

Advanced
**Synthesis &
Catalysis**

Supporting Information

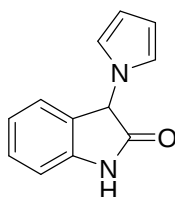
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SUPPORTING INFORMATION

Novel aqueous phase supramolecular synthesis of 3-pyrrolyl-indolin-2-ones and pyrrolyl-indeno [1,2-*b*] quinoxalines

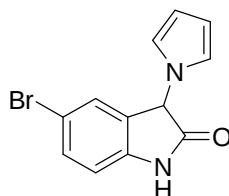
**R. Sridhar, B. Srinivas, V. Pavan Kumar, V. Prakash Reddy, A. Vijay Kumar and
K. Rama Rao***

*Organic Chemistry Division-I, Indian Institute of Chemical Technology, Uppal Road,
Hyderabad 500-007, India
E-mail: kakulapatirama@gmail.com*



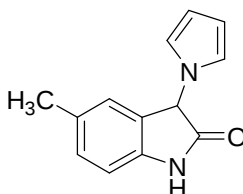
3-(1H-pyrrol-1-yl)indolin-2-one (3a): ¹

mp: 140-142 °C; IR: 3306, 3194, 1717, 1618, 1466 cm⁻¹; ¹H NMR (CDCl₃, 200MHz): δ 5.46 (s, 1H), 6.17 (t, 2H, *J* = 2.21 Hz), 6.63 (t, 2H, *J* = 2.21 Hz), 6.85-7.09 (m, 2H), 7.20-7.33 (m, 2H), 9.5 (brs, 1H); MS *m/z* (EI): 198 [M⁺]; Anal. Calcd for C₁₂H₁₀N₂O: C, 72.71; H, 5.08; N, 14.13. Found: C, 72.43; H, 5.19; N, 14.22.



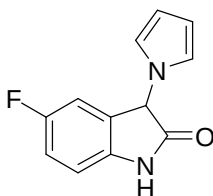
5-bromo-3-(1H-pyrrol-1-yl)indolin-2-one (3b): ¹

mp: 170-172 °C; IR: 3248, 2922, 1719, 1613, 1470 cm⁻¹; ¹H NMR (CDCl₃, 300MHz): δ 5.50 (s, 1H), 6.26 (t, 2H, *J* = 2.66 Hz), 6.67 (t, 2H, *J* = 2.66 Hz), 6.81 (d, 1H, *J* = 8.31 Hz), 7.37-7.47 (m, 2H), 8.90 (brs, 1H); MS *m/z* (EI): 278 [M⁺+2]; Anal. Calcd for C₁₂H₉BrN₂O: C, 52.01; H, 3.27; N, 10.11. Found: C, 52.32; H, 3.39; N, 10.19.



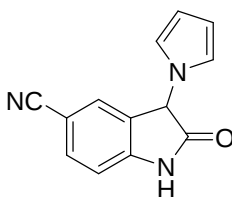
5-methyl-3-(1H-pyrrol-1-yl)indolin-2-one (3c): ¹

mp: 162-163 °C; IR: 3235, 2921, 1722, 1625, 1490 cm⁻¹; ¹H NMR (CDCl₃, 200MHz): δ 2.28 (s, 3H), 5.47 (s, 1H), 6.25 (t, 2H, *J* = 1.96 Hz), 6.71 (t, 2H, *J* = 1.96 Hz), 6.69-6.82 (m, 1H), 7.07-7.11 (m, 2H), 8.02 (brs, 1H); MS *m/z* (EI): 212 [M⁺]; Anal. Calcd for C₁₃H₁₂N₂O: C, 73.56; H, 5.70; N, 13.20. Found: 73.86; H, 5.80; N, 13.28.



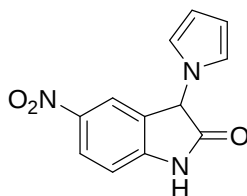
5-fluoro-3-(1H-pyrrol-1-yl)indolin-2-one (3d): ¹

mp: 170-172 °C; IR: 3256, 2923, 1726, 1630, 1487 cm⁻¹; ¹H NMR (CDCl₃, 200MHz): δ 5.45 (s, 1H), 6.19 (t, 2H, *J* = 2.17 Hz), 6.62 (t, 2H, *J* = 2.17 Hz), 6.78-6.87 (m, 1H), 6.93-7.05 (m, 2H), 9.45 (brs, 1H); MS *m/z* (EI): 216 [M⁺]; Anal. Calcd for C₁₂H₉FN₂O: C, 66.66; H, 4.20; N, 12.96. Found: C, 66.98; H, 4.21; N, 13.04.



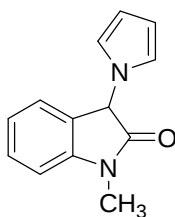
2-oxo-3-(1H-pyrrol-1-yl)indoline-5-carbonitrile (3e): ¹

mp: 160-161 °C; IR: 3256, 2395, 2923, 1726, 1630, 1487 cm⁻¹; ¹H NMR (CDCl₃, 200MHz): δ 5.40 (s, 1H), 6.17 (t, 2H, *J* = 2.16 Hz), 6.64 (t, 2H, *J* = 2.16 Hz), 6.79-6.84 (m, 1H), 6.93-7.02 (m, 2H), 9.40 (brs, 1H); MS *m/z* (EI): 223 [M⁺]; Anal. Calcd for C₁₃H₉N₃O: C, 69.95; H, 4.06; N, 18.82. Found: C, 69.62; H, 4.17; N, 18.91.



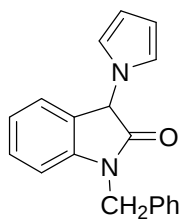
5-nitro-3-(1H-pyrrol-1-yl)indolin-2-one (3f): ¹

mp: 135-136 °C; IR: 3292, 2925, 1738, 1625, 1524, 1481, 1338 cm⁻¹; ¹H NMR (CDCl₃, 200MHz): d 5.60 (s, 1H), 6.25 (s, 2H), 6.66 (s, 2H), 6.97 (d, 1H, *J* = 8.59 Hz), 8.09-8.29 (m, 2H), 9.50 (brs, 1H); MS *m/z* (EI): 243 [M⁺]; Anal. Calcd for C₁₂H₉N₃O₃: C, 59.26; H, 3.73; N, 17.28. Found: C, 59.56; H, 3.63; N, 17.36.



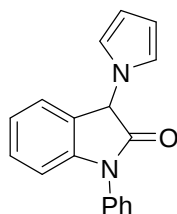
1-methyl-3-(1H-pyrrol-1-yl)indolin-2-one (3g): ¹

mp: 132-133 °C IR: 3090, 2924, 1720, 1615, 1489 cm⁻¹; ¹H NMR (CDCl₃, 300MHz): d 3.27 (s, 3H), 5.45 (s, 1H), 6.18 (t, 2H, *J* = 2.26 Hz), 6.64 (t, 2H, *J* = 2.26 Hz), 6.89 (d, 1H, *J* = 8.30 Hz), 7.10 (t, 1H, *J* = 7.55 Hz), 7.27-7.42 (m, 2H); MS *m/z* (EI): 212 [M⁺]; Anal. Calcd for C₁₃H₁₂N₂O: C, 73.56; H, 5.70; N, 13.20. Found: C, 73.86; H, 5.59; N, 13.29.



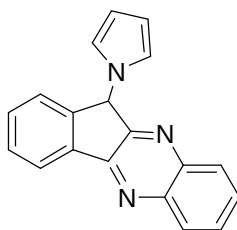
1-benzyl-3-(1H-pyrrol-1-yl)indolin-2-one (3h): ¹

mp: 124-125 °C, IR: 3091, 2922, 1721, 1612, 1489 cm⁻¹; ¹H NMR (CDCl₃, 200MHz): d 4.90 (s, 2H), 5.56 (s, 1H), 6.24 (t, 2H, *J* = 2.20 Hz), 6.70 (t, 2H, *J* = 2.20 Hz), 6.76-6.82 (m, 1H), 7.00-7.09 (m, 1H), 7.25-7.32 (m, 7H); MS *m/z* (EI): 288 [M⁺]; Anal. Calcd for C₁₉H₁₆N₂O: C, 79.14; H, 5.59; N, 9.72. Found: C, 79.35; H, 5.47; N, 9.81.



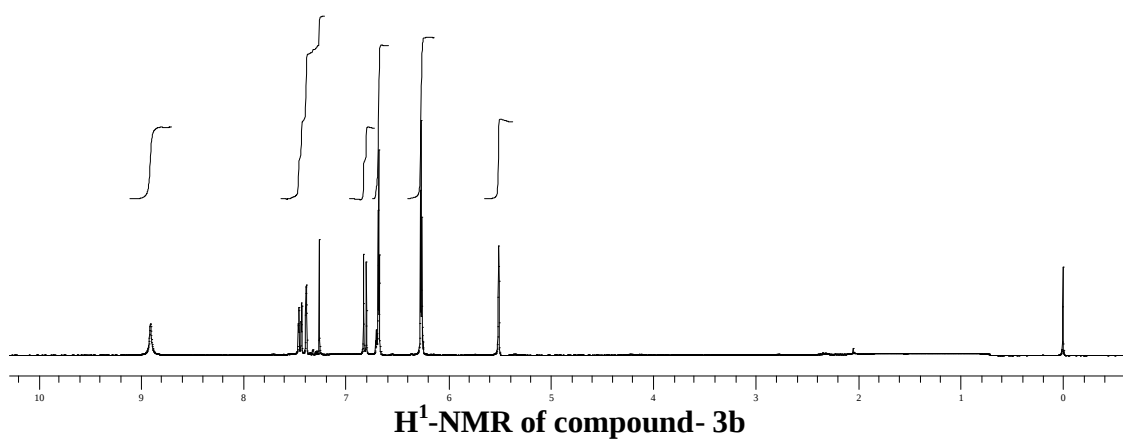
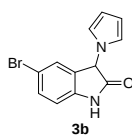
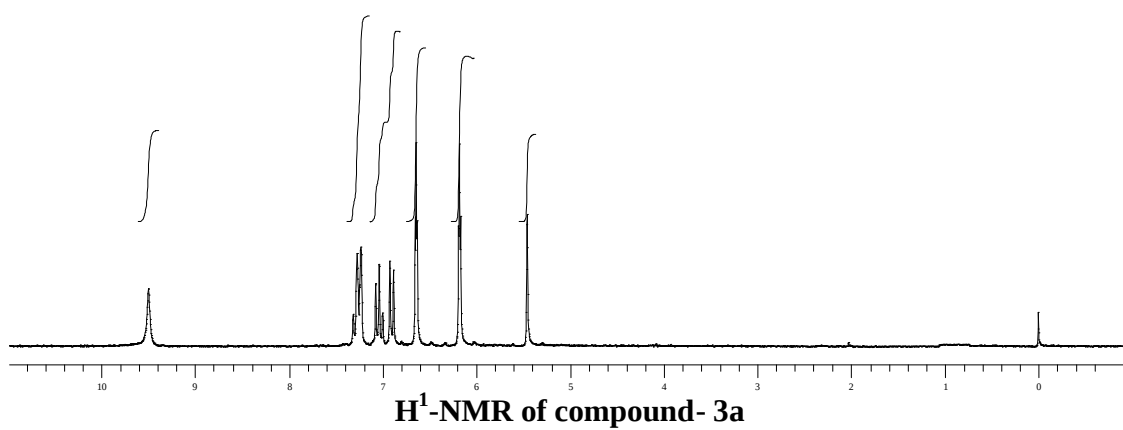
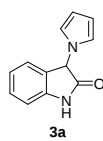
1-phenyl-3-(1H-pyrrol-1-yl)indolin-2-one (3i):

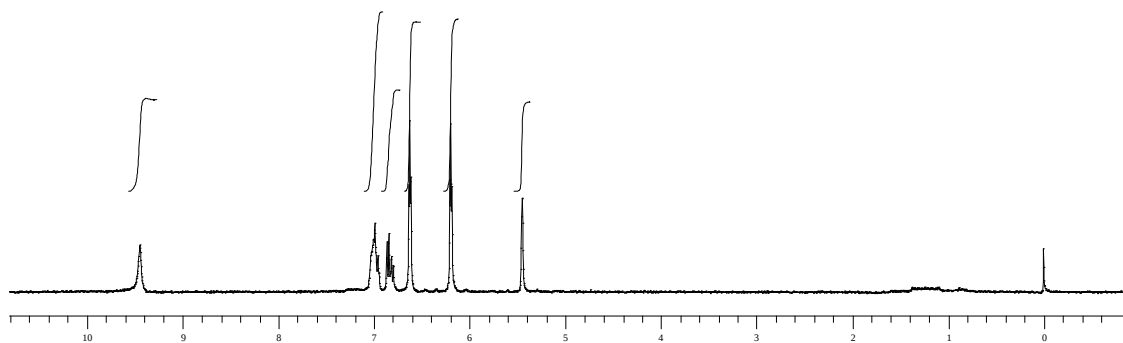
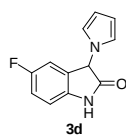
mp: 136-137 °C; IR: 3092, 2925, 1720, 1478 cm⁻¹; ¹H NMR (CDCl₃, 300MHz): d 5.69 (s, 1H), 6.29 (t, 2H, *J* = 2.26Hz), 6.81 (t, 2H, *J* = 2.26 Hz), 6.92 (d, 1H, *J* = 7.55 Hz), 7.17 (t, 1H, *J* = 7.55 Hz), 7.32-7.60 (m, 7H); MS *m/z* (EI): 274 [M⁺]; Anal. Calcd for C₁₈H₁₄N₂O: C, 78.81; H, 5.14; N, 10.31. Found: C, 78.51; H, 5.03; N, 10.39.



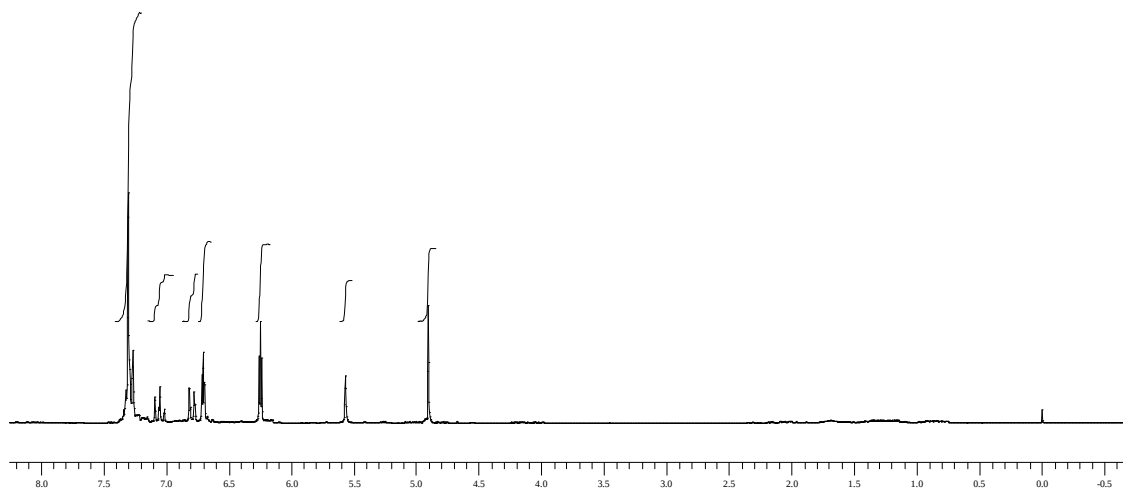
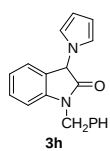
(6E,9Z)-N1-(1-(1H-pyrrol-1-yl)-1H-inden-2(3H)-ylidene)-N2-ethylidenebenzene-1,2-diamine (3j): ¹

mp: 180-181 °C, IR 3092, 2924, 1479 cm⁻¹; ¹H NMR (CDCl₃, 300MHz): d 6.19 (s, 1H), 6.22 (t, 2H, *J* = 2.26 Hz), 6.73 (t, 2H, *J* = 2.26 Hz), 7.49-7.74 (m, 5H), 8.04-8.26 (m, 3H); MS *m/z* (EI): 283 [M⁺]; Anal. Calcd for C₁₉H₁₃N₃: C, 80.54; H, 4.62; N, 14.83. Found: C, 80.88; H, 4.53; N, 14.91.

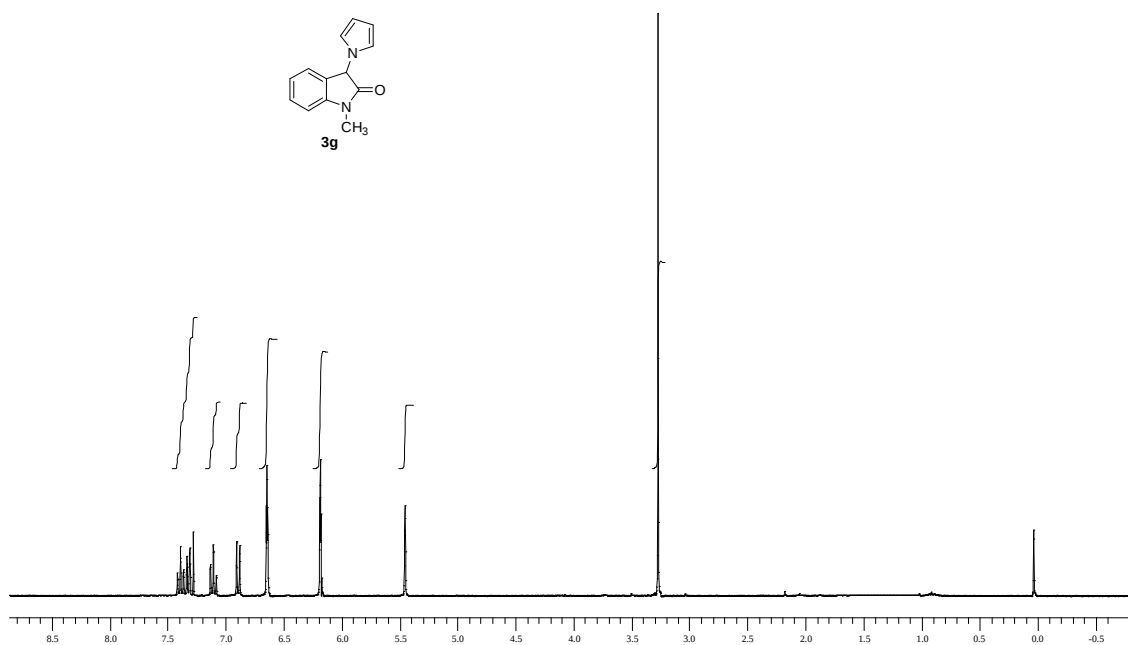




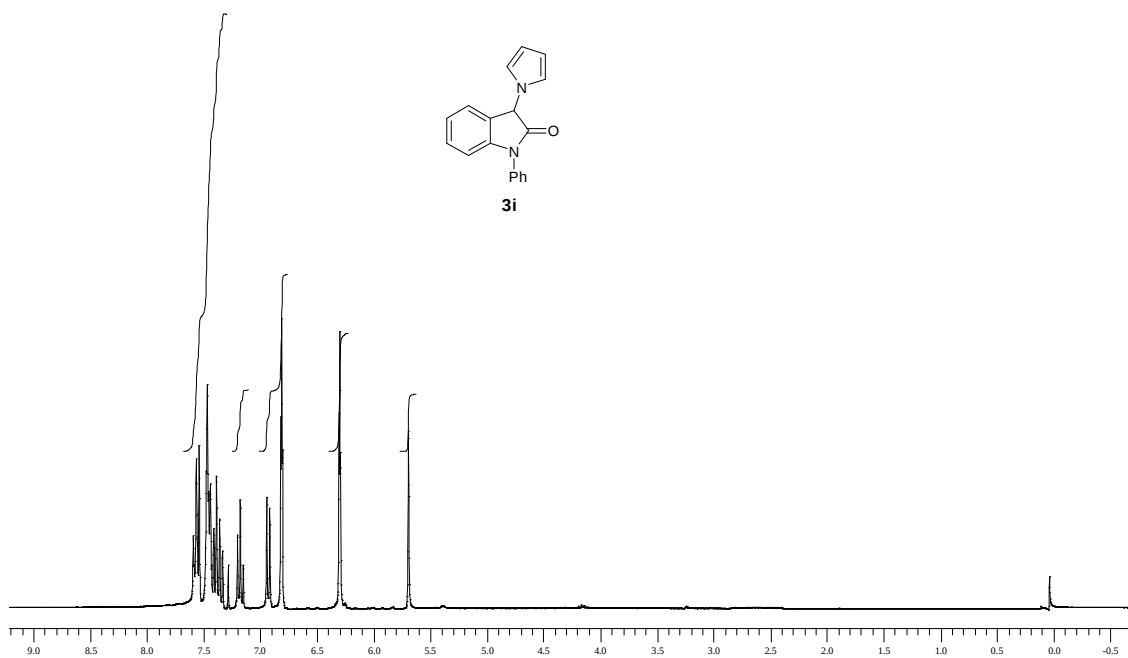
H^1 -NMR of compound- 3d



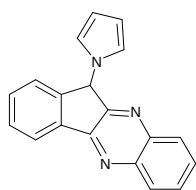
H^1 -NMR of compound- 3h



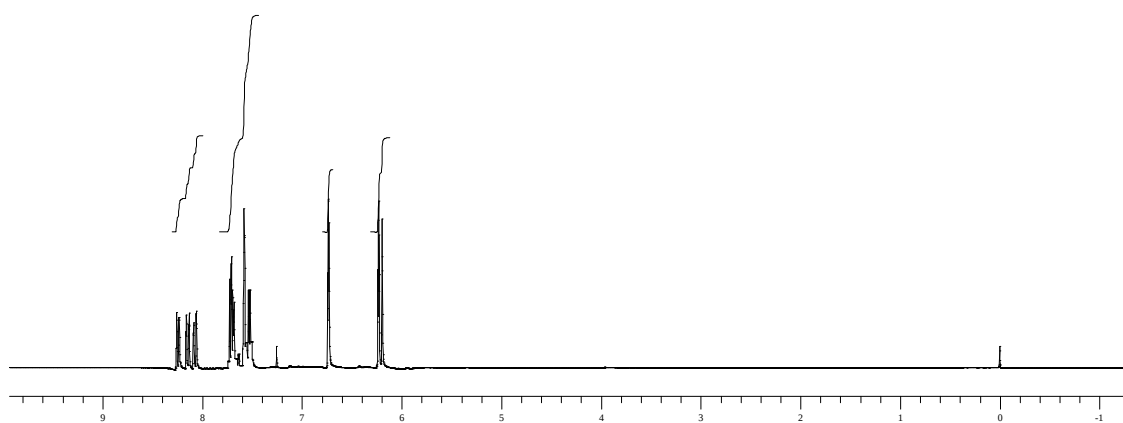
H¹-NMR of compound- 3g



H¹-NMR of compound- 3i

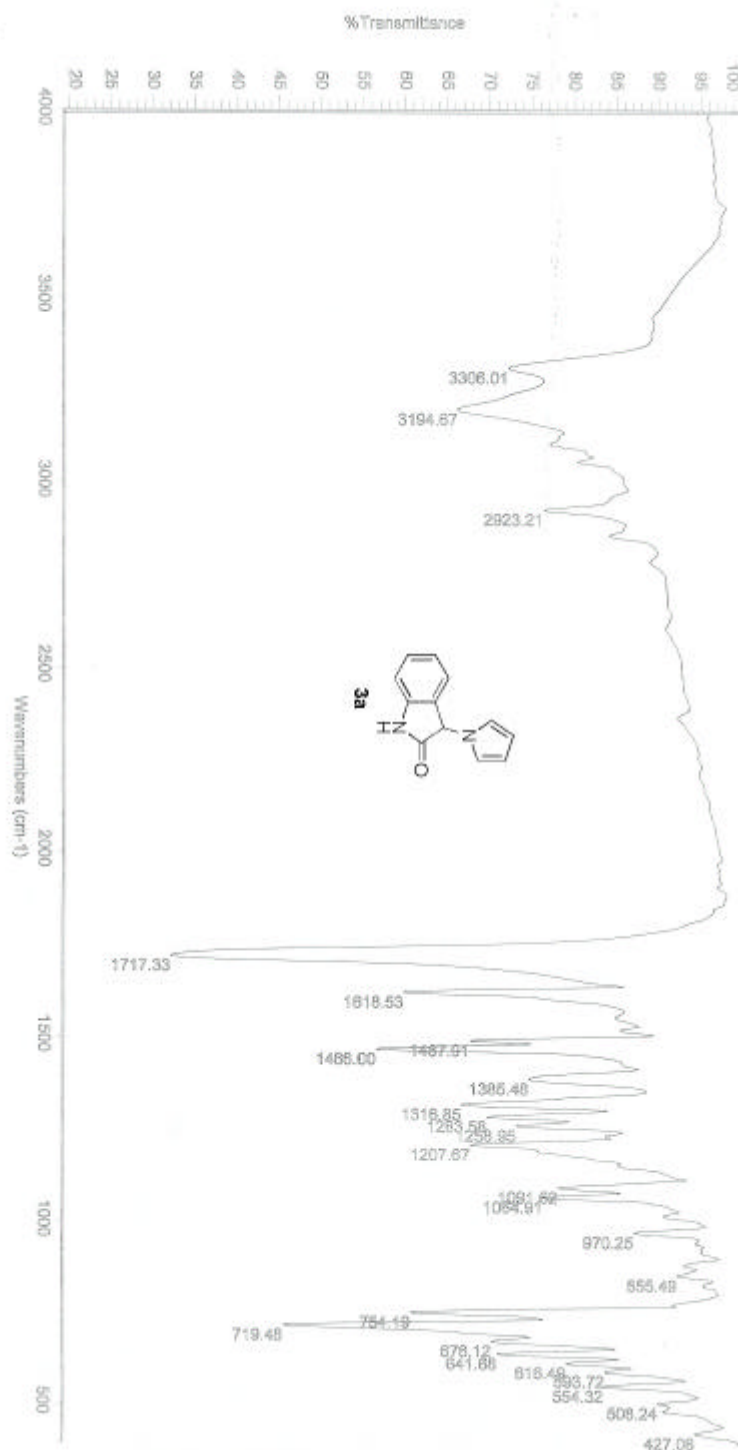


3j



^1H -NMR of compound- 3j

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FTIR Analysis Report

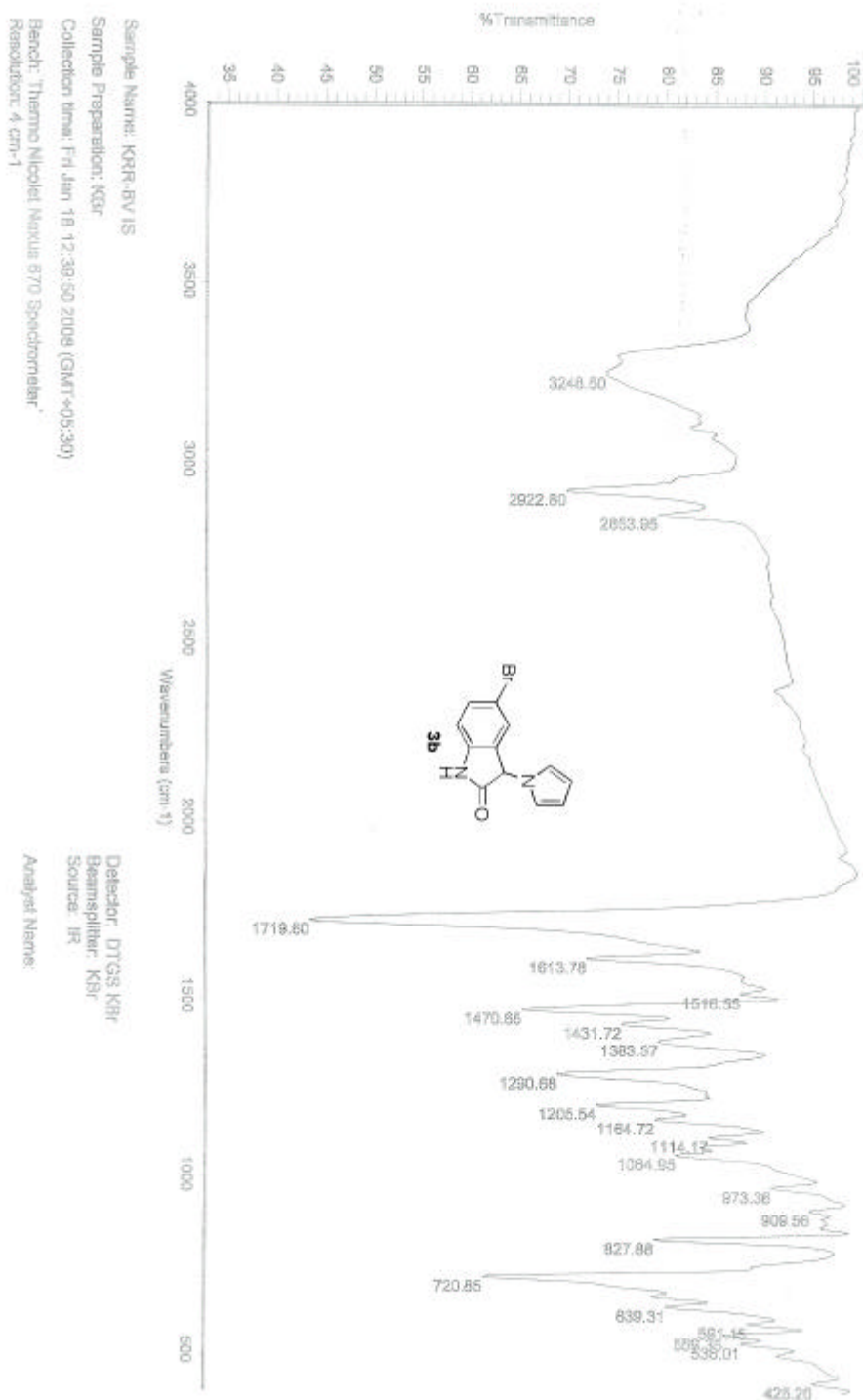


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Sample Preparation: KBr
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Bench: Thermo Nicolet Nexus 670 Spectrometer
Resolution: 4 cm⁻¹

Detector: DTGS KBr
Beam splitter: KBr
Source: IR
Analyst Name:

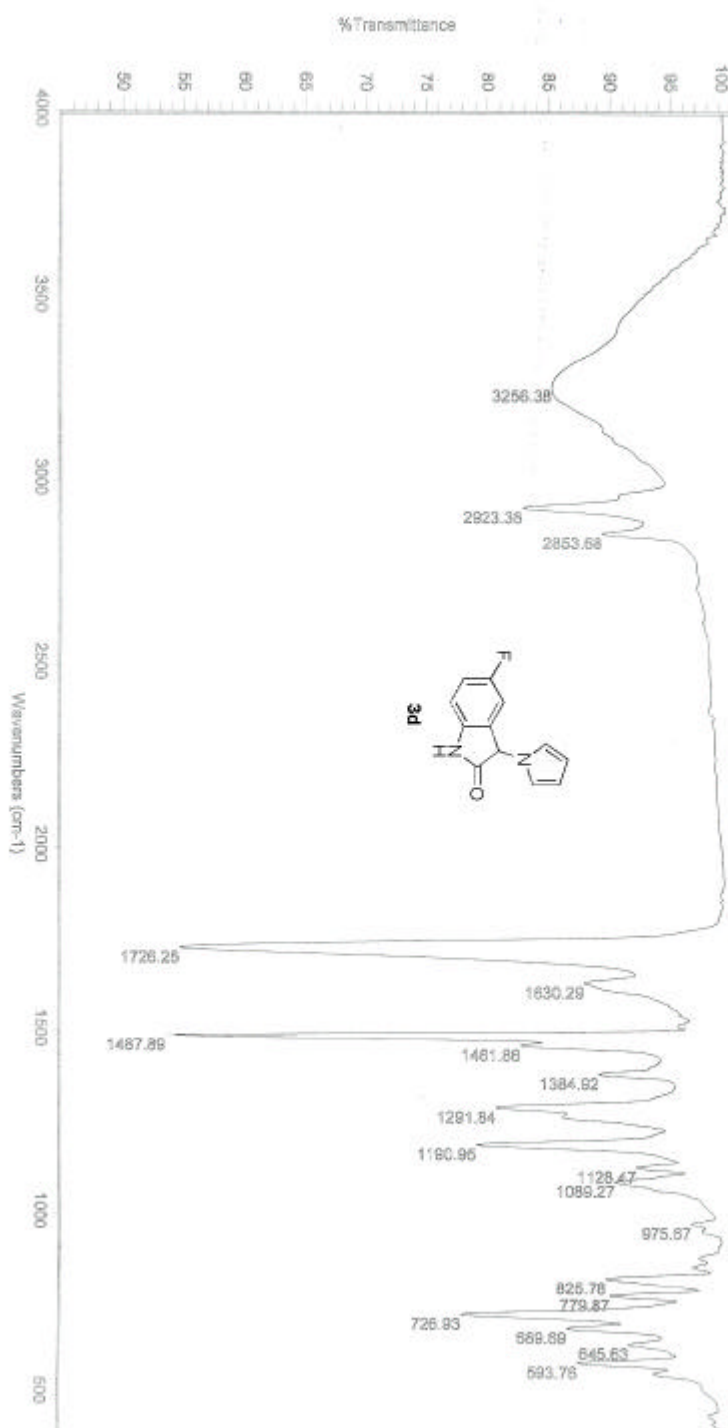
FT-IR spectra of compound- 3a

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FTIR Analysis Report



FT-IR spectra of compound- 3b

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FTIR Analysis Report

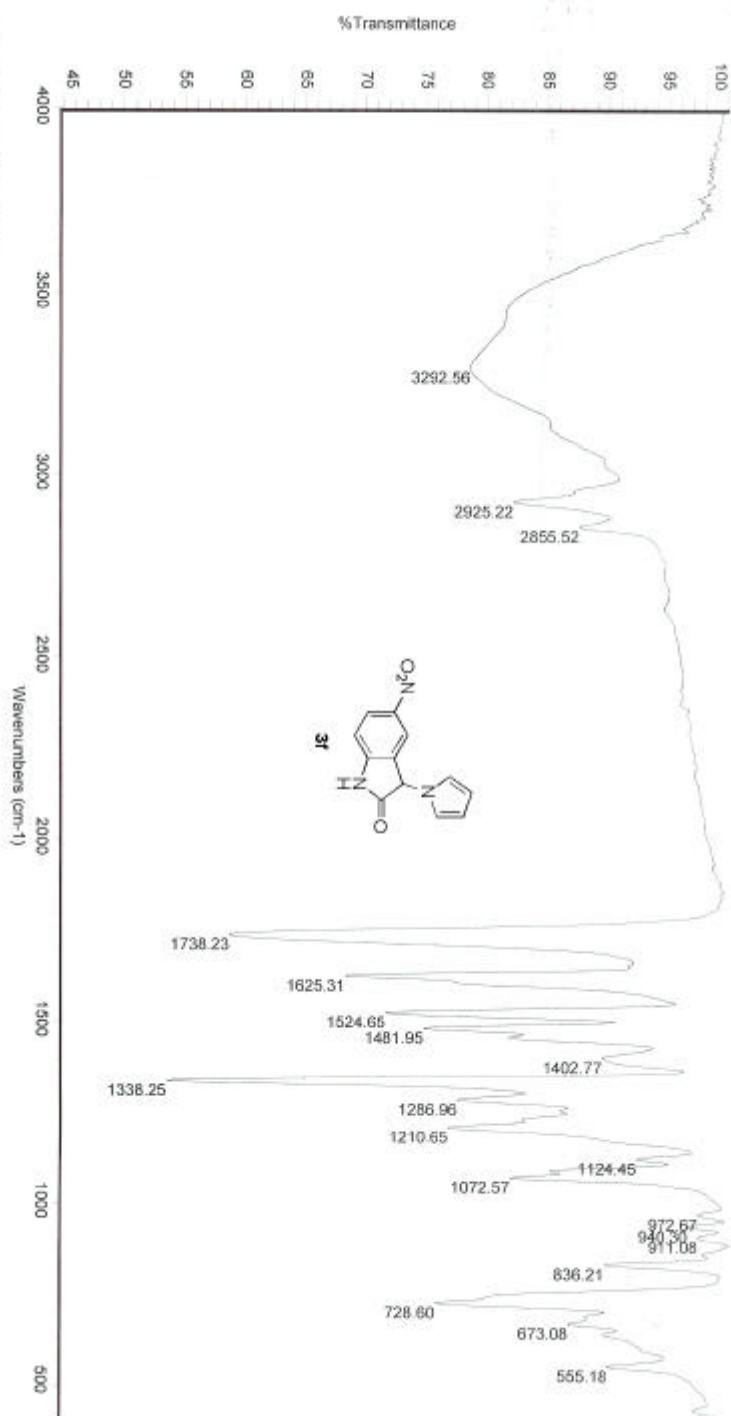


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Sample Preparation: NEAT
Collection time: Fri Jan 16 11:25:43 2008 (GMT+05:30)
Bench: Thermo Nicolet Nexus 670 Spectrometer
Resolution: 4 cm⁻¹

Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
Analyst Name:

FT-IR spectra of compound- 3d

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FTIR Analysis Report



Sample Name: KRR-NITRO
Sample Preparation: NEAT
Collection time: Tue Jan 22 11:57:39 2008 (GMT+05:30)
Bench: Thermo Nicolet Nexus 670 Spectrometer
Resolution: 4 cm⁻¹

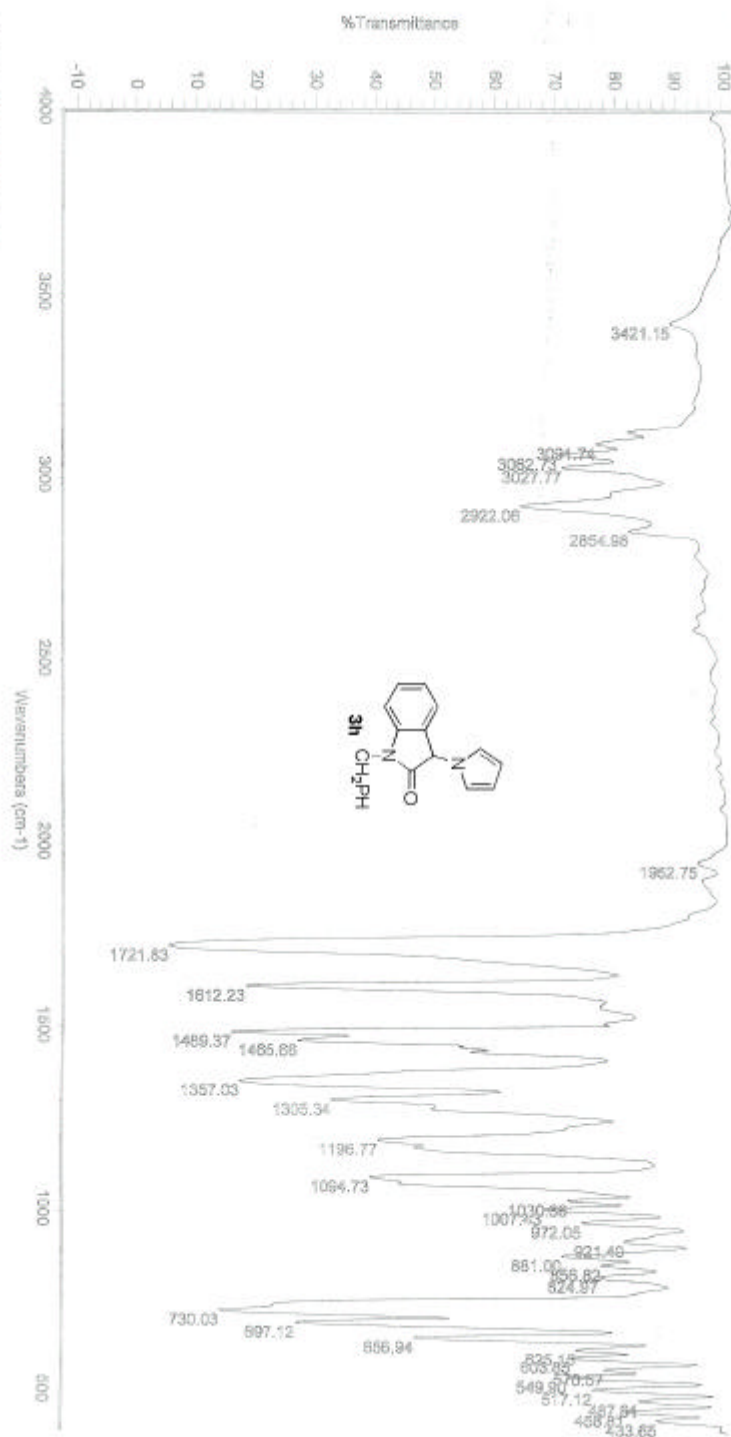
Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
Analyst Name:

FT-IR spectra of compound- 3f

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FTIR Analysis Report

Sample Name: KRR-BENG
Sample Preparation: NEAT
Collection time: Thu Jan 17 11:40:03 2008 (GMT+05:30)
Bench: Thermo Nicolet Nexus 670 Spectrometer
Resolution: 4 cm⁻¹

Detector: DTGS KBr
Beamsplitter: KBr
Source: IR
Analysis Name:



FT-IR spectra of compound- 3h

References and Notes:

1. (a) J. Azizian, A. R. Karimi, Z. Kazemizadeh, A. A. Mohammadi, M. R. Mohammadizadeh, *J. Org. Chem.*, **2005**, *70*, 1471; (b) B. K. Banik, M. Cardona, *Tetrahedron Lett.*, **2006**, *47*, 7385; (c) J. S. Yadav, B. V. Subba Reddy, Ruchi Jain, Ch. Suresh Reddy, *Tetrahedron Lett.*, **2007**, *48*, 3295.