

3-Nitroindoles Serving as *N*-Centered Nucleophiles for Aza-1,6-Michael Addition to *para*-Quinone Methides

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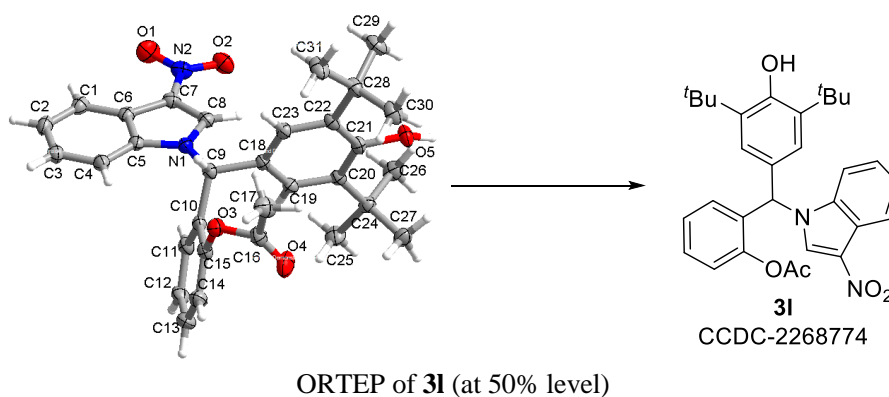
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Supporting Information

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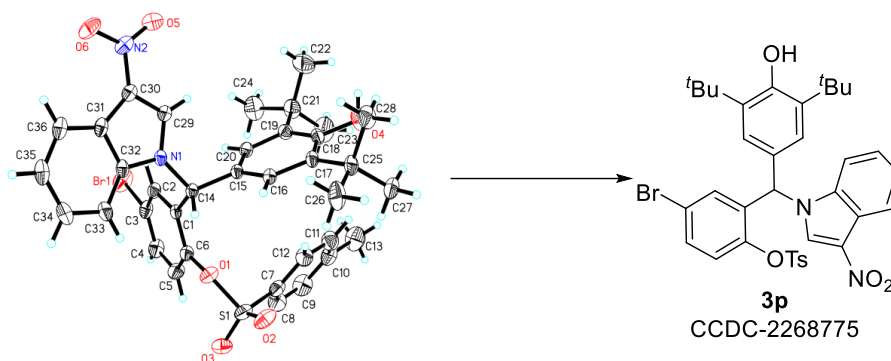
1. X-Ray crystal data for compounds **3l** and **3p**.



ORTEP of **3l** (at 50% level)

Table 1 Crystal data and structure refinement for 3l

Identification code	3l
Empirical formula	C ₃₁ H ₃₄ N ₂ O ₅
Formula weight	514.60
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	11.4957(2)
b/Å	22.7104(4)
c/Å	11.06142(18)
α/°	90
β/°	105.5630(18)
γ/°	90
Volume/Å ³	2781.95(9)
Z	4
ρ _{calc} /g/cm ³	1.229
μ/mm ⁻¹	0.672
F(000)	1096.0
Crystal size/mm ³	0.15 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)
2θ range for data collection/°	7.786 to 140.926
Index ranges	-9 ≤ h ≤ 13, -27 ≤ k ≤ 26, -13 ≤ l ≤ 11
Reflections collected	10598
Independent reflections	5213 [R _{int} = 0.0319, R _{sigma} = 0.0467]
Data/restraints/parameters	5213/0/351
Goodness-of-fit on F ²	1.027
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0520, wR ₂ = 0.1360
Final R indexes [all data]	R ₁ = 0.0666, wR ₂ = 0.1519
Largest diff. peak/hole / e Å ⁻³	0.30/-0.30



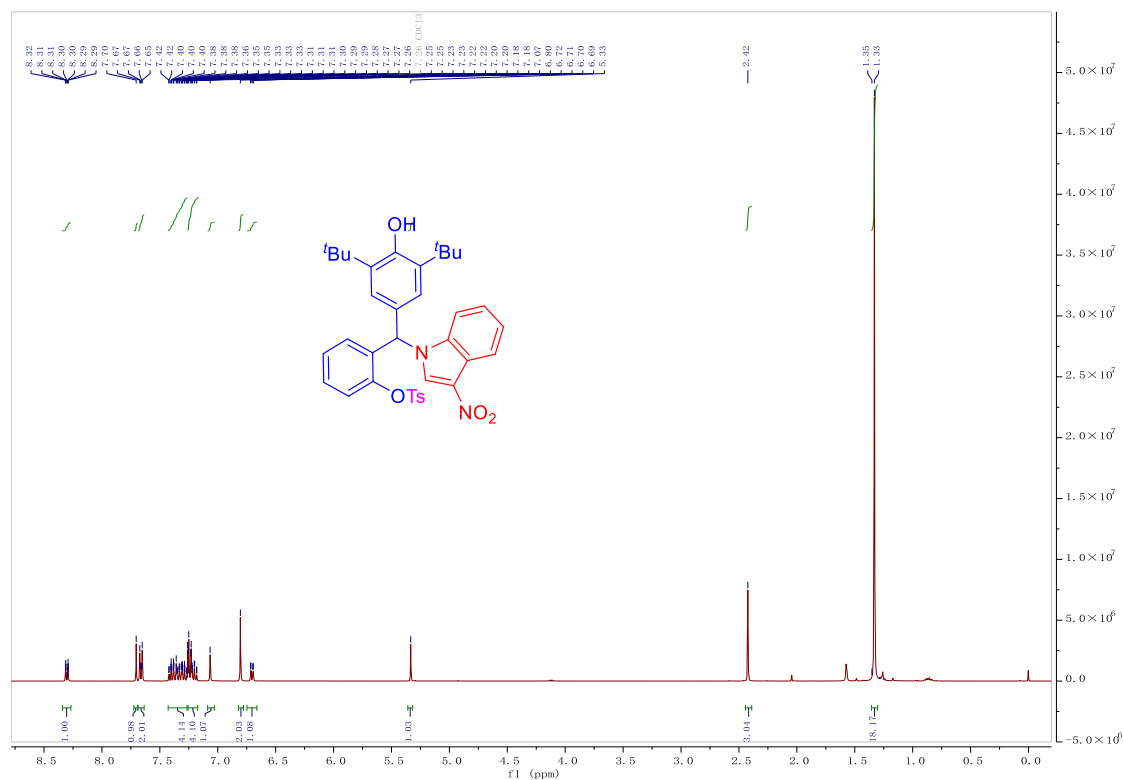
ORTEP of **3p** (at 50% level)

Table 1 Crystal data and structure refinement for 3p

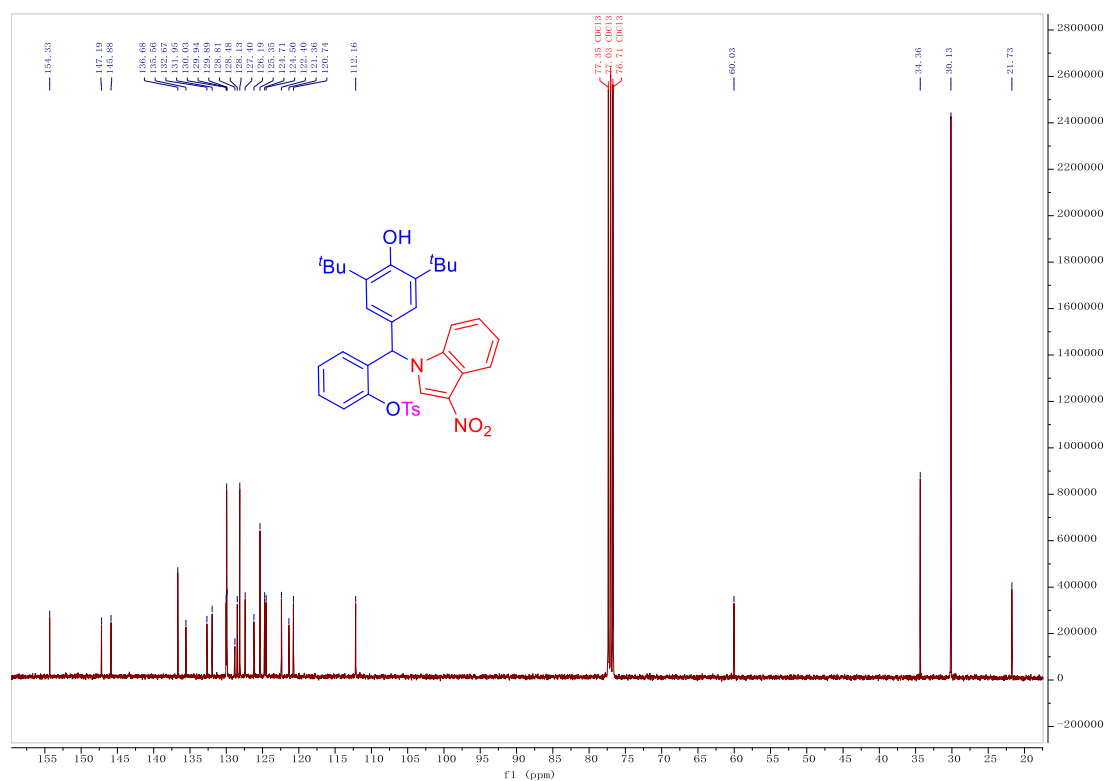
Identification code	3p
Empirical formula	C ₃₆ H ₃₇ BrN ₂ O ₆ S
Formula weight	705.64
Temperature/K	249.99(10)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	11.18050(10)
b/Å	16.1823(2)
c/Å	21.0128(2)
α/°	90
β/°	95.2830(10)
γ/°	90
Volume/Å ³	3785.62(7)
Z	4
ρ _{calc} /cm ³	1.238
μ/mm ⁻¹	2.346
F(000)	1464.0
Crystal size/mm ³	0.13 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	6.906 to 143.3
Index ranges	-13 ≤ h ≤ 9, -19 ≤ k ≤ 15, -25 ≤ l ≤ 25
Reflections collected	22216
Independent reflections	7234 [R _{int} = 0.0438, R _{sigma} = 0.0404]
Data/restraints/parameters	7234/0/423
Goodness-of-fit on F ²	1.070
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0482, wR ₂ = 0.1367
Final R indexes [all data]	R ₁ = 0.0529, wR ₂ = 0.1403
Largest diff. peak/hole / e Å ⁻³	0.68/-0.75

2. ^1H and ^{13}C NMR spectra for compounds **3**, **6**, and **11**

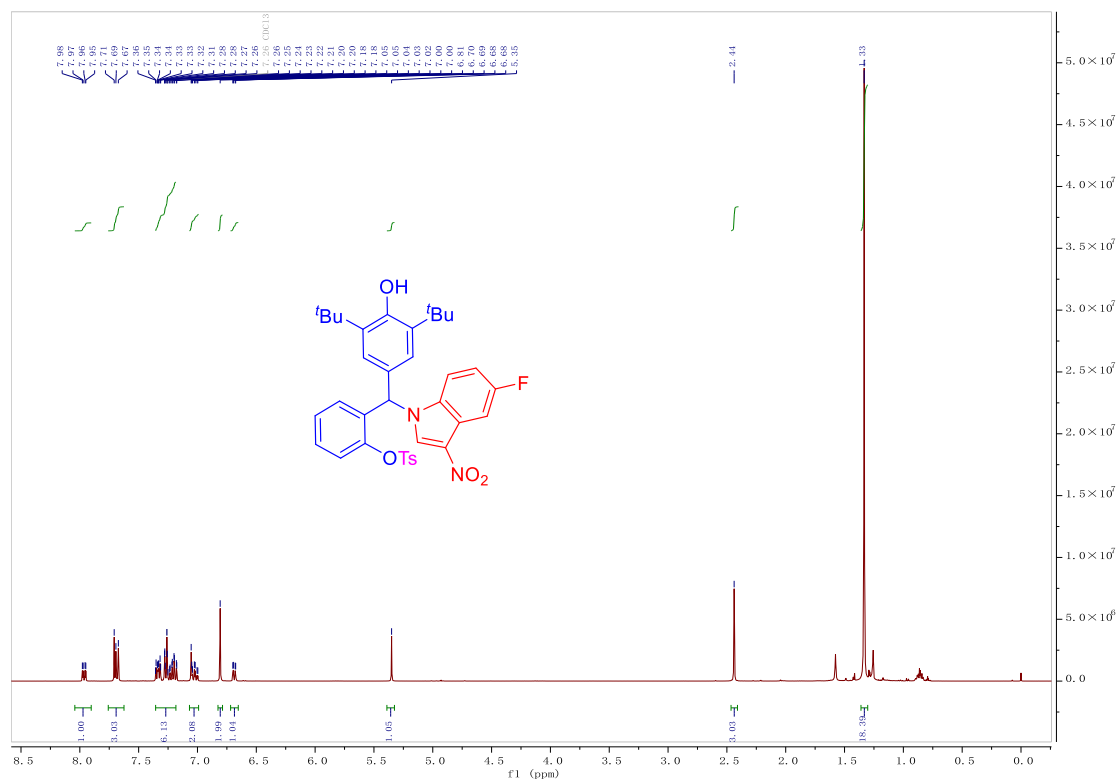
^1H NMR spectrum of **3a**



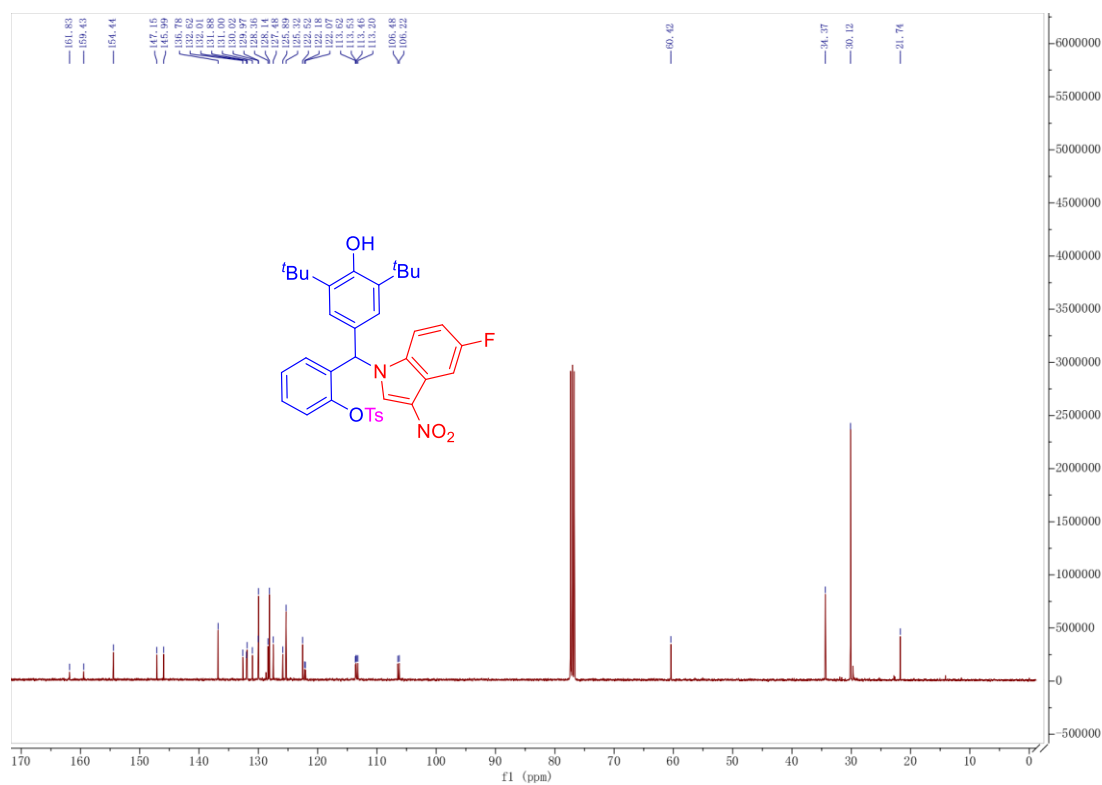
^{13}C NMR spectrum of **3a**



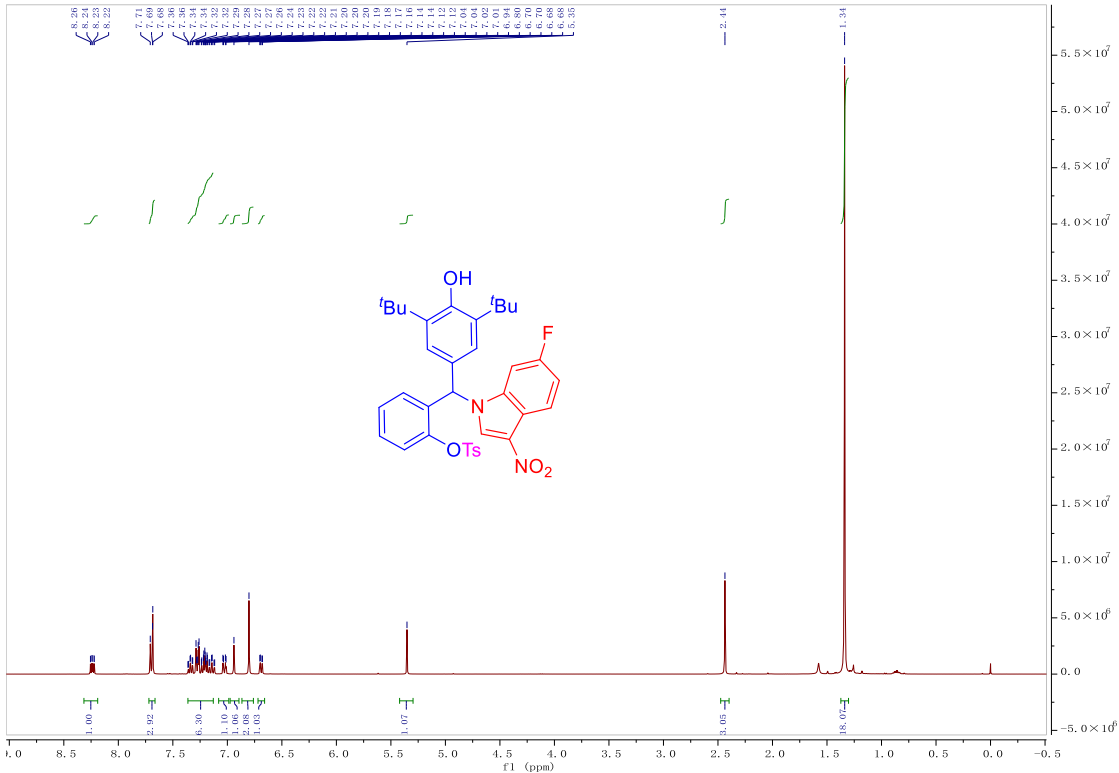
¹H NMR spectrum of 3b



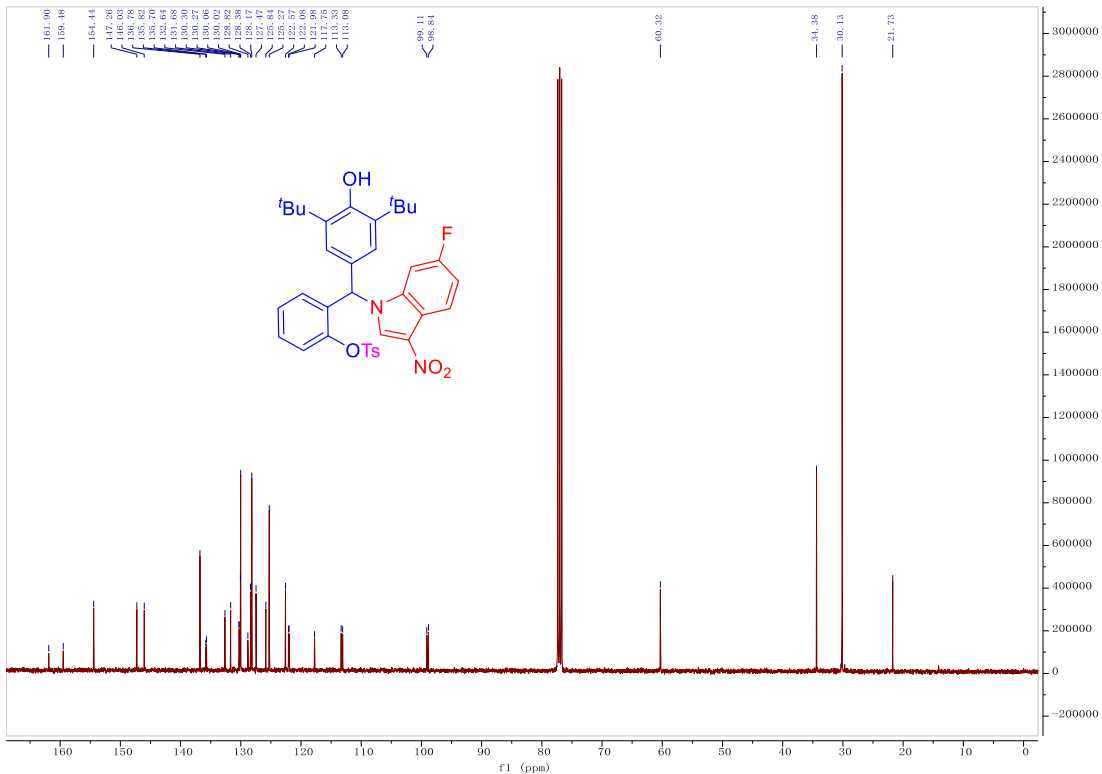
¹³C NMR spectrum of 3b



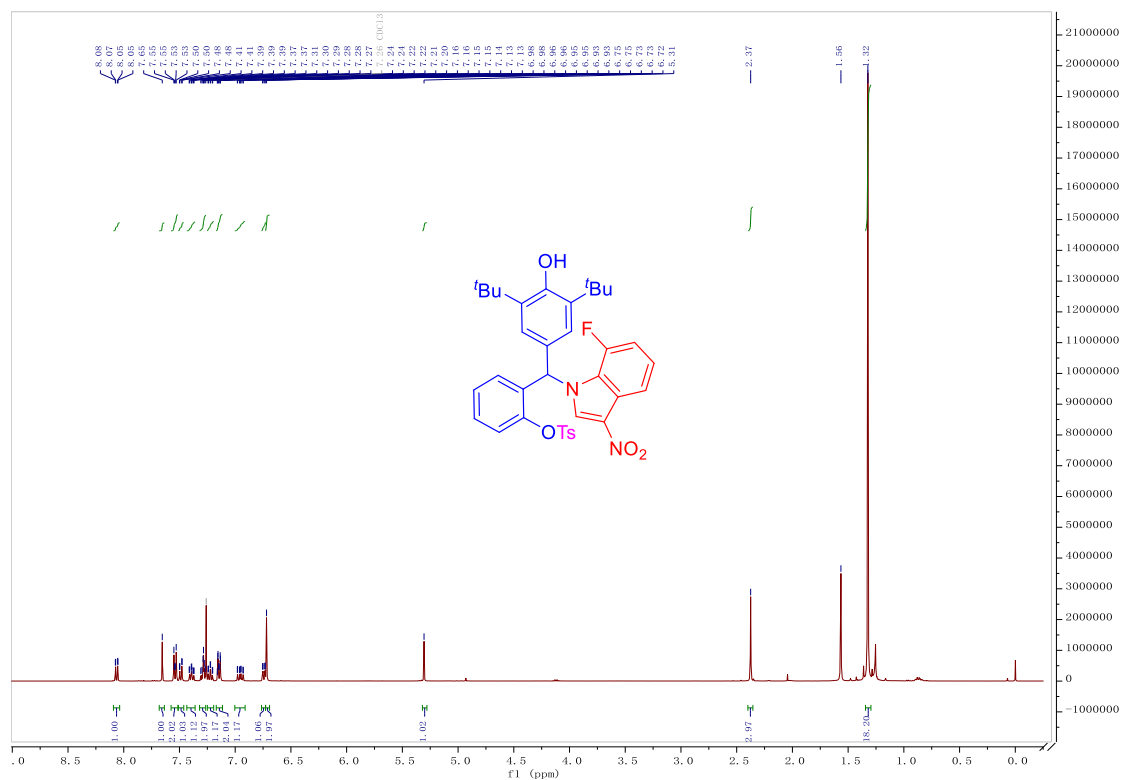
¹H NMR spectrum of 3c



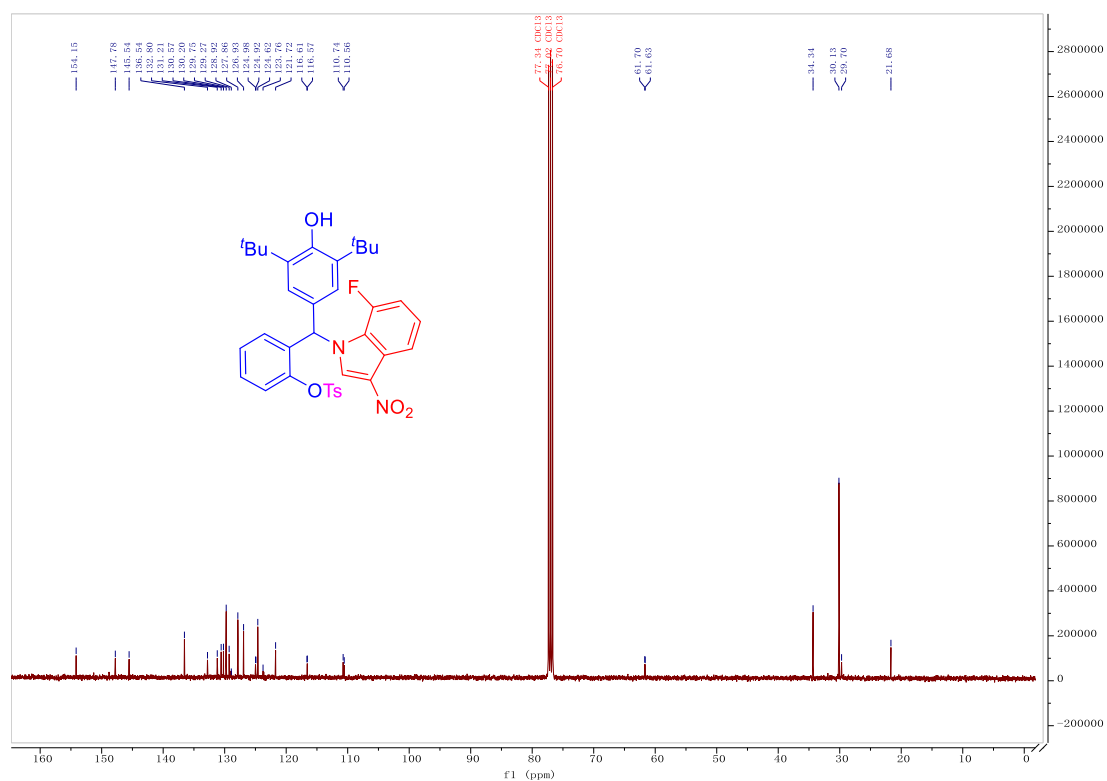
^{13}C NMR spectrum of 3c



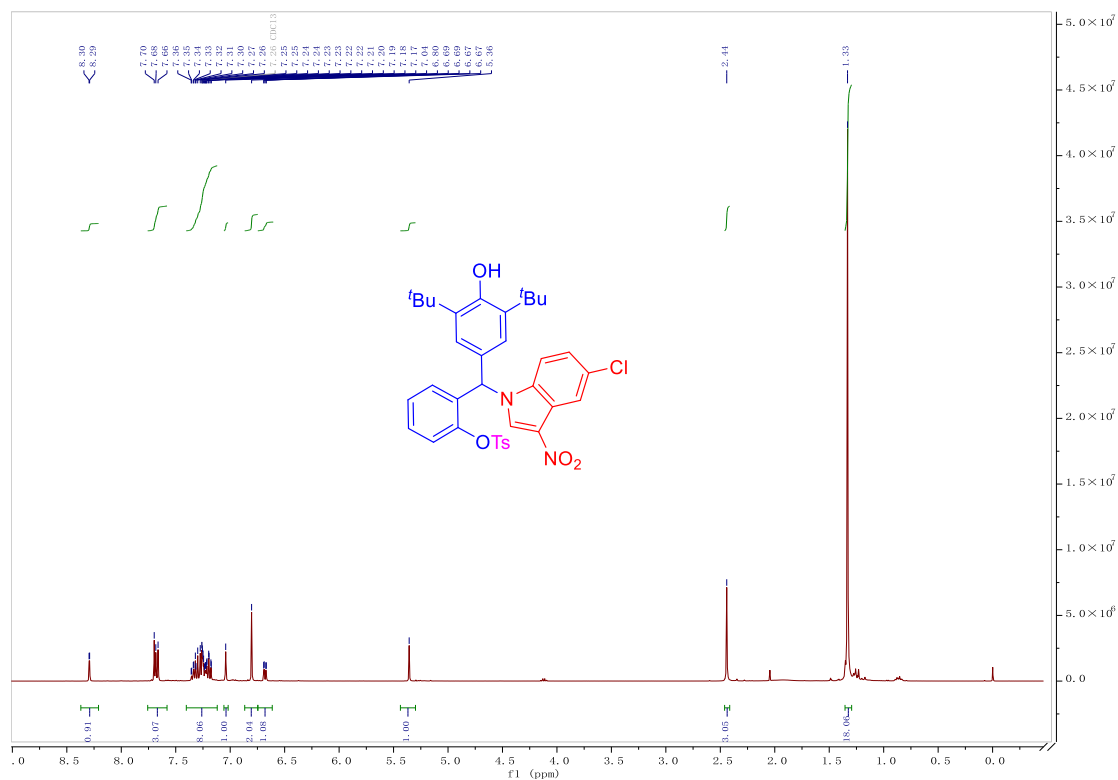
^1H NMR spectrum of 3d



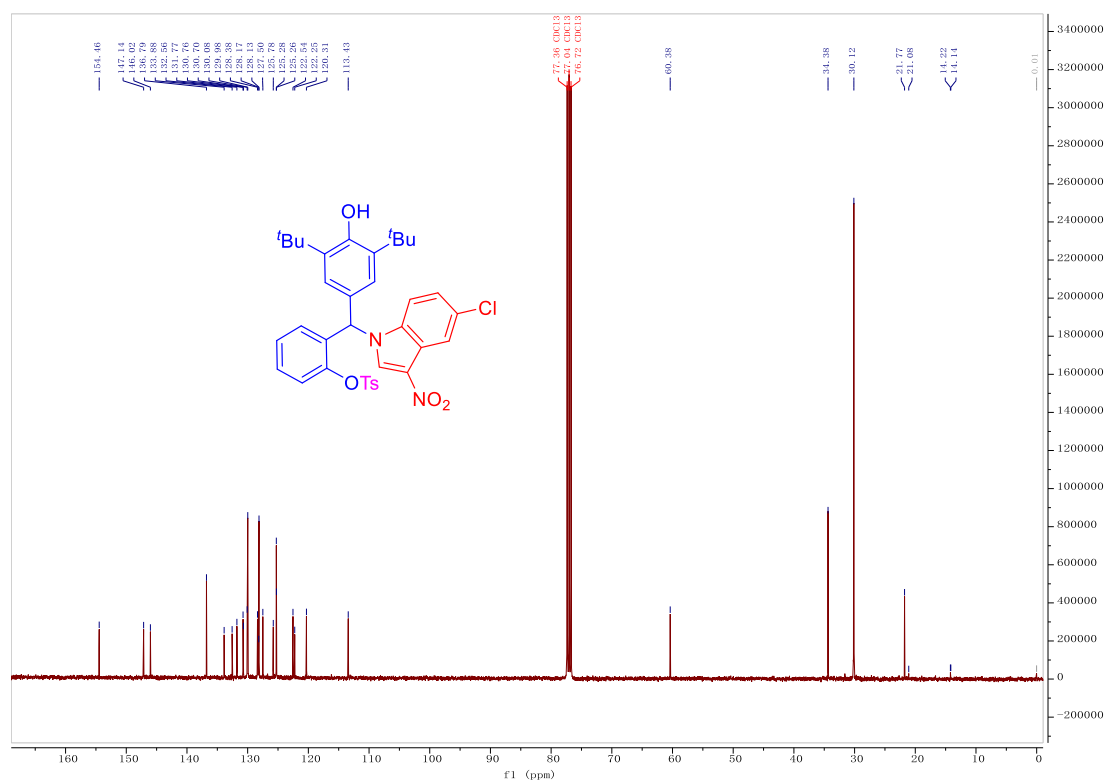
^{13}C NMR spectrum of 3d



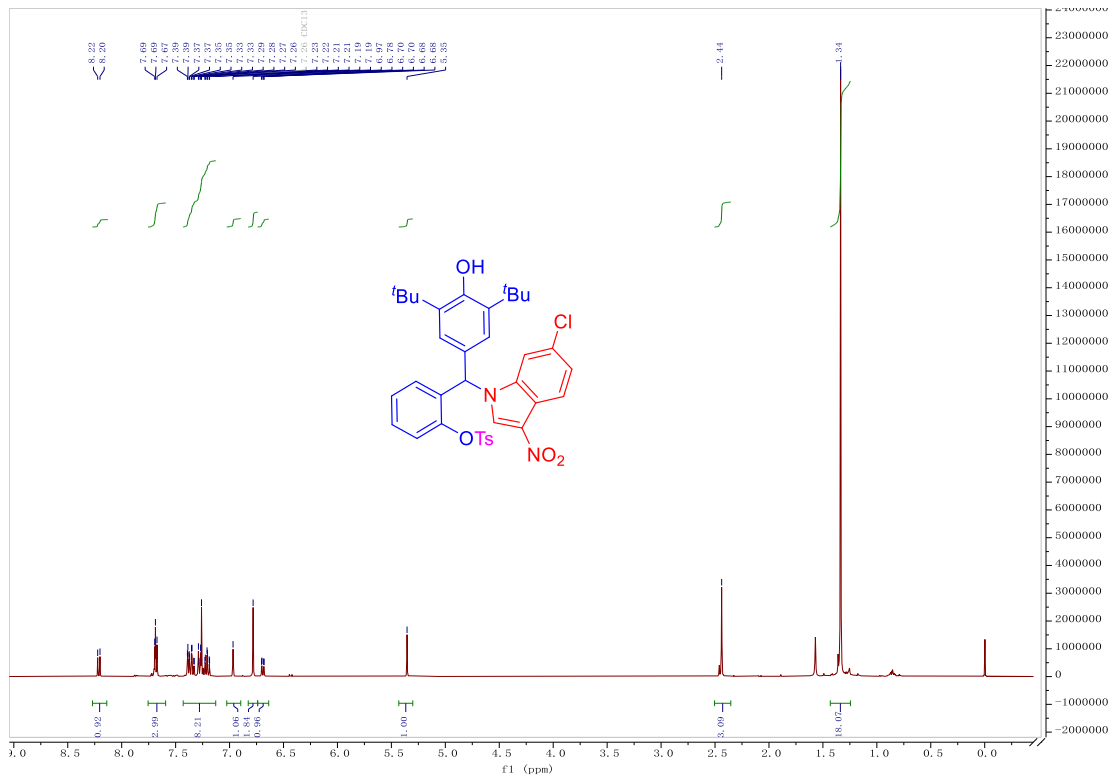
¹H NMR spectrum of 3e



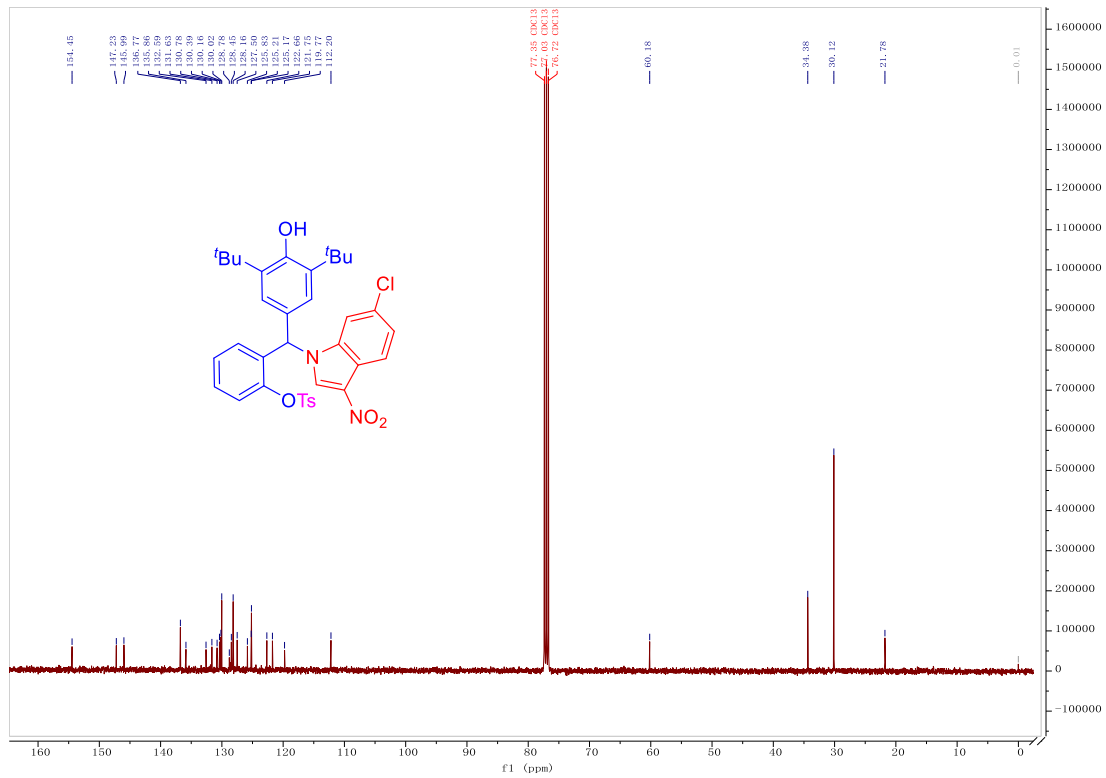
¹³C NMR spectrum of 3e



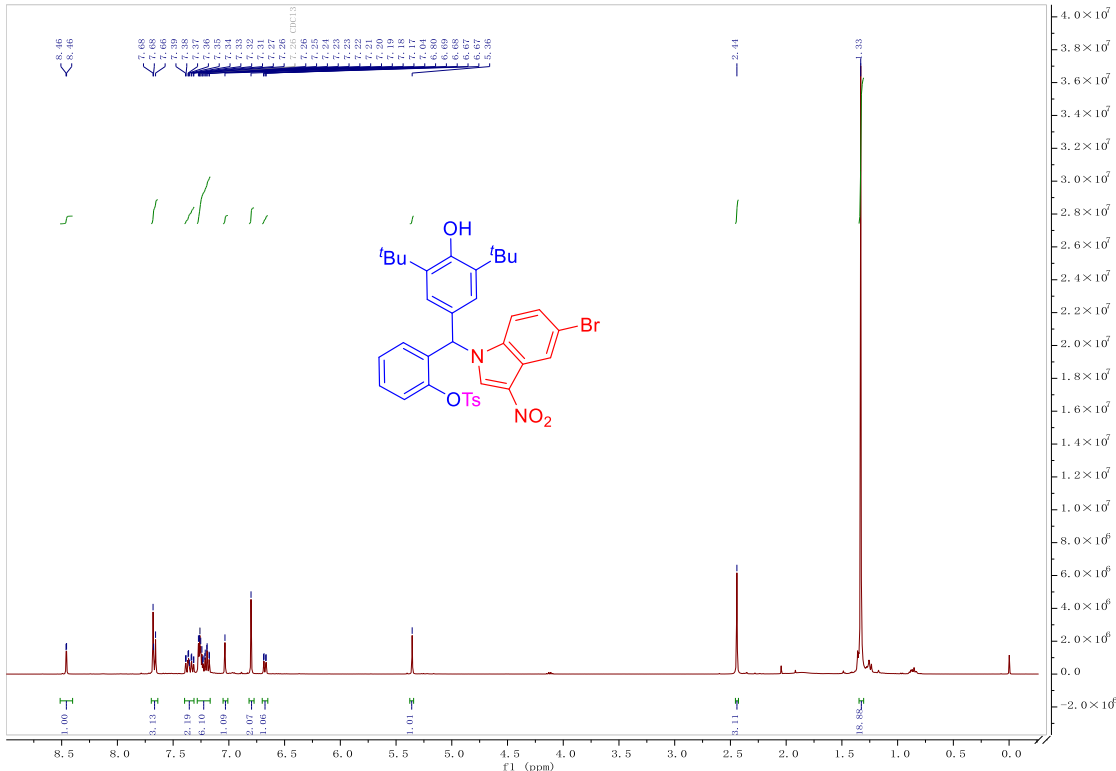
¹H NMR spectrum of 3f



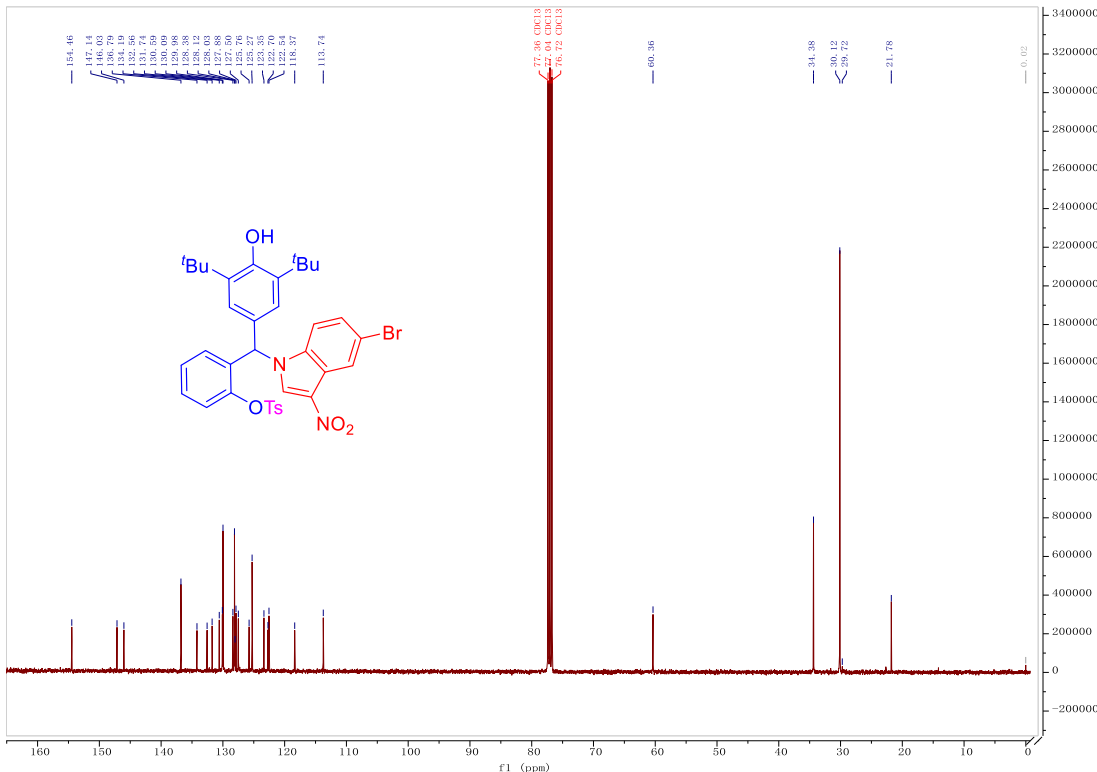
^{13}C NMR spectrum of 3f



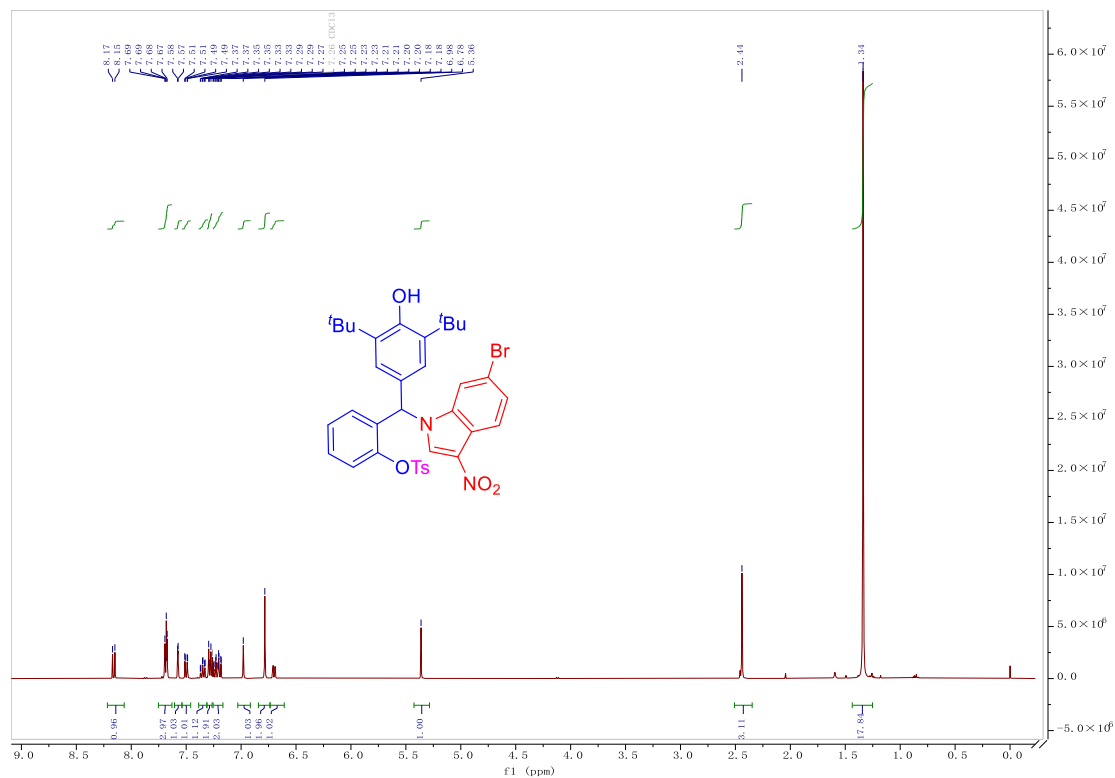
¹H NMR spectrum of 3g



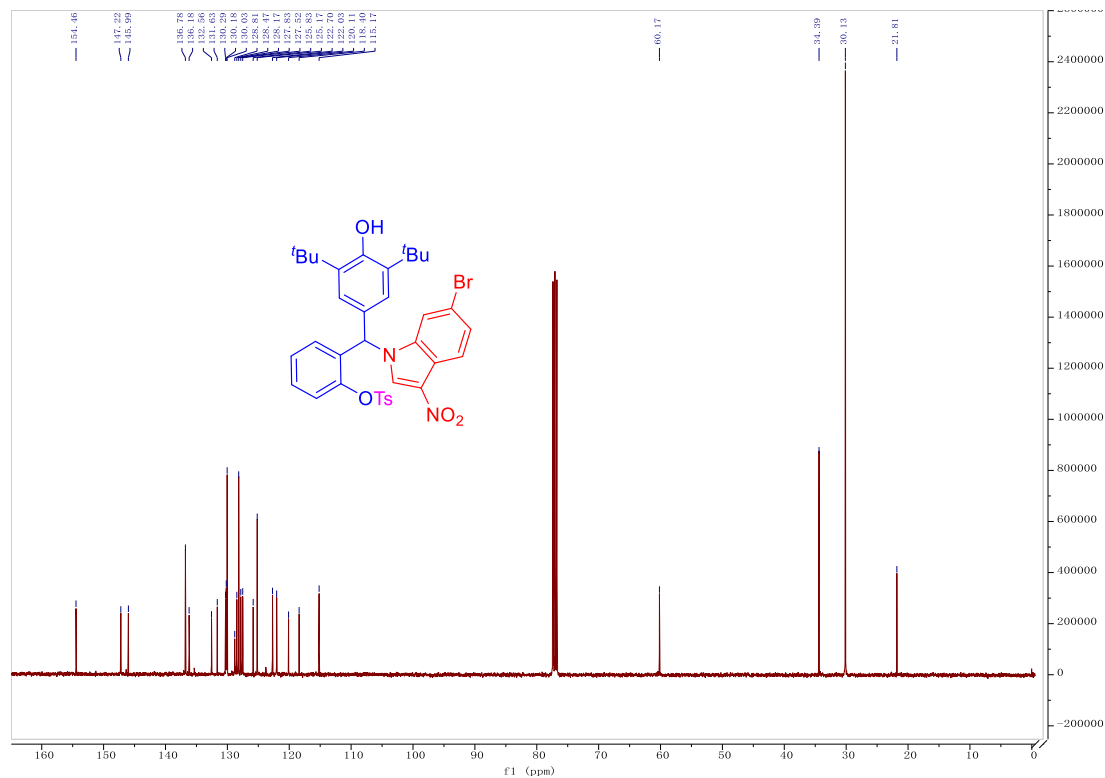
^{13}C NMR spectrum of 3g



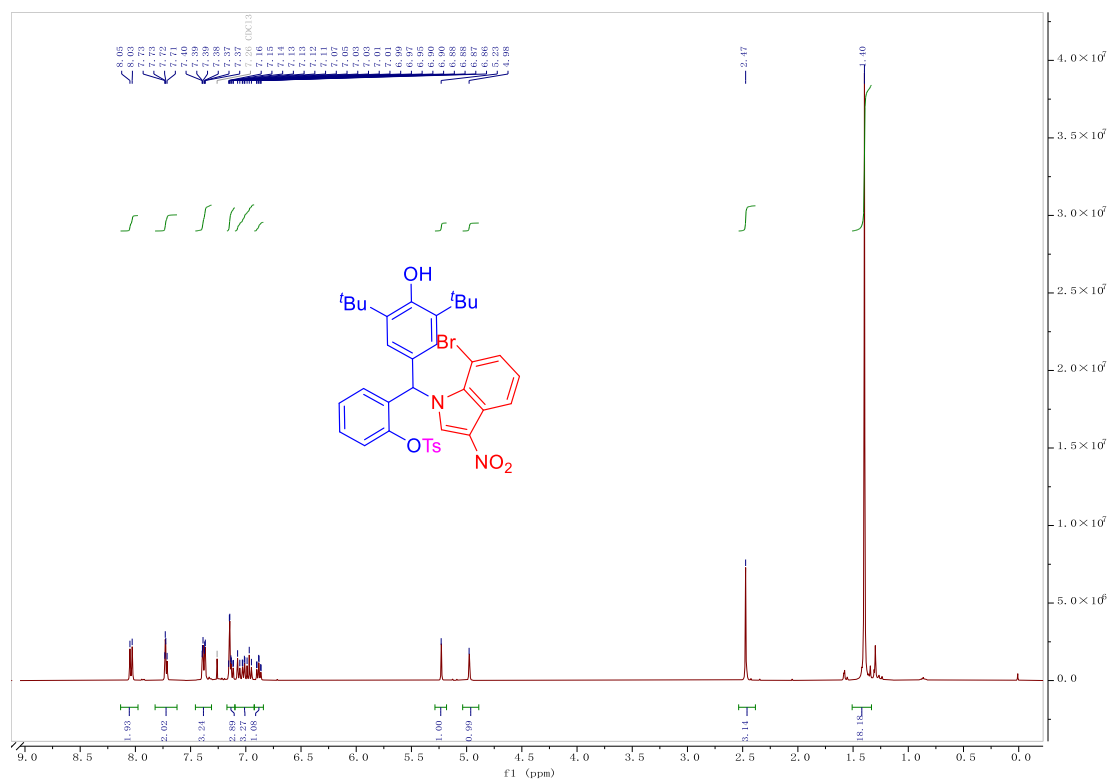
¹H NMR spectrum of 3h



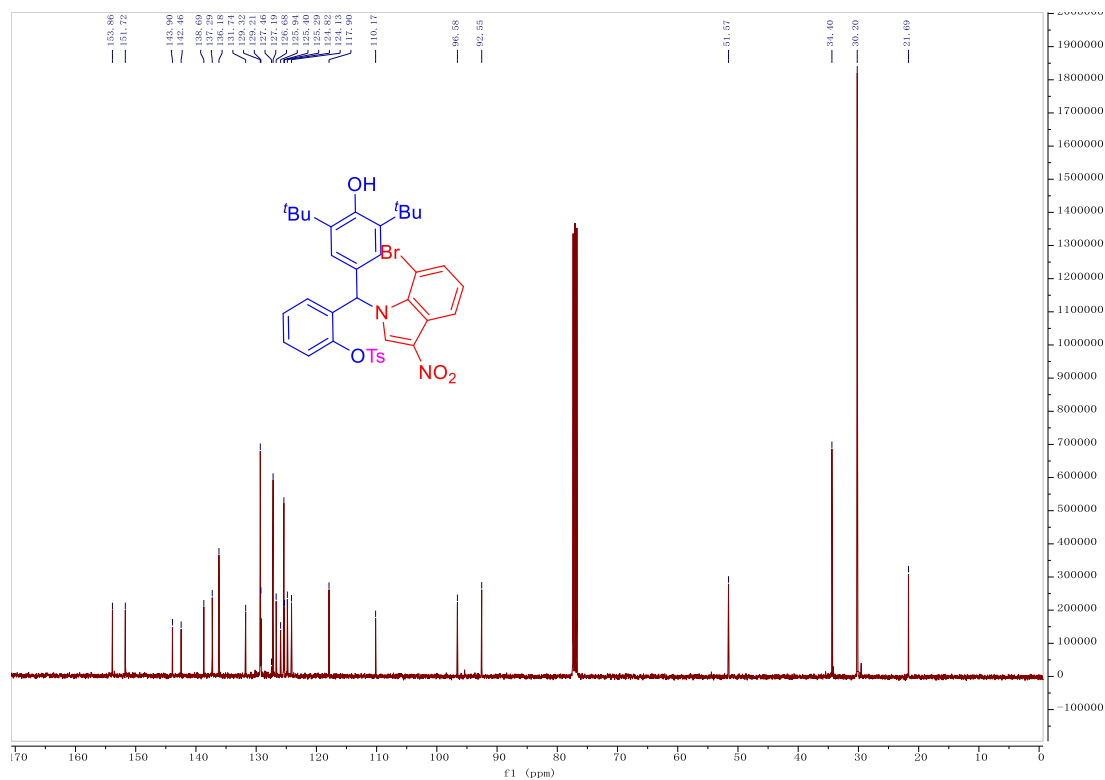
¹³C NMR spectrum of 3h



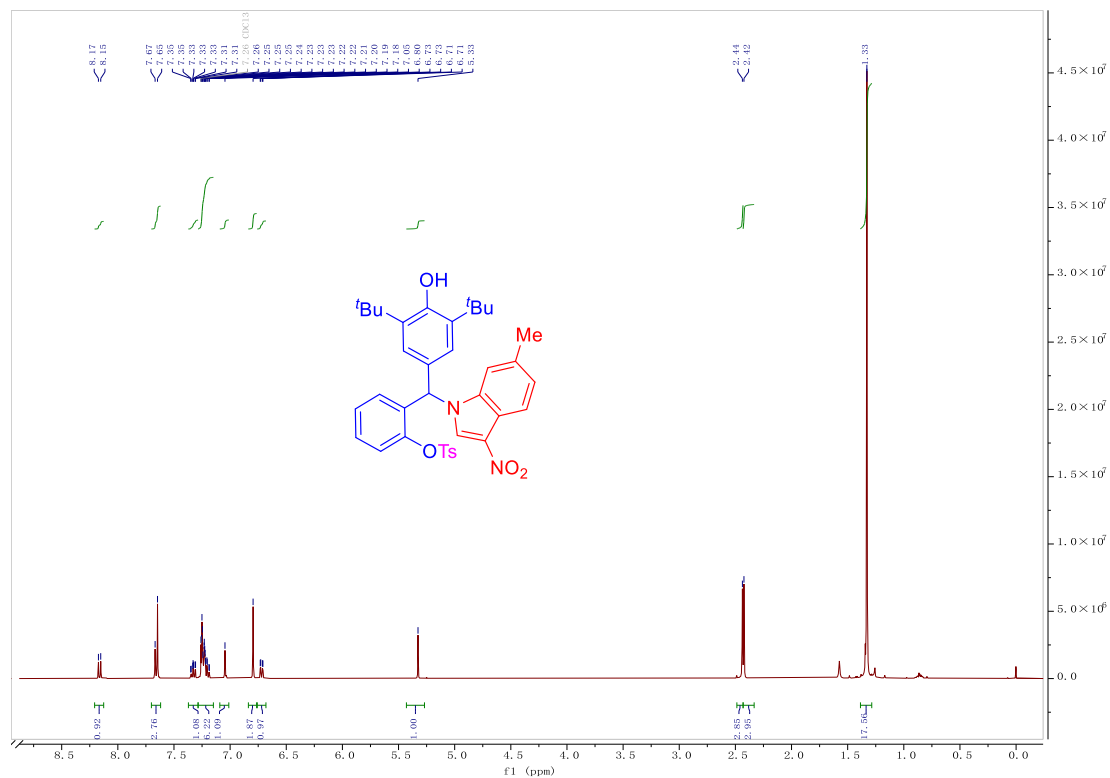
^1H NMR spectrum of 3i



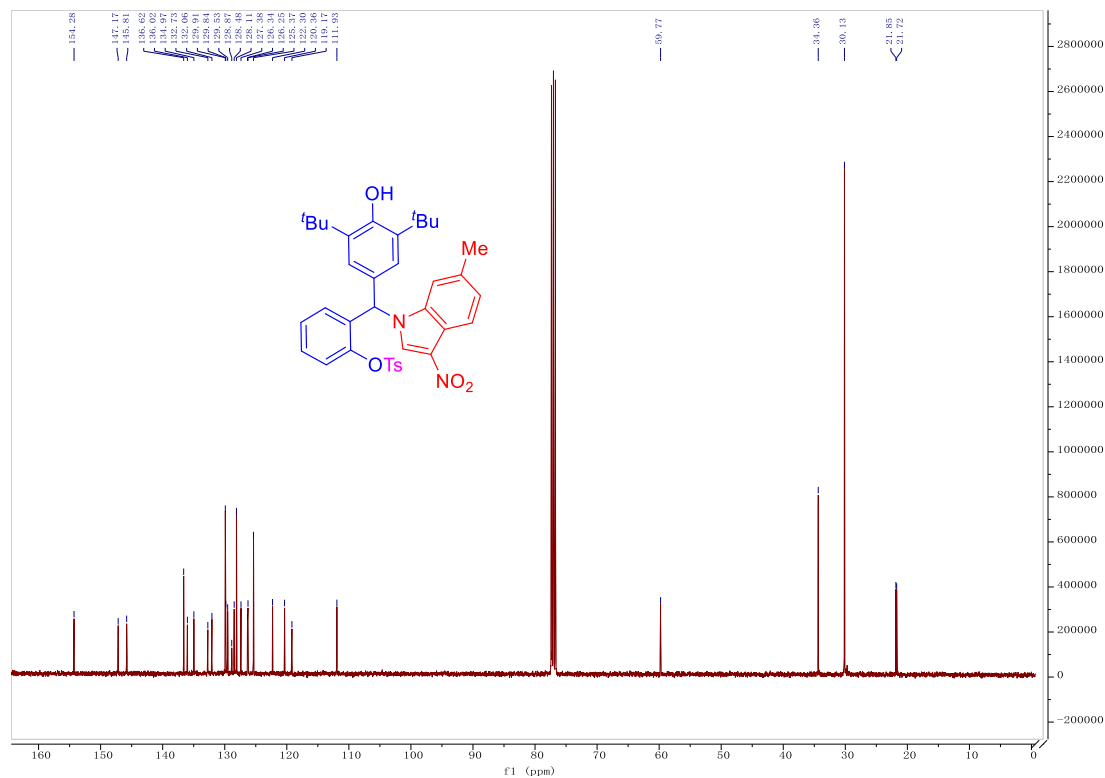
^{13}C NMR spectrum of 3i



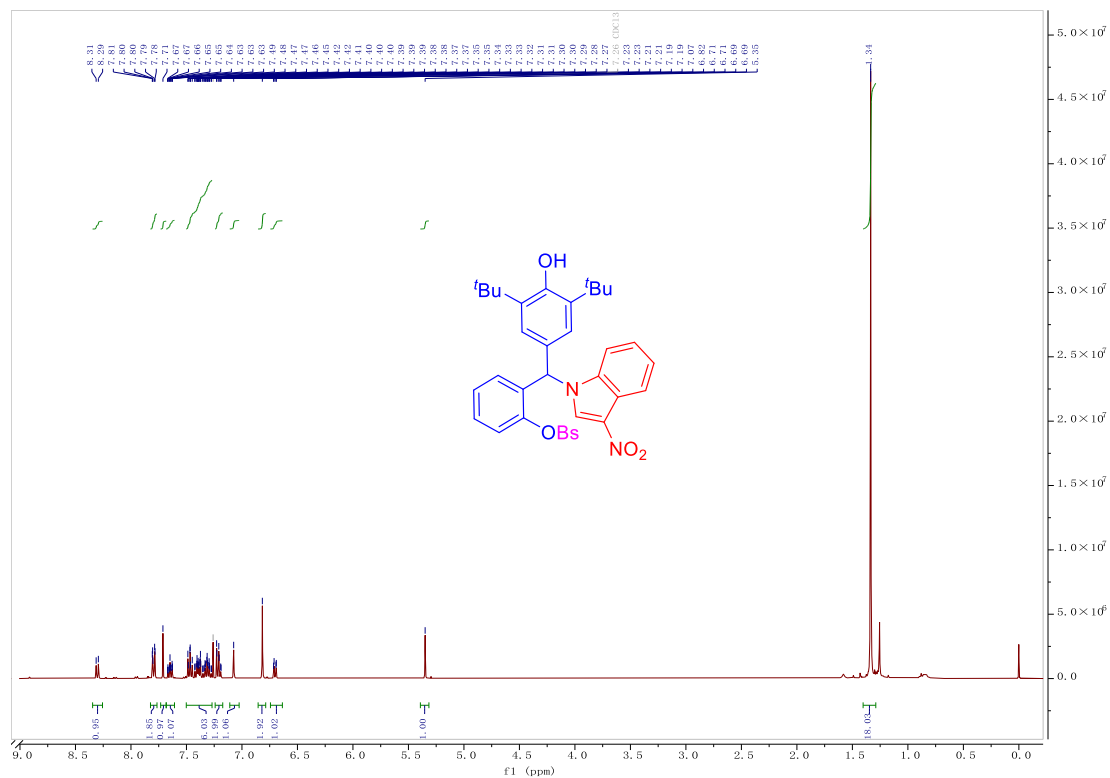
¹H NMR spectrum of 3j



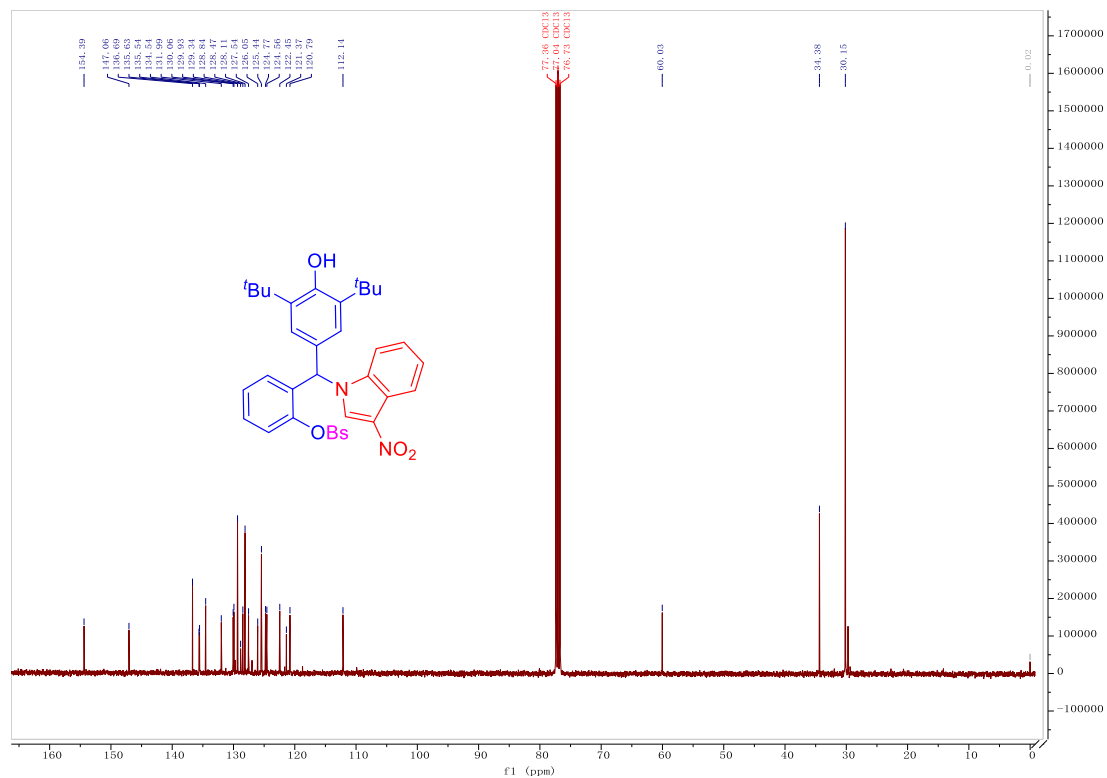
¹³C NMR spectrum of 3j



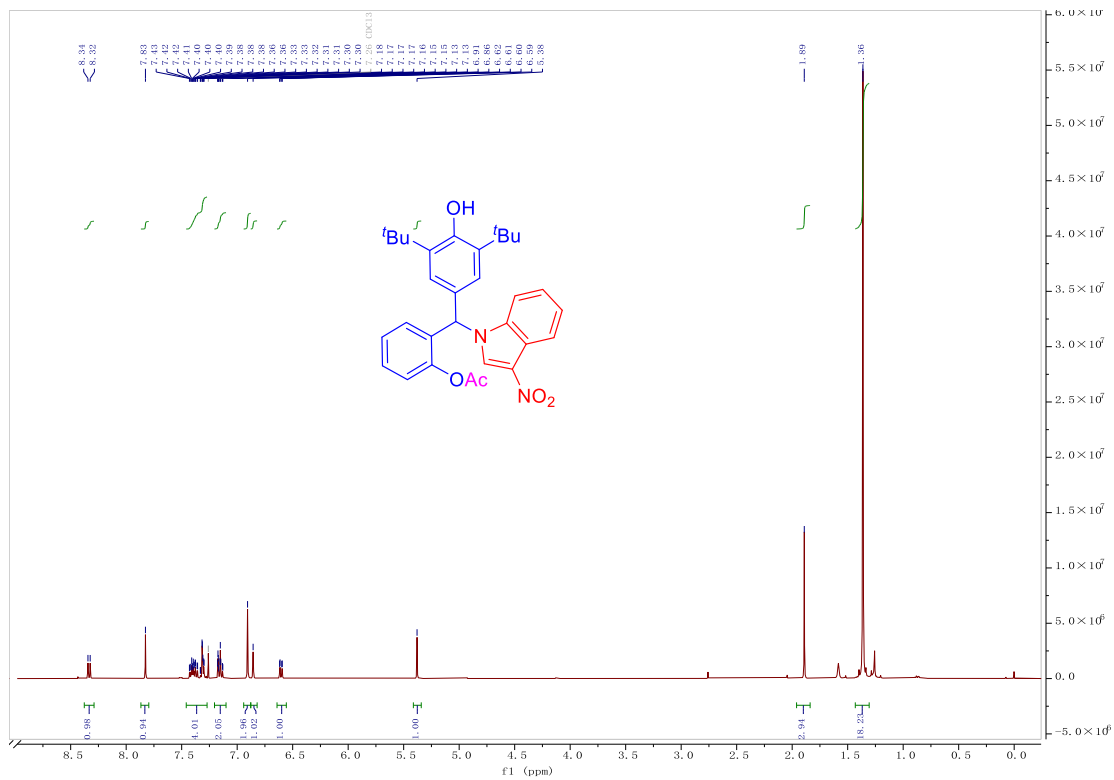
¹H NMR spectrum of 3k



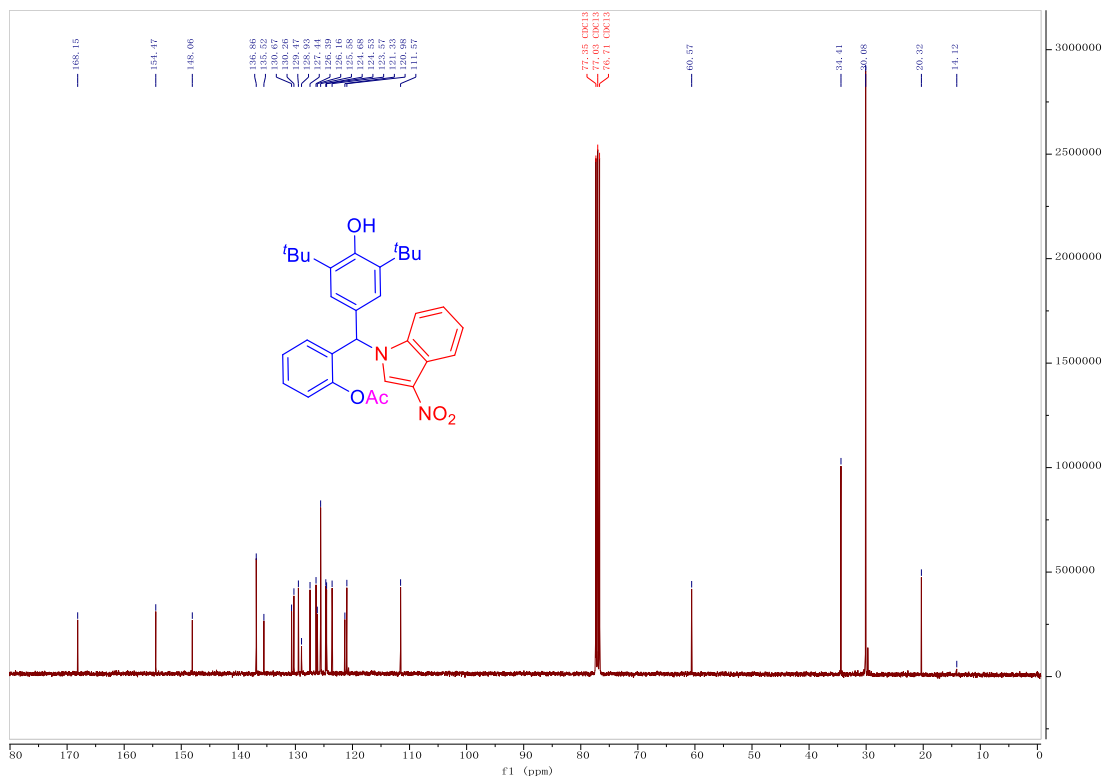
¹³C NMR spectrum of 3k



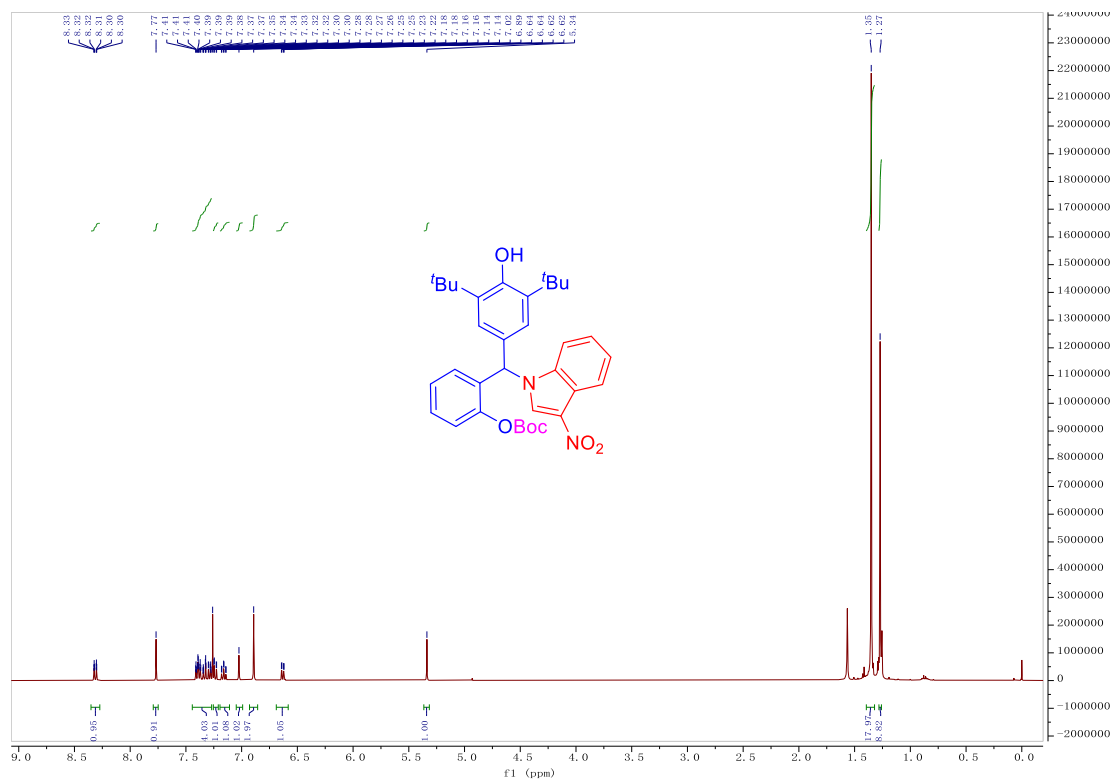
¹H NMR spectrum of 3l



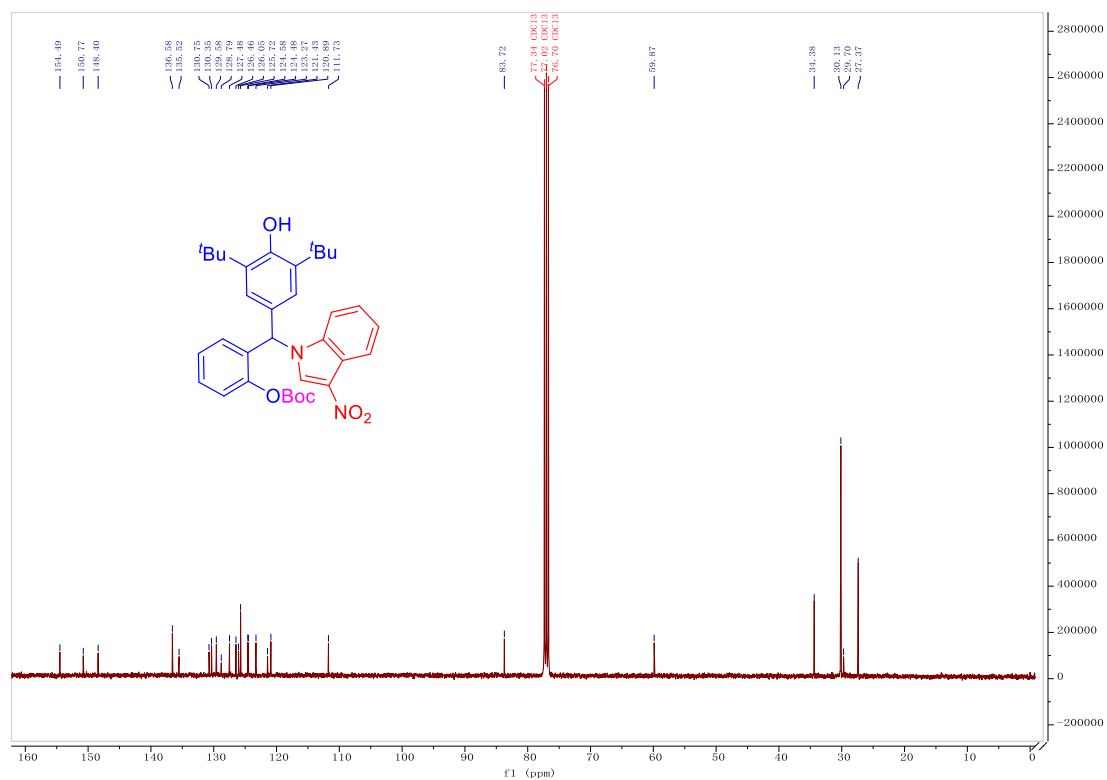
^{13}C NMR spectrum of 3l



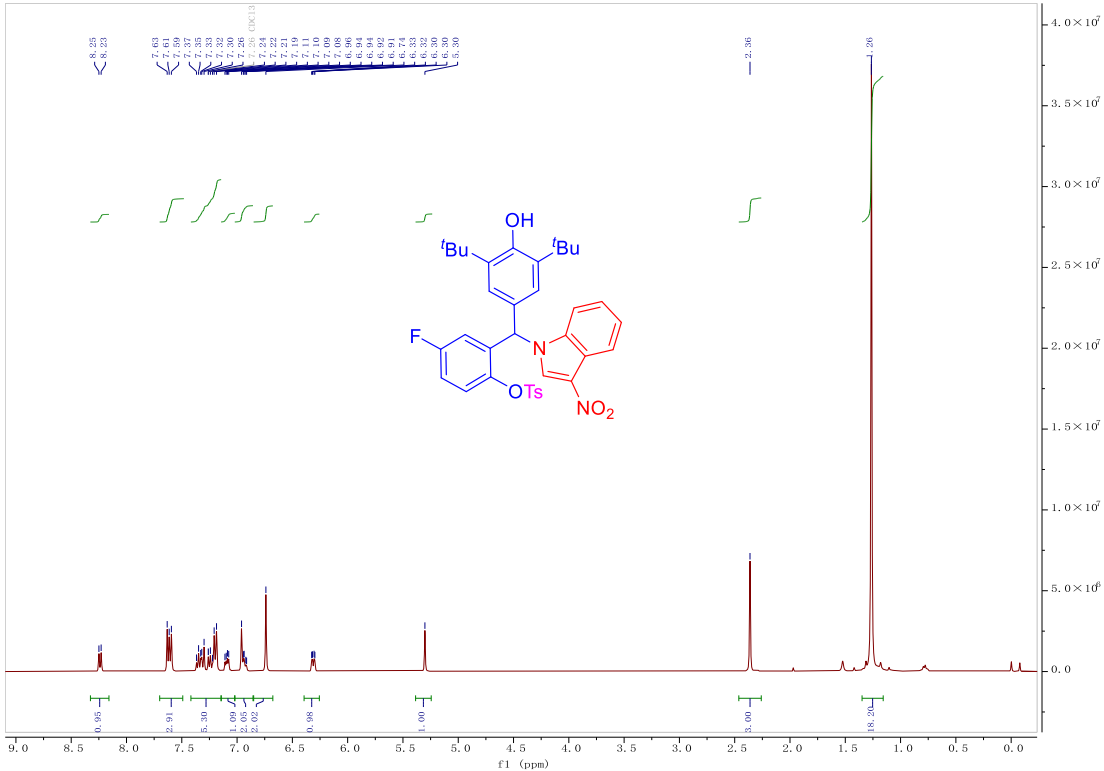
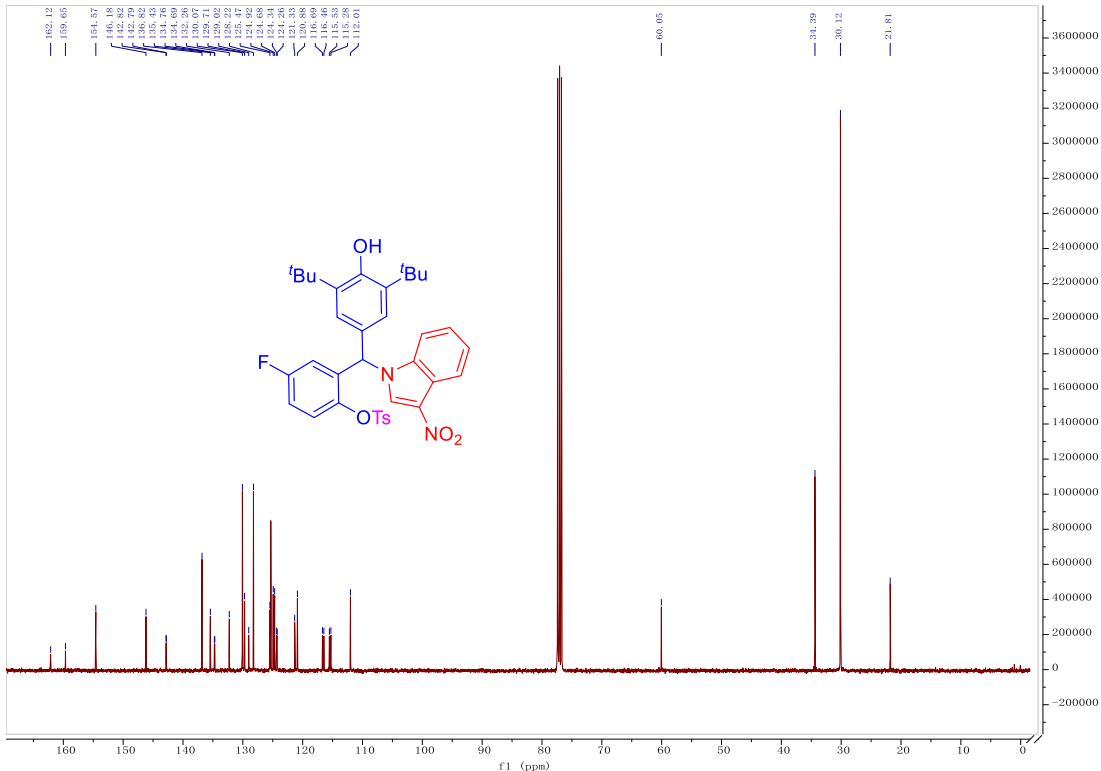
¹H NMR spectrum of 3m



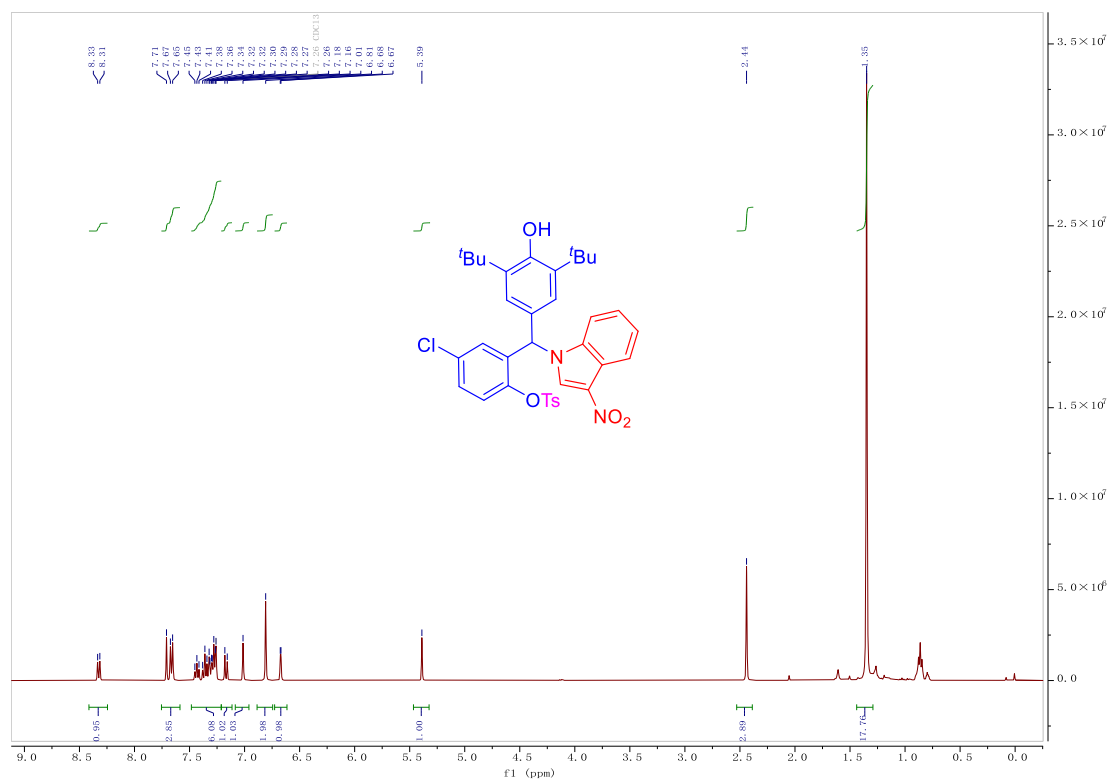
¹³C NMR spectrum of 3m



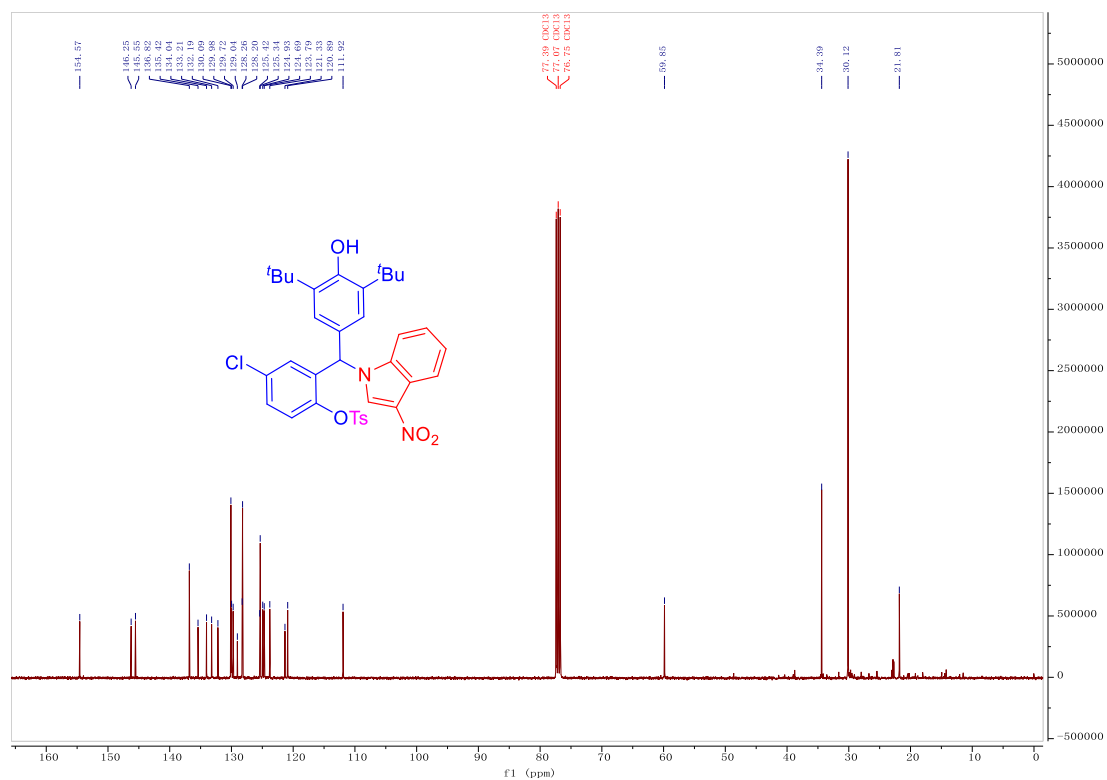
¹H NMR spectrum of 3n

¹³C NMR spectrum of 3n

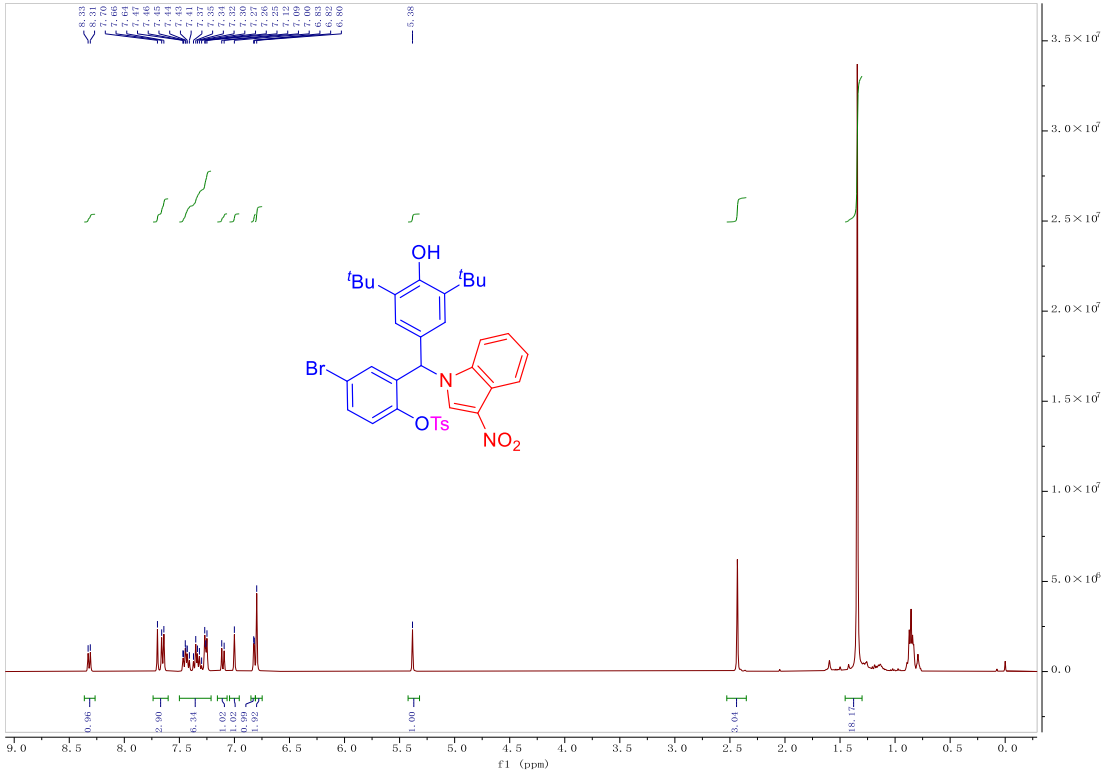
^1H NMR spectrum of 3o



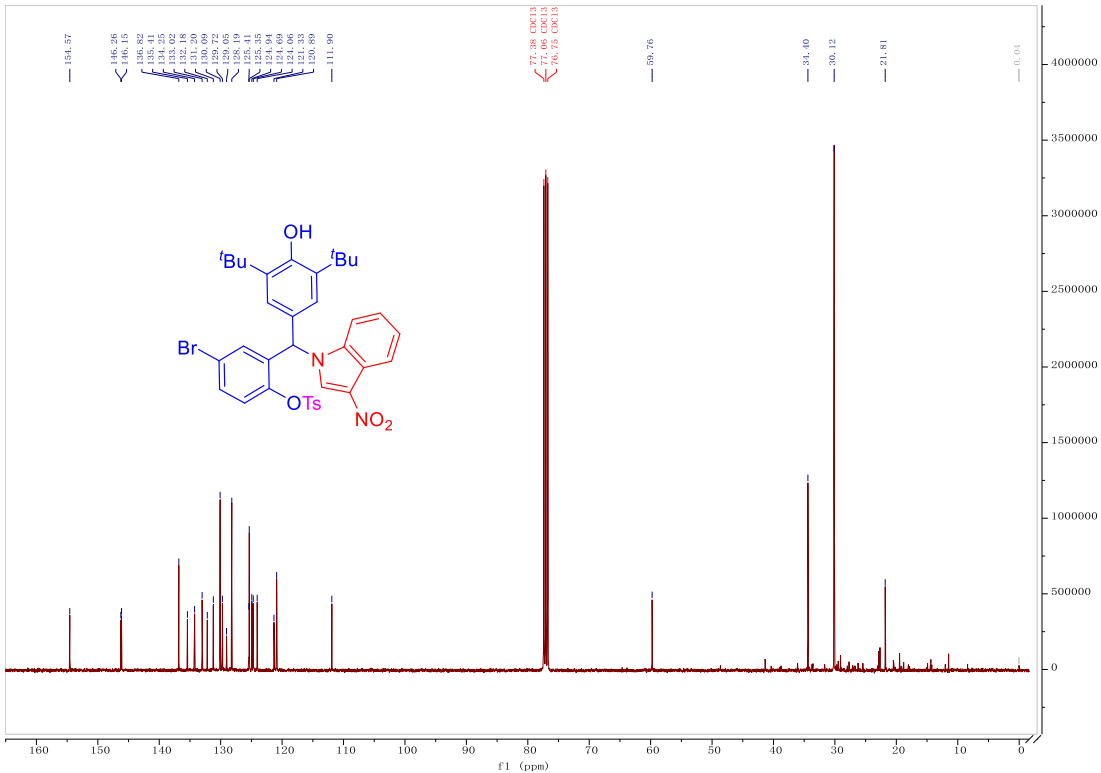
^{13}C NMR spectrum of 3o



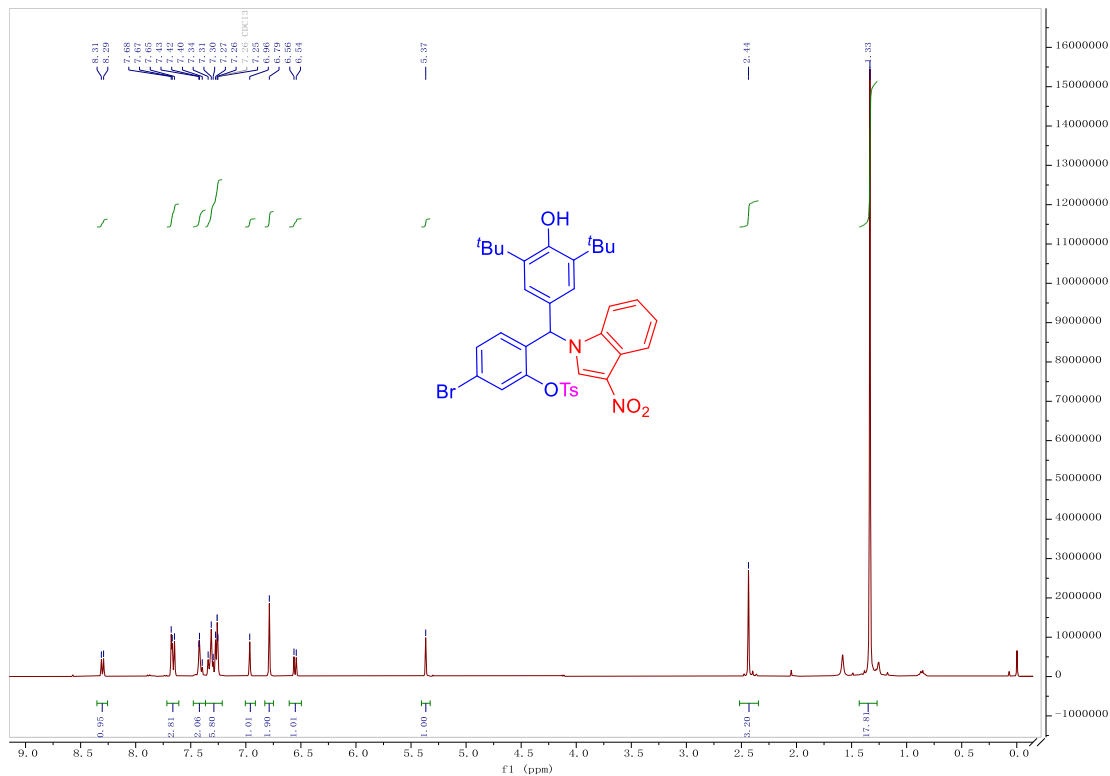
^1H NMR spectrum of 3p



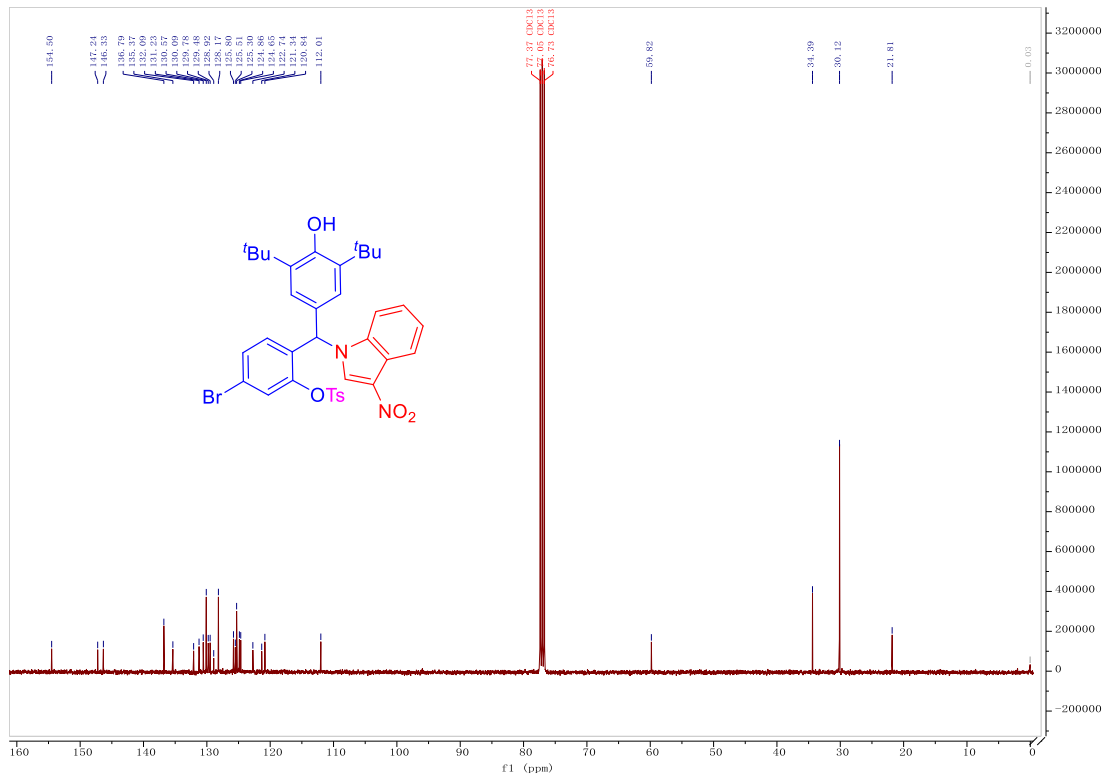
^{13}C NMR spectrum of 3p



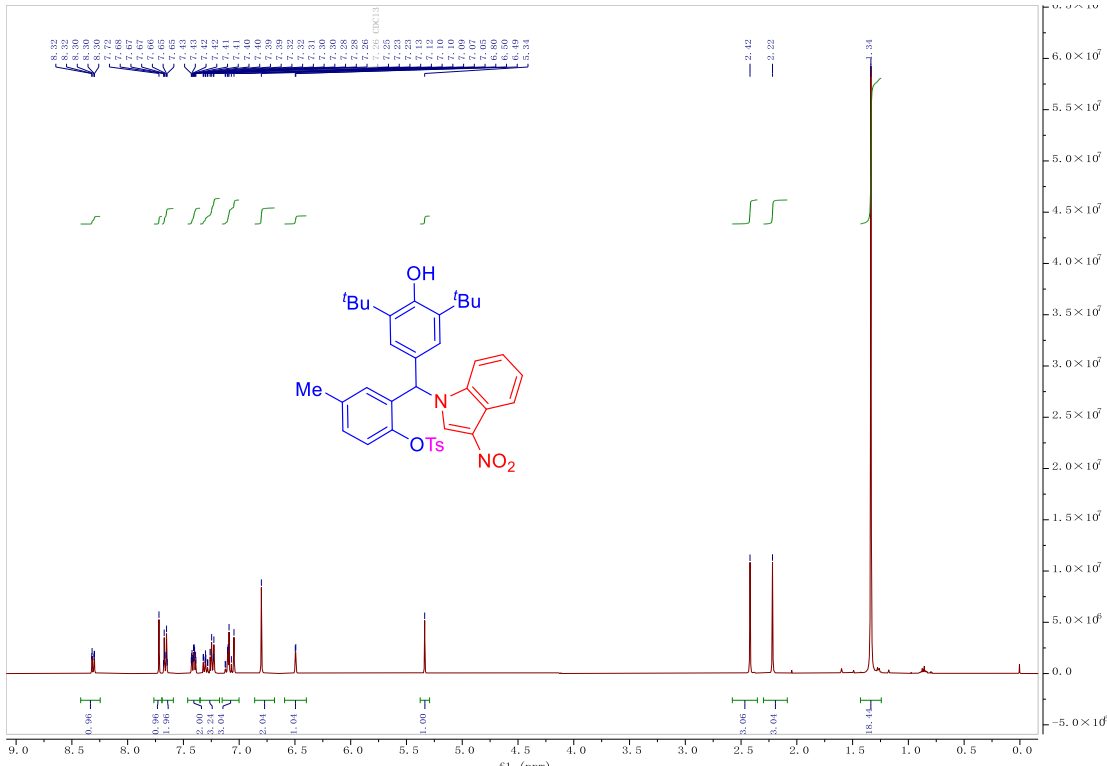
¹H NMR spectrum of 3q



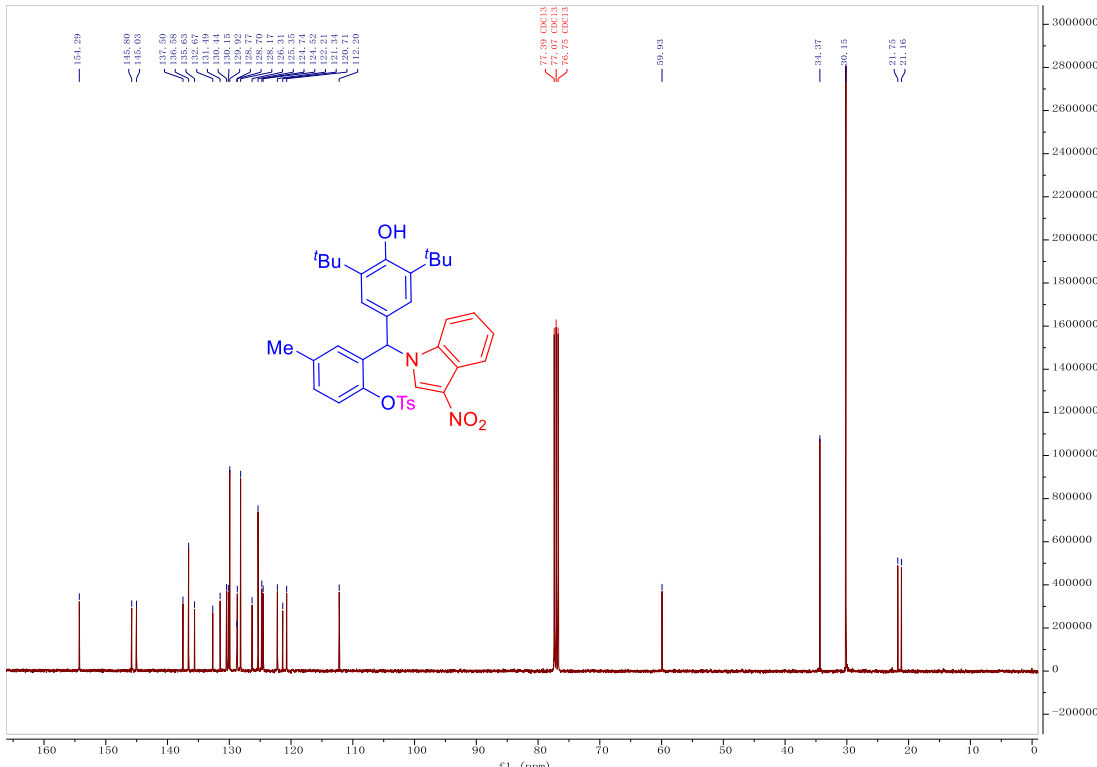
^{13}C NMR spectrum of 3q



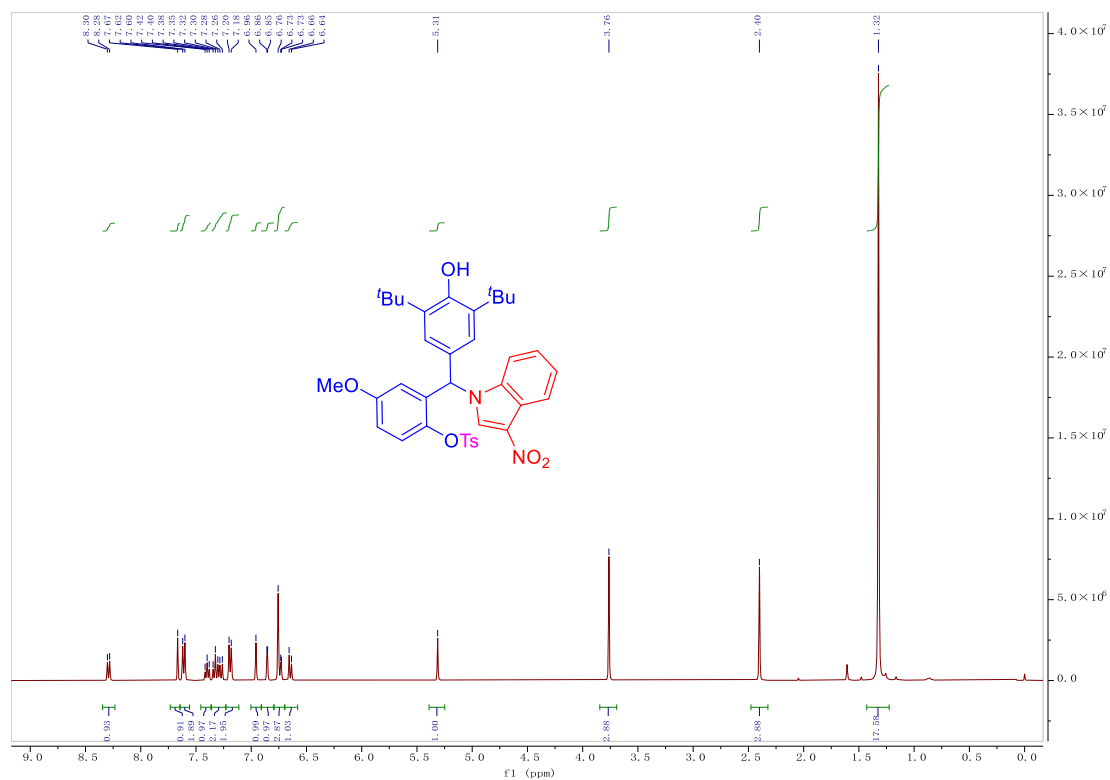
¹H NMR spectrum of 3r



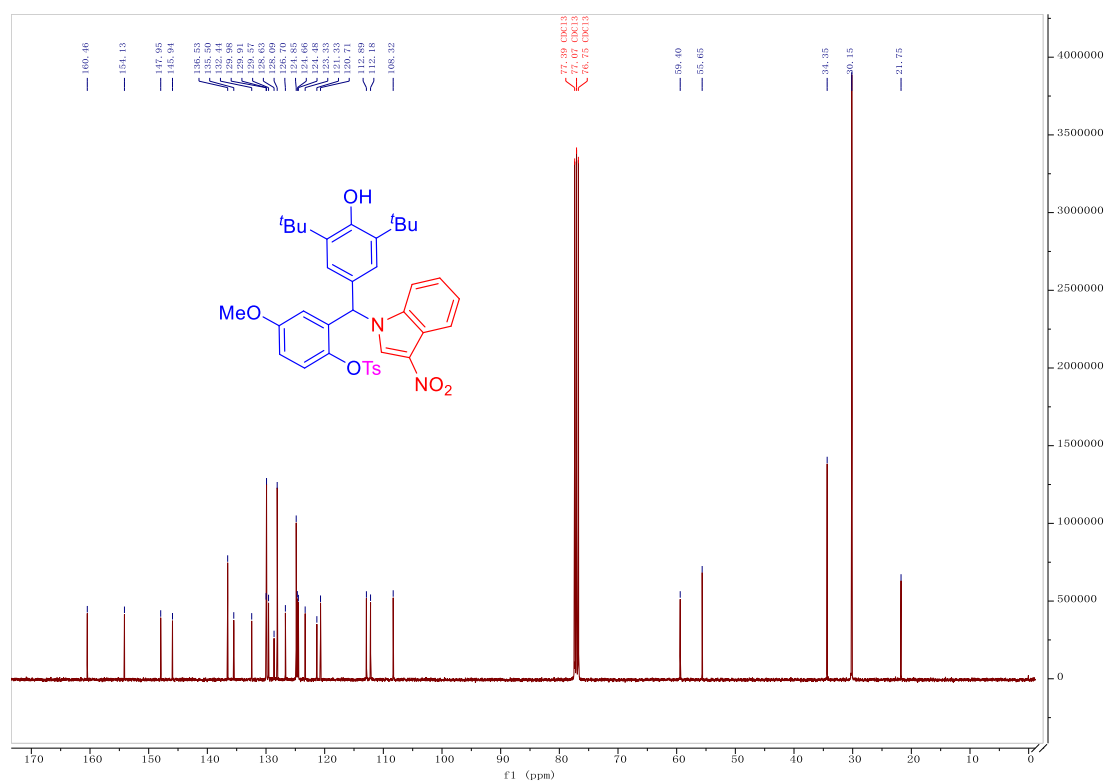
^{13}C NMR spectrum of 3r



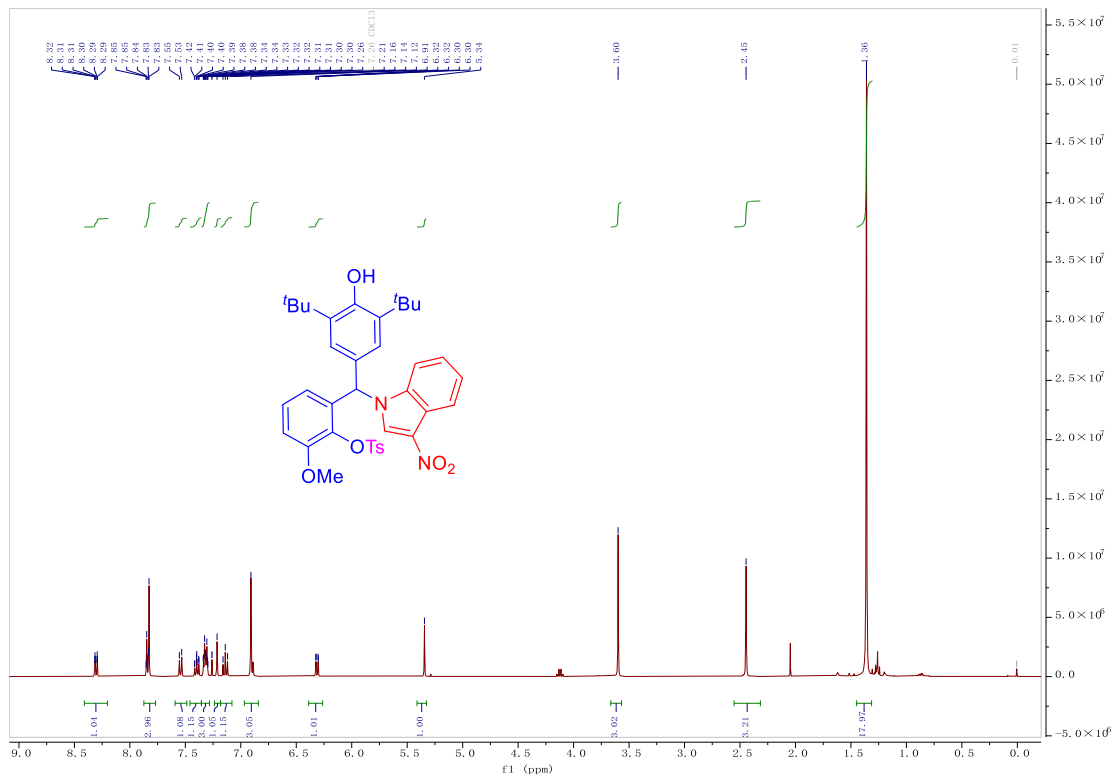
¹H NMR spectrum of 3s



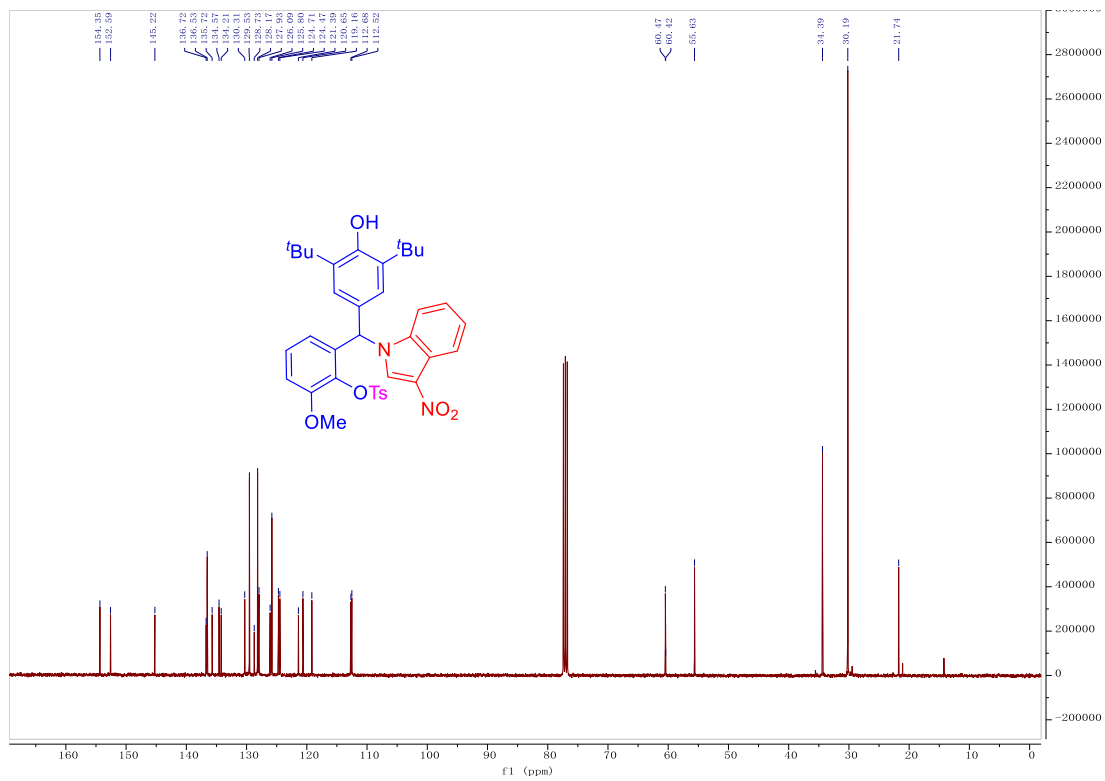
¹³C NMR spectrum of 3s



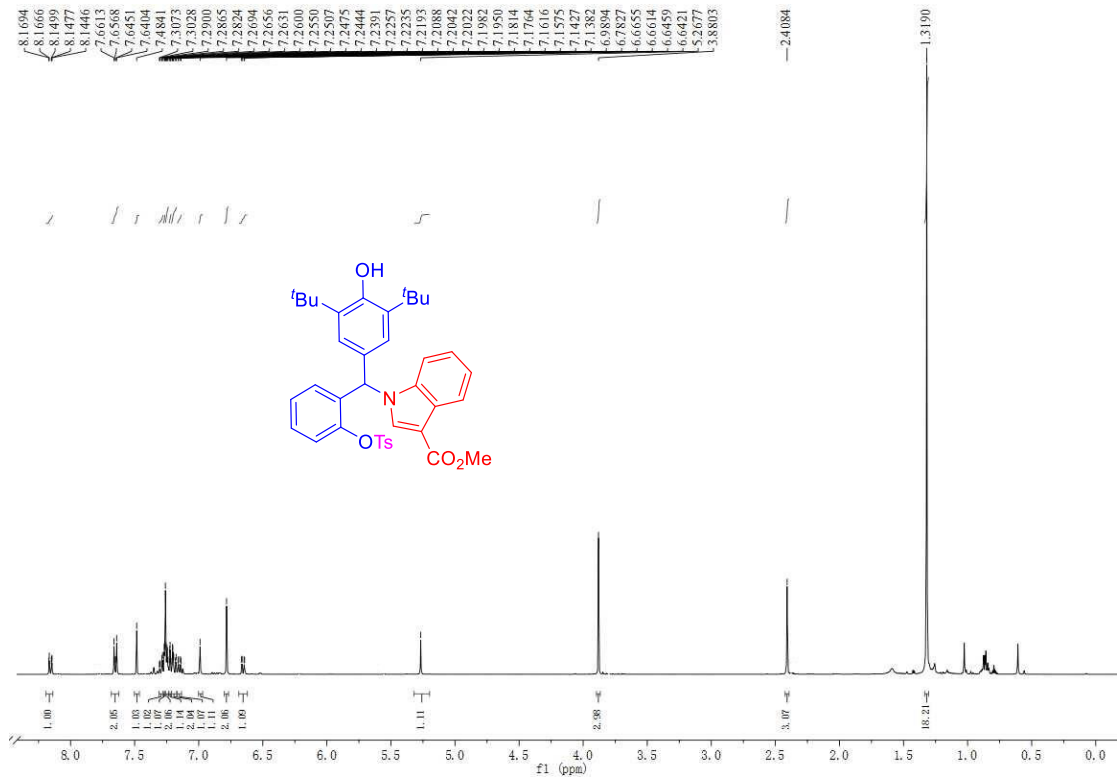
¹H NMR spectrum of 3t



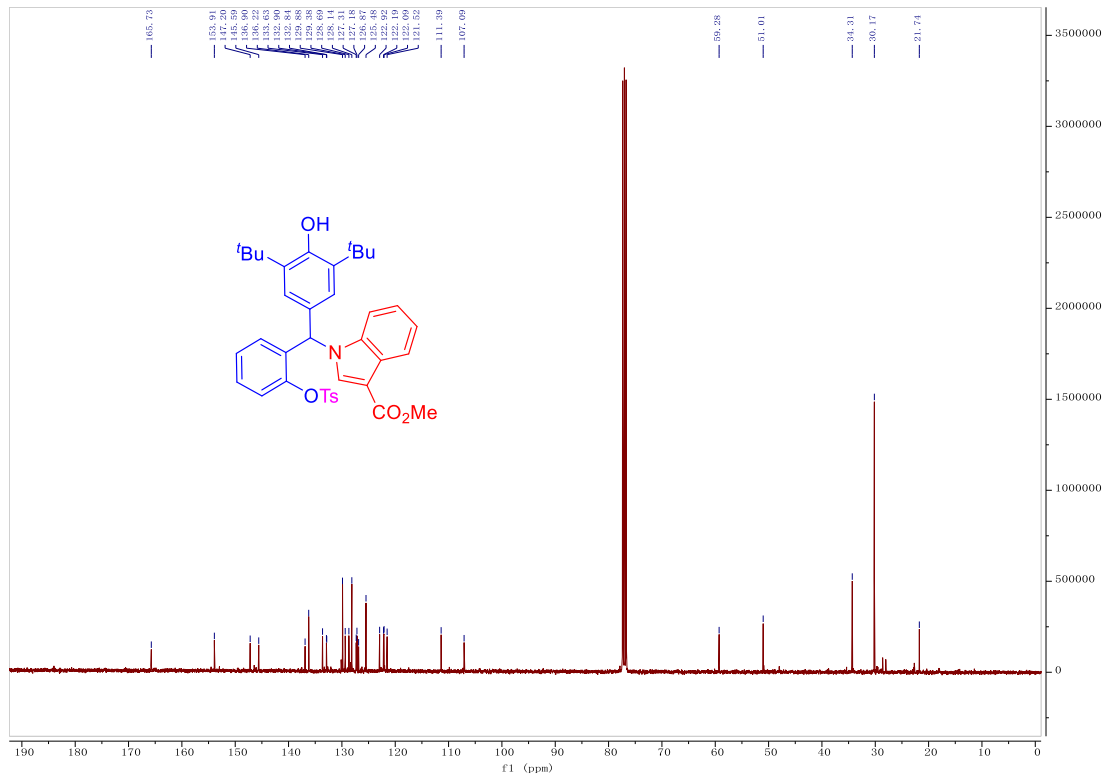
^{13}C NMR spectrum of 3t



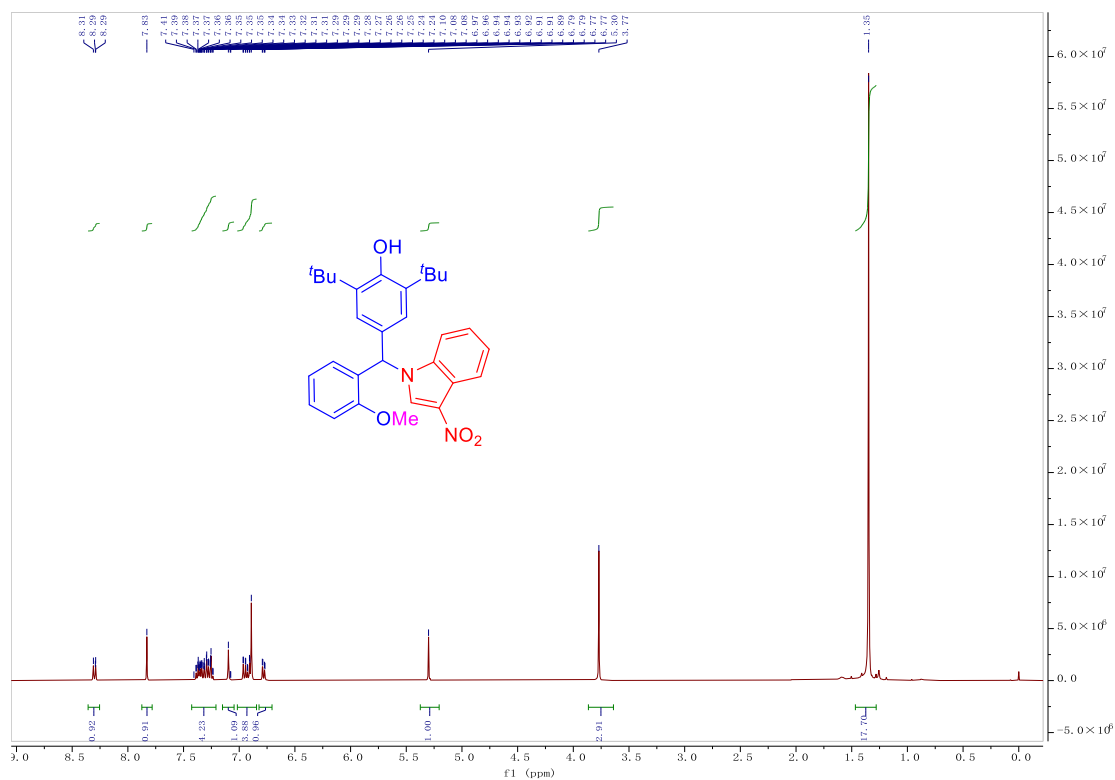
¹H NMR spectrum of 6



^{13}C NMR spectrum of 6



¹H NMR spectrum of 11



¹³C NMR spectrum of 11

