Electronic Supplementary Material (ESI) for Green Chemistry.

Supporting Information

Amide-Assisted Radical Strategy: Metal-free Direct Fluorination of Arenes in Aqueous Media

Deqiang Liang,*[,a,b] Yanni Li,[a] Shulin Gao,*[,a] Renlun Li,[a] Xiangguang Li,[a] Baoling Wang,[a] and Hai Yang[b]

[a]Department of Chemistry, Kunming University, Kunming 650214, China

[b]Key Laboratory of Yunnan Provincial Higher Education Institutions for Organic Optoelectronic Materials and Devices, Kunming University, Kunming 650214, China

E-mail: liangdq695@nenu.edu.cn (D. Liang); shulin.gao@yahoo.com (S. Gao)

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I. General information

Unless stated otherwise, chemicals were all purchased from commercial sources and used without treatment. Reactions were monitored by Thin Layer Chromatography (TLC) using silica gel F254 plates. Products were purified by column chromatography over 300-400 mesh silica gel under a positive pressure of air. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra were recorded at 25 °C on a Bruker Ascend^{TM} 400 spectrometer using TMS as internal standard. Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad), coupling constant (Hz), integration. High-resolution mass spectra (HRMS) were obtained using a Bruker microTOF II Focus spectrometer (ESI). Gas chromatography-mass spectrometry (GC-MS) analyses were performed on an Agilent 7890A gas chromatograph interfaced to a 5975C mass selective detector in electron impact ionization mode. *N*-(*p*-Tolyl)cinnamamide **1k** was prepared from *p*-toluidine and cinnamic acid, [1] and other anilides **1** were synthesized from anilines and acid chlorides.[2]

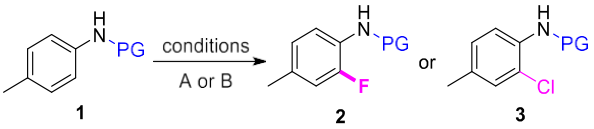
[1] Liang, D.; Li, X.; Lan, Q.; Huang, W.; Yuan, L.; Ma, Y. *Tetrahedron Lett.* **2016**, *57*, 2207–2210.

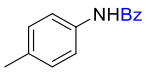
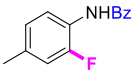
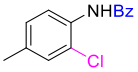
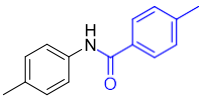
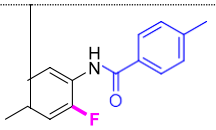
[2] (a) Sadig, J. E. R.; Foster, R.; Wakenhut, F.; Willis, M. C. *J. Org. Chem.* **2012**, *77*, 9473−9486. (b) Barbero, N.; Carril, M.; SanMartin, R.; Domínguez, E. *Tetrahedron* **2007**, *63*, 10425–10432.

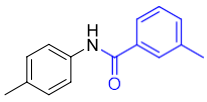
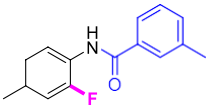
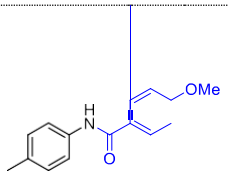
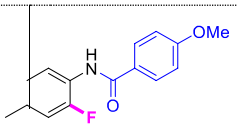
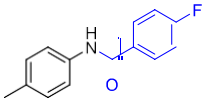
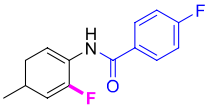
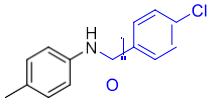
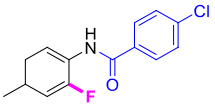
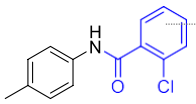
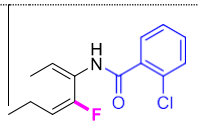
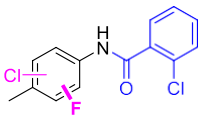
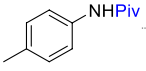
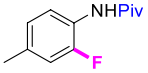
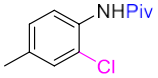
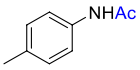
II. Detailed experimental data

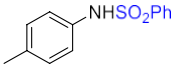
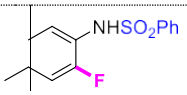
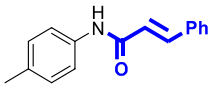
Though fluorination reactions of these anilides **1a-k** all proceeded smoothly under conditions A, disappointingly, desired chlorination reactions were challenging to effect with most substrates, the use of which delivered only poor yields of fluorinated products rather than chlorinated ones. Only *N*-(*p*-tolyl)benzamide **1a** (entry 1) and *N*-(*p*-tolyl)pivalamide **1h** (entry 8) reacted with Selectfluor under conditions B to afford the corresponding chlorides **3a,h** in 77% and 73% yields, respectively. In the case concerns 2-chloro-*N*-(*p*-tolyl)benzamide **1g**, stranger still, besides fluoride **2g** (18% yield), an inseparable dihalide **2g'** that was both fluorinated and chlorinated, was formed in 22% yield (entry 7, during substrate recovery, the dihalide **2g'** which possesses similar polarity to the substrate **1g** and was isolated together with **1g**. We were unable to purify **2g'** further, but it was identified by GC-MS and ^{19}F NMR analyses of the crude mixture. The yield was determined by ^{1}H NMR of this mixture.). In other cases, chloroanilide products were not detected or were present in only trace amounts, demonstrated by GC-MS and/or TLC analyses of the crude reaction mixtures. These are confusing, and we could not explain them at this stage.

Table S1. Scope of the *N*-protecting group[a,b]



	substrates	conditions (time)	products
1	 **1a**	A (9 h)	 **2a**, 83% (**3a**, trace)
		B (6 h)	 **3a**, 77% (**2a**, 7%)
2	 **1b**	A (9 h)	 **2b**, 85%[c,d]
		B (24 h)	**2b**, 21%[c-e]

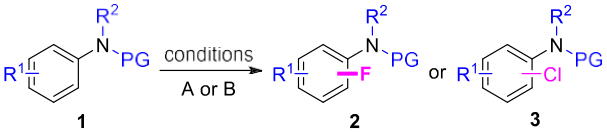
3		A (9 h)	 **2c**, 86%[c]
	1c	B (24 h)	**2c**, 17%[c,e]
4		A (9 h)	 **2d**, 82%[c]
	1d	B (24 h)	**2d**, 43%[c,e]
5		A (12 h)	 **2e**, 88%[c]
	1e	B (24 h)	**2e**, 21%[c,e]
6		A (24 h)	 **2f**, 81%[c]
	1f	B (24 h)	**2f**, 12%[c,e]
7		A (24 h)	 **2g**, 71%[c]
			2g, 18%[c,e]
	1g	B (24 h)	 **2g'**, 22%[f]
8		A (18 h)	 **2 ı**, 77% (**3h**, 0%)
	1h	B (9 h)	 **3 ı**, 73% (**2h**, 9%)
9		A (12 h)	 **2i**, 73%[c,g]
	1i	B (24 h)	**2i**, 18%[c-e]

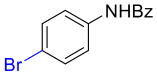
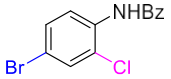
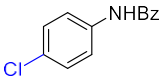
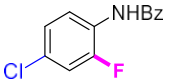
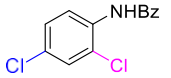
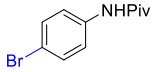
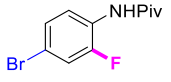
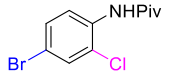
10		A (24 h)	
			2j, 77%[h]
	1j	B (24 h)	**2j**, 12%[e,h]
11		A (3 h)	
			2k, 86%[h]
	1k	B (24 h)	**2k**, 18%[e,h]

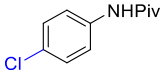
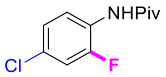
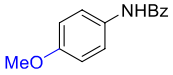
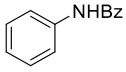
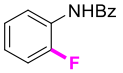
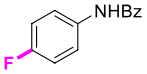
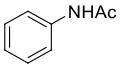
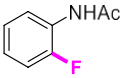
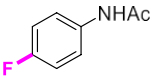
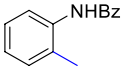
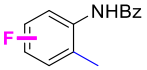
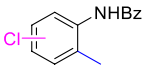
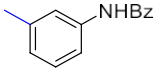
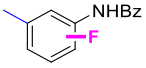
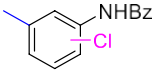
[a]Conditions A: **1** (1.0 mmol), Selectfluor (3.0 mmol), $MeNO_2$ (2.0 mL), H_2O (2.0 mL), 50 °C; Conditions B: **1** (1.0 mmol), Selectfluor (1.2 mmol), $MeNO_2$ (4.0 mL), 50 °C。 [b]Isolated yields. [c]No other noticeable product was observed by TLC. [d]Only minute quantities of chlorinated products were observed by GC-MS analysis of the crude reaction mixture. [e]Most of the substrate was recovered. [f]NMR yield, see reference 35. [g]No chlorinated product was detected by GC-MS analysis of the crude reaction mixture. [h]Trace amounts of other products were observed by TLC, which were not subjected to further analysis.

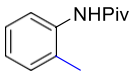
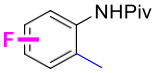
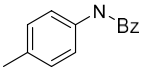
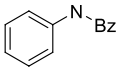
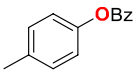
Ortho-chlorinations of **1l,m** under conditions B needed to be conducted at an elevated temperature of 90 °C, affording dihalide **3l,m** in high yields (entries 1 and 2). The use of *N*-(*o*-tolyl)benzamide **1s** also furnished chlorinated products in 71% yield (entry 8). With other substrates, however, chlorination reactions were again difficult to effect, affording corresponding chloroanilides in only very poor yields. Clearly, aryl substitution patterns of *N*-PGs and *N*-aryl groups both exert significant effect on the chlorination. Interestingly, the use of *N*-(4-bromophenyl)pivalamide **1n** (entry 3), *N*-(4-chlorophenyl)pivalamide **1o** (entry 4), *N*-phenylbenzamide **1q** (entry 6), or *N*-phenylacetamide **1r** (entry 7) all gave fluorinated products as major products under conditions both A and B, and in the cases concern **1n** or **1r**, reactions performed under conditons B even provided higher yields.

Table S2. Scope of the *N*-aryl group[a,b]



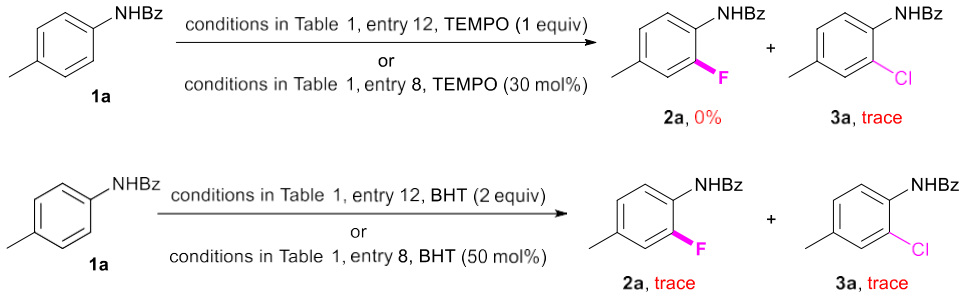
substrates	conditions (time)	products
1  **1l**	A (24 h)	 **2l**, 48% (**3l**, trace)
	B (24 h)[c]	 **3l**, 65% (**2l**, 13%)
2  **1m**	A (24 h)	 **2m**, 51% (**3m**, 6%)
	B (24 h)[c]	 **3m**, 73% (**2m**, 7%)
3  **1n**	A (24 h)	**2n**, 66% (**3n**, 12%)
	B (24 h)	 **2n**, 75%  **3n**, trace

4	 **1o**	A (24 h)	 **2o**, 50%[f]
		B (24 h)	**2o**, 44%[f]
5	 **1p**	A (6 h)[d]	complex
		B (10 h)[e]	
6	 **1q**	A (24 h)[g]	 **2q**, 77%  **2q'**, 9%
		B (24 h)[g]	**2q**, 69% **2q'**, 16%
7	 **1r**	A (24 h)[g]	**2r**, 46% **2r'**, 26%
		B (24 h)[g]	 **2r**, 20%  **2r'**, 58%
8	 **1s**	A (24 h)	 **2s** and **2s'**, 30%[h] **3s** and **3s'**, 34%[h]
		B (24 h)	**2s** and **2s'**, 8%[h]  **3s** and **3s'**, 71%[h]
9	 **1t**	A (24 h)	 **2t** and **2t'**, 43%[h] **3t**, **3t'** and **3t''**, 11%[h]
		B (24 h)	**2t** and **2t'**, 29%[h] 

			3t and **3t'**, 22%[h]
10	 **1u**	A (12 h)	 **2u** and **2u'**,[i] 61%
		B (24 h)	nr
11	 **1v**	A or B (24 h)[j]	nr
12	 **1w**	A or B (24 h)[j]	nr
13	 **4**	A or B (24 h)[j]	nr

[a]Conditions A: **1** (1.0 mmol), Selectfluor (3.0 mmol), $MeNO_2$ (2.0 mL), H_2O (2.0 mL), 50 °C; Conditions B: **1** (1.0 mmol), Selectfluor (1.2 mmol), $MeNO_2$ (4.0 mL), 50 °C。 [b]Isolated yields. [c]The reaction was run at 90 °C. [d]The reaction was run at room temperature. [e]No reaction occurred at room temperature after 24 h. [f]Trace amounts of other products were observed by TLC, and GC-MS analysis of the crude reaction mixture suggested that minute quantities of chloroanilide were generated. [g]Trace amounts of other products were observed by TLC, but were not subjected to further analysis. [h]Total GC yield of regioisomers. In this case, an inseparable complex mixture was yielded. [i]The two regioisomers possess similar polarities and were separated together. The resultant mixture was then subjected to GC-MS and ^{19}F NMR analyses. [j]The reaction was run at 130 °C.

III. Experiments of radical inhibition



Scheme S1. TEMPO and BHT experiments

It is true that Selectfluor might be consumed by TEMPO according to literature, we still take leave to argue that the radical nature of our reactions still could be probed by TEMPO, because in our studies **excess (3 equiv) Selectfluor was used but only 1 equiv of TEMPO was added. Even 1 equiv of Selectfluor was consumed, 2 equiv were left, and as shown in entry 7, Table 1, *the use of 2 equiv of Selectfluor should give fluorinated product in high yields*. But the fluorination was completely suppressed**. So, it is possible that *the suppression was the result of radical inhibition by TEMPO*.

On the other hand, recently there are also many reports that TEMPO does not consume Selectfluor under various conditions. For example, ***K. Sun and G. Zhang reported that TEMPO does NOT consume Selectfluor in $MeNO_2$*** (*ACS Catal.*, 2015, **5**, 7194). Last year, ***we also demonstrated that TEMPO does NOT consume Selectfluor in water*** (*Tetrahedron Lett.*, 2016, **57**, 5390, and LC-MS indicated that Selectfluor were mainly distributed in water). Our fluorination was run in $MeNO_2/H_2O$. So, the support for radical nature of our fluorination by TEMPO experiment might still be valid.

With respect to the BHT experiments, situations are similar. Selectfluor was excess, but the reactions were almost completely suppressed.

IV. General procedures

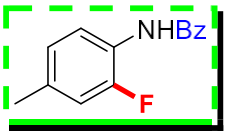
General procedure under conditions A (taking the fluorination of 1a as an example):

A 25-mL flask, equipped with a magnetic stirring bar and a reflux condenser, was charged with *N*-(*p*-tolyl)benzamide **1a** (211 mg, 1 mmol) and Selectfluor (1063 mg, 3 mmol), followed by addition of $MeNO_2$ (2.0 mL) and water (2.0 mL). The mixture was stirred at 50 °C for 9 h. After **1a** was consumed as indicated by TLC, the reaction mixture was quenched with saturated aqueous $Na_2S_2O_3$ (5.0 mL) and water (20.0 mL), and extracted with CH_2Cl_2 (10.0 mL) three times. The residue obtained after evaporation of the solvent was purified by column chromatography on silica gel (petroleum ether–ethyl acetate = 15:1, v/v) to afford *N*-(2-fluoro-4-methylphenyl)benzamide **2a** as a pale yellow solid (202 mg, 88% yield).

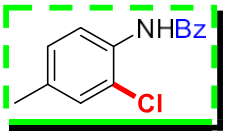
General procedure under conditions B (taking the chlorination of 1a as an example):

A 25-mL flask, equipped with a magnetic stirring bar and a reflux condenser, was charged with *N*-(*p*-tolyl)benzamide **1a** (211 mg, 1 mmol) and Selectfluor (425 mg, 1.2 mmol), followed by addition of $MeNO_2$ (4.0 mL). The mixture was stirred at 50 °C for 6 h. After **1a** was consumed as indicated by TLC, the reaction mixture was quenched with saturated aqueous $Na_2S_2O_3$ (5.0 mL) and water (20.0 mL), and extracted with CH_2Cl_2 (10.0 mL) three times. The residue obtained after evaporation of the solvent was purified by column chromatography on silica gel (petroleum ether–ethyl acetate = 15:1, v/v) to afford *N*-(2-chloro-4-methylphenyl)benzamide **3a** as a white solid (201 mg, 82% yield).

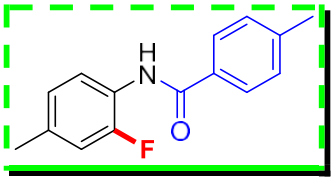
V. Spectral data of products



2a, *N*-(2-fluoro-4-methylphenyl)benzamide, pale yellow solid: mp 148-149 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.34 (s, 3H), 6.94-7.00 (m, 2H), 7.50 (dddd, *J* = 1.4, 1.6, 7.0, 7.6 Hz, 2H), 7.57 (dddd, *J* = 1.4, 1.4, 7.3, 7.3 Hz, 1H), 7.87-7.90 (m, 2H), 7.98 (brs, 1H), 8.30 (dd, *J* = 8.4, 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.36, 152.65 (d, $^{1}J_{(C–F)}$ = 241.0 Hz), 135.01 (d, $^{3}J_{(C–F)}$ = 7.3 Hz), 134.67, 132.04, 128.87, 127.07, 125.12 (d, $^{3}J_{(C–F)}$ = 3.2 Hz), 123.76 (d, $^{2}J_{(C–F)}$ = 10.1 Hz), 121.68 (d, $^{4}J_{(C–F)}$ = 1.1 Hz), 115.39 (d, $^{2}J_{(C–F)}$ = 18.8 Hz), 20.94 (d, $^{4}J_{(C–F)}$ = 1.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.82 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{14}H_{13}FNO^{+}$ ($[M+H]^{+}$) 230.0976. Found 230.0983.

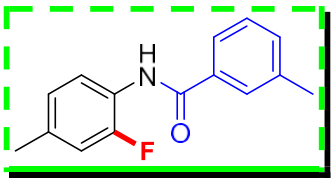


3a,[2] *N*-(2-chloro-4-methylphenyl)benzamide, white solid: mp 141-142 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.32 (s, 3H), 7.11-7.13 (m, 1H), 7.22 (d, *J* = 1.2 Hz, 1H), 7.50 (dddd, *J* = 1.4, 1.7, 7.0, 7.6 Hz, 2H), 7.57 (dddd, *J* = 1.4, 1.4, 7.3, 7.3 Hz, 1H), 7.89-7.92 (m, 2H), 8.36 (brs, 1H), 8.40 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.19, 134.91, 134.73, 132.17, 132.08, 129.35, 128.92, 128.49, 127.08, 122.96, 121.49, 20.70; HRMS (ESI-TOF) Calcd for $C_{14}H_{13}ClNO^{+}$ ($[M+H]^{+}$) 246.0680. Found 246.0696.

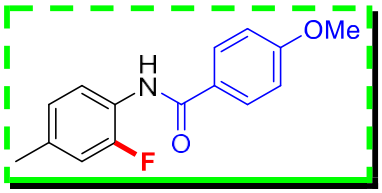


2b, *N*-(2-fluoro-4-methylphenyl)-4-methylbenzamide, white solid: mp 162-163 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.33 (s, 3H), 2.42 (s, 3H), 6.92-6.99 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.78 (ddd, *J* = 1.7, 1.7, 8.2 Hz, 2H), 7.97 (brs, 1H), 8.30 (dd, *J* = 8.4, 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.31, 153.62 (d, $^{1}J_{(C–F)}$ = 240.9 Hz), 142.60, 134.81 (d, $^{3}J_{(C–F)}$ = 7.3 Hz), 131.79, 129.51, 127.09, 125.09 (d, $^{3}J_{(C–F)}$ = 3.2 Hz), 123.87 (d, $^{2}J_{(C–F)}$ = 10.1 Hz), 121.66, 115.35 (d, $^{2}J_{(C–F)}$ = 18.8 Hz), 21.54, 20.94

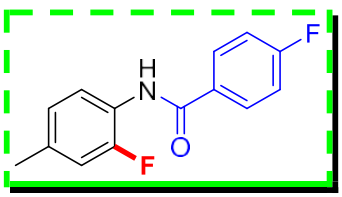
(d, $^{4}J_{(C–F)}$ = 1.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.90 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{15}H_{15}FNO^{+}$ ([M+H]$^{+}$) 244.1132. Found 244.1129.



2c, *N*-(2-fluoro-4-methylphenyl)-3-methylbenzamide, white solid: mp 126-127 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.34 (s, 3H), 2.44 (s, 3H), 6.94-7.00 (m, 2H), 7.36-7.41 (m, 2H), 7.65-7.67 (m, 1H), 7.69-7.71 (m, 1H), 7.97 (brs, 1H), 8.30 (dd, *J* = 8.4, 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.56, 152.60 (d, $^{1}J_{(C–F)}$ = 241.1 Hz), 138.80, 134.90 (d, $^{3}J_{(C–F)}$ = 7.4 Hz), 134.65, 132.78, 128.72, 127.80, 125.10 (d, $^{3}J_{(C–F)}$ = 3.2 Hz), 124.01, 123.81 (d, $^{2}J_{(C–F)}$ = 10.2 Hz), 121.64 (d, $^{4}J_{(C–F)}$ = 1.1 Hz), 115.36 (d, $^{2}J_{(C–F)}$ = 18.8 Hz), 21.42, 20.94 (d, $^{4}J_{(C–F)}$ = 1.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.87 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{15}H_{15}FNO^{+}$ ([M+H]$^{+}$) 244.1132. Found 244.1114.

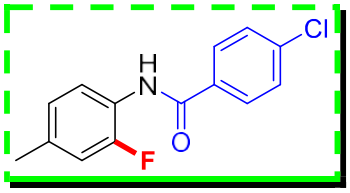


2d, *N*-(2-fluoro-4-methylphenyl)-4-methoxybenzamide, white solid: mp 134-135 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.34 (s, 3H), 3.88 (s, 3H), 6.93-7.00 (m, 4H), 7.84 (dd, *J* = 2.9, 2.1 Hz, 1H), 7.87 (dd, *J* = 2.1, 2.9 Hz, 1H), 7.91 (brs, 1H), 8.29 (dd, *J* = 8.4, 8.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.86, 162.63, 152.59 (d, $^{1}J_{(C–F)}$ = 240.9 Hz), 134.68 (d, $^{3}J_{(C–F)}$ = 7.3 Hz), 128.97, 126.85, 125.09 (d, $^{3}J_{(C–F)}$ = 3.1 Hz), 123.95 (d, $^{2}J_{(C–F)}$ = 10.1 Hz), 121.61 (d, $^{4}J_{(C–F)}$ = 1.2 Hz), 115.33 (d, $^{2}J_{(C–F)}$ = 18.9 Hz), 114.04, 55.50, 20.93 (d, $^{4}J_{(C–F)}$ = 1.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -132.05 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{15}H_{15}FNO_2^{+}$ ([M+H]$^{+}$) 260.1081. Found 260.1084.

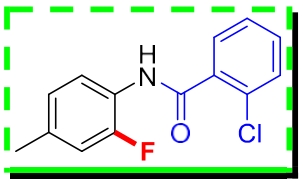


2e, 4-fluoro-*N*-(2-fluoro-4-methylphenyl)benzamide, white solid: mp 128-129 °C. ^{1}H

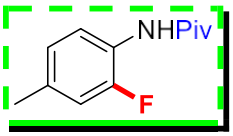
NMR (400 MHz, $CDCl_3$) δ = 2.34 (s, 3H), 6.94-7.00 (m, 2H), 7.15-7.21 (m, 2H), 7.88-7.93 (m, 3H), 8.26 (dd, J = 8.4, 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.03 (d, $^1J_{(C–F)}$ = 251.5 Hz), 164.28, 152.66 (d, $^1J_{(C–F)}$ = 241.3 Hz), 135.20 (d, $^3J_{(C–F)}$ = 7.4 Hz), 130.80 (d, $^4J_{(C–F)}$ = 3.2 Hz), 129.48 (d, $^3J_{(C–F)}$ = 9.0 Hz), 125.14 (d, $^3J_{(C–F)}$ = 3.2 Hz), 123.57 (d, $^2J_{(C–F)}$ = 10.1 Hz), 121.72 (d, $^4J_{(C–F)}$ = 0.9 Hz), 115.96 (d, $^2J_{(C–F)}$ = 21.9 Hz), 115.42 (d, $^2J_{(C–F)}$ = 18.8 Hz), 20.95 (d, $^4J_{(C–F)}$ = 1.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -107.10 (m, 1F), -131.72 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{14}H_{12}F_2NO^+$ ($[M+H]^+$) 248.0881. Found 248.0906.



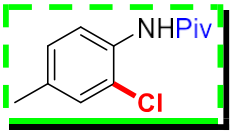
2f, 4-chloro-*N*-(2-fluoro-4-methylphenyl)benzamide, white solid: mp 149-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.34 (s, 3H), 6.94-7.00 (m, 2H), 7.47 (dd, J = 2.4, 2.0 Hz, 1H), 7.49 (dd, J = 2.0, 2.4 Hz, 1H), 7.82 (dd, J = 2.4, 2.0 Hz, 1H), 7.84 (dd, J = 2.0, 2.4 Hz, 1H), 7.92 (brs, 1H), 8.26 (dd, J = 8.4, 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.27, 152.64 (d, $^1J_{(C–F)}$ = 241.3 Hz), 138.37, 135.31 (d, $^3J_{(C–F)}$ = 7.4 Hz), 132.98, 129.14, 128.51, 125.16 (d, $^3J_{(C–F)}$ = 3.2 Hz), 123.49 (d, $^2J_{(C–F)}$ = 10.1 Hz), 121.71 (d, $^4J_{(C–F)}$ = 0.5 Hz), 115.44 (d, $^2J_{(C–F)}$ = 18.7 Hz), 20.96 (d, $^4J_{(C–F)}$ = 1.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.69 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{14}H_{12}ClFNO^+$ ($[M+H]^+$) 264.0586. Found 264.0590.



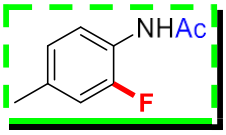
2g, 2-chloro-*N*-(2-fluoro-4-methylphenyl)benzamide, white solid: mp 118-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.35 (s, 3H), 6.94-7.01 (m, 2H), 7.37-7.48 (m, 3H), 7.80 (dd, J = 2.0, 7.6 Hz, 1H), 8.14 (brs, 1H), 8.32 (dd, J = 8.3, 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.15, 152.62 (d, $^1J_{(C–F)}$ = 242.2 Hz), 135.40 (d, $^3J_{(C–F)}$ = 7.4 Hz), 134.74, 131.91, 130.75, 130.59, 130.53, 127.33, 125.10 (d, $^3J_{(C–F)}$ = 3.1 Hz), 123.37 (d, $^2J_{(C–F)}$ = 10.3 Hz), 121.77 (d, $^4J_{(C–F)}$ = 0.8 Hz), 115.46 (d, $^2J_{(C–F)}$ = 18.7 Hz), 20.97 (d, $^4J_{(C–F)}$ = 1.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.23 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{14}H_{12}ClFNO^+$ ($[M+H]^+$) 264.0586. Found 264.0588.



2h,[3] *N*-(2-fluoro-4-methylphenyl)pivalamide, pale brown solid: mp 91-92 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.32 (s, 9H), 2.31 (s, 3H), 6.88-6.93 (m, 2H), 7.53 (brs, 1H), 8.17 (dd, J = 8.2, 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 176.52, 153.51 (d, $^{1}J_{(C–F)}$ = 240.5 Hz), 134.47 (d, $^{3}J_{(C–F)}$ = 7.4 Hz), 124.96 (d, $^{3}J_{(C–F)}$ = 3.2 Hz), 123.84 (d, $^{2}J_{(C–F)}$ = 10.0 Hz), 121.53 (d, $^{4}J_{(C–F)}$ = 1.4 Hz), 115.17 (d, $^{2}J_{(C–F)}$ = 18.9 Hz), 39.89, 27.59, 20.86 (d, $^{4}J_{(C–F)}$ = 1.5 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -132.59 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{12}H_{17}FNO^{+}$ ($[M+H]^{+}$) 210.1289. Found 210.1285.



3h,[4] *N*-(2-chloro-4-methylphenyl)pivalamide, pale yellow solid: mp 100-101 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.34 (s, 9H), 2.29 (s, 3H), 7.06-7.08 (m, 1H), 7.18 (d, J = 1.2 Hz, 1H), 7.92 (brs, 1H), 8.25 (d, J = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 176.53, 134.43, 132.19, 129.16, 128.34, 122.77, 121.32, 40.10, 27.60, 20.63; HRMS (ESI-TOF) Calcd for $C_{12}H_{17}ClNO^{+}$ ($[M+H]^{+}$) 226.0993. Found 226.0994.



2i,[5] *N*-(2-fluoro-4-methylphenyl)acetamide, white solid: mp 127-128 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.20 (s, 3H), 2.31 (s, 3H), 6.88-6.93 (m, 2H), 7.28 (brs, 1H), 8.11 (dd, J = 8.4, 8.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 168.15, 152.28 (d, $^{1}J_{(C–F)}$ = 241.0 Hz), 134.76 (d, $^{3}J_{(C–F)}$ = 7.4 Hz), 124.98 (d, $^{3}J_{(C–F)}$ = 3.1 Hz), 123.57 (d, $^{2}J_{(C–F)}$ = 10.4 Hz), 121.74, 115.29 (d, $^{2}J_{(C–F)}$ = 18.9 Hz), 24.59, 20.87 (d, $^{4}J_{(C–F)}$ = 1.2 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ = -131.94 (m, 1F); HRMS (ESI-TOF) Calcd for $C_9H_{11}FNO^{+}$ ($[M+H]^{+}$) 168.0819. Found 168.0813.

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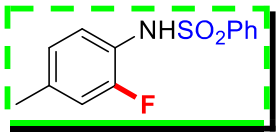
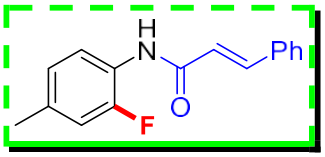
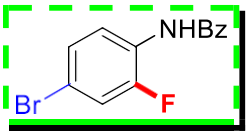


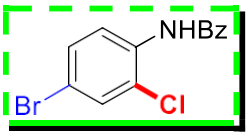
2j, *N*-(2-fluoro-4-methylphenyl)benzenesulfonamide, white solid: mp 110-111 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.27 (s, 3H), 6.67 (brs, 1H), 6.75 (dd, J = 0.8, 11.1 Hz, 1H), 6.90 (d, J = 8.2 Hz, 1H), 7.41-7.47 (m, 3H), 7.54 (dd, J = 7.5, 7.4 Hz, 1H), 7.74-7.76 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 154.31 (d, $^{1}J_{(C–F)}$ = 243.3 Hz), 138.85, 137.40 (d, $^{3}J_{(C–F)}$ = 7.2 Hz), 133.16, 129.01, 127.18, 125.35 (d, $^{3}J_{(C–F)}$ = 3.4 Hz), 124.24, 121.44 (d, $^{2}J_{(C–F)}$ = 12.7 Hz), 115.95 (d, $^{2}J_{(C–F)}$ = 19.1 Hz), 20.95 (d, $^{4}J_{(C–F)}$ = 1.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -129.86 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{13}H_{13}FNO_2S^+$ ([M+H]$^+$) 266.0646. Found 266.0660.



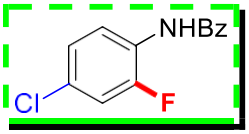
2k, *N*-(2-fluoro-4-methylphenyl)cinnamamide, white solid: mp 82-83 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.31 (s, 3H), 6.58 (d, J = 15.5 Hz, 1H), 6.90-6.95 (m, 2H), 7.35-7.41 (m, 3H), 7.51-7.54 (m, 3H), 7.75 (d, J = 15.5 Hz, 1H), 8.29 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.82, 152.41 (d, $^{1}J_{(C–F)}$ = 241.5 Hz), 142.67, 134.87 (d, $^{3}J_{(C–F)}$ = 7.0 Hz), 134.54, 130.05, 128.89, 128.02, 125.08 (d, $^{3}J_{(C–F)}$ = 3.2 Hz), 123.78 (d, $^{2}J_{(C–F)}$ = 10.1 Hz), 121.74, 120.54, 115.33 (d, $^{2}J_{(C–F)}$ = 18.8 Hz), 20.91 (d, $^{4}J_{(C–F)}$ = 1.4 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.65 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{16}H_{15}FNO^+$ ([M+H]$^+$) 256.1132. Found 256.1131.



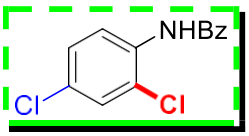
2l, *N*-(4-bromo-2-fluorophenyl)benzamide, white solid: mp 120-121 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.30-7.34 (m, 2H), 7.51 (dddd, J = 1.1, 1.6, 7.1, 7.7 Hz, 2H), 7.59 (dddd, J = 1.3, 1.3, 7.4, 7.4 Hz, 1H), 7.87-7.89 (m, 2H), 8.02 (brs, 1H), 8.40 (dd, J = 8.4, 9.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.39, 152.33 (d, $^{1}J_{(C–F)}$ = 246.0 Hz), 134.19, 132.38, 128.98, 127.91 (d, $^{3}J_{(C–F)}$ = 3.7 Hz), 127.10, 125.86 (d, $^{2}J_{(C–F)}$ = 9.8 Hz), 122.75 (d, $^{4}J_{(C–F)}$ = 1.4 Hz), 118.47 (d, $^{2}J_{(C–F)}$ = 22.3 Hz), 115.96 (d, $^{3}J_{(C–F)}$ = 9.3 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -128.57 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{13}H_{10}BrFNO^+$ ([M+H]$^+$) 293.9924. Found 293.9916.



3l,[6] *N*-(4-bromo-2-chlorophenyl)benzamide, white solid: mp 141-142 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.45 (dd, *J* = 2.2, 8.8 Hz, 1H), 7.52 (dddd, *J* = 1.5, 1.5, 7.1, 7.7 Hz, 2H), 7.57 (d, *J* = 2.3 Hz, 1H), 7.59 (dddd, *J* = 2.1, 2.3, 7.4, 7.3 Hz, 1H), 7.89-7.92 (m, 2H), 8.39 (brs, 1H), 8.49 (d, *J* = 8.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.23, 134.28, 133.99, 132.42, 131.50, 130.99, 129.03, 127.10, 123.71, 122.51, 116.40; HRMS (ESI-TOF) Calcd for $C_{13}H_{10}BrClNO^+$ ($[M+H]^+$) 309.9629. Found 309.9627.



2m,[7] *N*-(4-chloro-2-fluorophenyl)benzamide, white solid: mp 151-152 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.16-7.21 (m, 2H), 7.52 (dddd, *J* = 1.2, 1.6, 7.0, 7.7 Hz, 2H), 7.59 (dddd, *J* = 1.4, 1.3, 7.4, 7.3 Hz, 1H), 7.87-7.90 (m, 2H), 8.01 (brs, 1H), 8.46 (dd, *J* = 8.5, 9.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.40, 152.32 (d, $^{1}J_{(C-F)}$ = 244.9 Hz), 134.21, 132.36, 129.00 (d, $^{3}J_{(C-F)}$ = 9.9 Hz), 128.97, 127.09, 125.36 (d, $^{2}J_{(C-F)}$ = 10.0 Hz), 124.96 (d, $^{3}J_{(C-F)}$ = 3.6 Hz), 122.42 (d, $^{4}J_{(C-F)}$ = 1.7 Hz), 115.69 (d, $^{2}J_{(C-F)}$ = 22.6 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -128.68 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{13}H_{10}ClFNO^+$ ($[M+H]^+$) 250.0429. Found 250.0432.



3m,[8] *N*-(2,4-dichlorophenyl)benzamide, white solid: mp 122-123 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.32 (ddd, *J* = 0.2, 2.4, 8.9 Hz, 1H), 7.44 (d, *J* = 2.4 Hz, 1H), 7.53 (dddd, *J* = 1.3, 1.6, 7.0, 7.7 Hz, 2H), 7.60 (dddd, *J* = 1.4, 1.4, 7.4, 7.3 Hz, 1H),

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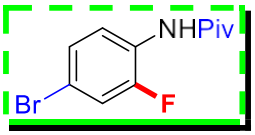
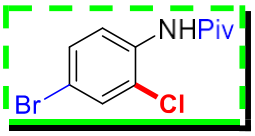
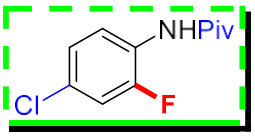
7.90-7.93 (m, 2H), 8.39 (brs, 1H), 8.55 (d, J = 8.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.25, 134.30, 133.53, 132.42, 129.22, 129.04, 128.76, 128.09, 127.10, 123.50, 122.18; HRMS (ESI-TOF) Calcd for $C_{13}H_{10}Cl_2NO^+$ ($[M+H]^+$) 266.0134. Found 266.0135.



2n,[9] *N*-(4-bromo-2-fluorophenyl)pivalamide, white solid: mp 79-80 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.32 (s, 9H), 7.25-7.28 (m, 2H), 7.56 (brs, 1H), 8.27 (dd, J = 8.6, 8.5 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 176.66, 152.20 (d, $^1J_{(C–F)}$ = 245.2 Hz), 127.75 (d, $^3J_{(C–F)}$ = 3.7 Hz), 125.94 (d, $^2J_{(C–F)}$ = 9.7 Hz), 122.60 (d, $^4J_{(C–F)}$ = 1.6 Hz), 118.25 (d, $^2J_{(C–F)}$ = 22.5 Hz), 115.46 (d, $^3J_{(C–F)}$ = 9.3 Hz), 40.05, 27.51; ^{19}F NMR (377 MHz, $CDCl_3$) δ = -129.37 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{11}H_{14}BrFNO^+$ ($[M+H]^+$) 274.0237. Found 274.0252.



3n, *N*-(4-bromo-2-chlorophenyl)pivalamide, white semisolid. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.35 (s, 9H), 7.43 (dd, J = 2.2, 8.9 Hz, 1H), 7.68 (d, J = 2.2 Hz, 1H), 7.96 (brs, 1H), 8.32 (d, J = 8.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 175.67, 134.06, 133.20, 130.38, 121.51, 115.28, 112.89, 39.24, 26.51; HRMS (ESI-TOF) Calcd for $C_{11}H_{14}BrClNO^+$ ($[M+H]^+$) 289.9942. Found 289.9940.



2o,[10] *N*-(4-chloro-2-fluorophenyl)pivalamide, white solid: mp 81-82 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 1.33 (s, 9H), 7.10-7.14 (m, 2H), 7.56 (brs, 1H), 8.31 (dd, J = 8.8, 8.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 176.66, 152.22 (d, $^1J_{(C–F)}$ = 244.3 Hz), 128.53 (d, $^3J_{(C–F)}$ = 10.0 Hz), 125.42 (d, $^2J_{(C–F)}$ = 9.8 Hz), 124.76 (d, $^3J_{(C–F)}$ = 3.6

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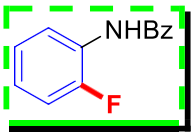
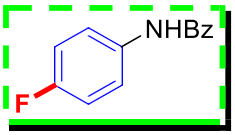
[10] (a) Christ, D. D.; Markwalder, J. A.; Fortunak, J. M.; Ko, S. S.; Mutlib, A. E.; Parsons, R. L., Jr.; Patel, M.; Seitz, S. P. European Patent EP 0929533 B1, **2003**. (b) Christ, D. D.; Cocuzza, A. J.; Ko, S. S.; Markwalder, J. A.; Mutlib, A. E.; Parsons, R. L., Jr.; Patel, M.; Seitz, S. P. U.S. Patent US 5874430 A1, **1999**.

Hz), 122.34 (d, $^{4}J_{(C–F)}$ = 1.8 Hz), 115.46 (d, $^{2}J_{(C–F)}$ = 22.8 Hz), 40.00, 27.50; ^{19}F NMR (377 MHz, $CDCl_3$) δ = -129.28 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{11}H_{14}ClFNO^+$ ($[M+H]^+$) 230.0742. Found 230.0746.



2q,[11] *N*-(2-fluorophenyl)benzamide, white solid: mp 113-114 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.06-7.16 (m, 2H), 7.17-7.21 (m, 1H), 7.51 (dddd, *J* = 1.3, 1.6, 7.0, 7.6 Hz, 2H), 7.58 (dddd, *J* = 1.4, 1.4, 7.3, 7.3 Hz, 1H), 7.87-7.92 (m, 2H), 8.07 (brs, 1H), 8.48 (ddd, *J* = 1.6, 8.1, 8.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 165.46, 152.70 (d, $^{1}J_{(C–F)}$ = 241.4 Hz), 134.57, 132.16, 128.91, 127.10, 126.56 (d, $^{2}J_{(C–F)}$ = 9.8 Hz), 124.73 (d, $^{3}J_{(C–F)}$ = 3.7 Hz), 124.50 (d, $^{3}J_{(C–F)}$ = 7.7 Hz), 121.79 (d, $^{4}J_{(C–F)}$ = 0.5 Hz), 114.84 (d, $^{2}J_{(C–F)}$ = 19.1 Hz); ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.43 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{13}H_{11}FNO^+$ ($[M+H]^+$) 216.0819. Found 216.0822.



2q',[12] *N*-(4-fluorophenyl)benzamide, white solid: mp 160-161 °C. ^{1}H NMR (400 MHz, DMSO) δ = 7.19 (dddd, *J* = 3.6, 2.2, 9.0, 8.9 Hz, 2H), 7.53 (dddd, *J* = 1.3, 1.6, 7.0, 7.6 Hz, 2H), 7.59 (dddd, *J* = 1.4, 1.4, 7.3, 7.2 Hz, 1H), 7.75-7.80 (m, 2H), 7.92-7.95 (m, 2H), 10.30 (brs, 1H); ^{13}C NMR (100 MHz, DMSO) δ = 166.00, 158.78 (d, $^{1}J_{(C–F)}$ = 238.8 Hz), 135.92 (d, $^{4}J_{(C–F)}$ = 2.6 Hz), 135.21, 132.11, 128.90, 128.07, 122.71 (d, $^{3}J_{(C–F)}$ = 7.8 Hz), 115.66 (d, $^{2}J_{(C–F)}$ = 22.1 Hz); ^{19}F NMR (377 MHz, DMSO) δ = -118.83 (m, 1F); HRMS (ESI-TOF) Calcd for $C_{13}H_{11}FNO^+$ ($[M+H]^+$) 216.0819. Found 216.0822.

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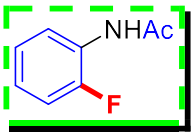
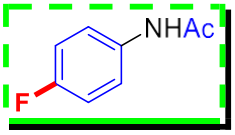


2r,[13] *N*-(2-fluorophenyl)acetamide, white solid: mp 77-78 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.22 (s, 3H), 7.01-7.14 (m, 3H), 7.42 (brs, 1H), 8.29 (dd, J = 7.9, 7.7 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 168.32, 152.31 (d, $^{1}J_{(C-F)}$ = 241.3 Hz), 126.37 (d, $^{2}J_{(C-F)}$ = 10.1 Hz), 124.58 (d, $^{3}J_{(C-F)}$ = 3.7 Hz), 124.28 (d, $^{3}J_{(C-F)}$ = 7.6 Hz), 121.82, 114.74 (d, $^{2}J_{(C-F)}$ = 19.2 Hz), 24.66; ^{19}F NMR (377 MHz, $CDCl_3$) δ = -131.28 (m, 1F); HRMS (ESI-TOF) Calcd for $C_8H_9FNO^+$ ($[M+H]^+$) 154.0663. Found 154.0684.



2r',[14] *N*-(4-fluorophenyl)acetamide, white solid: mp 149-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 2.16 (s, 3H), 7.00 (dd, J = 8.7, 8.6 Hz, 2H), 7.33 (brs, 1H), 7.43-7.47 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 168.34, 159.40 (d, $^{1}J_{(C-F)}$ = 242.0 Hz), 133.84 (d, $^{4}J_{(C-F)}$ = 2.6 Hz), 121.80 (d, $^{3}J_{(C-F)}$ = 7.8 Hz), 115.63 (d, $^{2}J_{(C-F)}$ = 22.4 Hz), 24.41; ^{19}F NMR (377 MHz, $CDCl_3$) δ = -118.00 (m, 1F); HRMS (ESI-TOF) Calcd for $C_8H_9FNO^+$ ($[M+H]^+$) 154.0663. Found 154.0666.

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VI. Computational details

General information

All species involved in the reactions were fully optimized without symmetry constraints with the M062X method[15] in combination with 6-311G(d) basis sets. The solvation effects on the structures and molecular properties were accounted using the integral-equation-formalism polarizable continuum model (IEF-PCM) [16] and the dielectric constant for 50% nitromethane/water solvent, ε= 57.46, were used for all calculations. Harmonic vibration frequencies and the intrinsic reaction coordinates (IRC) [17, 18] were computed at the same level (IEF-PCM/M062X/6-311G(d)) to characterize the stationary points and the reaction path, respectively. All the calculations have been carried out with the GAUSSIAN09 program.[19]

[15] Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215–241.
[16] Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999–3094.
[17] Gonzalez, C.; Schlegel, H. B. *J. Phys. Chem.* **1990**, *94*, 5523–5527.
[18] Gonzalez, C.; Schlegel, H. B. *J. Chem. Phys.* **1989**, *90*, 2154–2161.
[19] Gaussian 09, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Energy profile of the chain propagation steps

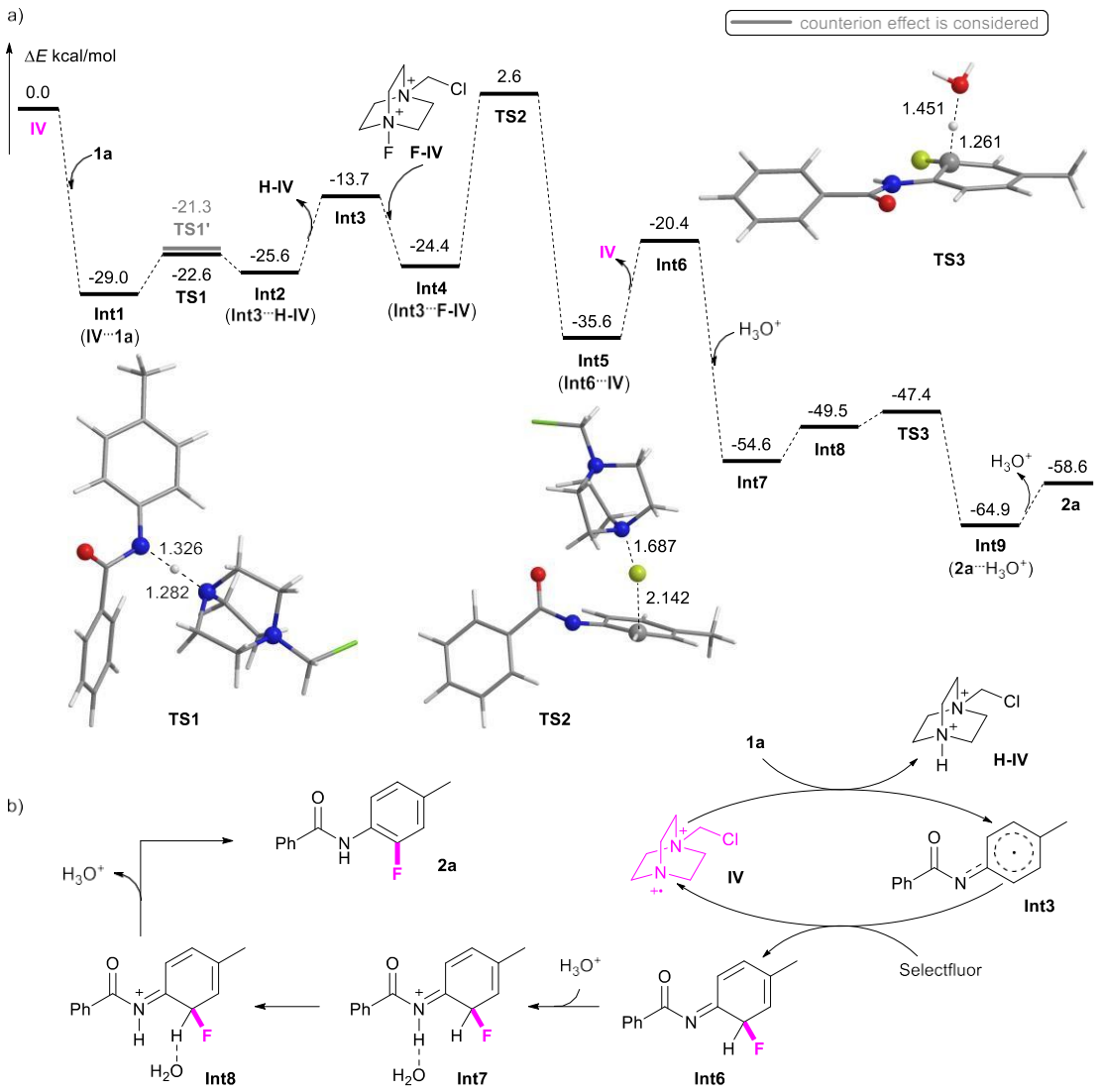


Figure S1. Energy profile, key optimized structures calculated at the IEF-PCM/M062X/6-311G(d) level, and proposed mechanism for the chain propagation steps. Δ*E* values are in kcal mol^{-1}. Distances are given in angstroms.

In the radical chain propagation steps, complex **Int1**, lying at -29.0 kcal mol^{-1} with respect to the initial radical **IV**, is first formed from **IV** and substrate **1a**, and then the hydrogen atom of the N-H bond transfers to **IV** through transition state **TS1** with a very small energy barrier of only 6.4 kcal mol^{-1}. The removal of the newly produced dication **H-IV** from the resultant intermediate **Int2** delivers radical intermediate **Int3**, which has an energy of -13.7 kcal mol^{-1} relative to **IV**. Complex **Int4** is then formed from **Int3** and the N−F reagent **F-IV**, and undergoes fluorine transfer from **F-IV** to **Int3** via the rate-determining transition state **TS2** by passing a barrier of 27.0 kcal

mol^{-1}. The breakup of the resultant intermediate **Int5** releases dearomatized intermediate **Int6** and simultaneously regenerates the key cationic N-radical **IV**, which propagates the chain. **Int6** isomerizes easily to the more stable final product **2a** with the assistance of a hydronium ion after crossing a barrier of 2.1 kcal mol^{-1} (**TS3**), through successive processes including proton migration from the hydronium ion to the nitrogen atom, dehydrogenative aromatization by complexed water, and the removal of the hydronium ion.

On the basis of Yan and Jiang's seminal work[20] together with the experimental and theoretical results, a plausible mechanism for the chain propagation steps of the title reaction is proposed.

Energy profile of the initiation steps

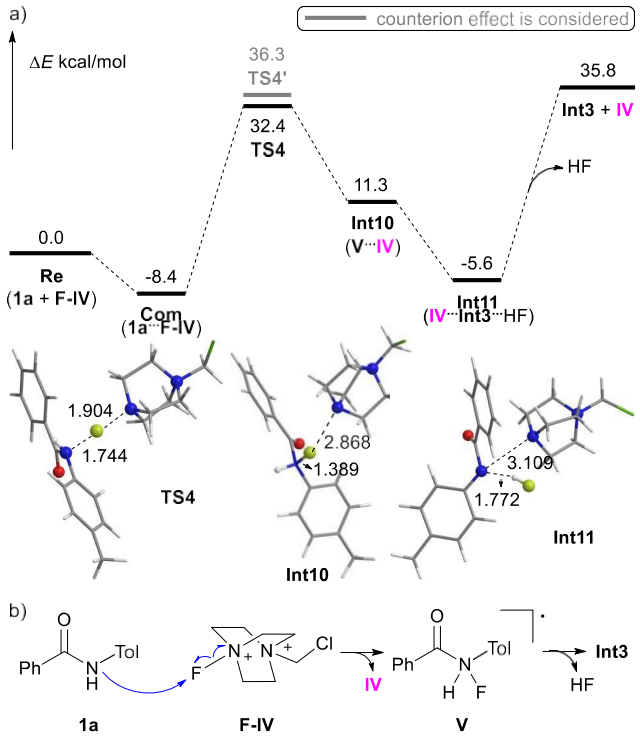


Figure S2. Energy profile, key optimized structures calculated at the IEF-PCM/M062X/6-311G(d) level, and proposed mechanism for the initiation steps. Δ*E* values are in kcal mol^{-1}. Distances are given in angstroms.

[20] Y. Ji, H. Yan, and Q. Jiang, *Eur. J. Org. Chem.*, 2015, 2051–2060.

To start with, complex **Com** is afforded from substrate **1a** and **F-IV**, with the amide group coordinated to the electrophilic fluorine via the nitrogen atom. Then, a new N-F bond is formed via the transition state **TS4** with an activation energy of 40.8 kcal mol^{-1}, delivering complex **Int10** having an energy of only 11.3 kcal mol^{-1} relative to reactants **Re**. Radical **IV** is generated in this step, judging by the N-F atomic distance of 2.868 Å, which is much longer than the N-F bond length in dication **F-IV** (1.365 Å). A novel radical **V**, which could be regarded as an amide-stabilized fluorine radical and is rather active, is simultaneously produced. It undergoes a spontaneous loss of HF immediately via H-N-F scissor vibration to afford radical **Int3** and finish SET, and complex **Int11** consisting of **IV**, **Int3**, and HF, is yielded. This process is further downhill by 16.9 kcal mol^{-1}, and attempt to locate a transition state for it met with no success since the kinetic barrier should be negligible. Impressively, **Int11** is significantly stabilized by complexing effect and lies at -5.6 kcal mol^{-1} relative to **Re**. At last, the endergonic breakup of **Int11** liberates both cationic *N*-radical **IV** and anilidyl radical **Int3**, which could participate in the chain propagation steps, resulting in a significant rise in energy (35.8 kcal mol^{-1} relative to **Re**). The energetic barrier of these steps is higher than that of the chain propagation steps by 9.2 kcal mol^{-1}. In all our computations, dication **F-IV** without $2BF_4^-$ was used instead of Selectfluor, for results from calculations with or without counterions differ only slightly. For example, transition states **TS4'** and **TS1'** located with the consideration of ion pairing effect lie only 3.9 or 1.3 kcal mol^{-1} higher in energy than **TS4** and **TS1**, respectively. A tentative mechanism for the chain initiation steps is outlined.

Energy profile of the ionic mechanism

The activation energy is 36.3 kcal mol^{-1}, 4.7 kcal mol^{-1} higher than that of the proposed chain propagation steps.

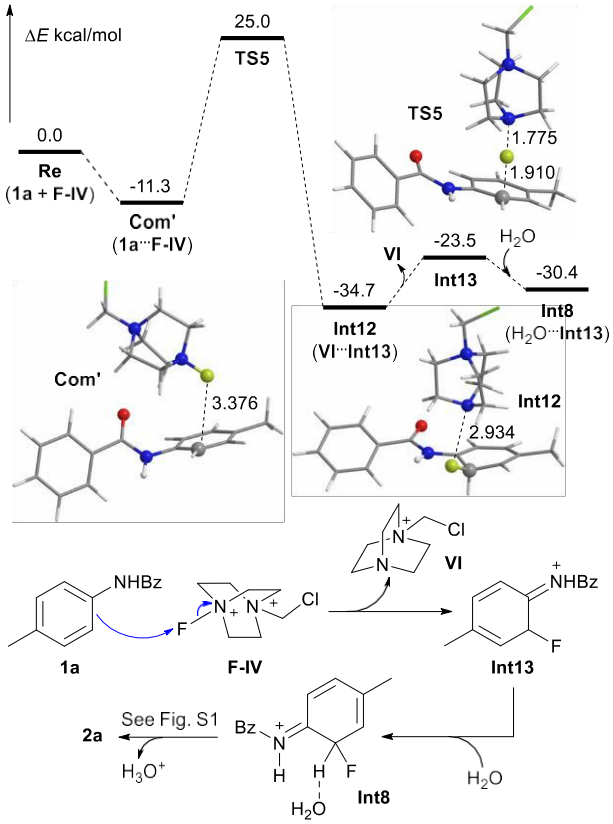


Figure S3. Energy profile, key optimized structures calculated at the IEF-PCM/M062X/6-311G(d) level, and proposed mechanism for the ionic mechanism. ΔE values are in kcal mol^{-1}. Distances are given in angstroms.

Reaction energy of the conventional single-electron transfer (SET) pathway

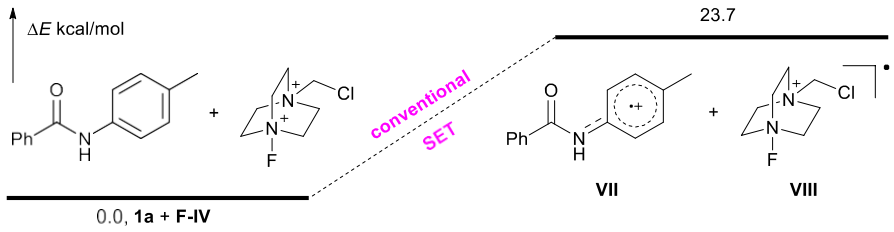


Figure S4. Reaction energy of the conventional SET pathway calculated at the IEF-PCM/M062X/6-311G(d) level. ΔE values are in kcal mol^{-1}.

Calculated homolytic bond dissociation energies

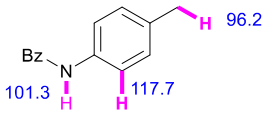


Figure S5. Calculated homolytic bond dissociation energies (kcal mol^{-1}) at the IEF-PCM/M062X/6-311G(d) level.

Energy profile for benzyl hydrogen abstraction

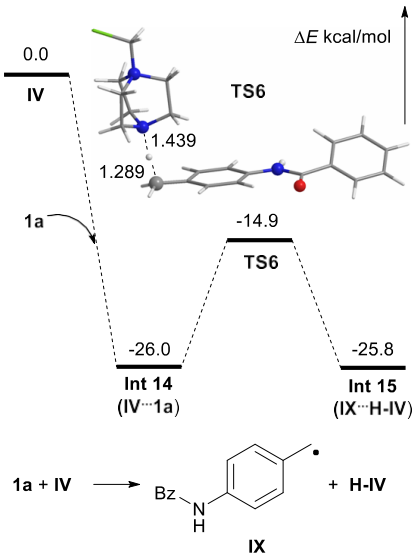
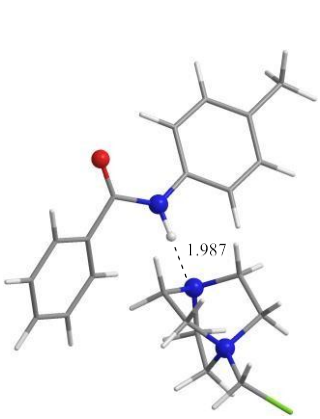
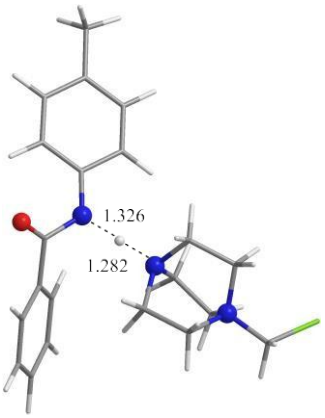


Figure S6. Energy profile for benzyl hydrogen abstraction at the IEF-PCM/M062X/6-311G(d) level. ΔE values are in kcal mol^{-1}.

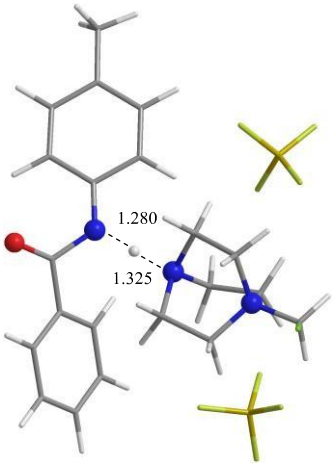
Figure S7. Key geometries optimized at the IEF-PCM/M062X/6-311G(d) level. Distances are given in angstroms.



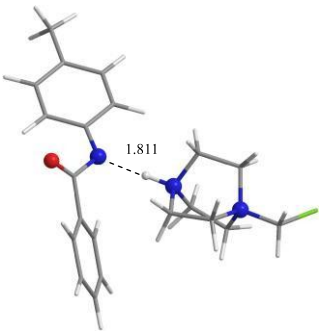
Int1



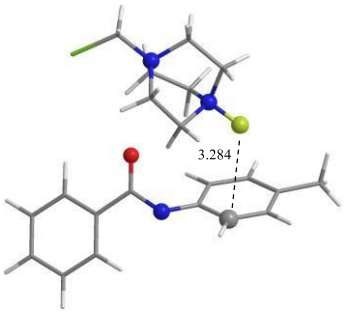
TS1



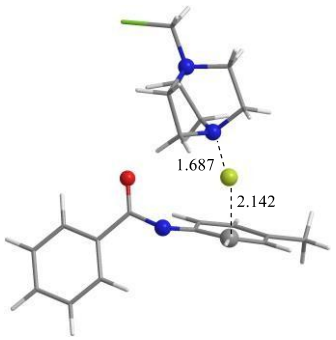
TS1'



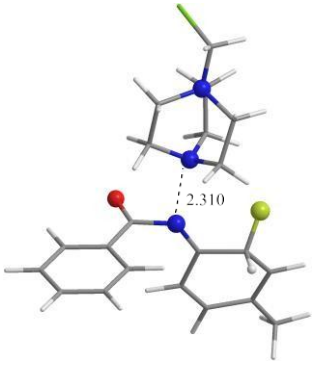
Int2



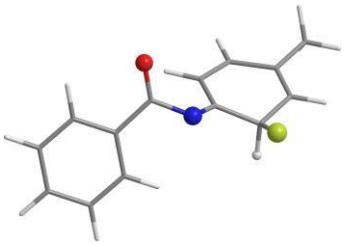
Int4



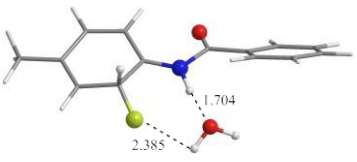
TS2



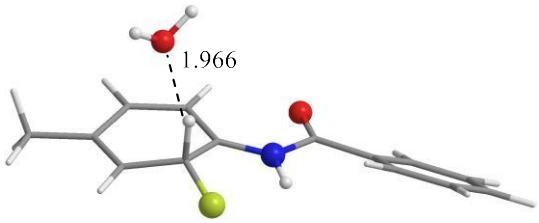
Int5



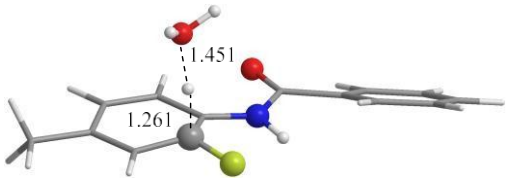
Int6



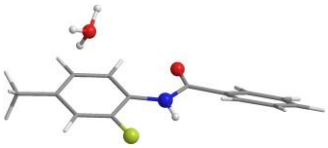
Int7



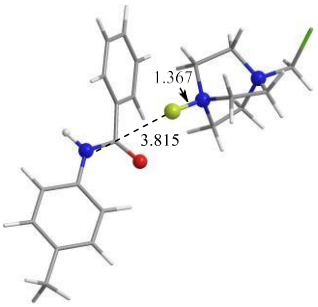
Int8



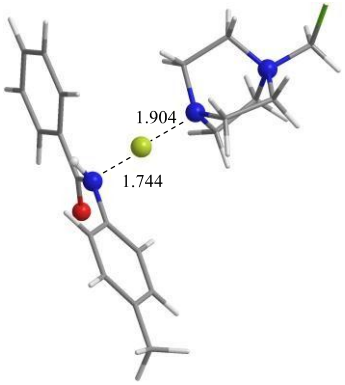
TS3



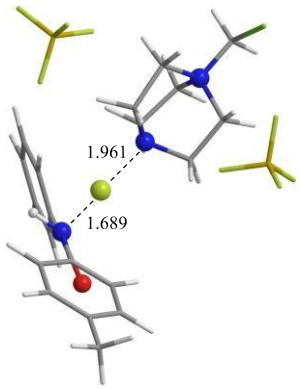
Int9



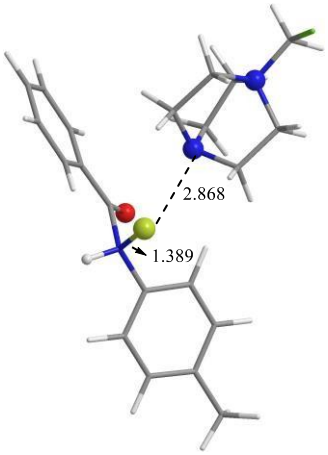
Com



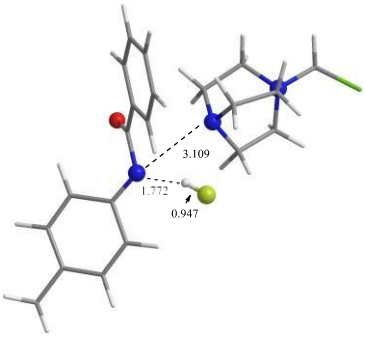
TS4



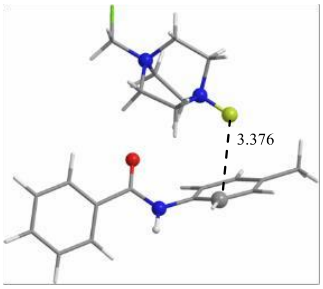
TS4'



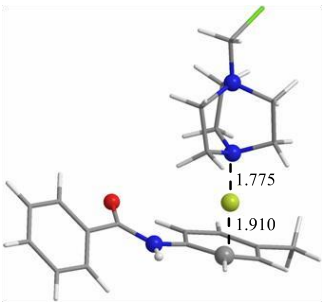
Int10



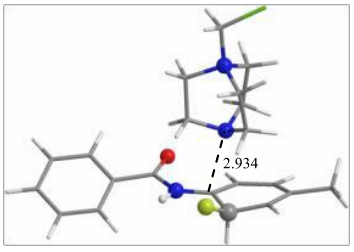
Int11



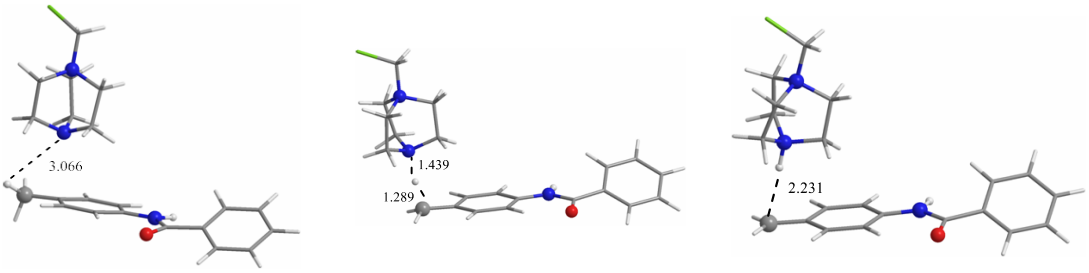
Com'



TS5



Int12



Int14 **TS6** **Int15**

Figure S7. Key geometries optimized at the IEF-PCM/M062X/6-311G(d) level. Distances are given in angstroms.

Table S3. Total energies (in Hartrees) of the optmized structures at the IEF-PCM/M062X/6-311G(d) level.

F-IV	-944.1754036	**Int10**	-1615.3540940
IV	-844.3487717	**Int1**	-1515.5917223
1a	-671.1967568	**TS1**	-1515.5815879
H-IV	-845.0301851	**Int2**	-1515.5863497
2a	-770.4352811	**Int4**	-1614.7295802
Int11	-1615.3810355	**TS2**	-1614.6865567
Int3	-670.5371070	**Int5**	-1614.7475423
TS1'	-2364.8630901	**Int7**	-847.2318675
Int6	-770.3745324	**Int8**	-847.2236650
H_3O^+	-76.8028454	**TS3**	-847.2204051
HF	-100.4292000	**Int9**	-847.2481901
Com	-1615.3855352	**Selectfluor**	-1793.4599905
TS4	-1615.3205899	**TS4'**	-2464.5988542
Com'	-1615.39013240	**Int12**	-1615.42743910
TS5	-1615.33231950	**VII**	-670.9713971
VIII	-944.3630732	**Int13**	-844.60467110
Int14	-1515.58697850	**TS6**	-1515.56926550
Int15	-1515.58671160		

Cartesian coordinates at the IEF-PCM/M062X/6-311G(d) level.

The cartesian coordinates of optimized structures at the IEF-PCM/M062X/6-311G(d) level are given below. The first line is structure number or name, and the second line corresponds to charge and multiplicity, respectively.

IV

2 2

C	-0.74888500	1.53265200	0.13903600
C	-2.19646400	1.00872900	-0.13758000
H	-0.65256700	1.92459400	1.14847900
H	-0.47896700	2.29749600	-0.58491700
H	-2.88600300	1.39427500	0.61054700
H	-2.53808100	1.25420200	-1.13924400
C	-0.00540800	-0.58564400	1.15638300
H	0.54040800	-1.50054000	0.94376200
H	0.37506900	-0.12747000	2.06645700
C	-1.54248900	-0.85332600	1.27886800
H	-1.72999400	-1.91492200	1.42652400
H	-1.99824400	-0.26740300	2.07185300
C	-1.45958100	-1.08241400	-1.14131100
H	-1.33927300	-2.14089600	-0.92861900
H	-2.07002400	-0.93494900	-2.02979300
C	-0.08426500	-0.35326800	-1.29754900
H	0.70292900	-1.07747200	-1.48845200
H	-0.10659000	0.39162900	-2.08980000
N	-2.06093900	-0.42463700	-0.00177300
N	0.21364500	0.36765500	-0.00008600
C	1.61244800	0.93586700	0.00080400
H	1.72159500	1.53745600	-0.89634600
H	1.72561000	1.53590800	0.89870900
Cl	2.83606200	-0.32874100	0.00070300

1a

0 1

C	4.07728700	1.46984300	0.42956700
C	2.73823900	1.09484400	0.46313800
C	2.35806400	-0.17768500	0.03240900
C	3.33004100	-1.07451200	-0.41265600
C	4.66480900	-0.69414700	-0.45682200
C	5.03988500	0.57997300	-0.03676000
H	4.36798900	2.45482700	0.77516300
H	2.00630400	1.78996200	0.86053900
H	3.02419200	-2.06628200	-0.72389400
H	5.41342000	-1.39083900	-0.81542100
C	0.93645200	-0.66235100	0.06655100
O	0.67630500	-1.84655200	0.19198100
N	-0.00659900	0.31539000	-0.06665500
C	-1.41015500	0.18321900	-0.04478000
C	-2.16217400	1.32374800	-0.35333900
C	-2.07728700	-0.99850800	0.28217700
C	-3.54611600	1.28048700	-0.33763800
H	-1.65442900	2.24989700	-0.60448200
C	-3.47061200	-1.01905300	0.29161300
H	-1.51803700	-1.88861900	0.52277700
C	-4.23158400	0.10519600	-0.01570500
H	-4.10572500	2.17871500	-0.58006700
H	-3.97211500	-1.94676400	0.54922100
H	0.33141100	1.23719400	-0.30124300
C	-5.73760600	0.06902200	-0.01384800
H	-6.11001900	-0.88493400	0.36092500
H	-6.15024800	0.86365100	0.61181000
H	-6.13460900	0.21146800	-1.02218000
H	6.08215900	0.87596100	-0.06586100

Int1

2 2

C	0.58707400	3.41829800	1.71924500
C	-0.42944200	2.57793200	1.28120300
C	-0.93879200	2.72772100	-0.01117400

C	-0.44495100	3.72276500	-0.85659700
C	0.58841400	4.54130700	-0.42240500
C	1.10443100	4.38792100	0.86336700
H	0.97409900	3.31660900	2.72599000
H	-0.83851900	1.83187500	1.95437800
H	-0.86112100	3.83014600	-1.85147700
H	0.99036800	5.29984900	-1.08271100
C	-2.02806900	1.85943000	-0.52007400
O	-2.86032300	2.19873500	-1.31604300
N	-1.98116800	0.53315900	0.00932600
C	-2.96760500	-0.37724600	0.03049000
C	-2.66330100	-1.64972300	0.61725200
C	-4.29112700	-0.13360500	-0.46214900
C	-3.61090000	-2.62707100	0.67833400
C	-5.21894300	-1.12998100	-0.38798700
H	-4.53752700	0.82239600	-0.89541900
C	-4.91453800	-2.40017400	0.17185000
H	-3.37246300	-3.58479600	1.12435900
H	-6.22035900	-0.95438300	-0.76335700
C	-5.96567300	-3.44924900	0.23939200
H	-5.57400700	-4.40142200	0.59046600
H	-6.76168600	-3.12460500	0.91808000
H	-6.42971200	-3.58638100	-0.74071900
H	1.90740200	5.03165000	1.20232700
H	-1.67519200	-1.81142600	1.03089200
N	0.87619800	-0.25879500	0.12724600
C	1.50870000	0.71296400	-0.78027900
C	1.66145100	-0.31636100	1.36919600
C	0.91174600	-1.58206700	-0.51745100
C	2.85488300	0.16644500	-1.29861700
H	1.65713500	1.64887800	-0.24073900
H	0.84945200	0.90845600	-1.62610800
C	3.16481000	-0.46435900	1.04906100
H	1.30479700	-1.15677100	1.96434100
H	1.50371800	0.59741500	1.94061800

H	0.30400000	-2.28659000	0.04812700
H	0.48371700	-1.48984800	-1.51588600
C	2.35757600	-2.11811800	-0.57868100
H	3.63342400	0.92778400	-1.29709900
H	2.77701700	-0.26518000	-2.29555500
N	3.29448500	-0.95143700	-0.37538400
H	3.65350900	-1.18674100	1.69865800
H	3.69912200	0.48400100	1.10135300
H	2.56242300	-2.83346700	0.21425300
H	2.59524400	-2.57420900	-1.53843700
C	4.70830200	-1.29057100	-0.72001000
H	4.75504600	-1.49985200	-1.78489600
H	5.33066100	-0.44086400	-0.45675300
Cl	5.29655300	-2.70825600	0.15714600
H	-1.04024200	0.22991800	0.32007000

TS1

2 2

C	0.20657100	3.47692800	1.84972000
C	-0.63963000	2.53759100	1.27134100
C	-1.02871100	2.68416800	-0.06264400
C	-0.58935500	3.77776800	-0.81004700
C	0.27532800	4.69983600	-0.23556100
C	0.67524100	4.54730900	1.09112700
H	0.50134400	3.37294000	2.88692600
H	-1.01652100	1.70766200	1.85996000
H	-0.91070000	3.87980600	-1.84015700
H	0.63832800	5.53703500	-0.81921300
C	-1.90954400	1.67915600	-0.71552600
O	-2.65147200	1.93164800	-1.63148300
N	-1.72287700	0.36572700	-0.20465100
C	-2.72115600	-0.51246600	-0.07788600
C	-2.40095500	-1.82585400	0.39971600
C	-4.10243000	-0.21016900	-0.33558300
C	-3.37292300	-2.77292700	0.56408800

C	-5.05432800	-1.17424100	-0.16137600
H	-4.38170600	0.77592100	-0.67477300
C	-4.72373100	-2.47793600	0.28091000
H	-3.10871100	-3.75972000	0.92488300
H	-6.09380800	-0.93910600	-0.36131300
C	-5.79540400	-3.50177400	0.44934900
H	-5.40376100	-4.44188800	0.83326200
H	-6.56729700	-3.13421400	1.13079700
H	-6.28624100	-3.69084600	-0.50970400
H	1.34863200	5.26956500	1.53735000
H	-1.37386400	-2.05487000	0.65456800
N	0.81305400	-0.21931000	-0.14077800
C	1.58630700	0.92071000	-0.70225600
C	1.33984800	-0.53265100	1.21081400
C	1.00164600	-1.39399600	-1.03335500
C	3.00230600	0.43927400	-1.05670600
H	1.60939700	1.71859100	0.03830900
H	1.08408000	1.28986000	-1.59479200
C	2.87447300	-0.61398700	1.15436700
H	0.90326200	-1.47458500	1.53799500
H	1.03159500	0.25115500	1.90003900
H	0.28353700	-2.16922500	-0.77433500
H	0.80464400	-1.07415200	-2.05534600
C	2.43008700	-1.93381100	-0.86613000
H	3.75214800	1.17868600	-0.78181100
H	3.10783600	0.19766900	-2.11276600
N	3.28393400	-0.83213500	-0.28290600
H	3.24864000	-1.44546200	1.74646400
H	3.35247900	0.30655100	1.48659200
H	2.47228600	-2.77424800	-0.17769800
H	2.86423700	-2.23127800	-1.81880600
C	4.74844500	-1.12618100	-0.40900200
H	4.99319100	-1.14355900	-1.46702500
H	5.29386600	-0.34416000	0.11073200
Cl	5.18079300	-2.68418400	0.29720900

H	-0.43987800	0.04937900	-0.09465100

TS1'

0 2

C	1.30521500	-3.65049900	-1.23555000
C	0.08480800	-3.13335000	-0.82222500
C	-0.43688300	-3.49593100	0.42297900
C	0.25121100	-4.39056000	1.24293100
C	1.48157100	-4.88898900	0.83379200
C	2.00893600	-4.51527700	-0.40068000
H	1.71647200	-3.36442600	-2.19514600
H	-0.46664500	-2.45823600	-1.46841700
H	-0.17288100	-4.66607300	2.20152300
H	2.03206000	-5.56446100	1.47752200
C	-1.72264300	-2.92817100	0.90466200
O	-2.44904300	-3.48090200	1.69332700
N	-1.97012600	-1.62502300	0.39686500
C	-3.19388500	-1.14497800	0.15390400
C	-3.30045800	0.21304100	-0.29382500
C	-4.40272300	-1.91405200	0.27172800
C	-4.52125000	0.77898100	-0.53724400
C	-5.60725500	-1.32751100	0.00777500
H	-4.35405400	-2.94735100	0.57938500
C	-5.70666100	0.02977700	-0.38860900
H	-4.57041700	1.81557100	-0.84761100
H	-6.51623100	-1.91133500	0.10155100
C	-7.04652100	0.63041000	-0.65211600
H	-7.57012800	0.06289800	-1.42645900
H	-7.66540800	0.57846200	0.24819800
H	-6.97131700	1.66947900	-0.96704900
H	2.97311500	-4.89819700	-0.71396900
H	-2.40470300	0.79582200	-0.46372500
H	-0.92228800	-0.88986200	0.41649300
N	0.13720600	-0.11259900	0.58591800
C	0.69079600	0.30801400	-0.72494400

C	-0.34779000	1.07471700	1.33880500
C	1.23543400	-0.74898600	1.35729900
C	1.56845500	1.54284800	-0.51027900
H	1.26921200	-0.52206500	-1.12796700
H	-0.12178300	0.55556200	-1.40485100
C	0.83728000	1.94256100	1.78989100
H	-0.91845200	0.72907300	2.20017900
H	-1.00413800	1.65259000	0.69401300
C	2.46455500	0.17959800	1.35114100
H	1.50336000	-1.69164900	0.88295500
H	0.87508100	-0.94457100	2.36686800
N	2.02139800	1.56125900	0.94167800
H	2.45182700	1.51485500	-1.14163200
H	1.01178000	2.46567700	-0.66511100
H	0.62725500	2.99771700	1.62763200
H	1.11011900	1.77184500	2.82883400
H	3.21111500	-0.13895100	0.62966000
H	2.91221600	0.25315500	2.33956500
C	3.14209500	2.54370500	1.02140200
H	2.79296100	3.48141700	0.59808900
H	3.97382100	2.12989600	0.45811400
Cl	3.66130600	2.84214700	2.68696100
F	-1.23878700	2.46140600	-1.60447300
B	-1.61466200	3.59241300	-0.84193800
F	-2.01630300	4.62369700	-1.67548900
F	-2.65301300	3.21080600	0.02206400
F	-0.49806100	3.98753000	-0.07104700
F	3.03832500	-0.01331600	-2.75250100
B	4.01668200	-0.51918400	-1.88437600
F	4.48464000	0.54286900	-1.06634300
F	5.07206800	-1.07228900	-2.59330300
F	3.42368900	-1.48623900	-1.04538500

Int2

2 2

C	0.30870200	3.22305900	1.85628100
C	-0.59846000	2.34702900	1.26873700
C	-0.98879100	2.53683100	-0.05916900
C	-0.48718900	3.61412900	-0.79011300
C	0.43759500	4.47268200	-0.20887600
C	0.83805000	4.27525100	1.11166400
H	0.60372700	3.08415600	2.88962900
H	-1.01915200	1.52833300	1.84364600
H	-0.81064800	3.75309500	-1.81521500
H	0.84667300	5.29550500	-0.78258800
C	-1.93387700	1.58968200	-0.72444500
O	-2.62007300	1.91093600	-1.66976500
N	-1.84829100	0.27904500	-0.23138600
C	-2.93734300	-0.48038400	-0.09798600
C	-2.75834200	-1.86486300	0.21921000
C	-4.28499100	0.00867000	-0.19655300
C	-3.83406000	-2.69756200	0.39111100
C	-5.34168100	-0.84134900	-0.01383600
H	-4.45878100	1.05319400	-0.41351900
C	-5.15008800	-2.21098300	0.27649000
H	-3.67323500	-3.74420700	0.62255900
H	-6.35404400	-0.45866200	-0.08630900
C	-6.33273200	-3.10624500	0.46560300
H	-6.03515200	-4.12886200	0.69181400
H	-6.96287300	-2.73719300	1.27928000
H	-6.95134000	-3.11355800	-0.43582000
H	1.55779700	4.94731100	1.56384400
H	-1.74973500	-2.24584500	0.31975600
N	0.96286200	-0.28405400	-0.17934400
C	1.69660200	0.86988200	-0.78799900
C	1.48596600	-0.52247400	1.20120400
C	1.17868200	-1.50354300	-1.02108000
C	3.11546900	0.39656800	-1.12776700
H	1.69727600	1.68587600	-0.06718300
H	1.17292300	1.18757900	-1.68659900

C	3.01888600	-0.53704000	1.13556400
H	1.07544700	-1.46488900	1.55597900
H	1.13901500	0.28307400	1.84388800
H	0.47273000	-2.26995600	-0.71218600
H	0.97696300	-1.23240100	-2.05548100
C	2.61985100	-1.98308800	-0.80873700
H	3.84569500	1.17029700	-0.90074300
H	3.21589000	0.10151100	-2.17015700
N	3.43528000	-0.82241000	-0.28746000
H	3.42760700	-1.31206400	1.77856100
H	3.45465800	0.42265400	1.40801200
H	2.68111400	-2.78193600	-0.07363500
H	3.06548500	-2.32190500	-1.74166300
C	4.91197400	-1.07627300	-0.39731000
H	5.15680500	-1.14584800	-1.45325000
H	5.42862600	-0.24670200	0.07622600
Cl	5.38824900	-2.57498200	0.39727400
H	-0.07740600	-0.08930300	-0.13900300

H-IV

2 1

C	-0.69543600	1.54130000	0.15571900
C	-2.11914700	1.06562100	-0.15799600
H	-0.59823900	1.90290000	1.17750400
H	-0.38871300	2.32613300	-0.53197700
H	-2.83412100	1.49617200	0.53795900
H	-2.42473800	1.29813300	-1.17532300
C	0.02251400	-0.58882500	1.14115700
H	0.54383900	-1.51234200	0.90282100
H	0.45275900	-0.16005600	2.04362300
C	-1.48836900	-0.80241000	1.29836000
H	-1.71503700	-1.84423500	1.50844200
H	-1.92054800	-0.17645900	2.07461800
C	-1.39807400	-1.06779300	-1.13859200
H	-1.26819000	-2.11880300	-0.89180800

H	-2.00204800	-0.98341300	-2.03747300
C	-0.06329200	-0.33070400	-1.29918700
H	0.73763100	-1.03256900	-1.51671900
H	-0.09540600	0.42931600	-2.07822200
N	-2.13971200	-0.42629100	-0.00122100
N	0.25571700	0.37288100	-0.00121800
C	1.65524600	0.92362200	-0.00222500
H	1.77192300	1.52051100	-0.90175100
H	1.77603100	1.52562800	0.89363000
Cl	2.86942700	-0.35231600	0.00176900
H	-3.10808200	-0.75253600	-0.00173900

Int3

0 2

C	3.78683800	1.56168500	0.53466700
C	2.52487300	1.18935600	0.08465900
C	2.25381200	-0.15034100	-0.19976300
C	3.25258800	-1.11181500	-0.03241900
C	4.51191000	-0.73820800	0.41671100
C	4.77975300	0.59991900	0.70043600
H	3.99688300	2.60219800	0.75315100
H	1.74945900	1.93256300	-0.05454700
H	3.02566600	-2.14737700	-0.25642500
H	5.28505800	-1.48653600	0.54627400
C	0.90572800	-0.60173900	-0.66651000
O	0.69370200	-1.75869800	-0.98635200
N	-0.03791600	0.40659600	-0.78531200
C	-1.30306100	0.22270000	-0.40976900
C	-2.24904200	1.22843400	-0.78394100
C	-1.78181100	-0.87658500	0.37599000
C	-3.56908000	1.13128900	-0.42001400
H	-1.88534100	2.06242500	-1.37253100
C	-3.10557400	-0.94738500	0.73365600
H	-1.09125900	-1.65040700	0.68355500
C	-4.02914400	0.04379000	0.34624100

H	-4.27142200	1.90022000	-0.72330300
H	-3.45361400	-1.78384000	1.33057700
C	-5.46224800	-0.03994400	0.77541500
H	-5.78649700	-1.07590300	0.87958900
H	-5.58960900	0.44279200	1.74972600
H	-6.12005600	0.46779700	0.06954100
H	5.76327100	0.89255000	1.05023400

F-IV

2 1

C	-0.28714500	1.64194600	0.16524800
C	-1.74654700	1.27392100	-0.14530800
H	-0.16139600	1.99058000	1.18787700
H	0.06370500	2.40720700	-0.52339500
H	-2.43204300	1.71742000	0.57254300
H	-2.05047500	1.52423200	-1.15936200
C	0.27383200	-0.54170200	1.13747700
H	0.72516800	-1.49874100	0.89203700
H	0.72522300	-0.15228500	2.04737600
C	-1.25135000	-0.65252000	1.29696200
H	-1.56227600	-1.68029600	1.46578200
H	-1.65611600	-0.00807000	2.07280600
C	-1.18494700	-0.90554100	-1.14752200
H	-1.14943400	-1.96468900	-0.90225700
H	-1.80198000	-0.74521400	-2.02781300
C	0.20408200	-0.26700200	-1.30147100
H	0.94609000	-1.03046700	-1.51988800
H	0.22596300	0.49140900	-2.08144500
N	-1.85153500	-0.21145600	-0.00098700
N	0.57469700	0.40745700	-0.00100800
F	-3.17343200	-0.55072200	-0.00267000
C	2.01698600	0.85084100	-0.00763000
H	2.17419300	1.43022700	-0.91233800
H	2.18318200	1.45108700	0.88195900
Cl	3.12467600	-0.51456200	0.00338600

Int4

2 2

C	5.62483200	-0.88431500	0.69441500
C	4.37646000	-0.27662200	0.74794800
C	3.31158600	-0.81268900	0.02029900
C	3.50106400	-1.95611700	-0.75932700
C	4.74941000	-2.56013400	-0.81052400
C	5.81102500	-2.02431000	-0.08328900
H	6.45136800	-0.47147900	1.26035100
H	4.22003000	0.60565200	1.35676800
H	2.66556000	-2.35719400	-1.32044500
H	4.89787300	-3.44675100	-1.41538400
C	1.96885100	-0.17507200	0.03540200
O	1.00665800	-0.66927600	-0.54786300
N	1.83439700	0.94728600	0.82479900
C	1.20462700	2.03589500	0.38406200
C	0.78955800	3.00420700	1.35052800
C	0.93593800	2.31334200	-0.99716200
C	0.11409100	4.13637200	0.96664900
C	0.27019800	3.45802200	-1.35630100
H	1.28186800	1.62081800	-1.75589800
C	-0.16947200	4.38652900	-0.38930400
H	-0.20755800	4.85190600	1.71519400
H	0.07927800	3.66024800	-2.40469100
C	-0.94372900	5.59958200	-0.80092700
H	-0.62400200	5.96239400	-1.77831700
H	-2.00707600	5.34953000	-0.87726600
H	-0.84532300	6.40381400	-0.07204800
H	6.78554200	-2.49738100	-0.12286100
N	-2.35300600	0.59355400	0.15252500
C	-3.82117000	0.38494100	0.33415700
C	-1.90879900	0.07853800	-1.17931300
C	-1.58543700	-0.06606300	1.25498900
C	-4.10001600	-1.08561100	-0.01761800

H	-4.33261100	1.06268000	-0.34441800
H	-4.05635500	0.63228400	1.36641100
C	-1.91610800	-1.45303200	-1.08179700
H	-0.89535100	0.43918800	-1.33970200
H	-2.59216700	0.48044700	-1.92345600
H	-0.53713100	-0.03040800	0.96809700
H	-1.76578000	0.50641200	2.16175600
C	-2.11969200	-1.50165100	1.36784700
H	-4.47835700	-1.19890300	-1.03065900
H	-4.81294700	-1.51334800	0.68357100
N	-2.80536300	-1.86474100	0.07171000
H	-0.91450100	-1.82628300	-0.88347900
H	-2.30721100	-1.89600200	-1.99518000
H	-1.29900500	-2.19516000	1.53361100
H	-2.85260500	-1.60619400	2.16547800
C	-3.14795000	-3.33118500	0.02317900
H	-3.68489700	-3.57420800	0.93519900
H	-3.76317300	-3.49721600	-0.85648400
Cl	-1.70697700	-4.33500500	-0.08299600
H	1.01143400	2.80288000	2.39188600
F	-2.09504000	1.93612400	0.20101100

TS2

2 2

C	5.37130200	-2.27255300	0.79193100
C	4.23171900	-1.47821400	0.82246200
C	3.10236800	-1.86182200	0.09576500
C	3.11453600	-3.03850100	-0.65750400
C	4.25460900	-3.82795600	-0.68458500
C	5.38226700	-3.44431800	0.04001200
H	6.24893600	-1.97983000	1.35543300
H	4.21530900	-0.56984400	1.41320600
H	2.22847500	-3.31773200	-1.21488000
H	4.26788800	-4.74044700	-1.26836200
C	1.87388600	-1.03234700	0.08018100

O	0.85559700	-1.35338200	-0.50570800
N	1.88869400	0.12828700	0.86158500
C	1.84090200	1.29938100	0.31934300
C	1.57957400	2.44097200	1.19430300
C	1.96446000	1.56707800	-1.10553100
C	1.58563900	3.73454200	0.69373800
C	1.91671300	2.84152500	-1.55786200
H	2.12496200	0.73932800	-1.78642800
C	1.73676400	3.95877700	-0.66865800
H	1.44394500	4.57076900	1.36726300
H	2.02838400	3.04439700	-2.61727000
C	1.72789200	5.33336500	-1.24532500
H	2.67216700	5.52796100	-1.76213800
H	0.93720200	5.41868900	-1.99634500
H	1.57750100	6.09567400	-0.48355200
H	6.27245100	-4.06231900	0.01876000
N	-1.83475600	0.95427500	0.57096400
C	-3.03218800	1.72810100	0.89225500
C	-1.74588100	0.62849100	-0.85412400
C	-1.69065700	-0.23708600	1.41054700
C	-4.22456600	0.90818900	0.34009800
H	-2.96547100	2.69762300	0.40460000
H	-3.08166200	1.85925400	1.97043900
C	-2.79521500	-0.47768400	-1.10897500
H	-0.74479500	0.25043500	-1.05435400
H	-1.93833700	1.53266900	-1.42688800
H	-0.83870800	-0.80262400	1.03688400
H	-1.51394400	0.07702400	2.43664100
C	-3.01985400	-1.01614400	1.28515700
H	-4.59652200	1.31021200	-0.59991400
H	-5.03516100	0.86263500	1.06414800
N	-3.75408500	-0.50832100	0.06336900
H	-2.32945900	-1.45784300	-1.17581900
H	-3.36962400	-0.28353100	-2.01242100
H	-2.83806900	-2.08014600	1.16086200

H	-3.67353100	-0.85534500	2.13984400
C	-4.97256400	-1.33626300	-0.23333600
H	-5.56978900	-1.38555200	0.67188100
H	-5.51437800	-0.84973700	-1.03893900
Cl	-4.55671100	-2.97421600	-0.73175900
H	1.52487100	2.24285000	2.25679300
F	-0.46917000	1.89102900	0.89503800

Int5

2 2

C	2.14434600	-3.63251100	1.69134700
C	1.80197500	-2.43315700	1.07956200
C	1.52656900	-2.41144000	-0.29125000
C	1.59192000	-3.58840600	-1.04413300
C	1.94069700	-4.78010000	-0.42822900
C	2.21643300	-4.80124700	0.93876700
H	2.35396400	-3.65510500	2.75364600
H	1.73730600	-1.52566000	1.66859600
H	1.37107900	-3.55073400	-2.10406500
H	1.99791200	-5.69285700	-1.00857400
C	1.14332600	-1.16293800	-0.99110400
O	0.75932400	-1.10637800	-2.13276500
N	1.14685300	0.01888100	-0.20105500
C	2.17355100	0.76258300	-0.05577600
C	2.09507000	1.99283100	0.82134300
C	3.47887600	0.47048500	-0.63815400
C	3.08770300	3.06152200	0.50329700
C	4.41816100	1.43129400	-0.67703600
H	3.63937700	-0.49283500	-1.10740500
C	4.21657000	2.79045500	-0.15712500
H	2.87770400	4.04064700	0.91982500
H	5.36673700	1.21462900	-1.15880800
C	5.29262900	3.80225700	-0.41617700
H	6.23231900	3.48495700	0.04268600
H	5.47324600	3.90186500	-1.48918800

H	5.02278800	4.77844400	-0.01567600
H	2.48704400	-5.73434500	1.41903500
N	-1.12058500	0.28361900	0.15094200
C	-1.37031500	0.59750800	1.55310400
C	-1.50131400	1.36573000	-0.75120300
C	-1.72884100	-0.98792900	-0.23639300
C	-2.85482900	1.03829800	1.62982100
H	-0.72275200	1.40900500	1.86996700
H	-1.17554900	-0.28970100	2.15129300
C	-3.05089100	1.35704900	-0.80574300
H	-1.08251100	1.17143300	-1.73694700
H	-1.10923200	2.30142900	-0.36399500
H	-1.61029300	-1.12486600	-1.30843100
H	-1.24765900	-1.80881100	0.29488500
C	-3.22357400	-0.89826500	0.16615300
H	-2.95929900	2.12066500	1.65990600
H	-3.35193900	0.60047900	2.49296400
N	-3.56367200	0.55913200	0.37627700
H	-3.42176000	0.87720000	-1.70732800
H	-3.45676100	2.36421900	-0.73883400
H	-3.86036600	-1.29491900	-0.62039200
H	-3.43082300	-1.41713200	1.09999200
C	-5.03621600	0.76043600	0.59179000
H	-5.34783400	0.09949300	1.39452900
H	-5.19207600	1.80250300	0.85472800
Cl	-5.97857000	0.39068700	-0.85100800
H	2.28216300	1.63579300	1.84533800
F	0.80878300	2.50615700	0.80457600

Int6

0 1

C	3.63735400	1.12712700	-1.26679100
C	2.44858700	0.95210300	-0.56719500
C	2.31188000	-0.12310800	0.31269200
C	3.36964200	-1.01728200	0.49138800

C	4.55511400	-0.84015600	-0.20802400
C	4.68876100	0.23239800	-1.08817500
H	3.74440000	1.96242400	-1.94866300
H	1.63177200	1.65214200	-0.69641500
H	3.24592300	-1.84575000	1.17866100
H	5.37473200	-1.53541600	-0.06995600
C	1.04662900	-0.36824200	1.06773200
O	0.92837000	-1.26859500	1.86973500
N	0.02641100	0.56221000	0.84450800
C	-1.02995100	0.24644300	0.20955700
C	-2.09659800	1.30424400	0.01618400
C	-1.30301600	-1.05181300	-0.41704200
C	-3.48591600	0.76372200	-0.11928400
C	-2.55864000	-1.37719400	-0.75975900
H	-0.49199900	-1.76393900	-0.51601400
C	-3.70959300	-0.48513100	-0.53673500
H	-4.29321800	1.46869600	0.05113300
H	-2.75956100	-2.35838000	-1.17949000
C	-5.07951500	-1.04548000	-0.78418400
H	-5.18335100	-1.35728100	-1.82685200
H	-5.25030100	-1.93022500	-0.16547600
H	-5.85450900	-0.31220000	-0.56337700
H	5.61477200	0.37105300	-1.63445000
H	-1.84050200	1.83544600	-0.91310300
F	-2.03538000	2.23565900	1.03470900

H_3O^+

1 1

H	0.00000000	0.93184400	-0.20630500
H	-0.80700100	-0.46592200	-0.20630500
H	0.80700100	-0.46592200	-0.20630500
O	0.00000000	0.00000000	0.07736400

Int7

1 1

C	-4.01278500	0.86275700	1.01863400
C	-2.68233800	0.53043600	0.79494900
C	-2.37345600	-0.55627700	-0.02745900
C	-3.39299700	-1.31606300	-0.60819000
C	-4.71778500	-0.96981100	-0.39172100
C	-5.02679000	0.11979300	0.42097800
H	-4.25651300	1.69929000	1.66196800
H	-1.89916500	1.10882600	1.26968100
H	-3.13340900	-2.16438000	-1.23017800
H	-5.50989400	-1.54729300	-0.85235200
C	-0.98046600	-0.99689500	-0.26083100
O	-0.65717000	-2.11008800	-0.56626600
N	0.00928600	0.04421500	-0.12043300
C	1.28724400	-0.15001900	0.11716700
C	2.14098700	1.08123600	0.23798200
C	1.91974200	-1.39916100	0.37365100
C	3.59980200	0.89180600	0.00995400
C	3.27919200	-1.44805800	0.39199000
H	1.33615100	-2.30001200	0.47008500
C	4.16198500	-0.31615000	0.14436900
H	4.17463300	1.79636700	-0.15423300
H	3.74630500	-2.41384500	0.56020400
C	5.63668600	-0.56950200	0.04323400
H	6.01822500	-0.97742300	0.98193400
H	5.84580900	-1.29994100	-0.74123500
H	6.17808300	0.34801100	-0.18181000
H	-6.06284700	0.38747300	0.59247700
O	-1.03928100	2.53676300	-0.59684900
H	-0.32693200	1.01838000	-0.29798300
H	-1.89579900	2.59044000	-1.03185300
H	-0.44823500	3.15218300	-1.04091000
H	2.02996900	1.37329400	1.29836300
F	1.63067800	2.10235300	-0.52716000

Int8

1 1

C	4.33010900	-1.47334400	0.16138100
C	3.01055700	-1.04290100	0.22033700
C	2.71469500	0.30852700	0.02233400
C	3.74247600	1.22354200	-0.22158100
C	5.05589500	0.78515500	-0.29284500
C	5.34949200	-0.56362100	-0.10250800
H	4.56082400	-2.51845600	0.32656800
H	2.23813900	-1.76416100	0.46304000
H	3.49658800	2.26923900	-0.36134900
H	5.85094300	1.49236000	-0.49501400
C	1.33831700	0.85646000	0.10063500
O	1.07709600	2.00240100	0.34428100
N	0.30255400	-0.08782600	-0.16951200
C	-1.01002200	0.11777700	-0.10951800
C	-1.85818600	-1.08178500	-0.33258300
C	-1.67573800	1.31258700	0.23345800
C	-3.24323700	-0.85209100	-0.78892700
C	-3.03066600	1.37275900	0.04051900
H	-1.12408000	2.17872900	0.55794700
C	-3.84544600	0.32183400	-0.52292700
H	-3.76755900	-1.70733500	-1.20081300
H	-3.52673400	2.30839700	0.28146900
C	-5.29499700	0.59691400	-0.79645100
H	-5.82492500	0.79290300	0.13838200
H	-5.40704800	1.47852800	-1.43040700
H	-5.76857400	-0.24998900	-1.29067300
H	6.37647100	-0.90549400	-0.15456200
H	0.58538500	-0.99678900	-0.52223200
F	-1.18890900	-2.05739800	-1.02738800
O	-2.89901300	-0.87143100	2.39287000
H	-2.36462900	-0.76090700	3.18449700
H	-3.65609800	-1.40773400	2.64558800
H	-2.01056600	-1.41656600	0.72548100

TS3

1 1

C	-4.28888900	1.47090400	-0.04981200
C	-2.96938900	1.04607000	0.04965500
C	-2.67657100	-0.31976300	0.02054600
C	-3.70951500	-1.25254600	-0.09571500
C	-5.02378000	-0.82288800	-0.20767900
C	-5.31379900	0.53950900	-0.18578700
H	-4.51531900	2.52953600	-0.01530800
H	-2.19214900	1.78946500	0.18972500
H	-3.46703500	-2.30832500	-0.10385600
H	-5.82191500	-1.54810800	-0.31032500
C	-1.29435100	-0.86069500	0.15018700
O	-1.05355700	-1.97420100	0.54593400
N	-0.27608200	0.01943500	-0.24690100
C	1.06097700	-0.19978900	-0.19628900
C	1.90890700	0.93587500	-0.45196200
C	1.71315800	-1.38874800	0.17990200
C	3.30762100	0.76350100	-0.72727000
C	3.08630800	-1.46105700	0.08353400
H	1.13644900	-2.24704200	0.48194200
C	3.91912900	-0.40818200	-0.38261200
H	3.85441200	1.62728500	-1.08931500
H	3.56005700	-2.39767000	0.36012000
C	5.40075100	-0.61978100	-0.51004200
H	5.84743900	-0.78767300	0.47209000
H	5.61184600	-1.49735200	-1.12360600
H	5.88416700	0.24426300	-0.96365900
H	-6.34070500	0.87559300	-0.26898100
H	-0.55670100	0.89219700	-0.67638700
H	2.06893800	1.17553400	0.77520700
F	1.28936500	2.01535100	-1.00316100
O	2.31521700	1.37587600	2.19085100
H	1.51276000	1.53327800	2.70214300
H	2.92942400	2.09696900	2.37274600

Int9

1 1

C	-4.38243900	1.38635600	0.56499900
C	-3.05434800	0.98138600	0.48820000
C	-2.73901700	-0.28152000	-0.01709200
C	-3.76099800	-1.13846500	-0.42771900
C	-5.08524700	-0.72687800	-0.36129300
C	-5.39699700	0.53712700	0.13417400
H	-4.62342400	2.36268700	0.96815700
H	-2.28030300	1.64404900	0.86014600
H	-3.50271700	-2.12237200	-0.80064200
H	-5.87455500	-1.39103200	-0.69293800
C	-1.33495400	-0.79725600	-0.10657500
O	-1.08489700	-1.98671800	-0.07713500
N	-0.37027200	0.16961400	-0.23745300
C	1.01026900	-0.02678700	-0.31181500
C	1.79977200	1.10785200	-0.54894800
C	1.67811300	-1.23984200	-0.15115300
C	3.17044900	1.07301200	-0.63141900
C	3.07589400	-1.28765900	-0.23333800
H	1.11412200	-2.13972400	0.03491000
C	3.84471200	-0.14707800	-0.48026300
H	3.70703400	1.99665600	-0.81642900
H	3.56855900	-2.24719600	-0.12037600
C	5.34195300	-0.21118900	-0.61238300
H	5.72840900	-1.16579600	-0.25633700
H	5.63234200	-0.09919000	-1.65963600
H	5.82336700	0.59046800	-0.05013100
H	-6.43089200	0.85721600	0.19116400
H	-0.68008400	1.11869700	-0.38835400
H	3.18483400	-0.42296600	1.59276500
F	1.15893900	2.28148400	-0.68930700
O	3.00143800	-0.00462600	2.48013300
H	3.75801600	0.51081000	2.81011500

H	2.70145300	-0.65656700	3.13727400

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C	4.14014600	1.39458200	0.50101500
C	2.81162400	0.98348100	0.51631600
C	2.46741500	-0.28377200	0.04180200
C	3.46412300	-1.13881500	-0.43004600
C	4.78842200	-0.72213800	-0.45502500
C	5.12769700	0.54655400	0.00934900
H	4.40313200	2.37491200	0.88024300
H	2.06137700	1.64589700	0.93471700
H	3.18537500	-2.12668300	-0.77694200
H	5.55659600	-1.38613500	-0.83362500
C	1.06044200	-0.80633200	0.04972200
O	0.82500900	-1.99997200	0.10283900
N	0.08952500	0.15273700	-0.02079300
C	-1.30025000	-0.04003900	0.00287900
C	-2.09653900	1.09230800	-0.19193600
C	-1.95933700	-1.25019600	0.21755000
C	-3.47036500	1.05938000	-0.18227300
C	-3.35297700	-1.29195400	0.22947200
H	-1.38345700	-2.14921700	0.36989800
C	-4.13037800	-0.15479800	0.03224800
H	-4.01645400	1.98297800	-0.34129700
H	-3.84001400	-2.24633200	0.39839800
H	0.38655700	1.10224100	-0.19182700
C	-5.63498800	-0.20591400	0.04539300
H	-5.99252900	-1.22003200	0.22416000
H	-6.04180700	0.44003200	0.82683900
H	-6.04682600	0.13630200	-0.90679500
H	6.16177200	0.87092900	-0.00497700
F	-1.46118700	2.26795900	-0.39719500

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C	-0.37822900	3.51579600	-1.15690500
C	0.61654200	2.56567300	-0.94358700
C	0.77650700	1.99939000	0.32247300
C	-0.06176700	2.38821400	1.37090500
C	-1.04576400	3.34704800	1.15740500
C	-1.20614300	3.90898800	-0.10875800
H	-0.51179700	3.94104800	-2.14423400
H	1.23639700	2.24326200	-1.77337500
H	0.06741200	1.93604600	2.34780900
H	-1.68708200	3.65391300	1.97481100
C	1.77872600	0.91718600	0.59915100
O	1.50859600	0.00547200	1.36985800
N	2.95743600	1.03705700	-0.06124200
C	4.07154400	0.16831300	-0.01161700
C	5.27895300	0.64655500	-0.52940000
C	4.01367900	-1.13074000	0.49514400
C	6.40766500	-0.15785200	-0.53395800
H	5.33101900	1.65336200	-0.93161100
C	5.15990600	-1.92049000	0.48282900
H	3.08994900	-1.51896600	0.89489000
C	6.37282400	-1.45767600	-0.02311400
H	7.33384300	0.23382200	-0.94246500
H	5.09894400	-2.92927700	0.87899500
H	3.10793000	1.90393200	-0.55840300
C	7.61193000	-2.31364800	-0.00021700
H	8.20769800	-2.17178500	-0.90356900
H	8.24606300	-2.05672500	0.85272300
H	7.36101000	-3.37192200	0.08154500
H	-1.97856600	4.64965000	-0.27820500
N	-1.48722800	-0.79984600	-0.68982400
C	-1.32634500	-1.12915200	0.76041500
C	-2.20942200	0.49928200	-0.86119500
C	-2.20872600	-1.90104700	-1.39943100
C	-2.71003800	-0.95735900	1.40259200

H	-0.58163200	-0.44775100	1.17431700
H	-0.95078000	-2.14835100	0.81258800
C	-3.68179500	0.24364300	-0.50087300
H	-2.09487100	0.79982500	-1.90008800
H	-1.72809800	1.21932500	-0.20317000
H	-2.42628100	-1.54918800	-2.40503100
H	-1.53932500	-2.75661000	-1.43662900
C	-3.46941000	-2.20522700	-0.57340900
H	-2.81580300	0.00472100	1.90017600
H	-2.89619400	-1.75681200	2.11586300
N	-3.76765500	-1.02292400	0.31874300
H	-4.29995400	0.11227100	-1.38447600
H	-4.07486500	1.06496100	0.09447900
H	-4.31825500	-2.36597100	-1.23264300
H	-3.34114000	-3.07323500	0.06984800
C	-5.10873500	-1.16950700	0.99267000
H	-5.12364600	-2.13801800	1.48373600
H	-5.20959400	-0.35933000	1.70870300
Cl	-6.43517500	-1.08325400	-0.15903400
F	-0.24249800	-0.67166700	-1.24136900

TS4

2 1

C	0.24793900	4.14943700	-1.30869300
C	0.85154200	2.92952300	-1.03533100
C	1.64090100	2.78946600	0.11131700
C	1.81791300	3.87420900	0.97660100
C	1.21450400	5.09000300	0.69549700
C	0.42939500	5.22764400	-0.44698900
H	-0.36694100	4.25559200	-2.19379400
H	0.67398700	2.10121500	-1.71022000
H	2.43112500	3.75040200	1.86073400
H	1.35562600	5.92966100	1.36472800
C	2.32035700	1.53396700	0.49391100
O	2.87339800	1.32180300	1.52878400

N	2.27491300	0.46056100	-0.51725500
C	2.98093600	-0.74769000	-0.34190400
C	3.71664500	-1.24904900	-1.41499400
C	2.89327000	-1.45356500	0.86310100
C	4.40081400	-2.44599300	-1.26697600
H	3.76637800	-0.70210700	-2.35004700
C	3.57608900	-2.64916400	0.98373500
H	2.29072300	-1.07571400	1.67732300
C	4.34554900	-3.16165800	-0.06984100
H	4.98290200	-2.82906700	-2.09717200
H	3.50956900	-3.20469400	1.91287700
H	2.29145900	0.80396700	-1.47615700
C	5.09098200	-4.45504600	0.10113200
H	5.54172300	-4.78347400	-0.83475500
H	5.88688000	-4.34054600	0.84123800
H	4.42523100	-5.24217000	0.46068600
H	-0.04331200	6.17769500	-0.66642000
N	-1.25869700	-0.32934400	-0.08774400
C	-1.39142400	-0.39905300	1.36181400
C	-2.08660400	0.73641700	-0.63992600
C	-1.56138700	-1.61384400	-0.70718400
C	-2.89836900	-0.49221800	1.69373400
H	-0.95974800	0.49748300	1.80419200
H	-0.84439800	-1.26990800	1.71912000
C	-3.56480400	0.28525800	-0.54332500
H	-1.81403500	0.90294200	-1.68069500
H	-1.90363000	1.64867100	-0.07336500
H	-1.56131100	-1.48687000	-1.78808800
H	-0.79160600	-2.33370300	-0.43355200
C	-2.94448000	-2.07583400	-0.18748700
H	-3.30766000	0.46136000	2.02161200
H	-3.10327600	-1.25085300	2.44633300
N	-3.63826400	-0.87737600	0.42490300
H	-3.94271600	-0.06807600	-1.49928000
H	-4.21431700	1.07503300	-0.16978100

H	-3.56908100	-2.45637400	-0.99169600
H	-2.86444800	-2.82732600	0.59657600
C	-5.04922500	-1.19743200	0.81382800
H	-5.02973400	-2.08983000	1.43206700
H	-5.44703400	-0.34678400	1.35929900
Cl	-6.08206000	-1.50220600	-0.58457200
F	0.57628400	0.09304400	-0.37286100

TS4'

0 1

C	0.72387900	3.71793200	1.59406800
C	1.43964800	2.64342200	1.08302500
C	2.20539400	1.85090800	1.94491700
C	2.24909500	2.14080100	3.31407600
C	1.53794300	3.21919200	3.81456600
C	0.77494800	4.00758600	2.95419000
H	0.12080300	4.31377100	0.92058900
H	1.34683800	2.43106500	0.02554100
H	2.84383200	1.51569700	3.96884800
H	1.57496200	3.44542400	4.87303600
C	2.98757900	0.68099000	1.50421800
O	3.53585200	-0.11426800	2.20071400
N	3.07354600	0.50290400	0.02905800
C	3.89732700	-0.49825000	-0.53536500
C	4.74239500	-0.14482100	-1.58455200
C	3.81985700	-1.81820800	-0.08135600
C	5.54469600	-1.11742000	-2.16287200
H	4.78198200	0.88017500	-1.93616000
C	4.62172400	-2.77186600	-0.67963600
H	3.13483600	-2.08735600	0.71085100
C	5.49962500	-2.44022500	-1.72092600
H	6.21108500	-0.84171400	-2.97201400
H	4.56567100	-3.79979600	-0.33834100
H	3.12181700	1.38884500	-0.47407600
C	6.36389000	-3.50067900	-2.34293700

H	6.95726300	-3.10124500	-3.16464000
H	7.04562900	-3.92309300	-1.60111300
H	5.75265800	-4.32096000	-2.72540700
H	0.21536200	4.84816000	3.34765300
F	1.46312400	0.09841100	-0.28268700
N	-0.43130900	-0.31078100	-0.58174500
C	-1.13829800	0.52559300	0.37884100
C	-0.78547300	0.04520000	-1.95150900
C	-0.67866700	-1.72209900	-0.31475500
C	-2.63595600	0.15436800	0.33149700
H	-0.74055700	0.33473500	1.37530200
H	-0.98694800	1.56776300	0.10677700
C	-2.32844900	-0.00500400	-2.09412600
H	-0.30230200	-0.66167100	-2.62499300
H	-0.42880200	1.05033000	-2.16481600
C	-2.13563300	-2.03657200	-0.72325700
H	-0.52810300	-1.90948200	0.74624200
H	0.01706500	-2.32640900	-0.89579600
N	-2.87450200	-0.72539000	-0.88517700
H	-2.94623700	-0.42139200	1.19799400
H	-3.25292100	1.04180700	0.20849100
H	-2.76419800	0.99138200	-2.09971600
H	-2.63389500	-0.55327600	-2.98225800
H	-2.65210900	-2.62525800	0.02950300
H	-2.18584600	-2.54283500	-1.68441600
C	-4.34910200	-0.94027300	-0.95757000
H	-4.82446400	0.02126100	-1.12661600
H	-4.65504200	-1.38651200	-0.01511800
Cl	-4.81421600	-2.02903800	-2.27492600
F	-0.29868800	3.23335900	-1.32559400
B	-1.59129400	3.49030100	-1.83994200
F	-1.79103300	4.85919200	-1.95891400
F	-1.71528400	2.85464800	-3.08392300
F	-2.54029600	2.93569900	-0.95240000
F	-3.76689900	-2.31629200	1.95121700

B	-2.57934300	-2.68062500	2.63895900
F	-1.92458900	-3.67600800	1.89949800
F	-2.89004300	-3.13157700	3.91331600
F	-1.74662700	-1.54416300	2.70719900

Int10

2 1

C	-0.70455600	4.05681500	-1.24720400
C	0.21449700	3.03422700	-1.06243600
C	0.47531700	2.57690600	0.23407000
C	-0.17054800	3.15539500	1.33704800
C	-1.09045000	4.17118400	1.13801700
C	-1.35991500	4.61809400	-0.15444500
H	-0.91259300	4.41151600	-2.24846900
H	0.68828800	2.60400500	-1.93543000
H	0.06153400	2.80651200	2.33609400
H	-1.59266400	4.61681000	1.98720900
C	1.40125000	1.49827300	0.56539300
O	1.71497100	1.03887300	1.59771700
N	2.21281800	0.90970400	-0.71346400
C	3.20577600	-0.10013600	-0.41810800
C	4.50131100	0.10157100	-0.86640900
C	2.82776500	-1.23766600	0.28805200
C	5.45176200	-0.87448200	-0.59463700
H	4.77222800	0.99582800	-1.41691300
C	3.78731000	-2.20104700	0.53432800
H	1.81146300	-1.35798500	0.63854200
C	5.11014500	-2.03432800	0.10031600
H	6.46934800	-0.73036800	-0.93747200
H	3.51194800	-3.09726500	1.07847700
H	2.64759100	1.68763900	-1.22435600
C	6.13193100	-3.09736400	0.38996000
H	7.10187800	-2.84642400	-0.03724700
H	6.25317500	-3.22646500	1.46771800
H	5.81181300	-4.05803700	-0.01864000

H	-2.08012700	5.41223000	-0.31020400
N	-0.89793000	-0.25554300	0.16065400
C	-1.26354100	-0.39537400	1.57072200
C	-1.91192900	0.56820900	-0.50841000
C	-0.89452900	-1.58192600	-0.46707300
C	-2.74583800	-0.80914800	1.70470200
H	-1.11064000	0.55421900	2.08535800
H	-0.61019300	-1.13731100	2.03064200
C	-3.25160700	-0.19460600	-0.61524900
H	-1.56445400	0.83033900	-1.50771400
H	-2.04385100	1.49079400	0.05863900
H	-0.79366100	-1.45191700	-1.54437700
H	-0.04121800	-2.16225300	-0.12003800
C	-2.18965200	-2.35033300	-0.12183300
H	-3.39452100	0.03356700	1.94021100
H	-2.89409100	-1.59274500	2.44574700
N	-3.20734300	-1.34607700	0.36308000
H	-3.40477000	-0.62260900	-1.60337900
H	-4.10957300	0.42562500	-0.35984900
H	-2.60752800	-2.86428100	-0.98429900
H	-2.04911500	-3.06590100	0.68780000
C	-4.54734400	-1.97221900	0.57071700
H	-4.41498600	-2.84594500	1.20221200
H	-5.19408500	-1.23797200	1.04183700
Cl	-5.29803900	-2.48659800	-0.94587400
F	1.26888400	0.40452400	-1.59899900

Int11

2 1

C	0.22043700	3.46216700	-1.78023400
C	0.79481400	2.31859400	-1.24060600
C	0.83475800	2.15684300	0.14738500
C	0.31305200	3.14359500	0.98919600
C	-0.26471600	4.28022600	0.44293400
C	-0.31320200	4.43715100	-0.94146500

H	0.18301600	3.58888600	-2.85513500
H	1.19166700	1.55912500	-1.90355900
H	0.36669000	3.00738800	2.06314900
H	-0.67478400	5.04378800	1.09241300
C	1.39623300	0.94725700	0.78223400
O	1.39598600	0.70571000	1.96049500
N	1.92577700	-0.01859400	-0.14529000
C	3.11304500	-0.48455000	-0.03782000
C	3.49050700	-1.53335200	-0.99615700
C	4.10575500	-0.04854100	0.95600000
C	4.71672800	-2.09713900	-0.94600800
H	2.74567600	-1.82580700	-1.72732900
C	5.32295100	-0.62902600	0.97296300
H	3.84754000	0.73589900	1.65464300
C	5.66079300	-1.65678800	0.02953200
H	5.00341800	-2.87288000	-1.64375600
H	6.07183300	-0.32067200	1.69163800
H	0.80792500	-0.56023800	-1.40907000
C	6.99217800	-2.27516200	0.09588200
H	7.25839500	-2.80503000	-0.81535800
H	7.75906700	-1.55197500	0.37643300
H	6.95255900	-3.00997500	0.91651200
H	-0.76653000	5.32438800	-1.36769600
N	-1.15292400	-0.26634000	0.20573000
C	-1.58262400	0.05881400	1.56721900
C	-1.97067400	0.50047300	-0.73943400
C	-1.37046100	-1.69931600	-0.02436100
C	-3.11925400	-0.04445100	1.68516900
H	-1.27375900	1.07372200	1.81798400
H	-1.09136900	-0.62396400	2.26033000
C	-3.42183600	-0.02980500	-0.74882400
H	-1.54428400	0.41199500	-1.73804400
H	-1.94355000	1.55204100	-0.44687100
H	-1.21414800	-1.90364400	-1.08194300
H	-0.63773200	-2.27093100	0.54569400

C	-2.79639300	-2.10852800	0.40694900
H	-3.60941900	0.92700900	1.63066400
H	-3.43249500	-0.55337700	2.59560600
N	-3.62670000	-0.85030800	0.50580300
H	-3.61256400	-0.69033900	-1.59161000
H	-4.16357400	0.76786000	-0.74569000
H	-3.27117000	-2.76857300	-0.31554700
H	-2.82317600	-2.57535000	1.39109800
C	-5.06703700	-1.15172800	0.75597200
H	-5.12979600	-1.81389900	1.61410900
H	-5.58029900	-0.21312700	0.94288200
Cl	-5.84354700	-1.94695800	-0.62024600
F	0.48887500	-0.83482500	-2.25713100

HF

0 1

F	0.00000000	0.00000000	0.09231900
H	0.00000000	0.00000000	-0.83086900

Selectfluor

0 1

N	0.24546000	1.01137100	0.06184700
C	0.14500000	-0.12956800	-0.92989800
H	1.14178400	-0.30194200	-1.32224500
H	-0.54093200	0.18070700	-1.71407100
C	1.26582200	0.69053100	1.12796800
H	2.25758800	0.75682400	0.69092900
H	1.15640800	1.43669300	1.91072100
C	-1.10065800	1.18062000	0.71666600
H	-1.84452600	1.25784800	-0.07152600
H	-1.08543400	2.09058400	1.31103600
C	-0.40925300	-1.37675300	-0.22655800
H	0.23295800	-2.23693200	-0.39886200
H	-1.44536000	-1.58411000	-0.48025400
C	-1.36382900	-0.04217800	1.61568000

H	-1.21418700	0.16205500	2.67326100
H	-2.35269200	-0.45765500	1.43976900
C	1.00980800	-0.72652600	1.66160500
H	1.68653100	-1.46070600	1.23306100
H	1.03543700	-0.75836900	2.74758600
N	-0.37353600	-1.09921000	1.23926100
C	0.65956100	2.21771100	-0.73229700
H	-0.13027900	2.43407500	-1.44492500
H	1.59425600	1.96125900	-1.22433500
Cl	0.91170400	3.63211400	0.28847500
B	3.64262300	-0.97271200	-0.66103700
F	3.21397700	0.25574400	-1.23199600
F	3.90531900	-0.75598400	0.69981300
F	4.75542000	-1.45030500	-1.32288600
F	2.56688900	-1.88821000	-0.76181900
B	-3.88171500	-0.38610300	-0.71522100
F	-5.04001000	-0.55011400	-1.45063800
F	-4.02131800	0.63648500	0.23762700
F	-2.79688000	-0.05038200	-1.56454800
F	-3.54177400	-1.57979000	-0.03949400
F	-0.72353700	-2.25081600	1.89175200

Com'

2 1

C	-5.79822057	-1.48091356	0.01913009
C	-4.75781022	-0.56972718	0.15982809
C	-3.43330919	-1.00868373	0.09926800
C	-3.16107672	-2.36554025	-0.08065118
C	-4.20188517	-3.27193269	-0.23119297
C	-5.52173525	-2.82958875	-0.18382649
H	-6.82415979	-1.13753234	0.07602928
H	-4.99070053	0.47190356	0.35130159
H	-2.13101548	-2.70021236	-0.10443836
H	-3.98537567	-4.32272286	-0.38247808
C	-2.27246421	-0.07984480	0.25446011
O	-1.17622161	-0.48186261	0.64037761
N	-2.49563909	1.21771090	-0.07320490
C	-1.52727684	2.24943970	0.06870236
C	-1.25634637	3.09561295	-1.00308584

C	-0.87818667	2.44702228	1.28762772
C	-0.34074717	4.13211570	-0.85254873
C	0.04532394	3.47521886	1.41794266
H	-1.10894153	1.80336958	2.12884055
C	0.33177125	4.33338079	0.35247463
H	-0.14109978	4.78784863	-1.69359060
H	0.54565788	3.61948898	2.37028193
H	-3.33970891	1.44333723	-0.57920621
C	1.36714953	5.41674945	0.49498988
H	2.36665739	5.01581140	0.30350563
H	1.19473799	6.22762330	-0.21335664
H	1.36883442	5.83341451	1.50320039
H	-6.33466940	-3.53738254	-0.29680160
F	1.92624419	2.02719867	-0.64416397
N	2.09511104	0.67656307	-0.51369654
C	1.14240330	0.00006738	-1.44401101
C	3.50719078	0.34065053	-0.86561757
C	1.79509092	0.30626103	0.90550157
C	1.14570990	-1.48802790	-1.06766602
H	1.48510866	0.19543398	-2.45735572
H	0.16403444	0.44511279	-1.27247327
C	3.58507890	-1.19173687	-0.97088938
H	4.13677372	0.75030527	-0.08018586
H	3.72910960	0.82163889	-1.81496973
H	2.35140331	0.99253615	1.53952011
H	0.72097859	0.42153007	1.03653431
C	2.25138638	-1.14956550	1.09422596
H	1.15176916	-2.10923313	-1.95973046
H	0.28885743	-1.72872921	-0.44089909
N	2.39385550	-1.79283404	-0.26536498
H	4.49096258	-1.55474270	-0.49252624
H	3.55725029	-1.53409862	-2.00304404
H	3.21287473	-1.21719463	1.59659907
H	1.50500723	-1.70654242	1.65755592
C	2.50889463	-3.29161953	-0.17078910
H	1.57143052	-3.66673760	0.22890488
H	2.69377404	-3.66944457	-1.17180233
Cl	3.82467764	-3.78854552	0.88571050
H	-1.76443485	2.94449820	-1.94941086

TS5

2 1

C	-5.18118375	-2.51686010	-1.17328585
C	-4.47774441	-1.38041405	-0.79065304

C	-3.62596389	-1.43072774	0.31511697
C	-3.49481607	-2.61645206	1.04091044
C	-4.18887467	-3.75188842	0.64768120
C	-5.03187496	-3.70263385	-0.46054637
H	-5.85082206	-2.47274181	-2.02362089
H	-4.63283493	-0.45630131	-1.33697850
H	-2.84373985	-2.63439341	1.90674146
H	-4.07656672	-4.67394860	1.20528315
C	-2.86329003	-0.24499830	0.80564787
O	-2.51724848	-0.12089394	1.95816379
N	-2.55397805	0.69805710	-0.17402603
C	-1.91553270	1.89908119	0.00274316
C	-1.32969481	2.49603276	-1.16010630
C	-1.73681604	2.52829878	1.24404040
C	-0.71986060	3.77537283	-1.07108269
C	-1.06532918	3.73104276	1.29089254
H	-2.12805089	2.08311281	2.14432894
C	-0.54360645	4.38554495	0.14191136
H	-0.35751099	4.23606552	-1.98279082
H	-0.94047169	4.21143506	2.25648920
H	-2.70168462	0.41250183	-1.13291476
C	0.14776737	5.71122203	0.29091069
H	1.02597616	5.61801021	0.93389618
H	0.47016301	6.09964845	-0.67465548
H	-0.51689526	6.44491322	0.75247992
H	-5.57832499	-4.58779534	-0.76447778
F	0.17689026	1.34514551	-0.93234613
N	1.51441695	0.20785824	-0.67248924
C	1.08183525	-1.08514938	-1.18636653
C	2.71240710	0.69407194	-1.34952525
C	1.67780074	0.18672164	0.77762894
C	2.09513214	-2.13203983	-0.66412398
H	1.06465608	-1.04027623	-2.27283515
H	0.08065006	-1.29708121	-0.81400762
C	3.77455104	-0.42847068	-1.24052147
H	3.03489832	1.60996915	-0.85943045
H	2.47512804	0.90118985	-2.39053347
H	1.77106982	1.21106545	1.13391651
H	0.79072234	-0.26759604	1.21500646
C	2.96172707	-0.62212713	1.07842327
H	2.40336978	-2.81428027	-1.45313027
H	1.70356176	-2.70061409	0.17649313
N	3.32986977	-1.39951551	-0.16860752
H	4.74442462	-0.02652754	-0.95934900

H	3.86910789	-0.99556828	-2.16436768
H	3.80146235	0.02478622	1.31765509
H	2.81093811	-1.33406101	1.88743550
C	4.37864710	-2.43677401	0.10852093
H	3.95632198	-3.15557506	0.80449155
H	4.64092049	-2.90615979	-0.83489623
Cl	5.83305403	-1.74321625	0.82399019
H	-1.59625427	2.10782180	-2.13569564

Int12

2 1

C	-5.55916856	-1.20382307	-1.27690545
C	-4.51409242	-0.39103202	-0.85749264
C	-3.86435411	-0.66887057	0.34860284
C	-4.27101836	-1.75148778	1.13420873
C	-5.30667550	-2.56587124	0.70309732
C	-5.94929618	-2.29269357	-0.50295180
H	-6.07097556	-0.98322315	-2.20534608
H	-4.25012058	0.47195557	-1.45839015
H	-3.76275035	-1.94586105	2.07090184
H	-5.61436132	-3.41210610	1.30491360
C	-2.75888785	0.16150926	0.87745330
O	-2.42122374	0.20472153	2.02783976
N	-2.04427601	0.91170062	-0.11604388
C	-1.12059407	1.83971180	0.09465276
C	-0.56281608	2.47908059	-1.13868511
C	-0.74322742	2.38783239	1.34570290
C	0.74370403	3.16351654	-0.97246717
C	0.32029778	3.24198419	1.38006514
H	-1.24595749	2.09063034	2.25119839
C	1.13930405	3.59611721	0.23587828
H	1.28125824	3.40124294	-1.88452564
H	0.61063157	3.64793976	2.34467356
H	-2.20025540	0.65258471	-1.08596680
C	2.38438743	4.40161175	0.46288425
H	3.04421672	3.89745938	1.17239688
H	2.92677045	4.55497772	-0.46878648
H	2.13409011	5.37746587	0.88449933
H	-6.76054654	-2.92810388	-0.83809740
F	-0.57339092	1.58483034	-2.18417288
N	1.11288663	0.19846777	-0.22340016
C	0.44160873	-1.05825540	-0.56666525
C	2.21184620	0.41597556	-1.17540972
C	1.67403074	0.08191183	1.12498679

C	1.35969837	-2.26132222	-0.26113259
H	0.17094722	-1.02938201	-1.62214678
H	-0.47155194	-1.16602299	0.01809345
C	3.07014993	-0.86046065	-1.31397430
H	2.81823287	1.24805401	-0.81615958
H	1.80134149	0.68619121	-2.14749204
H	2.02806072	1.05835233	1.45859389
H	0.88410621	-0.23987788	1.80487976
C	2.85618633	-0.91415312	1.13523360
H	1.34766582	-3.00544474	-1.05578284
H	1.11209570	-2.74377485	0.68316280
N	2.77741673	-1.74581854	-0.12574554
H	4.13507689	-0.63973593	-1.31656604
H	2.82202606	-1.43791618	-2.20402833
H	3.81890179	-0.40879148	1.12278316
H	2.82322560	-1.59556174	1.98414625
C	3.68097455	-2.93468170	-0.07979797
H	3.33477566	-3.58862256	0.71513272
H	3.63498815	-3.42890008	-1.04565548
Cl	5.36220021	-2.49749364	0.24851587
H	-1.29352474	3.27256969	-1.38374024

VII

1 2

C	3.98609200	1.49638600	0.49267800
C	2.65651300	1.09843200	0.43199300
C	2.34036400	-0.19009600	-0.00733500
C	3.35622500	-1.07814200	-0.37144800
C	4.68019200	-0.66983200	-0.32167000
C	4.99473500	0.61752900	0.10961800
H	4.23307500	2.49044900	0.84428600
H	1.88754600	1.78576400	0.76695600
H	3.09370000	-2.07709000	-0.69820100
H	5.46737800	-1.35289100	-0.61635600
C	0.94976800	-0.70190700	-0.06297800
O	0.65051200	-1.86383400	-0.01880600
N	-0.04904500	0.30952500	-0.21349800
C	-1.38521400	0.18421900	-0.11623200
C	-2.17311400	1.33426200	-0.45732700
C	-2.03949600	-1.01012400	0.32638000

C	-3.52912500	1.28125400	-0.37752400
H	-1.67191400	2.23798500	-0.78387200
C	-3.40300000	-1.03123500	0.40159400
H	-1.45635000	-1.87526600	0.59678000
C	-4.18736600	0.09645100	0.05312100
H	-4.12269200	2.14804400	-0.64254800
H	-3.90179900	-1.93081800	0.74100200
H	0.29249700	1.21975200	-0.50374600
C	-5.67062600	0.06260000	0.12928700
H	-6.04118200	-0.87809200	0.53008700
H	-6.03445900	0.88849600	0.74707300
H	-6.09232600	0.21427200	-0.86970700
H	6.03005400	0.93461100	0.15224500

VIII

1 2

C	0.19344900	1.66257900	-0.14916500
C	1.67635600	1.29531700	0.09240400
H	0.01720100	2.03397400	-1.15692500
H	-0.17279200	2.39048600	0.57221500
H	2.31462300	1.74837100	-0.66288300
H	2.01500700	1.60930500	1.07780900
C	-0.30954000	-0.53009800	-1.15502900
H	-0.78349300	-1.48509200	-0.94186200
H	-0.74658100	-0.10698200	-2.05788500
C	1.23074000	-0.65183800	-1.24481700
H	1.52919900	-1.68992100	-1.37302200
H	1.63699200	-0.06344100	-2.06528400
C	1.19387800	-0.80479300	1.15764800
H	1.22125500	-1.88079000	0.99788500
H	1.78180800	-0.56438600	2.04082100
C	-0.25510400	-0.28012500	1.30055700
H	-0.96383000	-1.08412300	1.48250100
H	-0.35053500	0.46990000	2.08433300
N	1.78460600	-0.15037300	0.00213700

N	-0.63709700	0.39739000	-0.00026700
C	-2.07516600	0.81219300	-0.00078700
H	-2.25370700	1.39860800	0.89535500
H	-2.25583200	1.39822000	-0.89700400
Cl	-3.17821200	-0.56715100	0.00009300
F	3.67556100	-0.58678800	-0.00173400

Int14

2 2

C	5.65508300	-2.42390500	1.18520800
C	4.63887000	-1.53060300	0.86905800
C	4.81708800	-0.62112600	-0.17677200
C	6.00714400	-0.61970700	-0.90888700
C	7.02308600	-1.50427900	-0.57969200
C	6.84741400	-2.40590400	0.46811500
H	5.51231400	-3.13659300	1.98810300
H	3.70602400	-1.58429000	1.41947700
H	6.12455200	0.08378000	-1.72428300
H	7.95072100	-1.49313500	-1.13877400
C	3.76828300	0.34306800	-0.59982600
O	3.69758800	0.81389800	-1.70472700
N	2.85068400	0.70385400	0.42011500
C	1.73220300	1.45701900	0.31763400
C	1.03189500	1.74184500	1.53414400
C	1.21312100	1.94947800	-0.91949900
C	-0.10924200	2.48256500	1.51517900
C	0.06512500	2.68793400	-0.91256100
H	1.73014300	1.73922700	-1.84135200
C	-0.63688000	2.97703100	0.28957900
H	-0.62708800	2.70321400	2.44129000
H	-0.32940800	3.06536300	-1.84927000
H	3.10331900	0.41611100	1.35856600
C	-1.81662100	3.88051400	0.28110600
H	-1.46705800	4.91357300	0.39334300
H	-2.48906000	3.67391300	1.11383900

H	7.64003500	-3.09964500	0.72257500
N	-2.23765600	0.83689900	0.02418000
C	-1.39409000	-0.26999800	-0.41598800
C	-2.82585300	0.50775000	1.32313300
C	-3.30191600	1.05244700	-0.95621800
C	-2.17234400	-1.60027700	-0.30419400
H	-0.50071500	-0.32227800	0.20933900
H	-1.08374900	-0.08787600	-1.44491300
C	-3.87741800	-0.61386700	1.16007800
H	-3.30466000	1.39145300	1.74477500
H	-2.02662000	0.19760100	1.99697900
H	-4.00781600	1.77712600	-0.55004000
H	-2.87636500	1.46275300	-1.87239000
C	-4.01103600	-0.28638600	-1.27177500
H	-1.90632400	-2.16637800	0.58725500
H	-2.04119800	-2.23066200	-1.18211900
N	-3.64838000	-1.27063800	-0.18284200
H	-4.89300600	-0.22540600	1.15400100
H	-3.79469700	-1.38458100	1.92502000
H	-5.09363800	-0.18464400	-1.28519500
H	-3.67990700	-0.72460000	-2.21231700
C	-4.40160100	-2.55446000	-0.31881400
H	-4.26109200	-2.92237100	-1.33064700
H	-4.00796600	-3.25359100	0.41323500
Cl	-6.13473200	-2.35839100	-0.03010600
H	-2.36206600	3.82265800	-0.66084700
H	1.42865500	1.36510200	2.46974800

TS6

2 2

C	6.58402700	-2.37255000	1.10137700
C	5.48058200	-1.58017800	0.80622900
C	5.56398600	-0.62257700	-0.20710300
C	6.74913300	-0.47578300	-0.93075200
C	7.85212900	-1.25997000	-0.62441600

C	7.77035200	-2.20808200	0.39314500
H	6.51332400	-3.12224200	1.88007800
H	4.55515000	-1.74749100	1.34666400
H	6.79321800	0.25977600	-1.72496200
H	8.77445100	-1.13486500	-1.17883200
C	4.41416500	0.24303200	-0.60498900
O	4.30311800	0.70884300	-1.71540900
N	3.49059600	0.49056300	0.41034400
C	2.30585000	1.18005000	0.33591400
C	1.59875100	1.37253700	1.55282600
C	1.76036300	1.68251400	-0.87200500
C	0.40849400	2.04100700	1.56807300
C	0.56297900	2.34829500	-0.84376400
H	2.29006300	1.54439500	-1.80012600
C	-0.15256400	2.56430100	0.36709700
H	-0.12136700	2.18278000	2.50331600
H	0.14526700	2.72995800	-1.76893000
H	3.76101900	0.18891500	1.33725400
C	-1.43096800	3.20038700	0.36569000
H	-1.67139800	3.81498100	-0.49977500
H	-2.24479900	2.21323100	0.20644400
H	-1.77926400	3.60140700	1.31617000
H	8.63020800	-2.82392000	0.62948400
N	-3.09665200	1.06328300	0.05120200
C	-2.23455700	-0.01322200	-0.46185100
C	-3.64078600	0.68357000	1.36689600
C	-4.19493100	1.32052300	-0.89564000
C	-2.99887500	-1.34667900	-0.35472400
H	-1.31978000	-0.05624400	0.13074000
H	-1.97059500	0.21818400	-1.49319200
C	-4.69087000	-0.42693100	1.16744700
H	-4.09980900	1.55611800	1.82822100
H	-2.81564900	0.34952000	1.99472000
H	-4.89644400	2.00670400	-0.42465500
H	-3.79273300	1.79182500	-1.79066000

C	-4.86489400	-0.02221500	-1.25269200
H	-2.70696600	-1.92403500	0.52084600
H	-2.87251700	-1.95634000	-1.24709900
N	-4.47572400	-1.03623000	-0.20053700
H	-5.70577000	-0.03760800	1.19084400
H	-4.59441800	-1.22086800	1.90572300
H	-5.94889800	0.06011000	-1.26007000
H	-4.52752600	-0.41611800	-2.21011400
C	-5.22165900	-2.32491400	-0.36613000
H	-5.09718800	-2.65497400	-1.39316000
H	-4.80431400	-3.04280800	0.33388600
Cl	-6.94635800	-2.15047000	-0.03380500
H	2.01810500	0.98483400	2.47433200

Int15

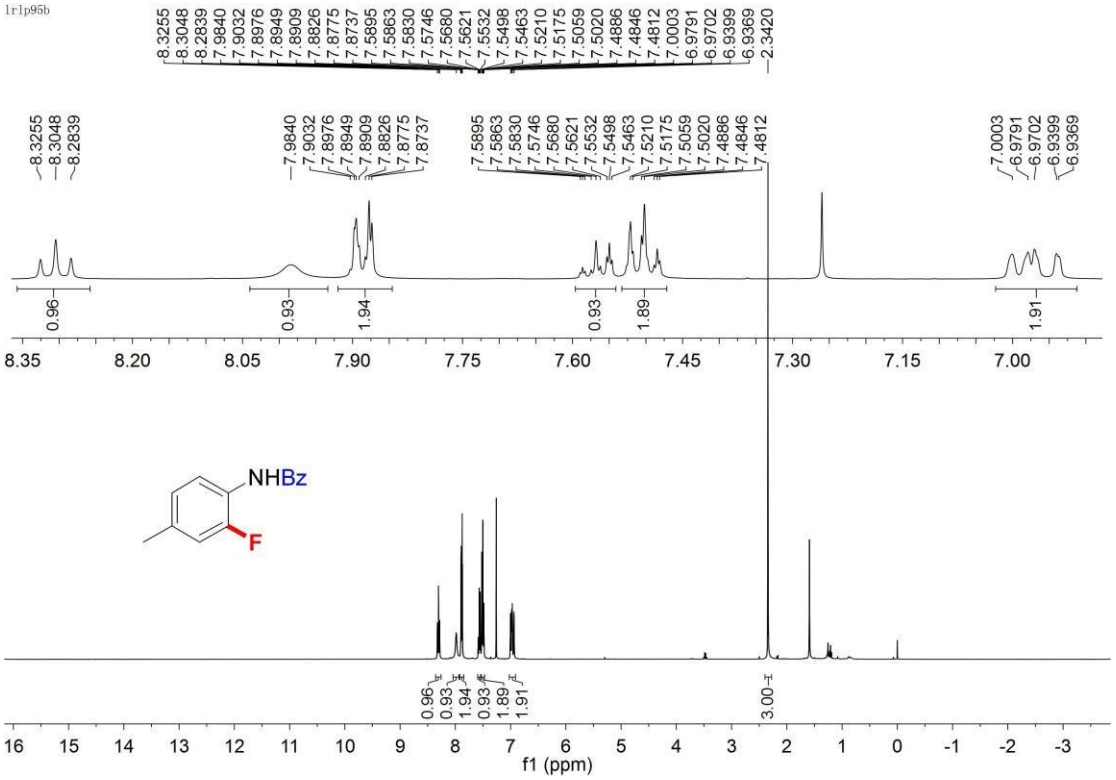
2 2

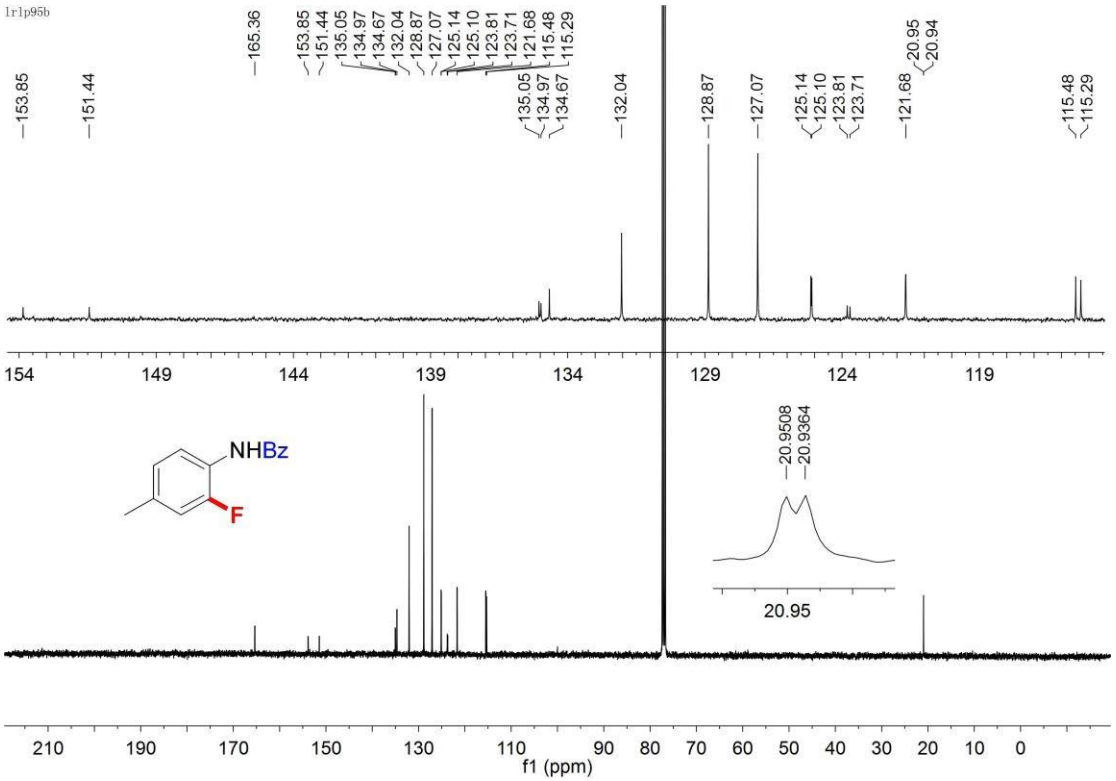
C	5.78586900	-2.39069400	1.31361600
C	4.74875700	-1.53500000	0.95854500
C	4.86125300	-0.73808200	-0.18252500
C	6.00913200	-0.81897500	-0.97231300
C	7.04809500	-1.66515500	-0.60907600
C	6.93790800	-2.45114000	0.53574700
H	5.68972100	-3.01453000	2.19422400
H	3.84581500	-1.52622200	1.55942400
H	6.07516900	-0.20929900	-1.86551500
H	7.94261700	-1.71426200	-1.21863300
C	3.77609900	0.18804100	-0.64362400
O	3.64440900	0.48210100	-1.81638500
N	2.97143000	0.67916500	0.35543400
C	1.87232800	1.53303800	0.23826700
C	1.28796400	1.99141400	1.43641100
C	1.32019600	1.94067400	-0.98954700
C	0.19706400	2.82761100	1.41796300
C	0.22402000	2.77990500	-1.00451200
H	1.75661400	1.60075100	-1.91506100

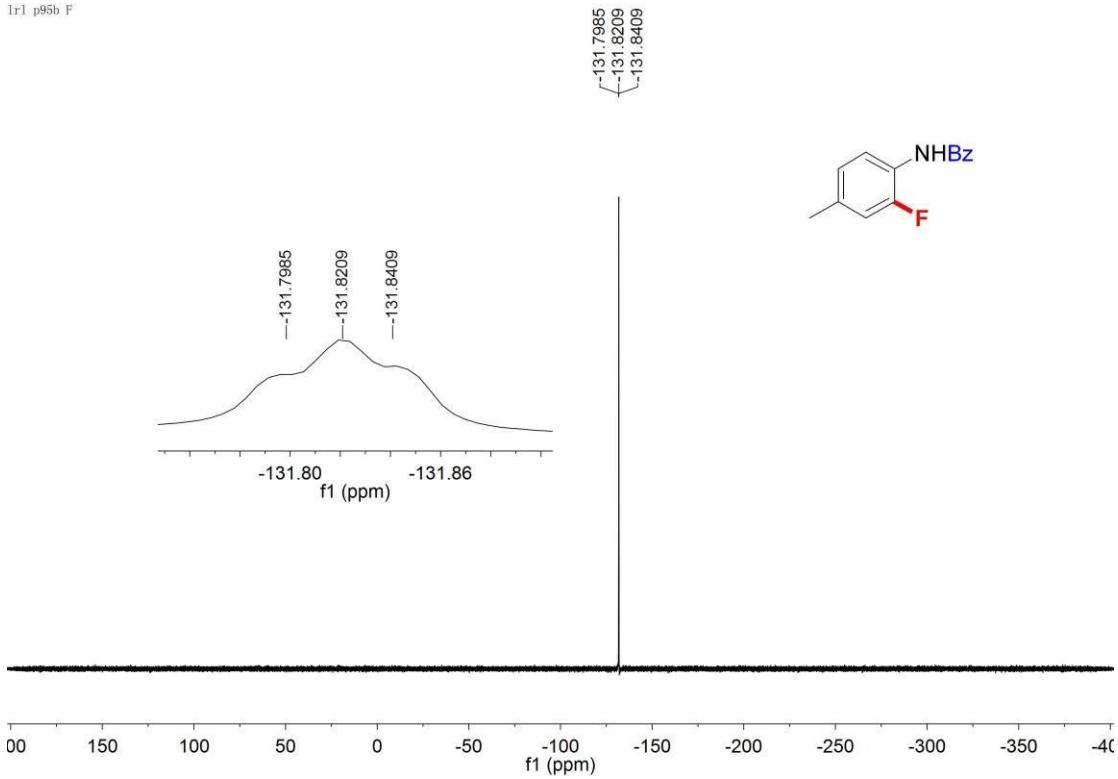
C	-0.38088600	3.25780400	0.18955100
H	-0.23426500	3.16763000	2.35335400
H	-0.19254000	3.08495500	-1.95915000
H	3.25903500	0.47857500	1.30271900
C	-1.51502100	4.09075200	0.16121200
H	-1.93042500	4.43155000	-0.77915500
H	-1.95161400	4.46672000	1.07807900
H	7.74670500	-3.11538800	0.81729400
N	-2.75386100	1.07395100	0.10936200
C	-1.64141700	0.10532500	-0.15172900
C	-3.43936200	0.71753700	1.39350300
C	-3.73356100	1.03035400	-1.02299400
C	-2.20320100	-1.30701400	0.04950500
H	-0.83271900	0.30887900	0.54838800
H	-1.28666500	0.27329000	-1.16595700
C	-4.26521400	-0.55141900	1.14529600
H	-4.07908500	1.54643000	1.68474100
H	-2.66902100	0.57360200	2.14817800
H	-4.60589000	1.60699500	-0.72473200
H	-3.27484300	1.49766800	-1.89136500
C	-4.06427500	-0.44161800	-1.30002400
H	-1.97694600	-1.70773100	1.03547200
H	-1.82193200	-1.98832900	-0.70765800
N	-3.71257200	-1.25278200	-0.07475800
H	-5.30985800	-0.32728800	0.94671300
H	-4.20145500	-1.23189000	1.99183900
H	-5.12480700	-0.56586400	-1.50317100
H	-3.48991200	-0.84767800	-2.13087300
C	-4.20732300	-2.66795400	-0.18786300
H	-3.84504300	-3.06938500	-1.12972700
H	-3.81402700	-3.22358900	0.65826300
Cl	-5.96594600	-2.76086100	-0.16149900
H	-2.36375000	2.02709700	0.17958500
H	1.70941100	1.68038500	2.38657900

VII. Copies of NMR spectra

2a



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NHBz
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-131.86
f1 (ppm)
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50
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-50
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-150
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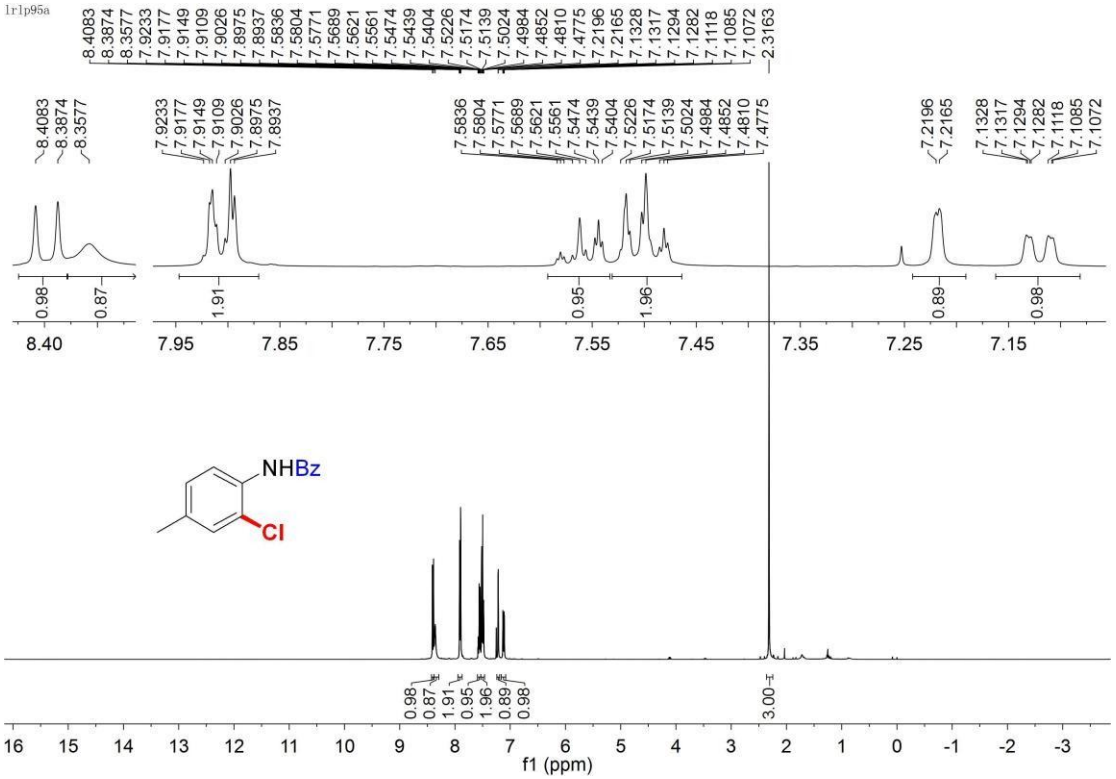
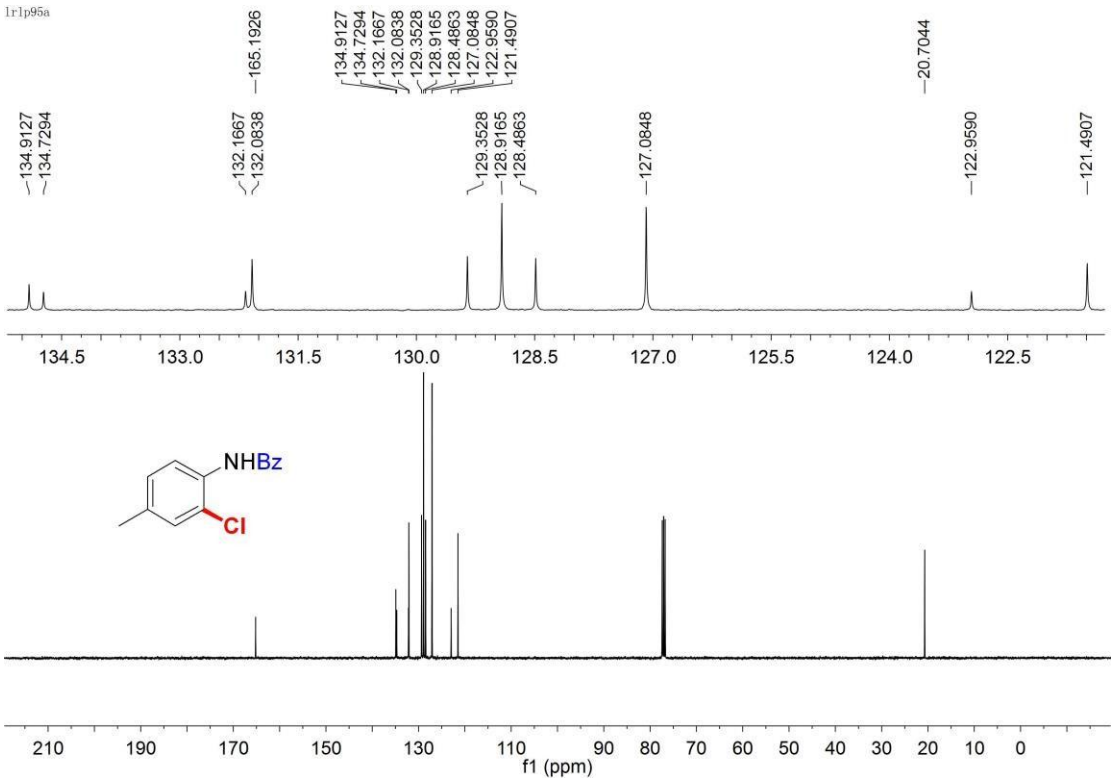
-250
-300
-350
-40
f1 (ppm)

3a





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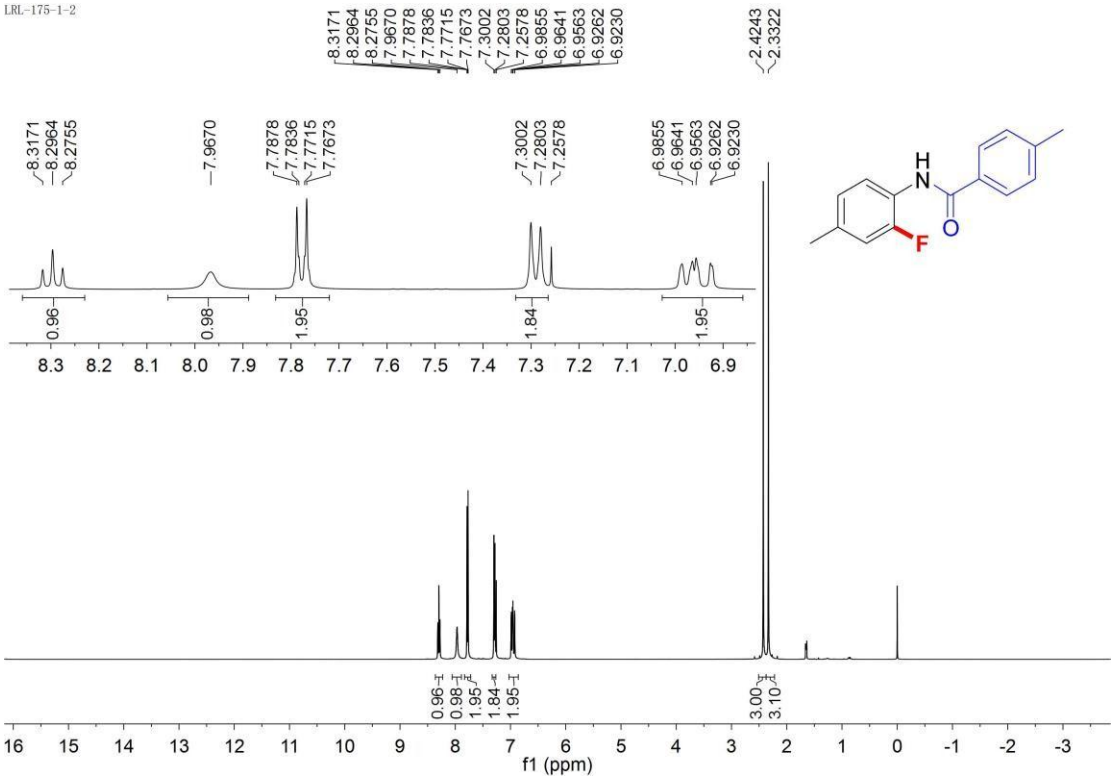
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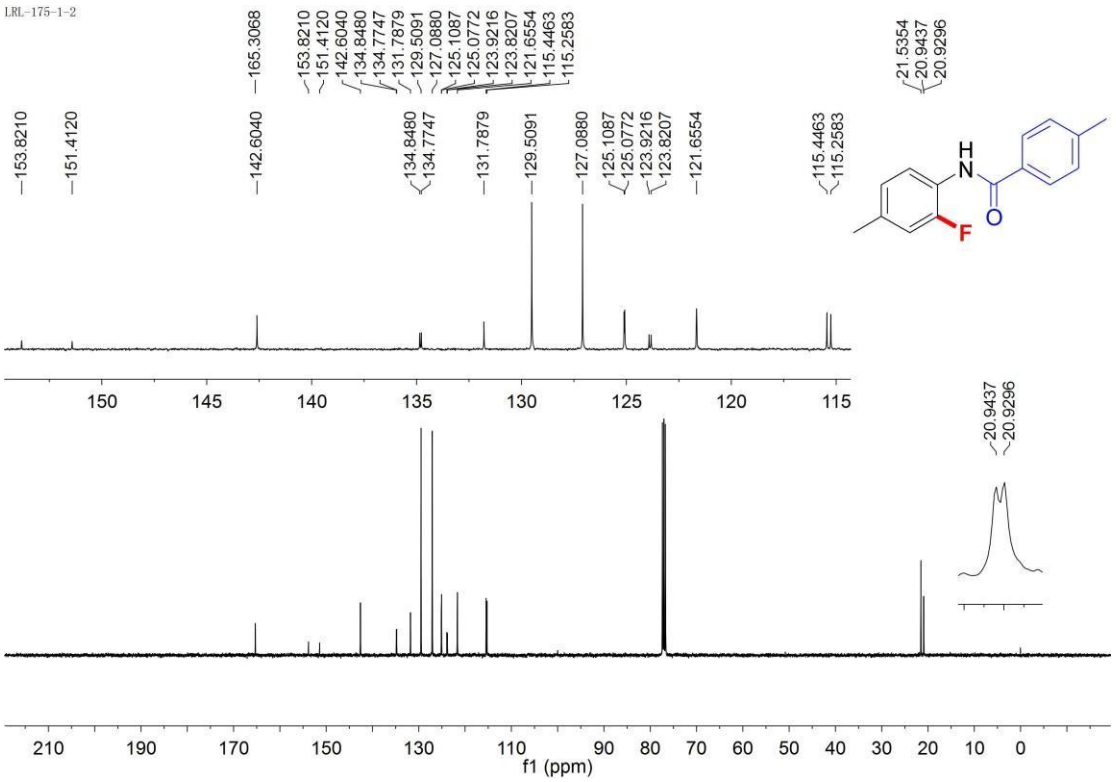
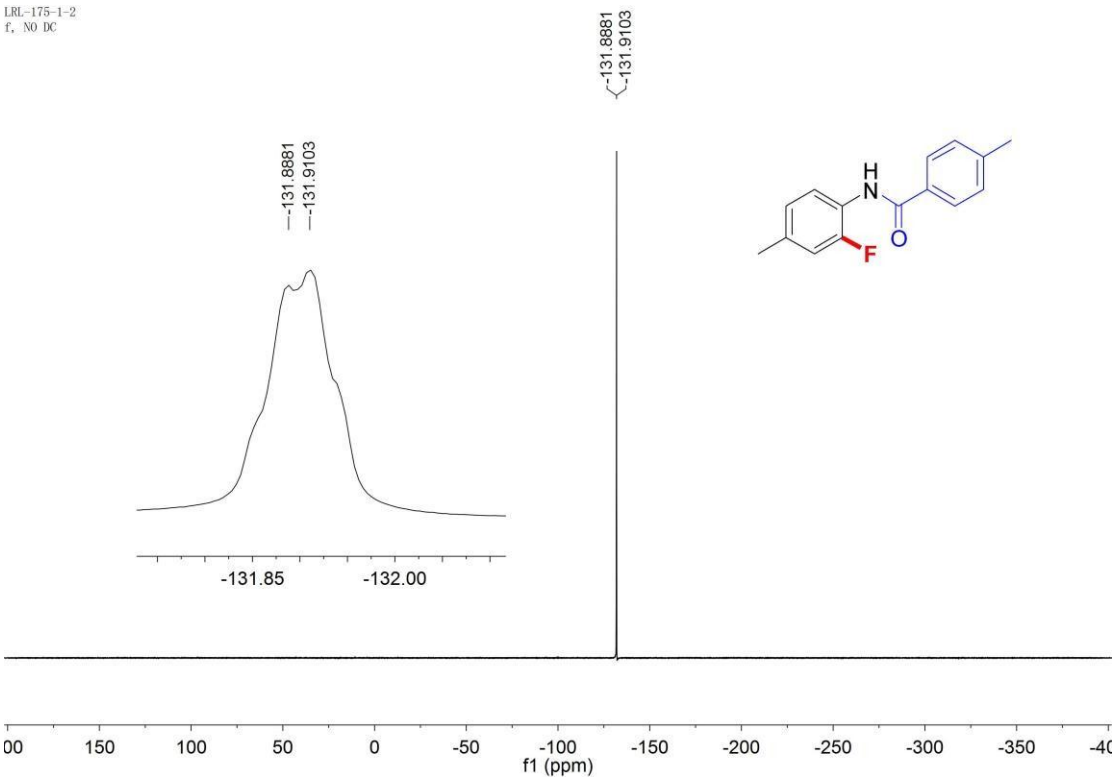
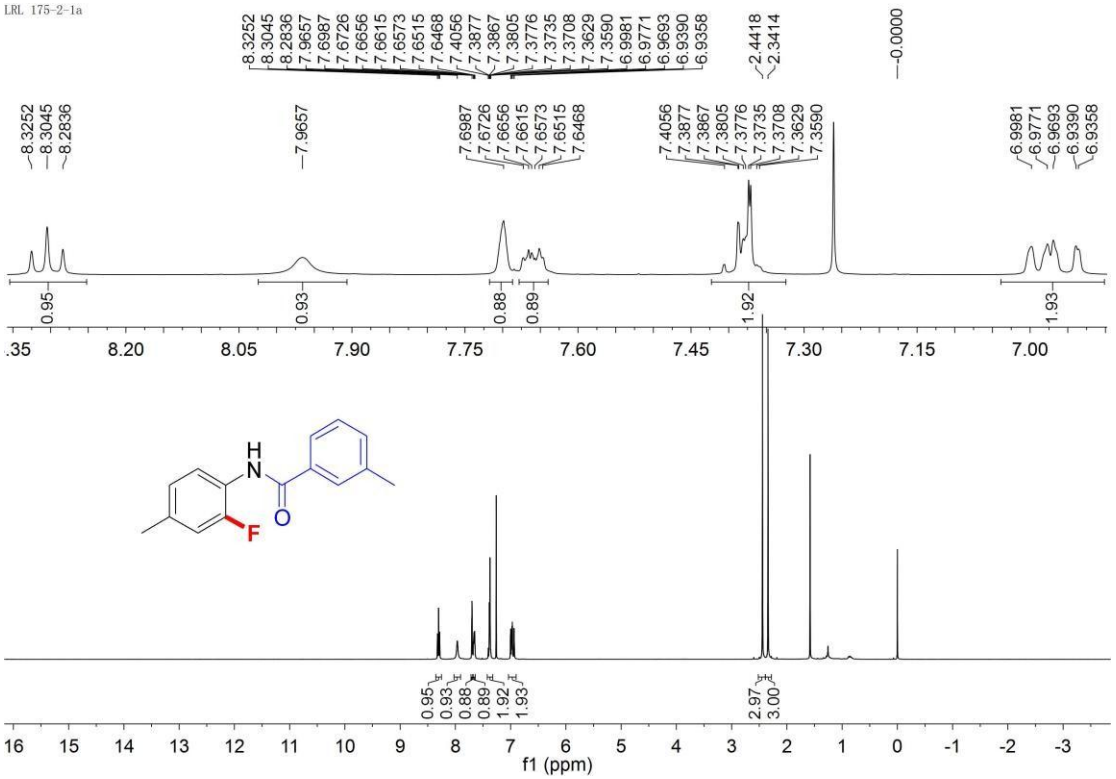
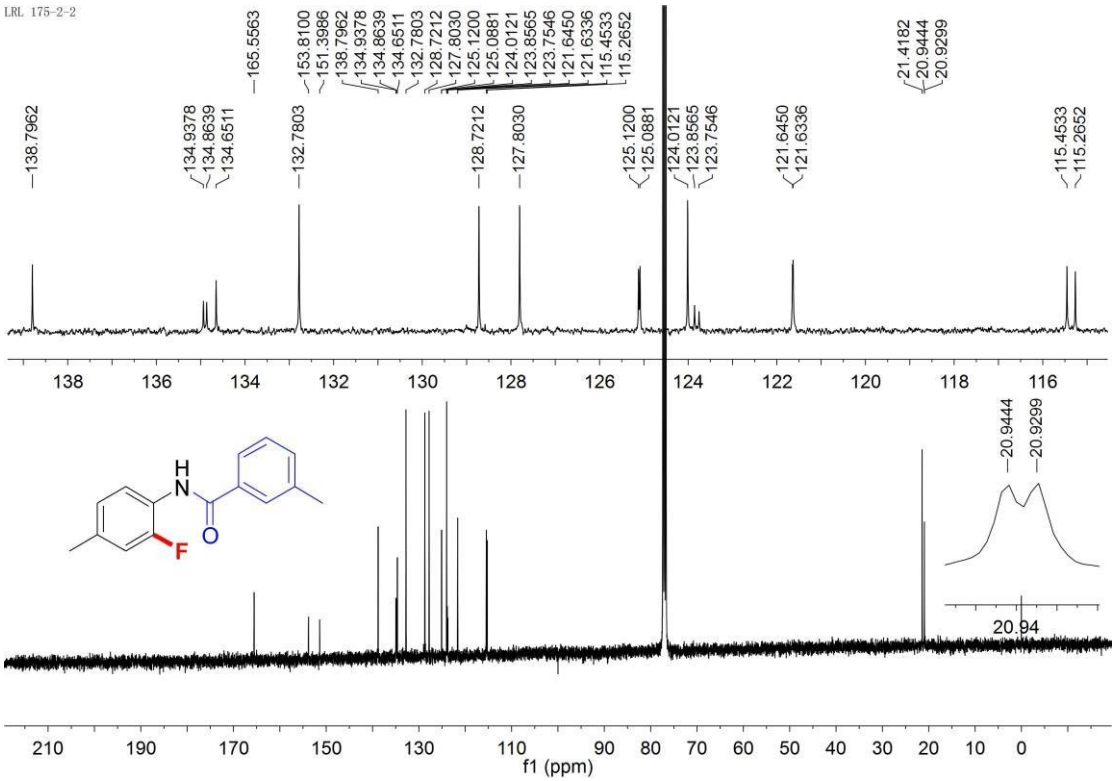
7.9670
7.7878
7.7836
7.7715
7.7673
7.3002
7.2803
7.2578
6.9855
6.9641
6.9563
6.9262
6.9230
2.4243
2.3322
0.96
0.98
1.95
1.84
1.95
3.00
3.10
f1 (ppm)

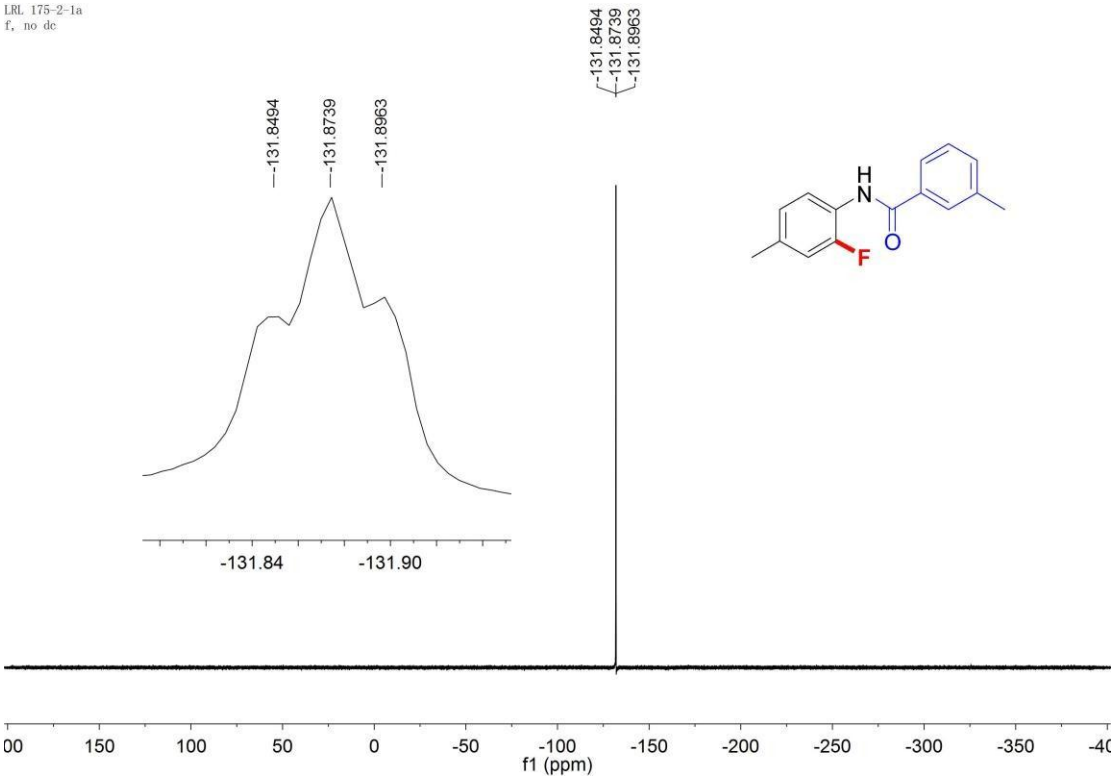

LRL-175-1-2
165.3068
153.8210
151.4120
142.6040
134.8480
134.7747
131.7879
129.5091
127.0880
125.1087
125.0772
123.9216
123.8207
121.6554
115.4463
115.2583
21.5354
20.9437
20.9296
f1 (ppm)


LRL-175-1-2
f, NO DC
-131.8881
-131.9103
-131.8881
-131.9103
H
N
O
F
-131.85
-132.00
00
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
-40
f1 (ppm)

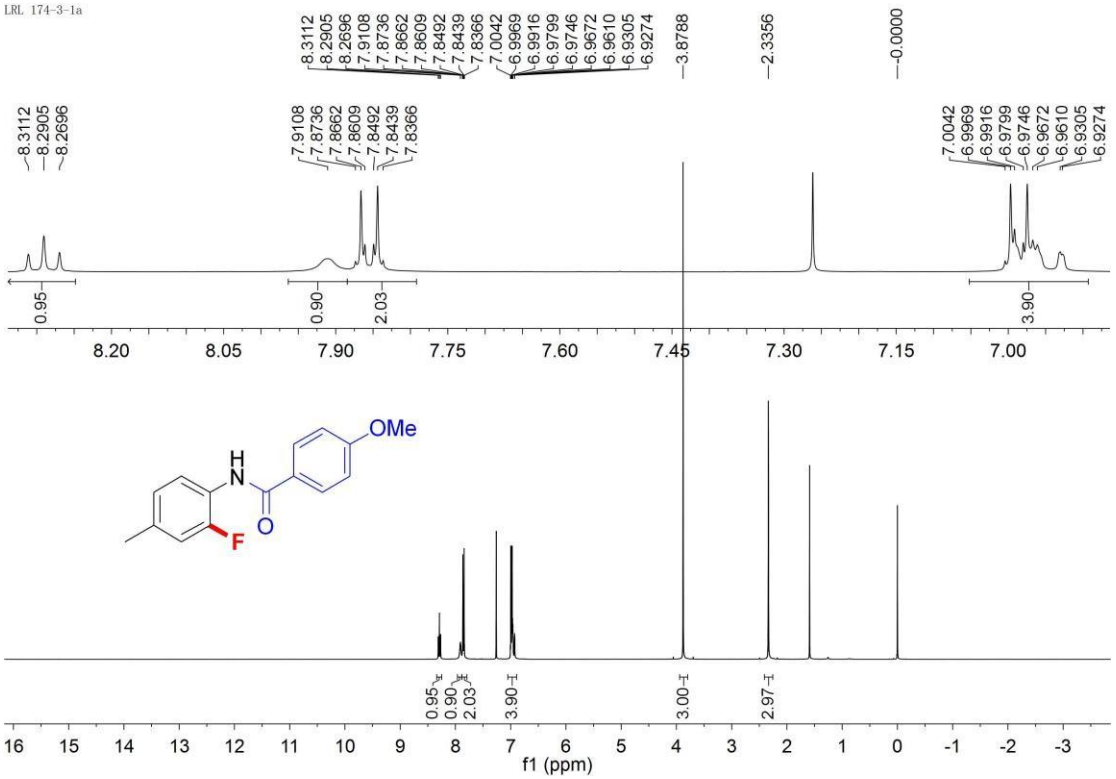
2c

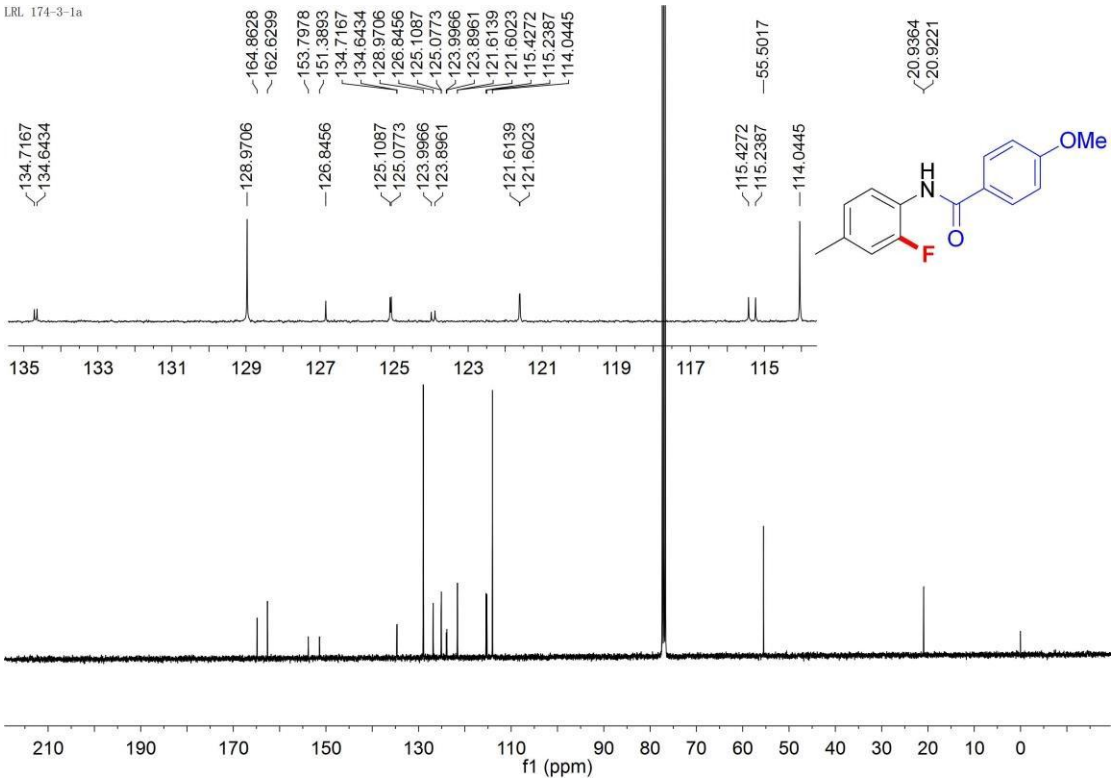

LRL 175-2-1a
8.3252
8.3045
8.2836
7.9657
7.6987
7.6726
7.6656
7.6615
7.6573
7.6515
7.6468
7.4056
7.3877
7.3867
7.3805
7.3776
7.3735
7.3708
7.3629
7.3590
6.9981
6.9771
6.9693
6.9390
6.9358
2.4418
2.3414
0.0000
0.95
0.93
0.88
0.89
1.92
1.93
2.97
3.00
f1 (ppm)

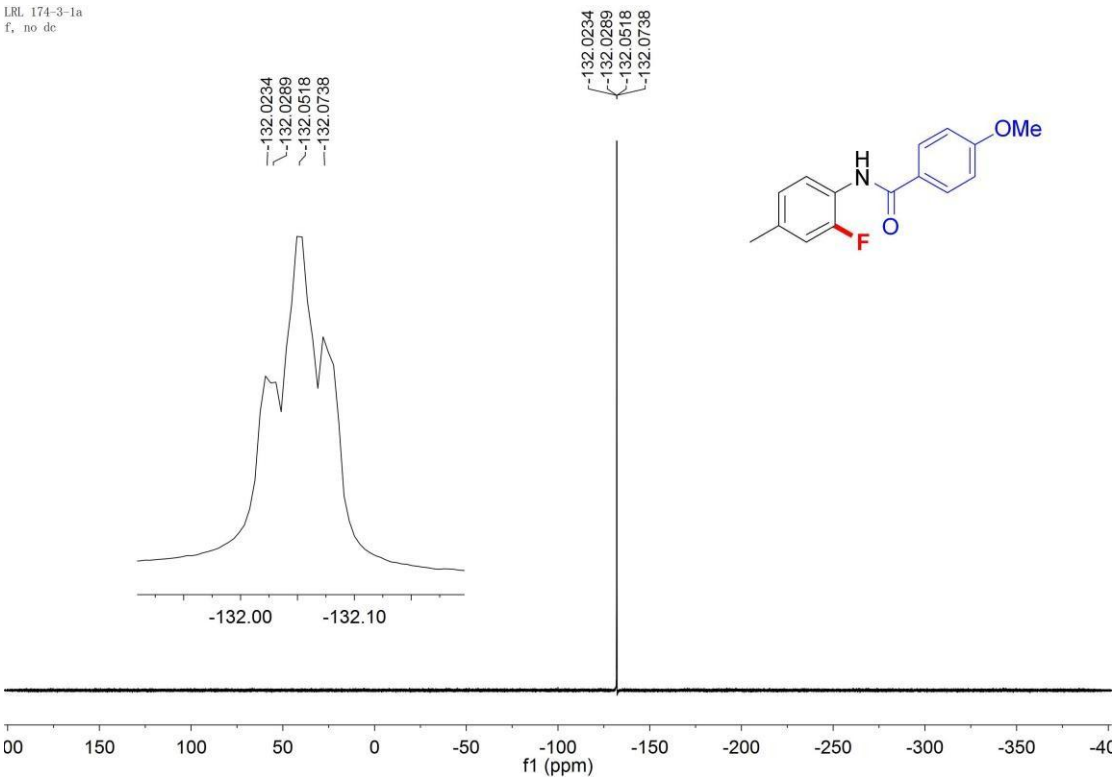

LRL 175-2-2
165.5563
153.8100
151.3986
138.7962
134.9378
134.8639
134.6511
132.7803
128.7212
127.8030
125.1200
125.0881
124.0121
123.8565
123.7546
121.6450
121.6336
115.4533
115.2652
21.4182
20.9444
20.9299
20.94
f1 (ppm)


LRL 175-2-1a
f, no dc
-131.8494
-131.8739
-131.8963
-131.84
-131.90
H
N
O
F
f1 (ppm)

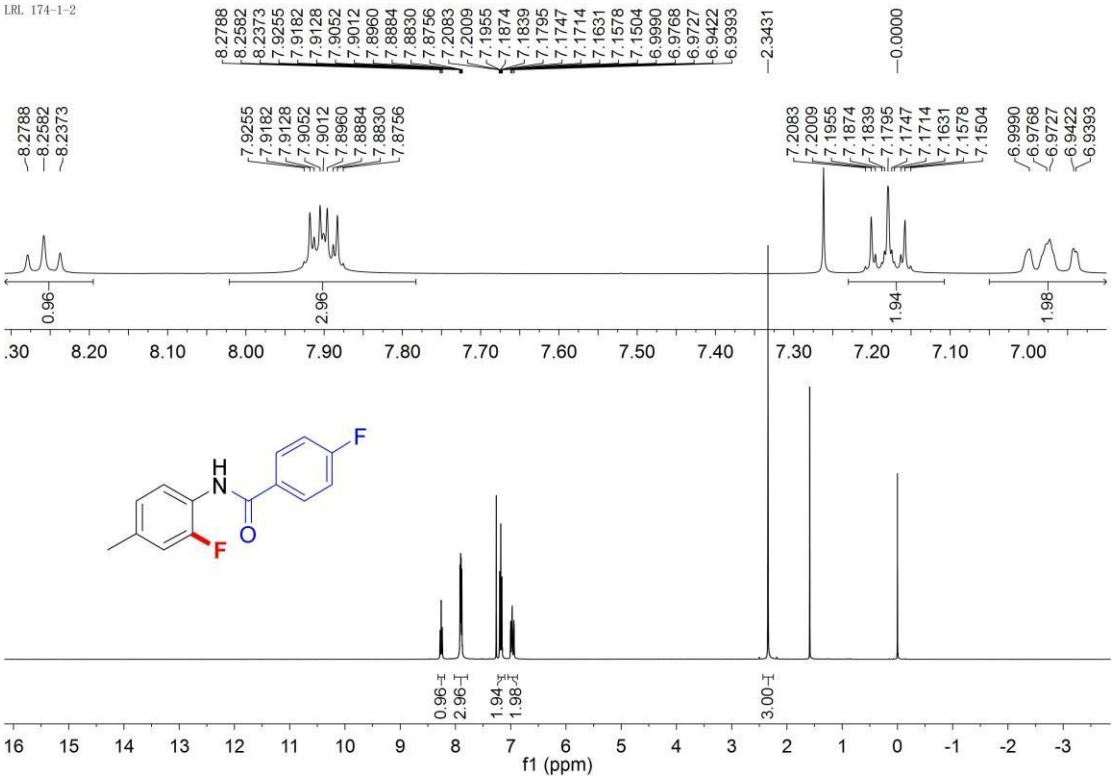
2d

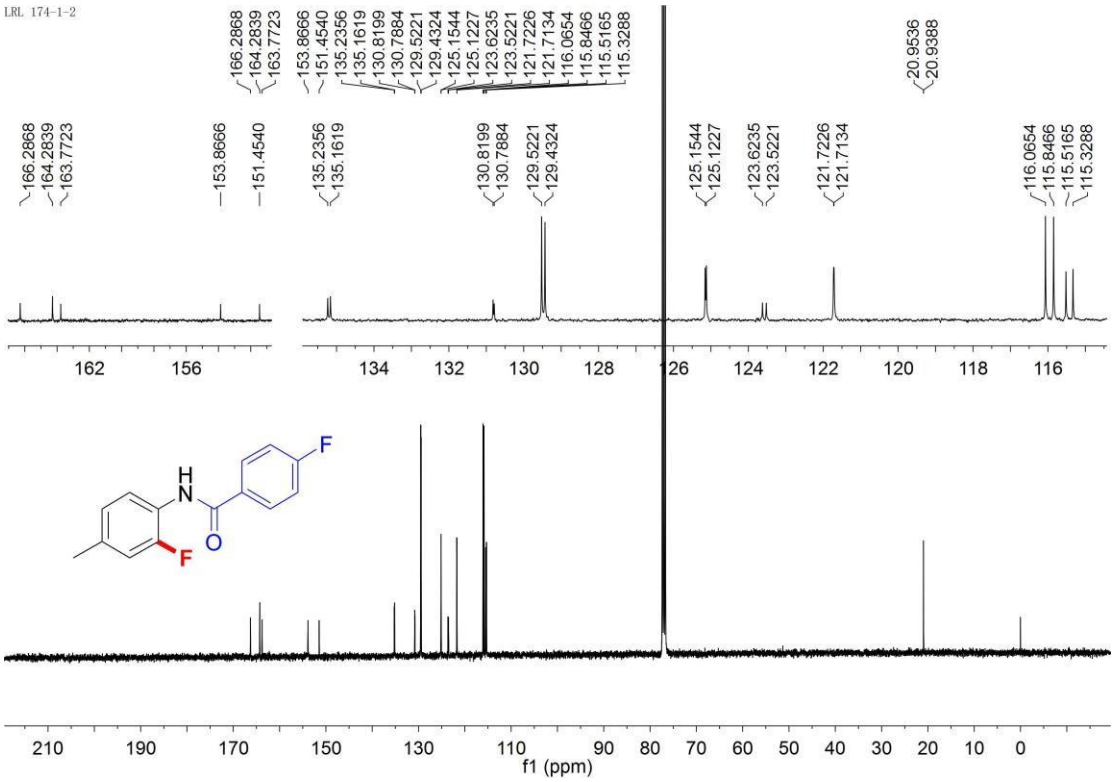

LRL 174-3-1a
8.3112
8.2905
8.2696
7.9108
7.8736
7.8662
7.8609
7.8492
7.8439
7.8366
7.0042
6.9969
6.9916
6.9799
6.9746
6.9672
6.9610
6.9305
6.9274
3.8788
2.3356
0.0000
0.95
0.90
2.03
3.90
3.00
2.97
OMe
H
N
O
F
f1 (ppm)

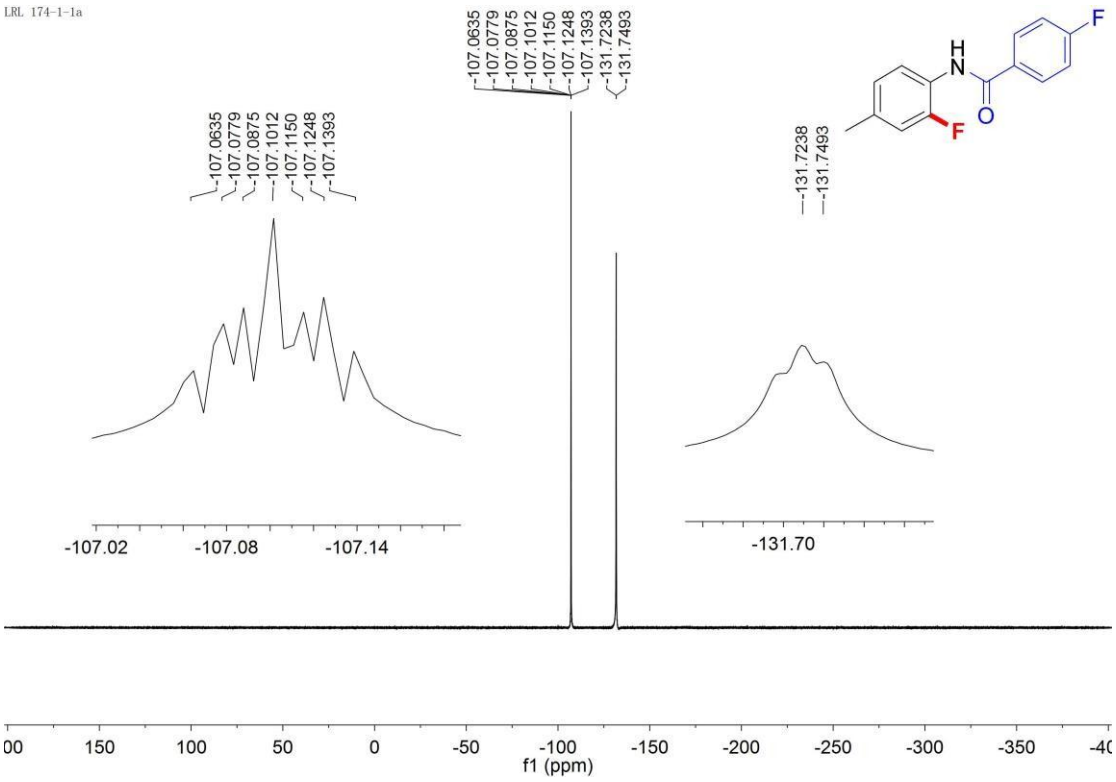

LRL 174-3-1a
164.8628
162.6299
153.7978
151.3893
134.7167
134.6434
128.9706
126.8456
125.1087
125.0773
123.9966
123.8961
121.6139
121.6023
115.4272
115.2387
114.0445
55.5017
20.9364
20.9221
OMe
H
N
O
F
f1 (ppm)


LRL 174-3-1a
f, no dc
-132.0234
-132.0289
-132.0518
-132.0738
-132.00
-132.10
OMe
H
N
O
F
f1 (ppm)

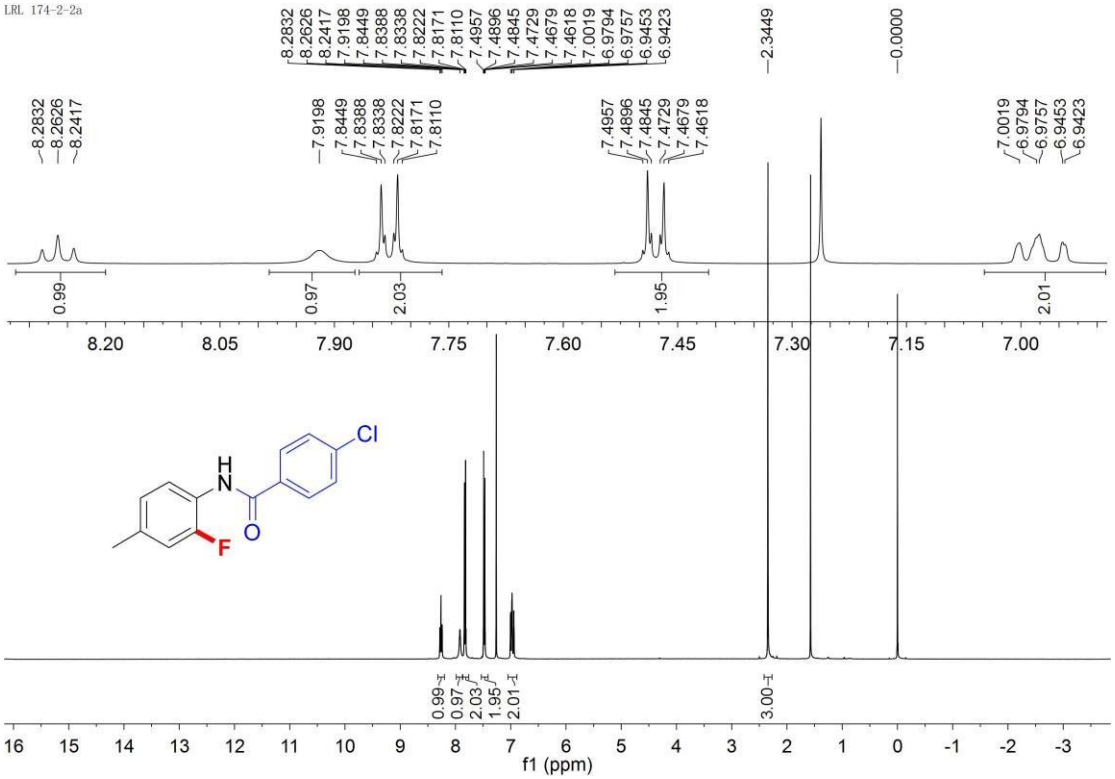
2e

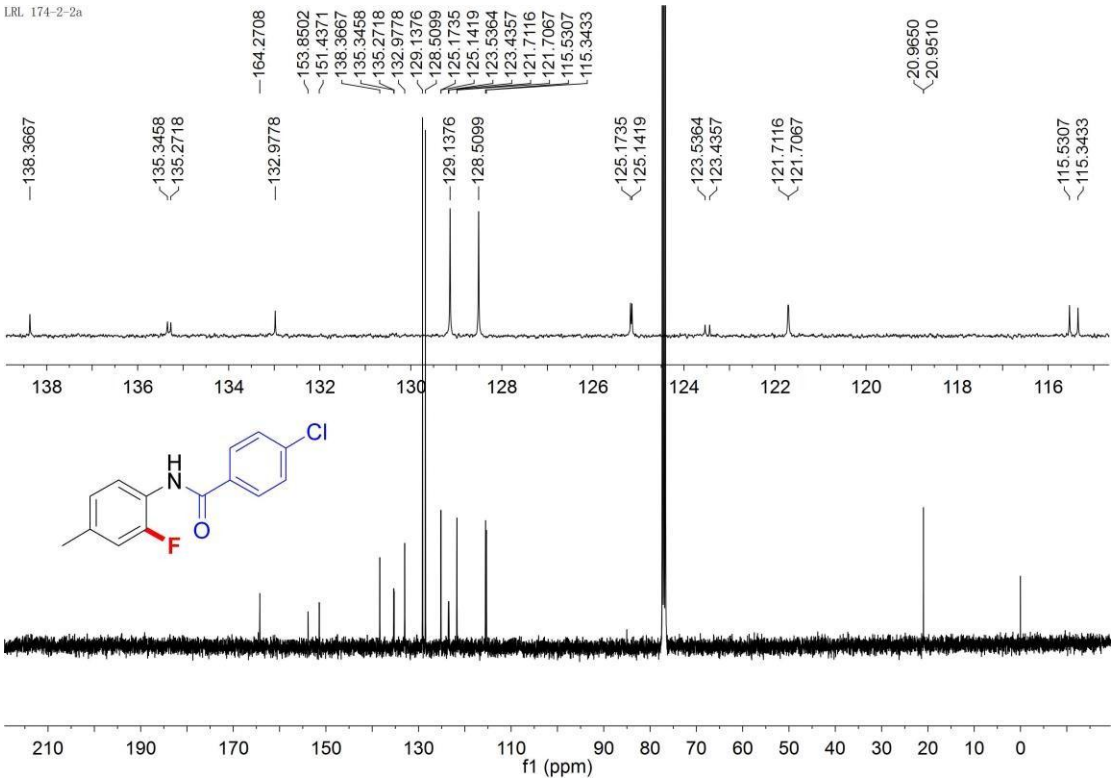

LRL 174-1-2
8.2788
8.2582
8.2373
7.9255
7.9182
7.9128
7.9052
7.9012
7.8960
7.8884
7.8830
7.8756
7.2083
7.2009
7.1955
7.1874
7.1839
7.1795
7.1747
7.1714
7.1631
7.1578
7.1504
6.9990
6.9768
6.9727
6.9422
6.9393
2.3431
0.0000
0.96
2.96
1.94
1.98
3.00
F
H
N
O
F
f1 (ppm)

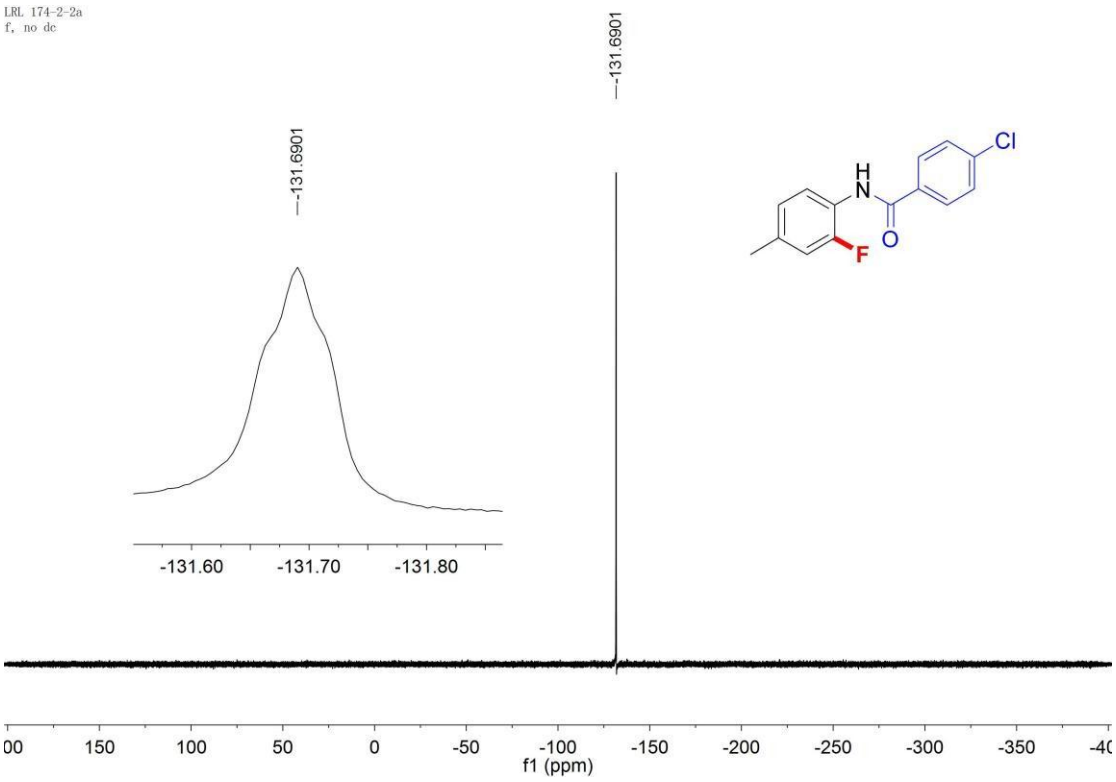

LRL 174-1-2
166.2868
164.2839
163.7723
153.8666
151.4540
135.2356
135.1619
130.8199
130.7884
129.5221
129.4324
125.1544
125.1227
123.6235
123.5221
121.7226
121.7134
116.0654
115.8466
115.5165
115.3288
20.9536
20.9388
F
H
N
O
F
f1 (ppm)


LRL 174-1-1a
-107.0635
-107.0779
-107.0875
-107.1012
-107.1150
-107.1248
-107.1393
-131.7238
-131.7493
-107.02
-107.08
-107.14
-131.70
f1 (ppm)

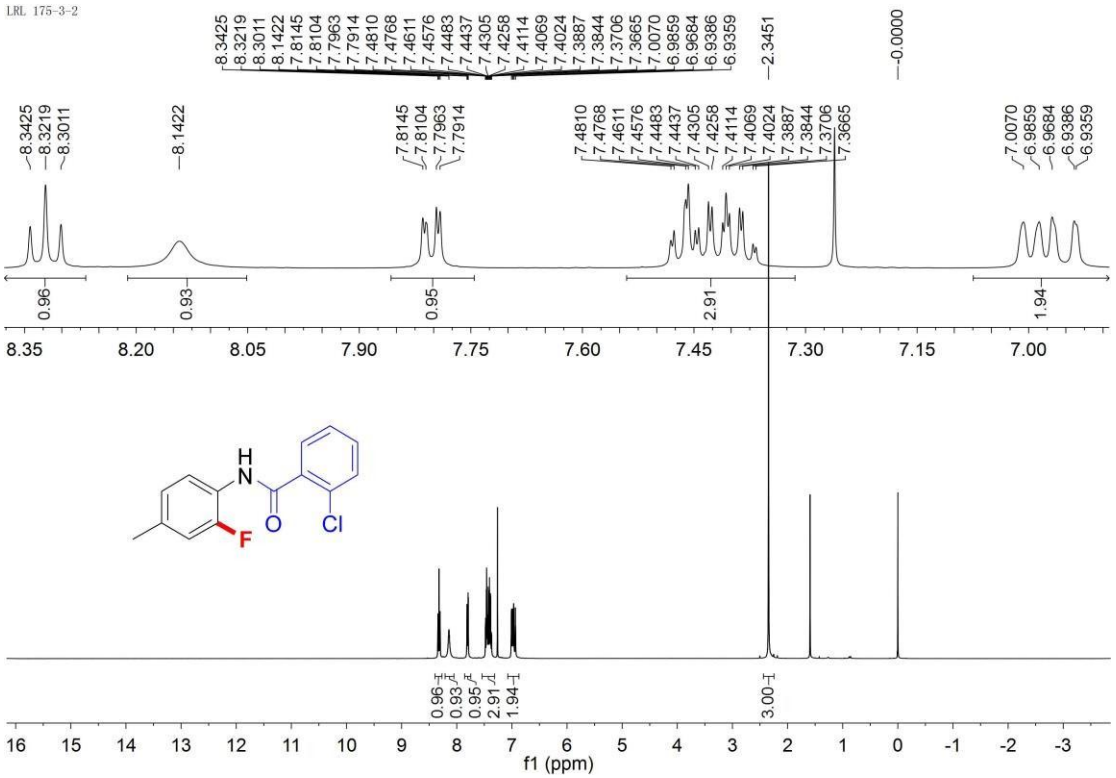
2f

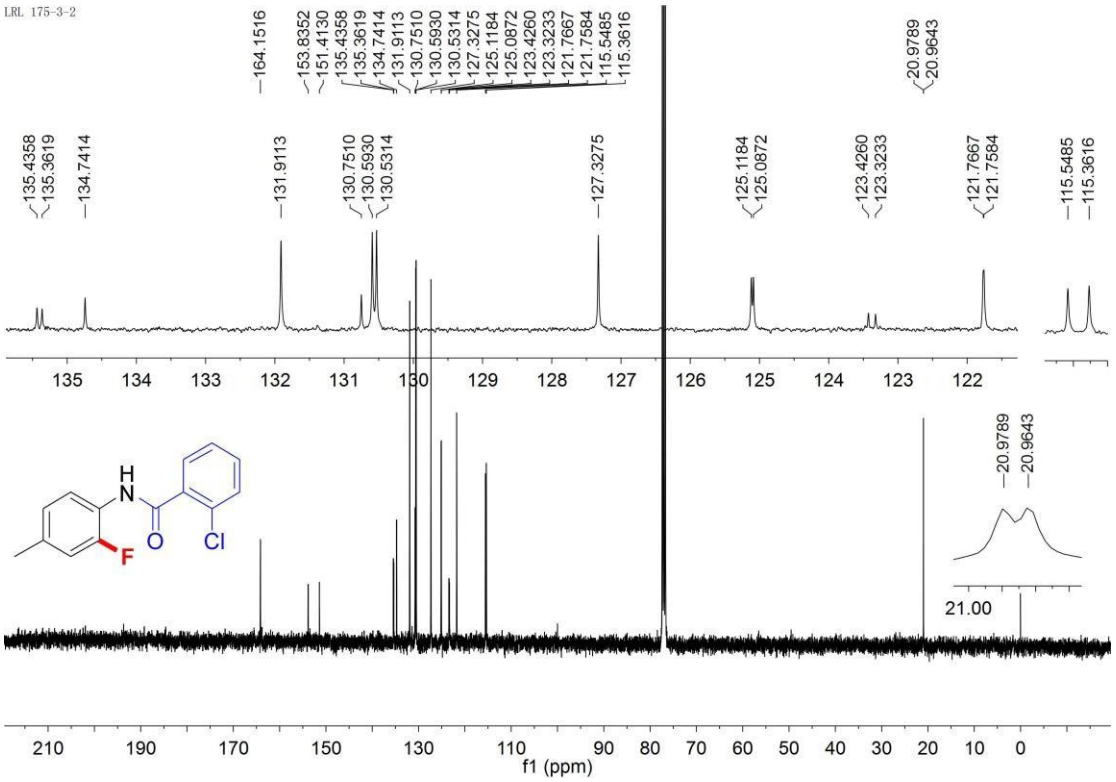

LRL 174-2-2a
8.2832
8.2626
8.2417
7.9198
7.8449
7.8388
7.8338
7.8222
7.8171
7.8110
7.4957
7.4896
7.4845
7.4729
7.4679
7.4618
7.0019
6.9794
6.9757
6.9453
6.9423
2.3449
0.0000
0.99
0.97
2.03
1.95
2.01
3.00
f1 (ppm)
Cl
H
N
O
F

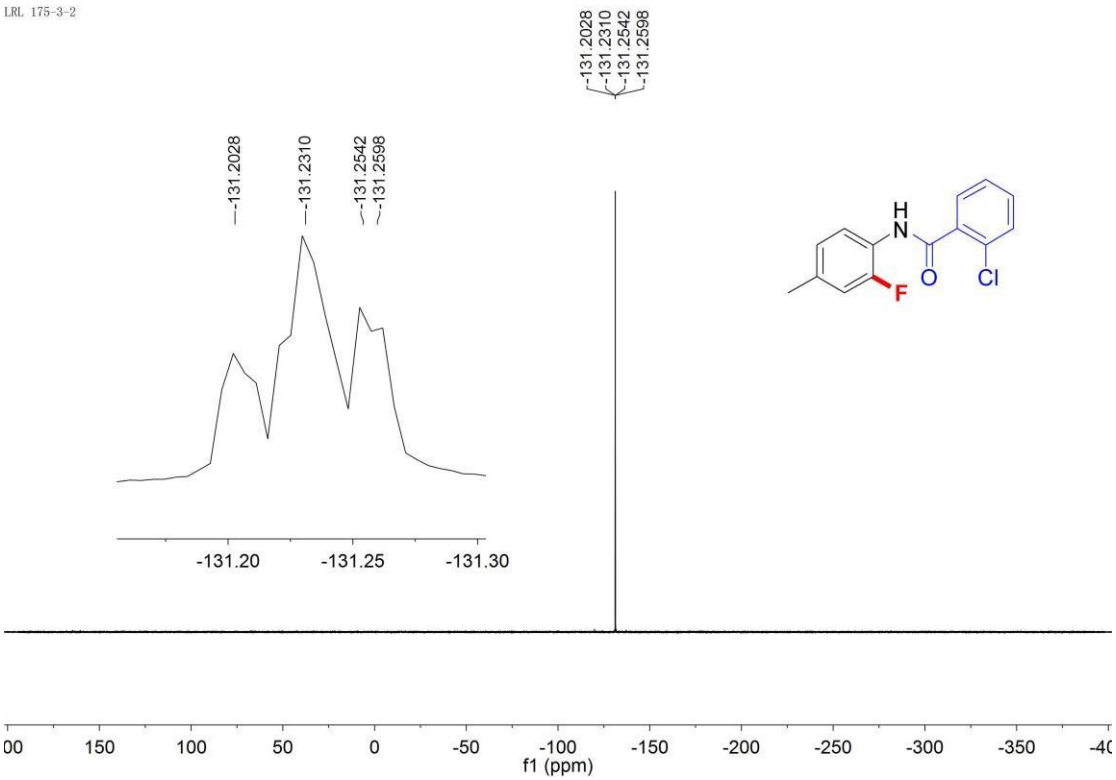

LRL 174-2-2a
164.2708
153.8502
151.4371
138.3667
135.3458
135.2718
132.9778
129.1376
128.5099
125.1735
125.1419
123.5364
123.4357
121.7116
121.7067
115.5307
115.3433
20.9650
20.9510
f1 (ppm)
Cl
H
N
O
F


LRL 174-2-2a
f, no dc
-131.6901
-131.6901
-131.60
-131.70
-131.80
Cl
H
N
O
F
f1 (ppm)

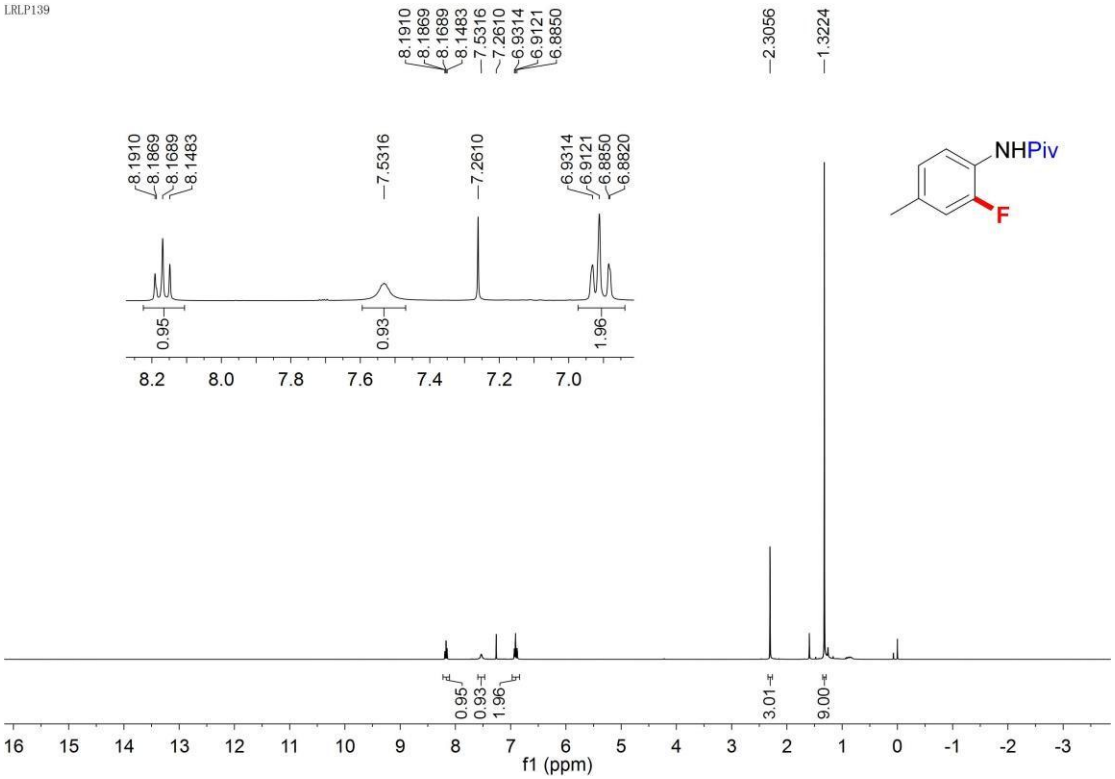
2g

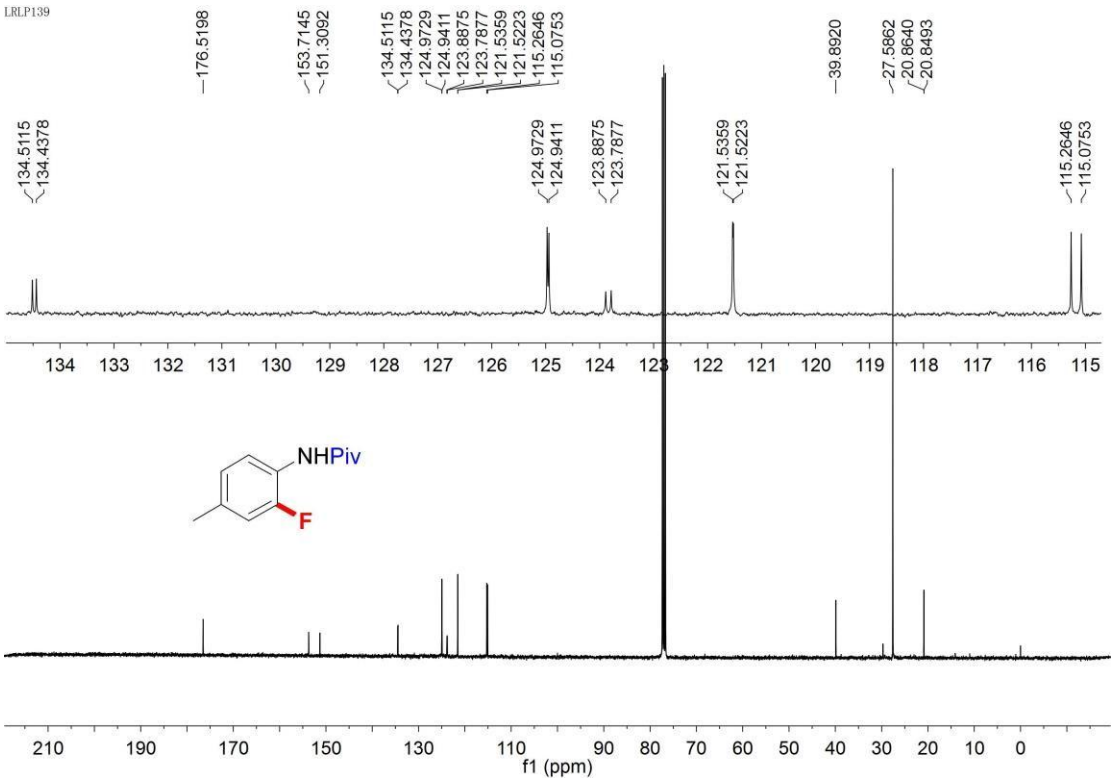

LRL 175-3-2
8.3425
8.3219
8.3011
8.1422
7.8145
7.8104
7.7963
7.7914
7.4810
7.4768
7.4611
7.4576
7.4483
7.4437
7.4305
7.4258
7.4114
7.4069
7.4024
7.3887
7.3844
7.3706
7.3665
7.0070
6.9859
6.9684
6.9386
6.9359
2.3451
0.0000
0.96
0.93
0.95
2.91
1.94
3.00
f1 (ppm)

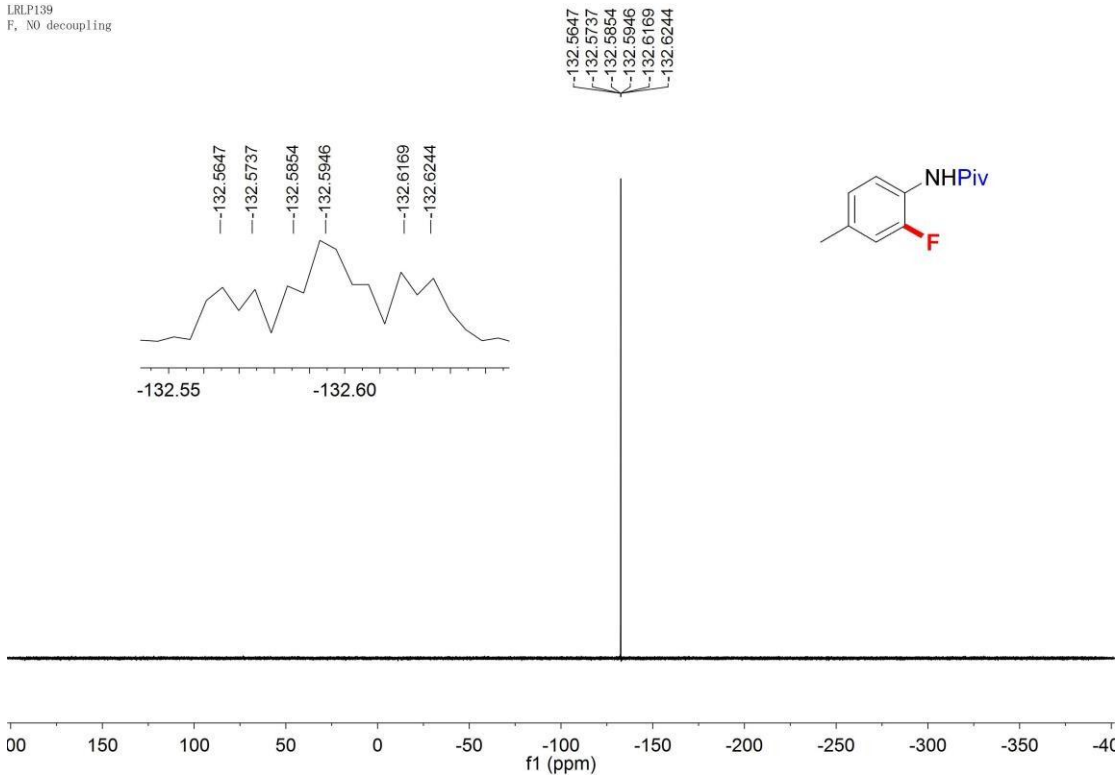

LRL 175-3-2
164.1516
153.8352
151.4130
135.4358
135.3619
134.7414
131.9113
130.7510
130.5930
130.5314
127.3275
125.1184
125.0872
123.4260
123.3233
121.7667
121.7584
115.5485
115.3616
20.9789
20.9643
21.00
f1 (ppm)


LRL 175-3-2
-131.2028
-131.2310
-131.2542
-131.2598
-131.20
-131.25
-131.30
H
N
O
F
Cl
f1 (ppm)

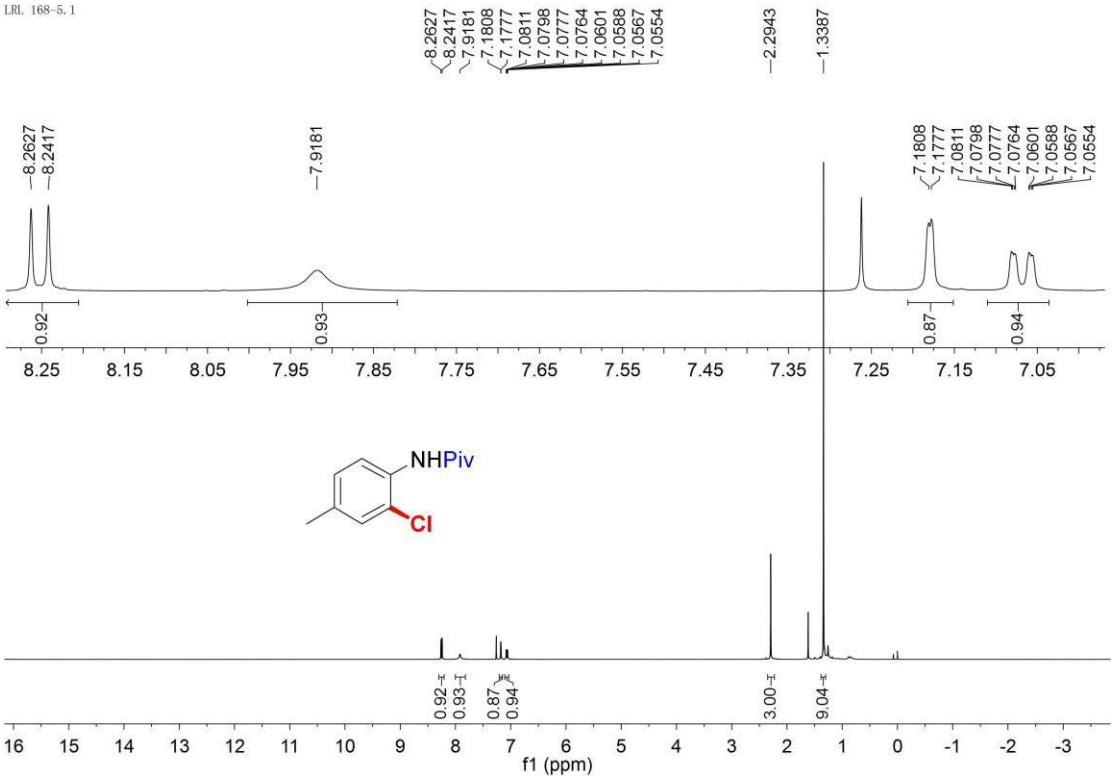
2h

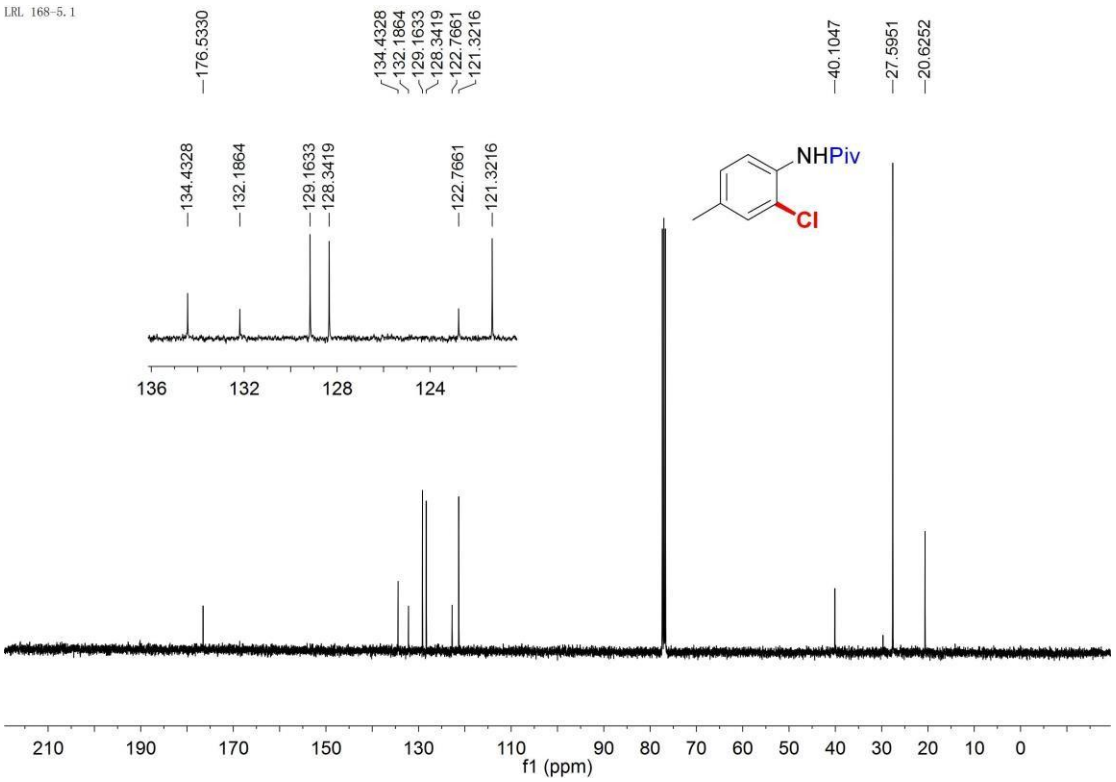

LRLP139
8.1910
8.1869
8.1689
8.1483
7.5316
7.2610
6.9314
6.9121
6.8850
6.8820
2.3056
1.3224
NHPiv
F
0.95
0.93
1.96
3.01
9.00
f1 (ppm)


LRLP139
176.5198
153.7145
151.3092
134.5115
134.4378
124.9729
124.9411
123.8875
123.7877
121.5359
121.5223
115.2646
115.0753
39.8920
27.5862
20.8640
20.8493
NHPiv
F
f1 (ppm)

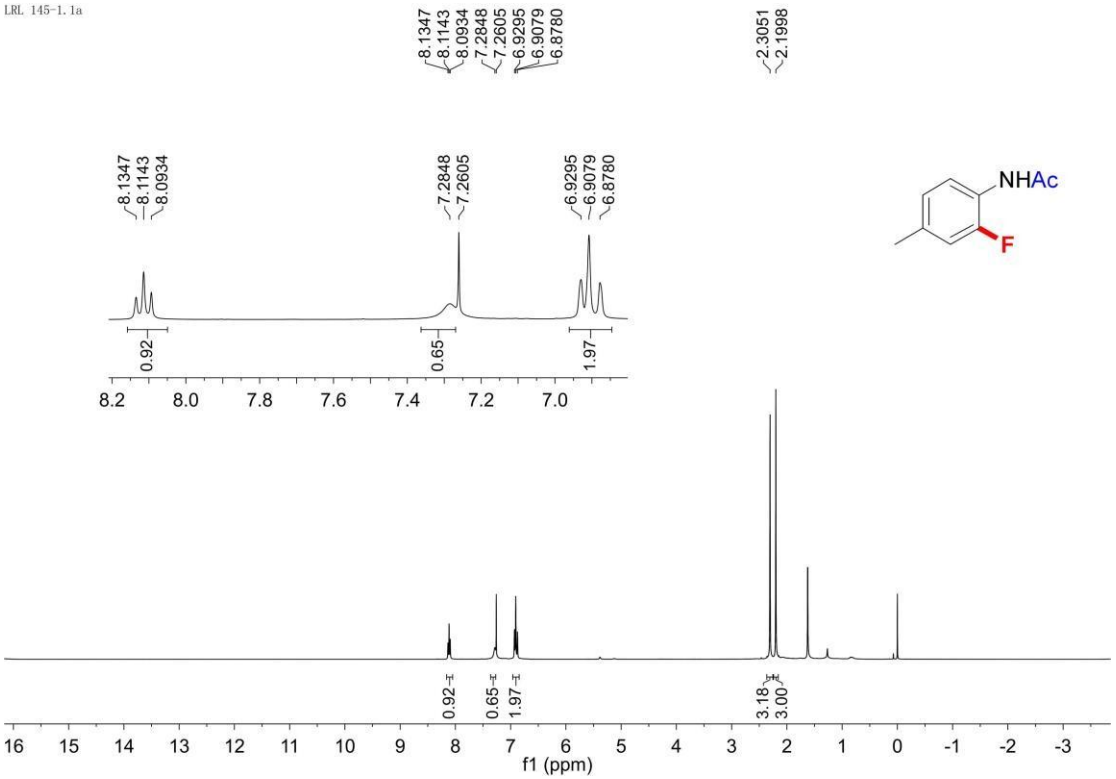

LRLP139
F, NO decoupling
-132.5647
-132.5737
-132.5854
-132.5946
-132.6169
-132.6244
NHPiv
F
-132.55
-132.60
f1 (ppm)

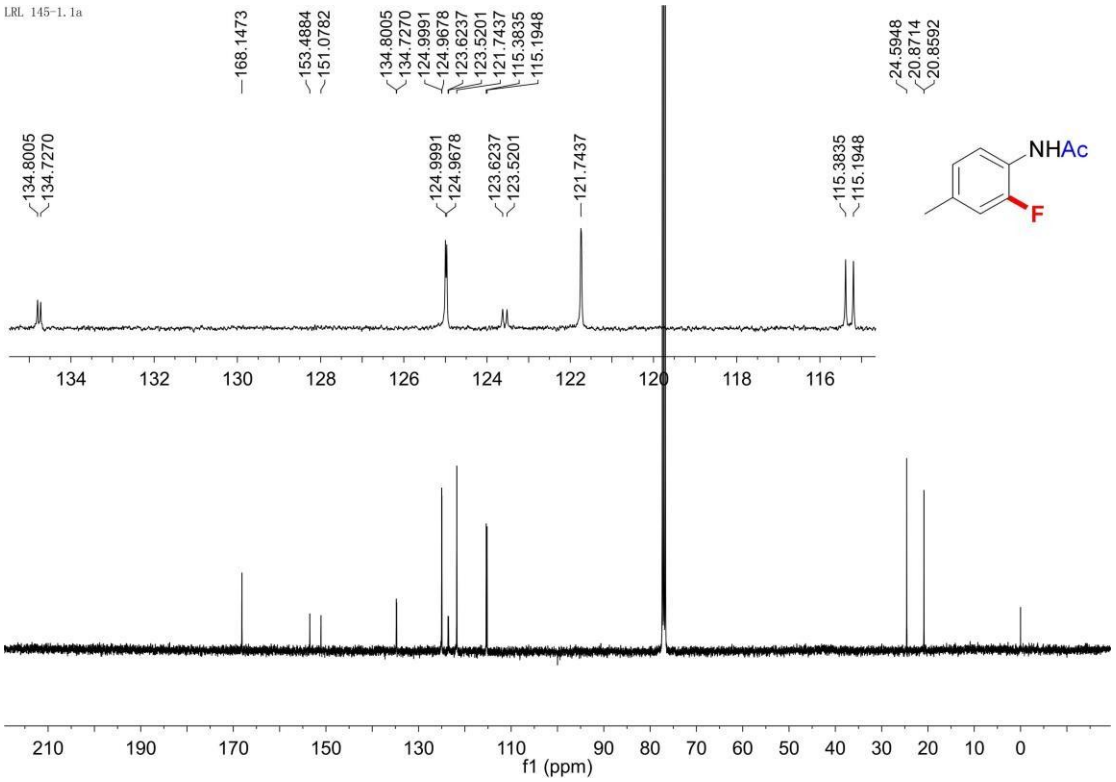
3h

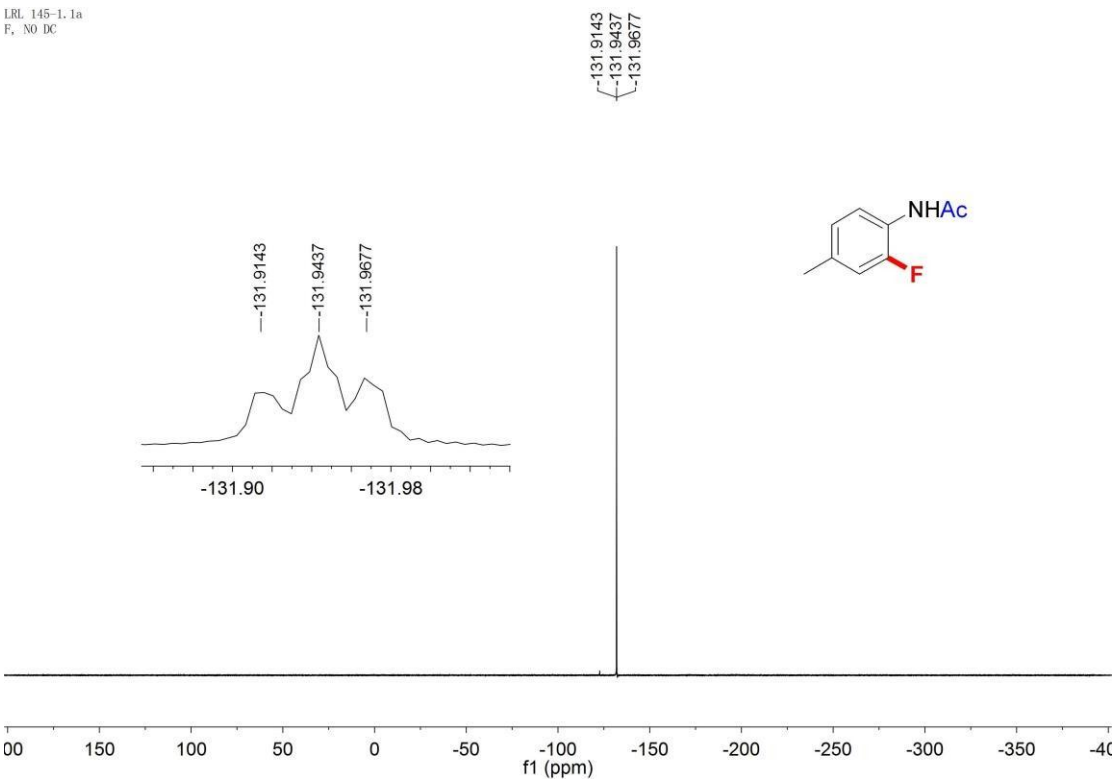

LRL 168-5.1
8.2627
8.2417
7.9181
7.1808
7.1777
7.0811
7.0798
7.0777
7.0764
7.0601
7.0588
7.0567
7.0554
2.2943
1.3387
0.92
0.93
0.87
0.94
3.00
9.04
NHPiv
Cl
f1 (ppm)


LRL 168-5.1
176.5330
134.4328
132.1864
129.1633
128.3419
122.7661
121.3216
40.1047
27.5951
20.6252
NHPiv
Cl
f1 (ppm)

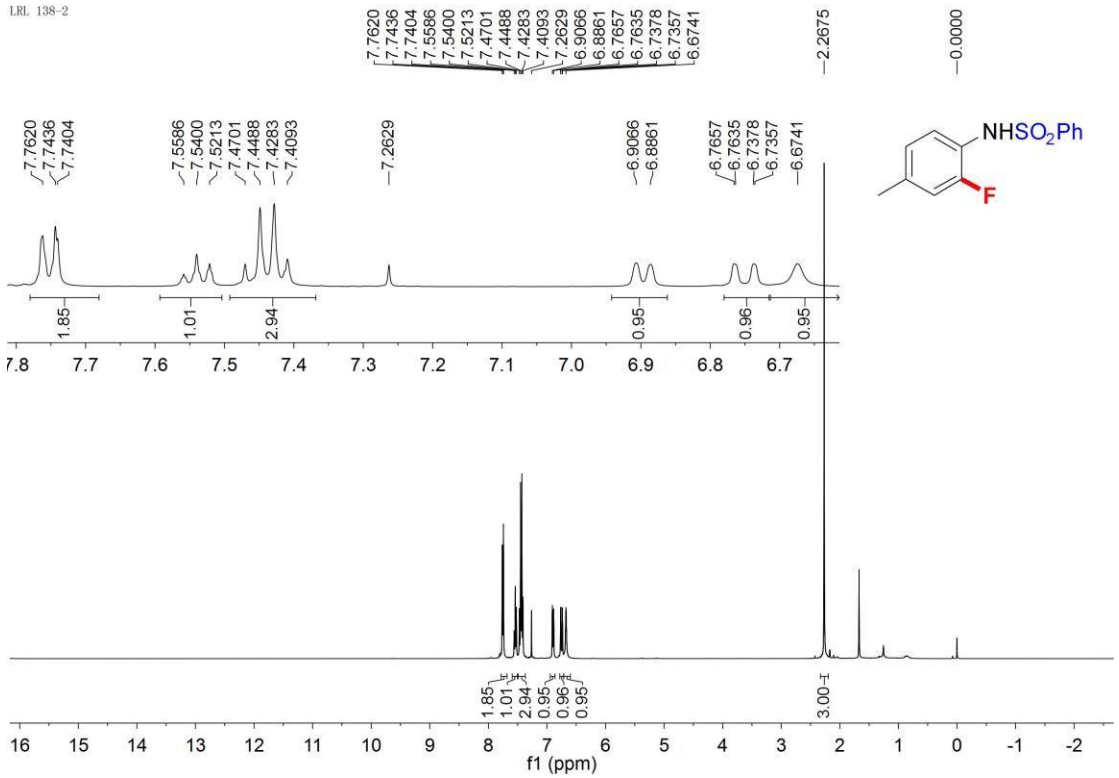
2i

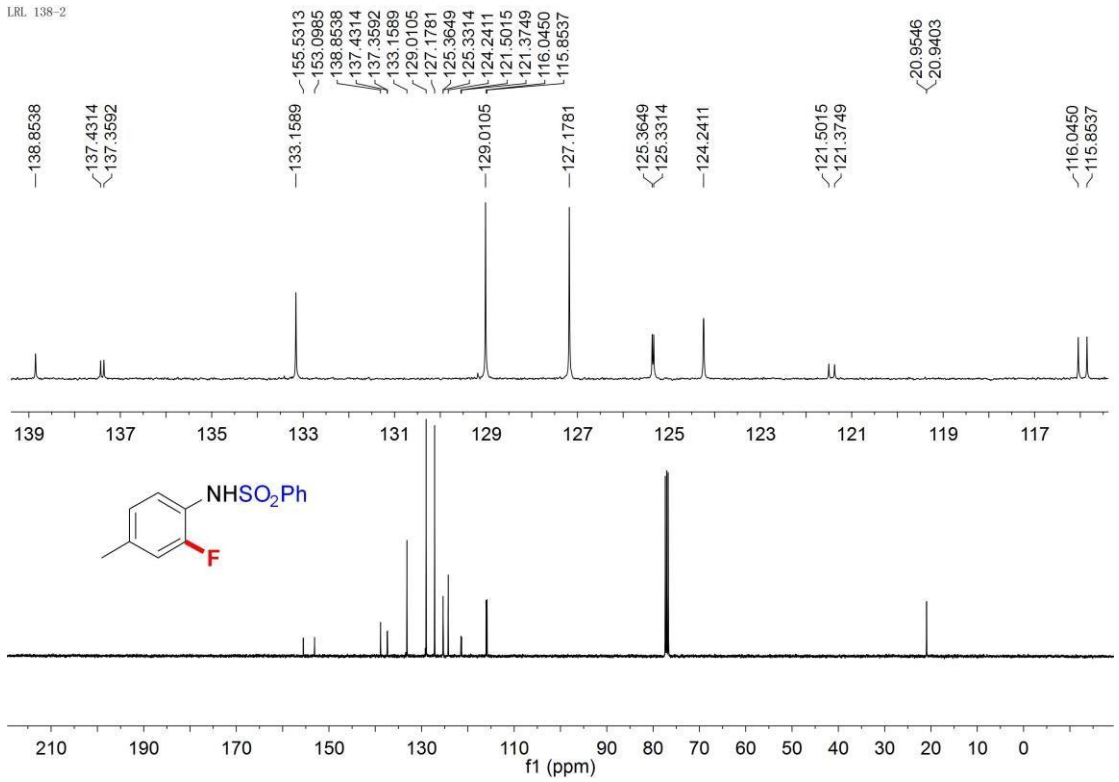

LRL 145-1.1a
8.1347
8.1143
8.0934
7.2848
7.2605
6.9295
6.9079
6.8780
2.3051
2.1998
NHAc
F
0.92
0.65
1.97
3.18
3.00
f1 (ppm)

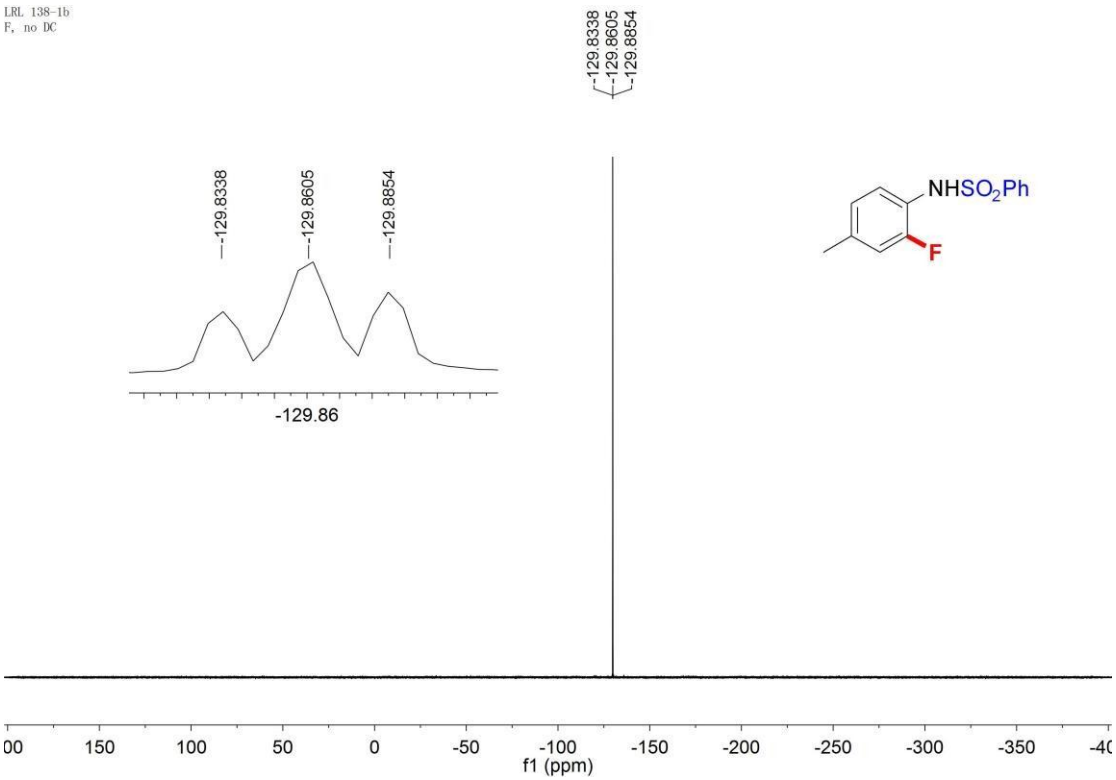

LRL 145-1.1a
168.1473
153.4884
151.0782
134.8005
134.7270
124.9991
124.9678
123.6237
123.5201
121.7437
115.3835
115.1948
24.5948
20.8714
20.8592
NHAc
F
f1 (ppm)


LRL 145-1.1a
F, NO DC
-131.9143
-131.9437
-131.9677
NHAc
F
-131.90
-131.98
f1 (ppm)

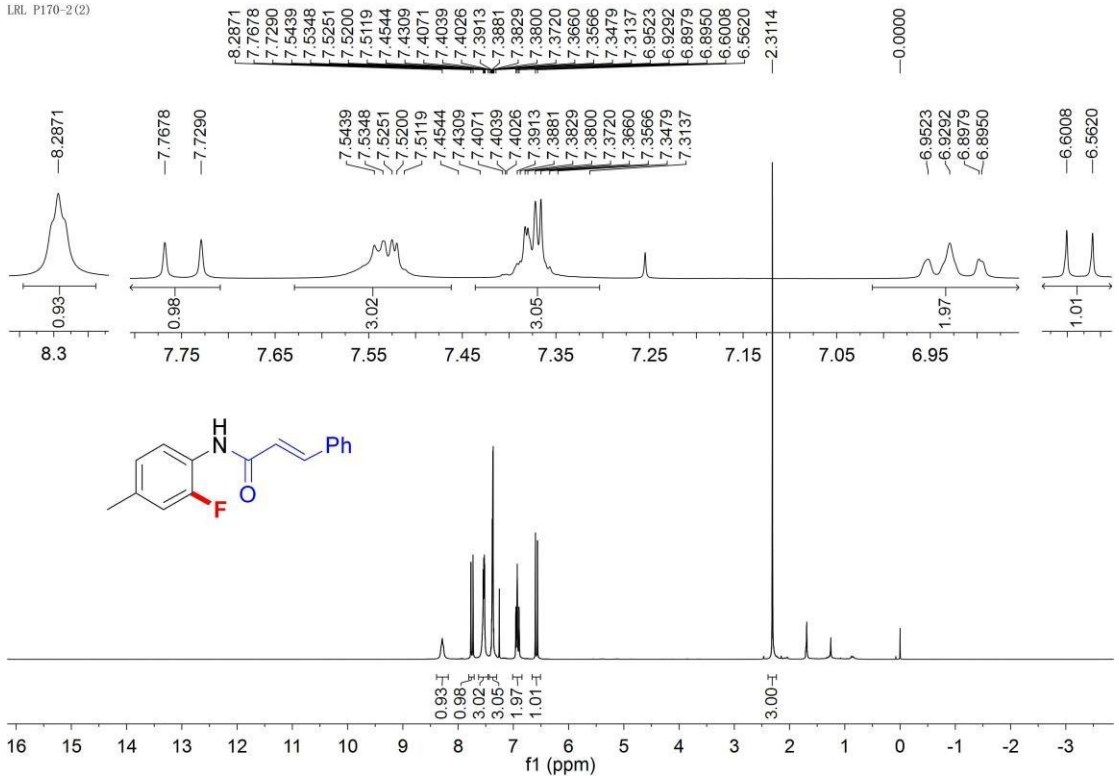
2j

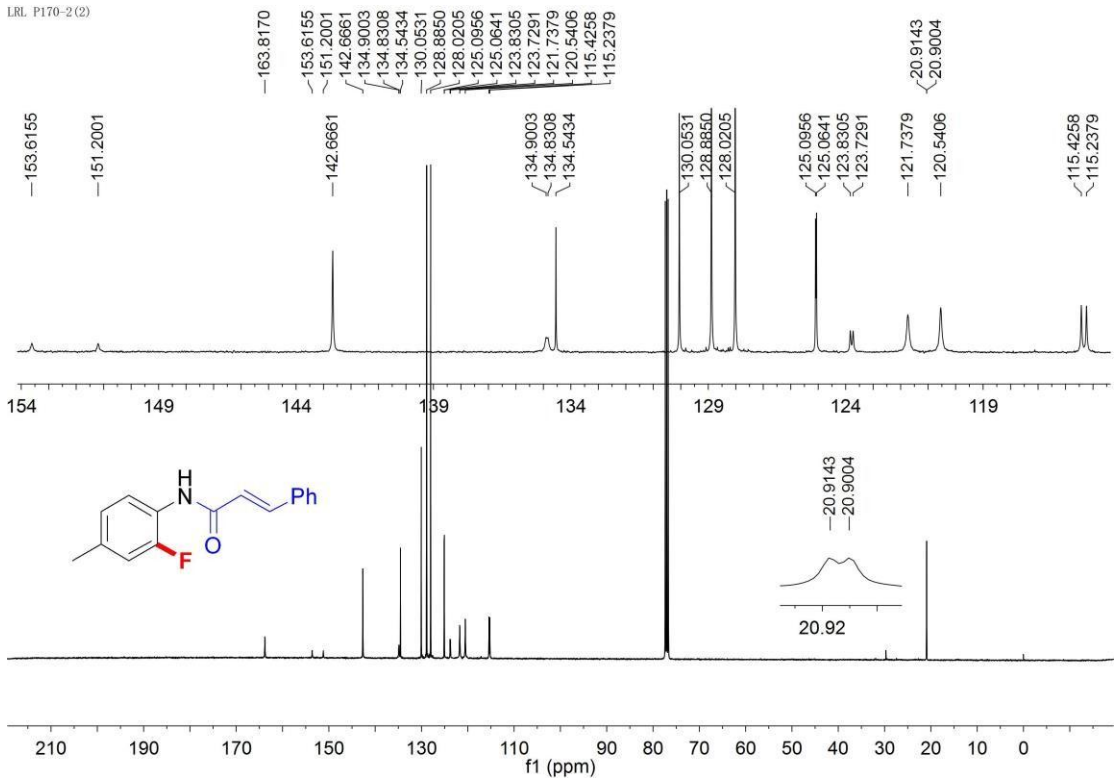

LRL 138-2
7.7620
7.7436
7.7404
7.5586
7.5400
7.5213
7.4701
7.4488
7.4283
7.4093
7.2629
6.9066
6.8861
6.7657
6.7635
6.7378
6.7357
6.6741
2.2675
0.0000
NHSO2Ph
F
1.85
1.01
2.94
0.95
0.96
0.95
3.00
f1 (ppm)

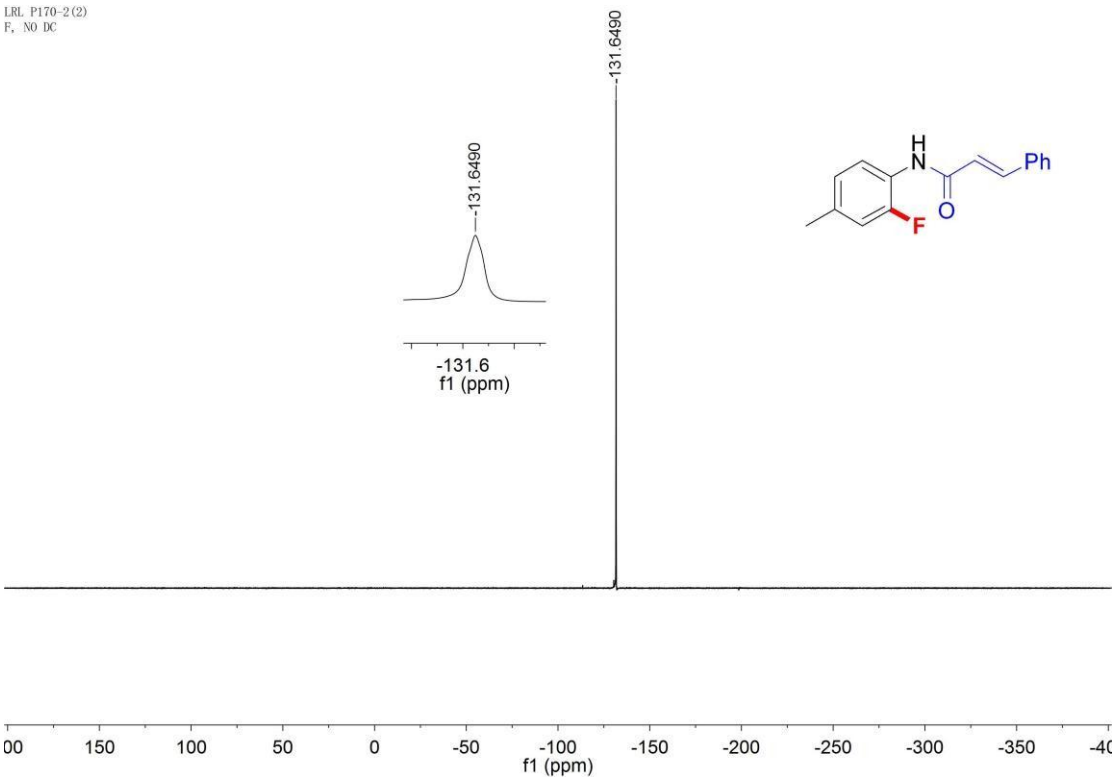

LRL 138-2
155.5313
153.0985
138.8538
137.4314
137.3592
133.1589
129.0105
127.1781
125.3649
125.3314
124.2411
121.5015
121.3749
116.0450
115.8537
20.9546
20.9403
NHSO2Ph
F
f1 (ppm)


LRL 138-1b
F, no DC
-129.8338
-129.8605
-129.8854
-129.8338
-129.8605
-129.8854
-129.86
NHSO2Ph
F
f1 (ppm)

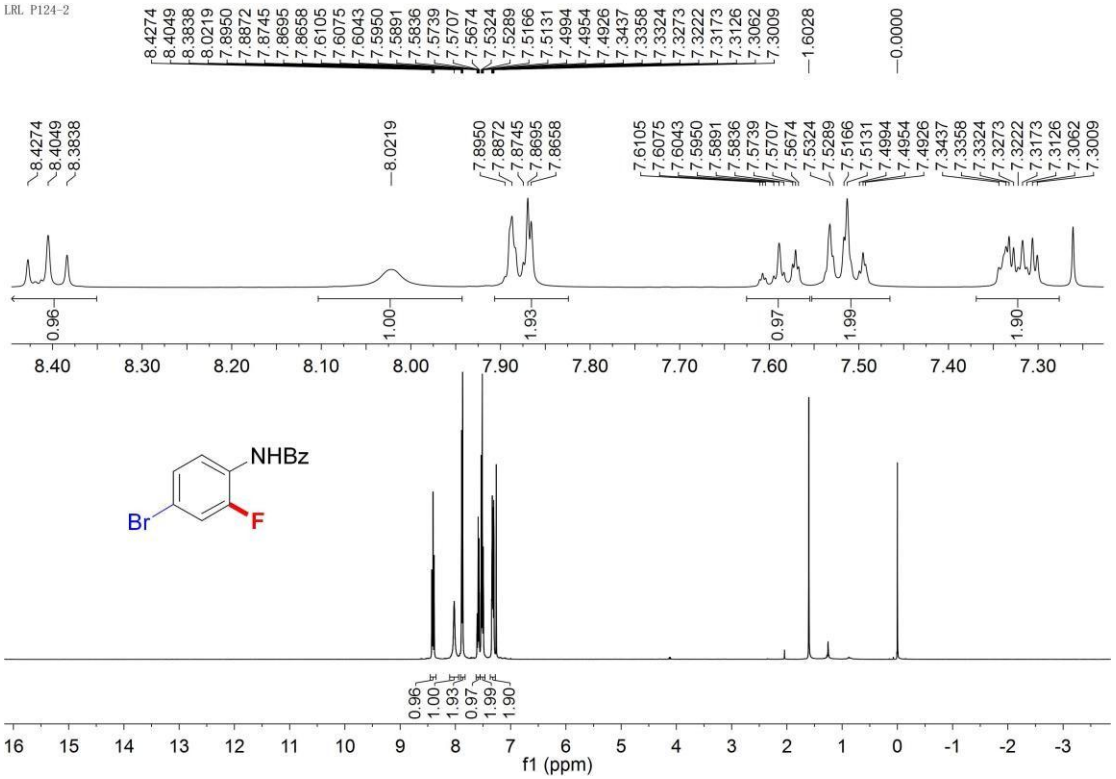
2k

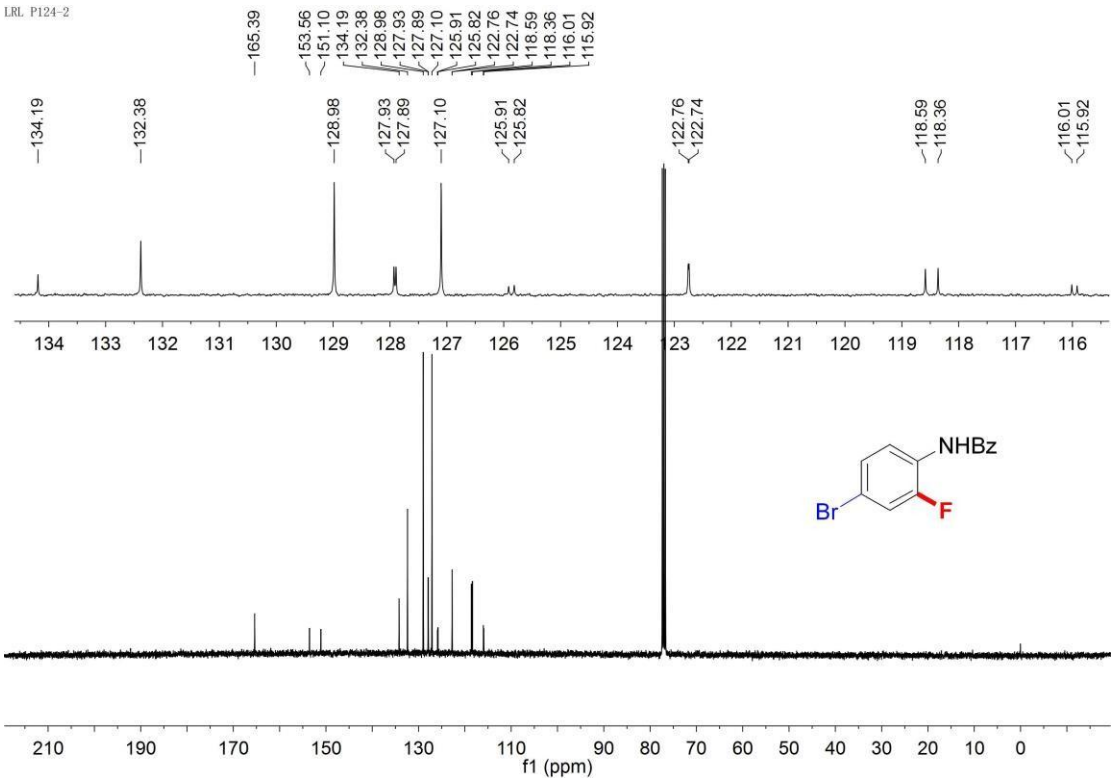


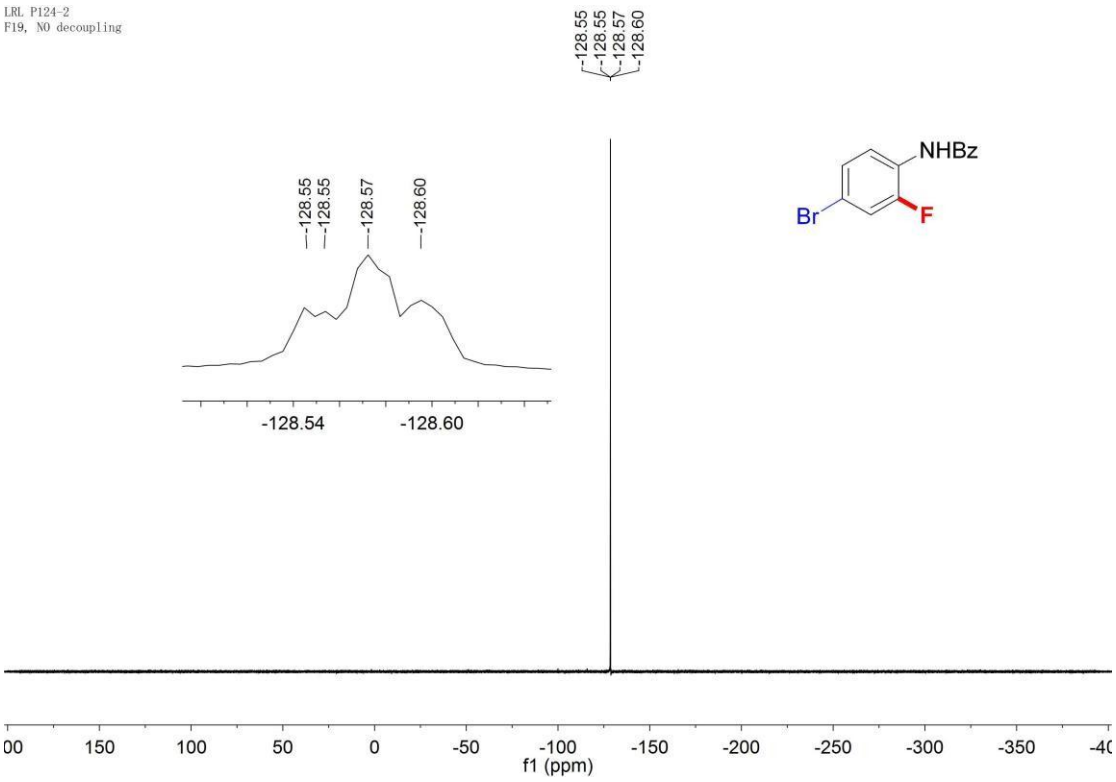



LRL P170-2(2)
F, NO DC
-131.6490
-131.6490
-131.6
f1 (ppm)
H
N
O
F
Ph
00
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
-40
f1 (ppm)

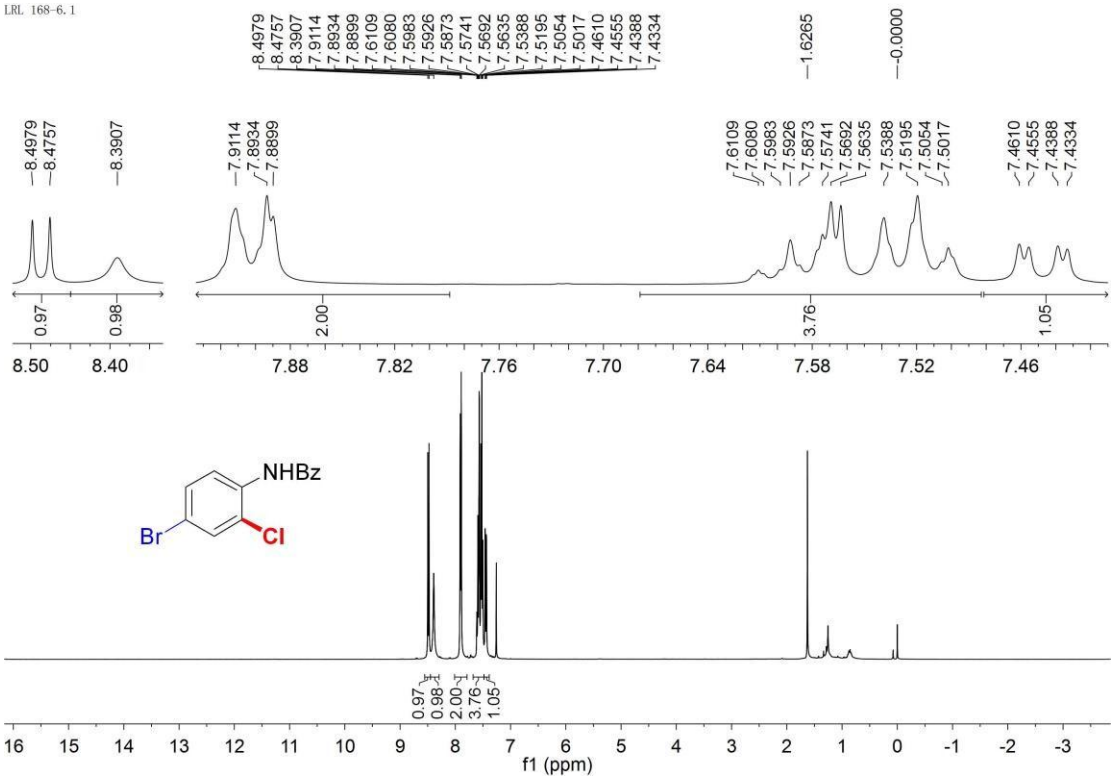
2l

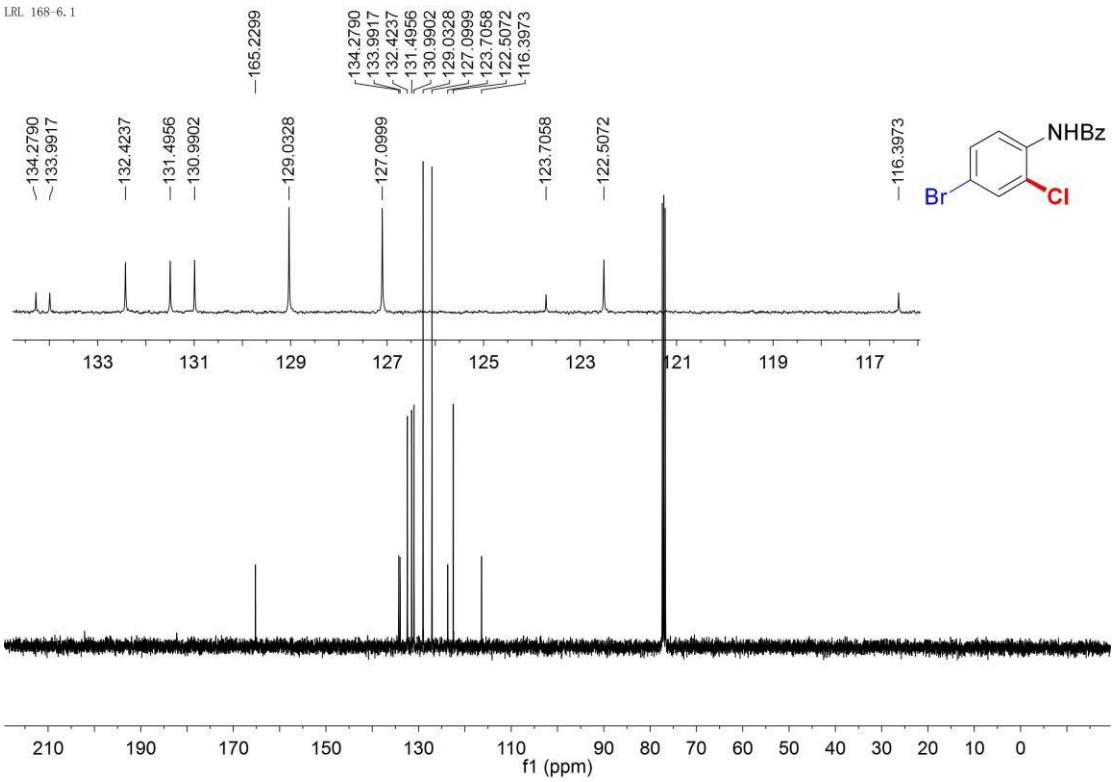




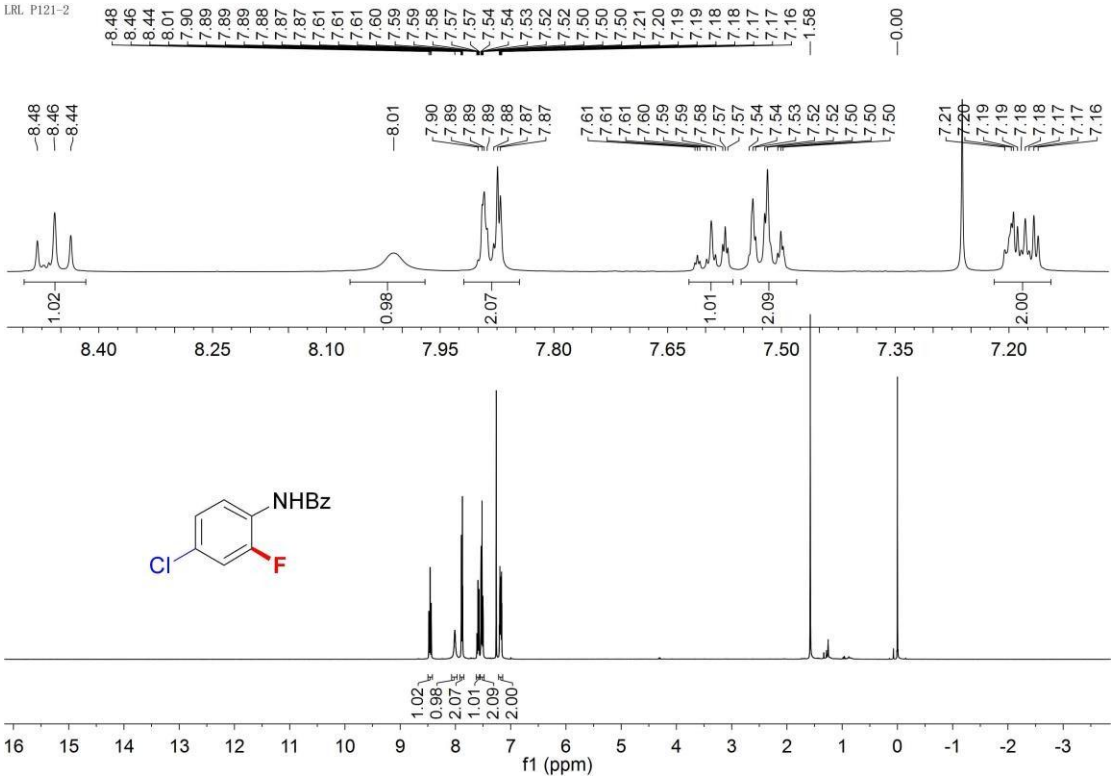

LRL P124-2
F19, NO decoupling
-128.55
-128.55
-128.57
-128.60
NHBz
Br
F
-128.54
-128.60
f1 (ppm)

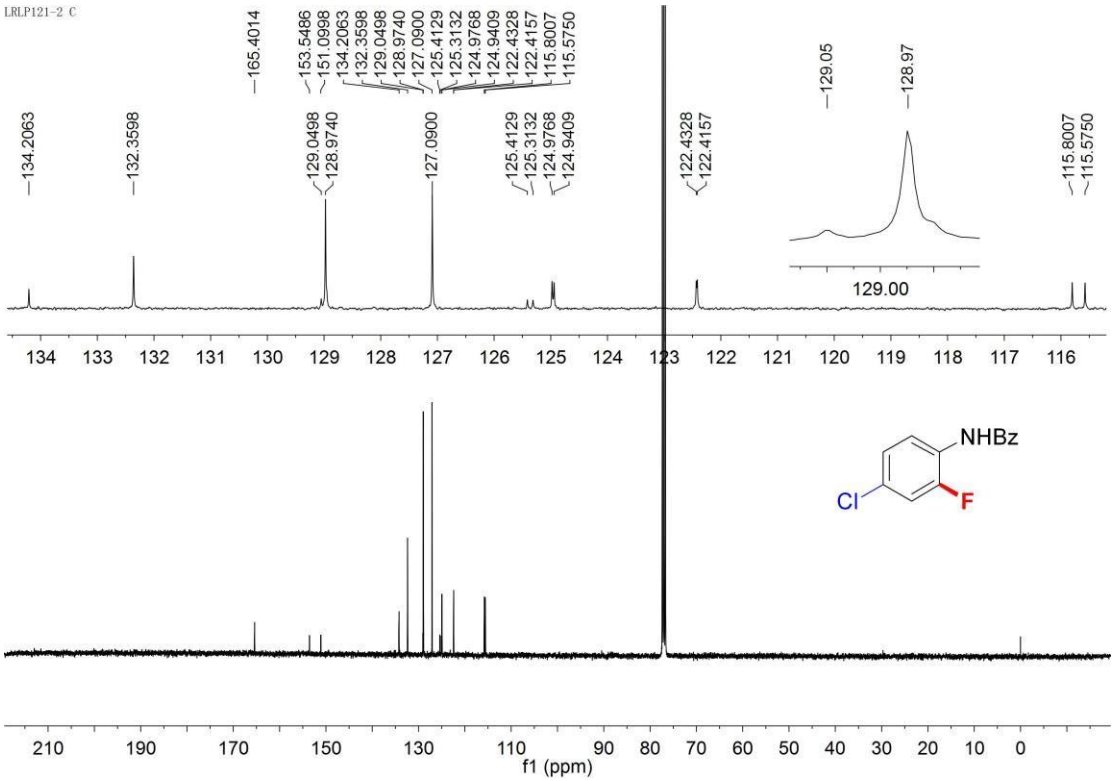
3l

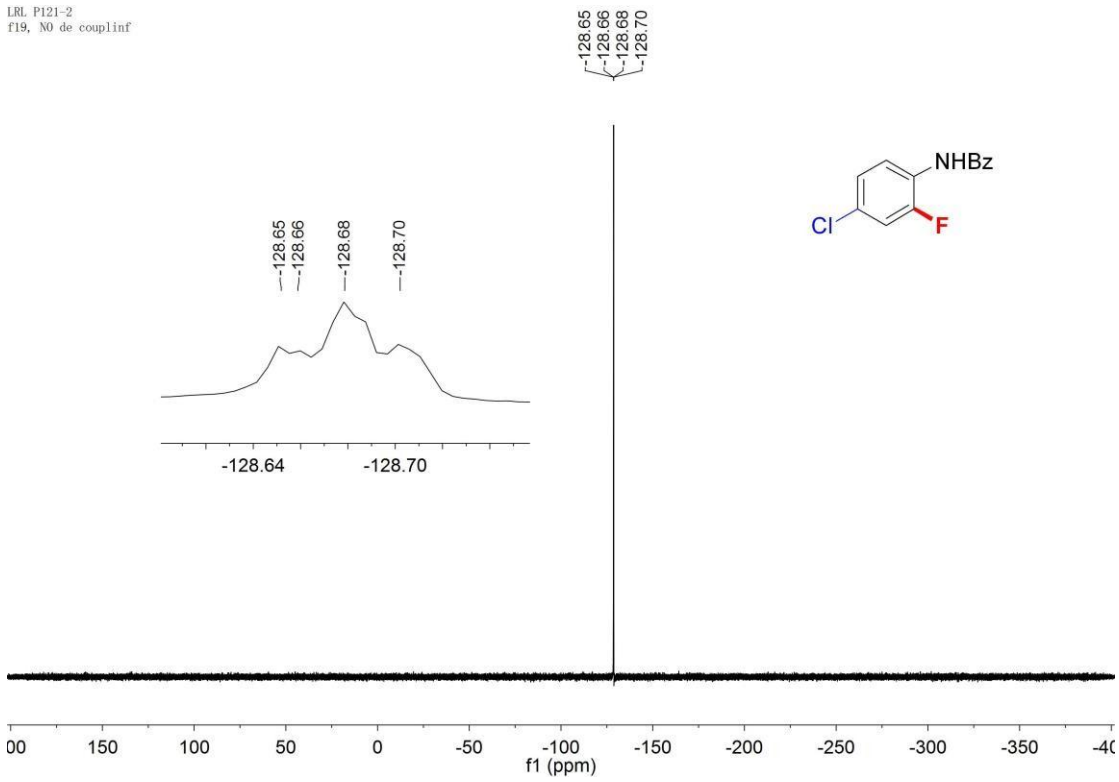

LRL 168-6.1
8.4979
8.4757
8.3907
7.9114
7.8934
7.8899
7.6109
7.6080
7.5983
7.5926
7.5873
7.5741
7.5692
7.5635
7.5388
7.5195
7.5054
7.5017
7.4610
7.4555
7.4388
7.4334
1.6265
0.0000
0.97
0.98
2.00
3.76
1.05
NHBz
Br
Cl
f1 (ppm)


LRL 168-6.1
165.2299
134.2790
133.9917
132.4237
131.4956
130.9902
129.0328
127.0999
123.7058
122.5072
116.3973
NHBz
Br
Cl
f1 (ppm)

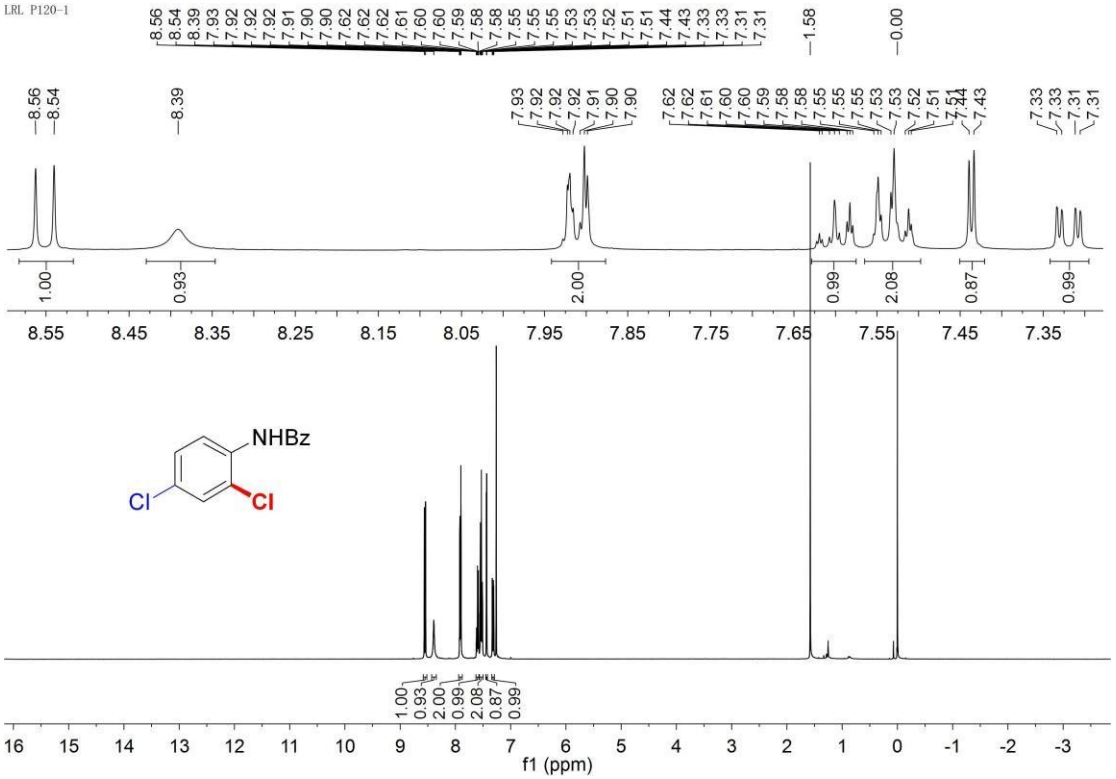
2m

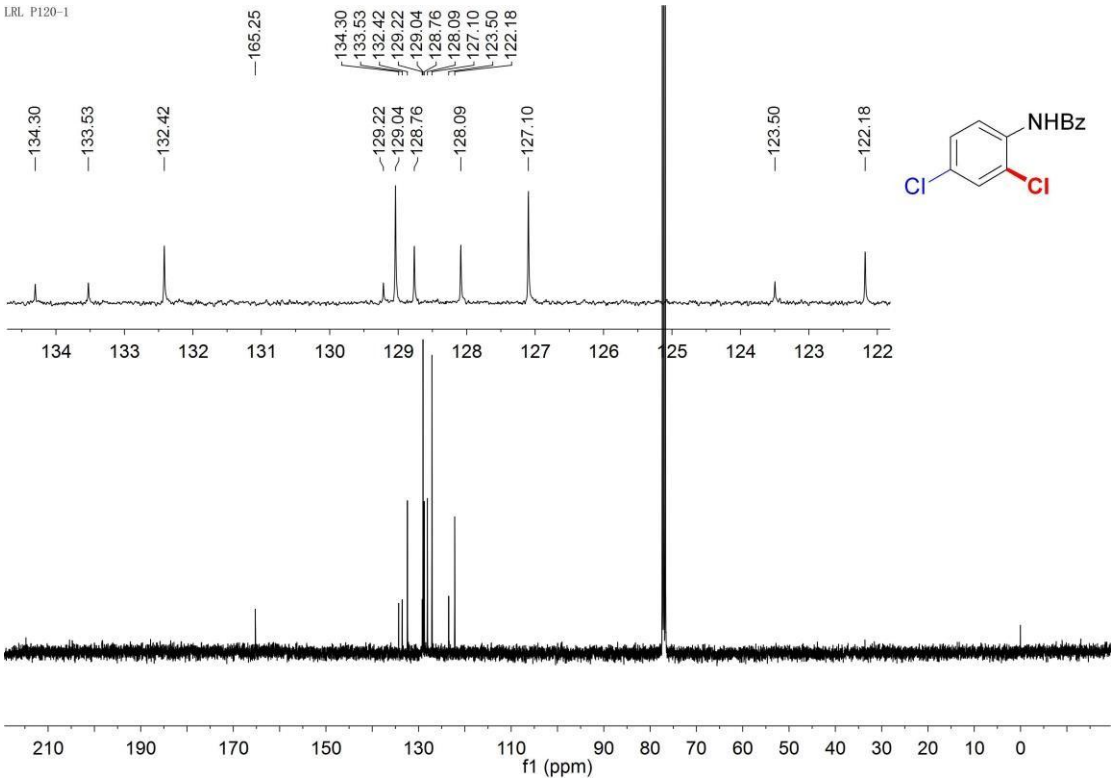




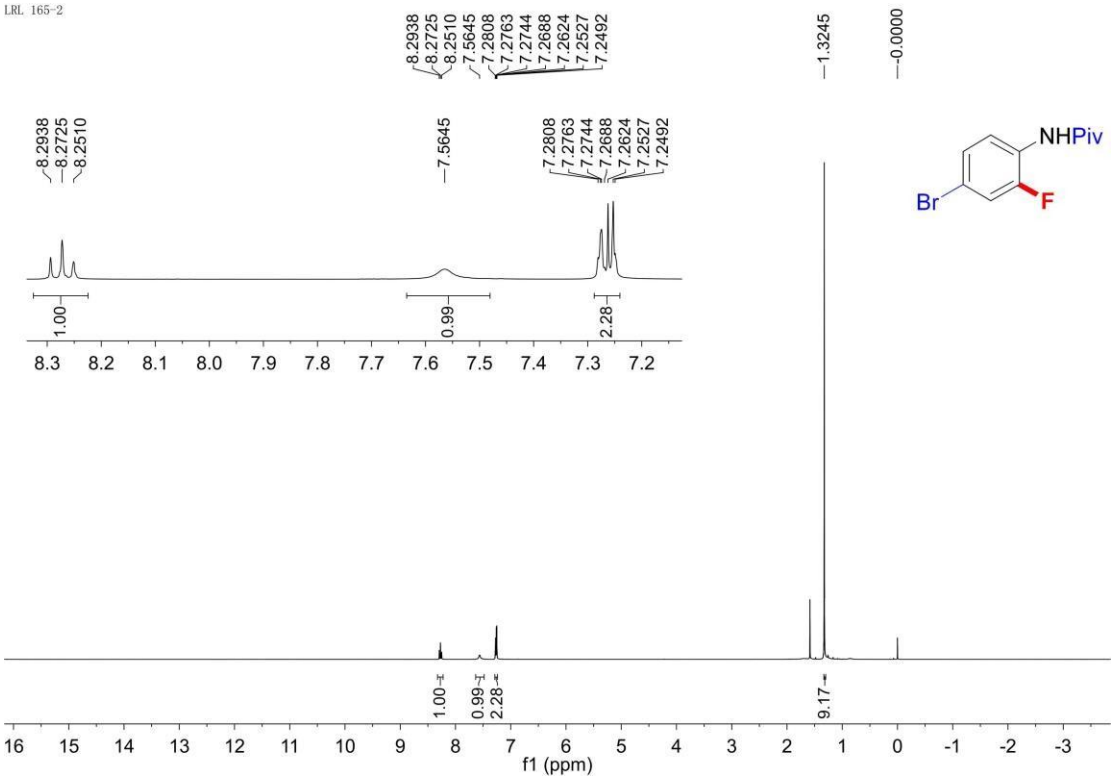

LRL P121-2
f19, N0 de couplinf
-128.65
-128.66
-128.68
-128.70
NHBz
Cl
F
-128.64
-128.70
f1 (ppm)

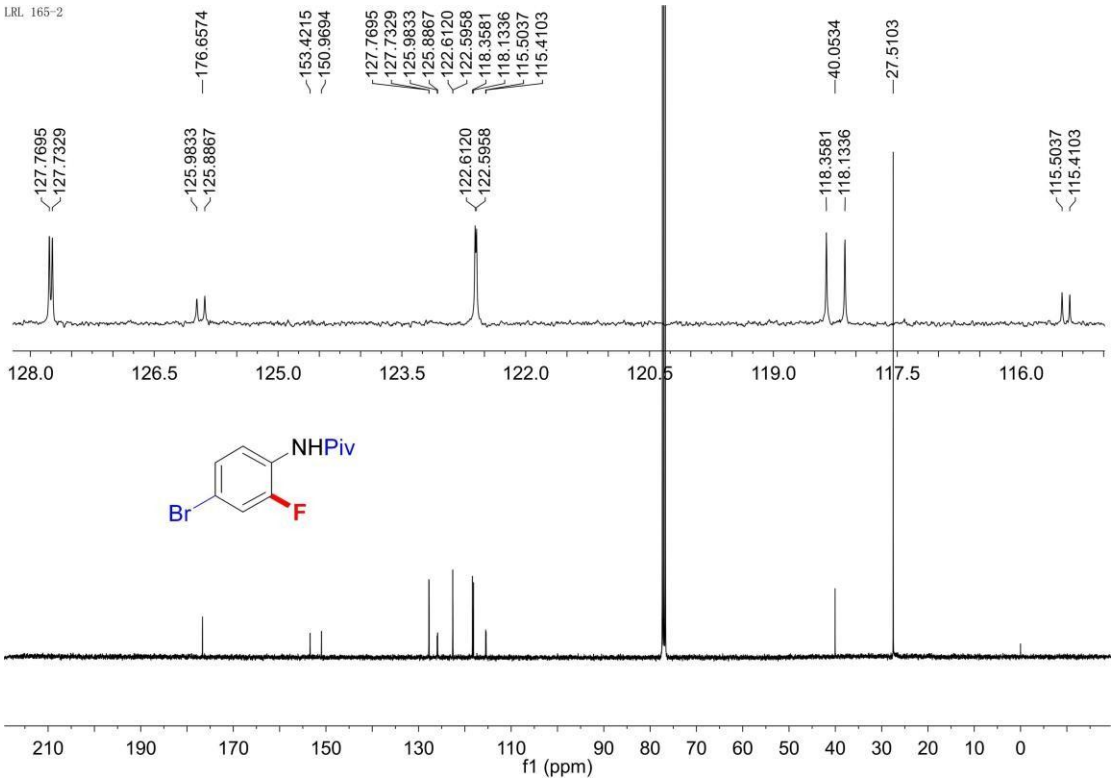
3m

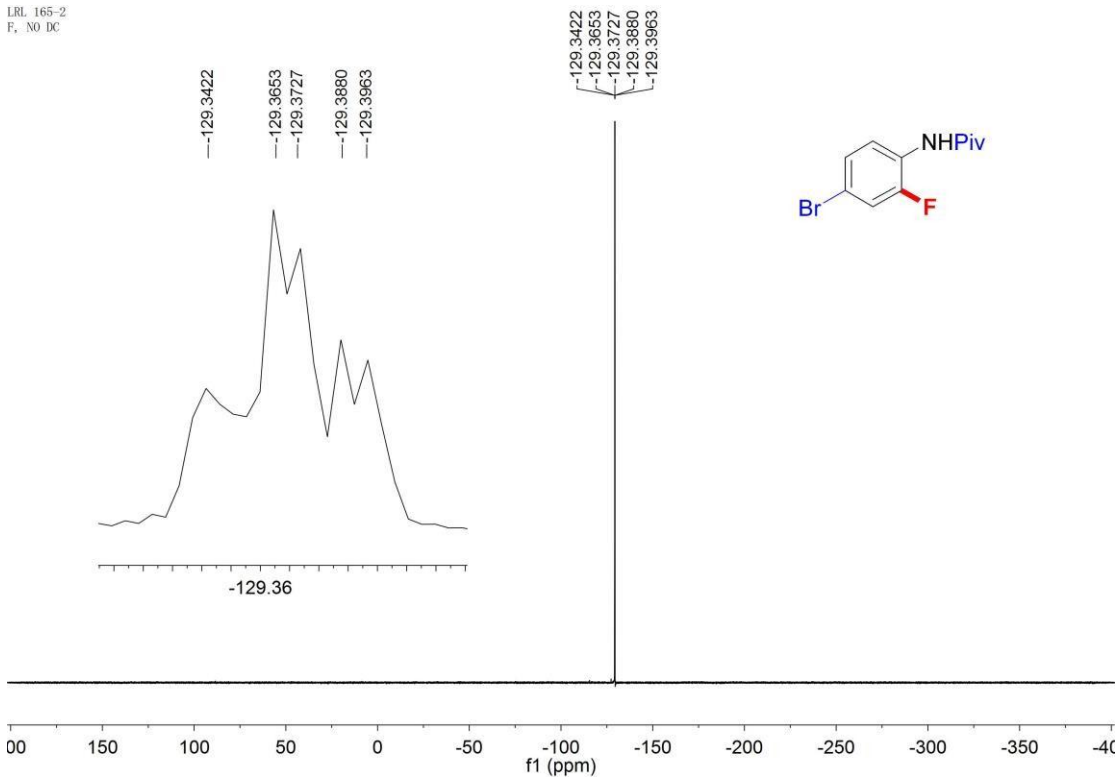




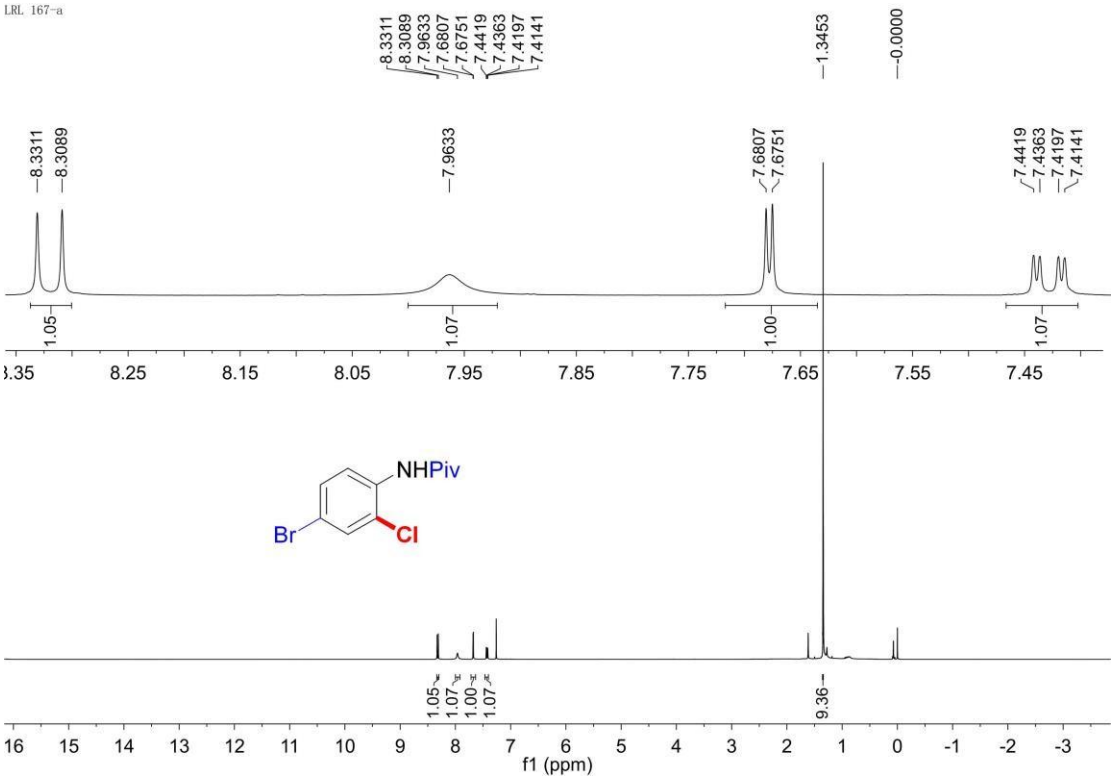
2n

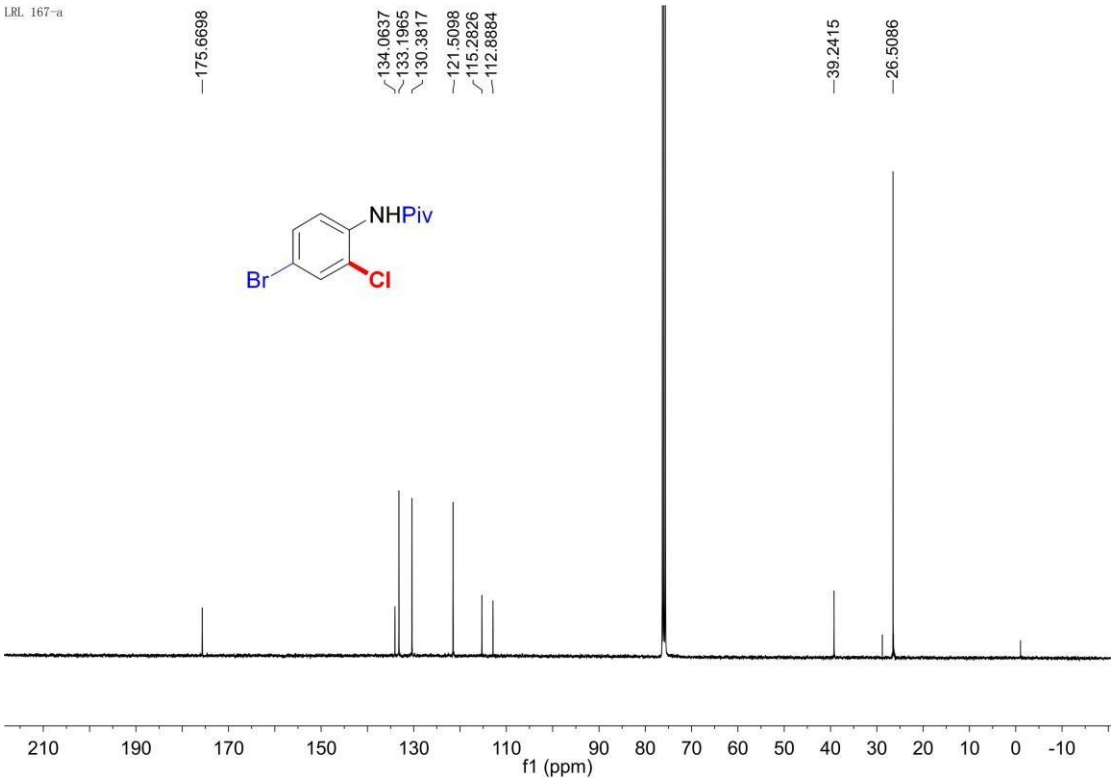

LRL 165-2
8.2938
8.2725
8.2510
7.5645
7.2808
7.2763
7.2744
7.2688
7.2624
7.2527
7.2492
1.3245
0.0000
NHPiv
Br
F
1.00
0.99
2.28
9.17
f1 (ppm)


LRL 165-2
176.6574
153.4215
150.9694
127.7695
127.7329
125.9833
125.8867
122.6120
122.5958
118.3581
118.1336
115.5037
115.4103
40.0534
27.5103
NHPiv
Br
F
f1 (ppm)

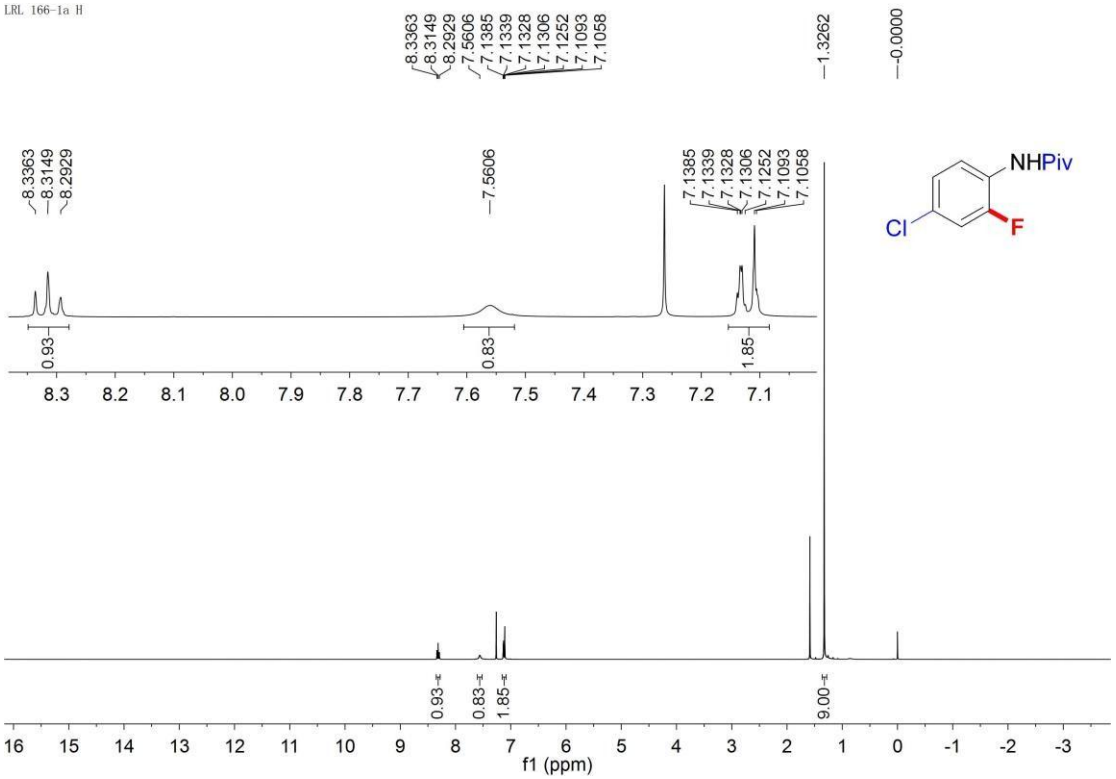

LRL 165-2
F, NO DC
-129.3422
-129.3653
-129.3727
-129.3880
-129.3963
-129.36
NHPiv
Br
F
f1 (ppm)

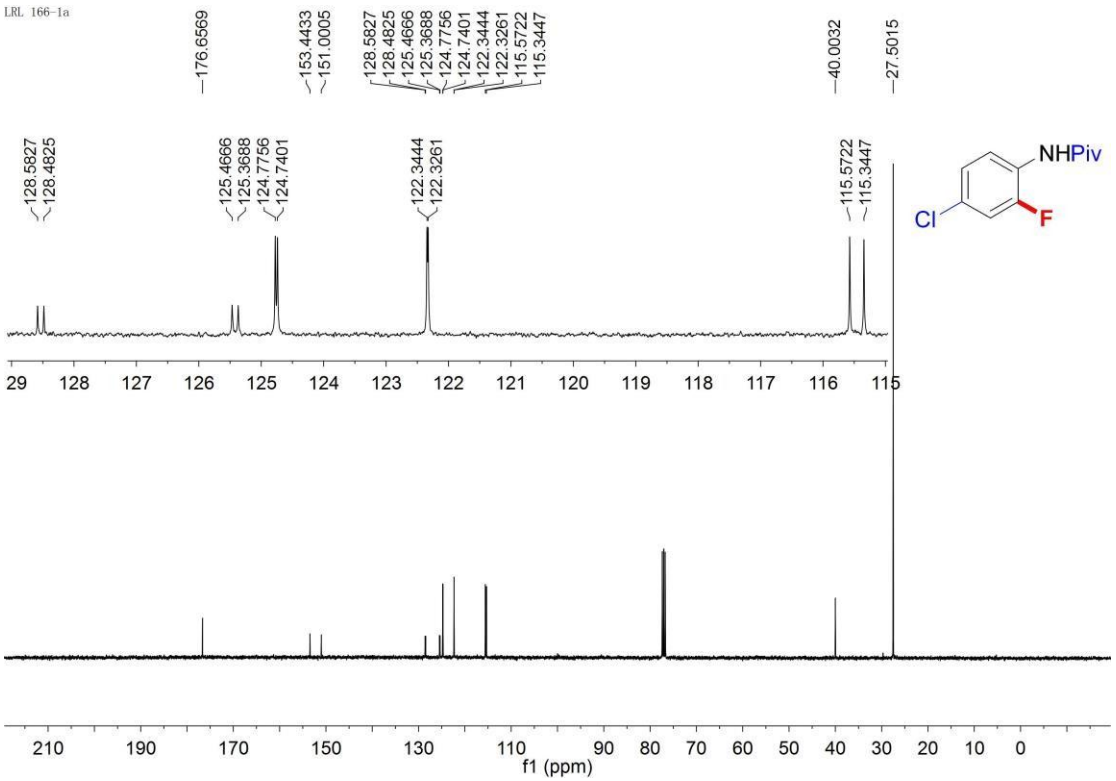
3n

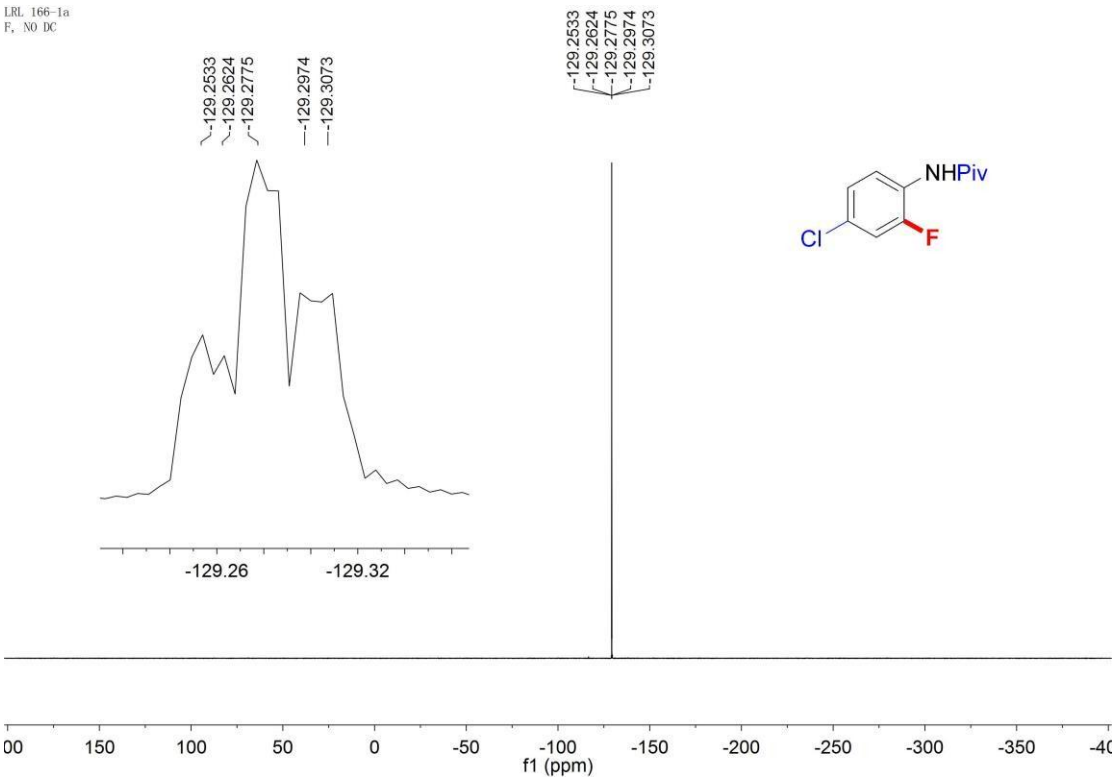

LRL 167-a
8.3311
8.3089
7.9633
7.6807
7.6751
7.4419
7.4363
7.4197
7.4141
1.3453
0.0000
1.05
1.07
1.00
1.07
9.36
NHPiv
Br
Cl
f1 (ppm)


LRL 167-a
175.6698
134.0637
133.1965
130.3817
121.5098
115.2826
112.8884
39.2415
26.5086
NHPiv
Br
Cl
f1 (ppm)

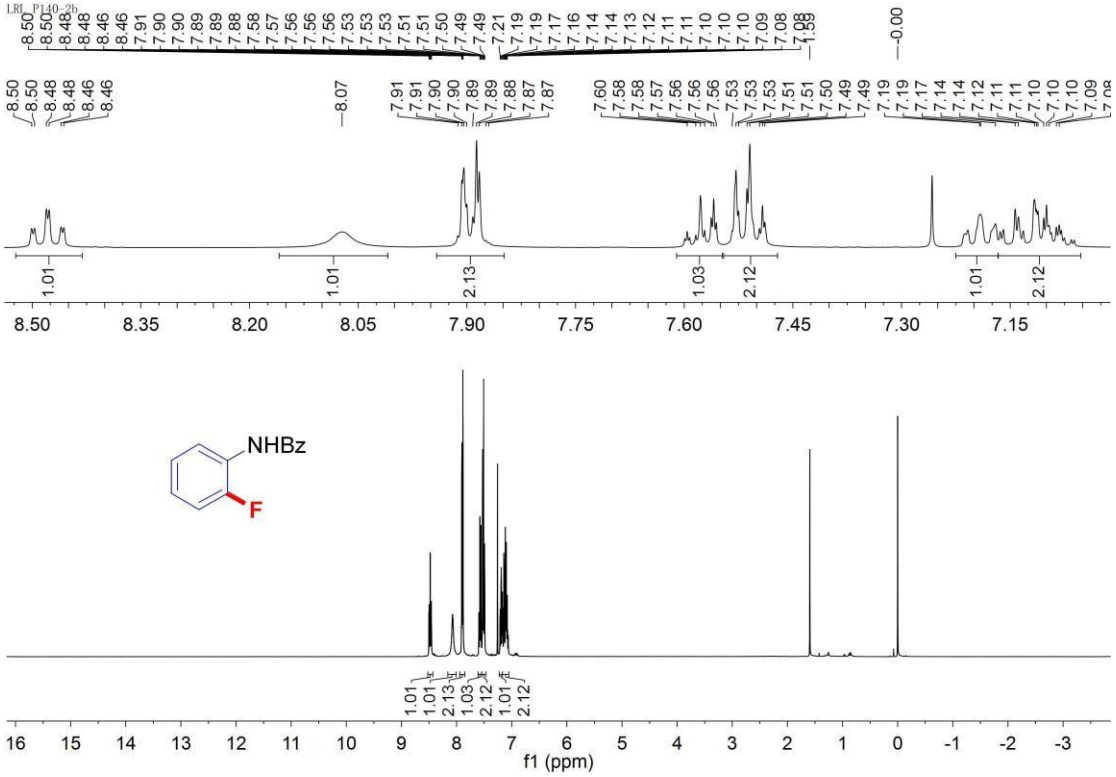
2o

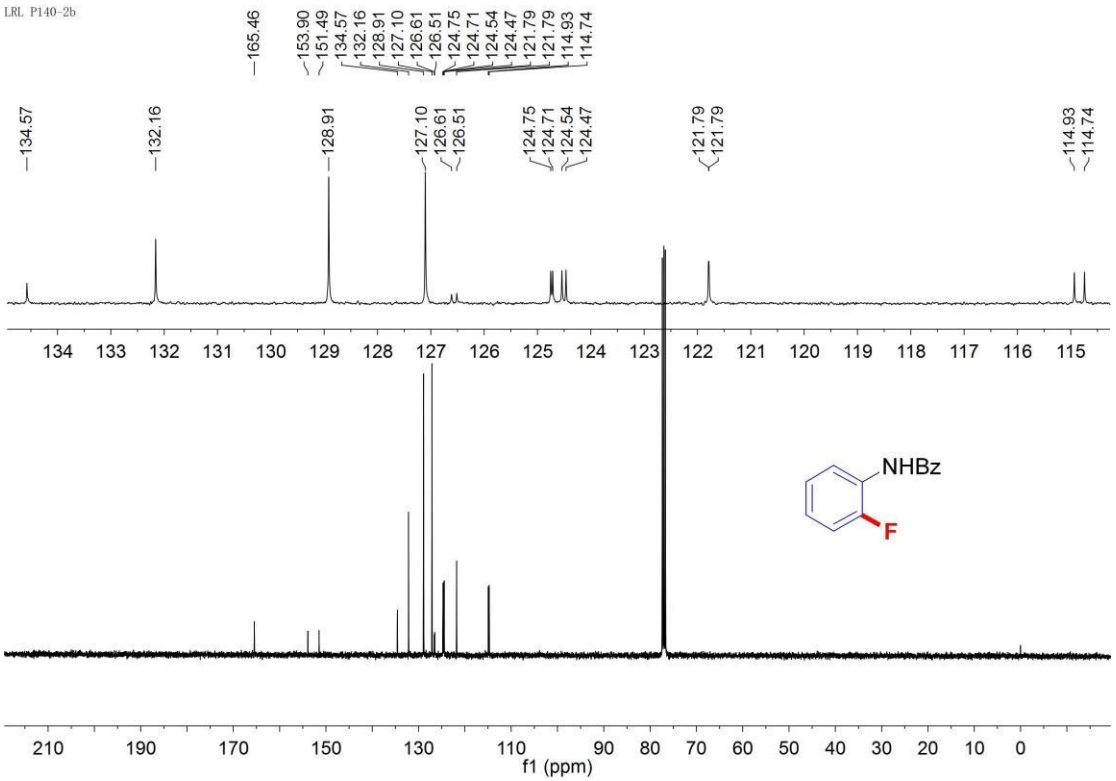

LRL 166-1a H
8.3363
8.3149
8.2929
7.5606
7.1385
7.1339
7.1328
7.1306
7.1252
7.1093
7.1058
1.3262
0.0000
NHPiv
Cl
F
0.93
0.83
1.85
9.00
f1 (ppm)

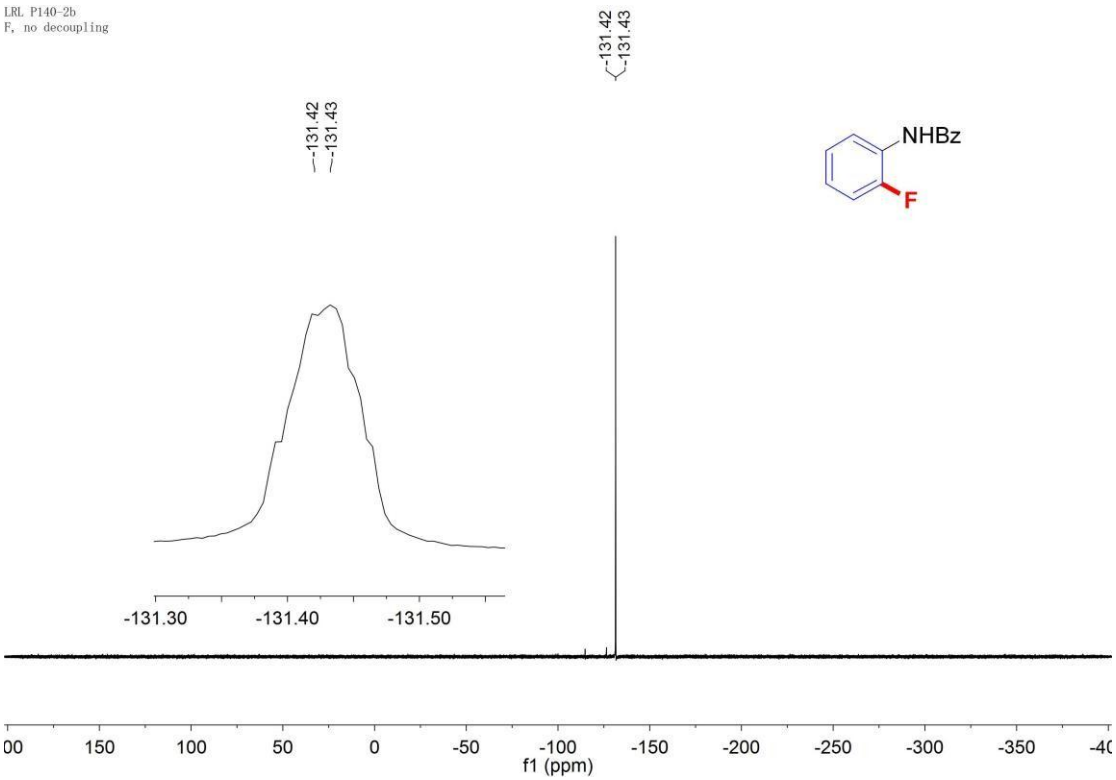

LRL 166-1a
176.6569
153.4433
151.0005
128.5827
128.4825
125.4666
125.3688
124.7756
124.7401
122.3444
122.3261
115.5722
115.3447
40.0032
27.5015
NHPiv
Cl
F
f1 (ppm)


LRL 166-1a
F, NO DC
-129.2533
-129.2624
-129.2775
-129.2974
-129.3073
-129.26
-129.32
NHPiv
Cl
F
f1 (ppm)

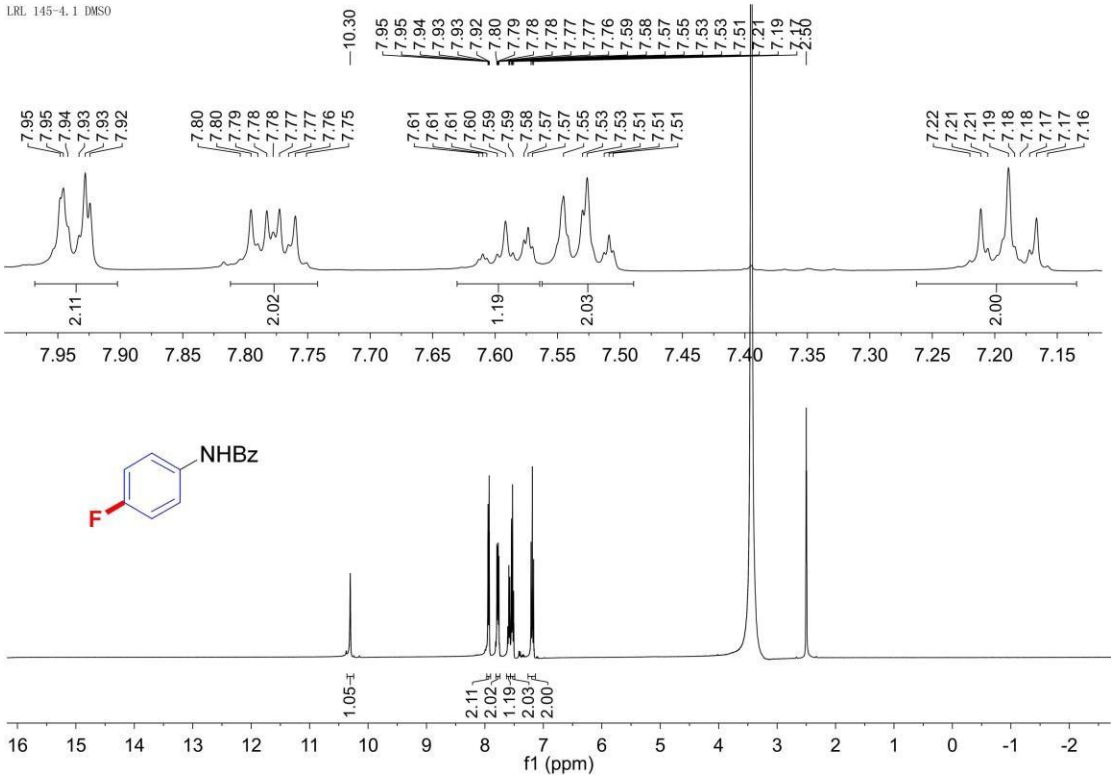
2q

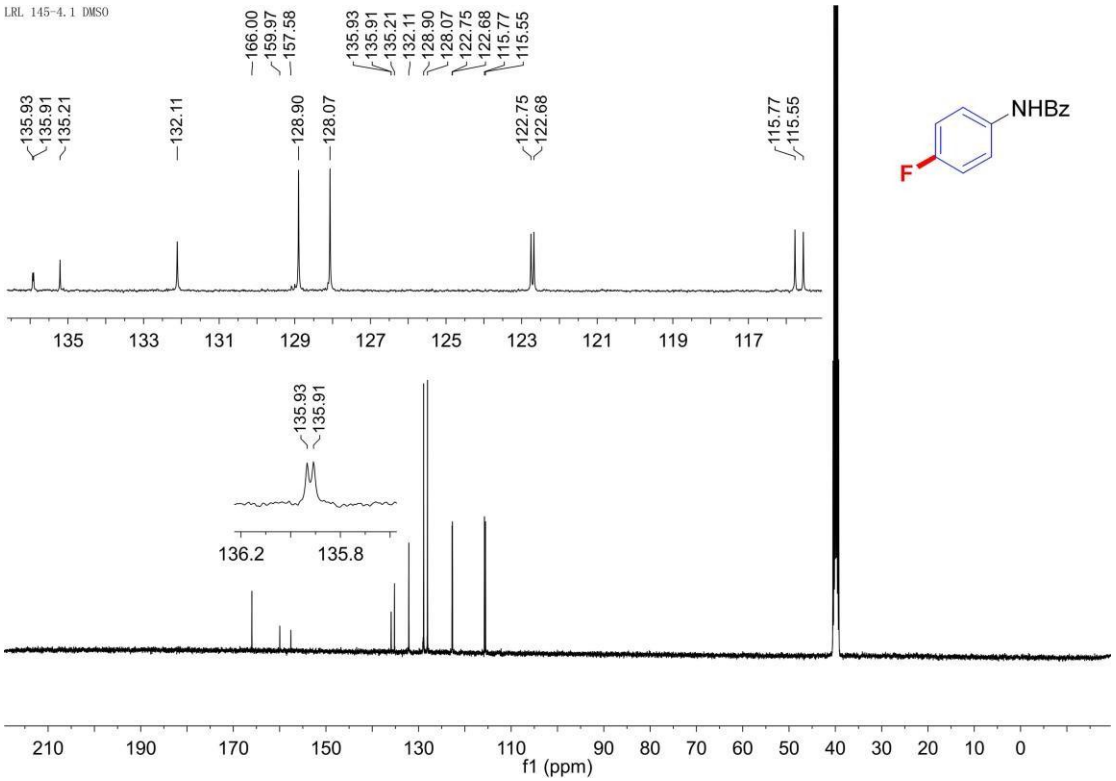


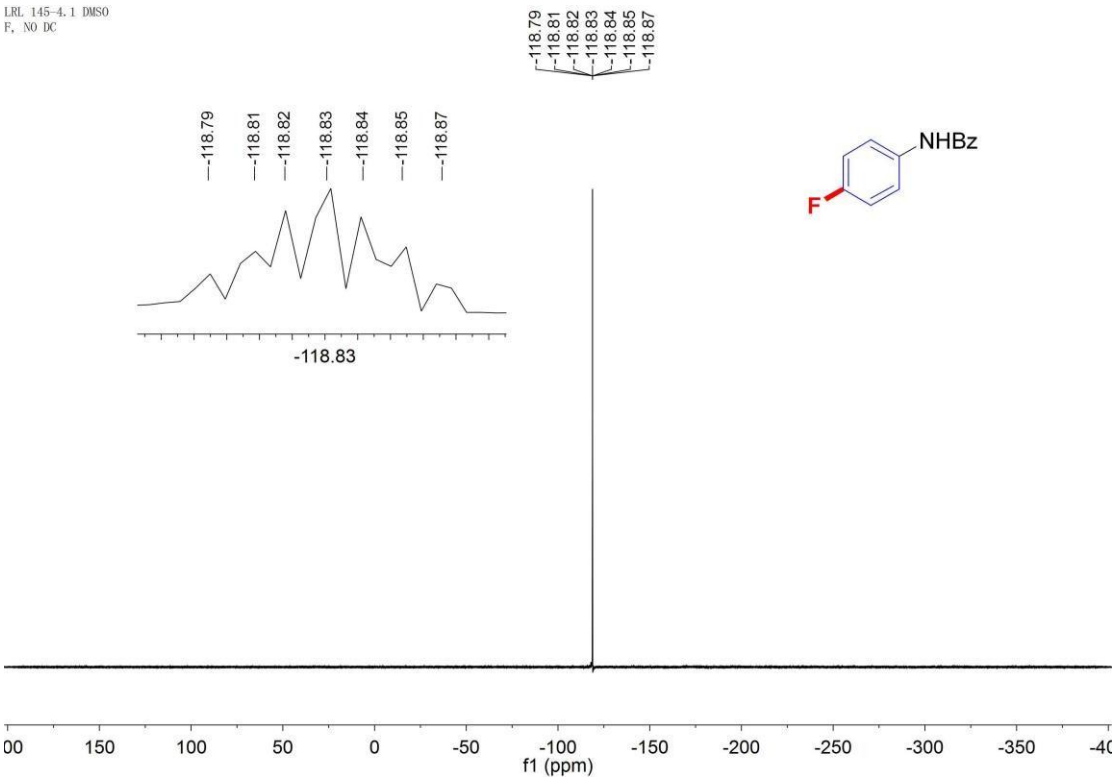



LRL P140-2b
F, no decoupling
-131.42
-131.43
-131.42
-131.43
NHBz
F
-131.30
-131.40
-131.50
00
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
-4(
f1 (ppm)

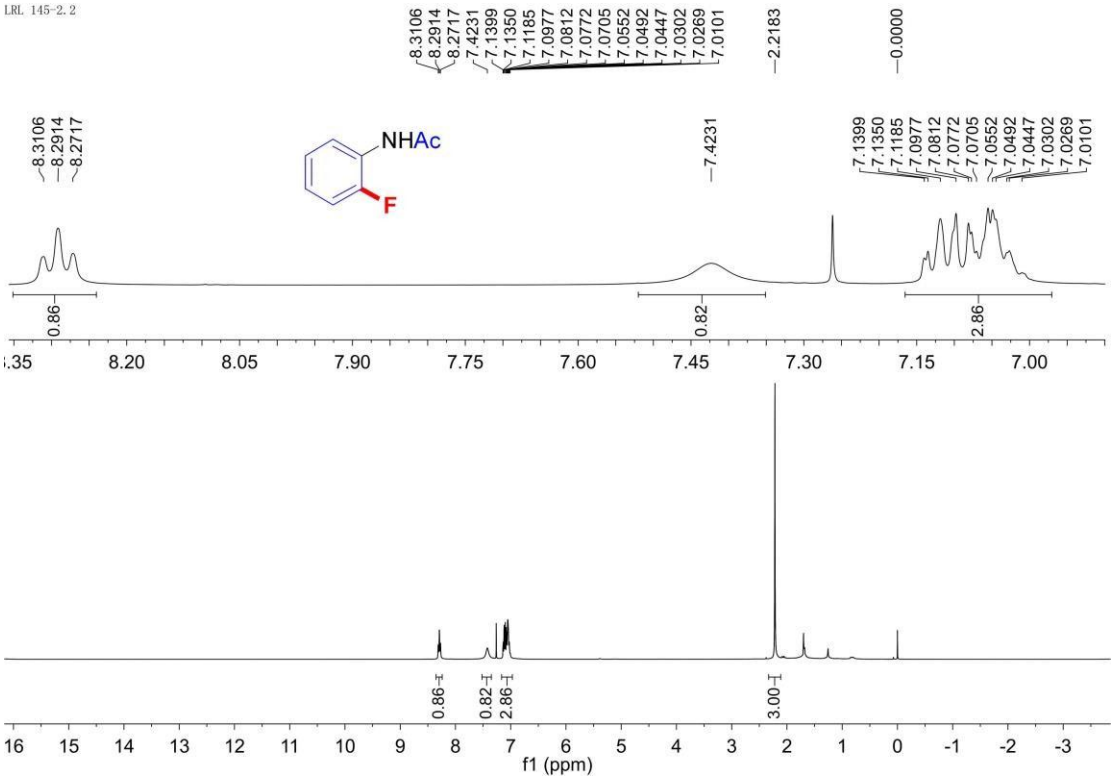
2q'

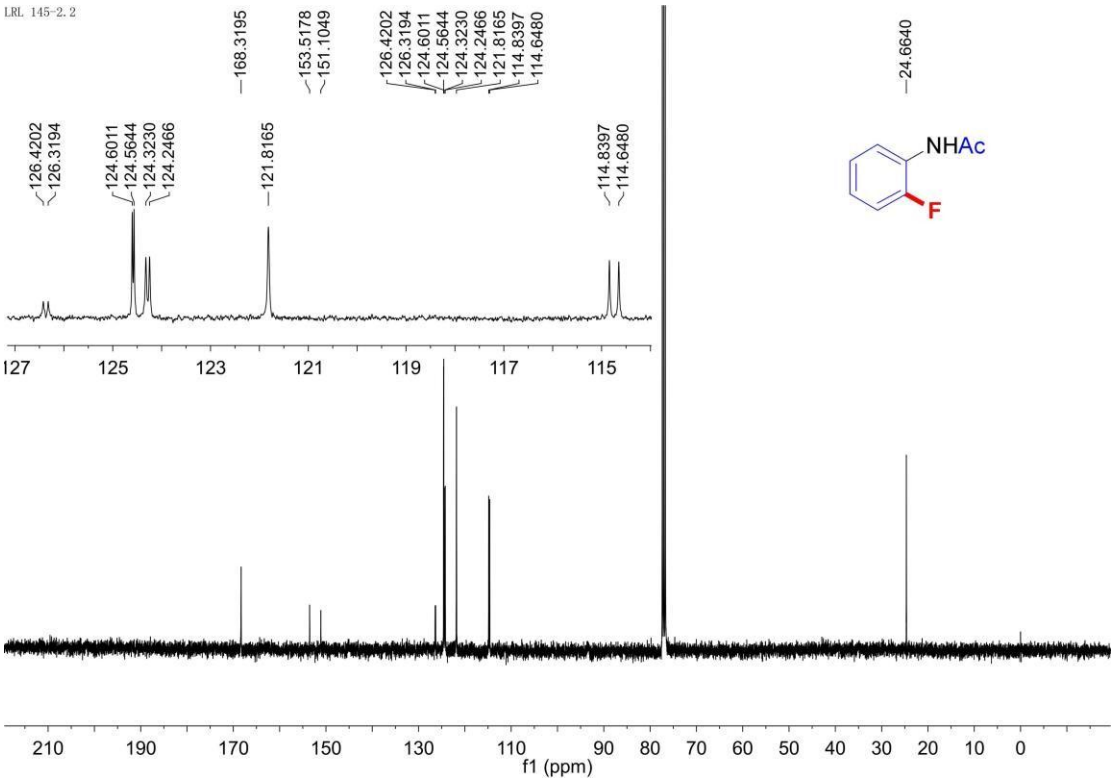


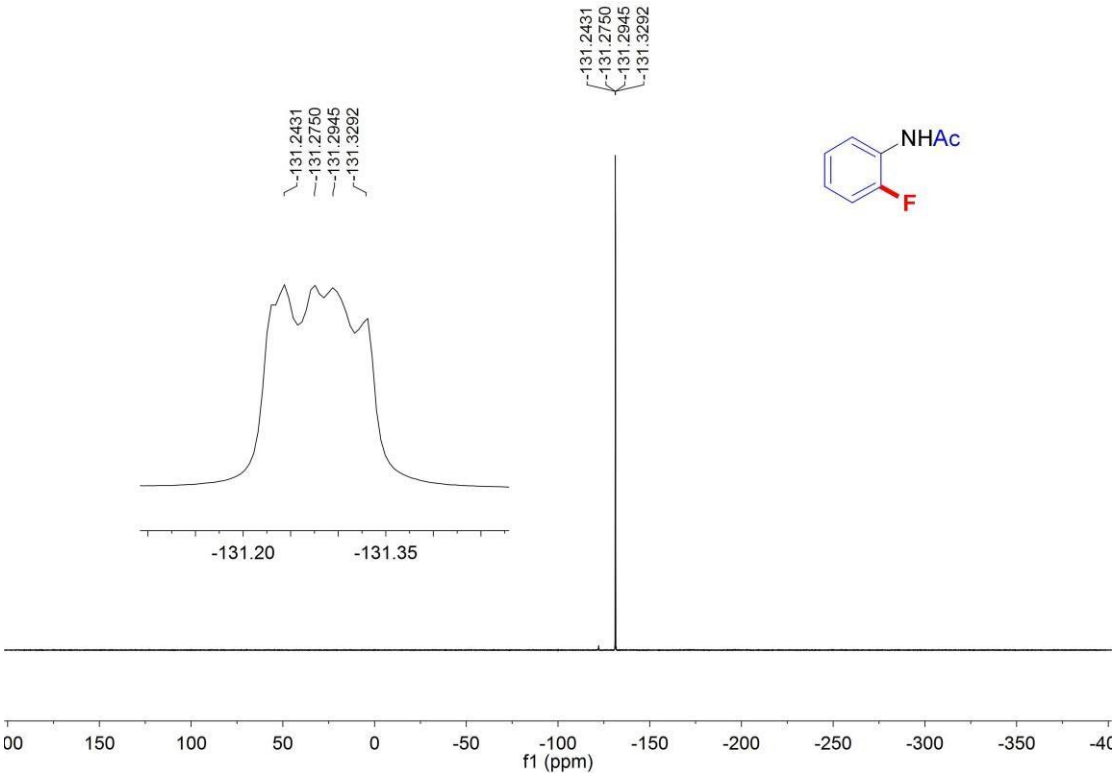



LRL 145-4.1 DMSO
F, NO DC
-118.79
-118.81
-118.82
-118.83
-118.84
-118.85
-118.87
-118.83
NHBz
F
00
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
-4(
f1 (ppm)

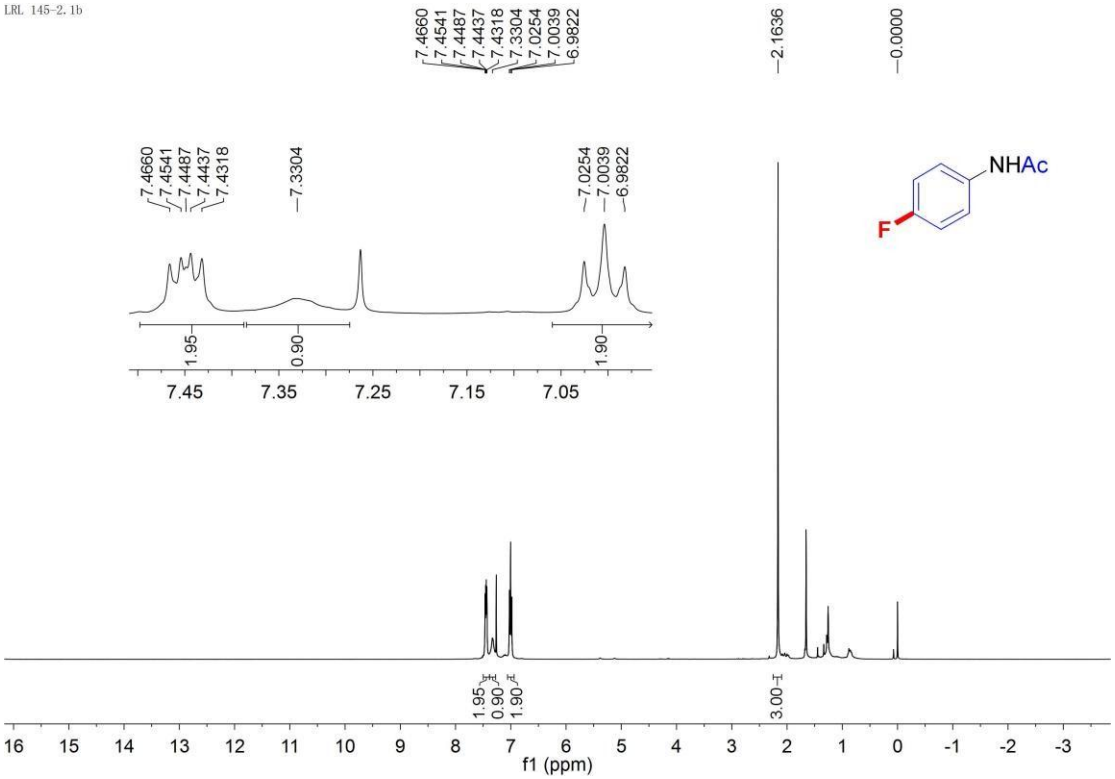
2r

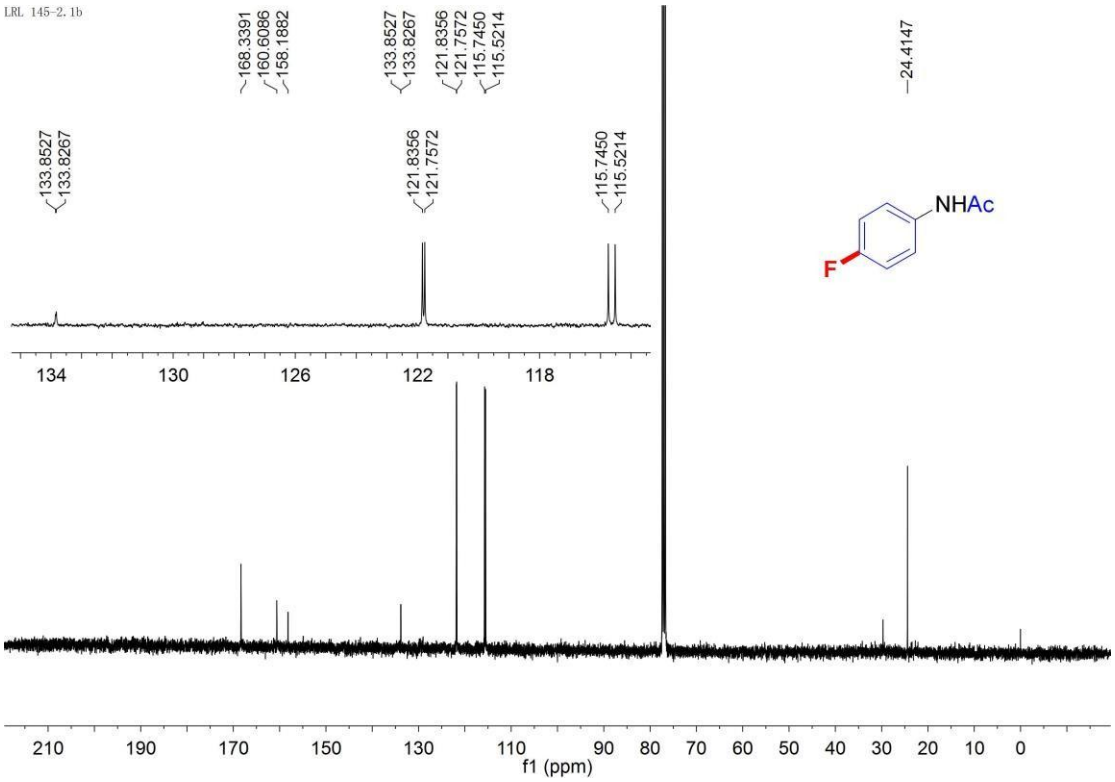

LRL 145-2.2
8.3106
8.2914
8.2717
7.4231
7.1399
7.1350
7.1185
7.0977
7.0812
7.0772
7.0705
7.0552
7.0492
7.0447
7.0302
7.0269
7.0101
2.2183
0.0000
NHAc
F
0.86
0.82
2.86
3.00
f1 (ppm)

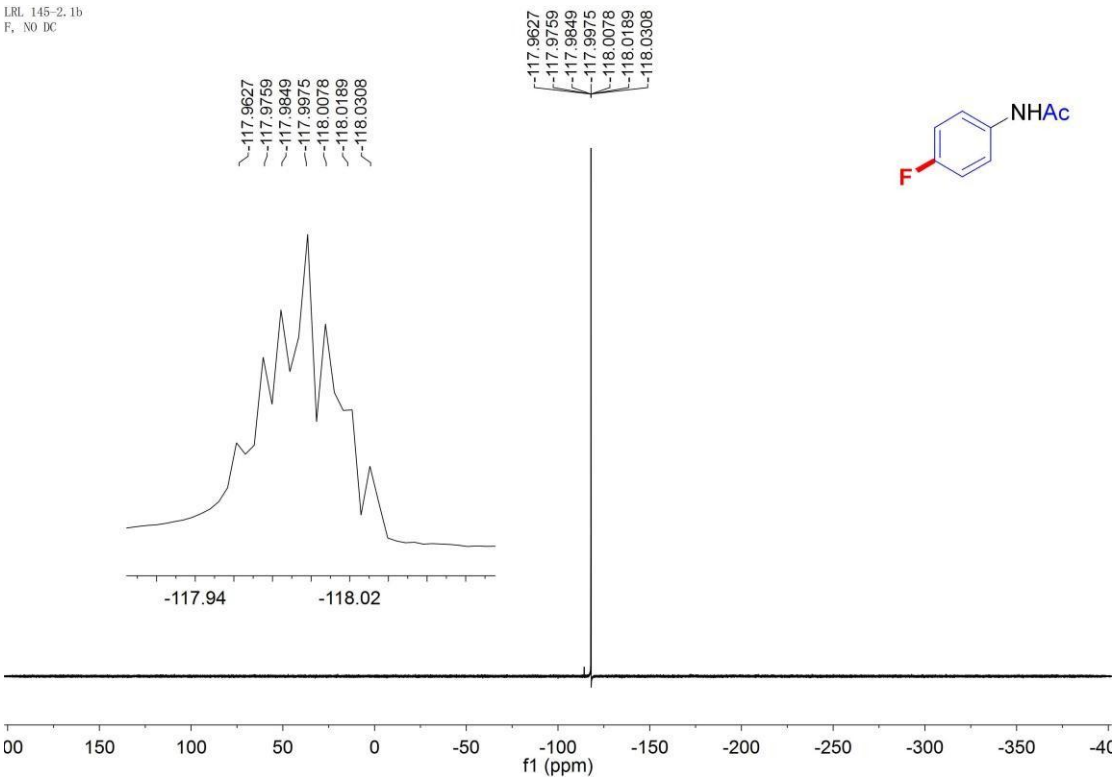

LRL 145-2.2
168.3195
153.5178
151.1049
126.4202
126.3194
124.6011
124.5644
124.3230
124.2466
121.8165
114.8397
114.6480
24.6640
NHAc
F
f1 (ppm)


-131.2431
-131.2750
-131.2945
-131.3292
-131.2431
-131.2750
-131.2945
-131.3292
NHAc
F
-131.20
-131.35
00
150
100
50
0
-50
-100
-150
-200
-250
-300
-350
-4(
f1 (ppm)

2r'

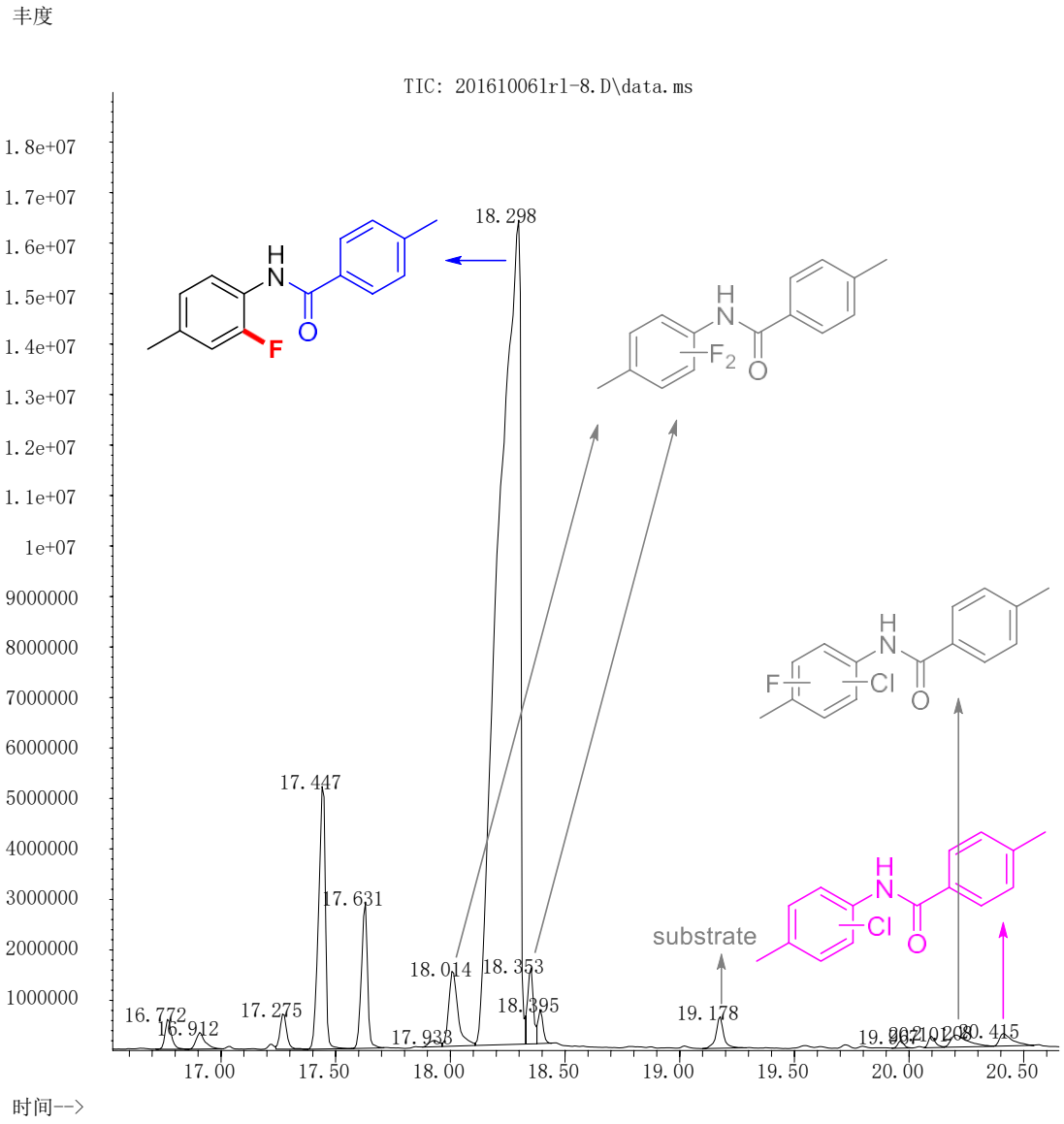

LRL 145-2.1b
7.4660
7.4541
7.4487
7.4437
7.4318
7.3304
7.0254
7.0039
6.9822
2.1636
0.0000
NHAc
F
1.95
0.90
1.90
3.00
f1 (ppm)


LRL 145-2.1b
168.3391
160.6086
158.1882
133.8527
133.8267
121.8356
121.7572
115.7450
115.5214
24.4147
NHAc
F
f1 (ppm)

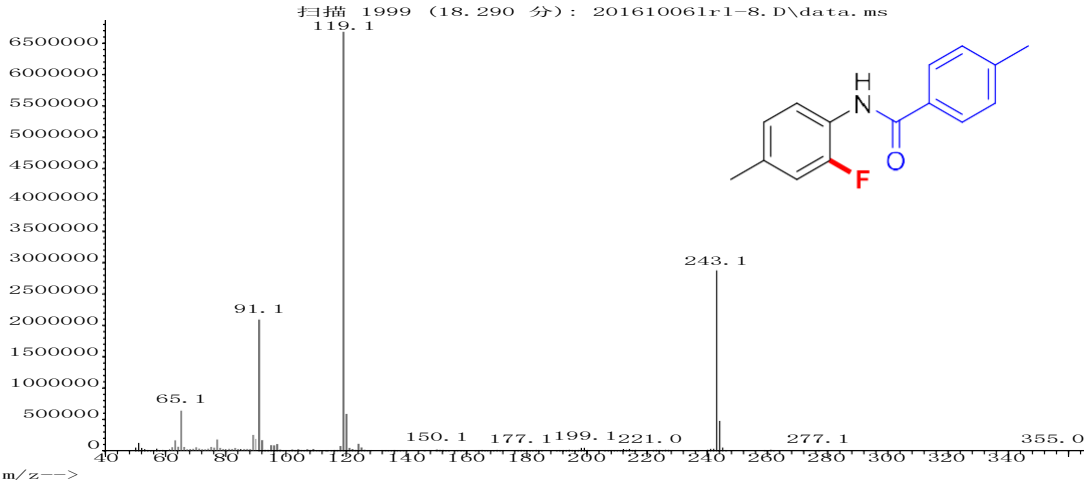

LRL 145-2.1b
F, NO DC
-117.9627
-117.9759
-117.9849
-117.9975
-118.0078
-118.0189
-118.0308
NHAc
F
-117.94
-118.02
f1 (ppm)

VIII. GC-MS experiments

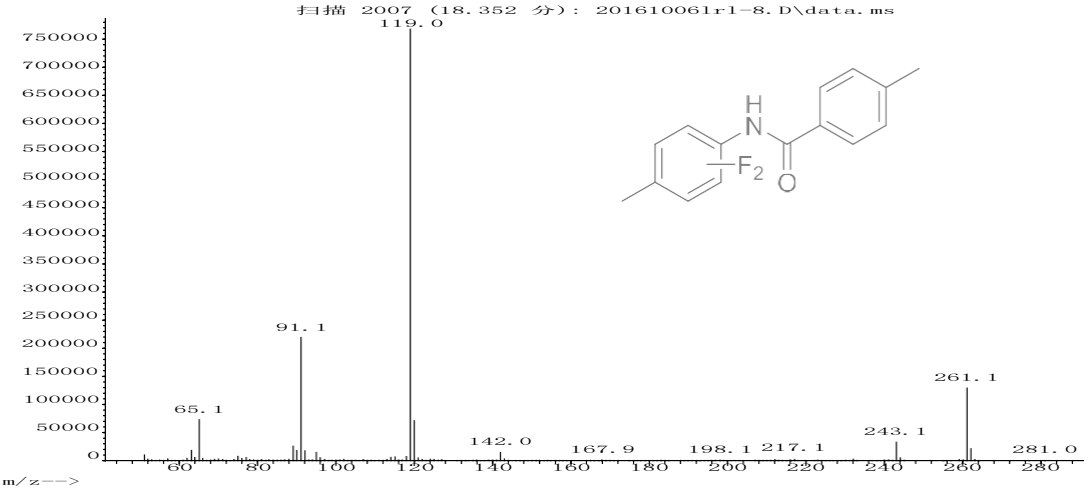
1. GC-MS analysis of the crude reaction mixture of 1b under conditions A



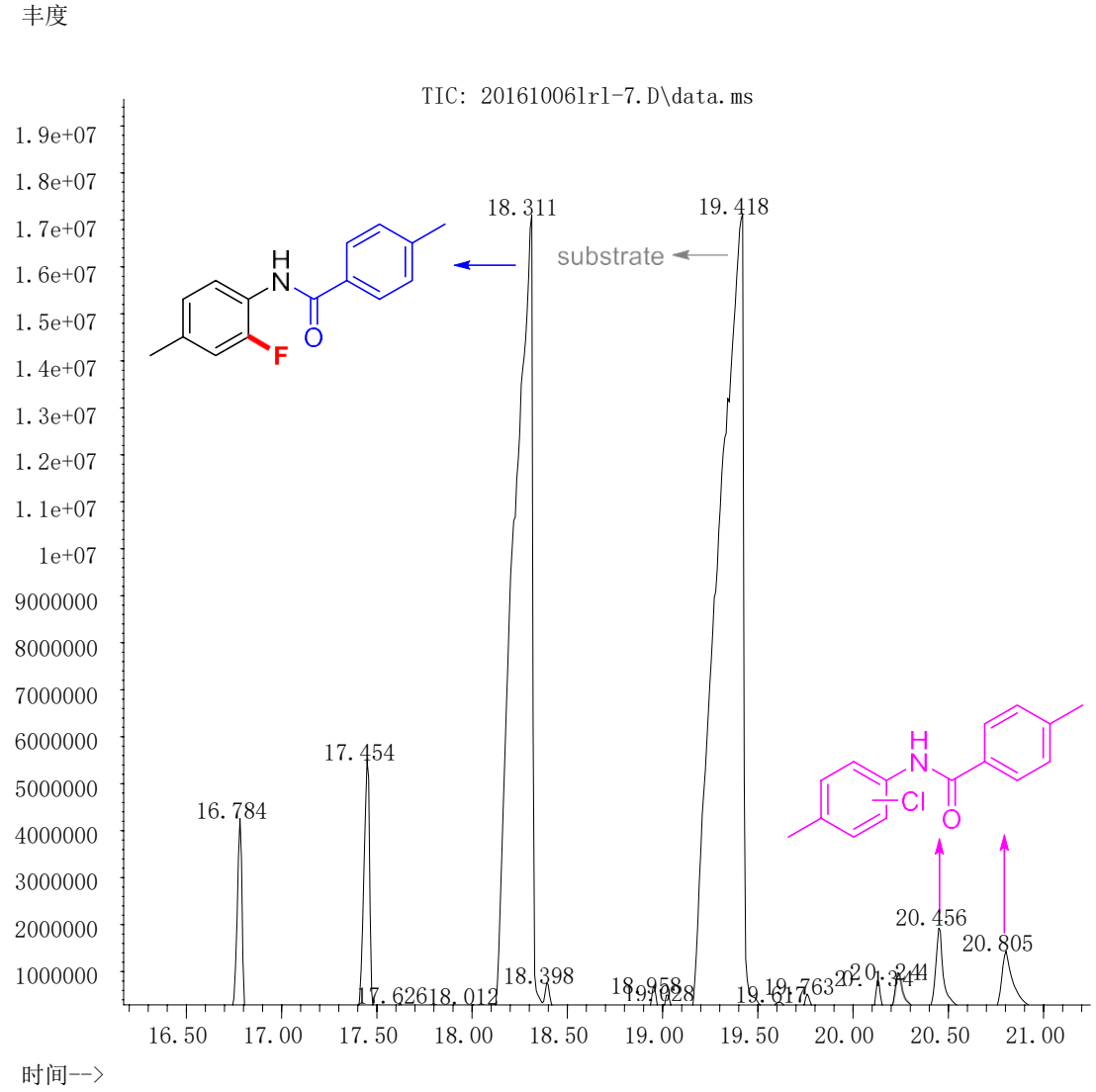
丰度

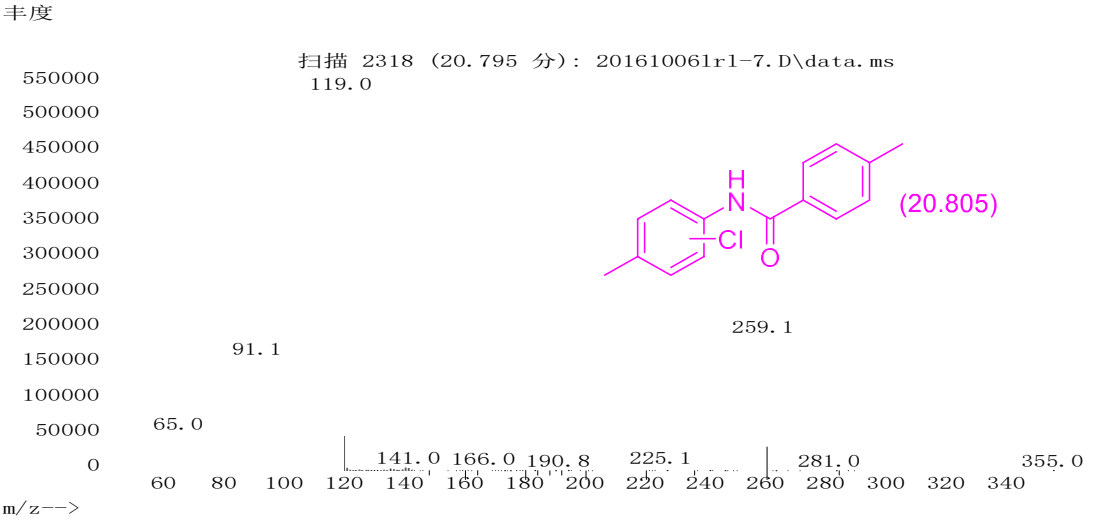

扫描 1999 (18.290 分): 201610061r1-8.D\data.ms
119.1
243.1
91.1
65.1
150.1
177.1
199.1
221.0
277.1
355.0
H
N
O
F
m/z-->
丰度
扫描 2269 (20.411 分): 201610061r1-8.D\data.ms
119.0
259.1
91.0
65.0
140.0
165.9
207.0
239.1
281.1
316.1
H
N
Cl
O
m/z-->
丰度
扫描 1964 (18.015 分): 201610061r1-8.D\data.ms
119.0
261.1
91.1
65.0
142.1
167.9
197.0
217.0
242.1
281.0
H
N
F2
O
m/z-->

丰度

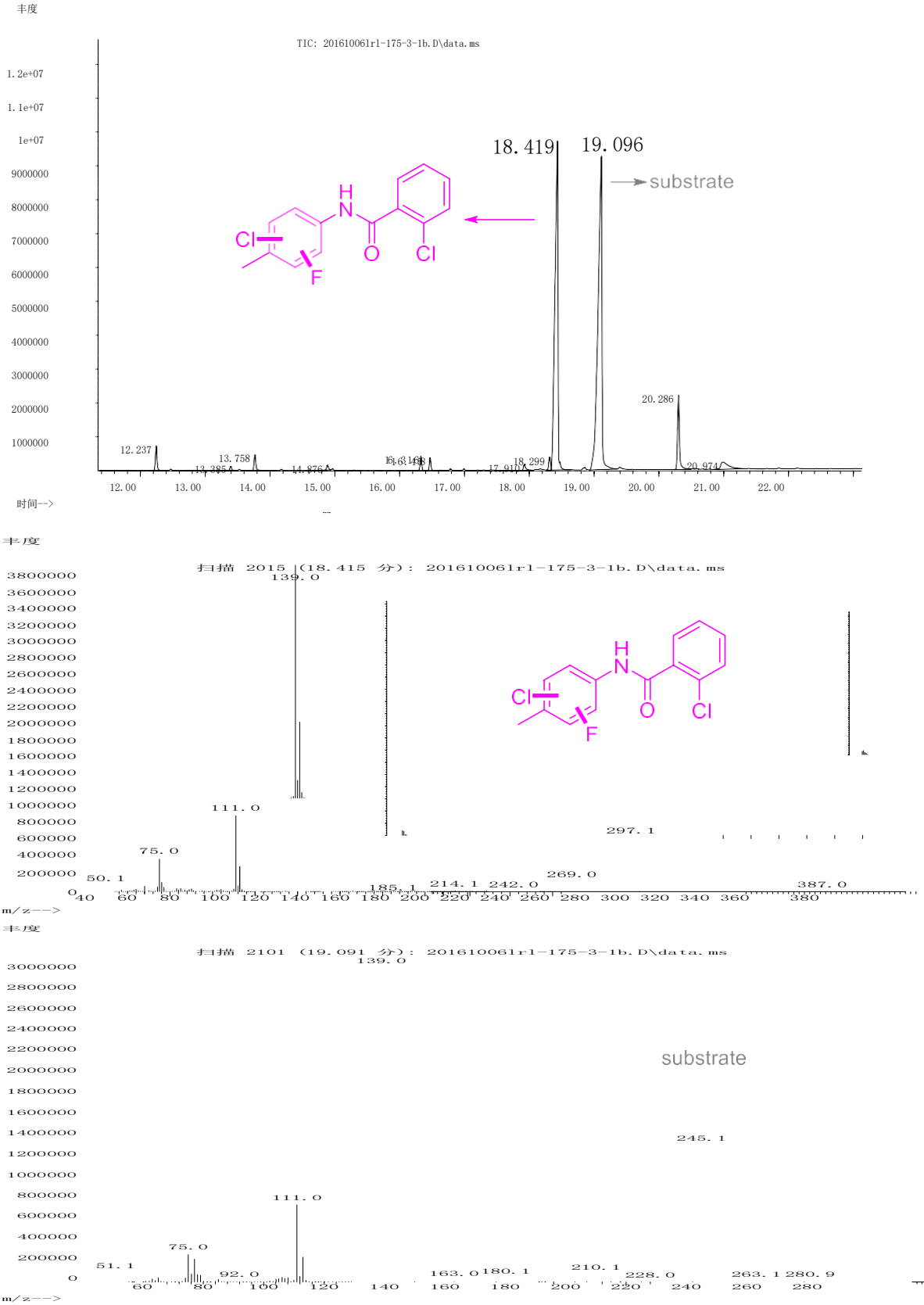

扫描 2007 (18.352 分): 201610061r1-8.D\data.ms
119.0
91.1
65.1
142.0
167.9
198.1
217.1
243.1
261.1
281.0
H
N
F2
O
m/z-->
丰度
扫描 2112 (19.177 分): 201610061r1-8.D\data.ms
119.0
substrate
225.1
91.1
65.0
139.0
180.0
207.0
243.1
261.0
281.0
m/z-->
丰度
扫描 2243 (20.206 分): 201610061r1-8.D\data.ms
119.0
91.1
65.0
136.0
158.1
184.0
207.0
239.0
257.1
277.1
H
N
F
Cl
O
m/z-->

2. GC-MS analysis of the crude reaction mixture of 1b under conditions B

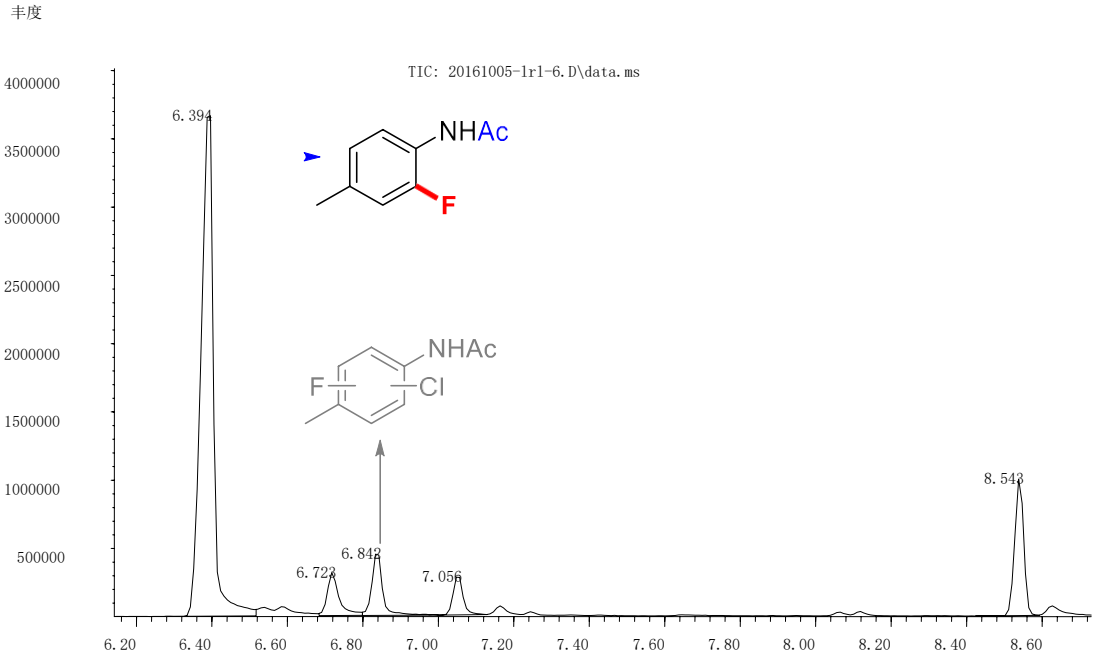




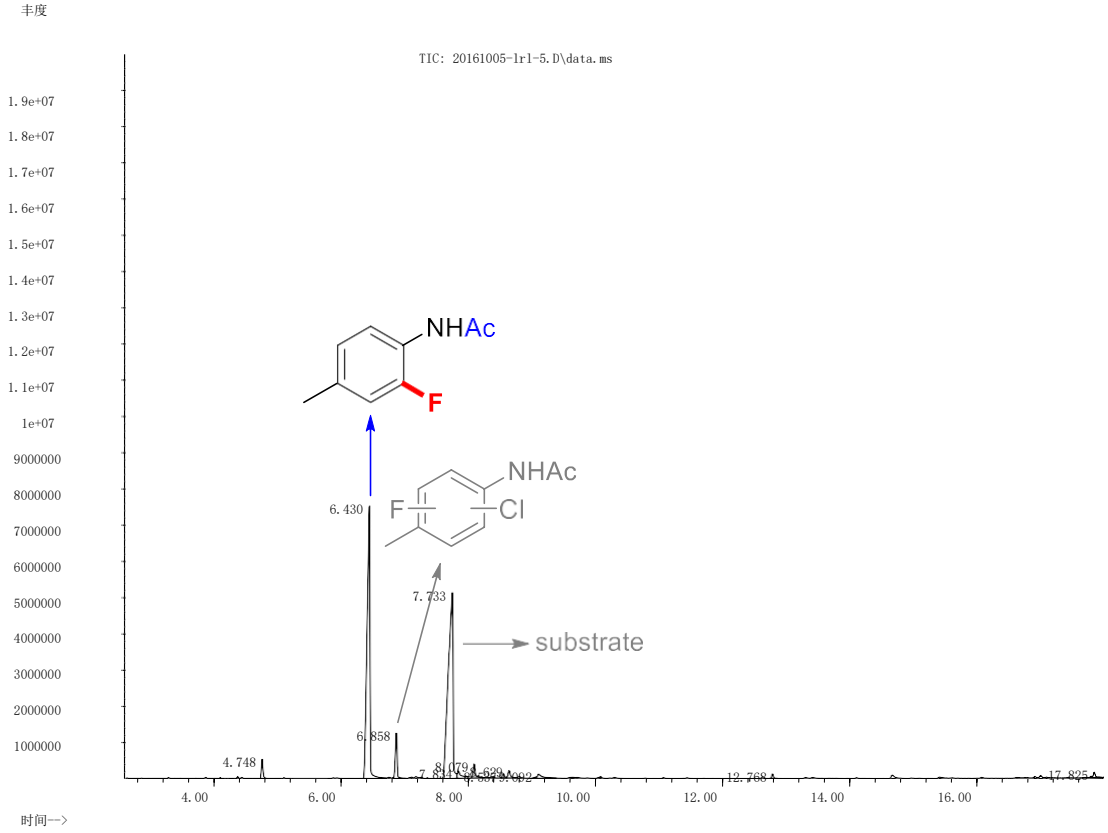
3. GC-MS analysis of the crude mixture of "recovered substrate 1g" under conditions B

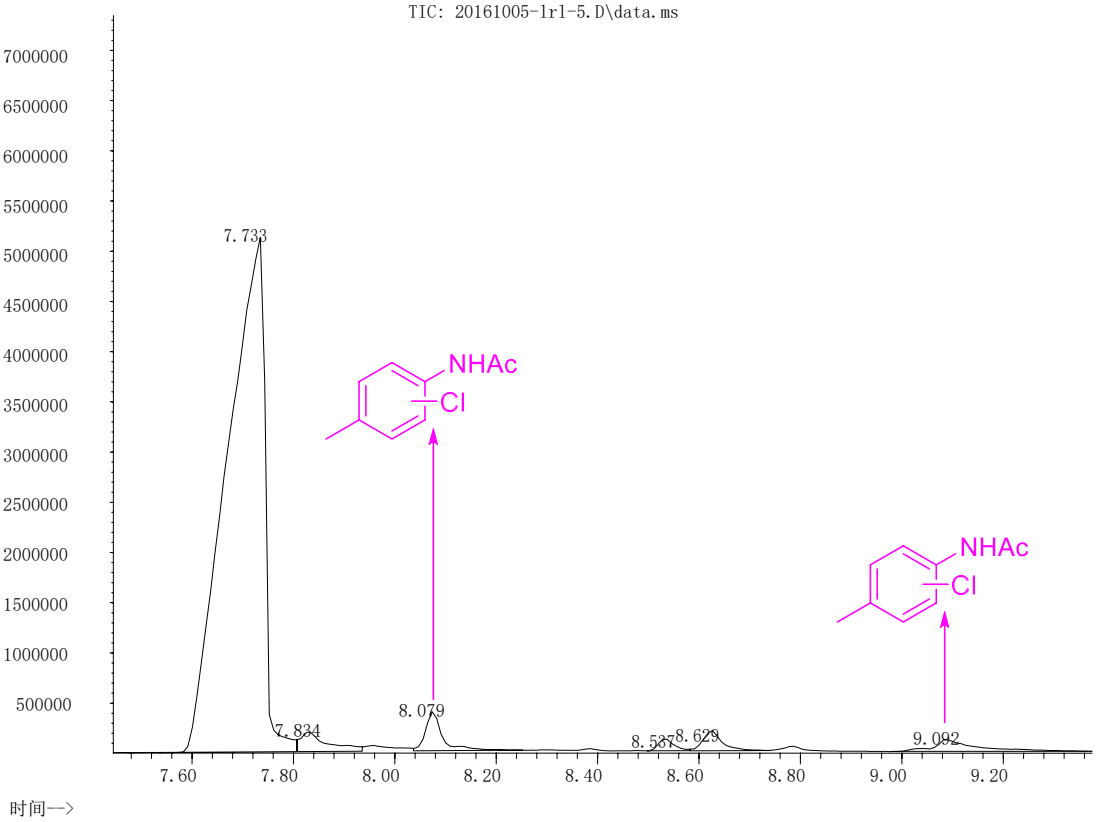


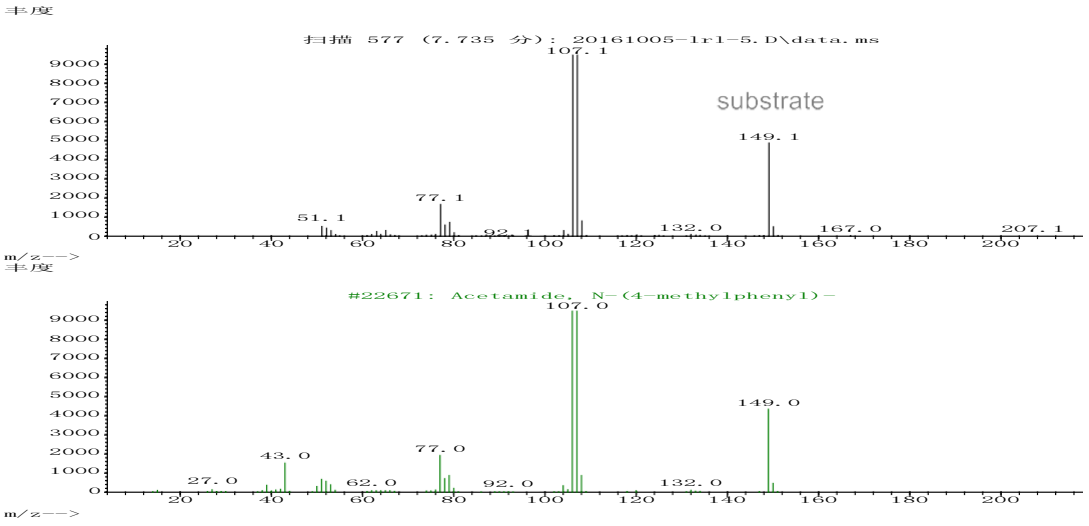
4. GC-MS analysis of the crude reaction mixture of 1i under conditions A

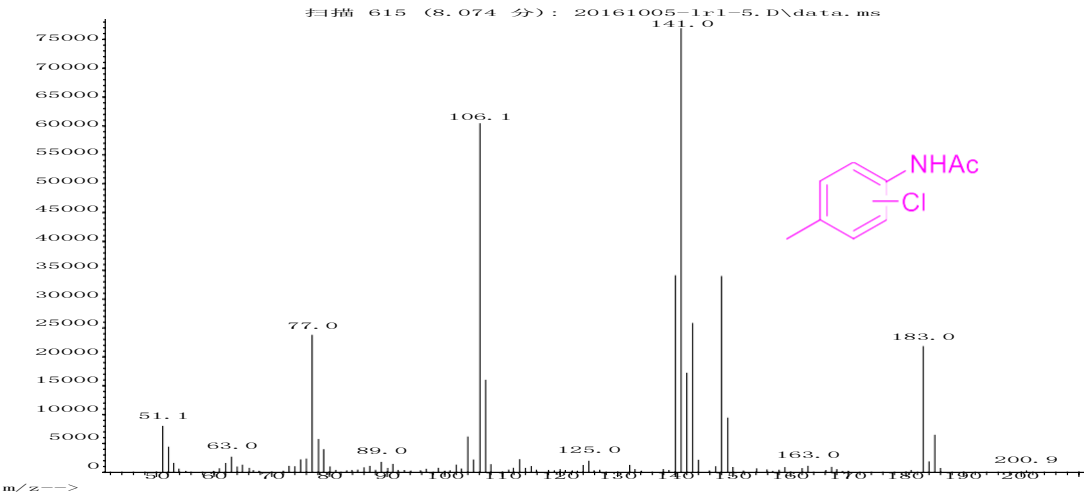


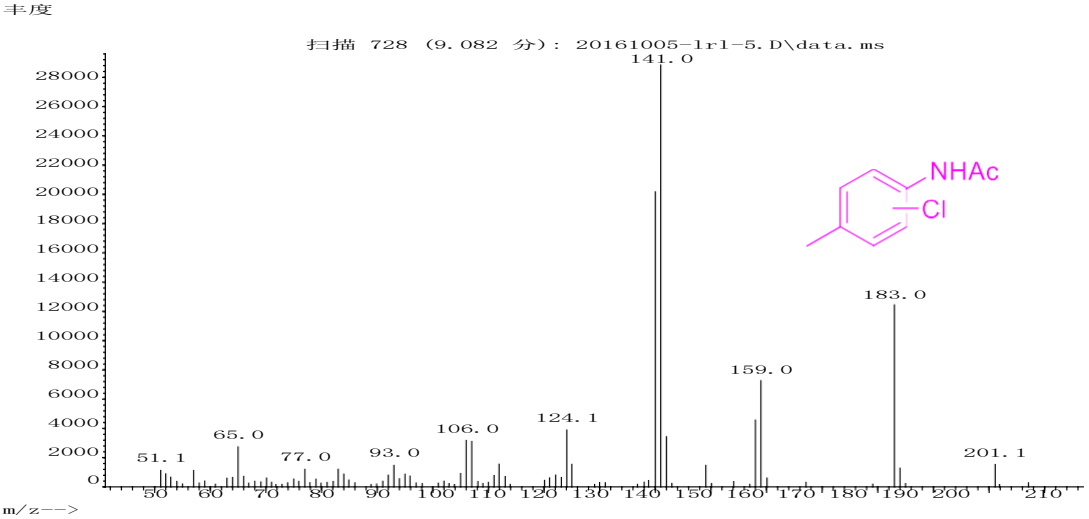
5. GC-MS analysis of the crude reaction mixture of 1i under conditions B



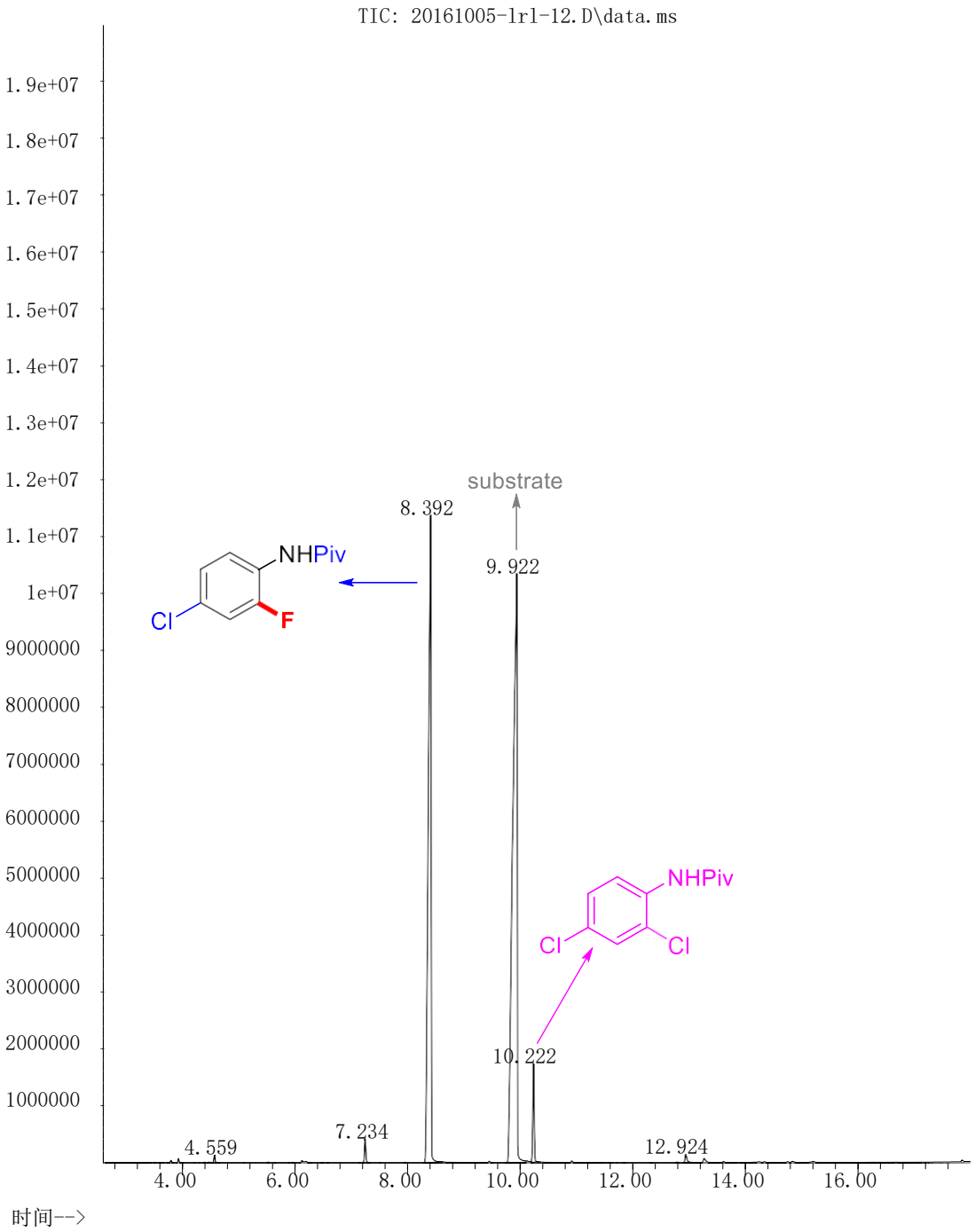


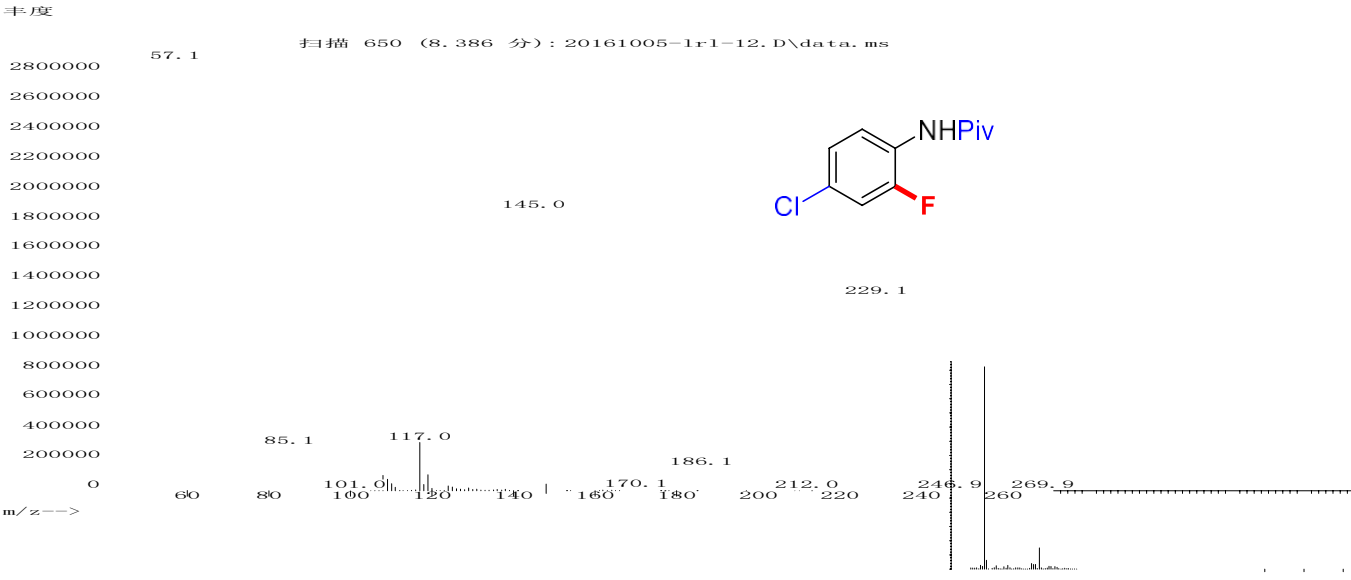

丰度
扫描 577 (7.735 分): 20161005-1r1-5.D\data.ms
substrate
107.1
149.1
77.1
51.1
132.0
167.0
207.1
m/z-->
丰度
#22671: Acetamide, N-(4-methylphenyl)-
107.0
149.0
43.0
77.0
27.0
62.0
92.0
132.0
m/z-->

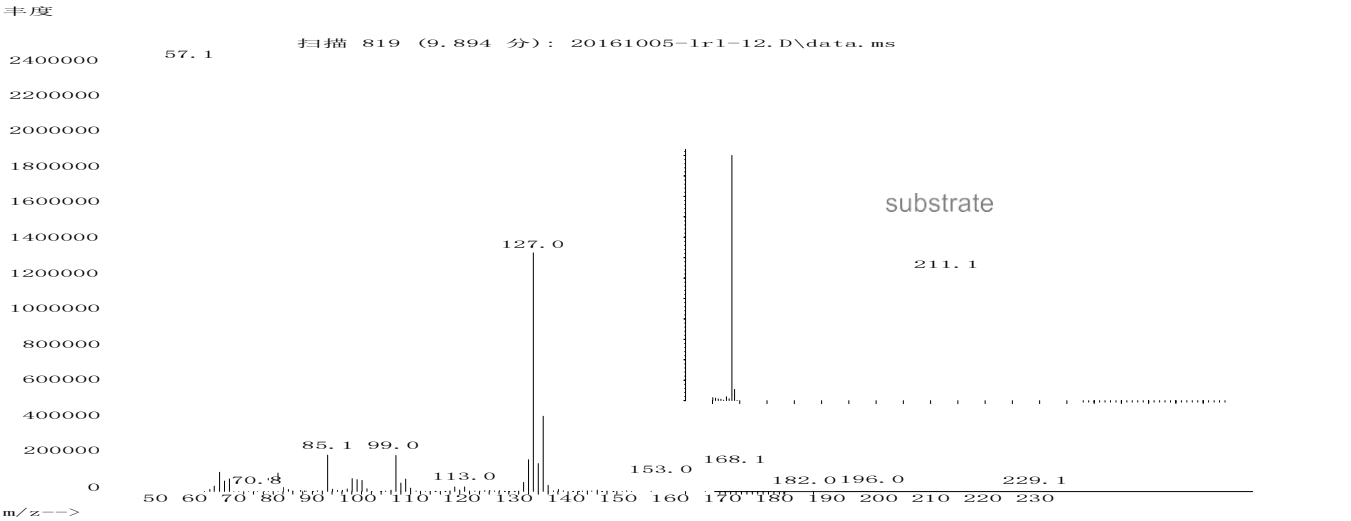

丰度
扫描 615 (8.074 分): 20161005-1r1-5.D\data.ms
141.0
106.1
NHAc
Cl
77.0
183.0
51.1
63.0
89.0
125.0
163.0
200.9
m/z-->

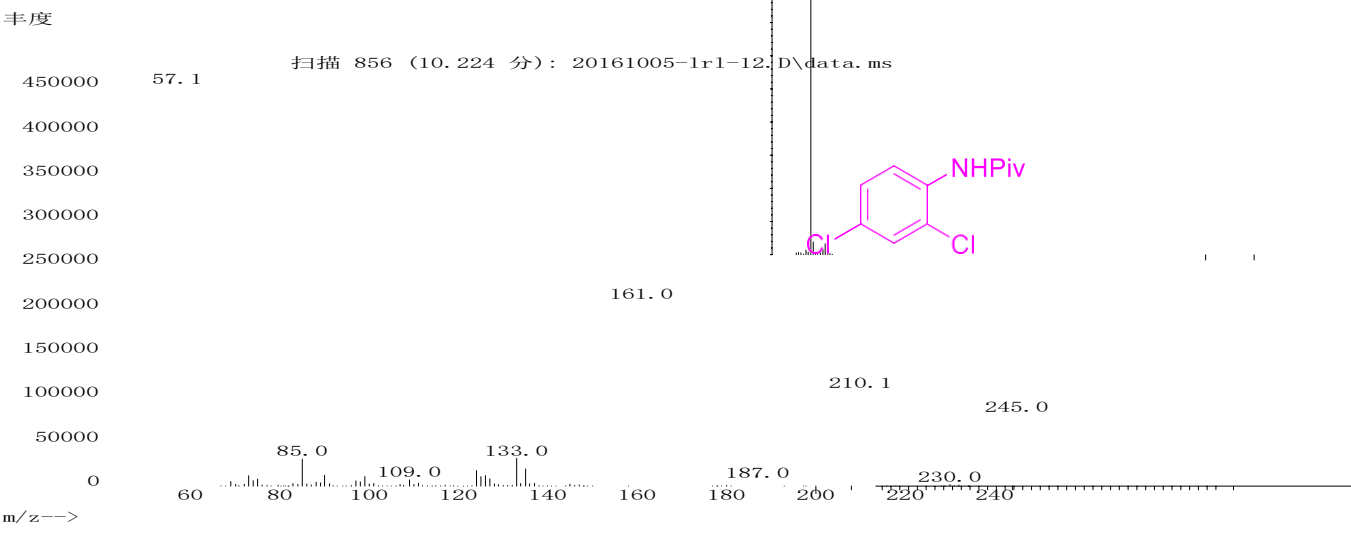

丰度
扫描 728 (9.082 分): 20161005-1r1-5.D\data.ms
141.0
NHAc
Cl
183.0
159.0
124.1
65.0
106.0
51.1
77.0
93.0
201.1
m/z-->

6. GC-MS analysis of the crude reaction mixture of 1p under conditions A

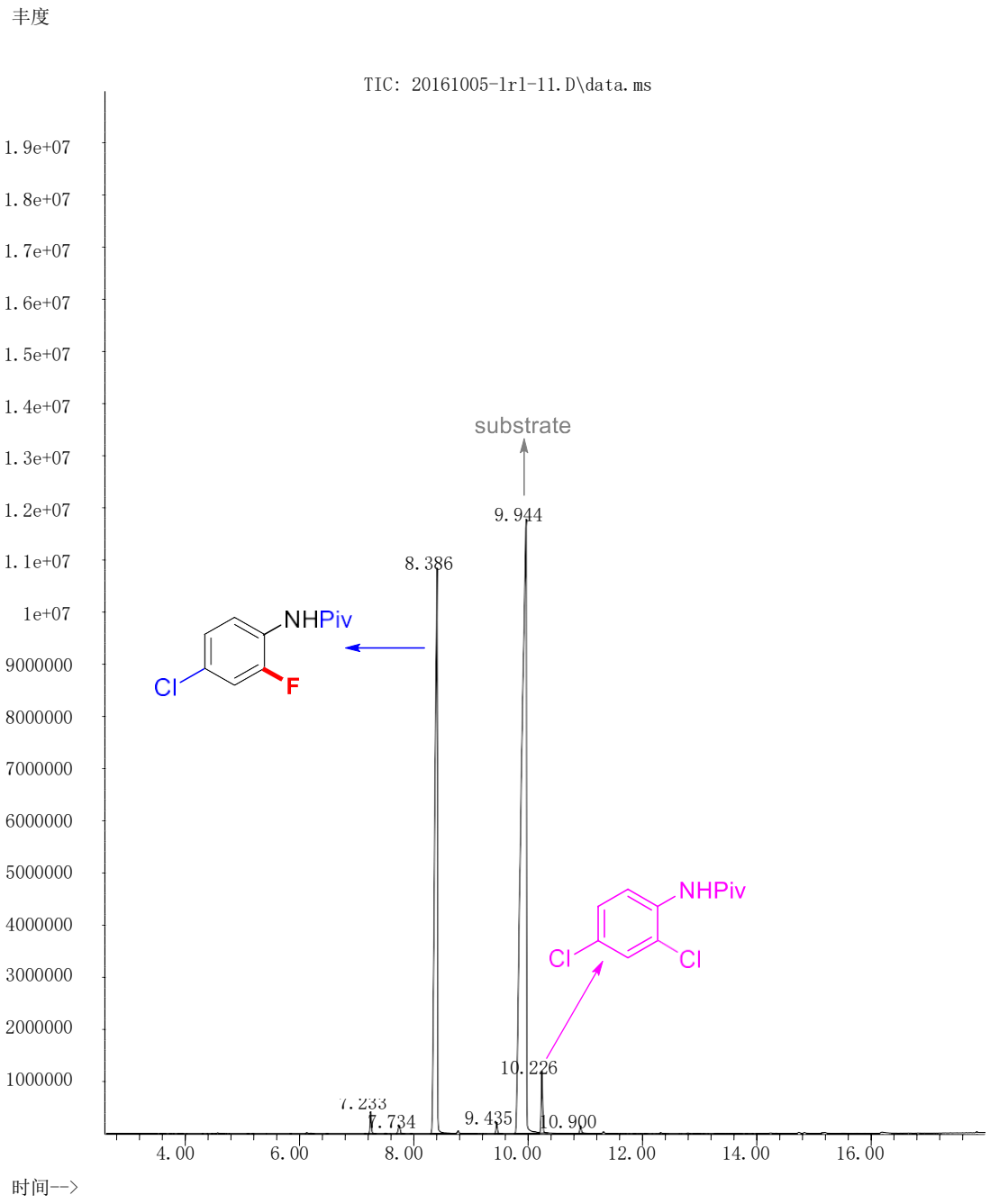



丰度
扫描 650 (8.386 分)：20161005-1r1-12.D\data.ms
57.1
145.0
NHPiv
Cl
F
229.1
85.1
117.0
186.1
101.0
170.1
212.0
246.9
269.9
m/z-->

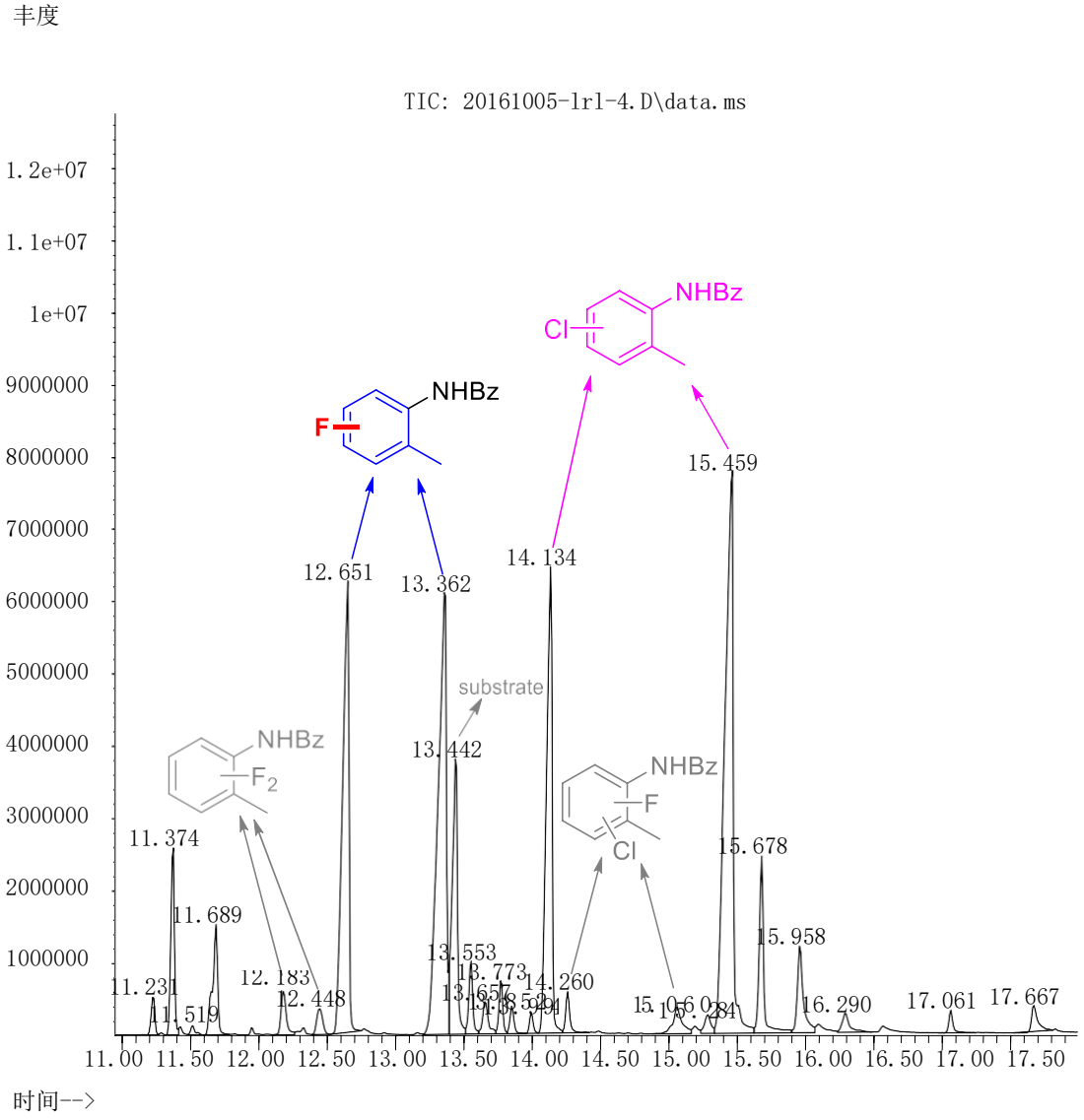

丰度
扫描 819 (9.894 分)：20161005-1r1-12.D\data.ms
57.1
substrate
211.1
127.0
85.1
99.0
70.8
113.0
153.0
168.1
182.0
196.0
229.1
m/z-->

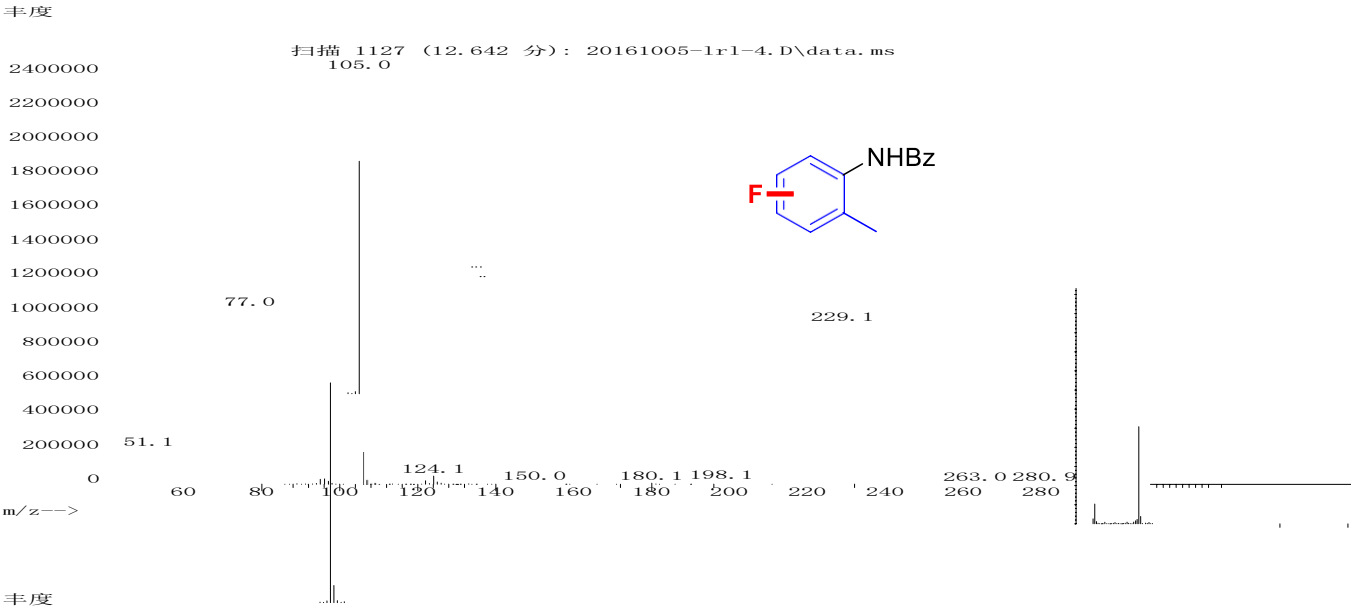

丰度
扫描 856 (10.224 分)：20161005-1r1-12.D\data.ms
57.1
NHPiv
Cl
Cl
161.0
210.1
245.0
85.0
133.0
109.0
187.0
230.0
m/z-->

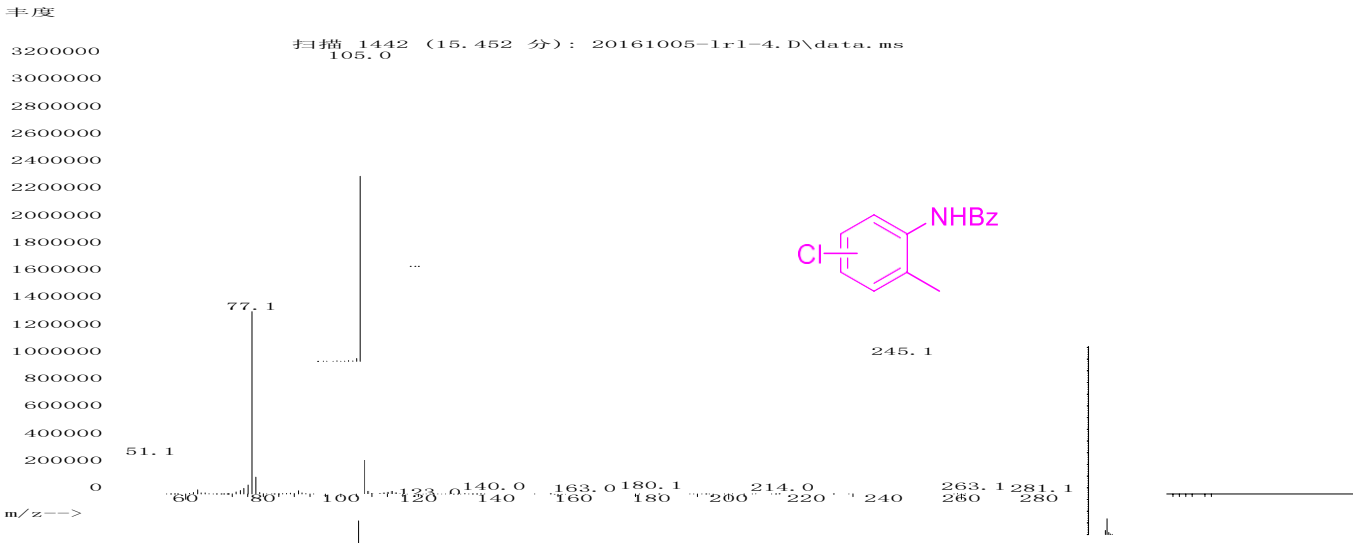
7. GC-MS analysis of the crude reaction mixture of 1p under conditions B

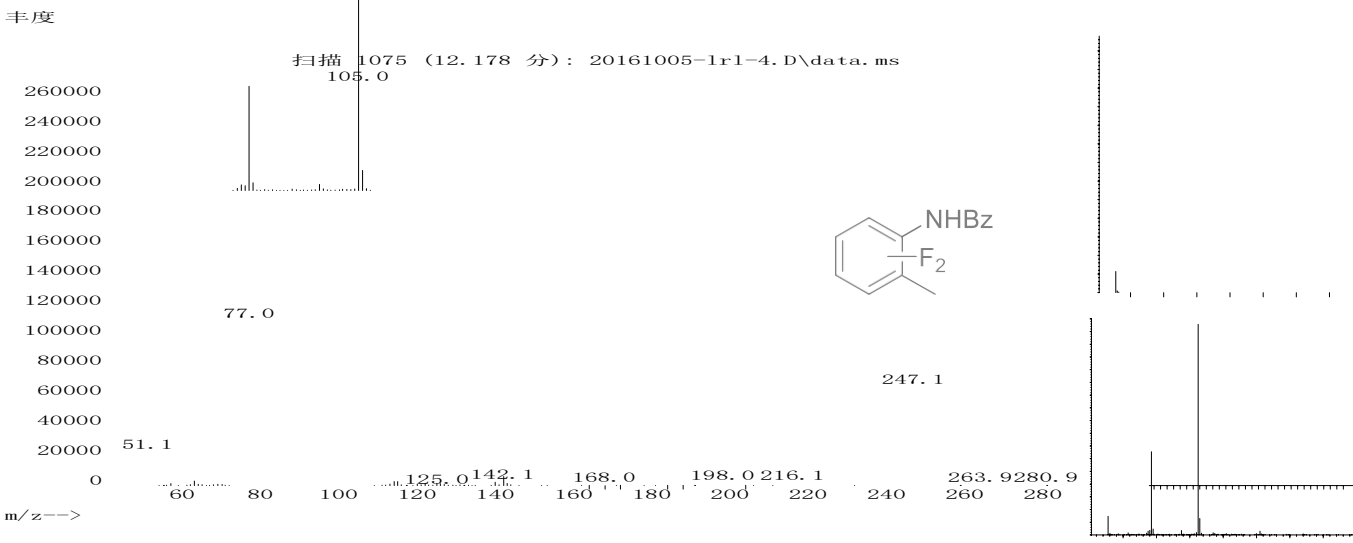


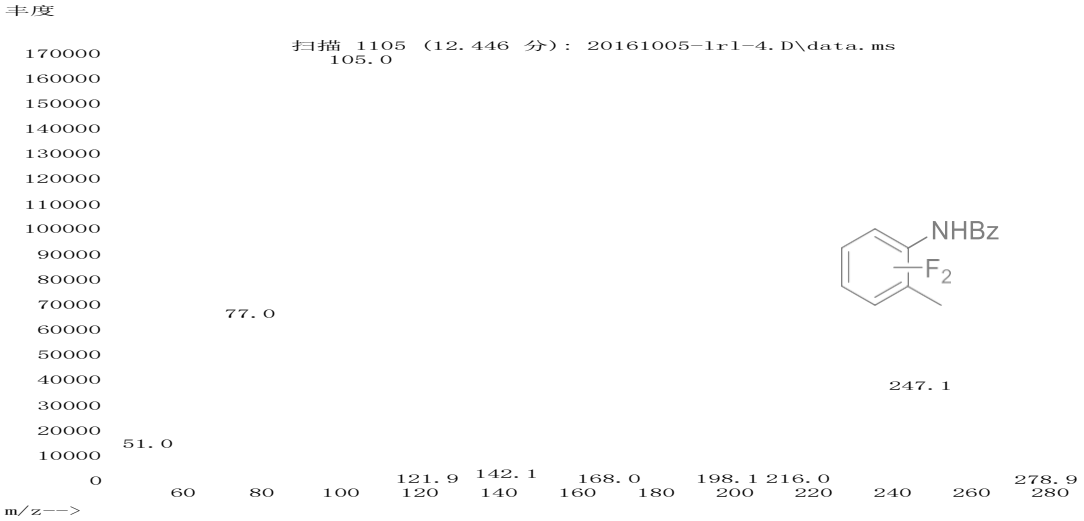
8. GC-MS analysis of the crude reaction mixture of 1s under conditions A

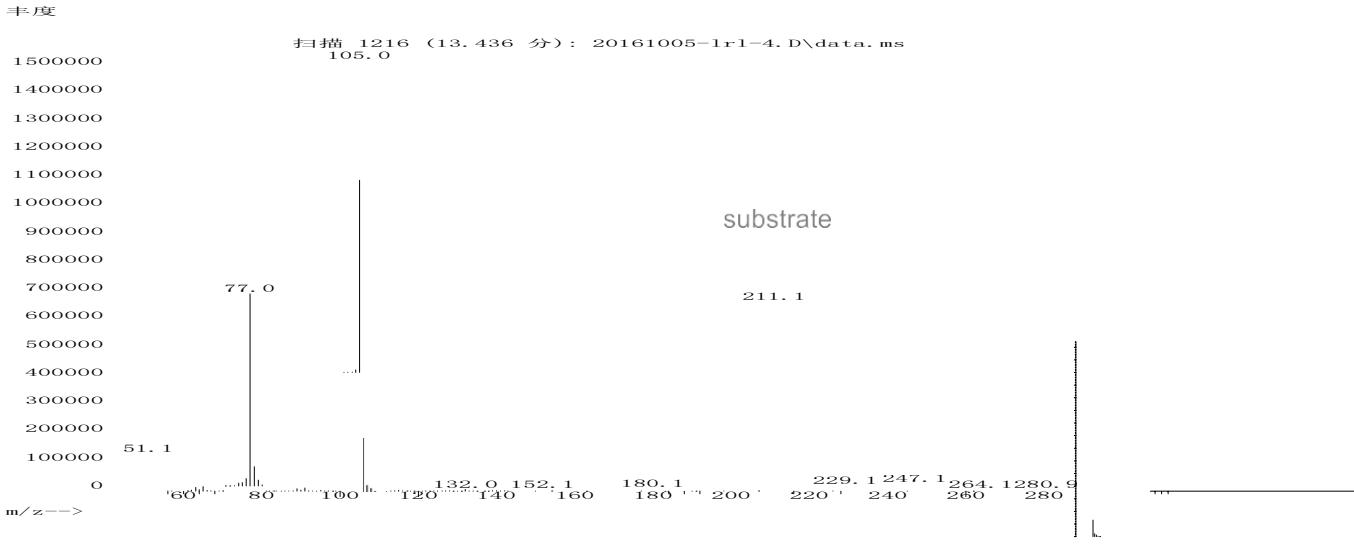


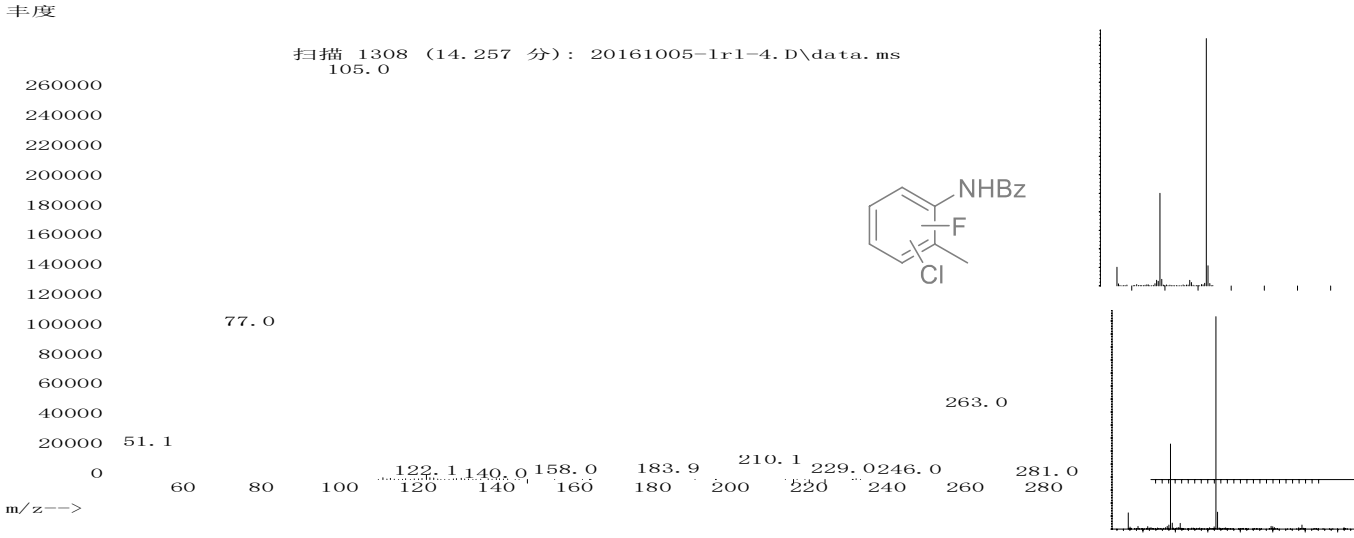

丰度
扫描 1127 (12.642 分): 20161005-1r1-4.D\data.ms
105.0
NHBz
F
77.0
229.1
51.1
124.1
150.0
180.1
198.1
263.0
280.9
m/z-->
丰度
扫描 1207 (13.356 分): 20161005-1r1-4.D\data.ms
105.0
NHBz
F
77.0
229.1
51.1
124.1
150.0
170.0
198.1
263.1
313.1
m/z-->
丰度
扫描 1294 (14.132 分): 20161005-1r1-4.D\data.ms
105.0
210.1
NHBz
Cl
77.1
51.1
122.9
140.0
163.1
180.1
228.0
245.1
263.0
281.0
m/z-->

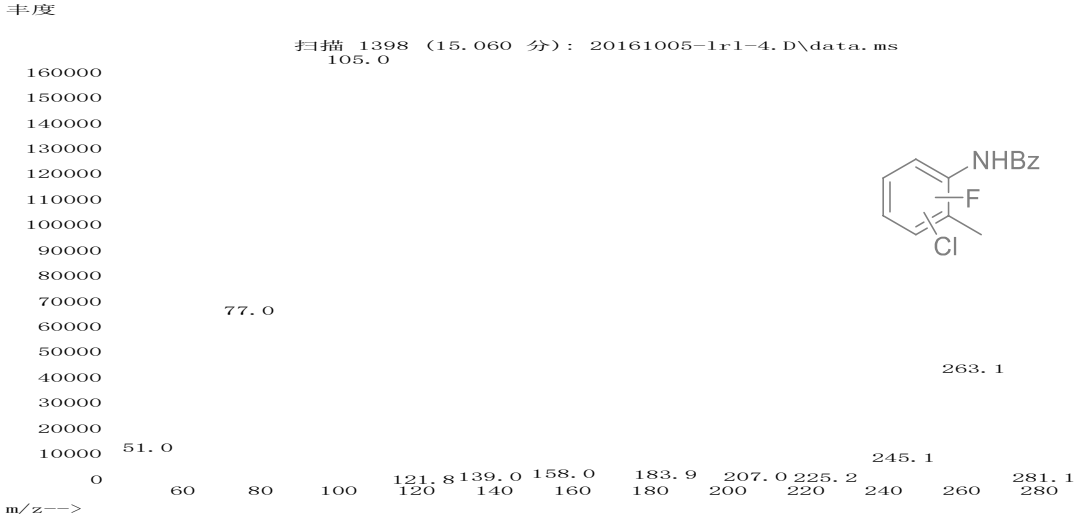

丰度
扫描 1442 (15.452 分): 20161005-1r1-4.D\data.ms
105.0
77.1
51.1
245.1
NHBz
Cl
m/z-->


丰度
扫描 1075 (12.178 分): 20161005-1r1-4.D\data.ms
105.0
77.0
51.1
247.1
NHBz
F2
m/z-->

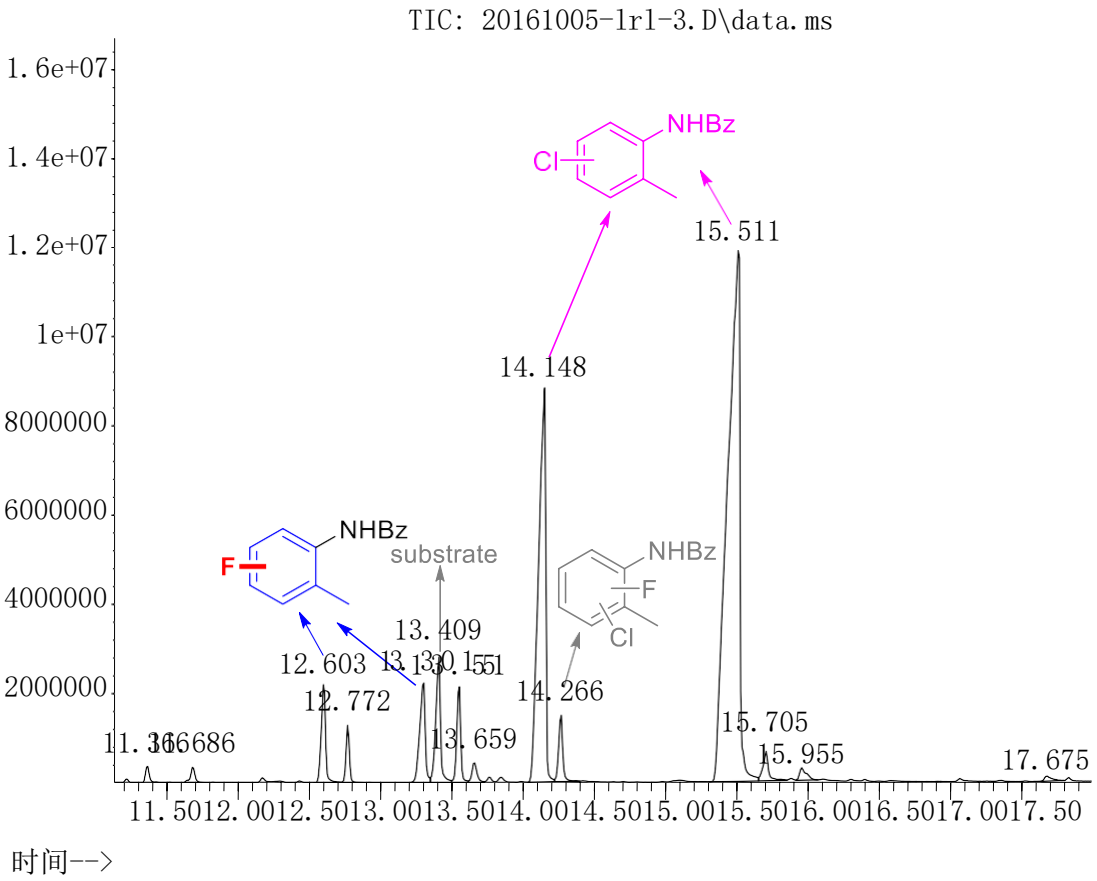

丰度
扫描 1105 (12.446 分): 20161005-1r1-4.D\data.ms
105.0
77.0
51.0
247.1
NHBz
F2
m/z-->


丰度
扫描 1216 (13.436 分): 20161005-1r1-4.D\data.ms
105.0
substrate
77.0
211.1
51.1
132.0
152.1
180.1
229.1
247.1
264.1
280.9
m/z-->

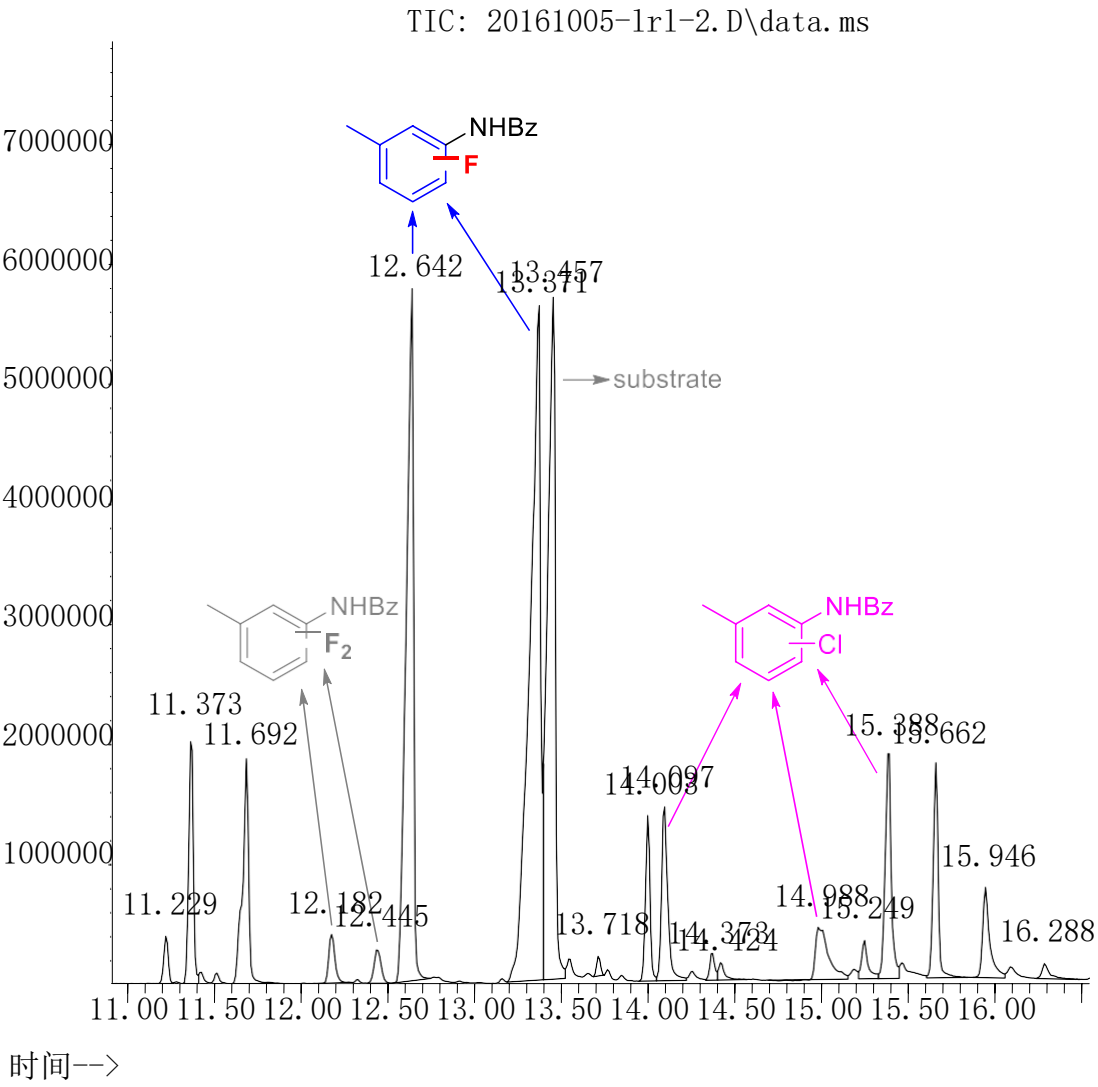

丰度
扫描 1308 (14.257 分): 20161005-1r1-4.D\data.ms
105.0
NHBz
F
Cl
77.0
263.0
51.1
122.1
140.0
158.0
183.9
210.1
229.0
246.0
281.0
m/z-->

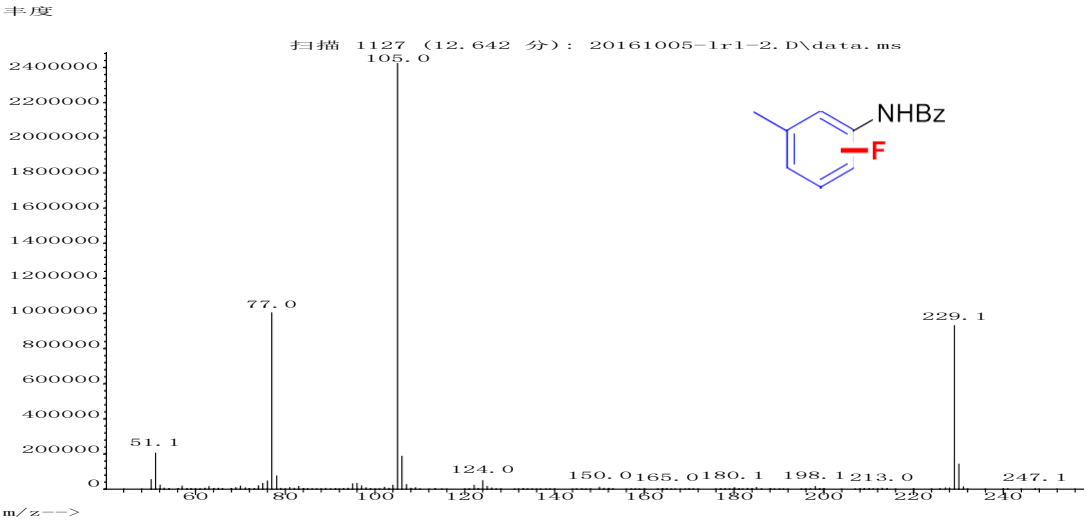

丰度
扫描 1398 (15.060 分): 20161005-1r1-4.D\data.ms
105.0
NHBz
F
Cl
77.0
263.1
51.0
121.8
139.0
158.0
183.9
207.0
225.2
245.1
281.1
m/z-->

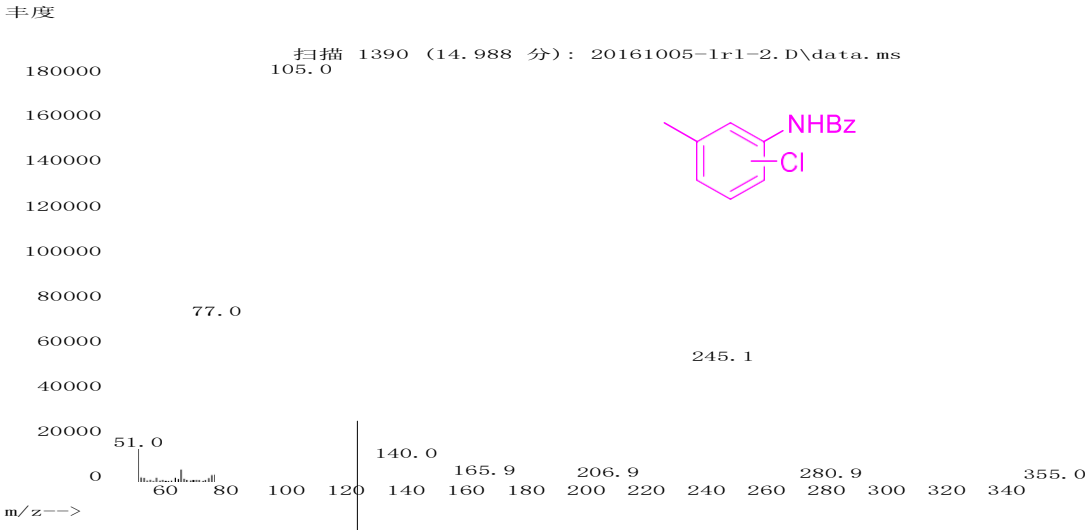
9. GC-MS analysis of the crude reaction mixture of 1s under conditions B



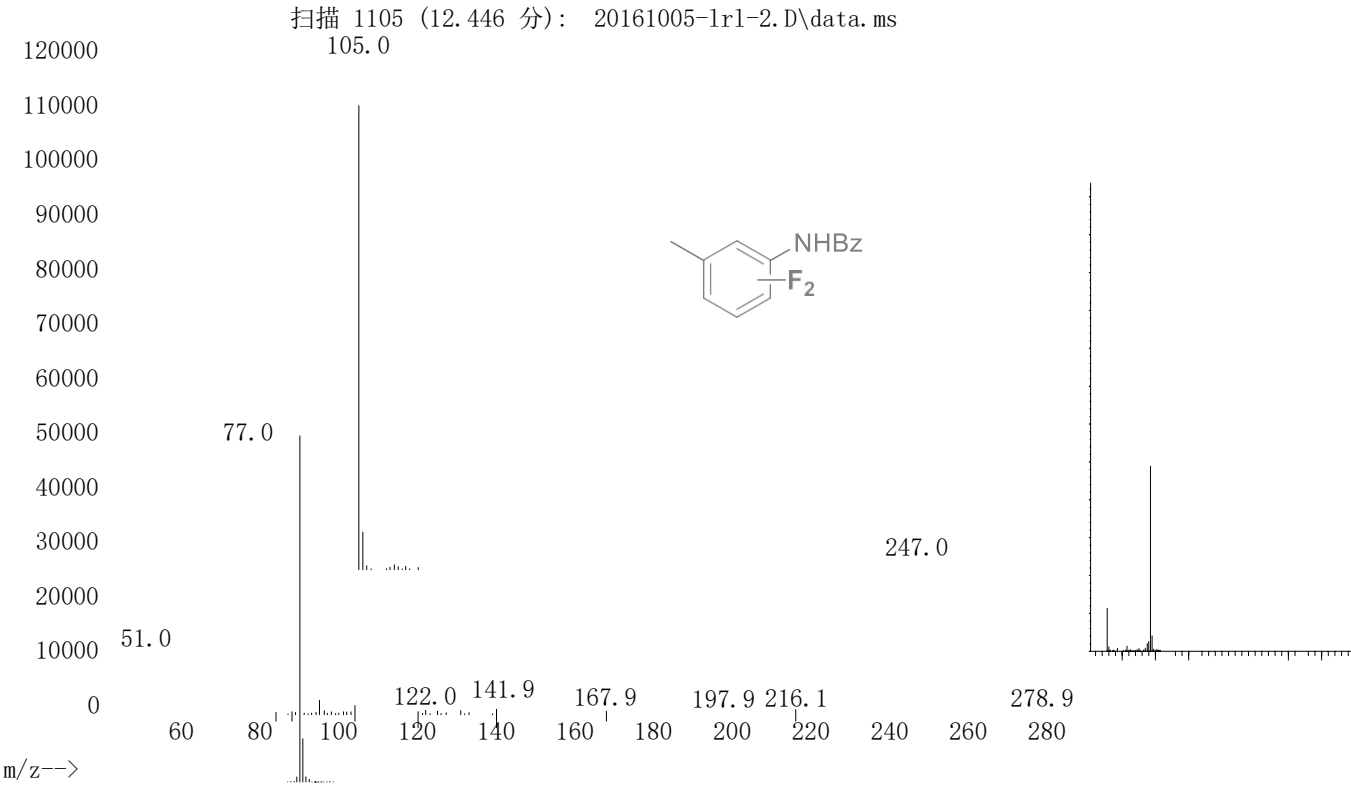
10. GC-MS analysis of the crude reaction mixture of 1t under conditions A



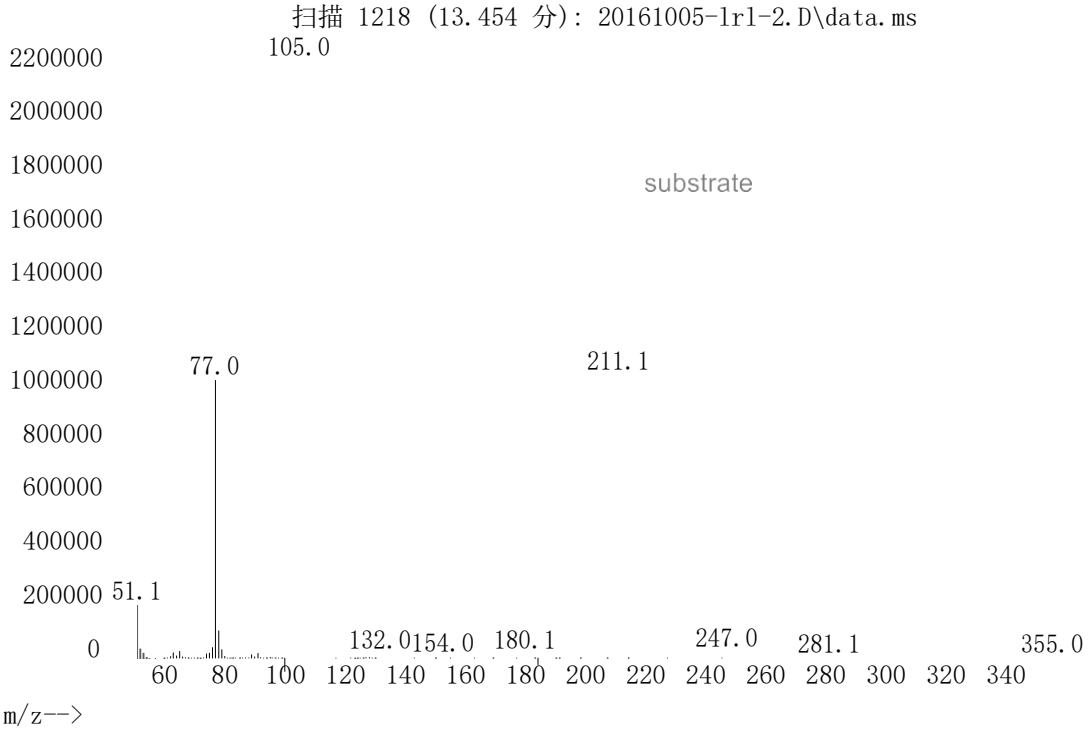

丰度
扫描 1127 (12.642 分): 20161005-1r1-2.D\data.ms
105.0
77.0
229.1
51.1
124.0
150.0
165.0
180.1
198.1
213.0
247.1
NHBz
F
m/z-->
丰度
扫描 1209 (13.374 分): 20161005-1r1-2.D\data.ms
105.0
77.0
229.1
51.1
124.1
150.0
166.9
185.0
211.1
247.0
280.9
NHBz
F
m/z-->
丰度
扫描 1290 (14.096 分): 20161005-1r1-2.D\data.ms
105.0
77.0
210.1
51.0
140.1
159.0
180.1
245.0
264.0
NHBz
Cl
m/z-->
丰度
#88500: 2'-Chloro-5'-methylbenzanilide
105.0
210.0
77.0
51.0
245.0
27.0
141.0
180.0
m/z-->


丰度
扫描 1390 (14.988 分): 20161005-1r1-2.D\data.ms
105.0
NHBz
Cl
77.0
245.1
51.0
140.0
165.9
206.9
280.9
355.0
m/z-->
丰度
扫描 1435 (15.390 分): 20161005-1r1-2.D\data.ms
105.0
NHBz
Cl
77.0
245.0
51.0
140.0
123.0
159.0
180.0
208.1
226.1
263.0
281.0
m/z-->
丰度
扫描 1075 (12.178 分): 20161005-1r1-2.D\data.ms
105.0
NHBz
F2
77.0
247.0
51.0
142.1
125.0
167.9
182.8
197.9
216.0
231.0
m/z-->

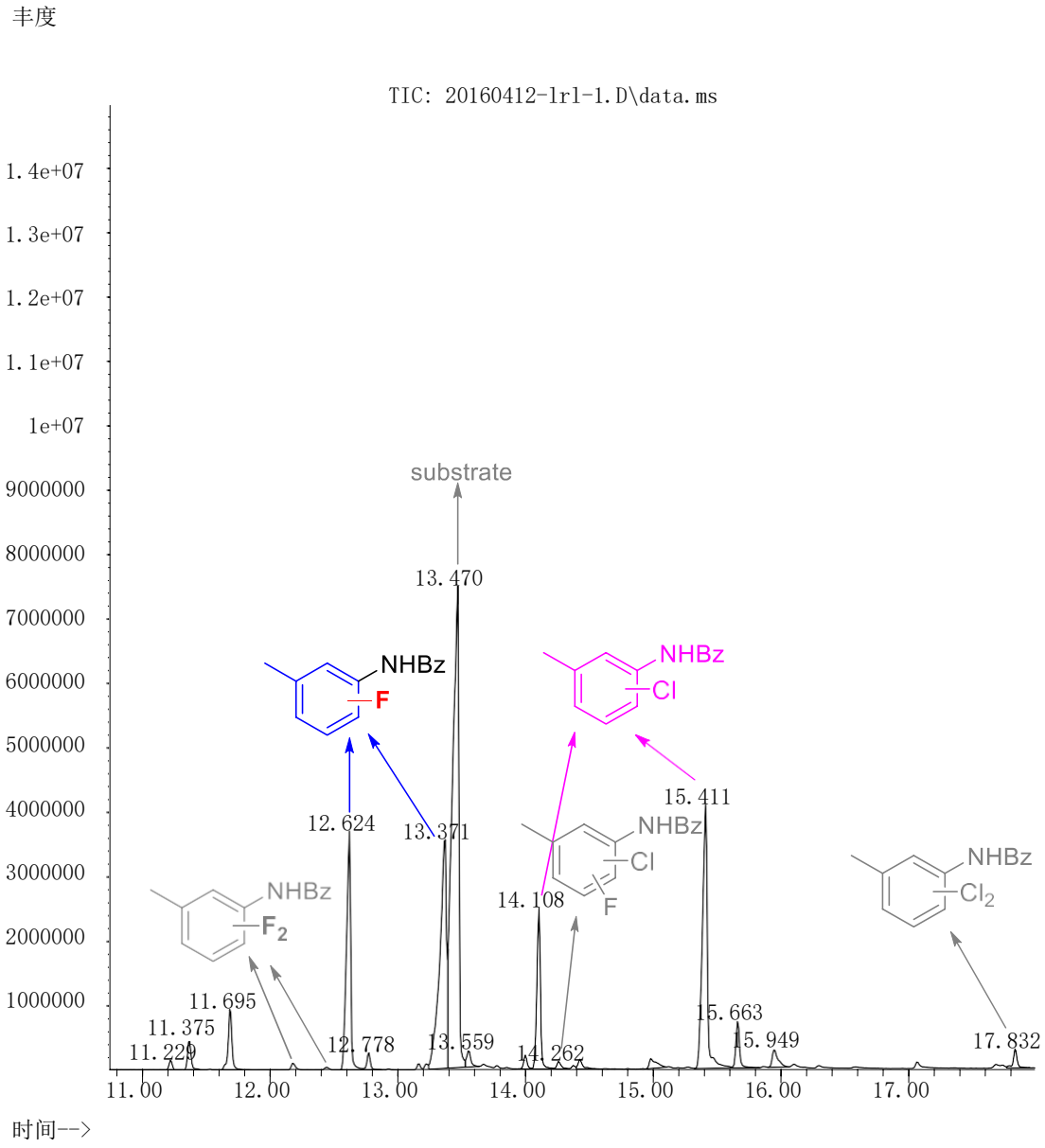
丰度


扫描 1105 (12.446 分): 20161005-lrl-2.D\data.ms
105.0
77.0
51.0
247.0
122.0
141.9
167.9
197.9
216.1
278.9
NHBz
F2
m/z-->

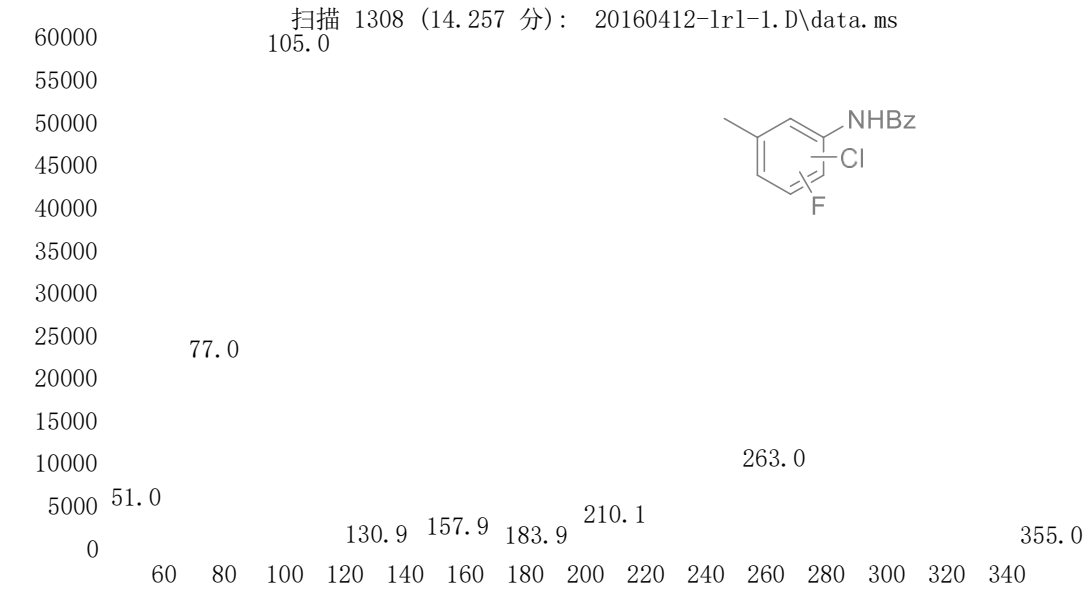
丰度


扫描 1218 (13.454 分): 20161005-lrl-2.D\data.ms
105.0
substrate
77.0
211.1
51.1
132.0
154.0
180.1
247.0
281.1
355.0
m/z-->

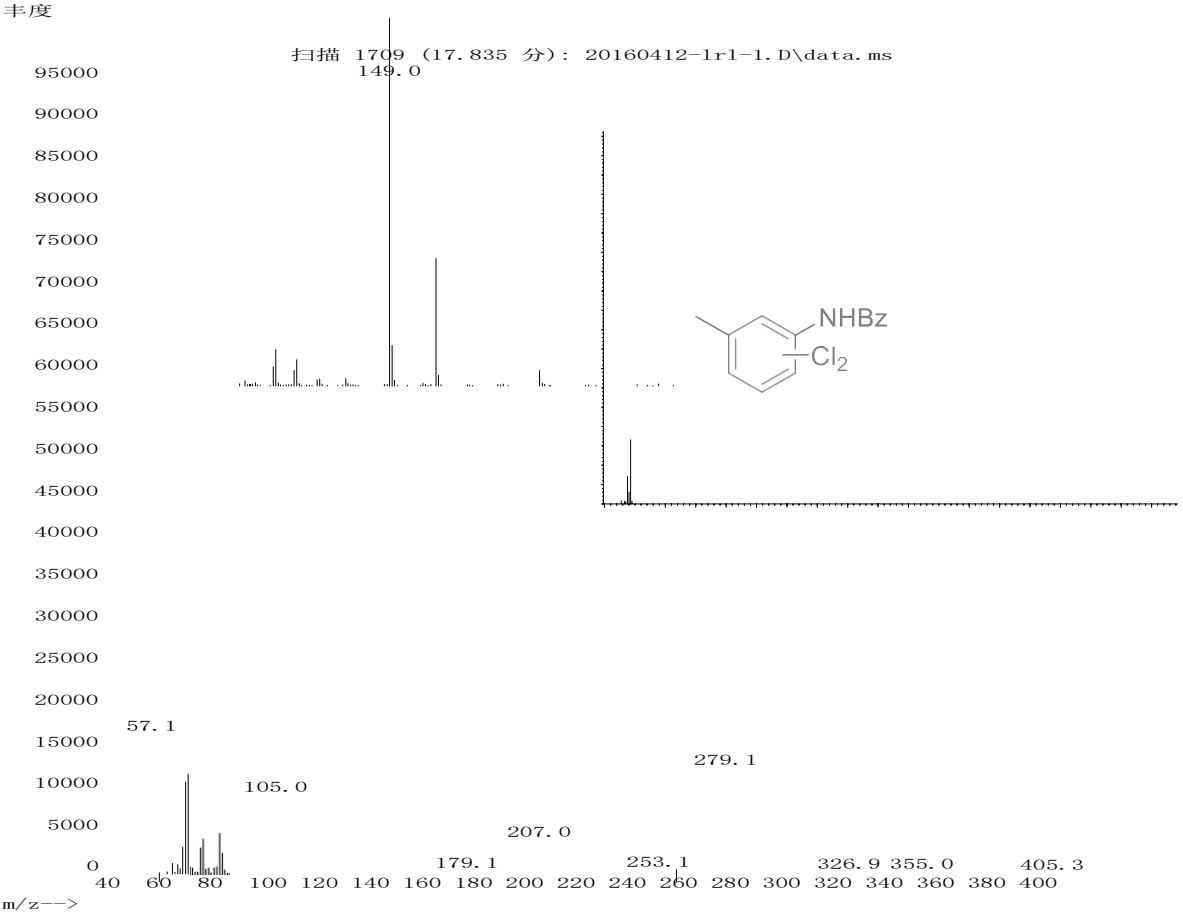
11. GC-MS analysis of the crude reaction mixture of 1t under conditions B



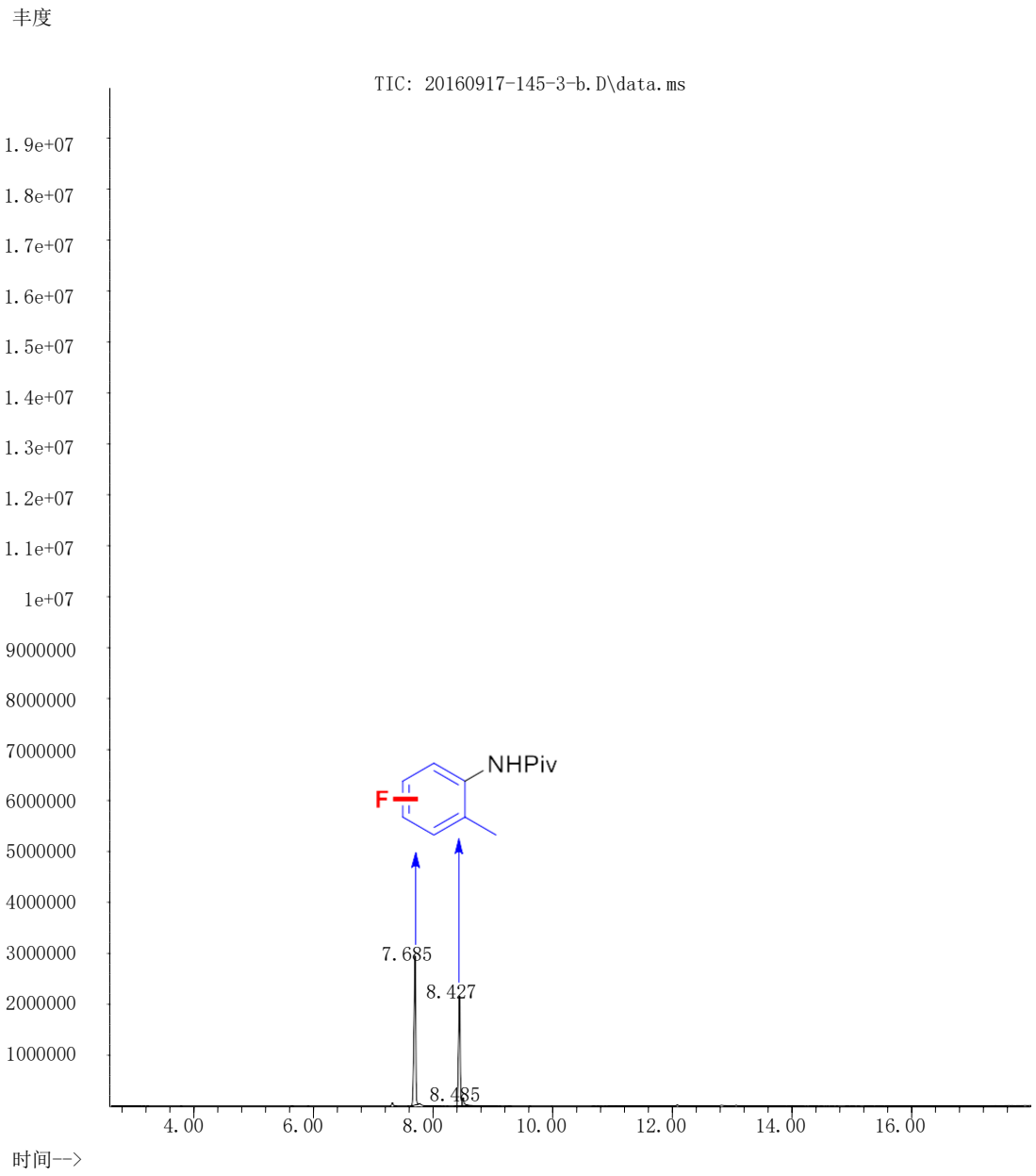
丰度

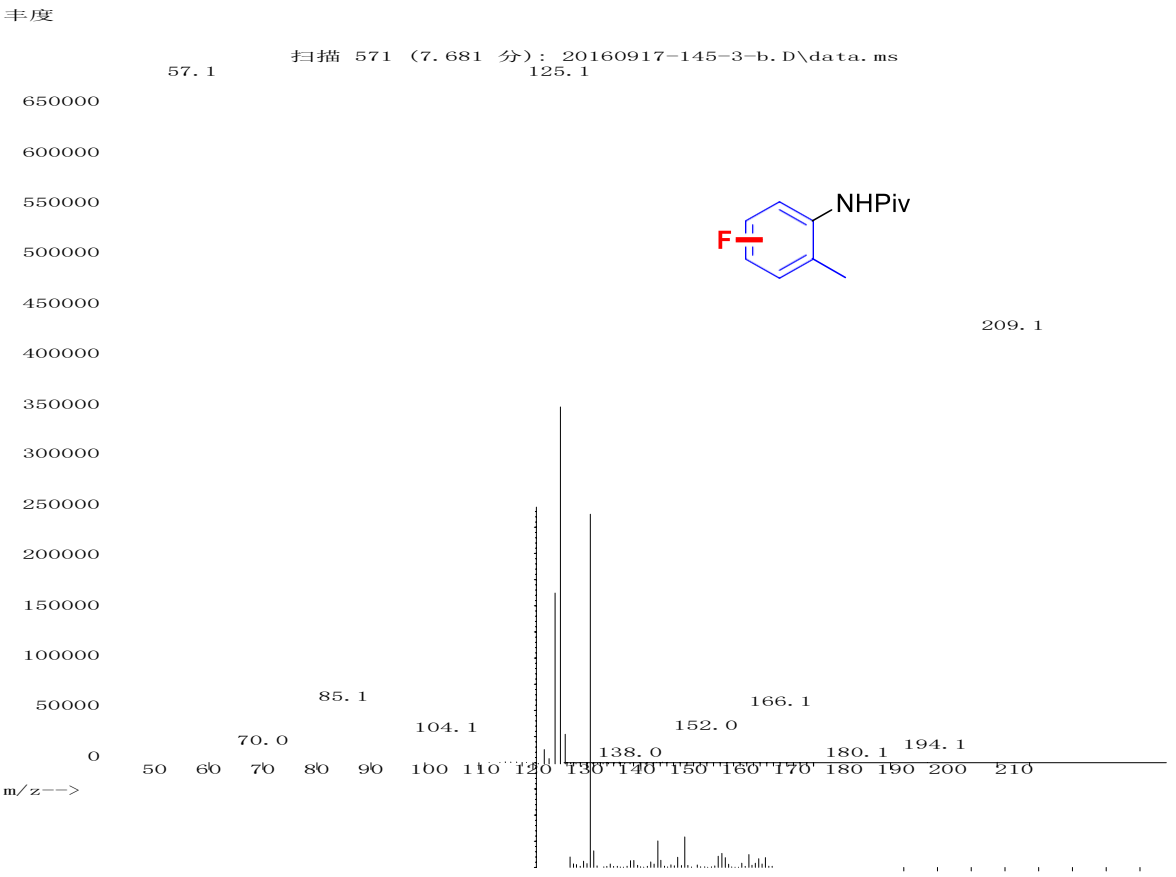

扫描 1308 (14.257 分): 20160412-lrl-1.D\data.ms
105.0
77.0
51.0
263.0
210.1
130.9
157.9
183.9
355.0
NHBz
Cl
F
m/z-->

丰度


扫描 1709 (17.835 分): 20160412-lrl-1.D\data.ms
149.0
57.1
105.0
207.0
179.1
279.1
253.1
326.9
355.0
405.3
NHBz
Cl2
m/z-->

12. GC-MS analysis of the crude product derived from 1u under conditions A

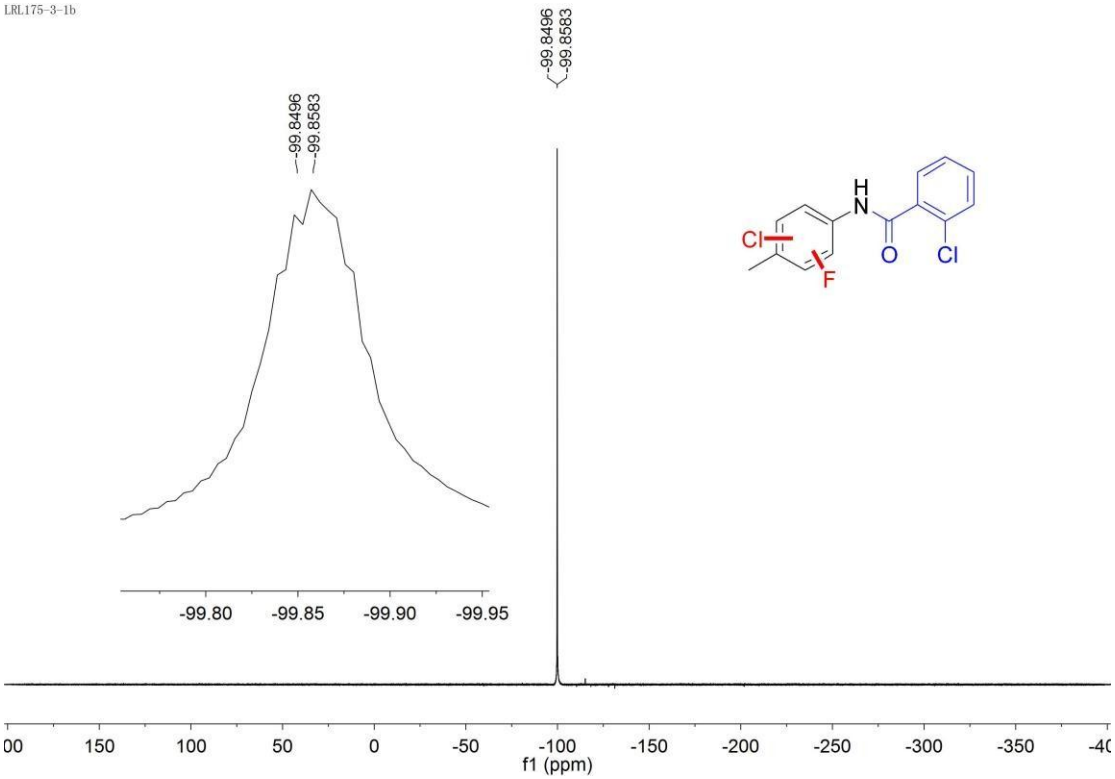



丰度
扫描 571 (7.681 分): 20160917-145-3-b.D\data.ms
57.1
125.1
NHPiv
F
209.1
85.1
166.1
104.1
152.0
70.0
138.0
180.1
194.1
m/z-->
丰度
扫描 654 (8.422 分): 20160917-145-3-b.D\data.ms
57.1
NHPiv
F
209.1
125.1
85.1
166.1
109.0
152.0
70.1
138.0
179.0
194.1
m/z-->

IX. ^{19}F NMR experiments

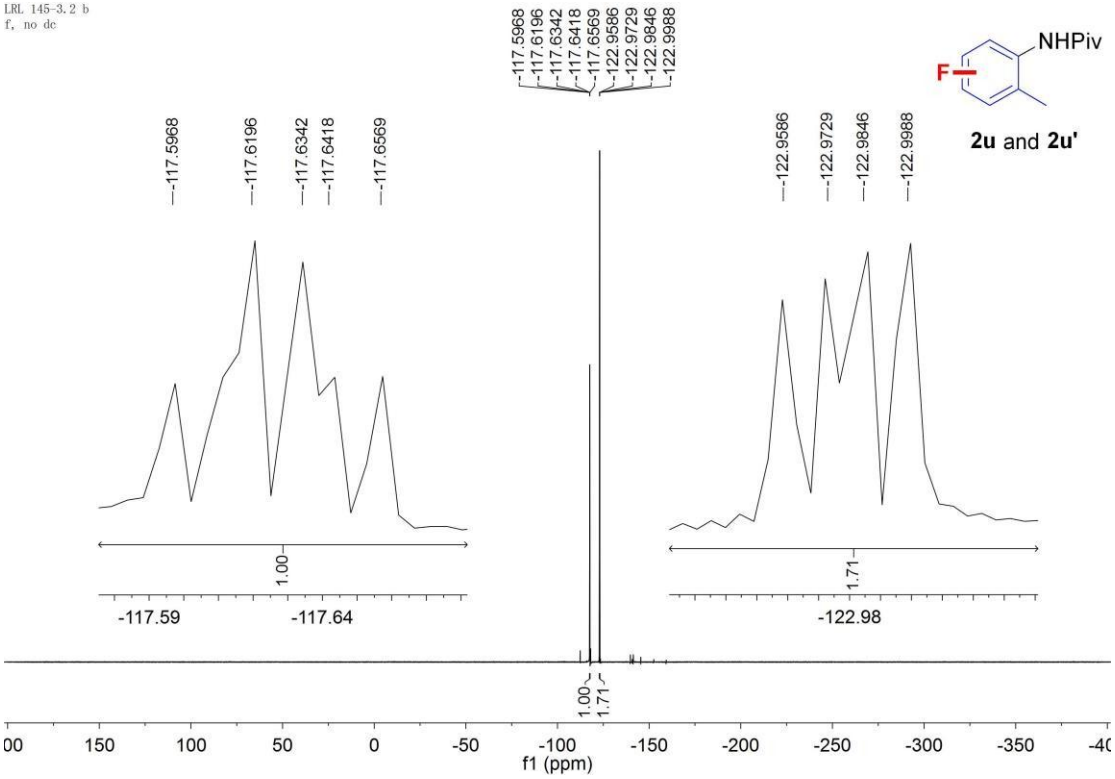
1. ^{19}F NMR analysis of the crude mixture of "recovered substrate 1g" under conditions B

^{19}F NMR, no decoupling



2. ^{19}F NMR analysis of the crude product derived from 1u under conditions A

^{19} F NMR, no decoupling



^{19} F NMR, with pulse decoupling