

Supporting Information

Synthesis of Phenylselanylisochroman-1-ones Through Highly Selective Selenolactonization of Styrene-Typed Carboxylic acids

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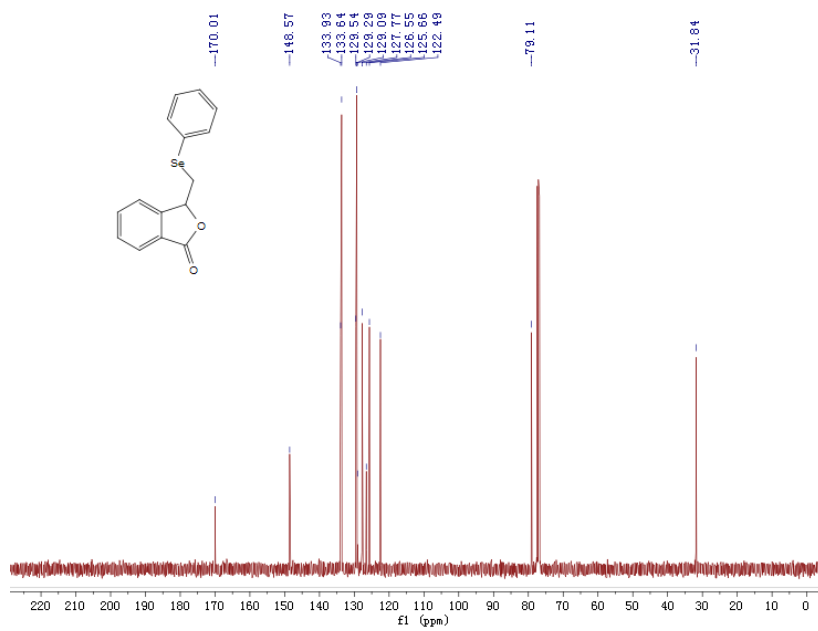
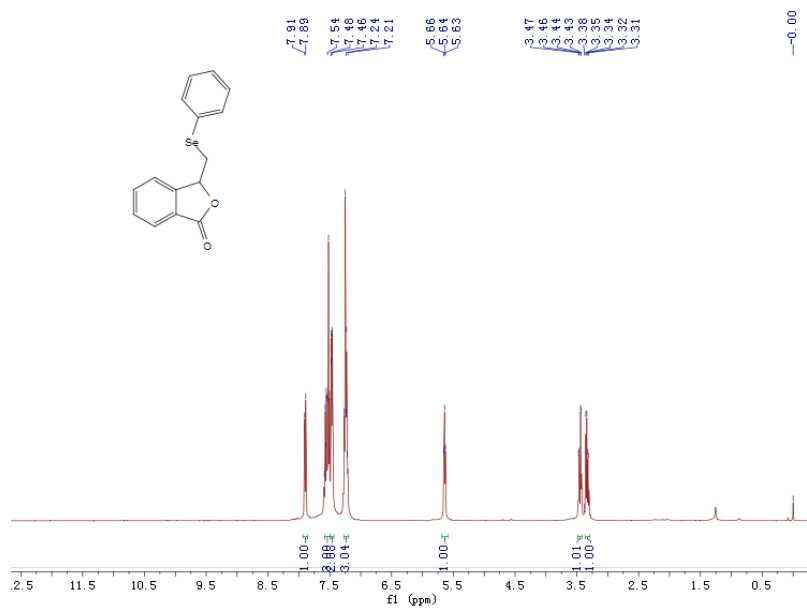
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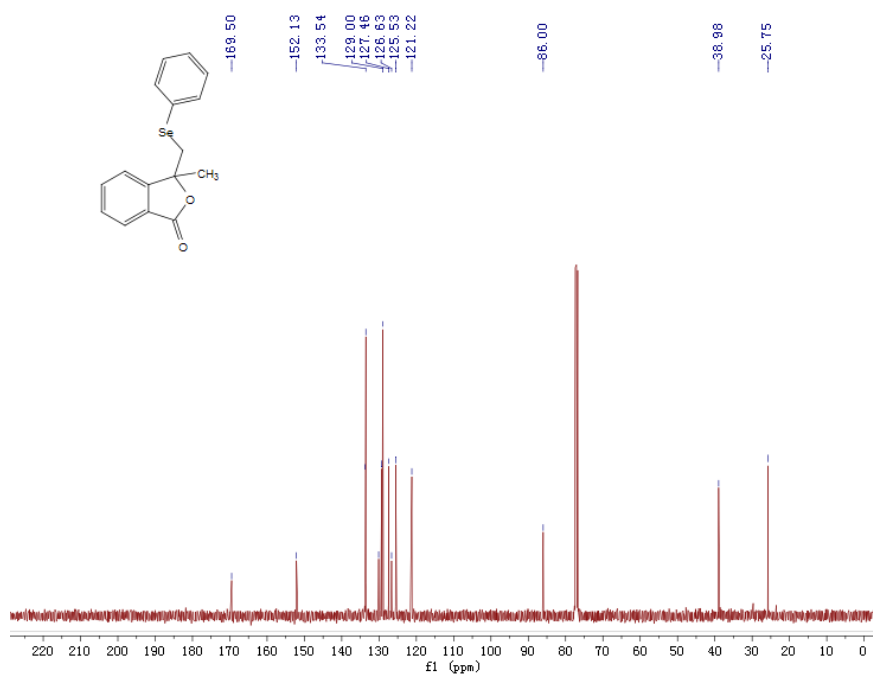
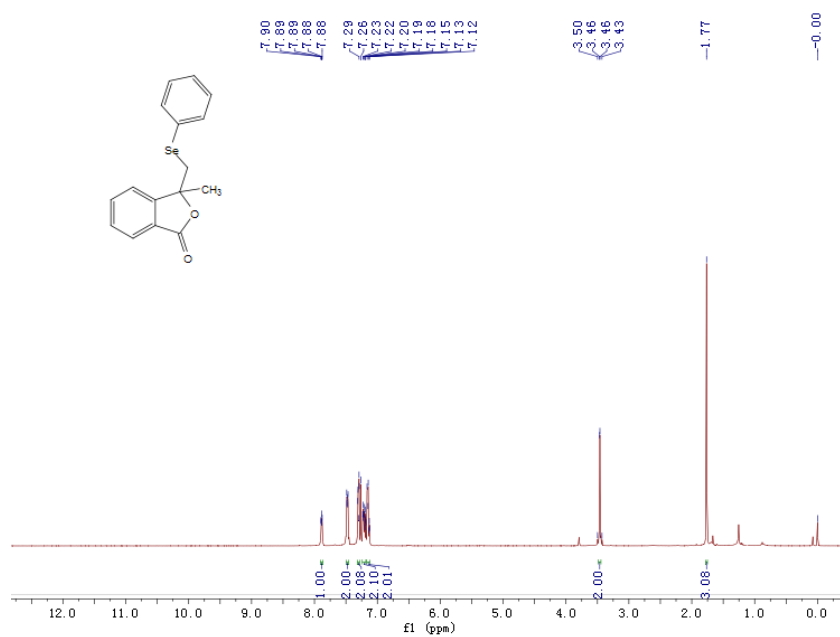
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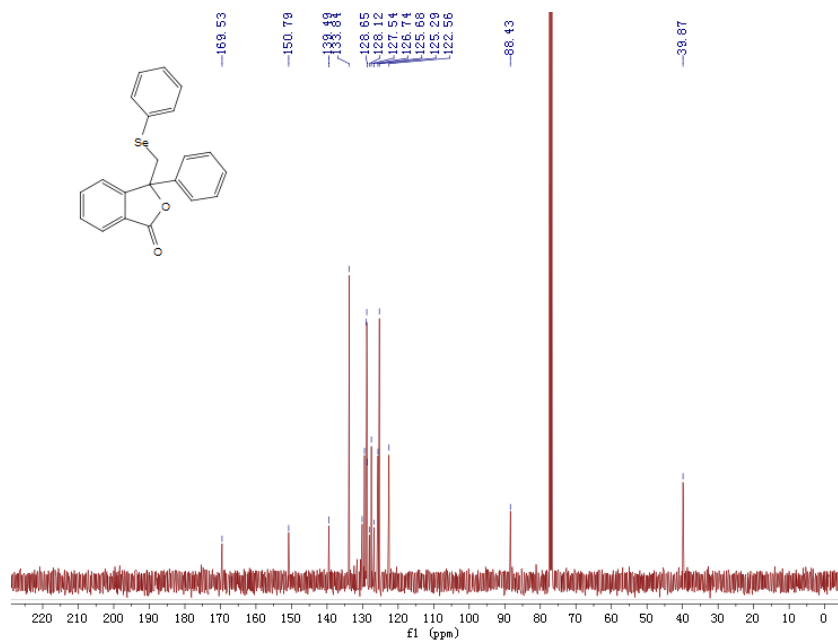
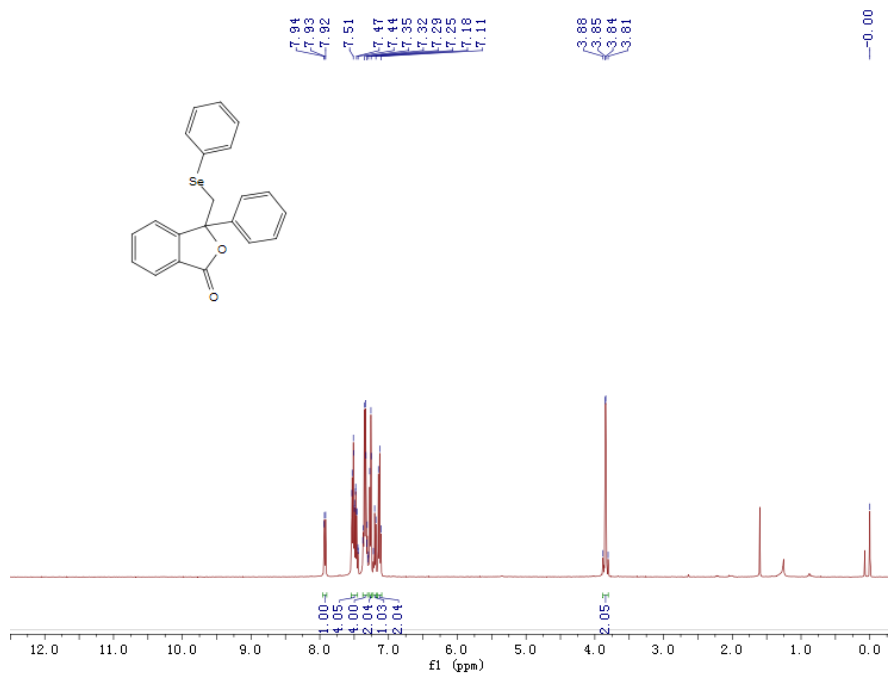
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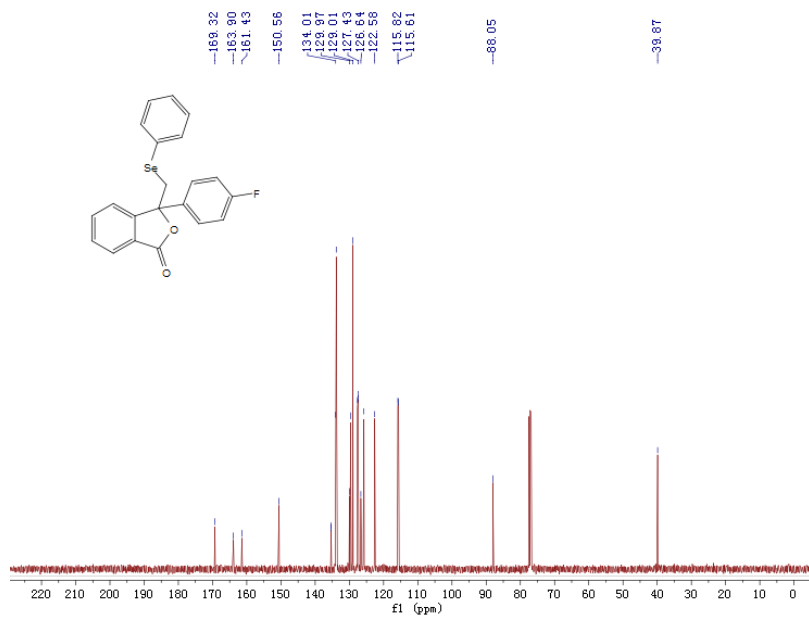
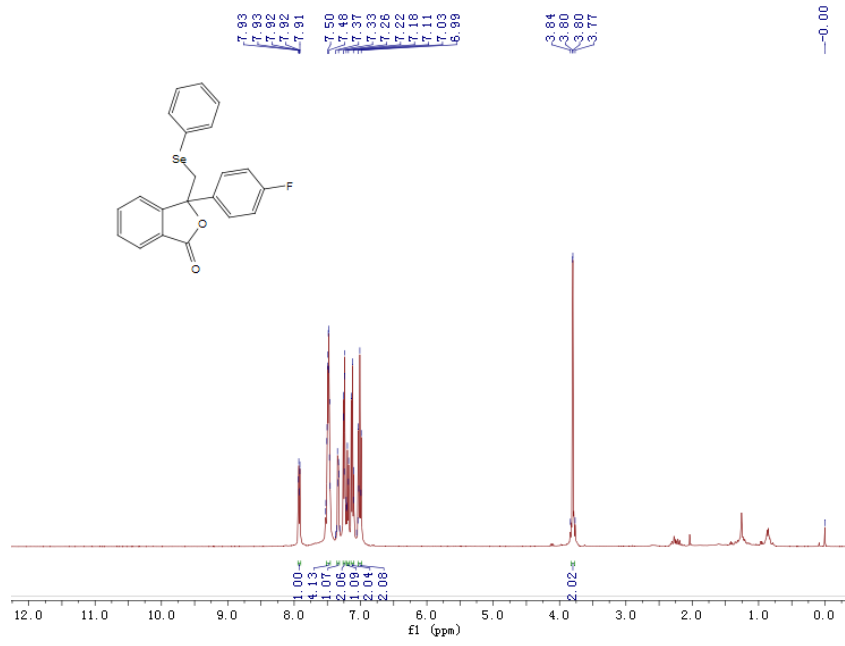
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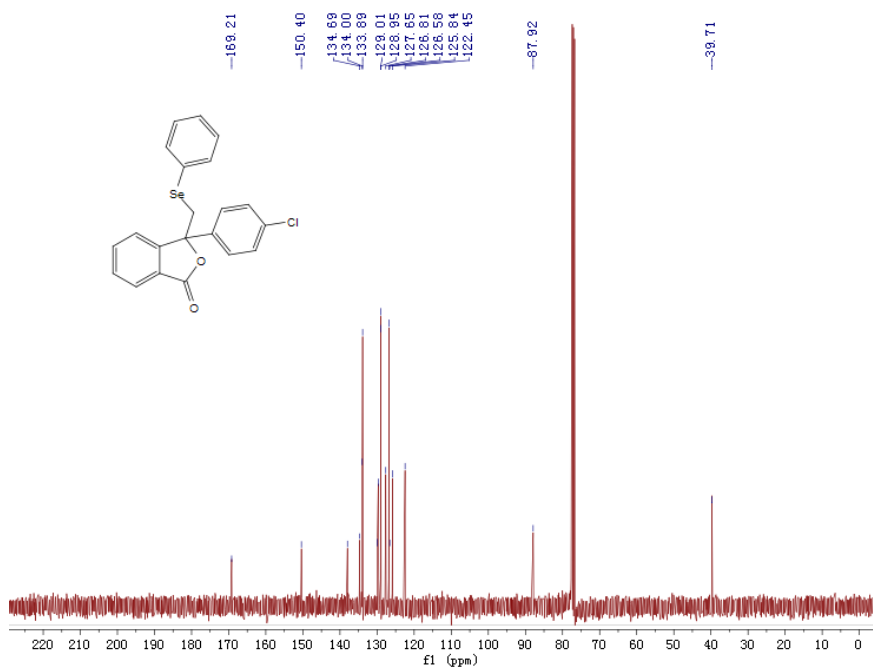
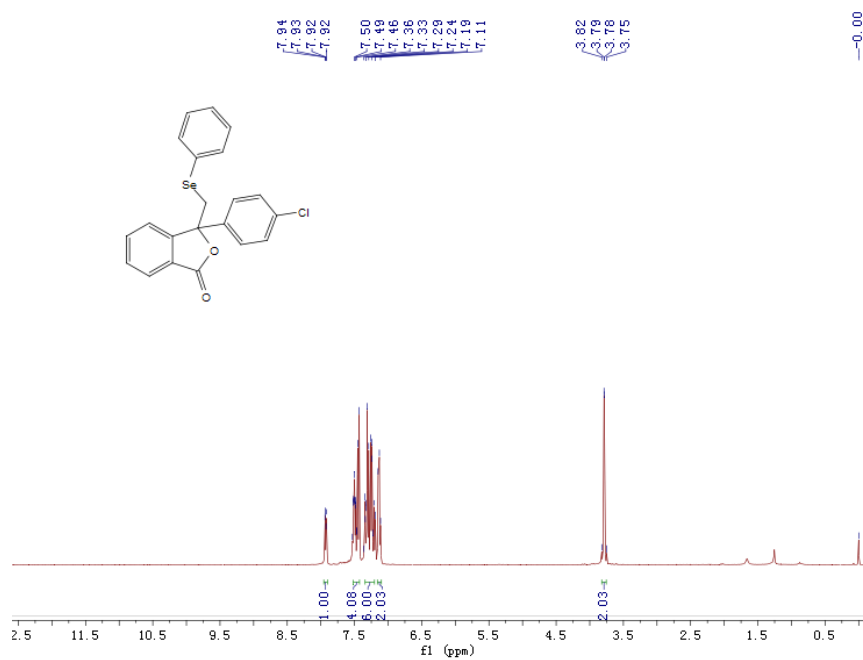
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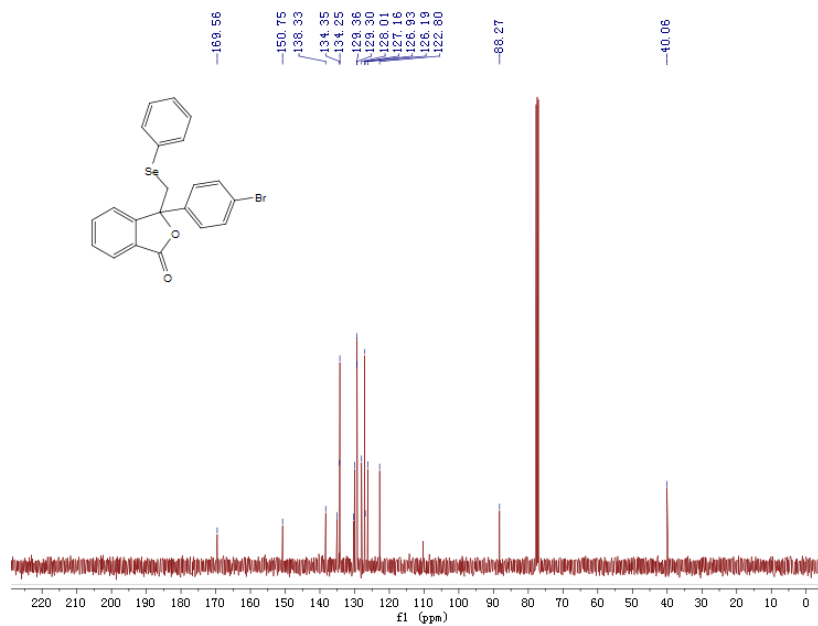
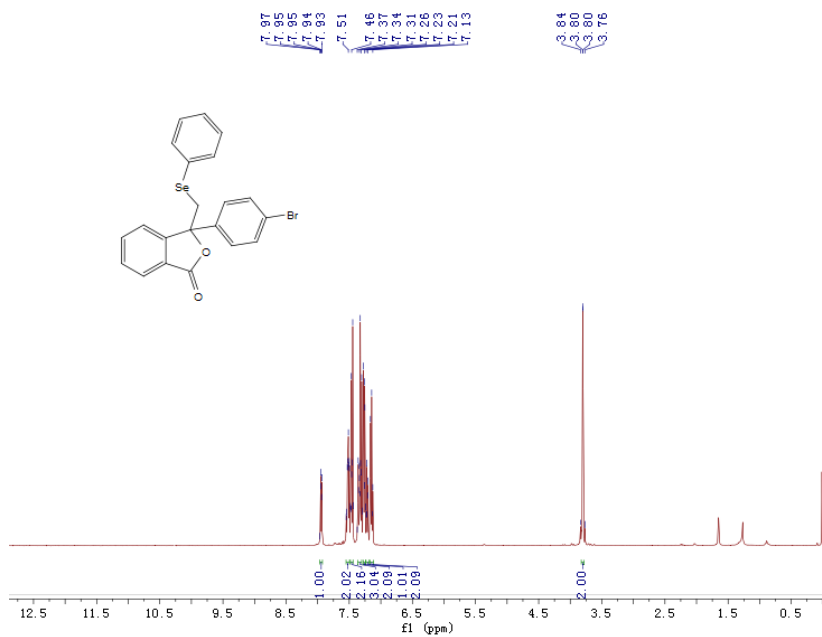
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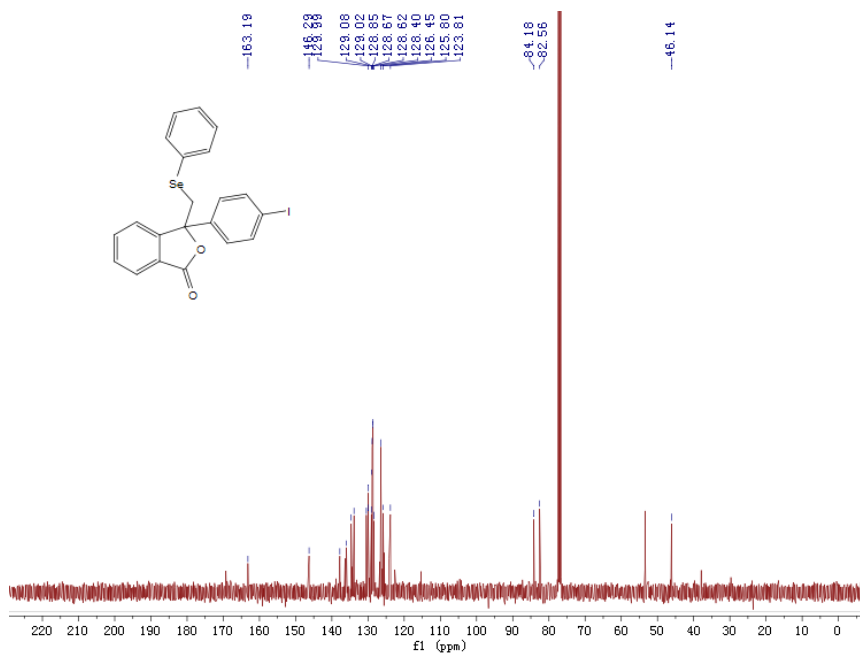
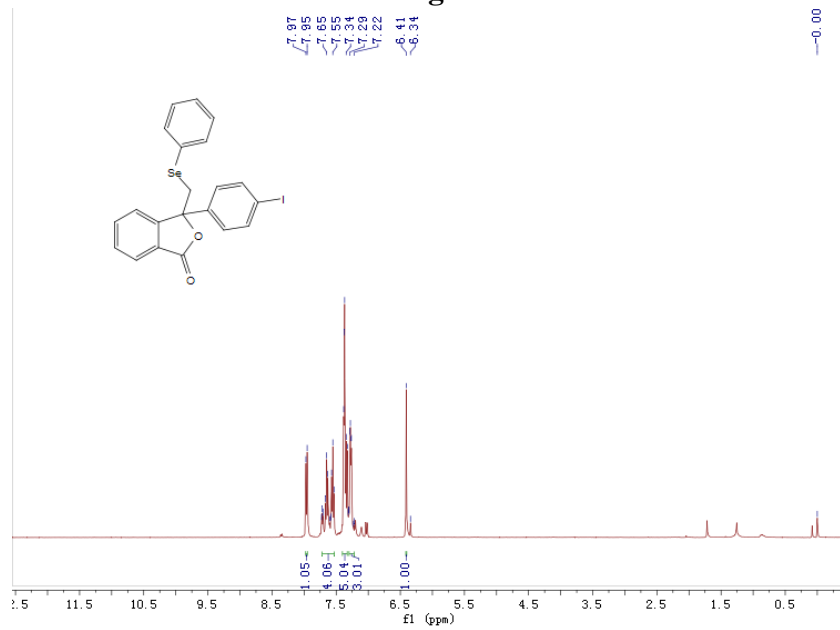
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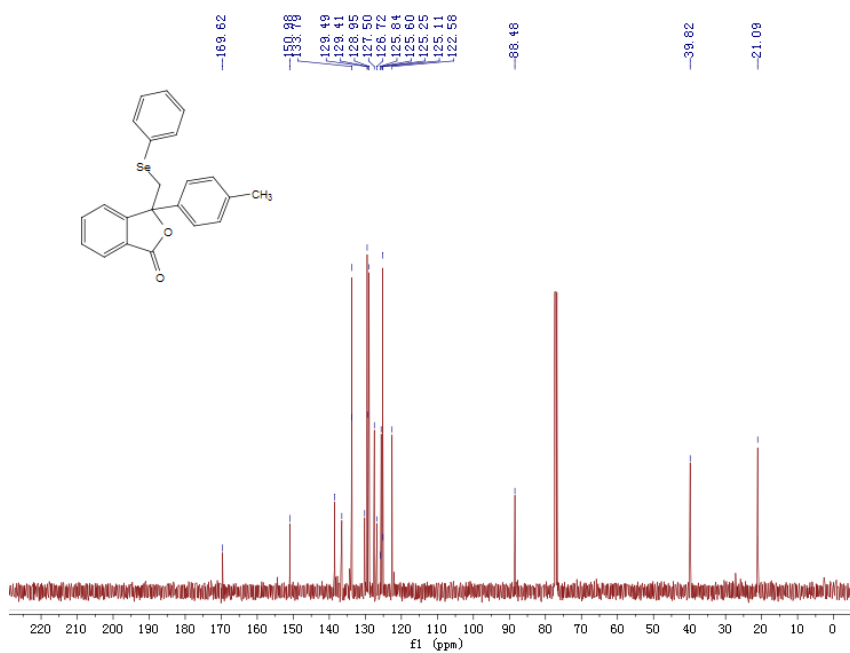
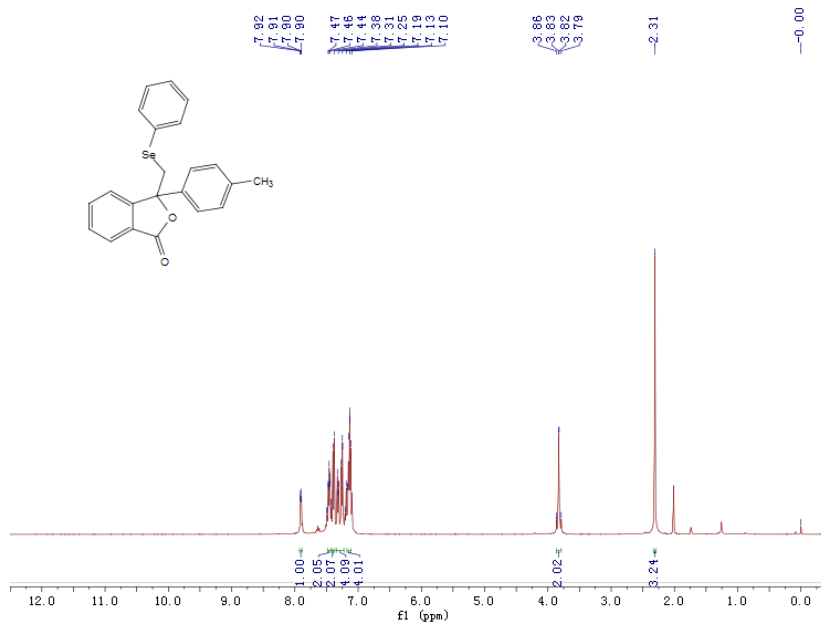
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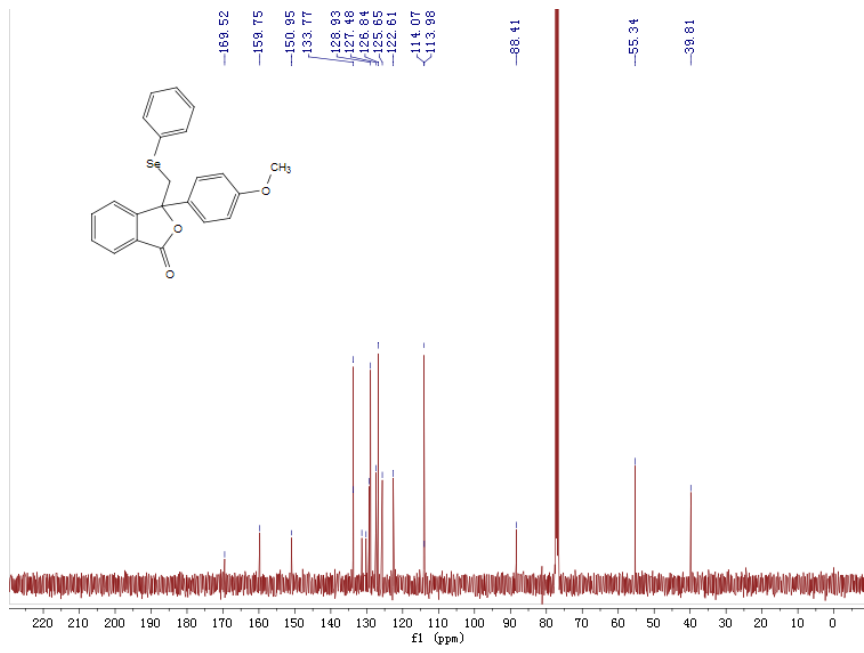
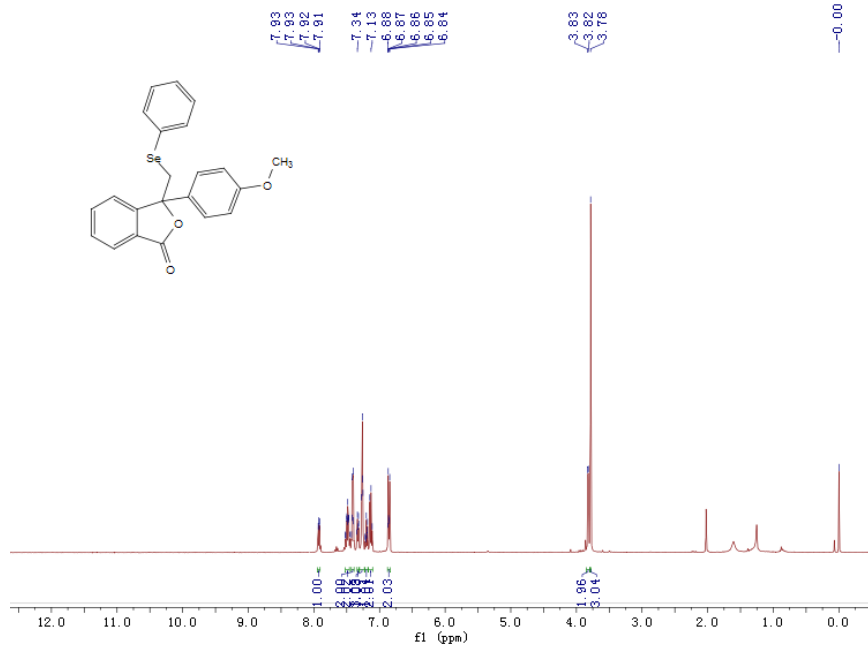
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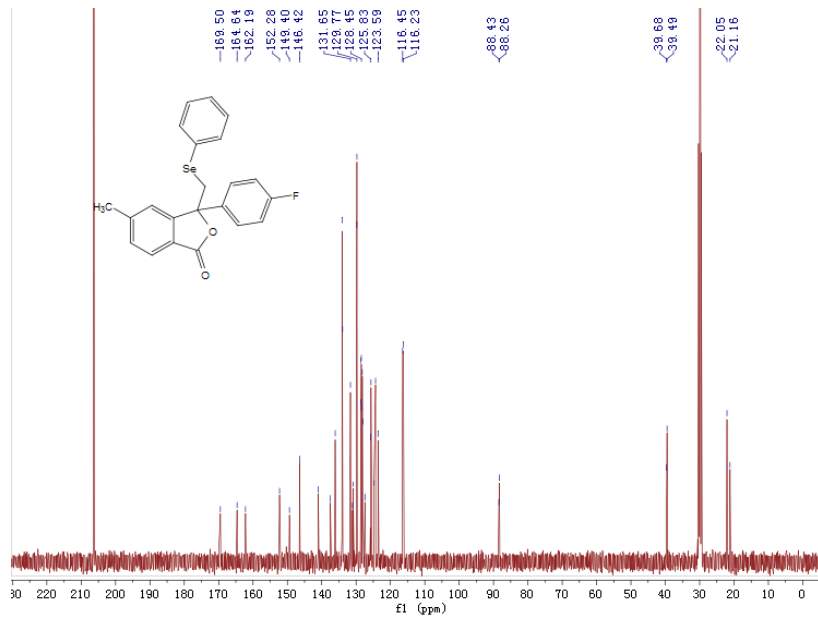
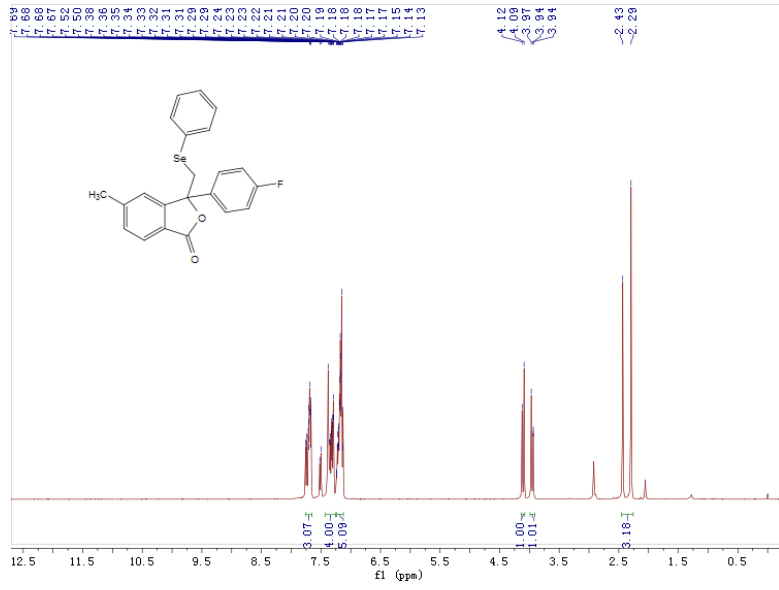
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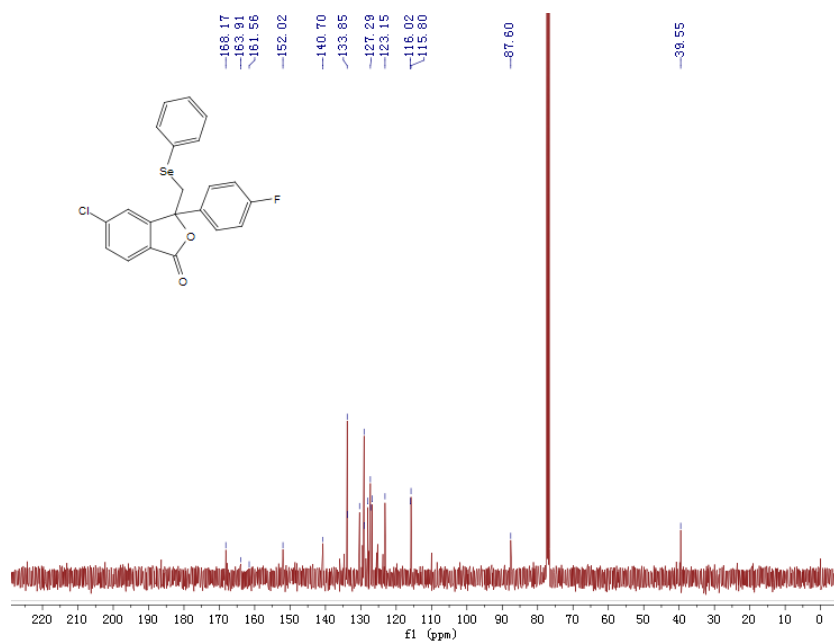
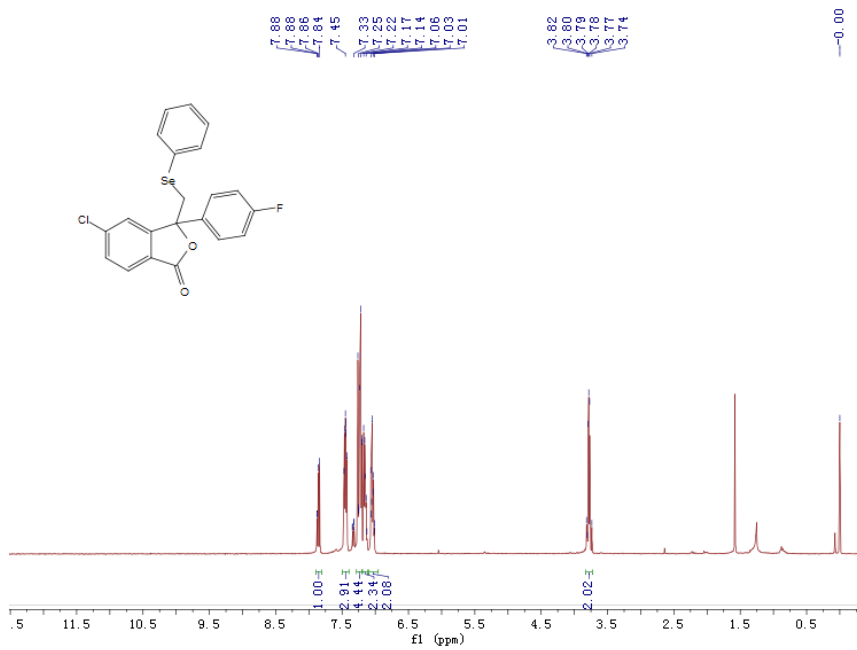
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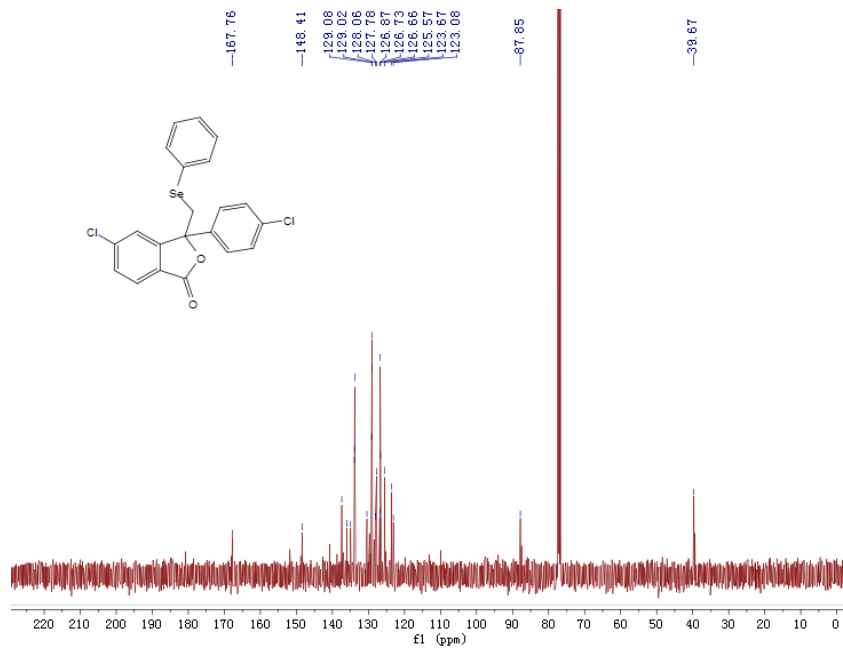
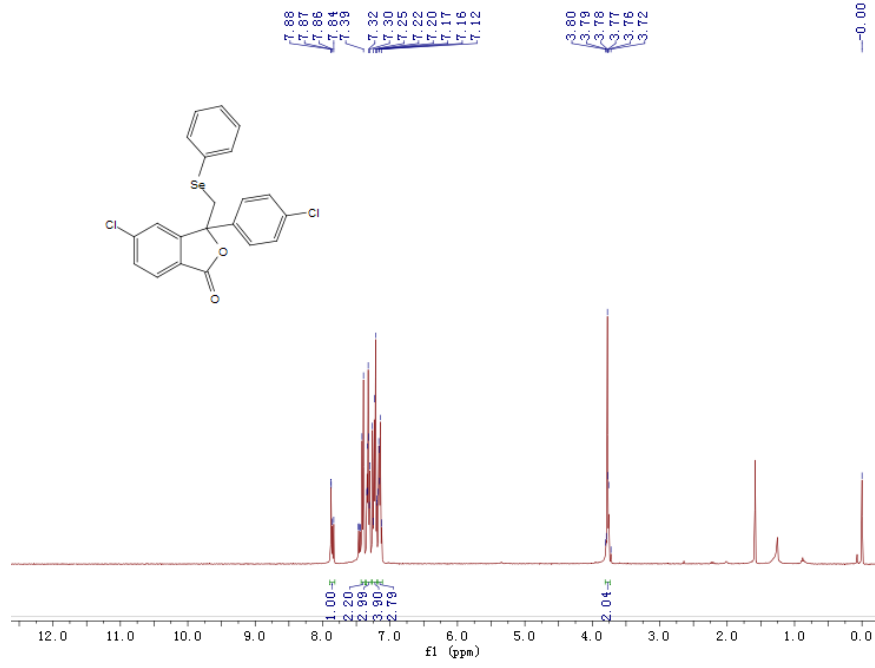
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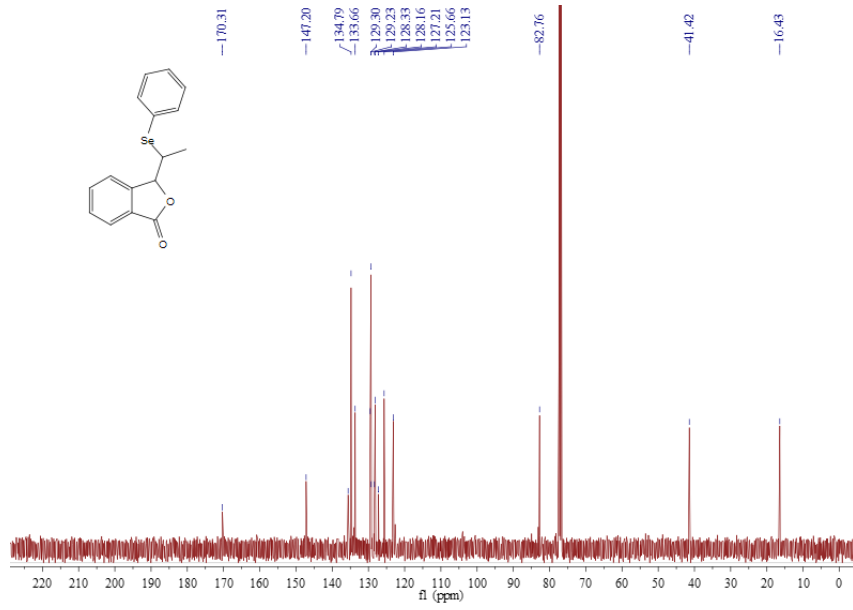
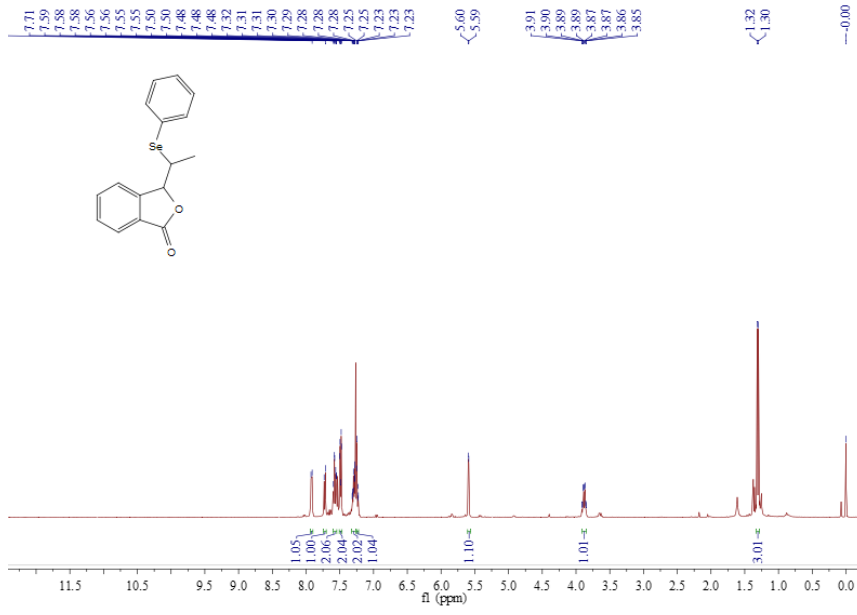
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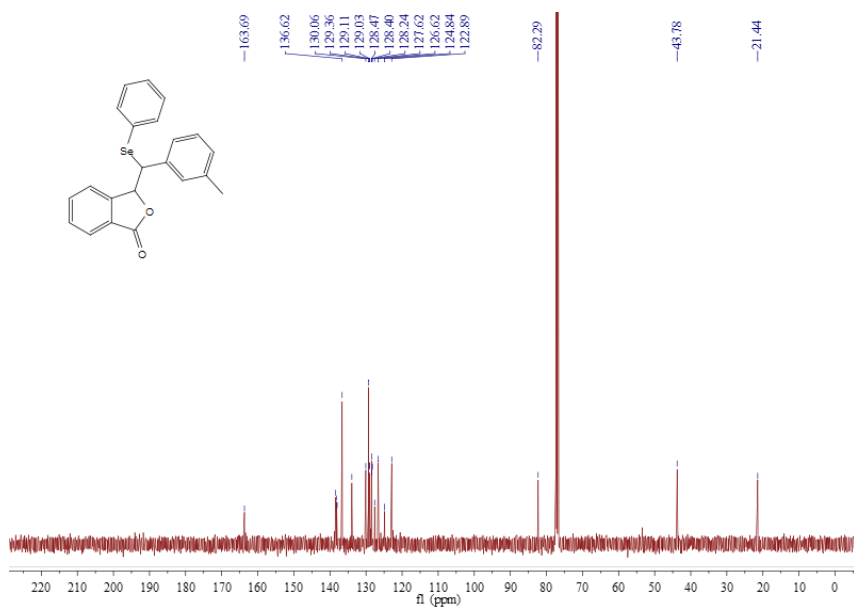
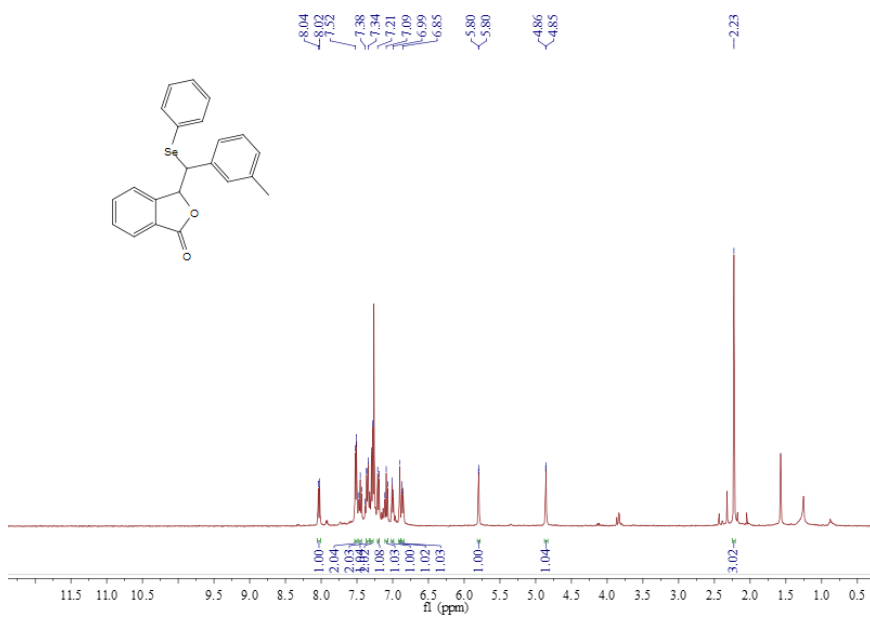
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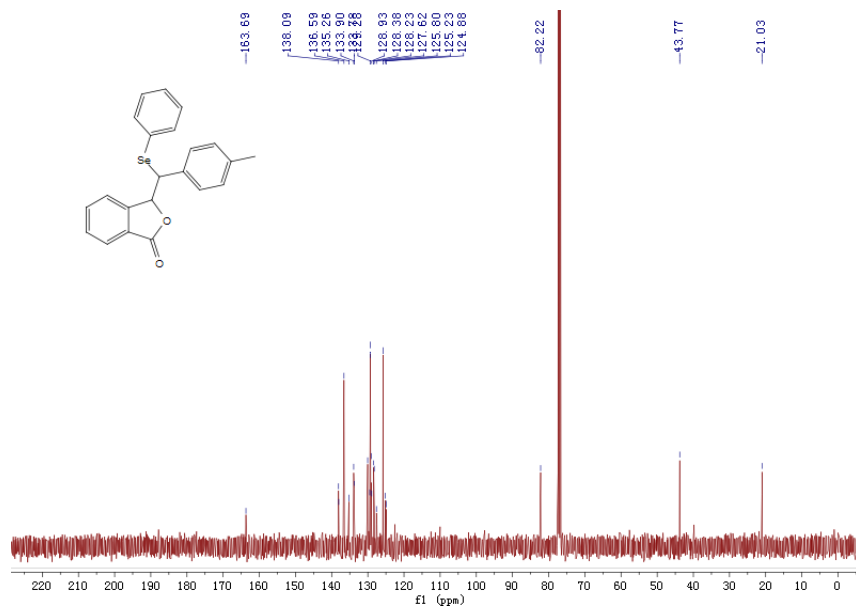
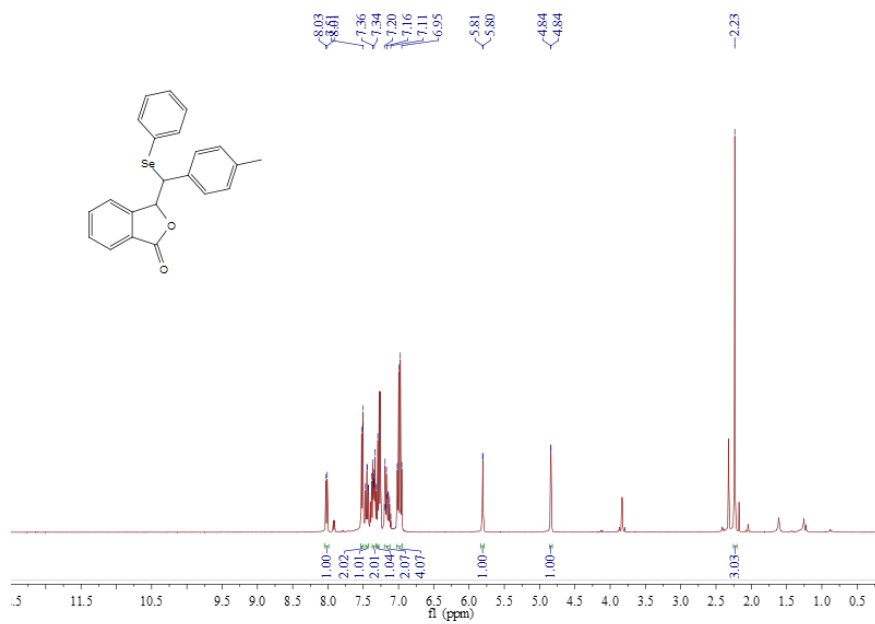
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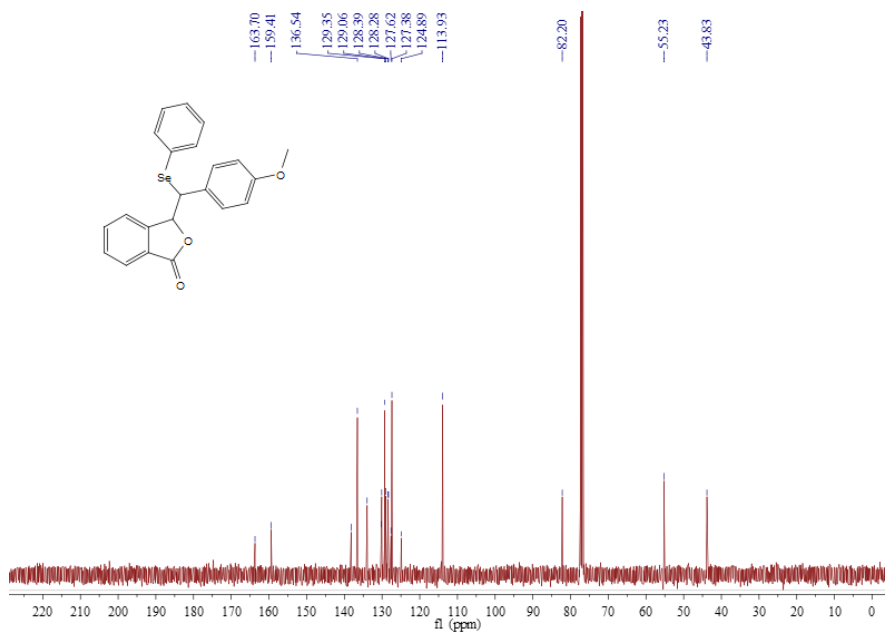
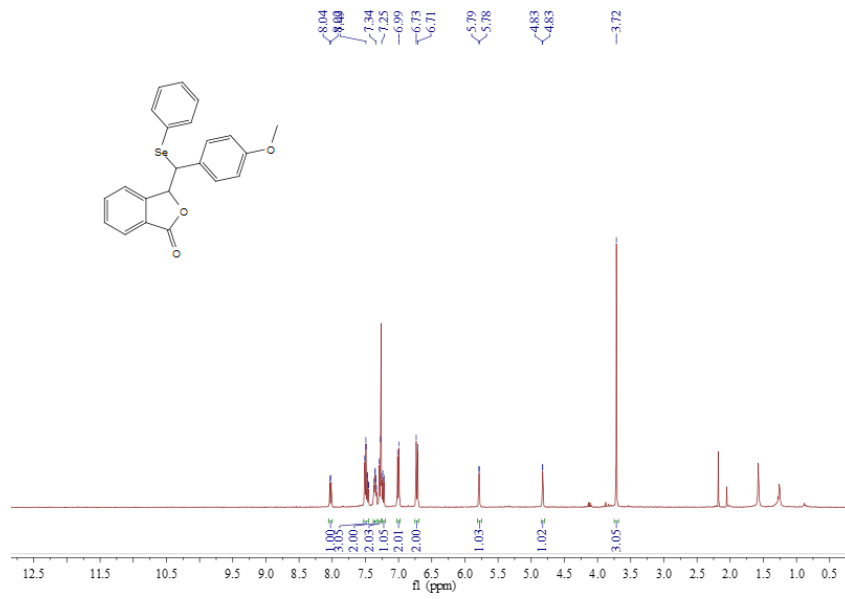
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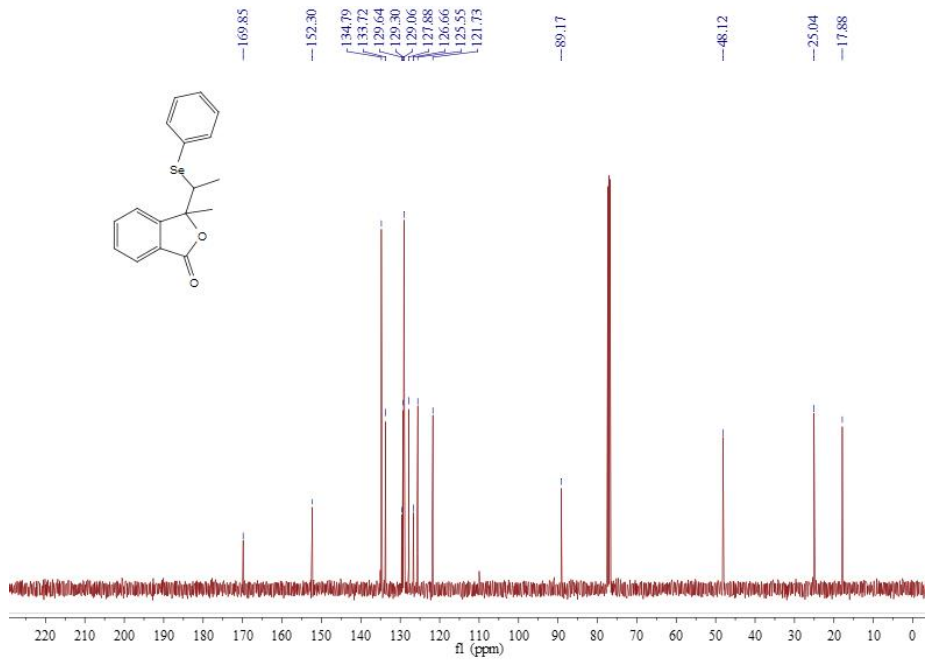
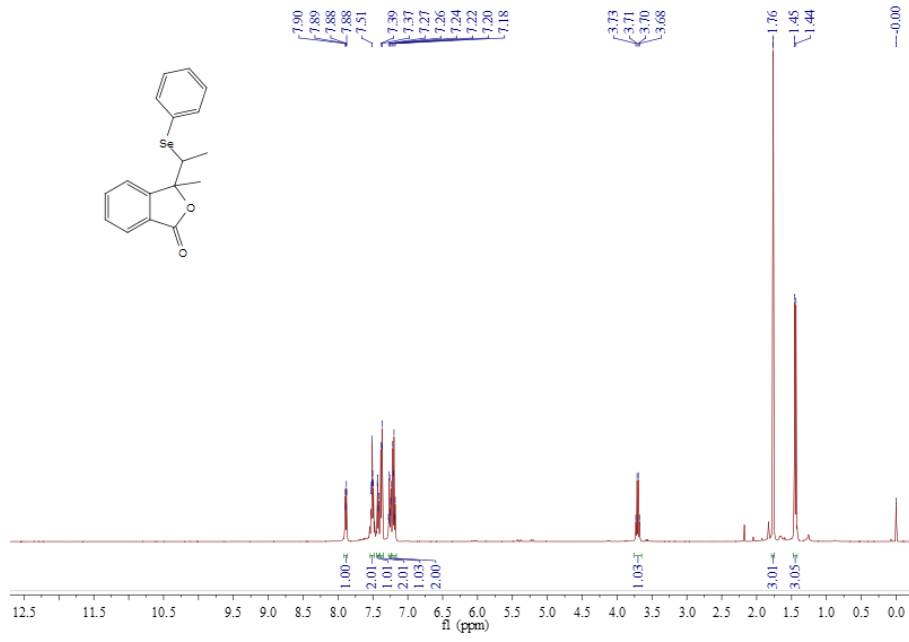
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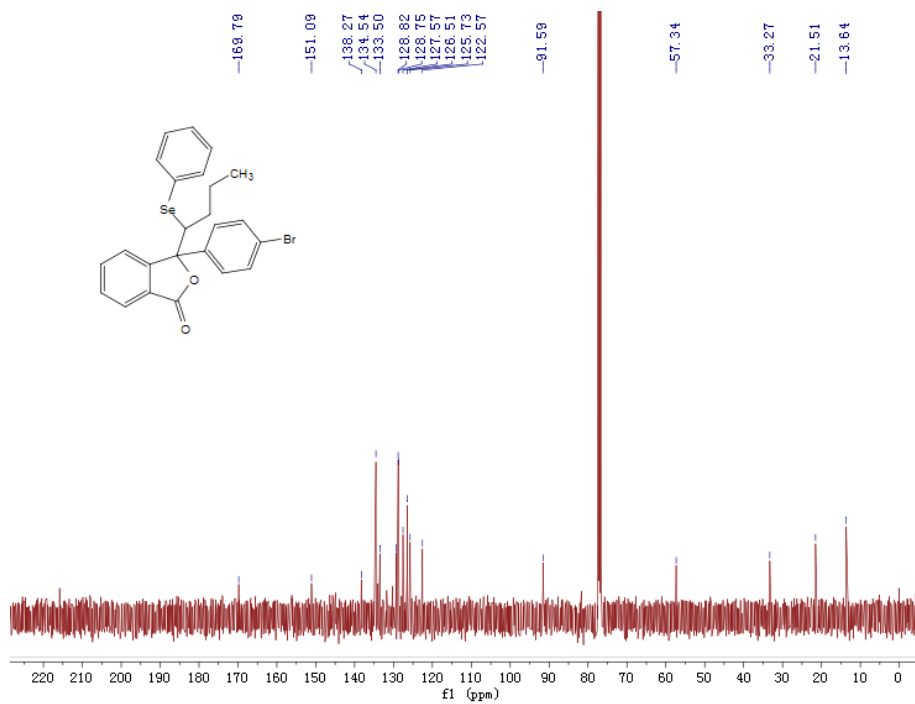
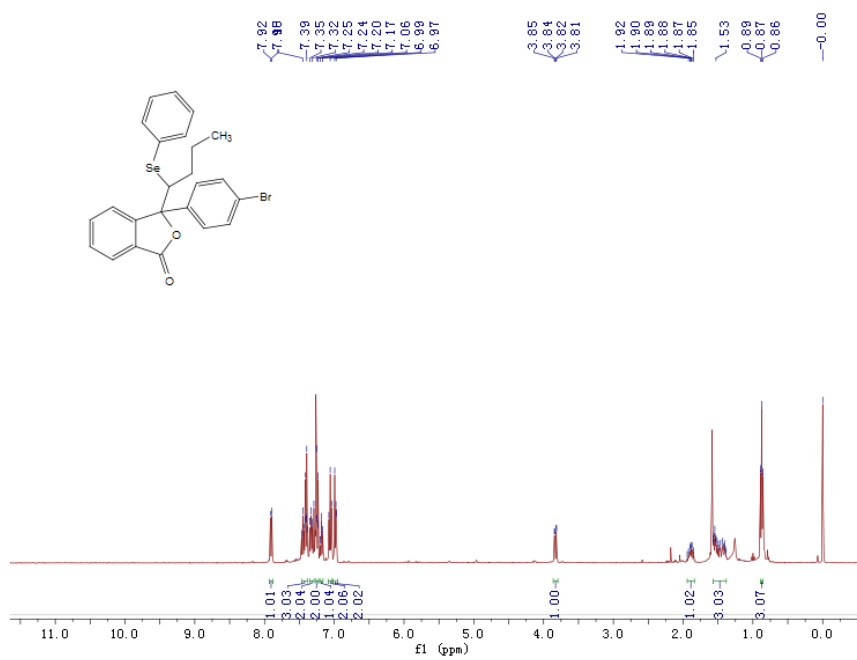
2p



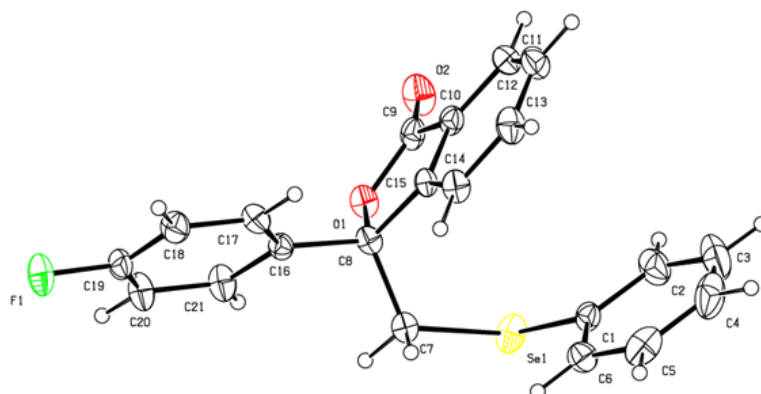
2q



2r



Crystal data and structure refinement for **2d**.



Identification code	1
Empirical formula	C ₂₁ H ₁₅ F O ₂ Se
Formula weight	397.29
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.1709(18) Å alpha = 64.078(3) deg. b = 10.707(2) Å beta = 66.282(3) deg. c = 10.708(2) Å gamma = 89.325(4) deg.
Volume	848.4(3) Å ³
Z, Calculated density	2, 1.555 Mg/m ³
Absorption coefficient	2.234 mm ⁻¹
F(000)	400
Crystal size	0.30 x 0.29 x 0.28 mm
Theta range for data collection	2.16 to 26.50 deg.
Limiting indices	-6 ≤ h ≤ 11, -13 ≤ k ≤ 13, -13 ≤ l ≤ 13
Reflections collected / unique	5596 / 3522 [R(int) = 0.0332]
Completeness to theta = 26.50	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.5735 and 0.5538
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3522 / 0 / 227
Goodness-of-fit on F ²	1.055
Final R indices [I > 2σ(I)]	R1 = 0.0435, wR2 = 0.1092
R indices (all data)	R1 = 0.0553, wR2 = 0.1151
Extinction coefficient	0.025(3)
Largest diff. peak and hole	0.761 and -0.860 e.Å ⁻³