

Literature Report

氟谱解析

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有机氟化学领域的重要性

有机氟化学作为有机化学的一门非常重要分支，历经百余年的发展，目前已全面渗透至农药、医药、材料、原子能和航天航空等各个领域，成为与生物化学、药物化学和材料化学等互相交叉与促进的重要学科。



氟元素-独特的角色与作用

原子	电负性 (Pauling)	Pauling原子 半径(Å)	Bonding原子 半径(Å)	键能(CH ₃ -X) (kcal/mol)	键长 CH ₃ -X(Å)
H	2.1	1.20	1.20	99	1.09
F	4.0	1.35	1.47	116	1.39
Cl	3.0	1.80	1.75	81	1.77
Br	2.8	1.95	1.85	68	1.93
O(OH)	3.5	1.40	1.52	86	1.43

- 独特的氟效应：**亲脂性、伪拟效应、阻断效应和氢键作用等方面。**
- 含氟农药具有**高选择性、高活性、高附加值、低成本、低毒、低残留和对环境友好**等优点，近十年来开发了大量杀菌、除草和杀虫等新型含氟农药品种。
- 含氟材料拥有优异的耐高低温、耐热、耐腐蚀、绝缘、抗粘、低摩擦、不燃和自润滑等性能，已成为国民经济中不可缺少的新型高分子合成材料。
- 医药方面，**已商品化的含氟药物所占比例高达25%**，其中含氟药物立普妥和百忧解均在全球畅销药物排行前列。

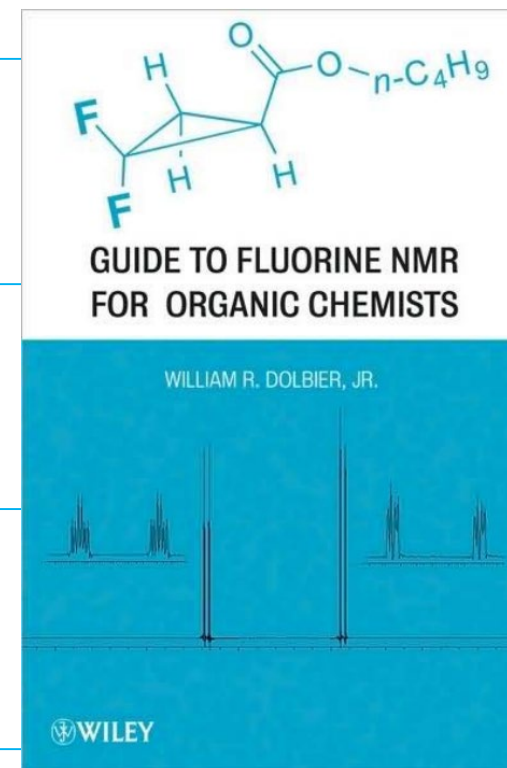
氟谱解析

1 氟谱的基本信息与特点

2 化学位移与偶合常数

3 分类详解

4 例题分析



所有具有磁活性的核的核磁数据

同位素	自旋量子数	天然丰度%	灵敏度		T = 7.0464对应的MHz	参比化合物	检测范围
			相对 ^a	绝对 ^b			
¹H	1/2	99.98	1.00	1.00	300.000	Si(CH ₃) ₄	10~0
² H	1	1.5 × 10 ⁻²	9.65 × 10 ⁻³	1.45 × 10 ⁻⁶	46.051	Si(CD ₃) ₄	10~0
³ H	1/2	0	1.21	0	319.990	Si(CT ₃) ₄	10~0
¹³C	1/2	1.108	1.59 × 10 ⁻²	1.76 × 10 ⁻⁴	75.432	Si(CH ₃) ₄	220~0
¹⁴ N	1	99.63	1.01 × 10 ⁻³	1.01 × 10 ⁻³	21.671	¹⁴ NH ₃ (l) ^c	900~0
¹⁵ N	1/2	0.37	1.04 × 10 ⁻³	3.85 × 10 ⁻⁶	30.398	¹⁵ NH ₃ (l) ^c	900~0
¹⁷ O	5/2	3.7 × 10 ⁻²	2.91 × 10 ⁻²	1.08 × 10 ⁻⁵	40.670	H ₂ O	1700~-50
¹⁹F	1/2	100	0.83	0.83	282.231	CFCl ₃	260~-280
²⁹ Si	1/2	4.7	7.84 × 10 ⁻³	3.69 × 10 ⁻⁴	59.595	Si(CH ₃) ₄	80~-380
³¹ P	1/2	100	6.63 × 10 ⁻²	6.63 × 10 ⁻²	121.442	85%H ₃ PO ₄	270~-480

^a 在原子核数量相同的条件下； ^b 相对灵敏度和天然丰度的产物； ^c 25 °C

氟谱的基本信息与特点

核	自旋量子数	相对灵敏度	天然丰度	V(MHz)
^1H	1/2	100	99.98	60.0
^{13}C	1/2	1.59	1.11	15.1
^{19}F	1/2	83.3	100	56.4

- 在核磁共振学中，除了碳和氢，氟大概是被研究最广泛的元素。这一方面是因为氟原子核本身的特殊性，另一方面就在于含氟活性分子的重要性；
- 氟的天然同位素只有 ^{19}F ，丰度为100%，是研究NMR的理想核；
- ^{19}F 灵敏度是 ^1H 的0.83倍，化学位移值范围> 350 ppm；
- 自旋量子数是1/2，因此氟与邻近的氢，碳的耦合类似于 ^1H ；
- ^{19}F 的化学位移较难预测与推理，因为含氟有机物中 ^{19}F 核的反磁性屏蔽少于1%，而顺磁性屏蔽是主要影响因素；
- ^{19}F 中一般不使用质子去偶技术，因此谱图中不仅会出现相邻F-F耦合，也会出现F-H耦合。但是峰面积积分比对计算相对原子数目的准确度并不如 ^1H 高。

化学位移

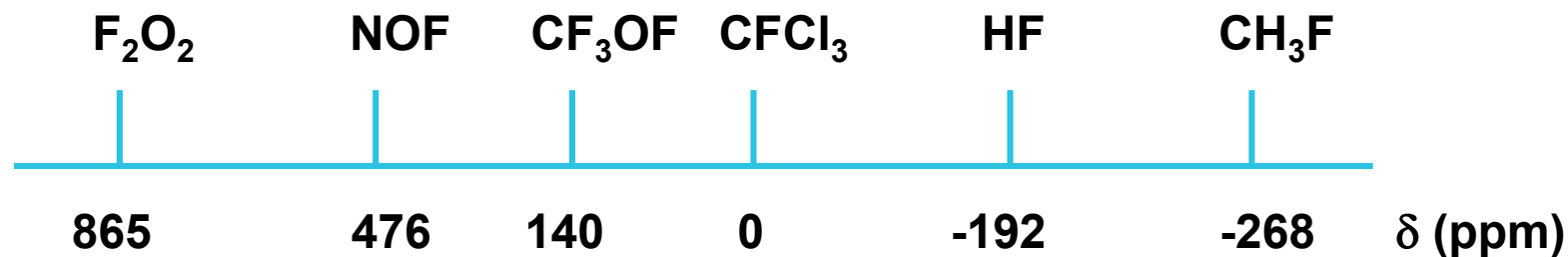
一氟三氯甲烷(CFCl_3)是氟谱中比较常用的内标试剂, 定标为0。 CFCl_3 峰($\delta = 0$) 往高场移动为负, 低场移动为正。其他内标试剂有:

$$\delta = \text{CF}_3\text{CO}_2\text{H}: -76.2 \text{ ppm}$$

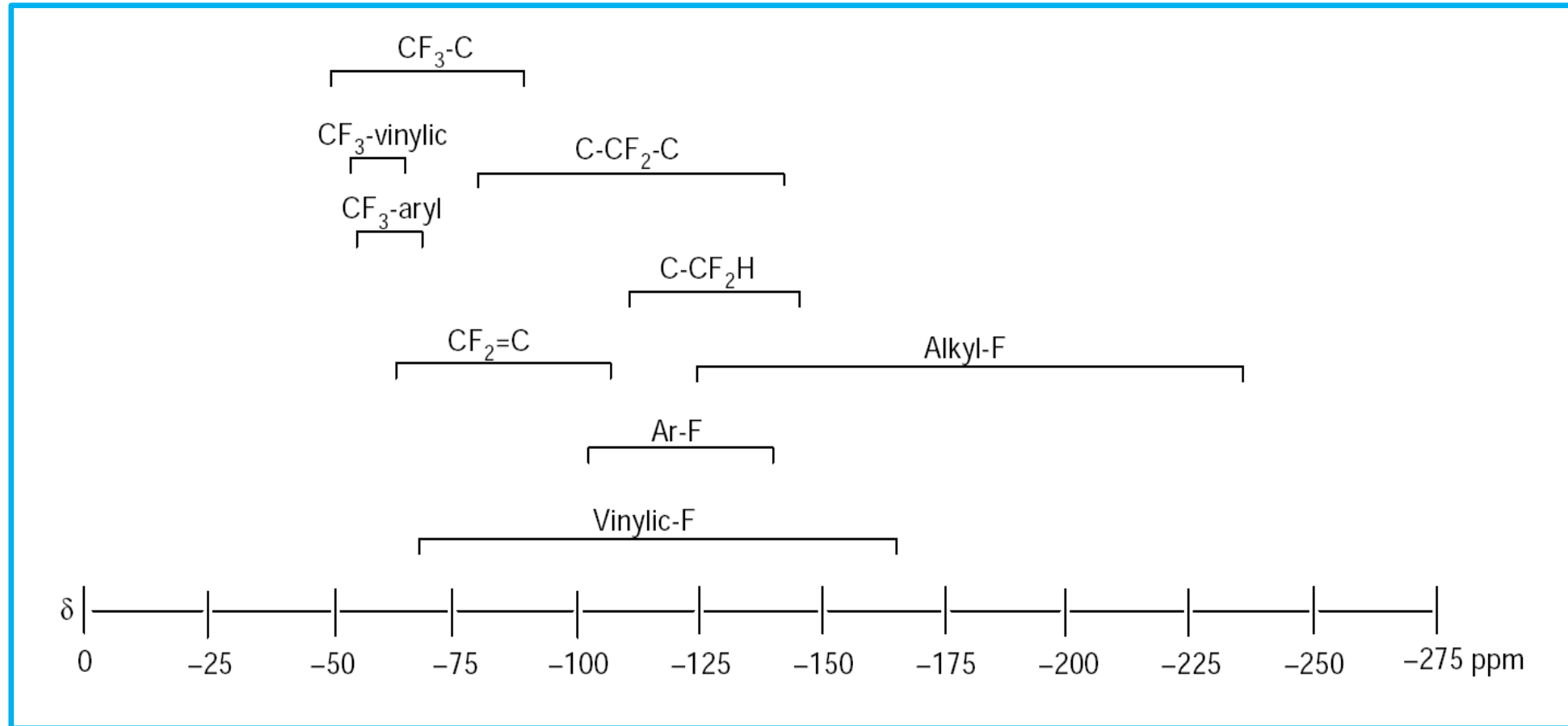
$$\delta = \text{PhCF}_3: -63.2 \text{ ppm}$$

$$\delta = \text{C}_6\text{F}_6: -162.2 \text{ ppm}$$

$$\delta = \text{CF}_3\text{COOC}_2\text{H}_5: -75.8 \text{ ppm}$$



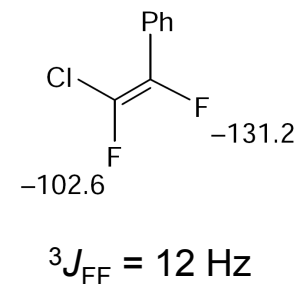
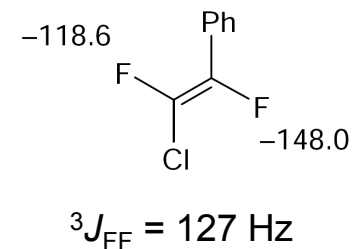
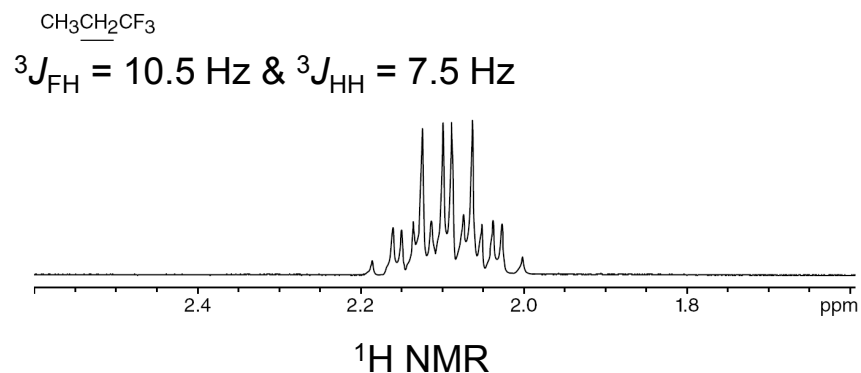
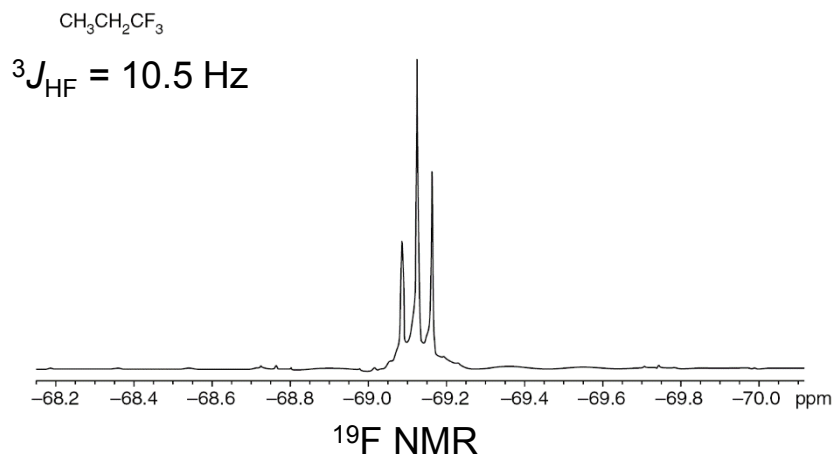
各类化合物的 ^{19}F 化学位移值图



绝大部分化合物的化学位移为负值，另有酰基氟、磺酰氟以及含 SF_5 类化合物为正值。

耦合常数

氟与氢核的自旋量子数都是1/2，因此F谱一般呈一级谱图。谱线裂分符合n+1规律。裂分峰强比也遵守帕斯卡三角的二项式展开 $[(a+b)^n]$ 展开式的各项系数。在非链状含氟化合物中影响F-F偶合和F-H偶合的主要因素是耦合的两个原子核之间的扭转角、化学环境以及邻近基团。



顺反异构的二氟烯烃偶合常数与化学位移都有很大差别。

氟-氟偶合

◆ 同碳偶合

${}^2J_{FF} = 100-290$ Hz (烷烃); 14-110 Hz (烯烃) 环状化合物同碳 J_{FF} 随环增大而增大, J_{FH} 变化不明显; 环上 J_{FF} 较烯烃 J_{FF} 大。



◆ 邻碳偶合

${}^3J_{FF} = 2-135$ Hz

一般饱和脂肪链化合物在15-16 Hz, 但是随着取代基吸电子效应的增强, 去屏蔽化增强, 偶合常数减小。



氟-氢偶合

◆ 同碳偶合 $^2J_{FH}$ 与氟个数有关。

-F: 47-55 Hz

-CF₂H: 57 Hz

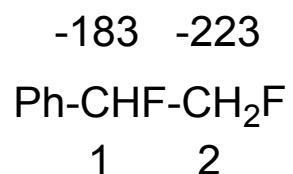
◆ 邻碳偶合 $^3J_{FH}$ 与碳上所连基团电负性有关。

-F: 21-27 Hz

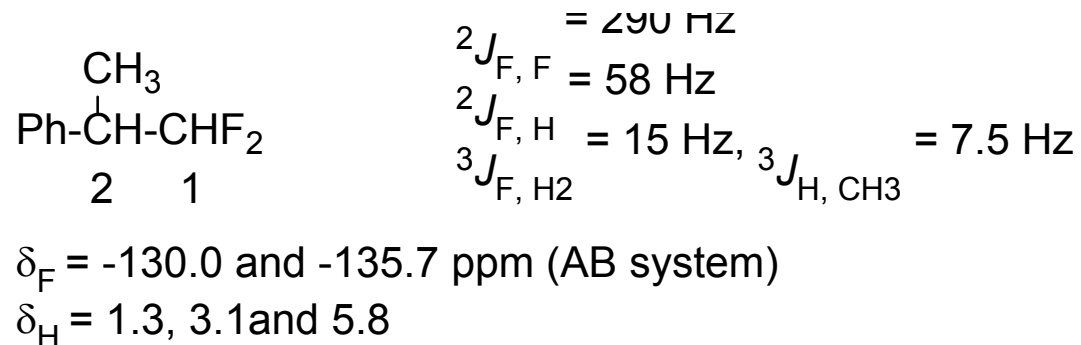
-CF₂H: 14-22 Hz

-CF₃: 7-11 Hz

反式烯基氟 $^3J_{FH}$: 35-52 Hz; 顺式烯基氟 $^3J_{FH}$: 14-20 Hz



$$\begin{aligned} ^2J_{F1, H1} &= 49 \text{ Hz}, & ^2J_{F2, H2} &= 47 \text{ Hz}, \\ ^3J_{F1, F2} &= 16 \text{ Hz} \\ ^3J_{F1, H2} &= 24 \text{ Hz}, & ^3J_{F2, H1} &= 17 \text{ Hz}, \end{aligned}$$

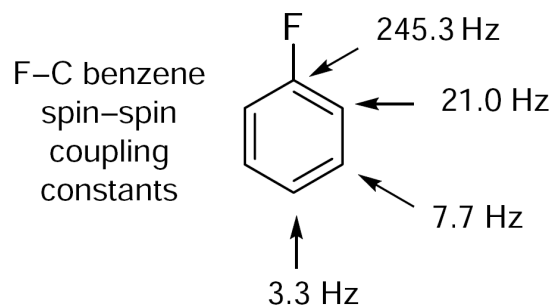


氟-碳偶合

- ◆ 氟-碳偶合常数最主要由碳上取代的氟个数决定，但是当氟被其他卤素取代后，偶合常数会增大(-CF₃、-CF₂H、-CH₂F都遵循这一规律)；被氧族元素取代的规律不统一。

X	F	Cl	Br	I
CF ₃ X, δ	122.4	118.0	112.9	78.2
¹ J _{FC} (Hz)	259	288	323	344
HCF ₂ X, δ	118.4	118.0	—	—
¹ J _{FC} (Hz)	274	288	—	—
H ₂ CFX, δ	109.4	—	—	—
¹ J _{FC} (Hz)	235	—	—	—

- ◆ 偶合常数会随着碳与氟之间键数增加而锐减，这是一个十分重要的判断含氟化合物结构信息的工具。

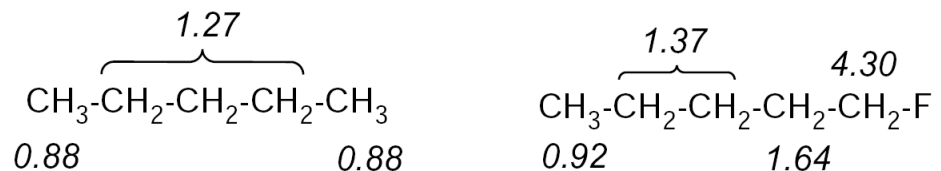


含氟化合物的氢谱

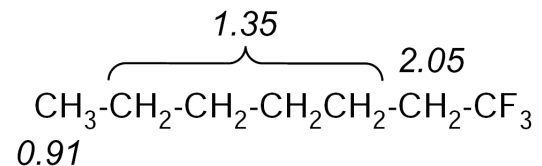
- ◆ 由于氟的强吸电子性，对氢核的去屏蔽作用较其他原子更强。



- ◆ 随着两核之间键数增加，化学位移值迅速减小。



- ◆ 三氟甲基效果类似于单氟取代。

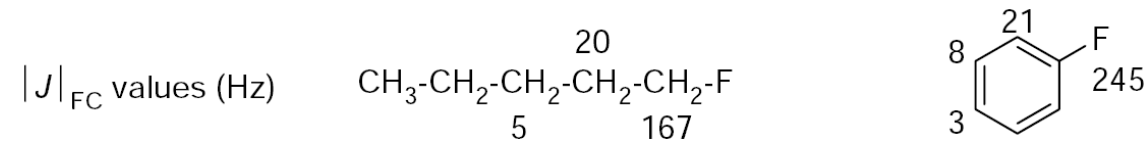


含氟化合物的碳谱

- ◆ 碳谱与氢谱类似，但是不与氟原子直接相连的碳化学位移偏移很小，只有与氟直接相连的碳会受到强的去屏蔽作用。



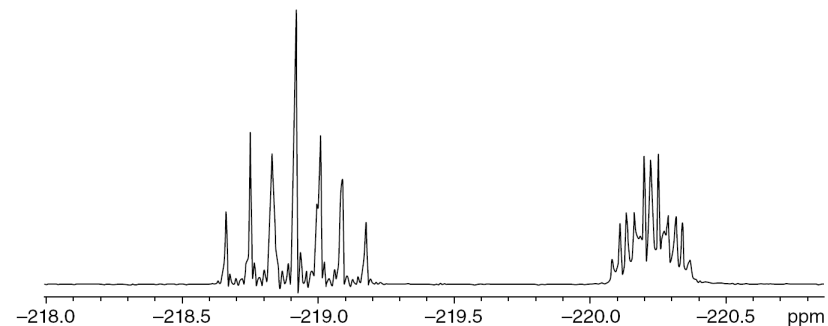
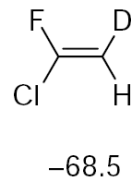
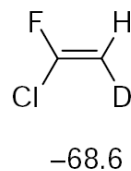
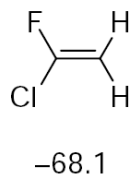
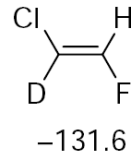
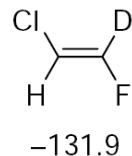
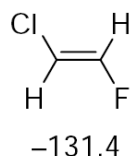
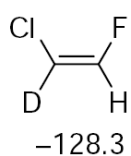
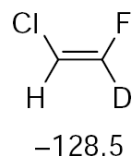
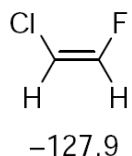
- ◆ 一个重要的另特征即是，F-C偶合常数($^2J_{FC}$, $^3J_{FC}$, $^4J_{FC}$)基本是恒定不变的。



氟谱的同位素效应

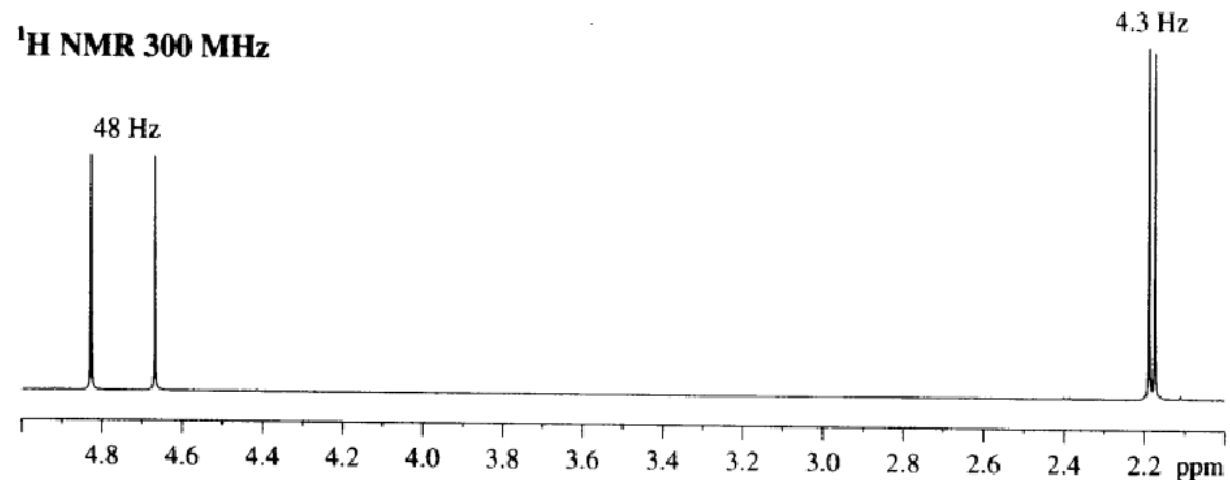
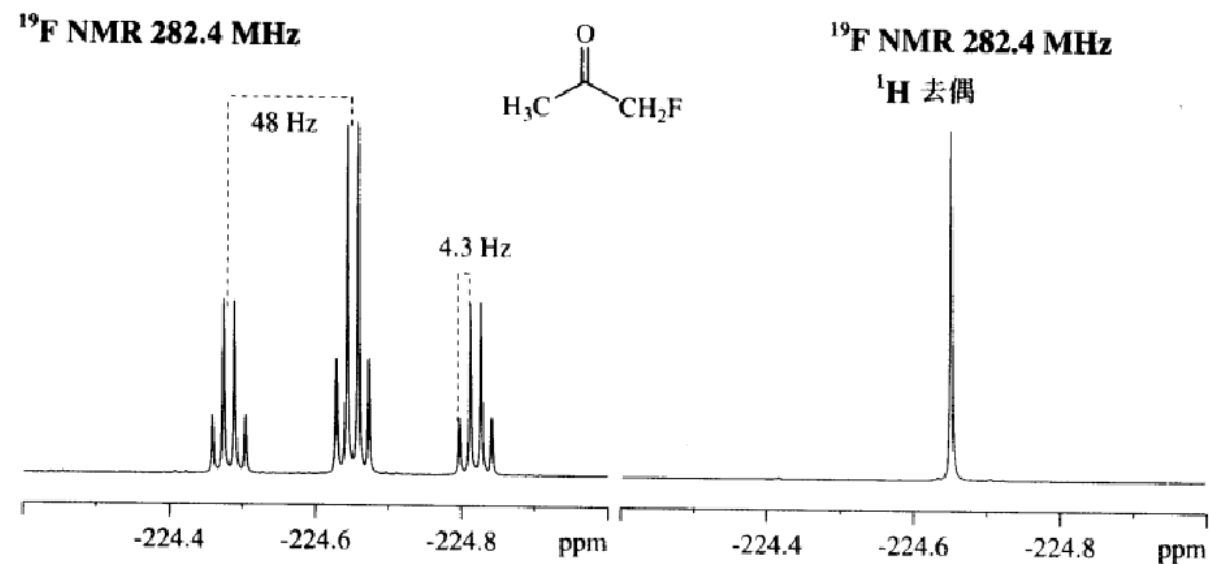
由于氟原子核对于周围环境的敏感性，以及氟化学位移的范围宽广，所以当附近的其他原子核被同位素原子核代替后，氟谱将会呈现明显不同。例如，将 ^1H 以 ^2H 代替后，氟化学位移将移向高场。

^{19}F of $\text{F-CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CD}_2\text{-F}$
显示：平均每氘代一个原子核会向高场移动0.65ppm (α -氘代效应)

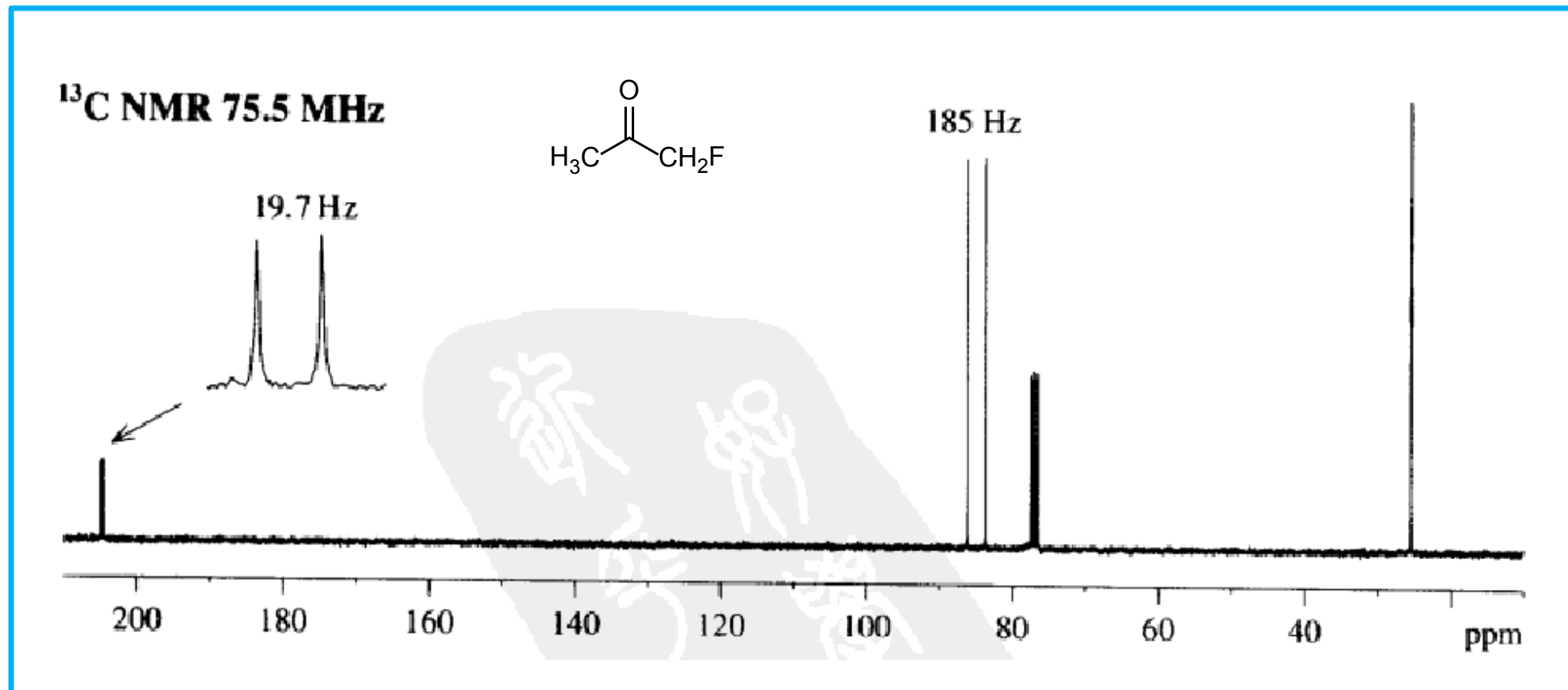


- ◆ 反式氘代比顺式氘代对于化学位移的影响更大。
- ◆ 这一规律也适用于对偶合常数的影响。
- ◆ α -氘代与 β -氘代对化学位移的影响也稍有不同。

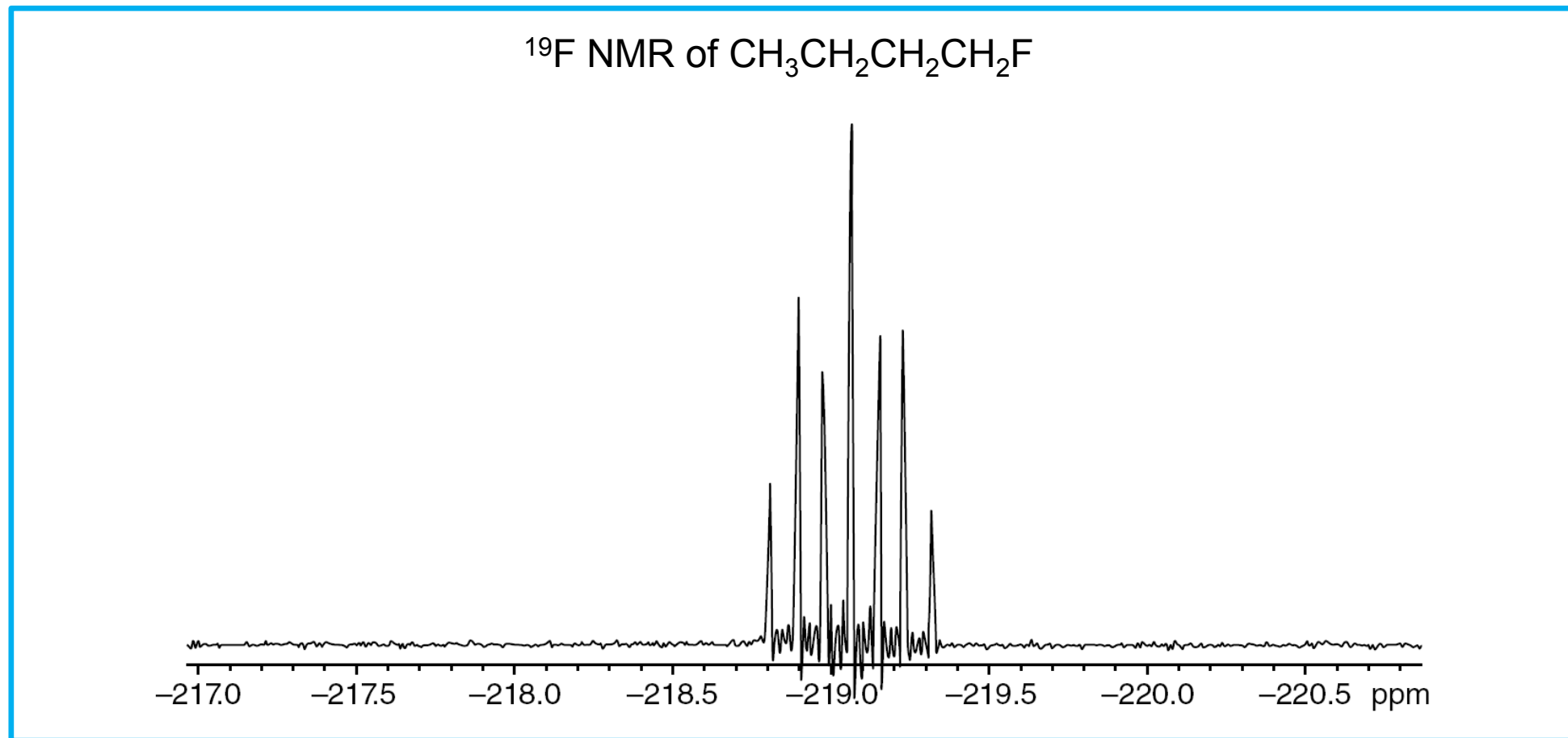
代表化合物举例



代表化合物举例



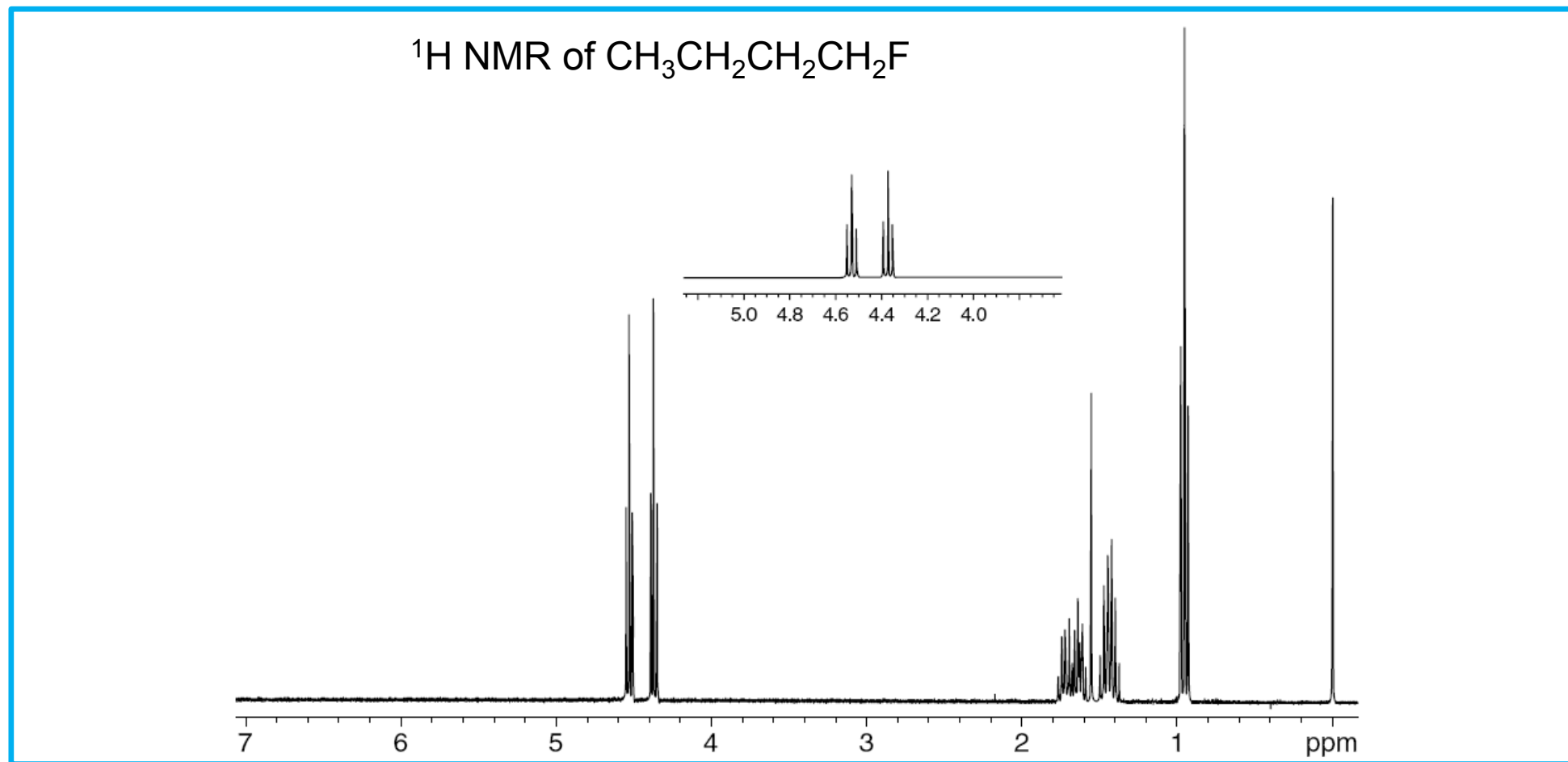
代表化合物举例



$\delta = -219 \text{ ppm}$ $^2J_{\text{FH}} = 47\text{-}49 \text{ Hz}$; $^3J_{\text{FH}} = 21\text{-}27 \text{ Hz}$

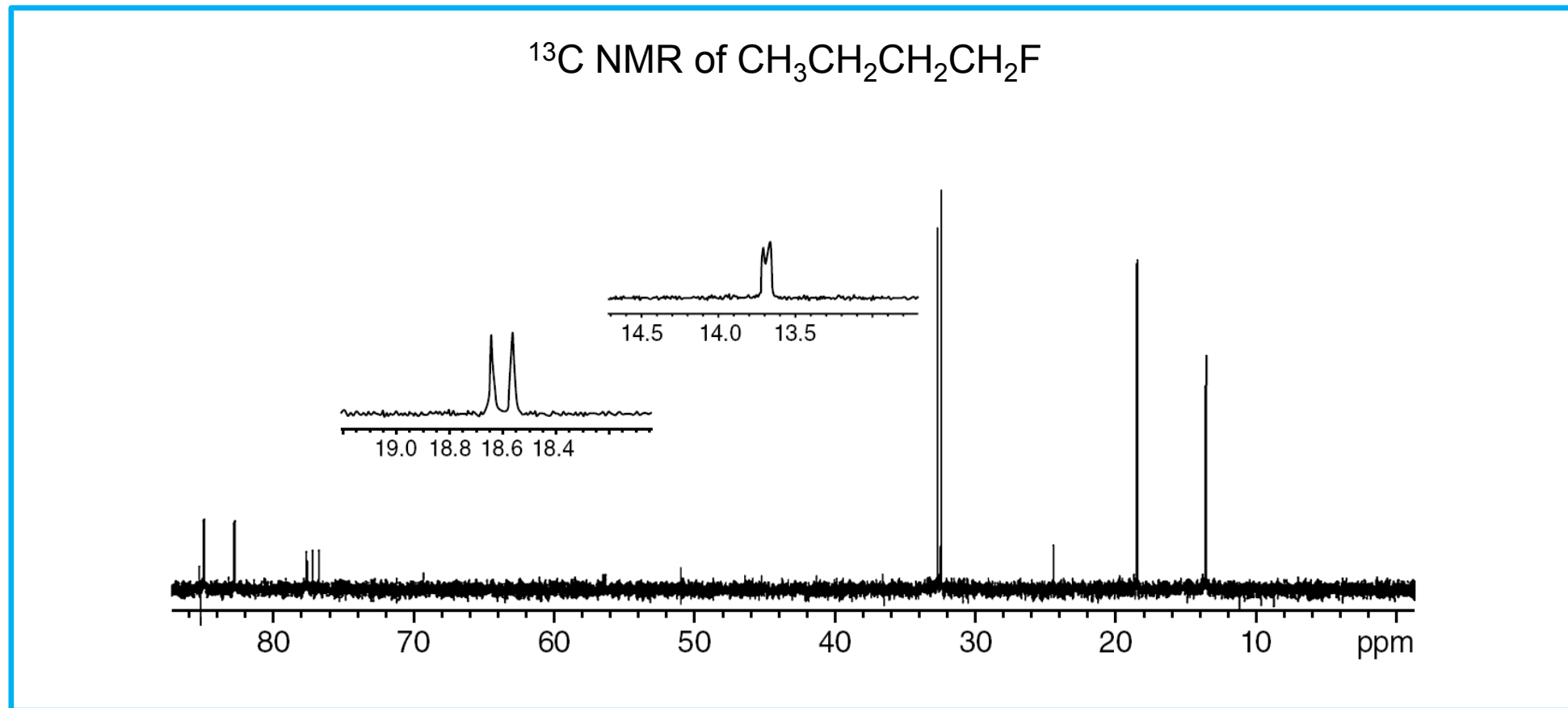
耦合常数差一倍的三重峰与三重峰的叠加，近似于一个七重峰

代表化合物举例



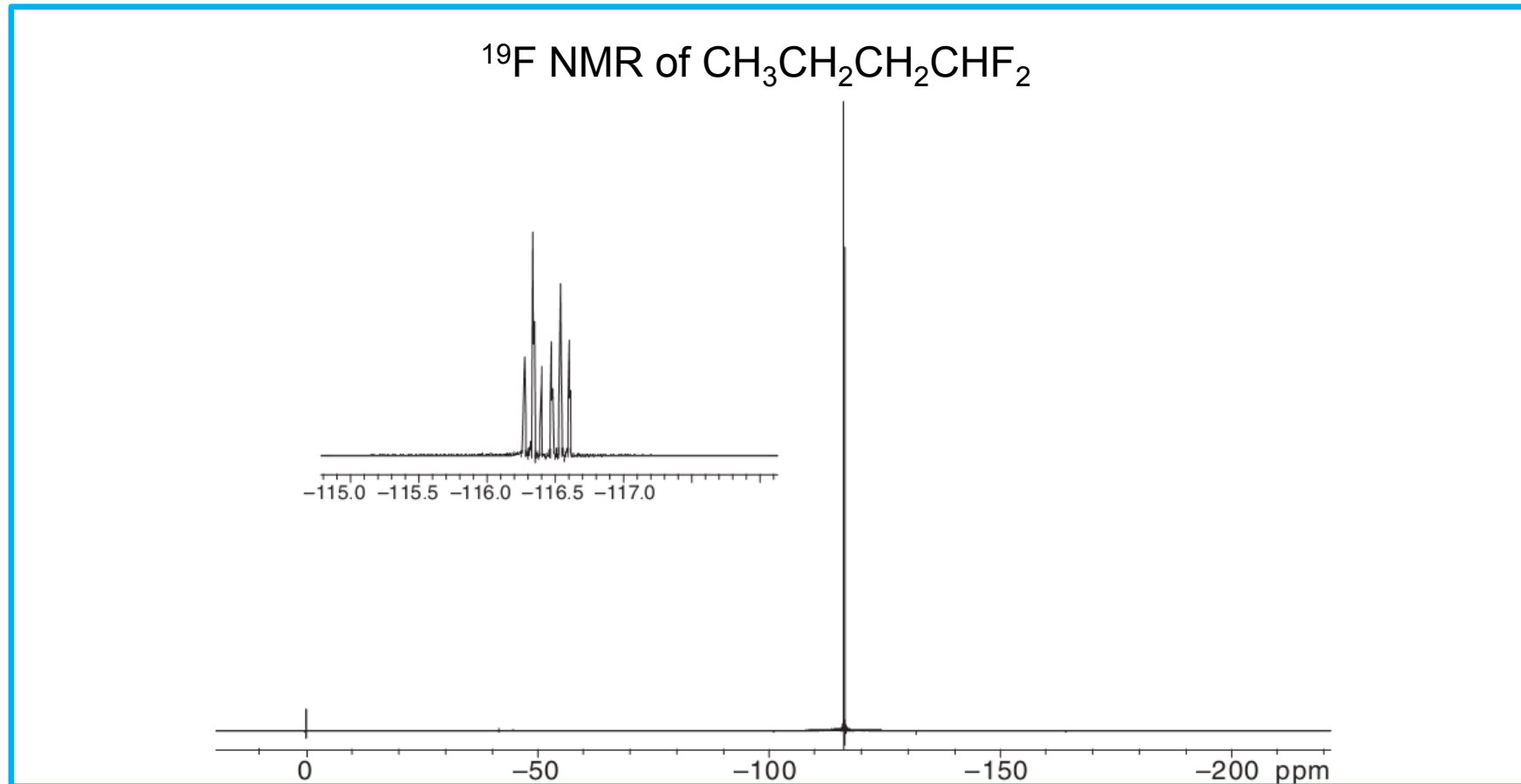
^1H NMR $\delta = 4.45$ (t, $^2J_{\text{HF}} = 47$, $^3J_{\text{HH}} = 6.0$ Hz, 2H), 1.70 (d, pent, $^3J_{\text{FH}} = 25$ Hz, $^3J_{\text{HH}} = 7$ Hz, 2H), 1.43 (sextet, $^3J_{\text{HH}} = 7.8$ Hz, 2H), 0.95 (t, $^3J_{\text{HH}} = 7.5$ Hz, 3H)

代表化合物举例



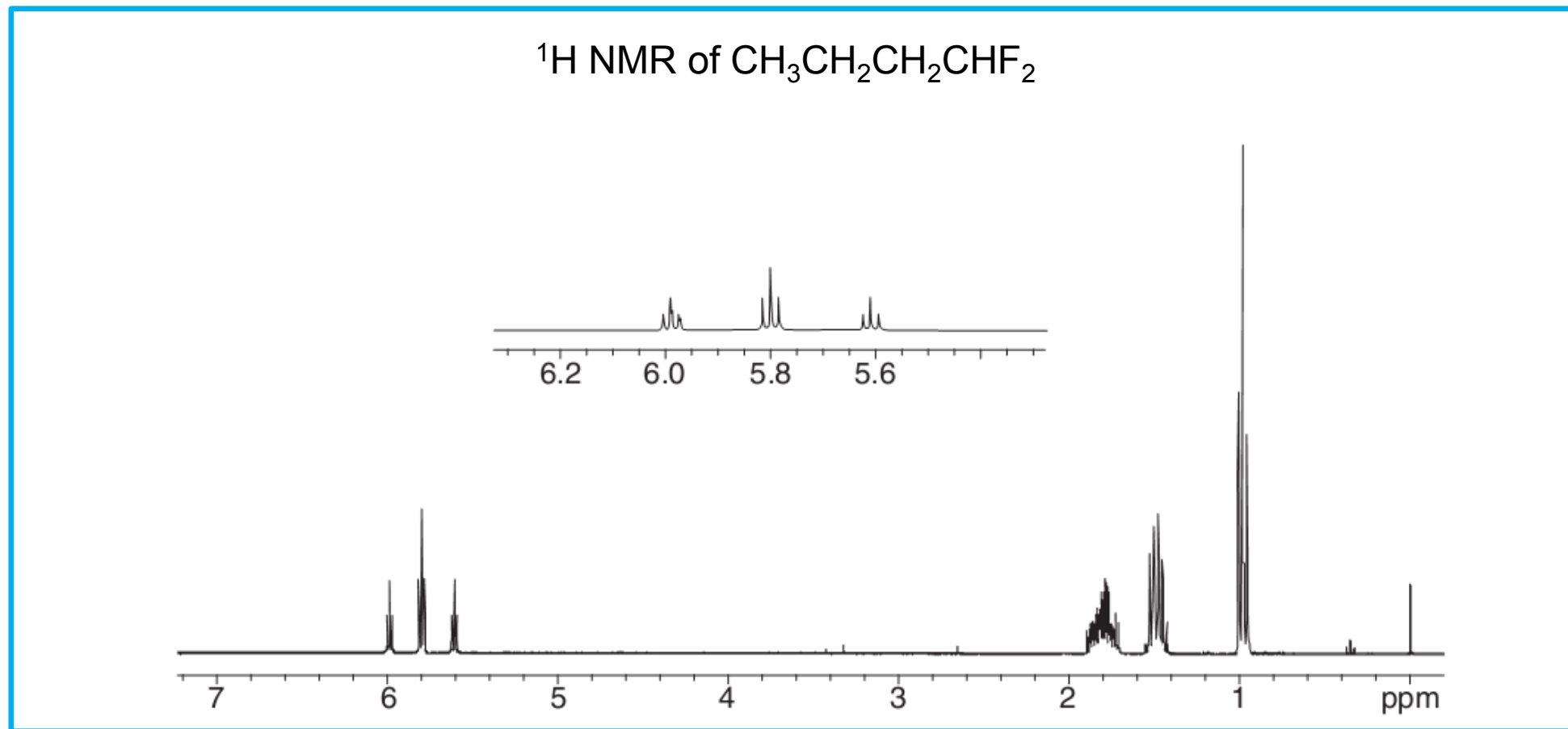
^{13}C NMR $\delta = 83.9$ (d, $^1J_{\text{FC}} = 165$ Hz), 32.7 (d, $^2J_{\text{FC}} = 19$ Hz), 18.6 (d, $^3J_{\text{FC}} = 6$ Hz), 13.7 (d, $^4J_{\text{FC}} = 3$ Hz)

代表化合物举例



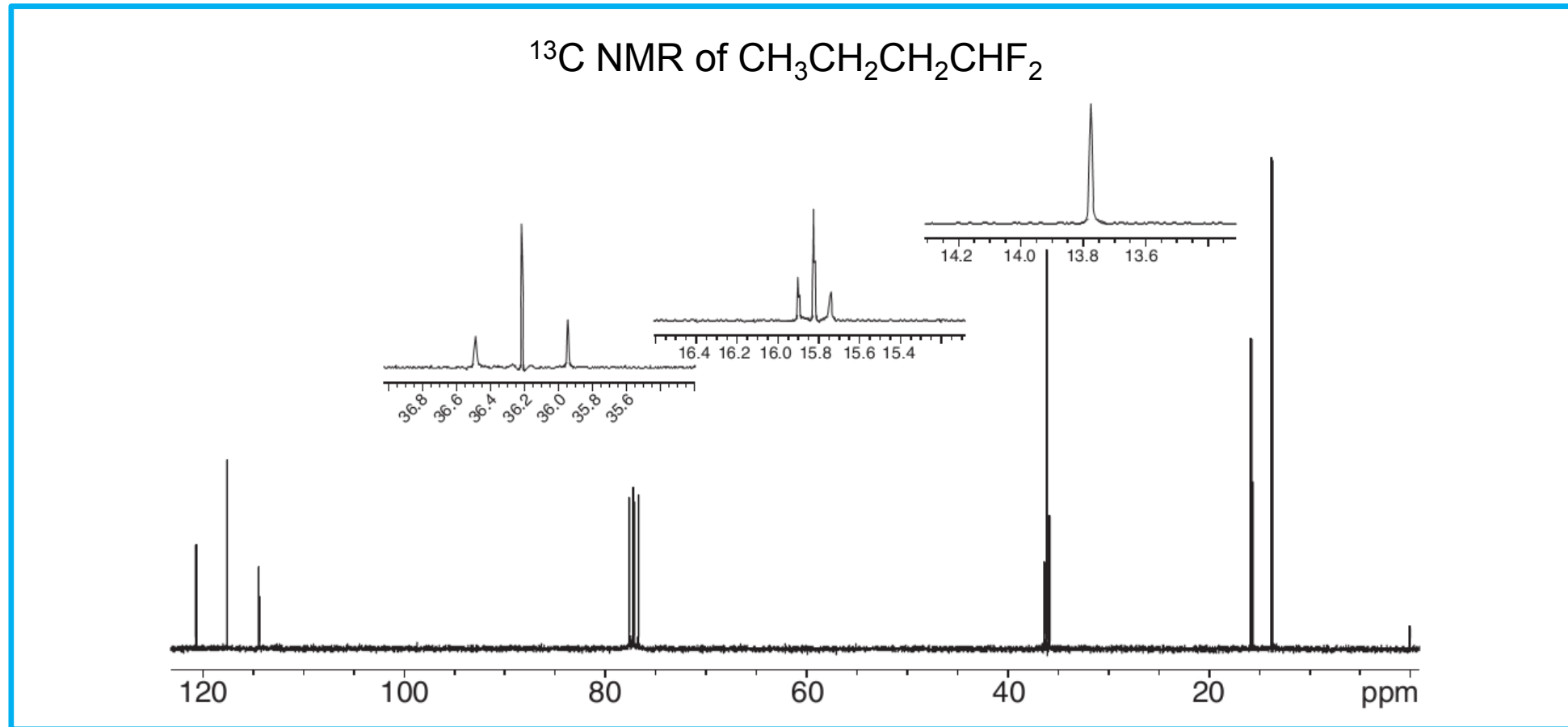
^{19}F NMR $\delta = -116.4$ ppm (d of t, $^2J_{\text{FH}} = 58$ Hz, $^3J_{\text{FH}} = 16.6$ Hz)

代表化合物举例



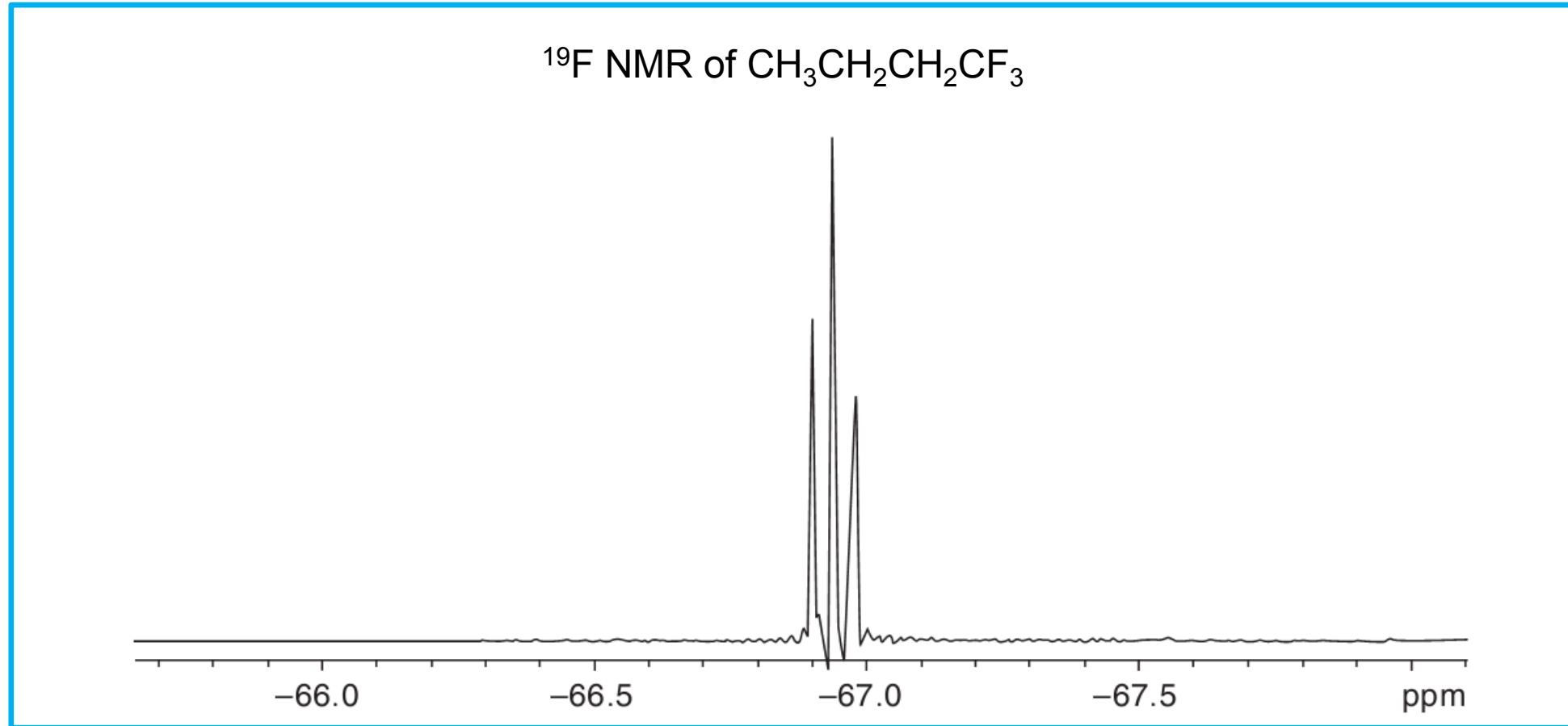
^1H NMR $\delta = 5.80$ (t of t, $^2J_{\text{FH}} = 57$ Hz, $^3J_{\text{HH}} = 4.5$ Hz, 1H), 1.80 (m, 2H), 1.49 (sextet, $^3J_{\text{HH}} = 7.5$ Hz, 2H), 0.98 (t, $^3J_{\text{HH}} = 7.2$ Hz, 3H)

代表化合物举例



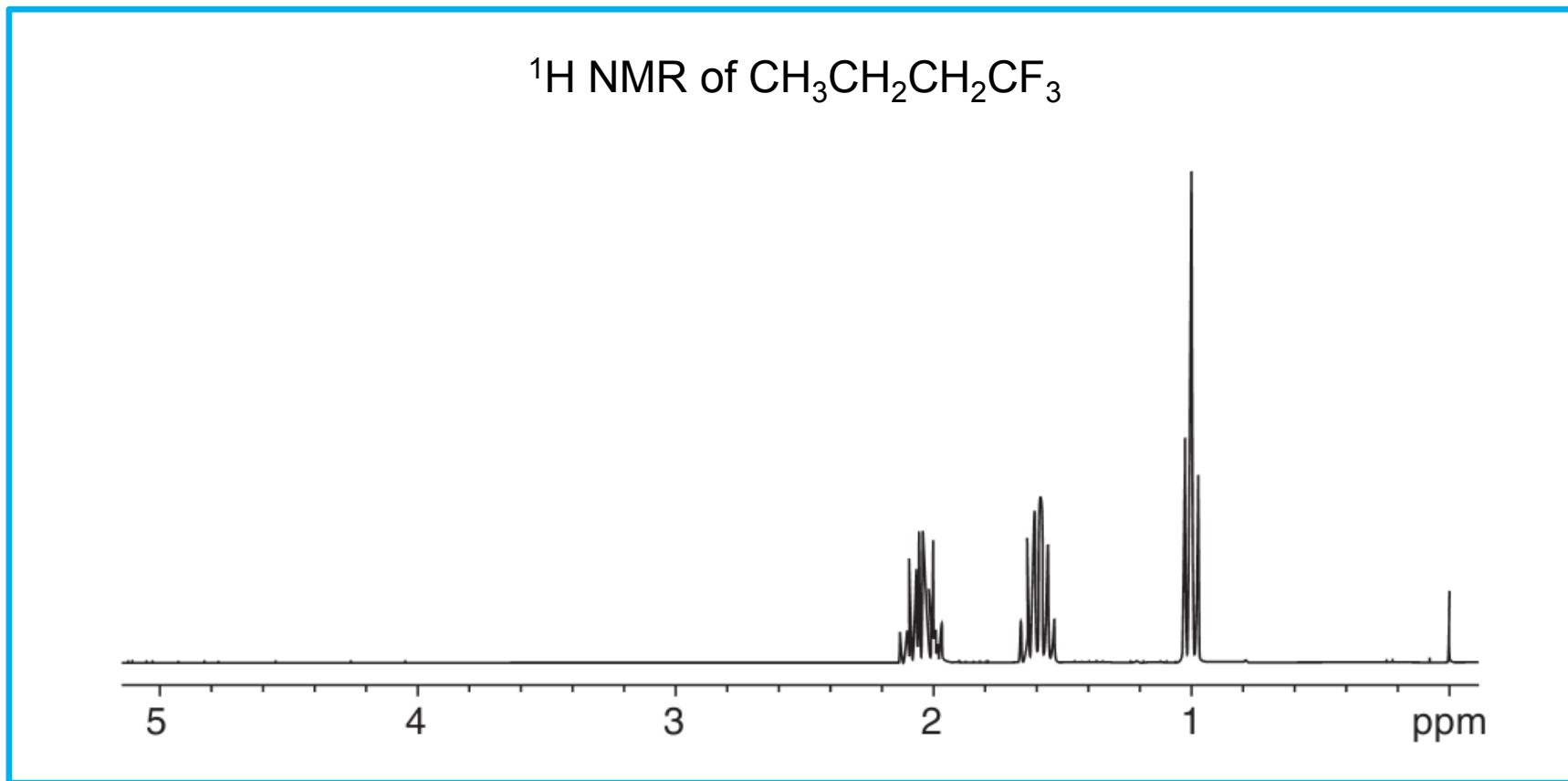
^{13}C NMR $\delta = 117.6$ (t, $^1J_{\text{FC}} = 239$ Hz), 13.8 (s), 36.2 (t, $^2J_{\text{FC}} = 20$ Hz), 15.8 (t, $^3J_{\text{FC}} = 6.0$ Hz)

代表化合物举例



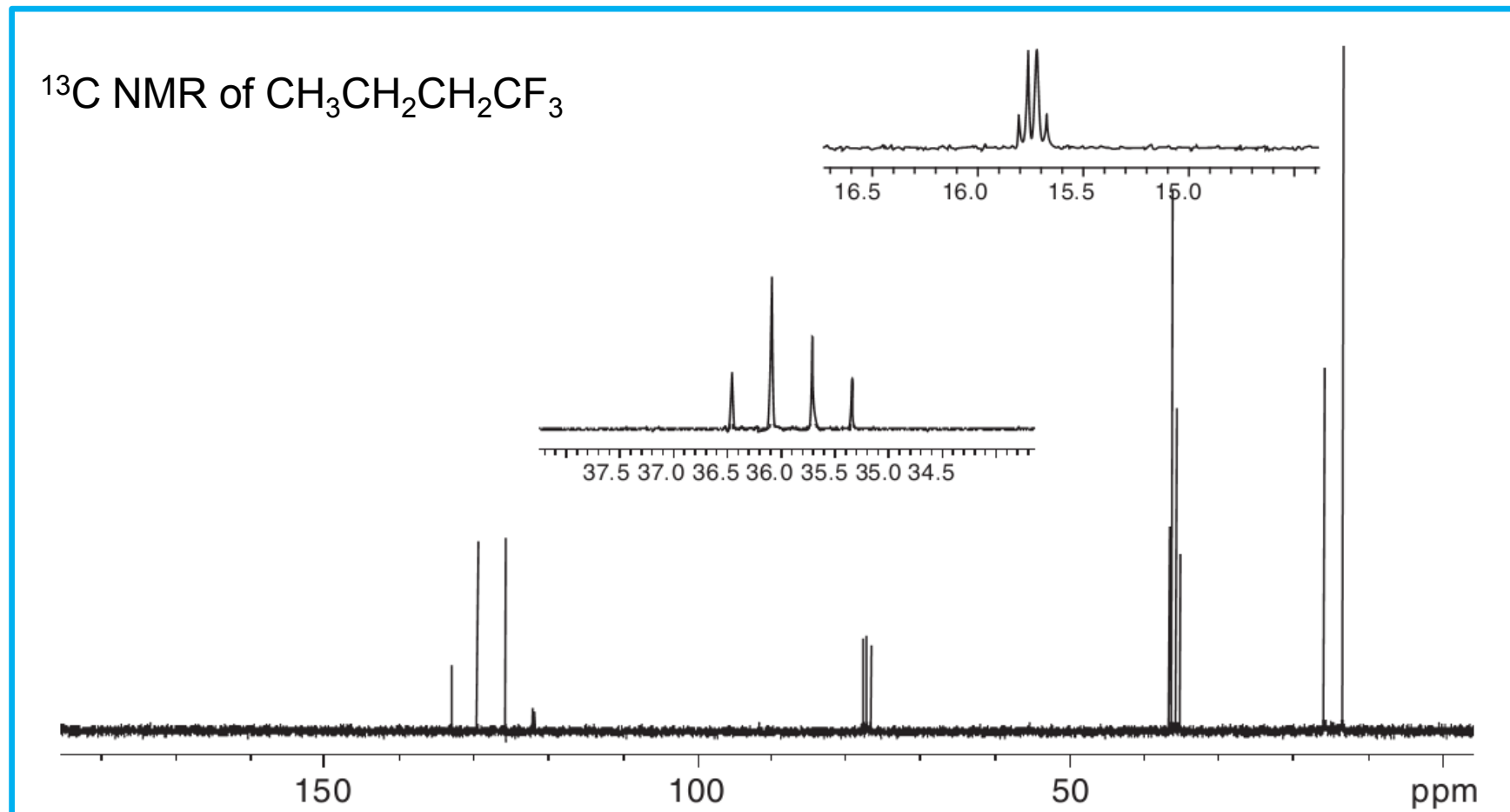
^{19}F NMR $\delta = -68$ ppm (t, $^3J_{\text{FH}} = 11$ Hz)

代表化合物举例



^1H NMR $\delta = 2.04$ (m, 2H), 1.59 (sextet, $^3J_{\text{HH}} = 8$ Hz, 2H), 1.01 (t, $^3J_{\text{HH}} = 7$ Hz, 3H)

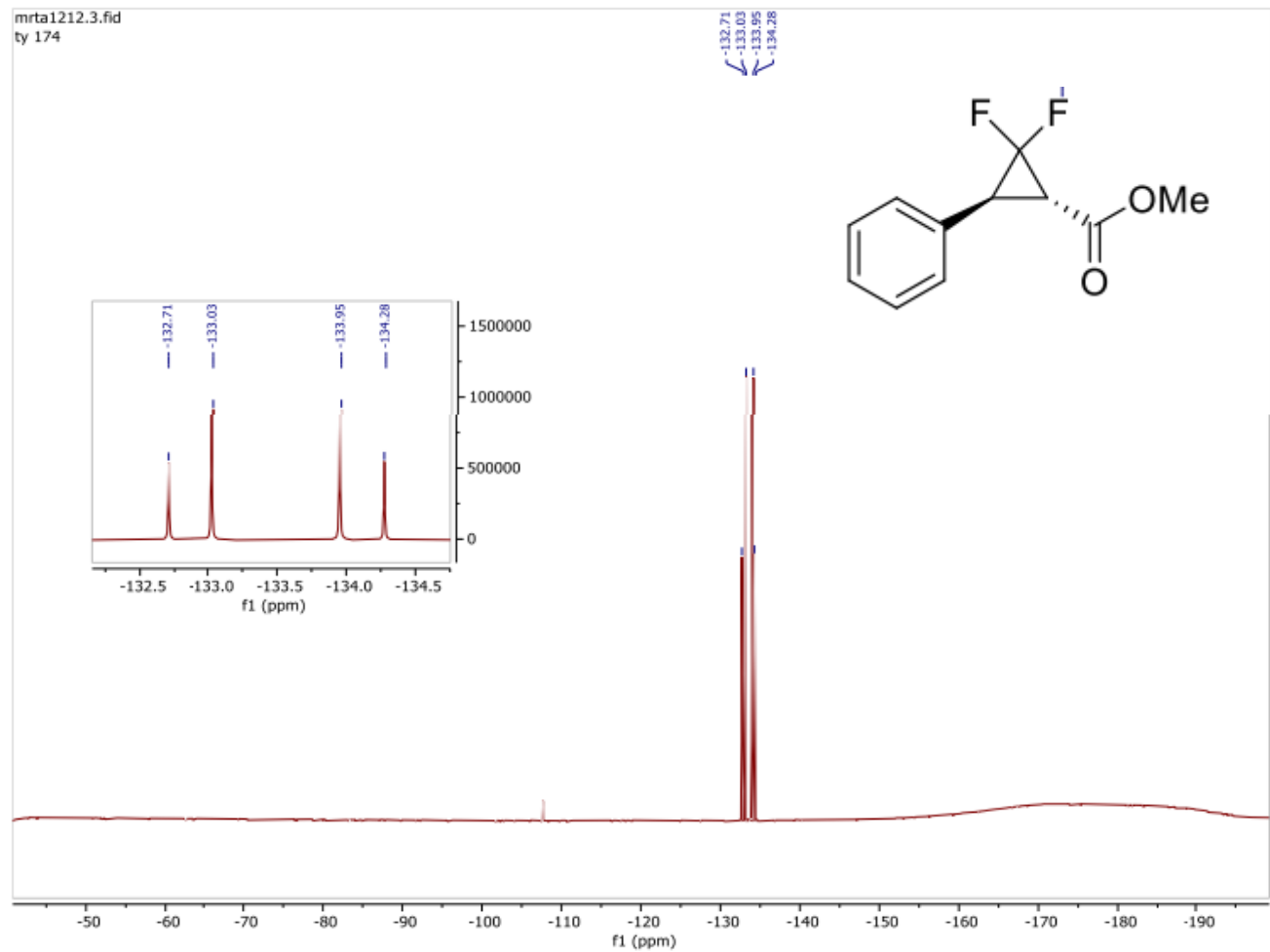
代表化合物举例



^{13}C NMR $\delta = 127.5$ (q, $^1J_{\text{FC}} = 276$ Hz), 35.9 (q, $^2J_{\text{FC}} = 28$ Hz), 15.7 (q, $^3J_{\text{FC}} = 2.6$ Hz), 13.4 (s)

代表化合物举例

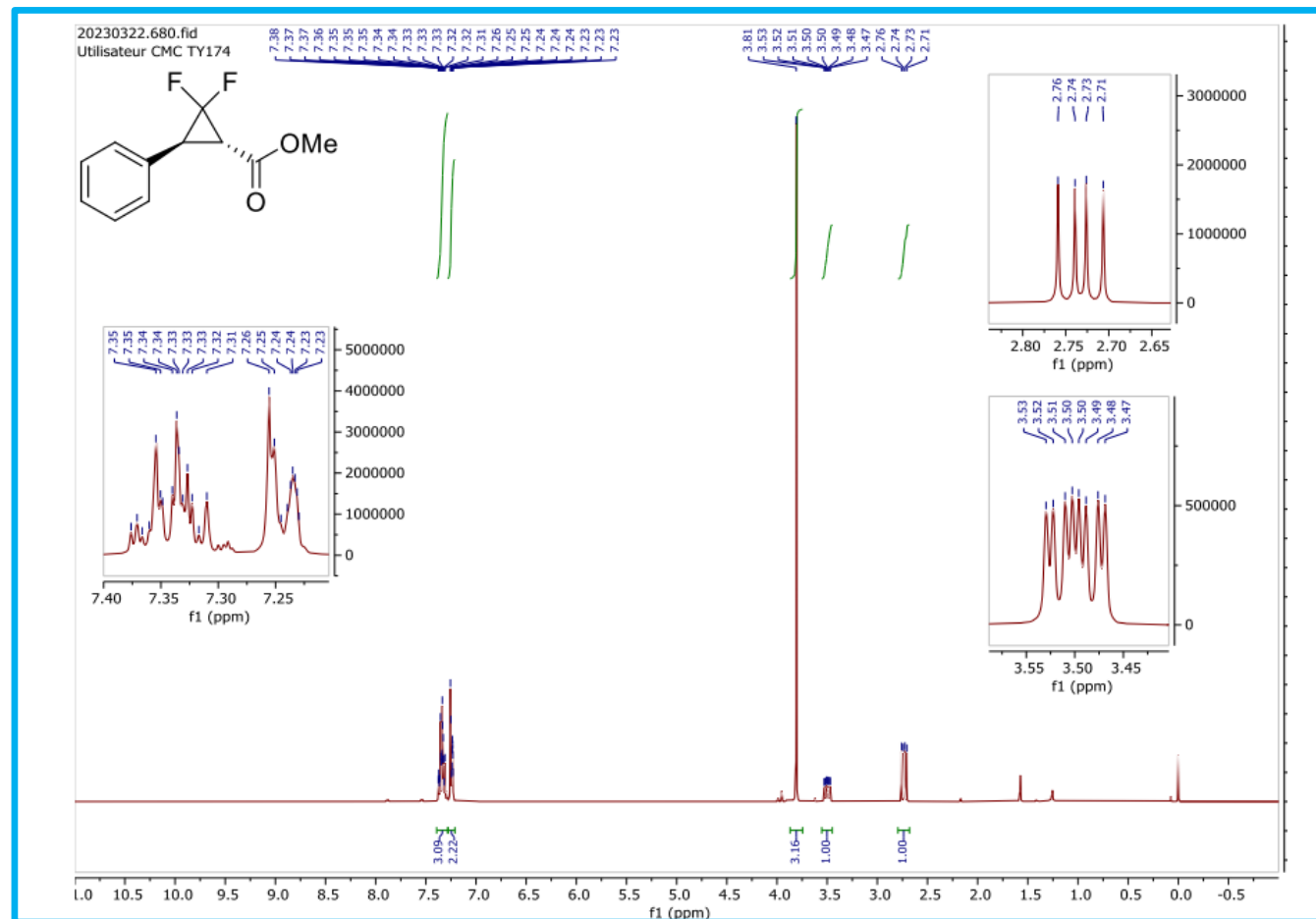
^{19}F NMR (471 MHz, CDCl_3)



^{19}F NMR (471 MHz, CDCl_3) $\delta = -132.9$ (d, $J = 151.6$ Hz), -134.1 (d, $J = 151.6$ Hz)

代表化合物举例

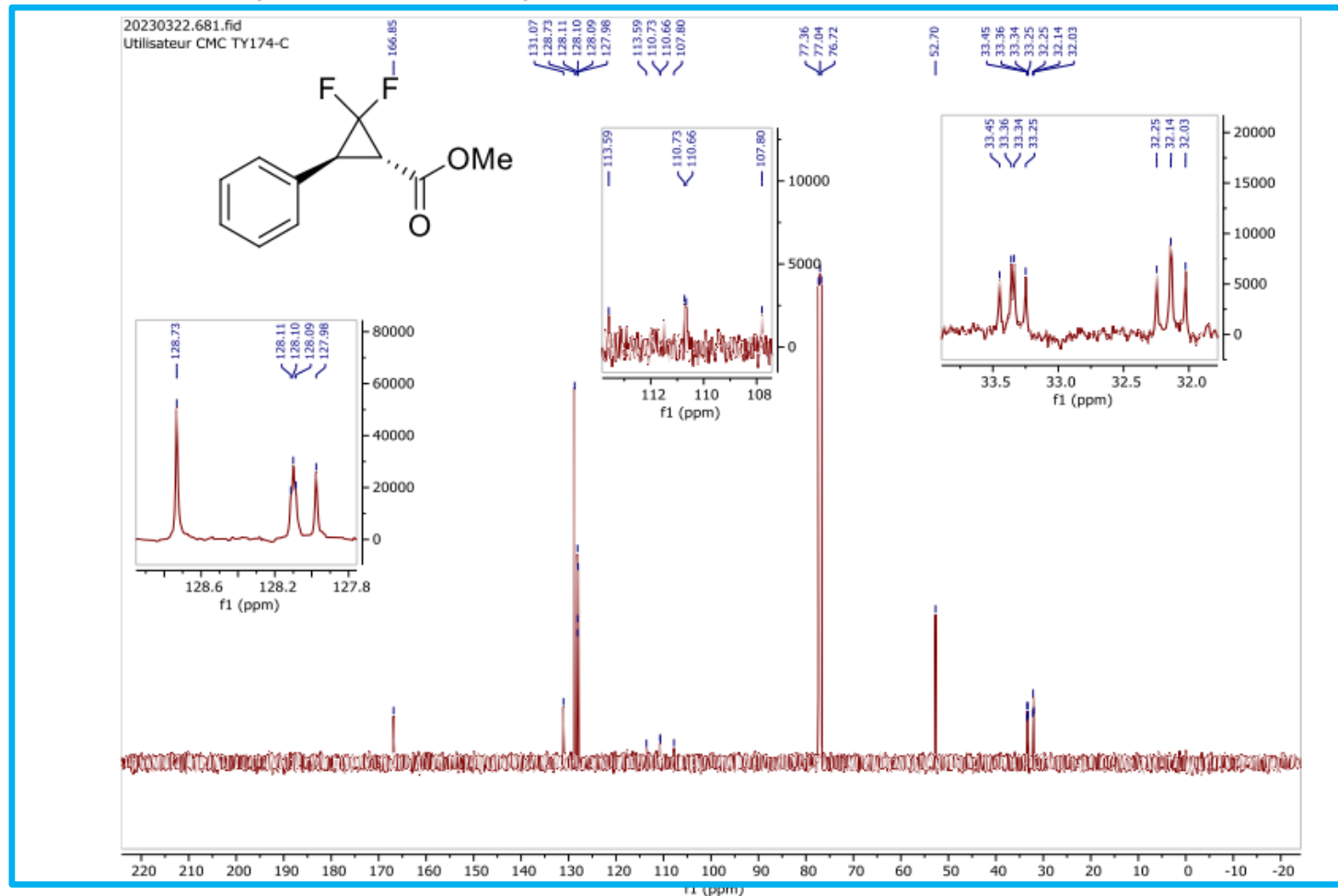
^1H NMR (400 MHz, CDCl_3)



^1H NMR (400 MHz, CDCl_3) δ = 7.39 – 7.28 (m, 3H), 7.28 – 7.21 (m, 2H), 3.81 (s, 3H), 3.50 (ddd, J = 13.6, 7.9, 2.9 Hz, 1H), 2.73 (dd, J = 13.1, 7.9 Hz, 1H)

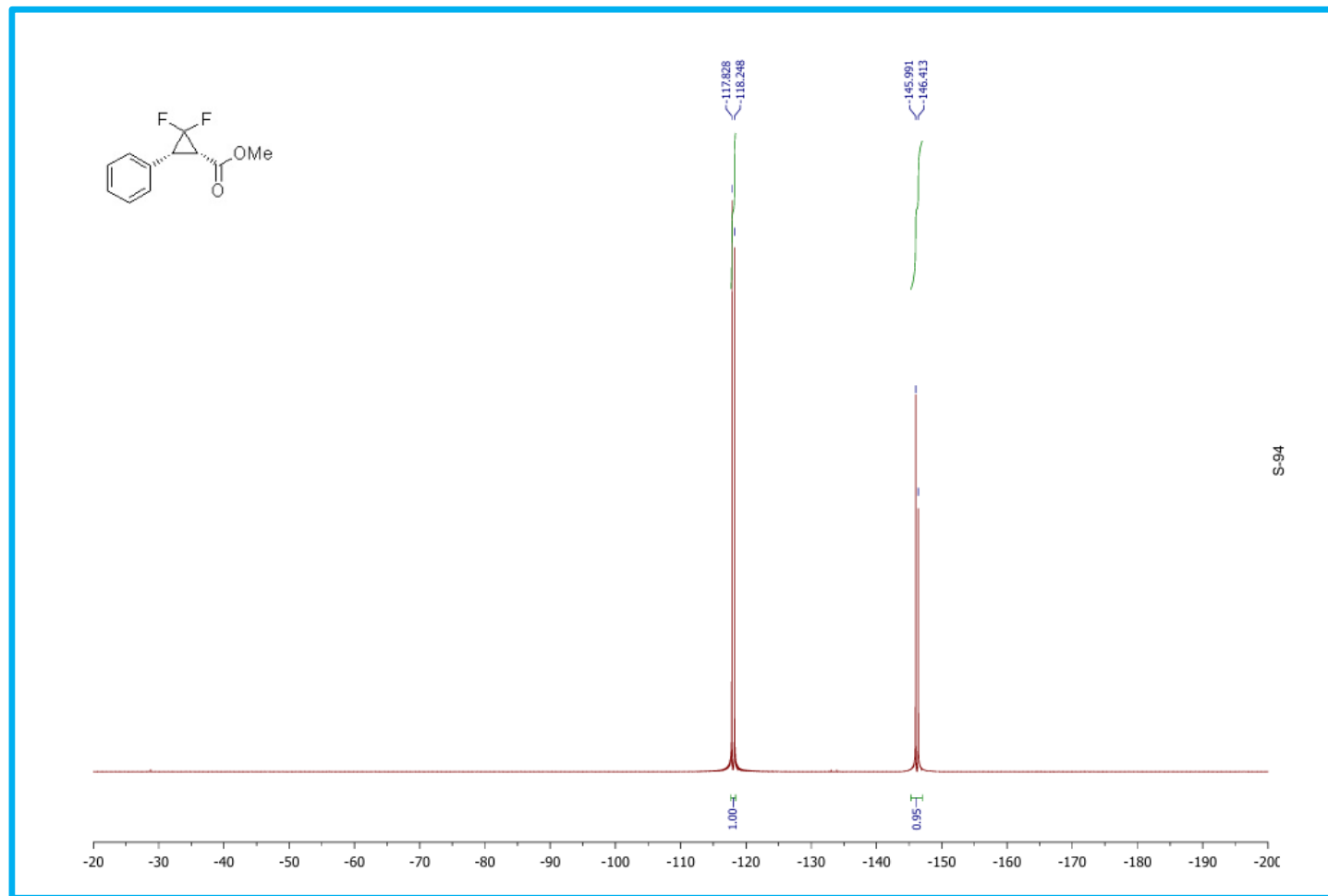
代表化合物举例

^{13}C NMR (100 MHz, CDCl_3)



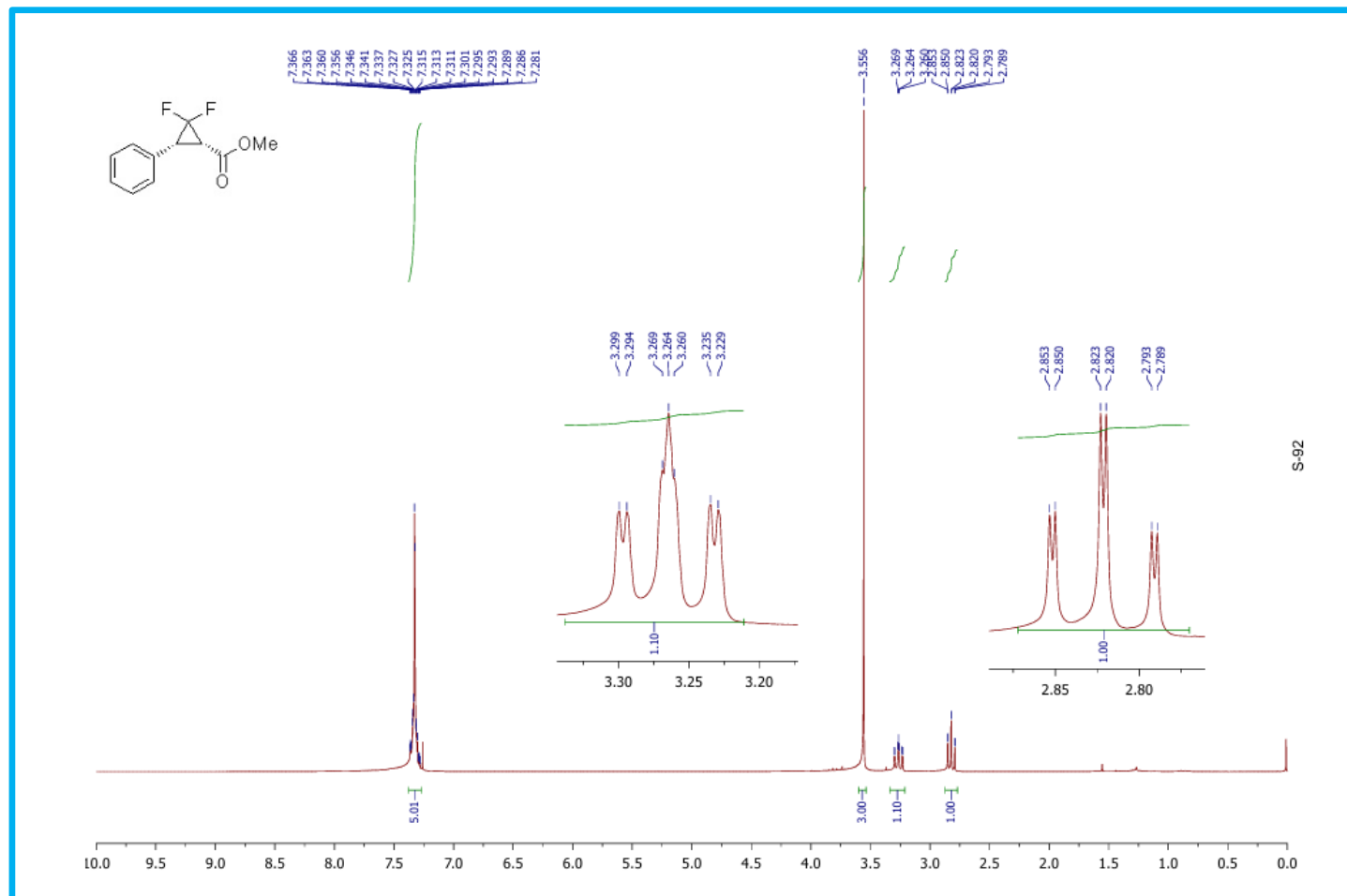
^{13}C NMR (100 MHz, CDCl_3) $\delta = 166.9, 131.1, 128.7$ (2C), 128.1 (t, $J = 1.4$ Hz, 2C), $128.0, 110.7$ (dd, $J = 294.7, 287.7$ Hz), $52.7, 33.3$ (dd, $J = 11.1, 8.9$ Hz), 32.1 (t, $J = 11.1$ Hz)

代表化合物举例



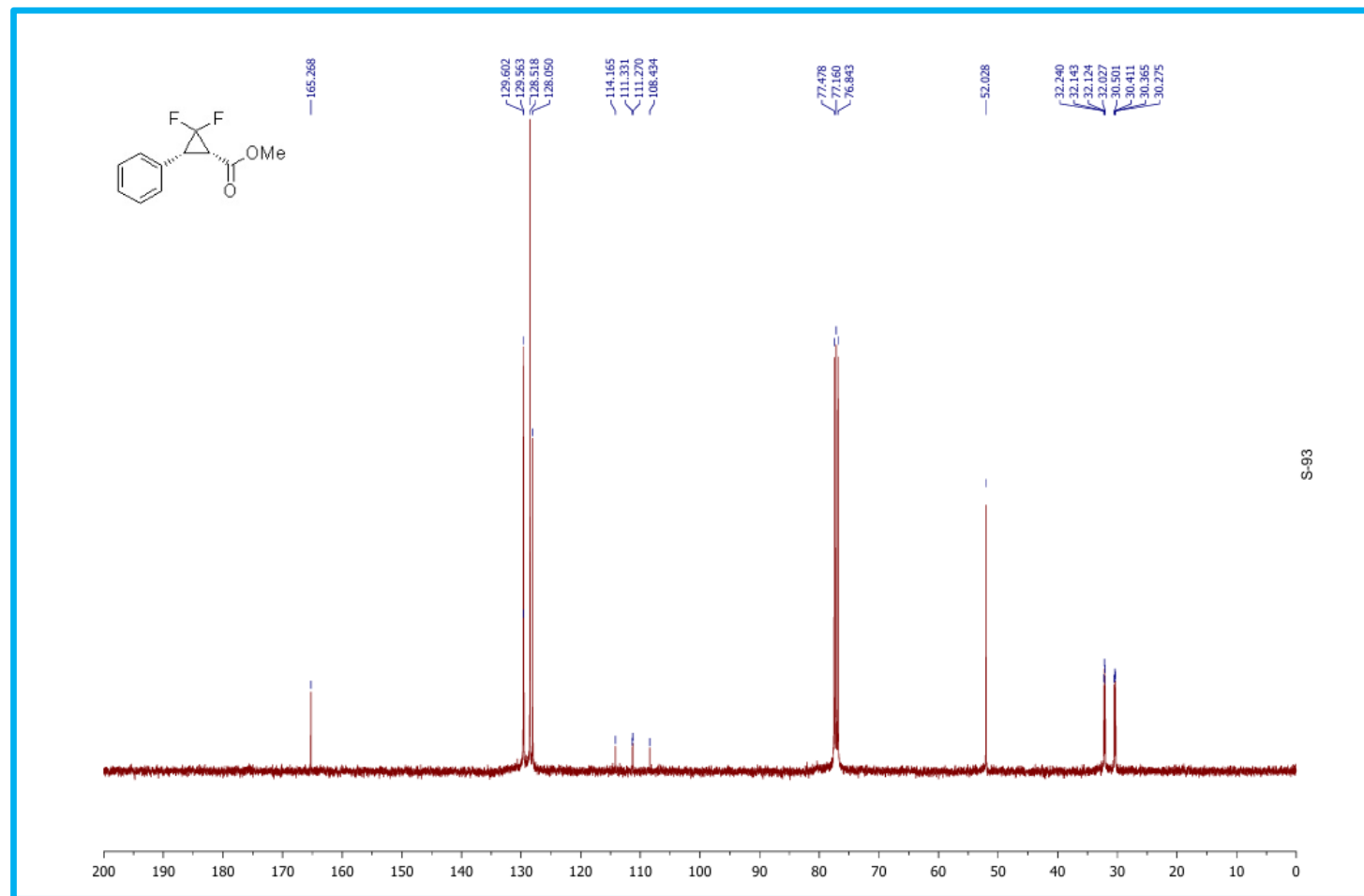
^{19}F NMR (471 MHz, CDCl_3) $\delta = -118.0$ (d, $^2J_{\text{F-F}} = 158$ Hz), -146.2 (d, $^2J_{\text{F-F}} = 159$ Hz)

代表化合物举例



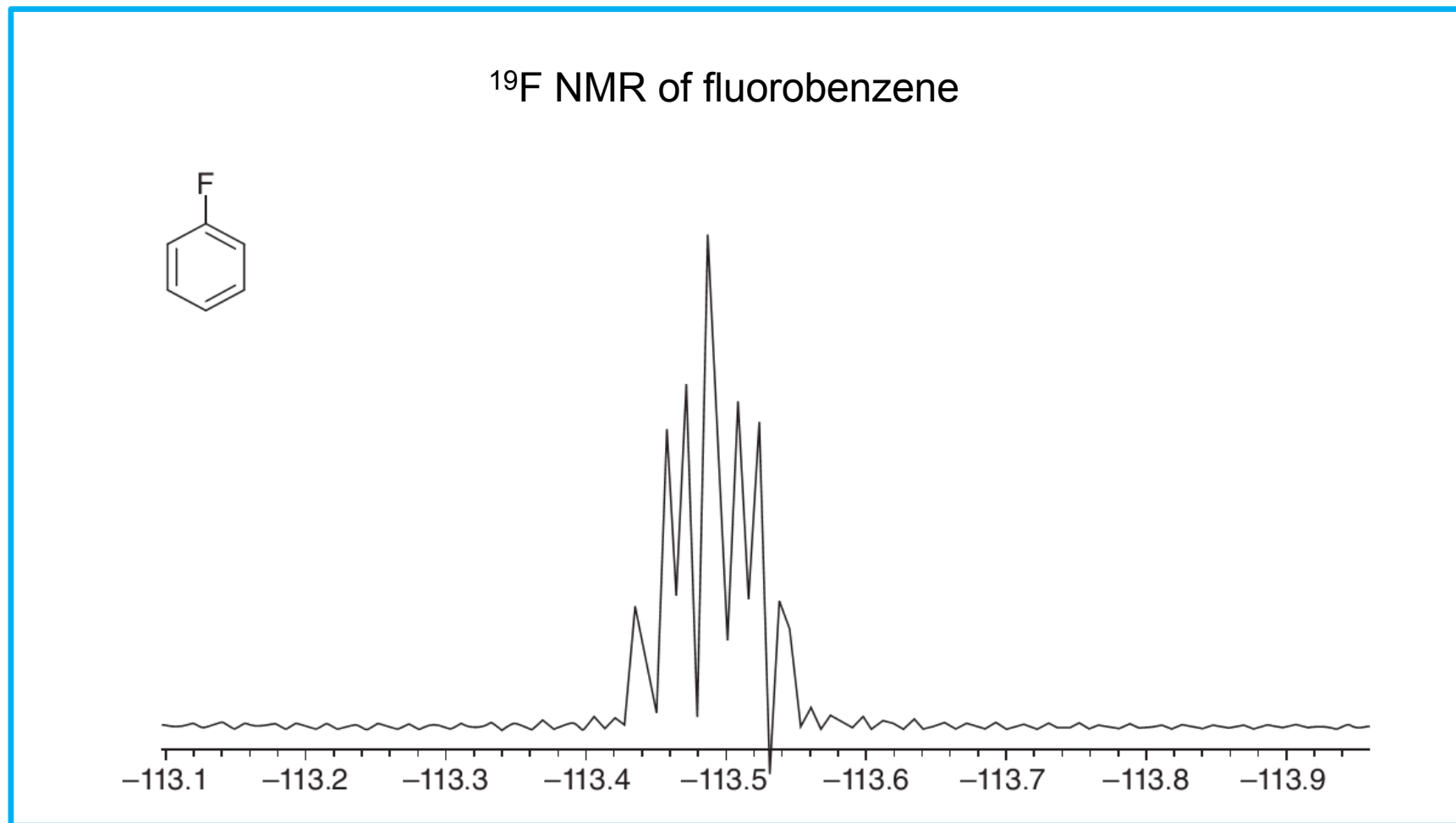
^1H NMR (400 MHz, CDCl_3) δ = 7.37–7.27 (m, 5H), 3.56 (s, 3H), 3.27 (ddd, J = 13.5, 12.5, 2.2 Hz, 1H), 2.82 (td, J = 12.2, 1.3 Hz, 1H)

代表化合物举例

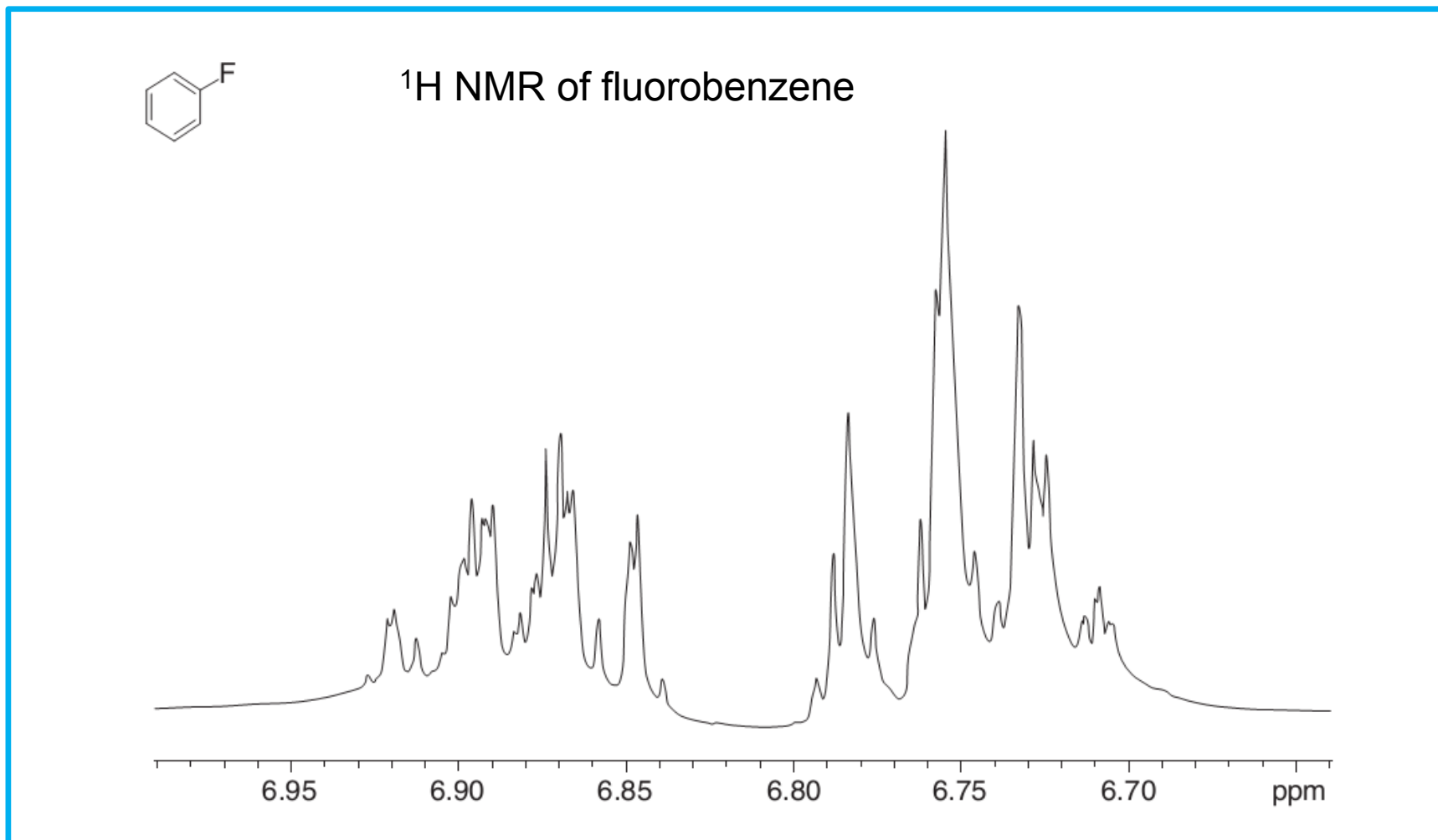


^{13}C NMR (100 MHz, CDCl_3) δ = 165.3, 129.6 (2C), 129.5, 128.5 (2C), 128.1, 111.3 (dd, $^1J_{\text{C-F}} = 291$ Hz and $^1J_{\text{C-F}} = 285$ Hz), 52.0, 32.1 (dd, $^2J_{\text{C-F}} = 11.7$ Hz and $^2J_{\text{C-F}} = 9.8$ Hz), 30.4 (dd, $^2J_{\text{C-F}} = 13.7$ Hz and $^2J_{\text{C-F}} = 9.0$ Hz)

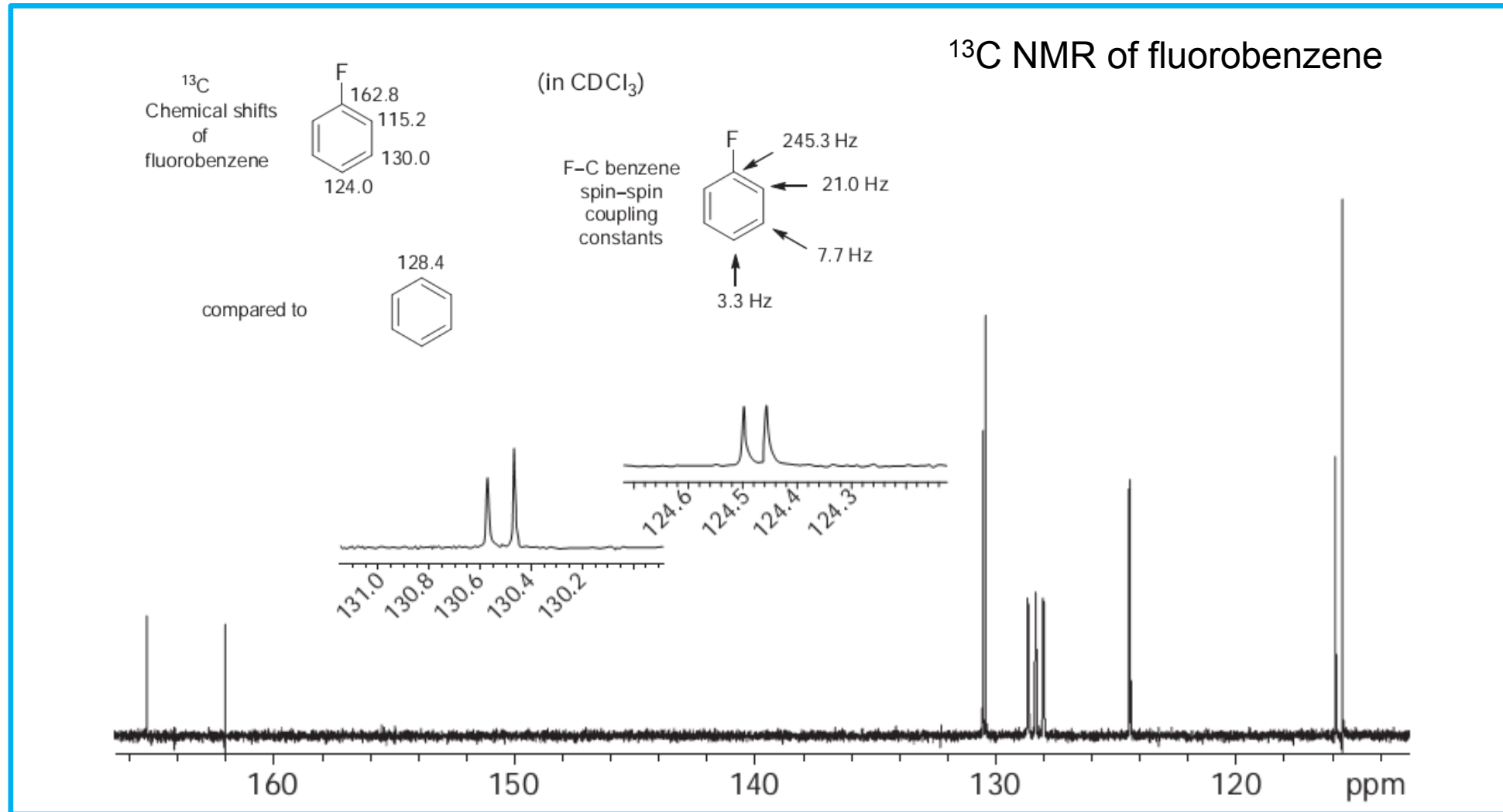
代表化合物举例



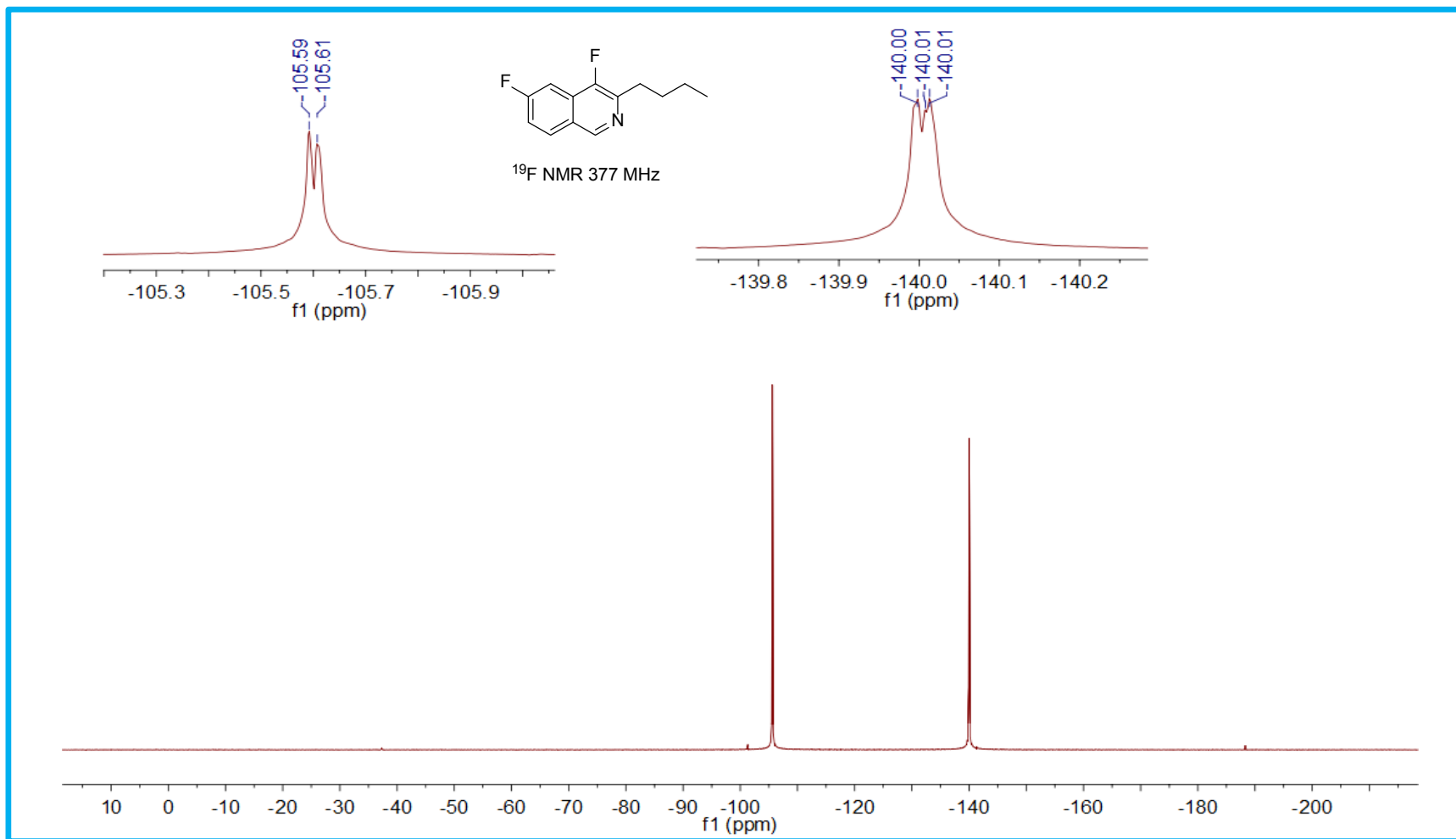
代表化合物举例



代表化合物举例

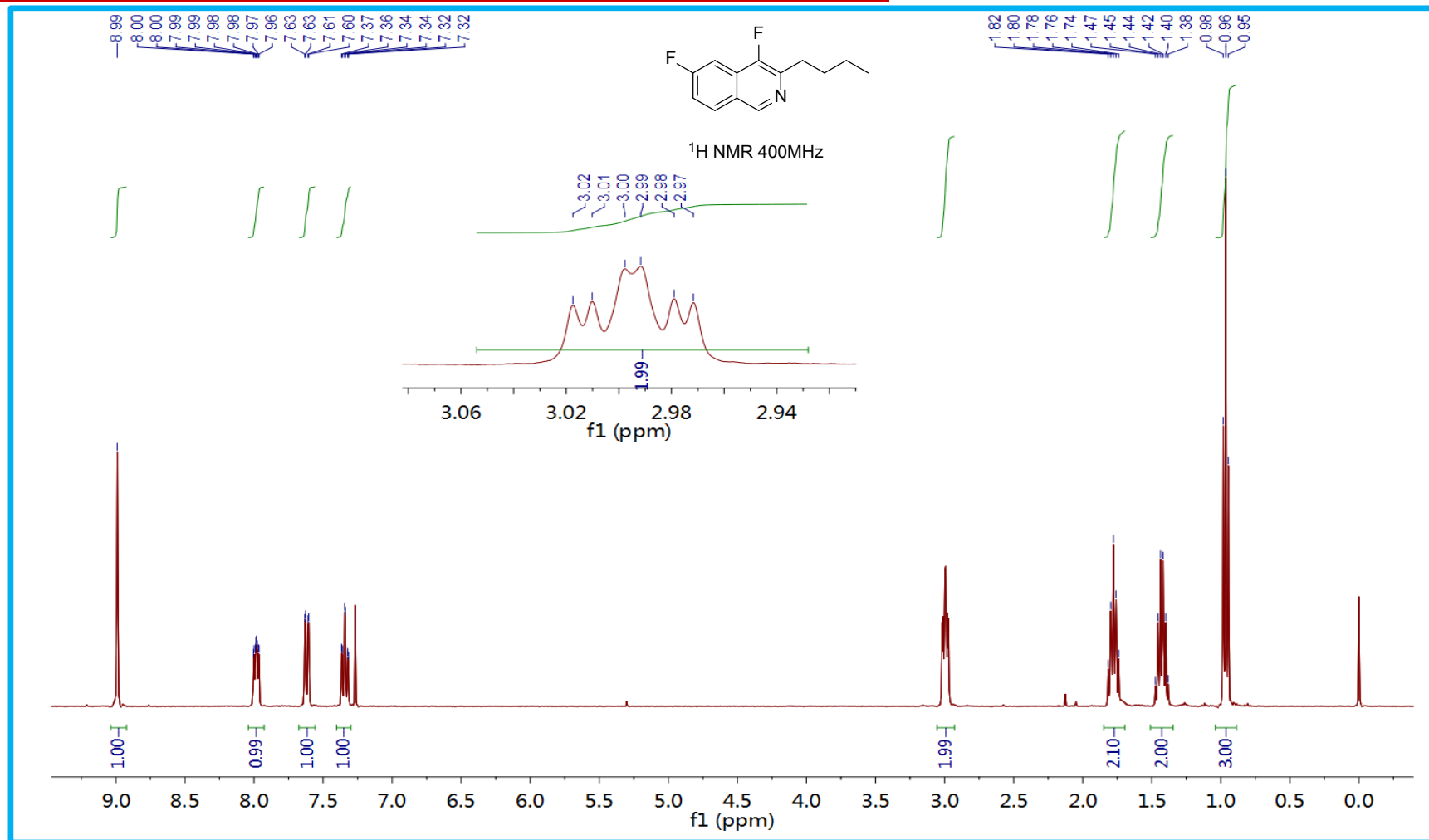


代表化合物举例



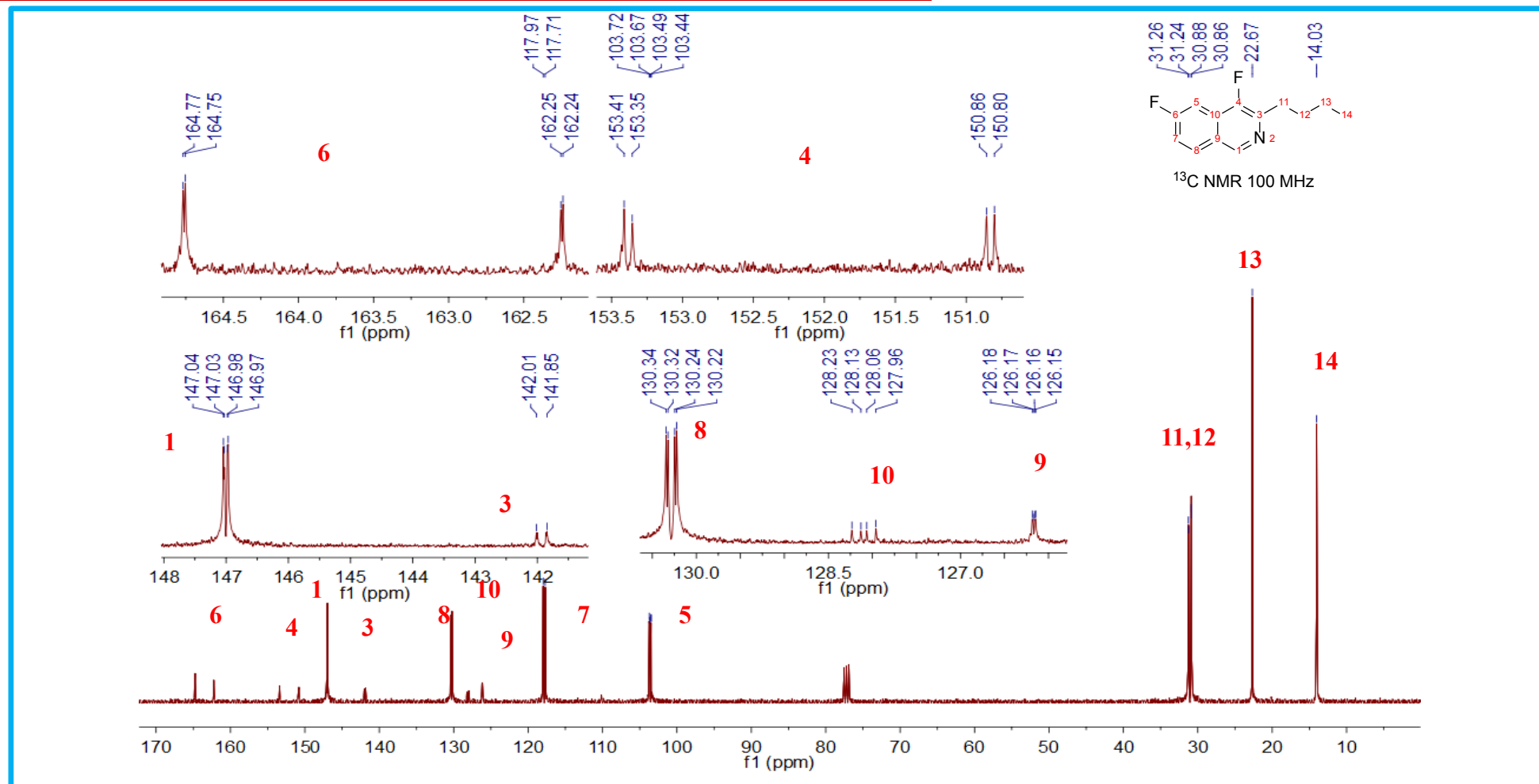
^{19}F NMR (376 MHz, CDCl_3) $\delta = -105.6$ (d, $^3J_{\text{FH}} = 5.9$ Hz), $-139.7 - -140.3$ (m)

代表化合物举例



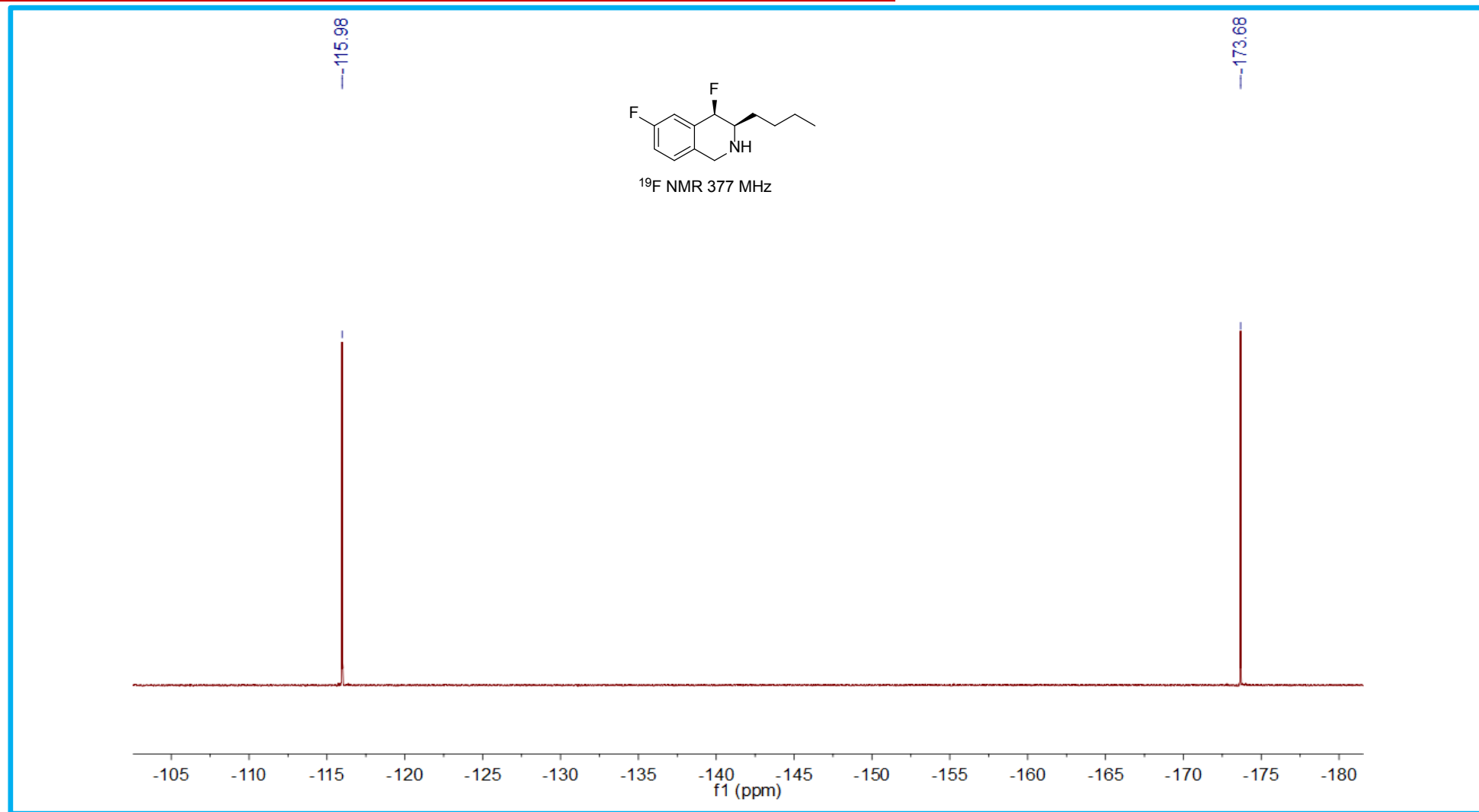
¹H NMR (400 MHz, CDCl₃) δ = 8.99 (s, 1H), 7.98 (ddd, J = 8.7, 5.2, 1.5 Hz, 1H), 7.62 (dd, J = 9.4, 2.0 Hz, 1H), 7.34 (td, J = 8.8, 2.3 Hz, 1H), 2.99 (td, J = 8.0, 2.9 Hz, 2H), 1.85-1.69 (m, 2H), 1.51-1.34 (m, 2H), 0.96 (t, J = 7.4 Hz, 3H)

代表化合物举例



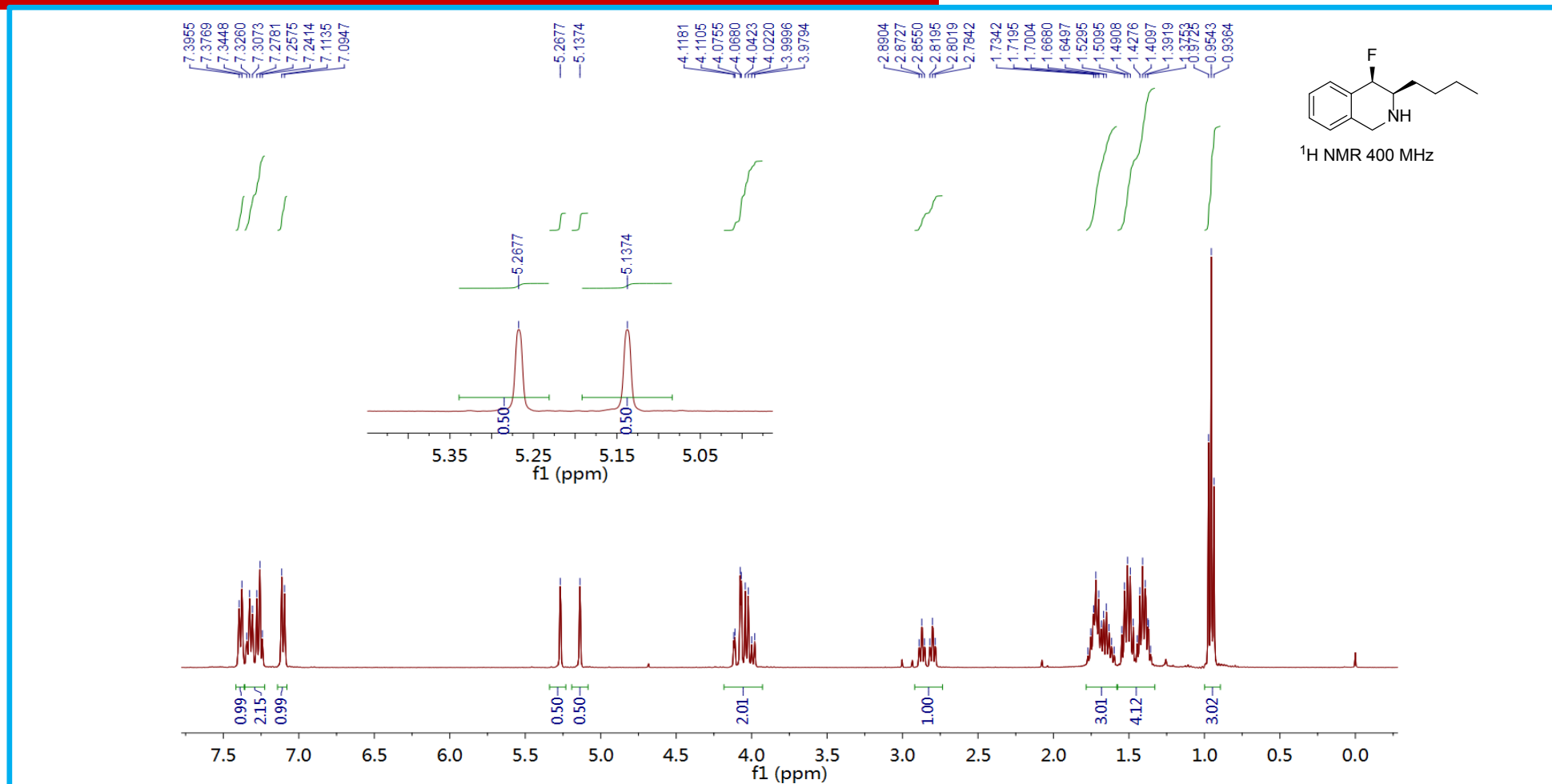
^{13}C NMR (100 MHz, CDCl_3) δ = 163.5 (dd, $^1J_{\text{FC}} = 253.1\text{ Hz}$, $^4J_{\text{FC}} = 1.4\text{ Hz}$), 152.1 (dd, $^1J_{\text{FC}} = 256.9\text{ Hz}$, $^4J_{\text{FC}} = 5.7\text{ Hz}$), 147.0 (dd, $^4J_{\text{FC}} = 6.2\text{ Hz}$, $^5J_{\text{FC}} = 1.4\text{ Hz}$), 141.9 (d, $^2J_{\text{FC}} = 16.9\text{ Hz}$), 130.3 (dd, $^3J_{\text{FC}} = 10.0$, $^4J_{\text{FC}} = 2.2\text{ Hz}$), 128.1 (dd, $^3J_{\text{FC}} = 17.0\text{ Hz}$, $^4J_{\text{FC}} = 10.4\text{ Hz}$), 126.2 (dd, $^3J_{\text{FC}} = 2.7\text{ Hz}$, $^4J_{\text{FC}} = 1.1\text{ Hz}$), 117.8 (d, $^2J_{\text{FC}} = 26.6\text{ Hz}$), 103.6 (dd, $^2J_{\text{FC}} = 23.5$, $^3J_{\text{FC}} = 5.1\text{ Hz}$), 31.3 (d, $^3J_{\text{FC}} = 2.0\text{ Hz}$), 30.9 (d, $^3J_{\text{FC}} = 1.7\text{ Hz}$), 22.7 (s), 14.0 (s)

代表化合物举例



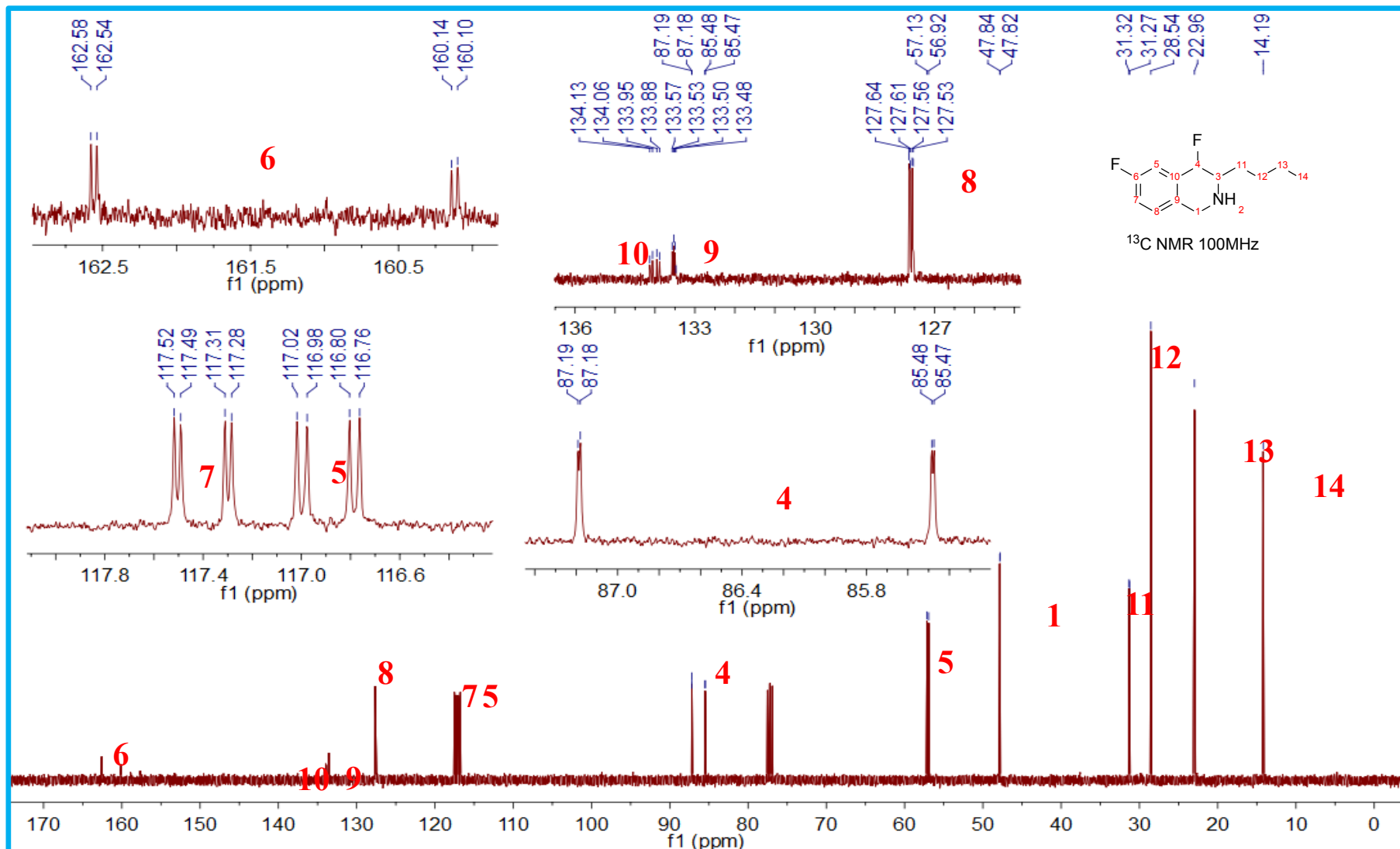
^{19}F NMR (376 MHz, CDCl_3) $\delta = -116.0$ (s), -173.7 (s)

代表化合物举例



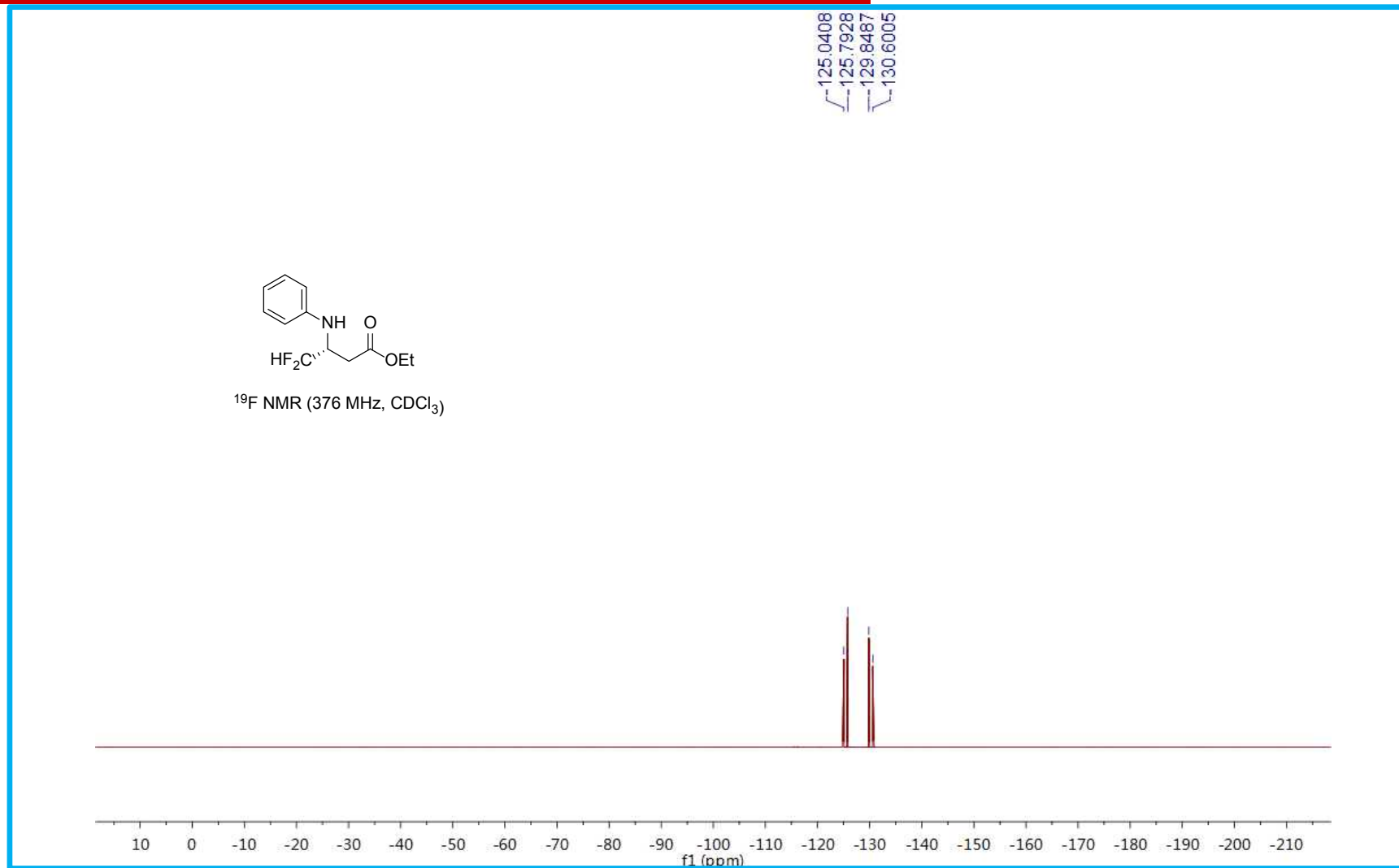
¹H NMR (400 MHz, CDCl₃) δ = 7.39 (d, J = 7.4 Hz, 1H), 7.33 (t, J = 7.5 Hz, 1H), 7.26 (t, J = 7.3 Hz, 1H), 7.10 (d, J = 7.5 Hz, 1H), 5.20 (d, $^2J_{\text{FH}}$ = 52.1 Hz, 1H), 4.05 (qd, $^5J_{\text{FH}}$ = 17.1, 5.6 Hz, 2H), 2.84 (dt, $^3J_{\text{FH}}$ = 28.3, 7.1 Hz, 1H), 1.90-1.58 (m, 3H), 1.59-1.28 (m, 4H), 0.95 (t, J = 7.2 Hz, 3H)

代表化合物举例



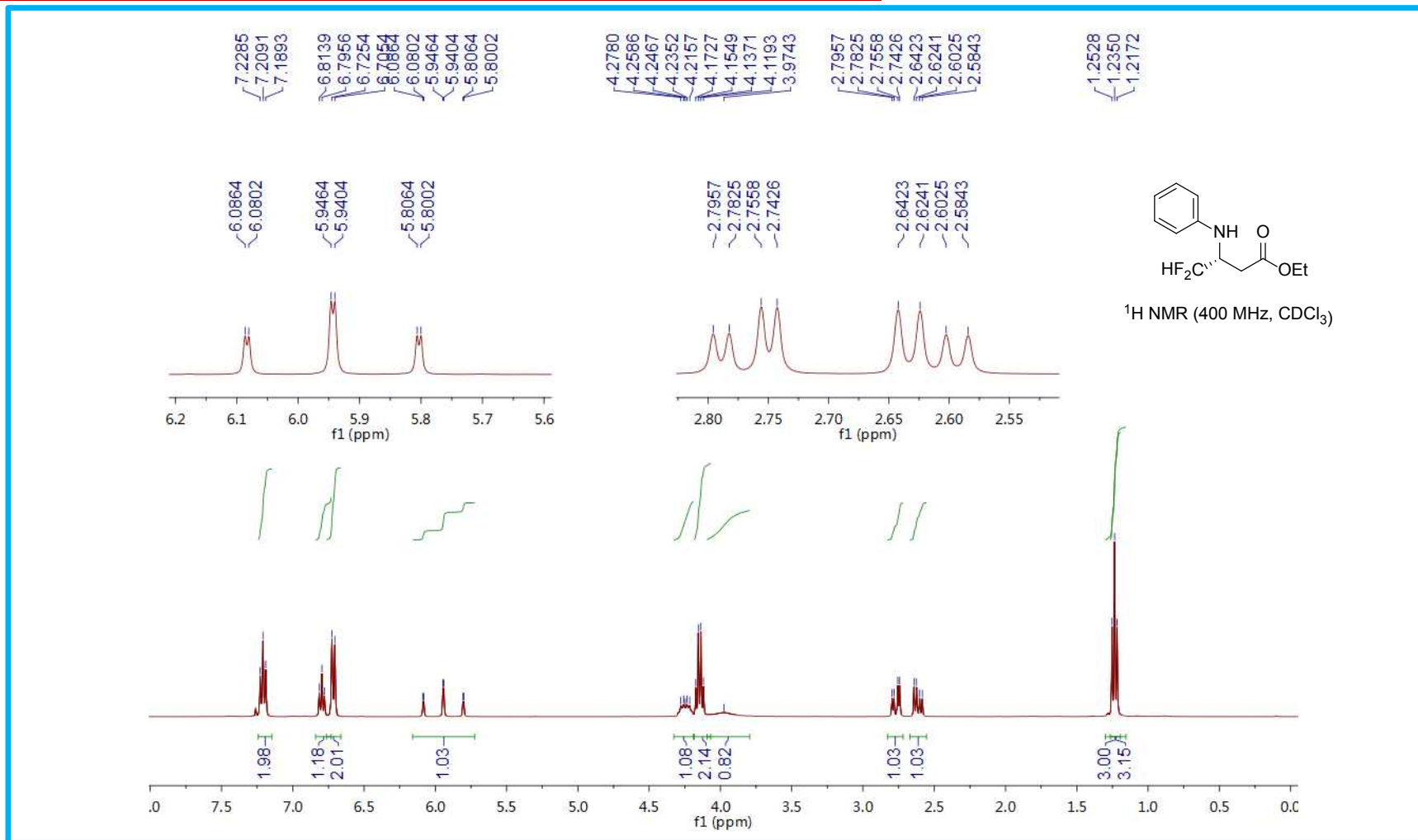
13C NMR (100 MHz, CDCl₃) δ = 161.3 (dd, ¹J_{FC} = 245.3 Hz, ⁴J_{FC} = 4.1 Hz), 134.0 (dd, J = 17.8, 7.1 Hz), 133.5 (dd, ³J_{FC} = 6.2 Hz, ⁴J_{FC} = 2.9 Hz), 127.6 (dd, ³J_{FC} = 7.7 Hz, ⁴J_{FC} = 2.5 Hz), 117.4 (dd, ²J_{FC} = 20.8 Hz, ⁴J_{FC} = 2.7 Hz), 116.9 (dd, ²J_{FC} = 21.5 Hz, ³J_{FC} = 4.1 Hz). 86.3 (dd, ¹J_{FC} = 171.7 Hz, ⁴J_{FC} = 1.1 Hz), 57.0 (d, ²J_{FC} = 20.9 Hz), 47.8 (d, ⁴J_{FC} = 1.7 Hz), 31.3 (d, ³J_{FC} = 4.8 Hz), 28.5 (s), 23.0 (s), 14.2 (s)

代表化合物举例



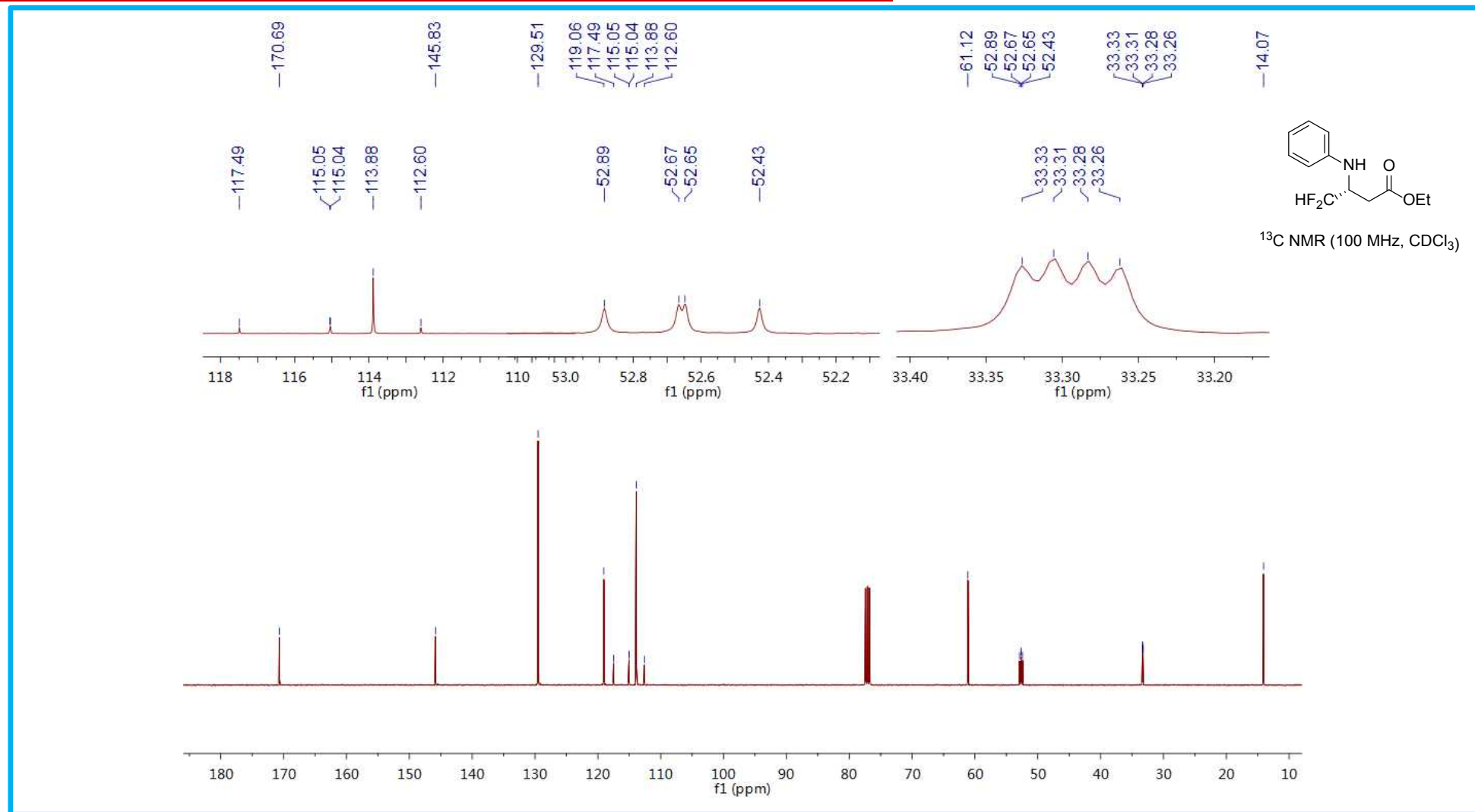
^{19}F NMR (376 MHz, CDCl₃) δ = -125.4 (d, J = 282.7 Hz, 1F), 130.2 (d, J = 282.7 Hz, 1F)

代表化合物举例



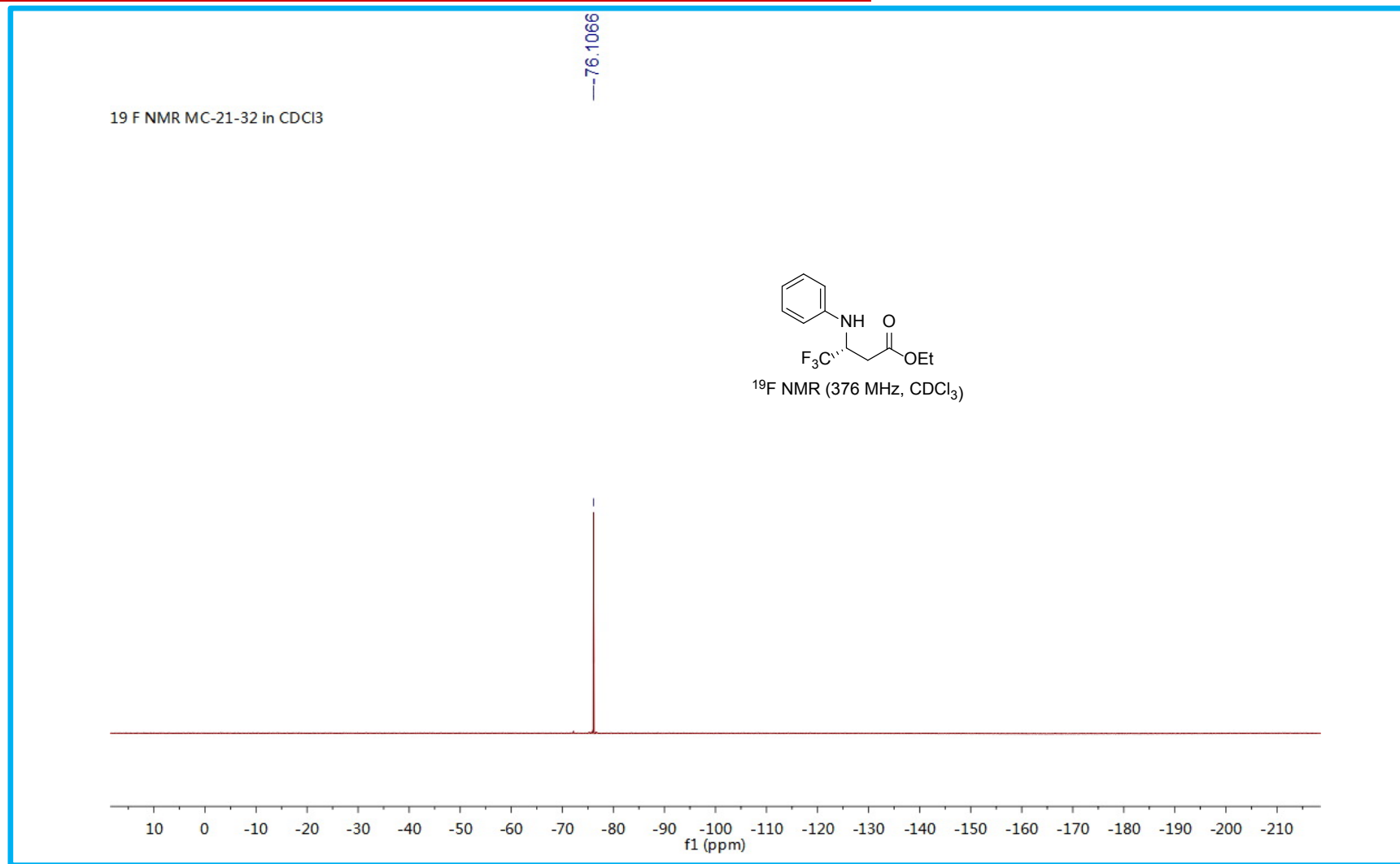
$^1\text{H NMR}$ (400 MHz, CDCl_3) δ = 7.21 (t, J = 7.8 Hz, 2H), 6.80 (t, J = 7.3 Hz, 1H), 6.72 (d, J = 8.0 Hz, 2H), 5.94 (td, J = 56.1, 2.5 Hz, 1H), 4.33 – 4.19 (m, 1H), 4.15 (q, J = 7.1 Hz, 2H), 3.97 (s, 1H), 2.77 (dd, J = 15.9, 5.3 Hz, 1H), 2.61 (dd, J = 15.9, 7.3 Hz, 1H), 1.24 (t, J = 7.1 Hz, 3H)

代表化合物举例



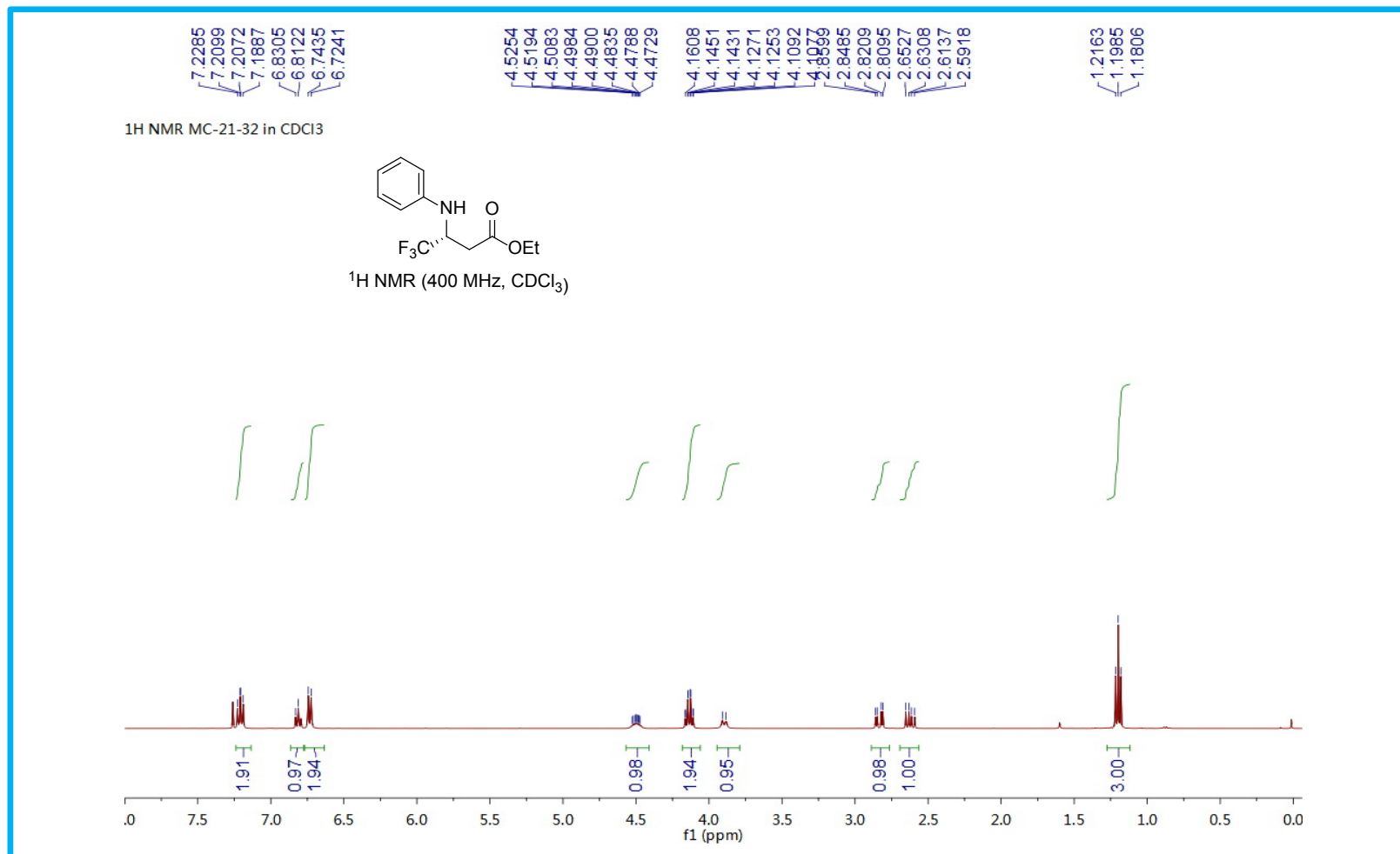
¹³C NMR (100 MHz, CDCl₃) δ = 170.7, 145.8, 129.5, 119.1, 115.1 (t, J = 245.0 Hz), 113.9, 61.1, 52.6 (dd, J = 24.0 Hz), 33.3 (dd, J = 5.0, 2.0 Hz), 14.1

代表化合物举例



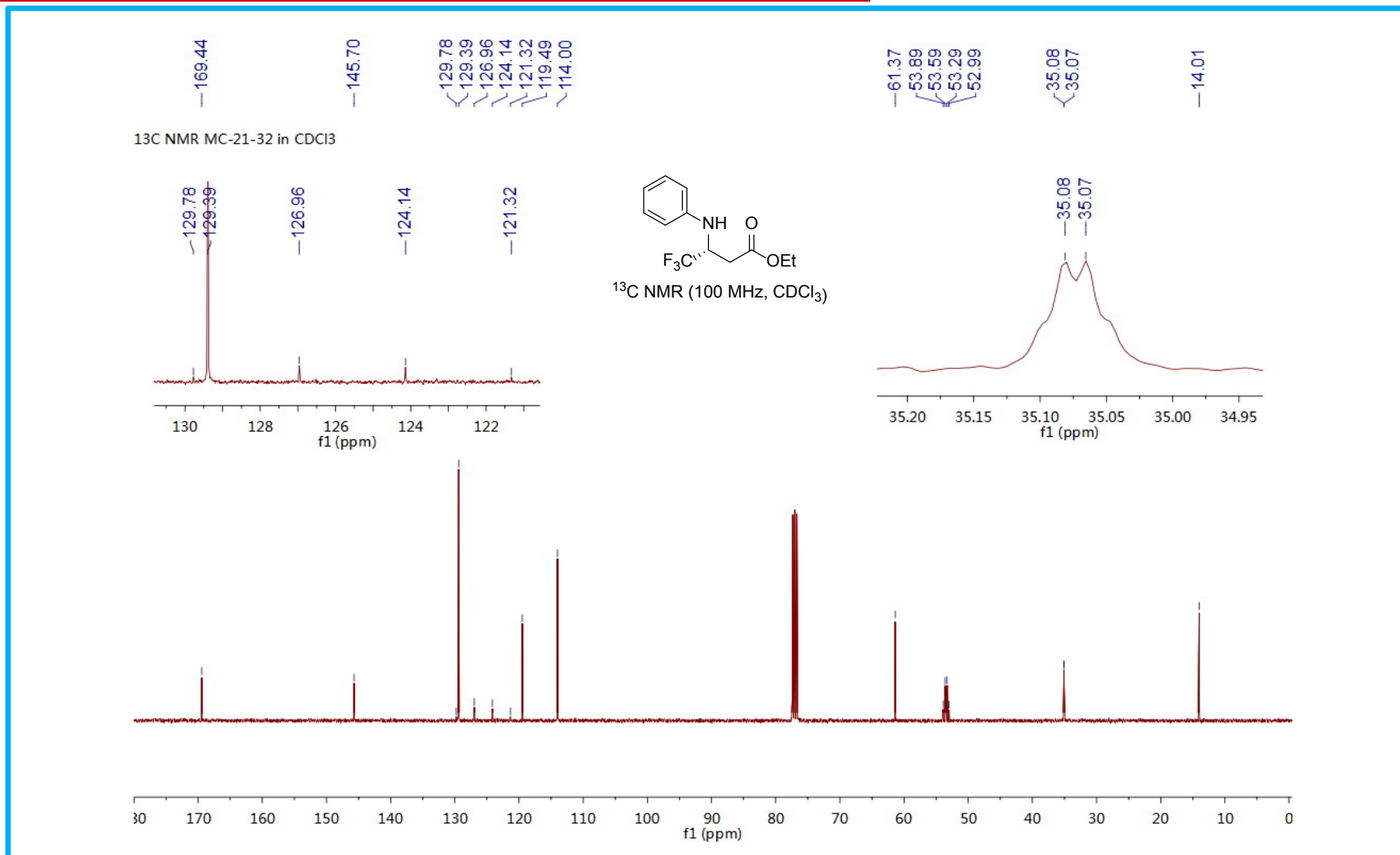
¹⁹F NMR (376 MHz, CDCl₃) $\delta = -76.1$

代表化合物举例



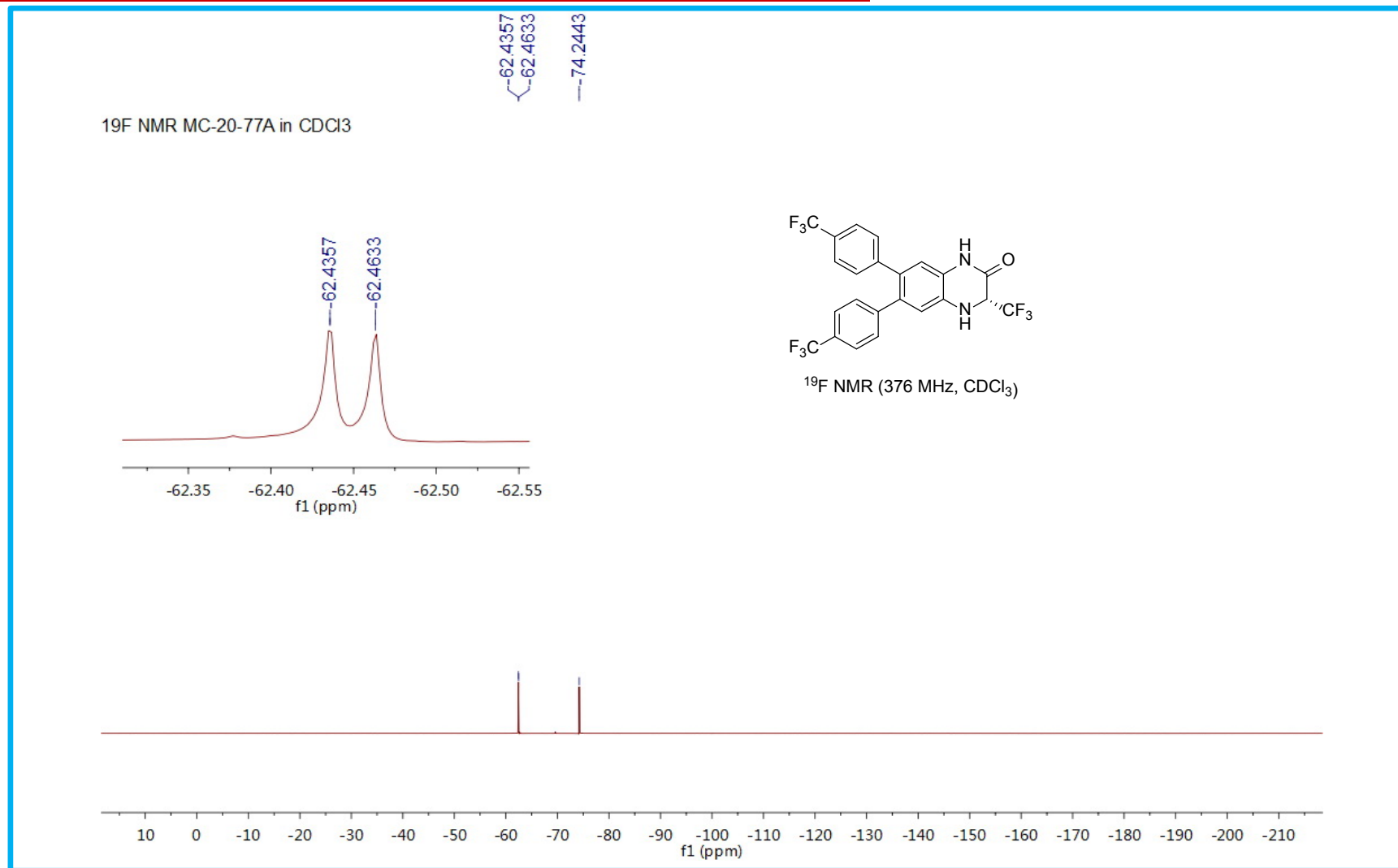
¹H NMR (400 MHz, CDCl₃) δ = 7.24 – 7.17 (m, 2H), 6.81 (t, J = 7.4 Hz, 1H), 6.73 (d, J = 7.8 Hz, 2H), 4.56 – 4.42 (m, 1H), 4.19 – 4.05 (m, 2H), 3.90 (d, J = 9.9 Hz, 1H), 2.83 (dd, J = 15.6, 4.5 Hz, 1H), 2.62 (dd, J = 15.6, 8.8 Hz, 1H), 1.20 (t, J = 7.1 Hz, 3H)

代表化合物举例



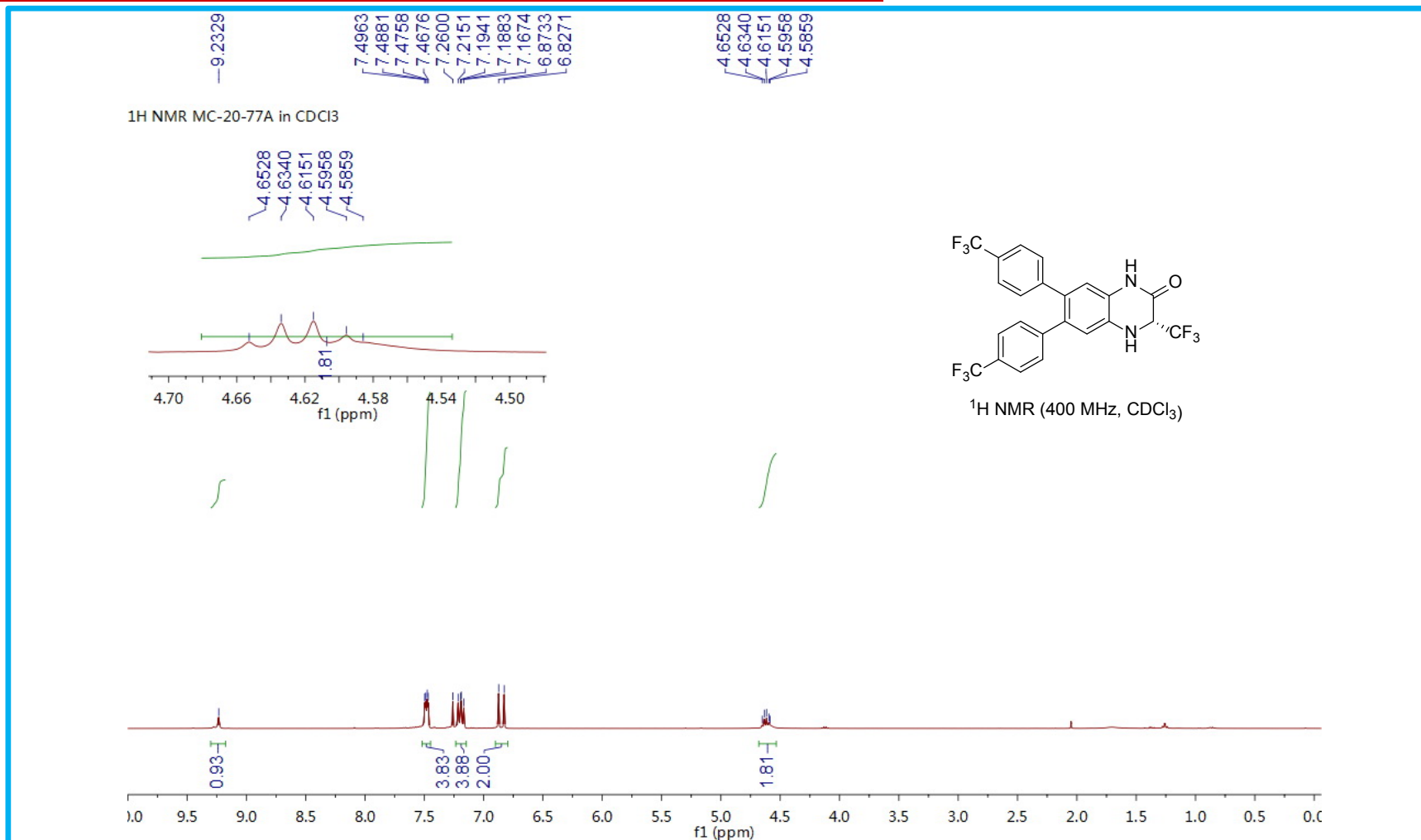
^{13}C NMR (100 MHz, CDCl_3) δ = 169.4, 145.7, 129.4, 125.6 (q, J = 282.0 Hz), 119.5, 114.0, 61.4, 53.4 (q, J = 30 Hz), 35.1 (q, J = 1.0 Hz), 14.0.

代表化合物举例



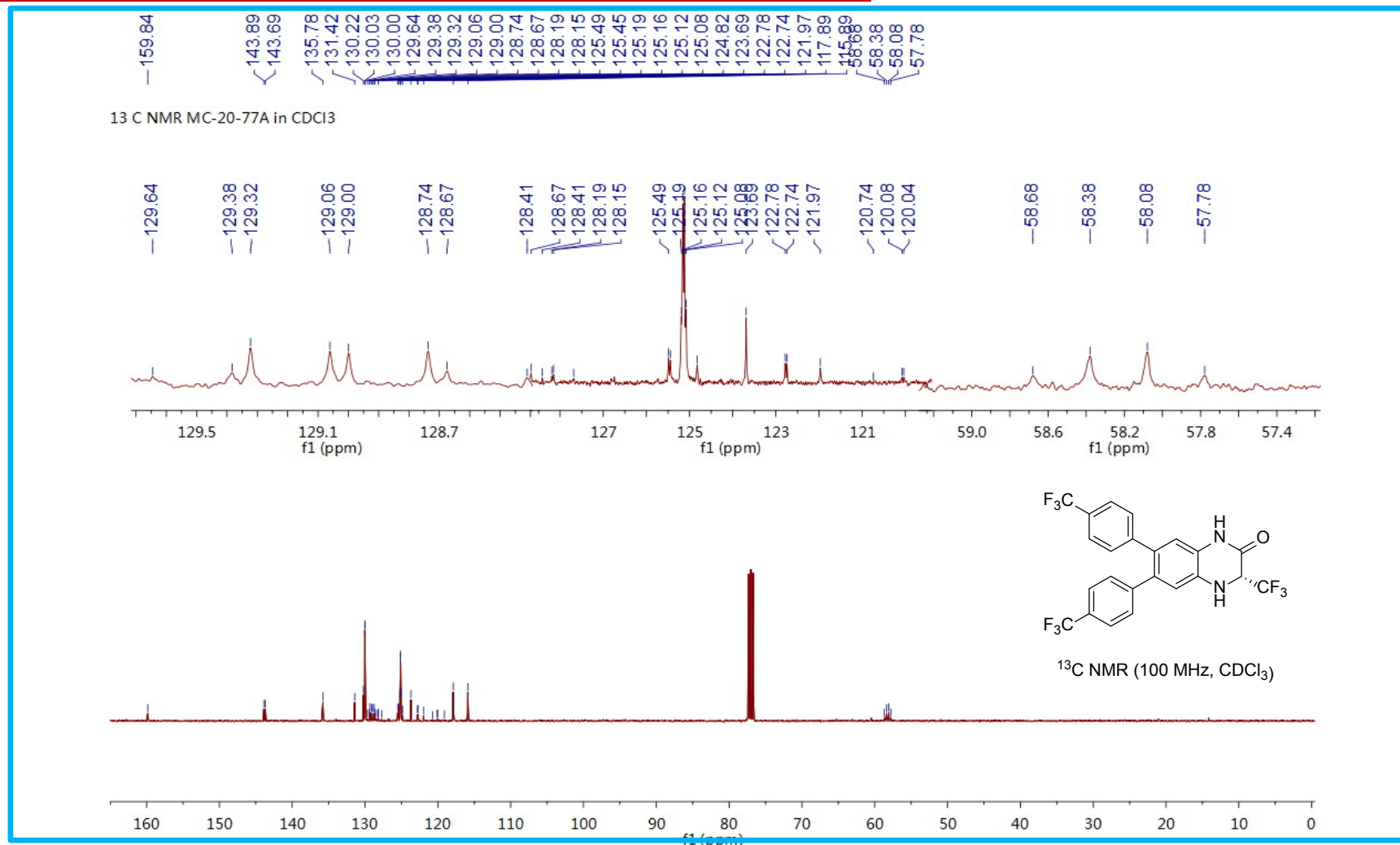
¹⁹F NMR (376 MHz, CDCl₃) $\delta = -62.4, -62.5, -74.2$

代表化合物举例



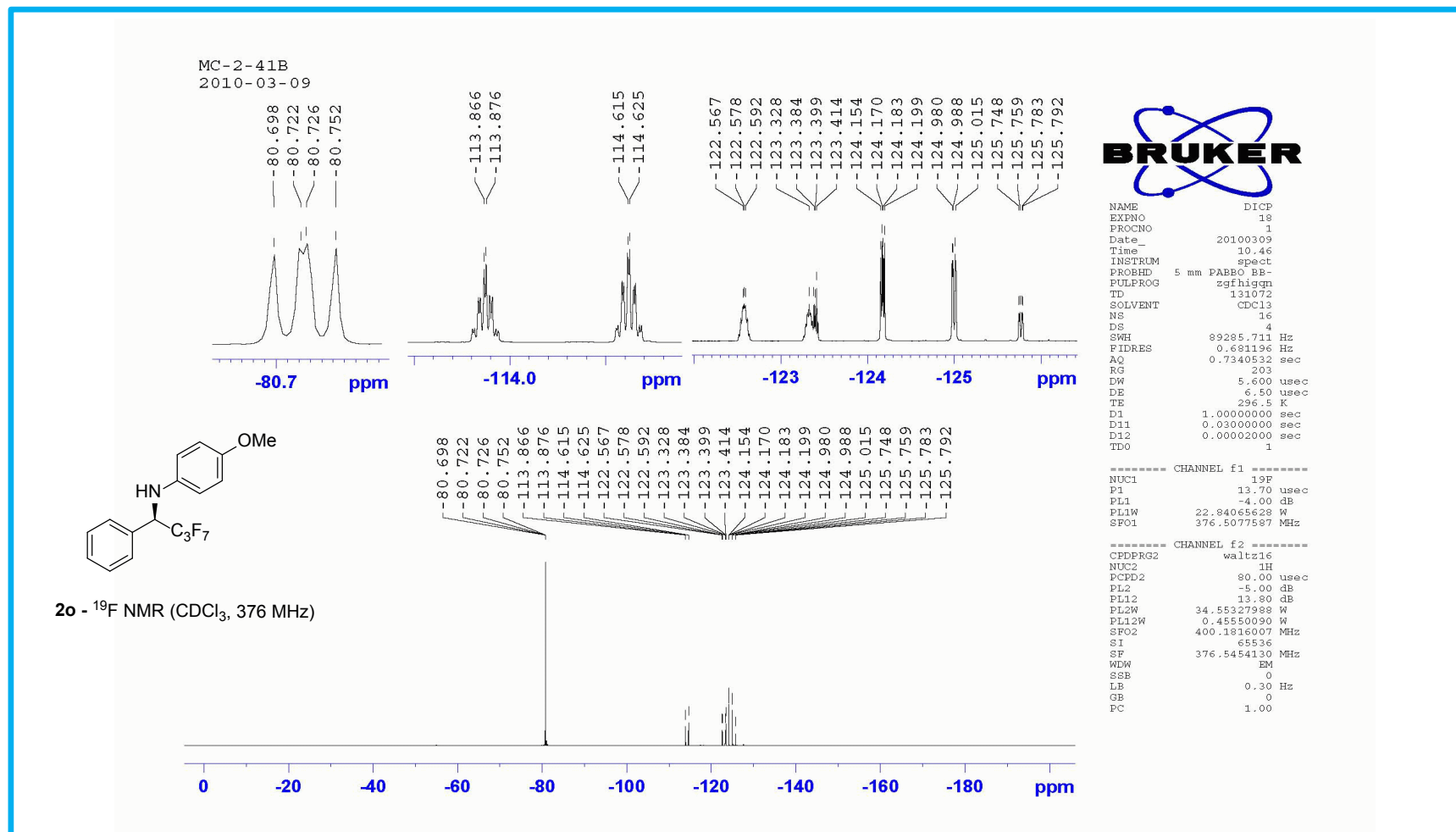
¹H NMR (400 MHz, CDCl₃) δ = 9.23 (brs, 1H), 7.48 (dd, J = 8.2, 3.3 Hz, 4H), 7.19 (dd, J = 10.7, 8.4 Hz, 4H), 6.85 (d, J = 18.5 Hz, 2H), 4.62 (q, J = 7.5 Hz, 1H), 4.59 (brs, 1H)

代表化合物举例



¹³C NMR (100 MHz, CDCl₃) δ = 159.8, 143.9, 143.7, 135.8, 131.4, 130.2, 130.1, 130.0, 129.2 (q, J = 32.0 Hz), 128.9 (q, J = 32.0 Hz), 125.1 (dq, J = 3.0 Hz, 2C), 124.1 (q, J = 271.0 Hz), 124.0 (q, J = 271.0 Hz), 123.7, 123.4 (q, J = 285.0 Hz), 117.9, 115.9, 58.2 (q, J = 30.0 Hz)

代表化合物举例



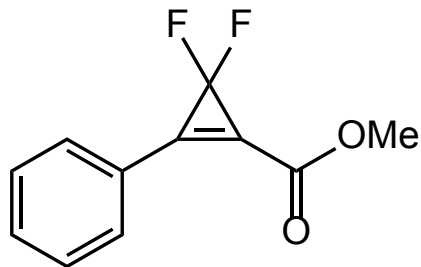
^{19}F NMR (376 MHz, CDCl_3) δ = -80.7 (q, 3F), -113.7 - 113.9 (m, 1F), -114.3-114.7 (m, 1F), -122.2 - 125.8 (m, 2F)

总结

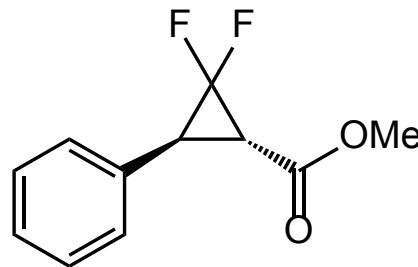
CH₃CH₂CH₂CH₂F: ¹³C NMR δ = 83.9 (d, $^1J_{FC}$ = 165 Hz); ¹⁹F NMR δ = - 219 ppm $^2J_{FH}$ = 47-49 Hz ; $^3J_{FH}$ = 21-27 Hz

CH₃CH₂CH₂CHF₂: ¹³C NMR δ = 117.6 (t, $^1J_{FC}$ = 239 Hz); ¹⁹F NMR δ = - 116.4 ppm (d of t, $^2J_{FH}$ = 58 Hz, $^3J_{FH}$ = 16.6 Hz)

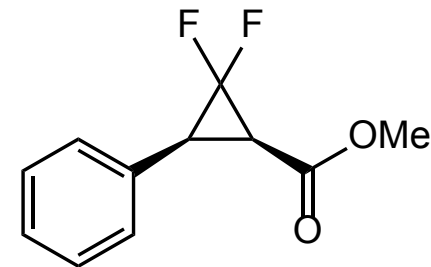
CH₃CH₂CH₂CF₃: ¹³C NMR δ = 127.5 (q, $^1J_{FC}$ = 276 Hz); ¹⁹F NMR δ = - 68 ppm (t, $^3J_{FH}$ = 11 Hz)



¹³C NMR δ = 98.85 (t, J = 276.4 Hz)
¹⁹F NMR δ = - 107.7

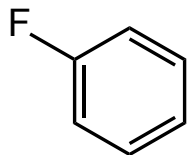


¹³C NMR δ = 110.7 (dd, J = 294.7, 287.7 Hz); ¹⁹F NMR δ = - 132.9 (d, J = 151.6 Hz), - 134.1 (d, J = 151.6 Hz)

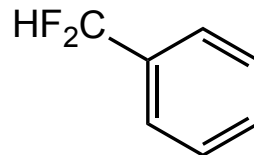


¹³C NMR δ = 111.3 (dd, J = 291 Hz and J = 285 Hz), ¹⁹F NMR δ = - 118.0 (d, J = 158 Hz), - 146.2 (d, J = 159 Hz).

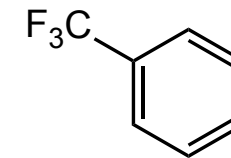
总结



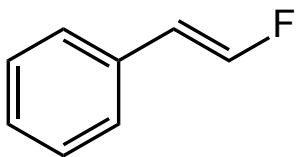
^{13}C NMR $\delta = 162.8$ (d, $J = 246.9$ Hz)
 ^{19}F NMR $\delta = -112.3$



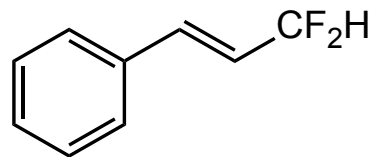
^{13}C NMR $\delta = 130.8$ (t, $J = 22.9$ Hz),
114.6 (t, $J = 238$ Hz); ^{19}F NMR
 $\delta = -109.28$ (d, $J = 56.6$ Hz)



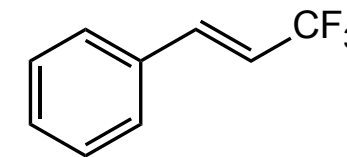
^{13}C NMR $\delta = 130.3$ (q, $J = 32.5$
Hz), 123.9 (q, $J = 272.7$ Hz);
 ^{19}F NMR $\delta = -62.7$



^{13}C NMR $\delta = 145.4$ (d, $J = 277$ Hz),
110.4 (d, $J = 19$ Hz), ^{19}F NMR $\delta = -$
113.1 (d, $J = 83$ Hz)



^{13}C NMR $\delta = 114.9$ (t, $J = 235.5$ Hz),
126.7 (t, $J = 22.6$ Hz); ^{19}F NMR
 $\delta = -108.2$ (d, $J = 57.4$ Hz,)



^{13}C NMR $\delta = 124.9$ (q, $J = 268.8$
Hz), 115.9 (q, $J = 33.8$ Hz); ^{19}F
NMR $\delta = -63.8$ (dd, $J = 6.5, 2.2$ Hz)

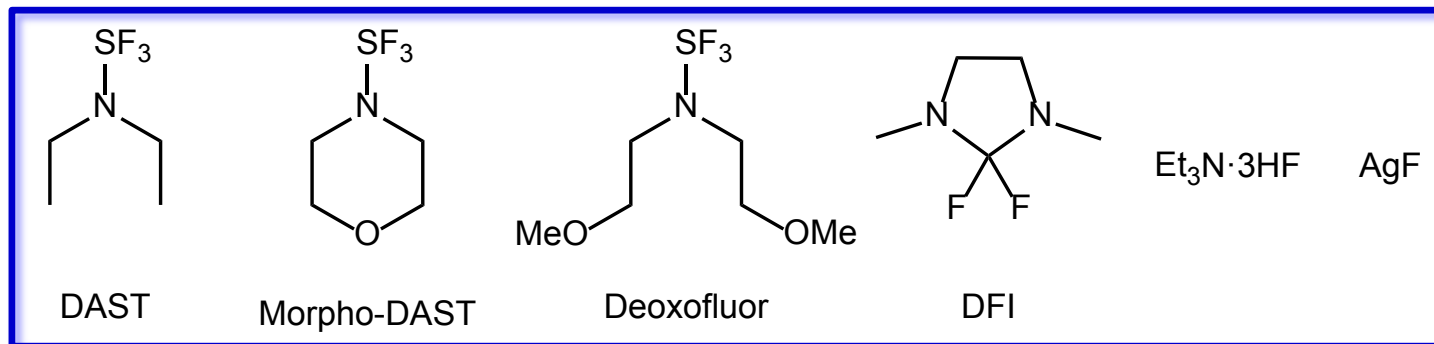
致 谢

本课件内容部分参考了上海有机所卿凤翎, 胡金波等老师的授课课件, 在此对所有有机所及国内从事氟化学研究的老师们表示敬意与感谢!

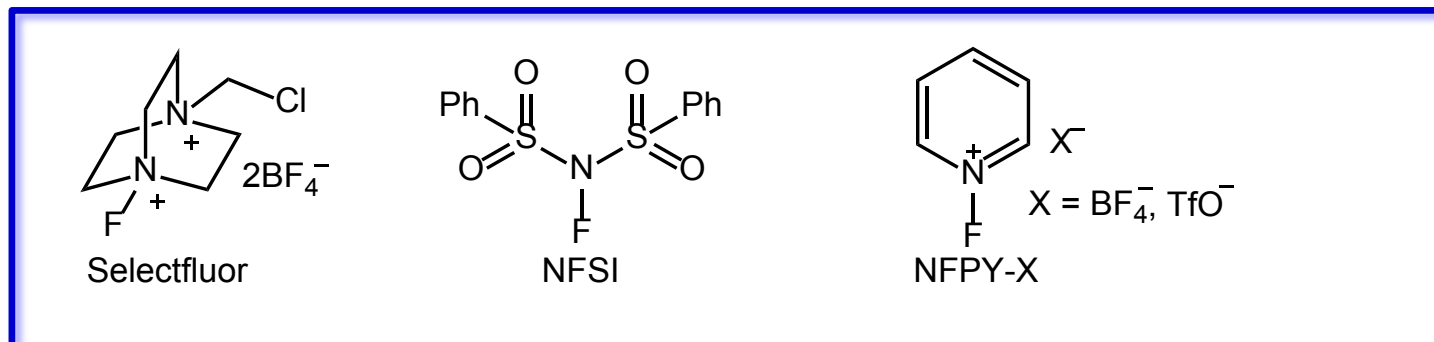


氟试剂

亲核氟化试剂

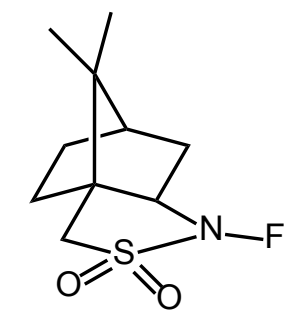


亲电氟化试剂

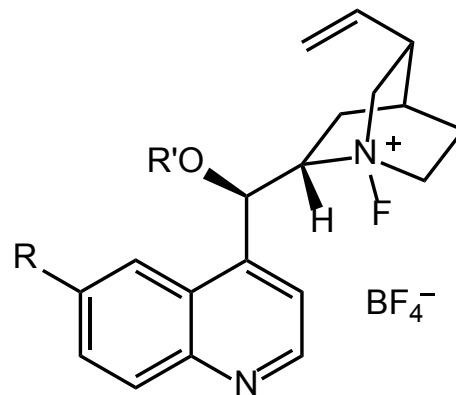


氟试剂

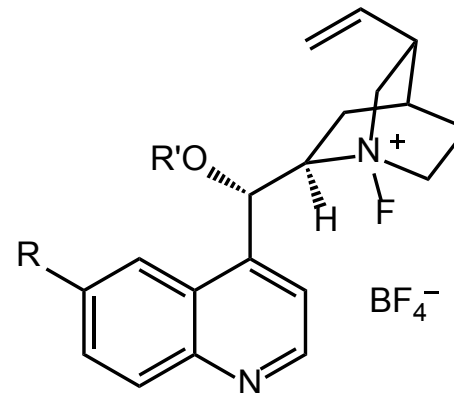
手性亲电氟化试剂



Differding & Lang

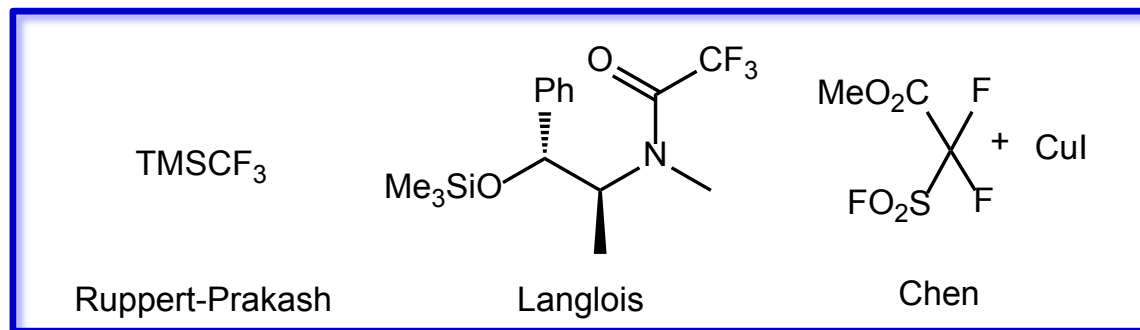


Cahard & Shibata

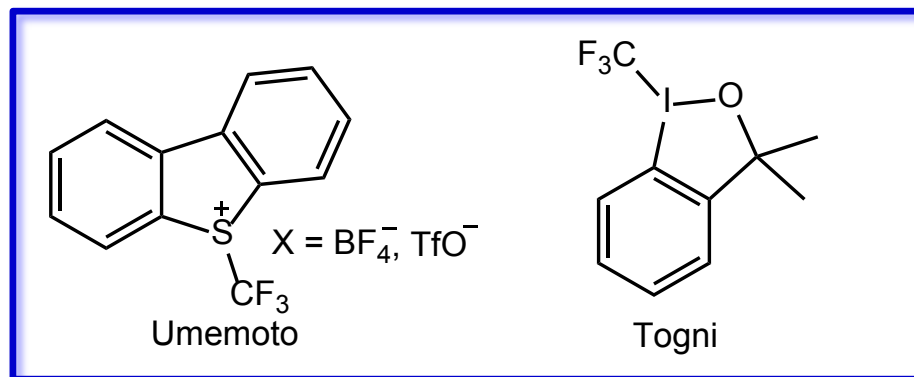


氟试剂

亲核三氟甲基化试剂

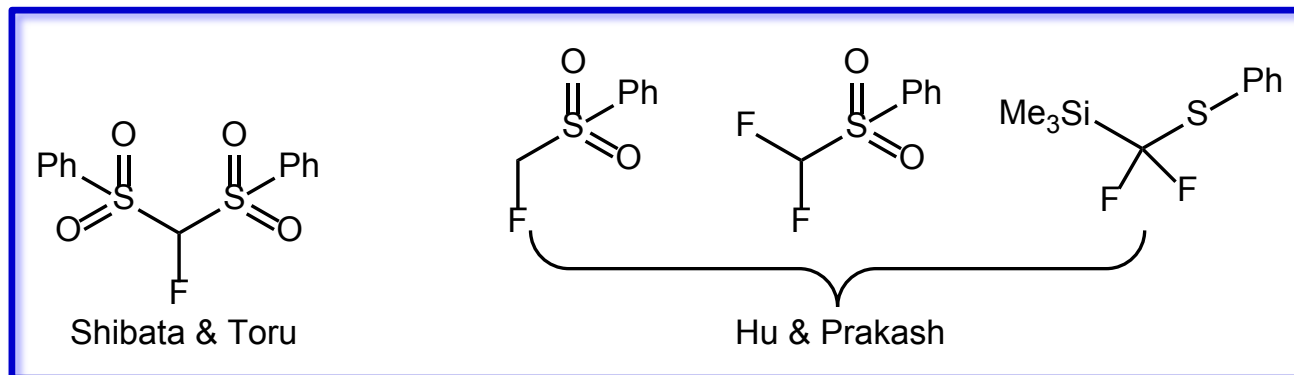


亲电三氟甲基化试剂



氟试剂

亲核单、双氟甲基化试剂



亲电双氟甲基化试剂

