Supporting Information

for

Fluorofluorophores: Fluorescent fluorous chemical tools spanning the visible spectrum

Ellen M. Sletten and Timothy M. Swager

Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139

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Supporting Tables

Table S1. Solubility of fluorofluorophores **2**–**7** in organic and semifluorinated solvents.

Fluorophore		**Solubility**							
#	wt% F	Acetone	EtOH	THF	DCM	PhMe	$PhCF_3$	TFE	HFIPA
2	59%	Y	M	Y	Y	Y	Y	Y	Y
3	61%	Y	M	Y	Y	Y	Y	Y	Y
4	54%	Y	S	Y	Y	M	Y	Y	Y
5	59%	Y	M	Y	Y	S	Y	Y	Y
6	60%	M	S	S	N	S	M	S	M
7	56%	Y	Y	M	Y	S	Y	Y	Y

Solubility key: N (no) = not soluble, Y (yes) = more than 1 mg/mL, S (sparingly) = less than 0.1 mg/mL, M (moderate) = between 0.1 mg/mL and 1 mg/mL. Solubilities determined by visual inspection.

Table S2. Solubility of fluorofluorophores **2**–**7** in fluorous solvents.

Fluorophore		**Solubility**					
#	wt% F	$MeOC_4F_9$	PFTPA	$F_{17}C_8I$[a]	PFMC[b]	PFD	PFH
2	59%	M	M	Y	S	S	S
3	61%	M	M	Y	M	S	S
4	54%	S	M	M	S	S	N
5	59%	S	M	Y	S	N	N
6	60%	S	S	S	N	S	N
7	56%	S	S	M	S	N	S

Solubility key: N (no) = not soluble, Y (yes) = more than 1 mg/mL, S (sparingly) = less than 0.1 mg/mL, M (moderate) = between 0.1 mg/mL and 1 mg/mL. Solubilities determined by visual inspection.
Abbreviation key: PFTPA = perfluorotripropylamine, PFMC = perfluoromethylcyclohexane, PFD = perfluorodecalin, PFH = perfluorohexanes.
[a]Good solubility was observed in perfluorooctyl iodide; however, it appeared to quench emission.
[b]We attempted to obtain f_i values[1] for the fluorofluorophores; however, their limited solubility in both toluene and perfluoromethylcyclohexane prevented us from obtaining accurate partition measurements.

[1] Kiss, L.E.; Kovesdi, I.; Rabai, J. "An improved design of fluorophilic molecules: prediction of the ln*P* fluorous partition coefficient, fluorophilicity, using 3D QSAR descriptors and neural networks." *J. Fluor. Chem.* **2001**, *108*, 95-109.

Supporting Figures

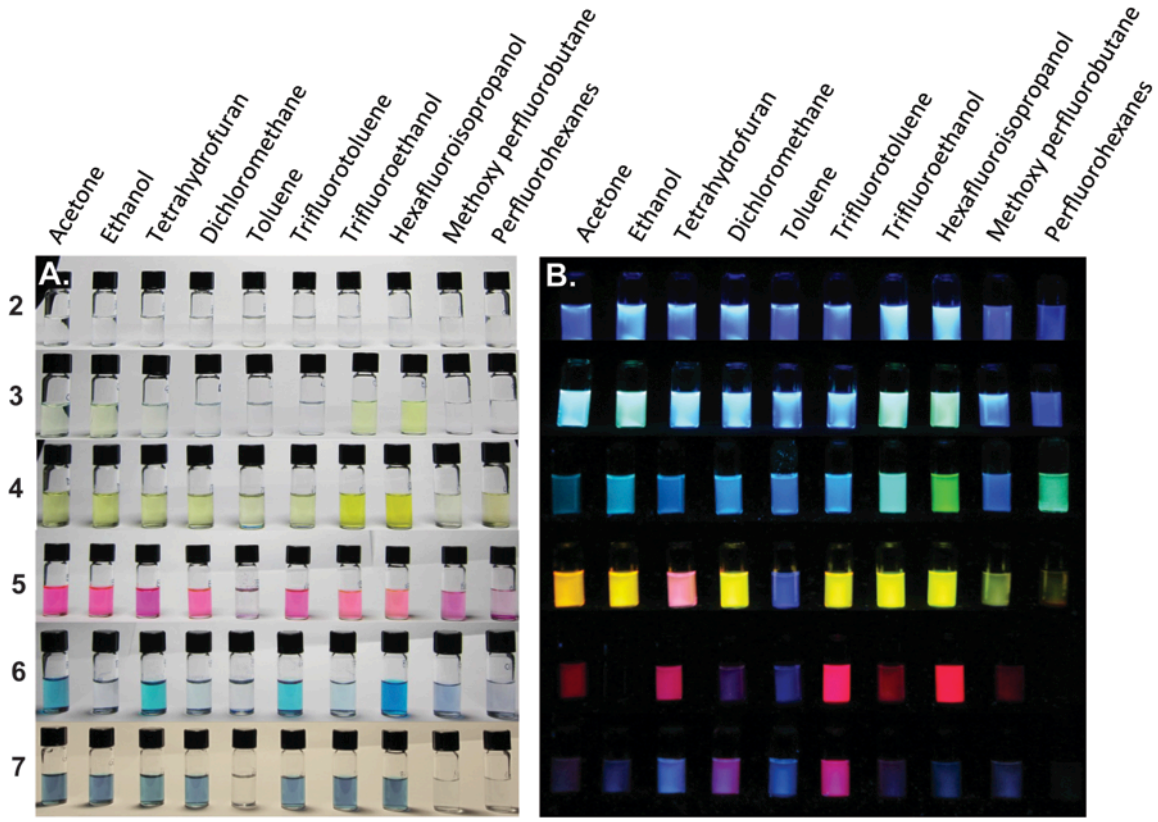


Figure S1. Solubility of fluororofluorophores **2**–**7**. 0.1 mg of **2**–**7** were dissolved in the indicated solvents (1 mL). Photographs were taken in visible (A) or long-wave UV (B) light.

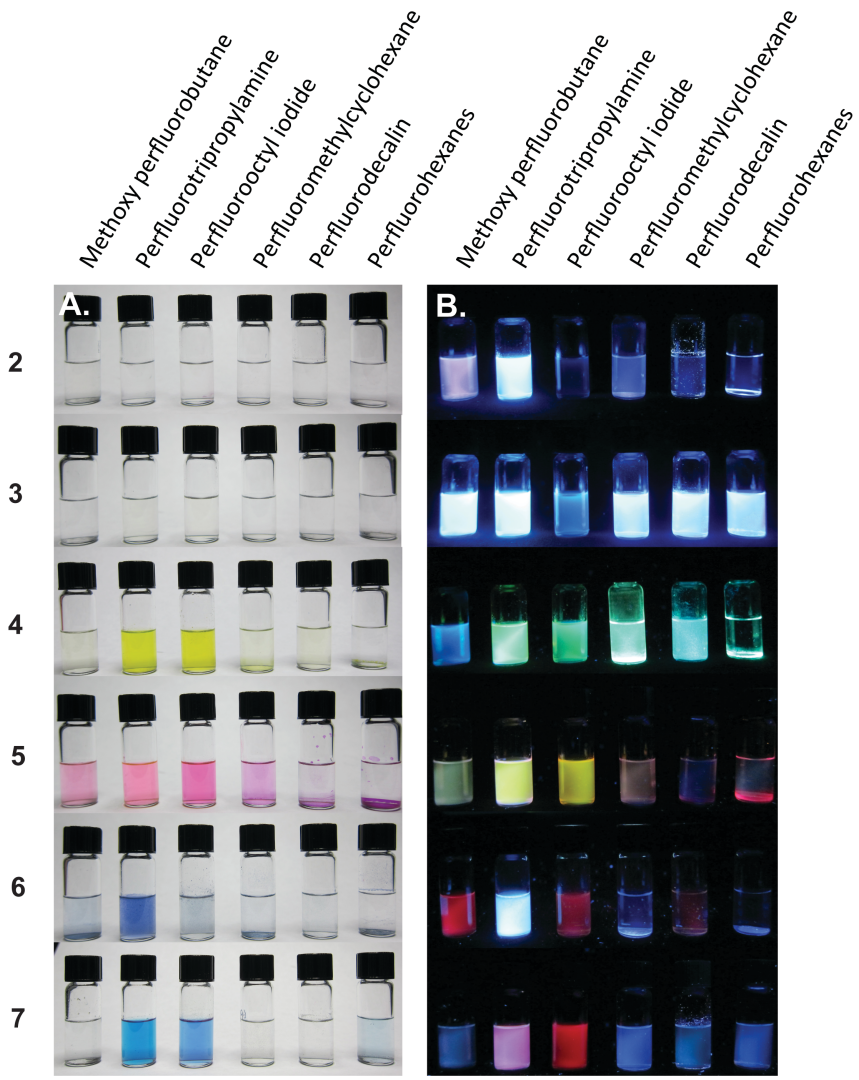


Figure S2. Solubility of fluororofluorophores **2**–**7** in fluorous solvents. 0.1 mg of **2**–**7** were dissolved in the indicated solvents (1 mL). Photographs were taken in visible (A) or long-wave UV (B) light.

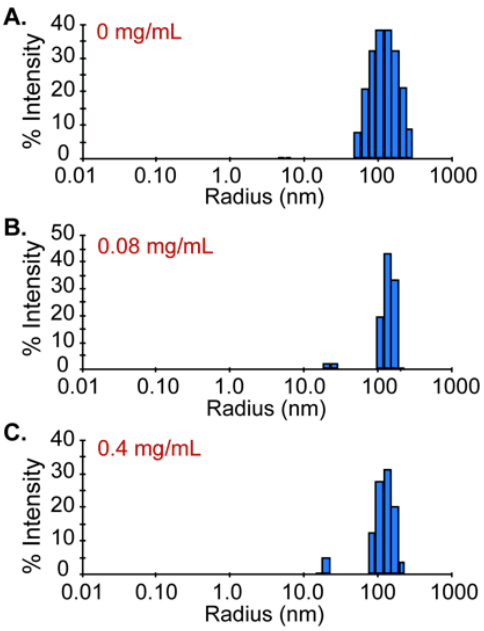


Figure S3. The addition of rhodamine **5** does not change the size of the emulsions. Dynamic light scattering of nanoemulsions (20 wt% 7:3 PFD/PFTPS, 2.8 wt% Plurnoic-F68 in PBS) containing 0 mg/mL (A), 0.08 mg/mL (B), or 0.4 mg/mL (C) rhodamine **5**.

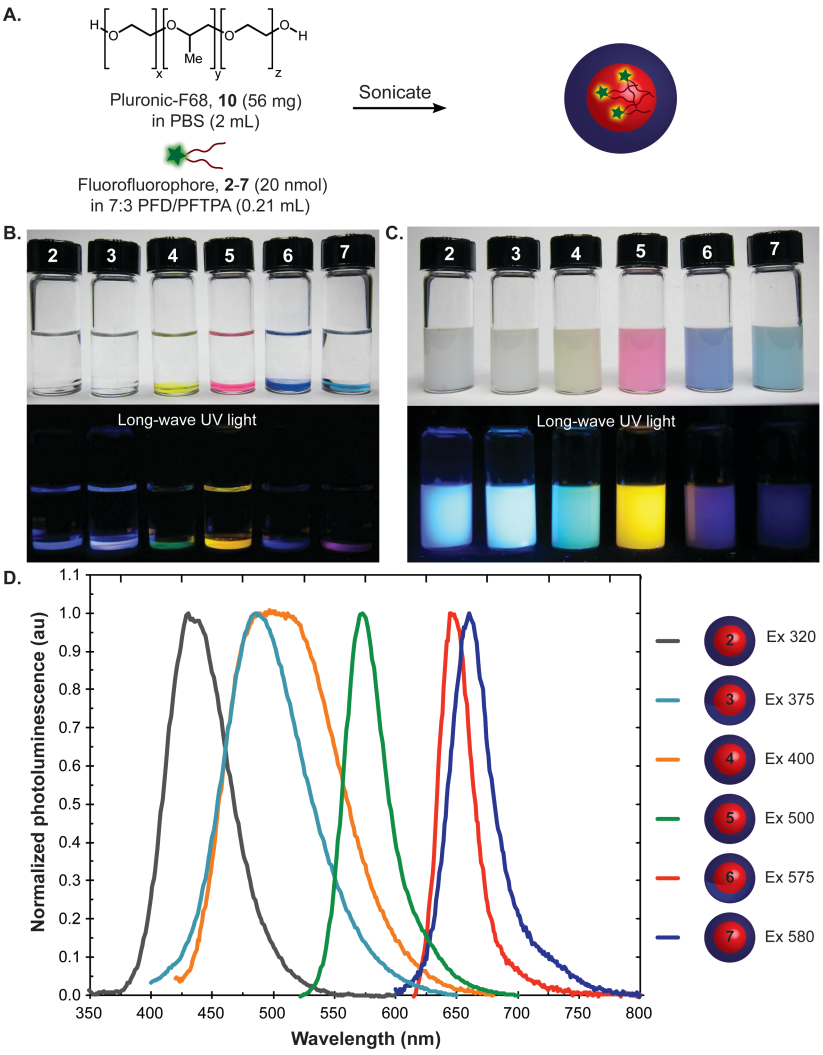


Figure S4. Fluorescent perfluorocarbon nanoemulsions. Fluorofluorophores **2–7** were dissolved in a 7:3 mixture of perfluorodecalin/perfluortripropylamine and a solution of Pluronic-F68 in PBS was added. The resulting biphasic solutions were sonicated (probe) to yield fluorescent nanoemulsions. (A) Schematic for preparation of nanoemulsions. (B) Visible and long-wave UV light photographs of the biphasic solutions prior to sonication. (C) Visible and long-wave UV light photographs of fluorescent nanoemulsions. (D) Normalized photoluminescence spectra of florescent nanoemulsions.

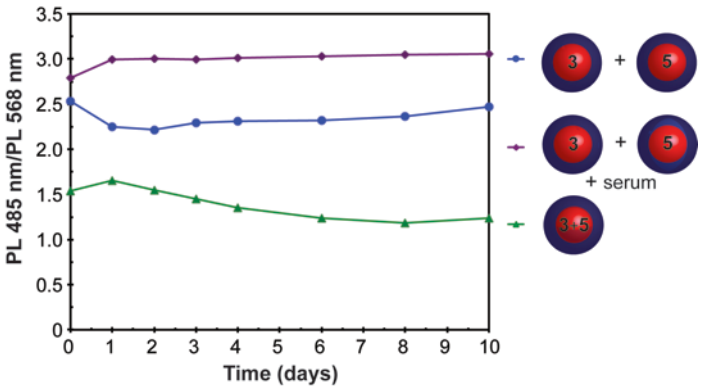


Figure S5. There is no significant exchange of fluorophores between emulsion droplets. Nanoemulsions were prepared as described in Figure 3A. Three samples were prepared: a 1:1 mixture of nanoemulsions containing **3** or **5** (blue line), a 1:1 mixture of nanoemulsions containing **3** or **5** plus serum (purple line), and nanoemulsions containing both **3** and **5** (green line). Each sample was excited at 375 nm and the photoluminescence was collected at various timepoints. The photoluminescence at 485 nm ($\lambda_{max,\ emulsion\ 3}$) was divided by the photoluminescence at 568 nm ($\lambda_{max,\ emulsion\ 5}$) and plotted vs. time. A smaller value represents more energy transfer between **3** and **5**.

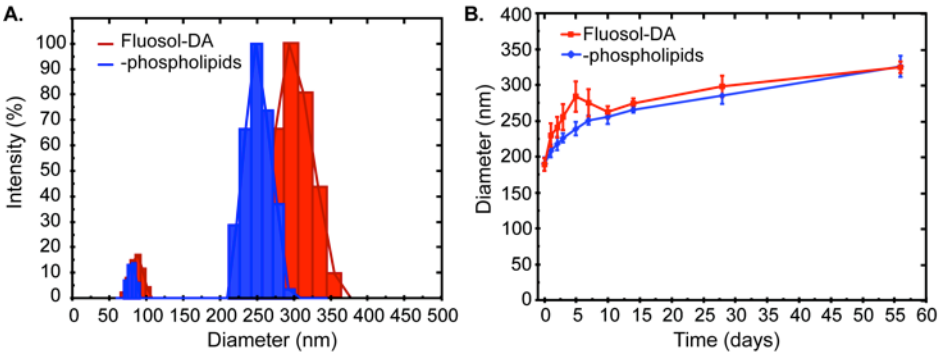
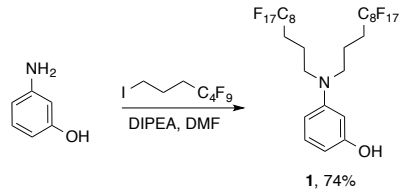


Figure S6. Comparison of Fluosol-DA 20[2] (red) and simplified formula without phospholipids and high ionic strength buffer (blue). (A) Raw dynamic light scattering data of Fluosol-DA 20 vs. nanoemulsions composed of 7:3 PFD/PFTPA (20 wt%) and Pluronic-F68 (2.8 wt%) in PBS. (B) The stability of the nanoemulsions in A over 2 months. Error bars represent the polydispersity as determined by dynamic light scattering.

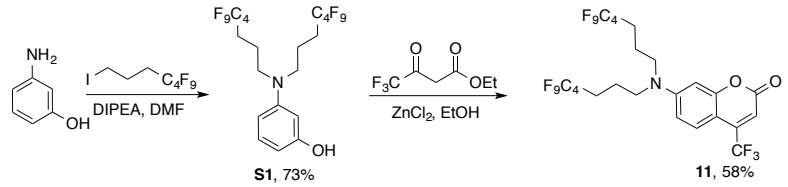
[2] Lowe, K.C. "Perfluorocarbons as Oxygen-transport fluids." *Comp. Biochem. Physiol.* **1987**, *87A*, 825-838.

Supporting Schemes

Scheme S1. Synthesis of fluorinated aminophenol **1**.



Scheme S2. Synthesis of coumarin **11**.



Scheme S3. Synthesis of coumarin **12**.

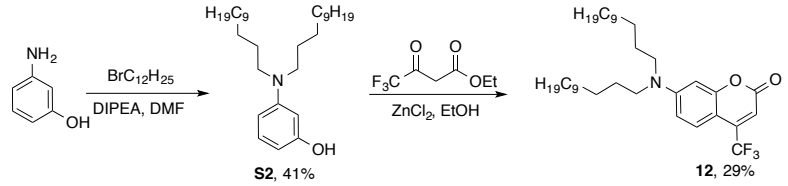


Figure Experimental Procedures

Figure 2A
$\sim 10^{-5}$ M solutions of **2**–**7** were prepared in ethanol (**2**–**5**, **7**) or acetone **6** and placed in quartz cuvettes. Absorbance spectra were obtained on a Cary 4000 UV/Vis spectrophotometer (Agilent Technologies) with a scan rate of 2000 nm/min. The instrument was blanked on the solvent prior to obtaining a spectrum. Photoluminescence spectra were obtained on a Jobin Yvon/Horiba Instruments spectrophotometer. For the photoluminescence spectra, 3 nm excitation slits and 5 nm emission slits were used. The integration time was 0.25 s. Spectra were normalized to the λ_{max} of the lowest energy transition and plotted.

Figure 2B/C
0.0001 mol **2**–**7** were placed in vials and dissolved in 1 mL trifluorotoluene (B) or toluene (C). The solutions were sonicated in a bath sonicator, allowed to settle and photographed under ambient and long-wave UV light.

Figure 3B/C
Rhodamine **5** (0.1 mg) was dissolved in PFD (18 μL, Synquest) and PFTPA (8 μL, Synquest) by bath sonication. To this solution, 28 mg/mL Pluronic-F68 (Sigma-Aldrich) in PBS (250 μL, Mediatech Inc.) was added and the biphasic mixture was sonicated (probe, 0.02 watts) at 0 °C for 15 minutes. The solution was diluted 1:100 in PBS and dropcast (5 μL) onto a clean glass slide (1 h bath sonication with acetone, 1 h bath sonication with isopropanol, dried with nitrogen) with a "window" of scotch tape. A coverslip was placed ontop and secured with clear nail polish before imaging. Confocal microscopy was performed on a Leica TCS SP2 Confocal Laser Scanning Microscope with a 63X oil objective. Excitation was performed with a 514 nm laser and emission between 530-650 nm was collected.

*As a result of the limits of optical imaging, we are only able to see the larger nanoemulsion droplets.[3] The confocal microscopy was aided by the ability to load significant amounts of fluorofluorophore in the emulsion droplets as we could not obtain images of perfluorocarbon nanoemulsions using 0.08 mg rhodamine **5** /mL total emulsion solution (350 μM **5** inside each droplet); however, when 0.4 mg **5**/mL total emulsion solution (1.7 mM **5** inside each droplet), was employed we observed images of spherical droplets. Thus, the microscopy was aided by the ability to load significant amounts of fluorofluorophore in the emulsion droplets, as we could no obtain images with*

[3] E. Abbe, *Arch. Mikrosk. Anat. Entwicklungsmech.,* 1893, **9**, 413-420.

Figure 3D

0.5 mL of three different nanoemulsions were prepared:

(A) rhodamine **5** only (0.02 mg)

(B) coumarin **3** only (0.01 mg)

(C) combination of rhodamine **5** (0.01 mg) and coumarin **3** (0.005 mg)

For each emulsion preparation, a stock solution of **3** or **5** in acetone was prepared and to eppendorf tubes, the appropriate amount to yield the above quantity was added. The acetone was allowed to evaporate and PFD (36 μL) and PFTPA (16 μL) were added and sonicated (bath) until all of the fluorophore was dissolved. A 28 mg/mL solution of Pluronic-F68 in PBS (0.5 mL) was added and the mixtures were sonicated (probe, 0.02 watts) for 15 minutes at 0 ^{o}C.

Five solutions were made from these three nanoemulsion:

(1) Nanoemulsion A (100 μL) in PBS (2.5 mL)

(2) Nanoemulsion B (100 μL) in PBS (2.5 mL)

(3) Nanoemulsion C (200 μL) in PBS (2.4 mL)

(4) Nanoemulsion A (100 μL) + B (100 μL) in PBS (2.4 mL)

(5) Nanoemulsion A (100 μL) + B (100 μL) were combined, sonicated (probe, 15 min, 0.02 watts, 0 ^{o}C) and then diluted with PBS (2.4 mL)

The photoluminescence of each mixture was measured (excitation = 375 nm, collection = 400-700 nm, excitation slit = 3 nm, emission slit = 5 nm, integration time 0.1 s). The green line represents the photoluminescence of solution (4) minus solution (1). The orange line represents the photoluminescence of solution (3) minus solution (1). The blue line represents the photoluminescence of solution (5) minus solution (1).

Figure 4B

Stock solution of coumarins **3**, **11**, and **12** were prepared in acetone. From these solutions, 0.04 μmol of each coumarin was added to an eppendorf tube and the acetone was allowed to evaporate. The resulting residue was sonicated in the presence of PFD (72 μL) and PFTPA (32 μL) until dissolved, at which point 28 mg/mL Pluronic-F68 in PBS (1 mL) was added. These mixtures (as well as a control containing no coumarin) were sonicated (probe, 0.02 watts) for 15 minutes at 0 ^{o}C. Each nanoemulsion was diluted ten-fold with PBS. Twelve samples were then prepared: 3 x (1 mL nanoemulsion with **3** plus 0.5 mL 1-octanol), 3 x (1 mL nanoemulsion with **11** plus 0.5 mL 1-octanol), 3 x (1 mL nanoemulsion with **12** plus 0.5 mL 1-octanol), 3 x (1 mL blank nanoemulsion plus 0.5 mL 1-octanol). Each solution was rocked continually and the photoluminescence of 60 μL of the 1-octanol layer was measured periodically over two weeks. Prior to the photoluminescence measurements, the samples were allowed to phase separate. Parameters for the photoluminescence spectra were: excitation at 375 nm, collection from 400-650 nm, excitation and emission slits were 7 nm, integration time was 0.25 s. The integrated photoluminescence over the entire range divided by the quantum yield of the coumarin was plotted vs. time. The integrated photoluminescence divided by the quantum yield was plotted so that the differences

between the photophysical properties (quantum yield and λ_{max}) of **3**, **11**, and **12** were accounted for.

Figure S1 and S2
0.1 mg **2–7** were placed in vials and 1 mL of each of the indicated solvents was added. The solutions were sonicated in a bath sonicator, allowed to settle and photographed under ambient (A) and long-wave UV (B) light.

Figure S3
A stock solution of rhodamine **5** was prepared in acetone. From this solution, 0, 0.02, or 0.1 mg of rhodamine **5** was added to an eppendorf tube. The acetone was allowed to evaporate, at which point the rhodamine **5** was dissolved in PFD (18 μL) and PFTPA (8μL). To these solutions, 28 mg/mL Pluronic-F68 in PBS (250 μL) was added and the mixture was sonicated (probe, 0.02 watts) for 15 minutes at 0 ^{o}C. Dynamic light scattering measurements were performed on each sample. The samples were measured on a DynaPro NanoStar (Wyatt) instrument. The measurements were taken on a 1:10 dilution of the nanoemulsions in PBS. The distribution data represents and average of 10, 5 sec acquisitions at 25 ^{o}C.

Figure S4
Each fluorofluorophore was aliquoted (20 nmol) into a 1 dram vial from an acetone stock solution. The acetone was evaporated and the residue was dissolved in 7:3 PFD/PFTPA (144 μL:64 μL). To these solutions, Pluronic-F68 in PBS (2 mL of 28 mg/mL solution) was added. Visible and UV light photographs were taken of these solutions (B). Each solution was sonicated (probe, 0.02 watts) for 15 min at 0 ^{o}C. Visible and UV light photographs were taken of the nanoemulsion solutions (C). The solutions were diluted 1:10 in PBS and the photoluminescence was collected in quartz cuvettes. Photoluminescence spectra were obtained on a Jobin Yvon/Horiba Instruments spectrophotometer with excitation as indicated in (D), 3 nm excitation slits, and 5 nm emission slits, and an integration time of 0.25 s. A nanoemulsion containing no fluorofluorophore was prepared as a control and the photoluminescence of the control at each indicated excitation was collected. Plotted in D are the photoluminescence of the fluorescent nanoemulsion minus the control nanoemulsion all normalized to one.

Figure S5
Nanoemulsions were prepared as described for Figure 3D and the following solutions were prepared:

(1) Nanoemulsion C (200 μL) in PBS (2.4 mL)
(2) Nanoemulsion A (100 μL) + B (100 μL) in PBS (2.4 mL)
(3) Nanoemulsion A (100 μL) + B (100 μL) + serum (100 μL, from human male AB plasma, Sigma) in PBS (2.3 mL)

The photoluminescence (excitation = 375 nm, collection = 400–700 nm, excitation slit = 3 nm, emission slit = 5 nm, integration time = 0.25 s) of each solution was measured. The process was repeated eight times over the course of ten days. Plotted is the photoluminescence at 485 nm divided by the photoluminescence at 568 nm vs, time for each sample. Sample (1) is the green line, sample (2) is the blue line and sample (3) is the purple line.

Figure S6
A mixture of PFD (18 μL), PFTPA (3 μL), phospholipids (0.1 mg, asolectin from soybean, Sigma), Pluronic-F68 (7 mg) and buffer A (250 μL) were combined and sonicated (probe, 0.02 watts) for 15 minutes at 0 ^{o}C. This sample is "Fluosol-DA" (red). A mixture of PFD (18 μL), PFTPA (3 μL), Pluronic-F68 (7 mg) and PBS (250 μL) were combined and sonicated (probe, 0.02 watts) for 15 minutes at 0 ^{o}C. This sample is "– phospholipids" (blue). The size of the emulsions were measured by dynamic light scattering on a NanoBrook Omni (Brookhaven) instrument. Samples were diluted 1:100 in 0.1x PBS and equilibrated (5 min) to 25 ^{o}C before measurement collection. Light scattering measurements were performed at 90^{o} and size distribution was determined by the NNLS algorithm. Error bars for DLS data represent one polydispersity unit (+/- 0.5 polydispersity) as determined from the average of five DLS experiments (100 s collection each).
Buffer A = 0.6 wt% NaCl, 0.034 wt% KCl, 0.02 wt% $MgCl_2$, 0.028 wt% $CaCl_2$, 0.21 wt% $NaHCO_3$, 0.18 wt% glucose

Scheme Experimental Procedures

General Procedure

All chemical reagents were purchased from Sigma-Aldrich, Acros or TCI and used without purification unless noted otherwise. Anhydrous DMF and MeOH were purchased from Aldrich in a sealed bottle. Anhydrous EtOH was prepared by drying over 3 Å molecular sieves. In all cases, solvent was removed by reduced pressure with an IKA RV-10 Rotovapor equipped with a Welch self-cleaning dry vacuum or house vacuum. Products were further dried by reduced pressure with a Maxima D2A high vacuum. Thin layer chromatography was performed with Baker-flex Silica Gel 1B-F plates (JT Baker). Flash chromatography was performed using technical grade silica gel with 60Å pores and 230-400 mesh particle size (Sigma-Aldrich, 717185). High performance liquid chromatography was performed on a semi-prep reverse phase (C_{18}) column using a Varian ProStar system equipped with refractive index and UV/Vis detectors. All ^{1}H, ^{19}F, and ^{13}C spectra are reported in ppm and referenced to solvent peaks. NMR spectra were obtained on Bruker Avance 400 or 600 instruments. High resolution electrospray ionization (ESI) mass spectra were obtained from the MIT Department of Chemistry Instrument Facility. Absorbance spectra were obtained on a Cary 4000 UV/Vis spectrophotometer (Agilent Technologies) with a scan rate of 2000 nm/min. The instrument was blanked on the solvent prior to obtaining a spectrum. Photoluminescence spectra were obtained on a Jobin Yvon/Horiba Instruments spectrophotometer. Absorbance and photoluminescence data were collected in quartz cuvettes. Extinction coefficients were determined using serial dilutions in volumetric flasks. Quantum yields were determined in ethanol or acetone by comparison to rhodamine 6G (Φ_f = 0.95), 7-diethylamino-4-methylcoumarin (Φ_f = 0.59), coumarin 153 (Φ_f = 0.38), coumarin 314 (Φ_f = 0.68), diphenylanthracene (Φ_f = 0.95), oxazine 170 (Φ_f = 0.60), or cresyl violet (Φ_f = 0.54) keeping all settings on the fluorimeter constant and all absorbance values under 0.1 au as described by Eaton.[4]

Phenol 1. 3-Aminophenol (410 mg, 3.8 mmol, 1.0 equiv.) was dissolved in DMF (8.0 mL, anhydrous). To this solution, 3-(perfluorooctyl)propyl iodide (5.0 g, 8.5 mmol, 2.2 equiv.) was added followed by *N*,*N*-diisopropylethylamine (0.80 mL, 4.6 mmol, 1.2 equiv.). The mixture was heated to 120 °C overnight. The following morning it was cooled to rt and loaded directly onto a silica gel column. Compound **1** was eluted from the silica gel column using a hexane/ethyl acetate solvent system with a gradient of 20:1, 15:1, 12:1, 10:1, and 8:1. This procedure resulted in pure **1** (2.9 g, 2.8 mmol, 74%). R_f = 0.8 in 4:1 hexane/ethyl acetate. ^{1}H NMR (400 MHz, Acetone-d_6): 8.01 (s, 1H), 6.99 (t, *J* = 8.0 Hz, 1H), 6.34- 6.30 (m, 2H), 6.19 (dd, *J* = 8.0 Hz, 2.0 Hz, 1H), 3.49 (t, *J* = 7.4 Hz, 4H), 2.34 (tt, *J* = 19.6, 7.9 Hz, 4H), 1.97-1.90 (m, 4H). ^{13}C NMR (101 MHz, Acetone-d_6): 159.5, 150.3, 130.8, 122.4-108.9 (m), 105.7, 105.3,

[4] Eaton, D.F. "Reference materials for fluorescence measurement." *Pure Appl. Chem.* **1988**, *60*, 1107-114.

101.2, 50.9, 28.9 (t, J = 22 Hz), 19.2. ^{19}F NMR (376 MHz, Acetone-d_6): -82.3 (t, J = 10.3 Hz, 6F), -114.7 (quint, J = 16 Hz, 4F), -122.5 (bs, 4F), -122.7 (bs, 8F), -123.6 (bs, 4F), -124.2 (bs, 4F), -127.1 - -127.2 (m, 4F). HRMS (ESI$^+$): Calculated for $C_{28}H_{17}F_{34}NO^+$ $[M+H]^+$: 1030.0840; found: 1030.0888.

Coumarin 2. Phenol **1** (250 mg, 0.24 mmol, 1.0 equiv.) was dissolved in ethanol (1.25 mL, anhydrous). To this solution, $ZnCl_2$ (40 mg, 0.29 mmol, 1.2 equiv.) and ethylacetoacetate (35 μL, 0.27 mmol, 1.1 equiv.) were added. The mixture was heated to 100 ^{o}C overnight, cooled to rt, and evaporated to dryness. The crude product was purified by silica gel chromatography using a hexane/ethyl acetate solvent system (20:1, 15:1, 10:1, 15:1). Coumarin **2** beings to elute at 10:1 hexane/ethyl acetate. This procedure resulted in 60 mg of **2** as a yellow solid (0.055 mmol, 23%). A small portion was purified by HPLC prior to photophysical characterization. HPLC conditions: MeOH/CH_2Cl_2 solvent system on a C_{18} column, using a gradient elution from 0-2% CH_2Cl_2 over 10 min. Coumarin **2** elutes at 5 min. R_f = 0.7 in 4:1 hexane/ethyl acetate. ^{1}H NMR (400 MHz, Acetone-d_6): 7.54 (d, J = 8.9 Hz, 1H), 6.86 (dd, J = 9.0, 2.6 Hz, 1H), 6.66 (d, J = 2.6 Hz, 1H), 5.92 (d, J = 1.3 Hz, 1H), 3.71 (t, J = 7.7 Hz, 4H), 2.50 – 2.37 (m, 4H), 2.37 (s, 3H), 2.06 - 1.99 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$): 162.0, 156.1, 152.9, 150.3, 126.4, 110.6, 110.3, 108.9, 98.9, 50.5, 28.4 (t, J = 22 Hz), 18.6, 18.5 (bs). CF_n carbons not observed due to low signal. ^{19}F NMR (376 MHz, Chloroform-d): -80.8 (t, J = 10 Hz, 6F), -113.8 (p, J = 16 Hz, 4F), -121.7 (bs, 4F), -121.9 (bs, 8F), -122.8 (bs, 4F), -123.4 (bs, 4F), -126.1 - -126.2 (m, 4F). HRMS (ESI$^+$): Calculated for $C_{32}H_{19}F_{34}NO_2^+$ $[M+H]^+$: 1096.0946; found: 1096.0957. Absorbance (EtOH): below 200 nm (ε > 75000 $M^{-1}cm^{-1}$), 233 nm (ε = 26600 $M^{-1}cm^{-1}$), 363 nm (ε = 21500 $M^{-1}cm^{-1}$). Emission (EtOH, Ex 350): 435 nm, Φ_f = 0.5. Quantum yield determined by reference to 7-diethylamino-4-methylcoumarin (Φ_f = 0.59).

Coumarin 3. Phenol **1** (250 mg, 0.24 mmol, 1.0 equiv.) was dissolved in ethanol (1.3 mL, anhydrous). To this solution, $ZnCl_2$ (40 mg, 0.29 mmol, 1.2 equiv.) and ethyl-4,4,4-trifluoromethyl acetoacetate (40 μL, 0.27 mmol, 1.1 equiv.) were added. The mixture was heated to 100 ^{o}C overnight. In the morning, the dried reaction mixture was dissolved in dichloromethane (5 mL) and water (5 mL) was added. The water was extracted with dichloromethane (6 x 5 mL) and perfluorohexane/ methoxyperfluorobutane (1 x 5 mL). The organics and fluorous layers were combined, dried with $MgSO_4$, decanted, and evaporated to dryness. The crude product was purified by silica gel chromatography using a hexane/ethyl acetate solvent system (25:1, 20:1, 17.5:1, 15:1, 10:1). Coumarin **3** beings to elute at 17.5:1 hexane/ethyl acetate. This procedure resulted in 126 mg of **3** as a yellow solid (0.11 mmol, 46%). R_f = 0.8 in 4:1 hexane/ethyl acetate. ^{1}H NMR (400 MHz, $CDCl_3$): 7.56 (dd, J = 9.1, 1.9 Hz, 1H), 6.63 (dd, J = 9.2, 2.6 Hz, 1H), 6.55 (d, J = 2.6 Hz, 1H), 6.46 (s, 1H), 3.49 (dd, J = 7.8, 7.6 Hz, 4H), 2.23 - 2.09 (m, 4H), 2.01 - 1.93 (m, 4H). ^{13}C NMR (101 MHz, Acetone-d_6): 160.1, 158.1, 152.5, 142.3, 141.6 (q, J = 32 Hz), 126.9, 124.5 – 109.6 (m, CF_n carbons), 110.7, 109.7 (q, J = 6 Hz), 103.5, 99.2, 50.3, 28.6 (t, J = 22

Hz), 18.9 (broad). ^{19}F NMR (376 MHz, $CDCl_3$): -64.7 (s, 3F), -80. 7 - -80.8 (m, 6F), -113.74 (td, *J* = 17.5, 15.5, 6.9 Hz, 4F), -121.6 - -122.0 (m, 12F), -122.7 (m, 4F), -123.3 (m, 4F), -126.1 - -126.4 (m, 4F). HRMS (ESI^+): Calculated for $C_{32}H_{16}F_{37}NO_2^+$ $[M+H]^+$: 1150.0663; found: 1150.0640. Absorbance (EtOH): 210 nm (ε = 38000 $M^{-1}cm^{-1}$), 253 nm (ε = 12900 $M^{-1}cm^{-1}$), 395 nm (ε = 19000 $M^{-1}cm^{-1}$). Emission (EtOH, Ex 375): 491 nm, Φ_f = 0.44±0.05. Quantum yield determined by reference to 7-diethylamino-4-methylcoumarin (Φ_f = 0.59), coumarin 153 (Φ_f = 0.38), and coumarin 314 (Φ_f = 0.68).

Chromene 4. Phenol **1** (50 mg, 0.049 mmol, 1.0 equiv.) was dissolved in ethanol (0.25 mL, anhydrous). To this solution, benzaldehyde (~6 μL, 0.06 mmol, 1.2 equiv., anhydrous), malononitrile (3.5 mg, 0.053 mmol, 1.1 equiv.) and piperidine (25 μL, 0.25 mmol., 5.2 equiv.) were added. This mixture was stirred for 16 h, at which point it was evaporated to dryness. The residue was dissolved in 95:5 CH_3CN/H_2O (10 mL) and extracted with $MeOC_4F_9$ (2 x 8 mL). The $MeOC_4F_9$ was combined and evaporated to dryness to yield 100 mg of 4-*H*-chromene intermediate. HRMS (ESI^+): Calculated for $C_{38}H_{23}F_{34}N_3O^+$ $[M+H]^+$: 1184.1371; found: 1184.1328. The crude 4-*H* chromene was dissolved in dichloromethane (5 mL, anhydrous). To this solution, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 13 mg, 0.057 mmol, 1.2 equiv.) was added and stirred at rt for 3 h. After 3 h, ethyl acetate (15 mL) was added and washed with sat. sodium bicarbonate (2 x 10 mL) and brine (1 x 10 mL). The organics were dried with $MgSO_4$, decanted, and evaporated to dryness to yield chromene **4** (49 mg, 0.041 mmol, 85%). R_f = 0.3 in 4:1 hexanes/ethyl acetate. A small portion was purified by HPLC prior to photophysical characterization. HPLC conditions: H_2O/MeOH solvent system on a C_{18} column, using a gradient elution from 90-100% MeOH over 18 min followed by a 5 min hold at 100% MeOH. Chromene **4** elutes at minute 22. ^{1}H NMR (400 MHz, Acetone-d_6): 7.82 (s, 1H), 7.62-7.59 (m, 3H), 7.51 - 7.48 (m, 2H), 6.90 (d, *J* = 9.1 Hz, 1H), 6.71 (dd, *J* = 9.2, 2.6 Hz, 1H), 6.63 (d, *J* = 2.5 Hz, 1H), 3.73 (t, *J* = 7.9 Hz, 4H), 2.40 (td, *J* = 19.3, 9.7 Hz, 4H), 2.04 – 1.99 (m, 4H). ^{13}C NMR (101 MHz, Acetone-d_6): 158.4, 157.2, 155.4, 153.3, 134.9, 130.7, 130.6, 129.7, 129.5, 116.2, 109.5, 108.8, 98.5, 97.4, 50.4, 28.65 (t, *J* = 22 Hz), 19.1. CF_n carbons not observed. ^{19}F NMR (376 MHz, Acetone-d_6): -81.7 (t, *J* = 10 Hz, 6F), -114.4 (p, *J* = 18 Hz, 4F), -122.2 (bs, 4F), -122.4 (bs, 8F), -123.3 (bs, 4F), -124.0 (bs, 4F), -126.7 - -126.9 (m, 4F). HRMS (ESI^+): Calculated for $C_{38}H_{21}F_{34}N_3O^+$ $[M+H]^+$: 1182.1214; found: 1182.1189. Absorbance (EtOH): 268 nm (ε = 14300 $M^{-1}cm^{-1}$), 308 nm (ε = 3700 $M^{-1}cm^{-1}$), 421 nm (ε = 26700 $M^{-1}cm^{-1}$). Emission (EtOH, Ex 375): 477 nm, Φ_f = 0.031±0.006. Quantum yield determined by reference to diphenylanthracene (Φ_f = 0.95) and coumarin 314 (Φ_f = 0.68).

Rhodamine 5. Zinc chloride (~50 mg, 0.4 mmol, 4 equiv.) was placed in a vial under high vacuum and heated with a flame until it stopped bubbling (but before it discolored). The $ZnCl_2$ was cooled to rt under vacuum. In a separate vial, phthalic anhydride (15 mg, 0.010 mmol, 1.0 equiv.) and compound **1** (200 mg, 0.19 mmol, 2.0 equiv.) were combined neat and heated to 120 °C. Once the phthalic anhydride and **1** had melted (approx. 25 min), the $ZnCl_2$ was added to the mixture and the temperature was raised to 180 °C. After 4 h, the reaction was cooled to rt, the solid was solubilized with a mixture of methanol/acetone/trifluoroethanol and evaporated onto silica gel for chromatography (it is important that the rhodamine is completely dissolved before evaporation onto silica gel or else the purification fails). The rhodamine free acid was eluted with a dichloromethane/methanol solvent system using a gradient of 100:1, 80:1, 60:1, 40:1, 20:1, 10:1, 5:1. The product begins eluting at 40:1 dichloromethane/methanol. This procedure resulted in 60 mg of rhodamine free acid (0.023 mmol, 24%) as a pink solid. R_f = 0.8 in MeOH. ^{1}H NMR (600 MHz, Acetone-d_6): 7.96 (d, J = 7.7 Hz, 1H), 7.79 (t, J = 7.5 Hz, 1H), 7.71 (t, J = 7.5 Hz, 1H), 7.28 (d, J = 7.6 Hz, 1H), 6.61-6.57(m, 6H), 3.62 (t, J = 7.6 Hz, 8H), 2.38 (dq, J = 19.4, 9.6, 7.8 Hz, 8H), 1.99 (p, J = 8.1 Hz, 8H). ^{13}C NMR (101 MHz, Acetone-d_6): 169.6, 154.0, 153.9, 150.5, 135.7, 130.5, 129.9, 128.5, 125.2, 125.0, 122.6-108.2 (m), 109.7, 108.2, 99.1, 84.9, 50.4, 28.7 (t, J = 22 Hz), 19.0. ^{19}F NMR (376 MHz, Acetone-d_6): -81.7 (apparent t, J = 10 Hz, 12F), -114.4 (p, J = 16 Hz, 8F), -122.2 - -122.6 (m, 24F), -123.33 (broad ddt, J = 25.0, 18.8, 9.0 Hz, 8F), -124.01 (broad s, 8F), -126.8 - -126.9 (m, 8F). HRMS (ESI$^+$): Calculated for $C_{64}H_{34}F_{68}N_2O_3^+$ $[M+H]^+$: 2171.1556; found, 2171.1529.

The rhodamine free acid (40 mg, 0.018 mmol, 1.0 equiv.) was dissolved in MeOH (5.0 mL, anhydrous) in a flame dried 3-neck flask with a reflux condenser under N_2. Acetyl chloride (0.10 mL, 1.4 mmol, 80 equiv.) was added and the mixture was heated to 60 °C for five days, at which point the mixture was cooled to rt, evaporated onto silica gel, and purified by flash chromatography using a dichloromethane/ methanol solvent system (50:1, 40:1, 30:1, 20:1). The product begins eluting at 30:1. This procedure resulted in pure esterified rhodamine **5** (28 mg, 0.013 mmol, 68%) as a pink solid. R_f = 0.5 in MeOH. ^{1}H NMR (400 MHz, Acetone-d_6): 8.35 (dm, J = 7.9 Hz, 1H), 7.95 (td, J = 7.5, 1.4 Hz, 1H), 7.88 (td, J = 7.7, 1.4 Hz, 1H), 7.56 (dm, J = 7.6 Hz, 1H), 7.36 (dd, J = 9.5, 2.5 Hz, 2H), 7.24-7.21 (m, 4H), 4.02 (t, J = 8.0 Hz, 8H), 3.65 (s, 3H), 2.59-2.46 (m, 8H), 2.19-2.12 (m, 8H). ^{13}C NMR (101 MHz, Acetone-d_6): 166.1, 161.0, 158.9, 157.4, 134.7, 134.0, 132.4, 131.9, 131.4, 131.3, 130.9, 115.9, 115.0, 97.6, 52.8, 51.0, 28.5 (t, J = 22 Hz), 19.2. CF_n carbons are not observed due to limited solubility of **5** in acetone. ^{19}F NMR (376 MHz, Acetone-d_6): -81.7 (t, J = 10 Hz, 12F), -114.5 (q, J = 18, 17 Hz, 8F), -122.2 - -122.5 (m, 24F), -123.3 (bs, 8F), -124.0 (bs, 8F), -126.7 - -126.9 (m, 8F). HRMS (ESI$^+$): Calculated for $C_{65}H_{37}F_{68}N_2O_3^+$: 2185.1713; found, 2185.1740. Absorbance (EtOH): 258 nm (ε = 30700 $M^{-1}cm^{-1}$), 354 nm (ε = 8630 $M^{-1}cm^{-1}$), 550 nm (ε = 97900 $M^{-1}cm^{-1}$). Emission (EtOH, Ex 500): 571 nm, Φ_f = 0.85 referenced to Rhodamine 6G (Φ_f = 0.95).

Squaraine 6. Phenol **1** (50 mg, 0.049 mmol, 1.0 equiv.) and squaric acid (2.8 mg, 0.025 mmol, 0.50 equiv.) were dissolved in 1-butanol (0.25 mL) and toluene (0.75 mL, anhydrous). This mixture was heated to 120 °C for 18 h, at which point it was cooled to rt. The blue precipitate was collected, washed with toluene, methanol, and acetone (carefully) and dried. This procedure resulted in 26 mg of pure **6** (0.012 mmol, 49% yield). R_f = 0.8 in 4:1 hexanes/ethyl acetate. ^{1}H NMR (600 MHz, HFIPA-d_2): 8.23 (bs, 2H), 6.93 (bs, 2H), 6.65 (bs, 2H), 3.96 (bs, 8H), 2.57 (bs, 8H), 2.42 (bs, 8H). Too low of solubility for ^{13}C. MS (MALDI$^+$): Calculated for $C_{62}H_{38}F_{68}N_2O_3^+$ [M+H-O]$^+$: 2151.1869; found: 2151.18. Absorbance (acetone): 392 nm (ε = 2100 $M^{-1}cm^{-1}$), 639 nm (ε = 168000 $M^{-1}cm^{-1}$). Emission (acetone, Ex 590): 657 nm, Φ_f = 0.89±0.09 referenced to oxazine 170 (Φ_f = 0.60) and cresyl violet (Φ_f = 0.54).

Oxazine 7. Phenol **1** (50 mg, 0.049 mmol, 1.0 equiv.) was dissolved in ethanol (1 mL, anhydrous). To this solution, *N*,*N*-dimethyl-4-nitrosoaniline (8 mg, 0.053 mmol, 1.1 equiv.) and perchloric acid (70%, 1 drop) were added. This mixture was heated to 100 °C for 36 h, at which point the reaction was cooled to rt and evaporated to dryness. The residue was dissolved in 95:5 CH_3CN/H_2O (20 mL) and extracted into $MeOC_4F_9$ (1 x 15 mL). The $MeOC_4F_9$ was evaporated to dryness and the residue was recrystallized from methanol to result in **7** (8 mg, 0.0063 mmol, 13% yield). R_f = 0.8 in 9:1 CH_2Cl_2/MeOH. ^{1}H NMR (600 MHz, Acetone-d_6): 7.86 (bs, 2H), 7.63 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.58 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.21 (bs, 1H), 7.00 (bs, 1H), 4.09 (bs, 4H), 3.57 (bs, 6H), 2.57-2.49 (m, 4H), 2.21-2.17 (m, 4H). ^{19}F NMR (376 MHz, Acetone-d_6): -81.7 (t, *J* = 10 Hz, 6F), -114.4 - -114.5 (m, 4F), -122.2 (bs, 4F), -122.4 (bs, 8F), -123.3 (bs, 4F), -123.9 (bs, 4F), -126.7 - -126.8 (m, 4F). HRMS (ESI$^+$): Calculated for $C_{32}H_{24}F_{34}N_3O^+$[M]$^+$: 1160.1371; found, 1160.1368. Absorbance (EtOH): below 200 nm (ε > 6000 $M^{-1}cm^{-1}$), 237 nm (ε = 24600 $M^{-1}cm^{-1}$), 259 nm (ε = 24400 $M^{-1}cm^{-1}$), 301 nm (ε = 8860 $M^{-1}cm^{-1}$), 389 nm (ε = 2300 $M^{-1}cm^{-1}$), 446 nm (ε = 2200 $M^{-1}cm^{-1}$), 641 nm (ε = 71900 $M^{-1}cm^{-1}$). Emission (EtOH, Ex 590): 664 nm, Φ_f = 0.16±0.02 referenced to oxazine 170 (Φ_f = 0.60) and cresyl violet (Φ_f = 0.54).

Phenol S1. 3-Aminophenol (205 mg, 1.88 mmol, 1.00 equiv.) was dissolved in DMF (4.0 mL, anhydrous). To this solution, 3-(perfluorobutyl)propyl iodide (1.46 g, 3.76 mmol, 2.00 equiv.) was added followed by *N*,*N*-diisopropylethylamine (0.40 mL, 2.3 mmol, 1.2 equiv.). The mixture was heated to 120 °C overnight. The following morning it was cooled to rt and loaded directly onto a silica gel column. Compound **S1** was eluted from the silica gel column using a hexane/ethyl acetate solvent system with a gradient of 20:1, 15:1, 12:1, 10:1, and 8:1. This procedure resulted in pure **S1** (0.866 g, 1.38 mmol, 73%). ^{1}H NMR (400 MHz, $CDCl_3$): 7.11 (t, *J* = 8.1 Hz, 1H), 6.29 (dd, *J* = 8.3, 2.4 Hz, 1H), 6.24 (dd, *J* = 7.8, 2.2 Hz, 1H), 6.21 (t, *J* = 2.3 Hz, 1H), 5.19 (s, 1H), 3.34 (t, *J* = 7.5 Hz, 4H), 2.10 (tt, *J* = 18.6, 8.0 Hz, 4H), 1.94-1.86 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$): 156.9, 149.2, 130.6, 121.8 - 109.1 (m, CF_n carbons), 105.9, 104.4, 100.1, 50.5, 28.3 (t, *J* = 22 Hz), 18.34 (t, *J* = 3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$) : -81.3 (tt, *J* = 10, 3 Hz, 6F), -114.2 - -114.4 (m, 4F), -124.5 - -124.6 m, 4F), -126.2 - -126.3 (m, 4F). HRMS (ESI$^+$): Calculated for $C_{20}H_{17}F_{18}NO^+$ [M+H]$^+$: 630.1095; found: 630.1090.

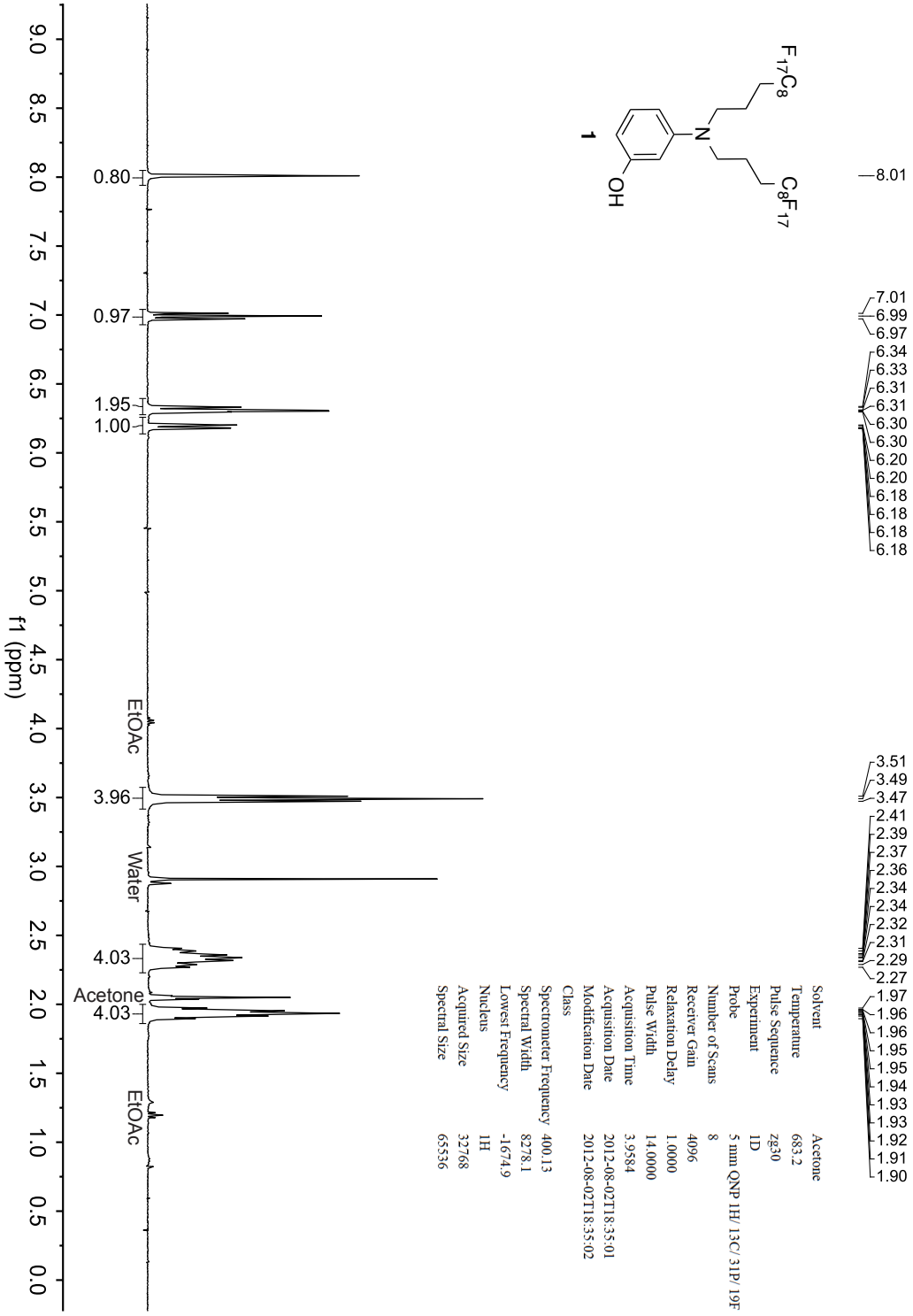
Coumarin 11. Zinc chloride (80 mg, 0.59 mmol, 1.18 equiv.) was placed in a vial under high vacuum and heated with a flame until it stopped bubbling (but before it discolored). The $ZnCl_2$ was cooled to rt and ethanol (2.5 mL, anhydrous) was added followed by phenol **S1** (315 mg, 0.50 mmol, 1.0 equiv.) and ethyl-4,4,4-trifluoroacetoacetate (85 μL, 0.58 mmol, 1.2 equiv.). The mixture was heated to 95 ^{o}C overnight. In the morning, the crude product was evaporated onto silica gel and chromatographed with a hexane/ethyl acetate solvent system (20:1, 15:1, 12:1, 10:1, 8:1). Coumarin **11** elutes at 10:1 hexane/ethyl acetate to yield 216 mg pure yellow solid (0.29 mmol, 58%). R_f = 0.6 in 4:1 hexane/ethyl acetate. ^{1}H NMR (600 MHz, $CDCl_3$): 7.56 (dd, *J* = 9.2, 1.9 Hz, 1H), 6.63 (dd, *J* = 9.2, 2.7 Hz, 1H), 6.54 (d, *J* = 2.6 Hz, 1H), 6.46 (s, 1H), 3.48 (t, *J* = 7.9 Hz, 4H), 2.15 (tt, *J* = 18.2, 7.8 Hz, 4H), 1.97 (quin, *J* = 8.2 Hz, 4H). ^{13}C NMR (101 MHz, $CDCl_3$): 160.2, 157.1, 150.8, 141.8 (q, *J* = 32 Hz), 126.8, 126.0 – 109.0 (m, CF_n carbons), 109.60 (q, *J* = 5 Hz), 109.55, 103.9, 98.8, 50.3, 28.2, (t, *J* = 23 Hz), 18.4. ^{19}F NMR (376 MHz, $CDCl_3$): -64.6 (s, 3F) , -81.3 (t, *J* = 10 Hz, 6F), -114.1 (quin, *J* = 16 Hz, 4F), -124.3 -124.4 (m, 4F), -125.96- -126.04 (m, 4F). HRMS (ESI^{+}): Calculated for $C_{24}H_{16}F_{21}NO_2^{+}$ $[M+H]^{+}$: 750.0995; found: 750.0980. Absorbance (EtOH): 210 nm (ε = 40200 $M^{-1}cm^{-1}$), 253 nm (ε = 13300 $M^{-1}cm^{-1}$), 395 nm (ε = 20300 $M^{-1}cm^{-1}$). Emission (EtOH, Ex 375): 491 nm, Φ_f = 0.45±0.05. Quantum yield determined by reference to 7-diethylamino-4-methylcoumarin (Φ_f = 0.59), coumarin 153 (Φ_f = 0.38), and coumarin 314 (Φ_f = 0.68).

Phenol S2. 3-Aminophenol (270 mg, 2.5 mmol, 1.0 equiv.) was dissolved in DMF (5.0 mL, anhydrous). To this solution, 1-bromodecane (1.3 mL, 4.7 mmol, 1.9 equiv.) was added followed by *N*,*N*-diisopropylethylamine (0.50 mL, 2.8 mmol, 1.21 equiv.). The mixture was heated to 120 ^{o}C overnight. The following morning it was cooled to rt and loaded directly onto a silica gel column. Compound **S2** was eluted from the silica gel column using a hexane/ethyl acetate solvent system with a gradient of 25:1, 20:1, 18:1, and 15:1. This procedure resulted in pure **S2** (0.4 g, 1.0 mmol, 41%). R_f = 0.8 in 5:1 hexane/ethyl acetate. ^{1}H NMR (400 MHz, $CDCl_3$): 7.06 (t, *J* = 8.1 Hz, 1H), 6.25 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.16 (t, *J* = 2.3 Hz, 1H), 6.12 (dd, *J* = 7.8, 2.2 Hz, 1H), 4.97 (bs, 1H), 3.23 (dd, *J* = 7.6, 7.8 Hz, 4H), 1.59 (p, *J* = 7.4 Hz, 4H), 1.34 - 1.30 (m, 38H), 0.92 (t, *J* = 6.7 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): 156.8, 149.9, 130.1, 104.9, 102.3, 98.8, 51.3, 32.1, 29.84, 29.82, 29.79, 29.78, 29.7, 29.5, 27.4, 27.3, 22.8, 14.3. HRMS (ESI^{+}): Calculated for $C_{30}H_{55}NO^{+}$ $[M+H]^{+}$: 446.4356; found, 446.4360.

Coumarin 12. Zinc chloride (80 mg, 0.59 mmol, 1.18 equiv.) was placed in a vial under high vacuum and heated with a flame until it stopped bubbling (but before it discolored). The $ZnCl_2$ was cooled to rt and phenol **S2** (210 mg, 0.47 mmol, 1.0 equiv.) was added and the vial was placed under vacuum. After ~ 1 h, ethanol (2.5 mL, anhydrous) was added followed by ethyl-4,4,4-trifluoroacetoacetate (85 μL, 0.58 mmol, 1.2 equiv.). The mixture was heated to 90 ^{o}C overnight. In the morning, the crude product was evaporated to dryness and purified by flash chromatography using a hexane/ethyl acetate solvent system (25:1, 20:1). This procedure gave coumarin **12** as a yellow oil in 29% yield (77 mg, 0.14 mmol). ^{1}H NMR (400 MHz, $CDCl_3$): 7.48 (dd, *J* = 9.2, 1.9 Hz, 1H), 6.59 (dd, *J* = 9.2, 2.6 Hz, 1H), 6.49 (d, *J* = 2.5 Hz,

1H), 6.35 (s, 1H), 3.32 (dd, 7.9, 67.6 Hz, 4H), 1.64-1.57 (m, 4H), 1.33-1.26 (m, 38H), 0.89 – 0.86 (m, 6H). ^{13}C NMR (101 MHz, $CDCl_3$): 160.7, 157.2, 151.7, 141.9 (q, *J* = 32 Hz), 126.2, 122.1 (q, *J* =275 Hz), 109.5, 107.69 (q, *J* = 6 Hz), 102.6, 98.0, 51.4, 32.1, 29.77, 29.76, 29.74, 29.71, 29.6, 29.5, 27.3, 27.2, 22.8, 14.2. ^{19}F NMR (376 MHz, $CDCl_3$): -64.52 (s, 3F). HRMS (ESI^+): Calculated for $C_{34}H_{54}F_3NO_2^+$ $[M+H]^+$: 566.4179; found: 566.4200. Absorbance (EtOH): 210 nm (ε = 47100 $M^{-1}cm^{-1}$), 259 nm (ε = 15800 $M^{-1}cm^{-1}$), 407 nm (ε = 20800 $M^{-1}cm^{-1}$). Emission (EtOH, Ex 375): 504 nm, Φ_f = 0.18$\pm$0.02. Quantum yield determined by reference to 7-diethylamino-4-methylcoumarin (Φ_f = 0.59), coumarin 153 (Φ_f = 0.38), and coumarin 314 (Φ_f = 0.68).

^{1}H-NMR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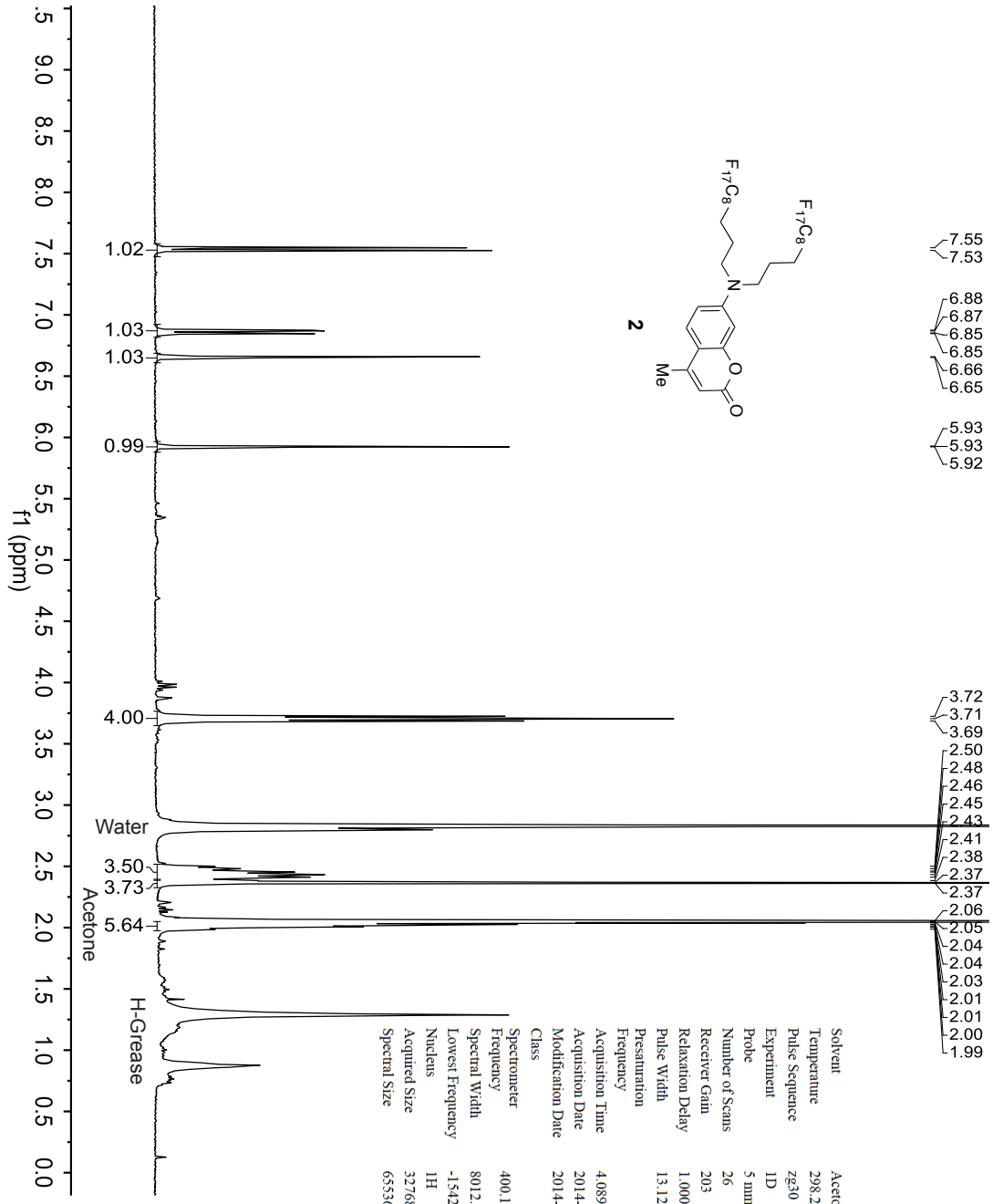
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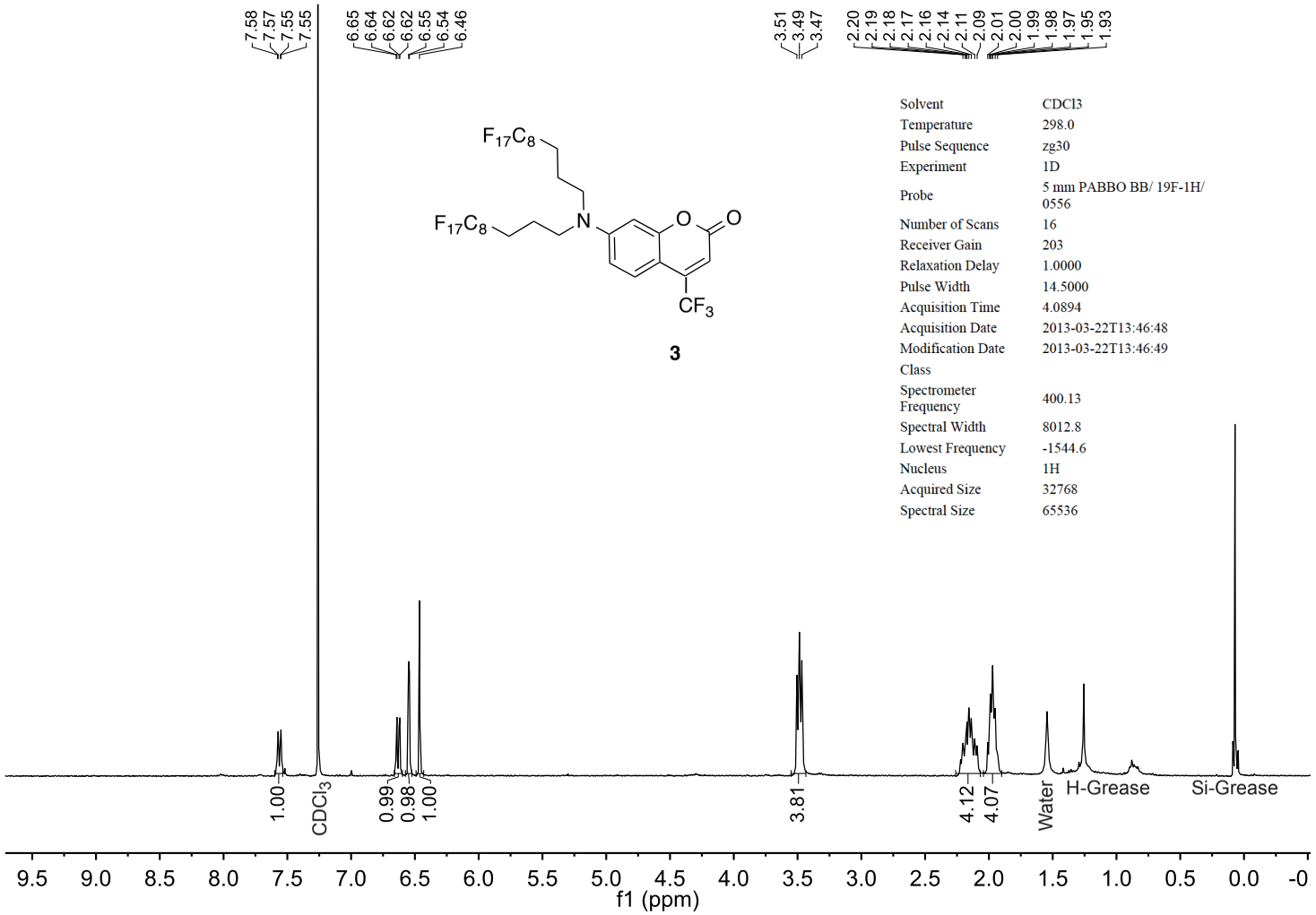
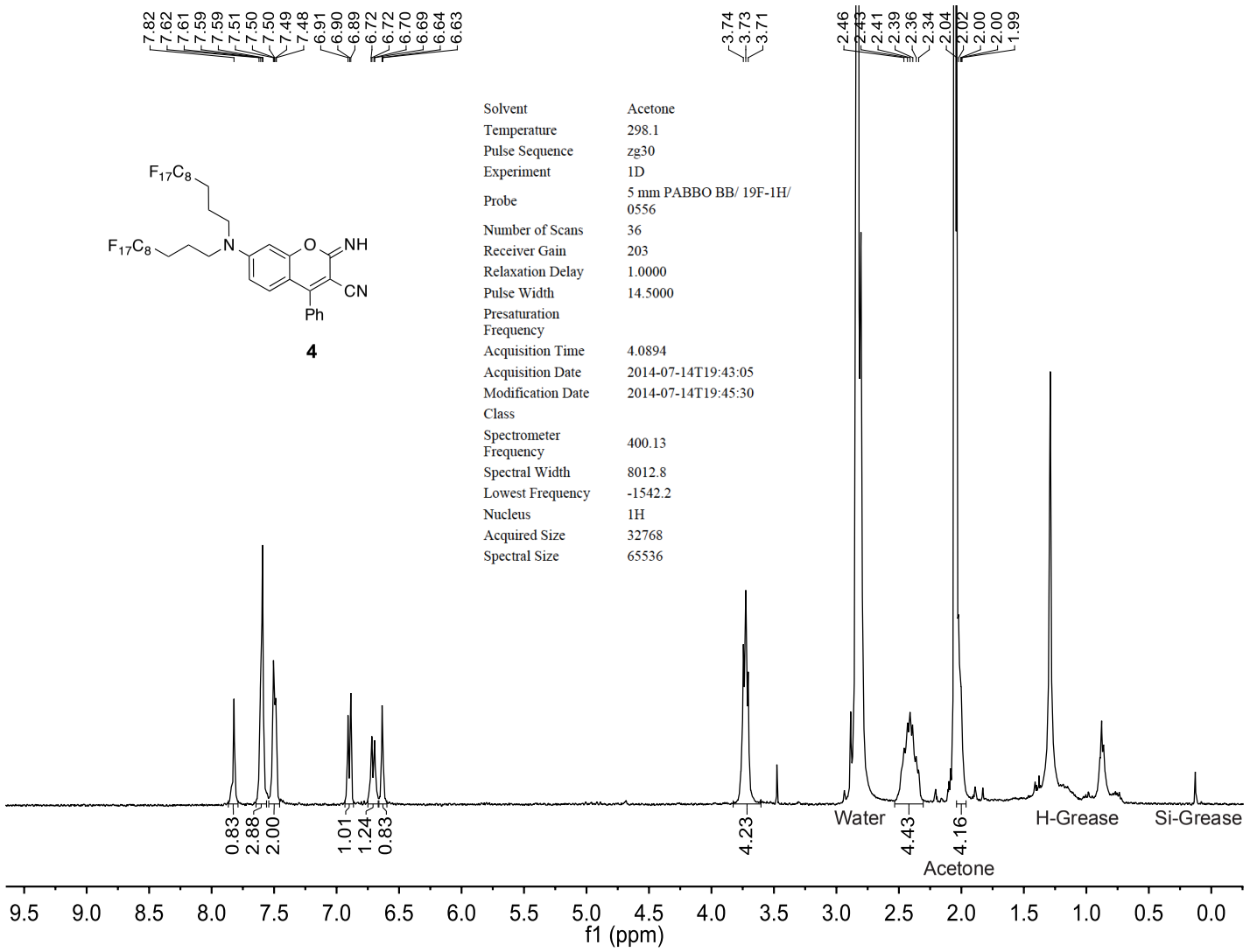
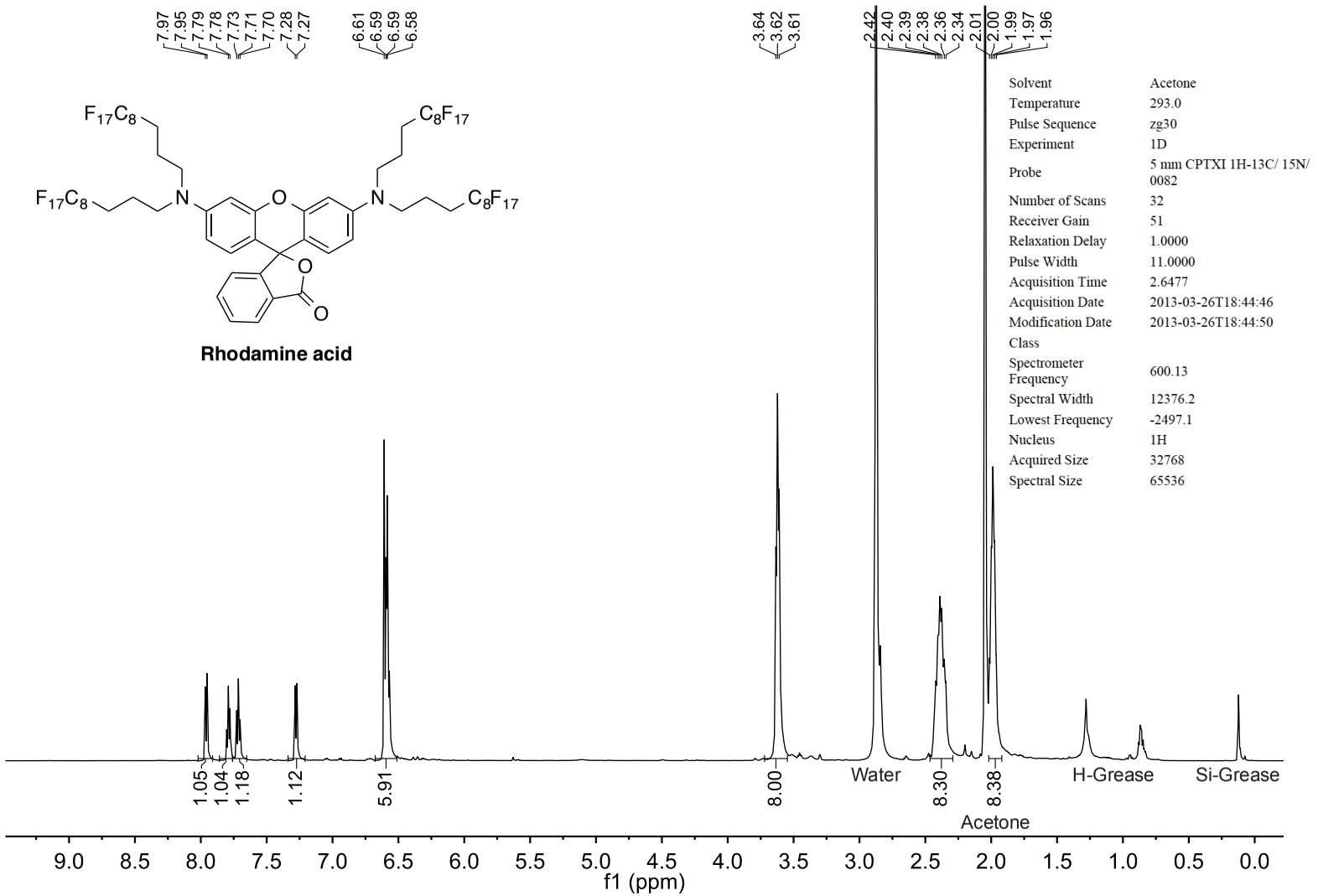
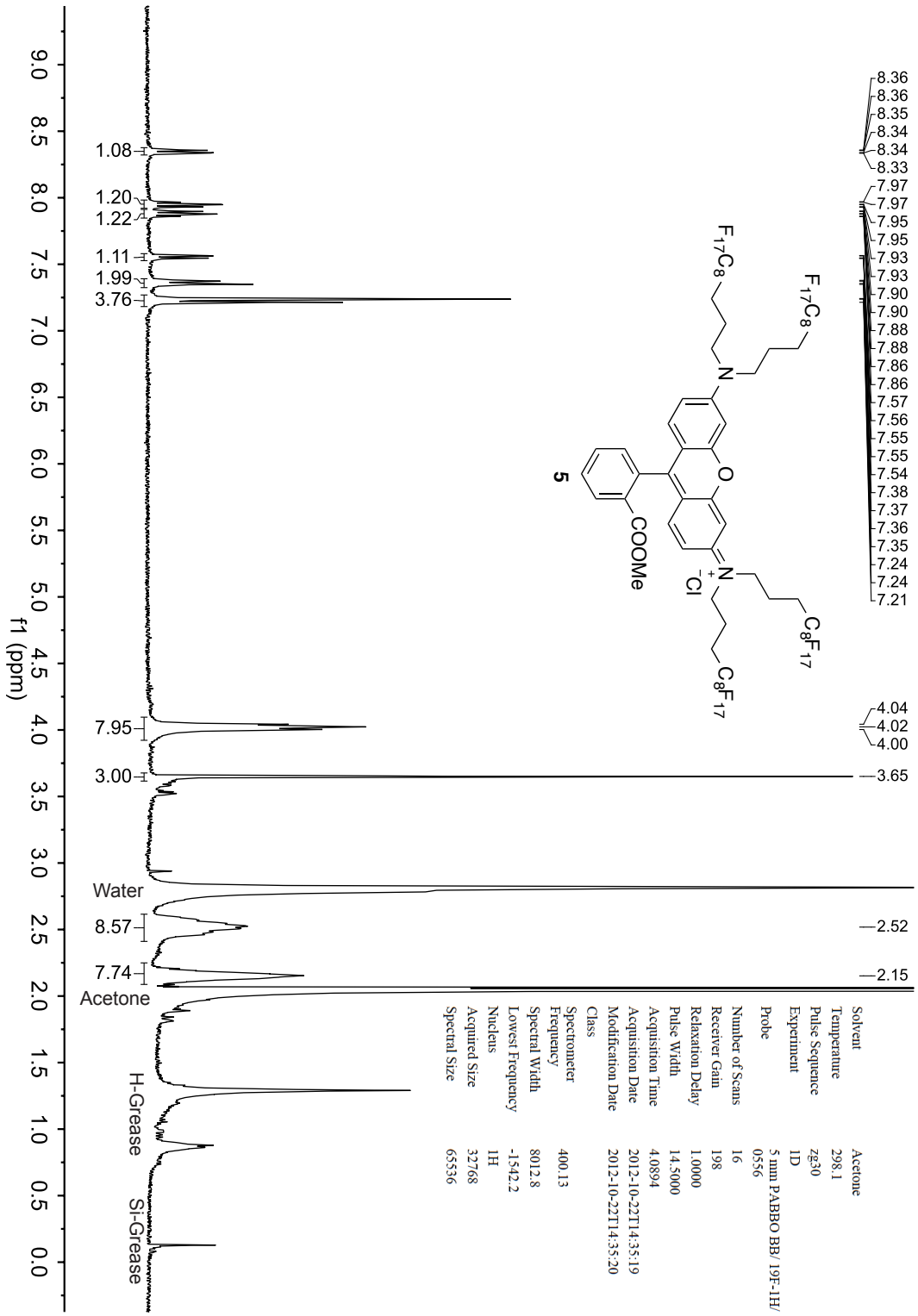
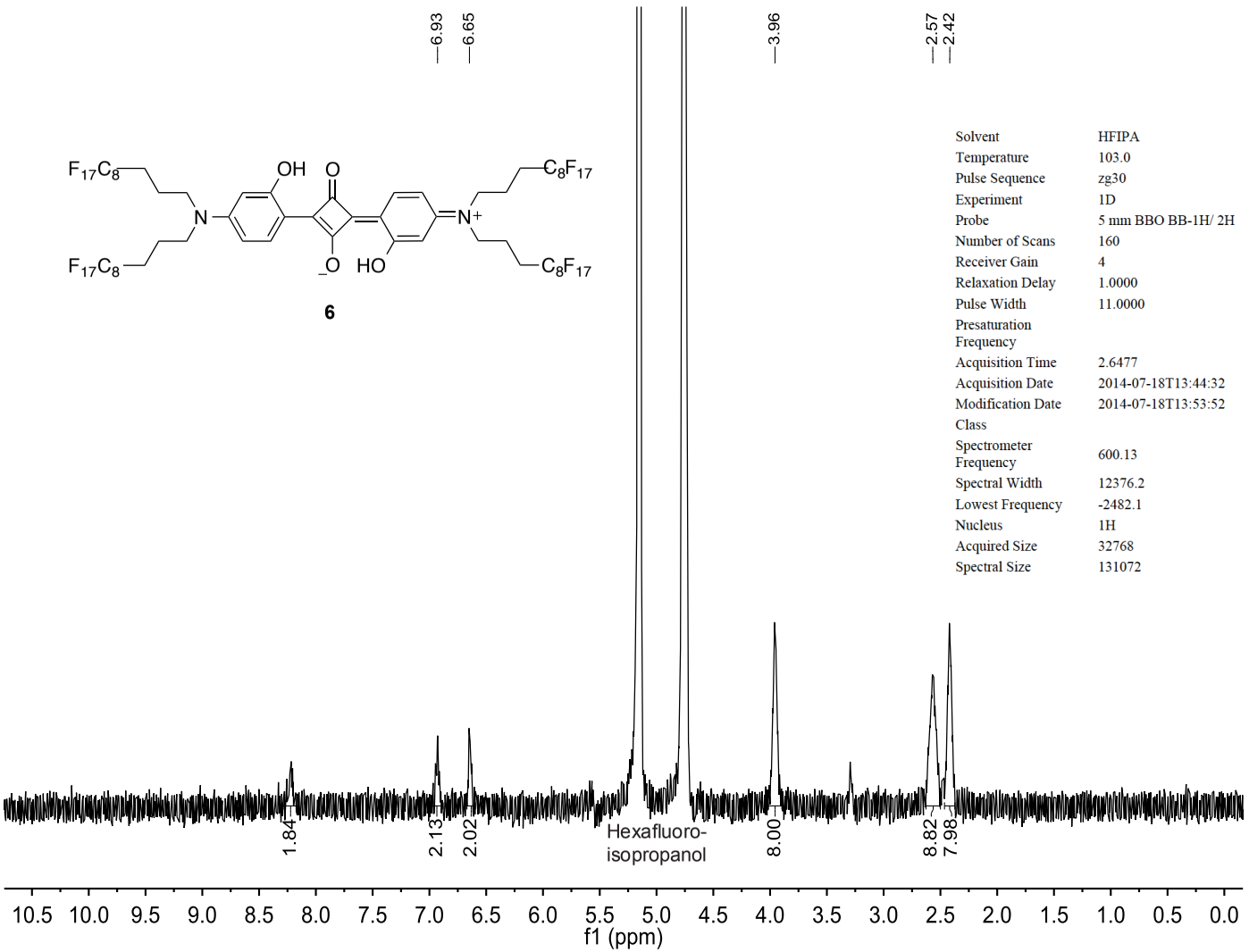
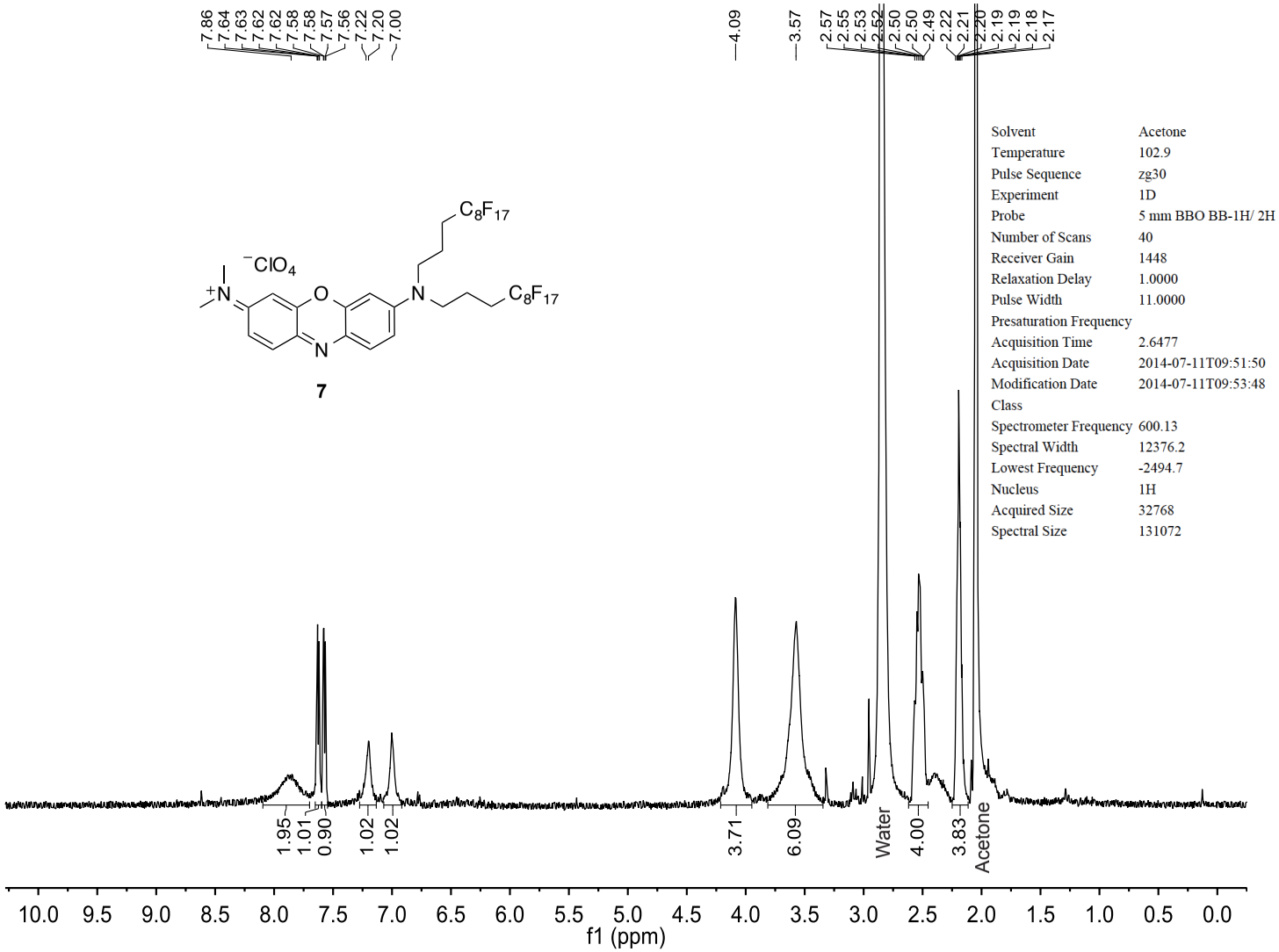

7.58
7.57
7.55
7.55
6.65
6.64
6.62
6.62
6.55
6.54
6.46
3.51
3.49
3.47
2.20
2.19
2.18
2.17
2.16
2.14
2.11
2.09
2.01
2.00
1.99
1.98
1.97
1.95
1.93
F17C8
F17C8
N
O
O
CF3
3
Solvent CDCl3
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 16
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 4.0894
Acquisition Date 2013-03-22T13:46:48
Modification Date 2013-03-22T13:46:49
Class
Spectrometer Frequency 400.13
Spectral Width 8012.8
Lowest Frequency -1544.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
1.00
CDCl3
0.99
0.98
1.00
3.81
4.12
4.07
Water
H-Grease
Si-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 0.5 0.0 -0
f1 (ppm)

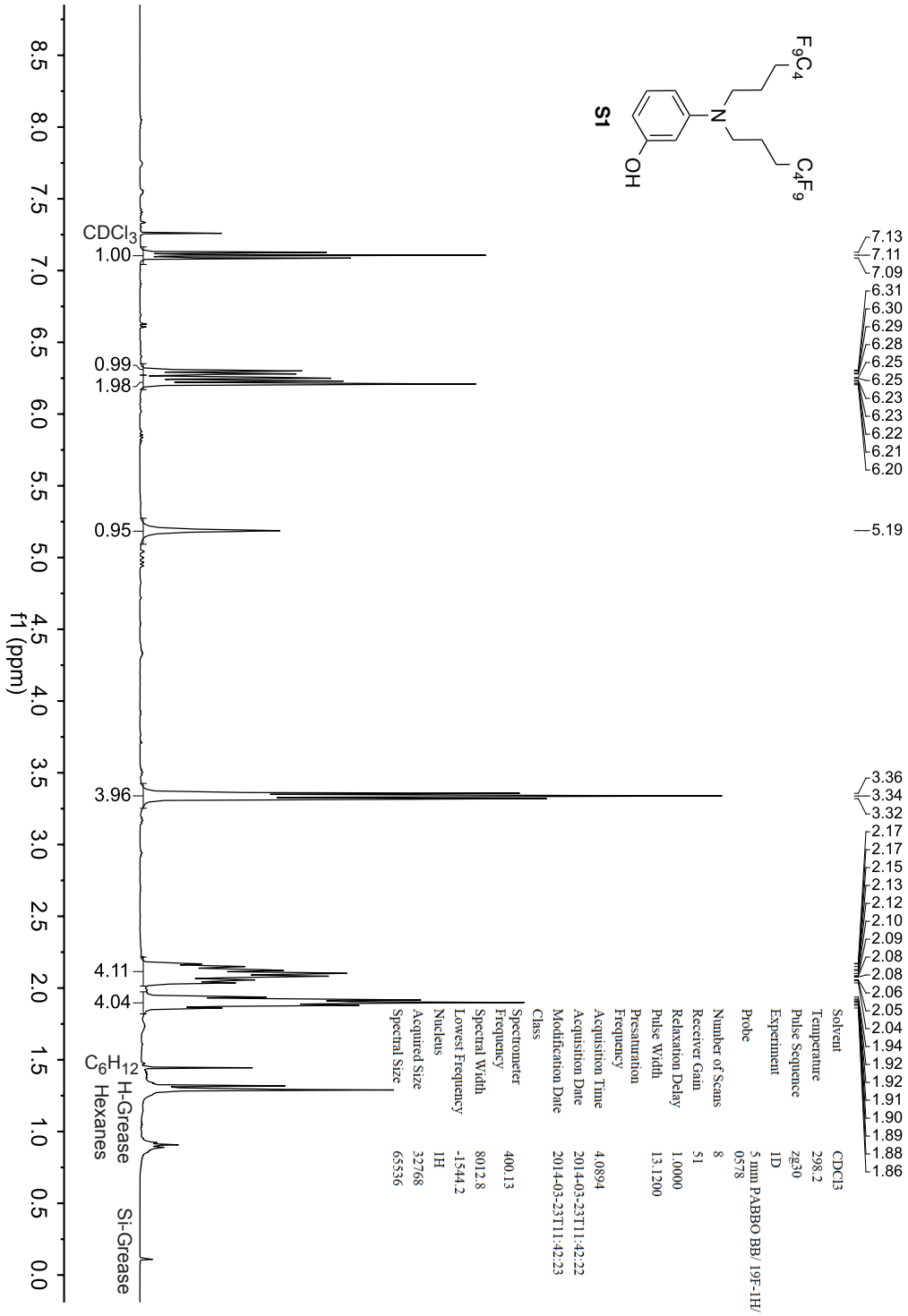

7.82
7.62
7.61
7.59
7.59
7.51
7.50
7.50
7.49
7.48
6.91
6.90
6.89
6.72
6.72
6.70
6.69
6.64
6.63
3.74
3.73
3.71
2.46
2.43
2.41
2.39
2.36
2.34
2.04
2.02
2.00
2.00
1.99
F17C8
F17C8
N
O
NH
CN
Ph
4
Solvent Acetone
Temperature 298.1
Pulse Sequence zg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 36
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.5000
Presaturation Frequency
Acquisition Time 4.0894
Acquisition Date 2014-07-14T19:43:05
Modification Date 2014-07-14T19:45:30
Class
Spectrometer Frequency 400.13
Spectral Width 8012.8
Lowest Frequency -1542.2
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
0.83
2.88
2.00
1.01
1.24
0.83
4.23
Water
4.43
4.16
Acetone
H-Grease
Si-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 0.5 0.0
f1 (ppm)

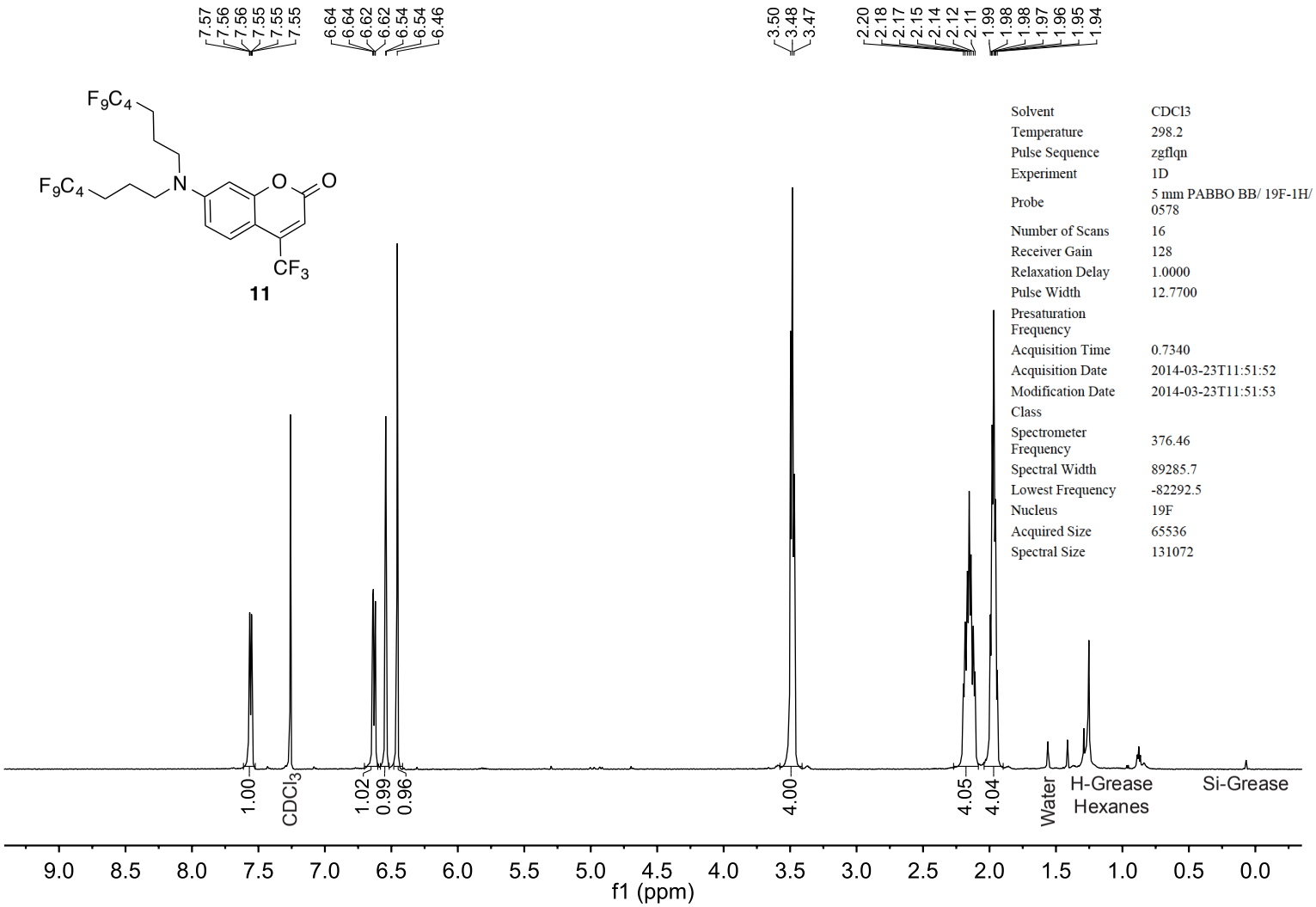

7.97
7.95
7.79
7.78
7.73
7.71
7.70
7.28
7.27
6.61
6.59
6.59
6.58
3.64
3.62
3.61
2.42
2.40
2.39
2.38
2.36
2.34
2.01
2.00
1.99
1.97
1.96
F17C8
C8F17
F17C8
C8F17
N
O
N
O
O
Rhodamine acid
Solvent Acetone
Temperature 293.0
Pulse Sequence zg30
Experiment 1D
Probe 5 mm CPTXI 1H-13C/ 15N/ 0082
Number of Scans 32
Receiver Gain 51
Relaxation Delay 1.0000
Pulse Width 11.0000
Acquisition Time 2.6477
Acquisition Date 2013-03-26T18:44:46
Modification Date 2013-03-26T18:44:50
Class
Spectrometer Frequency 600.13
Spectral Width 12376.2
Lowest Frequency -2497.1
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
1.05
1.04
1.18
1.12
5.91
8.00
Water
8.30
8.38
Acetone
H-Grease
Si-Grease
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)

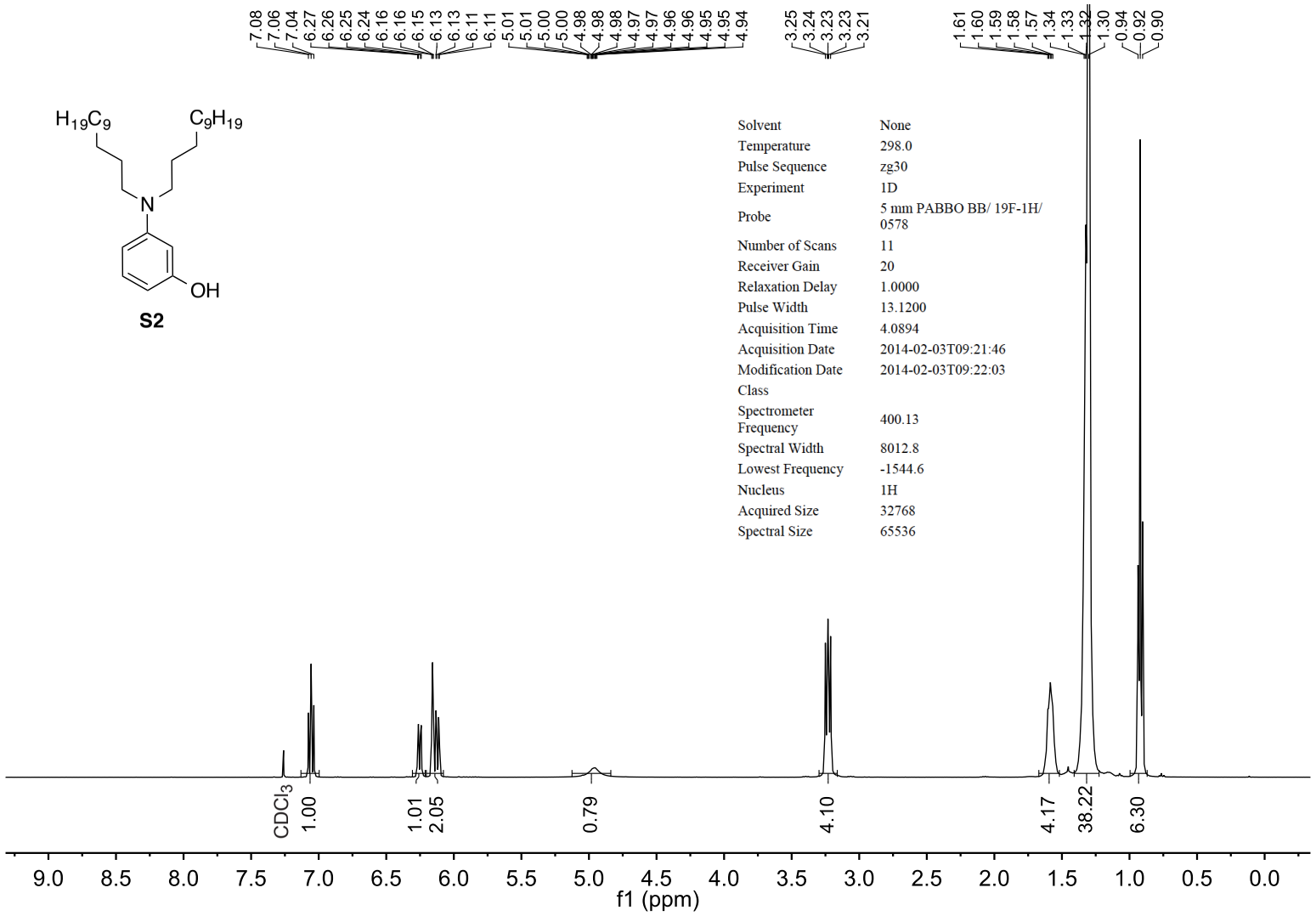

8.36
8.36
8.35
8.34
8.34
8.33
7.97
7.97
7.95
7.95
7.93
7.93
7.90
7.90
7.88
7.88
7.86
7.86
7.57
7.56
7.55
7.55
7.54
7.38
7.37
7.36
7.35
7.24
7.24
7.21
F17C8
N
F17C8
O
N
Cl
C8F17
C8F17
COOMe
5
4.04
4.02
4.00
3.65
2.52
2.15
1.08
1.20
1.22
1.11
1.99
3.76
7.95
3.00
Water
8.57
7.74
Acetone
H-Grease
Si-Grease
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)
Solvent Acetone
Temperature 298.1
Pulse Sequence zg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/
0556
Number of Scans 16
Receiver Gain 198
Relaxation Delay 1.0000
Pulse Width 14.5000
Acquisition Time 4.0894
Acquisition Date 2012-10-22T14:35:19
Modification Date 2012-10-22T14:35:20
Class
Spectrometer Frequency 400.13
Spectral Width 8012.8
Lowest Frequency -1542.2
Nucleus 1H
Acquired Size 32768
Spectral Size 65536

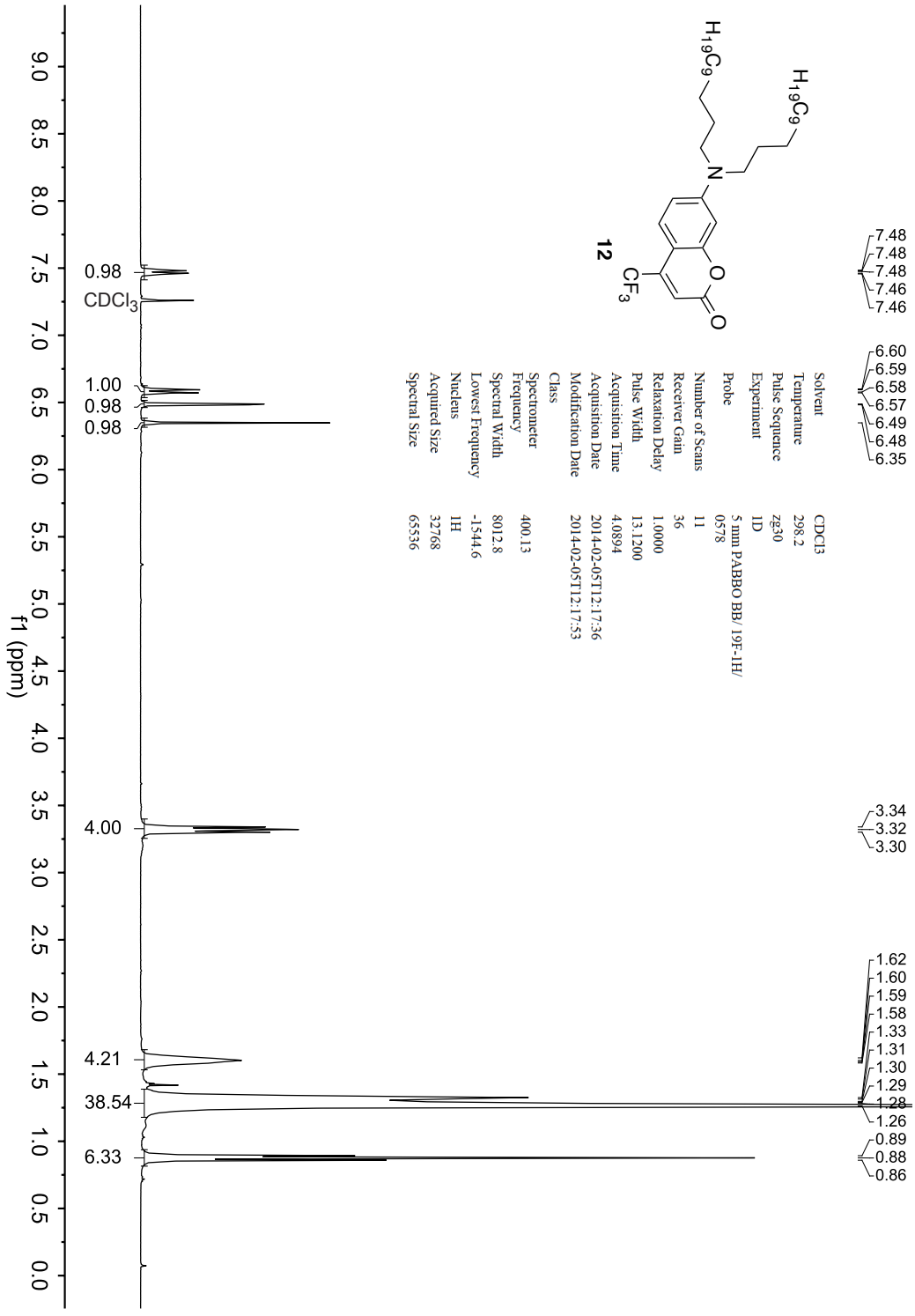

6.93
6.65
3.96
2.57
2.42
F17C8
OH
O
C8F17
N
N+
F17C8
O
HO
C8F17
6
Solvent HFIPA
Temperature 103.0
Pulse Sequence zg30
Experiment 1D
Probe 5 mm BBO BB-1H/ 2H
Number of Scans 160
Receiver Gain 4
Relaxation Delay 1.0000
Pulse Width 11.0000
Presaturation Frequency
Acquisition Time 2.6477
Acquisition Date 2014-07-18T13:44:32
Modification Date 2014-07-18T13:53:52
Class
Spectrometer Frequency 600.13
Spectral Width 12376.2
Lowest Frequency -2482.1
Nucleus 1H
Acquired Size 32768
Spectral Size 131072
1.84
2.13
2.02
Hexafluoro-
isopropanol
8.00
8.82
7.98
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
f1 (ppm)


7.86
7.64
7.63
7.62
7.62
7.58
7.58
7.57
7.56
7.22
7.20
7.00
4.09
3.57
2.57
2.55
2.53
2.52
2.50
2.50
2.49
2.22
2.21
2.20
2.19
2.19
2.18
2.17
C_8F_{17}
$^{-}ClO_4$
^{+}N
O
N
C_8F_{17}
N
7
Solvent Acetone
Temperature 102.9
Pulse Sequence zg30
Experiment 1D
Probe 5 mm BBO BB-1H/ 2H
Number of Scans 40
Receiver Gain 1448
Relaxation Delay 1.0000
Pulse Width 11.0000
Presaturation Frequency
Acquisition Time 2.6477
Acquisition Date 2014-07-11T09:51:50
Modification Date 2014-07-11T09:53:48
Class
Spectrometer Frequency 600.13
Spectral Width 12376.2
Lowest Frequency -2494.7
Nucleus 1H
Acquired Size 32768
Spectral Size 131072
1.95
1.01
0.90
1.02
1.02
3.71
6.09
Water
4.00
3.83
Acetone
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)

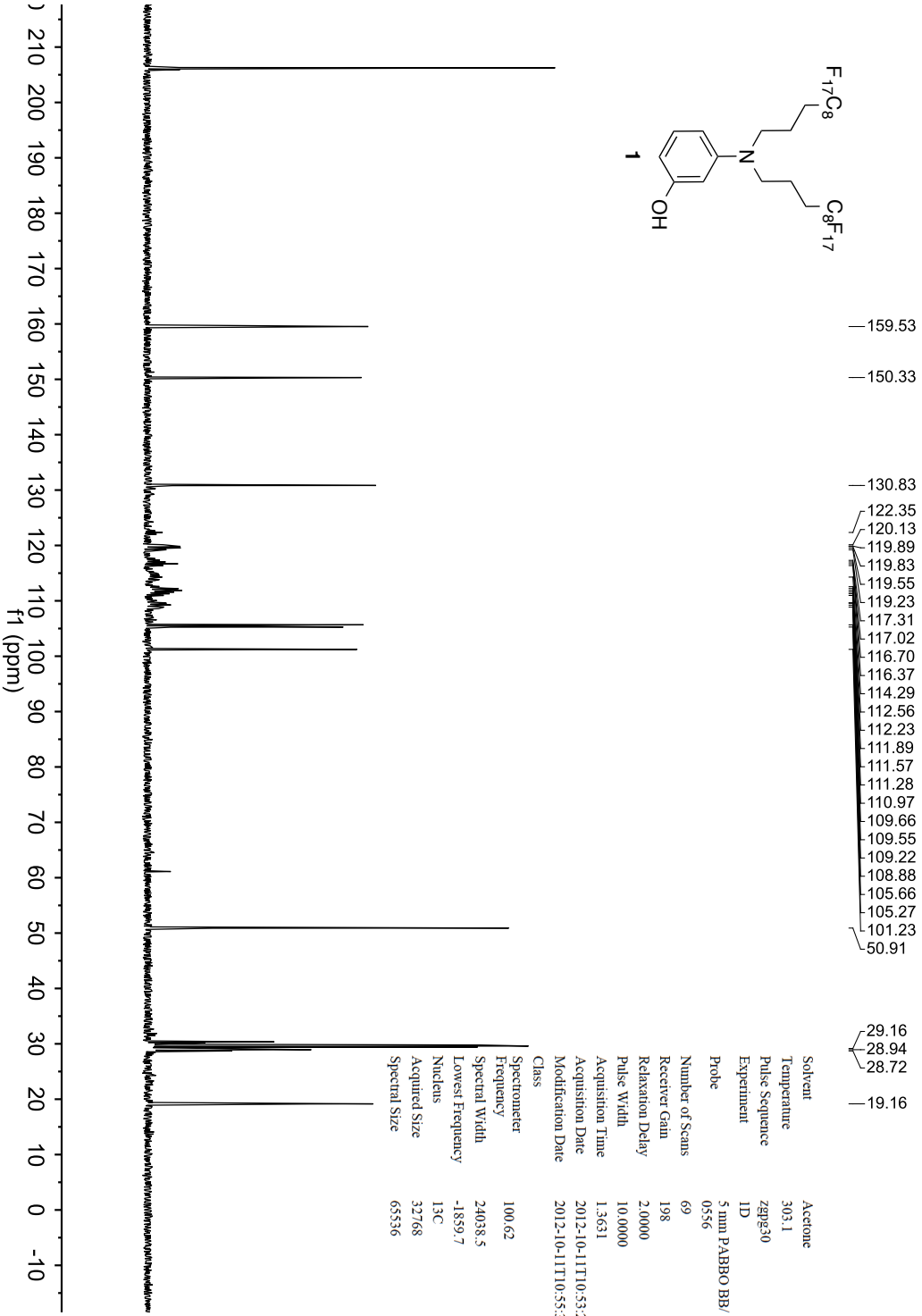

S1
F9C4
C4F9
N
OH
7.13
7.11
7.09
6.31
6.30
6.29
6.28
6.25
6.25
6.23
6.23
6.22
6.21
6.20
5.19
3.36
3.34
3.32
2.17
2.17
2.15
2.13
2.12
2.10
2.09
2.08
2.08
2.06
2.05
2.04
1.94
1.92
1.92
1.91
1.90
1.89
1.88
1.86
CDCl3
1.00
0.99
1.98
0.95
3.96
4.11
4.04
C6H12
H-Grease
Hexanes
Si-Grease
f1 (ppm)
Solvent CDCl3
Temperature 298.2
Pulse Sequence zg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/
0578
Number of Scans 8
Receiver Gain 51
Relaxation Delay 1.0000
Pulse Width 13.1200
Presaturation
Frequency
Acquisition Time 4.0894
Acquisition Date 2014-03-23T11:42:22
Modification Date 2014-03-23T11:42:23
Class
Spectrometer 400.13
Frequency 8012.8
Spectral Width -1544.2
Lowest Frequency 1H
Nucleus 32768
Acquired Size 65536
Spectral Size

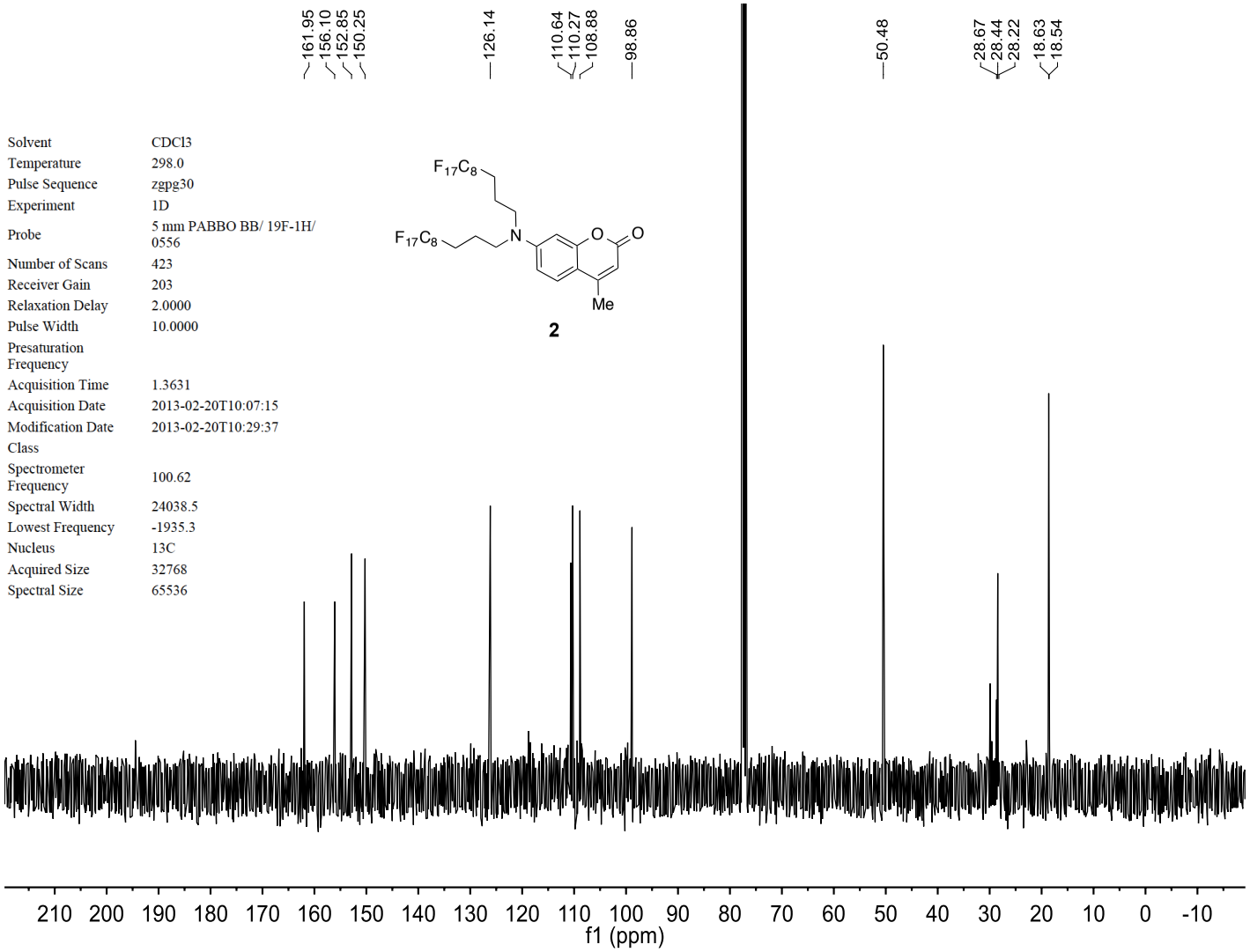

7.57
7.56
7.56
7.55
7.55
7.55
6.64
6.64
6.62
6.62
6.54
6.54
6.46
3.50
3.48
3.47
2.20
2.18
2.17
2.15
2.14
2.12
2.11
1.99
1.98
1.98
1.97
1.96
1.95
1.94
F9C4
F9C4
N
O
O
CF3
11
Solvent CDCl3
Temperature 298.2
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans 16
Receiver Gain 128
Relaxation Delay 1.0000
Pulse Width 12.7700
Presaturation Frequency
Acquisition Time 0.7340
Acquisition Date 2014-03-23T11:51:52
Modification Date 2014-03-23T11:51:53
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
1.00
CDCl3
1.02
0.99
0.96
4.00
4.05
4.04
Water
H-Grease
Hexanes
Si-Grease
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)

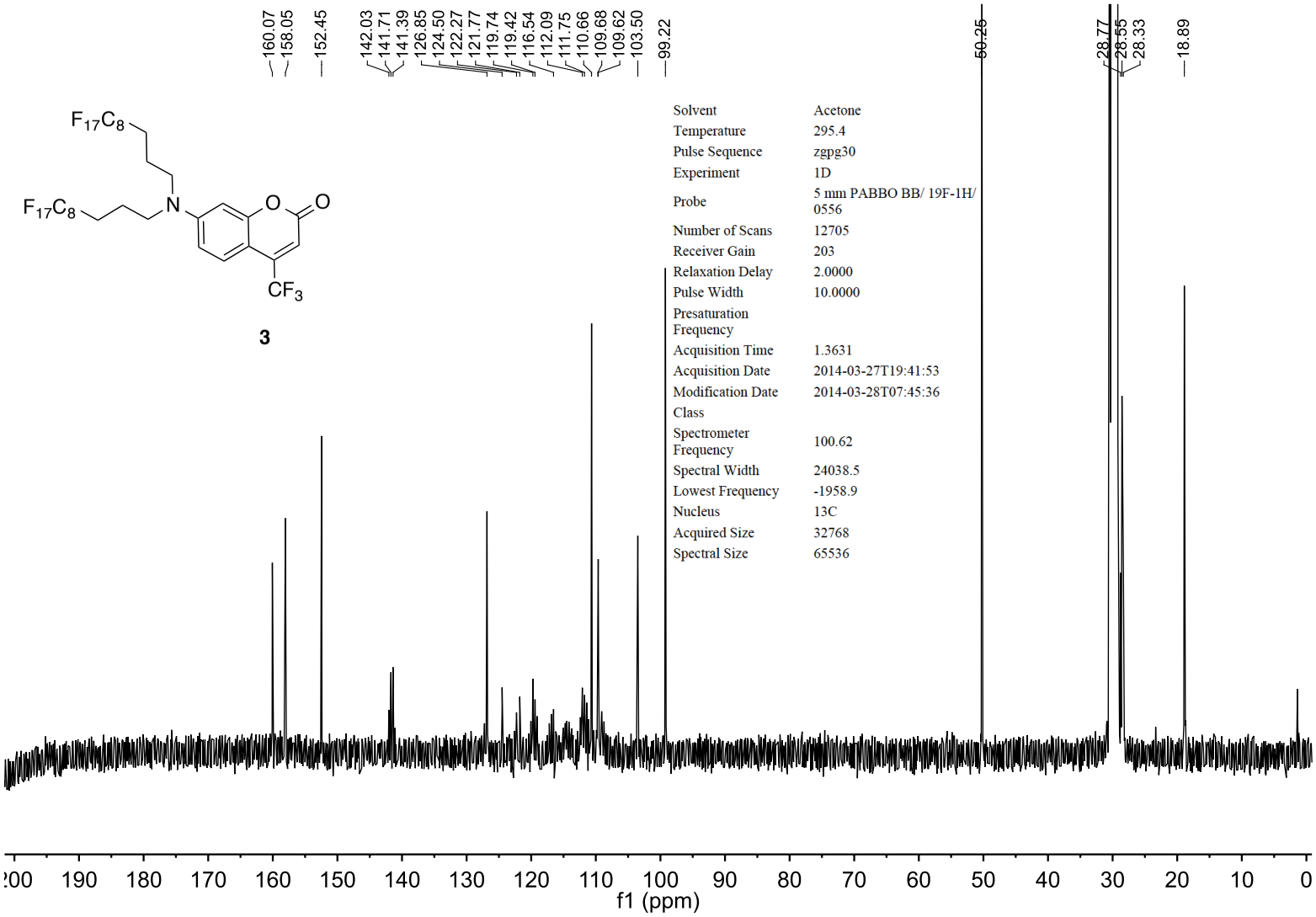

7.08
7.06
7.04
6.27
6.26
6.25
6.24
6.16
6.16
6.15
6.13
6.13
6.11
6.11
5.01
5.01
5.00
5.00
4.98
4.98
4.98
4.97
4.97
4.96
4.96
4.95
4.95
4.94
3.25
3.24
3.23
3.23
3.21
1.61
1.60
1.59
1.58
1.57
1.34
1.33
1.32
1.30
0.94
0.92
0.90
H19C9
C9H19
N
OH
S2
Solvent None
Temperature 298.0
Pulse Sequence zg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans 11
Receiver Gain 20
Relaxation Delay 1.0000
Pulse Width 13.1200
Acquisition Time 4.0894
Acquisition Date 2014-02-03T09:21:46
Modification Date 2014-02-03T09:22:03
Class
Spectrometer Frequency 400.13
Spectral Width 8012.8
Lowest Frequency -1544.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
CDCl3
1.00
1.01
2.05
0.79
4.10
4.17
38.22
6.30
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)

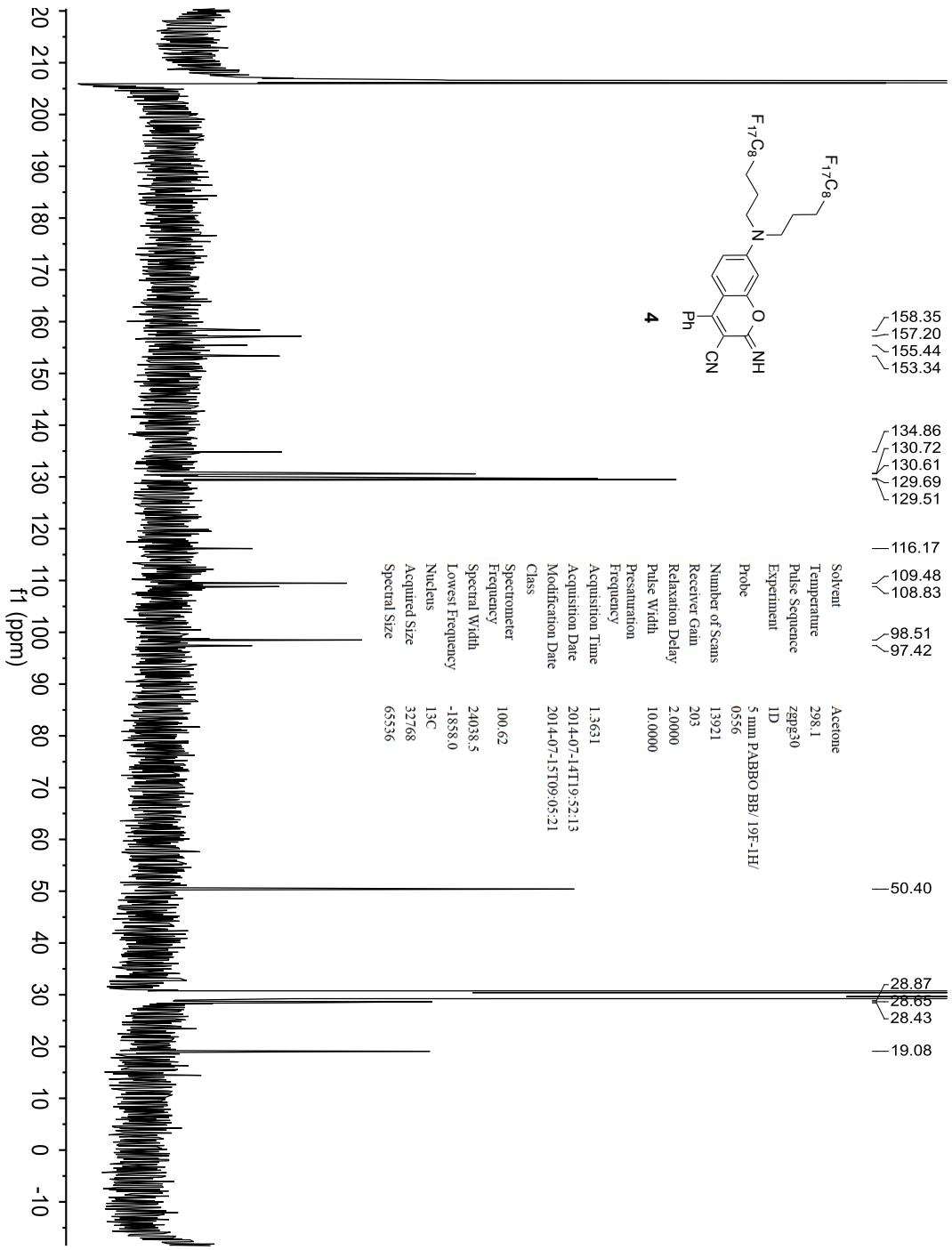

12
Solvent CDCl3
Temperature 298.2
Pulse Sequence zg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/
Number of Scans 11
Receiver Gain 36
Relaxation Delay 1.0000
Pulse Width 13.1200
Acquisition Time 4.0894
Acquisition Date 2014-02-05T12:17:36
Modification Date 2014-02-05T12:17:53
Class
Spectrometer Frequency 400.13
Spectral Width 8012.8
Lowest Frequency -1544.6
Nucleus 1H
Acquired Size 32768
Spectral Size 65536
7.48
7.48
7.48
7.46
7.46
6.60
6.59
6.58
6.57
6.49
6.48
6.35
3.34
3.32
3.30
1.62
1.60
1.59
1.58
1.33
1.31
1.30
1.29
1.28
1.26
0.89
0.88
0.86
0.98
CDCl3
1.00
0.98
0.98
4.00
4.21
38.54
6.33
f1 (ppm)

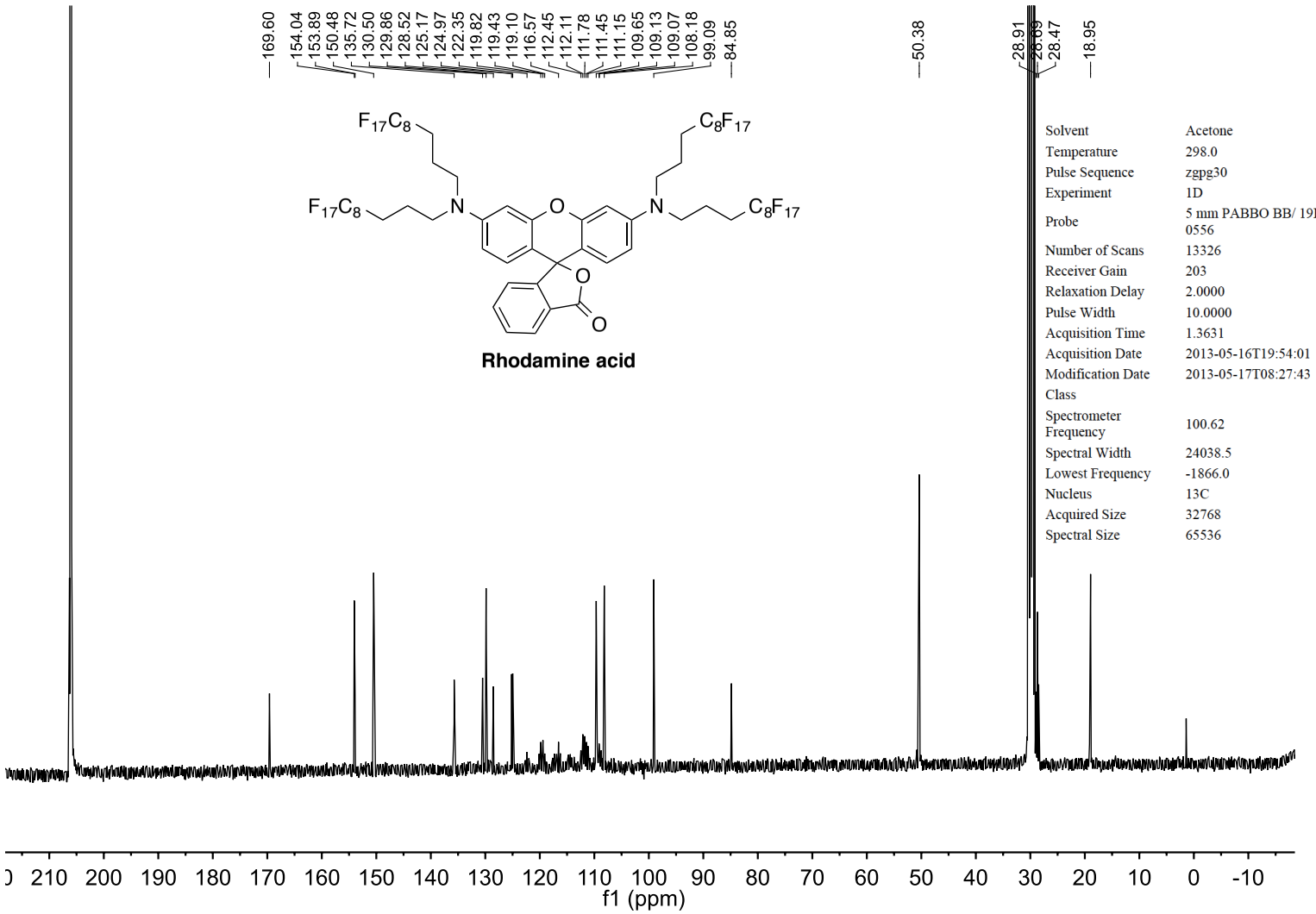
^{13}C-NMR

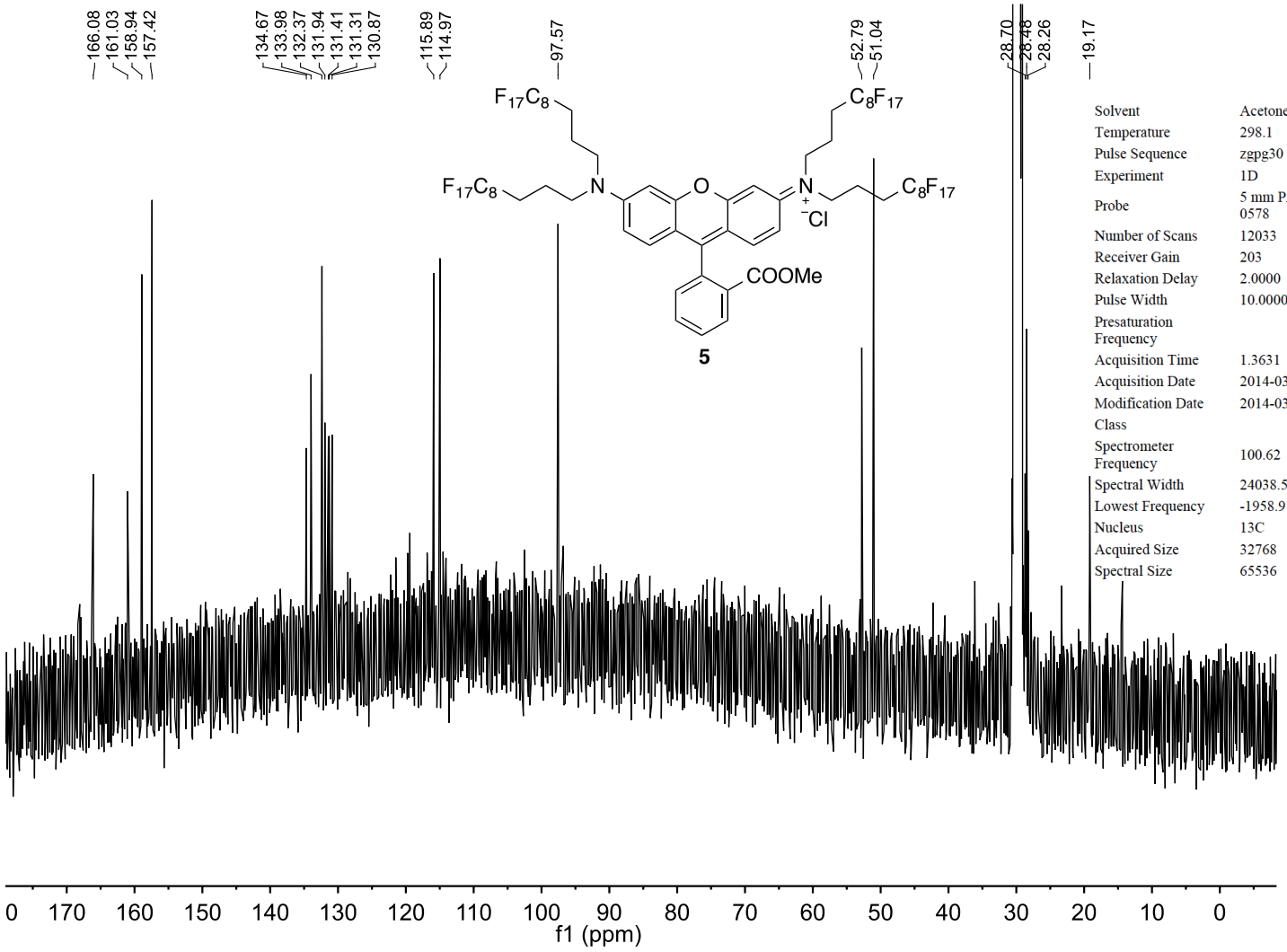

F17C8
C8F17
N
OH
1
159.53
150.33
130.83
122.35
120.13
119.89
119.83
119.55
119.23
117.31
117.02
116.70
116.37
114.29
112.56
112.23
111.89
111.57
111.28
110.97
109.66
109.55
109.22
108.88
105.66
105.27
101.23
50.91
29.16
28.94
28.72
19.16
Solvent Acetone
Temperature 303.1
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 69
Receiver Gain 198
Relaxation Delay 2.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Acquisition Date 2012-10-11T10:53:24
Modification Date 2012-10-11T10:55:33
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1859.7
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

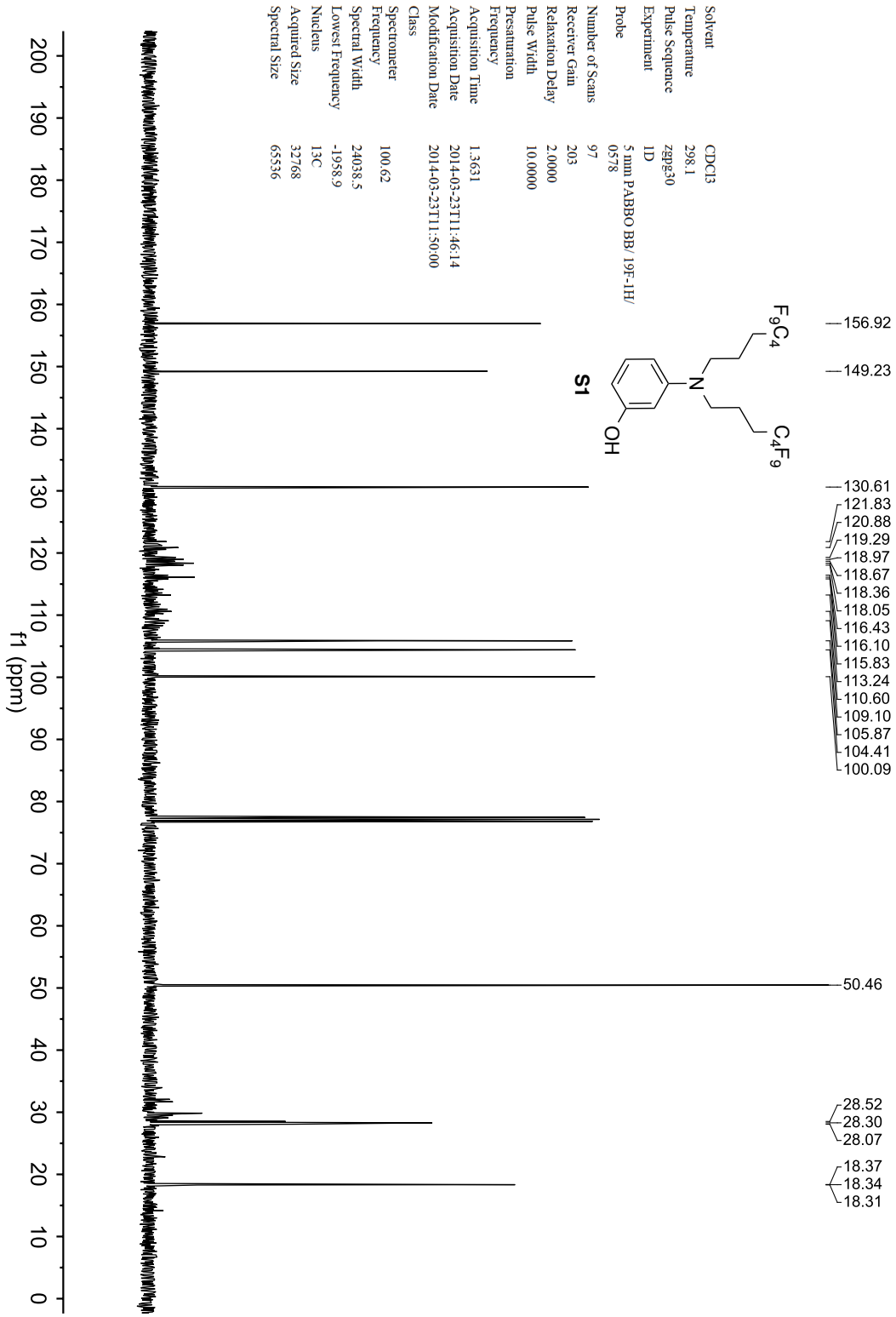

161.95
156.10
152.85
150.25
126.14
110.64
110.27
108.88
98.86
50.48
28.67
28.44
28.22
18.63
18.54
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 423
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Presaturation Frequency
Acquisition Time 1.3631
Acquisition Date 2013-02-20T10:07:15
Modification Date 2013-02-20T10:29:37
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1935.3
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
F17C8
F17C8
N
O
O
Me
2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

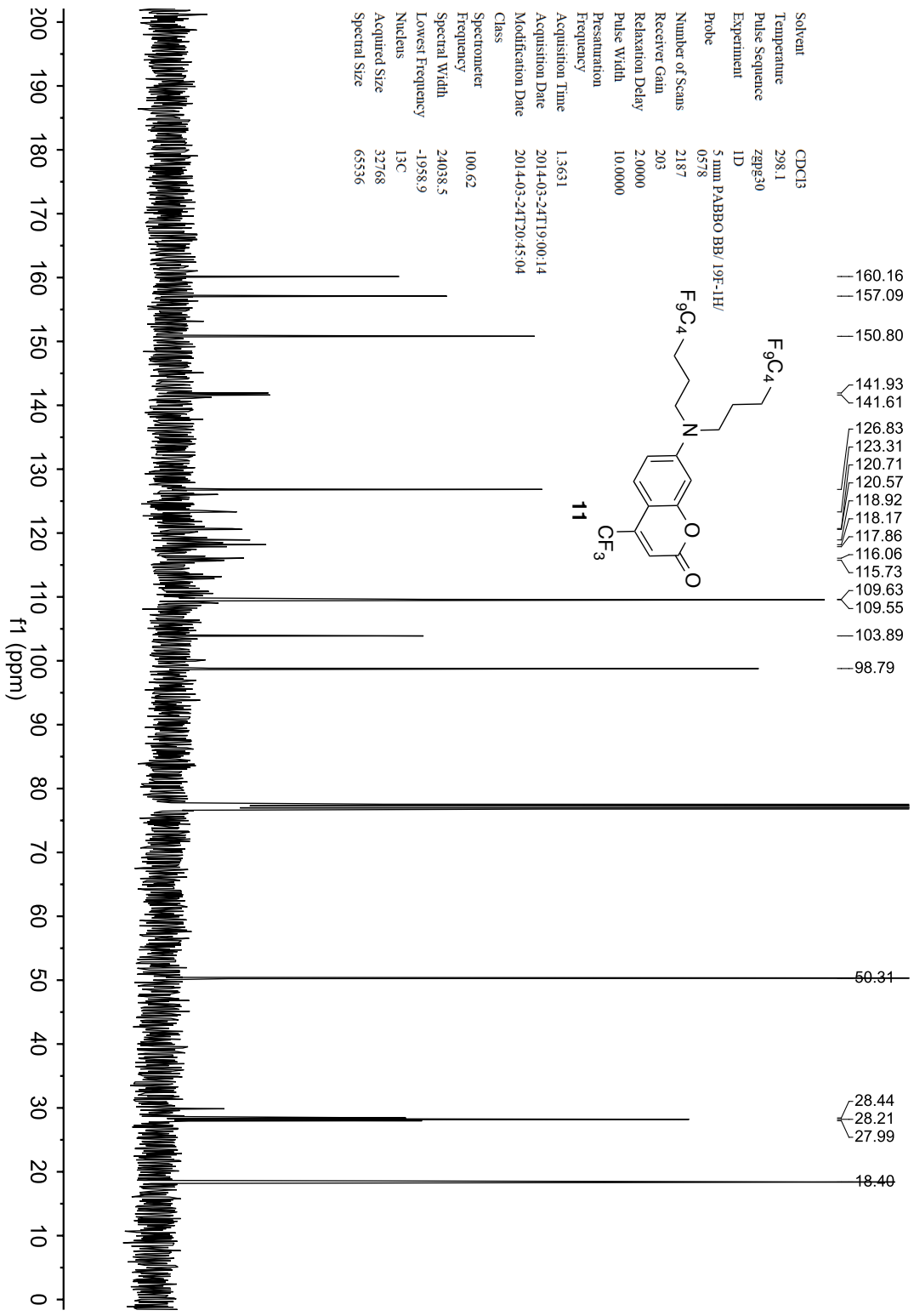

160.07
158.05
152.45
142.03
141.71
141.39
126.85
124.50
122.27
121.77
119.74
119.42
116.54
112.09
111.75
110.66
109.68
109.62
103.50
99.22
50.26
28.77
28.55
28.33
18.89
F17C8
F17C8
N
O
O
CF3
3
Solvent Acetone
Temperature 295.4
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 12705
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Presaturation Frequency
Acquisition Time 1.3631
Acquisition Date 2014-03-27T19:41:53
Modification Date 2014-03-28T07:45:36
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

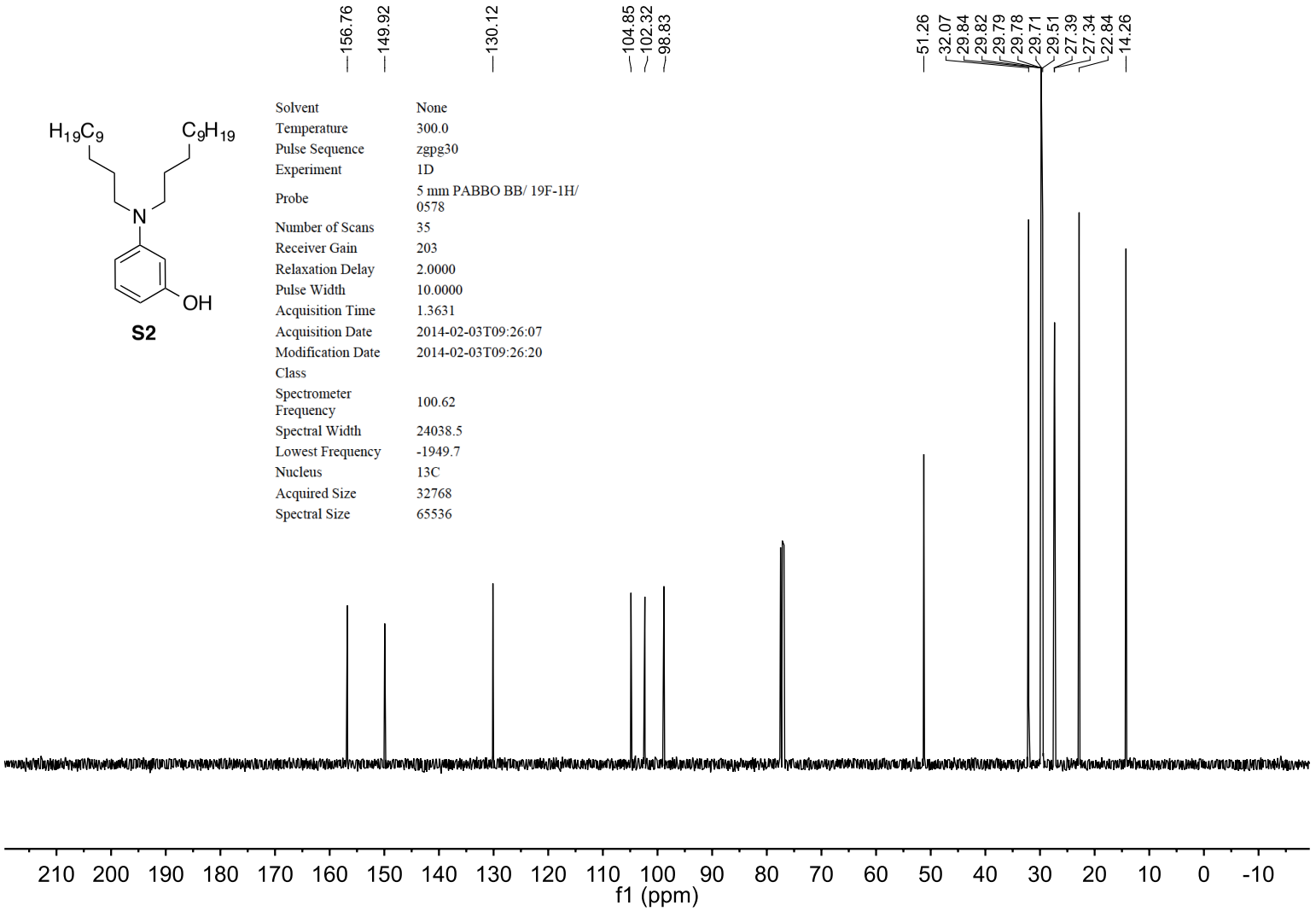

158.35
157.20
155.44
153.34
134.86
130.72
130.61
129.69
129.51
116.17
109.48
108.83
98.51
97.42
50.40
28.87
28.65
28.43
19.08
Solvent Acetone
Temperature 298.1
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/
0556
Number of Scans 13921
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Presaturation
Frequency
Acquisition Time 1.3631
Acquisition Date 2014-07-14T19:52:13
Modification Date 2014-07-15T09:05:21
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1858.0
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
4
Ph
CN
NH
O
N
F17C8
F17C8
f1 (ppm)

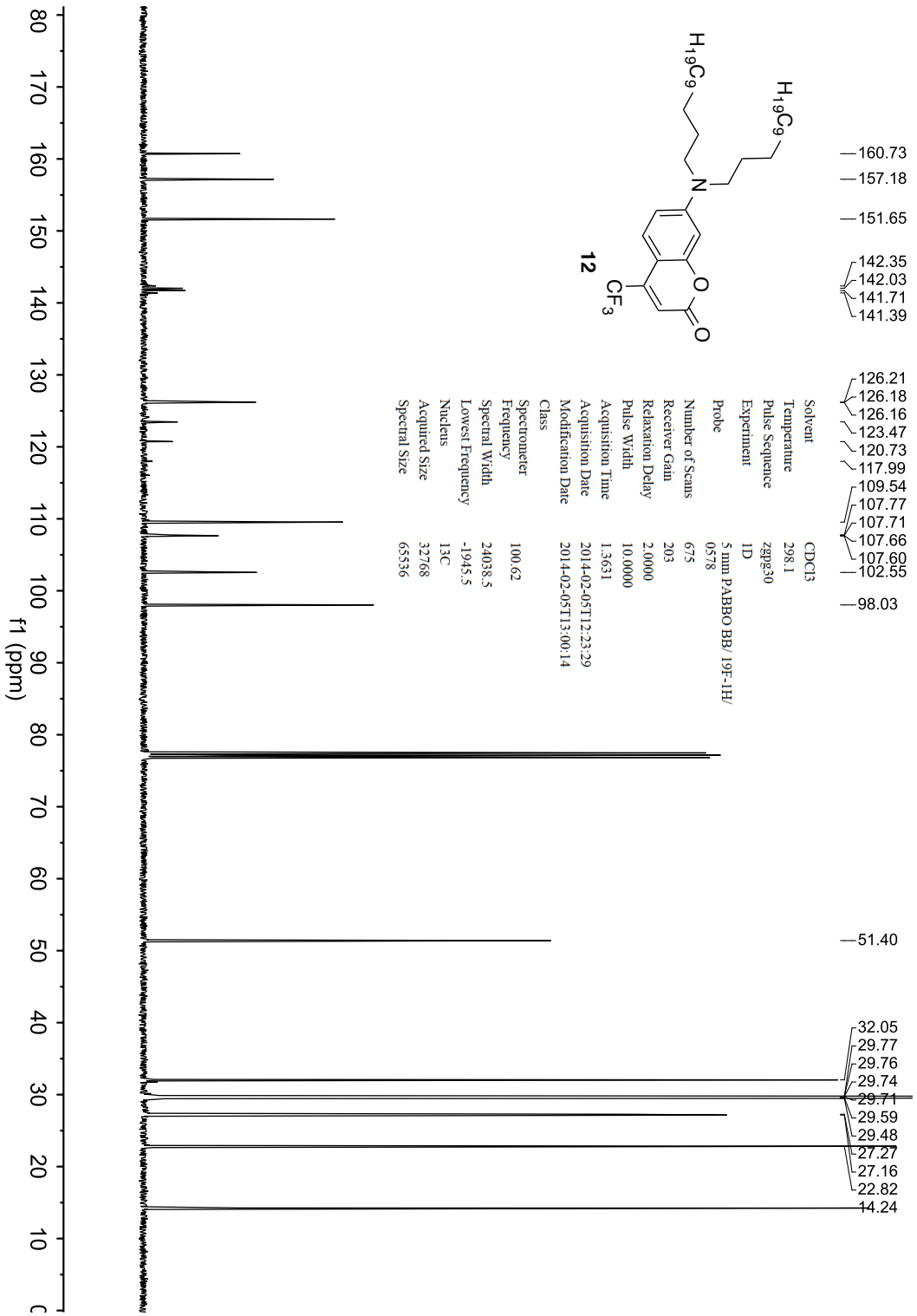

169.60
154.04
153.89
150.48
135.72
130.50
129.86
128.52
125.17
124.97
122.35
119.82
119.43
119.10
116.57
112.45
112.11
111.78
111.45
111.15
109.65
109.13
109.07
108.18
99.09
84.85
50.38
28.91
28.89
28.47
18.95
F17C8
C8F17
F17C8
N
O
N
C8F17
O
O
Rhodamine acid
Solvent Acetone
Temperature 298.0
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 13326
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Acquisition Date 2013-05-16T19:54:01
Modification Date 2013-05-17T08:27:43
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1866.0
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


166.08
161.03
158.94
157.42
134.67
133.98
132.37
131.94
131.41
131.31
130.87
115.89
114.97
97.57
52.79
51.04
28.70
28.48
28.26
19.17
F17C8
C8F17
F17C8
N
O
N
+
−Cl
C8F17
COOMe
5
Solvent Acetone
Temperature 298.1
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans 12033
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Presaturation Frequency
Acquisition Time 1.3631
Acquisition Date 2014-03-24T20:53:07
Modification Date 2014-03-25T08:18:27
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
0 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

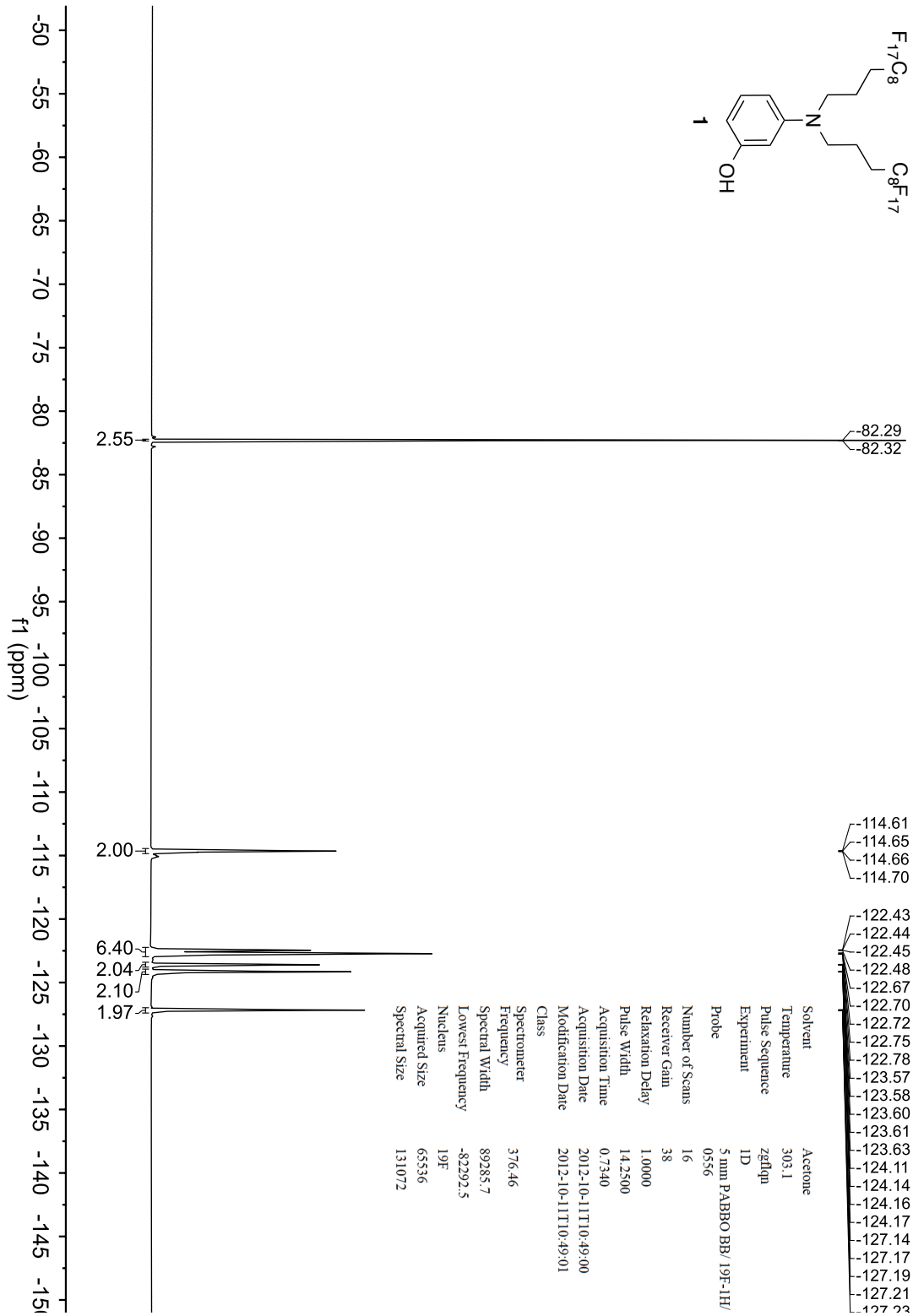

Solvent CDCl3
Temperature 298.1
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans 97
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Presaturation Frequency
Acquisition Time 1.3631
Acquisition Date 2014-03-23T11:46:14
Modification Date 2014-03-23T11:50:00
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
S1
OH
N
F9C4
C4F9
156.92
149.23
130.61
121.83
120.88
119.29
118.97
118.67
118.36
118.05
116.43
116.10
115.83
113.24
110.60
109.10
105.87
104.41
100.09
50.46
28.52
28.30
28.07
18.37
18.34
18.31
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

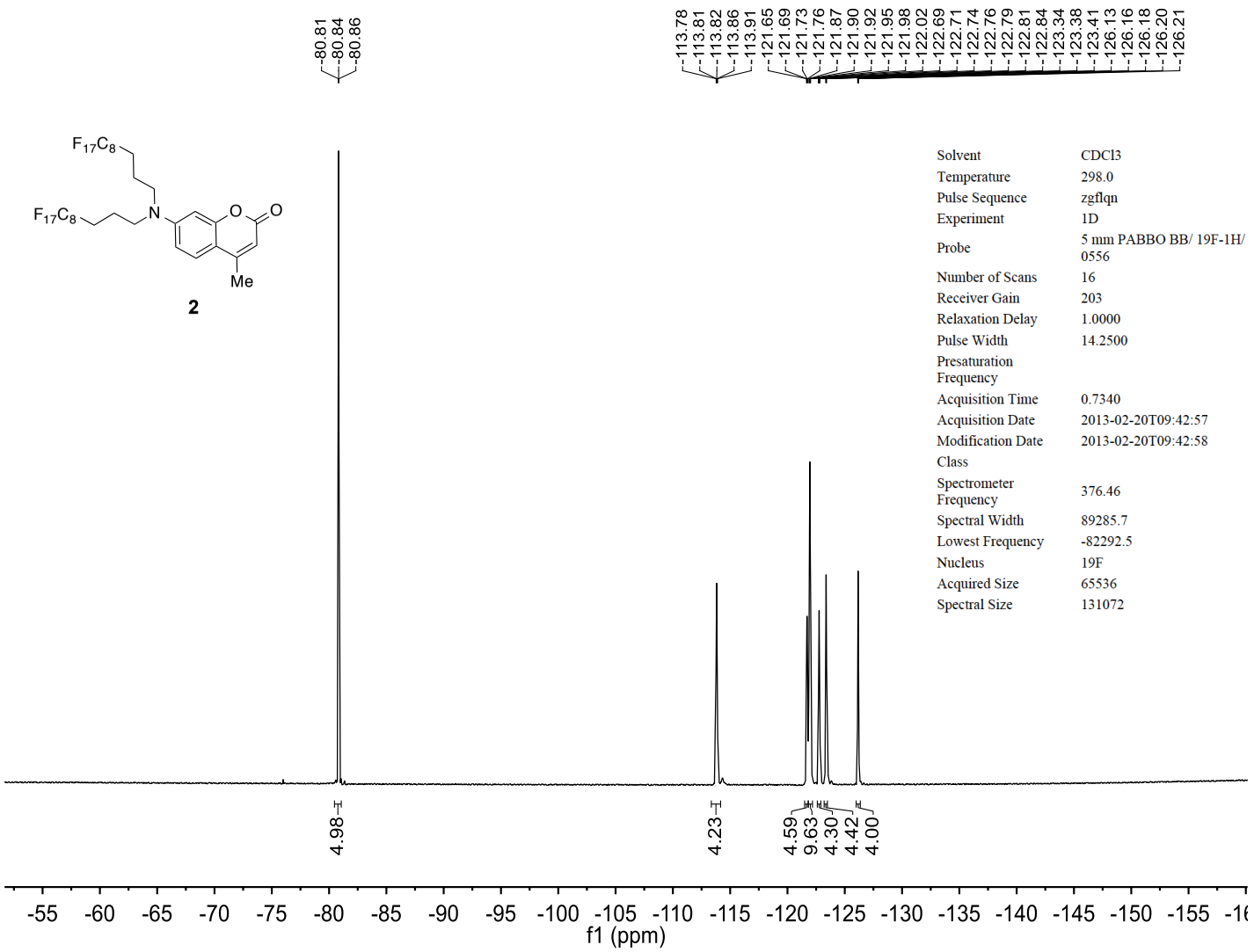

Solvent CDCl3
Temperature 298.1
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/
Number of Scans 2187
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Presaturation
Frequency
Acquisition Time 1.3631
Acquisition Date 2014-03-24T19:00:14
Modification Date 2014-03-24T20:45:04
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1958.9
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
F9C4
F9C4
N
O
O
CF3
11
160.16
157.09
150.80
141.93
141.61
126.83
123.31
120.71
120.57
118.92
118.17
117.86
116.06
115.73
109.63
109.55
103.89
98.79
50.31
28.44
28.21
27.99
18.40
f1 (ppm)

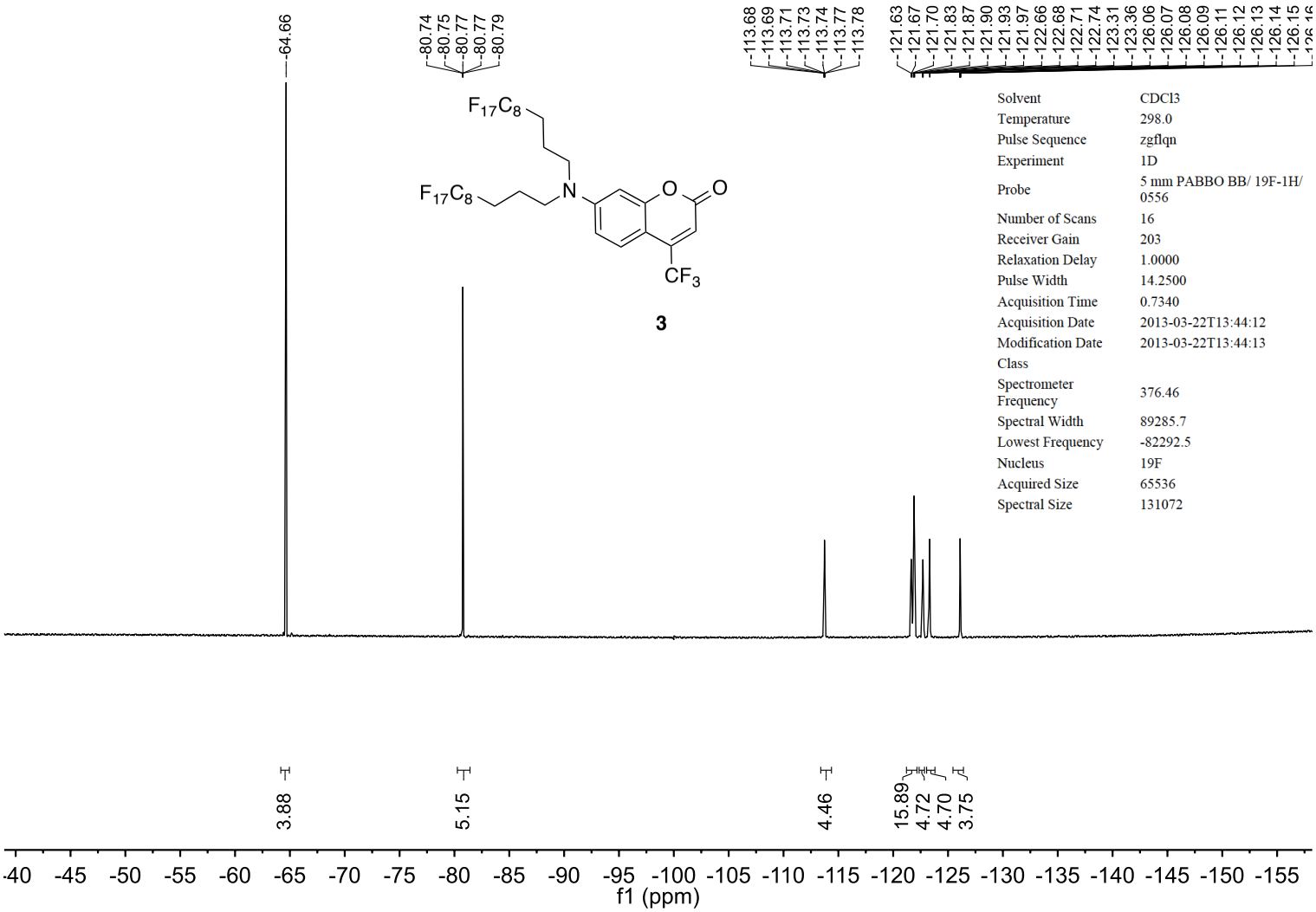

156.76
149.92
130.12
104.85
102.32
98.83
51.26
32.07
29.84
29.82
29.79
29.78
29.71
29.51
27.39
27.34
22.84
14.26
H19C9
C9H19
N
OH
S2
Solvent None
Temperature 300.0
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans 35
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Acquisition Date 2014-02-03T09:26:07
Modification Date 2014-02-03T09:26:20
Class
Spectrometer Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1949.7
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

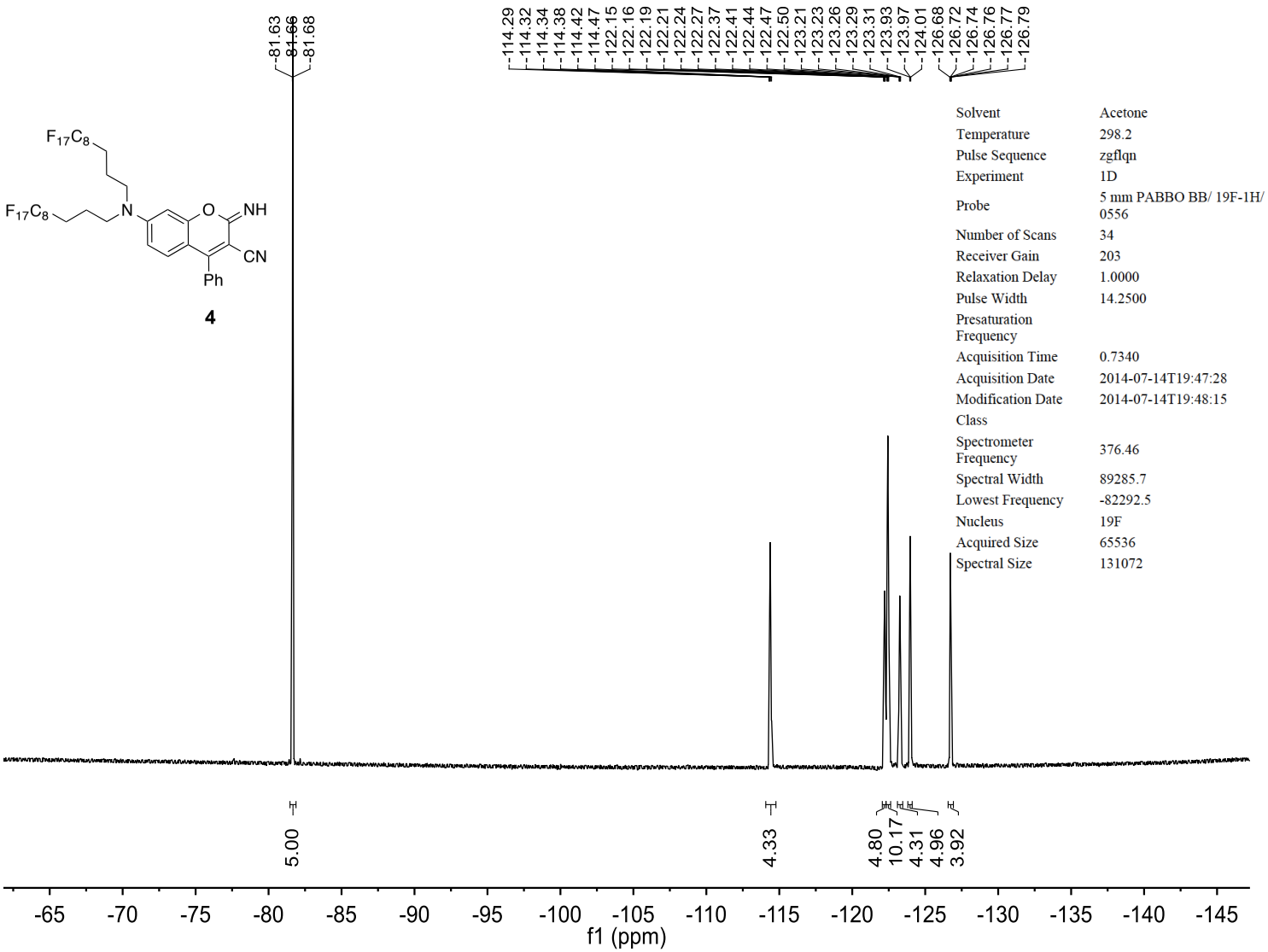

H19C9
H19C9
N
O
O
CF3
12
160.73
157.18
151.65
142.35
142.03
141.71
141.39
126.21
126.18
126.16
123.47
120.73
117.99
109.54
107.77
107.71
107.66
107.60
102.55
98.03
51.40
32.05
29.77
29.76
29.74
29.71
29.59
29.48
27.27
27.16
22.82
14.24
Solvent CDCl3
Temperature 298.1
Pulse Sequence zgpg30
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/
0578
Number of Scans 675
Receiver Gain 203
Relaxation Delay 2.0000
Pulse Width 10.0000
Acquisition Time 1.3631
Acquisition Date 2014-02-05T12:23:29
Modification Date 2014-02-05T13:00:14
Class
Spectrometer
Frequency 100.62
Spectral Width 24038.5
Lowest Frequency -1945.5
Nucleus 13C
Acquired Size 32768
Spectral Size 65536
f1 (ppm)
80
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

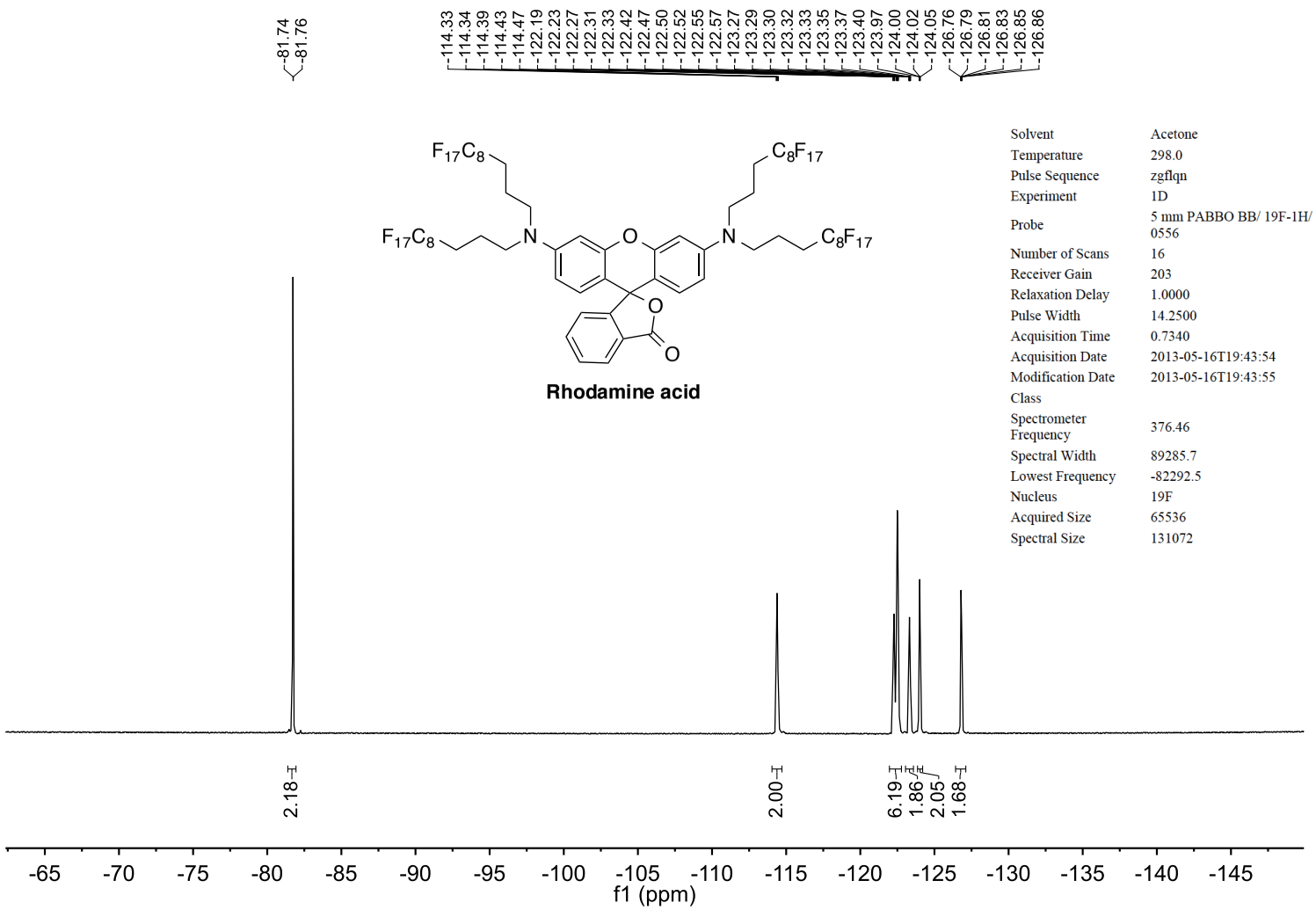
^{19}F-NMR

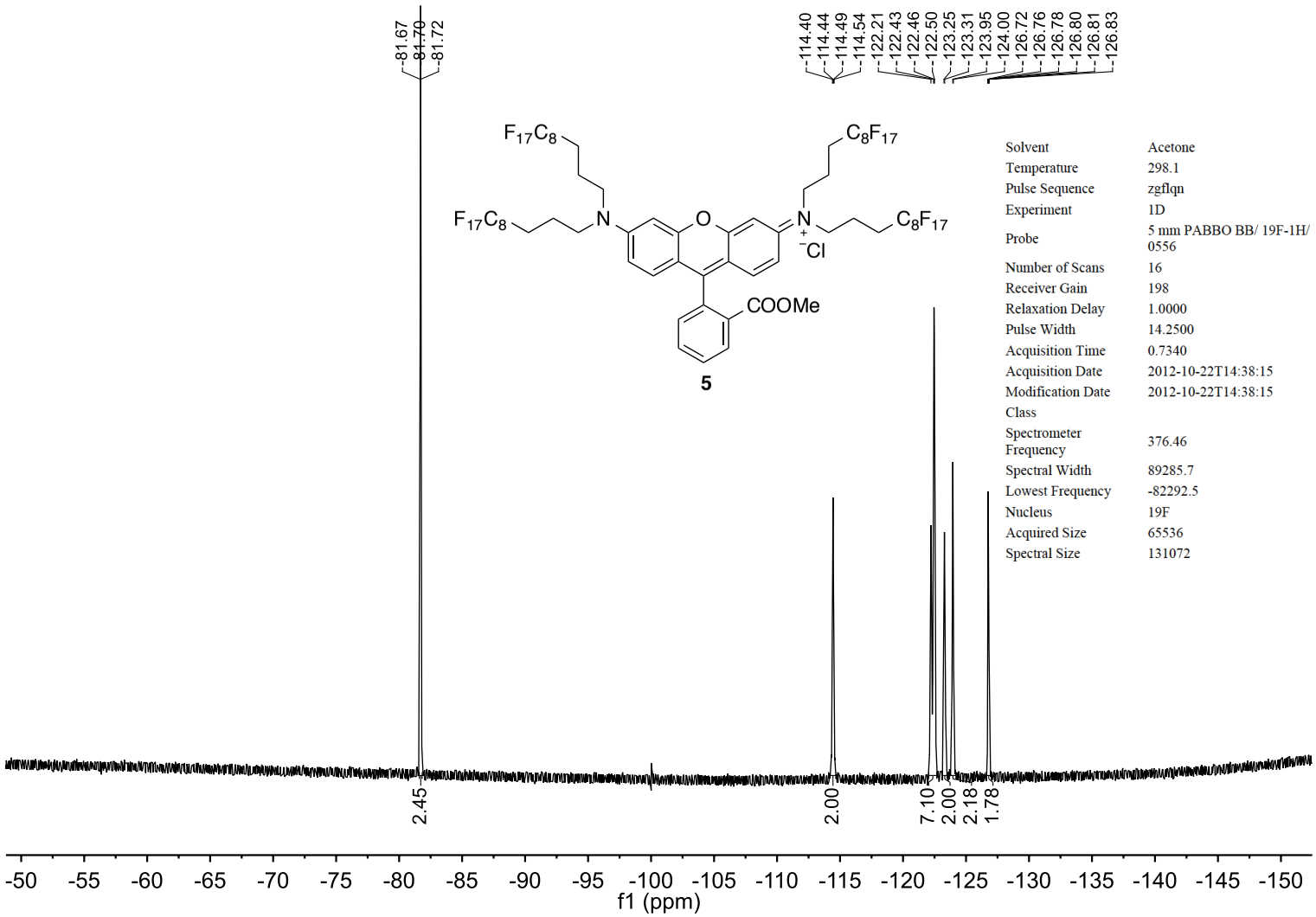

F17C8
C8F17
N
OH
1
-82.29
-82.32
-114.61
-114.65
-114.66
-114.70
-122.43
-122.44
-122.45
-122.48
-122.67
-122.70
-122.72
-122.75
-122.78
-123.57
-123.58
-123.60
-123.61
-123.63
-124.11
-124.14
-124.16
-124.17
-127.14
-127.17
-127.19
-127.21
2.55
2.00
6.40
2.04
2.10
1.97
f1 (ppm)
-50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145
Solvent Acetone
Temperature 303.1
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 16
Receiver Gain 38
Relaxation Delay 1.0000
Pulse Width 14.2500
Acquisition Time 0.7340
Acquisition Date 2012-10-11T10:49:00
Modification Date 2012-10-11T10:49:01
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072

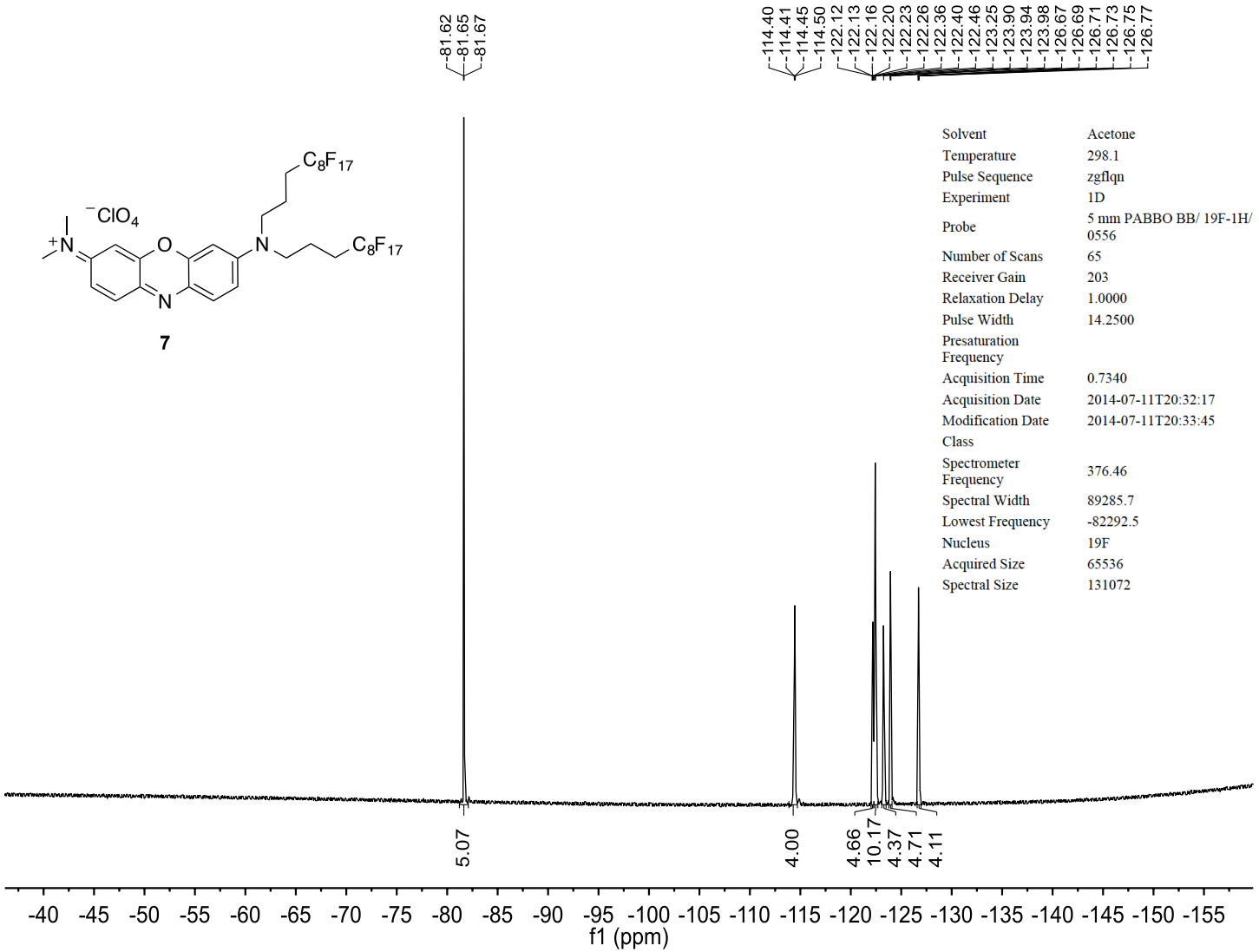

-80.81
-80.84
-80.86
-113.78
-113.81
-113.82
-113.86
-113.91
-121.65
-121.69
-121.73
-121.76
-121.87
-121.90
-121.92
-121.95
-121.98
-122.02
-122.69
-122.71
-122.74
-122.76
-122.79
-122.81
-122.84
-123.34
-123.38
-123.41
-126.13
-126.16
-126.18
-126.20
-126.21
F17C8
F17C8
N
O
O
Me
2
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 16
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.2500
Presaturation Frequency
Acquisition Time 0.7340
Acquisition Date 2013-02-20T09:42:57
Modification Date 2013-02-20T09:42:58
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
4.98
4.23
4.59
9.63
4.30
4.42
4.00
-55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155
f1 (ppm)

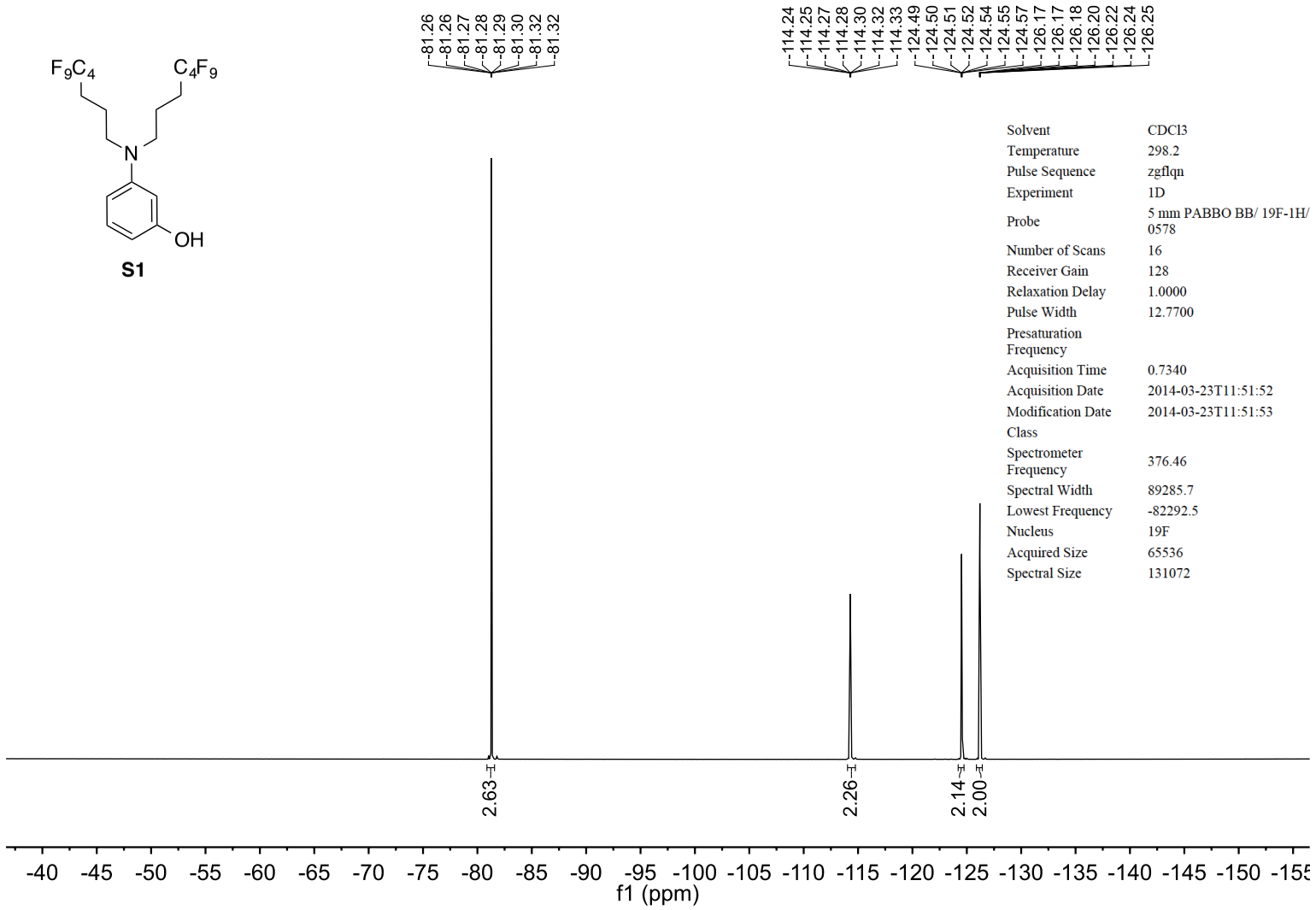

-64.66
-80.74
-80.75
-80.77
-80.77
-80.79
-113.68
-113.69
-113.71
-113.73
-113.74
-113.77
-113.78
-121.63
-121.67
-121.70
-121.83
-121.87
-121.90
-121.93
-121.97
-122.66
-122.68
-122.71
-122.74
-123.31
-123.36
-126.06
-126.07
-126.08
-126.09
-126.11
-126.12
-126.13
-126.14
-126.15
F17C8
F17C8
N
O
O
CF3
3
Solvent CDCl3
Temperature 298.0
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 16
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.2500
Acquisition Time 0.7340
Acquisition Date 2013-03-22T13:44:12
Modification Date 2013-03-22T13:44:13
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
3.88
5.15
4.46
15.89
4.72
4.70
3.75
-40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155
f1 (ppm)

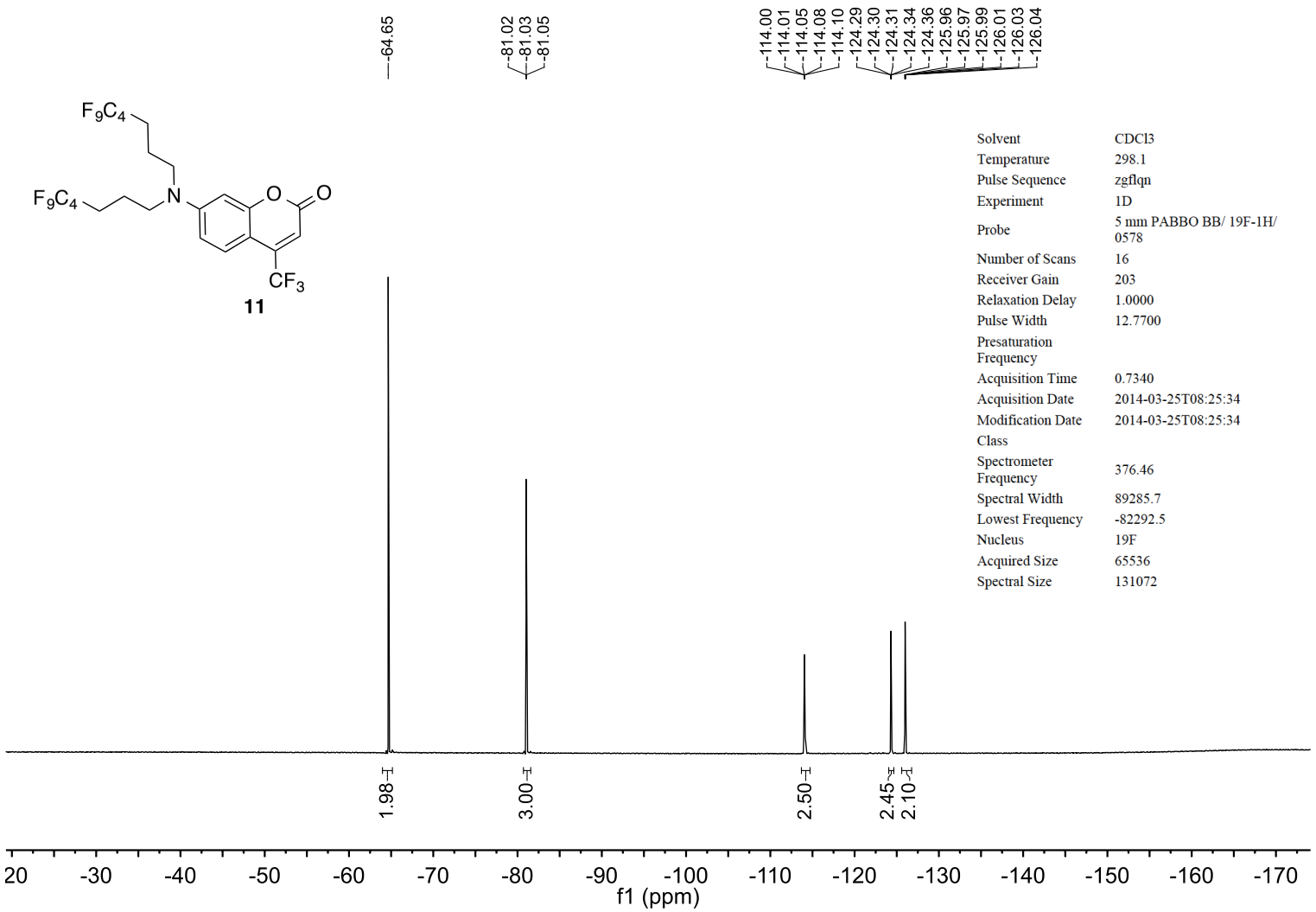

-81.63
-81.66
-81.68
-114.29
-114.32
-114.34
-114.38
-114.42
-114.47
-122.15
-122.16
-122.19
-122.21
-122.24
-122.27
-122.37
-122.41
-122.44
-122.47
-122.50
-123.21
-123.23
-123.26
-123.29
-123.31
-123.93
-123.97
-124.01
-126.68
-126.72
-126.74
-126.76
-126.77
-126.79
F17C8
F17C8
N
O
NH
CN
Ph
4
Solvent Acetone
Temperature 298.2
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 34
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.2500
Presaturation Frequency
Acquisition Time 0.7340
Acquisition Date 2014-07-14T19:47:28
Modification Date 2014-07-14T19:48:15
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
5.00
4.33
4.80
10.17
4.31
4.96
3.92
-65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145
f1 (ppm)

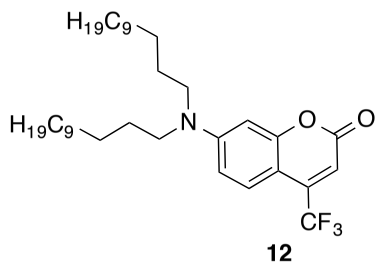

-81.74
-81.76
-114.33
-114.34
-114.39
-114.43
-114.47
-122.19
-122.23
-122.27
-122.31
-122.33
-122.42
-122.47
-122.50
-122.52
-122.55
-122.57
-123.27
-123.29
-123.30
-123.32
-123.33
-123.35
-123.37
-123.40
-123.97
-124.00
-124.02
-124.05
-126.76
-126.79
-126.81
-126.83
-126.85
-126.86
F17C8
C8F17
F17C8
C8F17
N
O
N
O
O
Rhodamine acid
Solvent Acetone
Temperature 298.0
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 16
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.2500
Acquisition Time 0.7340
Acquisition Date 2013-05-16T19:43:54
Modification Date 2013-05-16T19:43:55
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
2.18
2.00
6.19
1.86
2.05
1.68
-65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145
f1 (ppm)


-81.67
-84.70
-81.72
-114.40
-114.44
-114.49
-114.54
-122.21
-122.43
-122.46
-122.50
-123.25
-123.31
-123.95
-124.00
-126.72
-126.76
-126.78
-126.80
-126.81
-126.83
F17C8
C8F17
F17C8
N
O
N
+
−Cl
C8F17
COOMe
5
Solvent Acetone
Temperature 298.1
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 16
Receiver Gain 198
Relaxation Delay 1.0000
Pulse Width 14.2500
Acquisition Time 0.7340
Acquisition Date 2012-10-22T14:38:15
Modification Date 2012-10-22T14:38:15
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
2.45
2.00
7.10
2.00
2.18
1.78
-50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150
f1 (ppm)


-81.62
-81.65
-81.67
-114.40
-114.41
-114.45
-114.50
-122.12
-122.13
-122.16
-122.20
-122.23
-122.26
-122.36
-122.40
-122.46
-123.25
-123.90
-123.94
-123.98
-126.67
-126.69
-126.71
-126.73
-126.75
-126.77
$^{-}ClO_4$
^{+}N
O
N
N
C_8F_{17}
C_8F_{17}
7
Solvent Acetone
Temperature 298.1
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0556
Number of Scans 65
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 14.2500
Presaturation Frequency
Acquisition Time 0.7340
Acquisition Date 2014-07-11T20:32:17
Modification Date 2014-07-11T20:33:45
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
5.07
4.00
4.66
10.17
4.37
4.71
4.11
-40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155
f1 (ppm)


F9C4
C4F9
N
OH
S1
-81.26
-81.26
-81.27
-81.28
-81.29
-81.30
-81.32
-81.32
-114.24
-114.25
-114.27
-114.28
-114.30
-114.32
-114.33
-124.49
-124.50
-124.51
-124.52
-124.54
-124.55
-124.57
-126.17
-126.17
-126.18
-126.20
-126.22
-126.24
-126.25
Solvent CDCl3
Temperature 298.2
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans 16
Receiver Gain 128
Relaxation Delay 1.0000
Pulse Width 12.7700
Presaturation Frequency
Acquisition Time 0.7340
Acquisition Date 2014-03-23T11:51:52
Modification Date 2014-03-23T11:51:53
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
2.63
2.26
2.14
2.00
-40 -45 -50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155
f1 (ppm)

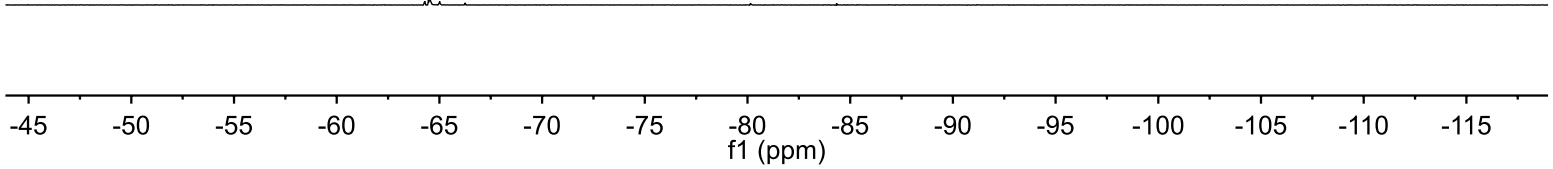

-64.65
-81.02
-81.03
-81.05
-114.00
-114.01
-114.05
-114.08
-114.10
-124.29
-124.30
-124.31
-124.34
-124.36
-125.96
-125.97
-125.99
-126.01
-126.03
-126.04
F9C4
F9C4
N
O
O
CF3
11
Solvent CDCl3
Temperature 298.1
Pulse Sequence zgflqn
Experiment 1D
Probe 5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans 16
Receiver Gain 203
Relaxation Delay 1.0000
Pulse Width 12.7700
Presaturation Frequency
Acquisition Time 0.7340
Acquisition Date 2014-03-25T08:25:34
Modification Date 2014-03-25T08:25:34
Class
Spectrometer Frequency 376.46
Spectral Width 89285.7
Lowest Frequency -82292.5
Nucleus 19F
Acquired Size 65536
Spectral Size 131072
1.98
3.00
2.50
2.45
2.10
20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170
f1 (ppm)



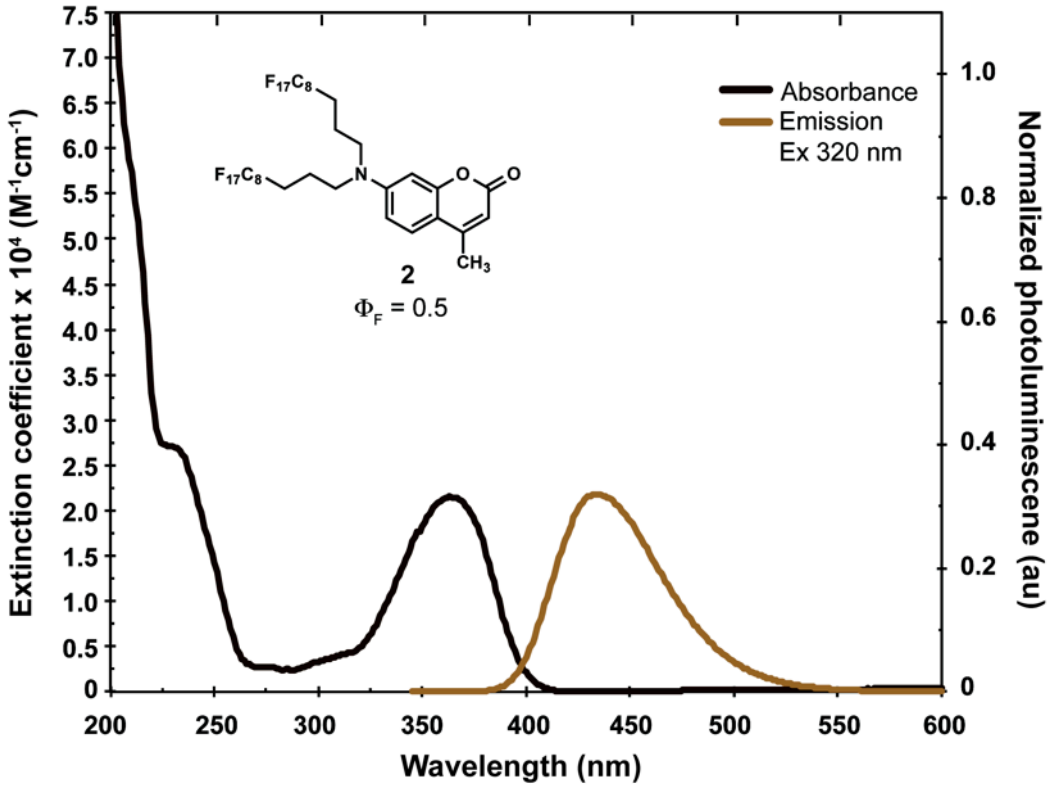
12

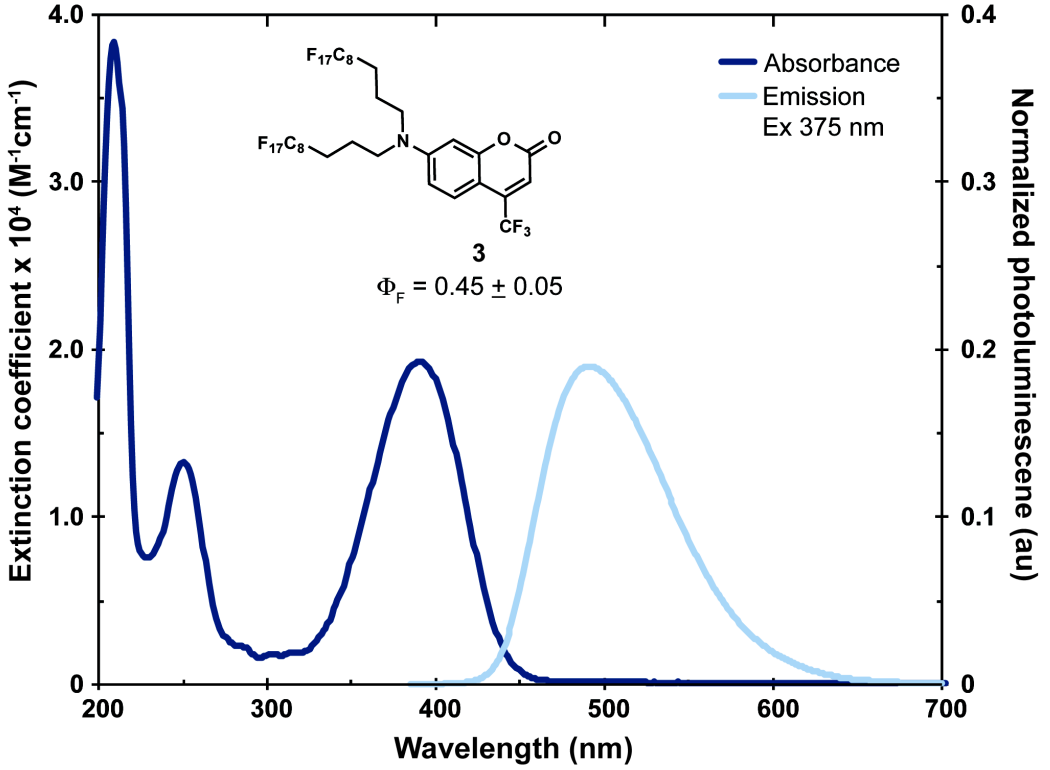
-64.52

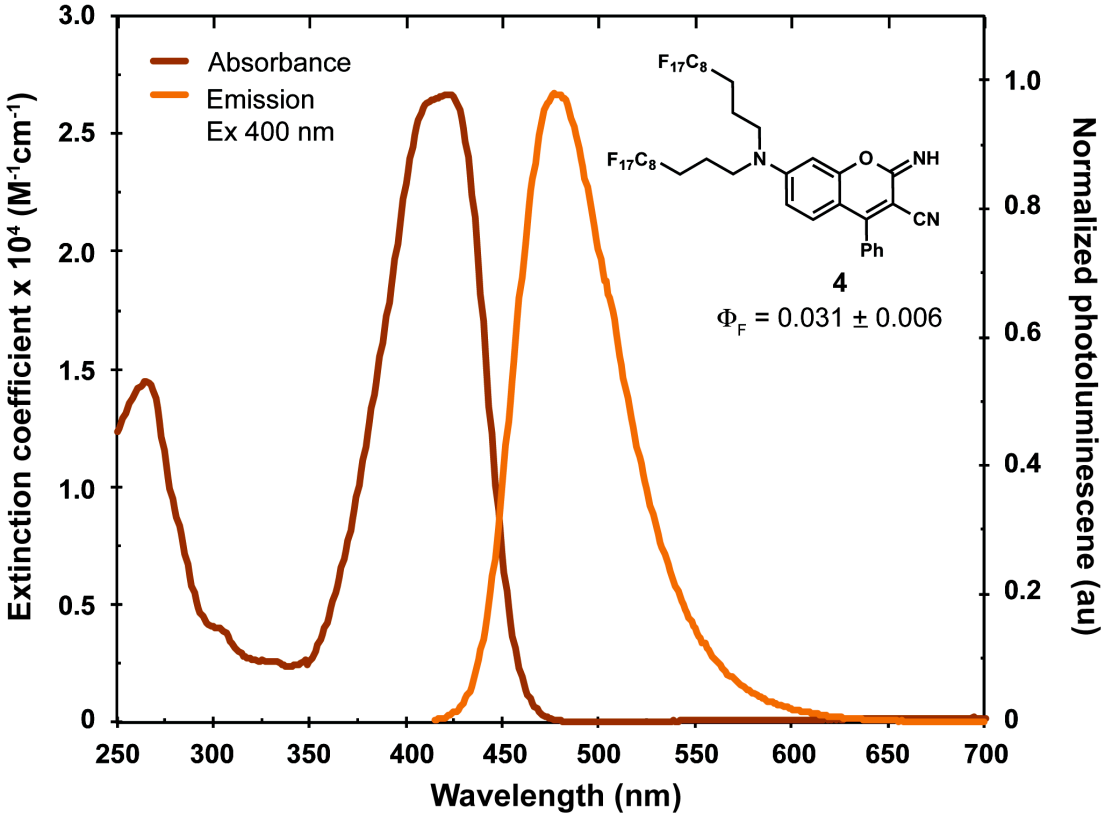
Solvent	CDCl3
Temperature	298.2
Pulse Sequence	zgflqn
Experiment	1D
Probe	5 mm PABBO BB/ 19F-1H/ 0578
Number of Scans	8
Receiver Gain	203
Relaxation Delay	1.0000
Pulse Width	12.7700
Acquisition Time	0.7340
Acquisition Date	2014-02-05T12:19:23
Modification Date	2014-02-05T12:19:24
Class	
Spectrometer Frequency	376.46
Spectral Width	89285.7
Lowest Frequency	-82292.5
Nucleus	19F
Acquired Size	65536
Spectral Size	131072

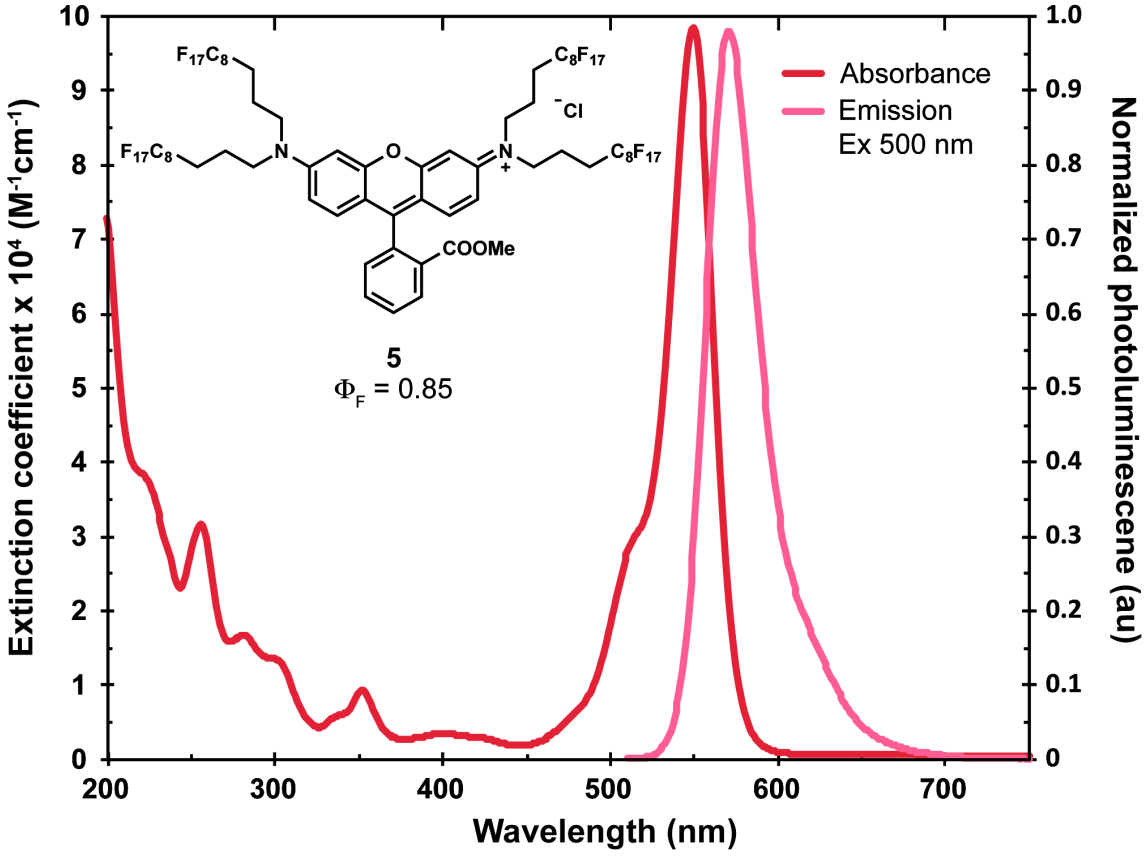


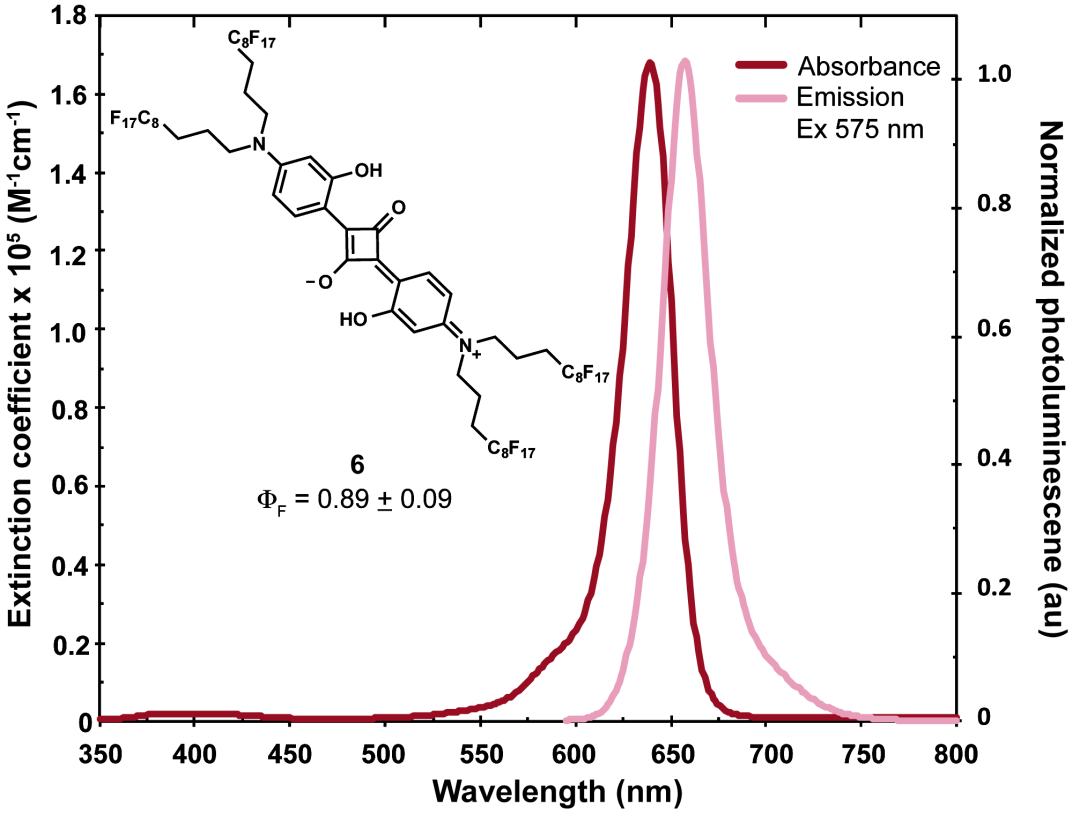
Photophysical Characterization

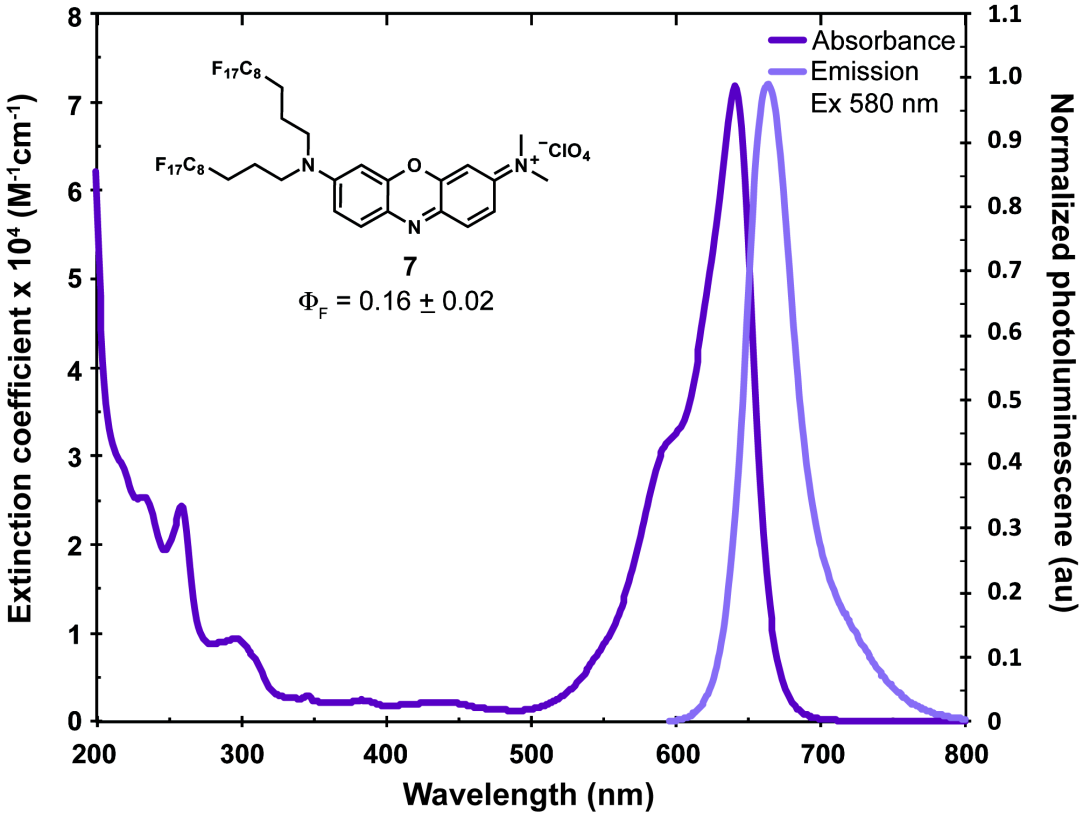


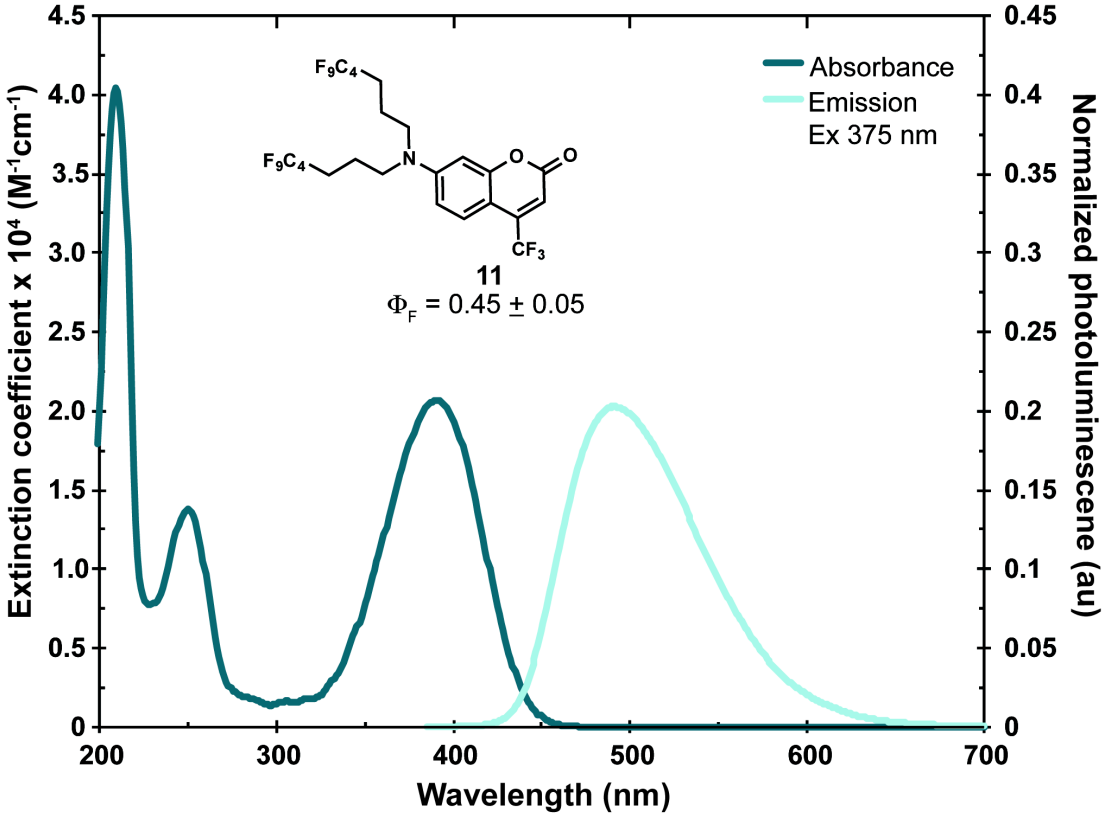


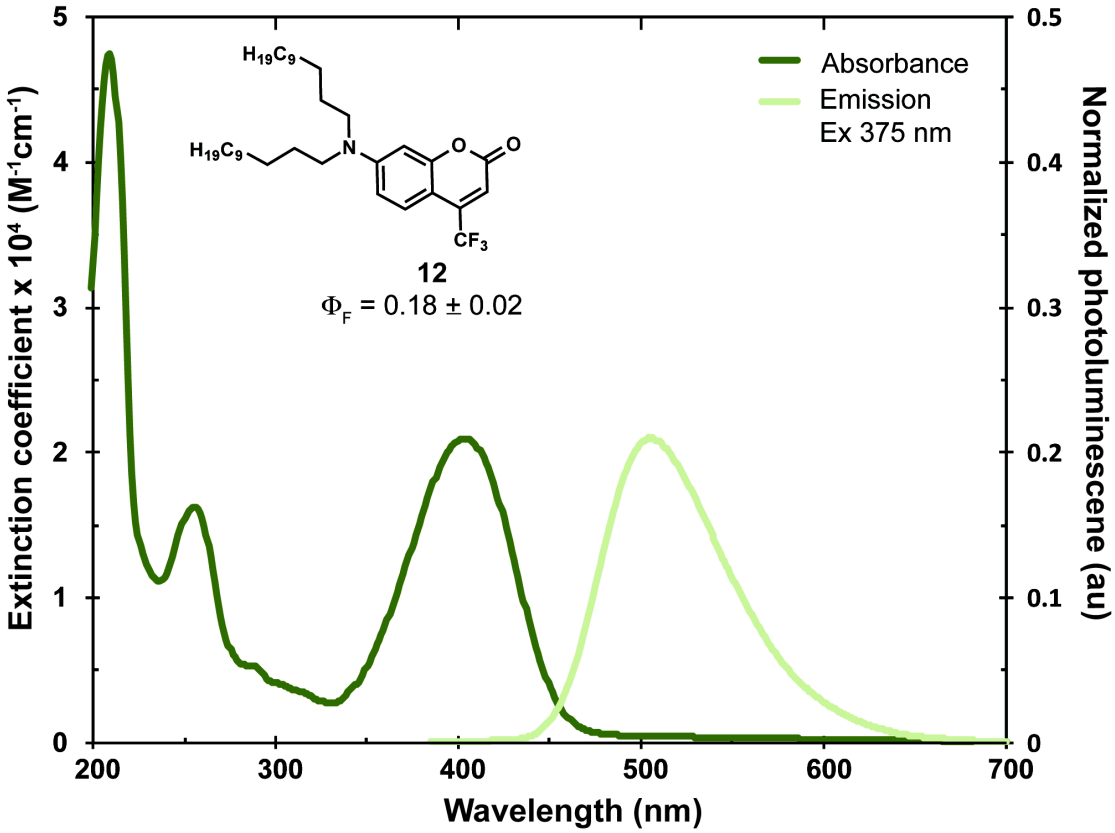

Absorbance
Emission
Ex 400 nm
Extinction coefficient x 10⁴ (M⁻¹cm⁻¹)
Normalized photoluminescene (au)
Wavelength (nm)
F17C8
F17C8
N
O
NH
CN
Ph
4
ΦF = 0.031 ± 0.006


Absorbance
Emission
Ex 500 nm
Extinction coefficient x 10⁴ (M⁻¹cm⁻¹)
Normalized photoluminescene (au)
Wavelength (nm)
F17C8
C8F17
-Cl
F17C8
N
O
N+
C8F17
COOMe
5
ΦF = 0.85


Absorbance
Emission
Ex 575 nm
Extinction coefficient x 10⁵ (M⁻¹cm⁻¹)
Normalized photoluminescene (au)
Wavelength (nm)
6
Φ_F = 0.89 ± 0.09


Absorbance
Emission
Ex 580 nm
Extinction coefficient x 10⁴ (M⁻¹cm⁻¹)
Normalized photoluminescene (au)
Wavelength (nm)
7
Φ_F = 0.16 ± 0.02


Absorbance
Emission
Ex 375 nm
11
Φ_F = 0.45 ± 0.05
Extinction coefficient x 10^4 ($M^{-1}cm^{-1}$)
Normalized photoluminescene (au)
Wavelength (nm)


Absorbance
Emission
Ex 375 nm
12
Φ_F = 0.18 ± 0.02
Extinction coefficient x 10^4 ($M^{-1}cm^{-1}$)
Normalized photoluminescene (au)
Wavelength (nm)