Supporting information

Nickel-mediated *N*-arylation with arylboronic acids: A new avenue to Chan-Lam coupling

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General Experimental:

All the reactions were carried out in 10 mL borosilicate vials with constant stirring using Teflon-coated magnetic stir bar in aerobic conditions. Solvents were freshly distilled according to standard procedures. Column chromatography was performed using Merck silica gel (100-200 mesh). Thin layer chromatography (TLC) was performed using Merck GF₂₅₄ plates (thickness 0.25 mm). Visualization of spots on TLC plate was accomplished with UV light and by staining in I₂ chamber.

All the melting points were determined in open capillary tubes and are uncorrected. ¹H and ¹³C NMR were recorded on 300 MHz and 75 MHz JEOL AL300 FTNMR spectrometer. NMR chemical shifts are expressed in δ values with reference to tetramethylsilane (TMS) as internal standard. Product yields refer to isolated yields after column chromatography.

Reagents:

All the chemicals including arylboronic acids, amines, amides, 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), 2,2'-bipyridyl, tetramethylethylenediamine (TMEDA), 1,10-phenanthroline and all metals salts including NiCl₂.6H₂O (99.999%) were procured from Sigma-Aldrich, USA and were used as received.

General Procedure for C-N Cross-Coupling: A 10 mL borosilicate vial containing arylboronic acid **1** (1 mmol), *N*-nucleophile **2** (2 mmol), NiCl₂.6H₂O (20 mol %), 2,2'-bipyridyl (20 mol %), DBU (2 mmol) and acetonitrile (1 mL) was stirred at room temperature under atmospheric conditions. The progress of the reaction was monitored by TLC using EtOAc and n-hexane as eluent. After completion, the reaction mixture was treated with EtOAc (5 mL) and water (5 mL). The organic layer was separated, and the aqueous layer was extracted with EtOAc (3 $\times$ 5 mL). The combined organic phase was washed with water (2 $\times$ 5 mL), dried over anhydrous Na₂SO₄, and concentrated to yield a residue, which was purified by silica gel column chromatography using hexane /ethyl acetate to yield clean product **3**.

Spectral data of the compounds:

1. Diphenylamine (3a)¹

Colorless solid; mp: 53-54 °C.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.26-7.17 (m, 4H, ArH), 7.05 (d, *J* = 7.8 Hz, 4H, ArH), 6.92 (t, *J* = 7.2 Hz, 2H, ArH), 5.63 (br s, 1H, NH).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 142.9, 129.2, 120.8, 117.7.

2. 4-Methyl-*N*-phenylaniline (3b)¹

White solid; mp: 86-87 °C.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.24-7.20 (m, 2H, ArH), 7.09-6.99 (m, 6H, ArH), 6.89 (t, *J* = 7.2 Hz, 1H, ArH), 5.59 (br s, 1H, NH), 2.30 (s, 3H, CH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 143.9, 140.2, 130.9, 129.8, 129.2, 120.2, 118.9, 116.8, 20.7.

3. 4-Methoxy-*N*-phenylaniline (3c)¹

White solid; mp: 105-107 °C.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.25-7.18 (m, 2H, ArH), 7.08 (d, *J* = 8.7 Hz, 2H, ArH), 6.91-6.80 (m, 5H, ArH), 5.48 (br s, 1H, NH), 3.79 (s, 3H, OCH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 155.2, 145.1, 135.6, 129.2, 122.1, 119.5, 115.5, 114.6, 55.5.

4. 4-Chloro-*N*-phenylaniline (3d)¹

Pale yellow solid; mp: 65-66 °C.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.29-7.18 (m, 4H, ArH), 7.04-6.92 (m, 5H, ArH), 5.65 (br s, 1H, NH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 142.5, 141.8, 129.4, 129.2, 125.4, 121.4, 118.7, 118.0.

5. 4-Nitro-*N*-phenylaniline (**3e**)²

Yellow solid; mp: 133-134 °C.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 8.12 (d, J = 9.0 Hz, 2H, ArH), 7.41 (t, J = 7.8 Hz, 2H, ArH), 7.25-7.13 (m, 3H, ArH), 6.95 (d, J = 9.3 Hz, 2H, ArH), 6.32 (br s, 1H, NH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 150.2, 139.5, 139.4, 129.6, 126.1, 124.5, 121.8, 113.6.

6. 3-Nitro-*N*-phenylaniline (**3f**)¹

Red solid; mp: 85-87 °C.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.82 (s, 1H, ArH), 7.70 (d, J = 7.8 Hz, 1H, ArH), 7.38-7.25 (m, 4H, ArH), 7.15-7.05 (m, 3H, ArH), 5.93 (br s, 1H, NH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 149.2, 145.0, 140.8, 129.9, 129.6, 123.1, 121.8, 119.8, 114.6, 110.2.

7. *N*-(2-Methylphenyl)aniline (**3g**)¹

Yellow oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.26-7.09 (m, 5H, ArH), 6.95-6.86 (m, 4H, ArH), 5.36 (br s, 1H, NH), 2.24 (s, 3H, CH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 143.9, 141.1, 130.9, 129.2, 128.2, 126.7, 121.9, 120.4, 118.7, 117.4, 17.8.

8. ***N*-(2-Methoxyphenyl)aniline (3h)**²

Brown oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.29-7.24 (m, 3H, ArH), 7.15 (d, J = 7.8 Hz, 2H, ArH), 6.95-6.85 (m, 4H, ArH), 6.14 (s, 1H, NH), 3.88 (s, 3H, OCH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 148.1, 142.6, 132.8, 129.2, 121.0, 120.7, 119.8, 118.4, 114.5, 110.4, 55.5.

9. **2-bromo-*N*-phenylaniline (3i)**¹

Brown oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.52 (d, J = 7.8 Hz, 1H, ArH), 7.34-7.23 (m, 4H, ArH), 7.16 (d, J = 7.5 Hz, 2H, ArH), 7.05 (t, J = 7.2 Hz, 1H, ArH), 6.75 (t, J = 6.9 Hz, 1H, ArH), 6.07 (s, 1H, NH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 141.5, 141.3, 132.9, 129.4, 128.0, 122.6, 120.8, 120.2, 115.7, 112.1, 55.5.

10. **2-(Phenylamino)phenol (3j)**³

Dark Brown oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.25-7.17 (m, 2H, ArH), 7.12 (t, J = 7.2 Hz, 1H, ArH), 6.99 (d, J = 7.5 Hz, 1H, ArH), 6.91-6.85 (m, 2H, ArH), 6.79-6.76 (m, 3H, ArH), 5.76 (br s, 1H, OH), 5.26 (br s, 1H, NH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 150.5, 145.1, 129.2, 125.5, 123.9, 120.8, 120.1, 115.8, 115.4.

11. N-Hexylaniline (3k)¹

Colorless oil.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.18 (t, *J* = 7.2 Hz, 2H, ArH), 6.69 (t, *J* = 6.9 Hz, 1H, ArH), 6.60 (d, *J* = 7.5 Hz, 2H, ArH), 3.57 (br s, 1H, NH), 3.11 (t, *J* = 6.9 Hz, 2H, CH₂), 1.65-1.56 (m, 2H, CH₂), 1.41-1.32 (m, 6H, CH₂), 0.91 (t, *J* = 5.4 Hz, 3H, CH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 148.5, 129.1, 117.0, 112.6, 43.9, 31.6, 29.5, 26.8, 22.6, 14.0.

12. N-Benzylaniline (3l)¹

Colorless oil.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.35-7.25 (m, 5H, ArH), 7.22-7.13 (m, 2H, ArH), 6.72 (t, *J* = 7.2 Hz, 1H, ArH), 6.68 (d, *J* = 7.8 Hz, 2H, ArH), 4.31 (s, 2H, CH₂), 4.0 (br s, 1H, NH).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 148.1, 139.4, 129.2, 128.5, 127.4, 127.1, 117.5, 112.8, 48.2.

13. N-Phenyl-morpholine (3m)⁴

Pale crystalline solid; mp: 51-53 °C.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.29 (t, *J* = 7.8 Hz, 2H, ArH), 6.92-6.85 (m, 3H, ArH), 3.87 (t, *J* = 4.8 Hz, 4H, CH₂), 3.16 (t, *J* = 4.8 Hz, 4H, CH₂).

¹³C NMR (100 MHz, CDCl₃, δ ppm): 151.2, 129.1, 120.0, 115.6, 66.9, 49.3.

14. N-Phenyl pyrazole (3p)¹

Light yellow oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.92 (d, $J = 2.1$ Hz, 1H, ArH), 7.72-7.68 (m, 3H, ArH), 7.47 (t, $J = 7.5$ Hz, 2H, ArH), 7.30-7.25 (m, 1H, ArH), 6.46 (s, 1H, ArH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 141.0, 140.2, 129.3, 126.6, 126.4, 119.1, 107.5.

15. ***N*-Phenylbenzamide (3q)**⁵

White solid; mp 161-163 °C.

^1H NMR (300 MHz, DMSO-d_6 , δ ppm): 10.24 (br s, 1H, NH), 7.97 (d, $J = 6.9$ Hz, 2H, ArH), 7.80 (d, $J = 7.8$ Hz, 2H, ArH), 7.59-7.51 (m, 3H, ArH), 7.38 (t, $J = 7.2$ Hz, 2H, ArH), 7.13 (t, $J = 7.2$ Hz, 1H, ArH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 165.7, 138.0, 135.1, 131.7, 129.0, 128.7, 127.0, 124.5, 120.3.

16. **2-Methyl-*N*-phenylbenzamide (3r)**⁶

White solid

^1H NMR (300 MHz, CDCl_3 , δ ppm): 10.27 (s, 1H, NH), 7.74 (d, $J = 7.8$ Hz, 2H, ArH), 7.44-7.28 (m, 6H, ArH), 7.09 (t, $J = 7.2$ Hz, 1H, ArH), 2.37 (s, 3H, CH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 168.1, 137.9, 136.2, 131.1, 130.1, 129.0, 126.5, 125.8, 124.4, 119.8, 19.7.

17. ***N*-Phenylacetamide (3t)**⁷

White solid; mp: 163-164 °C.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 8.25 (s, 1H, NH), 7.51 (d, J = 7.8 Hz, 2H, ArH), 7.29-7.24 (m, 2H, ArH), 7.09 (t, J = 7.5 Hz, 1H, ArH), 2.12 (s, 3H, CH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 169.1, 138.0, 128.6, 124.1, 120.1, 24.1.

18. Di-*p*-tolylamine (3u)⁸

Yellowish solid; mp: 79-80 °C.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.06 (d, J = 8.1 Hz, 4H, ArH), 6.95 (d, J = 8.4 Hz, 4H, ArH), 5.50 (s, 1H, NH), 2.28 (s, 6H, CH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 141.1, 130.1, 129.7, 117.8, 20.6.

19. 4-chloro-*N*-(*p*-tolyl)aniline (3v)⁹

White solid; mp: 82-83 °C.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.16 (d, J = 8.7 Hz, 2H, ArH), 7.09 (d, J = 8.1 Hz, 2H, ArH), 6.96-6.87 (m, 4H, ArH), 5.53 (s, 1H, NH), 2.29 (s, 3H, CH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 142.6, 139.7, 131.4, 129.9, 129.1, 124.6, 119.1, 117.8, 20.6.

20. 2-methoxy-*N*-(*p*-tolyl)aniline (3w)⁹

Yellow oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.23-7.18 (m, 1H, ArH), 7.07-7.03 (m, 4H, ArH), 6.84-6.79 (m, 3H, ArH), 6.06 (br s, 1H, NH), 3.87 (s, 3H, OCH_3), 2.30 (s, 3H, CH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 147.8, 139.8, 133.7, 130.9, 129.7, 120.7, 119.5, 119.1, 113.6, 110.3, 55.5, 20.6.

21. *N*-Benzyl-4-methylaniline (3x)¹⁰

Colourless oil.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.34-7.22 (m, 5H, ArH), 6.98 (d, *J* = 8.1 Hz, 2H, ArH), 6.56 (d, *J* = 8.1 Hz, 2H, ArH), 4.29 (s, 2H, CH₂), 3.88 (br s, 1H, NH), 2.22 (s, 3H, CH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 145.9, 139.6, 129.7, 128.5, 127.4, 127.1, 126.6, 112.9, 48.6, 20.3.

22. *N*-(*p*-tolyl)benzamide (3y)¹¹

White solid; mp: 158-159 °C.

¹H NMR (300 MHz, DMSO-d₆, δ ppm): 10.16 (s, 1H, NH), 7.95 (d, *J* = 7.2 Hz, 2H, ArH), 7.67 (d, *J* = 7.2 Hz, 2H, ArH), 7.58-7.51 (m, 3H, ArH), 7.16 (d, *J* = 7.8 Hz, 2H, ArH), 2.28 (s, 3H, CH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 165.6, 135.3, 135.0, 134.1, 131.6, 129.5, 128.6, 126.9, 120.3, 20.8.

23. *N*-phenyl-4-(trifluoromethyl)aniline (3z)¹

Colorless solid; mp: 59-60 °C.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.46 (d, *J* = 8.4 Hz, 2H, ArH), 7.33 (t, *J* = 7.5 Hz, 2H, ArH), 7.14 (d, *J* = 7.8 Hz, 2H, ArH), 7.05-7.01 (m, 3H, ArH), 5.89 (br s, 1H, NH).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 146.7, 141.1, 129.5, 126.7, 126.6, 126.4, 122.9, 121.8, 121.4, 120.0, 115.3.

24. 4-chloro-*N*-(4-(trifluoromethyl)phenyl)aniline (3aa)

Yellow oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.47 (d, J = 8.4 Hz, 2H, ArH), 7.27 (d, J = 8.7 Hz, 2H, ArH), 7.06-6.98 (m, 4H, ArH), 5.86 (br s, 1H, NH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 146.3, 139.8, 129.5, 127.7, 126.8, 126.7, 126.2, 122.4, 121.9, 121.1, 115.5.

25. *N*-(4-(trifluoromethyl)phenyl)benzamide (3ab)¹²

White solid; mp: 198-199 °C.

^1H NMR (300 MHz, DMSO-d_6 , δ ppm): 10.56 (br s, 1H, NH), 8.01-7.94 (m, 4H, ArH), 7.72 (d, J = 8.4 Hz, 2H, ArH), 7.60-7.51 (m, 3H, ArH).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 166.0, 142.8, 134.4, 131.9, 128.4, 127.7, 125.9, 125.8, 123.8, 120.0.

26. 3-methyl-*N*-phenylaniline (3ac)¹³

Yellow oil.

^1H NMR (300 MHz, CDCl_3 , δ ppm): 7.27-7.22 (m, 2H, ArH), 7.16 (t, J = 7.8 Hz, 1H, ArH), 7.06 (d, J = 7.8 Hz, 2H, ArH), 6.93-6.88 (m, 3H, ArH), 6.75 (d, J = 7.5 Hz, 1H, ArH), 5.64 (br s, 1H, ArH), 2.30 (s, 3H, CH_3).

^{13}C NMR (75 MHz, CDCl_3 , δ ppm): 143.1, 141.0, 139.1, 129.2, 129.1, 121.8, 120.8, 118.4, 117.7, 114.8, 21.5.

27. *N*-Benzyl-3-methylaniline (3ad)¹⁴

Yellow oil.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.35-7.23 (m, 5H, ArH), 7.07 (t, *J* = 7.5 Hz, 1H, ArH), 6.54 (d, *J* = 7.2 Hz, 1H, ArH), 6.46-6.43 (m, 2H, ArH), 4.30 (s, 2H, CH₂), 3.95 (br s, 1H, NH), 2.26 (s, 3H, CH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 148.1, 139.5, 139.0, 129.1, 128.5, 127.4, 127.1, 118.5, 113.6, 109.9, 48.3, 21.6.

28. Di(*o*-tolyl)amine (3ae)¹⁵

Colourless oil.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.19 (d, *J* = 7.2 Hz, 2H, ArH), 7.13 (t, *J* = 7.5 Hz, 2H, ArH), 6.98 (d, *J* = 7.8 Hz, 2H, ArH), 6.91 (t, *J* = 7.2 Hz, 2H, ArH), 5.13 (br s, 1H, NH), 2.26 (s, 6H, CH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 141.9, 130.7, 127.4, 126.7, 121.3, 118.2, 17.7.

29. *N*-benzyl-2-methylaniline (3af)¹⁰

Colourless oil.

¹H NMR (300 MHz, CDCl₃, δ ppm): 7.39-7.24 (m, 5H, ArH), 7.11 (t, *J* = 8.4 Hz, 2H, ArH), 6.69-6.59 (m, 2H, ArH), 4.37 (s, 2H, CH₂), 3.86 (br s, 1H, NH), 2.16 (s, 3H, CH₃).

¹³C NMR (75 MHz, CDCl₃, δ ppm): 146.0, 139.4, 130.0, 128.6, 127.5, 127.2, 127.1, 121.9, 117.1, 109.9, 48.3, 17.5.

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 PHPH 1H Mr. Amit K. Gupta

JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

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JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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MF 1.20 Hz
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MEPHNHPH 1H Mr. A.K. Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
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Operator : Nagendra Kumar
Shishir Singh

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SLVNT CDCL3
EXREF 0.00 ppm
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1H
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CTEMP CDCL3
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MEOPHNHPH02 1H Mr. A.K. Gupta

JEOL AL300 FTNMR
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VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

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DATIM Mon Oct 24 13:34:53 2011

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CTEMP	
SLVNT CDCL3	
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	22

C:\Amit Gupta\MEOPHNHPH 13C.ais
MEOPHNHPH 13C Mr. A.K. Gupta

DFILE C:\Amit Gupta\MEOPHNHPH 13C.
 COMNT MEOPHNHPH 13C Mr. A.K. Gupta
 DATIM Fri Dec 30 21:23:47 2011
 ORNUC 13C
 EXMOD BCM
 ORFRO 75.45 MHz
 ORSET 127.30 KHz
 ORFIN 44.7 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 3500
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 6.0 us
 IRNUC 1H
 CTEMP 17.9 c
 SLVNT CDCl3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 25

C:\Amit Gupta\CLPHNHPH 02 1H.als
CLPHNHPH 02 1H Mr.A.K.Gupta

JEOI AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\Amit Gupta\CLPHNHPH 02 1H
COMNT CLPHNHPH 02 1H Mr.A.K.Gupta
DATIM Thu Oct 20 16:37:34 2011
OBNUC 1H
EXMOD NON
OBFSQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
FOINT 32768
FREQU 9505.7 Hz
SCANS 32
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 17

C:\Amit Gupta\CINHPH 13C.als
CINHPH 13C Mr. A.K. Gupta

DFILE C:\Amit Gupta\CINHPH 13C.als
COMNT CINHPH 13C Mr. A.K. Gupta
DATIM Fri Mar 30 08:56:59 2012
OBNUC 13C
EXMOD BCM
OBFOQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 3500
ACQTM 1.606 sec
PD 1.394 sec
PWI 6.0 us
IRNUC 1H
CTEMP 18.1 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\WINNR98\COMMON\DEFAULT.ALS
NO2C 1H Mr.A.K.Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh

D:\WINNR98\COMMON\DEFAULT.
COMNT NO2C 1H Mr.A.K.Gupta
DATIM Tue May 08 14:12:42 2012
OBNUC 1H
EXMOD NON
OBFRC 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQ 9505.7 Hz
SCANS 18
ACQTM 3.447 sec
PD 1.547 sec
FW 5.2 us
IRNUC 1H
CTEMP 22.0 C
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 16

C:\Amit Gupta\NO2E_13C.als
NO2E 13C Mr.Amit Gupta

DFILE C:\Amit Gupta\NO2E_13C.als
COMNT NO2E 13C Mr.Amit Gupta
DATIM Fri Jun 01 14:34:25 2012
ORNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQ 20408.1 Hz
SCANS 250
ACQTM 1.606 sec
PD 1.394 sec
PWL 6.0 us
IRNUC 1H
CTEMP 22.1 c
SOLVT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh, I.T\MNO2B_1H.als
MNO2B 1H Mr.Dushyant singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Negendra Kumar
Shishir Singh

DEFILE C:\K.N. Singh, I.T\MNO2B_1H.
COMINT MNO2B_1H Mr.Dushyant singh
DATIM Fri May 25 15:43:52 2012
ORNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 55
ACQTM 3.47 sec
PD 1.547 sec
PWI 5.2 us
IRNUC 1H
CTEMP 21.8 C
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 20

C:\Amit Gupta\MNO2PHNHPH 13C.als
MNO2PHNHPH 13C Mr. Amit Gupta

DEFILE C:\Amit Gupta\MNO2PHNHPH 13C
COMNT MNO2PHNHPH 13C Mr. Amit Gupta
DATIM Thu Jan 12 22:54:57 2012
OBNUC 13C
EXMOD BCN
OSFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 3000
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.1 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh, I.T\Photo_1N.als
Photo 1N Dr.Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

D:\K.N. Singh, I.T\Photo_1N.
COMPT Photo 1N Dr.Dushyant Singh
DATIM Sat Jul 14 13:01:23 2012

ORNUC 1H
EXHOCO NON
ORNUC 300.40 MHz
ORSET 130.00 MHz
ORFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 46
ACQTM 3.447 sec
FO 1.547 sec
PM1 5.2 us
IRNUC 1H
CTEMP 20.0 C
SLVNT CDCL3
EXREF 0.00 ppm
RF 1.20 Hz
RGAIN 14

C:\K.N. Singh,.I.T\Photo_13C.ala
PhoANI 1H Dr.Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagnendra Kumar
Shishir Singh
D:\K.N. Singh,.I.T\Photo_13C
COMMENT PhoANI 1H Dr.Dushyant Singh
DATIM Sat Jul 12 13:23:50 2012
CQNUC 13C
EXMOC BCM
OBPRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 213
ACQTH 1.606 sec
PD 1.394 sec
PWI 6.0 us
IRNUC 1H
CTEMP 20.6 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh..I.T\PROANI-4_1H.alb
 PROANI-4 1H Dr.Dushyant Singh

JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005
 Operator : Nagendra Kumar
 Shahar Singh
 DFILE C:\K.N. Singh..I.T\PROANI-4
 COMMENT PROANI-4 1H Dr.Dushyant Singh
 DATIN Fri Jul 20 13:51:09 2012
 QBRUC 1H
 EXM00 NON
 CBF90 300.40 MHz
 OBSET 130.00 MHz
 CBFIN 1150.0 Hz
 POINT 32768
 FREQ0 9505.7 Hz
 SCANS 20
 ACQTH 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTENP 19.1 C
 SLVNT CDCL3
 EXREF 0.00 ppm
 RF 1.20 MHz
 RGAIN 16

C:\MINN898\COMMON\DEFAULT.ALS
PhoANI-1 13C Mr. Dushyant

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

D:\MINN898\COMMON\DEFAULT
COMPT PhoANI-1 13C Mr. Dushyant
DATIM Tue Jul 17 16:19:37 2012
CINUC 13C

EXMOD BOM
OBPRO 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 77
ACQTM 1.606 sec
PD 1.394 sec
PM1 6.0 us
IRSDC 1K
CTEMP 22.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh..1.T\CL-6_1H.a1s
CL-6 1H Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shahar Singh

DFILE C:\K.N. Singh..1.T\CL-6_1H.
COMMT CL-6 1H Mr. Dushyant Singh
DATIM Mon Jul 09 13:09:38 2012

EXNOUC 1H
EXNOCD NON
CHPRO 300.40 MHz
CHSET 130.00 MHz
CHFIN 1150.0 Hz
POINT 32768
FREQO 9505.7 Hz
SCANS 16
AQTM 3.447 sec
PD 1.547 sec
FWI 5.2 us
INNOUC 1H
CTEMP 19.4 c
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 21

C:\WINNOR98\COMMON\DEFAULT.ALS
 Probe: 13C Mr. Dushyant Singh

C:\K.N. Singh, I.T\CL-3 3C.als
CL-3 3C Mr.Dushyant K. Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\K.N. Singh, I.T\CL-3 3C..
COMNT CL-3 3C Mr.Dushyant K. Sing.
DATIM Sat Jul 07 12:43:27 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 759
ACQTN 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.9 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 24

C:\K.N. Singh,,I.T\HEX_1H.als
 HEX_1H Mr.D.S.Raghuvansi

JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

DFILE C:\K.N. Singh,,I.T\HEX_1H.als
 COMMENT HEX_1H Mr.D.S.Raghuvansi
 DATIM Mon Mar 26 13:28:14 2012
 ORNUC 1H
 EXMOC NON
 ORFRO 300.40 MHz
 ORSET 130.00 MHz
 ORFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 18
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTEMP 22.0 c
 SLVMT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 13

C:\K.N. Singh, I.T\HEX_13C.als
 HEX_13C Mr.Dubhyant K. singh

DFILE C:\K.N. Singh, I.T\HEX_13C.als
 COMPT HEX_13C Mr.Dubhyant K. singh
 DATIM Mon Mar 26 14:23:18 2012
 CNUC 13C
 EXMOD BCM
 CBFREQ 75.45 MHz
 ORSET 127.30 KHz
 CBFIN 44.7 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 250
 ACQTM 1.606 sec
 PD 1.394 sec
 FW1 6.0 us
 INUC 1H
 CTEMP 20.4 c
 SLVNT CDCL3
 EXPEF 77.00 ppm
 BF 1.20 Hz
 RGAIN 25

C:\K.N. Singh, I.T\PHB208_1H.als
PHB208_1H Mr. Dushyant Singh

JEOL AL300 ETNMR
CHEMISTRY DEPARTMENT
Benaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh, I.T\PHB208_1H
COMNT PHB208_1H Mr. Dushyant Singh
DATIM Fri May 25 14:04:05 2012
EXMOC 1H

EXMOC NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQ 9505.7 Hz
SCANS 32
ACQTM 3.447 sec
PD 1.547 sec
PWI 5.2 us
IRNUC 1H
CTEMP 21.7 C
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 13

NS-01

C:\Amit Gupta\MOR-07_1H.als
MOR-07_1H Mr.Amit Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\Amit Gupta\MOR-07_1H.als
CONNT MOR-07_1H Mr.Amit Gupta
DATIM Thu May 31 14:01:17 2012
OBNUC 1H

EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 MHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 34
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 21.8 c
SLVNT CDCL3
EXREF 0.00 ppm
Bf 1.20 Hz
RGAIN 14

C:\Amit Gupta\MOR_13C.als
MOR_13C Mr. Amit Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\Amit Gupta\MOR_13C.als
COMMT MOR_13C Mr. Amit Gupta
DATIM Wed May 02 11:39:15 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 489
ACQTM 1.606 sec
PD 1.394 sec
PWI 6.0 us
IRNUC 1H
CTEMP 20.6 c
SLUNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 15

C:\Amit Gupta\PY201 1H.als
PY201 1H Mr. A.K. Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\Amit Gupta\PY201 1H.als
COMNT PY201 1H Mr. A.K. Gupta
DATIM Wed Apr 25 17:04:55 2012

ORNUC 1H
EXMOD NON
ORFRO 300.40 MHz
ORSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 32
ACQTM 5.446 sec
PD 1.547 sec
PWL 5.2 us
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCl3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 18

NS 02

C:\Amit Gupta\PhCONHS_1H.a1s
PhCONHS 1H Mr. Amit K. Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\Amit Gupta\PhCONHS_1H.a1s
COMMT PhCONHS_1H Mr. Amit K. Gupta
DATIM Wed Jun 06 15:45:00 2012

OSNUC 1H	300.40 MHz
EXPOD NON	130.00 KHz
OSFRQ	1150.0 Hz
OSSET	32768
OSFTN	6016.8 Hz
POINT	32
FREQD	5.446 sec
SCANS	1.547 sec
ACQTM	5.2 us
PD	
PW1	23.0 c
IRNUC 1H	
CTEMP	0.00 ppm
SLVNT DMSO	1.20 Hz
EXREF	
BF	
RGAIN	16

C:\Amit Gupta\PHCONH_13C.als
PHCONH_13C Mr. Amit K. Gupta

DFile C:\Amit Gupta\PHCONH_13C.als
COMNT PHCONH_13C Mr. Amit K. Gupta
DATIM Tue Apr 17 11:49:14 2012
CENUC 13C
EXMOD BCM
OBPRO 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQ 20408.1 Hz
SCANS 200
ACQTM 1.606 sec
PD 1.394 sec
PWL 6.0 us
IRNUC 1H
CTEMP 37.6 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh,,1.T\Ph2MEAM_1H.a19
Ph2MEAM_1H Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VABANASI-221005
Operator : Nagesh Kumar
Shishir Singh
DFILE C:\K.N. Singh,,1.T\Ph2MEAM_1
CONNT Ph2MEAM_1H Mr. Dushyant Singh
DATIN Tue Jul 31 12:23:41 2012

EXMUC 1H
EXMUC NON
OBFTQ 300.40 MHz
OBSET 130.00 MHz
OBFIN 1150.0 Hz
POINT 32768
FREQ 9505.7 Hz
SCANS 32
ACQTM 3.447 sec
PD 1.547 sec
PWL 5.2 us
IRNUC 1H
CTEMP 20.5 C
SLANT DMSO
EXREF 2.49 ppm
BF 1.20 Hz
RGAIN 17

C:\WINNR98\Data\2MEAN_13C18CM El.als
2MEAN 13C Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VAPANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNR98\Data\2MEAN_13C1E
CONGT 2MEAN_13C Mr. Dushyant Singh
DATIM Wed Jul 25 20:25:34 2012

ORNUC	13C
EXMOD	BCN
ORFRO	75.45 MHz
ORSET	127.30 KHz
ORFIN	44.7 Hz
POINT	32768
FREQU	20408.1 Hz
SCANS	4000
ACQTM	1.606 sec
PD	1.394 sec
FWI	6.0 us
IRNUC	1H
CTEMP	19.1 C
SLVNT	CDCL3
EXREF	77.00 ppm
BF	1.20 Hz
RGAIN	24

C:\WINNMR98\COMMON\DEFAULT.ALS
ACIDE.1H Mr.Amit Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
D:\WINNMR98\COMMON\DEFAULT.ALS
COMPT ACIDE.1H Mr.Amit Gupta
DATIM Thu Apr 19 13:53:19 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
PUL 5.2 us
IRNUC 1H
CTEMP 21.3 C
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 12

C:\WINNR98\Data\AC-2_13C1BCH_E1.sls
AC-2 13C Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagerdra Kumar
Shishir Singh

OFILE C:\WINNR98\Data\AC-2_13C1B
COMNT AC-2 13C Mr. Dushyant Singh
DATIM Wed Jun 06 15:27:19 2012

ORNUC 13C
EXMOD ECM
ORFRO 75.45 MHz
ORSET 127.30 KHz
ORFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 500
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 24.0 C
SIVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,,I.T\MEME02_1H.a1a
MEME02_1H Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh,,I.T\MEME02_1H
CONST MEME02_1H Mr. Dushyant Singh
DATIM F11 Mar 23 15:48:55 2012

OBNUC	1H	
EXMOD	NON	
OBFRQ	300.40 MHz	
OBSET	130.00 KHz	
OBFIN	1150.0 Hz	
POINT	32768	
FREQU	9505.7 Hz	
SCANS	8	
ACQTM	3.447 sec	
PD	1.547 sec	
FW1	5.2 us	
IRNUC	1H	
CTEMP	21.7 C	
SLVNT	CDCL3	
EXREF	0.00 ppm	
BF	1.20 Hz	
RGAIN	19	

C:\K.N. Singh,,I.T\MEME02_13C.als
MEME02_13C Mr. Dushyant Singh

DFILE C:\K.N. Singh,,I.T\MEME02_12
 COMMENT MEME02_13C Mr. Dushyant Singh
 DATIM Sat Mar 24 17:31:21 2012
 ORNUC 13C
 EXMOD BCN
 OBFRQ 75.45 MHz
 OBSET 127.30 KHz
 OBFIN 44.7 Hz
 POINT 32768
 FREQU 20408.1 Hz
 SCANS 823
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 6.0 us
 INNUC 1H
 CTMP 20.8 C
 SLVT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 25

C:\Amit Gupta\MECL 1H.ais
MECL 1H Mr. Amit K. Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
D:\Amit Gupta\MECL 1H.ais
COMET MECL 1H Mr. Amit K. Gupta
DATIM Thu Apr 19 11:13:55 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 kHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 16
ACQTM 3.447 sec
PD 1.547 sec
FW 5.2 us
IRNUC 1H
CTEMP 24.0 C
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 12

C:\Amit Gupta\MECL-13C.als
MECL-13C Mr. Amit K. Gupta

OFIL C:\Amit Gupta\MECL-13C.als
COMT MECL-13C Mr. Amit K. Gupta
DATIM Thu Apr 19 11:07:57 2012
OENUC 13C
EXMOD BCM

OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 434
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.3 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,,I.T\p-TOOANI_1H.dls
p-TOOANI 1H Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh

DTITLE C:\K.N. Singh,,I.T\p-TOOANI_1H
COMMT p-TOOANI 1H Mr. Dushyant Singh
DATIN Wed Jul 25 12:07:08 2012

ORNUC 1H
EXMOD MCON
ORFRO 300.40 MHz
ORSET 130.00 KHz
ORFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 29
ACQTH 3.447 sec
PD 1.547 sec
FID 5.2 us
IRNUC 1H
CTEMP 21.3 C
SLVNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 14

C:\WINNMR98\COMMON\DEFAULT.ALS
MEPHOANI 13C Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagesh Kumar
Shishir Singh

C:\WINNMR98\COMMON\DEFAULT.
COMET MEPHOANI 13C Mr. Dushyant Si
DATIM Mon Jul 16 15:26:20 2012

GENUC 13C
EXMOC BCM
OBFRQ 75.45 MHz
OBSET 127.30 kHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 98
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 24.6 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\Amit Gupta\MEB206_1H.als
MEB206_1H Mr. Amit K. Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
DFILE C:\Amit Gupta\MEB206_1H.als
COMNT MEB206_1H Mr. Amit K. Gupta
DATIM Thu May 24 12:01:31 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQ 9509.7 Hz
SCANS 22
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 20.9 c
SLUNT CDCL3
EXREF 0.00 ppm
BF 1.20 Hz
RGAIN 15

NS 05

C:\WINNR98\COMMON\DEFAULT.ALS
MeCONH-5 1HMr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
D:\WINNR98\COMMON\DEFAULT.
COMNT MeCONH-5 1HMr. Dushyant Singh
DATIN Wed Jun 06 16:21:04 2012
GENUC 1H
EXMOD NON
GBFRQ 300.40 MHz
GBSET 130.00 KHz
GBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 32
ACQTM 5.446 sec
PD 1.547 sec
Pw1 5.2 us
IRNUC 1H
CTEMP 22.9 c
SLVNT CDCL3
EXREF 0.00 ppm
RF 1.20 Hz
RGAIN 15

C:\Amit Gupta\MECONH_1H.a1s
MECONH_1H Mr.Amit K. Gupta

DEFILE C:\Amit Gupta\MECONH_1H.a1s
COMNT MECONH_1H Mr.Amit K. Gupta
DATIM Fri Apr 20 12:09:46 2012
ORNUC 13C
EXMOD BCM
ORFRO 75.45 MHz
ORSET 127.30 KHz
ORFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 200
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 22.3 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 18

C:\Amit Gupta\CF3PHNPH 1H.als
CF3PHNPH 1H Mr.Amit K.Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
D:\Amit Gupta\CF3PHNPH 1H.4
COMET CF3PHNPH 1H Mr.Amit K.Gupta
DATIM Sat Oct 29 17:22:23 2011
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
ORSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 6016.8 Hz
SCANS 32
ACQTM 5.446 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 18.8 C
SLVNT CDCL3
EXREF 7.24 ppm
BF 1.20 Hz
RGAIN 22

NS 03

C:\WINNR98\COMMON_DEFAULT.ALS
CF3Cl 1H Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNR98\COMMON_DEFAULT.
COMNT CF3Cl 1H Mr. Dushyant Singh
DATIM Mon May 28 17:18:24 2012

OBNUC	1H
EXMOD	NON
OBFRQ	300.40 MHz
OBSET	130.00 KHz
OBFIN	1150.0 Hz
POINT	32768
FREQU	9505.7 Hz
SCANS	16
ACQTM	3.447 sec
PD	1.547 sec
PM1	5.2 us
IRNUC	1H
CTEMP	22.1 C
SLVNT	CDCL3
EXREF	0.00 ppm
BF	1.20 Hz
RGAIN	14

NS 04

C:\Amit Gupta\CF3AM_1H.als
CF3AM_1H Mr. A.K. Gupta

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\Amit Gupta\CF3AM_1H.als
COMMT CF3AM_1H Mr. A.K. Gupta
DATIM Tue May 22 12:32:39 2012
OBNUC 1H
EXMOD NON
OBFRQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQU 9505.7 Hz
SCANS 32
ACQTM 3.447 sec
PD 1.547 sec
PW1 5.2 us
IRNUC 1H
CTEMP 21.9 C
SLVNT DMSO
EXREF 2.49 ppm
BF 1.20 Hz
RGAIN 16

C:\Amit Gupta\CF3AM 13C.als
CF3AM 13C Mr. A.K. Gupta

DFile C:\Amit Gupta\CF3AM 13C.als
COMNT CF3AM 13C Mr. A.K. Gupta
DATIM Tue May 22 12:27:43 2012
OBNUC 13C
EXMOD BCM
OBFRQ 75.45 MHz
OBSET 127.30 KHz
OBFIN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 529
ACQTM 1.606 sec
PD 1.394 sec
PWL 6.0 us
IRNUC 1H
CTEMP 22.7 c
SLVNT DMSO
EXREF 39.50 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh, I.T\mPhANIL 1H.a1s
 mPhANIL 1H Mr. Dushyant Singh

JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005
 Operator : Nagendra Kumar
 Shishir Singh

DFILE C:\K.N. Singh, I.T\mPhANIL 1
 COMNT mPhANIL 1H Mr. Dushyant Sing
 DATIM Mon Jul 23 11:40:22 2012

OSNUC 1H
 EXMOD NON
 OSFREQ 300.40 MHz
 OSSET 130.00 MHz
 OSFIN 1150.0 Hz
 POINT 32768
 FREQ 9505.7 Hz
 SCANS 20
 ACQTM 3.447 sec
 PD 1.547 sec
 PW1 5.2 us
 INNUC 1H
 CTMP 21.2 c
 SLVT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 16

C:\WINNMR98\COMMON\DEFAULT.ALS
mPLANIL.13C Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\WINNMR98\COMMON\DEFAULT
COMNT mPLANIL.13C Mr. Dushyant S
DATIM Mon Jul 23 12:06:04 2012
ORNUC 13C
EXPOD BCM
ORFRO 75.45 MHz
ORSET 127.30 KHz
ORFTN 44.7 Hz
POINT 32768
FREQU 20408.1 Hz
SCANS 339
ACQTM 1.606 sec
PD 1.394 sec
PWL 6.0 us
IRNUC 1H
CTEMP 21.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh, I.T\m-PhBz_1H.als
m-PhBz 1H Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh, I.T\m-PhBz_1H
COMPT m-PhBz_1H Mr. Dushyant Singh
DATIM Mon Jul 23 15:39:49 2012

ORNUC 1H	EXMOC NON	300.40 MHz
	OBFSQ	130.00 KHz
	OBSET	1150.0 Hz
	OBFIN	32768
	POINT	9505.7 Hz
	FREQU	16
	SCANS	3.447 sec
	ACQTN	1.547 sec
	PD	5.2 us
	FW1	1H
	IRNUC	21.7 C
	CTEMP	CDCL3
	SLVNT	0.00 ppm
	EXREF	1.20 Hz
	BF	17
	RGAIN	

C:\WINNR98\COMMON\DEFAULT.ALS
m-PhBz 13C 1H Mr. Dushyant K. Singh

JKOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
D:\FILE C:\WINNR98\COMMON\DEFAULT.
COMPT m-PhBz 13C 1H Mr. Dushyant K.
DATIN Mon Jul 23 17:15:30 2012
ORNUC 13C
EXMOD BCM
ORFPO 75.45 MHz
ORSET 127.30 KHz
ORFIN 44.7 Hz
POINT 32768
FREQ 20408.1 Hz
SCANS 251
ACQTM 1.606 sec
PD 1.394 sec
FW 6.0 us
IRNUC 1H
CTEMP 22.3 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 25

C:\K.N. Singh,, I.T\OPHOTO-5.1H.als
 • OPHOTO-5.1H Mr.Dushyant Singh

JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005
 Operator : Nagendra Kumar
 Shiehir Singh

DFILE C:\K.N. Singh,, I.T\OPHOTO-5
 COMMENT OPHOTO-5.1H Mr.Dushyant Singh
 DATIM Thu Jul 26 14:54:04 2012
 ORNUC 1H
 EXMOC NON
 ORFRO 300.40 MHz
 ORSET 130.00 KHz
 ORFIN 1150.0 Hz
 POINT 32768
 FREQU 9505.7 Hz
 SCANS 16
 ACQTM 3.447 sec
 FO 1.547 sec
 PW1 5.2 us
 IRNUC 1H
 CTMP 21.6 C
 SLVNT CDCL3
 EXREF 0.00 ppm
 BF 1.20 Hz
 RGAIN 18

C:\WINNR98\COMMON\DEFAULT.ALS
OPHOTO 13C Dr.Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005
Operator : Nagendra Kumar
Shishir Singh
C:\WINNR98\COMMON\DEFAULT.
COMMENT OPHOTO 13C Dr.Dushyant Singh
DATEIN Fri Jul 20 13:44:36 2012
ORNDIC 13C
EXXOD BOM 75.45 MHz
ORFBO 127.30 MHz
ORSET 44.7 Hz
POINT 32768
FREQO 20408.1 Hz
SCANS 212
ACQTM 1.606 sec
PD 1.394 sec
PW1 6.0 us
IRNUC 1H
CTEMP 19.4 C
SLVNT CDCL3
EXREF 77.00 ppm
BF 1.20 Hz
RGAIN 23

C:\K.N. Singh, I.T\OPH2-4 1H.aie
OPH2-4 1H Mr. Dushyant Singh

JEOL AL300 FTNMR
CHEMISTRY DEPARTMENT
Banaras Hindu University,
VARANASI-221005

Operator : Nagendra Kumar
Shishir Singh

DFILE C:\K.N. Singh, I.T\OPH2-4 1
COMET OPH2-4 1H Mr. Dushyant Singh
DATIM Mon Jul 23 15:31:00 2012

OBNUC 1H
EXMOD NON
OBFTQ 300.40 MHz
OBSET 130.00 KHz
OBFIN 1150.0 Hz
POINT 32768
FREQ 9505.7 Hz
SCANS 35
ACQTM 3.447 sec
PD 1.547 sec
FW 5.2 us
IRNUC 1H
CTEMP 21.9 c
SLVNT CDCL3
EXREF 0.00 ppm
RF 1.20 Hz
PGAIN 19

C:\WINNOR99\Data\OPHBEZ_13CIBOM_E4.als
 OPHBEZ_13C Mr. Dushyant Singh

JEOL AL300 FTNMR
 CHEMISTRY DEPARTMENT
 Banaras Hindu University,
 VARANASI-221005

Operator : Nagendra Kumar
 Shishir Singh

DFILE C:\WINNOR99\Data\OPHBEZ_13C1
 COMNT OPHBEZ_13C Mr. Dushyant Singh
 DATIM Sat Jul 21 07:23:13 2012

OSNUC 13C
 EXNOO BOM
 OSFRO 75.45 MHz
 OSFET 127.30 MHz
 OSFPT 44.7 Hz
 POINT 32768
 FREQO 20408.1 Hz
 SCANS 3500
 ACQTM 1.606 sec
 PD 1.394 sec
 PW1 6.0 us
 INNUC 1H
 CTEDP 20.5 c
 SLVNT CDCL3
 EXREF 77.00 ppm
 BF 1.20 Hz
 RGAIN 24

Certificate of Analysis

SIGMA-ALDRICH

Product Name Nickel(II) chloride hexahydrate,
99.999% trace metals basis
Product Number 203866
Product Brand ALDRICH
CAS Number 7791-20-0
Molecular Formula $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$
Molecular Weight 237.69

TEST

APPEARANCE

GRAVIMETRIC ASSAY

TRACE ANALYSIS, ICP-MS

ICP ASSAY

PURITY

QC RELEASE DATE

SPECIFICATION

LIME GREEN CRYSTALS,
CRYSTALLINE POWDER
24.0% - 26.0% NI (WITH
DIMETHYLGLYOXIME)

CONFIRMS NICKEL COMPONENT.
PURITY BASED ON TRACE METALS
ANALYSIS

LOT 01301JV RESULTS

GREEN CRYSTALS

24.4% NI (WITH DIMETHYLGLYOXIME)

TRACE ELEMENTS IN PPB

BA 190 CO 3800 CR 90 CU 550 FE 210

CONFIRMS NICKEL COMPONENT

>99.999% BASED ON TRACE METAL
ANALYSIS

JULY 2008

Barbara Rajzor, Supervisor
Quality Control
Milwaukee, Wisconsin USA