

An unprecedented protocol for the synthesis of 3-hydroxy-3-phenacyloxindole derivatives with indolin-2-ones and α -substituted ketones

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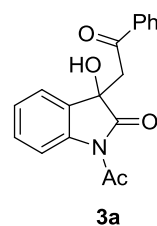
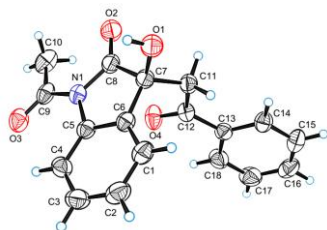
*E-mail: yzchen@zmc.edu.cn

Supporting Information

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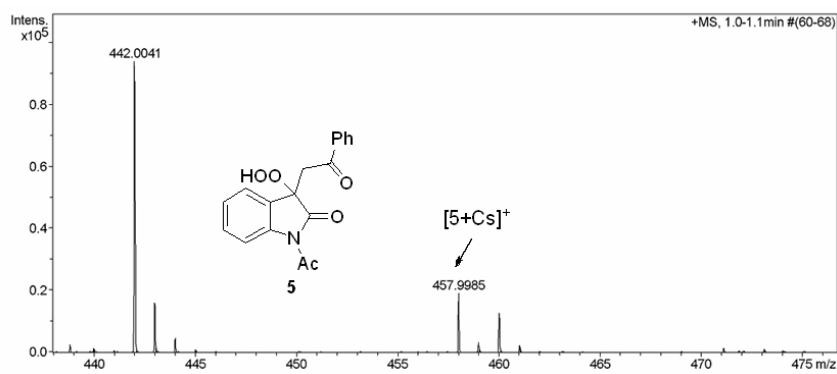
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1. X-ray crystallographic data of compound 3a (CCDC: 1437932)

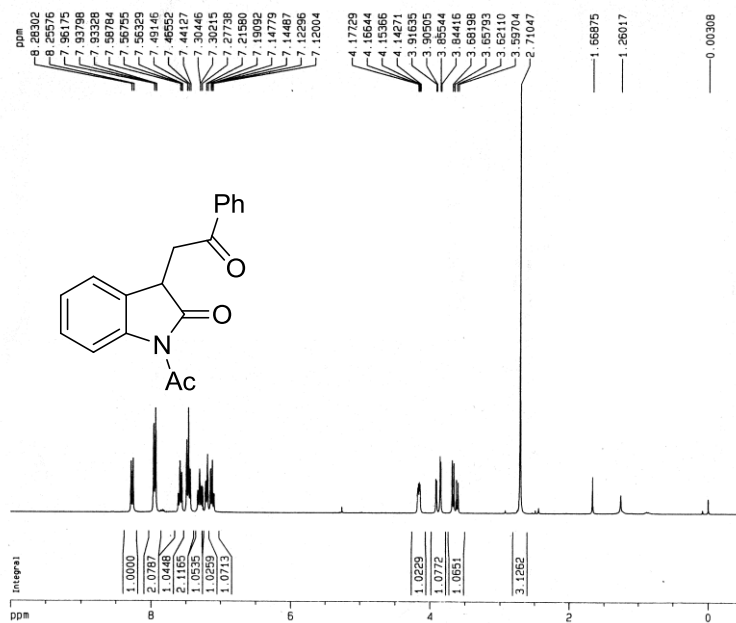


Empirical formula	C ₁₈ H ₁₅ NO ₄
Formula weight	309.31
Temperature/K	289(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å, b/Å, c/Å	11.1239(3), 8.9956(2), 15.6586(4)
α/°, β/°, γ/°	90, 105.218(2), 90
Volume/Å ³	1511.95(7)
Z	4
ρ _{calc} /cm ³	1.359
μ/mm ⁻¹	0.798
F(000)	648.0
Crystal size/mm ³	0.28 × 0.24 × 0.2
Radiation	CuKα (λ = 1.54184)
2θ range for data collection	12.432 to 139.398
Index ranges	-13 ≤ h ≤ 13, -10 ≤ k ≤ 9, -18 ≤ l ≤ 12
Reflections collected	6820
Independent reflections	2747 [R _{int} = 0.0135, R _{sigma} = 0.0143]
Data/restraints/parameters	2747/0/210
Goodness-of-fit on F ²	1.065
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0422, wR ₂ = 0.1106
Final R indexes [all data]	R ₁ = 0.0450, wR ₂ = 0.1128
Largest diff. peak/hole / e Å ⁻³	0.19/-0.15

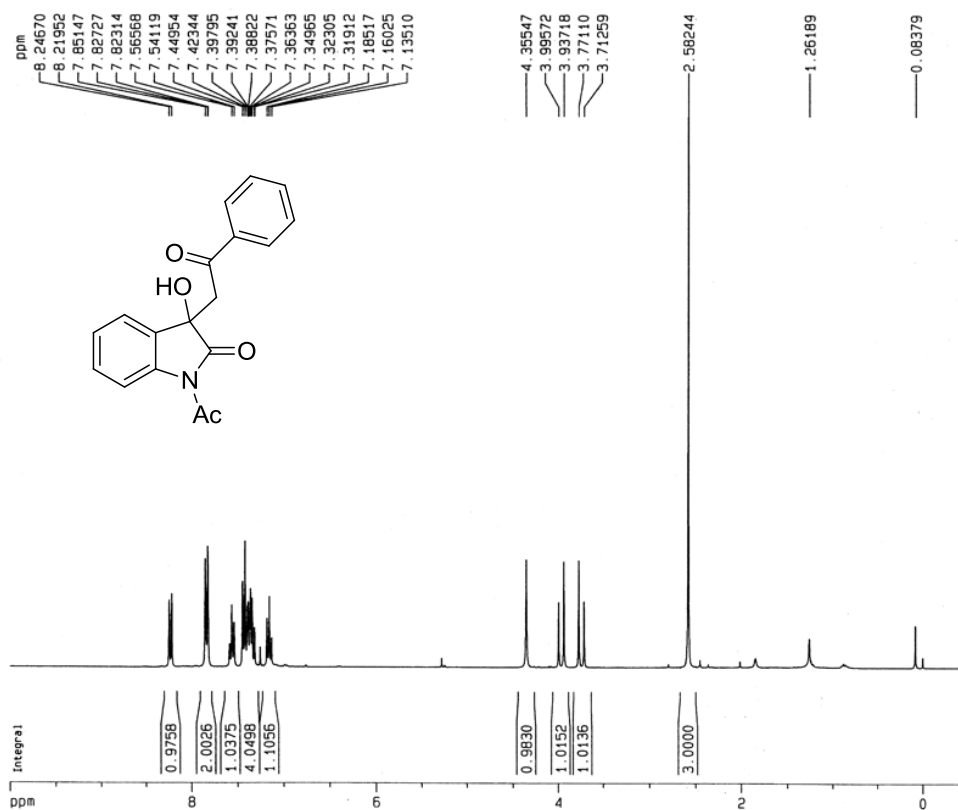
2. Mass Spectrum of hydroperoxide oxindoles 5 in the proposed pathway

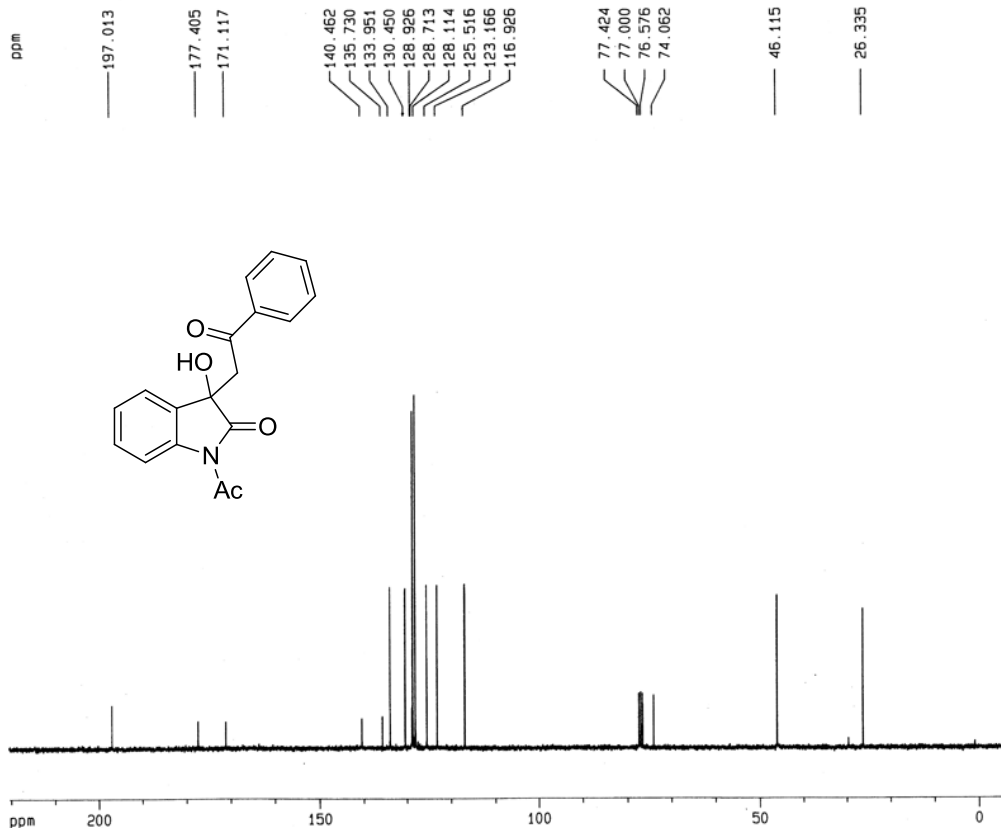


3. ^1H NMR of 3-monosubstituted oxindole 4 in the proposed pathway

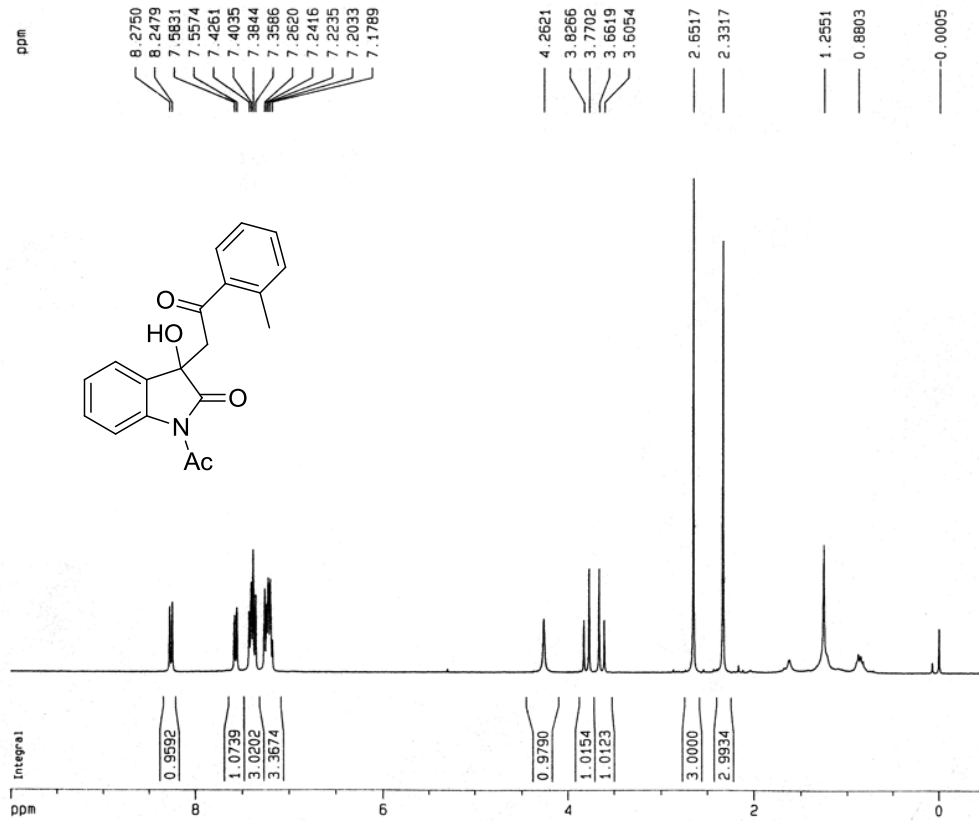


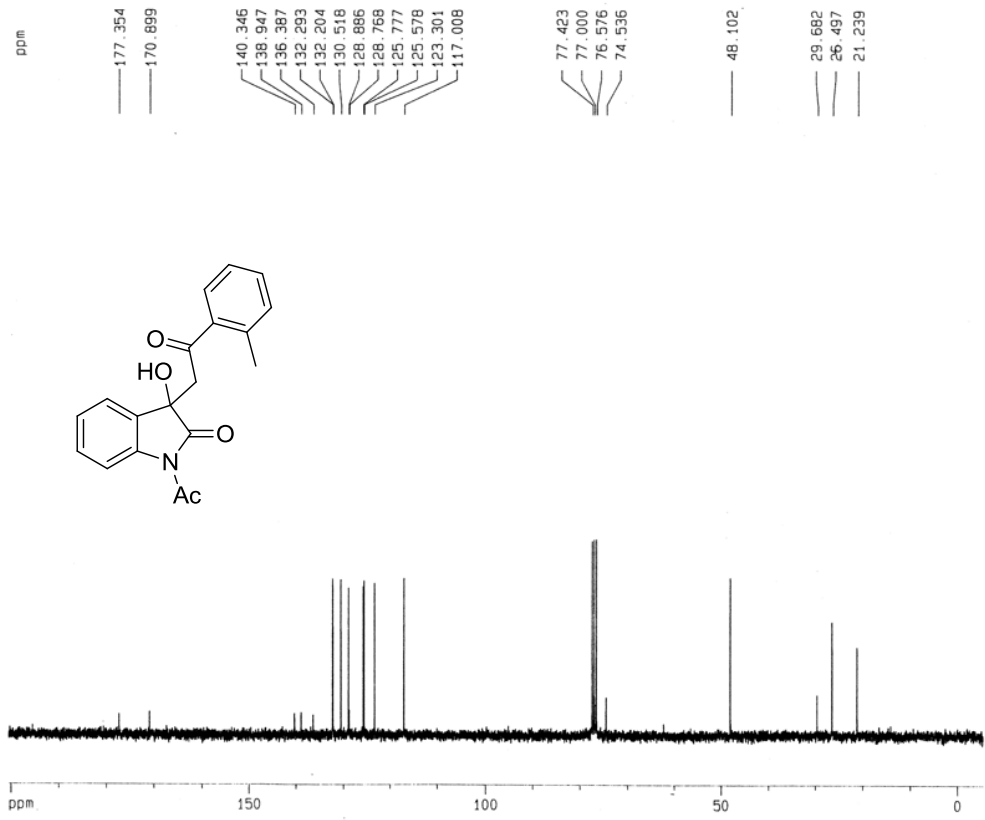
4. The copies of ^1H NMR, ^{13}C NMR spectra for compounds 3
 ^1H and ^{13}C NMR of 3a



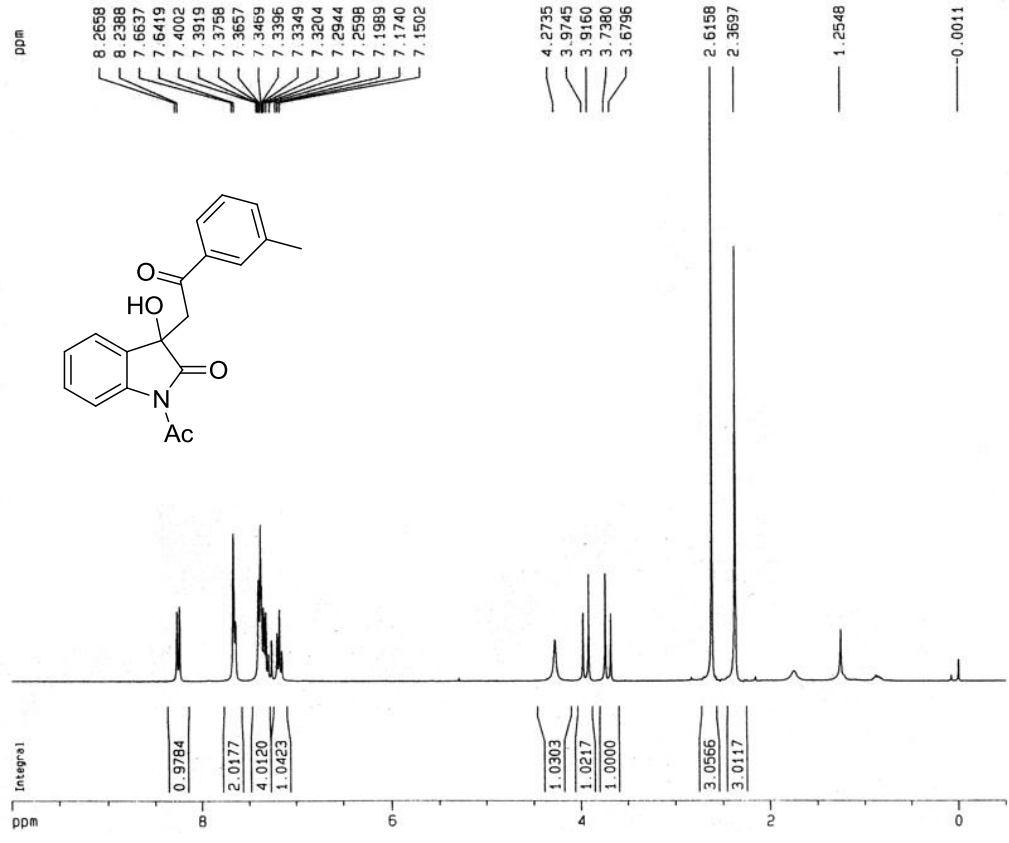


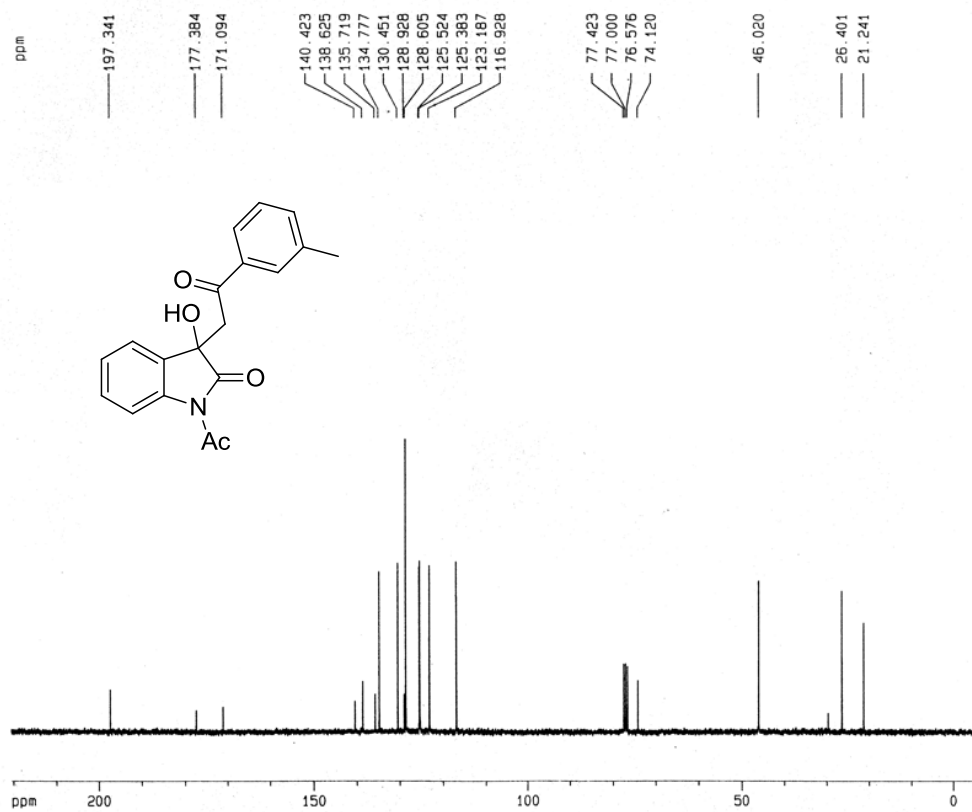
¹H and ¹³C NMR of 3b



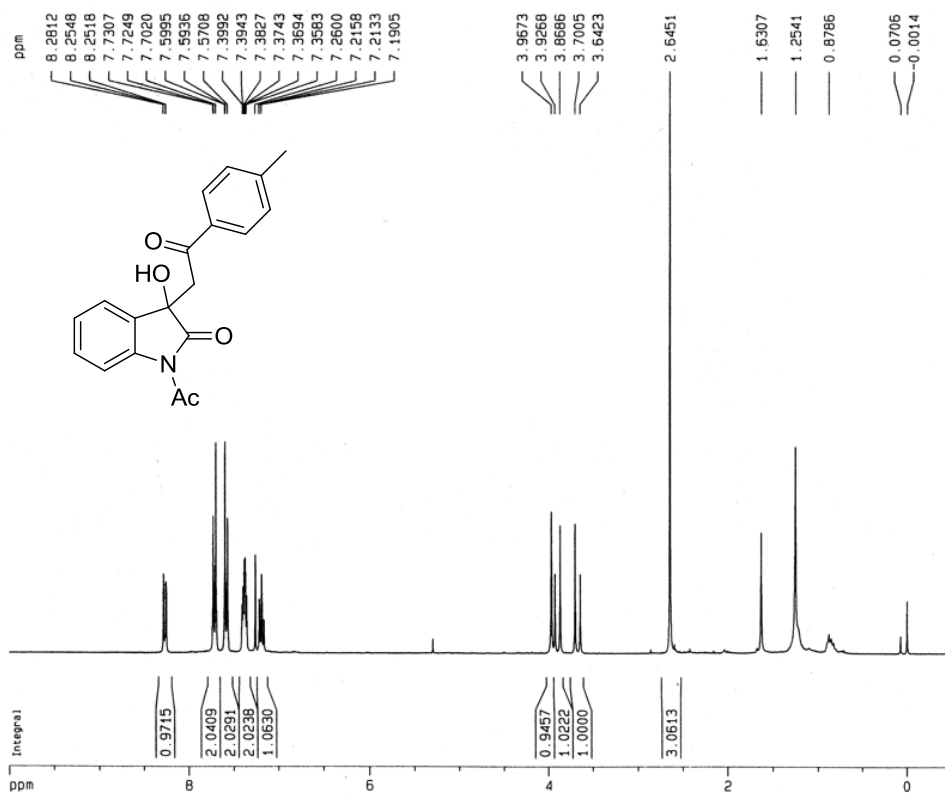


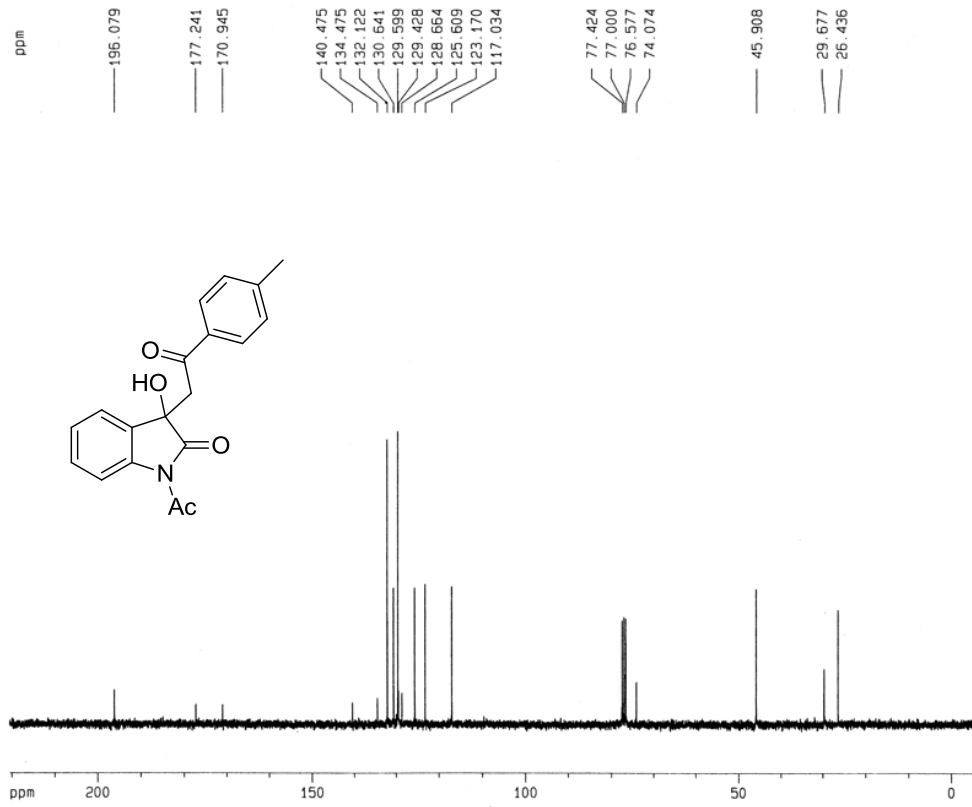
¹H and ¹³C NMR of 3c



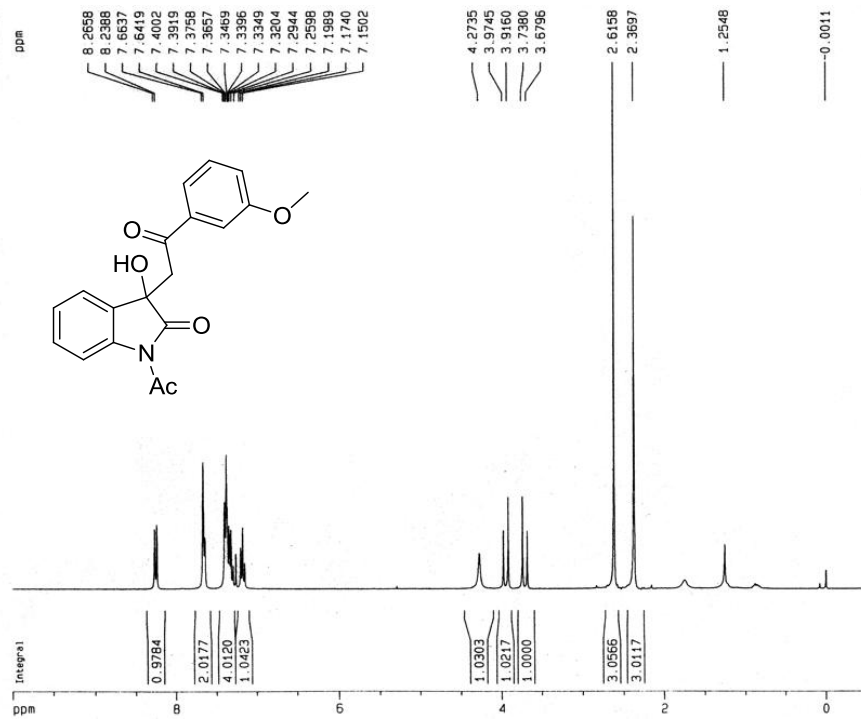


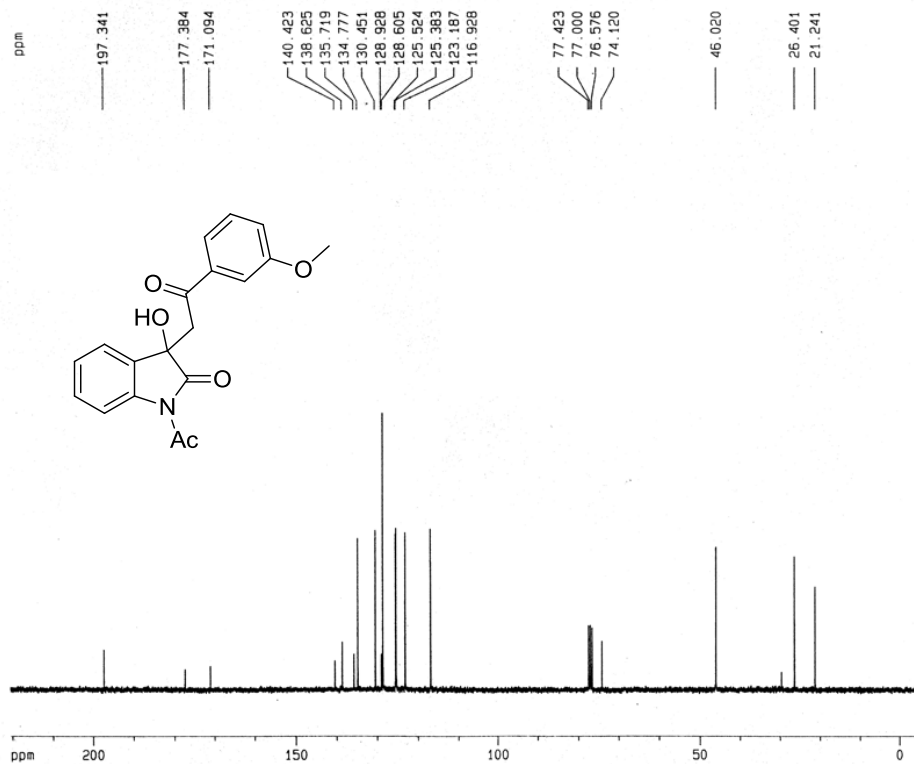
¹H and ¹³C NMR of 3d



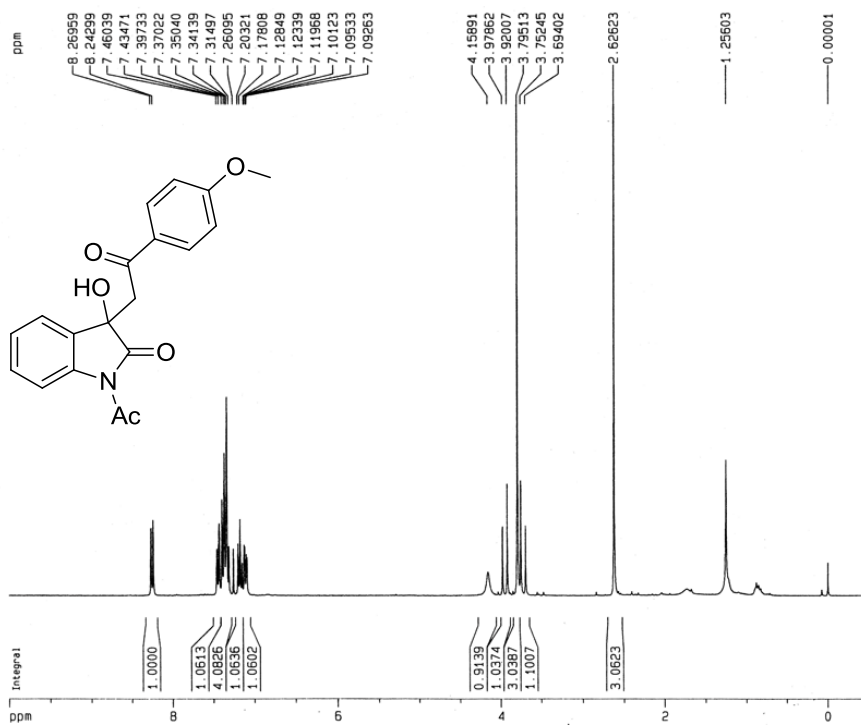


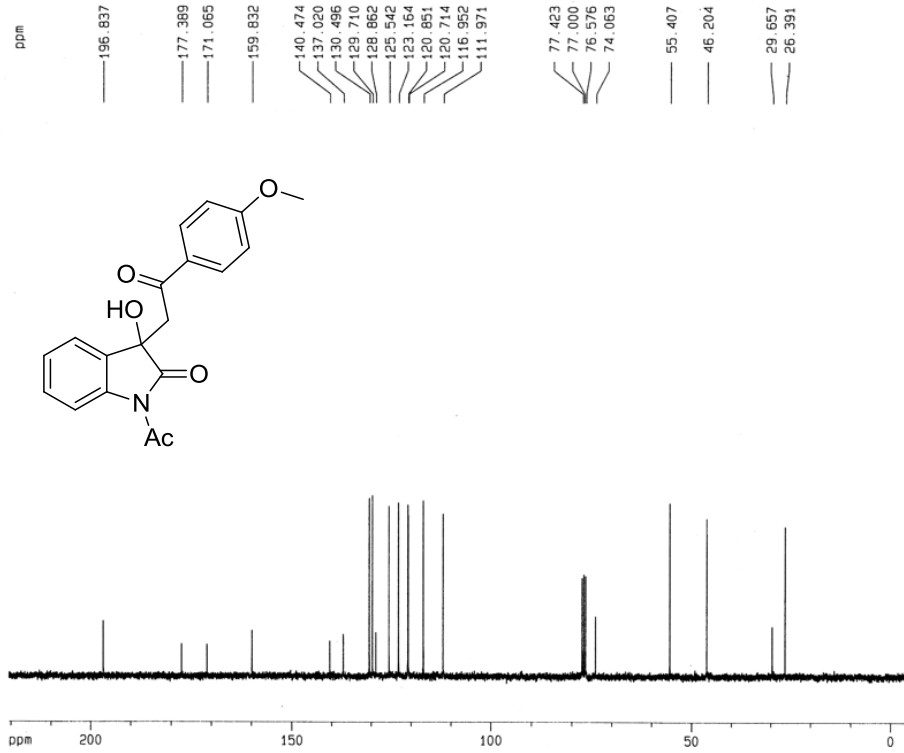
¹H and ¹³C NMR of 3e



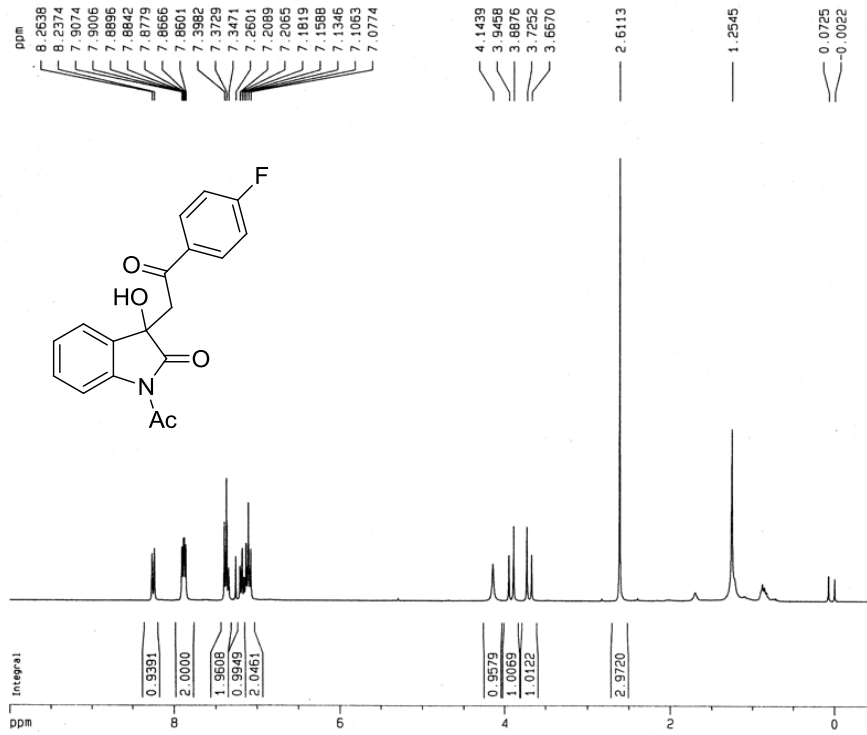


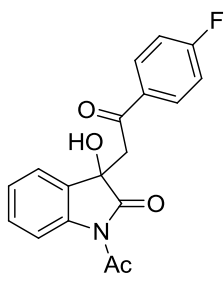
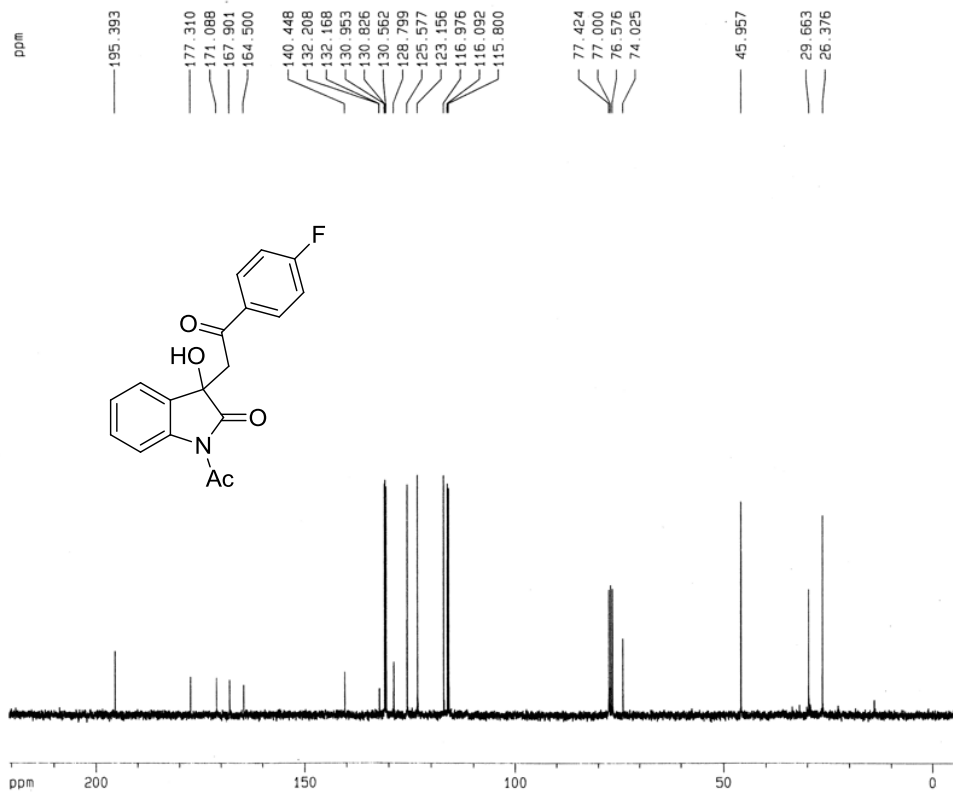
^1H and ^{13}C NMR of 3f



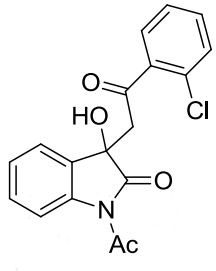
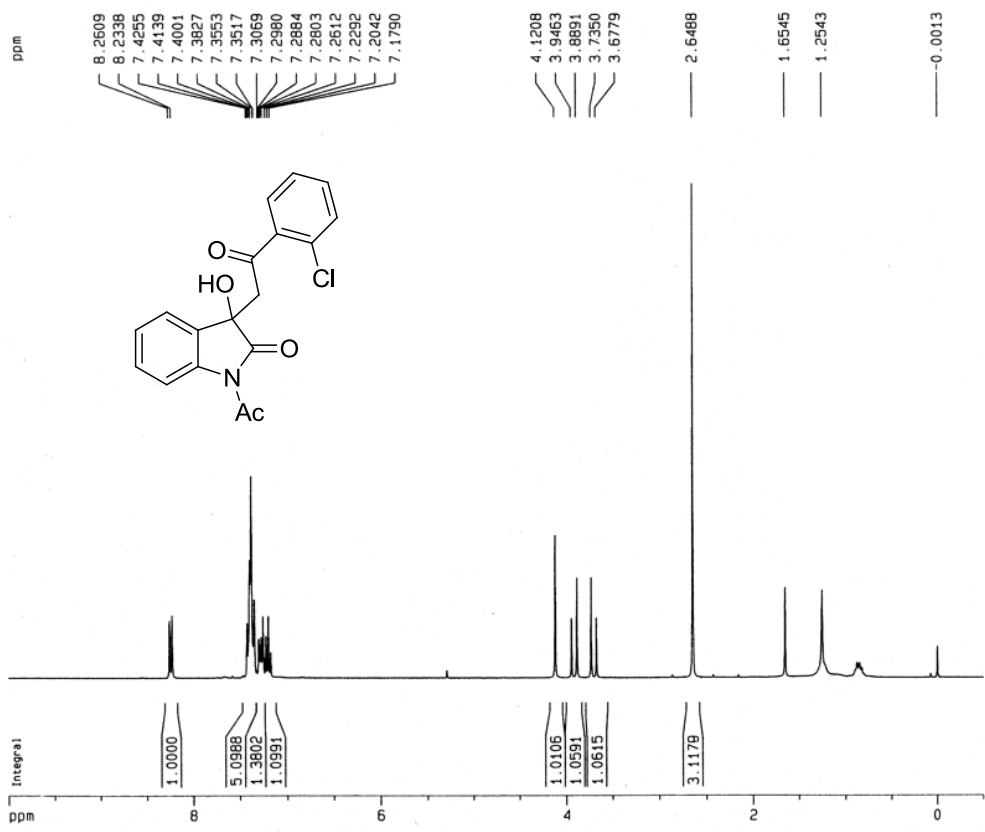


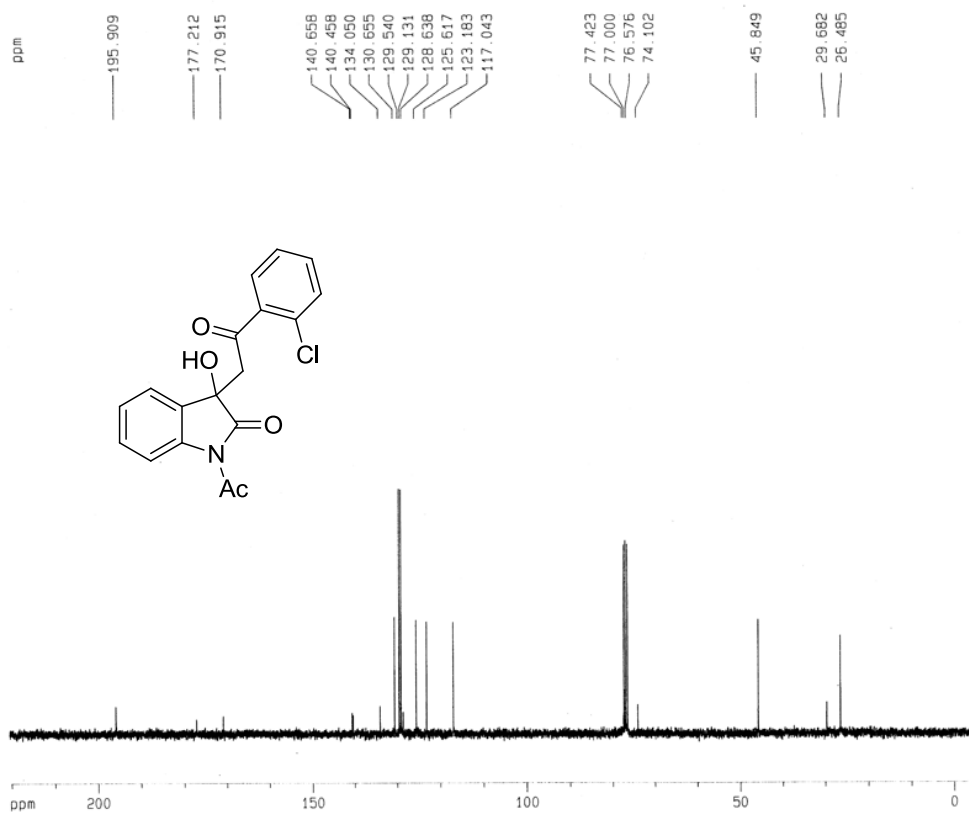
¹H and ¹³C NMR of 3g



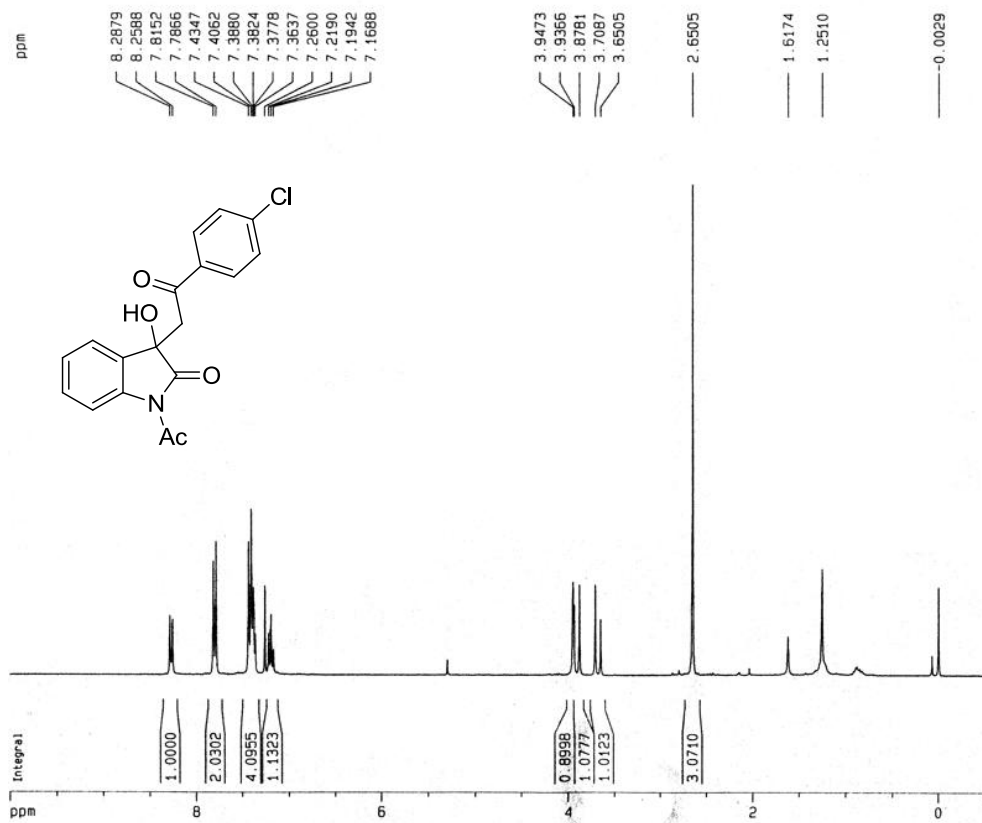


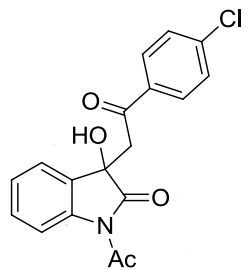
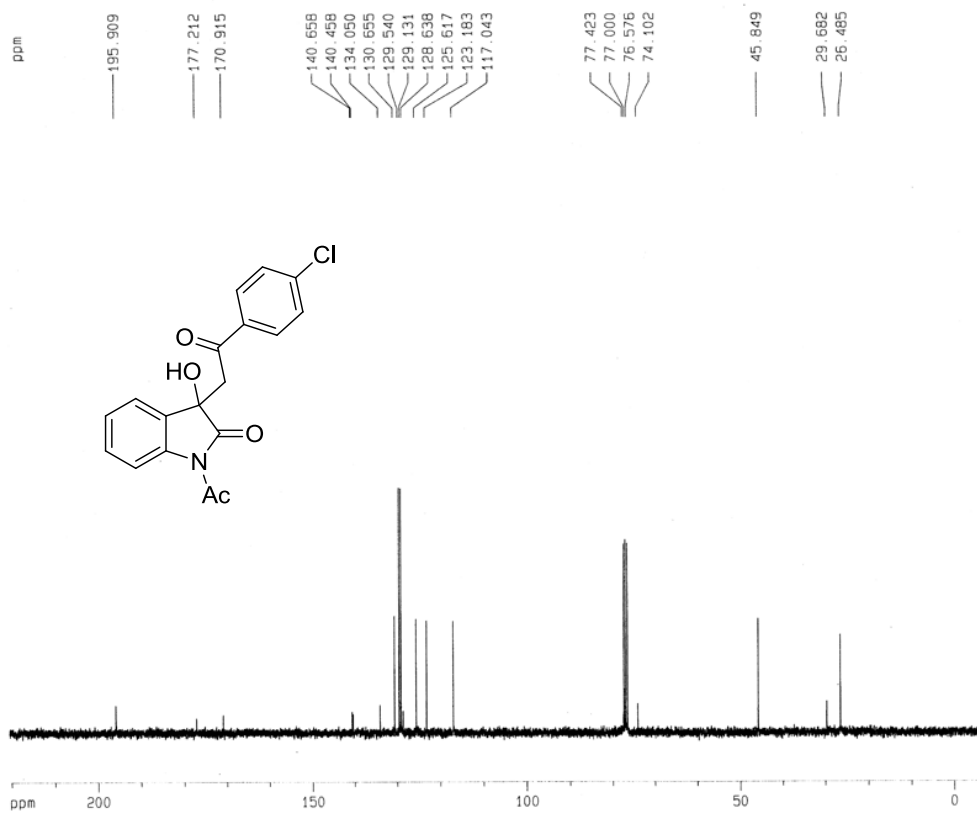
¹H and ¹³C NMR of 3h



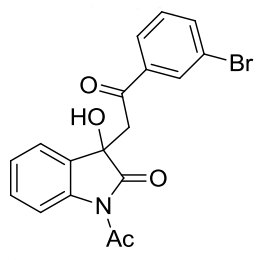
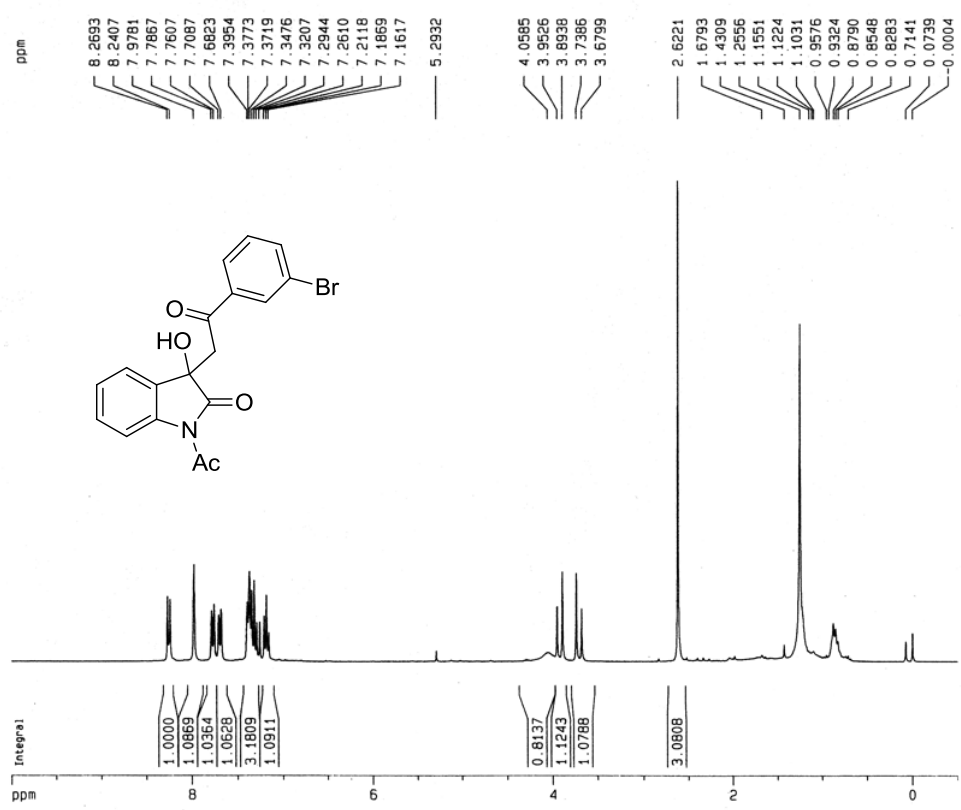


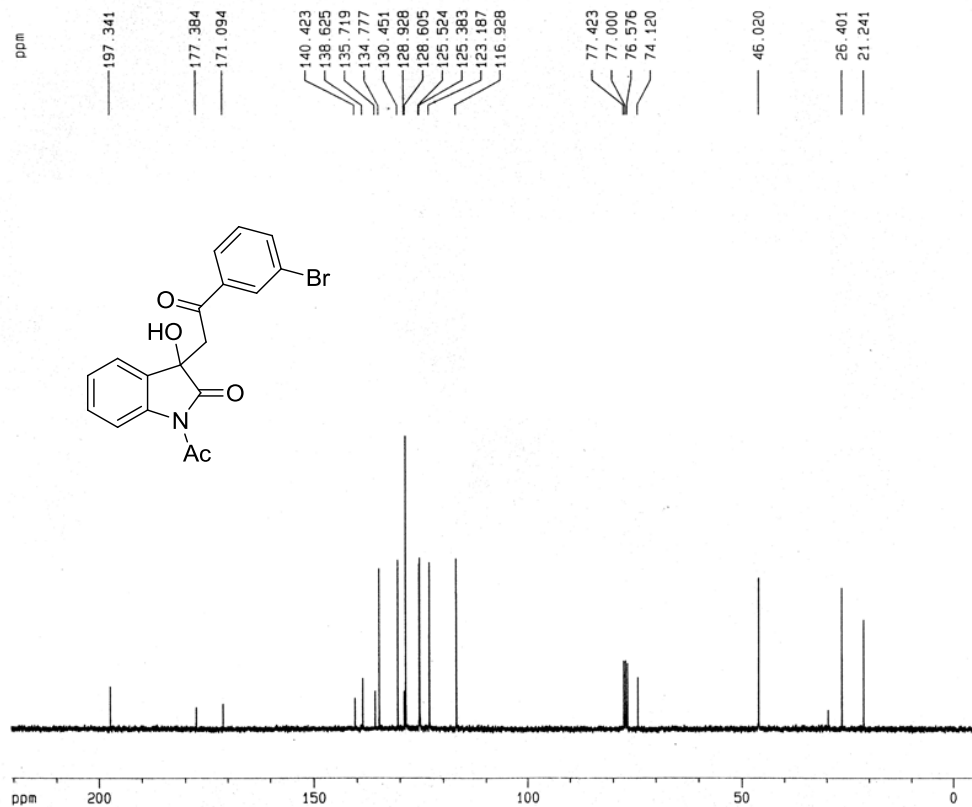
¹H and ¹³C NMR of 3i



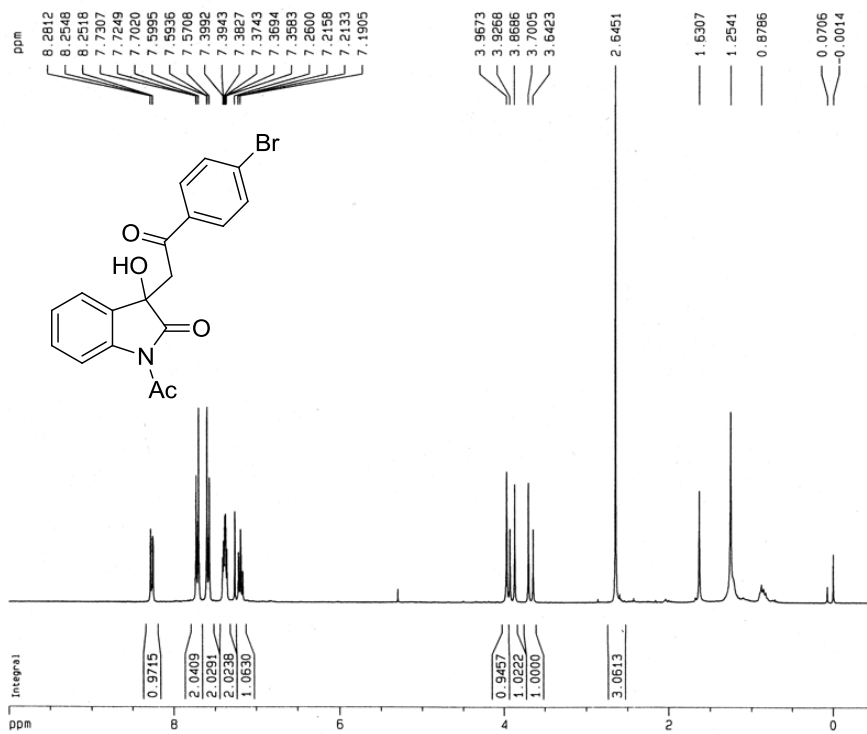


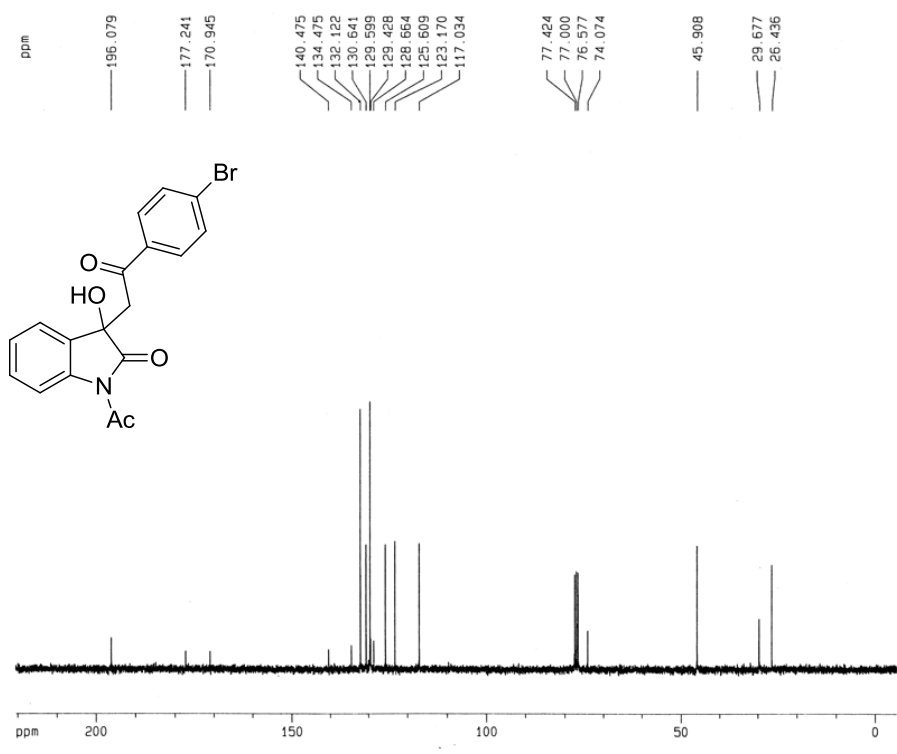
¹H and ¹³C NMR of 3j



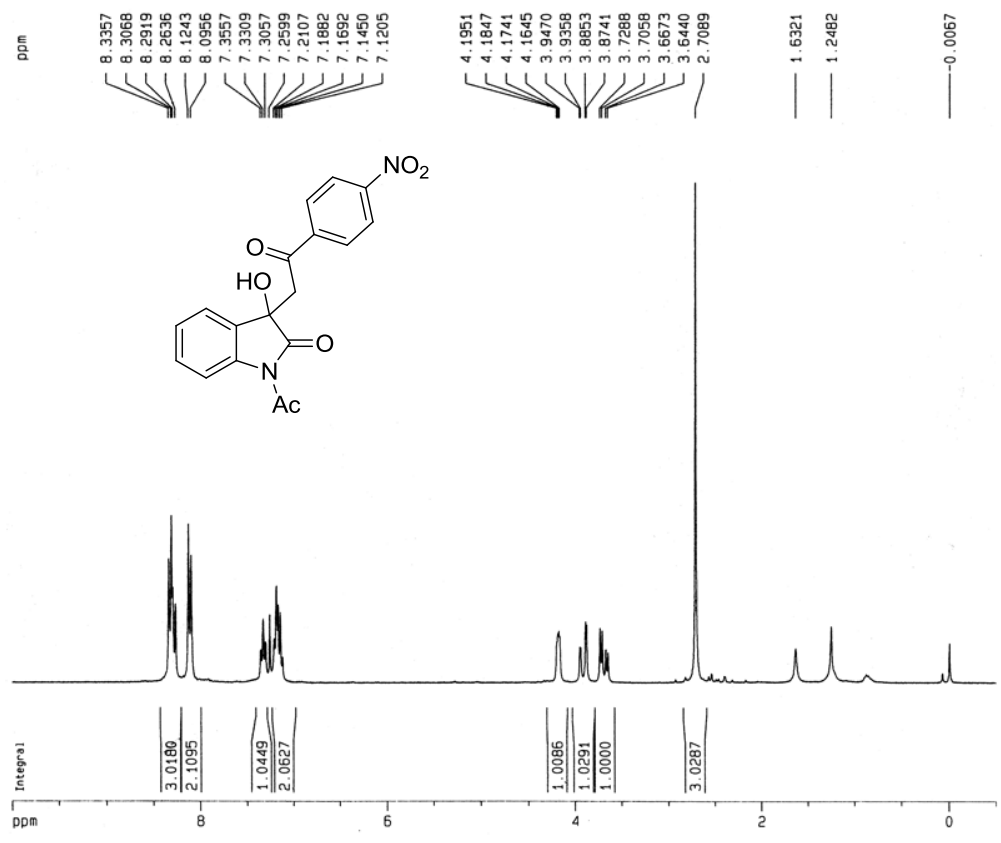


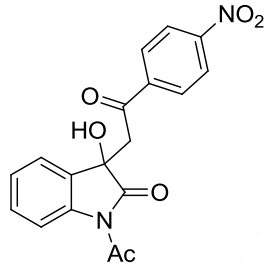
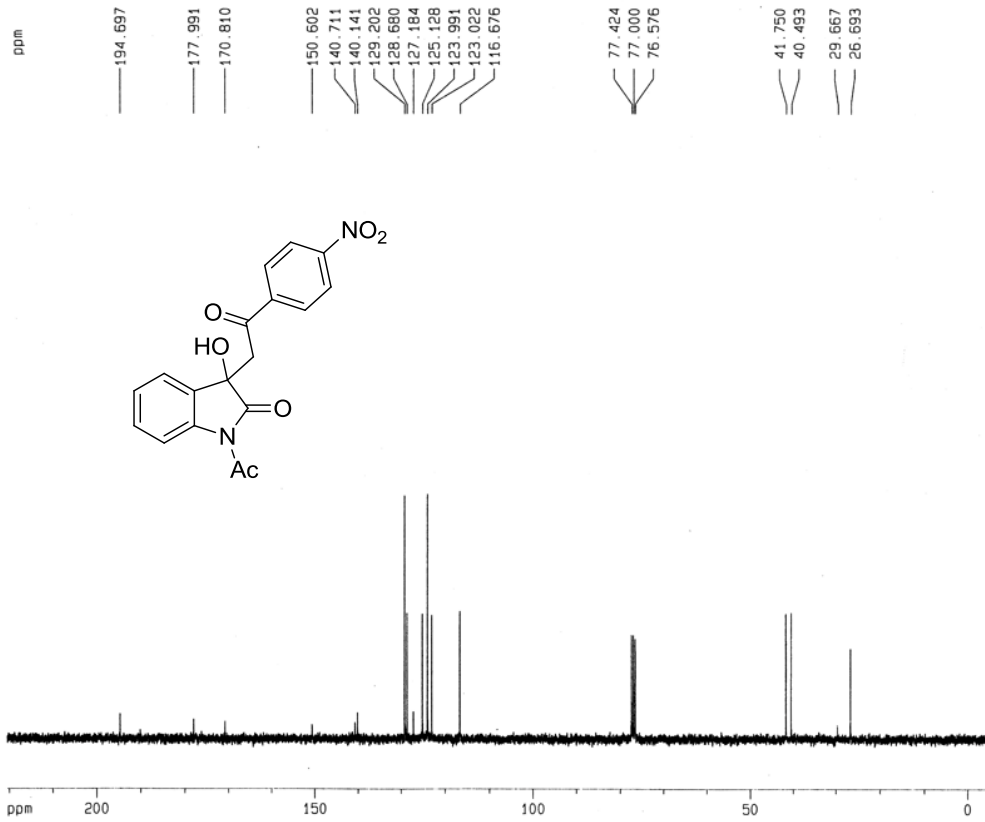
¹H and ¹³C NMR of 3k



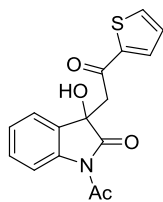
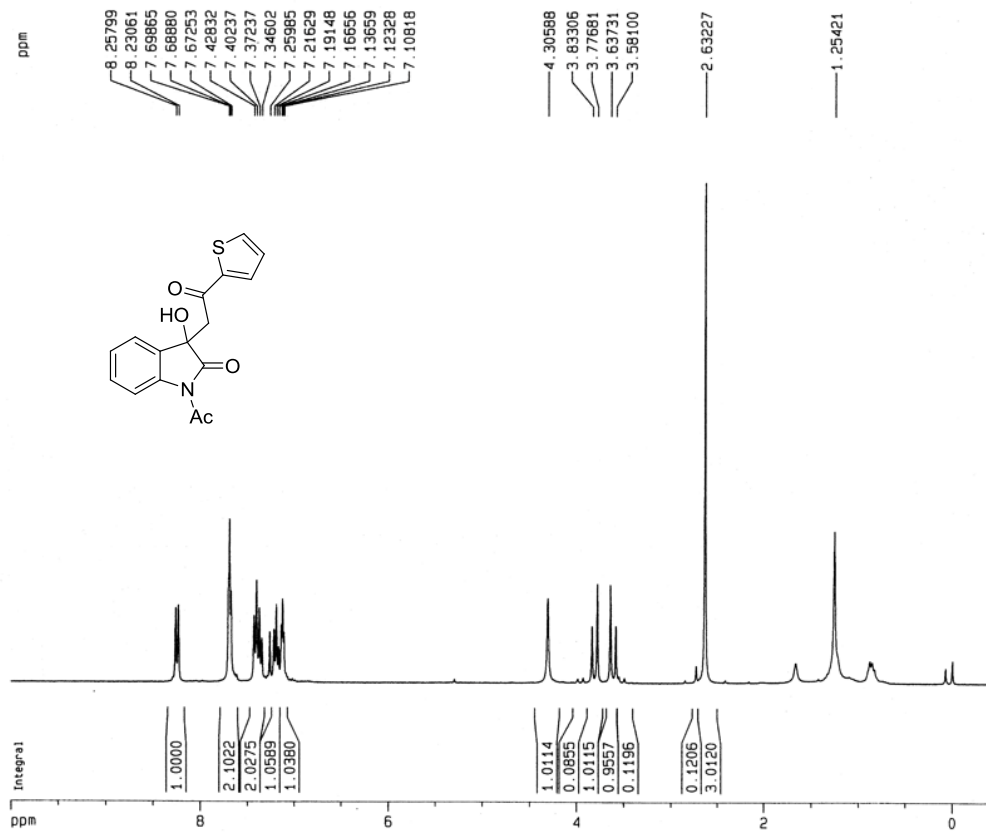


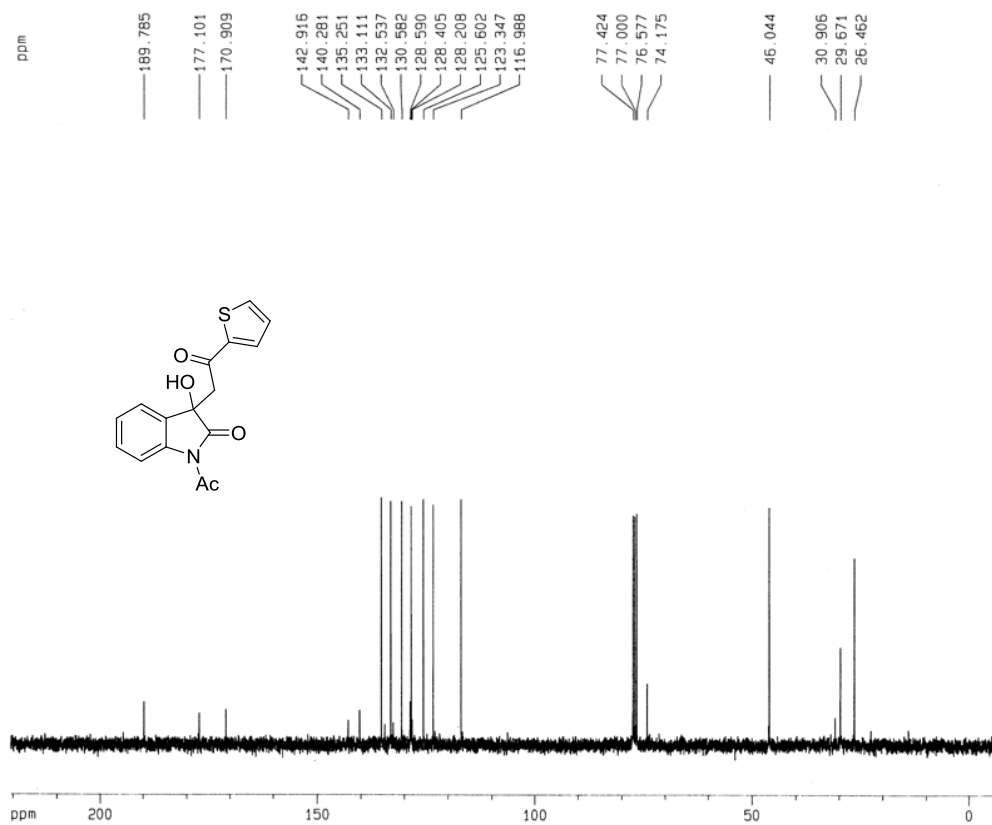
¹H and ¹³C NMR of 31



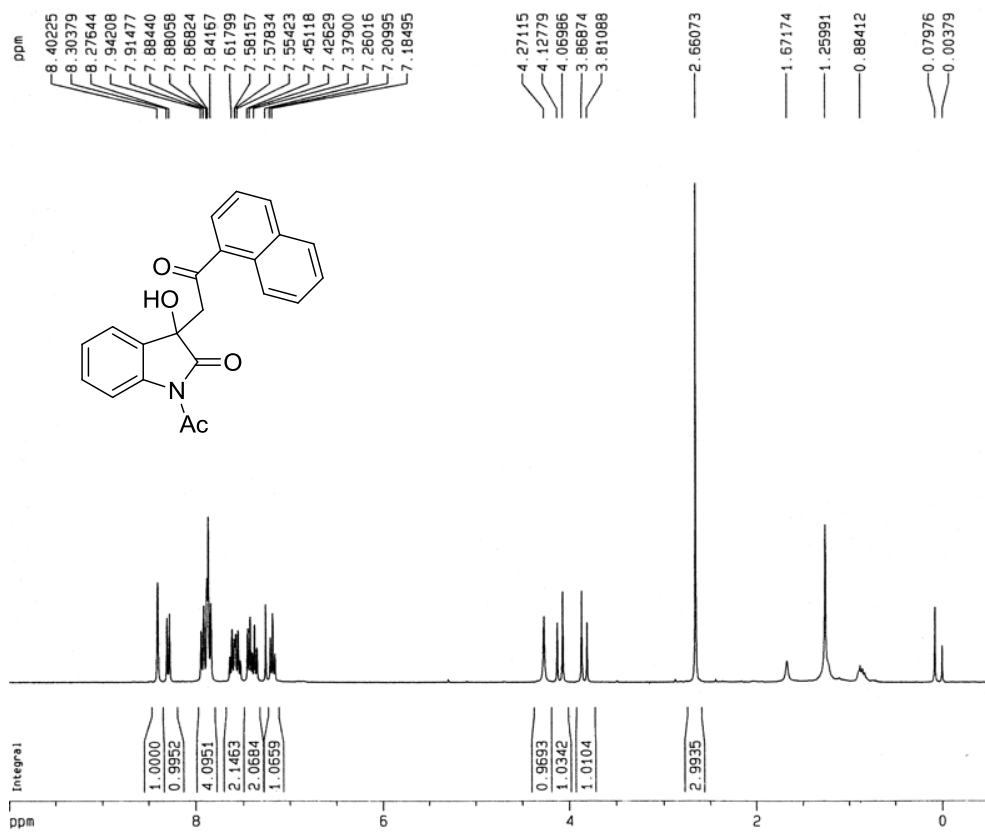


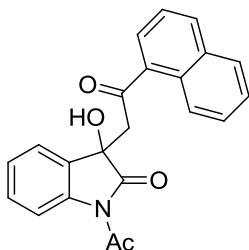
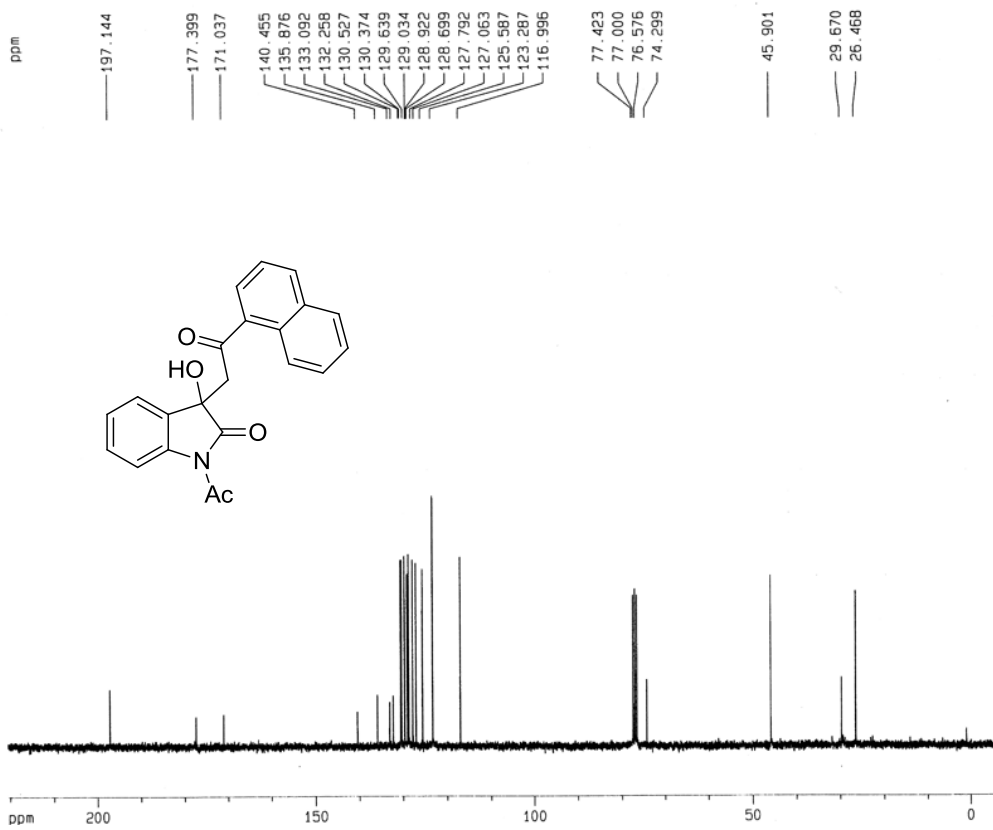
¹H and ¹³C NMR of 3m



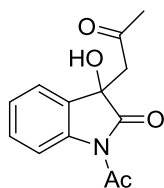
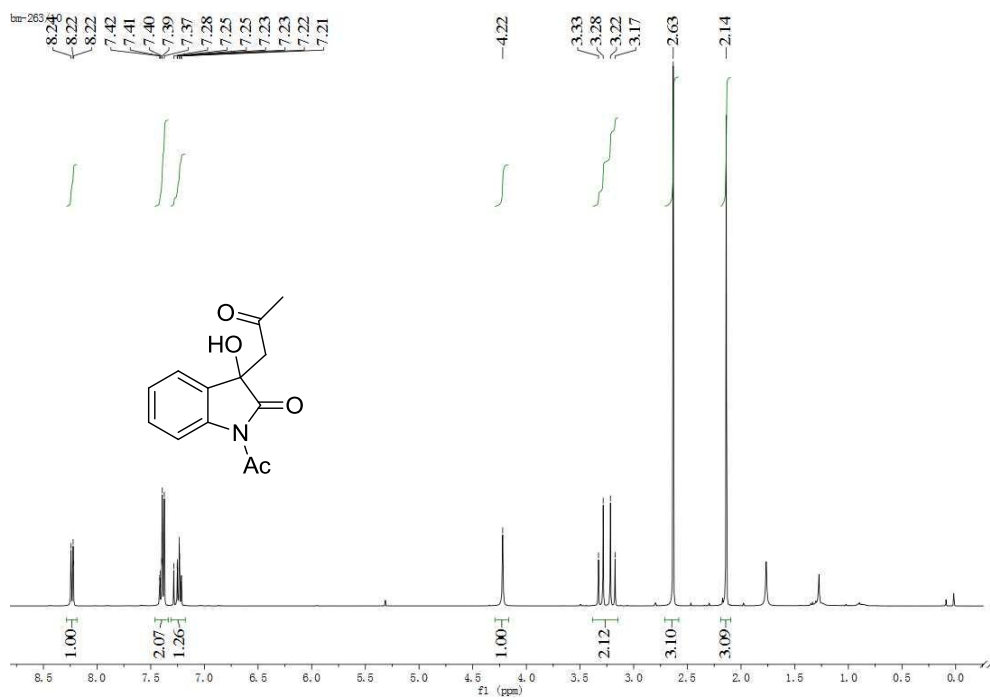


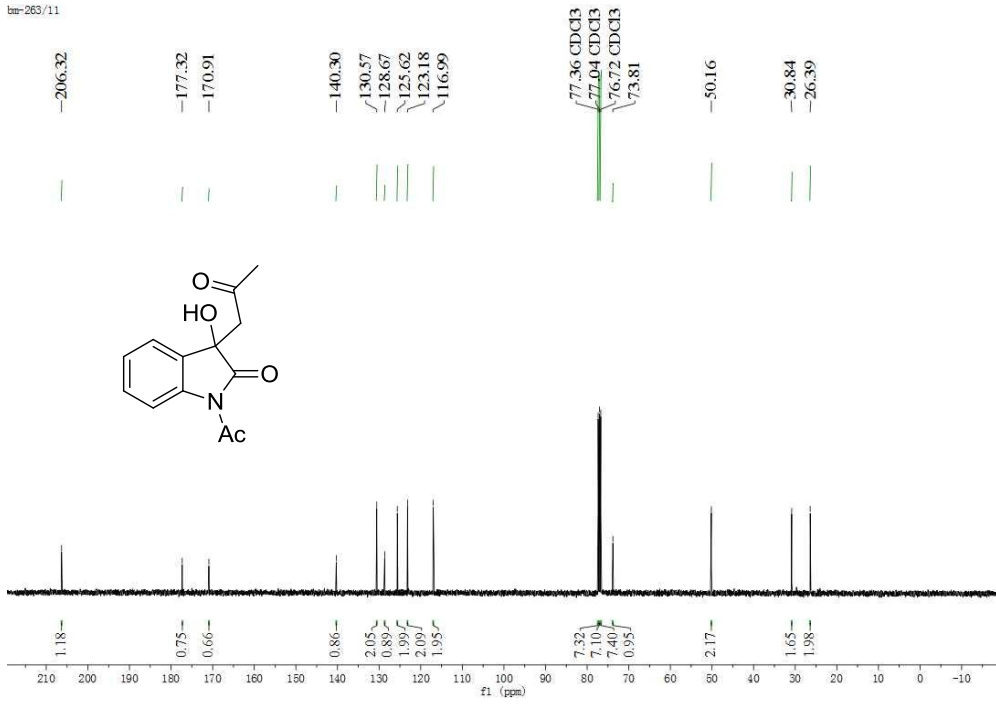
¹H and ¹³C NMR of 3n



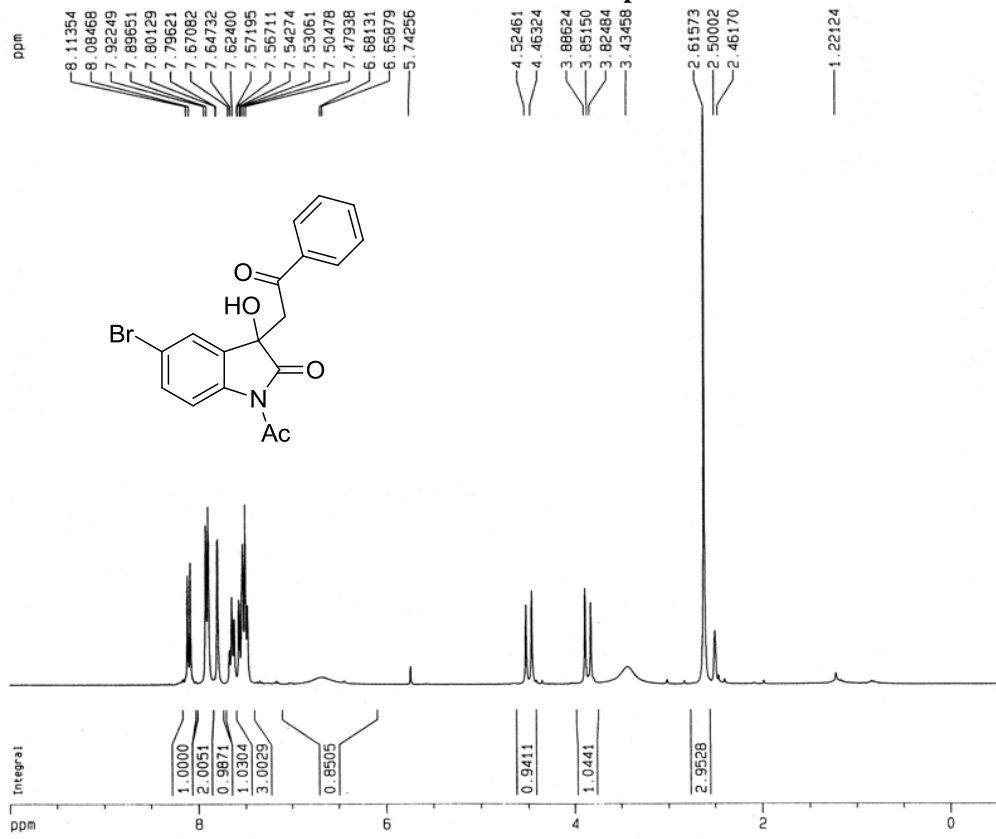


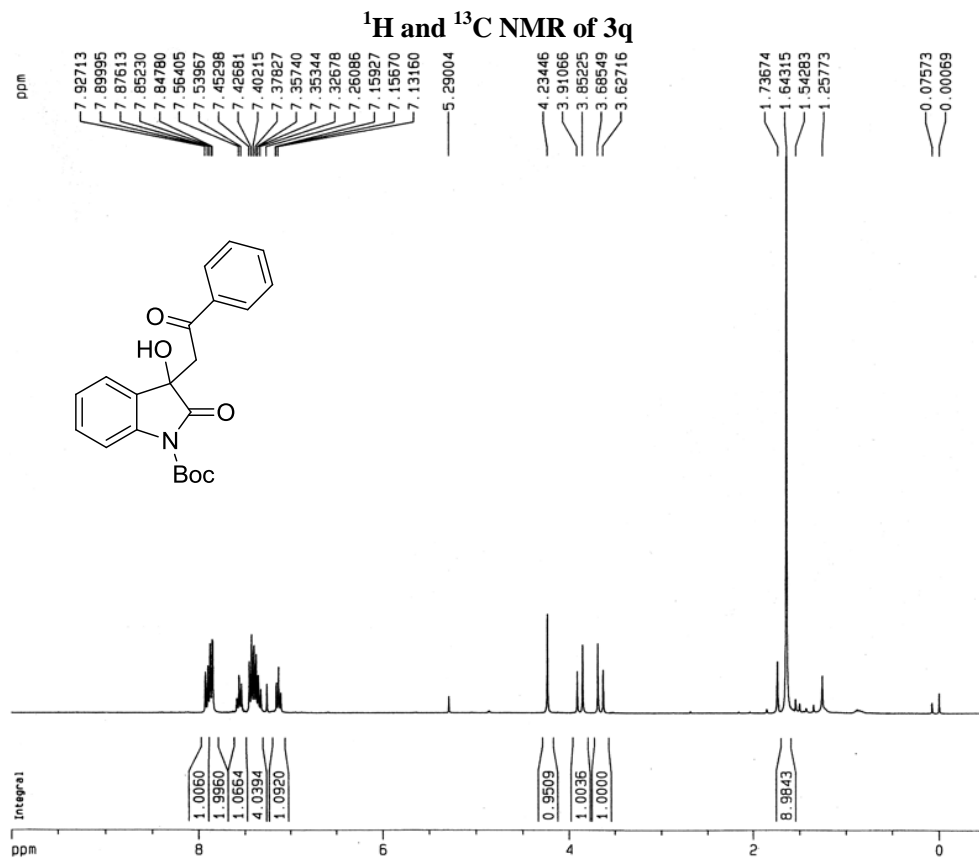
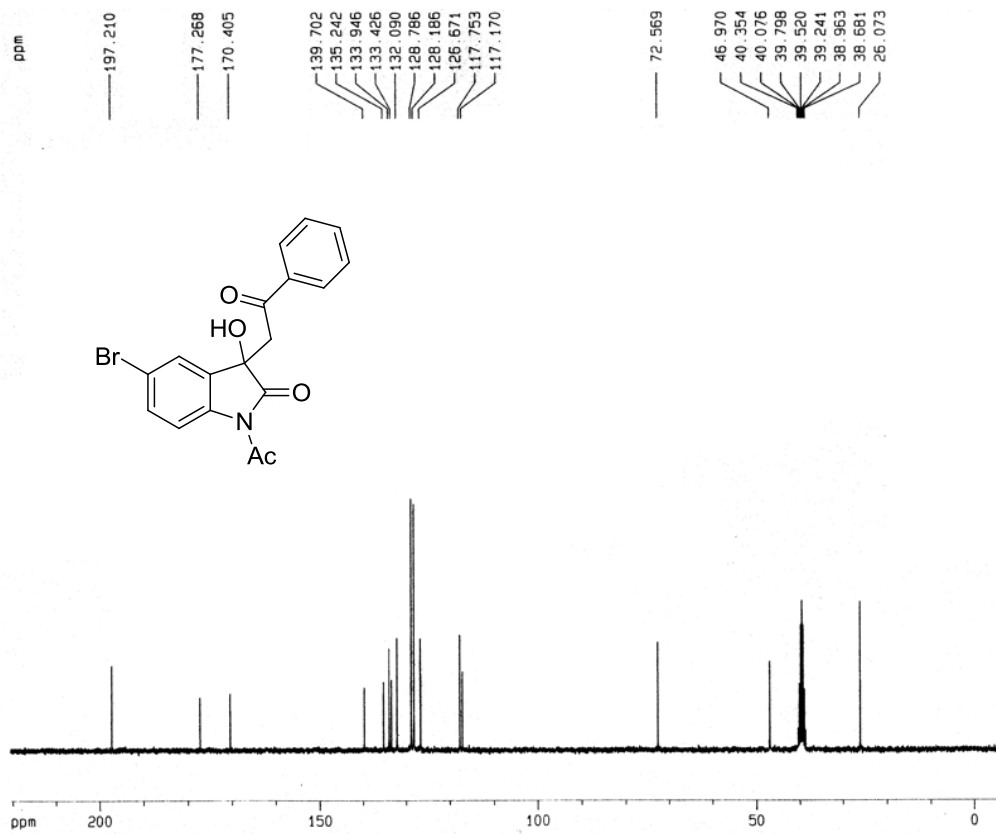
¹H and ¹³C NMR of 3o

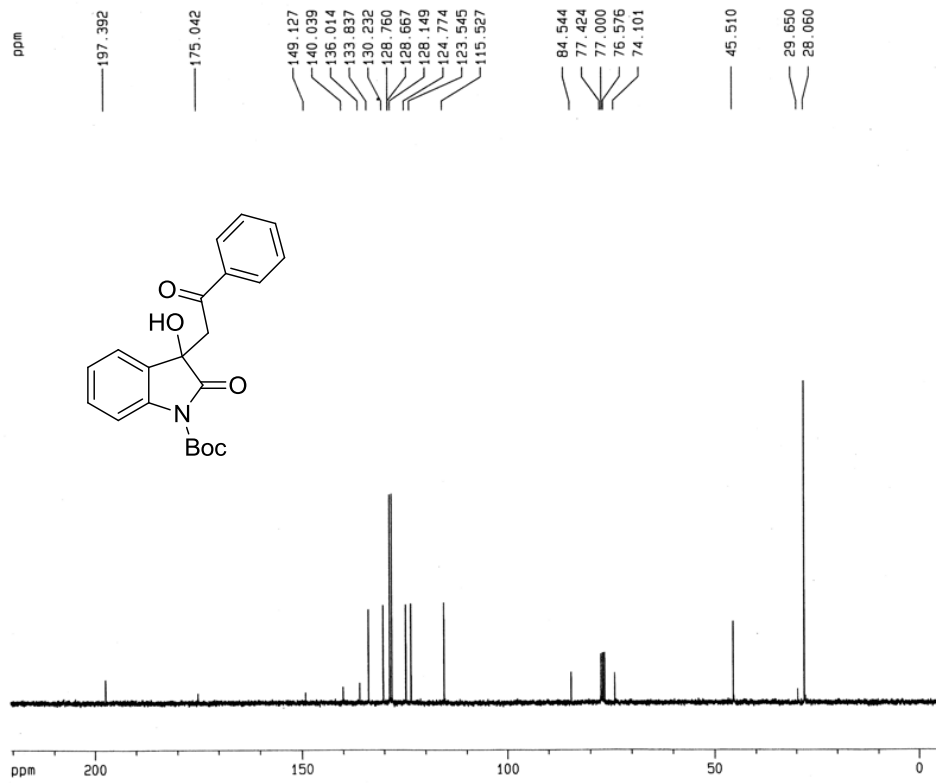




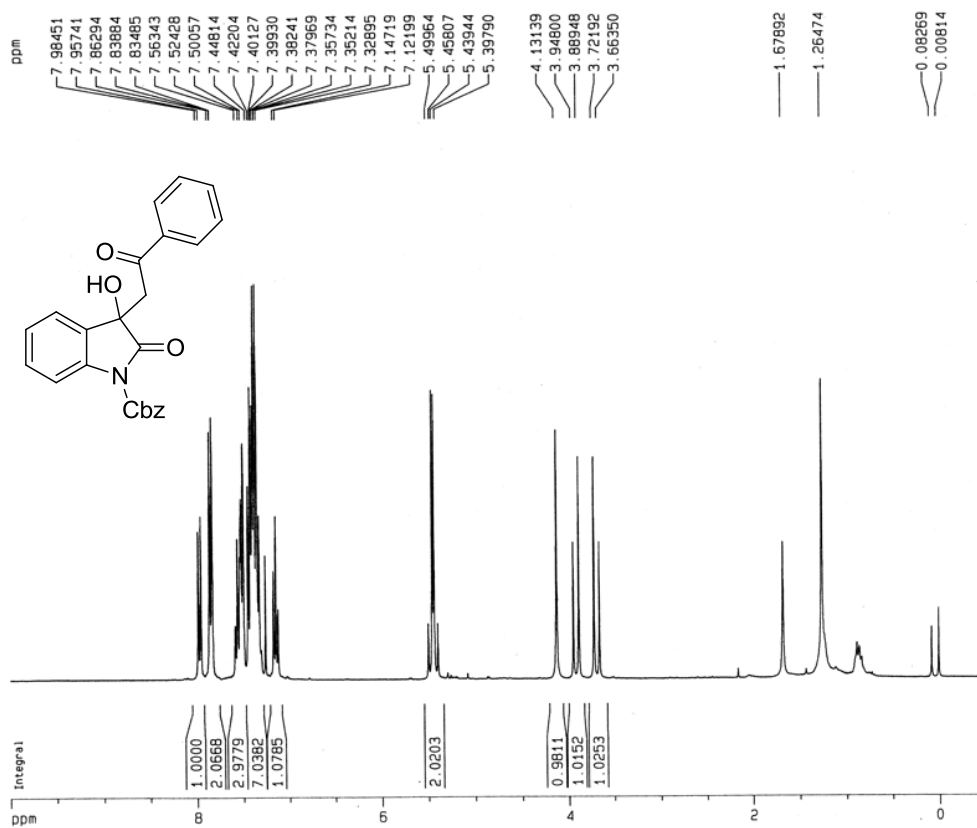
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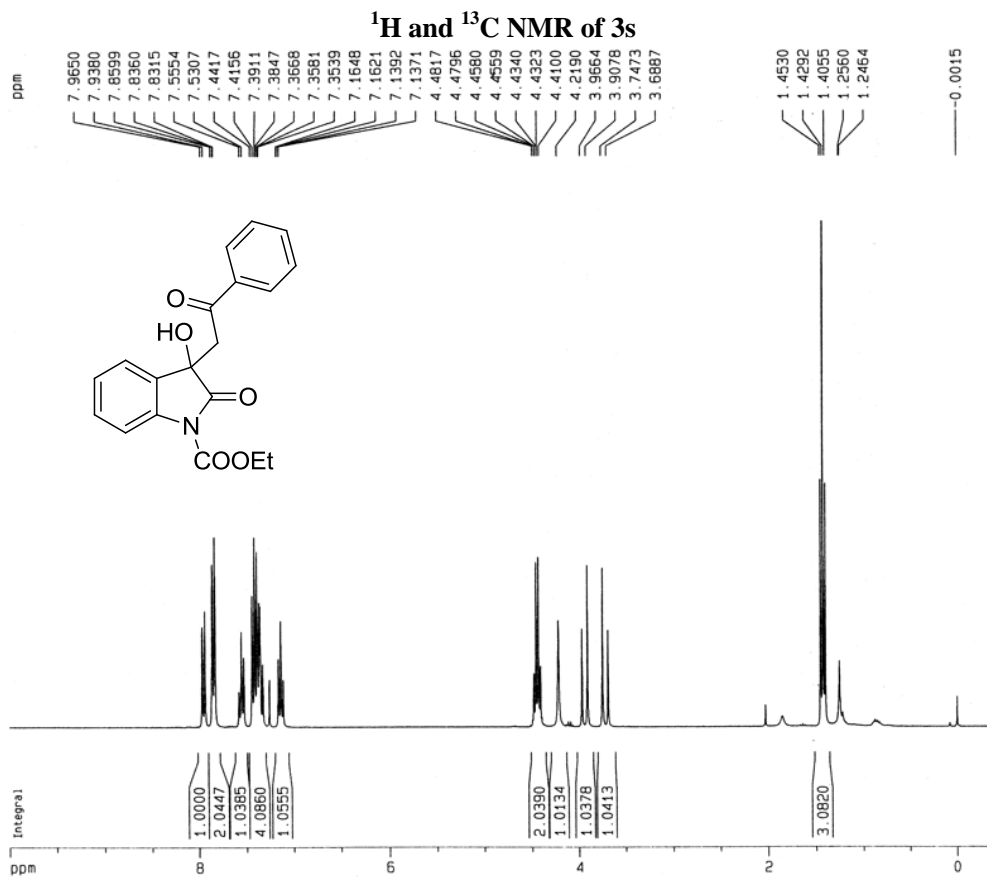
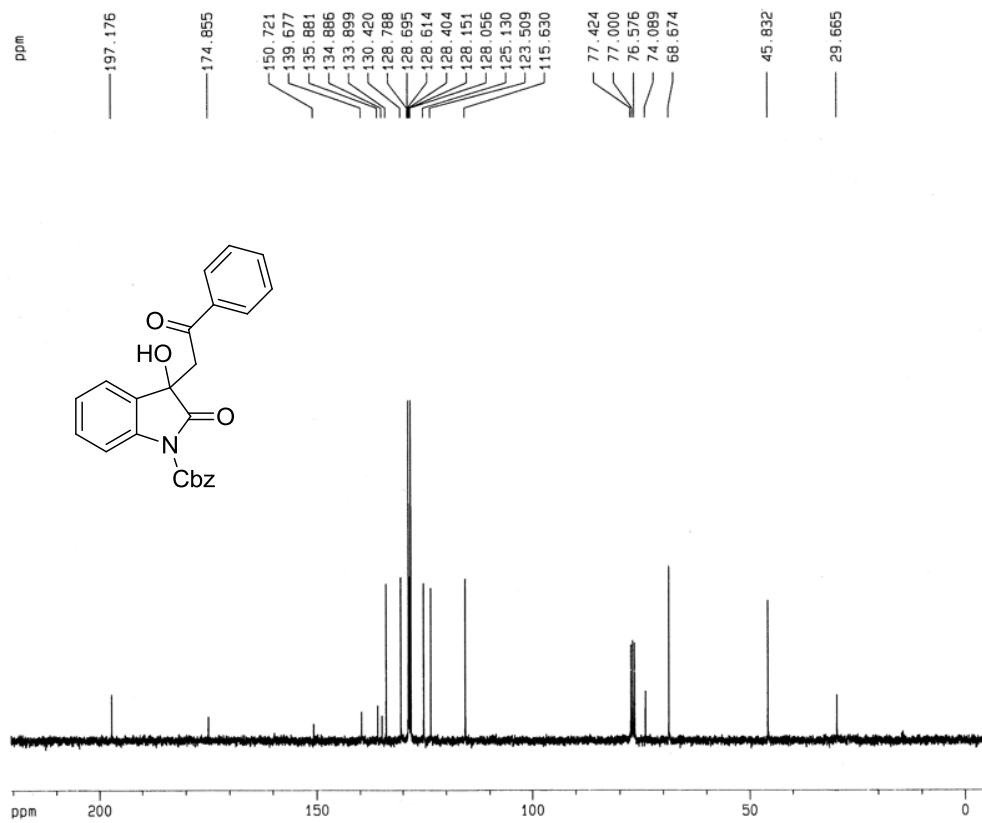


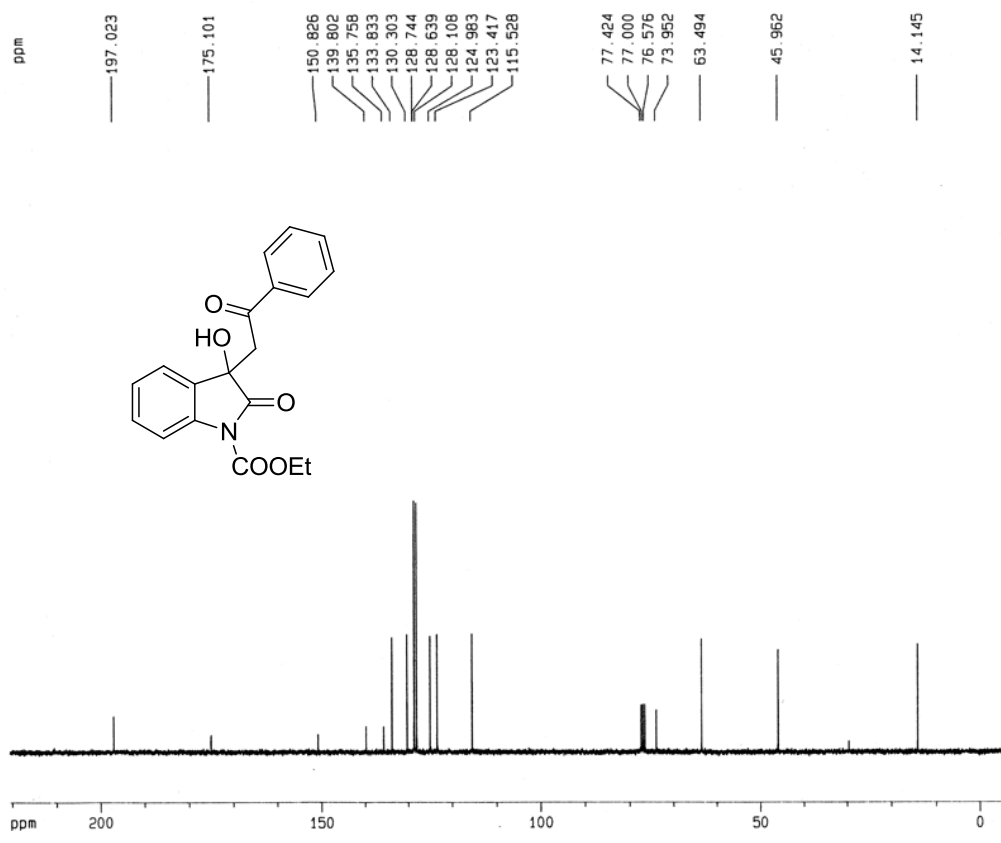




¹H and ¹³C NMR of 3r







¹H and ¹³C NMR of 3u

