

Supporting Information for

Halolactones are Potent HIV-1 Non-Nucleoside Reversed Transcriptase Inhibitors

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I NMR Spectra of 13 and 14

II HPLC of 13f, 13g, 13i and 14b

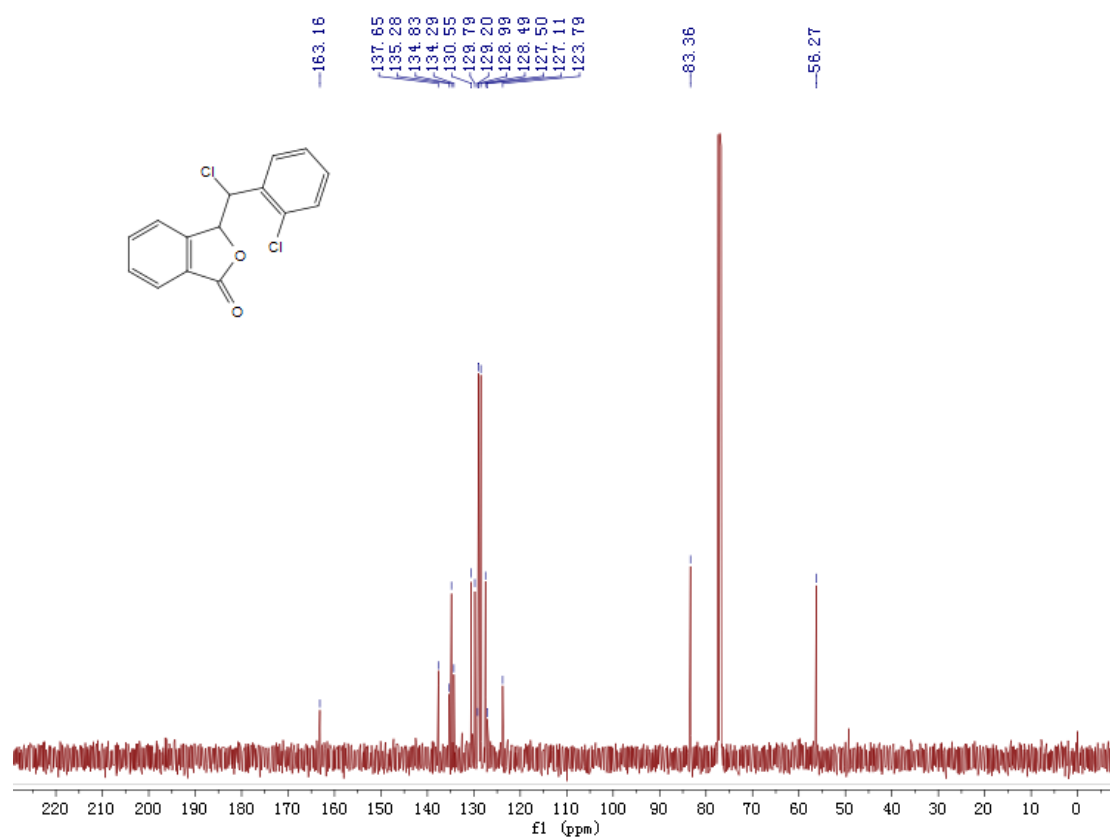
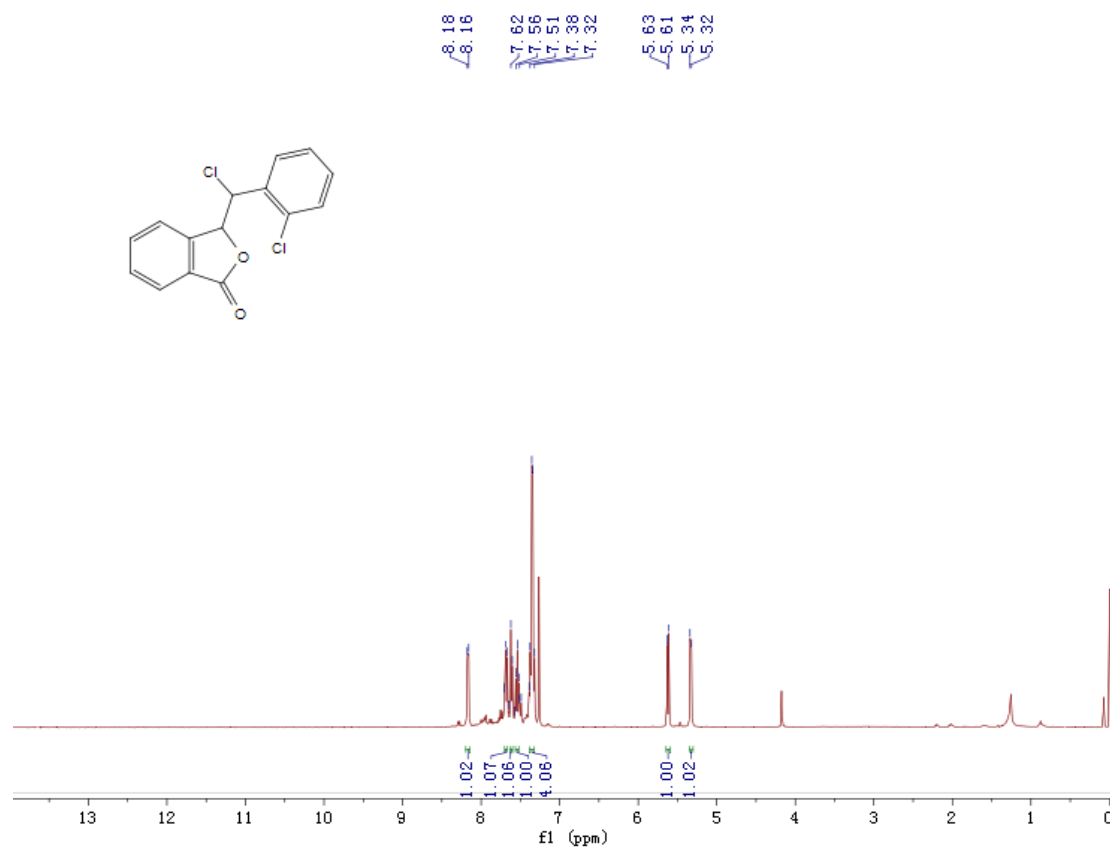
III X-ray crystallographic for 13k

* Prof. Hai-Bing Zhou, Tel.: +86-27-68759586; fax: +86-27-68759850; e-mail: zhouhb@whu.edu.cn

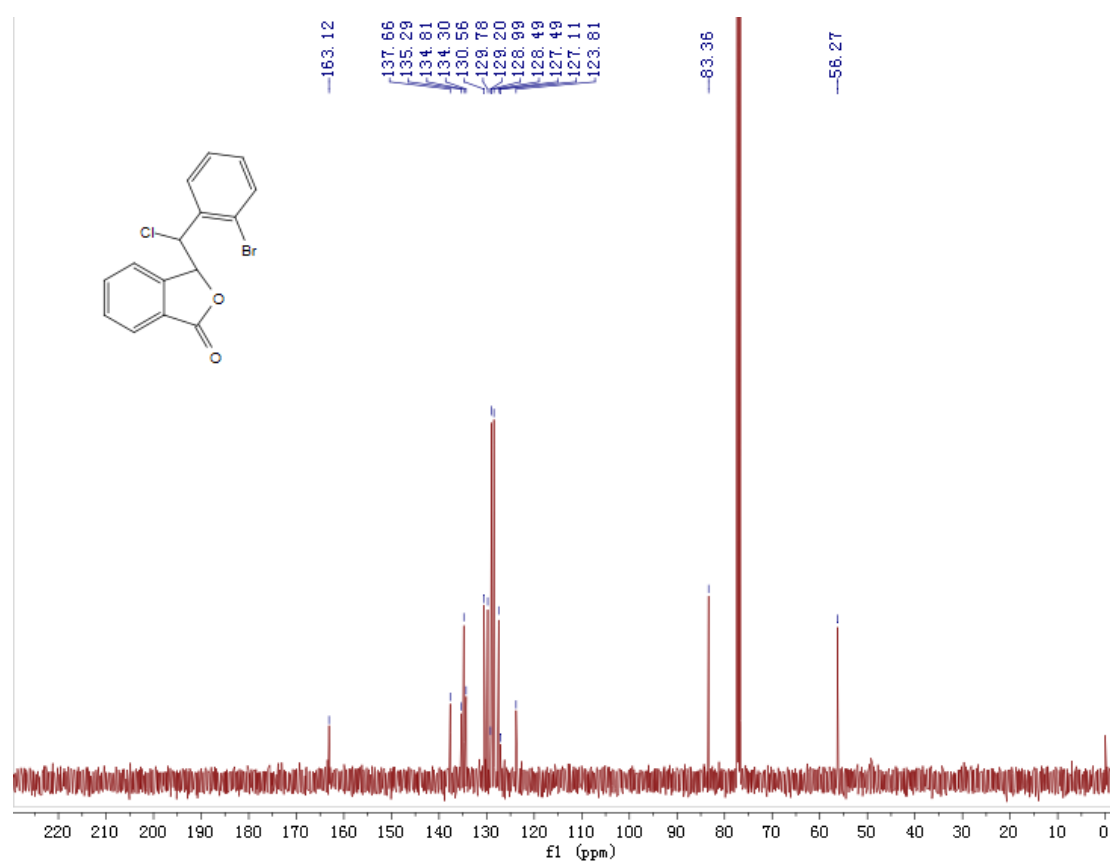
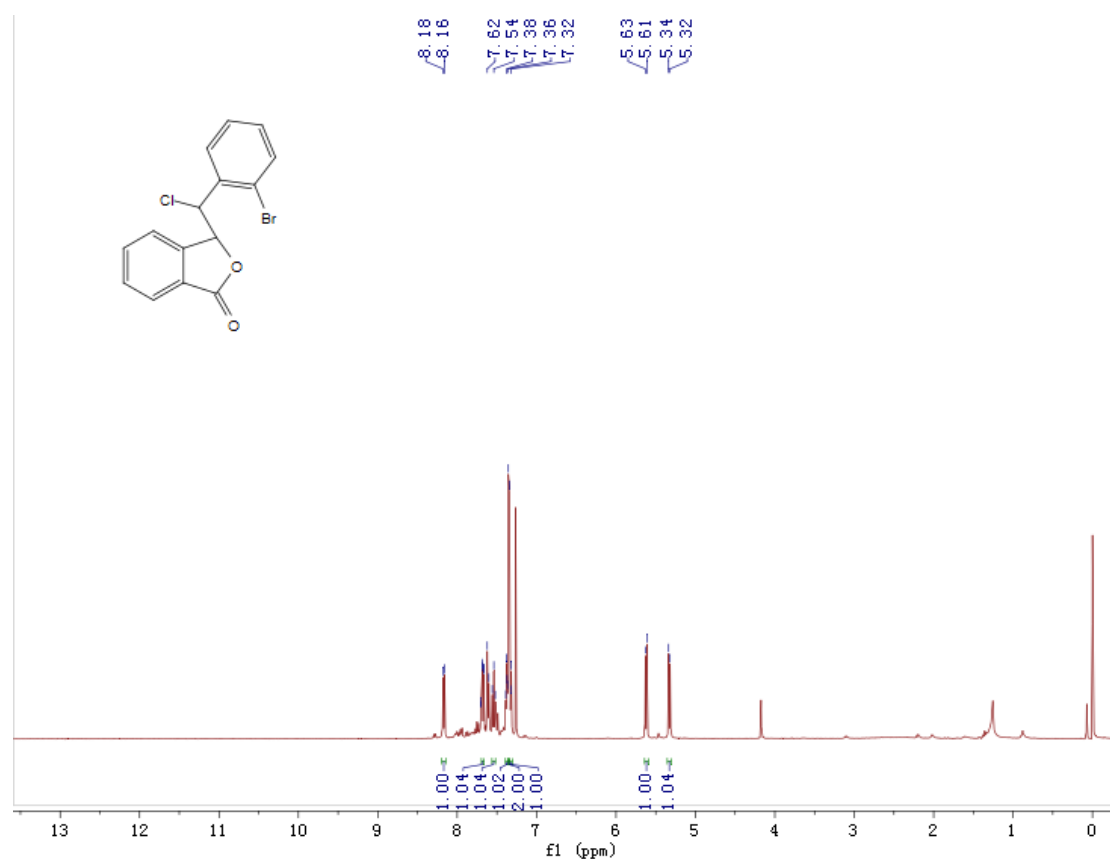
* Prof. Shuwen Wu, Tel.: +86-27-68759586; fax: +86-27-68759586; e-mail: shuwenwu@hotmail.com

I NMR Spectra of 13 and 14

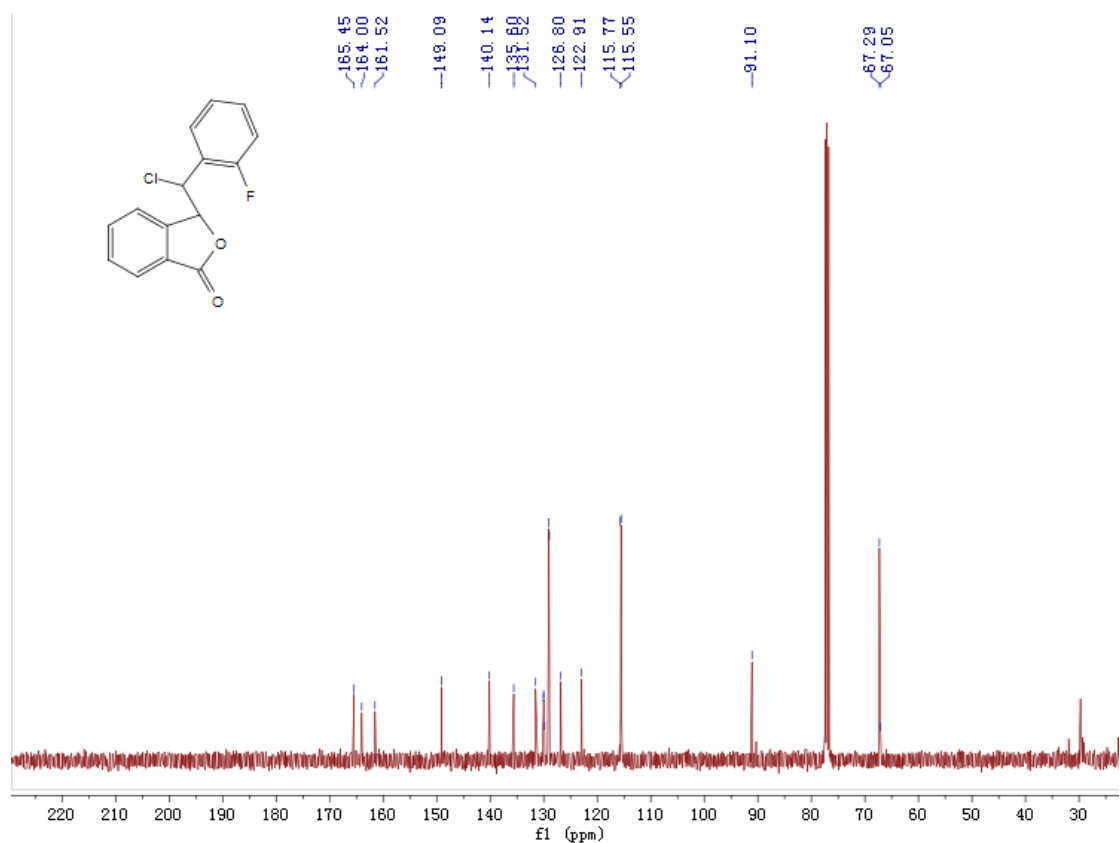
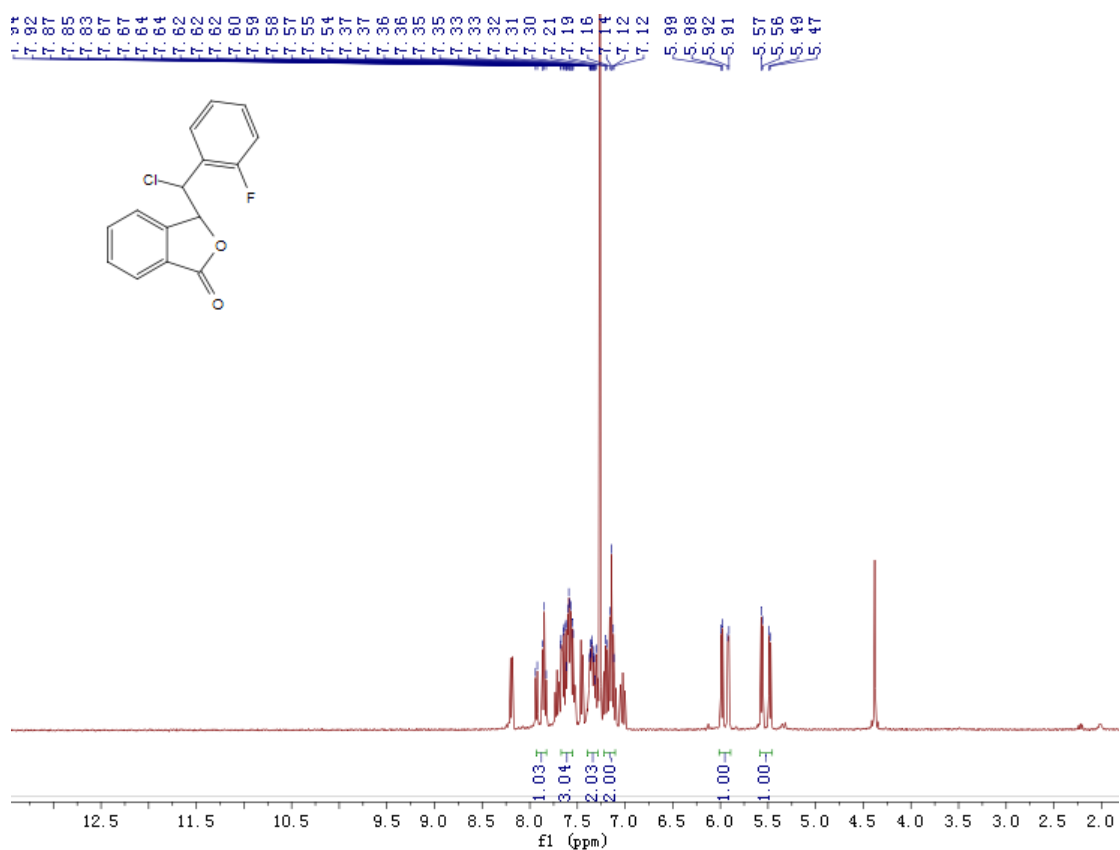
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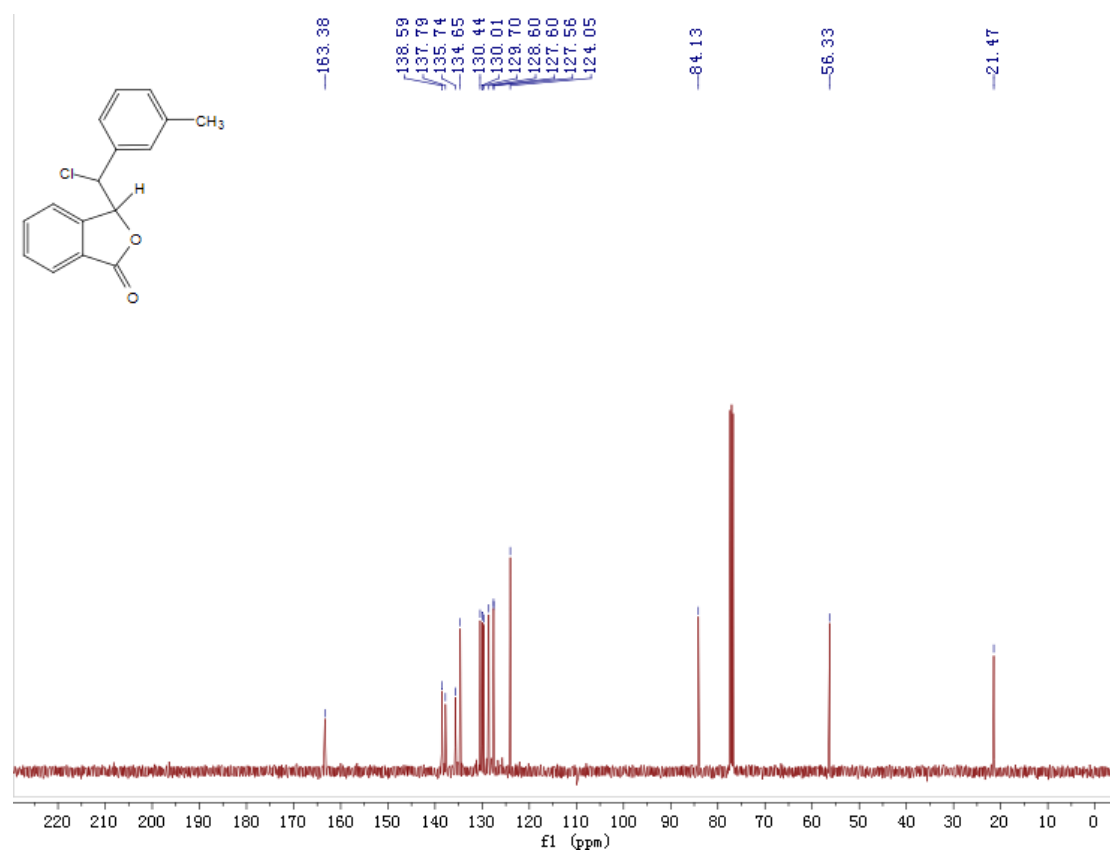
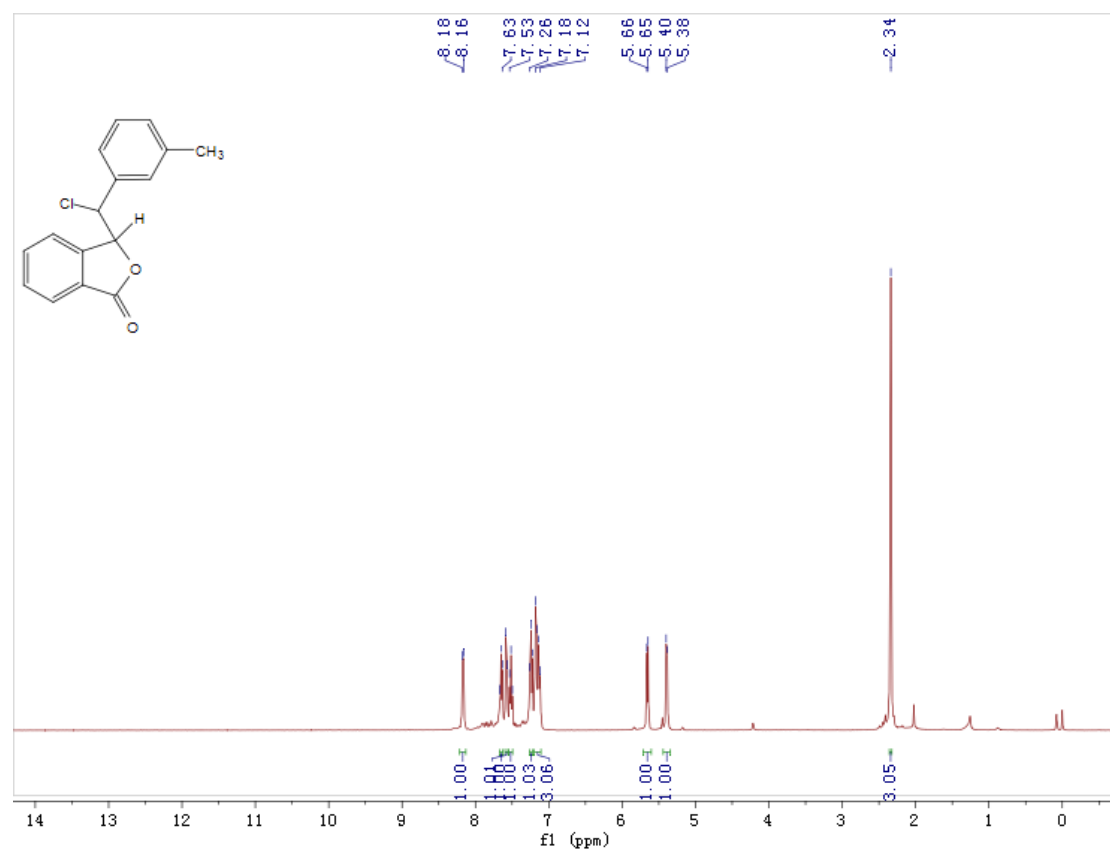
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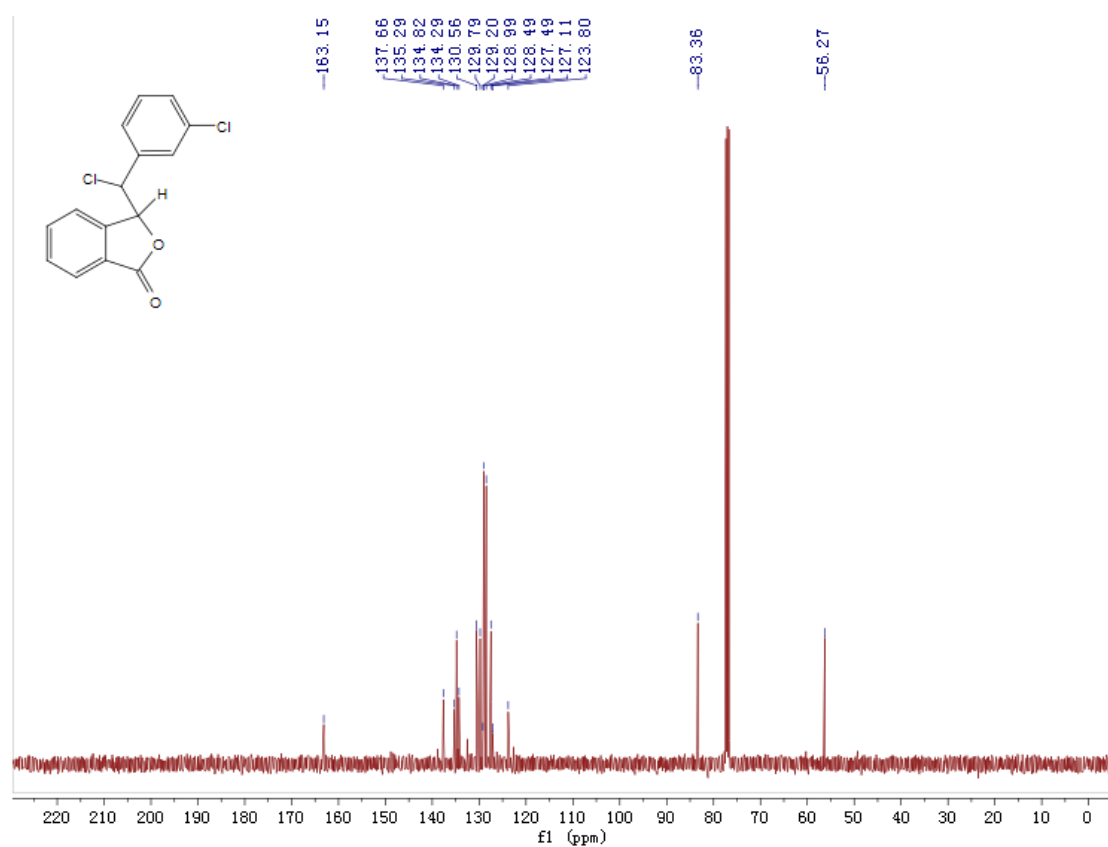
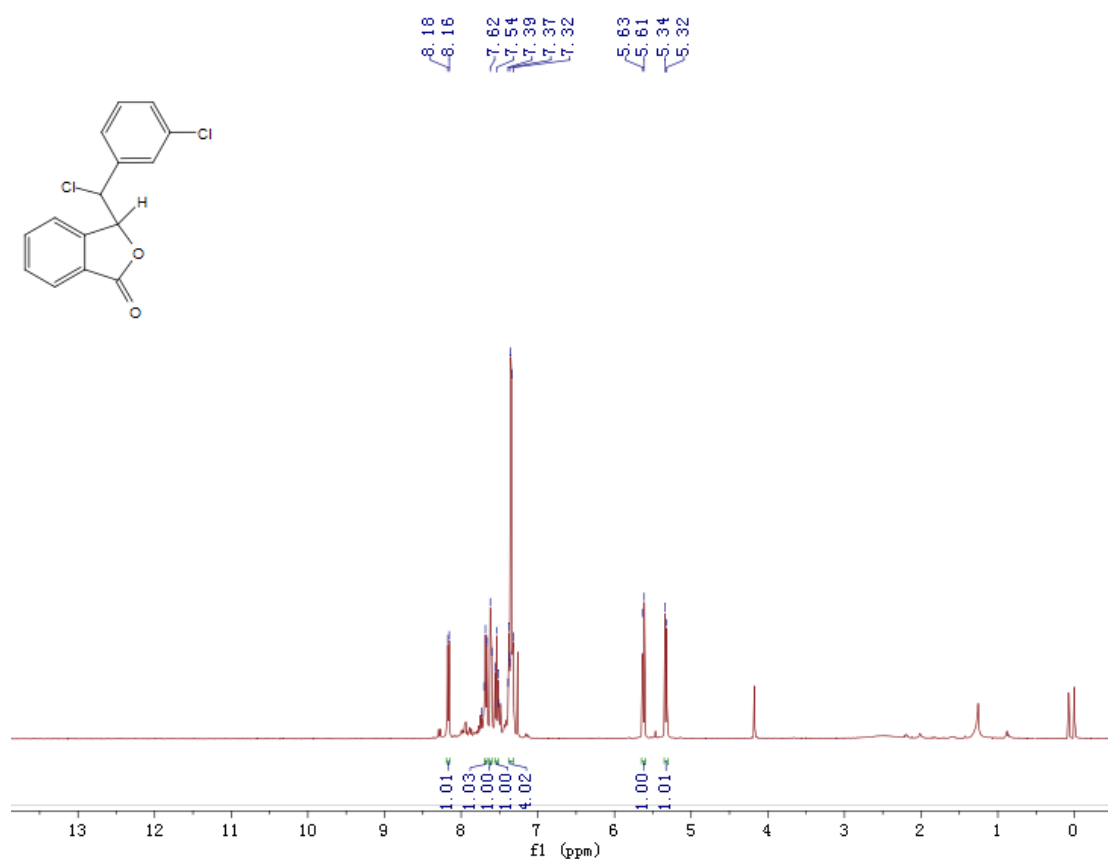
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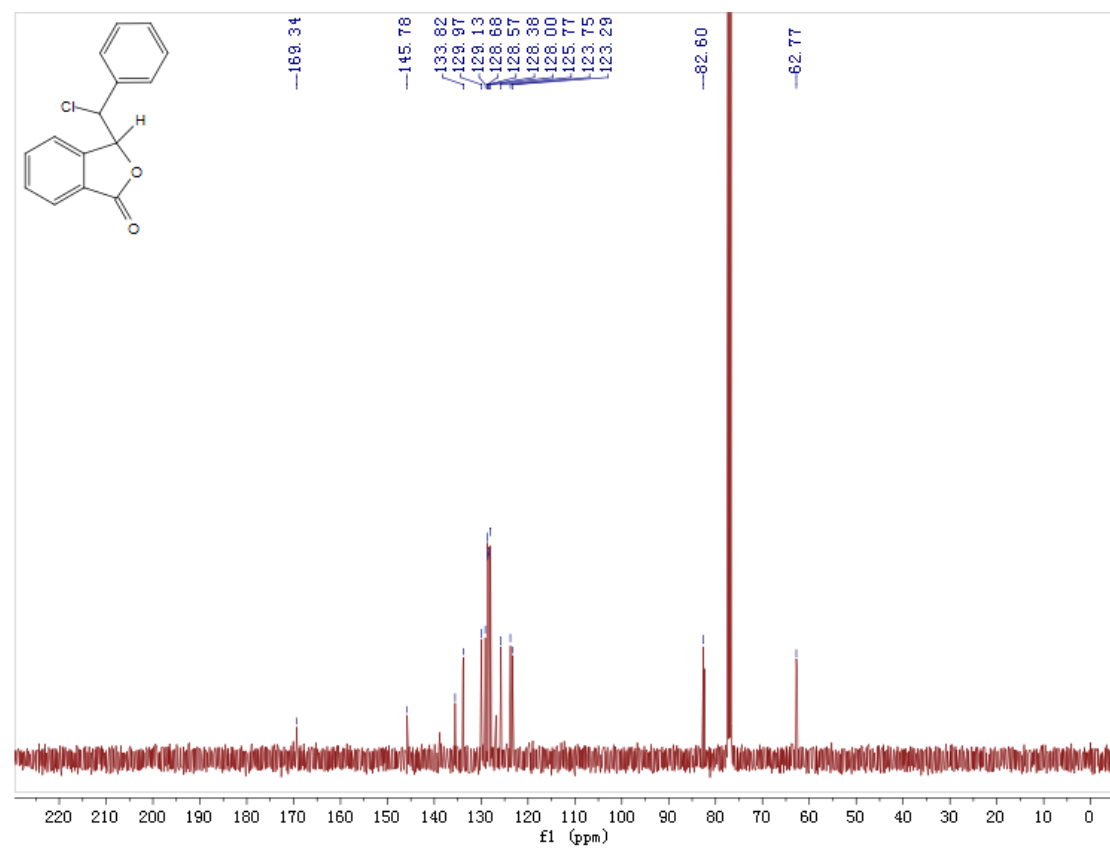
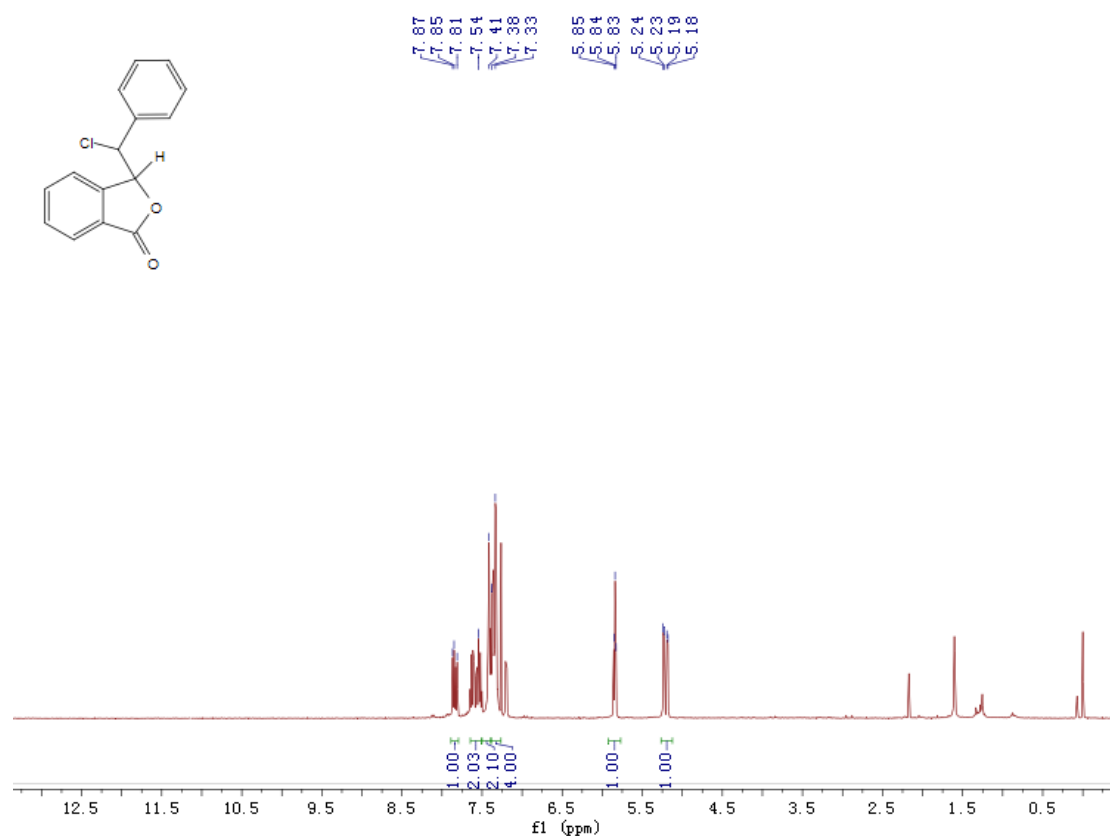
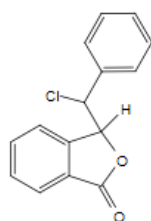
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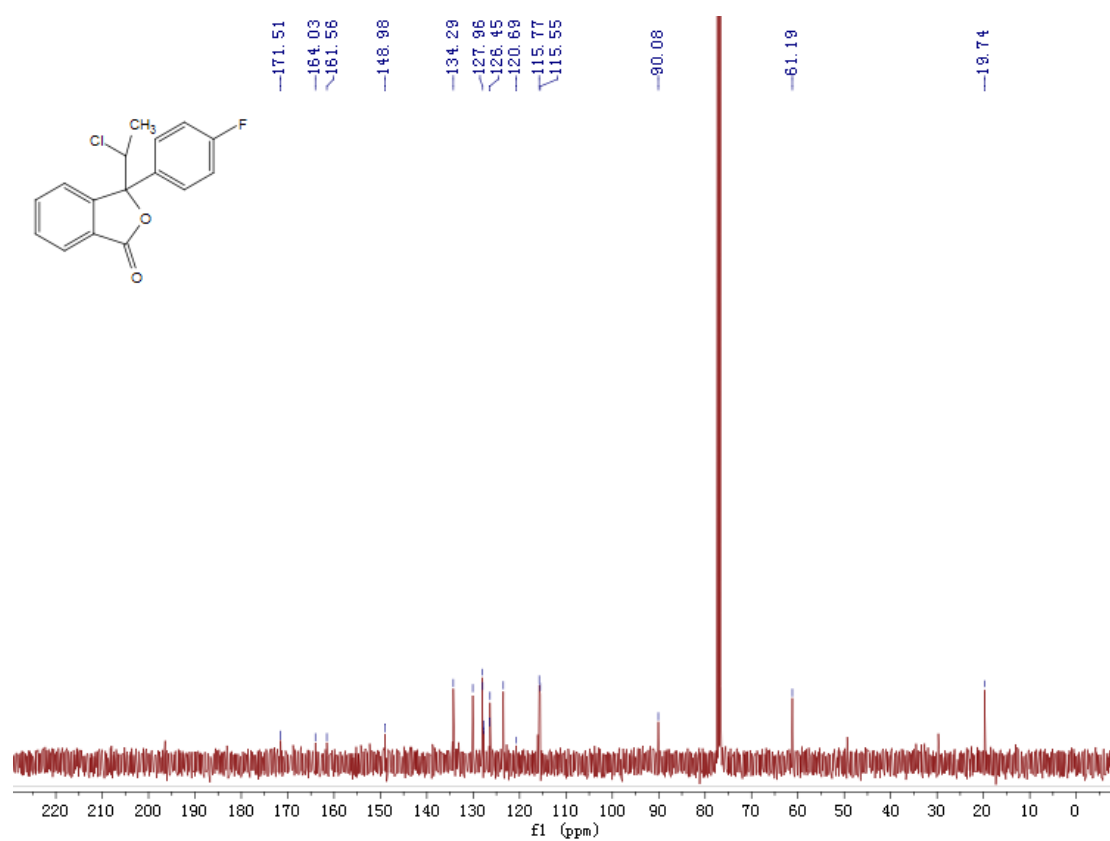
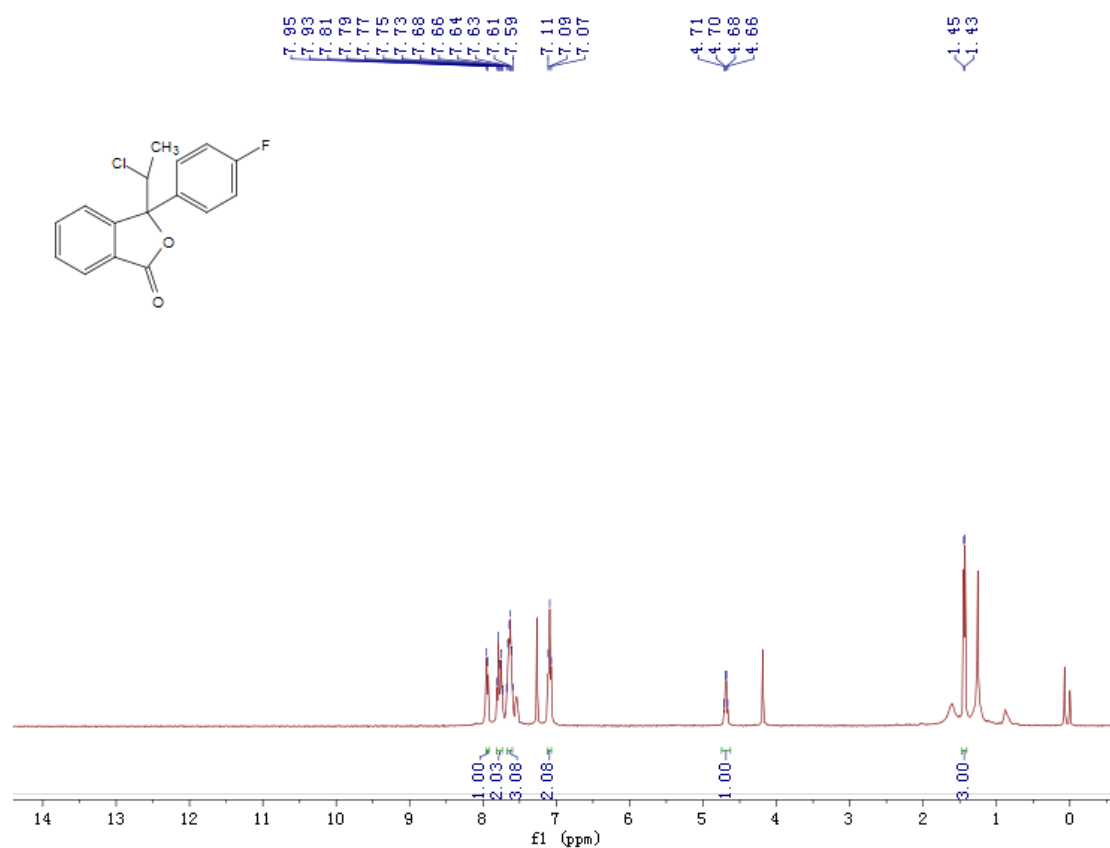
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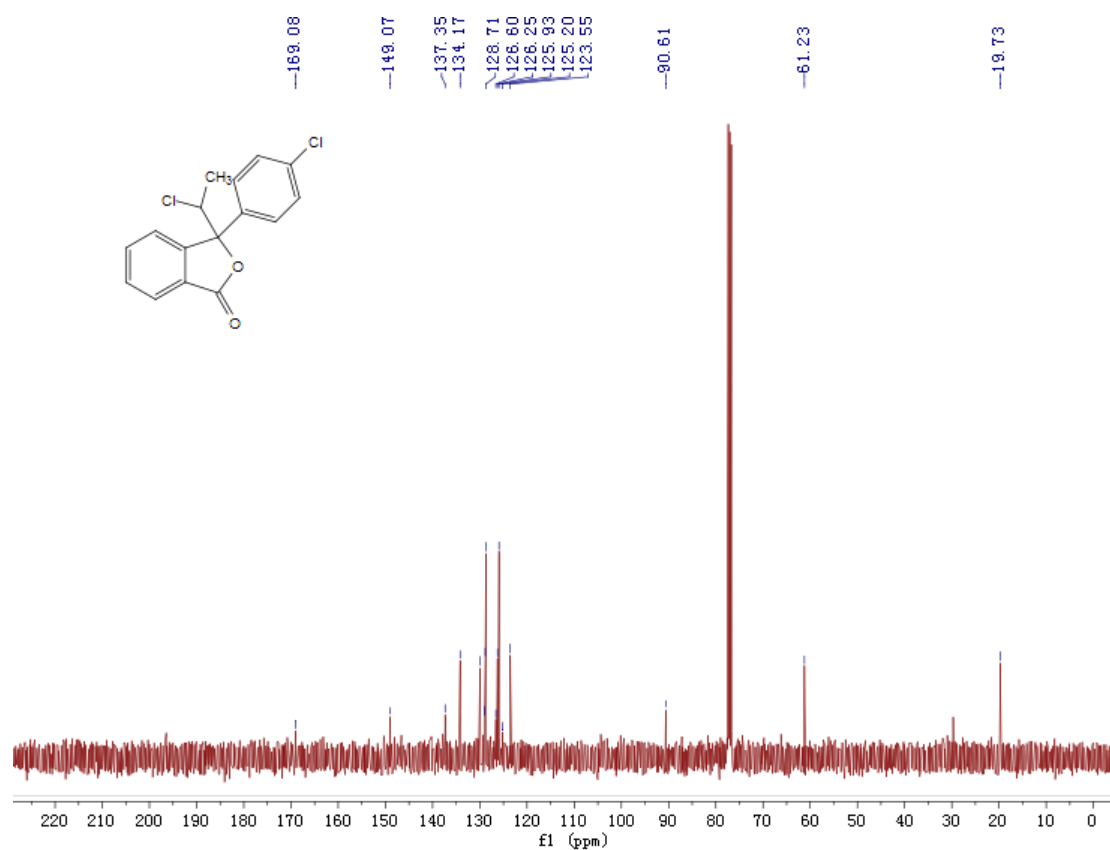
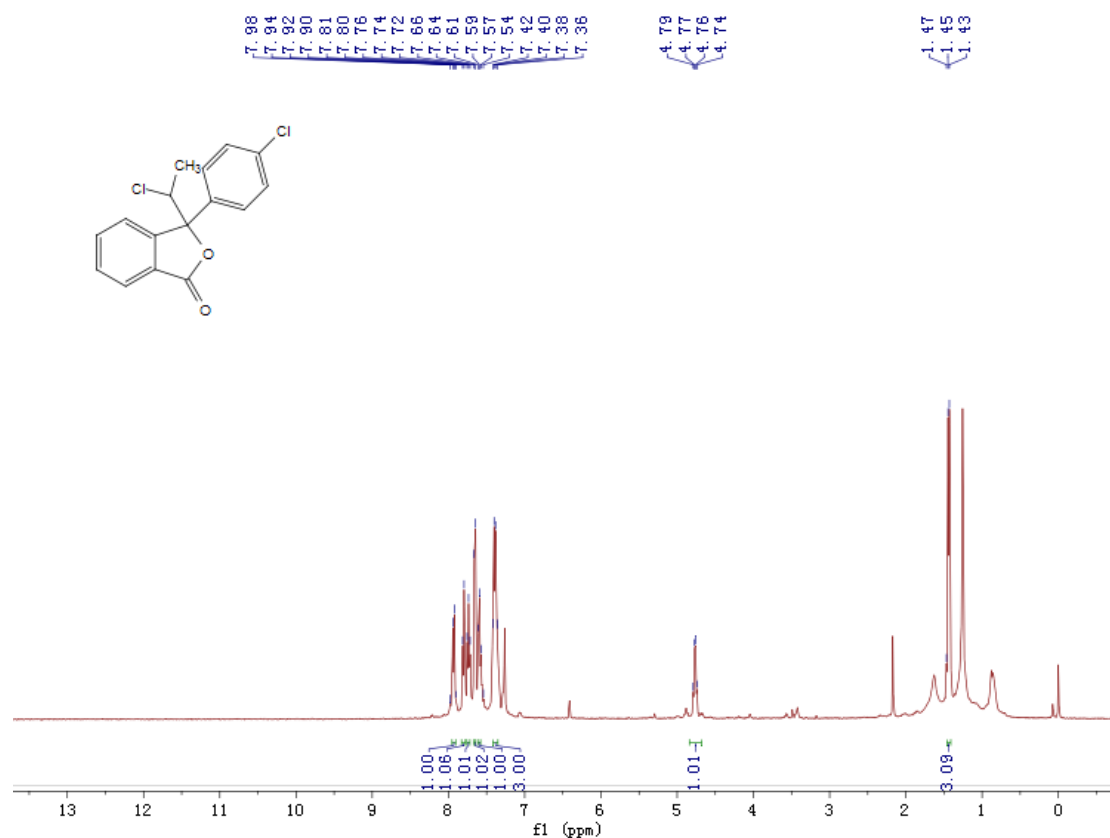
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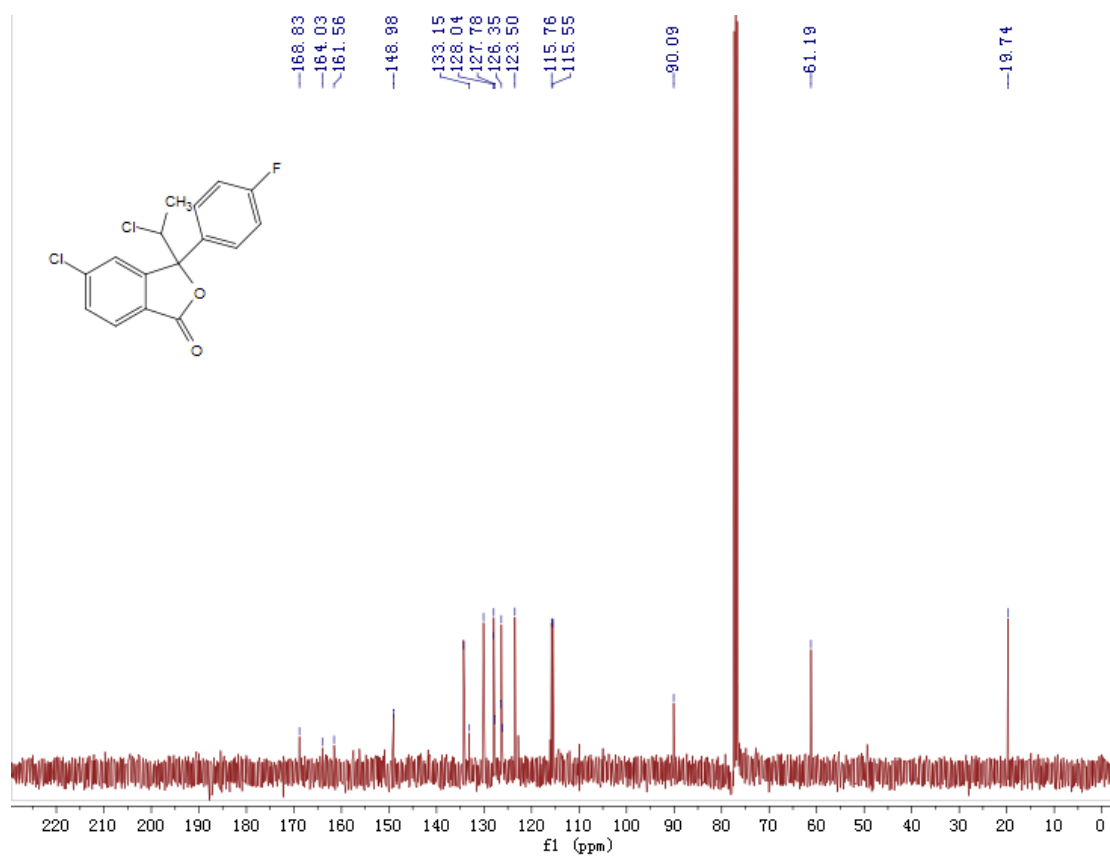
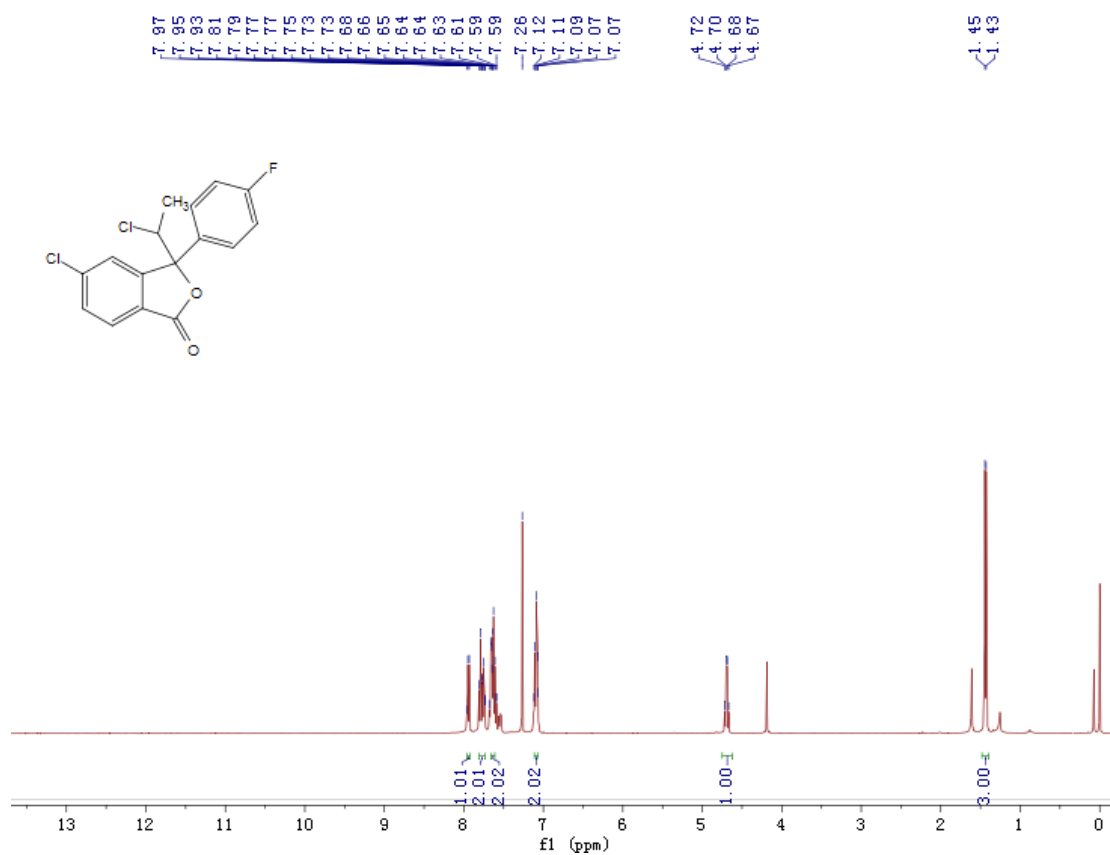
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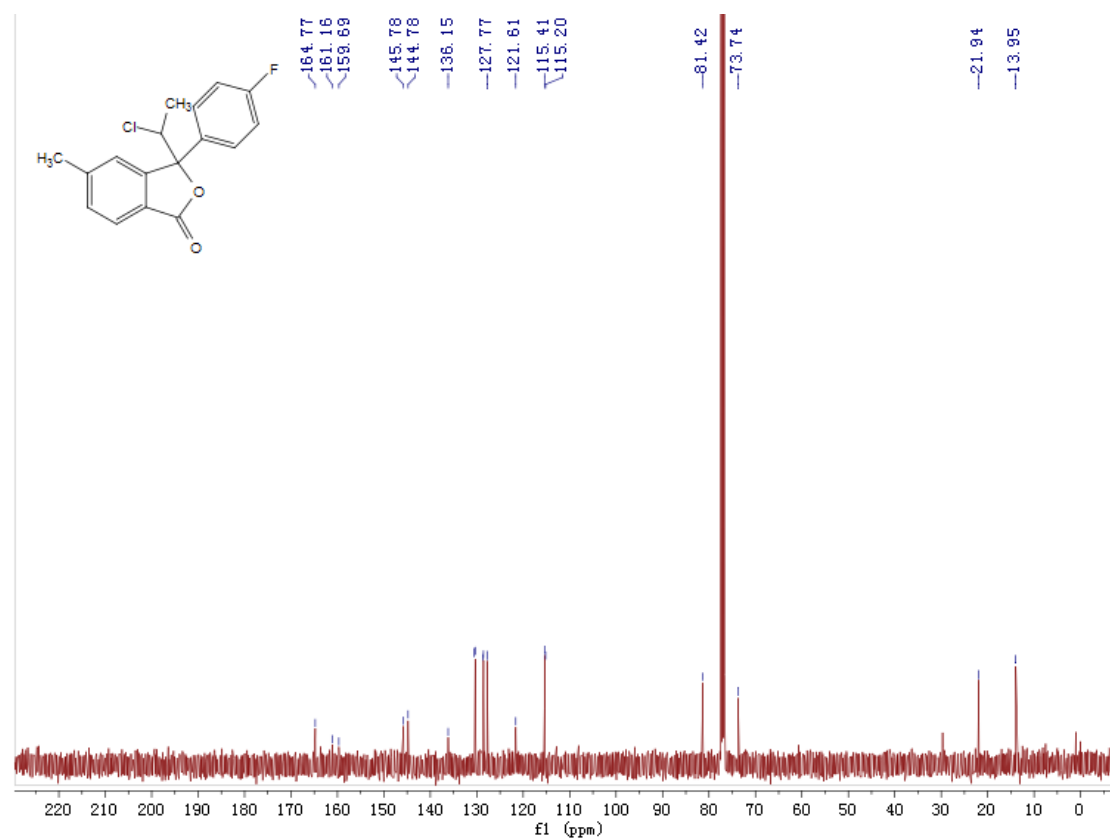
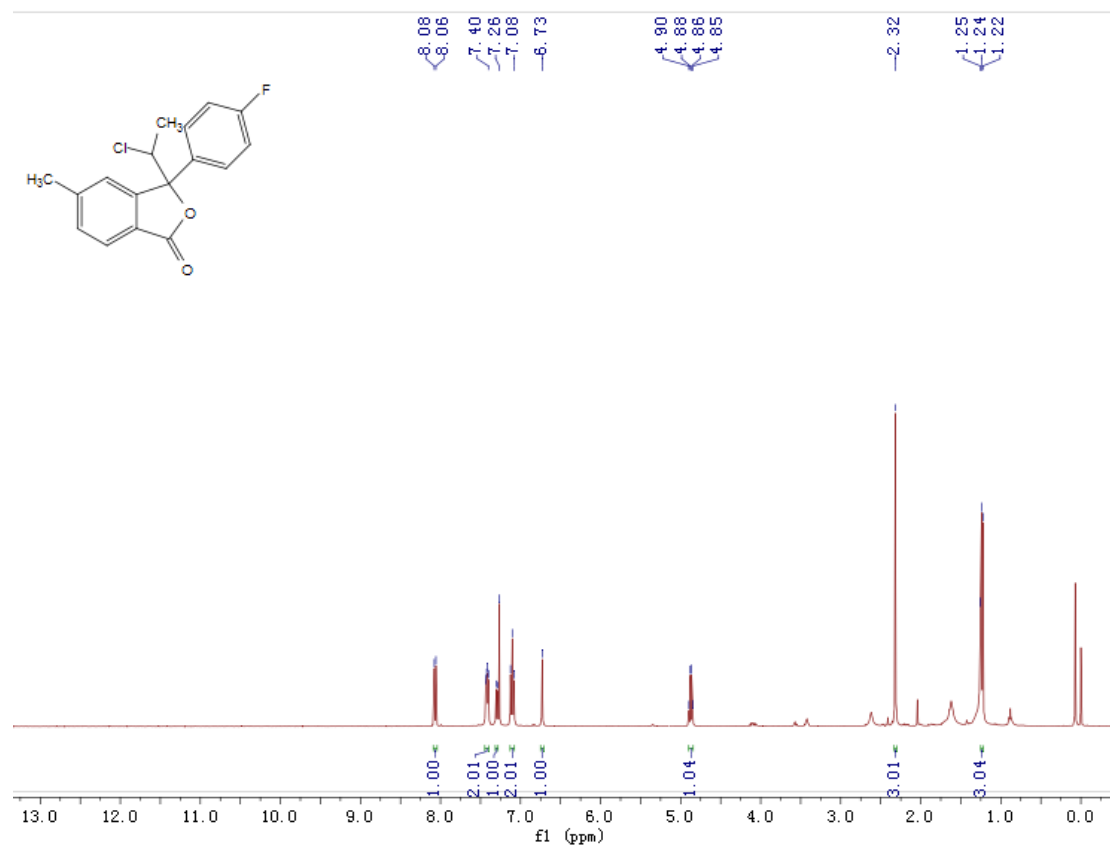
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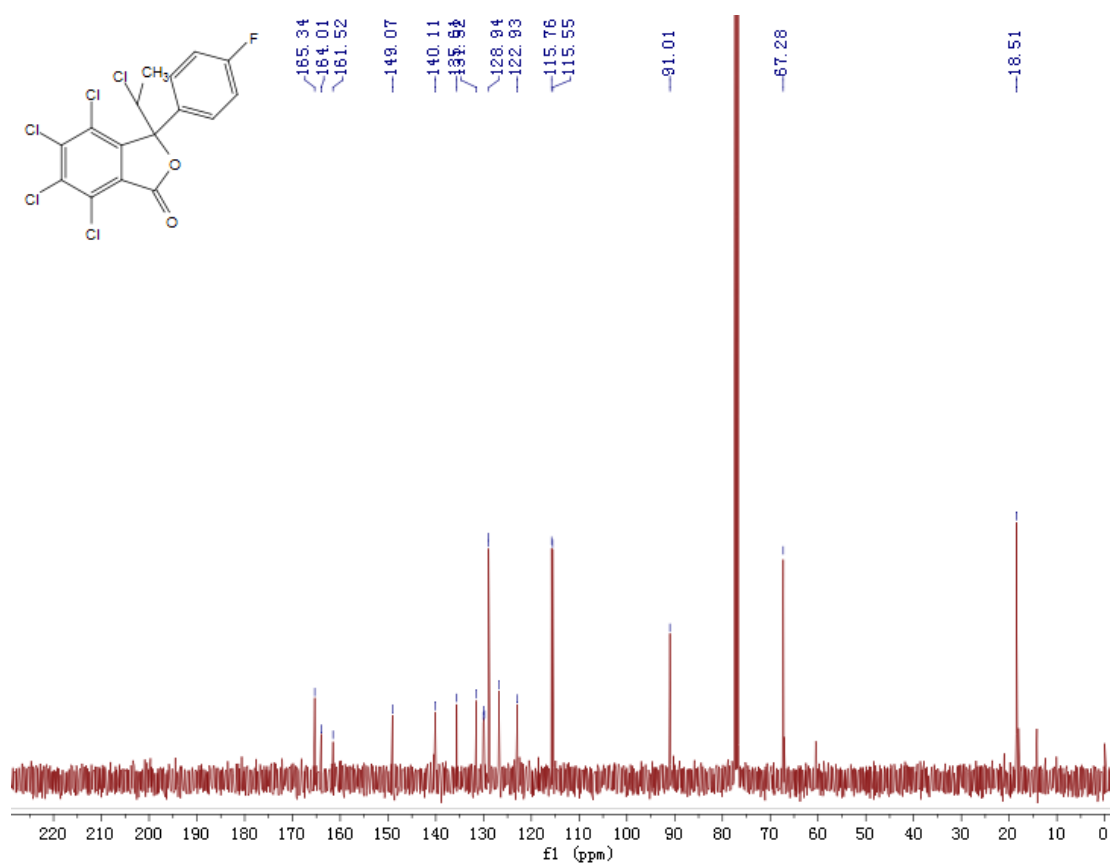
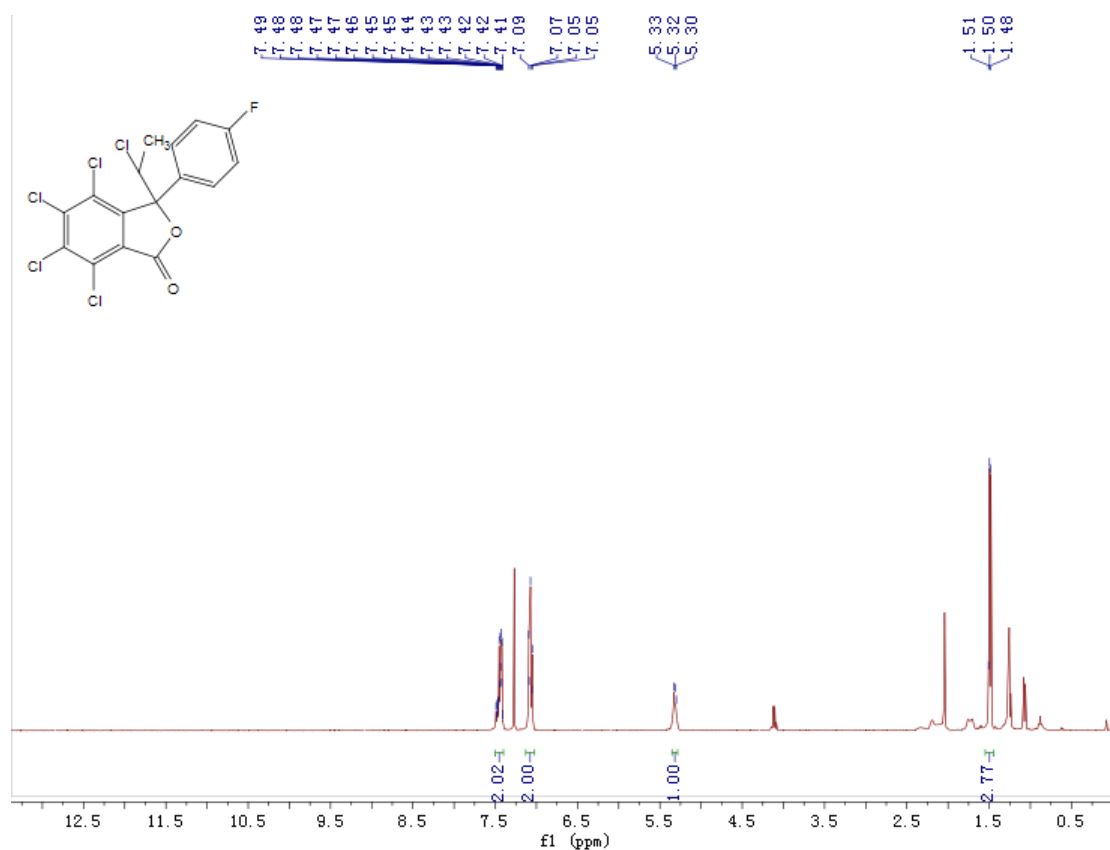
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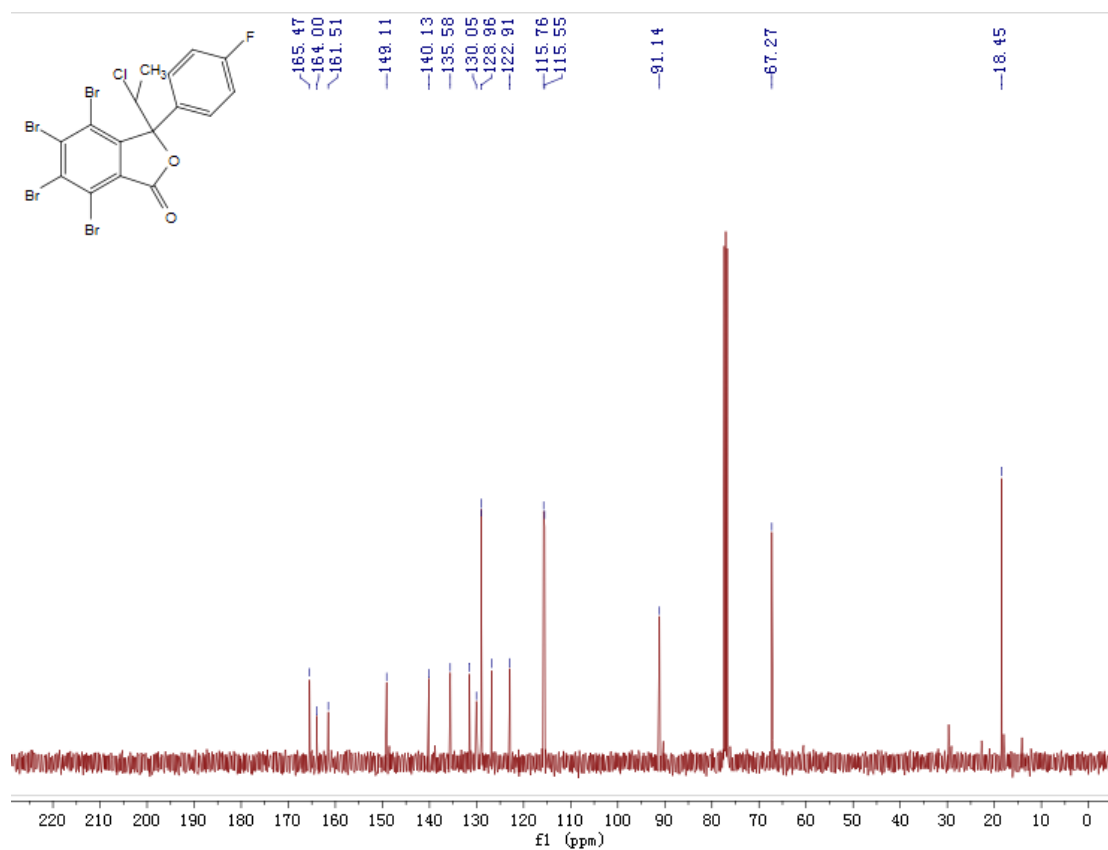
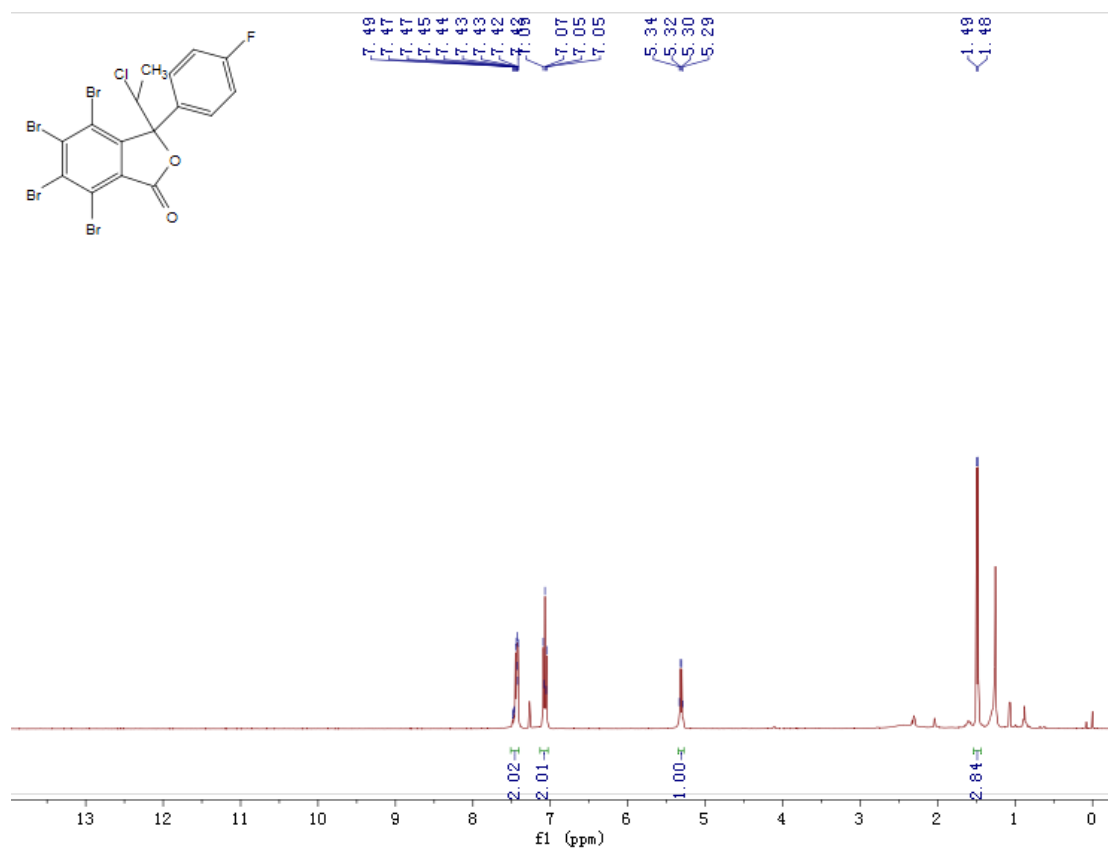
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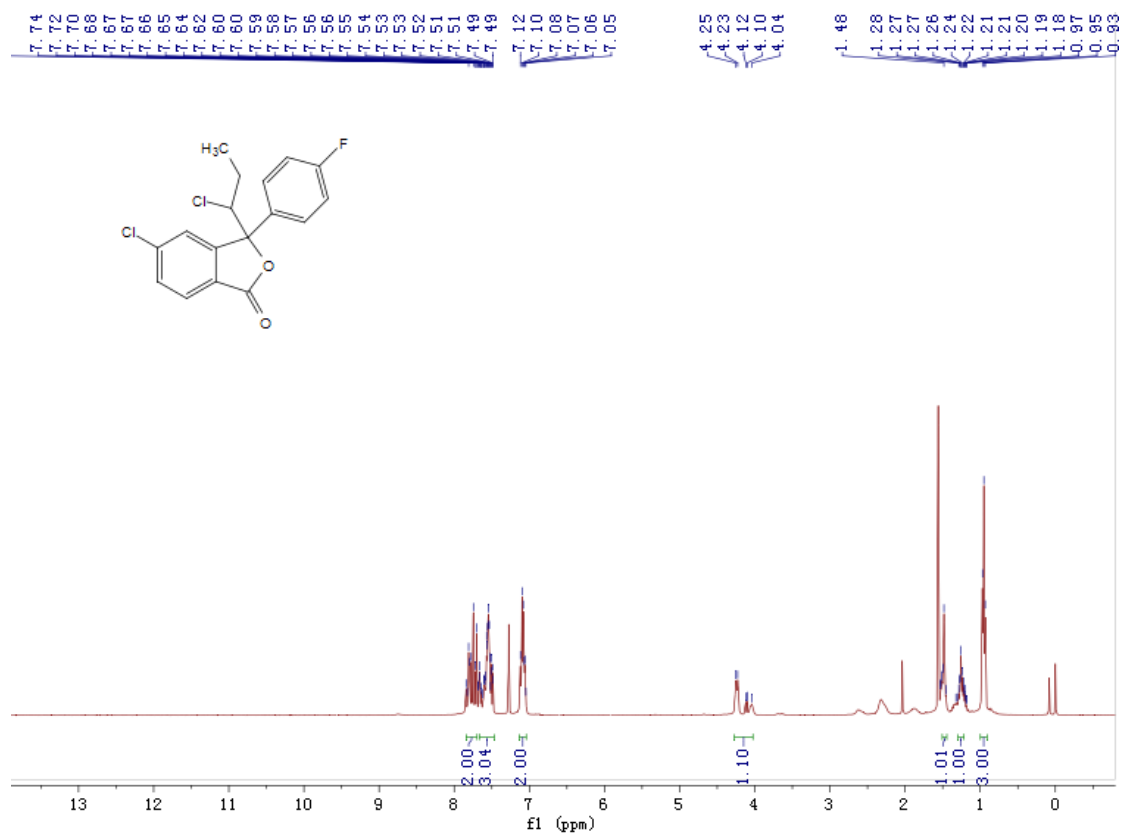
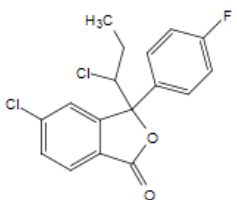
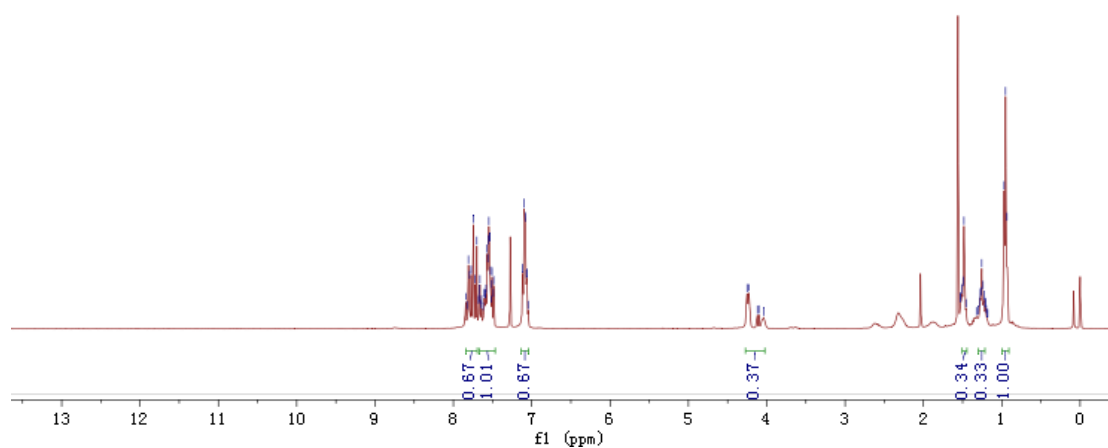
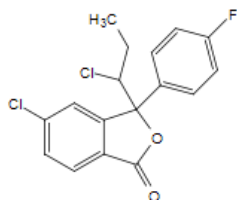
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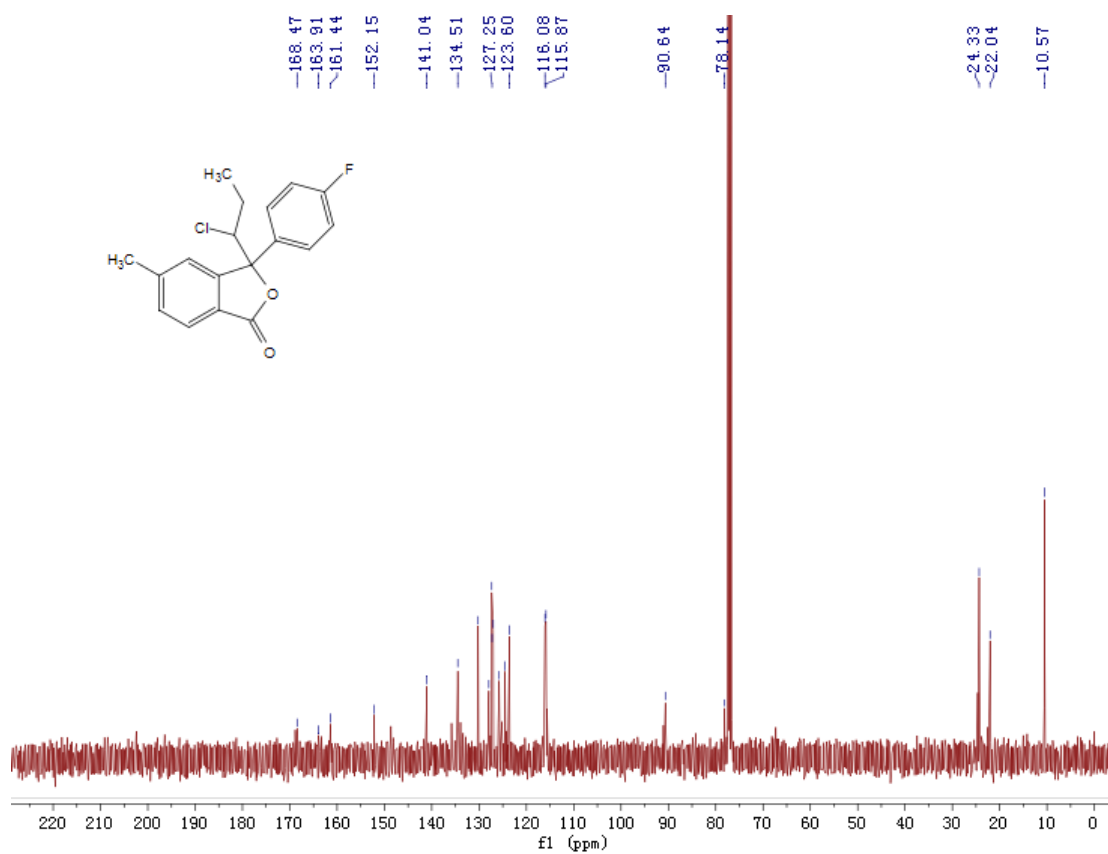
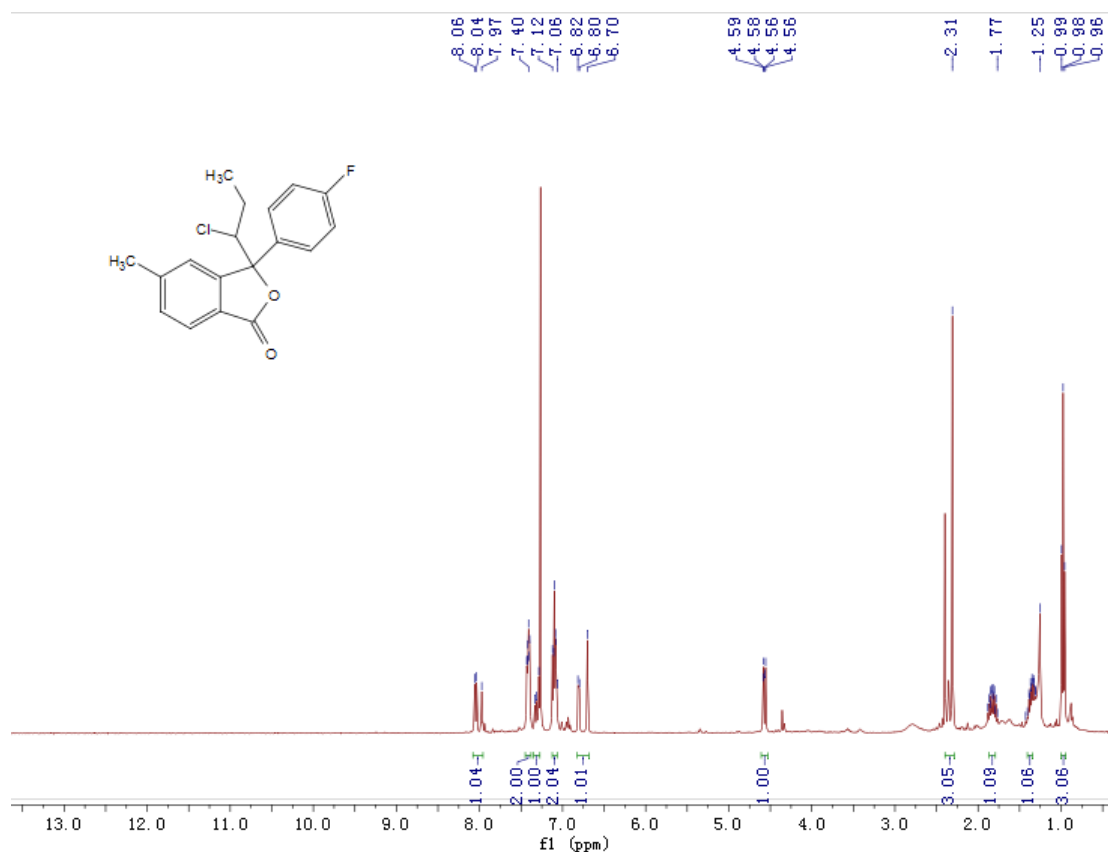
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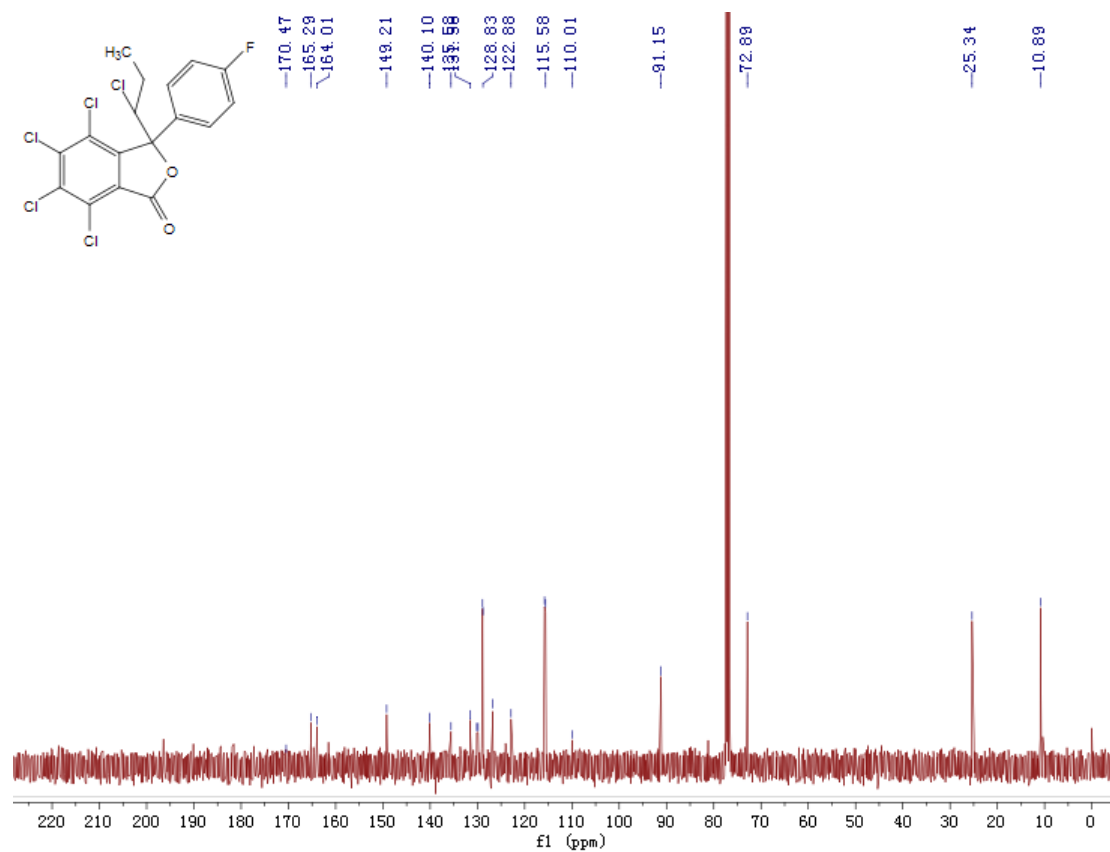
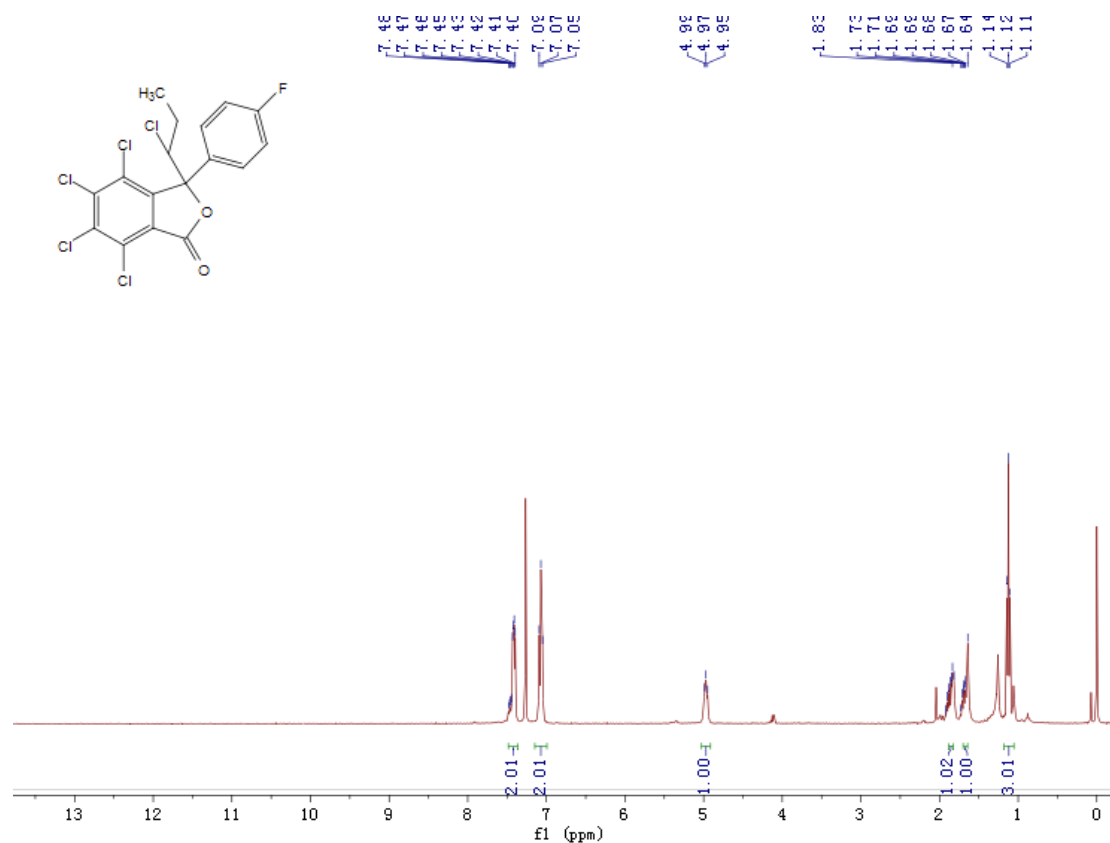
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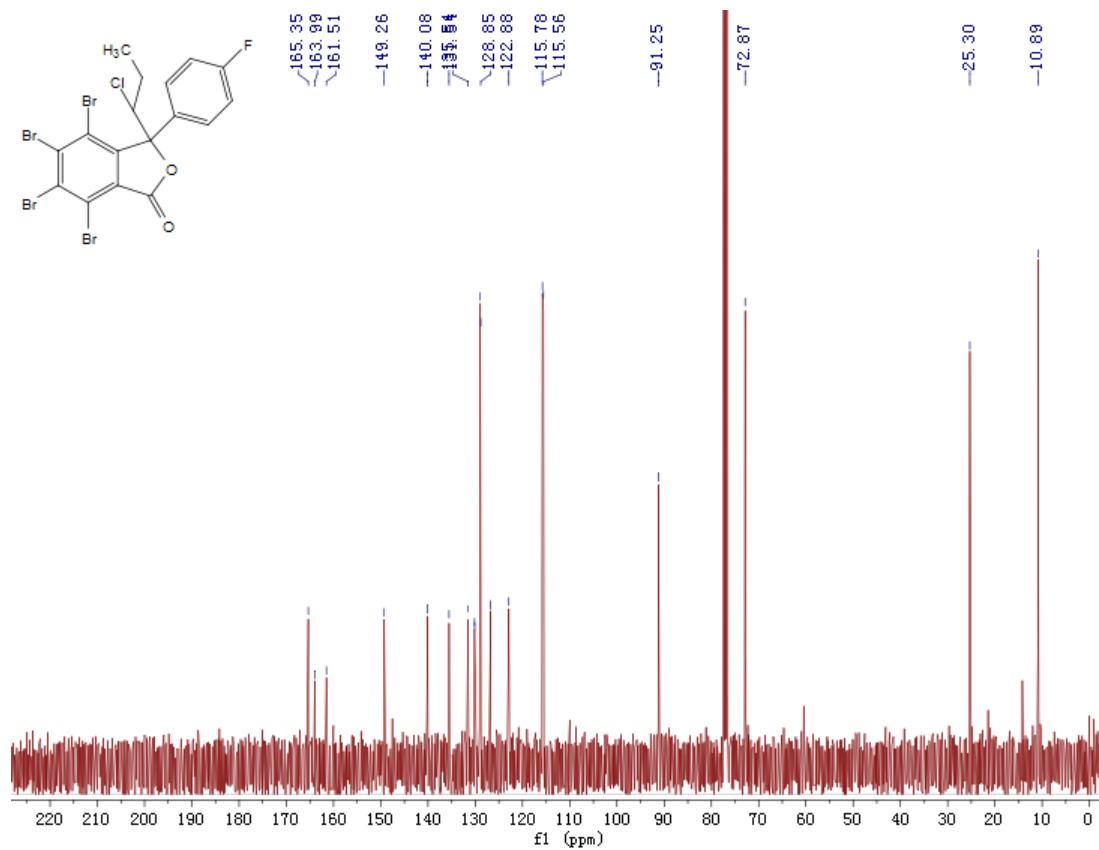
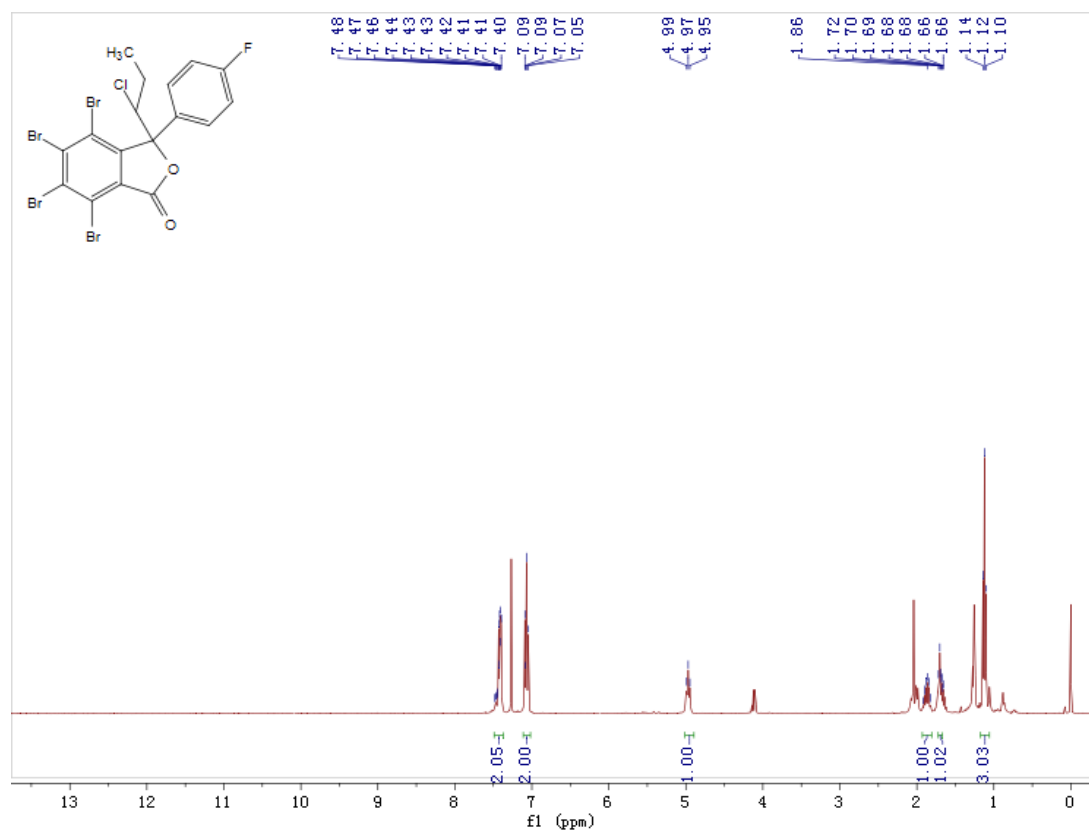
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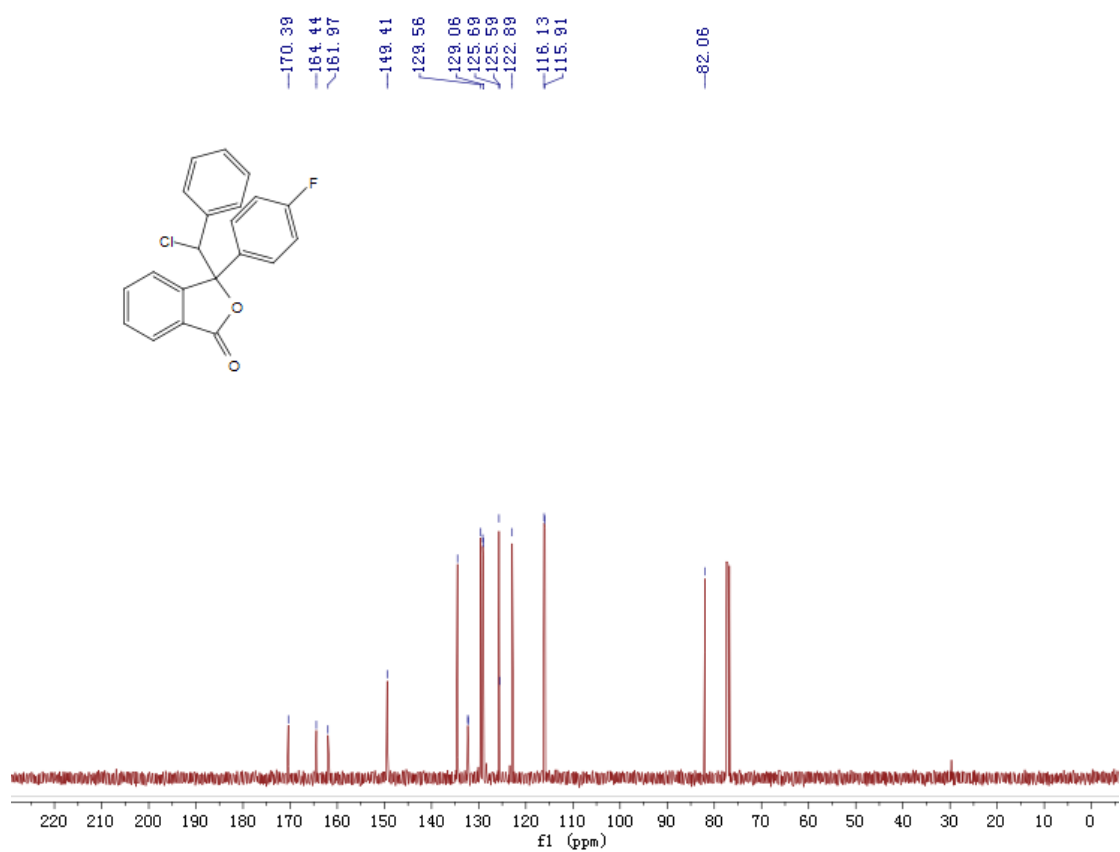
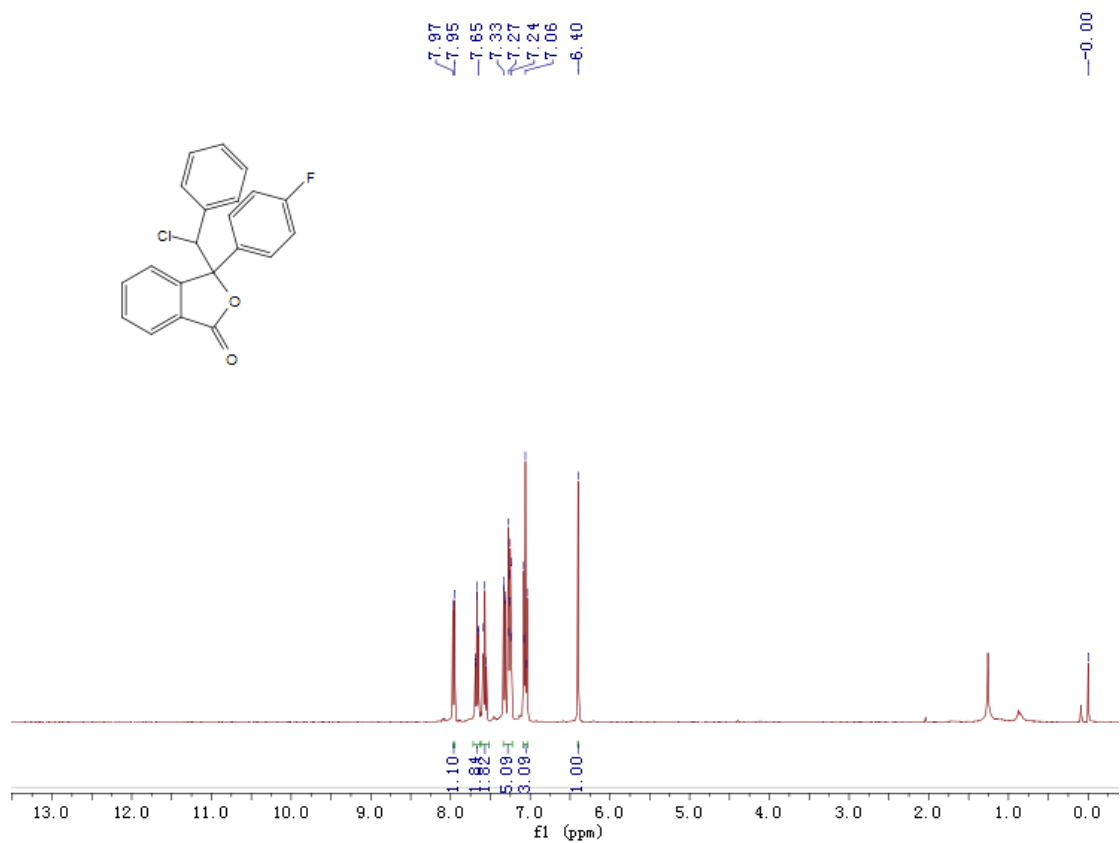
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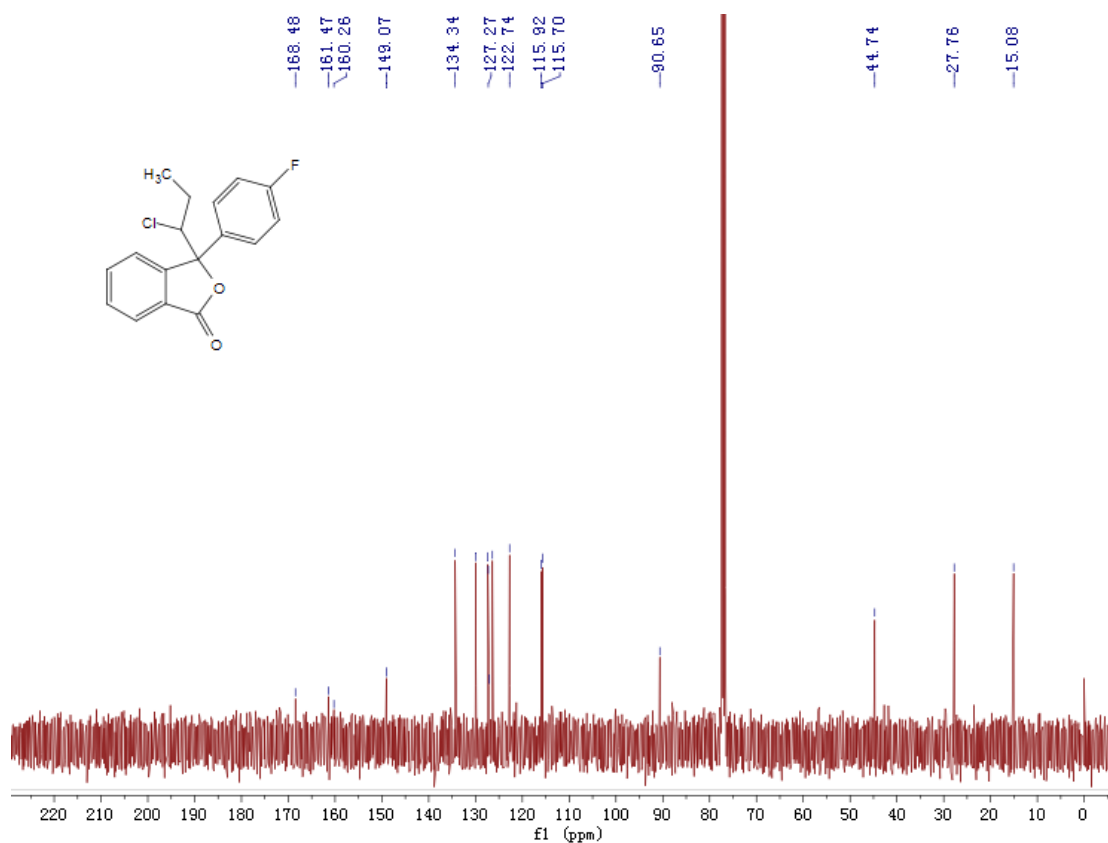
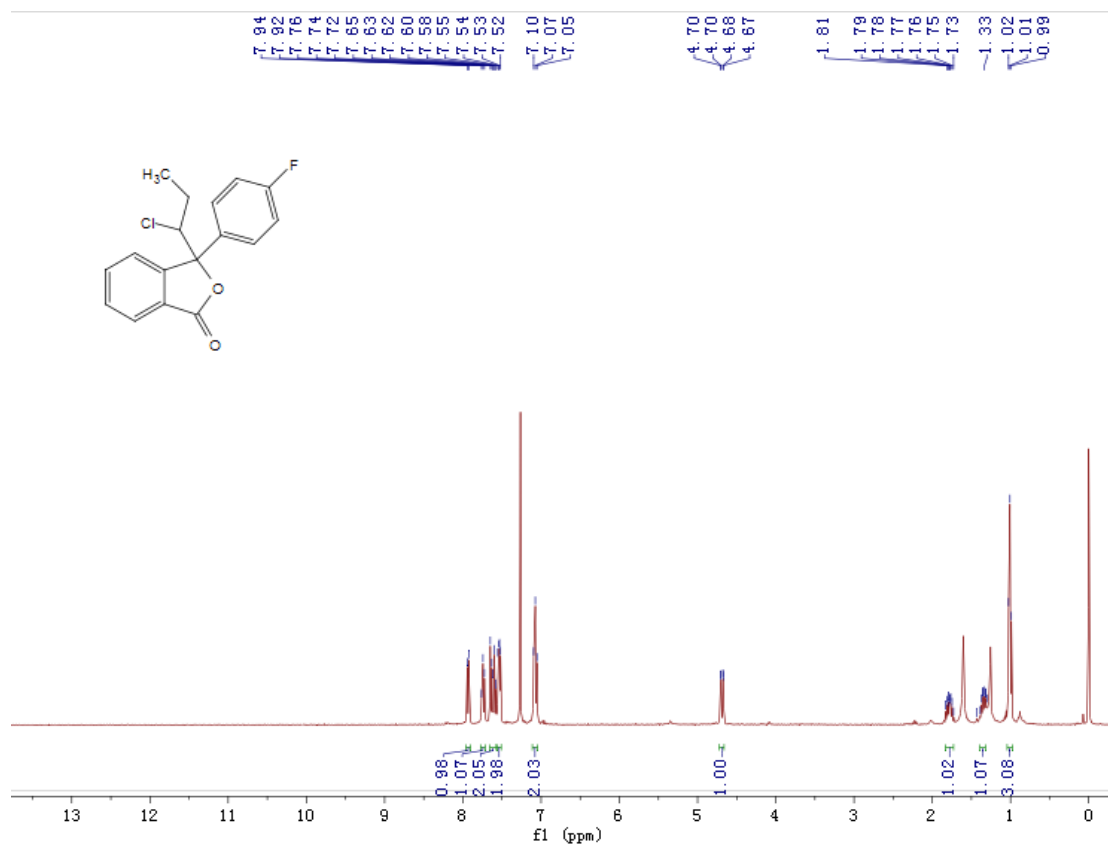
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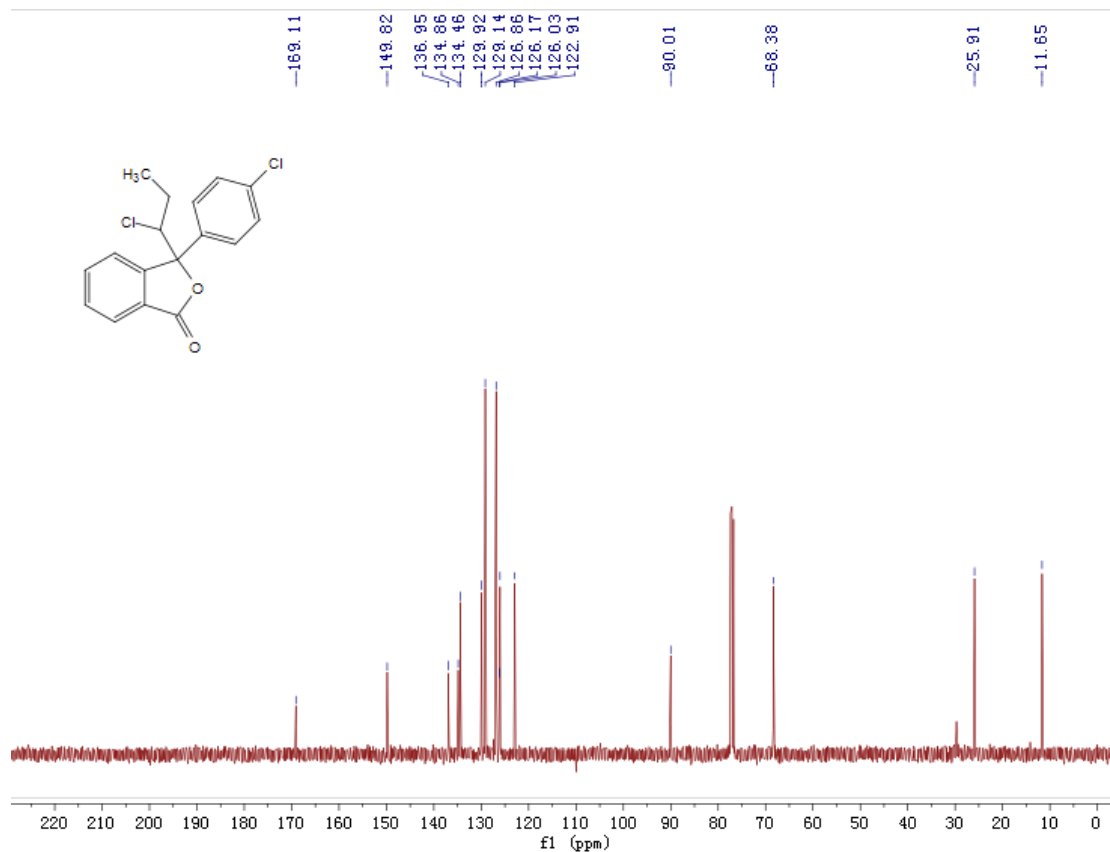
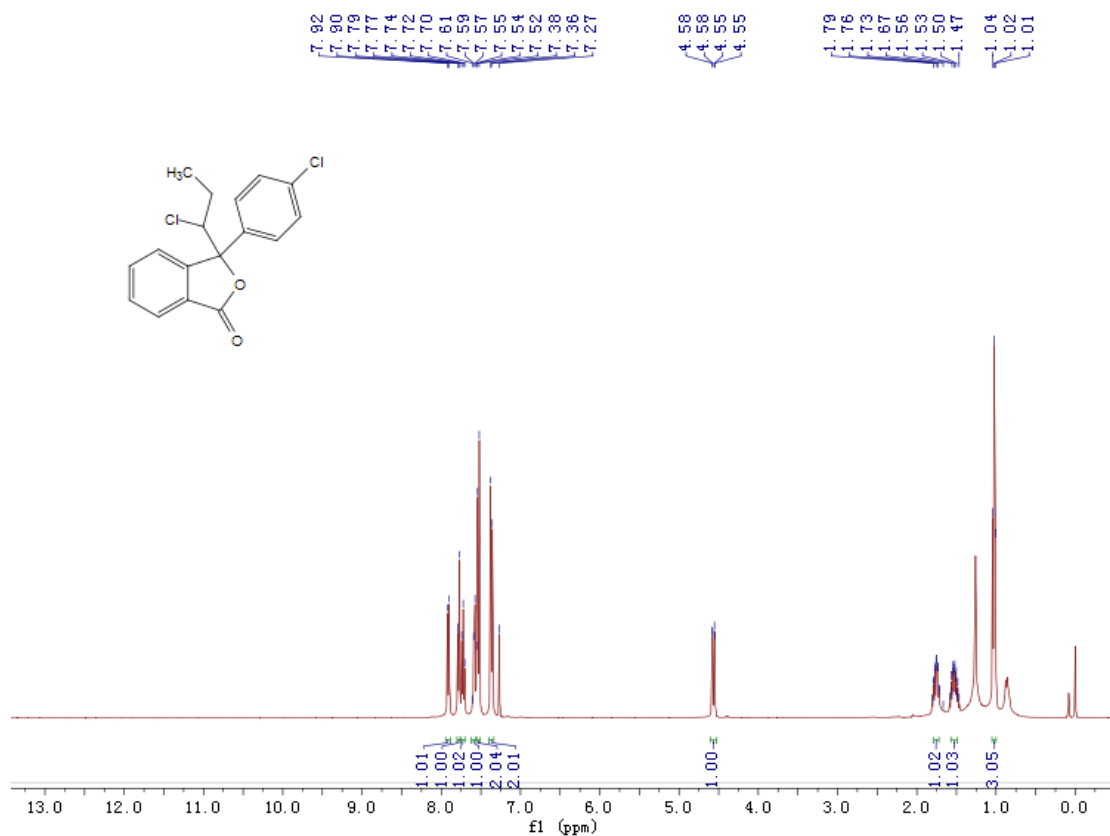
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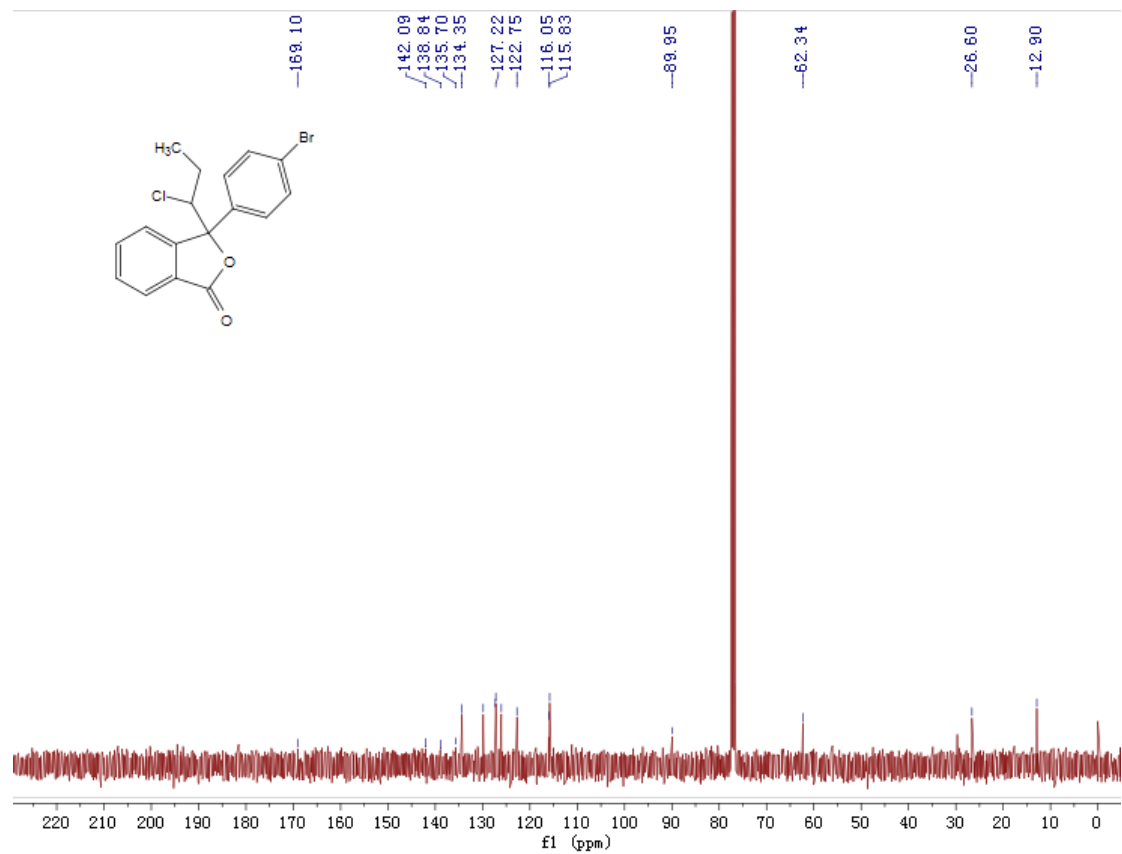
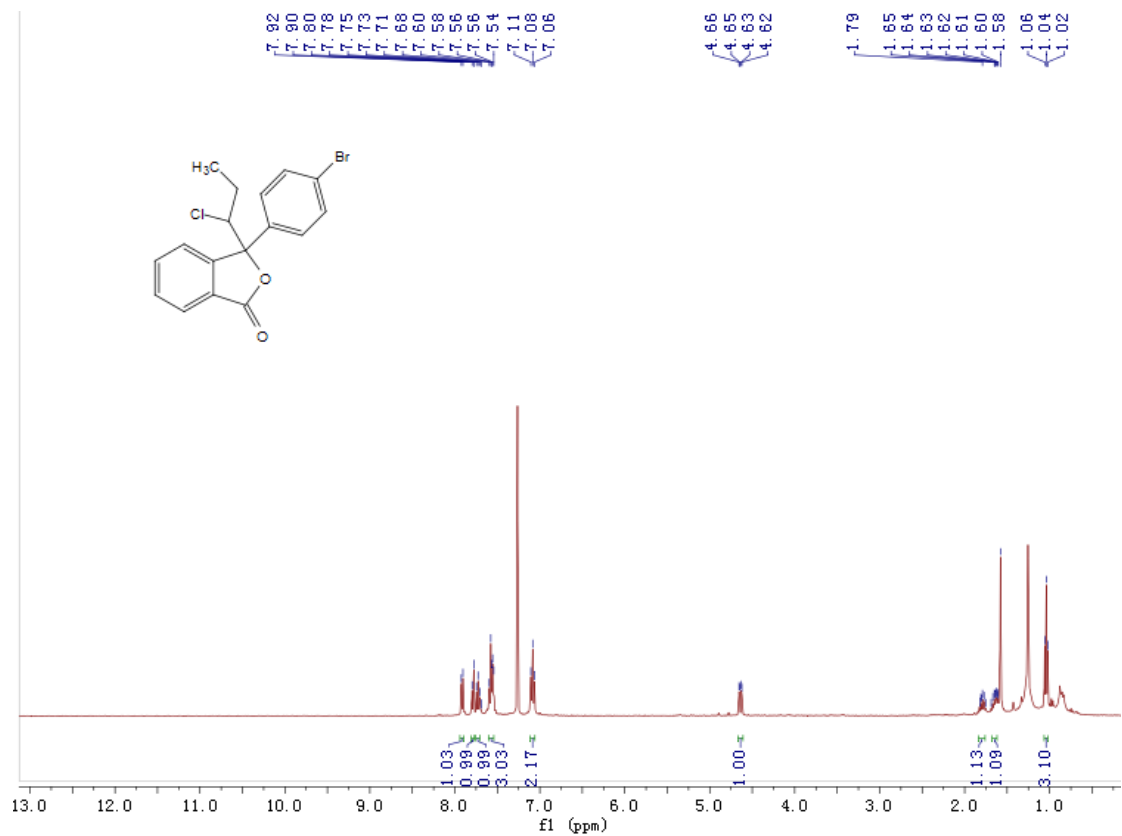
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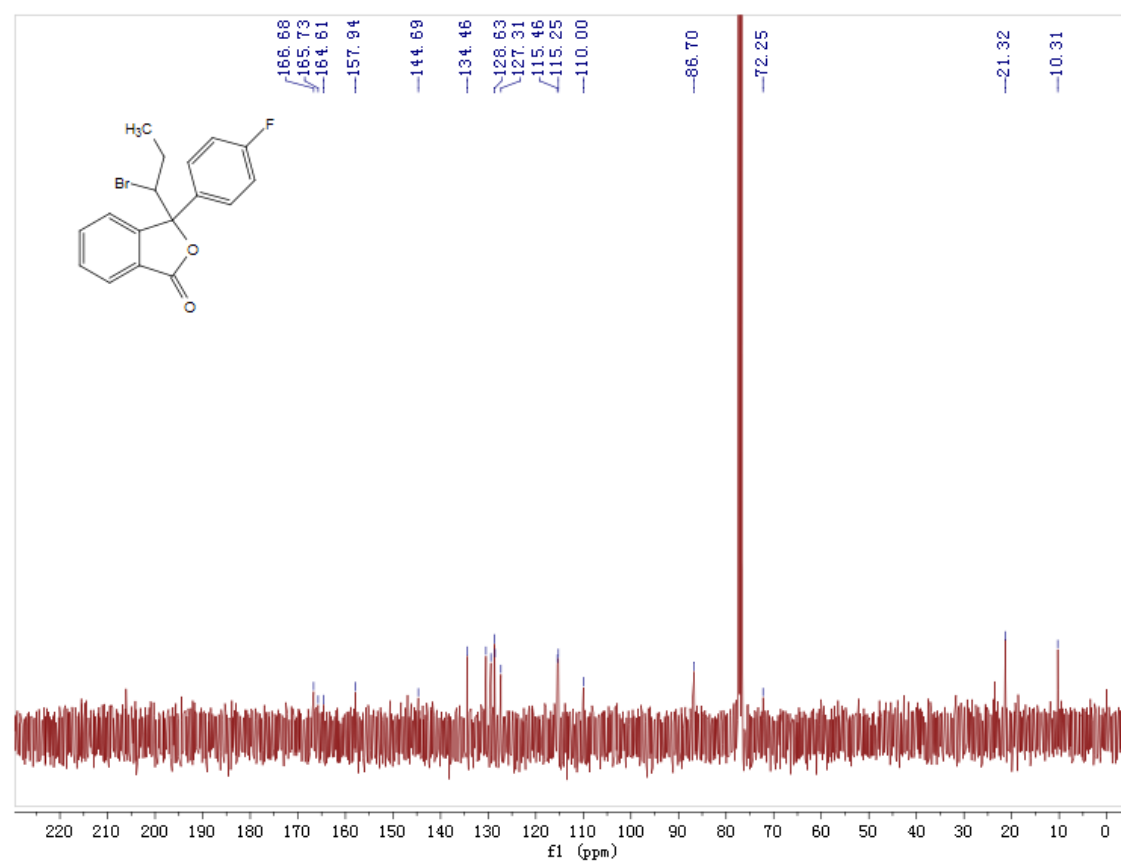
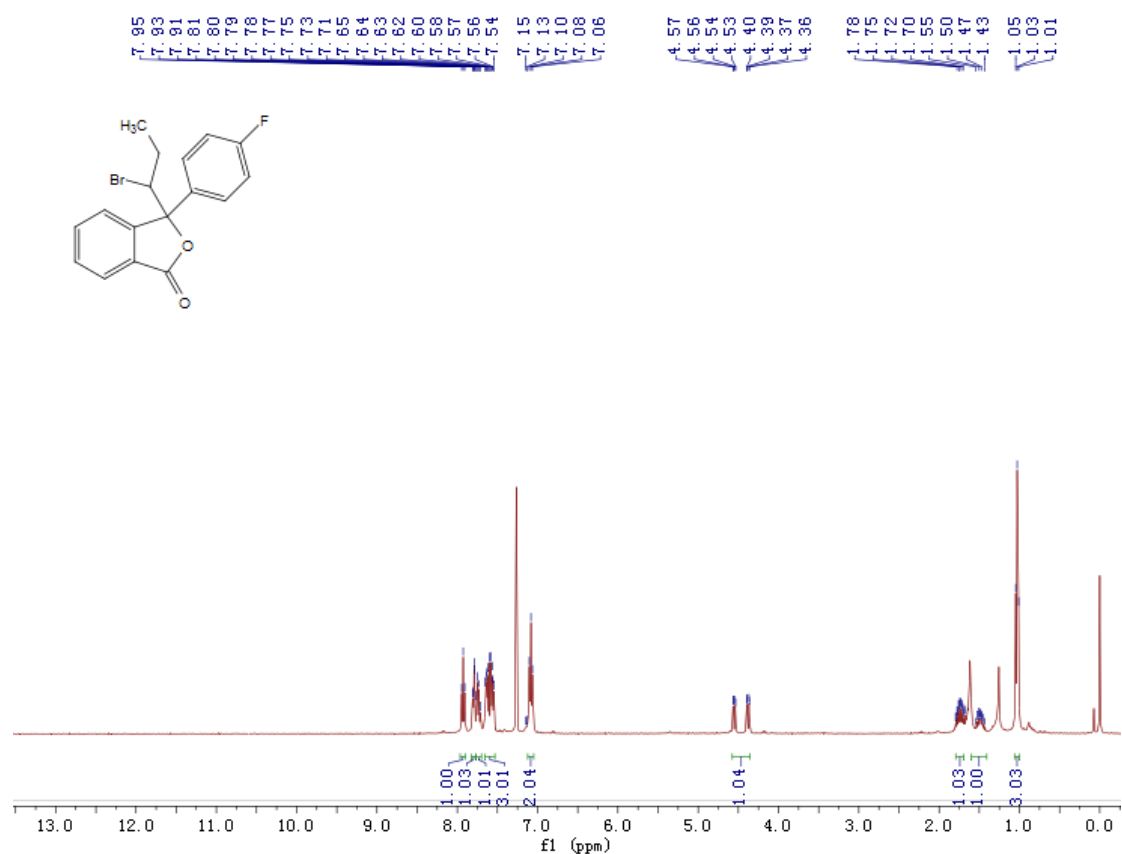
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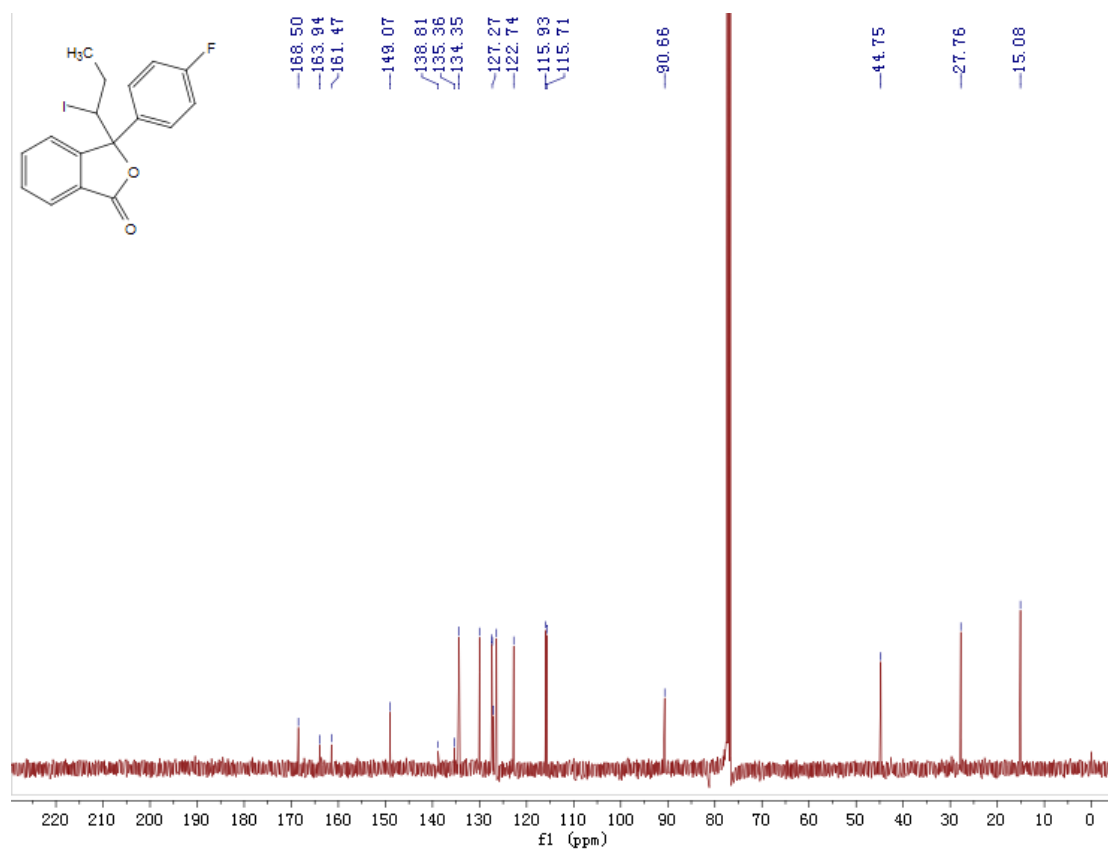
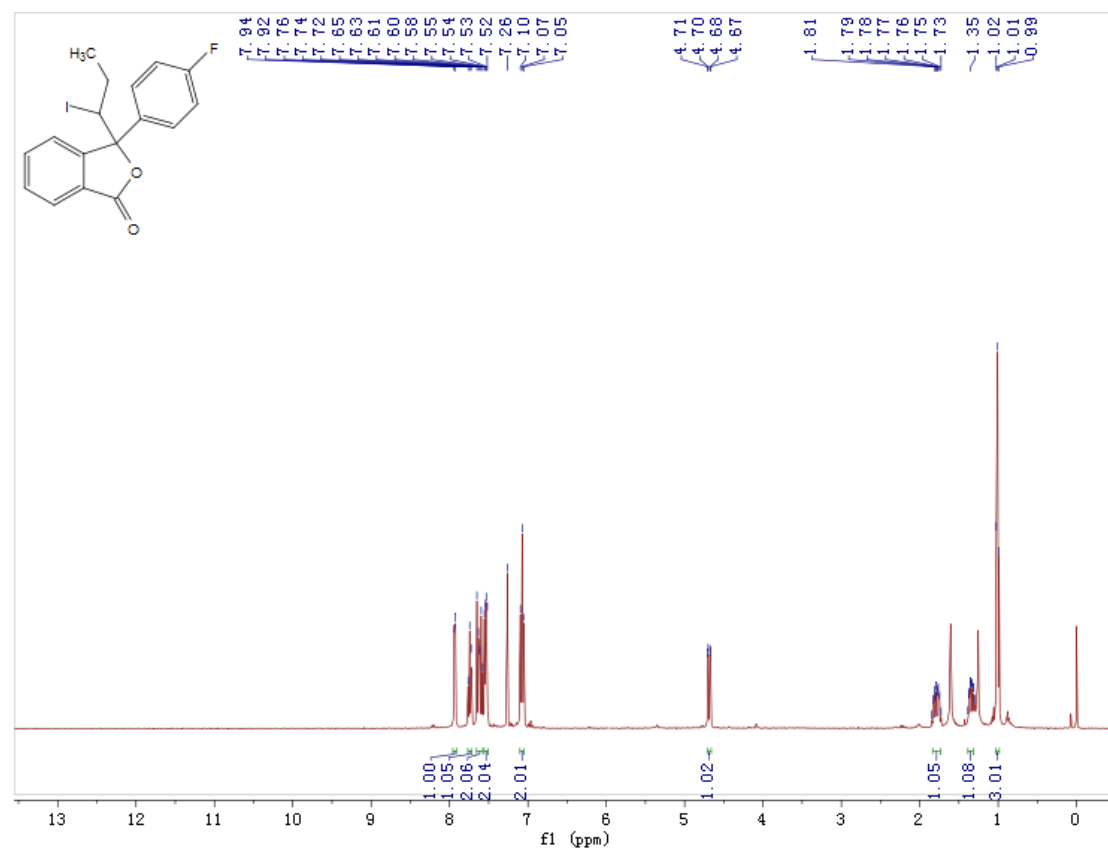
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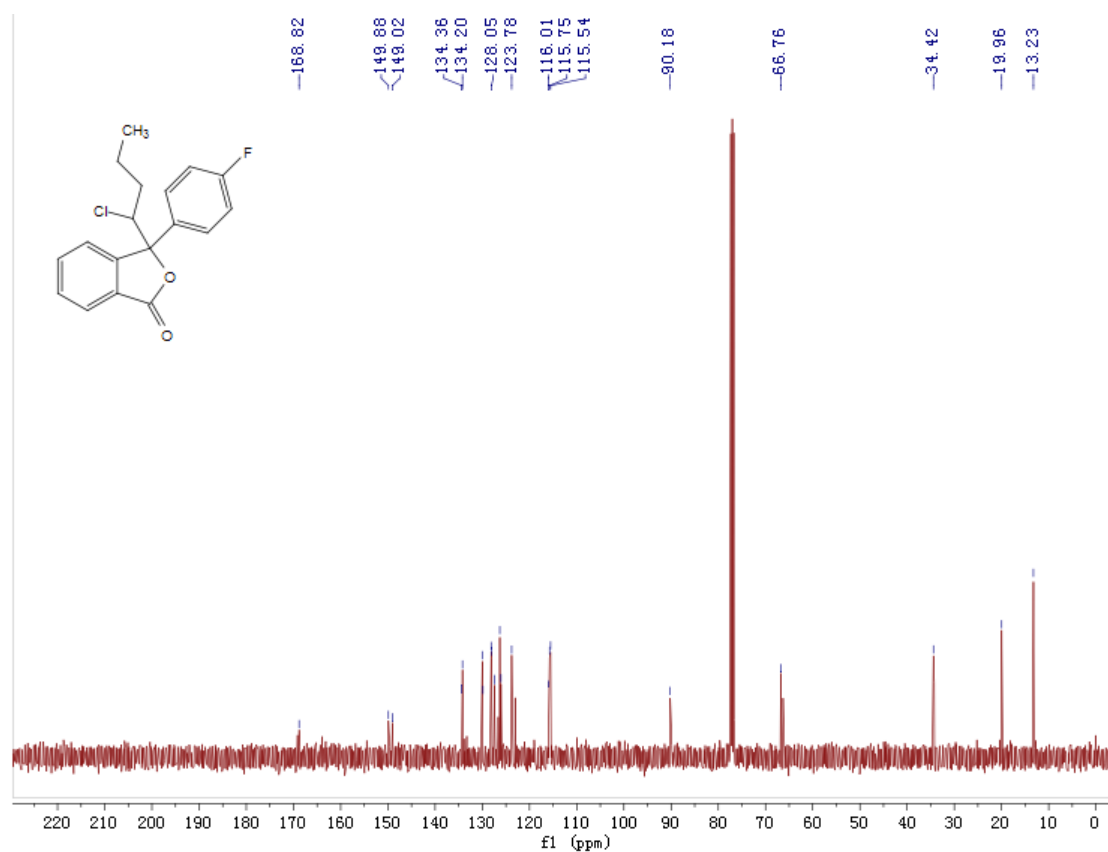
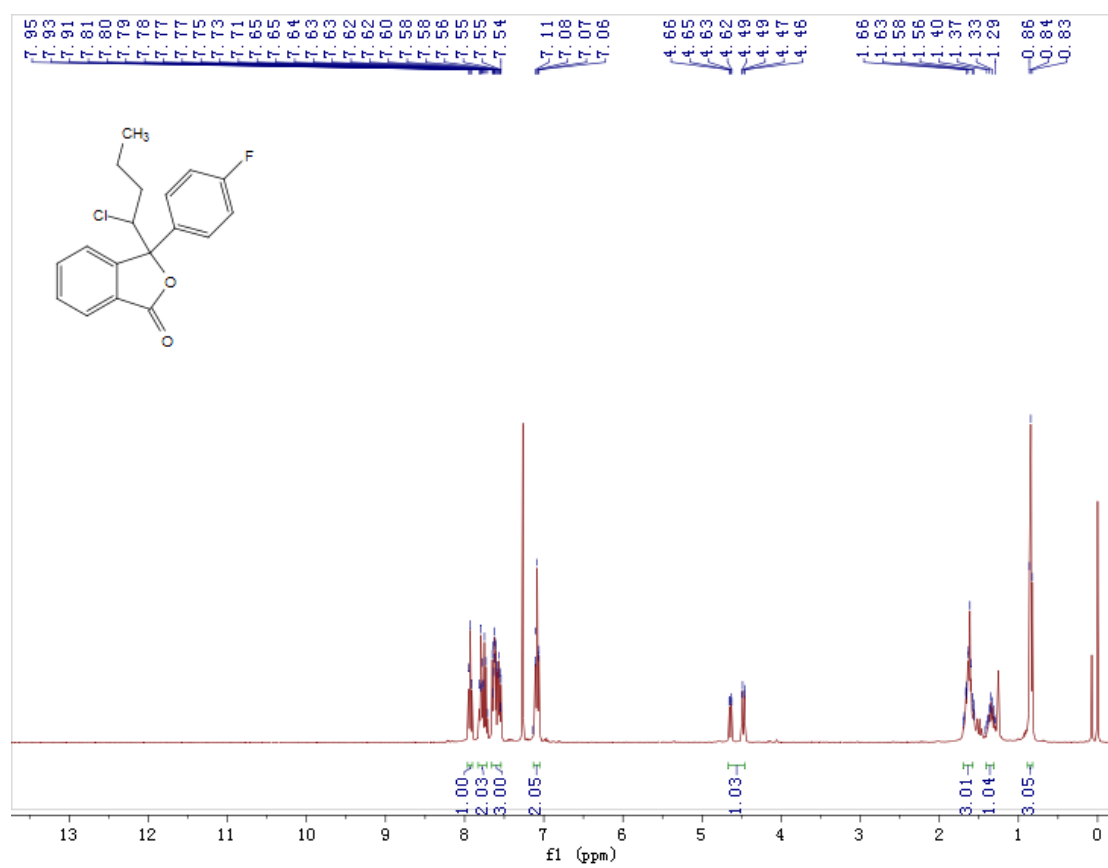
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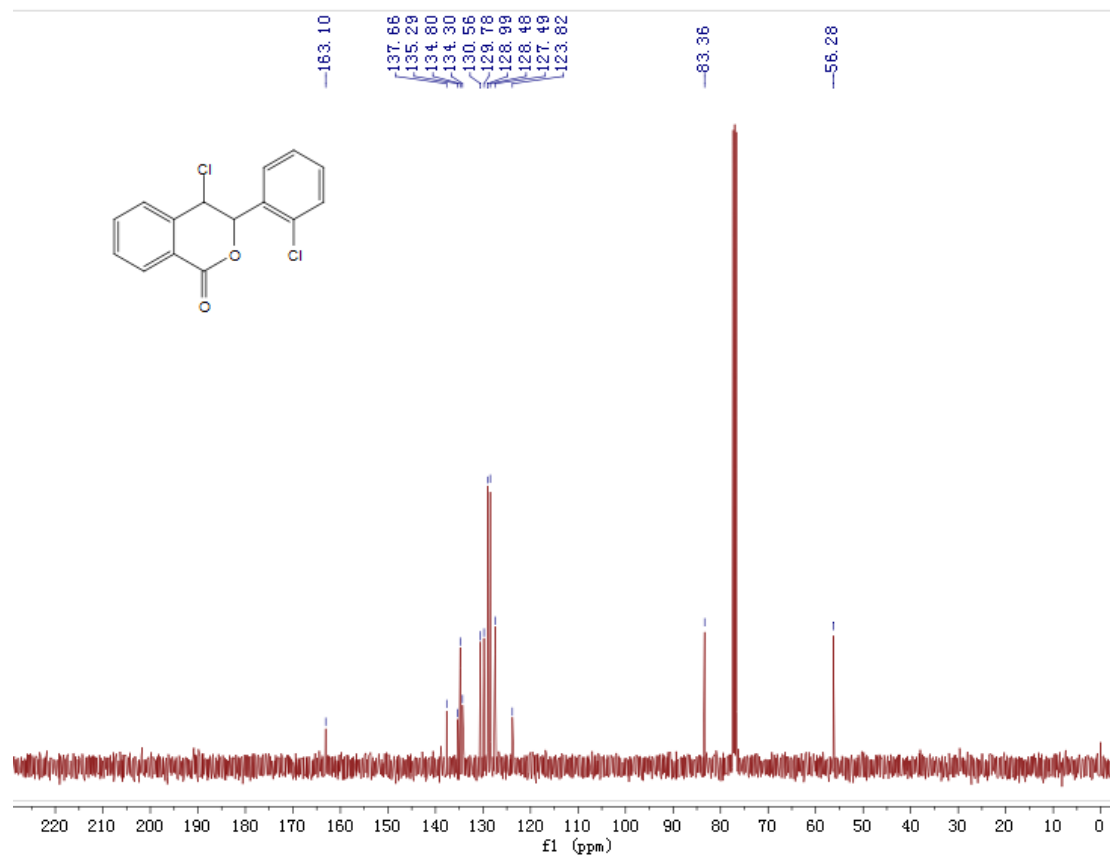
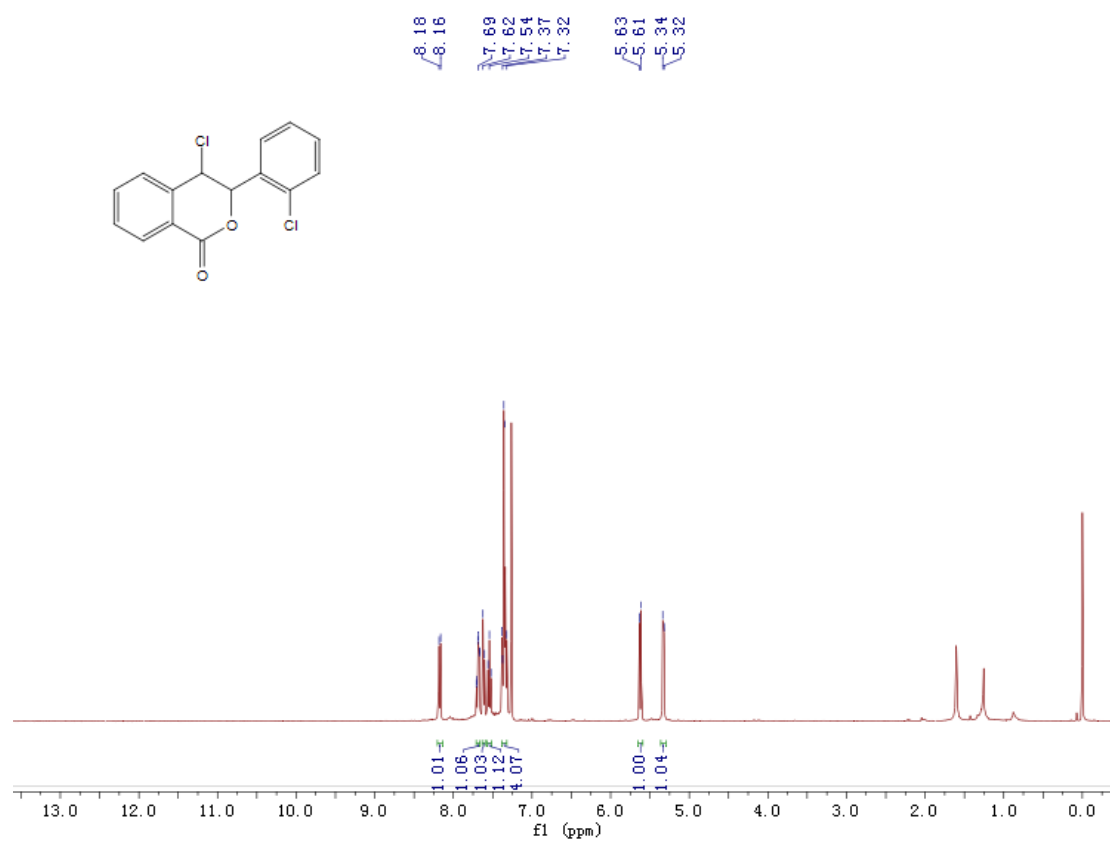
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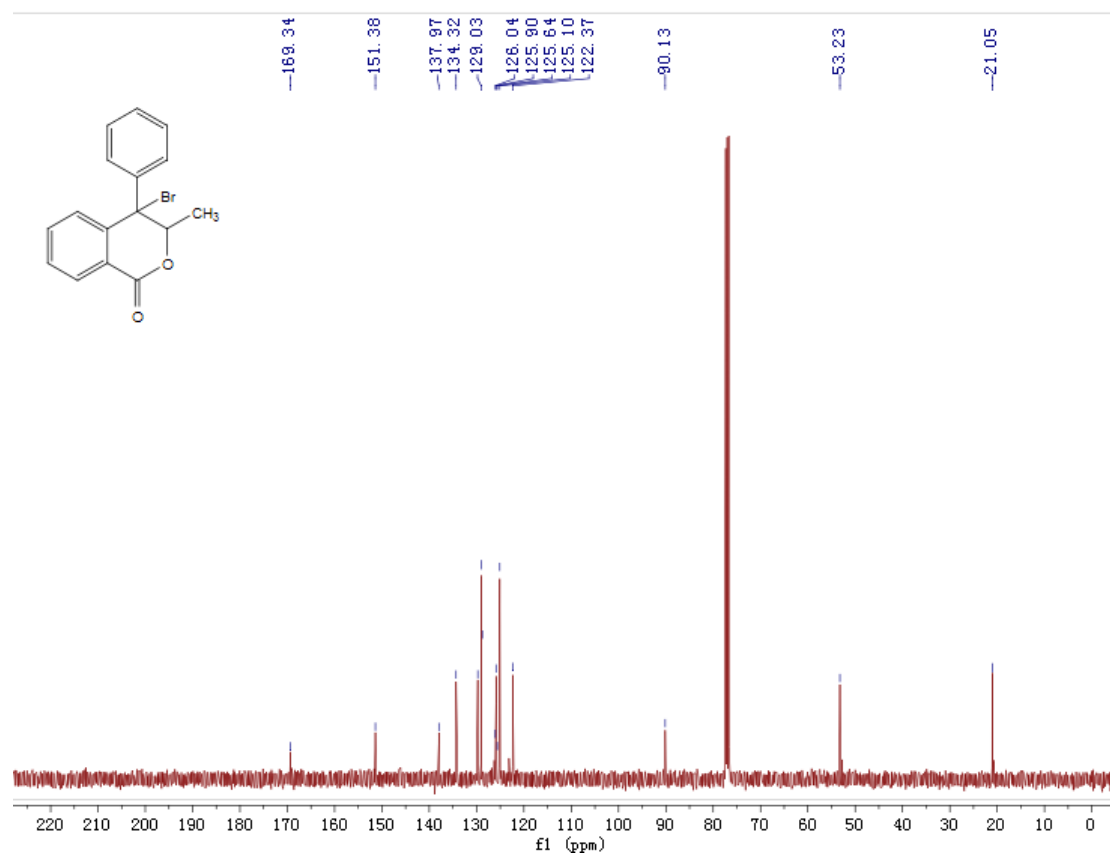
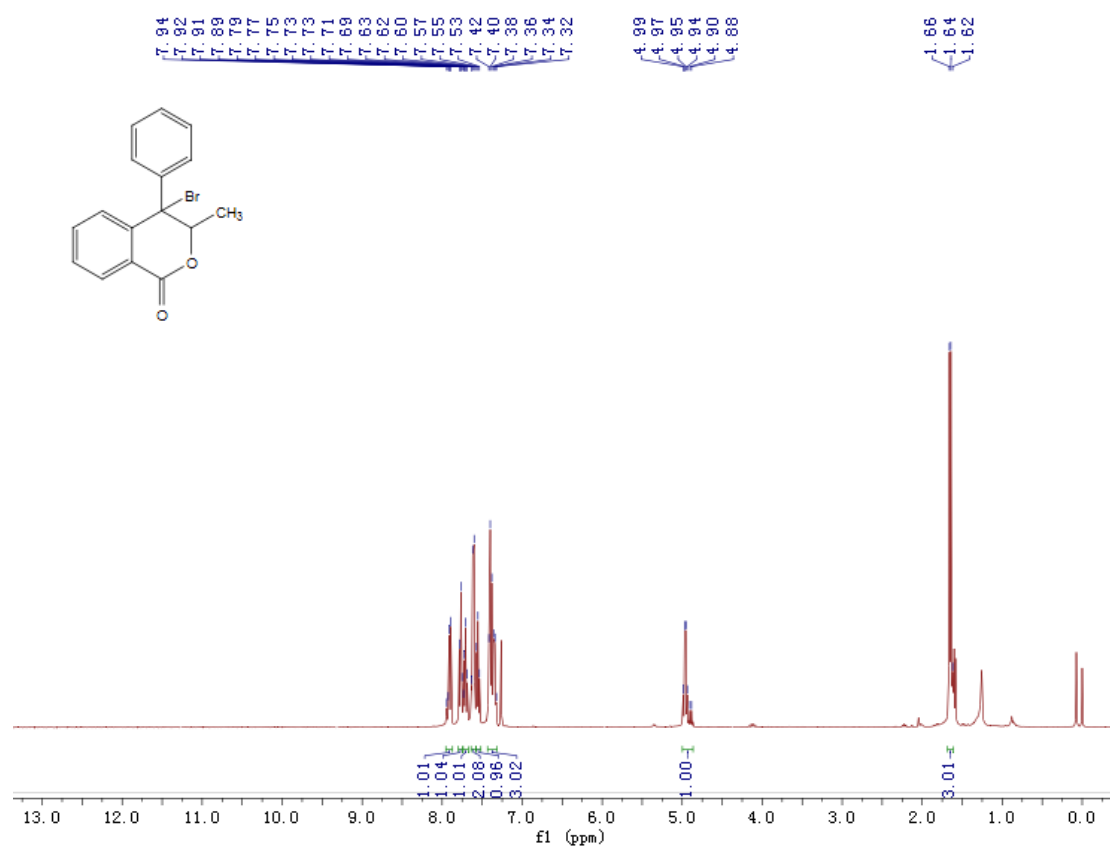
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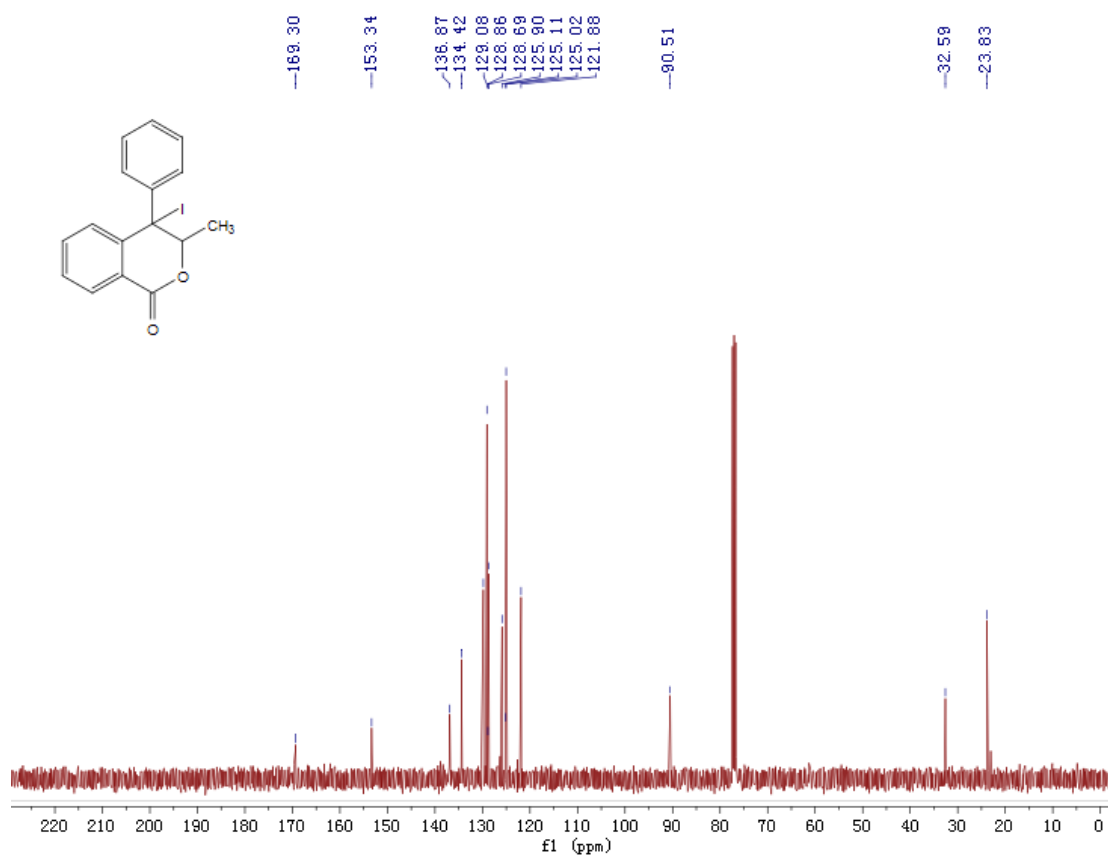
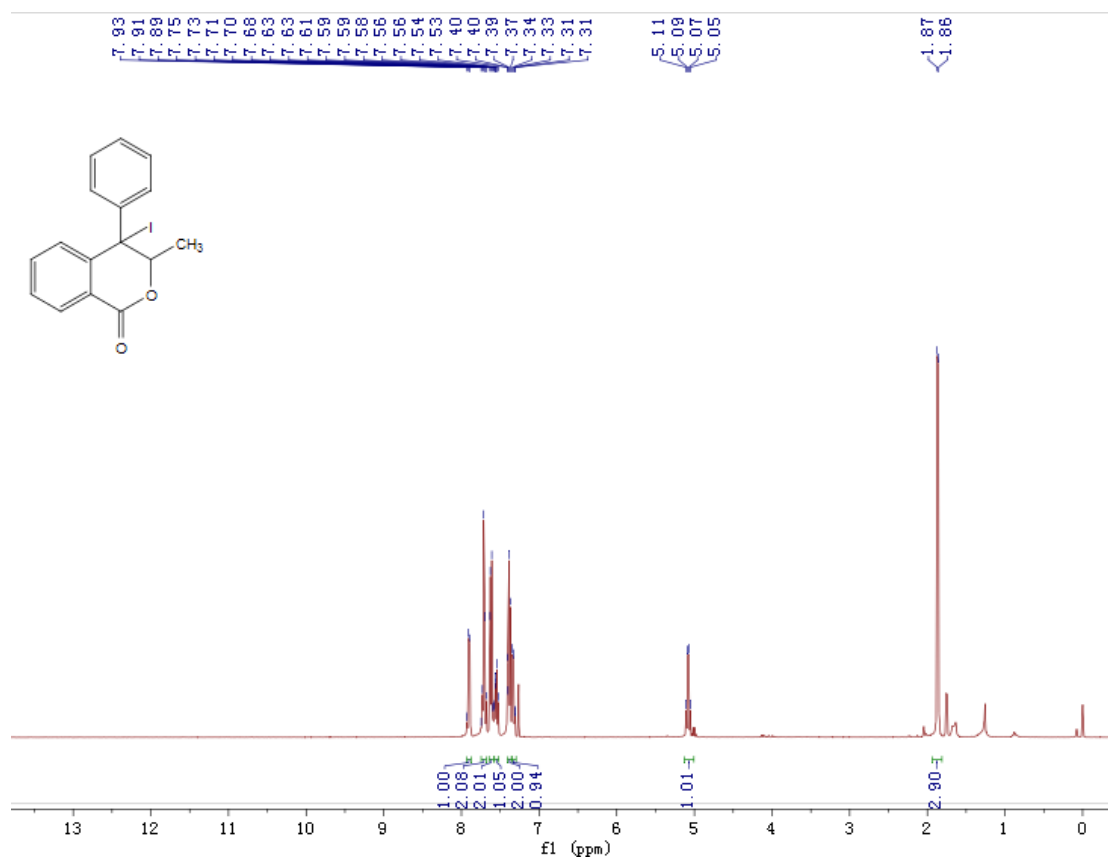
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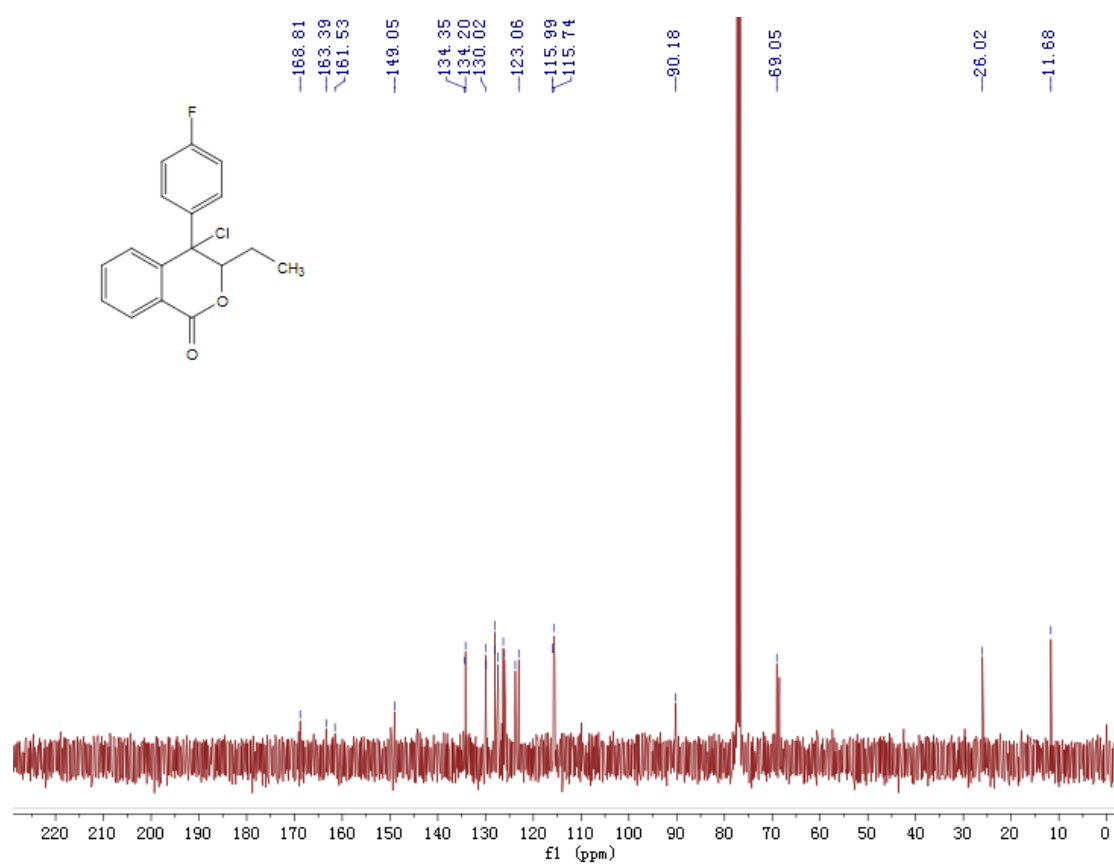
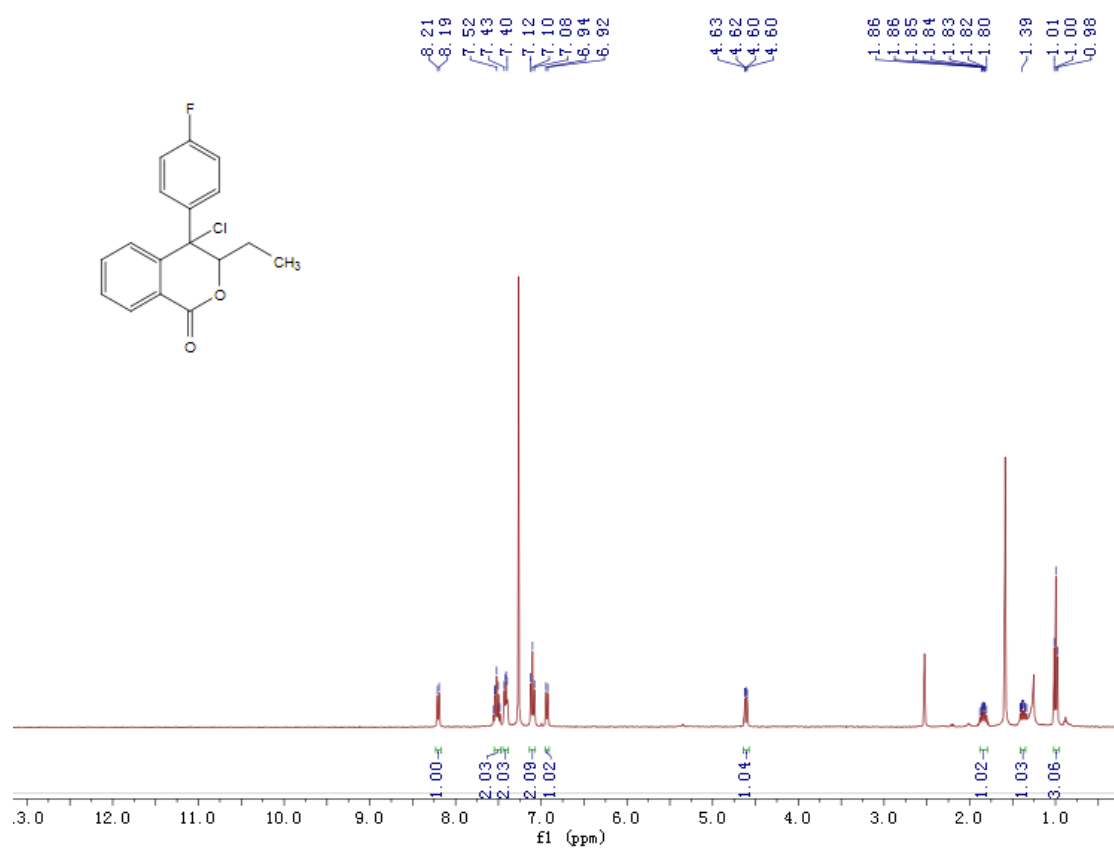
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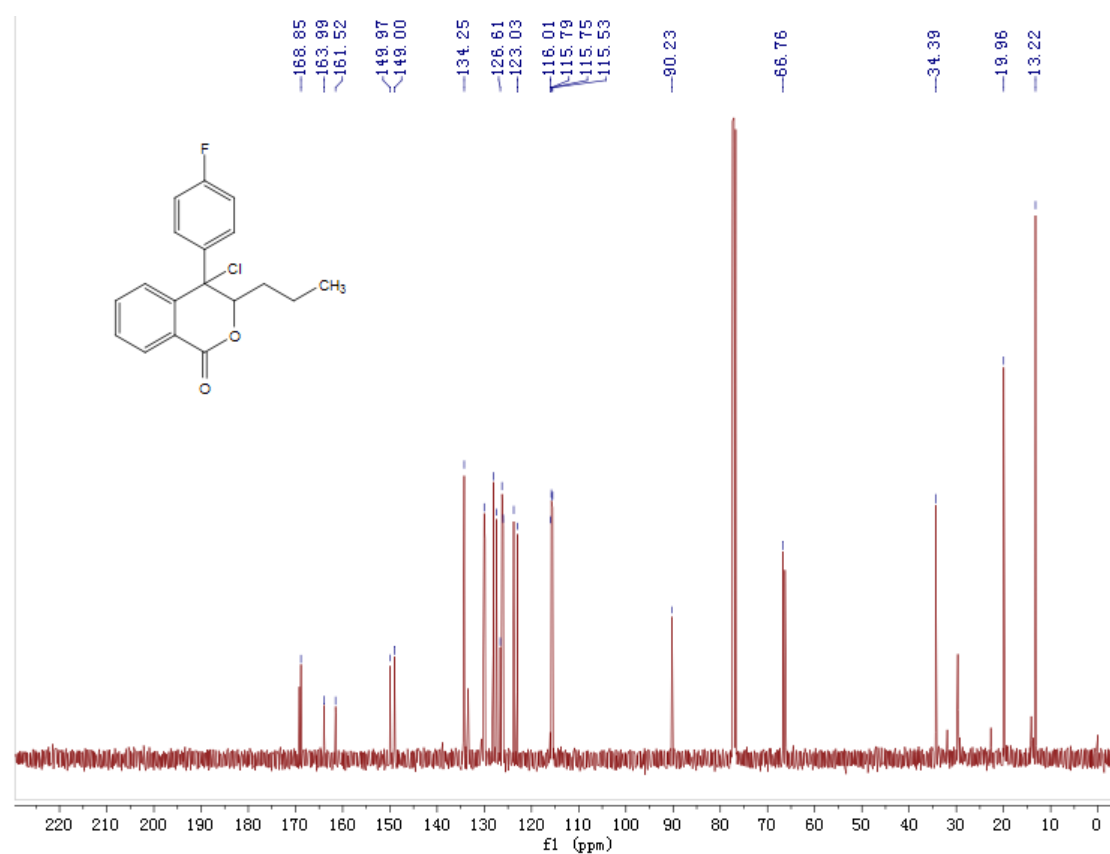
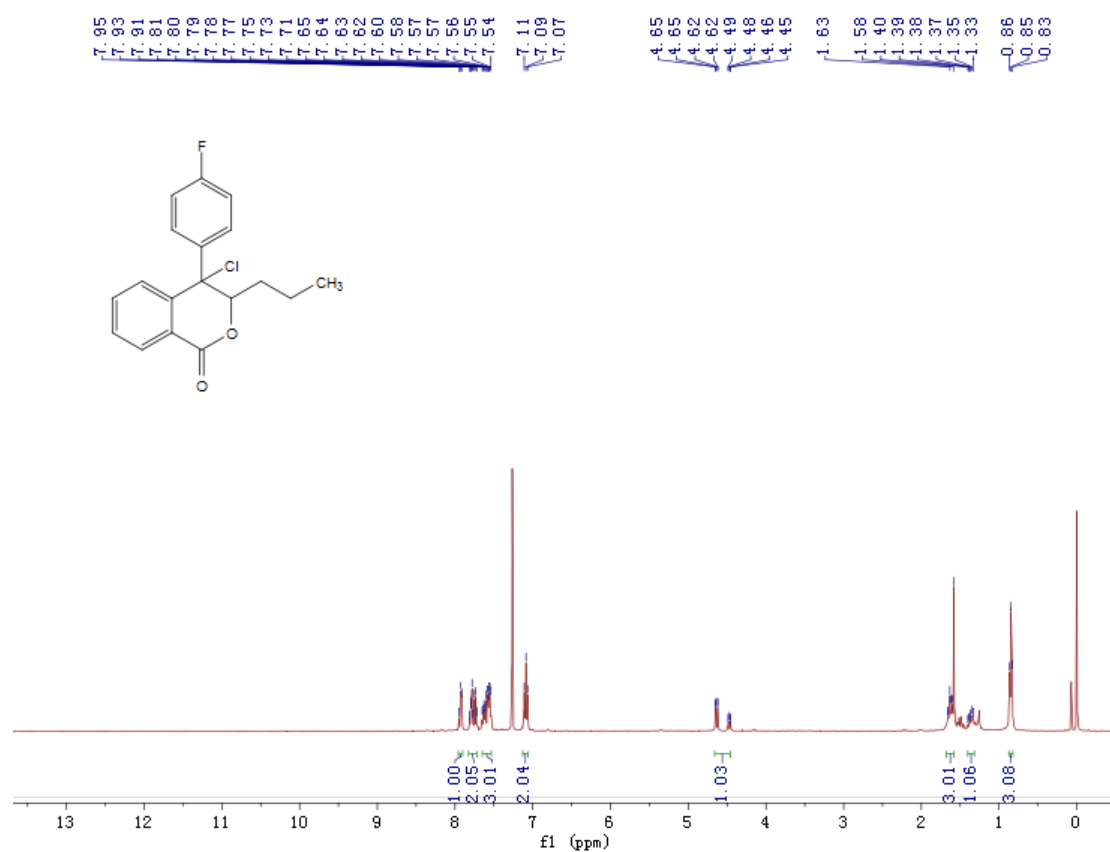
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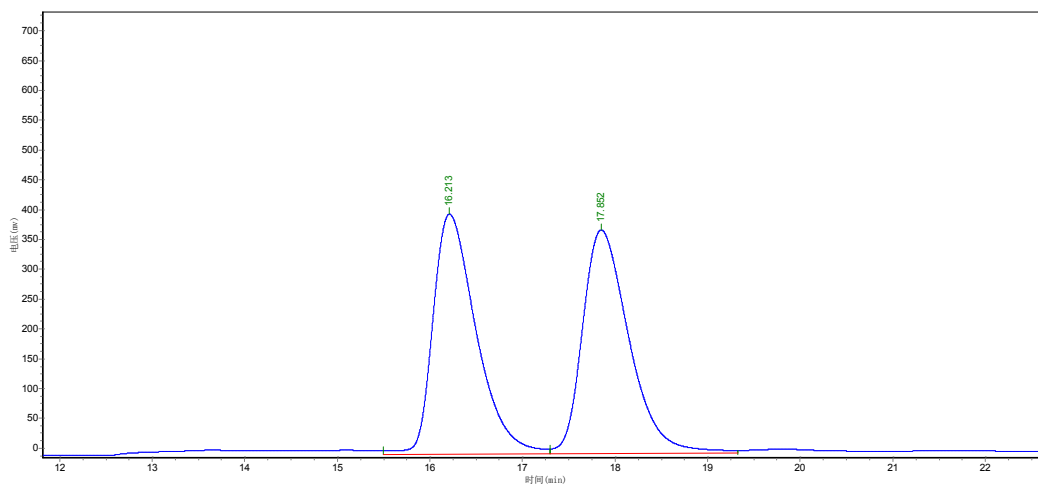
14m



II HPLC of 13f, 13g, 13i and 14b

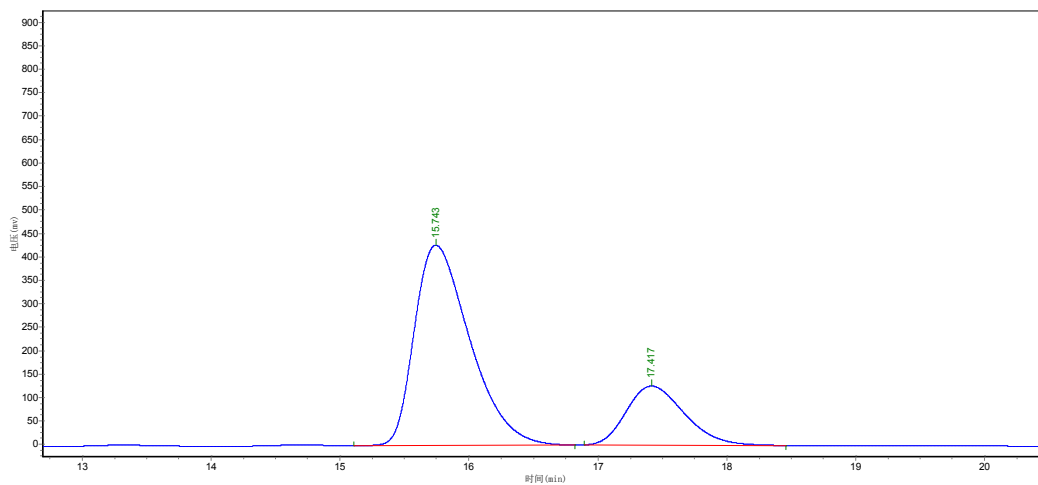
Compound 13f

Rac-13f



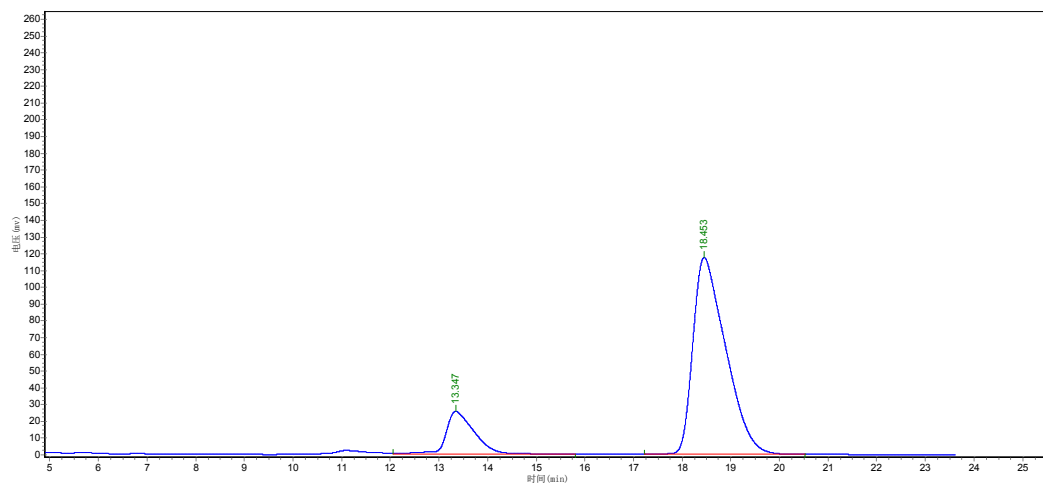
Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	16.213	402279.563	13037546.000	49.9217
2	17.852	374991.156	13078449.000	50.0783

R-13f



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	15.743	427406.844	12769922.000	78.5660
2	17.417	119965.406	3483834.500	21.4340

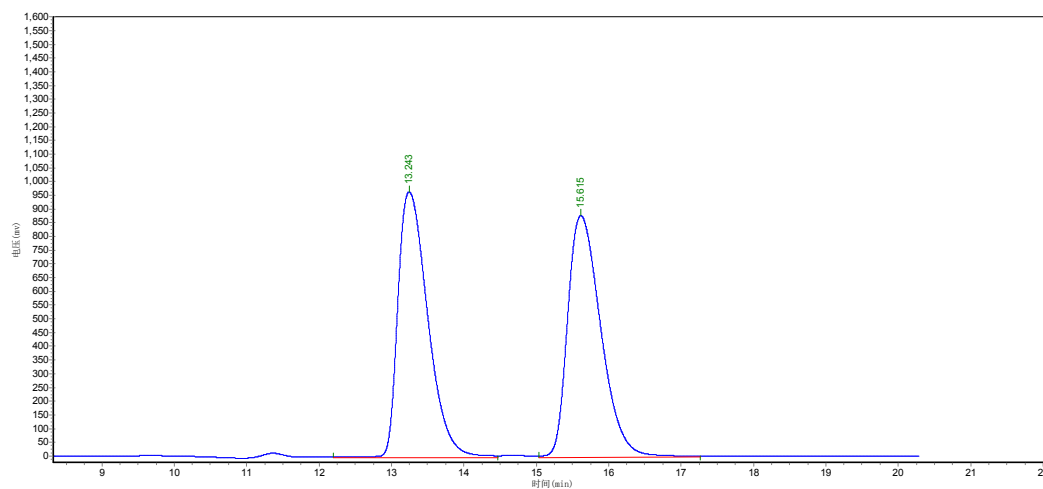
S-13f



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	13.347	25457.281	1029781.813	15.8229
2	18.453	117483.266	5478403.000	84.1771

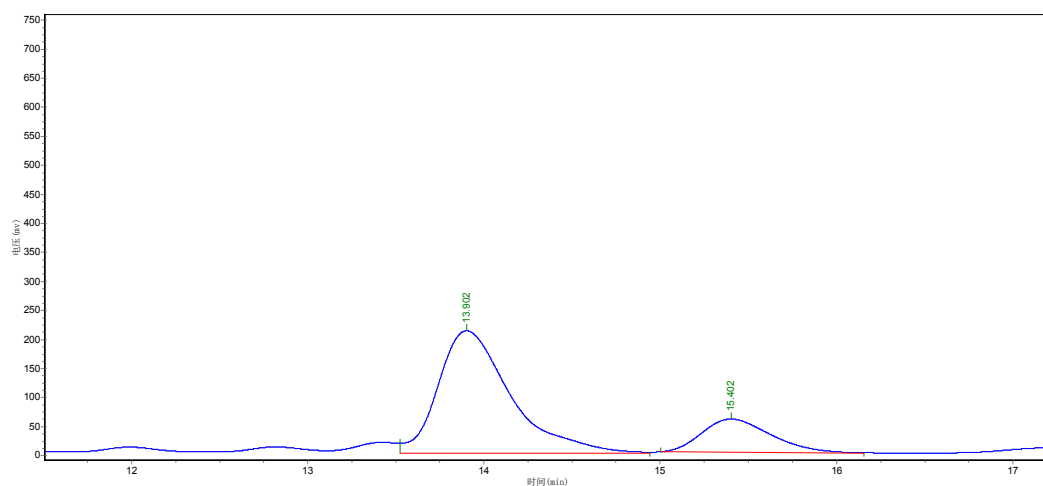
Compound 13g

Rac-13g



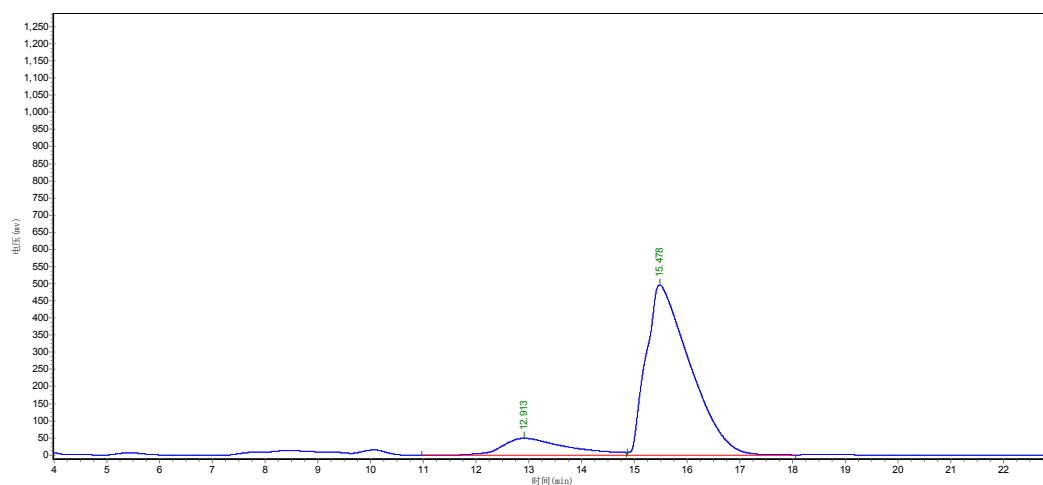
Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	13.243	968909.375	27941588.000	49.8642
2	15.615	880288.563	28093838.000	50.1359

R-13g



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	13.902	210706.109	5995384.500	80.8702
2	15.402	54928.629	1418200.875	19.1298

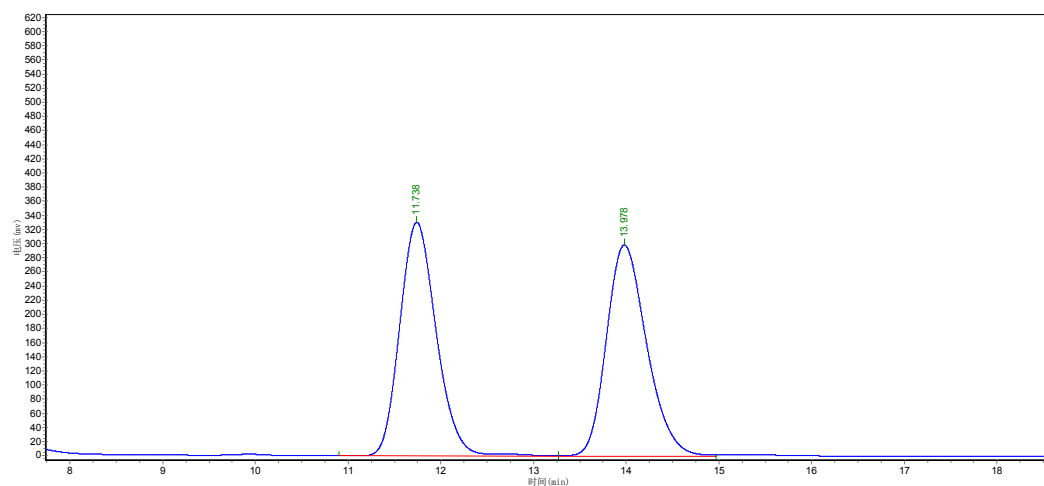
S-13g



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	12.913	49359.051	4216364.000	12.8665
2	15.478	496652.219	28553714.000	87.1335

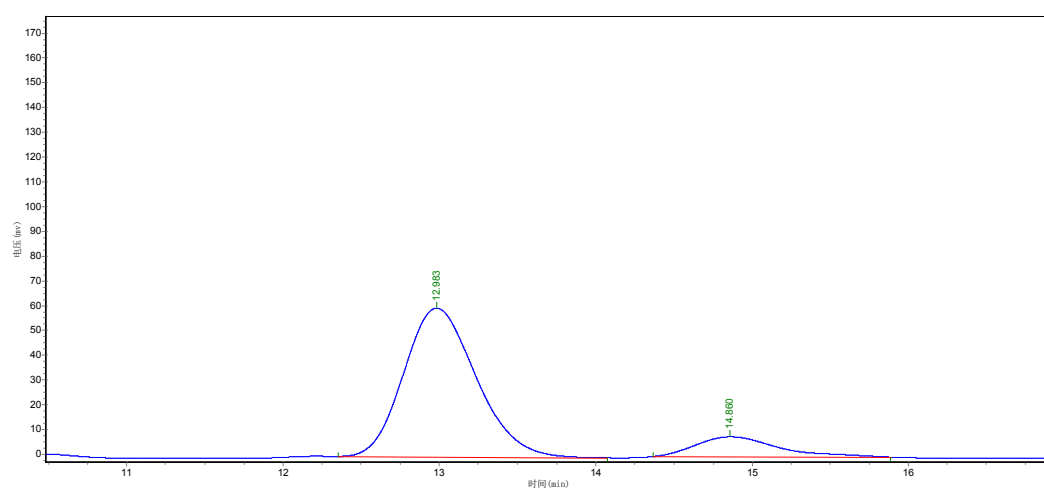
Compound 13i

Rac-13i



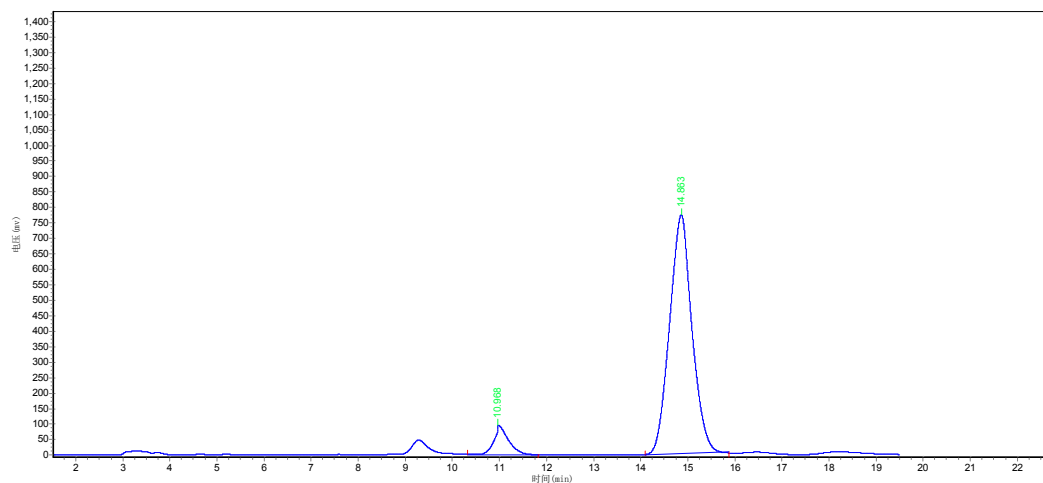
Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	11.738	330478.625	9044402.000	50.1464
2	13.978	298510.656	8991605.000	49.8536

R-13i



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	12.983	60044.742	1931425.250	88.4036
2	14.860	7619.948	253355.203	11.5964

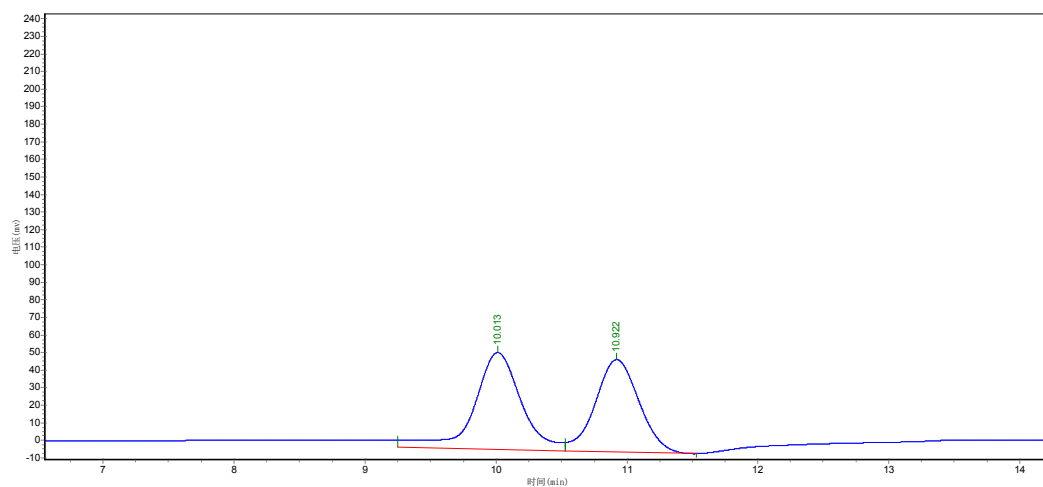
S-13i



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	10.968	95989.211	2087528.000	7.6265
2	14.863	770167.063	25284406.000	92.3735

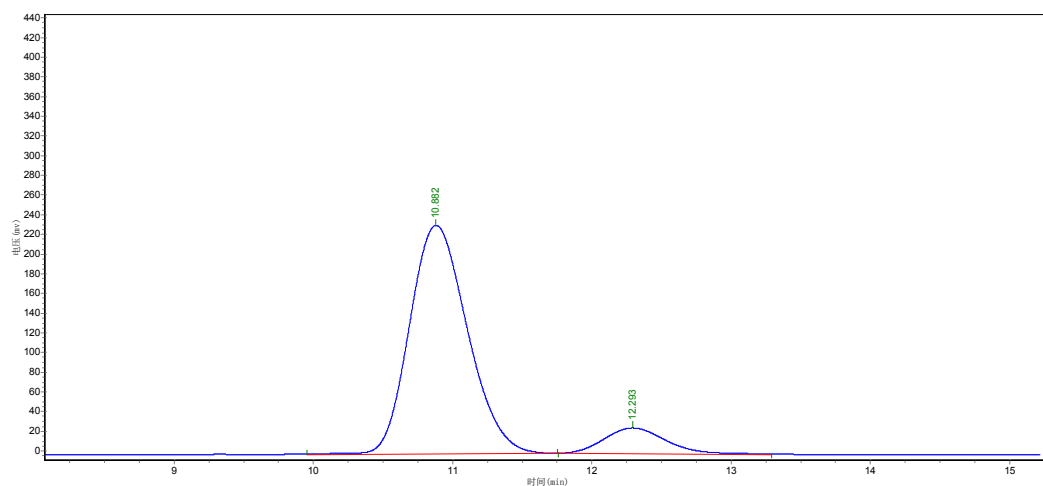
Compound 14b

Rac-14b



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	10.013	54955.035	1366839.250	53.0597
2	10.922	52516.375	1209201.750	46.9403

(3R, 4S)-14b



Peak	Ret Time (min)	Height (mAU)	Area (Mau *s)	Area (%)
1	10.882	232070.156	6682339.500	90.0322
2	12.293	25388.061	739827.563	9.9678

III X-ray crystallographic for 13k

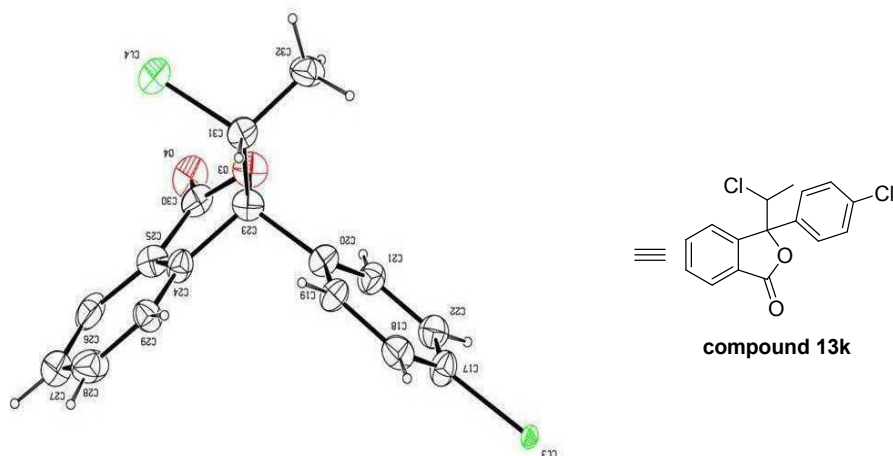


Table 1. Crystal data and structure refinement for 130618_0m.

Identification code	130618_0m
Empirical formula	C ₁₆ H ₁₁ Cl ₂ O ₂
Formula weight	306.15
Temperature	293(2) K

Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 11.158(3) Å alpha = 90 deg. b = 12.352(3) Å beta = 120.845(17) deg. c = 12.264(2) Å gamma = 90 deg.
Volume	1451.2(6) Å ³ , Z, Calculated density 4, 1.401 Mg/m ³
Absorption coefficient	0.444 mm ⁻¹
F(000)	628
Crystal size	0.29 x 0.28 x 0.27 mm
Theta range for data collection	2.13 to 26.50 deg.
Limiting indices	-14 ≤ h ≤ 10, -13 ≤ k ≤ 15, -12 ≤ l ≤ 15
Reflections collected / unique	8989 / 3003 [R(int) = 0.0820]
Completeness to theta = 26.50	100.0 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3003 / 0 / 183
Goodness-of-fit on F ²	1.744
Final R indices [I > 2σ(I)]	R1 = 0.1895, wR2 = 0.4577
R indices (all data)	R1 = 0.2580, wR2 = 0.5113
Extinction coefficient	0.64(7)
Largest diff. peak and hole	2.530 and -0.561 e.Å ⁻³