Electronic Supplementary Information

**P,N,N-pincer nickel-catalyzed cross-coupling of aryl fluorides and chlorides**

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**Synthesis and characterization of ligand precursors HL2 and HL3 and complexes 3a-3c**

![Scheme S-1. Synthesis of ligand precursors and complexes 3a-3c](image)

**Experimental details**

The reactions were performed under nitrogen atmosphere using standard Schlenk and vacuum line techniques. Solvents were distilled under nitrogen over sodium (toluene, hexane) or sodium/benzophenone (THF, Et₂O) and degassed prior to use. CDCl₃ was purchased from Cambridge Isotope Laboratories and used as received. (DME)NiCl₂,¹ 2-(Bromophenyl)-2'-(dimethylaminophenyl)amine,² and 2-diphenylphosphinophenyl)-2'-(dimethylaminophenyl)amine (HL1)² were prepared according to reported methods. M

Other chemicals were purchased from commercial vendors and used as received. NMR spectra were determined on a Bruker av300 or a Bruker Avance III 400 NMR spectrometer at room temperature using CDCl₃ as solvent. The chemical shifts of the ¹H
NMR spectra were referenced to TMS; the chemical shifts of the $^{13}$C NMR spectra were referenced to internal solvent resonances and the chemical shifts of the $^{31}$P NMR spectra were referenced to external 85% H$_3$PO$_4$. Elemental analysis was performed using an Elementar Vario EL Cube instrument.

**Preparation of (2-Diisopropylphosphinophenyl)-2'-/(dimethylaminophenyl)amine (HL2)**

A 2.4 M solution of Bu$n$Li in hexane (2.82 cm$^3$, 6.76 mmol) was added dropwise to a stirred solution of (2-bromophenyl-2'-dimethylaminophenyl)amine (0.98 g, 3.38 mmol) in Et$_2$O (20 cm$^3$) at about −80 °C. The mixture was allowed to warm to ambient temperature and stirred for 12 h. The resulting solution was recooled to −80 °C and chlorodiisopropylphosphine (0.53 cm$^3$, 3.38 mmol) was added into the cooled solution. The mixture was warmed to room temperature and stirred for 12 h. Degassed water (10 cm$^3$) and diethyl ether (10 cm$^3$) were added. The organic layer was separated and the aqueous phase was extracted with diethyl ether (5 cm$^3$ × 2). The combined organic phase was dried over MgSO$_4$ and evaporated to dryness under reduced pressure to give an off-white solid of HL2 (0.507 g, 46%). $^1$H NMR (CDCl$_3$): δ 0.96 (dd, $J = 6.8, 11.6$ Hz, 6H, CHMe$_2$), 1.12 (dd, $J = 6.8, 15.2$ Hz, 6H, CHMe$_2$), 2.08-2.18 (m, 2H, CHMe$_2$), 2.70 (s, 6H, NMe$_2$), 6.86 (t, $J = 7.4$ Hz, 2H, C$_6$H$_4$), 6.95 (t, $J = 7.6$ Hz, 1H, C$_6$H$_4$), 7.08 (d, $J = 8$ Hz, 1H, C$_6$H$_4$), 7.19-7.25 (m, 1H, C$_6$H$_4$), 7.30-7.41 (m, 2H, C$_6$H$_4$), 7.59 (d, $J = 8.4$ Hz, 1H, C$_6$H$_4$). $^{13}$C NMR (CDCl$_3$): δ 19.03 (d, $J = 8.9$ Hz), 20.19 (d, $J = 18.3$ Hz), 23.11 (d, $J = 10.7$ Hz), 44.04, 115.92 (d, $J = 2.4$ Hz), 116.00, 119.46 (d, $J = 6.7$ Hz), 120.50, 121.80, 121.95, 123.40, 129.55, 133.67, 137.46, 143.99, 148.63 (d, $J = 18.4$ Hz). $^{31}$P NMR (CDCl$_3$): δ −13.61.

**Preparation of (2-Dicyclohexylphosphinophenyl)-2'-/(dimethylaminophenyl)amine (HL3)**

A 2.4 M solution of Bu$n$Li in hexane (3.46 cm$^3$, 8.30 mmol) was added dropwise to a stirred solution of (2-bromophenyl-2'-dimethylaminophenyl)amine (1.21 g, 4.15 mmol) in Et$_2$O (20 cm$^3$) at about −80°C. The mixture was allowed to warm to ambient temperature and stirred for 12 h. After recooling this solution to −80°C chlorodicyclohexylphosphine (0.94 cm$^3$, 4.15 mmol) was added. The resulting mixture was warmed to room temperature and stirred for 12 h. Degassed water (10 cm$^3$) and diethyl ether (10 cm$^3$) were added. The organic phase was separated and the aqueous phase was extracted with diethyl ether (5 cm$^3$ × 2). The combined organic phase was dried over MgSO$_4$ and evaporated to dryness under reduced pressure to
afford a yellow oil. The yellow oil was dissolved in a mixed solvent of degassed ethanol (1 cm³) and hexane (8 cm³). The solution was cooled to −80 °C to give an off-white solid of HBL3 (0.857 g, 51%). ¹H NMR (CDCl₃): δ 0.99-1.38 (m, 10H, Cy), 1.55-1.80 (m, 8H, Cy), 1.82-2.03 (m, 4H, Cy), 2.69 (s, 6H, NMe₂), 6.81-6.99 (m, 3H, C₆H₄), 7.07 (d, J = 8.8 Hz, 1H, C₆H₄), 7.17-7.43 (m, 3H, C₆H₄), 7.55 (d, J = 9.6 Hz, 1H, C₆H₄). ¹³C NMR (CDCl₃): δ 26.52, 27.16 (d, J = 7.9 Hz), 27.37, 27.50, 28.92 (d, J = 7.5 Hz), 30.46 (d, J = 10.8 Hz), 33.02 (d, J = 16.7 Hz), 33.02 (d, J = 10.8 Hz), 44.00, 115.73, 116.25, 119.32, 119.35, 120.54, 121.47 (d, J = 16 Hz), 123.34, 129.47, 134.09, 137.42, 144.05, 148.76 (d, J = 18 Hz). ³¹P NMR (CDCl₃): δ −25.09.

**Preparation of [(L1)NiCl] (3a)**

A solution of compound HBL1 (0.86 g, 2.16 mmol) in THF (25 cm³) was cooled to about −80 °C. To the solution was added dropwise a 2.4 M solution of Bu"Li in hexane (0.9 cm³, 2.16 mmol) with stirring. The mixture was warmed to room temperature and stirred for 4 h. The resulting solution was added dropwise into a stirred suspension of (DME)NiCl₂ (0.48 g, 2.16 mmol) in THF (15 cm³) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo, and the residue was dissolved in toluene. The resulting solution was filtered and concentrated to afford green powder of 3a (0.73 g, 69%), mp 236-237 °C. Anal. Calcd for C₂₀H₂₄N₂PNiCl·0.1C₇H₈: C, 64.29; H, 5.01; N, 5.62. Found: C, 64.54; H, 4.92, N, 5.70. ¹H NMR (CDCl₃): δ 3.01 (d, J = 2 Hz, 6H, NMe₂), 6.47 (t, J = 7 Hz, 1H, Ar), 6.54-6.58 (m, 1H, Ar), 6.91-6.98 (m, 2H, Ar), 7.10-7.14 (m, 1H, Ar), 7.16 (dd, J = 1.2, 8 Hz, 1H, Ar), 7.40-7.47 (m, 5H, Ar), 7.48-7.54 (m, 3H, Ar), 7.84-7.92 (m, 4H, Ar). ¹³C NMR (CDCl₃): δ 49.03 (d, J = 2.3 Hz), 115.02, 115.52 (d, J = 11.8 Hz), 116.96, 117.09 (d, J = 7.7 Hz), 120.84, 122.14, 122.68, 127.38, 128.86 (d, J = 11 Hz), 129.15, 129.67, 131.06 (d, J = 2.9 Hz), 132.43 (d, J = 2 Hz), 133.50 (d, J = 10.4 Hz), 133.81, 146.52 (d, J = 2.8 Hz), 149.09 (d, J = 2 Hz), 159.89, 160.11. ³¹P NMR (CDCl₃): δ 26.67.

**Preparation of [(L2)NiCl] (3b)**
A solution of compound HL2 (0.51 g, 1.54 mmol) in THF (25 cm³) was cooled to about −80 °C. To the solution was added dropwise a 2.4 M solution Bu"Li in hexane (0.64 cm³, 1.54 mmol) with stirring. The mixture was warmed to room temperature and stirred for 4 h. The resulting solution was added dropwise into a stirred suspension of (DME)NiCl₂ (0.34 g, 1.54 mmol) in THF (15 cm³) at about −80 °C. The resulting mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo, and the residue was dissolved in Et₂O and then filtered. Hexane was added into the filtrate to form green crystals of 3b (0.42 g, 65%), mp 151-152 °C. Anal. Calcd for C₂₀H₂₈N₂PNiCl·0.2C₆H₁₄: C, 58.03; H, 7.07; N, 6.38. Found: C, 58.10; H, 6.68, N, 6.46. ¹H NMR (CDCl₃): δ 1.32 (dd, J = 6, 14.8 Hz, 6H, i-Pr), 1.50 (dd, J = 6, 16.4 Hz, 6H, i-Pr), 2.14-2.32 (m, i-Pr), 2.88 (s, 6H, NMe), 6.79-6.89 (m, 1H, Ar), 6.35-6.52 (m, 2H, Ar), 6.98-7.13 (m, 3H, Ar), 7.31-7.47 (m, 2H, Ar). ¹³C NMR (CDCl₃): δ 17.78, 18.70, 24.62 (d, J = 24.3 Hz), 48.50, 114.80, 115.30 (d, J = 10.8 Hz), 116.23 (d, J = 6.8 Hz), 116.45, 119.59, 120.02, 120.72, 127.18, 131.54, 131.87, 146.22, 149.42, 160.94, 161.12. ³¹P NMR (CDCl₃): δ 52.89.

Preparation of [(L₃)NiCl] (3c)

A solution of compound HL3 (0.86 g, 2.10 mmol) in THF (25 cm³) was cooled to about −80 °C. To the solution was added dropwise a 2.4 M solution of Bu"Li in hexane (0.86 cm³, 2.10 mmol) with stirring. The mixture was warmed to room temperature and stirred for 4 h. The resulting solution was added dropwise into a stirred suspension of (DME)NiCl₂ (0.46 g, 2.10 mmol) in THF (15 cm³) at about −80 °C. The mixture was warmed to room temperature and stirred overnight. Volatiles were removed in vacuo. The residue was dissolved in Et₂O and then filtered. Hexane was added into the filtrate to form green crystals of 3c (0.90 g, 86%), mp 180-181°C. Anal. Calcd for C₂₆H₃₆N₂PNiCl: C, 62.24; H, 7.23; N, 5.58. Found: C, 61.75; H, 7.23, N, 5.58. ¹H NMR (CDCl₃): δ 1.14-1.47 (m, 6H, C₆H₁₁), 1.55-2.16 (m, 14H, C₆H₁₁),
2.62 (b, 2H, C₆H₁₁), 2.95 (s, 6H, NMe), 6.42-6.61 (m, 2H, Ar), 6.83-6.97 (m, 1H, Ar), 7.03-7.21 (m, 3H, Ar), 7.35-7.54 (m, 2H, Ar). \(^{13}\)C NMR (CDCl₃): \(\delta\) 26.16, 26.99, 27.10, 27.25, 27.99, 28.53, 33.85, 34.11, 48.53, 114.77, 115.19 (d, \(J = 10.9\) Hz), 116.16 (d, \(J = 6.8\) Hz), 116.37, 120.02, 120.46, 120.69, 127.14, 131.65, 131.79, 146.27, 149.45, 161.00, 161.18. \(^{31}\)P NMR (CDCl₃): \(\delta\) 45.58.

**Crystal structure determination**

Single crystal of complex 3c was mounted in Lindemann capillaries under nitrogen. Diffraction data were collected at 290(2) K on an Oxford Diffraction Gemini S Ultra diffractometer with mirror-monochromated Cu K\(\alpha\) radiation (\(\lambda = 1.54184\) Å). The structures were solved by direct methods using SHELXS-97\(^3\) and refined against \(F^2\) by full-matrix least-squares using SHELXL-97.\(^4\) Hydrogen atoms were placed in calculated positions. Crystal data and experimental details of the structure determinations are listed in Table 1. CCDC 996222 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

**Table 1 Details of the X-ray structure determination of complex 3c**

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<th>Value</th>
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<td>(c) (Å)</td>
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no. of data/restraints/params 7437/1/563

goodness of fit on $F^2$ 1.033

final $R$ indices [$I > 2\sigma(I)$] $R1 = 0.0311$
wR2 = 0.0840

$R$ indices (all data) $R1 = 0.0326$
wR2 = 0.0856

largest diff peak and hole [e Å$^{-3}$] 0.33 and −0.19

References

Copies of $^1$H, $^{13}$C and $^{31}$P NMR spectra of complexes 3a-3c
1. [(L1)NiCl] (3a)
$^{31}$P NMR
Solvent: CDCl$_3$
[[L2]NiCl] (3b)
$^{31}$p NMR
Solvent: CDCl$_3$
[(L3)NiCl] (3c)

$^1$H NMR
Solvant: CDCl$_3$

$^{13}$C NMR
Solvant: CDCl$_3$
$^{31}$p NMR
Solvent: CDCl$_3$
Copies of $^1$H and $^{13}$C NMR spectra of the cross-coupling products

1. 4-Methoxy-4'-methylbiphenyl

$^1$H NMR (CDCl$_3$)

$^{13}$C NMR (CDCl$_3$)
2. 3-Methoxy-4'-methylbiphenyl

3-Methoxy-4'-methylbiphenyl

$^1$H NMR (CDCl$_3$)

3-Methoxy-4'-methylbiphenyl

$^{13}$C NMR (CDCl$_3$)
3. 4'-methyl-N,N-dimethylbiphenyl-4-amine

4'-methylN,N-dimethylbiphenyl-4-amine
$^1$H NMR (CDCl$_3$)
4. 3,4-dimethoxy-4'-methylbiphenyl

3,4-dimethoxy-4'-methylbiphenyl

$^1$H NMR (CDCl$_3$)

3,4-dimethoxy-4'-methylbiphenyl

$^{13}$C NMR (CDCl$_3$)
5. 3',4'- Dimethoxy- N,N-dimethylbiphenyl-4-amine

\[ \text{\^{1}H NMR (CDCl3)} \]

\[ \text{\^{13}C NMR (CDCl3)} \]
6. 1-Isopropyl-3-(4'-methylbiphenyl-4-yl)-1H-indole

\[ \text{H NMR (CDCl}_3) \]

\[ \text{C NMR (CDCl}_3) \]

1-Isopropyl-3-(4'-methylbiphenyl-4-yl)-1H-indole
7. (4'-Methylbiphenyl-4-yl)methanol

(4'-Methylbiphenyl-4-yl)methanol

$^1$H NMR (CDCl$_3$)

(4'-Methylbiphenyl-4-yl)methanol

$^{13}$C NMR (CDCl$_3$)
8. (4'-N, N-Dimethylaminobiphenyl-4-yl)methanol

^1H NMR (CDCl₃)

^13C NMR (CDCl₃)
9. 2'-Methyl-N,N-dimethylbiphenyl-4-amine

2'-MethylN,N-dimethylbiphenyl-4-amine

$^1$H NMR (CDCl$_3$)

2'-MethylN,N-dimethylbiphenyl-4-amine

$^{13}$C NMR (CDCl$_3$)
10. *N*,*N*-Dimethylbiphenyl-4-amine

*N*,*N*-Dimethylbiphenyl-4-amine

$^1$H NMR (CDCl$_3$)

$^1$C NMR (CDCl$_3$)
11. \(N,N\)-Dimethyl-(4-naphthalen-1-yl)aniline

\[\text{\(N,N\)-Dimethyl-(4-naphthalen-1-yl)aniline} \]

\[\text{\(^1\)H NMR (CDCl\textsubscript{3})} \]

\[\text{\(^1\)C NMR (CDCl\textsubscript{3})} \]
12. 4'-Methyl-4-(trifluoromethyl)biphenyl

4'-Methyl-4-(trifluoromethyl)biphenyl

$^1$H NMR (CDCl$_3$)

$^1$H NMR (CDCl$_3$)

4'-Methyl-4-(trifluoromethyl)biphenyl

$^{13}$C NMR (CDCl$_3$)

$^{13}$C NMR (CDCl$_3$)
13. 2-p-Tolylpyridine

2-p-Tolylpyridine

$^1$H NMR (CDCl$_3$)

2-p-Tolylpyridine

$^{13}$C NMR (CDCl$_3$)
14. 2-(4-Methoxy-phenyl)pyridine

1H NMR (CDCl3)

2-(4-Methoxy-phenyl)pyridine

13C NMR (CDCl3)
15. \(N,N\)-dimethyl-(4-pyridin-2-yl)benzenamine

\(^1\)H NMR (CDCl₃)
16. 4-Methyl-2-\textit{p}-tolylpyridine

\textbf{\textit{H} NMR (CDCl$_3$)}

\begin{itemize}
\item \textbf{4-Methyl-2-\textit{p}-tolylpyridine}
\item \textbf{C NMR (CDCl$_3$)}
\end{itemize}
17. 3-\textit{p}-Tolylpyridine

3-\textit{p}-Tolylpyridine

\textsuperscript{1}H NMR (CDCl\textsubscript{3})

3-\textit{p}-Tolylpyridine

\textsuperscript{13}C NMR (CDCl\textsubscript{3})
18. 1,4-Di(\(p\)-methylphenyl)benzene

\[ \text{1,4-Di}(p\text{-methylphenyl})\text{benzene} \]

\[ \begin{align*}
\text{\(^1\text{H NMR (CDCl}_3\))} \\
\text{\(^{13}\text{C NMR (CDCl}_3\))}
\end{align*} \]
19. 1,3,5-tris(\(\rho\)-methylphenyl)benzene

1,3,5-tris(\(\rho\)-methylphenyl)benzene

\(^1\)H NMR (CDCl\(_3\))

1,3,5-tris(\(\rho\)-methylphenyl)benzene

\({}^{13}\)C NMR (CDCl\(_3\))
20. 1-Methoxy-2-(p-toyl)benzoate

1H NMR (CDCl3)

13C NMR (CDCl3)
21. *N,N,2',5'-tetramethylbiphenyl-4-amine*

![N,N,2',5'-tetramethylbiphenyl-4-amine 1H NMR (CDCl3)](image)

![N,N,2',5'-tetramethylbiphenyl-4-amine 13C NMR (CDCl3)](image)
22. 4-Methoxybiphenyl

4-Methoxybiphenyl

$^1$H NMR (CDCl$_3$)

4-Methoxybiphenyl

$^{13}$C NMR (CDCl$_3$)
23. 4'-Methoxy-4-(trifluoromethyl)biphenyl
24. Dimethyl-(4'-trifluoromethylbiphenyl-4-yl)amine

[dimethyl-(4'-trifluoromethyl-biphenyl-4-yl)-amine 1

$^1$H NMR (CDCl$_3$)

[dimethyl-(4'-trifluoromethyl-biphenyl-4-yl)-amine 13

$^1$C NMR (CDCl$_3$)
25. (4'-Methylbiphenyl-4-yl)(phenyl)methanone

(4'-Methylbiphenyl-4-yl)(phenyl)methanone

$^1$H NMR (CDCl$_3$)

(4'-Methylbiphenyl-4-yl)(phenyl)methanone

$^{13}$C NMR (CDCl$_3$)
26. (4’-Methoxybiphenyl-4-yl)(phenyl)methanone

(4’-Methoxybiphenyl-4-yl)(phenyl)methanone

H NMR (CDCl₃)

(4’-Methoxybiphenyl-4-yl)(phenyl)methanone

C NMR (CDCl₃)
27. Ethyl 4'-methylbiphenyl-4-carboxylate

Ethyl 4'-Methylbiphenyl-4-carboxylate

$^1$H NMR (CDCl3)

Ethyl 4'-Methylbiphenyl-4-carboxylate

$^{13}$C NMR (CDCl3)
28. Ethyl 4'-methoxybiphenyl-4-carboxylate

Ethyl 4’-Methoxybiphenyl-4-carboxylate

$^1$H NMR (CDCl$_3$)

Ethyl 4’-methoxybiphenyl-4-carboxylate

$^{13}$C NMR (CDCl$_3$)
29. \(N,N\)-diethyl-4’-methylbiphenyl-4-carboxamide

\[\text{\(N,N\)-diethyl-4’-methylbiphenyl-4-carboxamide} \]

\[^1\text{H NMR (CDCl}_3\text{)}\]

\[\text{\(N,N\)-diethyl-4’-methylbiphenyl-4-carboxamide} \]

\[^13\text{C NMR (CDCl}_3\text{)}\]
30. N,N-Diethyl-4'-methoxybiphenyl-4-carboxamide
31. 4'-Methylbiphenyl-4-carbonitrile

4'-Methylbiphenyl-4-carbonitrile

$^1$H NMR (CDCl$_3$)

4'-Methylbiphenyl-4-carbonitrile

$^{13}$C NMR (CDCl$_3$)
32. (4'-Methylbiphenyl-2-yl)(phenyl)methanone

(4'-Methylbiphenyl-2-yl)(phenyl)methanone 
$^1$H NMR (CDCl$_3$)

(4'-Methylbiphenyl-2-yl)(phenyl)methanone 
$^{13}$C NMR (CDCl$_3$)
33. (4'-Methoxybiphenyl-2-yl)(phenyl)methanone

(4'-Methoxybiphenyl-2-yl)(phenyl)methanone

^1H NMR (CDCl3)

(4'-Methoxybiphenyl-2-yl)(phenyl)methanone

^13C NMR (CDCl3)
34. 4'-Methylbiphenyl-2-carbonitrile

4'-Methylbiphenyl-2-carbonitrile

$^1$H NMR (CDCl$_3$)

4'-Methylbiphenyl-2-carbonitrile

$^{13}$C NMR (CDCl$_3$)

4'-Methylbiphenyl-2-carbonitrile
35. 4'-methoxy-2-methylbiphenyl

**$^{1}$H NMR (CDCl$_3$)**

**$^{13}$C NMR (CDCl$_3$)**
36. (2'-Methylbiphenyl-4-yl)(phenyl)methanone

\[ (2'-\text{Methylbiphenyl}-4-\text{yl})(\text{phenyl})\text{methanone} \]

\( ^1H \text{NMR (CDCl}_3) \)

\[ \text{(2'-Methylbiphenyl-4-yl)(phenyl)methanone} \]

\( ^{13}C \text{NMR (CDCl}_3) \)
37. Ethyl 2’-methylbiphenyl-4-carboxylate

\[ \text{ethyl 2’-Methylbiphenyl-4-carboxylate} \]

\[ \text{\textsuperscript{1}H NMR (CDCl\textsubscript{3})} \]

\[ \text{ethyl 2’-Methylbiphenyl-4-carboxylate} \]

\[ \text{\textsuperscript{13}C NMR (CDCl\textsubscript{3})} \]
38. \( \text{N,N-Diethyl-2'}-\text{methylbiphenyl-4-carboxamide} \)

\[ \begin{array}{c}
\text{N,N-Diethyl-2'}-\text{methylbiphenyl-4-carboxamide} \\
\text{\( ^1 \)H NMR (CDCl₃)} \\
\end{array} \]

\[ \begin{array}{c}
\text{N,N-Diethyl-2'}-\text{methylbiphenyl-4-carboxamide} \\
\text{\( ^{13} \)C NMR (CDCl₃)} \\
\end{array} \]
39. 2-p-Tolyl-nicotinonitrile

$^1$H NMR (CDCl$_3$)

2-p-Tolyl-nicotinonitrile

$^{13}$C NMR (CDCl$_3$)

2-p-Tolyl-nicotinonitrile
40. 2-Methoxy-6-p-tolylpyridine

[Diagram of 1H NMR spectrum]

2-Methoxy-6-p-tolylpyridine  
$^1$H NMR (CDCl$_3$)

[Diagram of 13C NMR spectrum]

2-Methoxy-6-p-tolylpyridine  
$^{13}$C NMR (CDCl$_3$)
41. 2-(4-Methylphenyl)-4-methylquinoline

1H NMR (CDCl3)

13C NMR (CDCl3)
42. 2-(4-Methoxyphenyl)-4-methylquinoline

2-(4-Methoxyphenyl)-4-methylquinoline  $^1$H NMR (CDCl₃)

2-(4-Methoxyphenyl)-4-methylquinoline  $^{13}$C NMR (CDCl₃)
43. (4′-(Trifluoromethyl)biphenyl-4-yl)(phenyl)methanone

\((4'-(\text{trifluoromethyl})\text{biphenyl-4-yl})(\text{phenyl})\text{methanone}\)

\(^1\text{H NMR}\ (\text{CDCl}_3)

\[^{13}\text{C NMR}\ (\text{CDCl}_3)\)
44. Ethyl 4’-(trifluoromethyl)biphenyl-4-carboxylate

Ethyl 4’-(trifluoromethyl)biphenyl-4-carboxylate  $^1$H NMR (CDCl$_3$)

Ethyl 4’-(trifluoromethyl)biphenyl-4-carboxylate  $^{13}$C NMR (CDCl$_3$)
45. N,N-Diethyl-4'-{(trifluoromethyl)biphenyl-4-carboxamide

\( ^1H \text{ NMR (CDCl}_3 \) 

\( ^{13} \text{C NMR (CDCl}_3 \)
46. (4'- (trifluoromethyl) biphenyl-2-yl)(phenyl) methanone

(4'- (trifluoromethyl) biphenyl-2-yl)(phenyl) methanone

H NMR (CDCl₃)

(4'- (trifluoromethyl) biphenyl-2-yl)(phenyl) methanone

C NMR (CDCl₃)
47. 2-(4-(trifluoromethyl)phenyl)furan

2-(4-(trifluoromethyl)phenyl)furan

$^1$H NMR (CDCl$_3$)

2-(4-(trifluoromethyl)phenyl)furan

$^{13}$C NMR (CDCl$_3$)
48. (4-(Furan-2-yl)phenyl)(phenyl)methanone

(4-(Furan-2-yl)phenyl)(phenyl)methanone

$^1$H NMR (CDCl$_3$)

$^{13}$C NMR (CDCl$_3$)
49. Ethyl 4-(furan-2-yl)benzoate

Ethyl 4-(furan-2-yl)benzoate

$^1$H NMR (CDCl$_3$)

Ethyl 4-(furan-2-yl)benzoate

$^{13}$C NMR (CDCl$_3$)
50. N,N-Diethyl-4-(furan-2-yl)carboxamide

N,N-Diethyl-4-(furan-2-yl)carboxamide
$^1$H NMR (CDCl$_3$)

N,N-Diethyl-4-(furan-2-yl)carboxamide
$^{13}$C NMR (CDCl$_3$)
51. 2-Furan-2-yl-benzonitrile

2-Furan-2-yl-benzonitrile

$^1$H NMR (CDCl$_3$)

2-Furan-2-yl-benzonitrile

$^{13}$C NMR (CDCl$_3$)