Supporting Information

Ir(III)-Catalyzed C-H Functionalization of Triphenylphosphine Oxide Towards 3-Aryl Oxindoles

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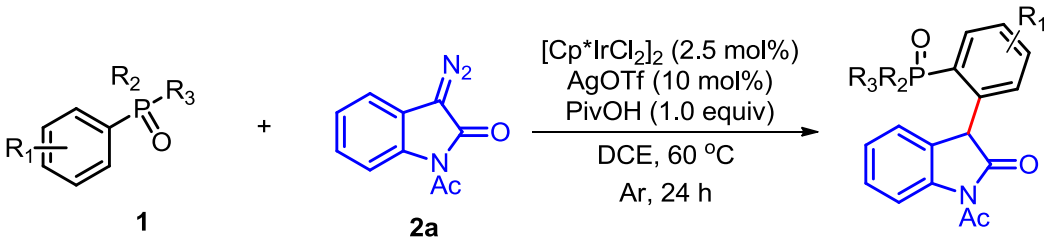
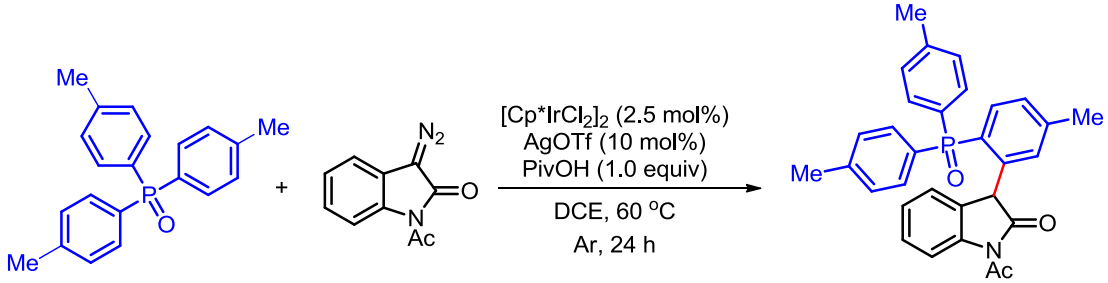
1. Scope of Phosphine oxides



entry	R_1	R_2	R_3	yield (%)
1	4-MeC_6H_4	4-MeC_6H_4	4-MeC_6H_4	n. r.
2	3- MeC_6H_4	3- MeC_6H_4	3- MeC_6H_4	n. r.
3	2- MeC_6H_4	2- MeC_6H_4	2- MeC_6H_4	n. r.
4	4,6-dimethoxyphenyl	4,6-dimethoxyphenyl	4,6-dimethoxyphenyl	n. r.
5	4-FC_6H_4	4-FC_6H_4	4-FC_6H_4	n. r.
6	4-ClC_6H_4	4-ClC_6H_4	4-ClC_6H_4	n. r.
7	4-BrC_6H_4	4-BrC_6H_4	4-BrC_6H_4	n. r.
8	4-$CF_3C_6H_4$	4-$CF_3C_6H_4$	4-$CF_3C_6H_4$	n. r.
9	2-naphthyl	2-naphthyl	2-naphthyl	n. r.
10	Ph	Me	Me	n. r.
11	Ph	C_6H_{11}	C_6H_{11}	n. r.
12	thienyl	thienyl	thienyl	n. r.

Reaction conditions: phosphine oxides (0.4 mmol), $[Cp^*IrCl_2]_2$ (2.5 mol%), AgOTf (10 mol%), PivOH (0.2 mmol), were carried out in 0.5 mL DCE under Ar atmosphere and stirred at 60 °C oil bath for 15 min, **2a** (0.2 mmol) was dissolved in 1.5 mL DCE and added over 6 h using a peristaltic pump.

2. Conditions screening



2a

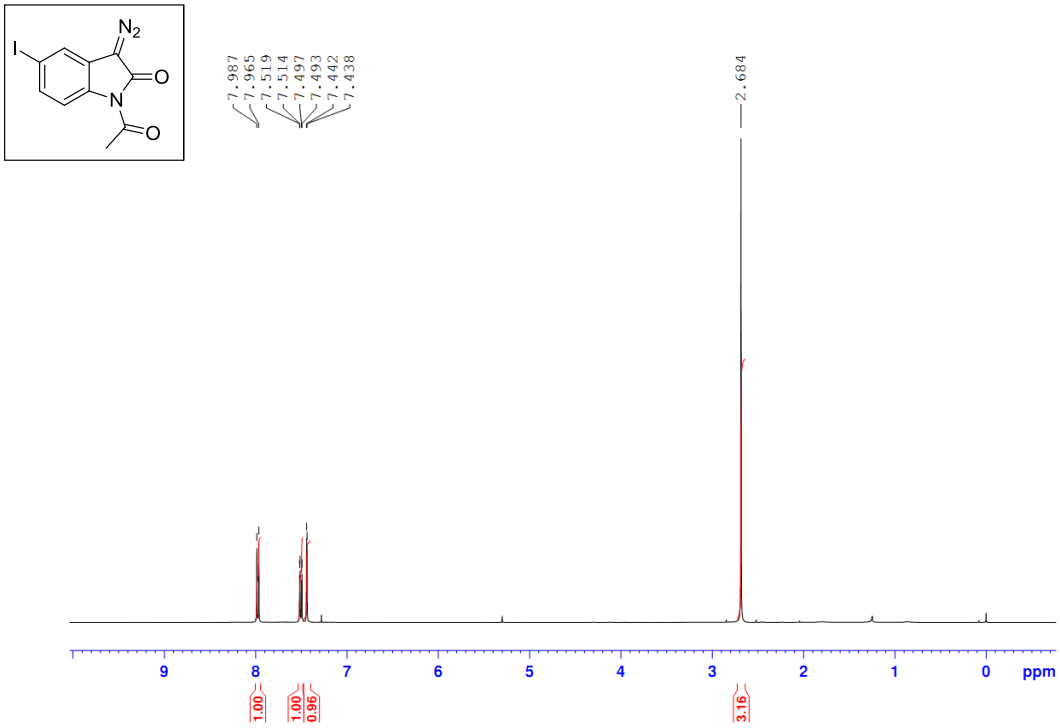
entry	Change conditions	Yield (%)[c]
1	none	0
2	$[Cp^*RhCl_2]_2$ instead of $[Cp^*IrCl_2]_2$	0
3	$AgSbF_6$ instead of AgOTf	0
4	$AgNTf_2$ instead of AgOTf	0
5	$AgPF_6$ instead of AgOTf	0
6	$AgBF_4$ instead of AgOTf	0
7	$AdCO_2H$ instead of PivOH	0
8	TMBzOH instead of PivOH	0
9	in THF	0
10	in Toluene	0
11	in 1,4-dioxane	0
12	in DME	0
13	80 °C instead of 60 °C	0
14	100 °C instead of 60 °C	0

Reaction conditions: tris(4-fluorophenyl)phosphine oxide (0.4 mmol), catalyst (2.5 mol%), silver salt (10 mol%), acid (0.2 mmol), were carried out in 0.5 mL solvent under Ar atmosphere and stirred at 60 °C oil bath for 15 min, **2a** (0.2 mmol) was dissolved in 1.5 mL solvent and added over 6 h using a peristaltic pump.

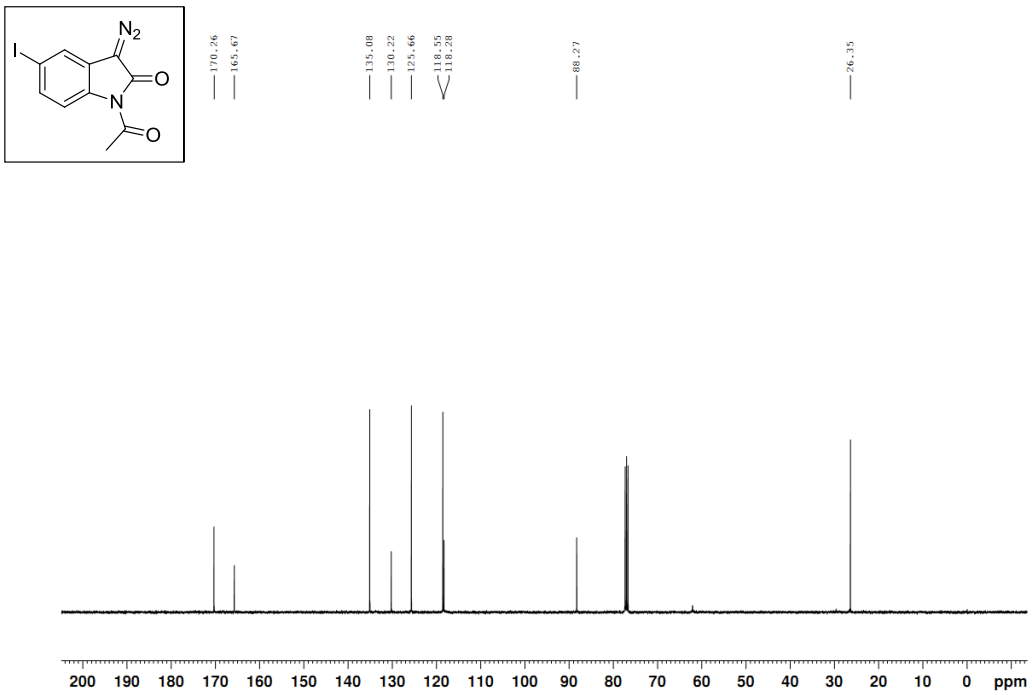
We added tris(4-methylphenyl)phosphine oxide to the reaction and screened a series of reaction conditions. However, experimental results show that undesired product was obtained.

3. NMR Data

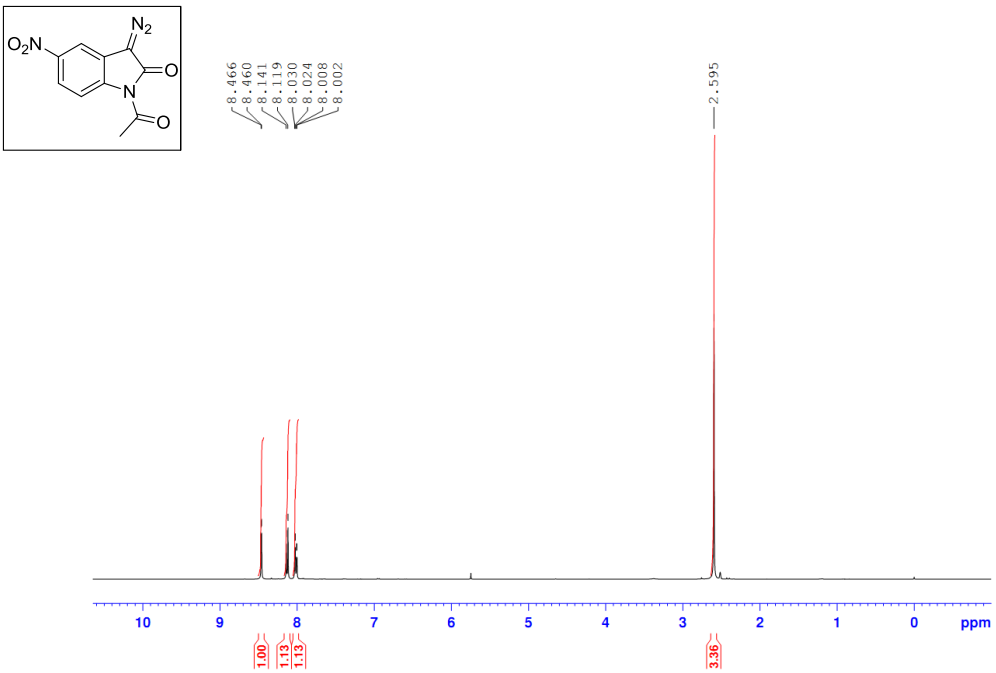
1-Acetyl-3-diazo-5-iodoindolin-2-one (2g) ^{1}H NMR (400 MHz, $CDCl_3$)



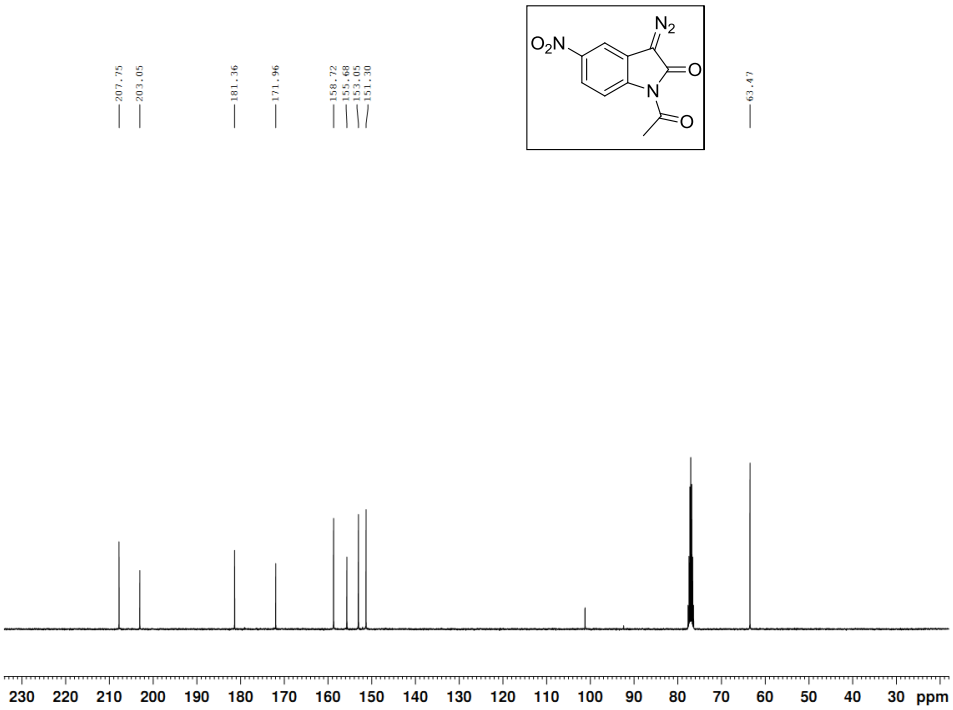
1-Acetyl-3-diazo-5-iodoindolin-2-one (2g) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



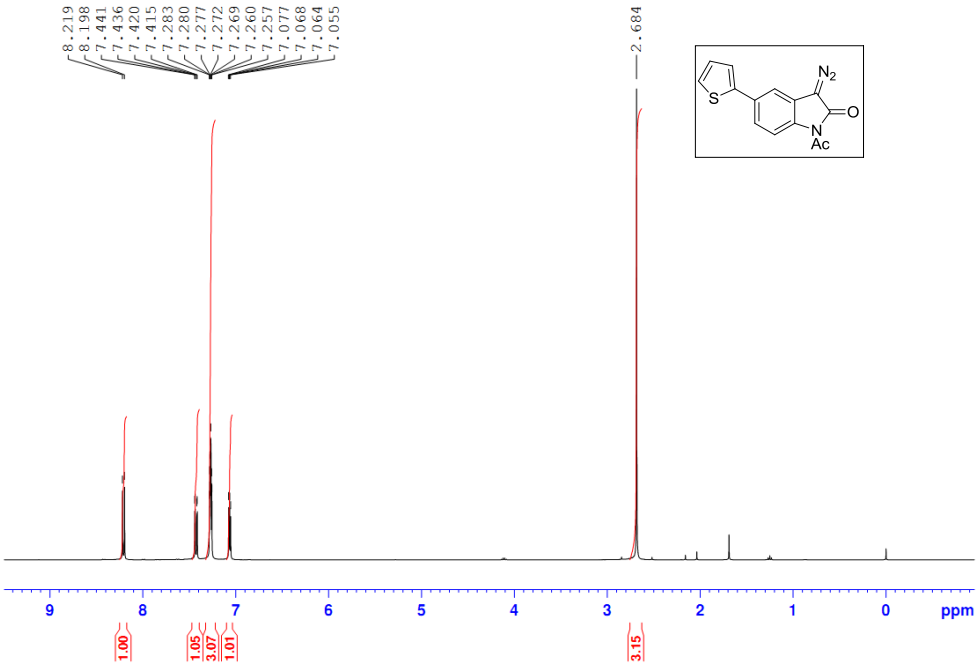
1-Acetyl-3-diazo-5-nitroindolin-2-one (2h) ^{1}H NMR (400 MHz, DMSO-*d6*)



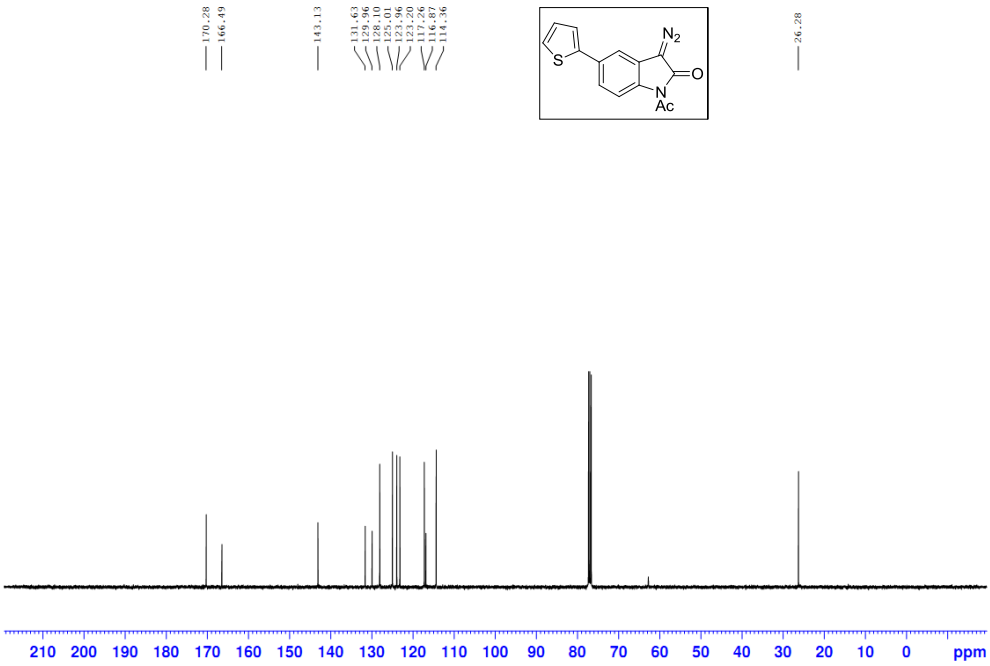
1-Acetyl-3-diazo-5-nitroindolin-2-one (2h) ^{13}C{^{1}H} NMR (100 MHz, DMSO-*d6*)



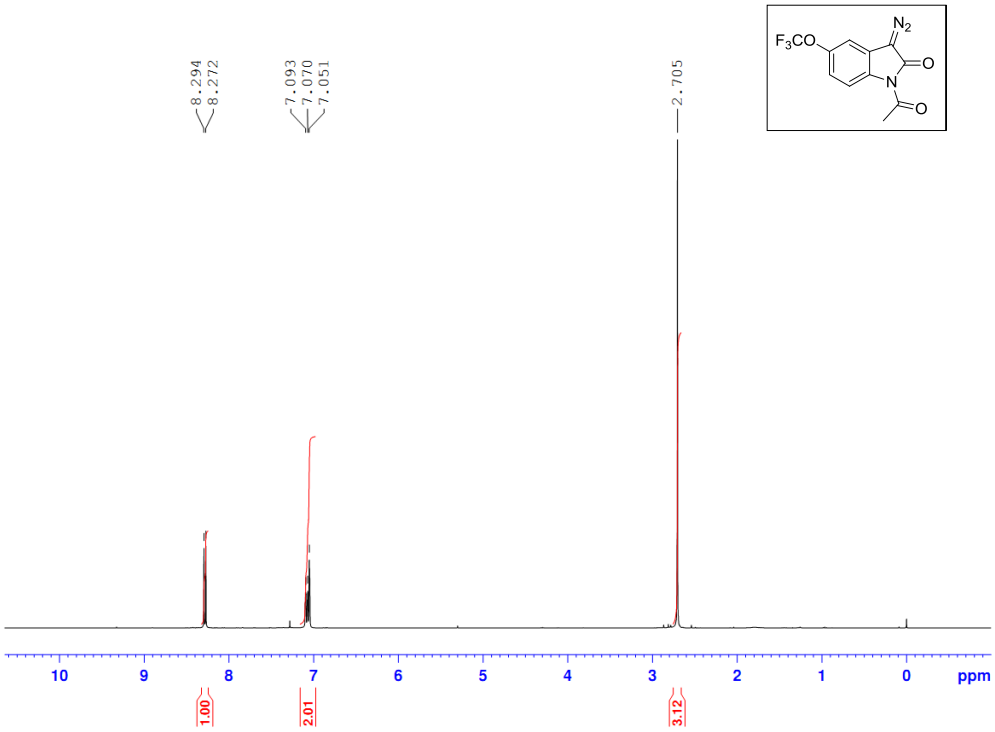
1-Acetyl-3-diazo-5-(thiophen-2-yl)indolin-2-one (2i) ^{1}H NMR (400 MHz, $CDCl_3$)



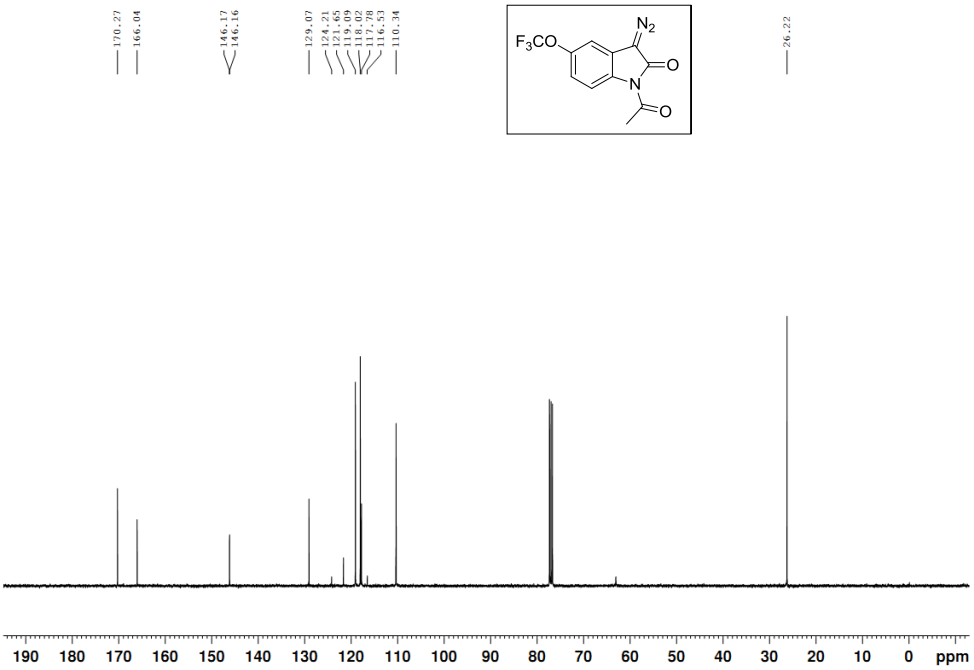
1-Acetyl-3-diazo-5-(thiophen-2-yl)indolin-2-one (2i) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



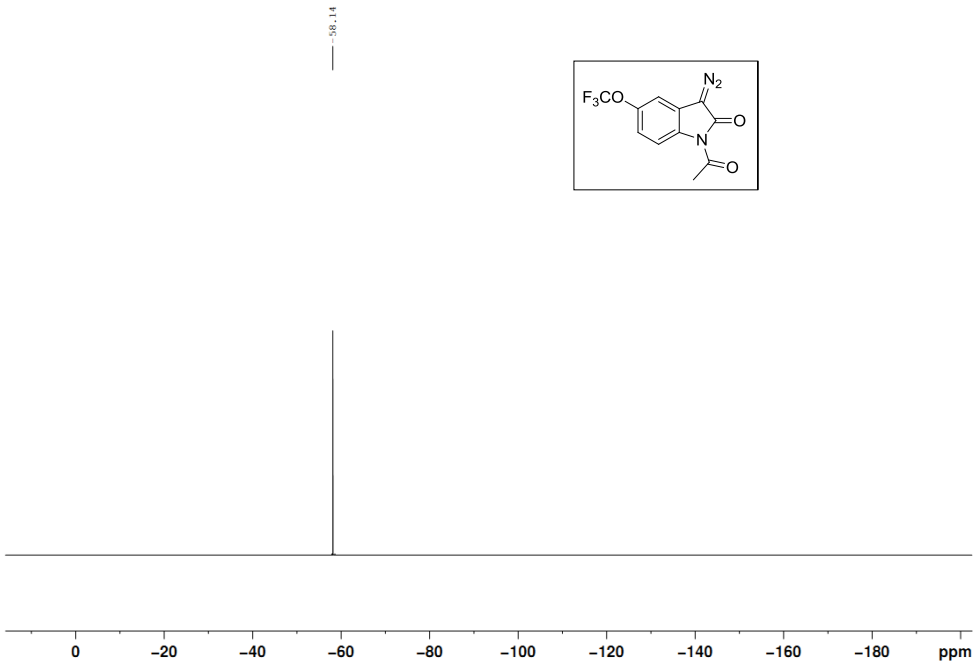
1-Acetyl-3-diazo-5-(trifluoromethoxy)indolin-2-one (2j) ^{1}H NMR (400 MHz, $CDCl_3$)



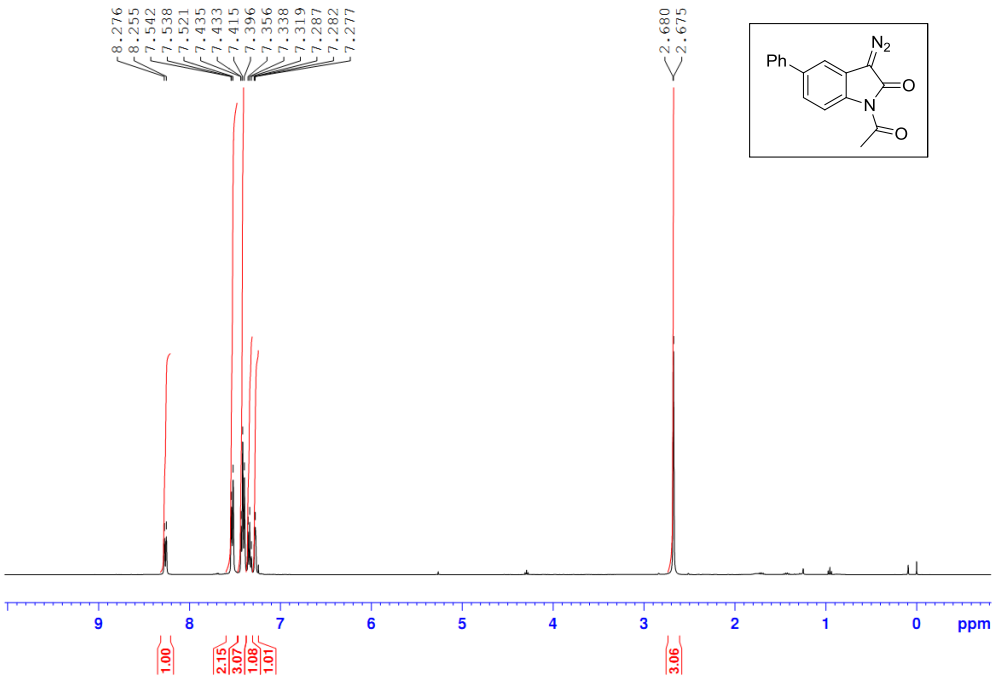
1-Acetyl-3-diazo-5-(trifluoromethoxy)indolin-2-one (2j) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



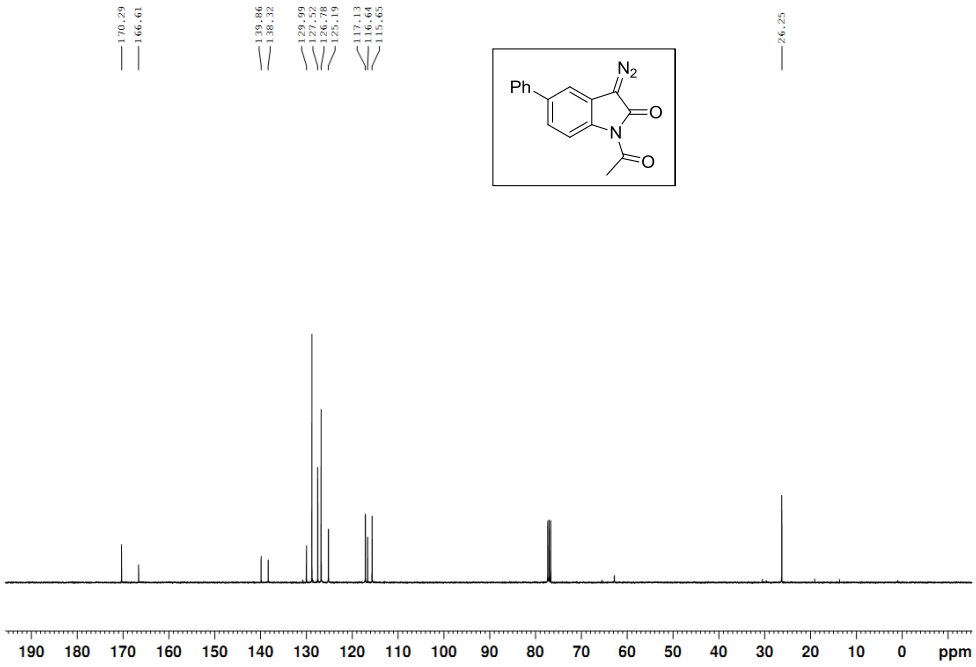
1-Acetyl-3-diazo-5-(trifluoromethoxy)indolin-2-one (2j) ^{19}F NMR (376 MHz, $CDCl_3$)



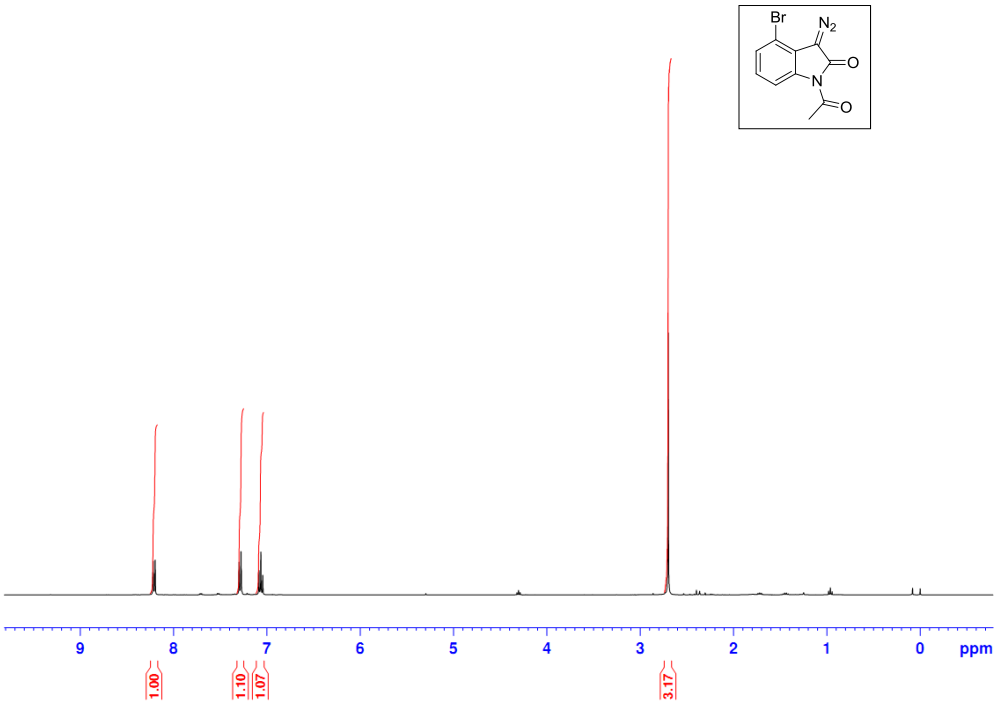
1-Acetyl-3-diazo-5-phenylindolin-2-one (2k) ^{1}H NMR (400 MHz, $CDCl_3$)



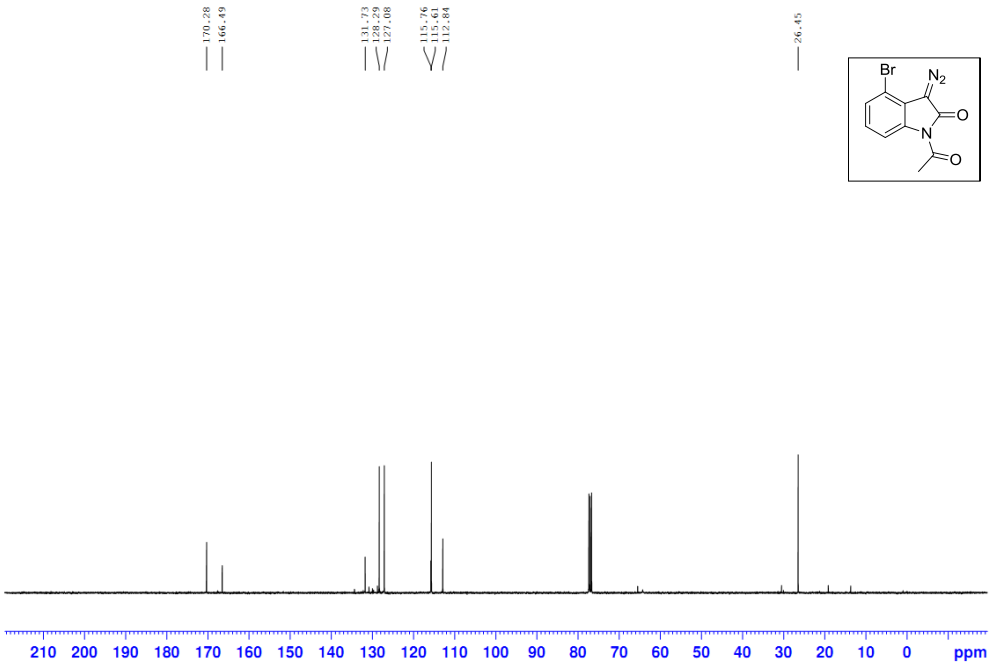
1-Acetyl-3-diazo-5-phenylindolin-2-one (2k) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



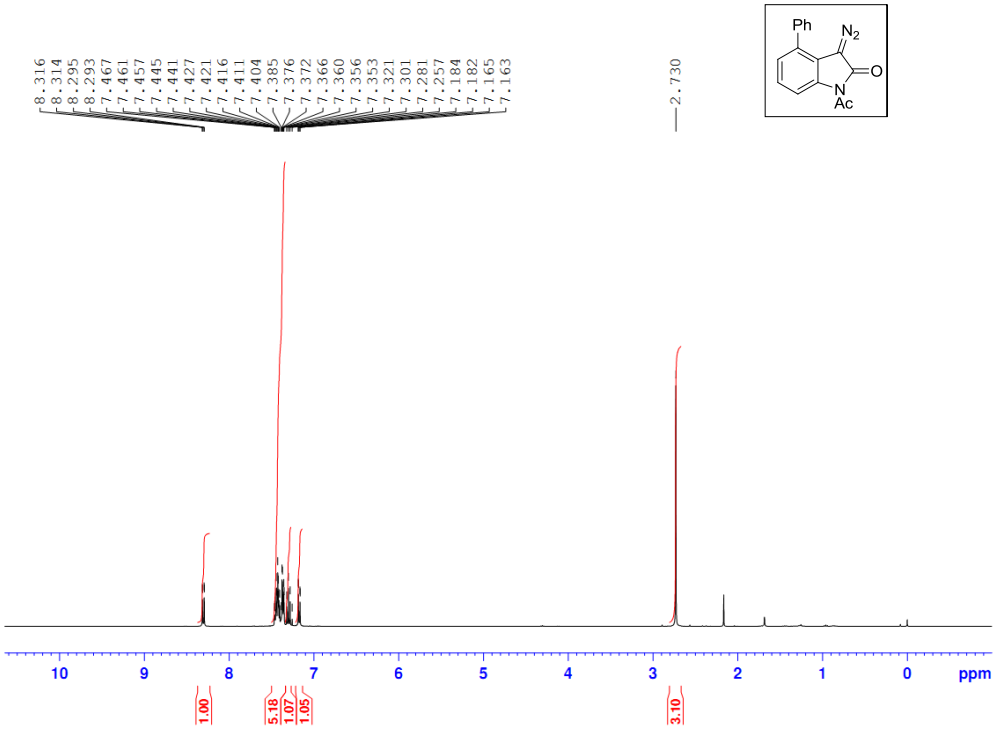
1-Acetyl-4-bromo-3-diazoindolin-2-one (2l) ^{1}H NMR (400 MHz, $CDCl_3$)



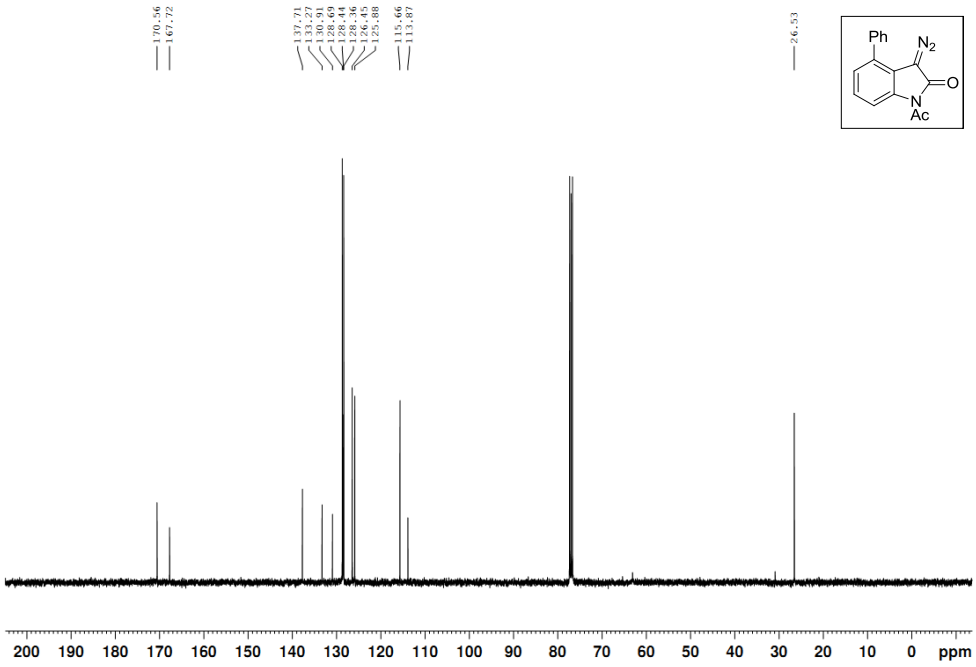
1-Acetyl-4-bromo-3-diazoindolin-2-one (2l) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



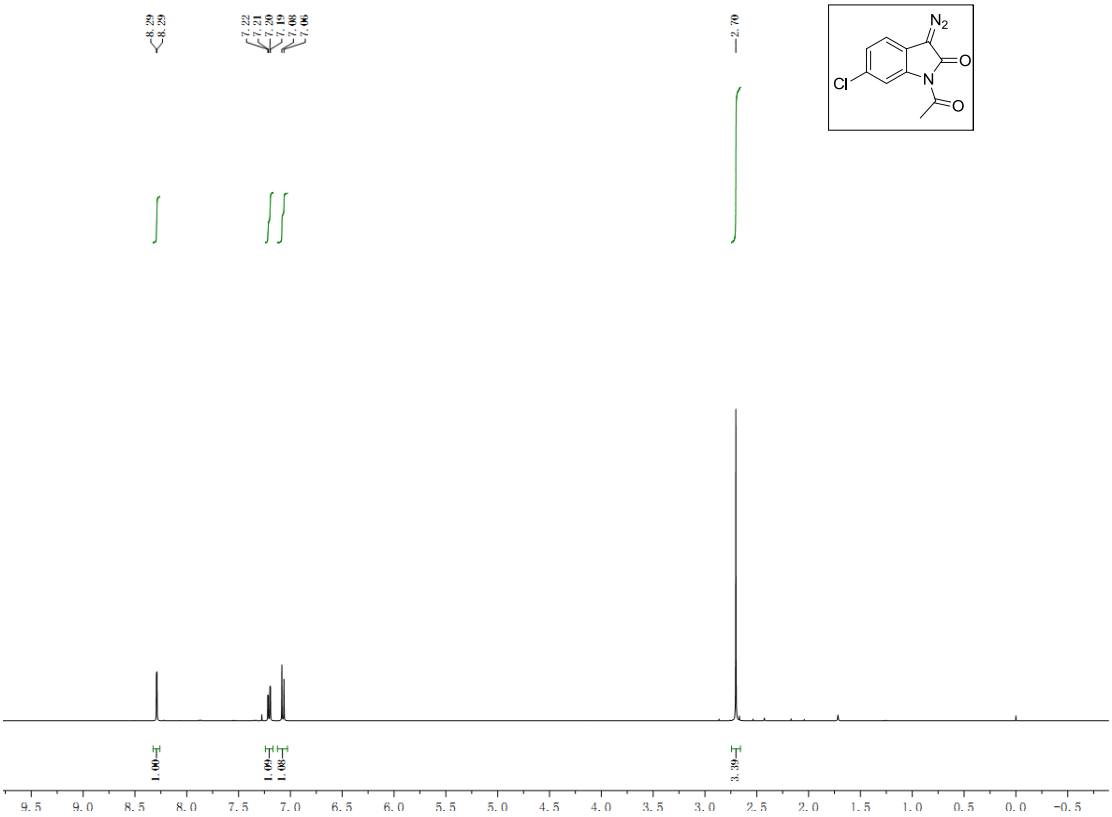
1-Acetyl-3-diazo-4-phenylindolin-2-one (2m) ^{1}H NMR (400 MHz, $CDCl_3$)



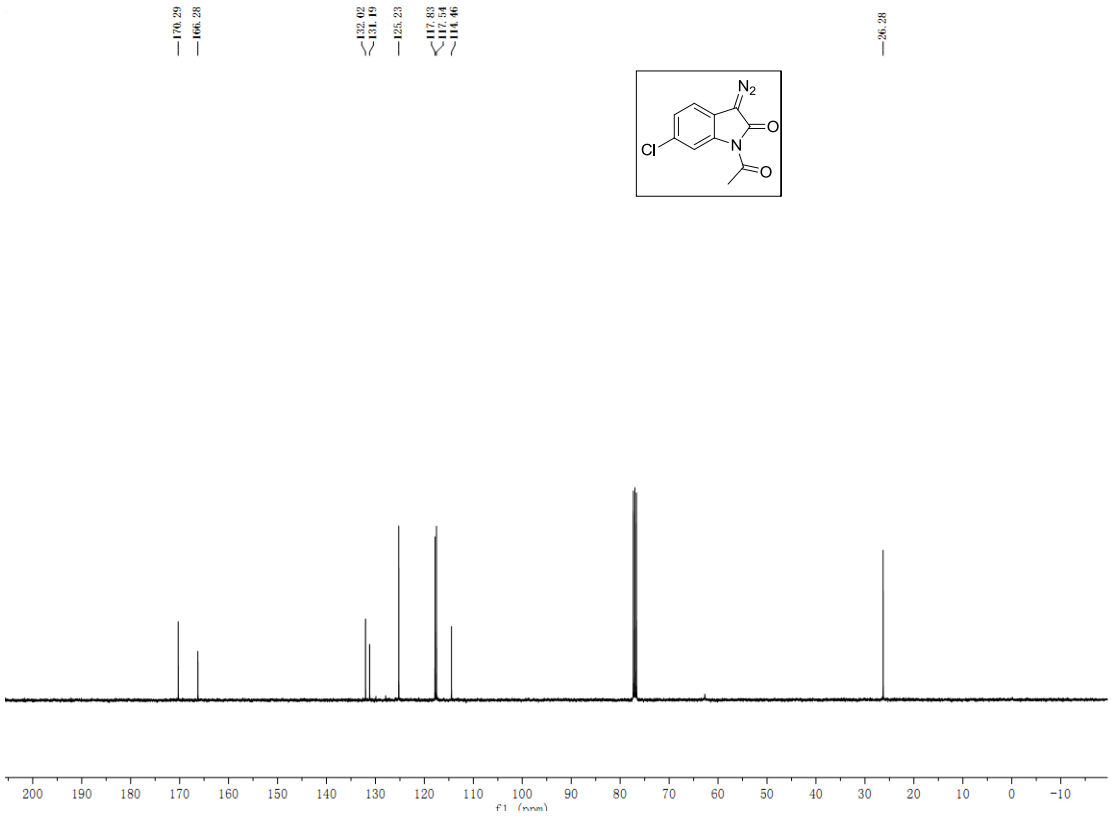
1-Acetyl-3-diazo-4-phenylindolin-2-one (2m) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



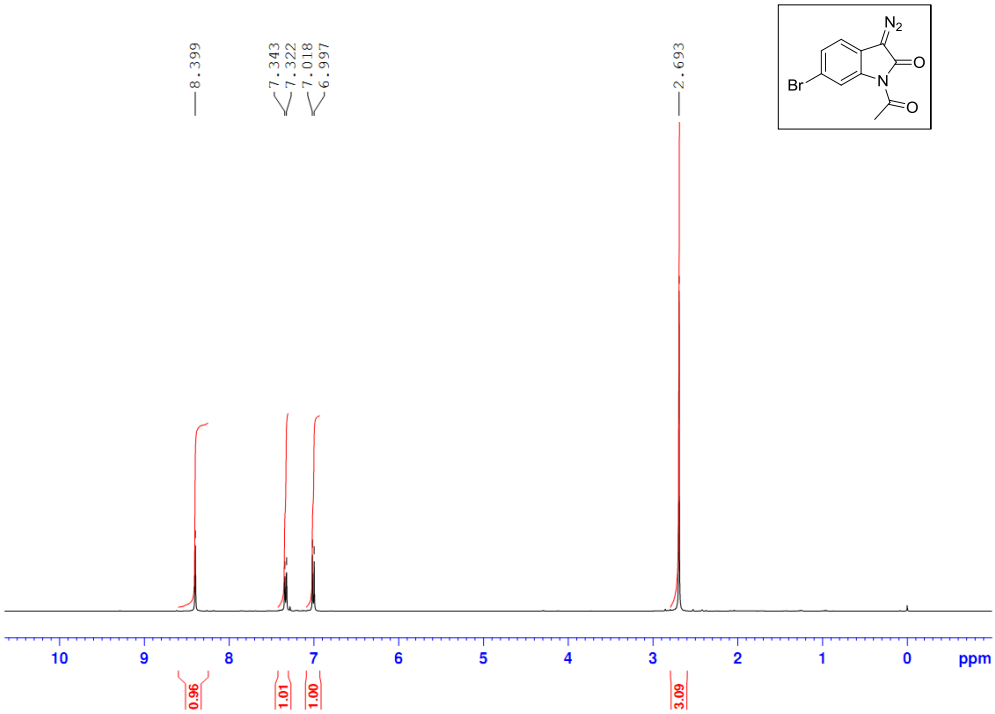
1-Acetyl-6-chloro-3-diazoindolin-2-one (2n) ^{1}H NMR (400 MHz, $CDCl_3$)



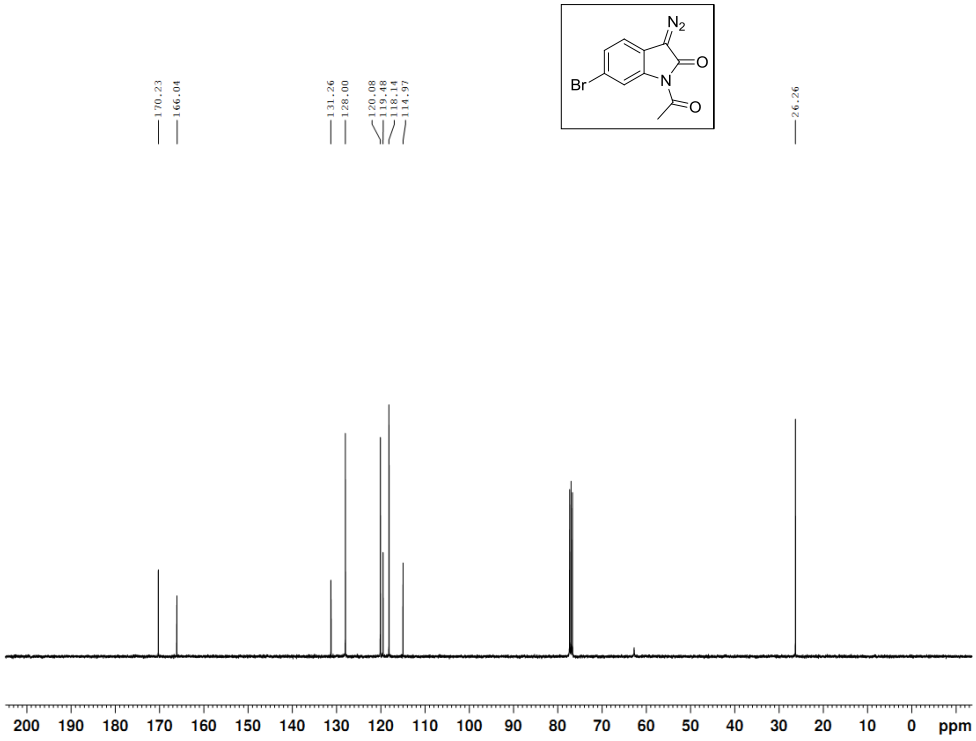
1-Acetyl-6-chloro-3-diazoindolin-2-one (2n) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



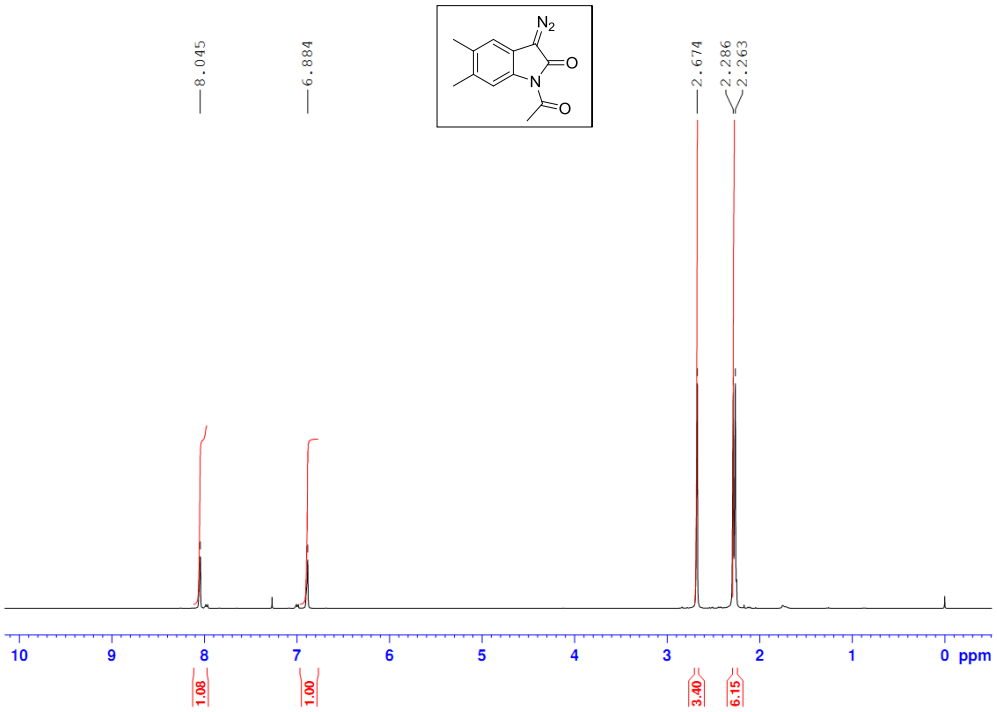
1-Acetyl-6-bromo-3-diazoindolin-2-one (2o) ^{1}H NMR (400 MHz, $CDCl_3$)



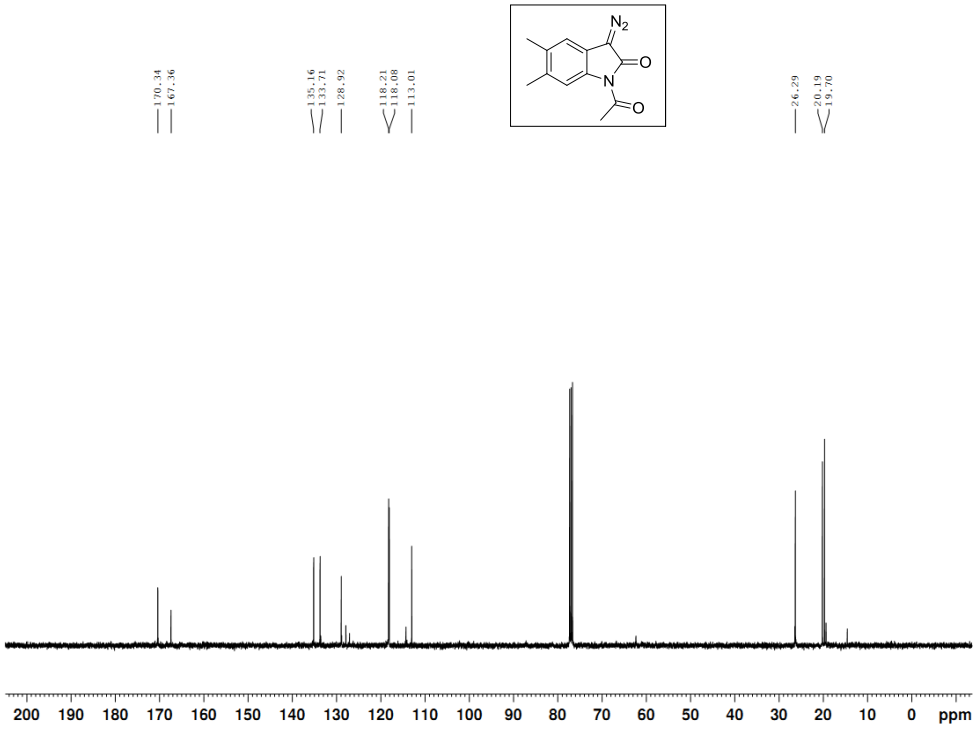
1-Acetyl-6-bromo-3-diazoindolin-2-one (2o) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



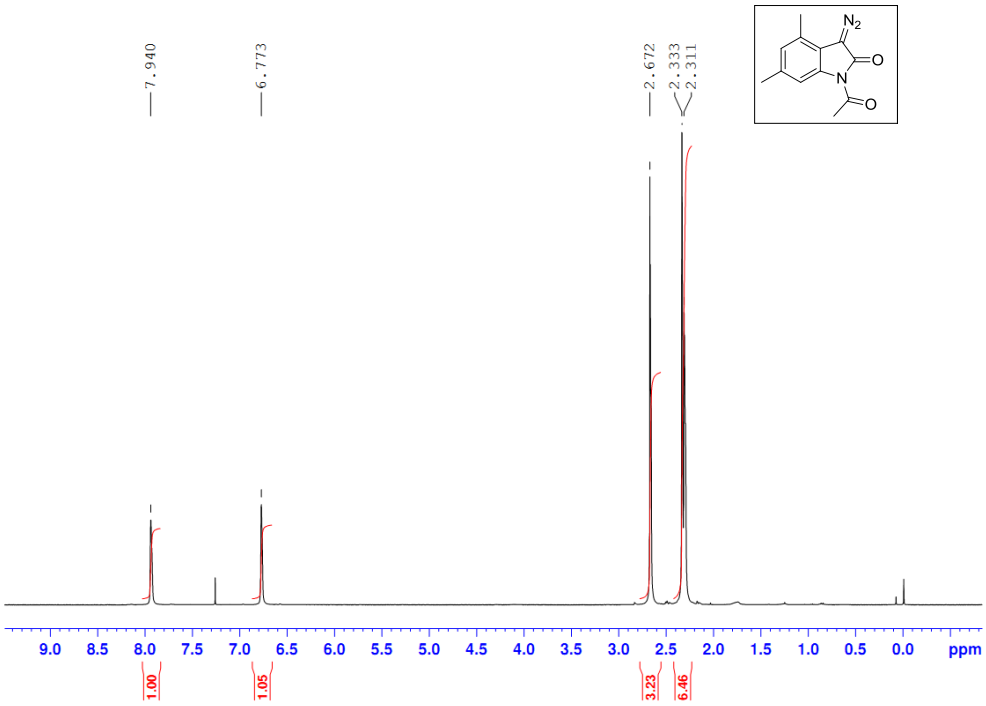
1-Acetyl-3-diazo-5,6-dimethylindolin-2-one (2r) ^{1}H NMR (400 MHz, $CDCl_3$)



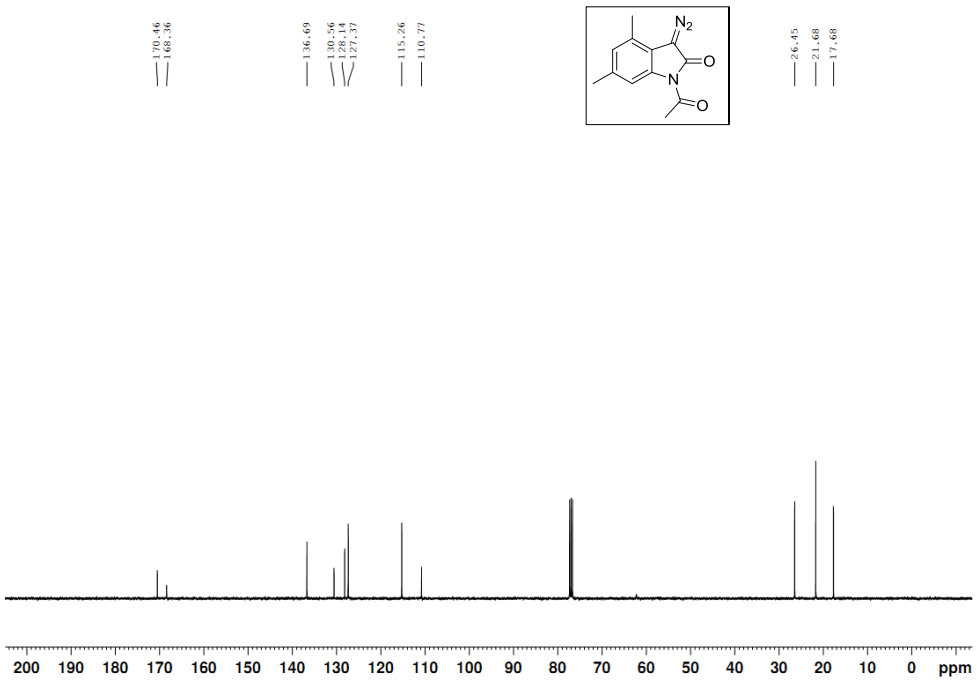
1-Acetyl-3-diazo-5,6-dimethylindolin-2-one (2r) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



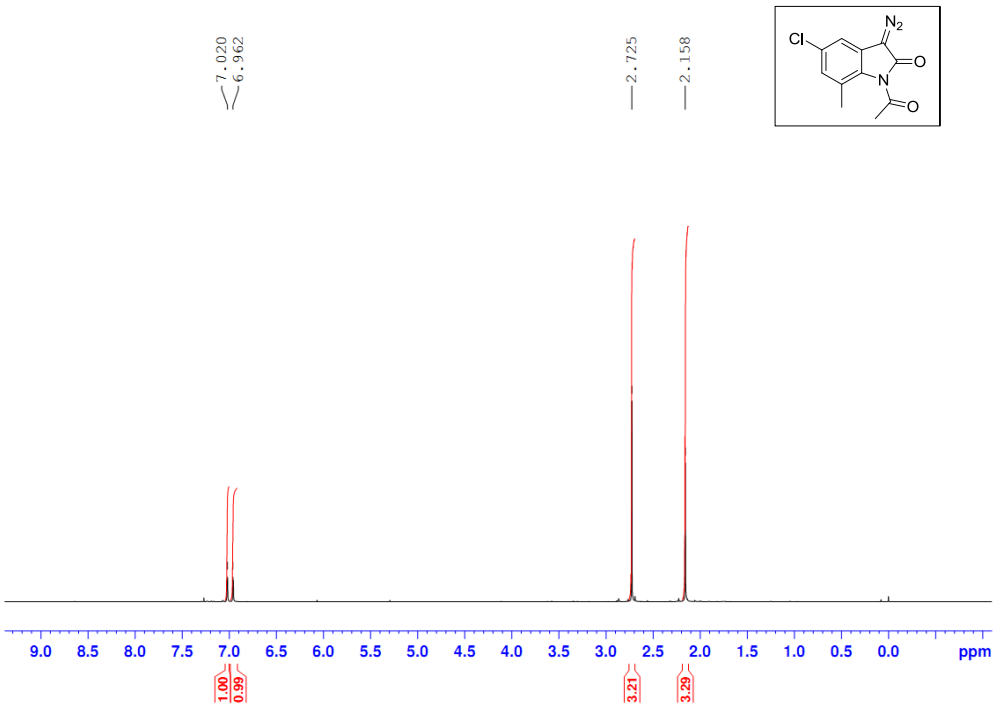
1-Acetyl-3-diazo-4,6-dimethylindolin-2-one (2s) ^{1}H NMR (400 MHz, $CDCl_3$)



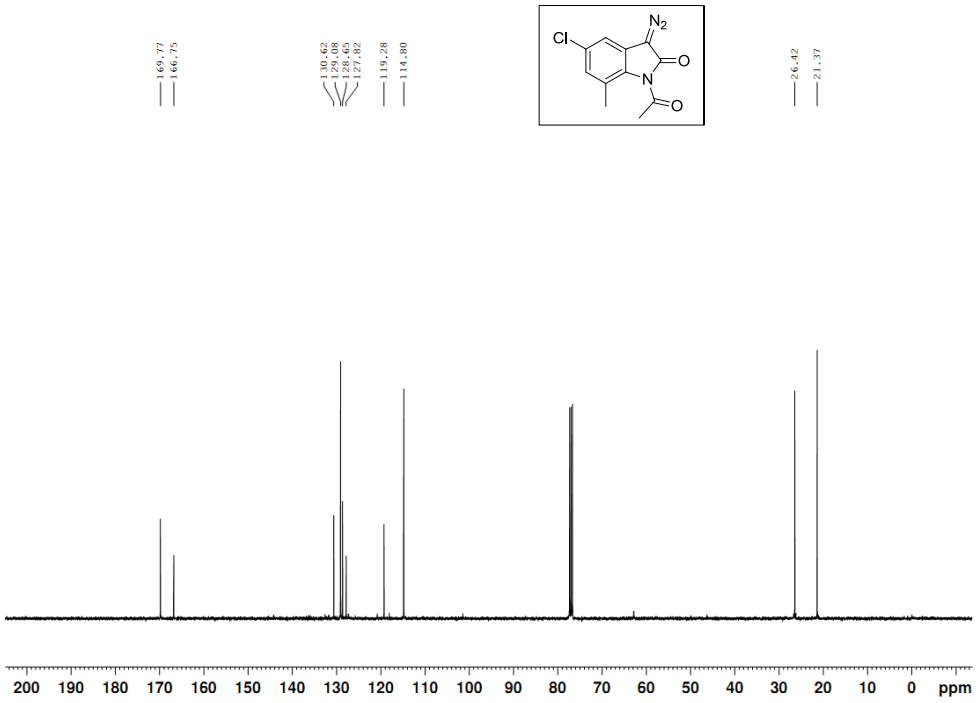
1-Acetyl-3-diazo-4,6-dimethylindolin-2-one (2s) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



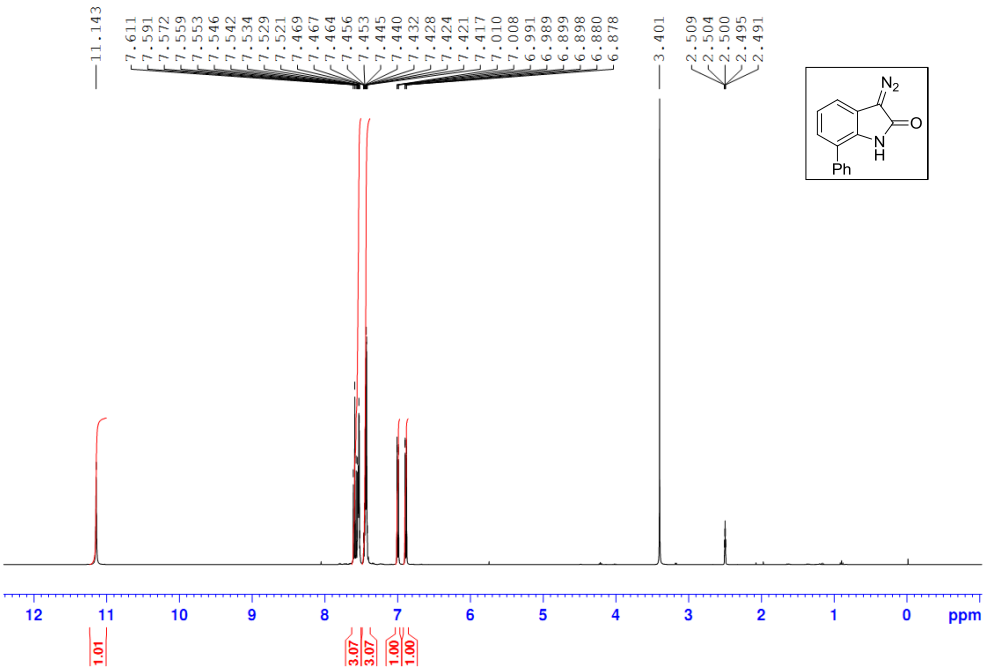
1-Acetyl-5-chloro-3-diazo-7-methylindolin-2-one (2t) ^{1}H NMR (400 MHz, $CDCl_3$)



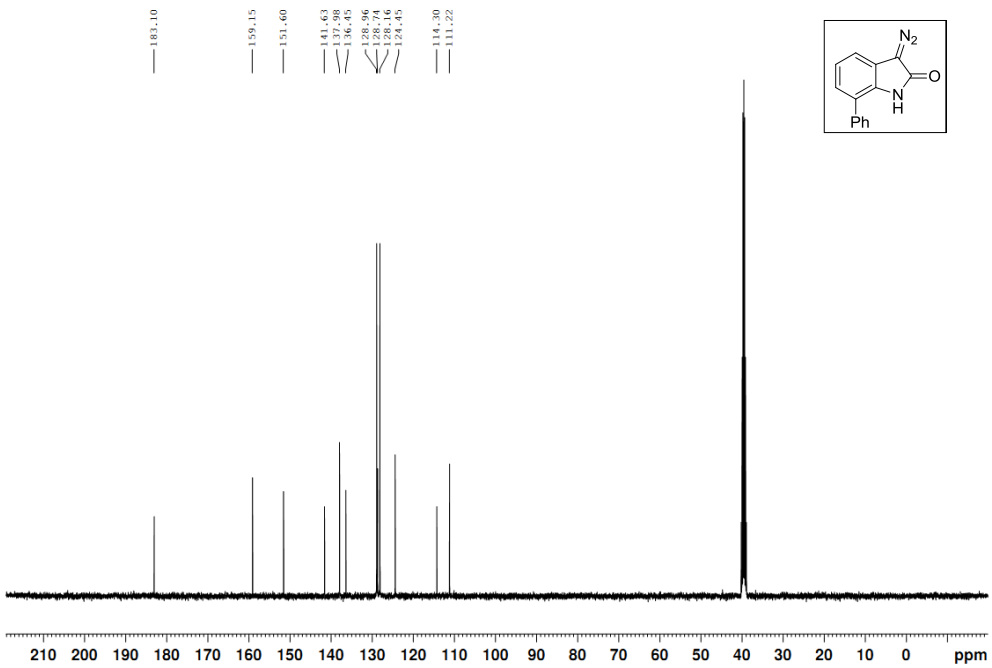
1-Acetyl-5-chloro-3-diazo-7-methylindolin-2-one (2t) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



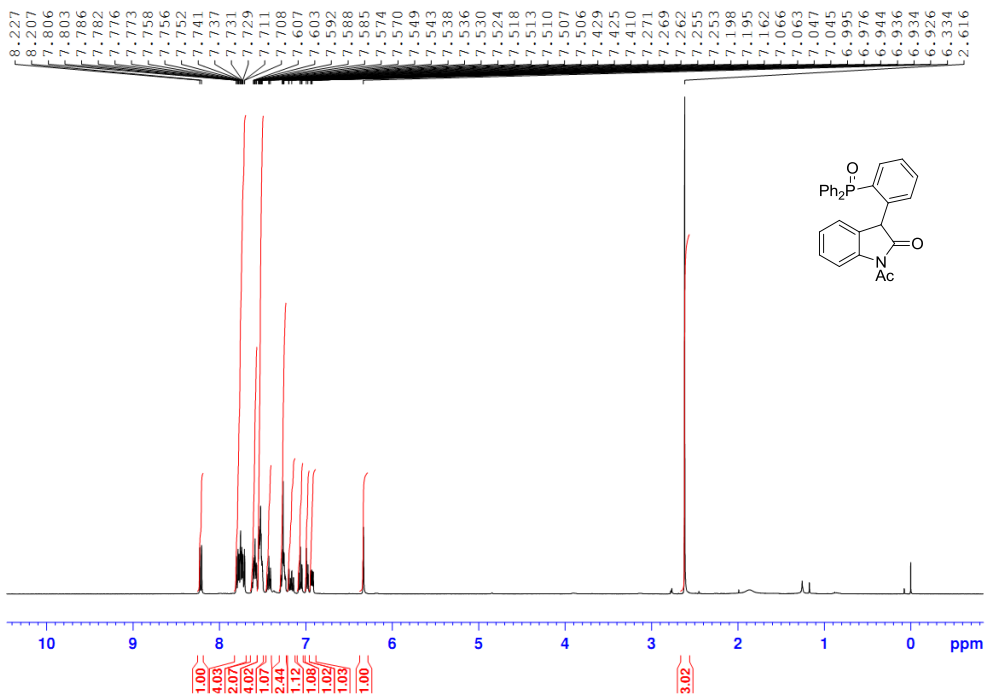
3-Diazo-7-phenylindolin-2-one (4b) ^{1}H NMR (400 MHz, DMSO-*d6*)



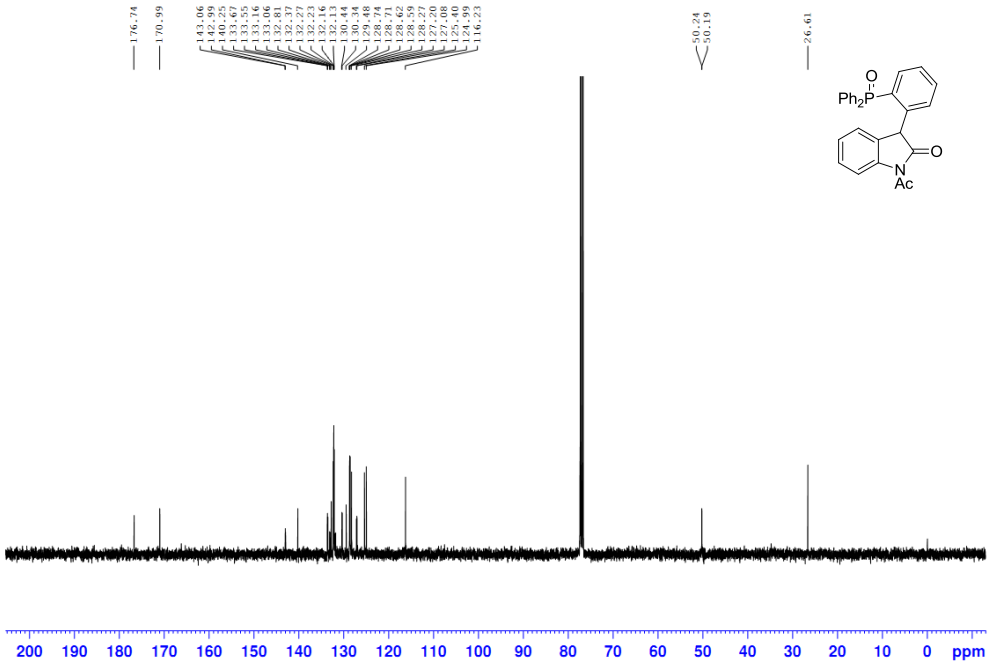
3-Diazo-7-phenylindolin-2-one (4b) $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-*d6*)



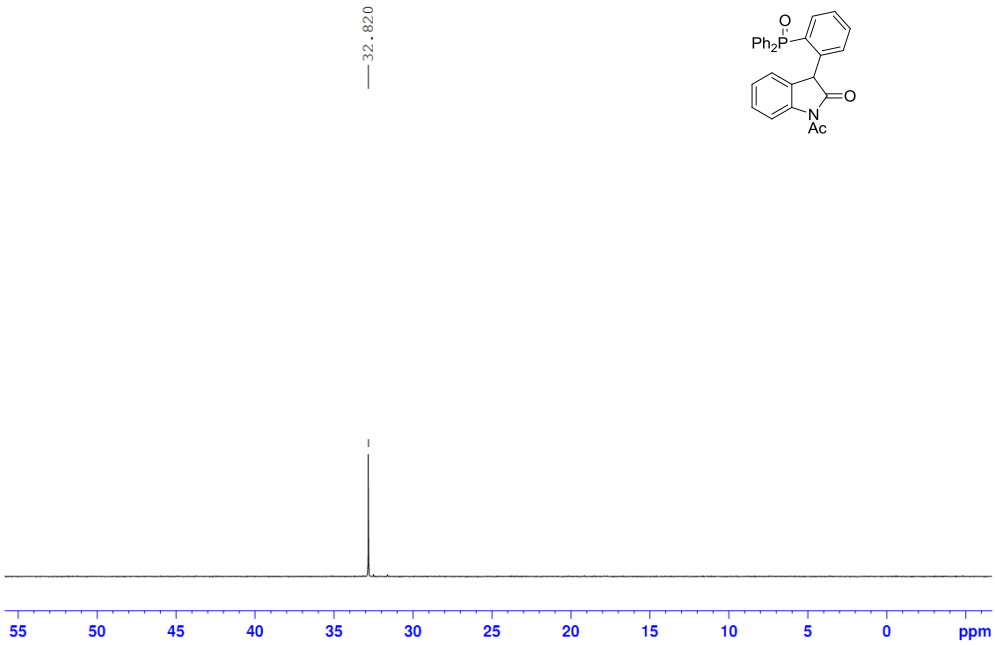
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3a) ^{1}H NMR (400 MHz, $CDCl_3$)



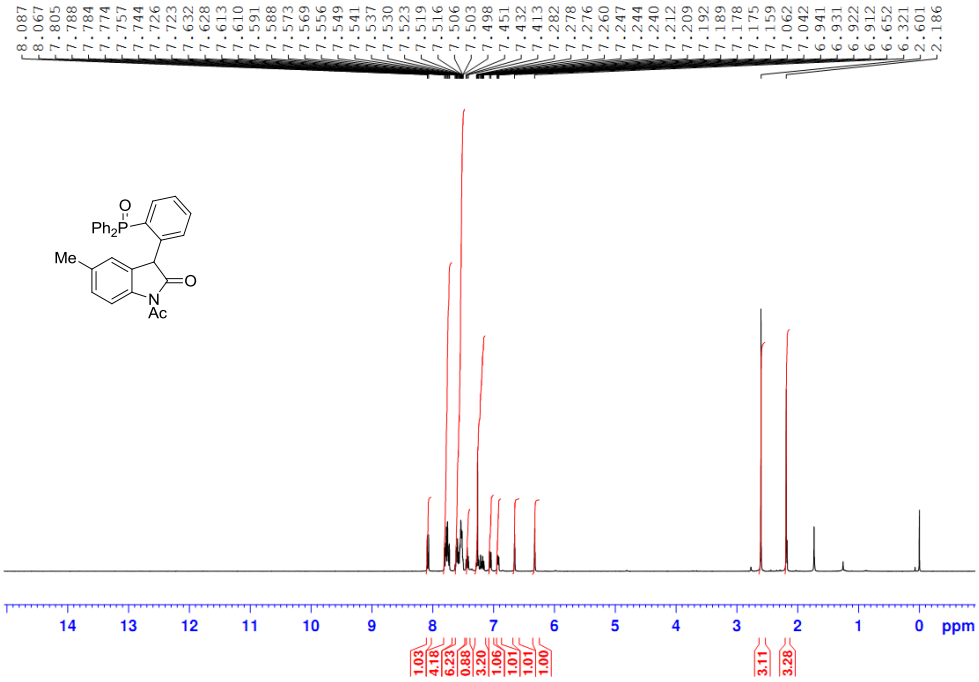
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3a) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



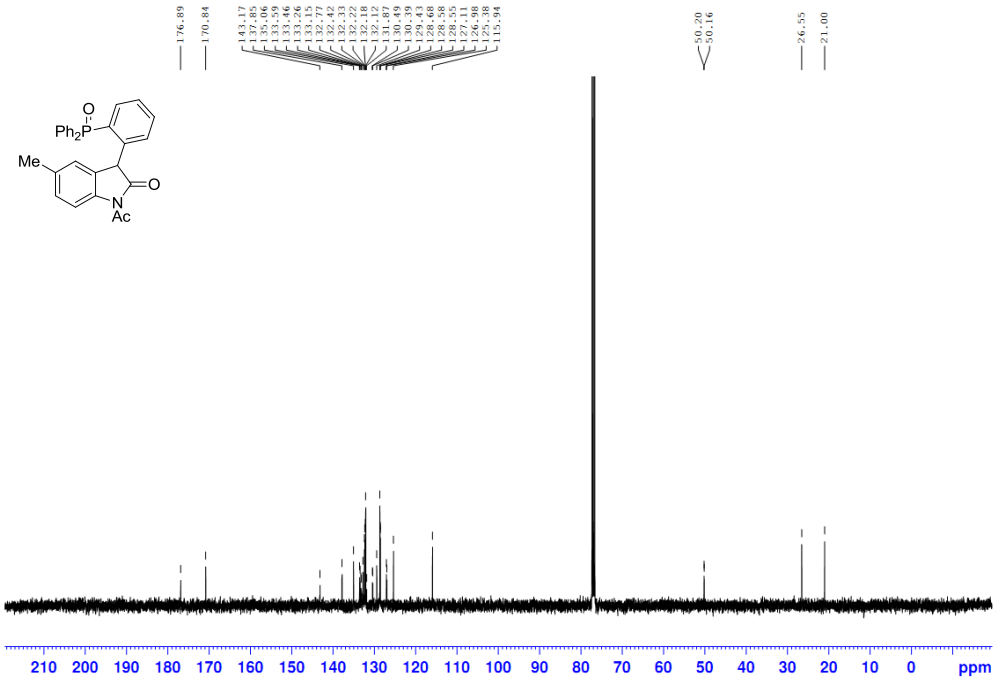
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3a) ^{31}P NMR (162 MHz, $CDCl_3$)



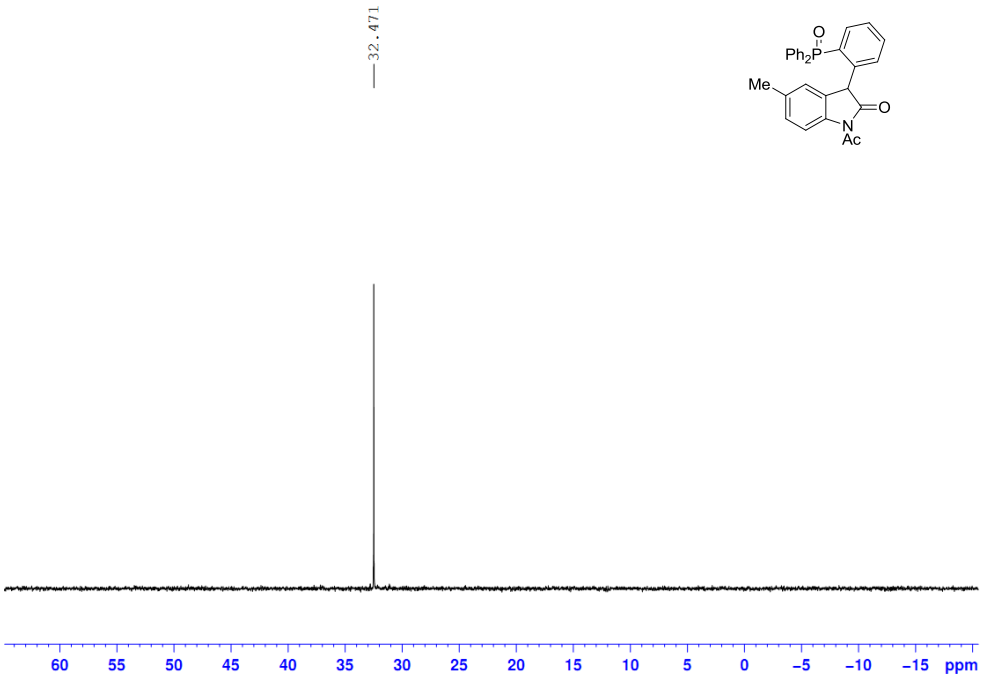
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-methylindolin-2-one (3b) ^{1}H NMR (400 MHz, $CDCl_3$)



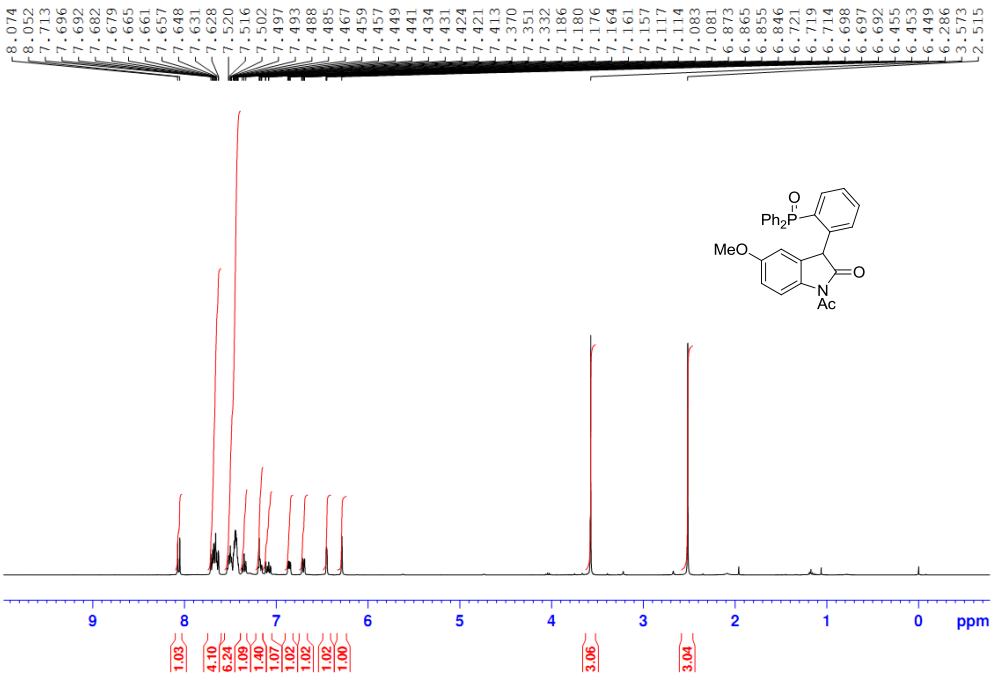
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-methylindolin-2-one (3b) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



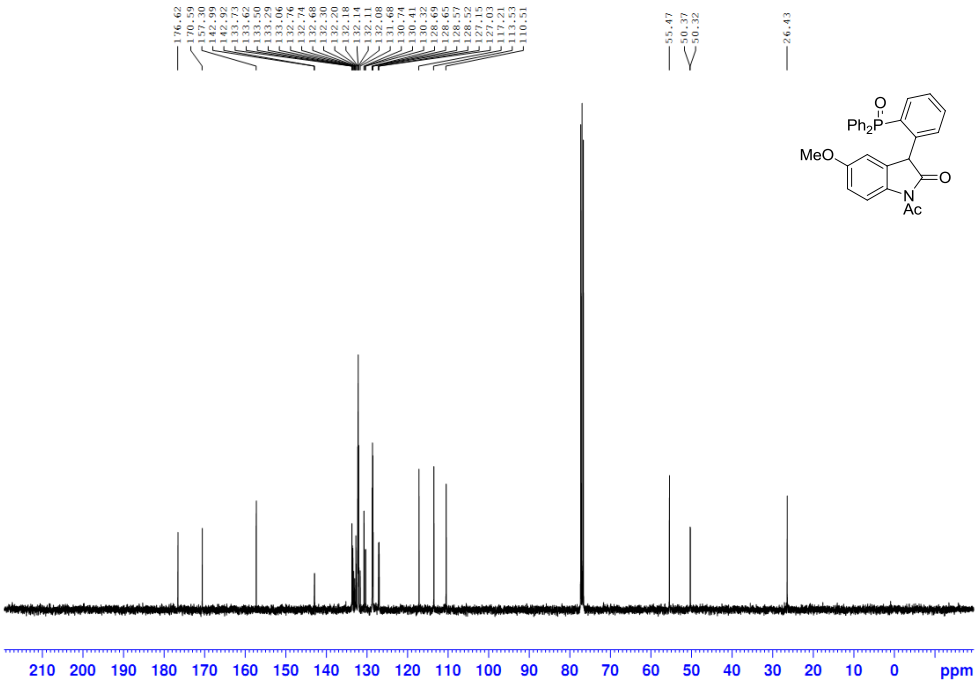
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-methylindolin-2-one (3b) ^{31}P NMR (162 MHz, $CDCl_3$)



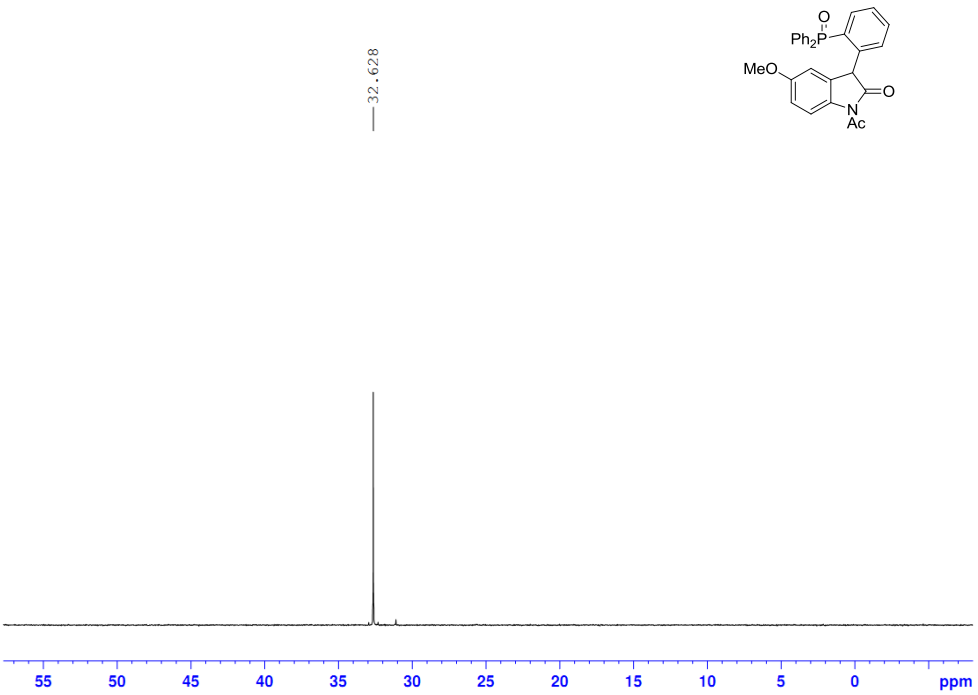
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-methoxyindolin-2-one (3c) ^{1}H NMR (400 MHz, $CDCl_3$)



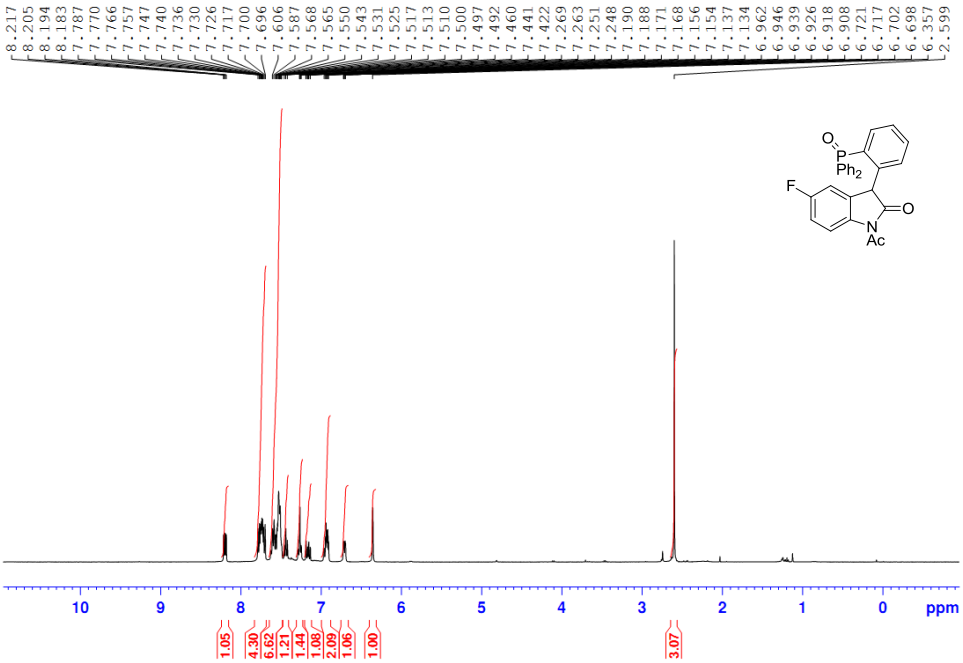
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-methoxyindolin-2-one (3c) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



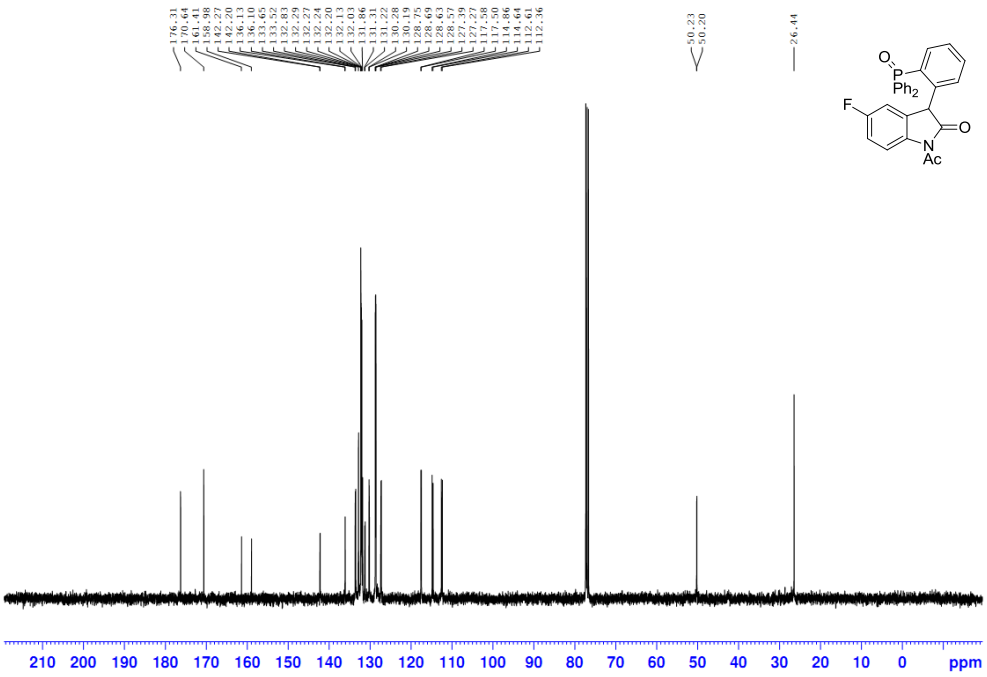
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-methoxyindolin-2-one (3c) ^{31}P NMR (162 MHz, $CDCl_3$)



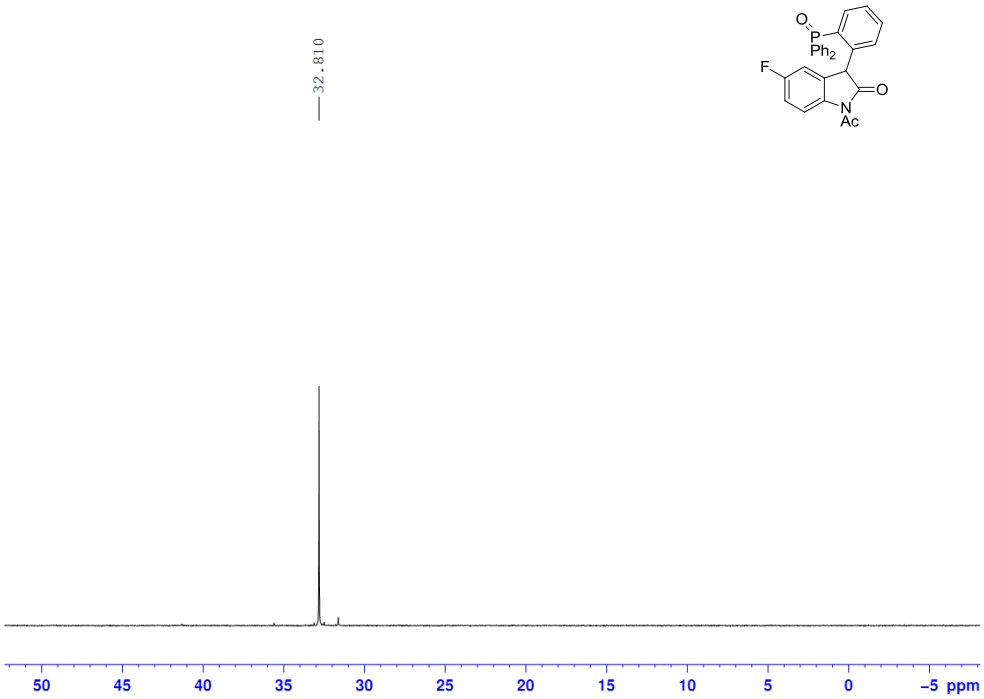
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-fluoroindolin-2-one (3d) ^{1}H NMR (400 MHz, $CDCl_3$)



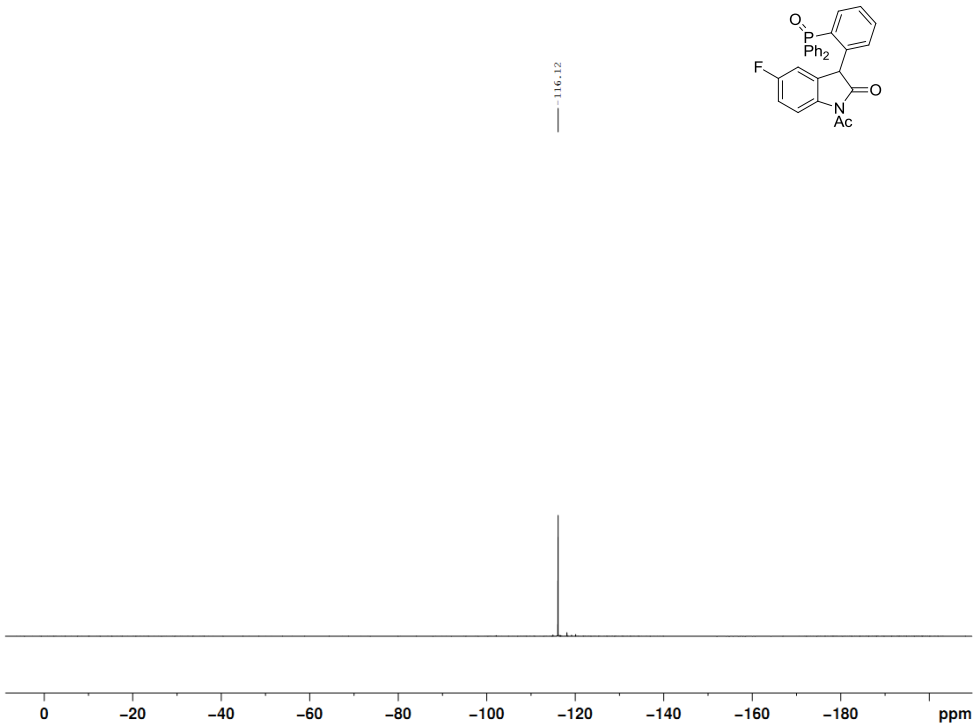
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-fluoroindolin-2-one (3d) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



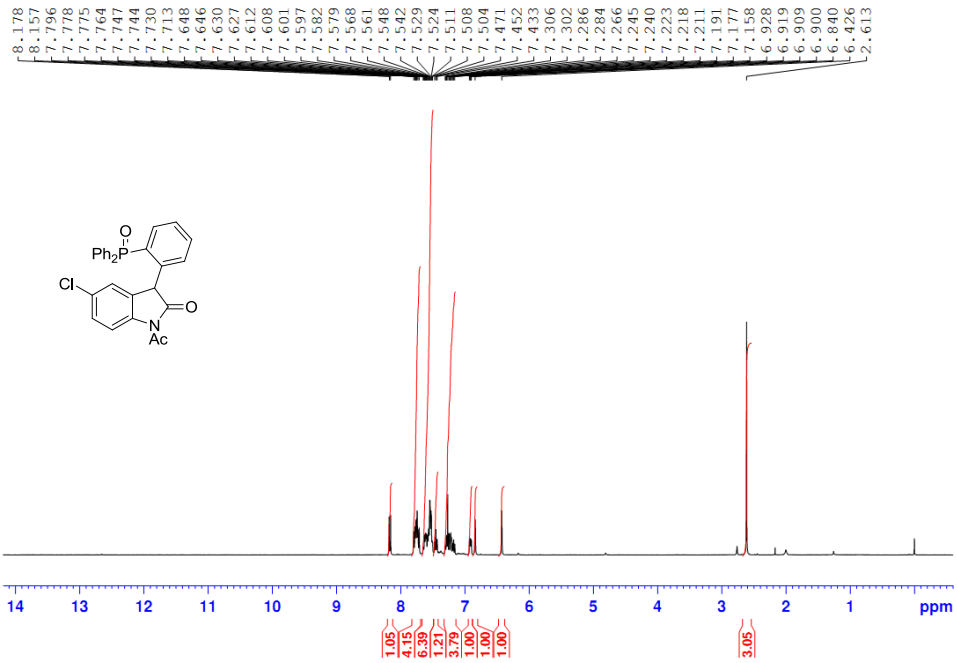
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-fluoroindolin-2-one (3d) ^{31}P NMR (162 MHz, $CDCl_3$)



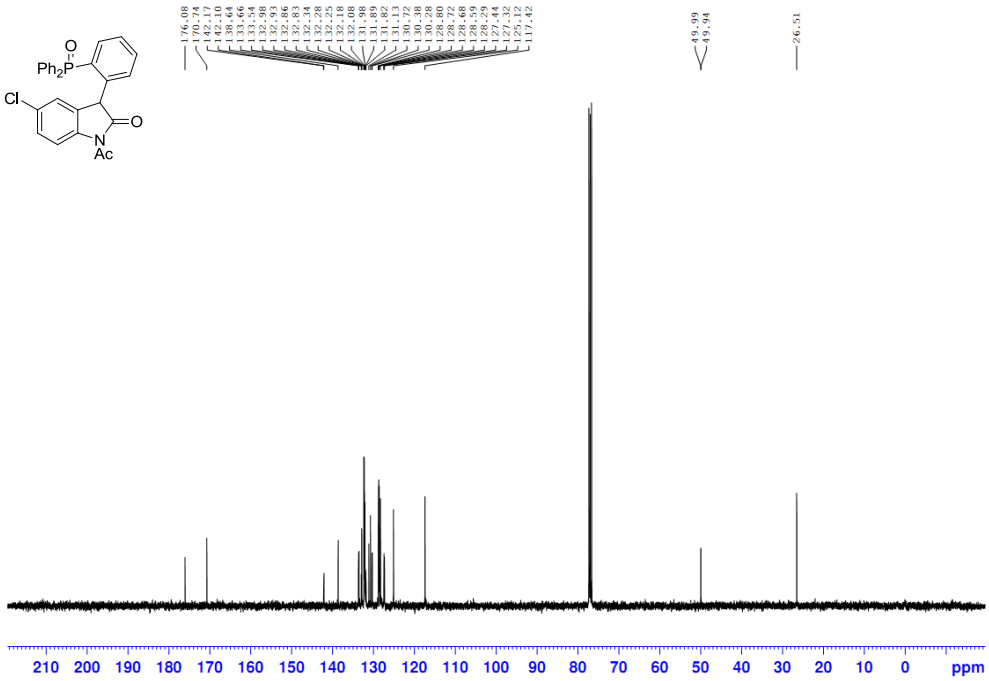
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-fluoroindolin-2-one (3d) ^{19}F NMR (376 MHz, $CDCl_3$)



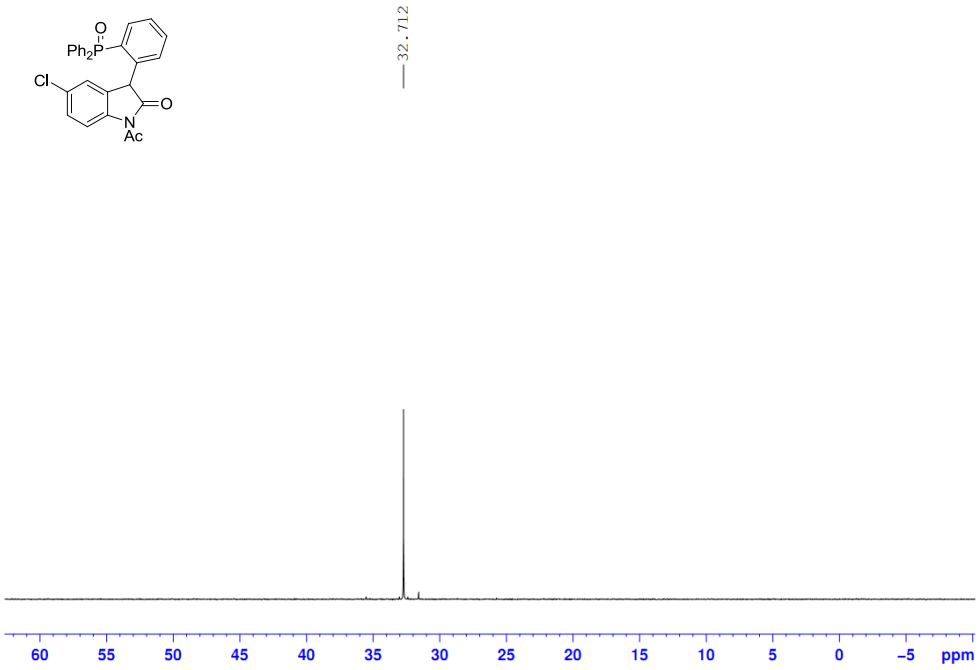
1-Acetyl-5-chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3e) ^{1}H NMR (400 MHz, $CDCl_3$)



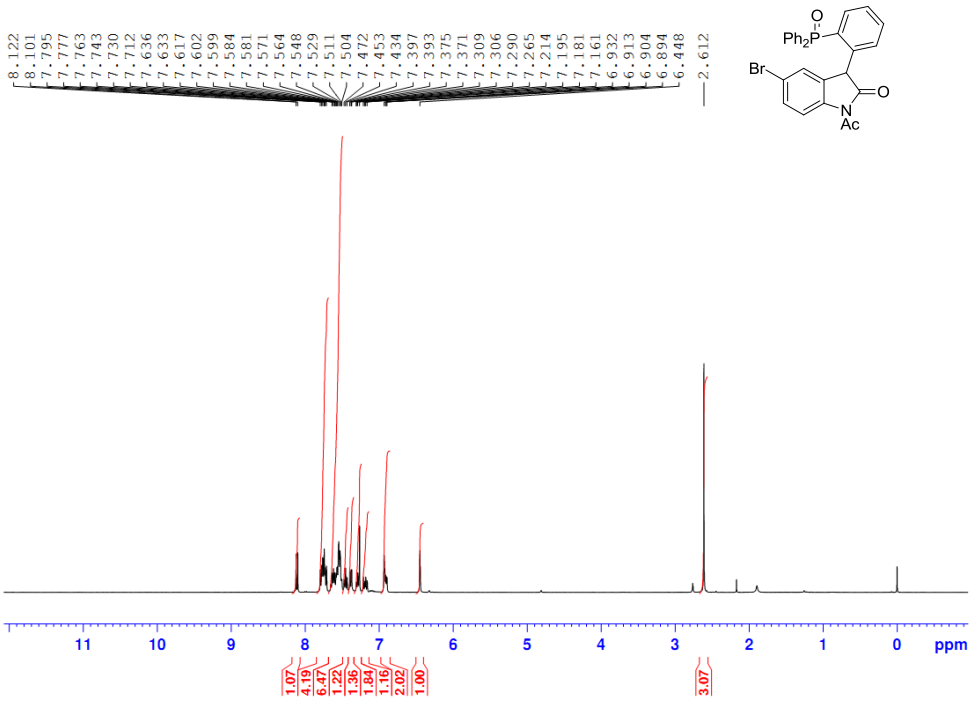
1-Acetyl-5-chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3e) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



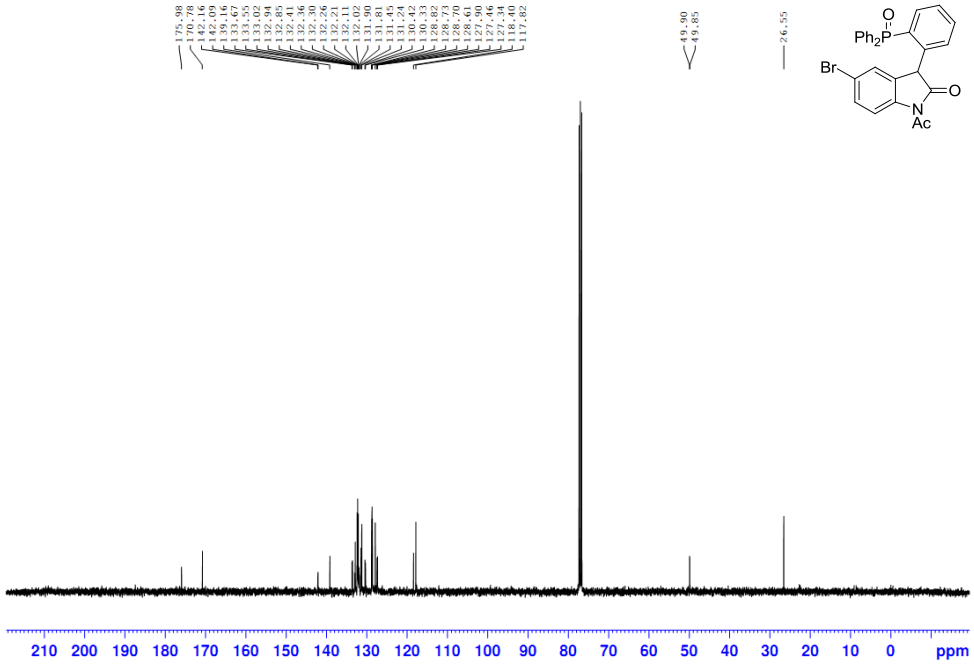
1-Acetyl-5-chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3e) ^{31}P NMR (162 MHz, $CDCl_3$)



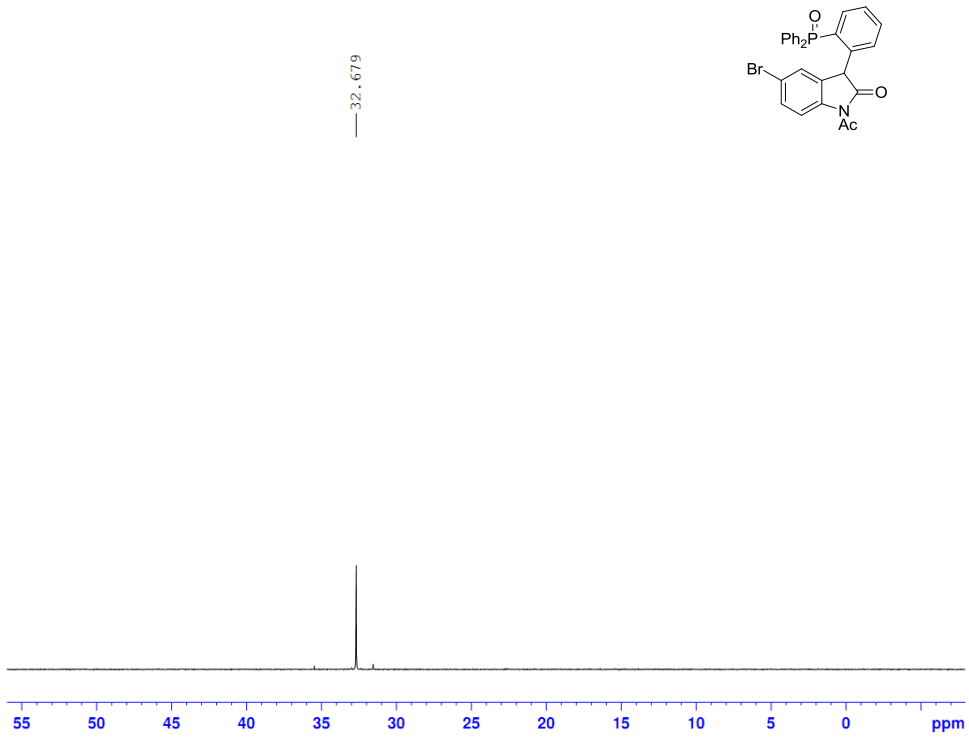
1-Acetyl-5-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3f) ^{1}H NMR (400 MHz, $CDCl_3$)



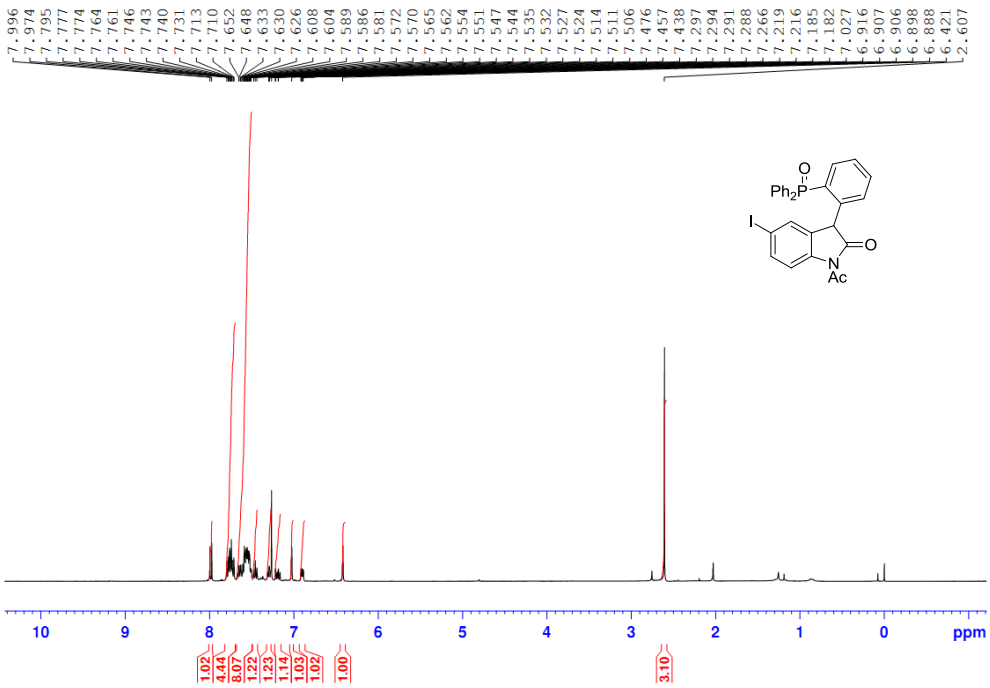
1-Acetyl-5-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3f) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



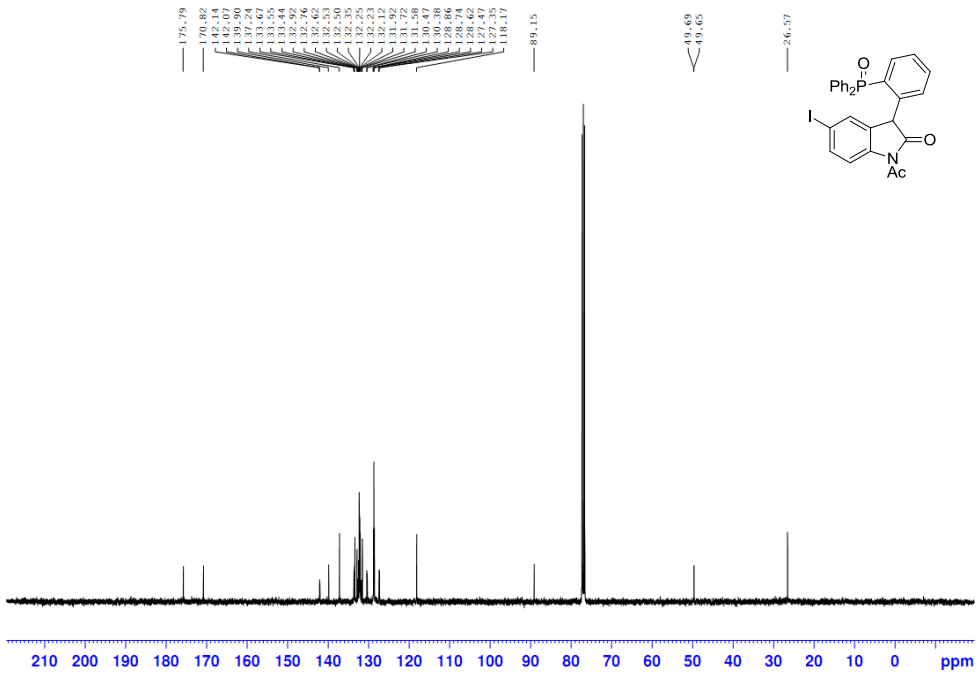
1-Acetyl-5-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3f) ^{31}P NMR (162 MHz, $CDCl_3$)



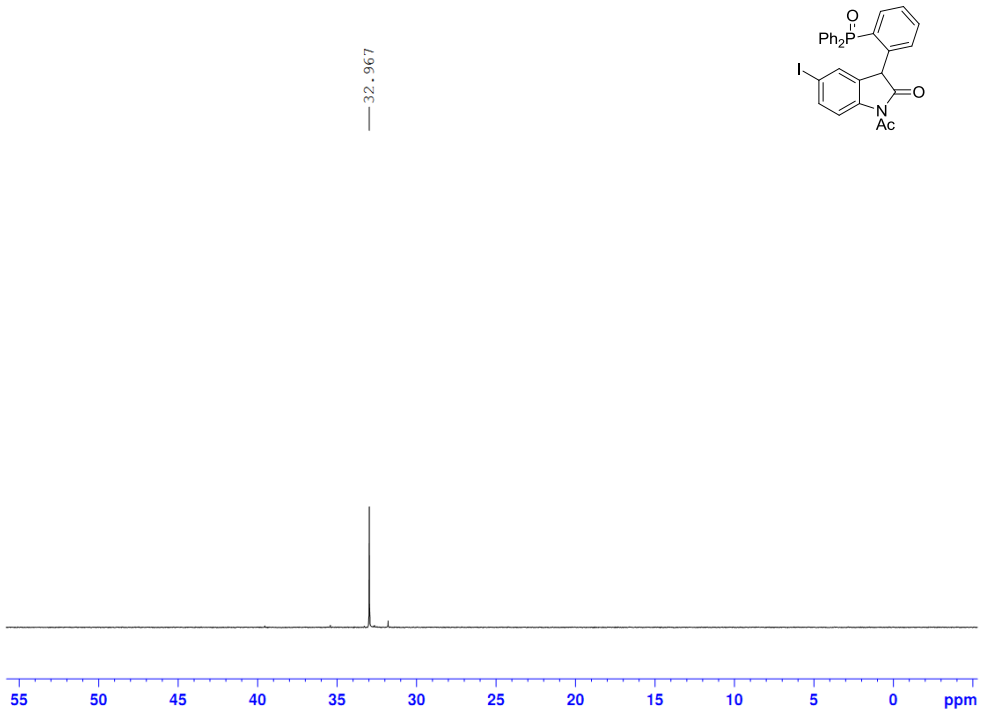
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-iodoindolin-2-one (3g) ^{1}H NMR (400 MHz, $CDCl_3$)



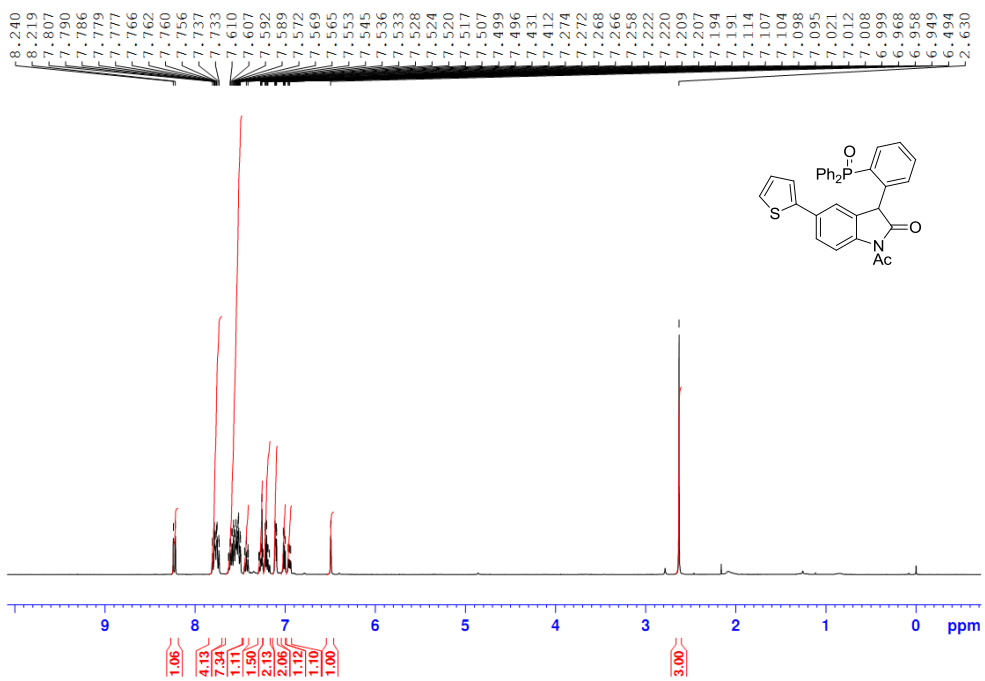
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-iodoindolin-2-one (3g) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



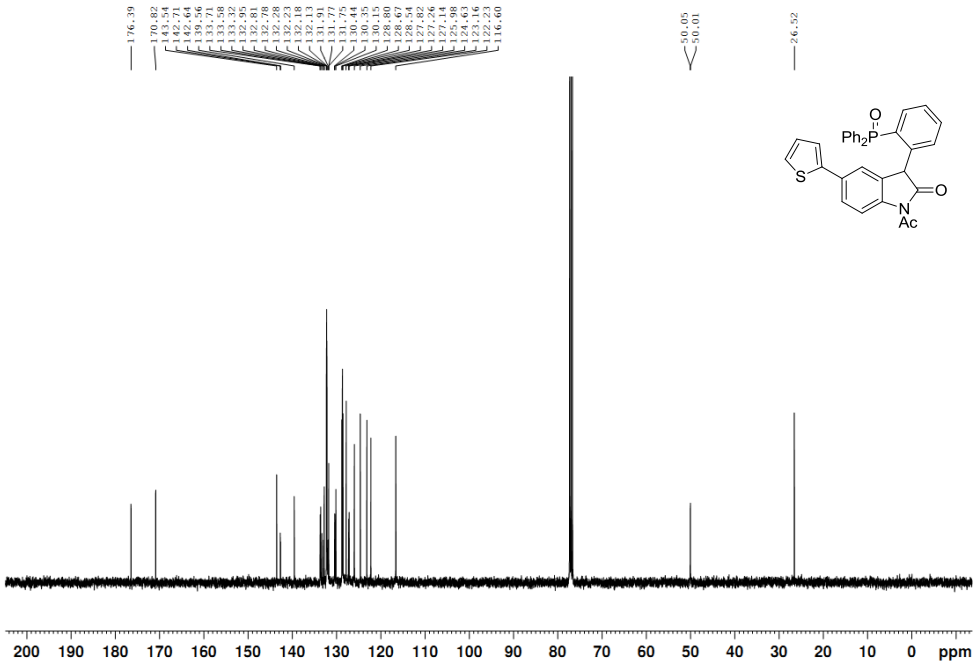
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-iodoindolin-2-one (3g) ^{31}P NMR (162 MHz, $CDCl_3$)



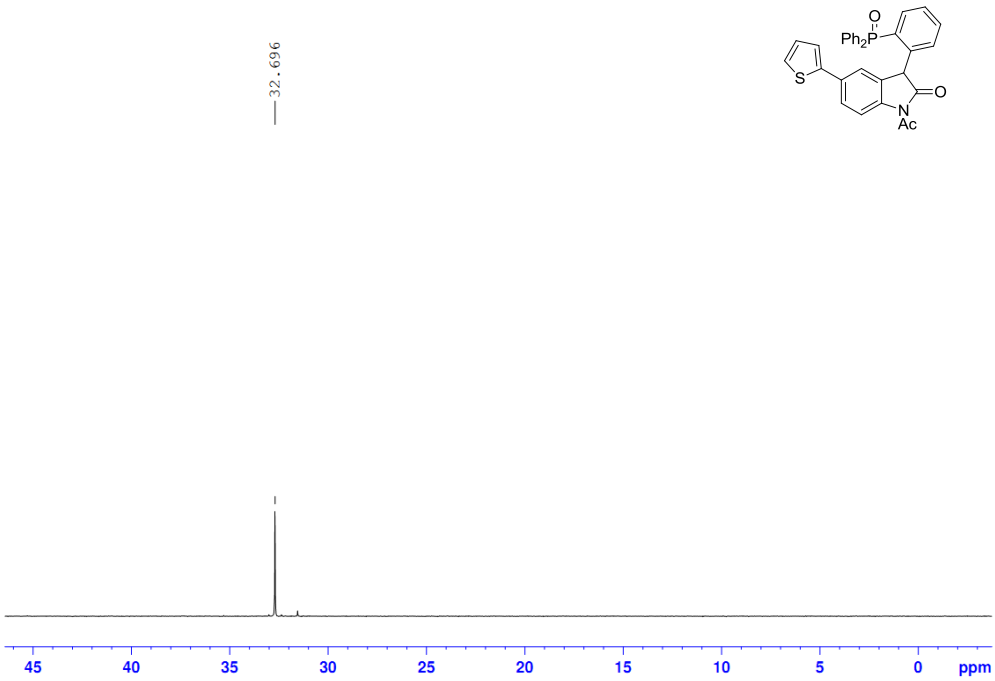
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-(thiophen-2-yl)indolin-2-one (3i) ^{1}H NMR (400 MHz, $CDCl_3$)



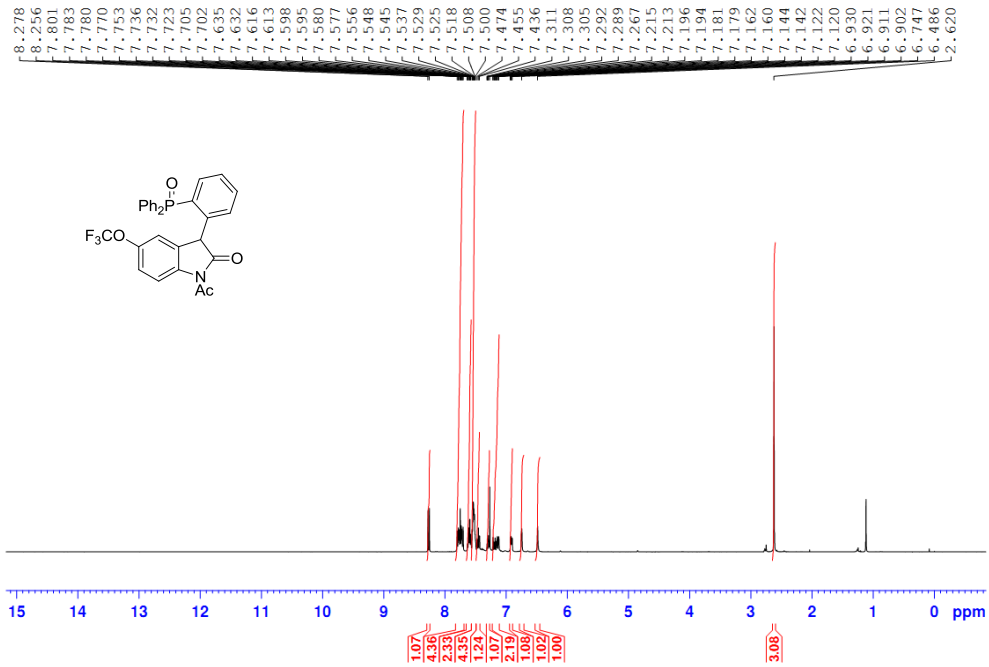
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-(thiophen-2-yl)indolin-2-one (3i) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



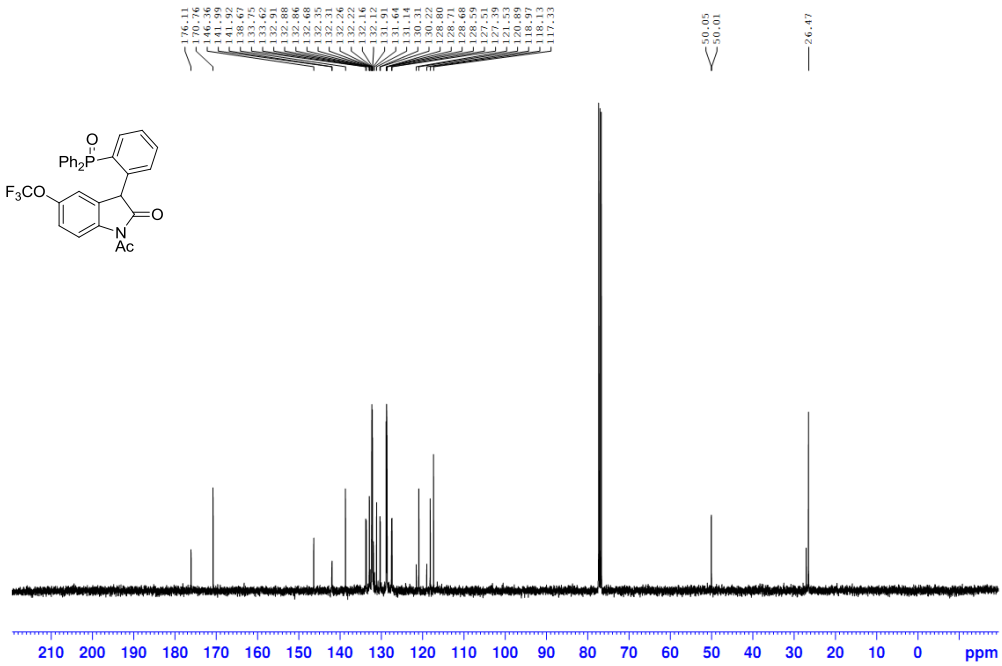
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-(thiophen-2-yl)indolin-2-one (3i) ^{31}P NMR (162 MHz, $CDCl_3$)



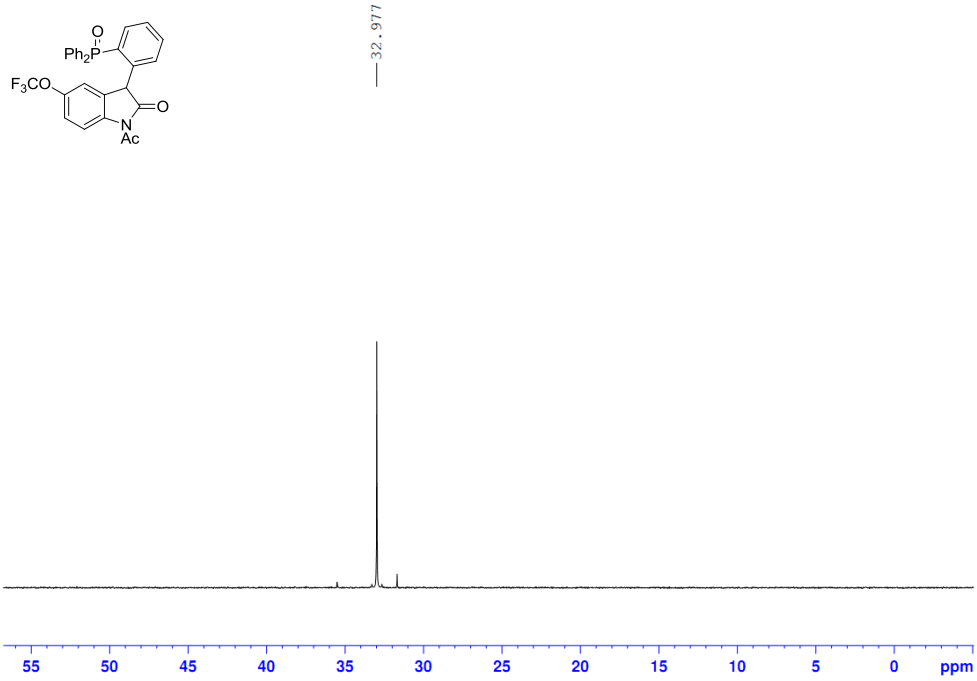
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-(trifluoromethoxy)indolin-2-one (3j) ^{1}H NMR (400 MHz, $CDCl_3$)



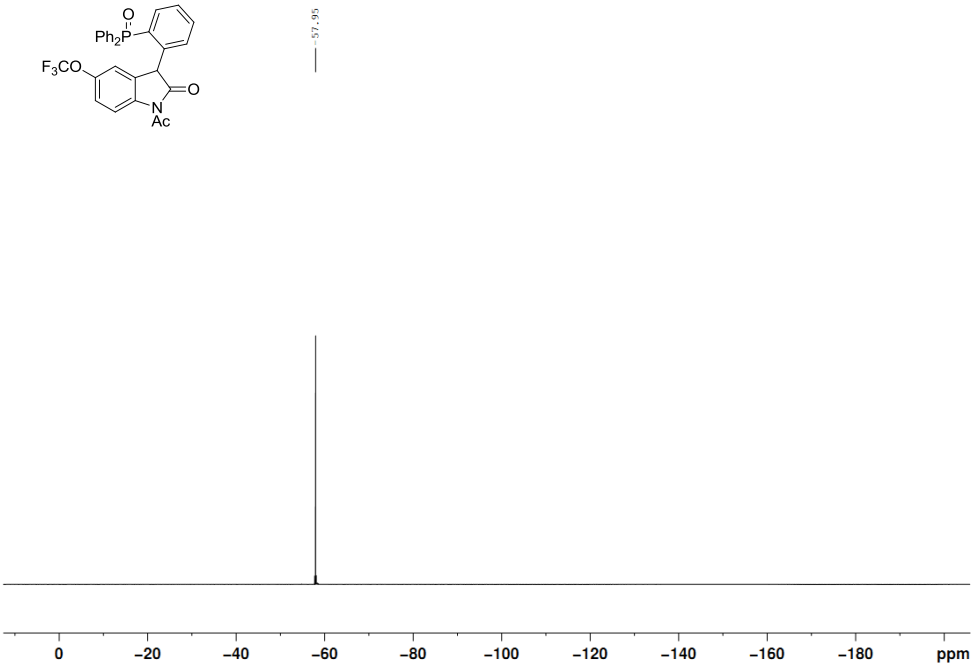
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-(trifluoromethoxy)indolin-2-one (3j) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



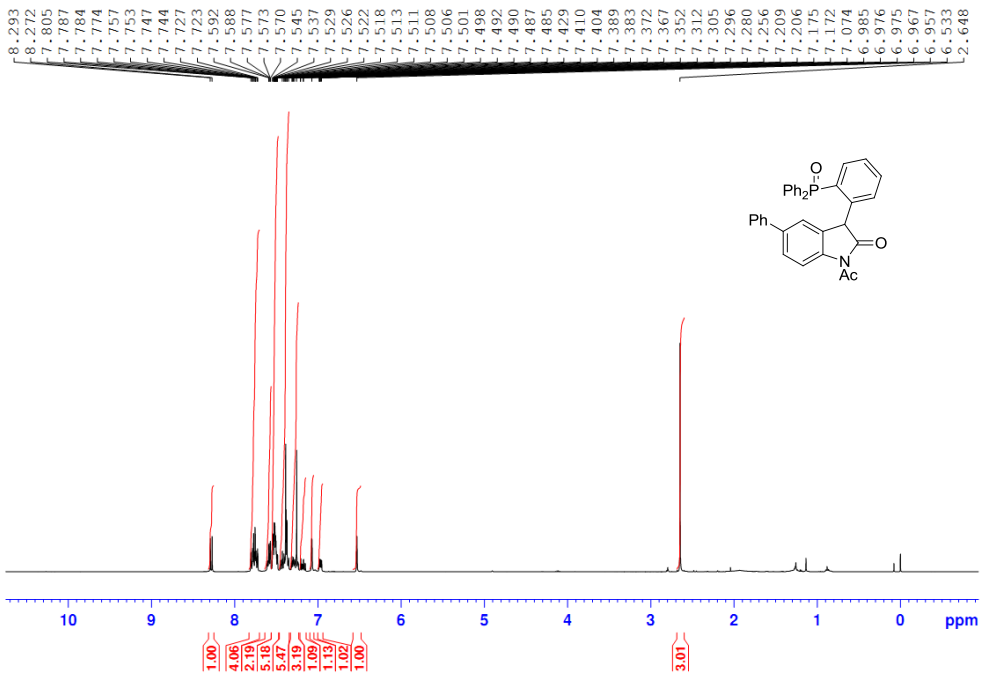
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-(trifluoromethoxy)indolin-2-one (3j) ^{31}P NMR (162 MHz, $CDCl_3$)



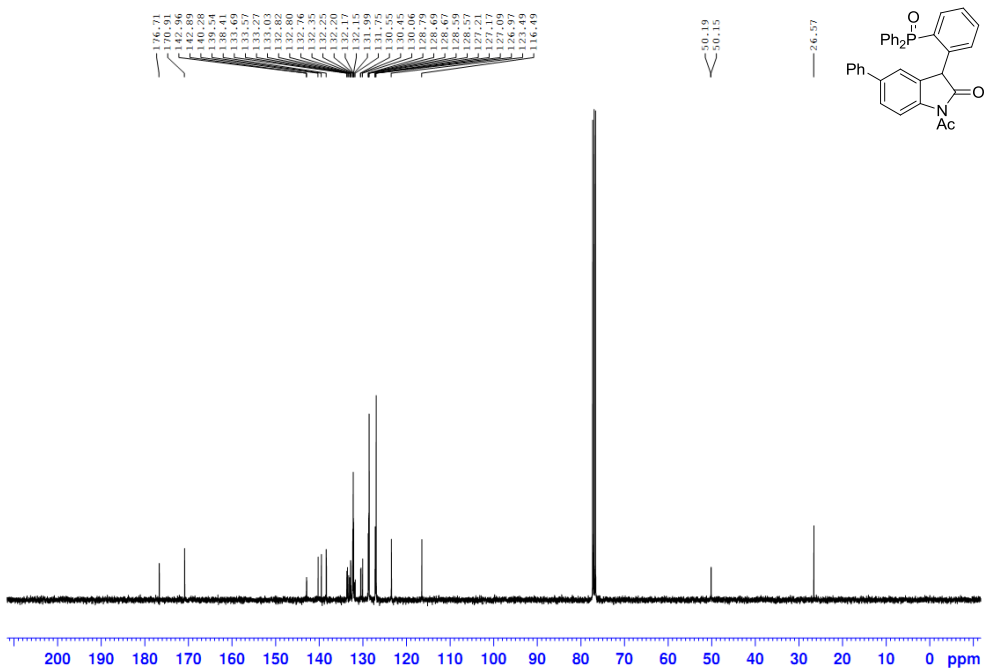
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-(trifluoromethoxy)indolin-2-one (3j) ^{19}F NMR (376 MHz, $CDCl_3$)



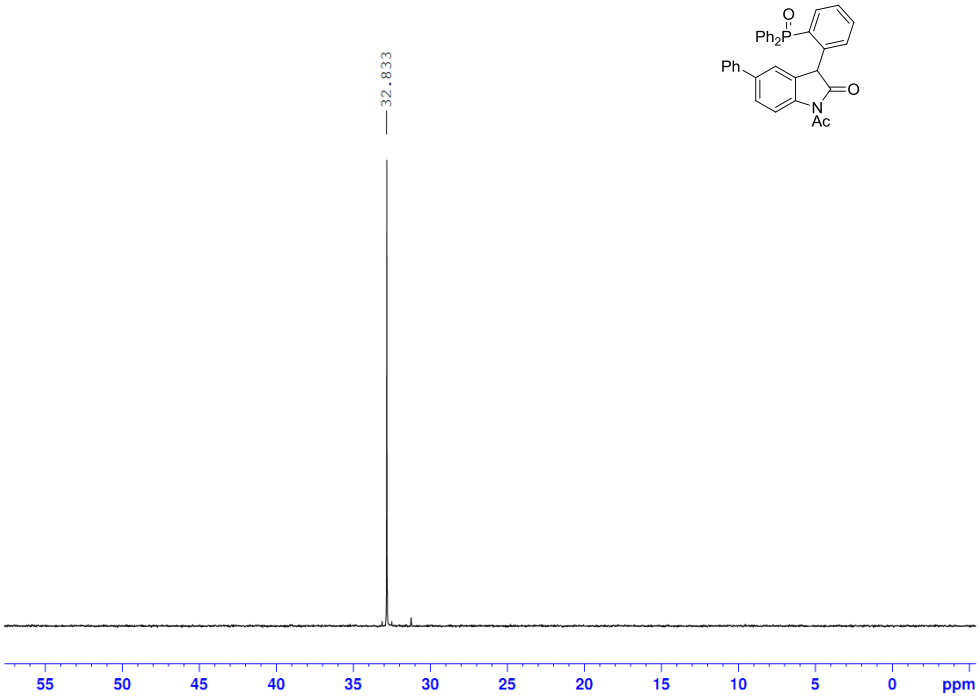
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-phenylindolin-2-one (3k) ^{1}H NMR (400 MHz, $CDCl_3$)



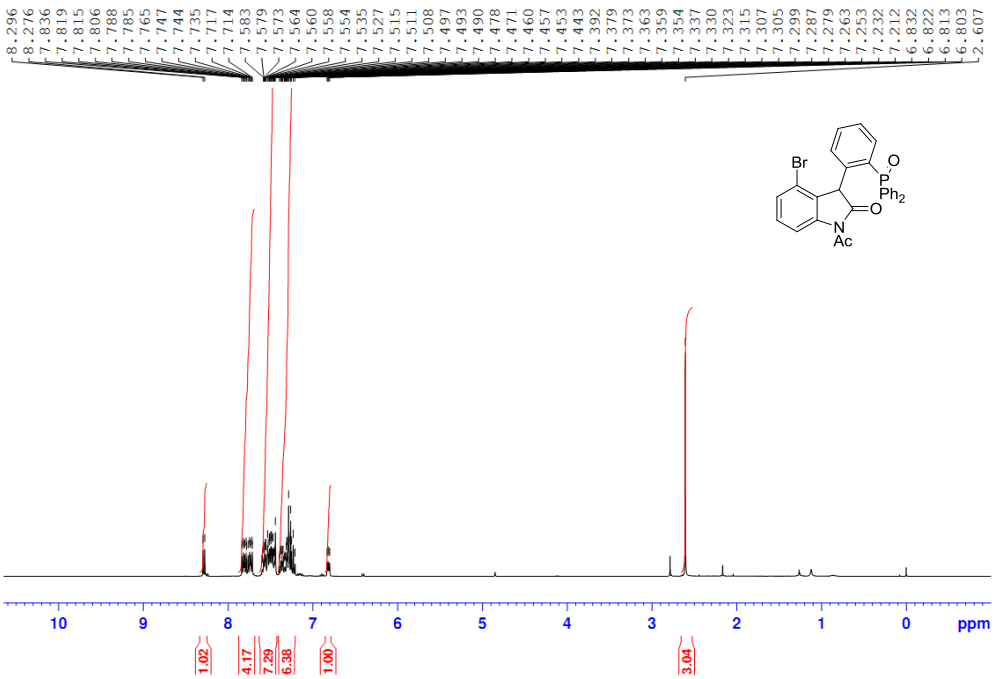
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-phenylindolin-2-one (3k) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



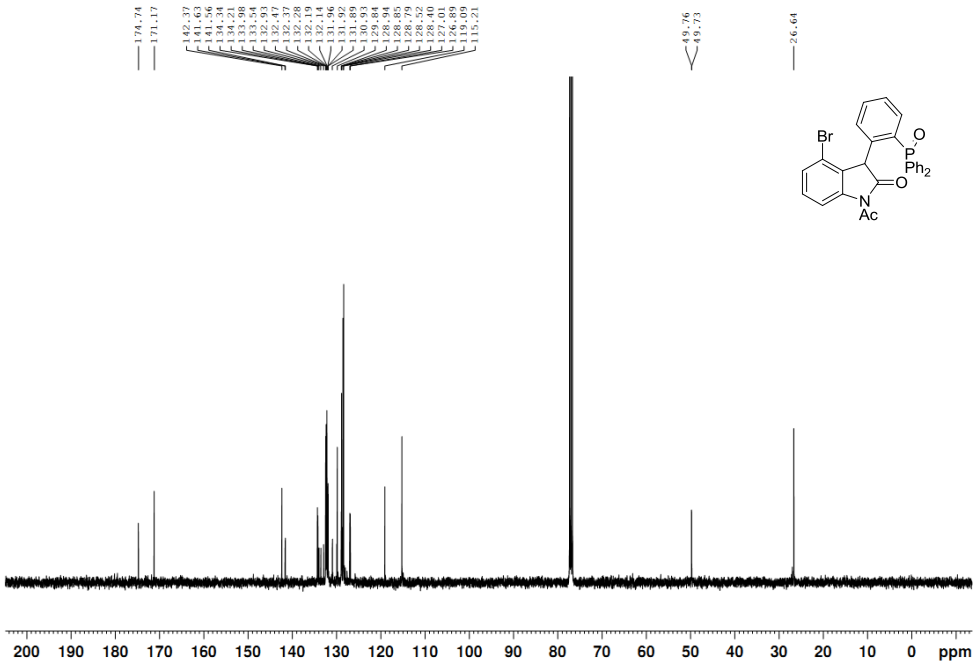
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5-phenylindolin-2-one (3k) ^{31}P NMR (162 MHz, $CDCl_3$)



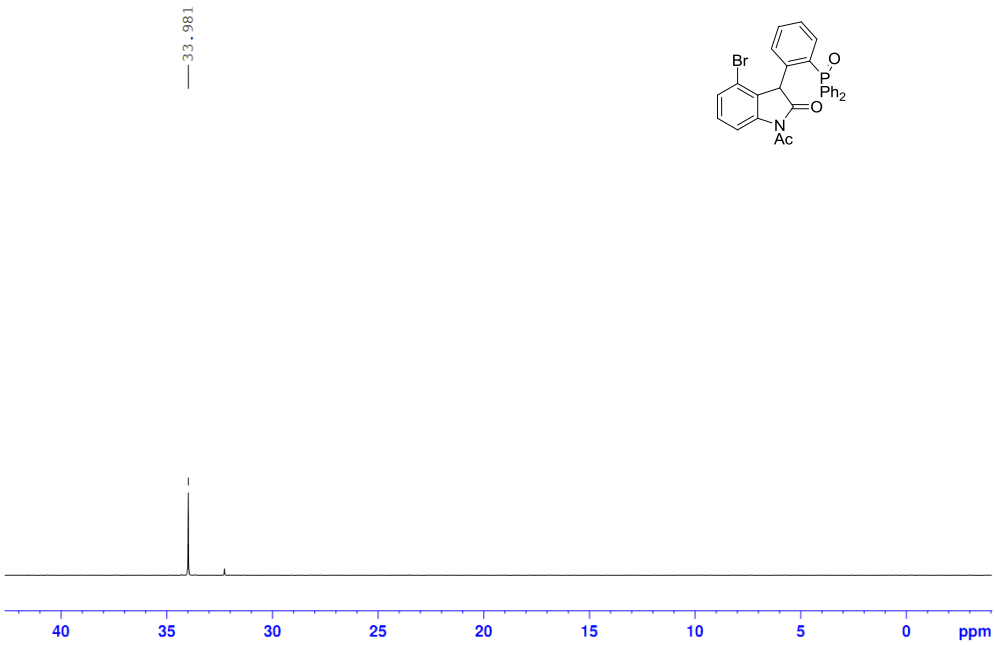
1-Acetyl-4-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3l) ^{1}H NMR (400 MHz, $CDCl_3$)



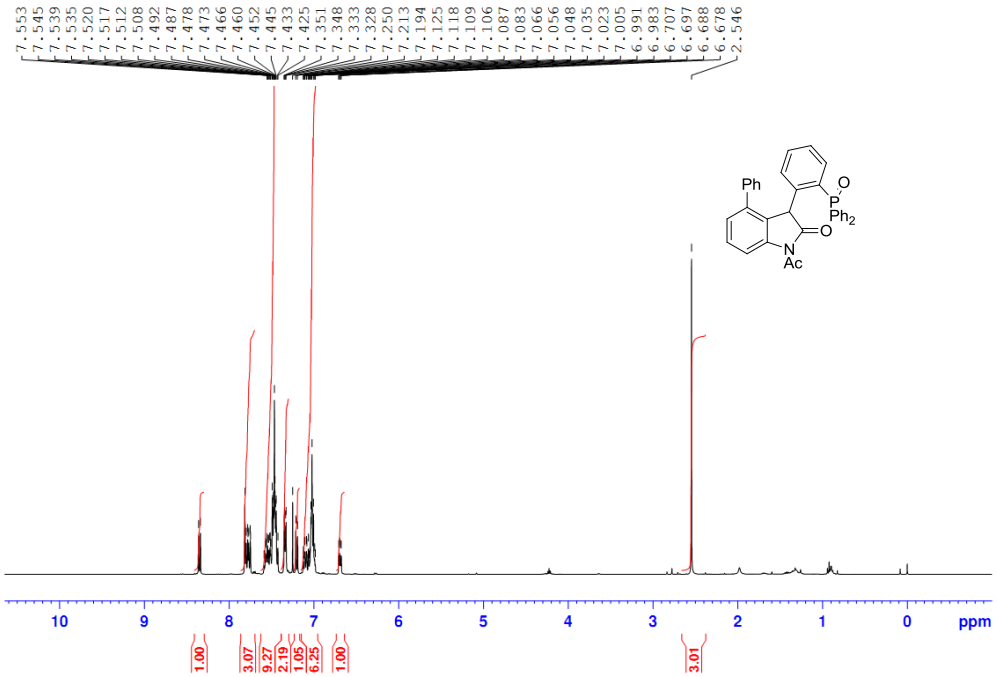
1-Acetyl-4-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3l) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



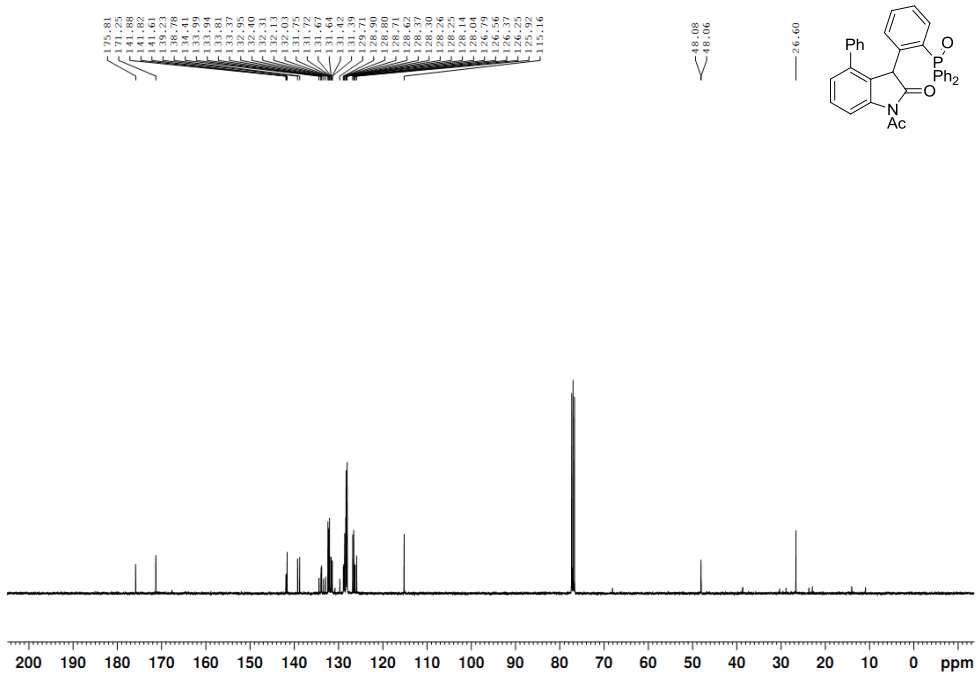
1-Acetyl-4-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3l) ^{31}P NMR (162 MHz, $CDCl_3$)



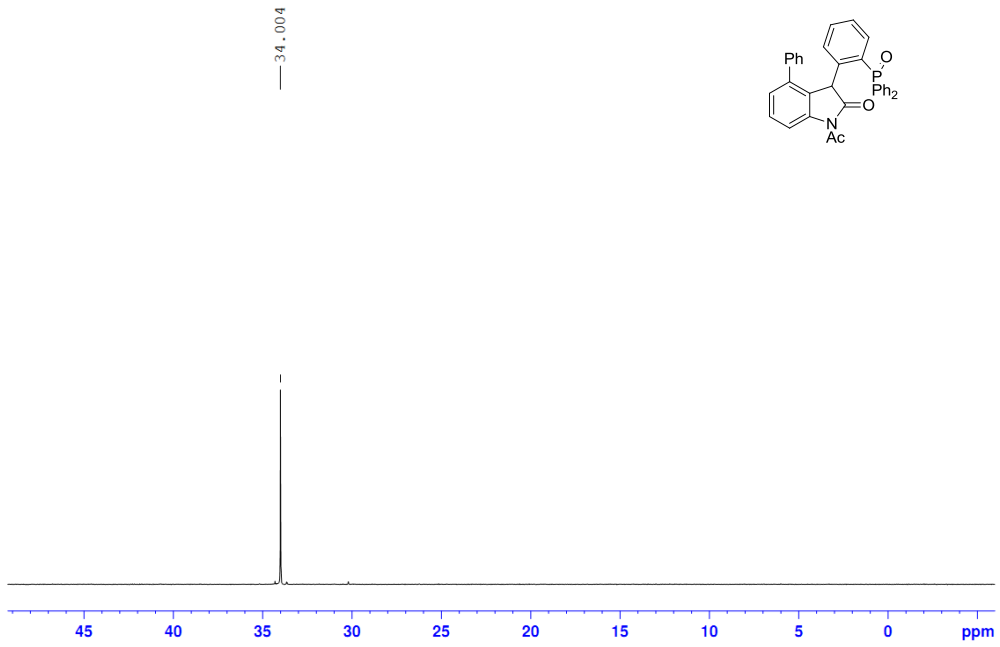
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-4-phenylindolin-2-one (3m) ^{1}H NMR (400 MHz, $CDCl_3$)



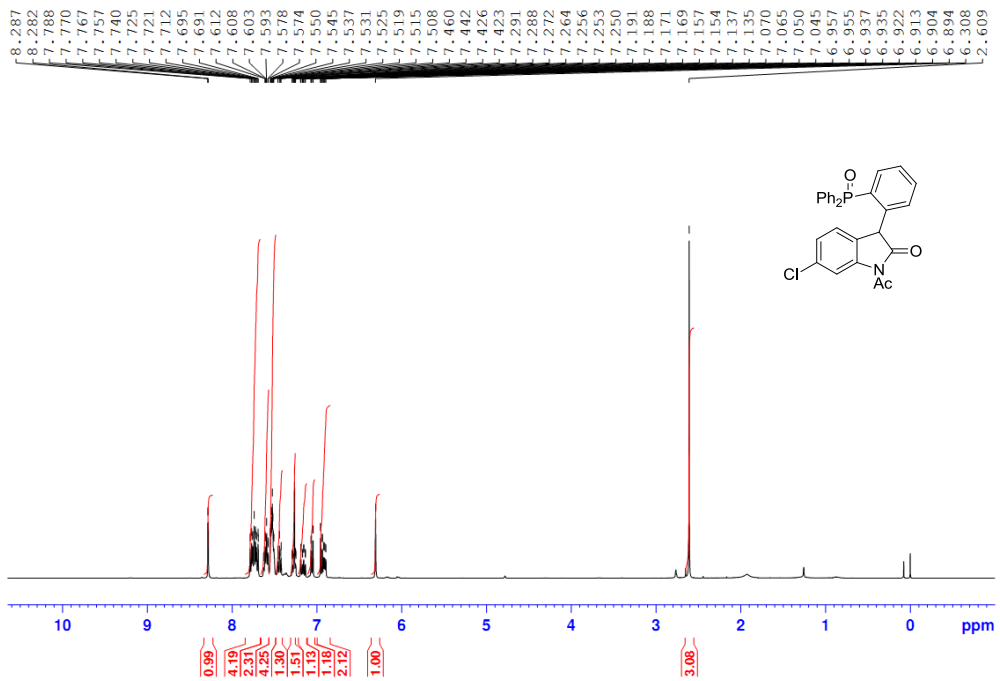
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-4-phenylindolin-2-one (3m) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



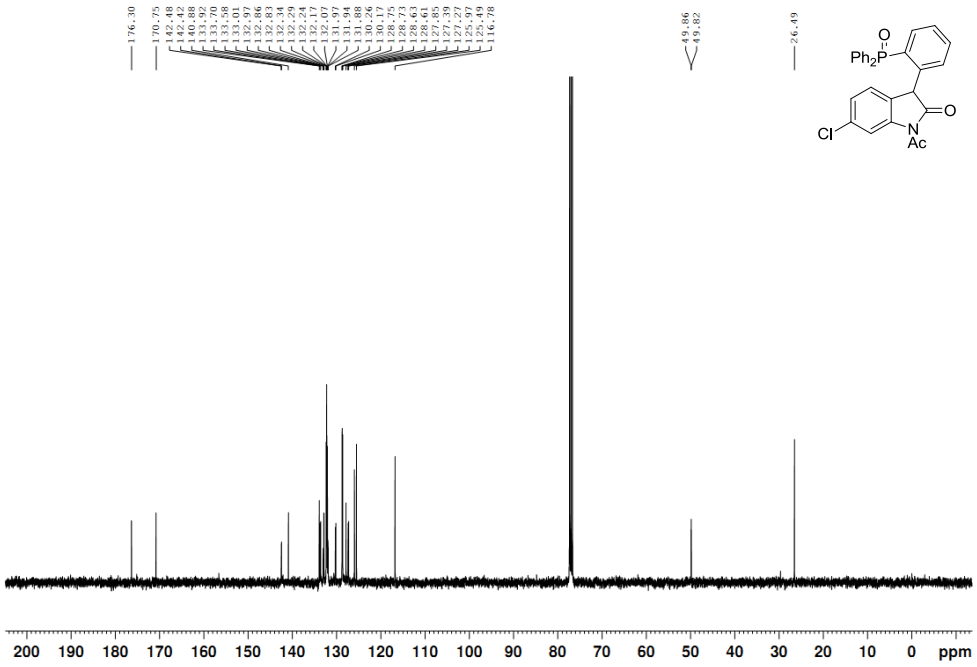
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-4-phenylindolin-2-one (3m) ^{31}P NMR (162 MHz, $CDCl_3$)



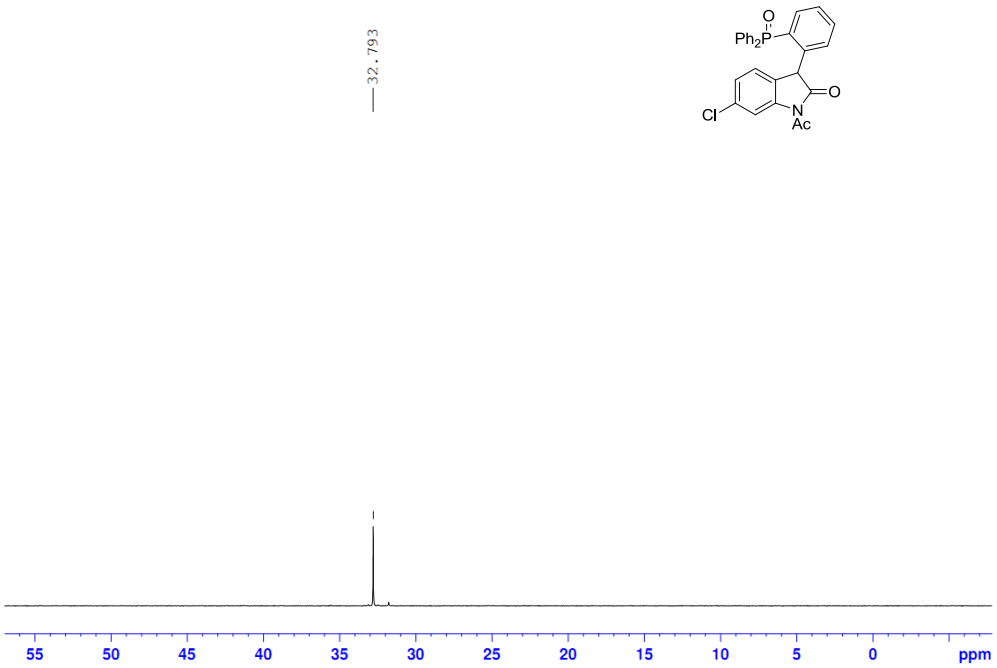
1-Acetyl-6- chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3n) ^{1}H NMR (400 MHz, $CDCl_3$)



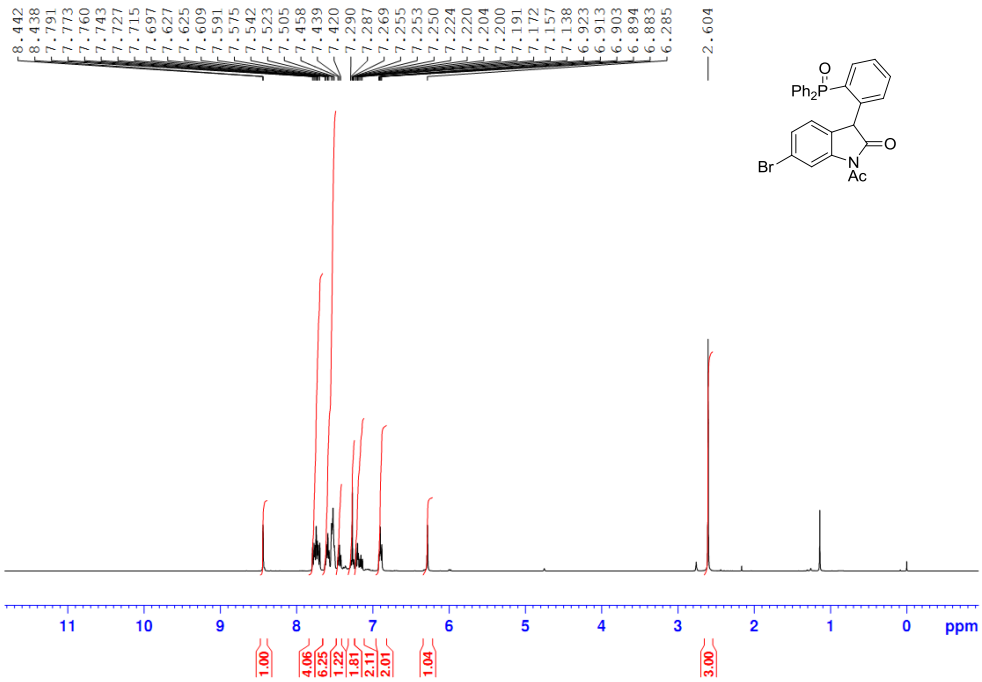
1-Acetyl-6- chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3n) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



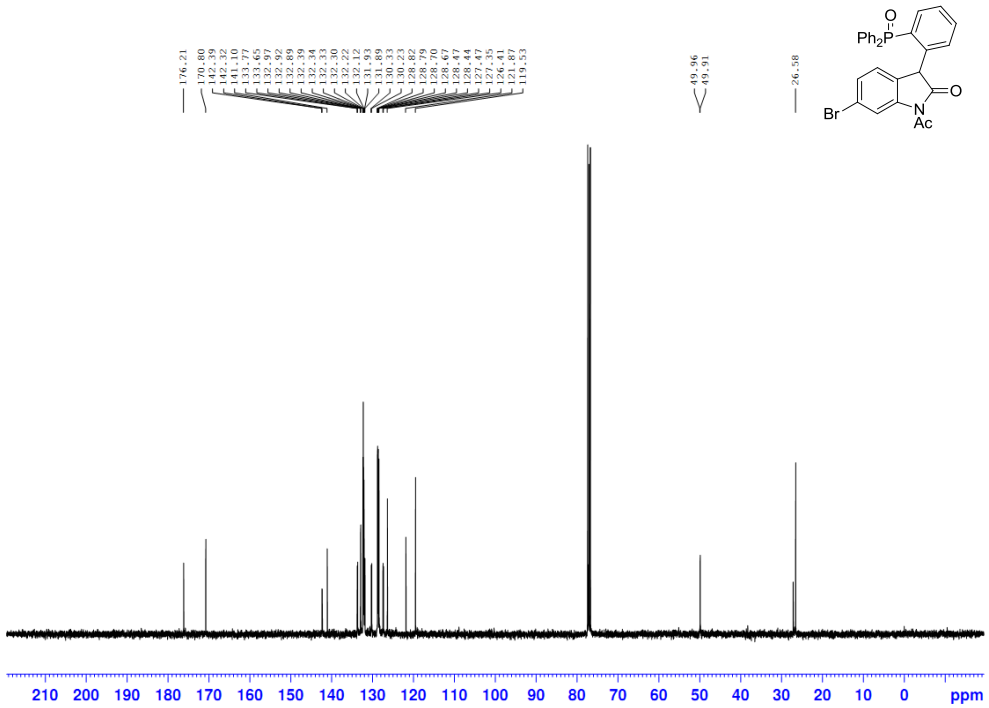
1-Acetyl-6- chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3n) ^{31}P NMR (162 MHz, $CDCl_3$)



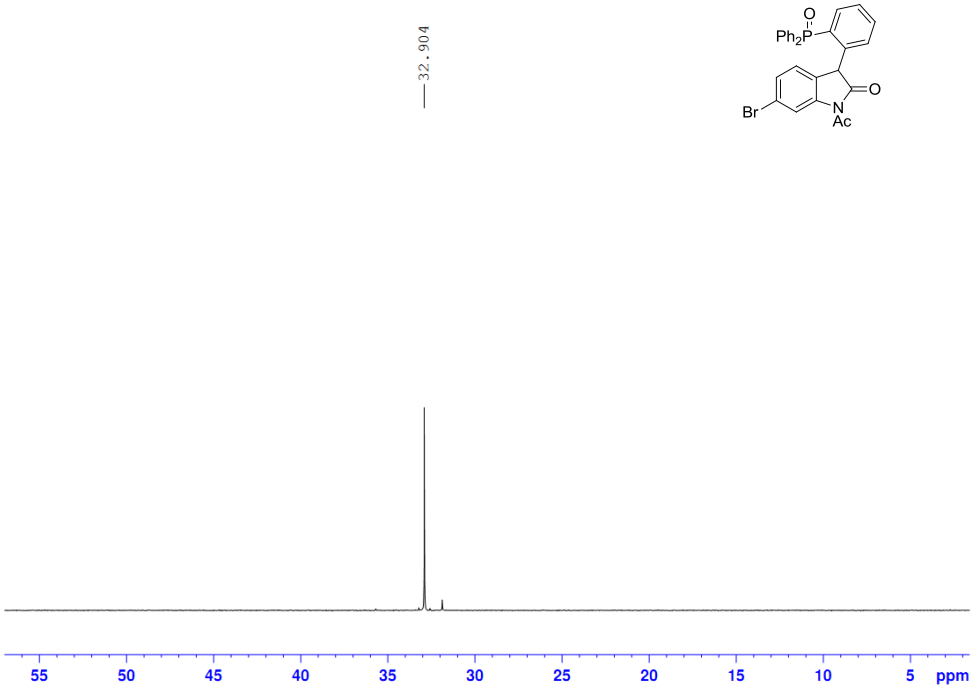
1-Acetyl-6-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3o) ^{1}H NMR (400 MHz, $CDCl_3$)



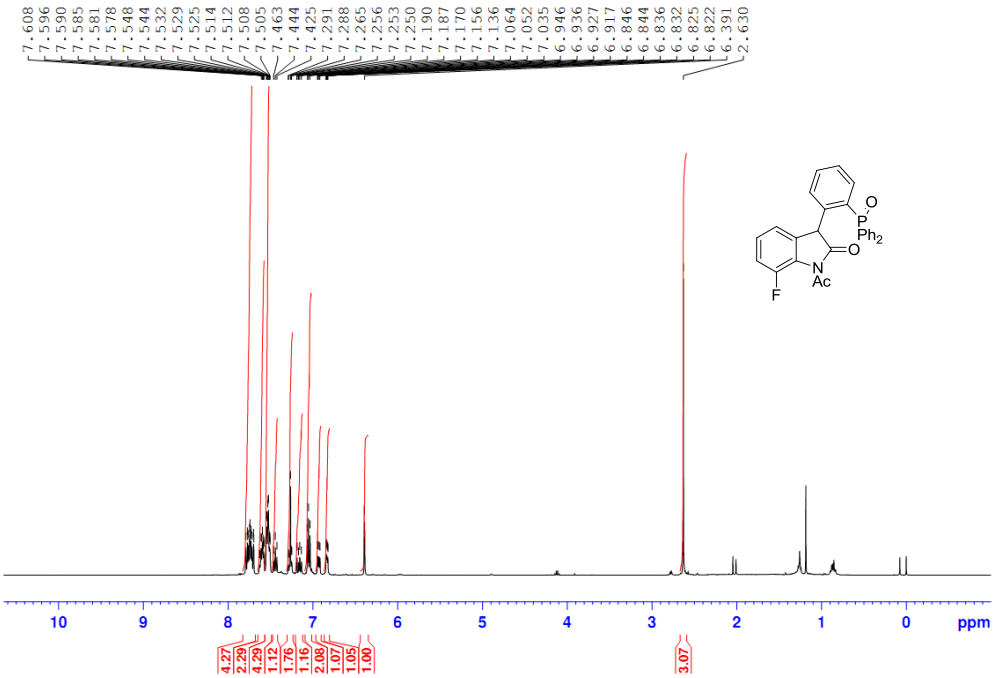
1-Acetyl-6-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3o) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



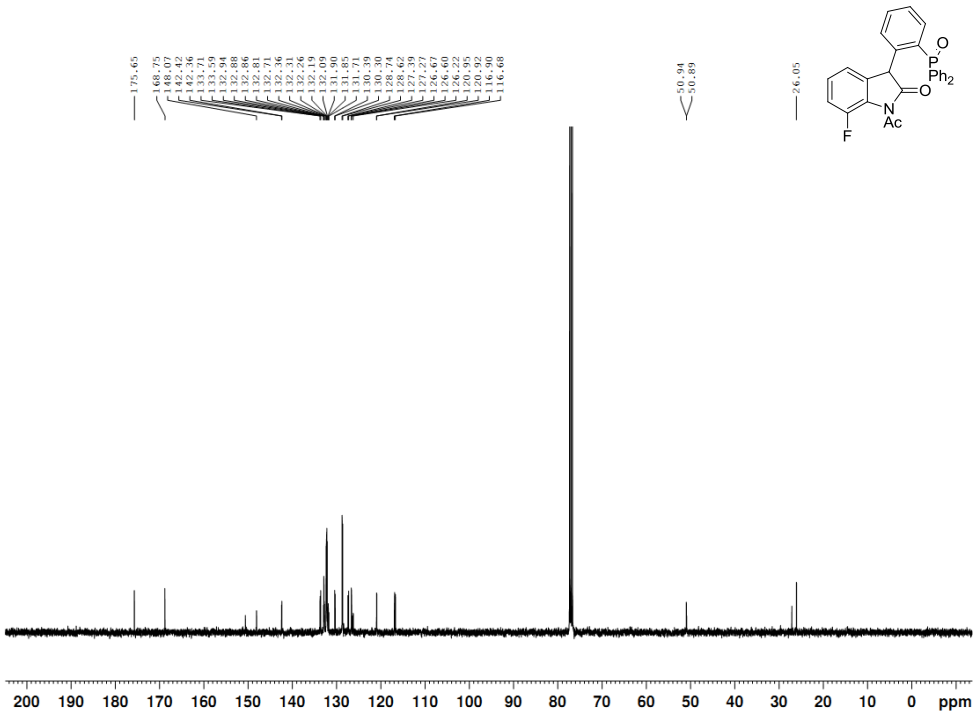
1-Acetyl-6-bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (3o) ^{31}P NMR (162 MHz, $CDCl_3$)



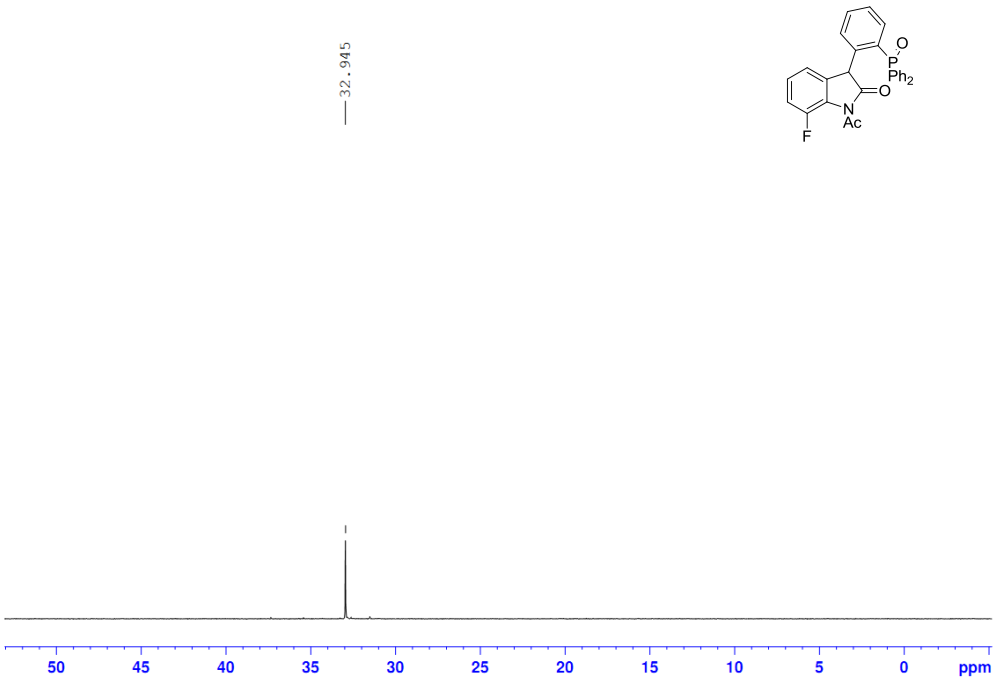
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-7-fluoroindolin-2-one (3q) ^{1}H NMR (400 MHz, $CDCl_3$)



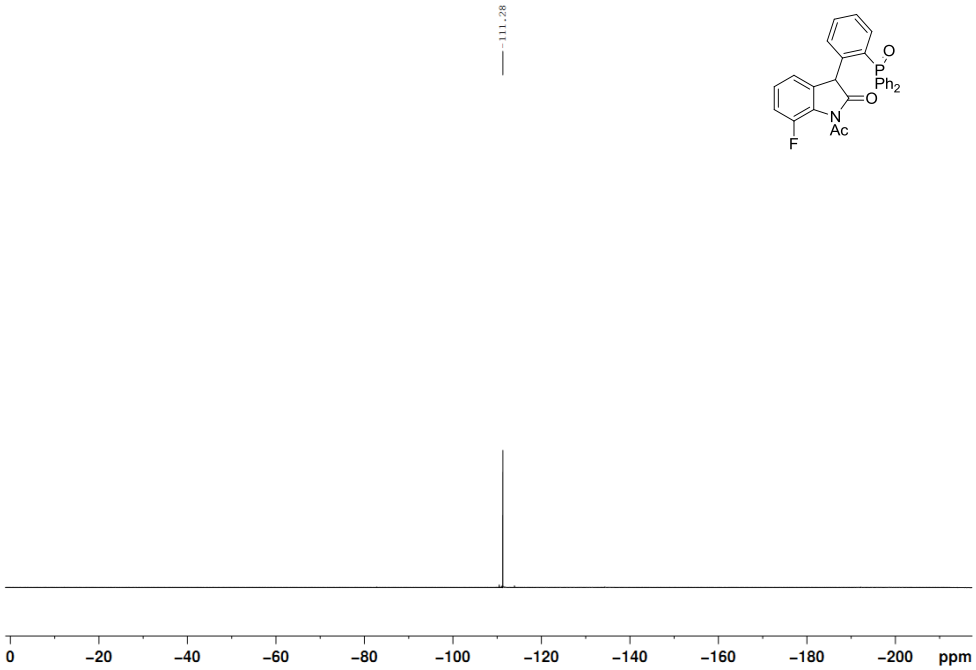
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-7-fluoroindolin-2-one (3q) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



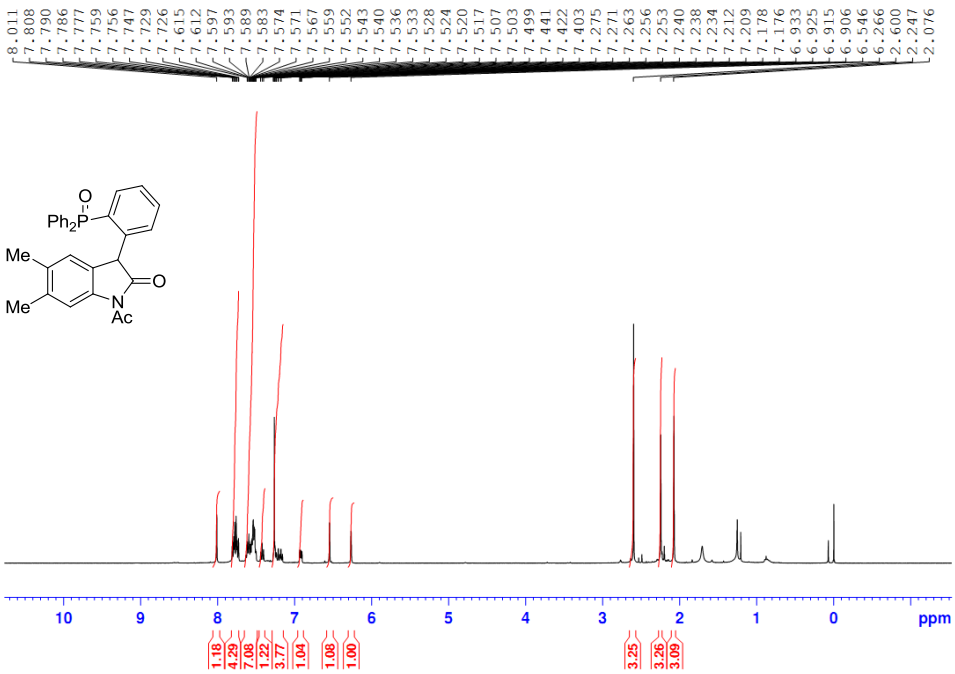
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-7-fluoroindolin-2-one (3q) ^{31}P NMR (162 MHz, $CDCl_3$)



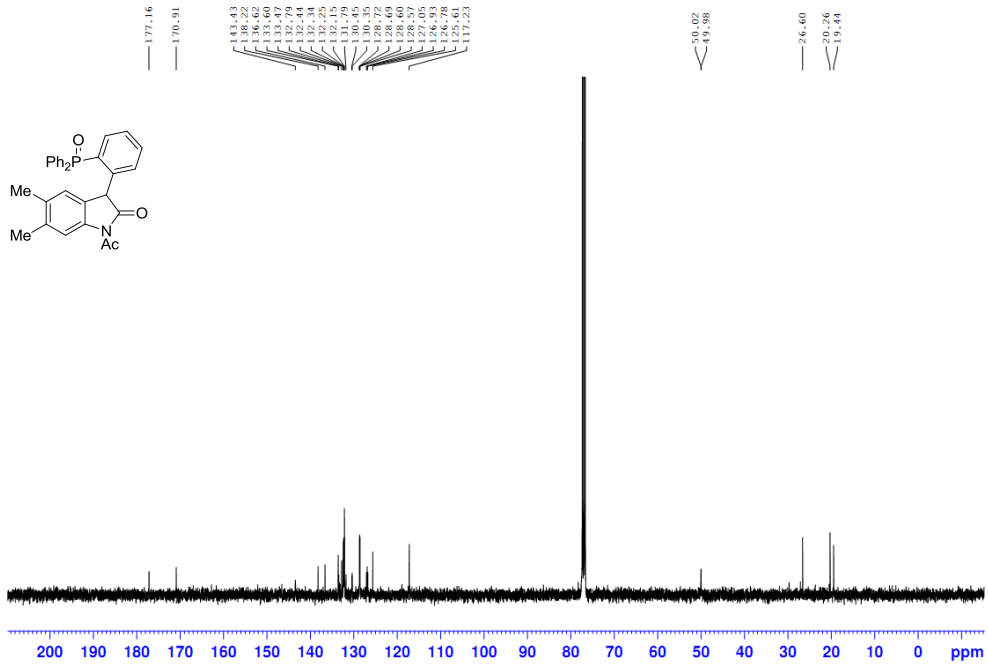
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-7-fluoroindolin-2-one (3q) ^{19}F NMR (376 MHz, $CDCl_3$)



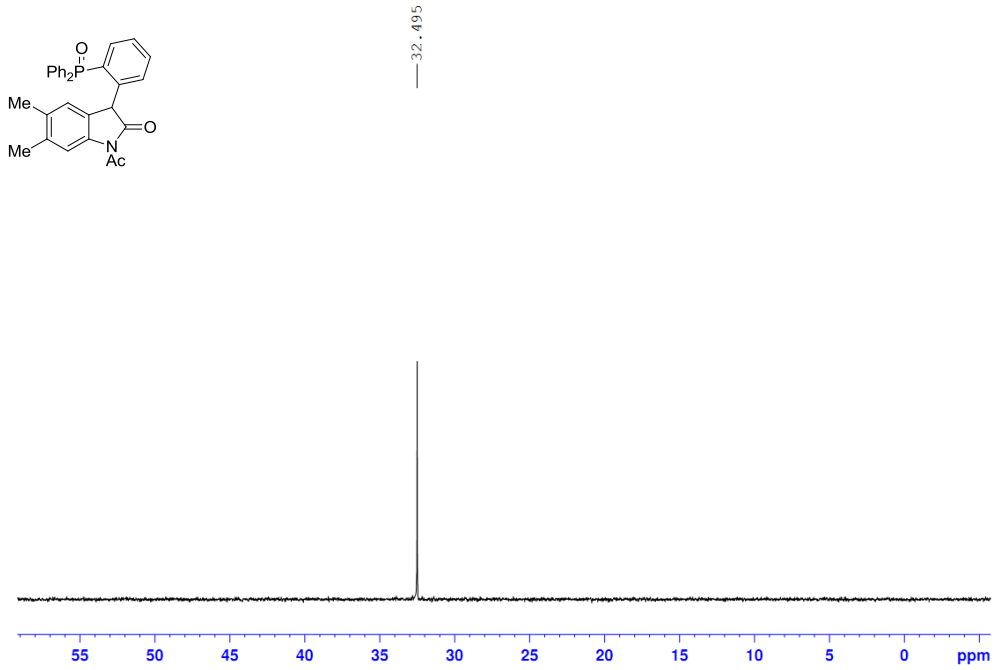
1-**Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5,6-dimethylindolin-2-one (3r)** ^{1}H NMR (400 MHz, $CDCl_3$)



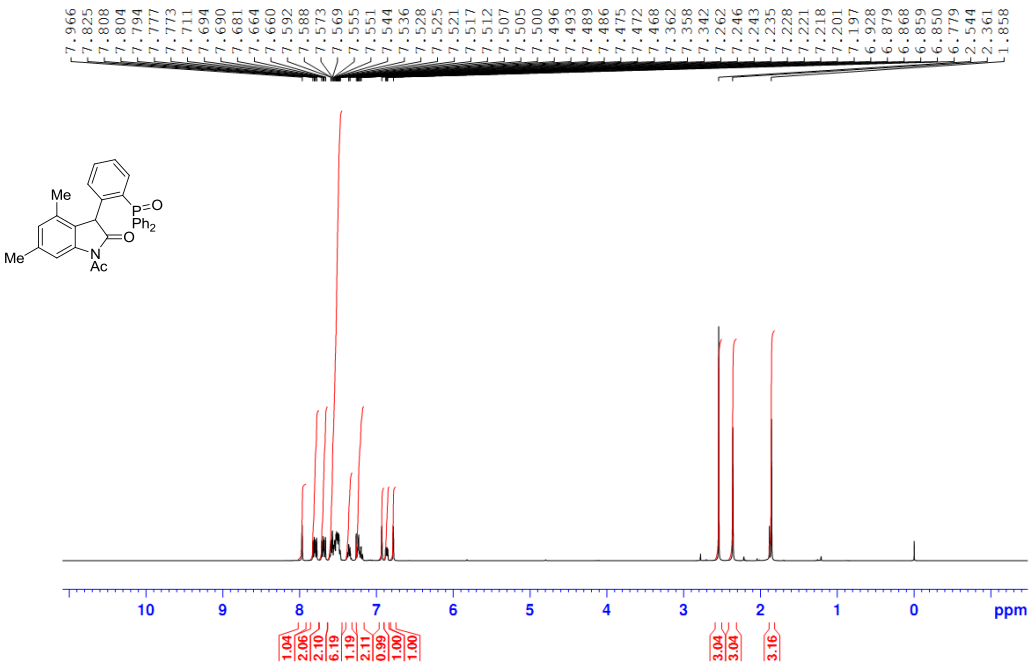
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5,6-dimethylindolin-2-one (3r) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



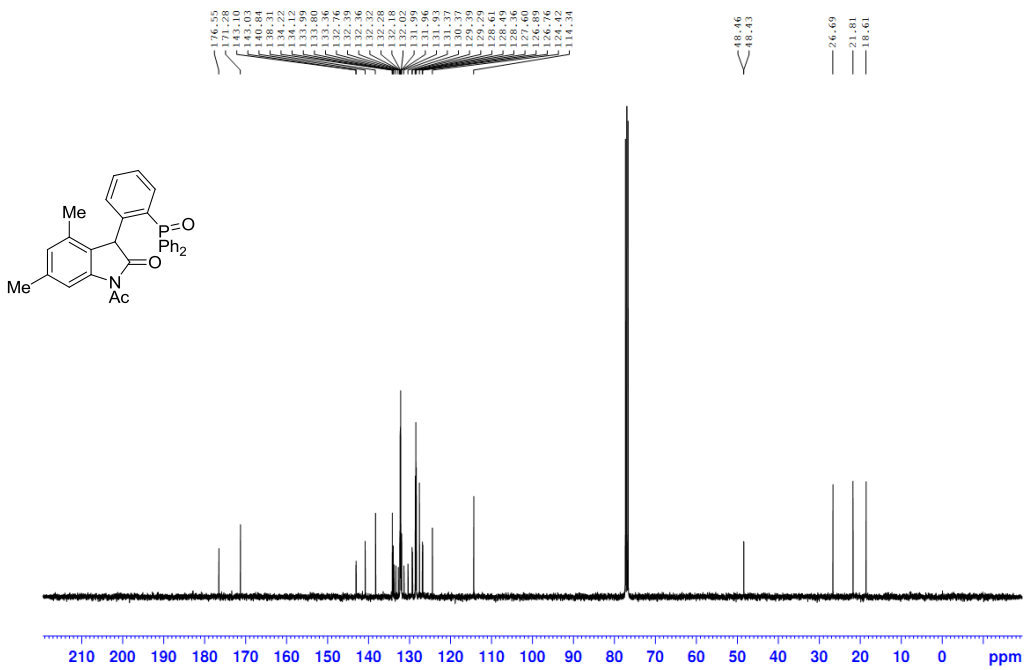
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-5,6-dimethylindolin-2-one (3r) ^{31}P NMR (162 MHz, $CDCl_3$)



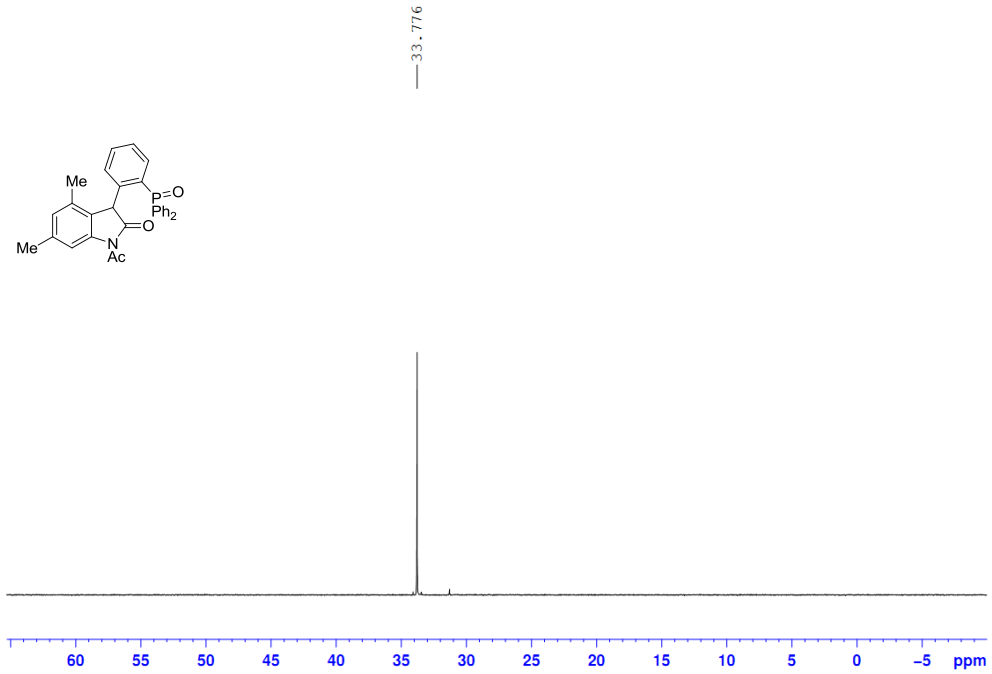
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-4,6-dimethylindolin-2-one (3s) ^{1}H NMR (400 MHz, $CDCl_3$)



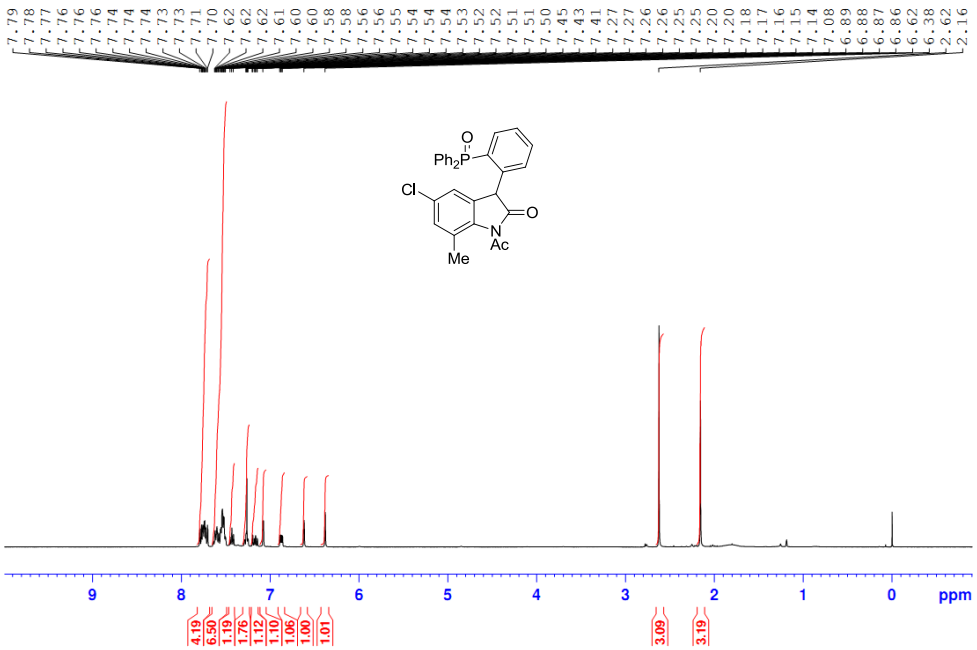
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-4,6-dimethylindolin-2-one (3s) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



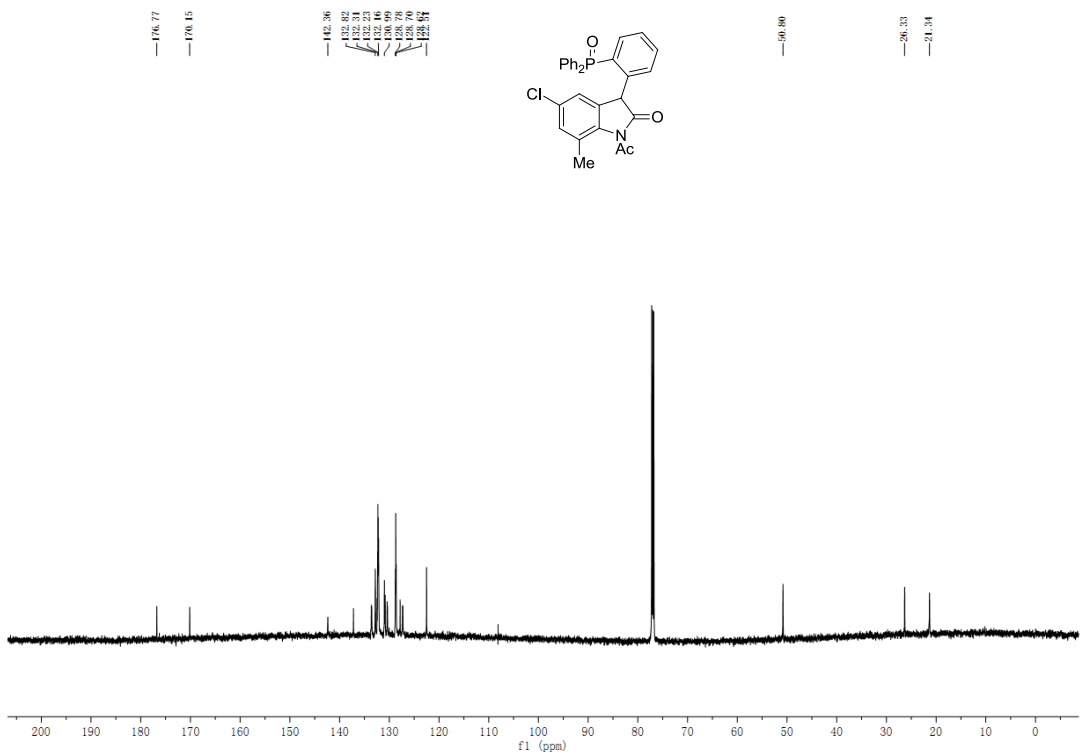
1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-4,6-dimethylindolin-2-one (3s) ^{31}P NMR (162 MHz, $CDCl_3$)



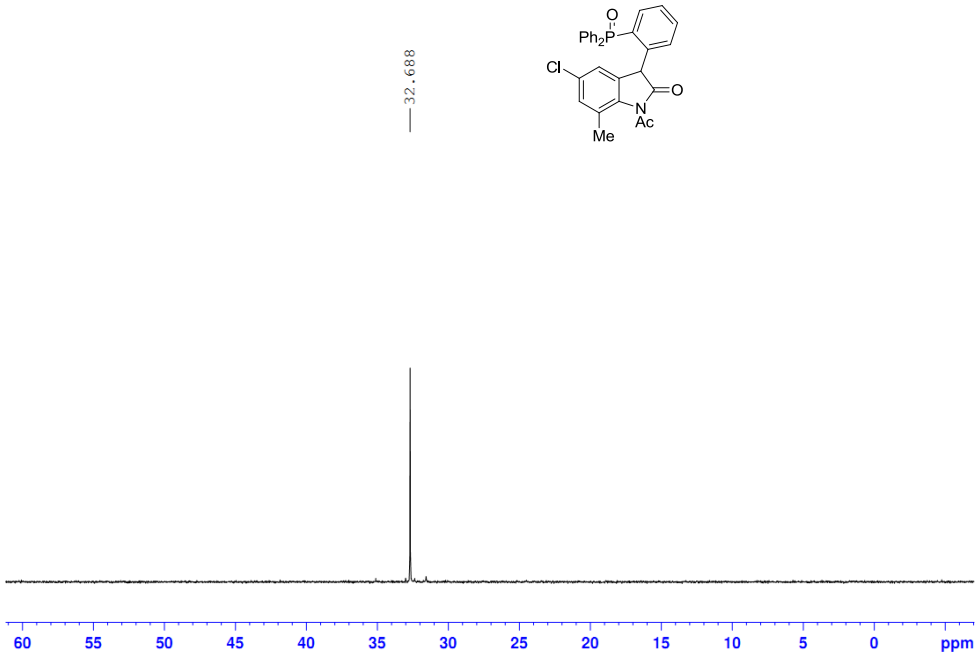
1-Acetyl-5-chloro-3-(2-(diphenylphosphoryl)phenyl)-7-methylindolin-2-one (3t) ^{1}H NMR (400 MHz, $CDCl_3$)



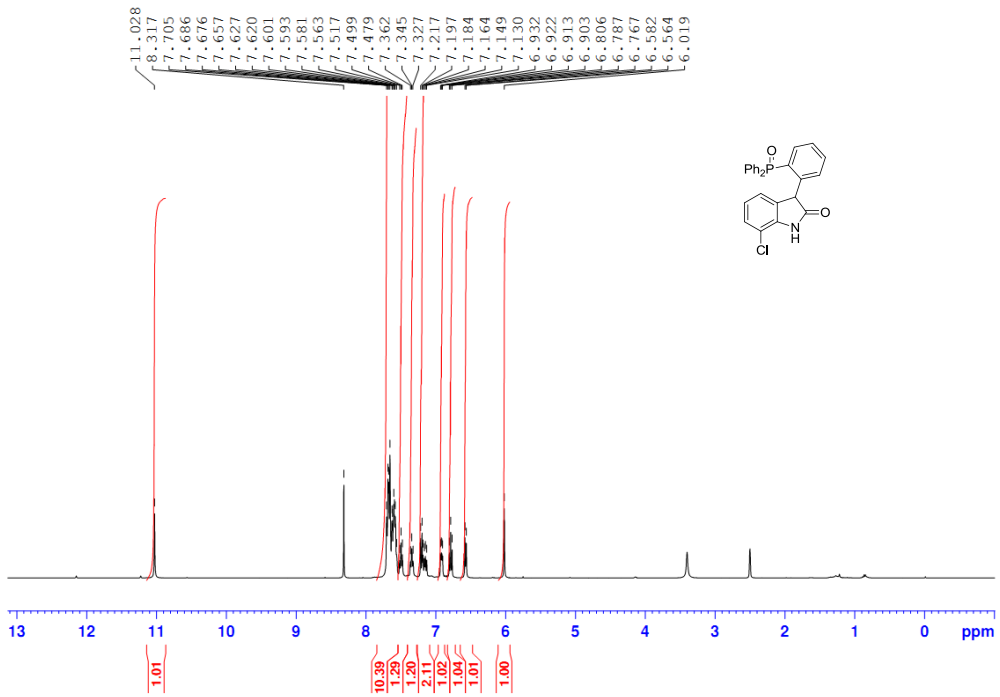
1-Acetyl-5-chloro-3-(2-(diphenylphosphoryl)phenyl)-7-methylindolin-2-one (3t) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



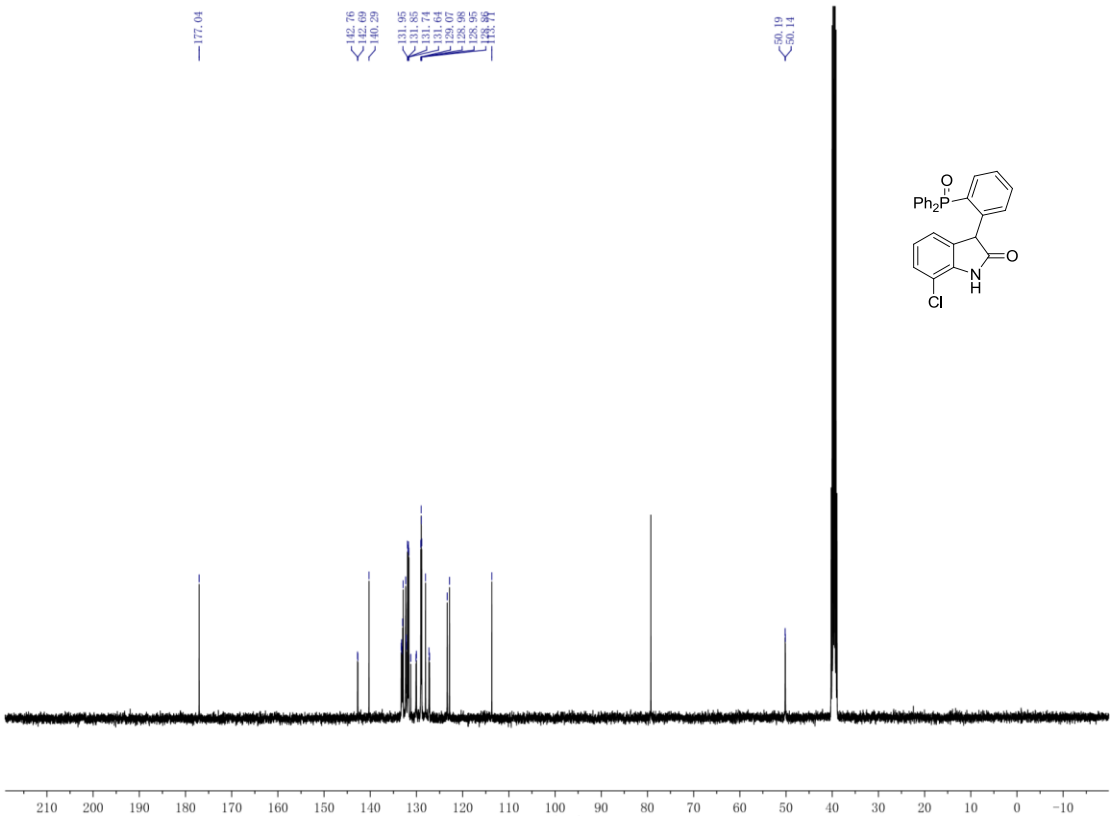
1-Acetyl-5-chloro-3-(2-(diphenylphosphoryl)phenyl)-7-methylindolin-2-one (3t) ^{31}P NMR (162 MHz, $CDCl_3$)



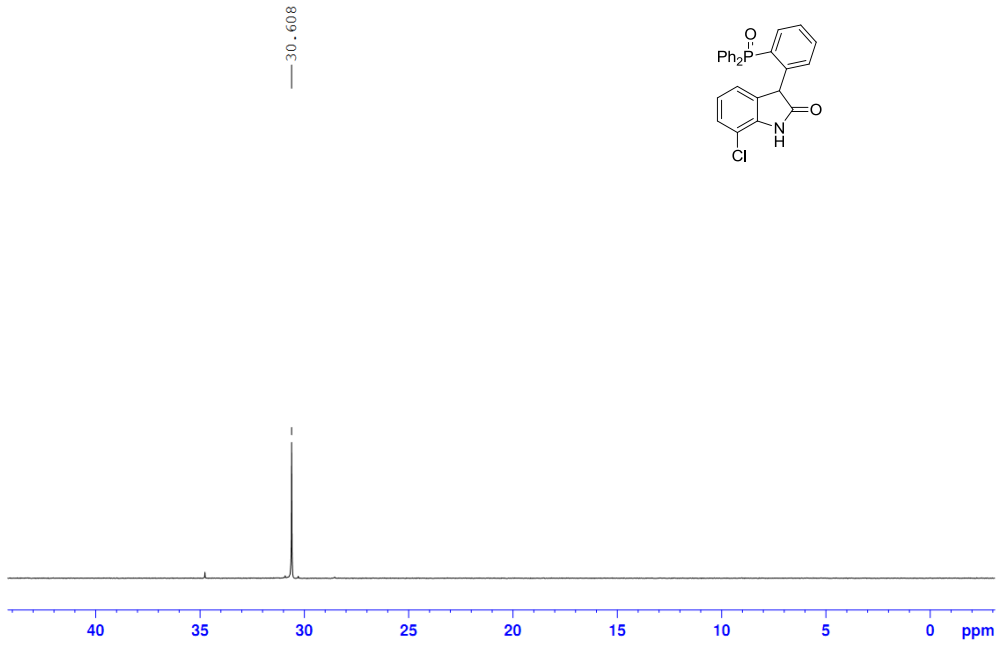
7-Chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5d) ^{1}H NMR (400 MHz, DMSO-*d6*)



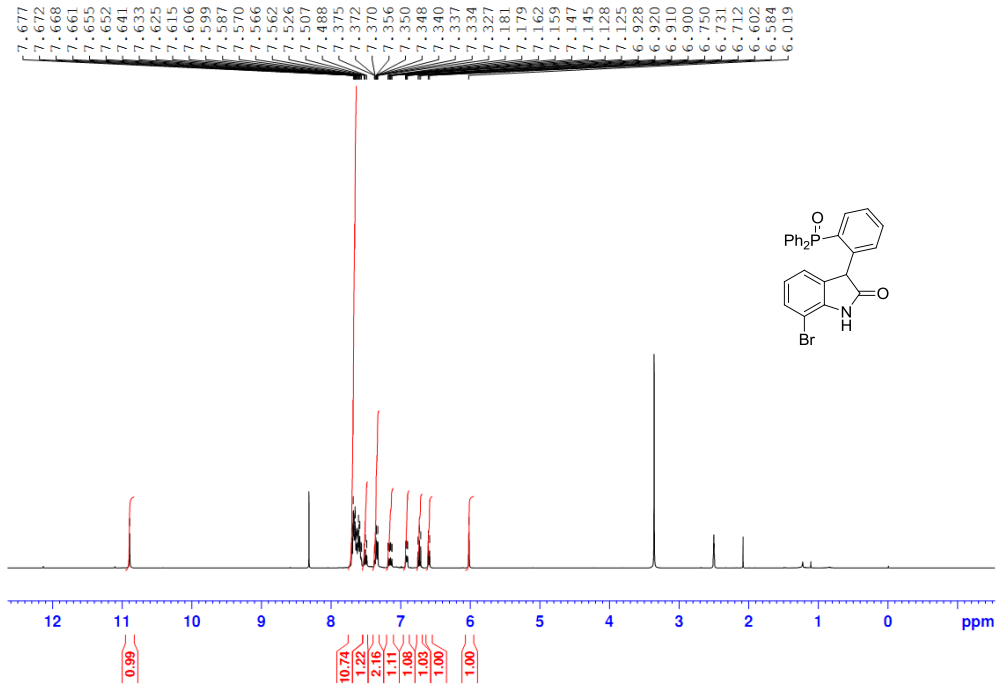
7-Chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5d) ^{13}C{^{1}H} NMR (100 MHz, DMSO-*d6*)



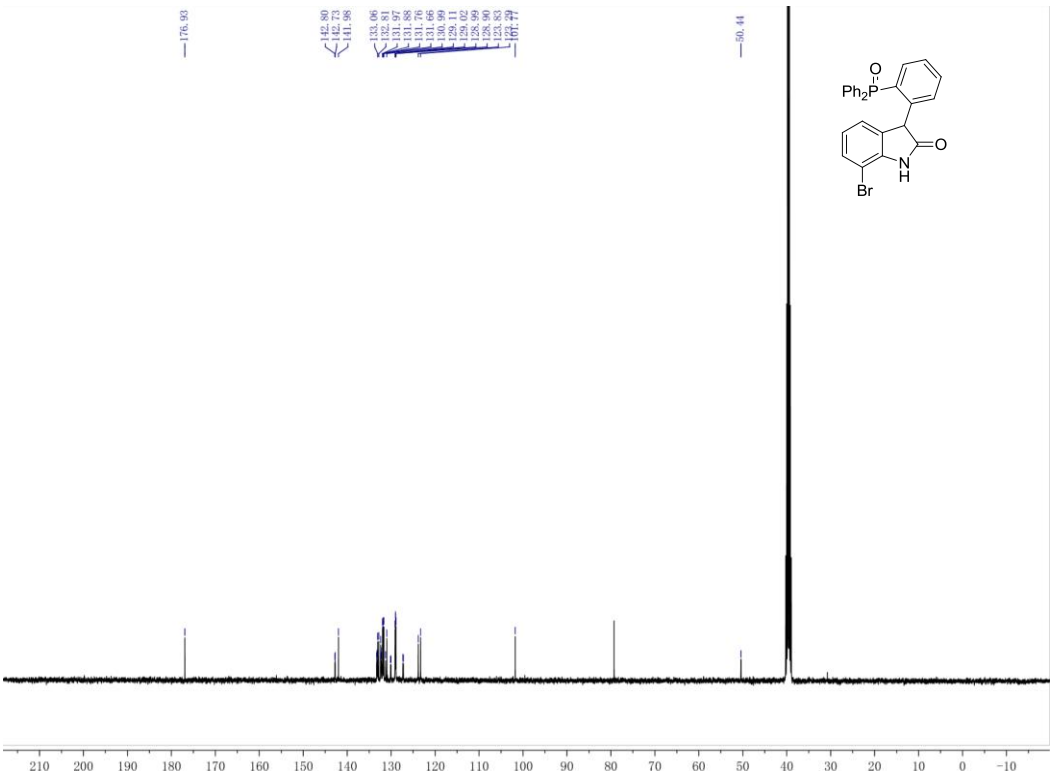
7-Chloro-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5d) ^{31}P NMR (162 MHz, DMSO-*d6*)



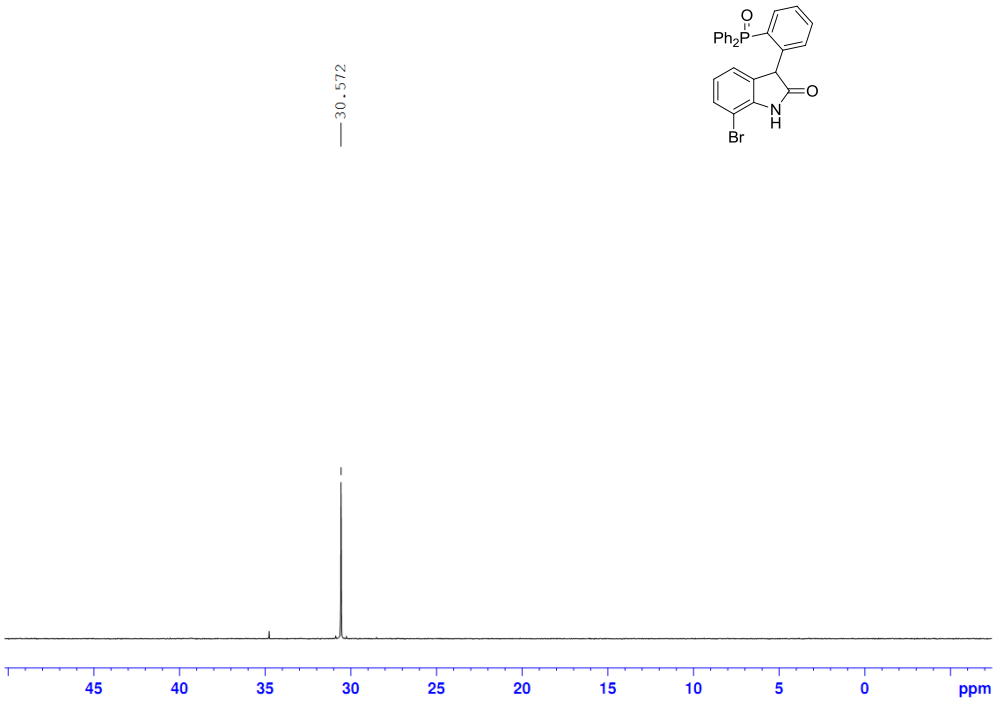
7-Bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5e) ^{1}H NMR (400 MHz, DMSO-*d6*)



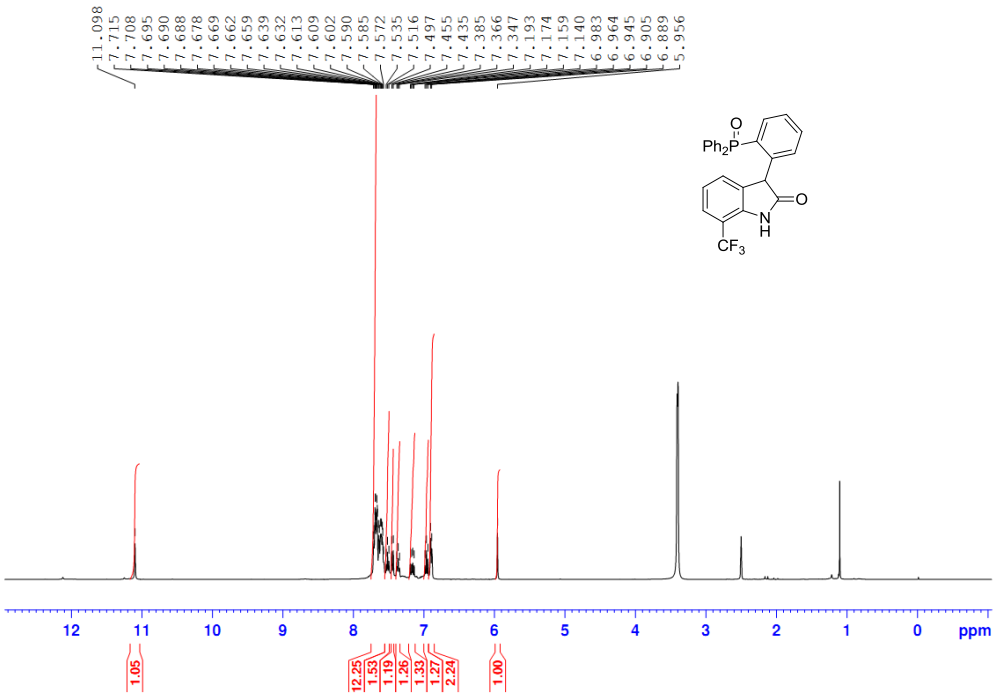
7-Bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5e) $^{13}C\{^{1}H\}$ NMR (100 MHz, DMSO-*d6*)



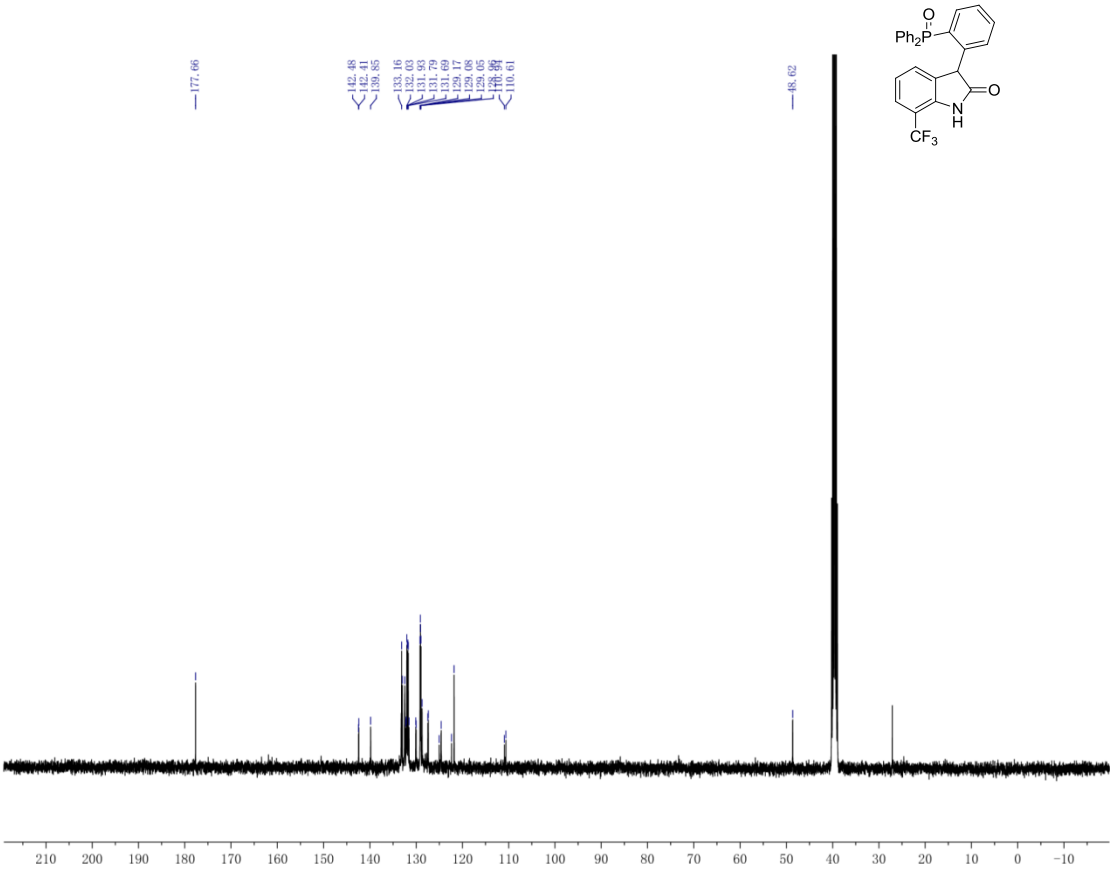
7-Bromo-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5e) ^{31}P NMR (162 MHz, DMSO-*d6*)



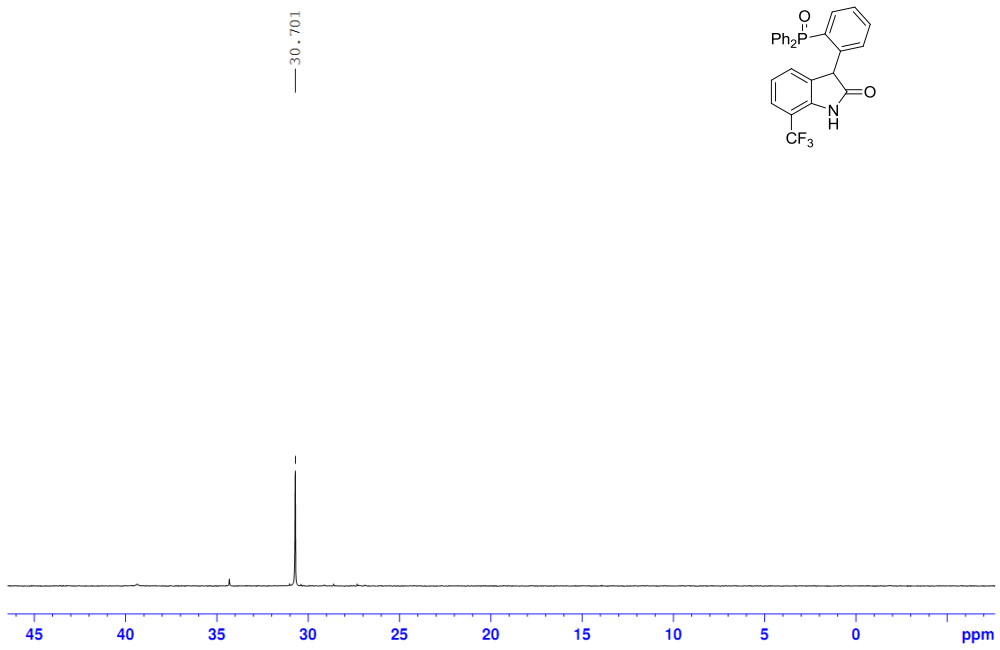
3-(2-(Diphenylphosphoryl)phenyl)-7-(trifluoromethyl)indolin-2-one (5g) ^{1}H NMR (400 MHz, DMSO-*d6*)



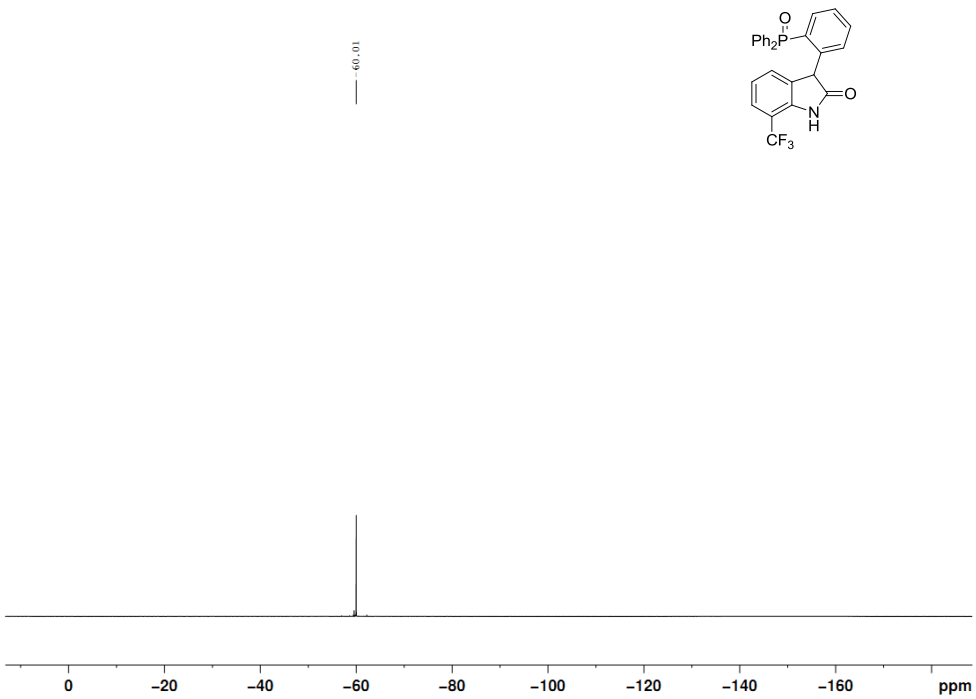
3-(2-(Diphenylphosphoryl)phenyl)-7-(trifluoromethyl)indolin-2-one (5g) ^{13}C{^{1}H} NMR (100 MHz, DMSO-*d6*)



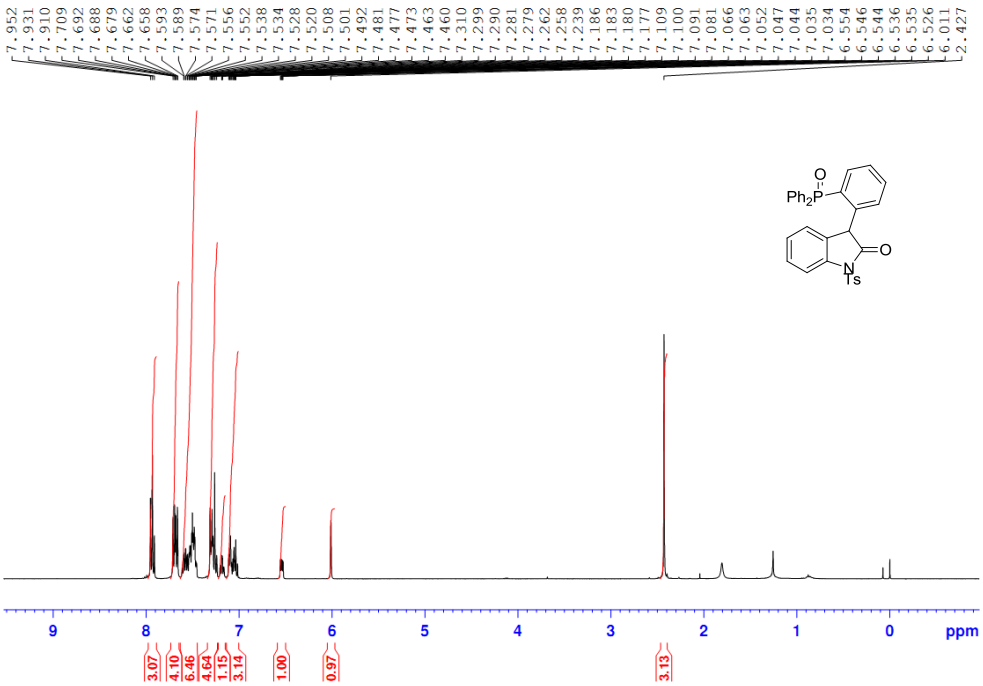
3-(2-(Diphenylphosphoryl)phenyl)-7-(trifluoromethyl)indolin-2-one (5g) ^{31}P NMR (162 MHz, DMSO-*d6*)



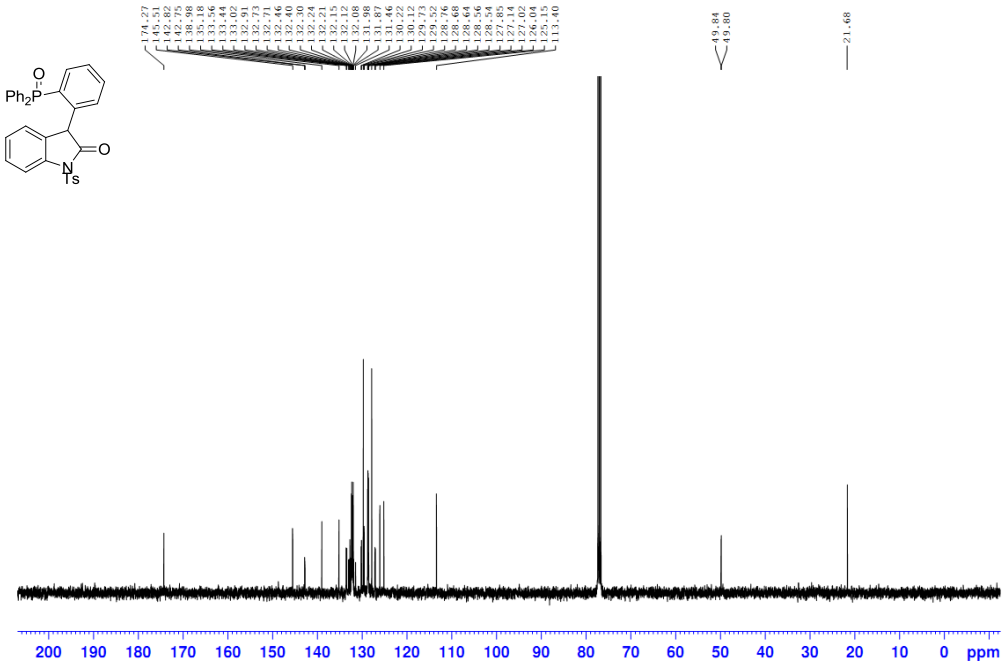
3-(2-(Diphenylphosphoryl)phenyl)-7-(trifluoromethyl)indolin-2-one (5g) ^{19}F NMR (376 MHz, DMSO-*d6*)



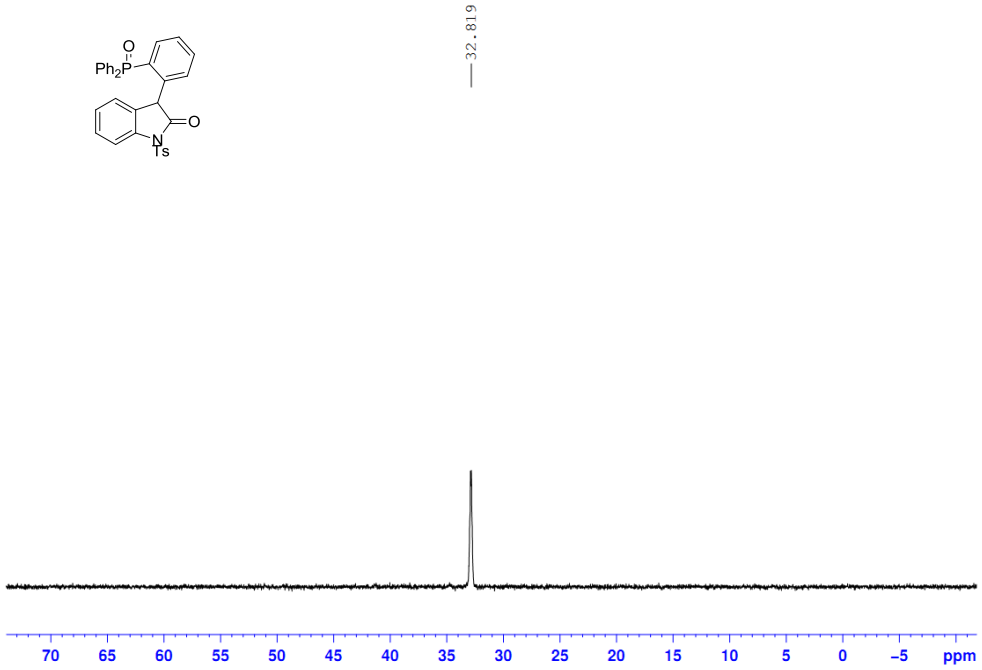
3-(2-(Diphenylphosphoryl)phenyl)-1-tosylindolin-2-one (5i) ^{1}H NMR (400 MHz, $CDCl_3$)



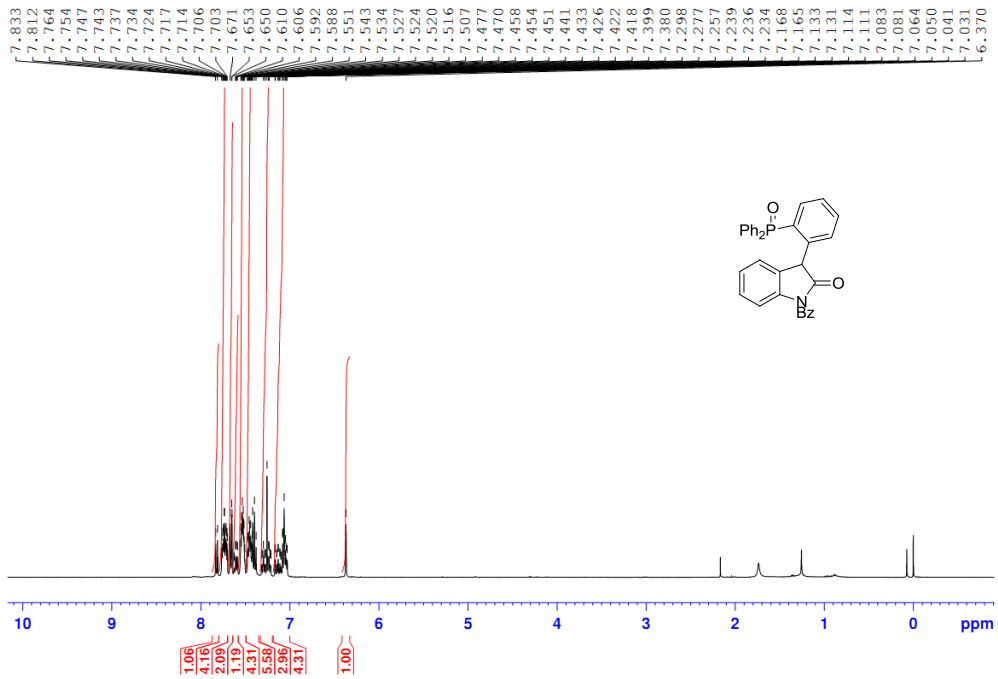
3-(2-(Diphenylphosphoryl)phenyl)-1-tosylindolin-2-one (5i) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



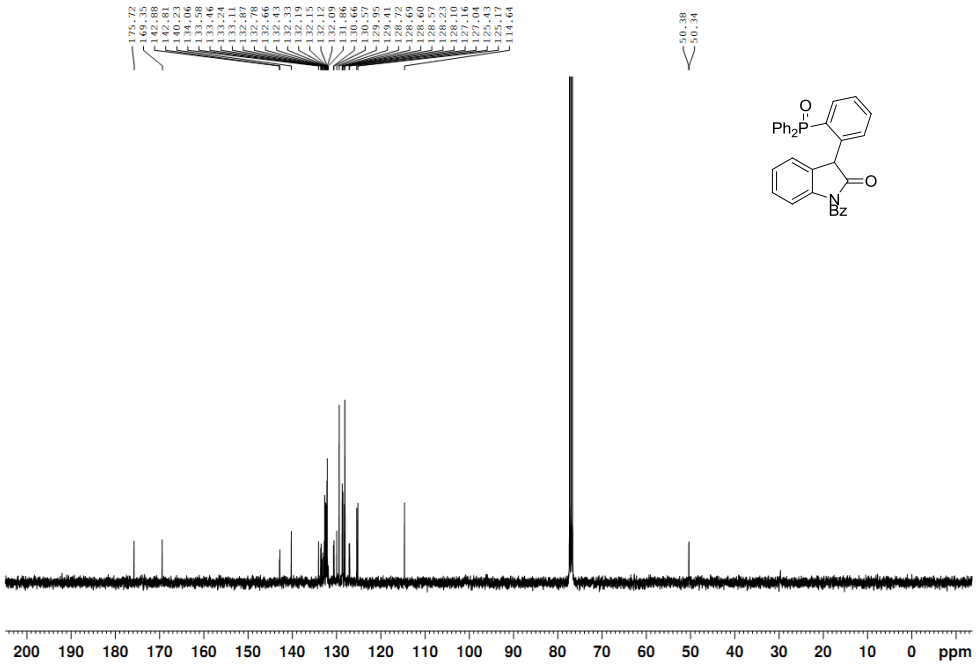
3-(2-(Diphenylphosphoryl)phenyl)-1-tosylindolin-2-one (5i) ^{31}P NMR (162 MHz, $CDCl_3$)



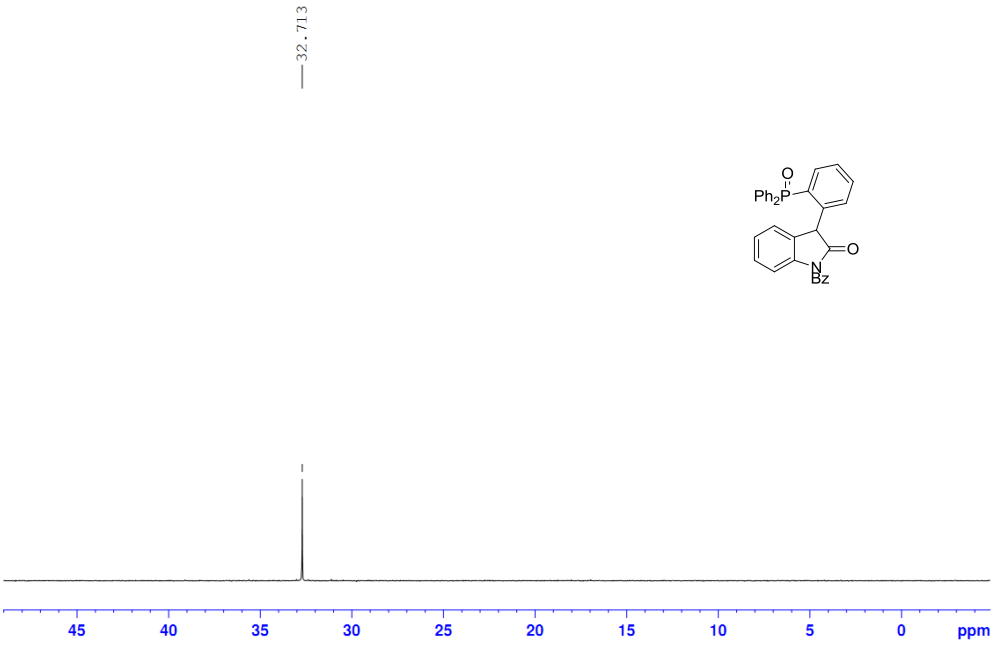
1-Benzoyl-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5j) ^{1}H NMR (400 MHz, $CDCl_3$)



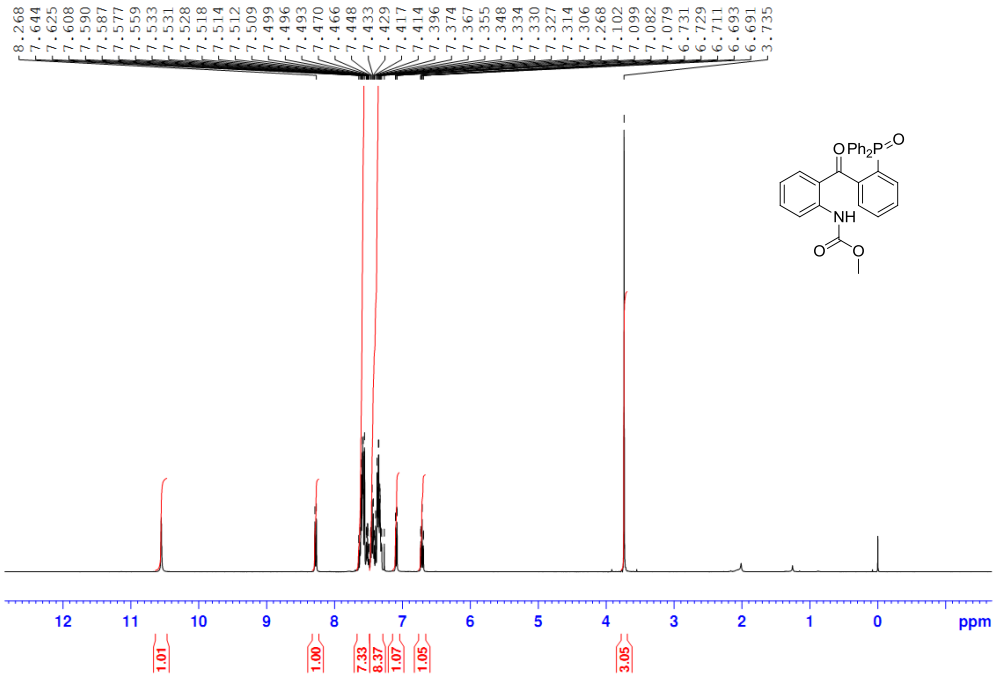
1-Benzoyl-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5j) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



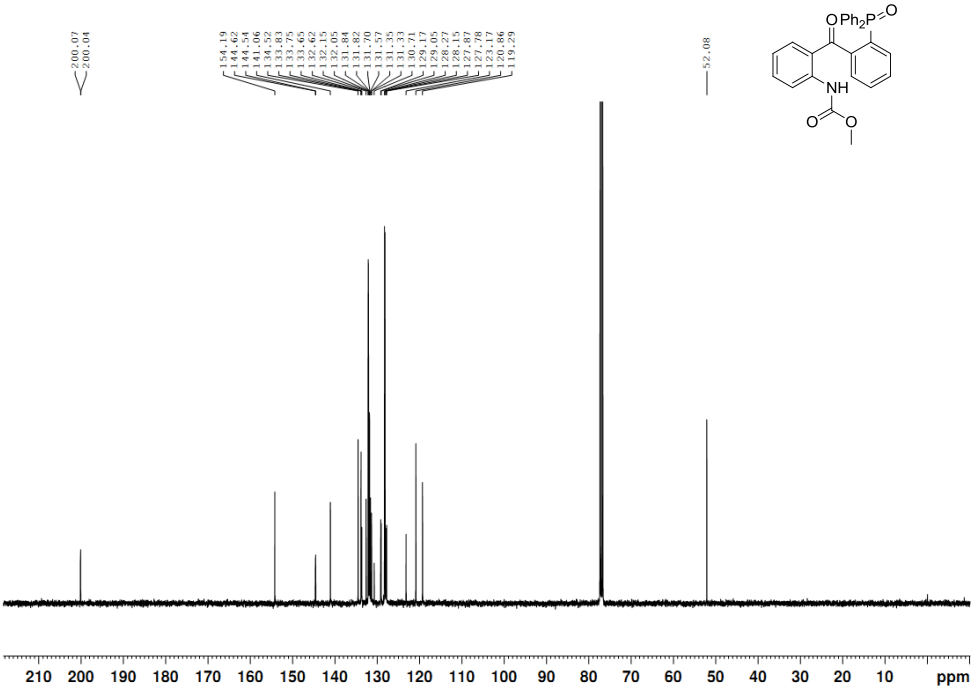
1-Benzoyl-3-(2-(diphenylphosphoryl)phenyl)indolin-2-one (5j) ^{31}P NMR (162 MHz, $CDCl_3$)



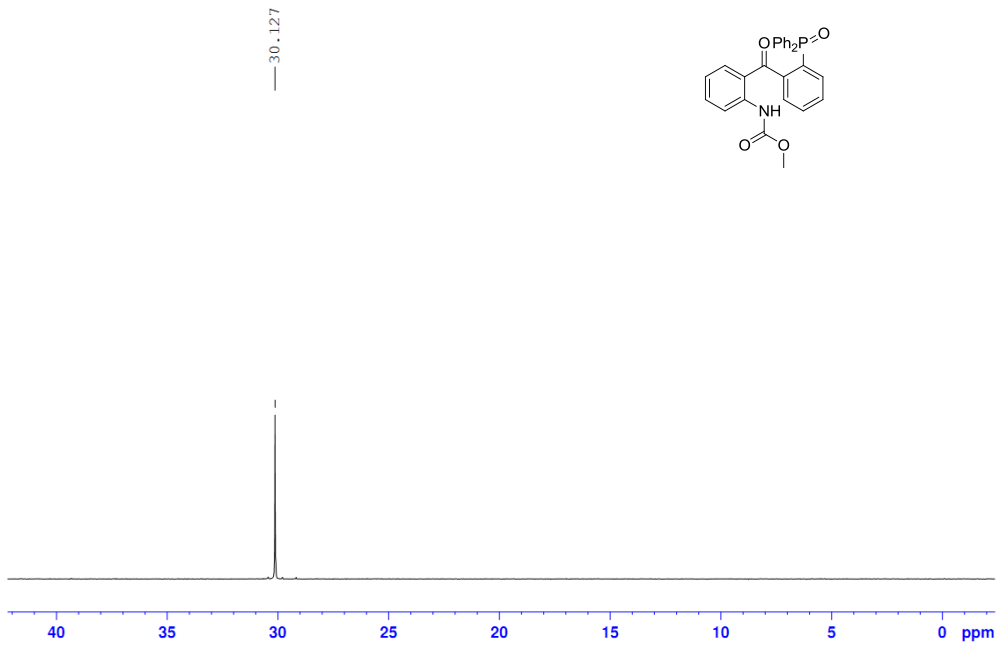
Methyl (2-(2-(diphenylphosphoryl)benzoyl)phenyl)carbamate (6a) ^{1}H NMR (400 MHz, $CDCl_3$)



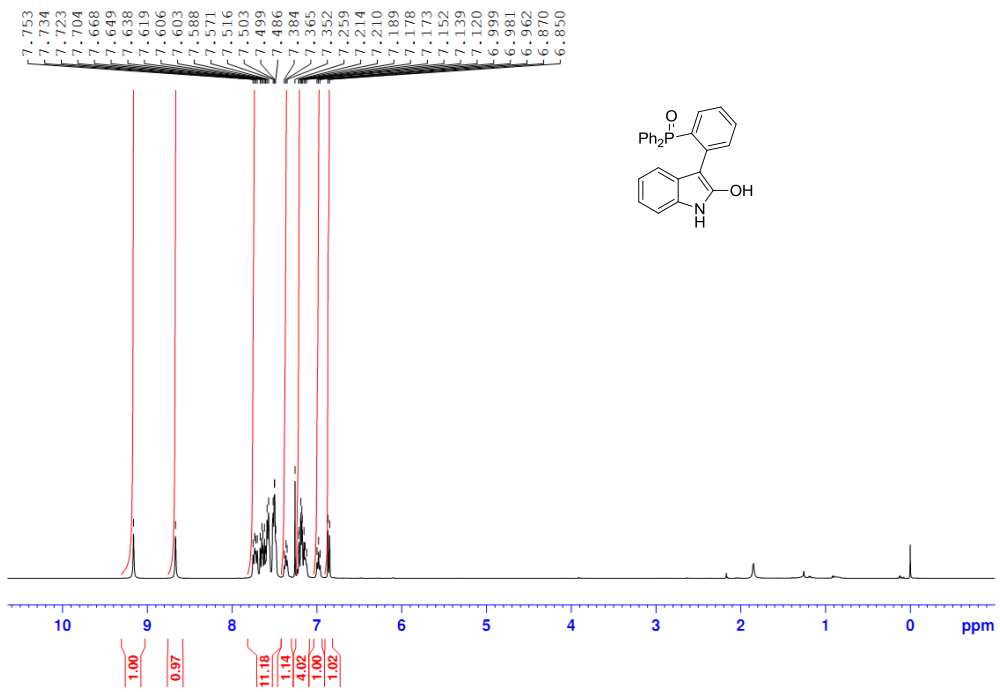
Methyl (2-(2-(diphenylphosphoryl)benzoyl)phenyl)carbamate (6a) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



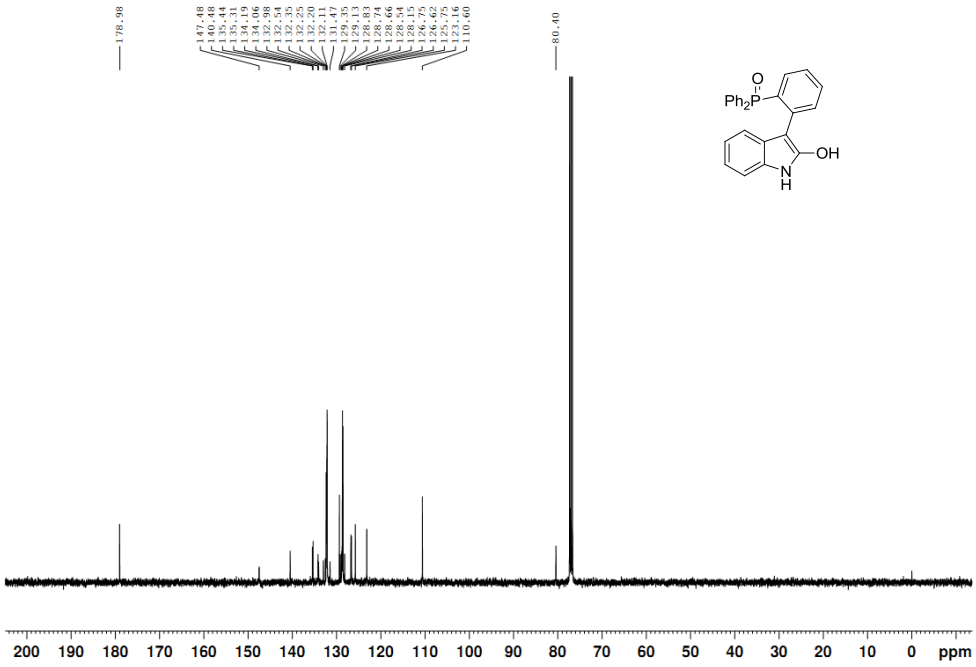
Methyl (2-(2-(diphenylphosphoryl)benzoyl)phenyl)carbamate (6a) ^{31}P NMR (162 MHz, $CDCl_3$)



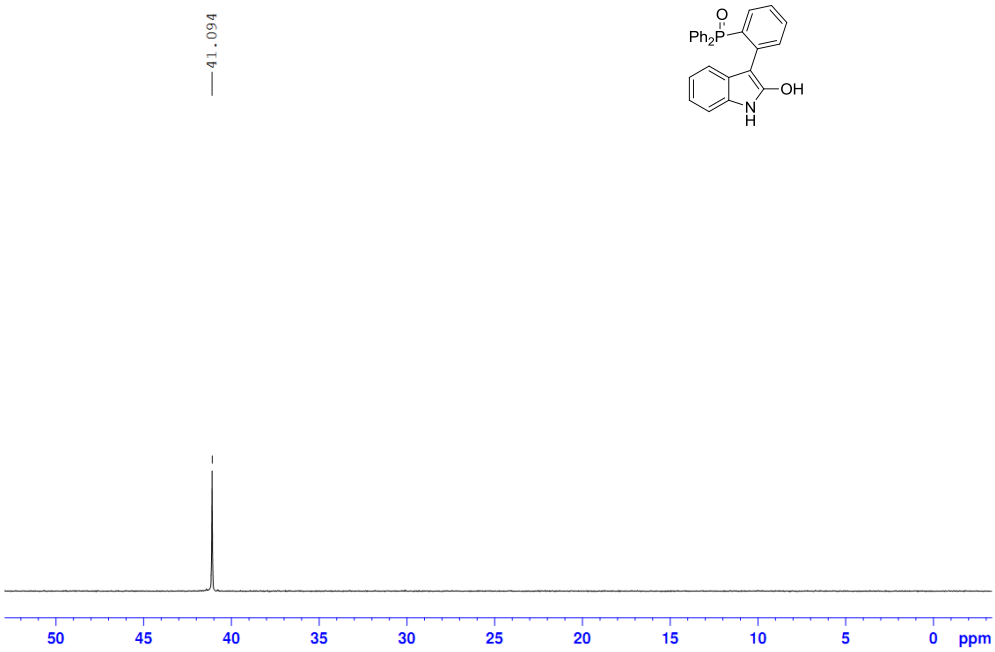
(2-(2-Hydroxy-1H-indol-3-yl)phenyl)diphenylphosphine oxide (7a) ^{1}H NMR (400 MHz, $CDCl_3$)



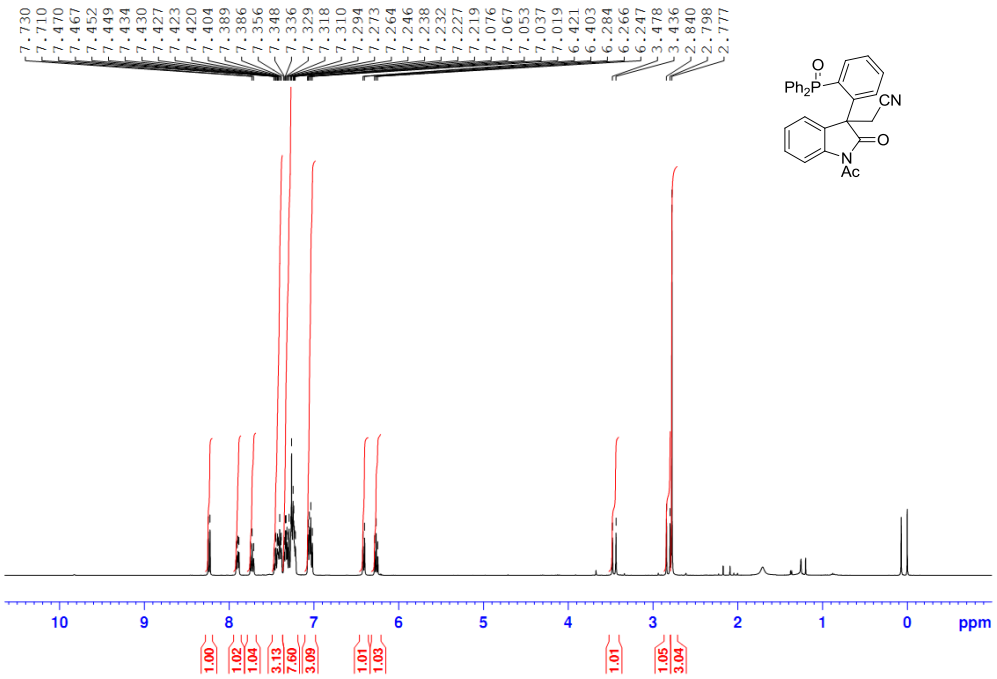
(2-(2-Hydroxy-1H-indol-3-yl)phenyl)diphenylphosphine oxide (7a) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



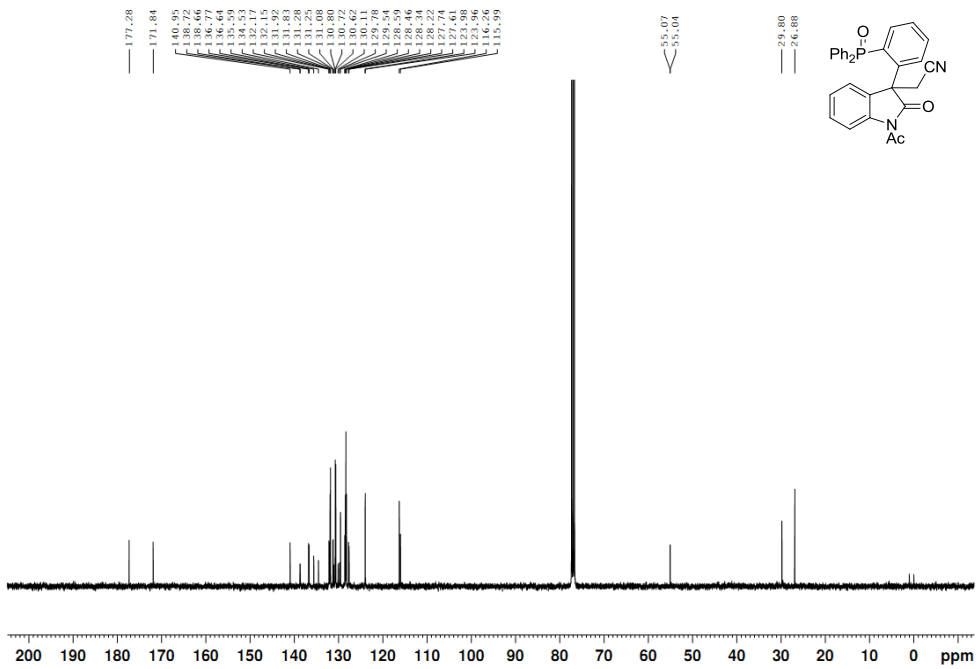
(2-(2-Hydroxy-1H-indol-3-yl)phenyl)diphenylphosphine oxide (7a) ^{31}P NMR (162 MHz, $CDCl_3$)



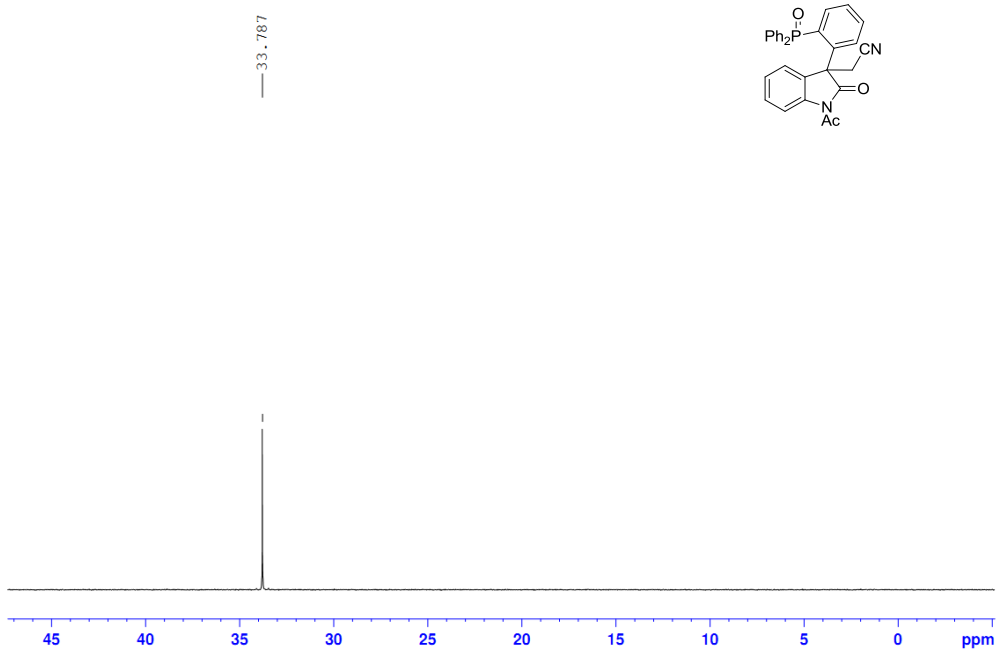
2-(1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-2-oxoindolin-3-yl)acetonitrile (8a) ^{1}H NMR (400 MHz, $CDCl_3$)



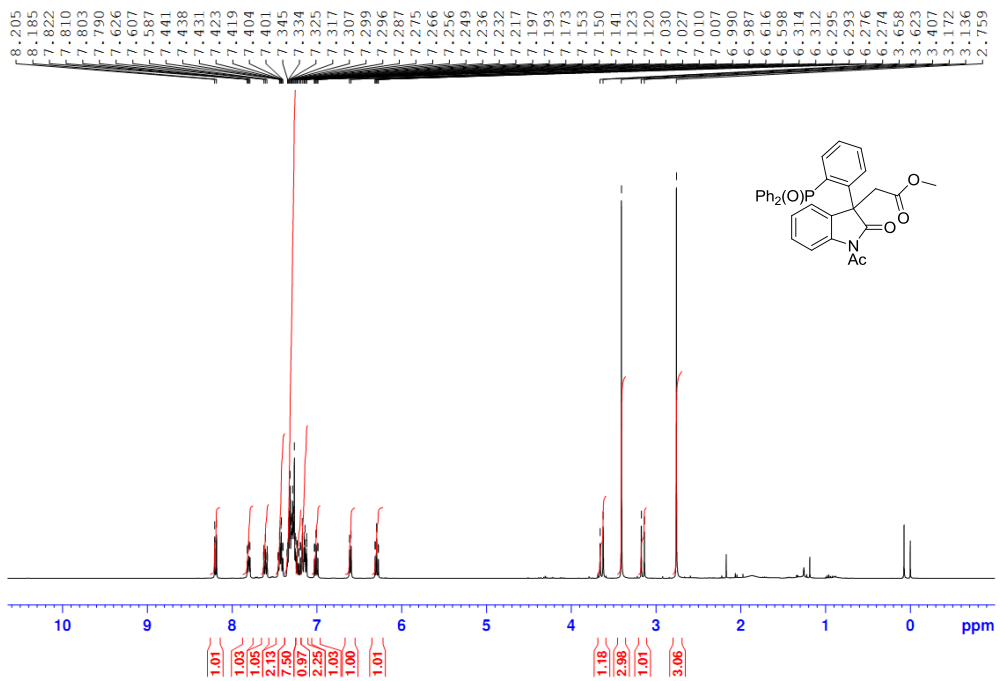
2-(1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-2-oxoindolin-3-yl)acetonitrile (8a) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



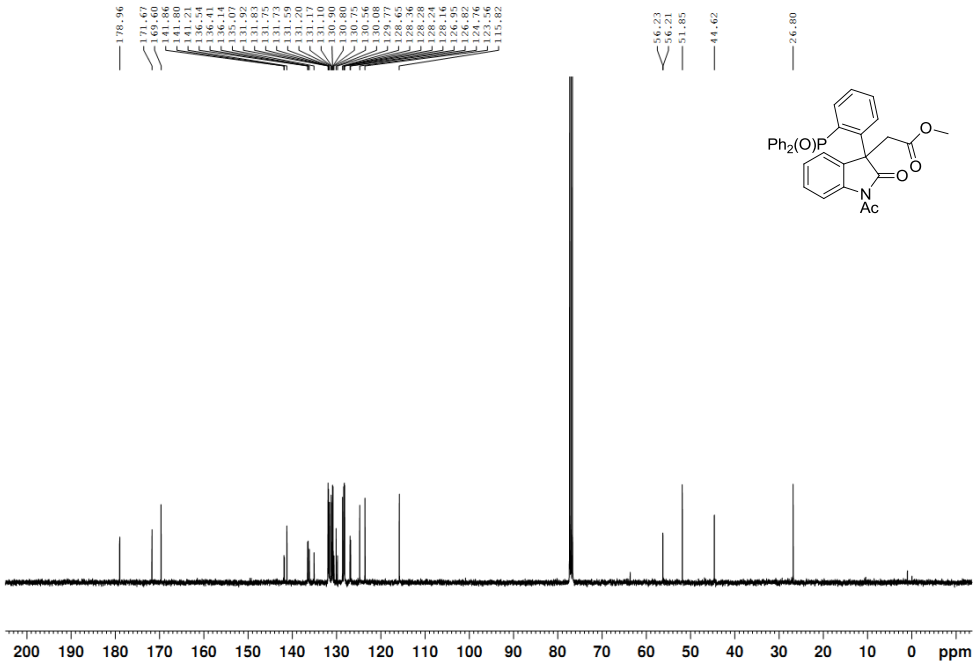
2-(1-Acetyl-3-(2-(diphenylphosphoryl)phenyl)-2-oxoindolin-3-yl)acetonitrile (8a) ^{31}P NMR (162 MHz, $CDCl_3$)



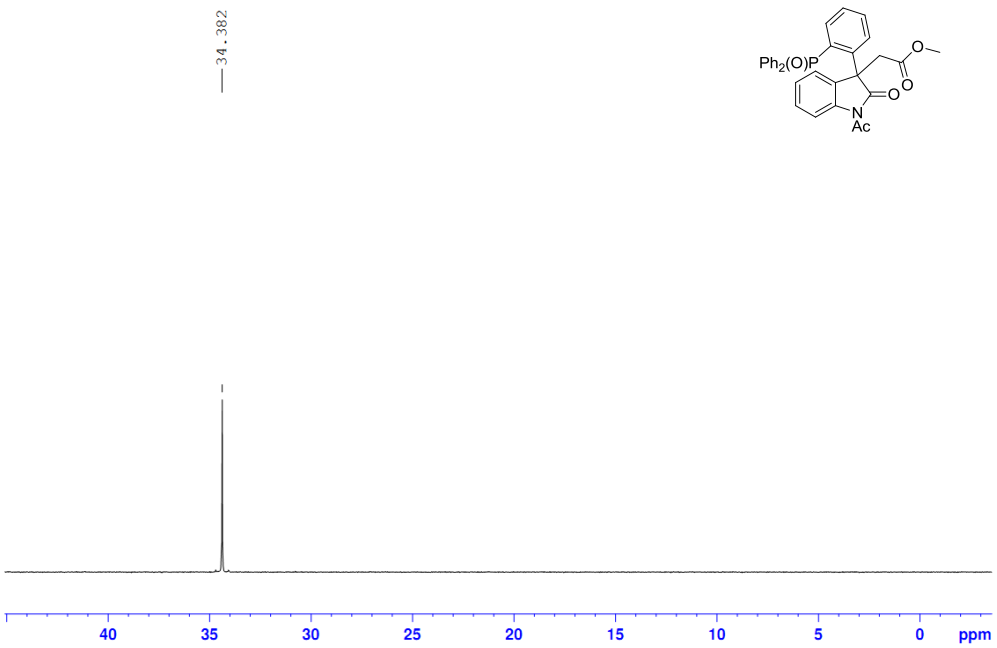
Methyl 2-(1-acetyl-3-(2-(diphenylphosphoryl)phenyl)-2-oxoindolin-3-yl)acetate (9a) ^{1}H NMR (400 MHz, $CDCl_3$)



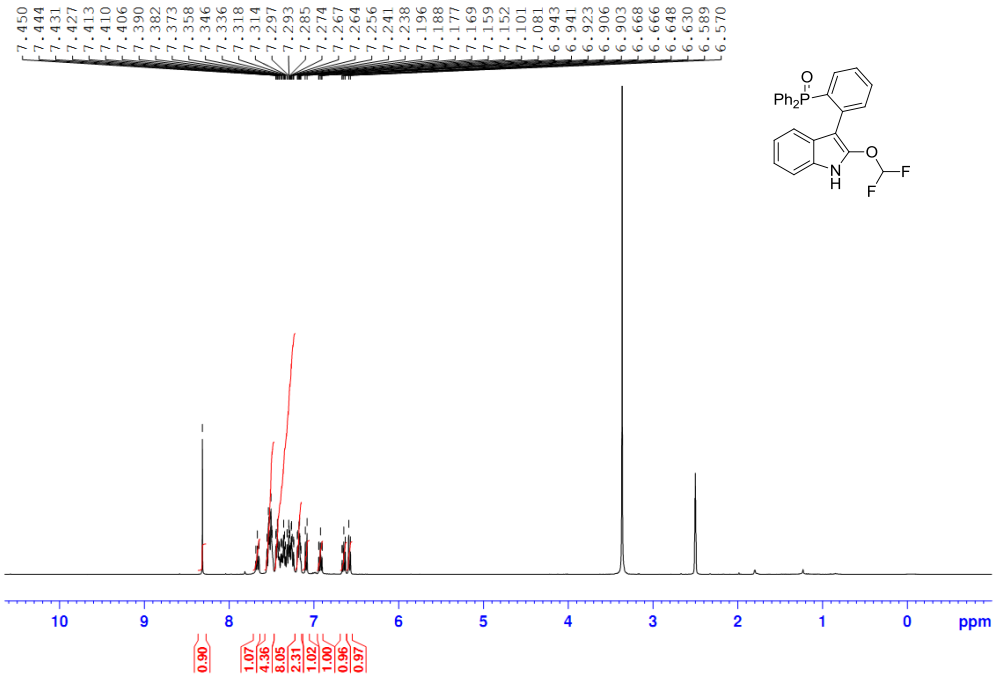
Methyl 2-(1-acetyl-3-(2-(diphenylphosphoryl)phenyl)-2-oxoindolin-3-yl)acetate (9a) $^{13}C\{^{1}H\}$ NMR (100 MHz, $CDCl_3$)



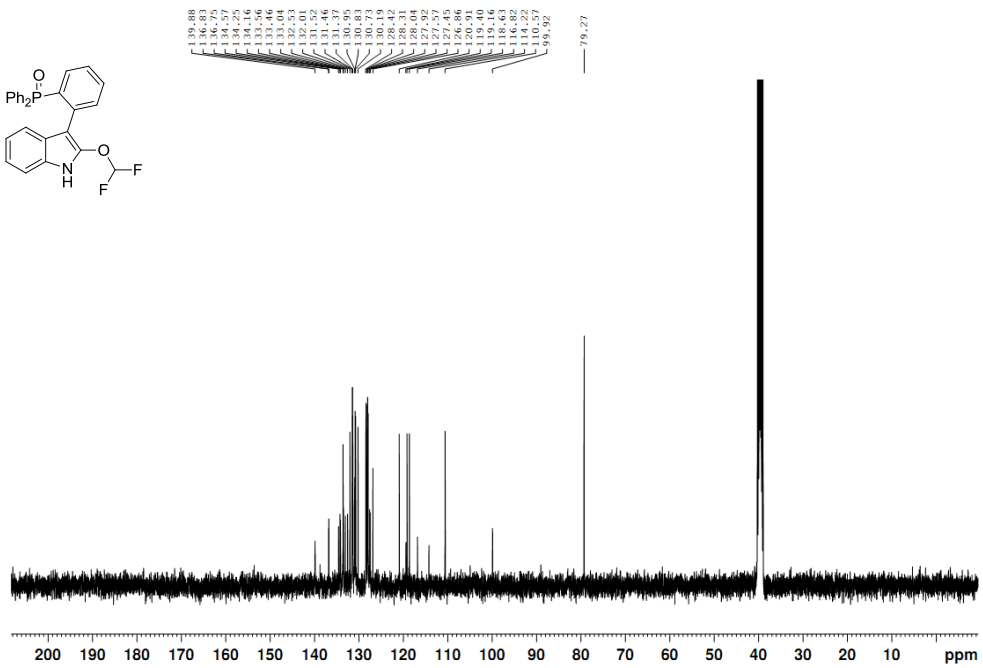
Methyl 2-(1-acetyl-3-(2-(diphenylphosphoryl)phenyl)-2-oxoindolin-3-yl)acetate (9a) ^{31}P NMR (162 MHz, $CDCl_3$)



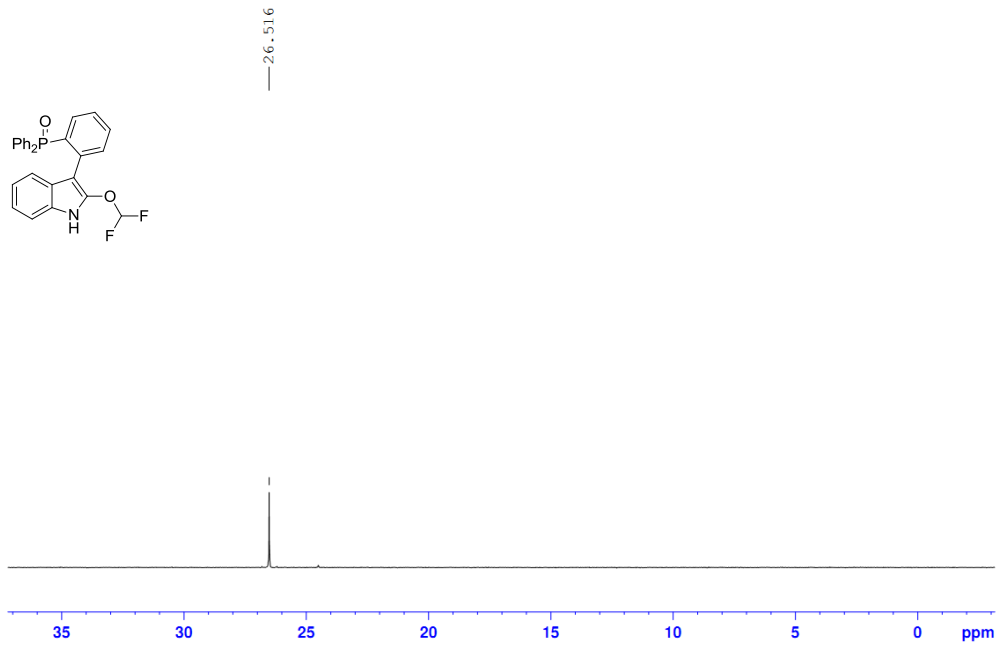
(2-(2-(Difluoromethoxy)-1H-indol-3-yl)phenyl)diphenylphosphine oxide (10a) ^{1}H NMR (400 MHz, $CDCl_3$)



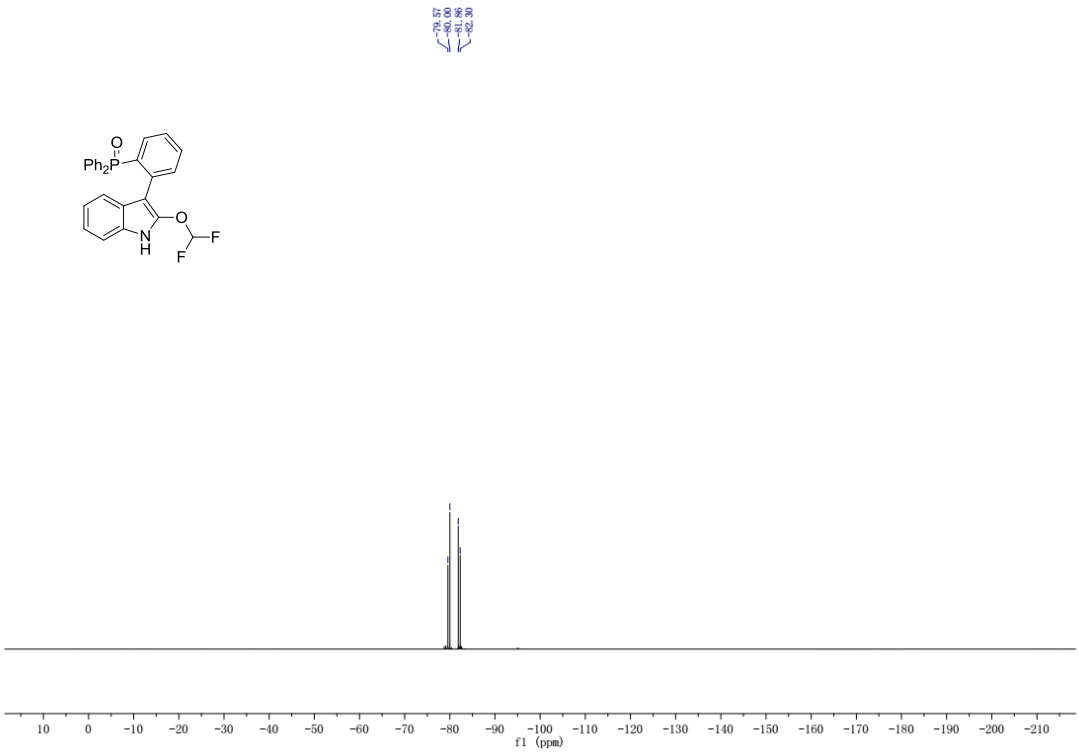
(2-(2-(Difluoromethoxy)-1H-indol-3-yl)phenyl)diphenylphosphine oxide (10a) ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$)



(2-(2-(Difluoromethoxy)-1H-indol-3-yl)phenyl)diphenylphosphine oxide (10a) ^{31}P NMR (162 MHz, $CDCl_3$)



(2-(2-(Difluoromethoxy)-1H-indol-3-yl)phenyl)diphenylphosphine oxide (10a) ^{19}F NMR (376 MHz, DMSO-*d6*)



4. *X*-ray structure of 3a

The absolute configuration of **3a** was determined by single crystal *X*-ray analysis. (CCDC 1959970 contains the supplementary crystallographic data for this structure. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre).

***X*-ray structure of product 3a (ellipsoid contour at 50% probability)**

Experimental

Single crystals of **3a** ($C_{28}H_{22}NO_3P$) were grown by slow evaporation in hexane/ dichloromethane = 3/1 under air atmosphere. A suitable crystal was selected and mounted on a XtaLAB Synergy R, DW system, HyPix diffractometer. The crystal was kept at 292(10) K during data collection. Using Olex2, the structure was solved with the ShelXS structure solution program using Direct Methods and refined with the ShelXL refinement package using Least Squares minimisation.

Crystal structure determination of 3a

Crystal Data for **3a** ($C_{28}H_{22}NO_3P$), MW = 451.43, triclinic, space group P-1, a = 8.3188(8) Å, b=9.3992(11) Å, c = 15.4909(9) Å, α = 75.866(7)°, β = 82.881(6)°, γ = 74.752(9)°, V = 1130.91(19) Å^3 , T = 292(10) K, Z = 2, μ(CuKα) = 1.542 mm^{-1}, *Dcalc* = 1.326 g/cm^3, 6616 reflections measured (9.843° ≤ 2Θ ≤ 69.741 °), 3867 unique (R_{int} = 0.0616, R_{sigma} = 0.0433) which were used in all calculations. The final R_1 was 0.0752 [I > 2σ(I)] and wR_2 was 0.2443 (all data).

Bond precision:	C-C = 0.0075 A		Wavelength = 1.54184
Cell:	a = 8.3188(8)	b = 9.3992(11)	c = 15.4909(9)
	alpha = 75.866(7)	beta = 82.881(6)	gamma = 74.752(9)
Temperature: 292 K			

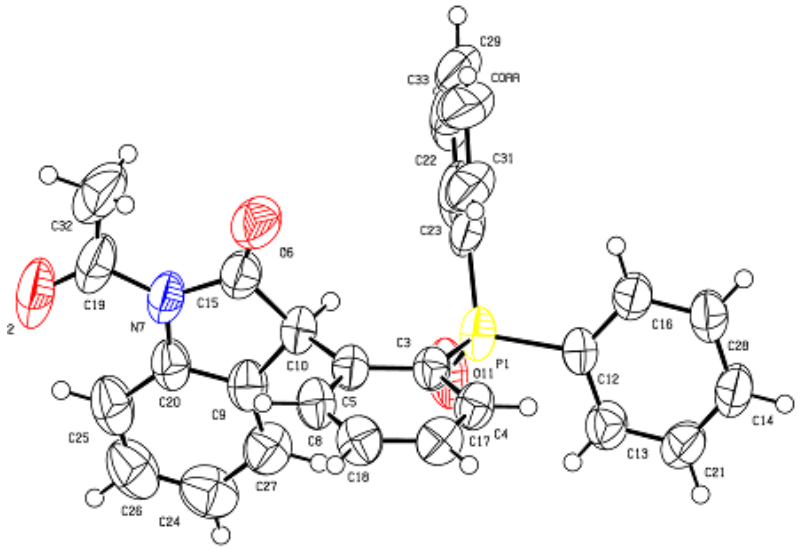
	Calculated	Reported
Volume	1130.91(19)	1130.91(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C28 H22 N O3 P	C28 H22 N O3 P
Sum formula	C28 H22 N O3 P	C28 H22 N O3 P
Mr	451.44	451.43
Dx,g cm-3	1.326	1.326
Z	2	2
Mu (mm-1)	1.326	1.326
F000	472.0	472.0
F000'	473.90	
h,k,lmax	9,11,18	9,11,18
Nref	3977	3867
Tmin,Tmax	0.788,0.853	0.705,1.000
Tmin'	0.788	

Correction method= # Reported T Limits: Tmin = 0.705 Tmax = 1.000 AbsCorr = MULTI-SCAN

Data completeness = 0.972 Theta(max) = 66.591

R(reflections) = 0.0752(2686) wR2(reflections) = 0.2443(3867)

S = 1.104 Npar = 299



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