Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Transition-Metal-Free Hydroamination/Defluorination/Cyclization of Perfluoroalkyl Alkynes with Amidines

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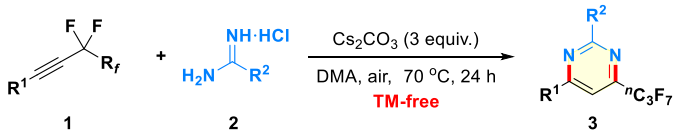
General information

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. All reactions were carried out under air atmosphere using undistilled solvent. Melting points were recorded on an Electrothermal digital melting point apparatus. IR spectra were recorded on a FT-IR spectrophotometer using KBr optics. ^{1}H, ^{19}F, and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker Avance or Joel 400 MHz spectrometers. The chemical shifts (δ) are reported in ppm and coupling constants (J) in Hz. High resolution mass spectra (HRMS) were obtained using a commercial apparatus (ESI Source). Column chromatography was generally performed on silica gel (300-400 mesh) and reactions were monitored by thin layer chromatography (TLC) using UV light to visualize the course of the reactions.

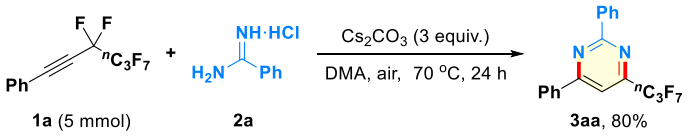
General procedure for the synthesis of perfluoroalkylated pyrimidines 3



1 2 3

A solution of perfluoroalkylethyne **1** (0.3 mmol), amidine hydrochloride **2** (0.36-0.45 mmol), and Cs_2CO_3 (293.2 mg, 0.9 mmol) in DMA (1.5 mL) was stirred at 70 °C under air for 24 h. The reaction was then quenched by saturated NH_4Cl solution (20 mL) and extracted with EtOAc (20 mL x 3). The organic layer was washed with saturated brine twice, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1 ~ 20/1) as eluent to afford the pure products **3**.

General procedure for the scale-up synthesis of product 3aa

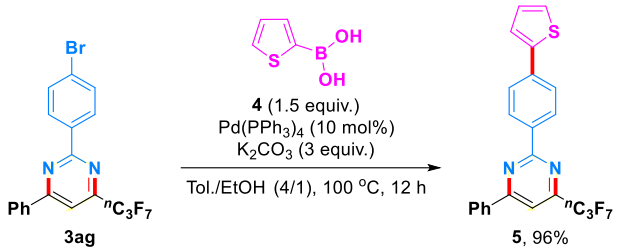


1a (5 mmol) **2a** **3aa**, 80%

A solution of (perfluorohex-1-yn-1-yl)benzene (1.60 g, 5 mmol, **1a**), benzamidine hydrochloride (0.94 g, 6 mmol, **2a**), and Cs_2CO_3 (4.89 g, 15 mmol) in DMA (30 mL) was stirred at 70 °C under air for 24 h. The reaction was then quenched by saturated NH_4Cl solution (100 mL) and extracted with EtOAc (100 mL x 3). The organic layer was washed with saturated brine twice, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1 ~ 20/1) as eluent to afford the pure product **3aa** (1.60 g, 80% yield).

Further transformation of products

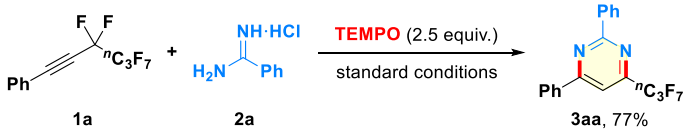
1) Cross-coupling reaction of product 3ag with thiophen-2-ylboronic acid 4



A solution of 2-(4-bromophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (95.8 mg, 0.2 mmol, **3ag**), thiophen-2-ylboronic acid (38.4 mg, 0.3 mmol, **4**), $Pd(PPh_3)_4$ (23.1 mg, 0.02 mmol), and K_2CO_3 (82.9 mg, 0.6 mmol) in toluene/EtOH (2 mL, 4/1) was stirred at 100 °C under N_2 for 12 h. The reaction was then quenched by saturated NH_4Cl solution (20 mL) and extracted with EtOAc (20 mL x 3). The organic layer was washed with saturated brine twice, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1 ~ 20/1) as eluent to afford the pure product **5** (92.9 mg, 96% yield).

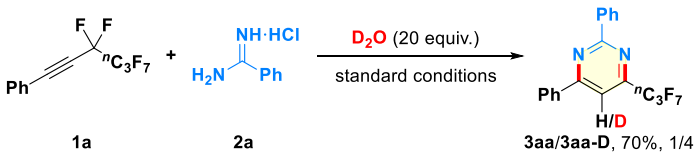
Mechanistic studies

1) Radical trapping experiment



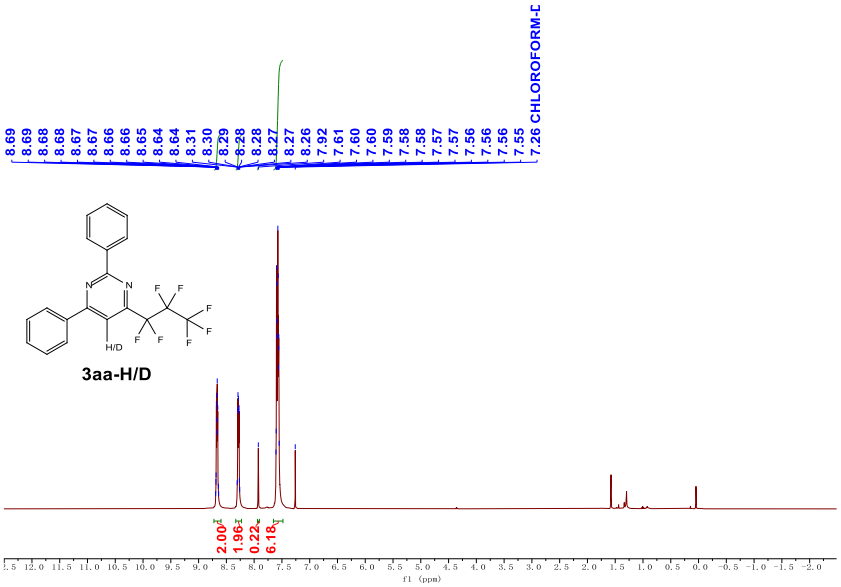
A solution of (perfluorohex-1-yn-1-yl)benzene (96.1 mg, 0.3 mmol, **1a**), benzamidine hydrochloride (56.4 mg, 0.36 mmol, **2a**), Cs_2CO_3 (293.2 mg, 0.9 mmol), and 2,2,6,6-tetramethylpiperidinooxy (117.2 mg, 0.75 mmol, TEMPO) in DMA (1.5 mL) was stirred at 70 °C under air for 24 h. The reaction was then quenched by saturated NH_4Cl solution (20 mL) and extracted with EtOAc (20 mL x 3). The organic layer was washed with saturated brine twice, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1 ~ 20/1) as eluent to afford the pure product **3aa** (92.6 mg, 77% yield). **This result suggested that radical intermediate was not involved in the reaction.**

2) D-labeling experiment

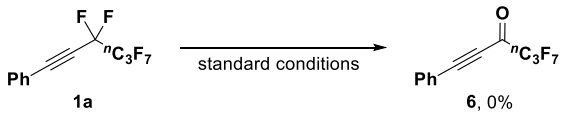


A solution of (perfluorohex-1-yn-1-yl)benzene (96.1 mg, 0.3 mmol, **1a**), benzamidine hydrochloride (56.4 mg, 0.36 mmol, **2a**), Cs_2CO_3 (293.2 mg, 0.9 mmol), and D_2O (108.0 mg, 6 mmol) in DMA (1.5 mL) was stirred at 70 °C under air for 24 h. The reaction was then quenched by saturated NH_4Cl solution (20 mL) and extracted with EtOAc (20 mL x 3). The organic layer was washed with saturated brine twice, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1 ~ 20/1) as eluent to afford the pure products **3aa**

and **3aa-D** (84.4 mg, 70% yield, **3aa**/ **3aa-D** = **1**/**4**). **This result suggested that water was the H atom source in the reaction.**

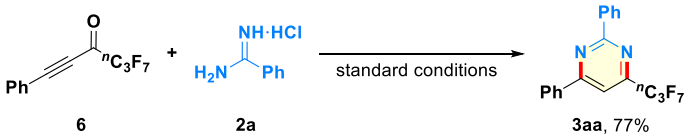


3) Hydrolysis of substrate 1a



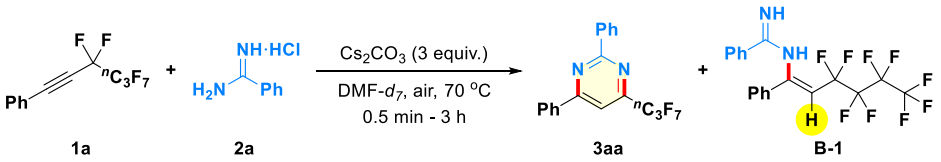
A solution of (perfluorohex-1-yn-1-yl)benzene (96.1 mg, 0.3 mmol, **1a**), and Cs_2CO_3 (293.2 mg, 0.9 mmol) in DMA (1.5 mL) was stirred at 70 °C under air for 24 h. No desired product **6** was observed. **This result suggested that defluorination step occurred after the intermolecular interaction of 1a and 2a during the reaction.**

4) Annulation of fluoroalkylated ynone 6 with amidine 2a

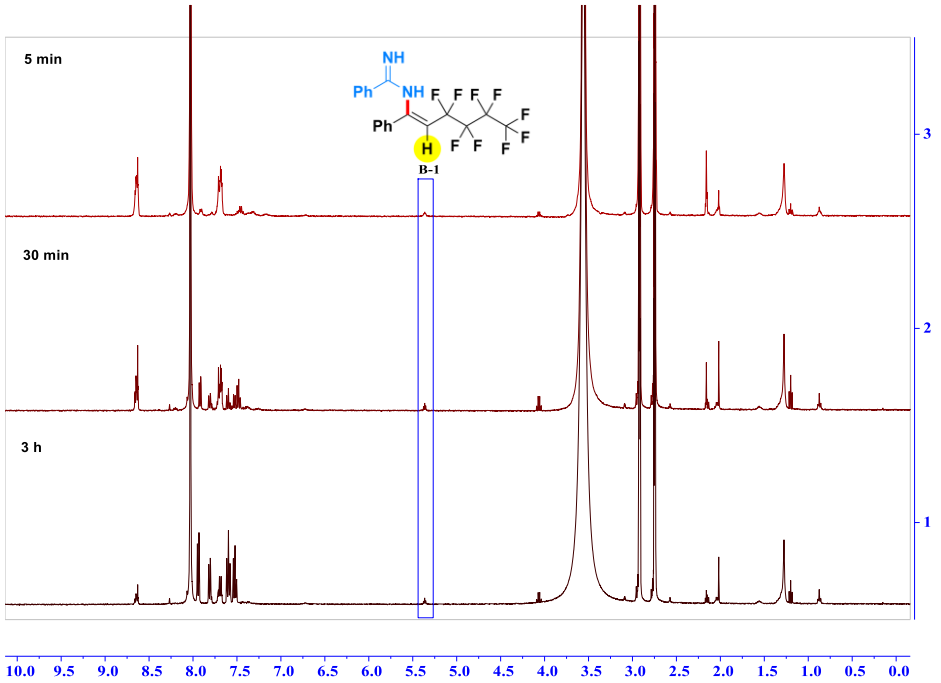


A solution of 4,4,5,5,6,6,6-heptafluoro-1-phenylhex-1-yn-3-one (89.4 mg, 0.3 mmol, **6**), and Cs_2CO_3 (293.2 mg, 0.9 mmol) in DMA (1.5 mL) was stirred at 70 °C under air for 24 h. The reaction was then quenched by saturated NH_4Cl solution (20 mL) and extracted with EtOAc (20 mL x 3). The organic layer was washed with saturated brine twice, dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude product was purified by flash column chromatography (300-400 mesh) using petroleum ether/ethyl acetate (100/1 ~ 20/1) as eluent to afford the pure product **3aa** (92.6 mg, 77% yield). **This result suggested that fluoroalkylated ynone 6 was not the reaction intermediate.**

5) ^{1}H NMR and HRMS analysis of the reaction mixture



A solution of (perfluorohex-1-yn-1-yl)benzene (96.1 mg, 0.3 mmol, **1a**), benzamidine hydrochloride (56.4 mg, 0.36 mmol, **2a**), and Cs_2CO_3 (293.2 mg, 0.9 mmol) in DMF-d_7 (1.5 mL) was stirred at 70 °C under air for 5 min, 0.5 h, or 3 h. The reaction mixture was analyzed by *in situ* ^{1}H NMR spectra. **The occurrence of ^{1}H NMR peak at 5.3 ppm indicated the involvement of hydroaminated intermediate B-1 (*Org. Lett.*, 2016, 18, 1422-1425).**

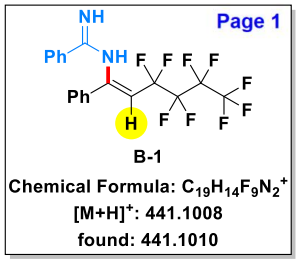


Proposed intermediate B-1 could also be detected by High Resolution Mass Spectrometry (HRMS), suggesting that intermediate B-1 might be involved in the reaction.

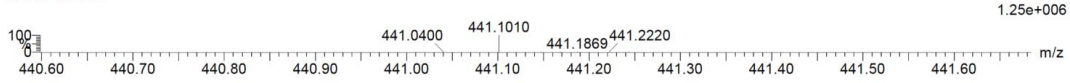
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 15-20 H: 12-15 N: 0-2 F: 5-10
2044-1 211 (1.585)
1: TOF MS ES+

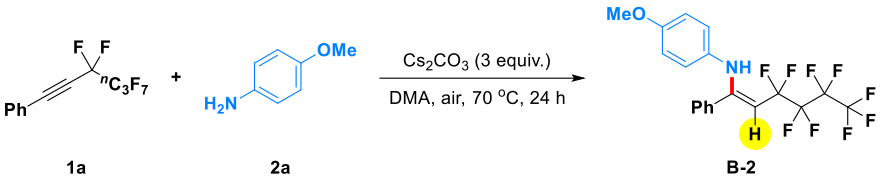


1.25e+006



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
441.1010	441.1013	-0.3	-0.7	9.5	111.1	n/a	n/a	C19 H14 N2 F9

6) The reaction of (perfluorohex-1-yn-1-yl)benzene (1a) with 4-methoxyaniline



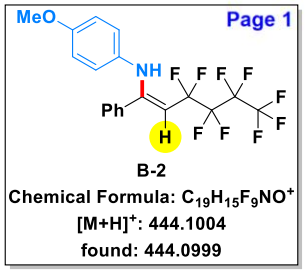
A solution of (perfluorohex-1-yn-1-yl)benzene (96.1 mg, 0.3 mmol, **1a**), 4-methoxyaniline (44.3 mg, 0.36 mmol), and Cs_2CO_3 (293.2 mg, 0.9 mmol) in DMA (1.5 mL) was stirred at 70 °C under air for 24 h. **No desired hydroaminated intermediate B-2 was obtained.**

However, proposed intermediate B-2 could be detected by High Resolution Mass Spectrometry (HRMS), suggesting that intermediate B-2 might be involved in the reaction.

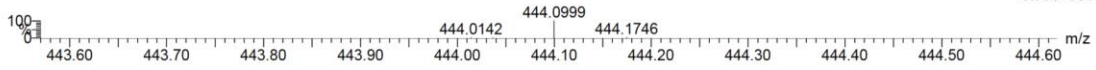
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
39 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 19-20 H: 14-16 N: 0-2 O: 0-2 F: 9-9 Na: 0-1 Si: 0-2
2044-2 332 (2.482)
1: TOF MS ES+



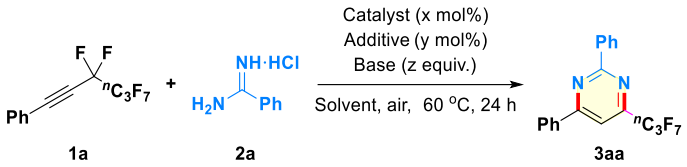
9.73e+004



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
444.0999	444.1010	-1.1	-2.5	8.5	51.6	n/a	n/a	C19 H15 N O F9

Optimization of reaction conditions

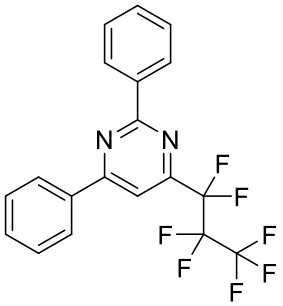
Table S1. Optimization of reaction conditions[a]



Entry	Catalyst (x mol%)	Additive (y mol%)	Base (z equiv.)	Solvent	Yield (%)[b]
1	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	--	THF	0
2	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	K_2CO_3 (3)	THF	33
3	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	Cs_2CO_3 (3)	THF	61
4	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	K_3PO_4 (3)	THF	43
5	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	K_2CO_3 (3)	THF	42
6	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	KO^tBu (3)	THF	43
7	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	NEt_3 (3)	THF	trace
8	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	DBU (3)	THF	trace
9	$Cu(OTf)_2$ (10)	$PMPNH_2$ (20)	DABCO (3)	THF	6
10	$Cu(OTf)_2$ (10)	--	Cs_2CO_3 (3)	THF	53
11	--	$PMPNH_2$ (20)	Cs_2CO_3 (3)	THF	62
12	--	--	Cs_2CO_3 (3)	THF	60
13	--	--	Cs_2CO_3 (4)	THF	43
14	--	--	Cs_2CO_3 (3)	THF	47[c]
15	--	--	Cs_2CO_3 (3)	THF	63[d]
16	--	--	Cs_2CO_3 (3)	MeCN	37[d]
17	--	--	Cs_2CO_3 (3)	DMF	67[d]
18	--	--	Cs_2CO_3 (3)	DMSO	50[d]
19	--	--	Cs_2CO_3 (3)	^{t}BuOH	37[d]
20	--	--	Cs_2CO_3 (3)	DCE	33[d]
21	--	--	Cs_2CO_3 (3)	H_2O	0[d,e]
22	--	--	Cs_2CO_3 (3)	toluene	58[d]
23	--	--	Cs_2CO_3 (3)	DMF	37[d,f]
24	--	--	Cs_2CO_3 (3)	DMF	54[d,g]
25	--	--	Cs_2CO_3 (3)	DMF	74[d,h] (73)[i]
26	--	--	Cs_2CO_3 (3)	DMF	70[d,j]
27	--	--	Cs_2CO_3 (3)	DMF	63[d,k]
28	--	--	Cs_2CO_3 (3)	DMF	65[d,e]
29	--	--	Cs_2CO_3 (3)	NMP	76[d,h]
30	--	--	Cs_2CO_3 (3)	DMA	79[d,h] (77)[i]
31	--	--	Cs_2CO_3 (2)	DMA	74[d,h,e]
32	--	--	Cs_2CO_3 (3)	DMA	74[d,h,l] (72)[i]

[a] Reaction conditions: **1a** (0.3 mmol), **2a** (0.3 mmol), catalyst (0.03 mmol), additive (0.06 mmol), and base (0.9-1.2 mmol) in solvent (1.5 mL) at 60 °C under air for 24 h. [b] Yields were determined by NMR analysis with 1,4-dimethoxybenzene (0.25 mmol) as an internal standard. [c] **1a** (0.36 mmol). [d] **2a** (0.36 mmol). [e] At 100 °C. [f] At room temperature. [g] At 40 °C. [h] At 70 °C. [i] Isolated yield. [j] At 80 °C. [k] At 90 °C. [l] 6 h.

Characterization data for products



4-(Perfluoropropyl)-2,6-diphenylpyrimidine (3aa):

Yield = 77% (91.9 mg). White solid. M.p. 59.6–60.2 °C.

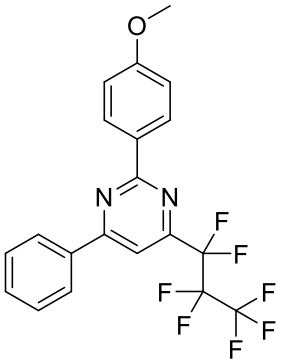
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.73-8.68 (m, 2H), 8.30-8.27 (m, 2H), 7.93 (s, 1H), 7.61-7.55 (m, 6H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.95 (s, 3F), -116.53 (s, 2F), -126.05 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 165.1, 156.8 (t, $J_{C\text{-}F}$ = 26.0 Hz), 136.5, 135.9, 131.9, 131.6, 129.1, 128.7, 128.7, 127.5, 111.6 (t, $J_{C\text{-}F}$ = 4.6 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{12}F_7N_2$ $[M+H]^+$ 401.0883, found: 401.0889.



2-(4-Methoxyphenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3ab):

Yield = 72% (92.9 mg). White solid. M.p. 87.2–88.3 °C.

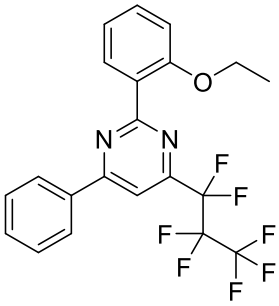
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.63-8.58 (m, 2H), 8.30-8.23 (m, 2H), 7.84 (s, 1H), 7.59-7.54 (m, 3H), 7.07-7.02 (m, 2H), 3.90 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.97 (s, 3F), -116.59 (s, 2F), -126.10 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.0, 164.8, 162.5, 156.6 (t, $J_{C\text{-}F}$ = 26.0 Hz), 136.0, 131.7, 130.0, 129.2, 129.0, 127.4, 113.9, 110.7 (t, $J_{C\text{-}F}$ = 4.4 Hz), 55.3 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{14}F_7N_2O$ $[M+H]^+$ 431.0989, found: 431.0994.



2-(2-Ethoxyphenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3ac):

Yield = 61% (81.2 mg). Yellow oil.

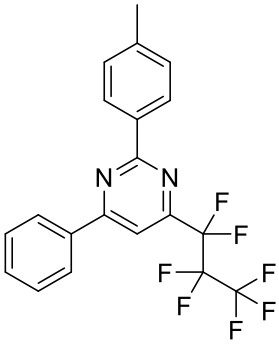
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.30-8.23 (m, 2H), 8.01-7.96 (m, 1H), 7.94 (d, J = 1.5 Hz, 1H), 7.59-7.52 (m, 3H), 7.51-7.43 (m, 1H), 7.15-7.05 (m, 2H), 4.17 (q, J = 7.0 Hz, 2H), 1.44 (td, J = 6.9, 1.4 Hz, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.00 (s, 3F), -116.47 (s, 2F), -125.86 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 165.9, 157.9, 156.2 (t, $J_{C\text{-}F}$ = 26.0 Hz), 136.0, 132.2, 131.7, 131.7, 129.0, 127.5, 127.4, 120.6, 113.5, 111.2 (t, $J_{C\text{-}F}$ = 5.0 Hz), 64.5, 14.7 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{21}H_{16}F_7N_2O$ $[M+H]^+$ 445.1145, found: 445.1151.



4-(Perfluoropropyl)-6-phenyl-2-(*p*-tolyl)pyrimidine (3ad):

Yield = 84% (104.2 mg). White solid. M.p. 101.2–101.9 °C.

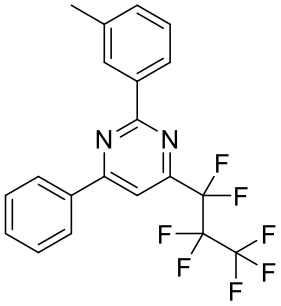
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 100/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56 (d, J = 8.2 Hz, 2H), 8.30-8.26 (m, 2H), 7.89 (s, 1H), 7.60-7.57 (m, 3H), 7.36 (d, J = 8.1 Hz, 2H), 2.47 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.95 (s, 3F), -116.53 (s, 2F), -126.07 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.1, 165.1, 156.7 (t, $J_{C\text{-}F}$ = 25.5 Hz), 142.0, 136.0, 133.9, 131.8, 129.4, 129.1, 128.7, 127.4, 111.2 (t, $J_{C\text{-}F}$ = 4.4 Hz), 21.5 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{14}F_7N_2$ $[M+H]^+$ 415.1040, found: 415.1045.



4-(Perfluoropropyl)-6-phenyl-2-(*m*-tolyl)pyrimidine (3ae):

Yield = 74% (92.1 mg). Colourless oil.

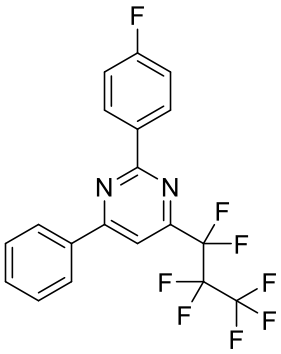
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 100/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.50-8.44 (m, 2H), 8.32-8.25 (m, 2H), 7.91 (s, 1H), 7.63-7.56 (m, 3H), 7.49-7.42 (m, 1H), 7.41-7.36 (m, 1H), 2.52 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.95 (t, J = 9.1 Hz, 3F), -116.53 (q, J = 9.1 Hz, 2F), -126.03 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.7, 165.2, 156.7 (t, $J_{C\text{-}F}$ = 26.0 Hz), 138.3, 136.5, 136.0, 132.4, 131.8, 129.2, 129.1, 128.6, 127.5, 126.0, 111.73 (t, $J_{C\text{-}F}$ = 4.3 Hz), 21.5 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{14}F_7N_2$ $[M+H]^+$ 415.1040, found: 415.1037.



2-(4-Fluorophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3af):

Yield = 84% (105.7 mg). White solid. M.p. 77.3–78.2 °C.

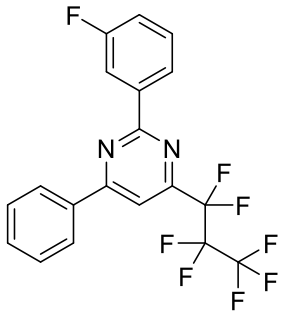
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.66-8.59 (m, 2H), 8.28-8.21 (m, 2H), 7.89 (s, 1H), 7.61-7.53 (m, 3H), 7.24-7.17 (m, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.99 (s, 3F), -108.58 (s, 1F), -116.60 (s, 2F), -126.08 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4 (d, $J_{C\text{-}F}$ = 17.3 Hz), 164.0 (d, $J_{C\text{-}F}$ = 14.6 Hz), 156.8 (t, $J_{C\text{-}F}$ = 24.8 Hz), 135.8, 132.7 (d, $J_{C\text{-}F}$ = 3.2 Hz), 132.0, 131.0, 130.9, 129.2, 127.5, 115.8, 111.5 (m) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{11}F_8N_2$ $[M+H]^+$ 419.0789, found: 419.0794.



2-(3-Fluorophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3ag):

Yield = 66% (82.6 mg). White solid. M.p. 71.3–71.8 °C.

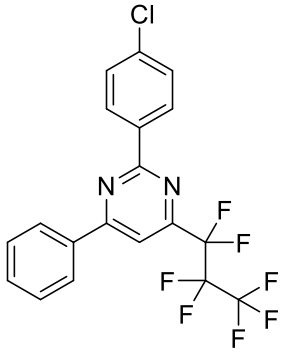
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.46-8.40 (m, 1H), 8.35-8.29 (m, 1H), 8.29-8.24 (m, 2H), 7.94 (s, 1H), 7.63-7.55 (m, 3H), 7.54-7.46 (m, 1H), 7.29-7.21 (m, 1H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.96 (t, J = 9.4 Hz, 3F), -112.67 (td, J = 9.0, 5.5 Hz, 1F), -116.54 (q, J = 9.0 Hz, 2F), -126.05 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 163.9 (d, $J_{C\text{-}F}$ = 3.3 Hz), 163.2 (d, $J_{C\text{-}F}$ = 243.5 Hz), 156.9 (t, $J_{C\text{-}F}$ = 26.3 Hz), 138.8 (d, $J_{C\text{-}F}$ = 7.7 Hz), 135.6, 132.0, 130.2 (d, $J_{C\text{-}F}$ = 7.7 Hz), 129.2, 127.5, 124.4 (d, $J_{C\text{-}F}$ = 2.9 Hz), 118.5 (d, $J_{C\text{-}F}$ = 21.2 Hz), 115.5 (d, $J_{C\text{-}F}$ = 23.6 Hz), 112.0 (t, $J_{C\text{-}F}$ = 4.6 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{11}F_8N_2$ $[M+H]^+$ 419.0789, found: 419.0788.



2-(4-Chlorophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3ah):

Yield = 69% (89.5 mg). White solid. M.p. 84.3–85.2 °C.

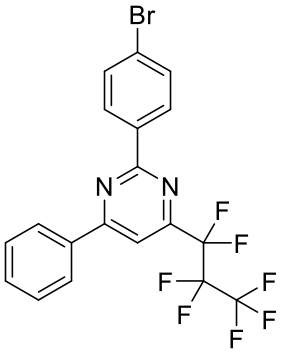
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.58-8.52 (m, 2H), 8.24 (dd, J = 7.6, 2.0 Hz, 2H), 7.90 (s, 1H), 7.61- 7.54 (m, 3H), 7.51-7.45 (m, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.96 (s, 3F), -116.54 (s, 2F), -126.06 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 164.1, 156.8 (t, $J_{C\text{-}F}$ = 25.8 Hz), 137.9, 135.7, 135.0, 132.0, 130.0, 129.2, 128.9, 127.5, 111.8 (t, $J_{C\text{-}F}$ = 4.5 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{11}ClF_7N_2$ $[M+H]^+$ 435.0493, found: 435.0499.



2-(4-Bromophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3ai):

Yield = 71% (102.5 mg). White solid. M.p. 90.1–92.2 °C.

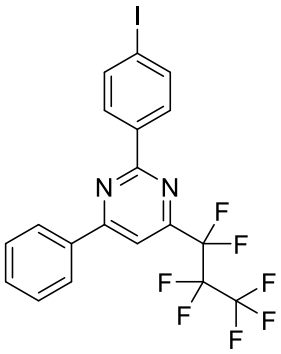
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.50-8.45 (m, 2H), 8.27-8.21 (m, 2H), 7.91 (s, 1H), 7.66-7.62 (m, 2H), 7.60-7.56 (m, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.95 (s, 3F), -116.53 (s, 2F), -126.03 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 164.2, 156.8 (t, $J_{C\text{-}F}$ = 27.0 Hz), 135.7, 135.4, 132.0, 131.9, 130.2, 129.2, 127.5, 126.5, 111.8 (t, $J_{C\text{-}F}$ = 4.5 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{11}BrF_7N_2$ $[M+H]^+$ 478.9988, found: 478.9994.



2-(4-Iodophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3aj):

Yield = 71% (111.7 mg; using 0.45 mmol **2h**). White solid. M.p. 121.5–122.5 °C.

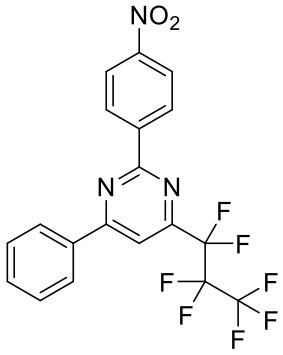
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.33 (d, J = 8.5 Hz, 2H), 8.24 (d, J = 10.0 Hz, 2H), 7.92 (s, 1H), 7.87 (d, J = 8.5 Hz, 2H), 7.62-7.52 (m, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.93 (s, 3F), -116.55 (s, 2F), -126.05 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 164.3, 156.8 (t, $J_{C\text{-}F}$ = 26.3 Hz), 137.9, 136.0, 135.6 132.0, 130.2, 129.2, 127.5, 111.9 (t, $J_{C\text{-}F}$ = 3.8 Hz), 99.0 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{11}F_7IN_2$ $[M+H]^+$ 526.9850, found: 526.9855.



2-(4-Nitrophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (3ak):

Yield = 54% (72.0 mg). Yellow solid. M.p. 58.0–59.2 °C.

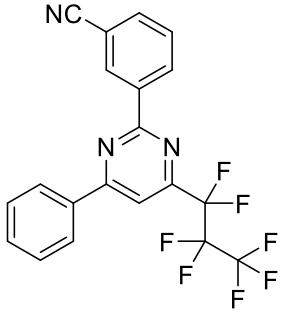
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1 ~10/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.78 (d, J = 8.8 Hz, 2H), 8.35 (d, J = 8.9 Hz, 2H), 8.30-8.24 (m, 2H), 8.01 (s, 1H), 7.67-7.56 (m, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.04 (t, J = 9.2 Hz, 3F), -116.59 (q, J = 9.3 Hz, 2F), -126.07 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 163.0, 157.1 (t, $J_{C\text{-}F}$ = 25.5 Hz), 149.8, 142.0, 135.3, 132.4, 129.6, 129.3, 127.5, 123.8, 112.8 (t, $J_{C\text{-}F}$ = 4.7 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{11}F_7N_3O_2$ $[M+H]^+$ 446.0734, found: 446.0739.



3-(4-(Perfluoropropyl)-6-phenylpyrimidin-2-yl)benzonitrile (3al):

Yield = 65% (82.3 mg). White solid. M.p. 140.4–140.9 °C.

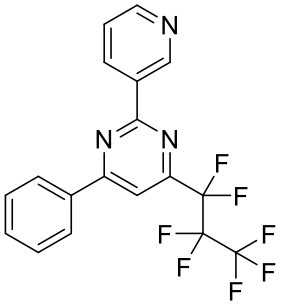
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1 ~30/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.92-8.89 (m, 1H), 8.86-8.81 (m, 1H), 8.29-8.23 (m, 2H), 7.97 (s, 1H), 7.84-7.78 (m, 1H), 7.69-7.55 (m, 4H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.94 (t, J = 9.4 Hz, 3F), -116.52 (q, J = 9.6 Hz, 2F), -125.98 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.6, 162.8, 157.0 (t, $J_{C\text{-}F}$ = 26.2 Hz), 137.6, 135.2, 134.5, 132.7, 132.3, 132.3, 129.6, 129.3, 127.5, 118.6, 113.0, 112.5 (t, $J_{C\text{-}F}$ = 4.7 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{11}F_7N_3$ $[M+H]^+$ 426.0836, found: 426.0835.



4-(Perfluoropropyl)-6-phenyl-2-(pyridin-3-yl)pyrimidine (3am):

Yield = 67% (81.1 mg). White solid. M.p. 68.1–69.2 °C.

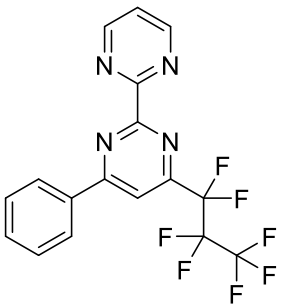
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 20/1 ~5/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.80 (s, 1H), 8.86-8.81 (m, 1H), 8.76 (d, J = 4.9 Hz, 1H), 8.31-8.19 (m, 2H), 7.95 (s, 1H), 7.63-7.50 (m, 3H), 7.49-7.43 (m, 1H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.98 (s, 3F), -116.55 (s, 2F), -126.04 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 163.3, 156.9 (t, $J_{C\text{-}F}$ = 26.5 Hz), 152.1, 150.2, 135.9, 135.3, 132.2, 132.1, 129.2, 127.5, 123.5, 112.3 (t, $J_{C\text{-}F}$ = 4.2 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{18}H_{11}F_7N_3$ $[M+H]^+$ 402.0836, found: 402.0841.



4-(Perfluoropropyl)-6-phenyl-2,2'-bipyrimidine (3an):

Yield = 35% (42.2 mg; using 0.45 mmol **2k**). White solid. M.p. 134.6-135.5 °C.

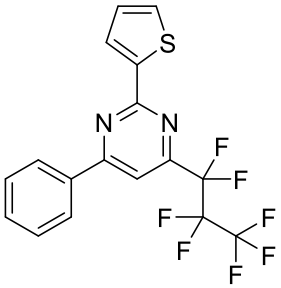
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 10/1 ~1/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.07 (d, J = 4.9 Hz, 2H), 8.25 (d, J = 8.2 Hz, 2H), 8.12 (s, 1H), 7.60-7.52 (m, 3H), 7.50-7.44 (m, 1H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.85 (s, 3F), -116.47 (s, 2F), -125.68 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.6, 163.5, 162.2, 158.1, 157.2 (t, $J_{C\text{-}F}$ = 25.2 Hz), 135.3, 132.2, 129.2, 127.9, 121.5, 114.5 (t, $J_{C\text{-}F}$ = 4.5 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{17}H_{10}F_7N_4$ $[M+H]^+$ 403.0788, found: 403.0794.



4-(Perfluoropropyl)-6-phenyl-2-(thiophen-2-yl)pyrimidine (3ao):

Yield = 83% (101.5 mg; using 0.45 mmol **2l**). White solid. M.p. 63.3–64.5 ºC.

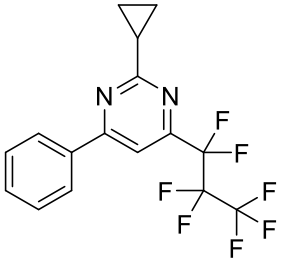
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 100/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.25-8.20 (m, 2H), 8.20-8.18 (m, 1H), 7.81 (s, 1H), 7.61-7.54 (m, 4H), 7.21-7.18 (m, 1H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.94 (s, 3F), -116.66 (s, 2F), -126.08 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 161.9, 156.6 (t, $J_{C\text{-}F}$ = 25.9 Hz), 142.3, 135.4, 132.0, 131.1, 130.5, 129.1, 128.4, 127.4, 110.8 (t, $J_{C\text{-}F}$ = 4.3 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{17}H_{10}F_7N_2S$ $[M+H]^+$ 407.0447, found: 407.0453.



2-Cyclopropyl-4-(perfluoropropyl)-6-phenylpyrimidine (3ap):

Yield = 76% (82.9 mg). White solid. M.p. 41.0–41.6 ºC.

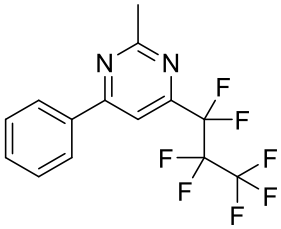
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.16-8.10 (m, 2H), 7.76 (s, 1H), 7.56-7.49 (m, 3H), 2.47-2.39 (m, 1H), 1.32-1.27 (m, 2H), 1.20-1.14 (m, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.08 (s, 3F), -116.84 (s, 2F), -126.21 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 173.3, 165.7, 156.1 (t, $J_{C\text{-}F}$ = 25.3 Hz), 135.9, 131.6, 129.1, 127.3, 110.7 (t, $J_{C\text{-}F}$ = 4.7 Hz), 18.4, 11.7 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{16}H_{12}F_7N_2$ $[M+H]^+$ 365.0883, found: 365.0889.



2-Methyl-4-(perfluoropropyl)-6-phenylpyrimidine (3aq):

Yield = 50% (51.0 mg). Colourless oil.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1).

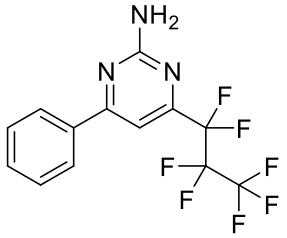
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.17-8.10 (m, 2H), 7.83 (s, 1H), 7.59-7.50 (m, 3H), 2.89 (s, 3H)

ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.05 (s, 3F), -116.88 (s, 2F), -126.11 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.3, 166.2, 156.2 (t, $J_{C\text{-}F}$ = 25.8 Hz), 135.8, 131.8, 129.2, 127.4, 111.4 (t, $J_{C\text{-}F}$ = 4.5 Hz), 26.2 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{14}H_{10}F_7N_2$ $[M+H]^+$ 339.0727, found: 339.0732.



4-(Perfluoropropyl)-6-phenylpyrimidin-2-amine (3ar):

Yield = 39% (39.6 mg; using 0.45 mmol **2o**). White solid. M.p. 84.8-86.0 °C.

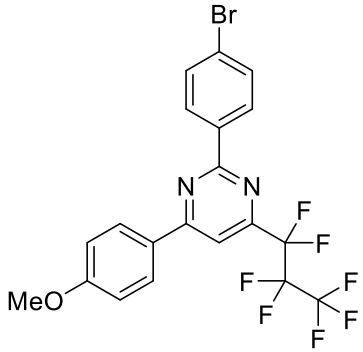
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 100/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.07-8.00 (m, 2H), 7.56-7.48 (m, 3H), 7.33 (s, 1H), 5.93 (s, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.94 (s, 3F), -116.69 (s, 2F), -126.08 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.8, 163.3, 157.1 (t, $J_{C\text{-}F}$ = 25.4 Hz), 136.1, 131.5, 129.0, 127.3, 104.8 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{13}H_9F_7N_3$ $[M+H]^+$ 340.0679, found: 340.0685.



2-(4-Bromophenyl)-4-(4-methoxyphenyl)-6-(perfluoropropyl)pyrimidine (3bi):

Yield = 79% (120.1 mg). White solid. M.p. 89.1-90.3 °C.

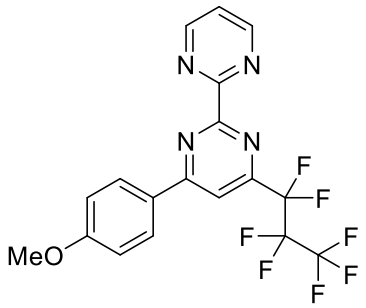
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.47-8.40 (m, 2H), 8.23-8.15 (m, 2H), 7.81 (s, 1H), 7.66-7.58 (m, 2H), 7.07-6.99 (m, 2H), 3.89 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.96 (t, J = 9.0 Hz, 3F), -116.61 (q, J = 9.3 Hz, 2F), -126.06 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.6, 163.9, 162.9, 156.4 (t, $J_{C\text{-}F}$ = 24.8 Hz), 135.6, 131.8, 130.1, 129.1, 128.0, 126.3, 114.5, 110.8, 55.4 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{13}BrF_7N_2O$ $[M+H]^+$ 509.0094, found: 509.0099.



4-(4-Methoxyphenyl)-6-(perfluoropropyl)-2,2'-bipyrimidine (3bn):

Yield = 28% (36.8 mg). White solid. M.p. 105.9–107.2 °C.

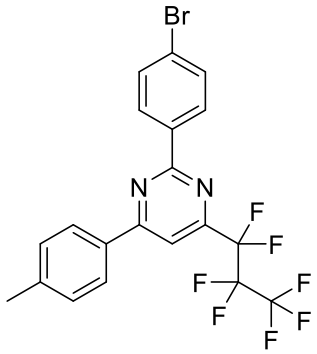
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 20/1~1/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.05 (d, J = 4.9 Hz, 2H), 8.28-8.23 (m, 2H), 8.04 (s, 1H), 7.46 (t, J = 4.9 Hz, 1H), 7.06-7.02 (m, 2H), 3.88 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.86 (s, 3F), -116.54 (s, 2F), -125.70 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.8, 163.4, 163.1, 162.5, 158.0, 156.9, 129.6, 127.6, 121.4, 114.6, 113.5 (t, $J_{C\text{-}F}$ = 4.5 Hz), 55.5 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{18}H_{12}F_7N_4O$ $[M+H]^+$ 433.0894, found: 433.0899.



2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(*p*-tolyl)pyrimidine (3ci):

Yield = 67% (98.4 mg). White solid. M.p. 97.5–98.8 °C.

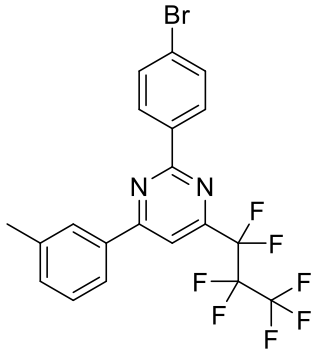
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.50-8.44 (m, 2H), 8.15-8.10 (m, 2H), 7.87 (s, 1H), 7.66-7.62 (m, 2H), 7.35 (d, J = 7.7 Hz, 2H), 2.46 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.96 (s, 3F), -116.57 (s, 2F), -126.05 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 164.1, 156.6 (t, $J_{C\text{-}F}$ = 26.4 Hz), 142.7, 135.5, 132.9, 131.8, 130.2, 129.9, 127.4, 126.4, 111.5 (t, $J_{C\text{-}F}$ = 4.2 Hz), 21.6 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{13}BrF_7N_2$ $[M+H]^+$ 493.0145, found: 493.0150.



2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(*m*-tolyl)pyrimidine (3di):

Yield = 71% (104.4 mg). White solid. M.p. 47.8-48.2 ºC.

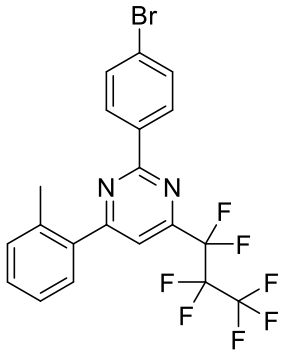
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.50-8.45 (m, 2H), 8.06-8.00 (m, 2H), 7.90 (s, 1H), 7.68-7.62 (m, 2H), 7.49-7.38 (m, 2H), 2.51 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.95 (s, 3F), -116.57 (s, 2F), -126.03 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.5, 164.1, 156.7 (t, $J_{C\text{-}F}$ = 26.6 Hz), 139.0, 135.6, 135.5, 132.8, 131.9, 130.2, 129.1, 128.0, 126.5, 124.7, 111.9 (t, $J_{C\text{-}F}$ = 3.9 Hz), 21.5 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{13}BrF_7N_2$ $[M+H]^+$ 493.0145, found: 493.0150.



2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(*o*-tolyl)pyrimidine (3ei):

Yield = 29% (42.6 mg; using 0.45 mmol **2g**). Yellow oil.

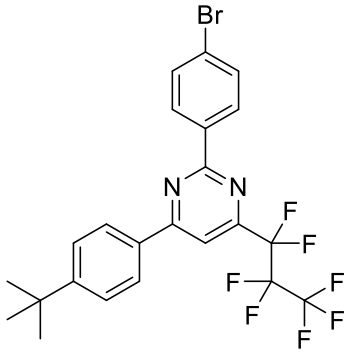
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.49-8.42 (m, 2H), 7.70 (s, 1H), 7.68-7.63 (m, 2H), 7.62-7.57 (m, 1H), 7.49-7.43 (m, 1H), 7.43-7.36 (m, 2H), 2.57 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.94 (s, 3F), -116.63 (s, 2F), -126.12 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.7, 163.8, 156.2 (t, $J_{C\text{-}F}$ = 26.5 Hz), 136.8, 136.7, 135.4, 131.9, 131.7, 130.4, 130.2, 129.9, 126.5, 126.5, 116.1 (t, $J_{C\text{-}F}$ = 4.3 Hz), 20.7 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{20}H_{13}BrF_7N_2$ $[M+H]^+$ 493.0145, found: 493.0150.



2-(4-Bromophenyl)-4-(4-(*tert*-butyl)phenyl)-6-(perfluoropropyl)pyrimidine (3fi):

Yield = 68% (109.0 mg). White solid. M.p. 110.9–111.9 ºC.

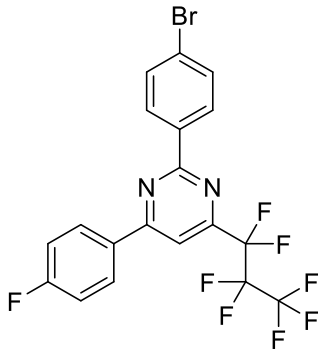
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.52-8.46 (m, 2H), 8.22-8.16 (m, 2H), 7.91 (s, 1H), 7.68-7.58 (m, 4H), 1.42 (s, 9H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.94 (s, 3F), -116.61 (s, 2F), -126.11 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 164.1, 156.7 (t, $J_{C\text{-}F}$ = 25.8 Hz), 155.8, 135.5, 132.9, 131.9, 130.2, 127.3, 126.4, 126.2, 111.6 (t, $J_{C\text{-}F}$ = 3.9 Hz), 35.0, 31.1 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{23}H_{19}BrF_7N_2$ $[M+H]^+$ 535.0614, found: 535.0620.



2-(4-Bromophenyl)-4-(4-fluorophenyl)-6-(perfluoropropyl)pyrimidine (3gi):

Yield = 80% (119.9 mg). White solid. M.p. 151.2–151.9 ºC.

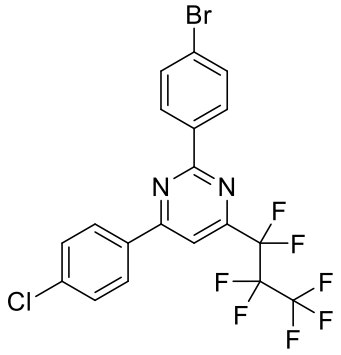
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.49-8.42 (m, 2H), 8.30-8.22 (m, 2H), 7.86 (s, 1H), 7.68-7.61 (m, 2H), 7.31-7.20 (m, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.93 (s, 3H), -107.14 (s, 1H), -116.59 (s, 2H), -126.03 (s, 2H) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.3 (d, $J_{C\text{-}F}$ = 251.9 Hz), 164.7 (d, $J_{C\text{-}F}$ = 98.1 Hz), 156.9 (t, $J_{C\text{-}F}$ = 25.8 Hz), 135.2, 131.9, 131.8 (d, $J_{C\text{-}F}$ = 3.0 Hz), 130.2, 129.7 (d, $J_{C\text{-}F}$ = 8.9 Hz), 126.6, 116.4 (d, $J_{C\text{-}F}$ = 21.8 Hz), 112.1 (t, $J_{C\text{-}F}$ = 30.9 Hz), 111.4 (t, $J_{C\text{-}F}$ = 4.7 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{10}BrF_8N_2$ $[M+H]^+$ 496.9894, found: 496.9900.



2-(4-Bromophenyl)-4-(4-chlorophenyl)-6-(perfluoropropyl)pyrimidine (3hi):

Yield = 78% (119.7 mg). White solid. M.p. 139.6–141.3 °C.

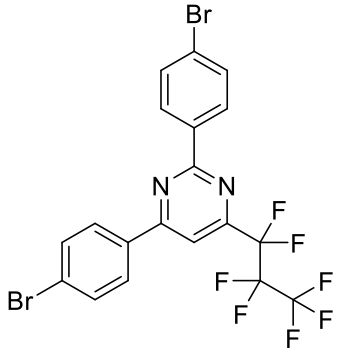
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.46-8.39 (m, 2H), 8.20-8.14 (m, 2H), 7.86 (s, 1H), 7.66-7.59 (m, 2H), 7.56-7.49 (m, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.93 (t, J = 9.0 Hz, 3F), -116.53 (q, J = 9.4 Hz, 2F), -125.99 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.2, 164.3, 157.1 (t, $J_{C\text{-}F}$ = 25.1 Hz), 138.4, 135.2, 134.1, 131.9, 130.2, 129.5, 128.7, 126.7, 111.5 (t, $J_{C\text{-}F}$ = 4.4 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{10}BrClF_7N_2$ $[M+H]^+$ 512.9599, found: 512.9604.



2,4-Bis(4-bromophenyl)-6-(perfluoropropyl)pyrimidine (3ii):

Yield = 76% (127.7 mg). White solid. M.p. 141.7–142.9 °C.

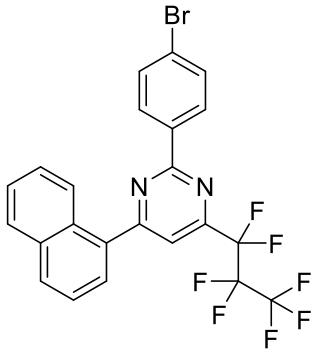
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.47-8.35 (m, 2H), 8.14-8.04 (m, 2H), 7.85 (s, 1H), 7.73-7.66 (m, 2H), 7.65-7.55 (m, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.93 (t, J = 9.2 Hz, 3F), -116.48 (q, J = 9.3 Hz, 2F), -125.95 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.2, 164.3, 157.1 (t, $J_{C\text{-}F}$ = 25.2 Hz), 135.1, 134.5, 132.4, 131.9, 130.2, 128.9, 127.0, 126.7, 111.5 (t, $J_{C\text{-}F}$ = 4.4 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{19}H_{10}Br_2F_7N_2$ $[M+H]^+$ 556.9093, found: 556.9099.



2-(4-Bromophenyl)-4-(naphthalen-1-yl)-6-(perfluoropropyl)pyrimidine (3ji):

Yield = 33% (52.3 mg; using 0.45 mmol **2g**). Yellow solid. M.p. 79.0–80.5 °C.

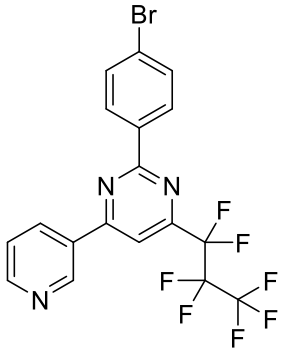
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.52-8.47 (m, 2H), 8.32-8.26 (m, 1H), 8.06 (d, J = 8.4 Hz, 1H), 8.03-7.95 (m, 1H), 7.87 (s, 1H), 7.80 (dd, J = 7.1, 1.3 Hz, 1H), 7.69-7.63 (m, 3H), 7.63-7.57 (m, 2H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.89 (s, 3F), -116.45 (s, 2F), -125.95 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.2, 164.1, 156.5 (t, $J_{C\text{-}F}$ = 27.2 Hz), 135.3, 134.9, 134.0, 132.0, 131.3, 130.4, 130.3, 128.8, 128.7, 127.5, 126.7, 126.6, 125.3, 124.6, 117.0 (t, $J_{C\text{-}F}$ = 3.6 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{23}H_{13}BrF_7N_2$ $[M+H]^+$ 529.0145, found: 529.0150.



2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(pyridin-3-yl)pyrimidine (3ki):

Yield = 81% (116.2 mg). White solid. M.p. 119.0-120.2 °C.

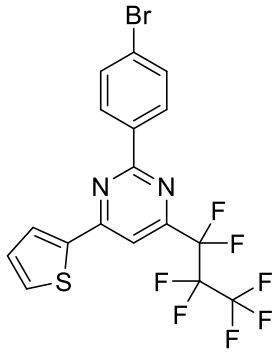
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 20/1~5/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.42 (d, J = 2.2 Hz, 1H), 8.83-8.78 (m, 1H), 8.54-8.48 (m, 1H), 8.44-8.39 (m, 2H), 7.92 (s, 1H), 7.63-7.57 (m, 2H), 7.54-7.47 (m, 1H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.95 (t, J = 9.1 Hz, 3F), -116.55 (q, J = 9.0 Hz, 2F), -125.99 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.3, 164.1, 157.1 (t, $J_{C\text{-}F}$ = 26.4 Hz), 152.6, 148.7, 134.8, 134.7, 131.9, 131.2, 130.1, 126.8, 123.8, 111.7 (t, $J_{C\text{-}F}$ =4.0 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{18}H_{10}BrF_7N_3$ $[M+H]^+$ 479.9941, found: 479.9946.



2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(thiophen-2-yl)pyrimidine (3li):

Yield = 60% (87.9 mg). White solid. M.p. 85.8–87.0 °C.

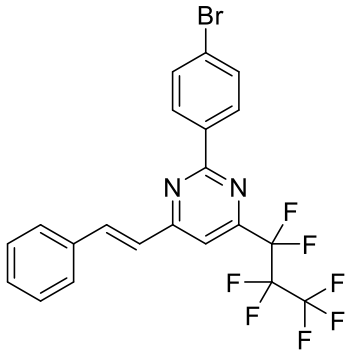
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.44-8.38 (m, 2H), 7.93-7.87 (m, 1H), 7.72 (s, 1H), 7.67-7.60 (m, 3H), 7.23-7.20 (m, 1H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.97 (s, 3F), -116.66 (s, 2F), -126.02 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.2, 161.2, 156.5 (t, $J_{C\text{-}F}$ = 25.8 Hz), 141.5, 135.0, 131.9, 131.8, 130.2, 128.9, 128.7, 126.6, 110.1 (t, $J_{C\text{-}F}$ = 4.8 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{17}H_9BrF_7N_2S$ $[M+H]^+$ 484.9553, found: 484.9558.



(*E*)-2-(4-bromophenyl)-4-(perfluoropropyl)-6-styrylpyrimidine (3mi):

Yield = 60% (90.9 mg). White solid. M.p. 106.4–107.0 °C.

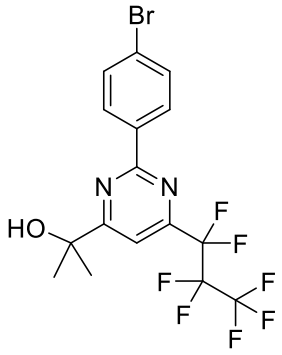
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.47-8.39 (m, 2H), 8.07 (d, J = 15.9 Hz, 1H), 7.69-7.62 (m, 4H), 7.49 (s, 1H), 7.48-7.39 (m, 3H), 7.16 (d, J = 15.9 Hz, 1H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.97 (s, 3F), -116.65 (s, 2F), -126.05 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.8, 163.9, 156.5 (t, $J_{C\text{-}F}$ = 26.5 Hz), 139.2, 135.5, 135.1, 131.8, 130.2, 130.0, 129.0, 128.0, 126.4, 125.0, 113.6 (t, $J_{C\text{-}F}$ = 3.7 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{21}H_{13}BrF_7N_2$ $[M+H]^+$ 505.0145, found: 505.0145.



2-(2-(4-Bromophenyl)-6-(perfluoropropyl)pyrimidin-4-yl)propan-2-ol (3ni):

Yield = 41% (57.3 mg). Yellow oil.

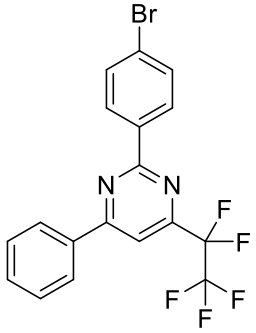
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1~20/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.43-8.35 (m, 2H), 7.74 (s, 1H), 7.67-7.61 (m, 2H), 3.64 (brs, 1H), 1.65 (s, 6H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.00 (t, J = 9.5 Hz, 3F), -116.34 (q, J = 9.5 Hz, 2F), -126.03 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 177.9, 163.3, 156.9 (t, $J_{C\text{-}F}$ = 26.7 Hz), 134.8, 132.0, 130.1, 126.8, 111.5 (t, $J_{C\text{-}F}$ = 4.6 Hz), 73.1, 30.0 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{16}H_{13}BrF_7N_2O$ $[M+H]^+$ 461.0094, found: 461.0099.



2-(4-Bromophenyl)-4-(perfluoroethyl)-6-phenylpyrimidine (3oi):

Yield = 79% (101.6 mg). White solid. M.p. 70.1–71.7 °C.

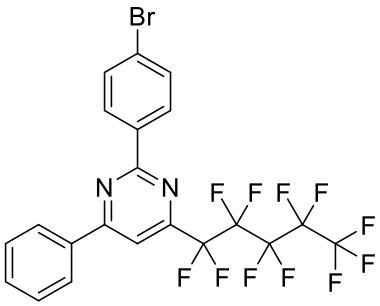
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.51-8.45 (m, 2H), 8.27-8.21 (m, 2H), 7.93 (s, 1H), 7.67-7.62 (m, 2H), 7.61-7.54 (m, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -82.42 (s, 3F), -118.70 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 164.2, 156.8 (t, $J_{C\text{-}F}$ = 26.3 Hz), 135.7, 135.4, 132.0, 131.9, 130.2, 129.2, 127.5, 126.5, 111.5 (t, $J_{C\text{-}F}$ = 4.3 Hz) ppm, carbons corresponding to the C_2F_5 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{18}H_{11}BrF_5N_2$ $[M+H]^+$ 429.0020, found: 429.0026.



2-(4-Bromophenyl)-4-(perfluoropentyl)-6-phenylpyrimidine (3pi):

Yield = 75% (129.9 mg). White solid. M.p. 88.5-90.0 °C.

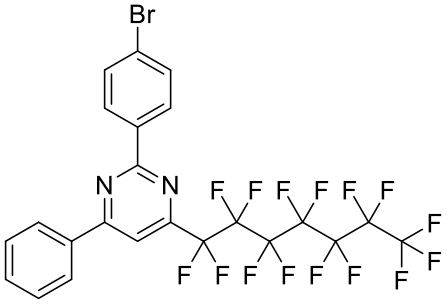
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.51-8.43 (m, 2H), 8.27-8.20 (m, 2H), 7.91 (s, 1H), 7.67-7.53 (m, 5H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.73 (s, 3F), -115.62 (s, 2F), -121.62 (s, 2F), -122.11 (s, 2F), -126.07 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 164.2, 157.0 (t, $J_{C\text{-}F}$ = 27.1 Hz), 135.7, 135.4, 132.0, 131.9, 130.2, 129.2, 127.5, 126.5, 111.9 (t, $J_{C\text{-}F}$ = 4.5 Hz) ppm, carbons corresponding to the C_5F_{11} group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{21}H_{11}BrF_{11}N_2$ $[M+H]^+$ 578.9924, found: 578.9930.



2-(4-Bromophenyl)-4-(perfluoroheptyl)-6-phenylpyrimidine (3qi):

Yield = 75% (153.8 mg). White solid. M.p. 74.4–76.0 °C.

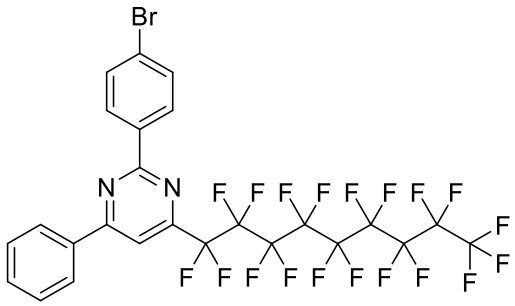
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.50-8.45 (m, 2H), 8.27-8.20 (m, 2H), 7.91 (s, 1H), 7.67-7.62 (m, 2H), 7.61-7.53 (m, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.76 (s, 3F), -115.55 (t, J = 5.1 Hz, 2F), -121.07 (s, 2F), -121.42 (s, 2F), -121.89 (s, 2F), -122.66 (s, 2F), -126.09 (t, J = 5.4 Hz, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 164.2, 157.0 (t, $J_{C\text{-}F}$ = 25.8 Hz), 135.6, 135.4, 132.0, 131.9, 130.2, 129.2, 127.4, 126.5, 111.8 (t, $J_{C\text{-}F}$ = 4.3 Hz) ppm, carbons corresponding to the C_7F_{15} group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{23}H_{11}BrF_{15}N_2$ $[M+H]^+$ 678.9861, found: 678.9866.



2-(4-Bromophenyl)-4-(perfluorononyl)-6-phenylpyrimidine (3ri):

Yield = 76% (177.7 mg). White solid. M.p. 92.7–94.0 °C.

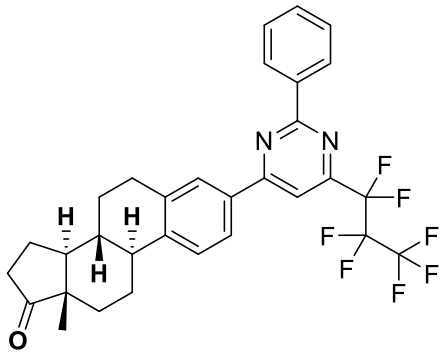
Purified by flash column chromatography through silica gel (petroleum ether).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.53-8.45 (m, 2H), 8.29-8.20 (m, 2H), 7.92 (s, 1H), 7.68-7.64 (m, 2H), 7.61-7.56 (m, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.67 (s, 3F), -115.53 (t, J = 4.7 Hz, 2F), -120.97 (s, 2F), -121.37 (s, 2F), -121.62 (s, 4F), -121.84 (s, 2F), -122.64 (s, 2F), -126.04 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 164.2, 157.1 (t, $J_{C\text{-}F}$ = 26.7 Hz), 135.7, 135.5, 132.0, 131.9, 130.2, 129.2, 127.5, 126.5, 111.9 (t, $J_{C\text{-}F}$ = 4.5 Hz) ppm, carbons corresponding to the C_9F_{19} group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{25}H_{11}BrF_{19}N_2$ $[M+H]^+$ 778.9797, found: 778.9802.



(8*R*,9*S*,13*S*,14*S*)-13-Methyl-3-(6-(perfluoropropyl)-2-phenylpyrimidin-4-yl)-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[*a*]phenanthren-17-one (3sa):

Yield = 38% (22.0 mg; using 0.1 mmol **1q**). White solid. M.p. 202.4-203.7 °C.

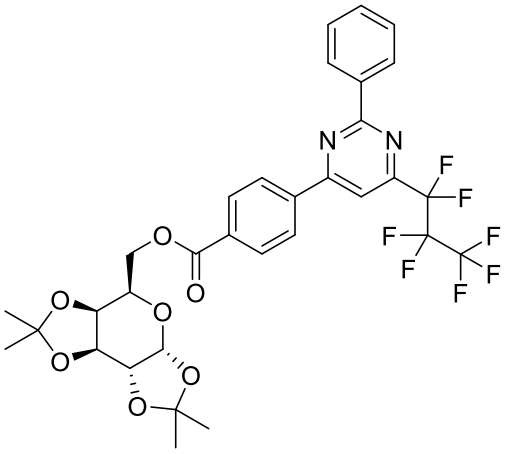
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1 ~ 30/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.67-8.59 (m, 2H), 8.04 (dd, J = 8.2, 2.0 Hz, 1H), 7.99 (d, J = 1.9 Hz, 1H), 7.87 (s, 1H), 7.57-7.52 (m, 3H), 7.49 (d, J = 8.2 Hz, 1H), 3.13-3.02 (m, 2H), 2.60-2.45 (m, 2H), 2.45-2.33 (m, 1H), 2.22-1.98 (m, 4H), 1.68-1.51 (m, 6H), 0.95 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.95 (t, J = 8.9 Hz, 3F), -116.56 (q, J = 9.0 Hz, 2F), -126.09 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 220.7, 166.1, 165.0, 156.3 (t, $J_{C\text{-}F}$ = 25.4 Hz), 144.2, 137.5, 136.6, 133.4, 131.5, 128.7, 128.0, 126.2, 124.0, 111.4 (t, $J_{C\text{-}F}$ = 4.8 Hz), 50.5, 47.9, 44.6, 37.9, 35.8, 31.5, 29.5, 26.3, 25.6, 21.6, 13.8 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{31}H_{28}F_7N_2O$ $[M+H]^+$ 577.2084, found: 577.2090.



((3*aR*,5*R*,5*aS*,8*aS*,8*bR*)-2,2,7,7-tetramethyltetrahydro-5*H*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-5-yl)methyl 4-(6-(perfluoropropyl)-2-phenylpyrimidin-4-yl)benzoate (3ta):

Yield = 72% (147.8 mg). White solid. M.p. 178.2-179.6 ºC.

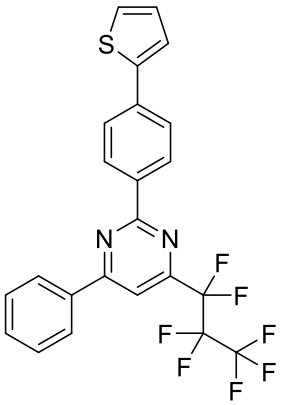
Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1 ~ 10/1).

^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.64-8.57 (m, 2H), 8.35-8.28 (m, 2H), 8.27-8.20 (m, 2H), 7.92 (s, 1H), 7.57-7.49 (m, 3H), 5.60 (d, *J* = 5.0 Hz, 1H), 4.68 (dd, *J* = 7.9, 2.5 Hz, 1H), 4.58 (dd, *J* = 11.5, 4.6 Hz, 1H), 4.51 (dd, *J* = 11.6, 7.7 Hz, 1H), 4.41-4.32 (m, 2H), 4.26-4.21 (m, 1H), 1.55 (s, 3H), 1.51 (s, 3H), 1.38 (s, 3H), 1.35 (s, 3H) ppm.

^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.96 (s, 3F), -116.44 (s, 2F), -125.99 (s, 2F) ppm.

^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.7, 165.2, 165.1, 157.1 (t, $J_{C\text{-}F}$ = 25.4 Hz), 139.8, 136.2, 132.8, 131.8, 130.4, 128.7, 127.4, 111.9, 109.7, 108.8, 96.3, 71.1, 70.7, 70.5, 66.1, 64.4, 26.0, 25.9, 24.9, 24.4 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling.

HRMS (m/z): calcd for $C_{32}H_{30}F_7N_2O_7$ $[M+H]^+$ 687.1936, found: 687.1942.



4-(Perfluoropropyl)-6-phenyl-2-(4-(thiophen-2-yl)phenyl)pyrimidine (5):

Yield = 96% (92.2 mg; using 0.2 mmol **3ag**). White solid. M.p. 119.3-120.5 ºC.

Purified by flash column chromatography through silica gel (petroleum ether/ethyl acetate, 50/1).

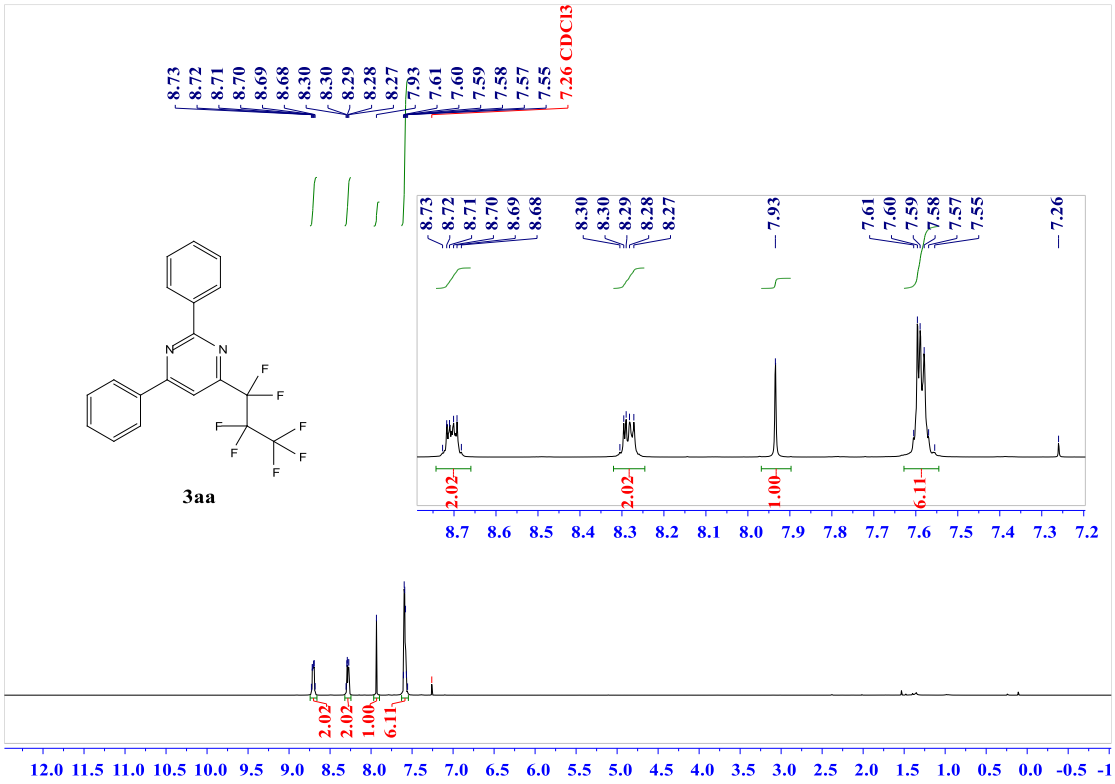
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.67-8.61 (m, 2H), 8.32-8.23 (m, 2H), 7.90 (s, 1H), 7.81-7.75 (m, 2H), 7.62-7.55 (m, 3H), 7.46 (d, *J* = 3.7 Hz, 1H), 7.38-7.34 (m, 1H), 7.14 (dd, *J* = 5.1, 3.7 Hz, 1H) ppm.

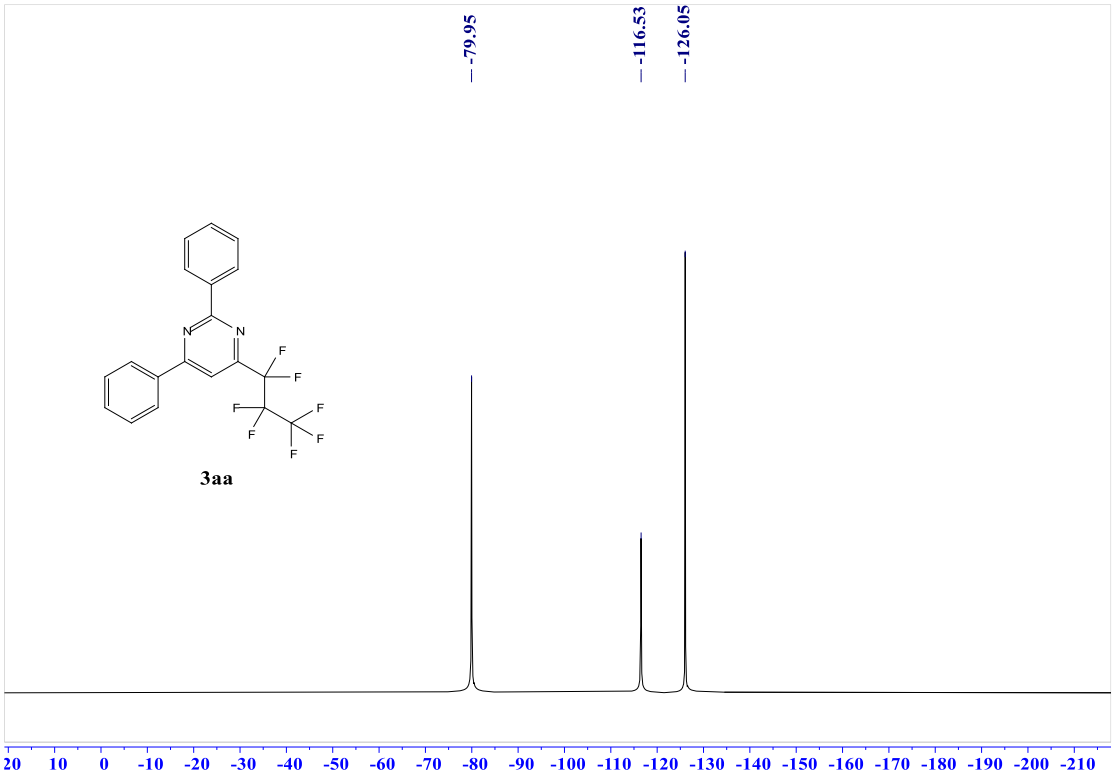
^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.91 (s, 3F), -116.43 (s, 2F), -125.97 (s, 2F) ppm.

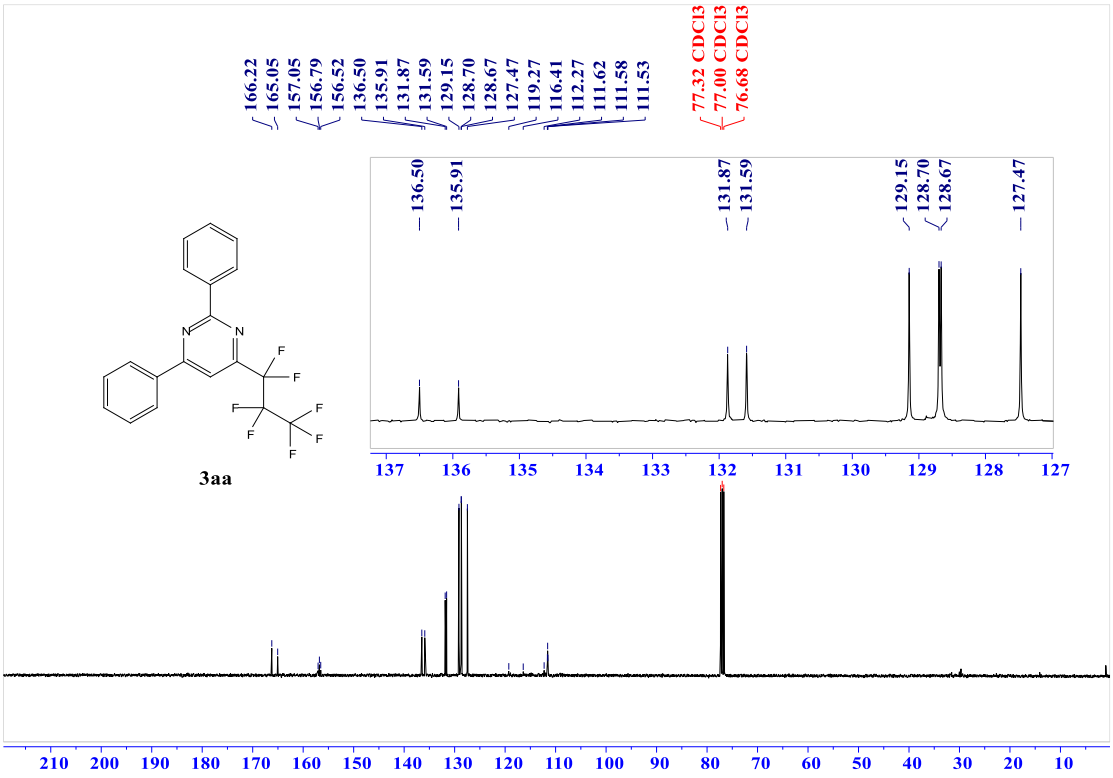
^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.2, 164.6, 156.8 (t, $J_{C\text{-}F}$ = 24.3 Hz), 143.6, 137.3, 135.9, 135.4, 131.9, 129.3, 129.2, 128.3, 127.5, 125.9, 125.8, 124.0, 111.5 ppm, carbons corresponding

to the C_3F_7 group cannot be identified due to C-F coupling.
HRMS (m/z): calcd for $C_{23}H_{14}F_7N_2S$ $[M+H]^+$ 483.0760, found: 483.0766.

^{1}H, ^{19}F, and ^{13}C NMR spectra of products



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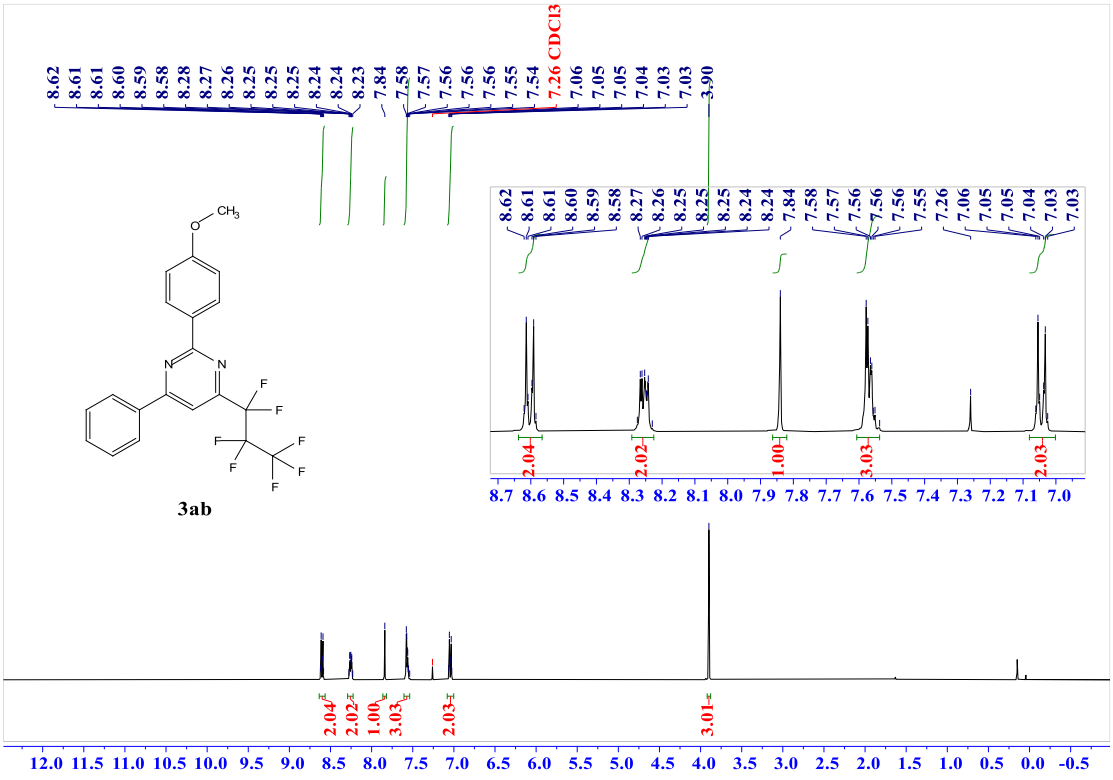
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7.03
3.90
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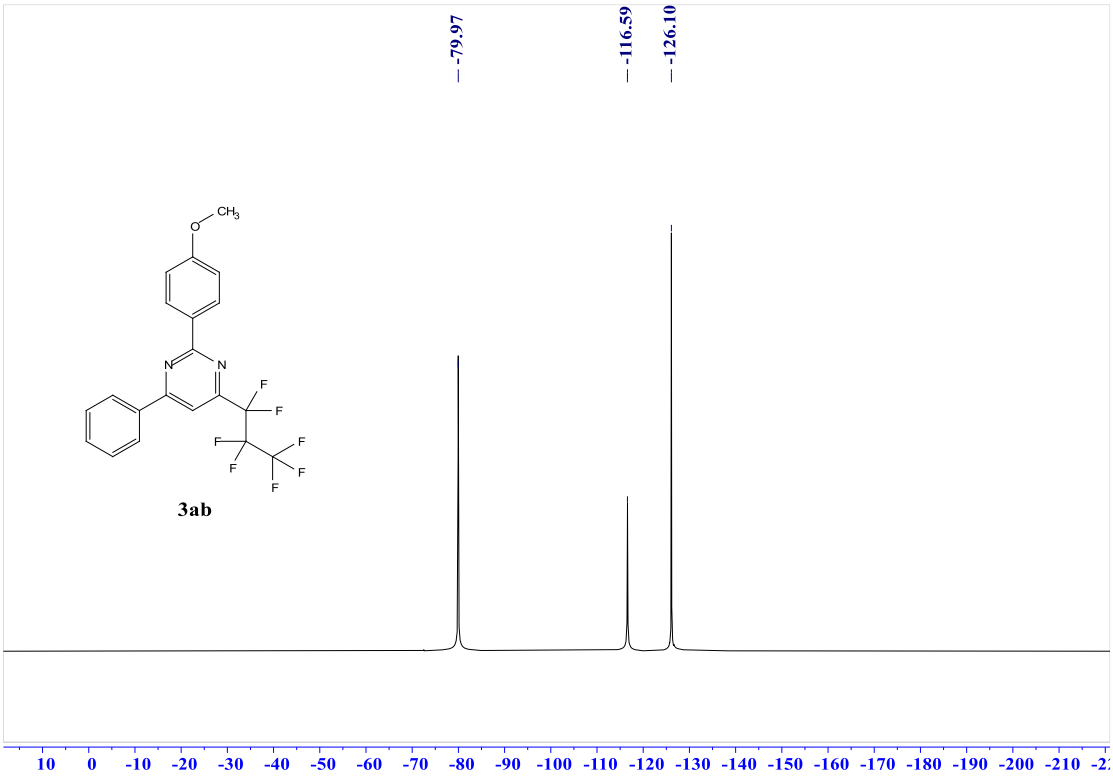
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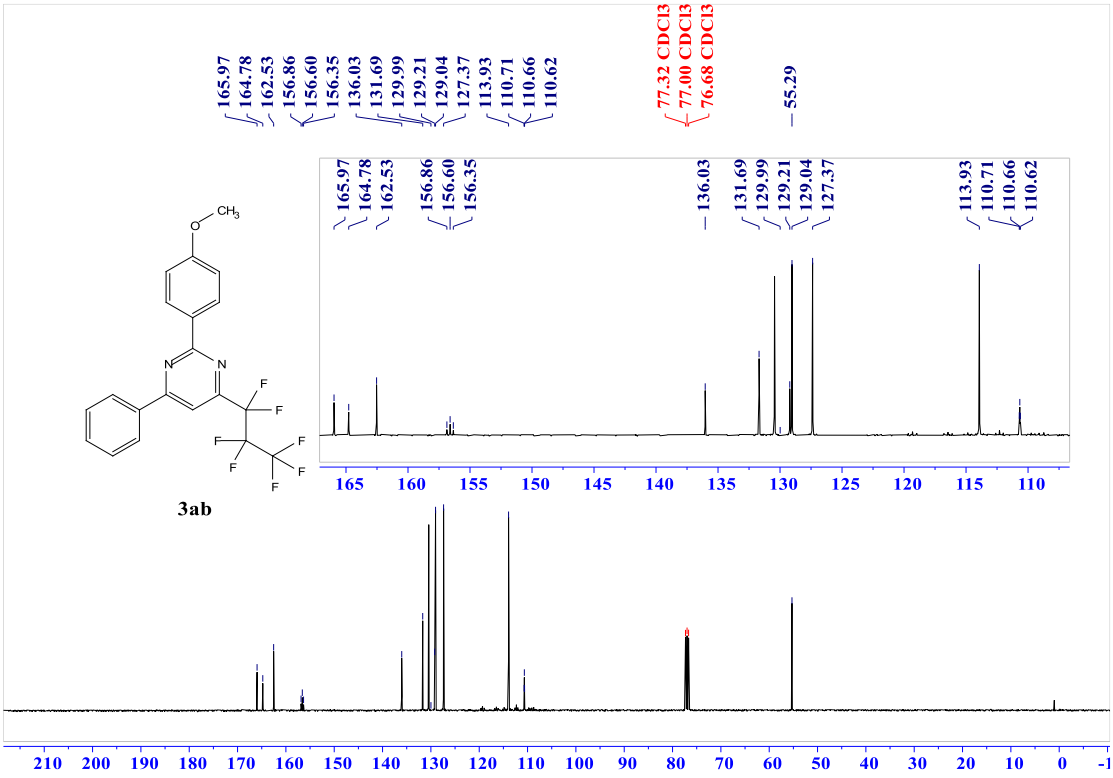
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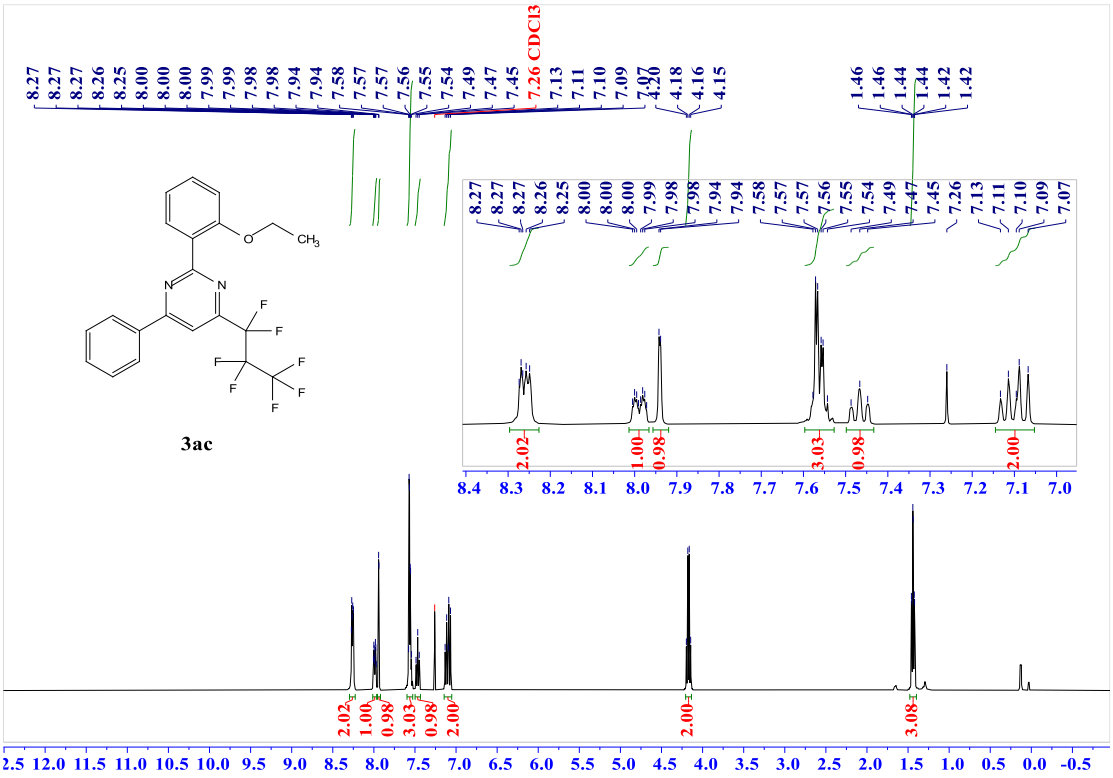
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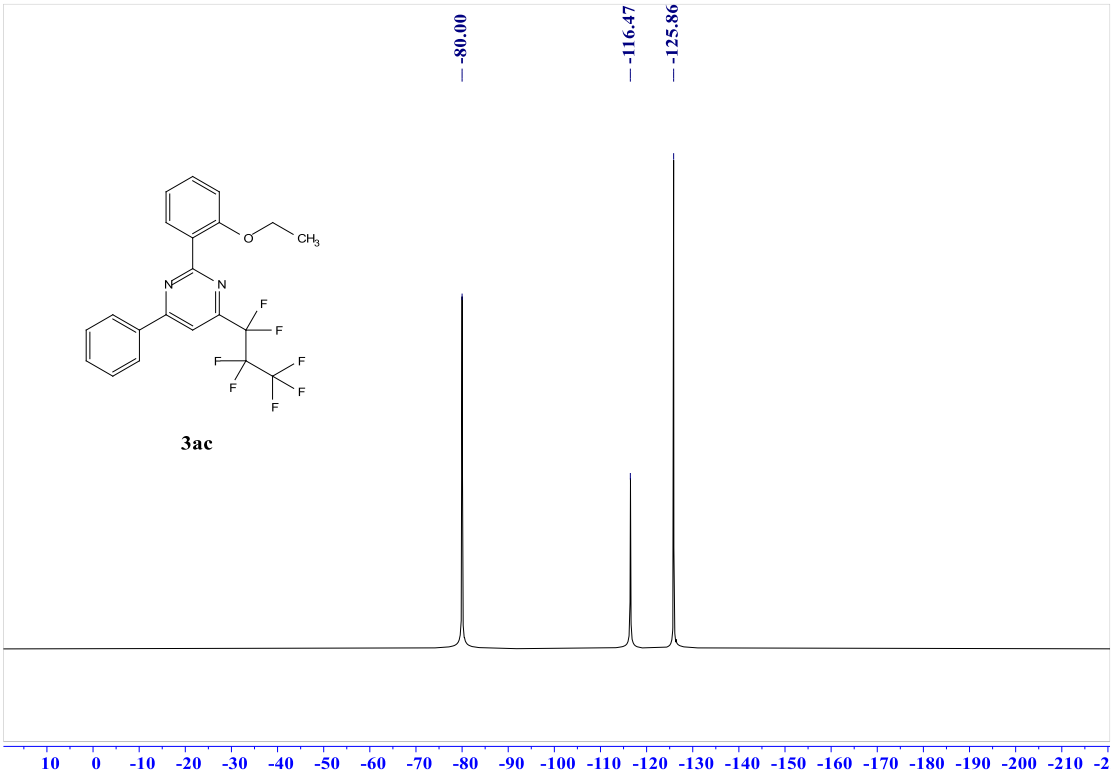
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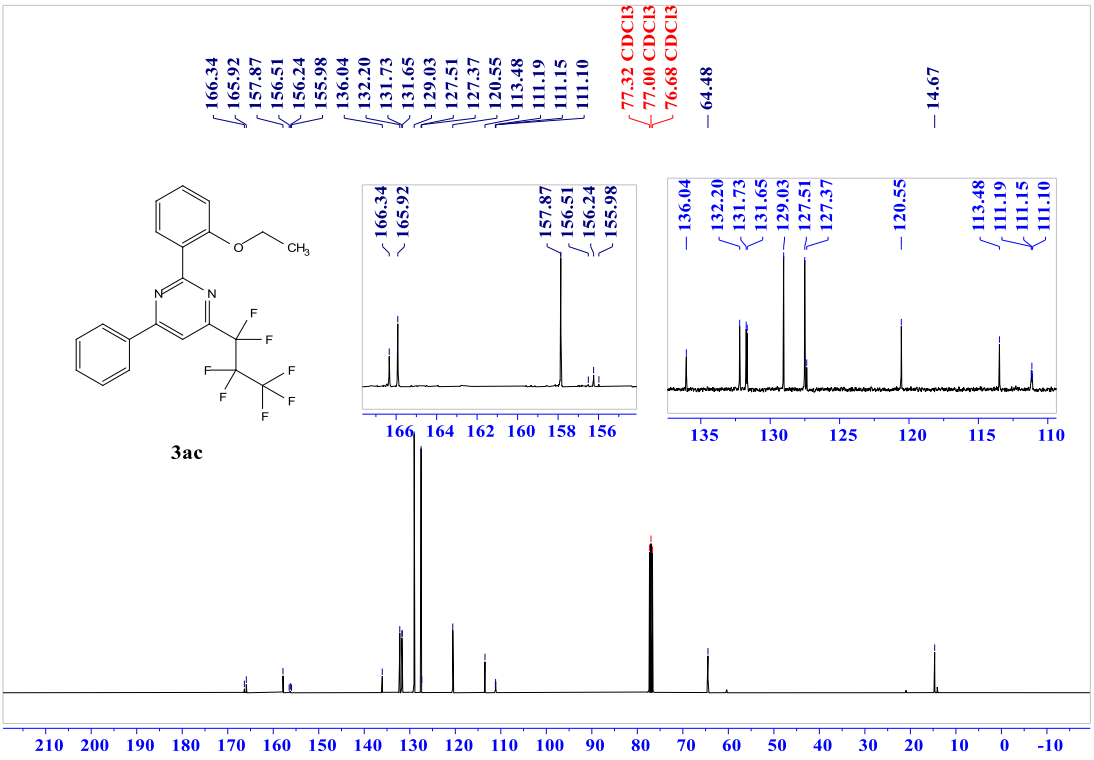
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111.15
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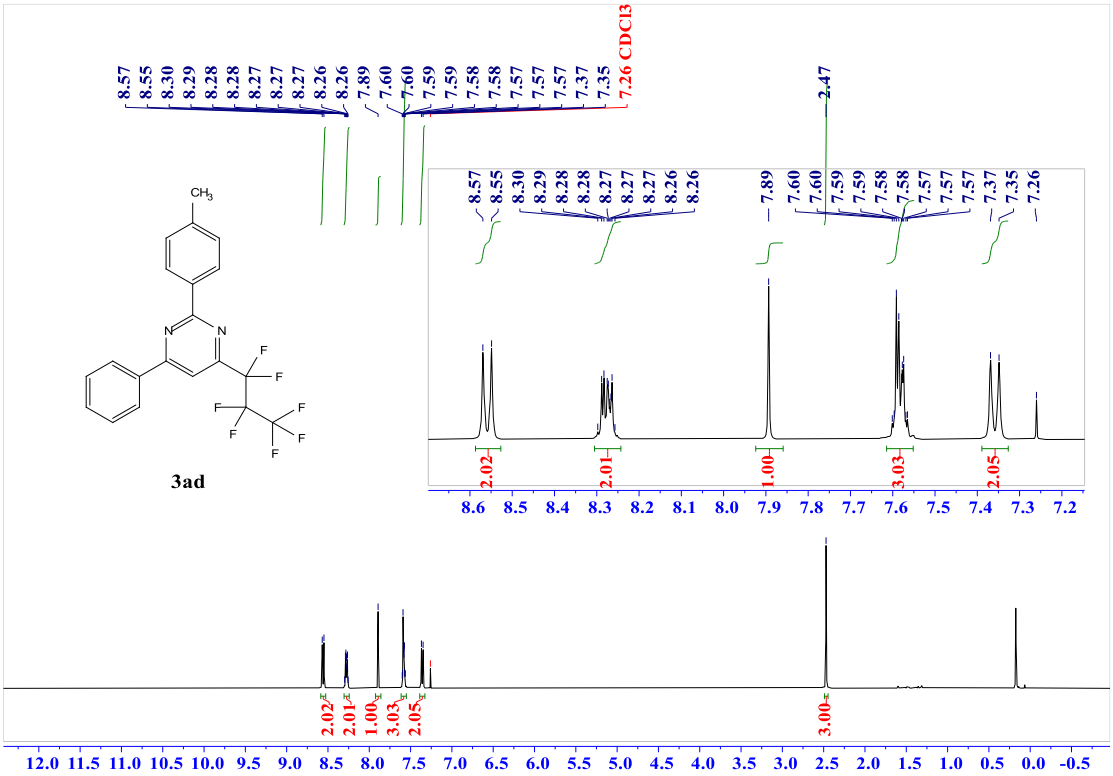
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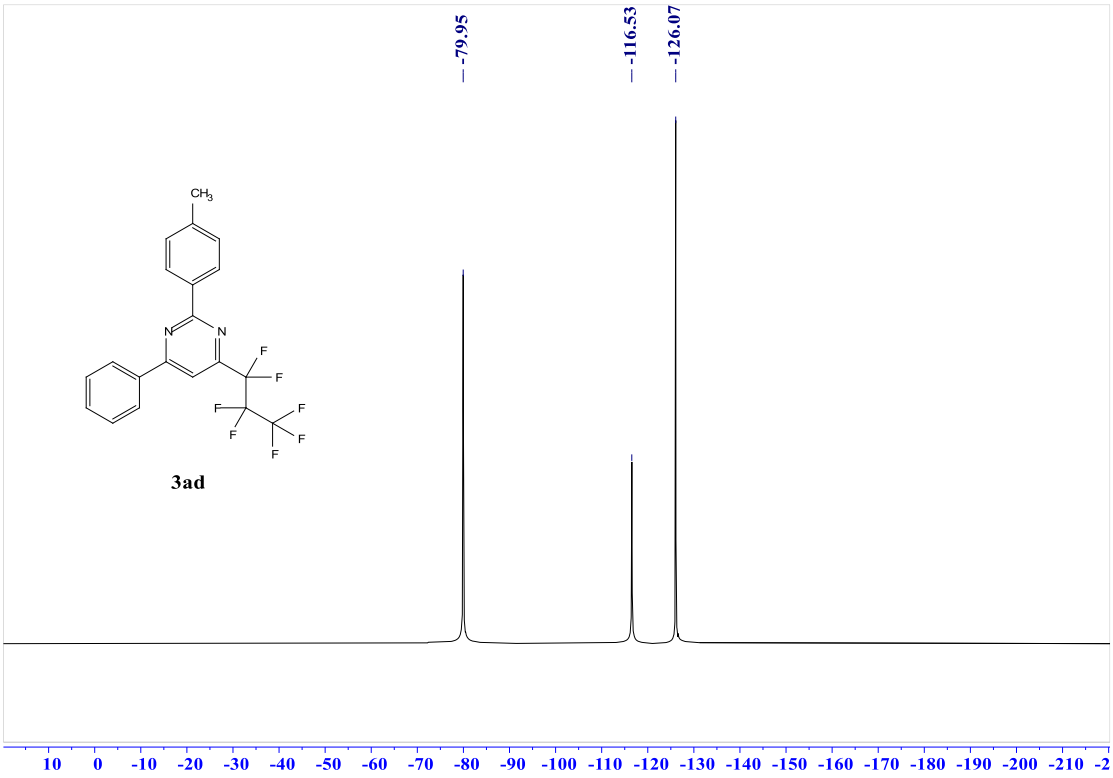
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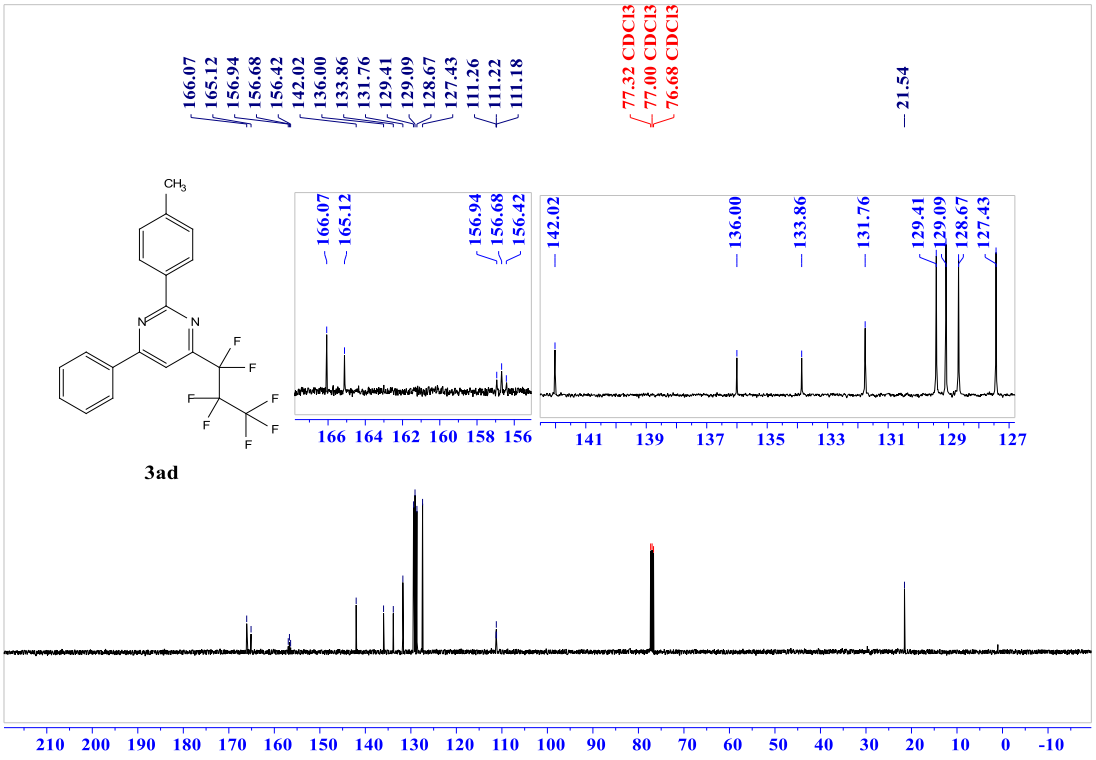
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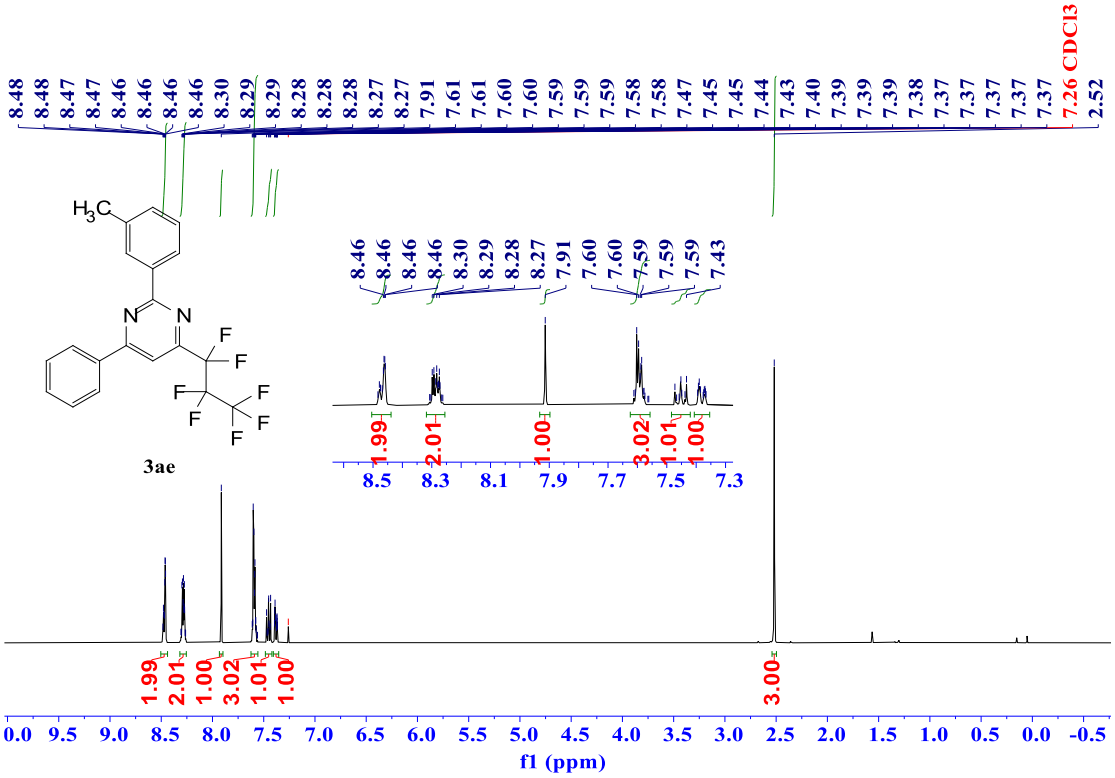
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H3C
N
N
F
F
F
F
F
F
F
3ae
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1.99 2.01 1.00 3.02 1.01 1.00
8.5 8.3 8.1 7.9 7.7 7.5 7.3
1.99 2.01 1.00 3.02 1.01 1.00 3.00
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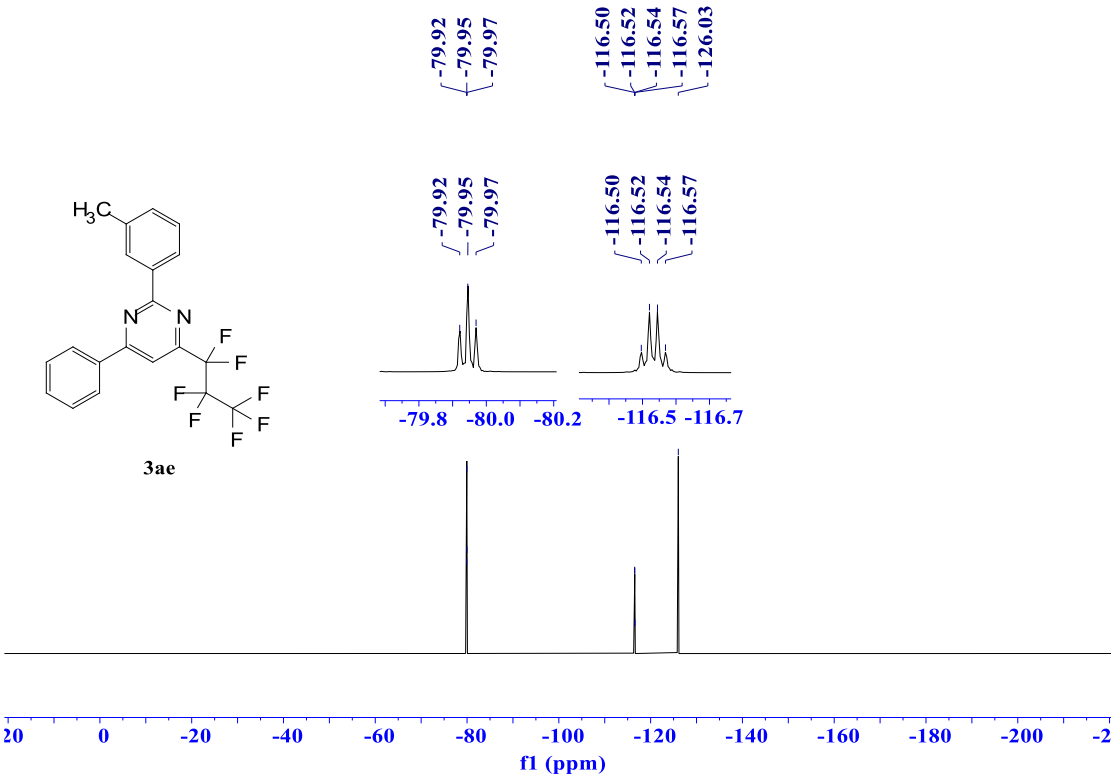
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3ae
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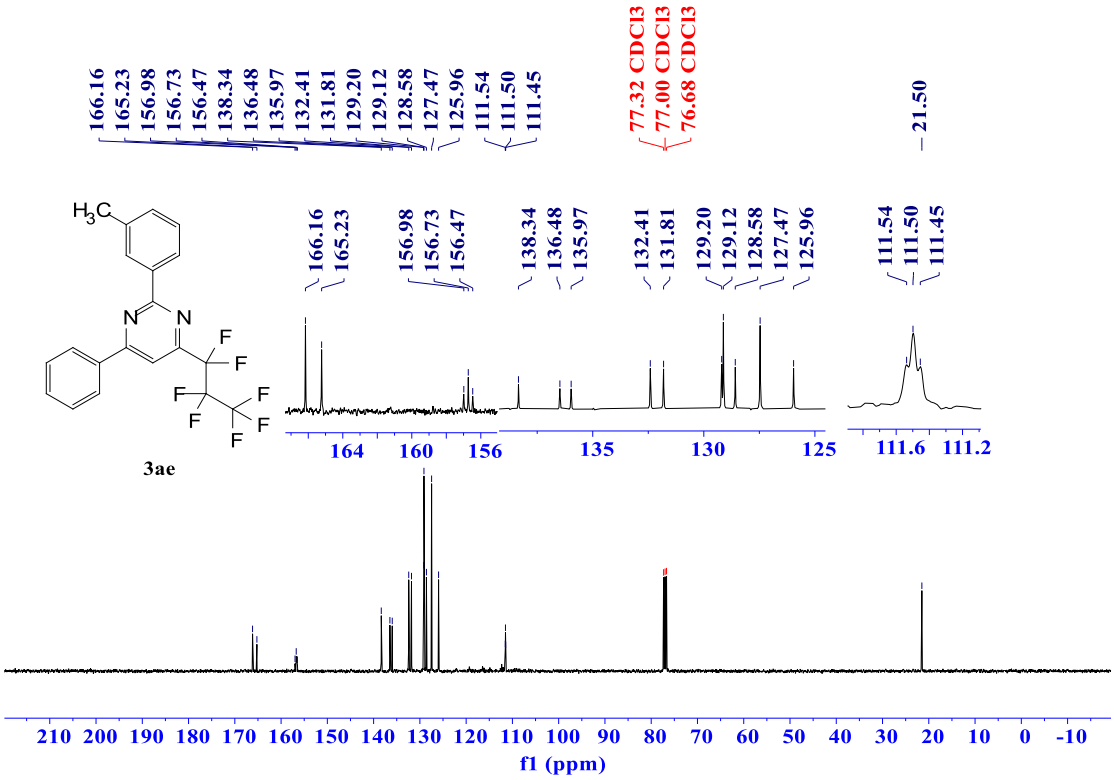
f1 (ppm)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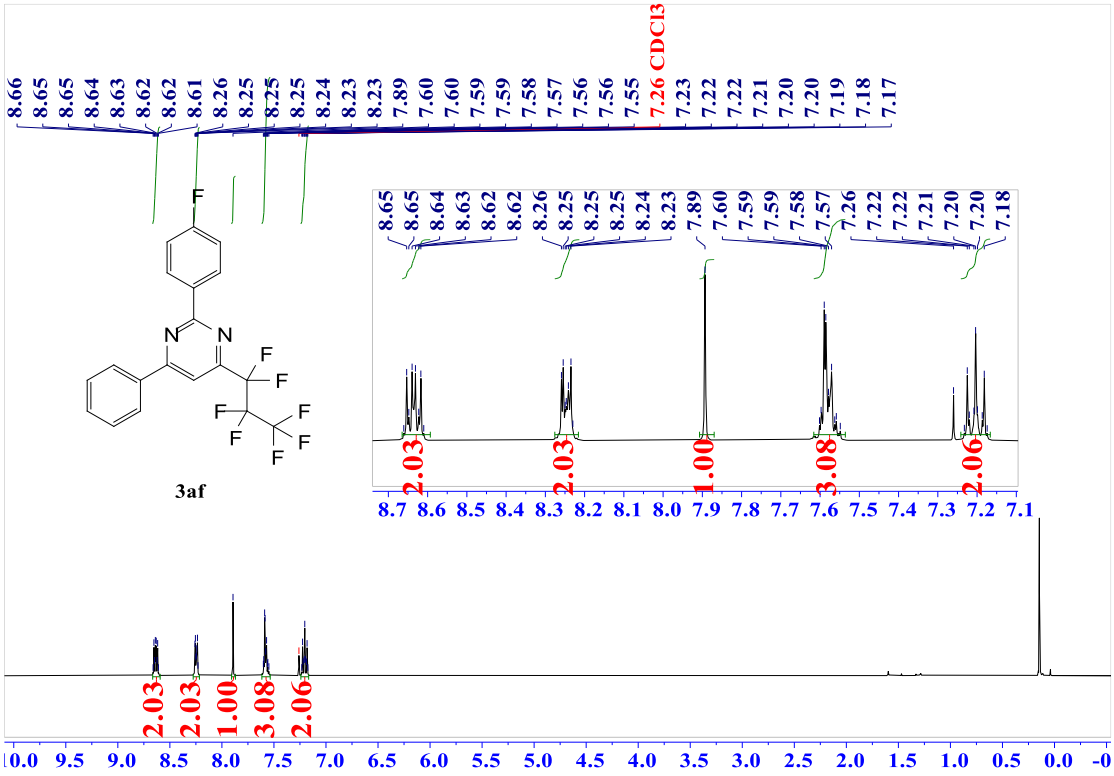
f1 (ppm)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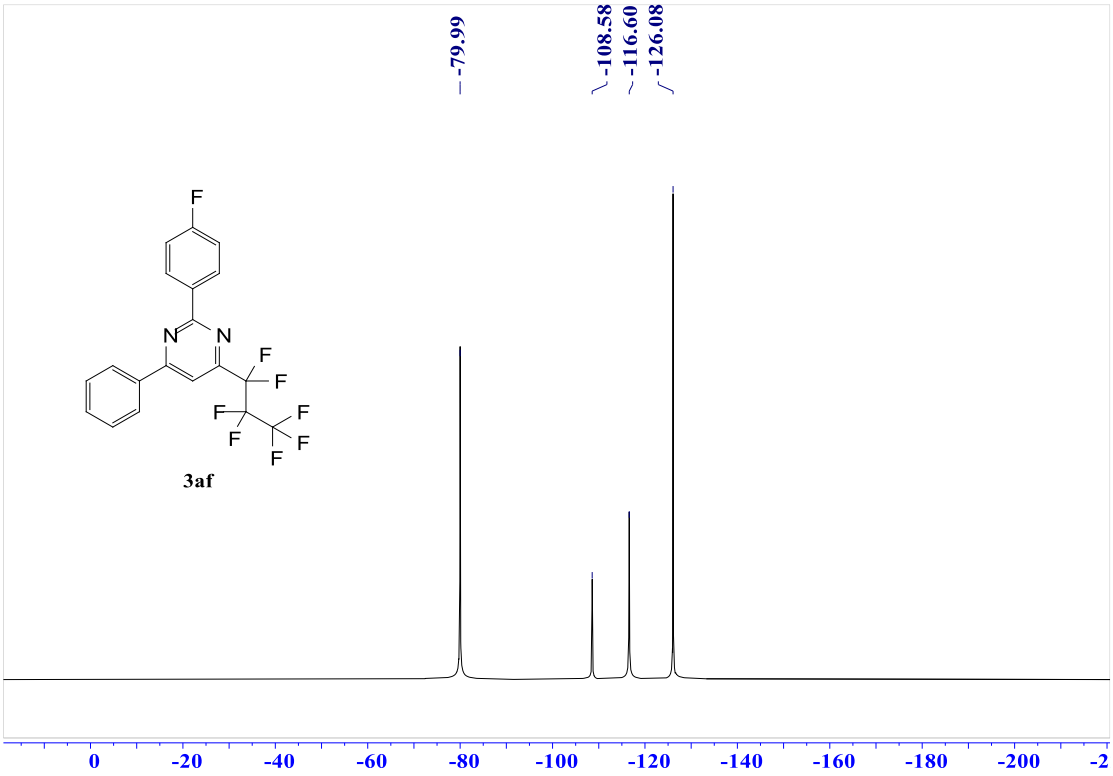
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0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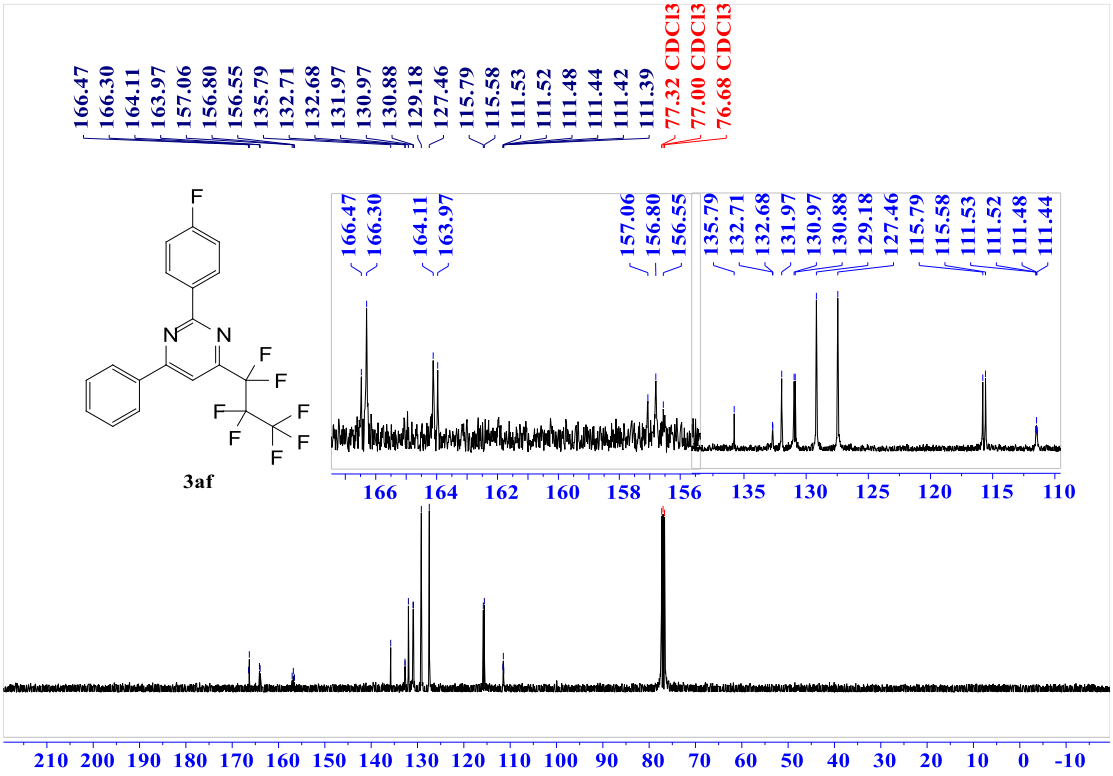
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77.00 CDCl3
76.68 CDCl3
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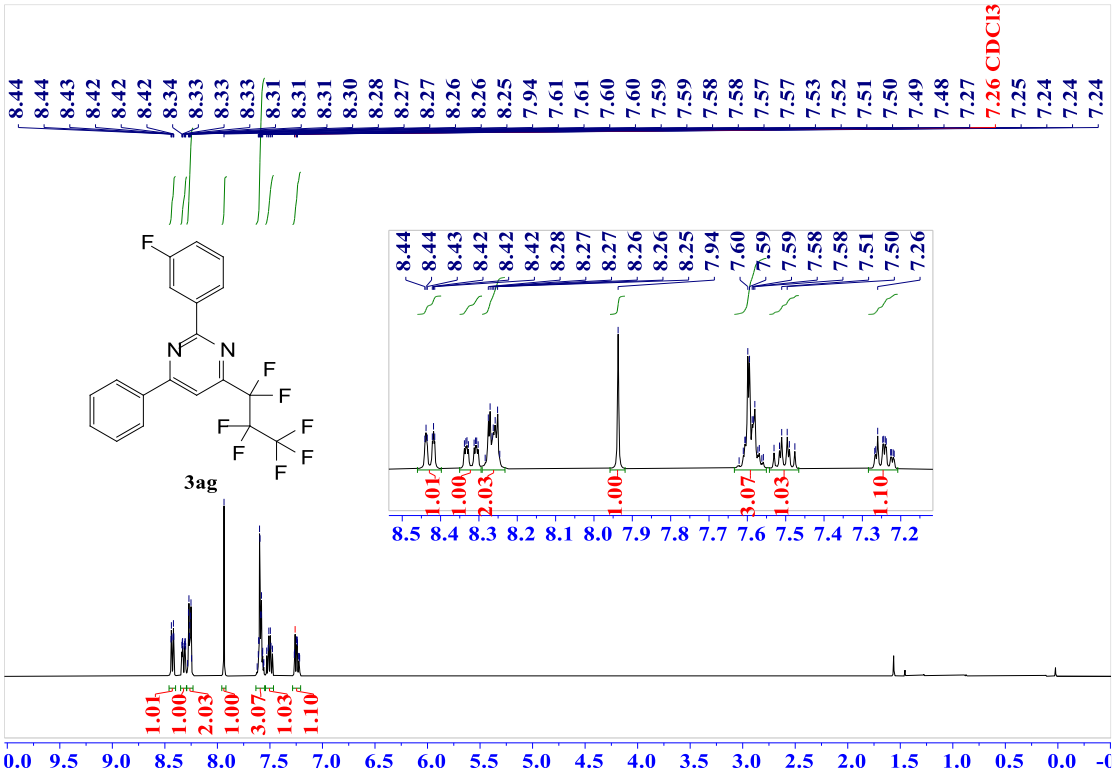
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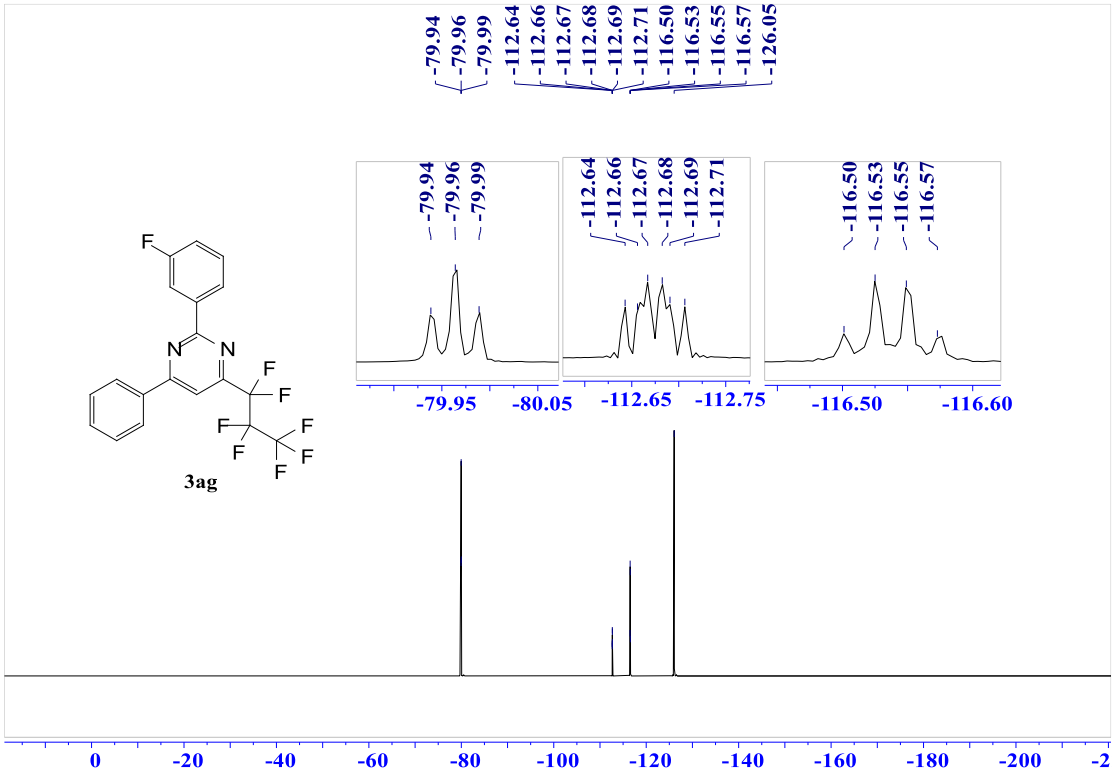
3ag
1.01 1.00 2.03 1.00 3.07 1.03 1.10
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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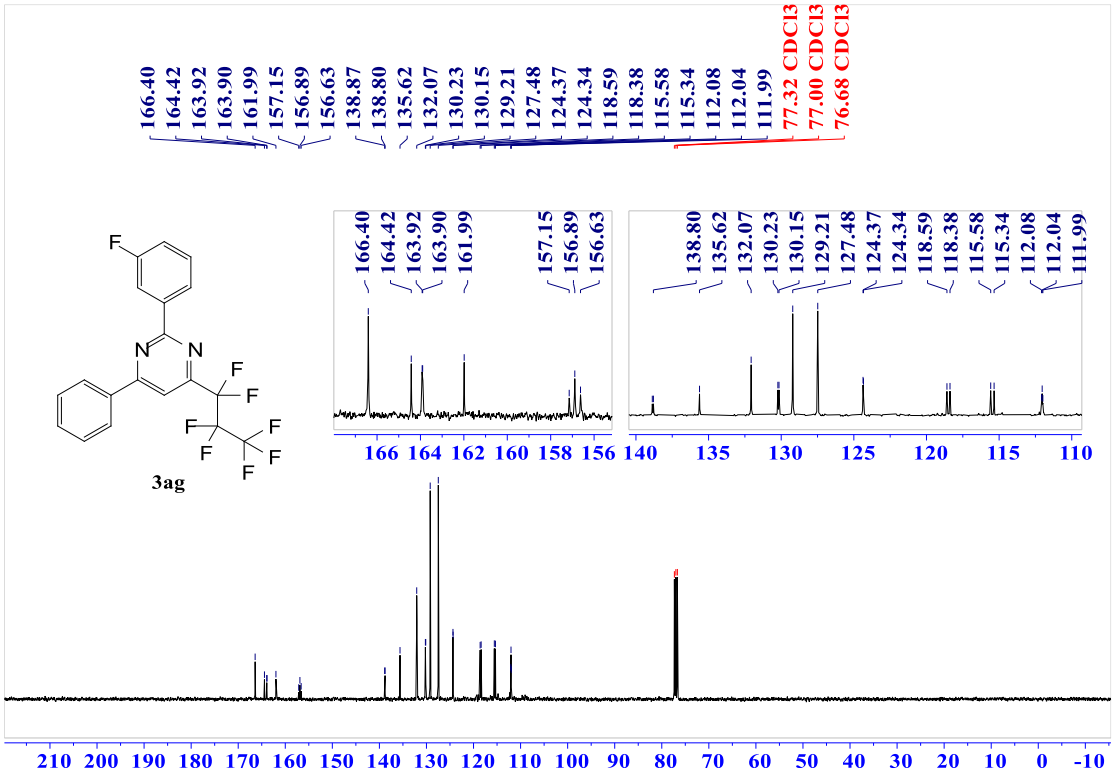
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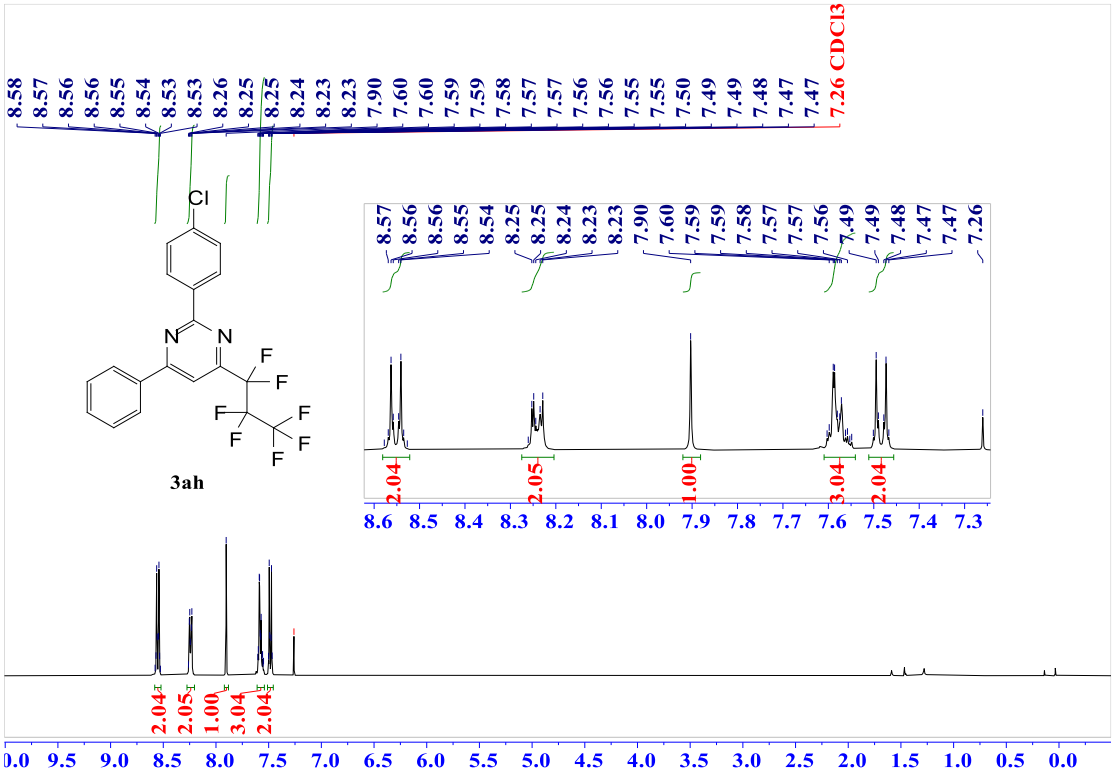
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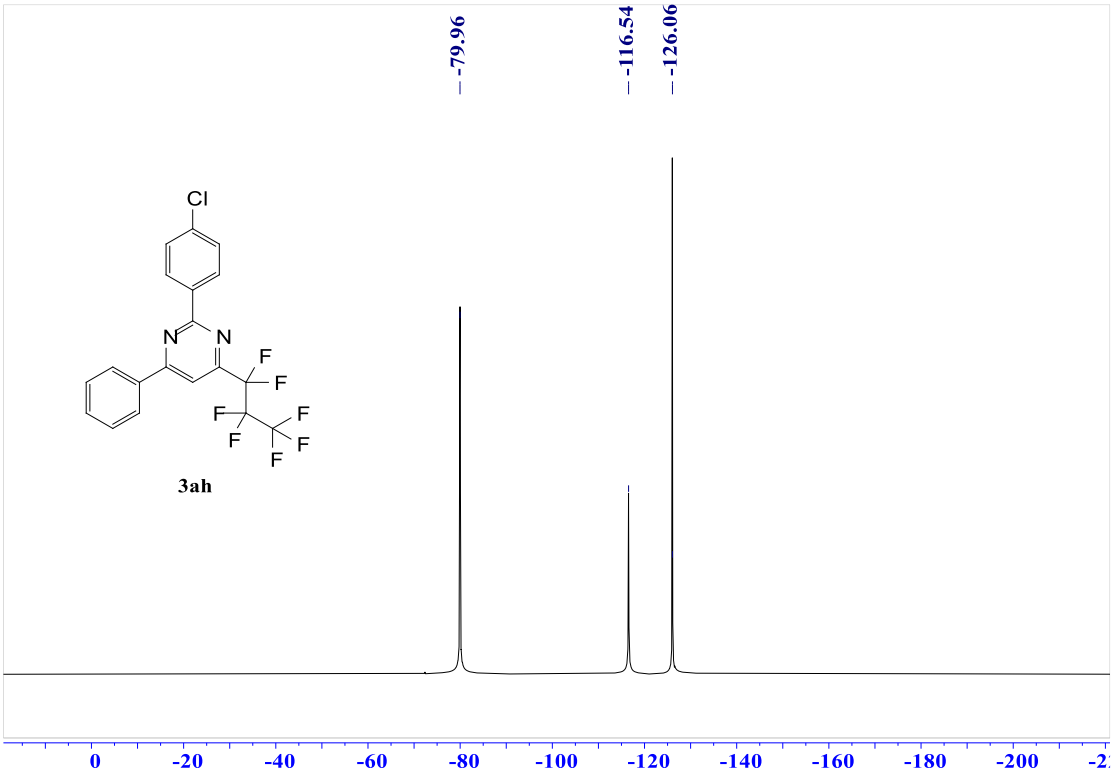
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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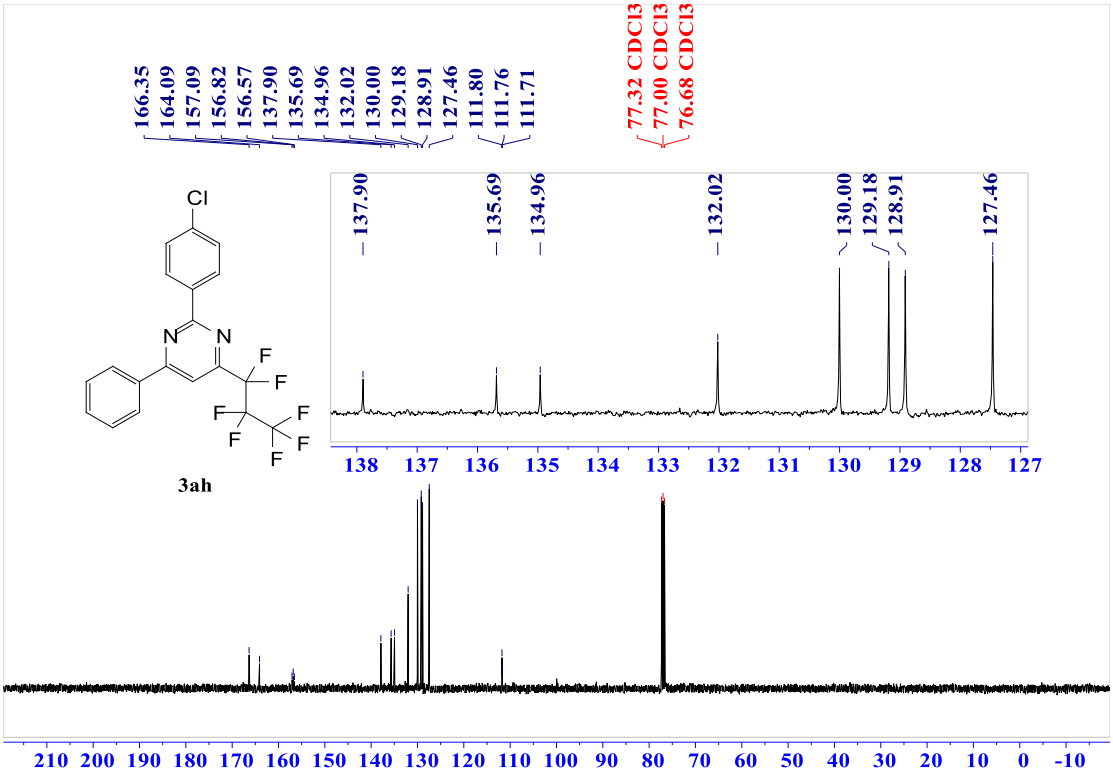
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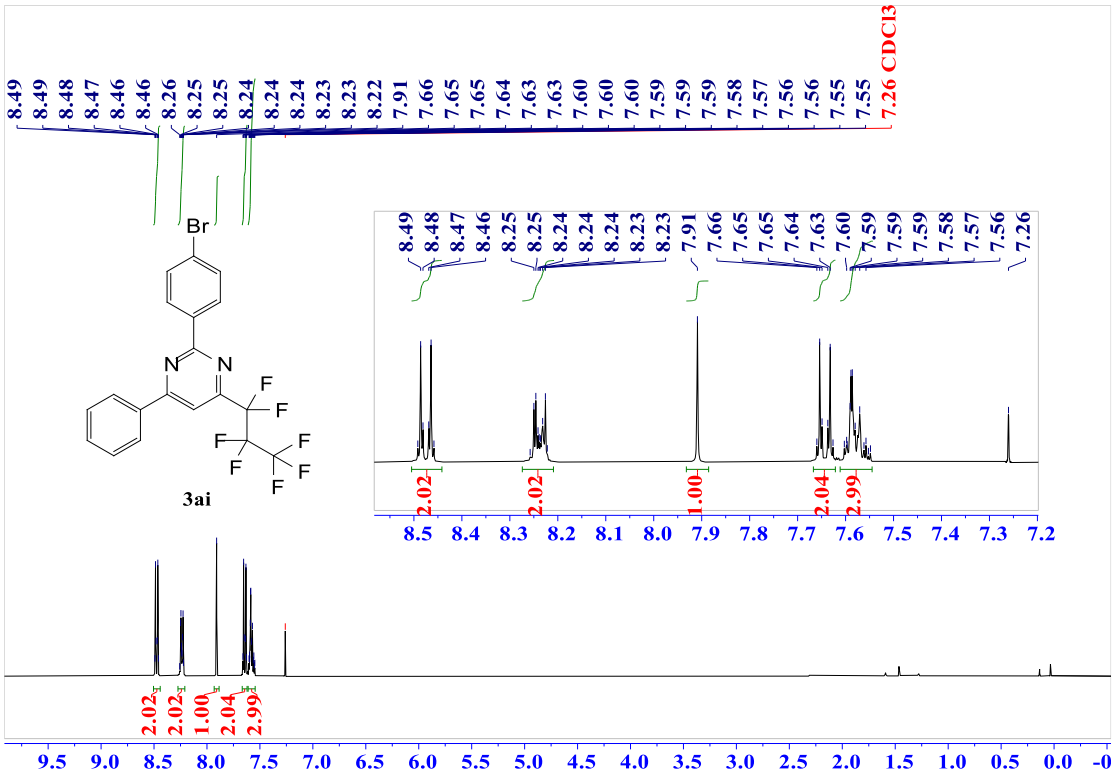
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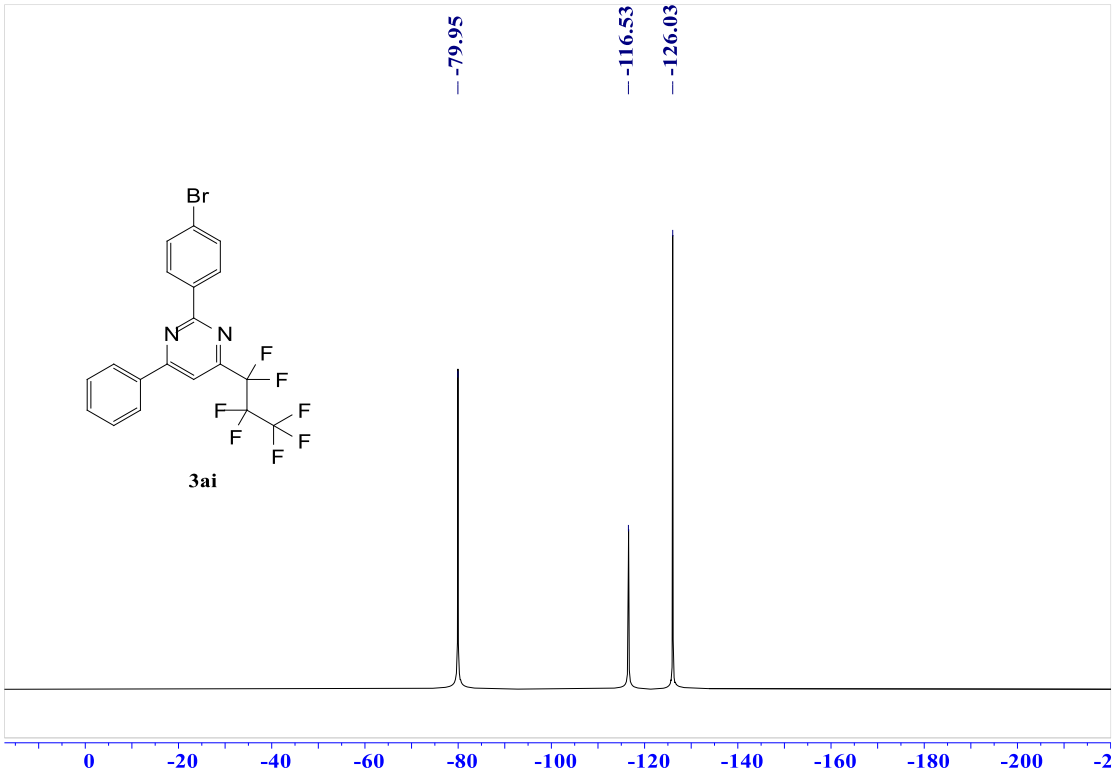
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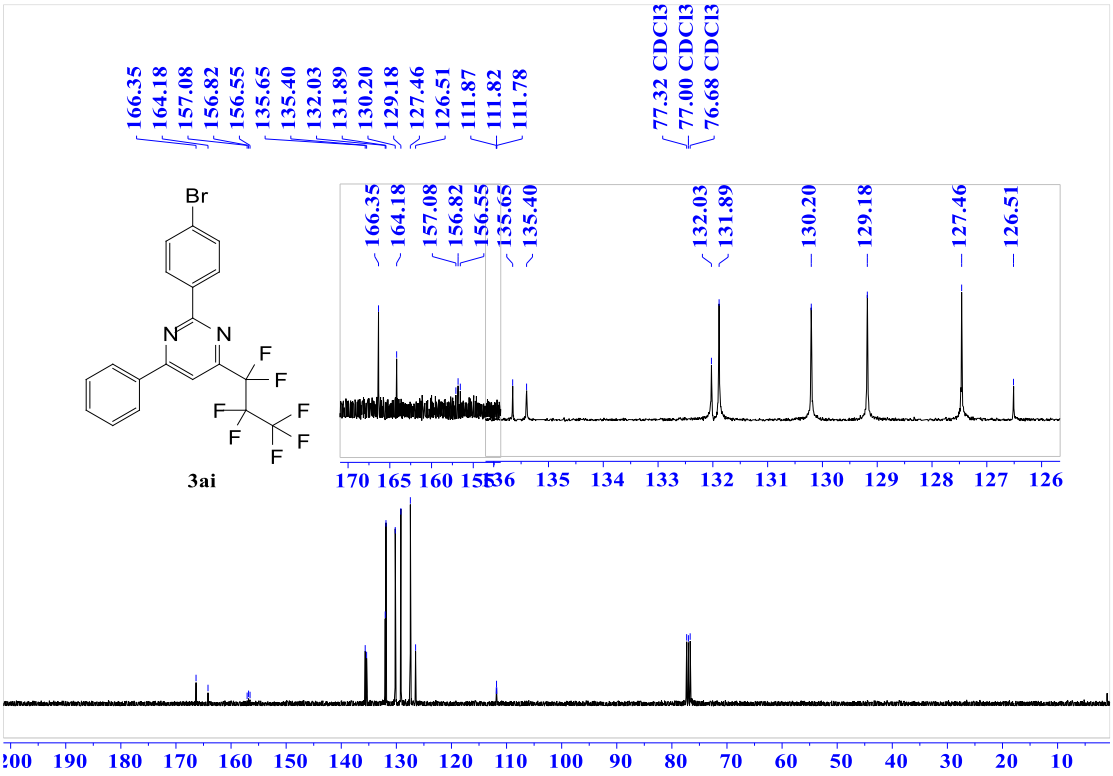
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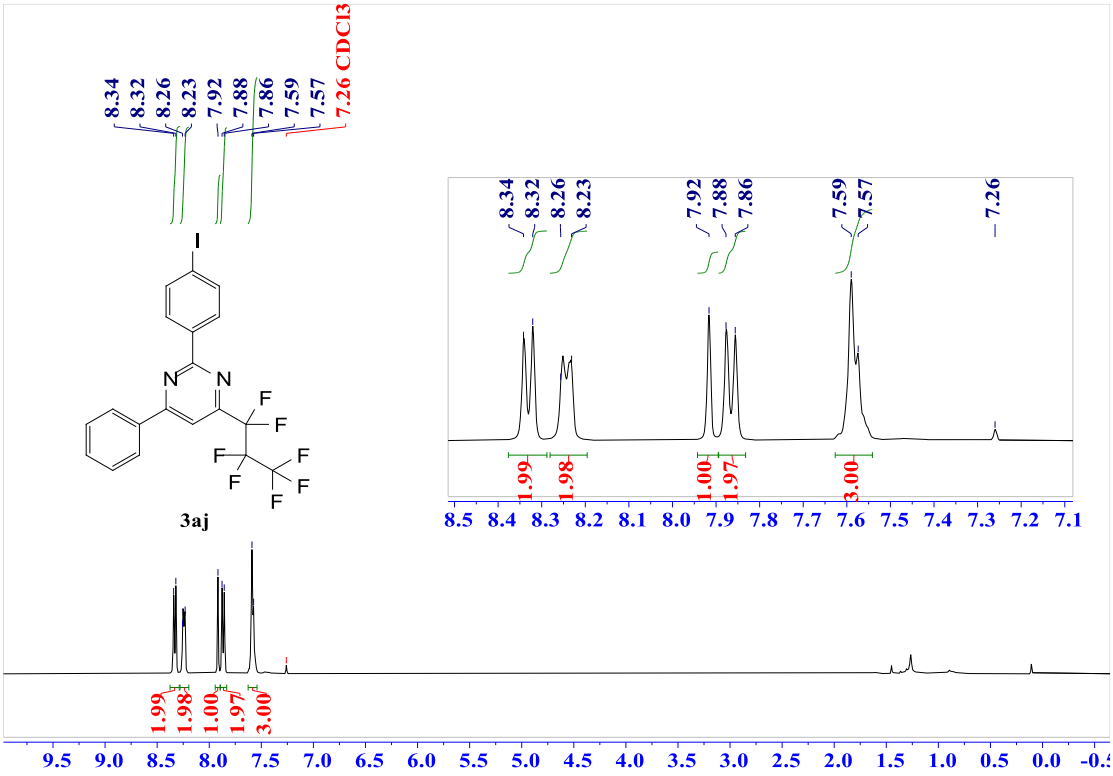
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1.97
3.00
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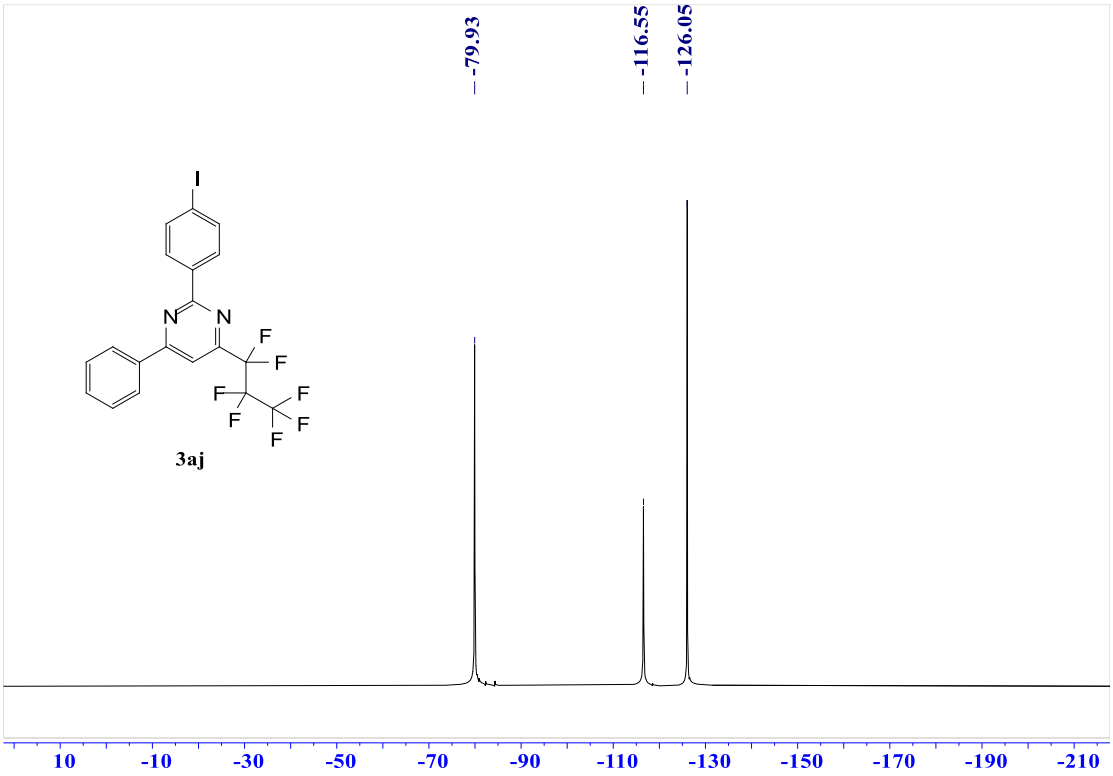
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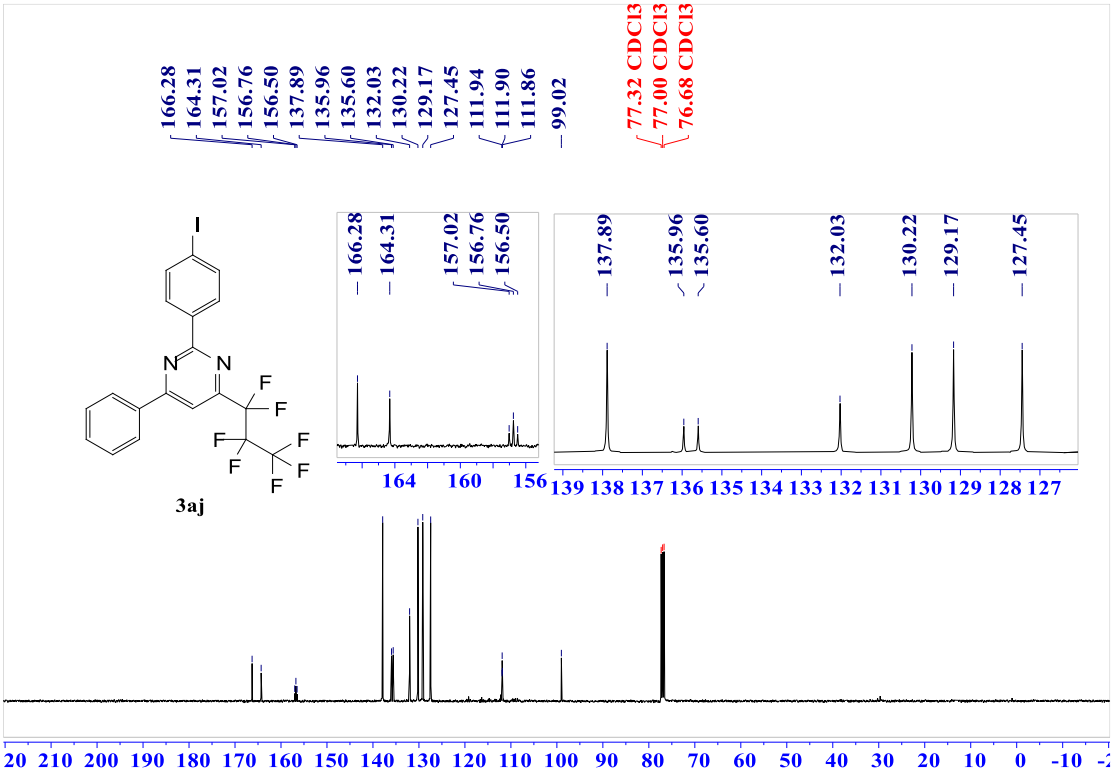
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76.68 CDCl3
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3aj
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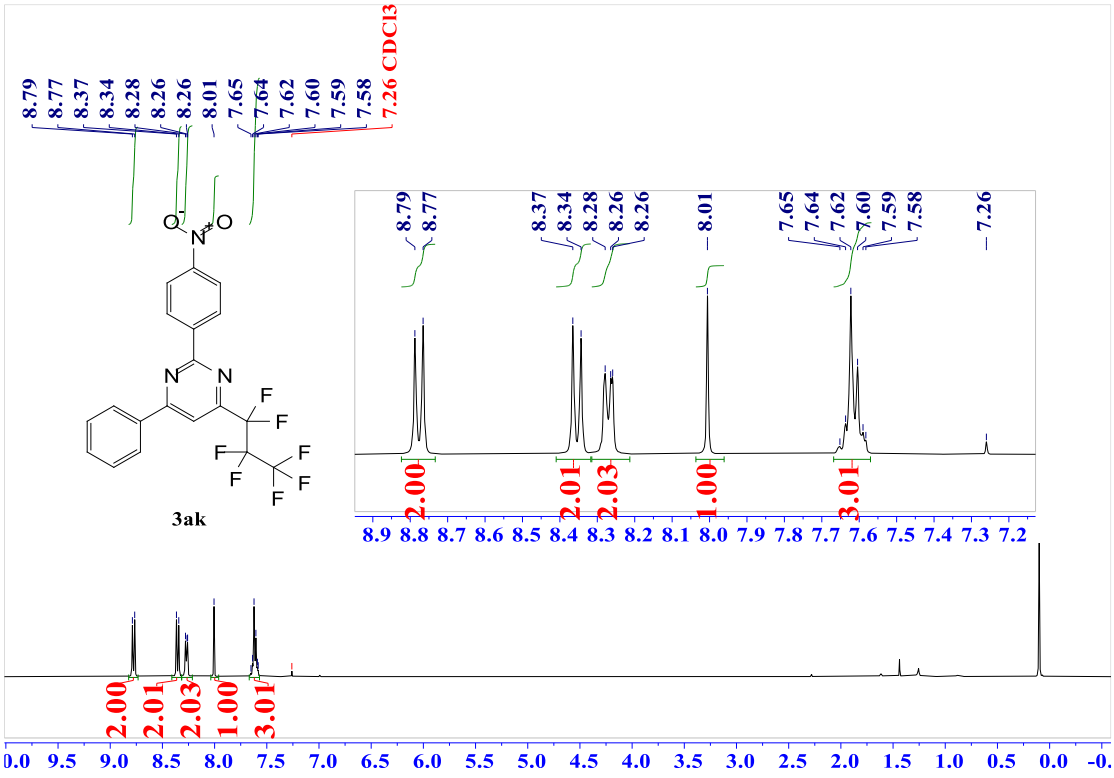
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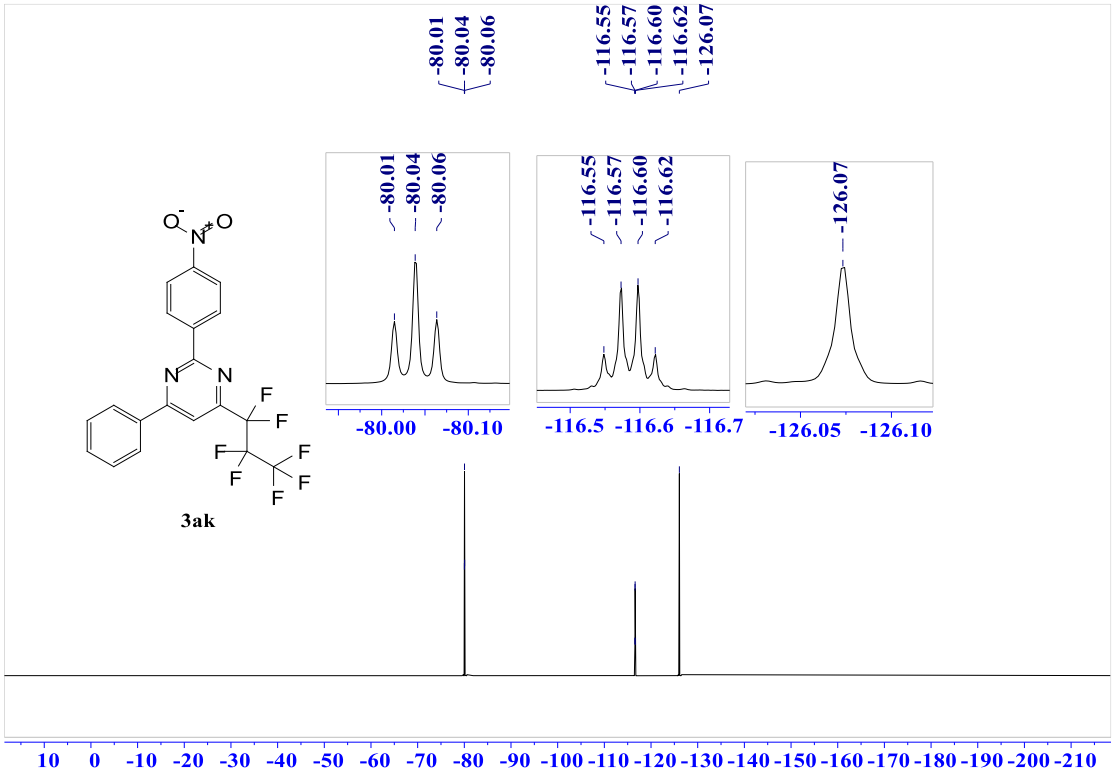
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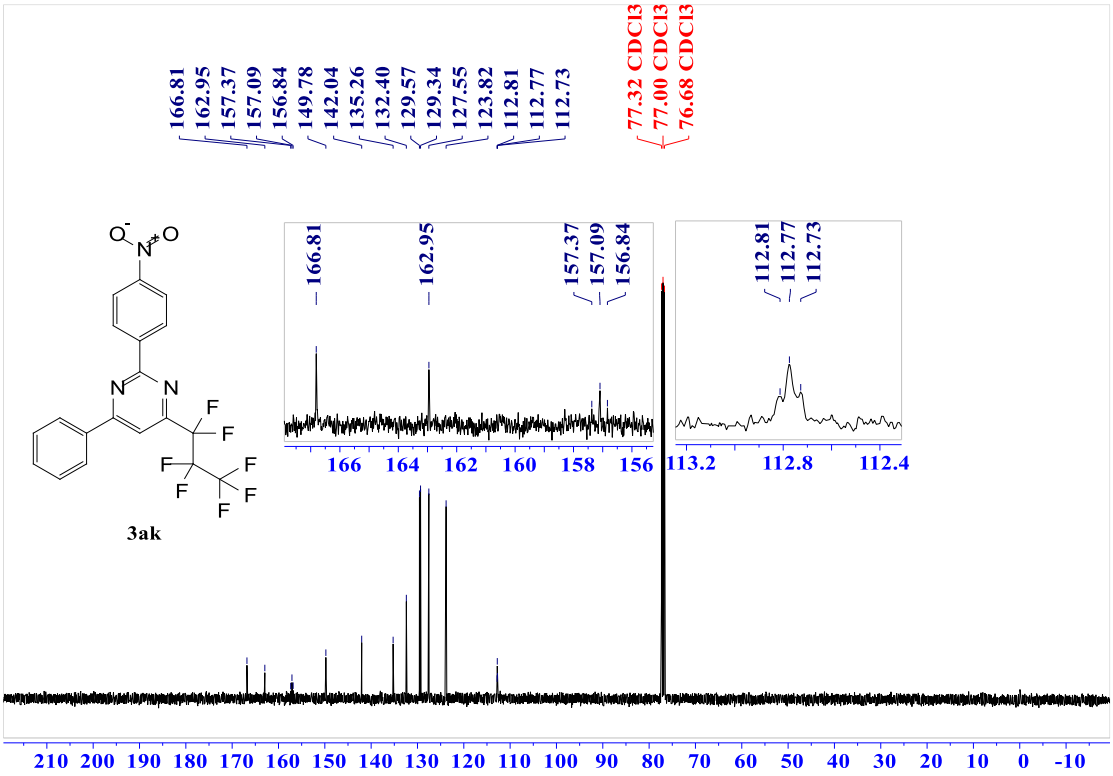
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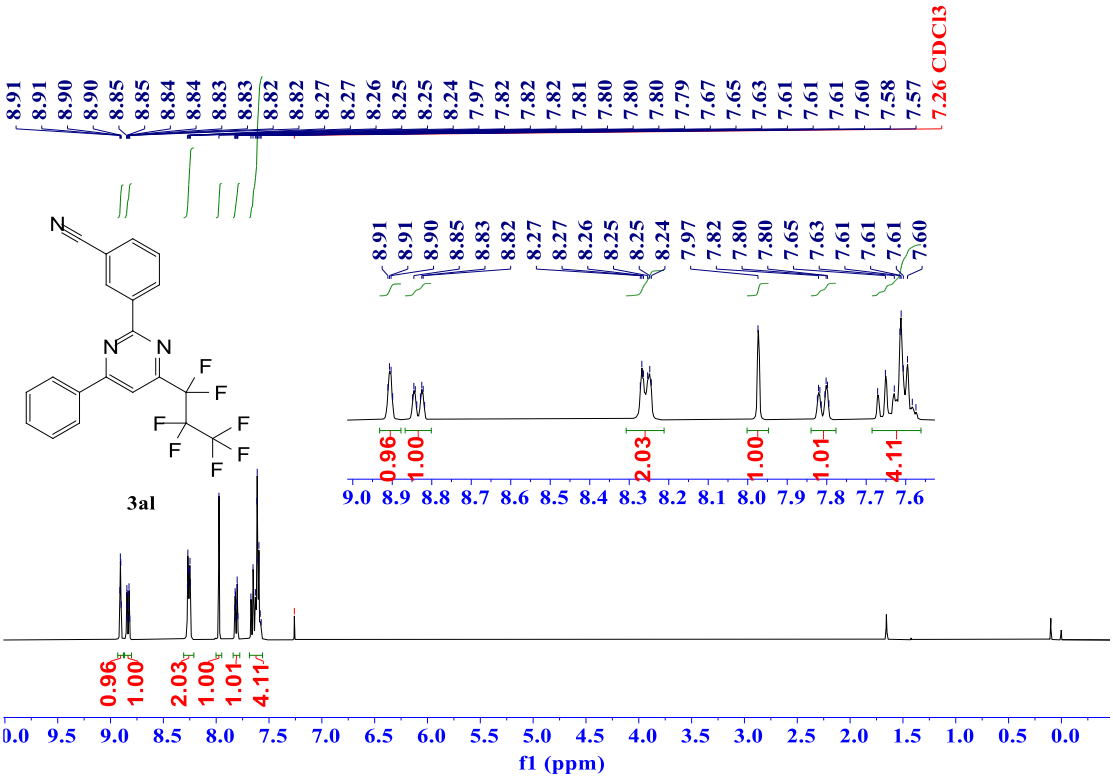
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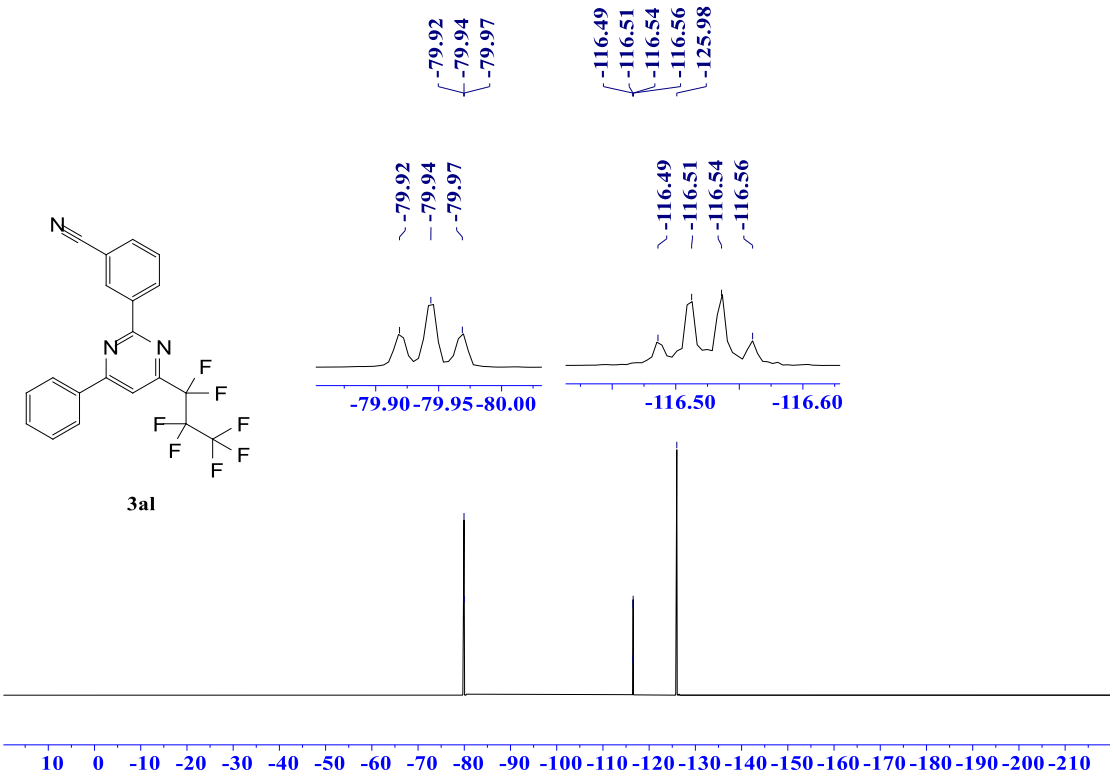
4.11
f1 (ppm)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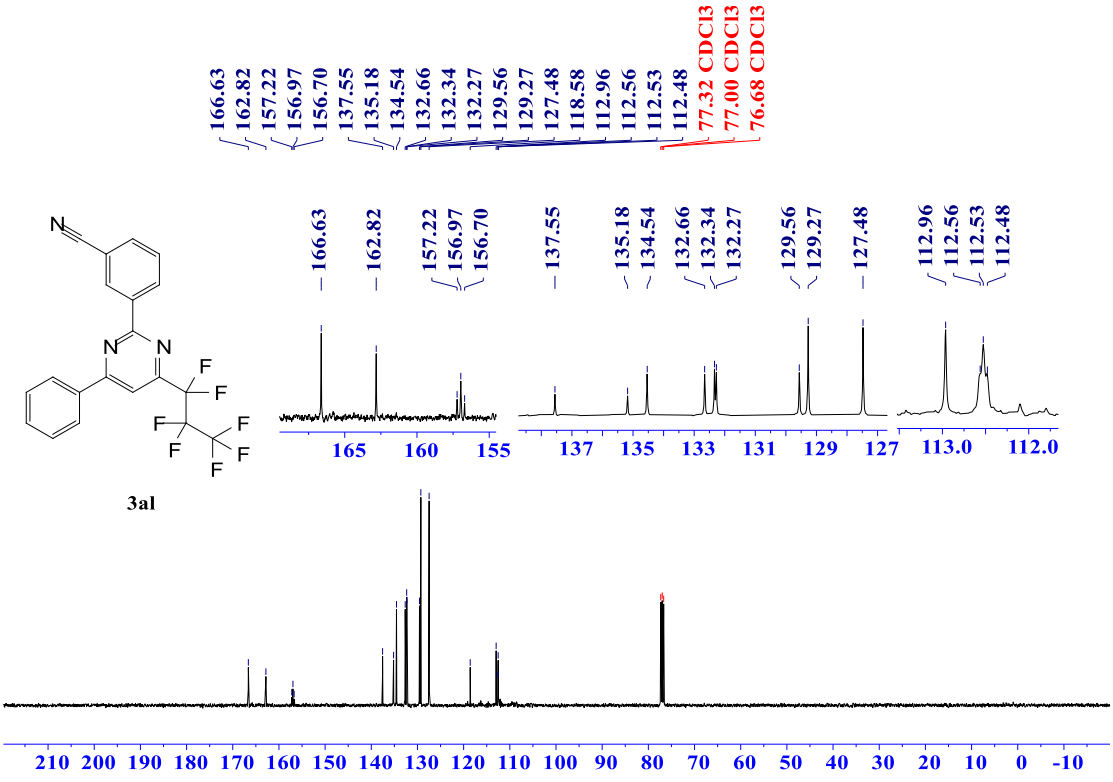
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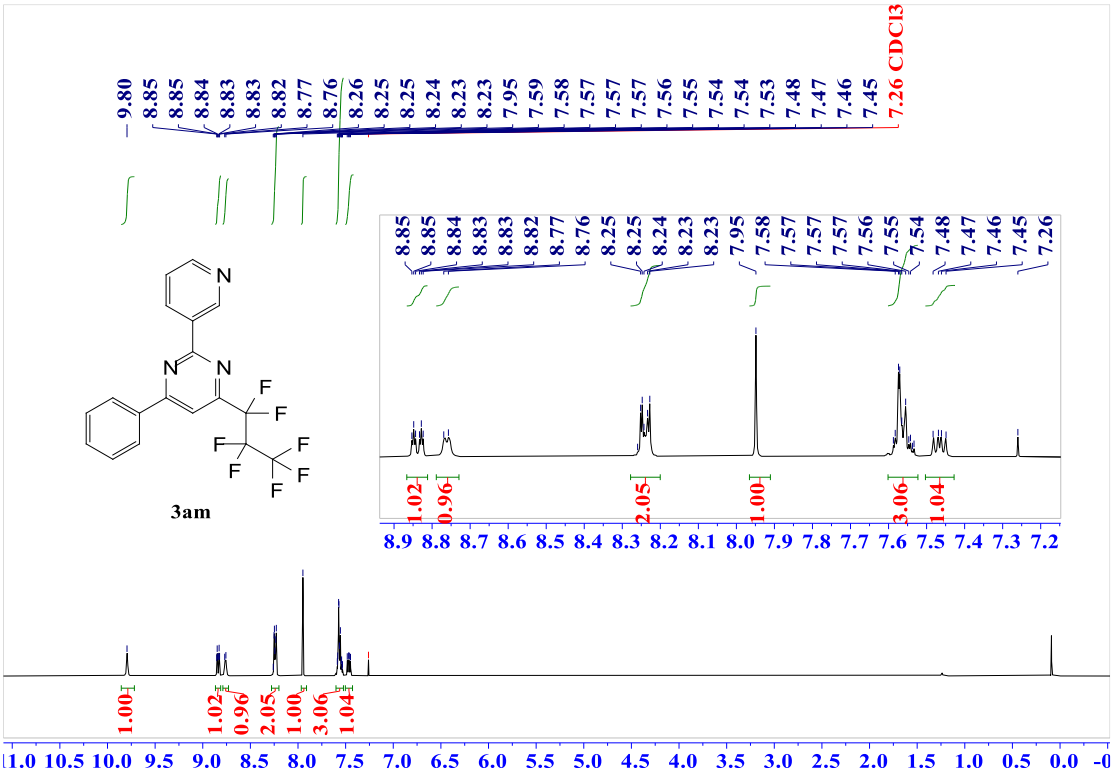
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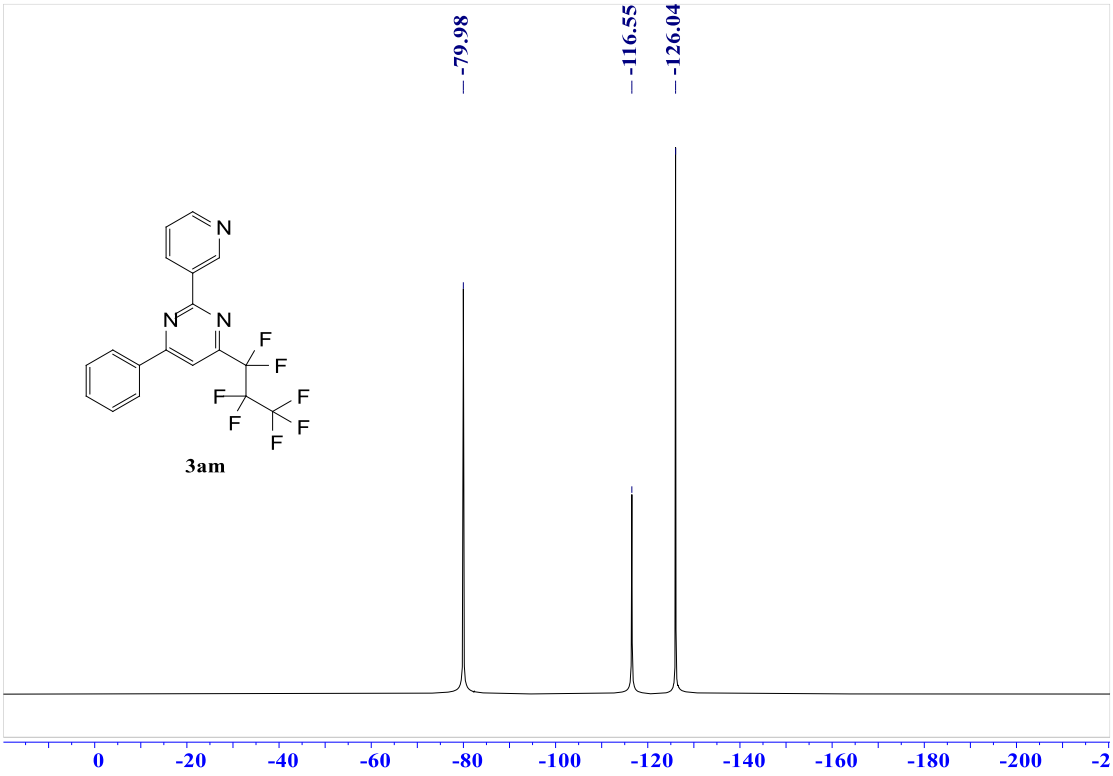
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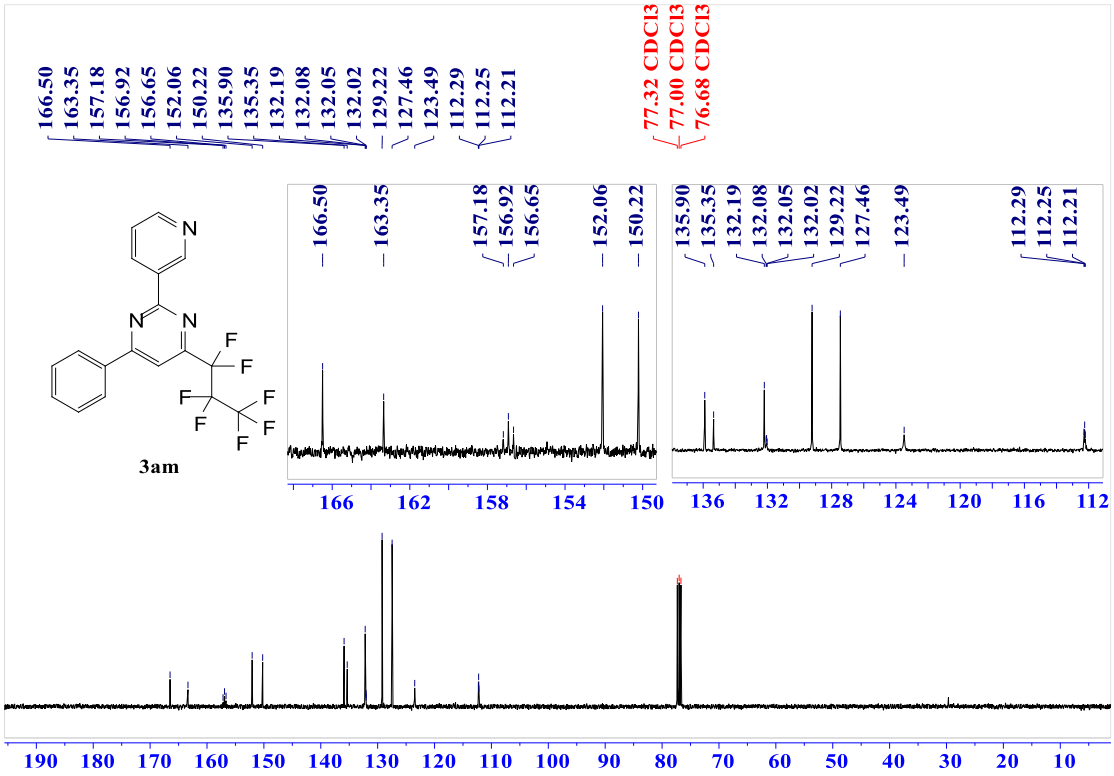
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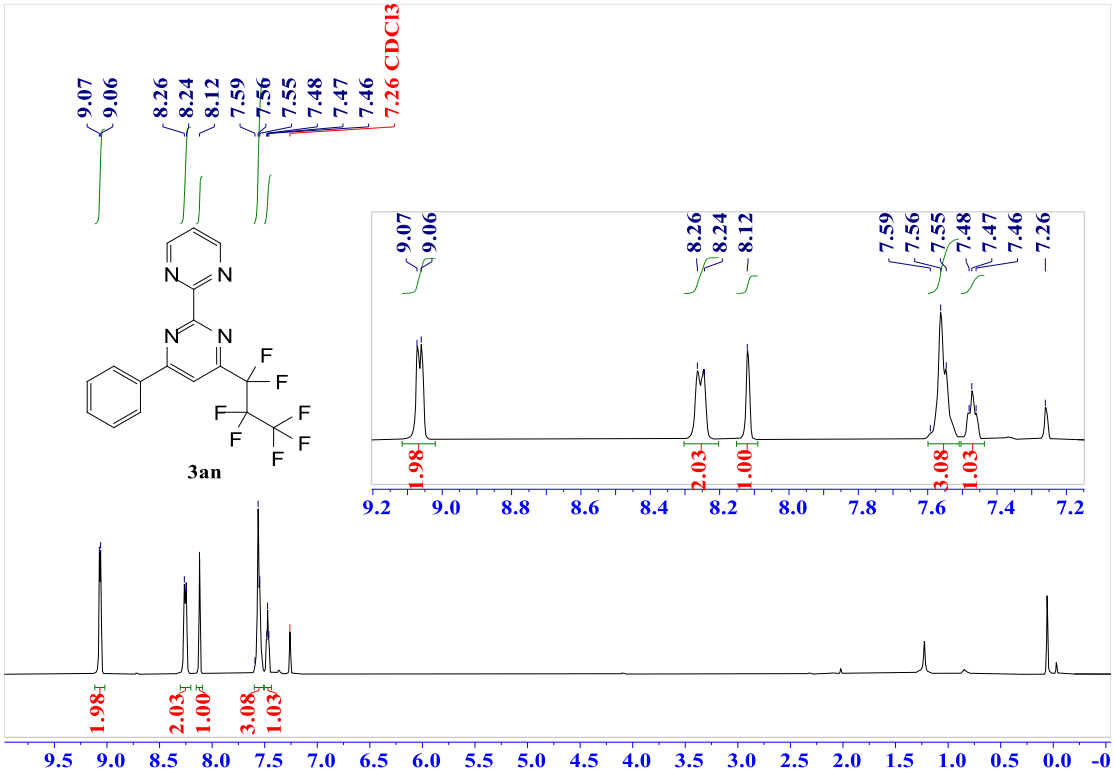
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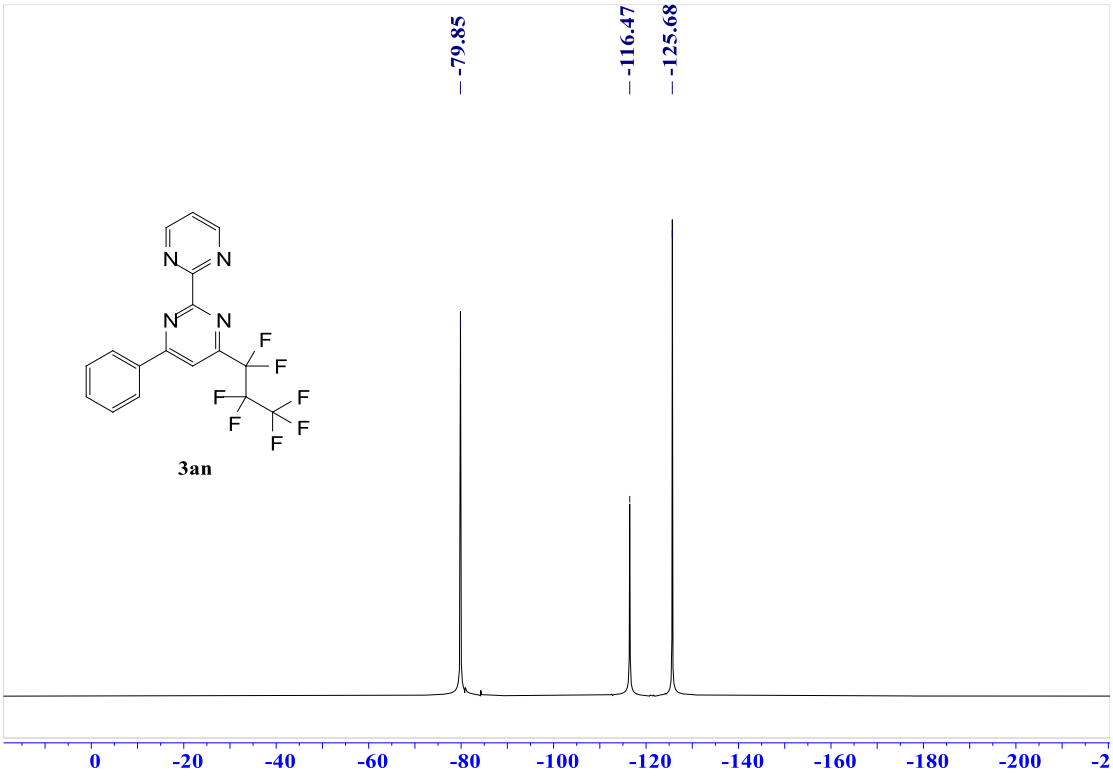
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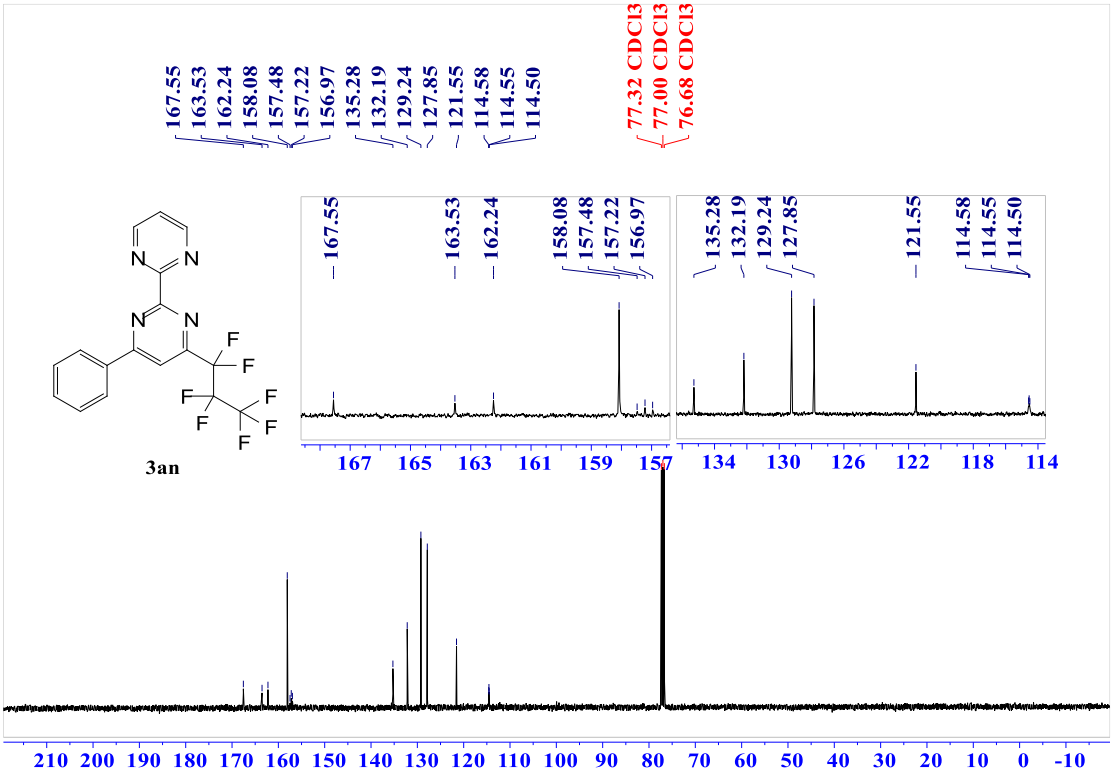
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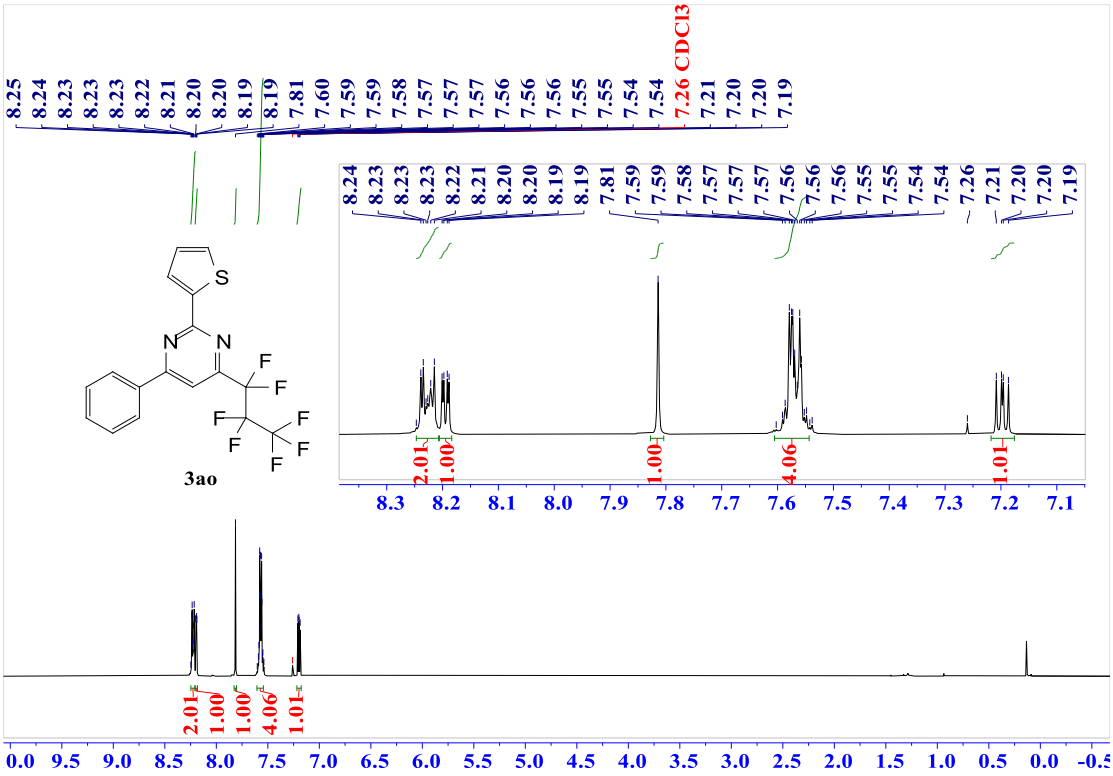
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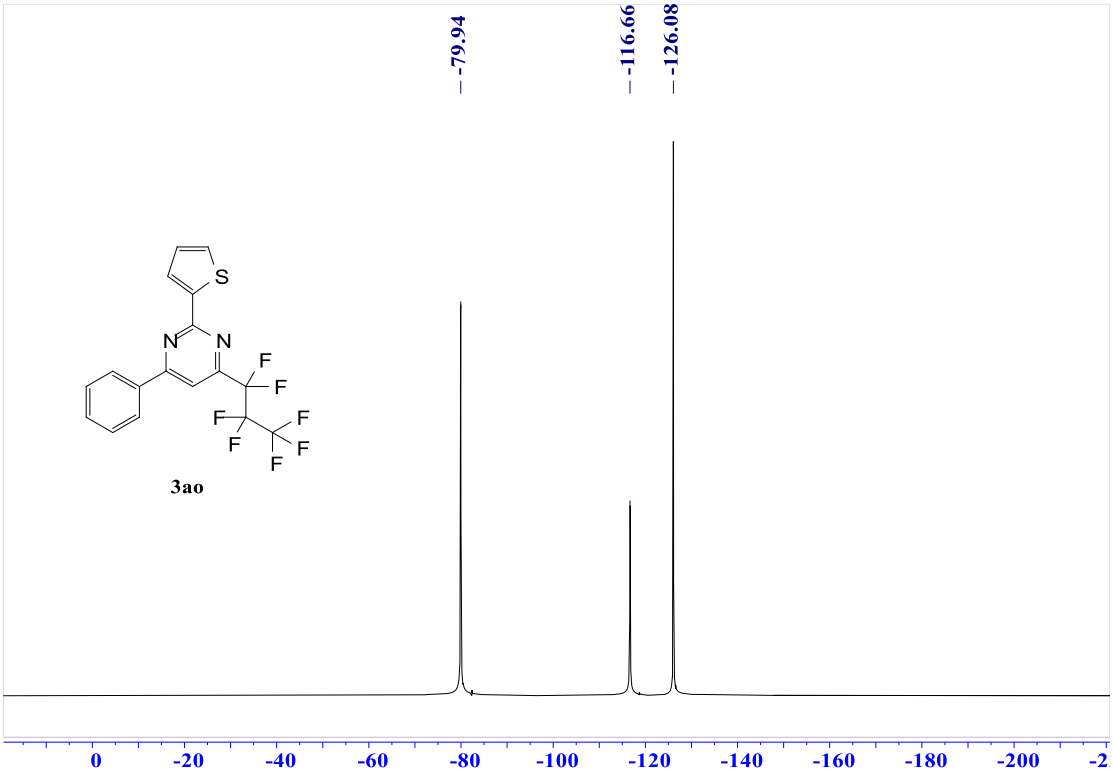
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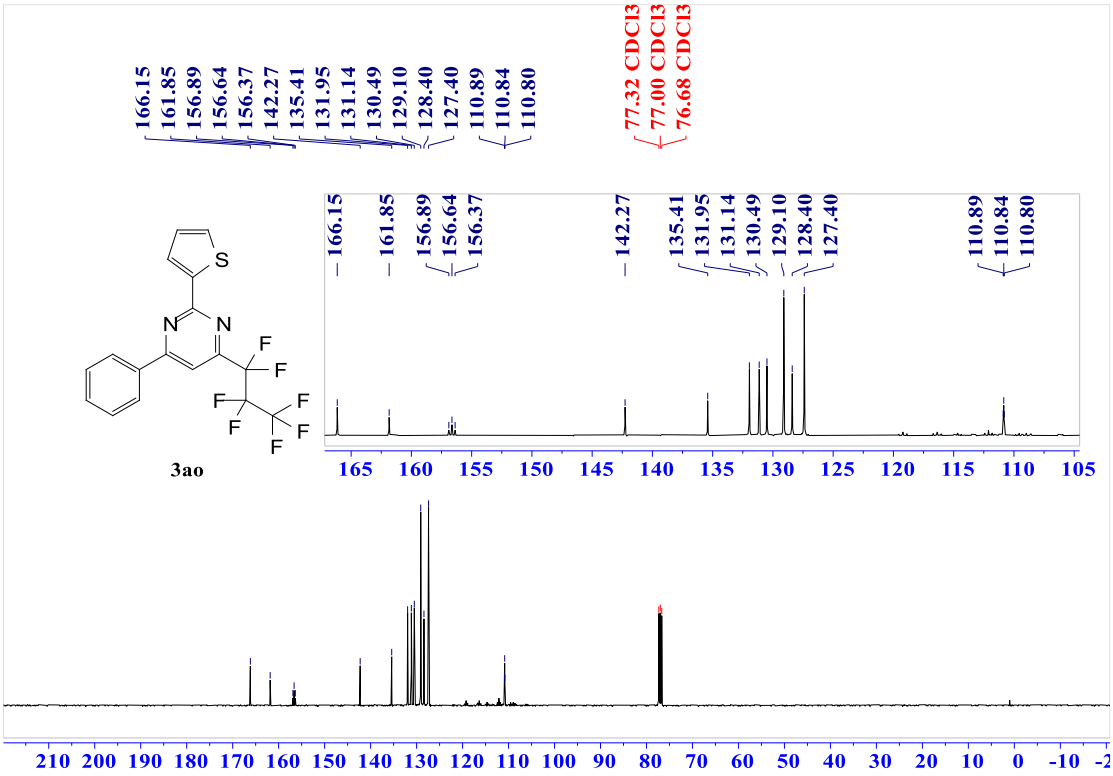
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110.80
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77.00 CDCl3
76.68 CDCl3
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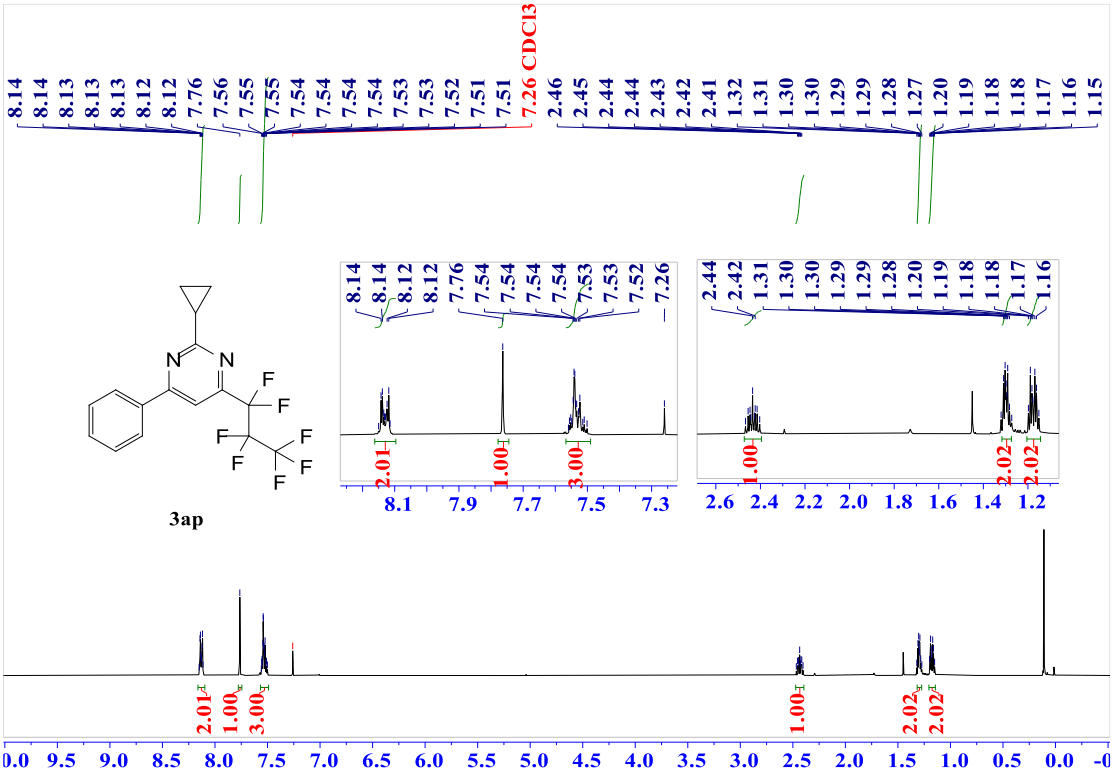
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7.51
7.26 CDCl3
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2.45
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1.17
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3ap
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1.00
3.00
1.00
2.02
2.02
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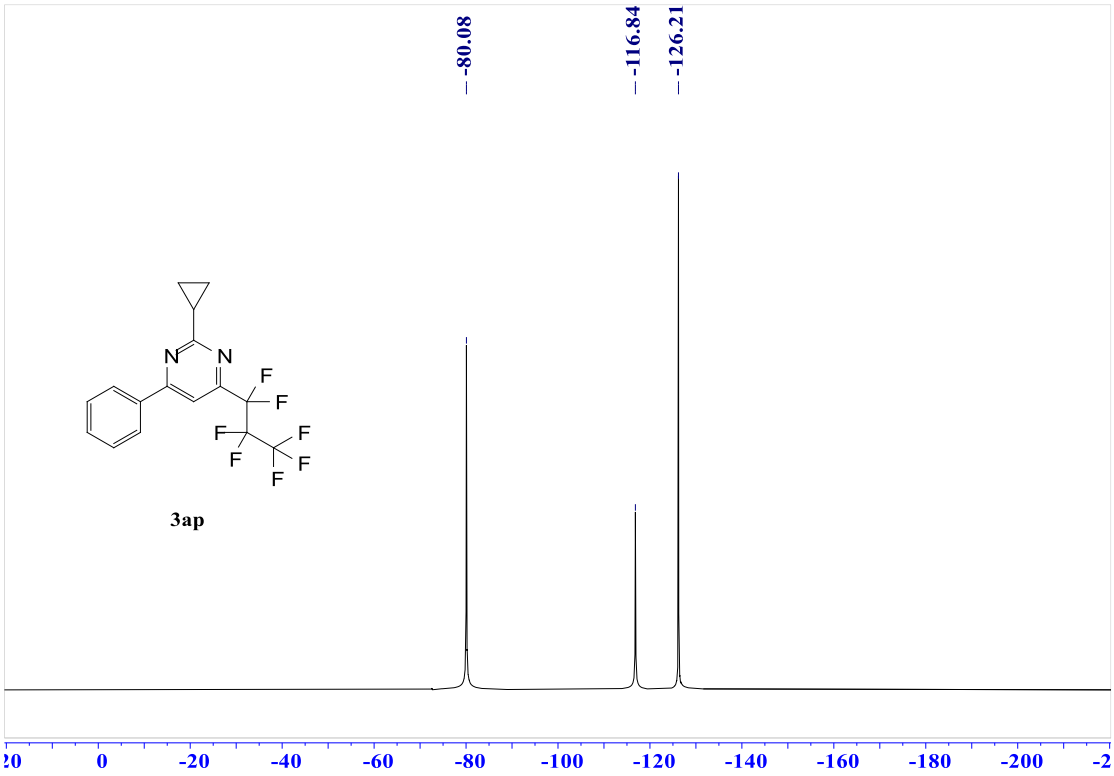
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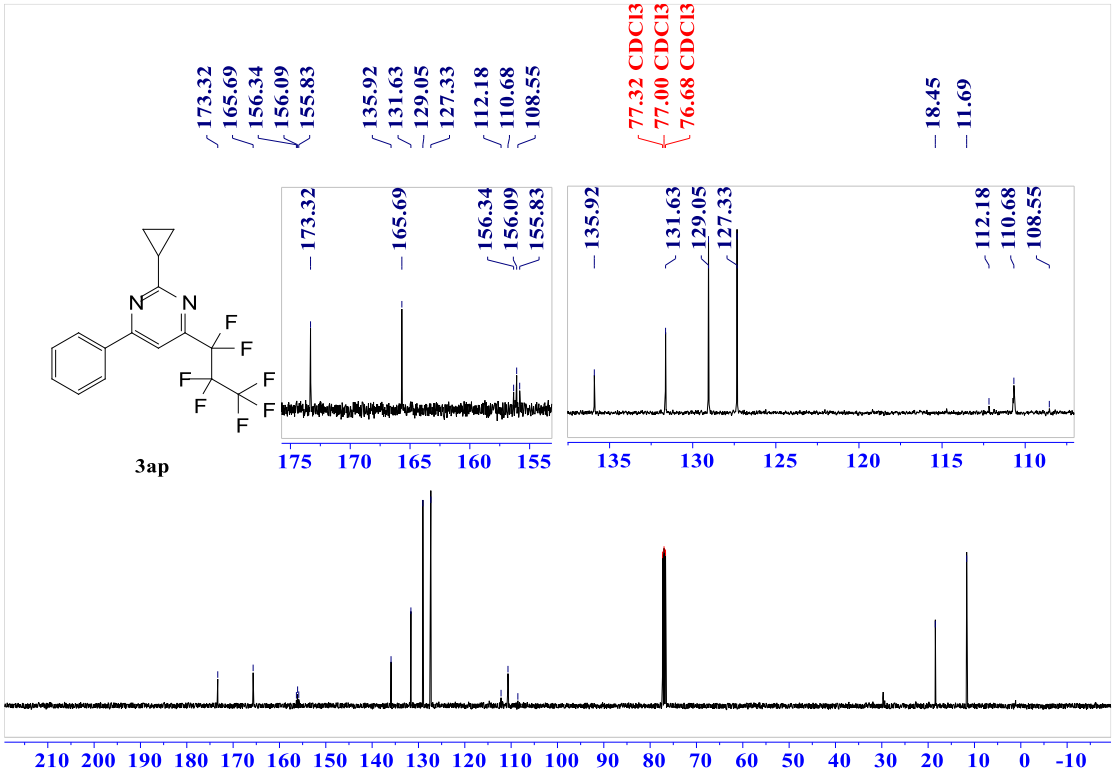
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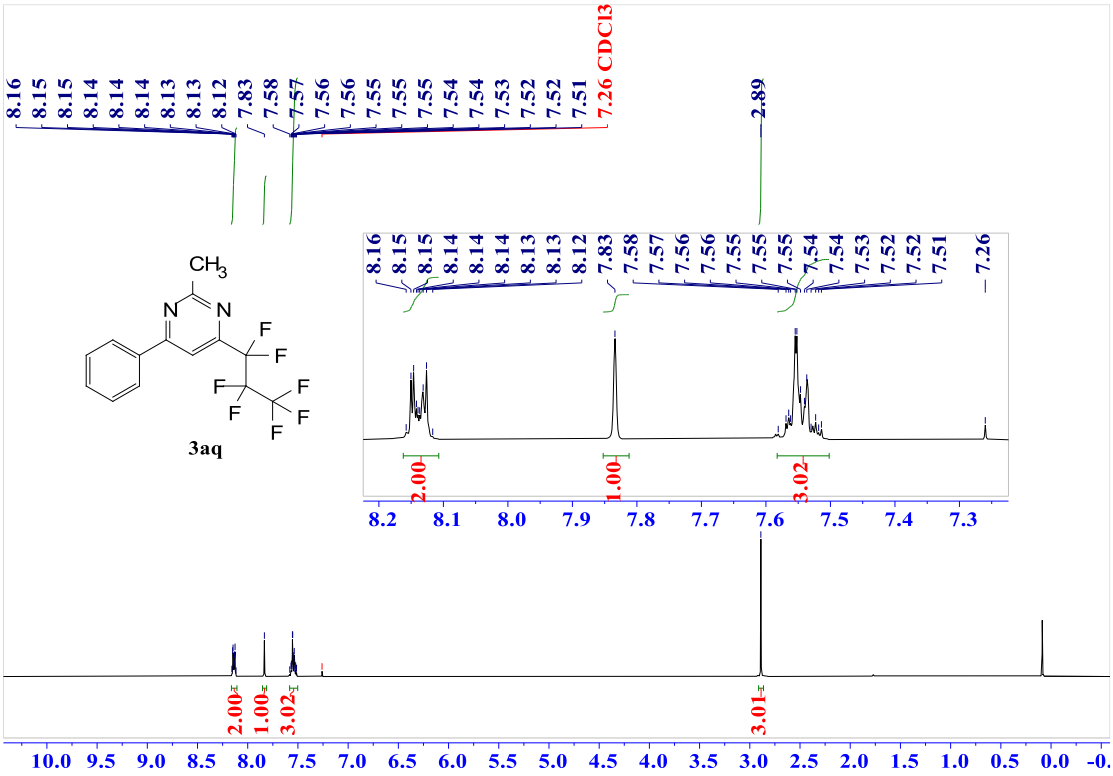
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2.89
CH3
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1.00
3.02
3.01
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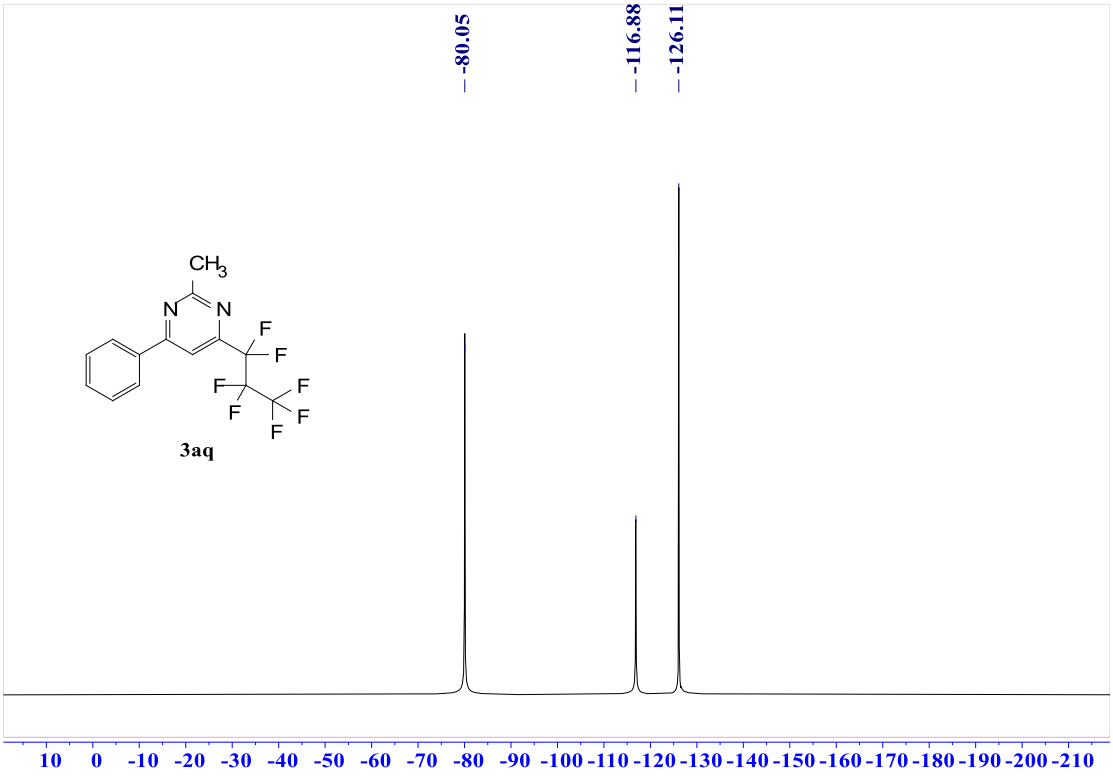
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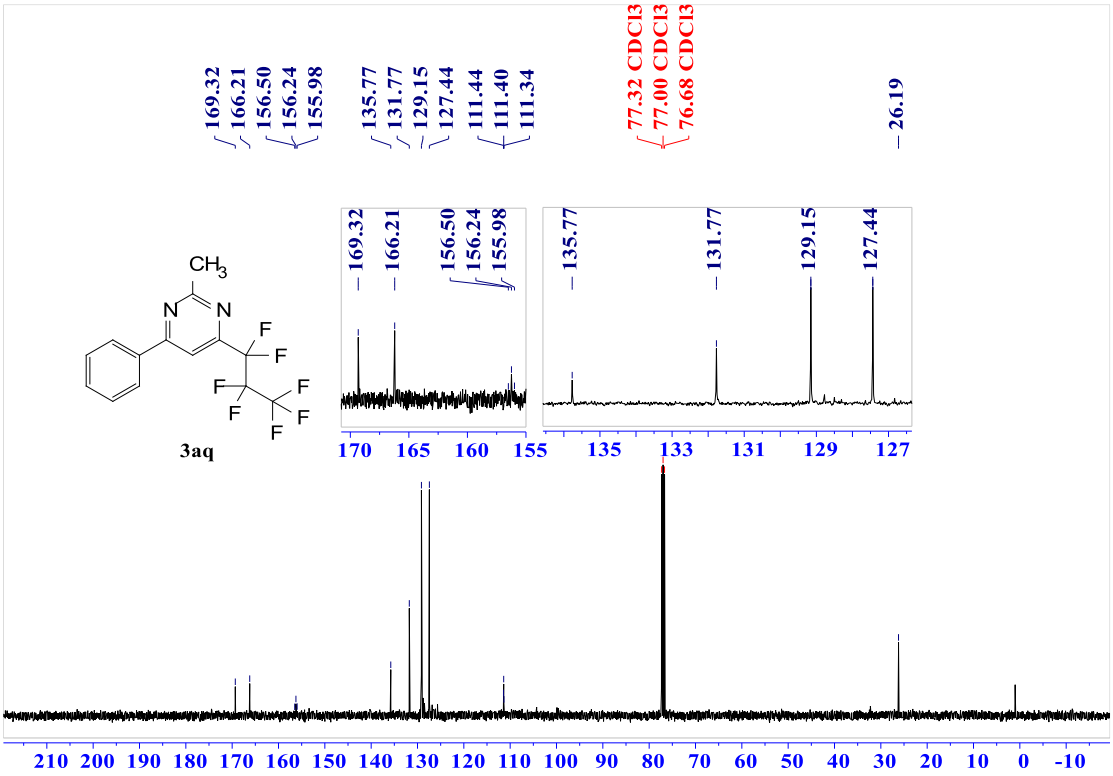
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77.00 CDCl3
76.68 CDCl3
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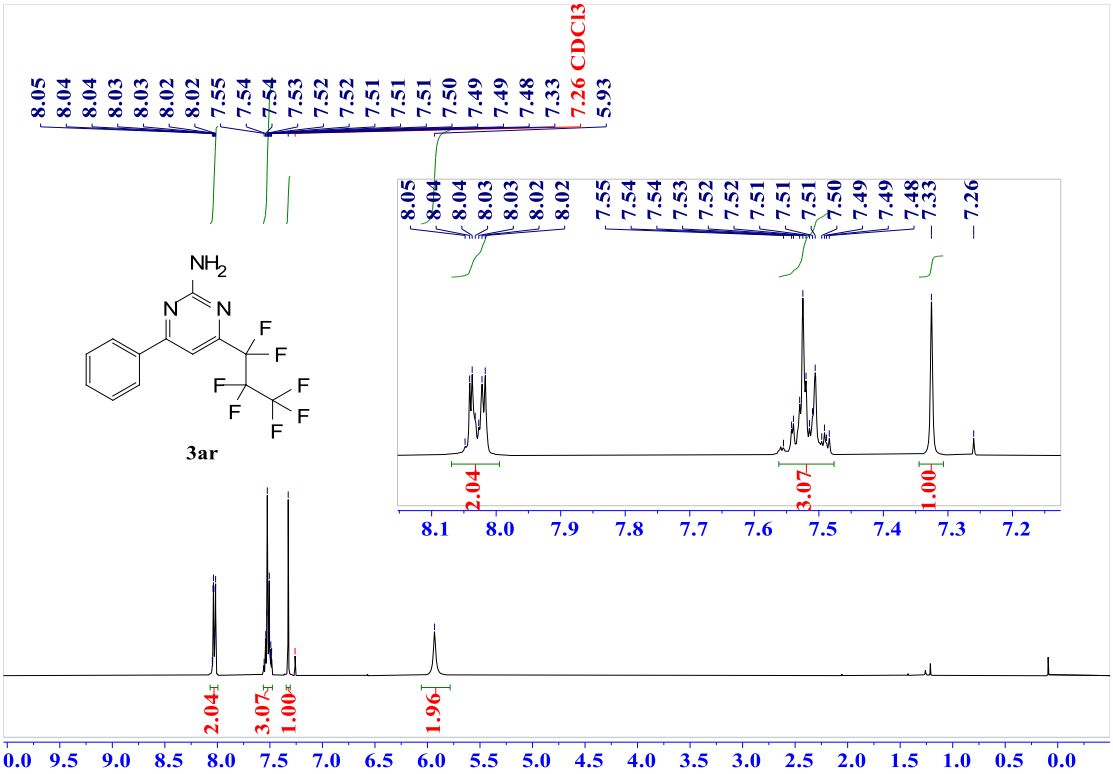
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7.48
7.33
7.26 CDCl3
5.93
NH2
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N
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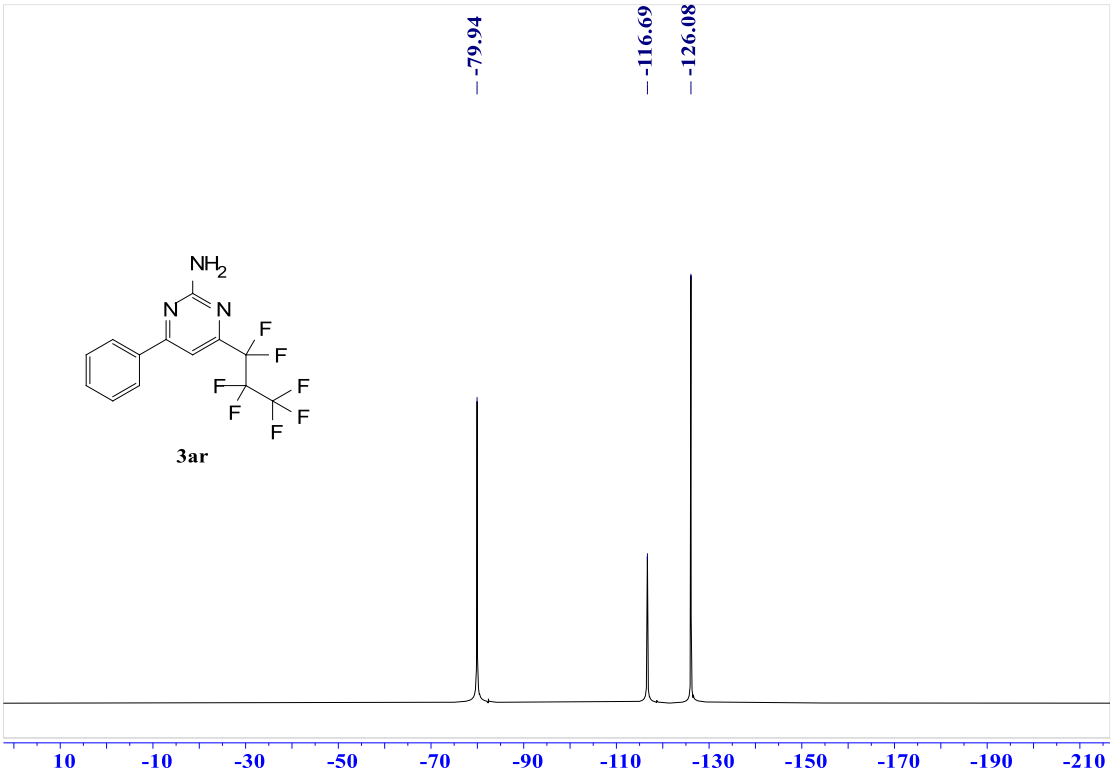
F
F
F
F
F
F
3ar
2.04
3.07
1.00
1.96
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0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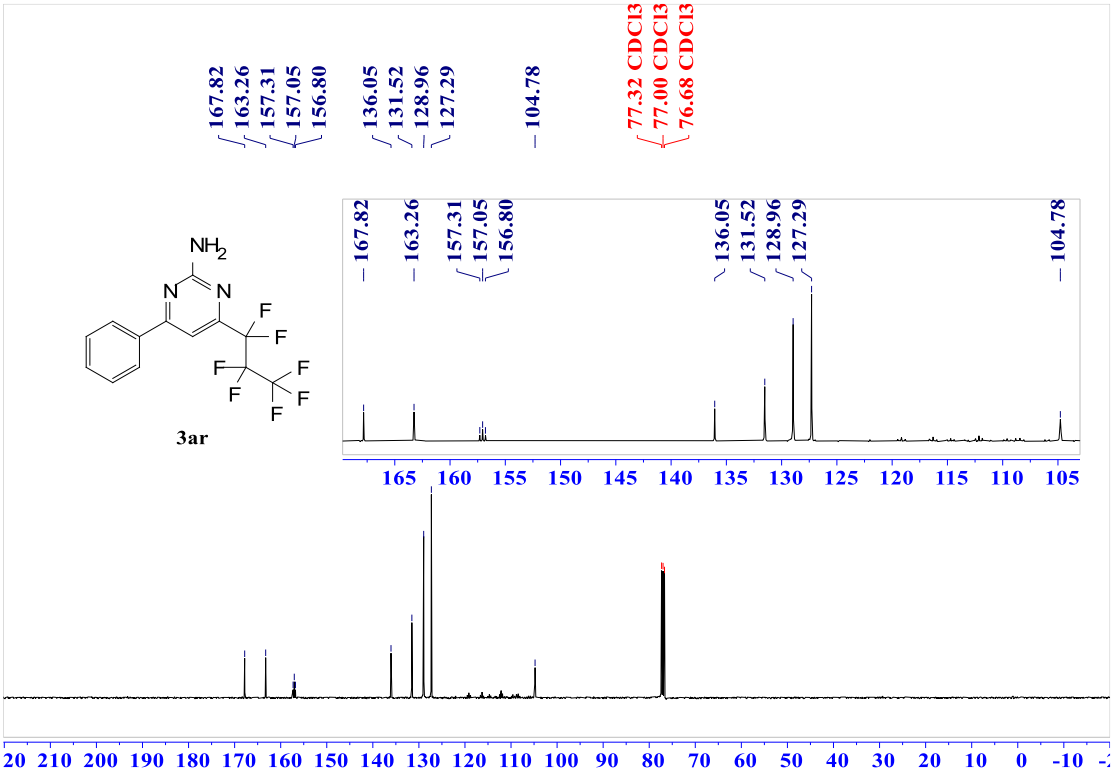
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77.00 CDCl3
76.68 CDCl3
NH2
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3ar
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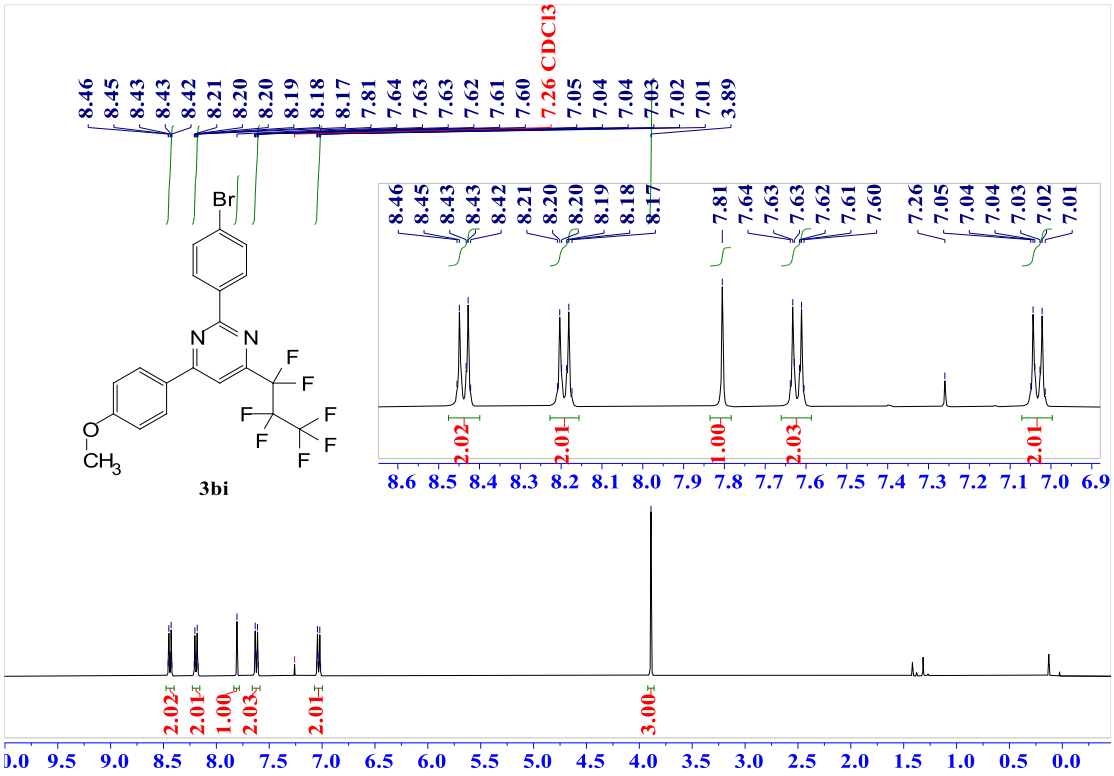
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Br
N
N
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F
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F
F
O
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3bi
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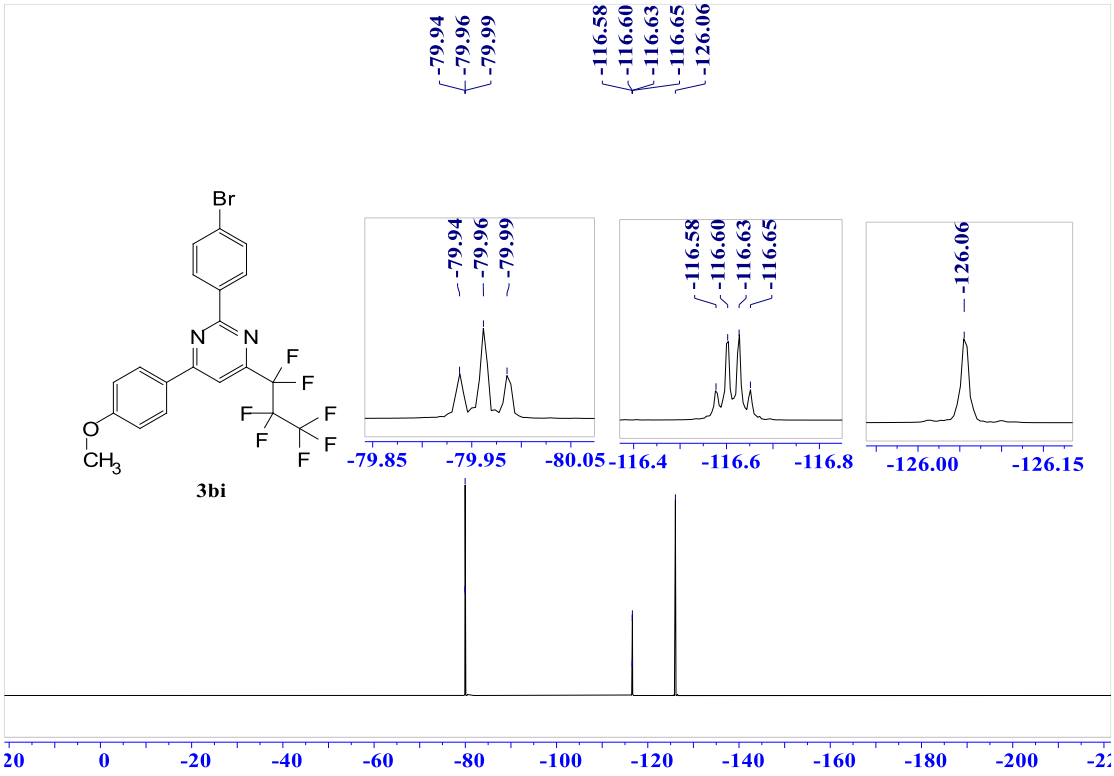
2.01
1.00
2.03
2.01
3.00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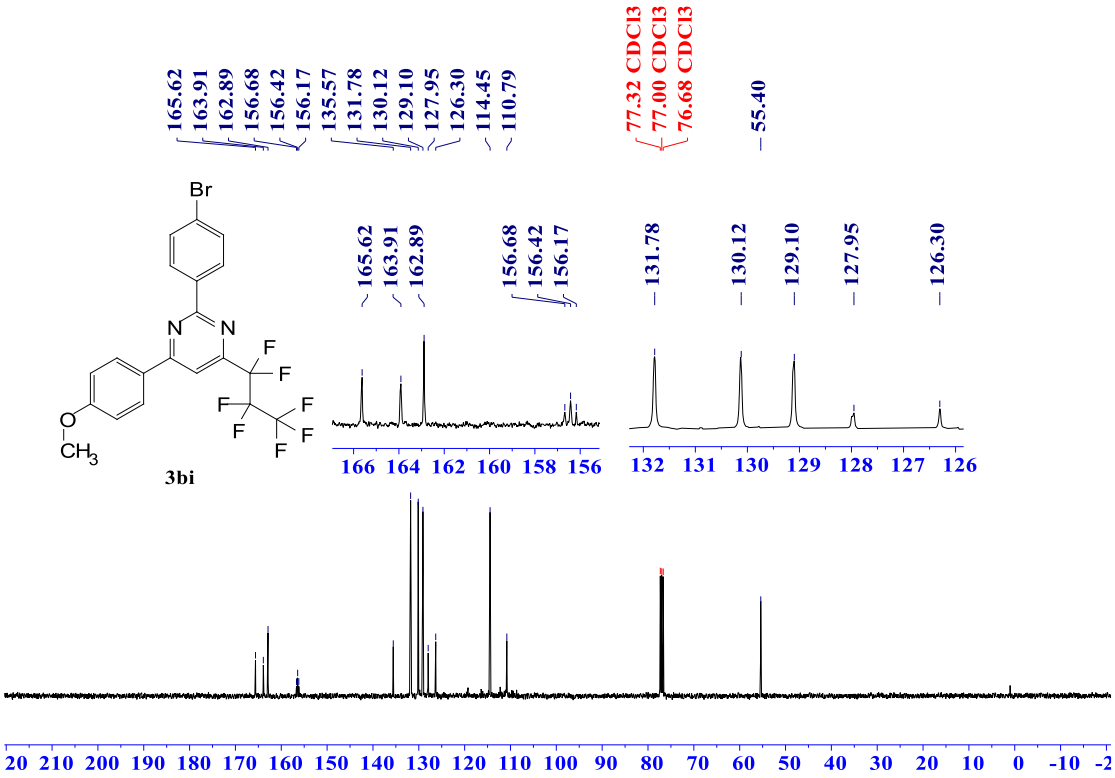
O
CH3
3bi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77.00 CDCl3
76.68 CDCl3
55.40
Br
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F
F
F
F
F
F
O
CH3
3bi
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163.91
162.89
156.68
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156.17
131.78
130.12
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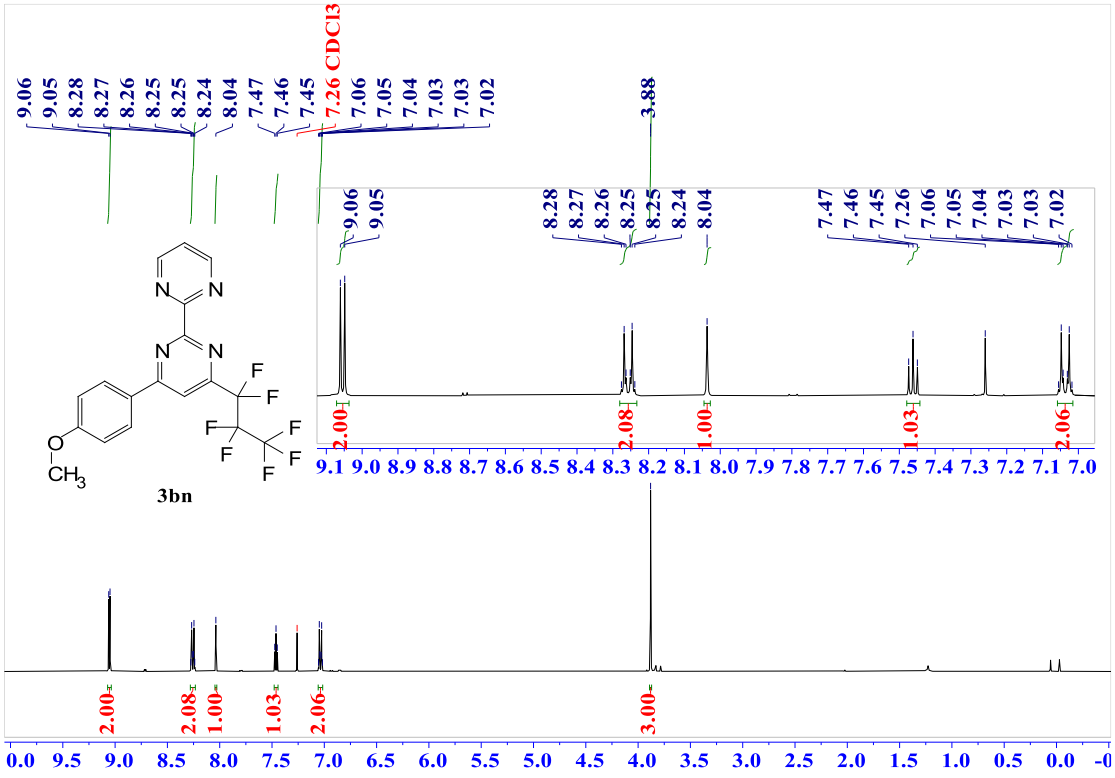
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7.05
7.04
7.03
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7.02
3.88
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N
N
N
F
F
F
F
F
F
O
CH3
3bn
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2.08
1.00
1.03
2.06
3.00
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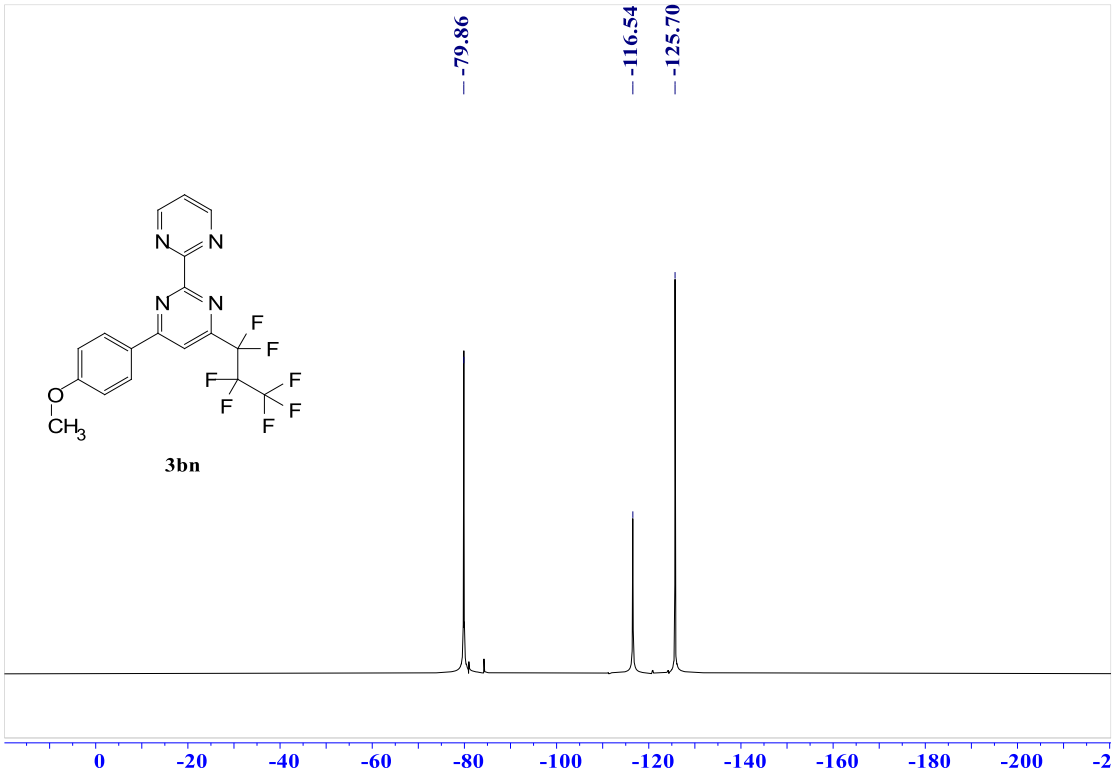
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0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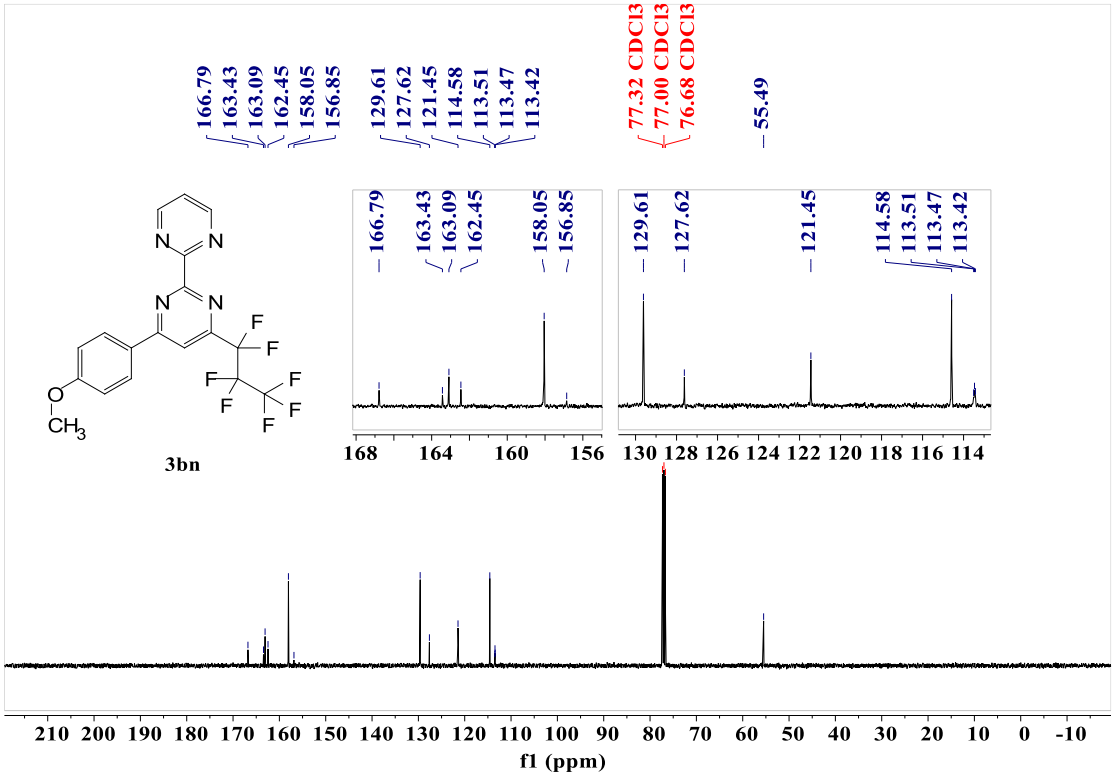
-200
-2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77.00 CDCl3
76.68 CDCl3
55.49
3bn
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164
160
156
130
128
126
124
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200
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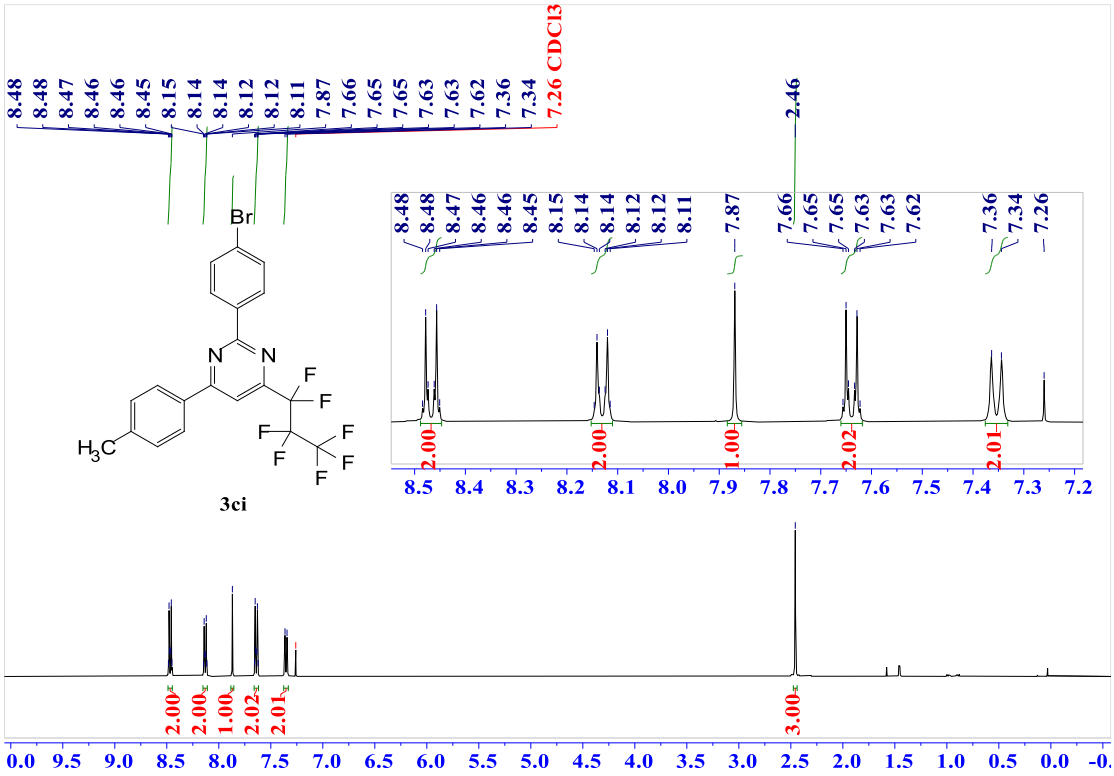
f1 (ppm)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F
F
F
F
F
F
H3C
3ci
2.00 2.00 1.00 2.02 2.01
3.00
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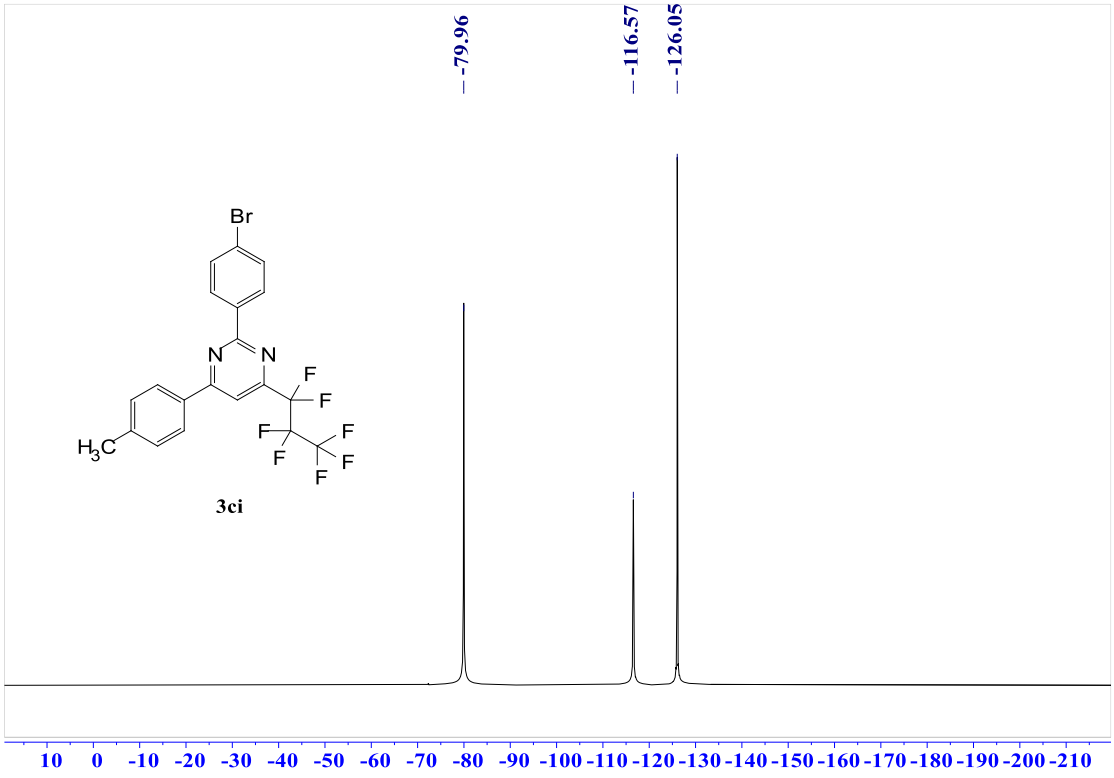
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F
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F
F
F
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3ci
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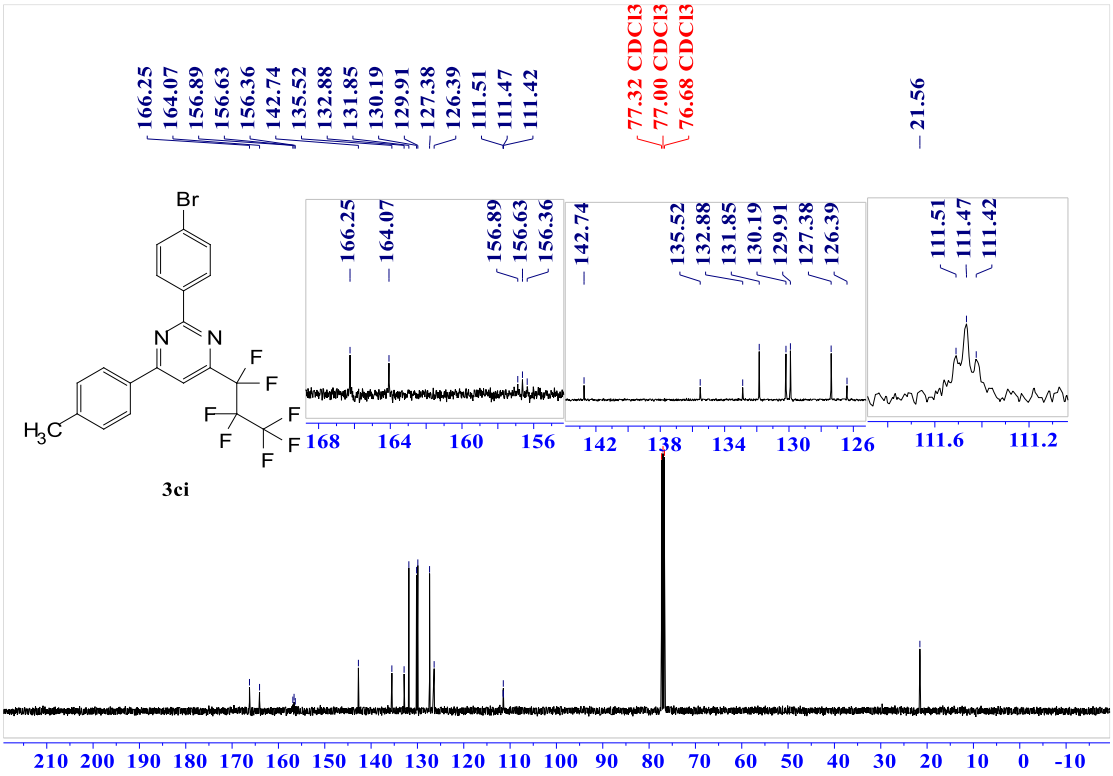
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77.00 CDCl3
76.68 CDCl3
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F
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F
H3C
3ci
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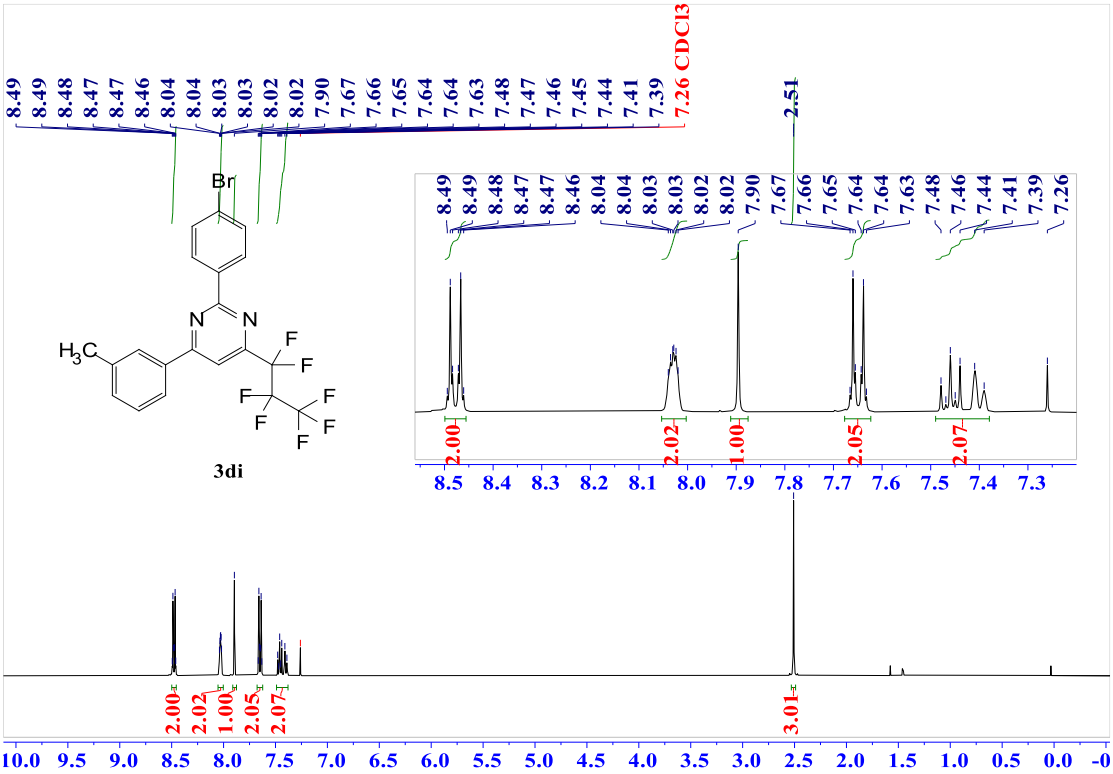
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7.46
7.45
7.44
7.41
7.39
7.26 CDCl3
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Br
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N
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F
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F
F
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H3C
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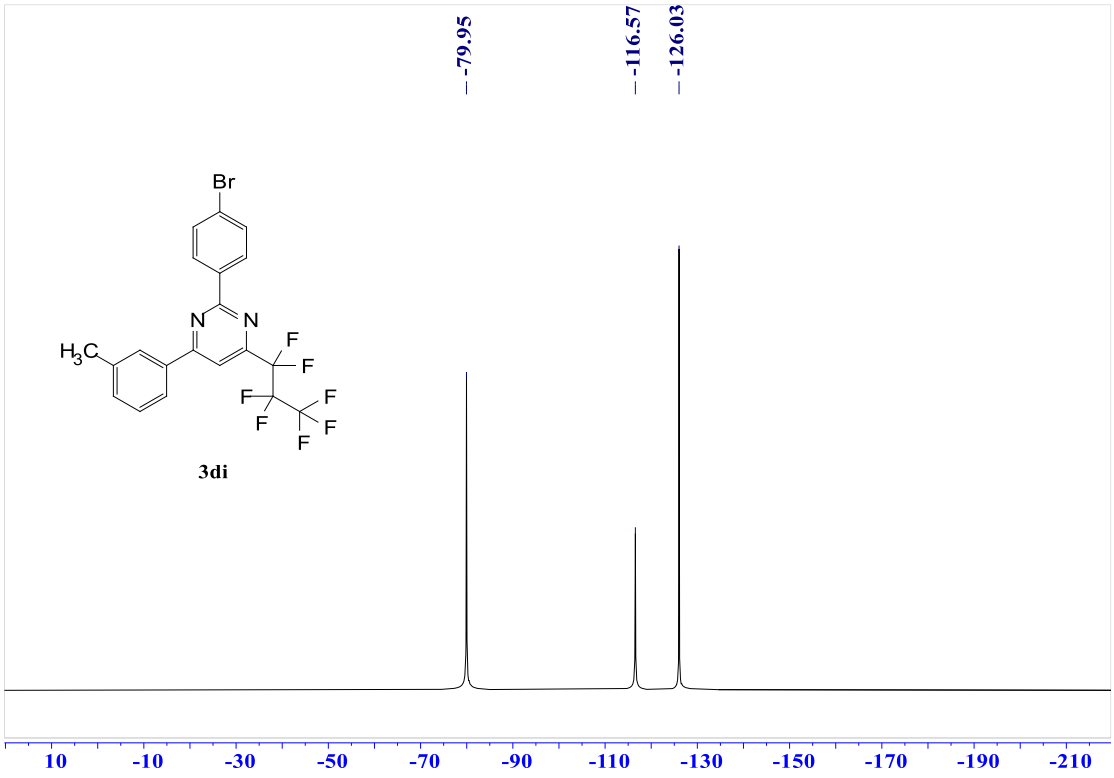
2.00
2.02
1.00
2.05
2.07
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0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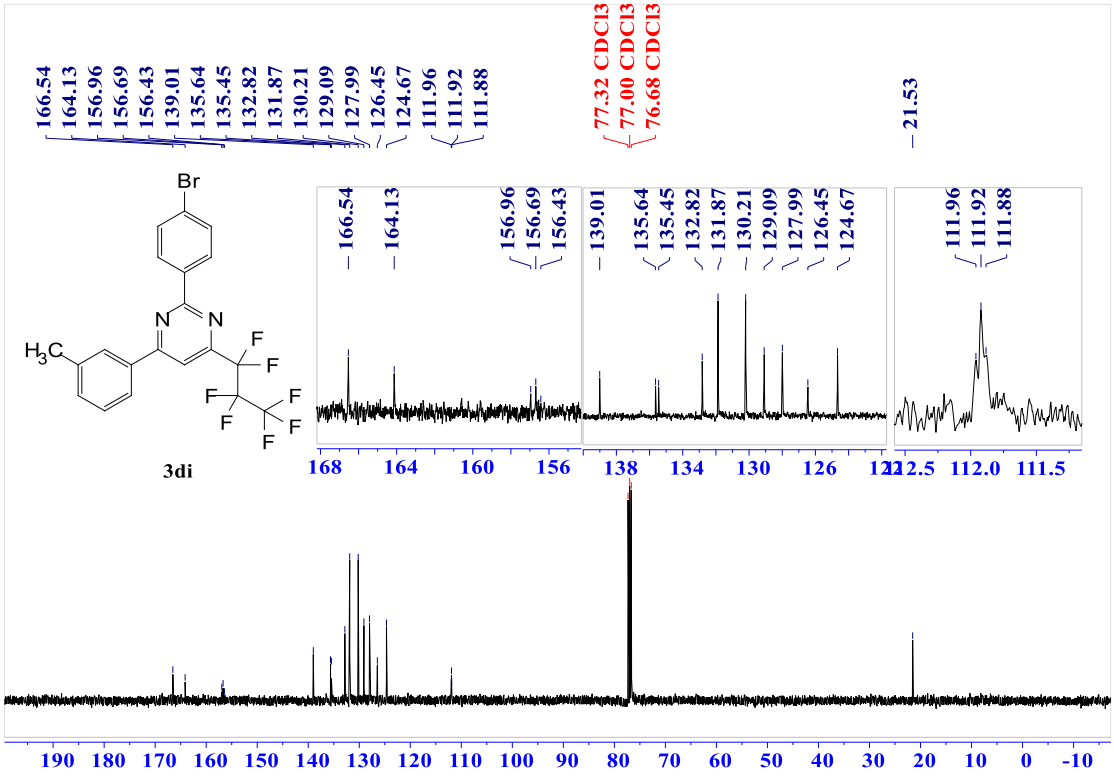
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F
F
F
F
F
3di
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134
130
126
112.5
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111.5
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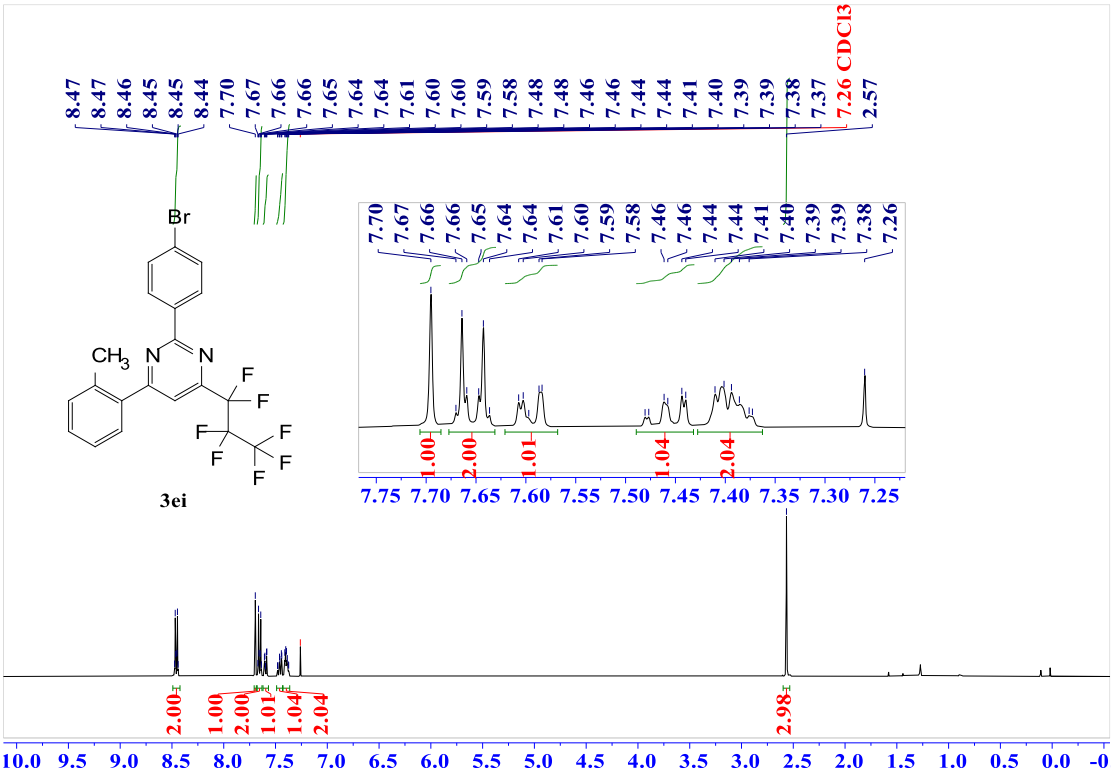
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Br
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3ei
7.70 7.67 7.66 7.66 7.65 7.64 7.64 7.61 7.60 7.59 7.58 7.46 7.46 7.44 7.44 7.41 7.40 7.39 7.39 7.38 7.26
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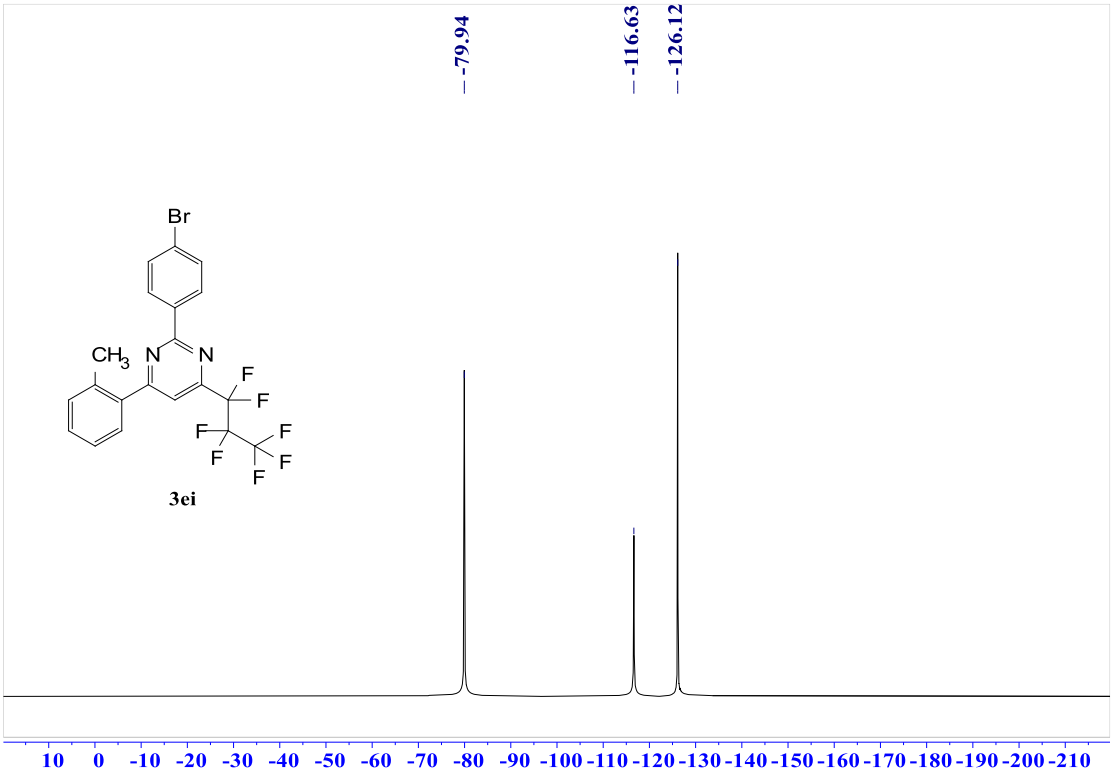
2.00 1.00 2.00 1.01 1.04 2.04 2.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0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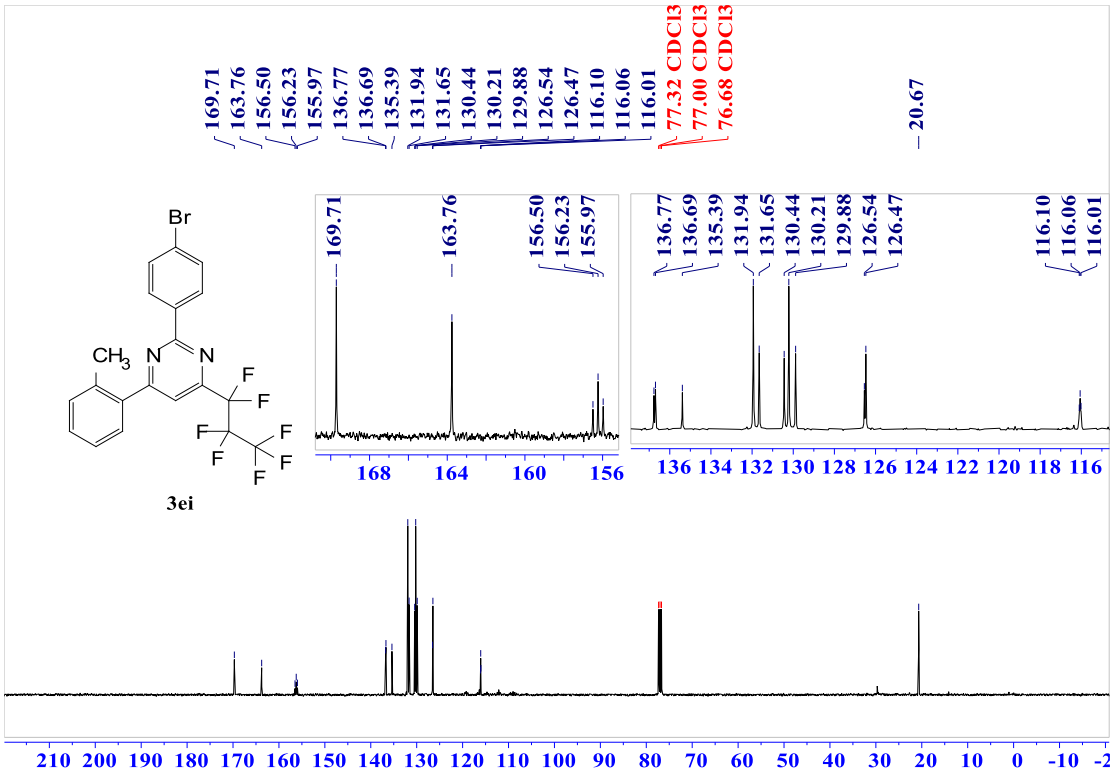
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77.00 CDCl3
76.68 CDCl3
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CH3
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F
F
F
F
3ei
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160
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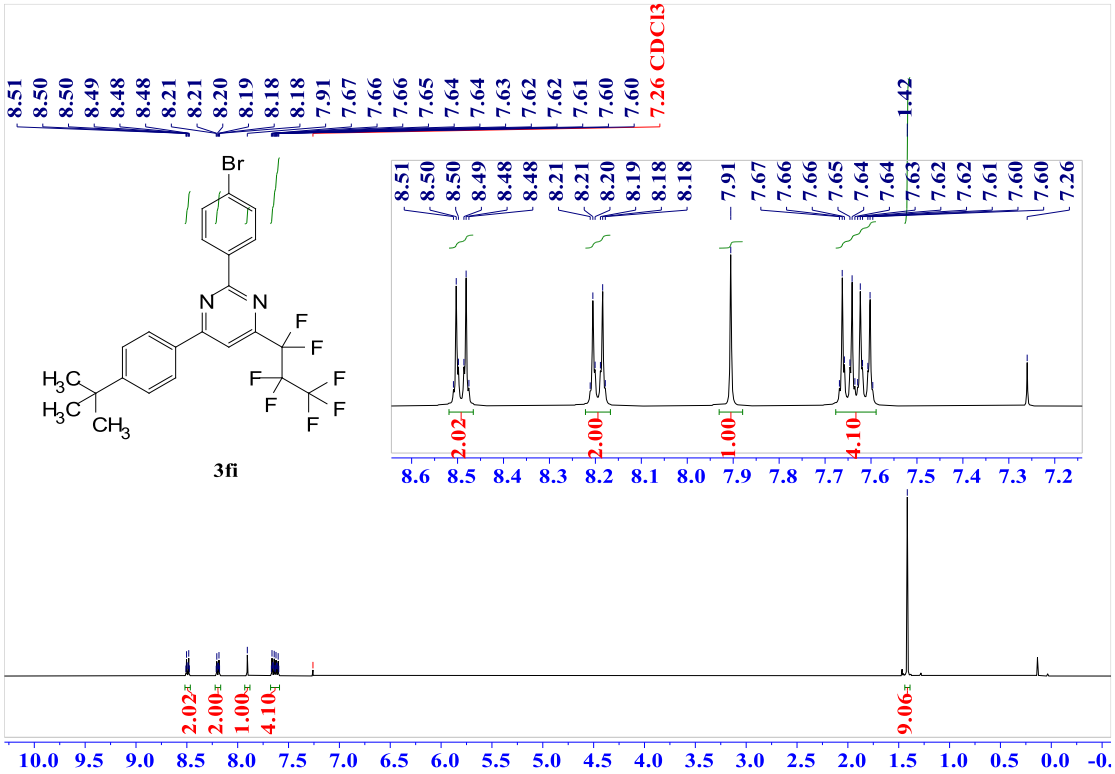
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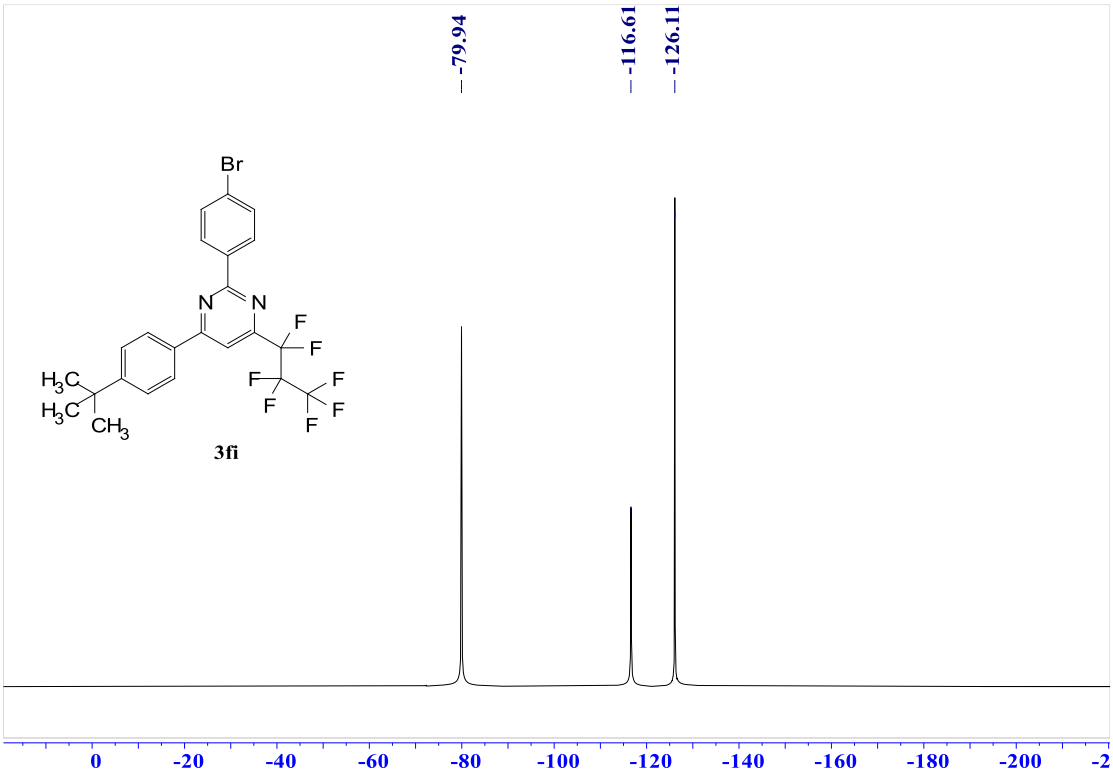
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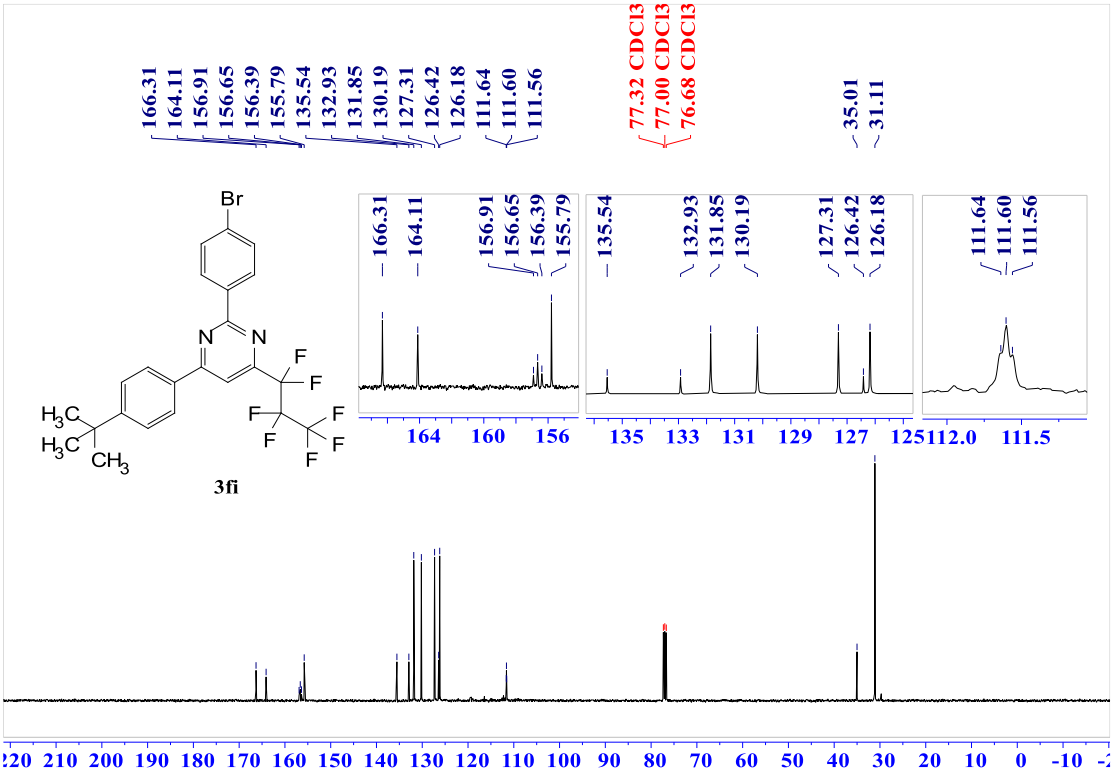
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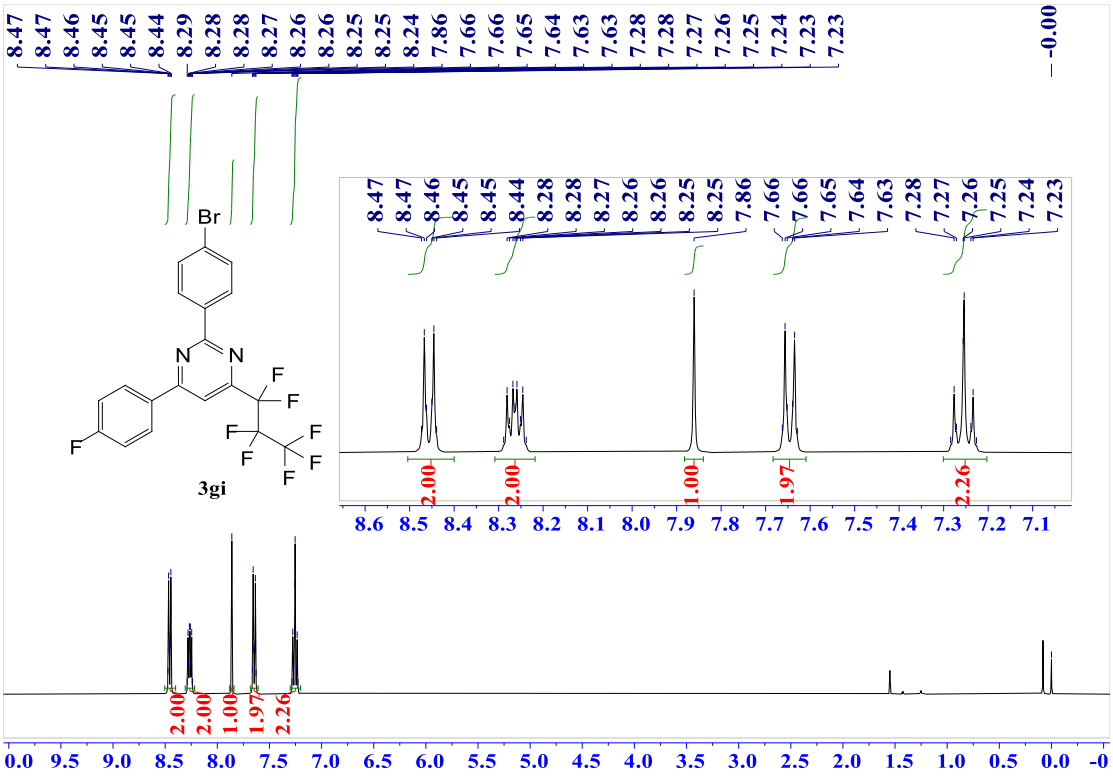
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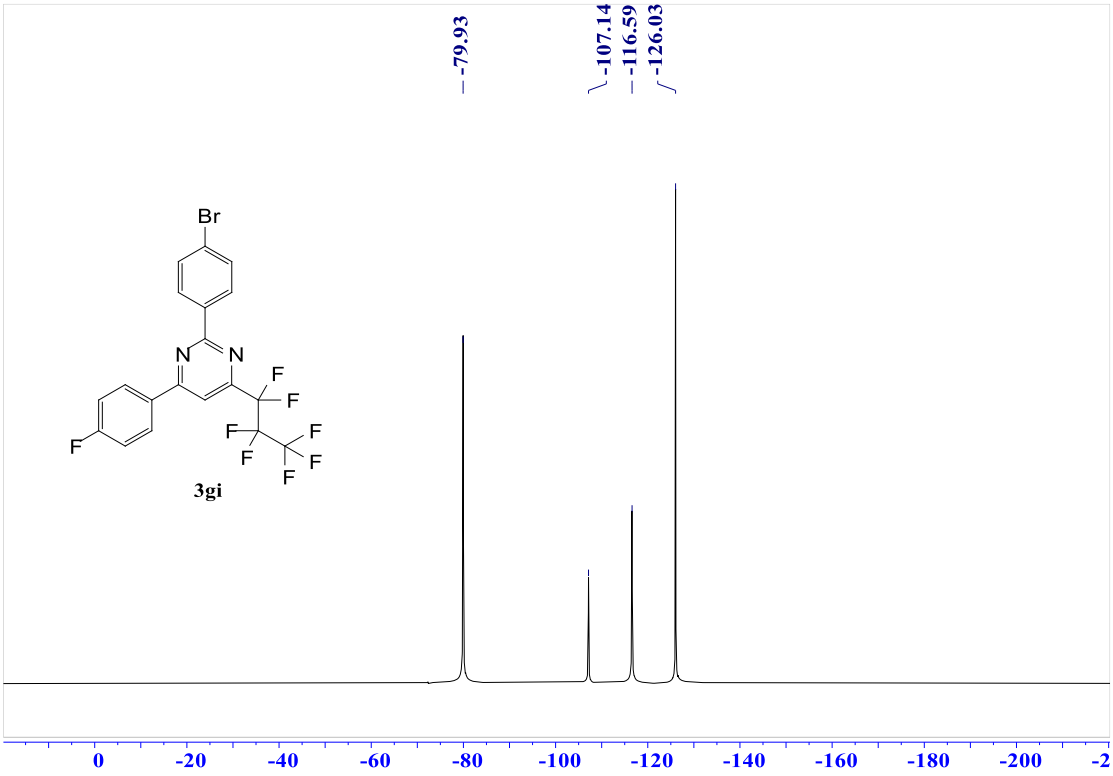
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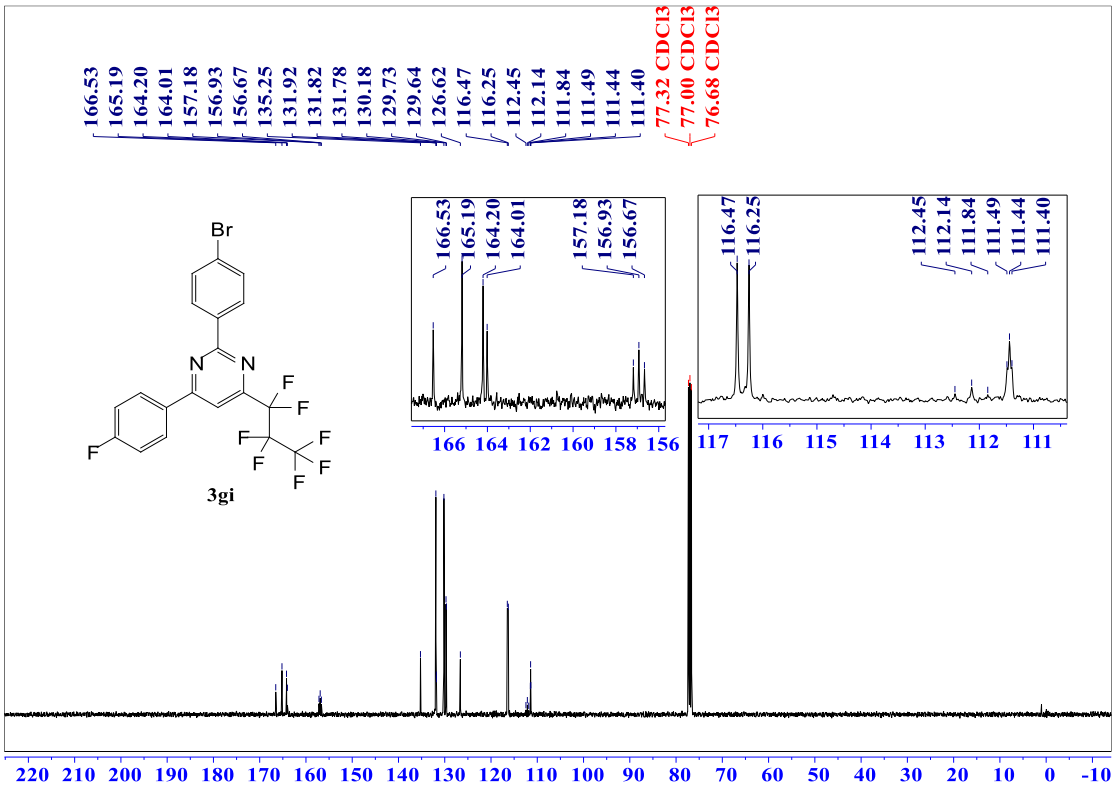
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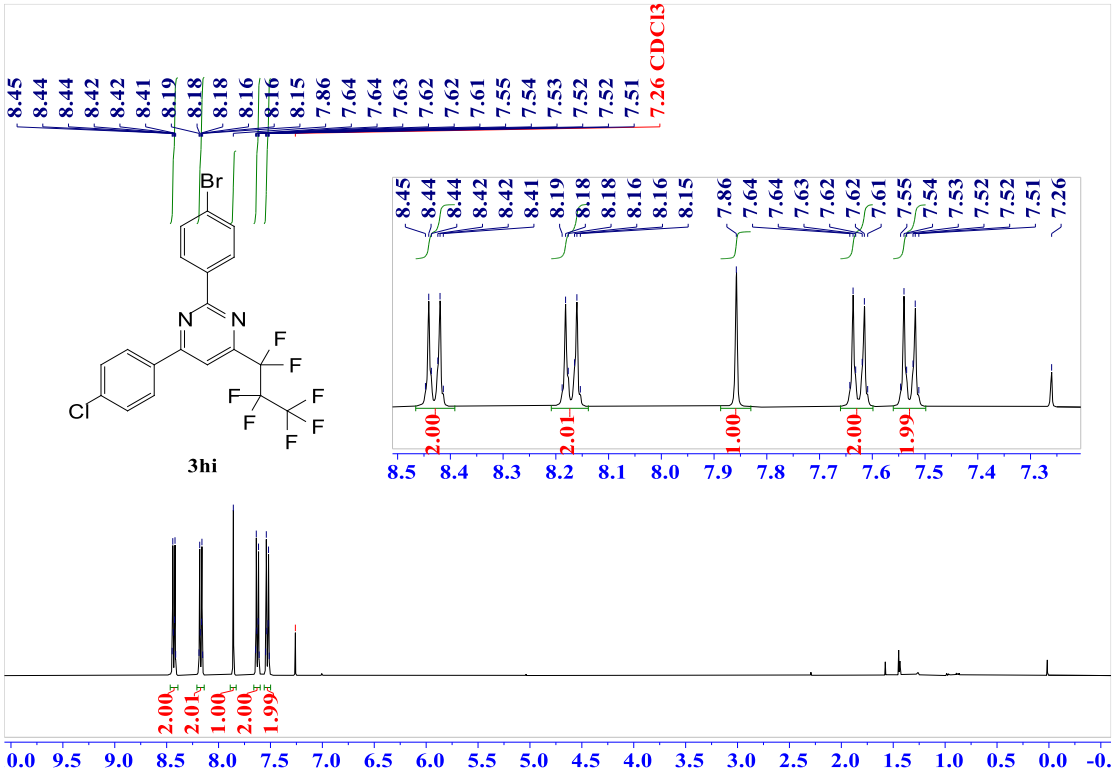
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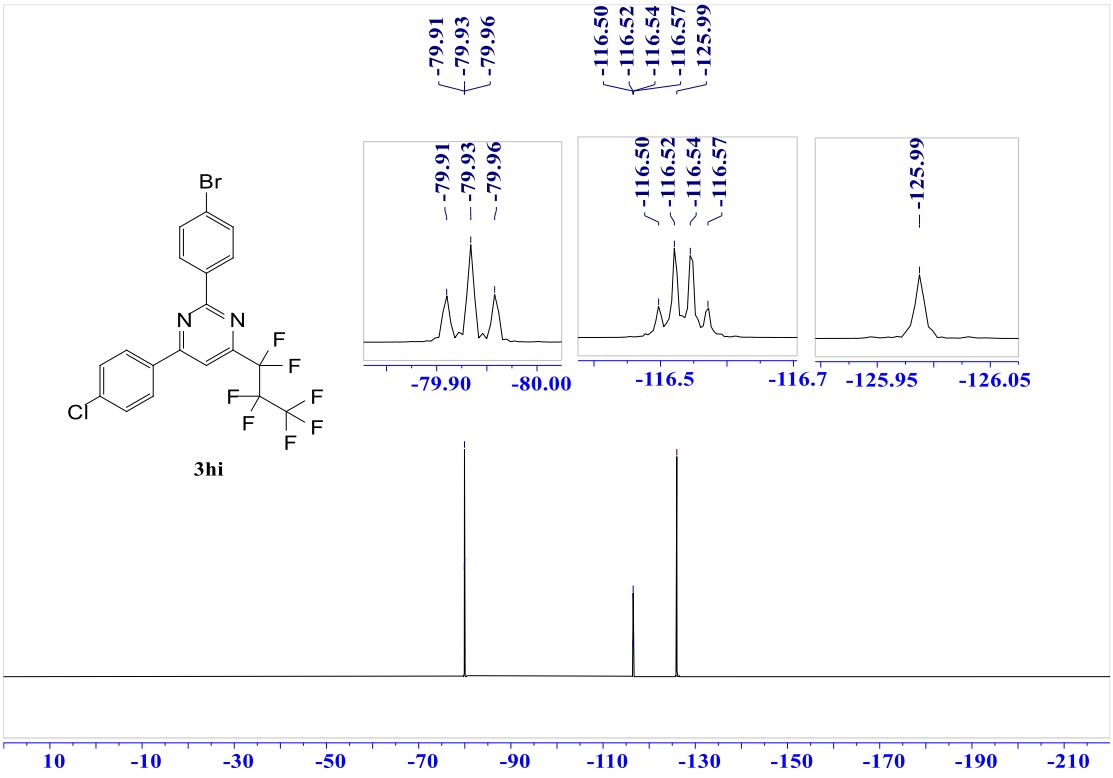
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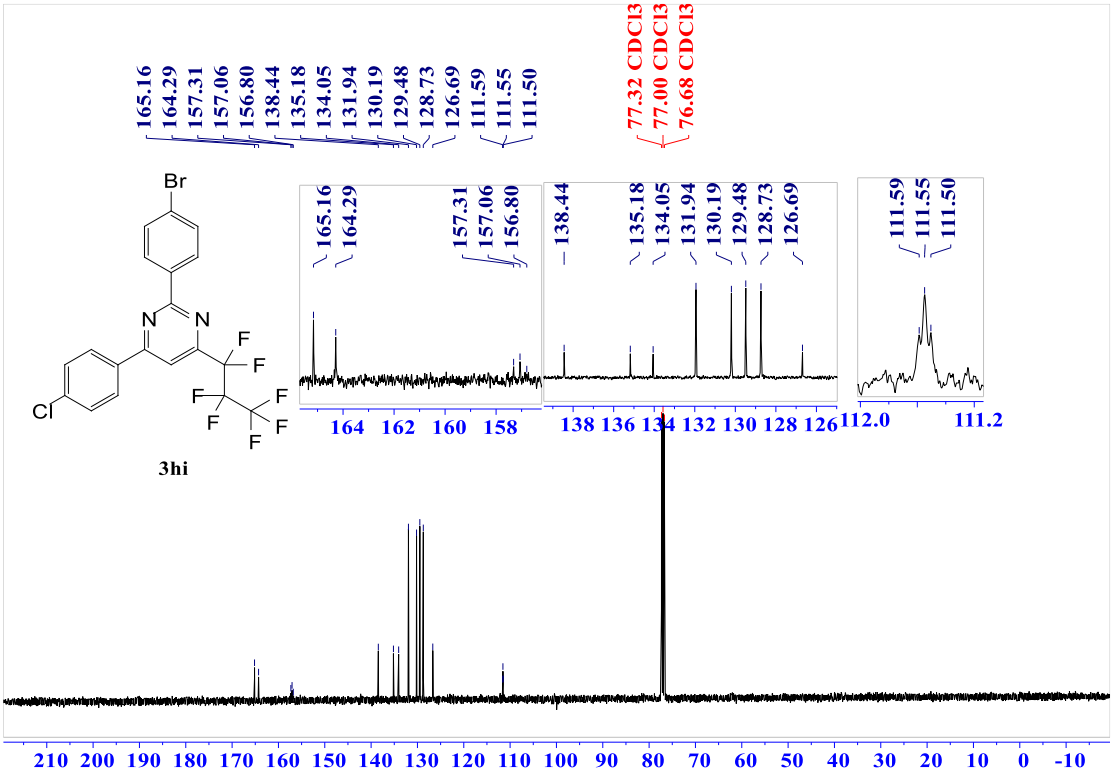
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Cl
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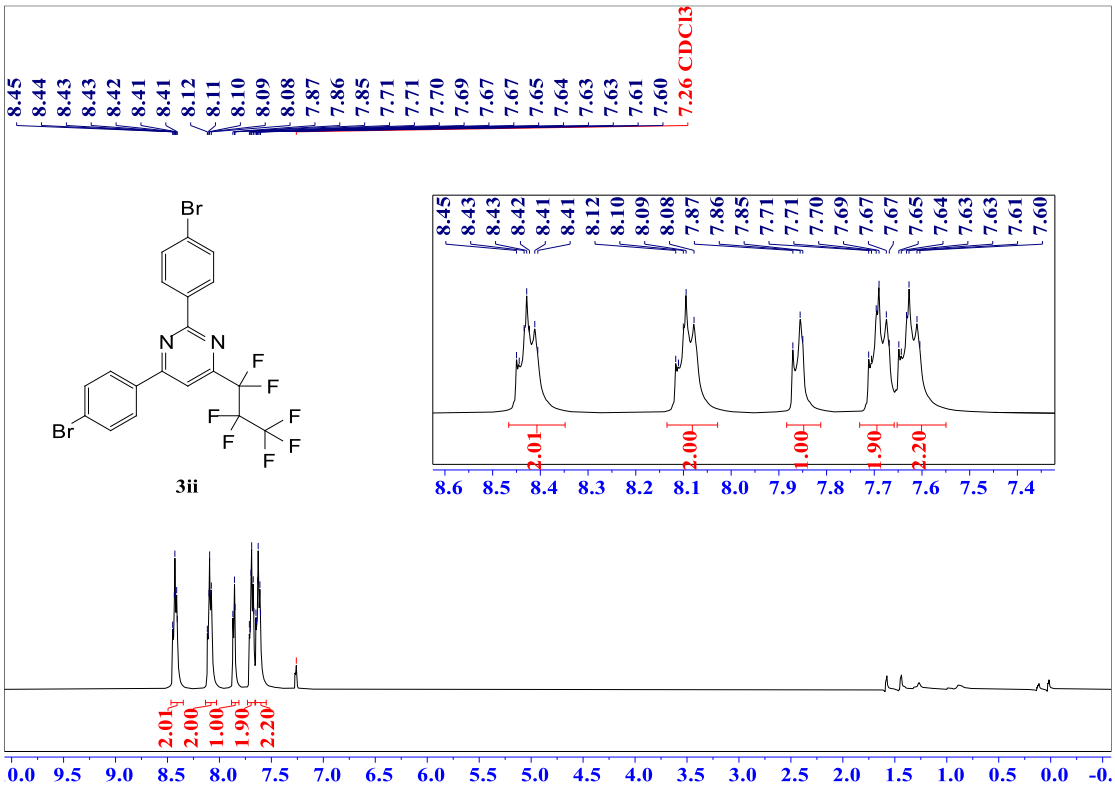
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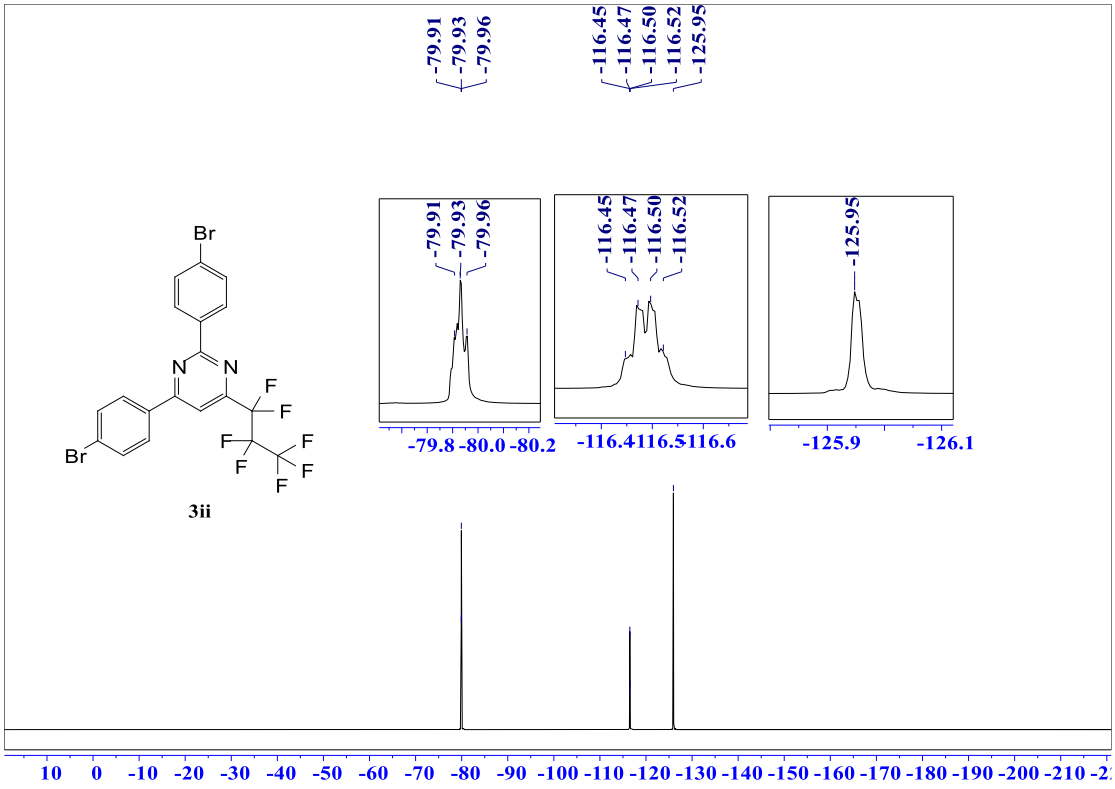
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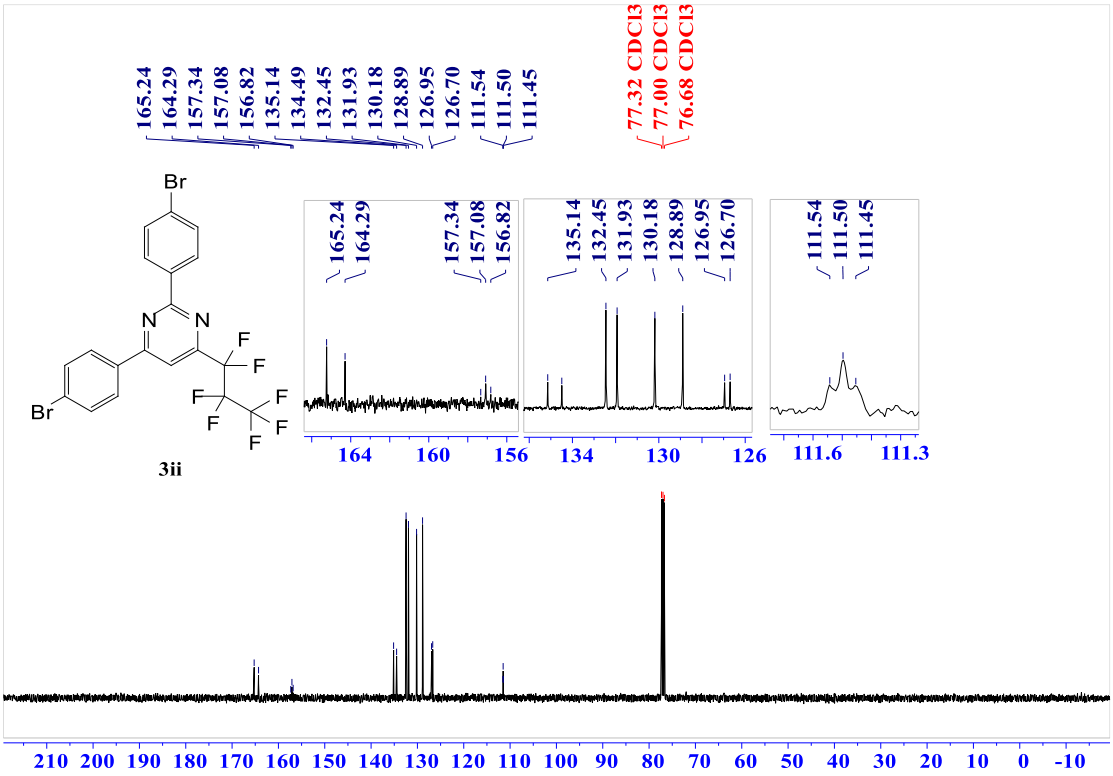
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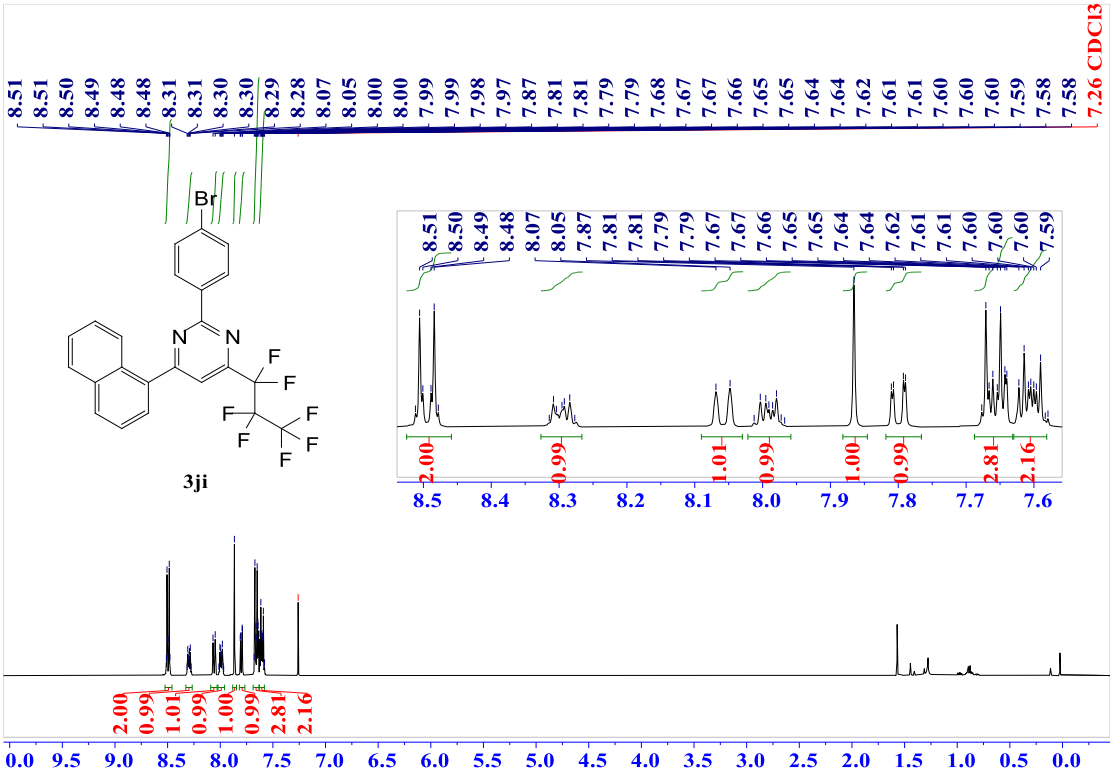
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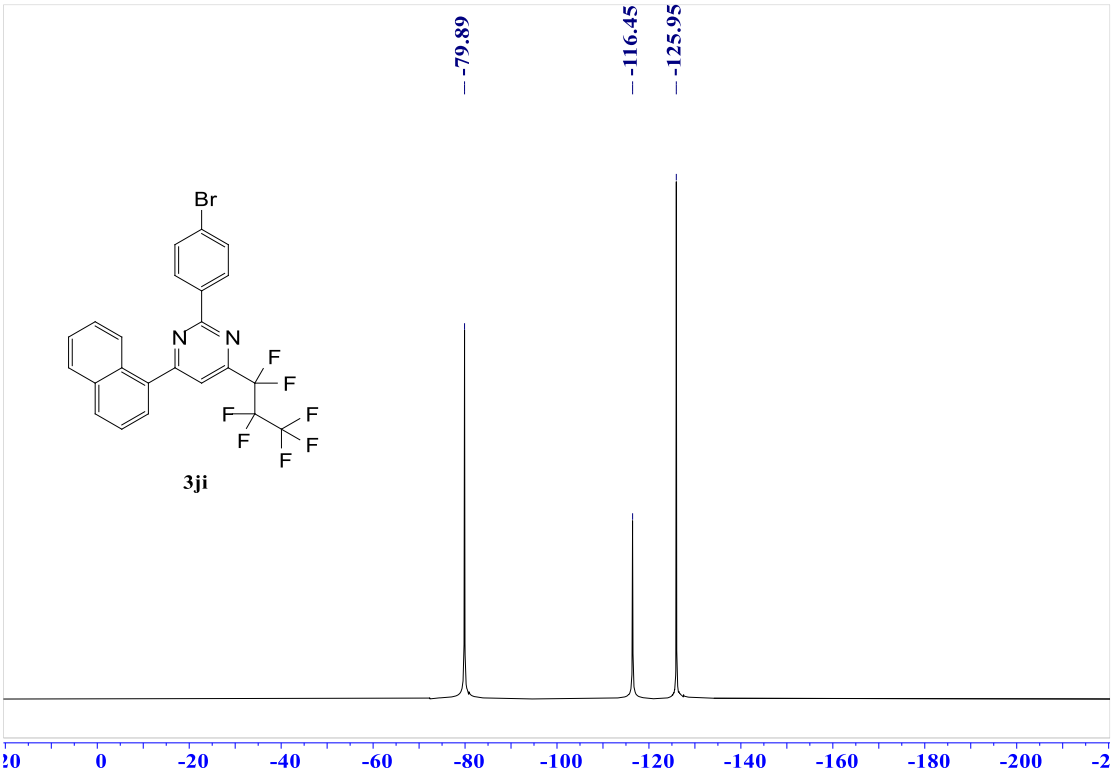
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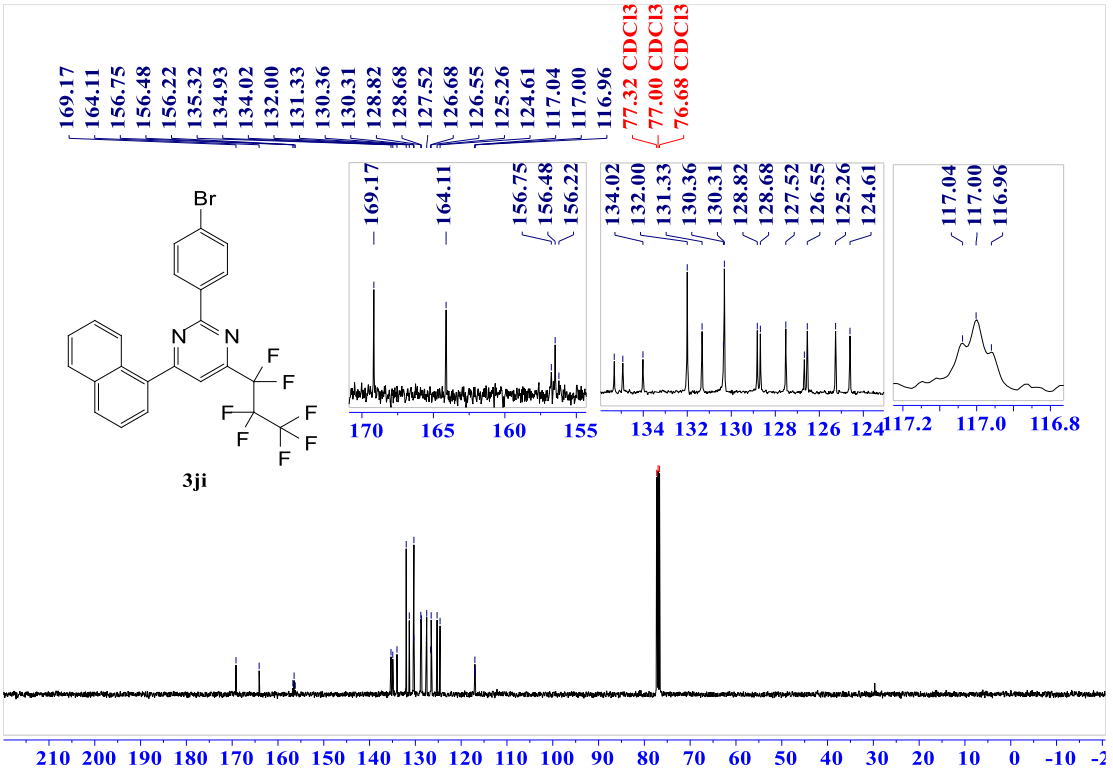
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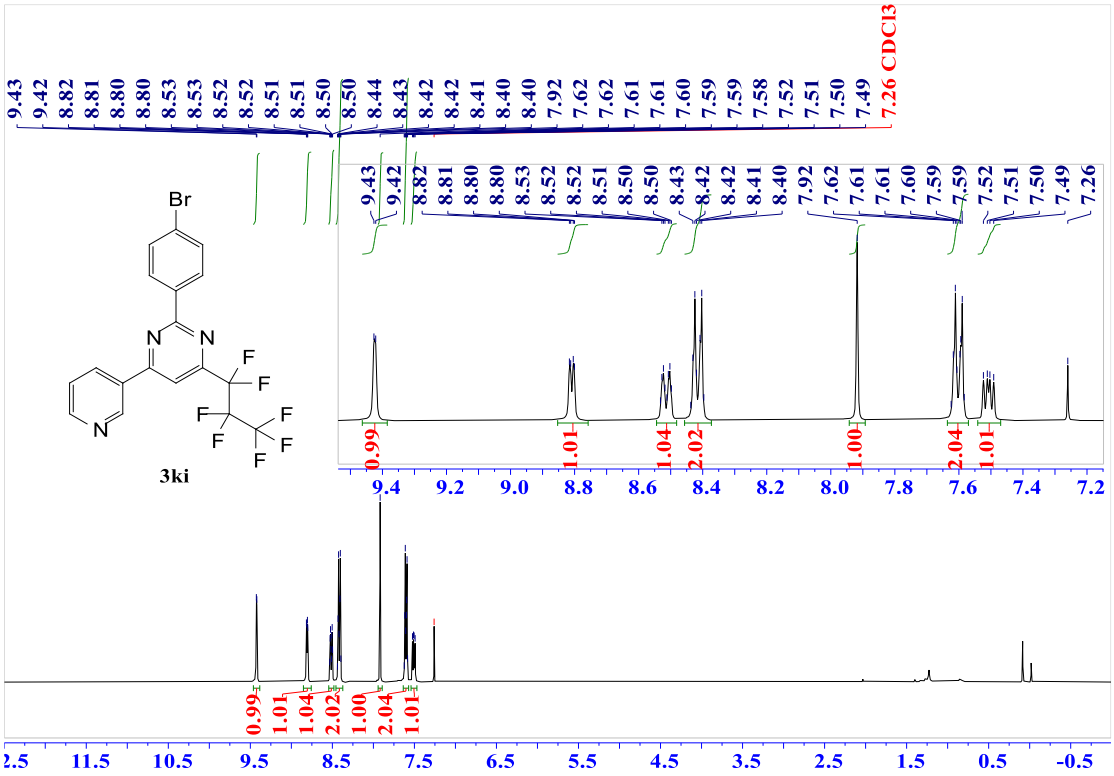
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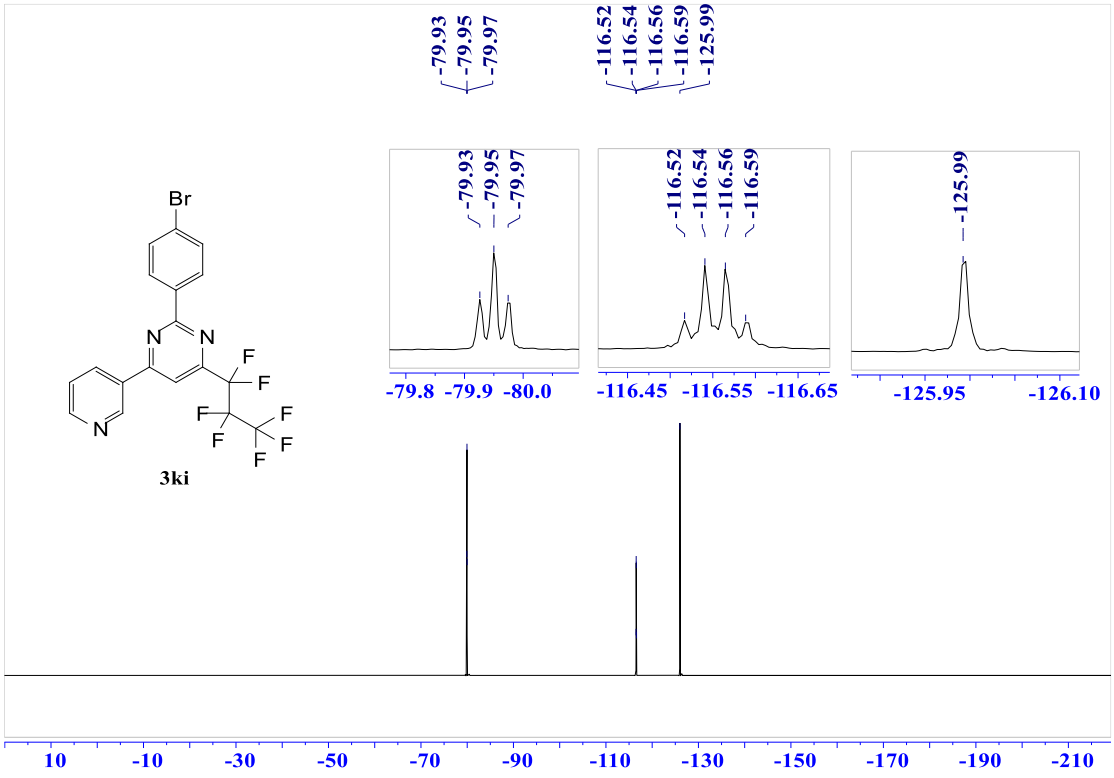
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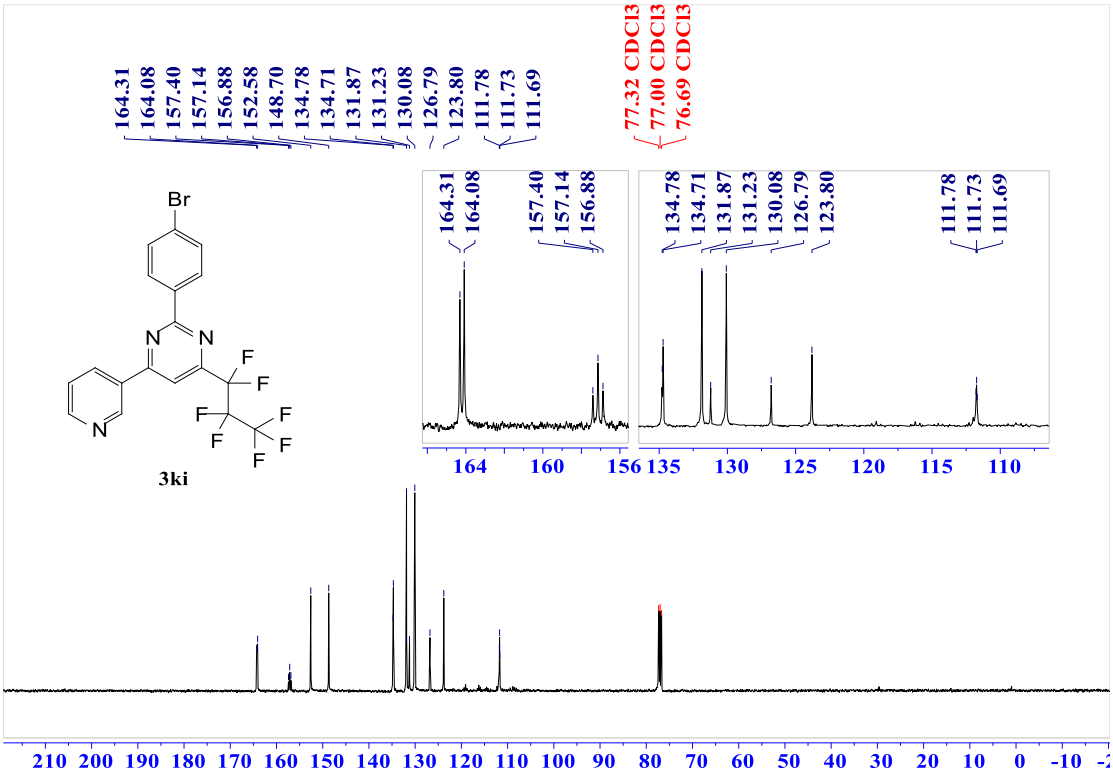
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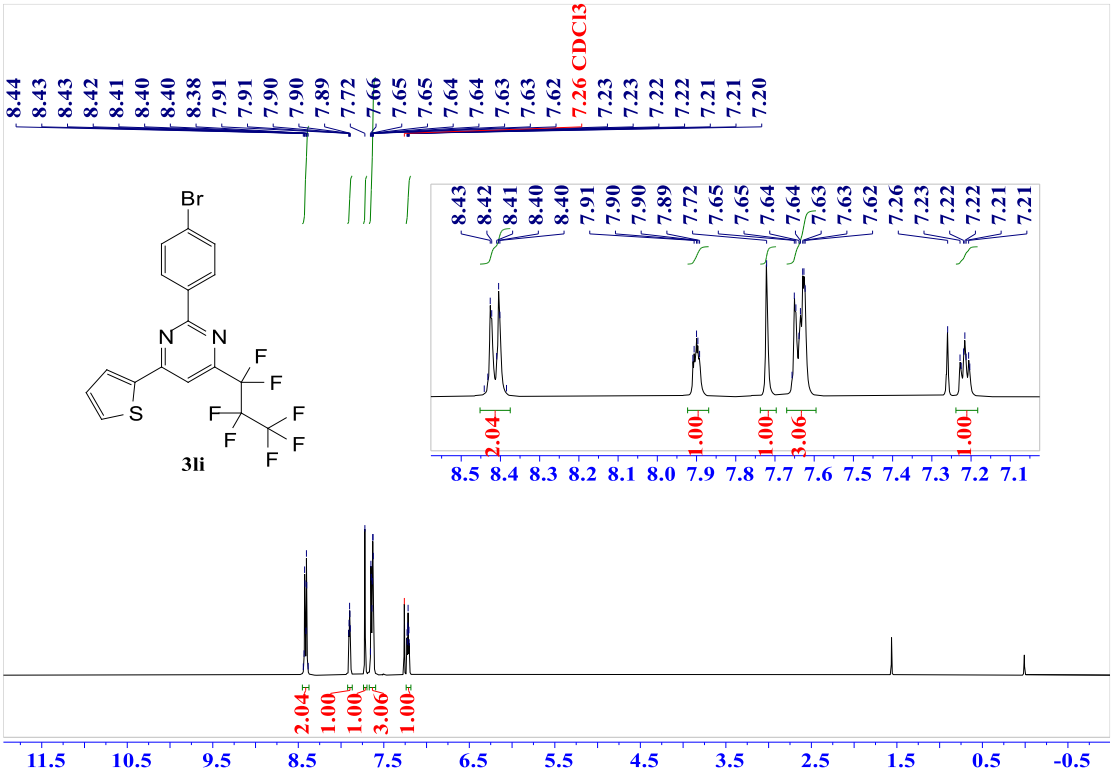
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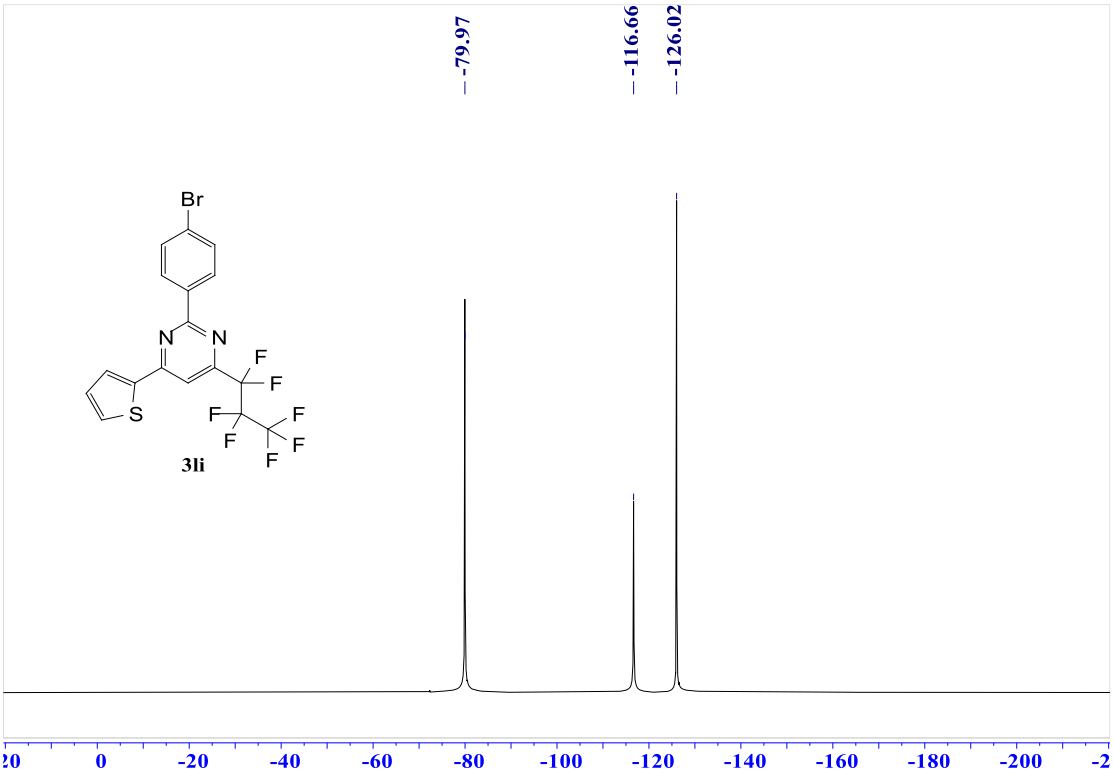
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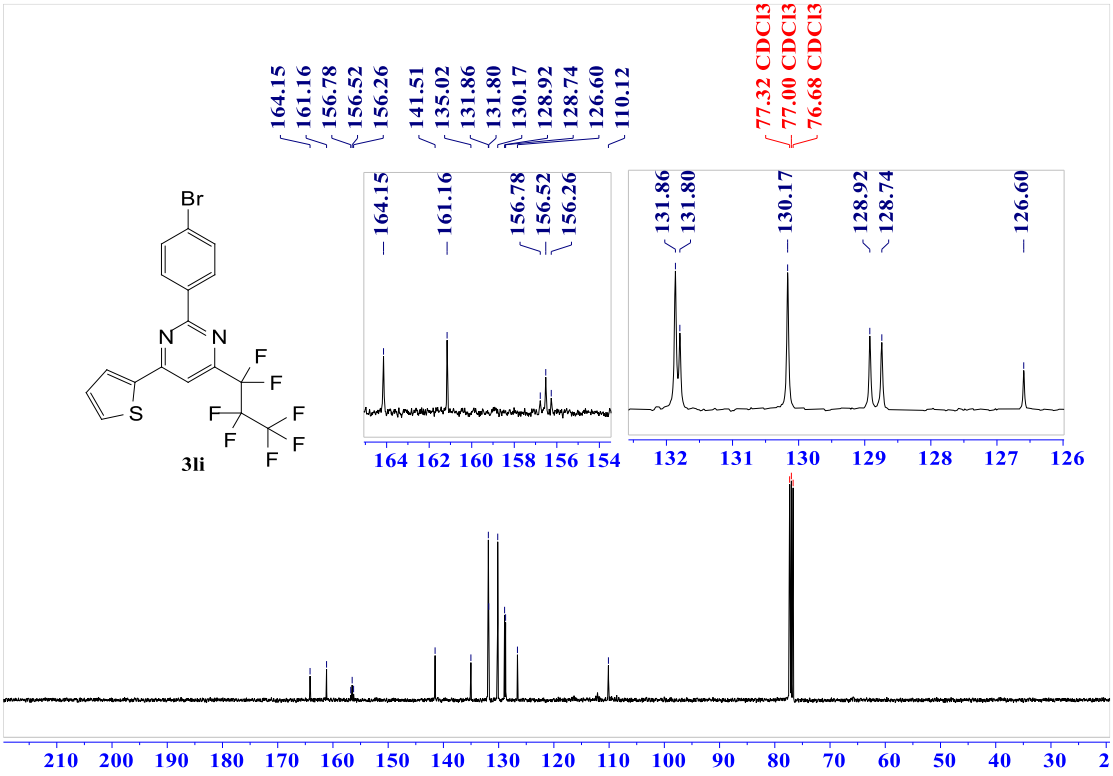
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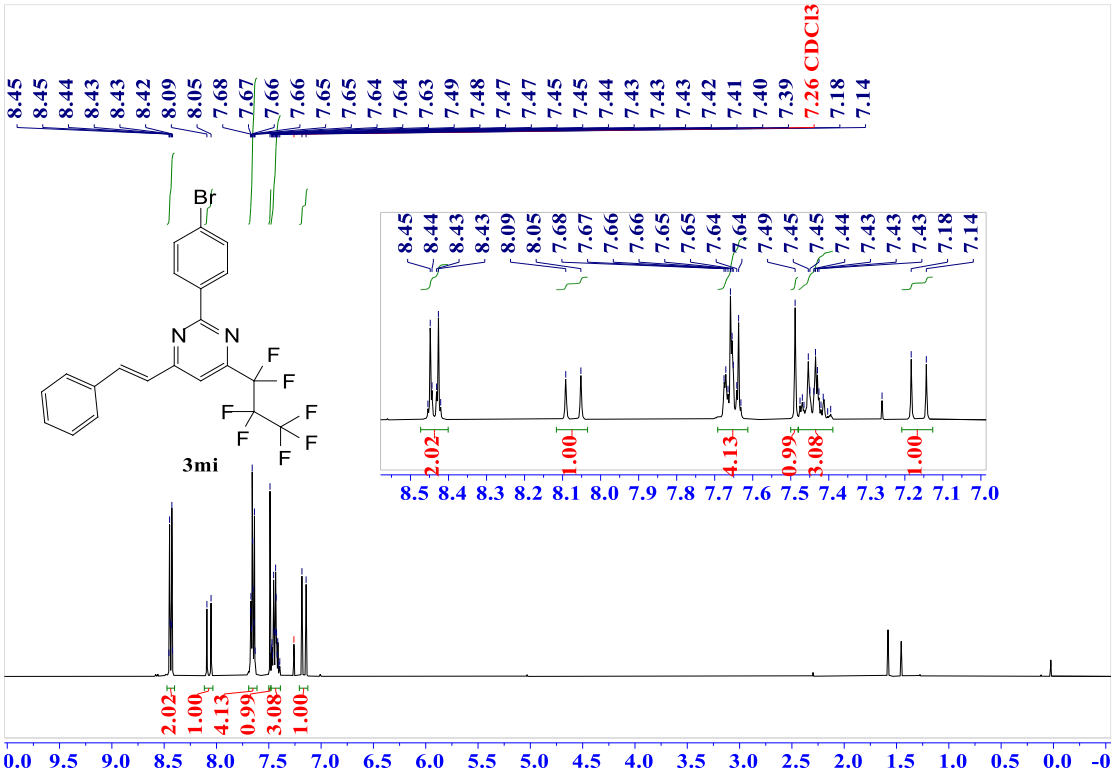
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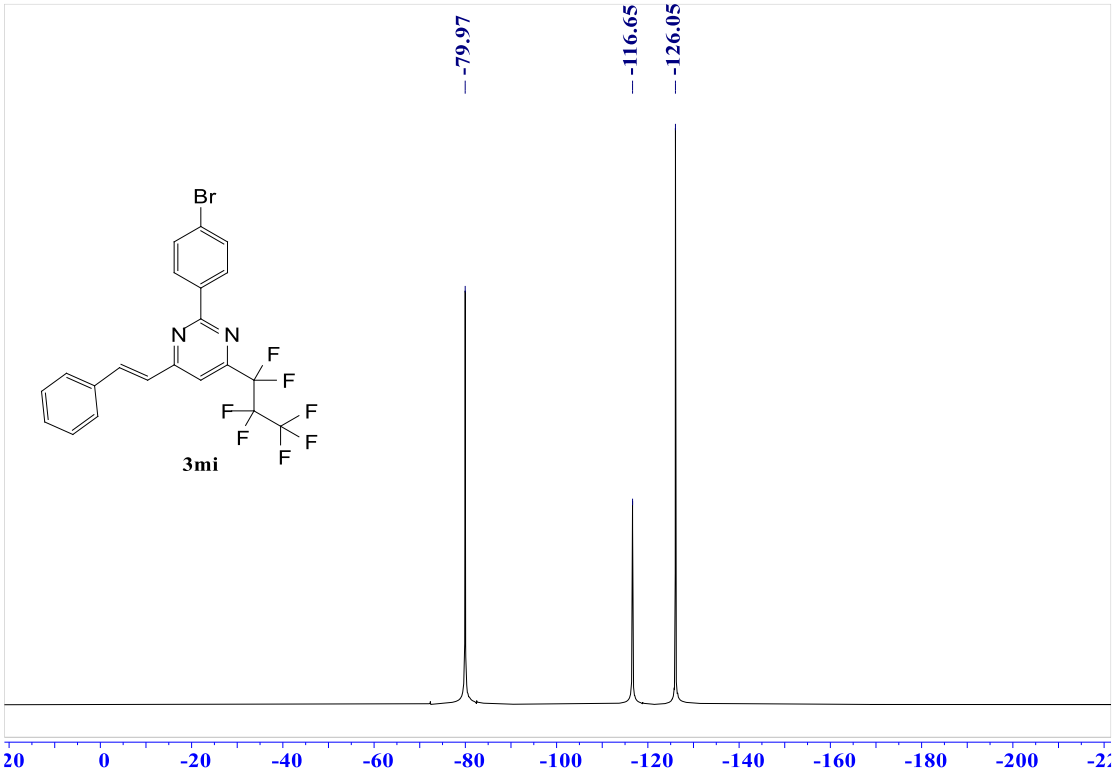
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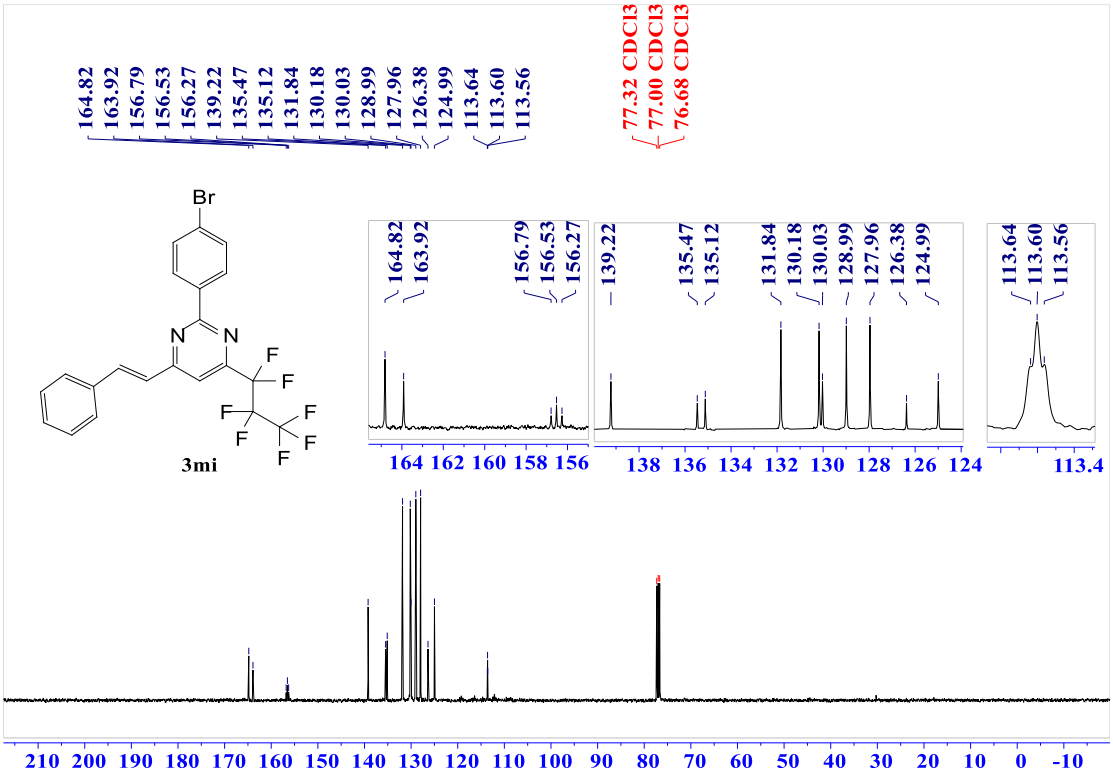
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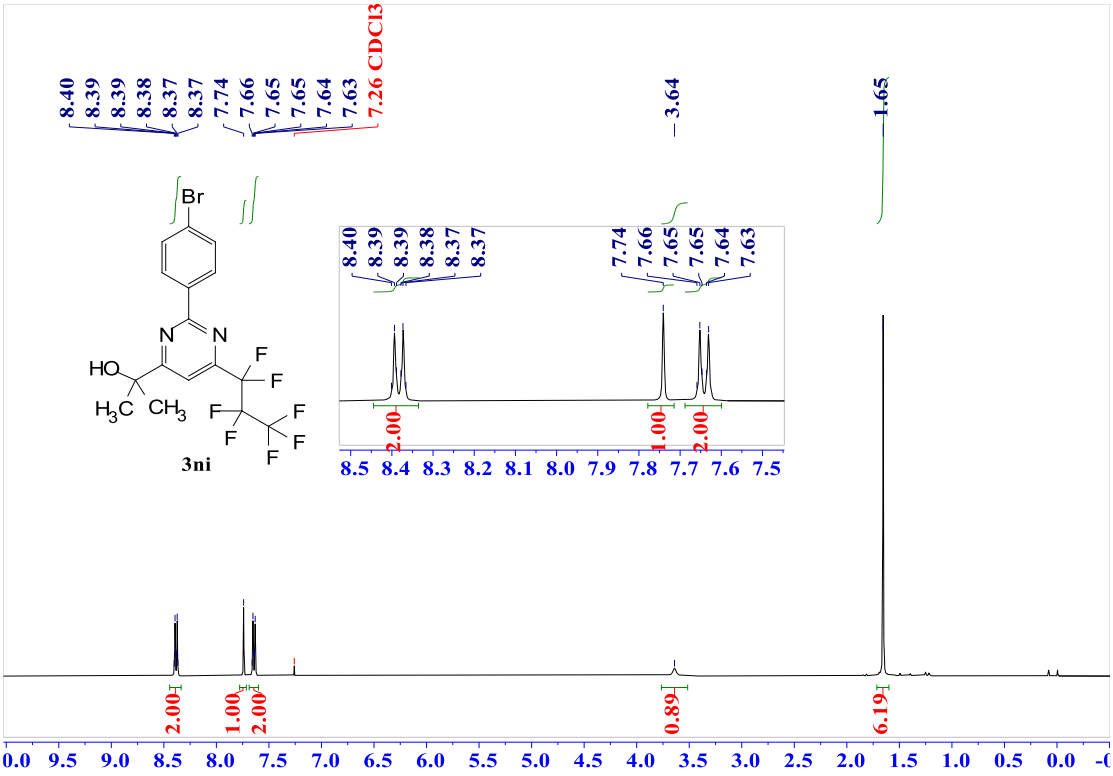
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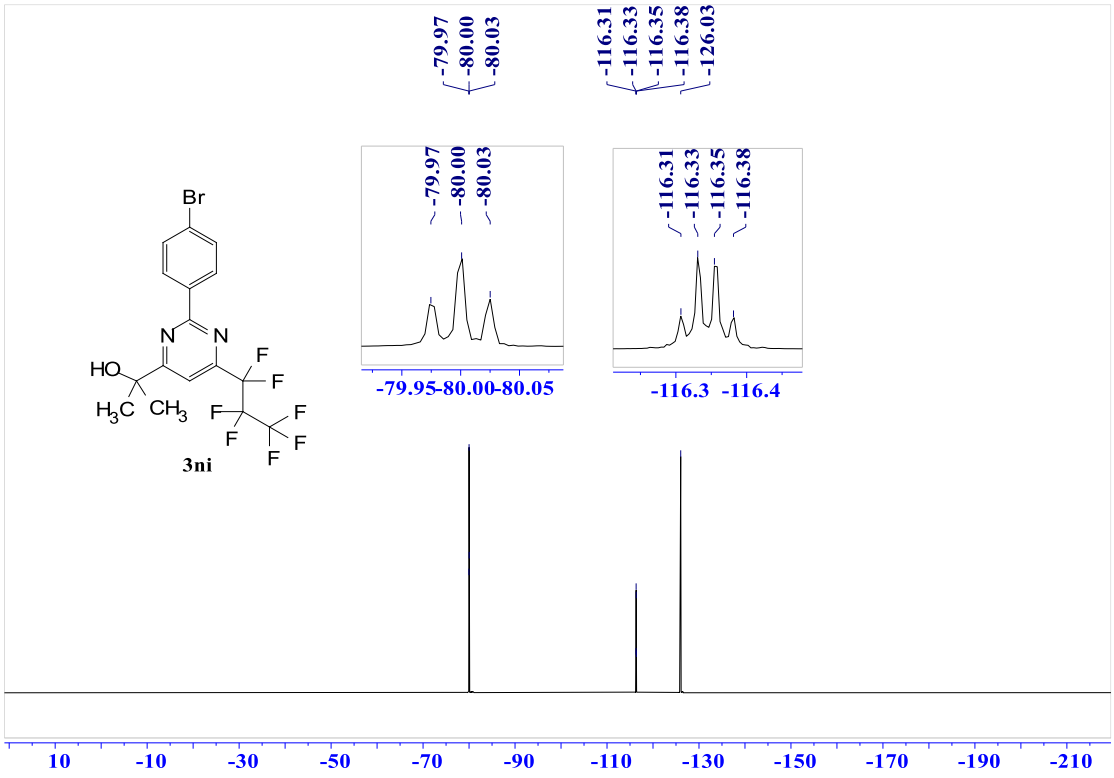
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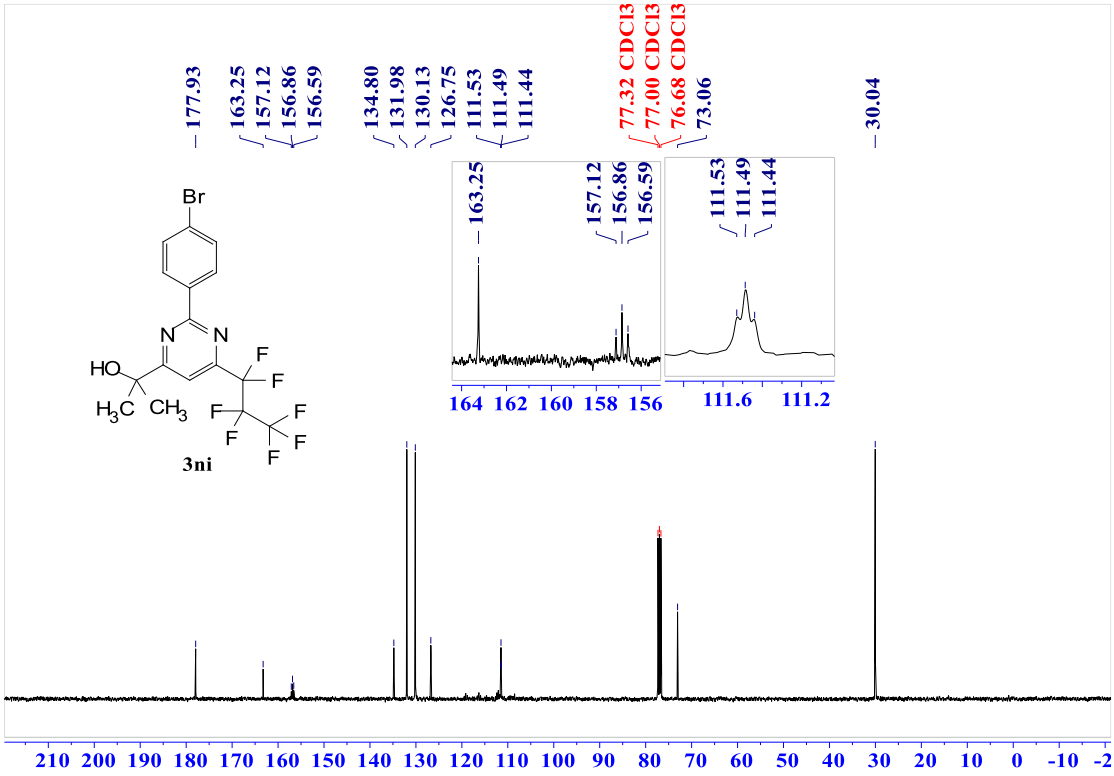
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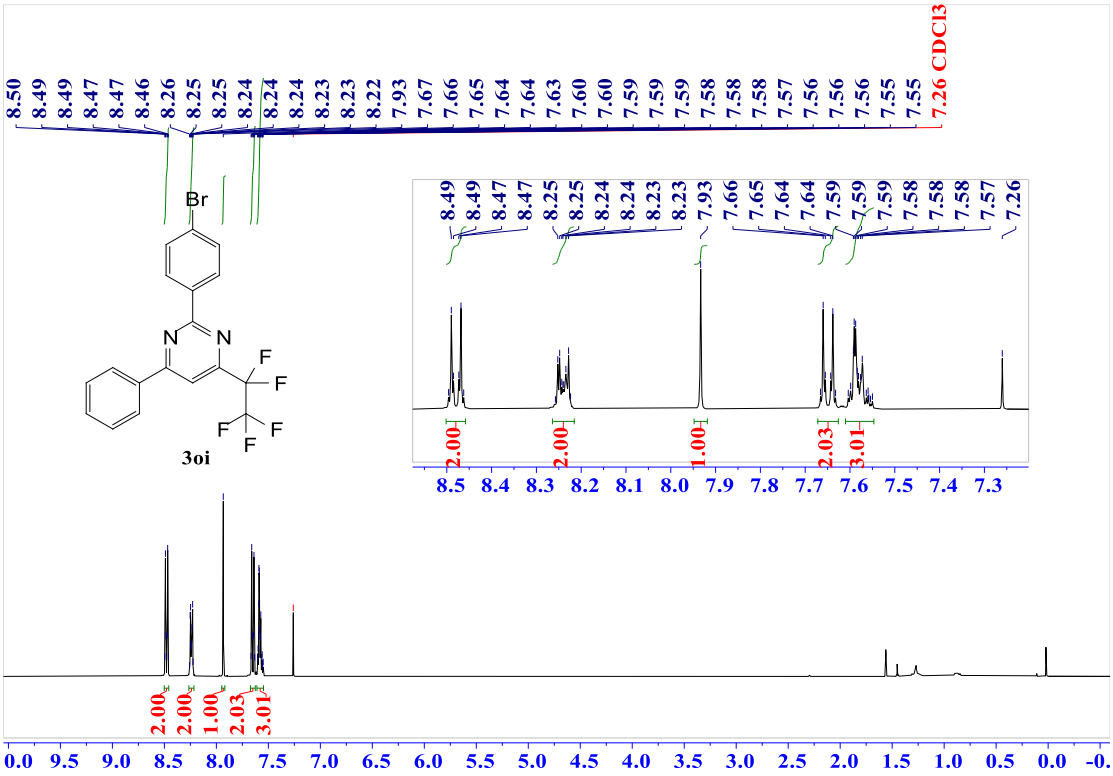
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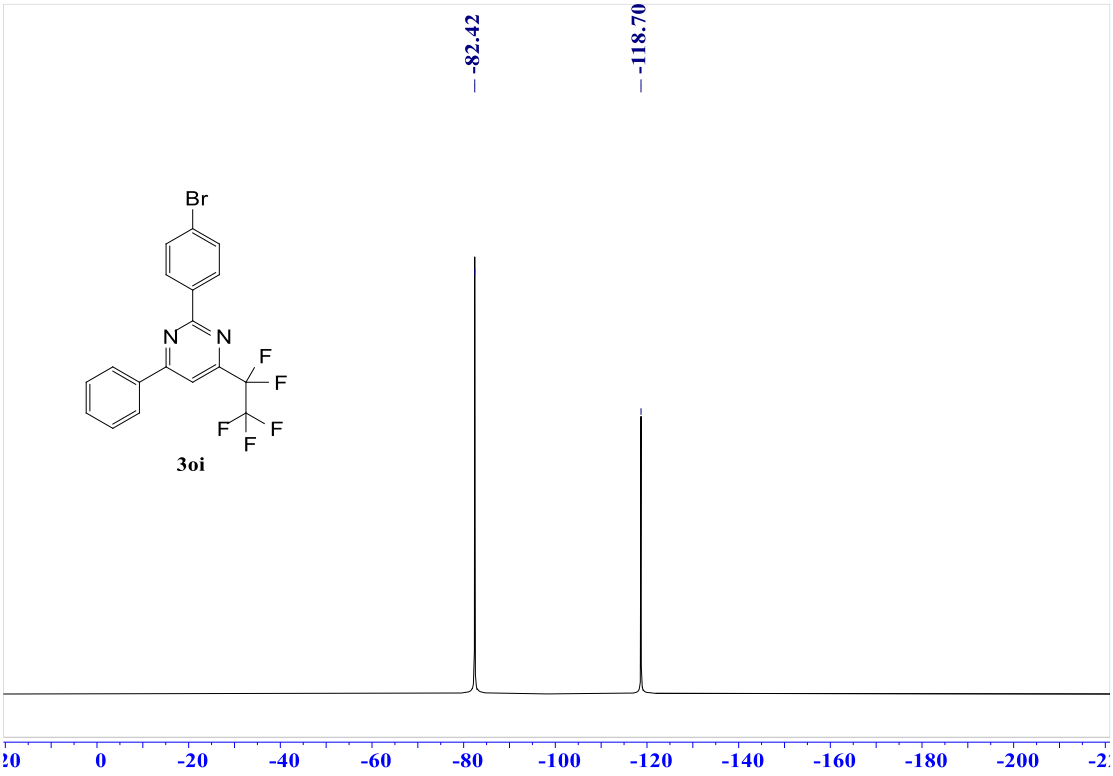
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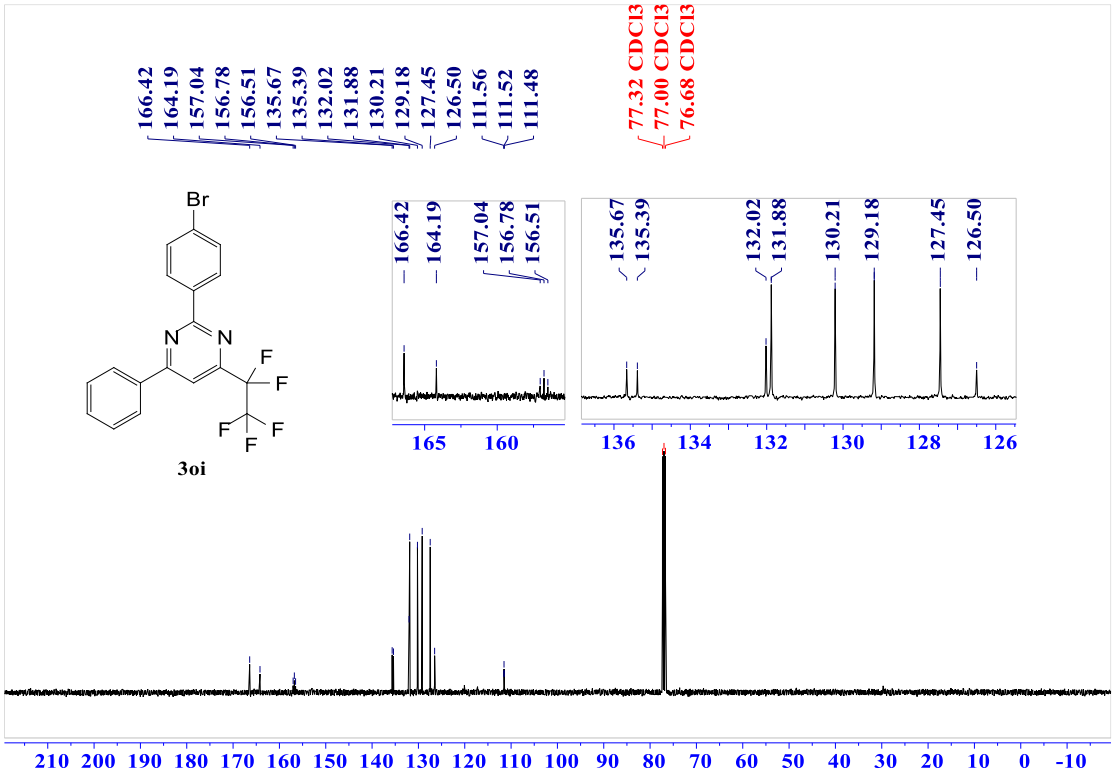
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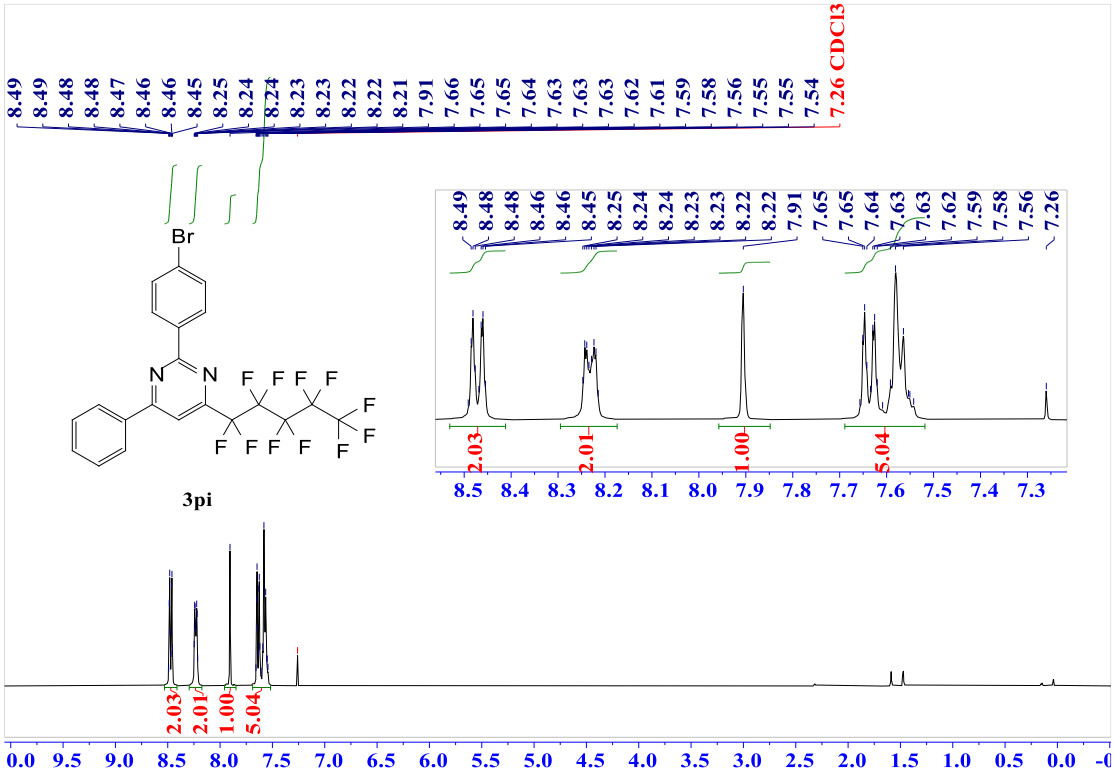
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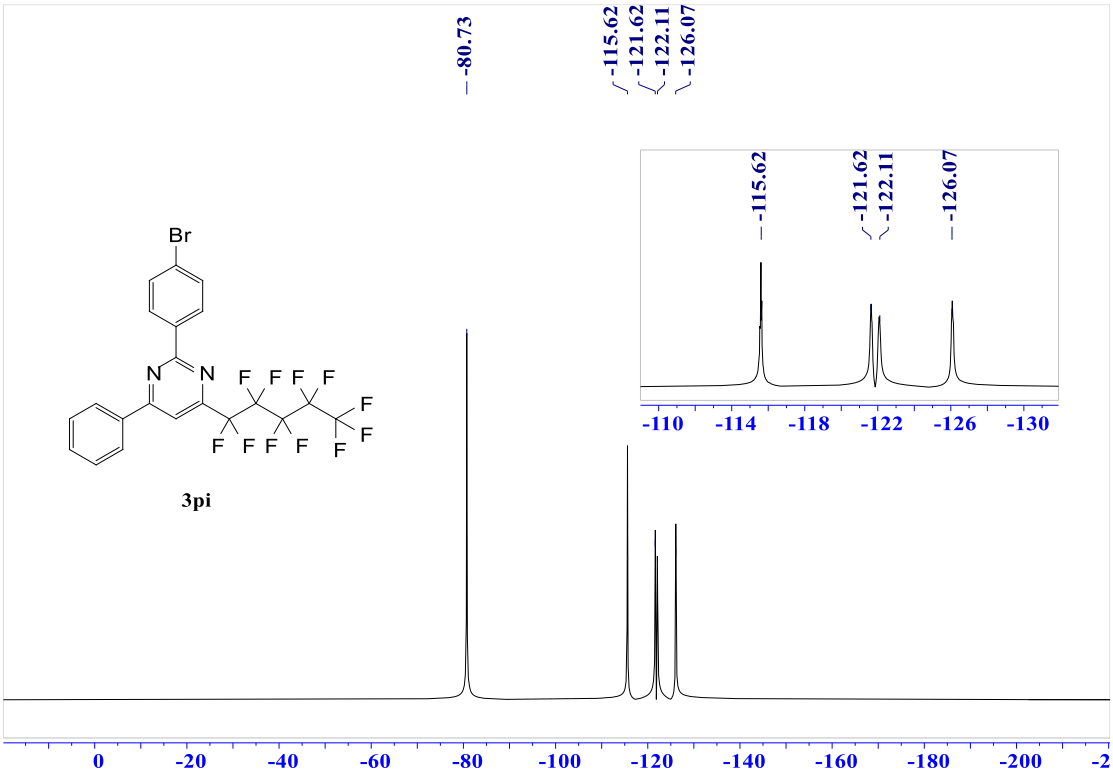
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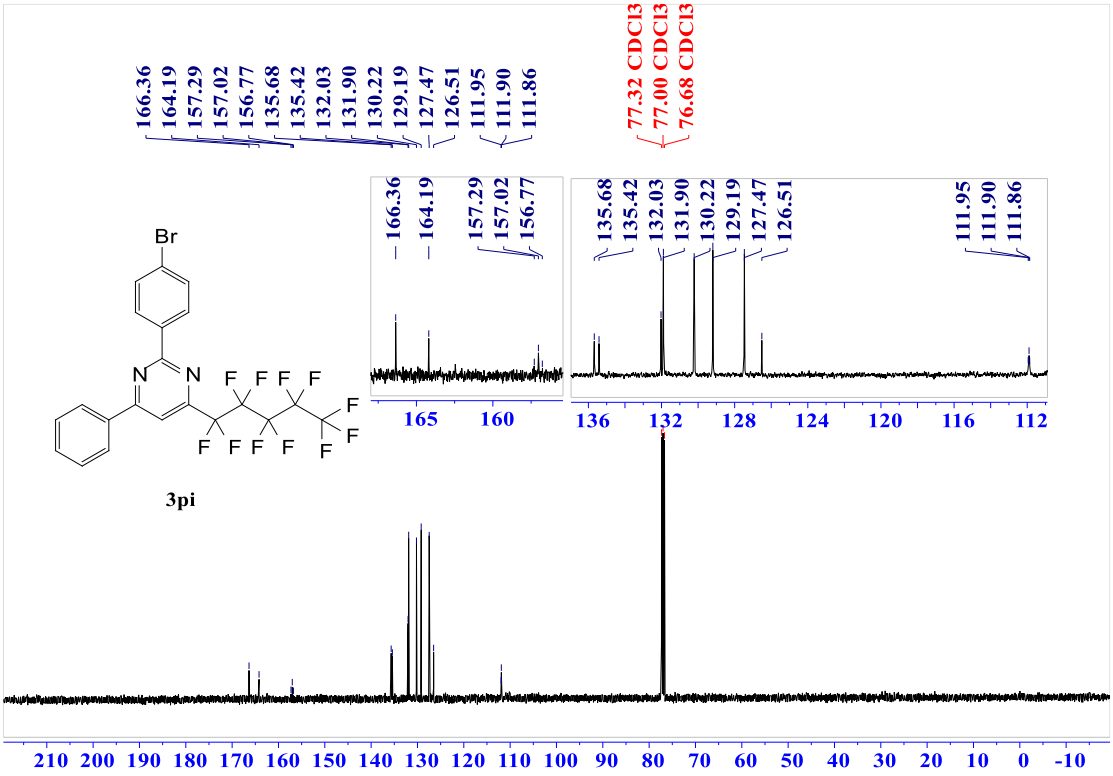
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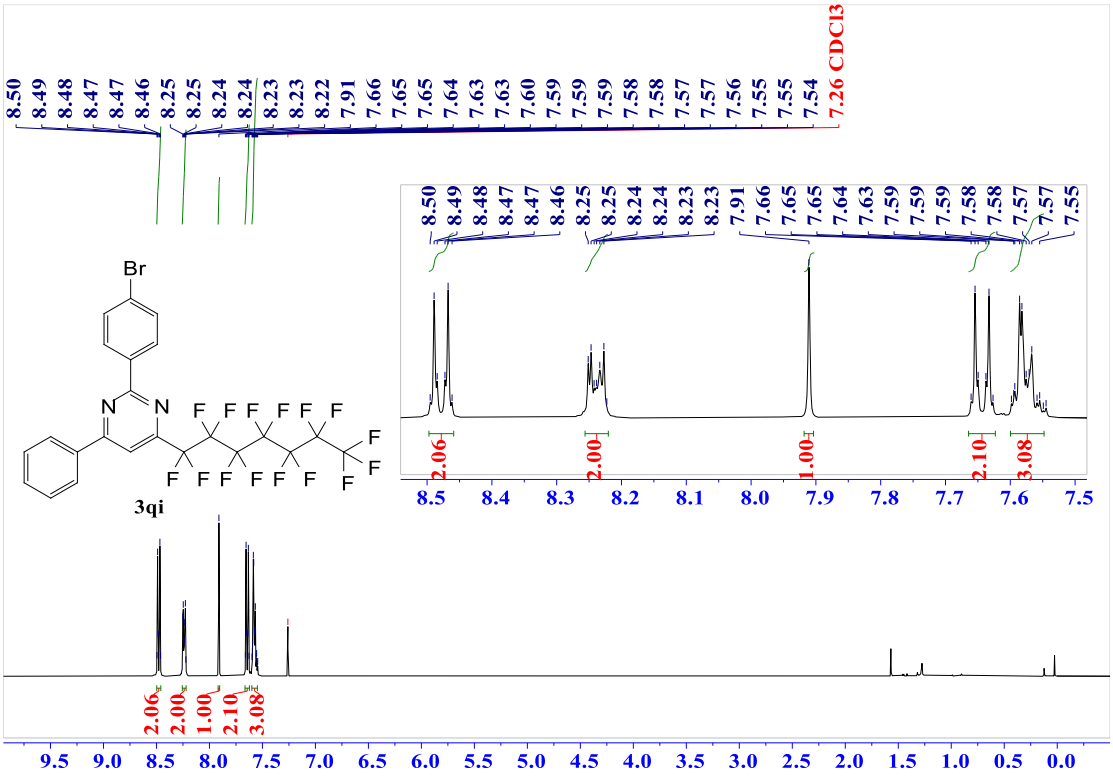
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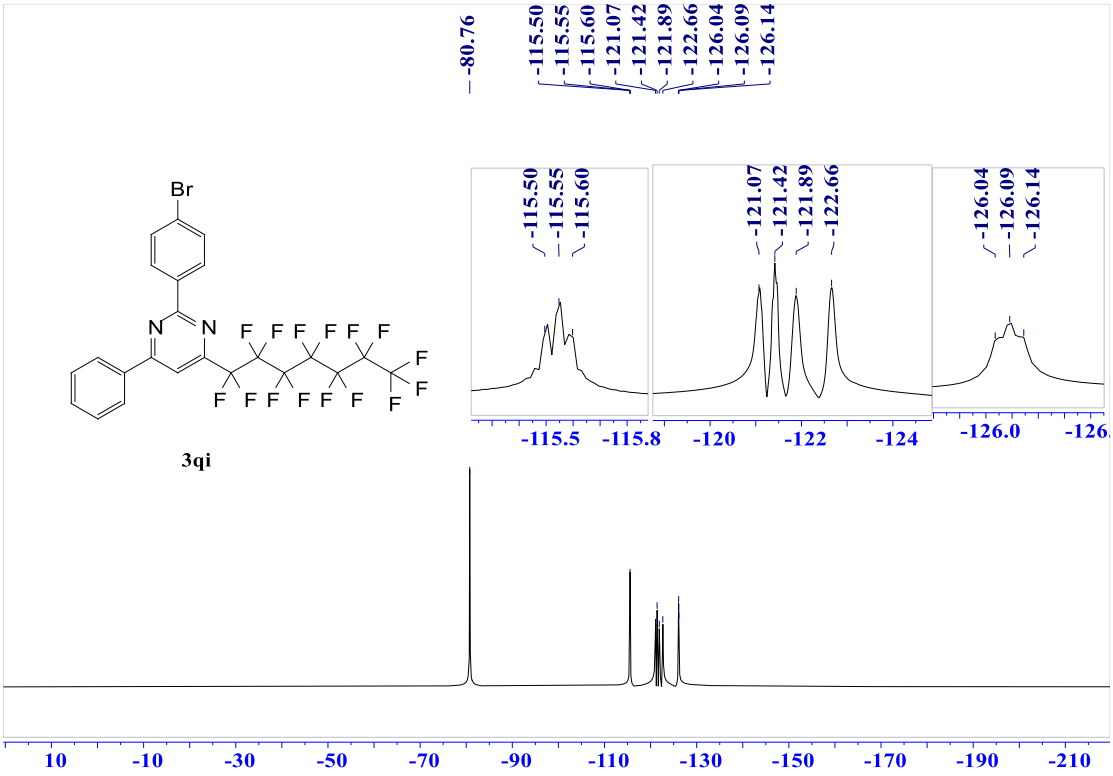
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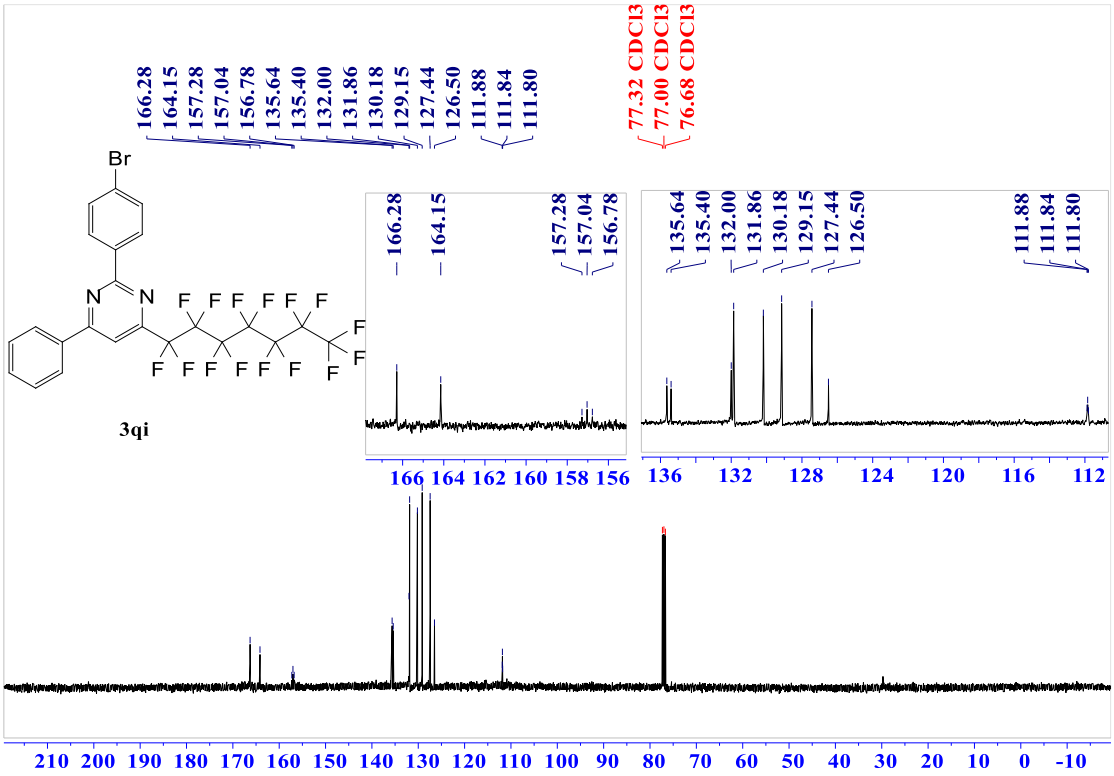
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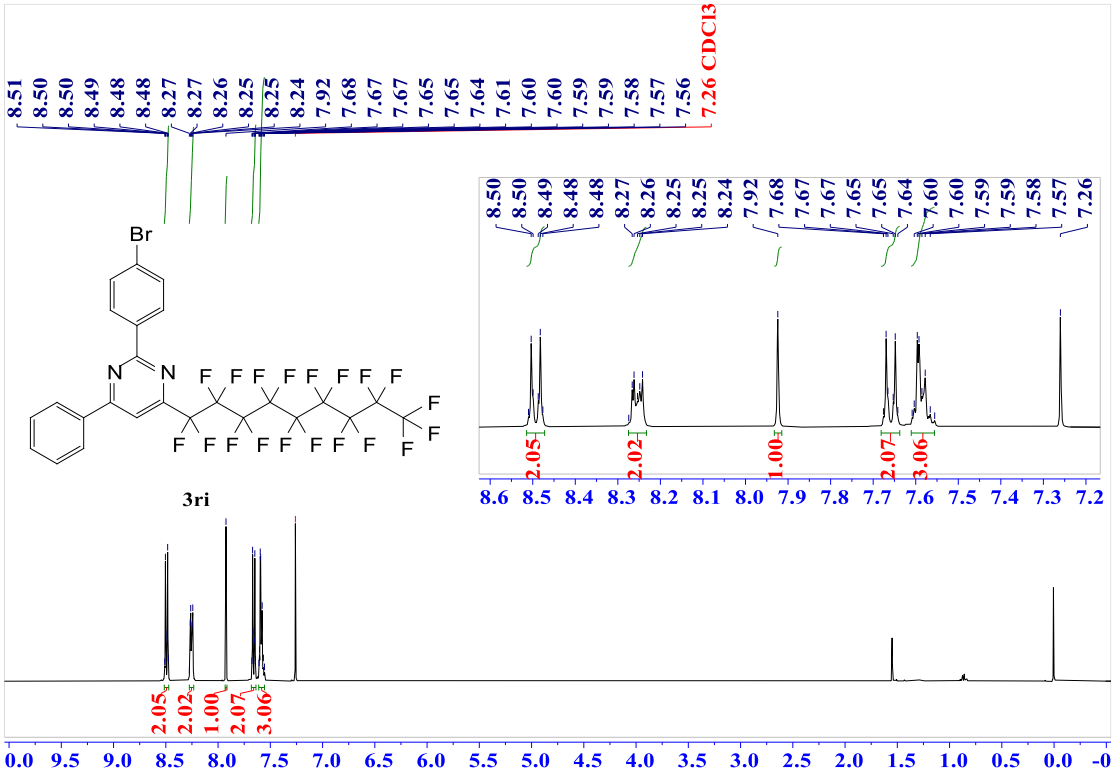
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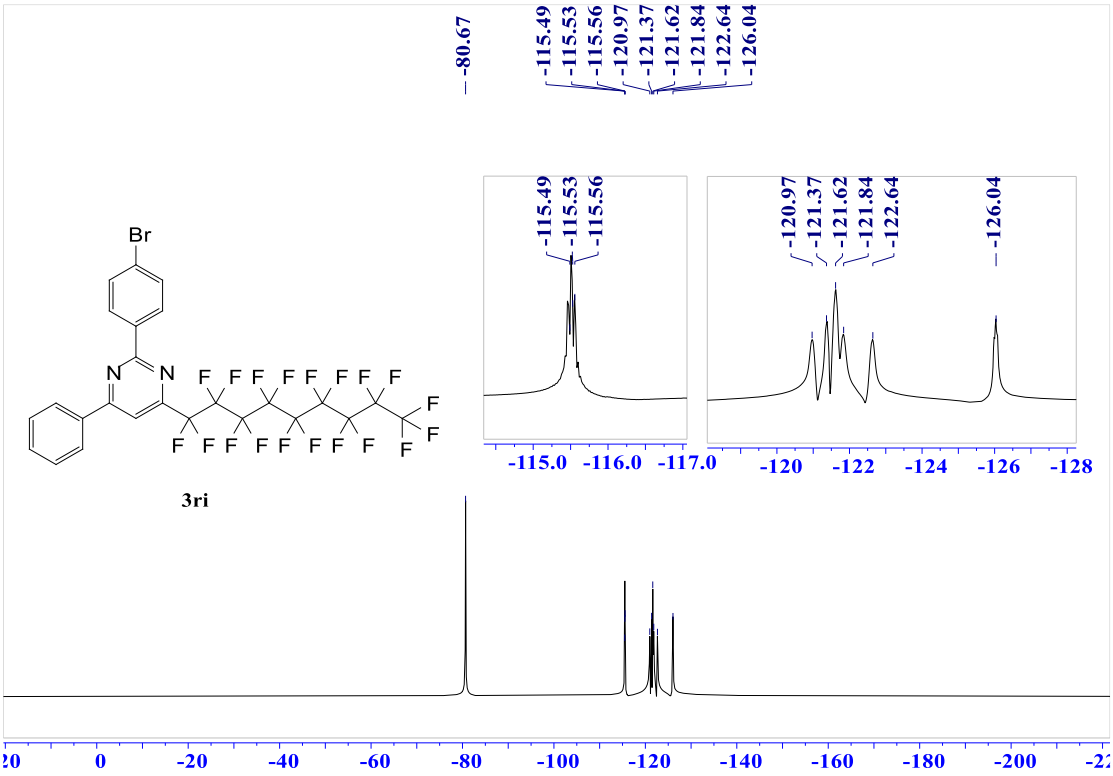
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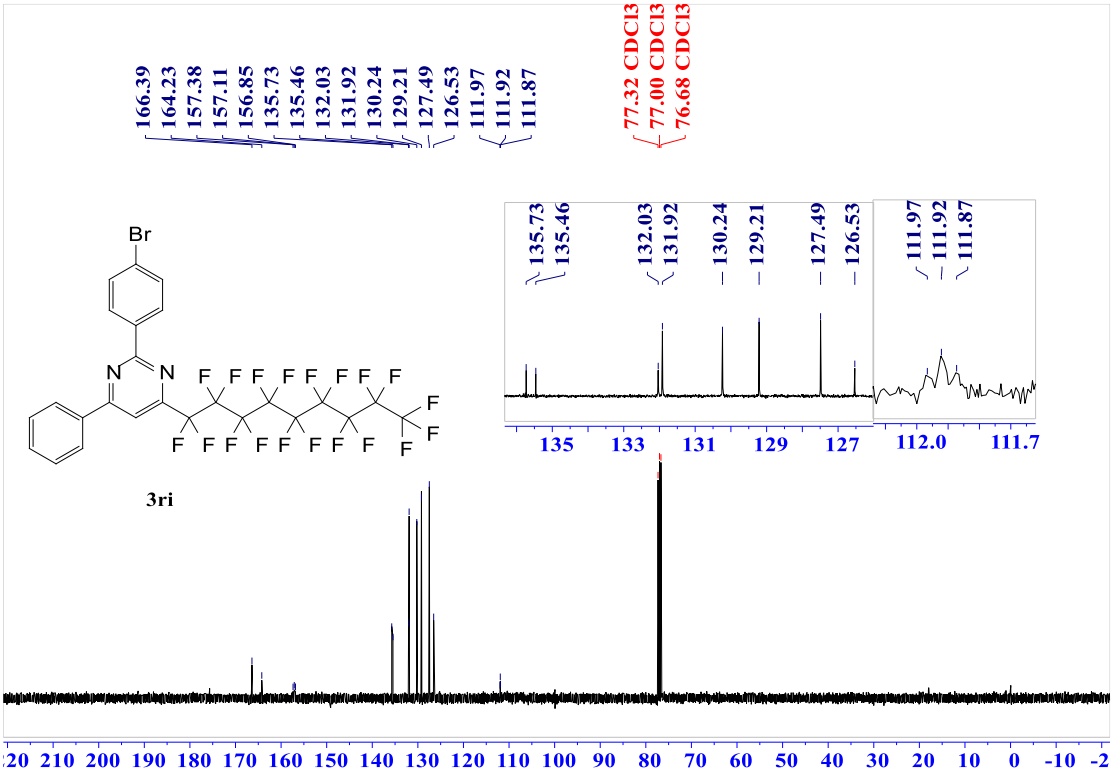
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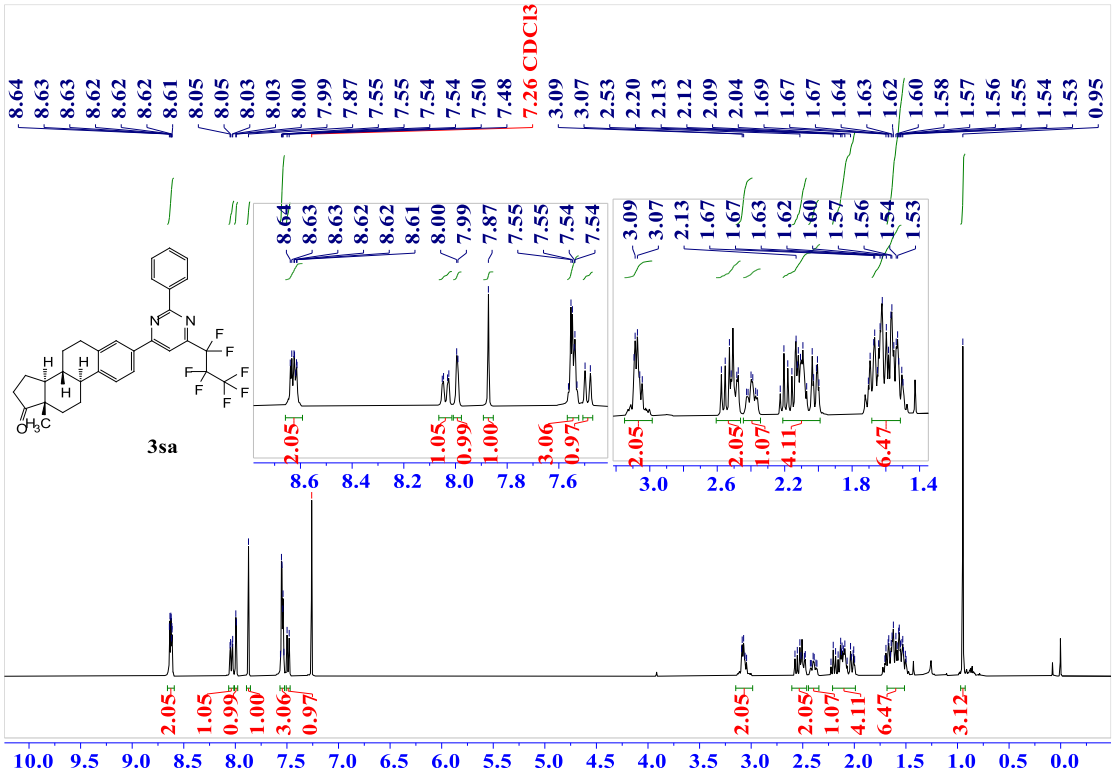
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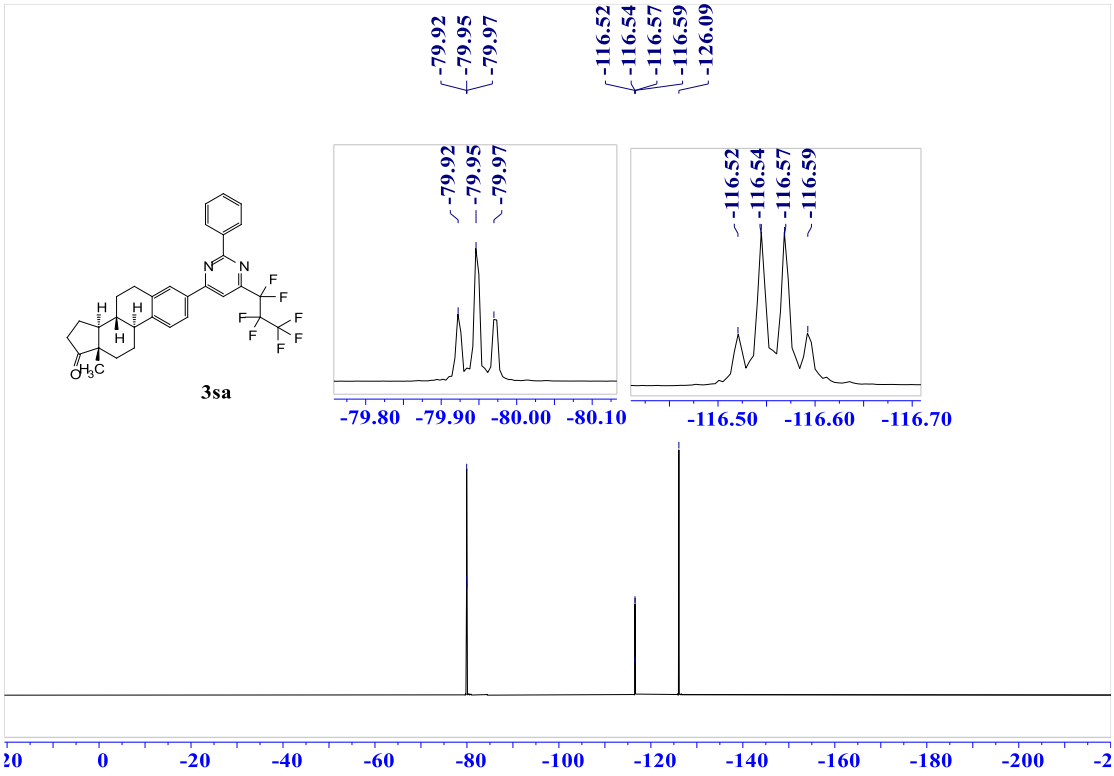
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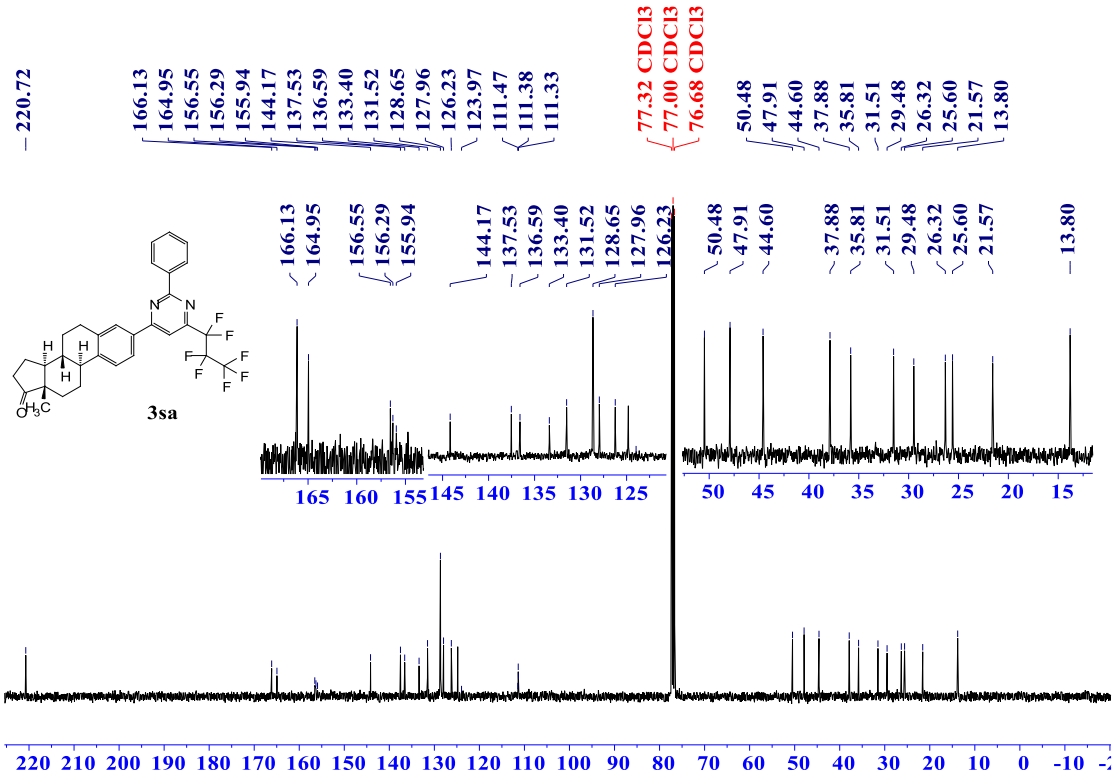
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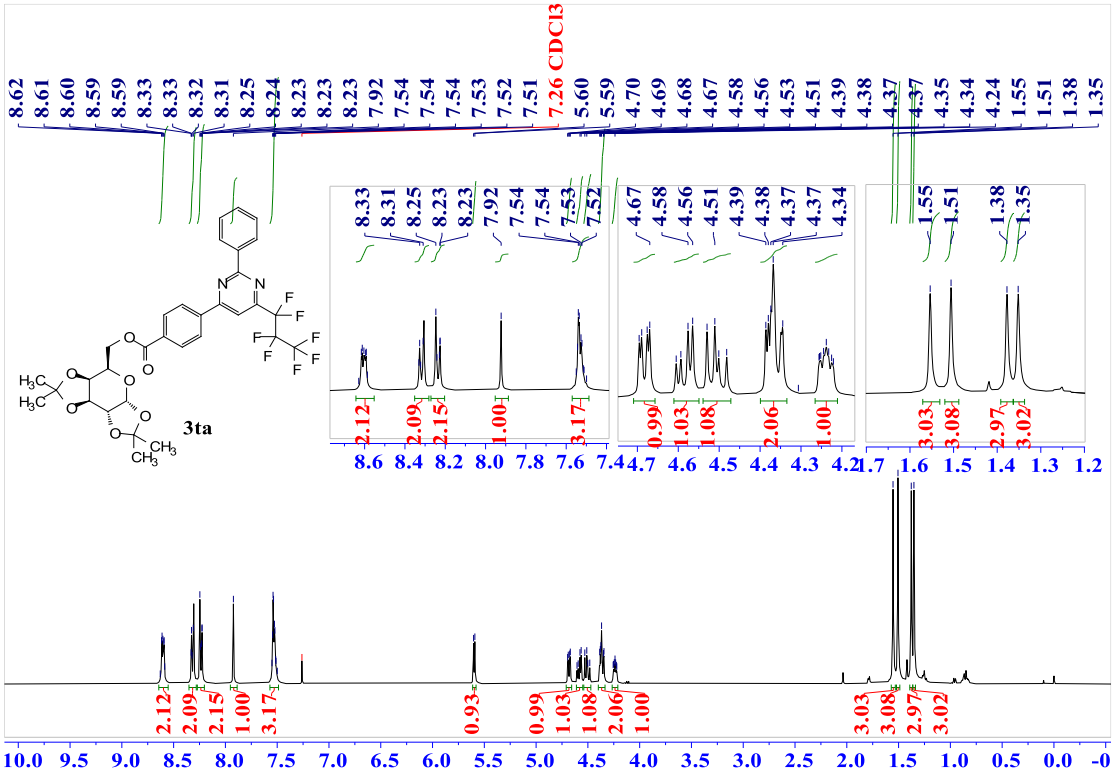
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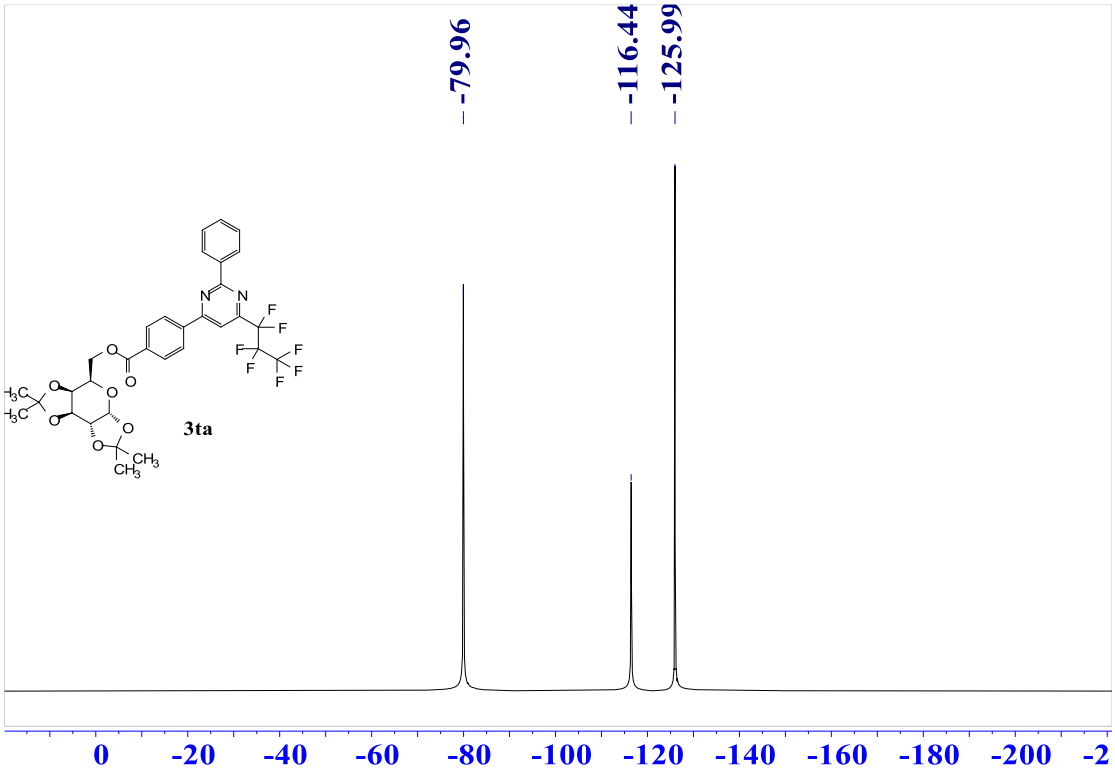
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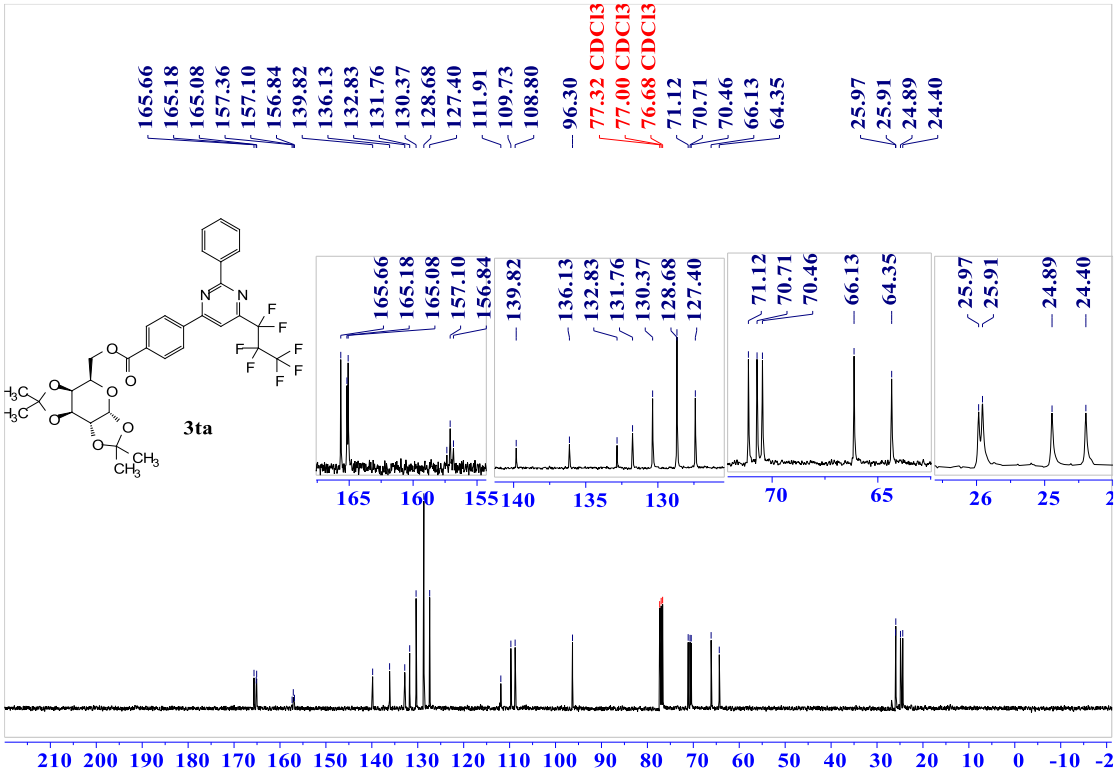
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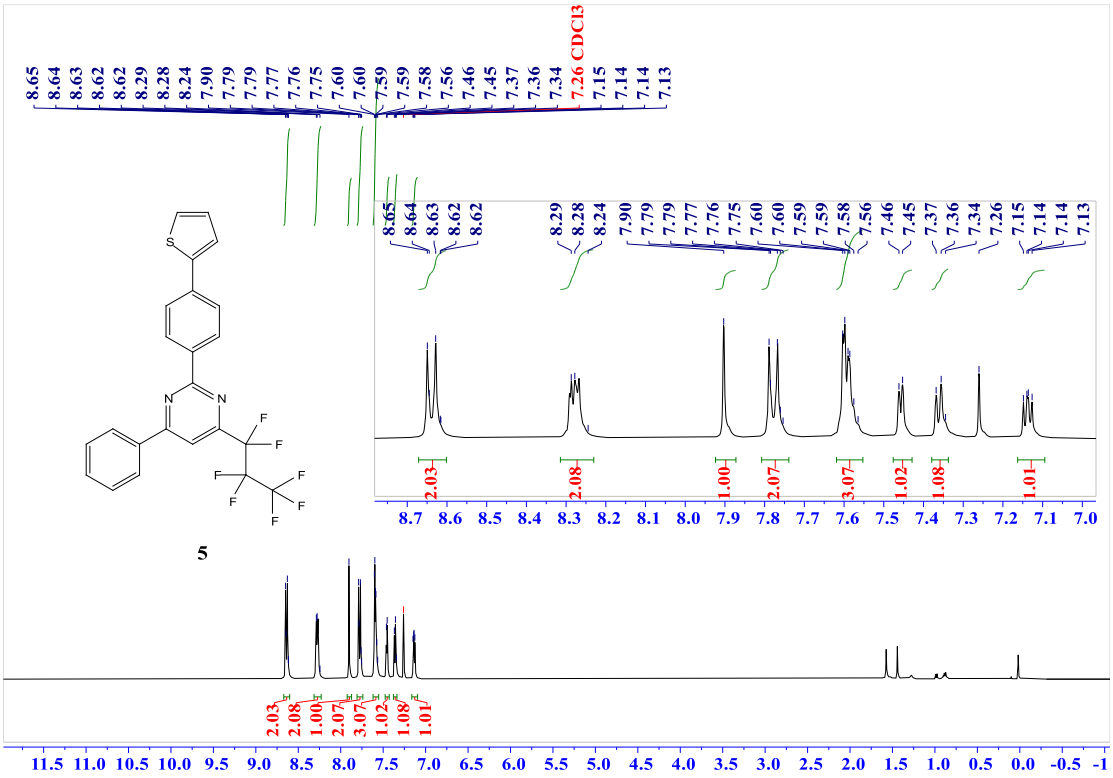
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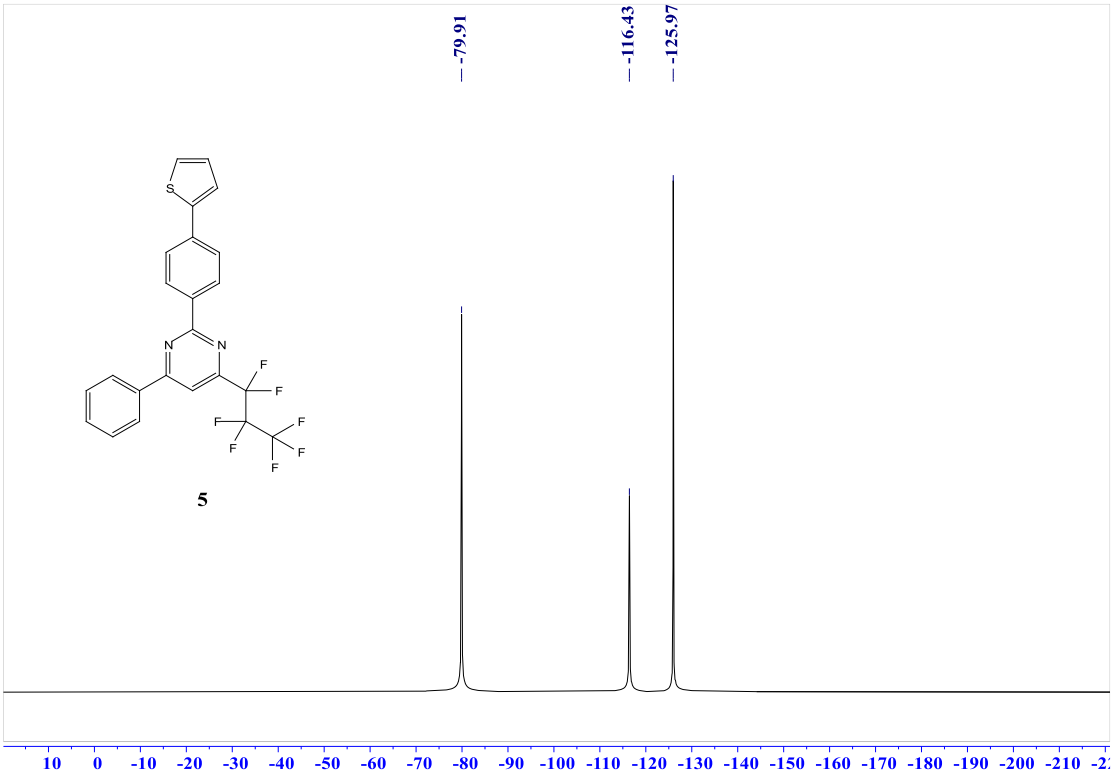
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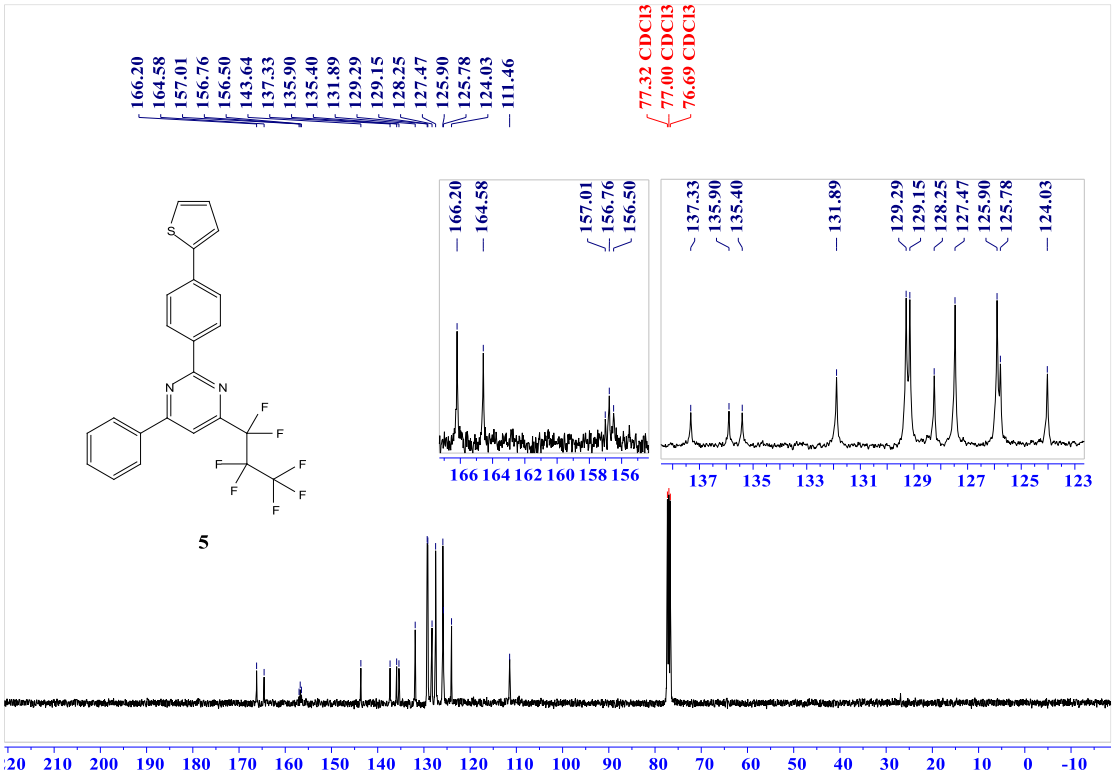
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