Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Dearomative *bis*-functionalization of quinoxalines and *bis*-*N*-arylation of (benz)imidazoles via Cu(II) mediated addition of boronic acids

Tamanna Khandelia, Subhendu Ghosh, and Bhisma K. Patel*

Department of Chemistry, Indian Institute of Technology Guwahati, Assam, India.

E-mail: patel@iitg.ac.in

Contents:

1. General Information and Instrumentation:

All chemicals were obtained from commercial sources and were used without further purification. The starting material **1** was synthesized according to previously described methods.[1] Reactions were monitored via TLC, prepared using silica gel 60 F_{254} (0.25 mm), and were detected under UV light at 254 nm. For chromatography, separation was carried out using 60−120 mesh-sized silica gel. Ethyl acetate/ hexane and methanol/ DCM mixtures were used as the eluent. ^{1}H, ^{13}C, and ^{19}F NMR spectra were recorded in 600, 500, and 400 MHz NMR in deuterated solvents, and the chemical shifts (δ) are given in ppm. The ^{1}H spectra were referenced to TMS (0 ppm) for $CDCl_3$ and H_2O in DMSO-d_6 (3.3 ppm) for DMSO-d_6; for ^{13}C $CDCl_3$ (77.16 ppm) and for DMSO-d_6 (39.5 ppm). IR spectra were recorded neat using an FT-IR spectrometer. HRMS was recorded using ESI (Q-TOF type mass analyzer) in positive modes.

2. Representative Hydroxy Group Containing Bio-Pharmaceuticals[2]:

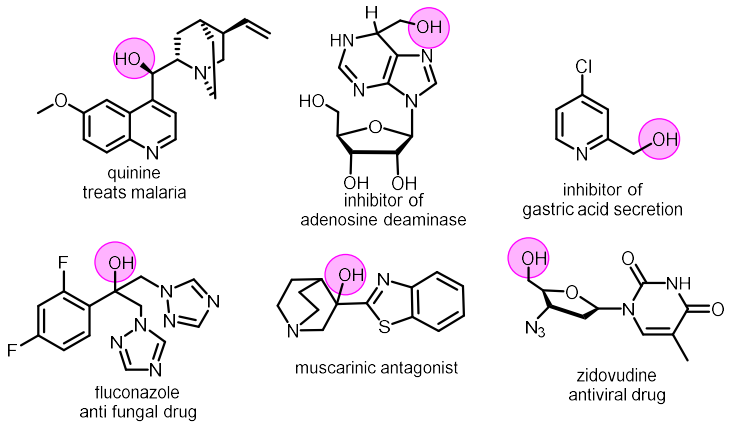


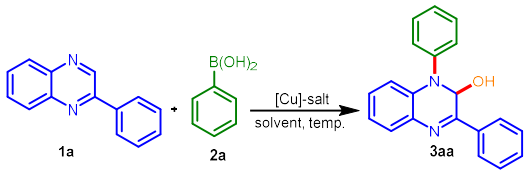
Figure S1: Hydroxy Group Containing Bio-Pharmaceuticals

3. Optimisation of Reaction Conditions

After confirming the structure of **3aa** (by ^{1}H, ^{13}C NMR, and X-ray crystallographic techniques) and to arrive at the optimal reaction conditions, various reaction parameters were tuned keeping **1a** and **2a** as the model coupling partners. At first a series of copper salts *viz.* CuF_2, $CuCl_2$, $Cu(acac)_2$, $CuBr_2$, and $Cu(OAc)_2$ were screened, but none could enhance the yield of **3aa** (Table S1, entries 2-6). A sequential enhancement in $Cu(OTf)_2$ loading from 0.2 to 1.2 equiv, improved the yield of **3aa** from 21% to 84% (Table S1, entries 7-9). However, a further enhancement in $Cu(OTf)_2$ loading to 1.5 and 2 equivalents did not improve the yield of **3aa**

significantly (Table S1, entry 10-11). The use of other solvents *viz.* *o*–xylene, *m*–xylene, 1,2-dichloroethane (DCE), chlorobenzene, 1,2-dichlorobenzene (DCB), tetrahydrofuran (THF), 2,2,2-trifluoroethanol (TFE), and DMSO were all found inferior to toluene (Table S1, entries 12-19). A control reaction in the absence of $Cu(OTf)_2$ yielded no trace of **3aa**, suggesting the crucial role of $Cu(OTf)_2$ in this protocol (Table S1, entry 20). Further, the reaction performed at a higher temperature (100 °C) failed to improve the yield (Table S1, entry 21), while there was no reaction at room temperature (Table S1, entry 22). No noticeable enhancement in the yield was observed by prolonging the reaction time to 20 h (Table S1, entry 23).

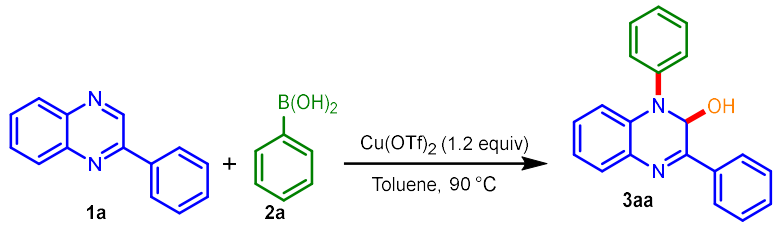
Table S1 Optimization of reaction conditions[a]



Entry	Cu salt (equiv)	Solvent	Yield of **3aa** (%)[b]
1	$Cu(OTf)_2$ (0.2)	Toluene	21
2	CuF_2 (0.2)	Toluene	13
3	$CuCl_2$ (0.2)	Toluene	nd
4	$Cu(acac)_2$ (0.2)	Toluene	nd
5	$CuBr_2$ (0.2)	Toluene	nd
6	$Cu(OAc)_2$ (0.2)	Toluene	nd
7	$Cu(OTf)_2$ (0.5)	Toluene	35
8	$Cu(OTf)_2$ (1.0)	Toluene	77
9	**$Cu(OTf)_2$ (1.2)**	**Toluene**	**84**
10	$Cu(OTf)_2$ (1.5)	Toluene	86
11	$Cu(OTf)_2$ (2)	Toluene	87
12	$Cu(OTf)_2$ (1.2)	*o*–Xylene	71
13	$Cu(OTf)_2$ (1.2)	*m*–Xylene	70
14	$Cu(OTf)_2$ (1.2)	1,2-DCE	57
15	$Cu(OTf)_2$ (1.2)	PhCl	61
16	$Cu(OTf)_2$ (1.2)	1,2-DCB	64
17	$Cu(OTf)_2$ (1.2)	THF	nd
18	$Cu(OTf)_2$ (1.2)	TFE	nd
19	$Cu(OTf)_2$ (1.2)	DMSO	nd
20	--	Toluene	nd
21[c]	$Cu(OTf)_2$ (1.2)	Toluene	84
22[d]	$Cu(OTf)_2$ (1.2)	Toluene	nd
23[e]	$Cu(OTf)_2$ (1.2)	Toluene	85

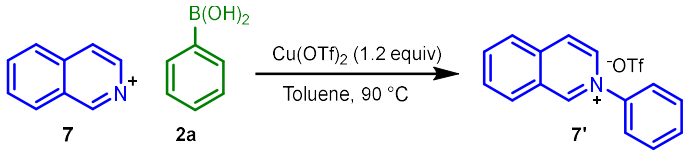
[a]Reaction Conditions: **1a** (0.35 mmol), **2a** (0.56 mmol), copper salt, solvent (1.5 mL), 90 °C, 15h. [b]Isolated yield. [c]Reaction carried out at 100 °C. [d]Reaction carried out at rt. [e]20 h. nd = not detected.

4. General Procedure for the Synthesis of 3aa



An oven-dried 5 mL round-bottom flask was charged with 2-phenylquinoxaline (**1a)** (0.35 mmol, 72 mg), phenylboronic acid **2a** (0.56 mmol, 68 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg), a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. The progress of the reaction was monitored via TLC. After completion of the reaction, the solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane: ethyl acetate (96:4) mixture to afford the desired product **3aa** as yellow solids in 84% yields (88 mg).

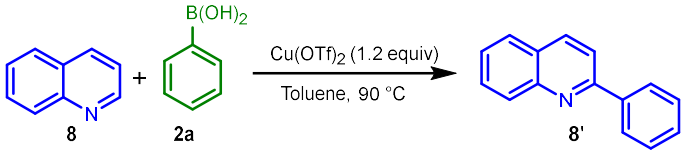
5. General Procedure for the Synthesis of 7'



An oven-dried 5 mL round-bottom flask was charged with isoquinoline (**7**) (0.35 mmol, 45 mg), phenylboronic acid **2a** (0.88 mmol, 68 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg), and a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. The progress of the reaction was monitored via TLC. After completion of the reaction, the solvent was removed by rotary evaporation. The reaction mixture was then purified over column chromatography by

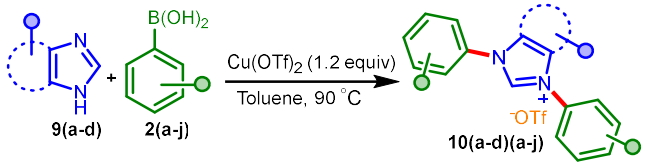
eluting with DCM: Methanol (95: 5) mixtures to afford the product **7'** as brown gummy solid in 81% yield.

6. General Procedure for the Synthesis of 8'



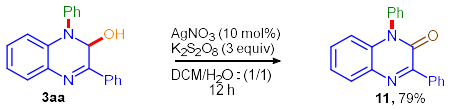
An oven-dried 5 mL round-bottom flask was charged with quinoline (**8**) (1.05 mmol, 135 mg), phenylboronic acid **2a** (0.56 mmol, 68 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg), and a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. The progress of the reaction was monitored via TLC. After completion of the reaction, the solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane: ethyl acetate (97:3) mixture to afford the product **8'** as white solid in 66% yield.

7. General Procedure for the Synthesis of 10



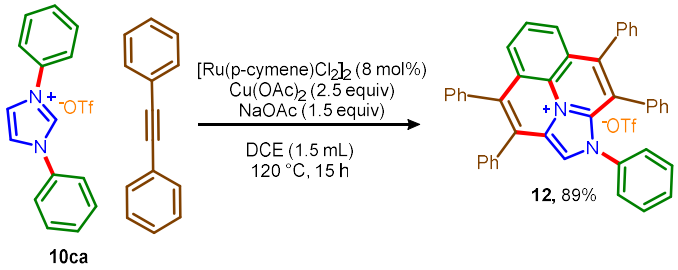
An oven-dried 5 mL round-bottom flask was charged with benzimidazole **9 a–b** (0.35 mmol) or imidazole **9 c–d** (0.35 mmol), phenylboronic acid **2a–j** (0.88 mmol), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol), and a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. The progress of the reaction was monitored via TLC. After completion of the reaction, the solvent was removed by rotary evaporation. The reaction mixture was then purified over column chromatography by eluting with DCM: Methanol (95: 5) mixtures to afford the desired products [**10(a–d)(a–j)**] as white and light brown solids in 58%–79% yields.

8. General procedure for the Synthesis of 11



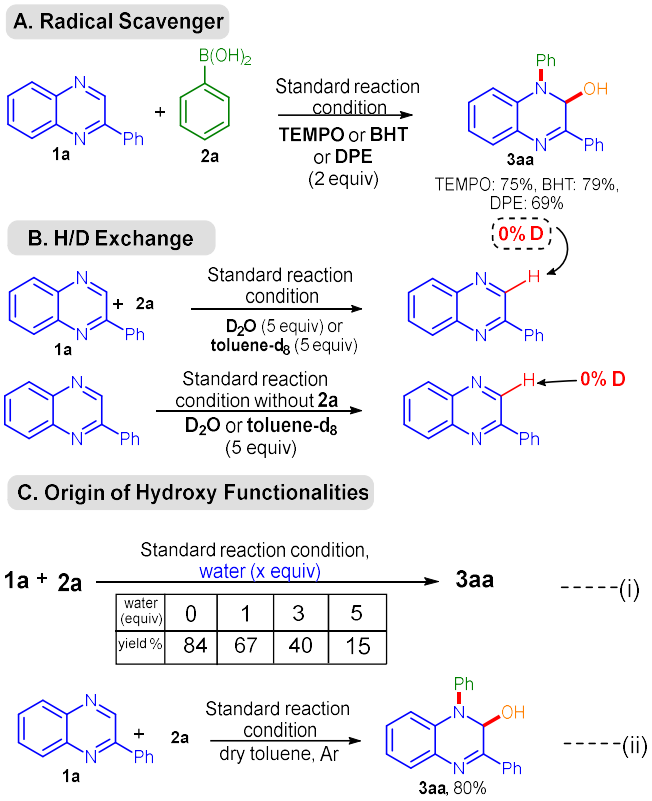
An oven-dried 5 mL round-bottom flask was charged with **3aa** (0.2 mmol, 60 mg), $AgNO_3$ (10 mol%, 3 mg), $K_2S_2O_8$ (3 equiv, 162 mg) and a magnetic stir bar in DCM/H_2O (1:1) (1.5 mL) and was stirred at rt for 12 h. The progress of the reaction was monitored via TLC. After completion of the reaction, the solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane: ethyl acetate (98:2) mixture to afford the product **11** as white solid in 79% yield (47 mg).

9. General procedure for the Synthesis of 12



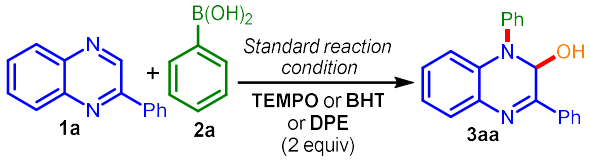
An oven-dried 5 mL round-bottom flask was charged with **10ca** (0.2 mmol, 74 mg), diphenylacetylene (0.4 mmol, 71 mg), $[Ru(p\text{-cymene})Cl_2]_2$ (8 mol%, 10 mg), $Cu(OAc)_2$ (2.5 equiv, 90 mg), NaOAc (1.5 equiv, 24 mg) and a magnetic stir bar in DCE (1.5 mL) and was refluxed at 120 °C for 15 h. The progress of the reaction was monitored via TLC. After completion of the reaction, the solvent was removed by rotary evaporation. The reaction mixture was then purified over column chromatography by eluting with DCM: Methanol (95: 5) mixtures to afford the product **12** as dark brown gummy solid in 89% yields (128 mg).

10. Mechanistic Studies



Scheme S1 Control reactions.

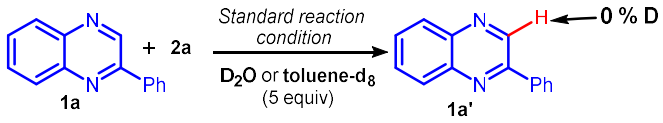
(A) Procedure for Addition of Radical Scavenger:



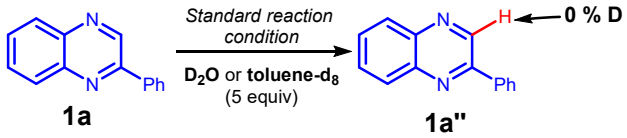
A 5 mL oven-dried round-bottom flask was charged with 2-phenylquinoxaline **1a** (0.35 mmol, 72 mg), phenylboronic acid **2a** (0.56 mmol, 68 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 151 mg), TEMPO (2 equiv, 0.7 mmol, 109 mg) or BHT (2 equiv, 0.7 mmol, 154 mg) or 1,1-diphenylethylene (DPE) (2 equiv, 0.7 mmol, 126 mg) and a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. The solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with

hexane: ethyl acetate (96:4) mixture to afford the desired product **3aa** as yellow solid in 78 mg (75% yield) for TEMPO, 83 mg (79% yield) for BHT and 72 mg (69% yield) for DPE. This observation suggests non-involvement of any radical path.

(B) Procedure for H/D exchange:



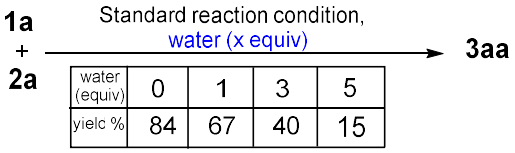
A 5 mL oven-dried round-bottom flask was charged with 2-phenylquinoxaline **1a** (0.35 mmol, 72 mg), phenylboronic acid **2a** (0.56 mmol, 68 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg), D_2O (5 equiv) or toluene-d_8 (5 equiv) and a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. The solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane: ethyl acetate (96: 4) mixture to afford an orange product. The extent of deuteration was determined by comparing the ^{1}H NMR of **1a'** to that of un-deuterated 2-phenylquinoxaline **1a**. Upon comparison, no deuteration was observed.



A 5 mL oven-dried round-bottom flask was charged with 2-phenylquinoxaline **1a** (0.35 mmol, 72 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg), D_2O (5 equiv) or toluene-d_8 (5 equiv) and a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. The solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane: ethyl acetate (96: 4) mixture to afford an orange product. The extent of deuteration was determined by comparing the ^{1}H NMR **1a''** to that of un-deuterated 2-phenylquinoxaline **1a**. Upon comparison, no deuteration was observed.

(C) Procedure for Investigation of Origin of Hydroxy Functionality

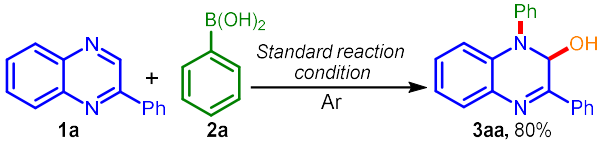
(i) Addition of External Water



water (equiv)	0	1	3	5
yielc %	84	67	40	15

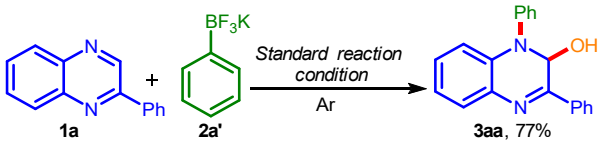
Four 5 mL oven-dried round-bottom flasks was charged with 2-phenylquinoxaline **1a** (0.35 mmol, 72 mg), phenylboronic acid **2a** (0.56 mmol, 68 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg), H_2O (0/ 1/ 3/ 5 equiv respectively) and a magnetic stir bar in toluene (1.5 mL) and was heated at 90 °C for 15 h. Solvents were removed by rotary evaporation. The reaction mixtures were then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layers were dried over anhydrous sodium sulfate and evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane: ethyl acetate (96: 4) mixtures to afford the product **3aa** as yellow solids in 84% (88 mg), 67% (70 mg), 40% (42 mg), 15% (16 mg) yields respectively for 0, 1, 3, 5 equiv of H_2O added.

(ii) Reaction in Dry Condition:



A 5 mL oven-dried round-bottom flask was charged with 2-phenylquinoxaline **1a** (0.35 mmol, 72 mg), purified phenylboronic acid **2a** (0.56 mmol, 68 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg), and a magnetic stir bar in anhydrous toluene (1.5 mL) under an argon atmosphere and was heated at 90 °C for 15 h. The solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane:ethyl acetate (96:4) mixture to afford the product **3aa** as yellow solids in 80% yield (84 mg).

(iii) Reaction with Phenyltrifluoroborate (2a') in Lieu of Phenylboronic acid (2a)



A 5 mL oven-dried round-bottom flask was charged with 2-phenyllquinoxaline **1a** (0.35 mmol, 72 mg), potassium phenyltrifluoroborate (**2a'**) (0.56 mmol, 103 mg), $Cu(OTf)_2$ (1.2 equiv, 0.42 mmol, 152 mg) and a magnetic stir bar in anhydrous toluene (1.5 mL) under an argon atmosphere and was heated at 90 °C for 15 h. The solvent was removed by rotary evaporation. The reaction mixture was then mixed with water (10 mL) and extracted with ethyl acetate (2 × 15 mL). The organic layer was dried over anhydrous sodium sulfate and was evaporated under reduced pressure. The residue so obtained was purified over column chromatography by eluting with hexane: ethyl acetate (96: 4) mixture to afford the product **3aa** as yellow solid in 77% yield (81 mg).

(iv) Thermogravimetric (TGA) Analysis:

The thermogravimetric analysis (TGA) of the air exposed $Cu(OTf)_2$ salt was conducted from 29 ° to 400 °C to ensure the presence of absorbed H_2O molecules in the metal salt (Figure S2). The TGA curve displays a single weight loss of 9% from 80 °C to 143 °C. This weight loss suggests the presence of two molecules of water per formula unit of $Cu(OTf)_2$.

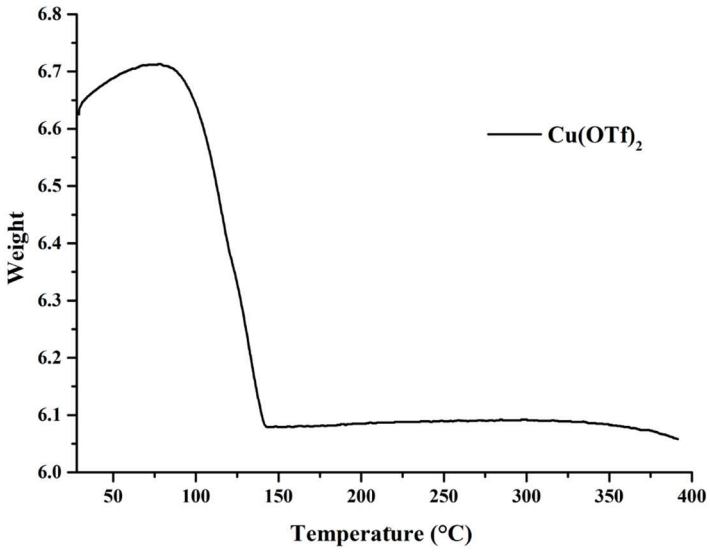


Figure S2: TGA curve of $Cu(OTf)_2$.

(D) HRMS analysis of crude reaction aliquot:

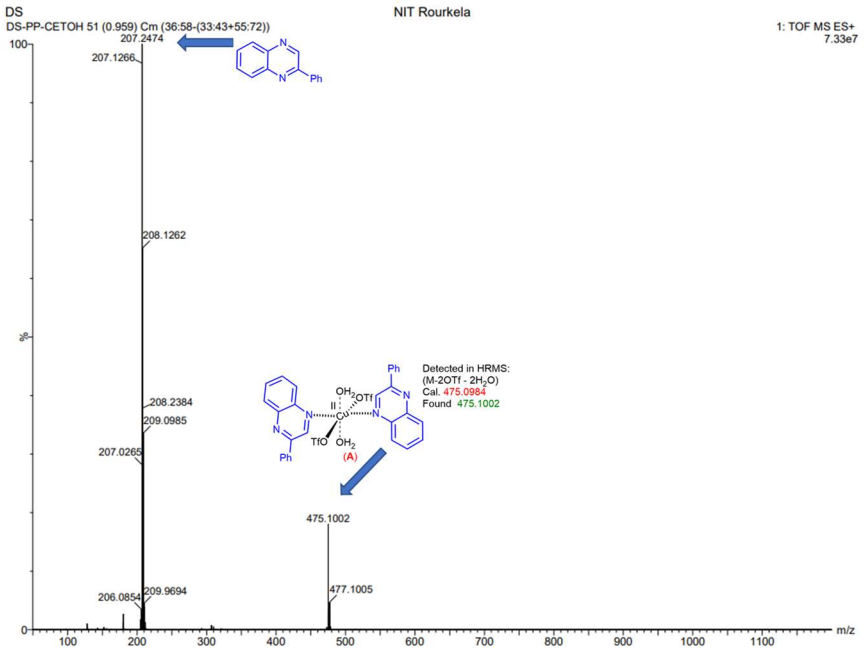
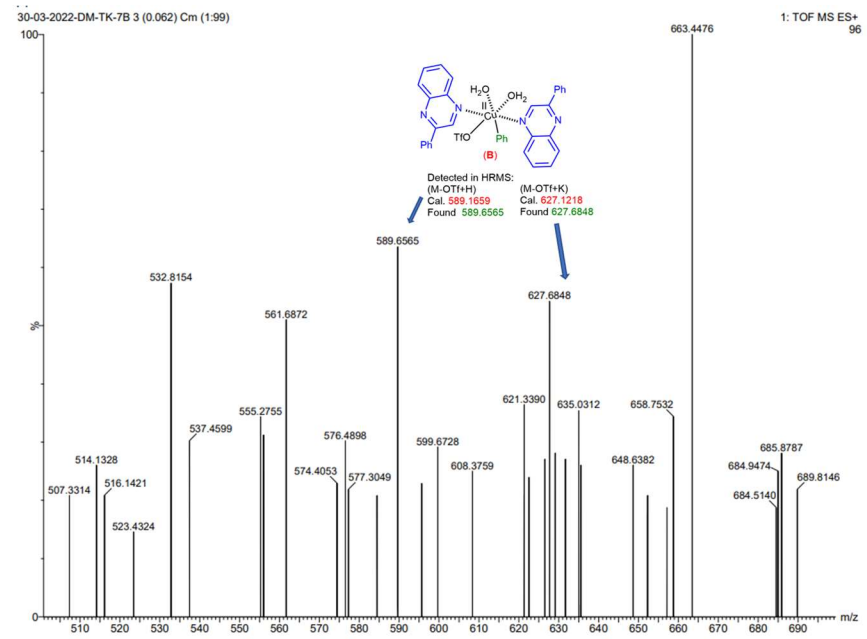


Figure S3: Detection of complex A



11. Crystallographic Description

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoK$_\alpha$ radiation (λ = 0.71073 Å) at 298 K for **10aa** and **10ca**. While **3aa** was collected with a XtaLAB Pro II AFC12 (RINC): Kappa single diffractometer. 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 SHELX-2014[c] program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions.

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.

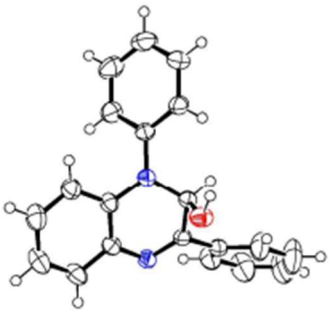


Figure S5. ORTEP diagram of **3aa** with ellipsoid probability 50%.

Table S2. **Crystal Data table for 3aa**

Empirical formula	$C_{20}H_{16}N_2O$
CCDC number	2215417
Formula weight	300.36
Temperature	298(2)
Wavelength	0.71073 Å
Crystal system	orthorhombic

Space group	Pbca
Unit cell dimensions	a = 9.0540(7) Å, b = 11.6026(5) Å, c = 29.7549(17) Å α= 90°, β= 90°, γ= 90°
Volume	3125.8 (3) $Å^3$
Z	8
Density (calculated)	1.276 g/cm^{-3}
Absorption coefficient	0.080
F(000)	1264
Theta range for data collection	2.614 to 26.521°
Index ranges	-7 < = h < = 10, -10 < = k < = 13, -31< = l < =35
Reflections collected	11732
Independent reflections	4877
Data completeness	1.00
Max. and min. transmission	0.975, 0.972
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	2761/ 0/ 212
Goodness-of-fit on F2	1.020
Final R indices [I>2sigma(I)]	0.0568, wR2 = 0.1140
R indices (all data)	0.0740, wR2 = 0.1215

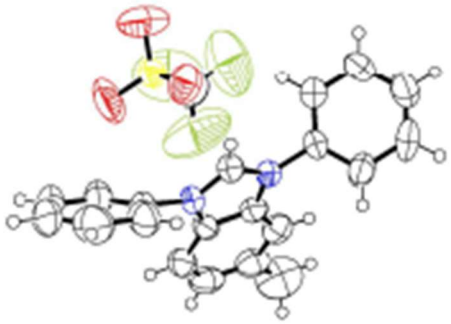


Figure S6. ORTEP diagram of **10aa** with ellipsoid probability 50%.

Table S3. Crystal Data table for 10aa

Empirical formula	$C_{21}H_{17}F_3O_3N_2S$
CCDC number	2215422
Formula weight	434.42
Temperature	298

Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	P 21/n
Unit cell dimensions	a = 11.7342(7) Å, b = 10.5428(6) Å, c = 16.8353(10) Å α = 90°, β = 90.689 (2)°, γ = 90°
Volume	2082.6 (2) $Å^3$
Z	4
Density (calculated)	1.386 g/cm^{-3}
Absorption coefficient	0.207
F(000)	896
Theta range for data collection	2.60 to 20.84°
Index ranges	-11 <= h <= 11, -10 <= k <= 10, -16 <= l <= 16
Reflections collected	38013
Independent reflections	9900
Data completeness	1
Max. and min. transmission	0.7446, 0.6005
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	2195/ 0/ 272
Goodness-of-fit on F2	1.027
Final R indices [I>2sigma(I)]	0.0963, wR2 = 0.1720
R indices (all data)	0.1158, wR2 = 0.1846

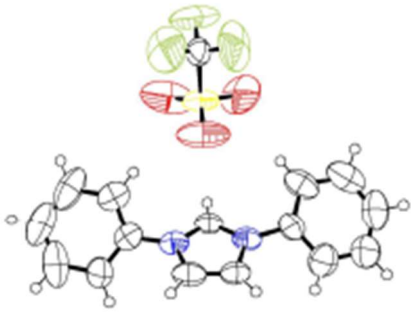


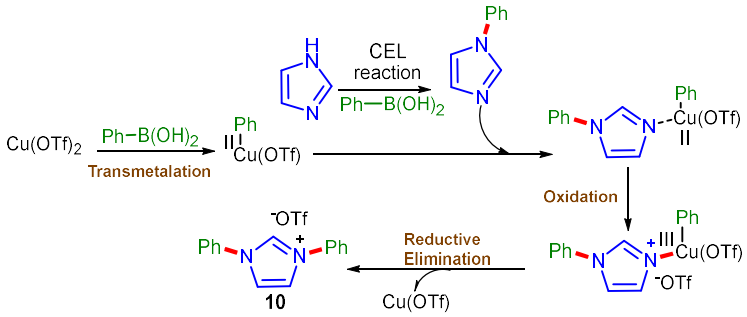
Figure S7. ORTEP diagram of **10ca** with ellipsoid probability 50%.

Table S4. Crystal Data table for **10ca**

Empirical formula	$C_{16}H_{13}F_3O_3N_2S$
CCDC number	2215420
Formula weight	370.34

Temperature	298
Wavelength	0.71073 Å
Crystal system	orthorhombic
Space group	Pnma
Unit cell dimensions	a = 10.1440 (5) Å, b = 17.4540 (9) Å, c = 9.2908 (5) Å α = 90° , β = 90° , γ = 90°
Volume	1644.97 (15) $Å^3$
Z	4
Density (calculated)	1.495 g/cm^{-3}
Absorption coefficient	0.247
F(000)	760
Theta range for data collection	2.97 to 26.10°
Index ranges	-12 <= h <= 12, -20 <= k <= 20, -11 <= l <= 11
Reflections collected	41668
Independent reflections	9788
Data completeness	1
Max. and min. transmission	0.7454, 0.5754
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	1499 / 0 / 121
Goodness-of-fit on F2	1.098
Final R indices [I>2sigma(I)]	0.0747, wR2 = 0.1379
R indices (all data)	0.0883, wR2 = 0. 1477

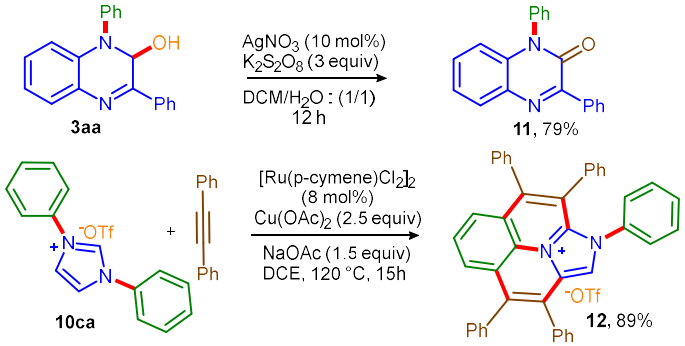
12. Plausible Mechanism for the Formation of 10:



Scheme S2. Plausible mechanism for **10**.

13. Post-Synthetic Modifications:

The C–OH group of **3aa** can be oxidized using $AgNO_3$/ $K_2S_2O_8$ to deliver amide **11** in good yield (79%) (Scheme S3).[3] Also, modification of **10ca** upon treatment with diphenyl acetylene under ruthenium catalysis offered a dual C–H/C–H annulated product **12** (89%).[4]



Scheme S3. Post-synthetic modification. Yield refers to the isolated product.

14. References:

1. K. Kumar, S. R. Mudshinge, S. Goyal, M. Gangar and V. A. Nair, *Tetrahedron Letters.* 2015 **56**, 1266.

2. (a) L. Niu, J. Liu, X. A. Liang, S. Wang and A. Lei, *Nat Commun* 2019, **10**, 467. (b) Y. Kong, W. Xu, X. Liu and J. Weng, *Chinese Chemical Letters* 2020, **31**, 3245.

3. J. Yu, H. Zhao, S. Liang, X. Bao and C. Zhu, *Org. Biomol. Chem.*, 2015, **13**, 7924.

4. (a) Q. Ge, B. Li, H. Song and B. Wang, Org. Biomol. Chem., 2015, 13, 7695. (b) R. Thenarukandiyil, S. K. Gupta and J. Choudhury, *ACS Catal.* 2016, **6**, 5132.

15. DFT calculation:

Input file of 3aa

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.500600	1.031300	0.000000
2	6	0	-2.500600	0.206200	0.000000

3	6	0	-1.786200	-0.206200	0.000000
4	6	0	-1.071700	0.206200	0.000000
5	6	0	-1.071700	1.031300	0.000000
6	6	0	-1.786200	1.443700	0.000000
7	7	0	-0.357200	-0.206200	0.000000
8	6	0	0.357200	0.206200	0.000000
9	6	0	0.357200	1.031300	0.000000
10	7	0	-0.357200	1.443700	0.000000
11	6	0	1.071700	-0.206200	0.000000
12	6	0	1.071700	-1.031300	0.000000
13	6	0	1.786200	-1.443700	0.000000
14	6	0	2.500600	-1.031300	0.000000
15	6	0	2.500600	-0.206200	0.000000
16	6	0	1.786200	0.206300	0.000000
17	1	0	-3.427231	1.566329	0.000000
18	1	0	-3.427231	-0.328829	0.000000
19	1	0	-1.786232	-1.276200	0.000000
20	1	0	-1.786232	2.513700	0.000000
21	1	0	1.283831	1.566329	0.000000
22	1	0	0.145086	-1.566357	0.000000
23	1	0	1.786232	-2.513700	0.000000
24	1	0	3.427231	-1.566329	0.000000
25	1	0	3.427259	0.328780	0.000000
26	1	0	1.786232	1.276300	0.000000

Input file of Pyridine:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.714500	0.412500	0.000000
2	6	0	-0.714500	-0.412500	0.000000
3	7	0	0.000000	-0.825000	0.000000
4	6	0	0.714500	-0.412500	0.000000
5	6	0	0.714500	0.412500	0.000000
6	6	0	0.000000	0.825000	0.000000
7	1	0	-1.641142	0.947508	0.000000
8	1	0	-1.641142	-0.947508	0.000000
9	1	0	1.641142	-0.947508	0.000000
10	1	0	1.641142	0.947508	0.000000
11	1	0	0.000000	1.895000	0.000000

Input file of 4:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z
1	6	0	-2.500600	1.031300	0.000000
2	6	0	-2.500600	0.206200	0.000000
3	6	0	-1.786200	-0.206200	0.000000
4	6	0	-1.071700	0.206200	0.000000
5	6	0	-1.071700	1.031300	0.000000
6	6	0	-1.786200	1.443700	0.000000
7	7	0	-0.357200	-0.206200	0.000000
8	6	0	0.357200	0.206200	0.000000
9	6	0	0.357200	1.031300	0.000000
10	7	0	-0.357200	1.443700	0.000000

11	6	0	1.071700	-0.206200	0.000000
12	6	0	1.071700	-1.031300	0.000000
13	6	0	1.786200	-1.443700	0.000000
14	6	0	2.500600	-1.031300	0.000000
15	6	0	2.500600	-0.206200	0.000000
16	6	0	1.786200	0.206300	0.000000
17	1	0	-3.427231	1.566329	0.000000
18	1	0	-3.427231	-0.328829	0.000000
19	1	0	-1.786232	-1.276200	0.000000
20	1	0	-1.786232	2.513700	0.000000
21	1	0	1.283831	1.566329	0.000000
22	1	0	0.145086	-1.566357	0.000000
23	1	0	1.786232	-2.513700	0.000000
24	1	0	3.427231	-1.566329	0.000000
25	1	0	3.427259	0.328780	0.000000
26	1	0	1.786232	1.276300	0.000000

Input file of 5:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.428900	0.412500	0.000000
2	6	0	-1.428900	-0.412500	0.000000
3	6	0	-0.714500	-0.825000	0.000000
4	6	0	0.000000	-0.412500	0.000000

5	6	0	0.000000	0.412500	0.000000
6	6	0	-0.714500	0.825000	0.000000
7	7	0	0.714500	-0.825000	0.000000
8	6	0	1.428900	-0.412500	0.000000
9	6	0	1.428900	0.412500	0.000000
10	7	0	0.714500	0.825000	0.000000
11	1	0	-2.355559	0.947480	0.000000
12	1	0	-2.355559	-0.947480	0.000000
13	1	0	-0.714532	-1.895000	0.000000
14	1	0	-0.714532	1.895000	0.000000
15	1	0	2.355559	-0.947480	0.000000
16	1	0	2.355559	0.947480	0.000000

Input file of 6:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.786200	0.412500	0.000000
2	6	0	-1.786200	-0.412500	0.000000
3	6	0	-1.071700	-0.825000	0.000000
4	6	0	-0.357200	-0.412500	0.000000
5	6	0	-0.357200	0.412500	0.000000
6	6	0	-1.071700	0.825000	0.000000
7	7	0	0.357200	-0.825000	0.000000
8	6	0	1.071700	-0.412500	0.000000
9	6	0	1.071700	0.412500	0.000000
10	7	0	0.357200	0.825000	0.000000
11	6	0	1.786200	-0.825000	0.000000

12	1	0	-2.712842	0.947508	0.000000
13	1	0	-2.712842	-0.947508	0.000000
14	1	0	-1.071700	-1.895000	0.000000
15	1	0	-1.071700	1.895000	0.000000
16	1	0	1.998342	0.947508	0.000000
17	1	0	2.599473	-0.129668	0.000000
18	1	0	1.842892	-1.440158	0.873651
19	1	0	1.842892	-1.440158	-0.873651

Input file of 7:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.428900	0.412500	0.000000
2	6	0	-1.428900	-0.412500	0.000000
3	6	0	-0.714500	-0.825000	0.000000
4	6	0	0.000000	-0.412500	0.000000
5	6	0	0.000000	0.412500	0.000000
6	6	0	-0.714500	0.825000	0.000000
7	6	0	0.714500	-0.825000	0.000000
8	7	0	1.428900	-0.412500	0.000000
9	6	0	1.428900	0.412500	0.000000
10	6	0	0.714500	0.825000	0.000000
11	1	0	-2.355559	0.947480	0.000000
12	1	0	-2.355559	-0.947480	0.000000
13	1	0	-0.714532	-1.895000	0.000000
14	1	0	-0.714532	1.895000	0.000000
15	1	0	0.714532	-1.895000	0.000000

16	1	0	2.355559	0.947480	0.000000
17	1	0	0.714532	1.895000	0.000000

Input file of 8:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.428900	0.412500	0.000000
2	6	0	-1.428900	-0.412500	0.000000
3	6	0	-0.714500	-0.825000	0.000000
4	6	0	0.000000	-0.412500	0.000000
5	6	0	0.000000	0.412500	0.000000
6	6	0	-0.714500	0.825000	0.000000
7	7	0	0.714500	-0.825000	0.000000
8	6	0	1.428900	-0.412500	0.000000
9	6	0	1.428900	0.412500	0.000000
10	6	0	0.714500	0.825000	0.000000
11	1	0	-2.355559	0.947480	0.000000
12	1	0	-2.355559	-0.947480	0.000000
13	1	0	-0.714532	-1.895000	0.000000
14	1	0	-0.714532	1.895000	0.000000
15	1	0	2.355559	-0.947480	0.000000
16	1	0	2.355559	0.947480	0.000000
17	1	0	0.714532	1.895000	0.000000

Input file of 9a$^{/}$:

Center	Atomic	Atomic	Coordinates (Angstroms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.349200	0.412500	0.000000
2	6	0	-1.349200	-0.412500	0.000000
3	6	0	-0.634800	-0.825000	0.000000
4	6	0	0.079700	-0.412500	0.000000
5	6	0	0.079700	0.412500	0.000000
6	6	0	-0.634800	0.825000	0.000000
7	7	0	0.864300	-0.667400	0.000000
8	6	0	1.349200	0.000000	0.000000
9	7	0	0.864300	0.667400	0.000000
10	1	0	-2.275859	0.947480	0.000000
11	1	0	-2.275859	-0.947480	0.000000
12	1	0	-0.634832	-1.895000	0.000000
13	1	0	-0.634832	1.895000	0.000000
14	1	0	2.419200	0.000000	0.000000
15	1	0	1.018816	1.142926	0.866025

Input file of 9c:

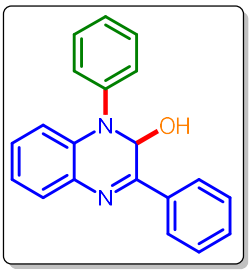
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.634800	0.412500	0.000000
2	6	0	-0.634800	-0.412500	0.000000
3	7	0	0.149800	-0.667400	0.000000
4	6	0	0.634800	0.000000	0.000000

5	7	0	0.149800	0.667400	0.000000
6	1	0	-1.500437	1.041446	0.000000
7	1	0	-1.500437	-1.041446	0.000000
8	1	0	0.304293	-1.142933	0.866025
9	1	0	1.704800	0.000000	0.000000

---

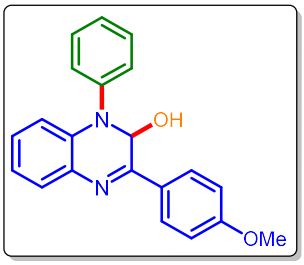
16. Spectral Data

*1,3-Diphenyl-1,2-dihydroquinoxalin-2-ol (**3aa**)*



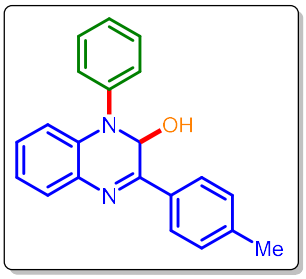
Yellow solid (88 mg, 84% yield), m.p. 150-153 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11-8.09 (m, 2H), 7.63 (d, J = 8 Hz, 1H), 7.55 (d, J = 7.5 Hz, 2H), 7.45–7.42 (m, 5H), 7.28 (t, J = 7.5 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 7.02–6.97 (m, 2H), 6.06 (s, 1H), 3.03 (s, 1H).; ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 153.6, 143.4, 136.1, 133.7, 132.4, 130.7, 129.7, 128.9, 128.6, 128.4, 127.5, 126.2, 125.3, 120.7, 115.8, 76.1. IR (neat, cm^{-1}) 3153, 3064, 1591, 1482, 1451, 1325, 1253, 1048, 750, 692. HRMS (ESI) [M - OH]$^+$ calcd for $C_{20}H_{15}N_2^+$ 283.1235, found 283.1237.

*3-(4-Methoxyphenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (**3ba**)*



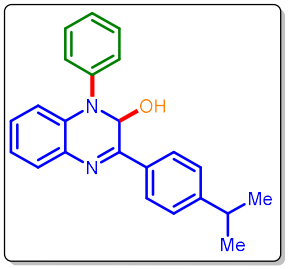
Yellow solid (90 mg, 78% yield); m.p. 145-150 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, J = 9 Hz, 2H), 7.59 (d, J = 8 Hz, 1H), 7.55 (d, J = 8 Hz, 2H), 7.43 (t, J = 7.7 Hz, 2H), 7.28 (d, J = 7.5 Hz, 1H), 7.11 (t, J = 7.5 Hz, 1H), 7.00 (d, J = 8 Hz, 1H), 6.96 (t, J = 7.8 Hz, 3H), 6.04 (s, 1H), 3.86 (s, 3H), 3.02 (s, 1H).; ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 161.8, 153.3, 143.6, 133.9, 132.2, 129.7, 129.2, 128.8, 128.3, 127.9, 126.0, 125.2, 120.7, 115.8, 114.2, 76.0, 55.6. IR (neat, cm^{-1}) 3319, 1601, 1486, 1306, 1250, 1023, 956, 834, 746. HRMS (ESI) [M - OH]$^+$ calcd for $C_{21}H_{17}N_2O^+$ 313.1341, found 313.1339.

*1-Phenyl-3-(p-tolyl)-1,2-dihydroquinoxalin-2-ol (**3ca**)*



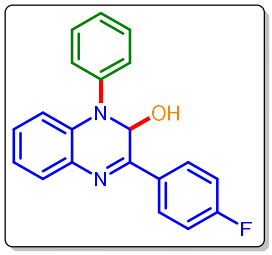
Yellow solid (88 mg, 80% yield); m.p. 190-192 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (d, J = 8.0 Hz, 2H), 7.54 (d, J = 8 Hz, 3H), 7.42 (t, J = 7.8 Hz, 2H), 7.27 (d, J = 7.5 Hz, 1H), 7.21 (d, J = 7.5 Hz, 2H), 7.09 (t, J = 7.7 Hz, 1H), 6.98 (d, J = 8 Hz, 1H), 6.92 (t, J = 7.5 Hz, 1H), 6.02 (s, 1H), 3.32 (s, 1H), 2.39 (s, 3H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 153.6, 143.5, 141.0, 133.8, 133.3, 132.3, 129.7, 129.5, 128.4, 128.2, 127.5, 126.1, 125.3, 120.6, 115.7, 76.1, 21.6. IR (neat, cm^{-1}) 3127, 1591, 1484, 1327, 1288, 1255, 1046, 1023, 750, 693, 473. HRMS (ESI) [M - OH]$^+$ calcd for $C_{21}H_{17}N_2^+$ 297.1392, found 297.1393.

*3-(4-Isopropylphenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (**3da**)*



Yellow solid (98 mg, 82% yield); m.p. 154- 158 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, J = 8.0 Hz, 2H), 7.65 (d, J = 8 Hz, 1H), 7.55 (d, J = 8 Hz, 2H), 7.44 (t, J = 7.7 Hz, 2H), 7.33–7.29 (m, 3H), 7.14 (t, J = 7.3 Hz, 1H), 7.03–7.00 (m, 2H), 6.06 (d, J = 8.5 Hz, 1H), 2.99–2.92 (m, 1H), 2.78 (d, J = 10.5 Hz, 1H), 1.27 (d, J = 7.0 Hz, 6H).; ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 153.7, 152.0, 143.5, 133.9, 133.8, 132.4, 129.7, 128.6, 128.2, 127.6, 127.0, 126.1, 125.3, 120.7, 115.9, 76.1, 34.3, 24.0, 23.9. IR (neat, cm^{-1}) 3335, 2960, 1667, 1595, 1491, 1329, 1017, 838, 750, 697. HRMS (ESI) [M - OH]$^+$ calcd for $C_{23}H_{21}N_2^+$ 325.1705, found 325.1712.

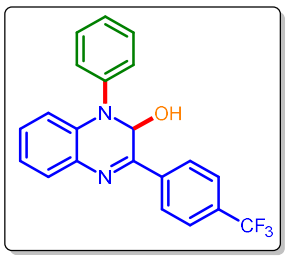
*3-(4-Fluoroophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (**3ea**)*



Yellow solid (84 mg, 75% yield); m.p. 127-130 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11–8.08 (m, 2H), 7.59 (d, J = 7.5 Hz, 1H), 7.55 (d, J = 7.5 Hz, 2H), 7.44 (t, J = 7.8 Hz, 2H), 7.29 (t, J = 7.5 Hz, 1H), 7.16– 7.10 (m, 3H), 7.01–6.96 (m, 2H), 6.01 (d, J = 10.5 Hz, 1H), 3.04 (d, J = 10.5 Hz, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 165.4, 163.4, 152.5, 143.4, 133.6, 132.4 (d, J = 3.2 Hz), 132.3, 129.8, 129.7

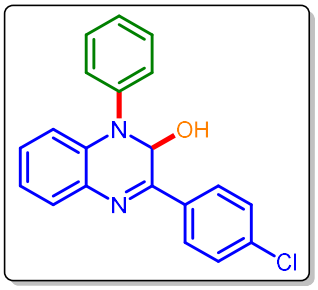
(d, J = 8.7 Hz), 128.5 (d, J = 8.8 Hz), 126.3, 125.3, 120.8, 116.0, 115.8 (d, J = 6.3 Hz), 76.1. ^{19}F NMR (471 MHz, $CDCl_3$) δ -109.68. IR (neat, cm^{-1}) 3194, 1592, 1490, 1318, 1225, 1155, 973, 831, 745, 697. HRMS (ESI) $[M - OH]^+$ calcd for $C_{20}H_{14}FN_2^+$ 301.1141, found 301.1142.

*1-Phenyl-3-(4-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (**3fa**)*



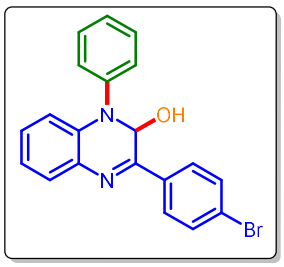
Yellow solid (82 mg, 64% yield); m.p. 70-72 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, J = 8 Hz, 2H), 7.67 (d, J = 8.4 Hz, 2H), 7.59–7.55 (m, 3H), 7.45 (t, J = 7.8 Hz, 2H), 7.31 (t, J = 7.2 Hz, 1H), 7.15 (t, J = 7.7 Hz, 1H), 6.99 (d, J = 8.4 Hz, 1H), 6.96 (t, J = 7.7 Hz, 1H), 6.02 (s, 1H), 3.38 (s, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 151.8, 143.2, 139.3, 133.4, 132.5, 132.0 (d, J = 32 Hz), 129.8, 129.2, 128.8, 127.8, 127.5, 126.5, 125.7 (q, J = 3.9 Hz), 125.5, 120.8, 115.9, 76.0. IR (neat, cm^{-1}) 3288, 1590, 1487, 1409, 1318, 1164, 1115, 1066, 1014, 747. HRMS (ESI) $[M - OH]^+$ calcd for $C_{21}H_{14}F_3N_2^+$ 351.1109, found. 351.1125.

*3-(4-Chlorophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (**3ga**)*



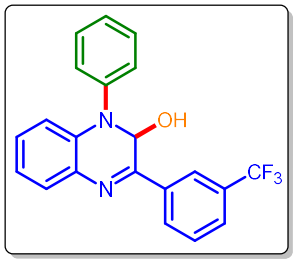
Yellow solid (93 mg, 79% yield); m.p. 147-148 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (d, J = 8.5 Hz, 2H), 7.61 (d, J = 8 Hz, 1H), 7.55 (d, J = 7.5 Hz, 2H), 7.46–7.41 (m, 4H), 7.30 (d, J = 7.5 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 7.02-6.98 (m, 2H), 6.01 (d, J = 9.5 Hz, 1H), 2.98 (d, J = 10 Hz, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 152.4, 143.3, 136.8, 134.6, 133.6, 132.4, 129.8, 129.1, 128.8, 128.7, 126.3, 125.4, 120.8, 115.9, 76.0. IR (neat, cm^{-1}) 3066, 1588, 1489, 1333, 1166, 1011, 865, 677. HRMS (ESI) $[M - OH]^+$ calcd for $C_{20}H_{14}ClN_2^+$ 317.0846, found 317.0923.

*3-(4-Bromophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (**3ha**)*



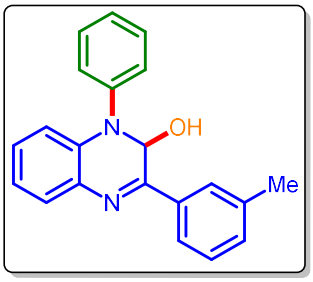
Yellow solid (110 mg, 83% yield); m.p. 155-163 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84 (d, J = 8.5 Hz, 2H), 7.54 (d, J = 7.5 Hz, 2H), 7.49 (d, J = 8.5 Hz, 2H), 7.42 (q, J = 8.0 Hz, 3H), 7.28 (t, J = 7.5 Hz, 1H), 7.07 (t, J = 7.3 Hz, 1H), 6.94 (d, J = 8 Hz, 1H), 6.81 (t, J = 7.5 Hz, 1H), 5.93 (d, J = 10.5 Hz, 1H), 3.89 (d, J = 10.5 Hz, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 152.1, 143.3, 134.7, 133.4, 132.3, 131.9, 129.7, 129.0, 128.7, 128.3, 126.3, 125.4, 125.4, 120.7, 115.6, 76.0. IR (neat, cm^{-1}) 3189, 1586, 1488, 1393, 1318, 1248, 1071, 1005, 827, 748. HRMS (ESI) $[M - OH]^+$ calcd for $C_{20}H_{14}BrN_2^+$ 361.0340, found 361.0342.

*1-Phenyl-3-(3-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (**3ia**)*



Yellow solid (99 mg, 77% yield); m.p. 127-130 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.28 (d, J = 8 Hz, 1H), 7.69 (d, J = 8 Hz, 1H), 7.65 (d, J = 7 Hz, 1H), 7.59–7.55 (m, 3H), 7.46 (t, J = 7.7 Hz, 2H), 7.31 (t, J = 7.3 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 7.01 (t, J = 7.5 Hz, 2H), 6.04 (d, J = 10.5 Hz, 1H), 2.99 (d, J = 10.6 Hz, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 151.8, 143.2, 136.9, 133.4, 132.5, 131.5, 131.3, 130.6, 129.8, 129.3, 129.1, 128.9, 127.0 (q, J = 3.7 Hz), 126.5, 125.5, 124.4 (q, J = 3.8 Hz), 120.9, 115.9, 76.0. ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.62. IR (neat, cm^{-1}) 3075, 1590, 1486, 1396, 1304, 1165, 1119, 978, 917, 799, 750, 694. HRMS (ESI) $[M - OH]^+$ calcd for $C_{21}H_{14}F_3N_2^+$ 351.1109, found 351.1106.

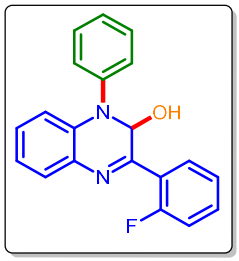
*1-Phenyl-3-(m-tolyl)-1,2-dihydroquinoxalin-2-ol (**3ja**)*



Yellow solid (88 mg, 80% yield); m.p. 90-93 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.84-7.82 (m, 2H), 7.54-7.50 (m, 3H), 7.41 (t, J = 7.7 Hz, 2H), 7.29-7.24 (m, 2H), 7.20 (d, J = 7.5 Hz, 1H), 7.06 (t, J = 7.5 Hz, 1H), 6.94 (d, J = 8 Hz, 1H), 6.89-6.85 (m, 1H), 6.00 (s, 1H), 3.67 (s, 1H), 2.36 (s, 3H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 153.7, 143.5,

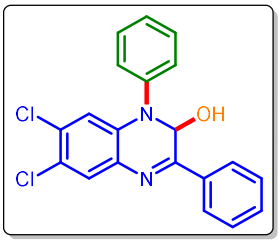
138.3, 136.0, 133.8, 132.4, 131.4, 129.6, 128.6, 128.3, 128.2, 128.1, 126.0, 125.3, 124.8, 120.6, 115.7, 76.1, 21.6. IR (neat, cm^{-1}) 3064, 2957, 1666, 1588, 1483, 1270, 1015, 954, 744, 693. HRMS (ESI) $[M - OH]^+$ calcd for $C_{21}H_{17}N_2^+$ 297.1392, found 297.1390.

*3-(2-Fluorophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (**3ka**)*



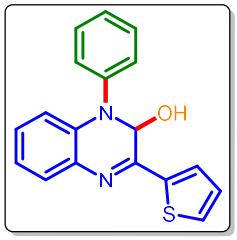
Yellow solid (73 mg, 64% yield); m.p. 140-145 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 8.12 (t, J = 7.5 Hz, 1H), 7.67 (d, J = 7.5 Hz, 1H), 7.54 (d, J = 8 Hz, 2H), 7.44 (t, J = 8 Hz, 3H), 7.30–7.26 (m, 2H), 7.19–7.11 (m, 2H), 7.03 (t, J = 7.5 Hz, 2H), 6.06 (d, J = 5 Hz, 1H), 2.81 (d, J = 6.5 Hz, 1H).; $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 162.5, 160.0, 151.0 (d, J = 3.2 Hz), 143.2, 133.8, 132.8, 132.1 (d, J = 8.9 Hz), 131.4 (d, J = 2.9 Hz), 129.7, 128.7, 128.7, 126.2, 125.3, 124.9 (d, J = 3.2 Hz), 120.7, 116.6 (d, J = 23.4 Hz), 115.8, 76.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.47. IR (neat, cm^{-1}) 3129, 1587, 1486, 1447, 1332, 1227, 1097, 976, 744, 696. HRMS (ESI) $[M + H]^+$ calcd for $C_{20}H_{16}FON_2^+$ 319.1241, found 319.1242.

*6,7-Dichloro-1,3-diphenyl-1,2-dihydroquinoxalin-2-ol (**3la**)*



Yellow solid (106 mg, 82% yield); m.p. 175-185 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.92–7.90 (m, 2H), 7.54–7.46 (m, 5H), 7.40–7.30 (m, 4H), 6.97 (s, 1H), 5.97 (d, J = 10.4 Hz, 1H), 4.18 (d, J = 10.0 Hz, 1H).; $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 154.6, 142.6, 135.0, 132.7, 132.2, 132.0, 131.2, 130.1, 129.0, 128.9, 127.7, 127.1, 125.8, 123.3, 116.5, 75.8. IR (neat, cm^{-1}) 3138, 1591, 1472, 1389, 1337, 1102, 975, 895, 701. HRMS (ESI) $[M - OH]^+$ calcd for $C_{20}H_{13}Cl_2N_2^+$ 351.0456, found. 351.0446

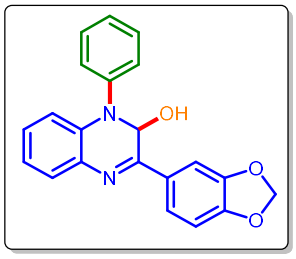
*1-Phenyl-3-(thiophen-2-yl)-1,2-dihydroquinoxalin-2-ol (**3ma**)*



Yellow solid (74 mg, 69% yield); m.p. 140-143 °C. ^1H NMR (400 MHz, $CDCl_3$) δ 7.62–7.60 (m, 2H), 7.57–7.54 (m, 2H), 7.49 (d, J = 5.0 Hz, 1H), 7.45 (t, J = 7.9 Hz, 2H), 7.31 (d, J = 7.6 Hz, 1H), 7.15–

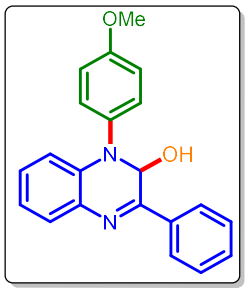
7.10 (m, 2H), 7.03–6.98 (m, 2H), 6.06 (s, 1H), 2.79 (s, 1H).; $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 149.4, 143.4, 142.9, 133.6, 132.6, 130.4, 129.8, 128.4, 128.3, 128.2, 128.1, 126.3, 125.4, 120.9, 115.9, 76.4. IR (neat, cm^{-1}) 3065, 1661, 1588, 1486, 1422, 1281, 1003, 938, 852, 742. HRMS (ESI) $[M - OH]^+$ calcd for $C_{18}H_{13}N_2S^+$ 289.0799, found 289.0789 .

*3-(Benzo[d][1,3]dioxol-5-yl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (**3na**)*



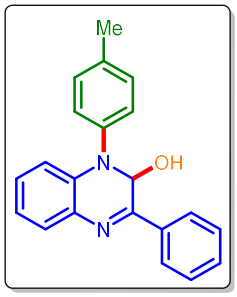
Yellow solid (49 mg, 41% yield); m.p. 138 -141 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.71 (s, 1H), 7.63–7.60 (m, 2H), 7.55 (d, J = 7.5 Hz, 2H), 7.44 (t, J = 7.7 Hz, 2H), 7.29 (d, J = 7.5 Hz, 1H), 7.14 (t, J = 7.7 Hz, 1H), 7.02 (d, J = 7.5 Hz, 2H), 6.87 (d, J = 8.5 Hz, 1H), 6.03 (d, J = 2.5 Hz, 2H), 5.99 (d, J = 17 Hz, 1H), 2.76 (d, J = 10.5 Hz, 1H).; $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$) δ 153.0, 150.0, 148.4, 143.5, 133.7, 132.2, 130.7, 129.7, 128.3, 128.1, 126.1, 125.2, 122.5, 120.8, 115.8, 108.3, 107.6, 101.7, 76.1. IR (neat, cm^{-1}) 3067, 1591, 1485, 1444, 1236, 1097, 1034, 933, 746, 696. HRMS (ESI) $[M - OH]^+$ calcd for $C_{21}H_{15}N_2O_2^+$ 327.1134, found 327.1128.

*1-(4-Methoxyphenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (**3ab**)*



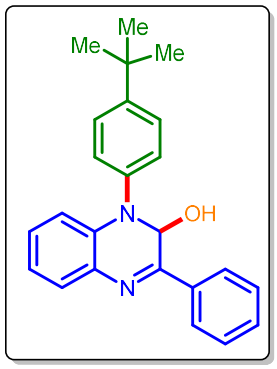
Yellow solid (93mg, 80% yield); m.p. 169-172 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13–8.11 (m, 2H), 7.65 (d, J = 8 Hz, 1H), 7.47-7.45 (m, 5H), 7.14 (t, J = 7.5 Hz, 1H), 7.00–6.97 (m, 3H), 6.85 (d, J = 8.5 Hz, 1H), 6.02 (d, J = 6 Hz, 1H), 3.86 (s, 3H), 2.78 (d, J = 9.5 Hz, 1H).; $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 158.3, 153.2, 136.3, 136.2, 133.4, 133.3, 130.6, 128.9, 128.8, 128.5, 127.7, 127.5, 120.2, 115.4, 115.0, 76.3, 55.7. IR (neat, cm^{-1}) 3118, 2935, 1590, 1483, 1326, 1253, 1048, 1024, 1000, 751, 693. HRMS (ESI) $[M - OH]^+$ calcd for $C_{21}H_{17}N_2O^+$ 313.1341, found 313.1340.

*3-Phenyl-1-(p-tolyl)-1,2-dihydroquinoxalin-2-ol (**3ac**)*



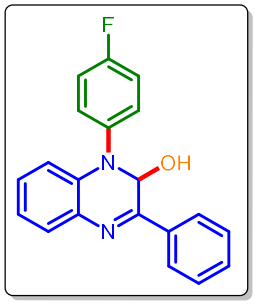
Yellow solid (86 mg, 78% yield); m.p. 150-155 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02–8.00 (m, 2H), 7.50 (dd, J = 9.7, 1.7 Hz, 1H), 7.43–7.35 (m, 5H), 7.22 (d, J = 10 Hz, 2H), 7.09–7.04 (m, 1H), 6.90 (dd, J = 10.5, 1.5 Hz, 1H), 6.88–6.84 (m, 1H), 5.98 (d, J = 9 Hz, 1H), 3.54 (d, J = 10 Hz, 1H), 2.38 (s, 3H).; ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 153.1, 140.8, 136.1, 136.0, 133.5, 132.7, 130.5, 130.2, 128.7, 128.4, 128.3, 127.5, 125.5, 120.3, 115.5, 76.2, 21.2. IR (neat, cm^{-1}) 3122, 1606, 1510, 1483, 1340, 1283, 1019, 970, 824, 750, 690. HRMS (ESI) [M - OH]$^{+}$ calcd for $C_{21}H_{17}N_2^{+}$ 297.1392, found 297.1396.

*1-(4-(Tert-butyl)phenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (**3ad**)*



Yellow solid (95 mg, 76% yield); m.p. 70-75 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.02-8.00 (m, 2H), 7.52 (d, J = 7.9 Hz, 1H), 7.43 (q, J = 8.5 Hz, 5H), 7.39–7.35 (m, 2H), 7.07 (t, J = 7.5 Hz, 1H), 6.96 (d, J = 8 Hz, 1H), 6.86 (t, J = 7.5 Hz, 1H), 6.00 (s, 1H), 3.59 (s, 1H), 1.35 (s, 9H).; ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$) δ 153.2, 149.2, 140.7, 136.0, 133.5, 132.6, 130.5, 128.7, 128.33, 128.31, 127.5, 126.5, 125.0, 120.3, 115.7, 76.1, 34.7, 31.5. IR (neat, cm^{-1}) 3517, 2955, 1602, 1510, 1479, 1371, 1265, 954, 748, 691. HRMS (ESI) [M - OH]$^{+}$ calcd for $C_{24}H_{23}N_2^{+}$ 339.1861 , found 339.1863.

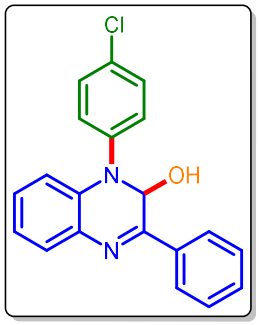
*1-(4-Fluorophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (**3ae**)*



Yellow solid (76 mg, 68% yield); m.p. 153-155 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09-8.07 (m, 2H), 7.60 (d, J = 7.5 Hz, 1H), 7.53-7.51 (m, 2H), 7.45–7.43 (m, 3H), 7.13 (t, J = 8.25 Hz, 3H), 6.97 (t, J = 7.5 Hz, 1H), 6.86 (d, J = 8 Hz, 1H), 5.98 (d, J = 10.5 Hz, 1H), 3.09 (d, J = 10.5 Hz, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 162.0, 160.1, 153.5, 139.4 (d, J = 3.0 Hz), 136.0, 133.5, 132.7, 130.7, 128.9, 128.7

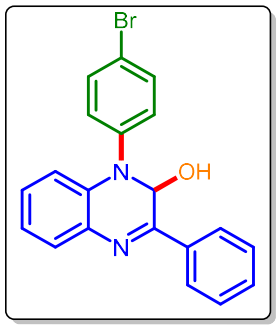
(d, J = 14.6 Hz), 127.7 (d, J = 8.3 Hz), 127.5, 120.7, 116.6 (d, J = 22.6 Hz),115.3, 76.2. ^{19}F NMR (471 MHz, $CDCl_3$) δ -120.20. IR (neat, cm^{-1}) 3074, 1611, 1502, 1338, 1288, 1158, 1104, 974, 836, 750, 695. HRMS (ESI) $[M - OH]^+$ calcd for $C_{20}H_{14}FN_2^+$ 301.1141, found 301.1144.

*1-(4-Chlorophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (**3af**)*



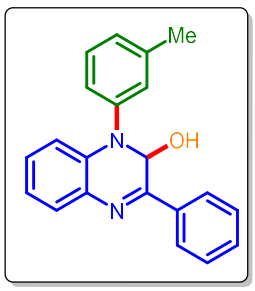
Yellow solid (79 mg, 68% yield); m.p. 160-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13–8.11 (m, 2H), 7.66 (dd, J = 7.6, 1.6 Hz, 1H), 7.50 (d, J = 8.8 Hz, 2H), 7.48–7.46 (m, 3H), 7.40 (d, J = 8.8 Hz, 2H), 7.19–7.14 (m, 1H), 7.04 (td, J = 7.5, 1.3 Hz, 1H), 7.00–6.98 (dd, J = 8.2, 1.2 Hz, 1H), 6.00 (d, J = 10 Hz, 1H), 2.88 (d, J = 10.8 Hz, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 153.8, 142.0, 136.0, 133.8, 132.1, 131.6, 130.8, 129.9, 128.9, 128.8, 128.6, 127.5, 126.5, 121.1, 115.7, 75.9. IR (neat, cm^{-1}) 3065, 1589, 1486, 1091, 1017, 976, 831, 749, 692. HRMS (ESI) $[M - OH]^+$ calcd for $C_{20}H_{14}ClN_2^+$ 317.0846 , found 317.0844.

*1-(4-Bromophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (**3ag**)*



Yellow solid (99 mg, 75% yield); m.p. 145-47 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12-8.10 (m, 2H), 7.65 (d, J = 7.5 Hz, 1H), 7.55 (d, J = 8.5 Hz, 2H), 7.47–7.44 (m, 5H), 7.16 (t, J = 7.5 Hz, 1H), 7.03 (t, J = 7.5 Hz, 1H), 7.00 (d, J = 8 Hz, 1H), 6.00 (d, J = 10.5 Hz, 1H), 2.89 (d, J = 10.5 Hz, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 153.8, 142.5, 136.0, 133.9, 132.8, 131.9, 130.8, 128.9, 128.8, 128.6, 127.5, 126.8, 121.2, 119.3, 115.7, 75.9. IR (neat, cm^{-1}) 3063, 1611, 1489, 1338, 1283, 1075, 977, 828, 749. HRMS (ESI) $[M - OH]^+$ calcd for $C_{20}H_{14}BrN_2^+$ 361.0340, found 361.0343.

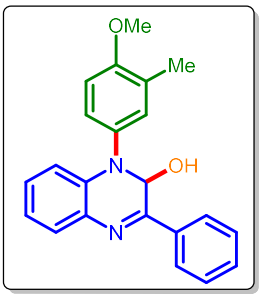
*3-Phenyl-1-(m-tolyl)-1,2-dihydroquinoxalin-2-ol (**3ah**)*



Yellow solid (87 mg, 79% yield); m.p. 90-95 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11–8.10 (m, 2H), 7.63 (dd, J = 8, 1.5 Hz, 1H), 7.45–7.43

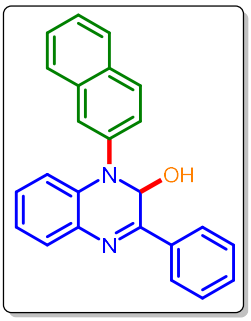
(m, 3H), 7.38 (s, 1H), 7.35–7.29 (m, 2H), 7.14 (t, J = 7.5 Hz, 1H), 7.09 (d, J = 7.0 Hz, 1H), 7.03–6.97 (m, 2H), 6.05 (d, J = 10 Hz, 1H), 2.98 (d, J = 10.5 Hz, 1H), 2.39 (s, 3H).; $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 153.5, 143.4, 139.8, 136.2, 133.7, 132.5, 130.6, 129.5, 128.8, 128.6, 128.4, 127.5, 127.0, 125.9, 122.4, 120.6, 116.0, 76.1, 21.6. IR (neat, cm^{-1}) 3056, 1596, 1482, 1330, 1177, 1018, 965, 692. HRMS (ESI) $[M - OH]^+$ calcd for $C_{21}H_{17}N_2^+$ 297.1392 , found 297.1393.

*1-(4-Methoxy-3-methylphenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (**3ai**)*



Yellow solid (98 mg, 81% yield); m.p. 152-156 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 8.12–8.10 (m, 2H), 7.63 (d, J = 7.5 Hz, 1H), 7.46–7.44 (m, 3H), 7.34–7.31 (m, 2H), 7.13 (t, J = 7.5 Hz, 1H), 6.96 (t, J = 7.3 Hz, 1H), 6.87 (t, J = 8 Hz, 2H), 6.02 (d, J = 9 Hz, 1H), 3.87 (s, 3H), 2.88 (d, J = 10.0 Hz, 1H), 2.25 (s, 3H).; $^{13}C\{^1H\}$ NMR (101 MHz, $CDCl_3$) δ 156.5, 153.0, 136.2, 135.7, 133.4, 133.2, 130.5, 128.8, 128.6, 128.5, 128.1, 127.5, 124.8, 120.0, 115.4, 110.7, 76.4, 55.7, 16.5. IR (neat, cm^{-1}) 3341, 2922, 1605, 1498, 1459, 1231, 1101, 1022, 940, 749. HRMS (ESI) $[M - OH]^+$ calcd for $C_{22}H_{19}N_2O^+$ 327.1497, found 327.1488.

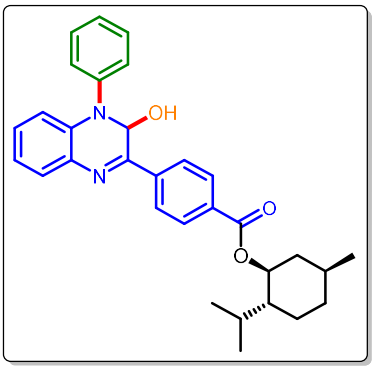
*1-(Naphthalen-2-yl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (**3aj**)*



Yellow solid (83 mg, 68% yield); m.p. 148-151 °C. ^1H NMR (500 MHz, $CDCl_3$) δ 8.18–8.16 (m, 2H), 8.11 (s, 1H), 7.87 (t, J = 8 Hz, 3H), 7.70 (d, J = 7.5 Hz, 1H), 7.57 (d, J = 8.5 Hz, 1H), 7.53 (t, J = 7 Hz, 1H), 7.51–7.46 (m, 4H), 7.17 (t, J = 7.5 Hz, 1H), 7.09–7.05 (m, 2H), 6.20 (d, J = 10 Hz, 1H), 2.92 (d, J = 10.5 Hz, 1H).; $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 153.8, 141.1, 136.1, 134.4, 134.0, 132.2, 131.7, 130.7, 129.2, 128.9, 128.8, 128.5, 127.9, 127.5, 126.9, 126.0, 124.3, 122.2, 121.1, 116.1, 76.4. IR (neat, cm^{-1}) 3072, 1576, 1451, 1319,

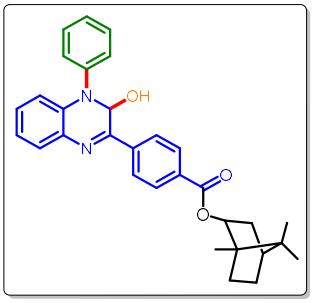
1168, 1027, 958, 638. HRMS (ESI) $[M - OH]^+$ calcd for $C_{24}H_{17}N_2^+$ 333.1392, found 333.1390.

*(1S,2R,5S)-2-Isopropyl-5-methylcyclohexyl 4-((S)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (**3oa**)*



Yellow solid (137 mg, 81% yield); m.p. 156-158 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (t, J = 8.5 Hz, 2H), 8.05 (t, J = 8.0 Hz, 2H), 7.58 –7.52 (m, 3H), 7.42 (t, J = 7.0 Hz, 2H), 7.28 (t, J = 7.7 Hz, 1H), 7.13 –7.08 (m, 1H), 6.96–6.90 (m, 2H), 6.0–6.00 (m, 1H), 4.97–4.91 (m, 1H), 3.75–3.50 (m, 1H), 2.16–2.13 (m, 1H), 1.98–1.92 (m, 1H), 1.80 –1.71 (m, 3H), 1.60–1.55 (m, 2H), 1.18– 1.09 (m, 2H), 0.93 (t, J = 7.2 Hz, 6H), 0.80 (dd, J = 7.2, 3.7 Hz, 3H).; $^{13}C\{^1H\}$ NMR (126 MHz, $CDCl_3$) δ 165.9, 165.8, 152.4, 152.3, 143.25, 139.82, 139.77, 133.5, 132.61, 132.55, 132.22, 132.19, 129.92, 129.91, 129.7, 128.9, 128.8, 128.7, 127.39, 127.38, 126.3, 125.4, 120.7, 115.81, 115.77, 75.97, 75.90, 75.37, 75.35, 47.39, 41.06, 34.4, 31.6, 26.8, 26.7, 23.94, 23.85, 22.2, 20.87, 20.84, 16.82, 16.73. IR (neat, cm^{-1}) 3339, 2912, 1655, 1478, 1454, 1222, 1214, 1007, 950, 782. HRMS (ESI) $[M - OH]^+$ calcd for $C_{31}H_{33}N_2O_2^+$ 465.2542, found 465.2471.

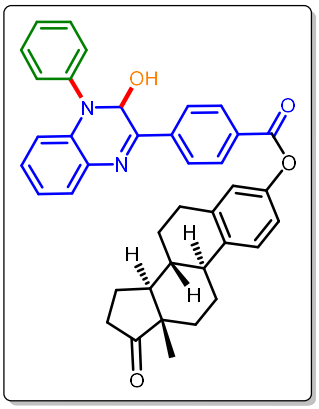
*(4R)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl 4-((S)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (**3pa**)*



Yellow solid (126 mg, 75% yield); m.p. 154-158 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 – 8.12 (m, 2H), 8.08 – 8.06 (m, 2H), 7.60–7.57 (m, 1H), 7.55 (d, J = 8 Hz, 2H), 7.44 (t, J = 7.8 Hz, 2H), 7.28 (t, J = 7.3 Hz, 1H), 7.13 (t, J = 7.5 Hz, 1H), 6.98–6.94 (m, 2H), 6.03 (d, J = 8 Hz, 1H), 5.14–5.10 (m, 1H), 3.47 (s, 1H), 2.51–2.45 (m, 1H), 2.16– .10 (m, 1H), 1.85–1.78 (m, 1H), 1.75 (t, J = 4.5 Hz, 1H), 1.46–1.39 (m, 1H), 1.36–1.31 (m, 1H), 1.14 (dd, J = 13.5, 3.5 Hz, 1H), 0.97 (s,

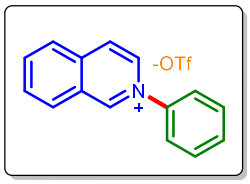
3H), 0.92 (s, 6H).; $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 166.6, 152.36, 152.32, 143.3, 139.89, 139.87, 133.6, 132.59, 132.58, 132.29, 132.26, 129.88, 129.75, 128.97, 128.83, 127.4, 126.3, 125.4, 120.8, 115.8, 81.0, 75.97, 75.96, 49.3, 48.0, 45.2, 37.0, 37.0, 28.2, 27.6, 19.9, 19.1, 13.8. IR (neat, cm^{-1}) 3439, 2913, 1675, 1454, 1426, 1208, 1157, 1009, 850, 672. HRMS (ESI) $[M - OH]^+$ calcd for $C_{31}H_{31}N_2O_2^+$ 463.2386 , found 463.2390.

*(8R,9S,13S,14S)-13-Methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl 4-((S)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (**3qa**)*



Yellow solid (86 mg, 41% yield); m.p. 140-146 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 (d, J = 8 Hz, 1H), 8.40–8.35 (m, 2H), 8.27 (d, J = 8 Hz, 1H), 8.19 (dd, J = 19.5, 8.0 Hz, 1H), 8.12 (d, J = 8.0 Hz, 1H), 7.85–7.98 (m, 1H), 7.72 (d, J = 8 Hz, 1H), 7.66 (t, J = 7.5 Hz, 1H), 7.54 (d, J = 7.5 Hz, 1H), 7.40–7.31 (m, 6H), 6.99 (d, J = 10.5 Hz, 1H), 4.16 (d, J = 5.5 Hz, 1H), 2.98– .93 (m, 3H), 2.36–2.29 (m, 3H), 2.08–1.98 (m, 6H), 1.26 (s, 3H), 0.94 (d, J = 3 Hz, 1H), 0.88 (t, J = 6.5 Hz, 2H).; $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 143.3, 131.1, 130.8, 130.6, 130.4, 130.3, 130.2, 129.98, 129.91, 129.7, 129.4, 129.1, 128.4, 127.8, 127.6, 126.7, 121.8, 120.3, 119.0, 115.7, 110.8, 77.4, 50.7, 48.1, 44.4, 38.2, 36.0, 29.8, 26.5, 25.96, 22.8, 21.8, 14.3, 14.0. IR (neat, cm^{-1}) 3349, 2930, 1657, 1480, 1447, 1209, 1201, 1021, 869, 632. HRMS (ESI) $[M - OH]^+$ calcd for $C_{39}H_{35}N_2O_3^+$ 579.2648, found 579.2664.

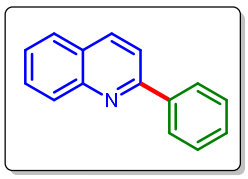
*2-Phenylisoquinolin-2-ium trifluoromethanesulfonate (**7′**)*



brown gummy solid (100 mg, 81% yield); ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.30 (s, 1H), 8.97 (dd, J = 6.8, 1.6 Hz, 1H), 8.65 (d, J = 6.8 Hz, 1H), 8.54 (d, J = 8.8 Hz, 1H), 8.37 (d, J = 8.4 Hz, 1H), 8.29–8.24 (m, 1H), 8.09– .05 (m, 1H), 7.93–7.90 (m, 2H), 7.74–7.68 (m, 3H).; $^{13}C\{^{1}H\}$ NMR (101 MHz, DMSO-d_6) δ 150.5, 143.0, 137.7,

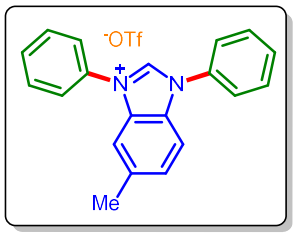
137.3, 135.0, 131.5, 131.2, 131.1, 130.3, 127.4, 127.3, 125.8, 125.0. ^{19}F NMR (471 MHz, DMSO) δ -78.10. IR (neat, cm^{-1}) 3229, 2940, 1690, 1468, 1432, 1278, 1211, 1001, 859, 659. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{15}H_{12}N^+$ 206.0964, found 206.1009.

*2-Phenylquinoline (**8l**)*



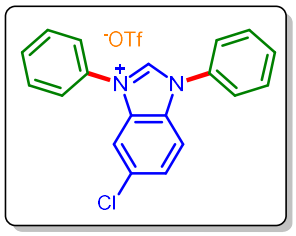
White solid (47 mg, 66% yield); m.p. 120-125 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (d, J = 8.4 Hz, 1H), 8.19–8.16 (m, 3H), 7.88 (d, J = 9 Hz, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.73 (t, J = 7.8 Hz, 1H), 7.55–7.52 (m, 3H), 7.47 (t, J = 7.6 Hz, 1H).; ^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$) δ 157.5, 148.4, 139.9, 136.9, 129.9, 129.8, 129.5, 129.0, 127.7, 127.6, 127.3, 126.4, 119.2. IR (neat, cm^{-1}) 3269, 2953, 1645, 1459, 1427, 1269, 1219, 1091, 779, 619. HRMS (ESI) [M + H]$^+$ calcd for $C_{15}H_{12}N^+$ 206.0964, found 206.1009.

*5-Methyl-1,3-diphenyl-1H-benzo[d]imidazol-3-ium trifluoromethanesulfonate (**10aa**)*



White solid (97 mg, 64% yield); m.p. 151-155 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.38 (s, 1H), 7.85–7.82 (m, 4H), 7.73 (d, J = 8.5 Hz, 1H), 7.72–7.68 (m, 4H), 7.66–7.64 (m, 2H), 7.52 (d, J = 9.5 Hz, 1H), 6.46 (s, 1H), 2.44 (s, 3H).; ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 142.3, 138.4, 133.13, 133.08, 131.5, 130.7, 130.459, 130.456, 129.4, 129.2, 125.5, 125.3, 113.4, 113.2, 21.1. ^{19}F NMR (471 MHz, DMSO-d_6) δ -78.20. IR (neat, cm^{-1}) 3139, 1570, 1289, 1219, 1119, 1104, 1021, 1001, 858, 720. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{20}H_{17}N_2^+$ 285.1392, found 285.1389.

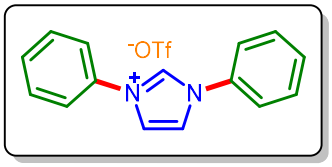
*5-Chloro-1,3-diphenyl-1H-benzo[d]imidazol-3-ium trifluoromethanesulfonate (**10ba**)*



White solid (92 mg, 58% yield); m.p. 149-156 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.56 (s, 1H), 8.02 (d, J = 1.5 Hz, 1H), 7.92 (d, J = 9.0 Hz, 1H), 7.90–7.86 (m, 3H), 7.78–7.70 (m, 7H), 6.47 (s, 1H).; ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 143.9, 132.72, 132.66, 132.4,

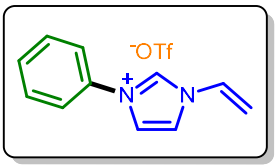
132.0, 130.9, 130.8, 130.5, 130.2, 128.2, 125.4, 125.3, 115.5, 113.7. ^{19}F NMR (471 MHz, DMSO-d$_6$) δ -72.99. IR (neat, cm^{-1}) 3138, 1579, 1248, 1211, 1169, 1144, 1023, 1007, 813, 758. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{19}H_{14}ClN_2^+$ 305.0846, found 305.0869.

*1,3-Diphenyl-1H-imidazol-3-ium trifluoromethanesulfonate (**10ca**)*



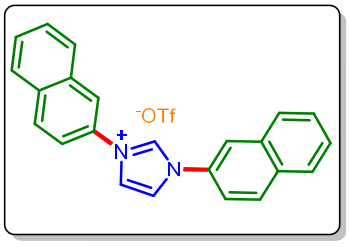
White solid (88 mg, 68% yield); m.p. 153-157 °C. ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 10.28 (t, J = 1.7 Hz, 1H), 8.52 (d, J = 1.6 Hz, 2H), 7.88–7.85 (m, 4H), 7.68–7.63 (m, 4H), 7.60–7.55 (m, 2H).; ^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$) δ 134.7, 134.6, 130.2, 130.1, 122.1, 122.0. ^{19}F NMR (471 MHz, DMSO-d$_6$) δ -77.97. IR (neat, cm^{-1}) 3128, 1552, 1285, 1257, 1147, 1120, 1067, 1060, 849, 755. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{15}H_{13}N_2^+$ 221.1079, found 221.1091.

*3-Phenyl-1-vinyl-1H-imidazol-3-ium trifluoromethanesulfonate (**10da**)*



Brown liquid (89 mg, 79% yield); ^{1}H NMR (500 MHz, DMSO-d$_6$) δ 9.97 (s, 1H), 8.33 (dt, J = 18, 2.0 Hz, 2H), 7.74–7.72 (m, 2H), 7.59 (t, J = 7.8 Hz, 2H), 7.54–7.51 (m, 1H), 7.23 (dd, J = 15.5, 9 Hz, 1H), 6.01 (dd, J = 15.7, 2.4 Hz, 1H), 5.46 (dd, J = 9, 2.5 Hz, 1H).; ^{13}C{^{1}H} NMR (101 MHz, DMSO-d$_6$) δ 134.6, 134.5, 130.2, 130.1, 128.8, 122.03, 121.99, 120.1, 109.8. ^{19}F NMR (471 MHz, DMSO-d$_6$) δ -78.03. IR (neat, cm^{-1}) 3133, 1559, 1228, 1217, 1148, 1146, 1053, 1018, 859, 756. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{11}H_{11}N_2^+$ 171.0922, found 171.0948.

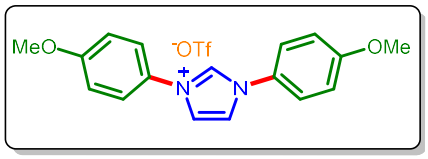
*1,3-Di(naphthalen-2-yl)-1H-imidazol-3-ium trifluoromethanesulfonate (**10cj**)*



Light brown solid (112 mg, 68% yield); m.p. 146-148 °C. ^{1}H NMR (500 MHz, DMSO-d$_6$) δ 10.57 (s, 1H), 8.74–8.72 (m, 2H), 8.55-8.54 (m, 2H), 8.28 (d, J = 8.5 Hz, 2H), 8.11–8.05 (m, 6H), 7.73–7.67 (m, 4H).; ^{13}C{^{1}H} NMR (126 MHz, DMSO-d$_6$) δ 134.9, 132.8, 132.5, 132.1, 130.3, 128.2, 128.01, 127.97, 127.78, 122.1, 120.5, 119.7. ^{19}F

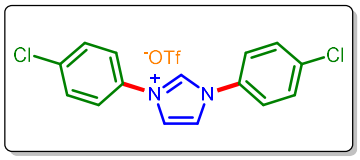
NMR (471 MHz, DMSO-d_6) δ -77.76. IR (neat, cm^{-1}) 3123, 1558, 1229, 1221, 1138, 1131, 1051, 1011, 852, 746. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{23}H_{17}N_2^+$ 321.1392, found.

*1,3-bis(4-Methoxyphenyl)-1H-imidazol-3-ium trifluoromethanesulfonate (**10cb**)*



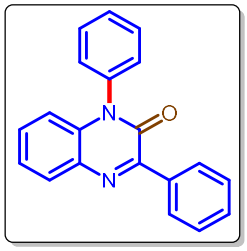
Light brown solid (99 mg, 66% yield); m.p. 145-149 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.05 (s, 1H), 8.36 (d, J = 2 Hz, 2H), 7.73 (d, J = 9.0 Hz, 4H), 7.15 (d, J = 9.0 Hz, 4H), 3.77 (s, 6H).; ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 160.2, 133.9, 127.8, 123.7, 122.0, 115.2, 55.8. ^{19}F NMR (471 MHz, DMSO-d_6) δ -77.75. IR (neat, cm^{-1}) 3123, 1561, 1227, 1216, 1149, 1143, 1042, 1017, 852, 750. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{17}H_{17}N_2O_2^+$ 281.1290, found 281.1315.

*1,3-bis(4-Chlorophenyl)-1H-imidazol-3-ium trifluoromethanesulfonate (**10cf**)*



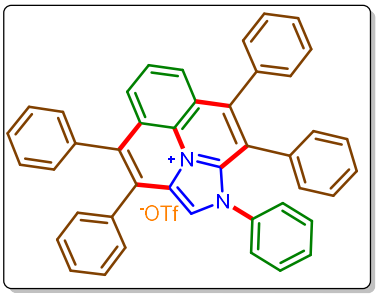
Light brown solid (104 mg, 68% yield); m.p. 150-153 °C. ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.38 (s, 1H), 8.53 (d, J = 1.6 Hz, 2H), 7.92 (d, J = 8.8 Hz, 4H), 7.76 (d, J = 8.8 Hz, 4H).; ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 135.1, 134.7, 133.5, 130.2, 124.0, 122.0. ^{19}F NMR (471 MHz, DMSO-d_6) δ -77.76. IR (neat, cm^{-1}) 3133, 1569, 1247, 1213, 1149, 1147, 1023, 1017, 812, 759. HRMS (ESI) [M - OTf]$^+$ calcd for $C_{15}H_{11}Cl_2N_2^+$ 289.0299, found 289.0356.

*1,3-Diphenylquinoxalin-2(1H)-one (**11**)*



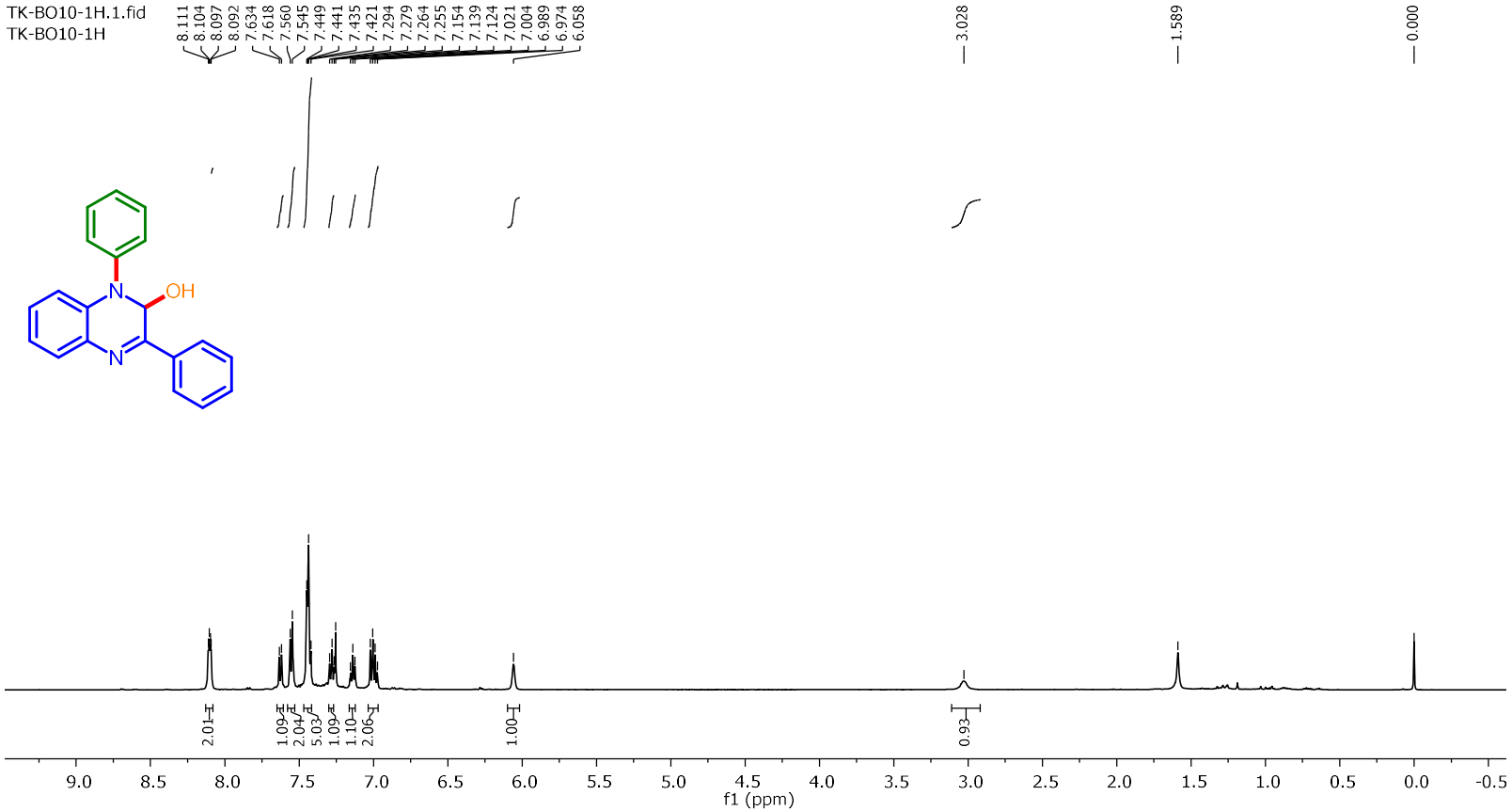
White solid (47 mg, 79% yield); m.p. 180-185 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.40 (m, 2H), 8.00–7.98 (m, 1H), 7.64 (t, J = 7.5 Hz, 2H), 7.57 (t, J = 7.5 Hz, 1H), 7.48–7.45 (m, 3H), 7.35–7.34 (m, 4H), 6.70–6.68 (m, 1H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 154.69, 154.67, 136.3, 135.9, 134.4, 133.2, 130.6, 130.4, 130.2, 130.1, 129.9, 129.6, 128.5, 128.2, 124.0, 115.5. IR (neat, cm^{-1}) 3065, 1657, 1597, 1581, 1457, 1291, 1216, 1150, 1073, 754. HRMS (ESI) [M + H]$^+$ calcd for $C_{20}H_{15}N_2O^+$ 299.1179, found 299.1172.

*1,3,4,8,9-Pentaphenyl-1H-benzo[ij]imidazo[2,1,5-de]quinolizin-10-ium trifluoromethanesulfonate (**12**)*

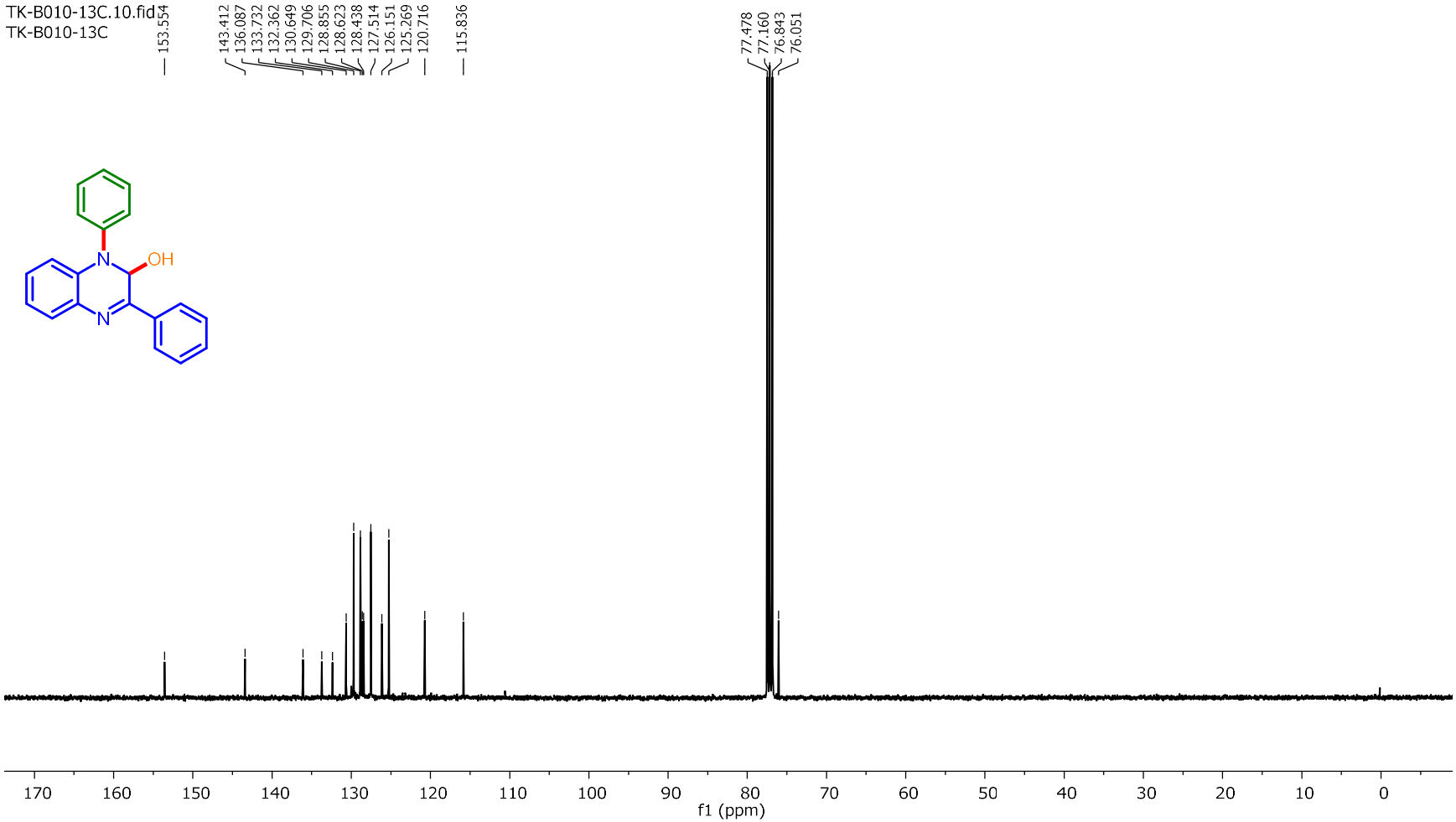


Dark brown gummy solid (128 mg, 89% yield); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.73 (d, J = 4.5 Hz, 2H), 7.65 (t, J = 4.7 Hz, 1H), 7.61 (s, 1H), 7.52–7.48 (m, 3H), 7.40–7.35 (m, 5H), 7.33–7.26 (m, 9H), 7.18 (t, J = 7.7 Hz, 1H), 7.08 (t, J = 7.7 Hz, 2H), 7.00 (d, J = 7.5 Hz, 2H), 6.89 (t, J = 7.5 Hz, 1H), 6.82 (t, J = 7.5 Hz, 2H).; ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 147.3, 137.9, 135.2, 134.7, 134.4, 134.0, 132.9, 131.7, 131.0, 130.6, 130.4, 129.95, 129.05, 128.92, 128.91, 128.8, 128.6, 128.6, 128.5, 128.2, 128.1, 128.0, 127.9, 127.1, 126.8, 126.6, 126.2, 125.5, 125.3, 124.6, 119.6. ^{19}F NMR (471 MHz, DMSO-d_6) δ -78.37. IR (neat, cm^{-1}) 3141, 1558, 1257, 1200, 1142, 1101, 1028, 1013, 802, 769. HRMS (ESI) $[M - OTf]^+$ calcd for $C_{43}H_{29}N_2^+$ 573.2325, found 573.2360.

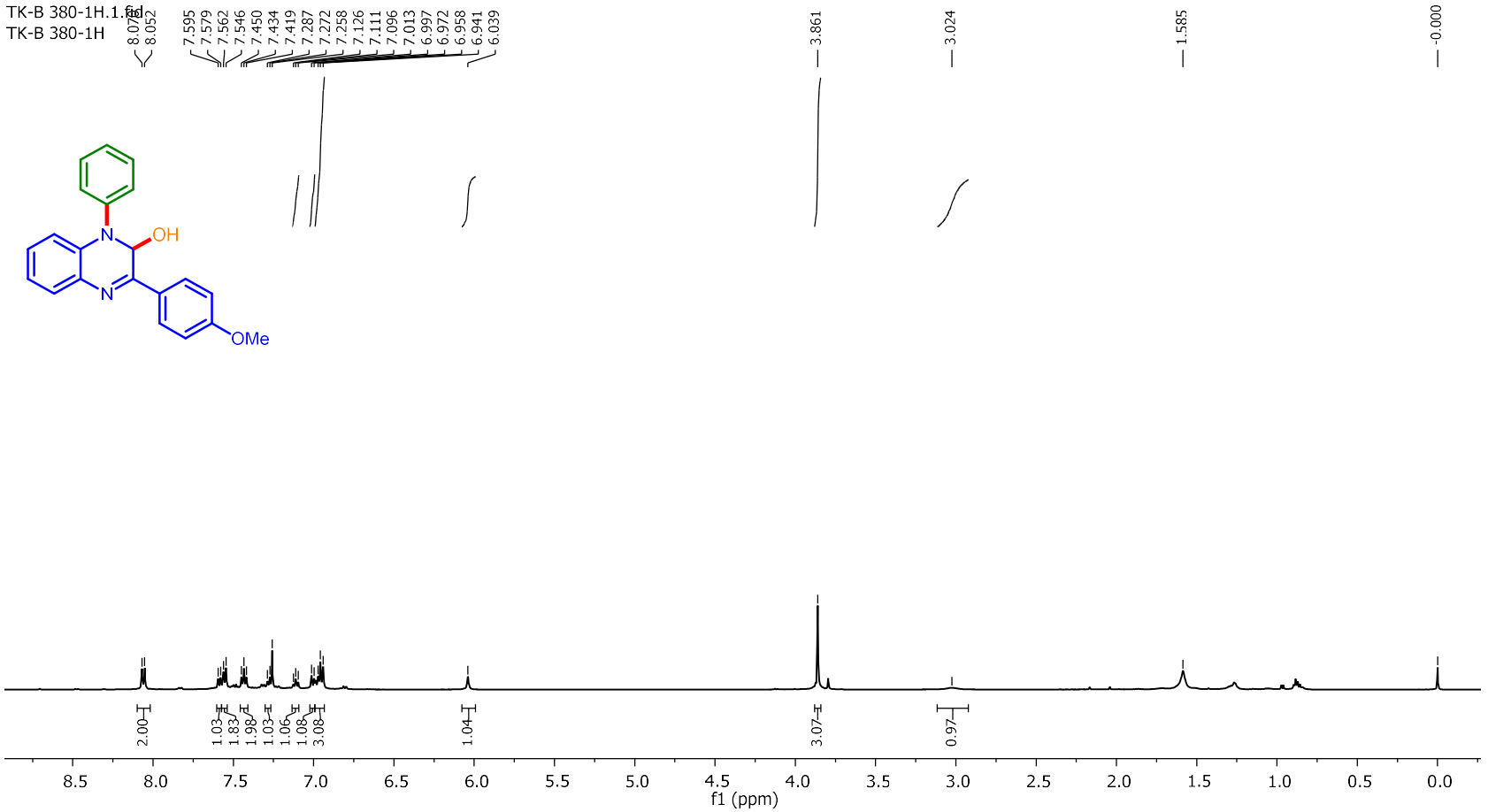
17. NMR Spectra



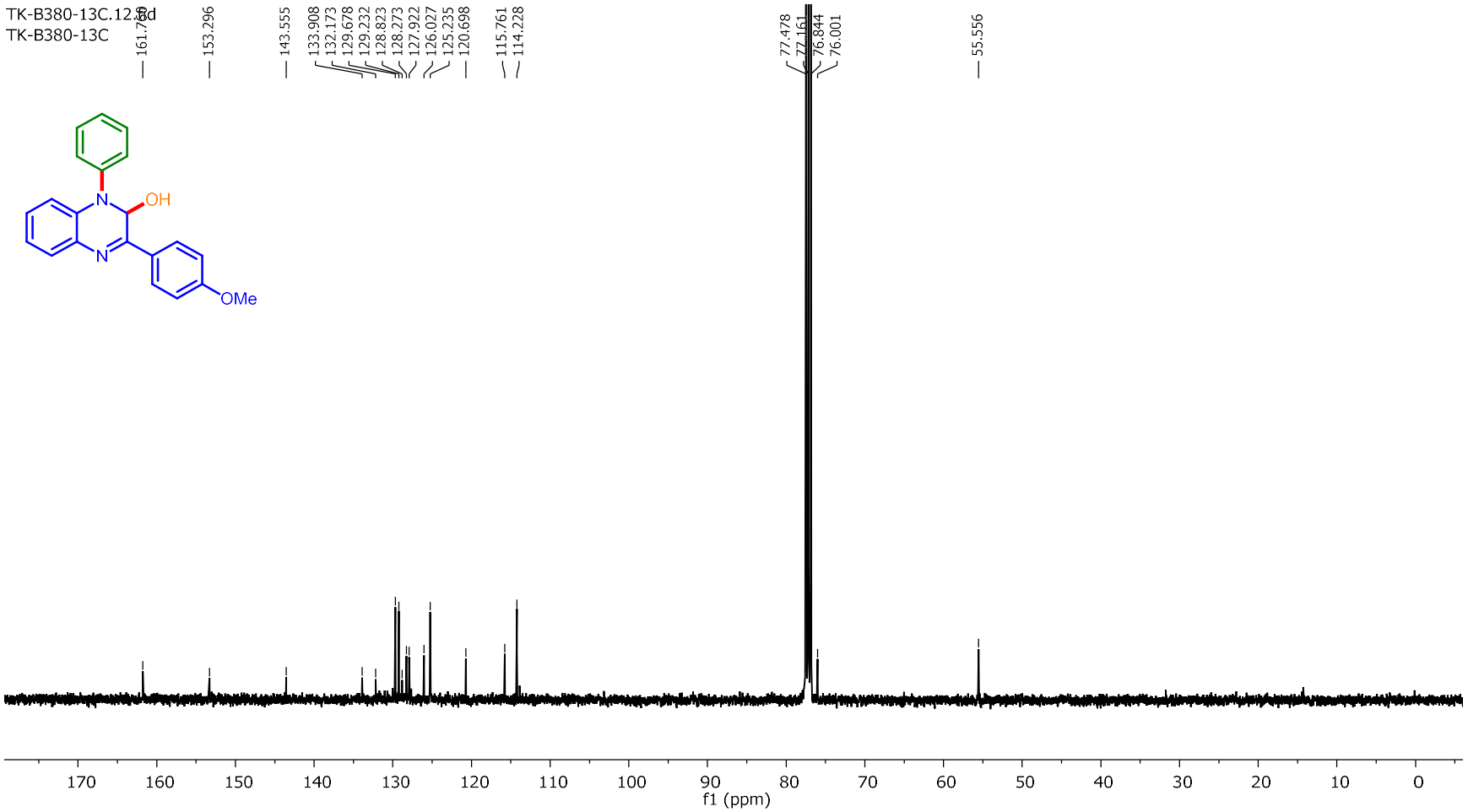
1,3-Diphenyl-1,2-dihydroquinoxalin-2-ol (3aa): ^{1}H NMR ($CDCl_3$, 500 MHz)



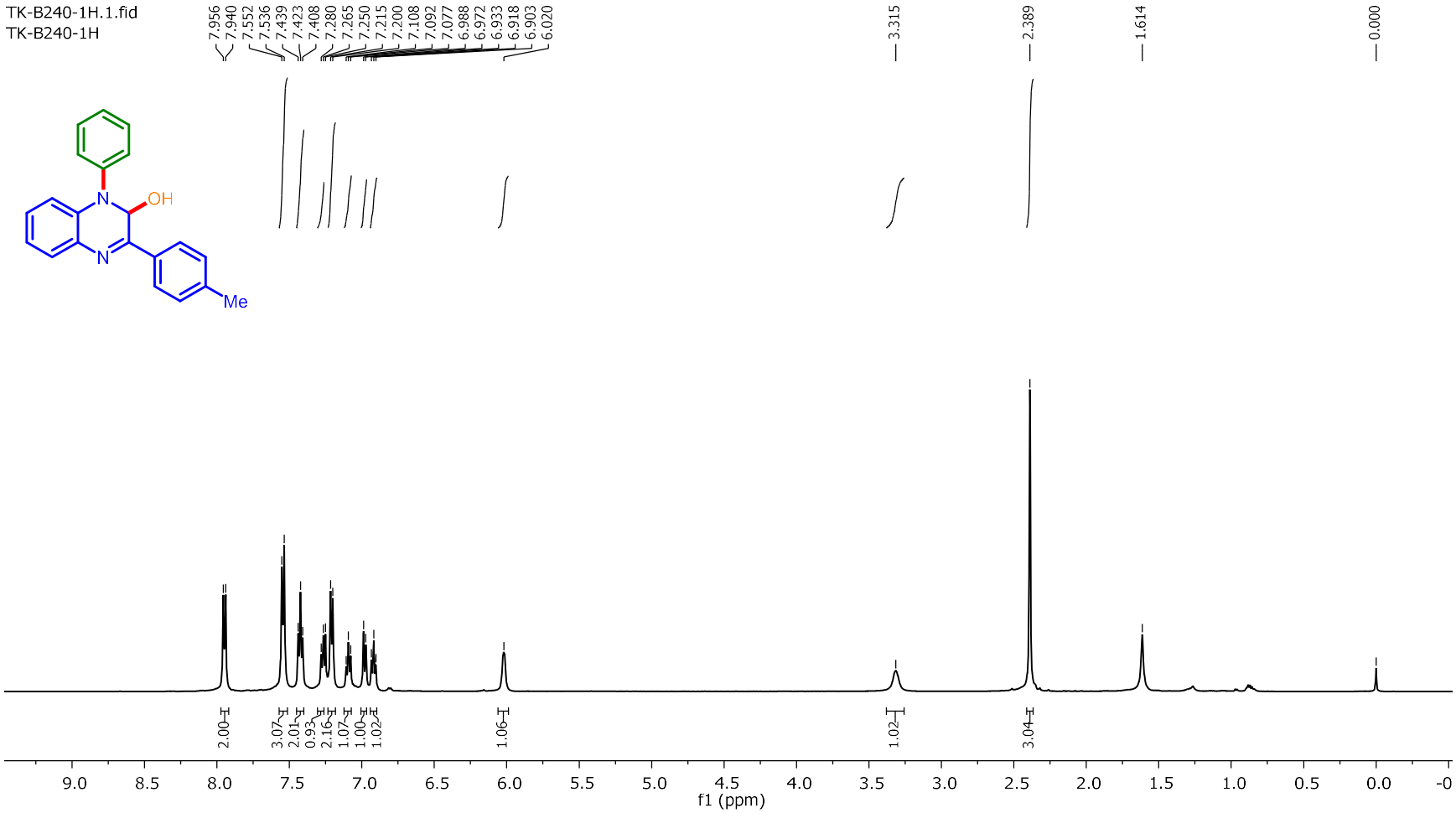
1,3-Diphenyl-1,2-dihydroquinoxalin-2-ol (3aa): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)



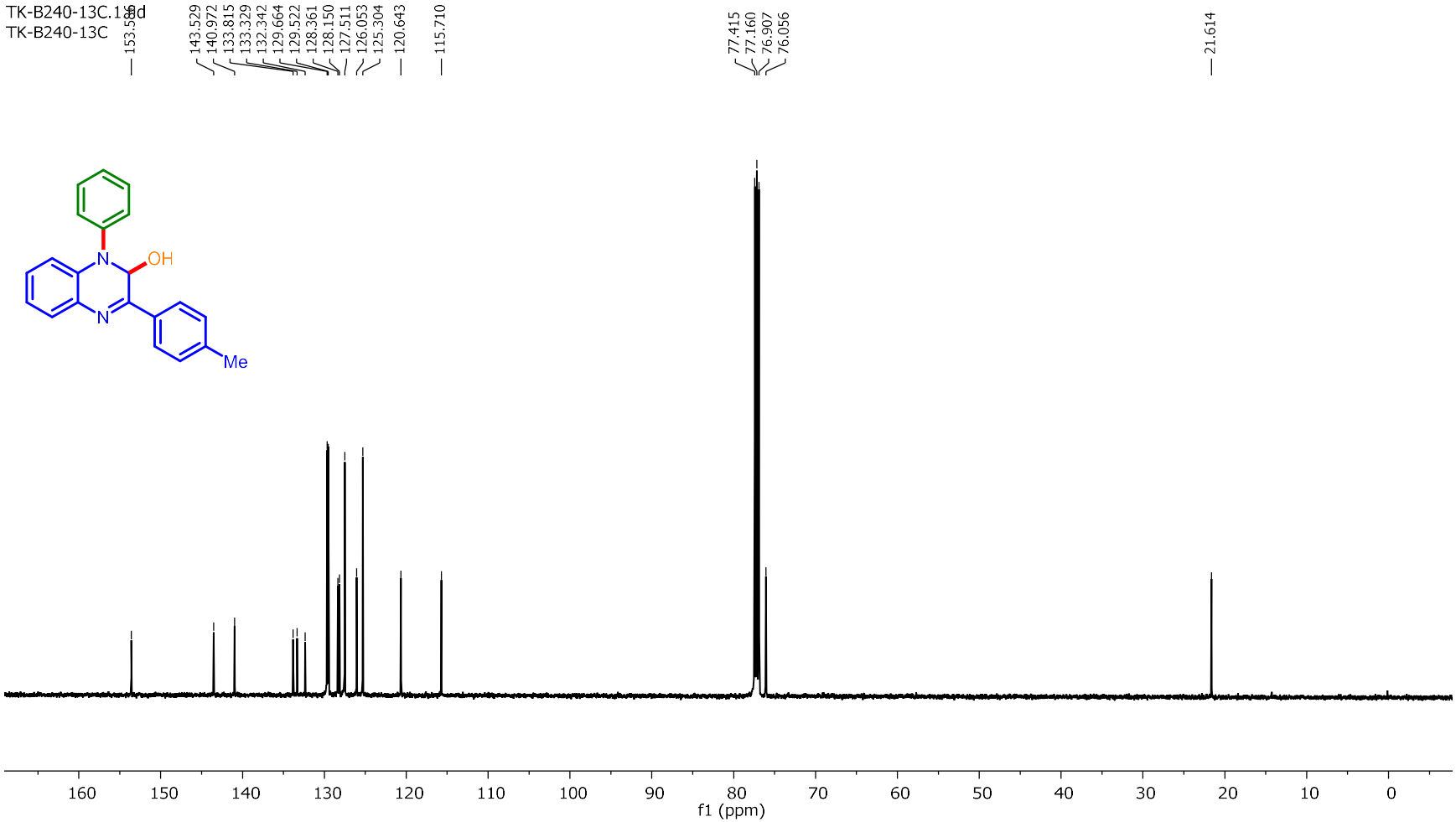
3-(4-Methoxyphenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ba): ^{1}H NMR ($CDCl_3$, 500 MHz)



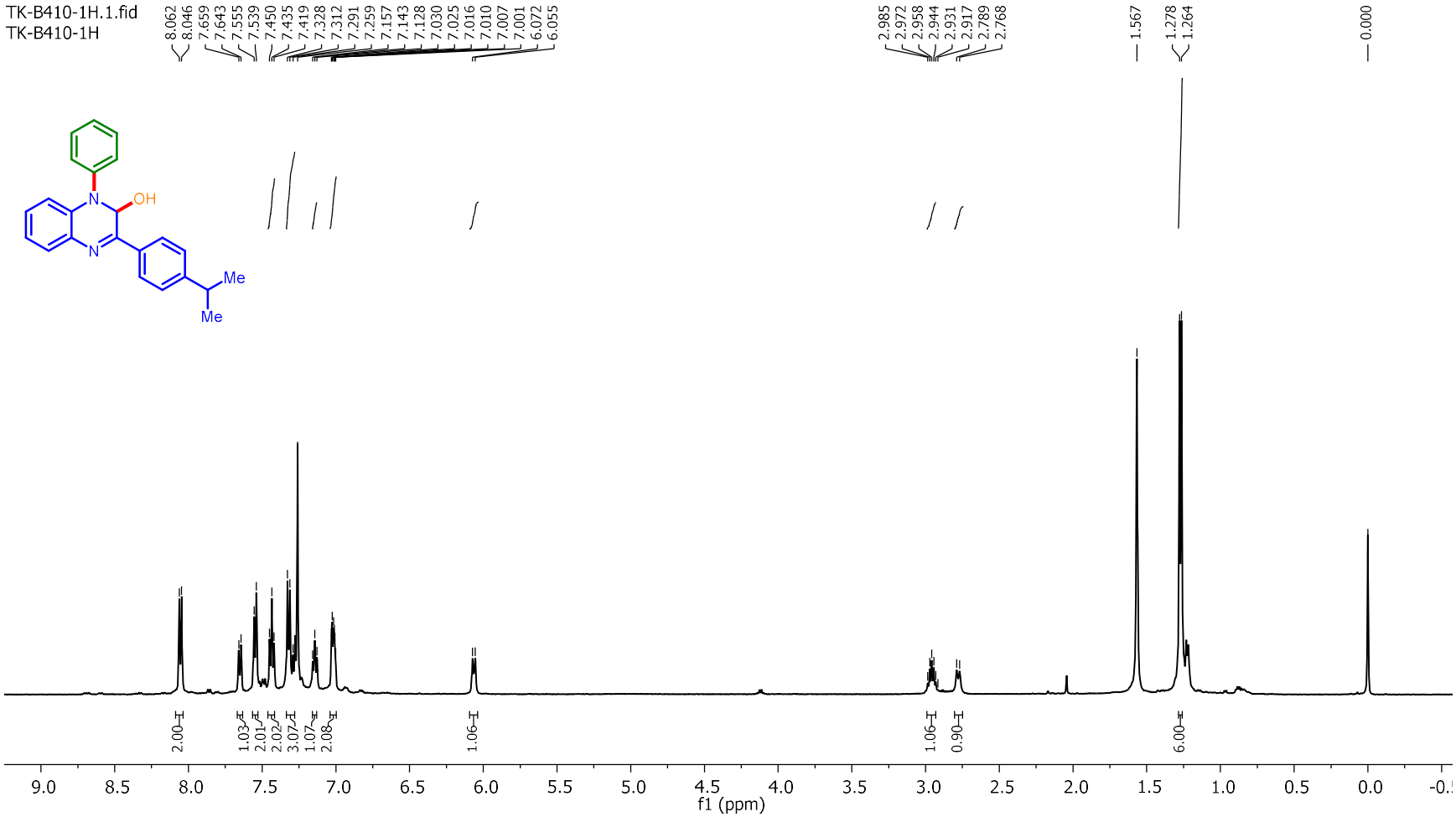
3-(4-Methoxyphenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ba): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101MHz)



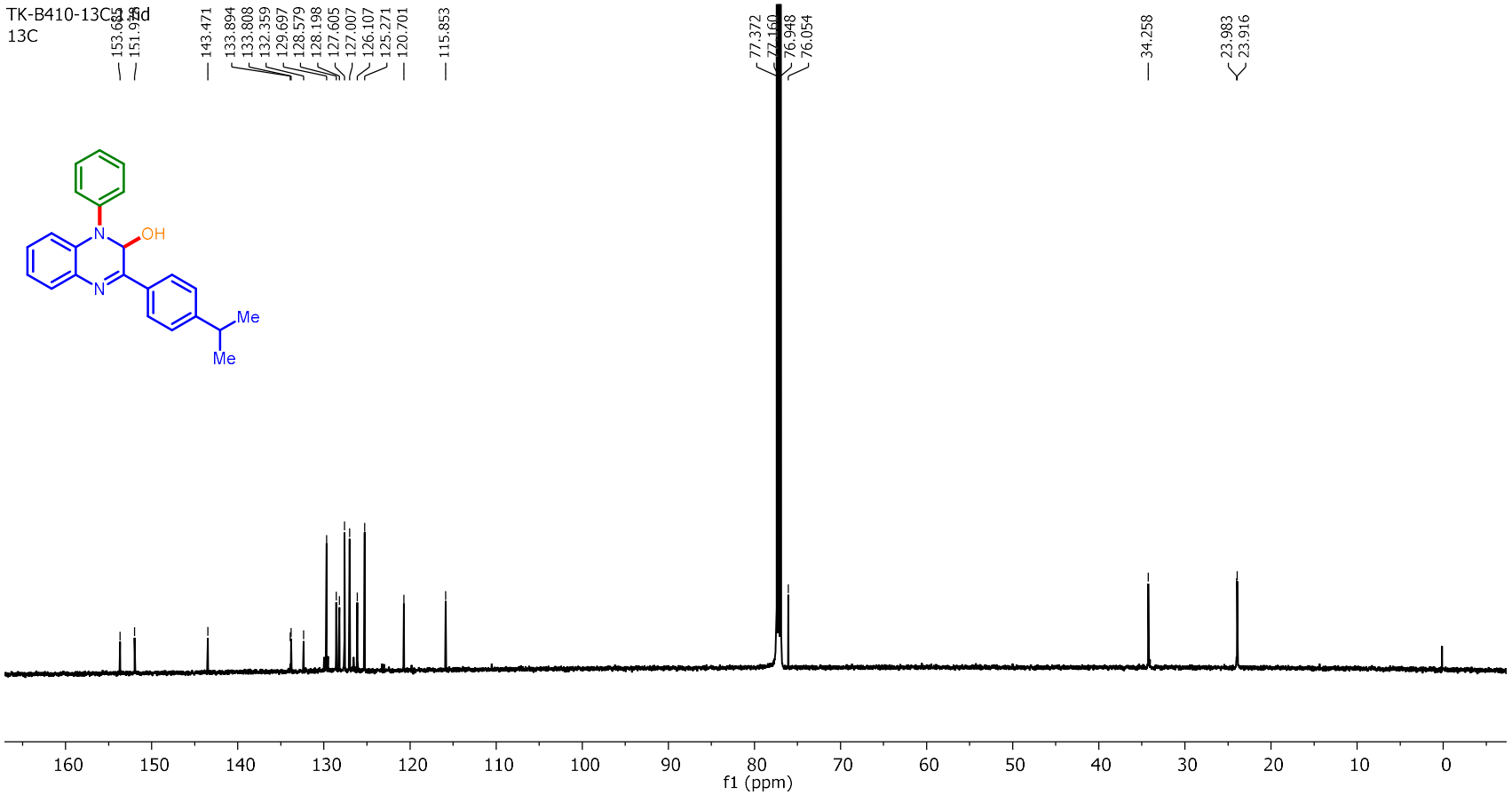
1-Phenyl-3-(*p*-tolyl)-1,2-dihydroquinoxalin-2-ol (3ca): ^{1}H NMR ($CDCl_3$, 500MHz)



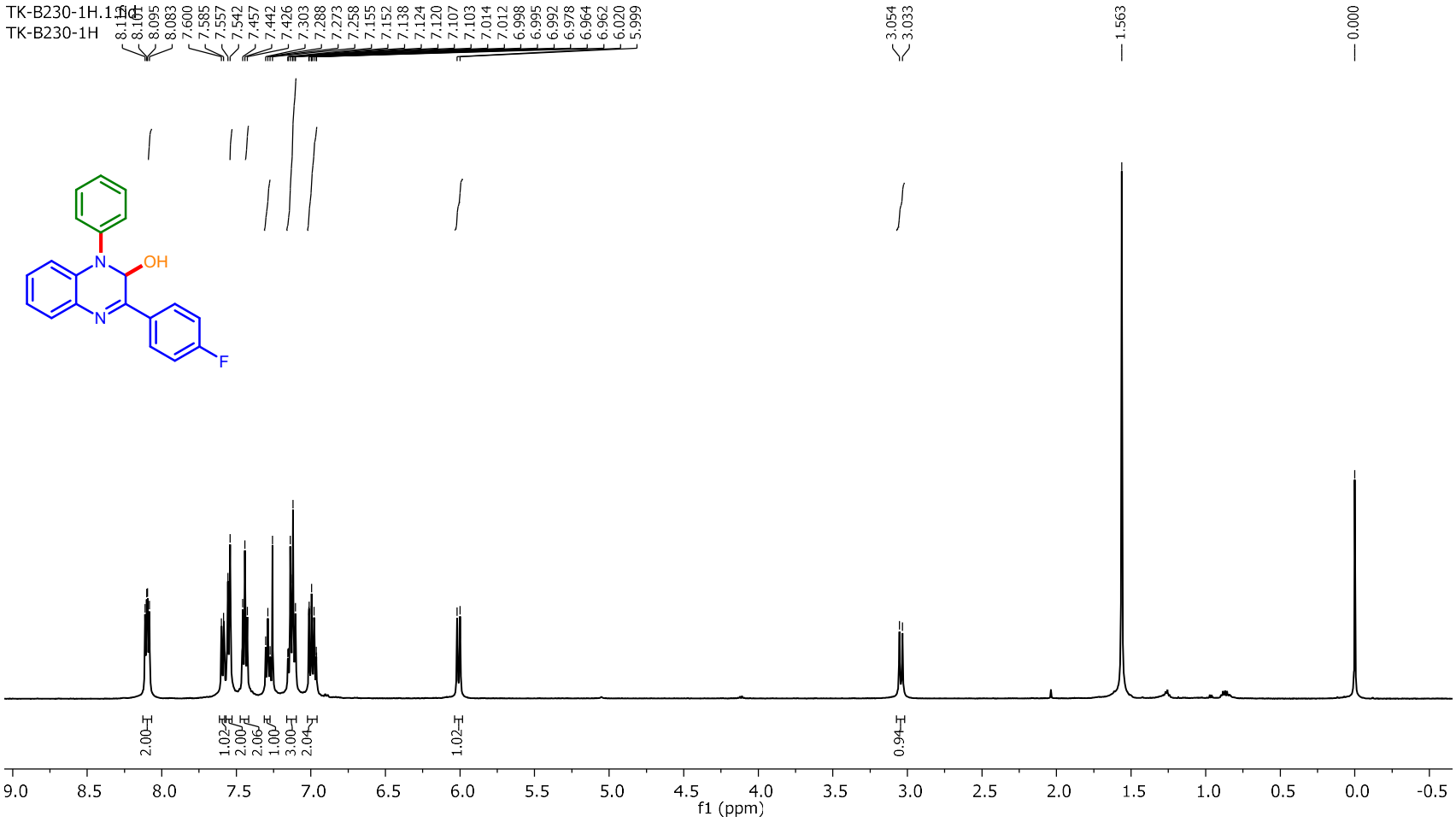
1-Phenyl-3-(*p*-tolyl)-1,2-dihydroquinoxalin-2-ol (3ca): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



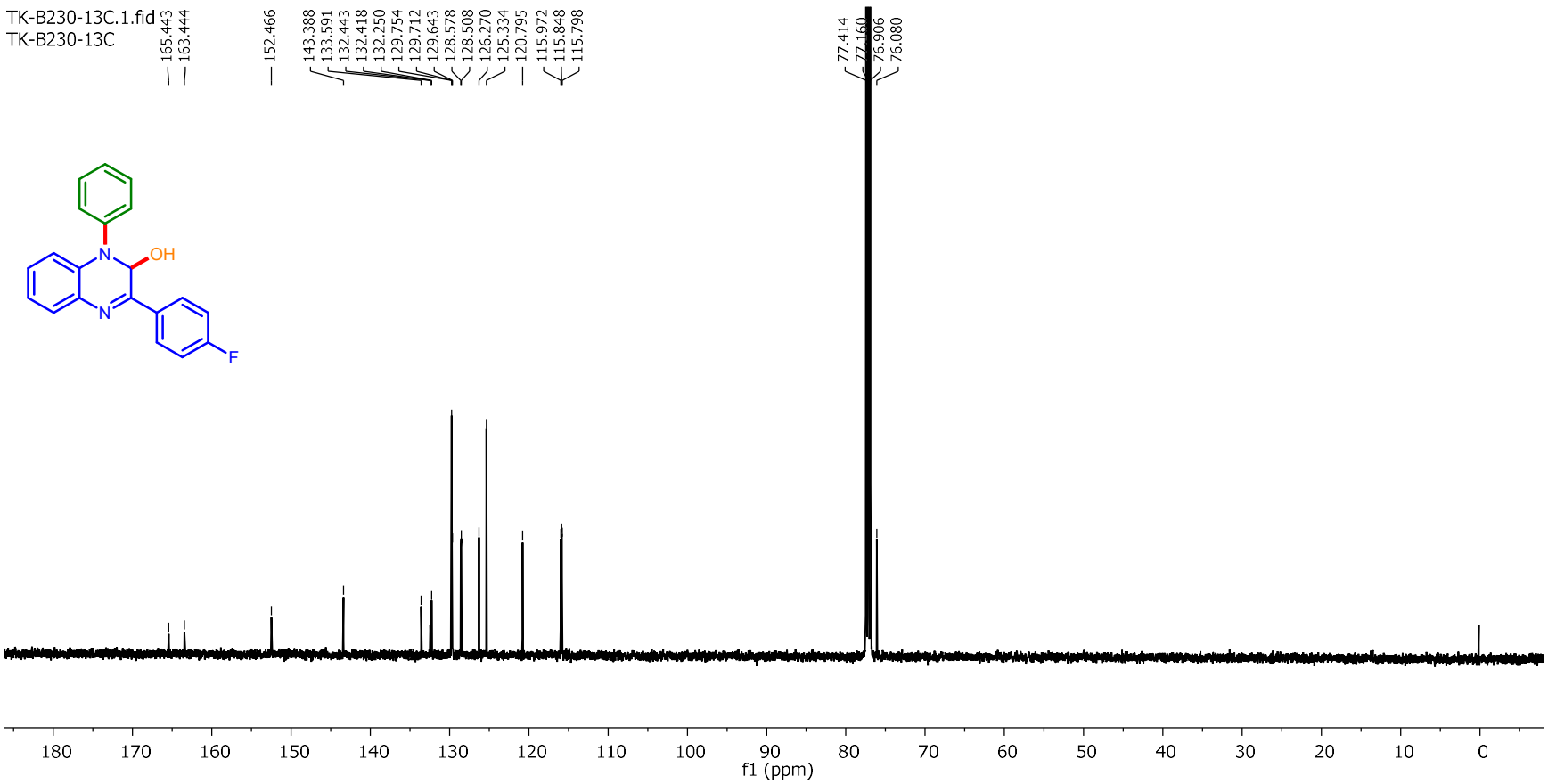
3-(4-Isopropylphenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3da): ^{1}H NMR ($CDCl_3$, 500 MHz)



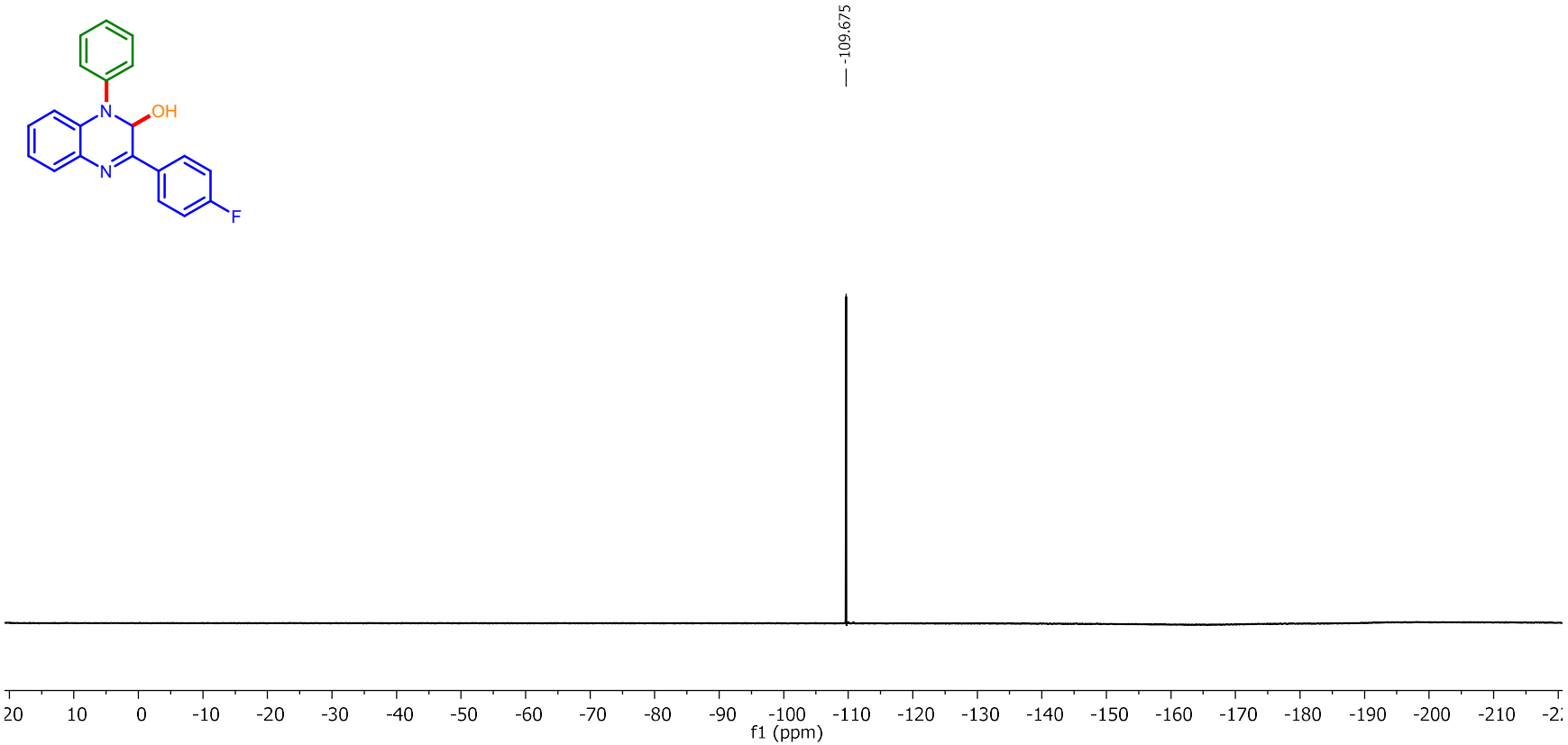
3-(4-Isopropylphenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3da): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz)



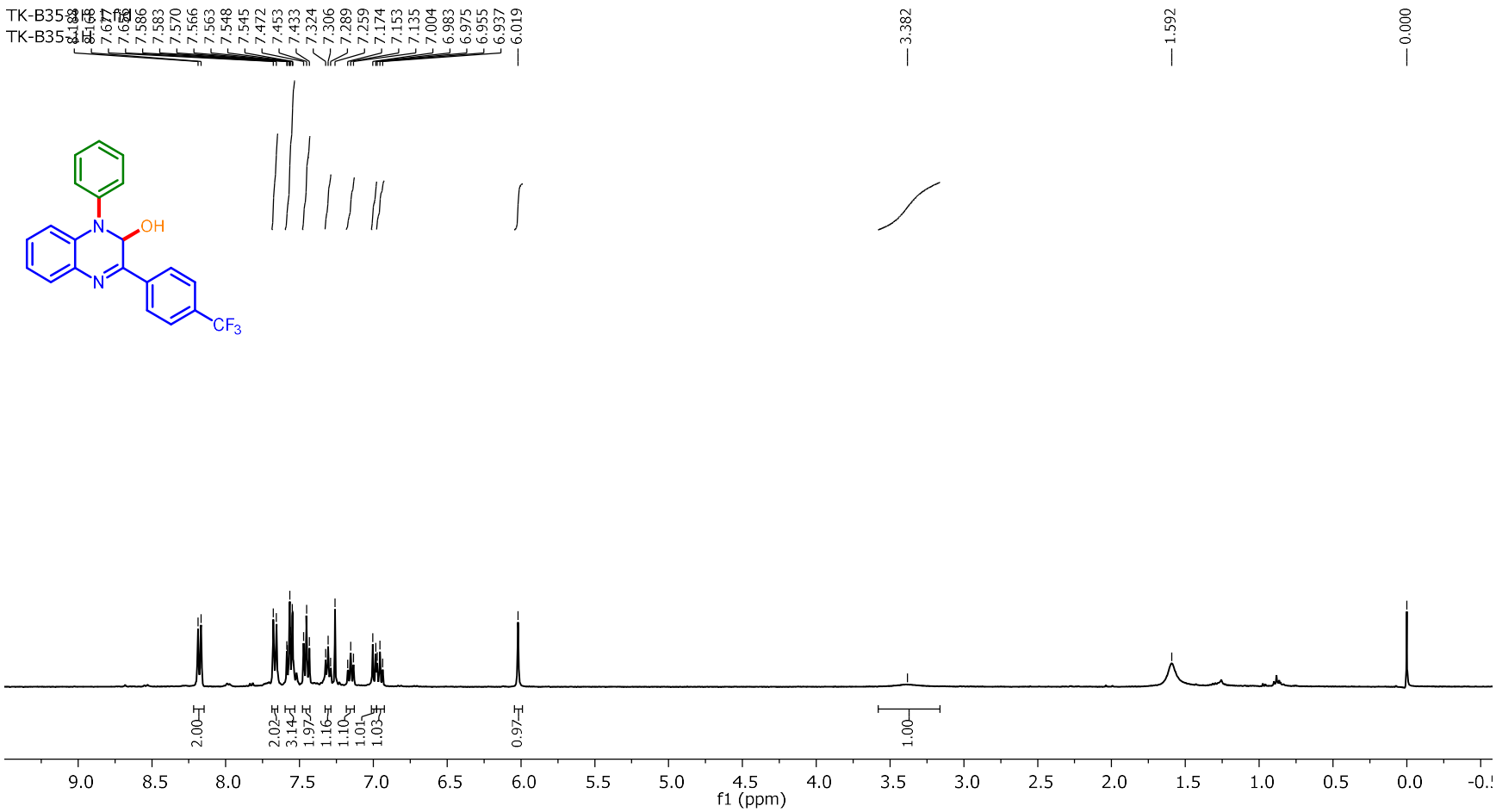
3-(4-Fluoroophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ea): ^{1}H NMR ($CDCl_3$, 500 MHz)



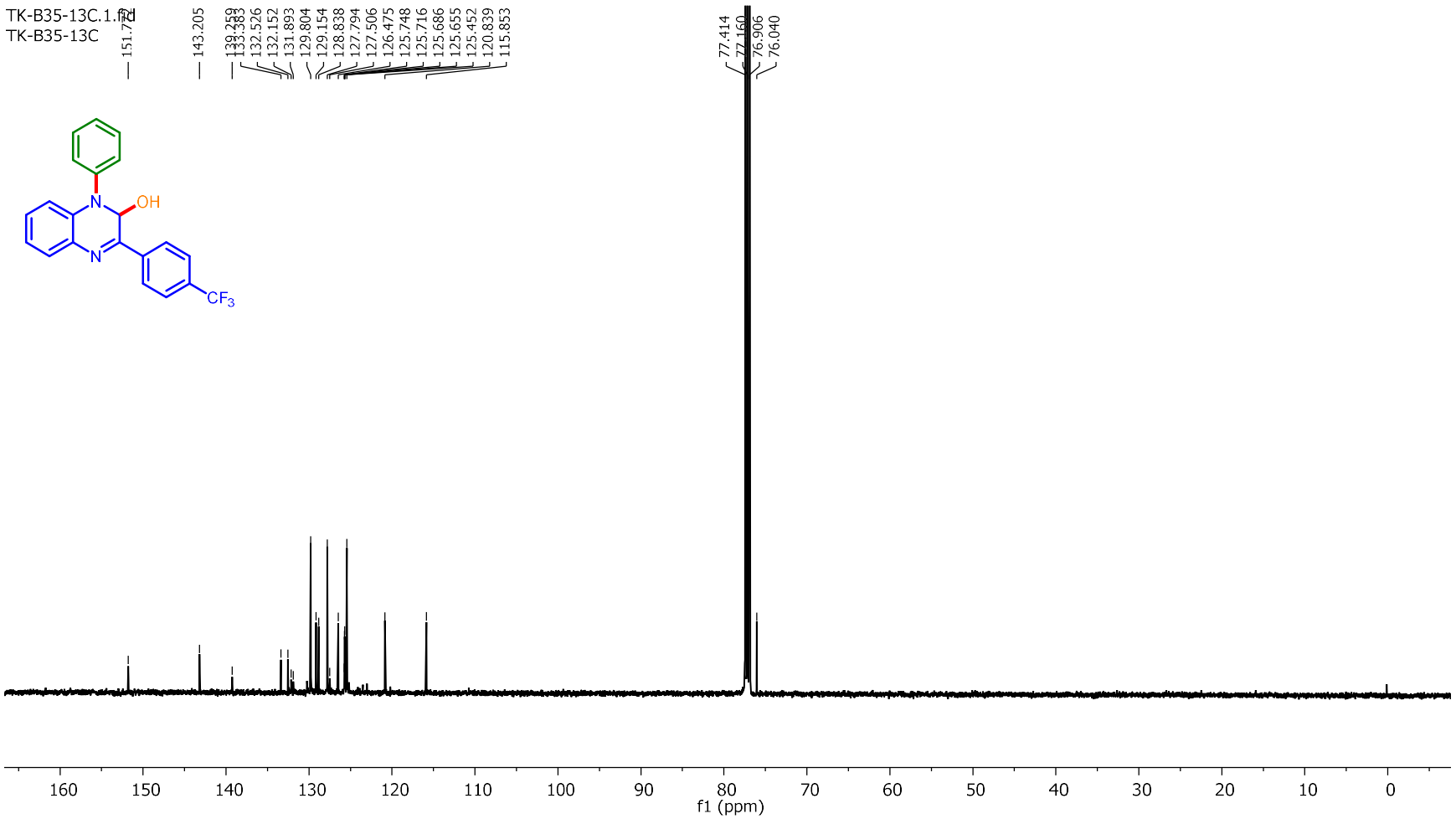
3-(4-Fluoroophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ea): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



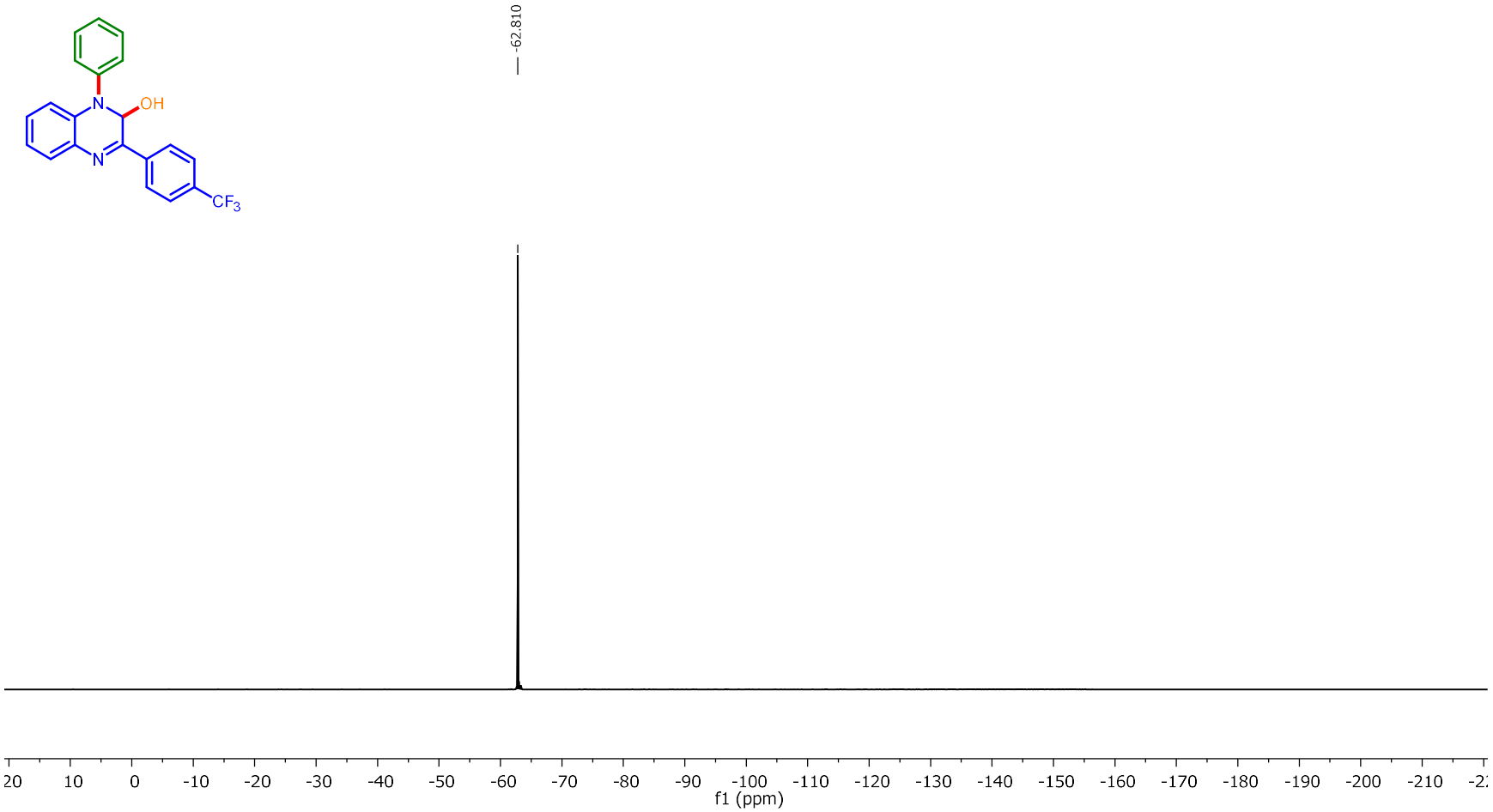
3-(4-Fluoroophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ea): ^{19}F NMR ($CDCl_3$, 471 MHz)



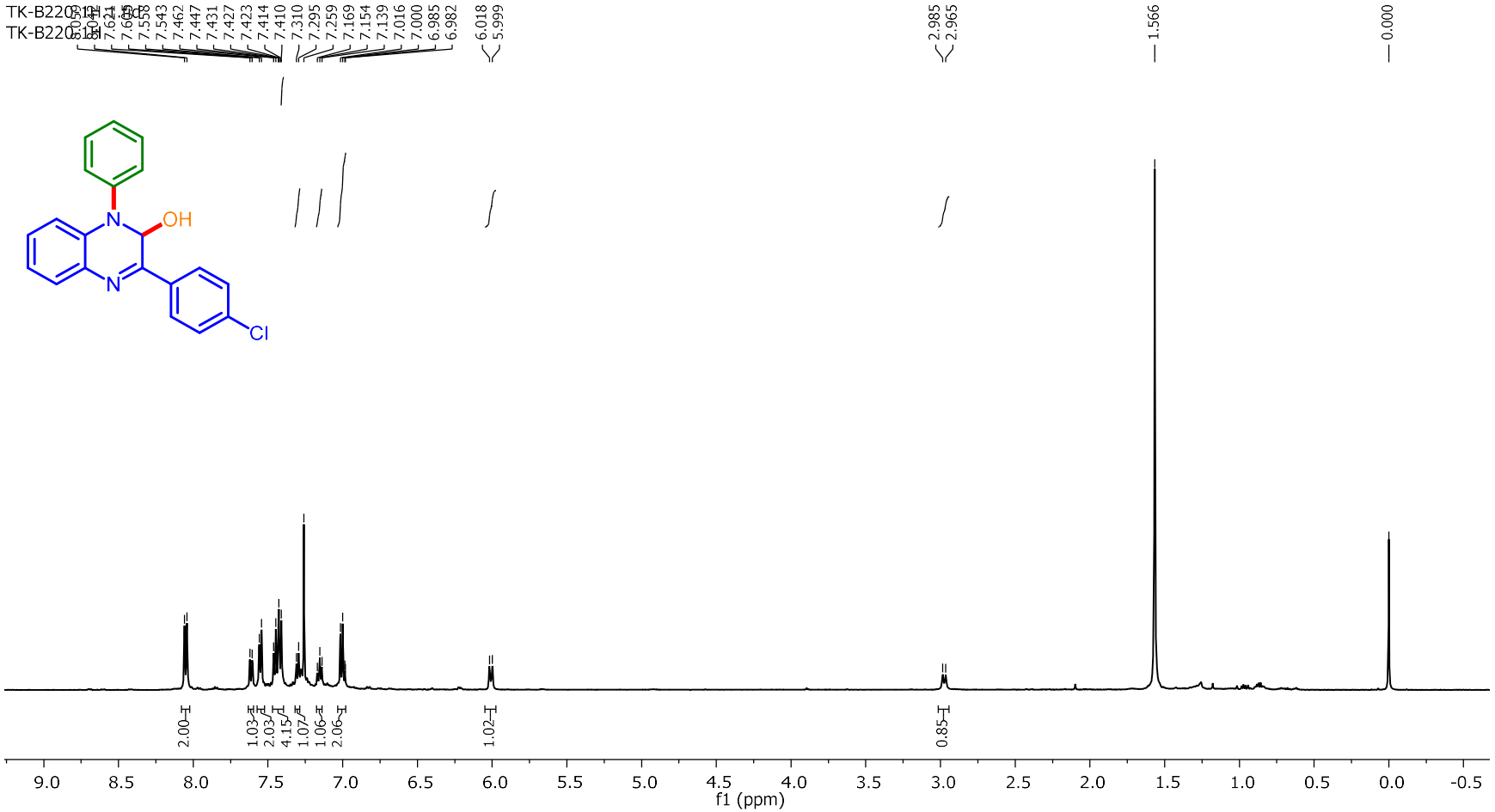
1-Phenyl-3-(4-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (3fa*):*[1]H NMR ($CDCl_3$, 500 MHz)



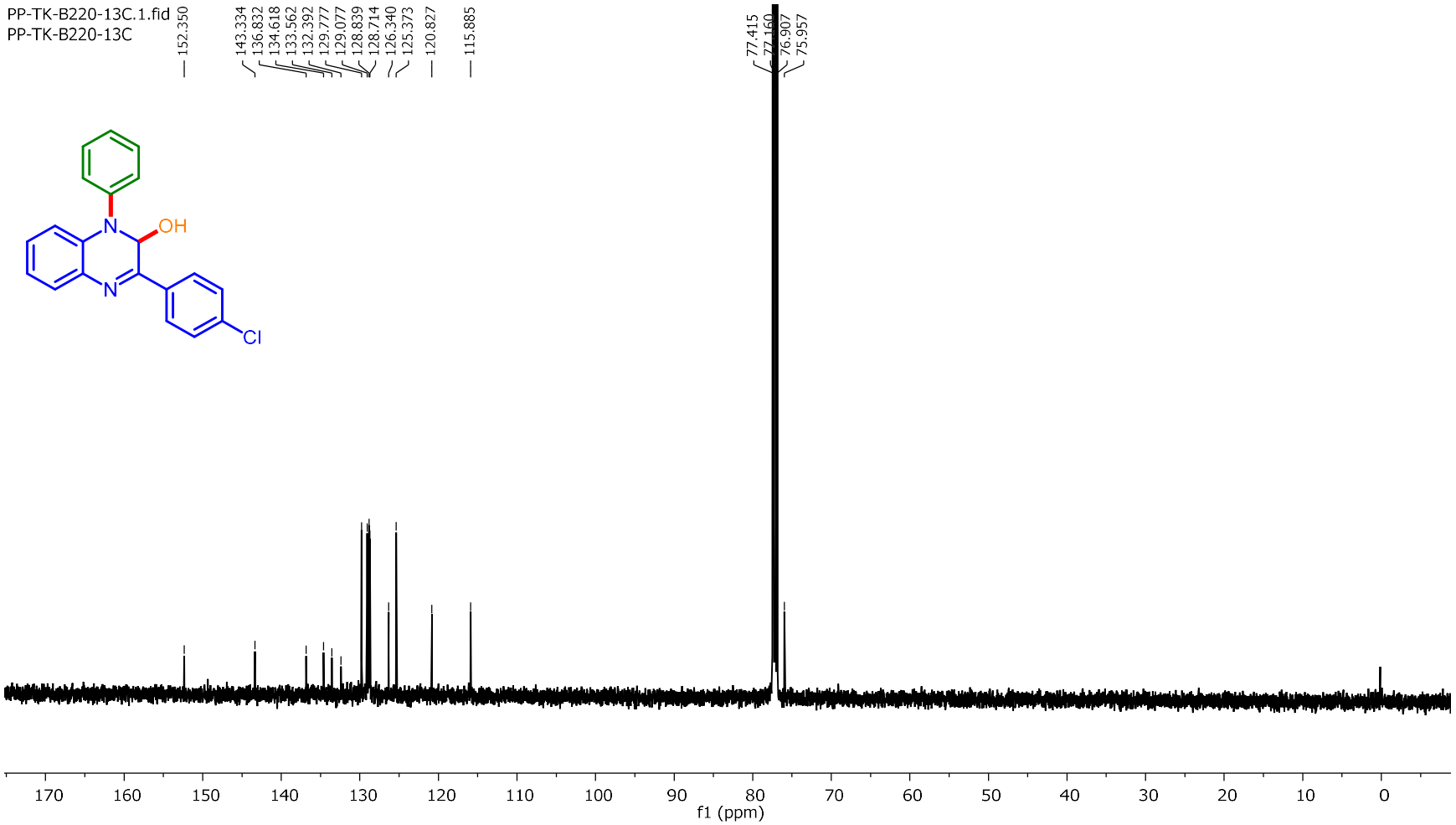
1-Phenyl-3-(4-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (3fa): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



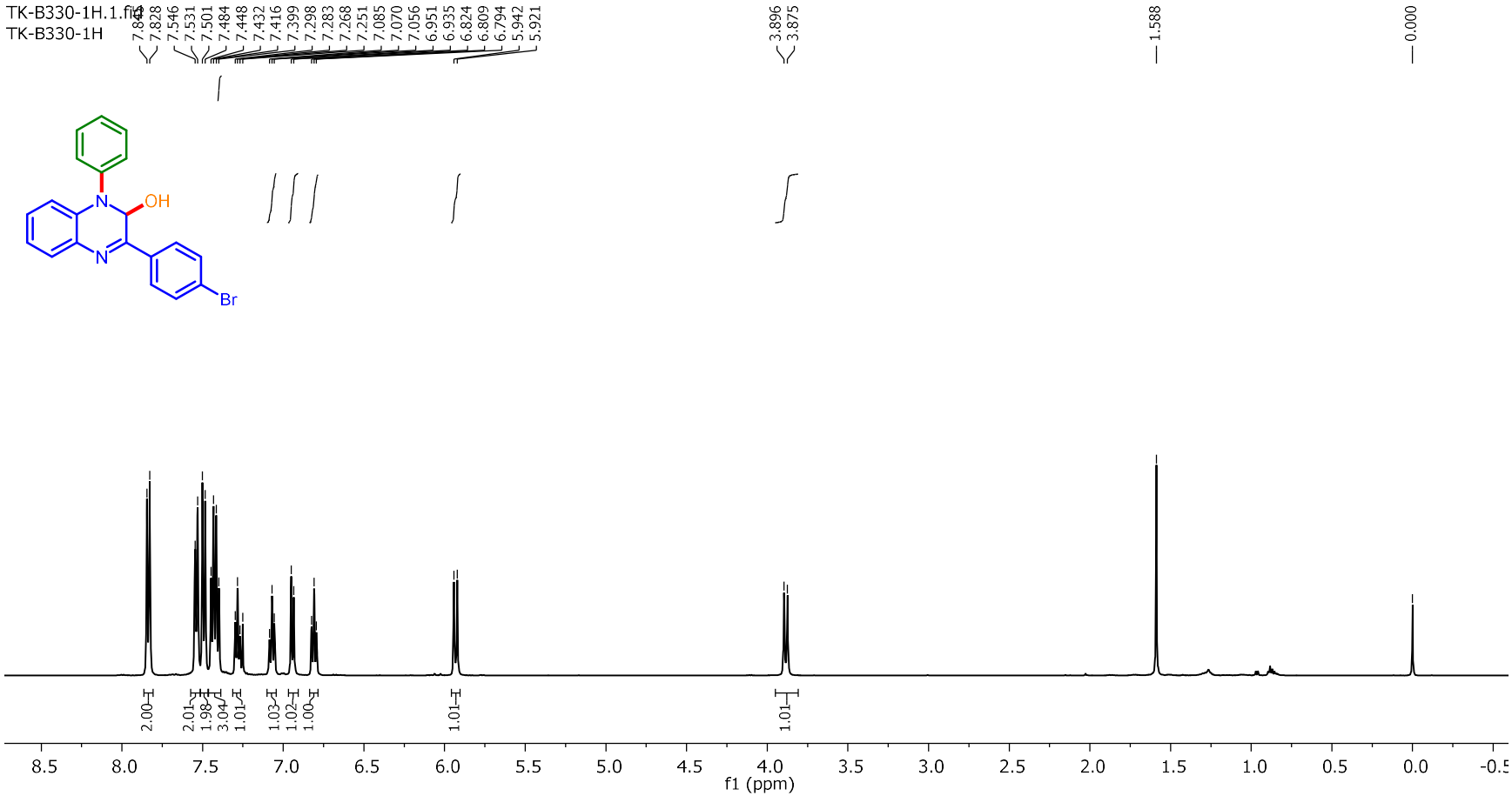
1-Phenyl-3-(4-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (3fa): ^{19}F NMR ($CDCl_3$, 471 MHz)



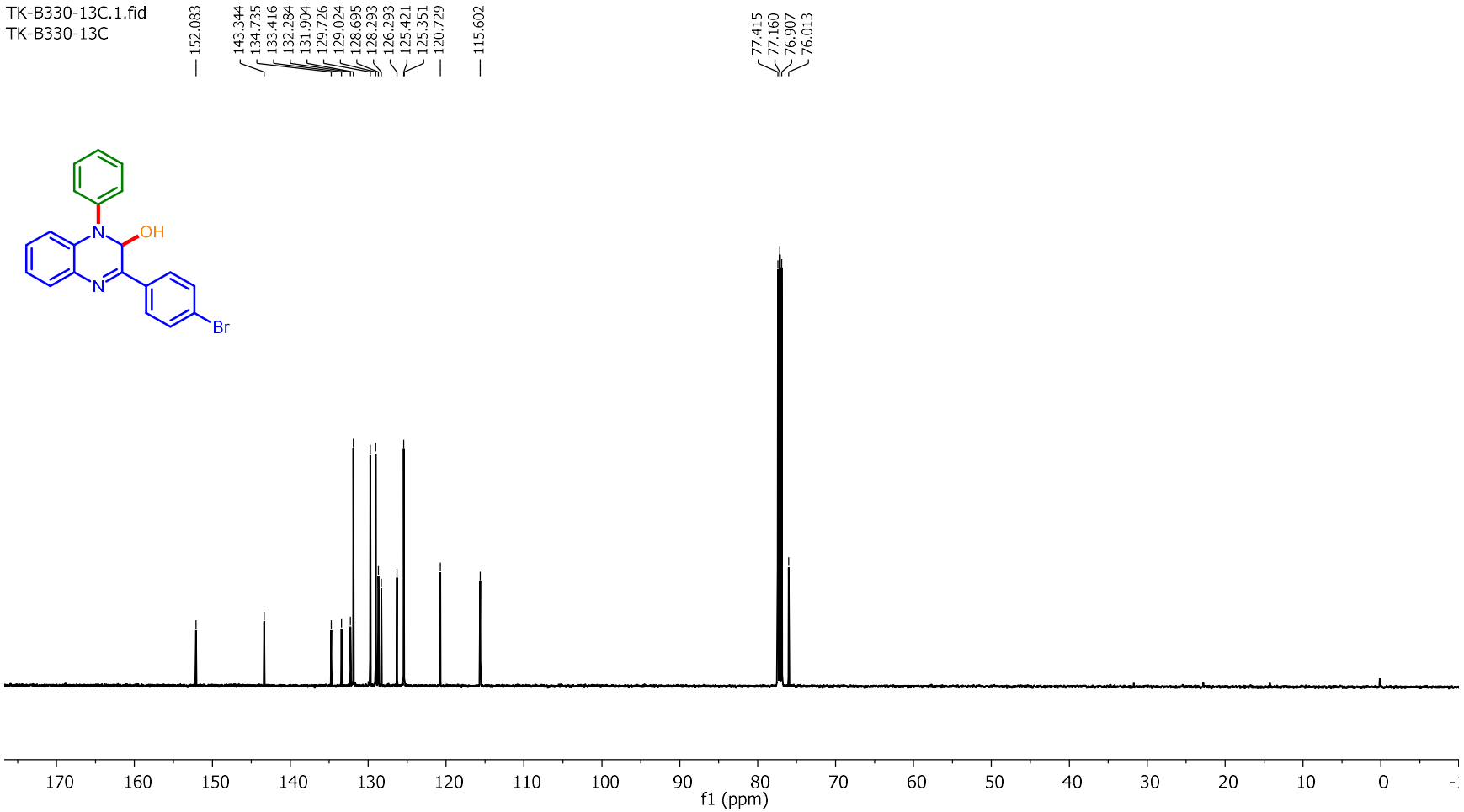
3-(4-Chlorophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ga): ^{1}H NMR ($CDCl_3$, 500 MHz)



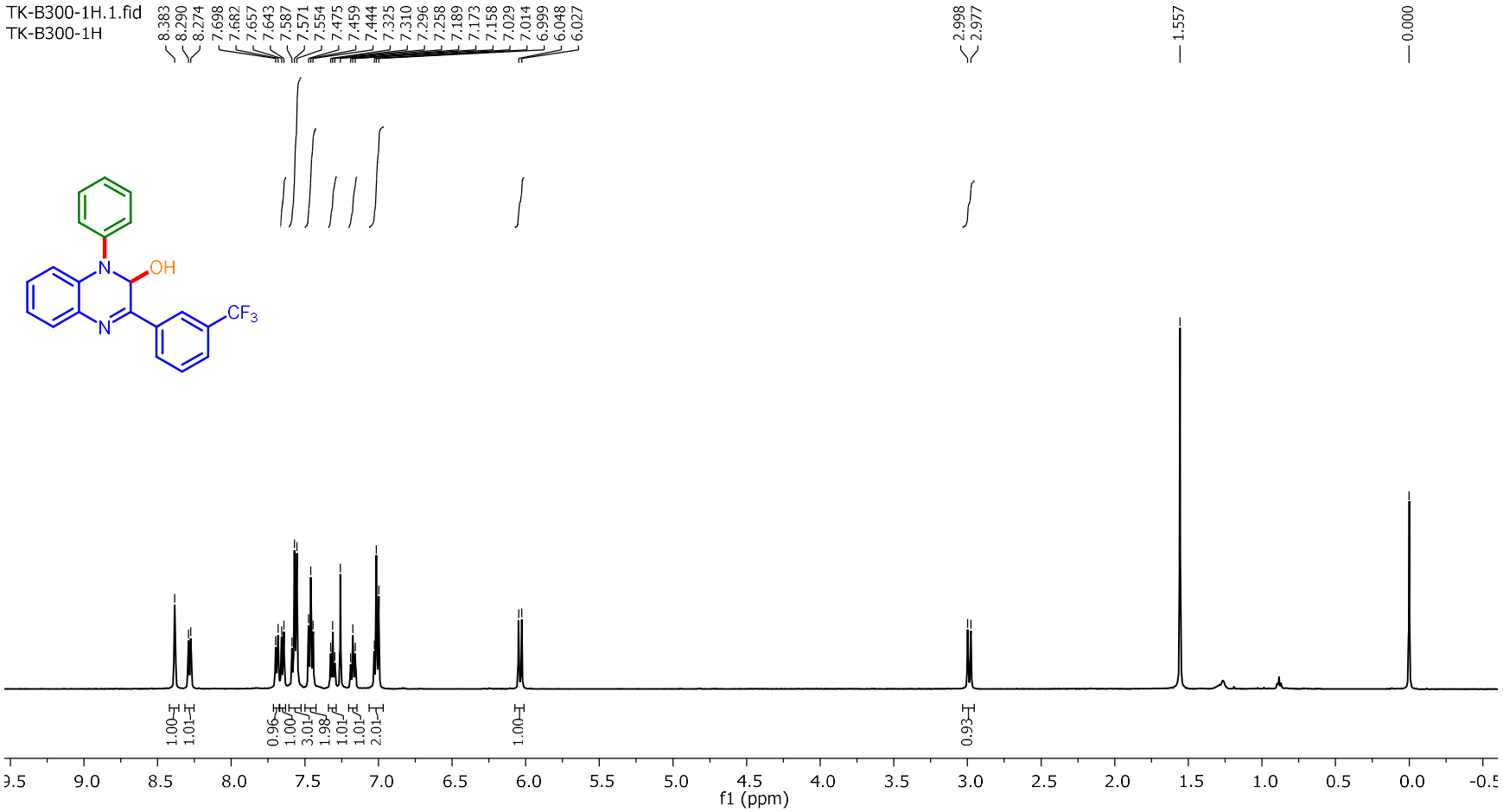
3-(4-Chlorophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ga): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



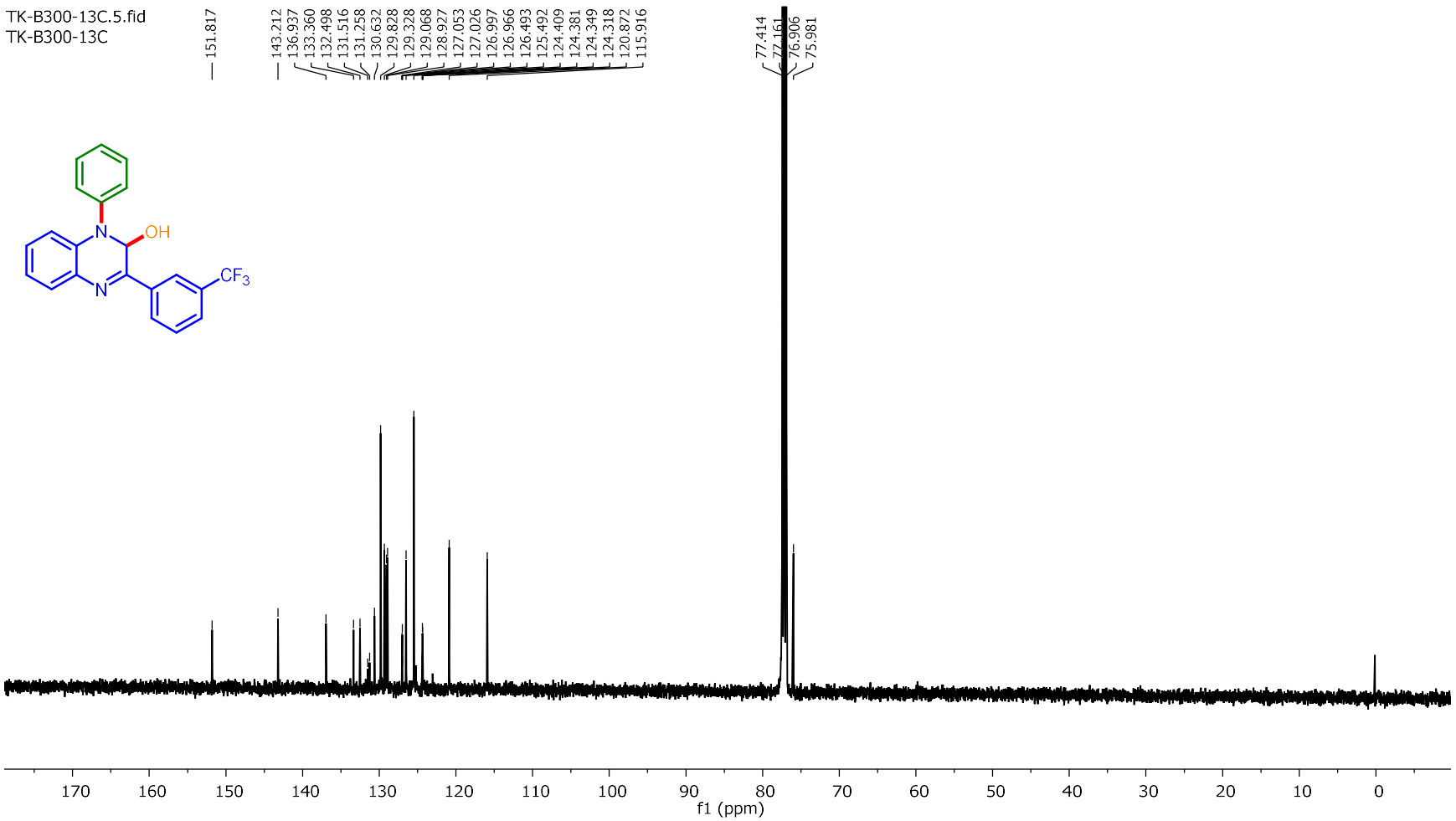
3-(4-Bromophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ha):^{1}H NMR ($CDCl_3$, 500 MHz)



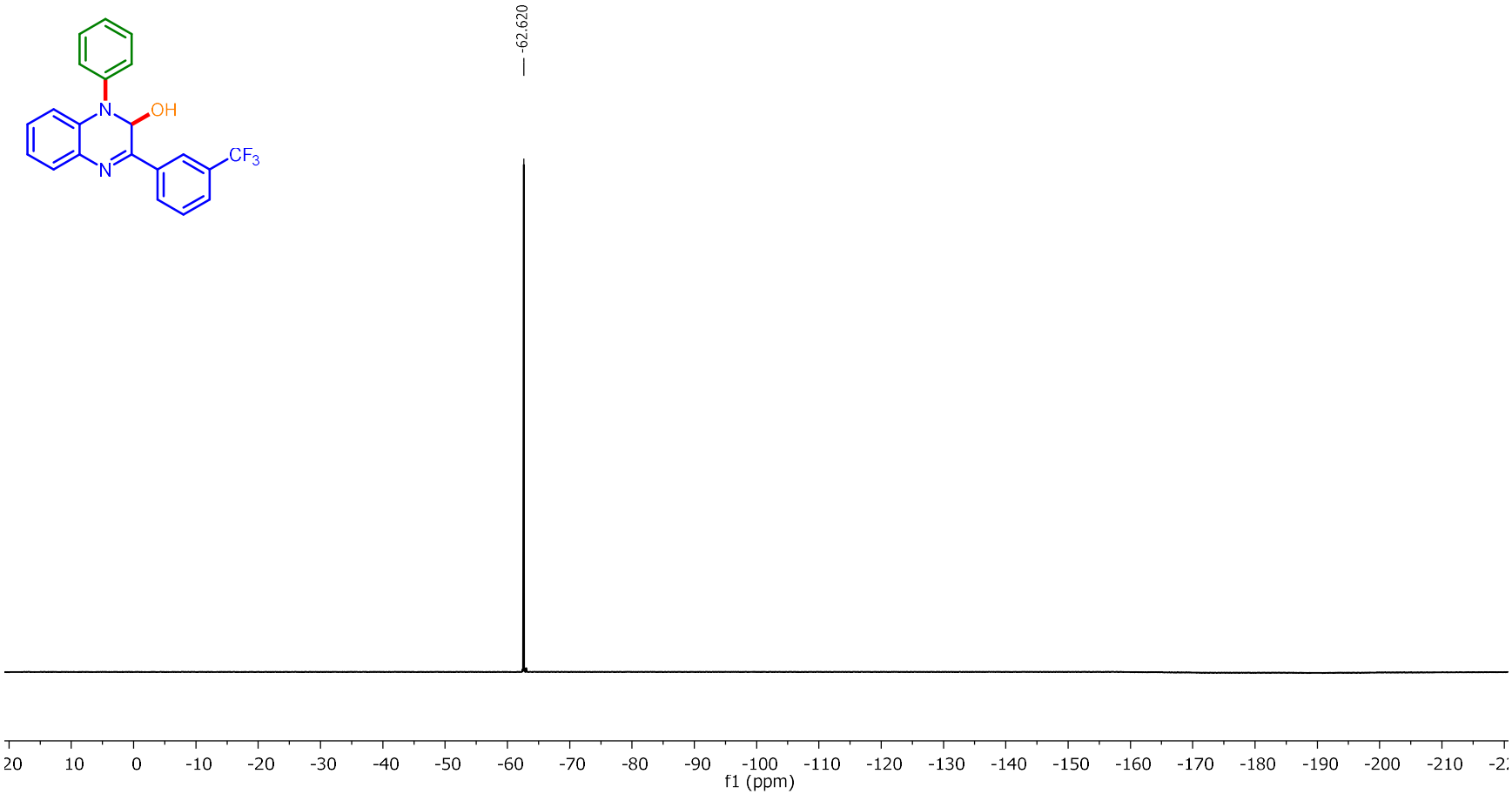
***3*-(4-Bromophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ha): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)**



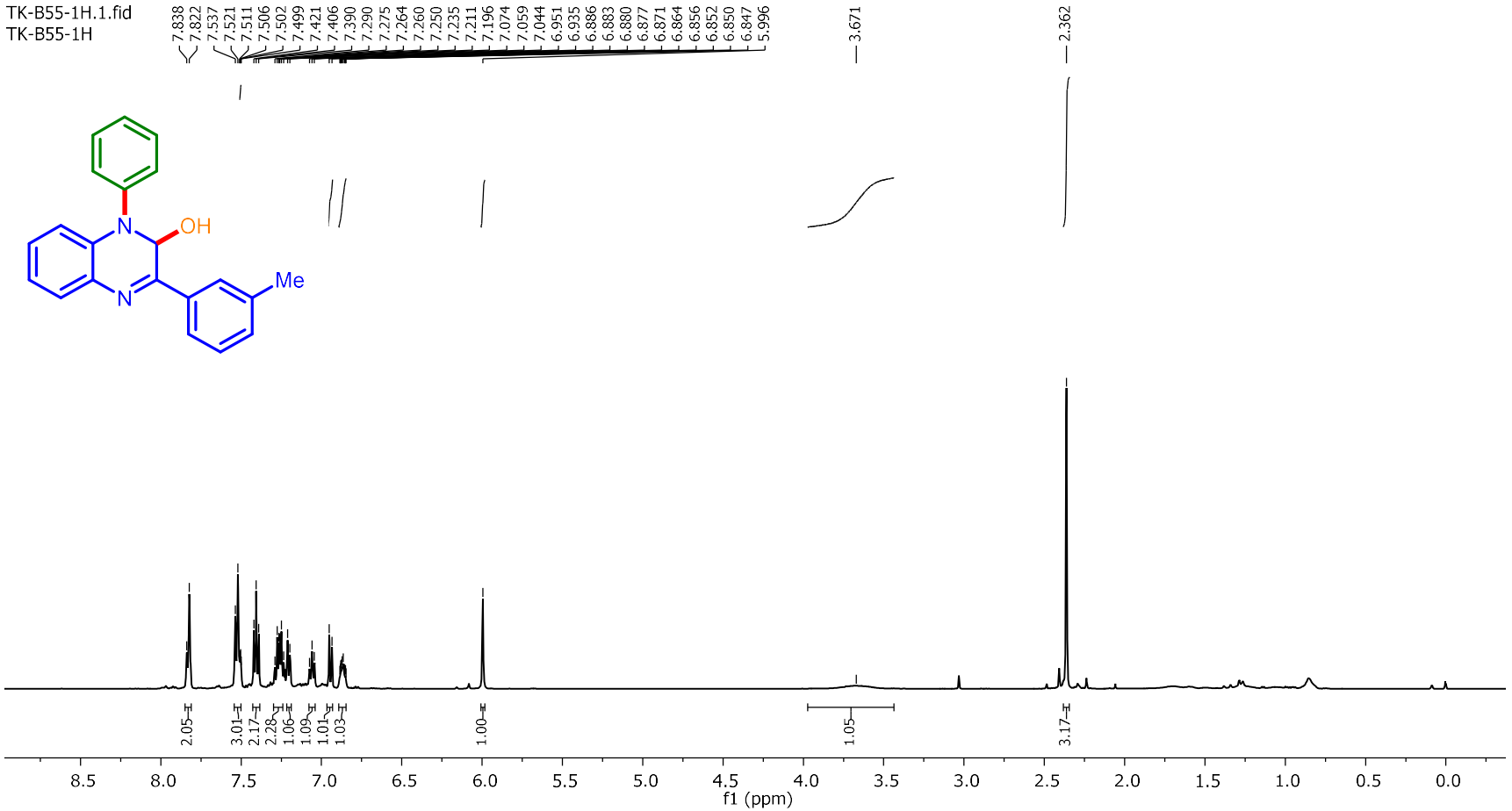
1-Phenyl-3-(3-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (3ia): ^{1}H NMR ($CDCl_3$, 500 MHz)



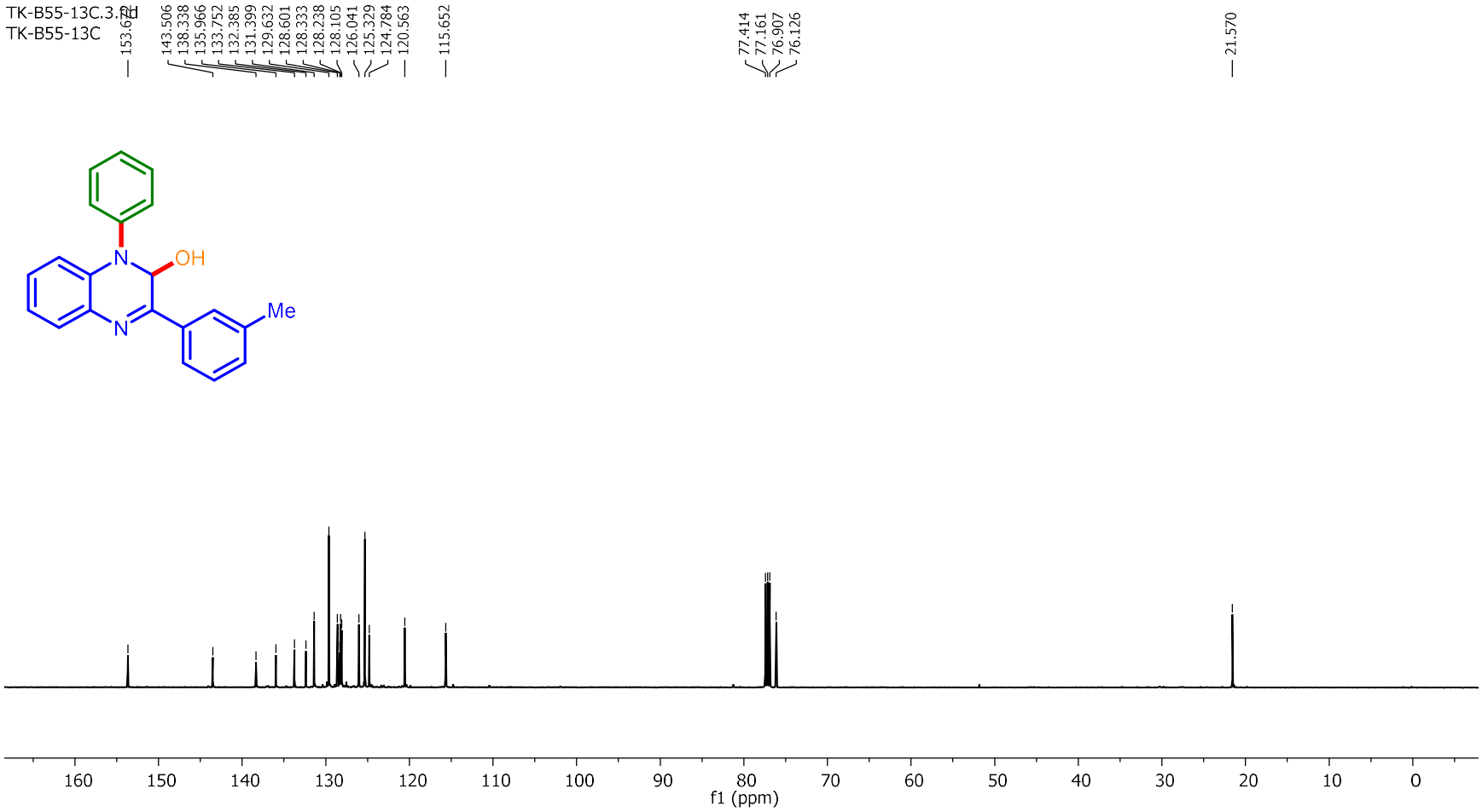
1-Phenyl-3-(3-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (3ia): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



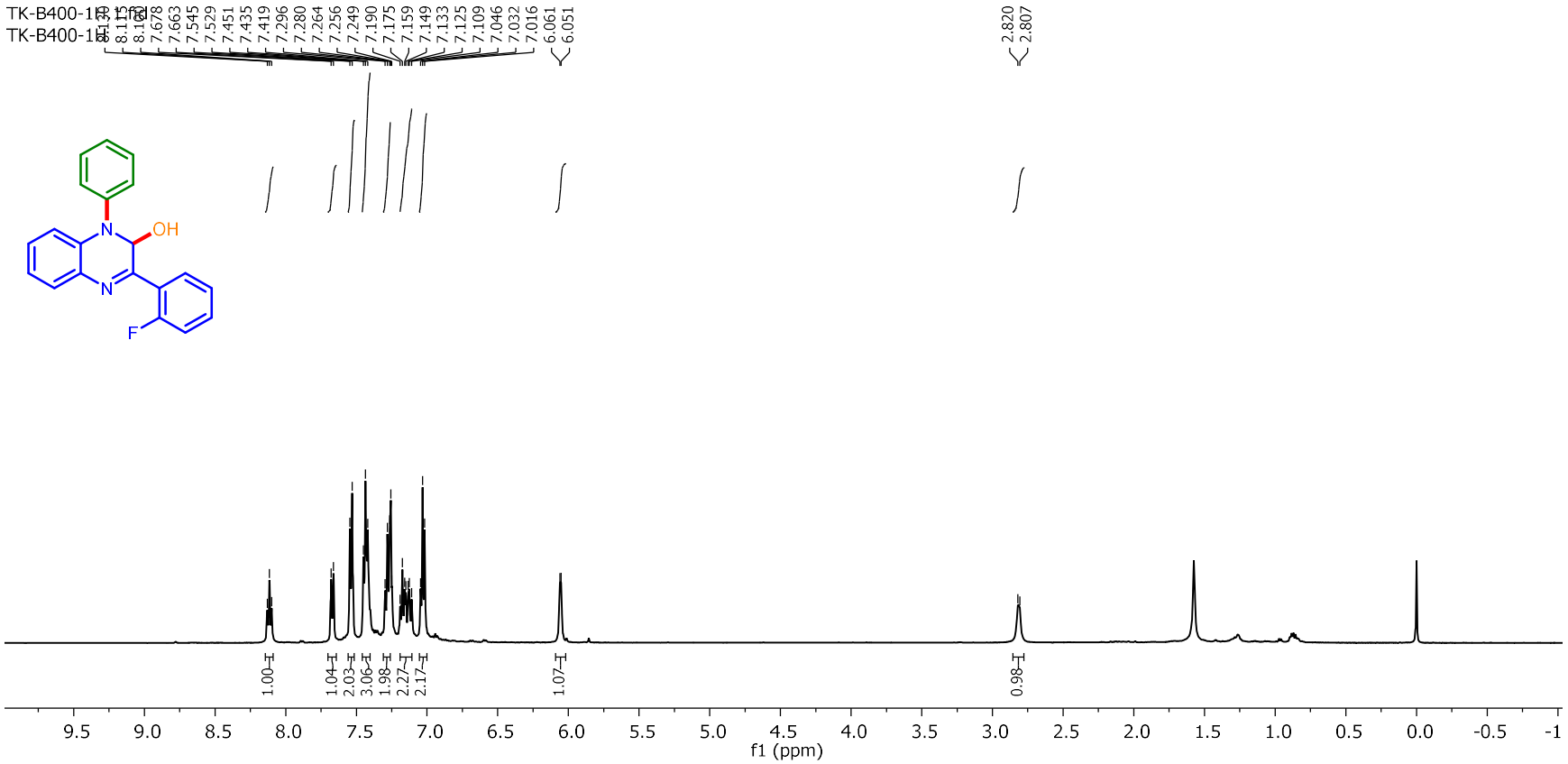
1-Phenyl-3-(3-(trifluoromethyl)phenyl)-1,2-dihydroquinoxalin-2-ol (3ia): ^{19}F NMR ($CDCl_3$, 471 MHz)



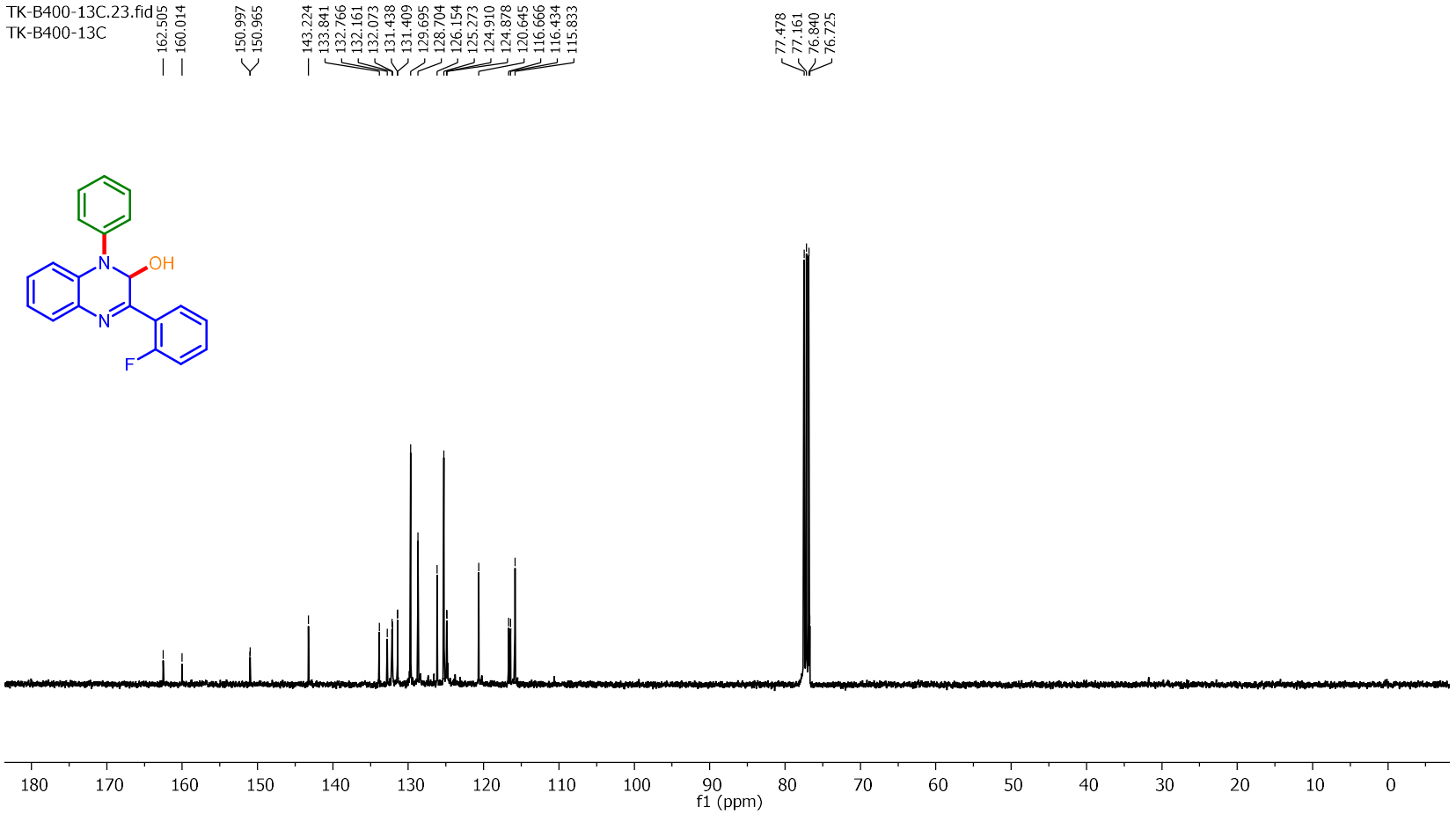
1-Phenyl-3-(*m*-tolyl)-1,2-dihydroquinoxalin-2-ol (3ja): ^{1}H NMR ($CDCl_3$, 500MHz)



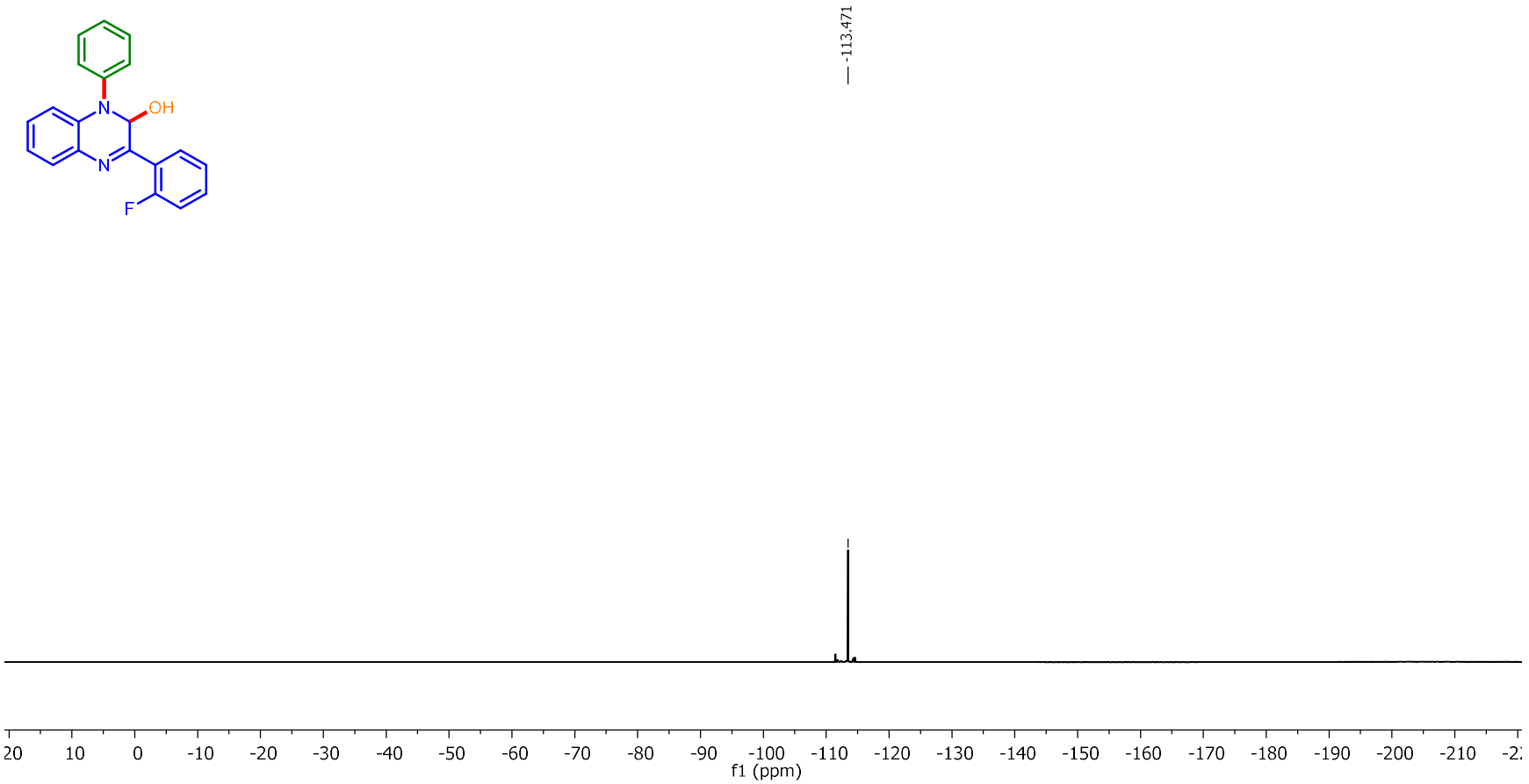
1-Phenyl-3-(m-tolyl)-1,2-dihydroquinoxalin-2-ol (3ja): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



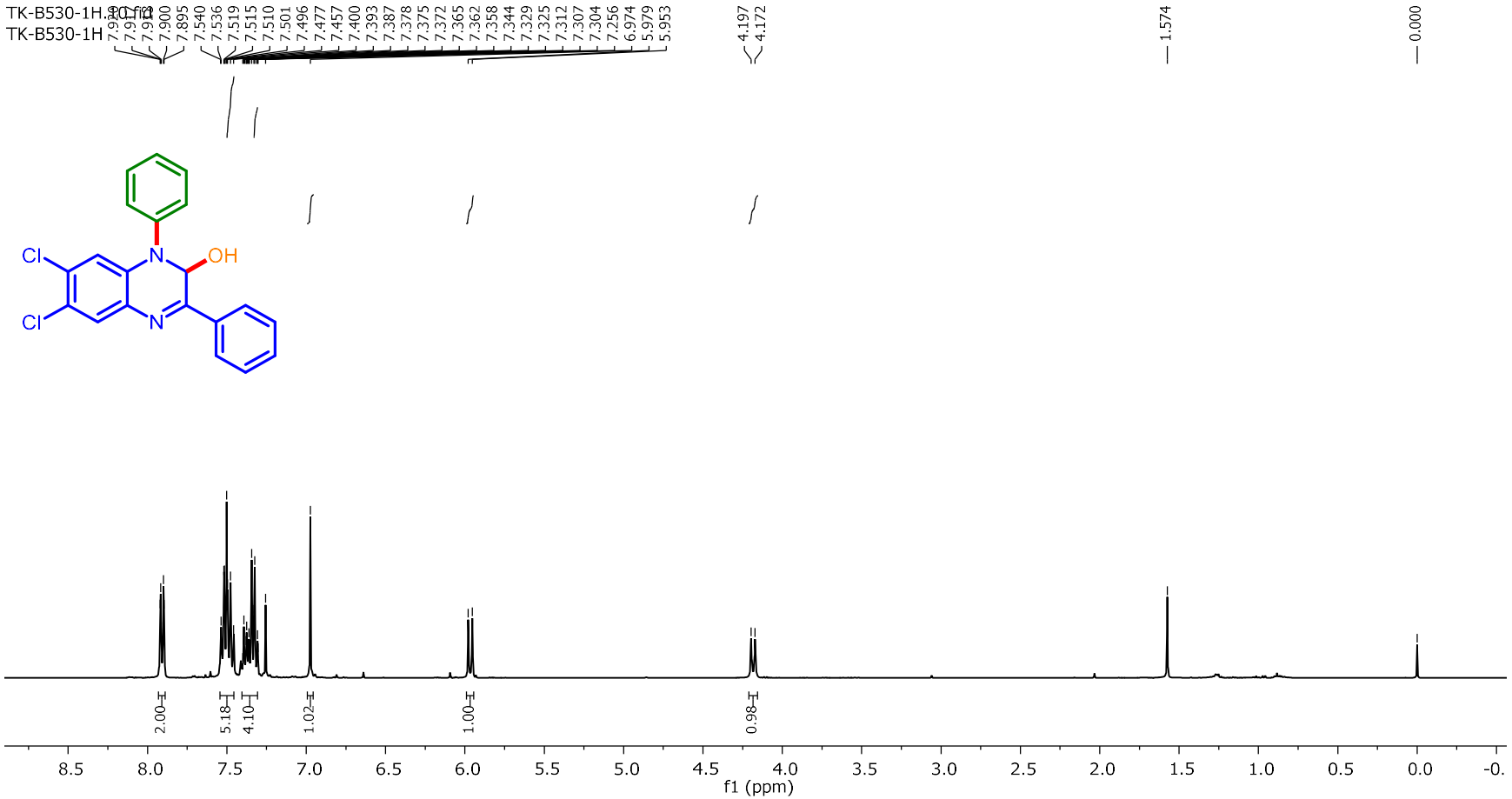
3-(2-Fluorophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ka): ^{1}H NMR ($CDCl_3$, 500MHz)



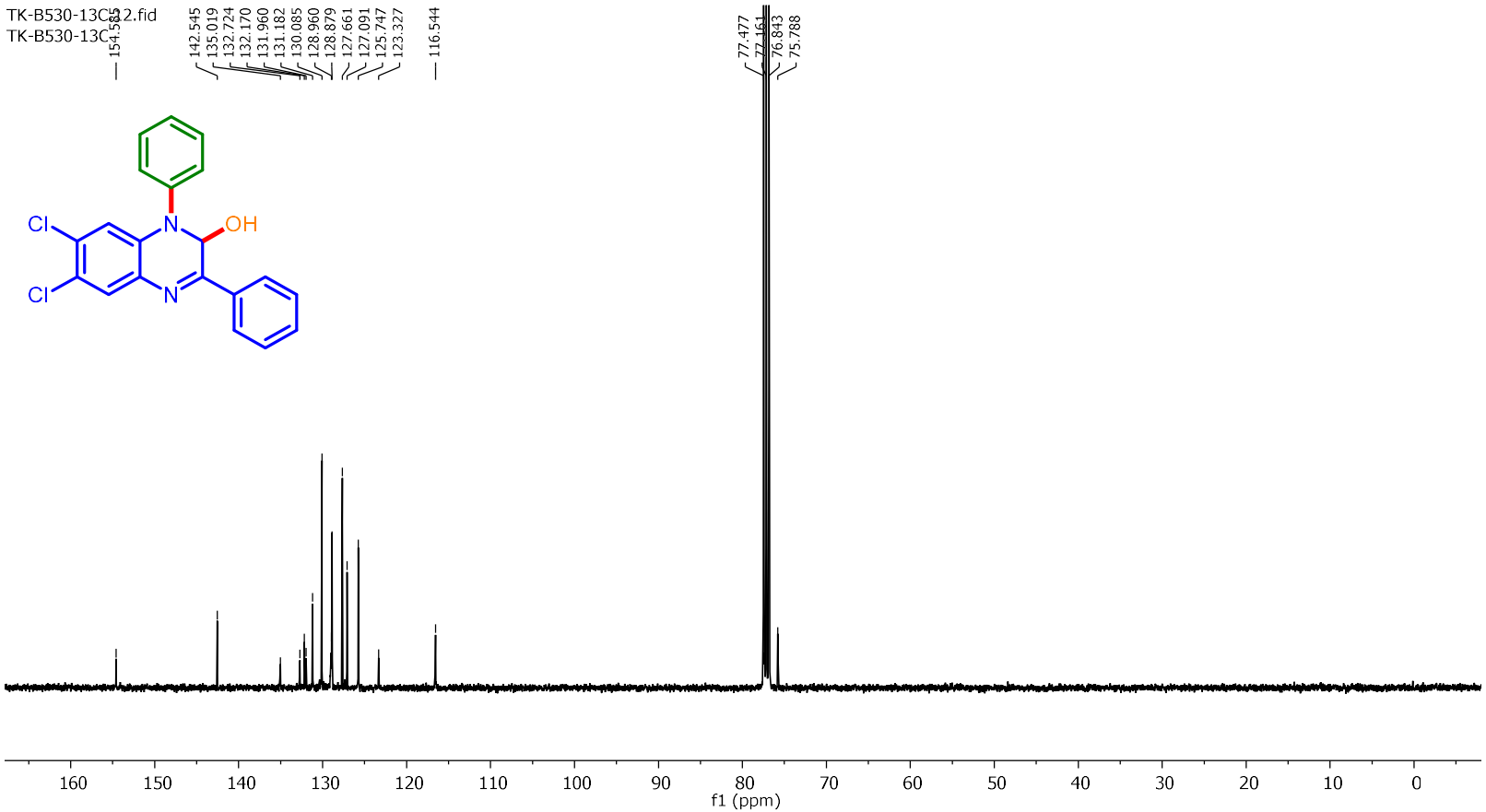
3-(2-Fluorophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ka): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)



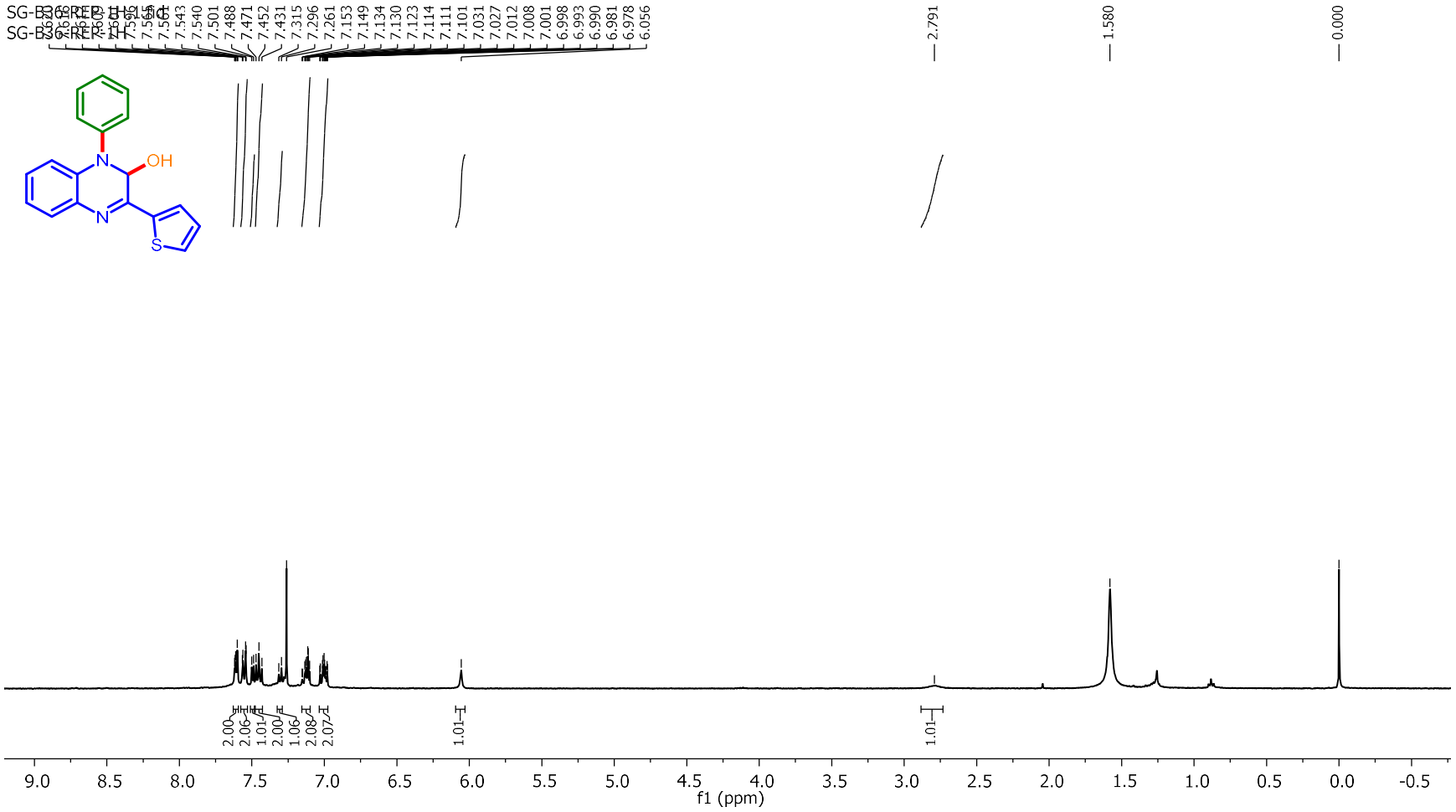
3-(2-Fluorophenyl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3ka): ^{19}F NMR ($CDCl_3$, 376 MHz)



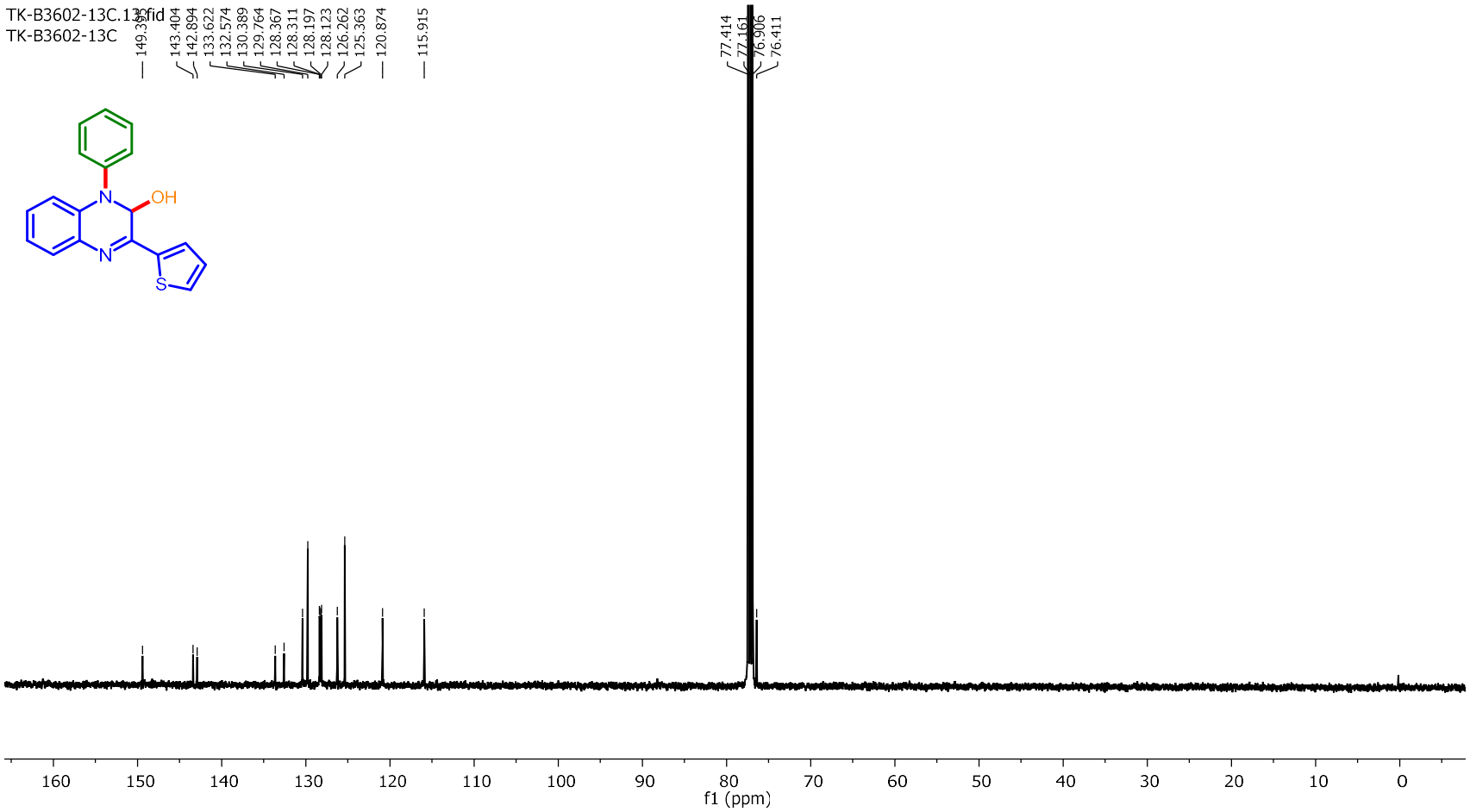
6,7-Dichloro-1,3-diphenyl-1,2-dihydroquinoxalin-2-ol (3la): ^{1}H NMR ($CDCl_3$, 400 MHz)



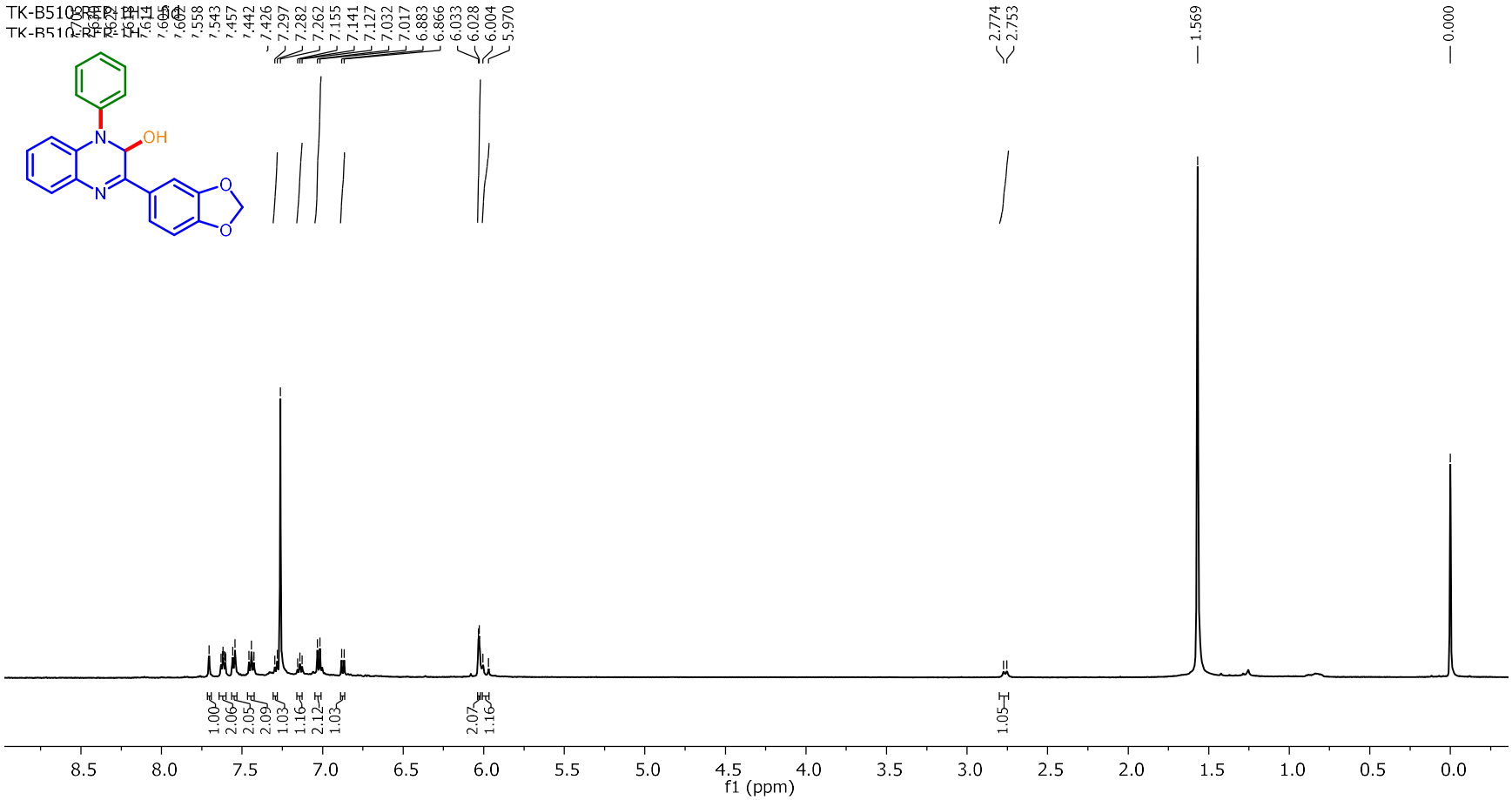
6,7-Dichloro-1,3-diphenyl-1,2-dihydroquinoxalin-2-ol (3la): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)



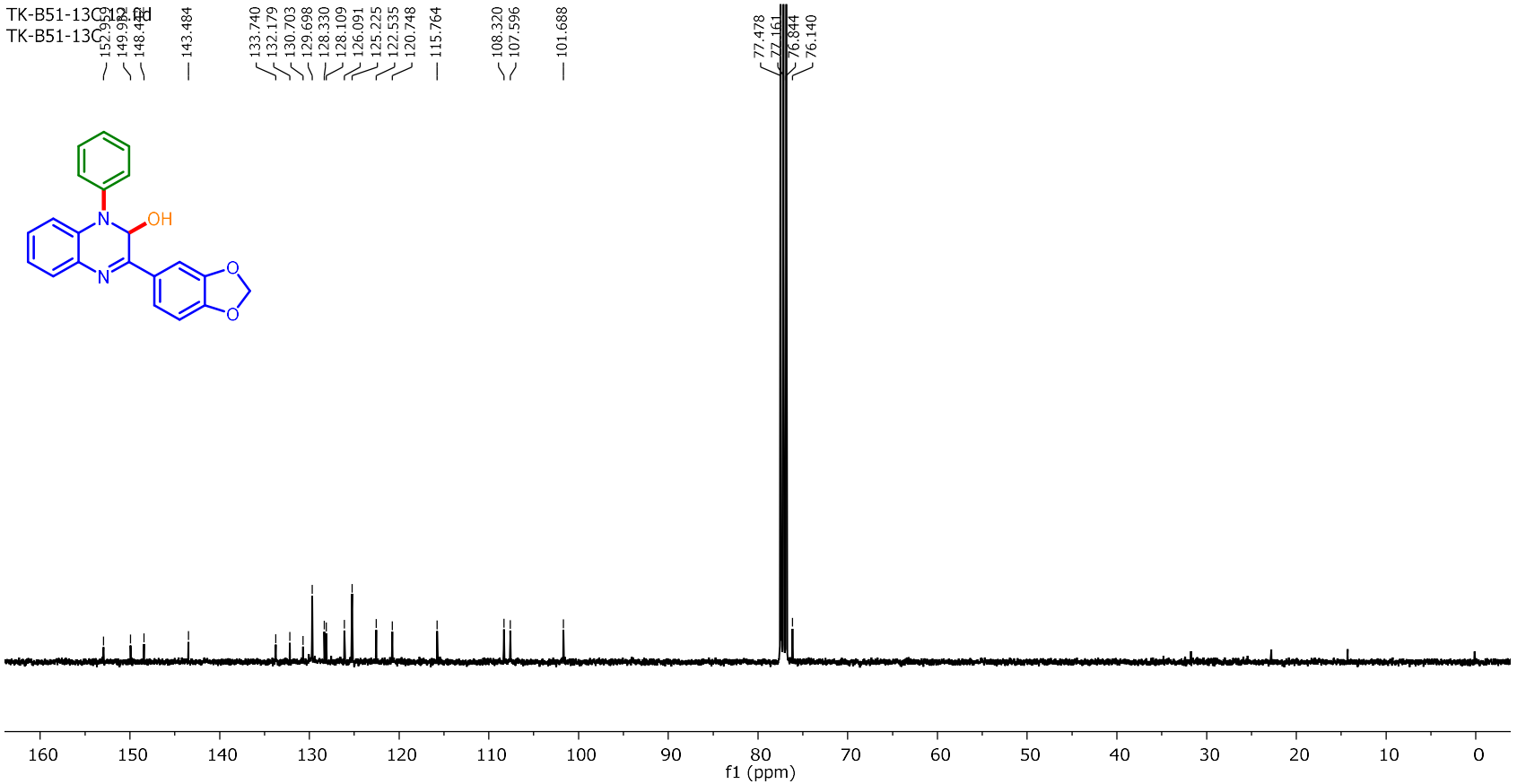
1-Phenyl-3-(thiophen-2-yl)-1,2-dihydroquinoxalin-2-ol (3ma): ^{1}H NMR ($CDCl_3$, 500MHz)



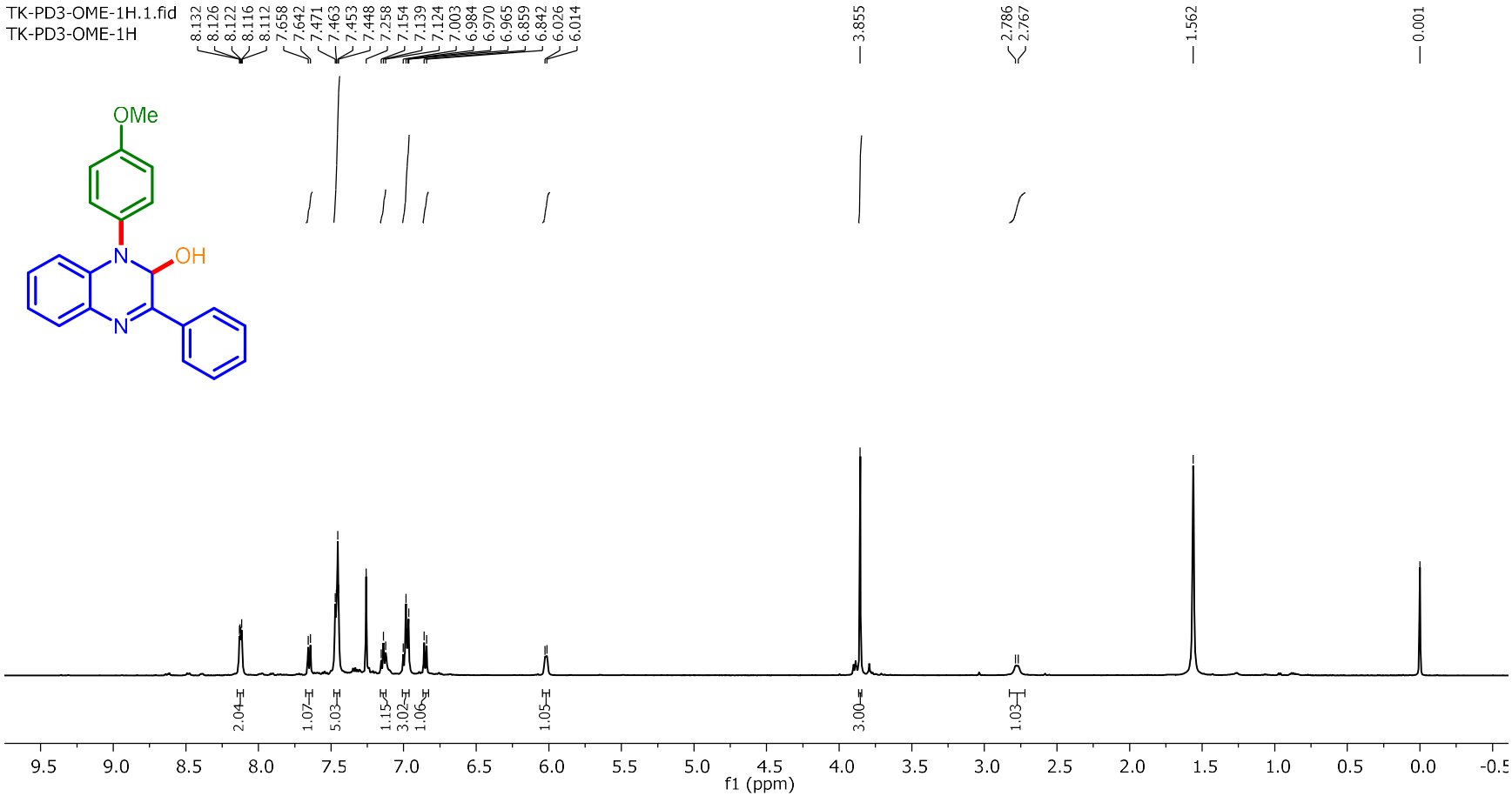
1-Phenyl-3-(thiophen-2-yl)-1,2-dihydroquinoxalin-2-ol (3ma): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



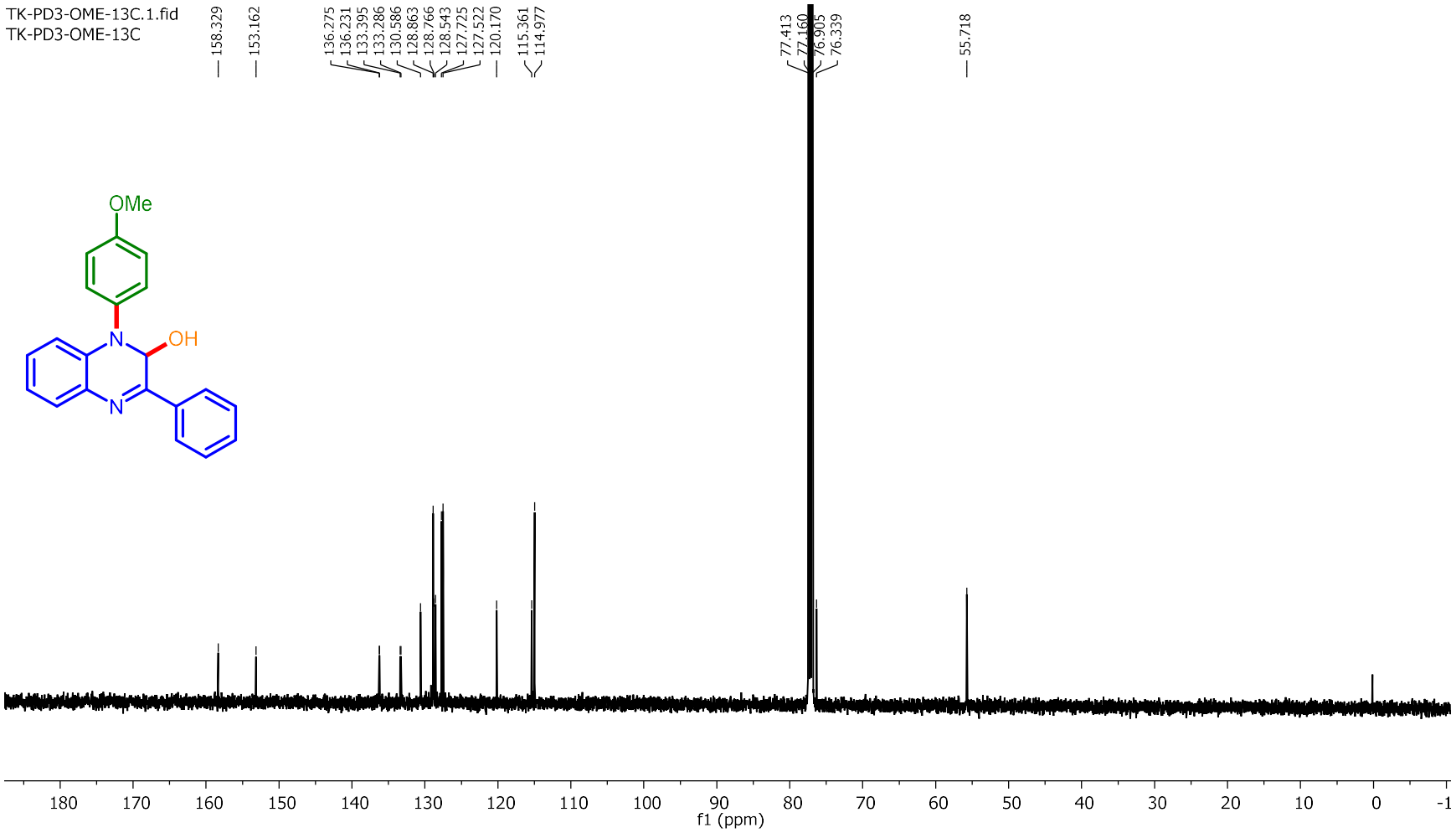
3-(Benzo[*d*][1,3]dioxol-5-yl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3na): ^{1}H NMR ($CDCl_3$, 400 MHz)



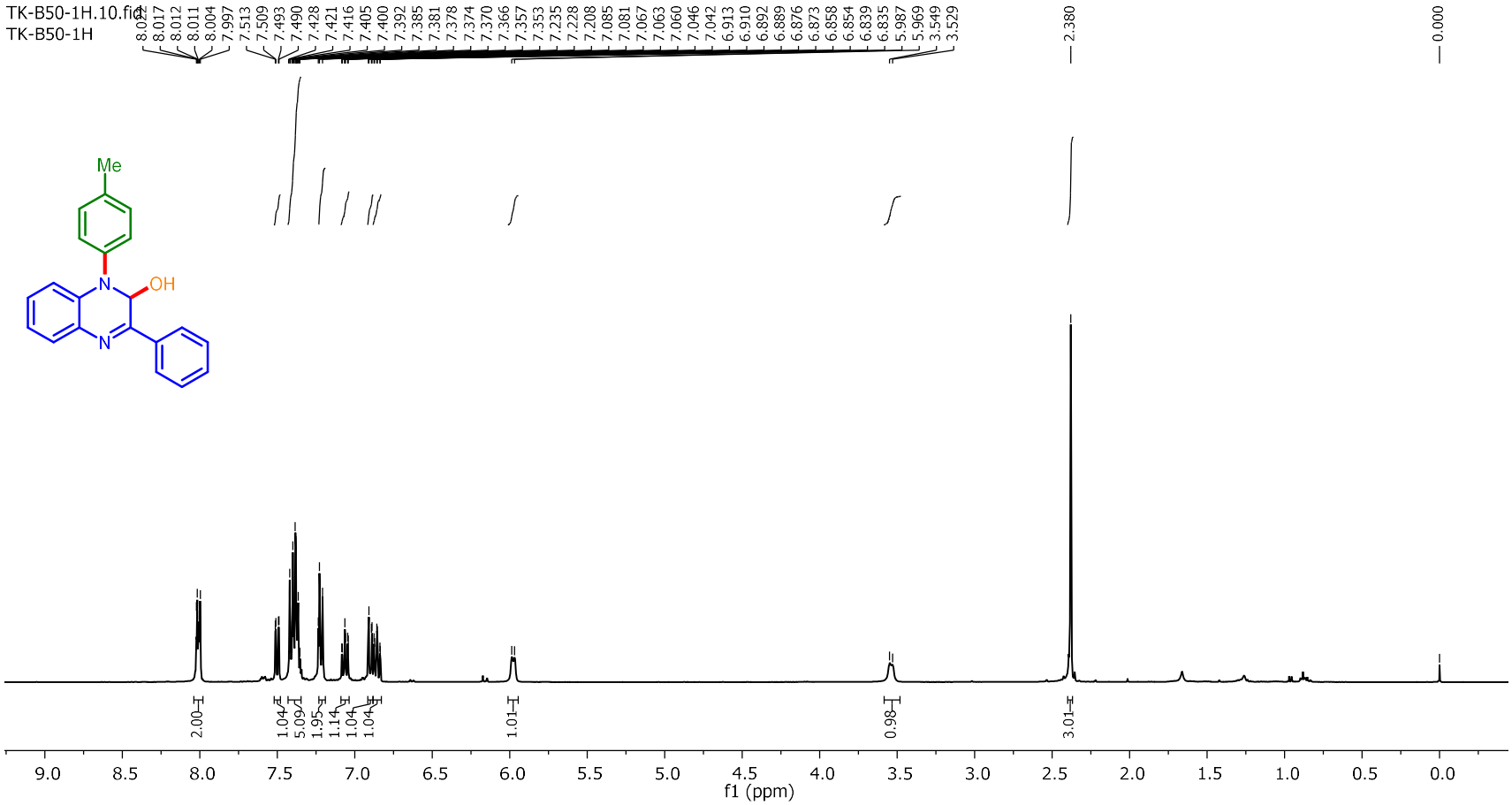
3-(Benzo[*d*][1,3]dioxol-5-yl)-1-phenyl-1,2-dihydroquinoxalin-2-ol (3na): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)



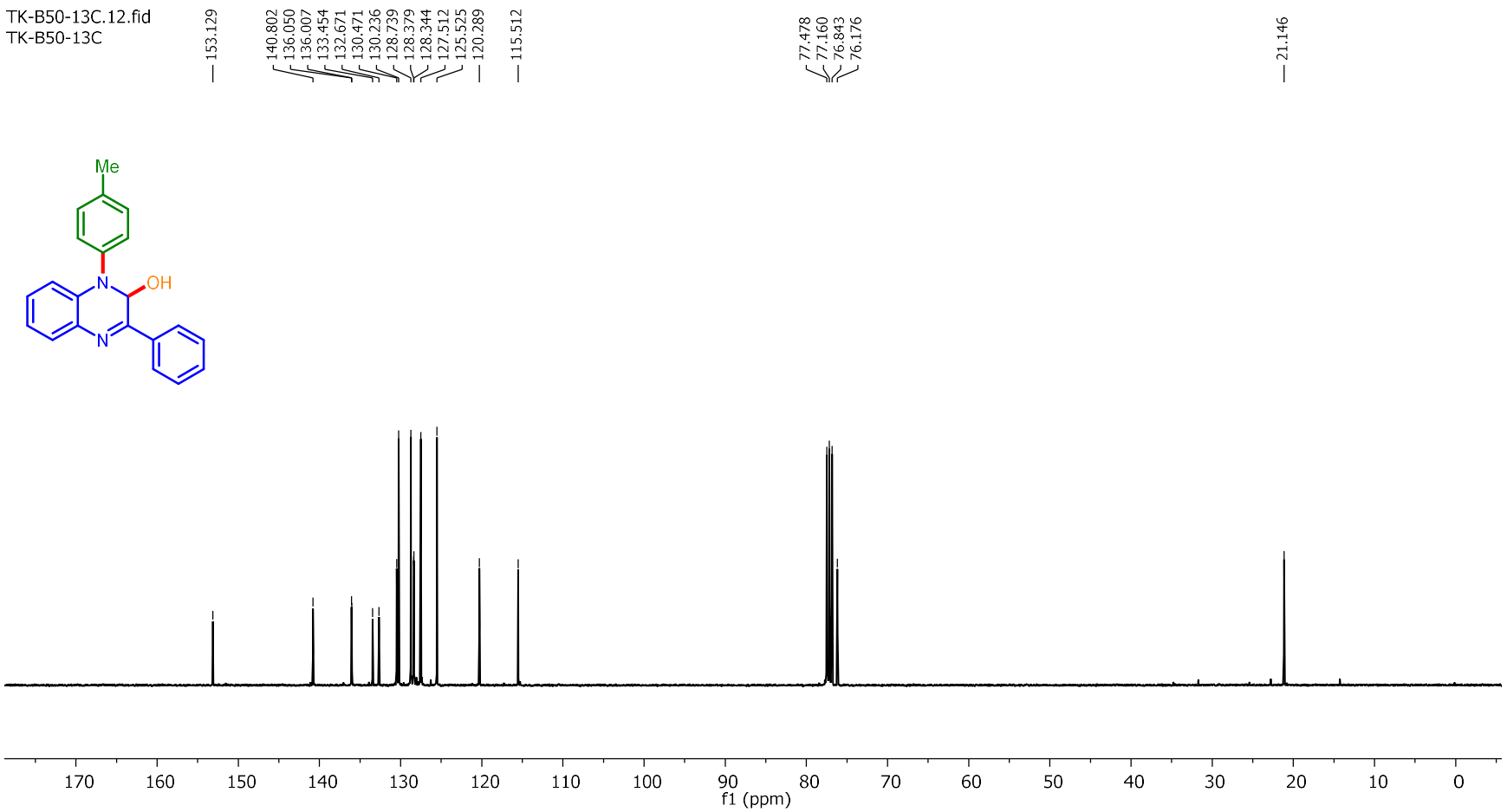
1-(4-Methoxyphenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ab): ^{1}H NMR ($CDCl_3$, 500 MHz)



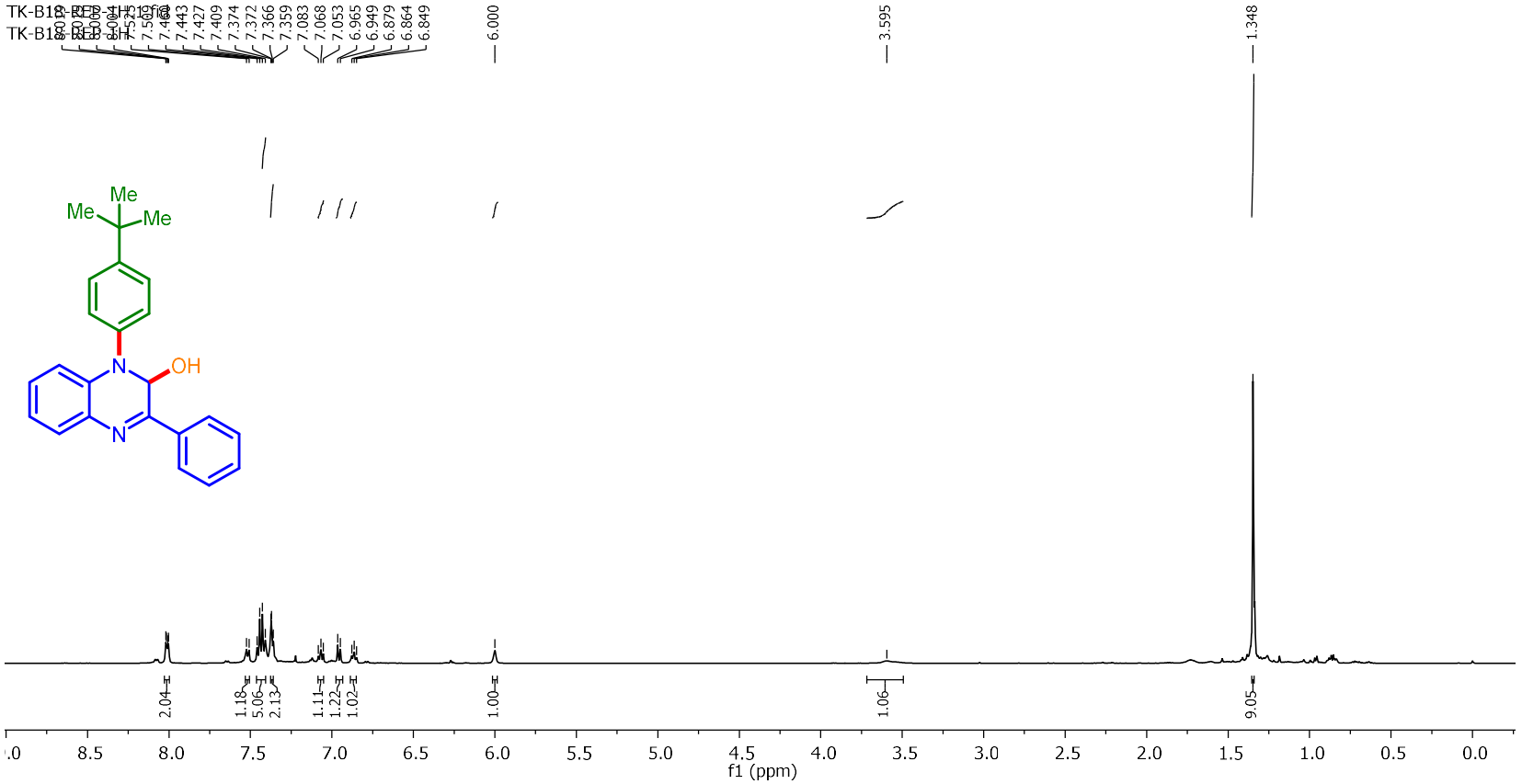
1-(4-Methoxyphenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ab): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



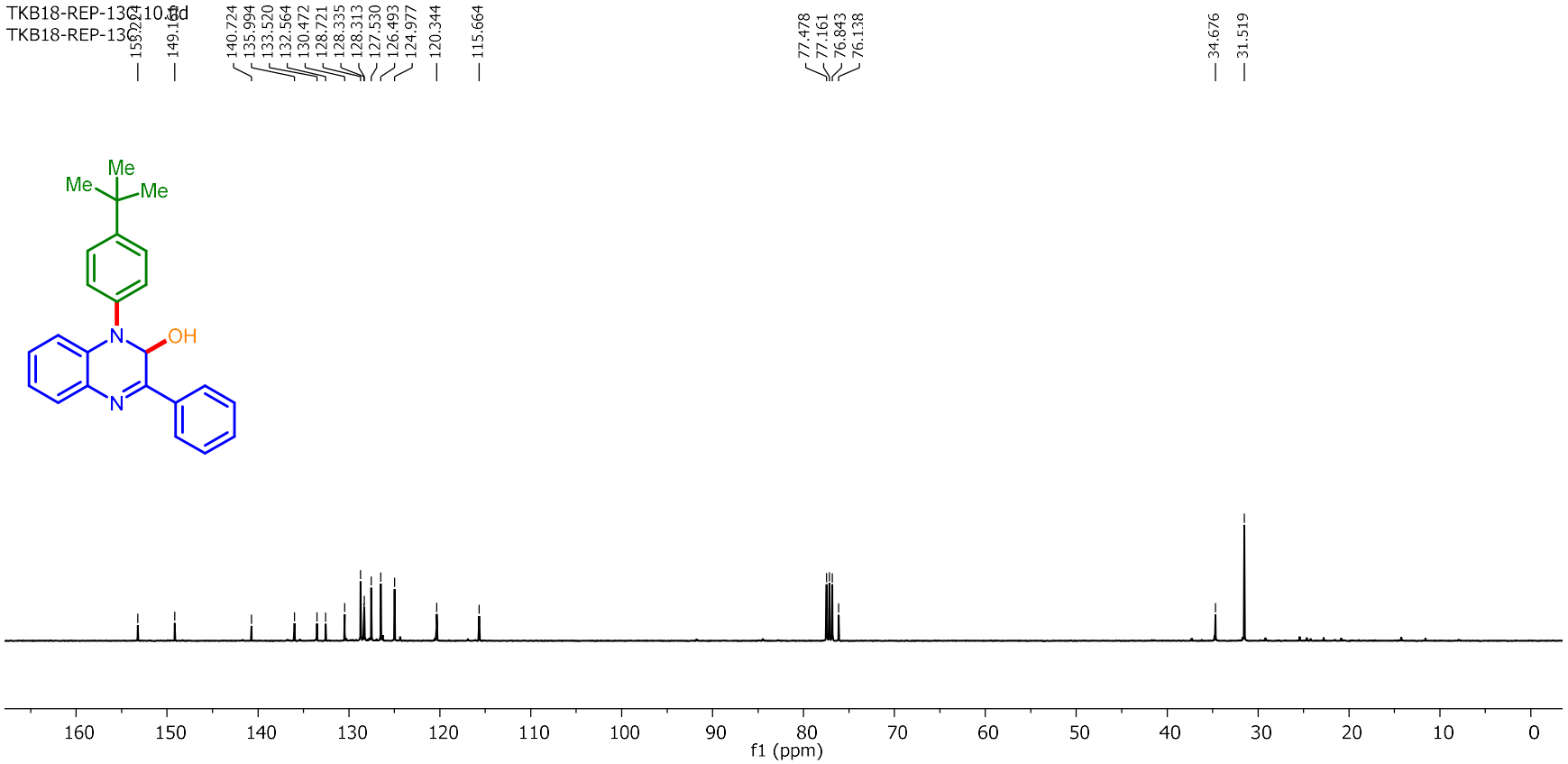
3-Phenyl-1-(p-tolyl)-1,2-dihydroquinoxalin-2-ol (3ac):^{1}H NMR ($CDCl_3$, 400 MHz)



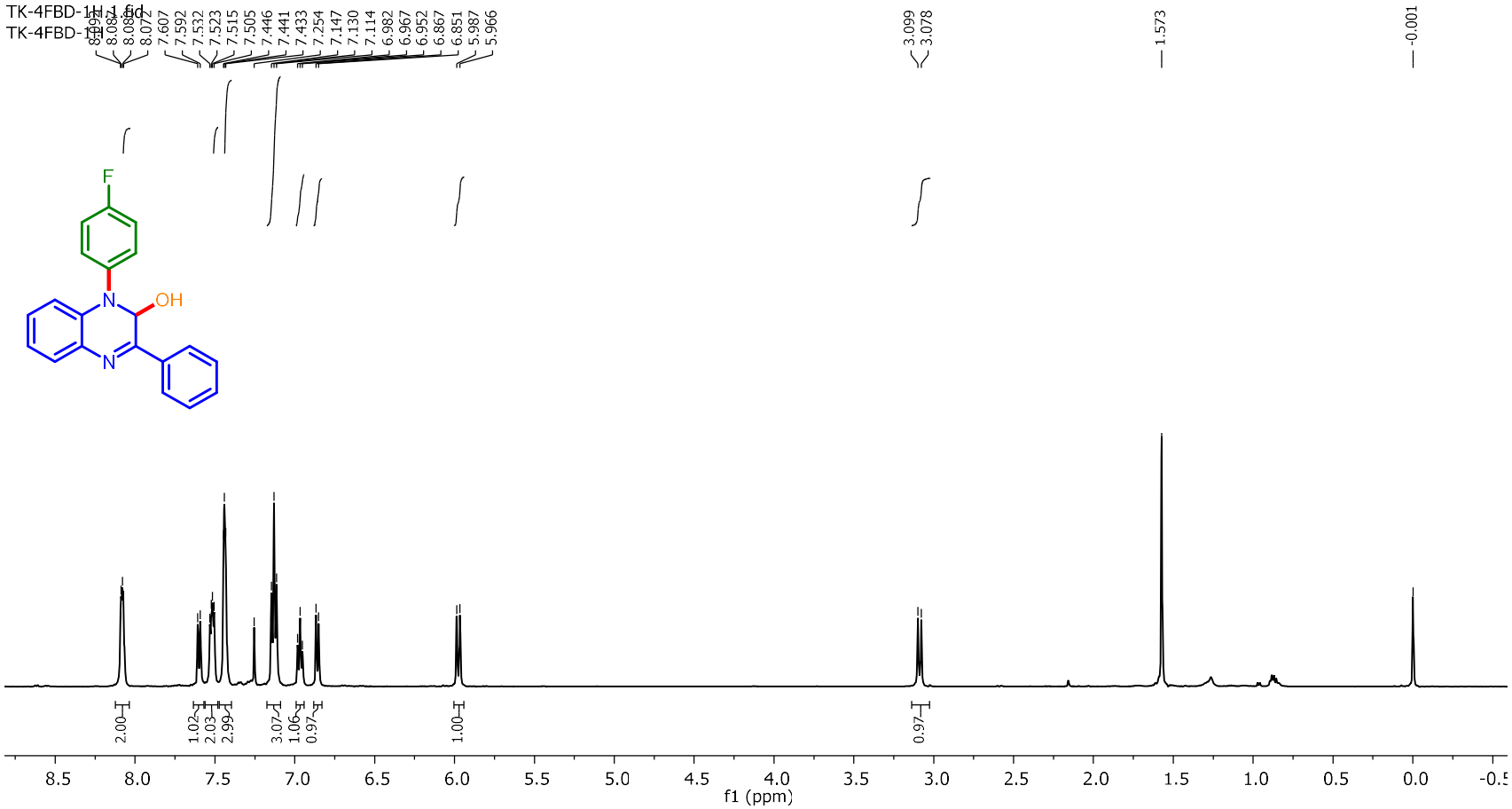
3-Phenyl-1-(p-tolyl)-1,2-dihydroquinoxalin-2-ol (3ac): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)



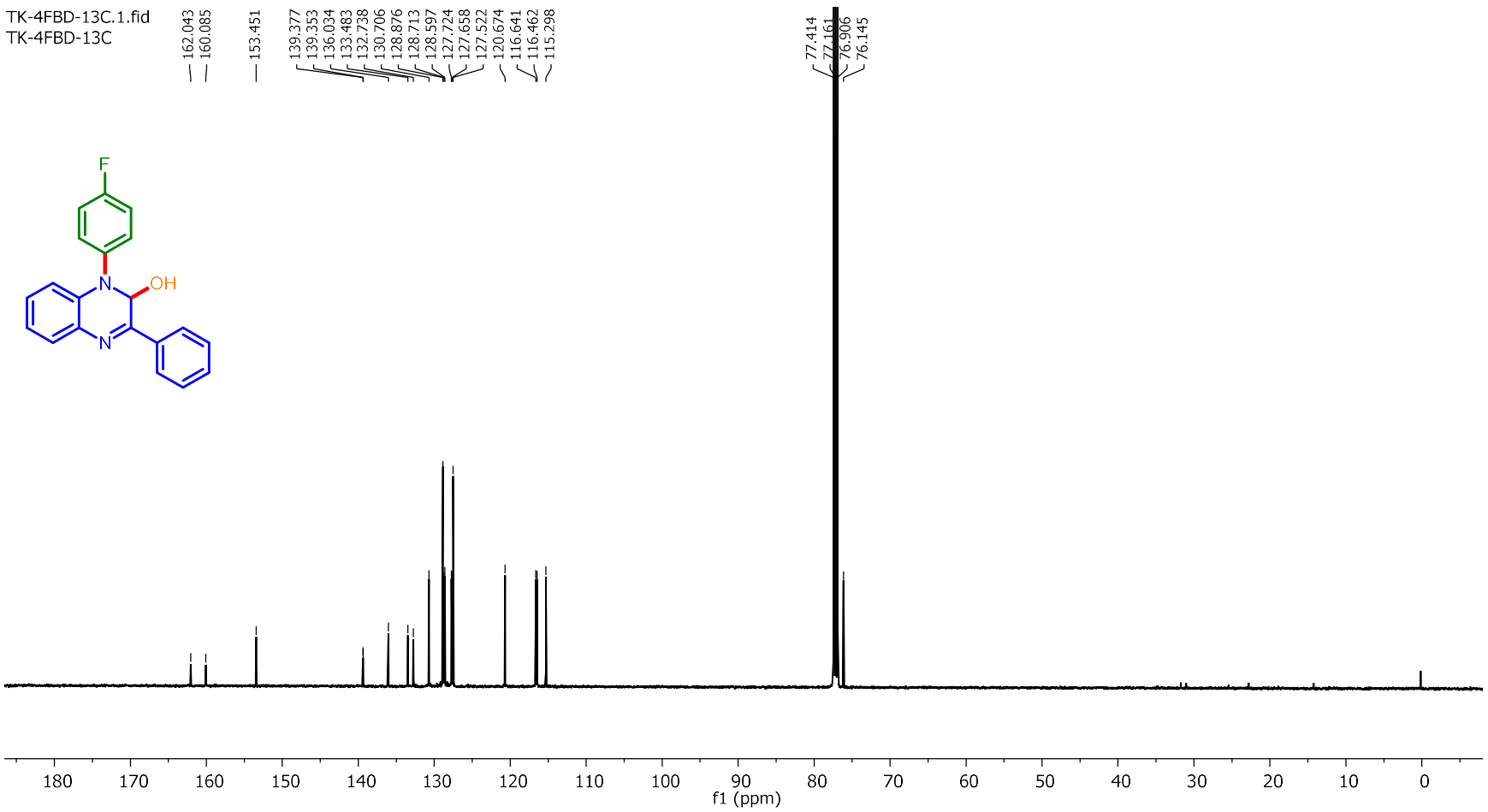
1-(4-(*tert*-Butyl)phenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ad): ^{1}H NMR ($CDCl_3$, 500 MHz)



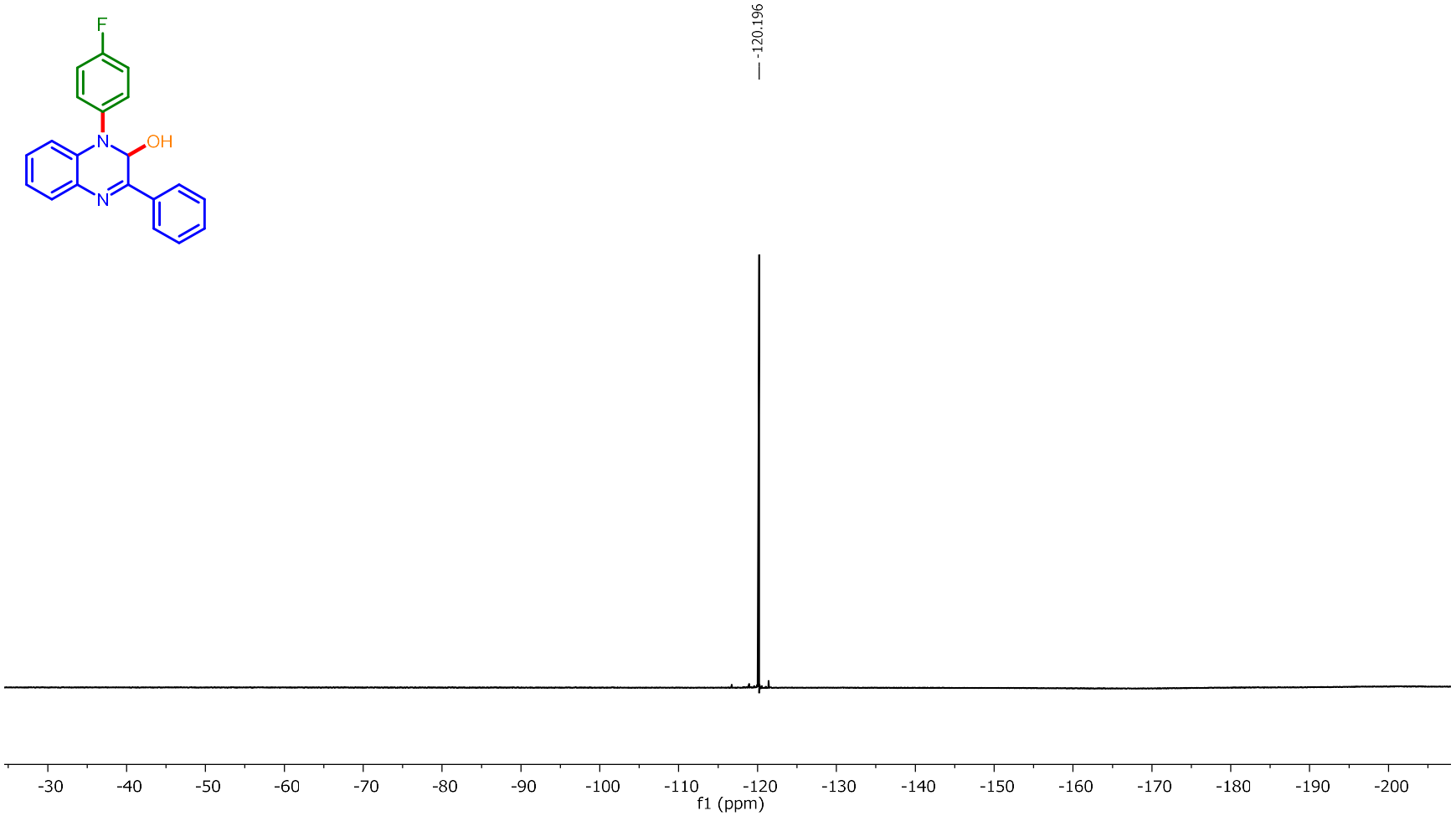
1-(4-(*tert*-Butyl)henyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ad): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)



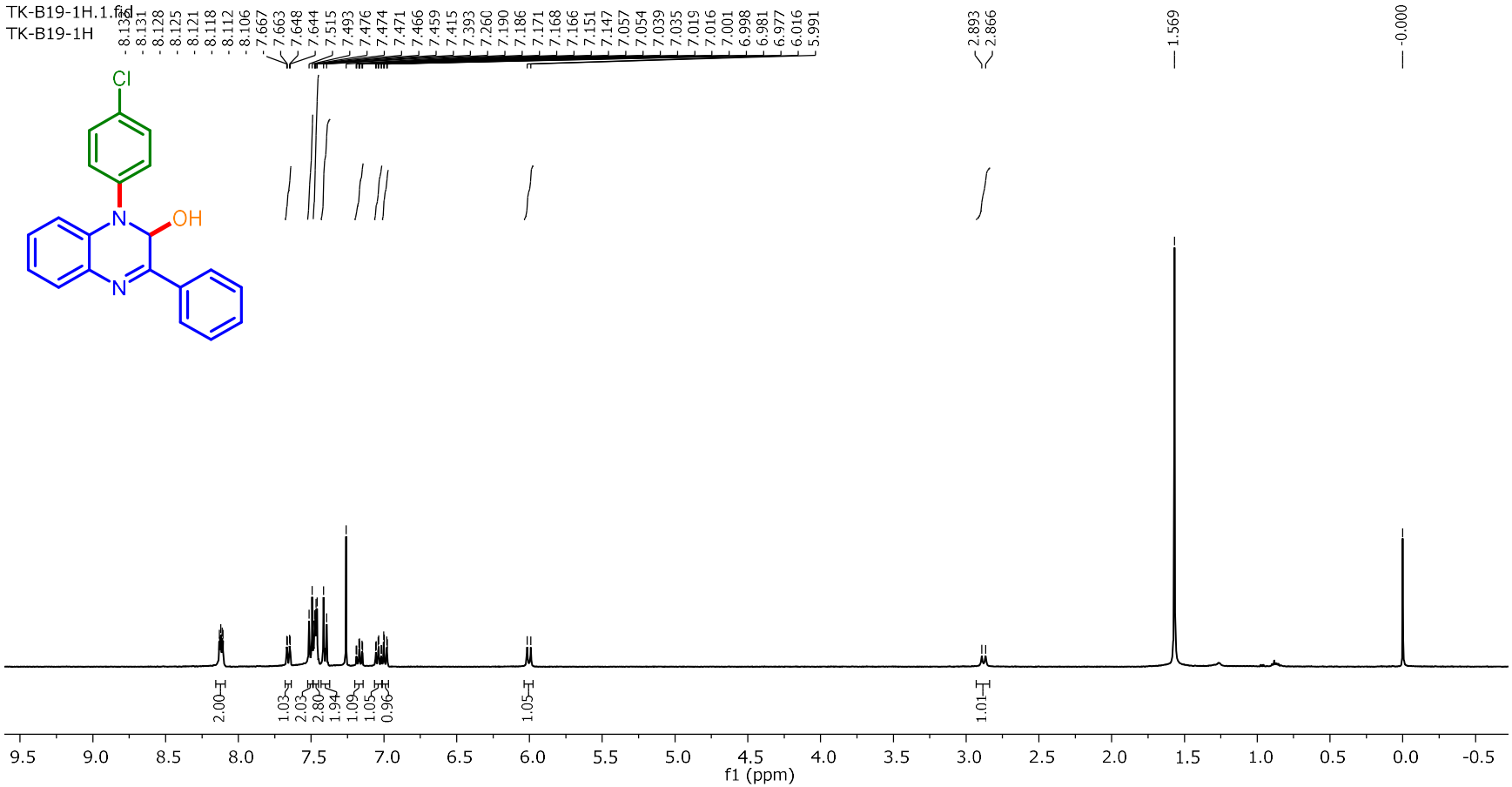
1-(4-Fluorophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ae): ^{1}H NMR ($CDCl_3$, 500 MHz)



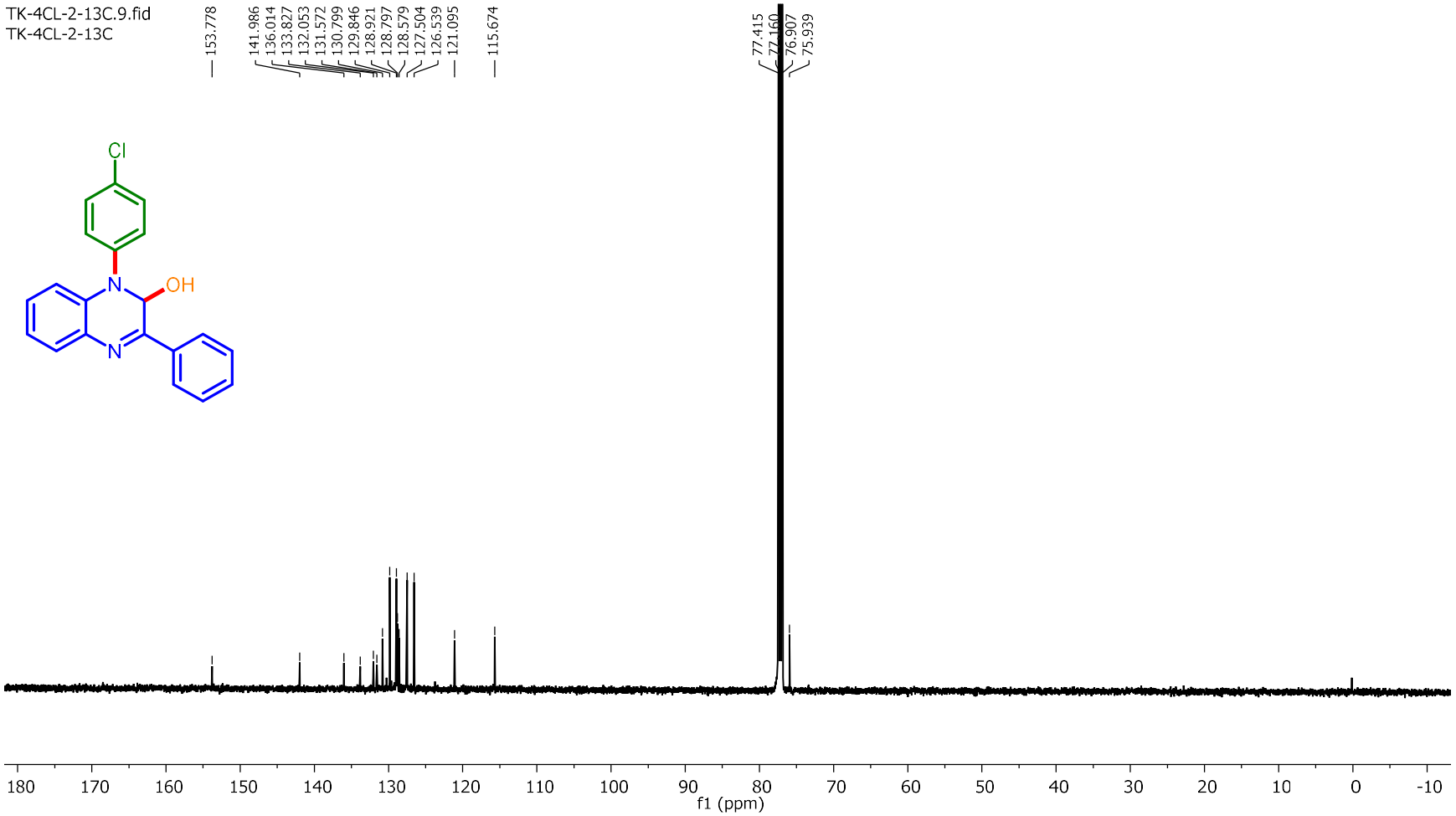
1-(4-Fluorophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ae): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



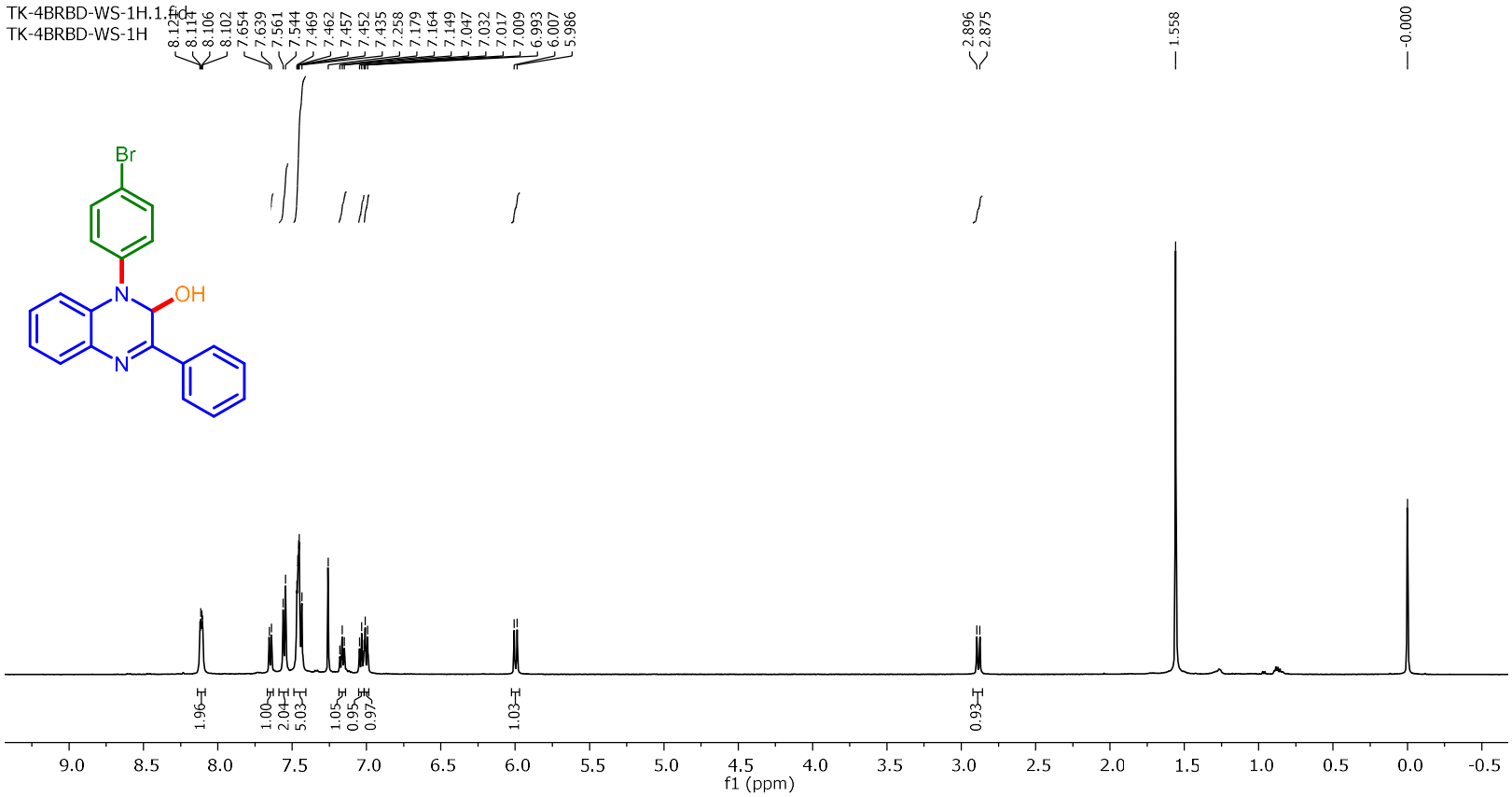
1-(4-Fluorophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ae): ^{19}F NMR ($CDCl_3$, 471 MHz)



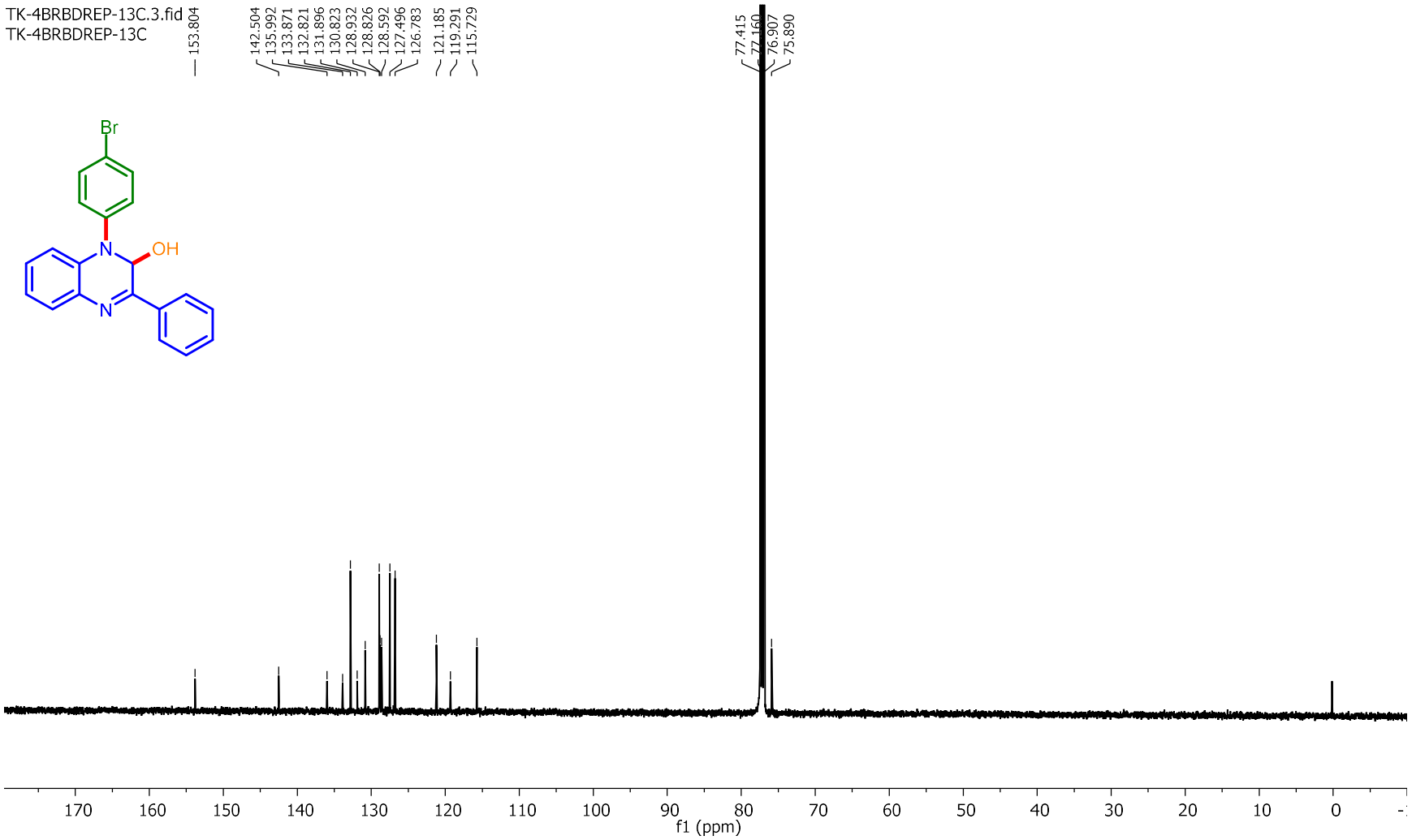
1-(4-Chlorophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3af): ^{1}H NMR ($CDCl_3$, 500 MHz)



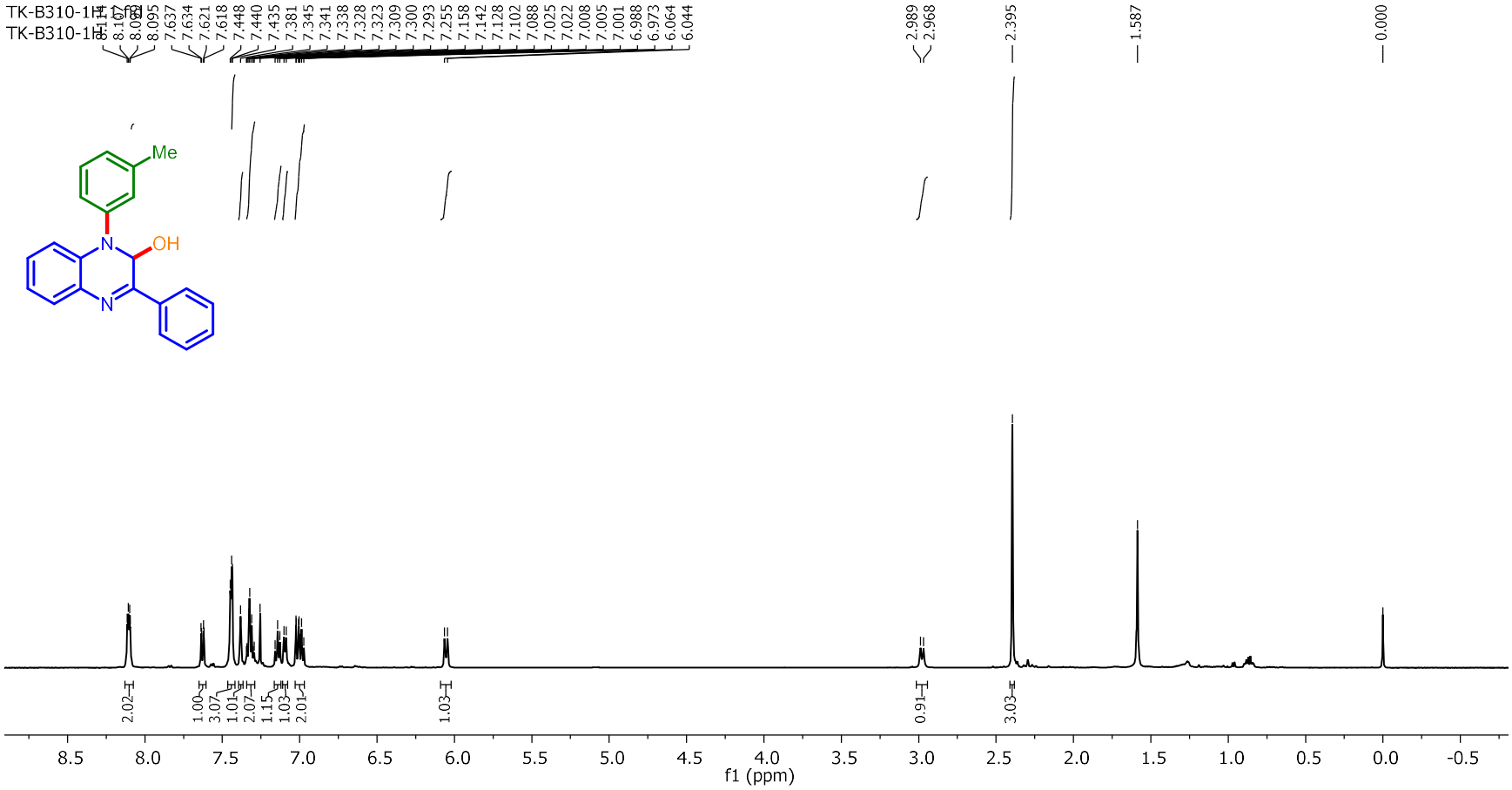
1-(4-Chlorophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3af): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



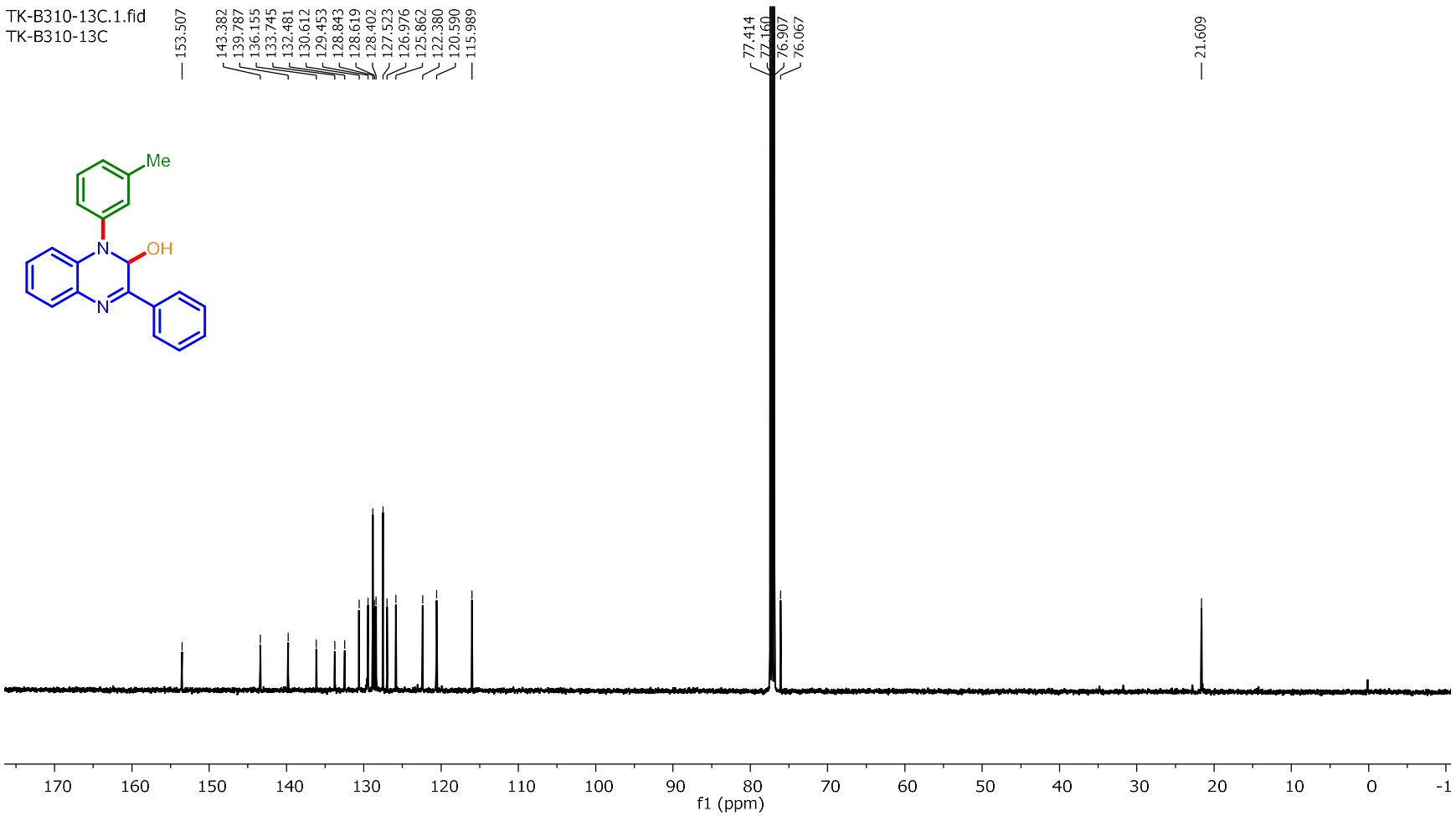
1-(4-Bromophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ag): ^{1}H NMR ($CDCl_3$, 500 MHz)



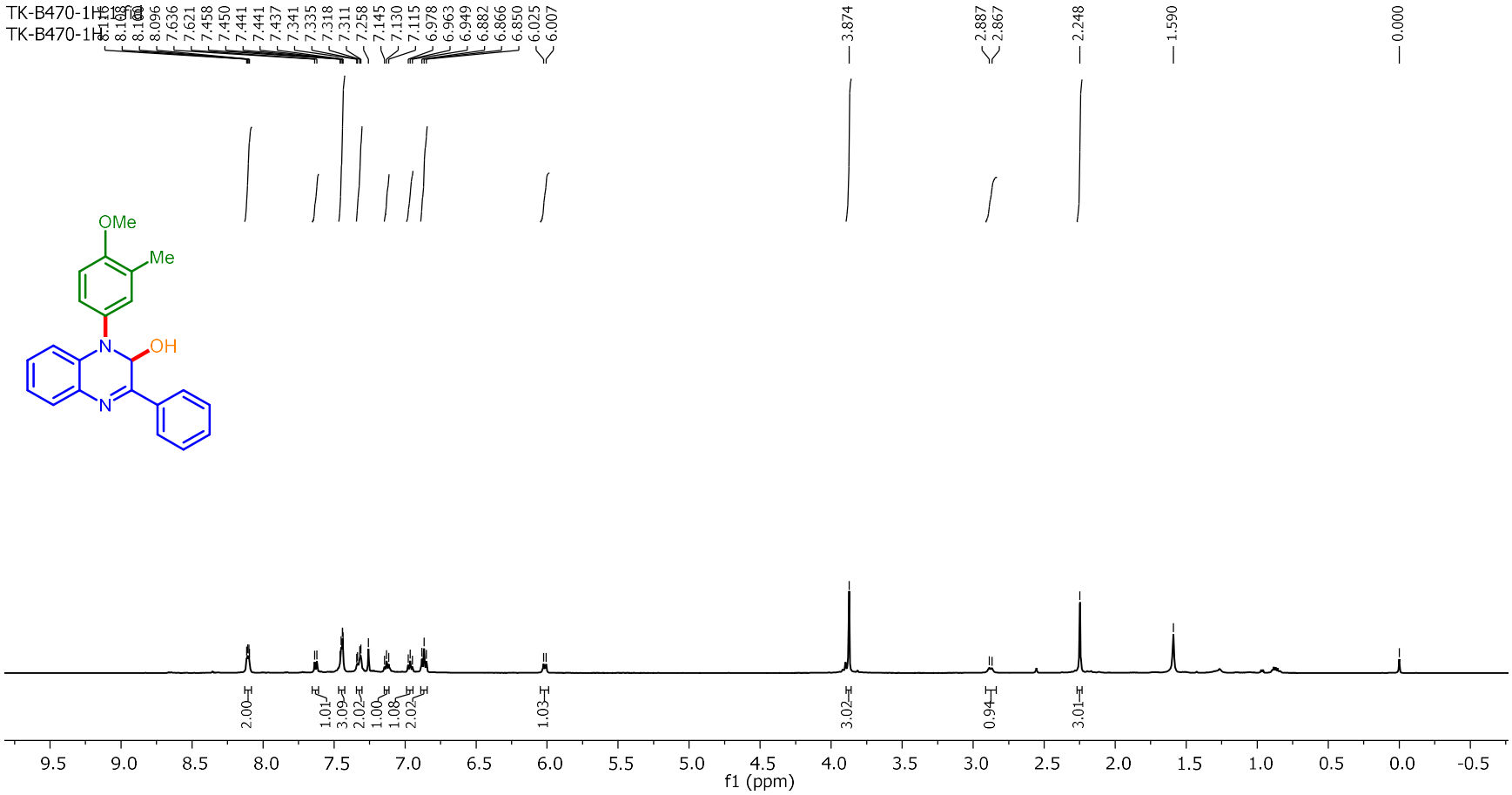
1-(4-Bromophenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ag): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



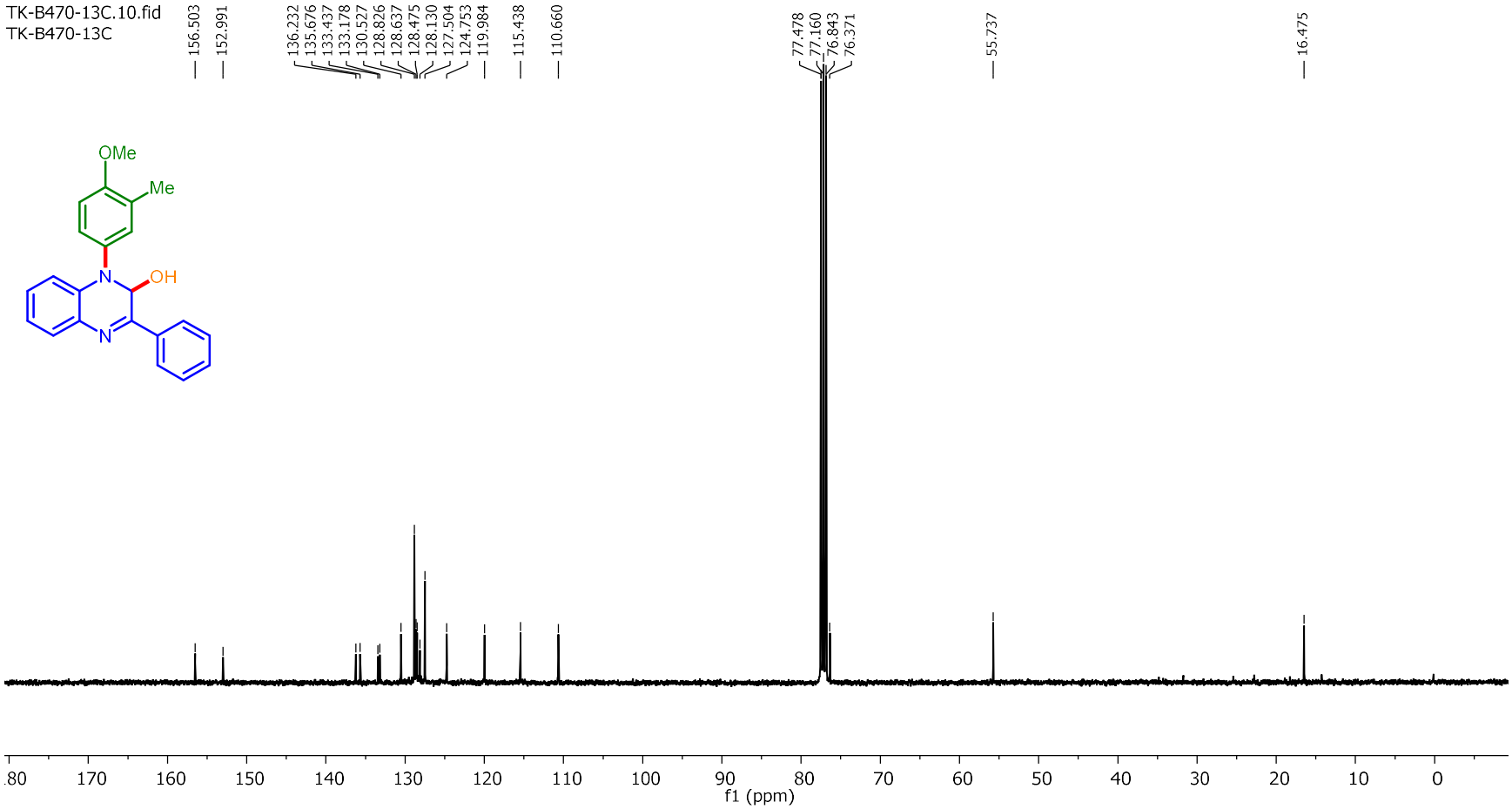
3-Phenyl-1-(m-tolyl)-1,2-dihydroquinoxalin-2-ol (3ah): ^{1}H NMR ($CDCl_3$, 500 MHz)



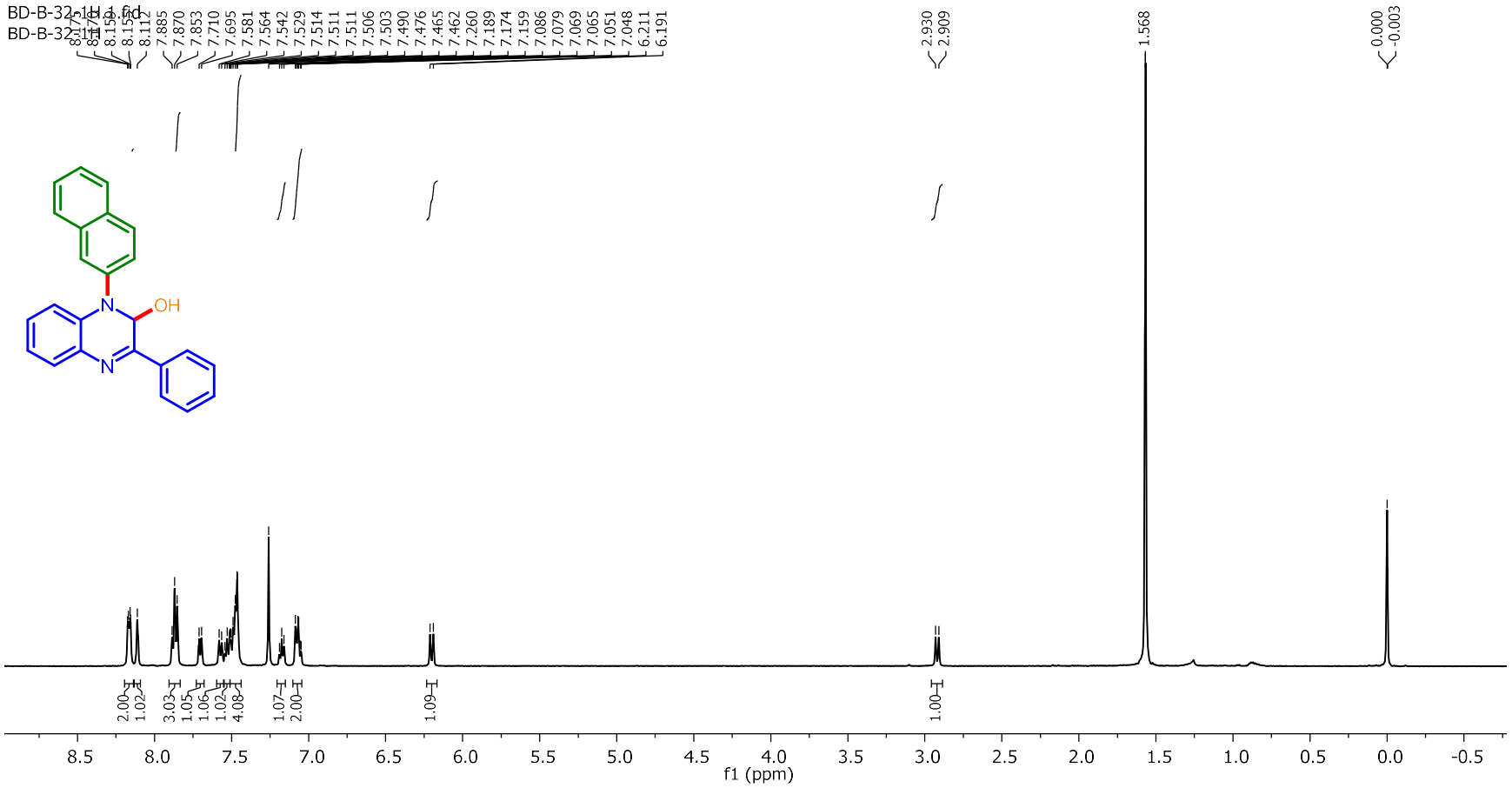
3-Phenyl-1-(m-tolyl)-1,2-dihydroquinoxalin-2-ol (3ah): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



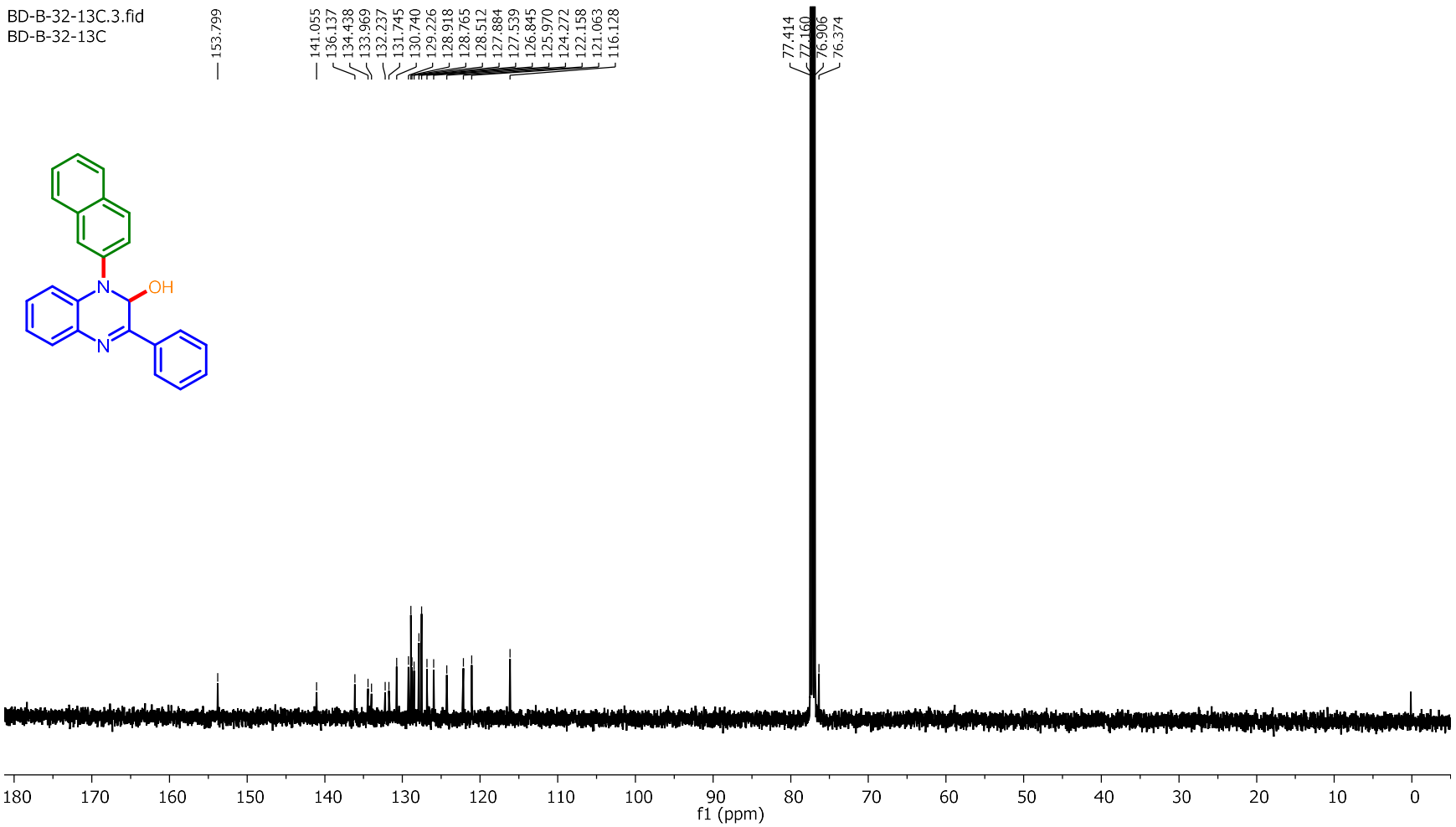
1-(4-Methoxy-3-methylphenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ai): ^{1}H NMR ($CDCl_3$, 500 MHz)



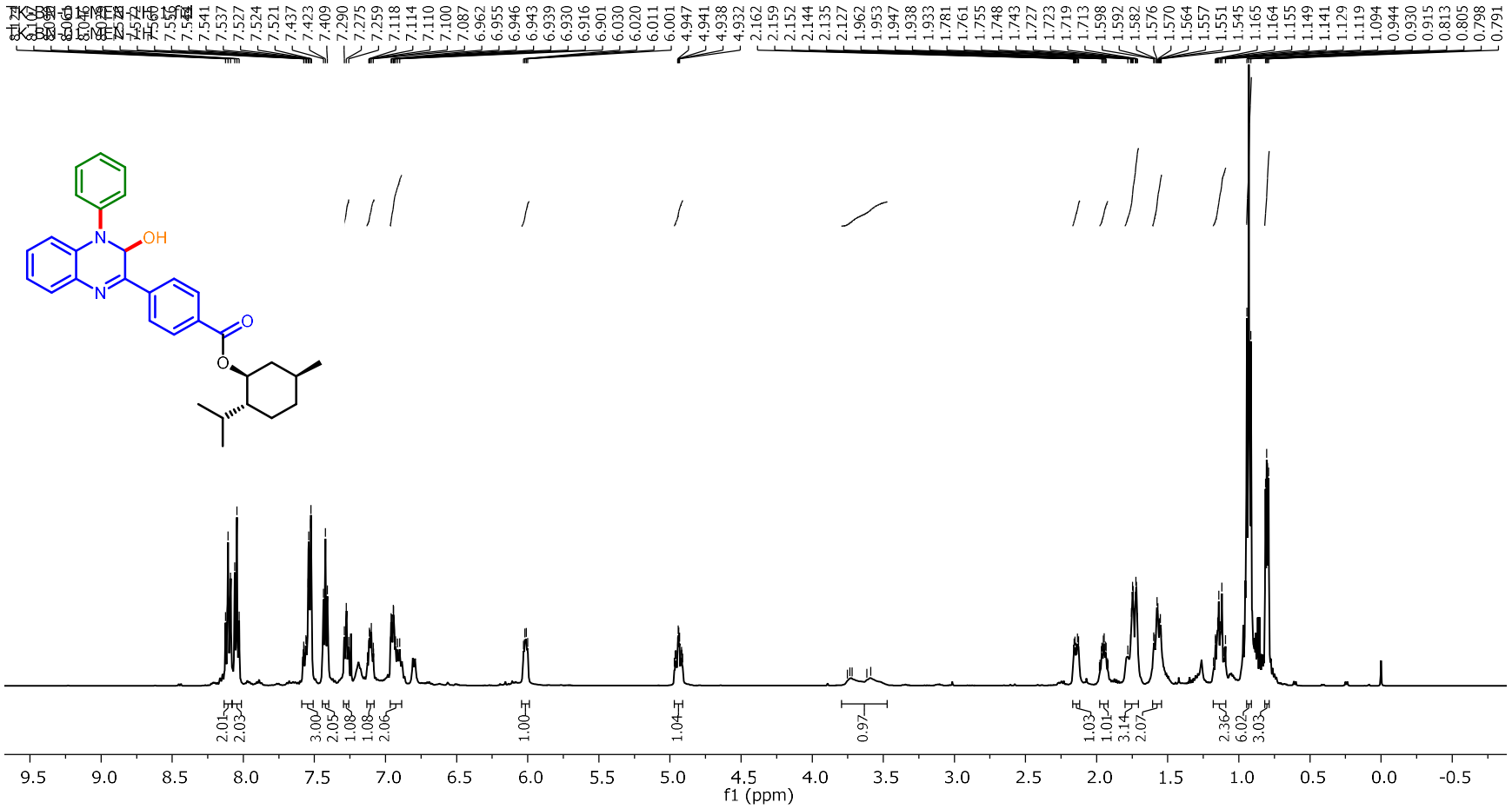
1-(4-Methoxy-3-methylphenyl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3ai): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 101 MHz)



1-(Naphthalen-2-yl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3aj):^{1}H NMR ($CDCl_3$, 500 MHz)

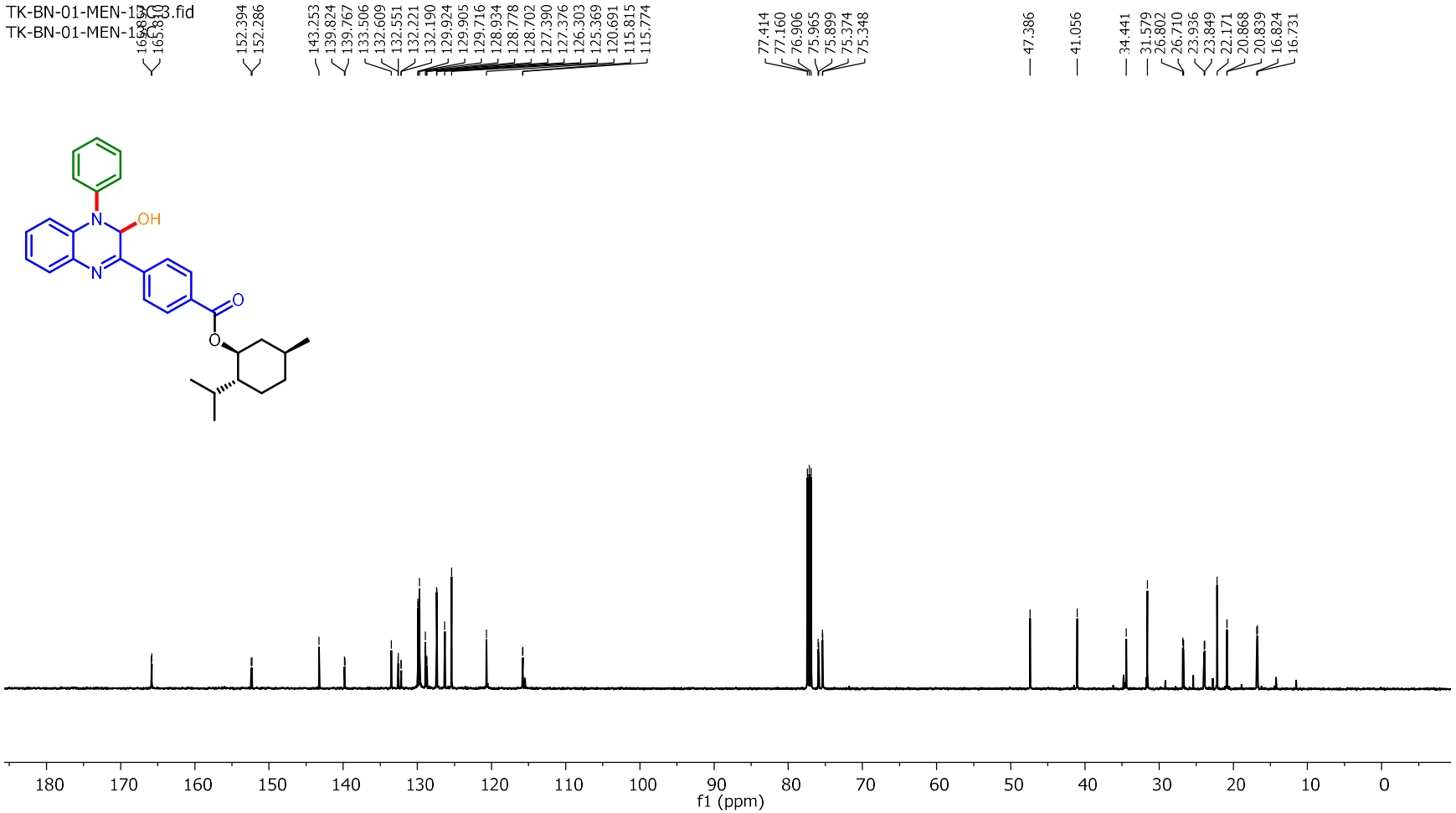


1-(Naphthalen-2-yl)-3-phenyl-1,2-dihydroquinoxalin-2-ol (3aj): **$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)**



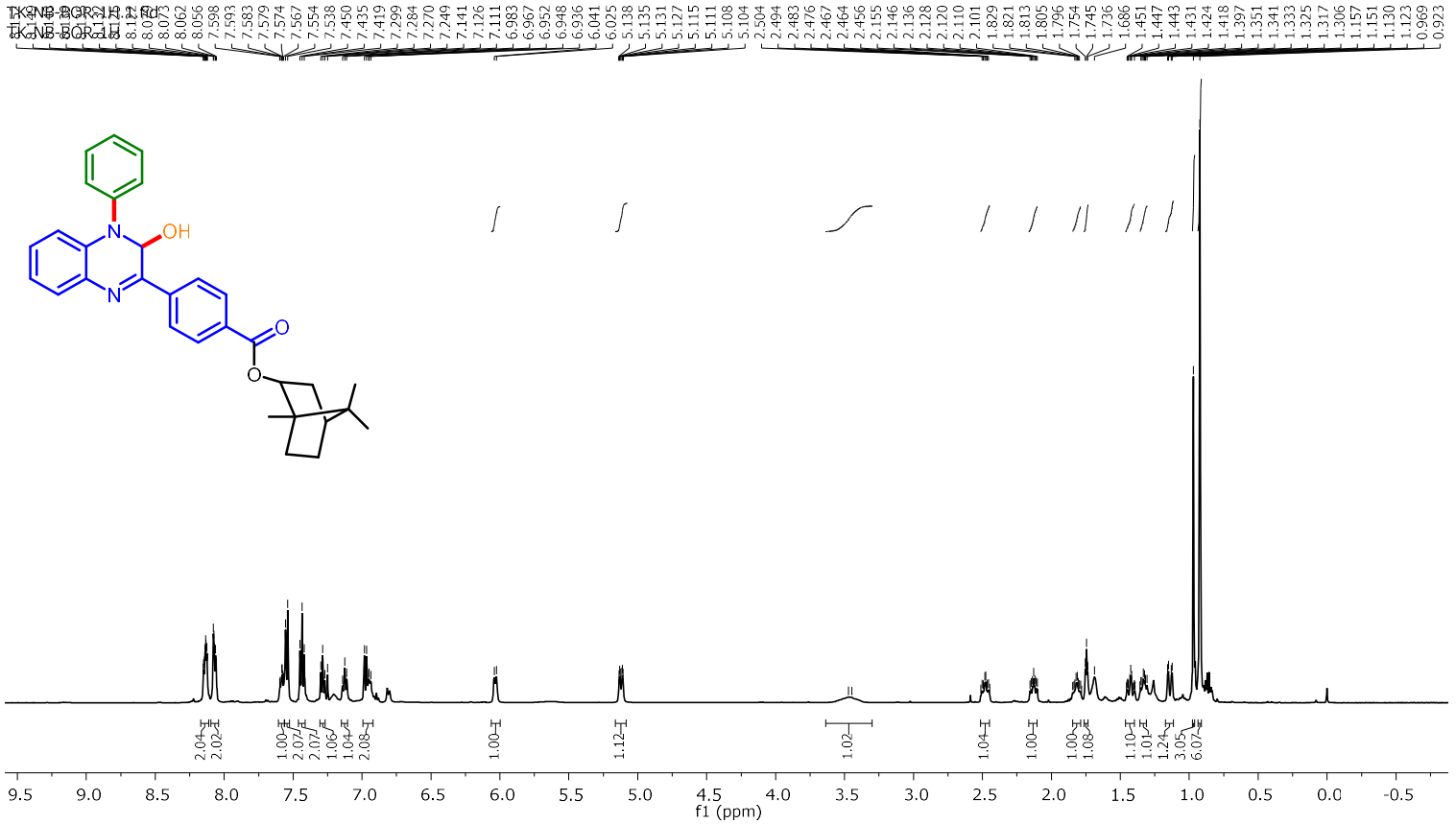
(1*S*, 2*R*, 5*S*)-2-Isopropyl-5-methylcyclohexyl 4-((*S*)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (3oa):

^{1}H NMR ($CDCl_3$, 500 MHz)



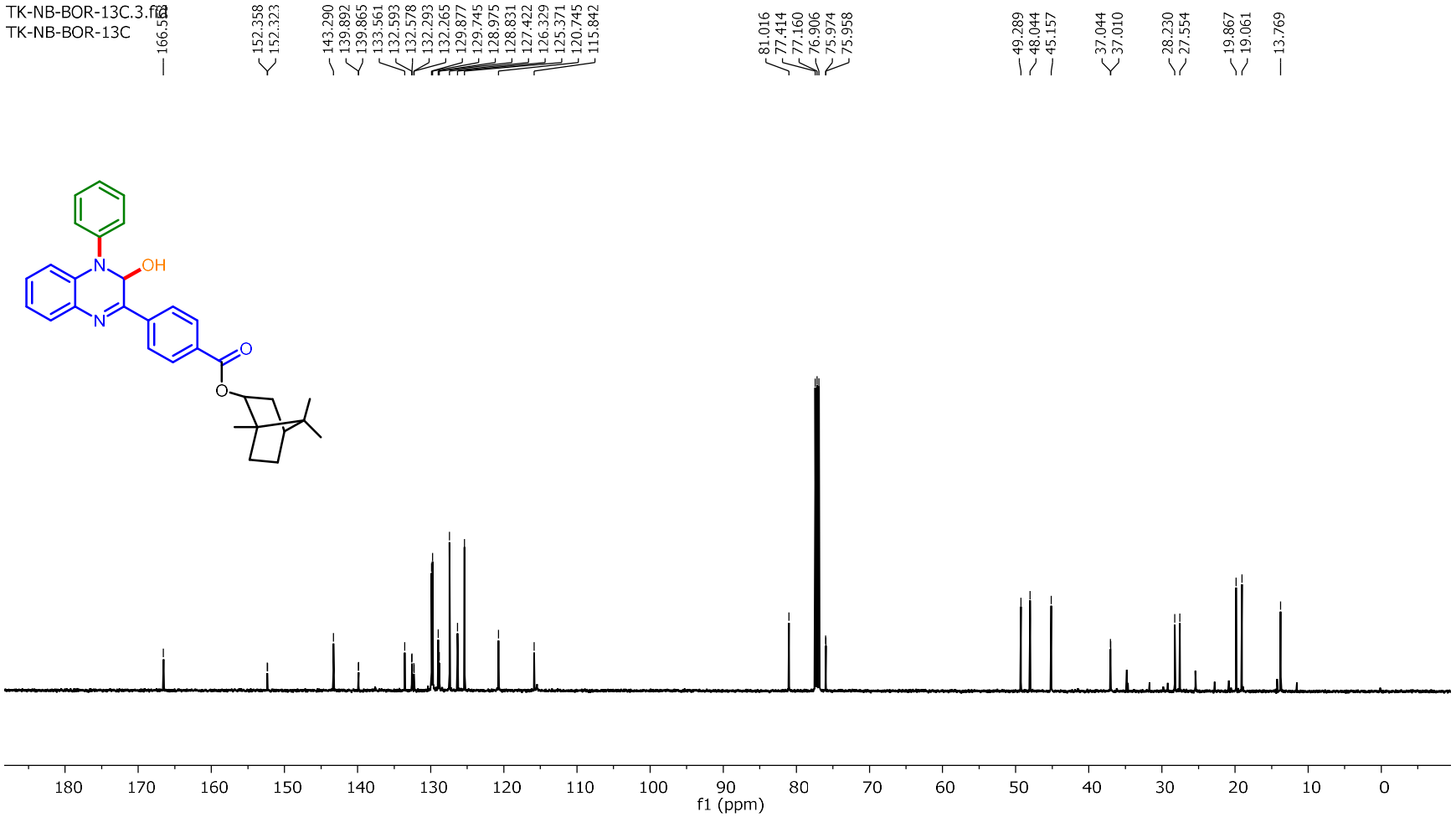
(1*S*, 2*R*, 5*S*)-2-Isopropyl-5-methylcyclohexyl 4-((*S*)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (3oa):

$^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)

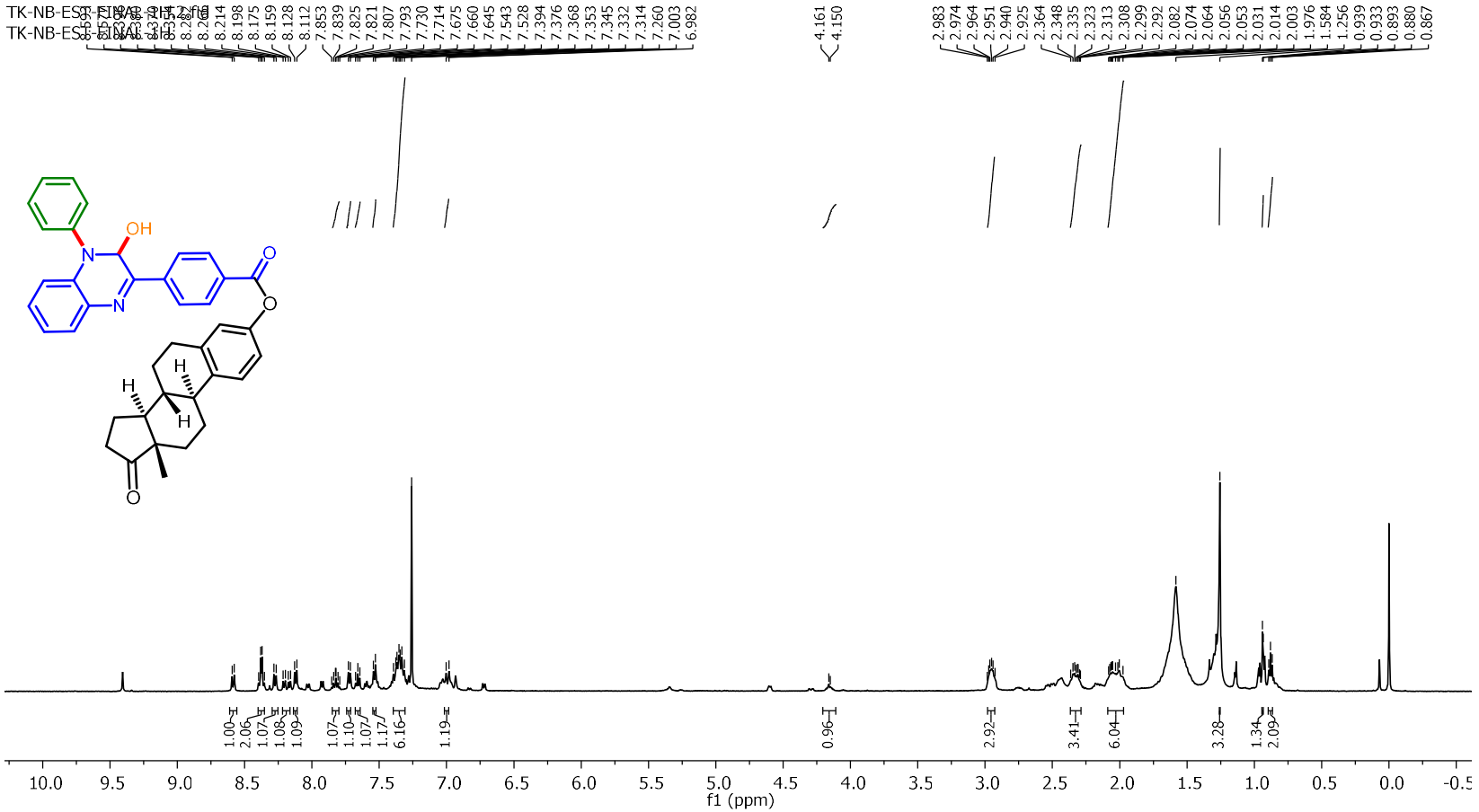


(4*R*)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl 4-((*S*)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (3pa):

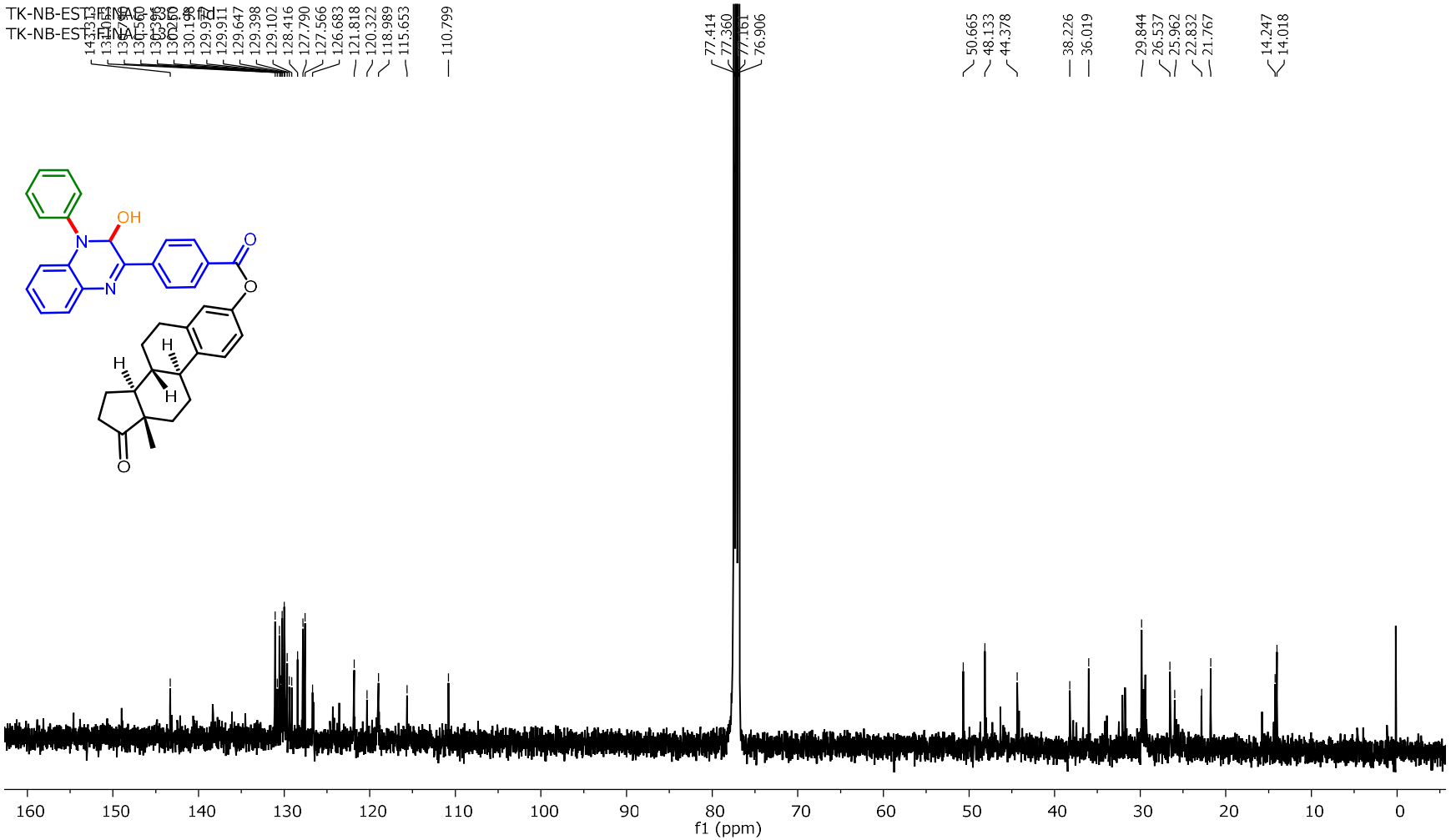
^{1}H NMR ($CDCl_3$, 500 MHz)



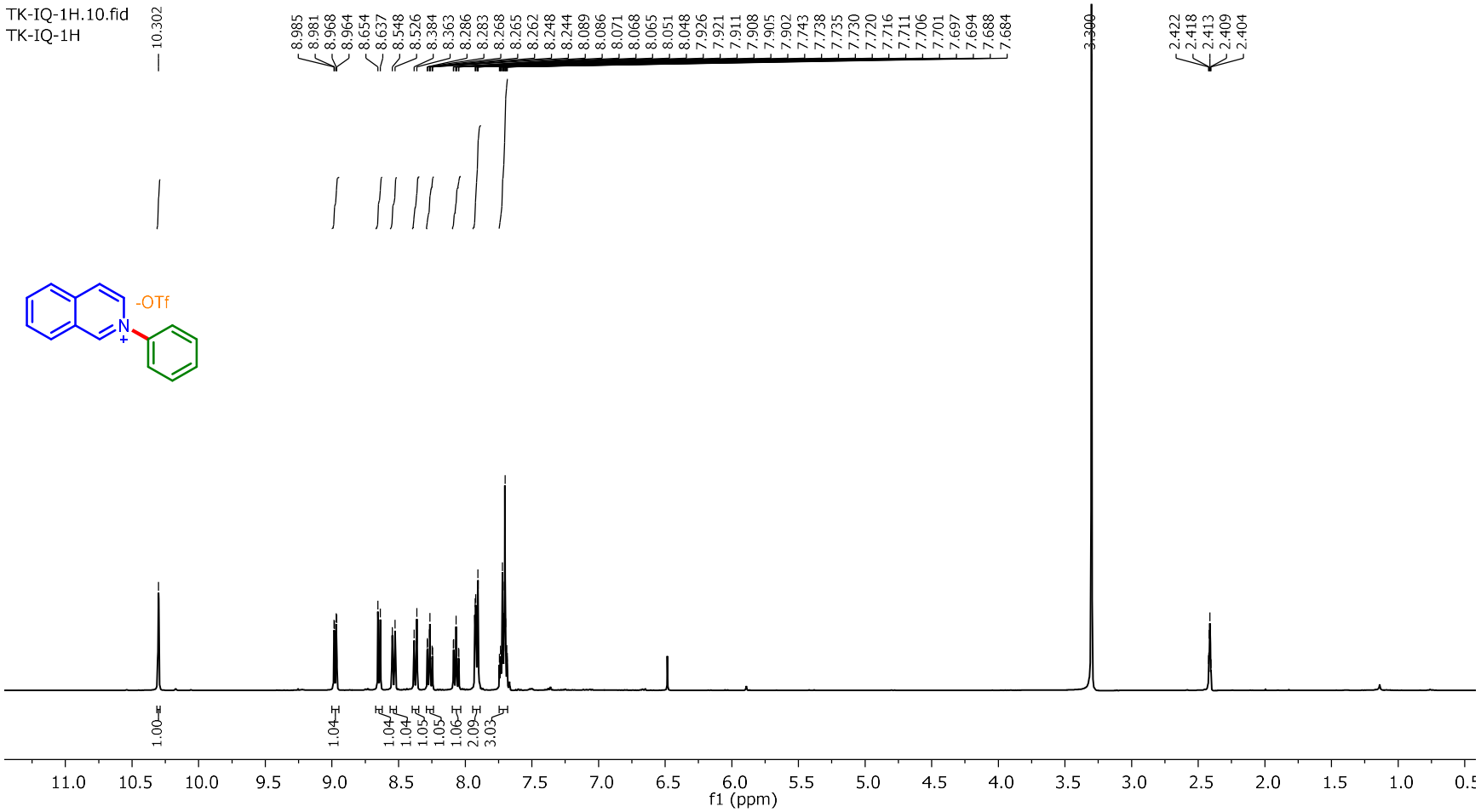
(4*R*)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl 4-((*S*)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (3pa): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



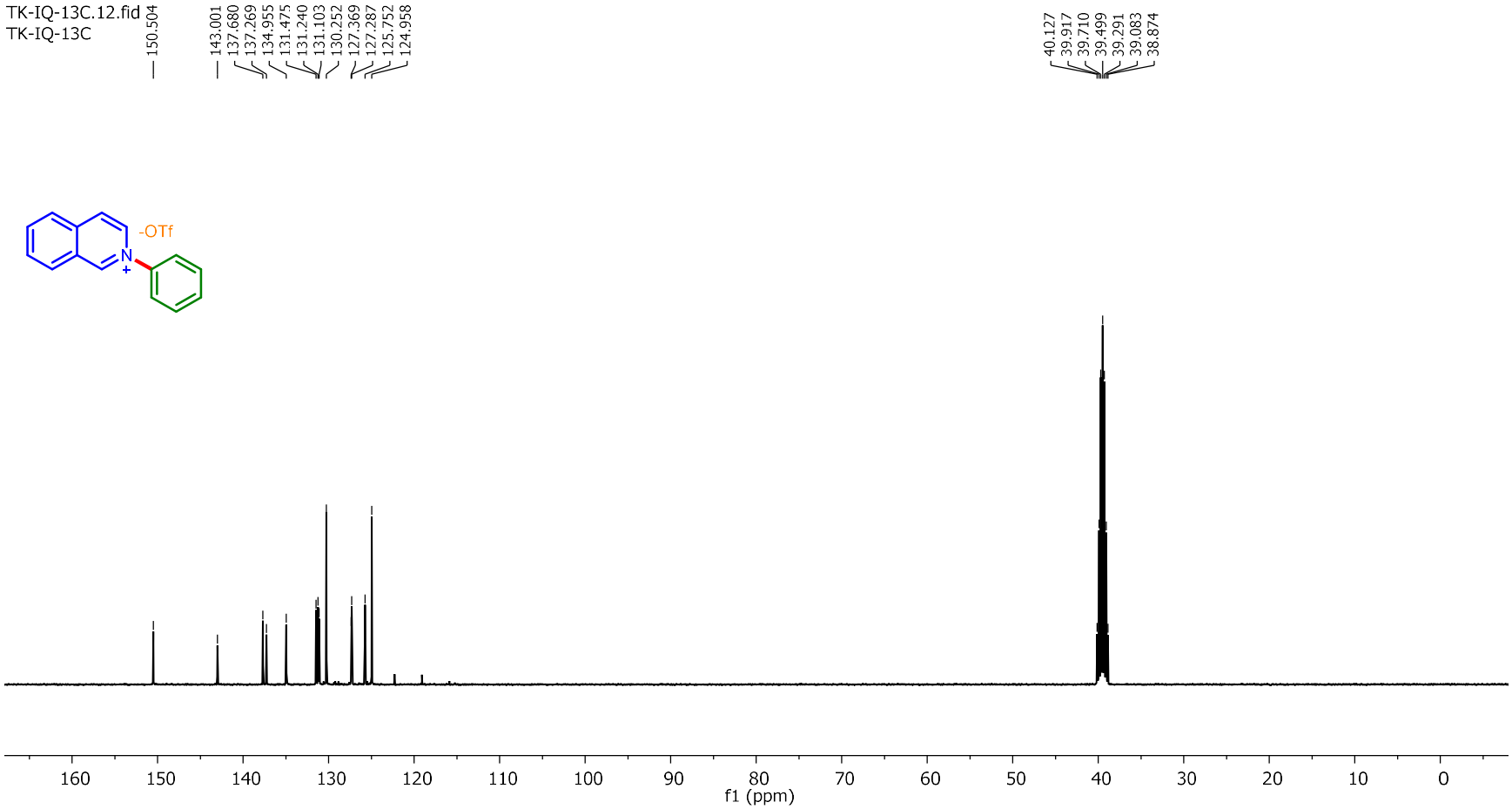
(8*R*,9*S*,13*S*,14*S*)-13-Methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-yl 4-((*S*)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (3qa): ^{1}H NMR ($CDCl_3$, 500 MHz)



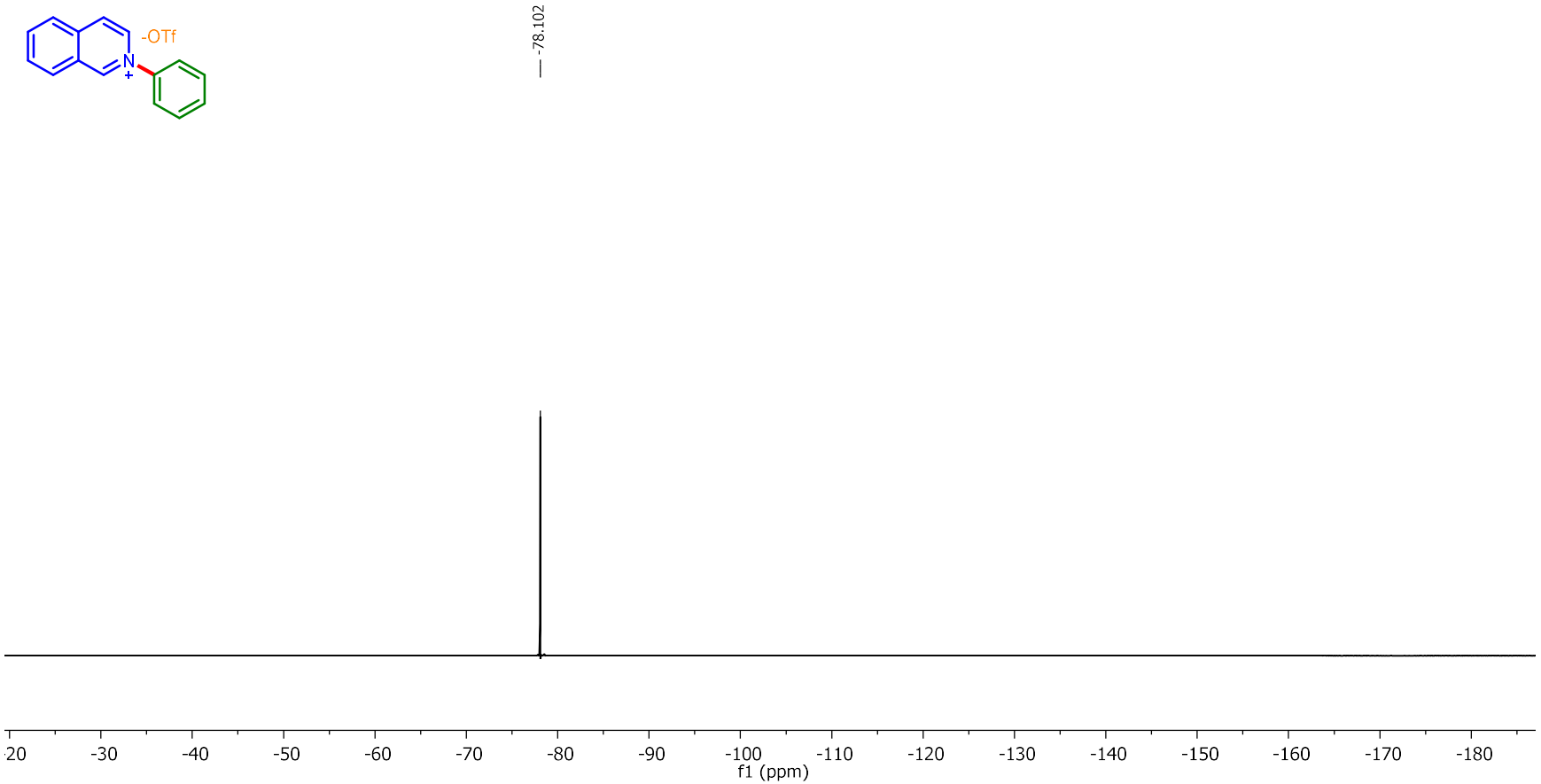
(8*R*,9*S*,13*S*,14*S*)-13-Methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6*H*-cyclopenta[a]phenanthren-3-yl 4-((*S*)-3-hydroxy-4-phenyl-3,4-dihydroquinoxalin-2-yl)benzoate (3qa): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



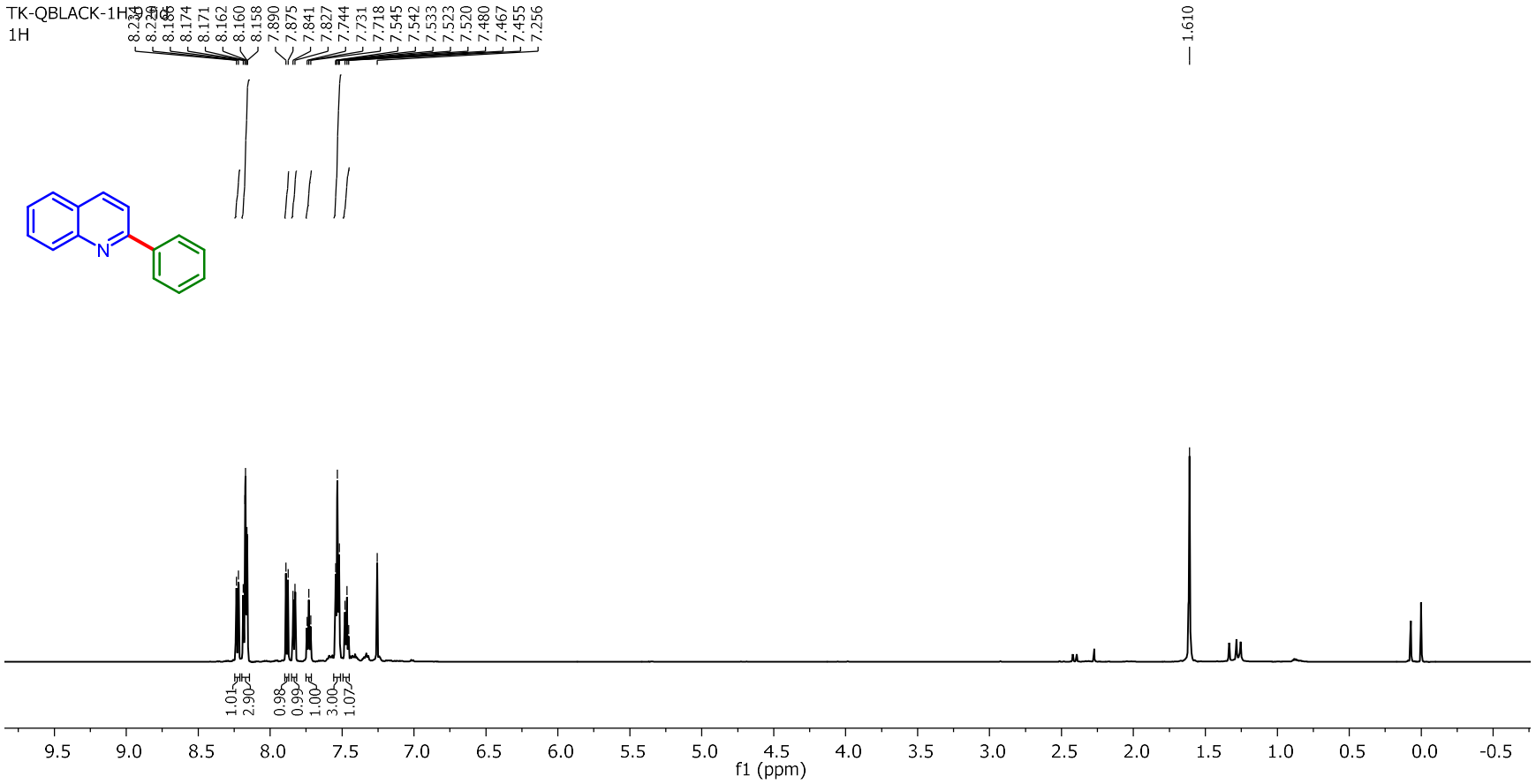
2-Phenylisoquinolin-2-ium trifluoromethanesulfonate (7'): ^{1}H NMR (DMSO-d$_6$, 400 MHz)



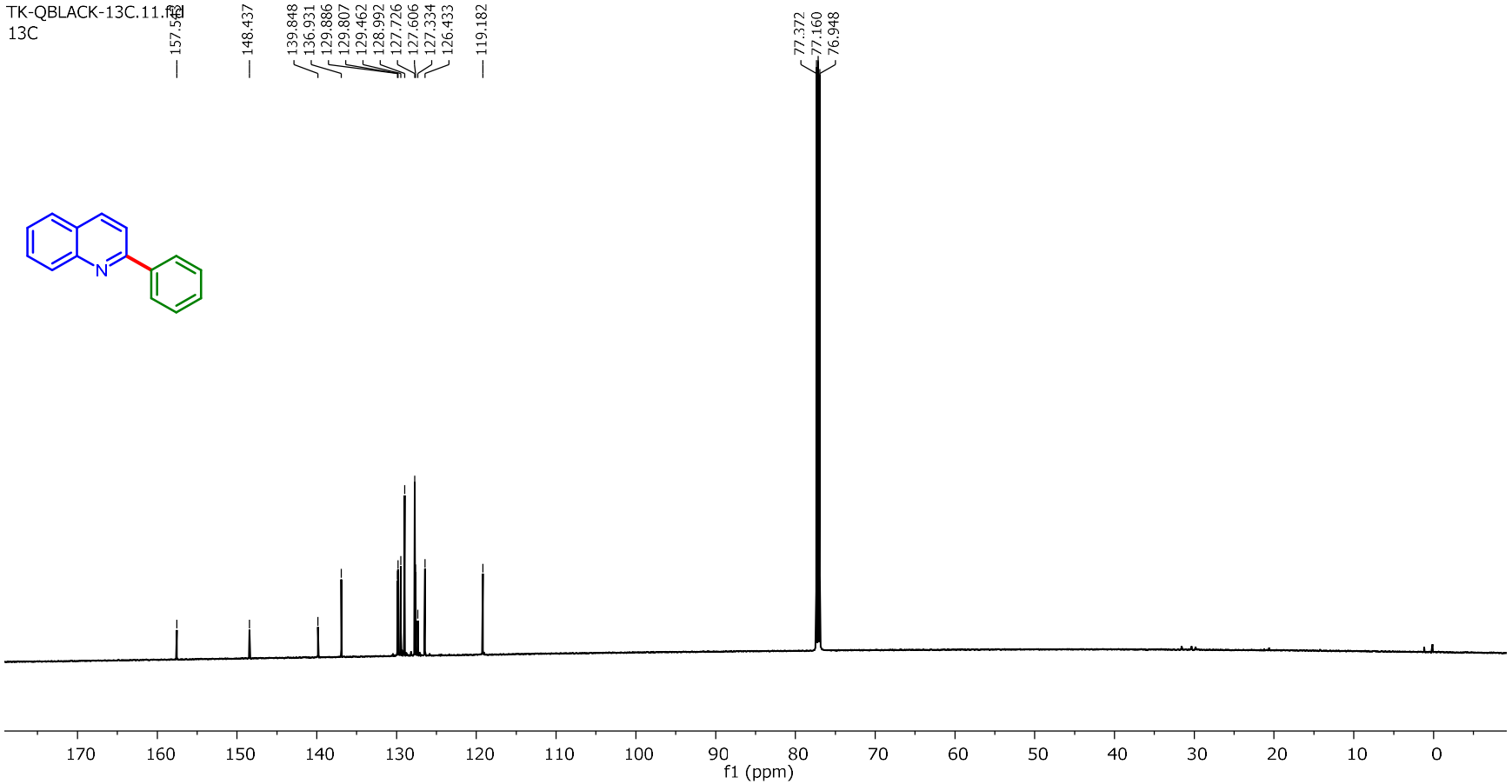
2-Phenylisoquinolin-2-ium trifluoromethanesulfonate (7'): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 101 MHz)



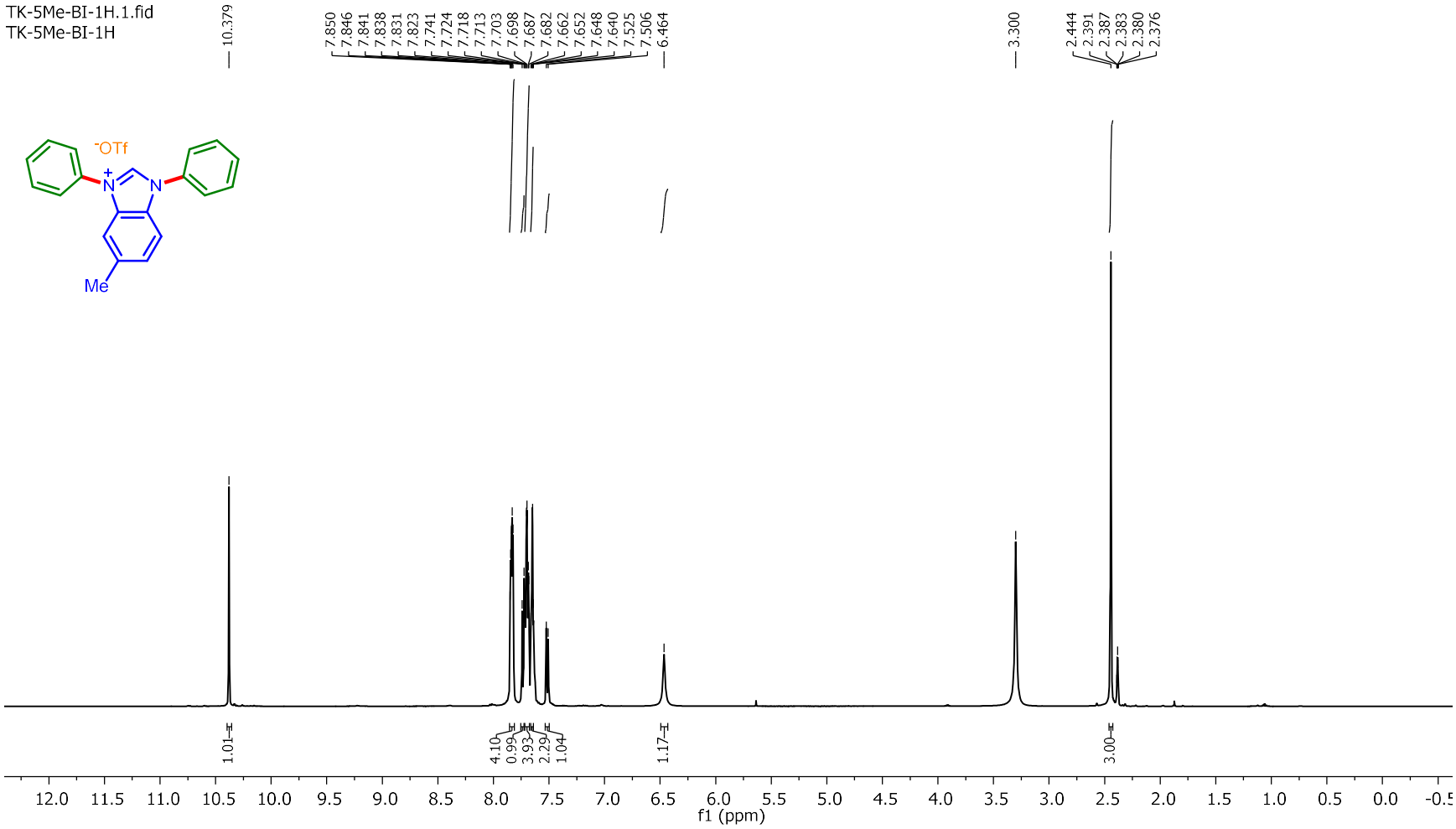
2-Phenylisoquinolin-2-ium trifluoromethanesulfonate (7'): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



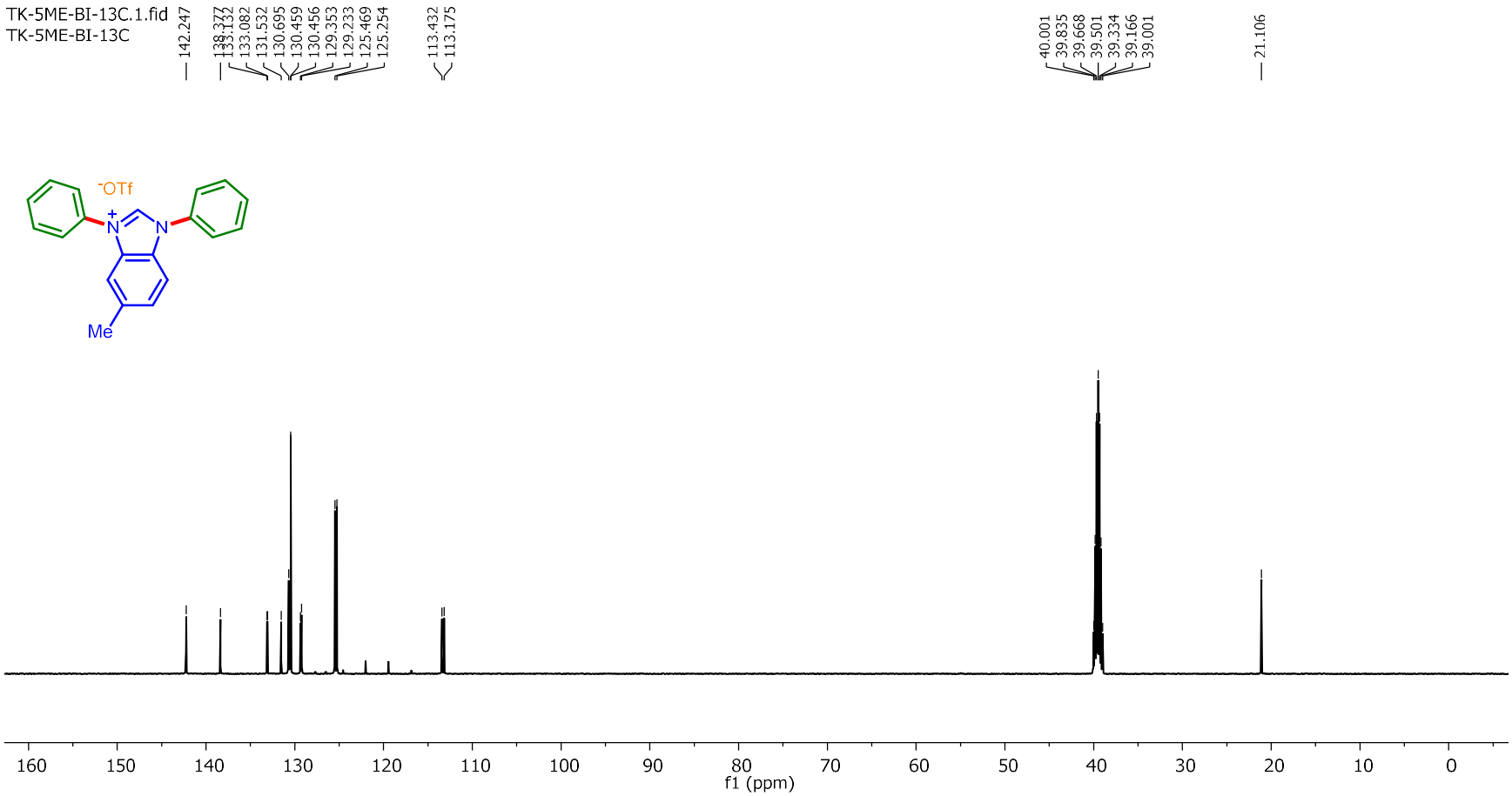
2-Phenylquinoline (8'): ^{1}H NMR ($CDCl_3$, 600 MHz)



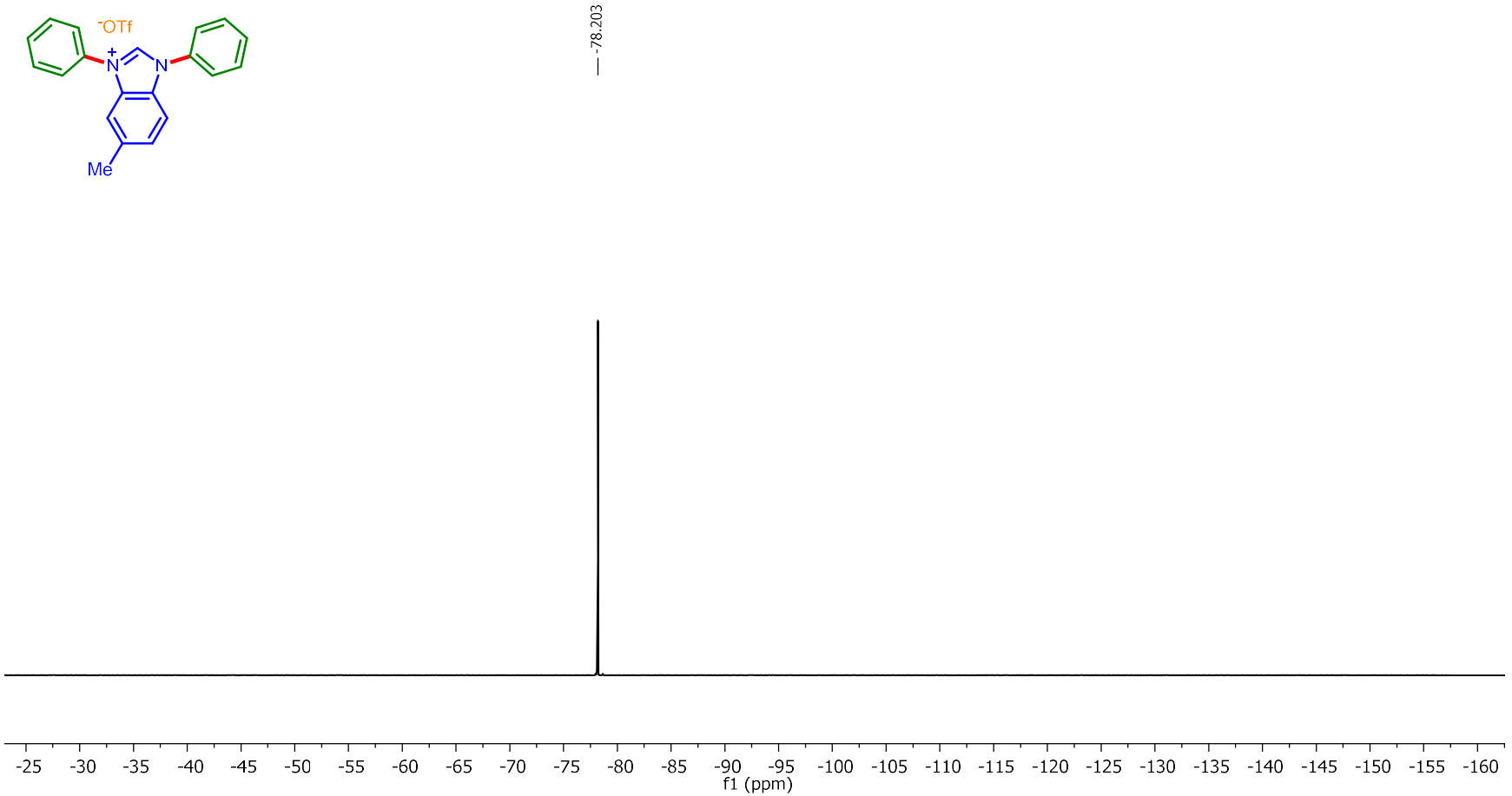
2-Phenylquinoline (8'): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 151 MHz)



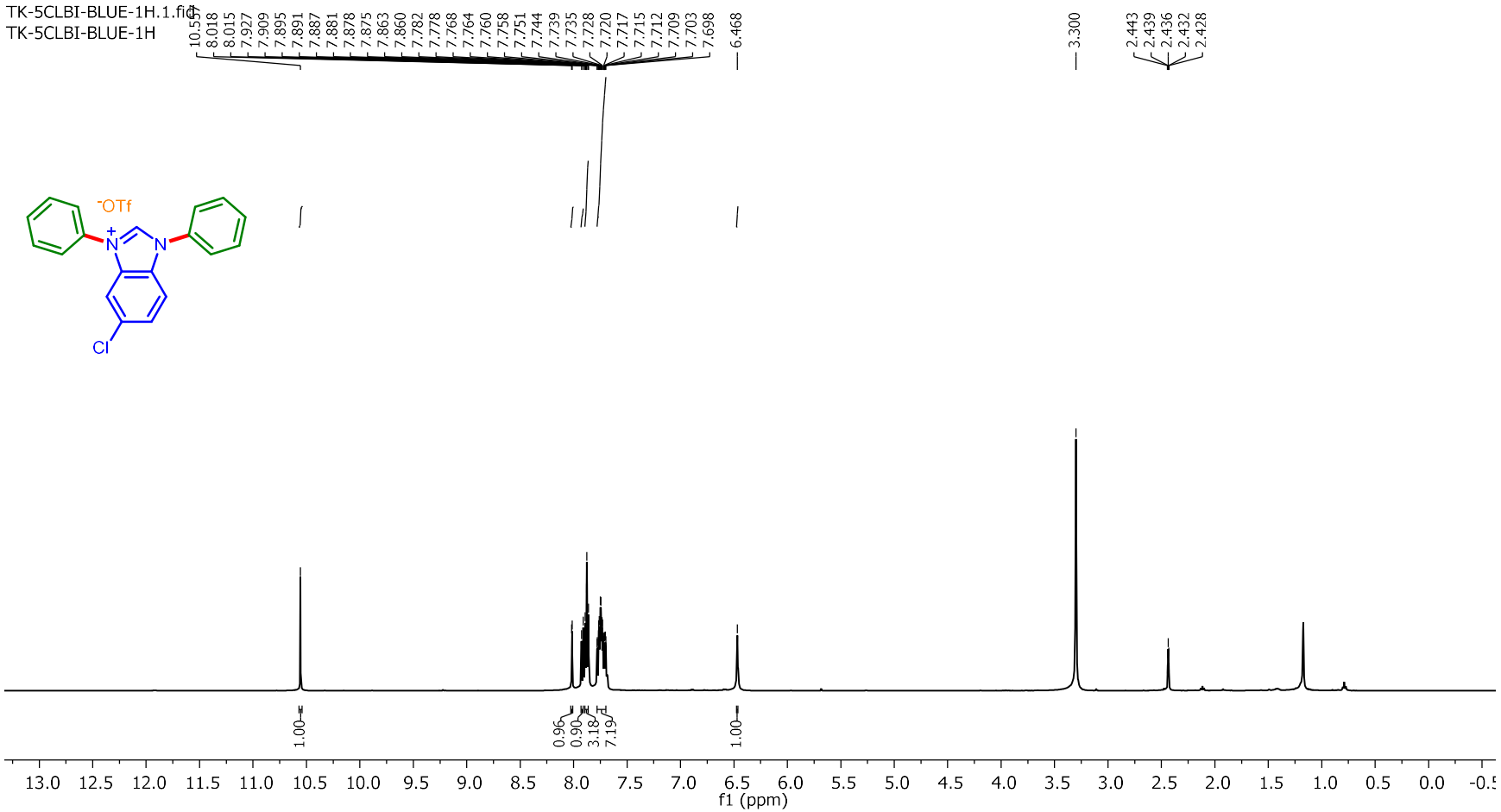
5-Methyl-1,3-diphenyl-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (10aa): ^{1}H NMR (DMSO-d$_6$, 500 MHz)



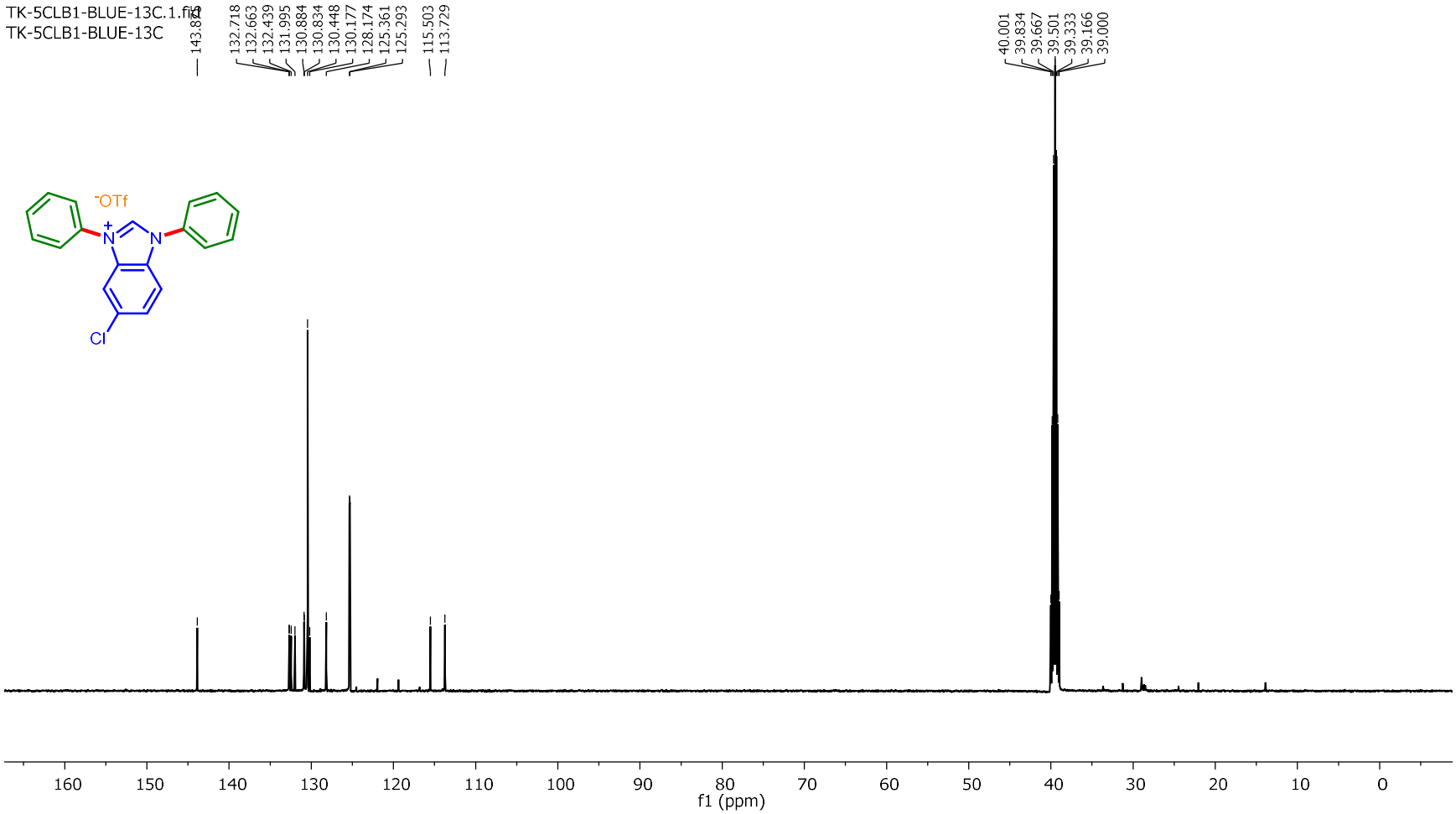
5-Methyl-1,3-diphenyl-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (10aa): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 126 MHz)



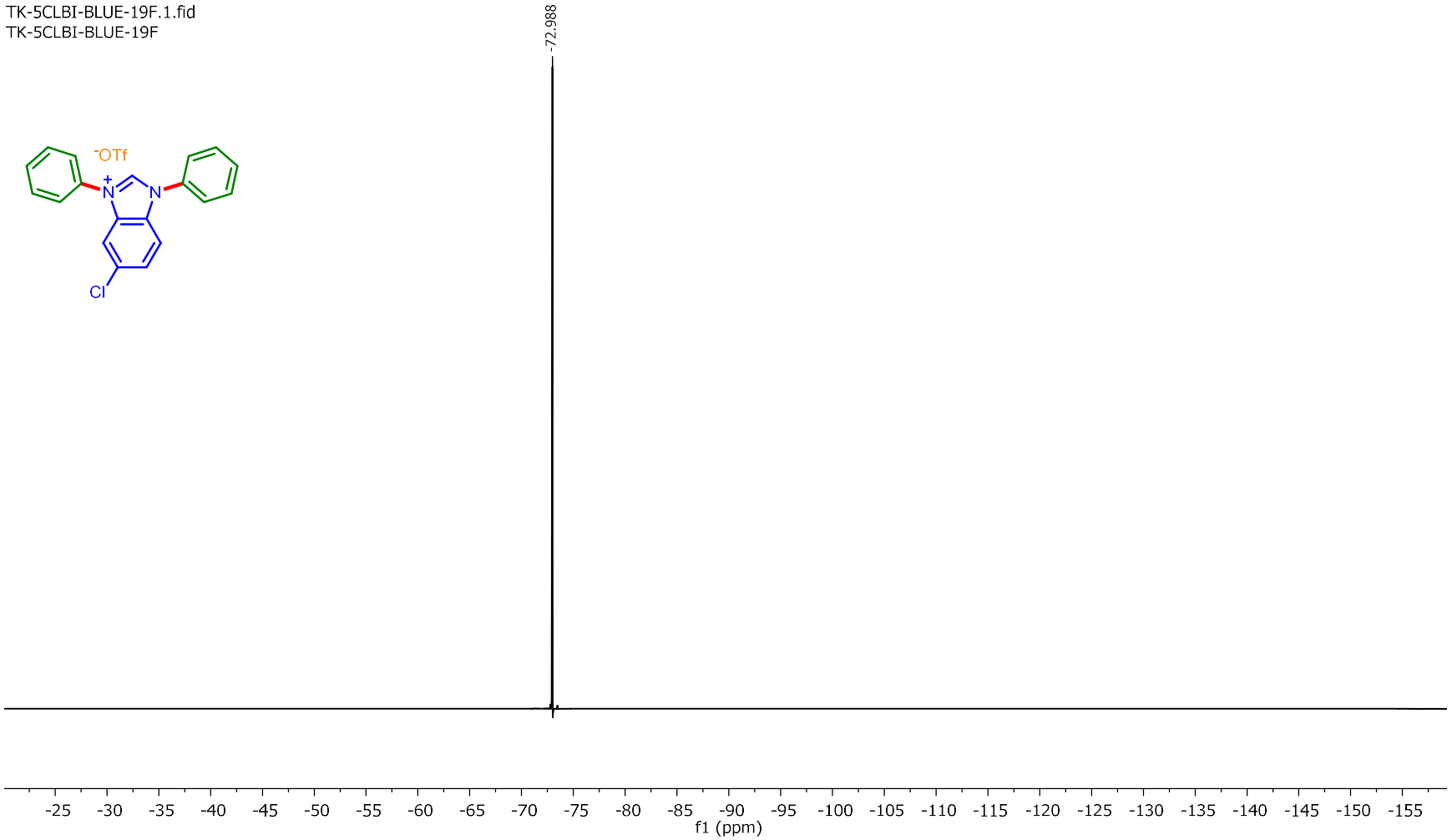
5-Methyl-1,3-diphenyl-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (10aa): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



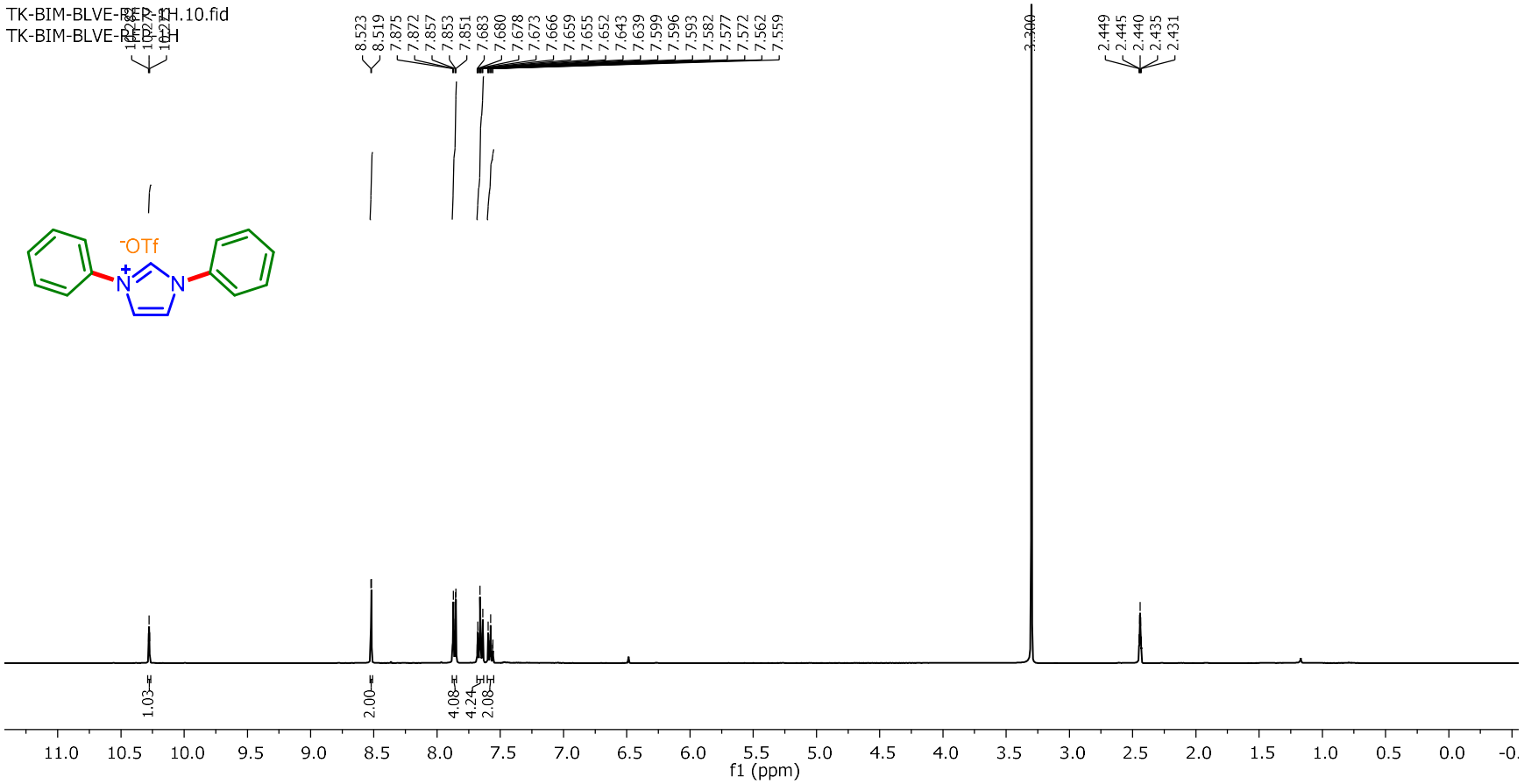
5-Chloro-1,3-diphenyl-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (10ba):^{1}H NMR (DMSO-d$_6$, 500 MHz)



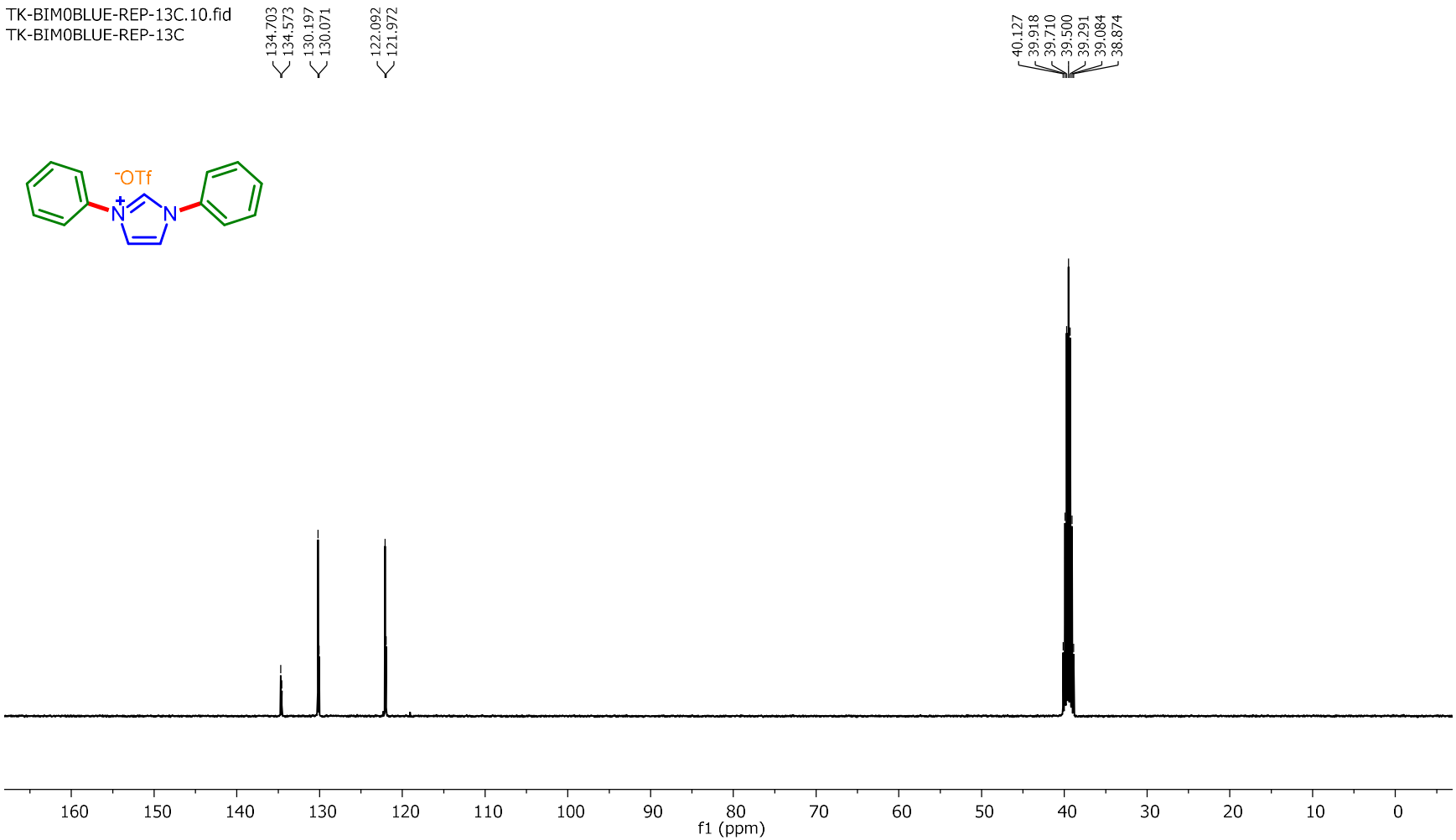
5-Chloro-1,3-diphenyl-1*H*-benzo[*d*]imidazol-3-ium trifluoromethanesulfonate (10ba): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 126 MHz)



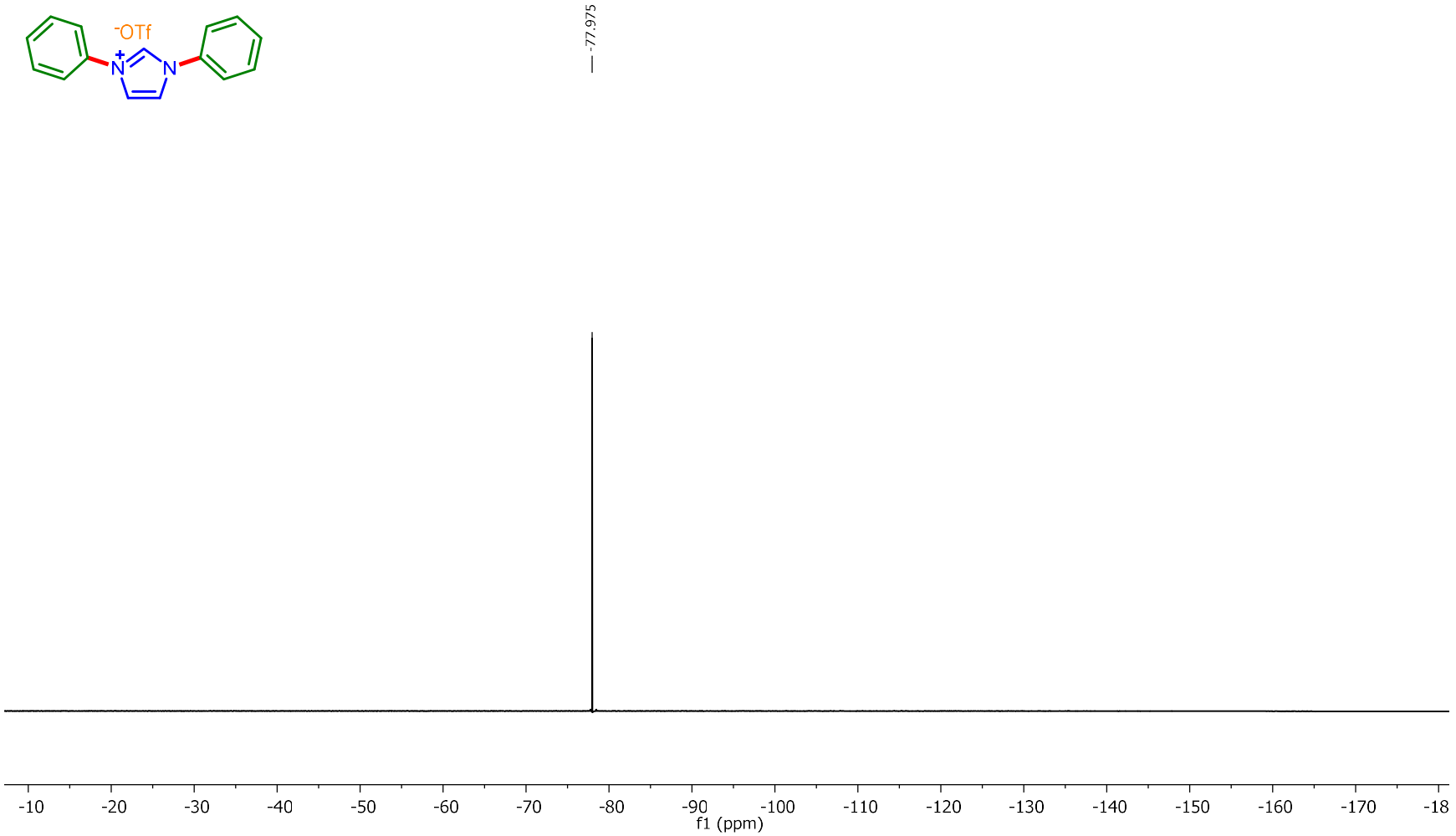
5-Chloro-1,3-diphenyl-1*H*-benzo[d]imidazol-3-ium trifluoromethanesulfonate (10ba): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



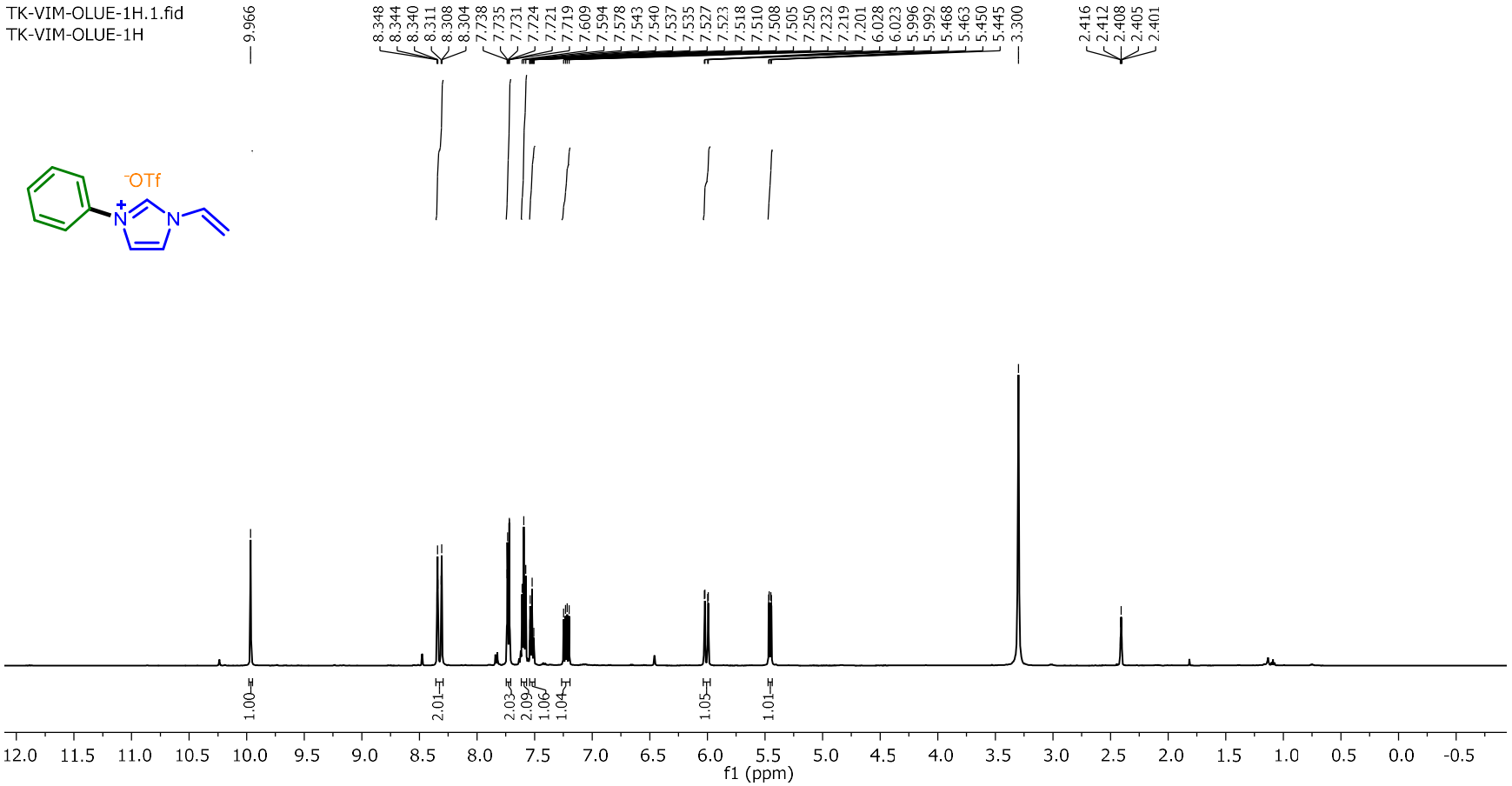
1,3-Diphenyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (10ca): ^{1}H NMR (DMSO-d$_6$, 400 MHz)



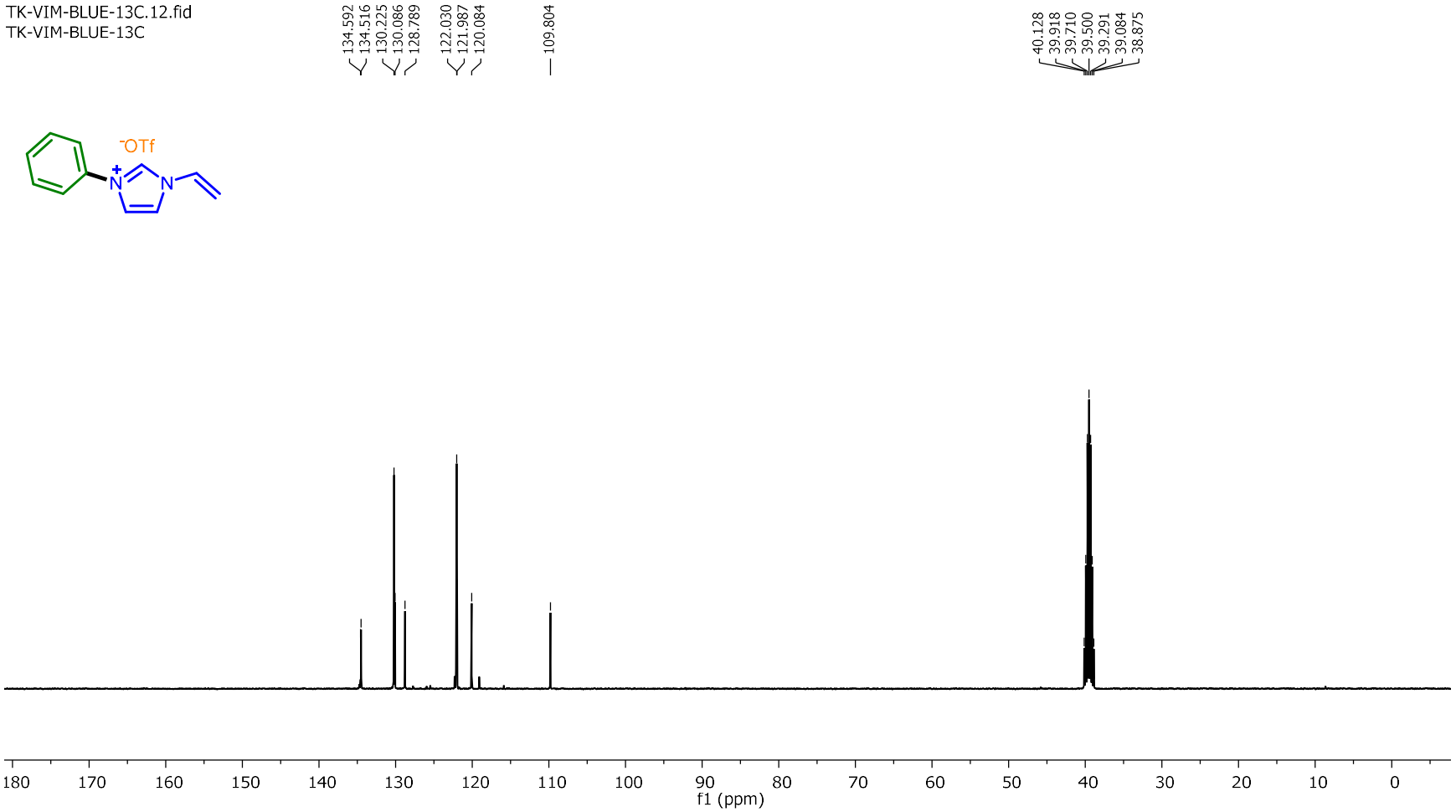
1,3-Diphenyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (10ca): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 101 MHz)



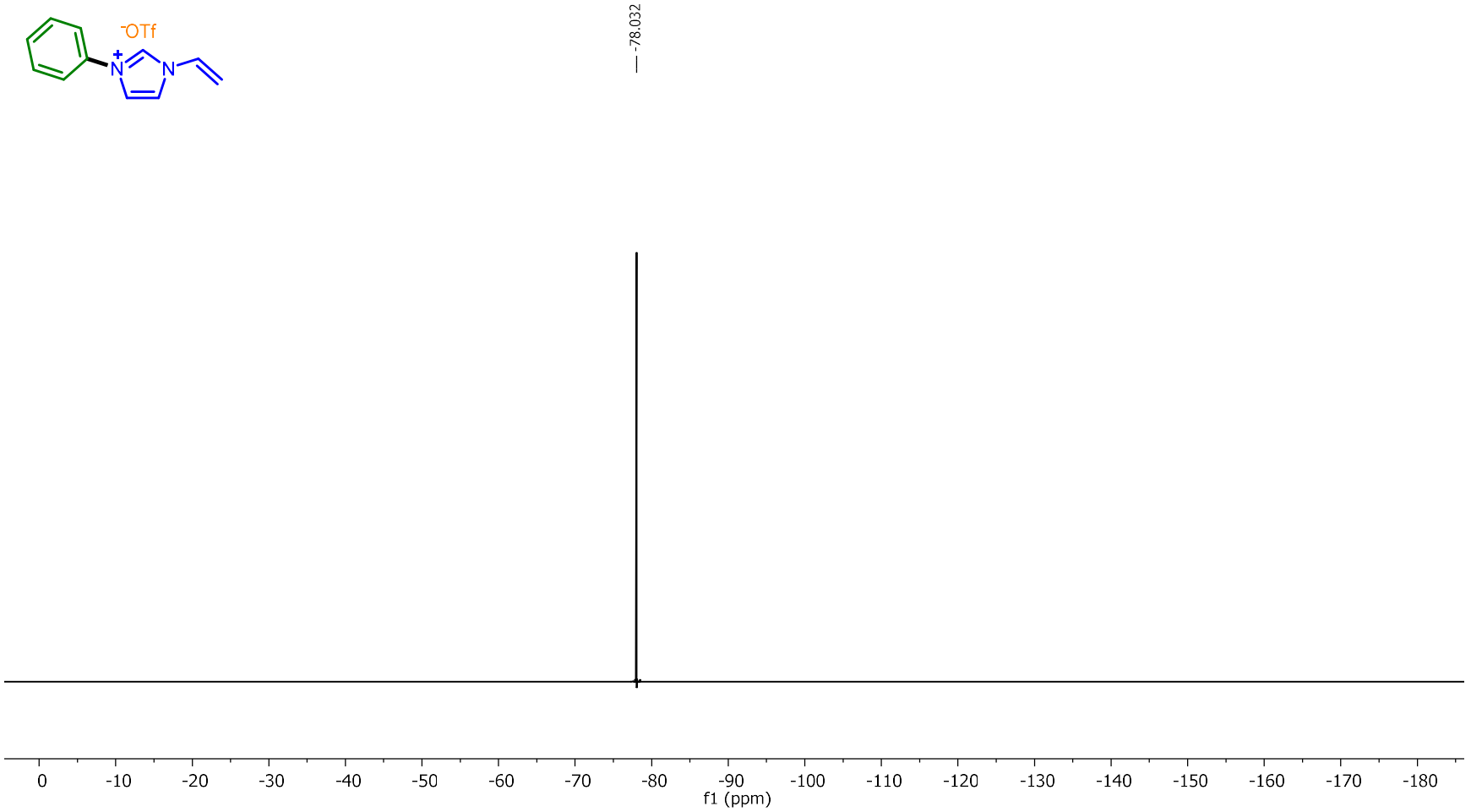
1,3-Diphenyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (10ca): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



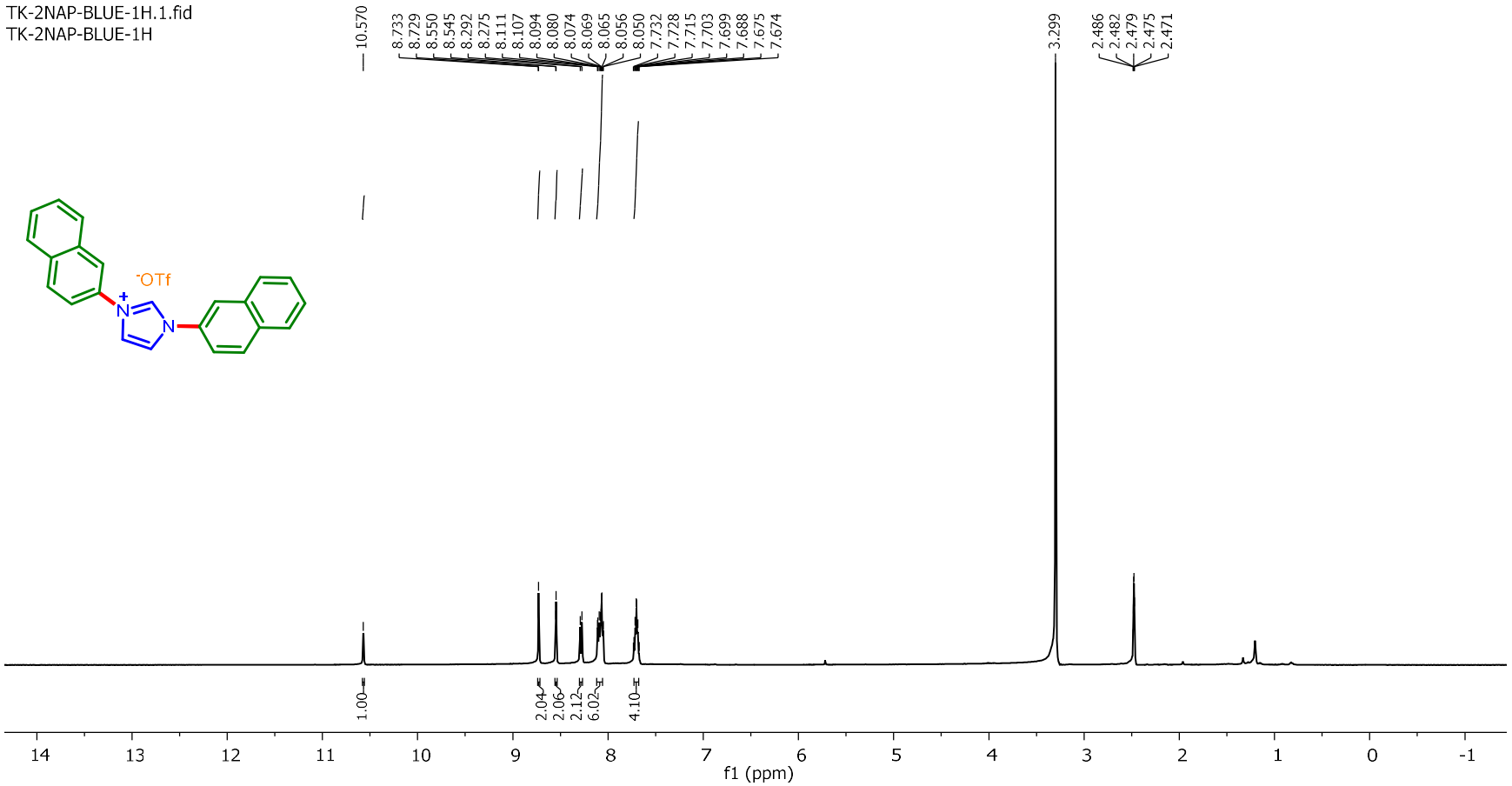
3-Phenyl-1-vinyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (10da): ^{1}H NMR (DMSO-d$_6$, 500 MHz)



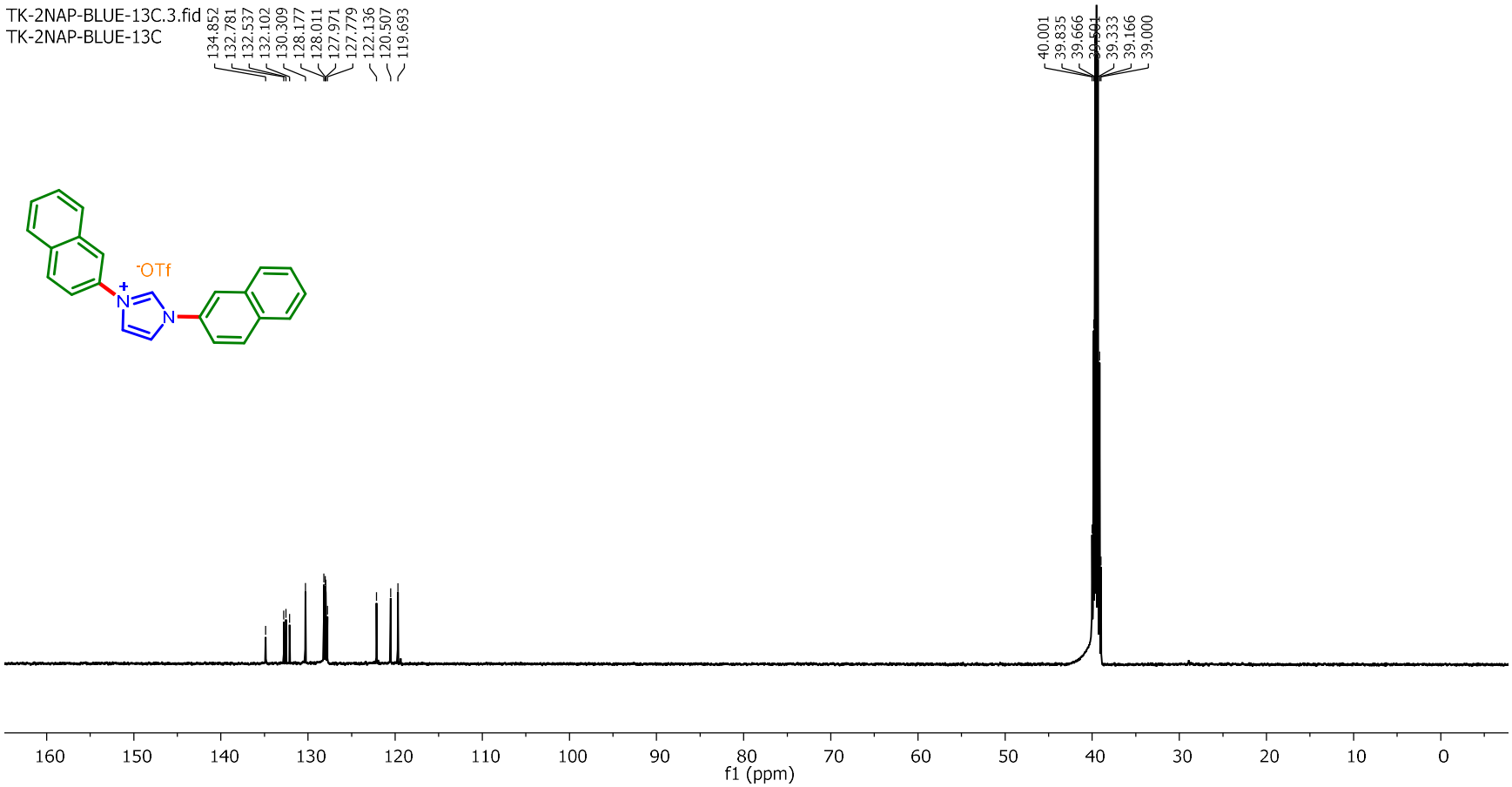
3-Phenyl-1-vinyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (10da): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 101 MHz)



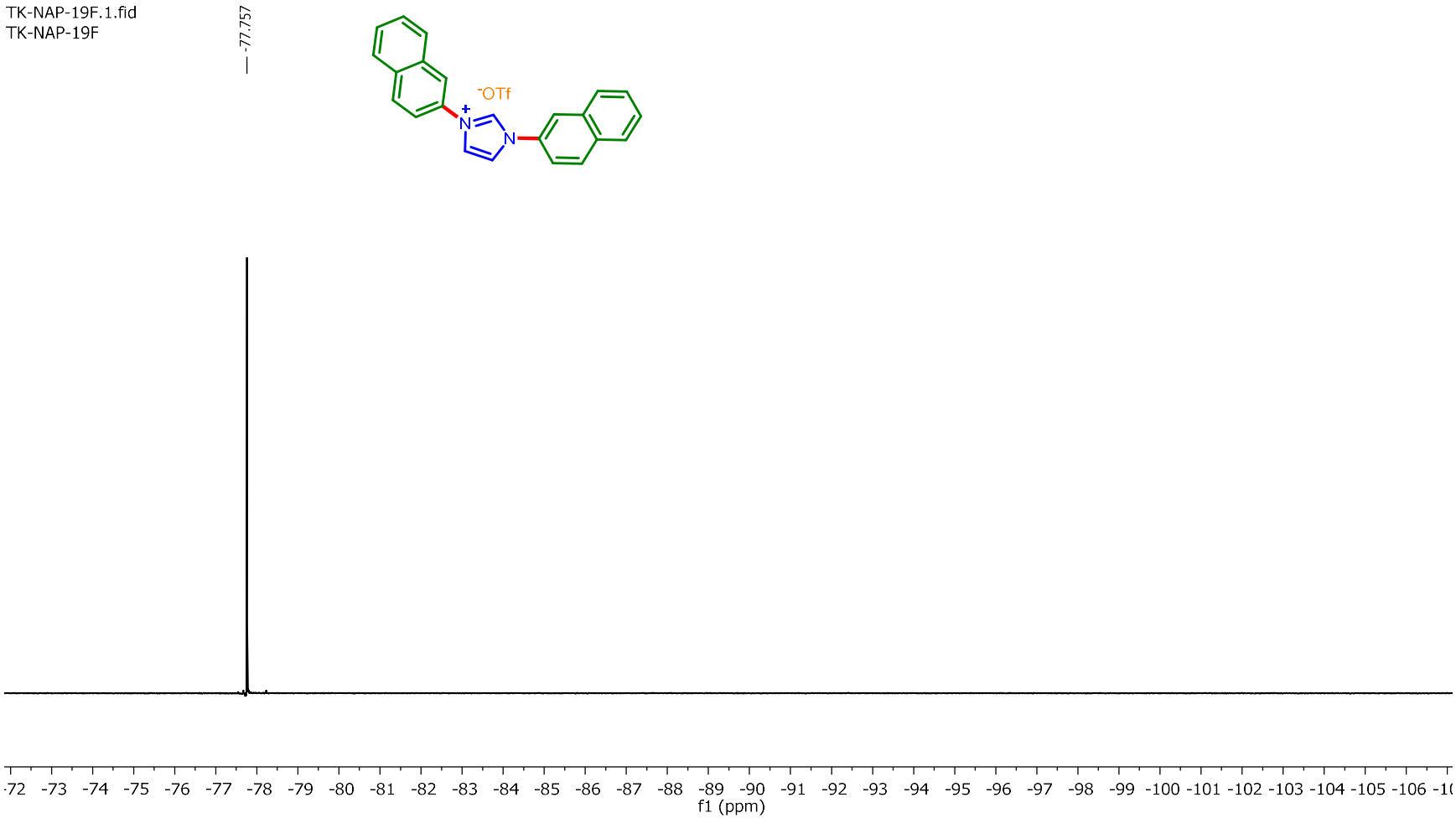
3-Phenyl-1-vinyl-1*H*-imidazol-3-ium trifluoromethanesulfonate (10da): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



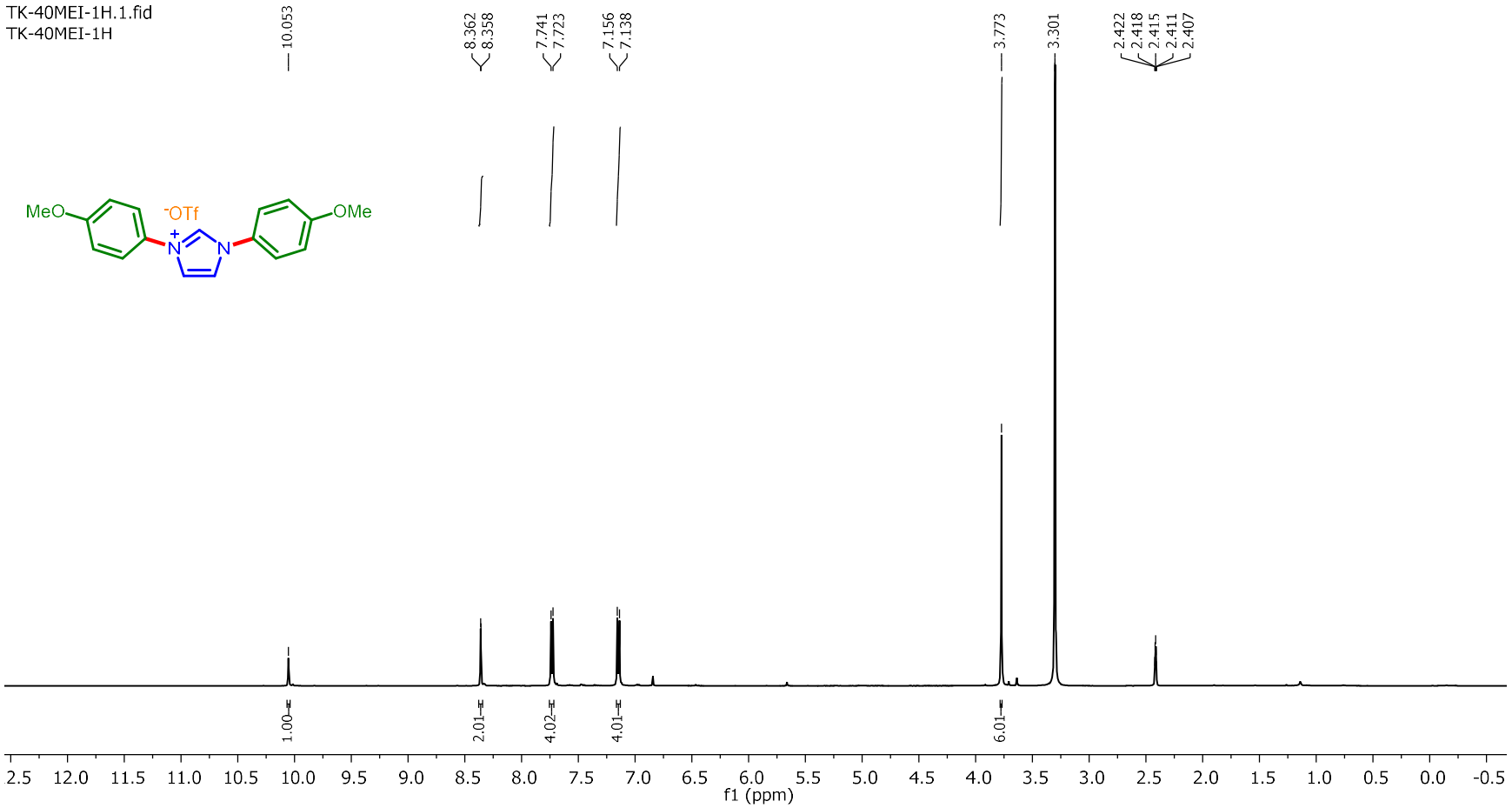
1,3-di(Naphthalen-2-yl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cj): ^{1}H NMR (DMSO-d$_6$, 500 MHz)



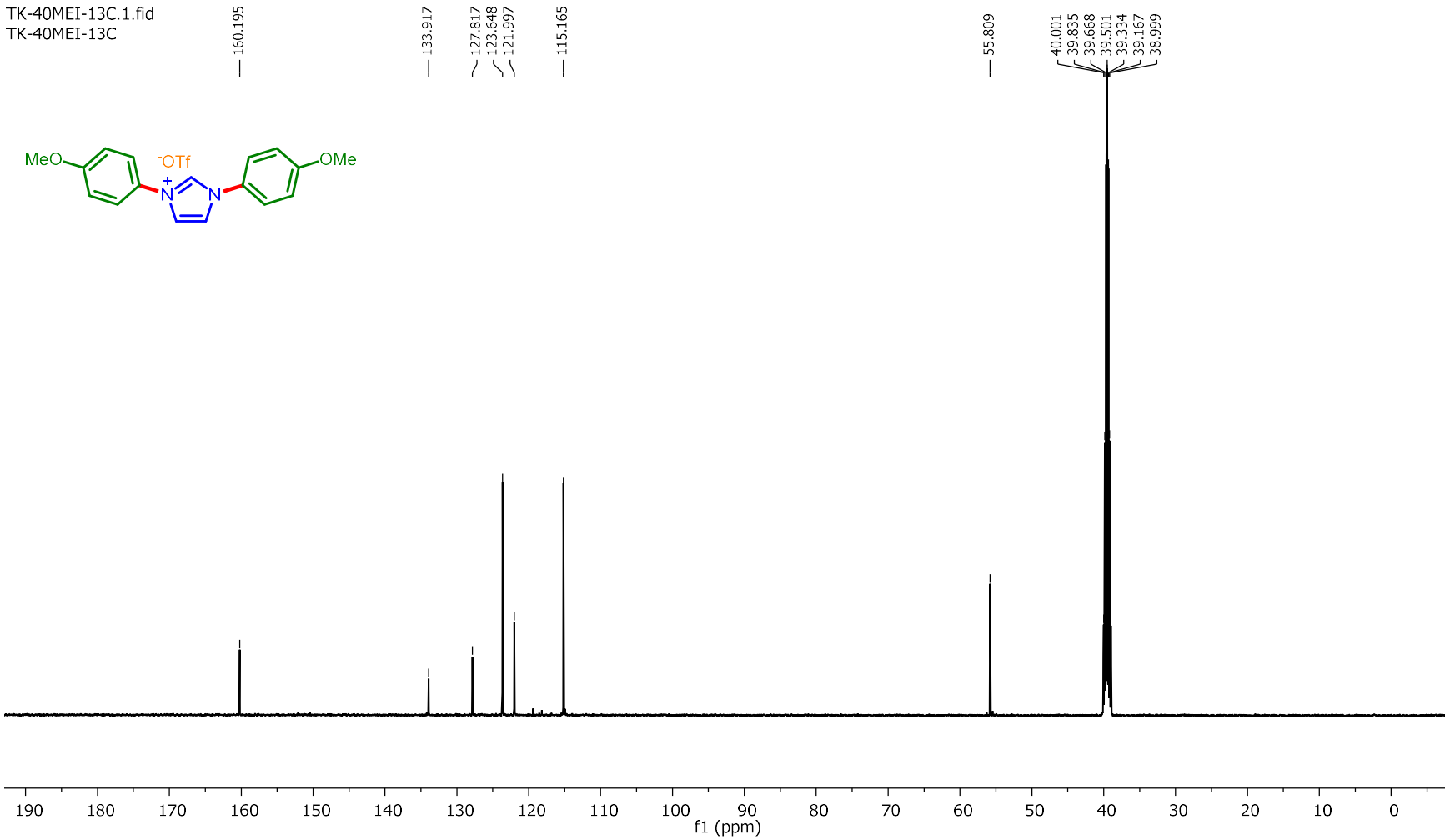
1,3-di(Naphthalen-2-yl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cj): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 126 MHz)



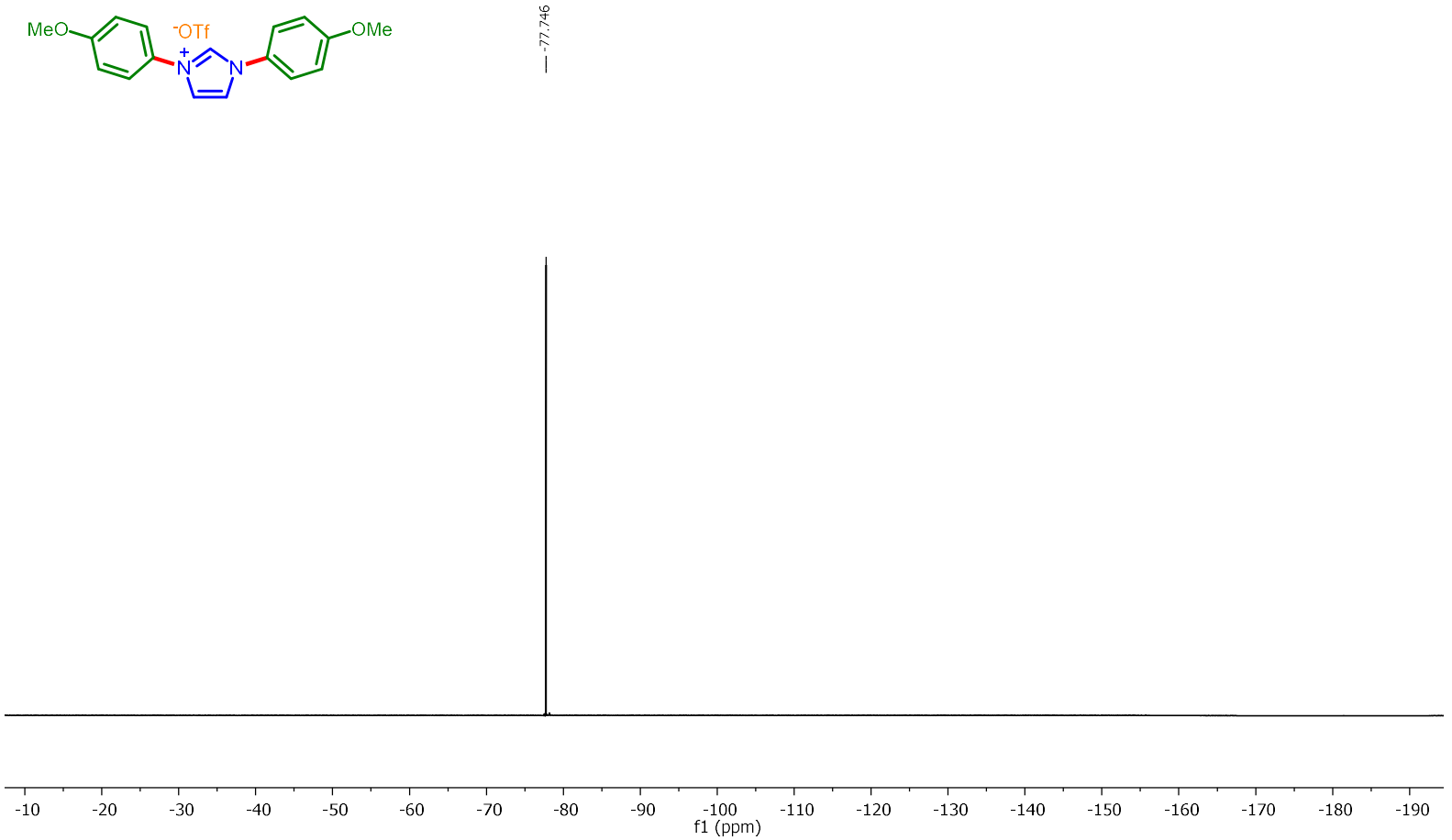
1,3-di(Naphthalen-2-yl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cj): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



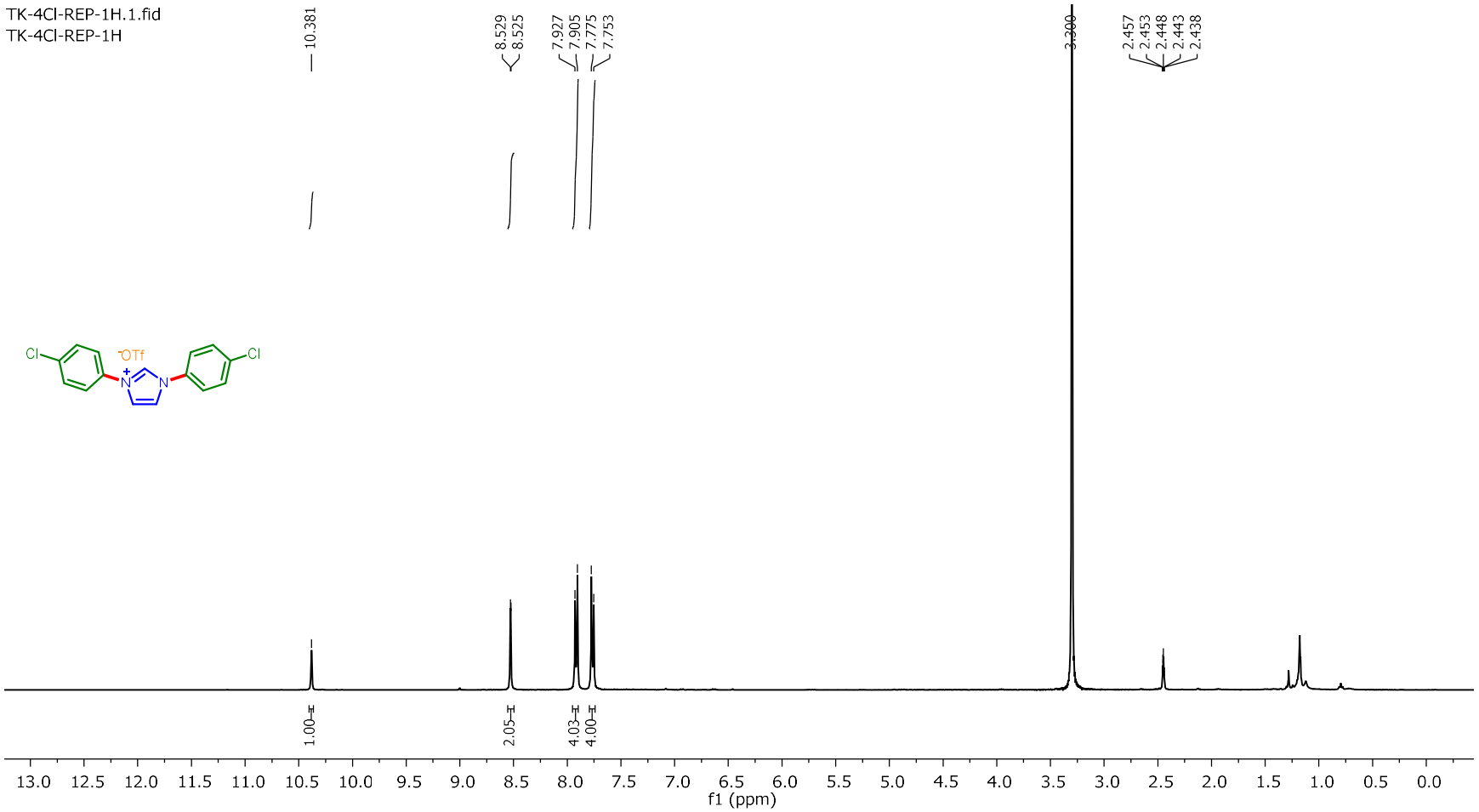
1,3-bis(4-Methoxyphenyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cb):^{1}H NMR (DMSO-d$_6$, 500 MHz)



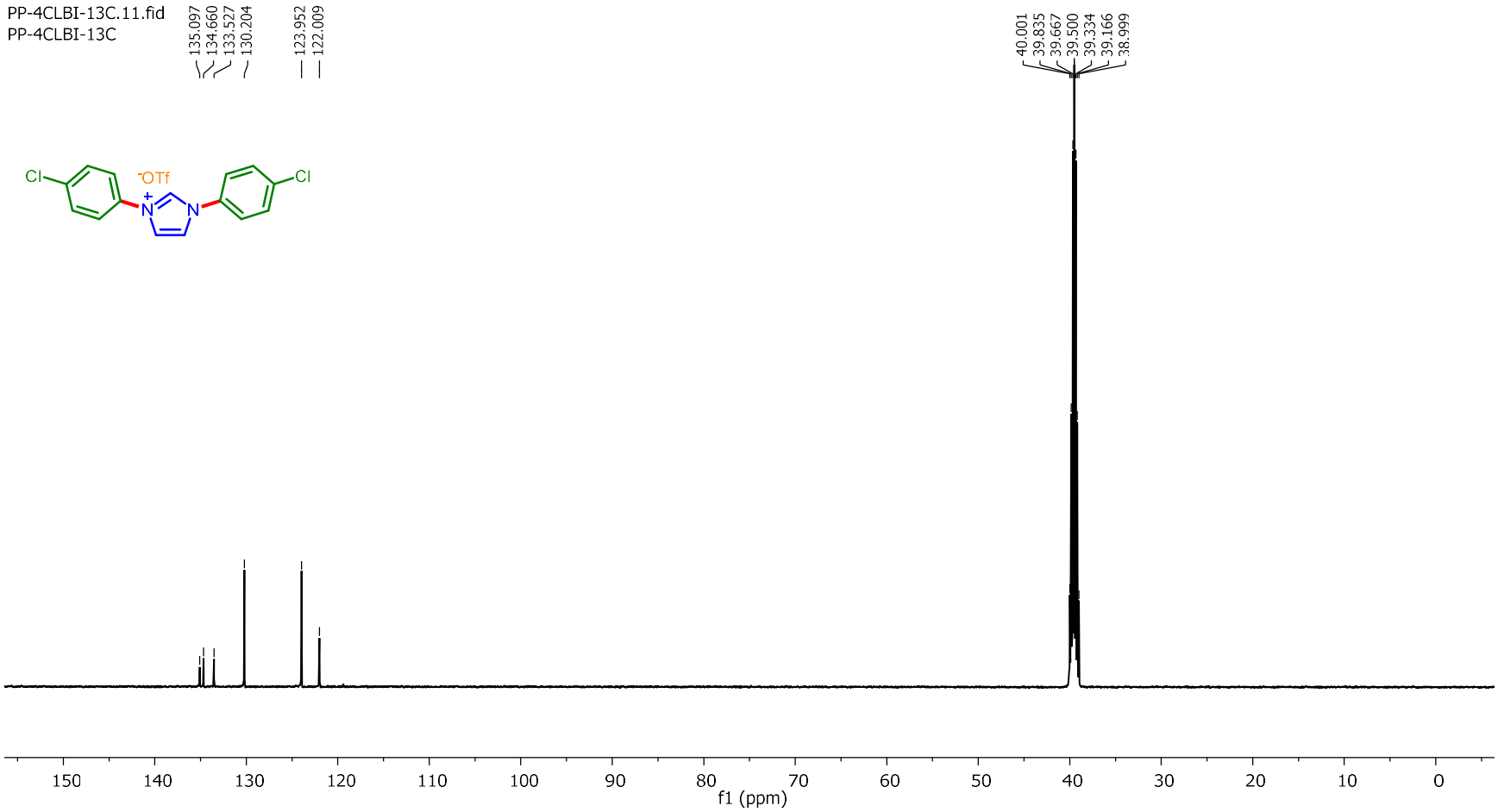
1,3-bis(4-Methoxyphenyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cb): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 126 MHz)



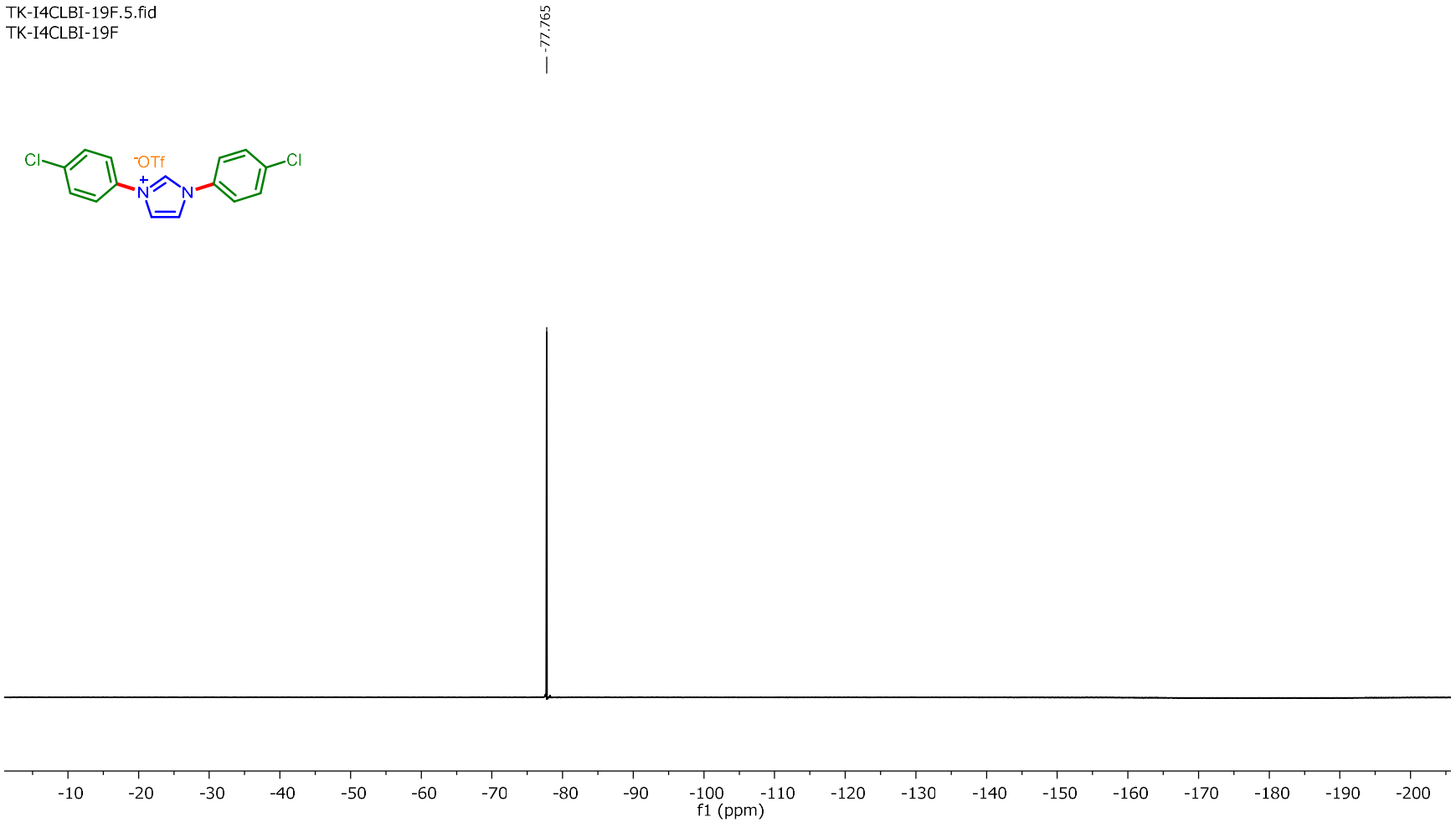
1,3-bis(4-Methoxyphenyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cb): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



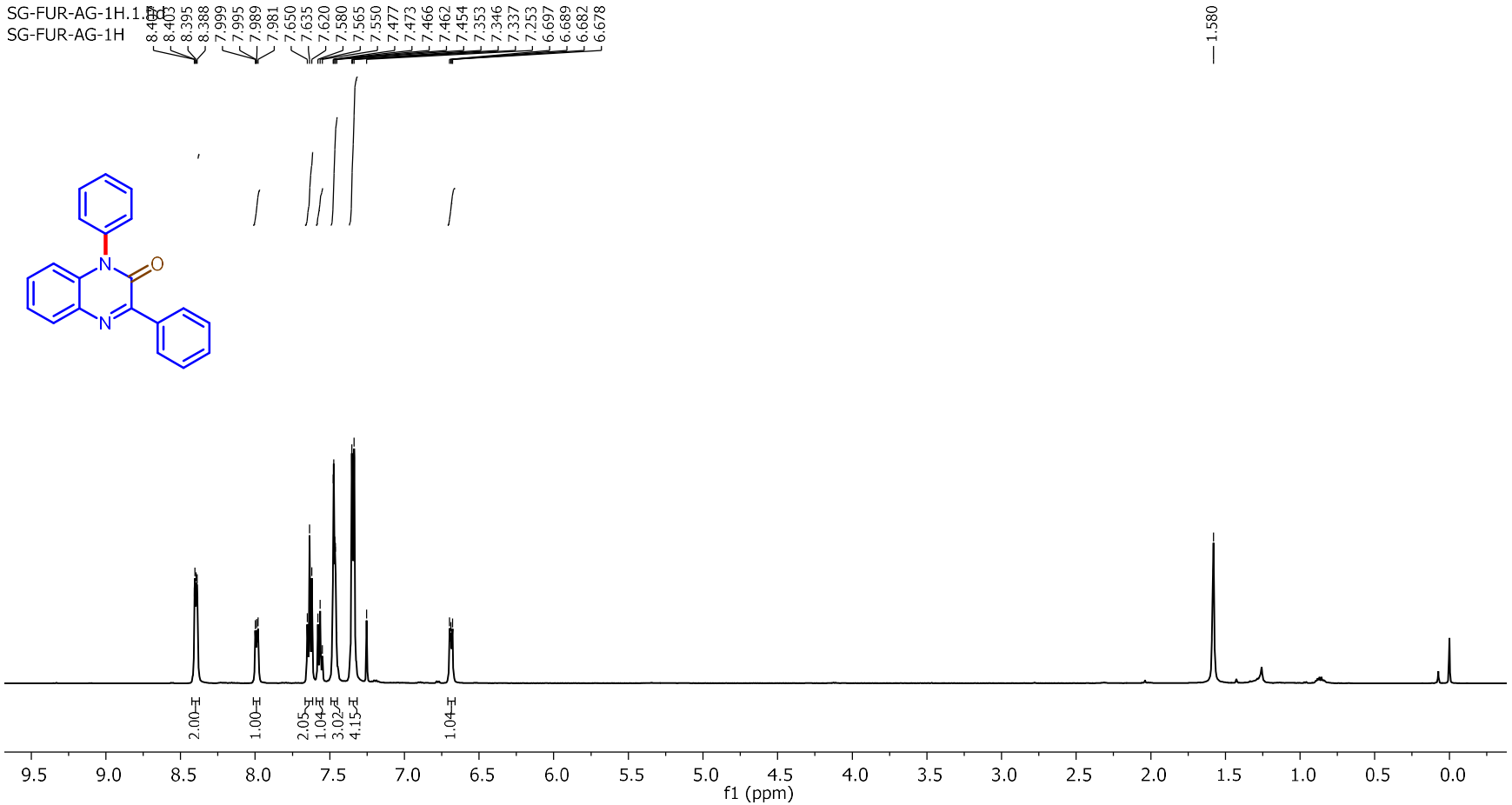
1,3-bis(4-Chlorophenyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cf): ^{1}H NMR (DMSO-d$_6$, 500 MHz)



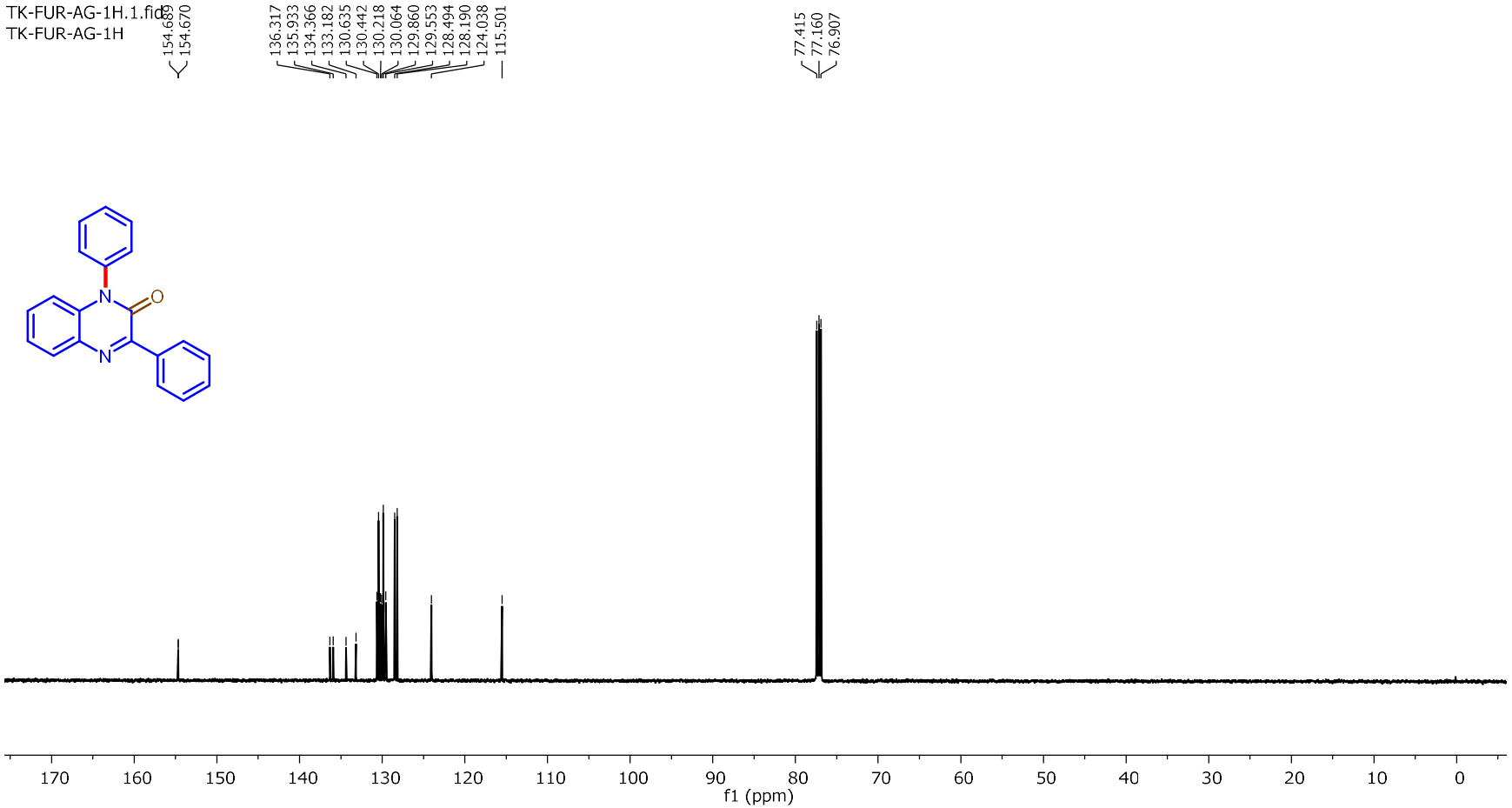
1,3-bis(4-Chlorophenyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cf): $^{13}C\{^{1}H\}$ NMR (DMSO-d_6, 126 MHz)



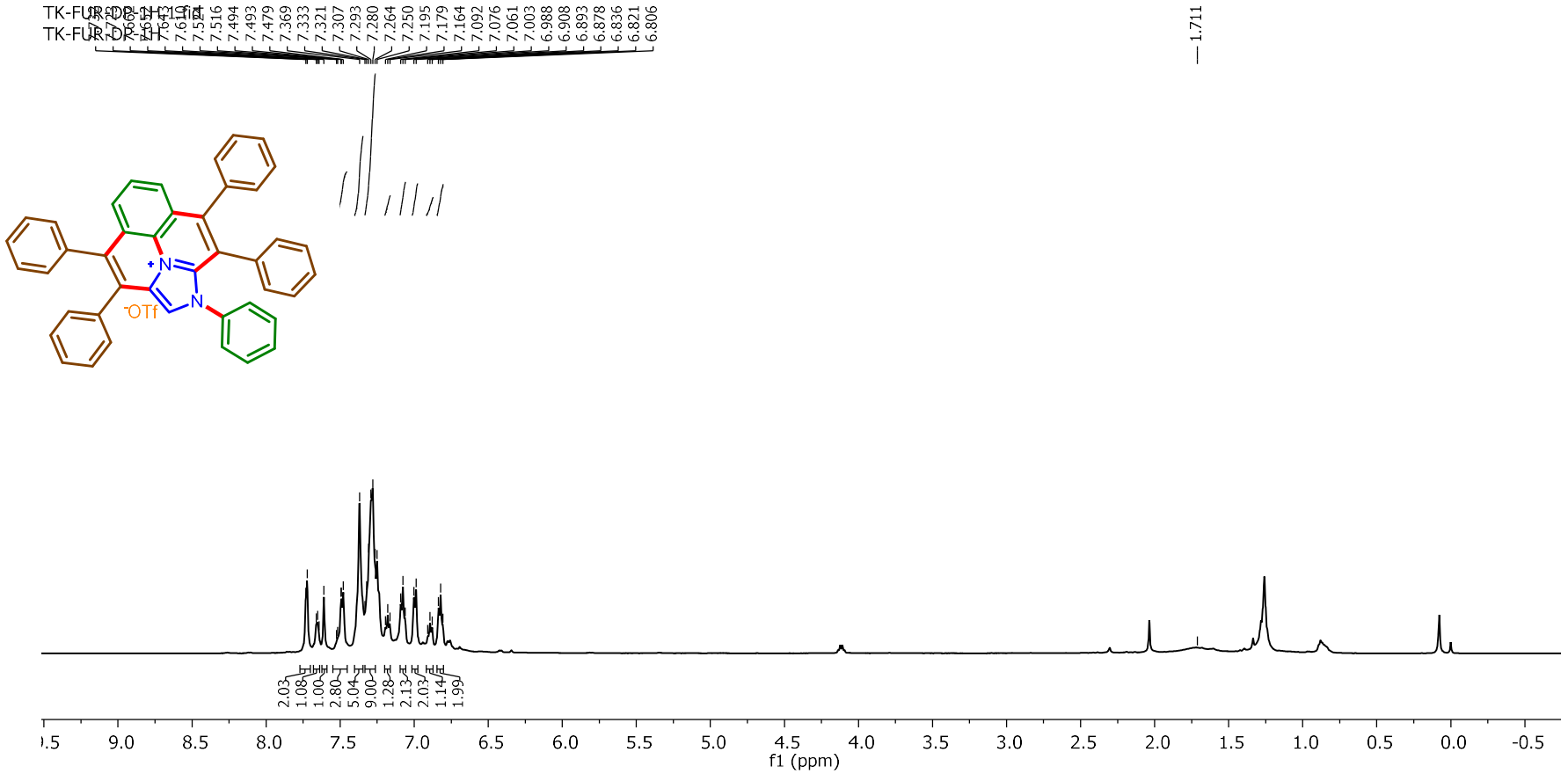
1,3-bis(4-Chlorophenyl)-1*H*-imidazol-3-ium trifluoromethanesulfonate (10cf): ^{19}F NMR (DMSO-d$_6$, 471 MHz)



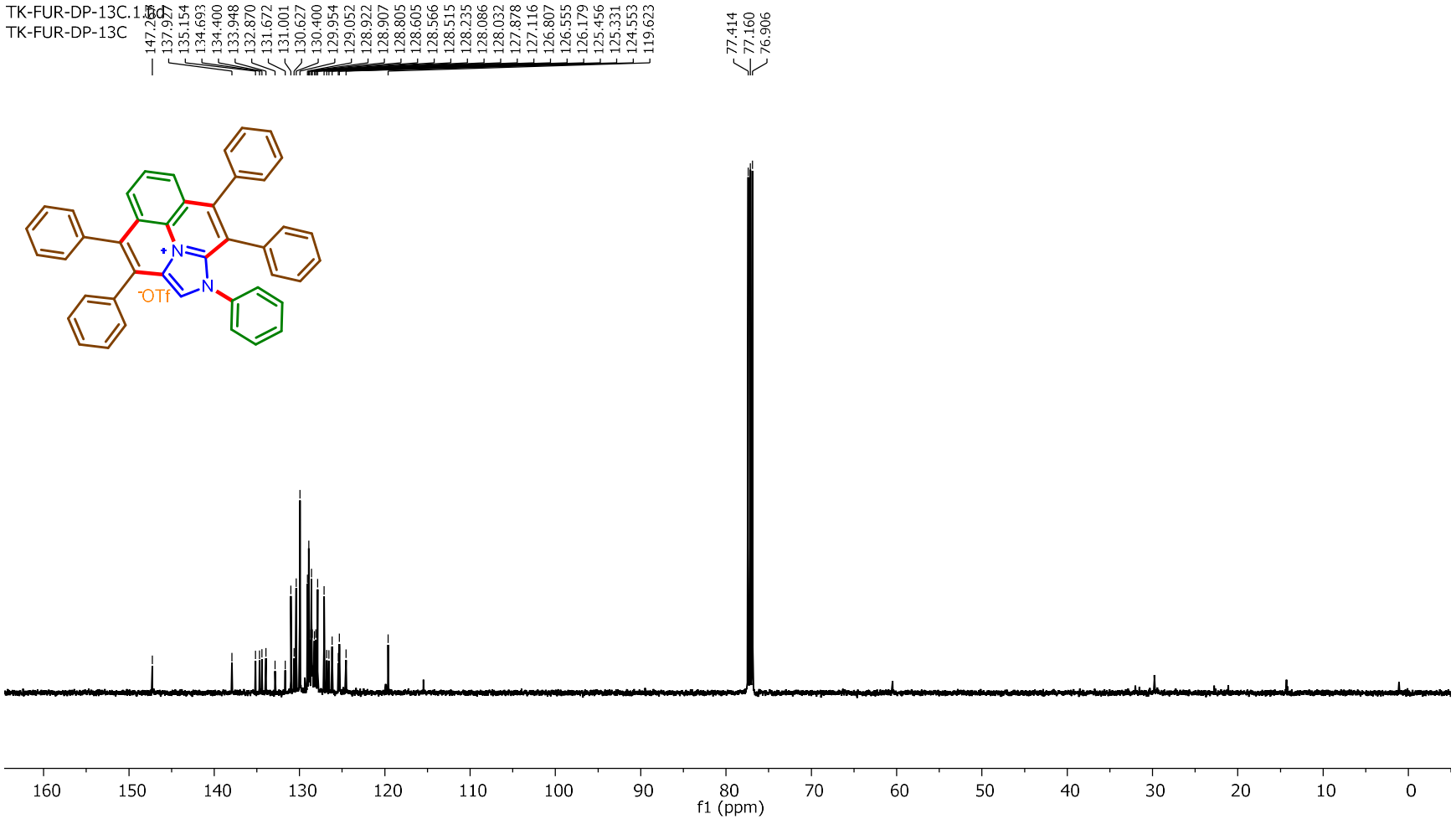
1,3-Diphenylquinoxalin-2(1*H*)-one (11): ^{1}H NMR ($CDCl_3$, 500 MHz)



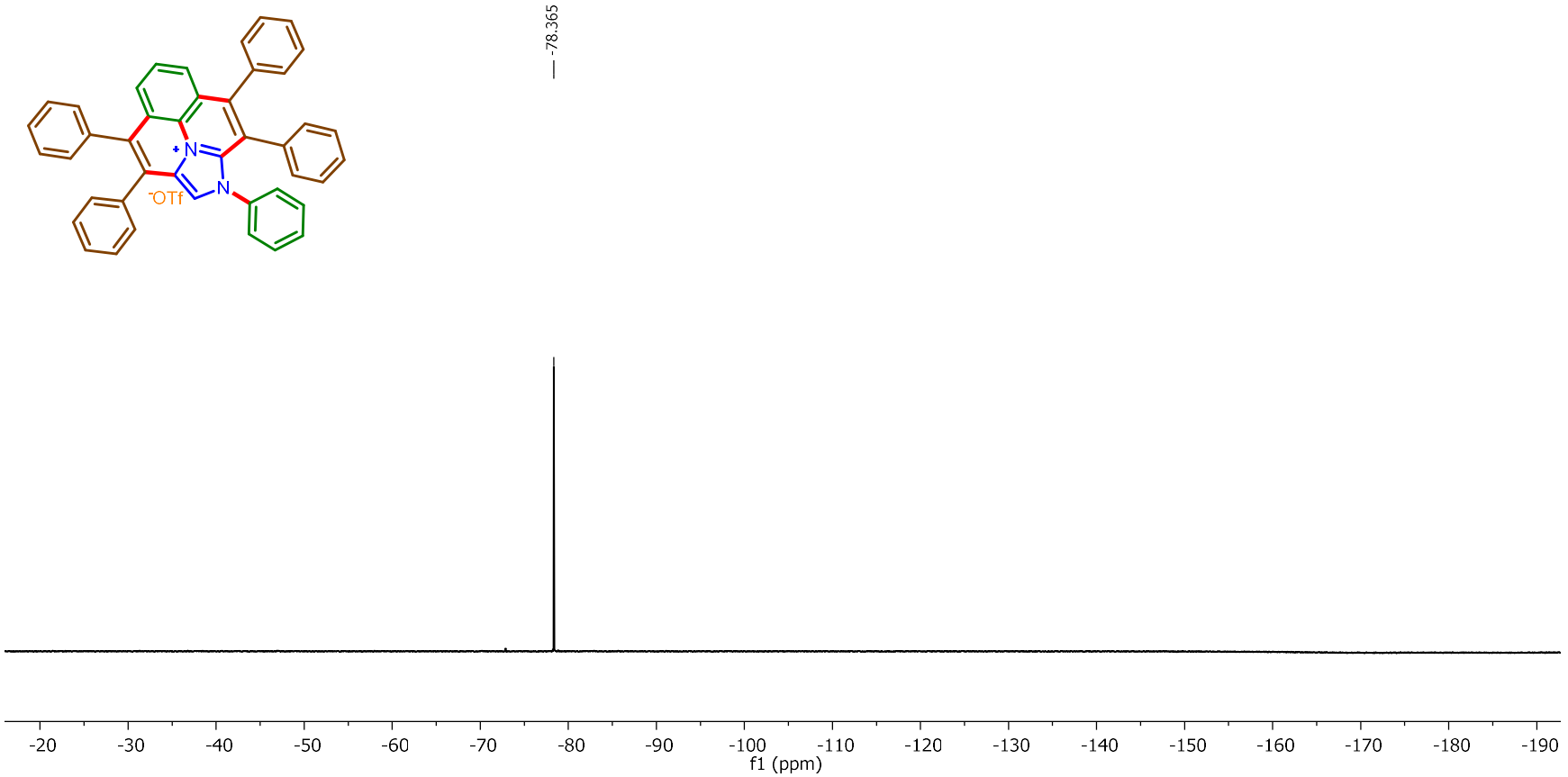
1,3-Diphenylquinoxalin-2(1*H*)-one (11): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



1,3,4,8,9-Pentaphenyl-1*H*-benzo[*ij*]imidazo[2,1,5-*de*]quinolizin-10-ium trifluoromethanesulfonate (12): ^{1}H NMR ($CDCl_3$, 500 MHz)



1,3,4,8,9-Pentaphenyl-1*H*-benzo[*ij*]imidazo[2,1,5-*de*]quinolizin-10-ium trifluoromethanesulfonate (12): $^{13}C\{^{1}H\}$ NMR ($CDCl_3$, 126 MHz)



1,3,4,8,9-Pentaphenyl-1*H*-benzo[*ij*]imidazo[2,1,5-*de*]quinolizin-10-ium trifluoromethanesulfonate (12): ^{19}F NMR ($CDCl_3$, MHz)