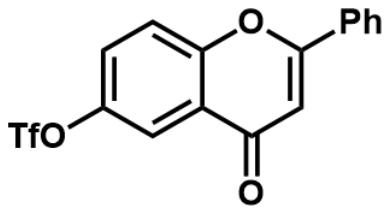

8.37
8.36
8.35
8.34
8.14
8.09
8.07
8.05
7.85
7.84
7.84
7.83
7.82
7.82
7.81
7.80
7.80
7.74
7.74
7.72
7.72
7.72
7.70
7.59
7.58
7.57
7.56
7.38
7.37
7.36
7.35
3.15
2.99
1H-NMR (400 MHz, Acetonitrile-d3)
−BF4
O+
Ph
N
8a
1.85
0.86
0.94
1.00
1.97
0.99
0.97
3.00
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

^{1}H-NMR (400 MHz, Methylene Chloride-d_2)

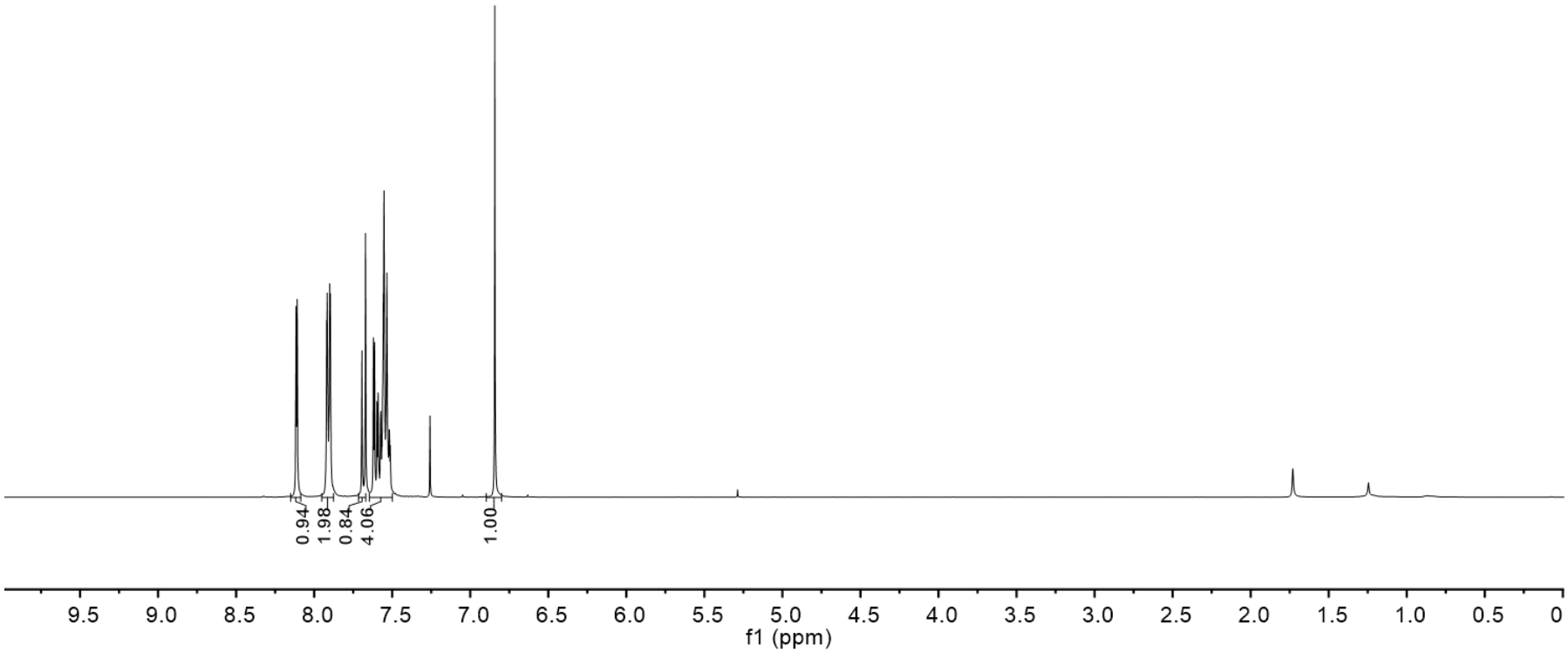


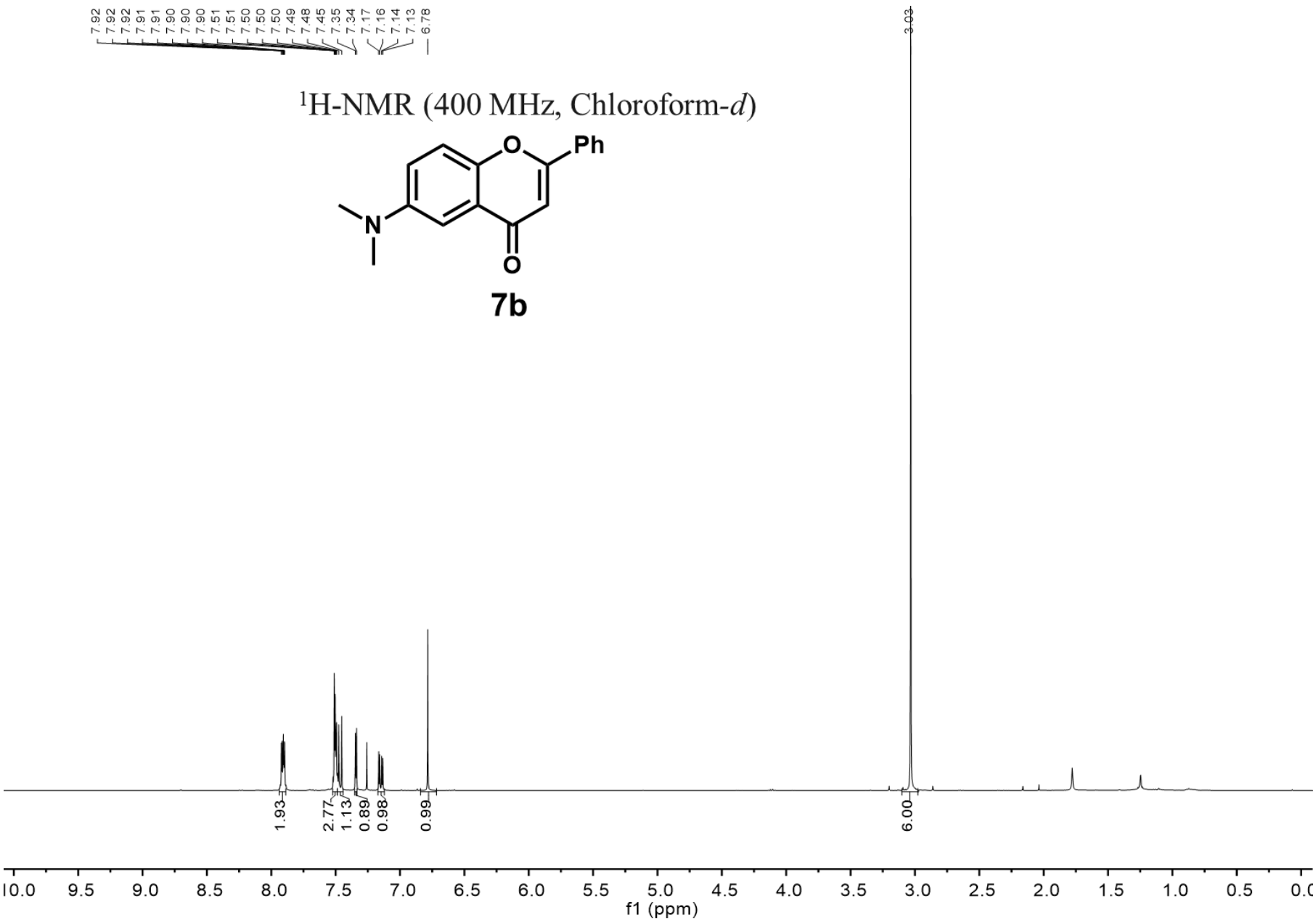


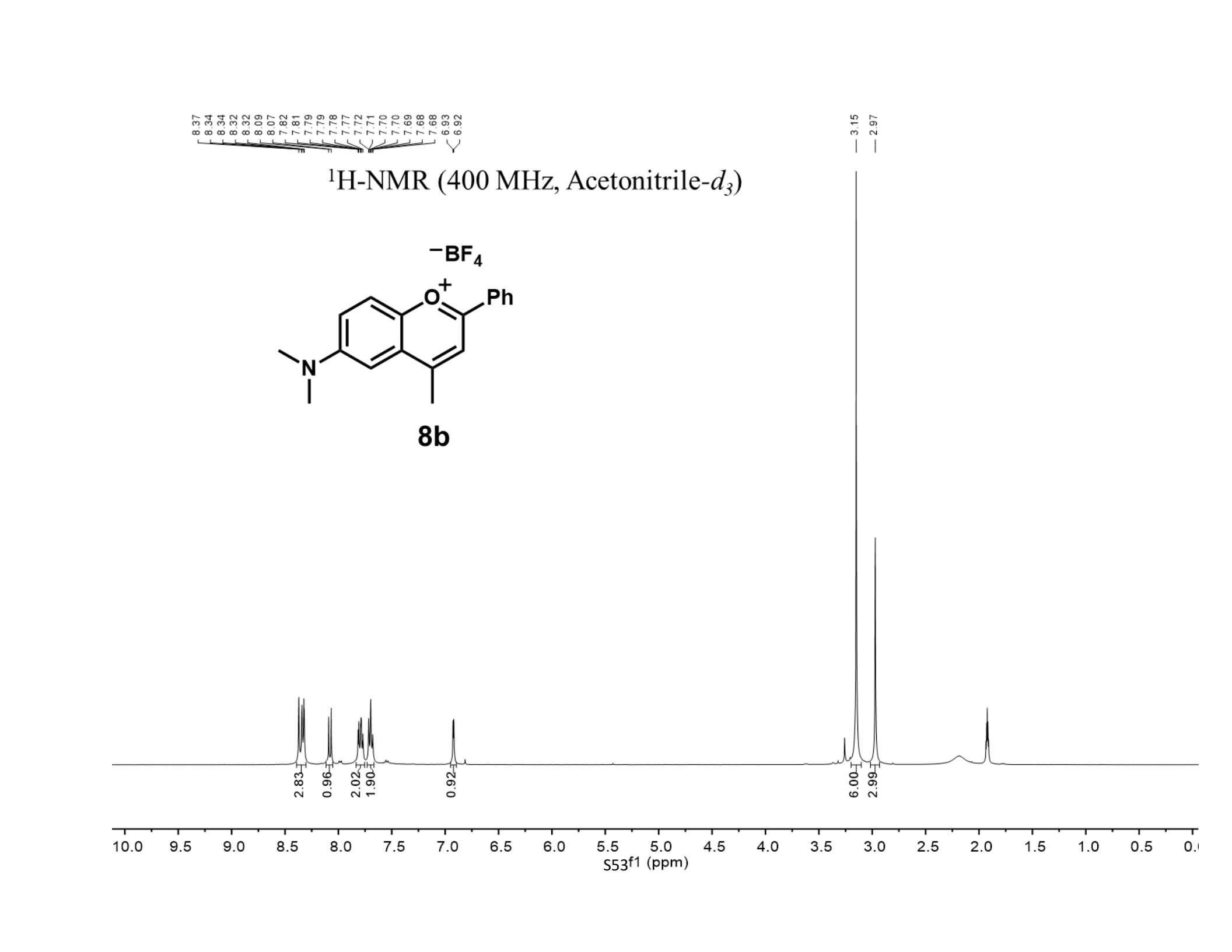
^{1}H-NMR (400 MHz, Chloroform-*d*)

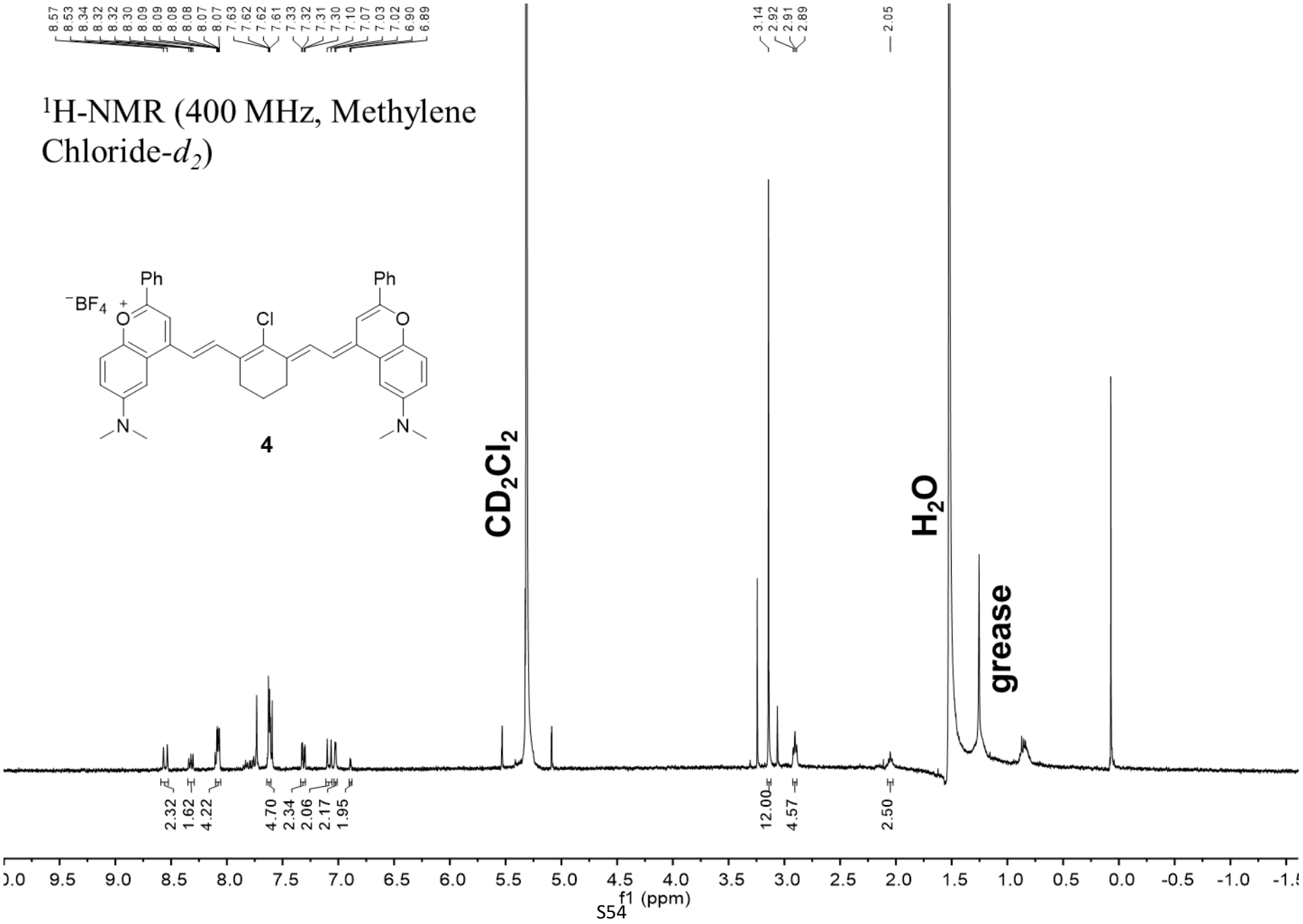


6b

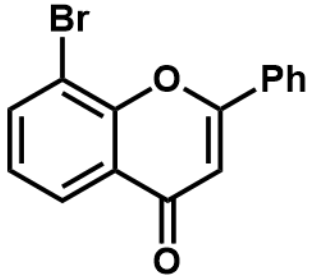



7.92
7.92
7.92
7.91
7.91
7.90
7.90
7.90
7.51
7.51
7.50
7.50
7.50
7.49
7.48
7.45
7.35
7.34
7.17
7.16
7.14
7.13
6.78
3.03
1H-NMR (400 MHz, Chloroform-d)
O
Ph
N
O
7b
1.93
2.77
1.13
0.89
0.98
0.99
6.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

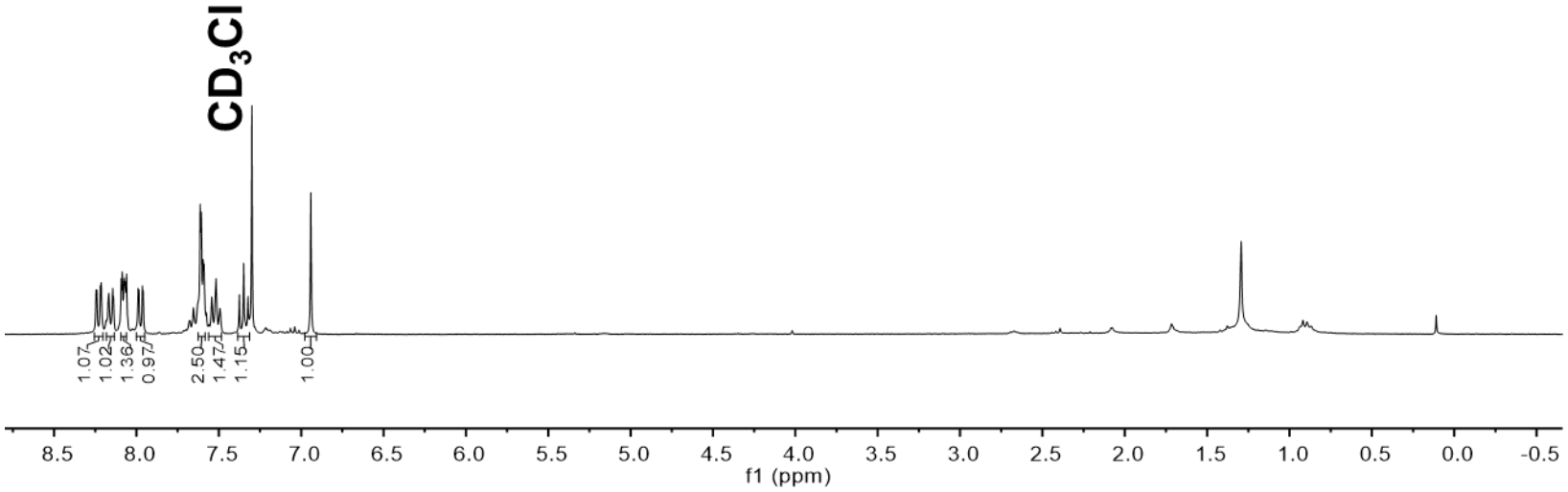

8.37
8.34
8.34
8.32
8.32
8.09
8.07
7.82
7.81
7.79
7.79
7.78
7.77
7.72
7.71
7.70
7.70
7.69
7.68
7.68
6.93
6.92
3.15
2.97
^{1}H-NMR (400 MHz, Acetonitrile-d_3)
$^-BF_4$
O
+
Ph
N
8b
2.83
0.96
2.02
1.90
0.92
6.00
2.99
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
S53f1 (ppm)

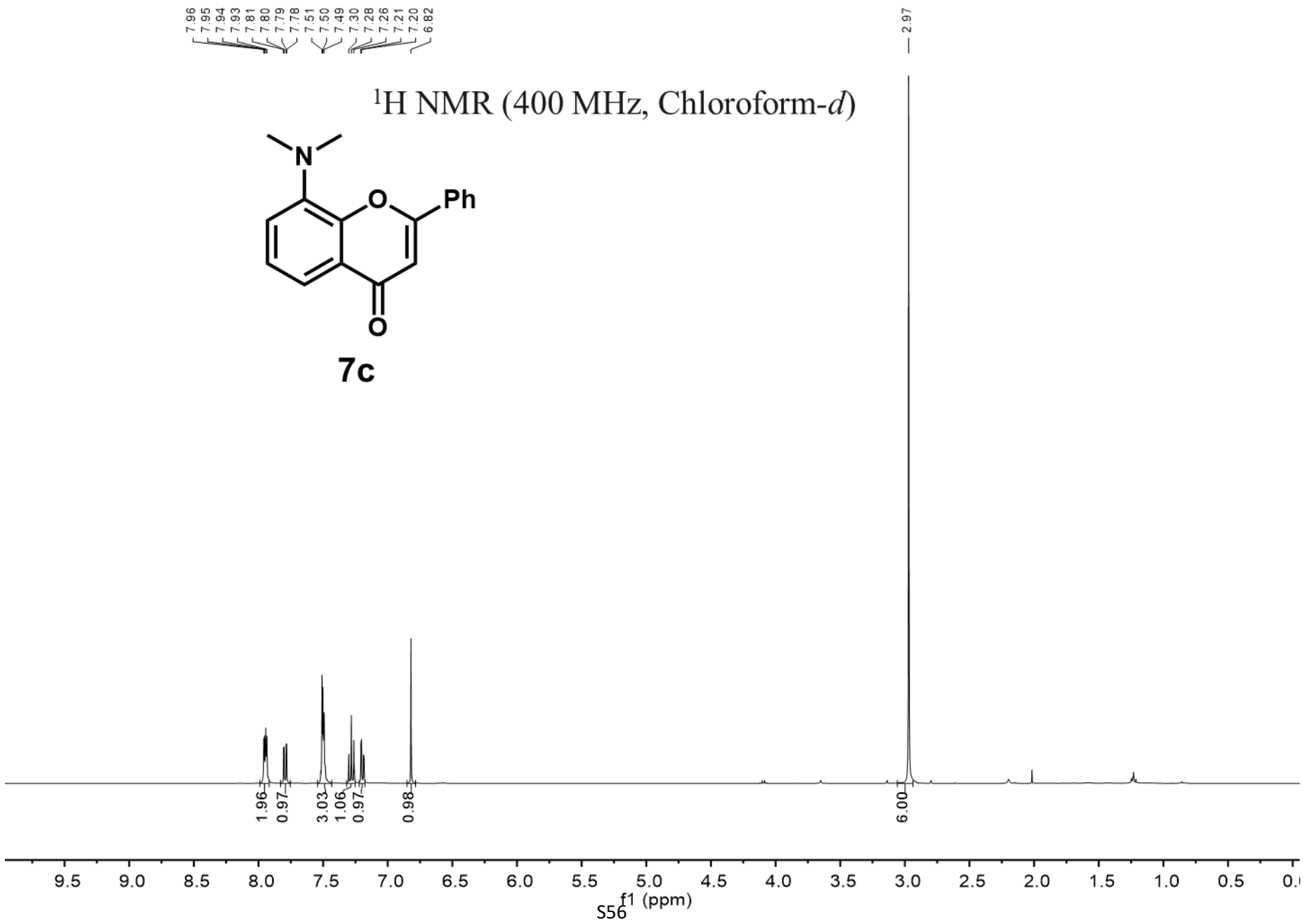

8.57
8.53
8.34
8.32
8.32
8.30
8.09
8.09
8.08
8.08
8.07
8.07
7.63
7.62
7.62
7.61
7.33
7.32
7.31
7.30
7.10
7.07
7.03
7.02
6.90
6.89
3.14
2.92
2.91
2.89
2.05
[1]H-NMR (400 MHz, Methylene Chloride-d_2)
Ph
$^{-}BF_4$
O
Cl
Ph
O
N
N
4
CD_2Cl_2
H_2O
grease
2.32
1.62
4.22
4.70
2.34
2.06
2.17
1.95
12.00
4.57
2.50
f1 (ppm)

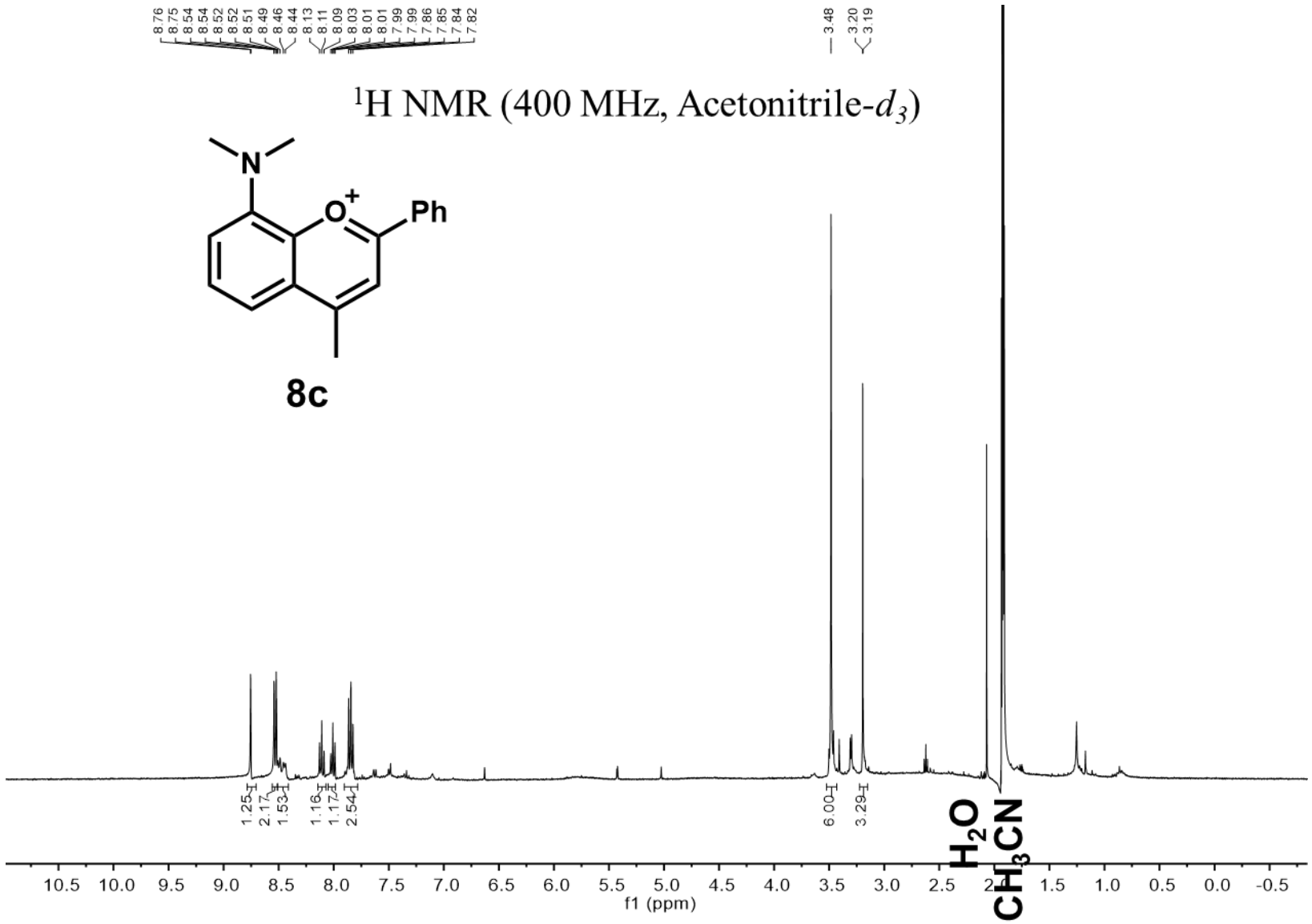
^{1}H-NMR (300 MHz, Chloroform-*d*)



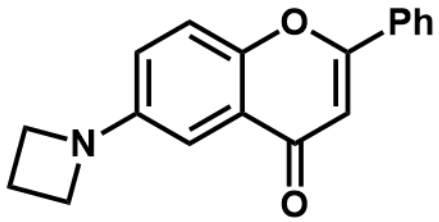
6c



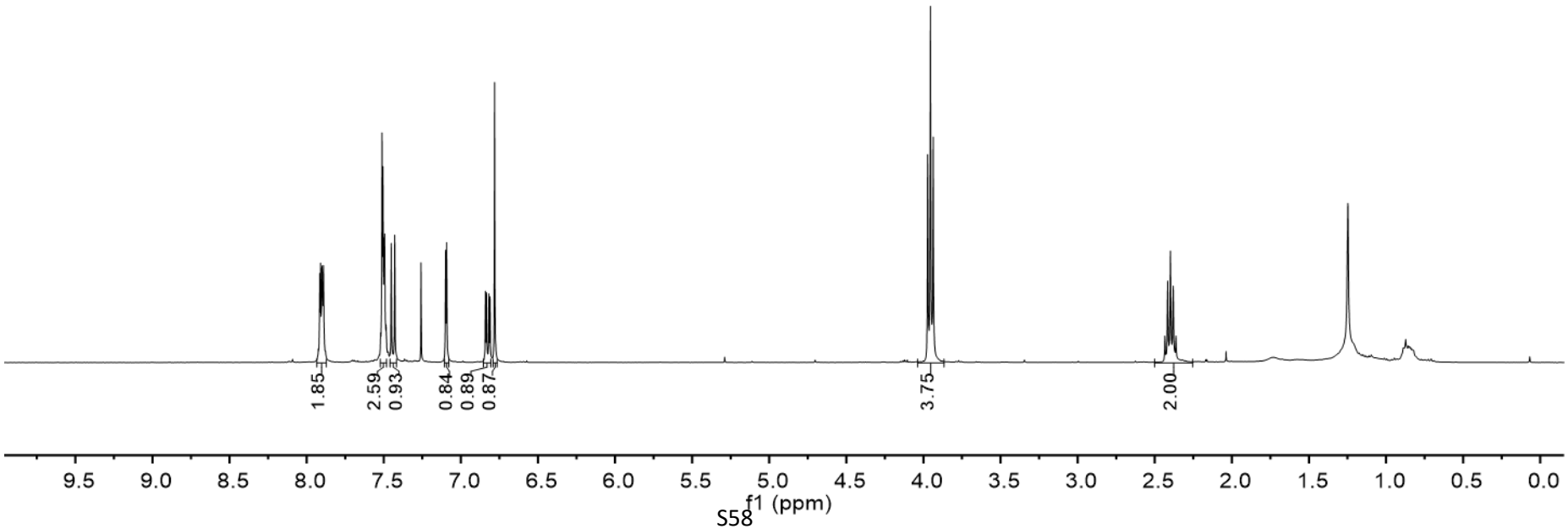

7.96
7.95
7.94
7.93
7.81
7.80
7.79
7.78
7.51
7.50
7.49
7.30
7.28
7.26
7.21
7.20
6.82
2.97
1H NMR (400 MHz, Chloroform-d)
N
O
Ph
O
7c
1.96
0.97
3.03
1.06
0.97
0.98
6.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

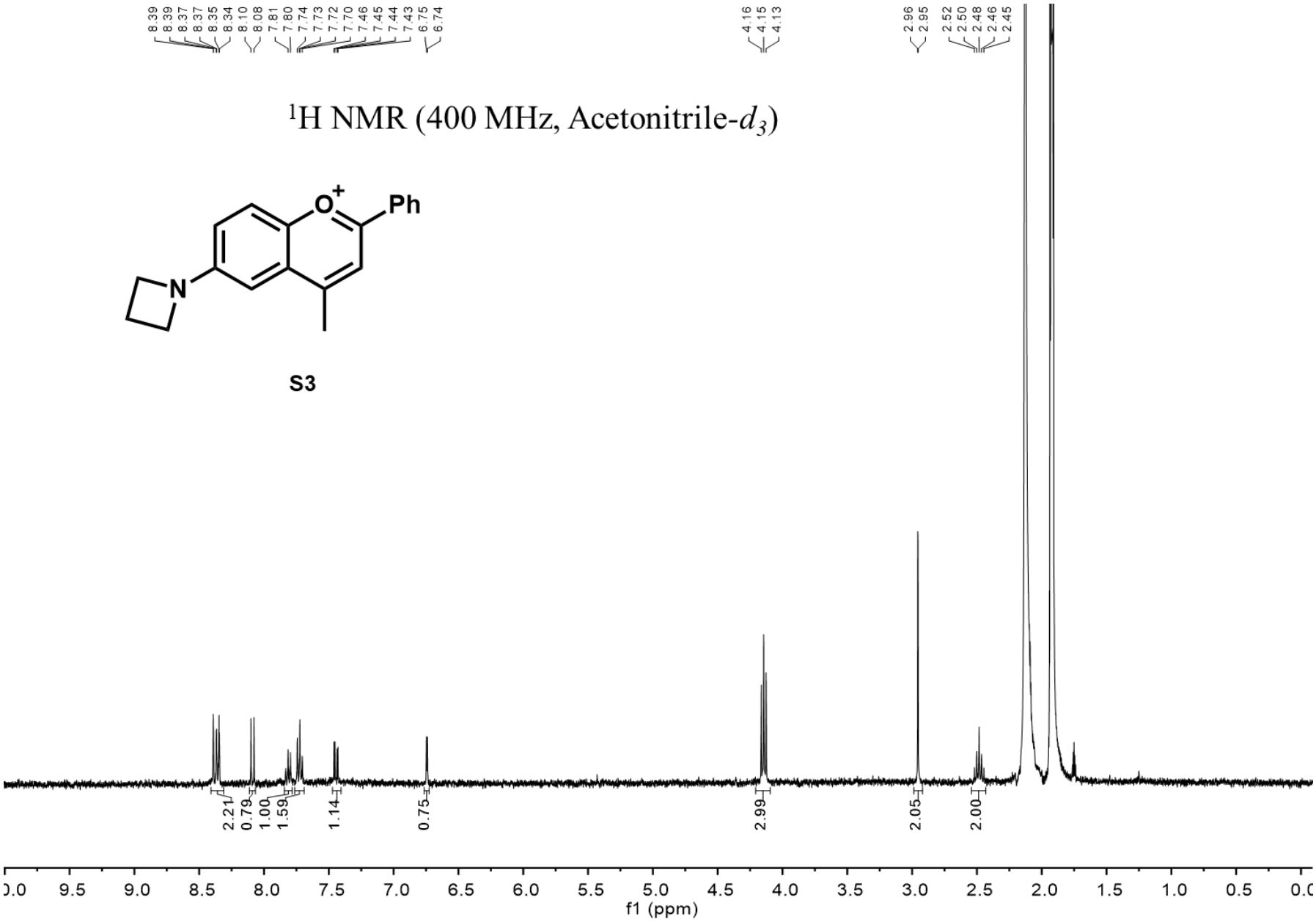

8.76
8.75
8.54
8.54
8.52
8.52
8.51
8.49
8.46
8.44
8.13
8.11
8.09
8.03
8.01
8.01
7.99
7.99
7.86
7.85
7.84
7.82
3.48
3.20
3.19
1H NMR (400 MHz, Acetonitrile-d3)
N
O+
Ph
8c
1.25
2.17
1.53
1.16
1.17
2.54
6.00
3.29
H2O
CH3CN
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

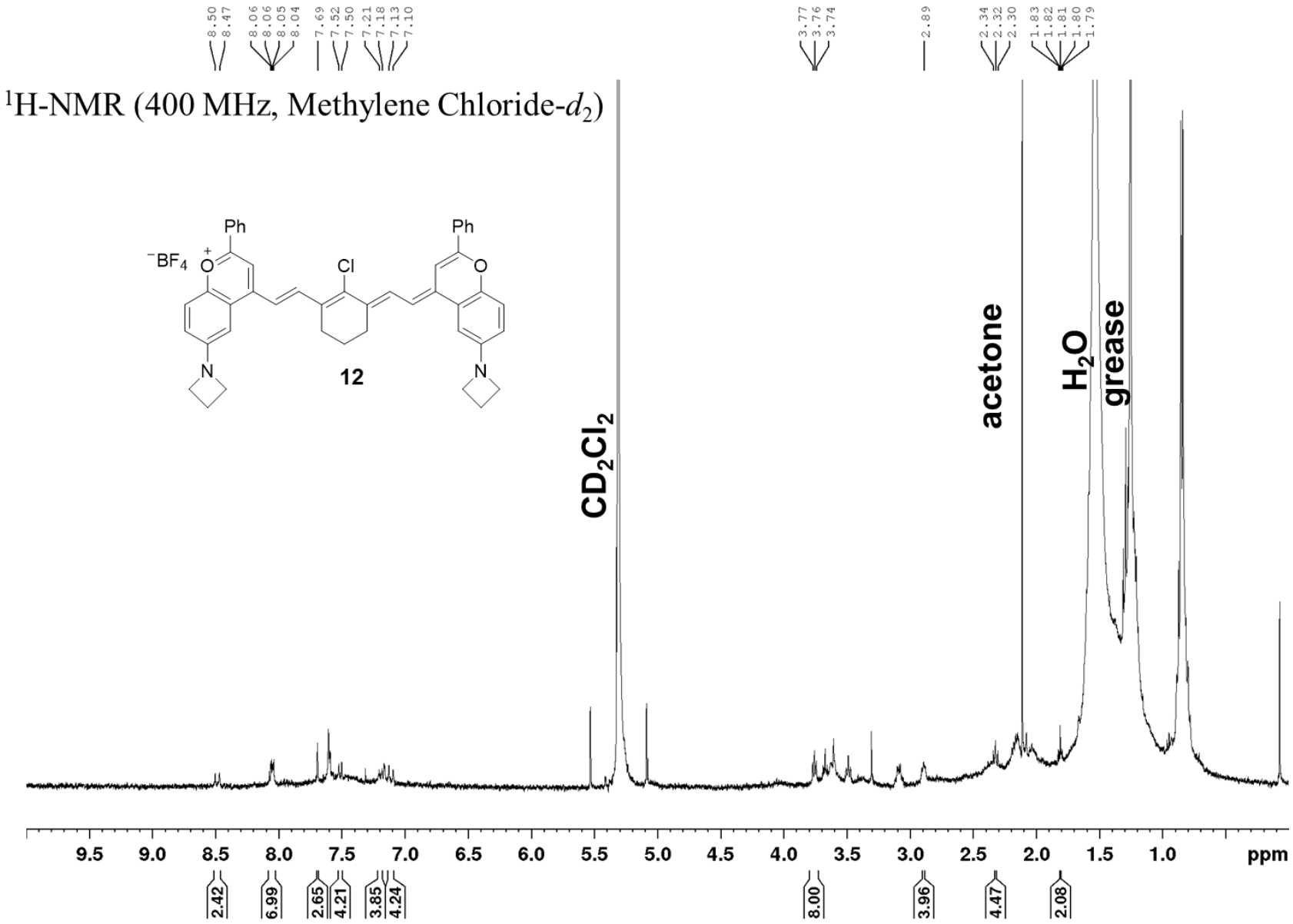
^{1}H NMR (400 MHz, Chloroform-*d*)

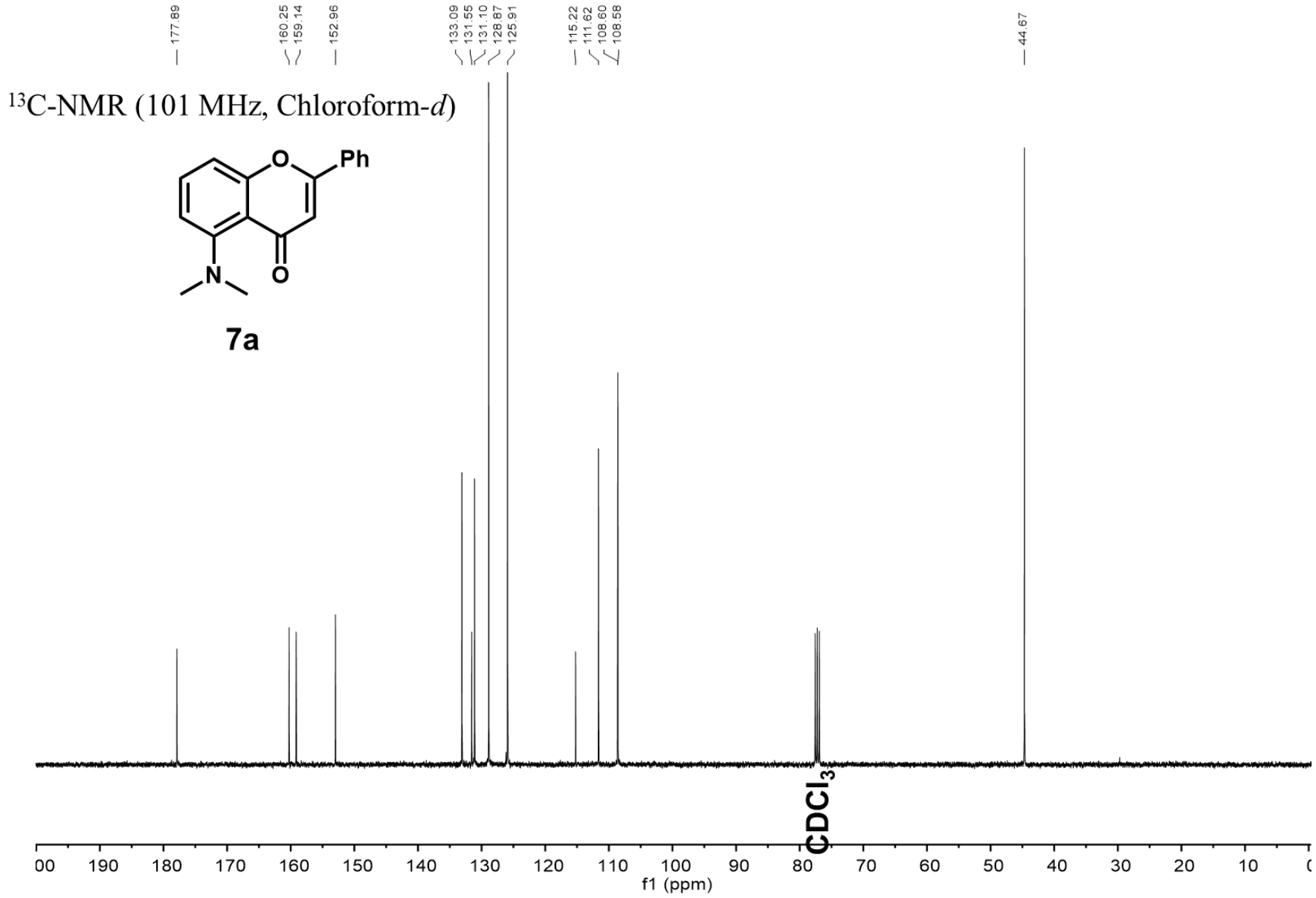


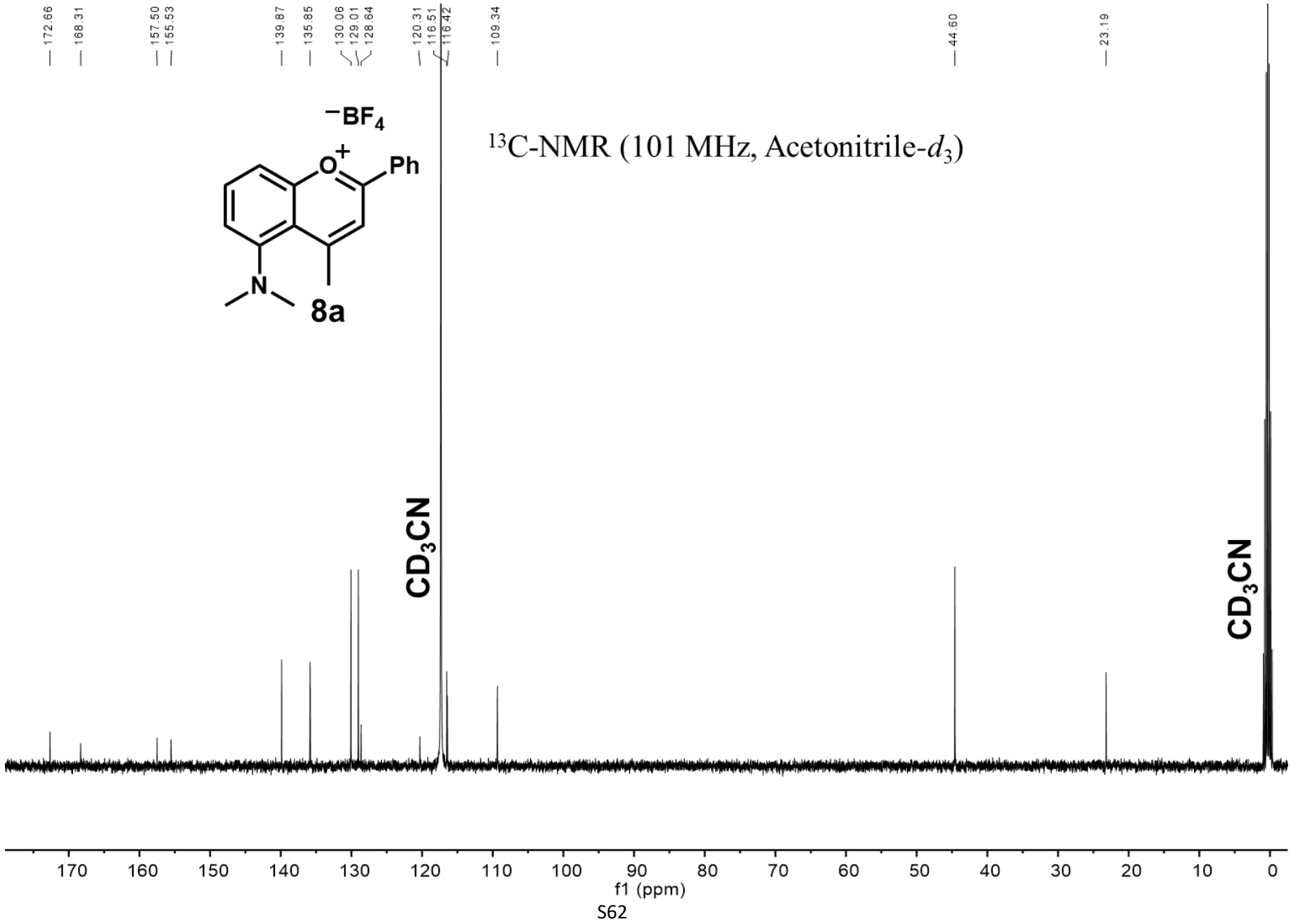
S2



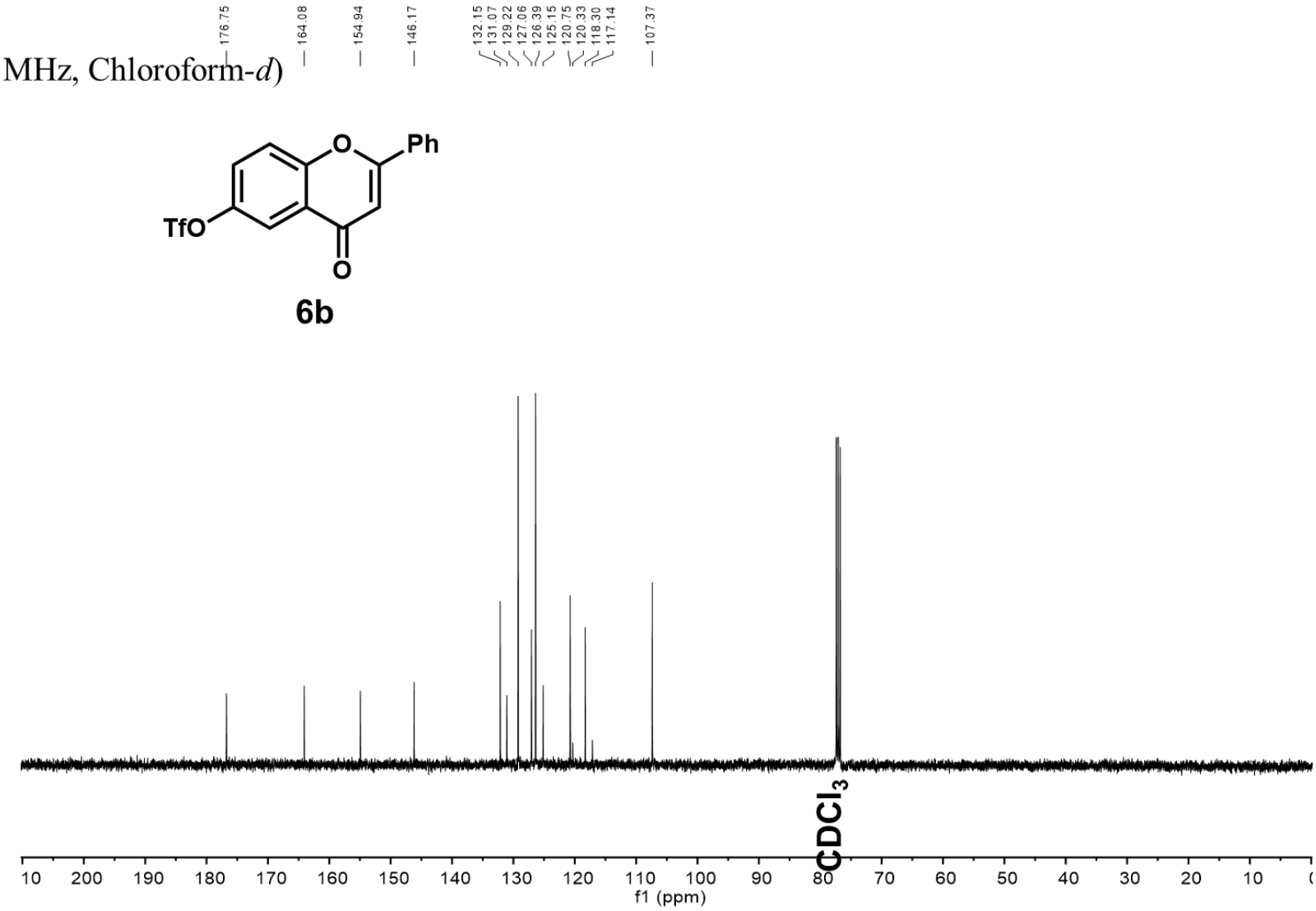

8.39
8.39
8.37
8.37
8.35
8.34
8.10
8.08
7.81
7.80
7.74
7.73
7.72
7.70
7.46
7.45
7.44
7.43
6.75
6.74
4.16
4.15
4.13
2.96
2.95
2.52
2.50
2.48
2.46
2.45
1H NMR (400 MHz, Acetonitrile-d3)
O+
Ph
N
S3
2.21
0.79
1.00
1.59
1.14
0.75
2.99
2.05
2.00
f1 (ppm)

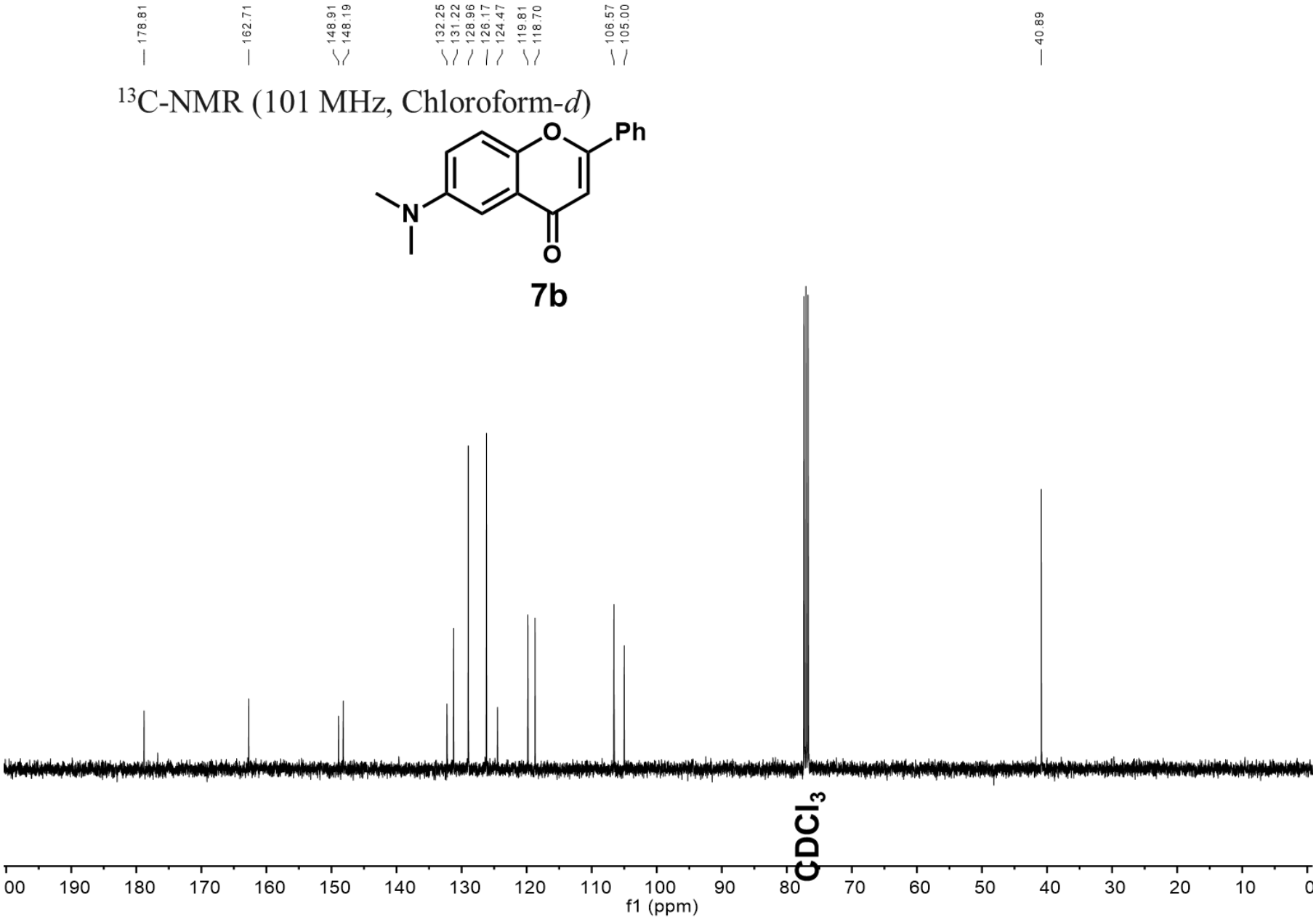

8.50
8.47
8.06
8.06
8.05
8.04
7.69
7.52
7.50
7.21
7.18
7.13
7.10
3.77
3.76
3.74
2.89
2.34
2.32
2.30
1.83
1.82
1.81
1.80
1.79
1H-NMR (400 MHz, Methylene Chloride-d2)
Ph
−BF4
O
+
Cl
Ph
O
N
N
12
CD2Cl2
acetone
H2O
grease
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.42
6.99
2.65
4.21
3.85
4.24
8.00
3.96
4.47
2.08

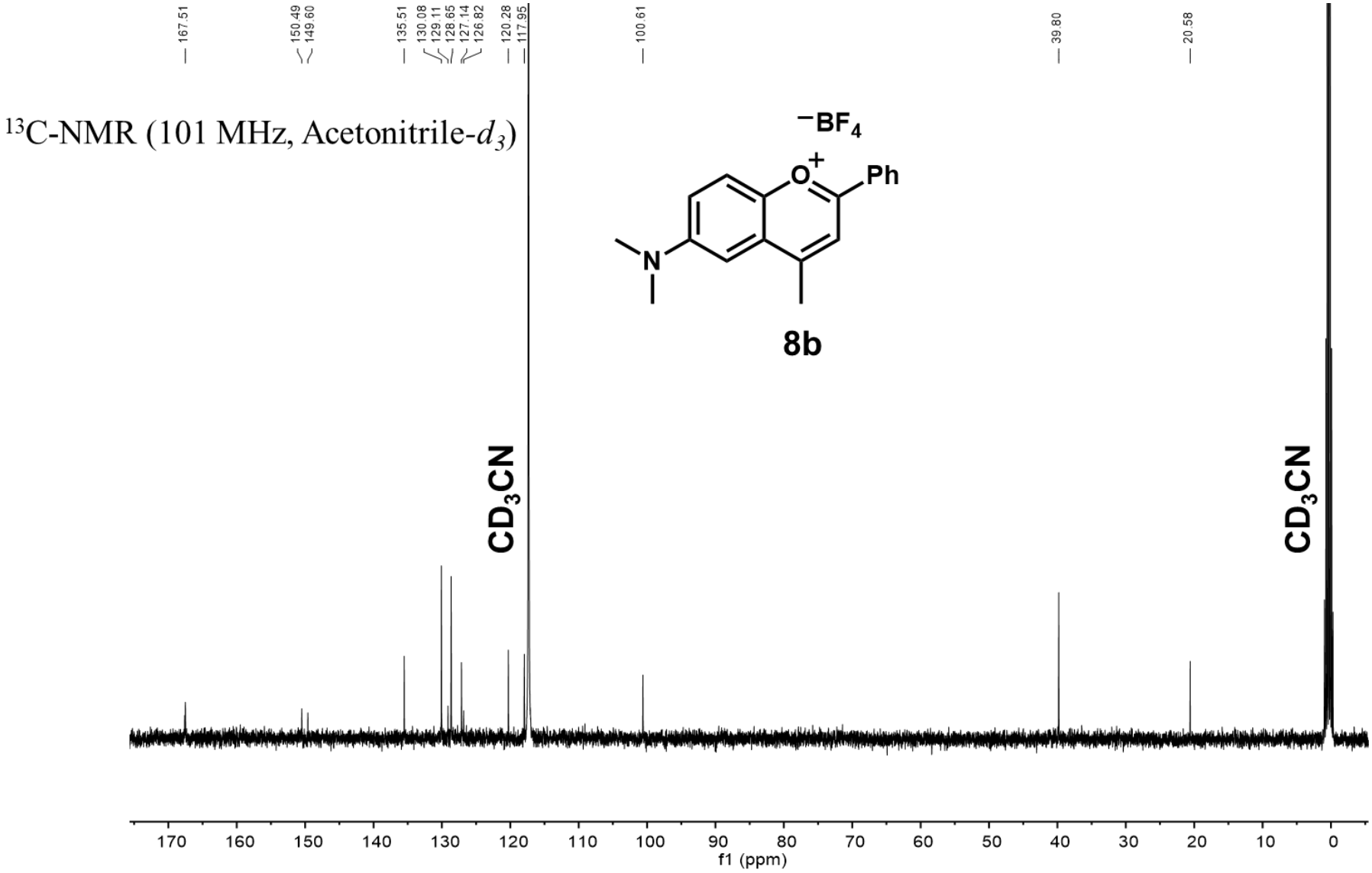

177.89
160.25
159.14
152.96
133.09
131.55
131.10
128.87
125.91
115.22
111.62
108.60
108.58
44.67
13C-NMR (101 MHz, Chloroform-d)
O
Ph
N
O
7a
CDCl3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


172.66
168.31
157.50
155.53
139.87
135.85
130.06
129.01
128.64
120.31
116.51
116.42
109.34
44.60
23.19
$^{-}BF_4$
O
+
Ph
N
8a
^{13}C-NMR (101 MHz, Acetonitrile-d_3)
CD_3CN
CD_3CN
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

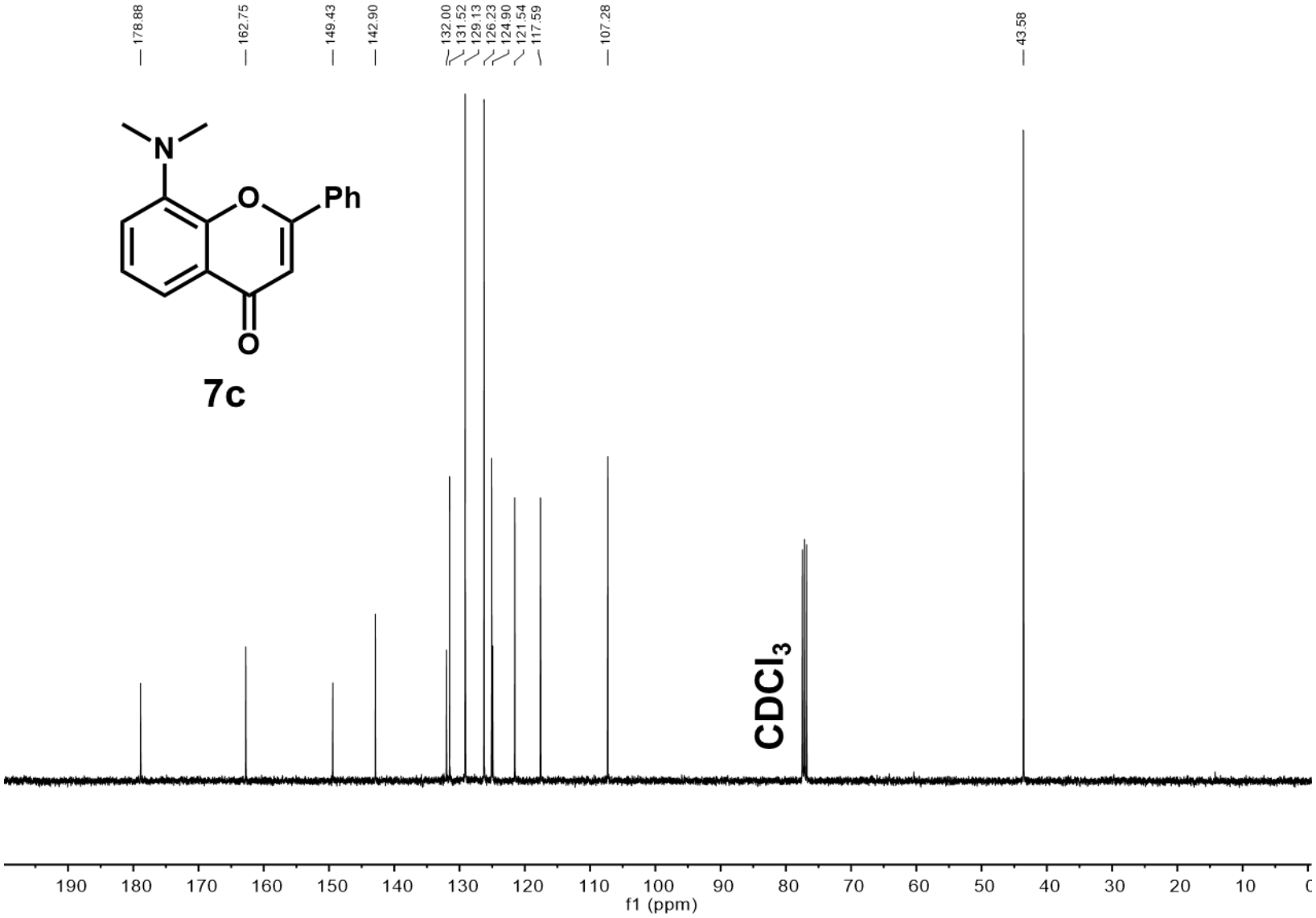
^{13}C-NMR (101 MHz, Chloroform-*d*)

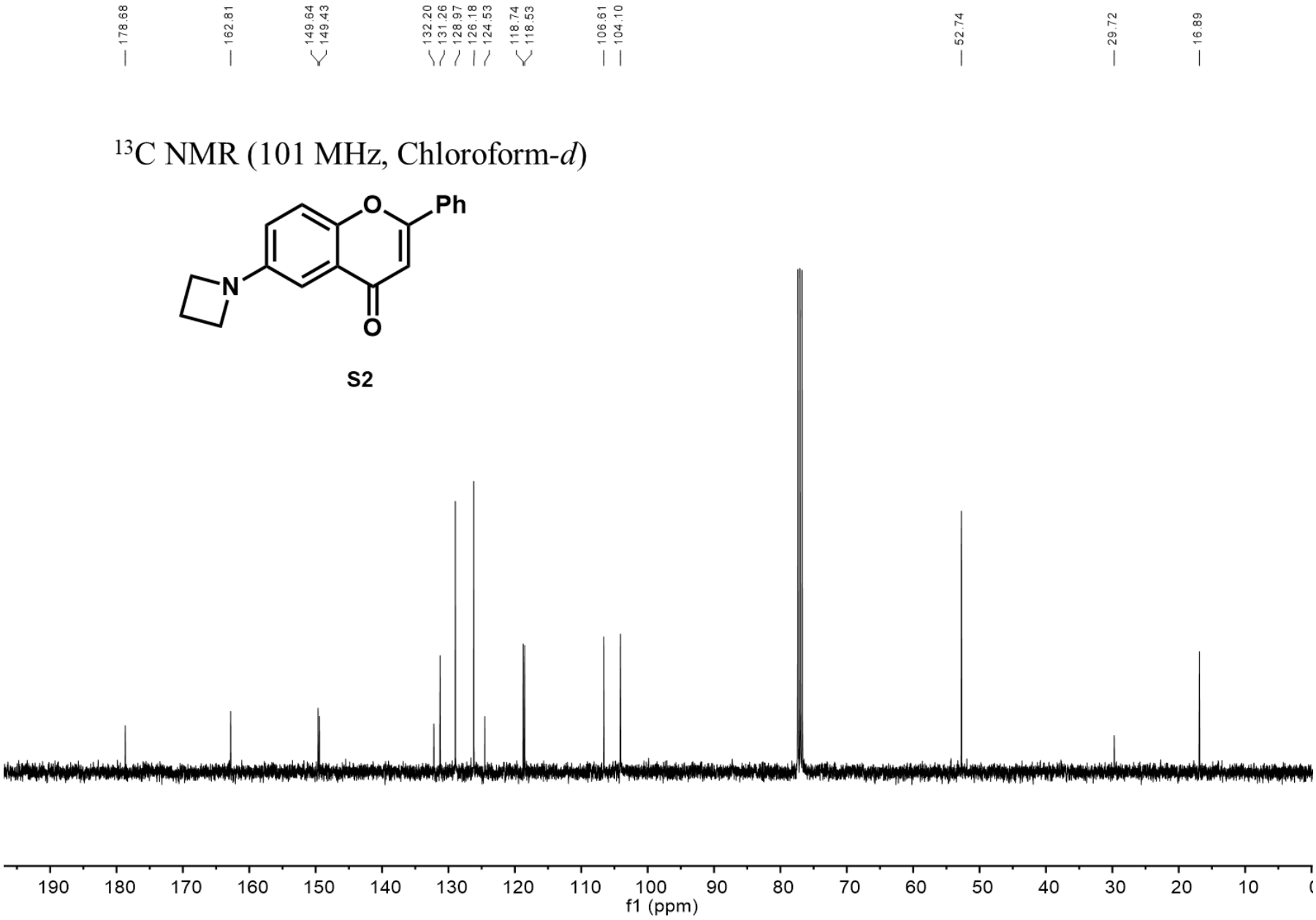



178.81
162.71
148.91
148.19
132.25
131.22
128.96
126.17
124.47
119.81
118.70
106.57
105.00
40.89
13C-NMR (101 MHz, Chloroform-d)
O
Ph
N
O
7b
CDCl3
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


167.51
150.49
149.60
135.51
130.08
129.11
128.65
127.14
126.82
120.28
117.95
100.61
39.80
20.58
13C-NMR (101 MHz, Acetonitrile-d3)
−BF4
O+
Ph
N
8b
CD3CN
CD3CN
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

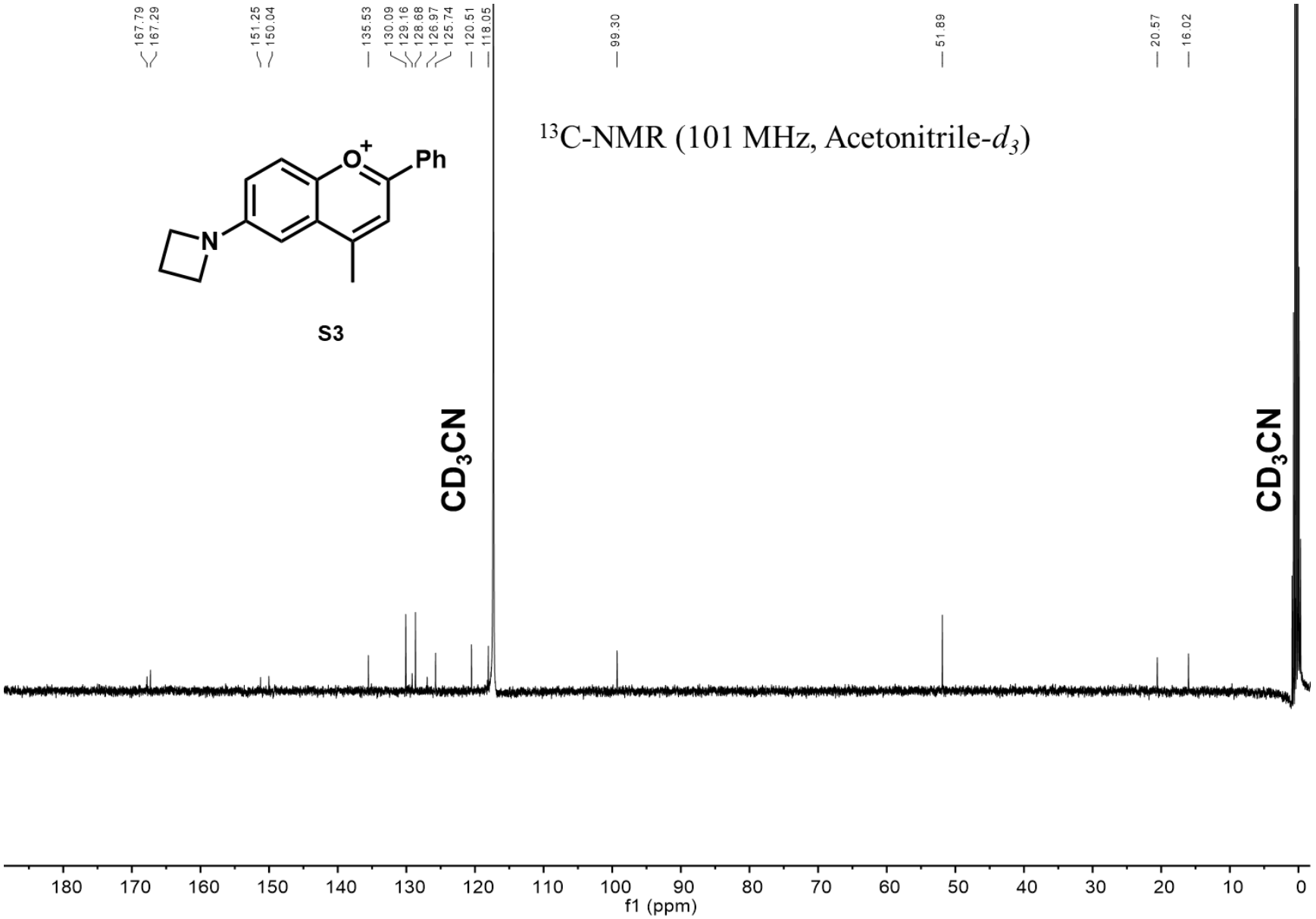
^{1}H NMR (400 MHz, Chloroform-*d*)



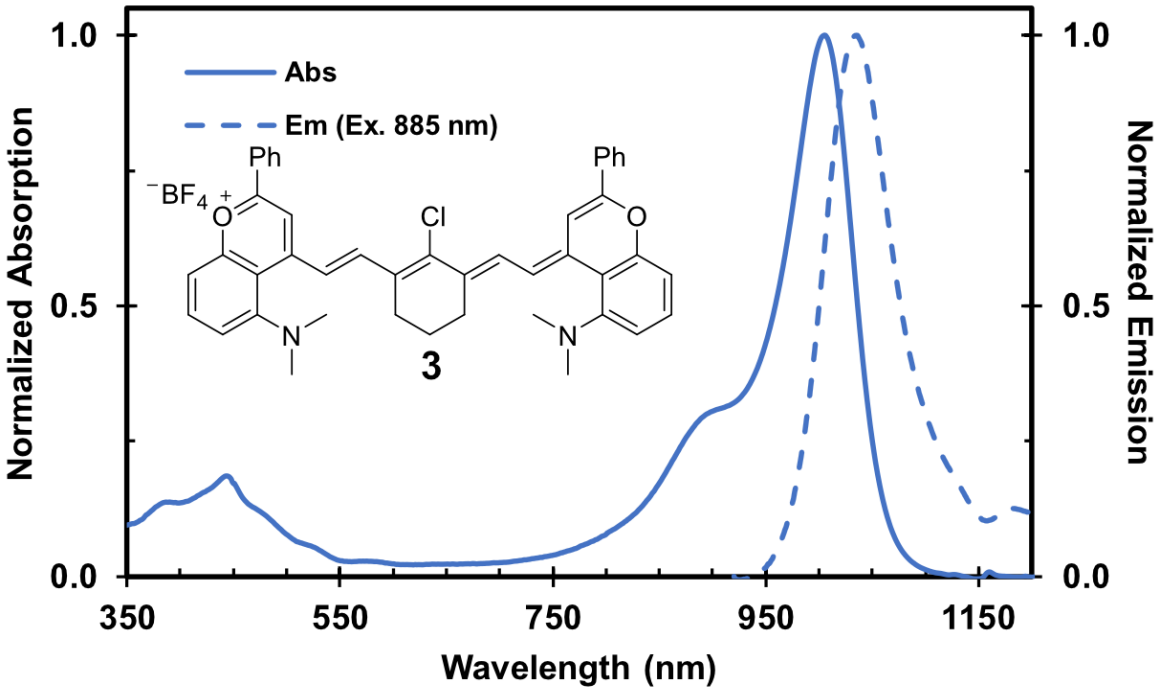


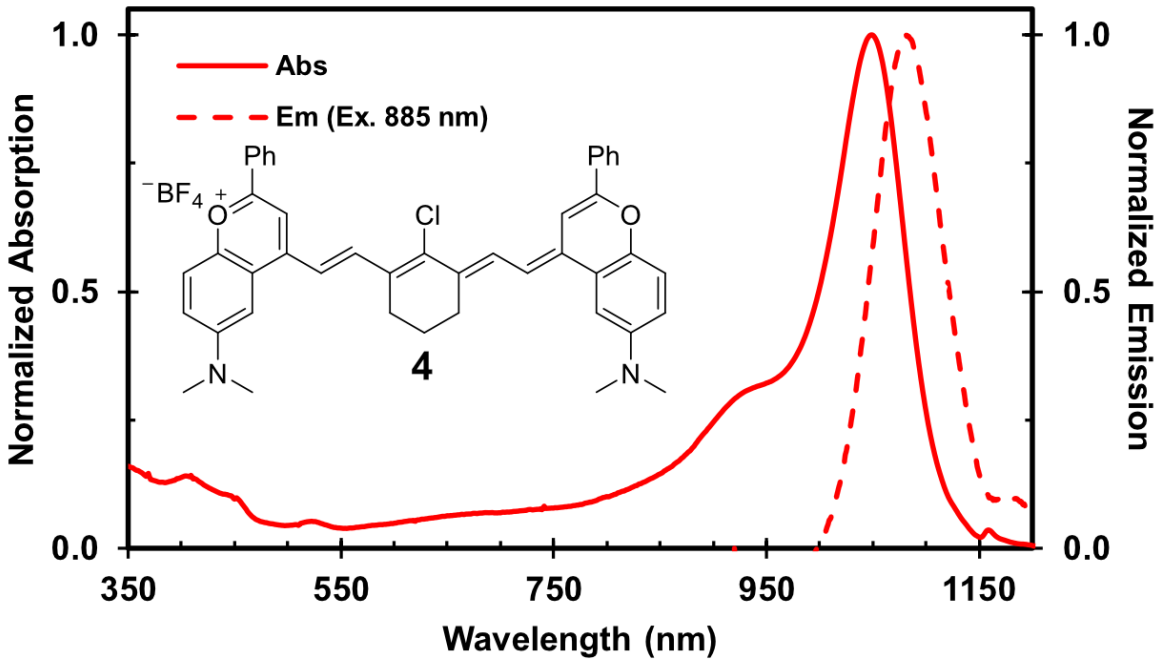
^{13}C NMR (101 MHz, Chloroform-*d*)

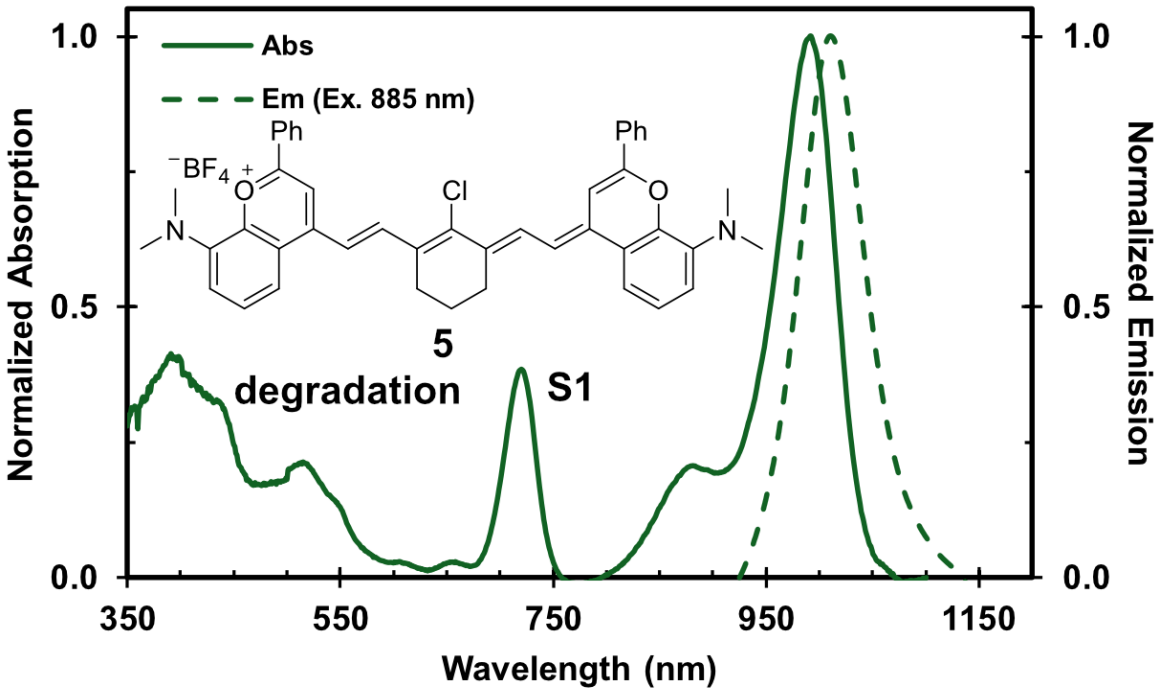
S2

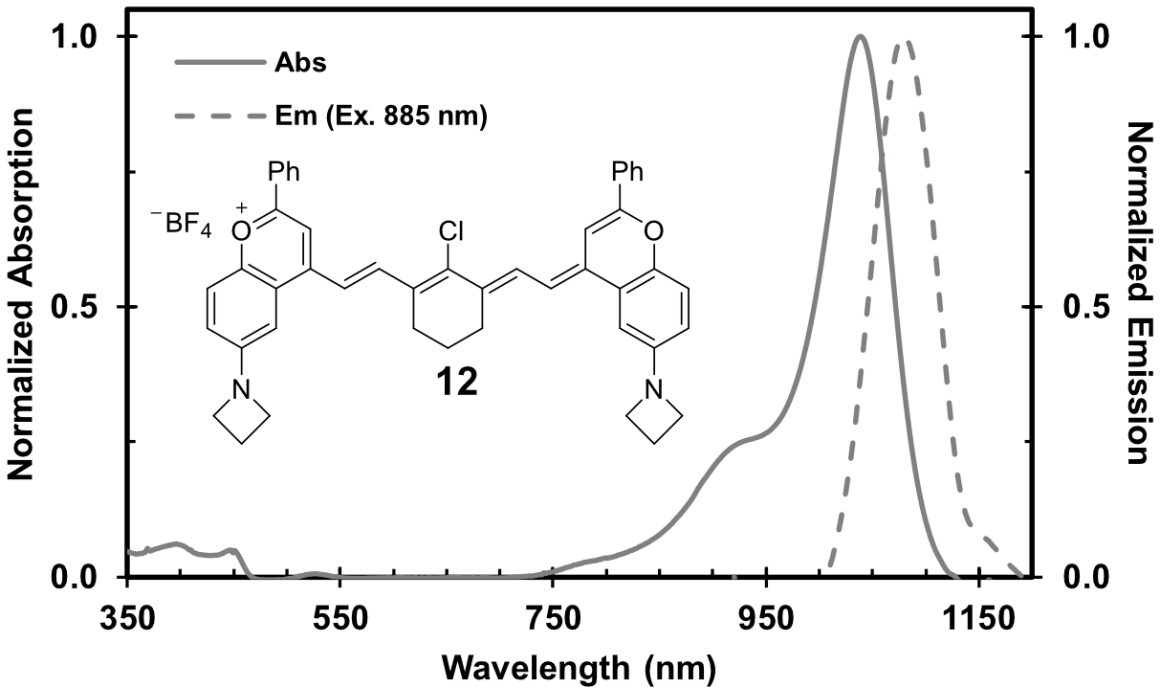

167.79
167.29
151.25
150.04
135.53
130.09
129.16
128.68
126.97
125.74
120.51
118.05
99.30
51.89
20.57
16.02
^{13}C-NMR (101 MHz, Acetonitrile-d_3)
Ph
O+
N
S3
CD3CN
CD3CN
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

Absorption/Emission Spectra :






Abs
Em (Ex. 885 nm)
Ph
Ph
$^{-}BF_4$ +
O
Cl
O
N
N
5
degradation
S1
Normalized Absorption
Normalized Emission
1.0
0.5
0.0
350
550
750
950
1150
Wavelength (nm)


Abs
Em (Ex. 885 nm)
Ph
Ph
$^{-}BF_4$ +
O
Cl
O
N
N
12
Normalized Absorption
Normalized Emission
1.0
0.5
0.0
350
550
750
950
1150
Wavelength (nm)

References:

(1) Semonin, O. E.; Johnson, J. C.; Luther, J. M.; Midgett, A. G.; Nozik, A. J.; Beard, M. C. Absolute Photoluminescence Quantum Yields of IR-26 Dye, PbS, and PbSe Quantum Dots. *J. Phys. Chem. Lett.* **2010**, *1* (16), 2445–2450.

(2) Fitzmaurice, R. J.; Etheridge, Z. C.; Jumel, E.; Woolfson, D. N.; Caddick, S. Microwave Enhanced Palladium Catalysed Coupling Reactions: A Diversity-Oriented Synthesis Approach to Functionalised Flavones. *Org. Lett.* **2006**, *8* (1), 11-13.

(3) Pajtás, D.; Patonay, T.; Kónya, K. Synthesis of 8-Bromoflavone and Its Buchwald-Hartwig Reaction with Amines. *Synth.* **2016**, *48* (1), 97–102.

(4) Schrödinger Release 2019-4: Maestro, Schrödinger, LLC, New York, NY, 2019. No Title.

(5) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. *Gaussian 16 Rev. B.01*, Wallingford, CT, **2016**.

(6) Neese, F. The ORCA Program System. *WIREs Comput. Mol. Sci.* **2012**, *2* (1), 73–78.