

Catalyst-free synthesis of α^1 -oxindole- α -hydroxyphosphonates via phospha-aldol reaction of isatins employing N-heterocyclic phosphine (NHP)-thiourea

Nagaraju Molleti and Jun Yong Kang^{*}

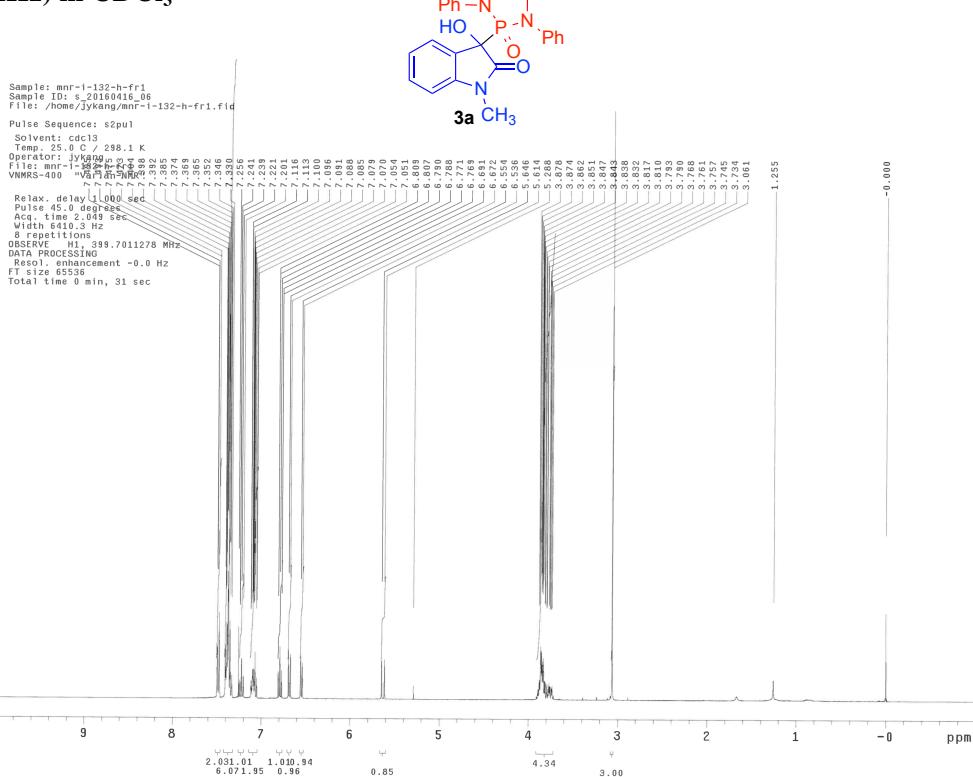
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4505 S. Maryland Parkway, Las Vegas, Nevada, 89154-4003, United States

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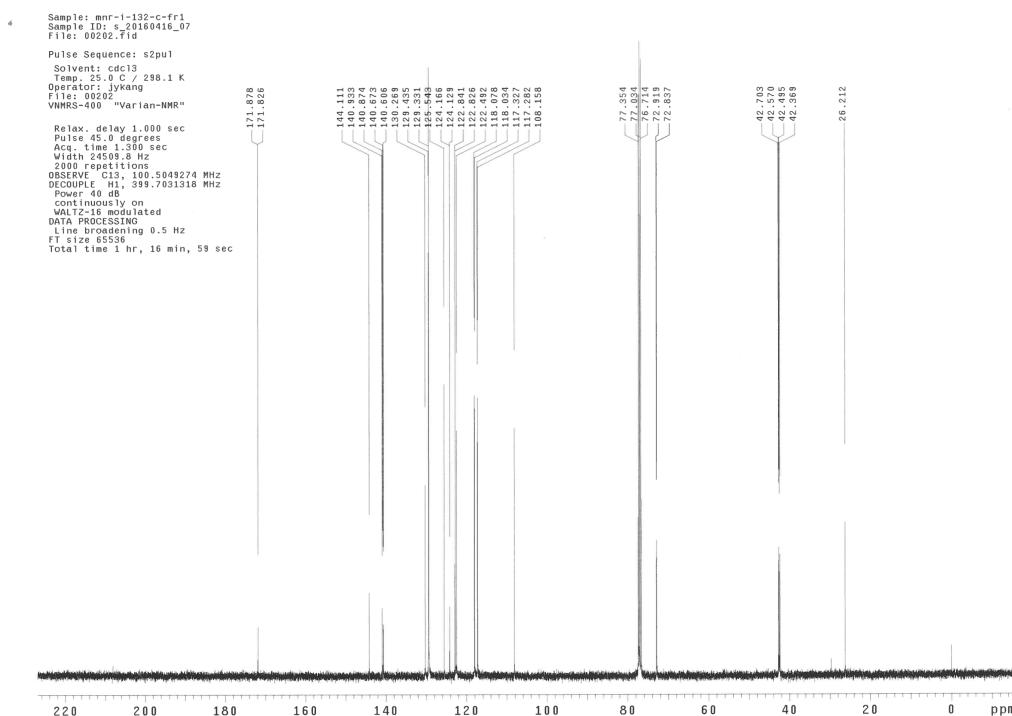
Supporting Information

^1H and ^{13}C NMR Spectra.....	S2
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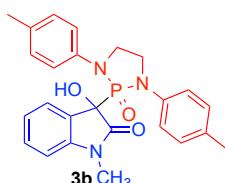
¹H NMR (400 MHz) in CDCl₃



¹³C NMR (100.5 MHz) in CDCl₃



¹H NMR (400 MHz) in CDCl₃



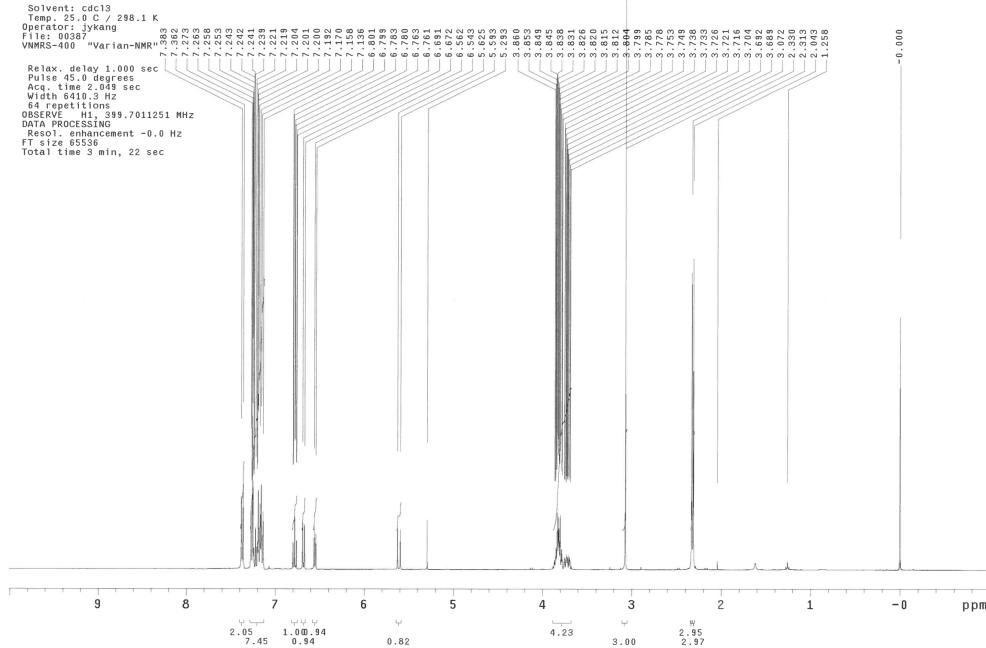
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Sample ID: s_20160504_10
File: 00387.fid

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Solvent: cdcl3
Tempr.: 25.0 C / 298.1 K
Operator: lykang
File #: 00387
VNMRGS-400 "Varian-NMR"

Relax, delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 6410.3 Hz
64 repetitions
OBSERVE F1 399.7011251 MHz
DATA POINTS 1024
RF enhancement -0.0 Hz
FT size 65536
Total time 3 min. 22 sec

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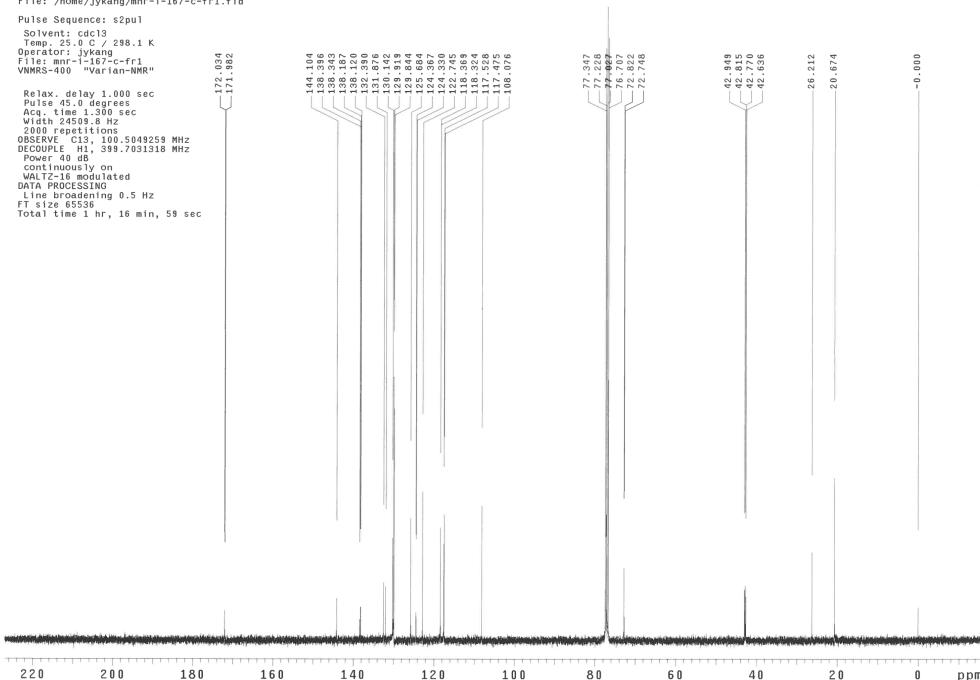
¹³C NMR (100.5 MHz) in CDCl₃

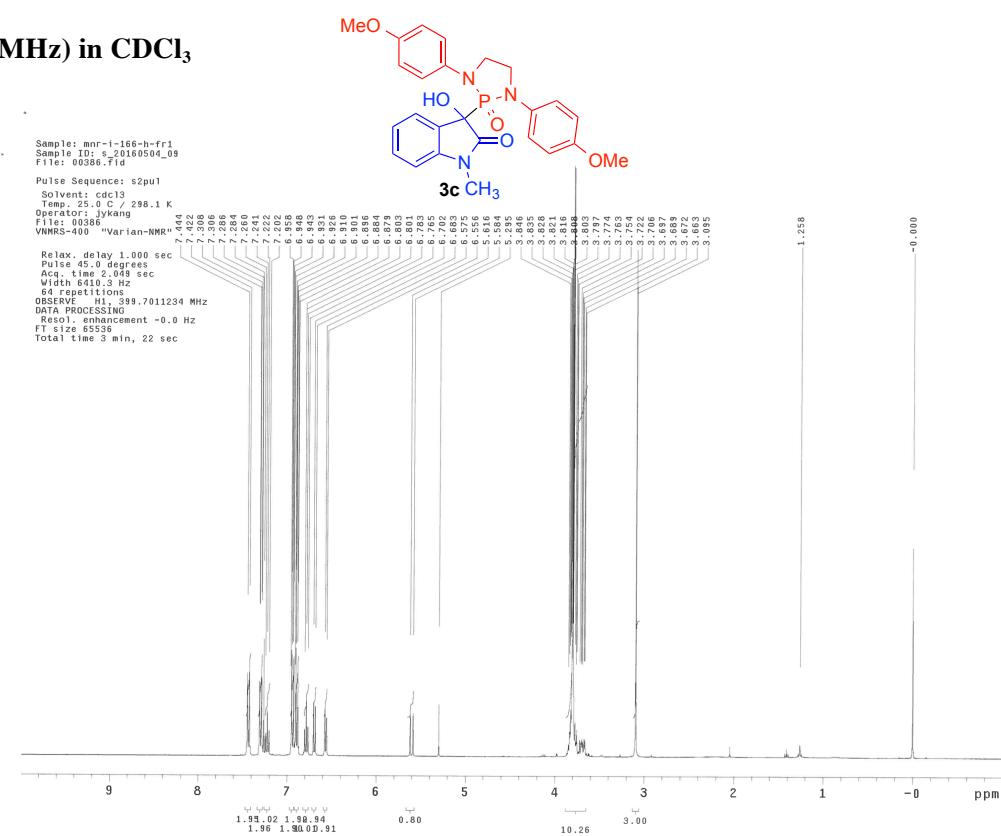
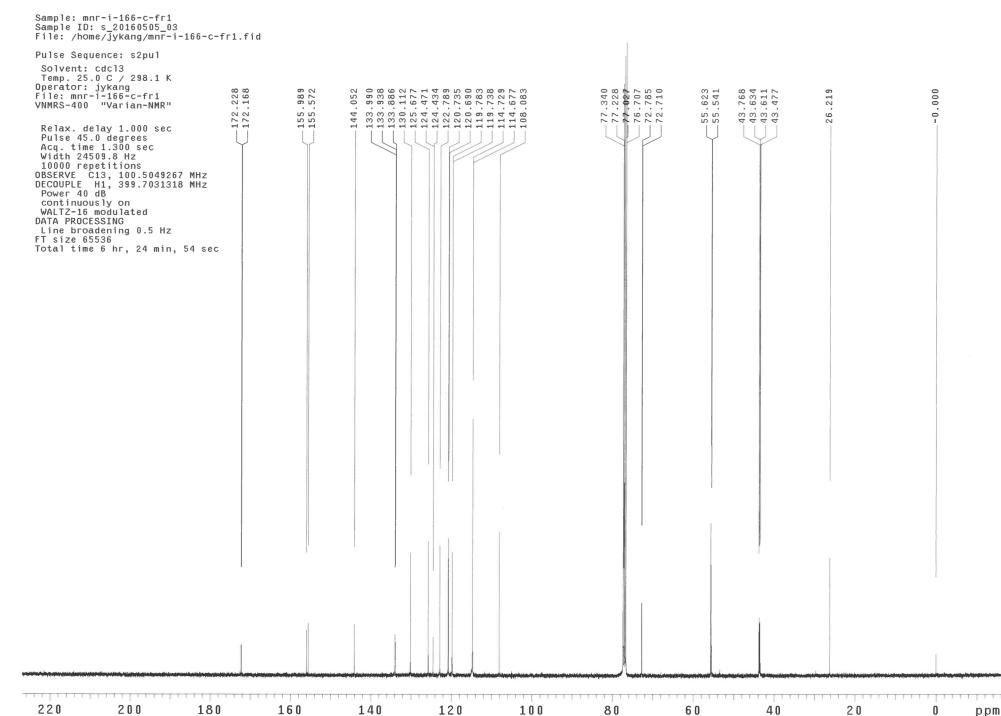
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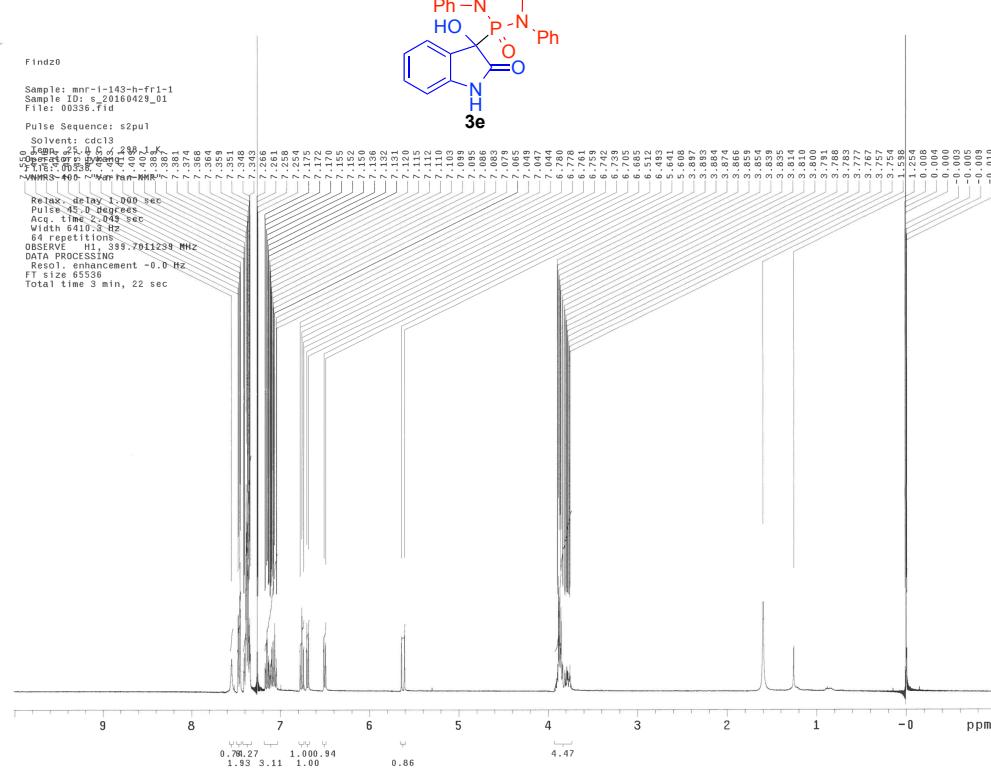
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Solvent: cdcl3
Temp: 25.0 C / 288.1 K
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Relax, delay 1.000 sec
Pulse, 45.0 degrees
AcqTime, 1.000 sec
Width 24509.8 Hz
2000 repetitions
CenterFreq, 300.5048259 MHz
DECcoupling, 399.7031318 MHz
Power 40 dB
CrossPolar, 1000
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
Filter, 100 Hz
Total time 1 hr, 16 min, 59 sec

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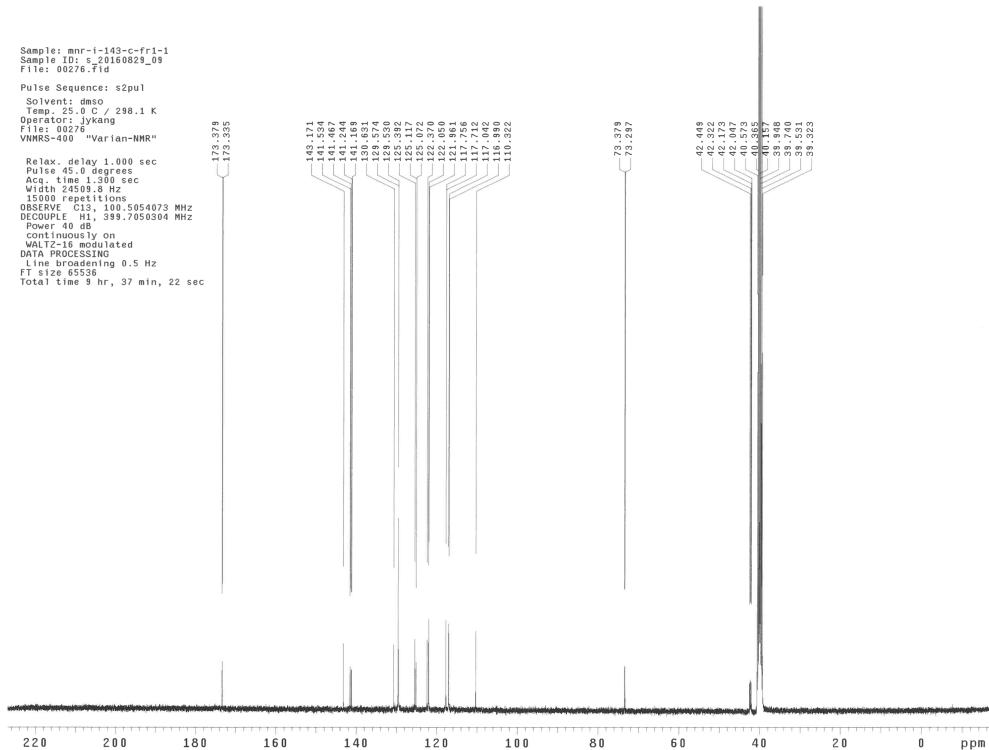


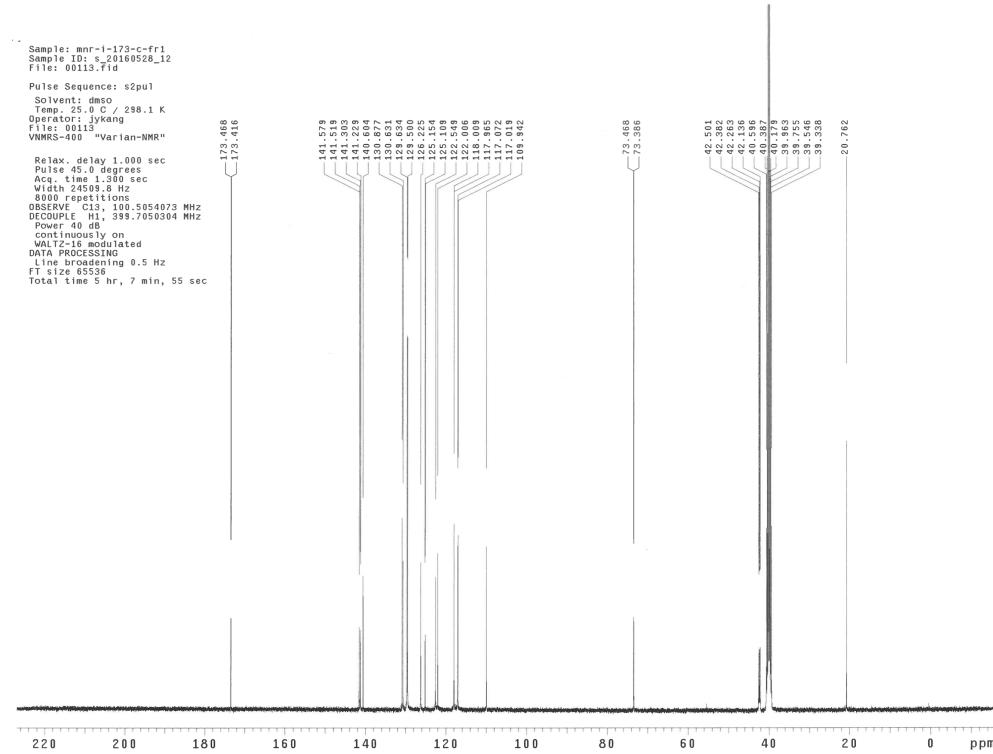
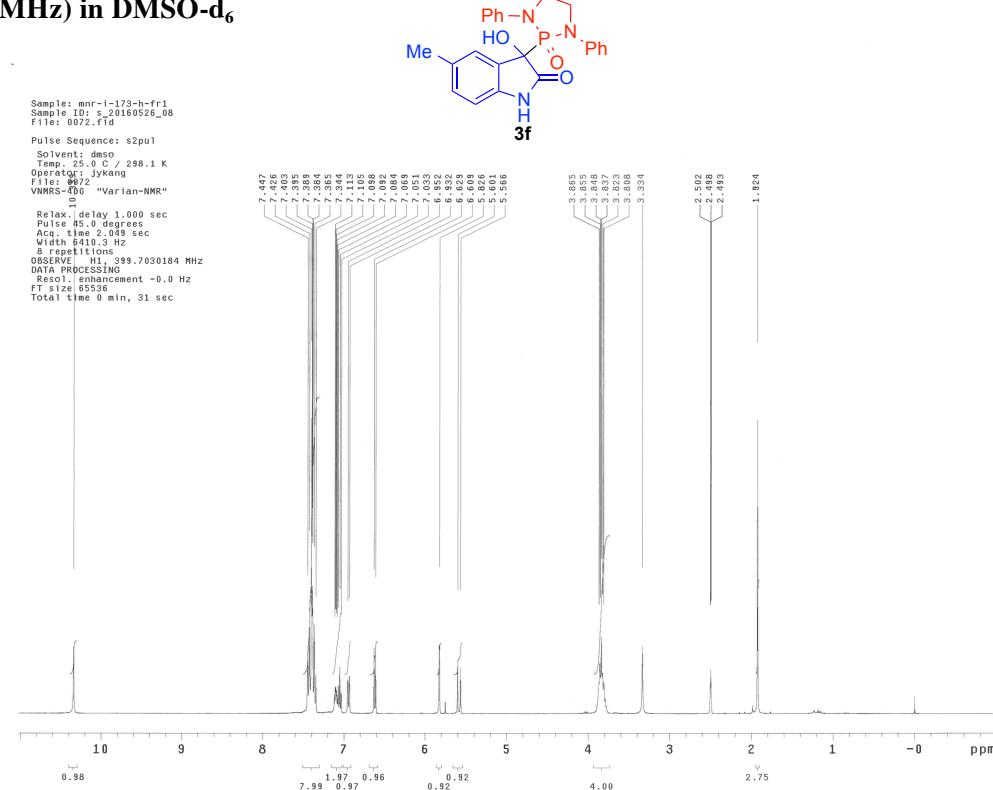
¹H NMR (400 MHz) in CDCl₃¹³C NMR (100.5 MHz) in CDCl₃

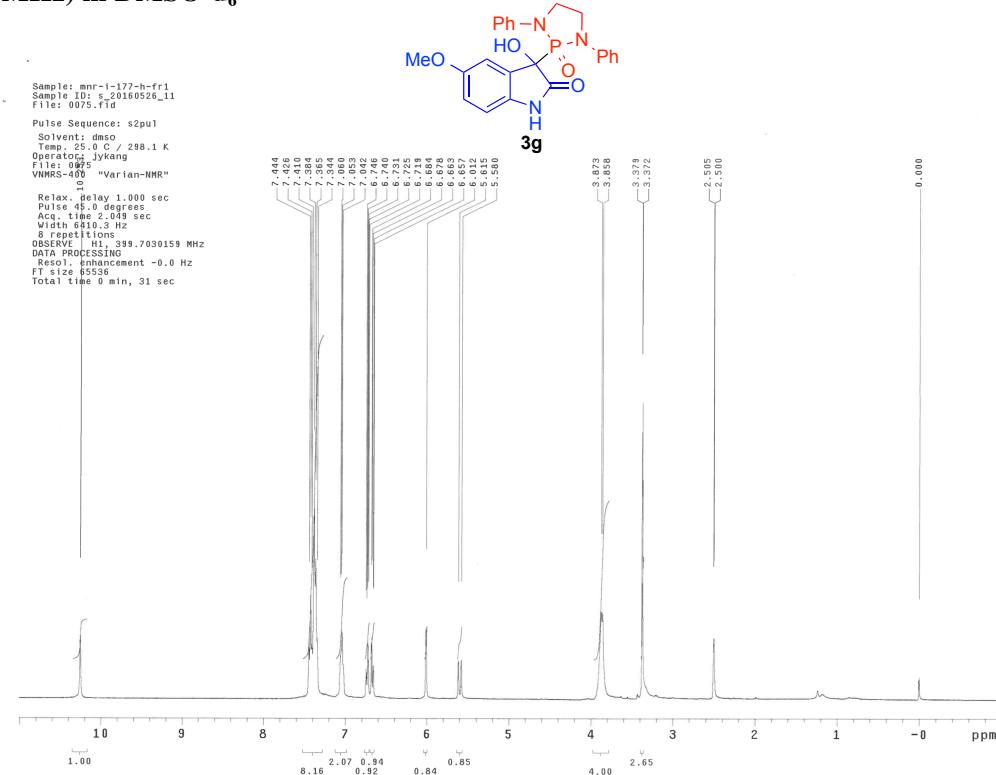
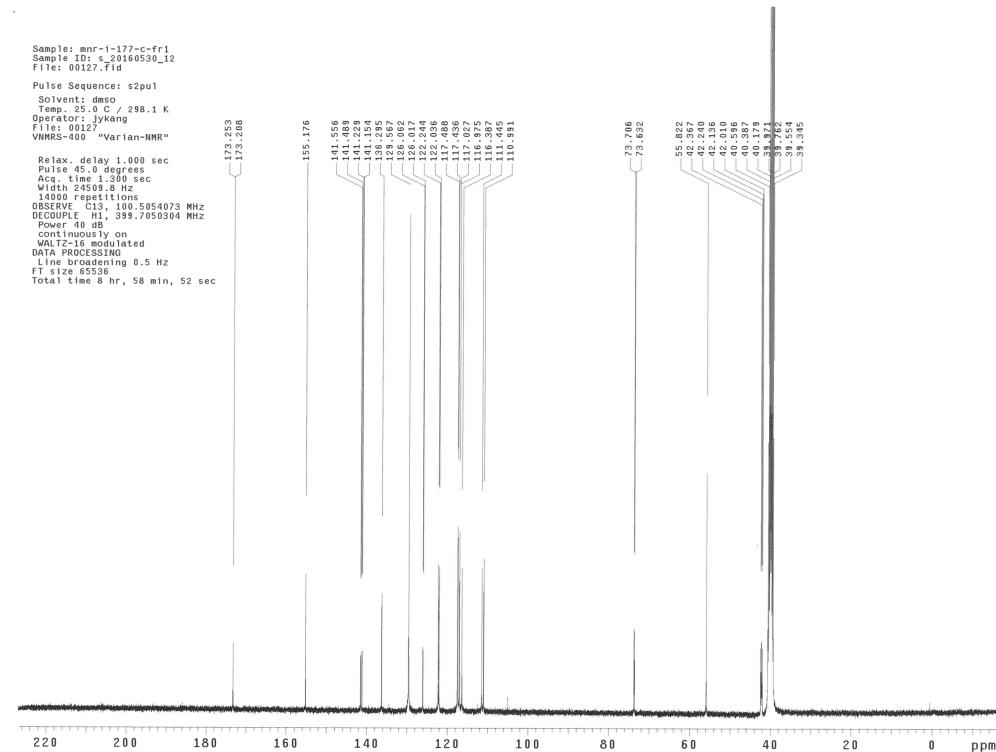
¹H NMR (400 MHz) in CDCl₃



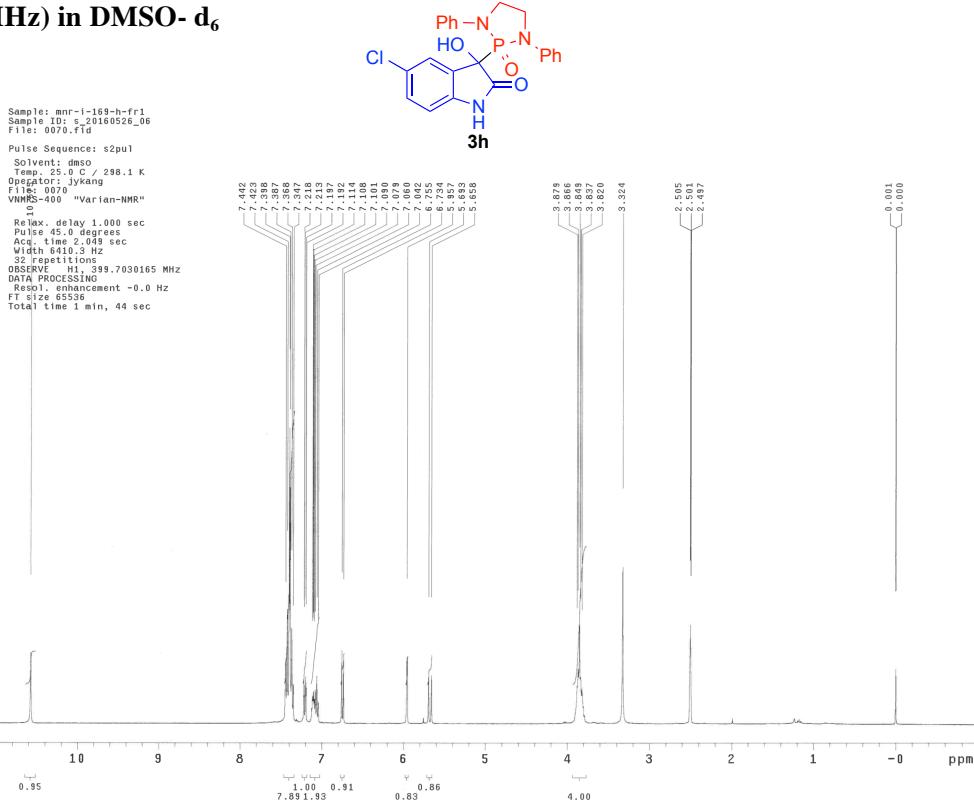
¹³C NMR (100.5 MHz) in DMSO-d₆



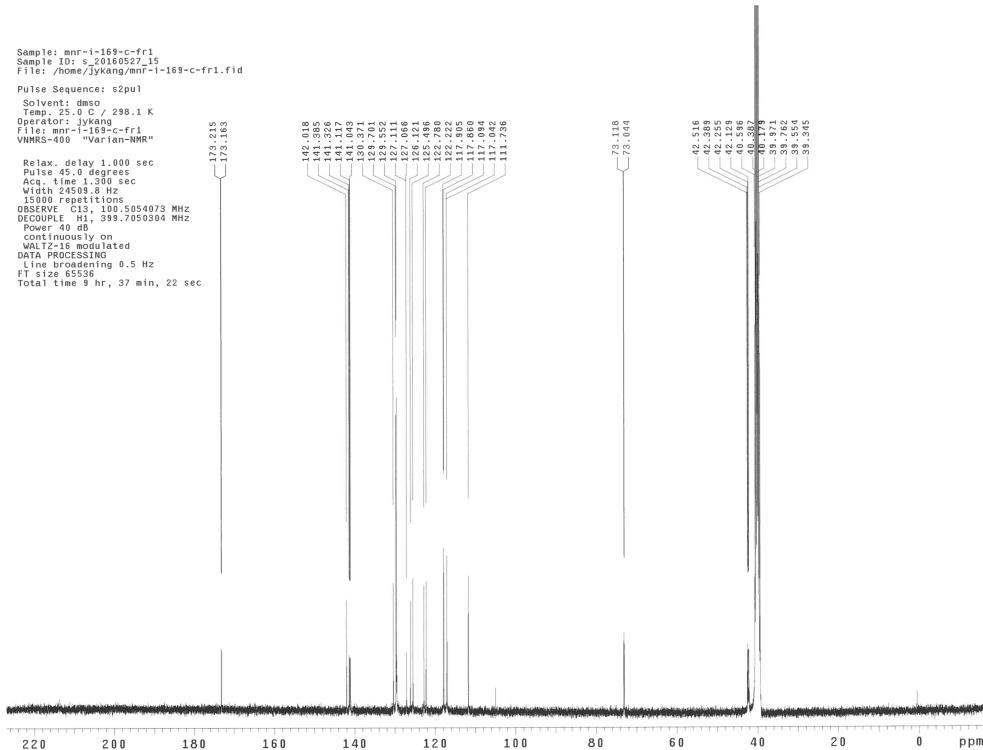
¹H NMR (400 MHz) in DMSO-d₆

¹H NMR (400 MHz) in DMSO-d₆**¹³C NMR (100.5 MHz) in DMSO-d₆**

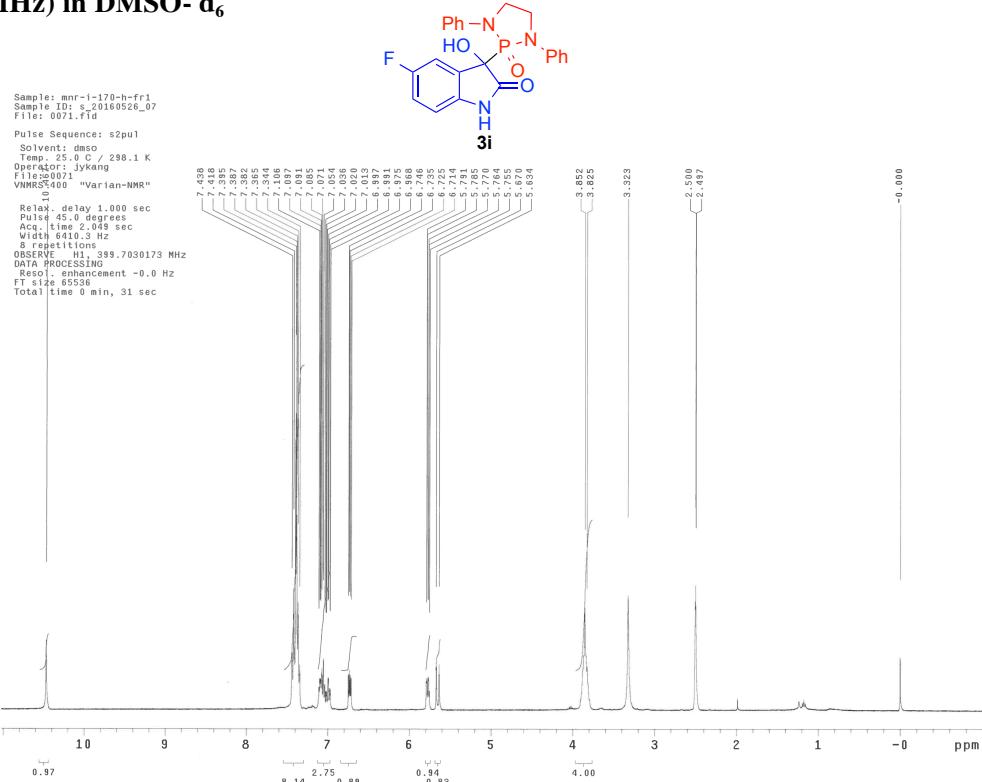
¹H NMR (400 MHz) in DMSO-d₆



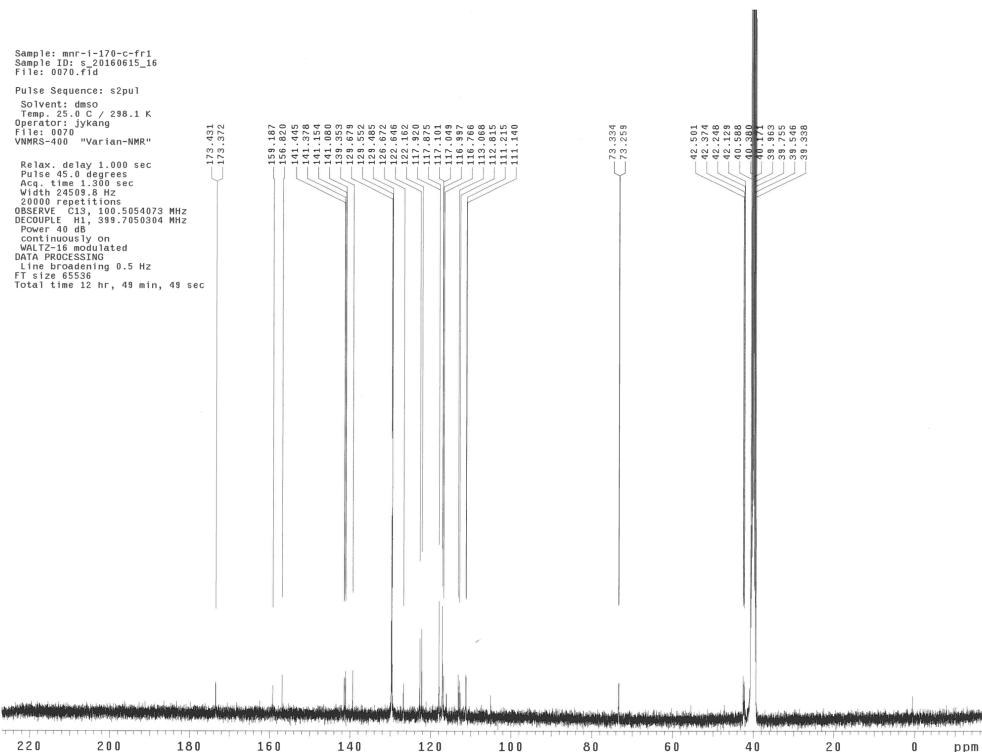
¹³C NMR (100.5 MHz) in DMSO-d₆

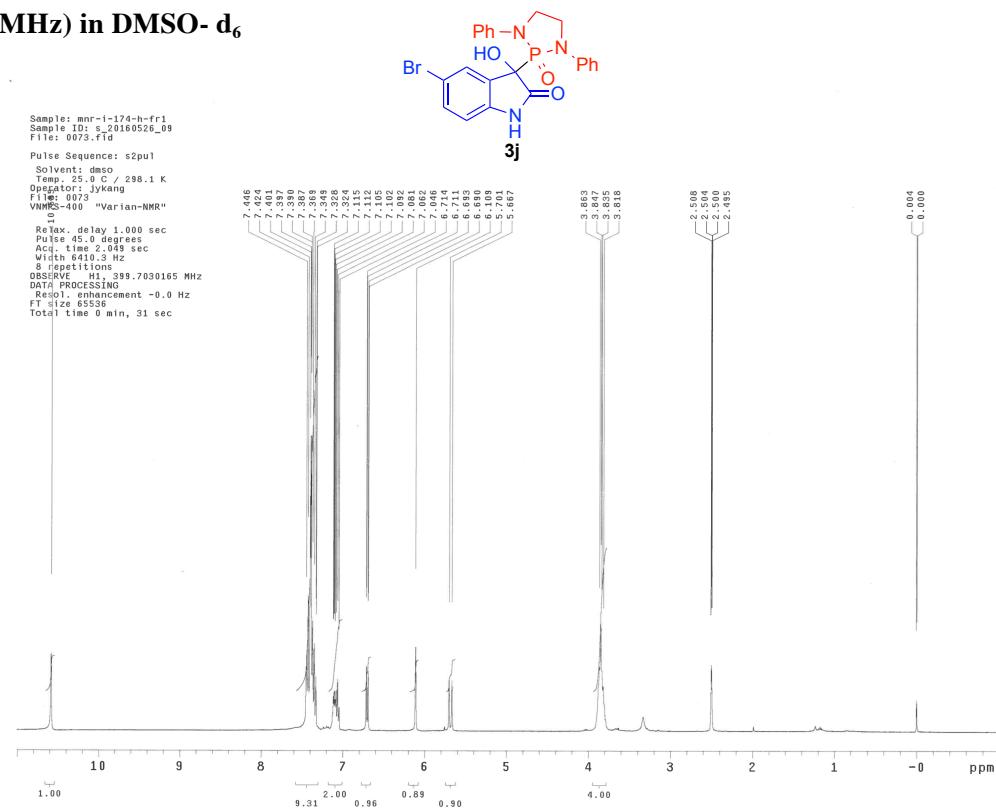
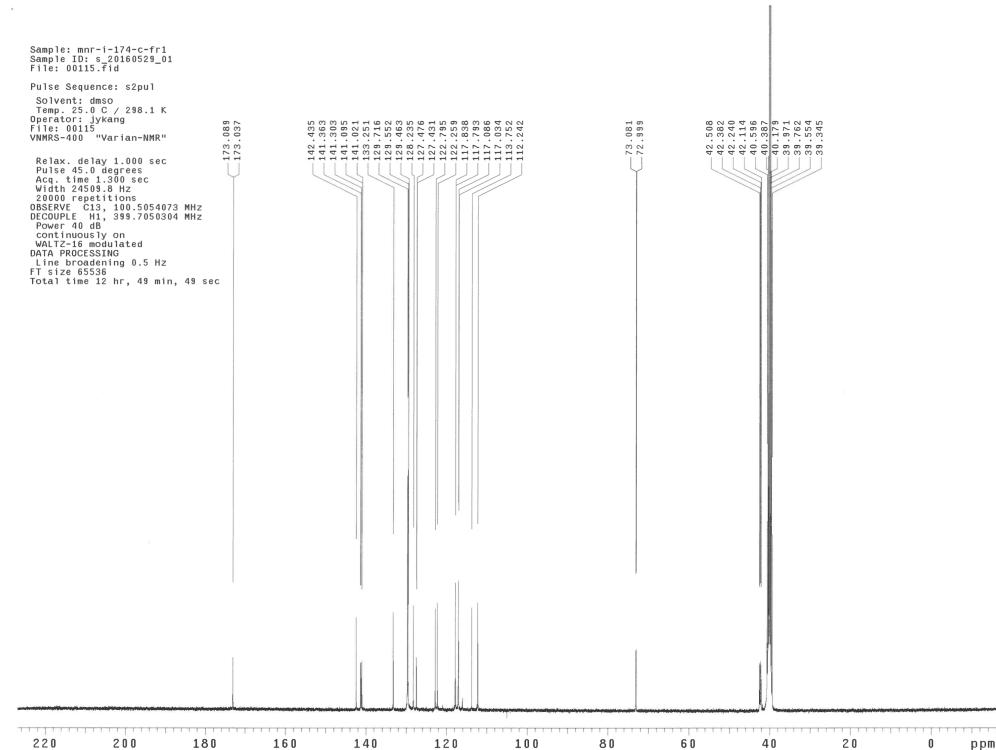


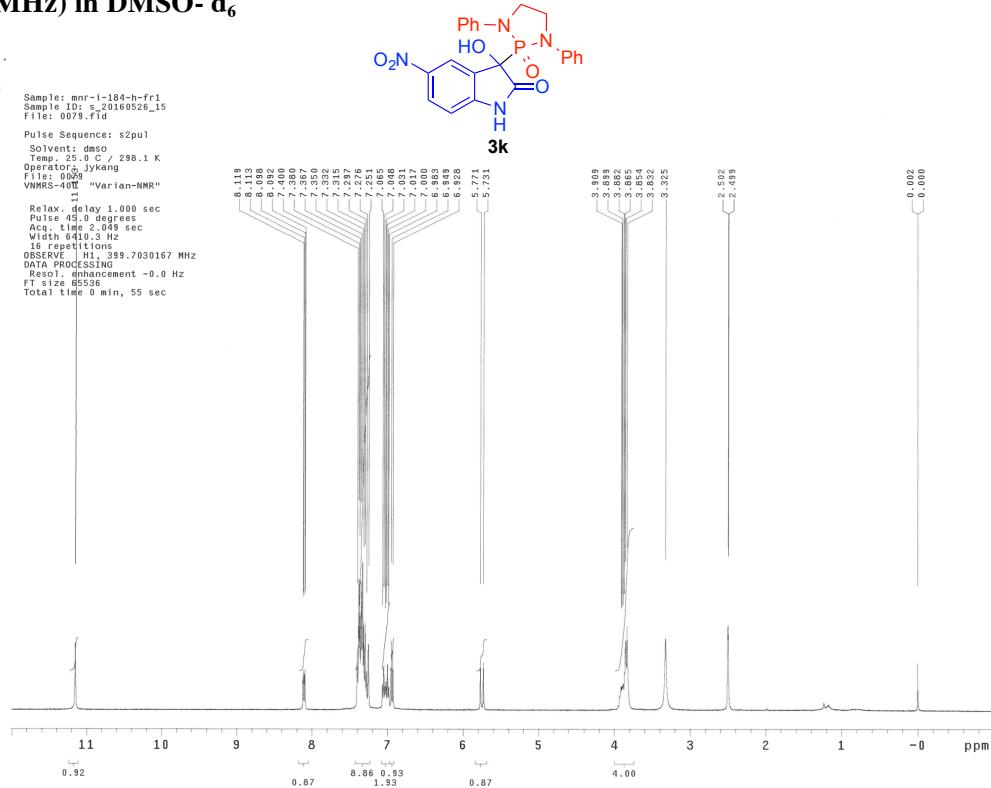
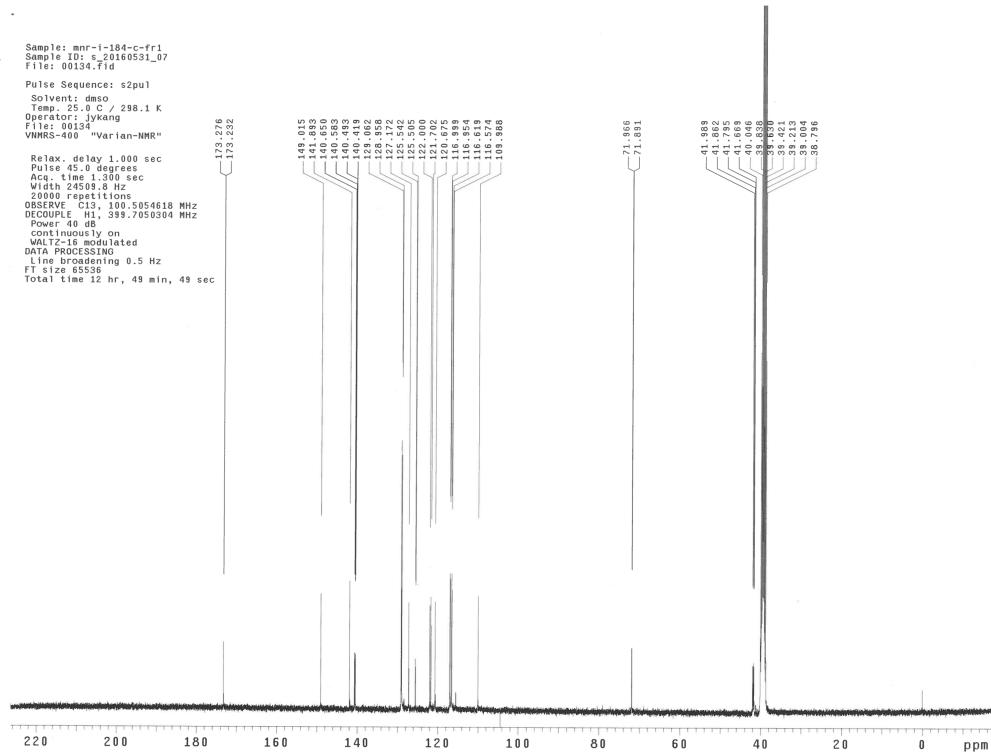
¹H NMR (400 MHz) in DMSO-d₆



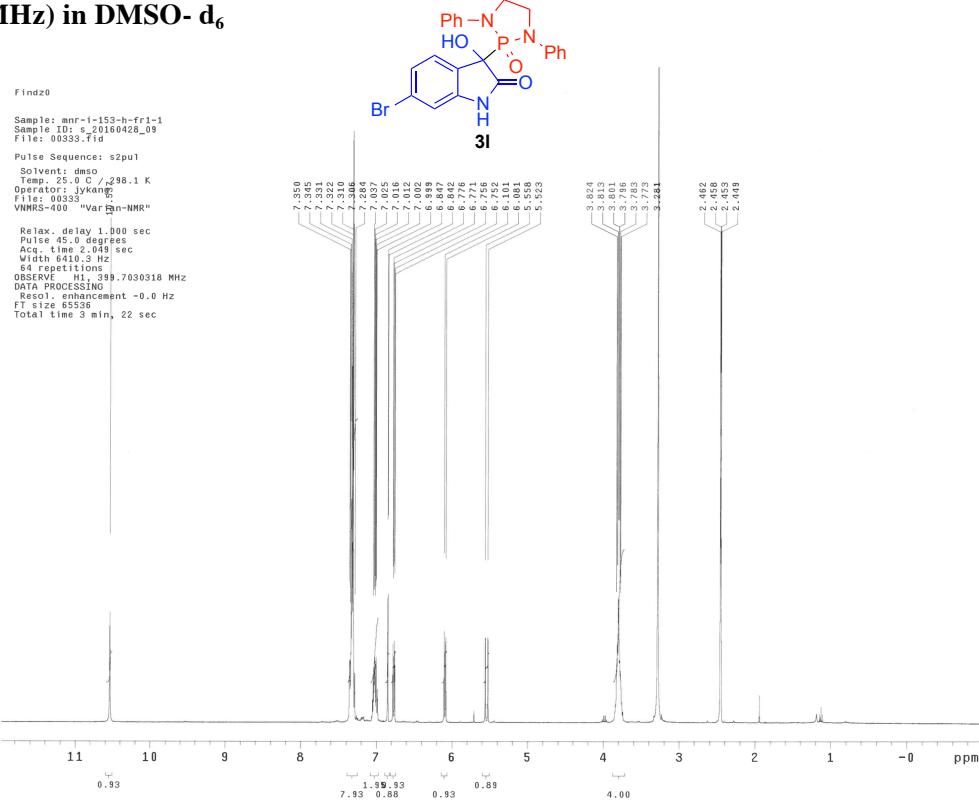
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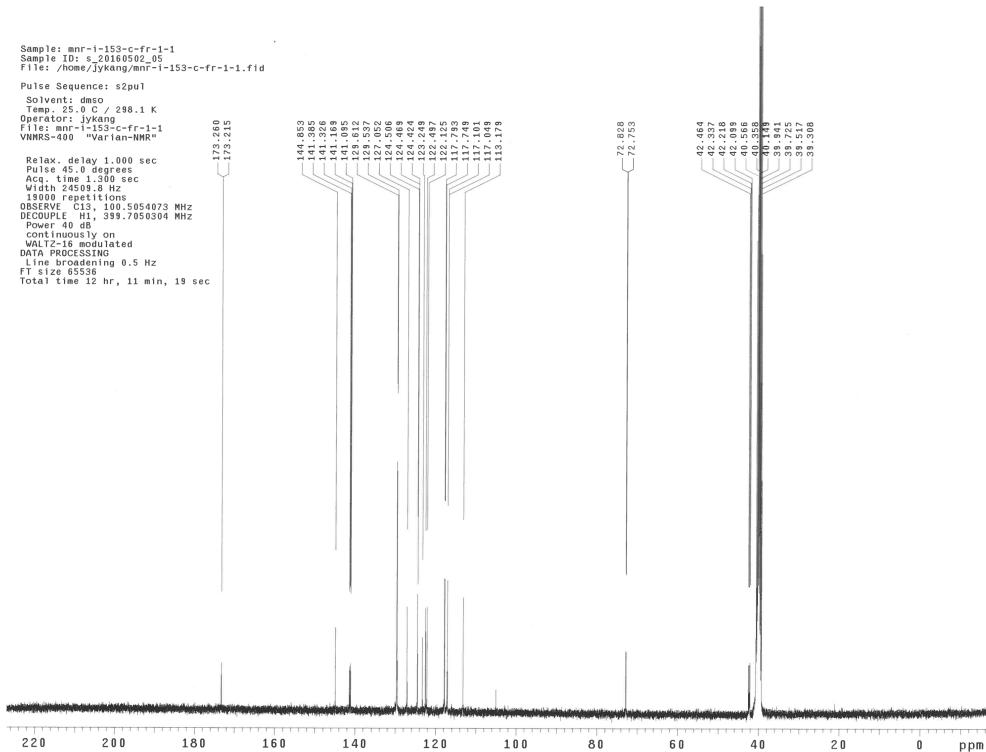
¹H NMR (400 MHz) in DMSO- d₆**¹³C NMR (100.5 MHz) in DMSO- d₆**

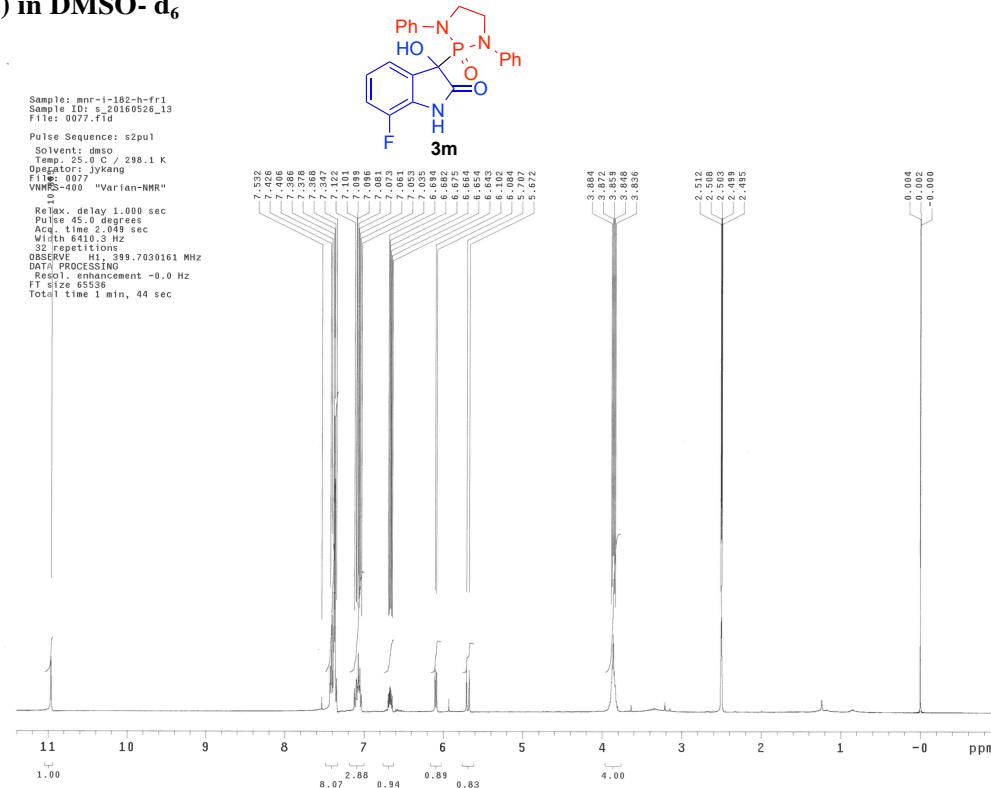
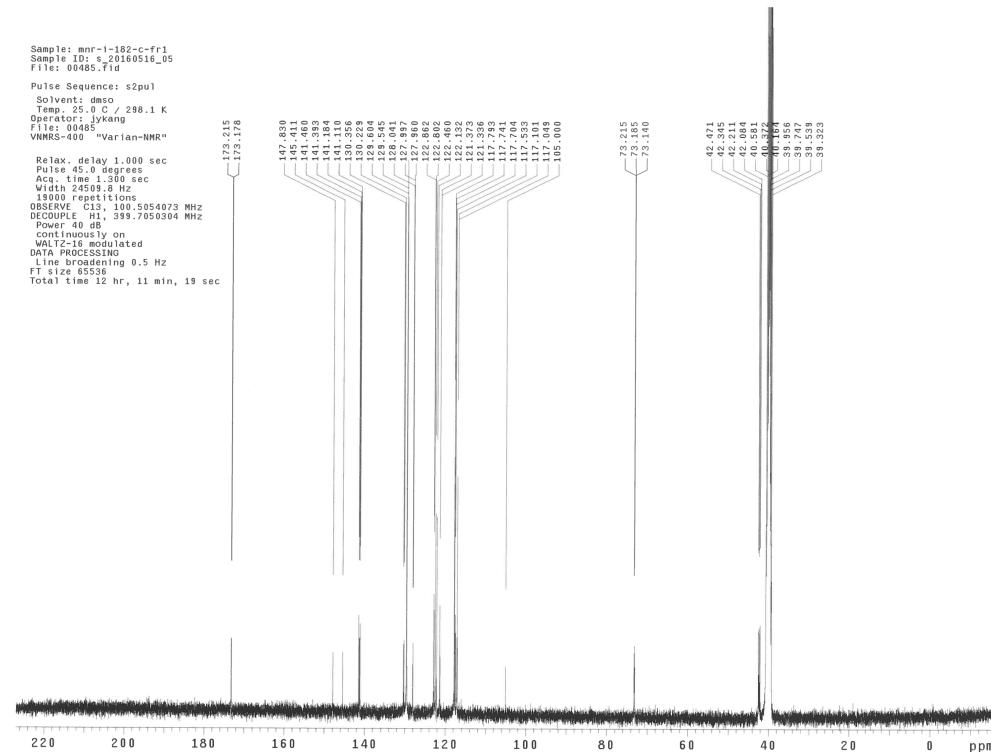
¹H NMR (400 MHz) in DMSO- d₆**¹³C NMR (100.5 MHz) in DMSO- d₆**

¹H NMR (400 MHz) in DMSO-d₆

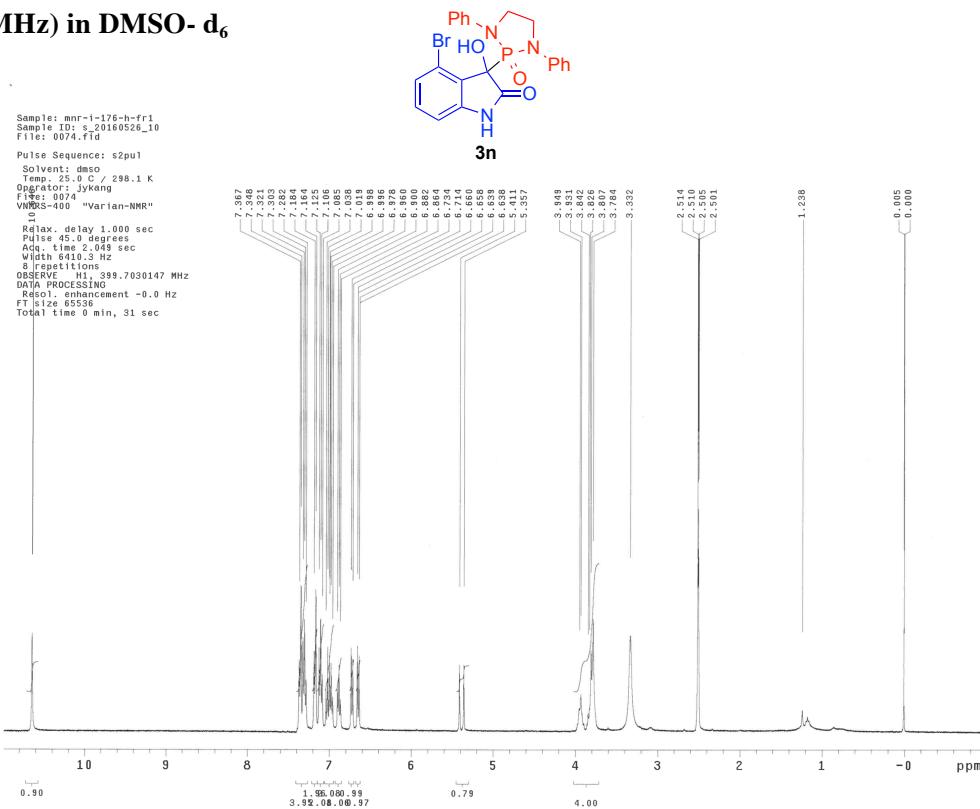


¹³C NMR (100.5 MHz) in DMSO-d₆

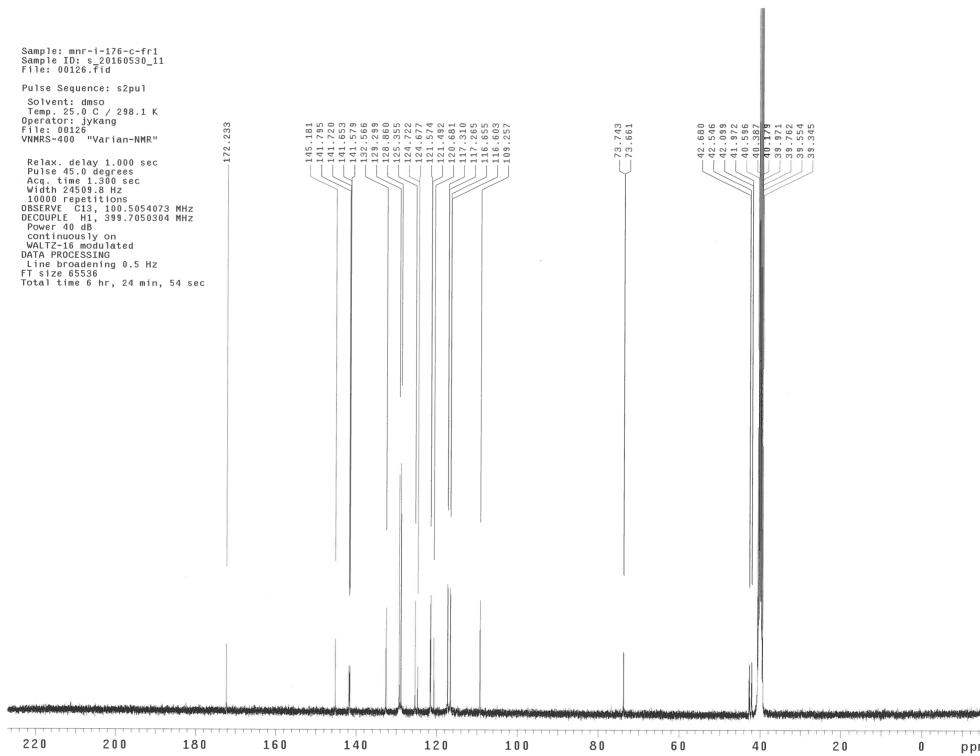


¹H NMR (400 MHz) in DMSO- d₆**¹³C NMR (100.5 MHz) in DMSO- d₆**

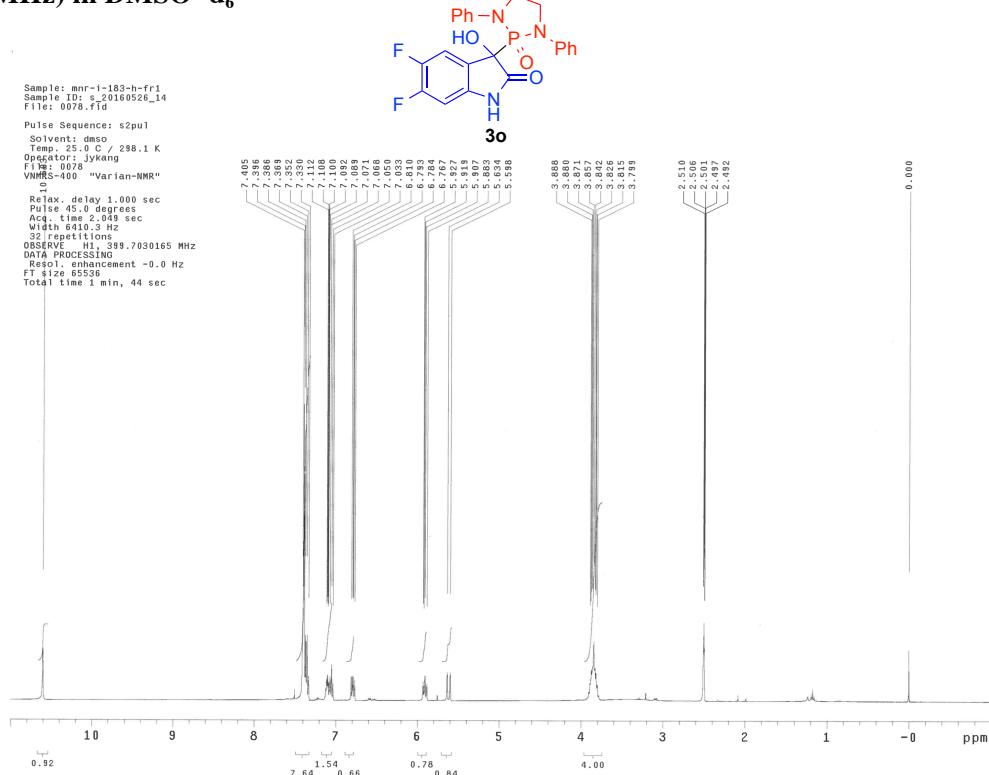
¹H NMR (400 MHz) in DMSO- d₆



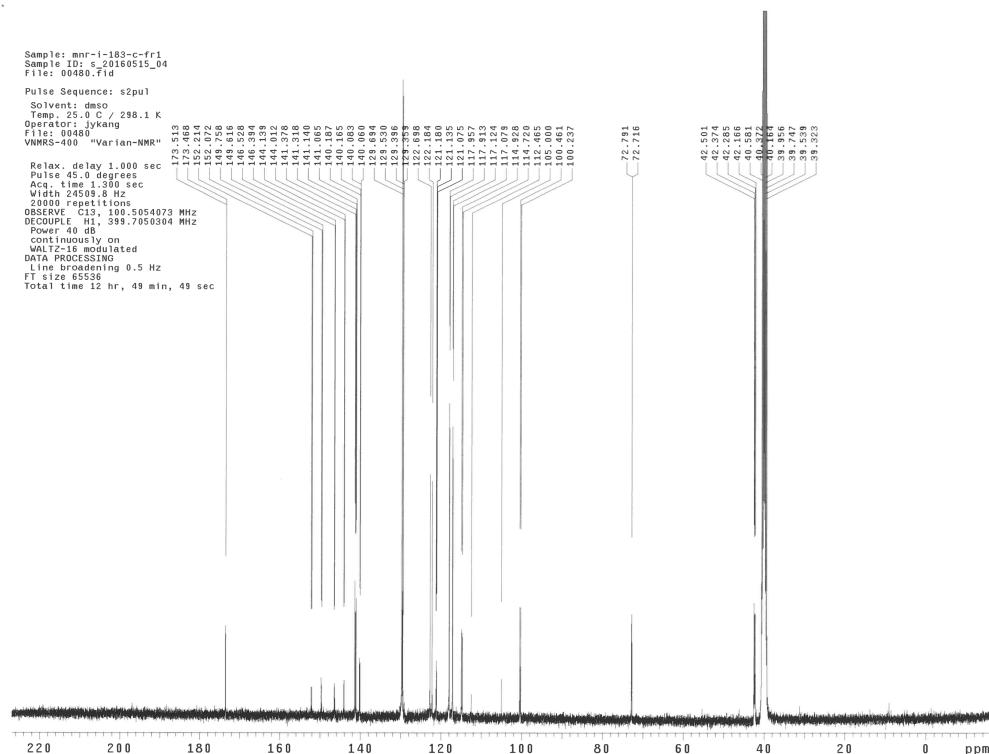
¹³C NMR (100.5 MHz) in DMSO-d₆

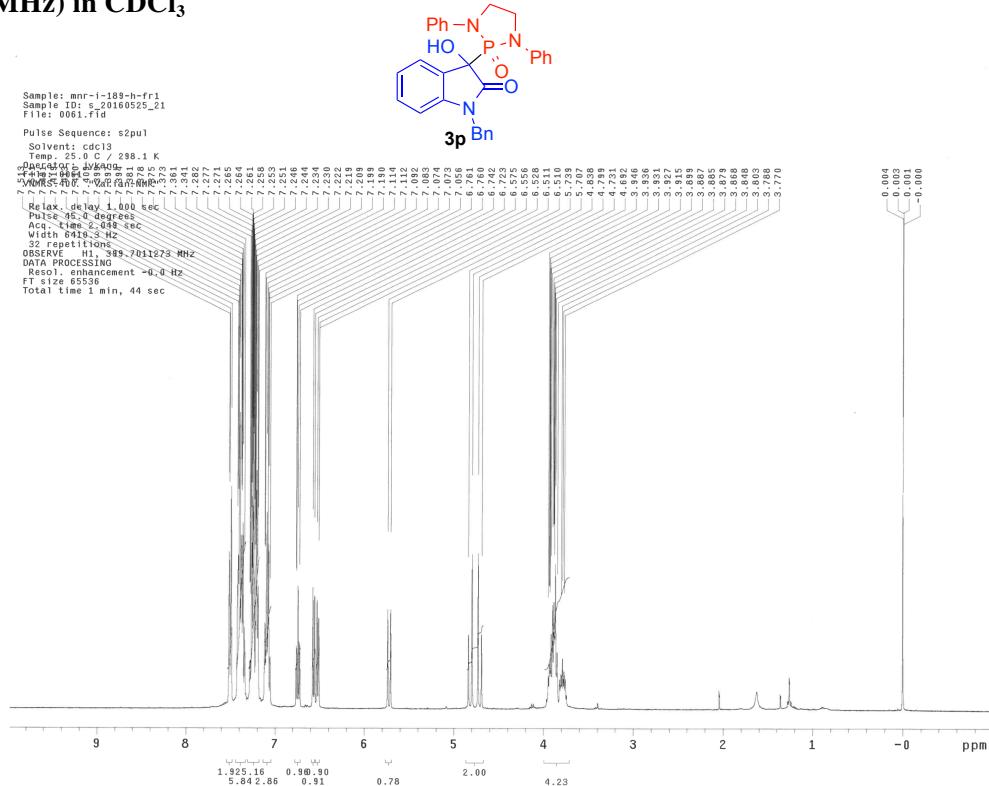
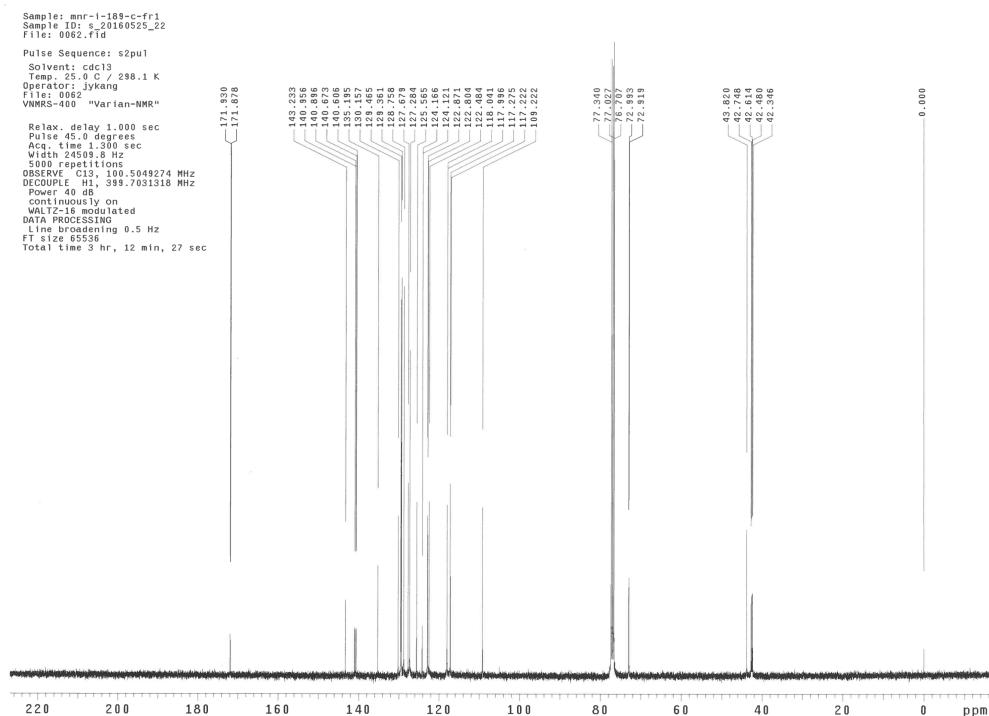


¹H NMR (400 MHz) in DMSO- d₆

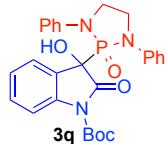


¹³C NMR (100.5 MHz) in DMSO-d₆



¹H NMR (400 MHz) in CDCl₃**¹³C NMR (100.5 MHz) in CDCl₃**

¹H NMR (400 MHz) in CDCl₃



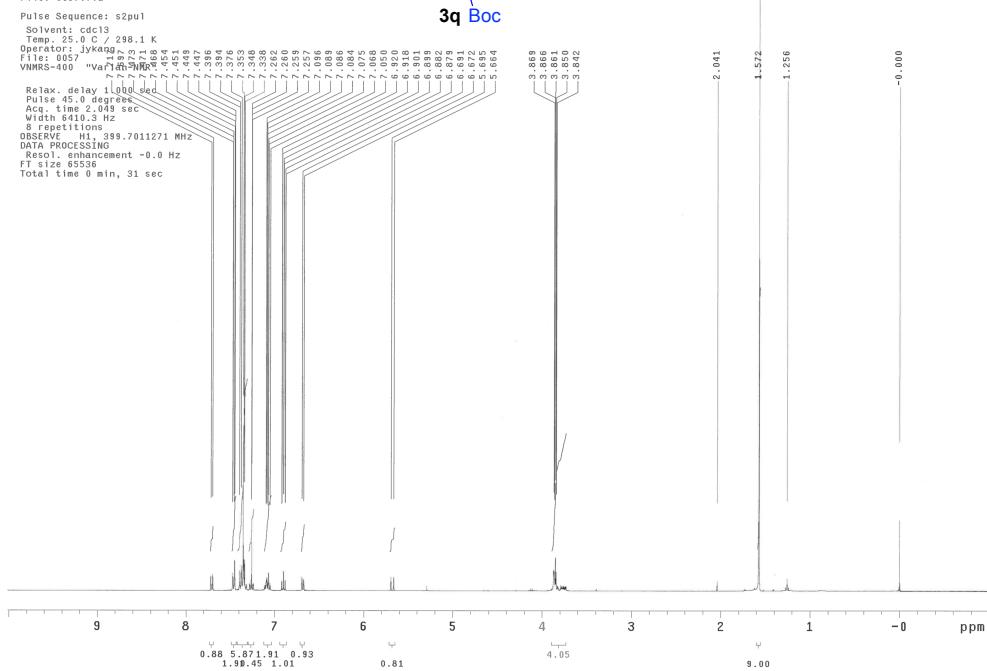
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Sample ID: s_20160525_17
File: 0057.fid

Pulse Sequence: s2pul

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1H NMR sequence: spqr
Solvent: cdc13
Temperature: 25.0 C
Integration: jkyang
File: 0057
VNMRX-400 "Varian NMR" JLab
Relax. delay 1.0lob1 sed
Pulse 45.0 degree
Acq. time 2.049 sec
Width 6410.3 Hz
8 repetitions
OBSERVE H1, 399.701127
DATA PROCESSING
Resol. enhancement -0.0
FT size 65536
Total time 0 min, 31 sec

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¹³C NMR (100.5 MHz) in CDCl₃

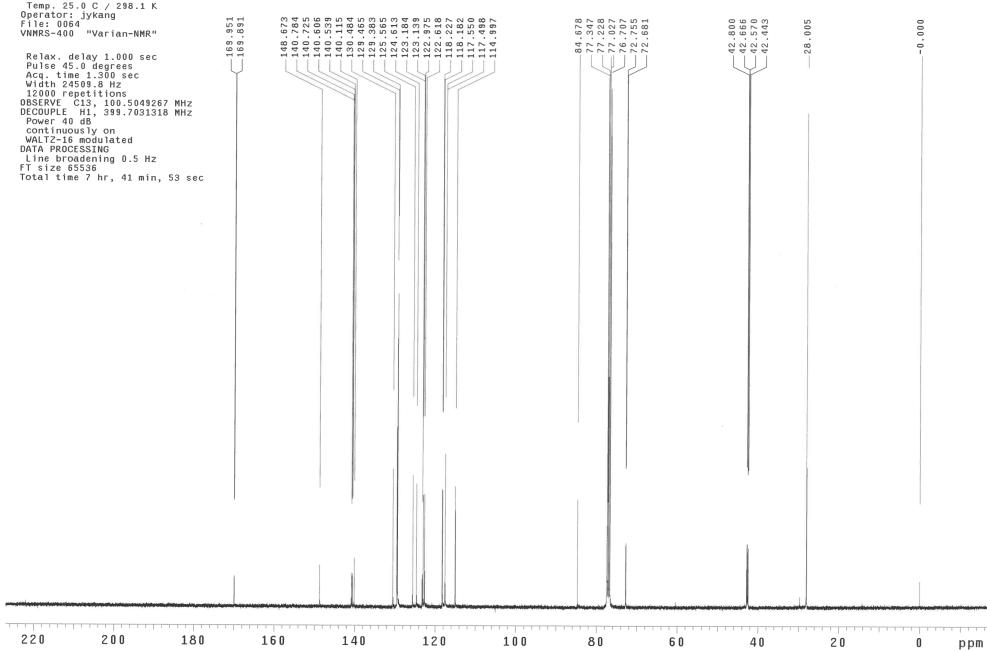
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Sample ID: s_20160525_23
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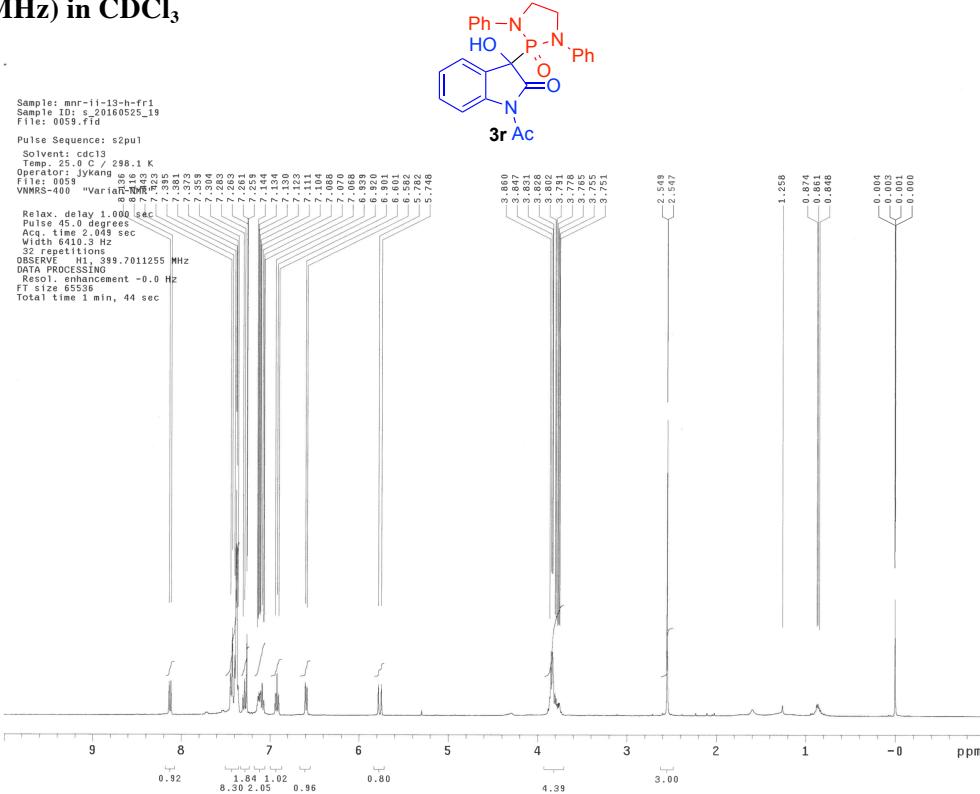
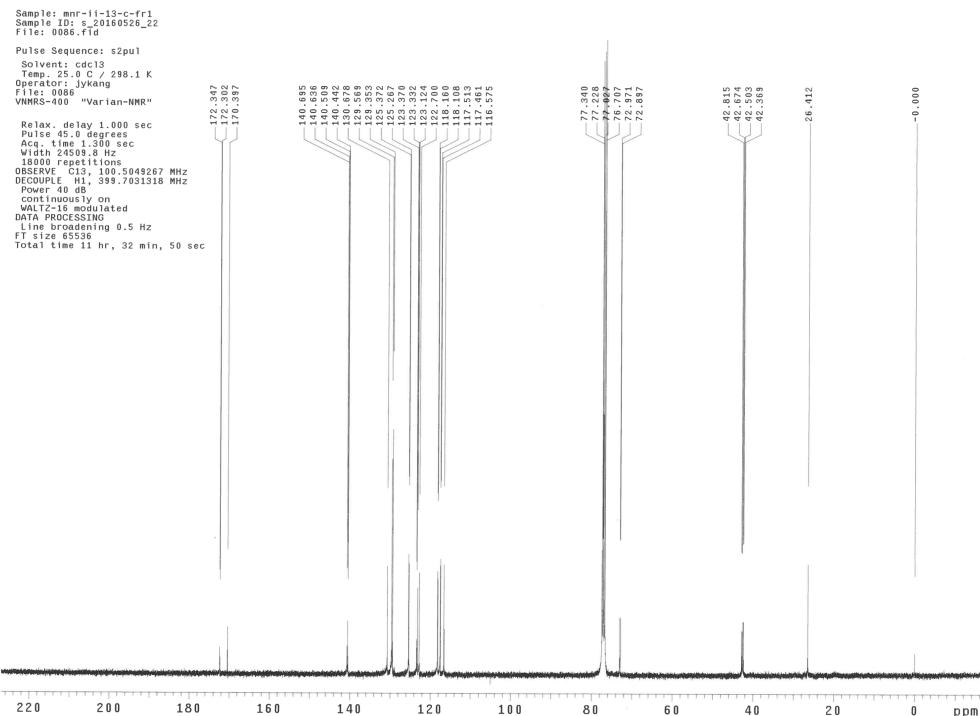
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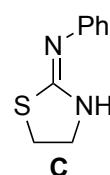
Pulse Sequence: s2pul
Solvent: cdc13
Temp. 25.0 C / 298.1 K
Operator: jykang
File: 0064
VNMRS-400 "Varian-NMR"

Relax, delay 1.000 sec
Pulse 45.0 degrees
Aq, time 1.300 sec
Width 24509.8 Hz
TE 1.000 sec
OBSERVE CHANNEL 504928
DECOUPLER H1, 399.703131
Power 40 dB
continuously on
Multi channel correlated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536

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¹H NMR (400 MHz) in CDCl₃**¹³C NMR (100.5 MHz) in CDCl₃**

¹H NMR (400 MHz) in CDCl₃

Sample: hh-i-50-h-fr2
Sample ID: s_20160219_01
File: /home/jykang/hh-i-50-h-fr2.fid

Pulse Sequence: s2pul

Solvent: cdcl₃

Temp: 25 °C / 298.1 K

Operator: jykang

File: hh-i-50-h-fr2

VNMR3-400 "Varian-NMR"

Relax. delay 1.000 sec

Pulse width 90°

Acq. time 2.049 sec

Width 6410.3 Hz

8 acquisitions

OBSERVE H1 399.7011277 MHz

DATA PROCESSING

Res. 1.0000000000000001 Hz

FT size 65536

Total time 0 min, 31 sec

