Supporting Information

Copper-Catalyzed Three-Component Cyclization of Amidines, Styrenes, and Fluoroalkyl Halides for The Synthesis of Modular Fluoroalkylated Pyrimidines

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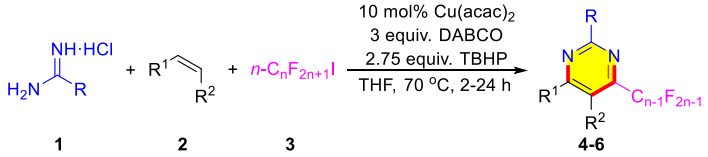
1. General information

Unless otherwise stated, all reagents were purchased from commercial suppliers and used without further purification. All reactions were carried out under air using undistilled solvent, without the need of precautions to exclude air and moisture unless otherwise noted. 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, ^{13}C NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 on Bruker Avance 400 MHz spectrometers. Tetramethylsilane (TMS) served as internal standard for ^{1}H NMR and ^{13}C NMR. High resolution mass spectra (HRMS) were obtained using a commercial apparatus (ESI or EI Source).

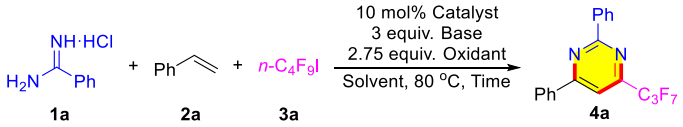
2. General procedures for the synthesis of perfluoroalkylated pyrimidine derivatives



1 **2** **3** **4-6**

Amidine **1** (0.3 mmol), alkene **2** (0.45 mmol), perfluoroalkyl halide **3** (0.75 mmol), $Cu(acac)_2$ (0.03 mmol), triethylenediamine (0.9 mmol) and TBHP (0.825 mmol, 5.5 M in decane) was stirred at 70 °C in THF (1.5 mL) for 2-24 h. Upon completion of the reaction (indicated by TLC), solvent was removed under vacuum and the residue was purified by flash silica gel column chromatography using petroleum ether/ethyl acetate as eluent to afford pure products **4-6**.

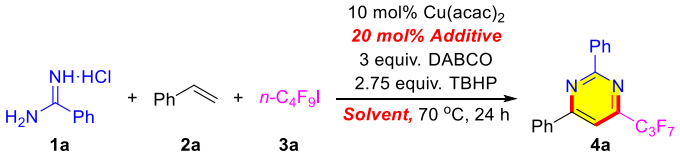
3. Table S1. Optimization of reaction conditions[a]



Entry	Catalyst	Base	Oxidant	Solvent	Time (h)	Yield (%)[b]
1	$Cu(acac)_2$	DABCO	TBHP	DME	12	74 (56)[c]
2	$Cu(acac)_2$	DABCO	TBHP	DME	7	58
3	$Cu(acac)_2$	--	TBHP	DME	12	0
4	$Cu(acac)_2$	DBU	TBHP	DME	12	42
5	$Cu(acac)_2$	K_2CO_3	TBHP	DME	12	21
6	$Cu(acac)_2$	DABCO	--	DME	12	25
7	$Cu(acac)_2$	DABCO	TBPB	DME	12	<10
8	$Cu(acac)_2$	DABCO	$K_2S_2O_8$	DME	12	trace
9	$Cu(acac)_2$	DABCO	TBHP	Toluene	12	71
10	$Cu(acac)_2$	DABCO	TBHP	Dioxane	12	69
11	$Cu(acac)_2$	DABCO	TBHP	DCE	12	(31)[c]
12	$Cu(acac)_2$	DABCO	TBHP	DMF	12	trace
13	$Cu(acac)_2$	DABCO	TBHP	MeCN	12	75
14	$Cu(acac)_2$	DABCO	TBHP	$MeNO_2$	12	0
15	--	DABCO	TBHP	DME	12	42
16	$Co(acac)_3$	DABCO	TBHP	DME	12	37
17	$CuBr_2$	DABCO	TBHP	DME	12	45
18	CuI	DABCO	TBHP	DME	24	(31)[c,d]
19	CuCl	DABCO	TBHP	DME	24	58 (42)[c,d]
20	CuBr·Me_2S	DABCO	TBHP	DME	24	65[d]
21	Cu	DABCO	TBHP	DME	24	40[e]
22	$Cu(acac)_2$	DABCO	TBHP	DME	24	79 (60)[c,e]
23	$Cu(acac)_2$	DABCO	TBHP	THF	24	80 (60)[c,f]

[a] Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), **3a** (0.75 mmol), catalyst (0.03 mmol), base (0.9 mmol) and oxidant (0.825 mmol) in solvent (1.5 mL) at 80 ℃ under air; TBPB = *tert*-butylperoxybenzoate; TBHP = *tert*-butyl hydroperoxide (5.5 M in decane). [b] Yields were determined by NMR analysis with 1,4-dimethoxybenzene as an internal standard. [c] Isolated yields. [d] 0.9 mmol of **2a** and 1.2 mmol of TBHP were used at 88 °C. [e] At 88 °C. [f] At 70 °C.

Table S2. Optimization of reaction conditions[a]

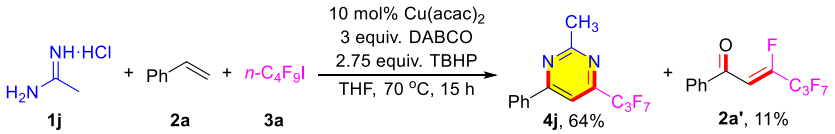


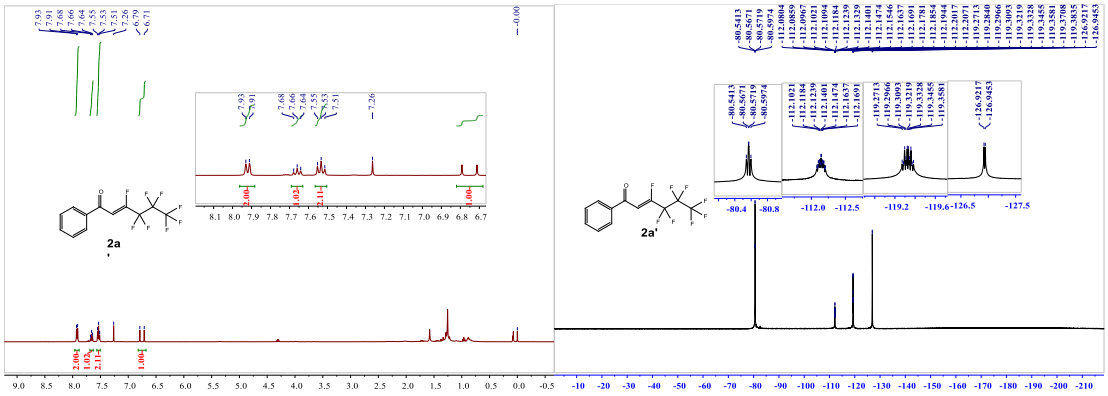
Entry	**Additive** (20 mol%)	**Solvent**	**Yield** (%)[b]
1	--	THF	80
2	TBAI	THF	73
3	$MnCl_2$	THF	52
4	$CeCl_3$	THF	50
5	--	THF-MeCN (2:1)	69
6	--	THF-DME (2:1)	58
7	--	THF-DMF (2:1)	41
8	--	THF-DCE (2:1)	60

[a] Reaction conditions: **1a** (0.3 mmol), **2a** (0.45 mmol), **3a** (0.75 mmol), $Cu(acac)_2$ (0.03 mmol), DABCO (0.9 mmol), additive (0.06 mmol) and TBHP (0.825 mmol) in solvent (1.5 mL) at 70 ℃ under air for 24 h. [b] Yields were determined by NMR analysis with 1,4-dimethoxybenzene as an internal standard.

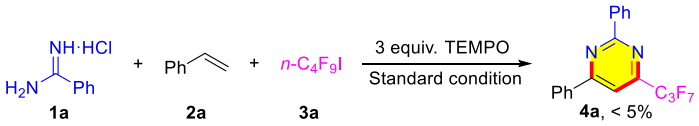
4. Mechanistic studies

1) Detection of the by-product (*Z*)-3,4,4,5,5,6,6,6-octafluoro-1-phenylhex-2-en-1-one (2a')



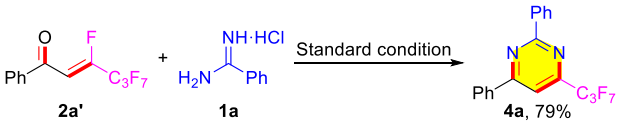


2) Trapping experiment with 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO)



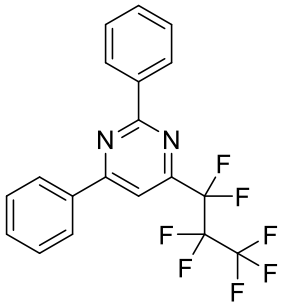
Amidine **1a** (0.3 mmol), alkene **2a** (0.45 mmol), perfluoroalkyl halide **3a** (0.75 mmol), 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO, 0.9 mmol), $Cu(acac)_2$ (0.03 mmol), triethylenediamine (0.9 mmol) and TBHP (0.825 mmol, 5.5 M in decane) was stirred at 70 °C in THF (1.5 mL) for 24 h.

3) The reaction of (*Z*)-3,4,4,4,5,5,6,6,6-octafluoro-1-phenylhex-2-en-1-one (2a') with 1a

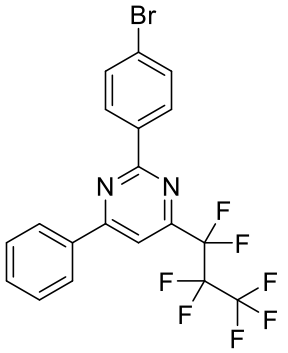


(*Z*)-3,4,4,4,5,5,6,6,6-Octafluoro-1-phenylhex-2-en-1-one (**2a'**, 0.36 mmol), amidine **1a** (0.3 mmol), $Cu(acac)_2$ (0.03 mmol), triethylenediamine (0.9 mmol) and TBHP (0.825 mmol, 5.5 M in decane) was stirred at 70 °C in THF (1.5 mL) for 24 h. Upon completion of the reaction (indicated by TLC), solvent was removed under vacuum and the residue was purified by flash silica gel column chromatography using petroleum ether/ethyl acetate as eluent, affording pure product **4a** in 79% yield.

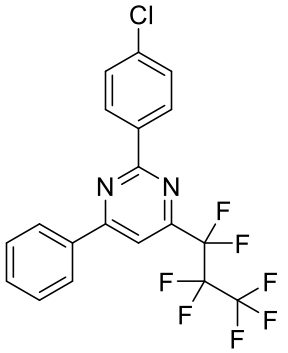
5. Characterization data for perfluoroalkylated pyrimidine derivatives



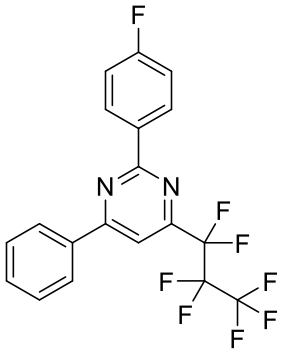
4-(Perfluoropropyl)-2,6-diphenylpyrimidine (4a): Yield = 60% . White solid. M.p. 59.6–60.2 ^{o}C. IR (KBr) ν = 3414, 3082, 1546, 1372, 1227, 928, 733 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.68–8.60 (m, 2H), 8.32–8.24 (m, 2H), 7.91 (s, 1H), 7.63–7.50 (m, 6H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.05 (t, J = 9.6 Hz, 3F), -116.65 (q, J = 9.6 Hz, 2F), -126.18 (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.



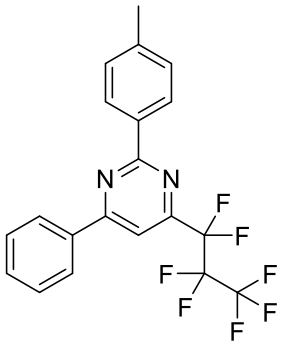
2-(4-Bromophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (4b): Yield = 73%. White solid. M.p. 90.1–92.2 ^{o}C. IR (KBr) ν = 3414, 2929, 1588, 1373, 1140, 740 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.64–8.36 (m, 5H), 7.90–7.78 (m, 2H), 7.72–7.58 (m, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.04 (t, J = 9.2 Hz, 3F), -116.64 (q, J = 9.1 Hz, 2F), -126.14 (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: 478.9963.



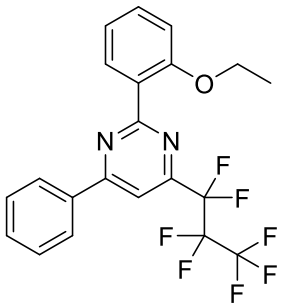
2-(4-Chlorophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (4c): Yield = 62%. White solid. M.p. 84.3–85.2 ºC. IR (KBr) ν = 3443, 2922, 1586, 1384, 1231, 929, 741 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.57–8.48 (m, 5H), 7.71–7.61 (m, 5H) ppm. ^{19}F NMR (376 MHz, DMSO-d_6): δ = -79.61 (t, J = 9.6 Hz, 3F), -115.52 (q, J = 9.5 Hz, 2F), -125.78 (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: 435.0492.



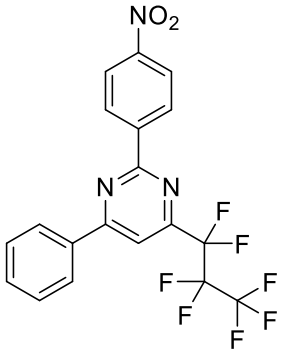
2-(4-Fluorophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (4d): Yield = 61%. White solid. M.p. 77.3–78.2 ºC. IR (KBr) ν = 3572, 2928, 1546, 1371, 1227, 1116, 931, 771 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.63–8.54 (m, 2H), 8.54–8.46 (m, 3H), 7.71–7.59 (m, 3H), 7.49–7.38 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -74.82 (t, J = 8.8 Hz, 3F), -103.78 – -103.99 (m, 1F), -110.74 (q, J = 8.6 Hz, 2F), -120.94– -121.13 (m, 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: 419.0809.



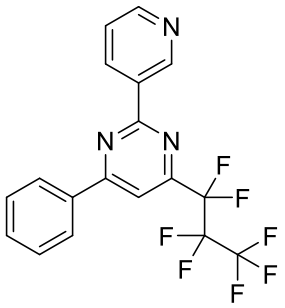
4-(Perfluoropropyl)-6-phenyl-2-(*p*-tolyl)pyrimidine (4e): Yield = 62%. White solid. M.p. 101.2–101.9 °C. IR (KBr) ν = 2924, 1544, 1371, 1229, 1117, 927, 739 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.41 (d, J = 8.2 Hz, 2H), 8.16–8.11 (m, 2H), 7.75 (s, 1H), 7.48–7.40 (m, 3H), 7.21 (d, J = 8.1 Hz, 2H), 2.33 (s, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.07 (t, J = 9.6 Hz, 3F), -116.64 (q, J = 9.6 Hz, 2F), -126.17 (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: 415.1028.



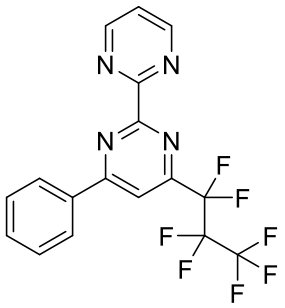
2-(2-Ethoxyphenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (4f): Yield = 75%. Yellow oil. IR (KBr) ν = 3411, 2979, 1585, 1374, 1234, 753 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.50 (s, 1H), 8.44 (dd, J = 8.0, 1.5 Hz, 2H), 7.80 (dd, J = 7.6, 1.7 Hz, 1H), 7.68–7.58 (m, 3H), 7.57–7.50 (m, 1H), 7.22 (d, J = 8.2 Hz, 1H), 7.12 (t, J = 7.1 Hz, 1H), 4.13 (q, J = 6.9 Hz, 2H), 1.28 (t, J = 6.9 Hz, 3H) ppm. ^{19}F NMR (376 MHz, DMSO-d_6): δ = -79.69 (t, J = 9.0 Hz, 3F), -115.42 (q, J = 9.0 Hz, 2F), -125.67 (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: 445.1133.



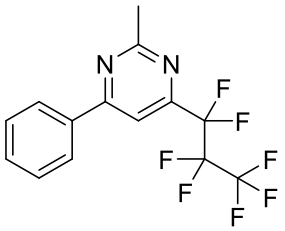
2-(4-Nitrophenyl)-4-(perfluoropropyl)-6-phenylpyrimidine (4g): Yield = 63%. Yellow solid. M.p. 58.0–60.2 °C. IR (KBr) ν = 3419, 3090, 1580, 1341, 1233, 1120, 734 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.79 (d, J = 8.9 Hz, 2H), 8.37 (d, J = 8.9 Hz, 2H), 8.31–8.25 (m, 2H), 8.01 (s, 1H), 7.67–7.57 (m, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.02 (t, J = 9.7 Hz, 3F), -116.57 (q, J = 9.7 Hz, 2F), -126.06 (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.



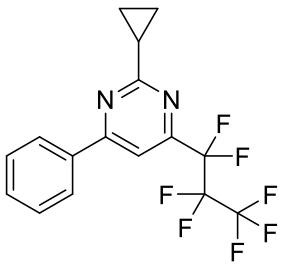
4-(Perfluoropropyl)-6-phenyl-2-(pyridin-3-yl)pyrimidine (4h): Yield = 52%. White solid. M.p. 68.1–69.2 °C. IR (KBr) ν = 3072, 2922, 1587, 1375, 1223, 1117, 928, 738 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.82 (s, 1H), 8.85 (d, J = 8.0 Hz, 1H), 8.79 (s, 1H), 8.33–8.23 (m, 2H), 7.97 (s, 1H), 7.64–7.56 (m, 3H), 7.51–7.44 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.05 (t, J = 9.6 Hz, 3F), -116.62 (q, J = 9.6 Hz, 2F), -126.12 (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: 402.0840.



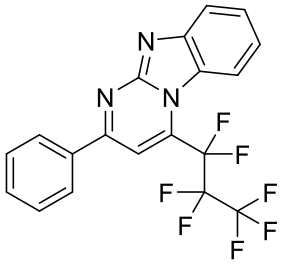
4-(Perfluoropropyl)-6-phenyl-2,2'-bipyrimidine (4i): Yield = 60%. White solid. M.p. 134.6–135.5 °C. IR (KBr) ν = 3419, 3065, 1582, 1374, 1224, 1123, 933, 739 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.09 (d, J = 4.9 Hz, 2H), 8.28 (dd, J = 7.6, 2.0 Hz, 2H), 8.13 (s, 1H), 7.63–7.55 (m, 3H), 7.49 (t, J = 4.9 Hz, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.94 (t, J = 9.8 Hz, 3F), -116.50 (q, J = 9.7 Hz, 2F), -125.73 (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: 403.0796.



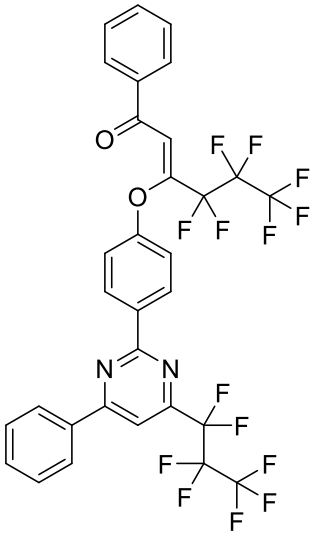
2-Methyl-4-(perfluoropropyl)-6-phenylpyrimidine (4j): Yield = 64%. Colourless oil. IR (KBr) ν = 3421, 2951, 1617, 1232, 799, 733 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.18–8.10 (m, 2H), 7.83 (s, 1H), 7.60–7.49 (m, 3H), 2.89 (s, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.16 (t, J = 9.5 Hz, 3F), -116.96 (q, J = 9.8 Hz, 2F), -126.22 (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: 339.0729.



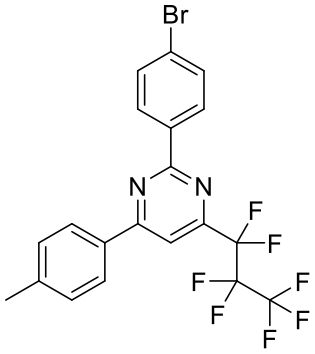
2-Cyclopropyl-4-(perfluoropropyl)-6-phenylpyrimidine (4k): Yield = 58%. M.p. 41.0–41.6 °C. IR (KBr) ν = 3410, 2925, 1578, 1373, 1226, 1116, 952, 741 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.16–8.08 (m, 2H), 7.75 (s, 1H), 7.59–7.50 (m, 3H), 2.47–2.37 (m, 1H), 1.31–1.26 (m, 2H), 1.20–1.14 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.11 (t, J = 9.6 Hz, 3F), -116.93 (q, J = 9.6 Hz, 2F), -126.27 (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: 365.0882.



4-(Perfluoropropyl)-2-phenylbenzo[4,5]imidazo[1,2-*a*]pyrimidine (4l): Yield = 65%. Yellow solid. M.p. 80.9–82.3 °C. IR (KBr) ν = 3412, 3146, 1629, 1399, 1223, 1122, 1025, 741 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.50–8.43 (m, 2H), 8.20 (s, 1H), 8.00 (d, J = 8.2 Hz, 1H), 7.97–7.90 (m, 1H), 7.70–7.62 (m, 4H), 7.59–7.52 (m, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.56 (t, J = 10.4 Hz, 3F), -109.98 (q, J = 10.4 Hz, 2F), -123.39 (s, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 159.2, 151.2 (t, $J_{C\text{-}F}$ = 25.1 Hz), 145.3, 135.1, 132.0, 129.5, 129.1, 128.0, 127.6, 126.6, 123.4, 120.9, 114.9 (m), 105.7 (t, $J_{C\text{-}F}$ = 8.8 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling. HRMS m/z: calcd for $C_{19}H_{11}F_7N_3$ $[M+H]^+$ 414.0836, found: 414.0831.

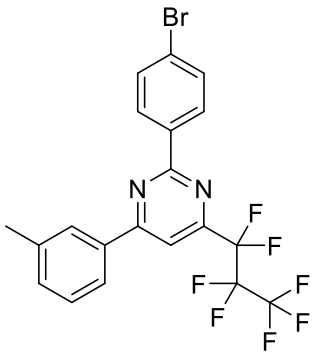


(*Z*)-4,4,5,5,6,6,6-Heptafluoro-3-(4-(4-(perfluoropropyl)-6-phenylpyrimidin-2-yl)phenoxy)-1-phenylhex-2-en-1-one (4m): Yield = 47%. White solid. M.p. 116.2–117.1 °C. IR (KBr) ν = 3410, 3064, 1690, 1548, 1229, 1116, 930, 772 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.51–8.46 (m, 3H), 8.43–8.37 (m, 2H), 7.85 (dd, J = 8.2, 1.4 Hz, 2H), 7.77 (s, 1H), 7.70–7.60 (m, 4H), 7.56–7.50 (m, 2H), 7.21 (d, J = 8.9 Hz, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.06 (t, J = 9.6 Hz, 3F), -80.30 (t, J = 9.9 Hz, 3F), -116.40 (q, J = 9.9 Hz, 2F), -116.71 (q, J = 9.5 Hz, 2F), -125.95 (s, 2F), -126.22 (s, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 188.2, 166.1, 164.0, 158.8, 156.7 (t, $J_{C\text{-}F}$ = 26.0 Hz), 147.2 (t, $J_{C\text{-}F}$ = 26.7 Hz), 136.3, 135.8, 134.0, 132.2, 131.9, 130.4, 129.1, 128.8, 128.5, 127.4, 116.6 (t, $J_{C\text{-}F}$ = 4.4 Hz), 116.4, 111.3 (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 $C_{31}H_{17}F_{14}N_2O_2$ $[M+H]^+$ 715.1061, found: 715.1088.

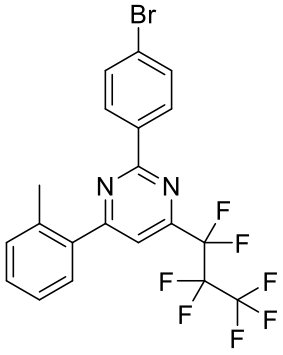


2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(*p*-tolyl)pyrimidine (5a): Yield = 56%. White solid. M.p. 97.5–99.8 °C. IR (KBr) ν = 3414, 2924, 1583, 1385, 1227, 1117, 1010, 926, 740 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.49 (s, 1H), 8.41 (t, J = 8.7 Hz, 4H), 7.88–7.79 (m, 2H), 7.43 (d,

J = 8.0 Hz, 2H), 2.43 (s, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.06 (t, J = 9.7 Hz, 3F), -116.69 (q, J = 9.7 Hz, 2F), -126.17 (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: 493.0168.

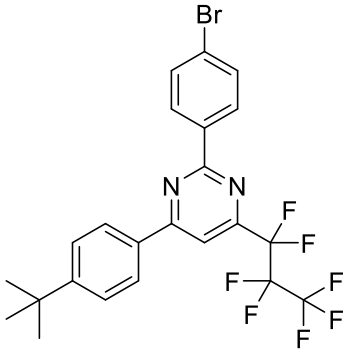


2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(m-tolyl)pyrimidine (5b): Yield = 63%. White solid. M.p. 47.8–49.2 °C. IR (KBr) ν = 3415, 2923, 1588, 1380, 1184, 1120, 936, 745 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.52 (s, 1H), 8.47–8.40 (m, 2H), 8.34–8.27 (m, 2H), 7.85–7.79 (m, 2H), 7.55–7.45 (m, 2H), 2.47 (s, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.05 (t, J = 9.8 Hz, 3F), -116.67 (q, J = 9.6 Hz, 2F), -126.16 (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: 493.0144.

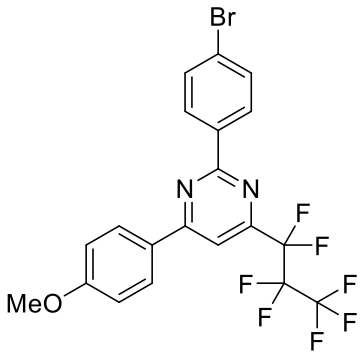


2-(4-Bromophenyl)-4-(perfluoropropyl)-6-(*o*-tolyl)pyrimidine (5c): Yield = 51%. Yellow oil. IR (KBr) ν = 3455, 2923, 1583, 1387, 1232, 1010, 741 cm^{-1}. ^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.33–8.28 (m, 2H), 8.11 (s, 1H), 7.77–7.71 (m, 2H), 7.67 (dd, J = 8.1, 1.4 Hz, 1H), 7.48–7.42 (m,

1H), 7.37 (dd, J = 7.8, 6.5 Hz, 2H), 2.46 (s, 3H) ppm. ^{19}F NMR (376 MHz, DMSO-d_6): δ = -74.98 (t, J = 8.9 Hz, 3F), -111.05 (q, J = 8.9 Hz, 2F), -121.22 (s, 2F) ppm. ^{13}C NMR (100 MHz, DMSO-d_6): δ = 169.7, 162.8, 155.0 (t, $J_{C\text{-}F}$ = 25.5 Hz), 136.6, 136.2, 135.1, 132.2, 131.4, 130.6, 130.4, 130.0, 126.5, 125.9, 116.8 (t, $J_{C\text{-}F}$ = 4.0 Hz), 20.3 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling. HRMS m/z: calcd for $C_{20}H_{13}BrF_7N_2$ $[M+H]^+$ 493.0145, found: 493.0135.

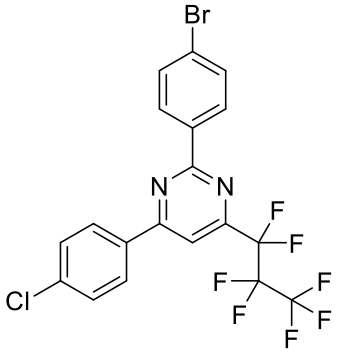


2-(4-Bromophenyl)-4-(4-(*tert*-butyl)phenyl)-6-(perfluoropropyl)pyrimidine (5d): Yield = 57%. White solid. M.p. 110.9–111.9 ºC. IR (KBr) ν = 3410, 2960, 1590, 1390, 1220, 1120, 928, 840, 741 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.53–8.44 (m, 2H), 8.24–8.14 (m, 2H), 7.89 (s, 1H), 7.68–7.63 (m, 2H), 7.63–7.56 (m, 2H), 1.39 (s, 9H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.06 (t, J = 9.1 Hz, 3F), -116.72 (q, J = 9.2 Hz, 2F), -126.21 (s, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 164.1, 155.8, 155.4 (t, $J_{C\text{-}F}$ = 25.6 Hz), 135.5, 132.9, 131.9, 130.2, 127.3, 126.4, 126.2, 111.6 (t, $J_{C\text{-}F}$ = 4.9 Hz), 35.0, 31.1ppm, 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: 535.0587.

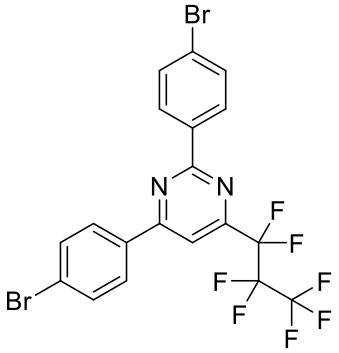


2-(4-Bromophenyl)-4-(4-methoxyphenyl)-6-(perfluoropropyl)pyrimidine (5e): Yield = 63%. White solid. M.p. 89.1–90.3 ºC. IR (KBr) ν = 3414, 2955, 1584, 1544, 1388, 1212, 923, 834 cm^{-1}.

^{1}H NMR (400 MHz, DMSO-d_6): δ = 8.52–8.47 (m, 2H), 8.45 (s, 1H), 8.44–8.40 (m, 2H), 7.85–7.78 (m, 2H), 7.19–7.13 (m, 2H), 3.89 (s, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.07 (t, J = 9.7 Hz, 3F), -116.73 (q, J = 9.5 Hz, 2F), -126.18 (s, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.7, 164.0, 162.9, 156.5 (t, $J_{C\text{-}F}$ = 27.2 Hz), 135.6, 131.8, 130.2, 129.2, 128.0, 126.3, 114.5, 110.9 (t, $J_{C\text{-}F}$ = 4.6 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 $C_{20}H_{13}BrF_7N_2O$ $[M+H]^+$ 509.0094, found: 509.0092.

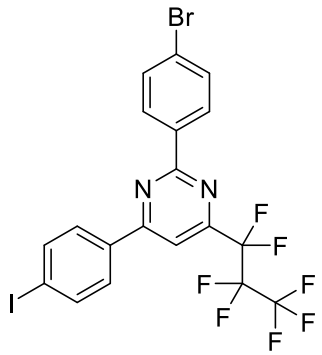


2-(4-Bromophenyl)-4-(4-chlorophenyl)-6-(perfluoropropyl)pyrimidine (5f): Yield = 64%. White solid. M.p. 139.6–141.3 °C. IR (KBr) ν = 3413, 2925, 1583, 1382, 1231, 1010, 830, 744 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.50–8.43 (m, 2H), 8.23–8.16 (m, 2H), 7.87 (s, 1H), 7.69–7.62 (m, 2H), 7.58–7.50 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.04 (t, J = 9.7 Hz, 3F), -116.64 (q, J = 9.8 Hz, 2F), -126.11 (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: 512.9626.

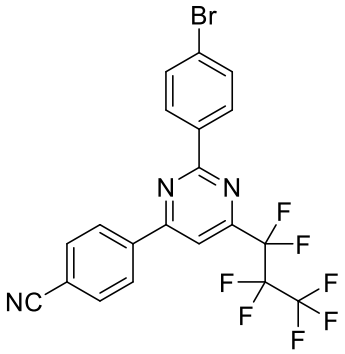


2,4-Bis(4-bromophenyl)-6-(perfluoropropyl)pyrimidine (5g): Yield = 64%. White solid. M.p. 141.7–142.9 °C. IR (KBr) ν = 3412, 3086, 1585, 1385, 1230, 1009, 926, 826, 742 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.49–8.40 (m, 2H), 8.15–8.07 (m, 2H), 7.87 (s, 1H), 7.73–7.67 (m, 2H),

7.67–7.60 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.04 (t, J = 9.7 Hz, 3F), -116.63 (q, J = 9.8 Hz, 2F), -126.09 (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: 556.9105.

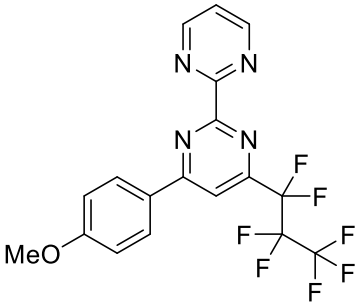


2-(4-Bromophenyl)-4-(4-iodophenyl)-6-(perfluoropropyl)pyrimidine (5h): Yield = 53%. White solid. M.p. 110.7–112.3 °C. IR (KBr) ν = 3412, 2934, 1588, 1385, 1228, 1118, 1004, 741 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.50–8.41 (m, 2H), 8.01–7.88 (m, 4H), 7.87 (s, 1H), 7.69–7.61 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 165.5, 164.3, 157.1 (t, $J_{C\text{-}F}$ = 26.3 Hz), 138.5, 135.2, 135.1, 132.0, 130.2, 128.9, 126.7, 111.5 (t, $J_{C\text{-}F}$ = 4.5 Hz), 99.3 ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling. HRMS m/z: calcd for $C_{19}H_{10}BrF_7IN_2$ $[M+H]^+$ 604.8955, found: 604.8955.

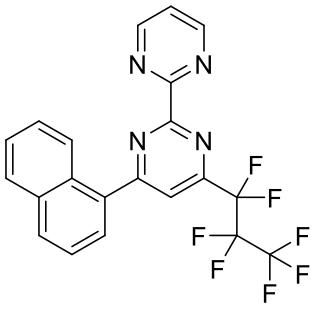


4-(2-(4-Bromophenyl)-6-(perfluoropropyl)pyrimidin-4-yl)benzonitrile (5i): Yield = 58%. White solid. M.p. 212.1–212.6 °C. IR (KBr) ν = 3410, 3075, 2230, 1543, 1389, 1185, 1010, 841, 739 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.51–8.43 (m, 2H), 8.40–8.33 (m, 2H), 7.95 (s, 1H), 7.92–7.85 (m, 2H), 7.71–7.63 (m, 2H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.01 (t, J = 9.2 Hz, 3F), -116.55 (q, J = 9.5 Hz, 2F), -126.03 (s, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 164.6,

164.4, 157.6 (t, J_{C-F} = 26.3 Hz), 139.6, 134.8, 132.9, 132.1, 130.2, 128.0, 127.0, 118.0, 115.4, 112.2 (t, J_{C-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 $C_{20}H_{10}BrF_7N_3$ $[M+H]^+$ 503.9941, found: 503.9936.

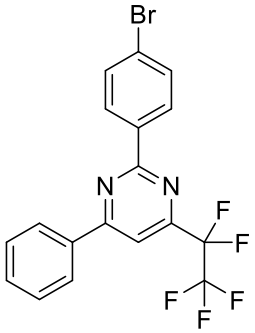


4-(4-Methoxyphenyl)-6-(perfluoropropyl)-2,2'-bipyrimidine (5m): Yield = 42%. White solid. M.p. 105.9–107.2 °C. IR (KBr) ν = 3411, 3068, 2941, 1563, 1374, 1230, 1117, 930, 855, 731 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 9.08 (d, J = 4.9 Hz, 2H), 8.33–8.23 (m, 2H), 8.05 (s, 1H), 7.48 (t, J = 4.9 Hz, 1H), 7.11–7.01 (m, 2H), 3.91 (s, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.98 (t, J = 9.3 Hz, 3F), -116.58 (q, J = 9.5 Hz, 2F), -125.78 (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-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.

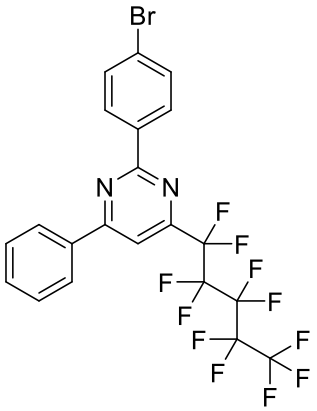


4-(Naphthalen-1-yl)-6-(perfluoropropyl)-2,2'-bipyrimidine (5n): Yield = 38%. White solid. M.p. 102.8–104.0 °C. IR (KBr) ν = 3419, 3046, 2924, 1562, 1374, 1223, 930, 779 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 9.08 (d, J = 4.9 Hz, 2H), 8.21–8.15 (m, 1H), 8.08 (s, 1H), 8.04 (d, J = 8.2 Hz, 1H), 7.99–7.93 (m, 1H), 7.83 (dd, J = 7.1, 1.3 Hz, 1H), 7.66–7.54 (m, 3H), 7.48 (t, J = 4.9 Hz, 1H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -79.90 (t, J = 10.0 Hz, 3F), -116.46 (q, J = 10.0 Hz, 2F), -125.68 (s, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 169.9, 163.5, 162.2, 158.2, 156.3 (t, J_{C-F} = 27.9 Hz), 134.6, 133.9, 131.4, 130.4, 129.0, 128.8, 127.7, 126.5, 125.3, 124.3, 121.6, 119.7

(t, J_{C-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 $C_{21}H_{12}F_7N_4$ $[M+H]^+$ 453.0945, found: 53.0951.

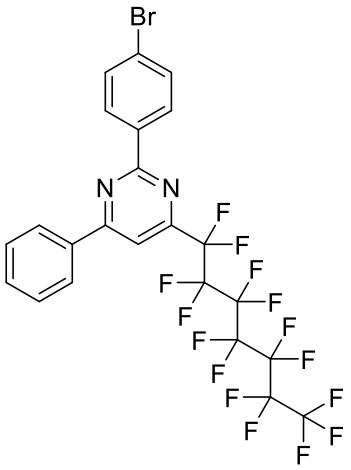


2-(4-Bromophenyl)-4-(perfluoroethyl)-6-phenylpyrimidine (6a): Yield = 62%. White solid. M.p. 70.1–71.7 °C. IR (KBr) ν = 3426, 2934, 1586, 1384, 1208, 1004, 769, 686 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 8.51–8.48 (m, 2H), 8.29–8.22 (m, 2H), 7.93 (s, 1H), 7.68–7.65 (m, 2H), 7.63–7.55 (m, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -82.50 – -82.58 (m, 3F), -118.82 – -118.90 (m, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 164.2, 156.8 (t, J_{C-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-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 $C_{18}H_{11}BrF_5N_2$ $[M+H]^+$ 429.0020, found: 429.0033.



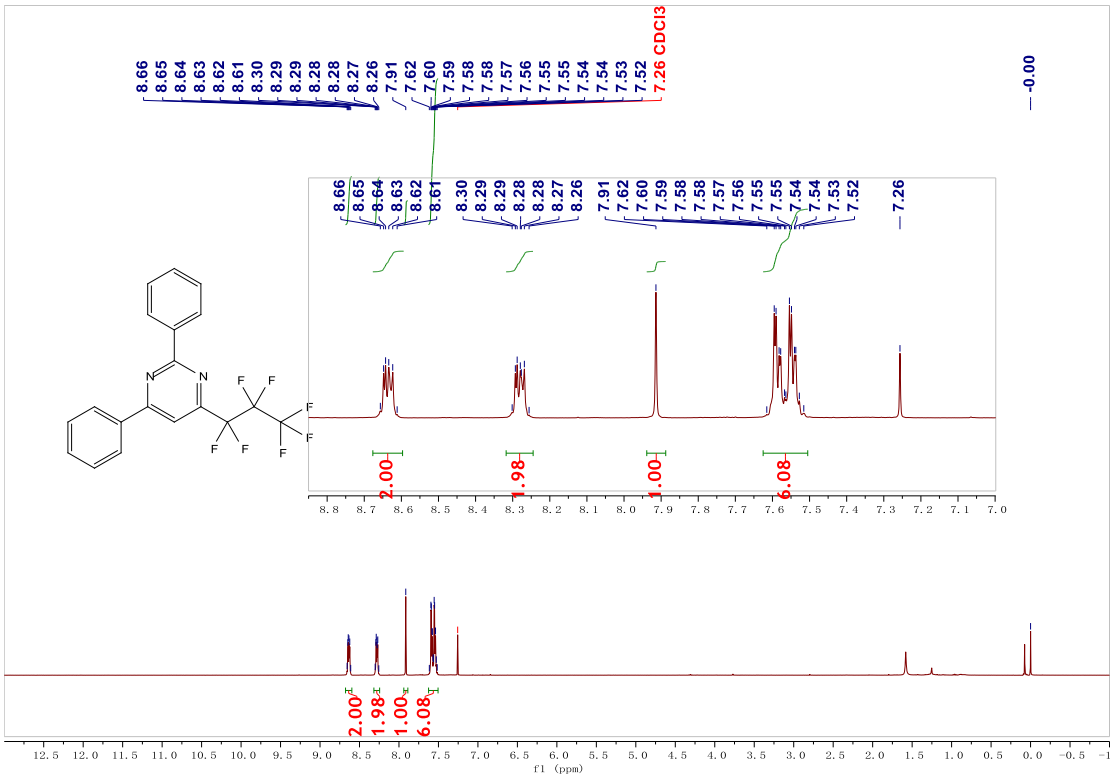
2-(4-Bromophenyl)-4-(perfluoropentyl)-6-phenylpyrimidine (6b): Yield = 59%. White solid. M.p. 88.5–90.0 °C. IR (KBr) ν = 3412, 2915, 1587, 1386, 1198, 1137, 734 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ = 8.51–8.46 (m, 2H), 8.28–8.22 (m, 2H), 7.92 (s, 1H), 7.68–7.63 (m, 2H), 7.62–7.54 (m, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -80.84 (t, J = 9.9 Hz, 3F), -115.73 (t, J = 13.5 Hz, 2F), -121.69 – -121.90 (m, 2F), -122.10 – -122.30 (m, 2F), -126.11 – -126.33 (m, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.4, 164.2, 157.0, 135.7 (t, J_{C-F} = 27.1 Hz), 135.4, 132.0,

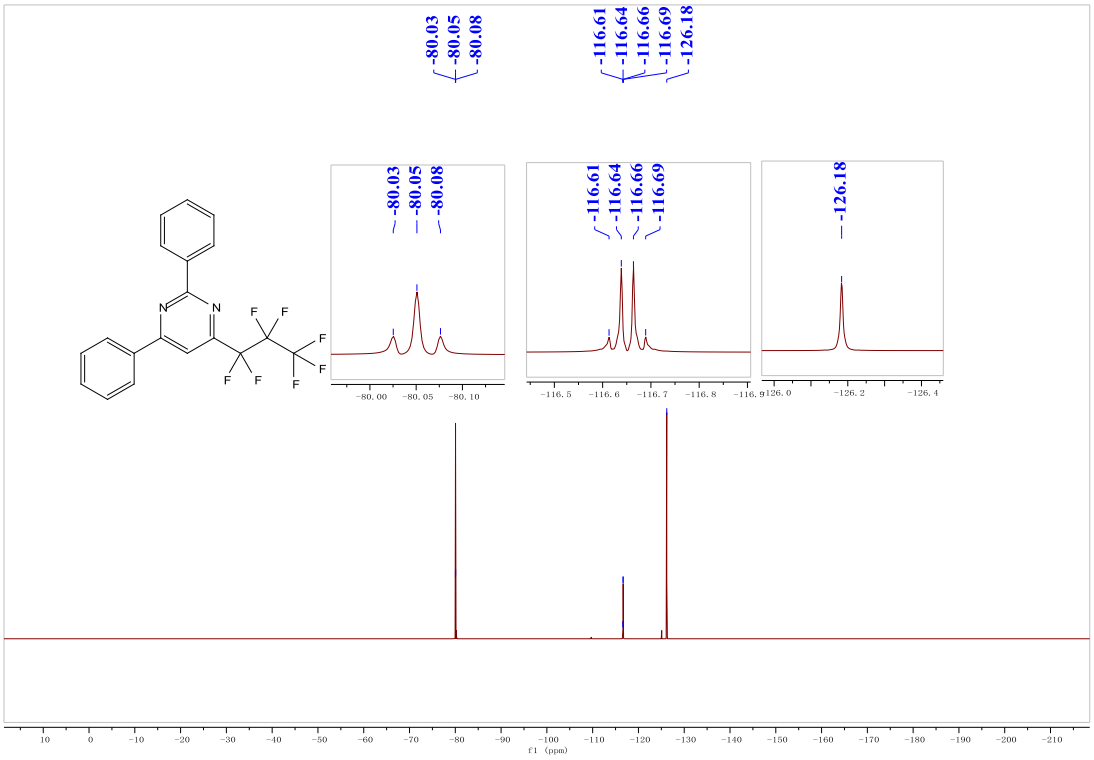
131.9, 130.2, 129.2, 127.5, 126.5, 111.9 (t, J_{C-F} = 4.5 Hz) ppm, carbons corresponding to the C_3F_7 group cannot be identified due to C-F coupling. HRMS m/z: calcd for $C_{21}H_{11}BrF_{11}N_2$ $[M+H]^+$ 578.9924, found: 578.9925.

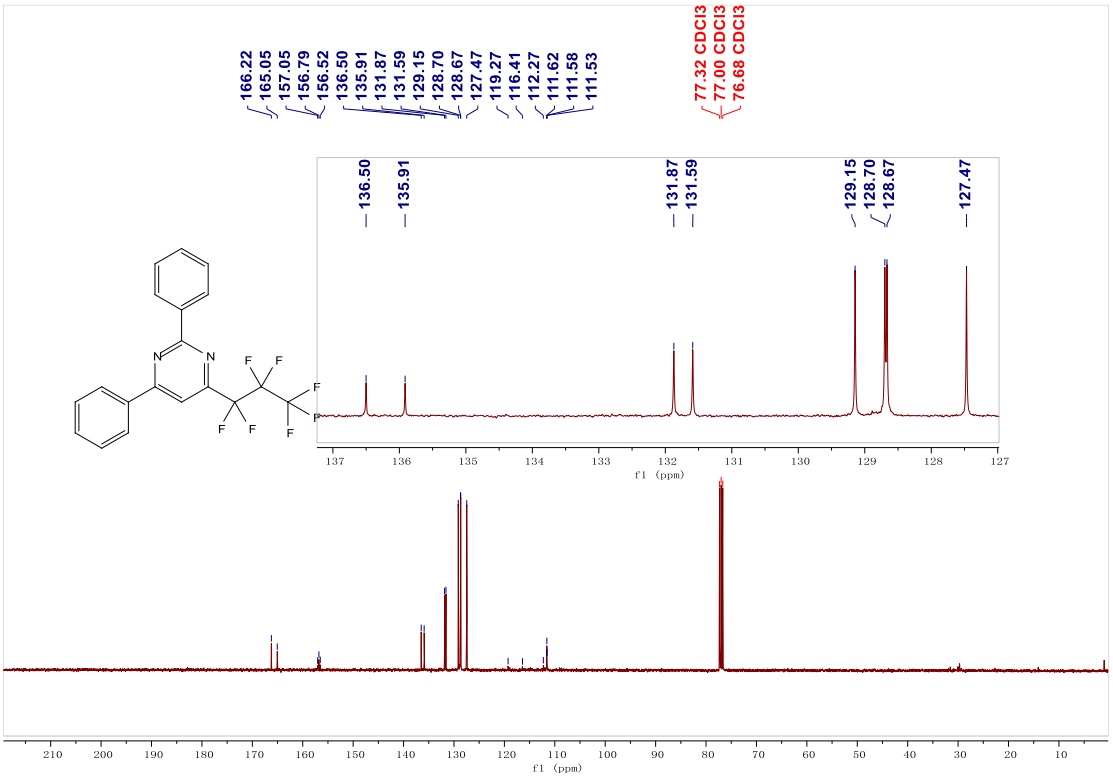


2-(4-Bromophenyl)-4-(perfluoroheptyl)-6-phenylpyrimidine (6c): Yield = 67%. White solid. M.p. 74.4–76.0 °C. IR (KBr) ν = 3420, 2928, 1586, 1384, 1218, 1141, 771 cm^{-1}. ^1H NMR (400 MHz, DMSO-d_6): δ = 8.56 (s, 1H), 8.54–8.49 (m, 2H), 8.49–8.42 (m, 2H), 7.86–7.81 (m, 2H), 7.71–7.61 (m, 3H) ppm. ^{19}F NMR (376 MHz, $CDCl_3$): δ =-80.89 (t, J = 9.8 Hz, 3F), -115.69 (t, J = 13.8 Hz, 2F), -121.07 – -121.40 (m, 2F), -121.47 – -121.68 (m, 2F), -121.86 – -122.15 (m, 2F), -122.68 – -122.96 (m, 2F), -126.14 – -126.36 (m, 2F) ppm. ^{13}C NMR (100 MHz, $CDCl_3$): δ = 166.3, 164.2, 157.0 (t, J_{C-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-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 $C_{23}H_{11}BrF_{15}N_2$ $[M+H]^+$ 678.9861, found: 678.9861.

6. The ^{1}H , ^{19}F, ^{13}C spectra of products 4-6:



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112.27
111.62
111.58
111.53
77.32 CDCl3
77.00 CDCl3
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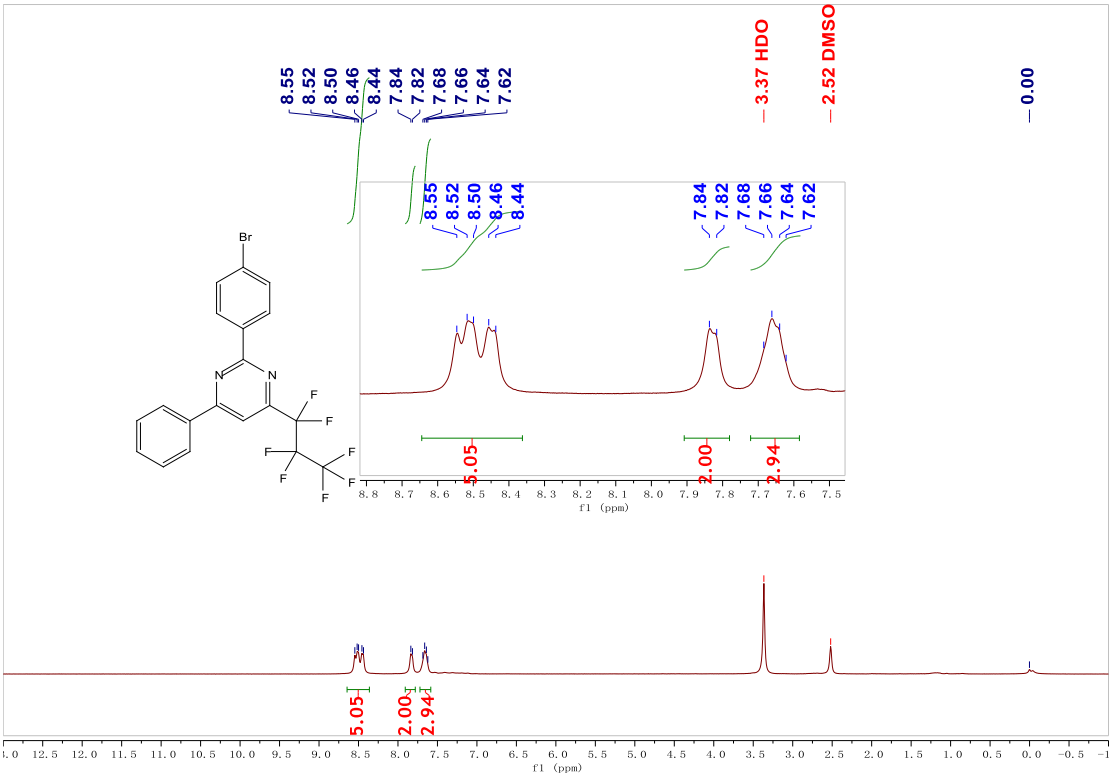
128.67
127.47
f1 (ppm)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7.62
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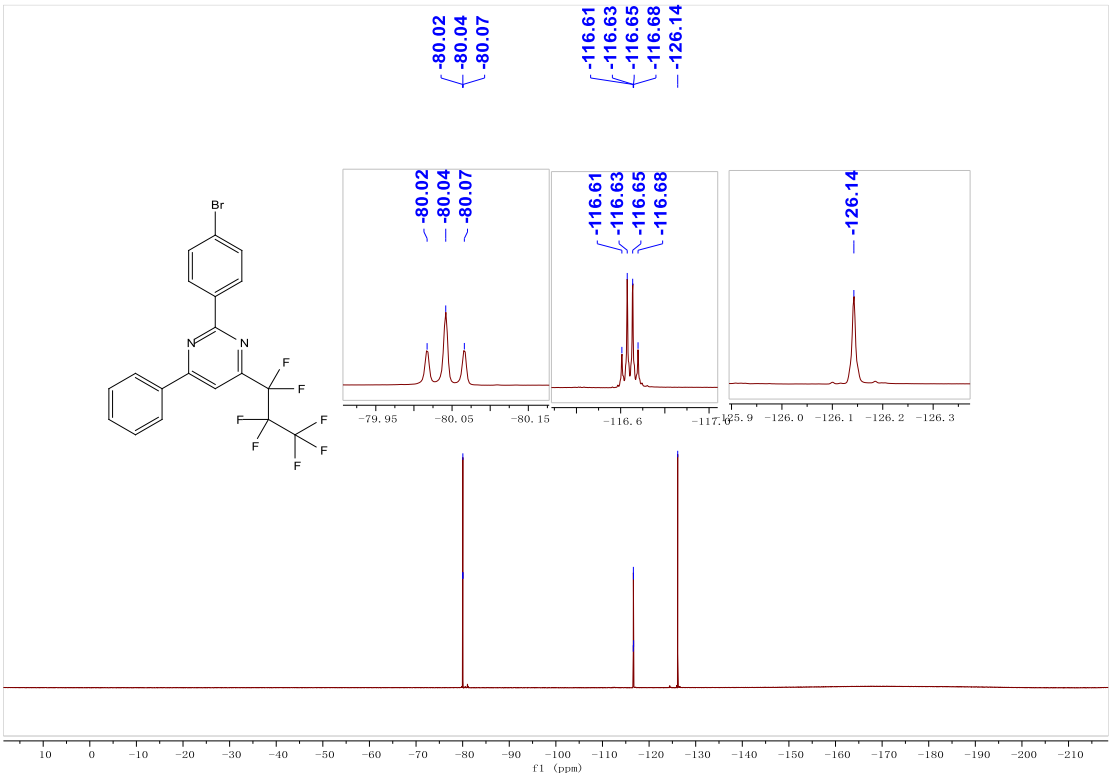
2.00
2.94
f1 (ppm)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F
F
F
F
F
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-80.15
-116.6
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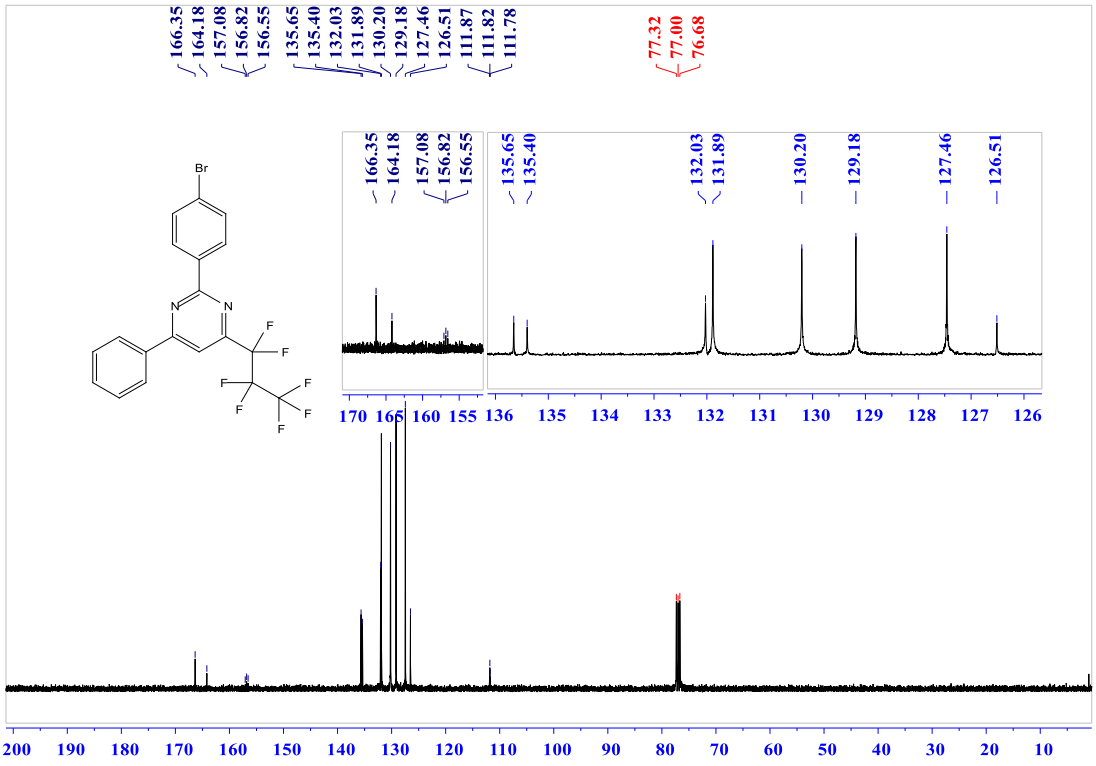
-126.1
-126.2
-126.3
f1 (ppm)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F
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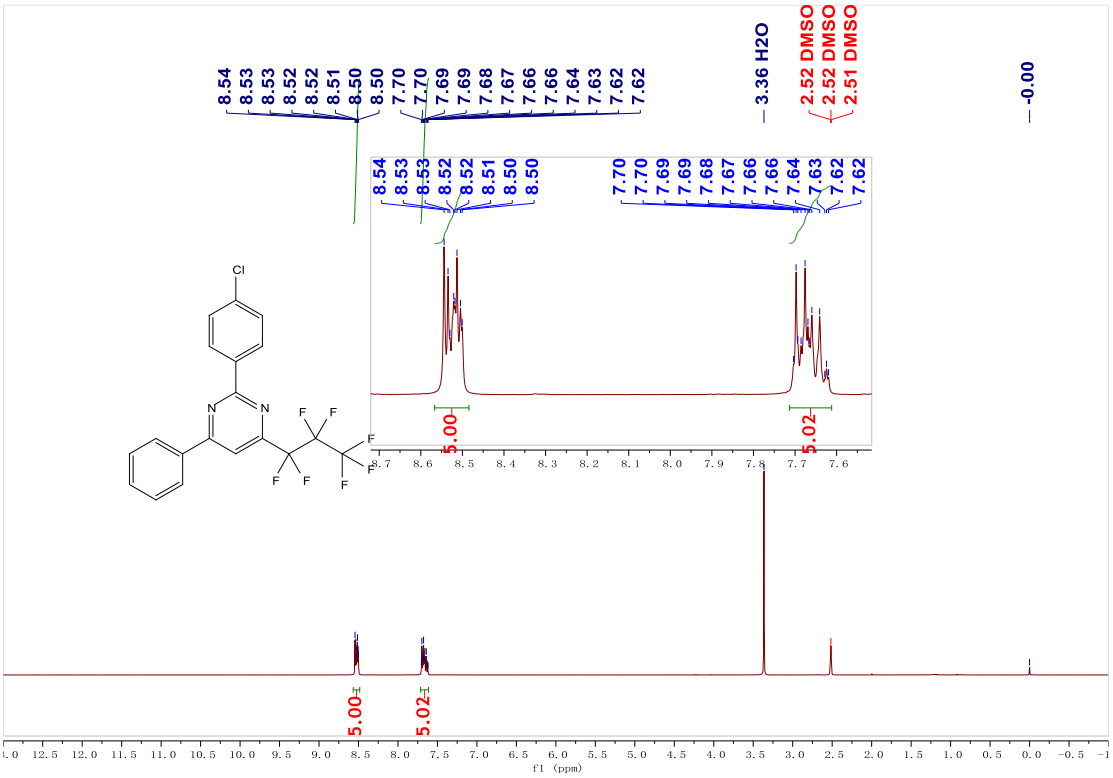
40
30
20
10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7.66
7.64
7.63
7.62
7.62
3.36 H2O
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F
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F
F
F
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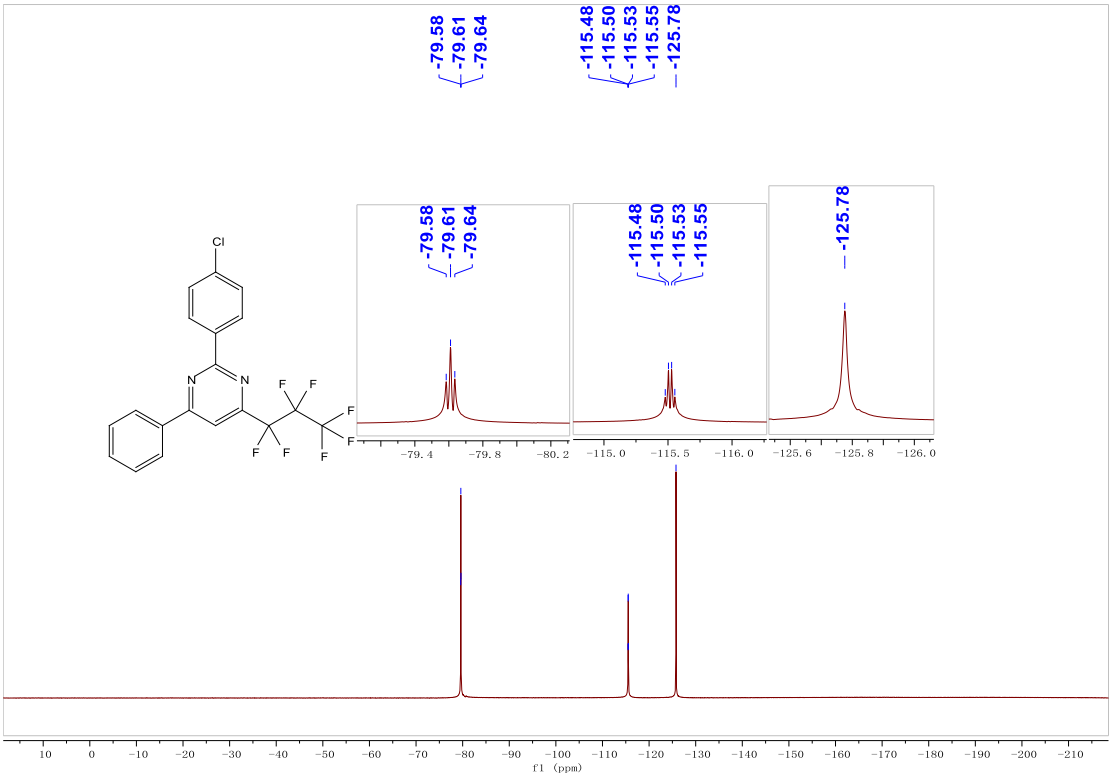
5.02
f1 (ppm)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-115.50
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-115.55
-125.78
Cl
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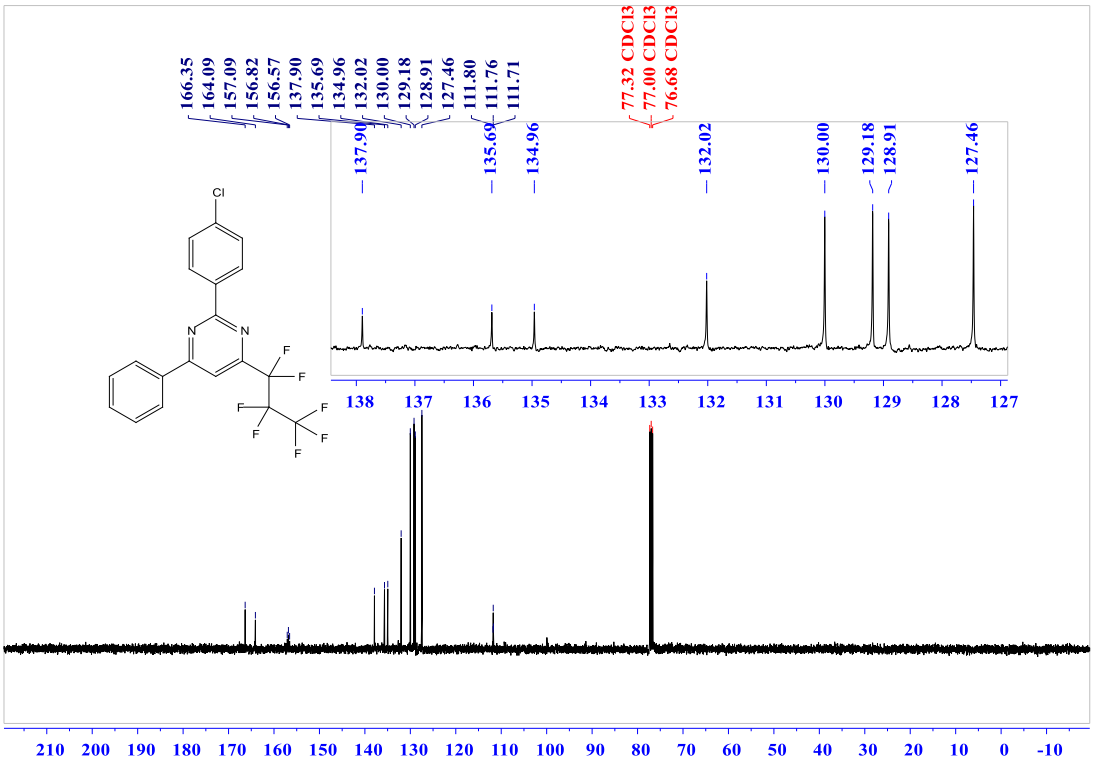
F
F
F
F
F
F
f1 (ppm)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77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
Cl
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F
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F
F
F
F
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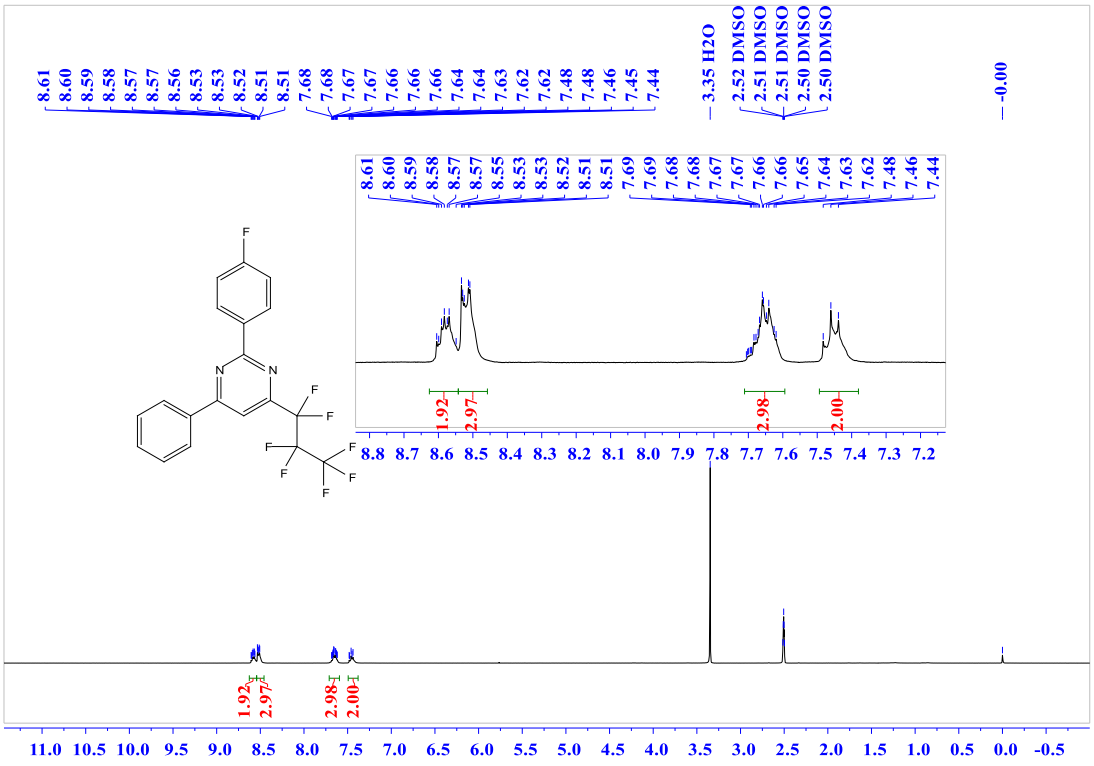
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2.51 DMSO
2.51 DMSO
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N
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F
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F
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2.98
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8.1
8.0
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7.4
7.3
7.2
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10.5
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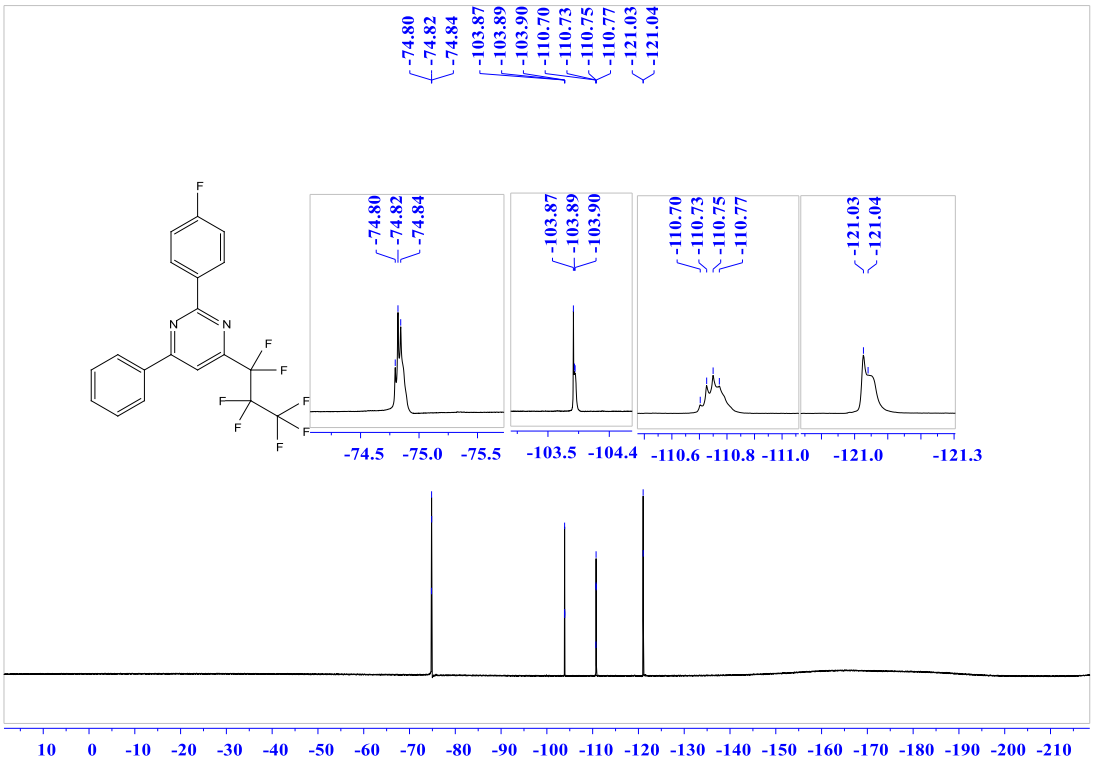
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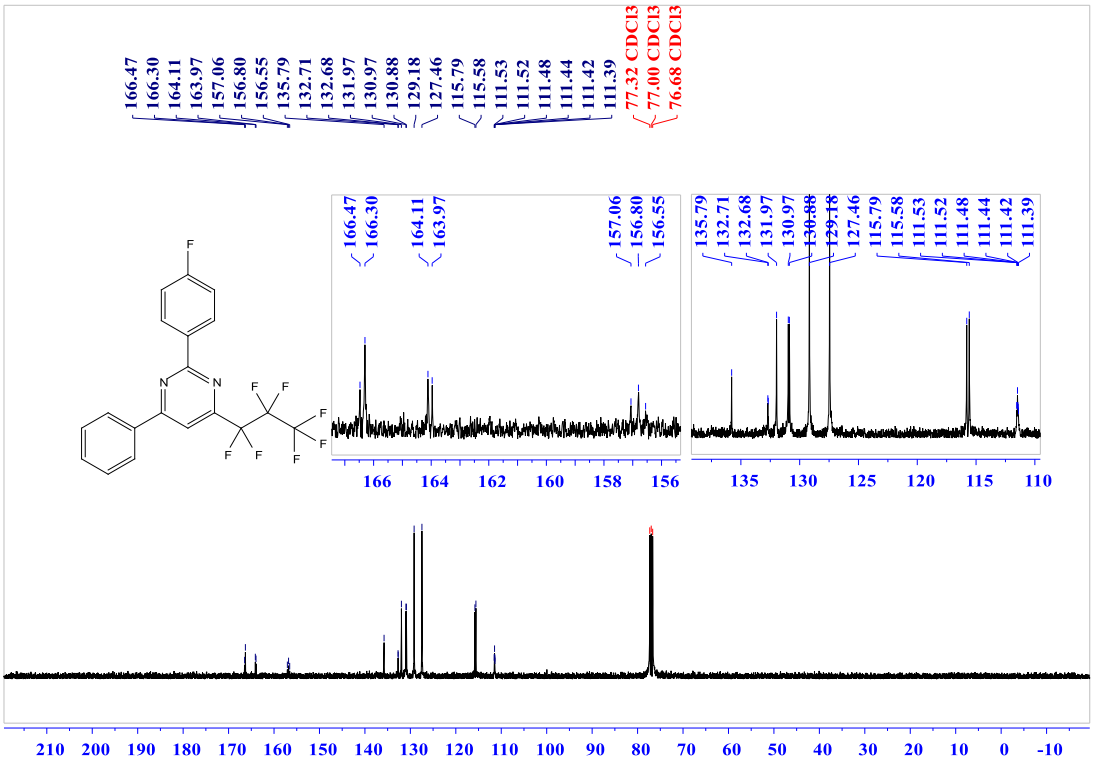
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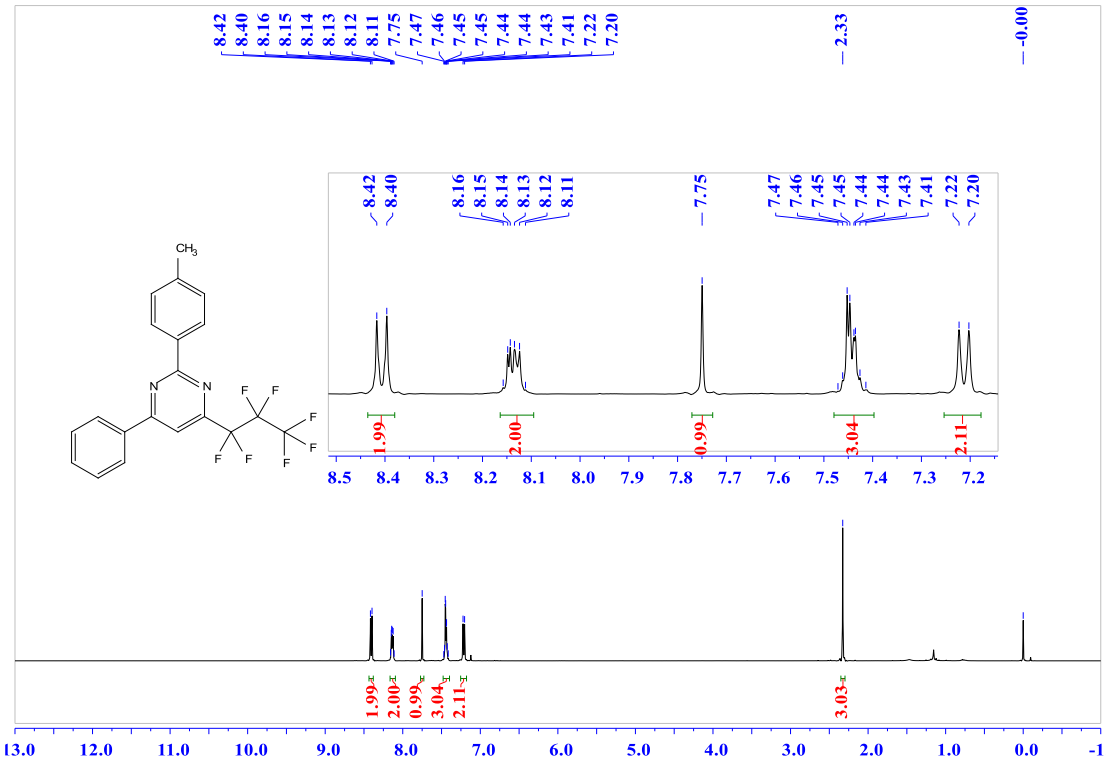
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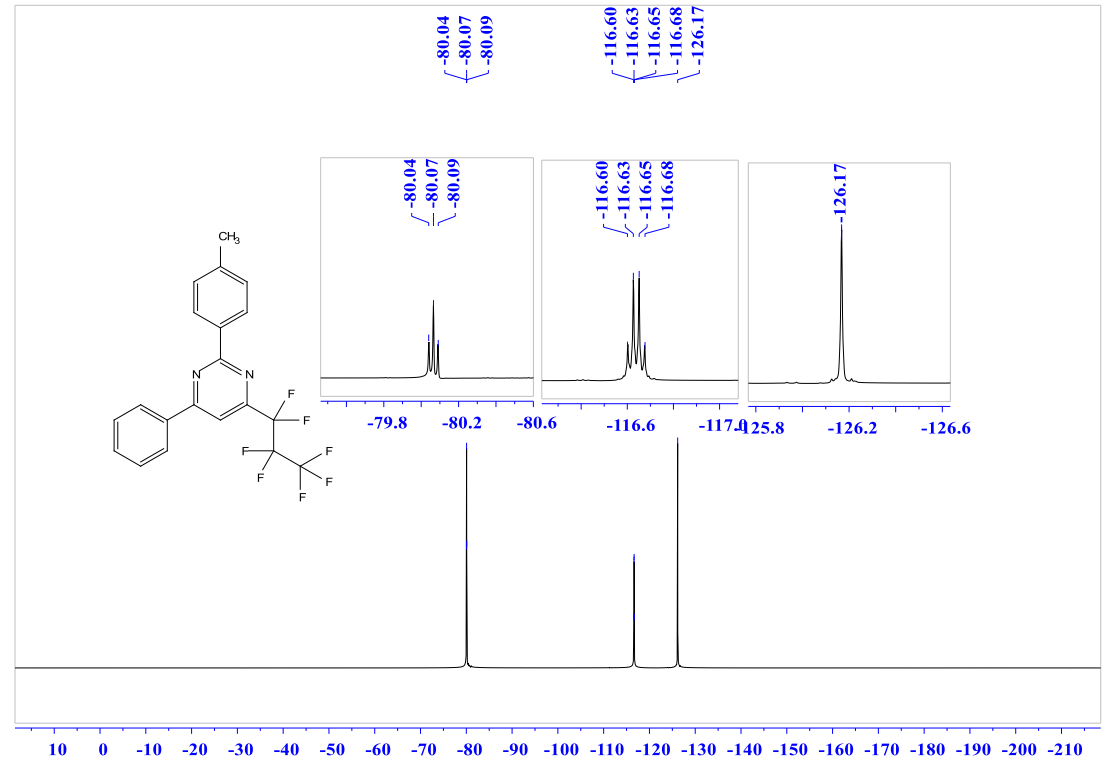
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-60
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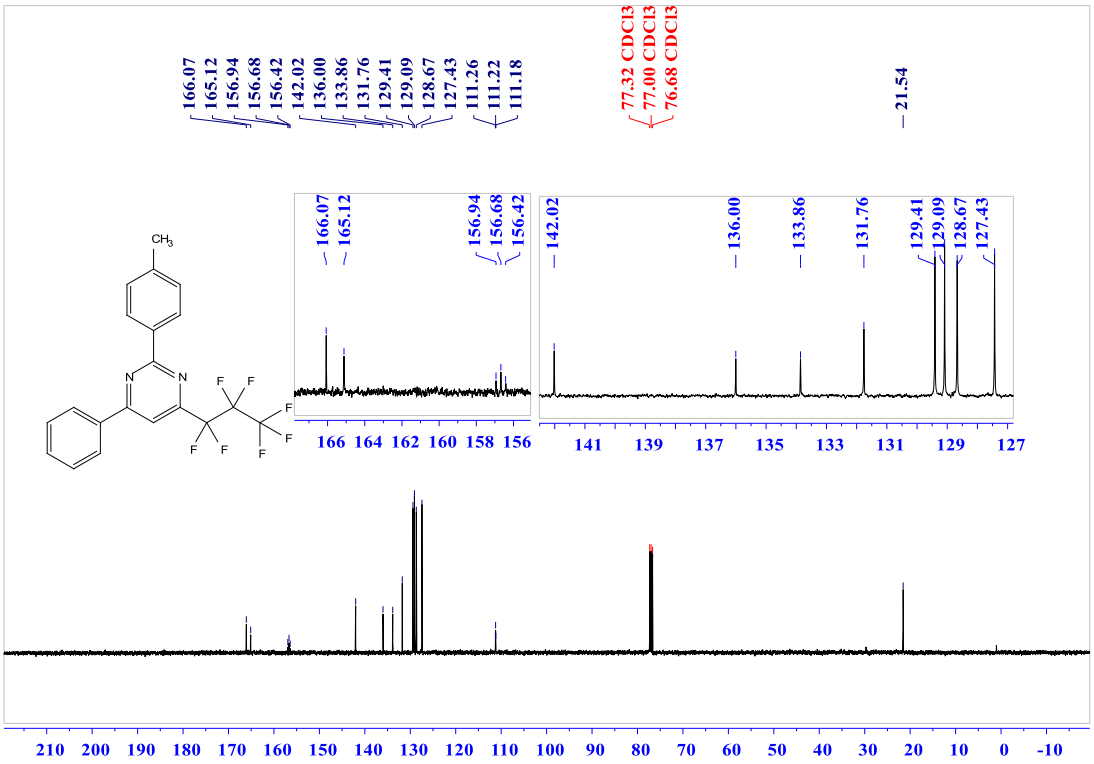

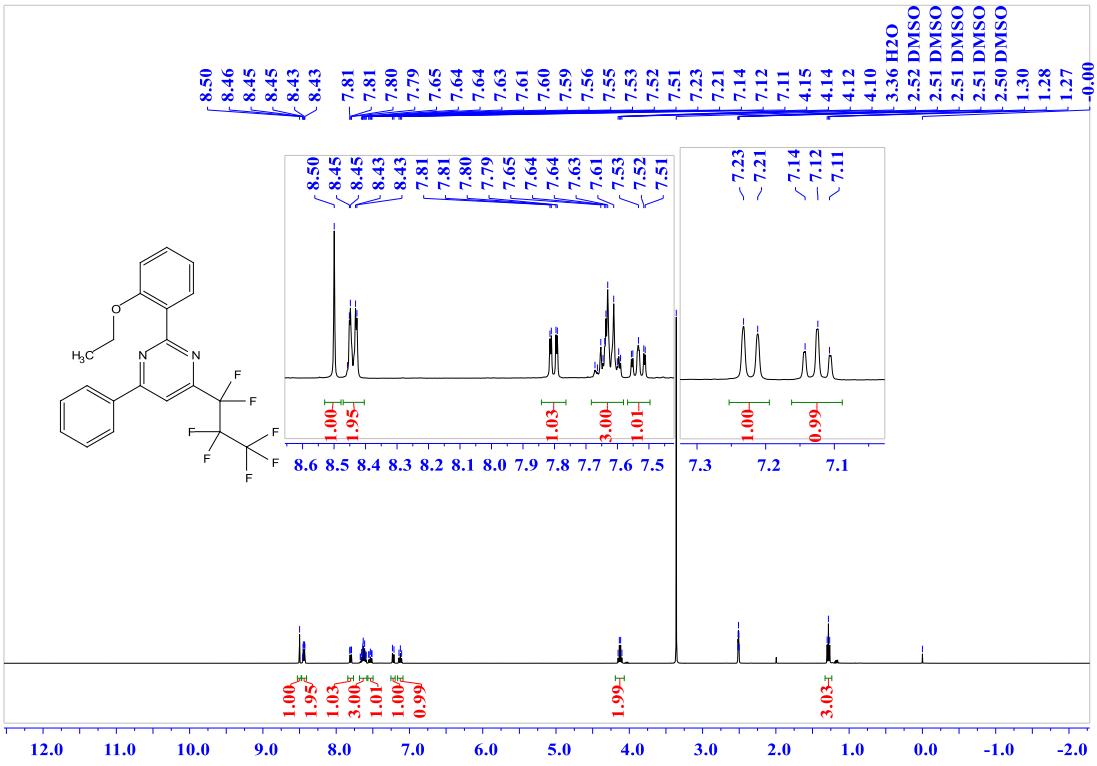

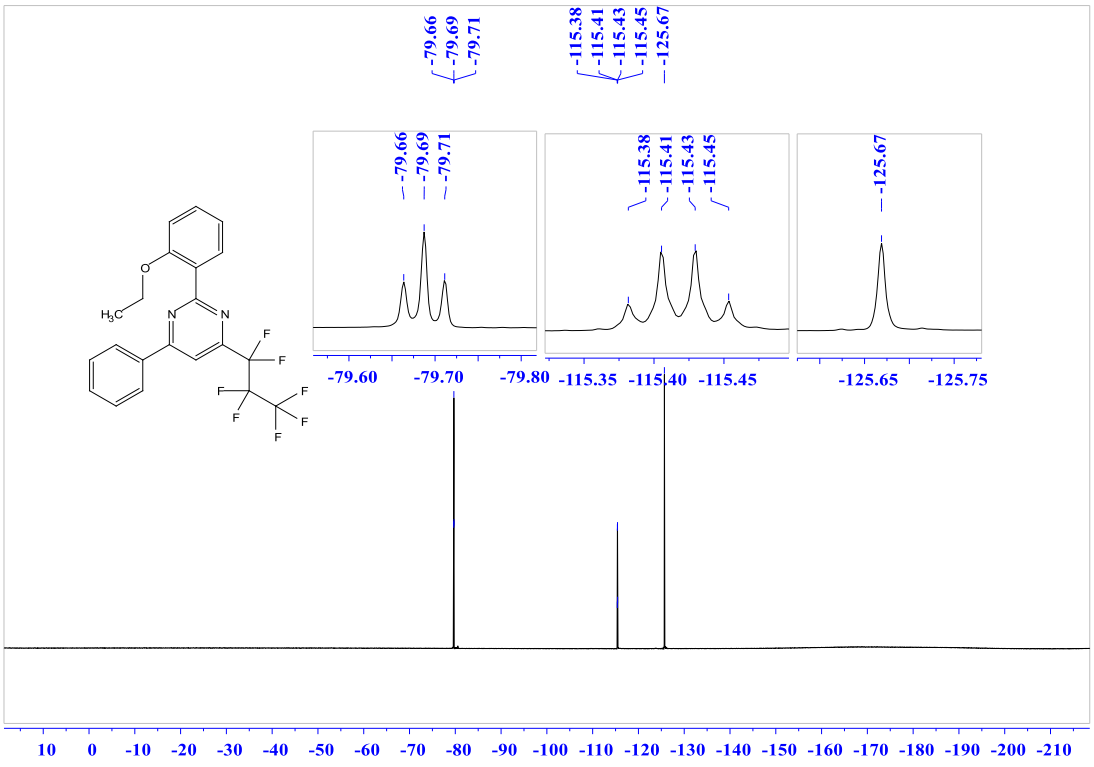
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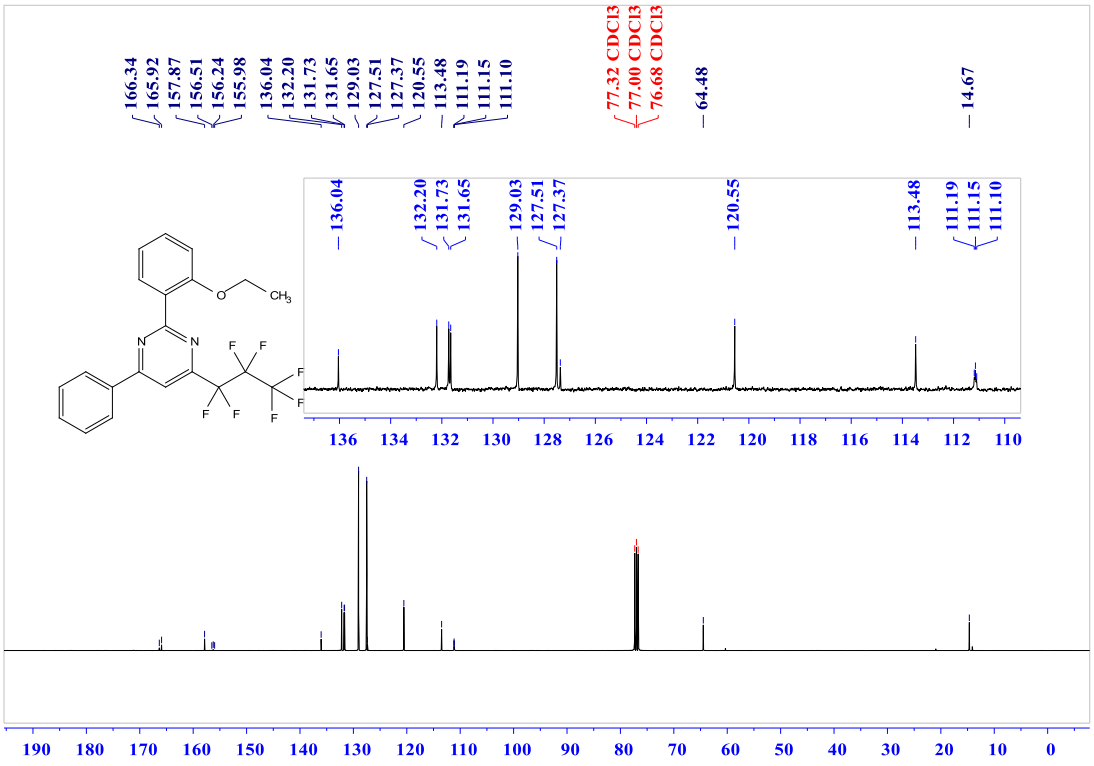
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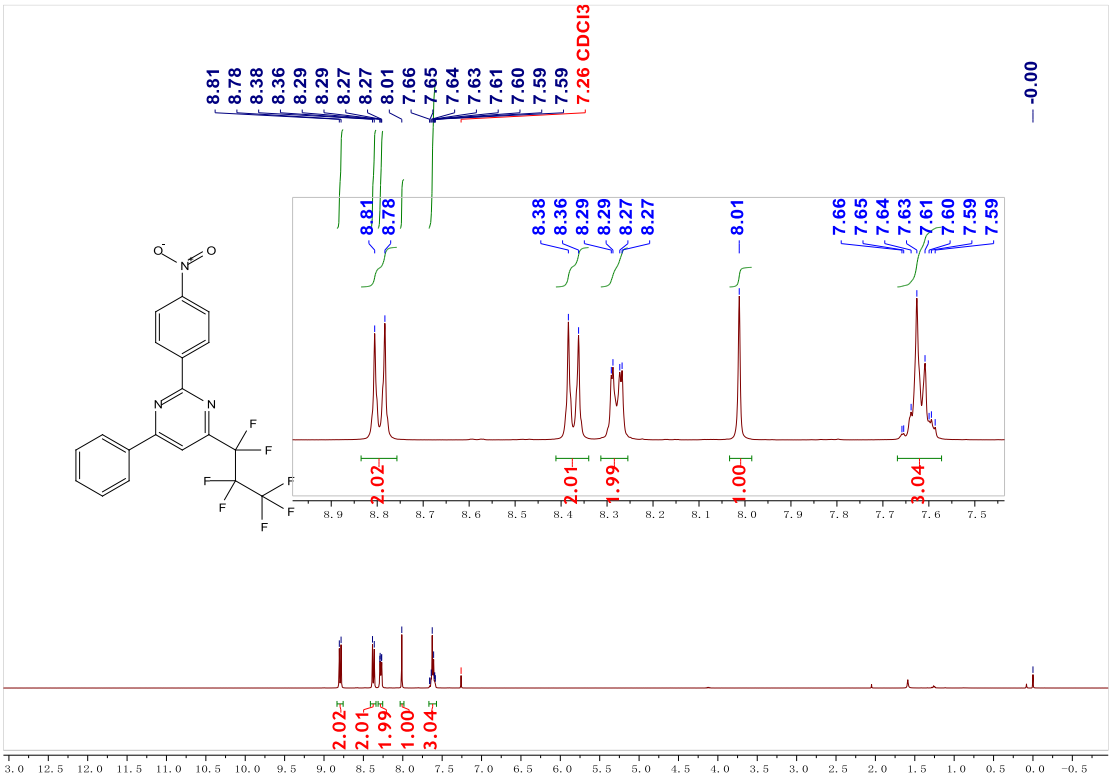
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7.63
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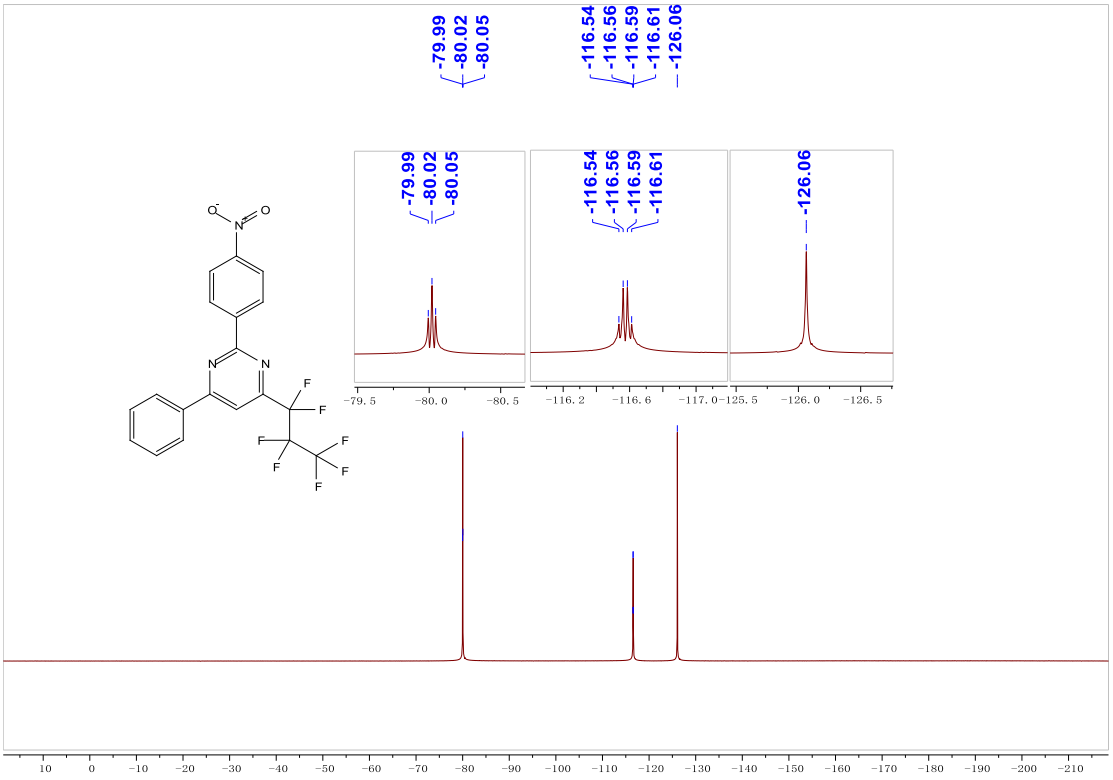
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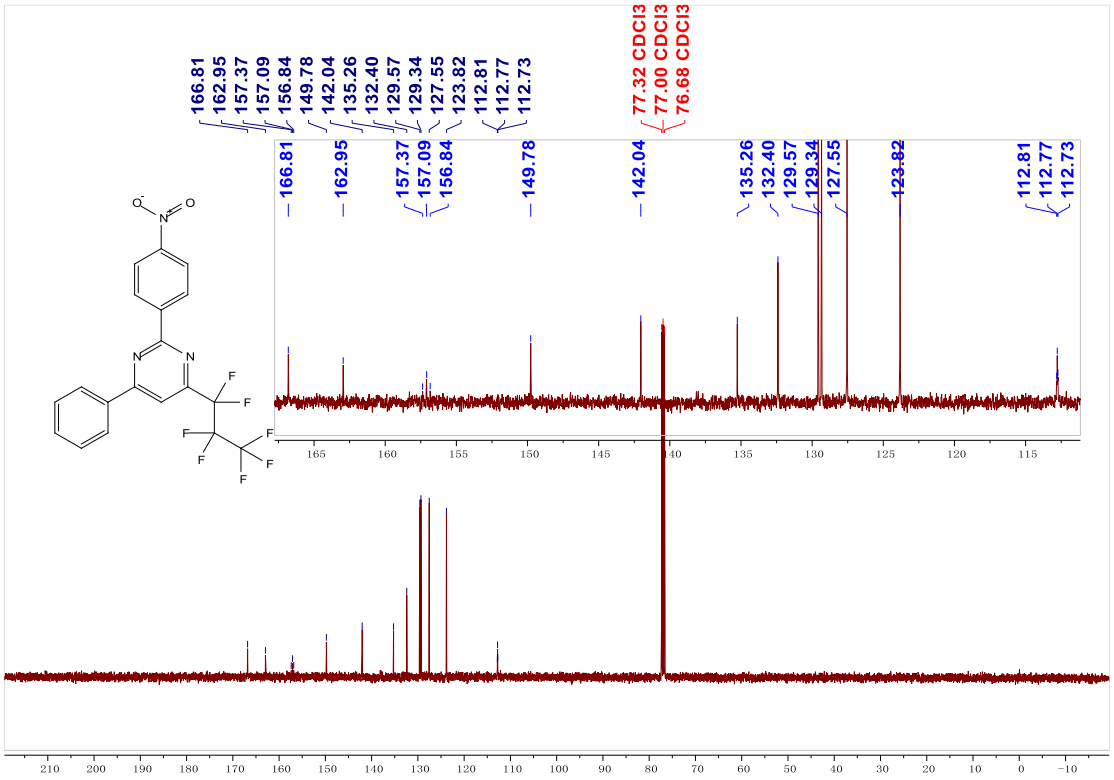
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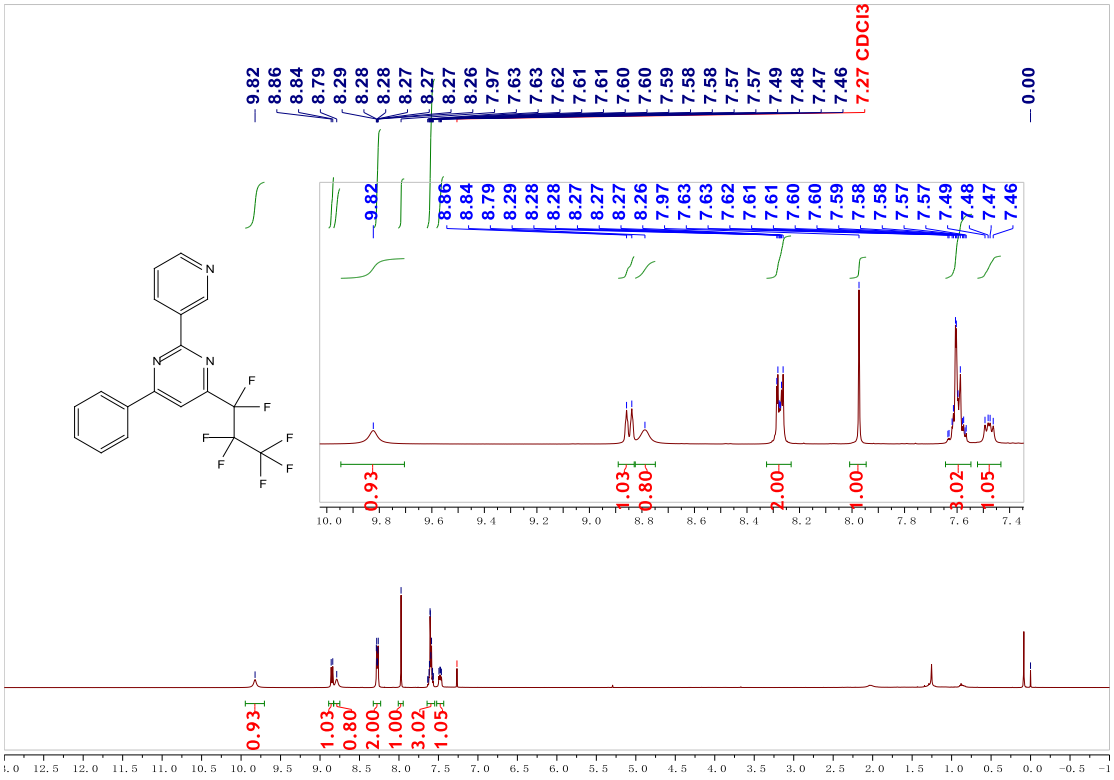
76.68 CDCl3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7.63
7.62
7.61
7.61
7.60
7.60
7.59
7.58
7.58
7.57
7.57
7.49
7.48
7.47
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7.27 CDCl3
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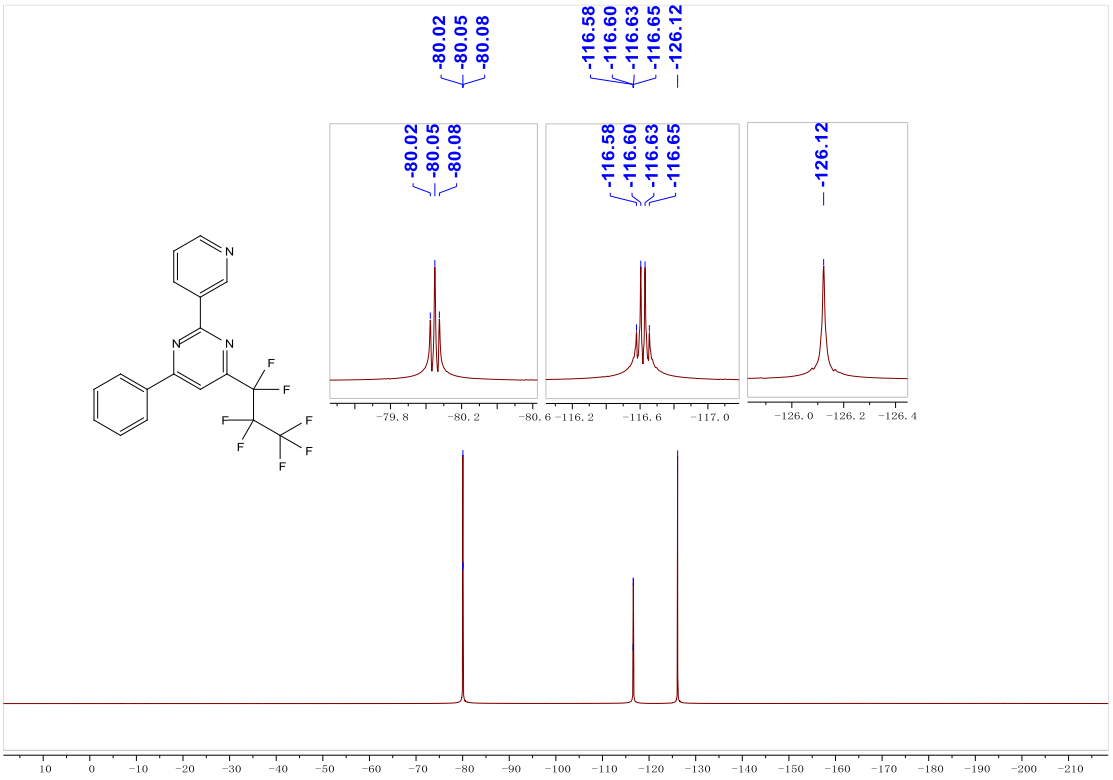
1.03
0.80
2.00
1.00
3.02
1.05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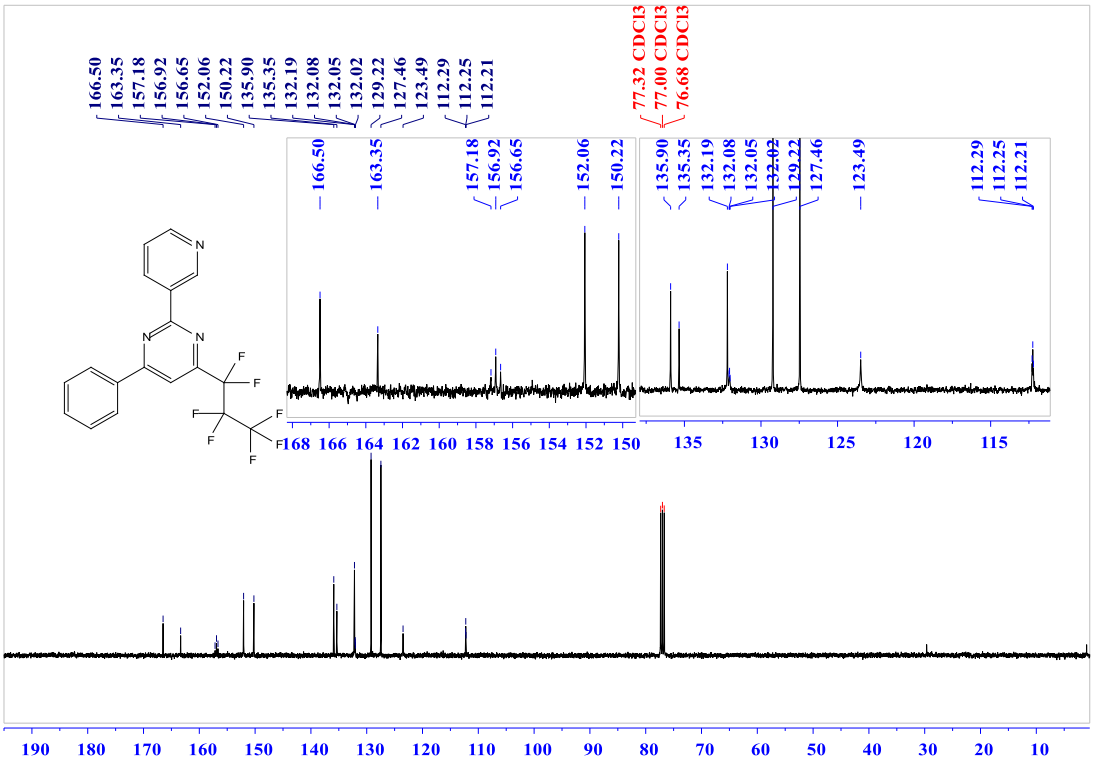
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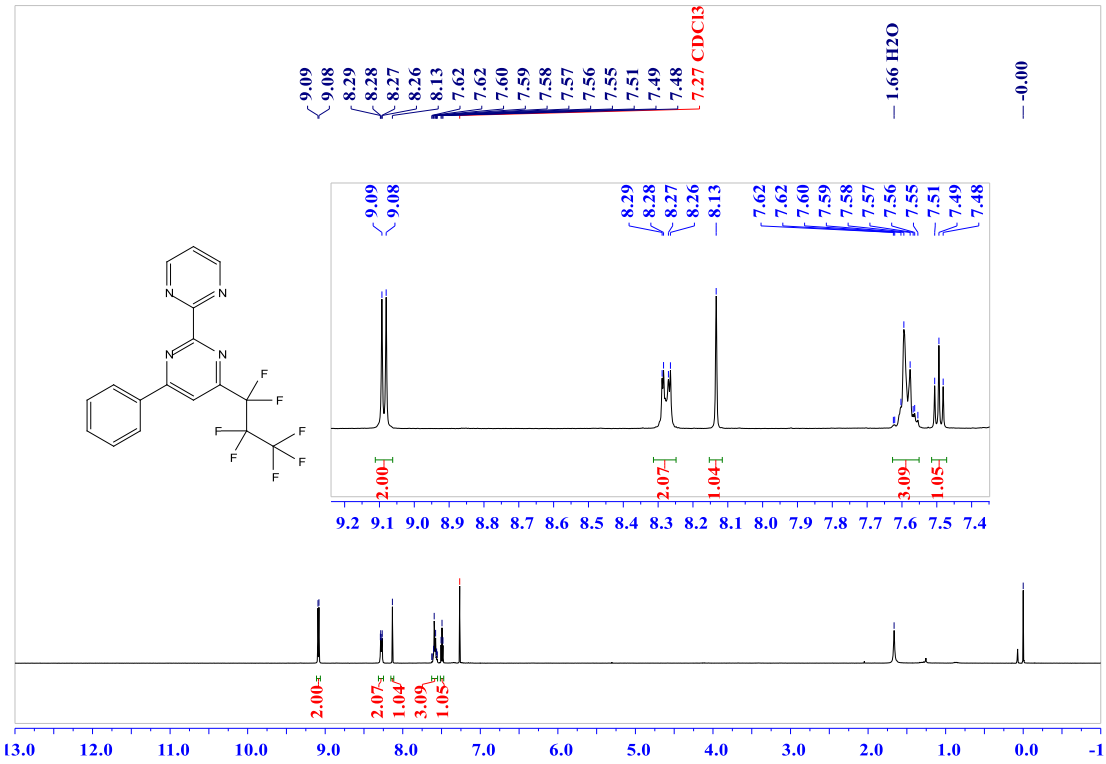
77.00 CDCl3
76.68 CDCl3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8.26
8.13
7.62
7.62
7.60
7.59
7.58
7.57
7.56
7.55
7.51
7.49
7.48
7.27 CDCl3
1.66 H2O
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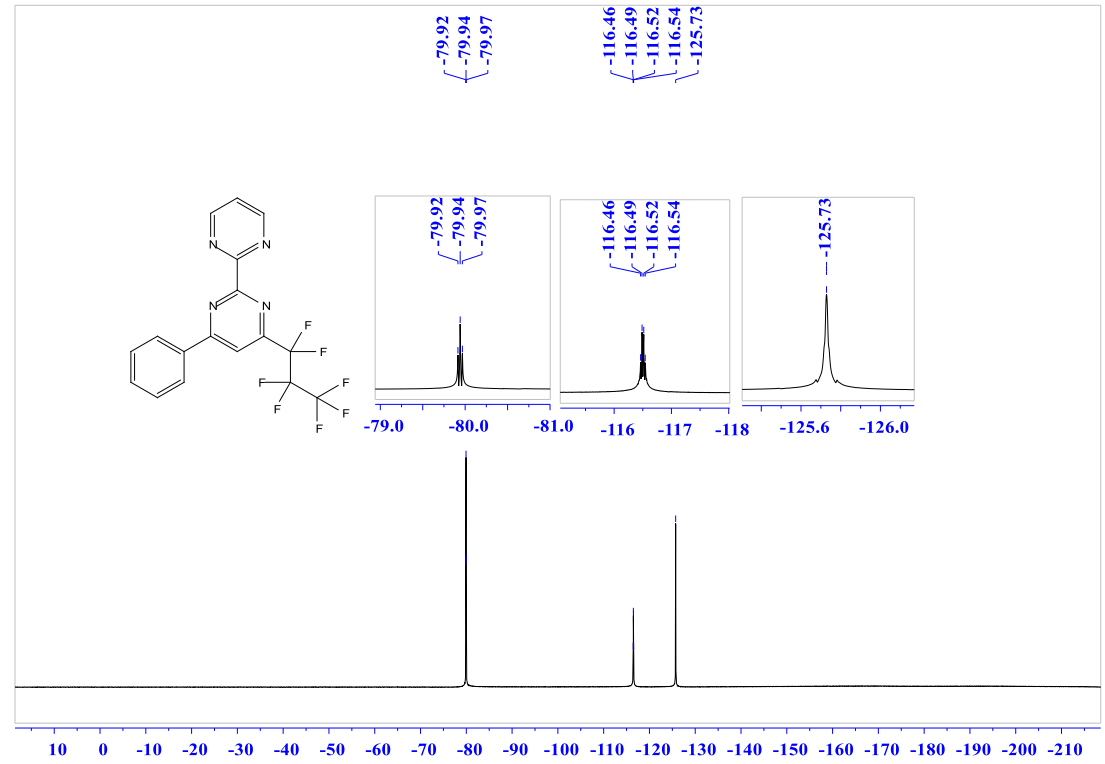
2.00
2.07
1.04
3.09
1.05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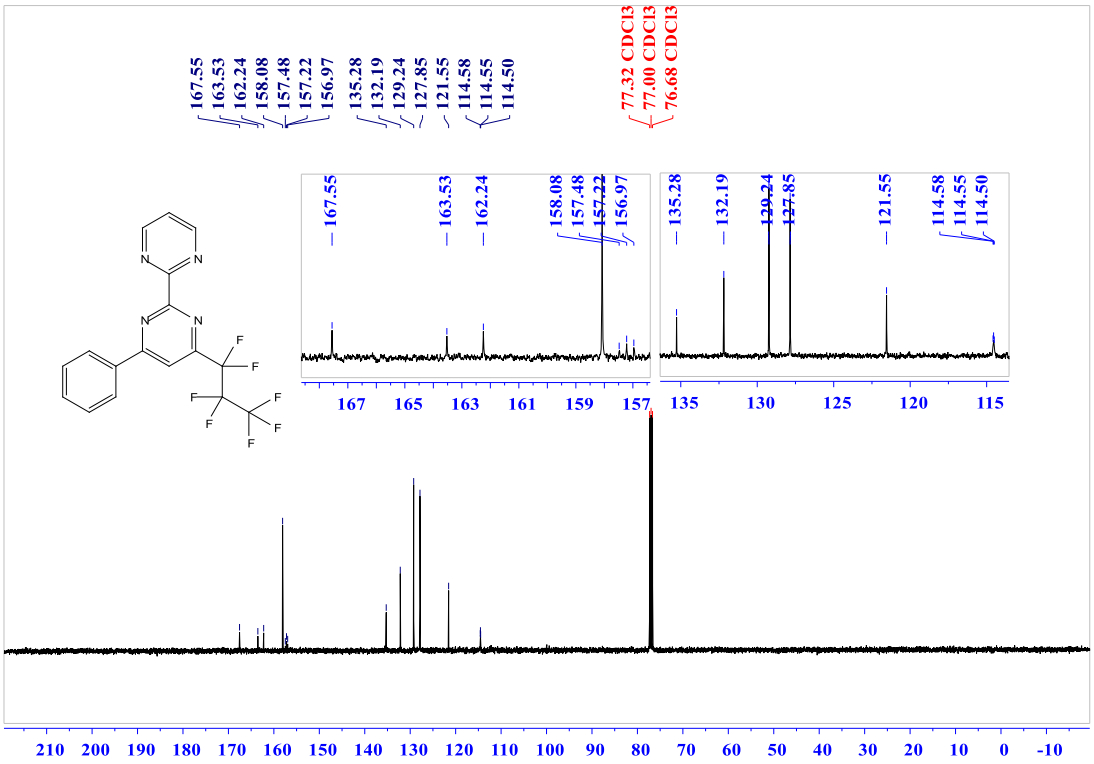
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135.28
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129.24
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121.55
114.58
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114.50
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
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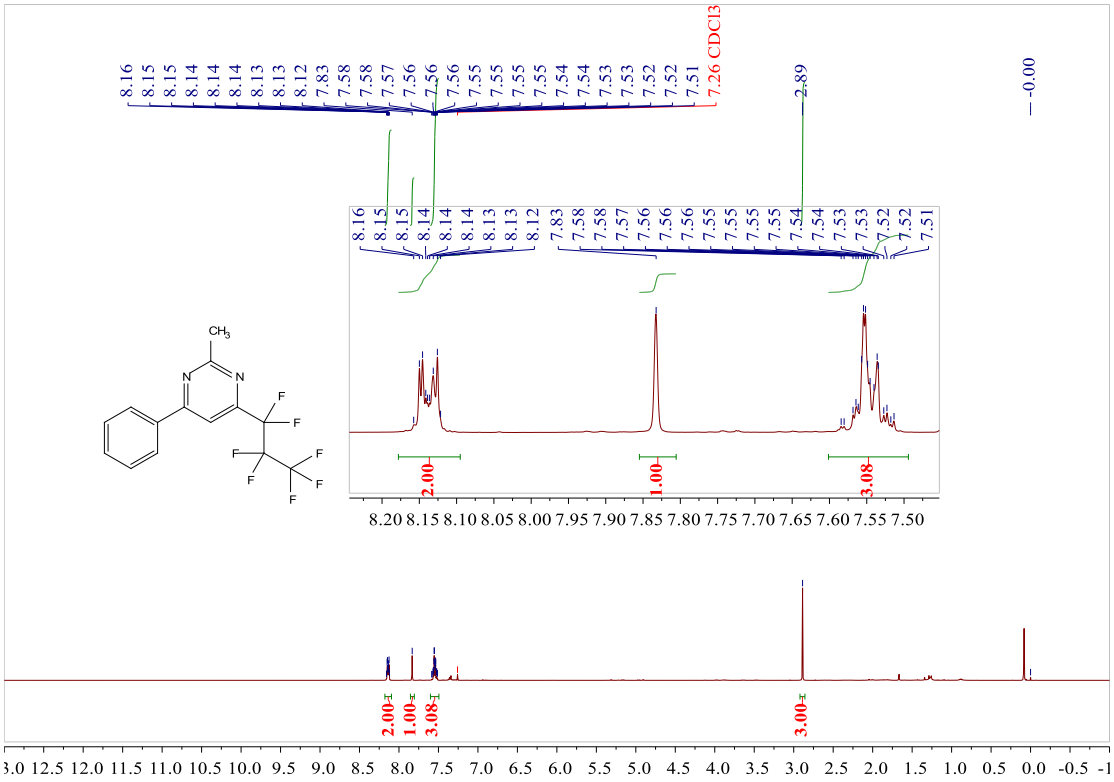
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2.00
1.00
3.08
3.00
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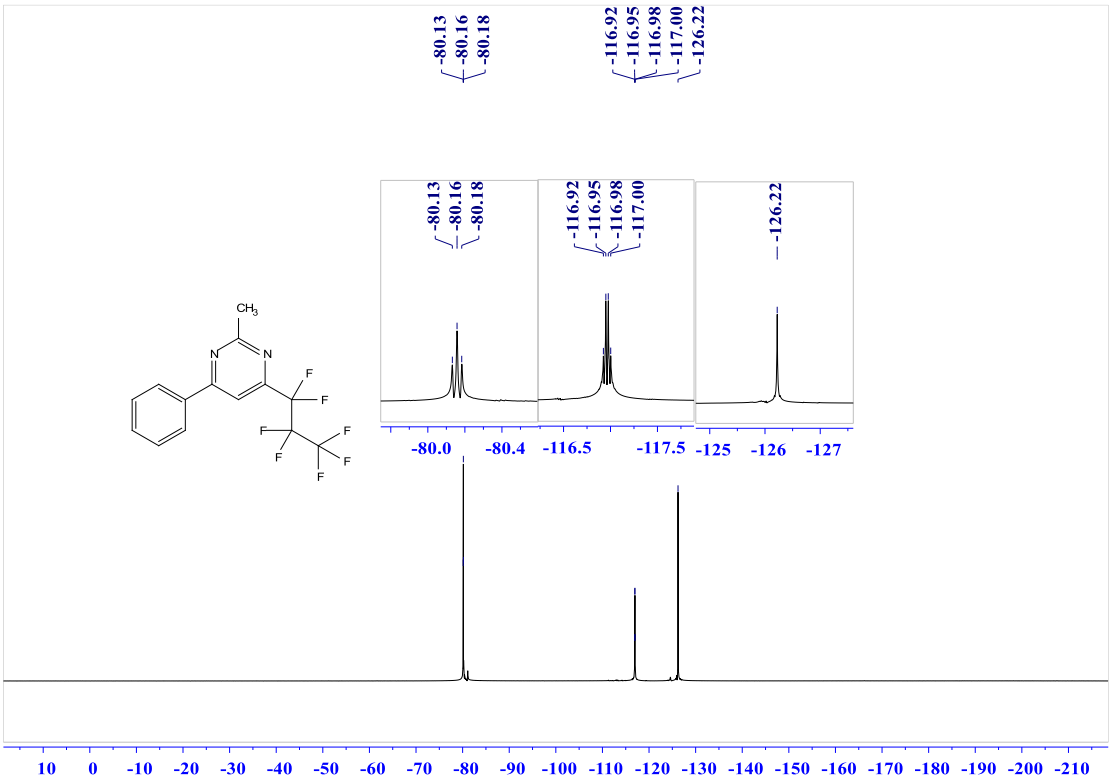
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-80.16
-80.18
-116.92
-116.95
-116.98
-117.00
-126.22
CH3
N
N
F
F
F
F
F
F
-80.0
-80.4
-116.5
-117.5
-125
-126
-127
10
0
-10
-20
-30
-40
-50
-60
-70
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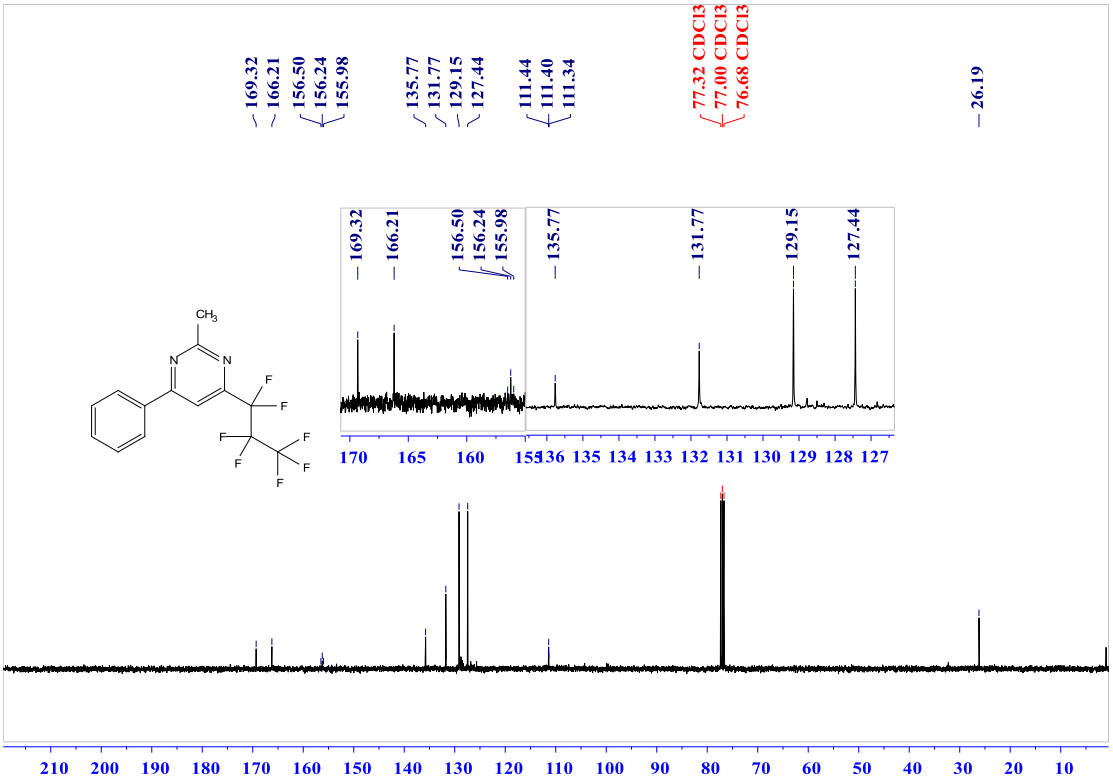
-150
-160
-170
-180
-190
-200
-210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156.24
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135.77
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111.44
111.40
111.34
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
26.19
CH3
N
N
F
F
F
F
F
F
170
165
160
155
136
135
134
133
132
131
130
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128
127
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20
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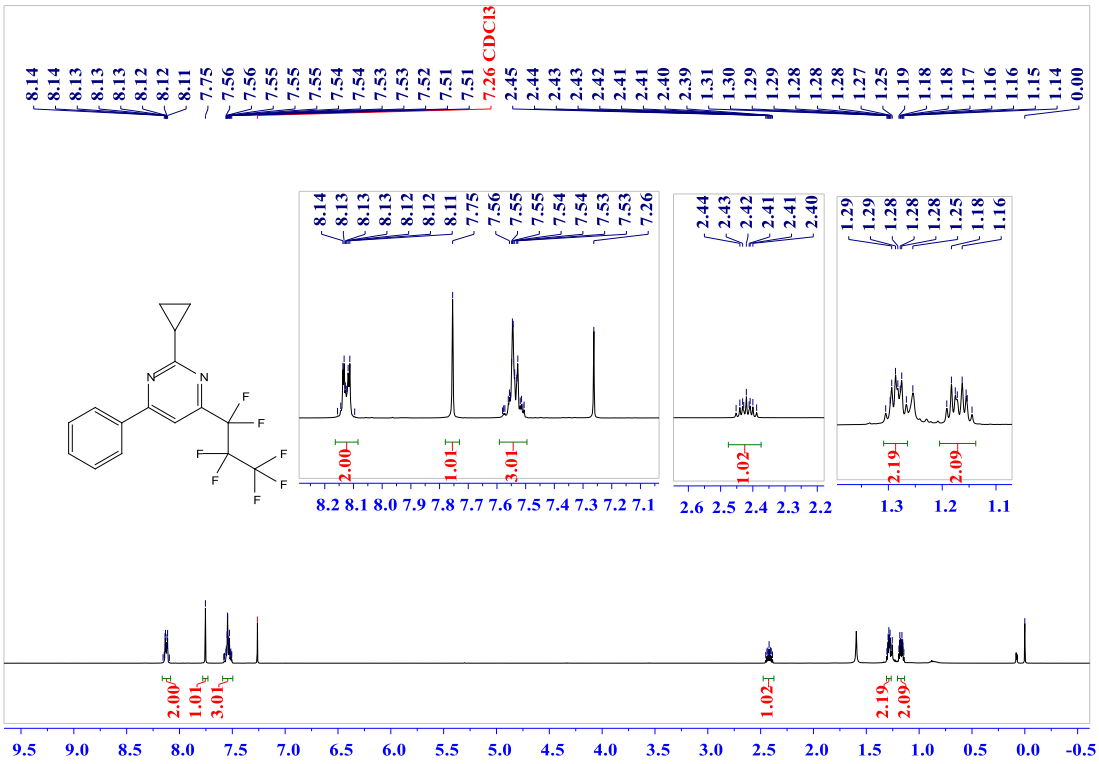

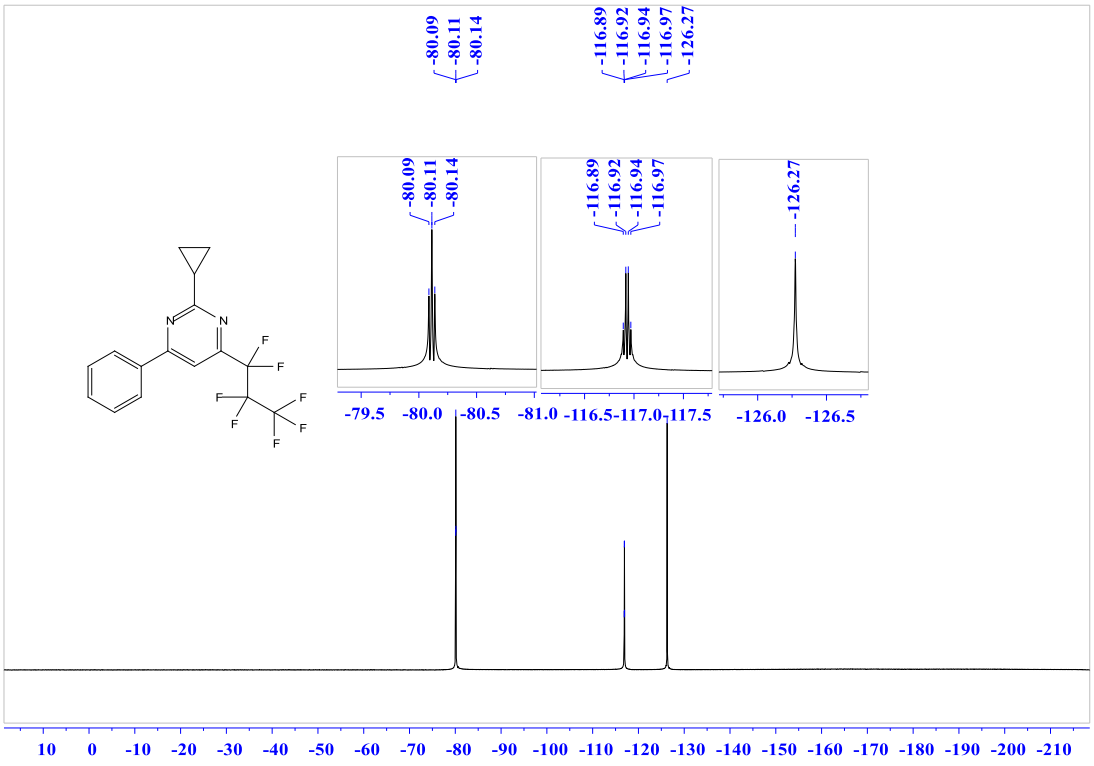

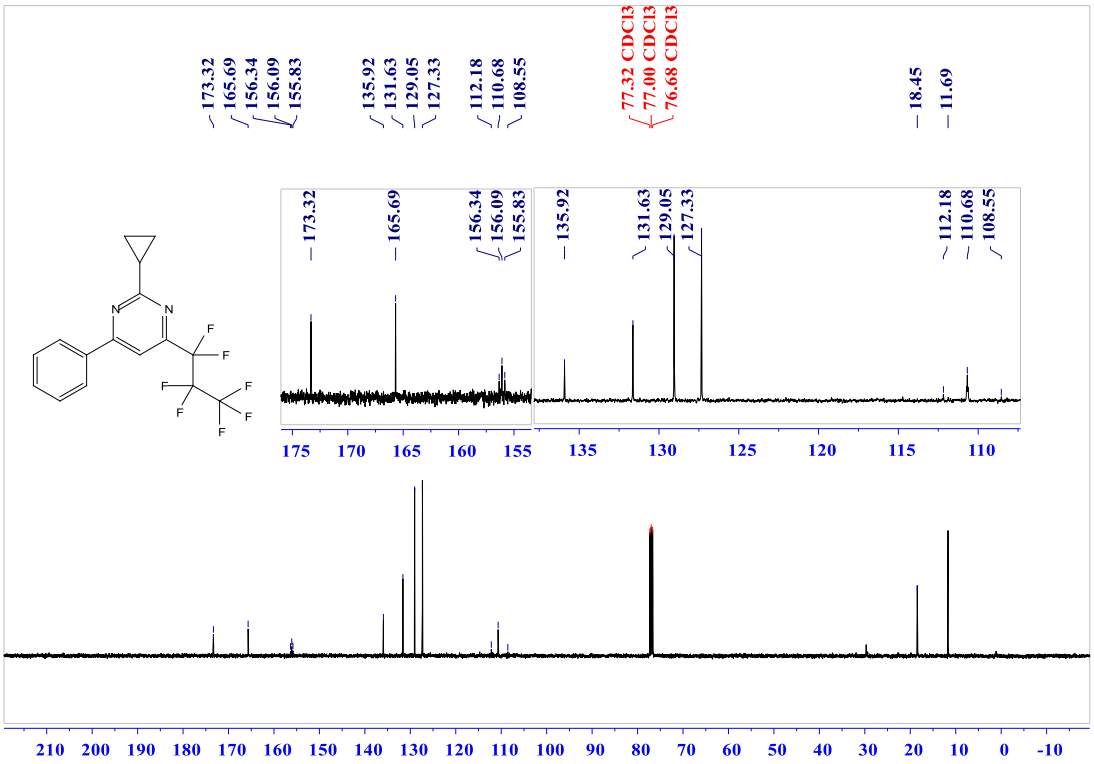
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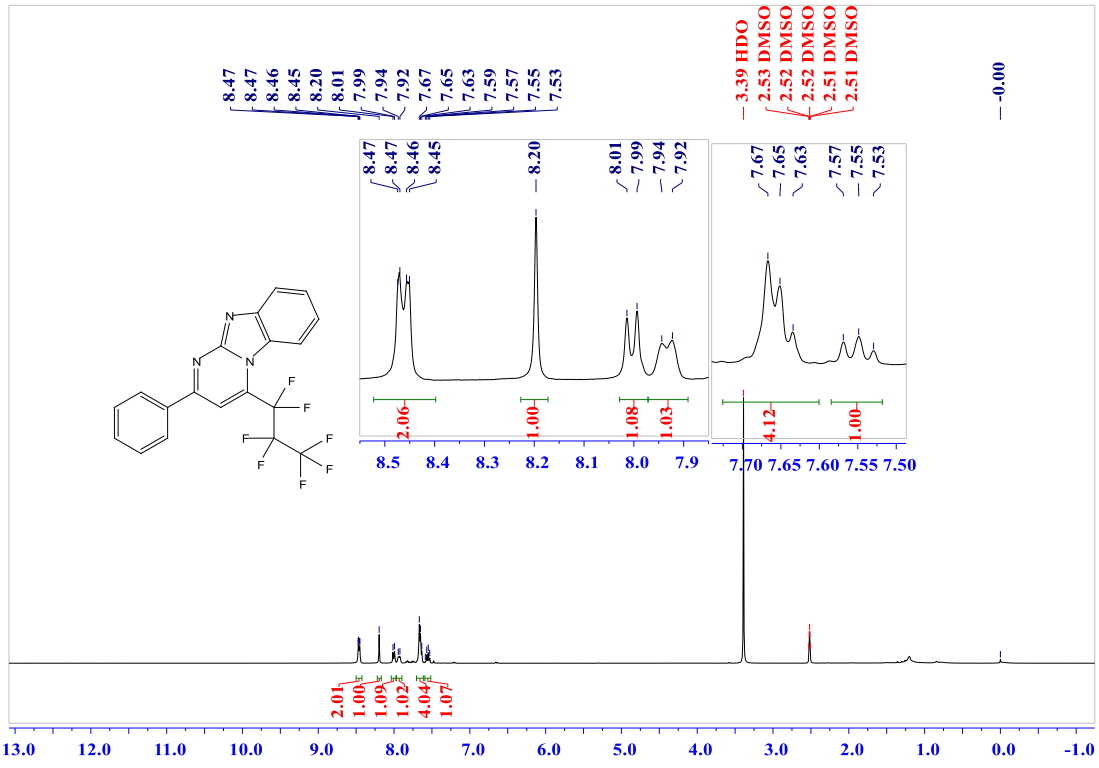
77.00 CDCl3
76.68 CDCl3
18.45
11.69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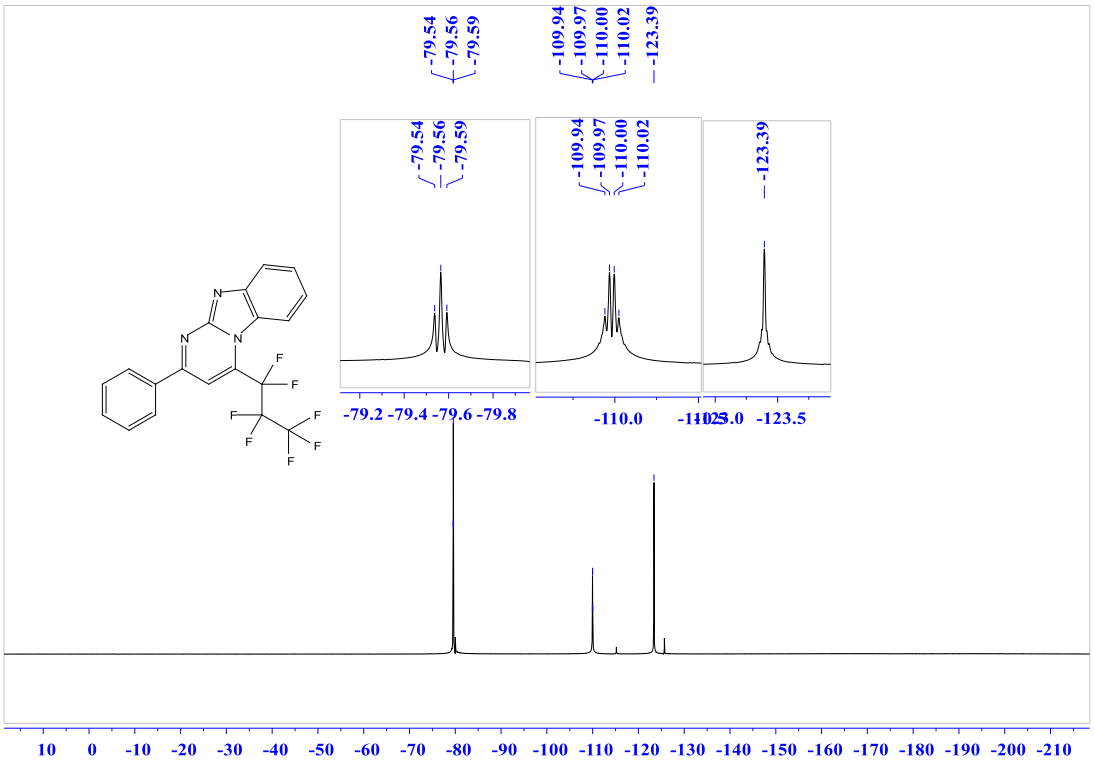
7.65
7.63
7.59
7.57
7.55
7.53
3.39 HDO
2.53 DMSO
2.52 DMSO
2.52 DMSO
2.51 DMSO
2.51 DMSO
-0.00
2.06
1.00
1.08
1.03
4.12
1.00
2.01
1.00
1.09
1.02
4.04
1.07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-79.56
-79.59
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-110.00
-110.02
-123.39
-79.2 -79.4 -79.6 -79.8
-110.0
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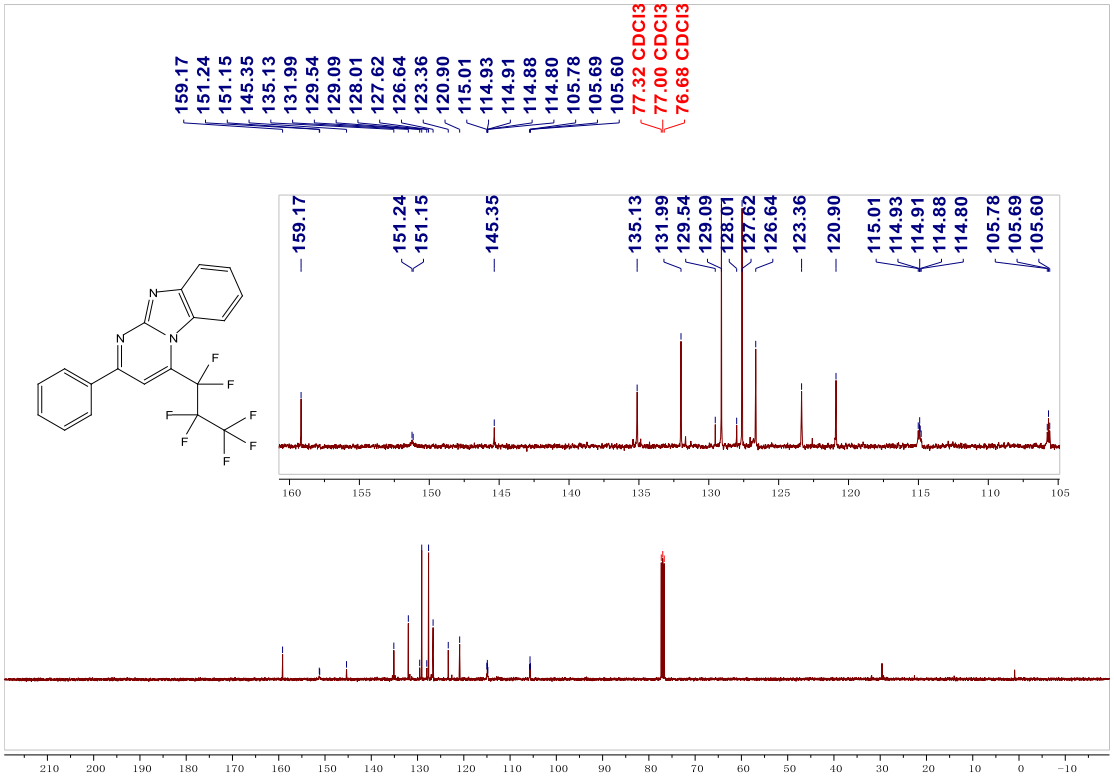
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210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127.62
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115.01
114.93
114.91
114.88
114.80
105.78
105.69
105.60
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
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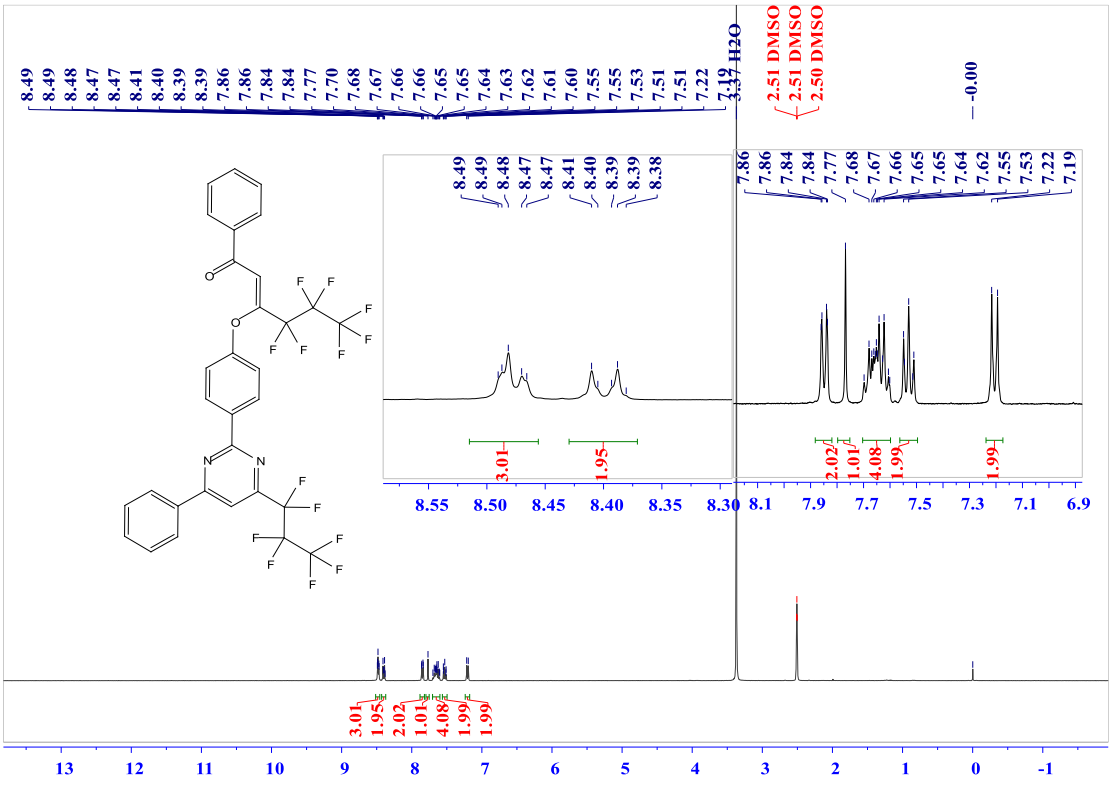

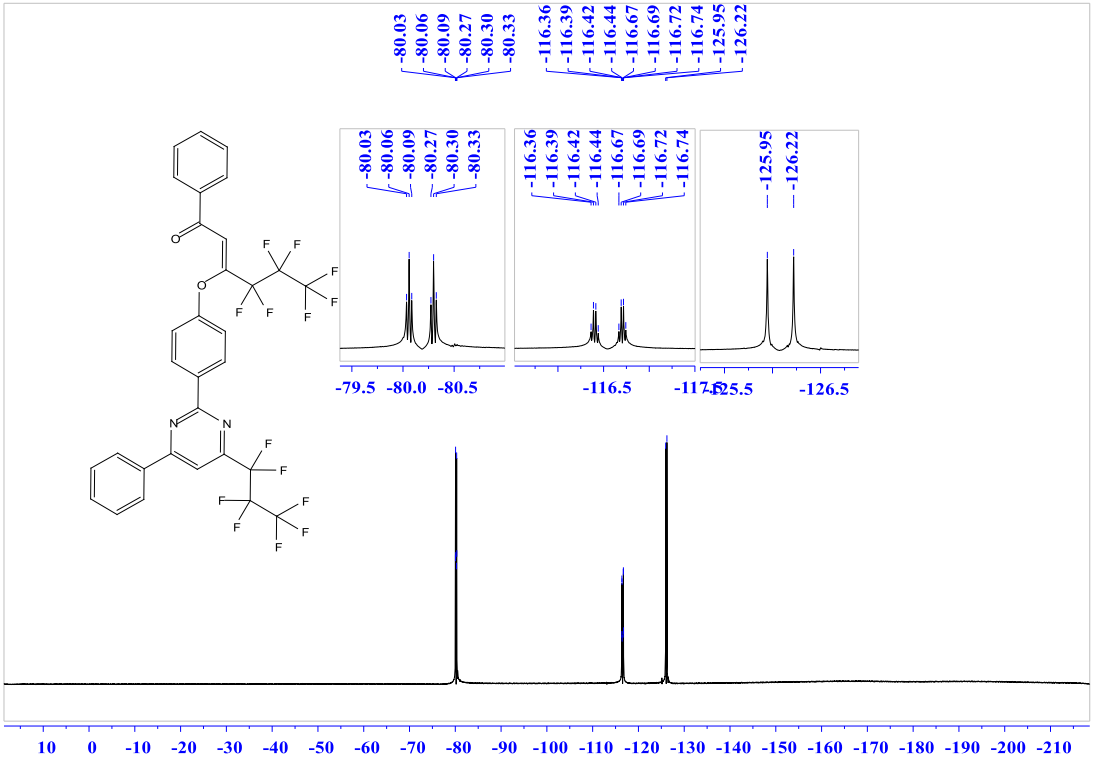

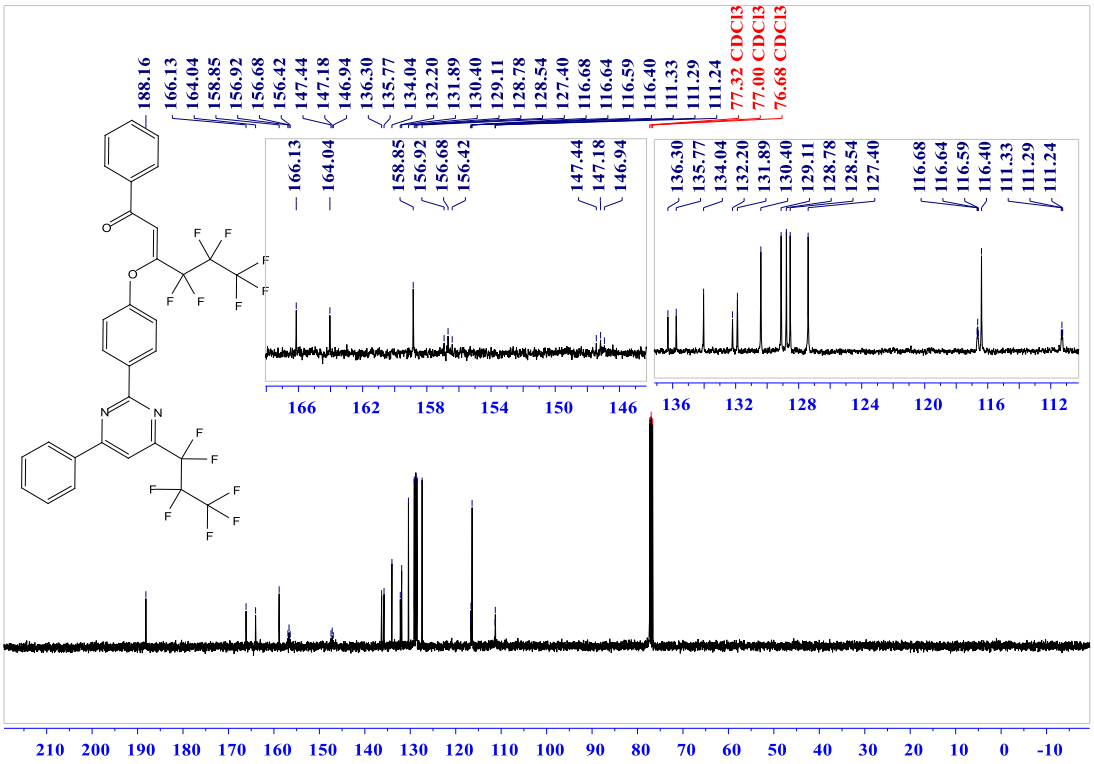
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111.33
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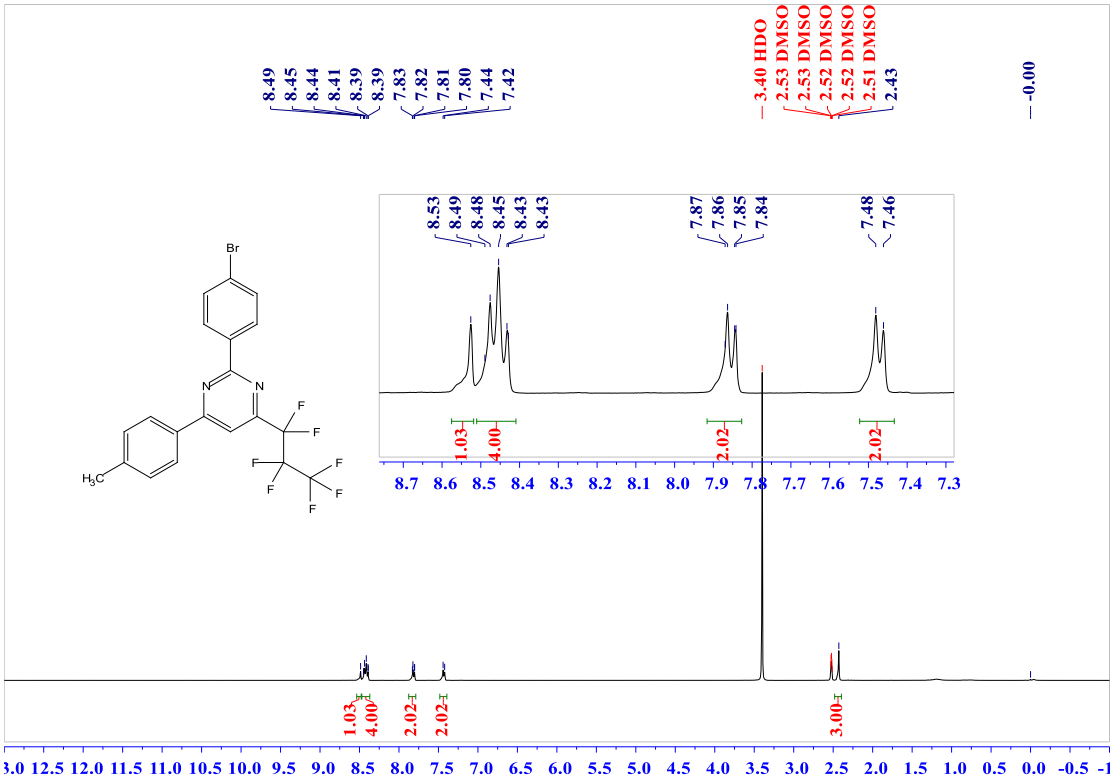
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7.80
7.44
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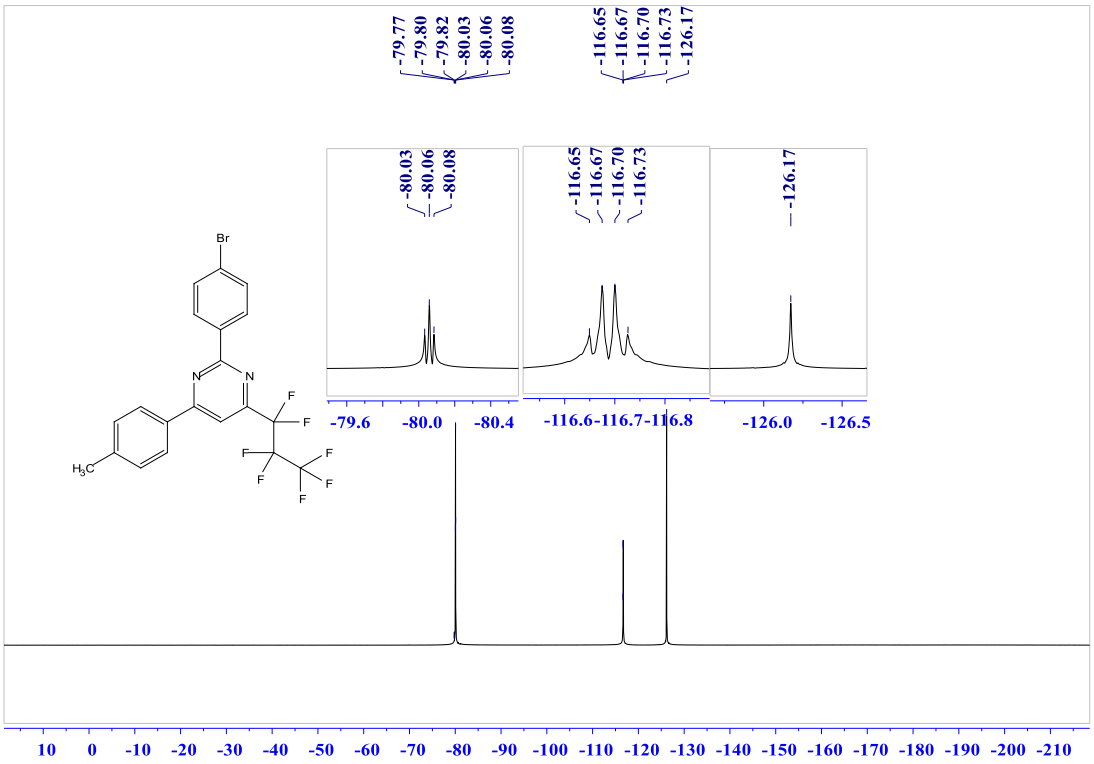
2.53 DMSO
2.53 DMSO
2.52 DMSO
2.52 DMSO
2.51 DMSO
2.43
-0.00
1.03
4.00
2.02
2.02
3.00
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1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F
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F
F
F
H3C
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-80.4
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-116.7
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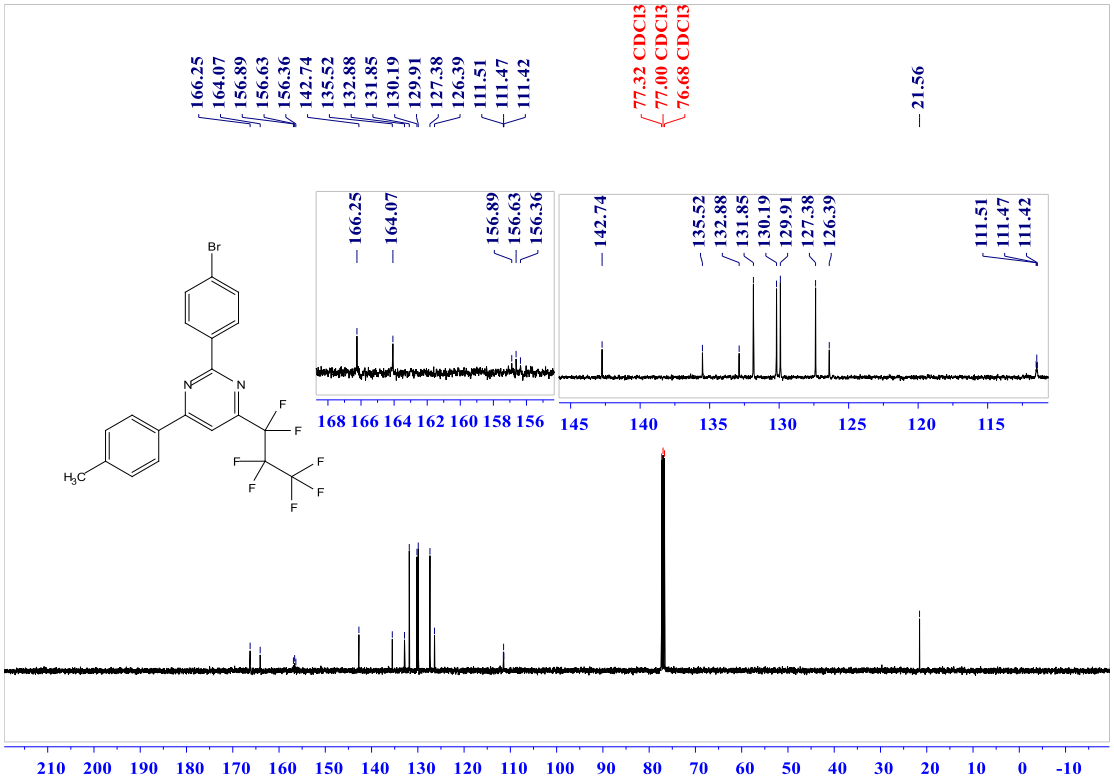
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111.47
111.42
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
21.56
Br
N
N
F
F
F
F
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H3C
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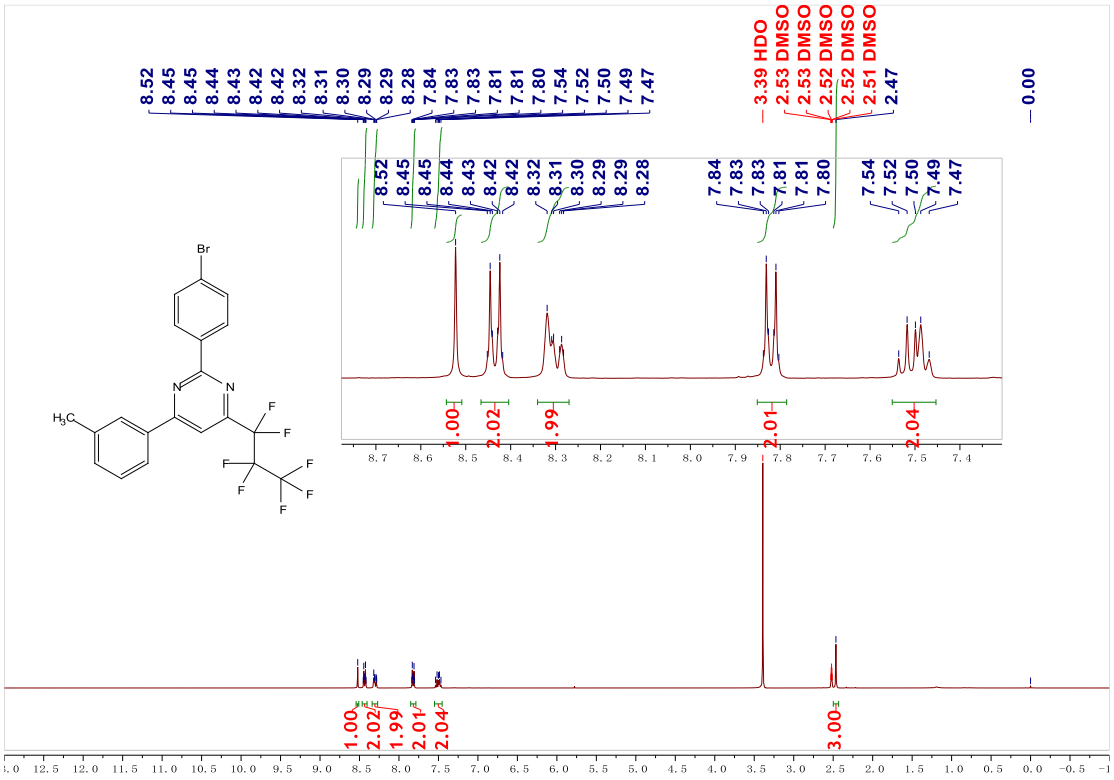
145 140 135 130 125 120 115
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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3.39 HDO 2.53 DMSO 2.53 DMSO 2.52 DMSO 2.52 DMSO 2.51 DMSO 2.47
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1.00 2.02 1.99 2.01 2.04
3.00
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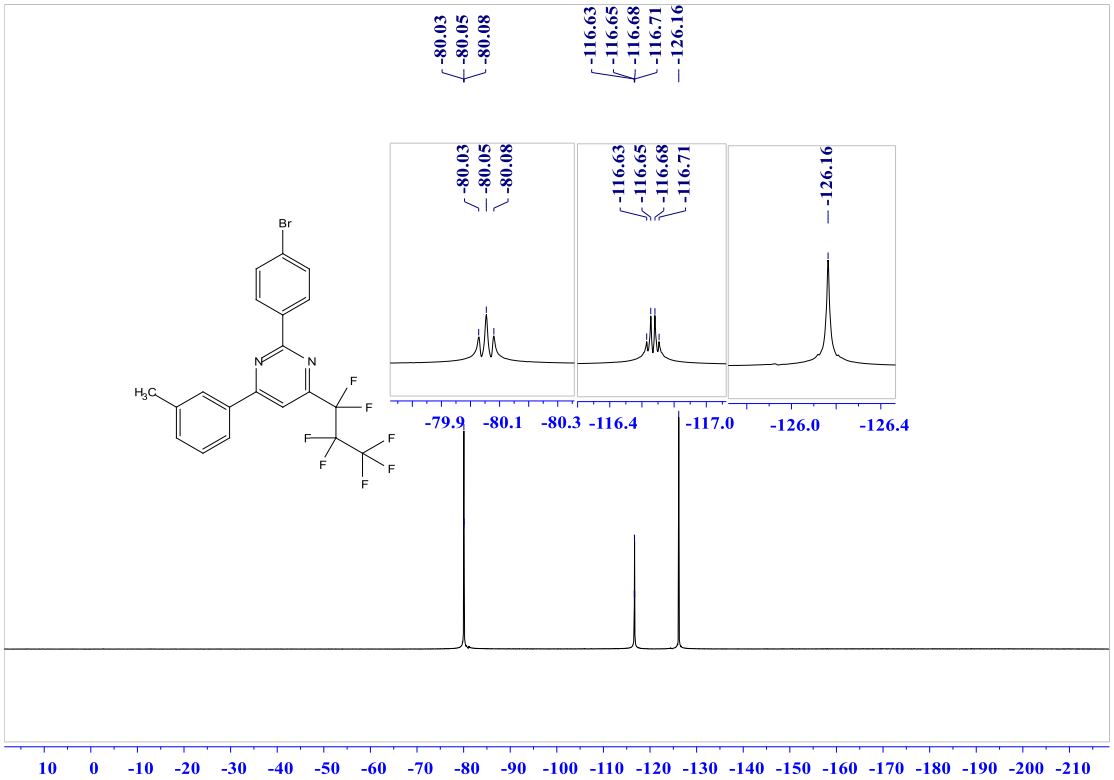
F
F
F
F
F
F
H3C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-79.9 -80.1 -80.3 -116.4 -117.0 -126.0 -126.4
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
Br
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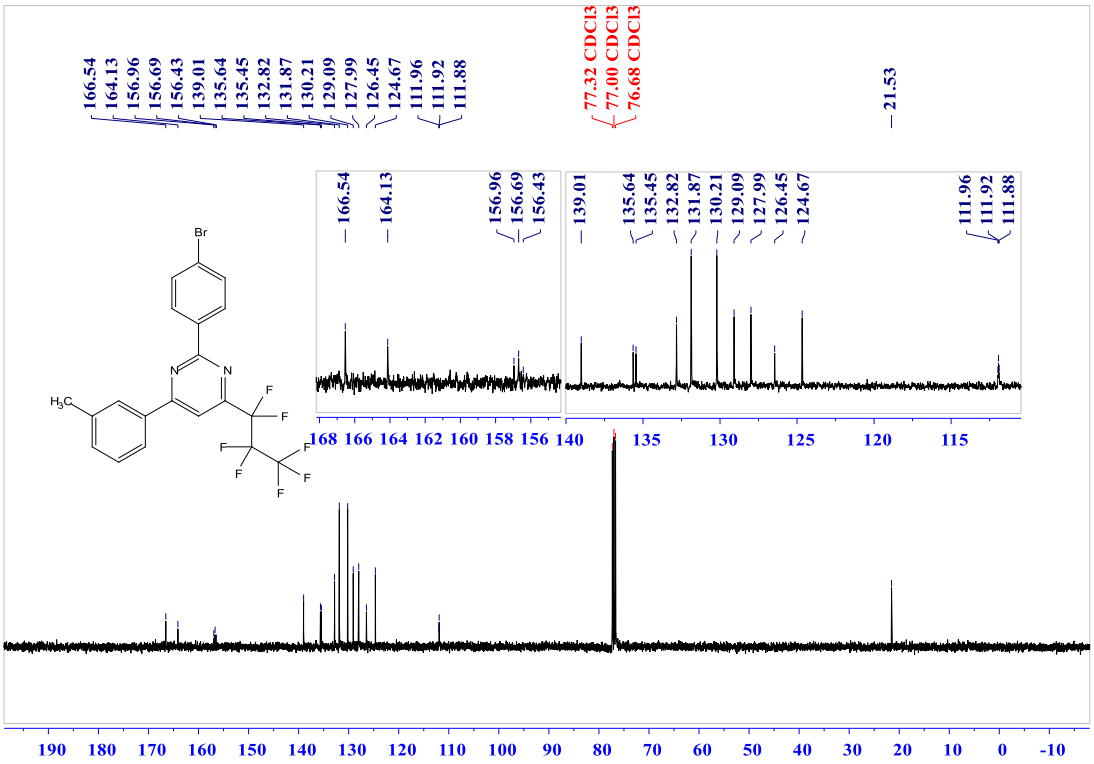
F
H3C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124.67
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111.88
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
21.53
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F
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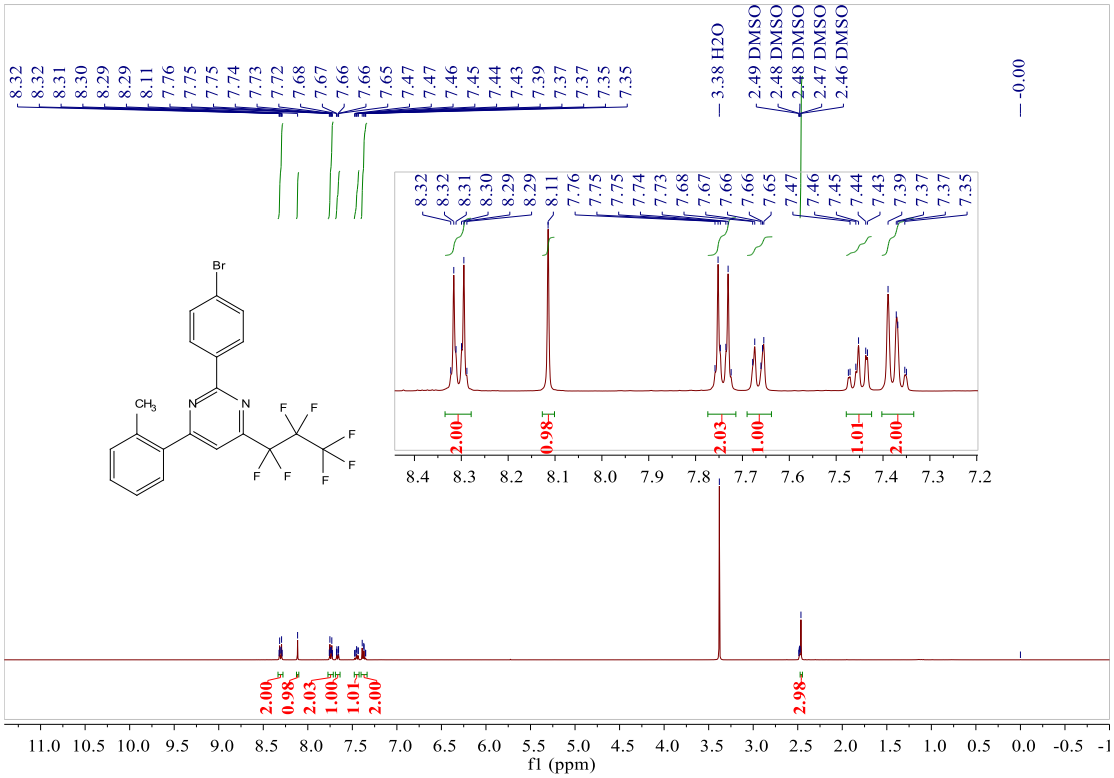
F
F
F
H3C
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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7.75
7.74
7.73
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7.66
7.65
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7.47
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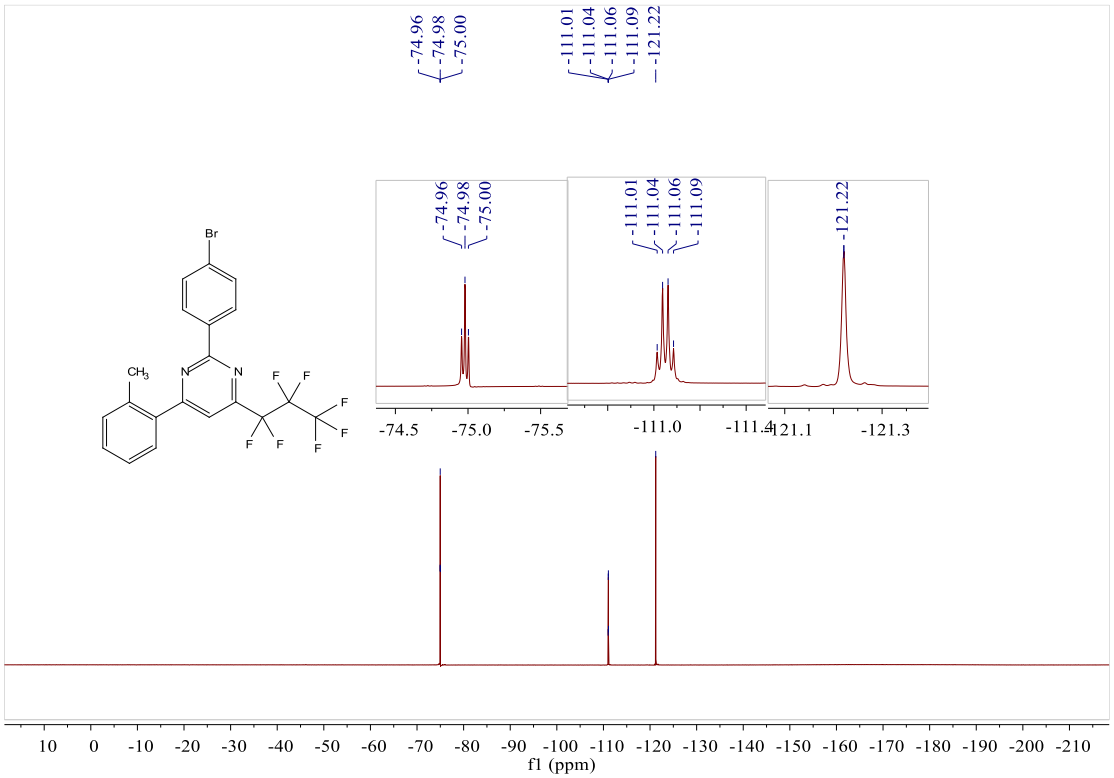
7.45
7.44
7.43
7.39
7.37
7.37
7.35
7.35
3.38 H2O
2.49 DMSO
2.48 DMSO
2.48 DMSO
2.47 DMSO
2.46 DMSO
-0.00
Br
N
N
CH3
F
F
F
F
F
F
2.00
0.98
2.03
1.00
1.01
2.00
2.98
fl (ppm)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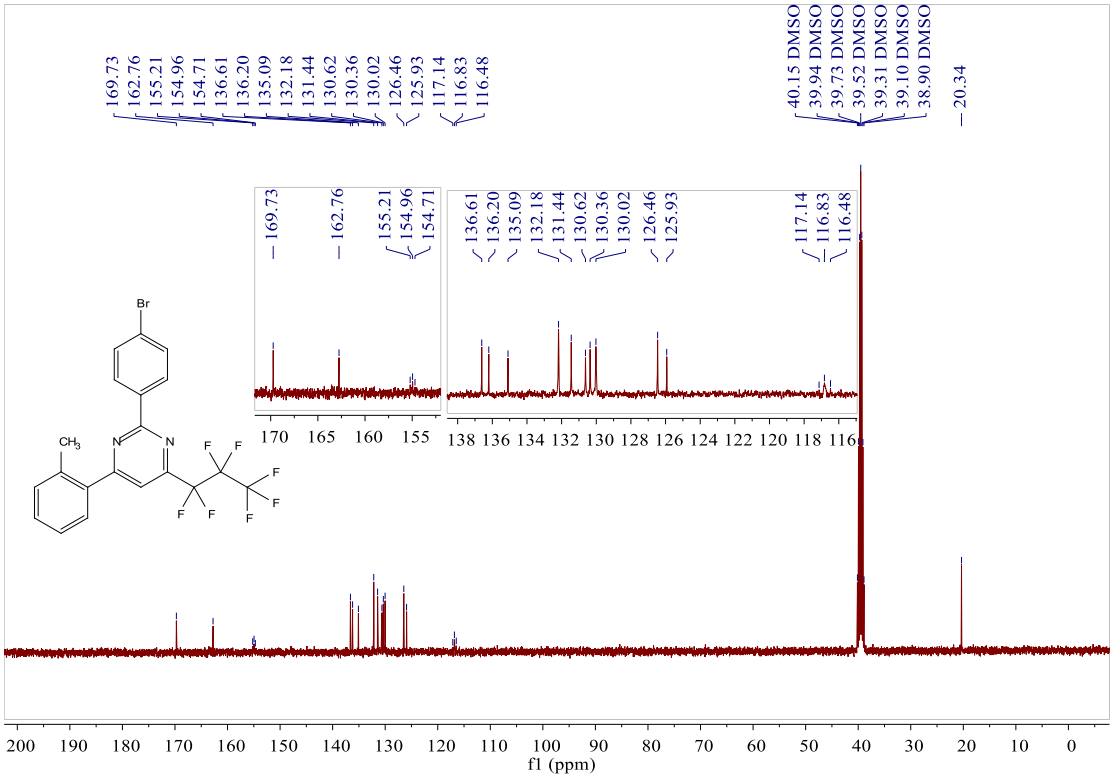
-74.98
-75.00
-111.01
-111.04
-111.06
-111.09
-121.22
Br
CH3
N
N
F
F
F
F
F
F
F
-74.5
-75.0
-75.5
-111.0
-111.4
-121.1
-121.3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)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135.09
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131.44
130.62
130.36
130.02
126.46
125.93
117.14
116.83
116.48
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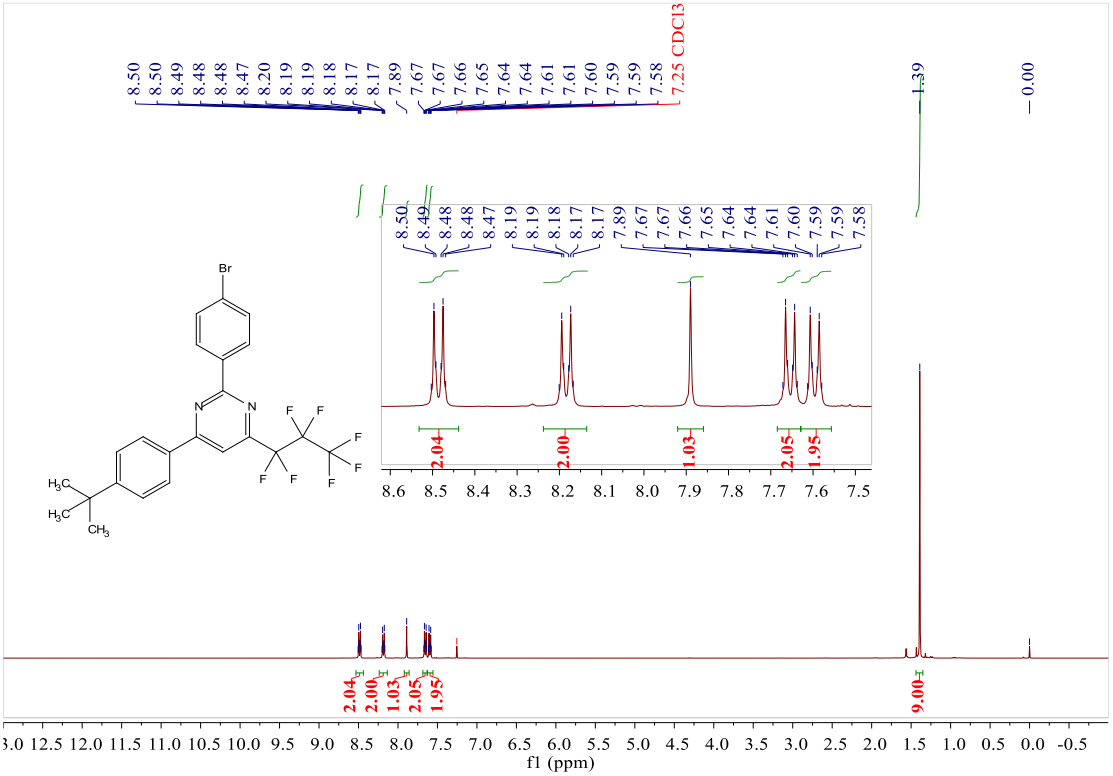
39.94 DMSO
39.73 DMSO
39.52 DMSO
39.31 DMSO
39.10 DMSO
38.90 DMSO
20.34
Br
CH3
N
N
F
F
F
F
F
F
F
170 165 160 155
138 136 134 132 130 128 126 124 122 120 118 116
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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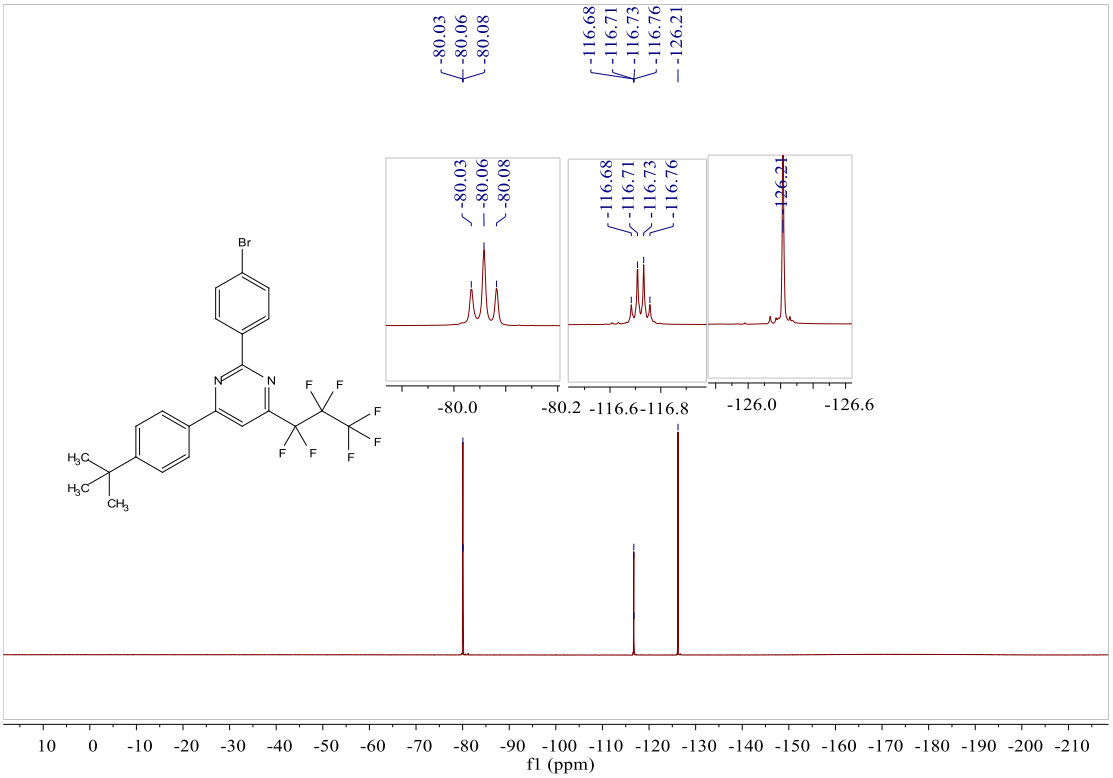
1.39
0.00
Br
N
N
F
F
F
F
F
F
F
H3C
H3C
CH3
2.04
2.00
1.03
2.05
1.95
9.00
f1 (ppm)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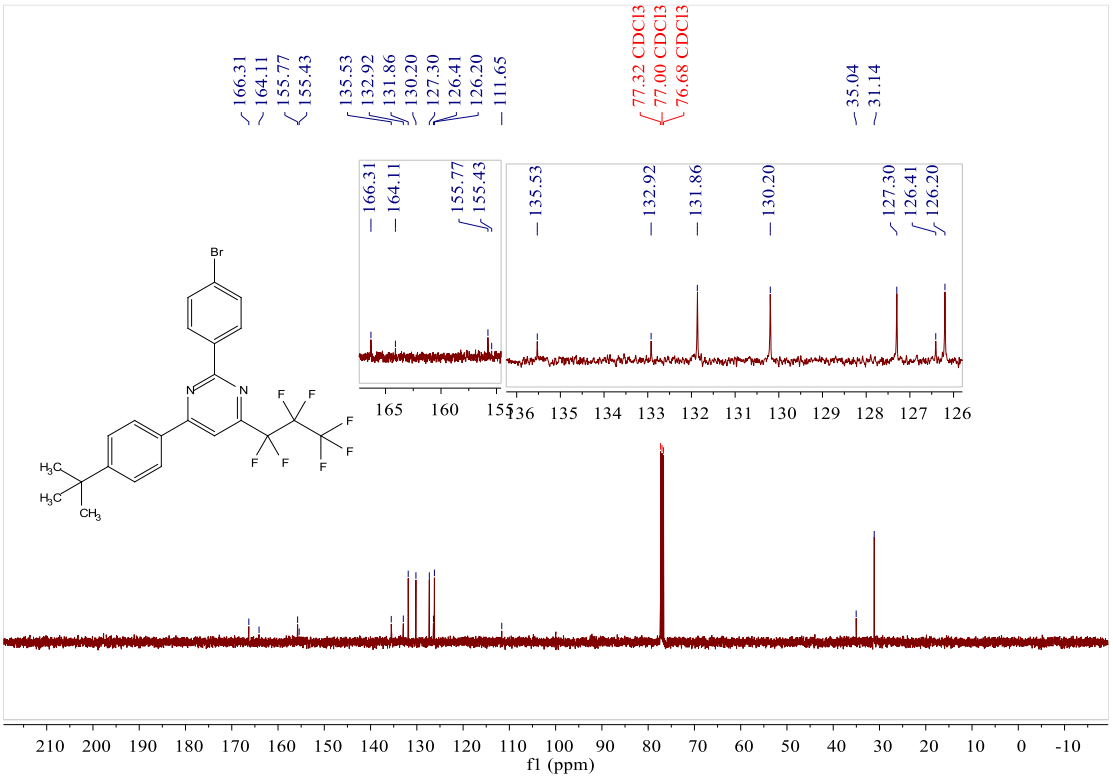
-80.06
-80.08
-116.68
-116.71
-116.73
-116.76
-126.21
Br
N
N
F
F
F
F
F
F
F
H3C
H3C
CH3
f1 (ppm)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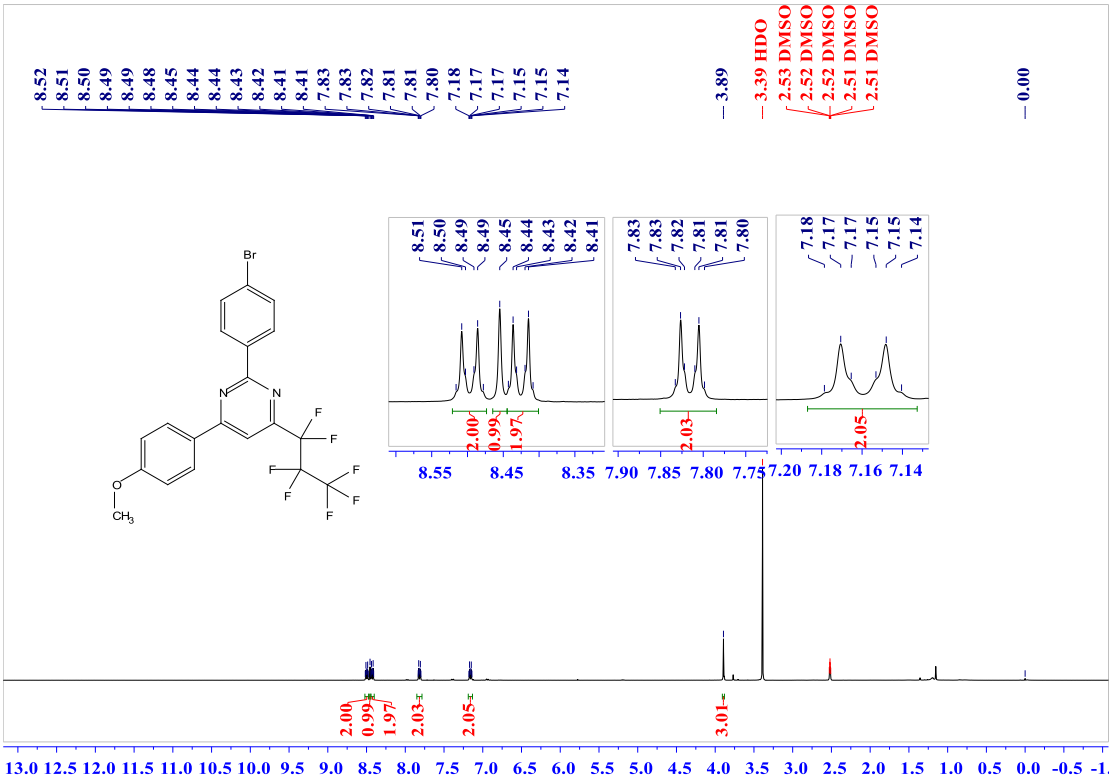
132.92
131.86
130.20
127.30
126.41
126.20
111.65
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
35.04
31.14
Br
N
N
F
F
F
F
F
F
H3C
H3C
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.48
8.45
8.44
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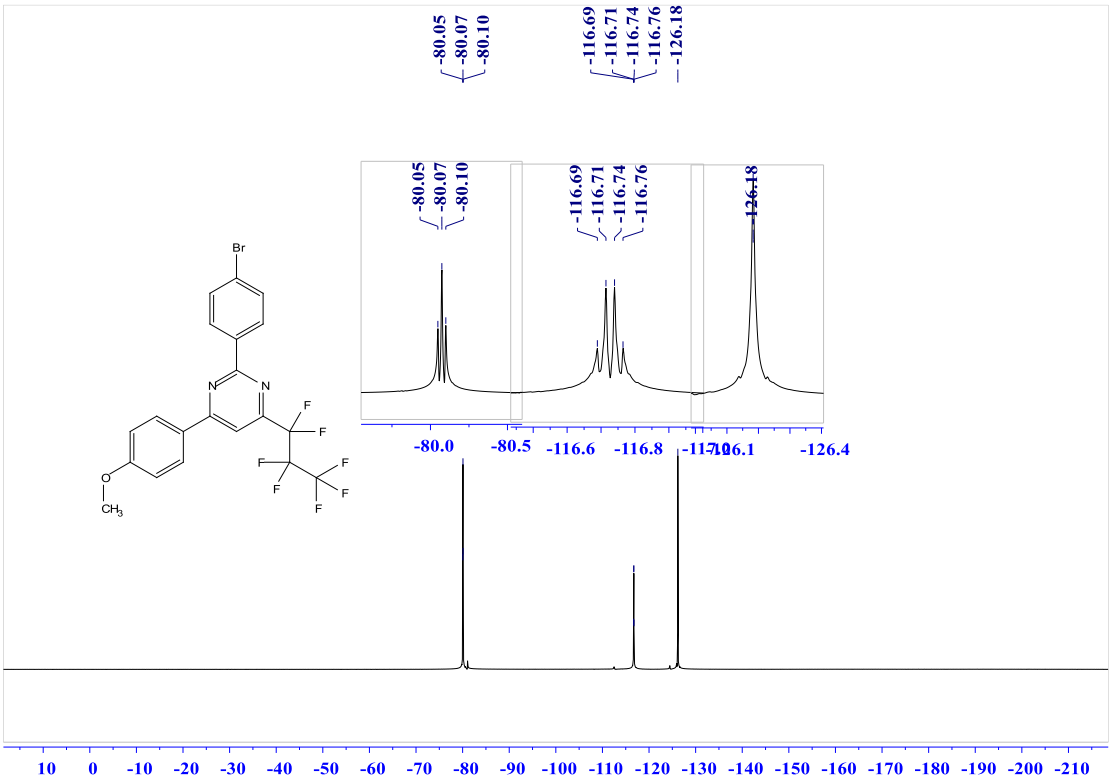
8.42
8.41
8.41
7.83
7.83
7.82
7.81
7.81
7.80
7.18
7.17
7.17
7.15
7.15
7.14
3.89
3.39 HDO
2.53 DMSO
2.52 DMSO
2.52 DMSO
2.51 DMSO
2.51 DMSO
0.00
Br
N
N
F
F
F
F
F
F
O
CH3
2.00
0.99
1.97
2.03
2.05
3.01
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5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-80.10
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-116.76
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Br
N
N
F
O
CH3
-80.0
-80.5
-116.6
-116.8
-126.1
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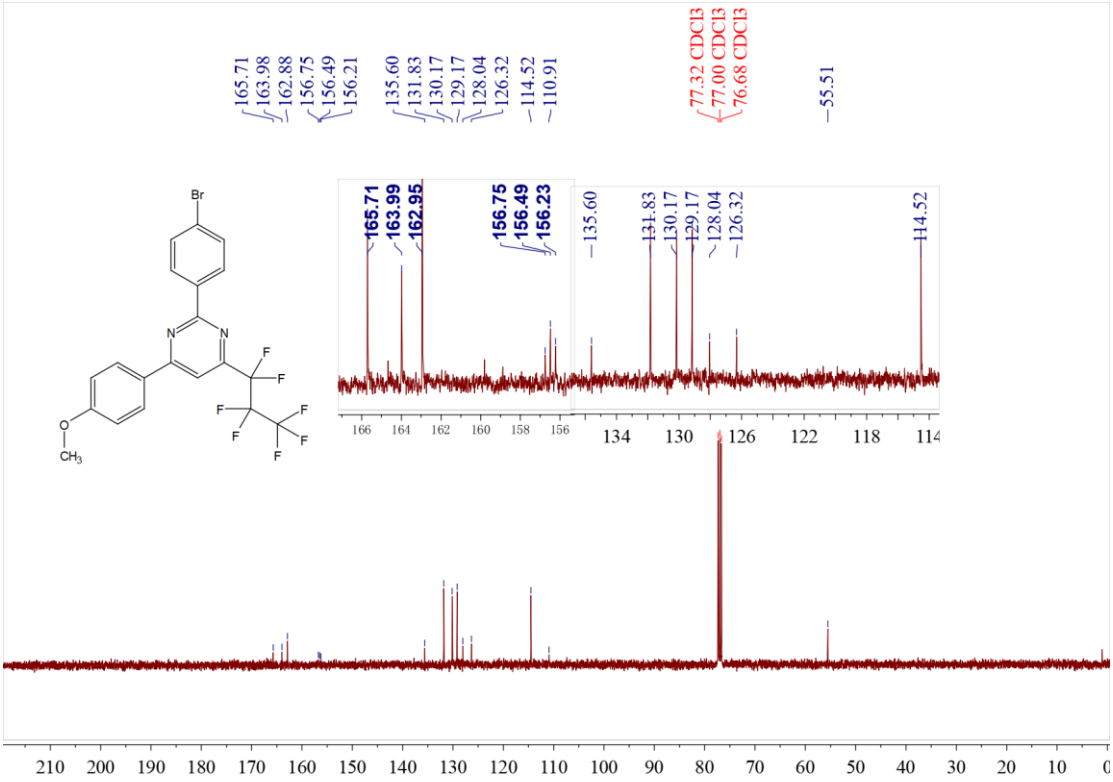
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210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131.83
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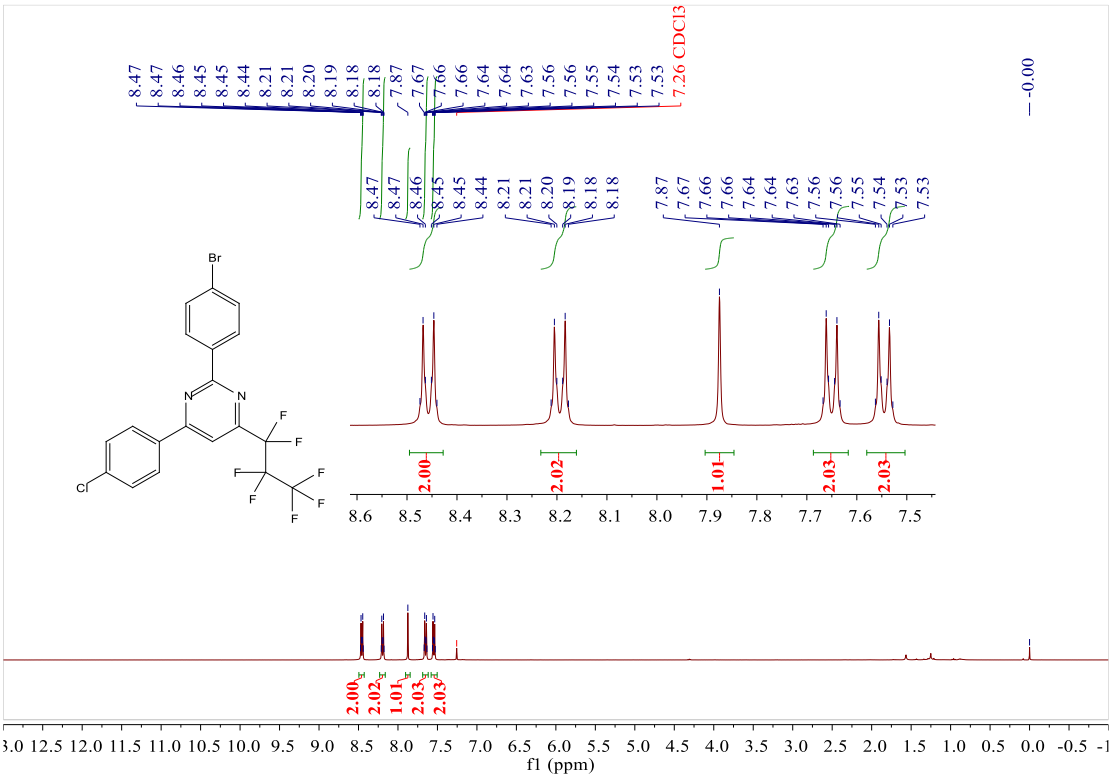
129.17
128.04
126.32
114.52
110.91
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
55.51
Br
N
N
F
O
CH3
134 130 126 122 118
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10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8.44
8.21
8.21
8.20
8.19
8.18
8.18
7.87
7.67
7.66
7.66
7.64
7.64
7.63
7.56
7.56
7.55
7.54
7.53
7.53
7.26 CDCl3
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Br
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N
F
F
F
F
F
F
F
Cl
2.00
2.02
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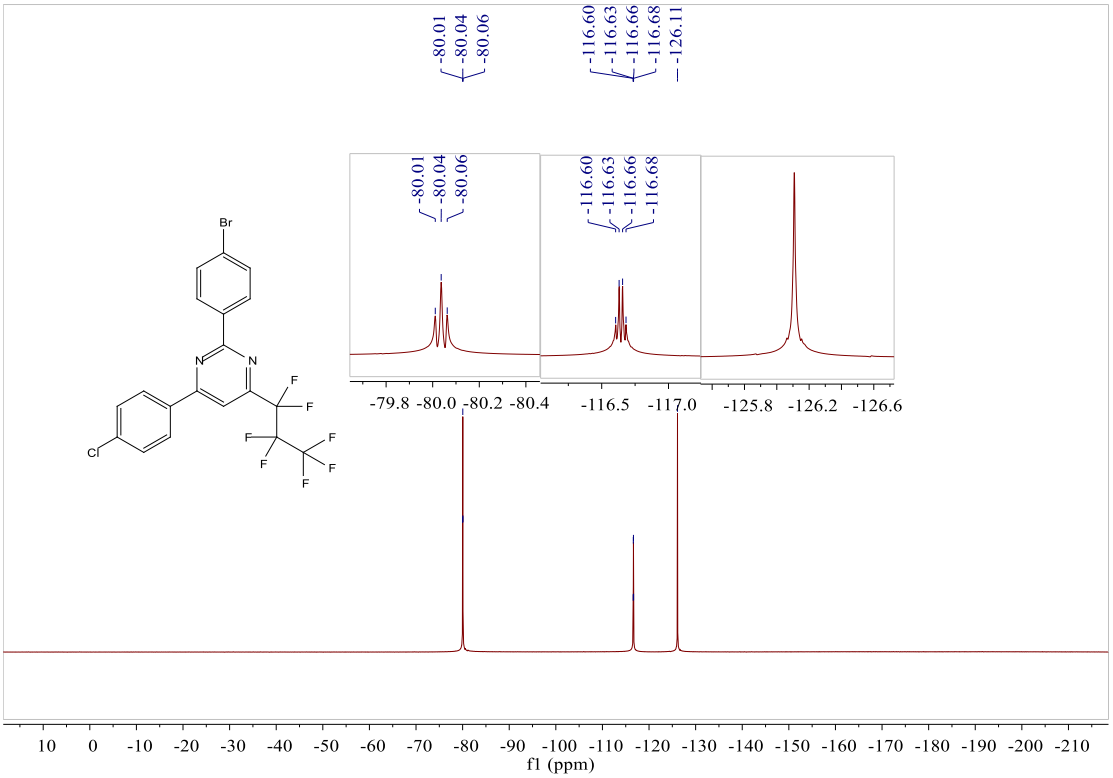
f1 (ppm)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-80.04
-80.06
-116.60
-116.63
-116.66
-116.68
-126.11
Br
N
N
F
F
F
F
F
F
F
Cl
-79.8 -80.0 -80.2 -80.4
-116.5 -117.0
-125.8 -126.2 -126.6
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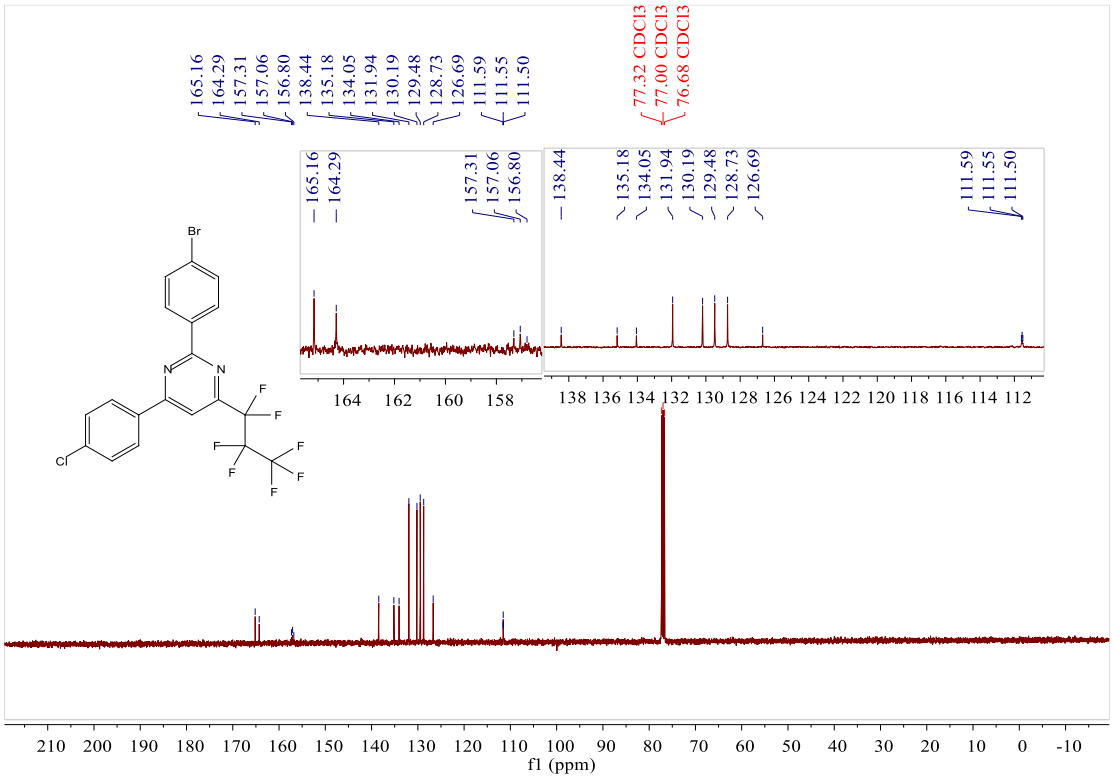
f1 (ppm)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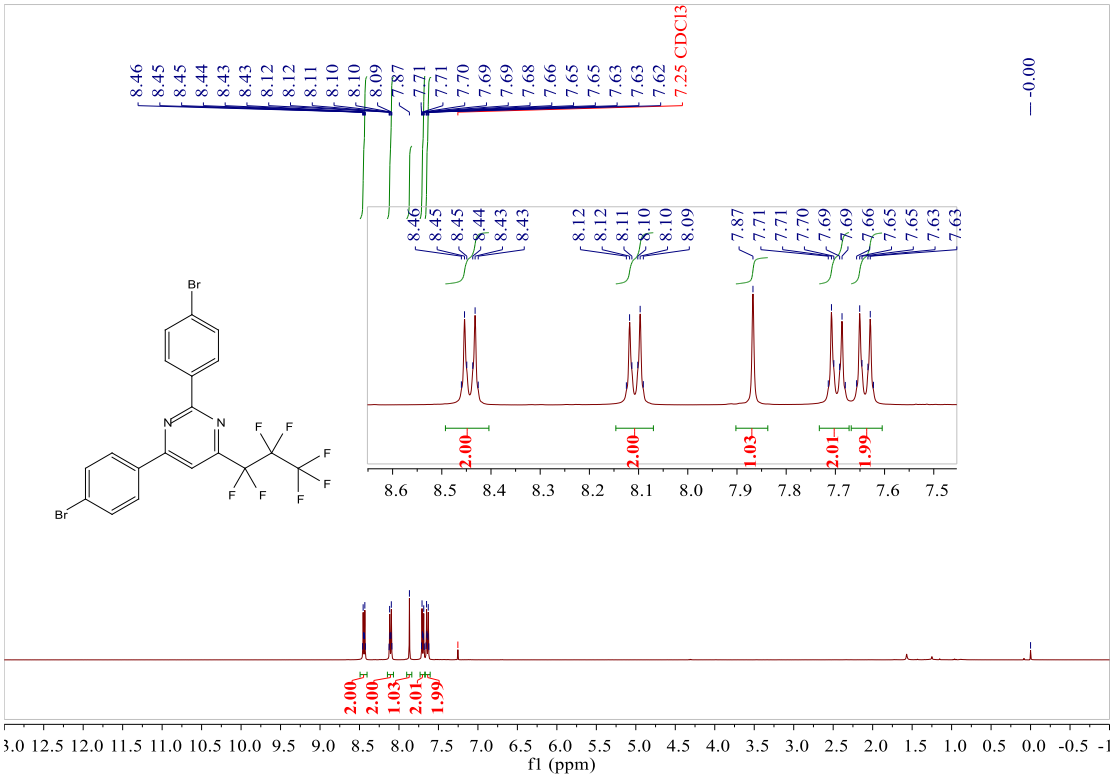
157.06
156.80
138.44
135.18
134.05
131.94
130.19
129.48
128.73
126.69
111.59
111.55
111.50
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
Br
N
N
F
F
F
F
F
F
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.45
8.45
8.44
8.43
8.43
8.12
8.12
8.11
8.10
8.10
8.09
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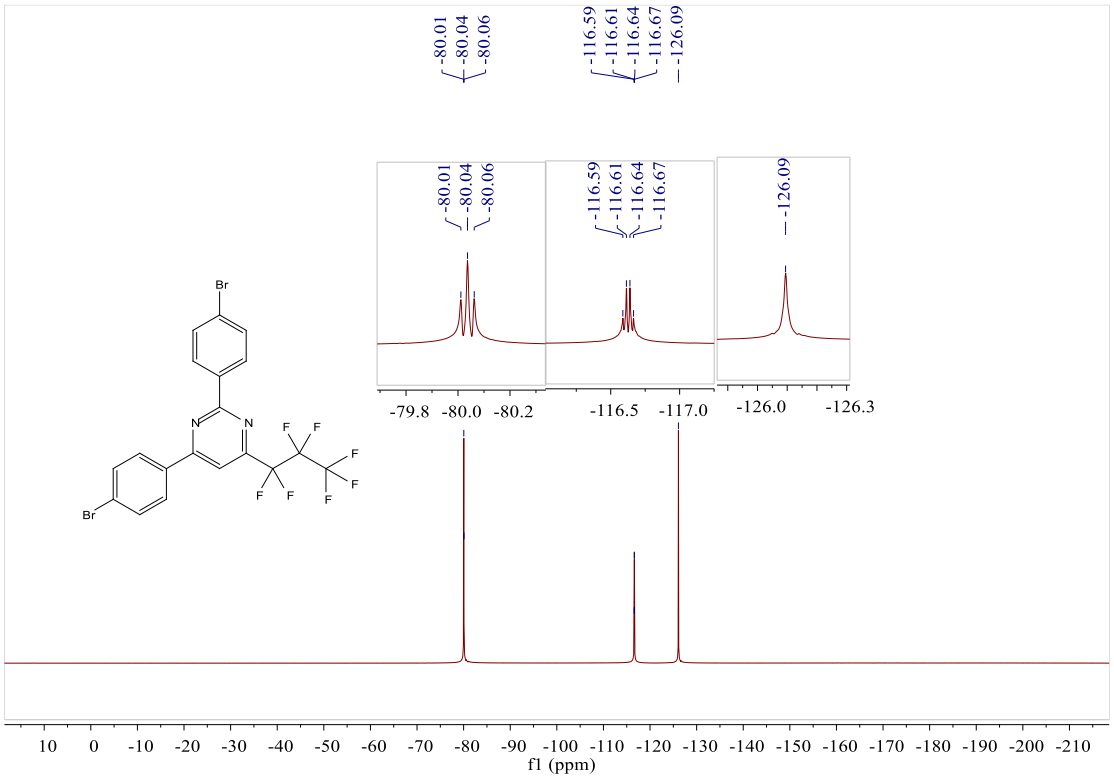
7.71
7.71
7.70
7.69
7.69
7.68
7.66
7.65
7.65
7.63
7.63
7.62
7.25 CDCl3
-0.00
Br
N
N
F
F
F
F
F
F
Br
2.00
2.00
1.03
2.01
1.99
8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
f1 (ppm)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-80.06
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-116.61
-116.64
-116.67
-126.09
Br
N
N
F
Br
-79.8 -80.0 -80.2
-116.5 -117.0
-126.0 -126.3
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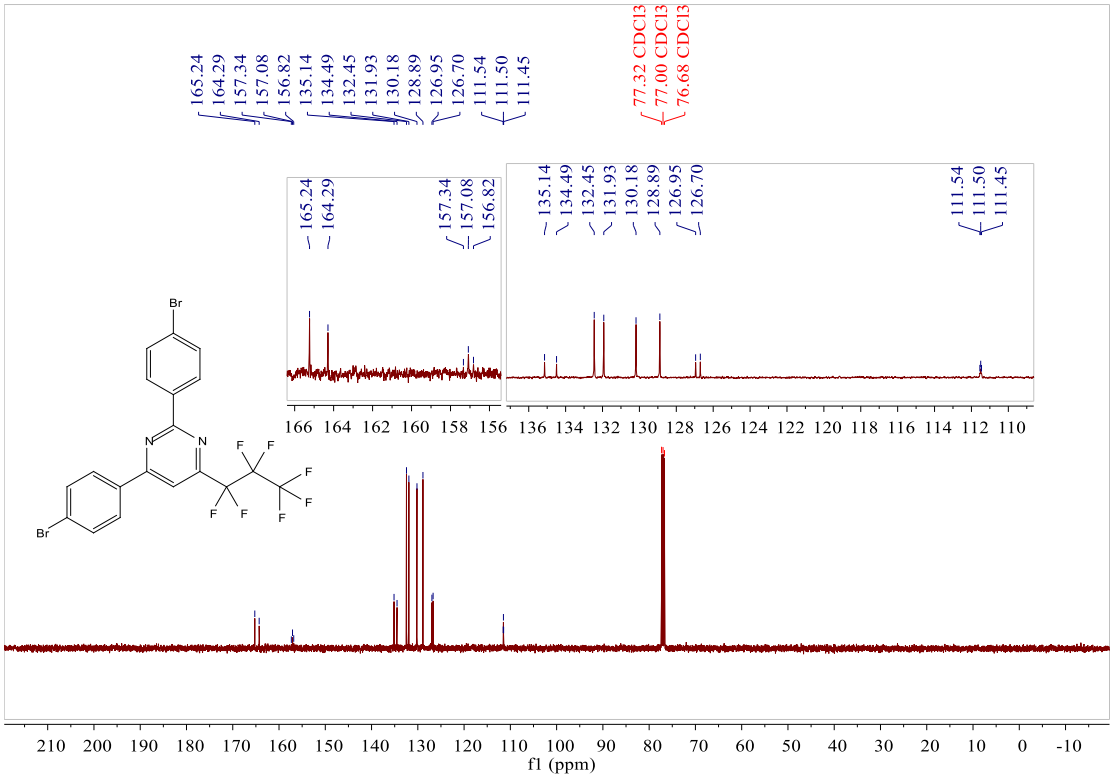
f1 (ppm)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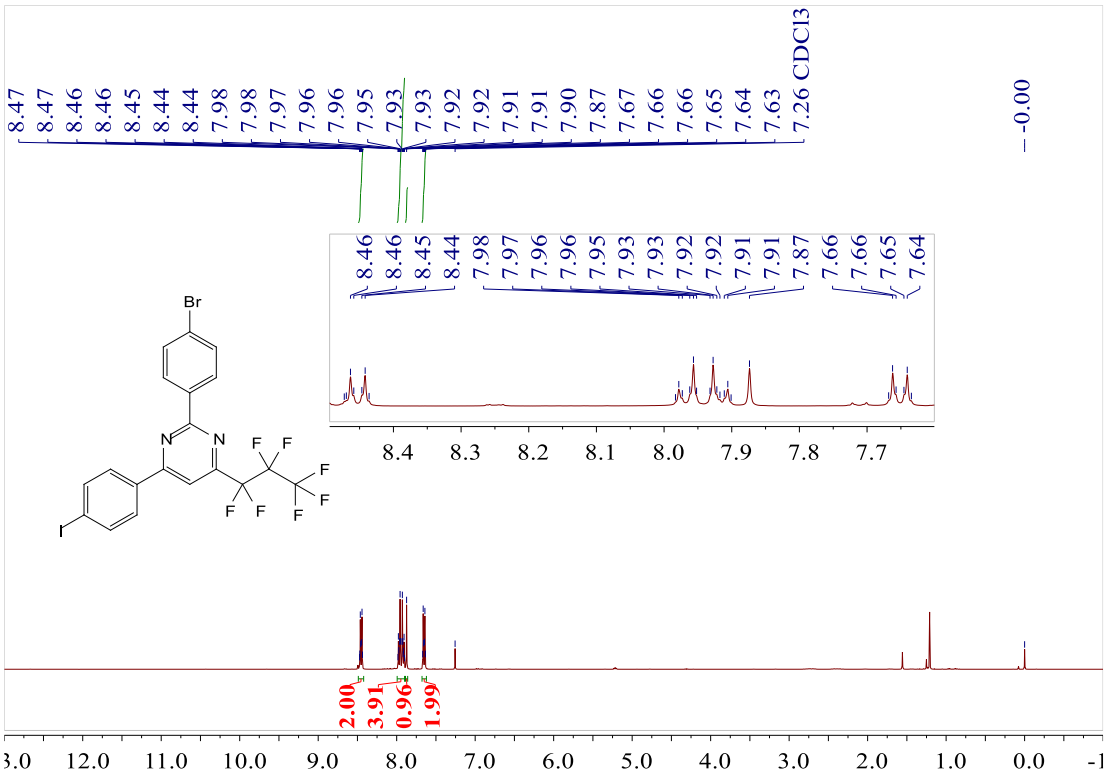
135.14
134.49
132.45
131.93
130.18
128.89
126.95
126.70
111.54
111.50
111.45
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
Br
N
N
F
Br
166 164 162 160 158 156
136 134 132 130 128 126 124 122 120 118 116 114 112 110
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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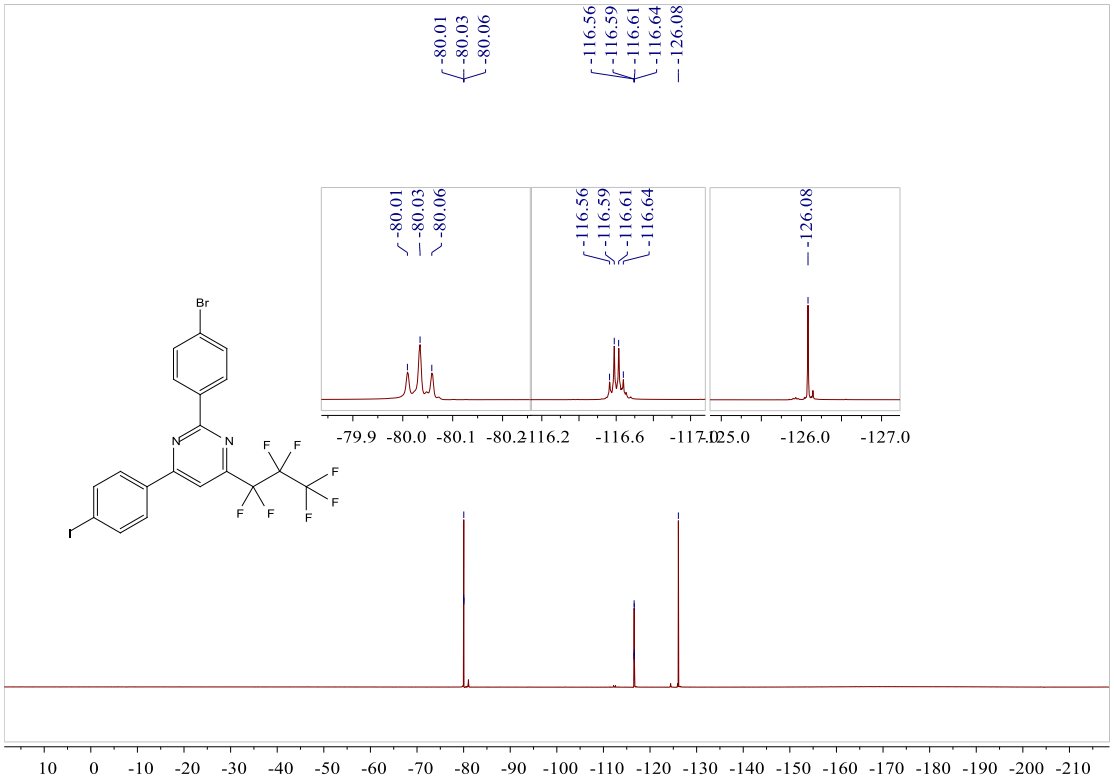
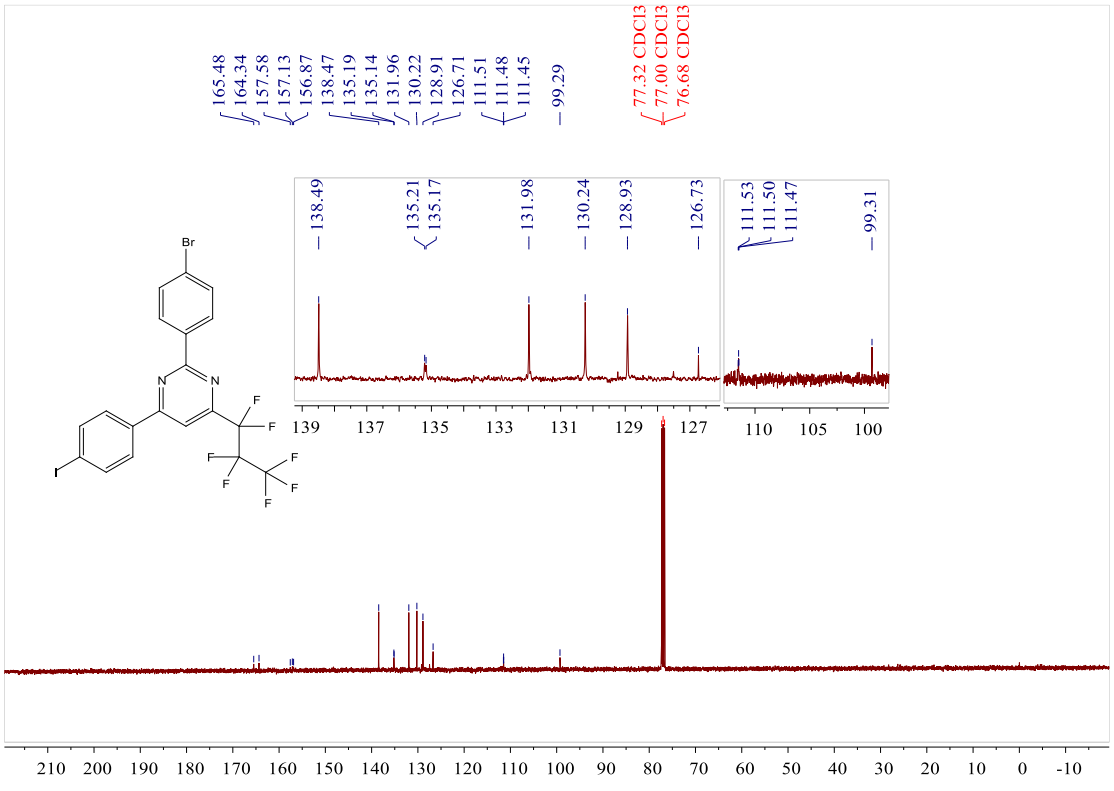
-0.00
8.46 8.46 8.45 8.44 7.98 7.97 7.96 7.96 7.95 7.93 7.93 7.92 7.92 7.91 7.91 7.87 7.66 7.66 7.65 7.64
Br
N N F F F F F F F F
I
2.00 3.91 0.96 1.99


-80.01 -80.03 -80.06 -116.56 -116.59 -116.61 -116.64 -126.08
Br
N N F F F F F F F F
I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135.14
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111.48
111.45
99.29
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
138.49
135.21
135.17
131.98
130.24
128.93
126.73
111.53
111.50
111.47
99.31
Br
F
F
F
F
F
F
F
I
N
N
139
137
135
133
131
129
127
110
105
100
210
200
190
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50
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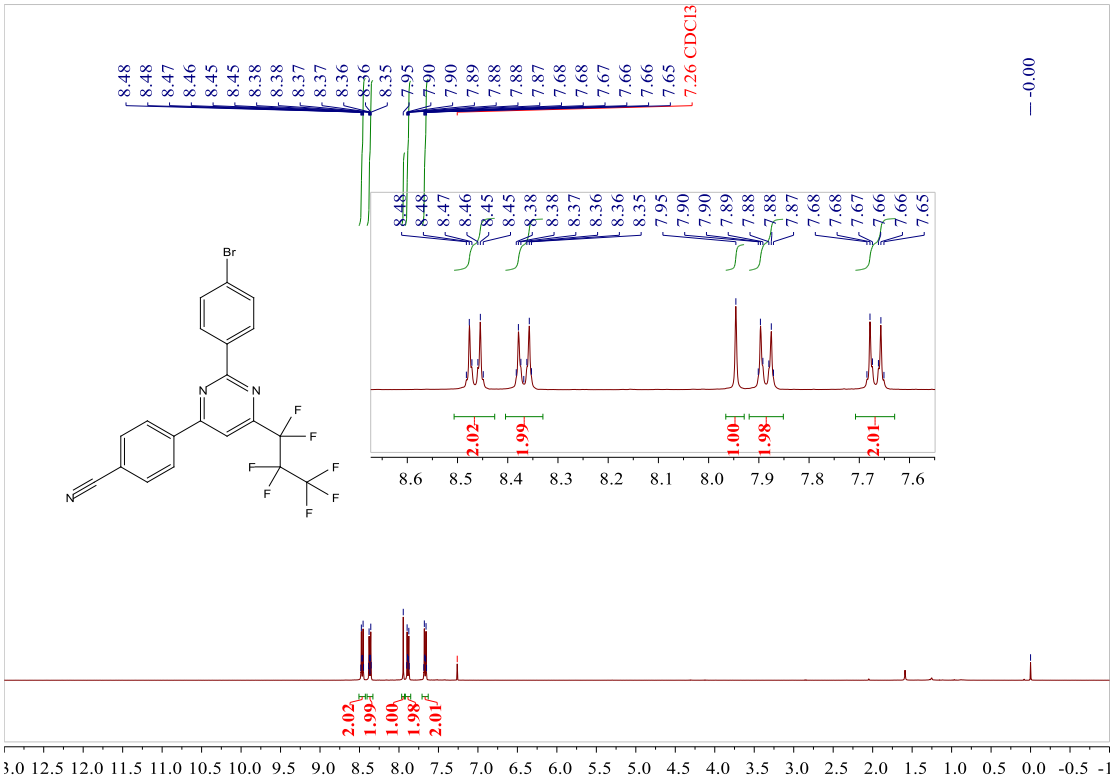
20
10
0
-10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8.36
8.35
7.95
7.90
7.90
7.89
7.88
7.88
7.87
7.68
7.68
7.67
7.66
7.66
7.65
7.26 CDCl3
-0.00
Br
F
F
F
F
F
F
F
N
N
N
2.02
1.99
1.00
1.98
2.01
8.6
8.5
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
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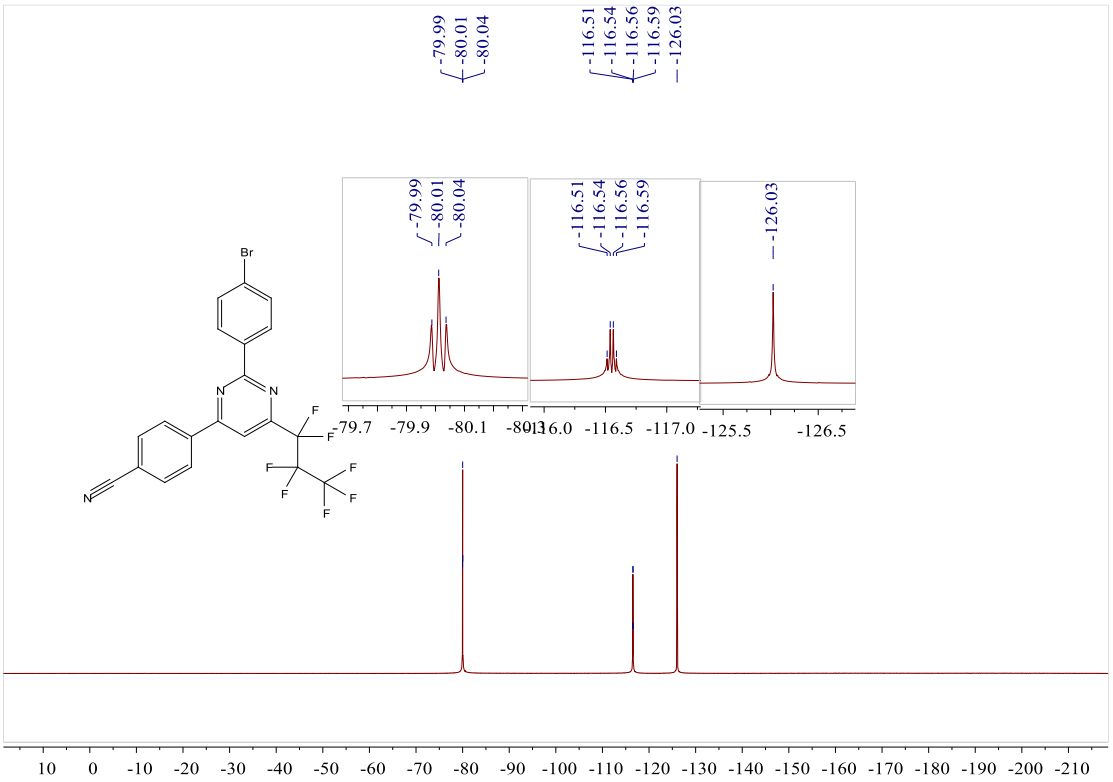
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1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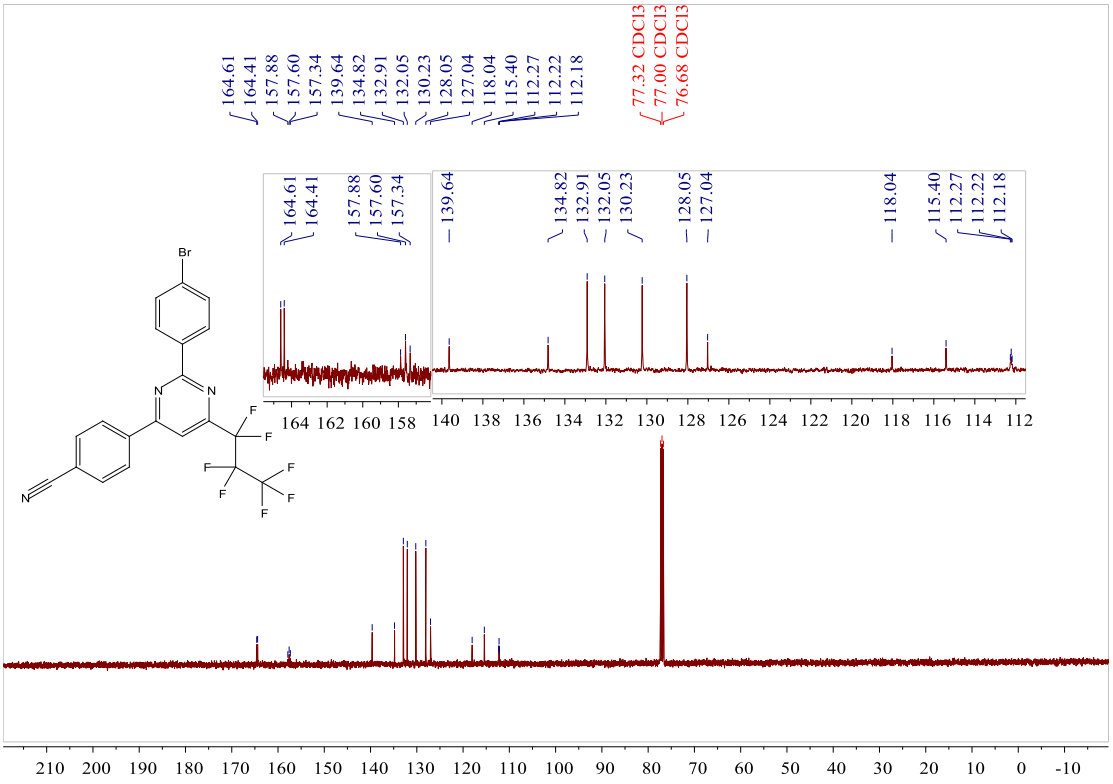
-80.04
-116.51
-116.54
-116.56
-116.59
-126.03
Br
N
N
F
F
F
F
F
F
N
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210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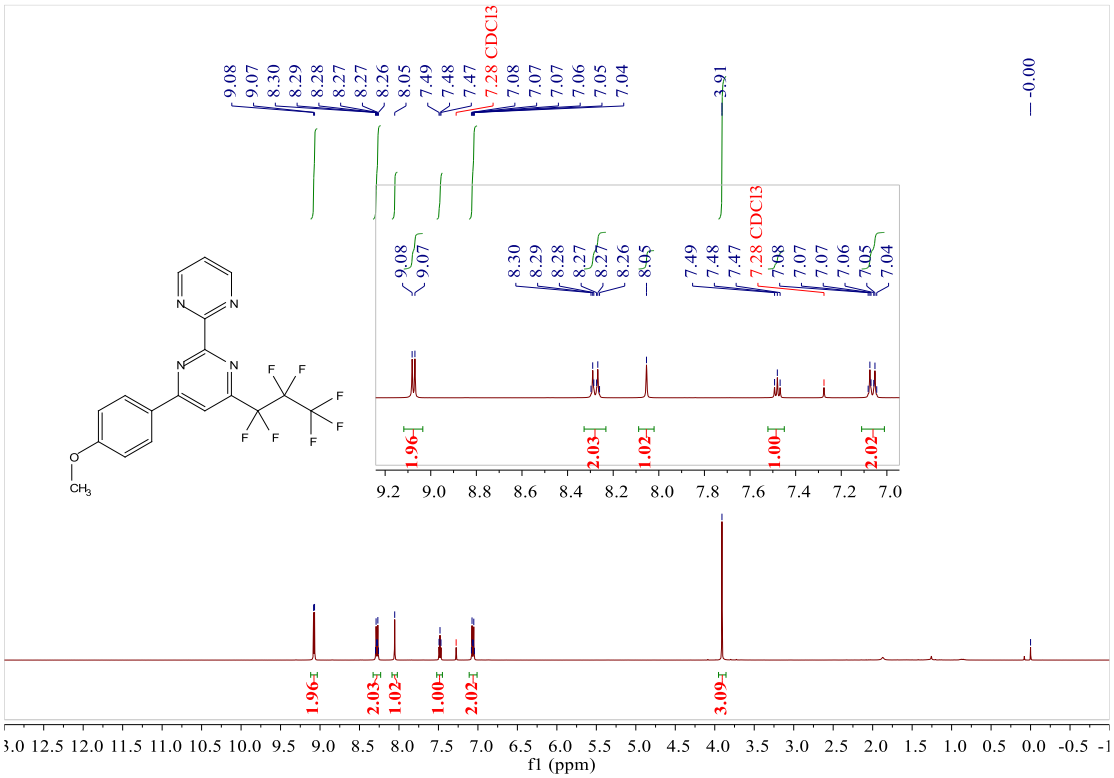
139.64
134.82
132.91
132.05
130.23
128.05
127.04
118.04
115.40
112.27
112.22
112.18
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
Br
N
N
F
F
F
F
F
F
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10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9.07
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8.29
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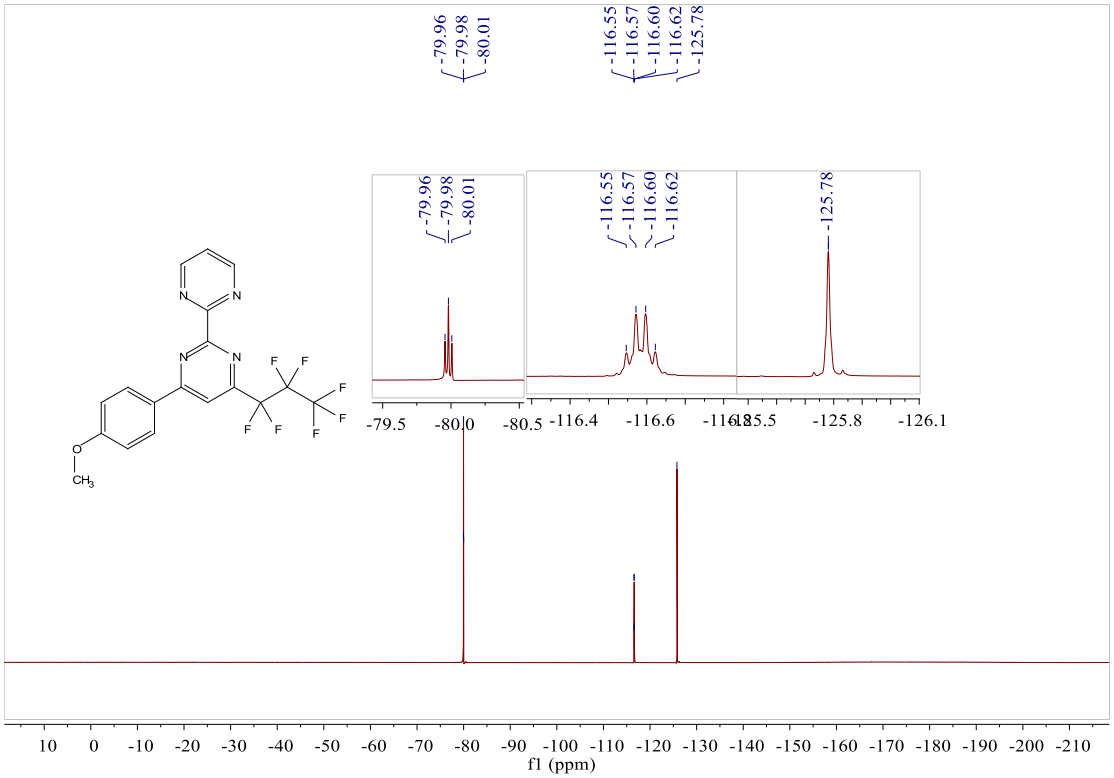
8.27
8.27
8.26
8.05
7.49
7.48
7.47
7.28 CDCl3
7.08
7.07
7.07
7.06
7.05
7.04
3.91
-0.00
1.96
2.03
1.02
1.00
2.02
3.09
f1 (ppm)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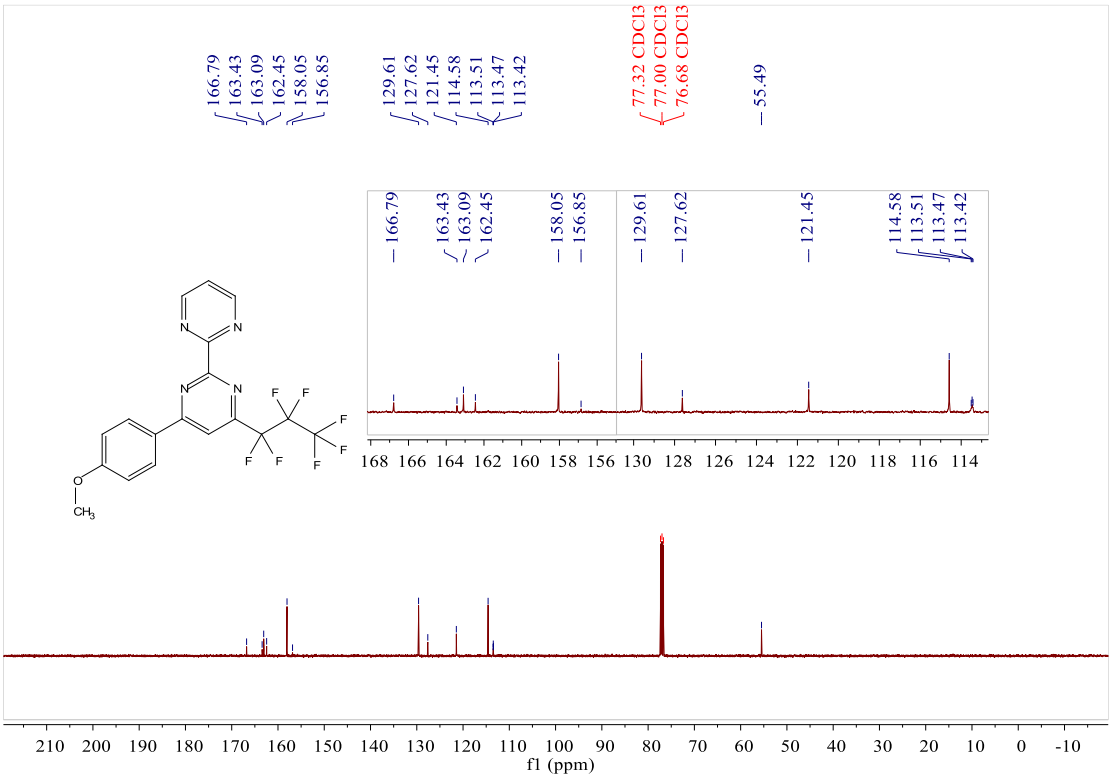
-79.98
-80.01
-116.55
-116.57
-116.60
-116.62
-125.78
f1 (ppm)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127.62
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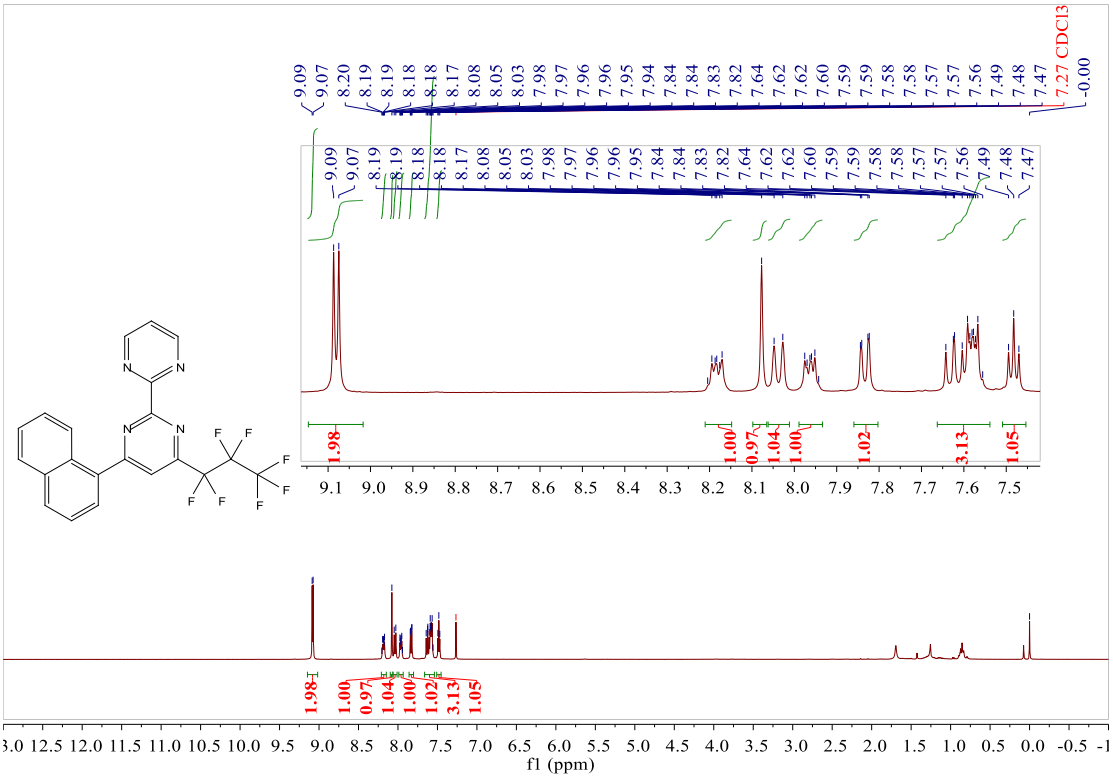
114.58
113.51
113.47
113.42
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
55.49
f1 (ppm)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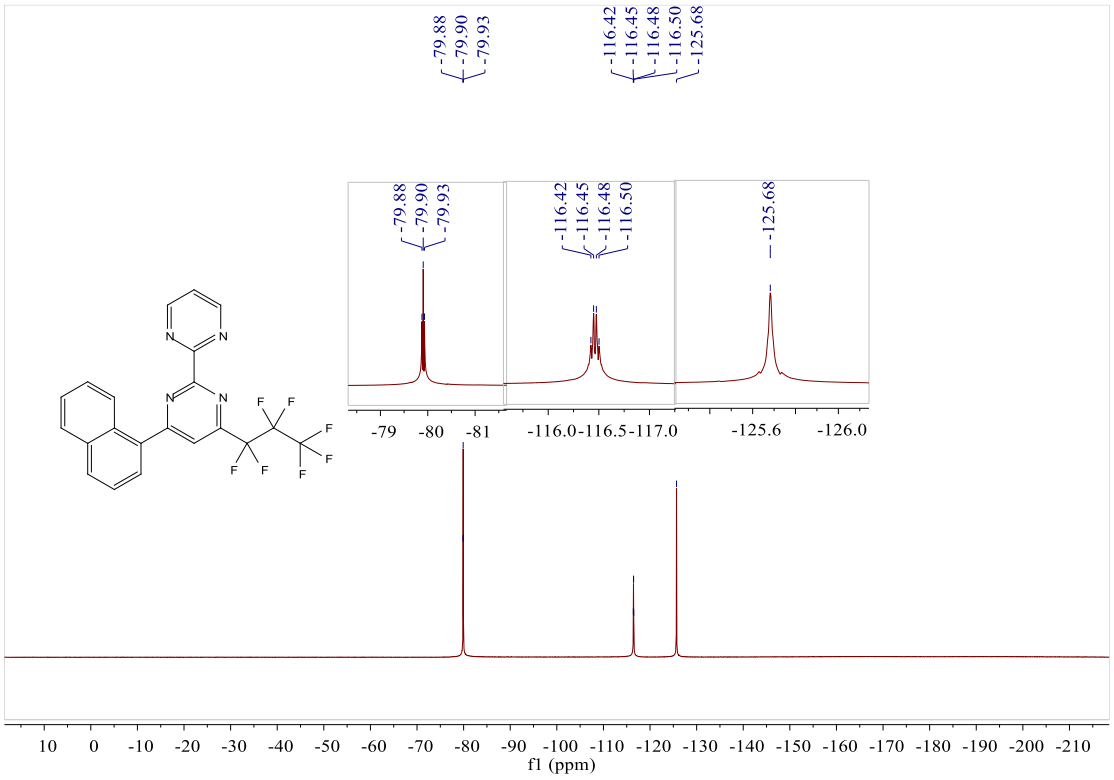
8.18
8.17
8.08
8.05
8.03
7.98
7.97
7.96
7.95
7.94
7.84
7.83
7.82
7.64
7.62
7.60
7.59
7.58
7.57
7.56
7.49
7.48
7.47
7.27 CDCl3
-0.00
1.98
1.00
0.97
1.04
1.00
1.02
3.13
1.05
f1 (ppm)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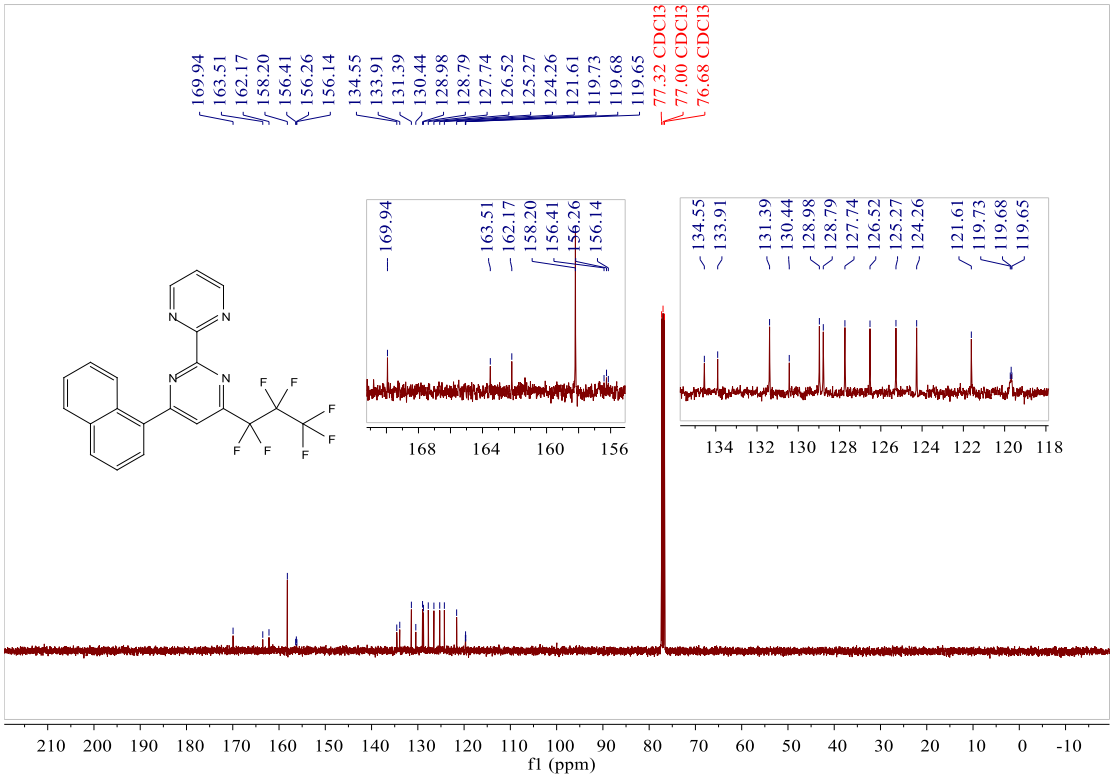
-79.90
-79.93
-116.42
-116.45
-116.48
-116.50
-125.68
f1 (ppm)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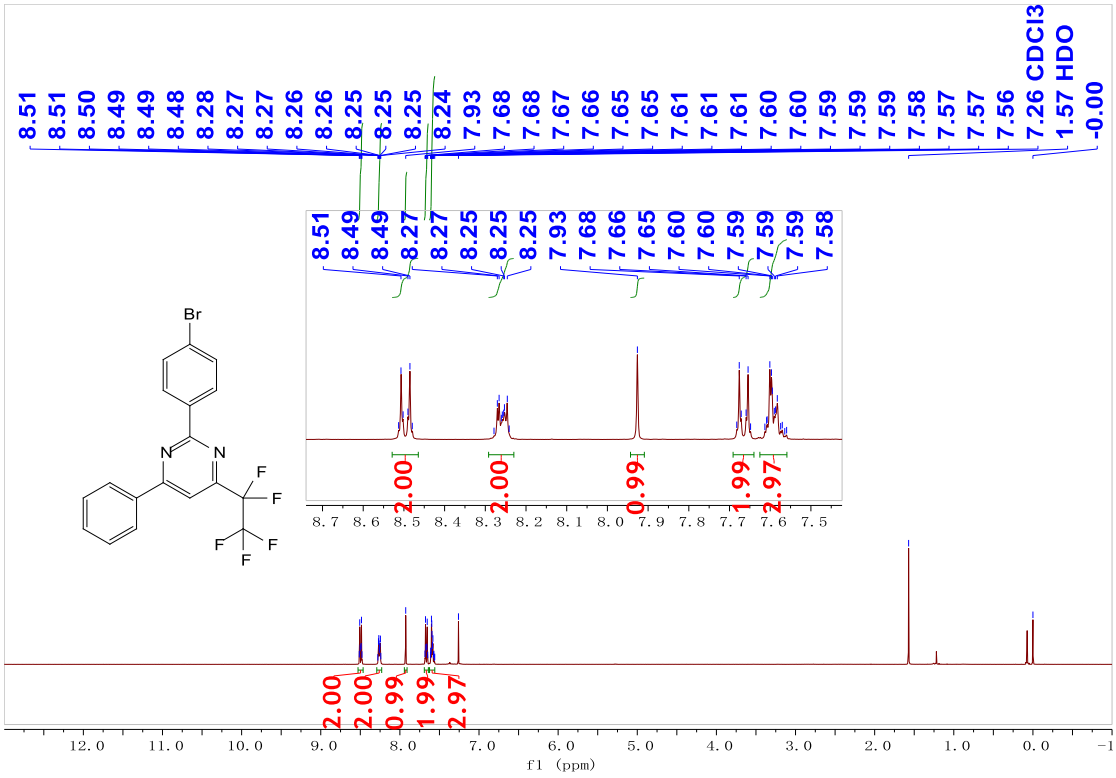
131.39
130.44
128.98
128.79
127.74
126.52
125.27
124.26
121.61
119.73
119.68
119.65
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
f1 (ppm)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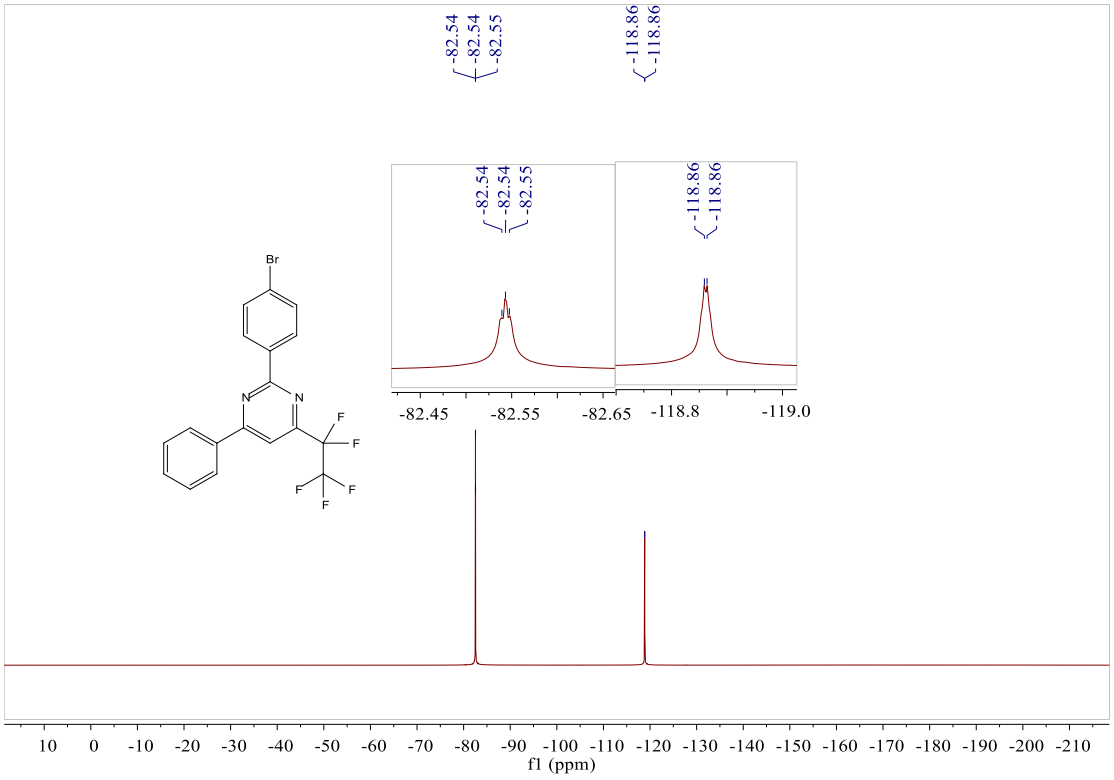
Br
N
N
F
F
F
F
F
2.00 2.00 0.99 1.99 2.97
f1 (ppm)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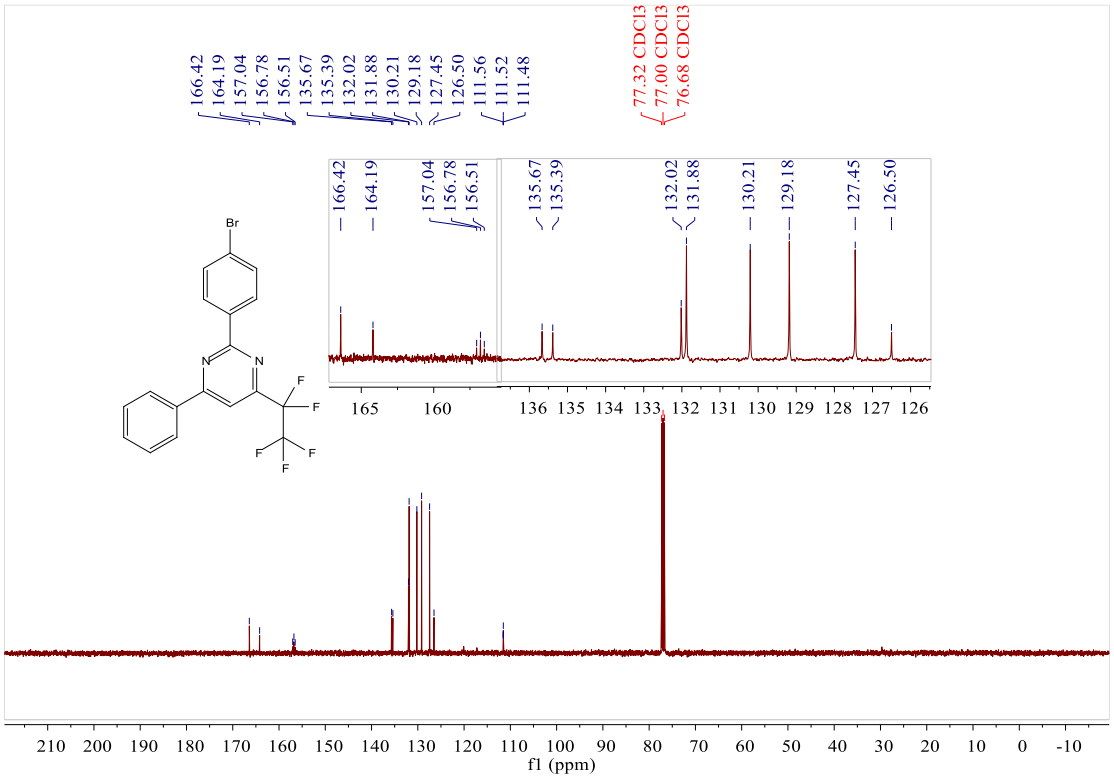
Br
N
N
F
F
F
F
F
-82.45 -82.55 -82.65 -118.8 -119.0
f1 (ppm)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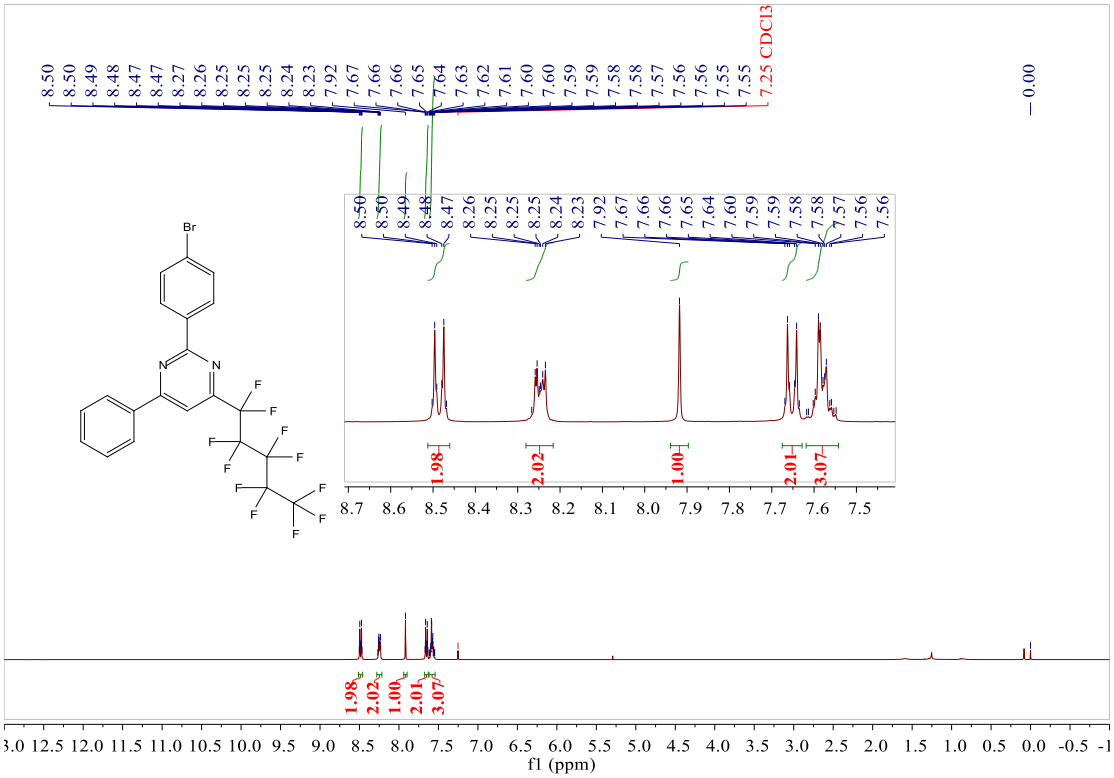
135.39
132.02
131.88
130.21
129.18
127.45
126.50
111.56
111.52
111.48
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
Br
N
N
F
F
F
F
F
165
160
136 135 134 133 132 131 130 129 128 127 126
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.59
7.58
7.58
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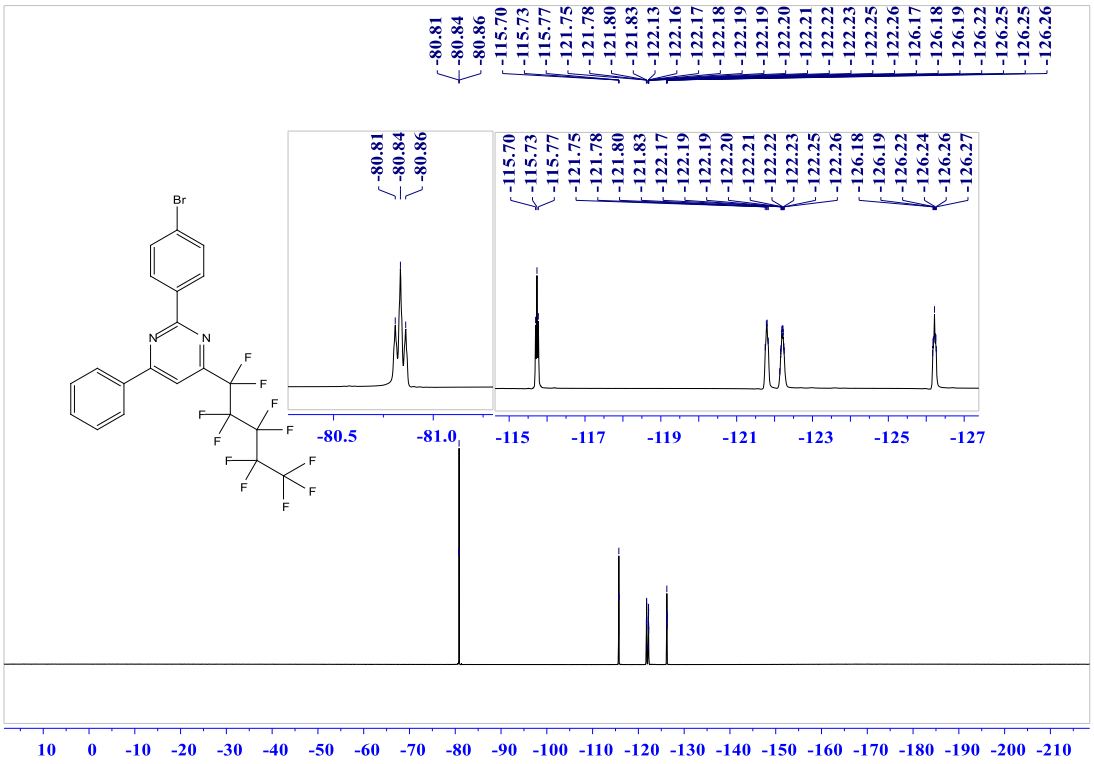
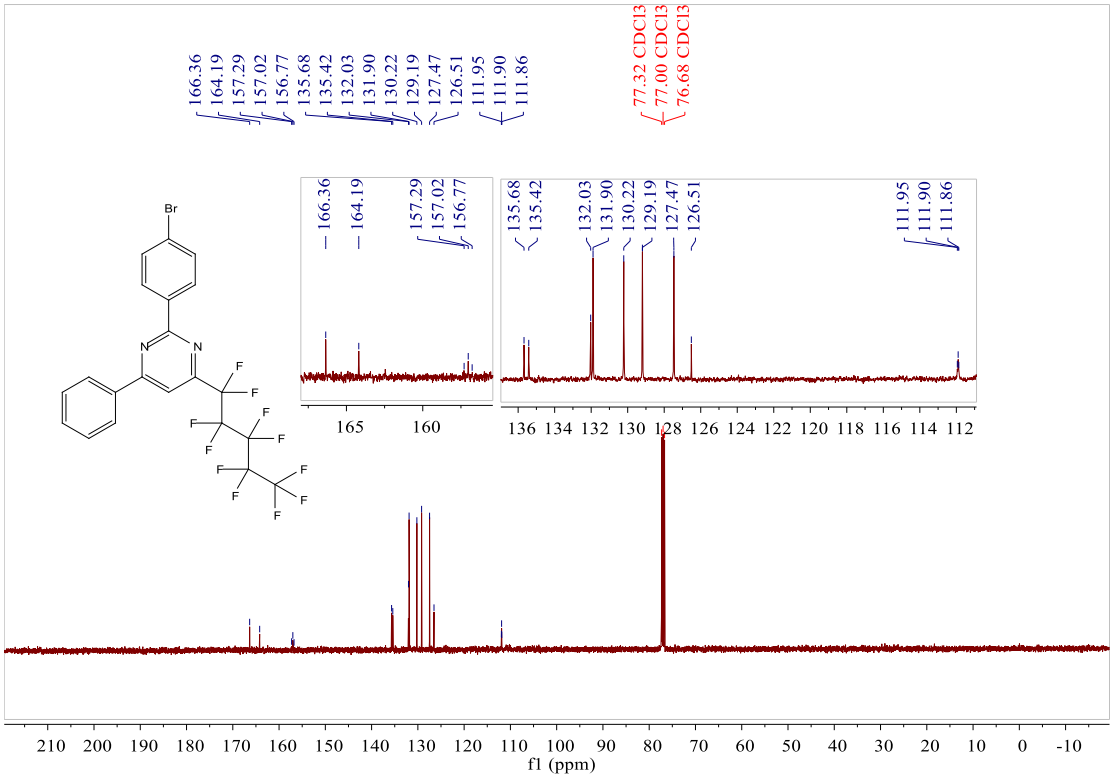
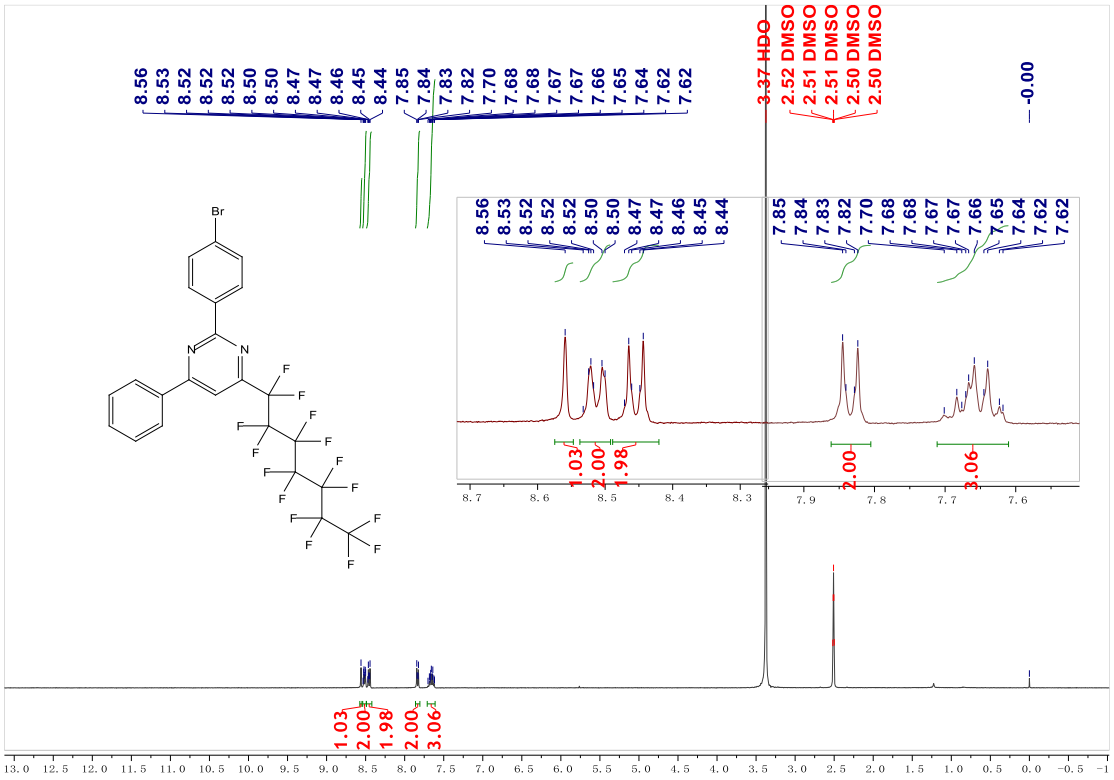
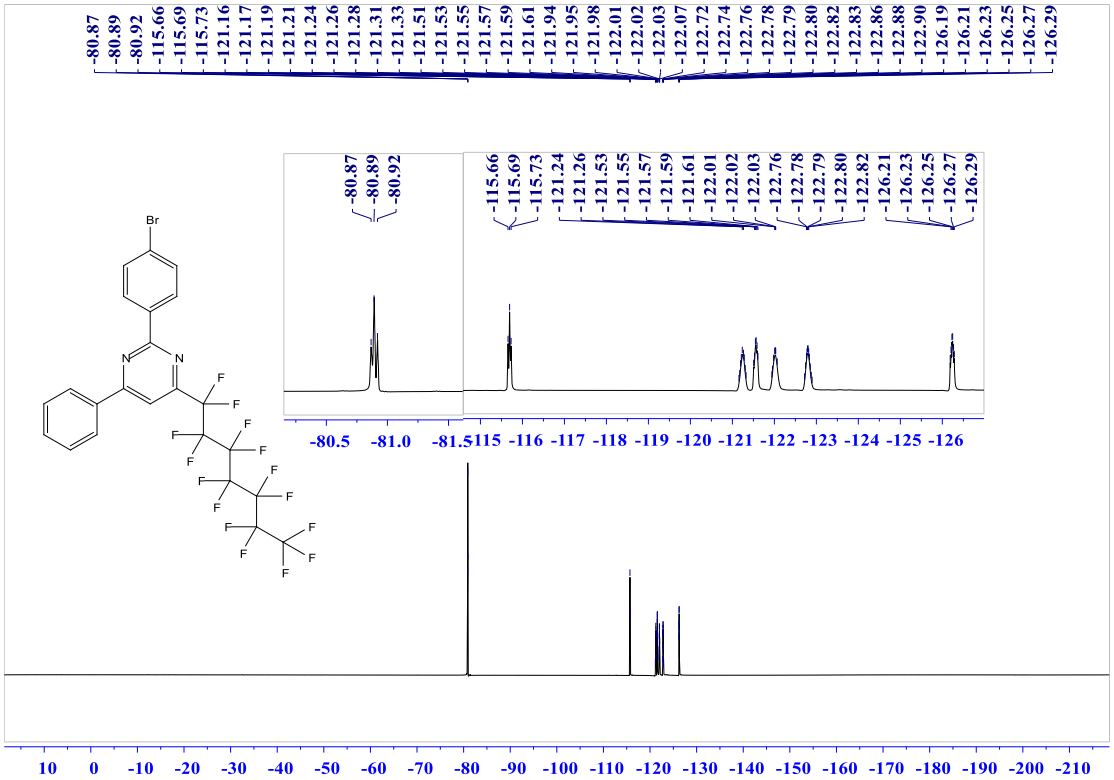
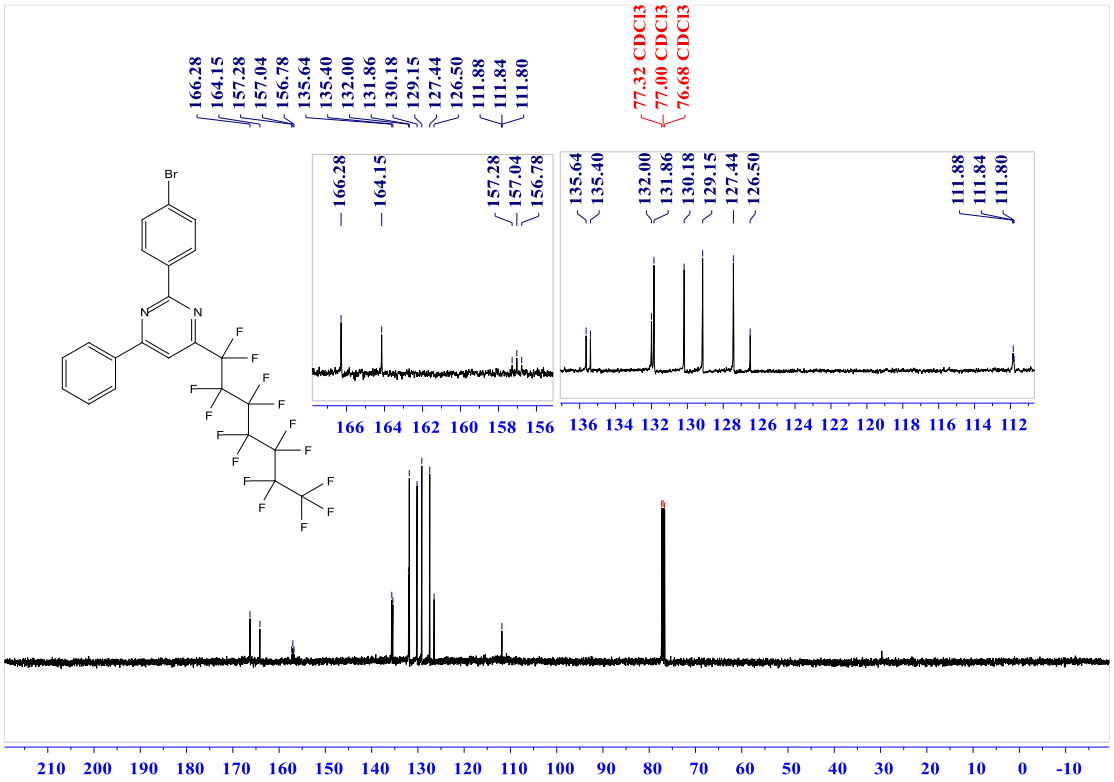
7.56
7.56
7.55
7.25 CDCl3
0.00
Br
N
N
F
F
F
F
F
F
F
F
F
1.98
2.02
1.00
2.01
3.07
8.7 8.6 8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5
3.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


-80.81
-80.84
-80.86
-115.70
-115.73
-115.77
-121.75
-121.78
-121.80
-121.83
-122.13
-122.16
-122.17
-122.18
-122.19
-122.19
-122.20
-122.21
-122.22
-122.23
-122.25
-122.26
-126.17
-126.18
-126.19
-126.22
-126.25
-126.25
-126.26
Br
N
N
F
-80.5
-81.0
-115
-117
-119
-121
-123
-125
-127
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210


166.36
164.19
157.29
157.02
156.77
135.68
135.42
132.03
131.90
130.22
129.19
127.47
126.51
111.95
111.90
111.86
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
Br
N
N
F
165
160
136 134 132 130 128 126 124 122 120 118 116 114 112
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.56 8.53 8.52 8.52 8.52 8.50 8.50 8.47 8.47 8.46 8.45 8.44 7.85 7.84 7.83 7.82 7.70 7.68 7.68 7.67 7.67 7.66 7.65 7.64 7.62 7.62
3.37 HDO
2.52 DMSO
2.51 DMSO
2.51 DMSO
2.50 DMSO
2.50 DMSO
-0.00
Br
1.03 2.00 1.98 2.00 3.06


-80.87 -80.89 -80.92 -115.66 -115.69 -115.73 -121.16 -121.17 -121.19 -121.21 -121.24 -121.26 -121.28 -121.31 -121.33 -121.51 -121.53 -121.55 -121.57 -121.59 -121.61 -121.94 -121.95 -121.98 -122.01 -122.02 -122.03 -122.07 -122.72 -122.74 -122.76 -122.78 -122.79 -122.80 -122.82 -122.83 -122.86 -122.88 -122.90 -126.19 -126.21 -126.23 -126.25 -126.27 -126.29
Br


166.28
164.15
157.28
157.04
156.78
135.64
135.40
132.00
131.86
130.18
129.15
127.44
126.50
111.88
111.84
111.80
77.32 CDCl3
77.00 CDCl3
76.68 CDCl3
Br
N
N
F
166 164 162 160 158 156
136 134 132 130 128 126 124 122 120 118 116 114 112
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10