Supporting Information

Harnessing Reductive BF_2-Complexation *via* Ru(II)-Catalyzed N–O Cleavage of Isoxazoles

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1. General Information:

All the reagents were commercial grade and purified according to the established procedures. All the reactions were carried out in oven-dried glassware. The highest commercial quality reagents were purchased and were used without further purification unless otherwise stated. Reactions were monitored by thin-layer chromatography (TLC) on a 0.25 mm silica gel plates ($60F_{254}$) visualized under UV illumination at 254 nm. Organic extracts were dried over anhydrous sodium sulfate (Na_2SO_4). Solvents were removed using a rotary evaporator under reduced pressure. Column chromatography was performed to purify the crude product on silica gel 60–120 mesh using a mixture of hexane and ethyl acetate as eluent. All the isolated compounds were characterized by ^{1}H, $^{13}C\{^{1}H\}$ NMR and IR spectroscopic (HRMS-spectrometric) techniques. NMR spectra for all the samples were recorded in deuterochloroform ($CDCl_3$). ^{1}H, $^{13}C\{^{1}H\}$ were recorded in 500 (126) or 400 (101) MHz spectrometer and were calibrated using tetramethylsilane for ^{1}H NMR, deuterochloroform for ^{13}C NMR as an internal reference {$Si(CH_3)_4$: 0.00 ppm for ^{1}H NMR, 77.16 ppm for ^{13}C NMR. The chemical shifts are quoted in δ units, parts per million (ppm). ^{1}H NMR data is represented as follows: Chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublet, integration and coupling constant(s) *J* in hertz (Hz). High-resolution mass spectra (HRMS) were recorded on a mass spectrometer using electrospray ionization-time of flight (ESI-TOF) reflection experiments. FT-IR spectra were recorded as neat and reported in the frequency of absorption (cm^{-1}). All UV–vis experiments were performed in 1 mL quartz cuvettes with a path length equal to 1 cm. Photoluminescence was carried out upon exciting at suitable wavelength in 1 mL quartz cuvettes.

2. Representative BF_2 Complexes:

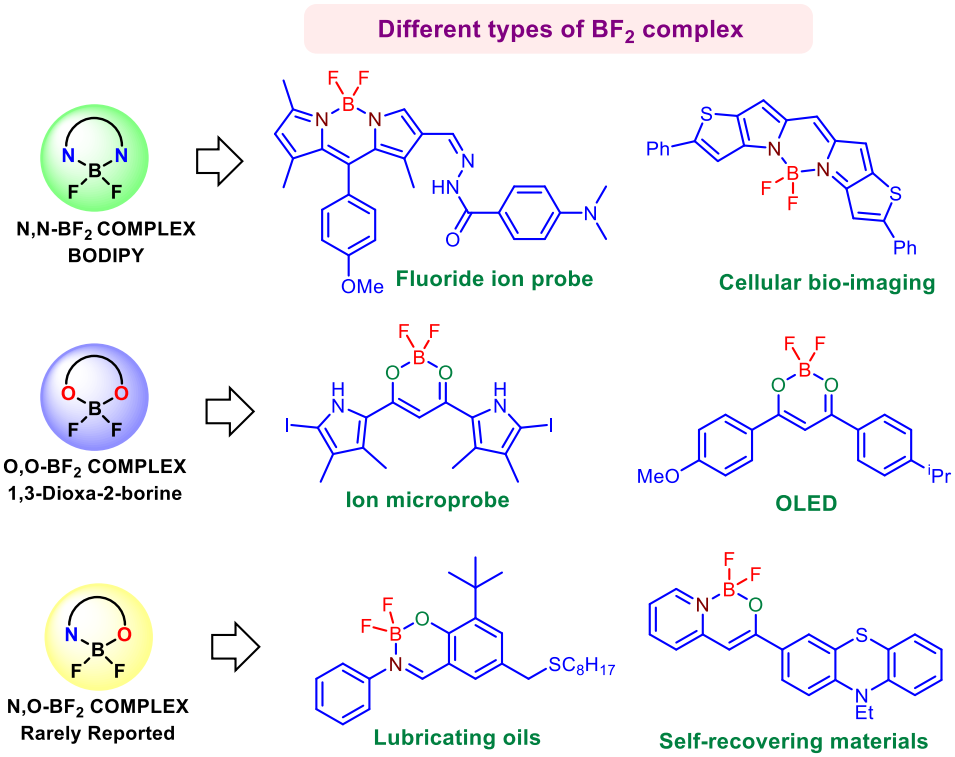
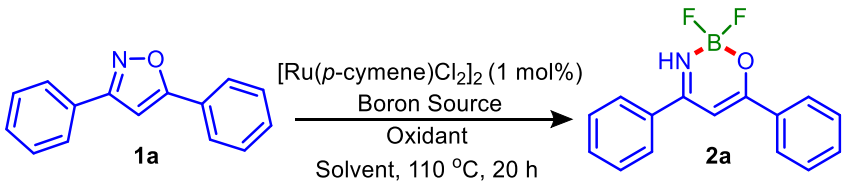


Fig S1. Representative BF_2 Complex

3. Optimization of Reaction Condition:

Table S1. Optimization of Reaction Conditions.[a,b]



Entry	Boron Source (equiv.)	Oxidant (equiv.)	Solvent	Yield[b] (%)
1	$BF_3.OEt_2$(2.0)	$Cu(OAC)_2.H_2O$ (1.0)	1,2-DCE	30
2	$Cu(BF_4)_2$ (2.0)	-	1,2-DCE	47
3	$Cu(MeCN)_4BF_4$ (2.0)	-	1,2-DCE	42
4	$Co(BF_4)_2.6H_2O$ (2.0)	-	1,2-DCE	n.d.
5	$AgBF_4$ (0.2)	$Cu(OAC)_2.H_2O$ (1.0)	1,2-DCE	55
6	$NaBF_4$ (2.0)	$Cu(OAC)_2.H_2O$ (1.0)	1,2-DCE	n.d.
7	$N(Bu)_4BF_4$ (2.0)	$Cu(OAC)_2.H_2O$ (1.0)	1,2-DCE	n.d.

8	HBF_4 (2.0)	$Cu(OAC)_2.H_2O$ (1.0)	1,2-DCE	57
9	HBF_4 (5.0)	$Cu(OAC)_2.H_2O$ (1.0)	1,2-DCE	68
10	HBF_4 (7.0)	$Cu(OAC)_2.H_2O$ (1.0)	1,2-DCE	73
11	HBF_4 (7.0)	--	1,2-DCE	n.d.
12	HBF_4 (7.0)	$Cu(OAc)_2$ (1.0)	1,2-DCE	76
13	HBF_4 (7.0)	CuO (1.0)	1,2-DCE	20
14	HBF_4 (7.0)	Cu_2O (1.0)	1,2-DCE	79
15	**HBF_4 (7.0)**	**Cu_2O (2.0)**	**1,2-DCE**	**87**
16	HBF_4 (7.0)	Cu_2O (2.0)	PhCl	20
17	HBF_4 (7.0)	Cu_2O (2.0)	TFE	40
18	HBF_4 (7.0)	Cu_2O (2.0)	THF	50
19	HBF_4 (7.0)	Cu_2O (2.0)	1,4-Dioxane	30
20	HBF_4 (7.0)	Cu_2O (2.0)	$CHCl_3$	50
21	HBF_4 (7.0)	Cu_2O (2.0)	MeCN	traces
22	HBF_4 (7.0)	Cu_2O (2.0)	MeOH	45
23	HBF_4 (7.0)	Cu_2O (2.0)	1,2-DCB	46
24	HBF_4 (7.0)	Cu_2O (2.0)	Toluene	55

[a]Reaction Conditions unless specified otherwise: **1a** (0.2 mmol), [Ru(*p*-cymene)Cl_2]$_2$ (1 mol%), boron source, oxidants, solvent (1.5 ml) for 20 h. [b]Isolated yield. n.d. = not detected.

At first a series of boron sources *viz.* $Cu(BF_4)_2$, $Cu(MeCN)_4BF_4$, $Co(BF_4)_2.6H_2O$, $AgBF_4$, $NaBF_4$, $N(Bu)_4BF_4$, HBF_4 were screened, among which HBF_4 gave better yield (57%) of **2a** (Table S1, entries 2-8). Notably, when the loading of HBF_4 was enhanced from 2 equiv. to 5 equiv., the yield was increased to 68%, and on further increment to 7 equiv., 73% of the product was obtained (Table S1, entries 9-10). In the absence of copper salt, no trace of product **2a** was observed (Table S1, entry 11). Considering its importance, a series of copper salts such as $Cu(OAc)_2$, CuO, Cu_2O were examined instead of $Cu(OAc)_2.H_2O$ (Table S1, entries 12-14). A notable enhancement in the yield of the product to 79% was observed using Cu_2O (entry 14). Interestingly, when the loading of Cu_2O was enhanced from 1 to 2 equivalent, the yield of **2a** improved to 87% (Table S1, entry 15). Now, various solvents such as PhCl, TFE, THF, 1,4-dioxane, $CHCl_3$, MeCN, MeOH, 1,2-DCB, and toluene were screened. However, all the solvents provided a lesser yield of products compared to 1,2-DCE (Table S1, entries 16-24). The best optimized condition for the synthesis of 2,2-difluoro-4,6-diphenyl-2*H*-1,3,2λ^4-oxazaborinine (**2a**) was 3,5-diphenylisoxazole (**1a**) (1 equiv.), [Ru(*p*-cymene)Cl_2]$_2$ (1 mol%), HBF_4 (7 equiv.) and oxidant Cu_2O (2 equiv.) at 110 ^oC in 1,2-DCE in a sealed tube.

4. General Procedure:

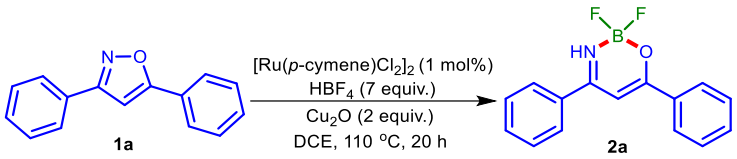
(A) General Procedure for the Synthesis of Isoxazoles:

All isoxazole derivatives (**1a**-**1y**) were synthesized by following the previous reported procedure.[1]

(B) General Procedure for the Synthesis of 1′a:

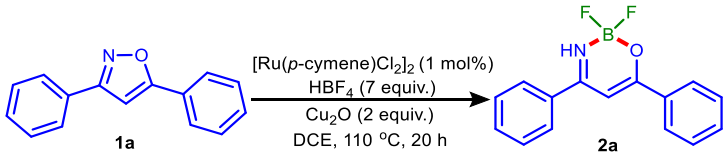
1′a was synthesized by following previously reported procedure.[2]

(C) General Procedure for the Synthesis of 2a:



To an oven-dried pressure tube (20.3 cm x 19 mm, 21 mL) containing a magnetic bead was added 3,5-diphenylisoxazole **1a** (0.2 mmol, 44.2 mg), $[RuCl_2(p\text{-cymene})]_2$ (0.002 mmol, 1.2 mg), HBF_4 (1.4 mmol, 122.9 mg), Cu_2O (0.4 mmol, 57.2 mg) and DCE (1.5 mL). After that, the reaction mixture was stirred at 110 °C on a preheated oil bath for 20 h. After completion of the reaction (monitored by TLC), the solvent (1,2-DCE) was evaporated under reduced pressure. After evaporation, the reaction mixture was admixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). Then the organic layer was dried over anhydrous Na_2SO_4, and the solvent was evaporated under reduced pressure. Then the crude mixture was purified over column chromatography (60-120 mesh silica) by eluting it with 10% ethyl acetate in hexane to afford 2,2-difluoro-4,6-diphenyl-2*H*-1,3,2λ^4-oxazaborinine (**2a**) as a yellow solid with 87% yield (47 mg). The identity and purity of the product was confirmed by spectroscopic analysis.

(D) Procedure for 1 mmol scale synthesis of 2a:



To an oven-dried pressure tube (20.3 cm x 19 mm, 21 mL) containing a magnetic bar was added 3,5-diphenylisoxazole **1a** (1 mmol, 221 mg), $[RuCl_2(p\text{-cymene})]_2$ (0.01 mmol, 6.1 mg), HBF_4 (7 mmol, 614.7 mg), Cu_2O (2 mmol, 286.2 mg) and DCE (2 mL). After that, the reaction mixture was stirred at 110

^{o}C on a preheated oil bath for 20 h. After completion of the reaction (monitored by TLC), the solvent (1,2-DCE) was evaporated under reduced pressure. After evaporation, the reaction mixture was admixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). Then the organic layer was dried over anhydrous Na_2SO_4, and the solvent was evaporated under reduced pressure. Then the crude mixture was purified over column chromatography (60-120 mesh silica) by eluting it with 10% ethyl acetate in hexane to afford 2,2-difluoro-4,6-diphenyl-2*H*-1,3,2λ^4-oxazaborinine (**2a**) as a yellow solid with 83% yield (224 mg).

5. Crystallographic Information:

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å) at 296 K. Cell parameters were retrieved using SMART [a] software and refined with SAINT[a] on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS[b]. The structure was solved by direct methods implemented in the SHELX-2014[c] program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in different Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. yellow crystals of **2s** were isolated from $CHCl_3$ solvent at 120 K temperature.

a. SMART V 4.043 Software for the CCD Detector System; Siemens Analytical Instruments Division: Madison, WI, 2008.

b. SAINT Plus (v 6.14) Bruker AXS Inc., Madison, WI, 2008.

c. Sheldrick, G. M. SHELXL-2014, Program for the Refinement of Crystal Structures; University of Göttingen: Göttingen (Germany), 1997.

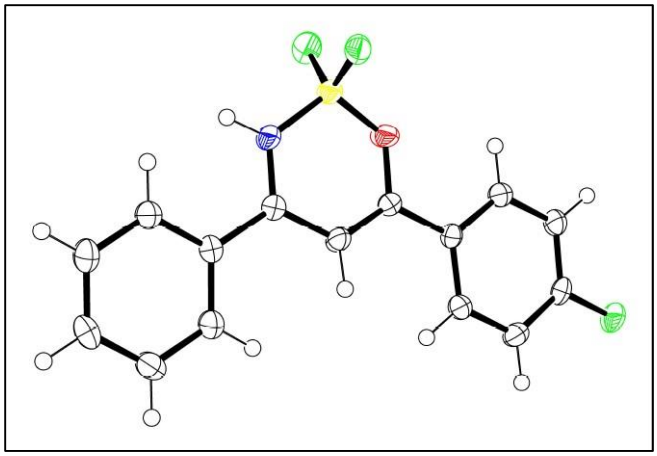
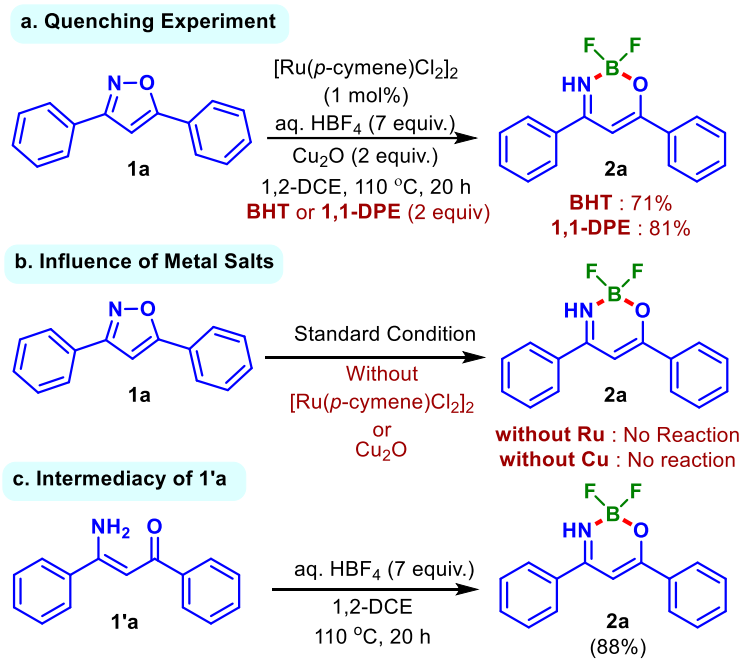


Figure S2. ORTEP diagram of **2s** with the thermal ellipsoids set at 50% probability.

Table S2. Crystal Data table for 2s

Empirical formula	$C_{15}H_{11}BF_3NO$
CCDC number	2341722
Formula weight	289.09
Temperature	120(2)
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/n
Unit cell dimensions	a = 9.3925(17) Å, b = 12.469(2) Å, c = 11.765(2) Å α= 90°, β= 106.136(5)°, γ= 90°
Volume	1323.6(4) $Å^3$
Z	4
Density (calculated)	1.451 g/cm^{-3}
Absorption coefficient	0.120
F (000)	612
Theta range for data collection	2.432 to 24.995 °
Index ranges	-11 < = h < = 11, -14 < = k < = 14, -13< = l < = 13
Reflections collected	25123
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	2317 / 0 / 191
Goodness-of-fit on F2	1.053
Final R indices [I>2sigma(I)]	0.0344, wR2 = 0.0880
R indices (all data)	0.0404, wR2 = 0.0939

6. Control Experiment for Elucidation of Mechanism:



Scheme S1. Control reactions.

(a) Procedure of quenching experiment:

To an oven-dried pressure tube (20.3 cm x 19 mm, 21 mL) containing a magnetic bar was added 3,5-diphenylisoxazole **1a** (0.2 mmol, 44.2 mg), $[RuCl_2(p\text{-cymene})]_2$ (0.002 mmol, 1.2 mg), HBF_4 (1.4 mmol, 122.9 mg), Cu_2O (0.4 mmol, 57.2 mg), BHT (0.4 mmol, 88 mg) or 1,1-DPE (0.4 mmol, 72 mg,) and DCE (1.5 mL). After that, the reaction mixture was stirred at 110 °C in a preheated oil bath for 20 h. The solvent (1,2-DCE) was evaporated under reduced pressure. After evaporation, the reaction mixture was mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). Then the organic layer was dried over anhydrous Na_2SO_4, and the solvent was evaporated under reduced pressure. Then the crude mixture was purified over column chromatography (60-120 mesh silica) by eluting it with 10% ethyl acetate in hexane to afford 2,2-difluoro-4,6-diphenyl-2*H*-1,3,2λ^4-oxazaborinine (**2a**) as a yellow solid compound with 71% (38 mg) (for BHT) and 81% (44 mg) (for 1,1-DPE). This observation suggests the non-involvement of any radical pathway.

(b) Influence of metal salt:

(i) In the absence of [$RuCl_2$(*p*-cymene)]$_2$:

To an oven-dried pressure tube (20.3 cm x 19 mm, 21 mL) containing a magnetic bar was added 3,5-diphenylisoxazole **1a** (0.2 mmol, 44.2 mg), HBF_4 (1.4 mmol, 122.9 mg), Cu_2O (0.4 mmol, 57.2 mg) and DCE (1.5 mL). After that, the reaction mixture was stirred at 110 ^oC on a preheated oil bath for 20 h. After 20 h of reaction, TLC was checked and no product was formed. This observation suggests that 1 mol% [$RuCl_2$(*p*-cymene)]$_2$ is necessary for the reaction.

(ii) In the absence of Cu_2O:

To an oven-dried pressure tube (20.3 cm x 19 mm, 21 mL) containing a magnetic bar was added 3,5-diphenylisoxazole **1a** (0.2 mmol, 44.2 mg), [$RuCl_2$(*p*-cymene)]$_2$ (0.002 mmol, 1.2 mg), HBF_4 (1.4 mmol, 122.9 mg) and DCE (1.5 mL). After that, the reaction mixture was stirred at 110 ^oC on a preheated oil bath for 20 h. After 20 h of reaction, TLC was checked and no product was formed. This observation suggests that Cu_2O is necessary for the reaction.

(c) Intermediacy of 1′a:

To an oven-dried pressure tube (20.3 cm x 19 mm, 21 mL) containing a magnetic bar was added (*Z*)-3-amino-1,3-diphenylprop-2-en-1-one **1′a** (0.2 mmol, 44.6 mg), HBF_4 (1.4 mmol, 122.9 mg) and DCE (1.5 mL). After that, the reaction mixture was stirred at 110 ^oC on a preheated oil bath for 20 h. After completion of the reaction (monitored by TLC), the solvent (1,2-DCE) was evaporated under reduced pressure. After evaporation, the reaction mixture was admixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). Then the organic layer was dried over anhydrous Na_2SO_4, and the solvent was evaporated under reduced pressure. Then the crude mixture was purified over column chromatography (60-120 mesh silica) by eluting it with 10% ethyl acetate in hexane to afford 2,2-difluoro-4,6-diphenyl-2*H*-1,3,2λ^4-oxazaborinine (**2a**) as a yellow solid with 88% yield (48 mg). The identity and purity of the product was confirmed by spectroscopic analysis. This observation suggests that ruthenium (catalyst) and copper (oxidant) are crucial for N–O bond cleavage of isoxazole ring.

7. HRMS Analysis of Crude Reaction Mixture:

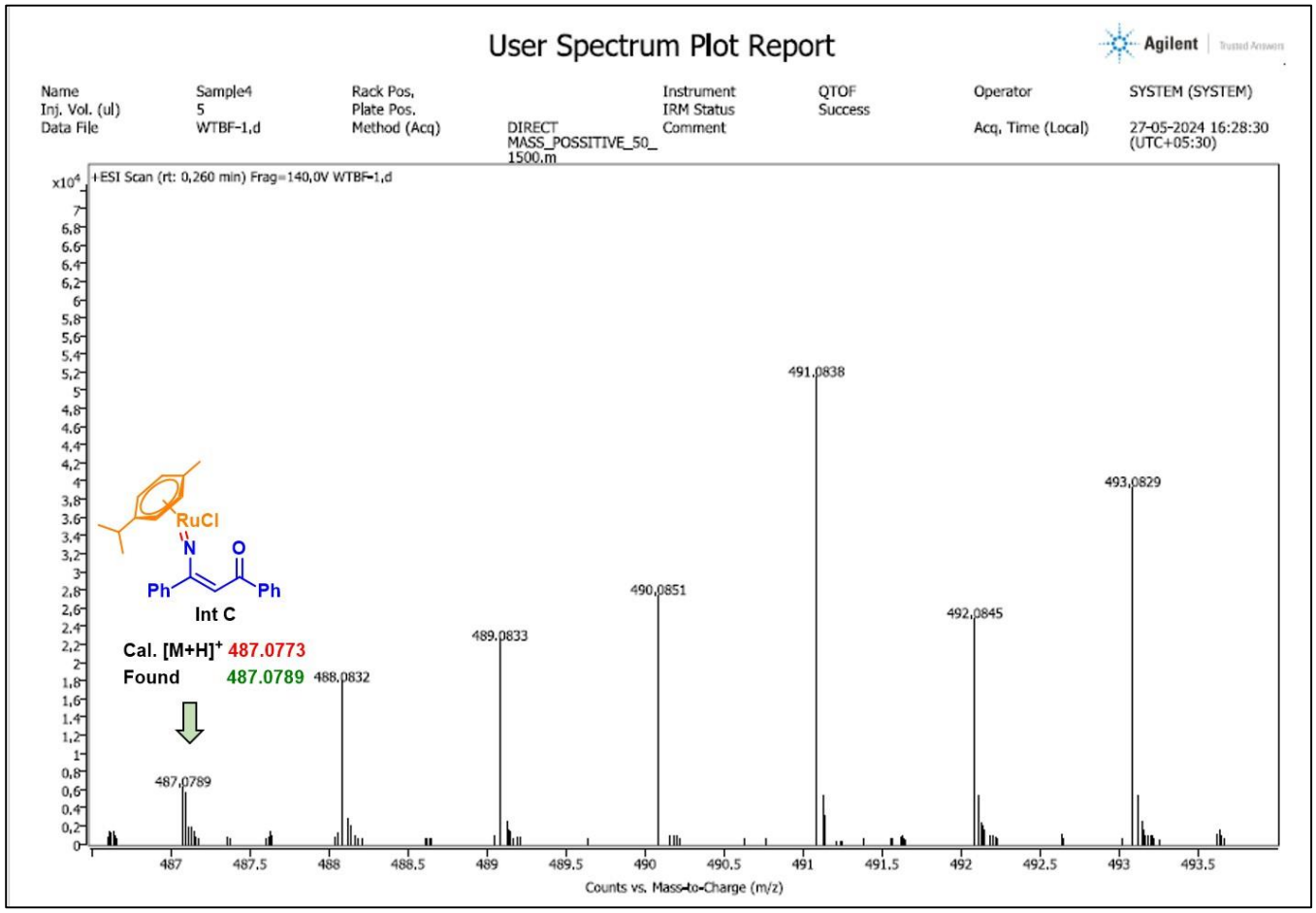


Figure S3. HRMS spectra of the crude reaction mixture (Int. **C**)

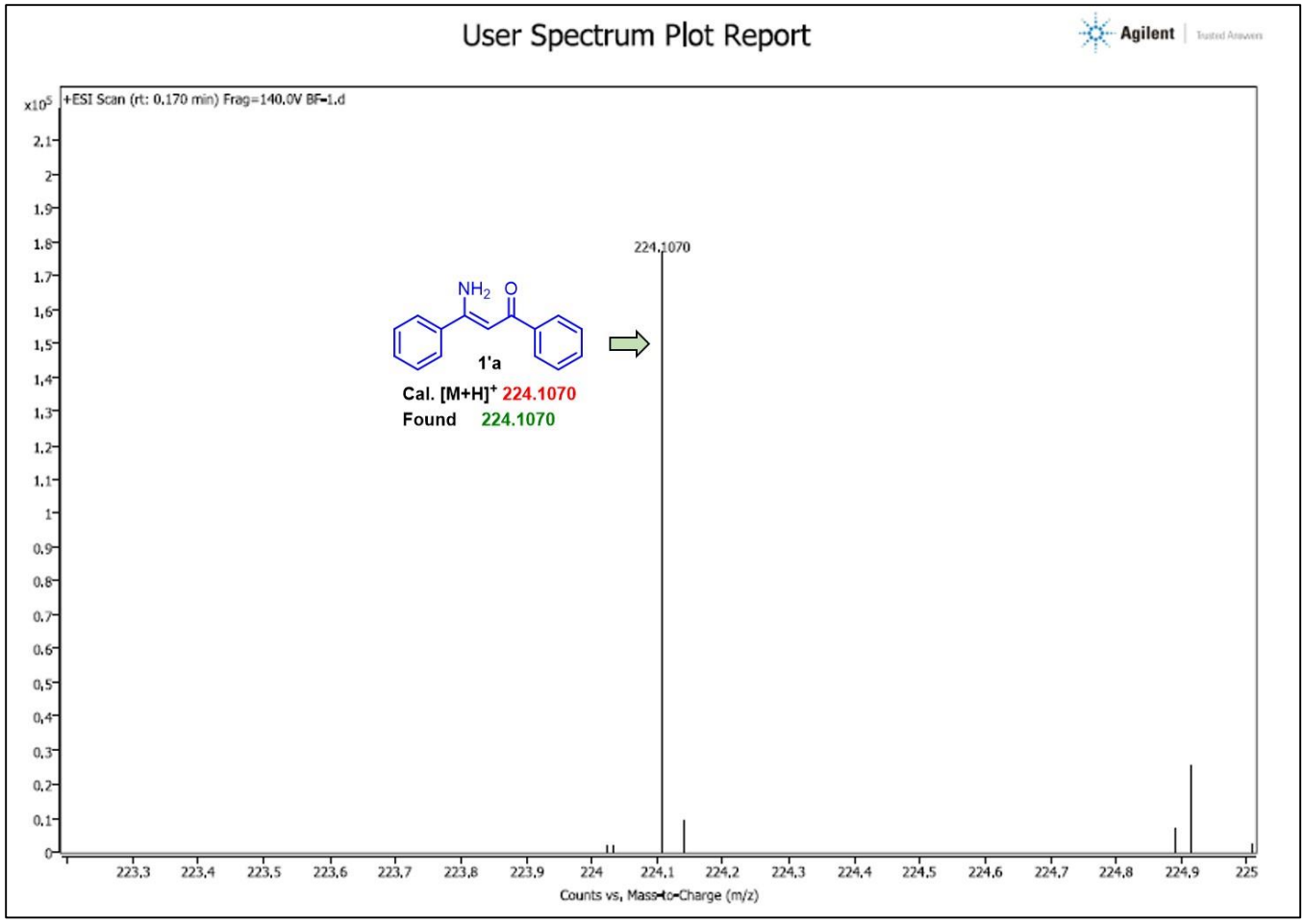


Figure S4. HRMS spectra of the crude reaction mixture (Int. **E**)

8. DFT Calculation:

To gain insight into the geometry and electronic structure of these synthesized BF_2 complexes, the density functional theory (DFT) calculations were performed using the B3LYP/6-31G+ (d) basis set level in DCM modelled by PCM approach (Figure S5, Table S3).

Table S3. DFT Calculation of Some Selected BF_2 Complex

Compound	HOMO (eV)[a]	LUMO (eV)[a]	ΔE (LUMO - HOMO) (eV)[b]
2a	-6.739	-2.672	4.067
2c	-6.691	-2.629	4.062
2g	-6.765	-2.704	4.061
2q	-6.578	-2.617	3.961
2s	-6.751	-2.694	4.057
2u	-6.523	-2.648	3.875
[a]DFT calculation using the B3LYP/6-31G+ (d) basis set level in DCM solvent modelled by PCM approach. [b]ΔE = LUMO – HOMO			

1. (a) C. Lee, W. Yang, and R. G. Parr, Phys. Rev. B., 1988, 37, 785–789; (b) A. D. Becke, J. Chem. Phys., 1993, 98, 5648–5652; (c) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, and M. J. Frisch, J. Phys. Chem., 1994, 98, 11623-11627.

2. Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

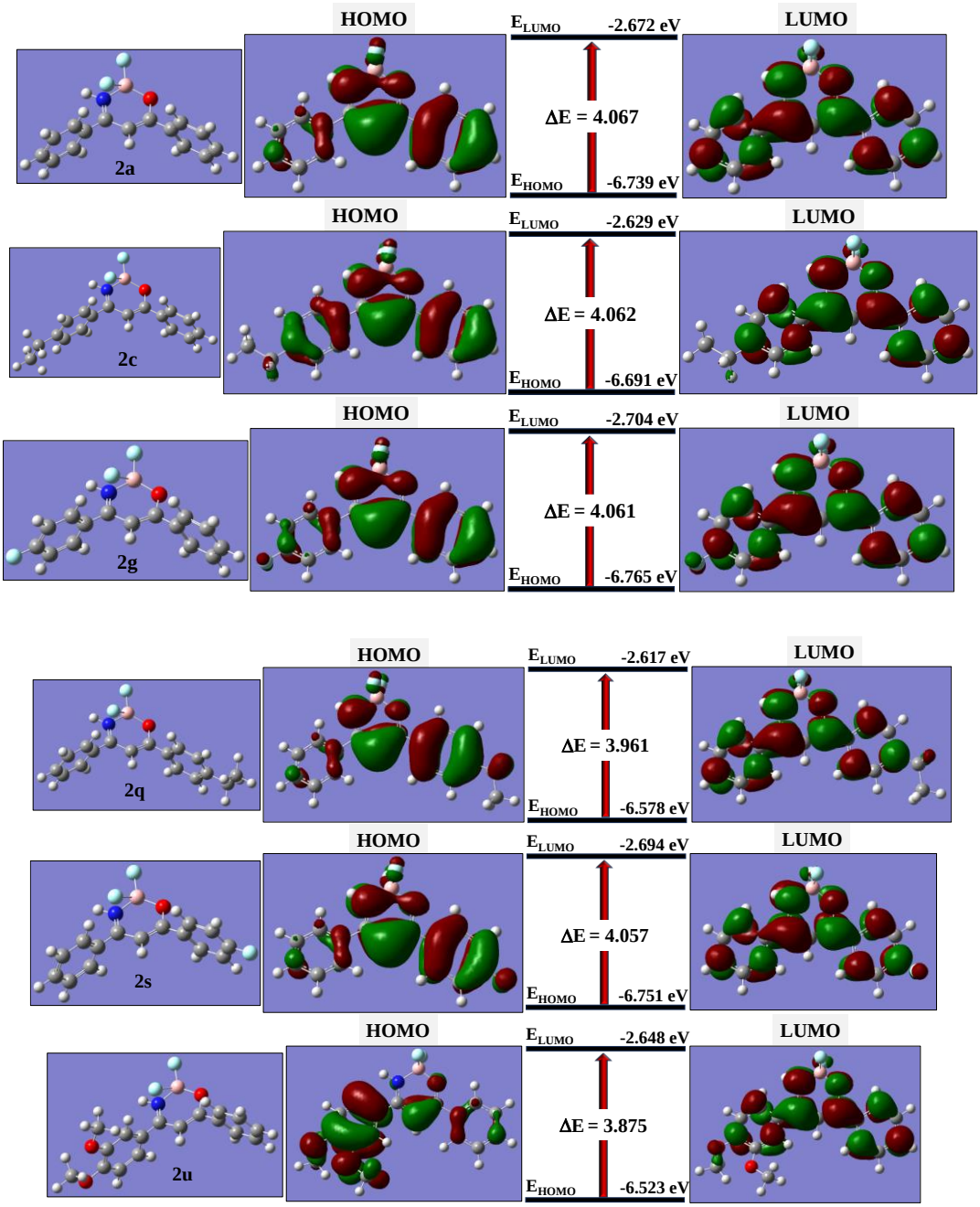


Figure S5. DFT optimized structures and HOMO-LUMO energy level diagrams of synthesized compounds **2a**, **2c**, **2g, 2q**, **2s**, **2u** respectively using the B3LYP/6-31G+ (d) basis set level in DCM solvent modelled by PCM approach.

9. Photophysical Studies:

Photophysical properties of a few representative BF_2 complexes have been investigated. In DCM, they exhibit absorption $\lambda_{max,abs}$ in the region of 352−363 nm with an extinction coefficient (ε) in the range of 8000−64000 $M^{-1}cm^{-1}$ (Figure S6A) (Table S4) and the fluorescence emission $\lambda_{max,em}$ ranging between 413−485 nm with a Stokes shift of 61−125 nm (Figure S6B) (Table S4). Apart from the solution state, the solid BF_2 complex **2u** exhibit absorption at 405 nm (Figure S6C) and a strong fluorescence emission at 550 nm (Figure S6D).

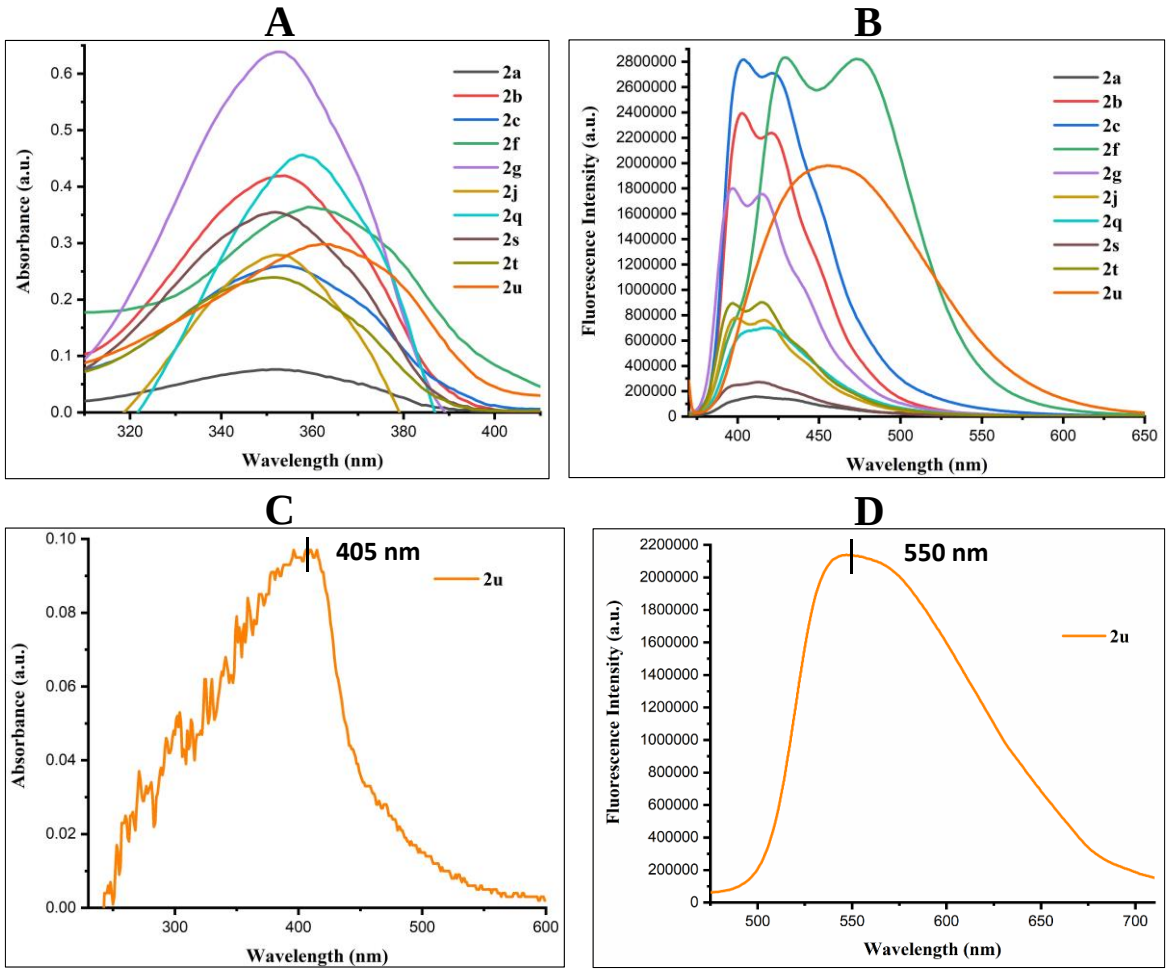


Figure S6. (**A**) UV−visible and (**B**) Fluorescence spectra of some selected BF_2 complex in DCM at a concentration of 10μM at room temperature. (**C**) UV−visible and (**D**) Fluorescence spectra of **2u** in solid state at room temperature.

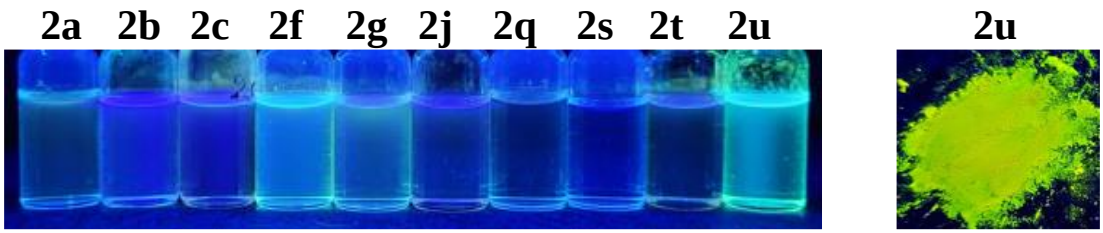


Figure S7. Images of some selected BF_2 complex in solution and solid state under 365 nm UV lamp.

Fluorescence quantum yields of some synthesized compounds were investigated by standard methods using Quinine sulphate as the reference (Φ_F = 0.55 in 0.1 M H_2SO_4, λ_{ex} = 353 nm) in HPLC grade DCM solvent. The synthesized compound exhibit quantum yield upto 33% in DCM (Table S4) whereas in solid state one compound **2u** exhibit 26.9% quantum yield.

Quantum yield of a probe:

$$QY = QY_{ref} (\eta^2 / \eta_{ref}^2)(I/A)(A_{ref}/I_{ref})$$

Here, QY_{ref} is the quantum yield of reference compound, η denote the refractive index of solvent, η_{ref} is the refractive index of the solvent of dissolved reference compound, I and I_{ref} denotes the integrated fluorescence intensity of the probe and reference respectively. Whereas A and A_{ref} are the absorbances of the probe and reference at the excitation wavelength.

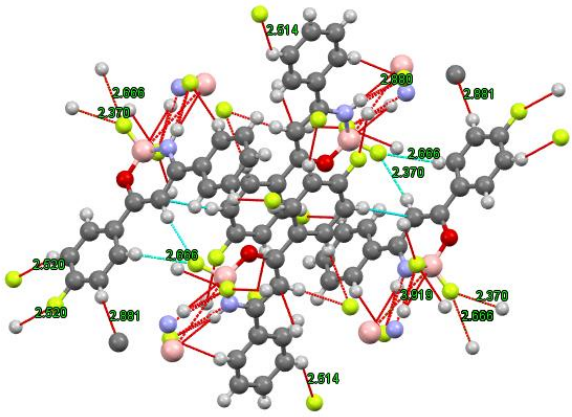
Table S4. Photophysical Properties of Selected Products

Compound	$\lambda_{max,abs}$ (nm)[a]	ε ($M^{-1}cm^{-1}$)	$\lambda_{max,em}$ (nm)[b]	Stokes shift (nm)[c]	Quantum yield[d] (Φ_F)
2a	353	8000	435 (410)	82 (57)	0.018
2b	354	42000	421 (403)	67 (49)	0.071
2c	353	26000	441 (393)	88 (40)	0.194
2f	360	36000	485 (422)	125 (62)	0.337
2g	353	64000	415 (396)	62 (43)	0.066
2j	352	28000	416 (398)	64 (46)	0.039
2q	358	46000	420	62	0.019
2s	352	36000	413 (397)	61 (45)	0.019
2t	352	24000	415 (397)	63 (45)	0.036

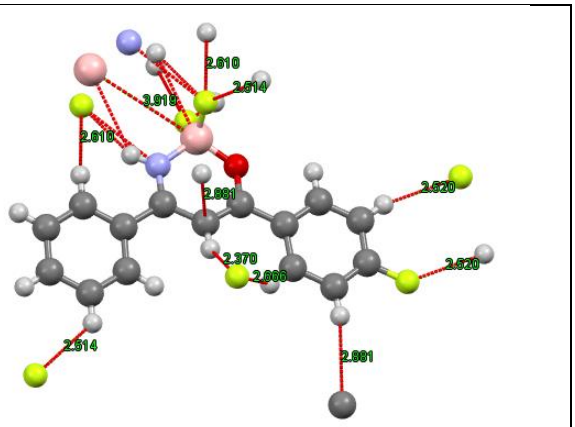
2u	363	30000	469	106	0.117

[a]Recorded at 10 µM in HPLC grade DCM at 25 °C. [b]Measured at 10 µM in HPLC grade DCM at 25 °C excited at 353 nm. [c]Stokes shift = $\lambda_{max,abs}$ - $\lambda_{max,em}$ (nm), $\lambda_{max,abs}$ are their π-π* absorption wavelengths. [d]Determined by quinine sulfate (Φ_F = 0.55) as standard in 0.1 M H_2SO_4 solution on excitation at 353 nm.

10. Intermolecular Non-Covalent Interactions in 2s Crystal:



Inside Crystal Lattice



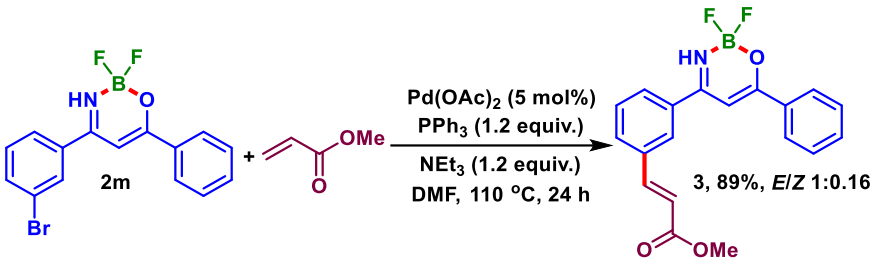
Asymmetric Unit

	Number	Atom1	Atom2	Length	Length-VdW	Symm. op. 1	Symm. op. 2
1	1	F003	H00B	2.370	-0.300	x,y,z	1/2-x,-1/2+y,1/2-z
2	2	F003	H00C	2.666	-0.004	x,y,z	1/2-x,-1/2+y,1/2-z
3	3	F001	N005	2.970	-0.050	x,y,z	-x,1-y,-z
4	4	F001	H005	2.142	-0.528	x,y,z	-x,1-y,-z
5	5	F001	H00I	2.610	-0.060	x,y,z	-x,1-y,-z
6	6	H005	B00L	2.880	-0.320	x,y,z	-x,1-y,-z
7	7	B00L	B00L	3.919	-0.081	x,y,z	-x,1-y,-z
8	8	F002	H00D	2.520	-0.150	x,y,z	2-x,1-y,1-z
9	9	C00B	H00F	2.881	-0.019	x,y,z	-1/2+x,1.5-y,-1/2+z
10	10	H00J	F001	2.514	-0.156	x,y,z	-1/2+x,1.5-y,1/2+z

Figure S8. Intermolecular Non-Covalent Interactions in **2s** Crystal

11. Synthetic Utilization:

Heck reaction of 4-(3-bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2m**) with methyl acrylate in the presence of palladium catalyst, triphenylphosphine and base triethylamine at 110 °C to synthesize a *m*-alkenylated N,O bidentate organic BF_2 complex **3** with 89% yield.[3]



Scheme S2. Post-synthetic modification. Yield refers to the isolated product. The *E*/*Z* ratio was determined by ^{1}H NMR.

An oven-dried 10 mL round-bottom flask containing a magnetic bead was charged with 4-(3-bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2m**) (0.2 mmol, 69.8 mg), methyl acrylate (0.3 mmol, 25.8 mg) $Pd(OAc)_2$ (0.01 mmol, 2.2 mg), PPh_3 (0.24 mmol, 63 mg), NEt_3 (0.24 mmol, 24.2 mg) and DMF (1 mL). After that, the reaction mixture was stirred at 110 °C in a preheated oil bath for 24 h. After completion of the reaction (monitored by TLC), the reaction mixture was admixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). Then the organic layer was dried over anhydrous Na_2SO_4, and the solvent was evaporated under reduced pressure. Then the crude mixture was purified over column chromatography (60-120 mesh silica) by eluting it with 12% ethyl acetate in hexane to afford methyl (*E*)-3-(3-(2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinin-4-yl)phenyl)acrylate (**3**) as a brown gummy compound with 89% yield (63 mg). The identity and purity of the product was confirmed by spectroscopic analysis.

12. References:

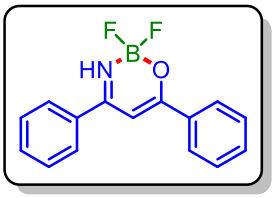
1. P. Kumar and M. Kapur, *Org. Lett.*, 2019, **21**, 2134.

2. S. Kovacs and Z. Novak, *Tetrahedron*, 2013, **69**, 8987.

3. H. A. Dieck and R. F. Heck, *J. Am. Chem. Soc.*, 1974, **96**, 1133.

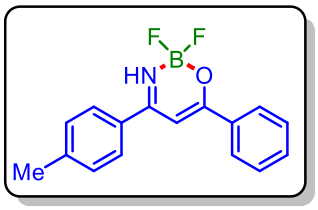
13. Spectral Data:

2,2-Difluoro-4,6-diphenyl-2*H*-1,3,2λ^4-oxazaborinine (2a):



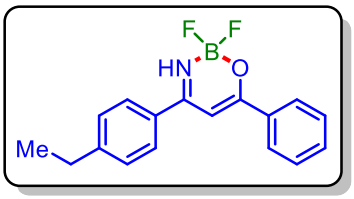
A yellow solid compound (47 mg, 87% yield); mp 158–161 °C; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 2H), 7.67 (t, J = 7.4 Hz, 1H), 7.58 (q, J = 7.3 Hz, 3H), 7.49 (t, J = 7.6 Hz, 2H), 7.41 (s, 1H), 6.55 (s, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.3, 170.5, 134.4, 133.6, 133.3, 132.9, 129.8, 128.9, 127.9, 126.9, 92.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -131.18, -131.21, -131.24, -131.27; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.09, 1.00, 0.91; IR (neat, cm^{-1}): 3343, 2915, 1579, 1609, 1524, 1493, 1422, 1373, 1036, 768, 684; HRMS (ESI-TOF) calcd for $C_{15}H_{12}BF_2NO$ $[M + Na]^+$ 294.0872, found 294.0871.

2,2-Difluoro-6-phenyl-4-(p-tolyl)-2*H*-1,3,2λ^4-oxazaborinine (2b):



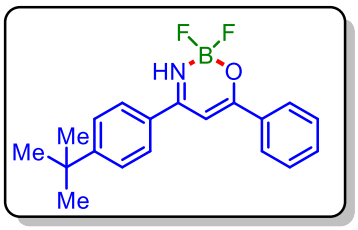
A yellow solid compound (51 mg, 90% yield); mp 171–173 °C; purified over a column of silica gel (8% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, J = 7.5 Hz, 2H), 7.65 (d, J = 8.5 Hz, 2H), 7.56 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.5 Hz, 2H), 7.41 (s, 1H), 7.38 (d, J = 8.0 Hz, 2H), 6.54 (s, 1H), 2.47 (s, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 173.9, 170.1, 144.4, 133.8, 132.8, 131.3, 130.5, 128.9, 127.8, 126.8, 92.0, 21.8; ^{19}F NMR (471 MHz, $CDCl_3$) δ -131.64, -131.67, -131.70, -131.74; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.10, 1.01, 0.91; IR (neat, cm^{-1}): 3345, 2920, 1578, 1605, 1523, 1491, 1425, 1373, 1039, 767, 694; HRMS (ESI-TOF) calcd for $C_{16}H_{14}BF_2NO$ $[M + Na]^+$ 308.1029, found 308.1028.

4-(4-Ethylphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2c):



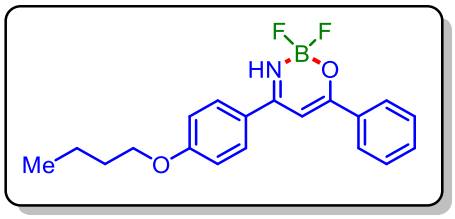
A light yellow solid compound (53 mg, 88% yield); mp 170–173 °C; purified over a column of silica gel (8% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 7.2 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.55 (t, J = 7.2 Hz, 1H), 7.48 (t, J = 7.6 Hz, 2H), 7.40 (d, J = 8.0 Hz, 3H), 6.54 (s, 1H), 2.76 (q, J = 7.6 Hz, 2H), 1.29 (t, J = 7.8 Hz, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 173.9, 170.2, 150.6, 133.8, 132.8, 131.5, 129.3, 128.9, 127.8, 127.0, 92.1, 29.0, 15.3; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.11, 1.02, 0.92; IR (neat, cm^{-1}): 3347, 2924, 1579, 1605, 1524, 1495, 1425, 1374, 1038, 766, 695; HRMS (ESI-TOF) calcd for $C_{17}H_{16}BF_2NO$ [M + Na]$^+$ 322.1185, found 322.1184.

4-(4-(Tert-butyl)phenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2d):



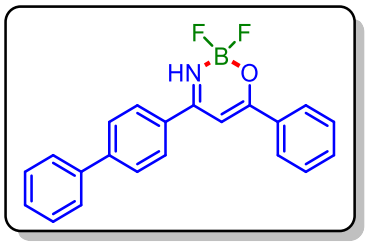
A light yellow solid compound (56 mg, 85% yield); mp 189–191 °C; purified over a column of silica gel (7% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 8.5 Hz, 2H), 7.59 (d, J = 8.0 Hz, 2H), 7.55 (d, J = 7.5 Hz, 1H), 7.48 (t, J = 7.8 Hz, 2H), 7.42 (s, 1H), 6.55 (s, 1H), 1.37 (s, 9H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 173.9, 170.2, 157.5, 133.8, 132.8, 131.3, 128.9, 127.8, 126.81, 126.75, 92.1, 35.4, 31.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -131.49, -131.52, -131.55, -131.58; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.10, 1.01, 0.91; IR (neat, cm^{-1}): 3386, 2921, 1605, 1515, 1466, 1434, 1375, 1036, 776, 688; HRMS (ESI-TOF) calcd for $C_{19}H_{20}BF_2NO$ [M + Na]$^+$ 350.1498, found 350.1503.

4-(4-Butoxyphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2e):



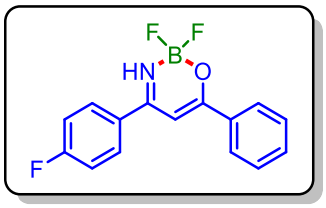
A light brown solid compound (58 mg, 85% yield); mp 181–183 °C; purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 7.2 Hz, 2H), 7.71 (d, J = 8.8 Hz, 2H), 7.55 (t, J = 7.4 Hz, 1H), 7.48 (t, J = 8.0 Hz, 2H), 7.32 (s, 1H), 7.04 (d, J = 8.8 Hz, 2H), 6.53 (d, J = 2.0 Hz, 1H), 4.06 (t, J = 6.6 Hz, 2H), 1.85 – 1.78 (m, 2H), 1.52 (q, J = 7.5 Hz, 2H), 1.00 (t, J = 7.6 Hz, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 173.4, 169.2, 163.6, 133.9, 132.6, 129.8, 128.9, 127.7, 125.6, 115.6, 91.7, 68.4, 31.2, 19.3, 13.9; ^{19}F NMR (471 MHz, $CDCl_3$) δ -132.03, -132.06, -132.09, -132.13. ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.11, 1.01, 0.91; IR (neat, cm^{-1}): 3363, 2931, 1607, 1520, 1469, 1439, 1378, 1026, 768, 684; HRMS (ESI-TOF) calcd for $C_{19}H_{20}BF_2NO_2$ $[M + Na]^+$ 366.1447, found 366.1447.

4-([1,1'-Biphenyl]-4-yl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2f):



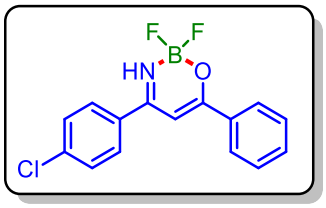
A light orange solid compound (56 mg, 81% yield); mp 175–178 °C; purified over a column of silica gel (14% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, J = 7.5 Hz, 2H), 7.81 (q, J = 9.0 Hz, 4H), 7.64 (d, J = 7.5 Hz, 2H), 7.56 (t, J = 7.3 Hz, 1H), 7.50 (q, J = 6.8 Hz, 4H), 7.44 (t, J = 7.5 Hz, 2H), 6.59 (s, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.2, 169.9, 146.3, 139.3, 133.7, 132.9, 132.7, 129.8, 129.3, 129.1, 128.9, 128.8, 128.3, 127.9, 127.5, 127.4, 92.1; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.15, 1.06, 0.96; IR (neat, cm^{-1}): 3365, 2929, 1579, 1625, 1529, 1490, 1426, 1378, 1049, 765, 698; HRMS (ESI-TOF) calcd for $C_{21}H_{16}BF_2NO$ $[M + Na]^+$ 370.1185, found 370.1187.

2,2-Difluoro-4-(4-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2g):



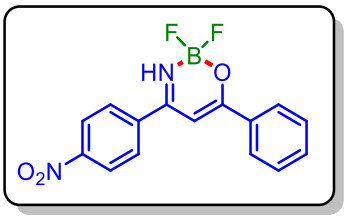
A yellow solid compound (46 mg, 79% yield); mp 211–213 °C; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 7.6 Hz, 2H), 7.78 (dd, J = 8.6, 5.0 Hz, 2H), 7.57 (t, J = 7.4 Hz, 1H), 7.49 (t, J = 7.6 Hz, 2H), 7.44 (s, 1H), 7.30 – 7.25 (m, 2H), 6.50 (s, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.5, 169.3, 165.8 (d, J = 255.8 Hz), 133.5, 133.1, 130.5, 129.4 (d, J = 8.8 Hz), 129.0, 127.9, 117.2 (d, J = 21.4 Hz), 92.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ -104.51, -131.08, -131.11, -131.14, -131.18; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.08, 0.98, 0.89; IR (neat, cm^{-1}): 3358, 2921, 1597, 1531, 1493, 1432, 1372, 1043, 772, 686; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BF_3NO$ $[M + Na]^+$ 312.0778, found 312.0780.

4-(4-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2h):



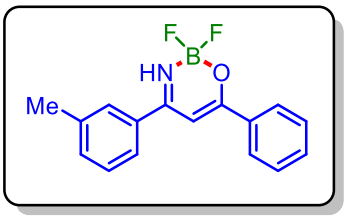
A light yellow solid compound (46 mg, 76% yield); mp 161–164 °C; purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, J = 8.0 Hz, 2H), 7.70 (d, J = 8.5 Hz, 2H), 7.59 – 7.56 (m, 3H), 7.49 (t, J = 7.6 Hz, 2H), 7.45 (s, 1H), 6.50 (d, J = 1.5 Hz, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.7, 169.3, 139.8, 133.5, 133.1, 133.0, 130.2, 129.0, 128.3, 127.9, 92.0; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.83, -130.86, -130.89, -130.92; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.08, 0.99, 0.89; IR (neat, cm^{-1}): 3339, 2914, 1614, 1525, 1486, 1437, 1378, 1034, 767, 683; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BClF_2NO$ $[M + Na]^+$ 328.0482, found 328.0482.

2,2-Difluoro-4-(4-nitrophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2i):



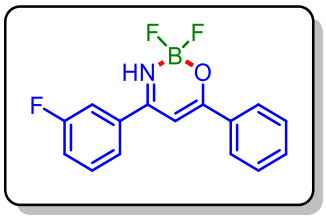
A yellow solid compound (47 mg, 74% yield); mp 161–163 ºC; purified over a column of silica gel (13% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, J = 8.5 Hz, 2H), 8.06 (d, J = 7.5 Hz, 2H), 7.92 (d, J = 8.5 Hz, 2H), 7.61 (t, J = 7.3 Hz, 1H), 7.52 (t, J = 7.5 Hz, 2H), 7.43 (s, 1H), 6.51 (s, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 176.2, 168.6, 150.5, 145.5, 140.3, 133.7, 129.1, 128.2, 128.1, 125.0, 92.4; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.19, -130.21, -130.25, -130.28; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.02, 0.92, 0.84; IR (neat, cm^{-1}): 3359, 3066, 1609, 1531, 1464, 1430, 1379, 1038, 779, 686; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BF_2N_2O_3$ $[M + Na]^+$ 339.0723, found 339.0724.

2,2-Difluoro-6-phenyl-4-(*m*-tolyl)-2*H*-1,3,2λ^4-oxazaborinine (2j):



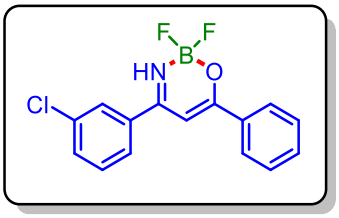
A yellow solid compound (51 mg, 89% yield); mp 166–169 ºC; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 7.2 Hz, 2H), 7.58 – 7.46 (m, 7H), 7.38 (s, 1H), 6.53 (d, J = 1.6 Hz, 1H), 2.48 (s, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.2, 170.7, 139.9, 134.4, 134.1, 133.7, 132.9, 129.7, 128.9, 127.9, 127.4, 124.0, 92.3, 21.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -131.40, -131.43, -131.47, -131.50; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.07, 0.98, 0.89; IR (neat, cm^{-1}): 3346, 2920, 1579, 1605, 1528, 1491, 1420, 1373, 1039, 765, 692; HRMS (ESI-TOF) calcd for $C_{16}H_{14}BF_2NO$ $[M + Na]^+$ 308.1029, found 308.1027.

2,2-Difluoro-4-(3-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2k):



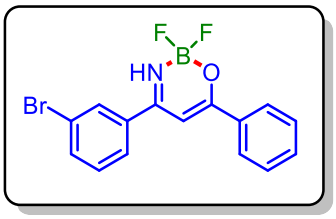
A yellow solid compound (45 mg, 78% yield); mp 177–179 ºC; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 7.2 Hz, 2H), 7.60 – 7.43 (m, 7H), 7.38 – 7.33 (m, 1H), 6.50 (d, J = 2.0 Hz, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 175.1, 169.3, 163.2 (d, J = 249.5 Hz), 136.5, 133.4, 133.2, 131.7 (d, J = 8.8 Hz), 129.0, 128.0, 122.6, 120.3 (d, J = 21.4 Hz), 114.2 (d, J = 23.9 Hz), 92.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ -109.59, -130.72, -130.76, -130.79, -130.82; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.06, 0.96, 0.87; IR (neat, cm^{-1}): 3351, 2919, 1614, 1526, 1484, 1437, 1377, 1037, 766, 688; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BF_3NO$ $[M + Na]^+$ 312.0778, found 312.0782.

4-(3-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2l):



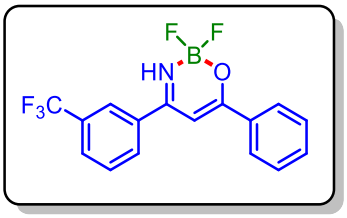
A yellow solid compound (47 mg, 77% yield); mp 167–169 ºC; purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.04 (d, J = 7.5 Hz, 2H), 7.72 (t, J = 1.8 Hz, 1H), 7.64 – 7.48 (m, 7H), 6.49 (d, J = 1.5 Hz, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 175.1, 169.3, 136.2, 136.0, 133.4, 133.2, 133.1, 131.1, 129.0, 128.0, 127.2, 124.9, 92.1; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.64, -130.67, -130.71, -130.74; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.06, 0.97, 0.88; IR (neat, cm^{-1}): 3338, 2918, 1615, 1522, 1480, 1433, 1375, 1031, 766, 683; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BClF_2NO$ $[M + Na]^+$ 328.0482, found 328.0481.

4-(3-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2m):



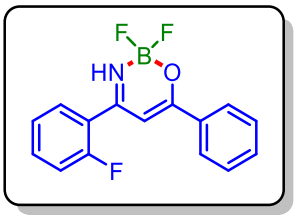
A light brown solid compound (55 mg, 78% yield); mp 120 –123 °C; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, J = 7.5 Hz, 2H), 7.87 (s, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.67 (d, J = 9.0 Hz, 1H), 7.59 (t, J = 7.5 Hz, 1H), 7.52 – 7.45 (m, 3H), 7.36 (s, 1H), 6.49 (d, J = 2.0 Hz, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 175.2, 169.2, 136.5, 136.1, 133.4, 133.3, 131.3, 130.0, 129.0, 128.0, 125.4, 123.9, 92.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.82, -130.85, -130.88, -130.92. ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.03, 0.93, 0.84; IR (neat, cm^{-1}): 3335, 2922, 1613, 1510, 1478, 1427, 1377, 1030, 759, 688; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BBrF_2NO$ $[M + Na]^+$ 371.9977, found 371.9974.

2,2-Difluoro-6-phenyl-4-(3-(trifluoromethyl)phenyl)-2*H*-1,3,2λ^4-oxazaborinine (2n):



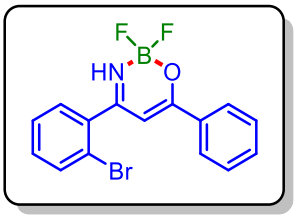
A yellow solid compound (51 mg, 75% yield); mp 158–160 °C; purified over a column of silica gel (15% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, J = 8.0 Hz, 2H), 7.99 (s, 1H), 7.95 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 7.5 Hz, 1H), 7.75 (t, J = 7.8 Hz, 1H), 7.62 – 7.57 (m, 2H), 7.50 (t, J = 7.5 Hz, 2H), 6.52 (s, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 175.3, 169.3, 135.4, 133.3, 132.4 (d, J = 32.8 Hz), 130.6, 130.1, 129.7 (d, J = 3.8 Hz), 129.0, 128.0, 124.6, 124.0 (q, J = 3.4 Hz), 122.4, 92.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.85, -130.28, -130.32, -130.36; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.09, 1.01, 0.92; IR (neat, cm^{-1}): 3375, 2923, 1619, 1536, 1486, 1433, 1381, 1039, 766, 685; HRMS (ESI-TOF) calcd for $C_{16}H_{11}BF_5NO$ $[M + Na]^+$ 362.0746, found 362.0748.

2,2-Difluoro-4-(2-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2o**):



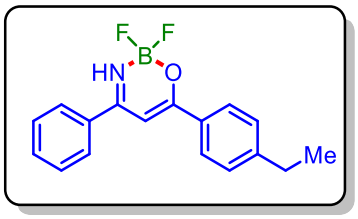
A brown solid compound (45 mg, 78% yield); mp 165–167 ^{o}C; purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.00 – 7.99 (m, 2H), 7.75 (s, 1H), 7.71 – 7.68 (m, 1H), 7.62 – 7.58 (m, 1H), 7.56 – 7.53 (m, 1H), 7.46 (t, J = 7.5 Hz, 2H), 7.35 (t, J = 7.8 Hz, 1H), 7.28 – 7.24 (m, 1H), 6.52 (s, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.1, 166.5, 160.4 (d, J = 255.8 Hz), 134.8 (d, J = 8.8 Hz), 133.5, 132.9, 129.5, 128.9, 127.8, 125.5 (d, J = 3.8 Hz), 121.8 (d, J = 8.8 Hz), 117.4 (d, J = 21.4 Hz), 93.5; ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.80, -130.37, -130.40, -130.44, -130.47; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.03, 0.93, 0.83; IR (neat, cm^{-1}): 3350, 2923, 1612, 1519, 1465, 1427, 1374, 1051, 762, 686; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BF_3NO$ $[M + Na]^+$ 312.0778, found 312.0781.

4-(2-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2p**):



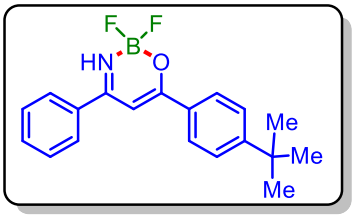
A brown gummy compound (53 mg, 76% yield); purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.2 Hz, 2H), 7.74 (d, J = 7.6 Hz, 1H), 7.56 (t, J = 7.4 Hz, 1H), 7.49 – 7.40 (m, 6H), 6.35 (d, J = 1.6 Hz, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.4, 171.2, 136.3, 134.4, 133.1, 132.8, 129.8, 129.5, 128.9, 128.3, 128.0, 127.8, 126.9, 120.2, 94.9; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.30, -130.33, -130.36, -130.39; ^{11}B NMR (160 MHz, $CDCl_3$) δ 0.97, 0.88, 0.79; IR (neat, cm^{-1}): 3338, 2922, 1612, 1515, 1473, 1429, 1376, 1027, 757, 686; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BBrF_2NO$ $[M + Na]^+$ 371.9977, found 371.9976.

6-(4-Ethylphenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2q**):



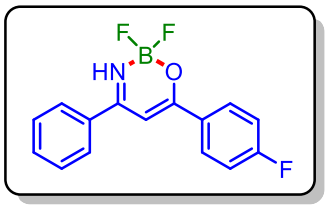
A light yellow solid compound (52 mg, 87% yield); mp 175–177 ^{o}C; purified over a column of silica gel (8% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.96 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 7.5 Hz, 2H), 7.64 (t, J = 7.3 Hz, 1H), 7.57 (t, J = 7.5 Hz, 2H), 7.42 (s, 1H), 7.31 (d, J = 8.0 Hz, 2H), 6.51 (s, 1H), 2.72 (q, J = 7.5 Hz, 2H), 1.27 (t, J = 7.5 Hz, 3H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.4, 170.2, 150.1, 134.5, 133.2, 131.1, 129.7, 128.5, 128.0, 126.9, 91.8, 29.1, 15.3; ^{19}F NMR (471 MHz, $CDCl_3$) δ -131.17, -131.20, -131.24, -131.27; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.12, 1.03, 0.93; IR (neat, cm^{-1}): 3348, 2925, 1578, 1606, 1527, 1496, 1428, 1375, 1037, 768, 694; HRMS (ESI-TOF) calcd for $C_{17}H_{16}BF_2NO$ [M + Na]$^+$ 322.1185, found 322.1185.

6-(4-(*tert*-Butyl)phenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2r**):



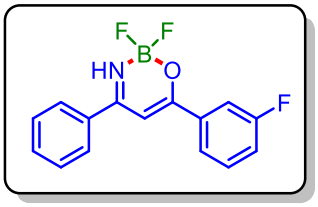
A yellow solid compound (55 mg, 84% yield); mp 187–189 ^{o}C; purified over a column of silica gel (8% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, J = 8.8 Hz, 2H), 7.75 – 7.72 (m, 2H), 7.64 (t, J = 7.4 Hz, 1H), 7.57 (t, J = 7.4 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 7.46 (s, 1H), 6.51 (d, J = 2.4 Hz, 1H), 1.35 (s, 9H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.2, 170.2, 156.8, 134.4, 133.1, 130.8, 129.7, 127.7, 126.9, 125.9, 91.8, 35.3, 31.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.97, -131.00, -131.03, -131.06; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.14, 1.04, 0.95; IR (neat, cm^{-1}): 3335, 2958, 1609, 1517, 1494, 1454, 1379, 1049, 762, 665; HRMS (ESI-TOF) calcd for $C_{19}H_{20}BF_2NO$ [M + Na]$^+$ 350.1498, found 350.1506.

2,2-Difluoro-6-(4-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2s**):



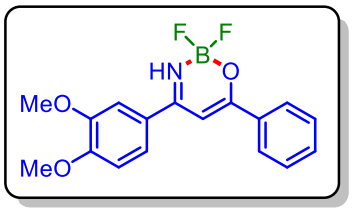
A yellow solid compound (44 mg, 76% yield); mp 191–194 ºC; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (dd, J = 9.0, 5.5 Hz, 2H), 7.74 (d, J = 7.5 Hz, 2H), 7.66 (t, J = 7.5 Hz, 1H), 7.58 (t, J = 7.8 Hz, 2H), 7.50 (s, 1H), 7.17 (t, J = 8.5 Hz, 2H), 6.48 (d, J = 2.0 Hz, 1H); ^{13}C {^{1}H} NMR (126 MHz, $CDCl_3$) δ 173.0, 170.6, 165.7 (d, J = 255.8 Hz), 134.3, 133.4, 130.3 (d, J = 8.8 Hz), 129.8, 126.9, 116.2 (d, J = 21.4 Hz), 91.9; ^{19}F NMR (471 MHz, $CDCl_3$) δ -105.50, -131.18, -131.21, -131.24, -131.27; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.06, 0.97, 0.88; IR (neat, cm^{-1}): 3358, 2921, 1597, 1531, 1493, 1432, 1372, 1043, 772, 686; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BF_3NO$ $[M + Na]^+$ 312.0778, found 312.0783.

2,2-Difluoro-6-(3-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2t**):



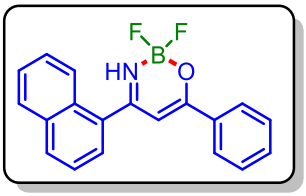
A yellow solid compound (43 mg, 75% yield); mp 181–183 ºC; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, J = 8.0 Hz, 1H), 7.77 – 7.65 (m, 5H), 7.59 (t, J = 7.4 Hz, 2H), 7.48 – 7.42 (m, 1H), 7.27 – 7.22 (m, 1H), 6.52 (d, J = 2.0 Hz, 1H); ^{13}C {1H} NMR (126 MHz, $CDCl_3$) δ 172.39, 170.77, 163.0 (d, J = 247.0 Hz), 134.0, 133.5, 132.7, 130.5 (d, J = 7.6 Hz), 129.9, 126.9, 123.4 (d, J = 2.5 Hz), 119.7 (d, J = 21.4 Hz), 114.7 (d, J = 22.7 Hz), 92.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -111.73, -130.71, -130.74, -130.77, -130.80; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.06, 0.97, 0.88; IR (neat, cm^{-1}): 3362, 2919, 1611, 1522, 1487, 1416, 1374, 1040, 756, 683; HRMS (ESI-TOF) calcd for $C_{15}H_{11}BF_3NO$ $[M + Na]^+$ 312.0778, found 312.0779.

4-(3,4-Dimethoxyphenyl)-2,2-difluoro-6- phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2u**):



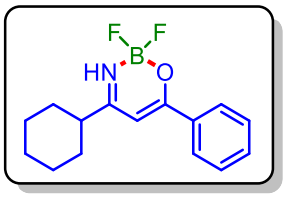
A dark yellow solid compound (59 mg, 89% yield); mp 211–213 ºC; purified over a column of silica gel (18% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, J = 7.0 Hz, 2H), 7.56 (t, J = 7.3 Hz, 1H), 7.49 (t, J = 7.8 Hz, 2H), 7.41 – 7.39 (m, 1H), 7.34 (s, 1H), 7.17 (s, 1H), 7.01 (d, J = 8.5 Hz, 1H), 6.51 (s, 1H), 3.99 (d, J = 3.0 Hz, 6H); ^{13}C {1H} NMR (126 MHz, $CDCl_3$) δ 173.5, 169.6, 153.6, 150.0, 133.9, 132.7, 128.9, 127.7, 126.4, 121.1, 111.5, 109.1, 91.9, 56.5, 56.4; ^{19}F NMR (471 MHz, $CDCl_3$) δ -131.84, -131.87, -131.90, -131.94; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.11, 1.02, 0.92; IR (neat, cm^{-1}): 3372, 2920, 1599, 1517, 1492, 1440, 1380, 1256, 1043, 764, 682; HRMS (ESI-TOF) calcd for $C_{17}H_{16}BF_2NO_3$ [M + Na]$^+$ 354.1084, found 354.1086.

2,2-Difluoro-4-(naphthalen-1-yl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2v**):



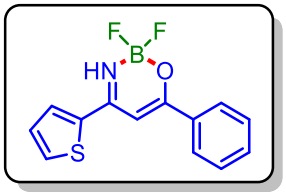
A brown gummy compound (55 mg, 85% yield); purified over a column of silica gel (14% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 – 7.94 (m, 5H), 7.66 – 7.53 (m, 6H), 7.46 (t, J = 7.5 Hz, 2H), 6.47 (s, 1H); ^{13}C {1H} NMR (126 MHz, $CDCl_3$) δ 173.8, 172.3, 133.9, 133.4, 133.0, 132.2, 129.4, 129.1, 128.9, 128.2, 127.9, 127.2, 126.2, 125.2, 124.3, 95.5; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.45, -130.48, -130.52, -130.55; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.11, 1.02, 0.92; IR (neat, cm^{-1}): 3332, 2924, 1615, 1517, 1491, 1435, 1379, 1023, 773, 689; HRMS (ESI-TOF) calcd for $C_{19}H_{14}BF_2NO$ [M + Na]$^+$ 344.1029, found 344.1031.

4-Cyclohexyl-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2w**):



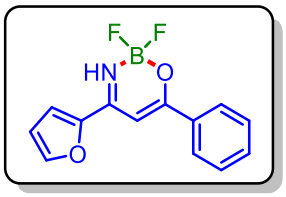
A white solid compound (50 mg, 90% yield); mp 165–167 ^{o}C; purified over a column of silica gel (10% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.94 (d, J = 8.0 Hz, 2H), 7.52 – 7.42 (m, 4H), 6.12 (s, 1H), 2.40 (t, J = 11.0 Hz, 1H), 1.96 – 1.87 (m, 4H), 1.78 – 1.75 (m, 1H), 1.44 – 1.33 (m, 4H), 1.29 – 1.22 (m, 1H); ^{13}C {1H} NMR (126 MHz, $CDCl_3$) δ 180.5, 172.6, 133.6, 132.4, 128.7, 127.5, 92.3, 45.8, 30.2, 25.7, 25.5; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.76, -130.79, -130.82, -130.86; ^{11}B NMR (160 MHz, $CDCl_3$) δ 0.93, 0.84, 0.74; IR (neat, cm^{-1}): 3348, 2934, 1530, 1472, 1438, 1391, 1019, 773, 692; HRMS (ESI-TOF) calcd for $C_{15}H_{18}BF_2NO$ $[M + Na]^+$ 300.1342, found 300.1348.

2,2-Difluoro-6-phenyl-4-(thiophen-2-yl)-2*H*-1,3,2λ^4-oxazaborinine (**2x**):



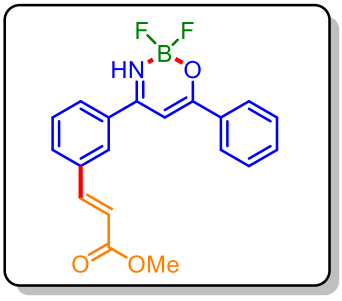
A brown solid compound (46 mg, 84% yield); mp 199–201 ^{o}C; purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 7.6 Hz, 2H), 7.80 (d, J = 3.6 Hz, 1H), 7.74 (d, J = 5.2 Hz, 1H), 7.57 (t, J = 6.8 Hz, 1H), 7.49 (t, J = 7.4 Hz, 2H), 7.31 – 7.27 (m, 2H), 6.54 (d, J = 1.6 Hz, 1H); ^{13}C {1H} NMR (126 MHz, $CDCl_3$) δ 174.1, 162.3, 136.7, 133.6, 133.0, 132.9, 130.8, 129.5, 128.9, 127.8, 91.6; ^{19}F NMR (471 MHz, $CDCl_3$) δ -132.18, -132.21, -132.24, -132.28; ^{11}B NMR (160 MHz, $CDCl_3$) δ 0.98, 0.89, 0.79; IR (neat, cm^{-1}): 3364, 2930, 1596, 1532, 1499, 1431, 1375, 1045, 778, 681; HRMS (ESI-TOF) calcd for $C_{13}H_{10}BF_2NOS$ $[M + Na]^+$ 300.0436, found 300.0436.

2,2-Difluoro-4-(furan-2-yl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (**2y**):



A brown solid compound (44 mg, 85% yield); mp 155–157 ºC; purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, J = 7.6 Hz, 2H), 7.76 (s, 1H), 7.57 – 7.47 (m, 4H), 7.31 (d, J = 3.6 Hz, 1H), 6.70 (d, J = 2.0 Hz, 1H), 6.49 (d, J = 2.0 Hz, 1H); ^{13}C {1H} NMR (126 MHz, $CDCl_3$) δ 173.9, 157.0, 148.0, 133.6, 132.8, 129.1, 128.9, 127.7, 117.6, 113.7, 89.0; ^{19}F NMR (471 MHz, $CDCl_3$) δ -132.06, -132.09, -132.12, -132.15; ^{11}B NMR (160 MHz, $CDCl_3$) δ 0.93, 0.83, 0.74; IR (neat, cm^{-1}): 3354, 2923, 1599, 1537, 1496, 1435, 1371, 1049, 774, 689; HRMS (ESI-TOF) calcd for $C_{13}H_{10}BF_2NO_2$ $[M + Na]^+$ 284.0665, found 284.0664.

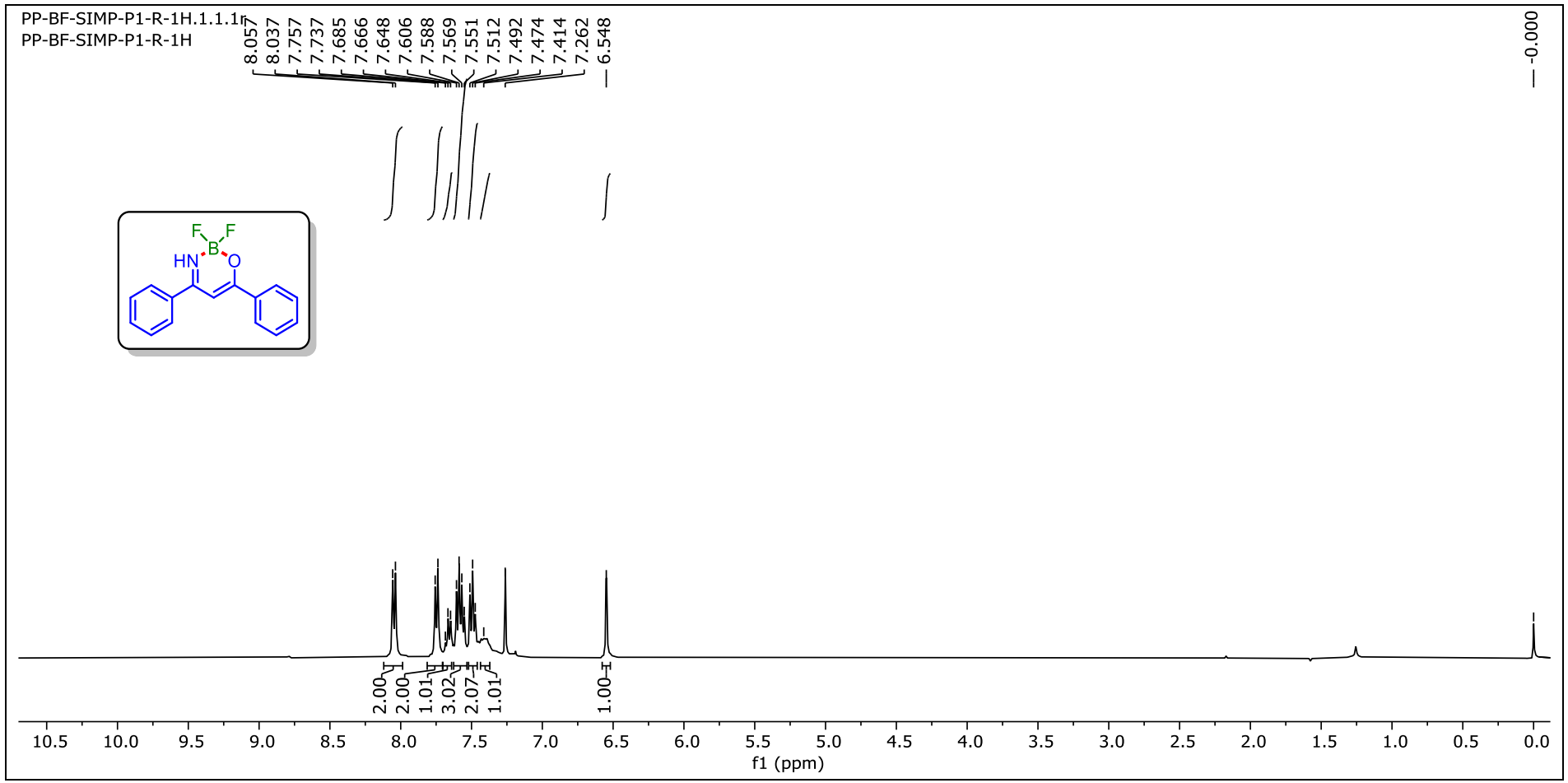
Methyl (*E*)-3-(3-(2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinin-4-yl)phenyl)acrylate (**3**):



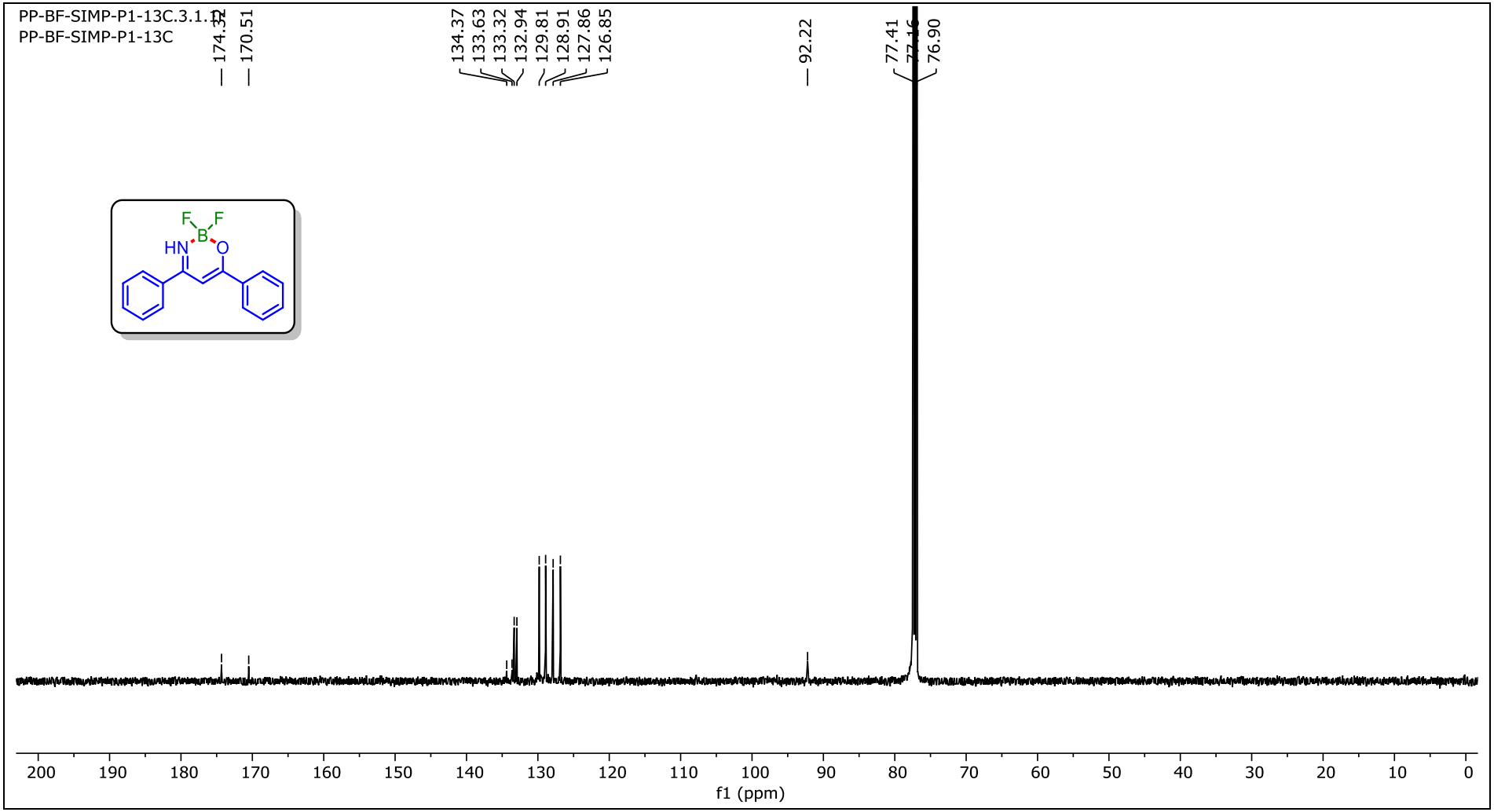
A brown gummy compound (63 mg, 89% yield, *E*/*Z* 1:0.16); purified over a column of silica gel (12% EtOAc in hexane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, J = 7.5 Hz, 2H), 7.76 (d, J = 6.5 Hz, 1H), 7.72 (s, 1H), 7.68 – 7.64 (m, 3H), 7.56 – 7.50 (m, 3H), 7.47 – 7.44 (m, 5H), 6.52 (d, J = 16.0 Hz, 1H), 6.14 (s, 1H), 3.83 (s, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.5, 167.2, 162.1, 143.8, 140.3, 138.7, 135.4, 132.3, 132.2, 132.13, 132.10, 131.4, 130.1, 129.8, 129.0, 128.7, 128.6, 128.5, 128.2, 127.4, 126.1, 119.4, 92.3, 52.0; ^{19}F NMR (471 MHz, $CDCl_3$) δ -130.87, -130.90, -130.93, -131.21, -131.24, -131.27, -131.30; ^{11}B NMR (160 MHz, $CDCl_3$) δ 1.09, 1.00, 0.91; IR (neat, cm^{-1}): 3339, 2924, 2853, 1715, 1606, 1525, 1436, 1312, 1175, 751, 694.

14. NMR Spectra:

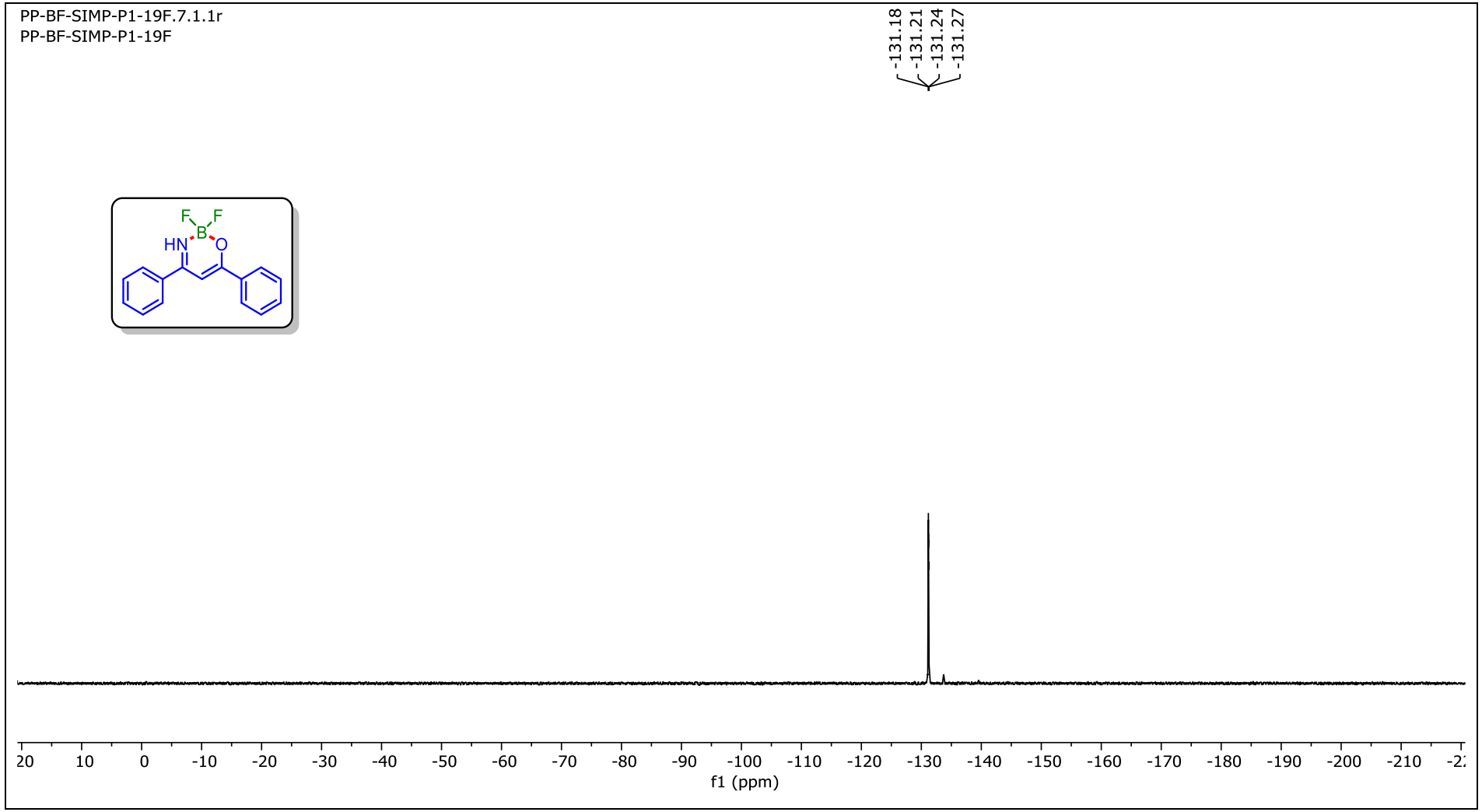
^{1}H NMR of **2,2-Difluoro-4,6-diphenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2a)** ($CDCl_3$, 400 MHz)



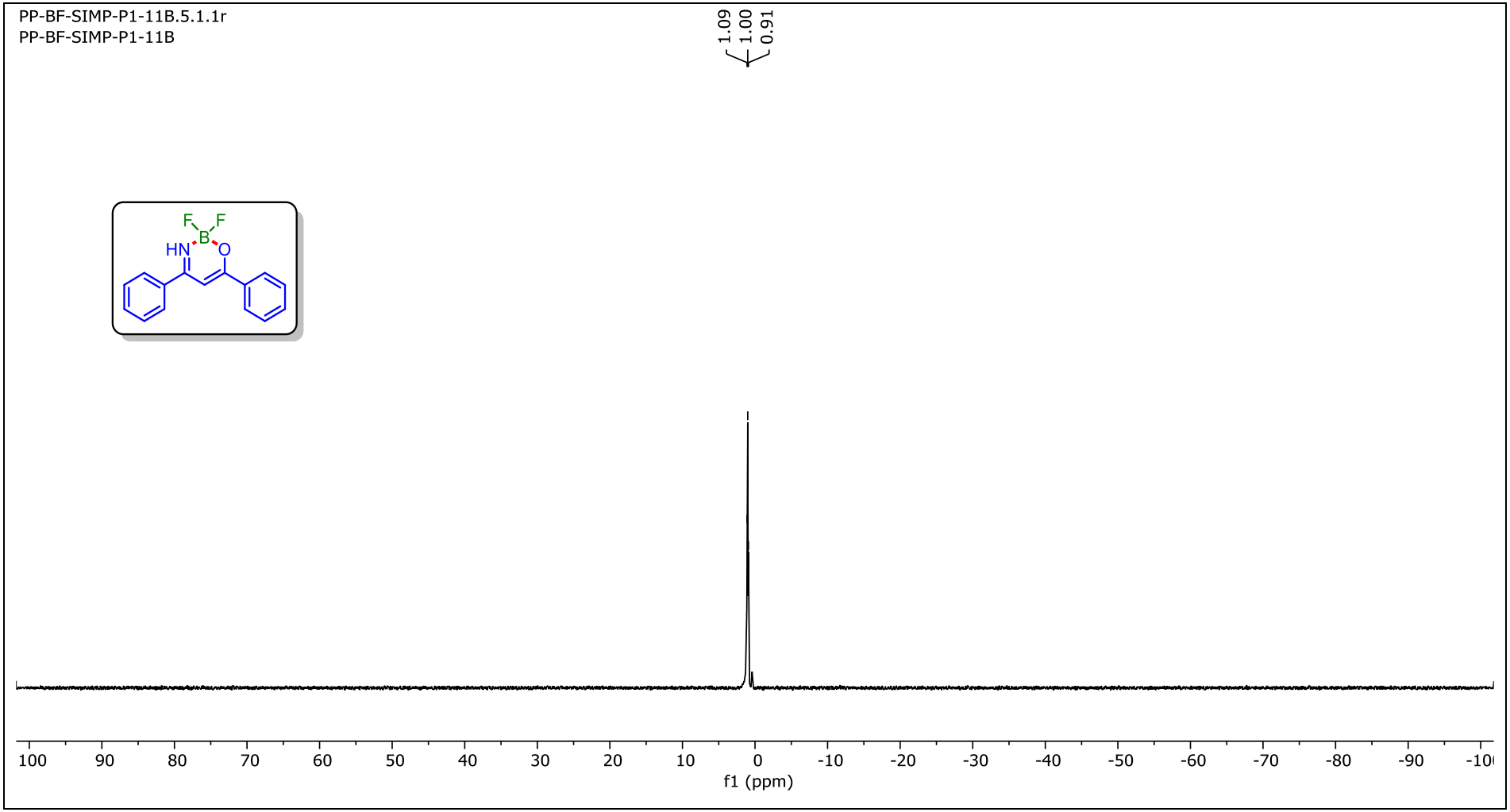
^{13}C {^{1}H} NMR of **2,2-Difluoro-4,6-diphenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2a)** ($CDCl_3$, 126 MHz)



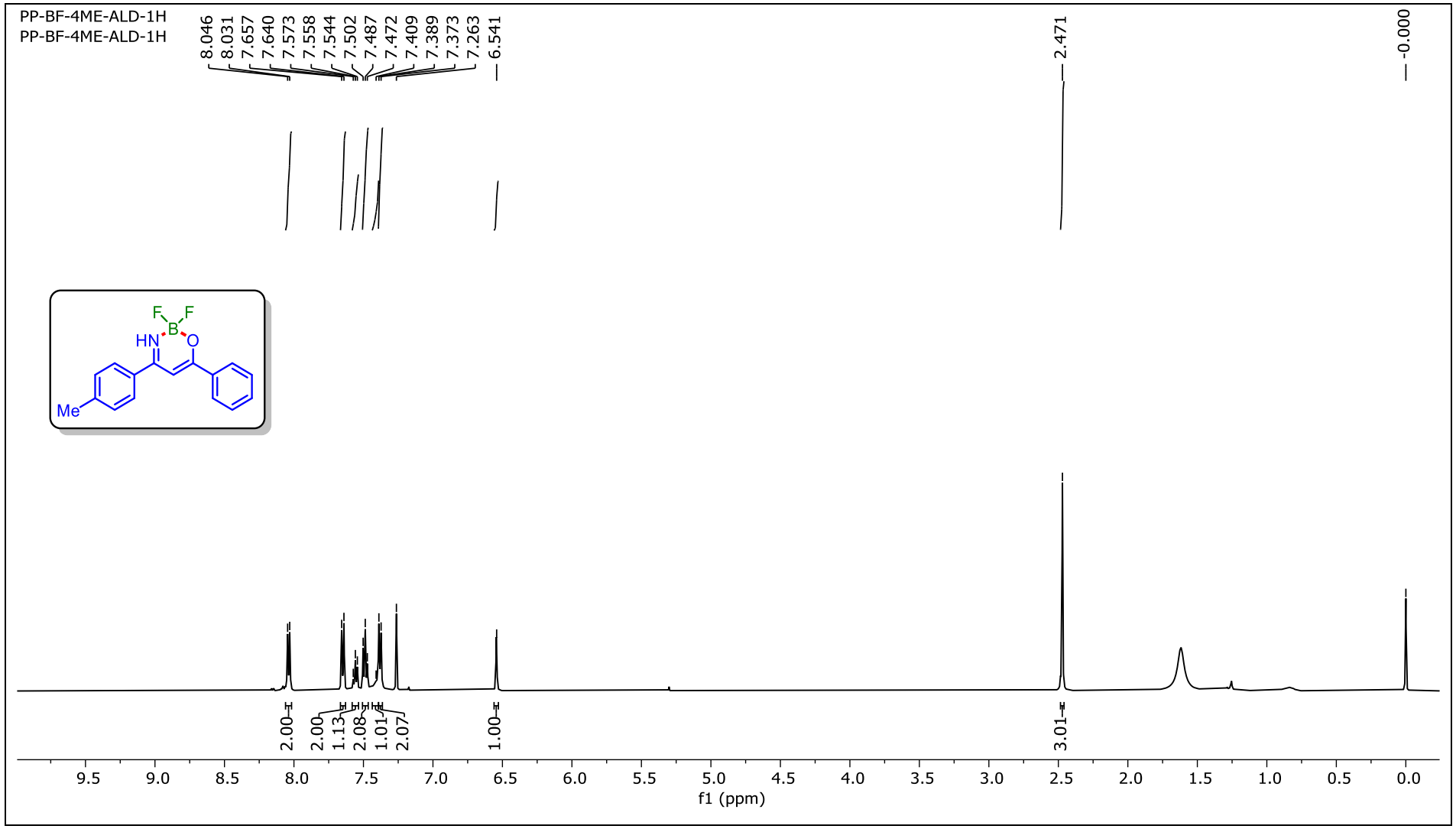
^{19}F NMR of **2,2-Difluoro-4,6-diphenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2a)** ($CDCl_3$, 471 MHz)



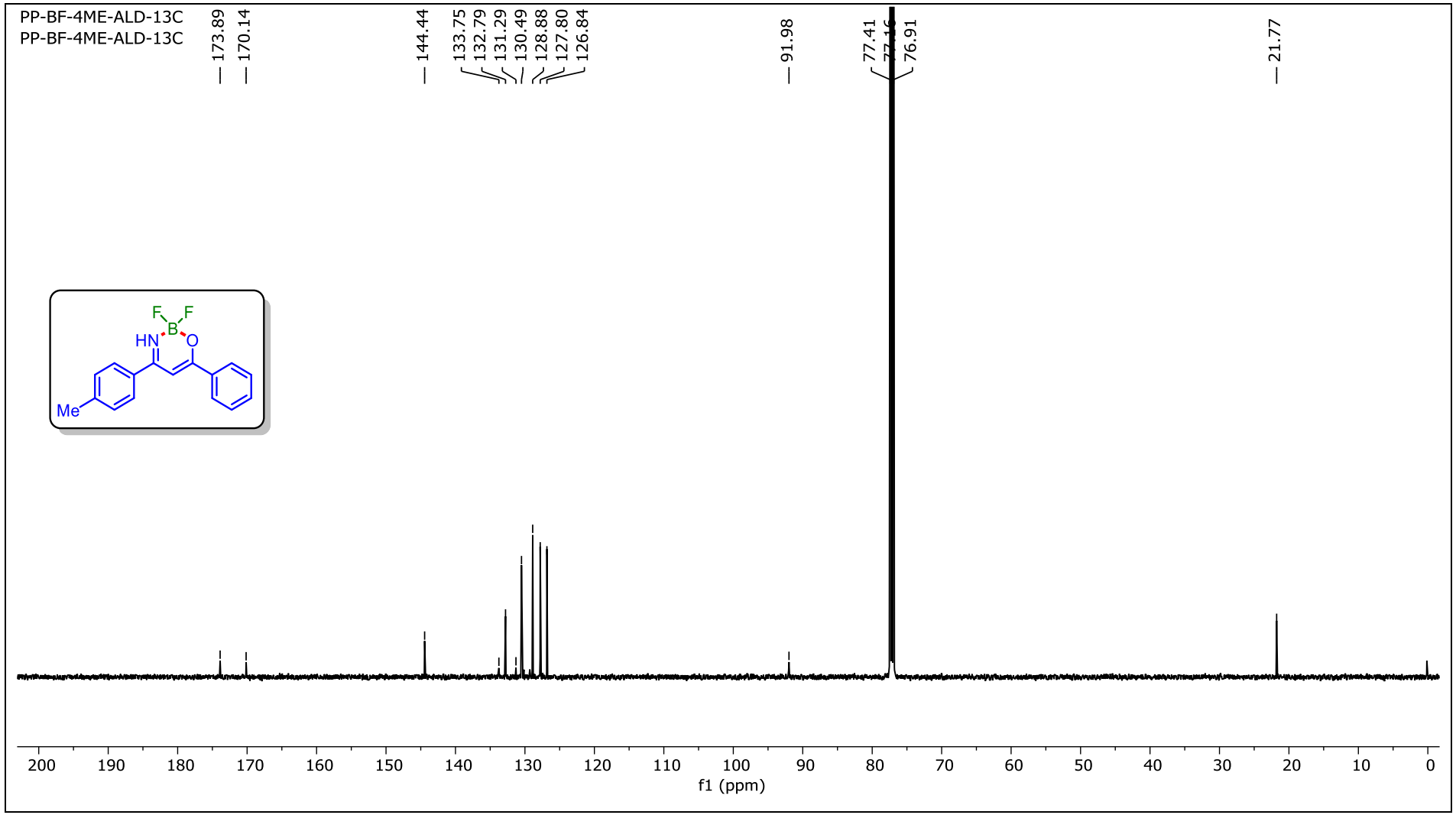
^{11}B NMR of **2,2-Difluoro-4,6-diphenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2a)** ($CDCl_3$, 160 MHz)



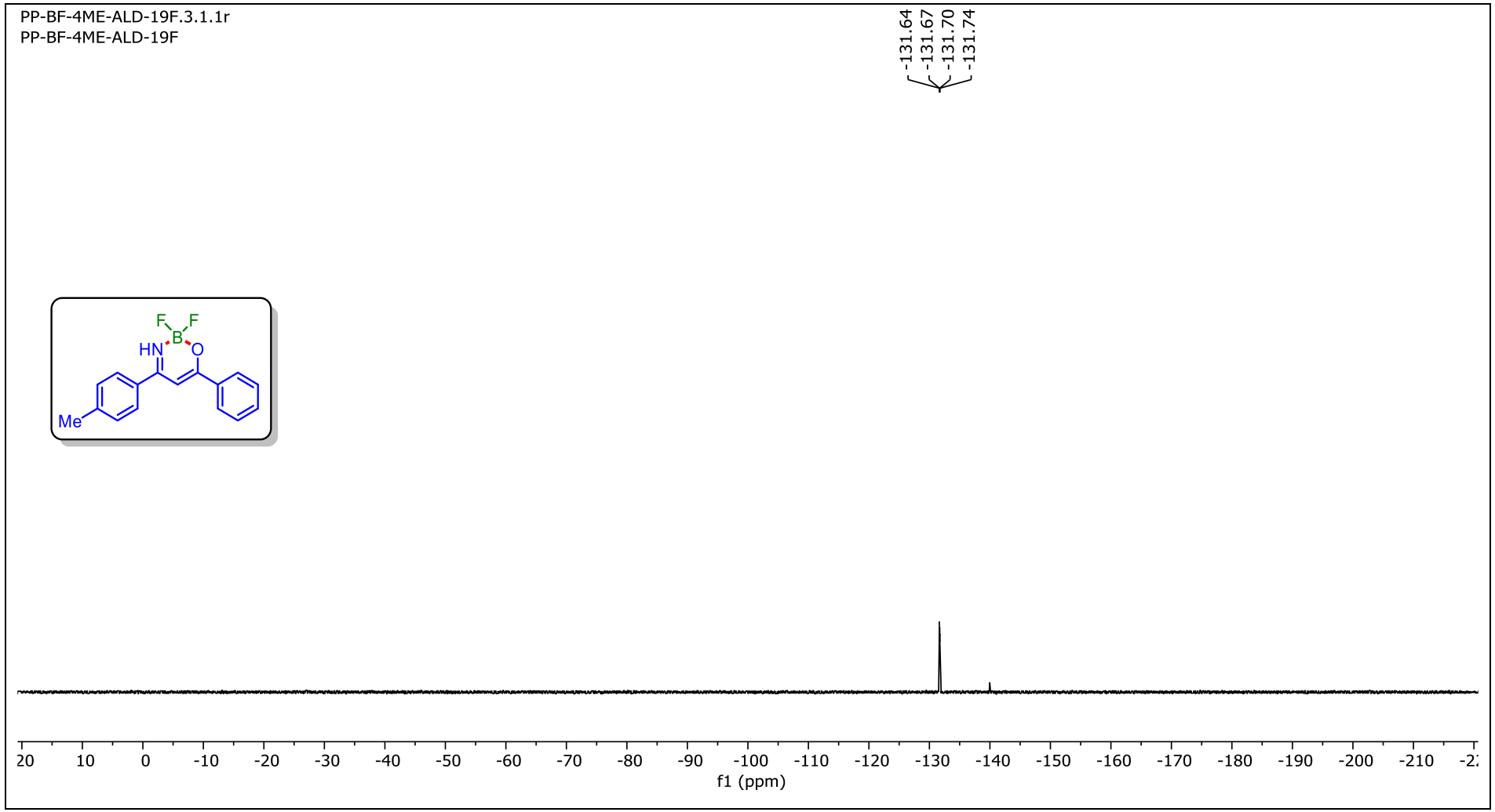
^{1}H NMR of **2,2-Difluoro-6-phenyl-4-(p-tolyl)-2*H*-1,3,2λ^{4}-oxazaborinine (2b)** ($CDCl_3$, 500 MHz)



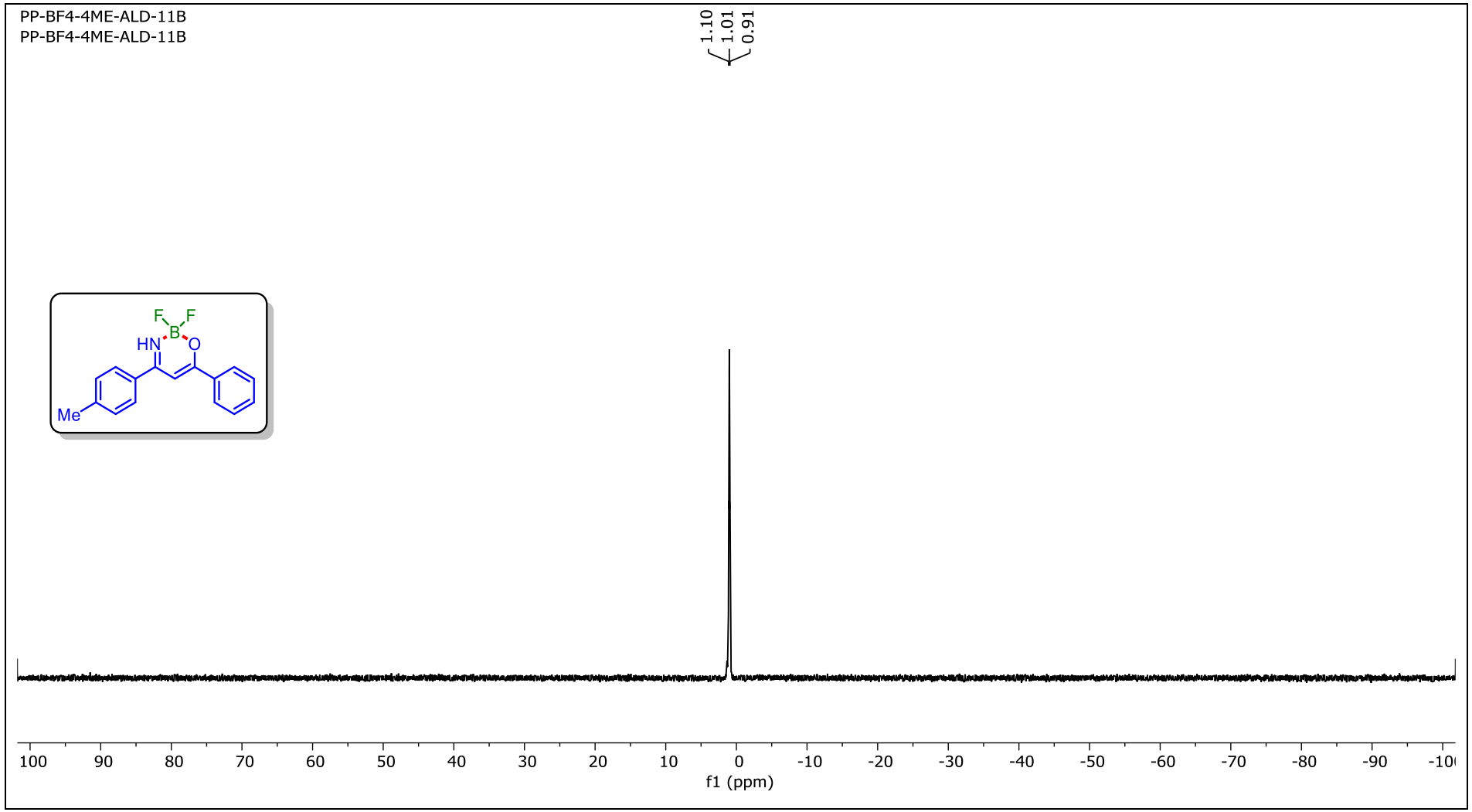
^{13}C {^{1}H} NMR of **2,2-Difluoro-6-phenyl-4-(p-tolyl)-2*H*-1,3,2λ^{4}-oxazaborinine (2b)** ($CDCl_3$, 126 MHz)



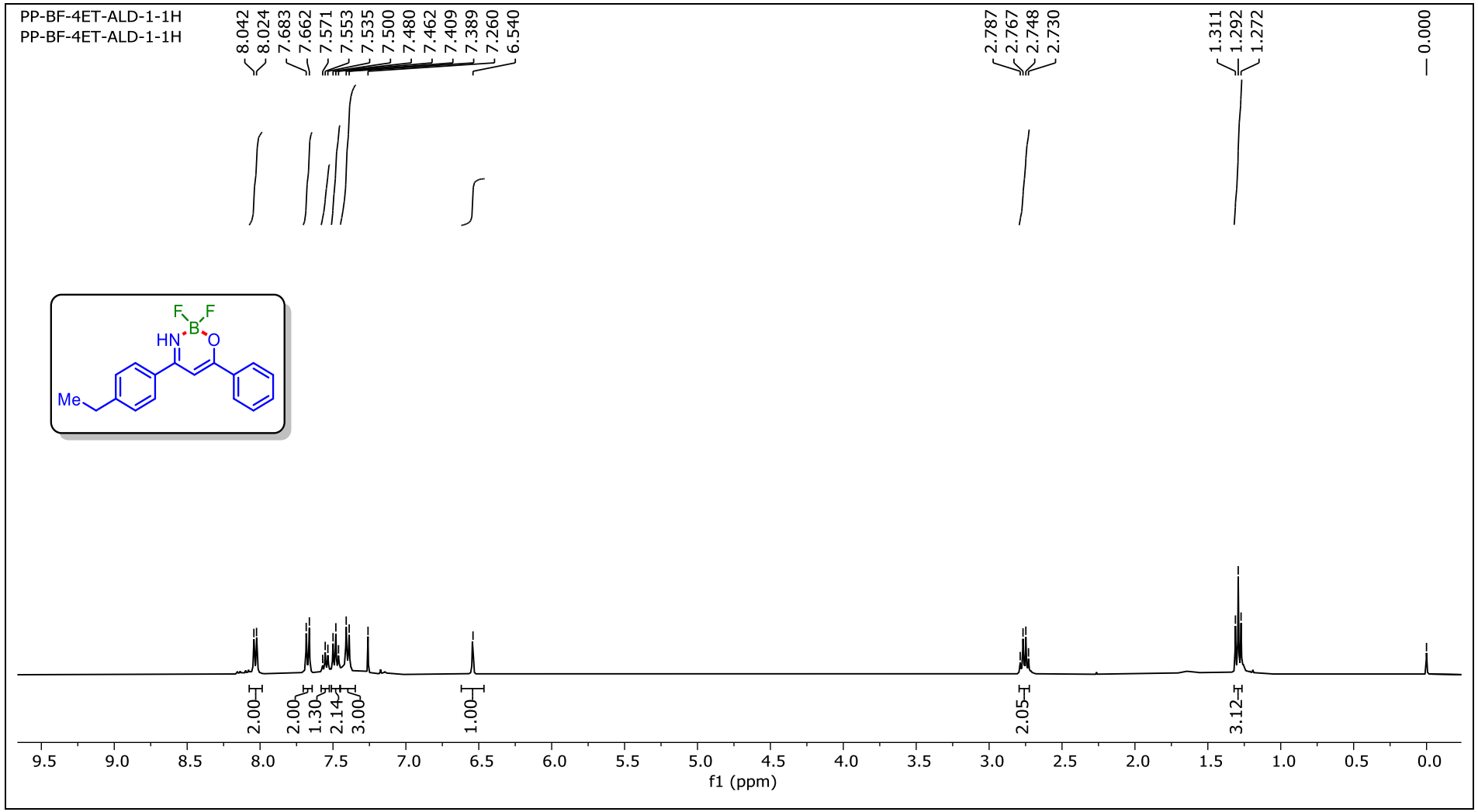
^{19}F NMR of **2,2-Difluoro-6-phenyl-4-(p-tolyl)-2*H*-1,3,2λ^{4}-oxazaborinine (2b)** ($CDCl_3$, 471 MHz)



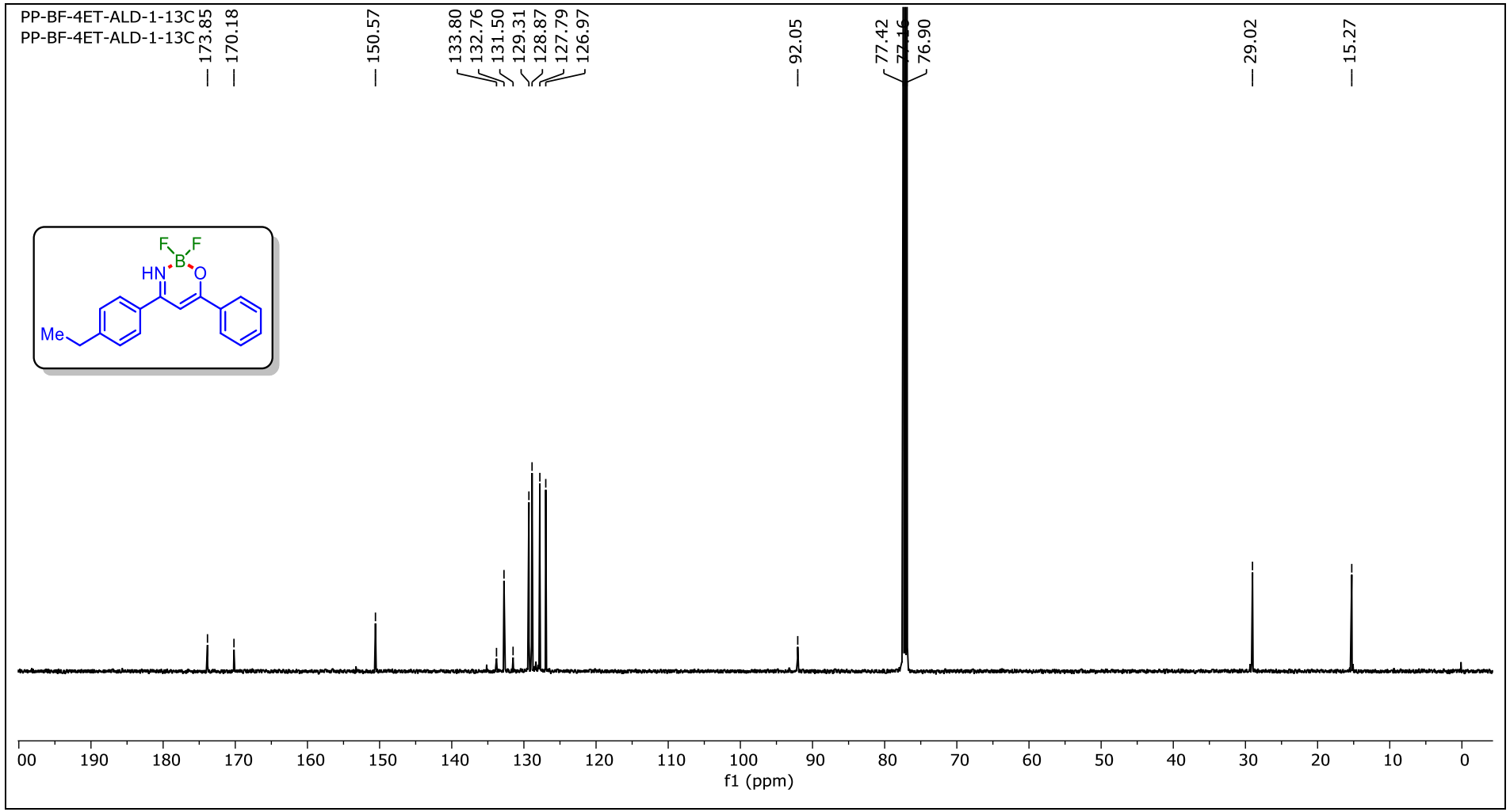
^{11}B NMR of **2,2-Difluoro-6-phenyl-4-(p-tolyl)-2*H*-1,3,2λ^4-oxazaborinine (2b)** ($CDCl_3$, 160 MHz)



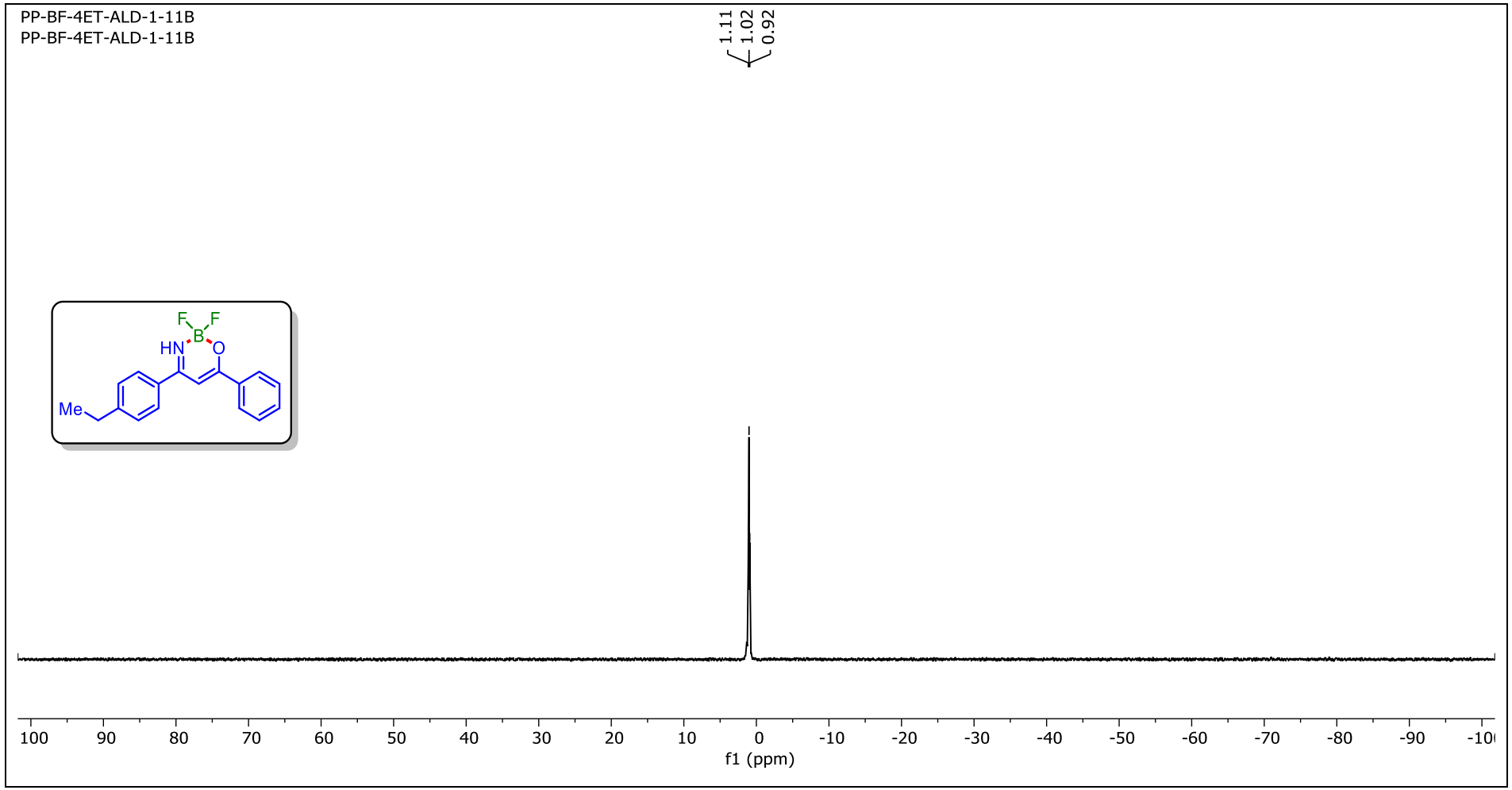
^{1}H NMR of **4-(4-Ethylphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2c)** ($CDCl_3$, 400 MHz)



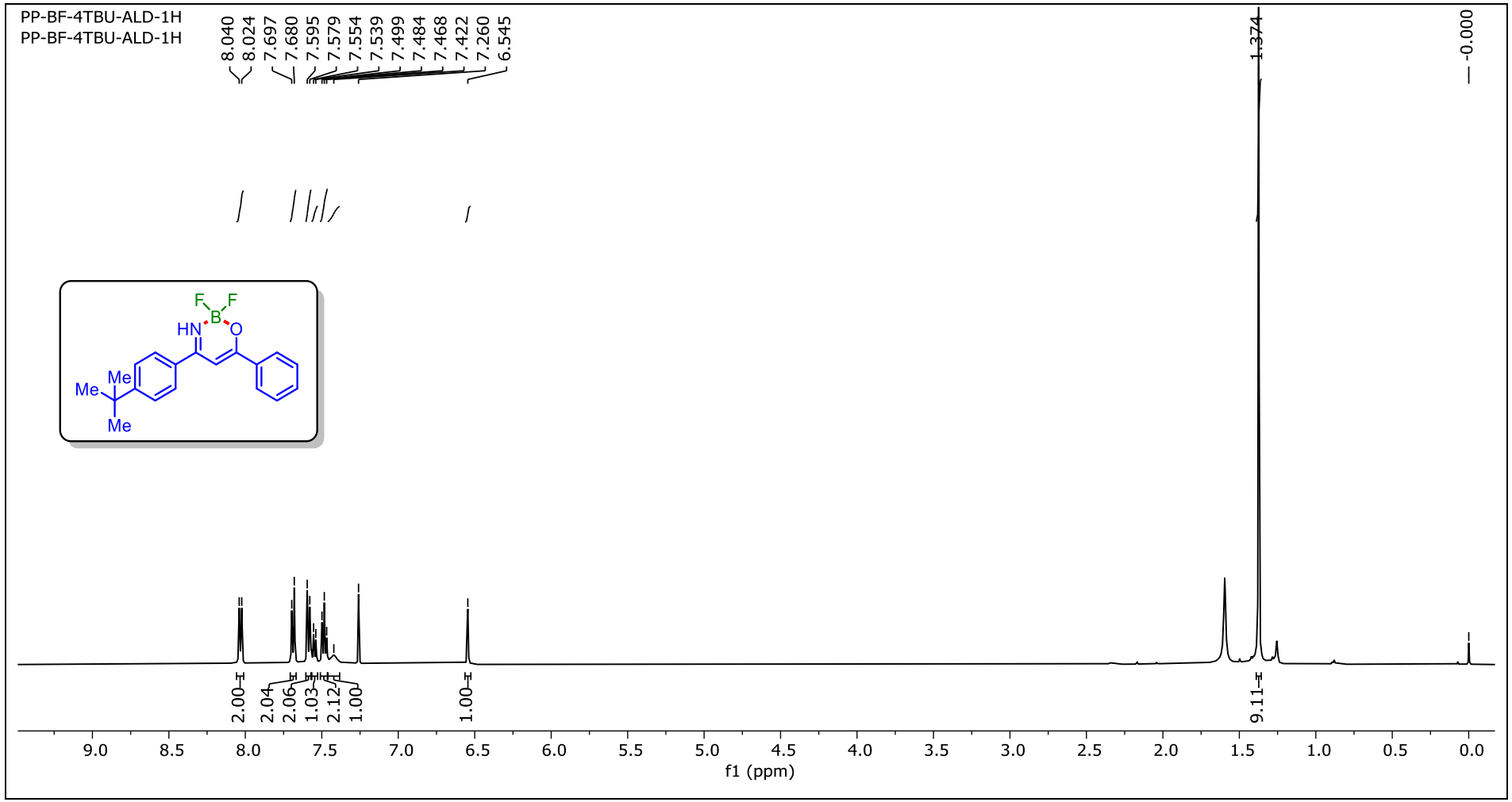
^{13}C {^{1}H} NMR of **4-(4-Ethylphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2c)** ($CDCl_3$, 126 MHz)



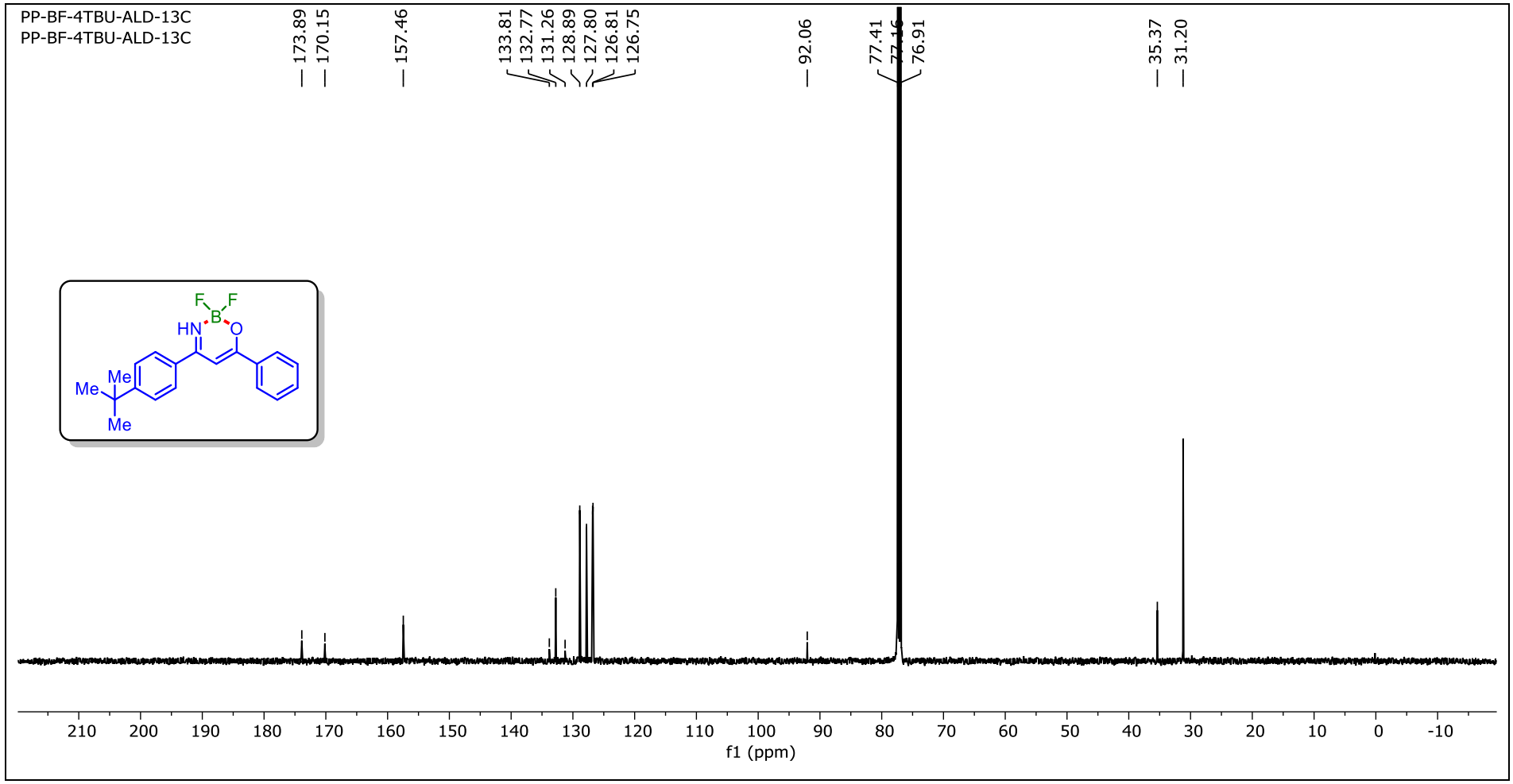
^{11}B NMR of **4-(4-Ethylphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2c)** ($CDCl_3$, 160 MHz)



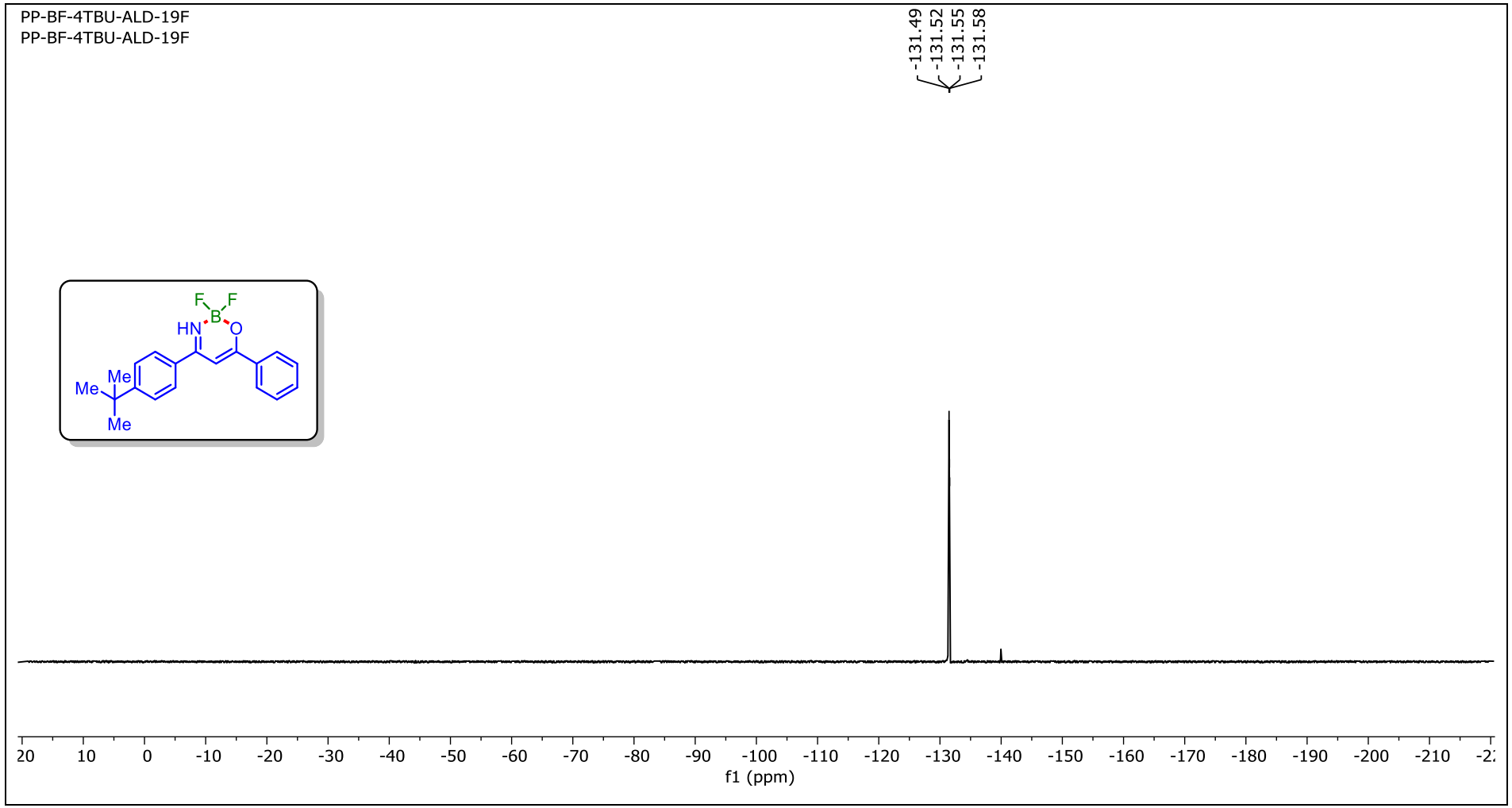
^{1}H NMR of **4-(4-(Tert-butyl)phenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2d)** ($CDCl_3$, 500 MHz)



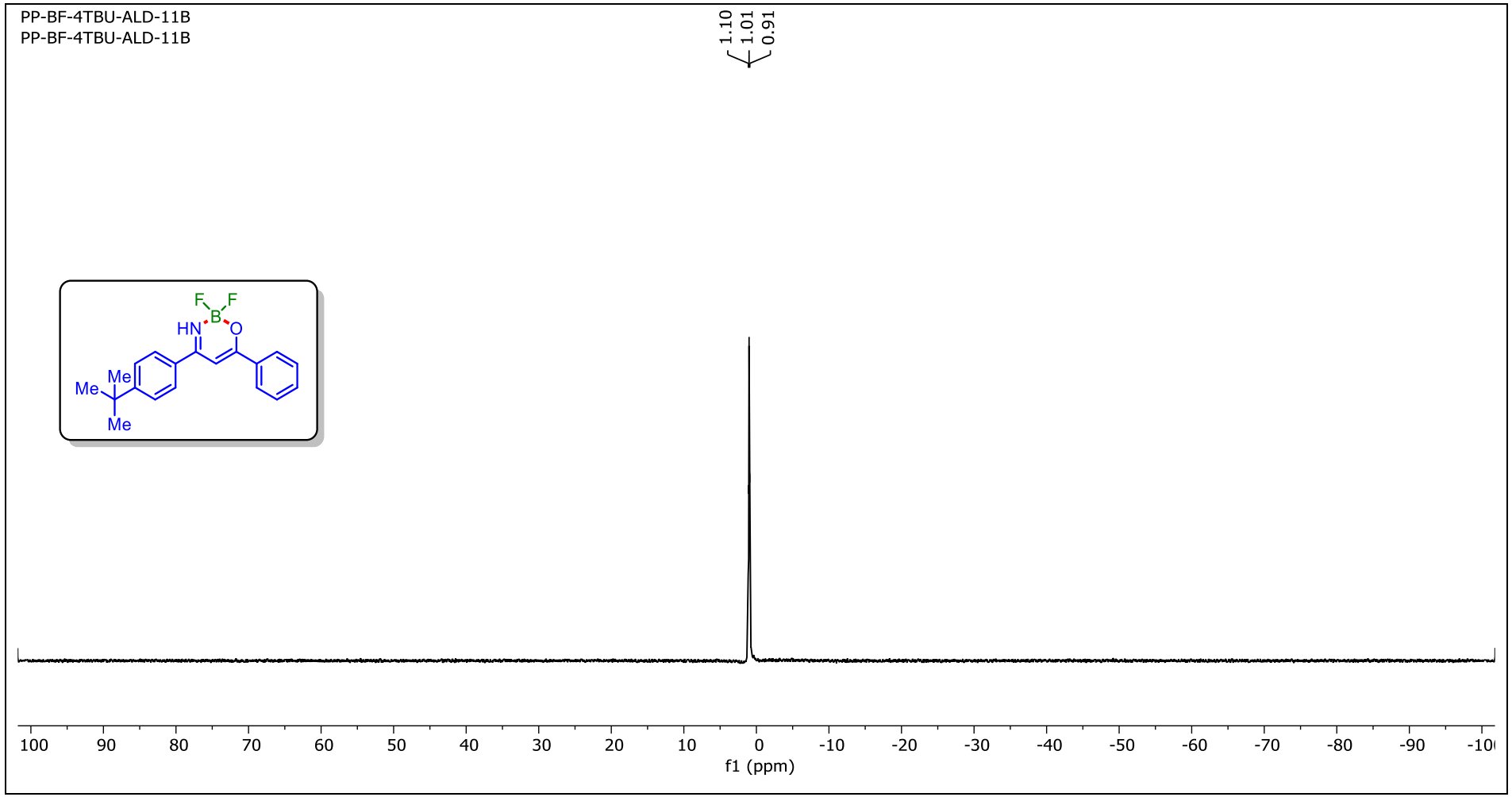
^{13}C {^{1}H} NMR of **4-(4-(Tert-butyl)phenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2d)** ($CDCl_3$, 126 MHz)



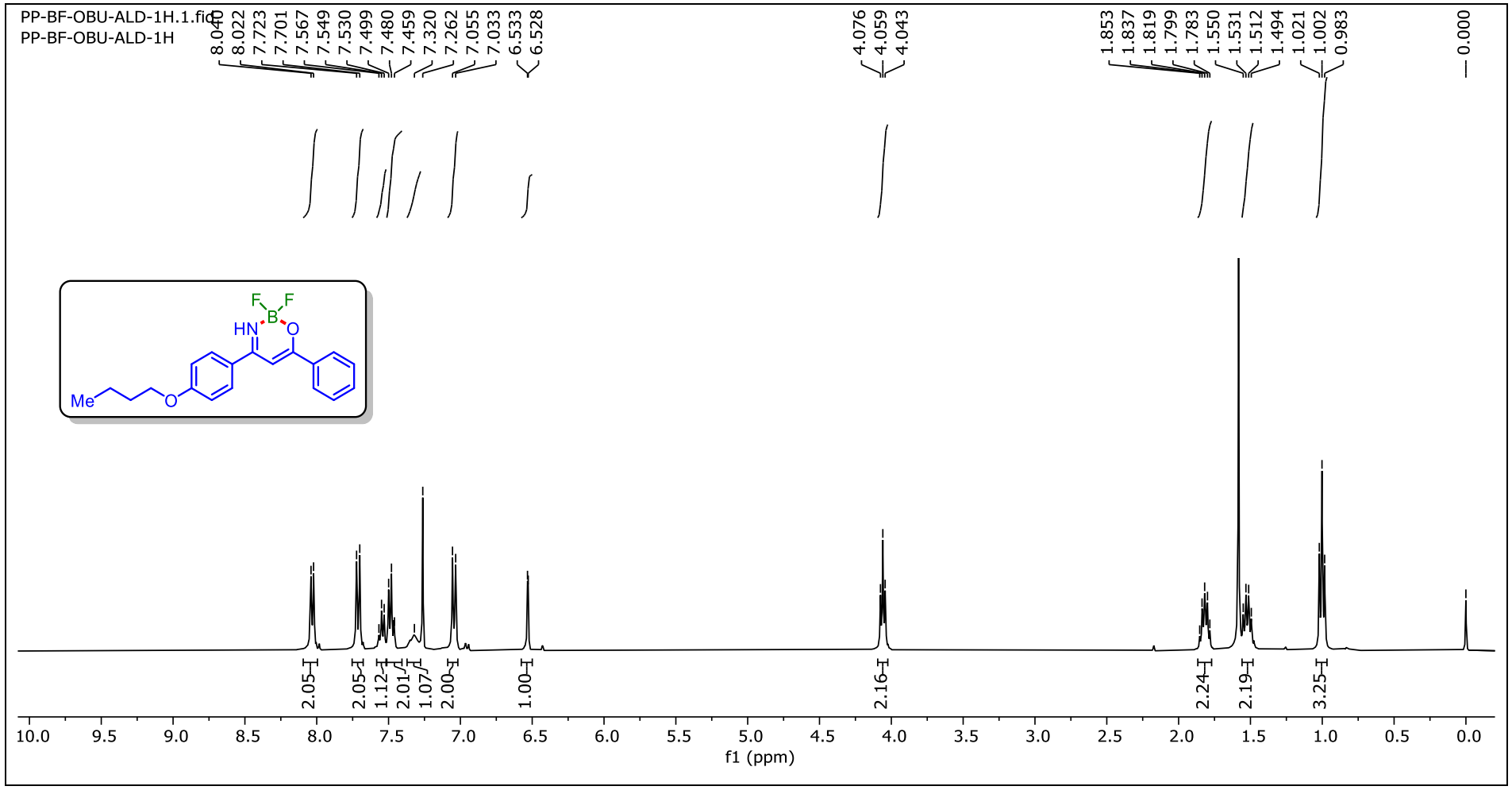
^{19}F NMR of **4-(4-(Tert-butyl)phenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2d)** ($CDCl_3$, 471 MHz)



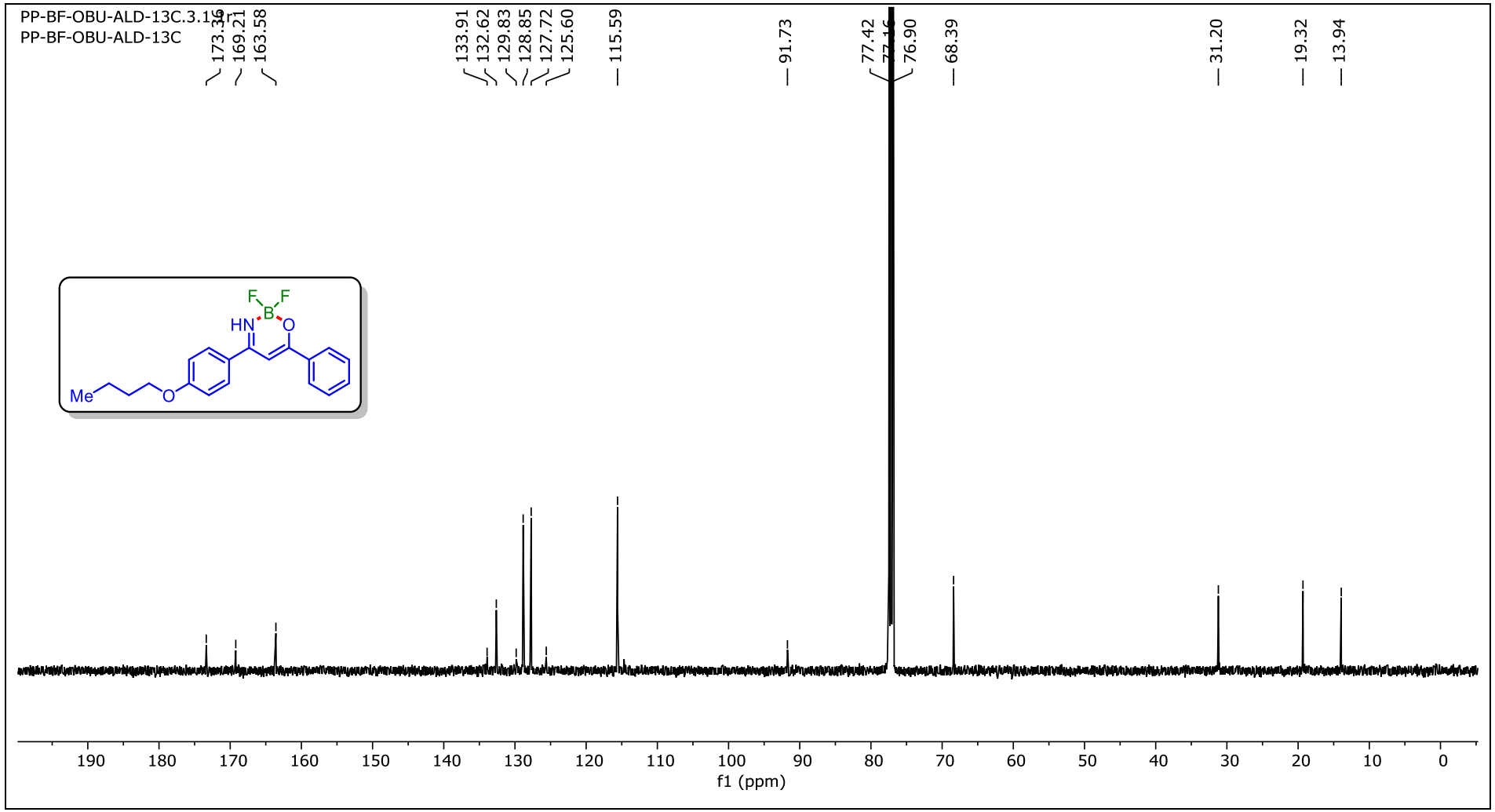
^{11}B NMR of **4-(4-(Tert-butyl)phenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2d)** ($CDCl_3$, 160 MHz)



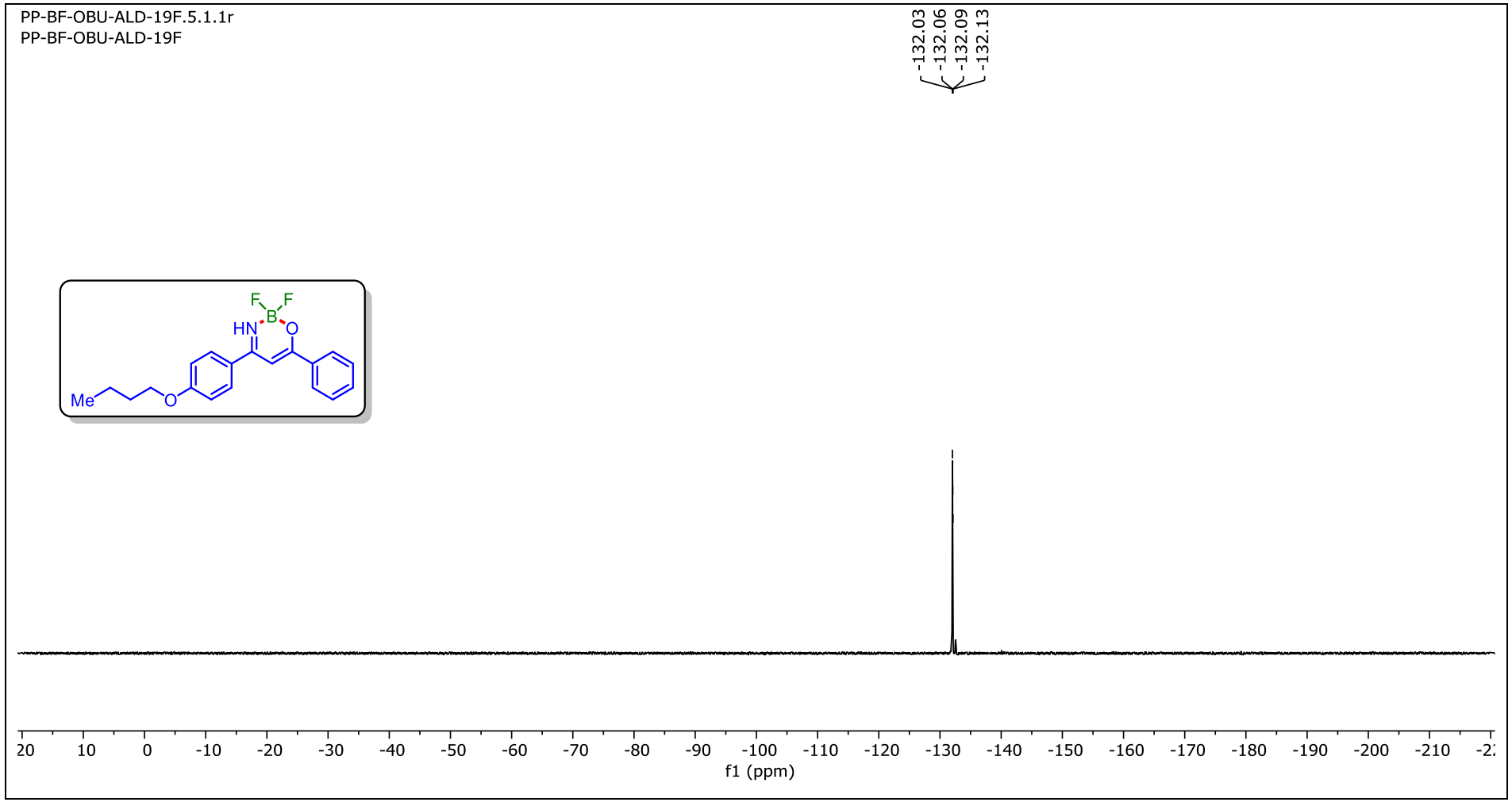
^{1}H NMR of **4-(4-Butoxyphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2e)** ($CDCl_3$, 400 MHz)



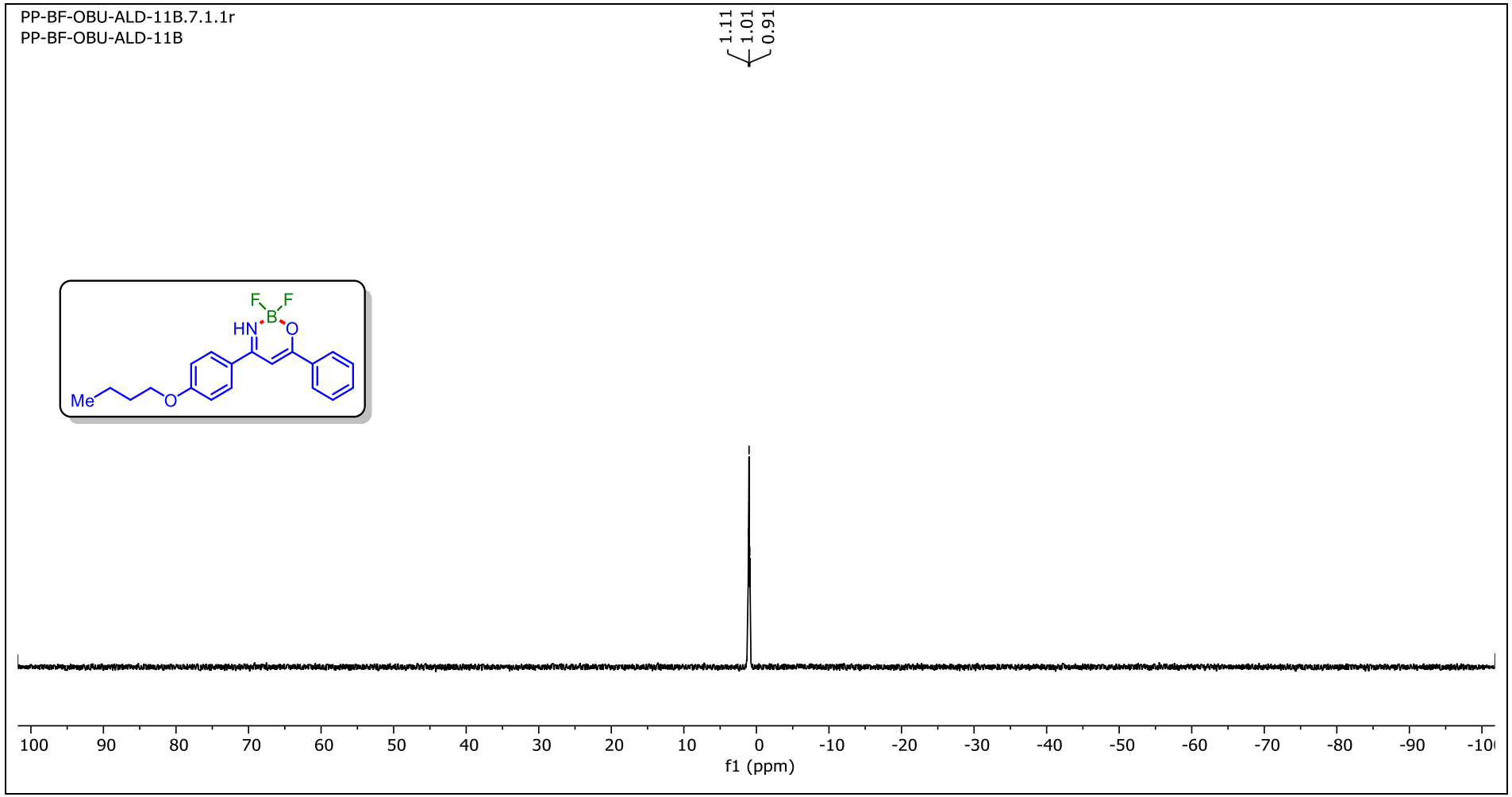
^{13}C {^{1}H} of **4-(4-Butoxyphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2e)** ($CDCl_3$, 126 MHz)



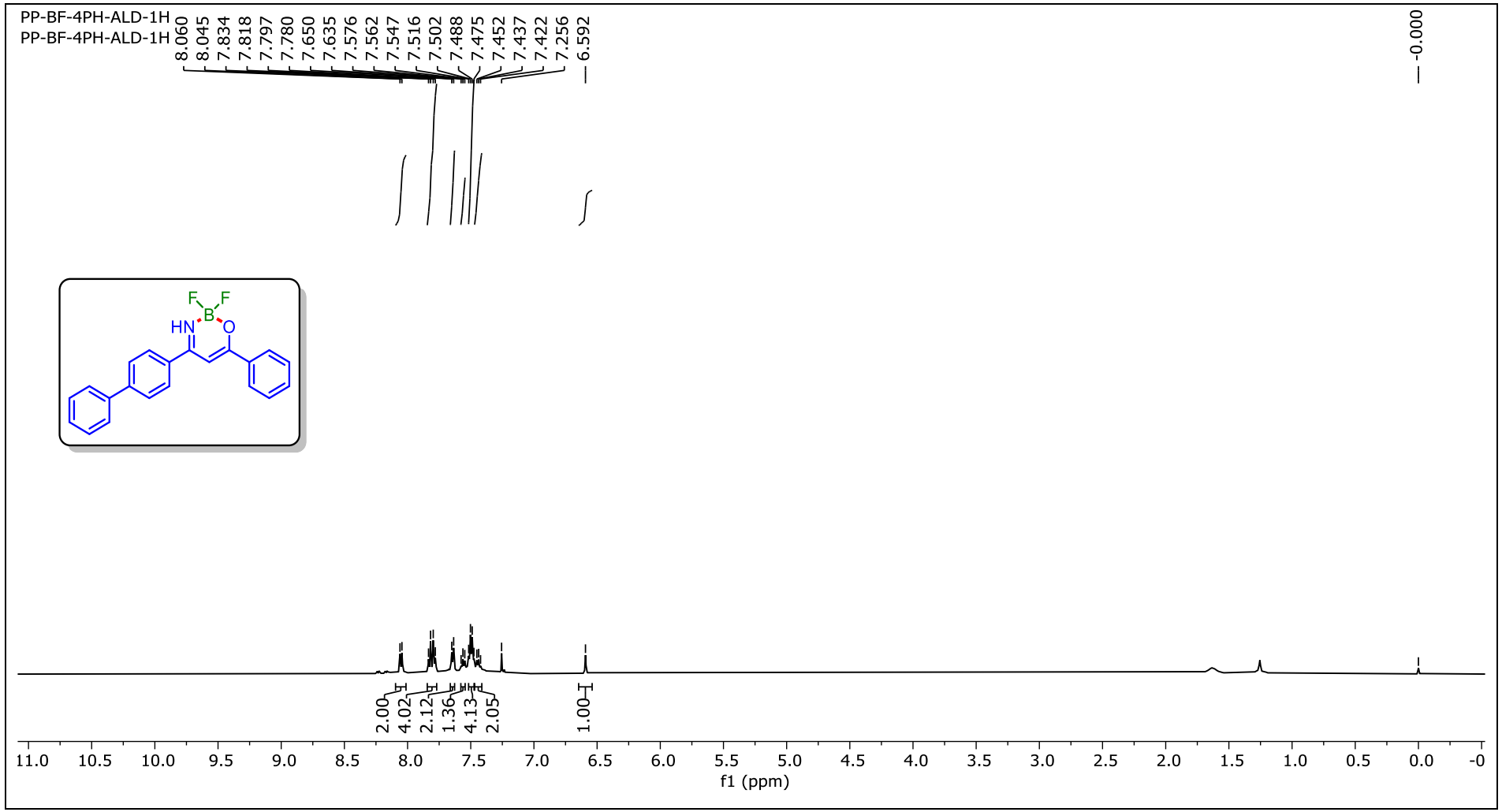
^{19}F NMR of **4-(4-Butoxyphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2e)** ($CDCl_3$, 471 MHz)



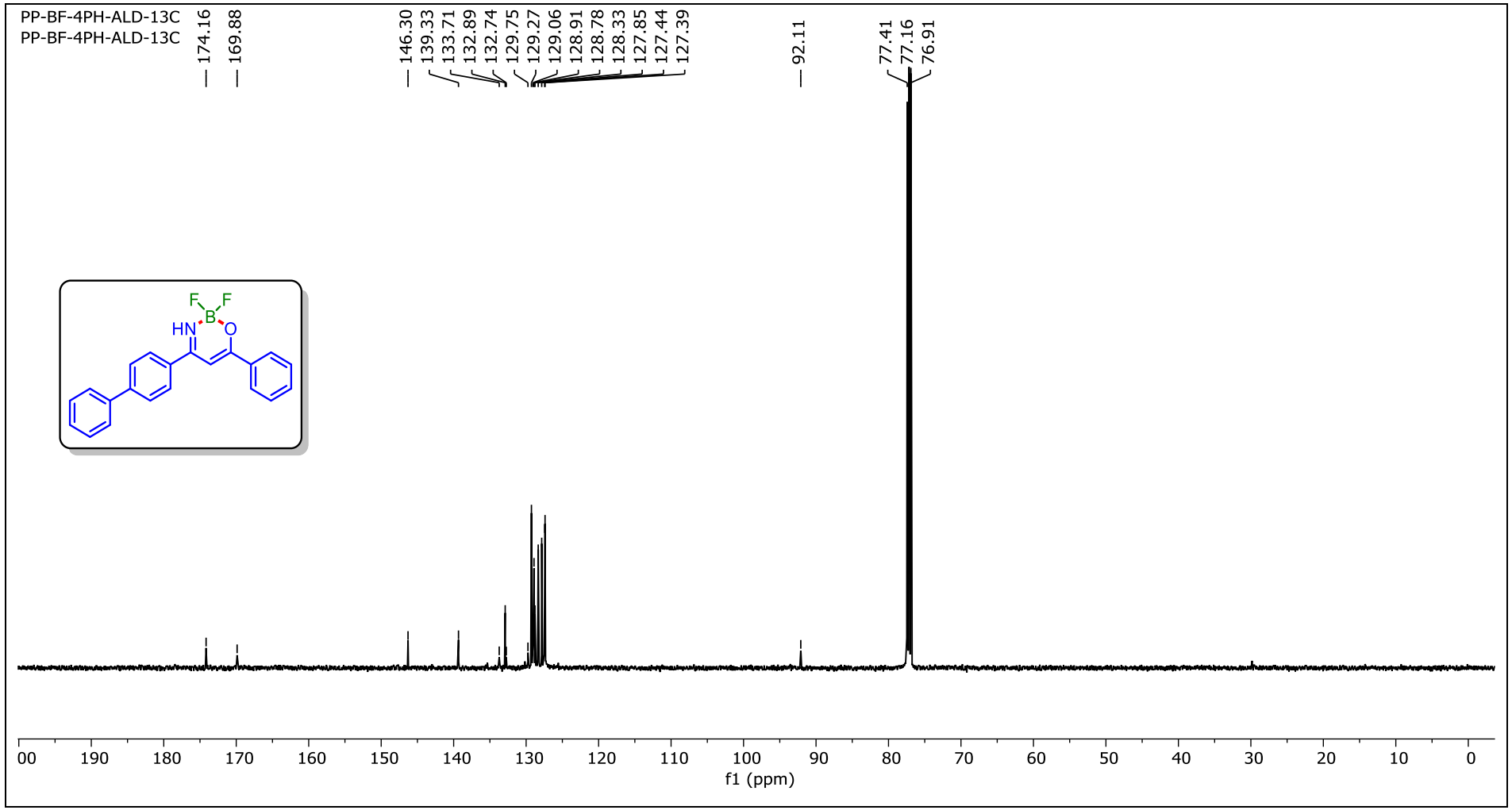
^{11}B NMR of **4-(4-Butoxyphenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2e)** ($CDCl_3$, 160 MHz)



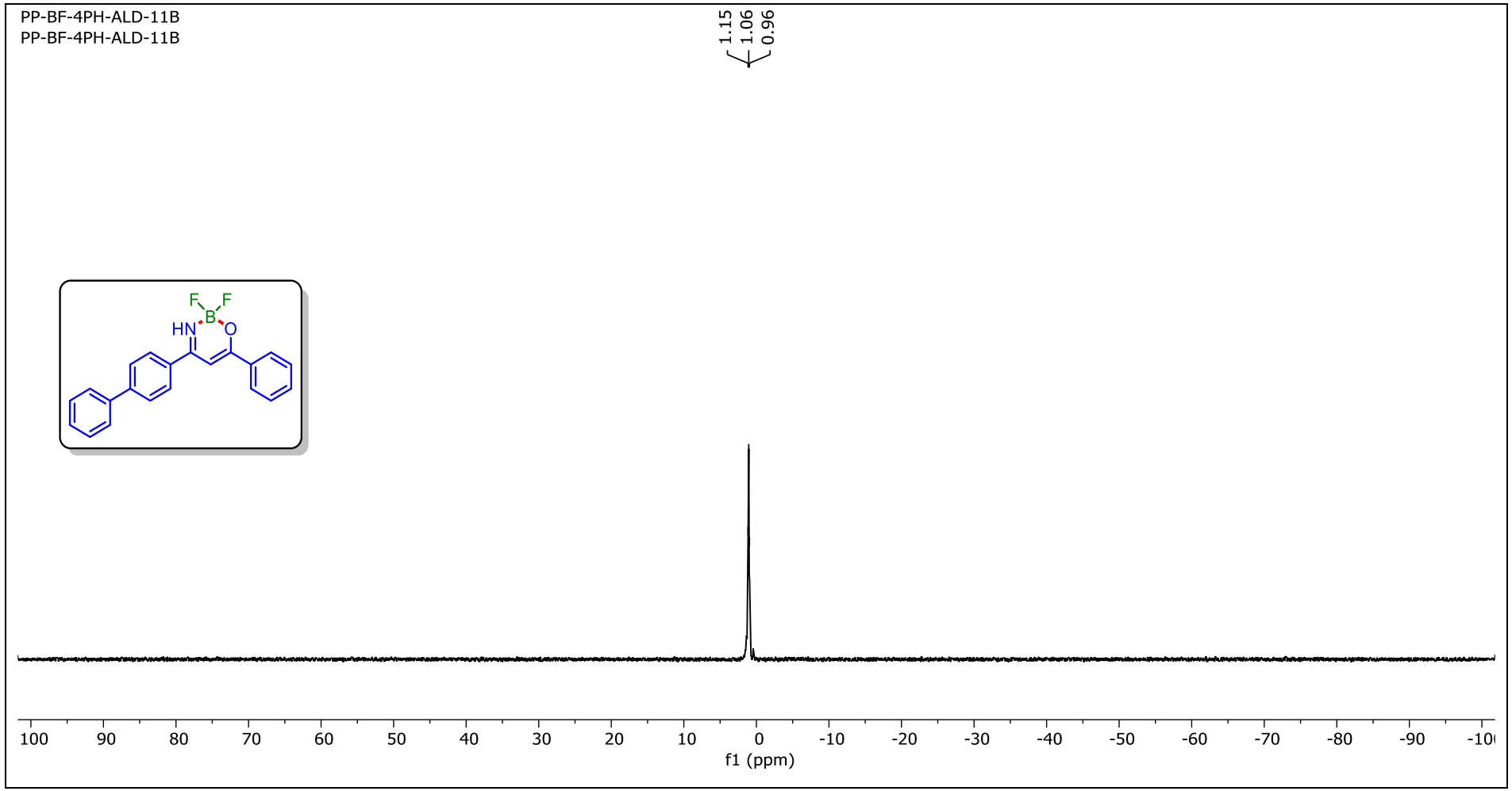
^{1}H NMR of **4-([1,1'-Biphenyl]-4-yl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2f)** ($CDCl_3$, 500 MHz)



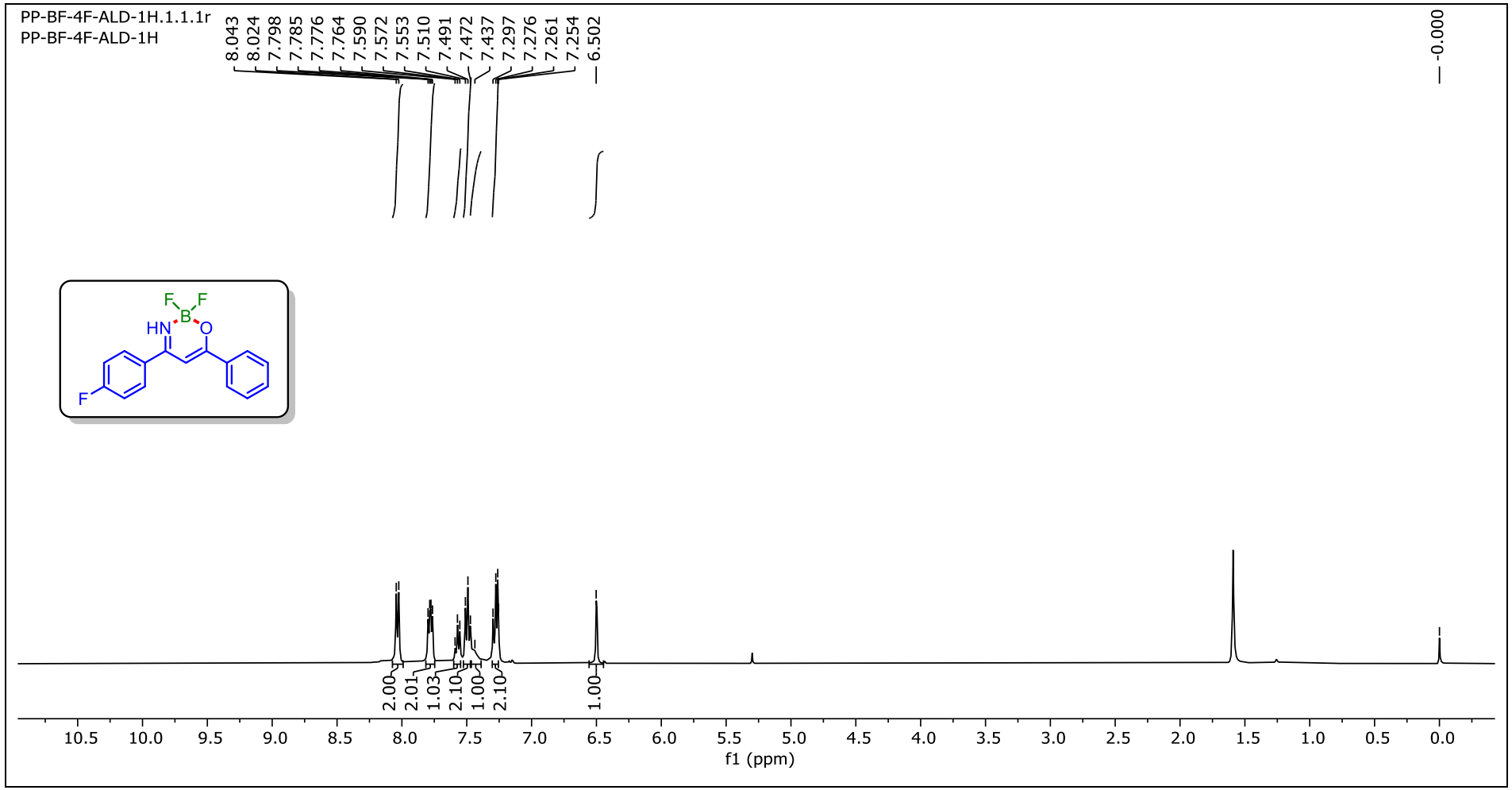
^{13}C {^{1}H} of **4-([1,1'-Biphenyl]-4-yl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2f)** ($CDCl_3$, 126 MHz)



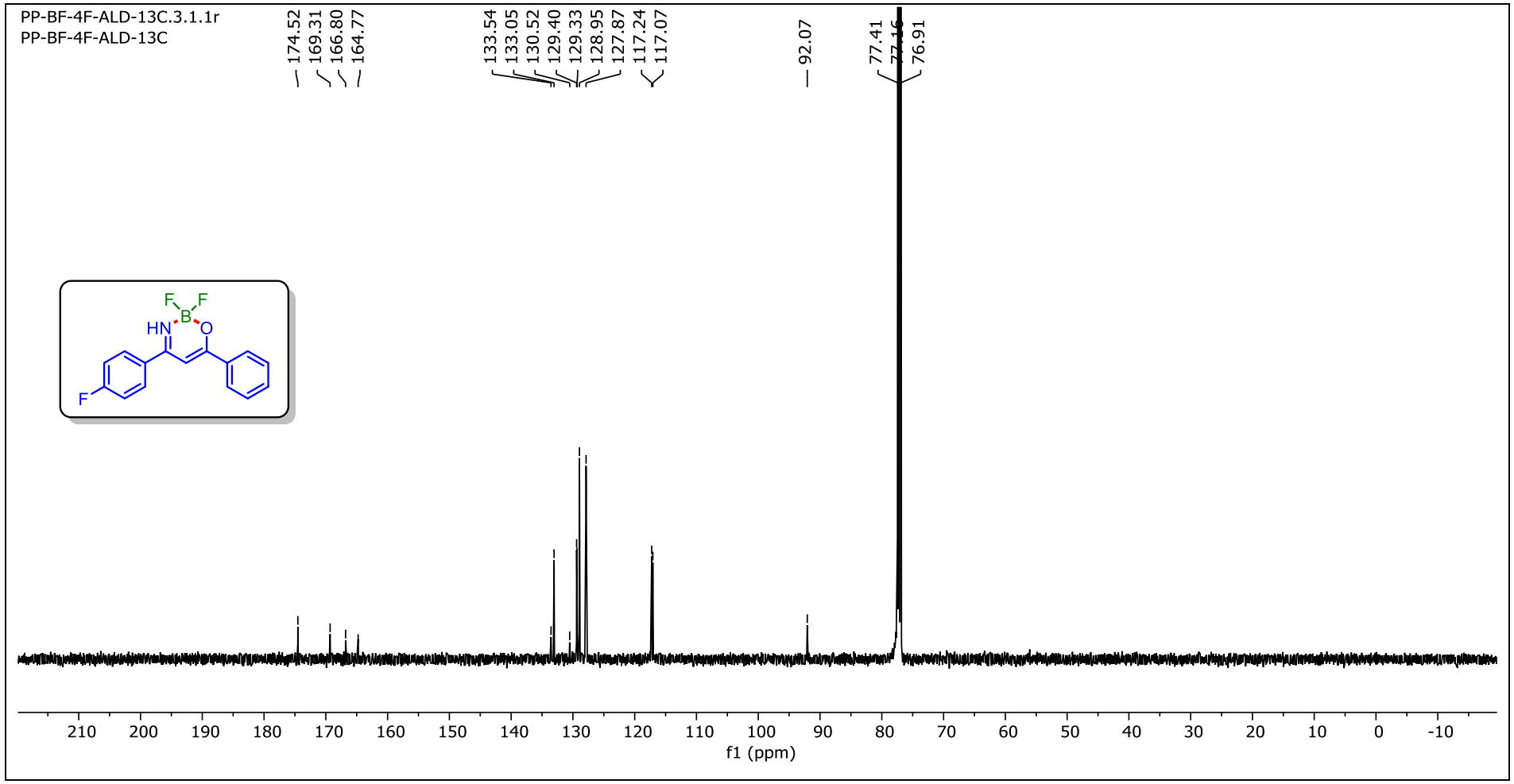
^{11}B NMR of **4-([1,1'-Biphenyl]-4-yl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2f)** ($CDCl_3$, 160 MHz)



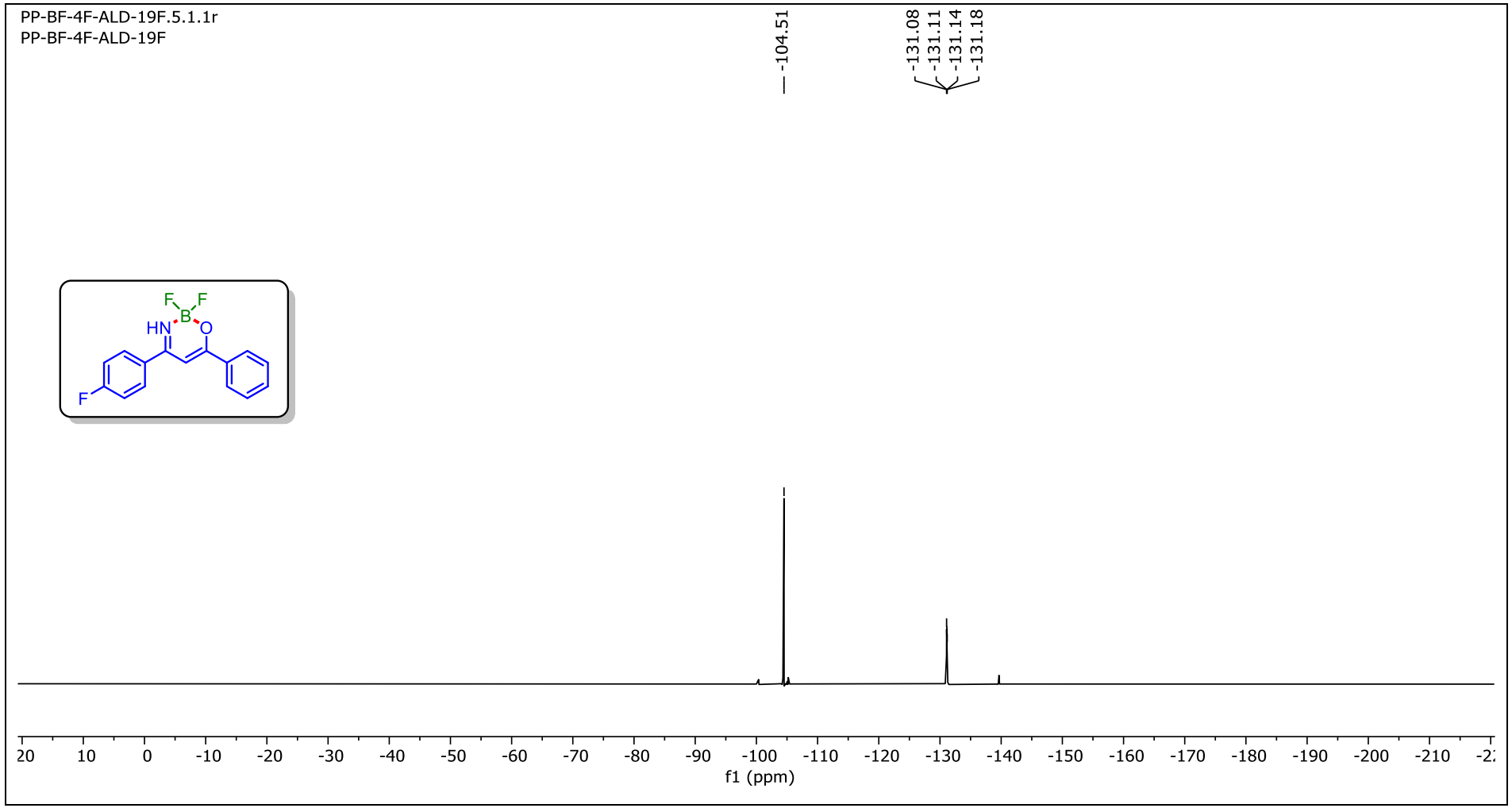
^{1}H NMR of **2,2-Difluoro-4-(4-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2g)** ($CDCl_3$, 400 MHz)



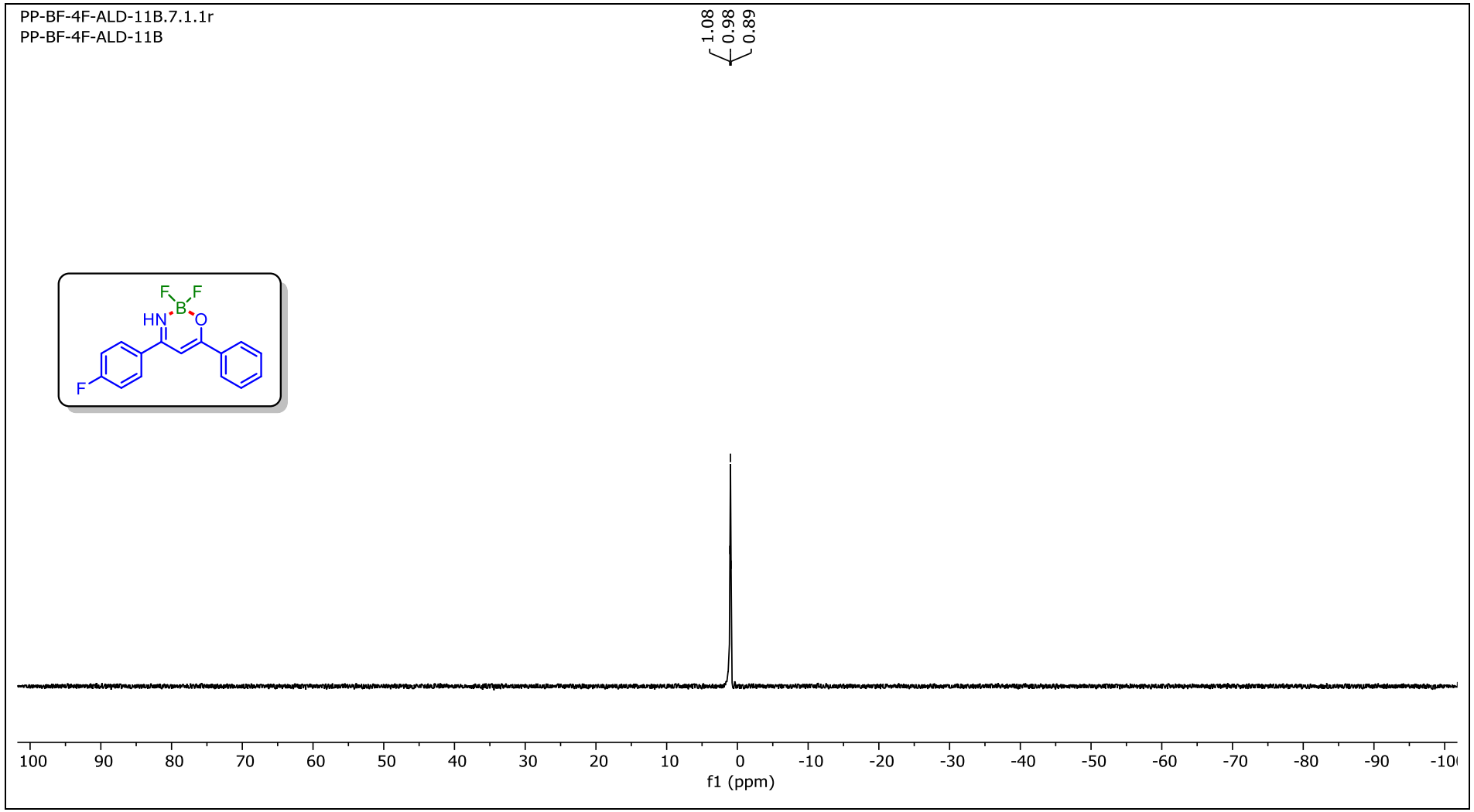
^{13}C {^{1}H} NMR of **2,2-Difluoro-4-(4-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2g)** ($CDCl_3$, 126 MHz)



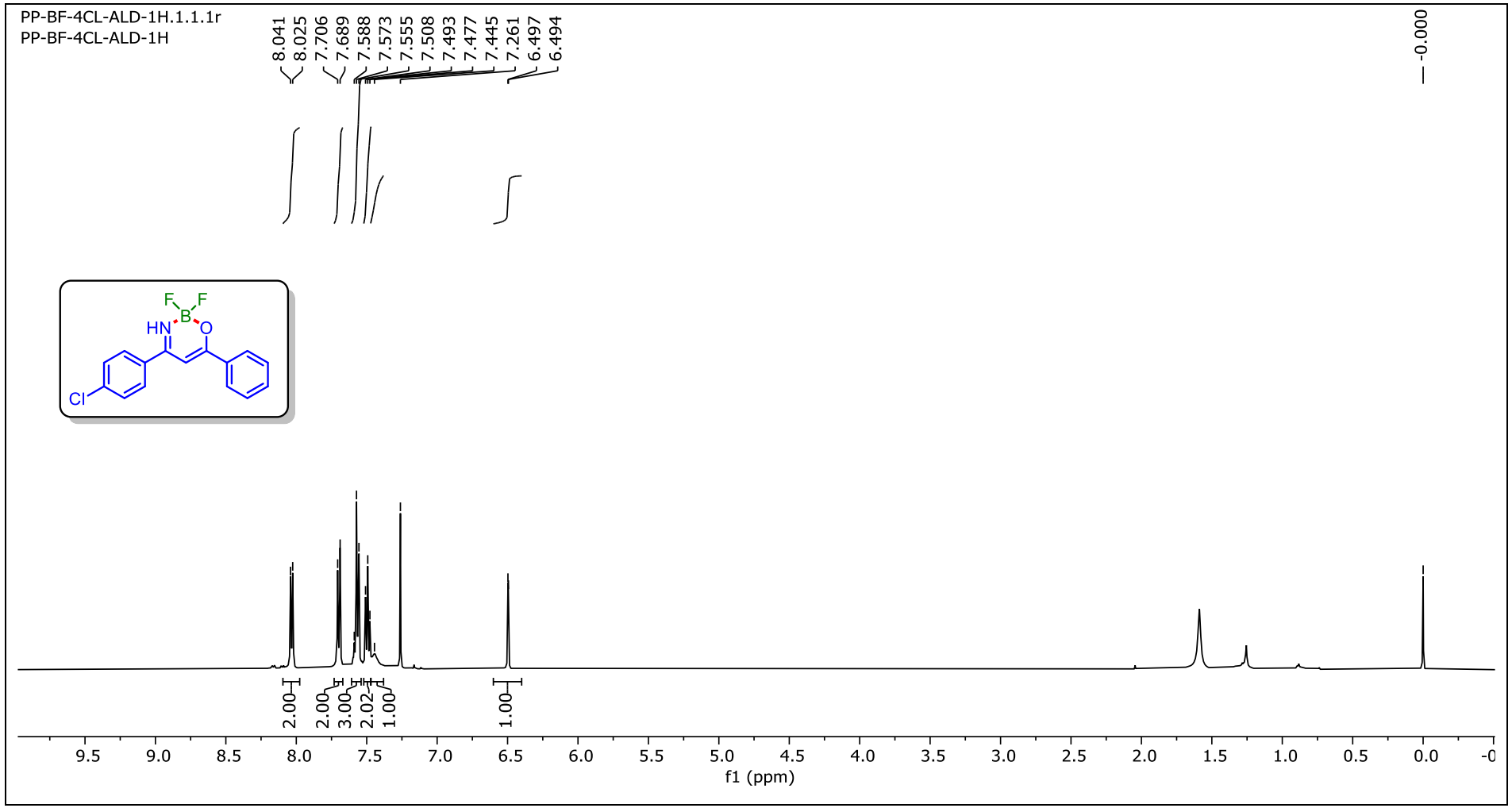
^{19}F NMR of **2,2-Difluoro-4-(4-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2g)** ($CDCl_3$, 471 MHz)



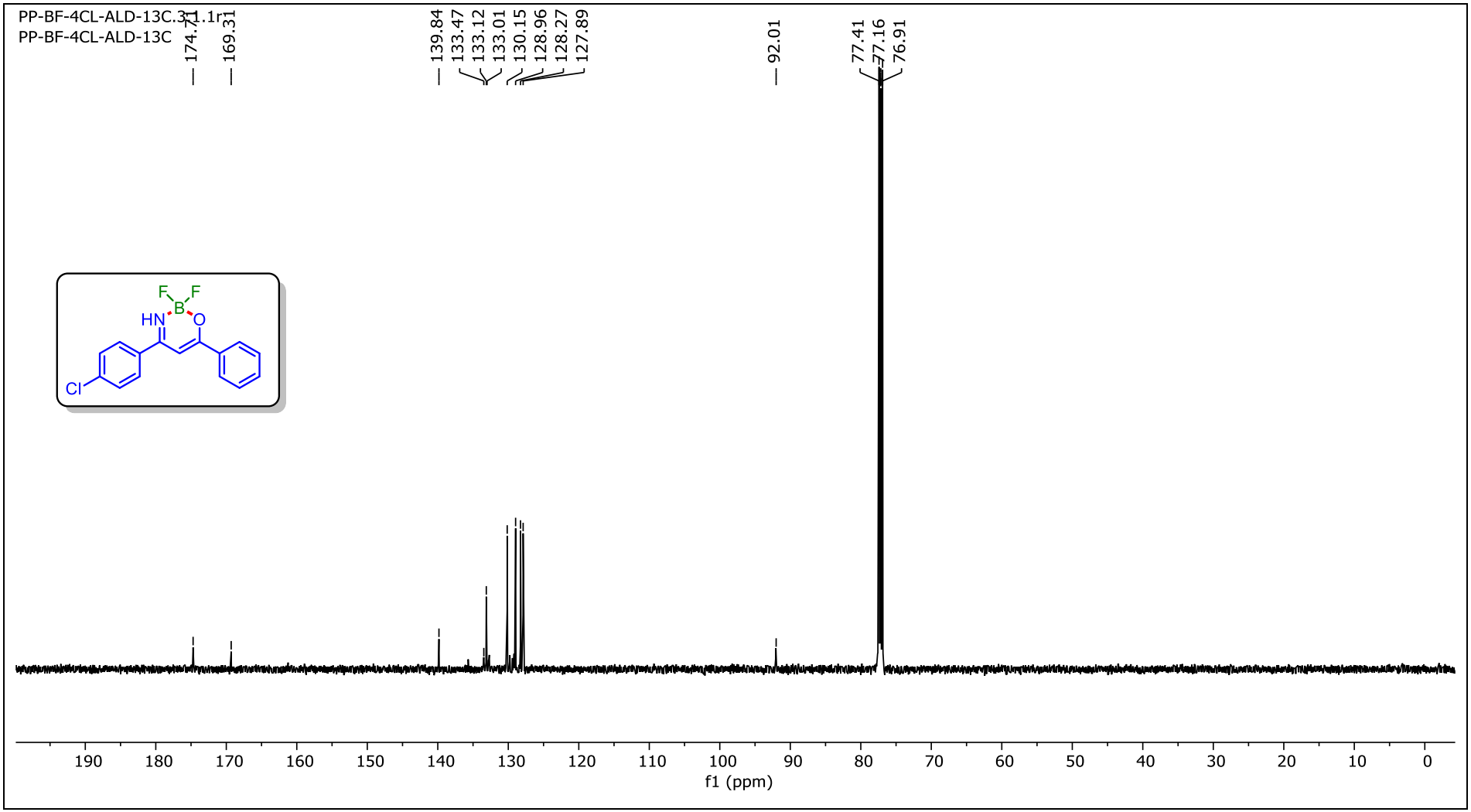
^{11}B NMR of **2,2-Difluoro-4-(4-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2g)** ($CDCl_3$, 160 MHz)



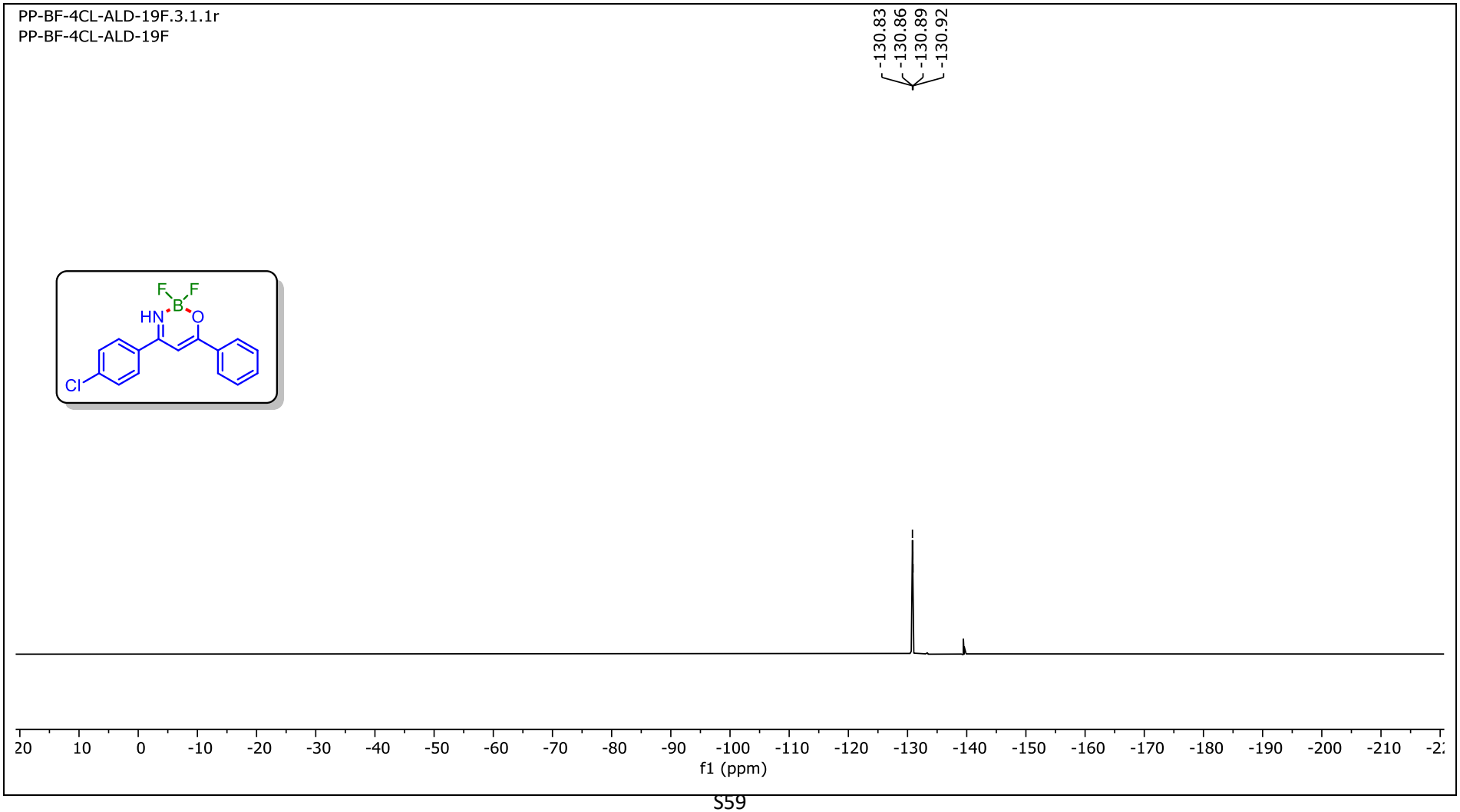
^{1}H NMR of **4-(4-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2h)** ($CDCl_3$, 500 MHz)



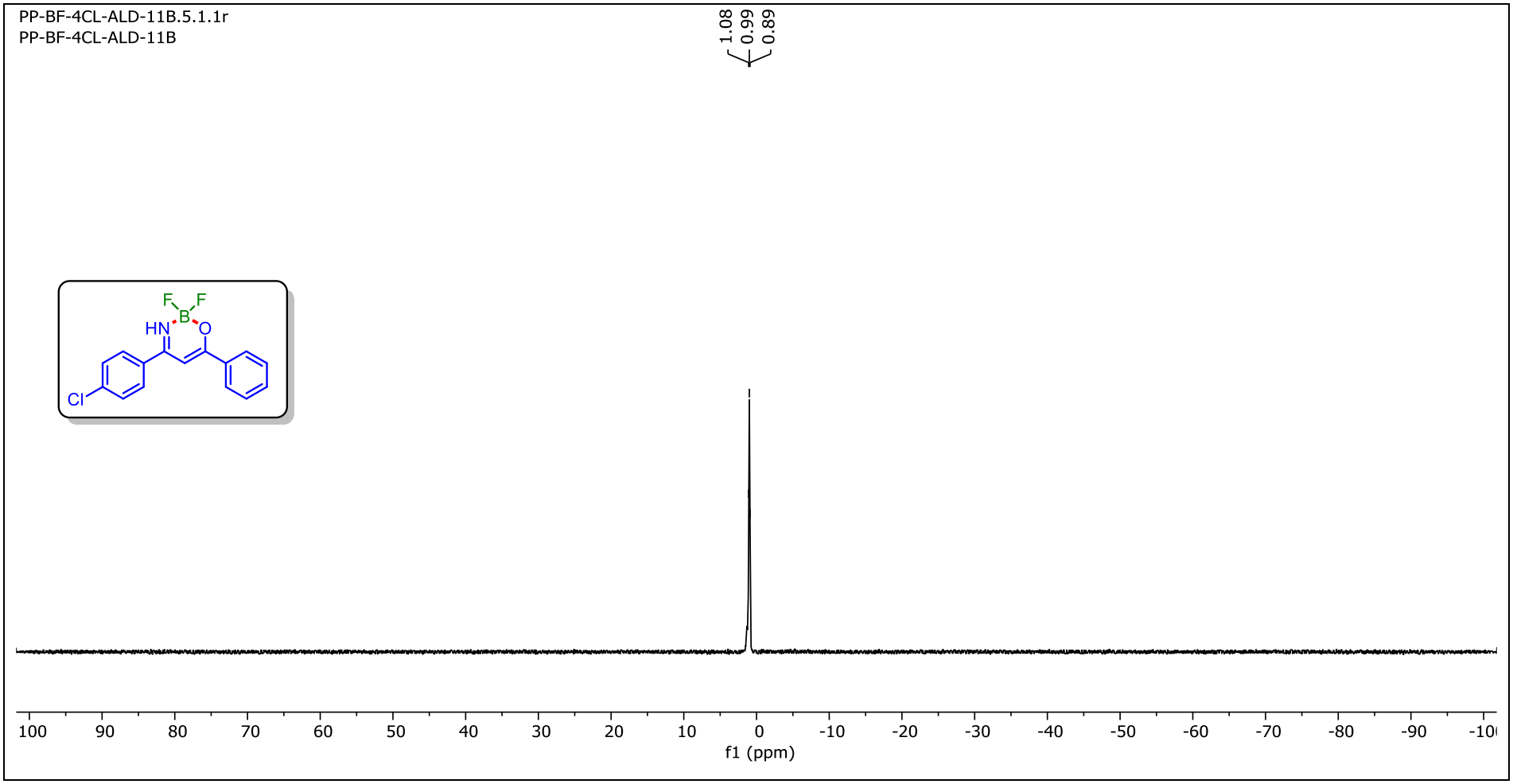
^{13}C {^{1}H} NMR of **4-(4-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2h)** ($CDCl_3$, 126 MHz)



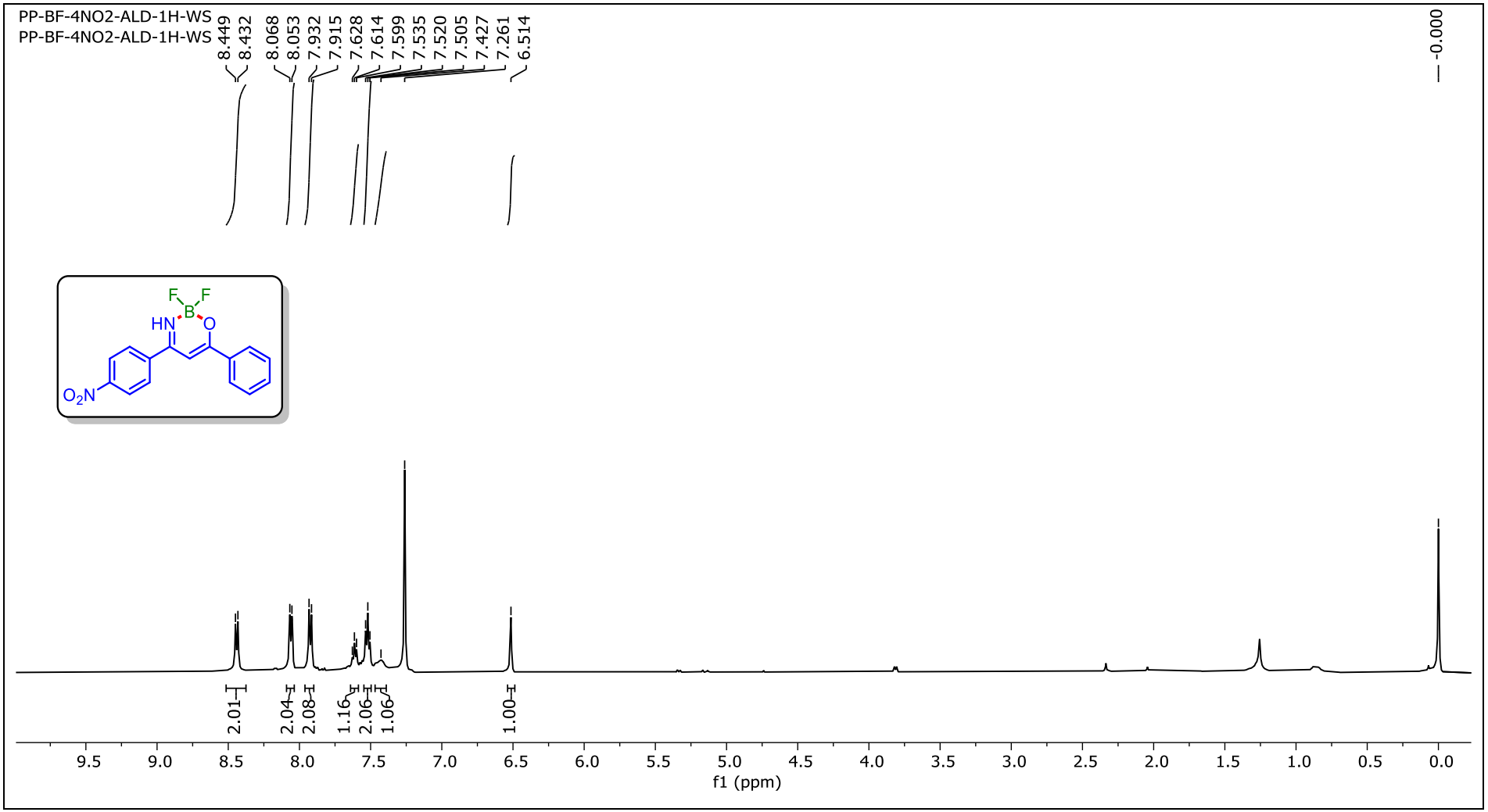
^{19}F NMR of **4-(4-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2h)** ($CDCl_3$, 471 MHz)



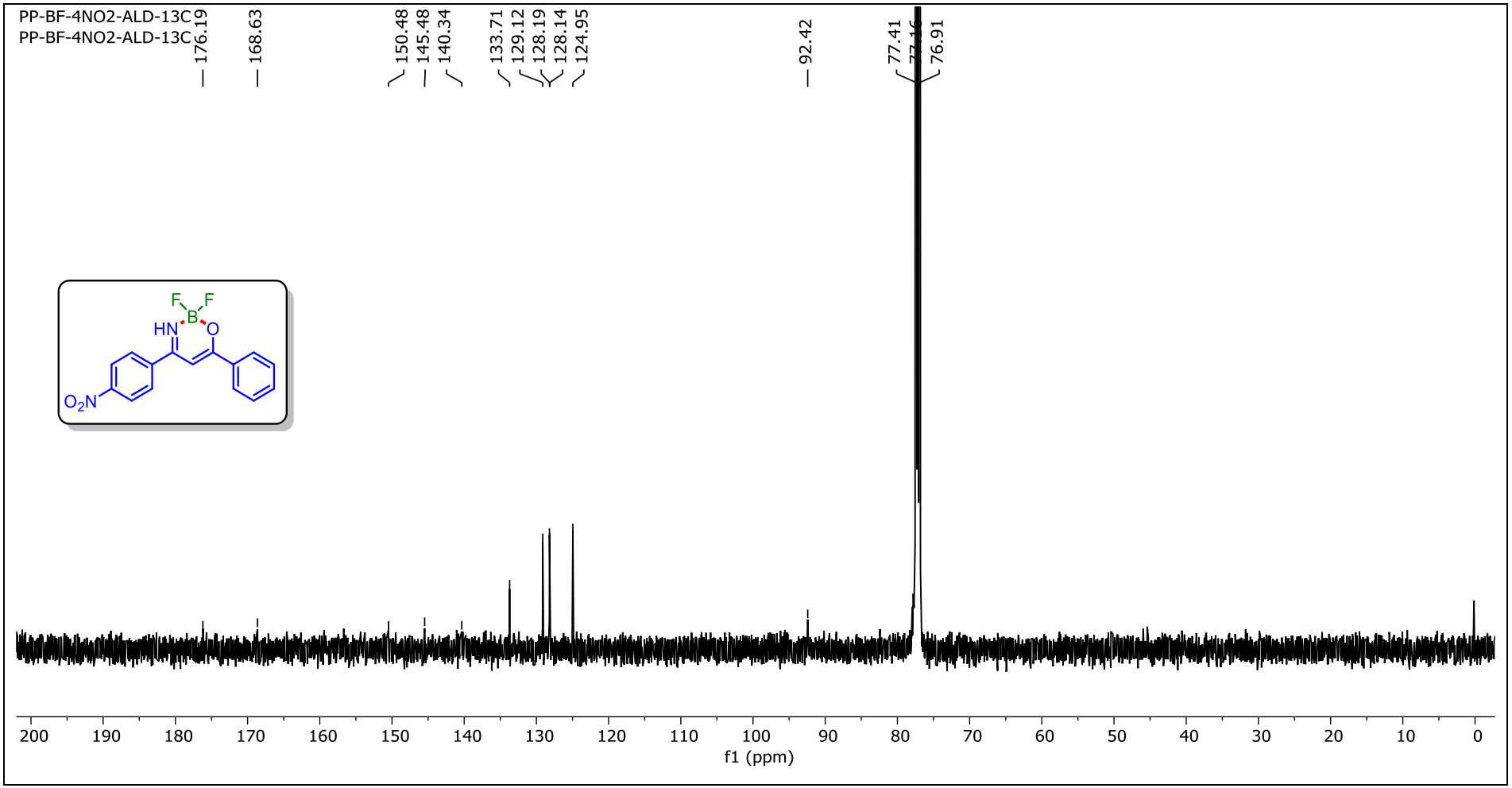
^{11}B NMR of **4-(4-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2h)** ($CDCl_3$, 160 MHz)



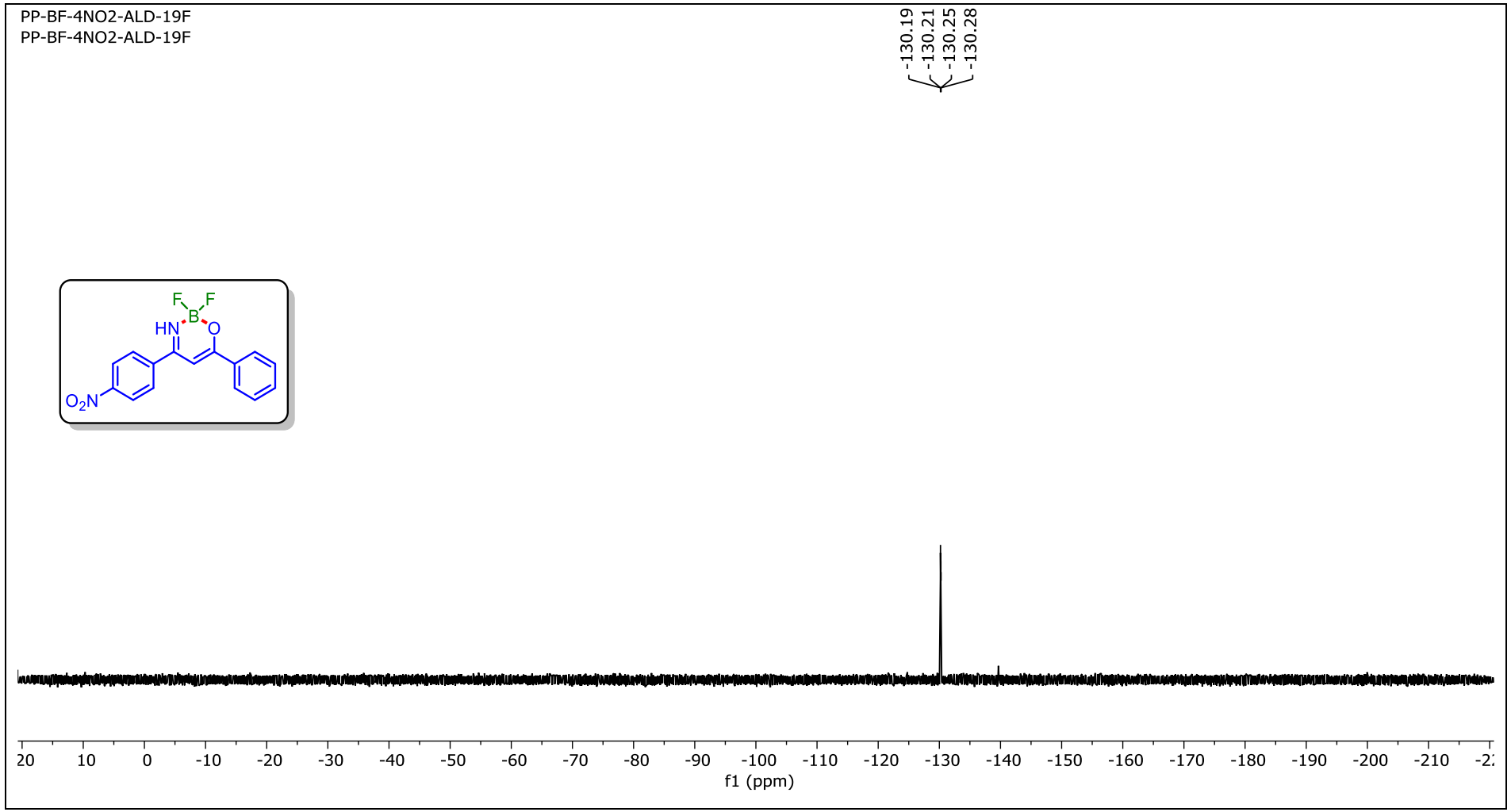
^{1}H NMR of **2,2-Difluoro-4-(4-nitrophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2i)** ($CDCl_3$, 500 MHz)



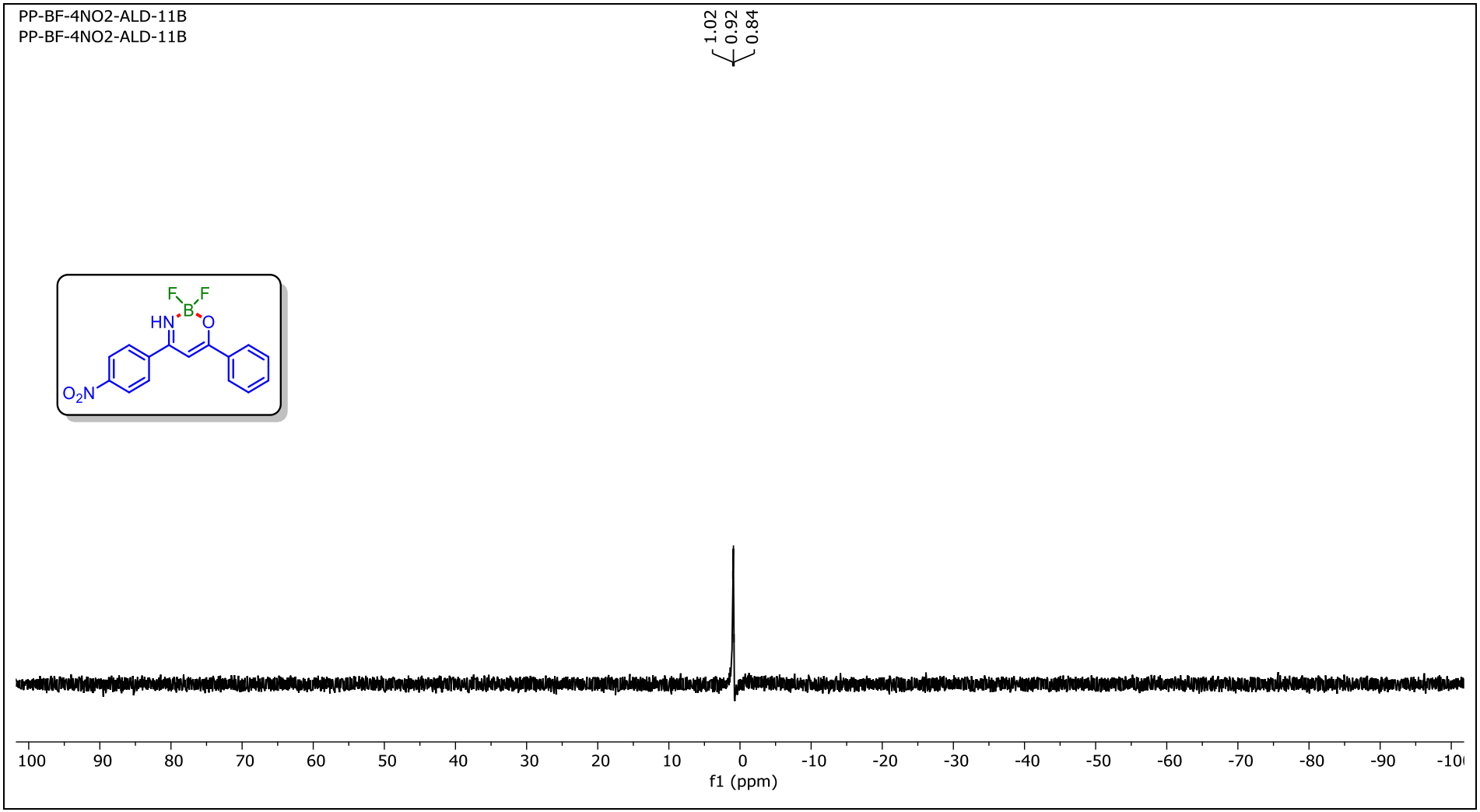
^{13}C {^{1}H} NMR of **2,2-Difluoro-4-(4-nitrophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2i)** ($CDCl_3$, 126 MHz)



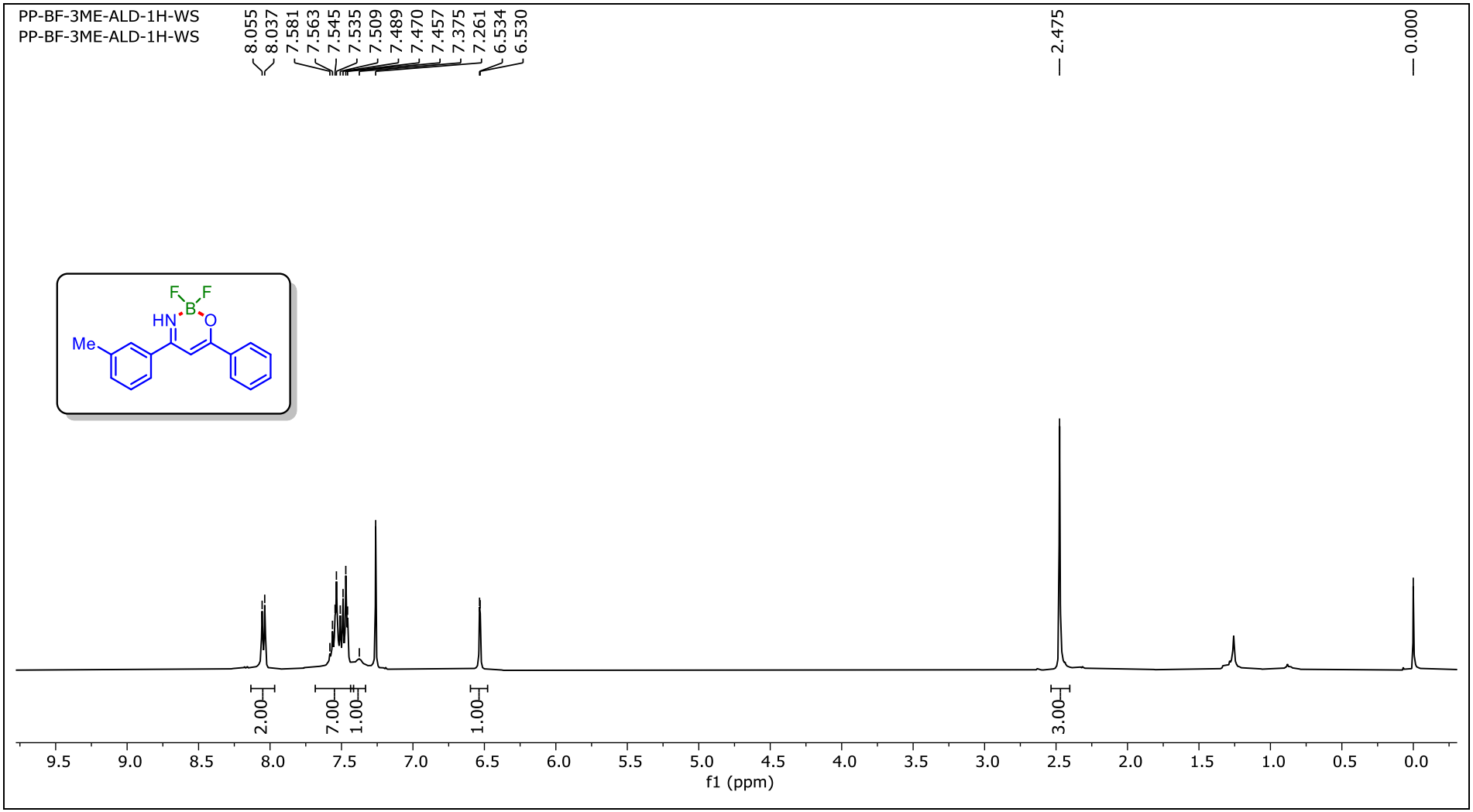
^{19}F NMR of **2,2-Difluoro-4-(4-nitrophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2i)** ($CDCl_3$, 471 MHz)



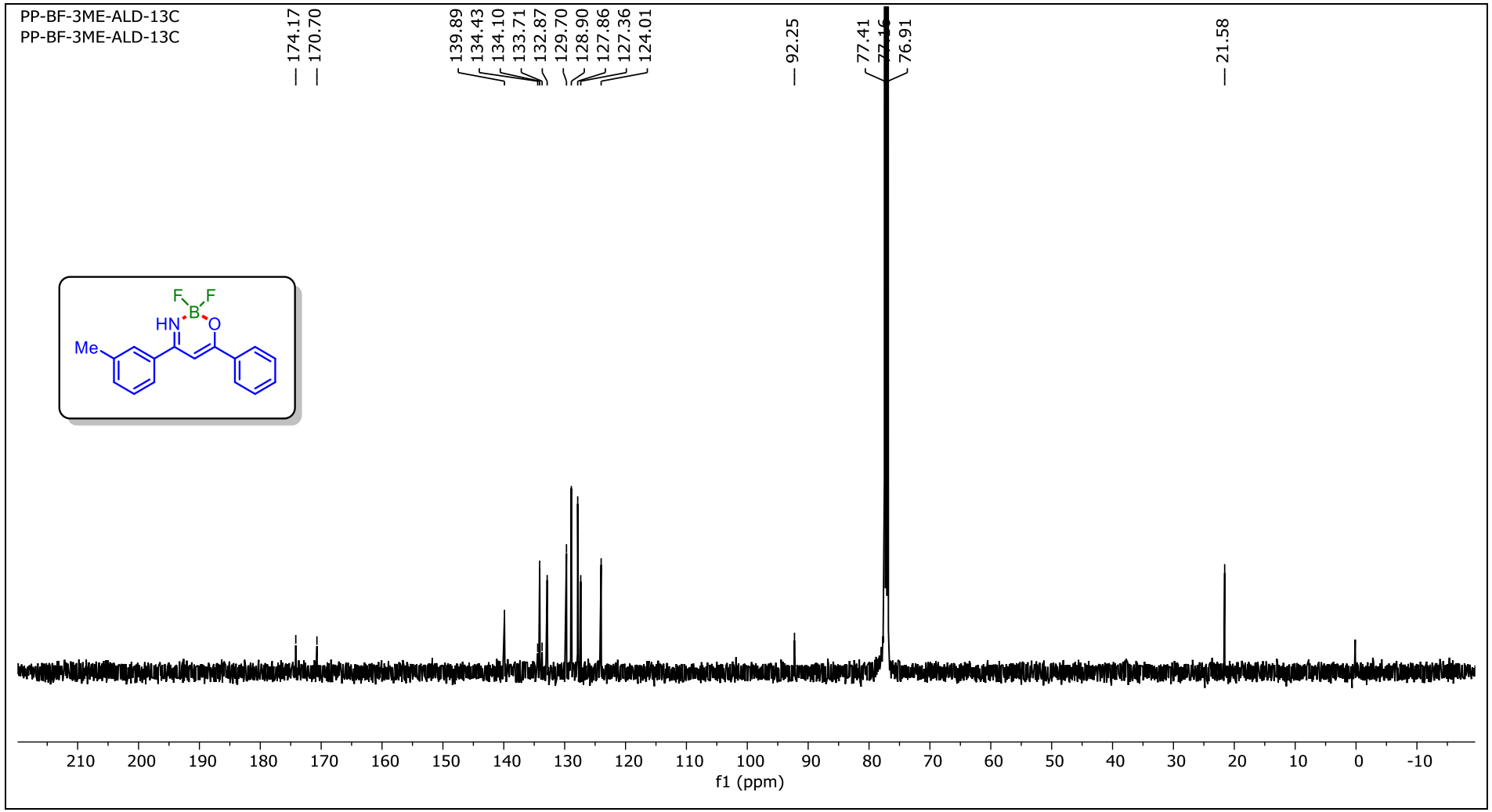
^{11}B NMR of **2,2-Difluoro-4-(4-nitrophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2i)** ($CDCl_3$, 160 MHz)



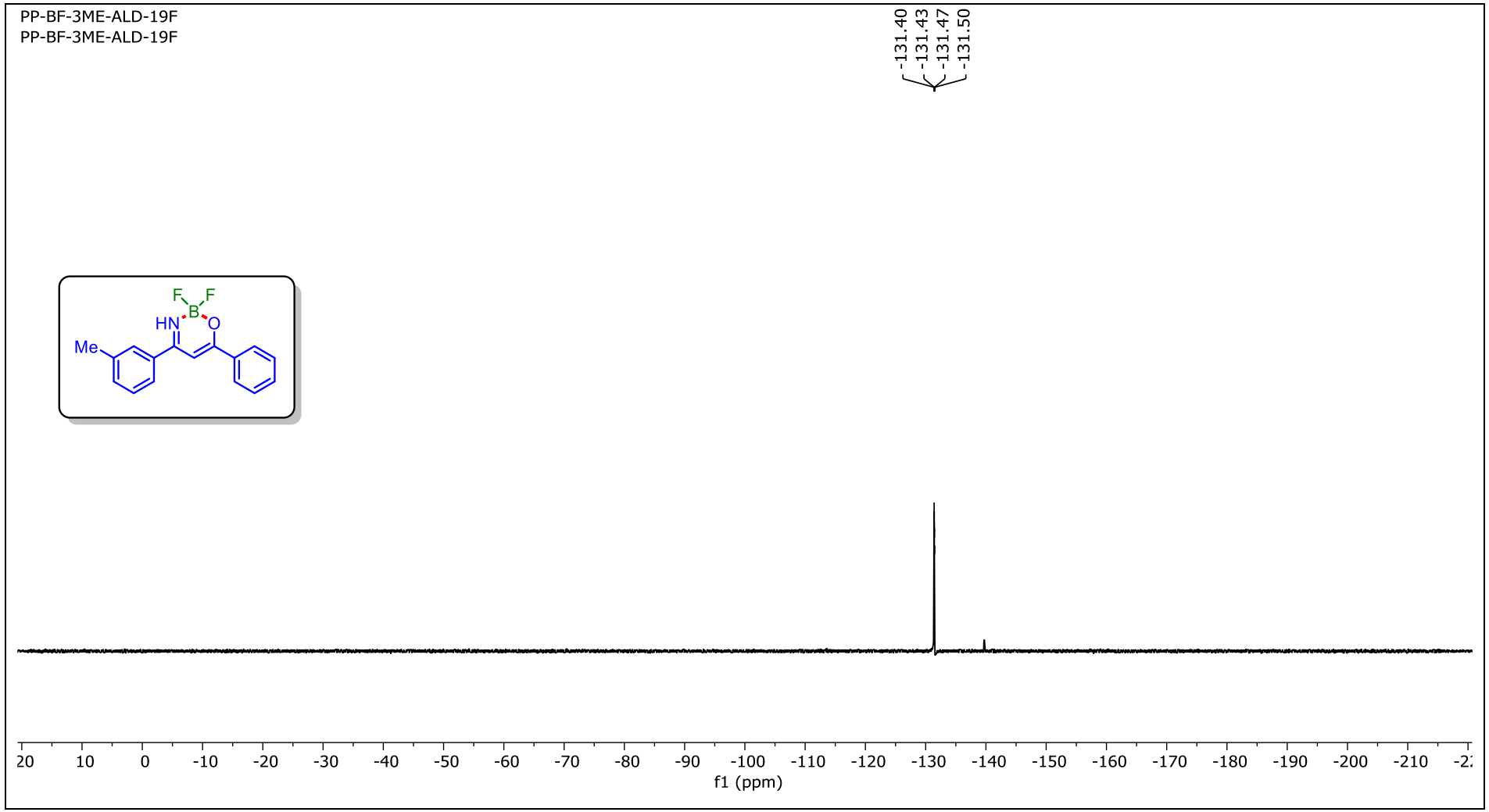
^{1}H NMR of **2,2-Difluoro-6-phenyl-4-(m-tolyl)-2*H*-1,3,2λ^{4}-oxazaborinine (2j)** ($CDCl_3$, 400 MHz)



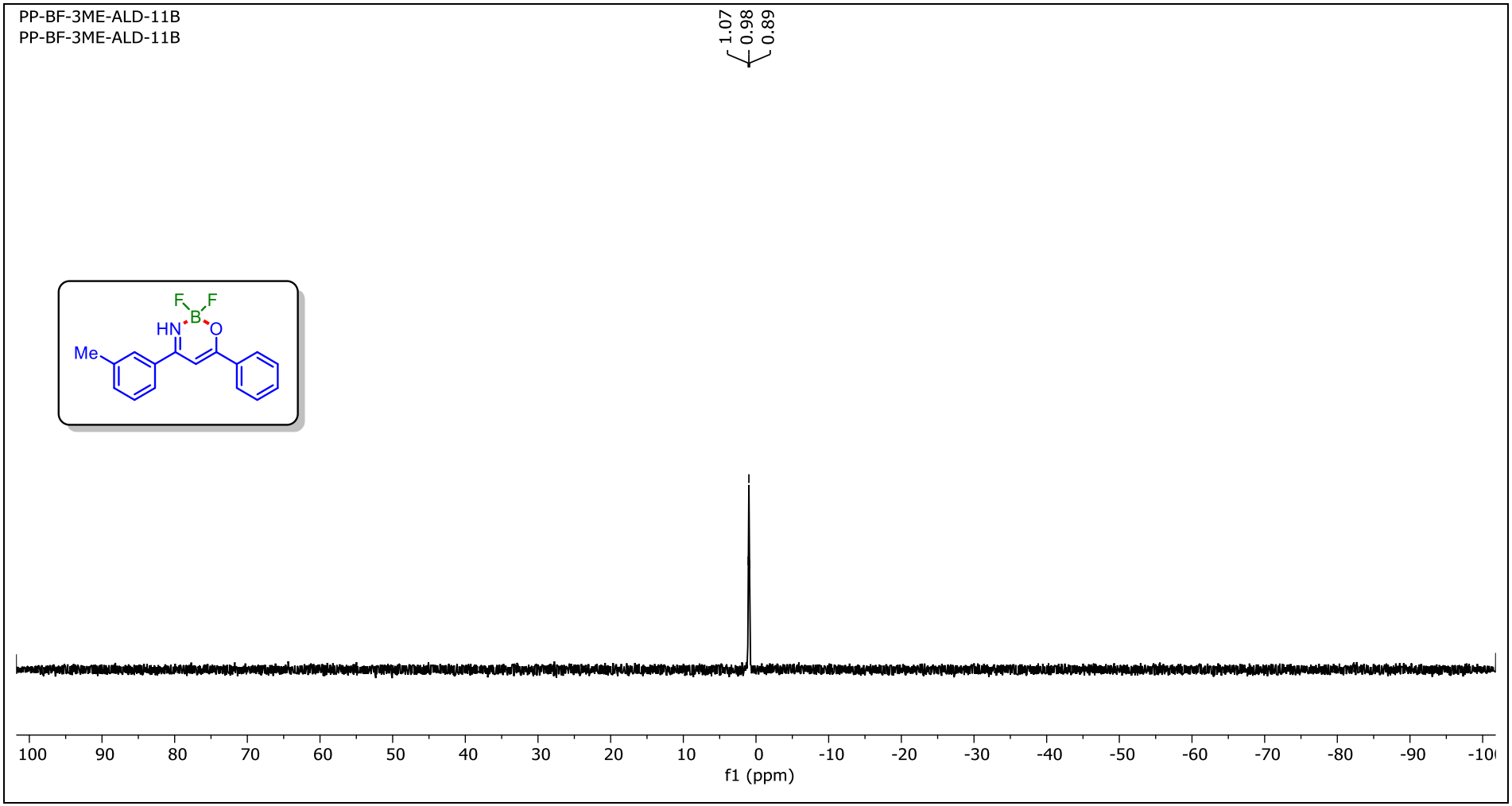
^{13}C {^{1}H} NMR of **2,2-Difluoro-6-phenyl-4-(m-tolyl)-2*H*-1,3,2λ^{4}-oxazaborinine (2j)** ($CDCl_3$, 126 MHz)



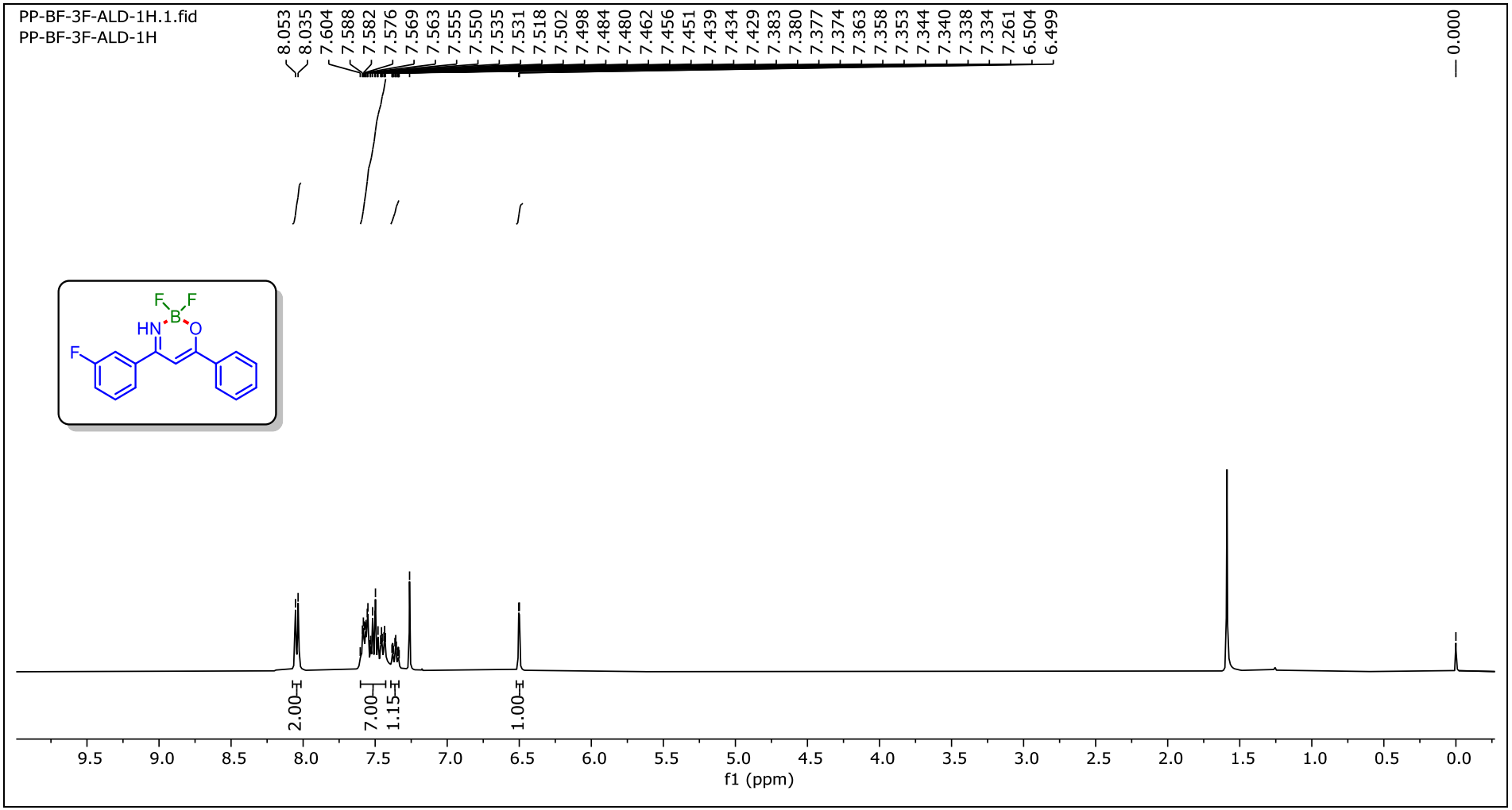
^{19}F NMR of **2,2-Difluoro-6-phenyl-4-(m-tolyl)-2*H*-1,3,2λ^4-oxazaborinine (2j)** ($CDCl_3$, 471 MHz)



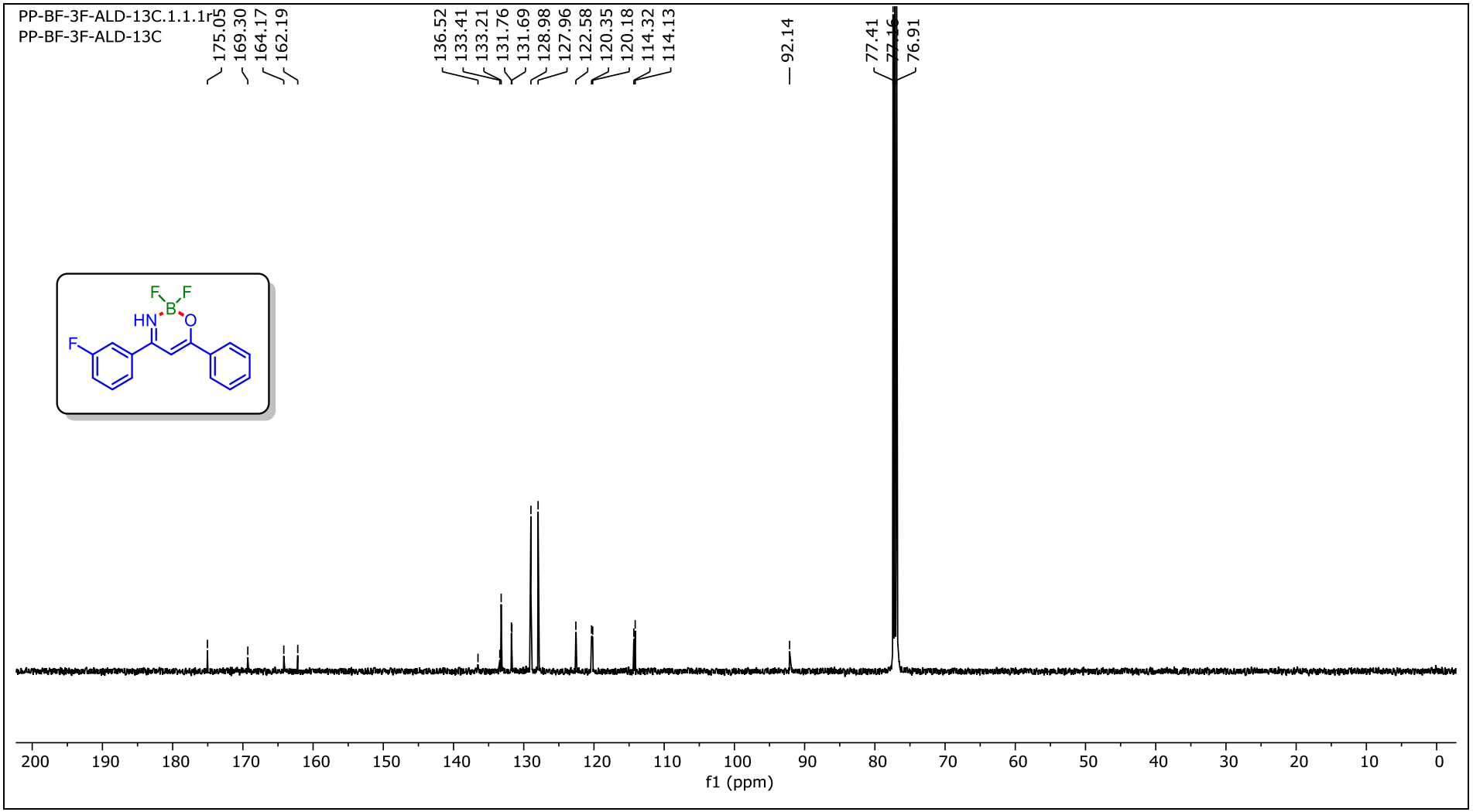
^{11}B NMR of **2,2-Difluoro-6-phenyl-4-(m-tolyl)-2*H*-1,3,2λ^4-oxazaborinine (2j)** ($CDCl_3$, 160 MHz)



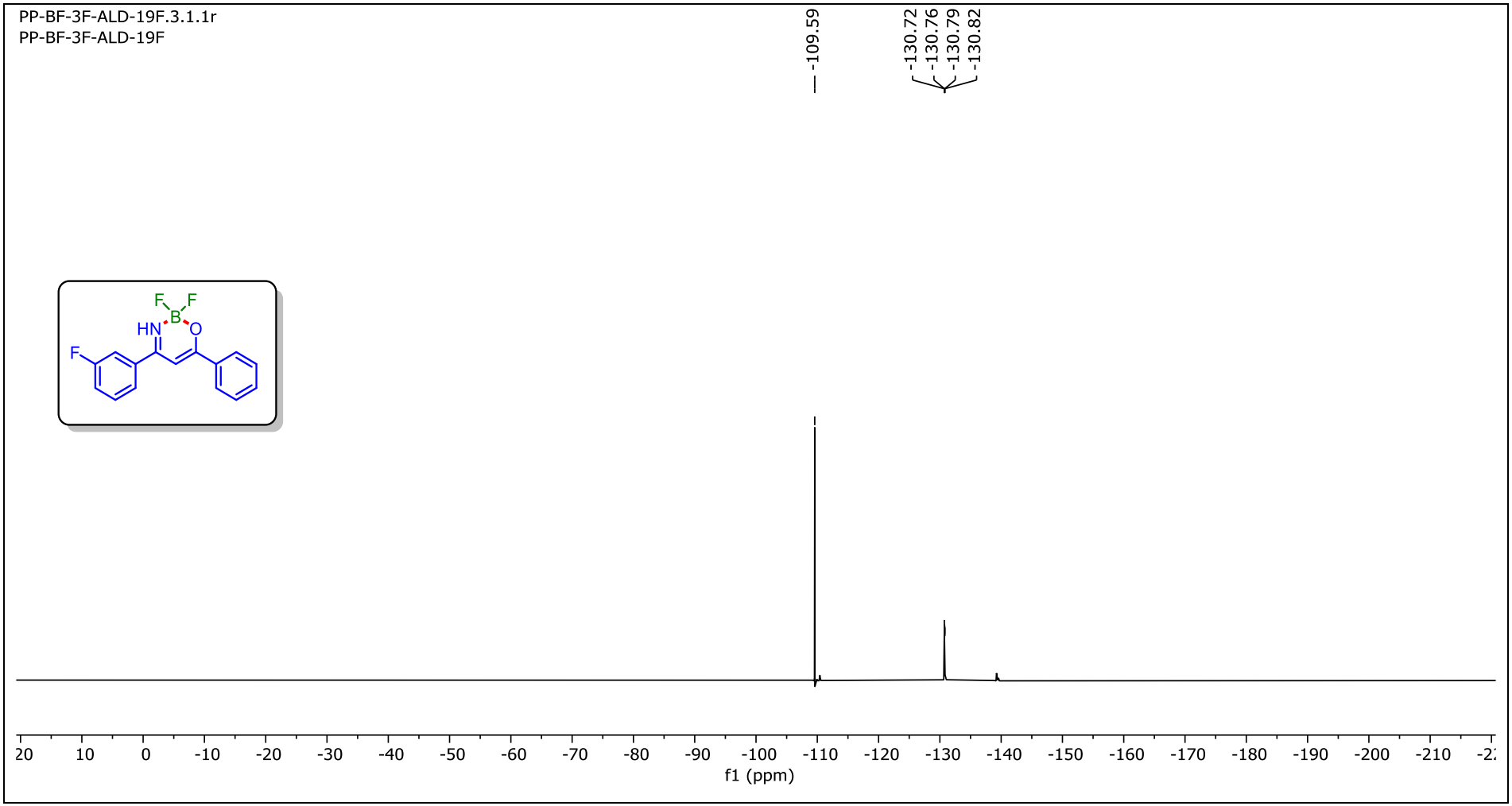
^{1}H NMR of **2,2-Difluoro-4-(3-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2k)** ($CDCl_3$, 400 MHz)



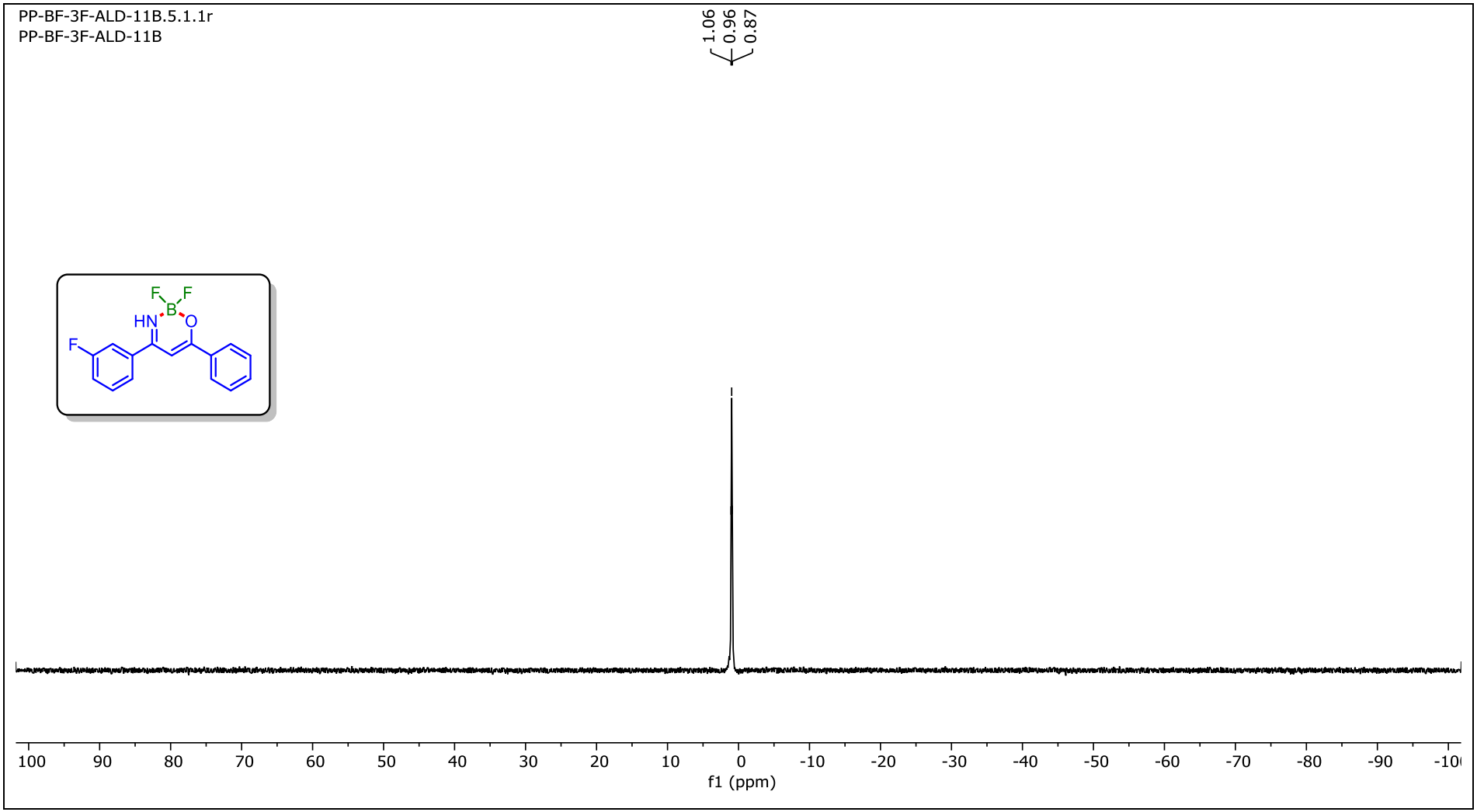
^{13}C {^{1}H} NMR of **2,2-Difluoro-4-(3-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2k)** ($CDCl_3$, 126 MHz)



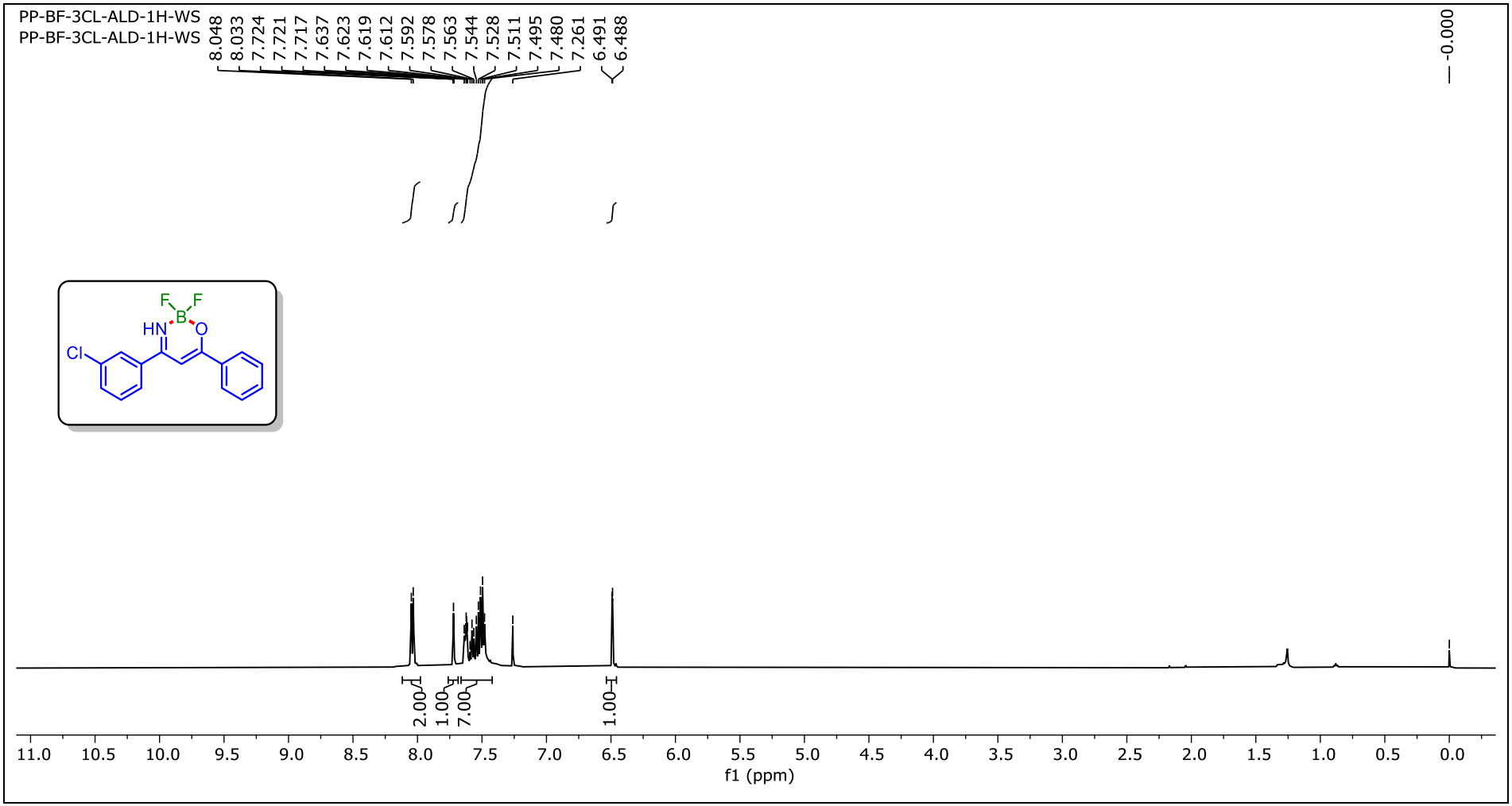
^{19}F NMR of **2,2-Difluoro-4-(3-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2k)** ($CDCl_3$, 471 MHz)



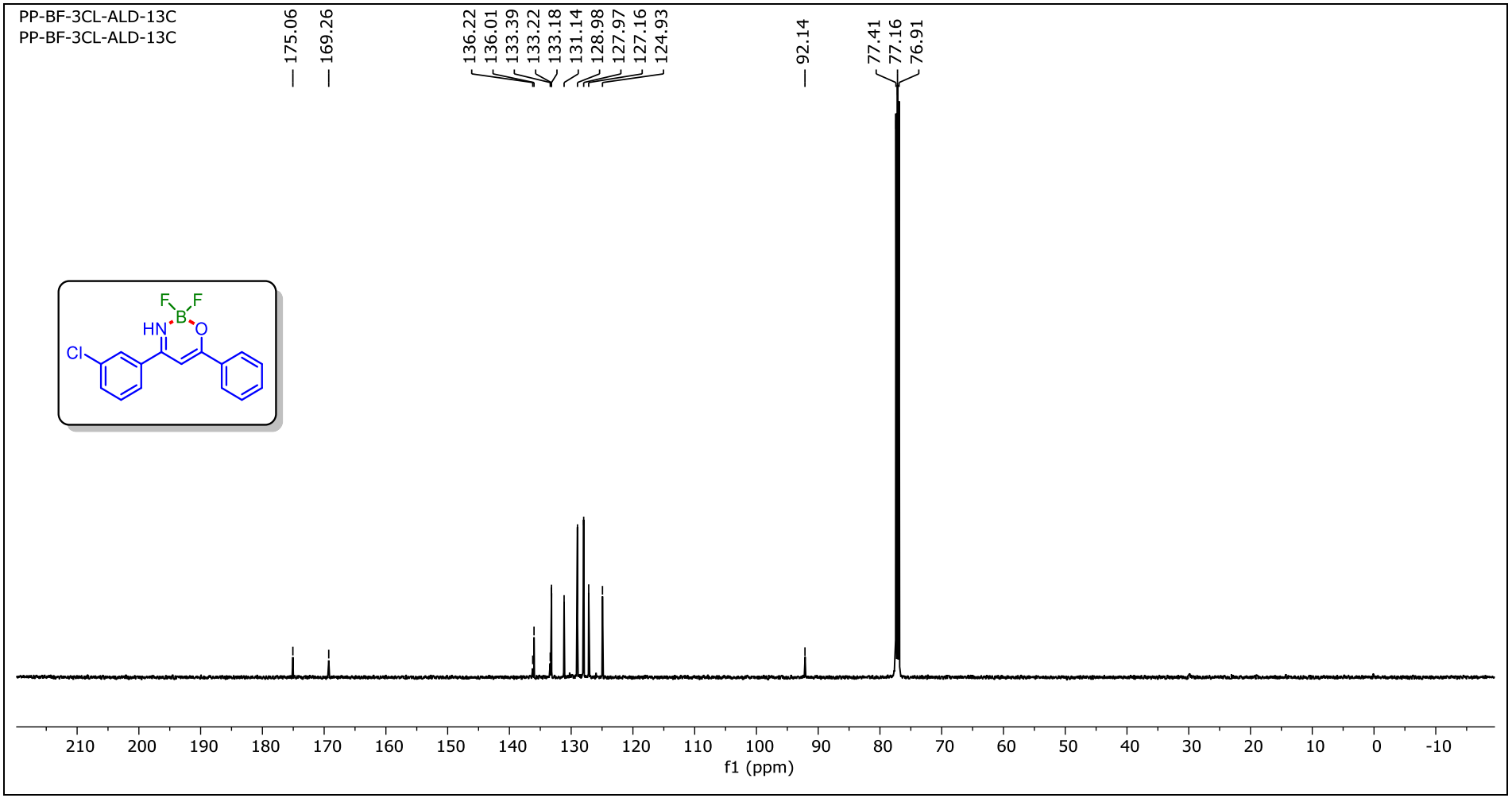
^{11}B NMR of **2,2-Difluoro-4-(3-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2k)** ($CDCl_3$, 160 MHz)



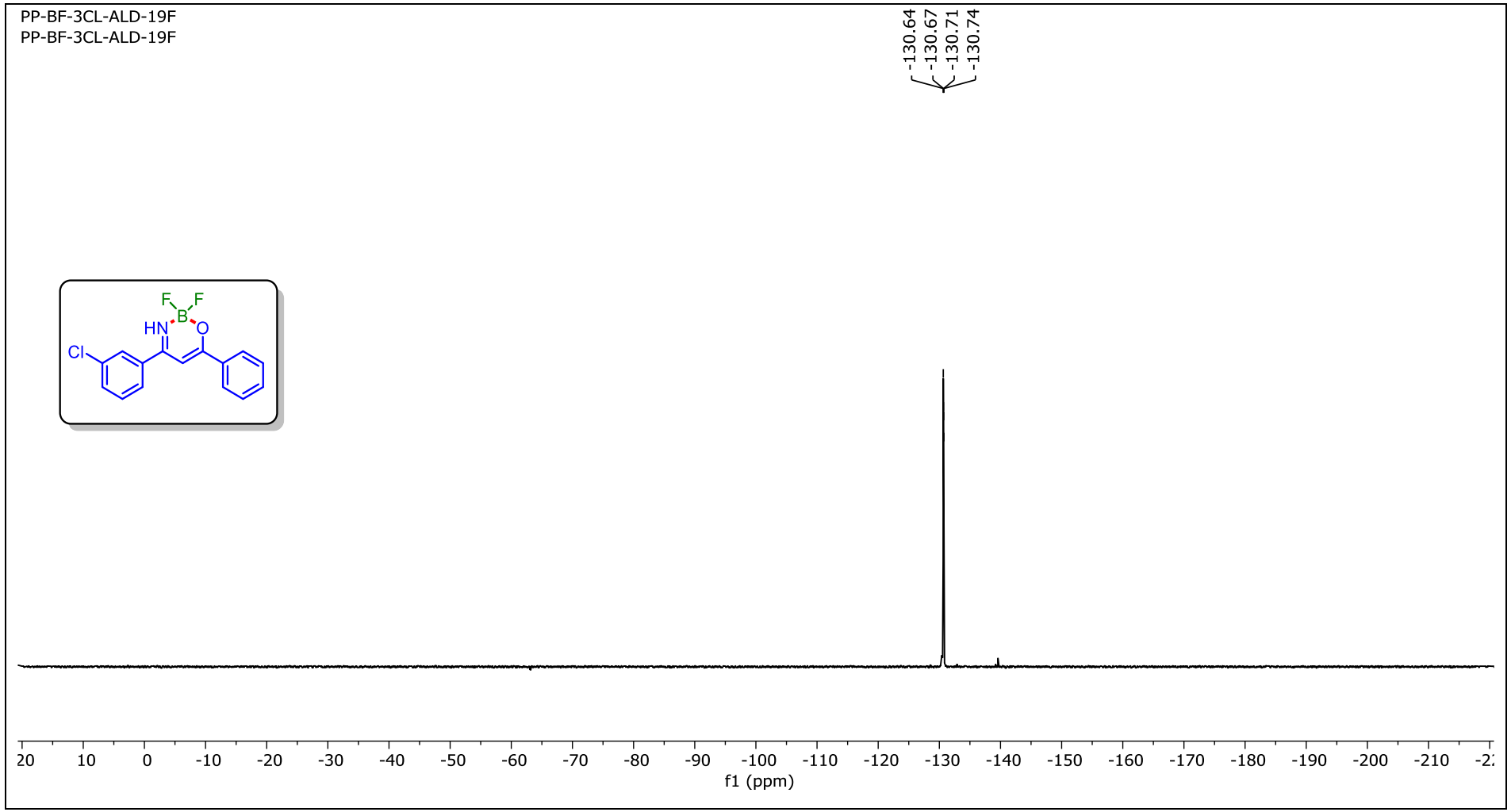
^{1}H NMR of **4-(3-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2l)** ($CDCl_3$, 500 MHz)



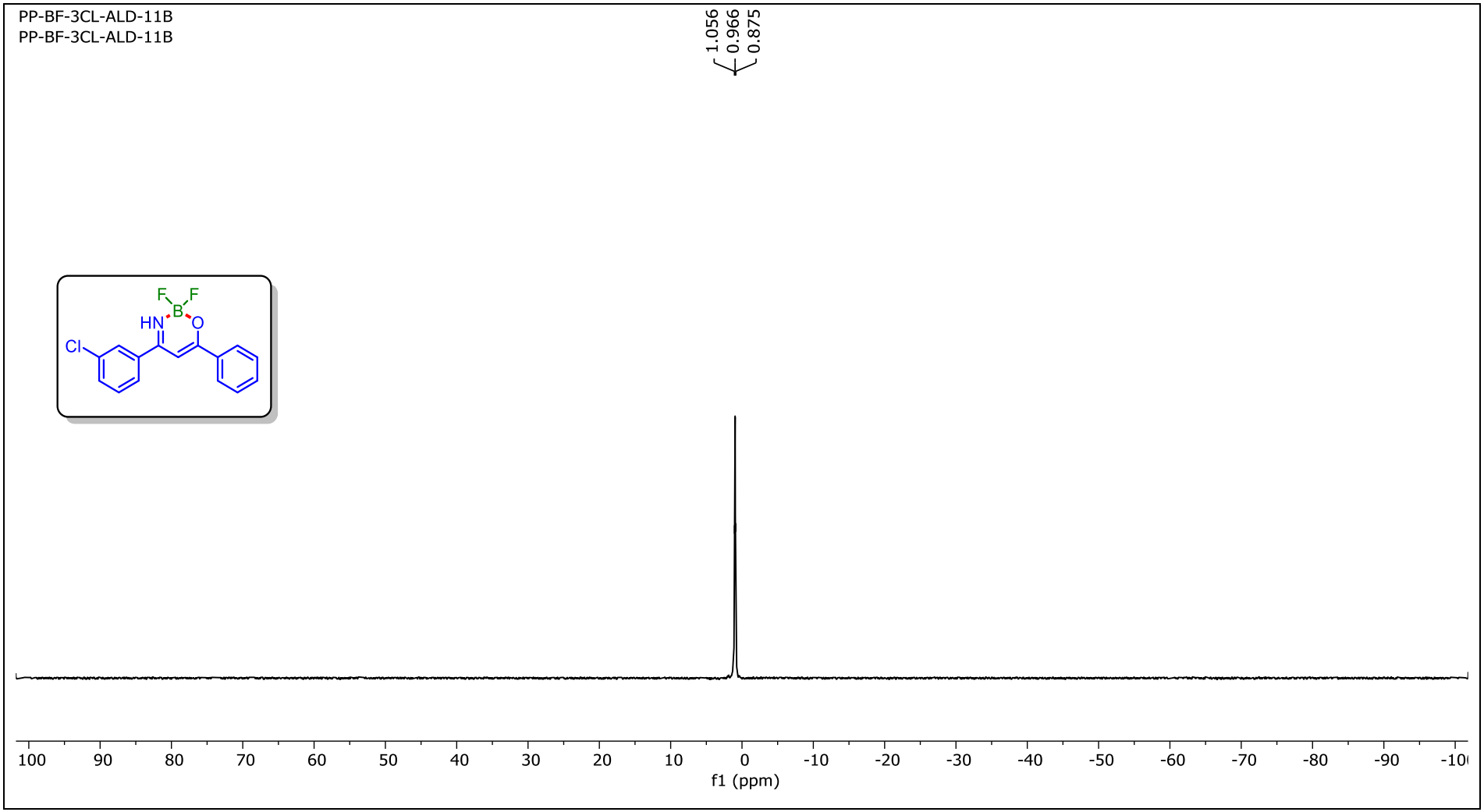
^{13}C {^{1}H} NMR of **4-(3-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2l)** ($CDCl_3$, 126 MHz)



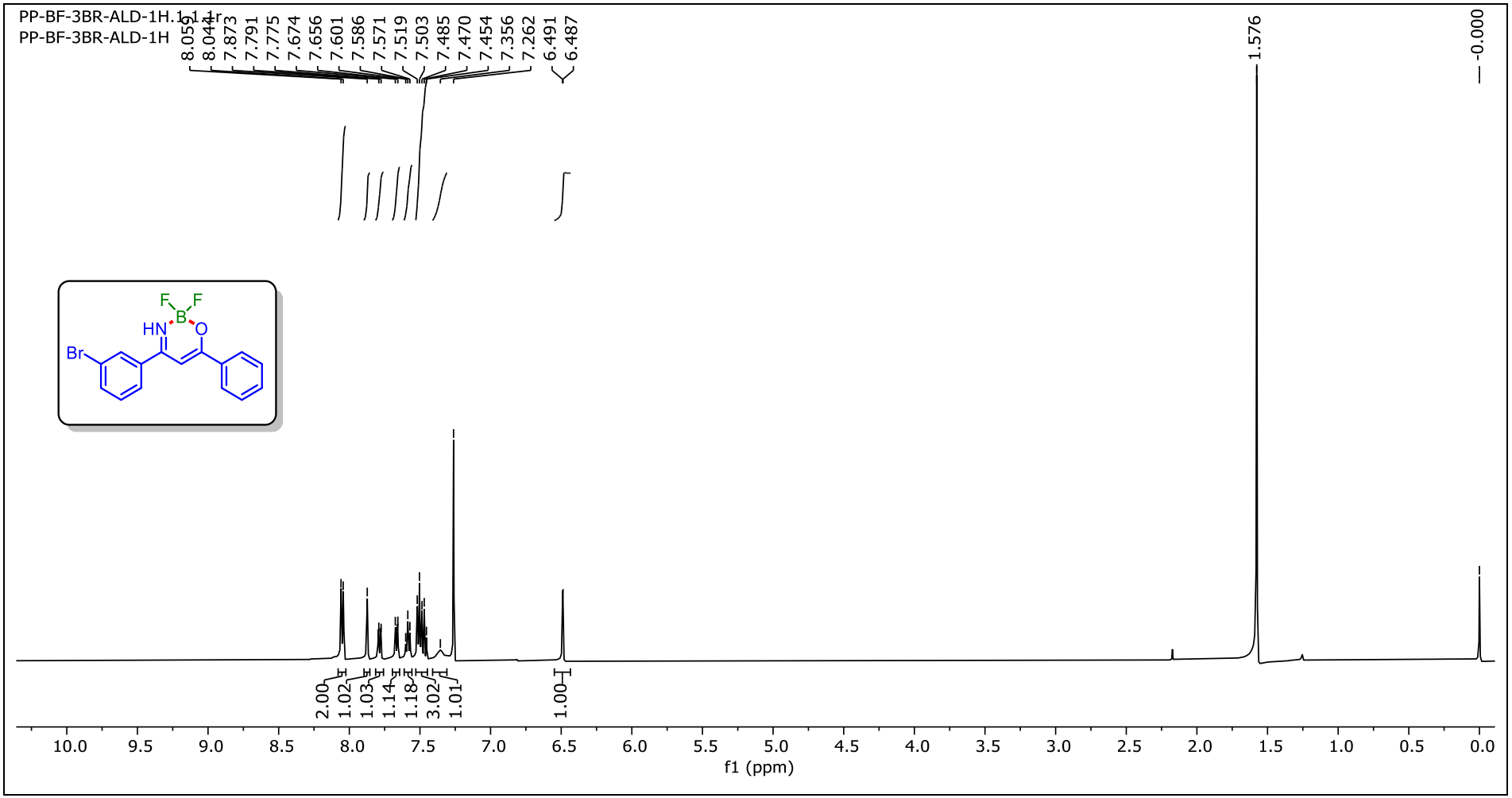
^{19}F NMR of **4-(3-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2l)** ($CDCl_3$, 471 MHz)



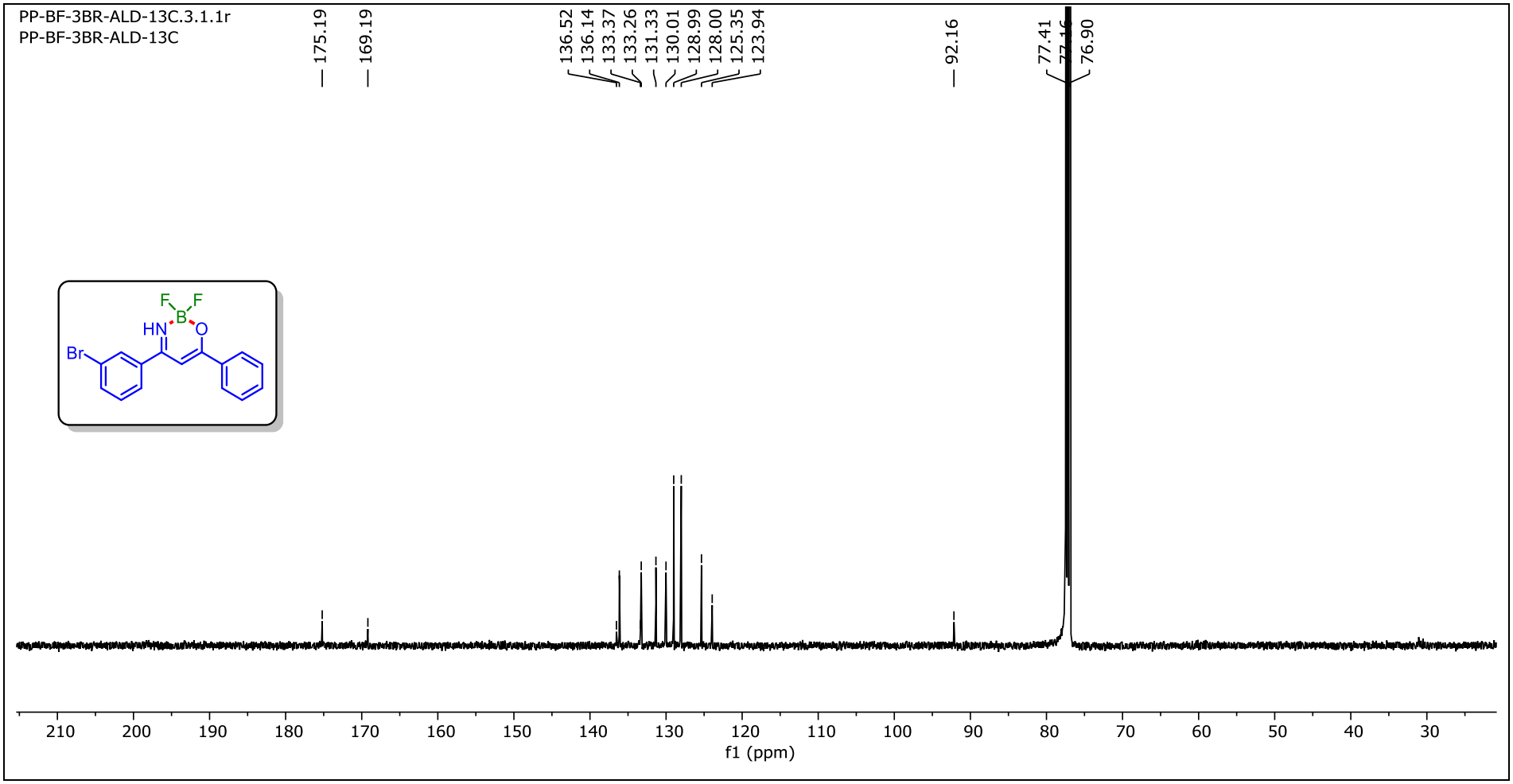
^{11}B NMR of **4-(3-Chlorophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2l)** ($CDCl_3$, 160 MHz)



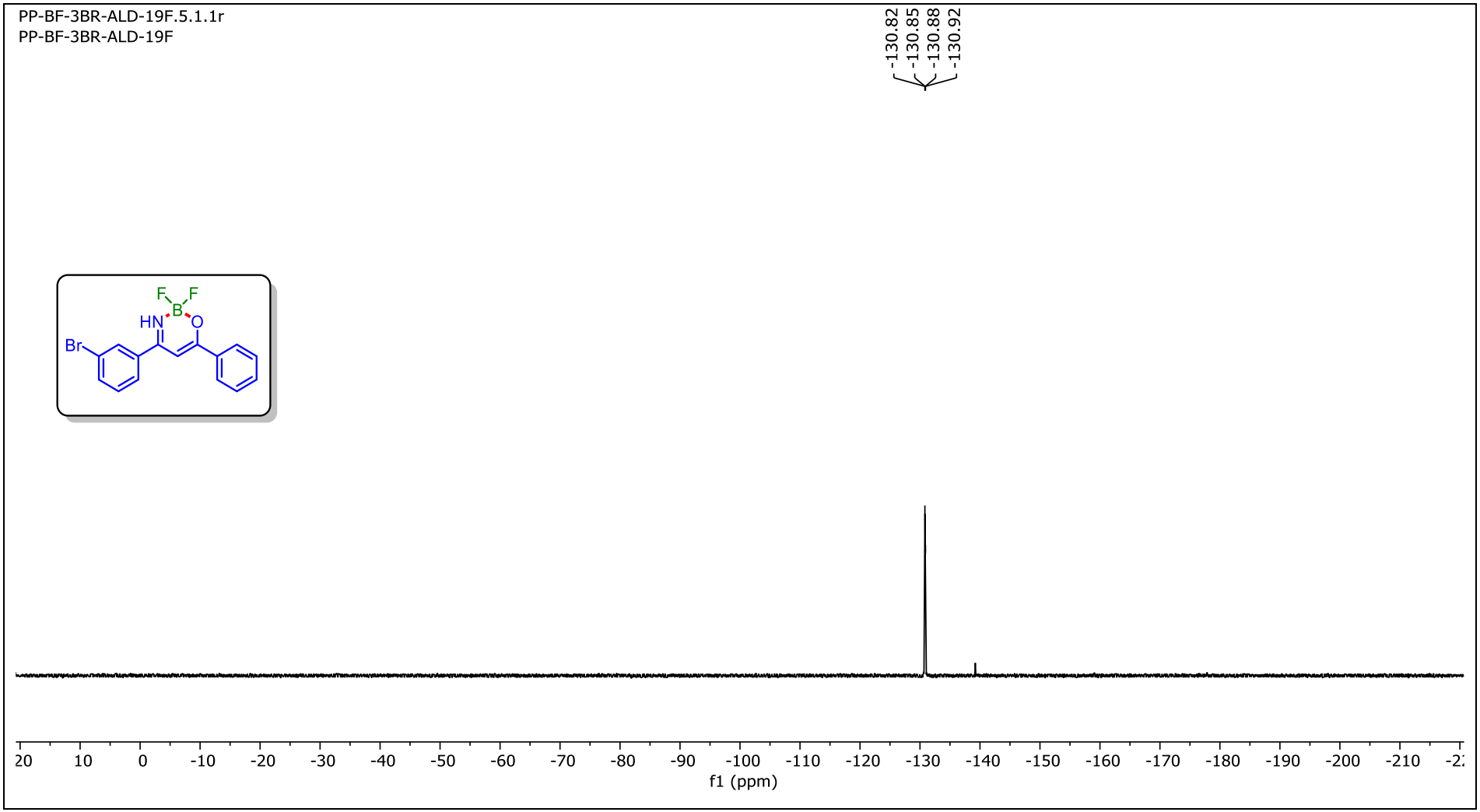
^{1}H NMR of **4-(3-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2m)** ($CDCl_3$, 500 MHz)



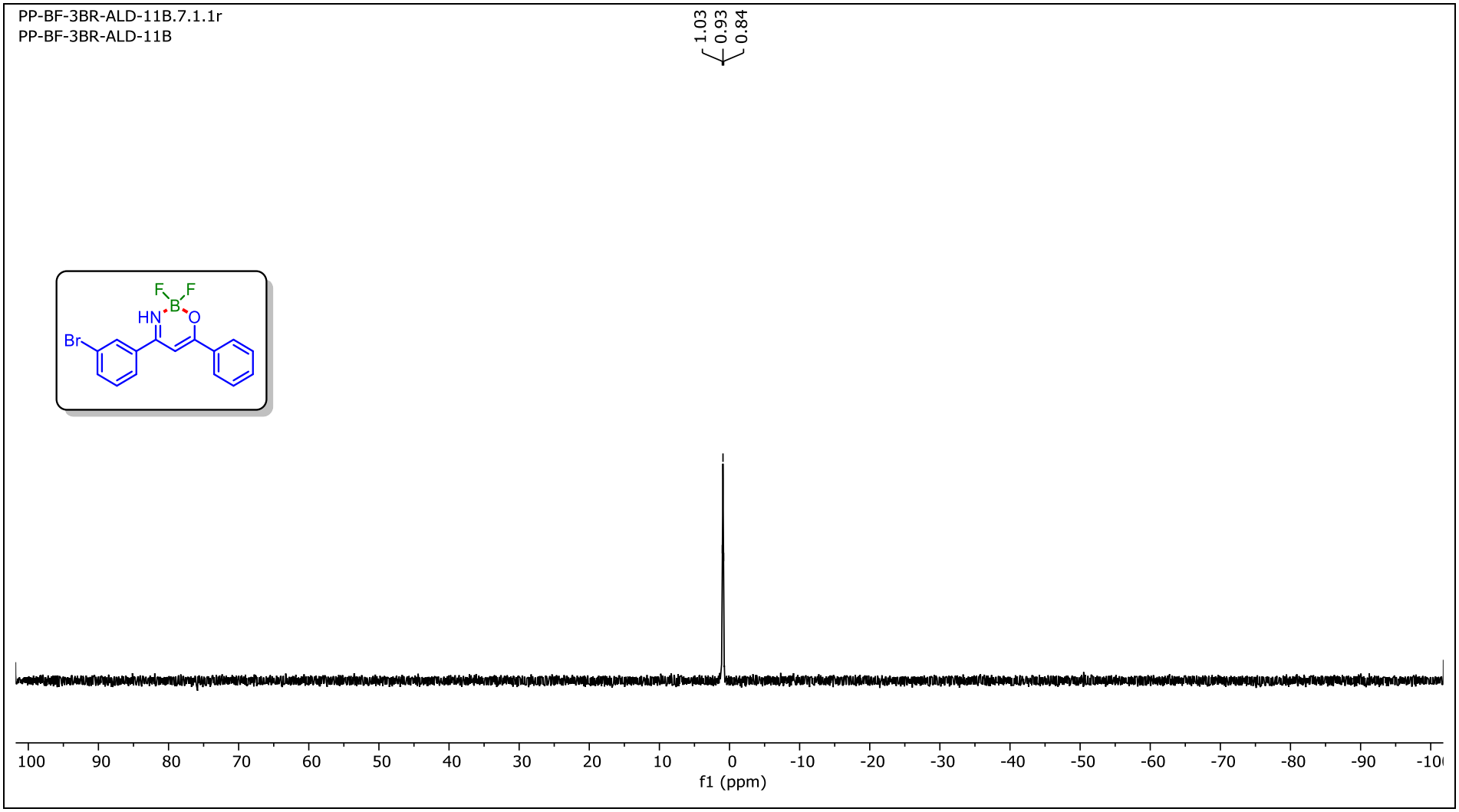
^{13}C {^{1}H} NMR of **4-(3-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2m)** ($CDCl_3$, 126 MHz)



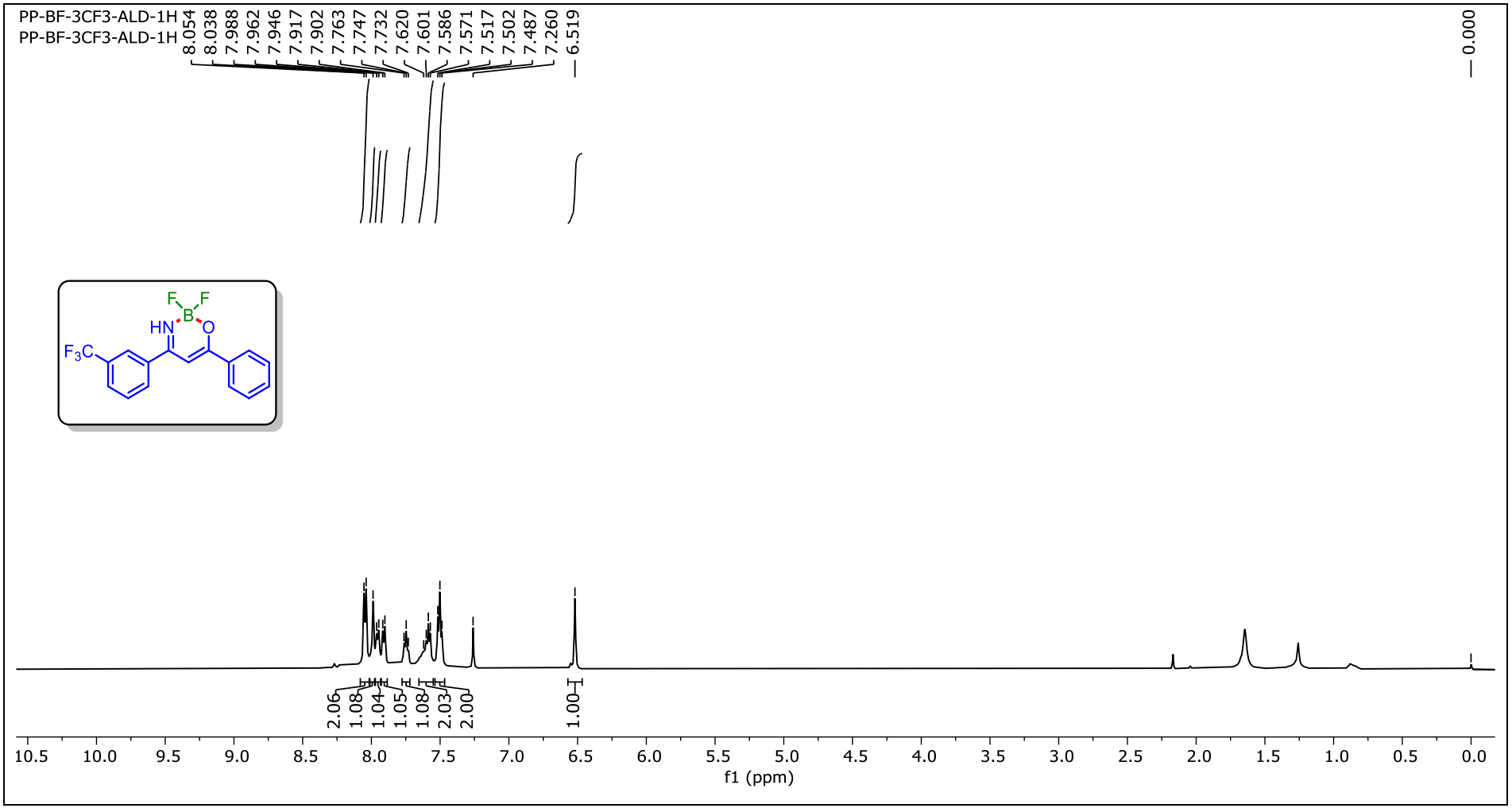
^{19}F NMR of **4-(3-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2m)** ($CDCl_3$, 471 MHz)



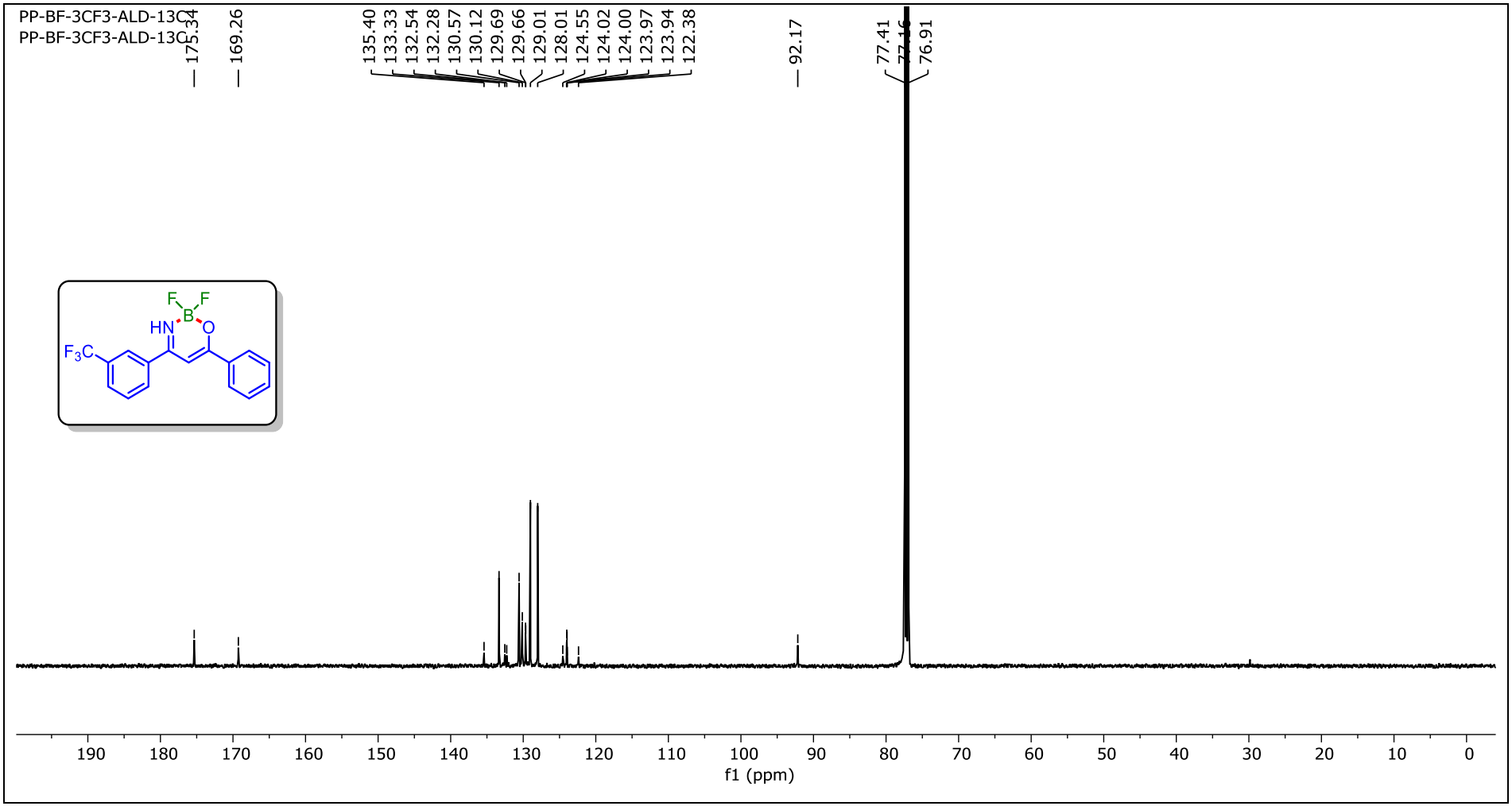
^{11}B NMR of **4-(3-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2m)** ($CDCl_3$, 160 MHz)



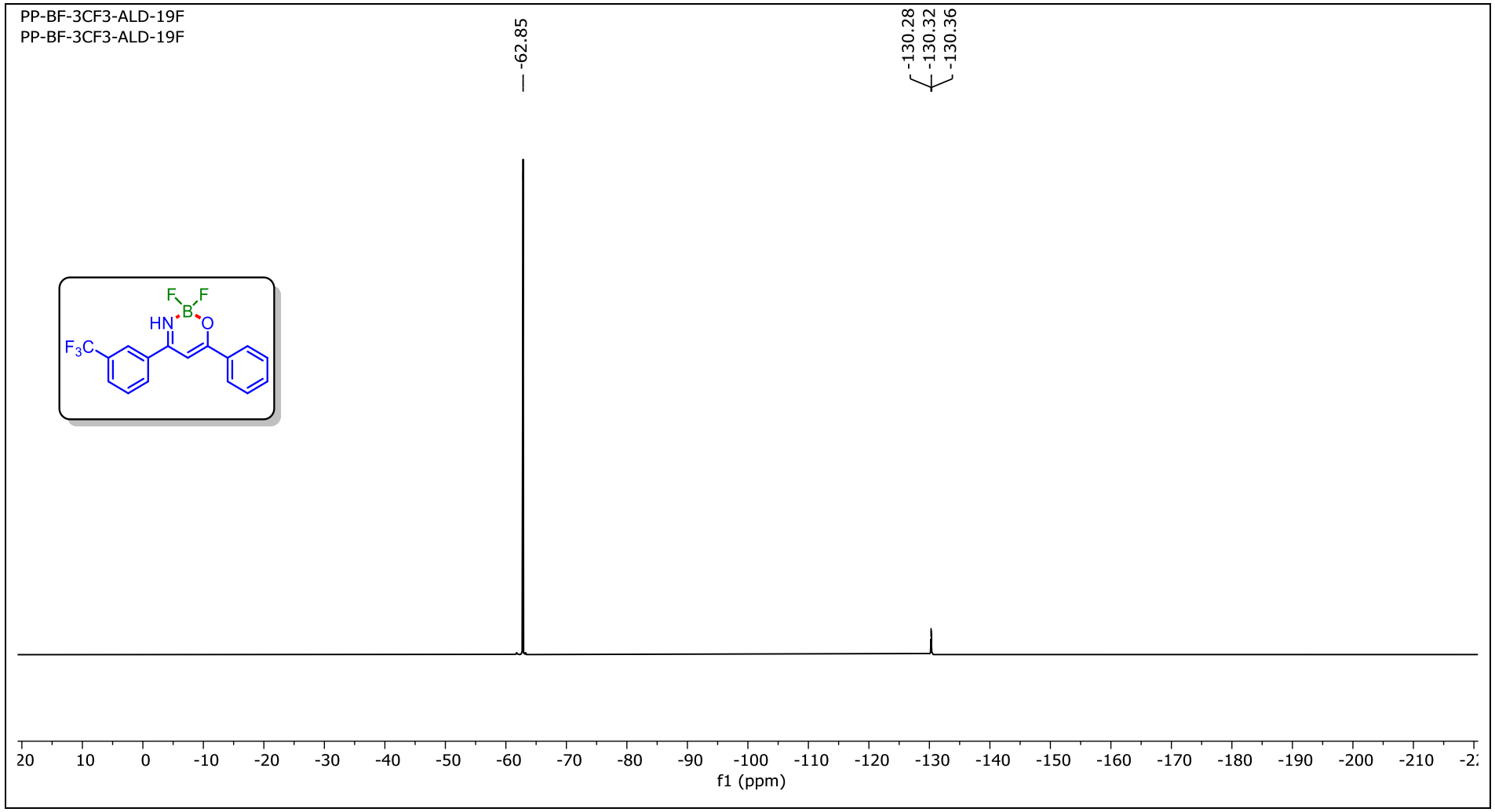
^{1}H NMR of **2,2-Difluoro-6-phenyl-4-(3-(trifluoromethyl)phenyl)-2*H*-1,3,2λ^{4}-oxazaborinine (2n)** ($CDCl_3$, 500 MHz)



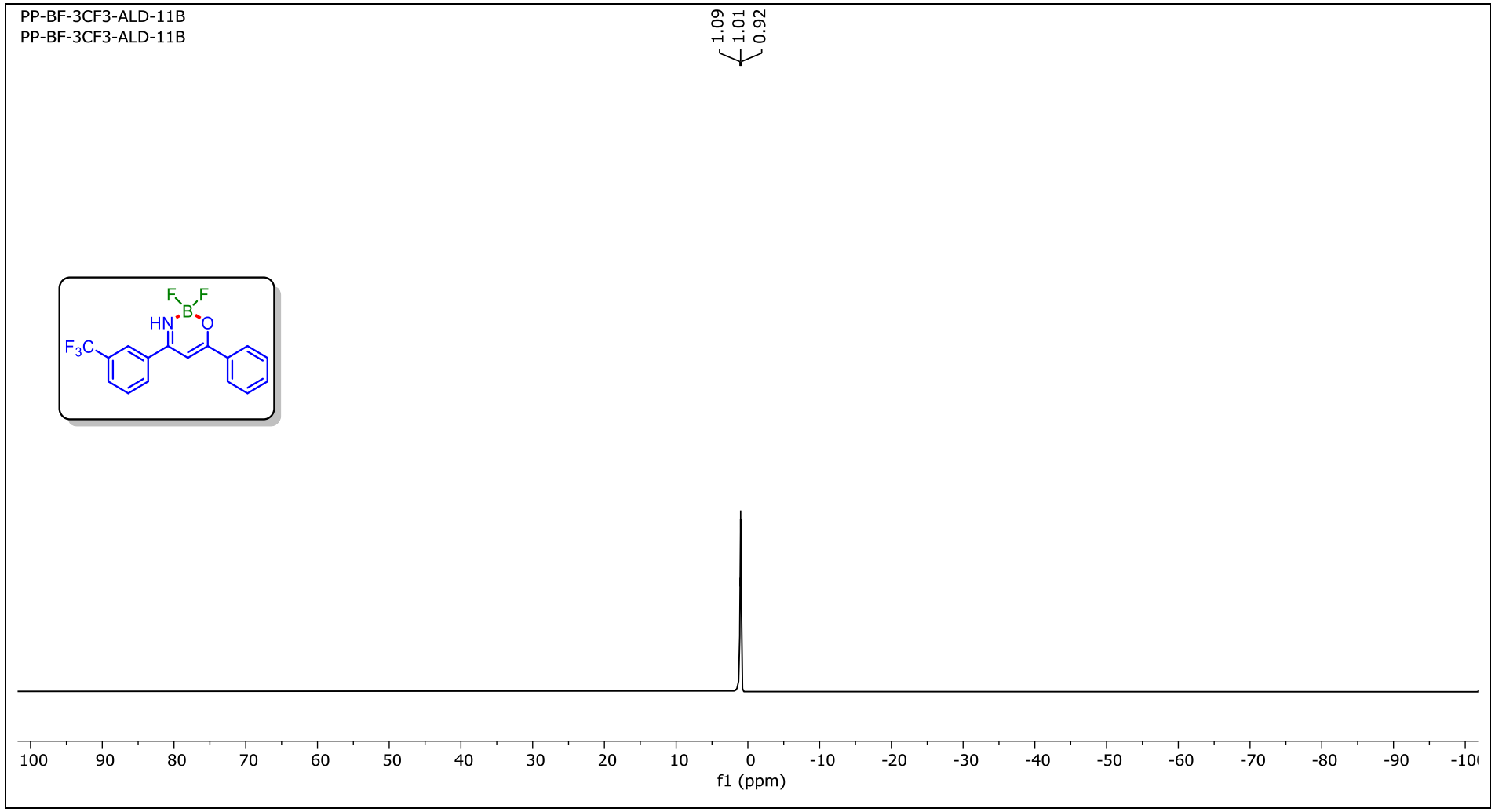
^{13}C {^{1}H} of **2,2-Difluoro-6-phenyl-4-(3-(trifluoromethyl)phenyl)-2*H*-1,3,2λ^{4}-oxazaborinine (2n)** ($CDCl_3$, 126 MHz)



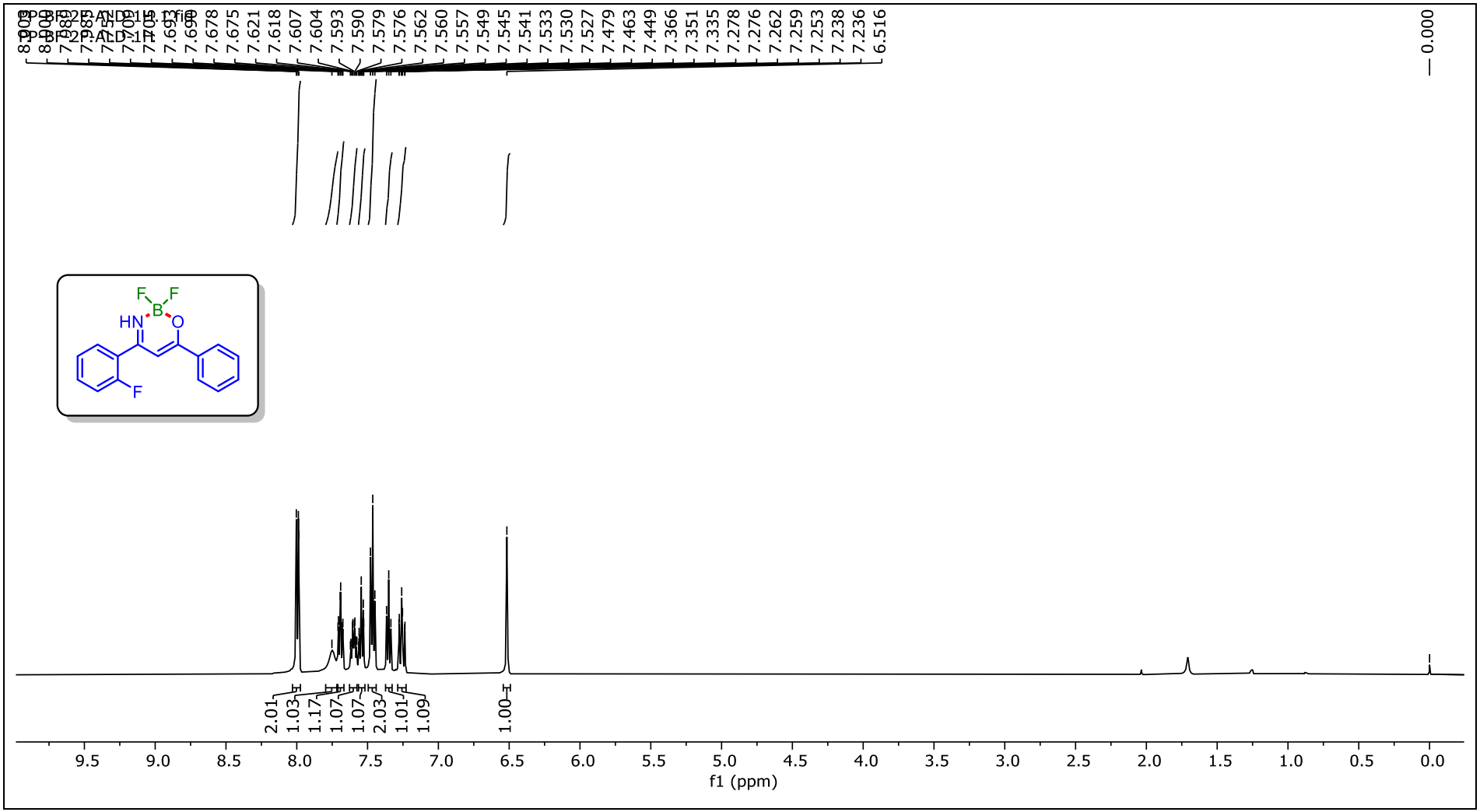
^{19}F NMR of **2,2-Difluoro-6-phenyl-4-(3-(trifluoromethyl)phenyl)-2*H*-1,3,2λ^4-oxazaborinine (2n)** ($CDCl_3$, 471 MHz)



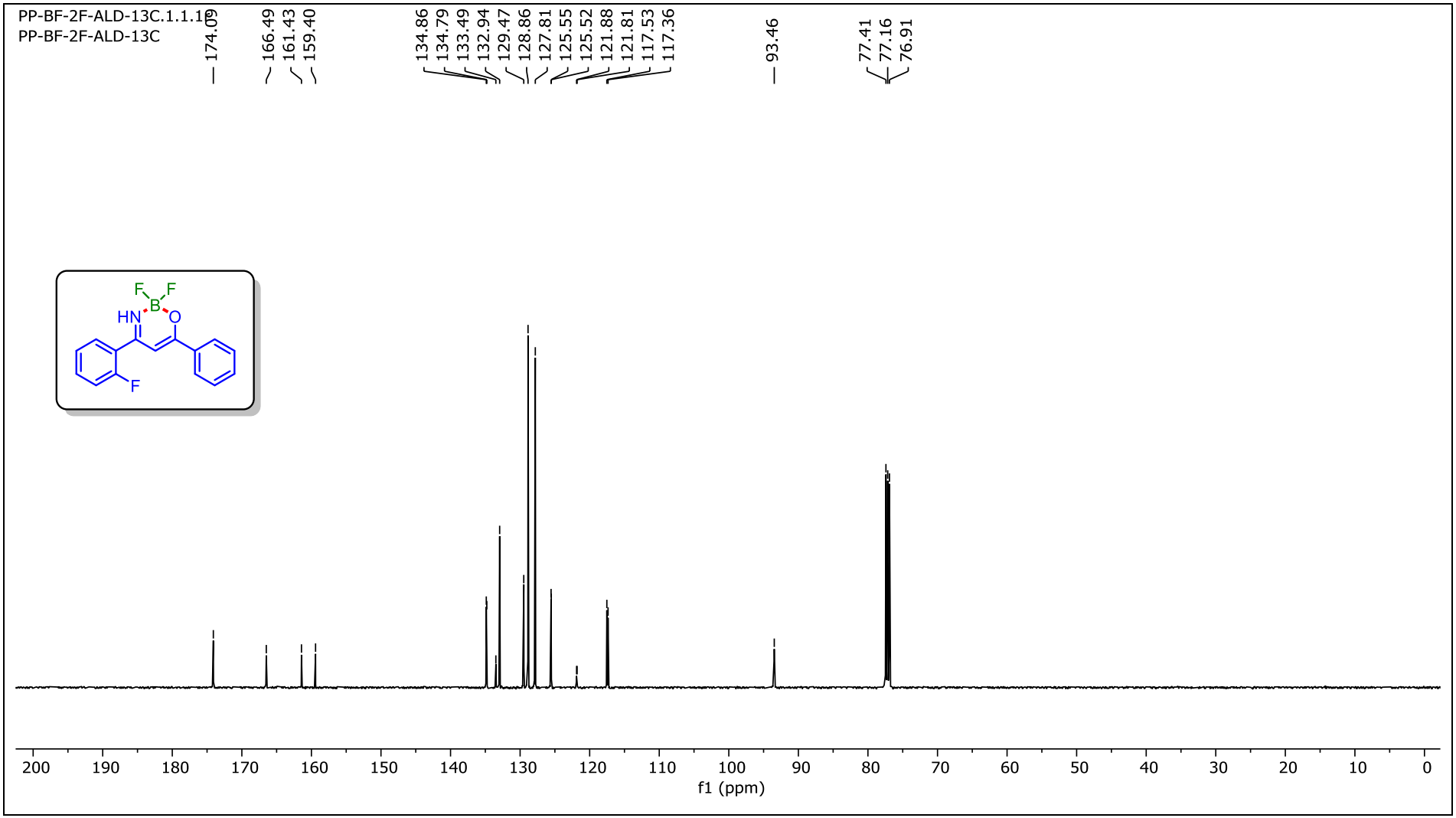
^{11}B NMR of **2,2-Difluoro-6-phenyl-4-(3-(trifluoromethyl)phenyl)-2*H*-1,3,2λ^4-oxazaborinine (2n)** ($CDCl_3$, 160 MHz)



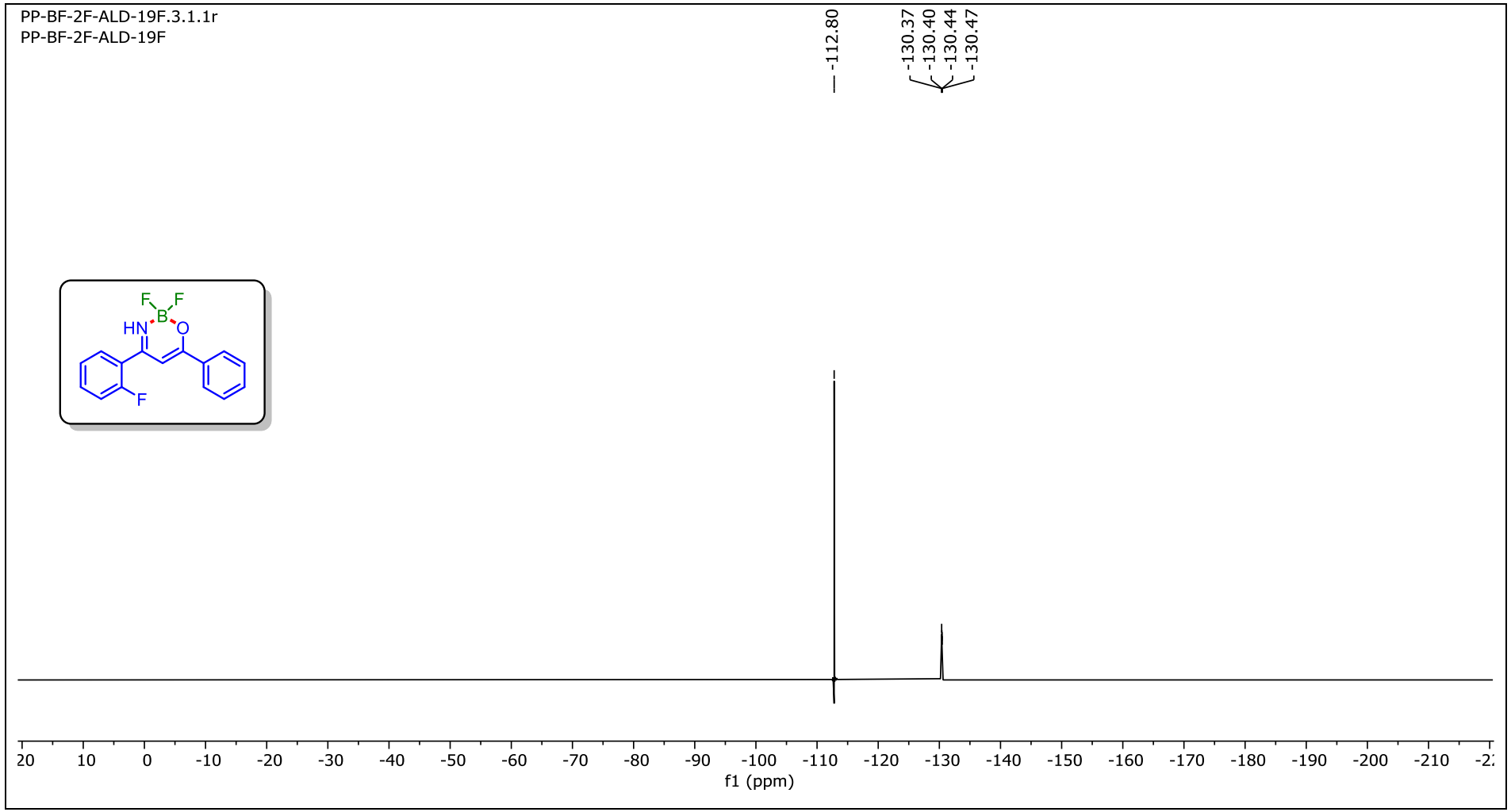
^{1}H NMR of **2,2-Difluoro-4-(2-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2o)** ($CDCl_3$, 500 MHz)



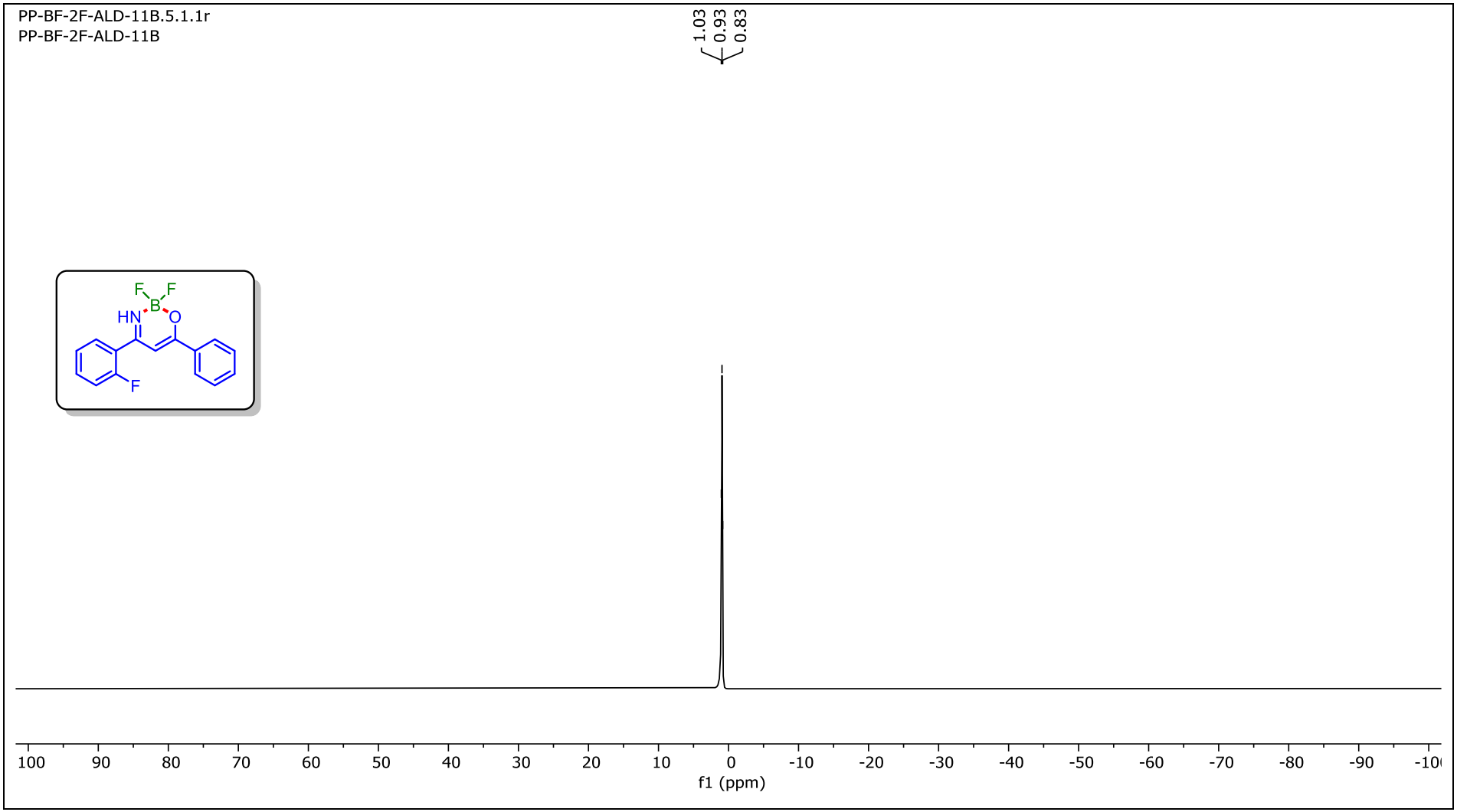
^{13}C {^{1}H} NMR of **2,2-Difluoro-4-(2-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2o)** ($CDCl_3$, 126 MHz)



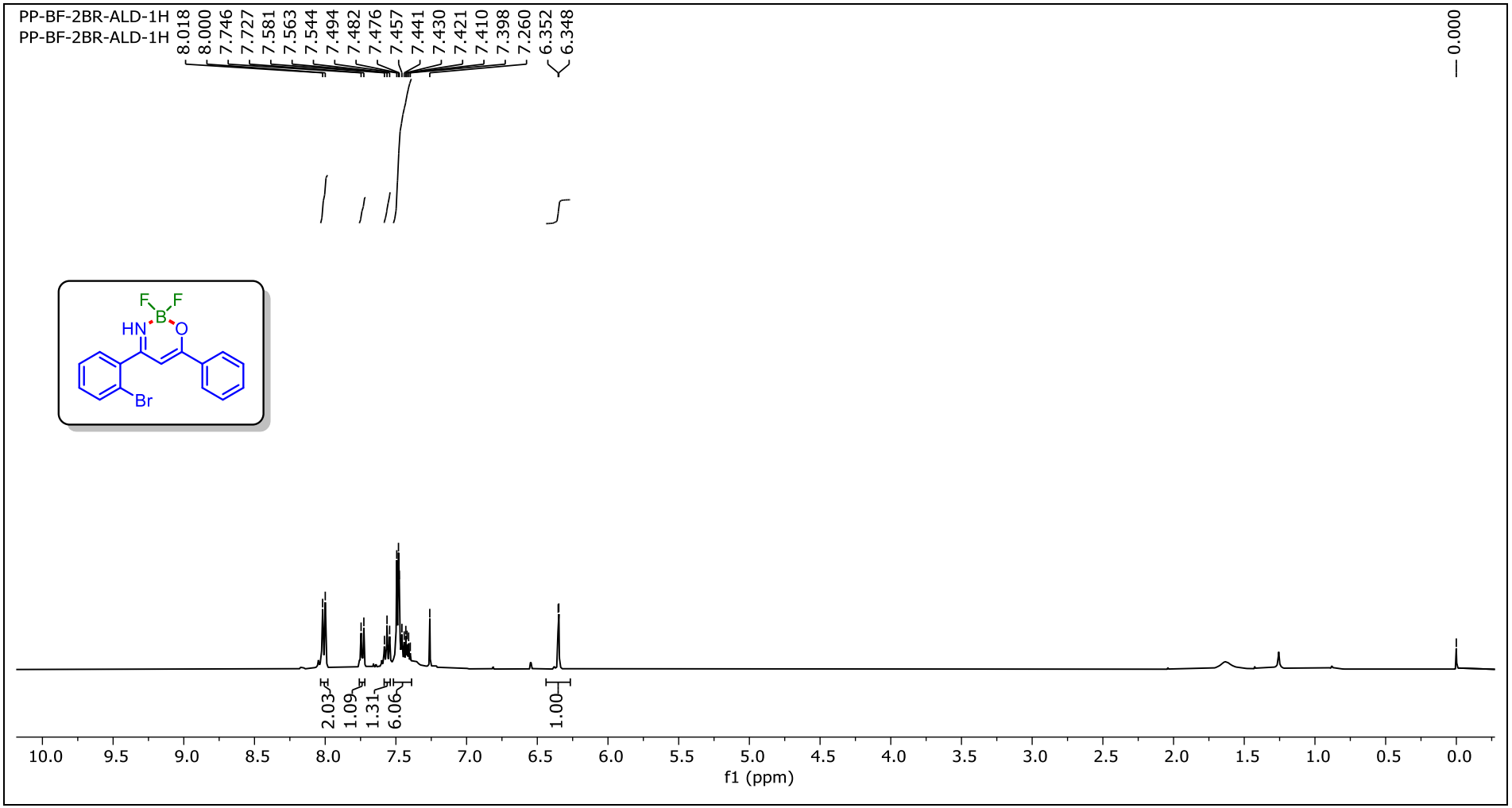
^{19}F NMR of **2,2-Difluoro-4-(2-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2o)** ($CDCl_3$, 471 MHz)



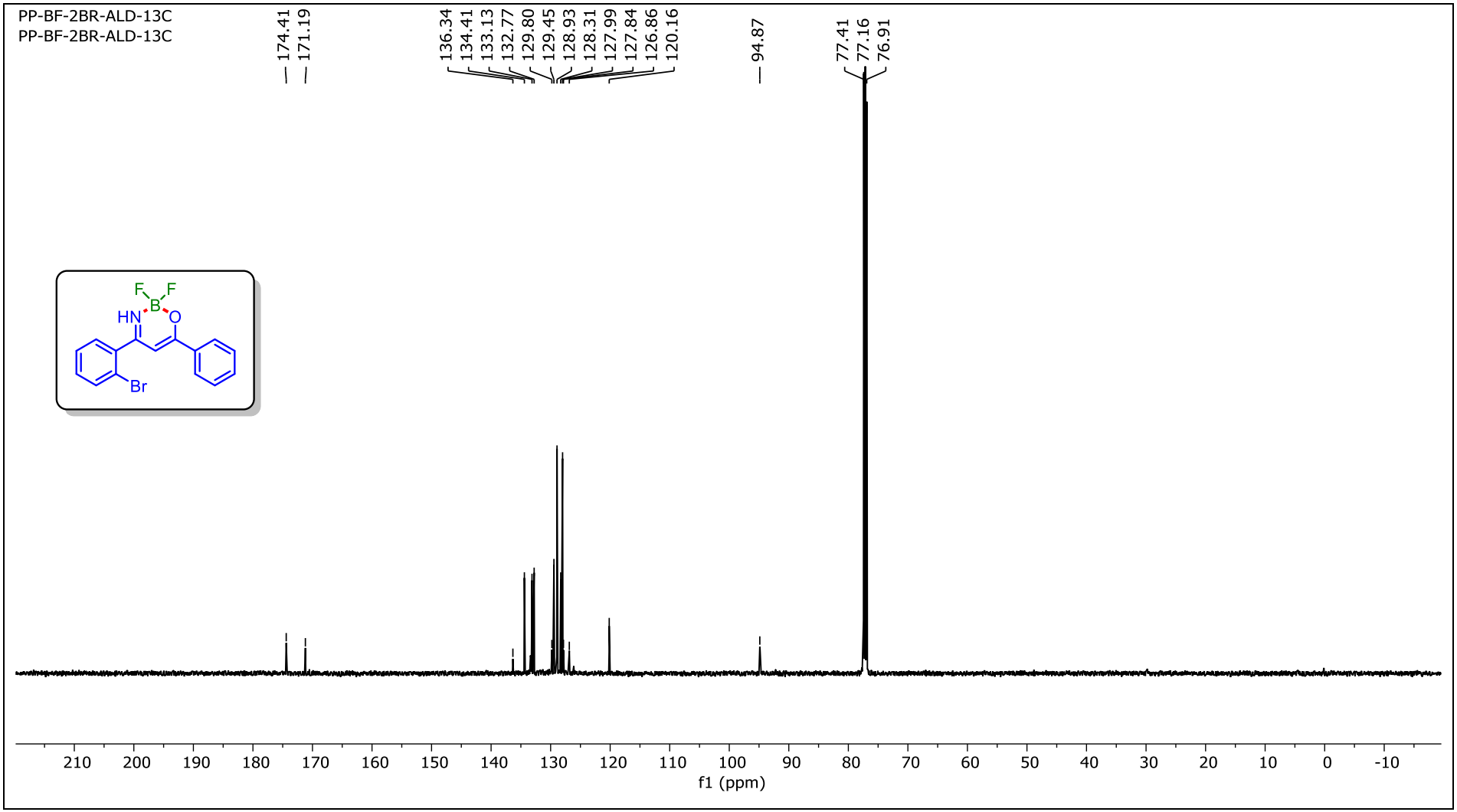
^{11}B NMR of **2,2-Difluoro-4-(2-fluorophenyl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2o)** ($CDCl_3$, 160 MHz)



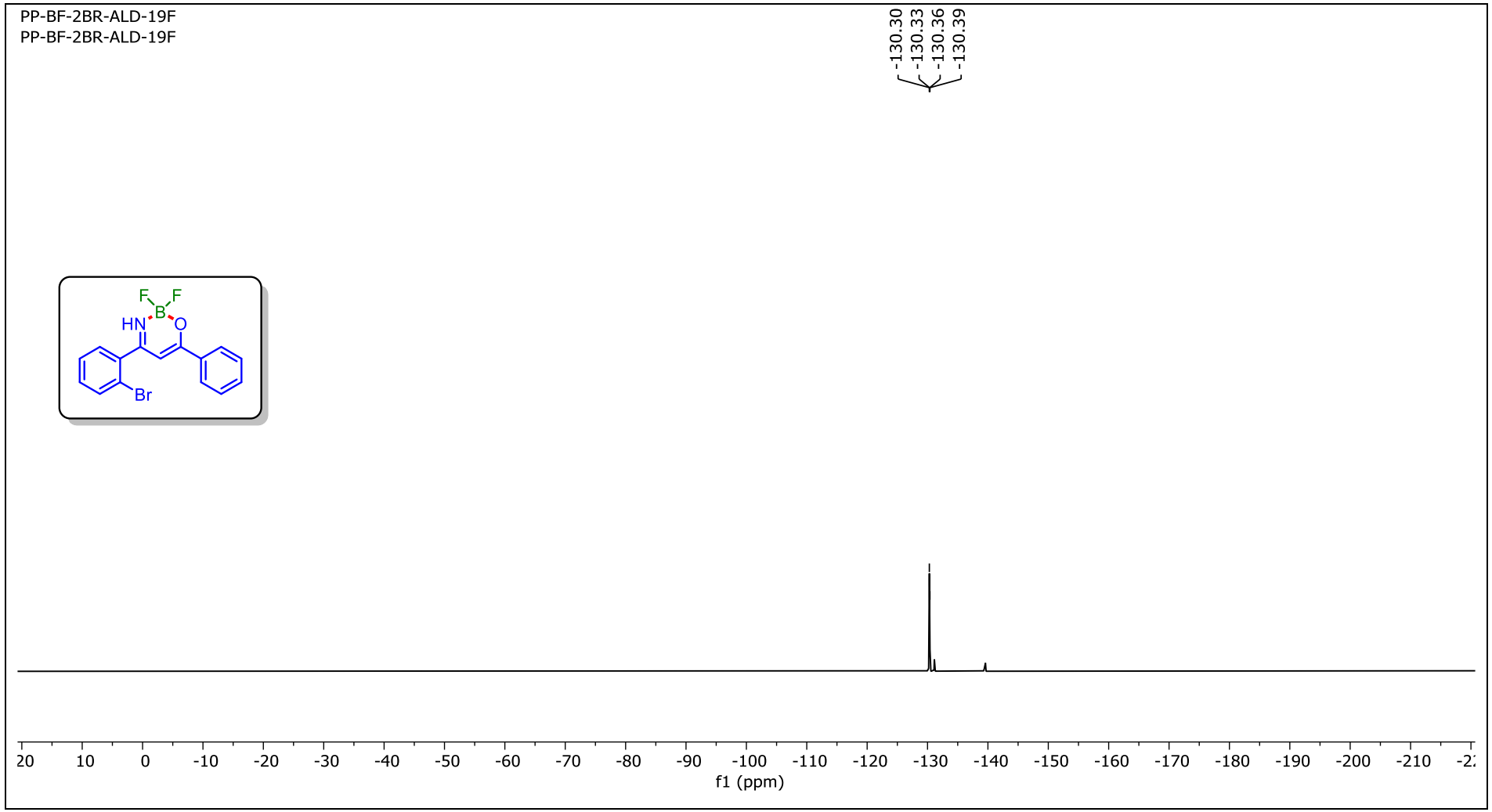
^{1}H NMR of **4-(2-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2p)** ($CDCl_3$, 400 MHz)



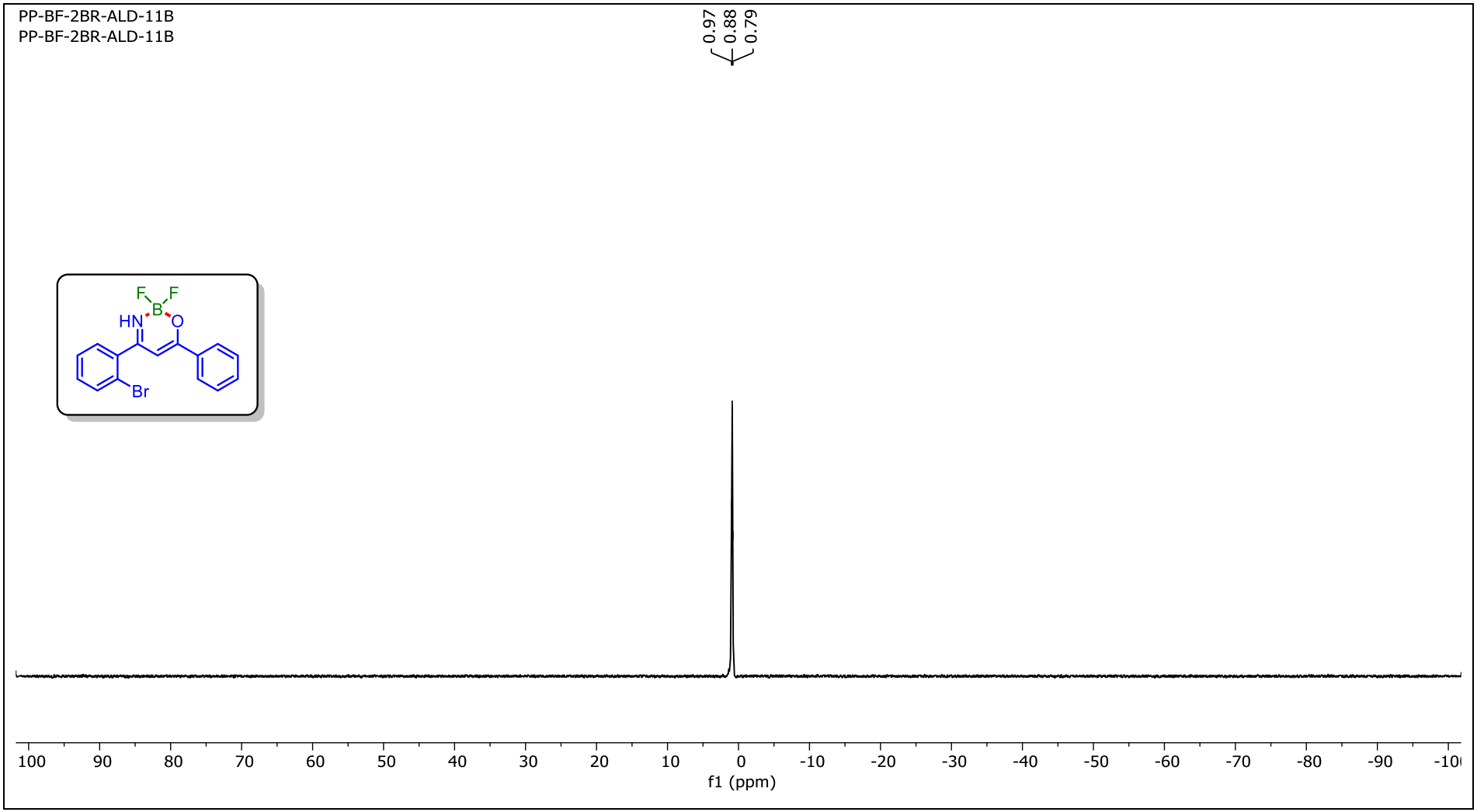
^{13}C {^{1}H} NMR of **4-(2-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2p)** ($CDCl_3$, 126 MHz)



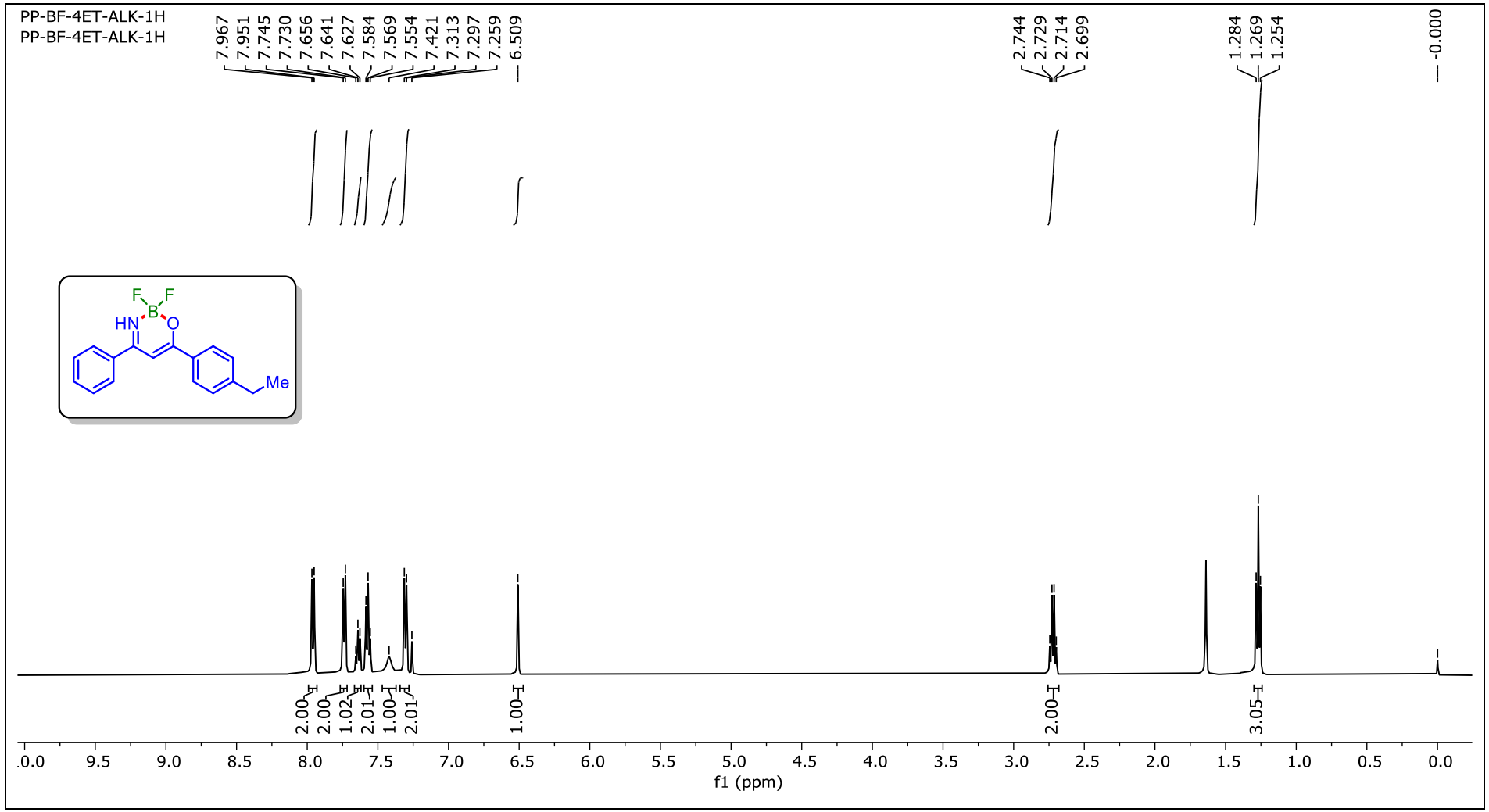
^{19}F NMR of **4-(2-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2p)** ($CDCl_3$, 471 MHz)



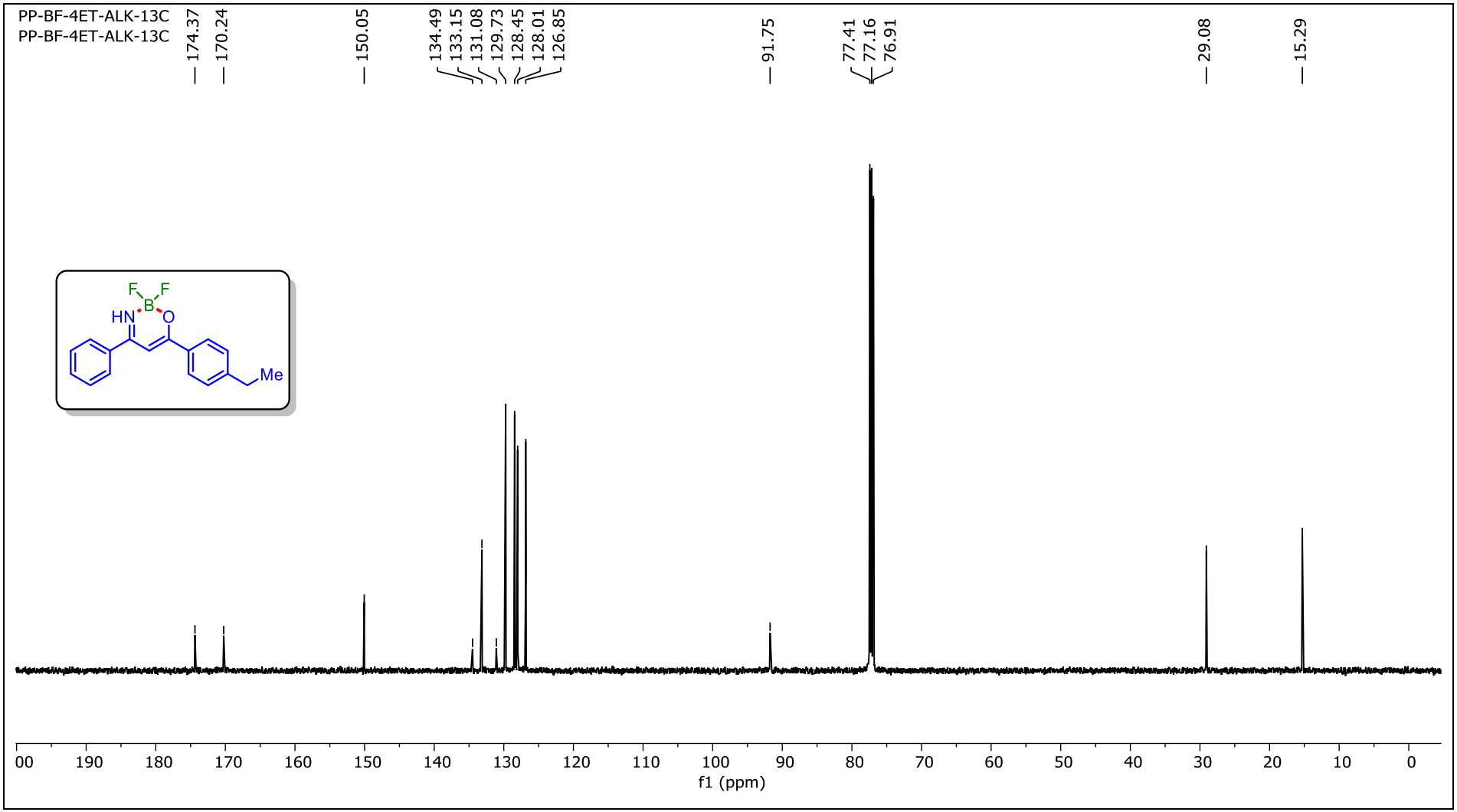
^{11}B NMR of **4-(2-Bromophenyl)-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2p)** ($CDCl_3$, 160 MHz)



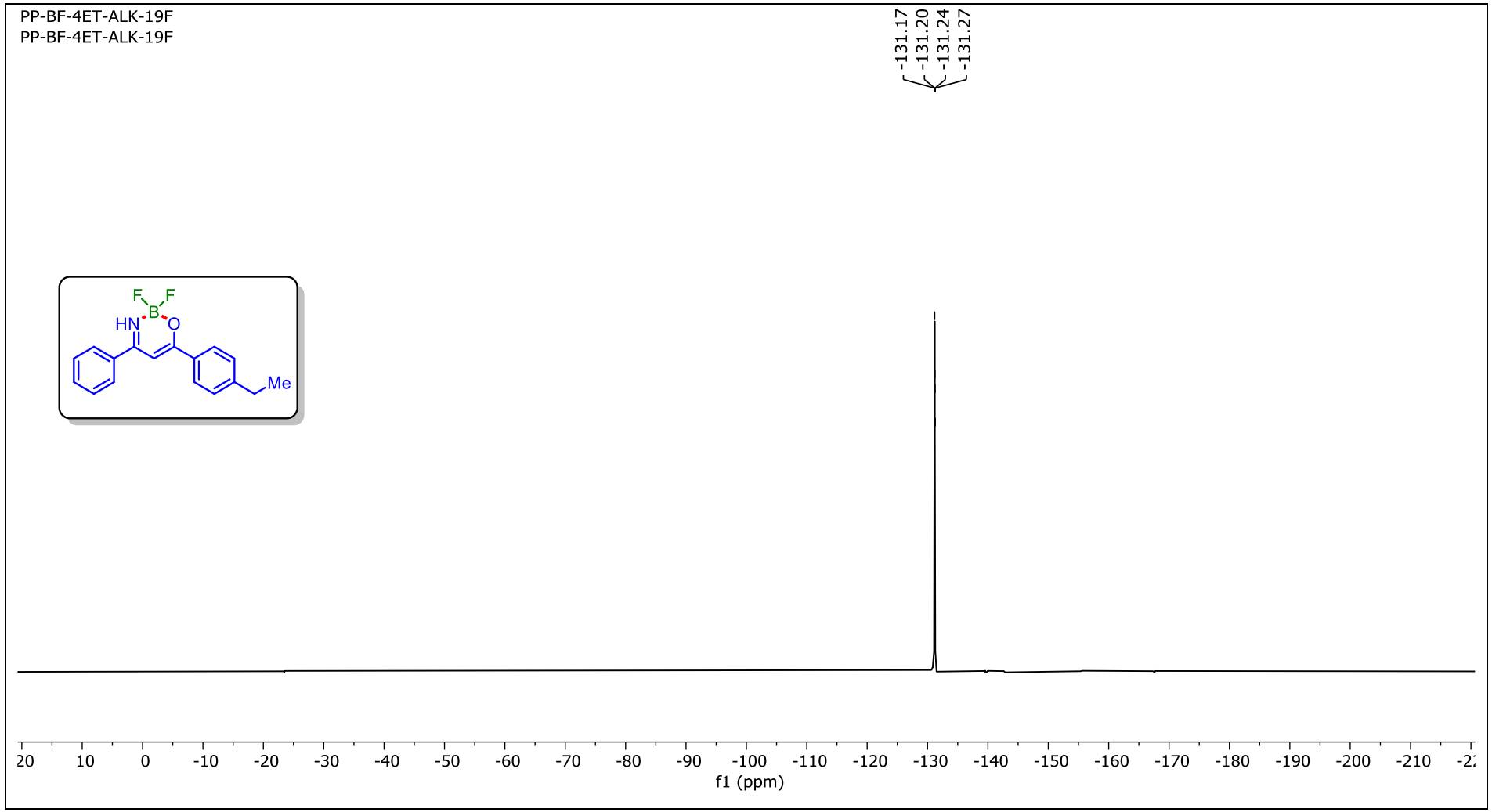
^{1}H NMR of **6-(4-Ethylphenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2q)** ($CDCl_3$, 500 MHz)



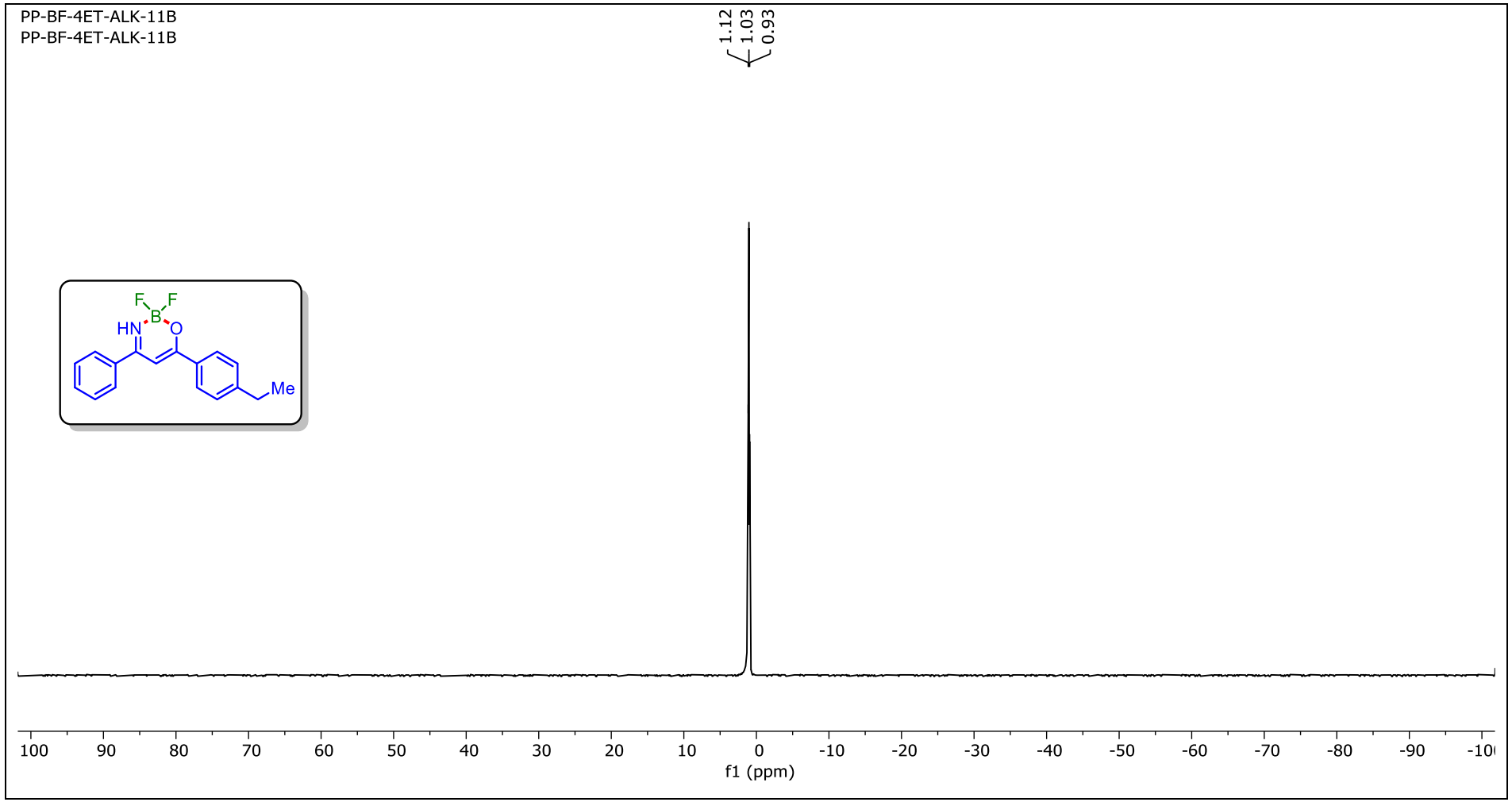
^{13}C {^{1}H} NMR of **6-(4-Ethylphenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2q)** ($CDCl_3$, 126 MHz)



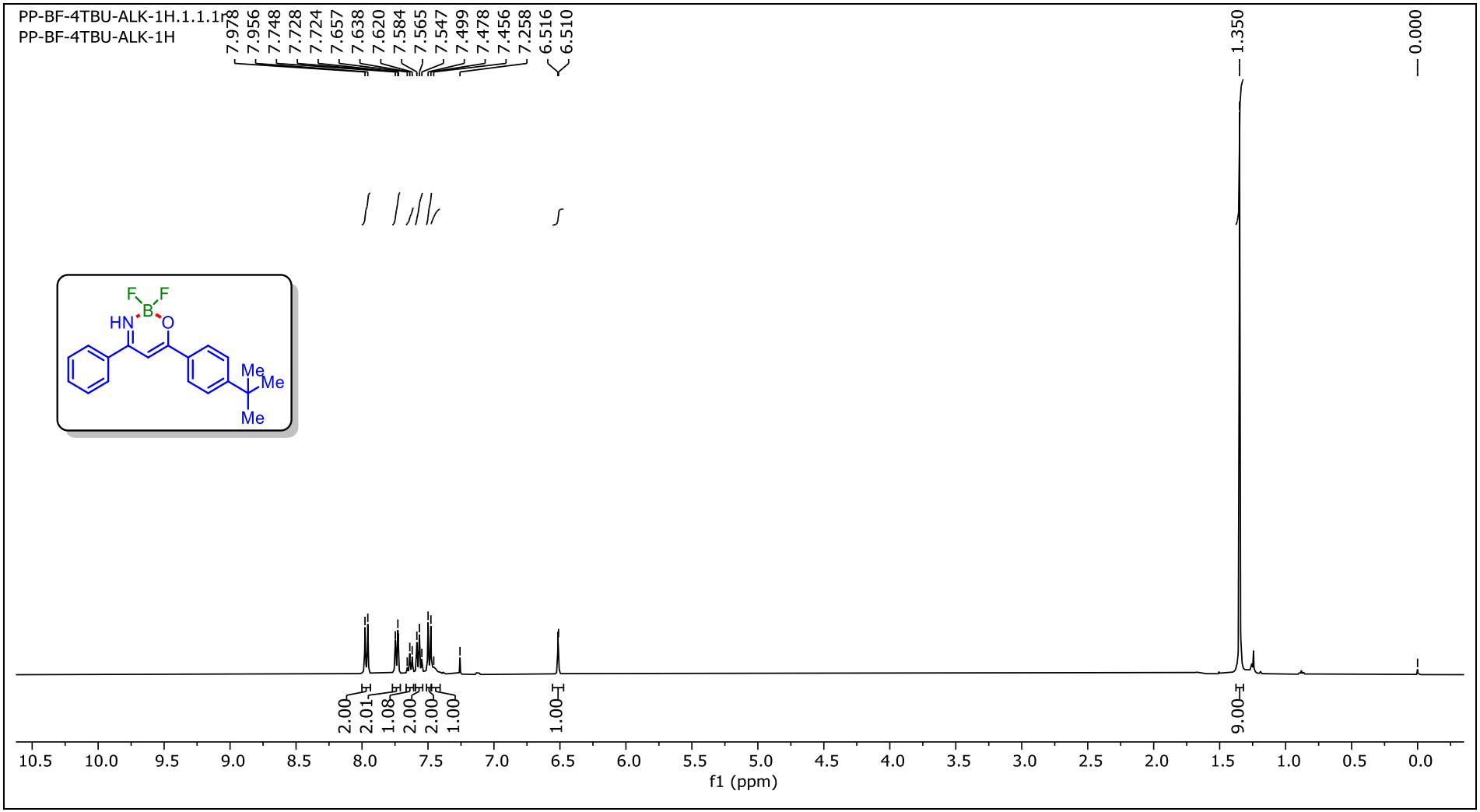
^{19}F NMR of **6-(4-Ethylphenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2q)** ($CDCl_3$, 471 MHz)



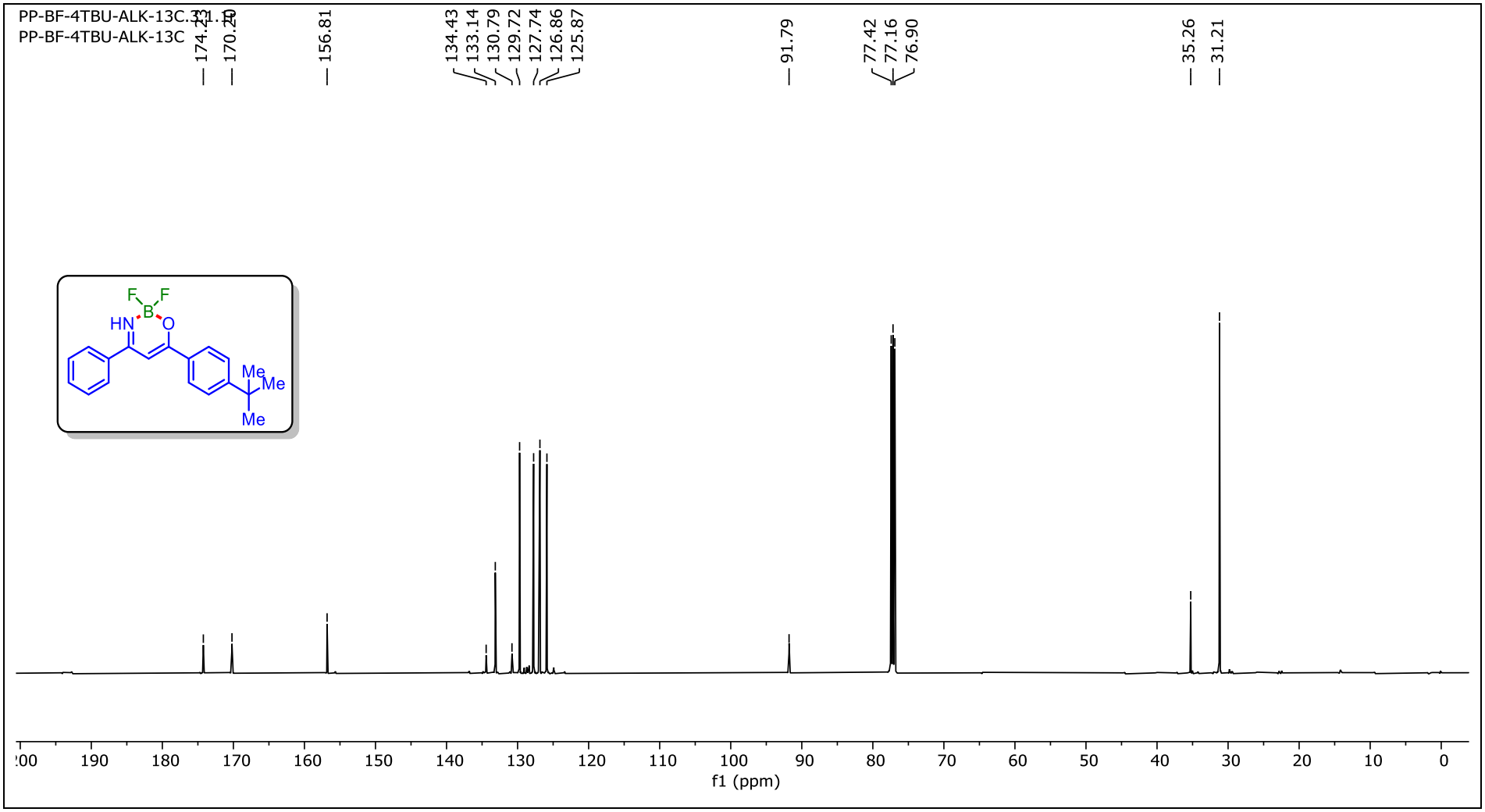
^{11}B NMR of **6-(4-Ethylphenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2q)** ($CDCl_3$, 160 MHz)



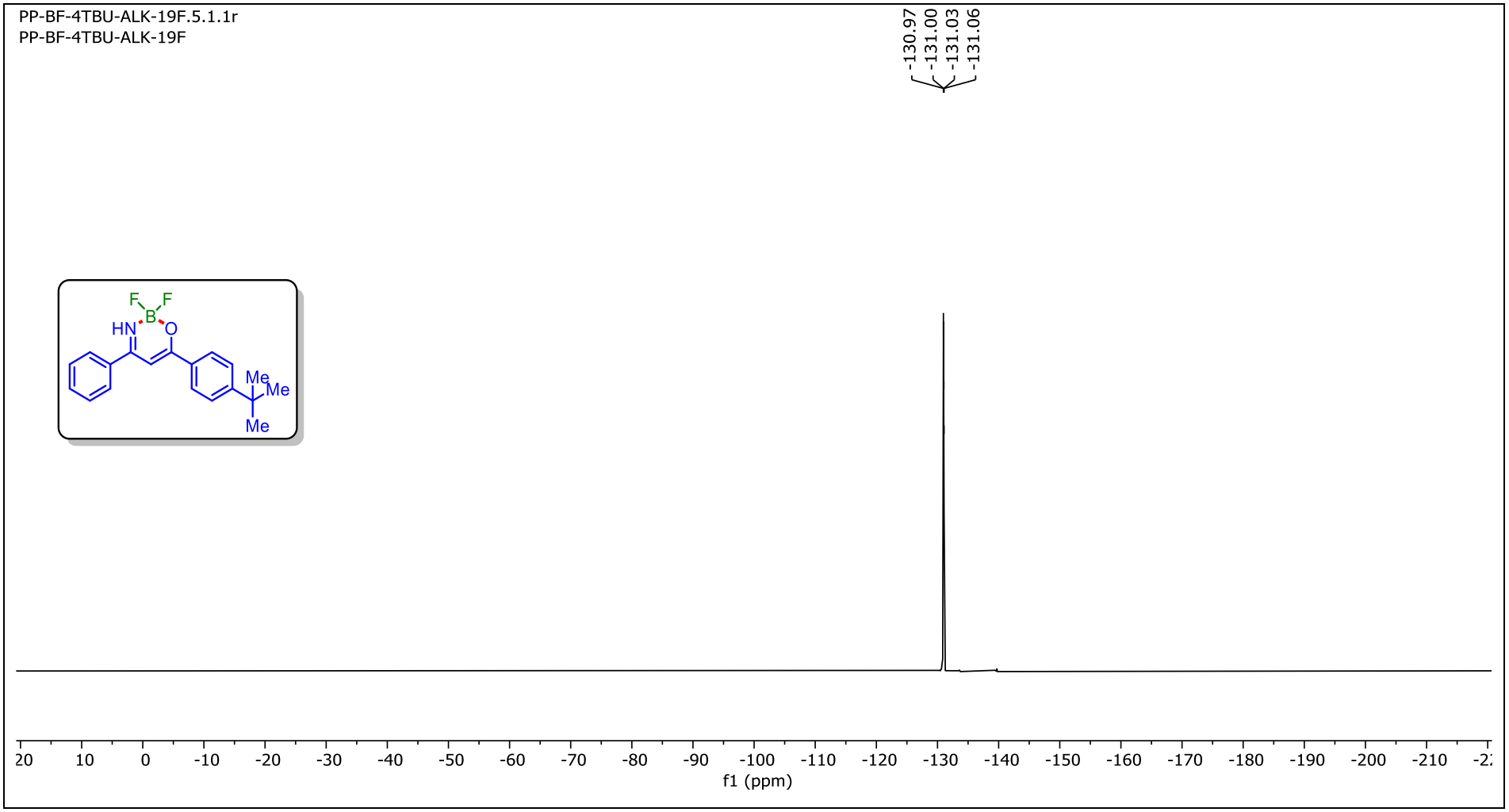
^{1}H NMR of **6-(4-(*tert*-Butyl)phenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2r)** ($CDCl_3$, 400 MHz)



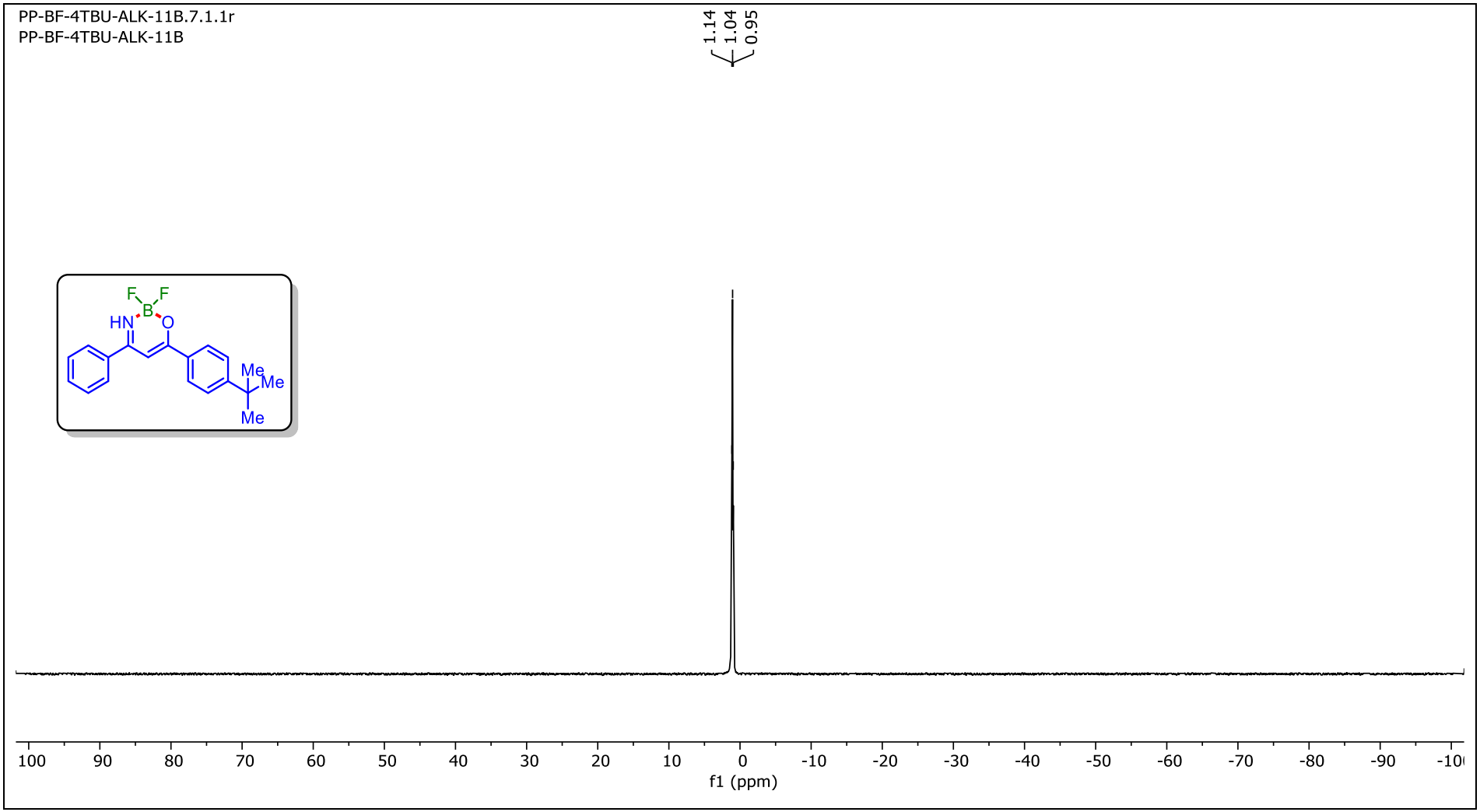
^{13}C {^{1}H} NMR of **6-(4-(*tert*-Butyl)phenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2r)** ($CDCl_3$, 126 MHz)



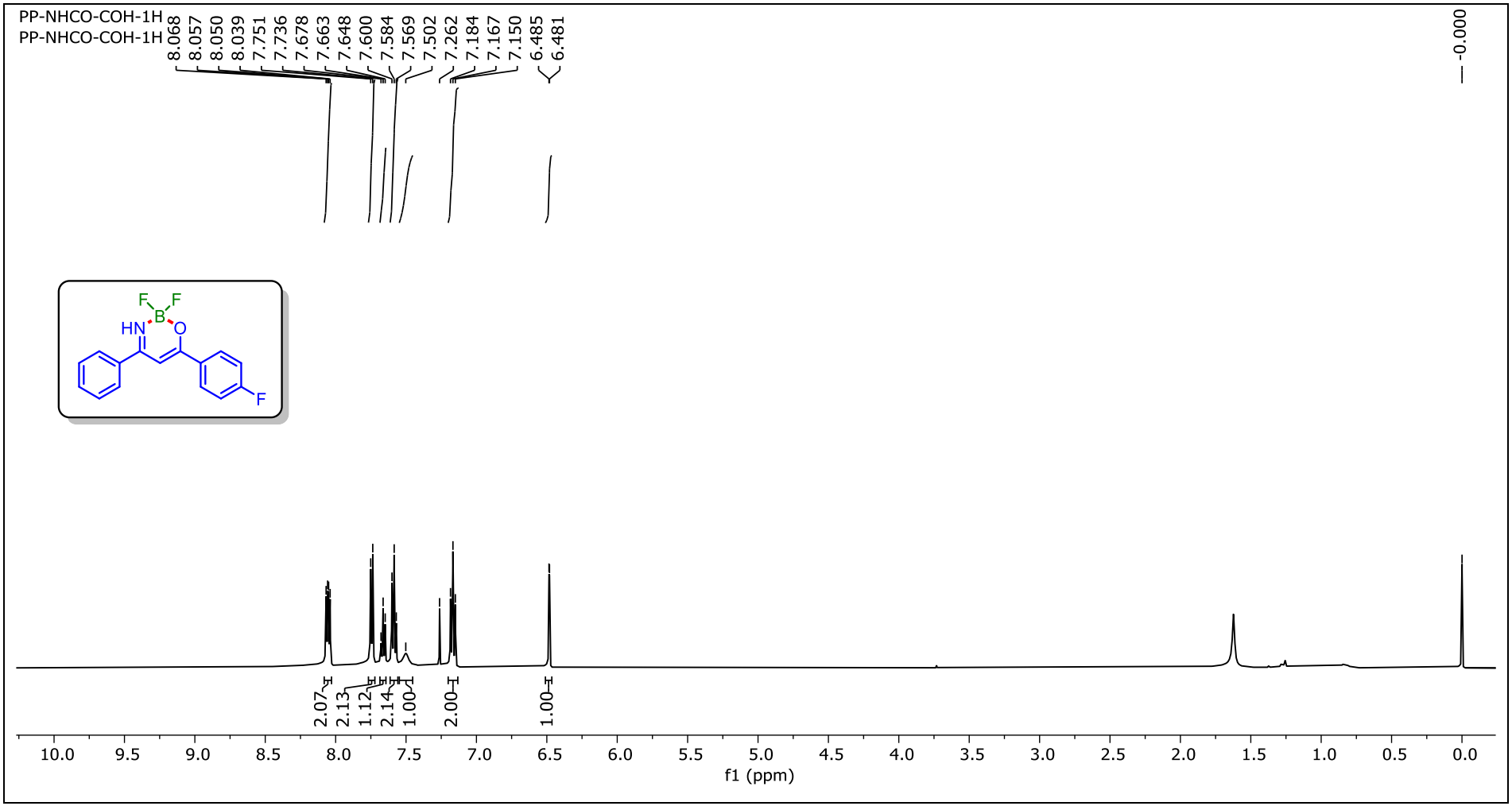
^{19}F NMR of **6-(4-(*tert*-Butyl)phenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2r)** ($CDCl_3$, 471 MHz)



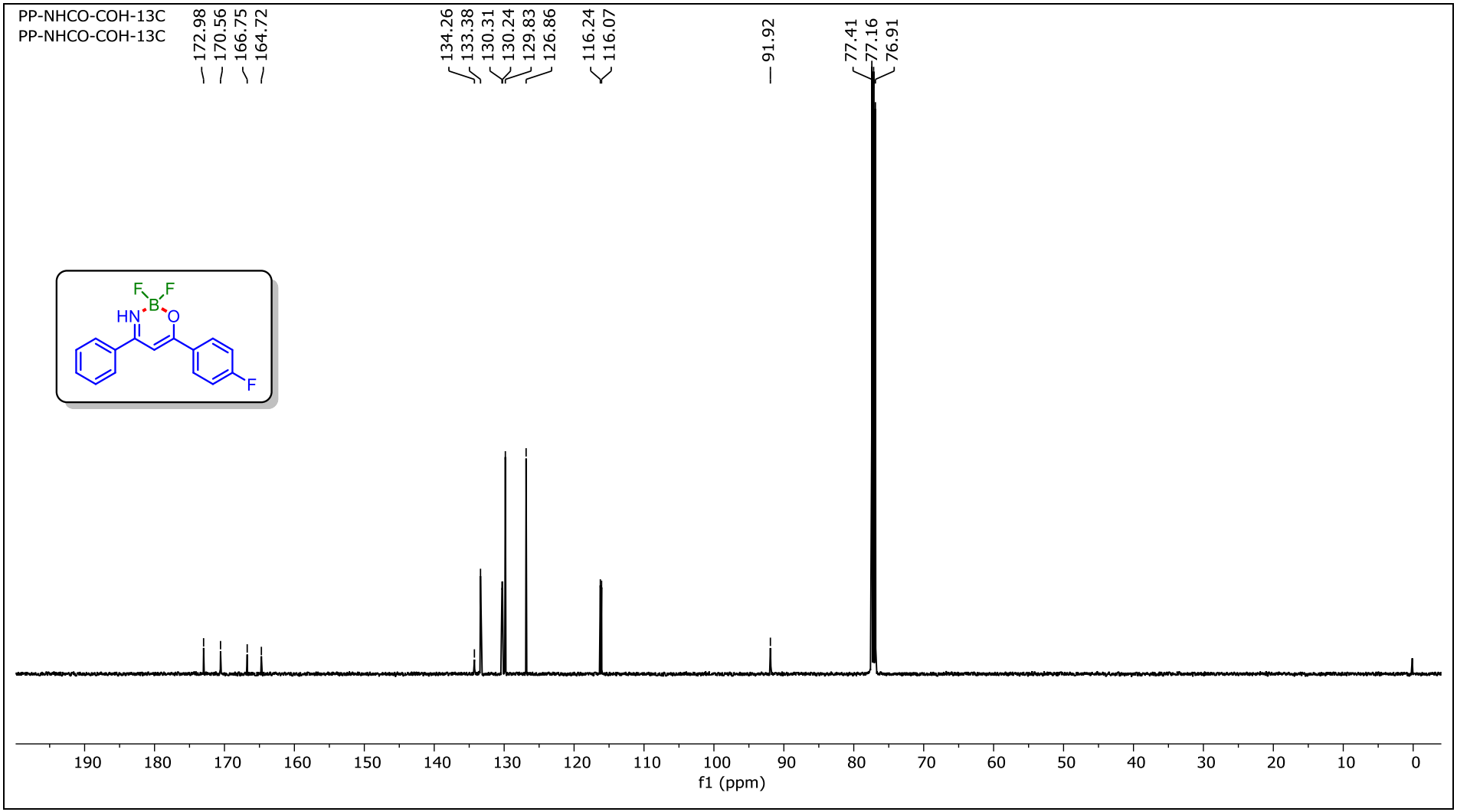
^{11}B NMR of **6-(4-(*tert*-Butyl)phenyl)-2,2-difluoro-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2r)** ($CDCl_3$, 160 MHz)



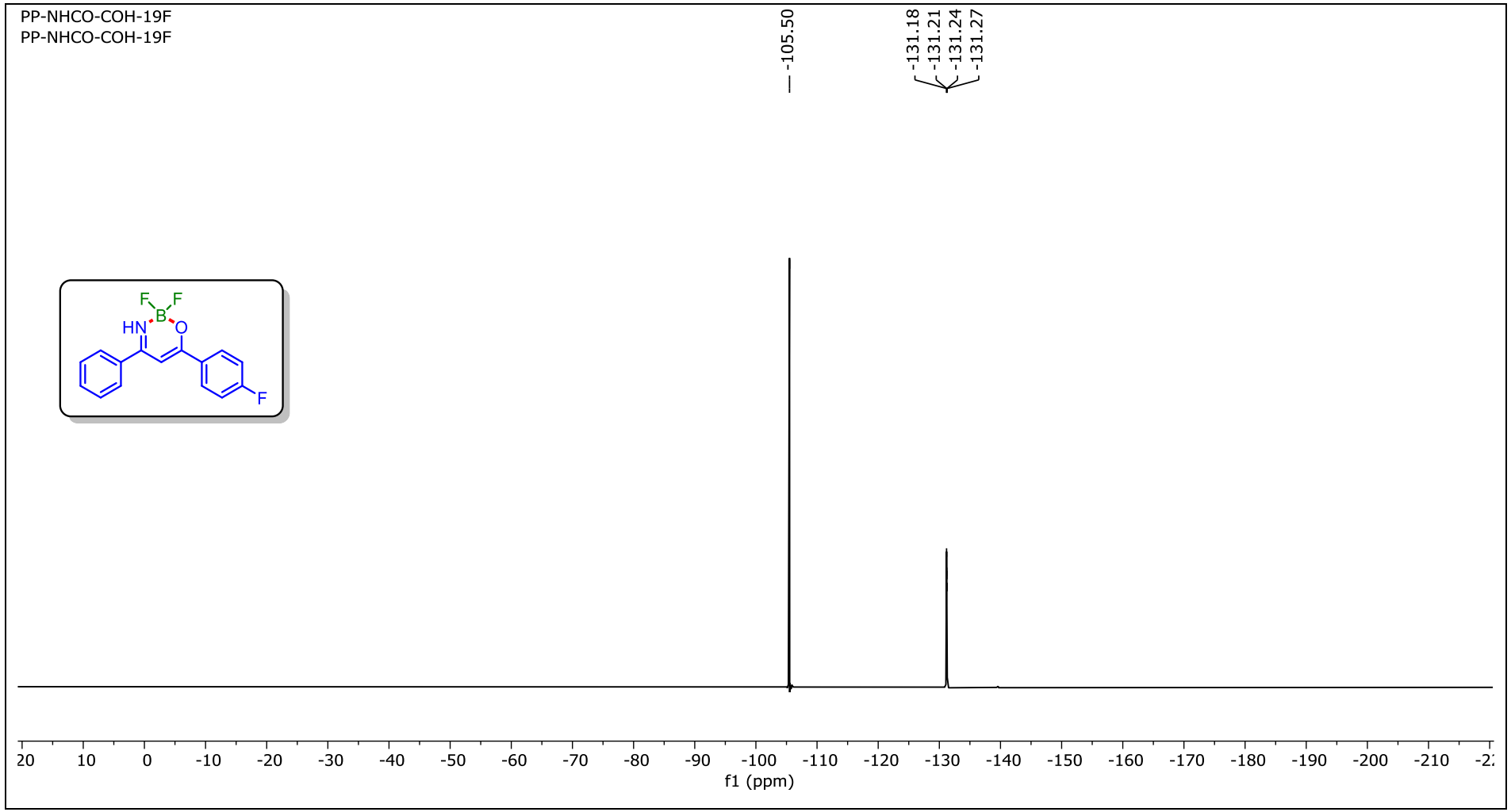
^{1}H NMR of **2,2-Difluoro-6-(4-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2s)** ($CDCl_3$, 500 MHz)



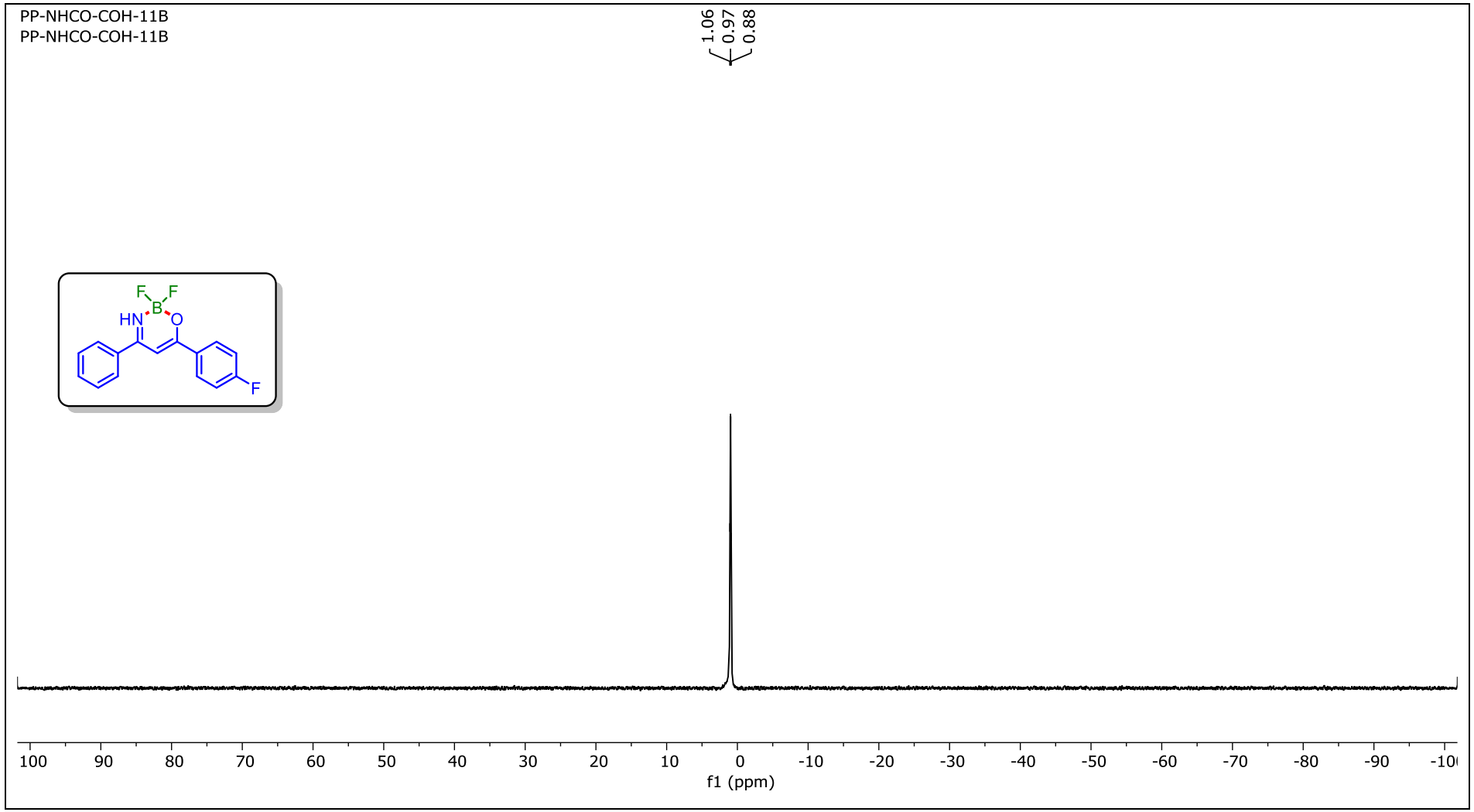
^{13}C {^{1}H} NMR of **2,2-Difluoro-6-(4-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2s)** ($CDCl_3$, 126 MHz)



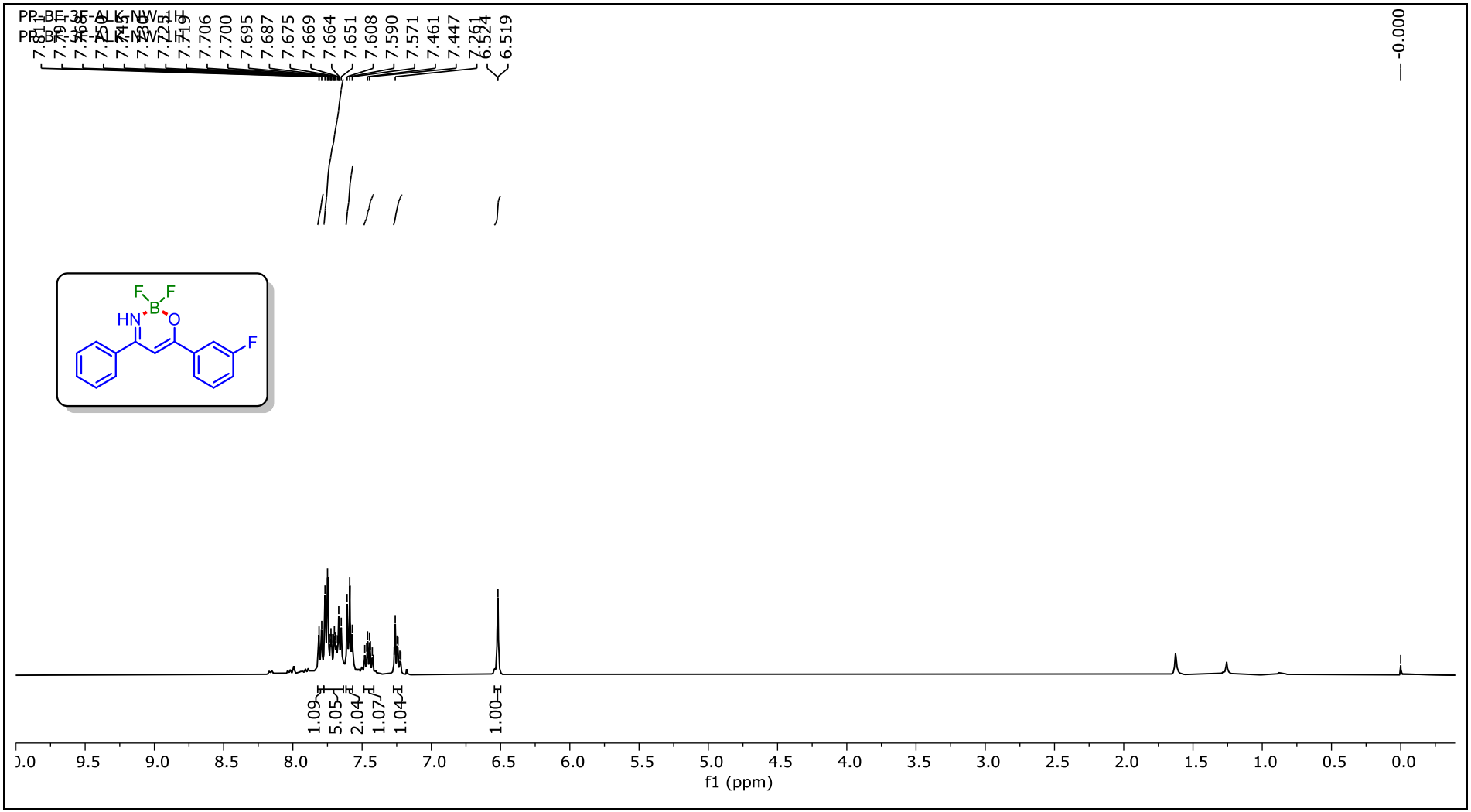
^{19}F NMR of **2,2-Difluoro-6-(4-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2s)** ($CDCl_3$, 471 MHz)



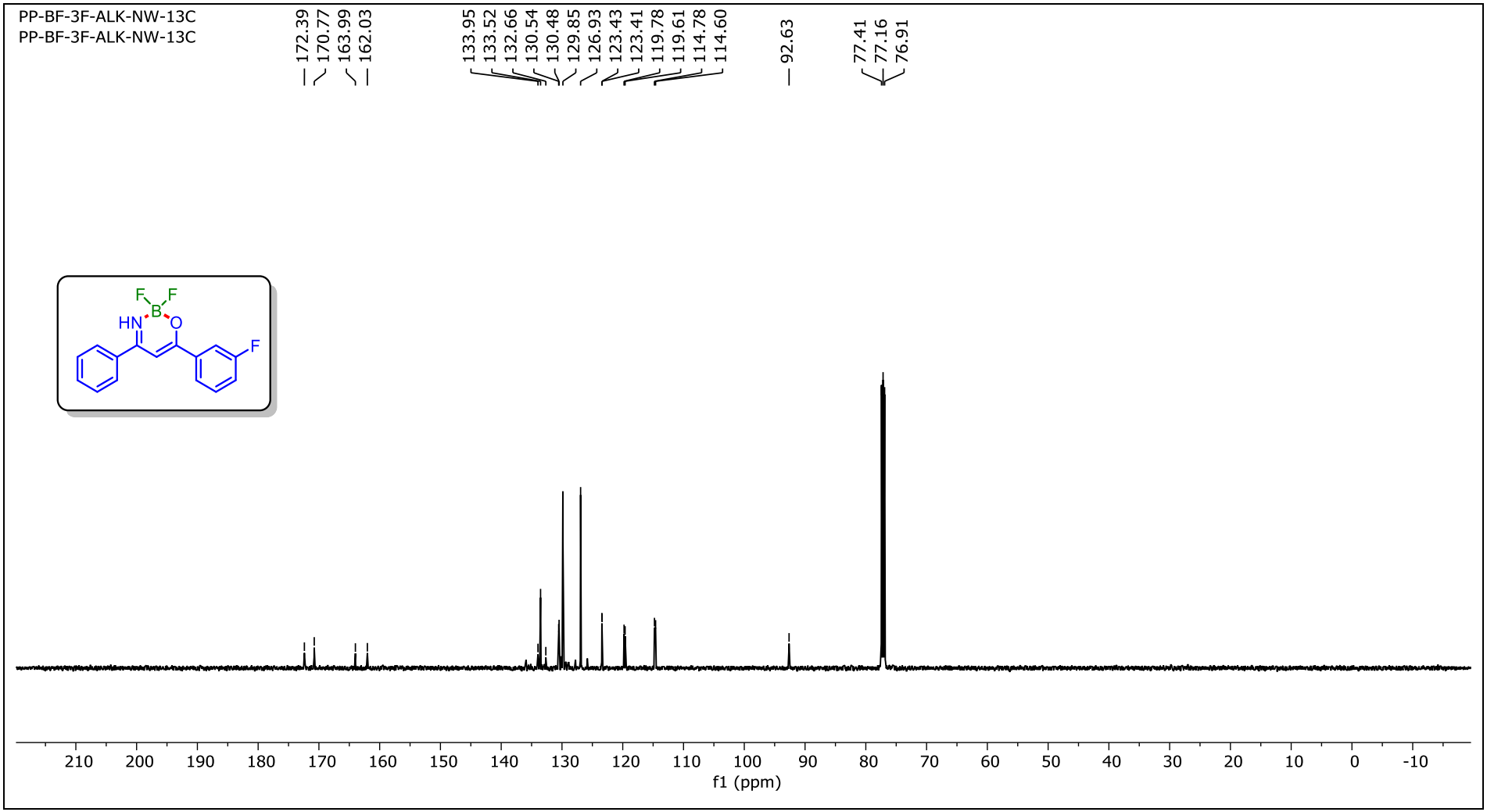
^{11}B NMR of **2,2-Difluoro-6-(4-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2s)** ($CDCl_3$, 160 MHz)



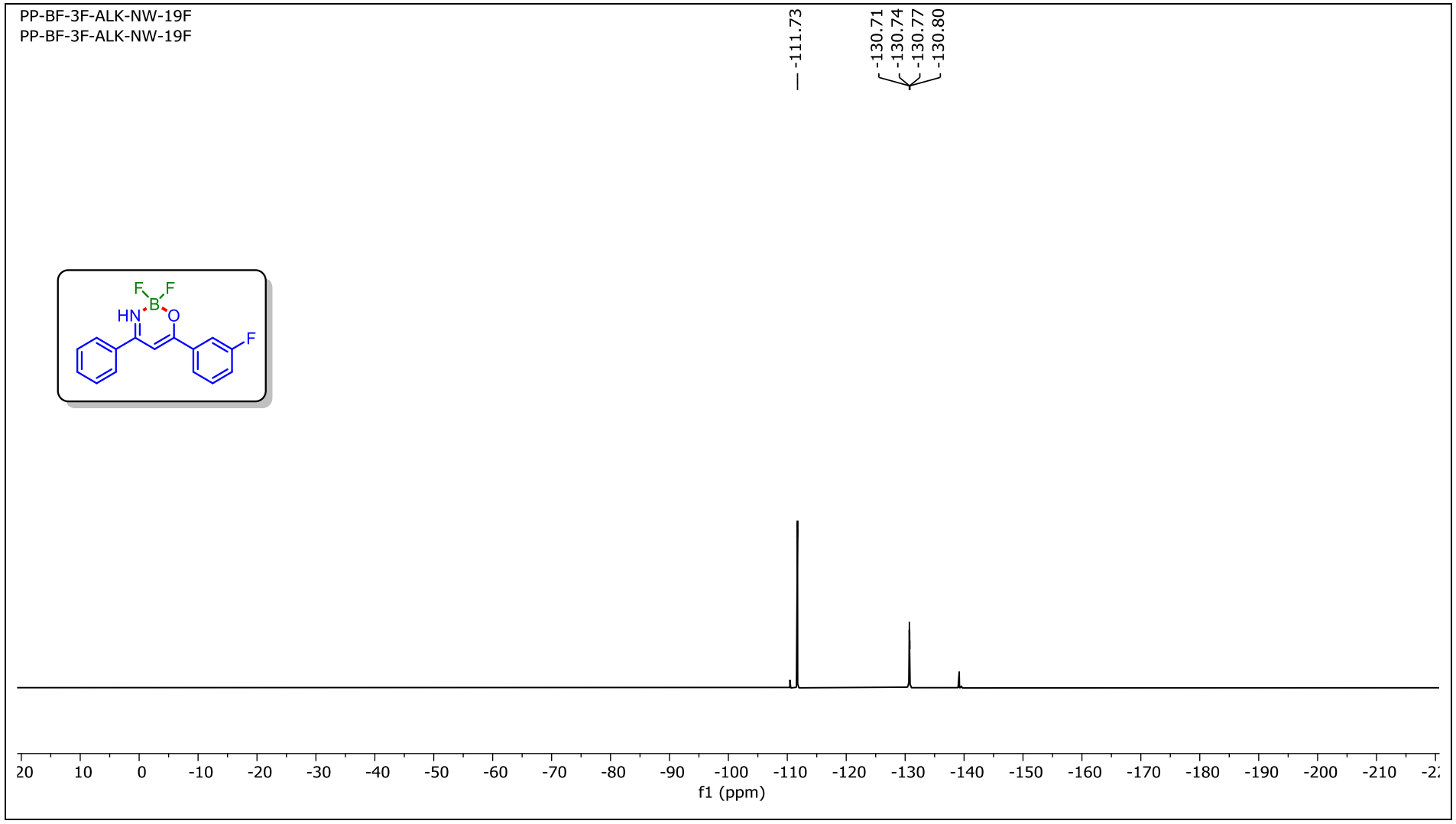
^{1}H NMR of **2,2-Difluoro-6-(3-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2t)** ($CDCl_3$, 400 MHz)



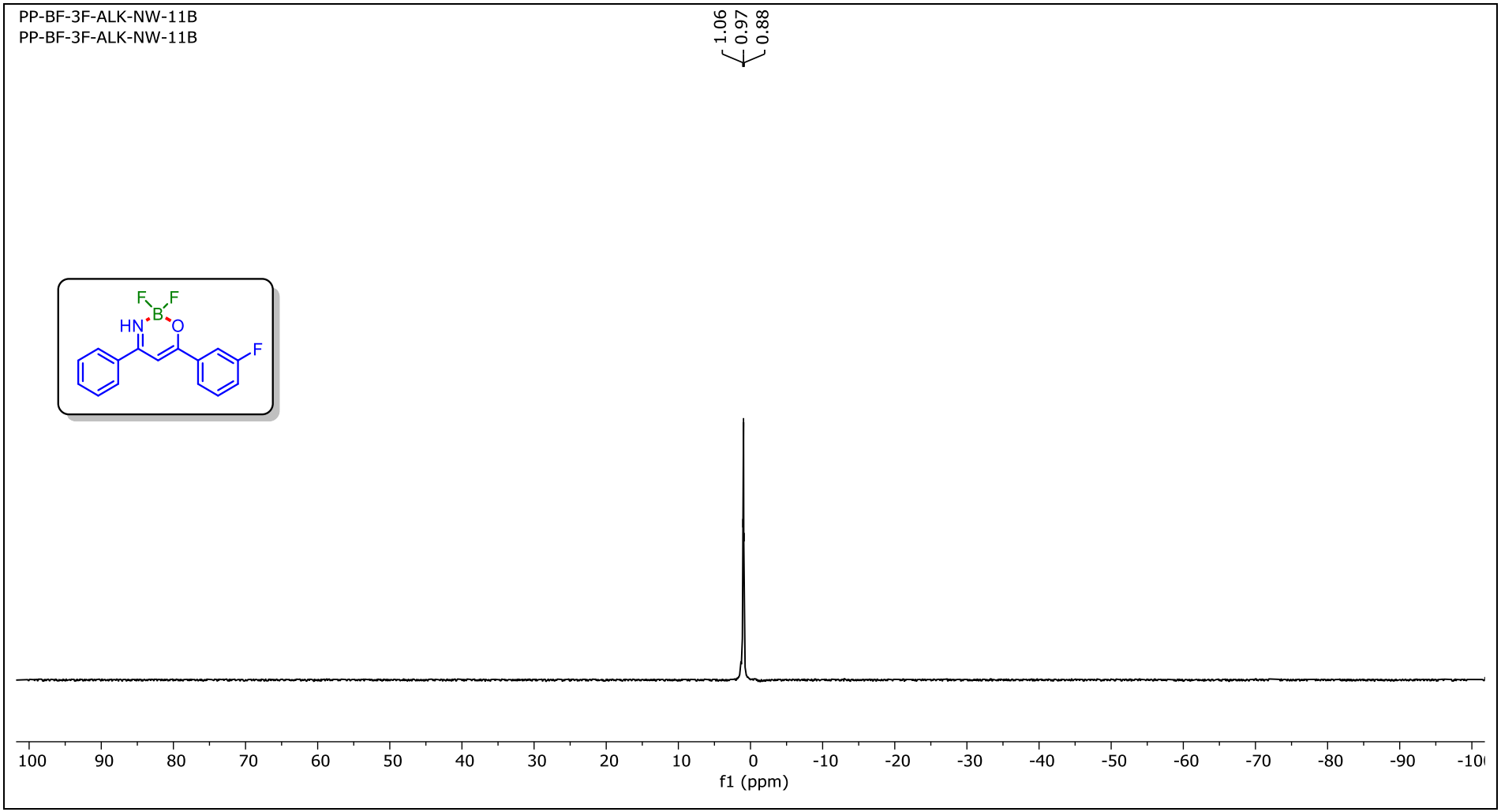
^{13}C {^{1}H} NMR of **2,2-Difluoro-6-(3-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2t)** ($CDCl_3$, 126 MHz)



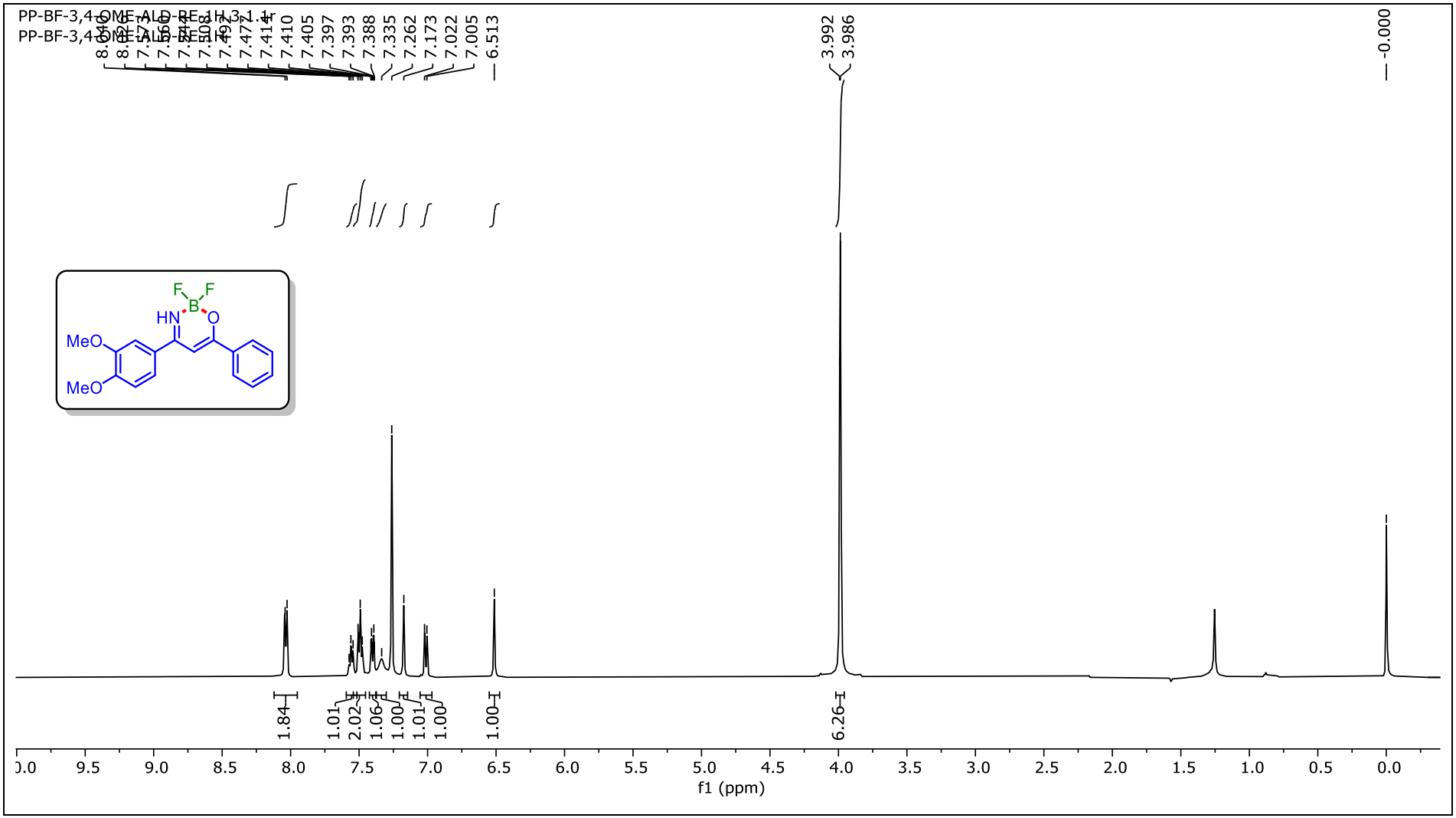
^{19}F NMR of **2,2-Difluoro-6-(3-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2t)** ($CDCl_3$, 471 MHz)



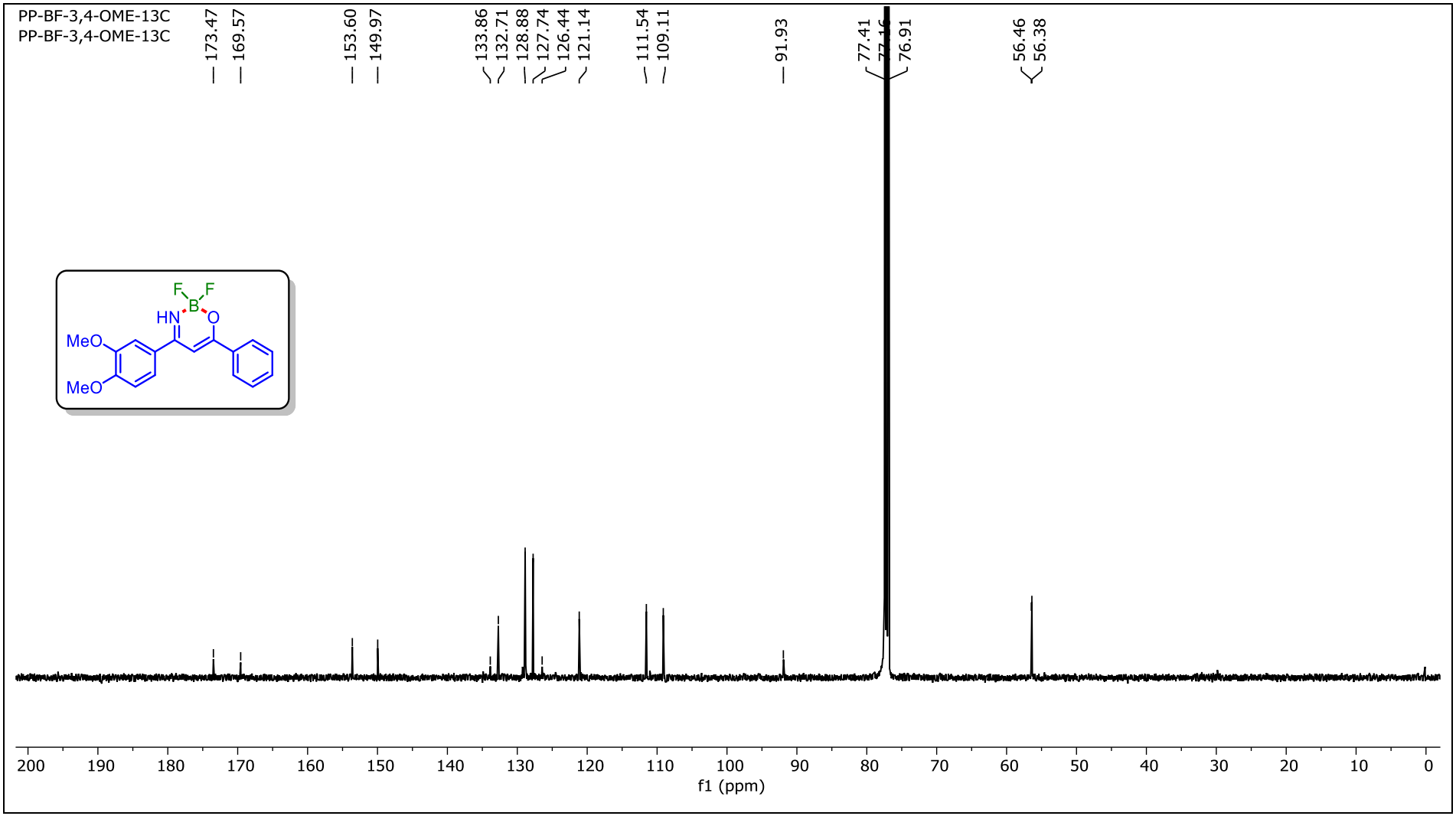
^{11}B NMR of **2,2-Difluoro-6-(3-fluorophenyl)-4-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2t)** ($CDCl_3$, 260 MHz)



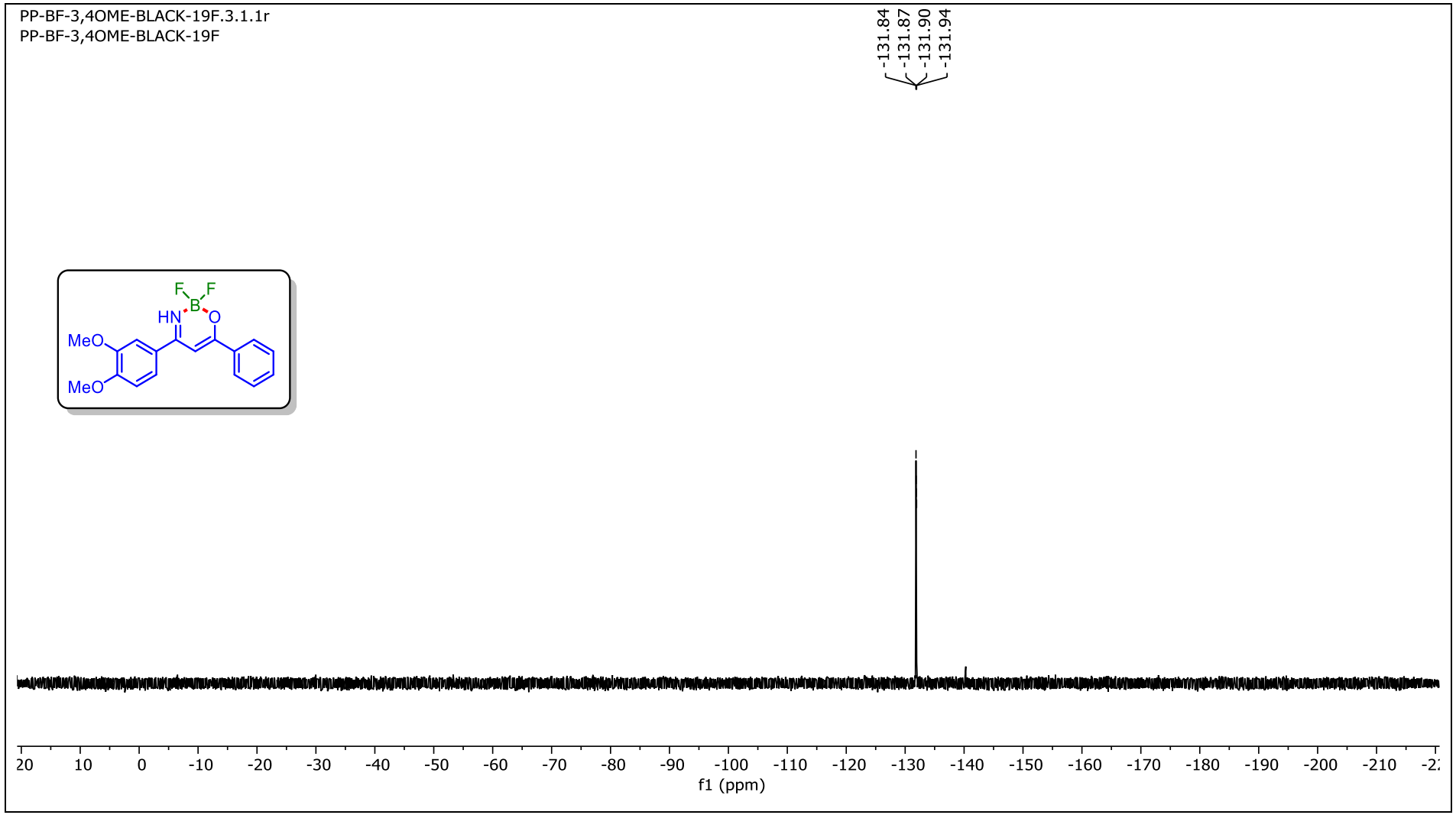
^{1}H NMR of **4-(3,4-Dimethoxyphenyl)-2,2-difluoro-6- phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2u)** ($CDCl_3$, 500 MHz)



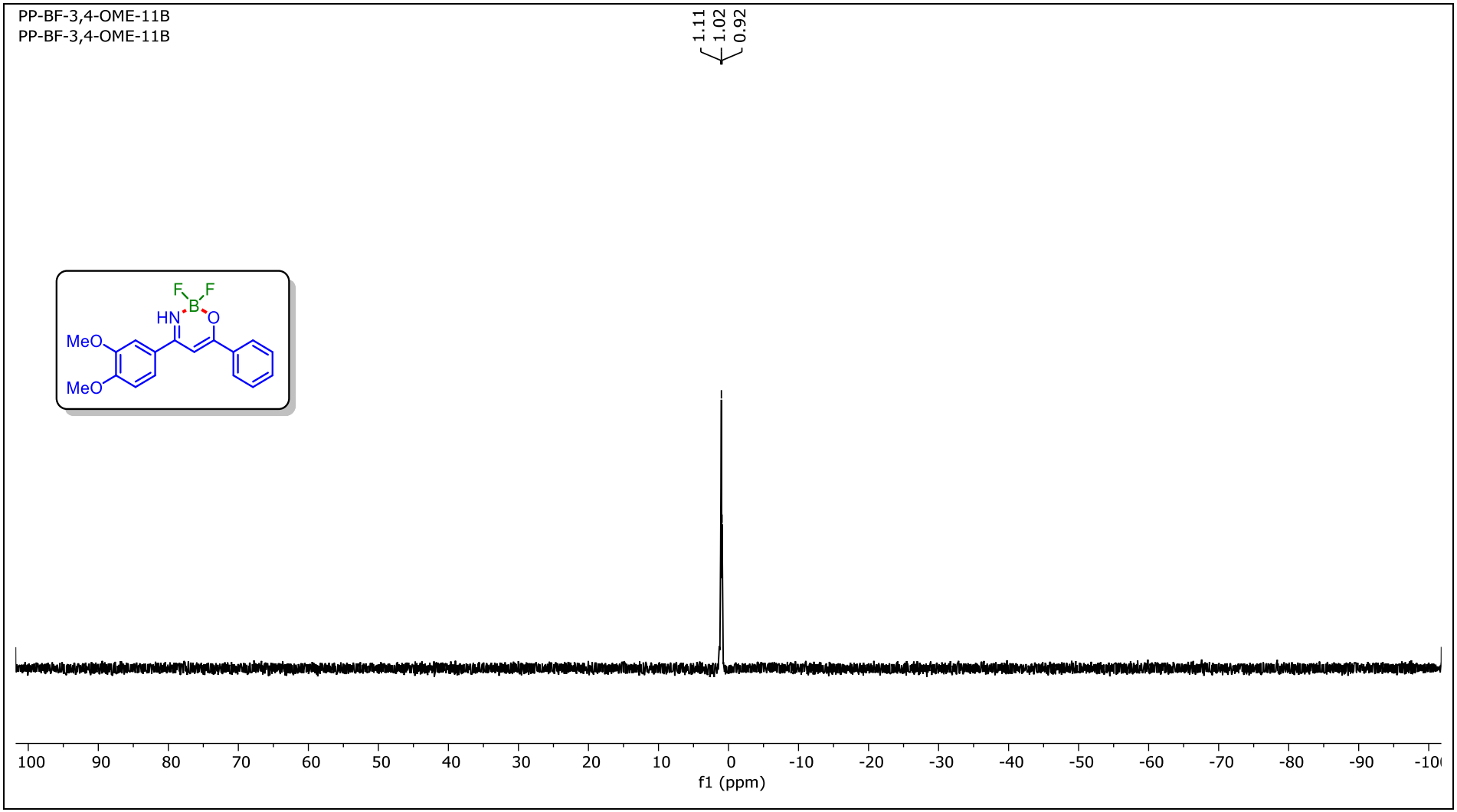
^{13}C {^{1}H} NMR of **4-(3,4-Dimethoxyphenyl)-2,2-difluoro-6- phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2u)** ($CDCl_3$, 126 MHz)



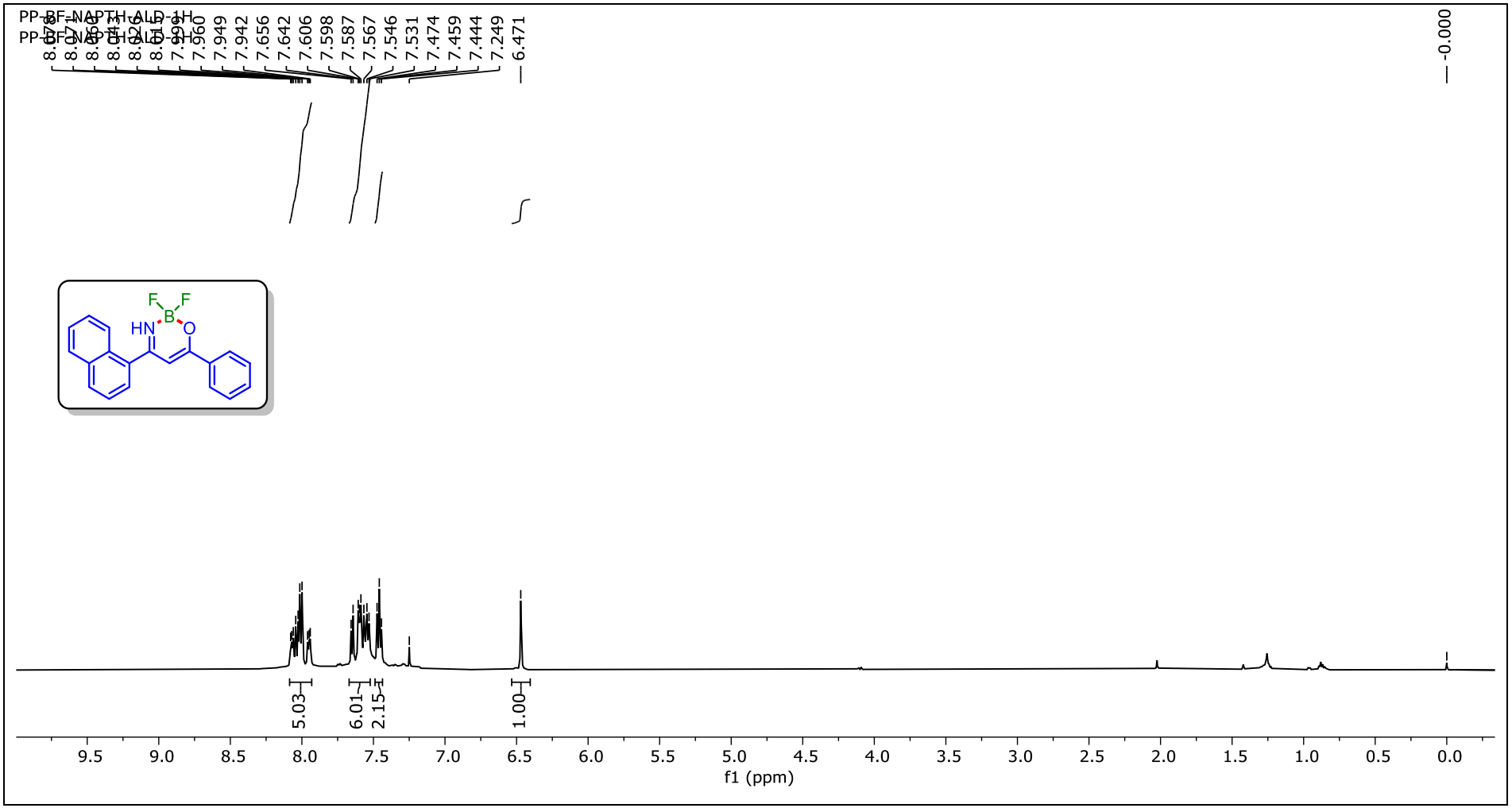
^{19}F NMR of **4-(3,4-Dimethoxyphenyl)-2,2-difluoro-6- phenyl-2*H*-1,3,2λ^4-oxazaborinine (2u)** ($CDCl_3$, 471 MHz)



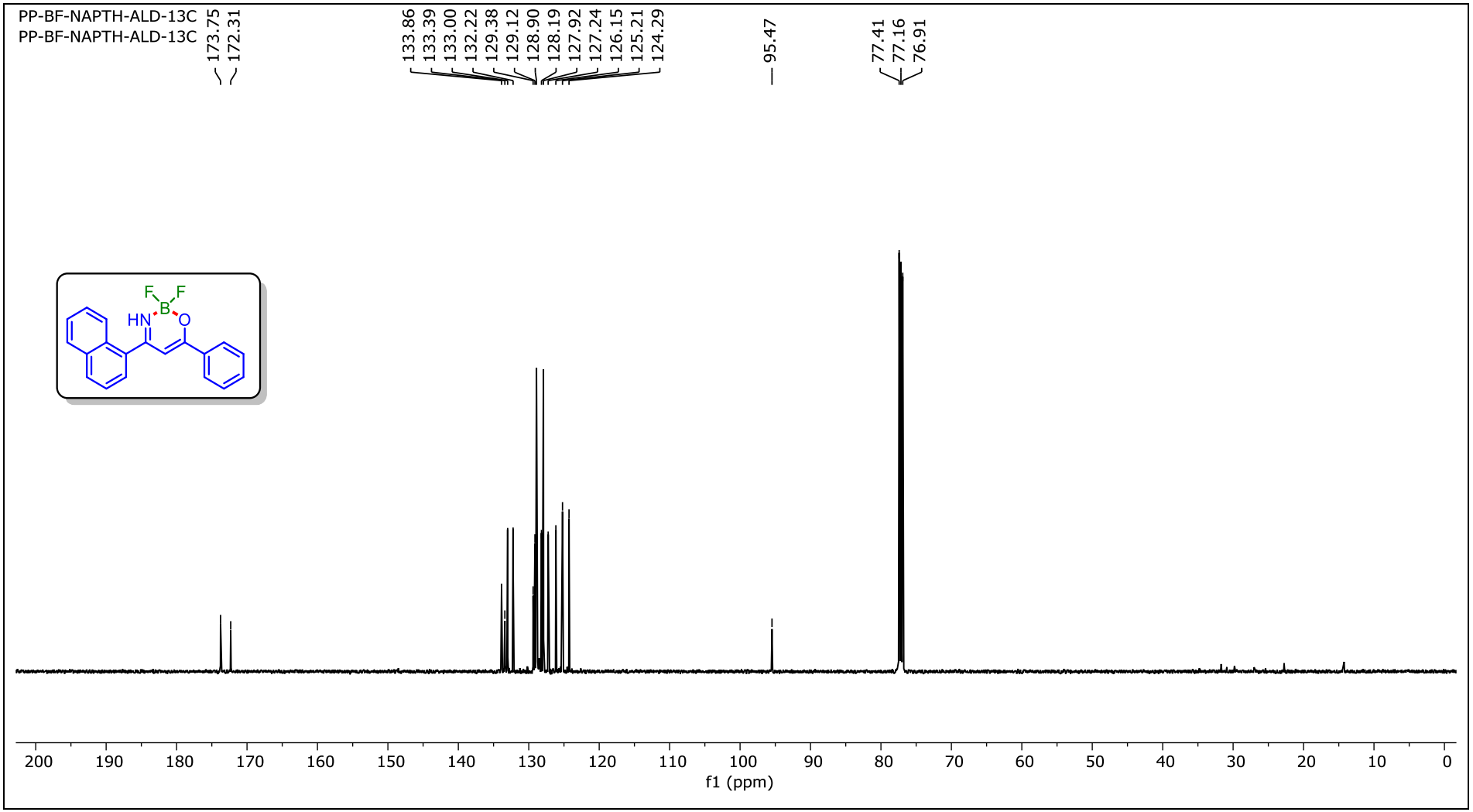
^{11}B NMR of **4-(3,4-Dimethoxyphenyl)-2,2-difluoro-6- phenyl-2*H*-1,3,2λ^4-oxazaborinine (2u)** ($CDCl_3$, 160 MHz)



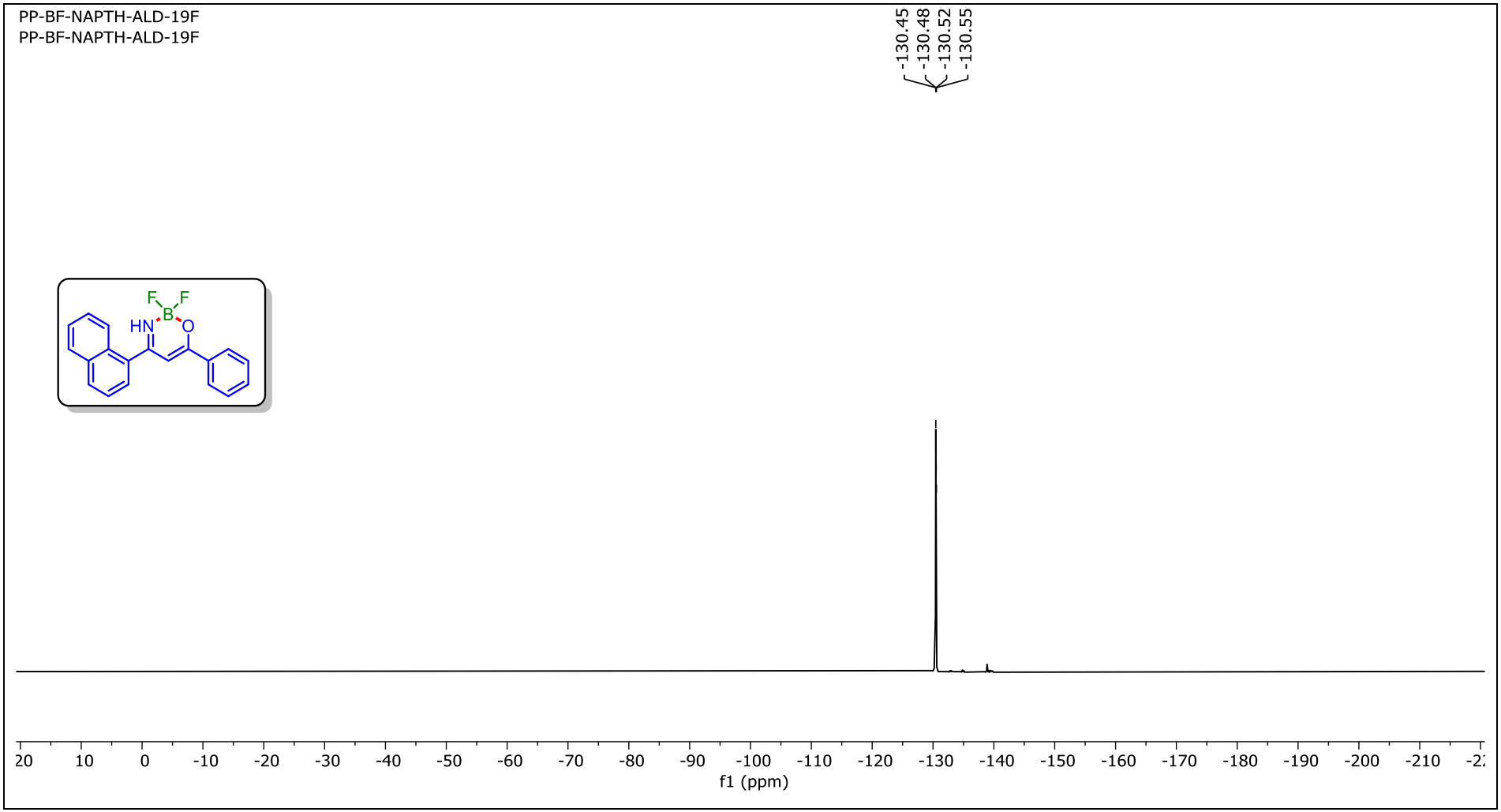
^{1}H NMR of **2,2-Difluoro-4-(naphthalen-1-yl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2v)** ($CDCl_3$, 500 MHz)



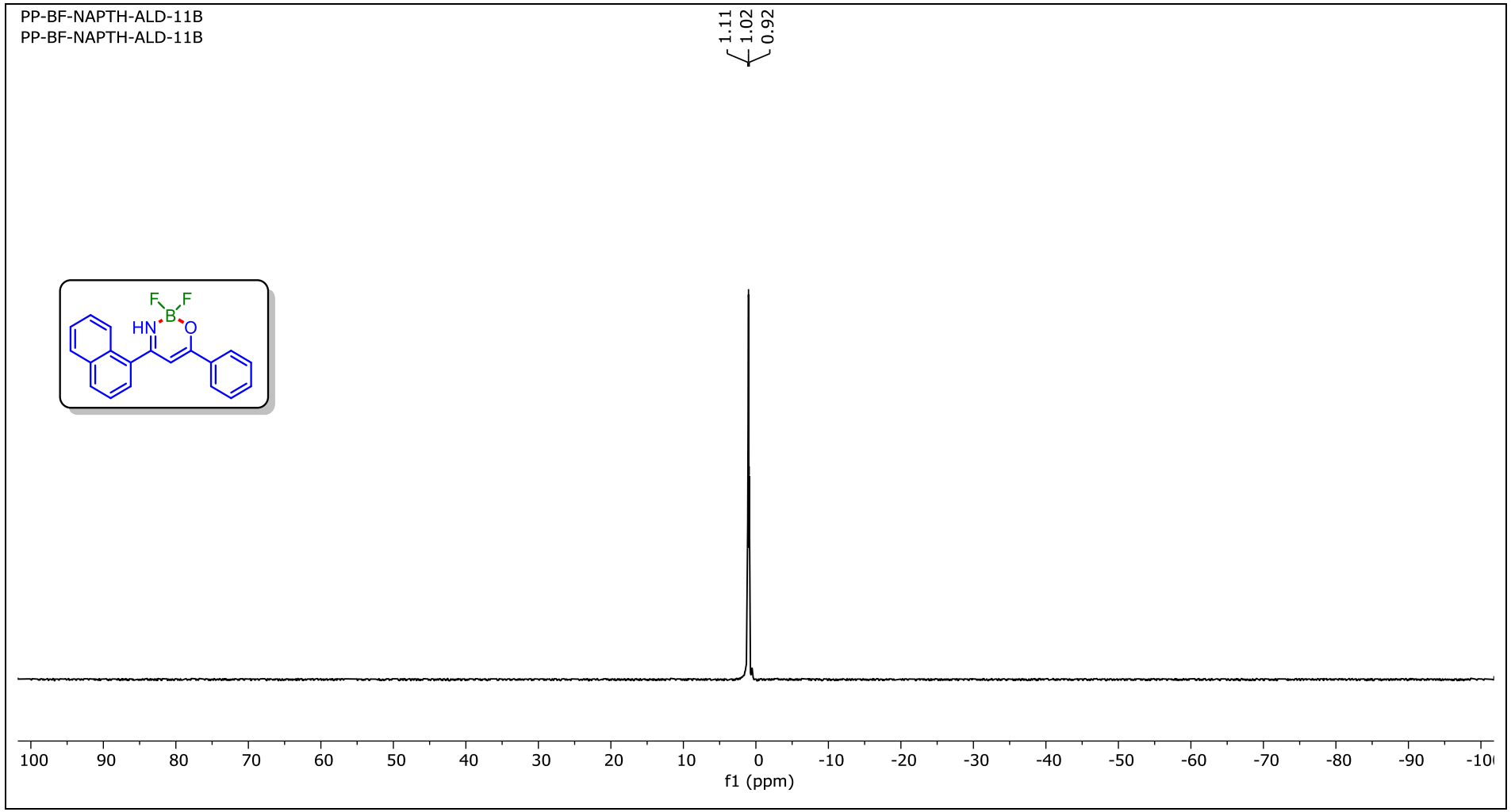
^{13}C {^{1}H} NMR of **2,2-Difluoro-4-(naphthalen-1-yl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2v)** ($CDCl_3$, 126 MHz)



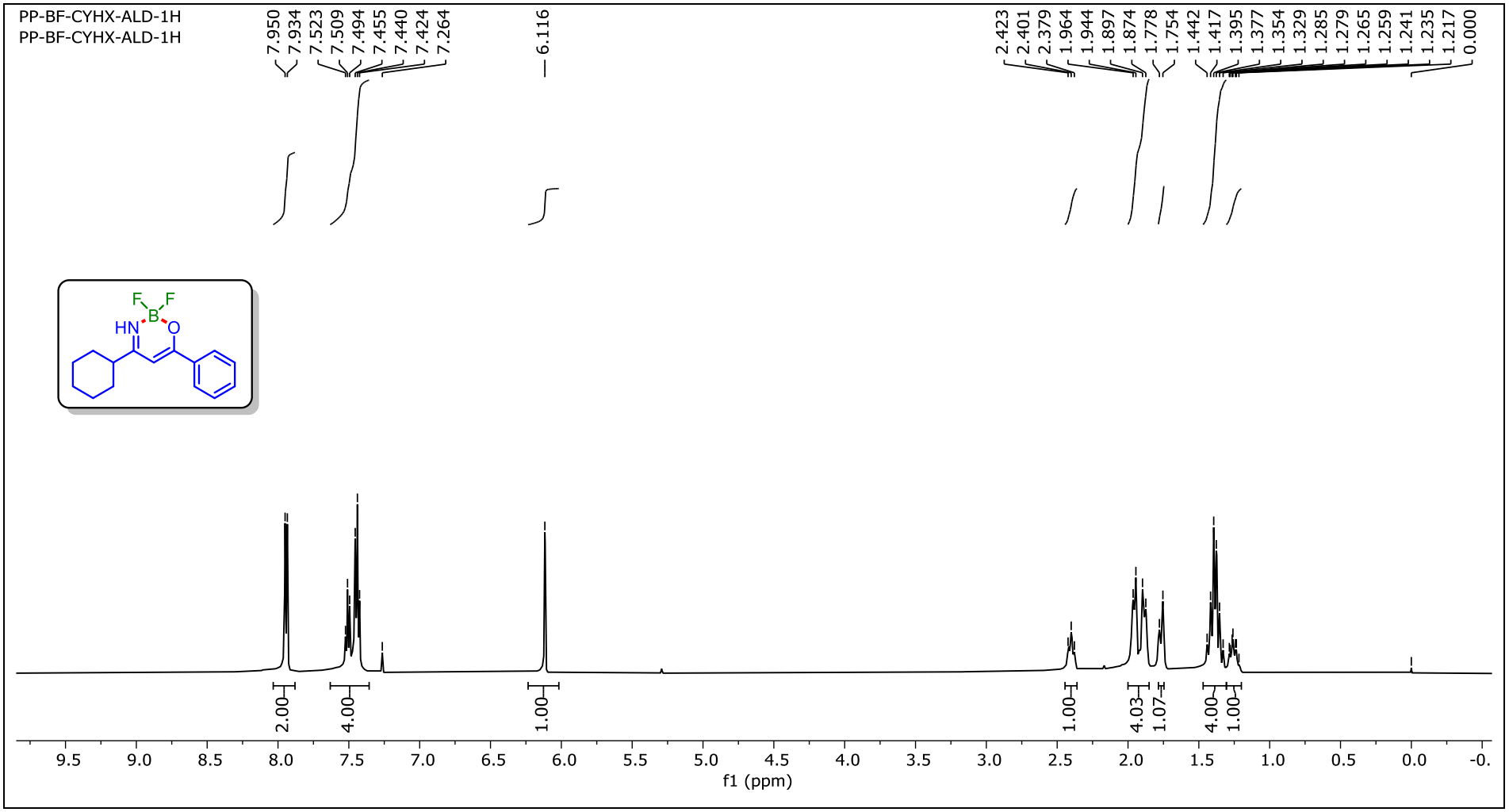
^{19}F NMR of **2,2-Difluoro-4-(naphthalen-1-yl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2v)** ($CDCl_3$, 471 MHz)



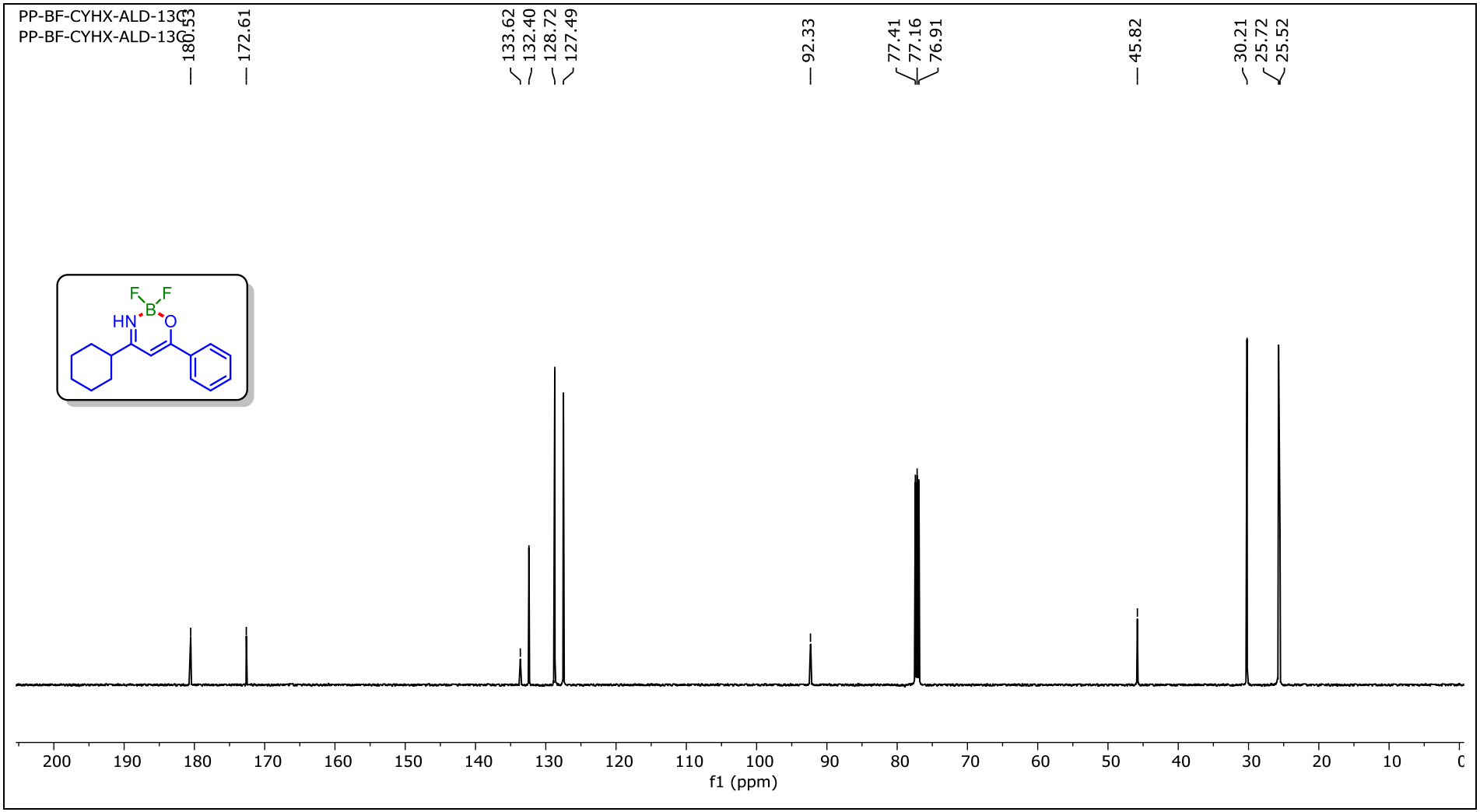
^{11}B NMR of **2,2-Difluoro-4-(naphthalen-1-yl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2v)** ($CDCl_3$, 160 MHz)



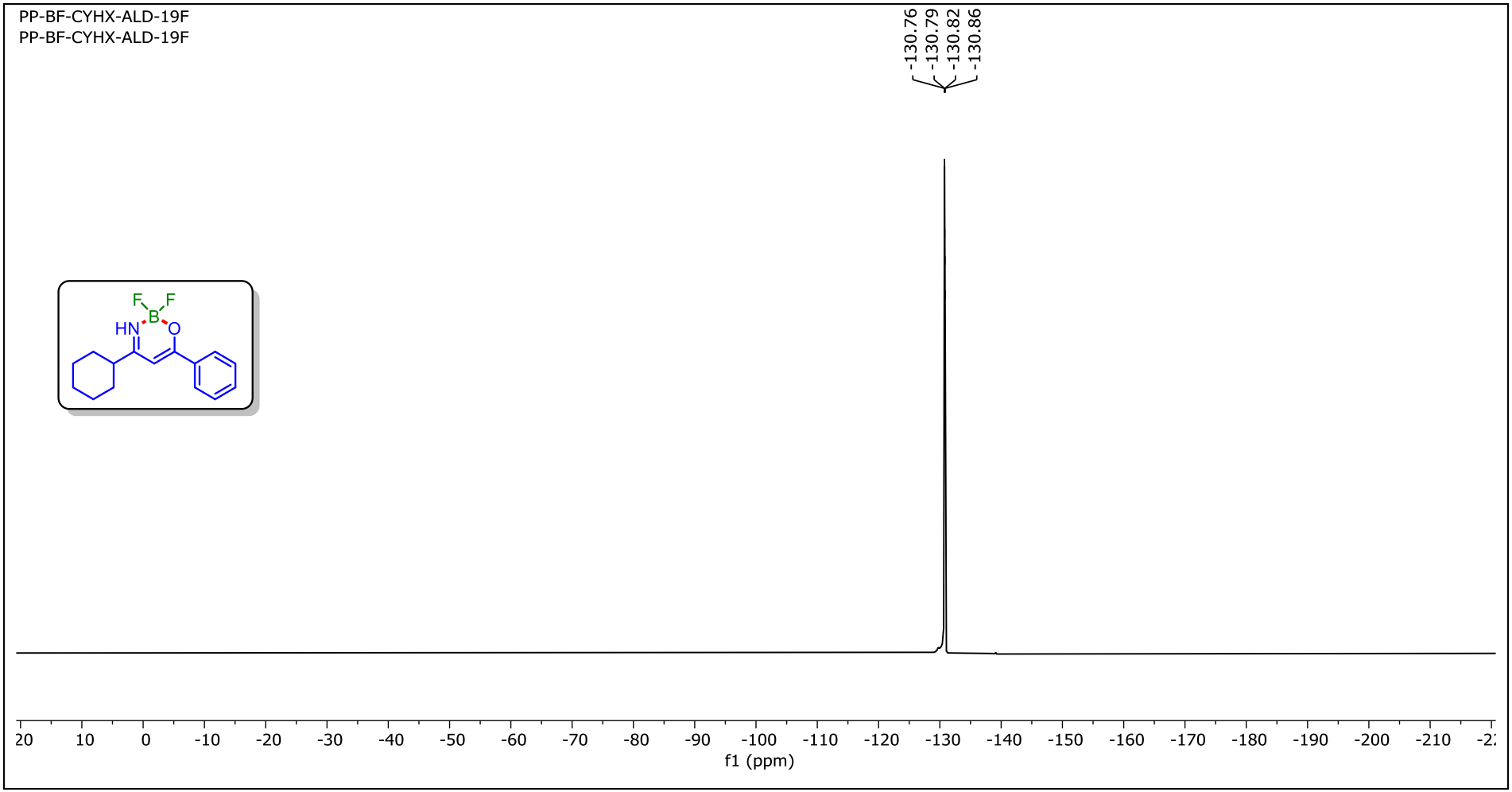
^{1}H NMR of **4-Cyclohexyl-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2w)** ($CDCl_3$, 500 MHz)



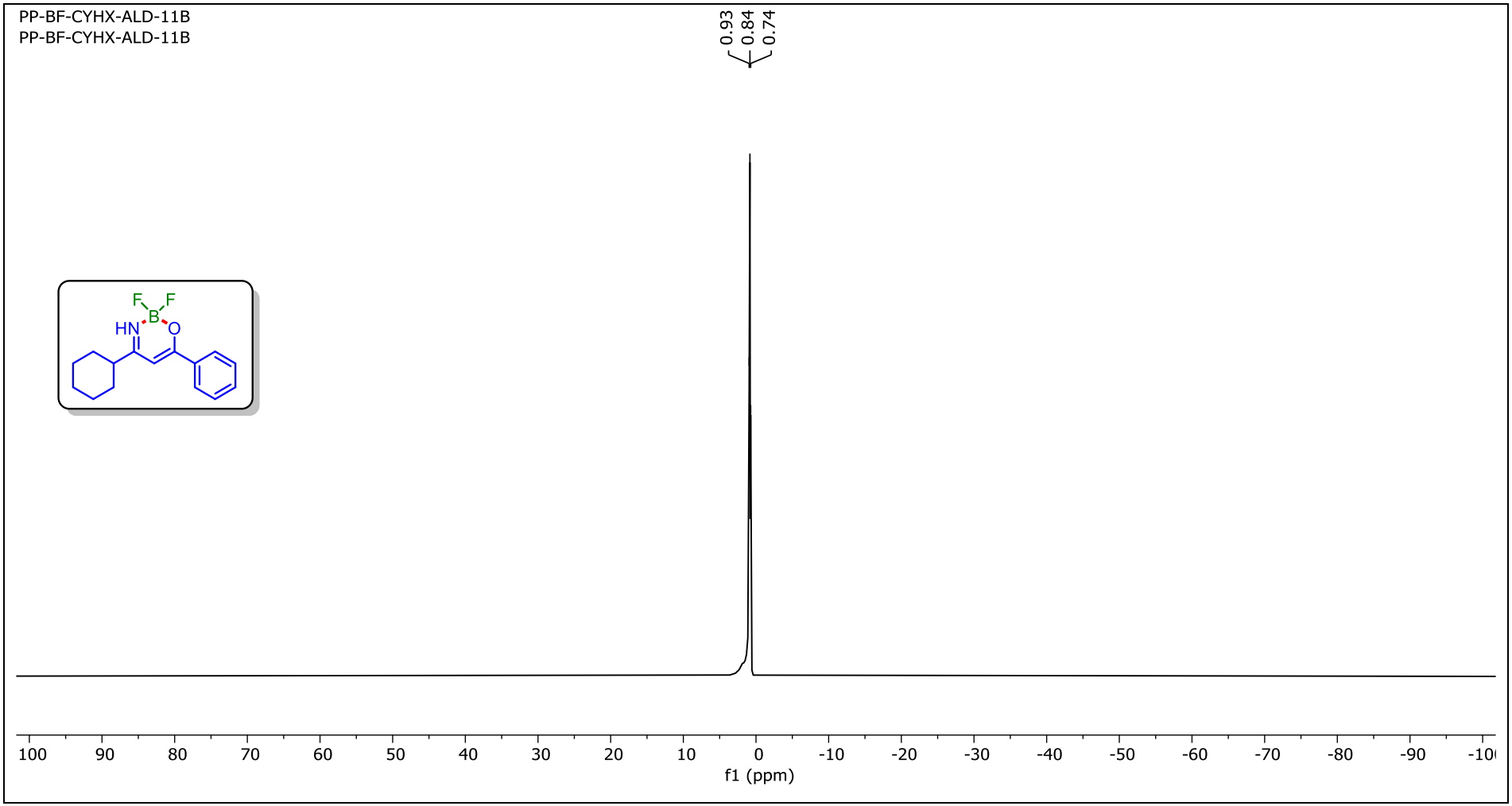
^{13}C {^{1}H} NMR of **4-Cyclohexyl-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2w)** ($CDCl_3$, 126 MHz)



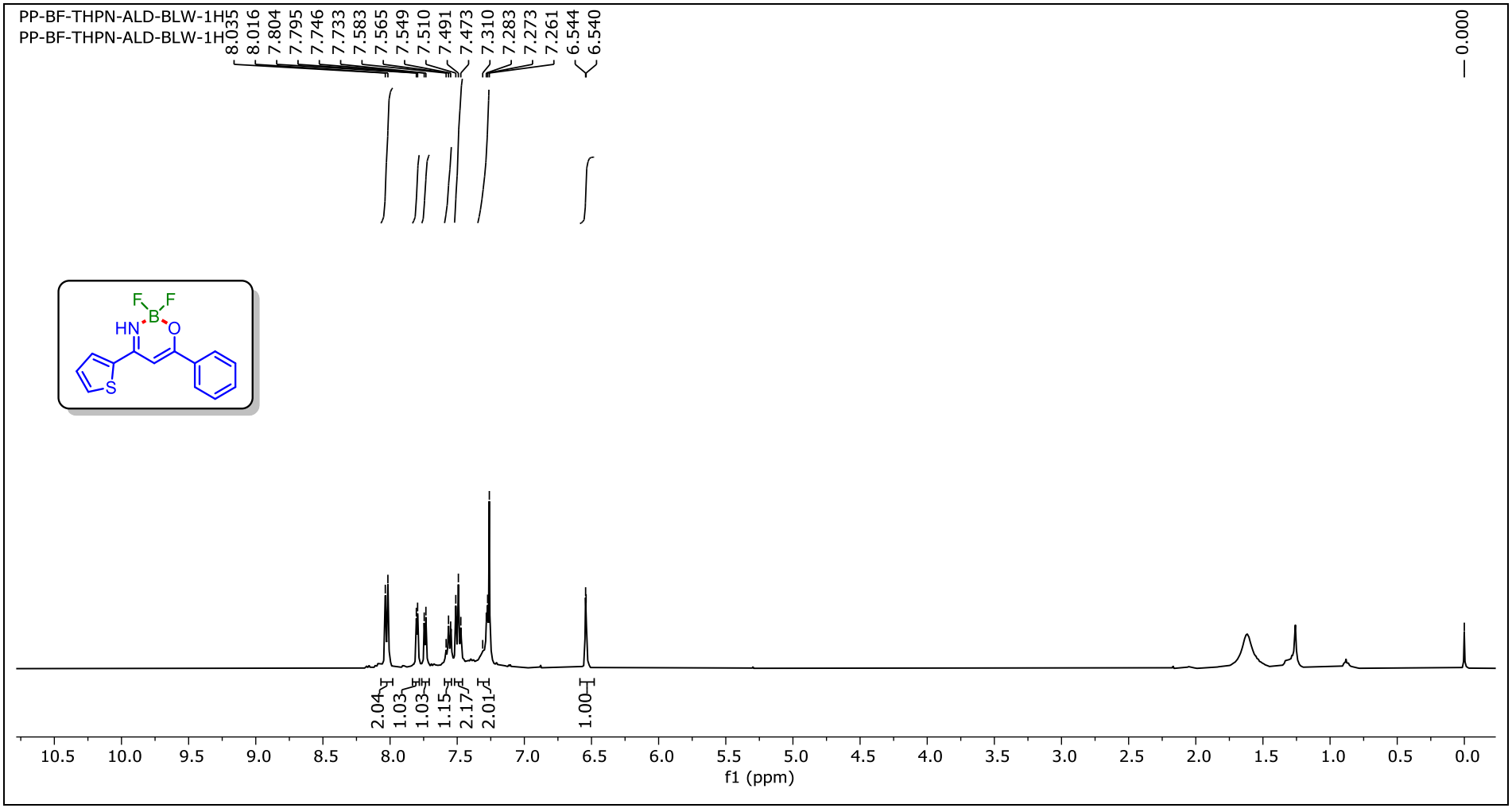
^{19}F NMR of **4-Cyclohexyl-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2w)** ($CDCl_3$, 471 MHz)



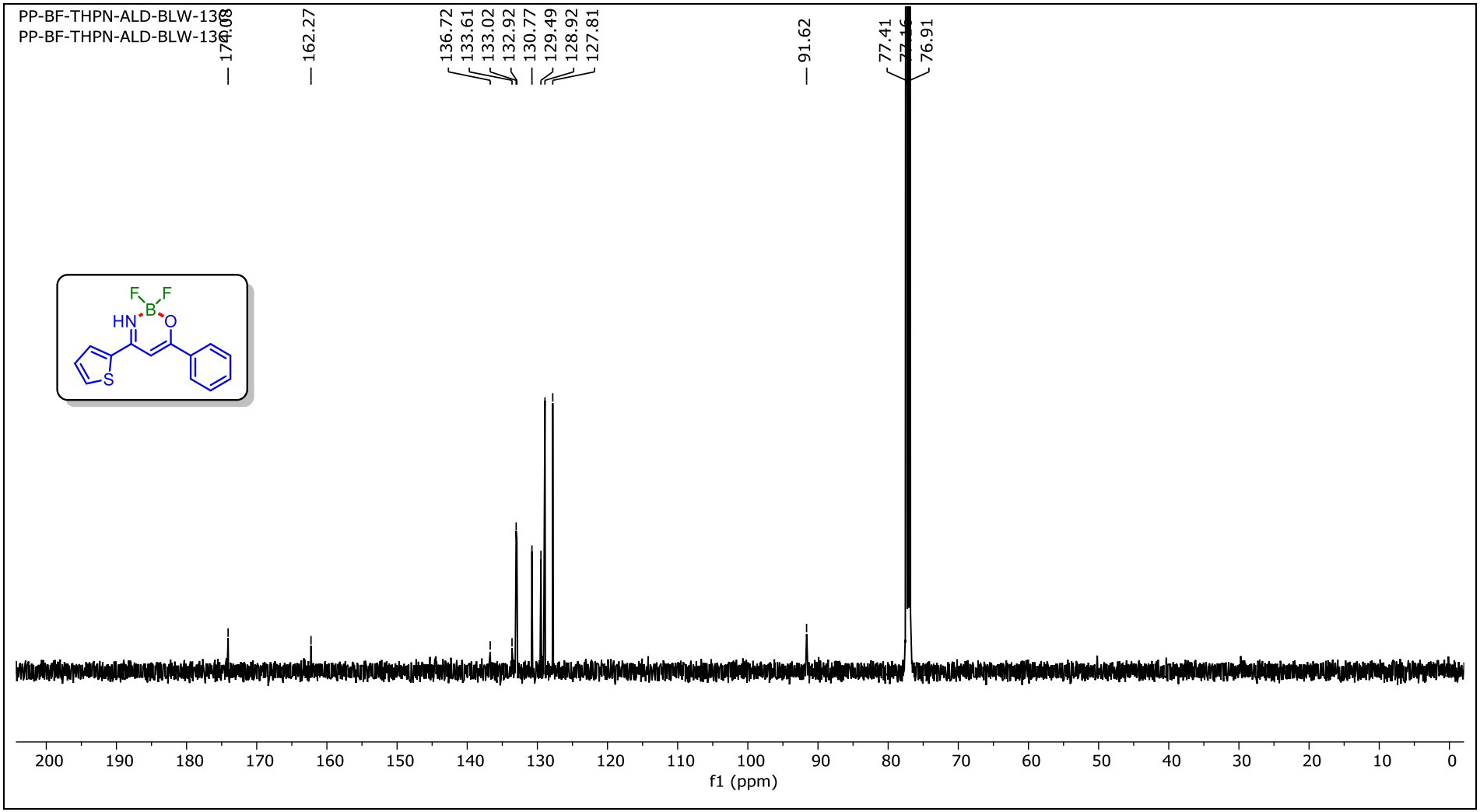
^{11}B NMR of **4-Cyclohexyl-2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2w)** ($CDCl_3$, 160 MHz)



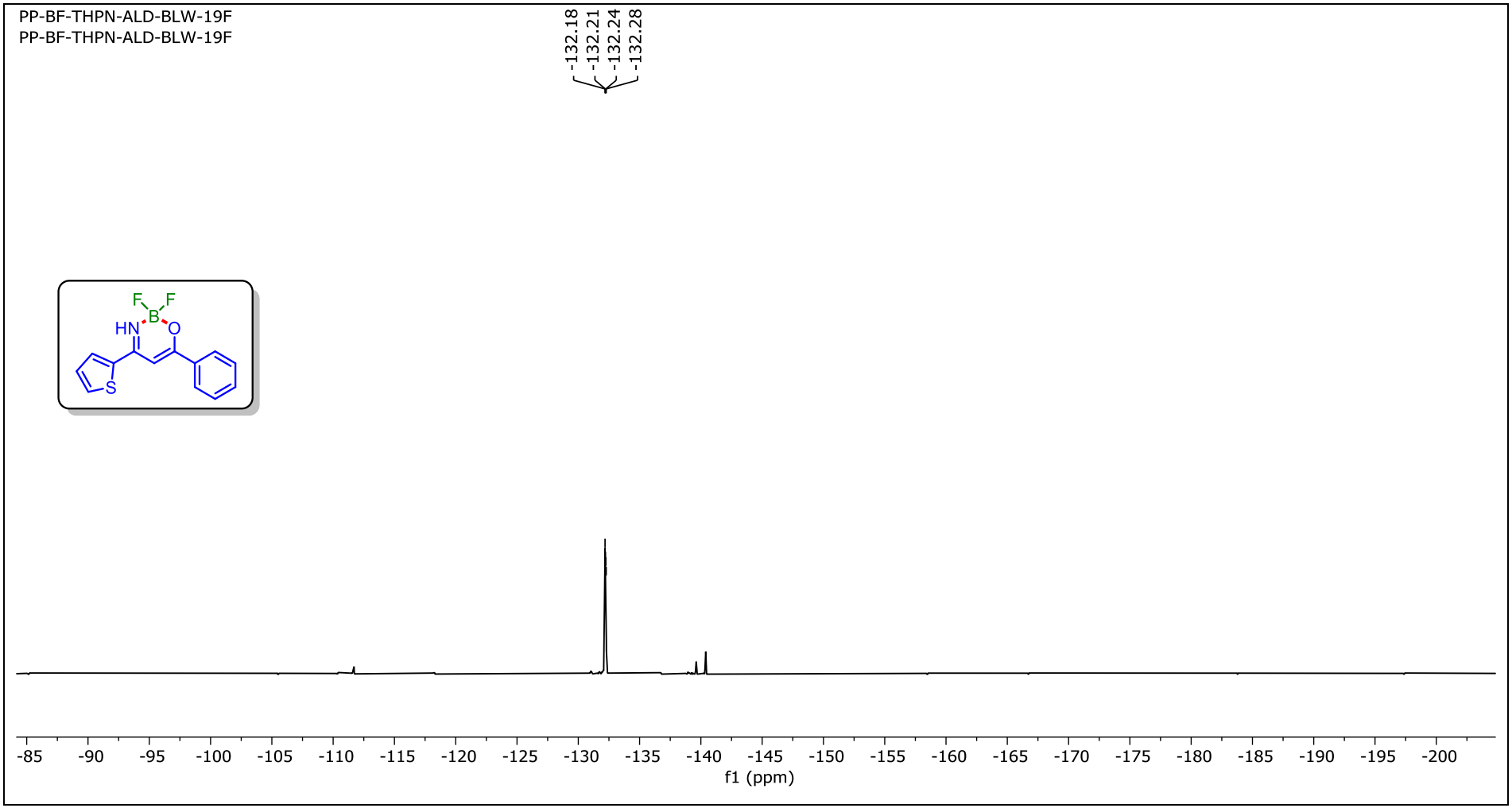
^{1}H NMR of **2,2-Difluoro-6-phenyl-4-(thiophen-2-yl)-2*H*-1,3,2λ^{4}-oxazaborinine (2x)** ($CDCl_3$, 400 MHz)



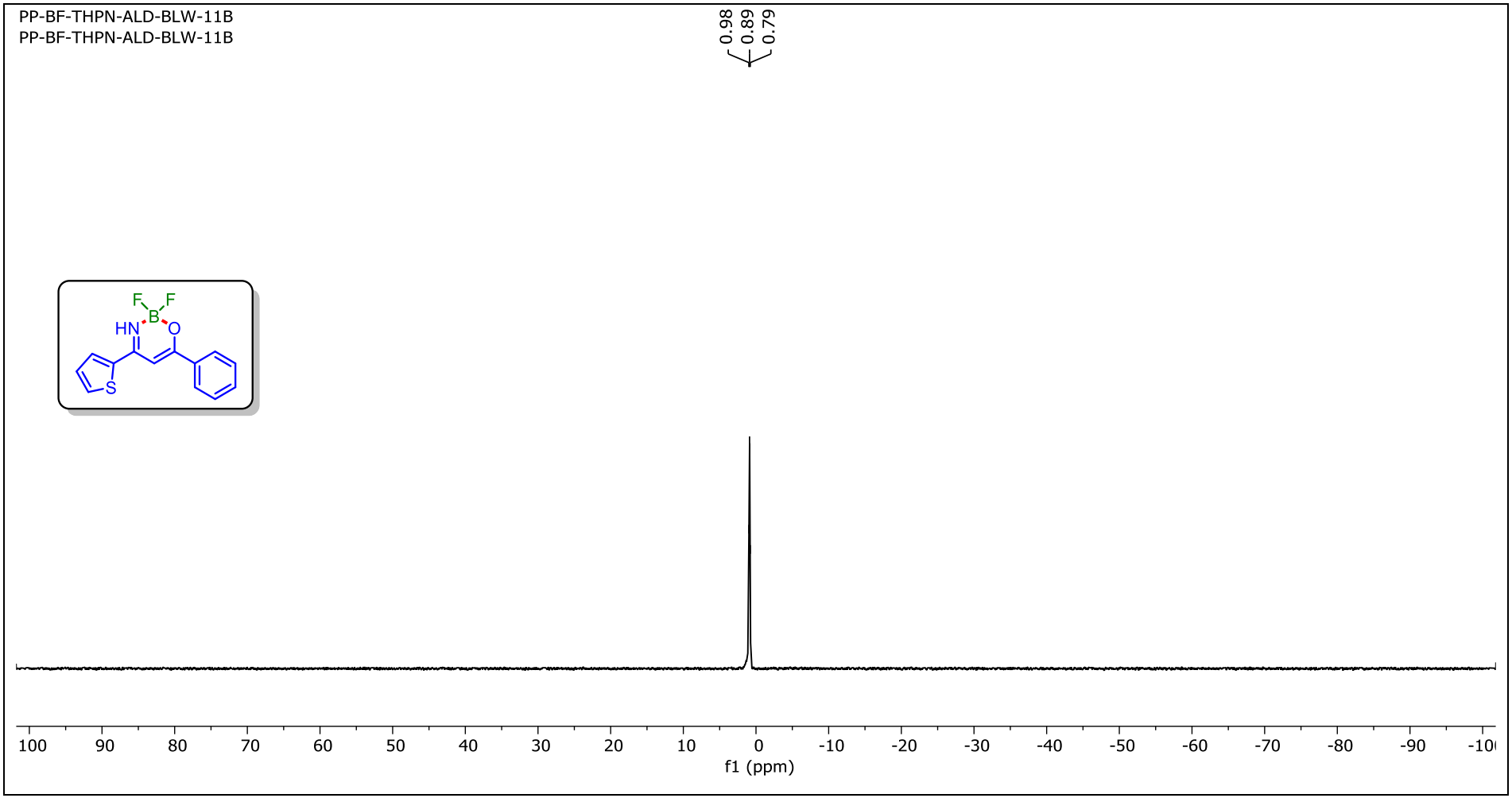
^{13}C {^{1}H} NMR of **2,2-Difluoro-6-phenyl-4-(thiophen-2-yl)-2*H*-1,3,2λ^{4}-oxazaborinine (2x)** ($CDCl_3$, 126 MHz)



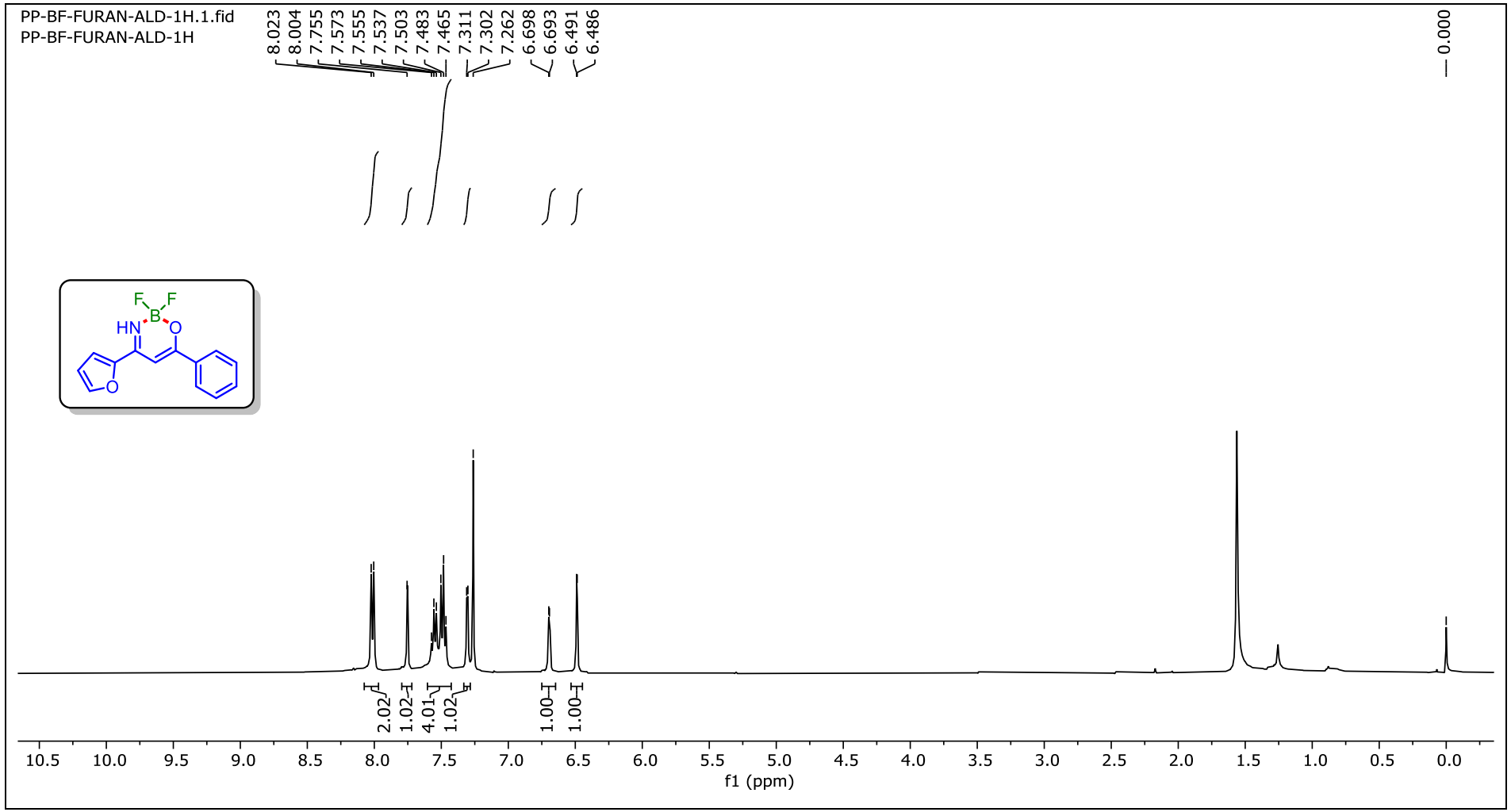
^{19}F NMR of **2,2-Difluoro-6-phenyl-4-(thiophen-2-yl)-2*H*-1,3,2λ^4-oxazaborinine (2x)** ($CDCl_3$, 471 MHz)



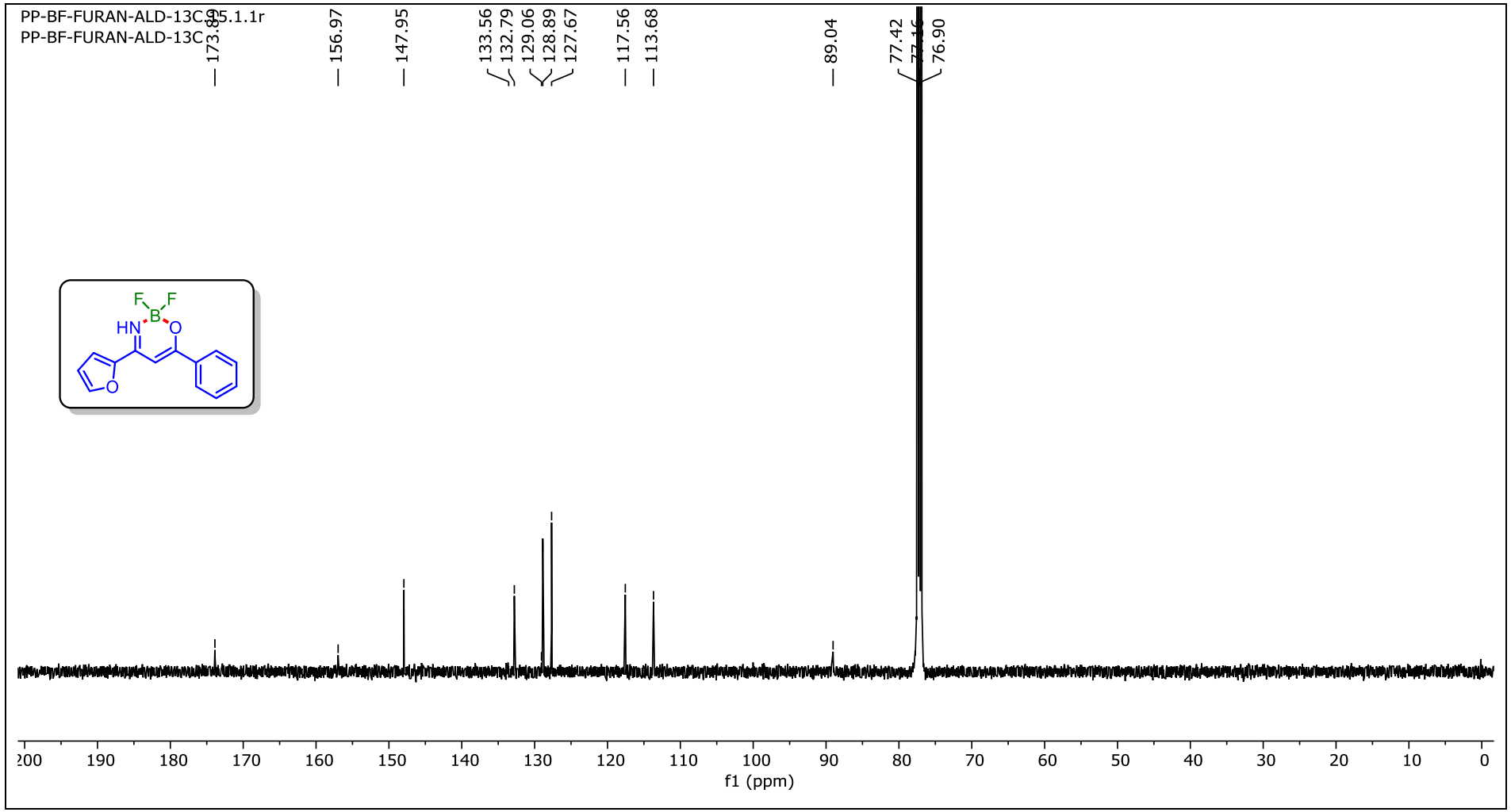
^{11}B NMR of **2,2-Difluoro-6-phenyl-4-(thiophen-2-yl)-2*H*-1,3,2λ^4-oxazaborinine (2x)** ($CDCl_3$, 160 MHz)



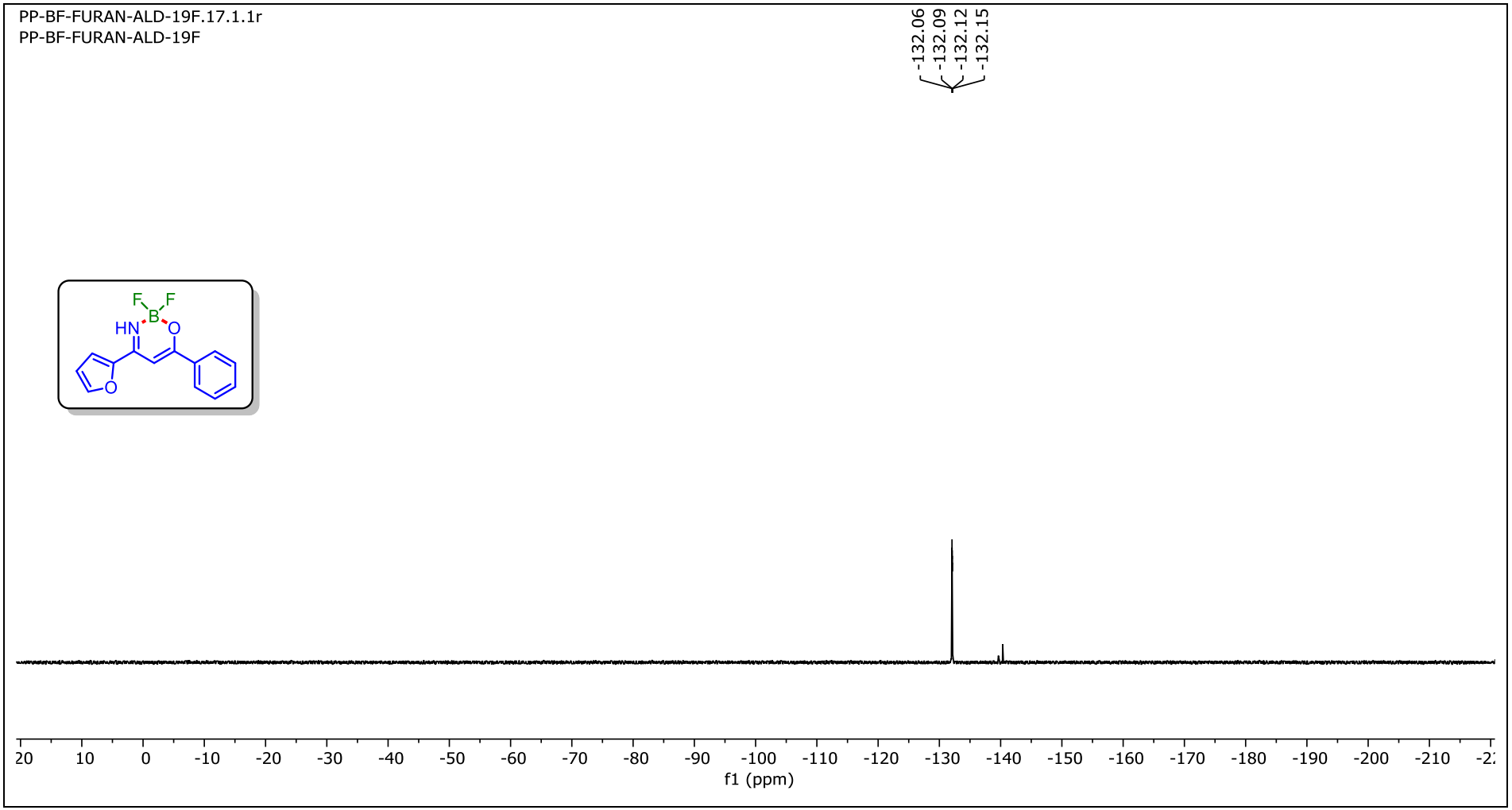
^{1}H NMR of **2,2-Difluoro-4-(furan-2-yl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2y)** ($CDCl_3$, 400 MHz)



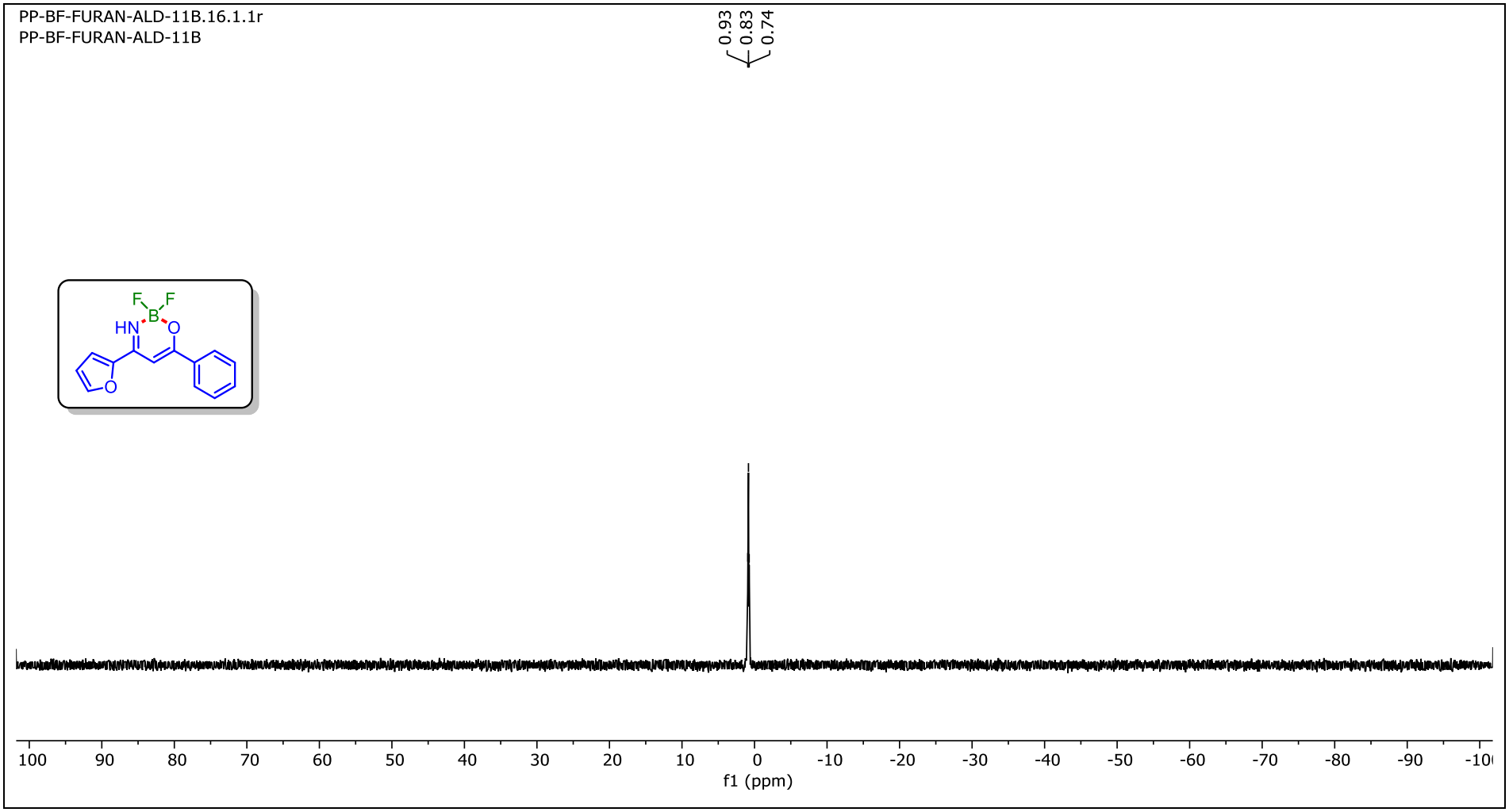
^{13}C {^{1}H} NMR of **2,2-Difluoro-4-(furan-2-yl)-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinine (2y)** ($CDCl_3$, 126 MHz)



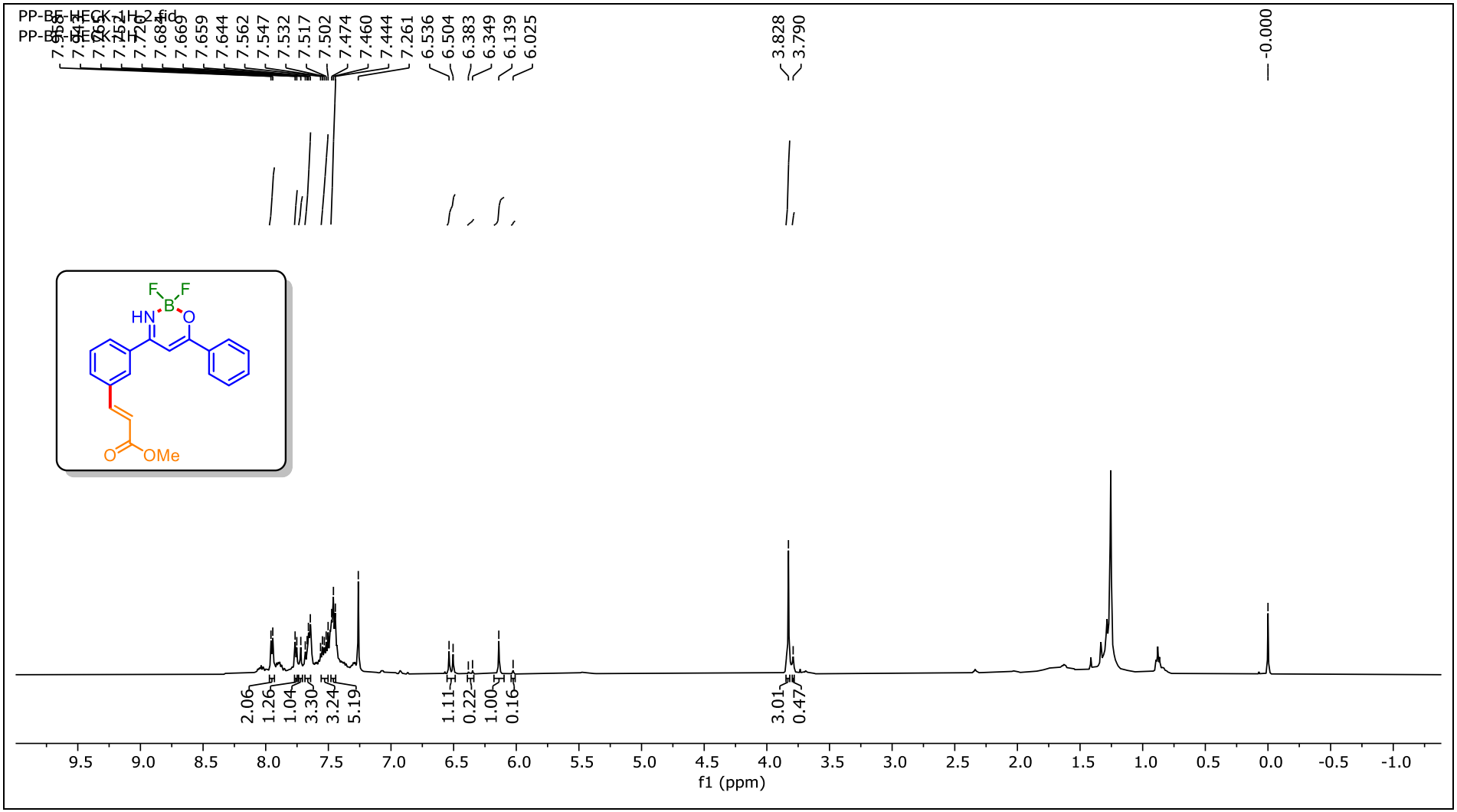
^{19}F NMR of **2,2-Difluoro-4-(furan-2-yl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2y)** ($CDCl_3$, 471 MHz)



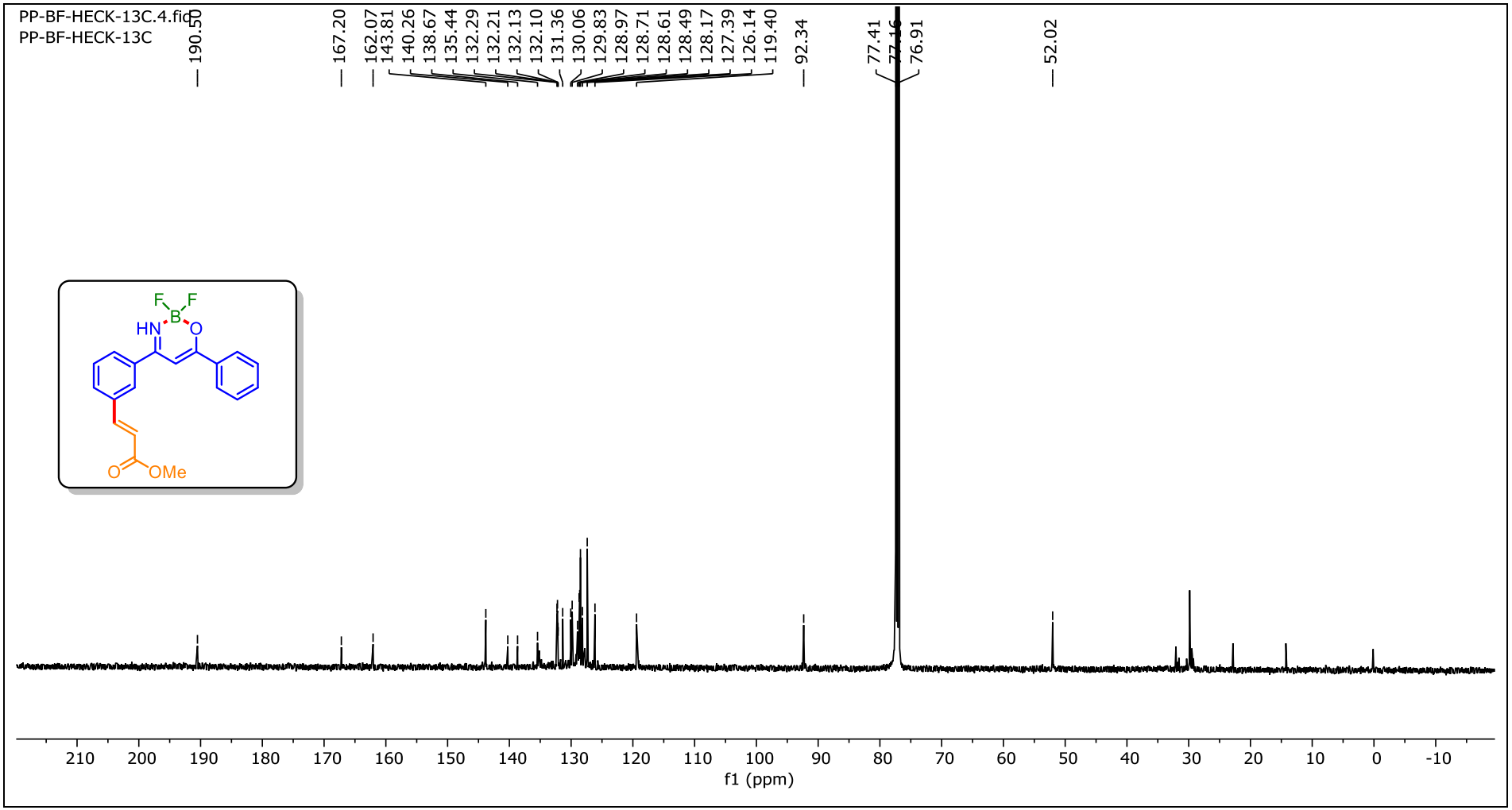
^{11}B NMR of **2,2-Difluoro-4-(furan-2-yl)-6-phenyl-2*H*-1,3,2λ^4-oxazaborinine (2y)** ($CDCl_3$, 160 MHz)



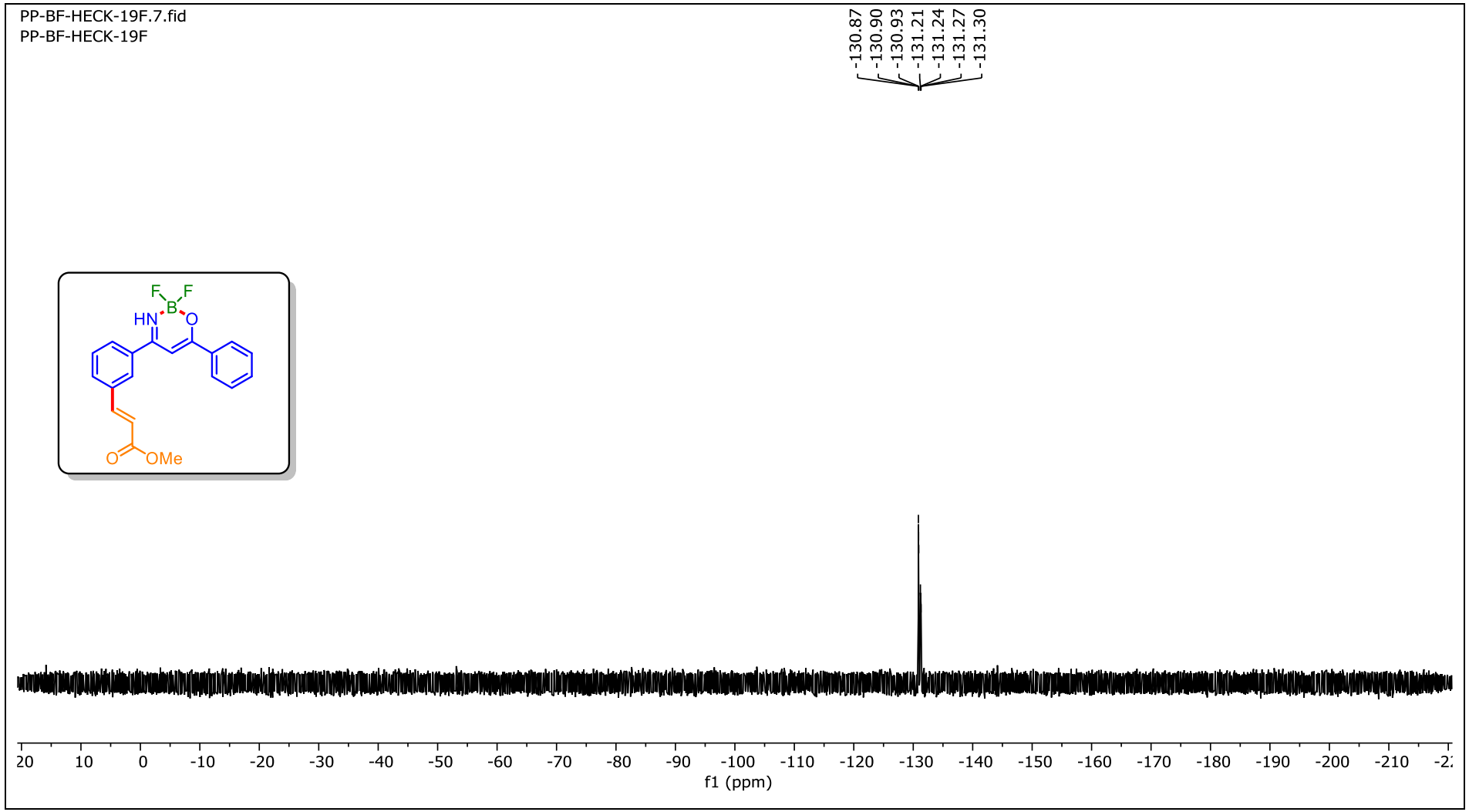
^{1}H NMR of **Methyl (*E*)-3-(3-(2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinin-4-yl)phenyl)acrylate** (**3**) ($CDCl_3$, 500 MHz)



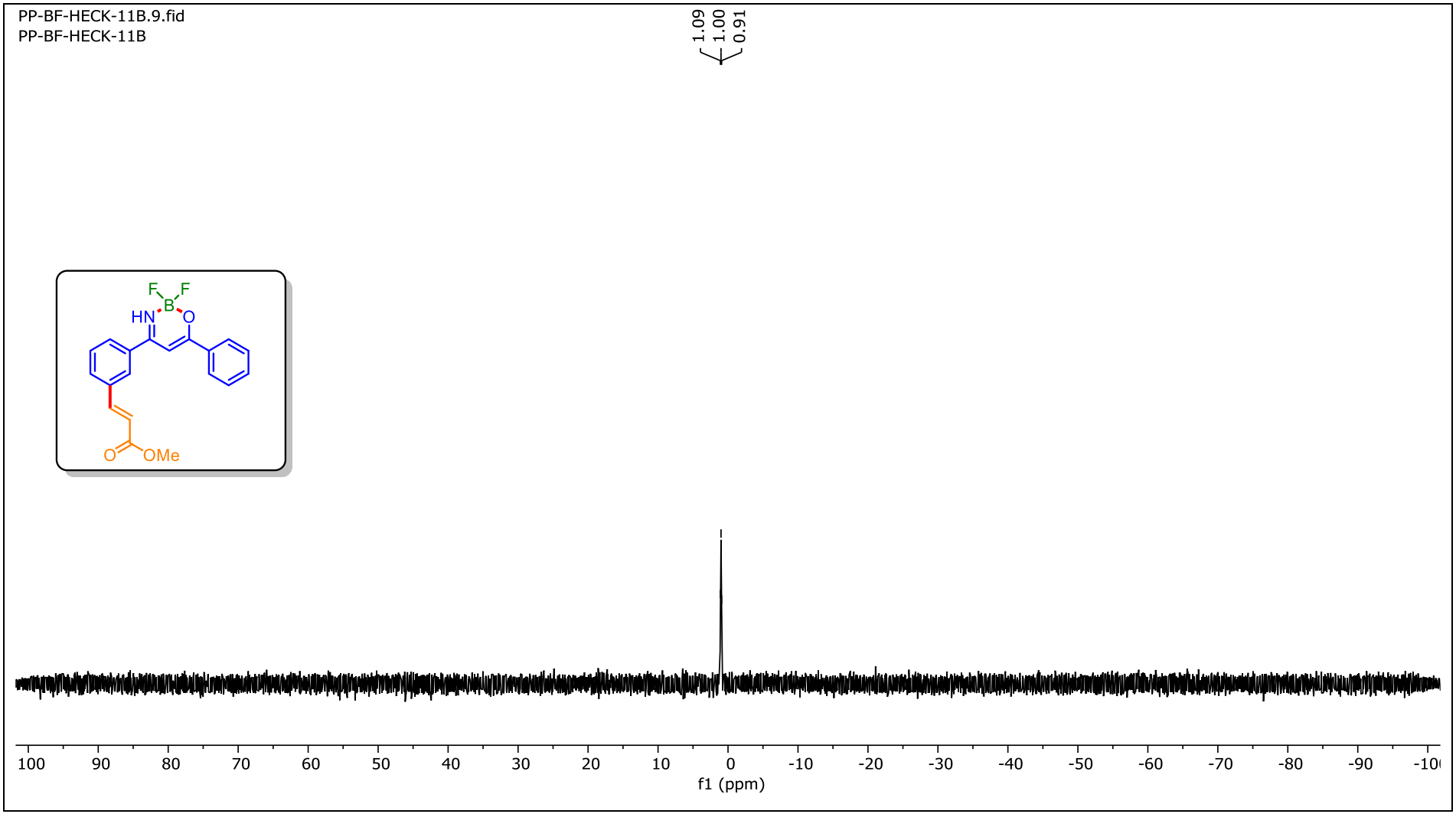
^{13}C NMR of **Methyl (*E*)-3-(3-(2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinin-4-yl)phenyl)acrylate** (**3**) ($CDCl_3$, 126 MHz)



^{19}F NMR of **Methyl (*E*)-3-(3-(2,2-difluoro-6-phenyl-2*H*-1,3,2λ^{4}-oxazaborinin-4-yl)phenyl)acrylate** (**3**) ($CDCl_3$, 471 MHz)



^{11}B NMR of **Methyl (*E*)-3-(3-(2,2-difluoro-6-phenyl-2*H*-1,3,2λ^4-oxazaborinin-4-yl)phenyl)acrylate** (**3**) ($CDCl_3$, 160 MHz)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f1 (ppm)