Supporting Information for

Synthesis of Spiro[pyrazolin-3,3'-oxindoles] and 3-Arylcarbonylmethyl Substituted Ylideneoxindoles by 1,3-Dipolar Cycloadditions of 3-Ylideneoxindoles and in situ-generated α-Diazoketones

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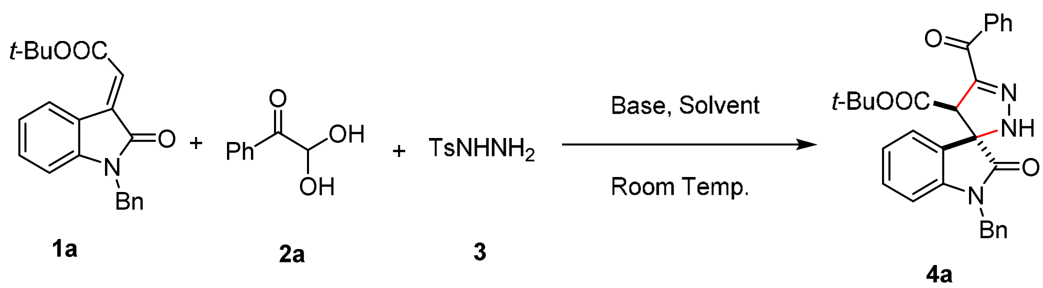
1. Detailed optimization of reaction conditions:

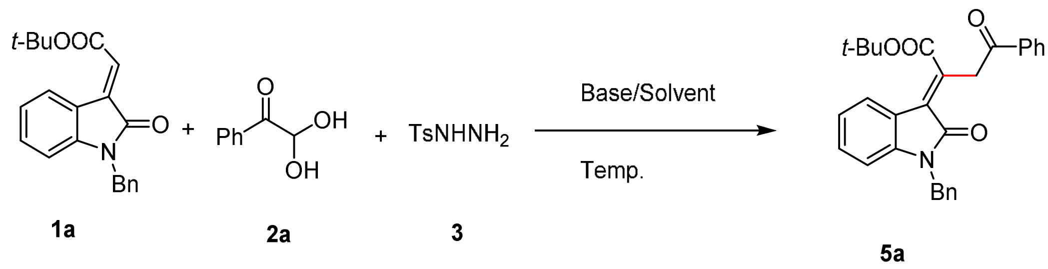
Table S1: Optimization of the condition of 1,3-diploar cycloaddition of **1a**, phenylglyoxal monohydrate **2a** with 4-methylbenzenesulfonohydrazide **3**[a]



Entry	Temp./^{o}C	Base	Sol.	Time (min)	Yield [%][b]	d.r.[c]
1	Room Temp.	Cs_2CO_3	DMSO	20	80	>20:1
2	Room Temp.	K_2CO_3	DMSO	20	77	>20:1
3	Room Temp.	KOH	DMSO	20	72	>20:1
4	Room Temp.	DBU	DMSO	20	83	>20:1
5	Room Temp.	DMAP	DMSO	20	45	n.d.
6	Room Temp.	Et_3N	DMSO	20	15	n.d.
7	Room Temp.	DBU	EtOH	20	40	n.d.
8	Room Temp.	DBU	CH_3CN	20	70	>20:1
9	Room Temp.	DBU	THF	20	62	>20:1
10	Room Temp.	DBU	DCM	20	46	n.d.

[a] General reaction conditions: **1a** (0.5 mmol), **2a** (0.5 mmol), **3** (0.5 mmol), solvent (2.5 mL). n. d.= no detected. [b] Isolated yields. [c] Determined by ^{1}H NMR analysis.

Table S2: Optimization of the reaction condition for the synthesis of **5a**[a]



Entry	Temp./°C	Base	Sol.	Time (min)	Yield [%][b]
1	80	Cs_2CO_3	DMSO	20	70
2	80	NaOH	DMSO	20	85
3	80	Na_2CO_3	DMSO	120	58
4	80	DBU	DMSO	120	62
5	80	NaOH	DMF	20	78
6	80	NaOH	EtOH	20	36
7	80	NaOH	CH_3CN	60	42
8	80	NaOH	Dioxane	120	38
9	80	NaOH	Toluene	120	25
10	60	NaOH	DMSO	60	35
11	100	NaOH	DMSO	20	81
12	110	NaOH	DMSO	20	78

[a] General reaction conditions: **1a** (0.5 mmol), **2a** (0.5 mmol), **3** (0.5 mmol), solvent (2.5 mL). [b] Isolated yields.

3. Copies of ^{1}H NMR, ^{13}C NMR and HRMS of 4 and 5

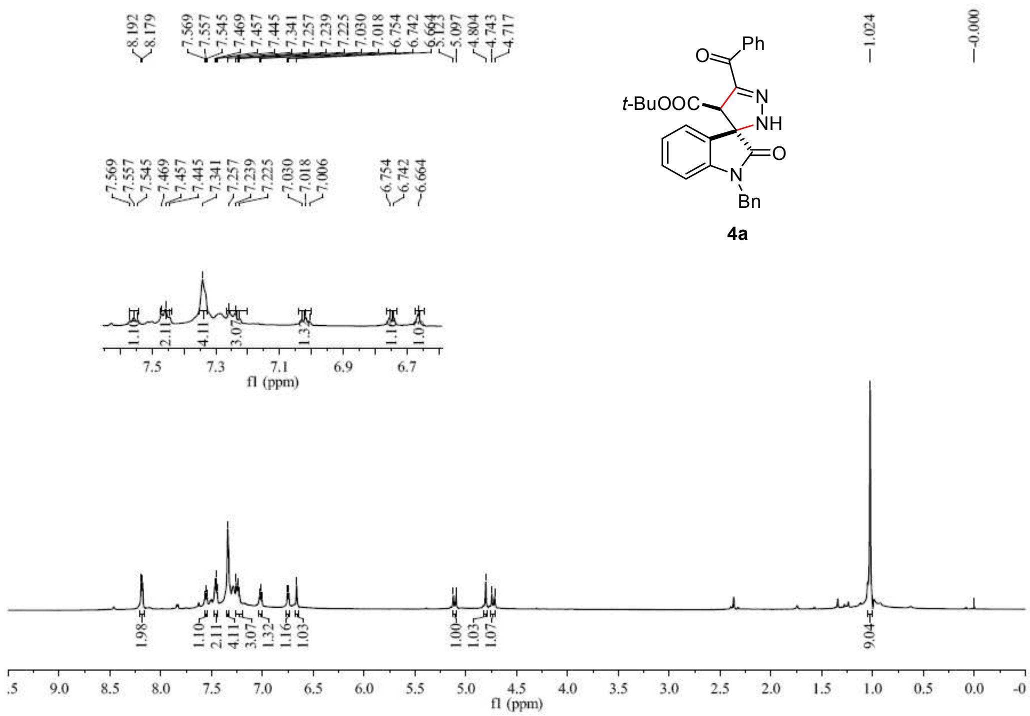


Figure S1. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4a**.

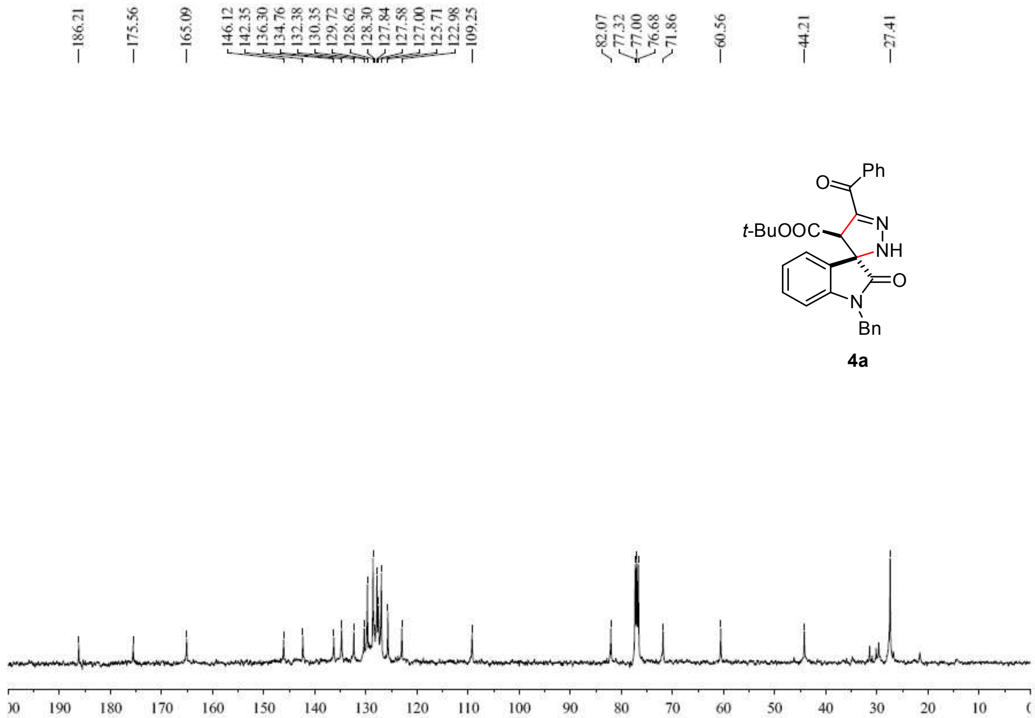


Figure S2. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4a**.

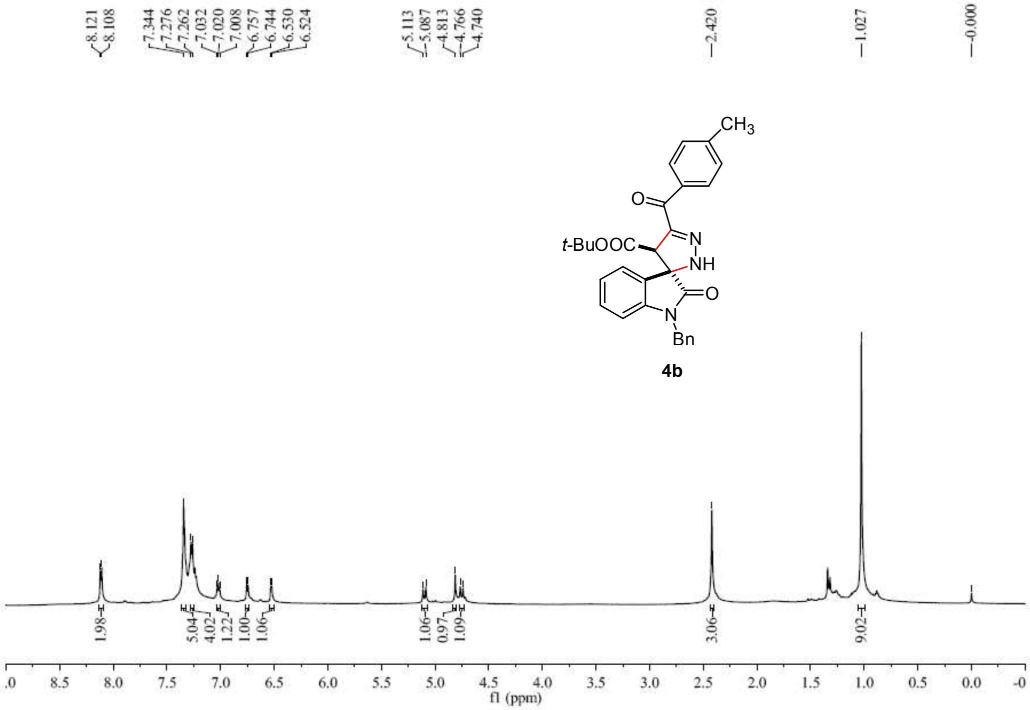


Figure S3. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4b**.

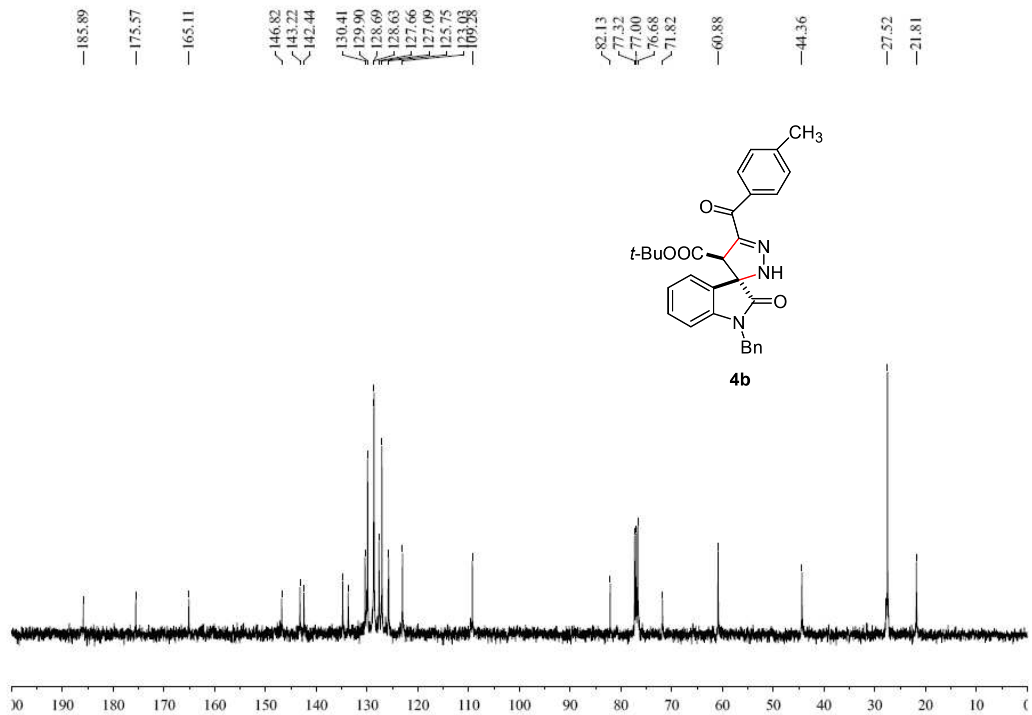


Figure S4. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4b**.

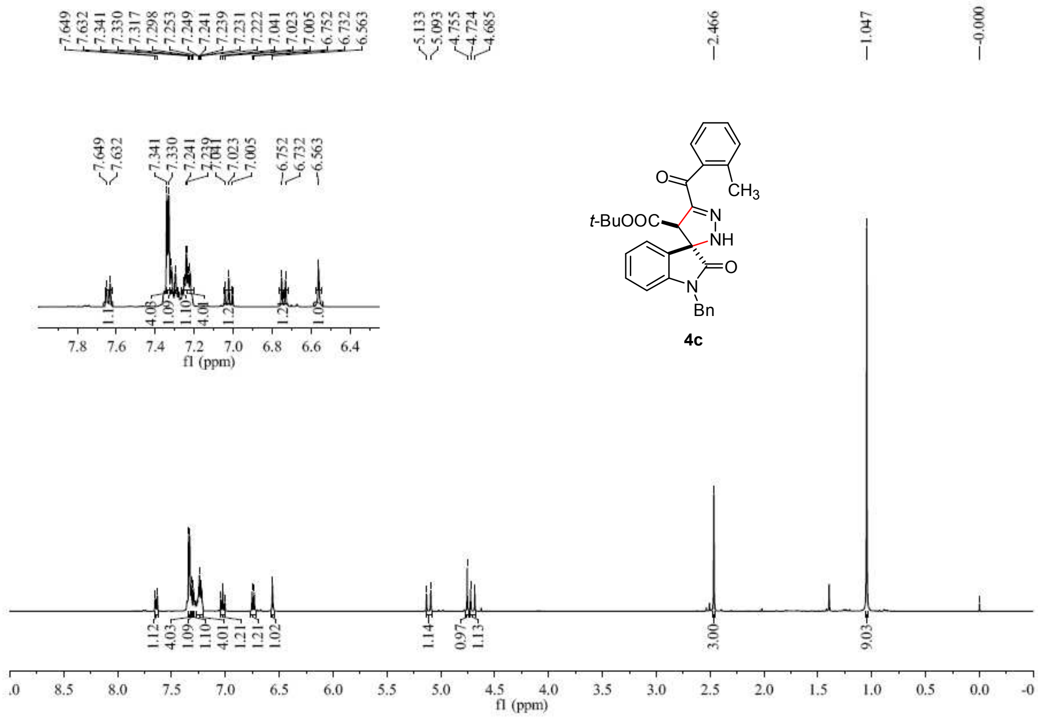


Figure S5. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4c**.

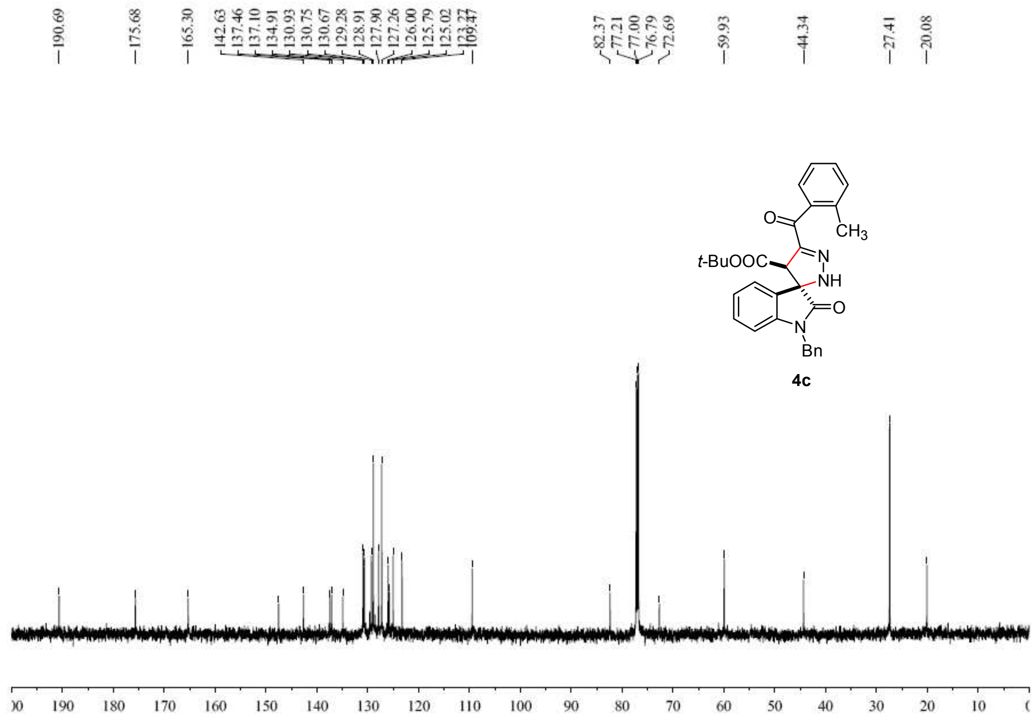


Figure S6. The ^{13}C NMR (150M Hz, $CDCl_3$) of **4c**.

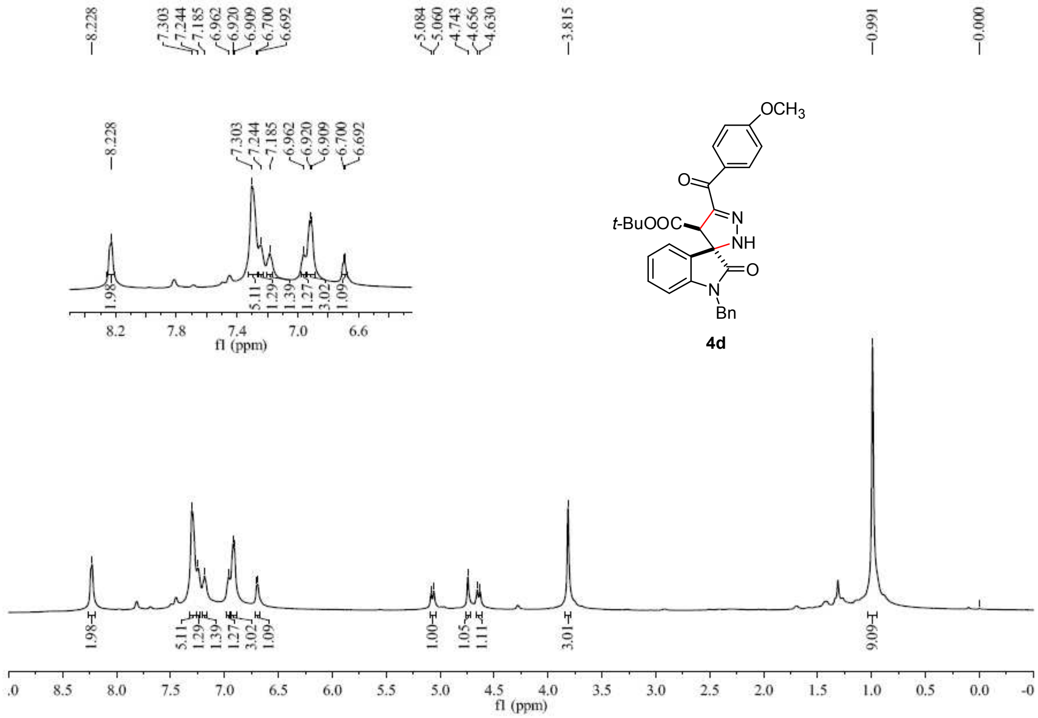


Figure S7. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4d**.

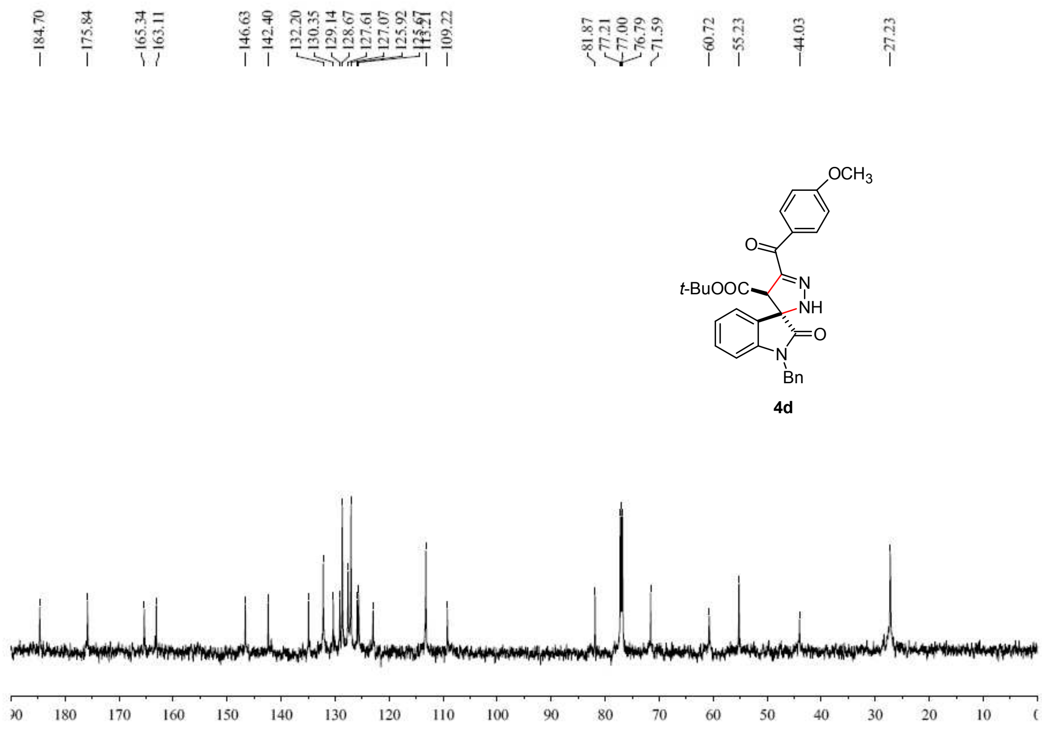


Figure S8. The ^{13}C NMR (150M Hz, $CDCl_3$) of **4d**.

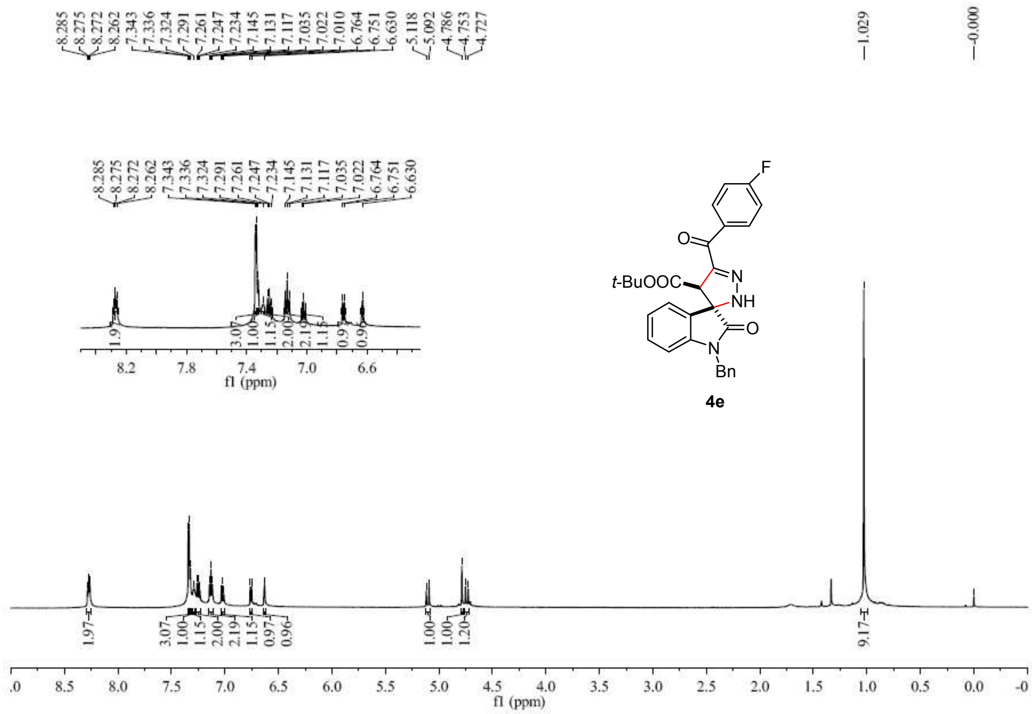


Figure S9. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4e**.

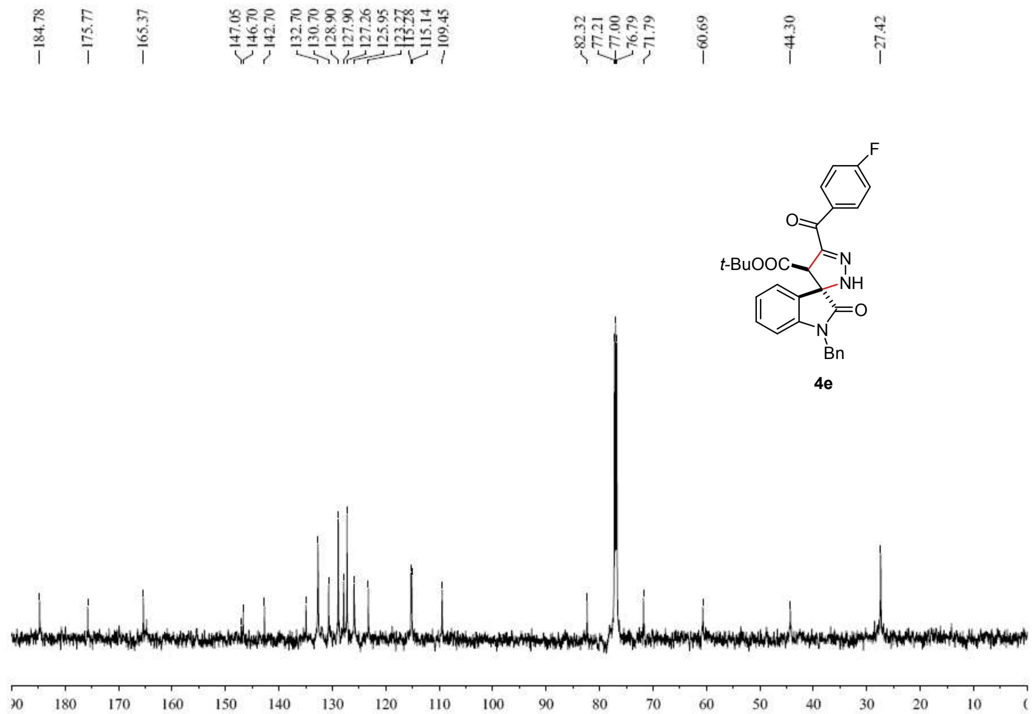


Figure S10. The ^{13}C NMR(150M Hz, $CDCl_3$) of **4e**.

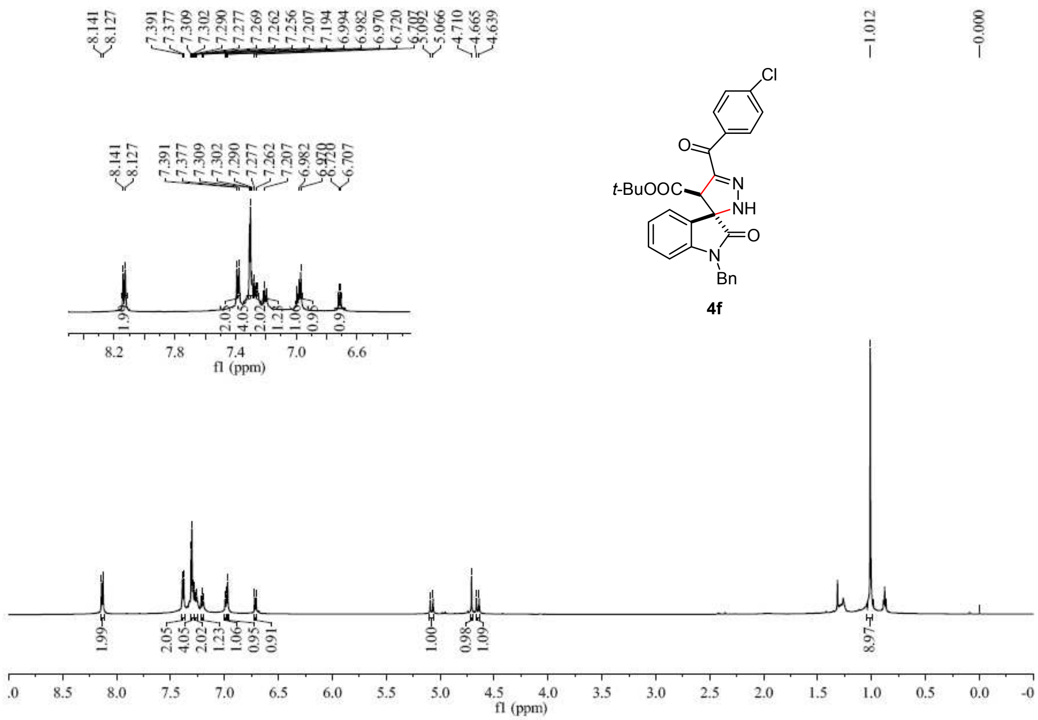


Figure S11. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4f**.

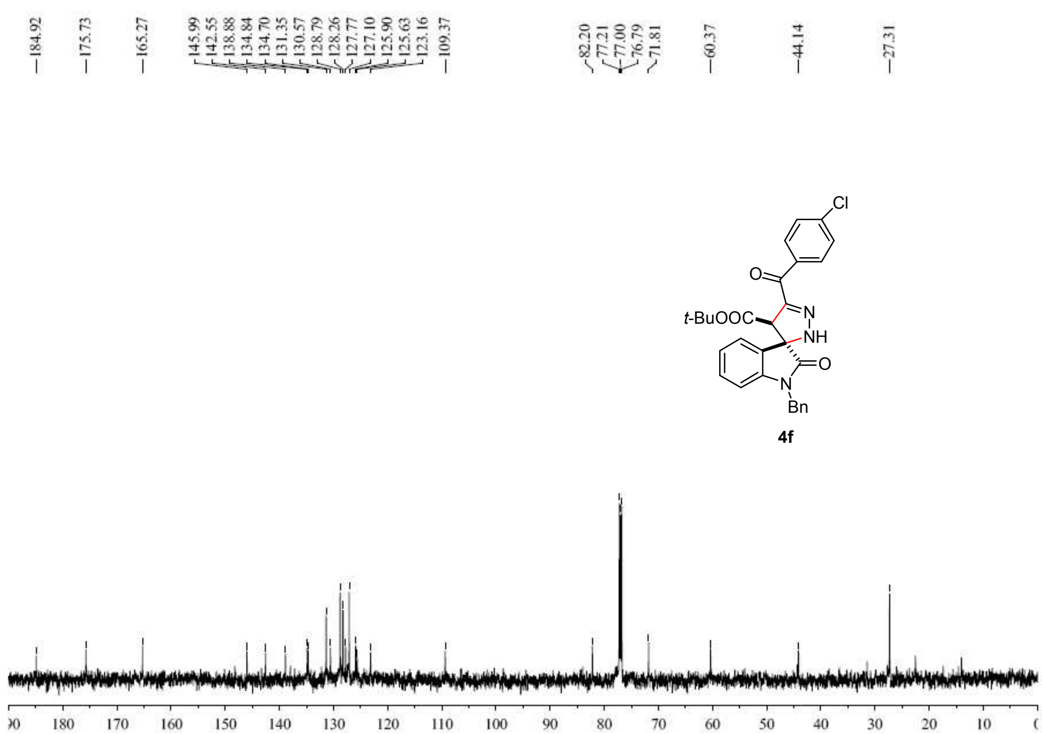


Figure S12. The ^{13}C NMR(150M Hz, $CDCl_3$) of **4f**.

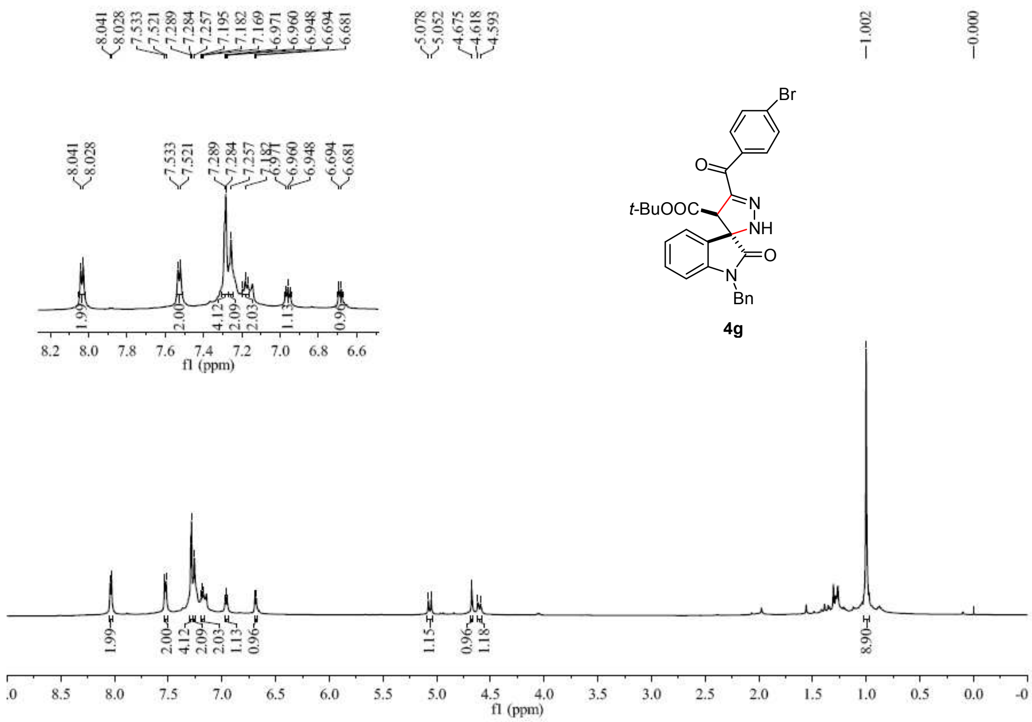


Figure S13. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4g**.

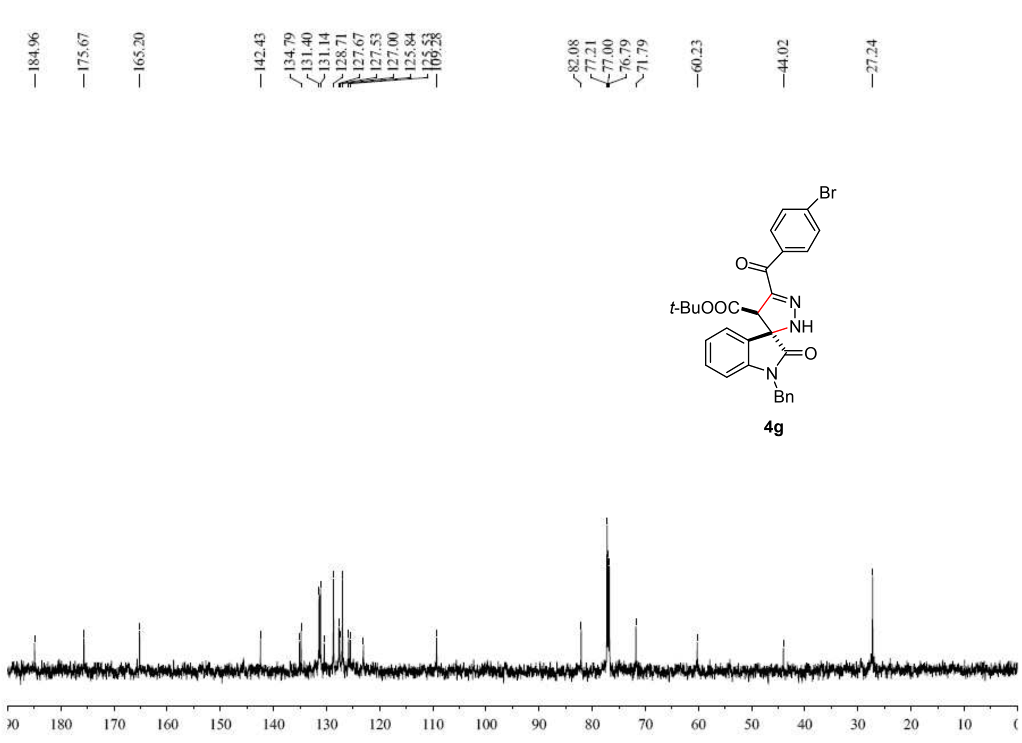


Figure S14. The ^{13}C NMR(150M Hz, $CDCl_3$) of **4g**.

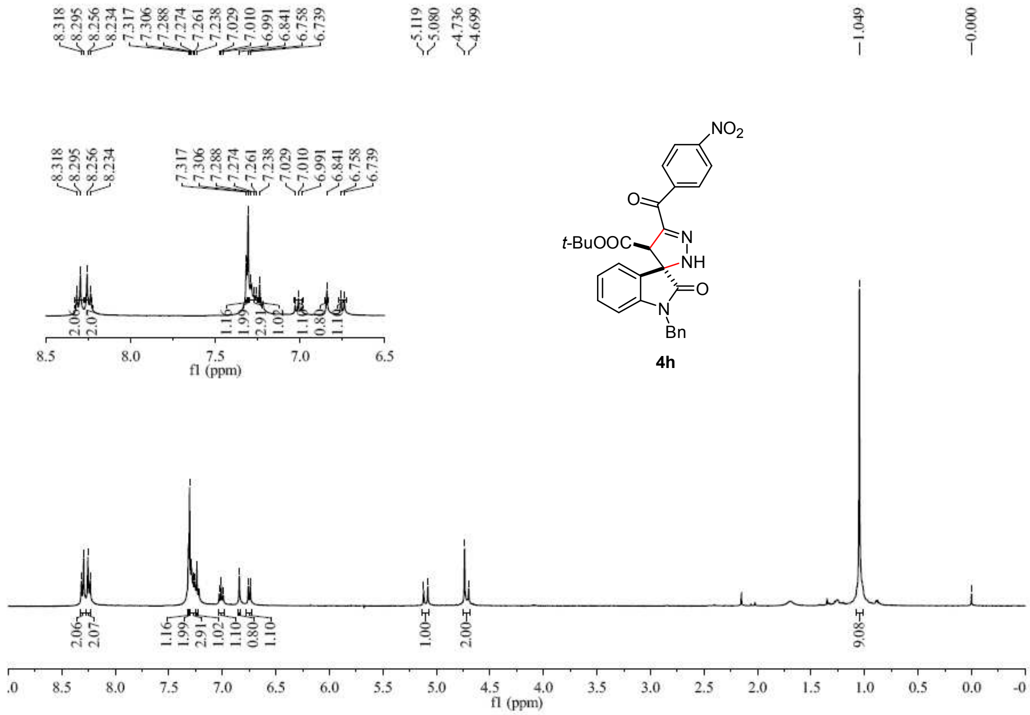


Figure S15. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4h**.

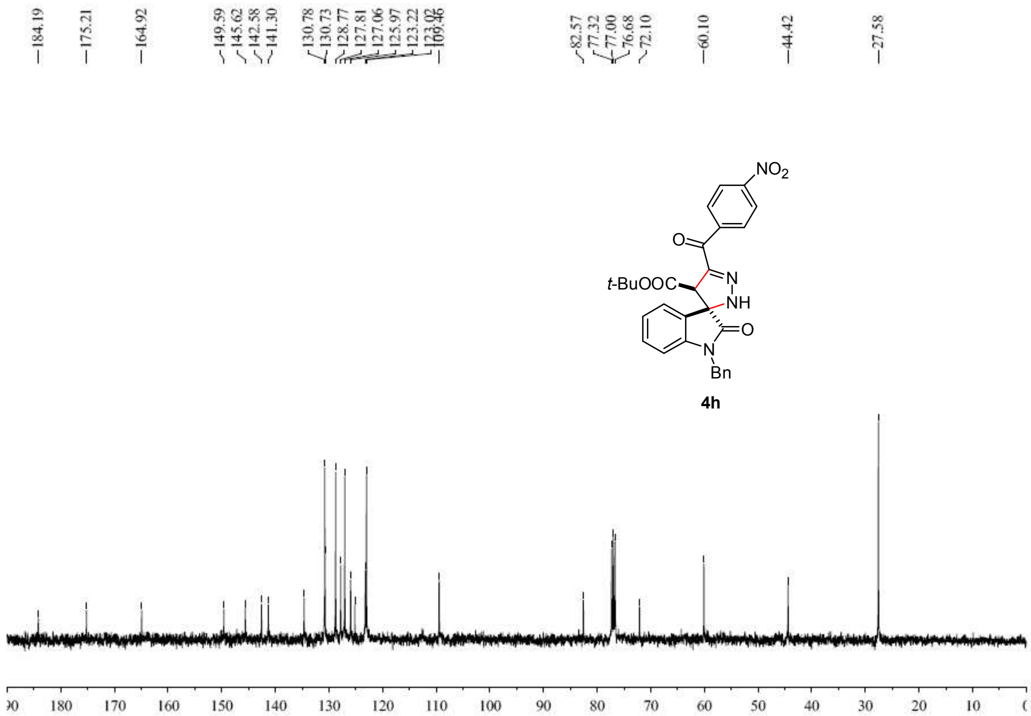


Figure S16. The ^{13}C NMR(100M Hz, $CDCl_3$) of **4h**.

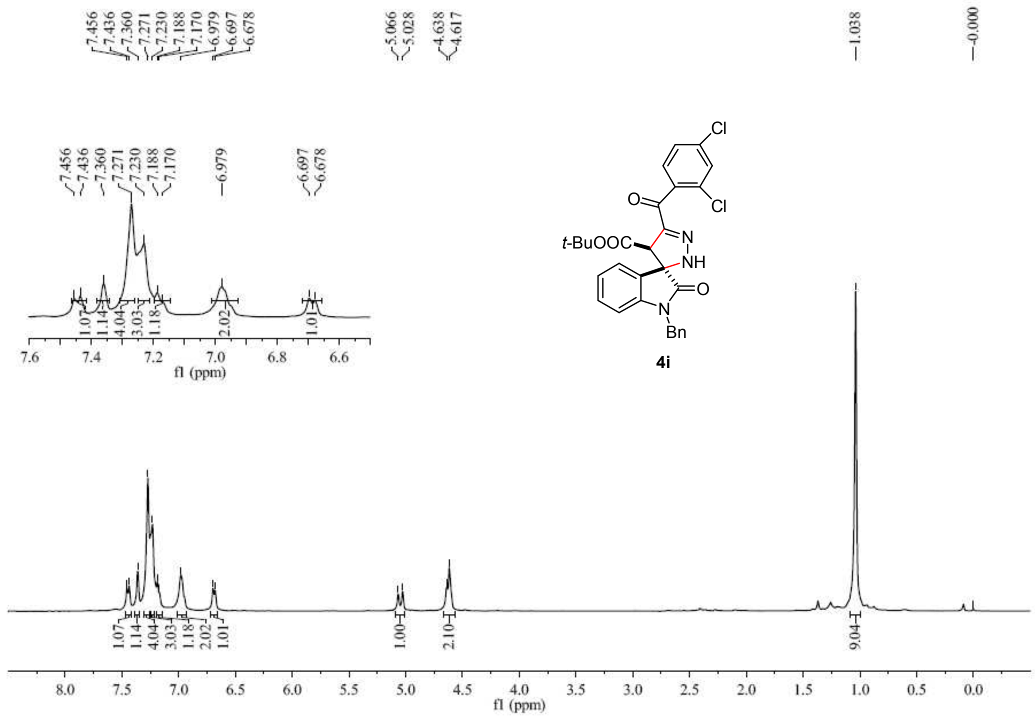


Figure S17. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4i**.

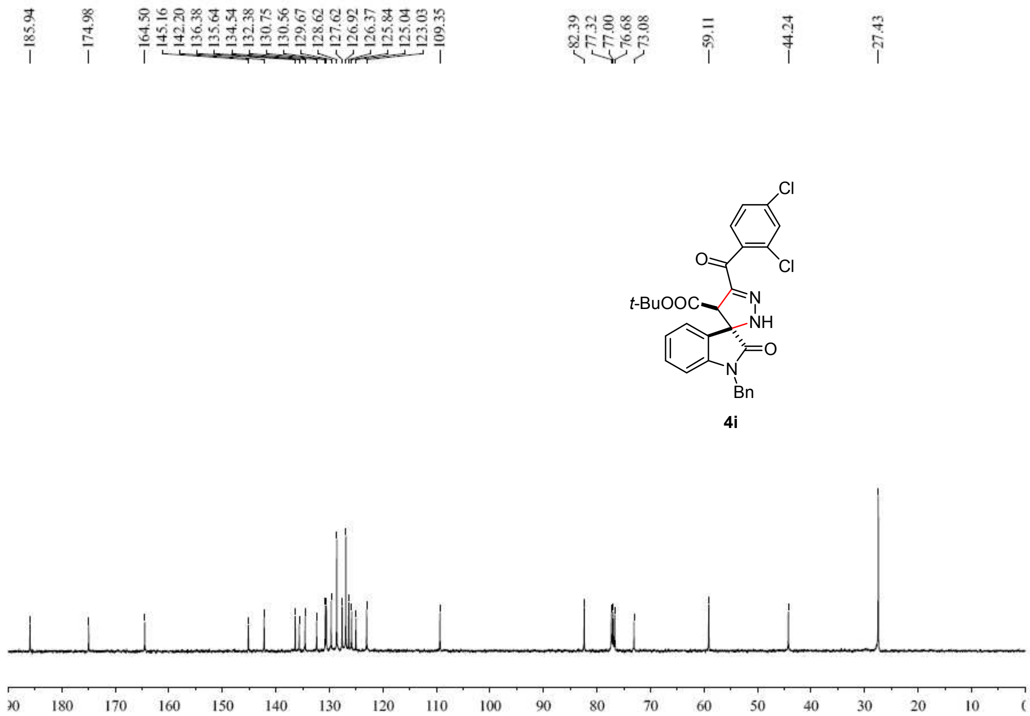


Figure S18. The ^{13}C NMR(100M Hz, $CDCl_3$) of **4i**.

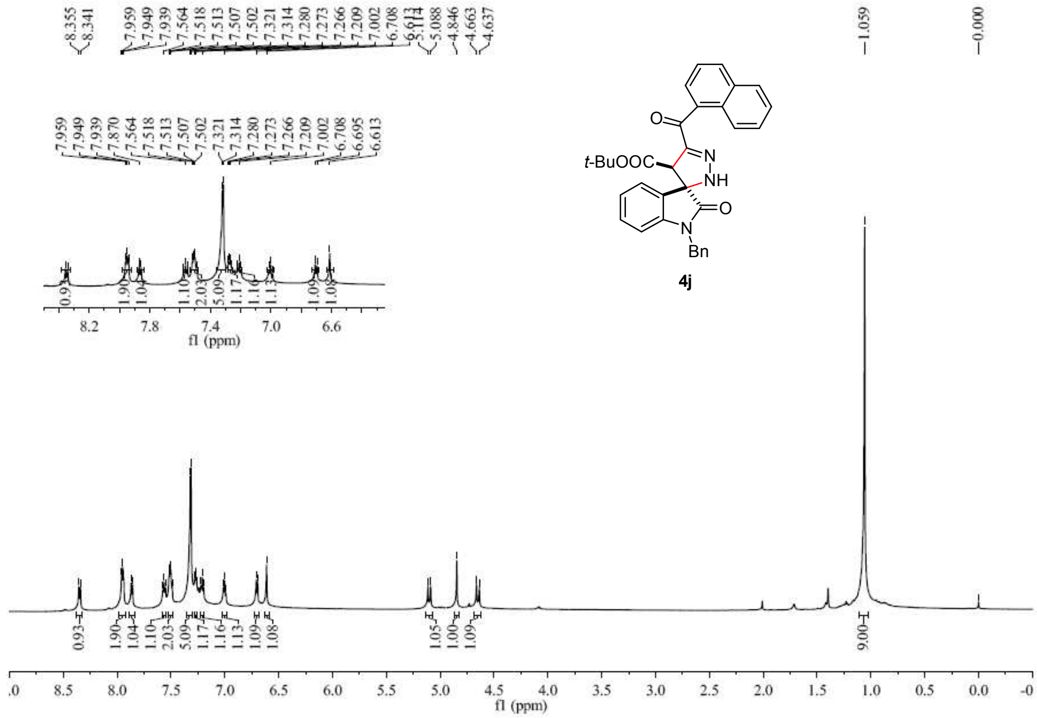


Figure S19. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4j**.

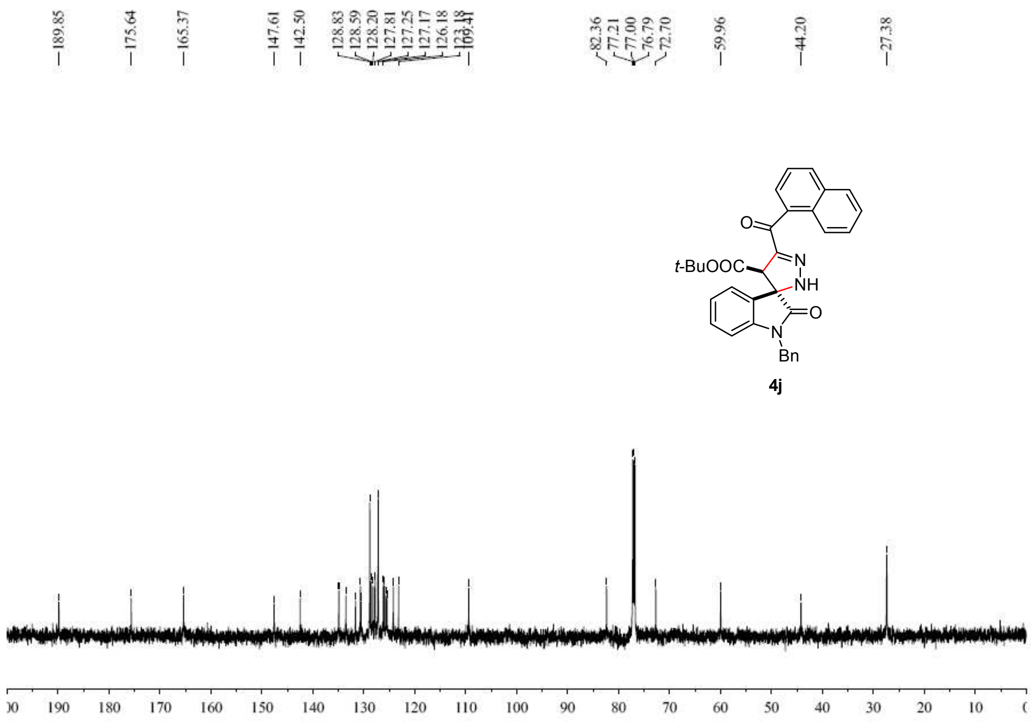


Figure S20. The ^{13}C NMR(150M Hz, $CDCl_3$) of **4j**.

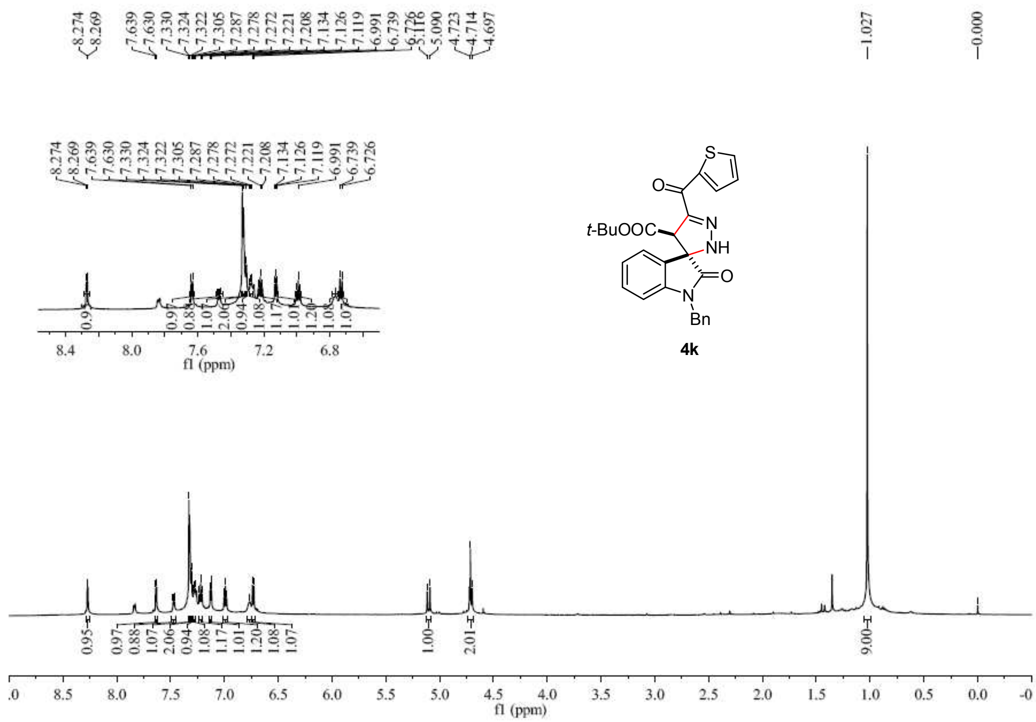


Figure S21. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4k**.

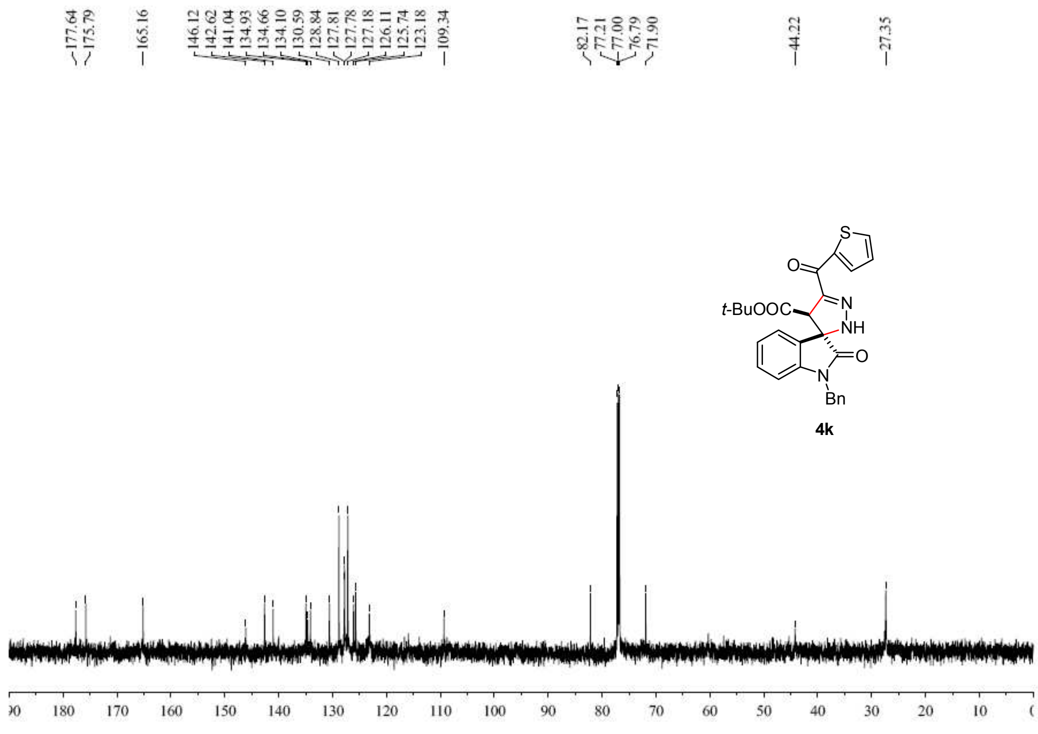


Figure S22. The ^{13}C NMR(150M Hz, $CDCl_3$) of **4k**.

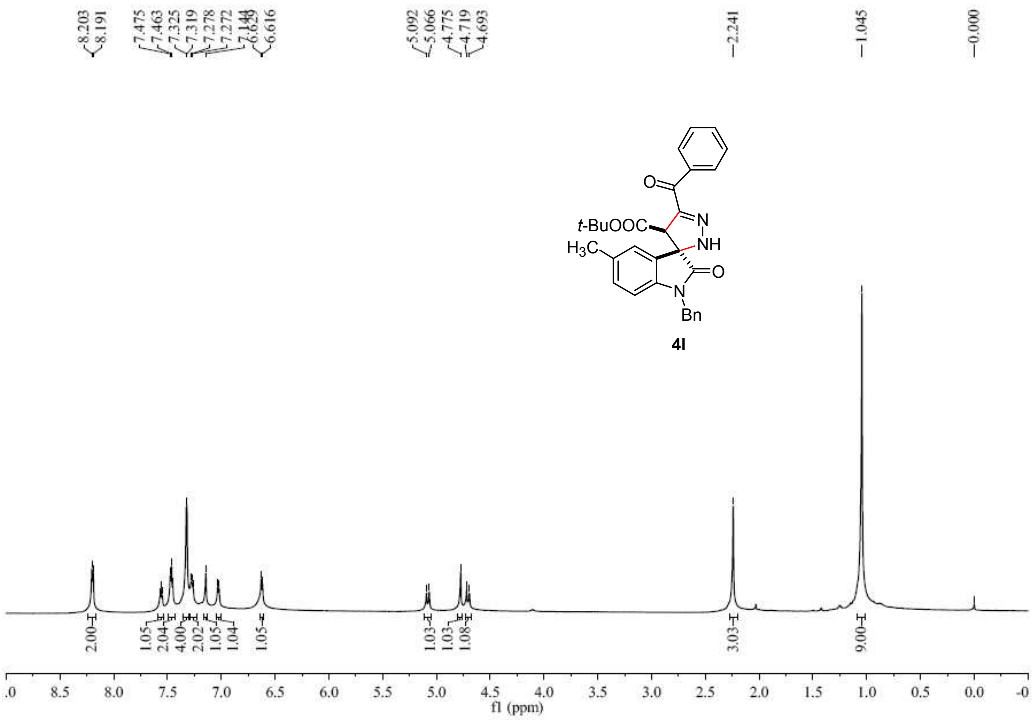


Figure S23. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4l**.

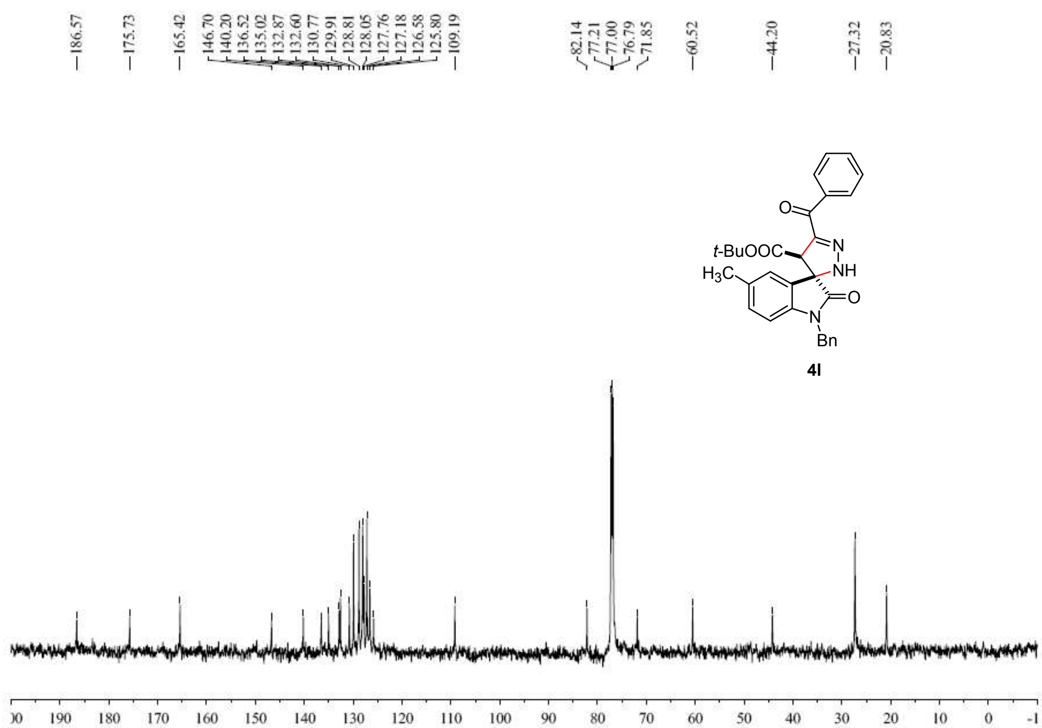


Figure S24. The ^{13}C NMR (150M Hz, $CDCl_3$) of **4l.**

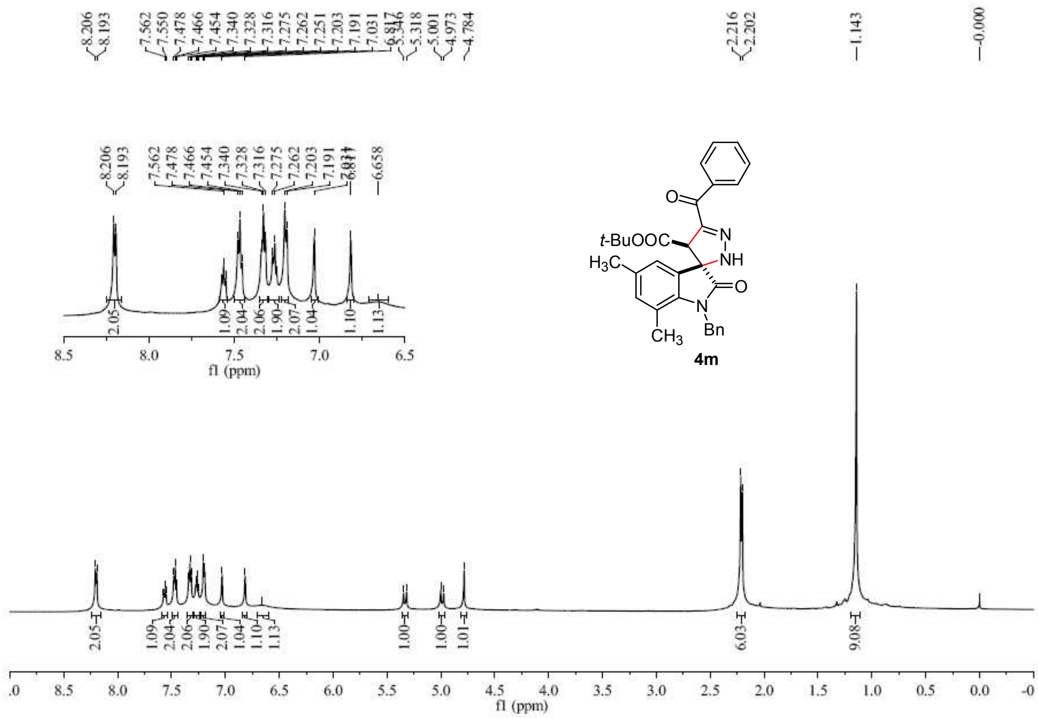


Figure S25. The [1]H NMR (600M Hz, $CDCl_3$) of **4m**.

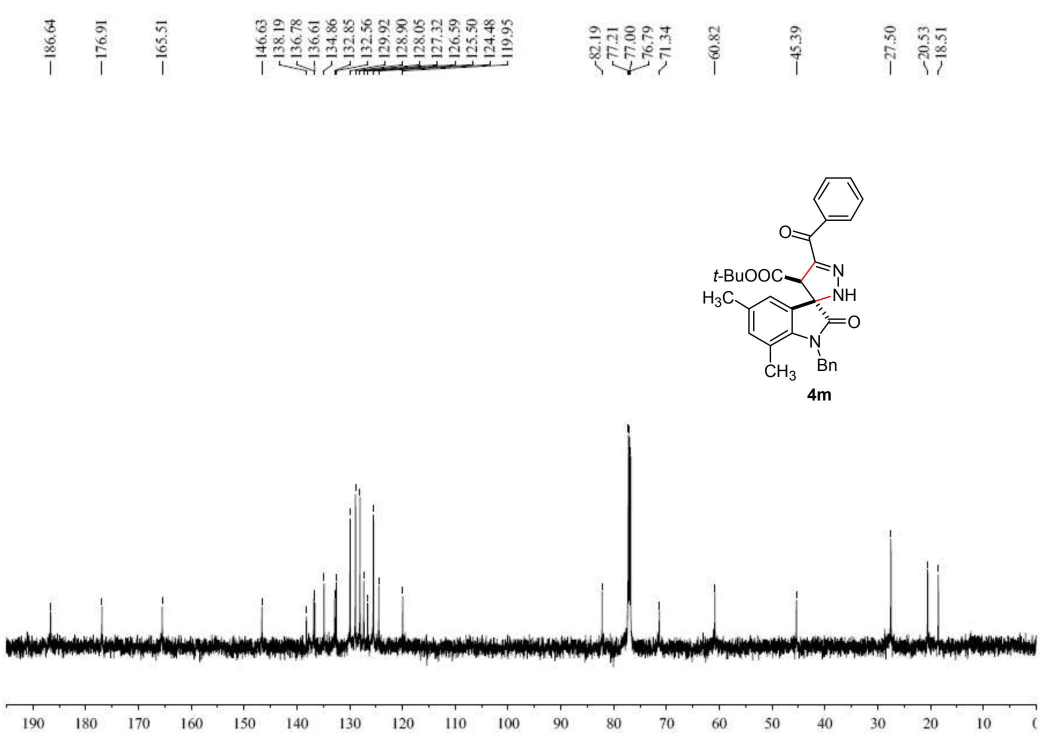


Figure S26. The [13]C NMR (150M Hz, $CDCl_3$) of **4m.**

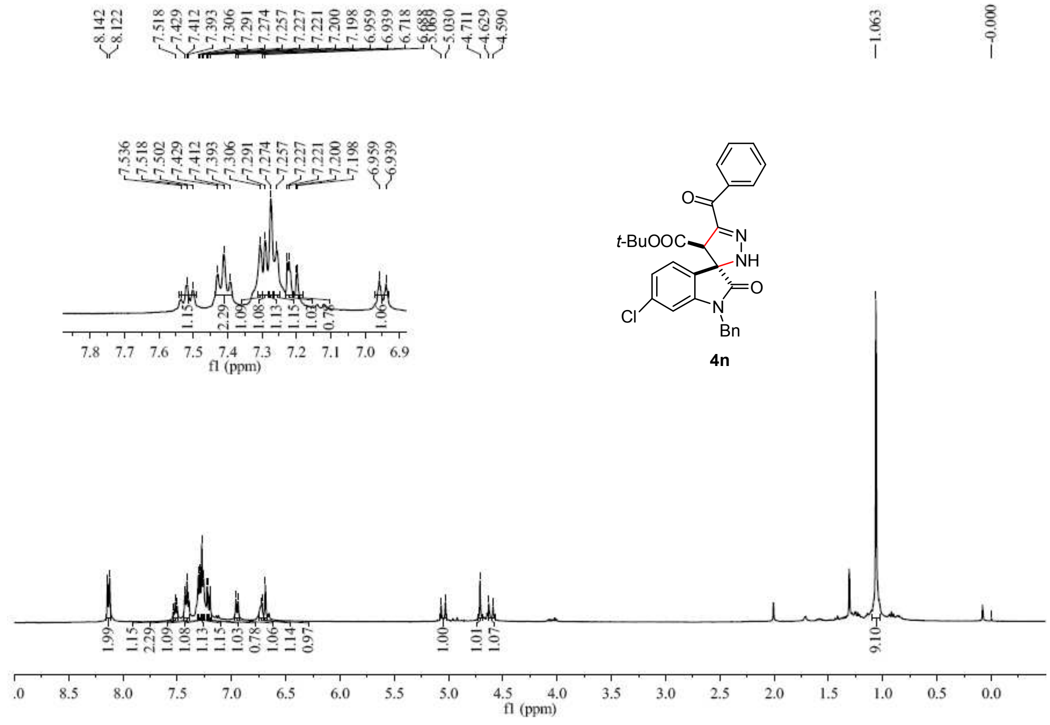


Figure S27. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4n**.

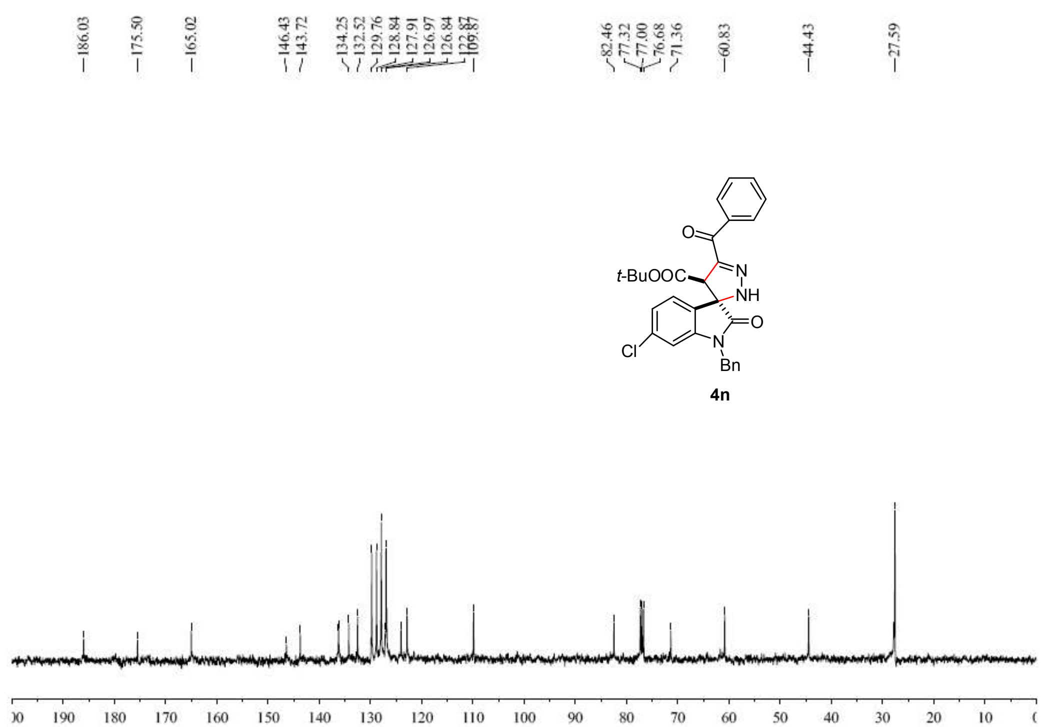


Figure S28. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4n.**

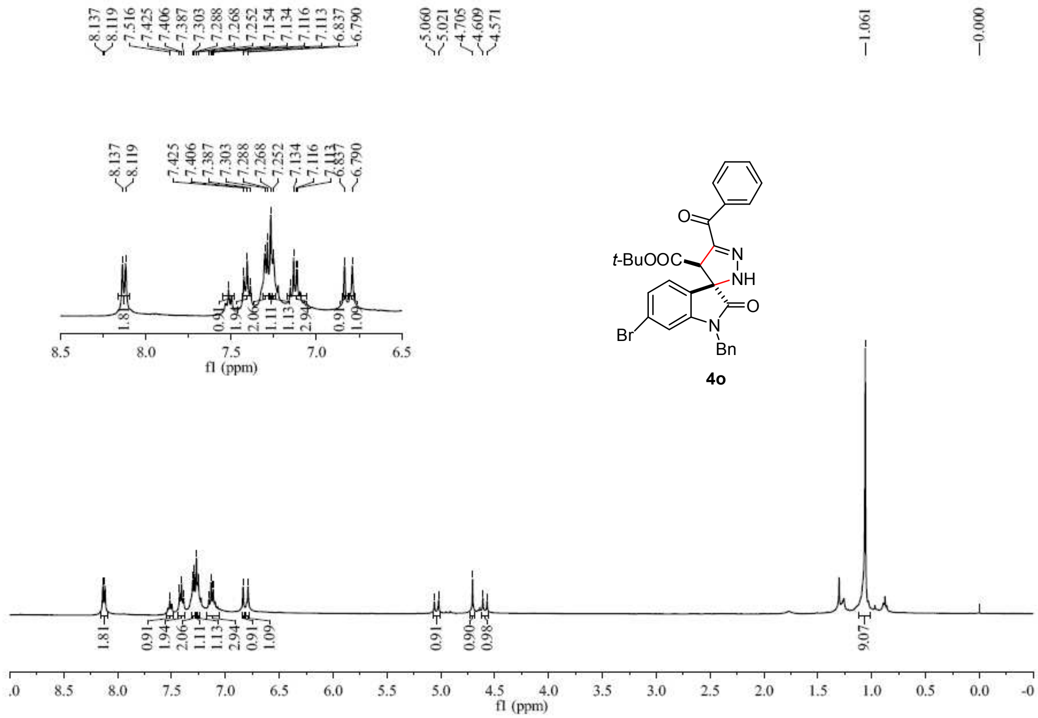


Figure S29. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4o**.

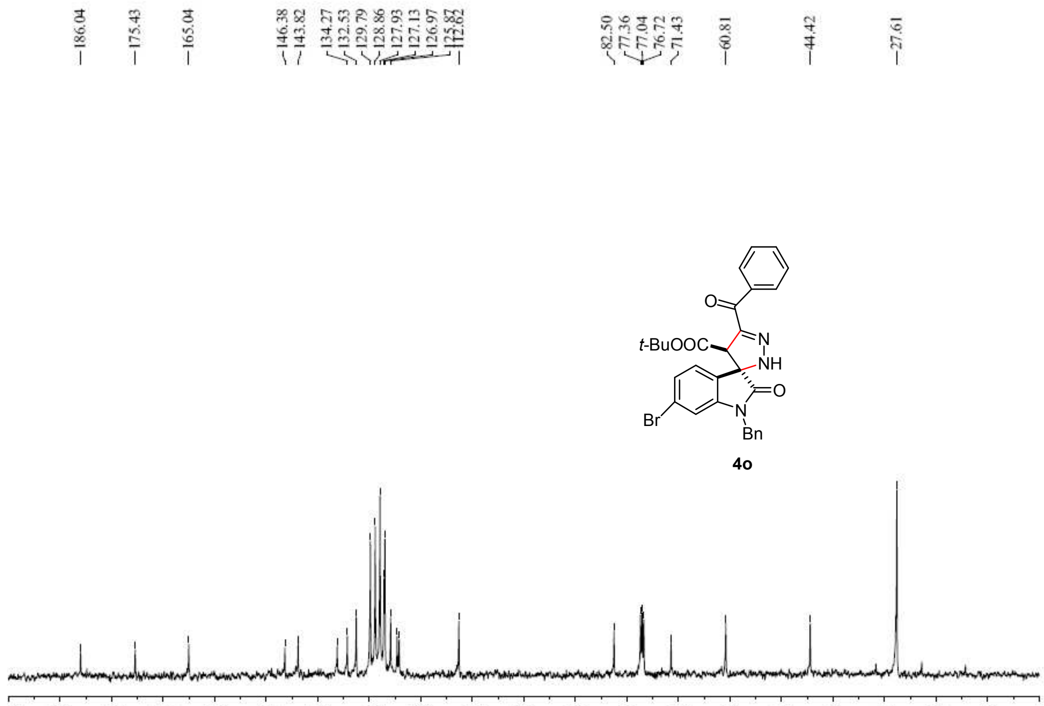


Figure S30. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4o.**

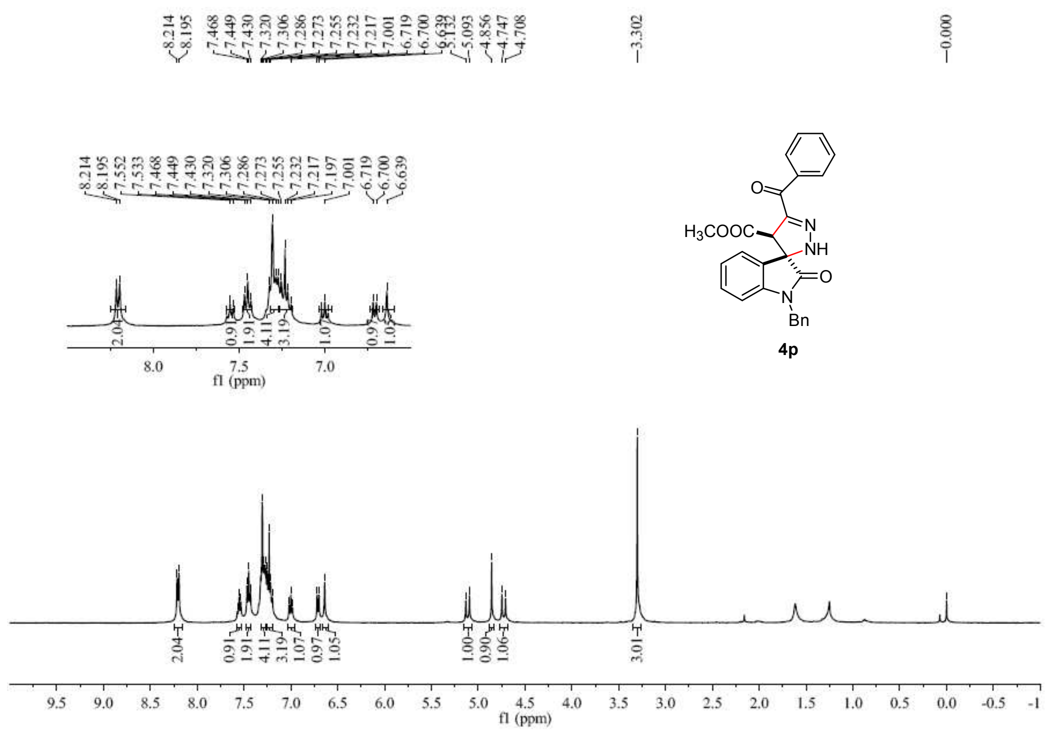


Figure S31. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4p**.

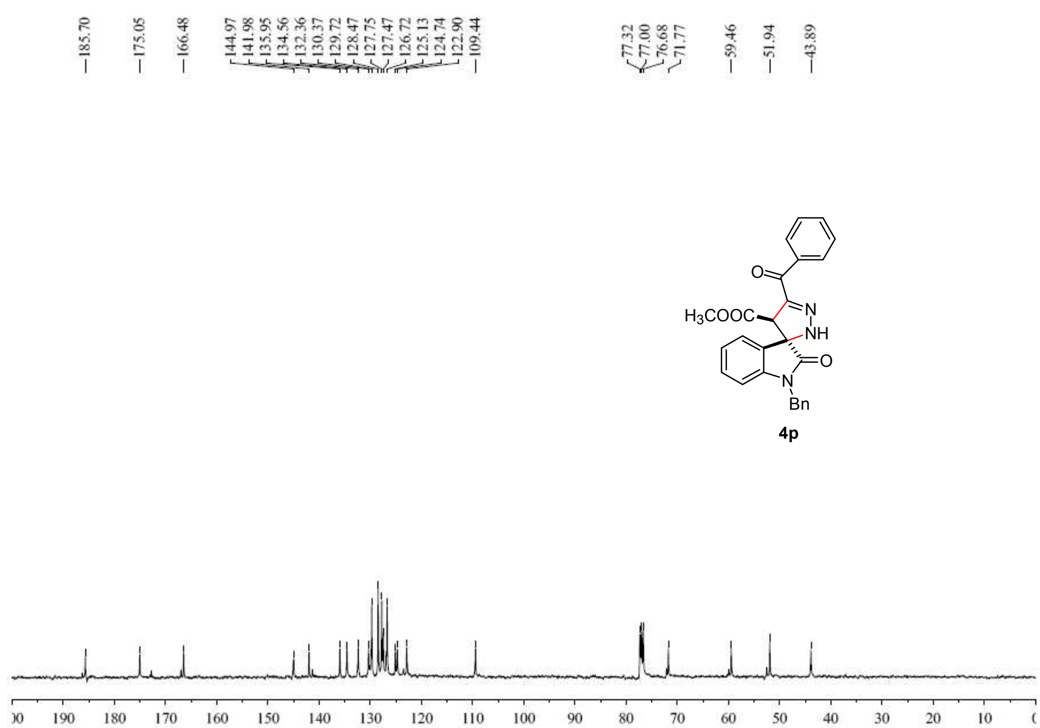


Figure S32. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4p.**

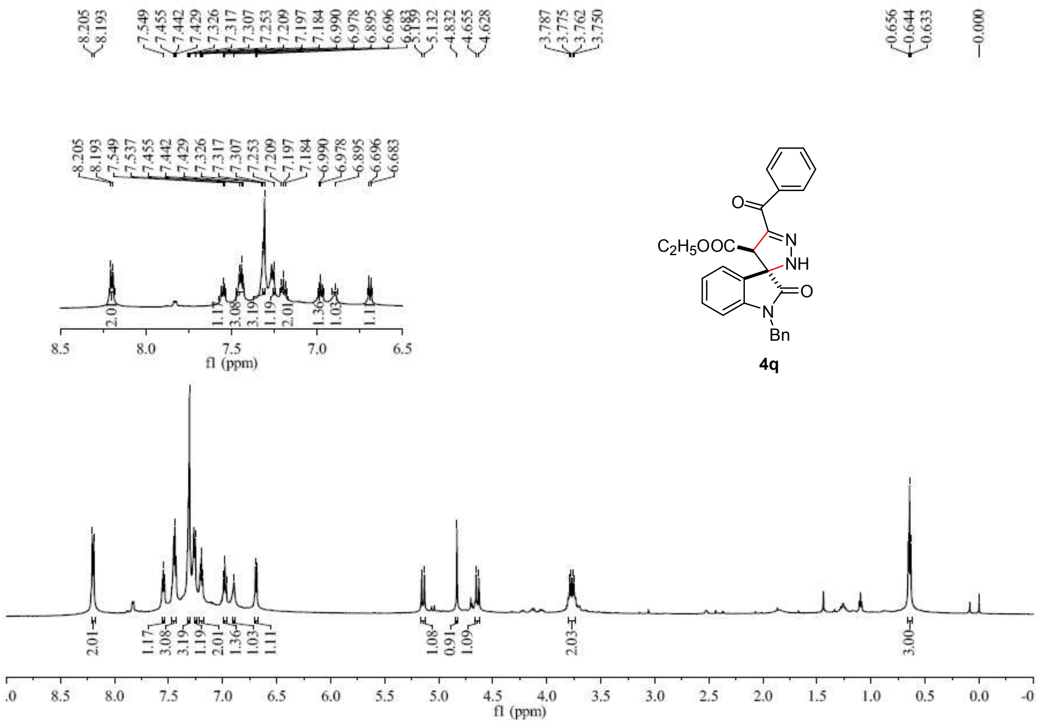


Figure S33. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4q**.

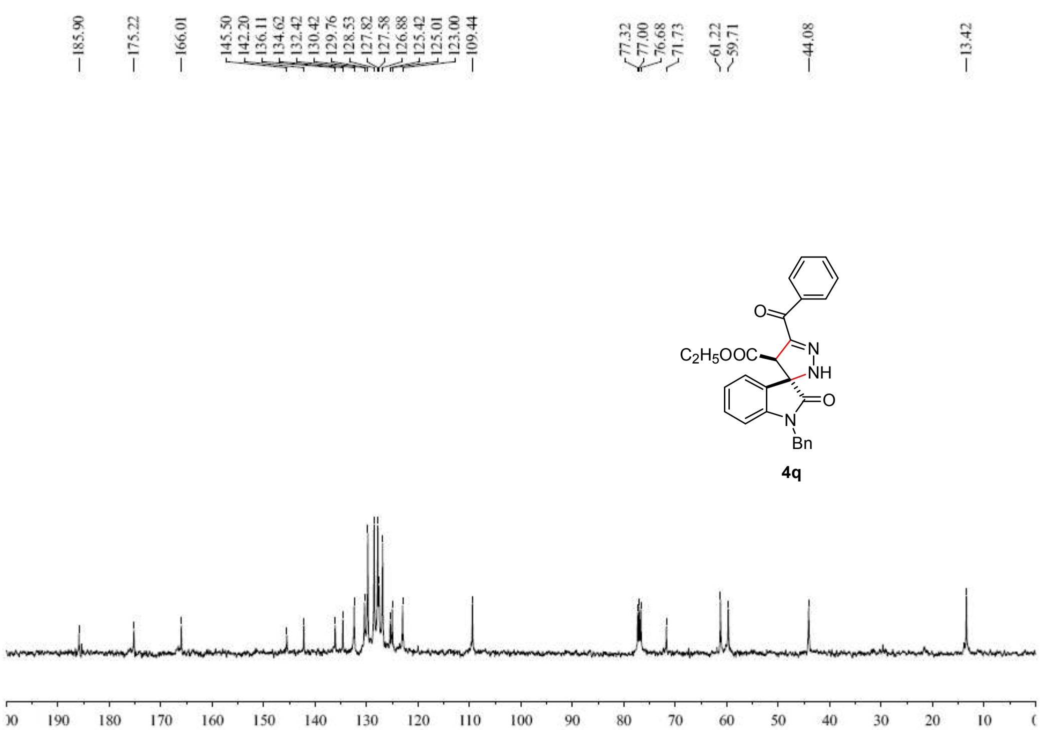


Figure S34. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4q.**

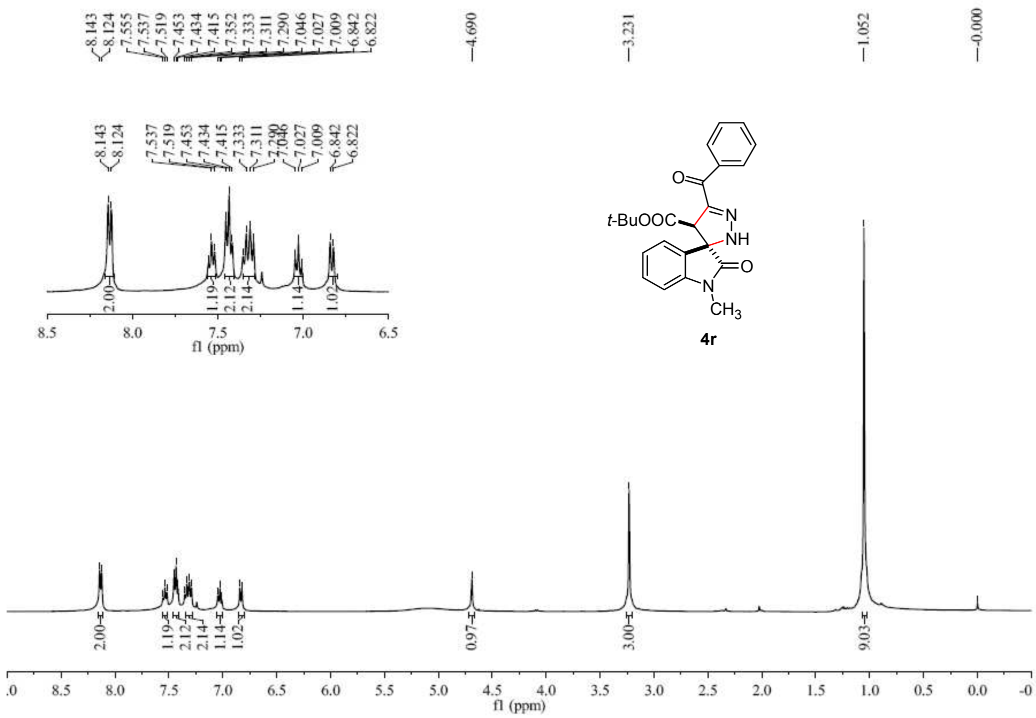


Figure S35. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4r**.

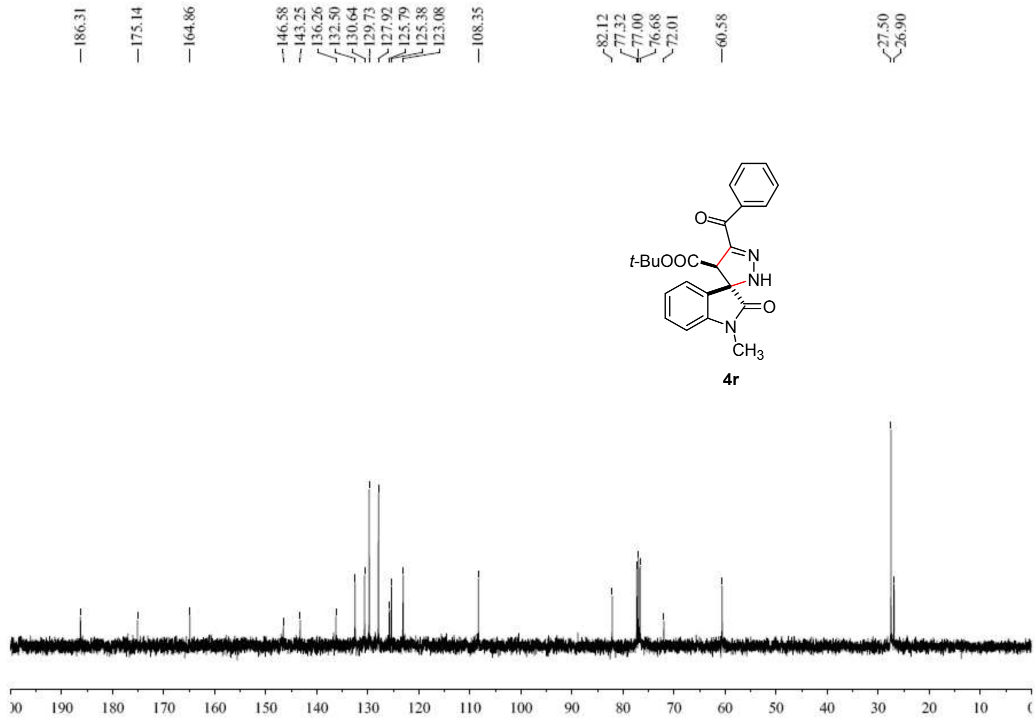


Figure S36. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4r.**

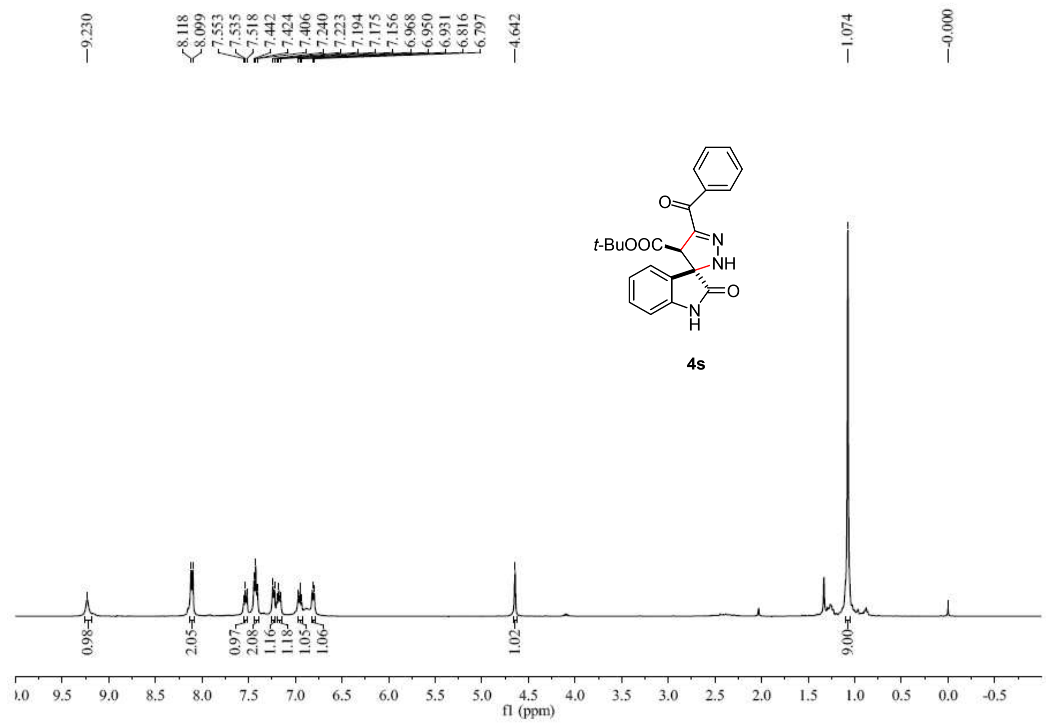


Figure S37. The ^{1}H NMR (400M Hz, $CDCl_3$) of **4s**.

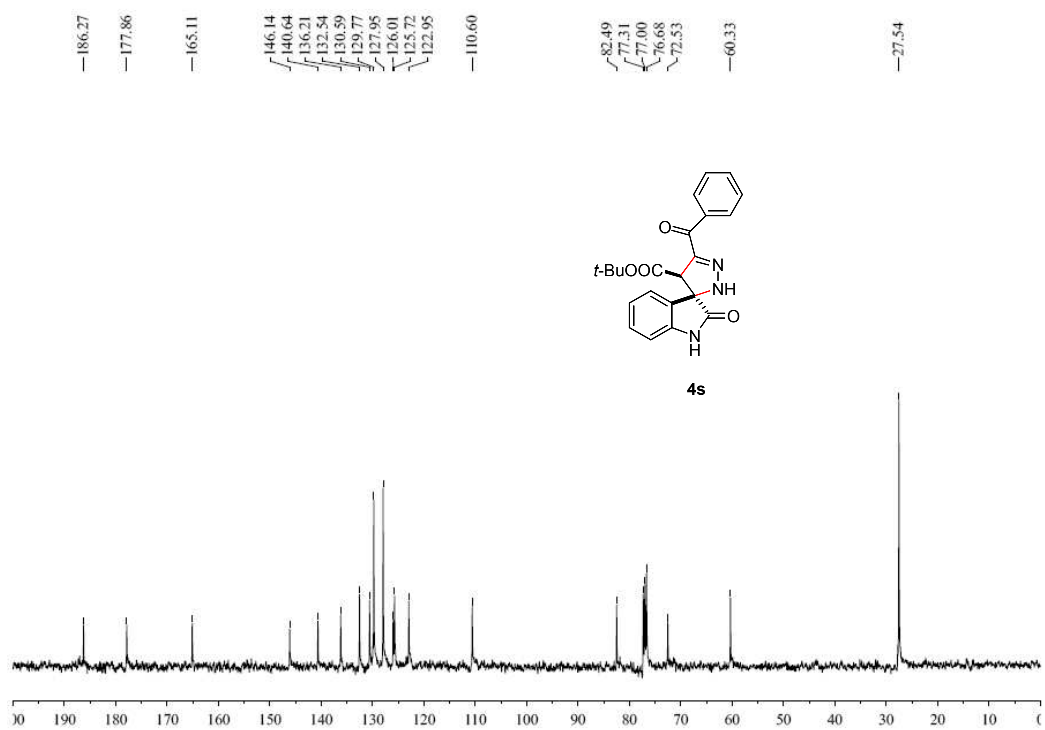


Figure S38. The ^{13}C NMR (100M Hz, $CDCl_3$) of **4s.**

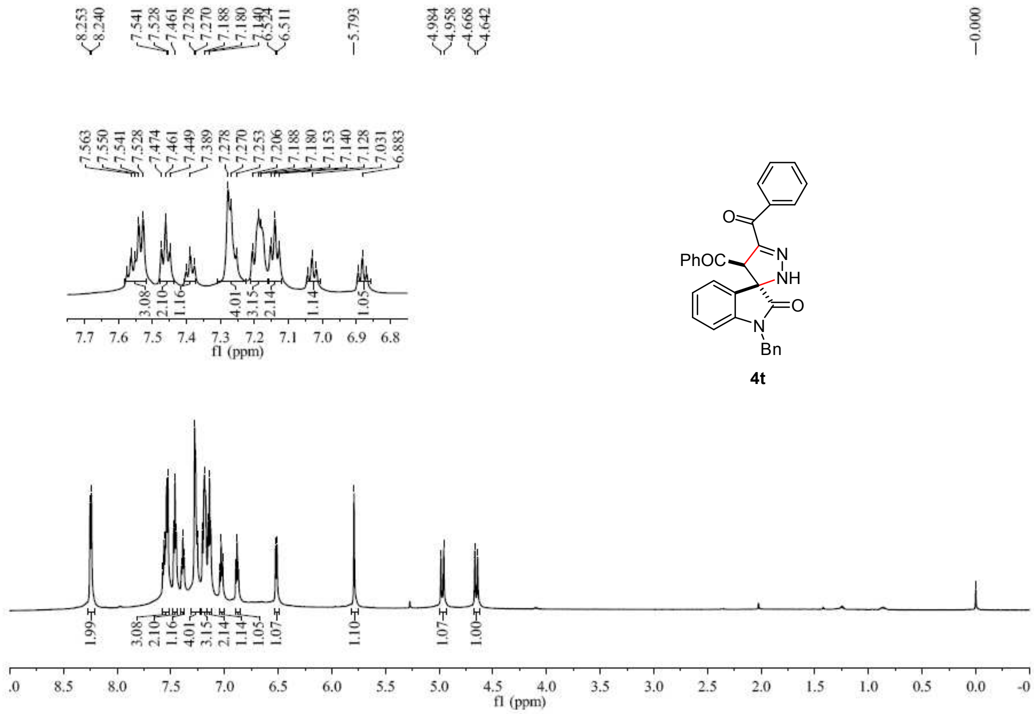


Figure S39. The ^{1}H NMR (600M Hz, $CDCl_3$) of **4t.**

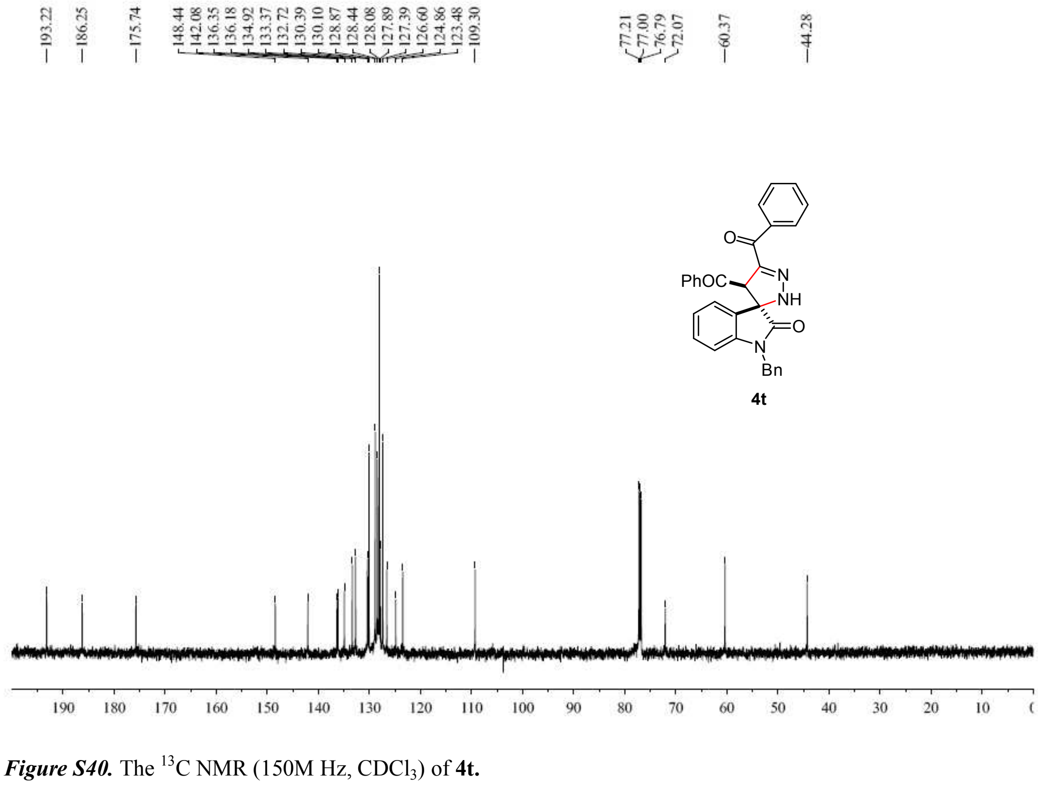


Figure S40. The ^{13}C NMR (150M Hz, $CDCl_3$) of **4t.**

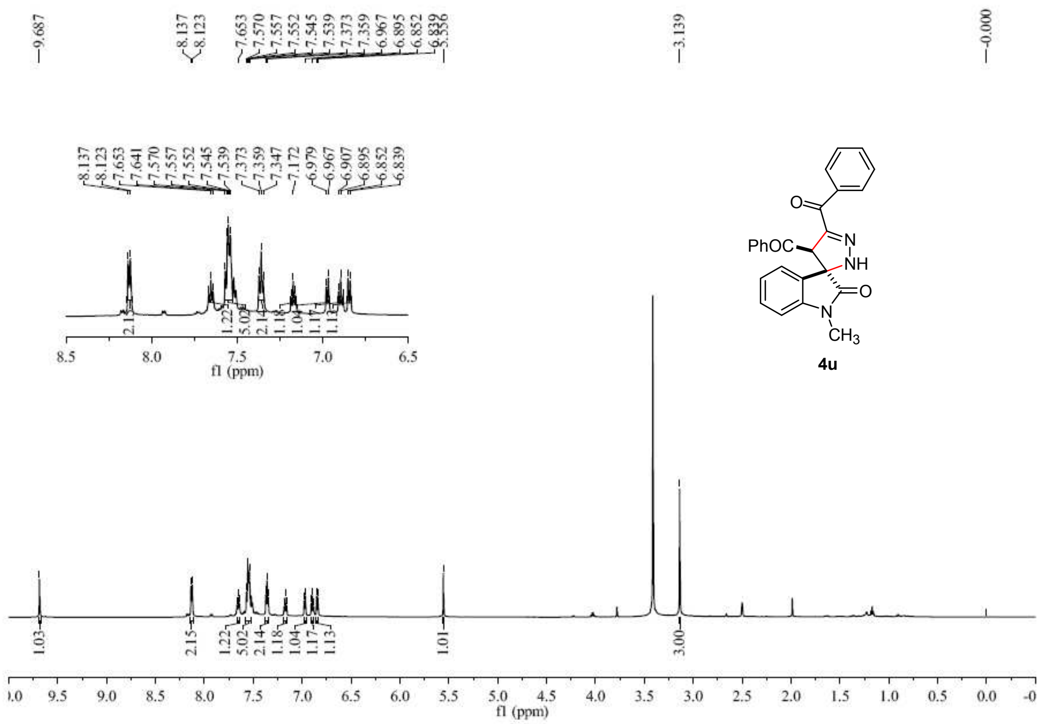


Figure S41. The ^{1}H NMR (600M Hz, DMSO-d_6) of **4u.**

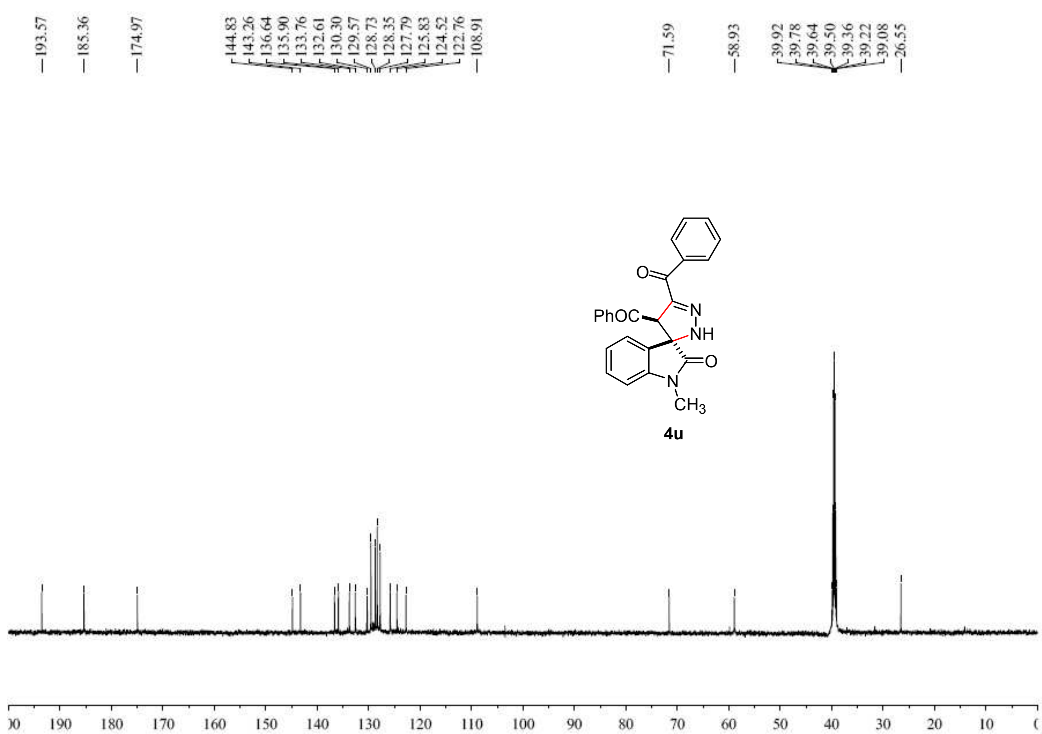


Figure S42. The ^{13}C NMR (150M Hz, DMSO-d_6) of **4u.**

Copies of ^{1}H NMR and ^{13}C NMR Spectra of 5

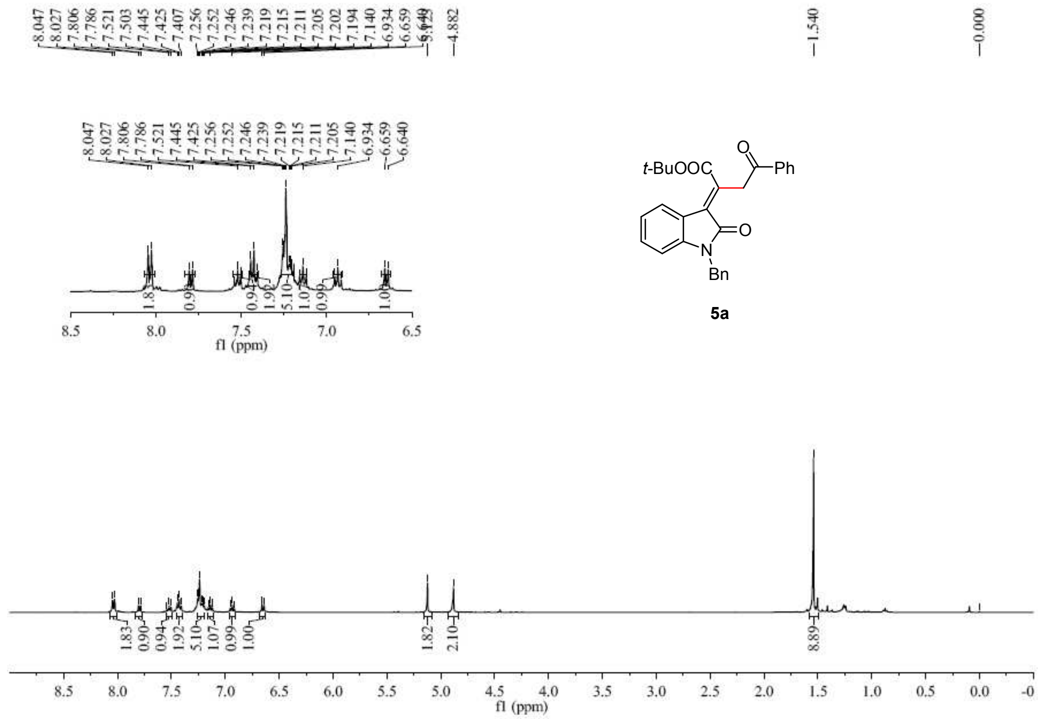


Figure S43. The ^{1}H NMR (400M Hz, $CDCl_3$) of **5a.**

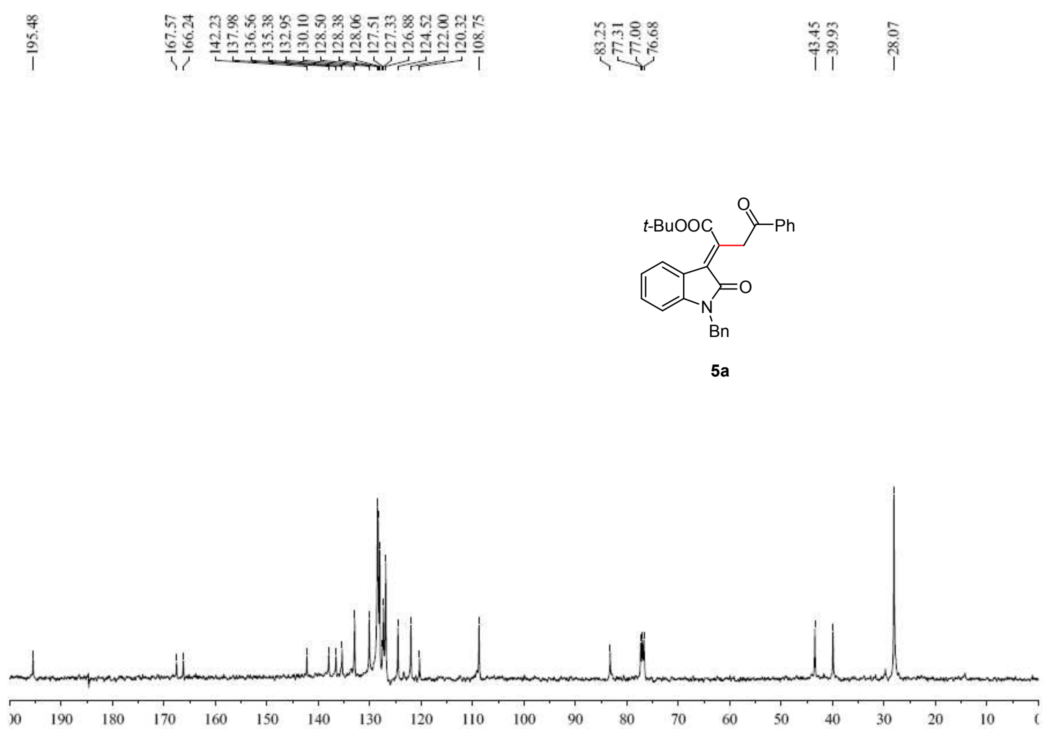


Figure S44. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5a.**

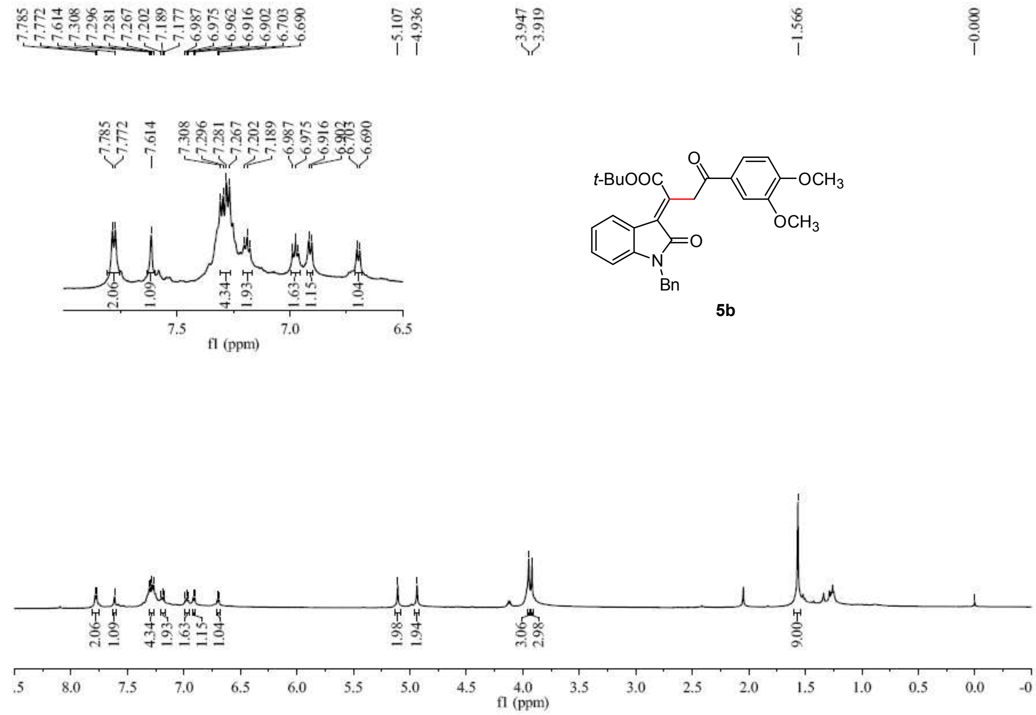


Figure S45. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5b.**

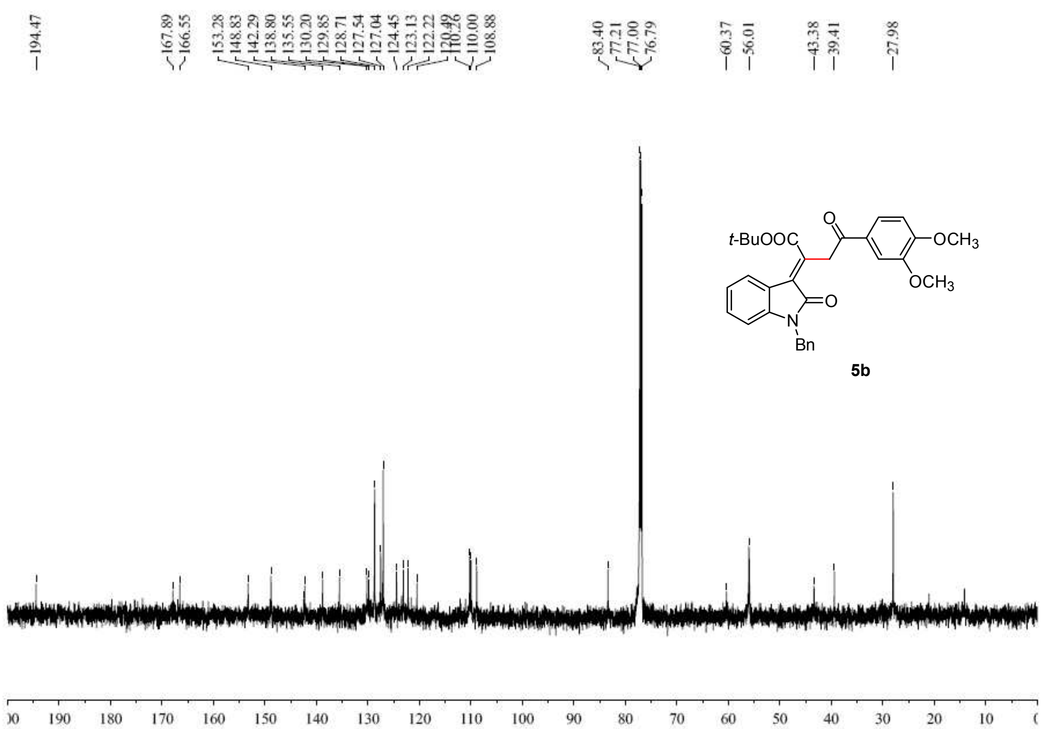


Figure S46. The ^{13}C NMR (150M Hz, $CDCl_3$) of **5b.**

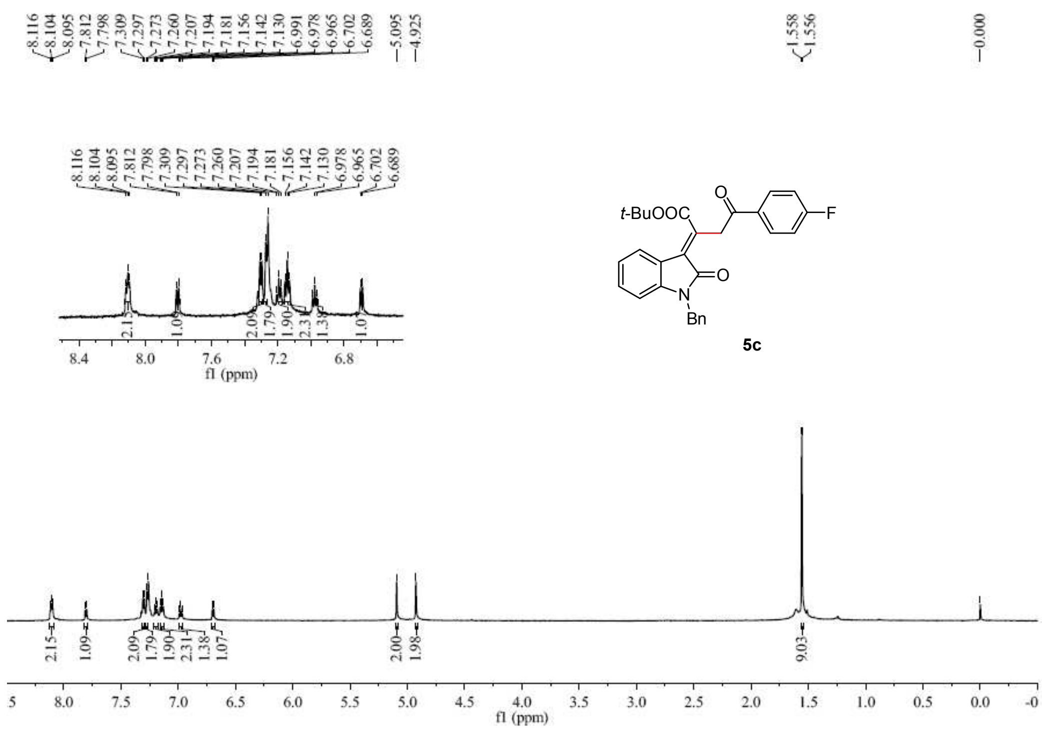


Figure S47. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5c.**

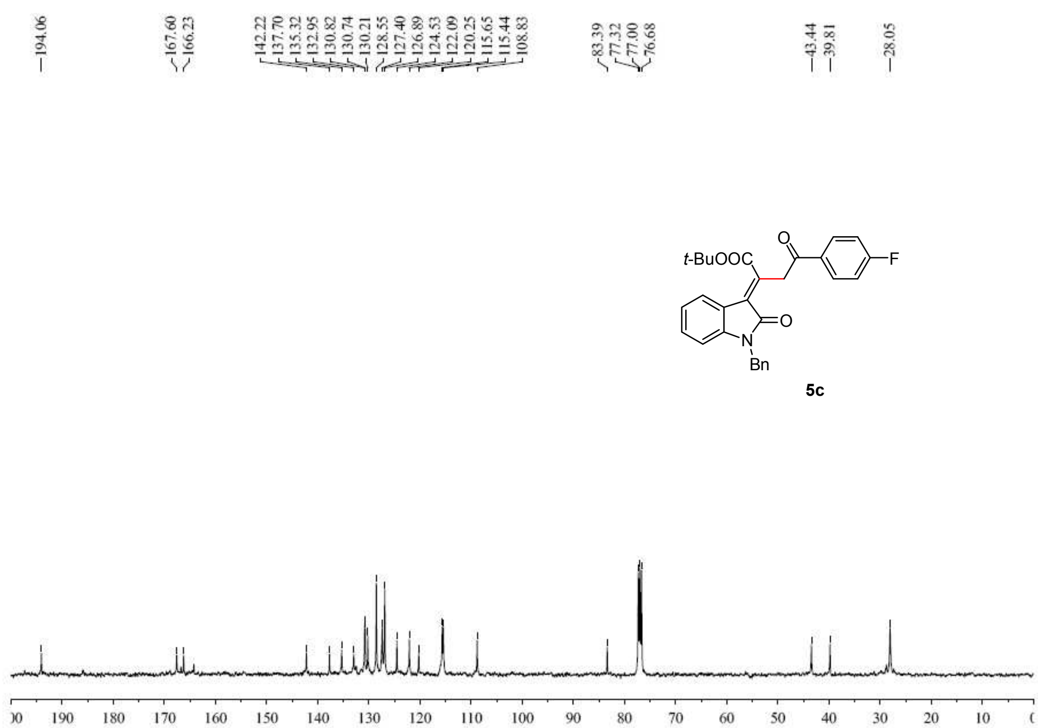


Figure S48. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5c.**

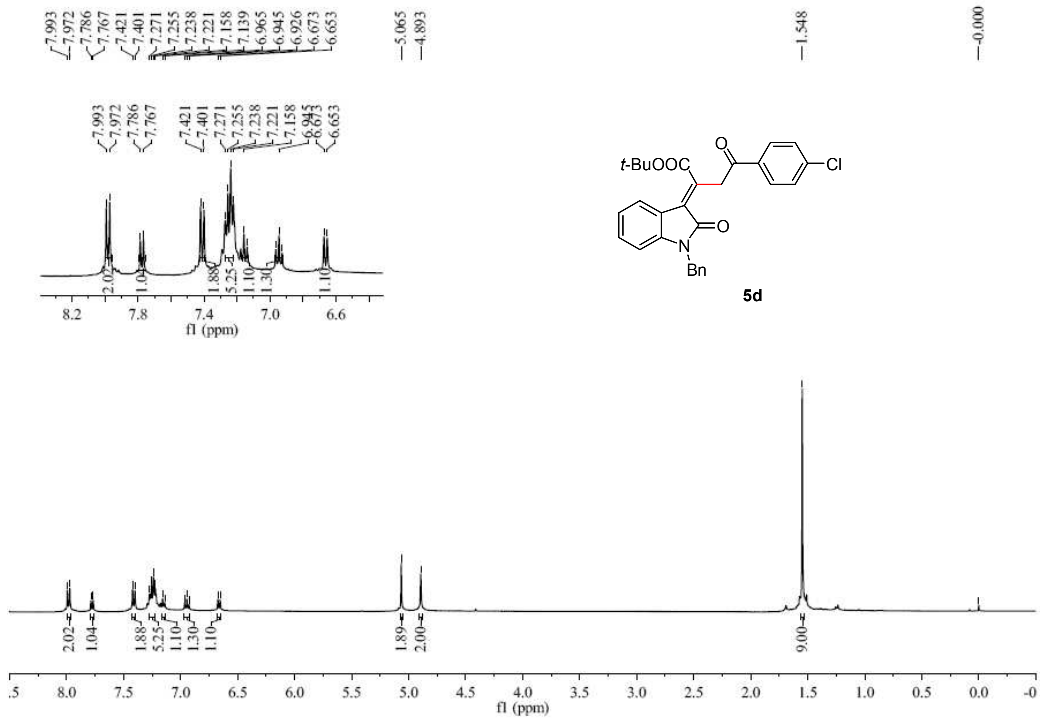


Figure S49. The ^{1}H NMR (400M Hz, $CDCl_3$) of **5d.**

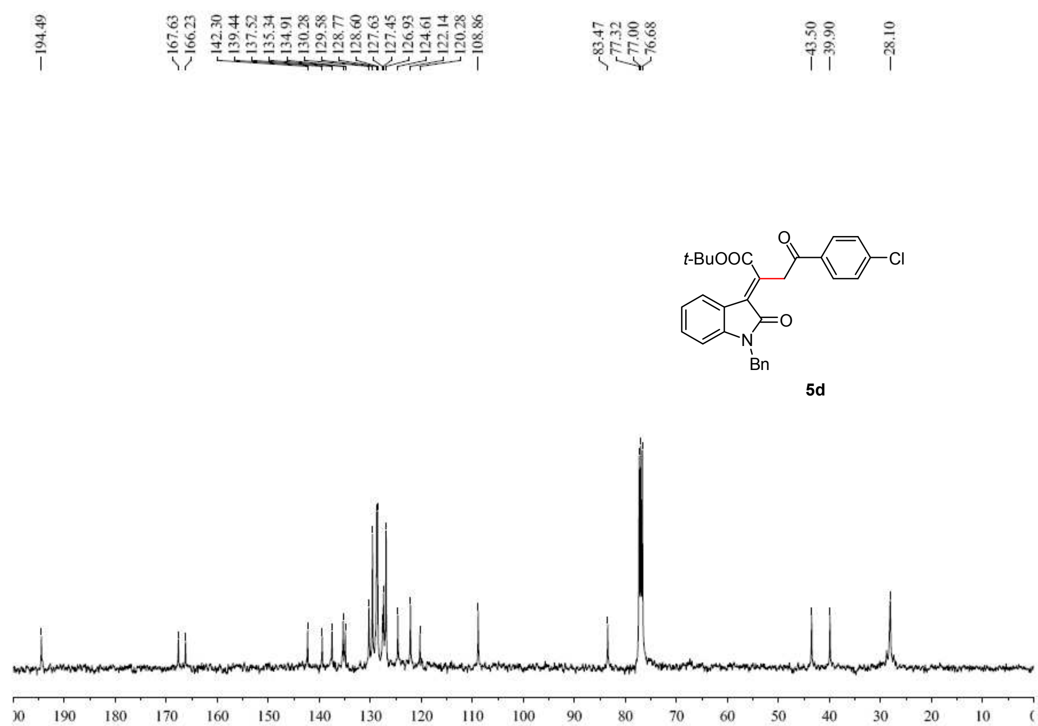


Figure S50. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5d.**

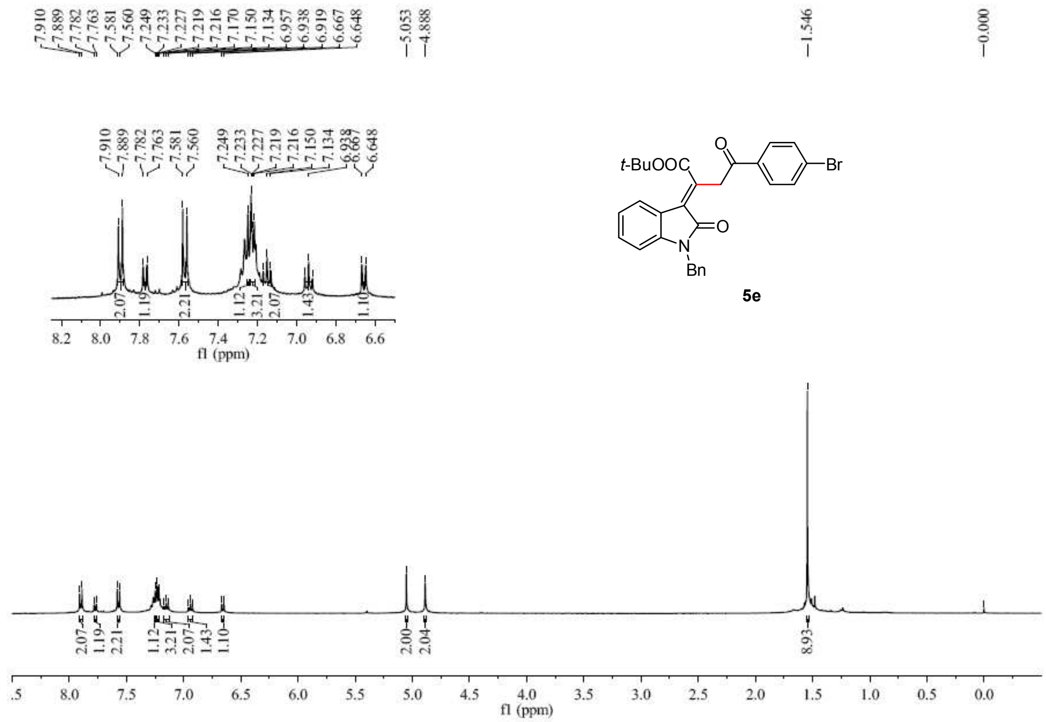


Figure S51. The ^{1}H NMR (400M Hz, $CDCl_3$) of **5e.**

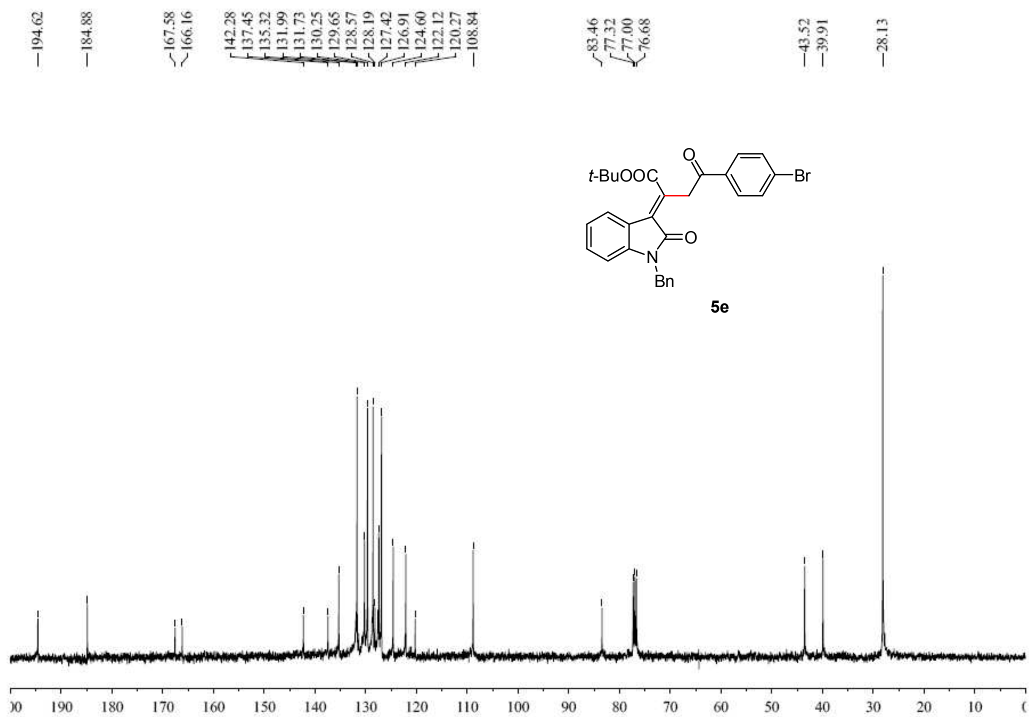


Figure S52. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5e.**

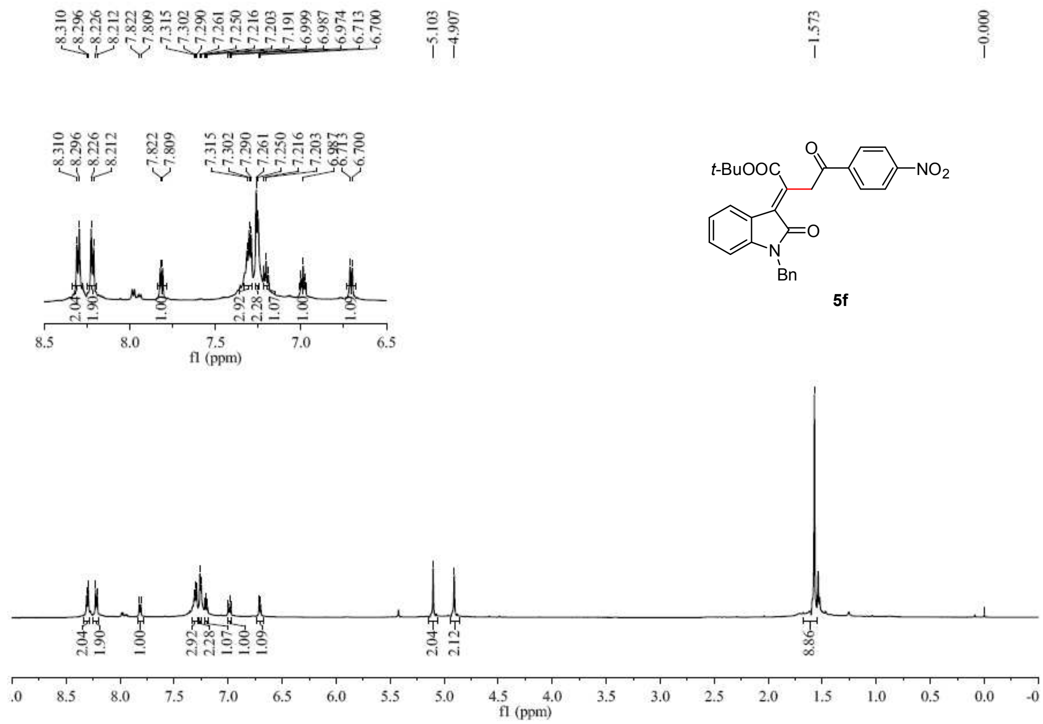


Figure S53. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5f.**

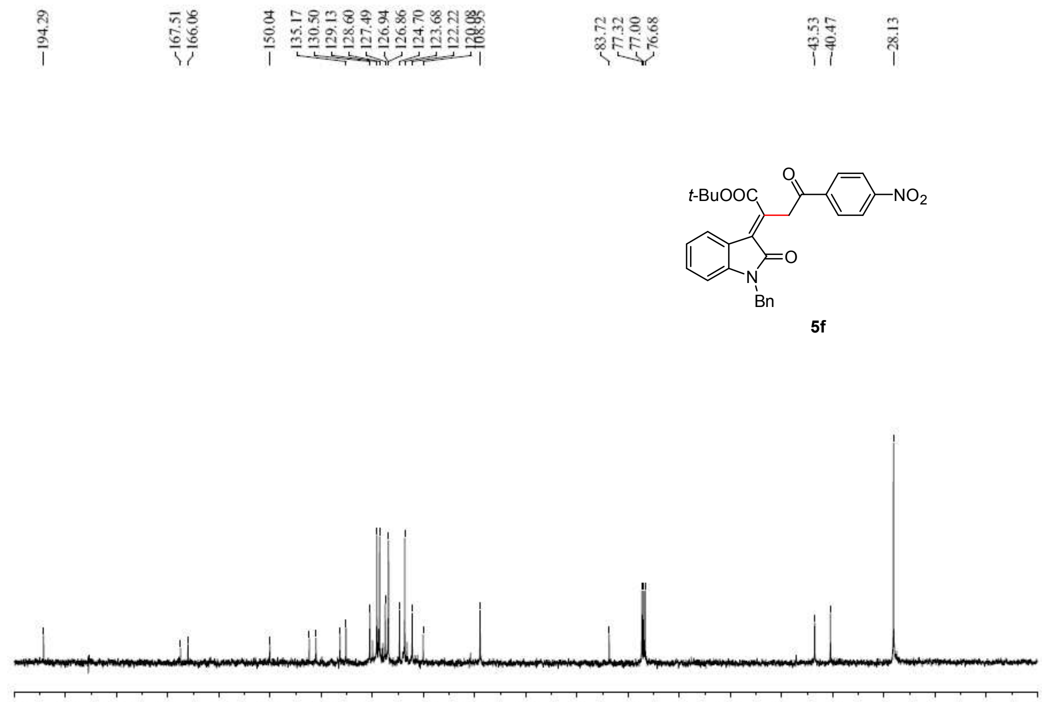


Figure S54. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5f.**

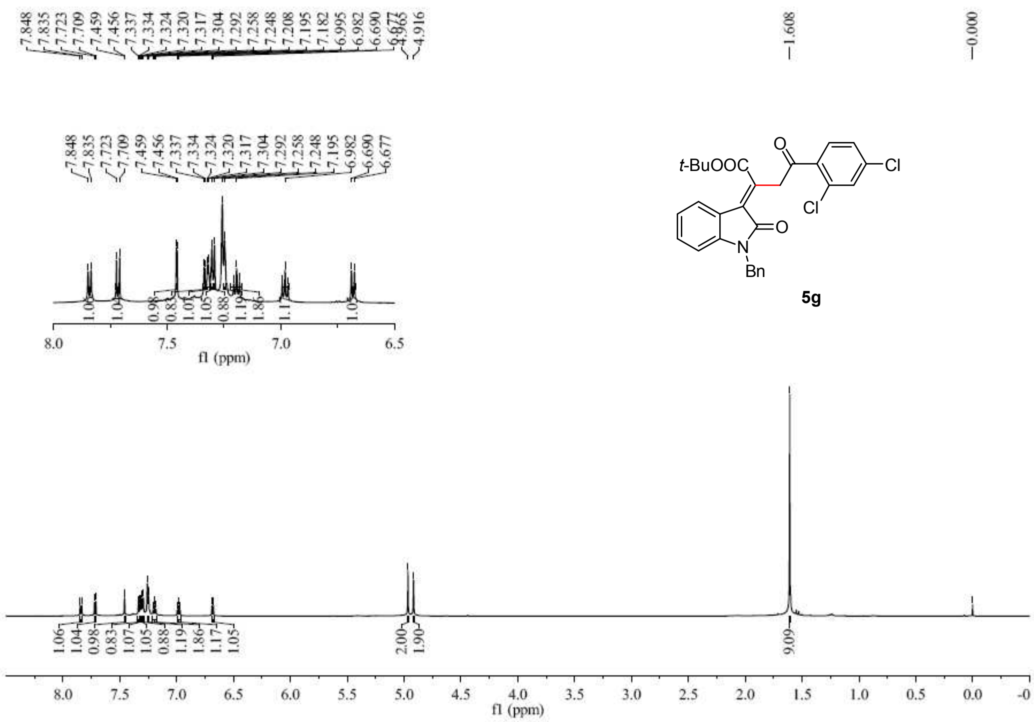


Figure S55. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5g.**

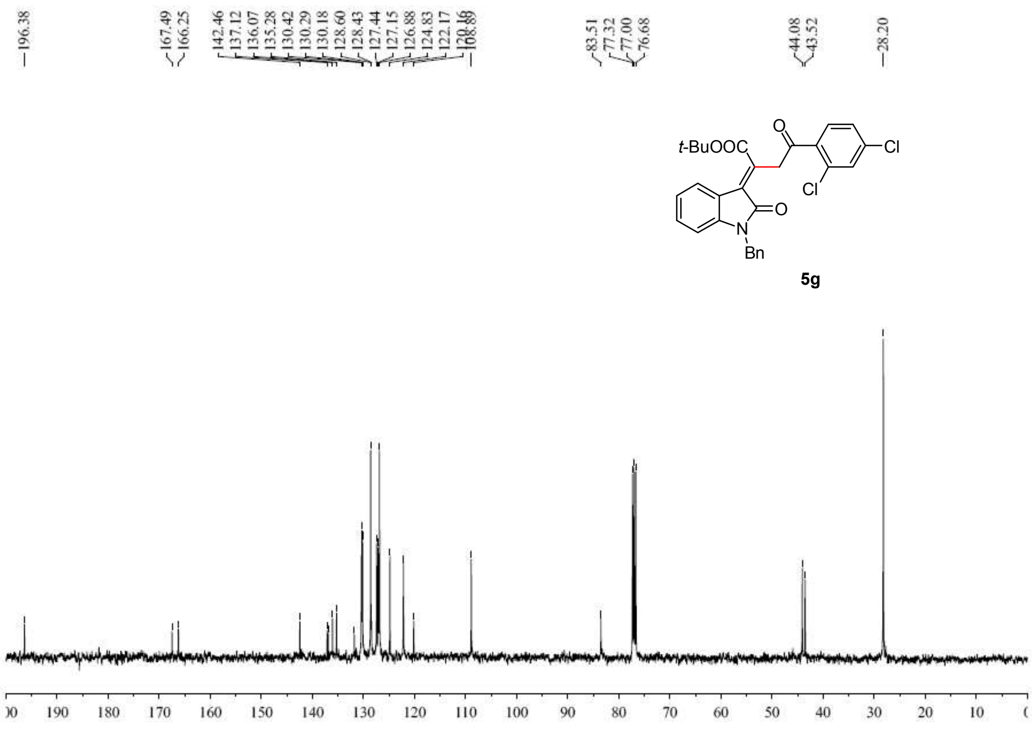
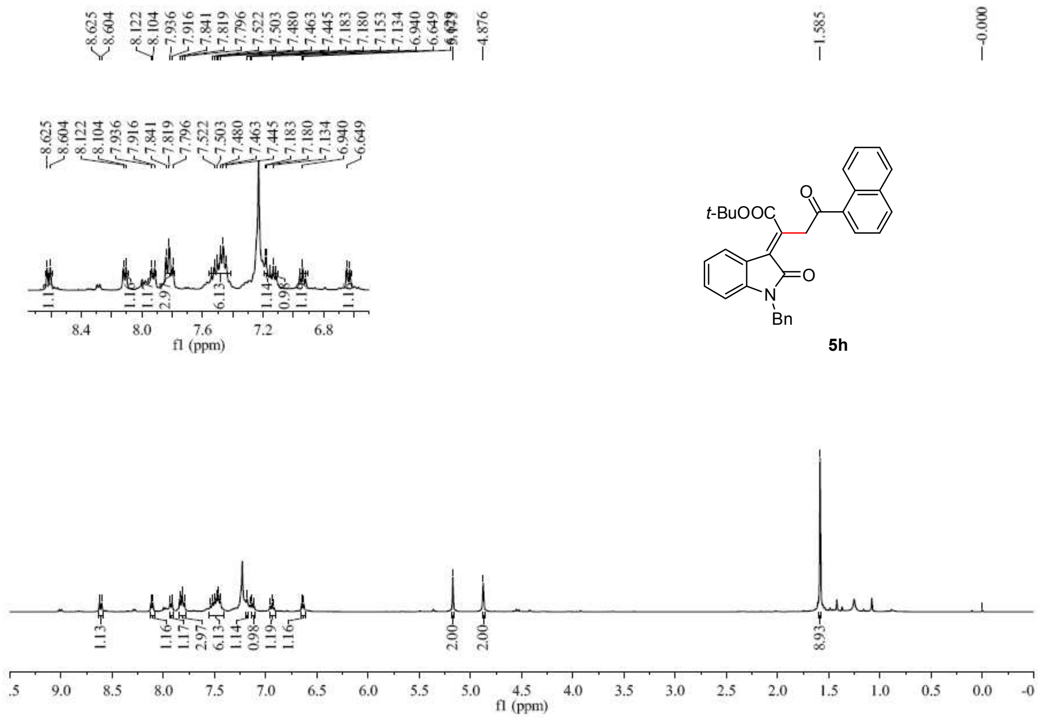
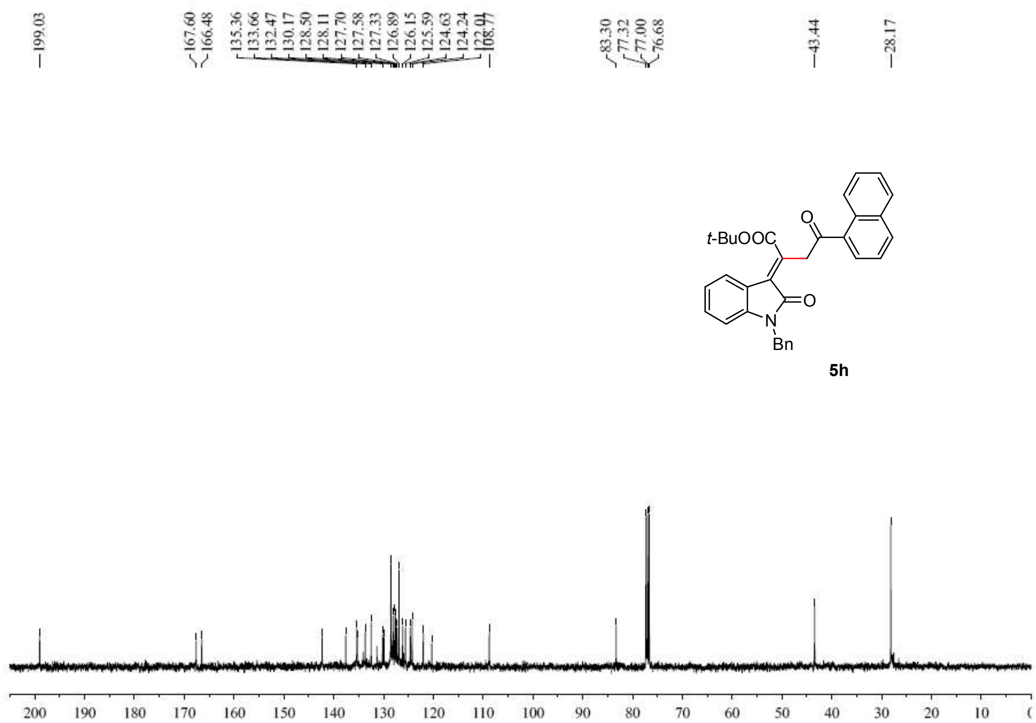


Figure S56. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5g.**



5h

Figure S57. The ^{1}H NMR (400M Hz, $CDCl_3$) of **5h.**



5h

Figure S58. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5h.**

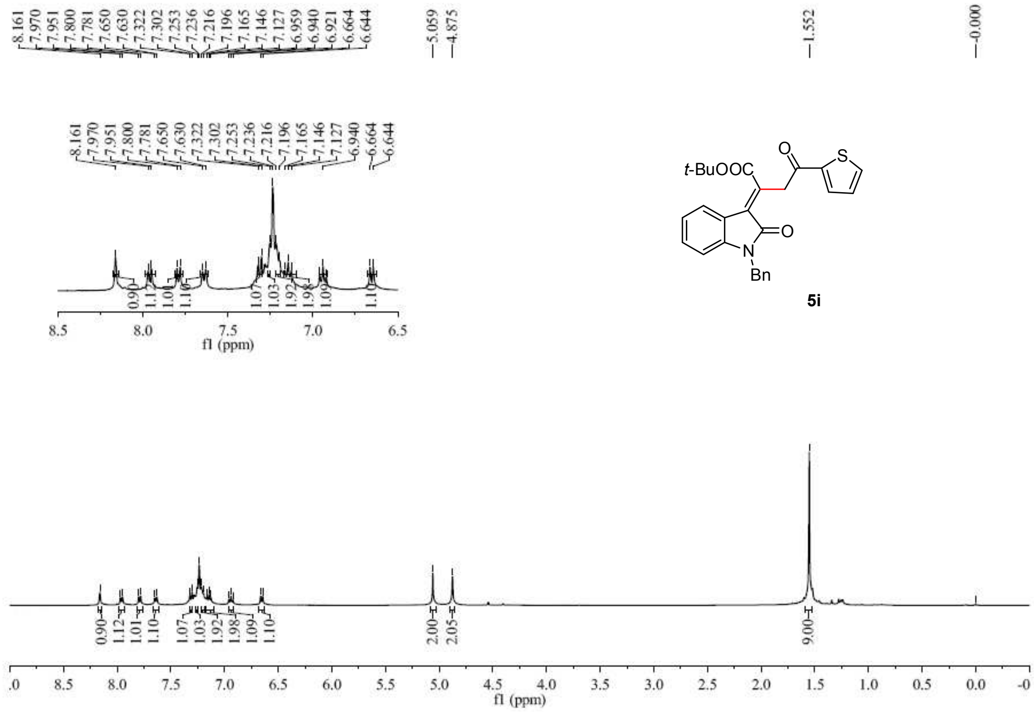


Figure S59. The ^{1}H NMR (400M Hz, $CDCl_3$) of **5i.**

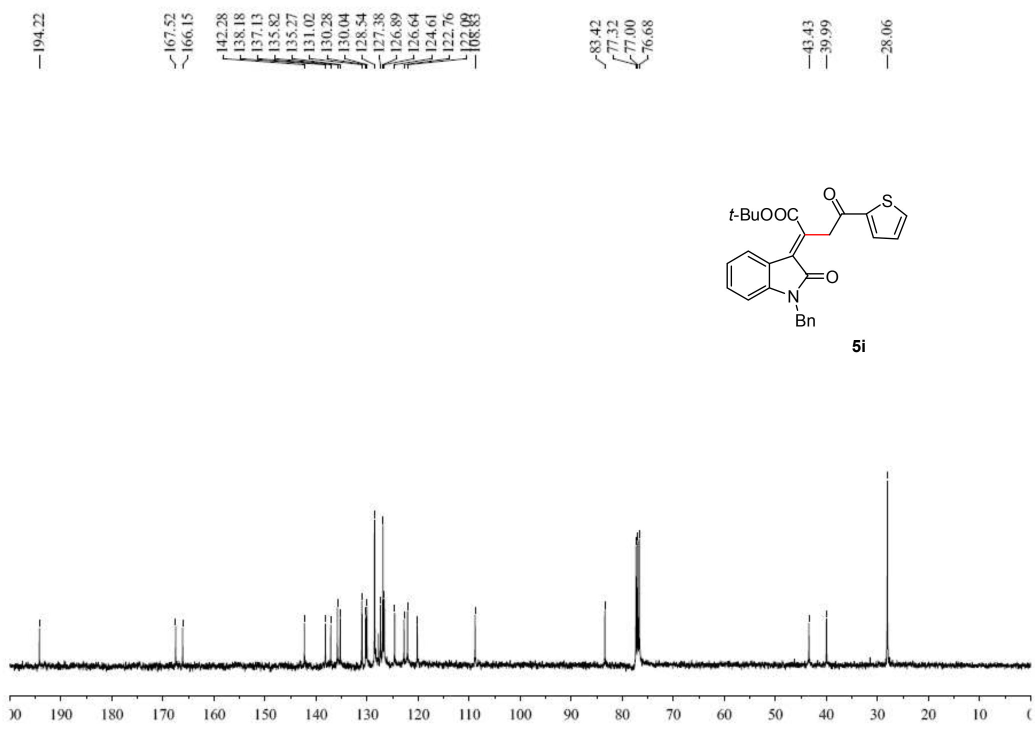


Figure S60. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5i.**

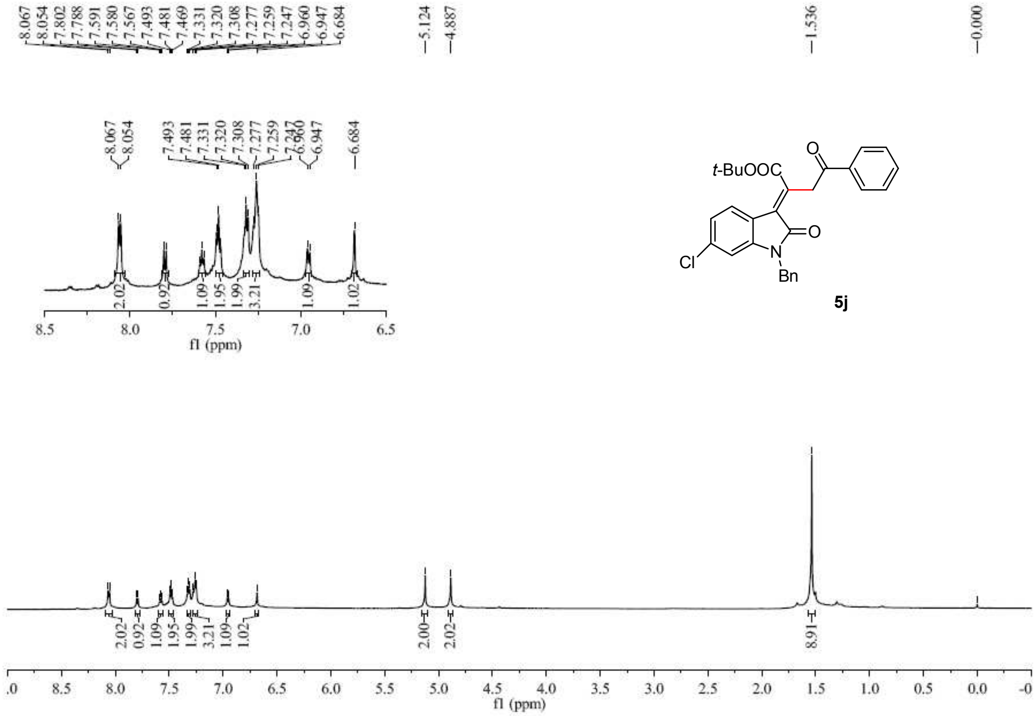


Figure S61 The ^{1}H NMR (600M Hz, $CDCl_3$) of **5j.**

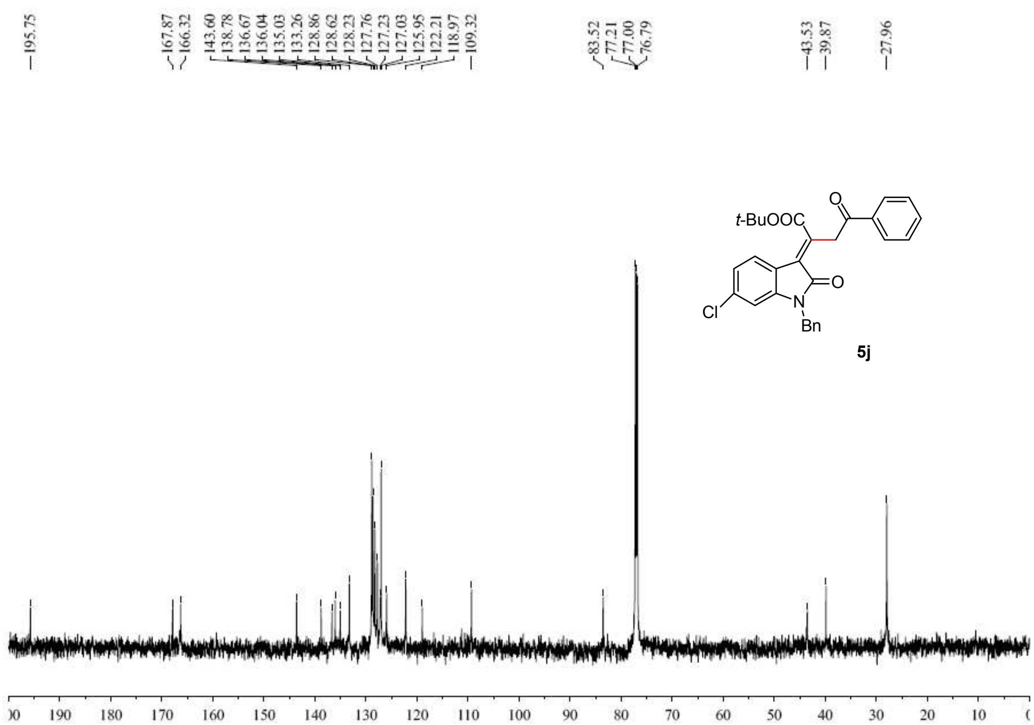


Figure S62. The ^{13}C NMR (150M Hz, $CDCl_3$) of **5j.**

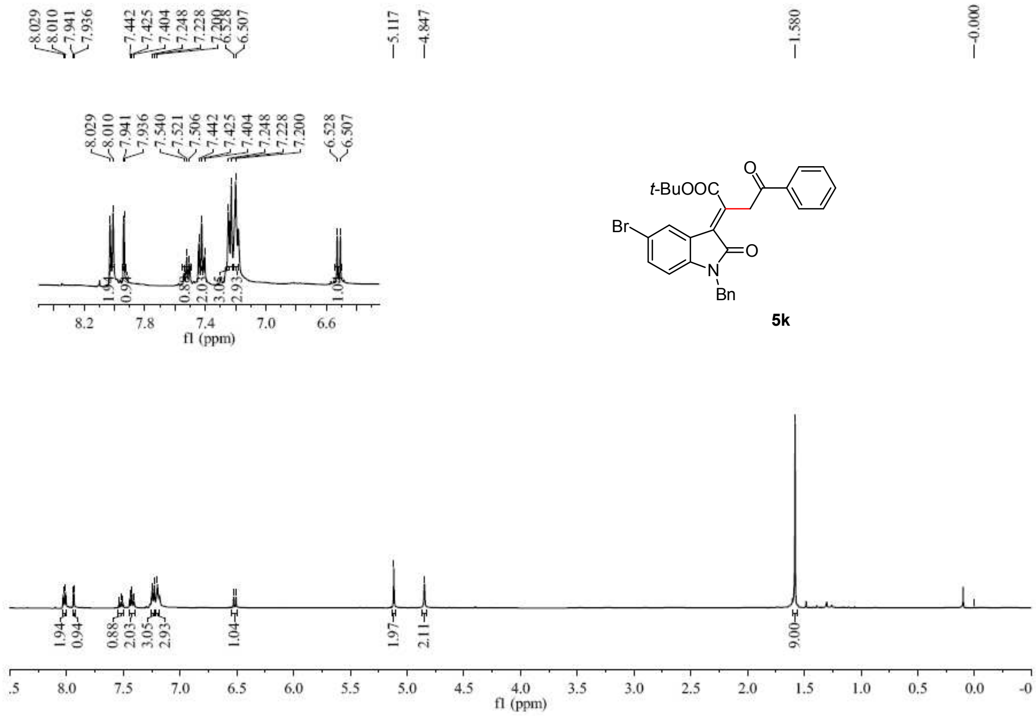


Figure S63. The ^{1}H NMR (400M Hz, $CDCl_3$) of **5k.**

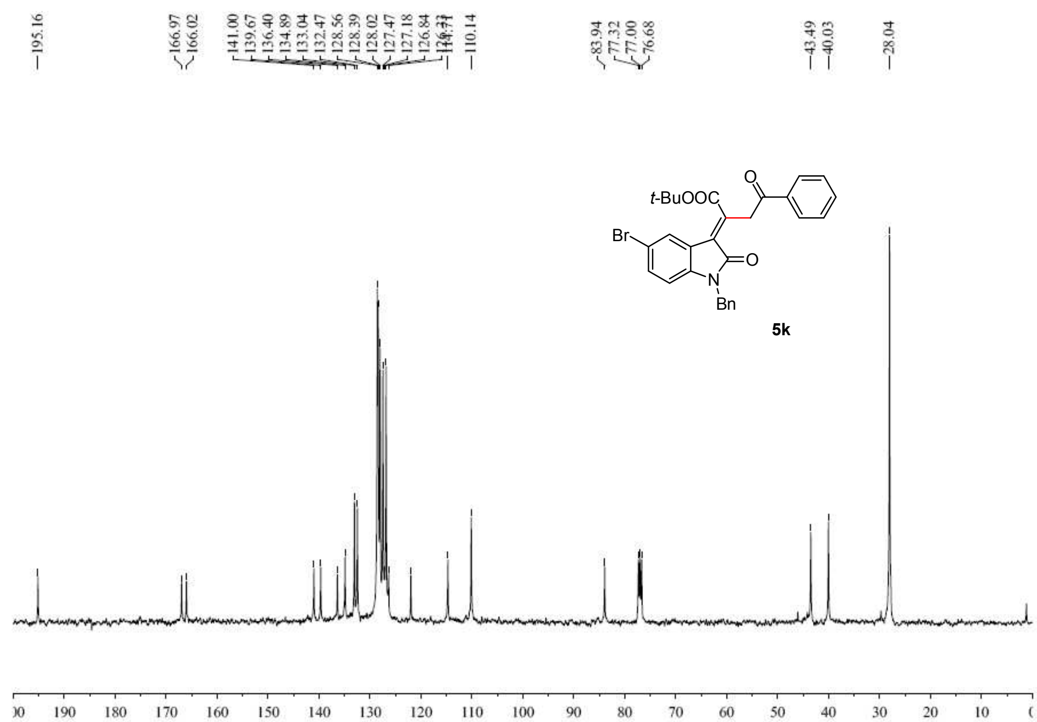


Figure S64. The ^{13}C NMR (100M Hz, $CDCl_3$) of **5k.**

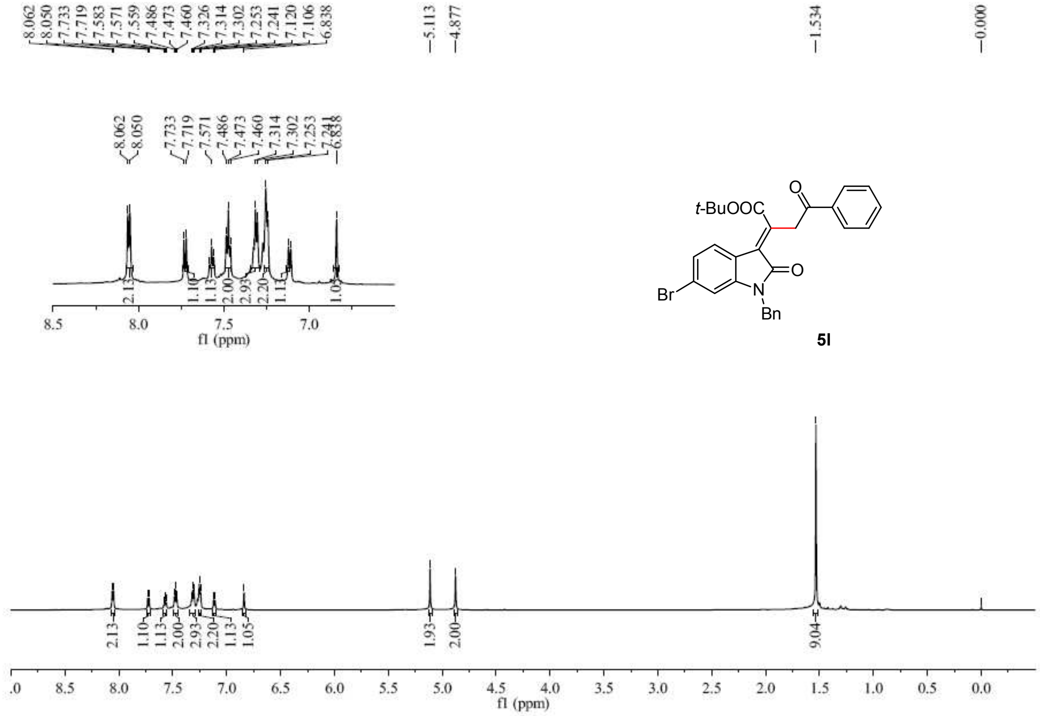


Figure S65. The [1]H NMR (600M Hz, $CDCl_3$) of **5l.**

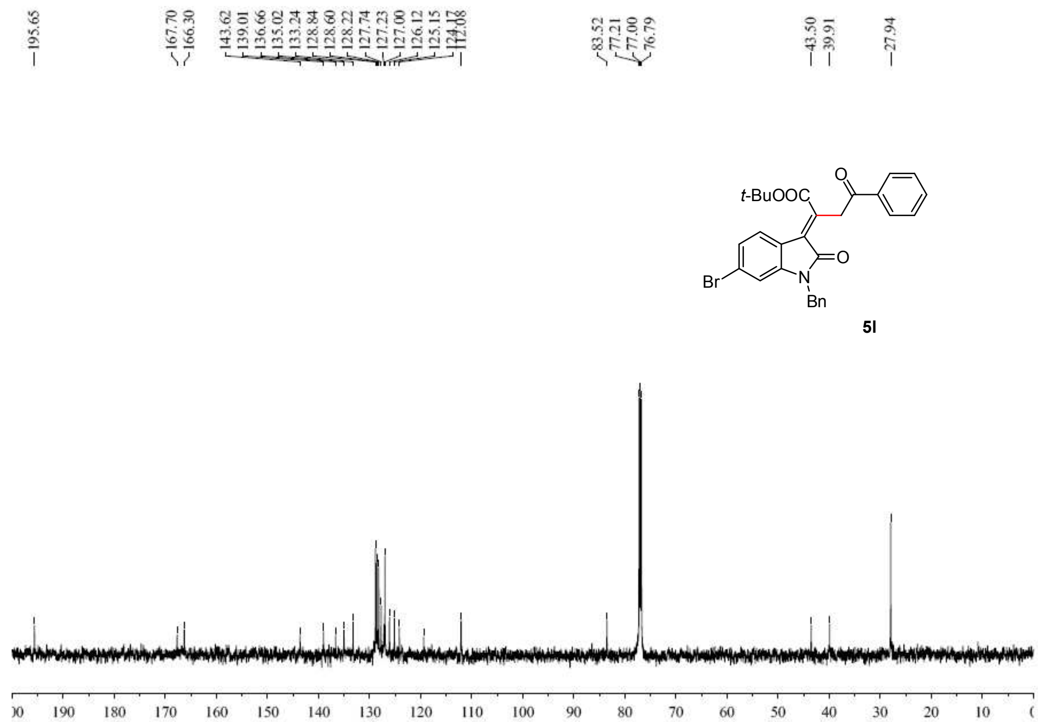


Figure S66. The [13]C NMR (150M Hz, $CDCl_3$) of **5l.**

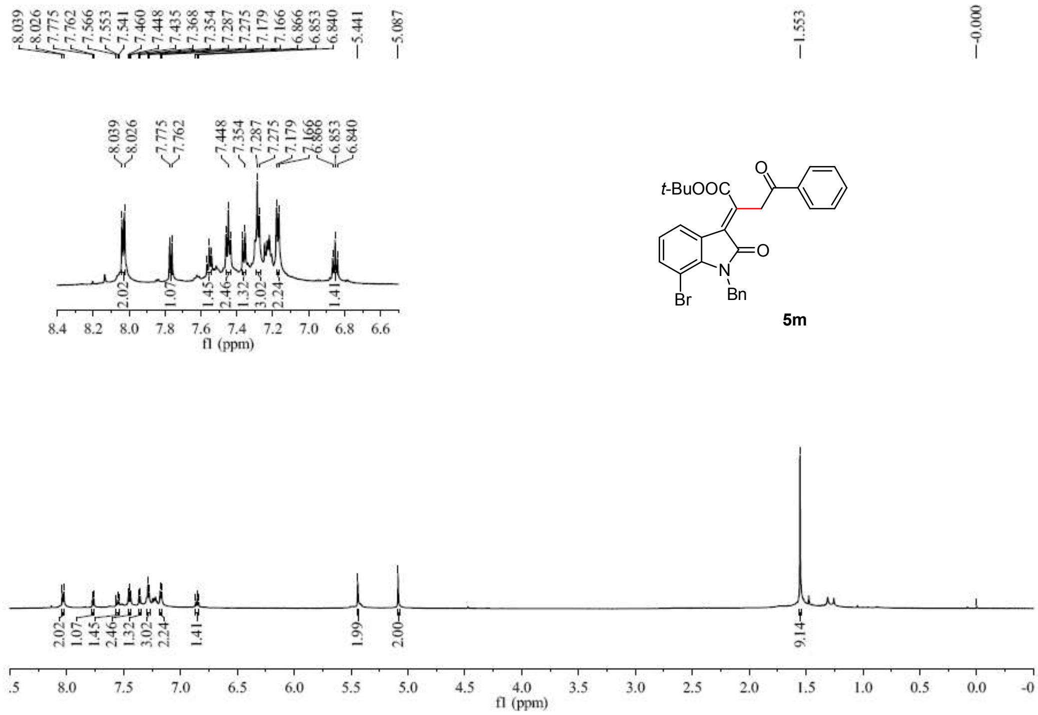


Figure S67. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5m.**

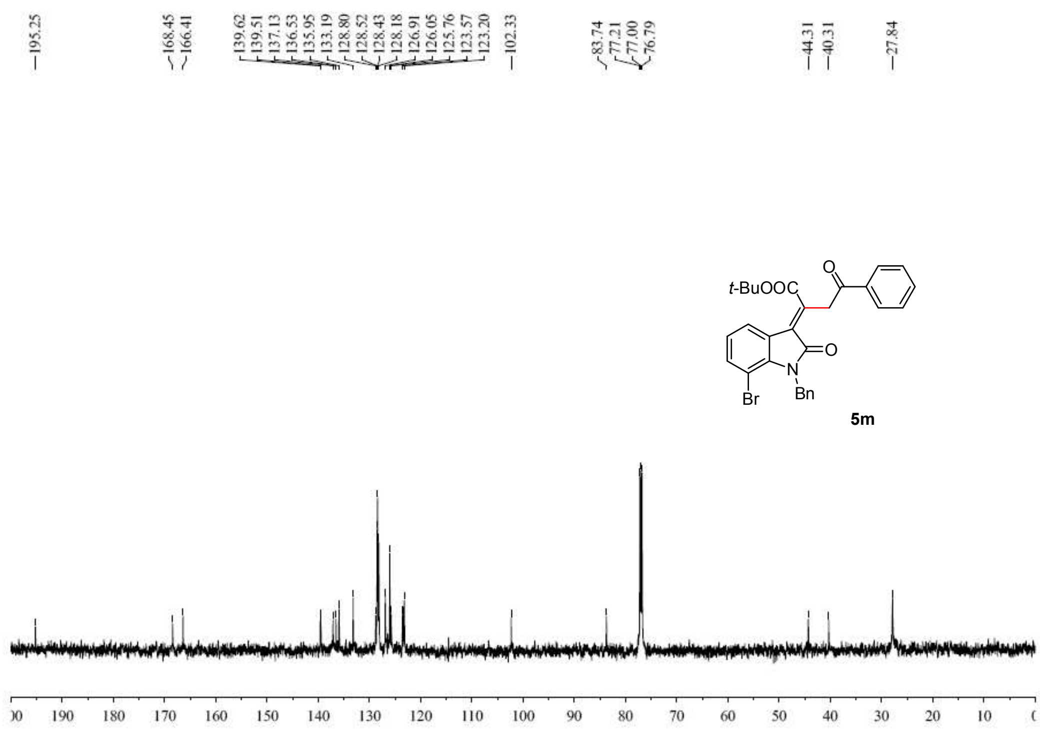


Figure S68. The ^{13}C NMR (150M Hz, $CDCl_3$) of **5m.**

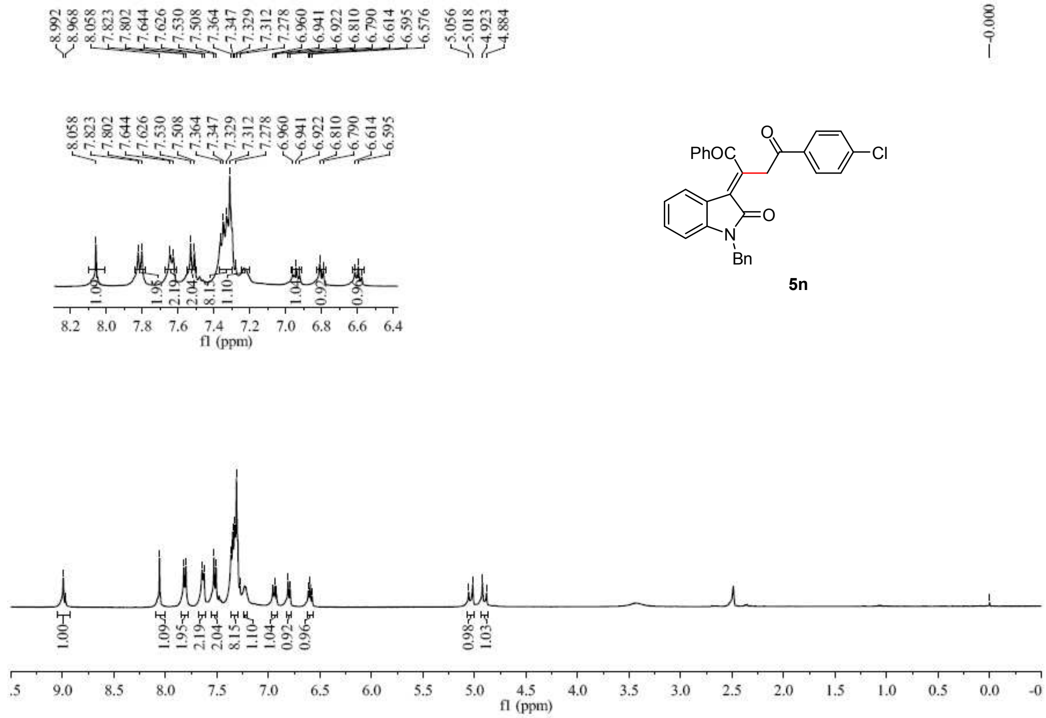


Figure S69. The ^{1}H NMR (400M Hz, DMSO-*d6*) of **5n.**

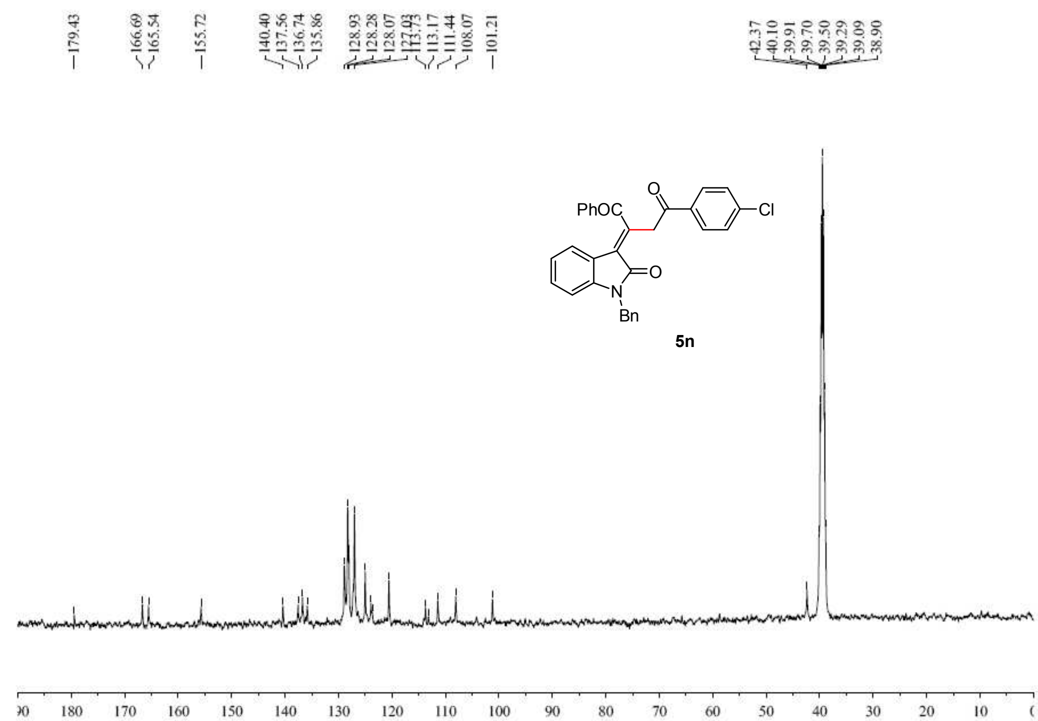


Figure S70. The ^{13}C NMR (100M Hz, DMSO-*d6*) of **5n.**

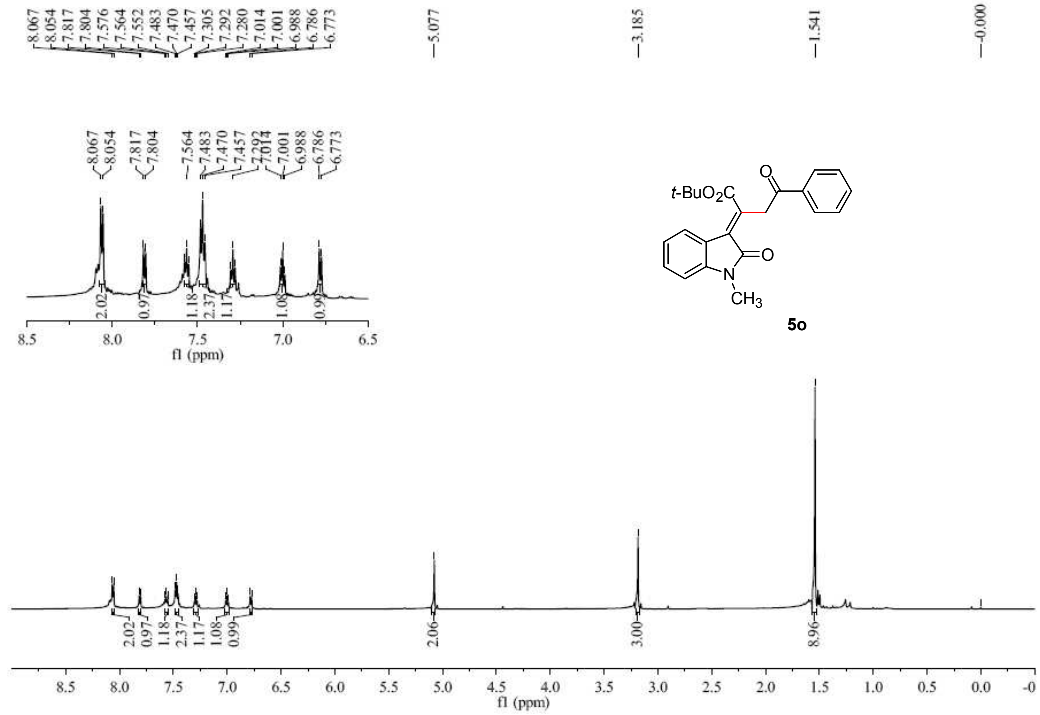


Figure S71. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5o.**

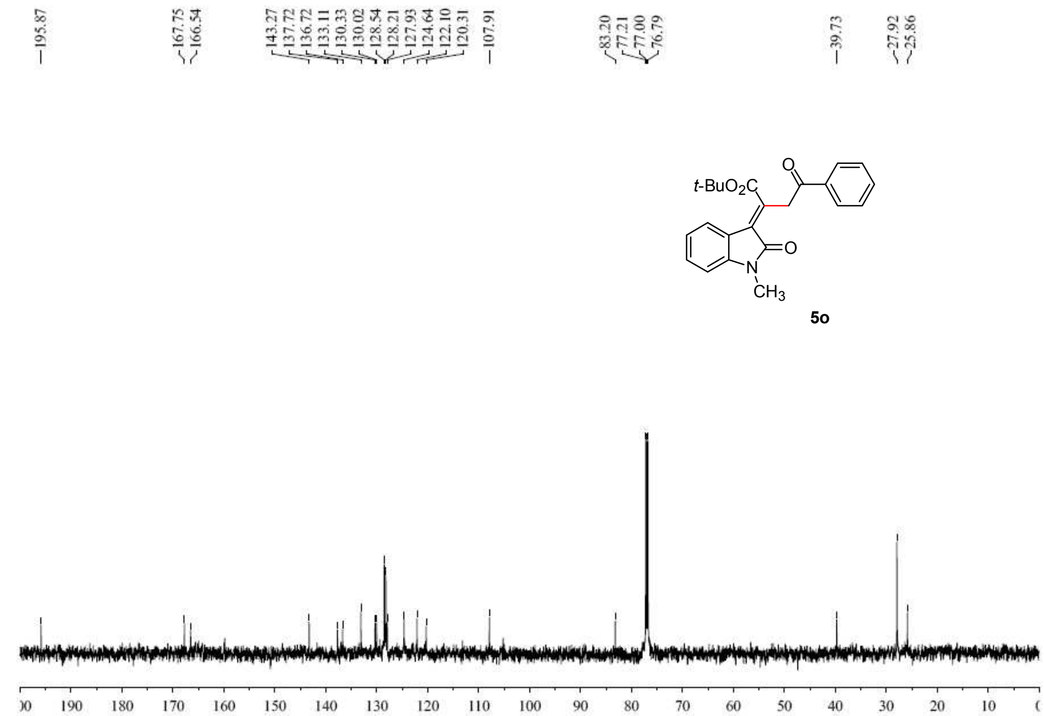


Figure S72. The ^{13}C NMR (150M Hz, $CDCl_3$) of **5o.**

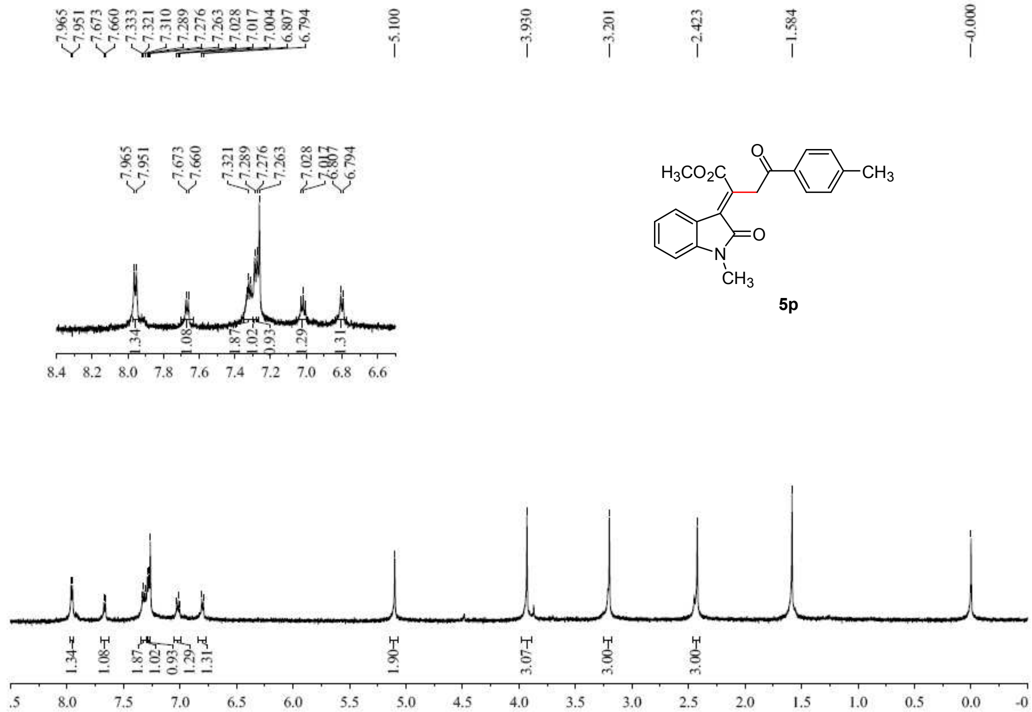


Figure S73. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5p.**

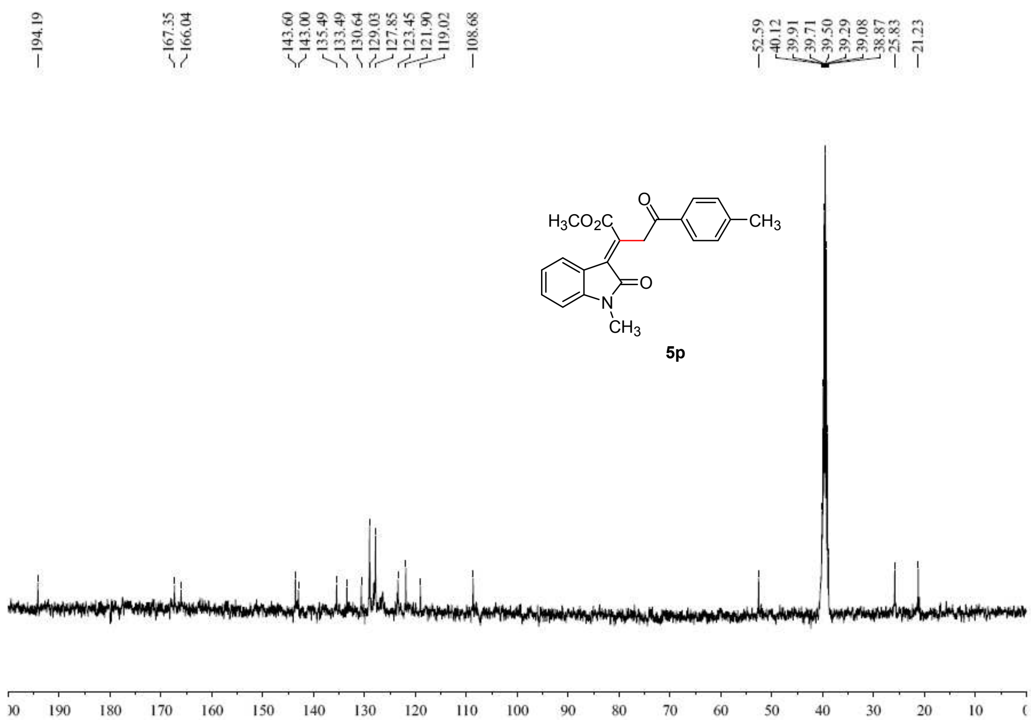


Figure S74. The ^{13}C NMR (100M Hz, DMSO-d_6) of **5p.**

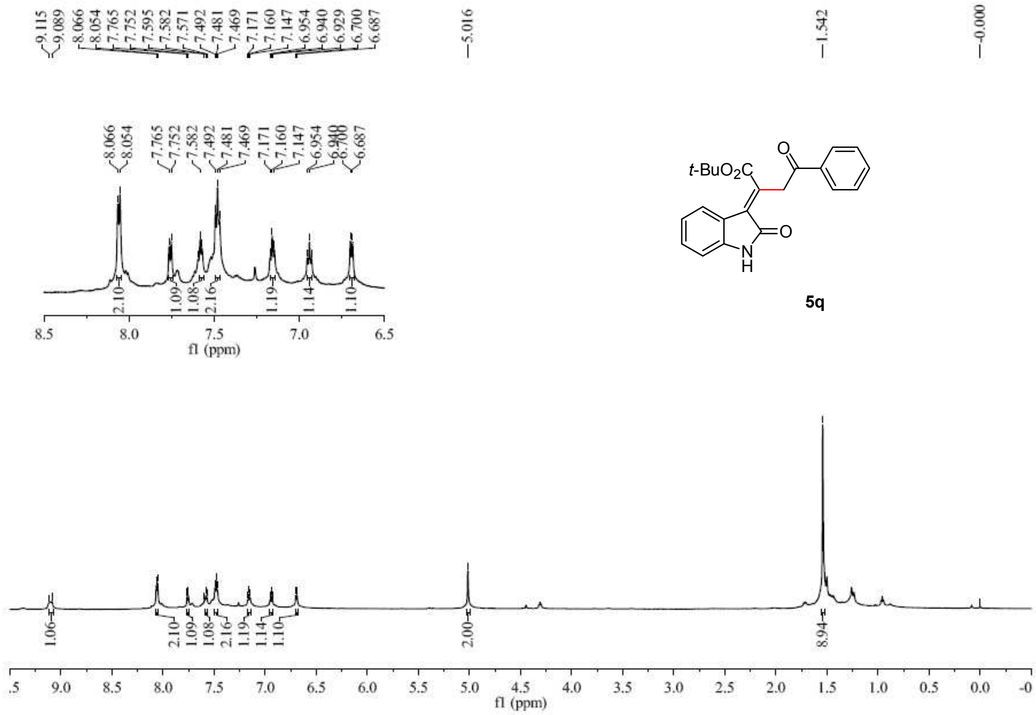


Figure S75. The ^{1}H NMR (600M Hz, $CDCl_3$) of **5q.**

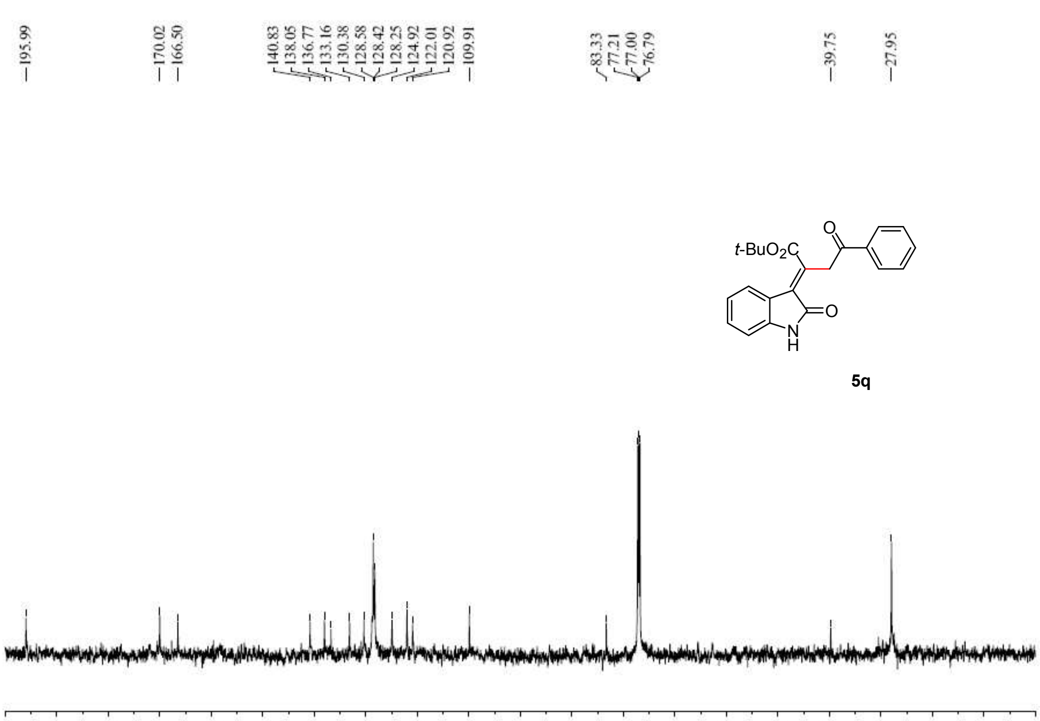


Figure S76. The ^{13}C NMR (150M Hz, $CDCl_3$) of **5q.**

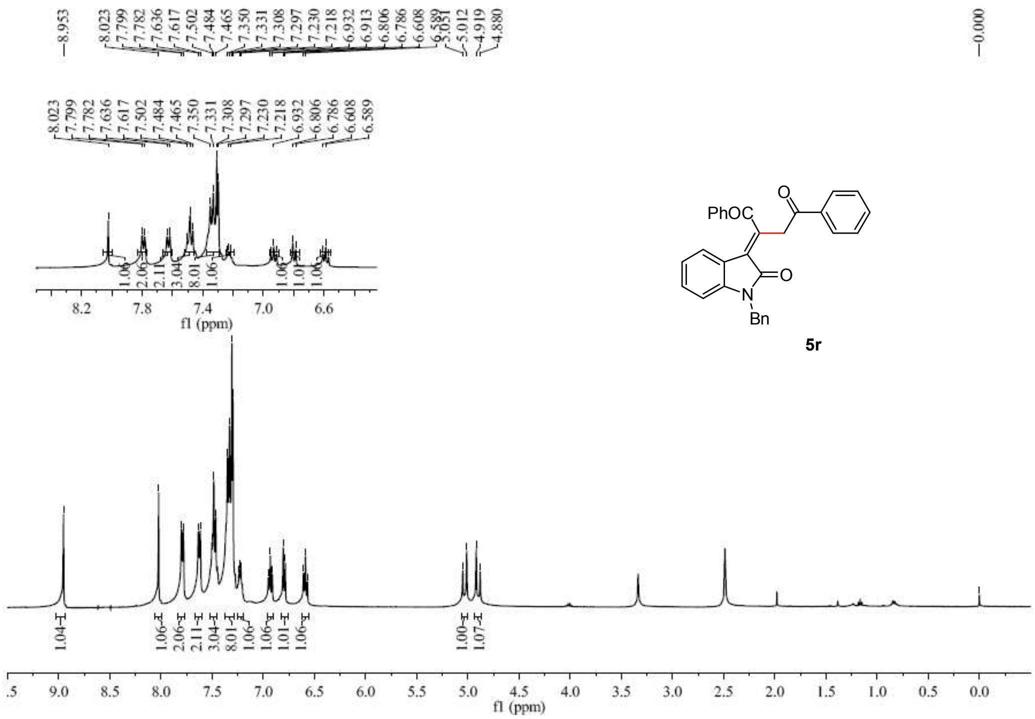


Figure S77. The ^{1}H NMR (400M Hz, DMSO-*d6*) of **5r.**

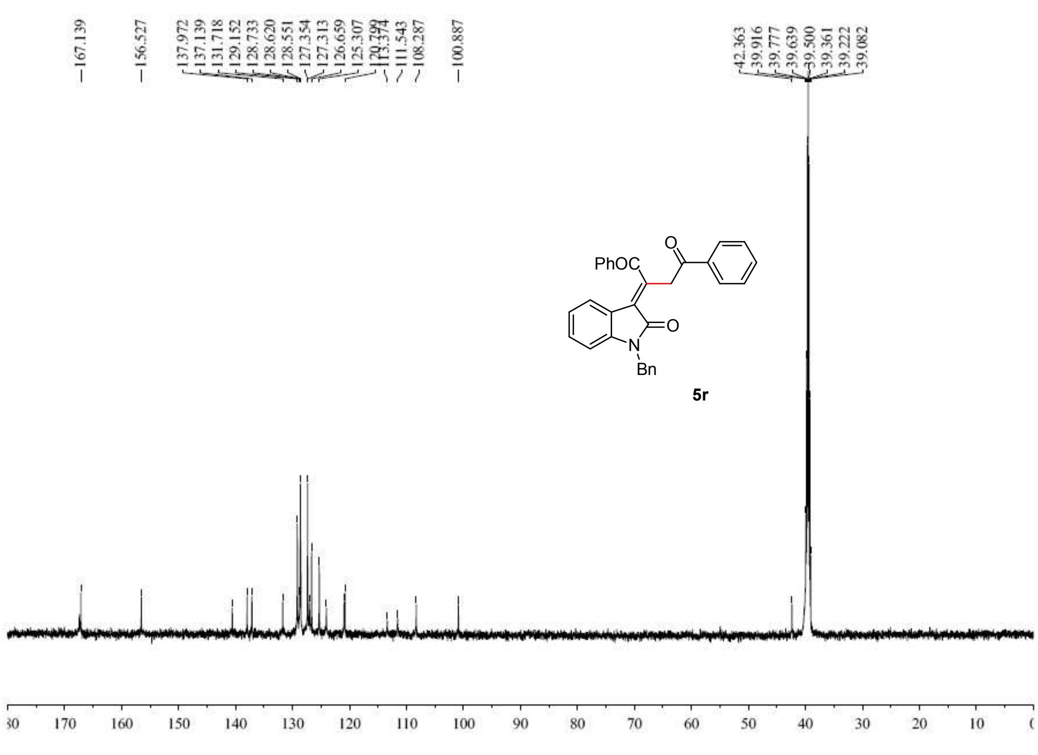
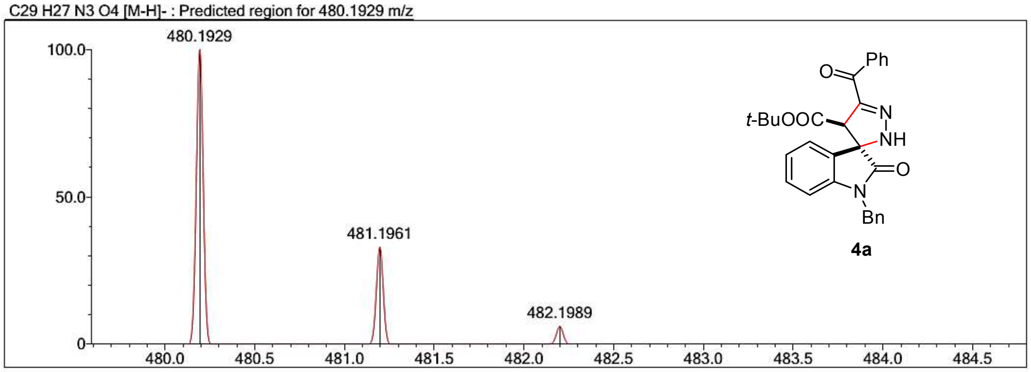


Figure S78. The ^{13}C NMR (150M Hz, DMSO-*d6*) of **5r.**

HRMS spectra of 4 and 5

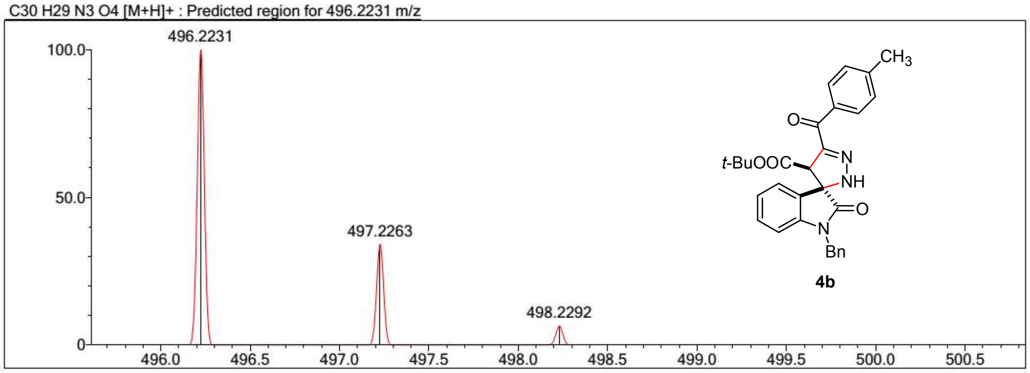
C29 H27 N3 O4 [M-H]- : Predicted region for 480.1929 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	82.12	C29 H27 N3 O4	[M-H]-	480.1942	480.1929	1.3	2.71	85.79	18.0

Figure S79. The HRMS spectra of **4a.**

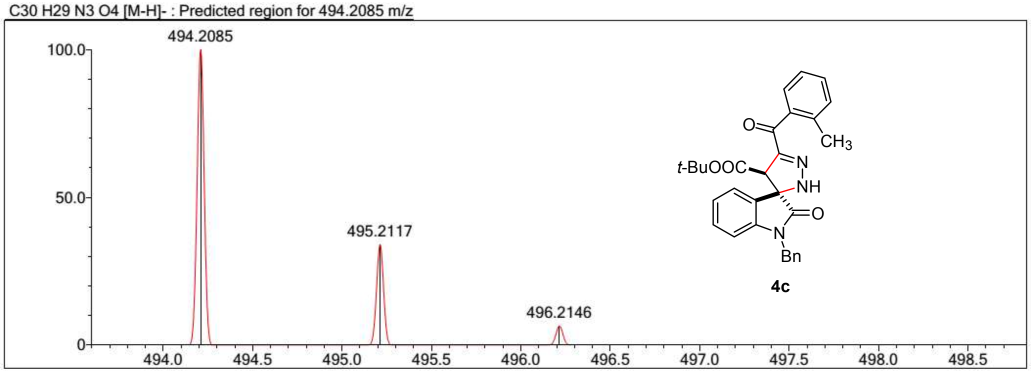
C30 H29 N3 O4 [M+H]+ : Predicted region for 496.2231 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	99.97	C30 H29 N3 O4	[M+H]+	496.2226	496.2231	-0.5	-1.01	100.00	18.0

Figure S80. The HRMS spectra of **4b.**

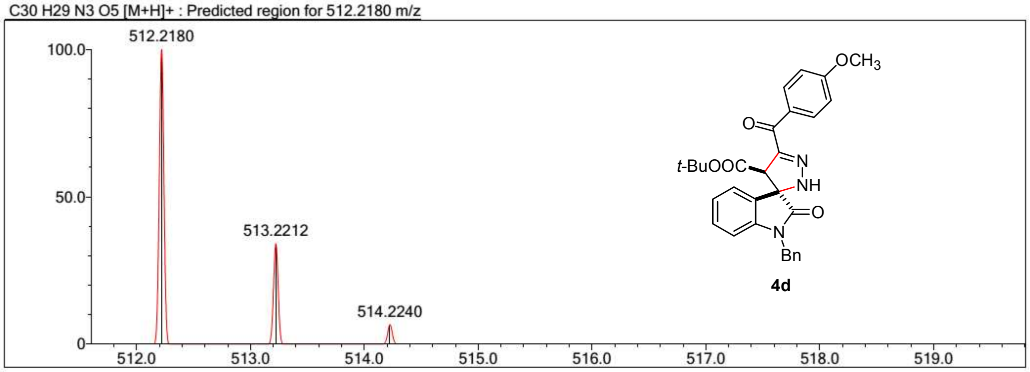
C30 H29 N3 O4 [M-H]- : Predicted region for 494.2085 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
3	91.39	C30 H29 N3 O4	[M-H]-	494.2097	494.2085	1.2	2.43	94.78	18.0

Figure S81. The HRMS spectra of **4c.**

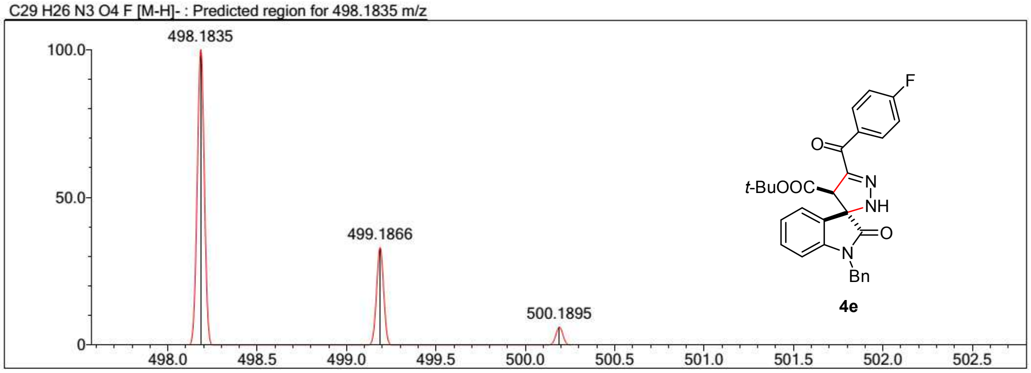
C30 H29 N3 O5 [M+H]+ : Predicted region for 512.2180 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.21	C30 H29 N3 O5	[M+H]+	512.2169	512.2180	-1.1	-2.15	73.32	18.0

Figure S82. The HRMS spectra of **4d.**

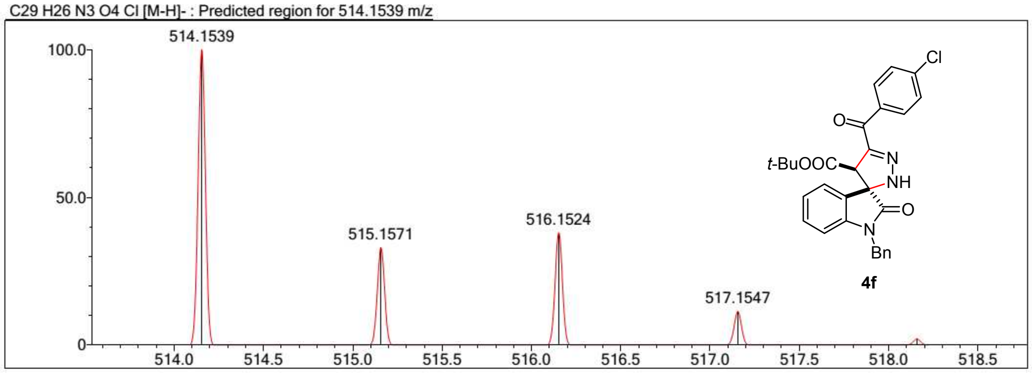
C29 H26 N3 O4 F [M-H]- : Predicted region for 498.1835 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	81.27	C29 H26 N3 O4 F	[M-H]-	498.1846	498.1835	1.1	2.21	83.81	18.0

Figure S83. The HRMS spectra of **4e.**

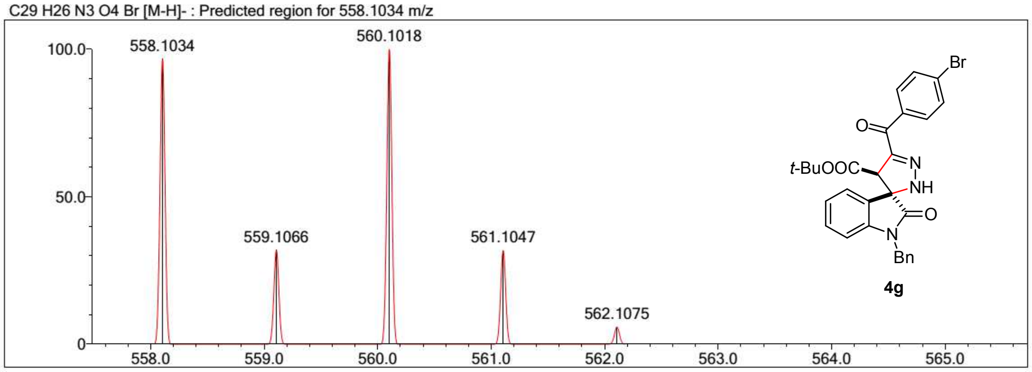
C29 H26 N3 O4 Cl [M-H]- : Predicted region for 514.1539 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
4	63.07	C29 H26 N3 O4 Cl	[M-H]-	514.1553	514.1539	1.4	2.72	65.91	18.0

Figure S84. The HRMS spectra of **4f.**

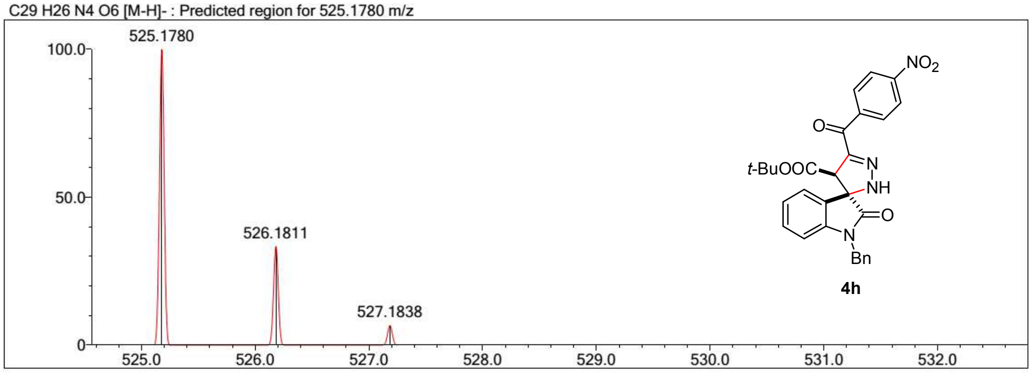
C29 H26 N3 O4 Br [M-H]- : Predicted region for 558.1034 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.34	C29 H26 N3 O4 Br	[M-H]-	558.1042	558.1034	0.8	1.43	89.30	18.0

Figure S85. The HRMS spectra of **4g.**

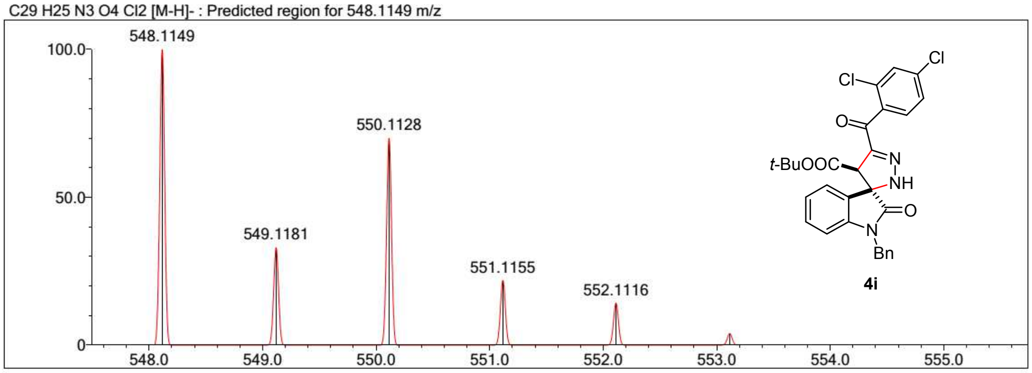
C29 H26 N4 O6 [M-H]- : Predicted region for 525.1780 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	89.51	C29 H26 N4 O6	[M-H]-	525.1784	525.1780	0.4	0.76	89.51	19.0

Figure S86. The HRMS spectra of **4h.**

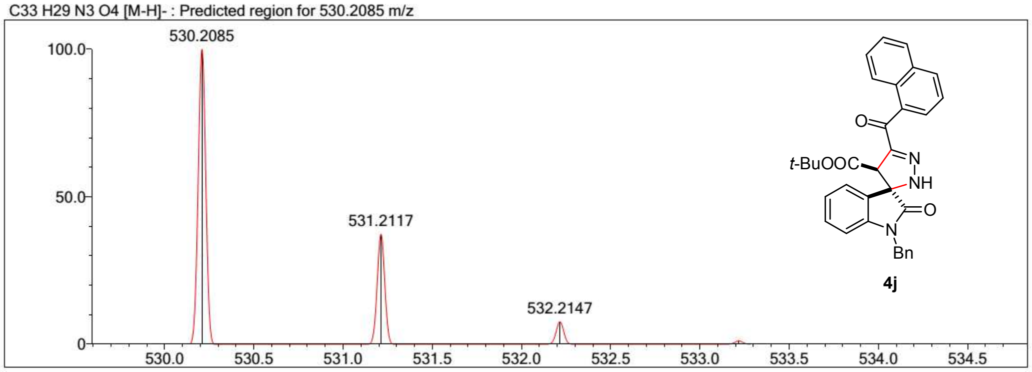
C29 H25 N3 O4 Cl2 [M-H]- : Predicted region for 548.1149 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	95.49	C29 H25 N3 O4 Cl2	[M-H]-	548.1163	548.1149	1.4	2.55	99.34	18.0

Figure S87. The HRMS spectra of **4i.**

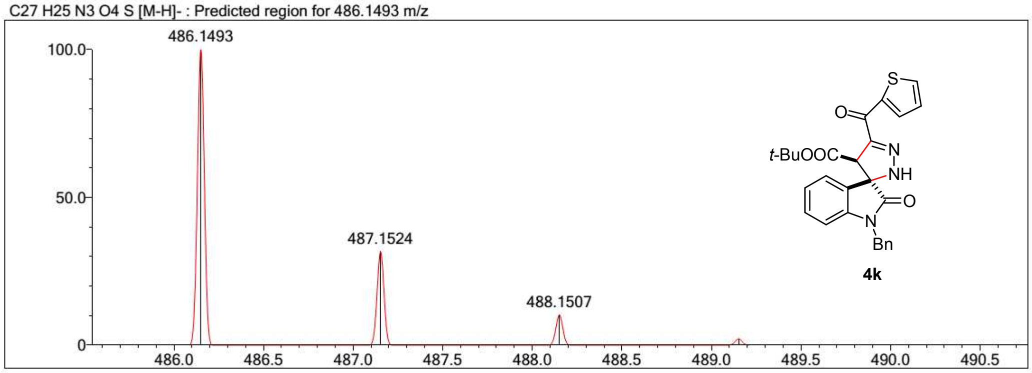
C33 H29 N3 O4 [M-H]- : Predicted region for 530.2085 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	88.23	C33 H29 N3 O4	[M-H]-	530.2099	530.2085	1.4	2.64	92.00	21.0

Figure S88. The HRMS spectra of **4j.**

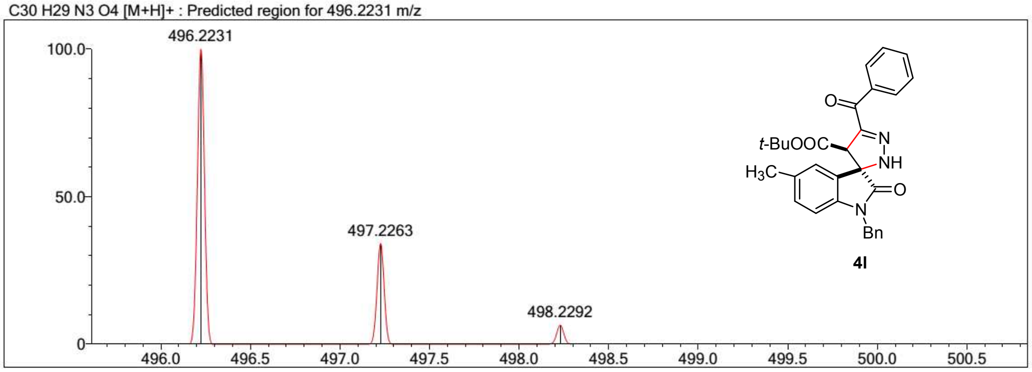
C27 H25 N3 O4 S [M-H]- : Predicted region for 486.1493 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	82.85	C27 H25 N3 O4 S	[M-H]-	486.1507	486.1493	1.4	2.88	86.93	17.0

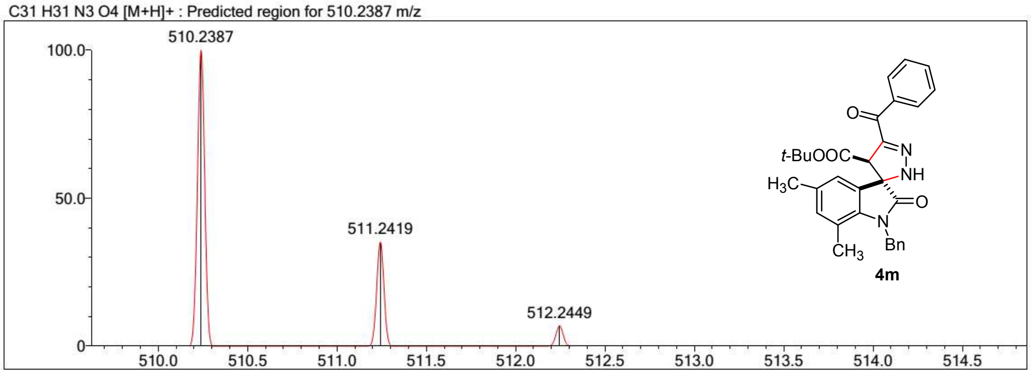
Figure S89. The HRMS spectra of **4k.**

C30 H29 N3 O4 [M+H]+ : Predicted region for 496.2231 m/z



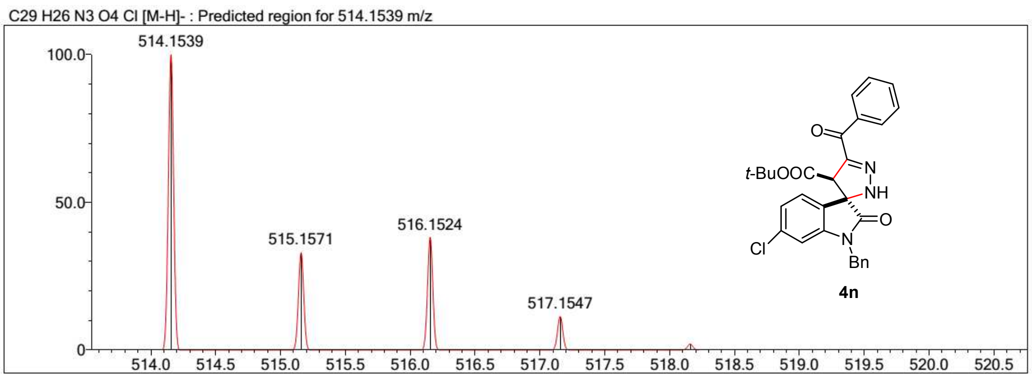
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	96.04	C30 H29 N3 O4	[M+H]+	496.2226	496.2231	-0.5	-1.01	96.07	18.0

Figure S90. The HRMS spectra of **4l.**



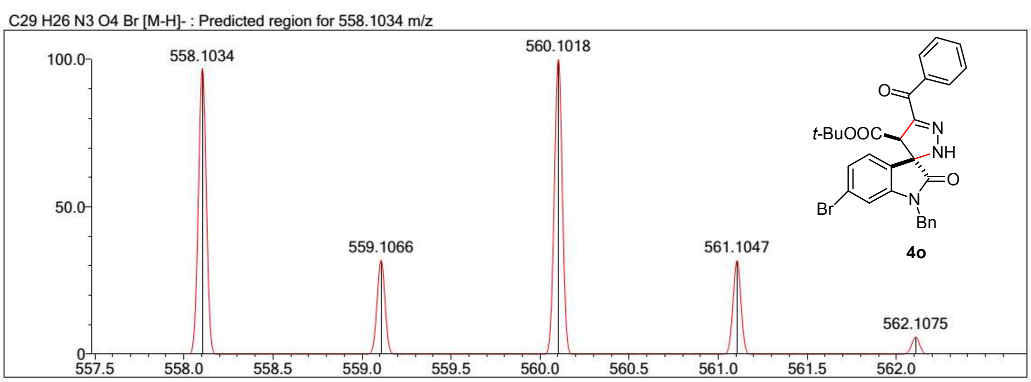
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	99.55	C31 H31 N3 O4	[M+H]+	510.2393	510.2387	0.6	1.18	100.00	18.0

Figure S91. The HRMS spectra of **4m.**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
5	29.05	C29 H26 N3 O4 Cl	[M-H]-	514.1551	514.1539	1.2	2.33	30.05	18.0

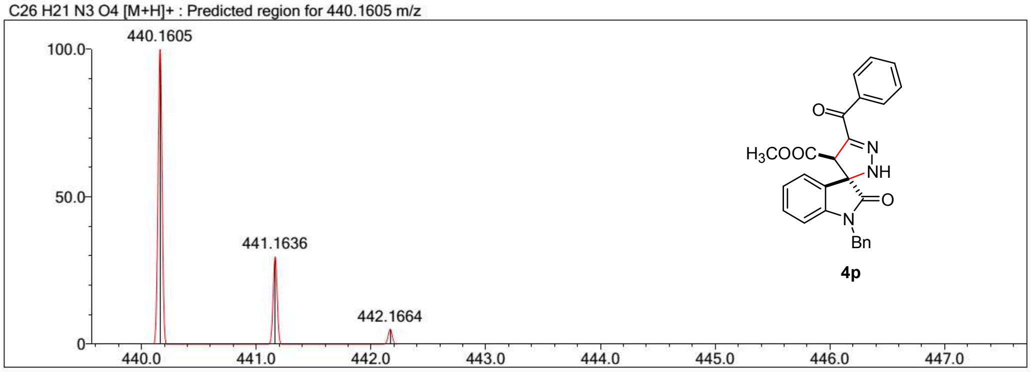
Figure S92. The HRMS spectra of **4n.**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	57.27	C29 H26 N3 O4 Br	[M-H]-	558.1040	558.1034	0.6	1.08	57.38	18.0

Figure S93. The HRMS spectra of **4o.**

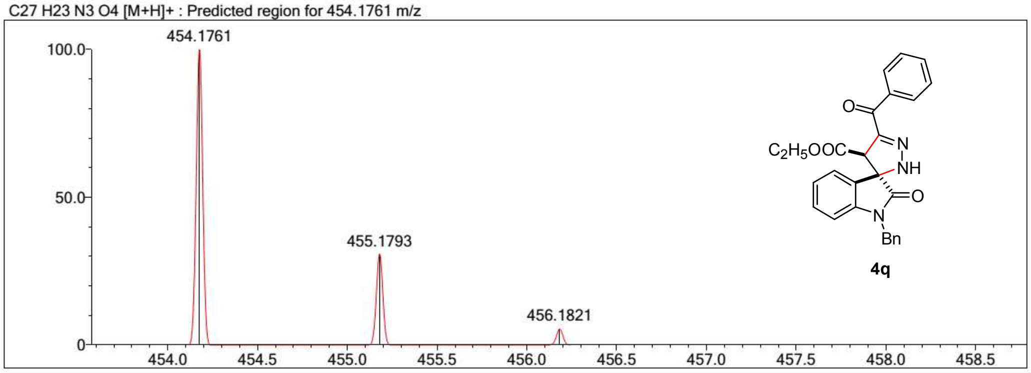
C26 H21 N3 O4 [M+H]+ : Predicted region for 440.1605 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	91.75	C26 H21 N3 O4	[M+H]+	440.1607	440.1605	0.2	0.45	91.75	18.0

Figure S94. The HRMS spectra of **4p.**

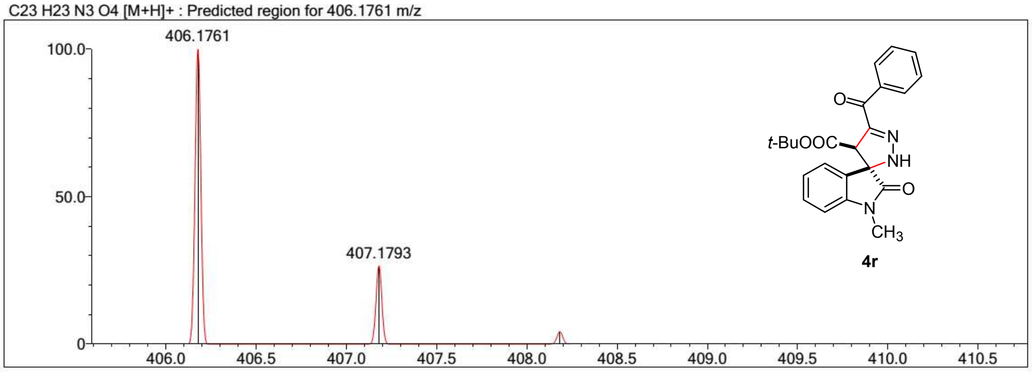
C27 H23 N3 O4 [M+H]+ : Predicted region for 454.1761 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	99.29	C27 H23 N3 O4	[M+H]+	454.1765	454.1761	0.4	0.88	99.29	18.0

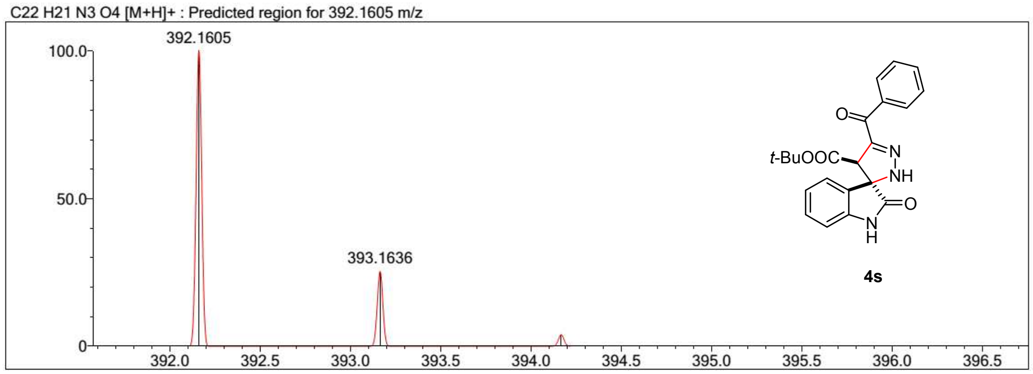
Figure S95. The HRMS spectra of **4q.**

C23 H23 N3 O4 [M+H]+ : Predicted region for 406.1761 m/z



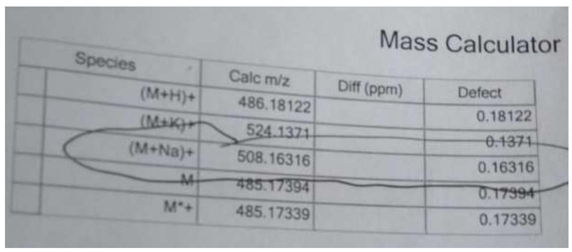
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	95.74	C23 H23 N3 O4	[M+H]+	406.1769	406.1761	0.8	1.97	98.12	14.0

Figure S96. The HRMS spectra of **4r.**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	80.94	C22 H21 N3 O4	[M+H]+	392.1612	392.1605	0.7	1.78	82.55	14.0

Figure S97. The HRMS spectra of **4s.**



Mass Calculator

Species	Calc m/z	Diff (ppm)	Defect
(M+H)+	486.18122		0.18122
(M+K)+	524.1371		0.1371
(M+Na)+	508.16316		0.16316
M	485.17394		0.17394
M*+	485.17339		0.17339

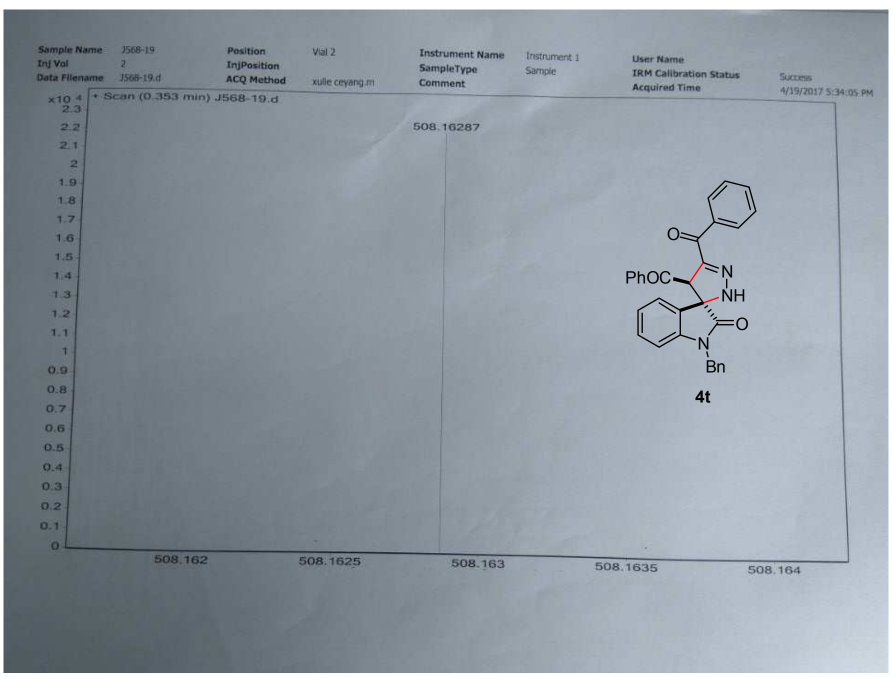


Figure S98. The HRMS spectra of **4t.**

Mass Calculator

Species	Calc m/z	Diff (ppm)	Defect
(M+H)+	410.14992		0.14992
(M+K)+	448.1058		0.1058
(M+Na)+	432.13186		0.13186
M	409.14264		0.14264
M*+	409.14209		0.14209

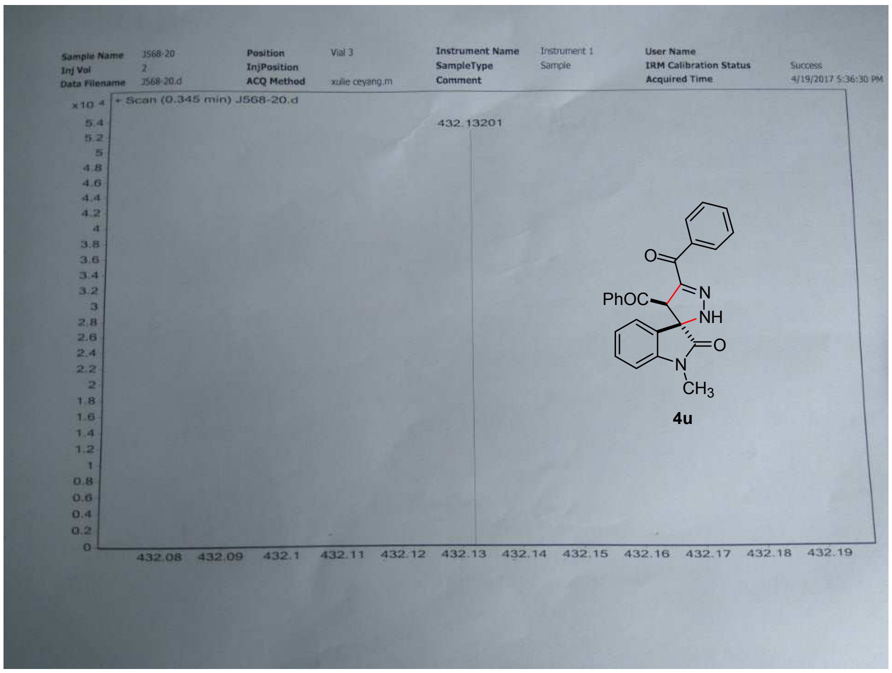
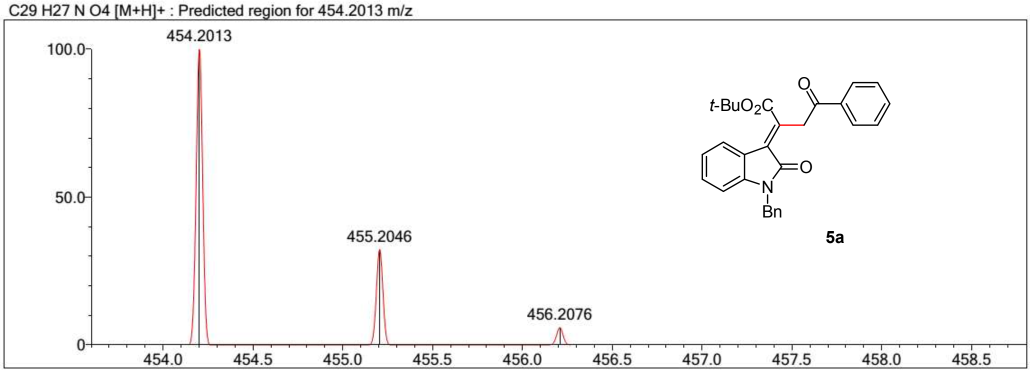


Figure S99. The HRMS spectra of **4u.**

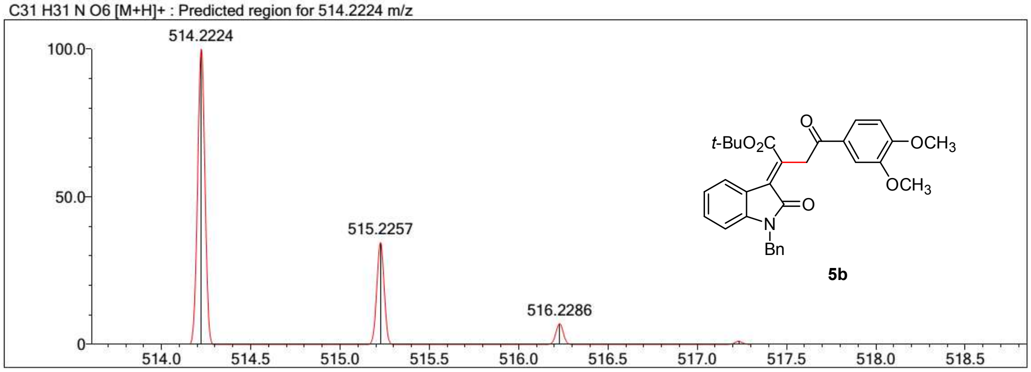
C29 H27 N O4 [M+H]+ : Predicted region for 454.2013 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	94.00	C29 H27 N O4	[M+H]+	454.2012	454.2013	-0.1	-0.22	94.00	17.0

Figure S100. The HRMS spectra of **5a.**

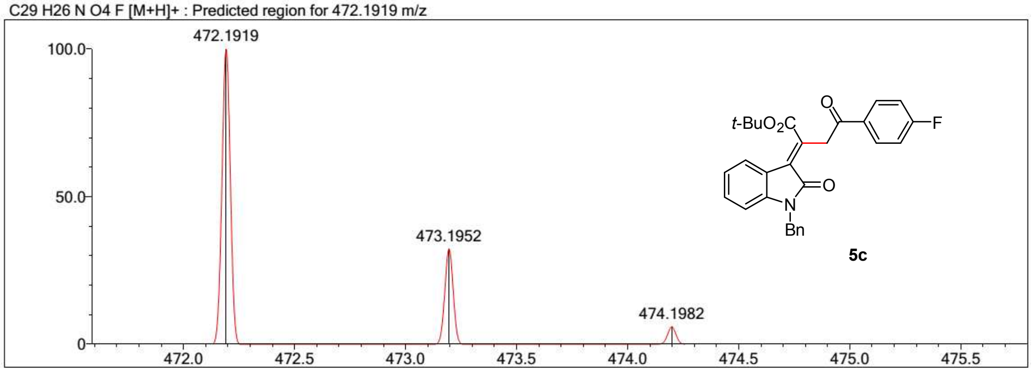
C31 H31 N O6 [M+H]+ : Predicted region for 514.2224 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
6	98.13	C31 H31 N O6	[M+H]+	514.2233	514.2224	0.9	1.75	100.00	17.0

Figure S101. The HRMS spectra of **5b.**

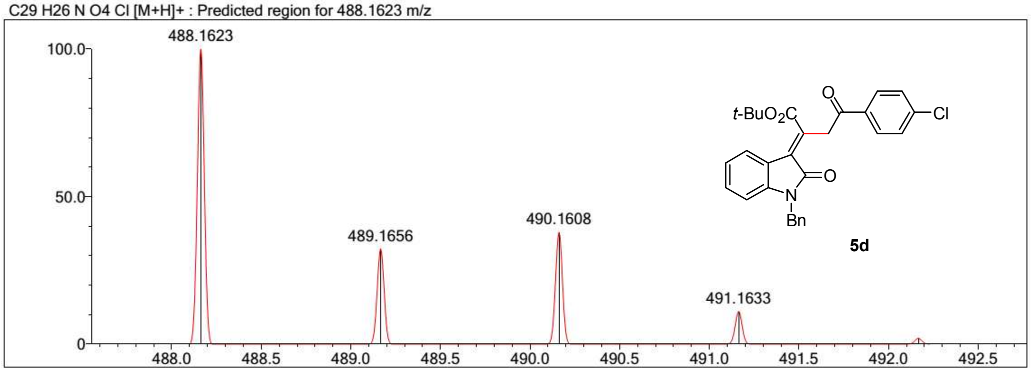
C29 H26 N O4 F [M+H]+ : Predicted region for 472.1919 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	89.93	C29 H26 N O4 F	[M+H]+	472.1911	472.1919	-0.8	-1.69	91.50	17.0

Figure S102. The HRMS spectra of **5c.**

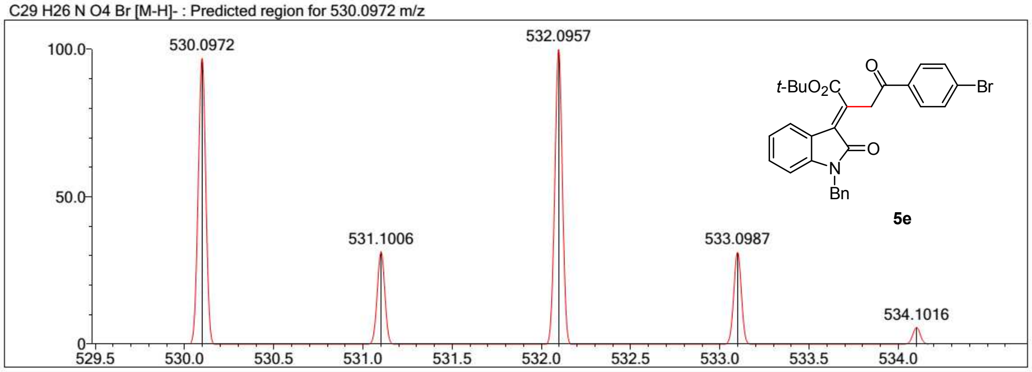
C29 H26 N O4 Cl [M+H]+ : Predicted region for 488.1623 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
5	50.66	C29 H26 N O4 Cl	[M+H]+	488.1609	488.1623	-1.4	-2.87	53.14	17.0

Figure S103. The HRMS spectra of **5d.**

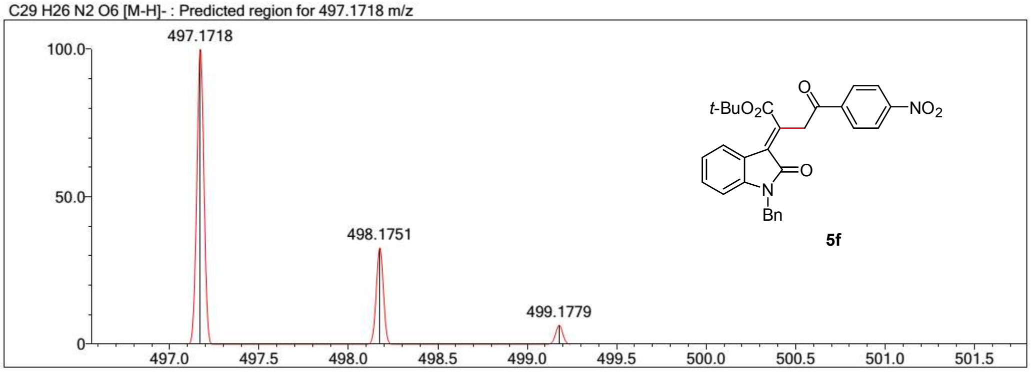
C29 H26 N O4 Br [M-H]- : Predicted region for 530.0972 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	91.85	C29 H26 N O4 Br	[M-H]-	530.0980	530.0972	0.8	1.51	93.04	17.0

Figure S104. The HRMS spectra of **5e.**

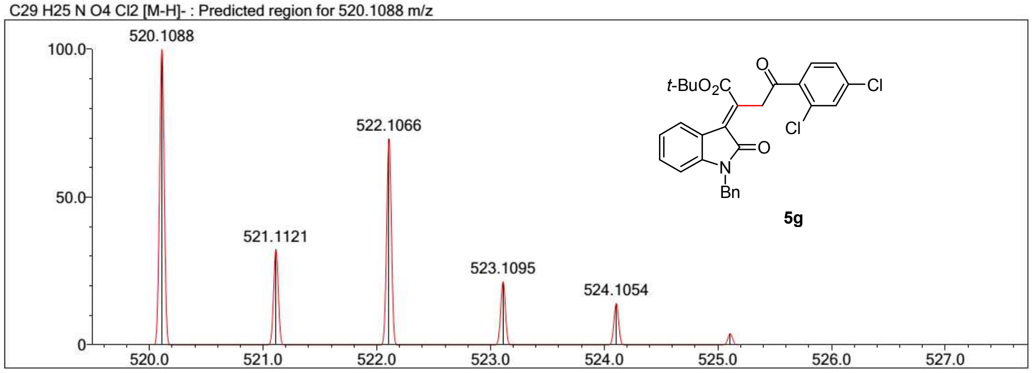
C29 H26 N2 O6 [M-H]- : Predicted region for 497.1718 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	86.08	C29 H26 N2 O6	[M-H]-	497.1737	497.1718	1.9	3.82	92.61	18.0

Figure S105. The HRMS spectra of **5f.**

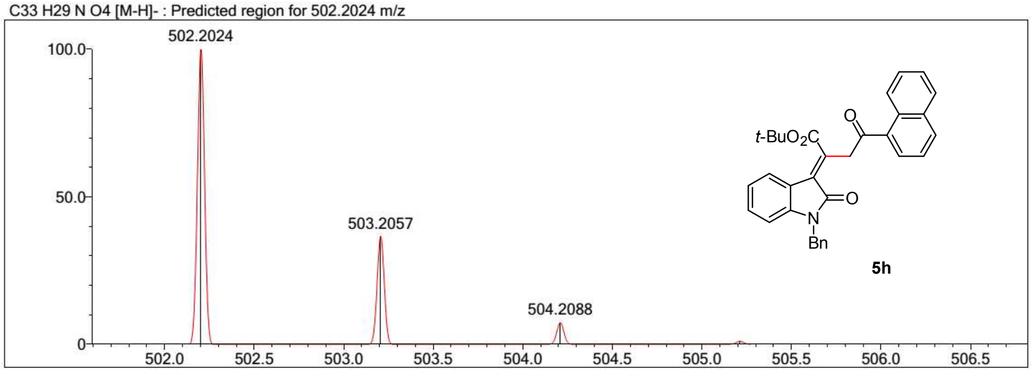
C29 H25 N O4 Cl2 [M-H]- : Predicted region for 520.1088 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	90.82	C29 H25 N O4 Cl2	[M-H]-	520.1098	520.1088	1.0	1.92	92.96	17.0

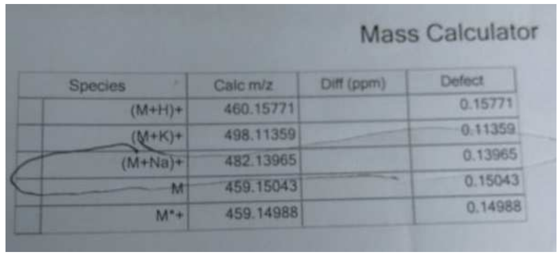
Figure S106. The HRMS spectra of **5g.**

C33 H29 N O4 [M-H]- : Predicted region for 502.2024 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	83.84	C33 H29 N O4	[M-H]-	502.2026	502.2024	0.2	0.40	83.84	20.0

Figure S107. The HRMS spectra of **5h.**



Mass Calculator

Species	Calc m/z	Diff (ppm)	Defect
(M+H)+	460.15771		0.15771
(M+K)+	498.11359		0.11359
(M+Na)+	482.13965		0.13965
M	459.15043		0.15043
M*+	459.14988		0.14988

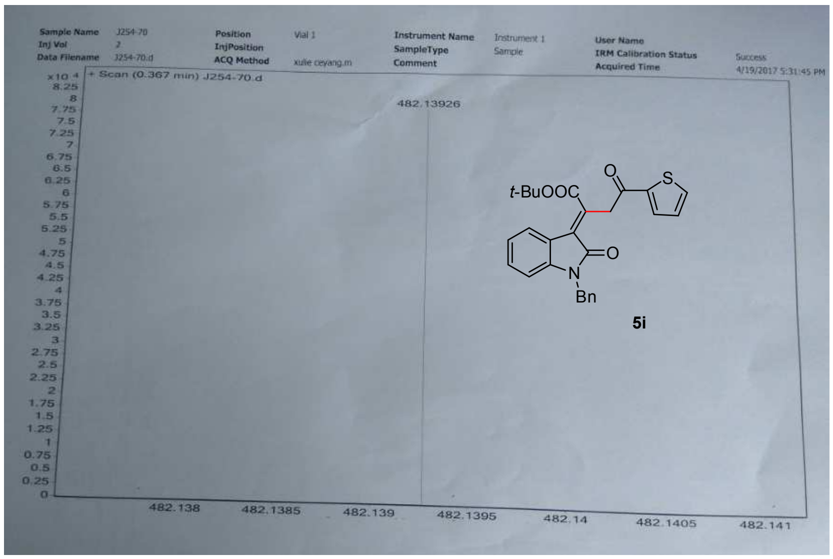
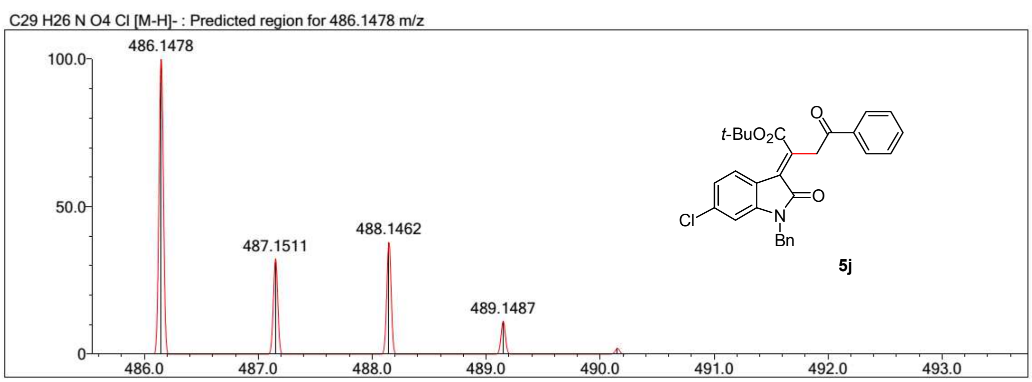


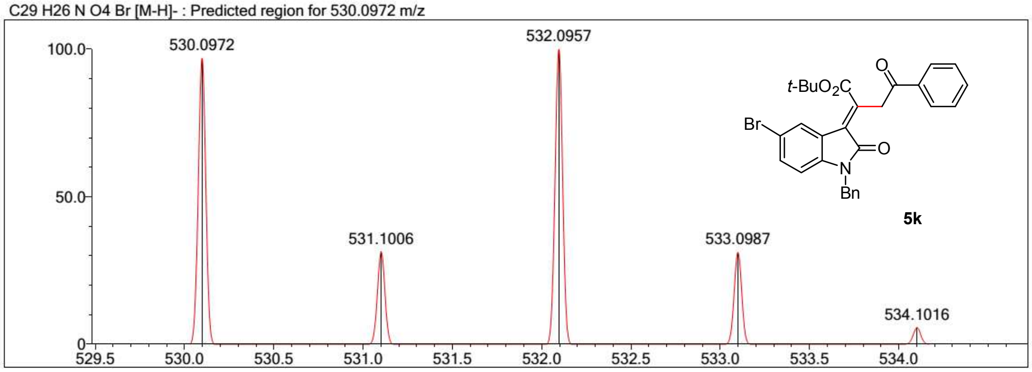
Figure S108. The HRMS spectra of **5i.**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	84.64	C29 H26 N O4 Cl	[M-H]-	486.1483	486.1478	0.5	1.03	84.70	17.0

Figure S109. The HRMS spectra of **5j.**

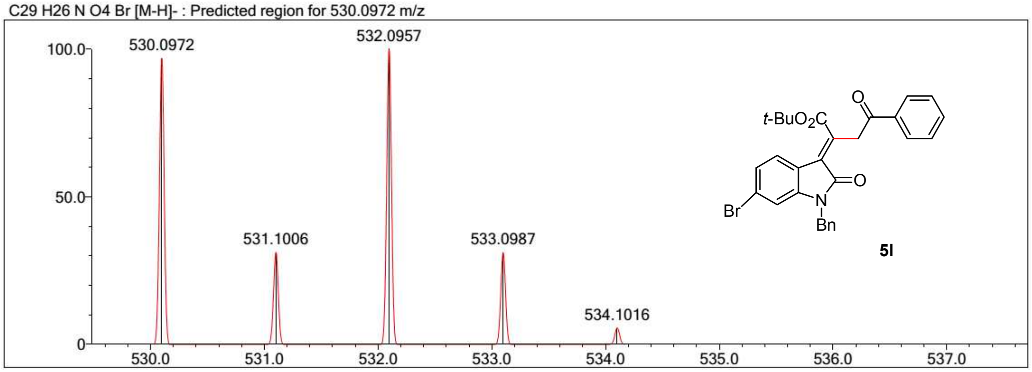
C29 H26 N O4 Br [M-H]- : Predicted region for 530.0972 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	81.80	C29 H26 N O4 Br	[M-H]-	530.0983	530.0972	1.1	2.08	84.07	17.0

Figure S110. The HRMS spectra of **5k.**

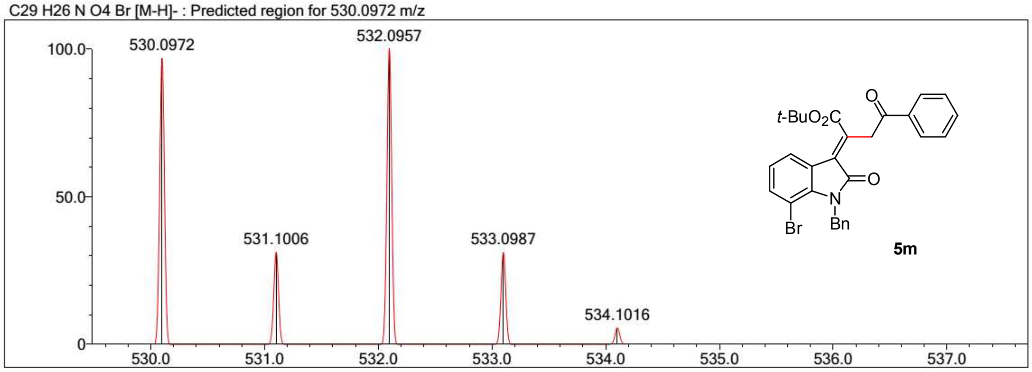
C29 H26 N O4 Br [M-H]- : Predicted region for 530.0972 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	98.02	C29 H26 N O4 Br	[M-H]-	530.0980	530.0972	0.8	1.51	99.28	17.0

Figure S111. The HRMS spectra of **5l.**

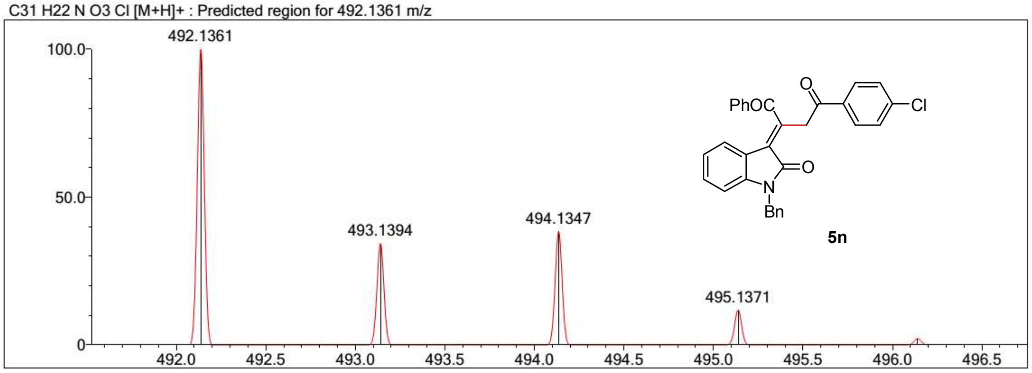
C29 H26 N O4 Br [M-H]- : Predicted region for 530.0972 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.30	C29 H26 N O4 Br	[M-H]-	530.0976	530.0972	0.4	0.75	88.30	17.0

Figure S112. The HRMS spectra of **5m.**

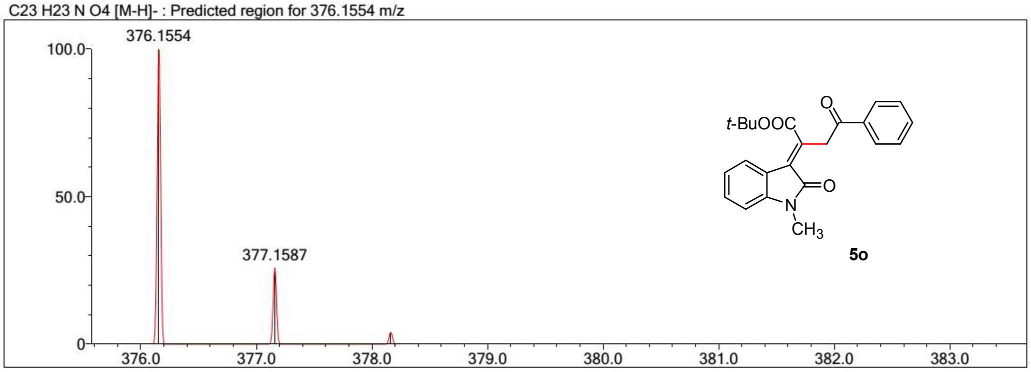
C31 H22 N O3 Cl [M+H]+ : Predicted region for 492.1361 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	71.88	C31 H22 N O3 Cl	[M+H]+	492.1363	492.1361	0.2	0.41	71.88	21.0

Figure S113. The HRMS spectra of **5n.**

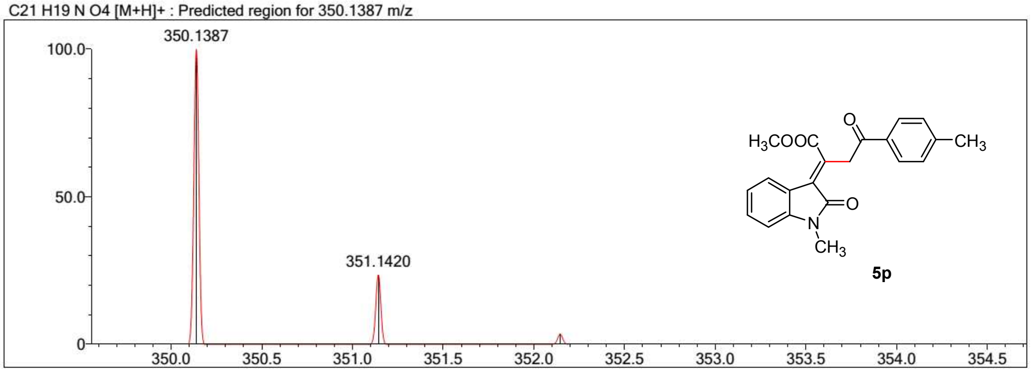
C23 H23 N O4 [M-H]- : Predicted region for 376.1554 m/z



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	79.83	C23 H23 N O4	[M-H]-	376.1554	376.1554	-0.0	0.00	79.83	13.0

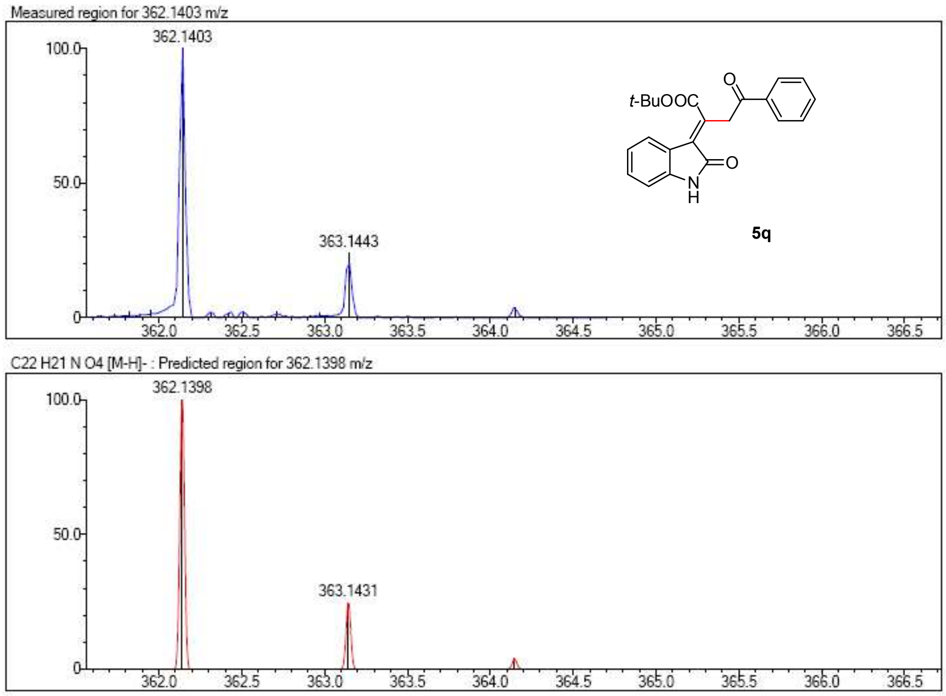
Figure S114. The HRMS spectra of **5o.**

C21 H19 N O4 [M+H]+ : Predicted region for 350.1387 m/z



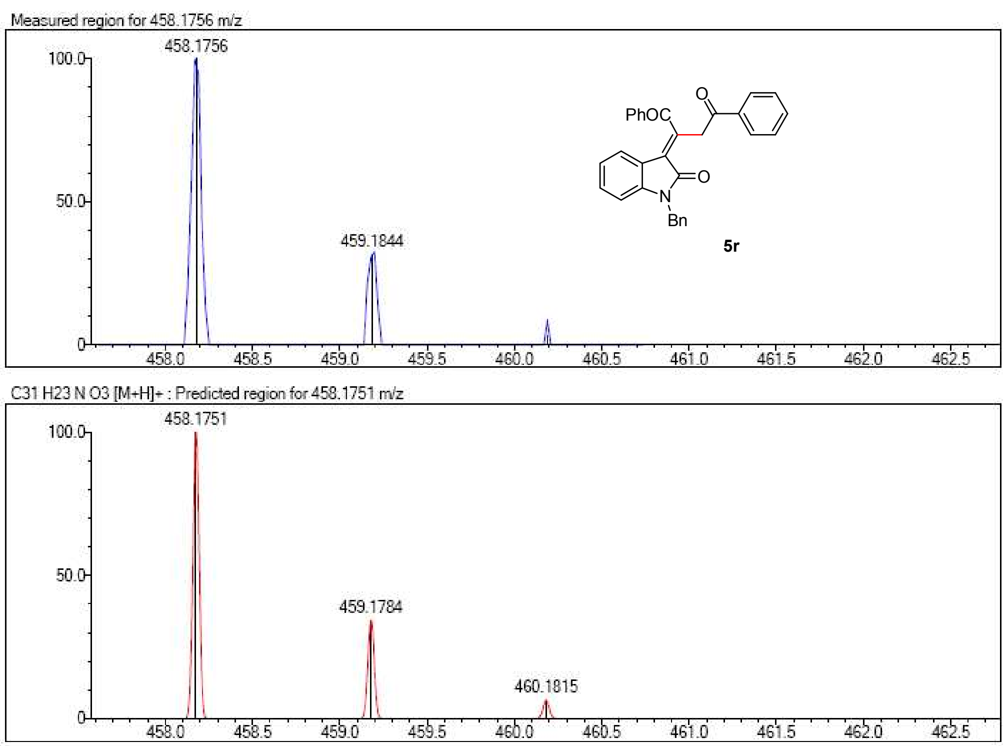
Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	100.00	C21 H19 N O4	[M+H]+	350.1384	350.1387	-0.3	-0.86	100.00	13.0

Figure S115. The HRMS spectra of **5p.**



Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	80.30	C22 H21 N O4	[M-H]-	362.1403	362.1398	0.5	1.38	81.07	13.0

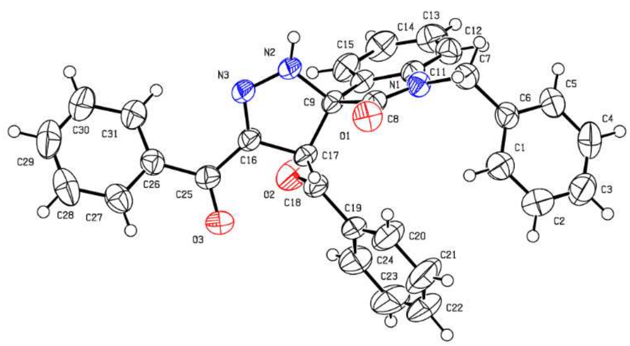
Figure S116. The HRMS spectra of **5q.**

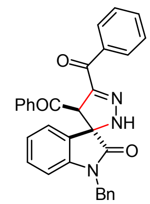


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
2	78.54	C31 H23 N O3	[M+H]+	458.1756	458.1751	0.5	1.09	78.72	21.0

Figure S117. The HRMS spectra of **5r.**

5. X-ray crystal structure of 4t and 5p.



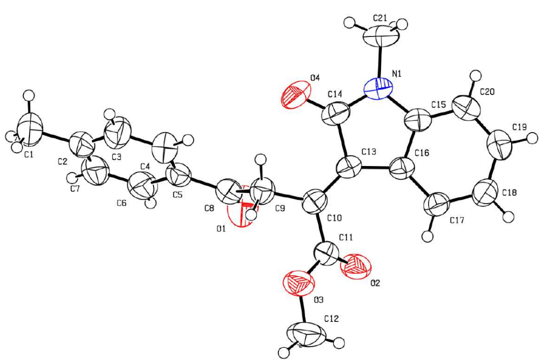


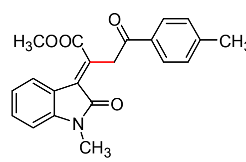
4t

Figure S118. ORTEP diagram of the X-ray crystal structure of **4t**. Platon plot of **4t** (298 k) with thermal ellipsoids at the 50% probability level.

Single crystal of compound **4t** was obtained from the mixed petroleum ether and ethyl acetate (V/V, 5:1). CCDC 1551876 contains the supplementary crystallographic data which can be obtained free of charge from The Cambrige Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data. $C_{31}\,H_{23}\,N_3\,O_3$, M = 485.52, monoclinic, a = 13.431(2) Å, b = 8.930(2) Å, c = 21.363(4) Å, V = 2462.8(7) Å^3.





5p

Figure S119. ORTEP diagram of the X-ray crystal structure of **5p**. Platon plot of **5p** (298 k) with thermal ellipsoids at the 50% probability level.

Single crystal of compound **5p** was obtained from the mixed petroleum ether and ethyl acetate (V/V, 2:1). CCDC 1551878 contains the supplementary crystallographic data which can be obtained free of charge from The Cambrige Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Crystal data. $C_{21}\,H_{19}\,N\,O_4$, M = 349.37, triclinic, a = 8.481(2) Å, b = 8.527(2) Å, c = 13.607(3) Å, V = 893.2(4) Å^3.