Supplementary Information

Ni-Catalyzed Reductive Decyanation of Nitriles with Ethanol as the Reductant

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1. General
All $^1$H and $^{13}$C NMR spectra were recorded on Bruker ADVANCE III 500 MHz/400 MHz/600 MHz spectrometer in deuterium solvents with tetramethylsilane (TMS) as internal standard. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad signal. Chemical shifts are given in ppm and are referenced to TMS ($^1$H, $^{13}$C, $^{31}$P). All spectra were obtained at 25 °C in the solvent indicated. Coupling constants $J$ are given in Hz. GC analyses were performed on Agilent 7890 A instrument with FID detector using an SE-54 capillary column (30 m x 0.32 mm (i.d.), 0.25 μm). Column chromatography was performed on neutral silica gel or Al$_2$O$_3$ (200-300 mesh) with ethyl acetate/petroleum ether or toluene/petroleum ether as eluent. All reactions were carried out under nitrogen atmosphere. Alcohols and solvents were dried following the general procedure and distilled before utilization. Nickel complexes, bases, ligands and other reagents were commercial available and used directly unless otherwise noted. Most of nitriles were prepared through Suzuki coupling or Pd-catalyzed cyanation of aryl bromides according to the reported literature unless otherwise noted.\(^1\)

2. The synthesis of nitriles

2,3,3-triphenylacrylonitrile (3j): Benzophenone (5.5 g, 30 mmol), t-BuOK (1.2 eq., 4.0 g) and benzylcyanide (40 mL) were added to a flask. The mixture was heated to 160 °C and stirred for 4 hours. The mixture was added to HCl aq. (100 mL, 1 mol/L). Extracted the crude product with ethyl acetate (3 x 100 mL) and washed the organic phase with saturated NaHCO$_3$ aq. 3.4 g of light pink solid was obtained in 40% isolated yield by column chromatography on silica gel (petroleum ether as the eluent).

$^1$H NMR (CDCl$_3$, 600 MHz): δ 7.47-7.39 (m, 5H), 7.28-7.16 (m, 8H), 7.00 (d, $J$=7.6 Hz, 2H). $^{13}$C NMR (CDCl$_3$, 150 MHz) δ 157.9, 140.5, 139.2, 135.0, 130.9, 130.0, 129.8, 129.1, 128.6, 128.6, 128.5, 128.4, 120.2, 111.8.
3. Optimization of reductive decyanation of 1-naphthonitrile

Table S1 Effect of different pre-catalysts, ligands and bases

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<th>Base</th>
<th>Ligand/ 12 mol%</th>
<th>Yield %$^b$</th>
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<td>74</td>
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<tr>
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<td>KHMDS</td>
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<td>58</td>
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$^a$ Reaction conditions: 1a (0.5 mmol), Cat.[Ni] (10 mol%), Ligand (12 mol%), t-AmOK (1 mmol), EtOH (0.75 mmol), Toluene (3 mL), 140 °C for 8 h. $^b$ GC yield with biphenyl as the internal standard.
Table S2 Control experiments

![Chemical structure](image)

<table>
<thead>
<tr>
<th>Entry</th>
<th>Cat.[Ni]/ 10 mol%</th>
<th>Reductant/ 3 eq.</th>
<th>Base/ 2 eq.</th>
<th>Time/ h</th>
<th>Yield %b</th>
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<td>KHMDS</td>
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<td>4</td>
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<td>3</td>
<td>-</td>
<td>EtOH</td>
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<td>4</td>
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<td>KHMDS</td>
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<td>82</td>
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a Reaction conditions: 1a (0.5 mmol), Cat.[Ni] (10 mol%), KHMDS (1 mmol, 0.5 mol/L in toluene, 2 mL), EtOH (1.5 mmol), Toluene (1 mL), 140 °C. b GC yield with biphenyl as the internal standard.

4. General procedure for Ni-catalyzed reductive decyanation of nitriles
To a Young tube was added 1-naphthonitrile (153.0 mg, 1 mmol), NiCl₂(dpff) (68 mg, 10 mol%), KHMDS (2 mmol, 0.5 mol/L in toluene, 4 mL), toluene (2.0 mL) and EtOH (173 μL, 3 mmol). The mixture was stirred at 140 °C for 8 hours. Then removed the solvent in vacuo. Extracted the resulting mixture by ethyl acetate (50 mL) for three times. After drying and concentration, 90 mg of naphthalene was obtained in 70% isolated yield by column chromatography on silica gel (petroleum ether as the eluent, product 2t was isolated by Al₂O₃).

Other reactions employing different aryl and alkyl nitriles and the deuterium-labelling experiments followed the similar procedure unless otherwise noted.

5. The investigation for the formation of 9-methylanthracene
Initially, we proposed that the methylated product was formed because of the presence of HMDS in the reaction. However, as the following Figure S1 shows, when t-AmOK was utilized instead as the base, methylated product was also detected in a considerable amount (Eq 1). To our surprise, with EtOH- d₆ as the hydride donor and t-AmOK as the base, 9-(methyl-d₃)anthracene was detected as well in 30% selectivity (Eq 2). Therefore,
we concluded that EtOH was assigned as the methyl source.

Figure S1. Decyanation of 9-anthracenecarbonitrile with t-AmOK as the base
Figure S2. Decyanation of 9-anthracenecarbonitrile with EtOH-d6 as the hydride donor
6. Stochiometric experiments

6.1 Synthesis of the Complex I

To a Young tube was added phenanthrene-9-carbonitrile (61 mg, 0.3 mmol), Ni(COD)$_2$ (69 mg, 0.25 mmol), dcyph (106 mg, 0.25 mmol) and toluene (5 mL). After stirring at 100 °C for 8 hours, the mixture was then allowed to cool to room temperature. The solvent was removed by vacuum and the residue was washed with hexane for three times under nitrogen atmosphere. Complex I was obtained as a yellow solid (145 mg, 85% yield). The crystals of complex I was grown from the saturated toluene solution of complex I.

6.2 Stochiometric experiments of Complex I

To a Young tube was added Complex I (50 mg, 0.07 mmol), KHMDS (0.3 mL, 0.5 mol/L in toluene, 0.14 mmol), EtOH (9.8 mg, 0.21 mmol) and toluene (0.1 mL). The mixture was stirred at 140 °C for 8 hours. 79% GC yield was obtained with biphenyl as the internal standard.

6.3 Decyanation of 1-naphthonitrile with complex I as the catalyst.

GC Yield = 70%
To a Young tube was added 1-naphthonitrile (77 mg, 0.5 mmol), Comples I (34 mg, 10 mol%), KHMDS (2.0 mL, 0.5 mol/L in toluene, 1 mmol), EtOH (69.1 mg, 1.5 mmol) and toluene (1.0 mL). The mixture was stirred at 140 °C for 8 hours. 70% GC yield was attained with biphenyl as the internal standard.

6.4 X-ray crystal structure of Complex I

Figure S3. Solid structure of complex I. Hydrogen atoms were emitted for clarity.

Table S3. Crystal data and structure refinement for Complex I.

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<th>Identification code</th>
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<td>Empirical formula</td>
<td>C41 H55 N Ni P2</td>
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<tr>
<td>Wavelength</td>
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<tr>
<td>Crystal system</td>
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<tr>
<td>Space group</td>
<td>P2/n</td>
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<tr>
<td>Unit cell dimensions</td>
<td>a = 9.0356(3) Å, α= 90°.</td>
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<tr>
<td></td>
<td>b = 26.9308(9) Å, β=101.7300(10)°.</td>
</tr>
<tr>
<td></td>
<td>c = 17.7744(5) Å, γ = 90°.</td>
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<td>Volume</td>
<td>4234.8(2) Å³</td>
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<td>Z</td>
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<tr>
<td>Density (calculated)</td>
<td>1.070 Mg/m³</td>
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<tr>
<td>Absorption coefficient</td>
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</table>
Crystal size: 0.120 x 0.110 x 0.080 mm$^3$

Theta range for data collection: 2.361 to 27.506°.

Index ranges: -11 <= h <= 11, -31 <= k <= 34, -23 <= l <= 21

Reflections collected: 39082

Independent reflections: 9697 [R(int) = 0.0744]

Completeness to theta = 25.242°: 99.8%

Refinement method: Full-matrix least-squares on F$^2$

Data / restraints / parameters: 9697 / 0 / 406

Goodness-of-fit on F$^2$: 1.029

Final R indices [I>2sigma(I)]: R1 = 0.0543, wR2 = 0.1524

R indices (all data): R1 = 0.0868, wR2 = 0.1728

Extinction coefficient: n/a

Largest diff. peak and hole: 0.966 and -0.531 e.Å$^{-3}$

Table S4. Selected bond lengths [Å] and angles [°] for Complex I.

<table>
<thead>
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<th>selected angles [°]</th>
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<td>C(38)-C(39)</td>
<td>1.463(4)</td>
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6.5 Deuterium-labelling experiments

Following the general procedure, we performed the decyanation of 1e in the presence of EtOH-d6, which gave the deuterated product 2e-d in 63% yield with 89% deuterium incorporation. Since deuterium-labeled molecules now receive significant attention as
the drug candidates, 1f and 1i were employed to undergo decyanation in the presence of EtOH-d6 as well. 51% and 35% of the deuterated products were isolated with 83% deuterium incorporation, respectively.

6.6 Proposed mechanism
According to the mechanistic experiments, the proposed mechanism for this Ni-catalyzed reductive decyanation reaction was shown in the following Scheme S1. The Ni(0) species (A) in situ generated from nickel precatalyst first coordinated with the C=C double bond of aromatic ring adjacent to cyano group to afford intermediate B (complex I if substrate 1c). The intermediate B underwent oxidative addition to break C-CN bond affording the intermediate C. The alcoholysis of C in the presence of base produced the intermediate D, which could undergo β-H elimination to form nickel hydride species E. A reductive elimination of E finally released the desired decyanated product and regenerated Ni(0) species to run into the next catalytic cycle.
**Scheme S1.** Proposed mechanism of this Ni-catalyzed reductive decyanation of nitrile.
7. NMR spectra of reductive decyanation products

Naphthalene (2a, 2a')\textsuperscript{3}: \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): \( \delta \) 7.90-7.85 (m, 4H), 7.54-7.48 (m, 4H).

Phenanthrene (2b)\textsuperscript{3}: \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): \( \delta \) 8.71 (d, \( J =8.3 \) Hz, 2H), 7.91 (d, \( J =8.0 \) Hz, 2H), 7.75 (s, 2H), 7.71-7.65 (m, 2H), 7.65-7.58 (m, 2H).
Anthracene (2c): $^1$H NMR (CDCl$_3$, 500 MHz): δ 8.44 (s, 2H), 8.05-7.99 (m, 4H), 7.50-7.45 (m, 4H).

9-Methylanthracene: δ 8.35 (s, 0.38H), 8.30 (d, J = 8.6 Hz, 0.76H), 8.06-7.98 (m, 0.76H), 7.55-7.50 (m, 0.76H), 7.50-7.46 (m, 0.76H), 3.12 (s, 1.14H).

Biphenyl (2d, 2d'): $^1$H NMR (CDCl$_3$, 500 MHz): δ 7.62 (d, J = 7.5 Hz, 4H), 7.49-7.42 (m, 4H), 7.37 (t, J = 7.3 Hz, 2H).
4-Methyl-1,1'-biphenyl (2e, 2e', 2e'')$^6$: $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.58 (d, $J$ = 7.5 Hz, 2H), 7.49 (d, $J$ = 7.5 Hz, 2H), 7.42 (t, $J$ = 7.5 Hz, 2H), 7.32 (d, $J$ = 7.5 Hz, 1H), 7.25 (d, $J$ = 7.7 Hz, 2H), 2.39 (s, 3H).

![4-Methyl-1,1'-biphenyl](image)

4-Butyl-1,1'-biphenyl (2f)$^7$: $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.58 (d, $J$ = 7.8 Hz, 2H), 7.50 (d, $J$ = 7.5 Hz, 2H), 7.42 (t, $J$ = 7.5 Hz, 2H), 7.31 (t, $J$ = 7.4 Hz, 1H), 7.25 (d, $J$ = 7.8 Hz, 2H), 2.65 (t, $J$ = 7.6 Hz, 2H), 1.67-1.59 (m, 2H), 1.43-1.34 (m, 2H), 0.95 (t, $J$ = 7.3 Hz, 3H).

![4-Butyl-1,1'-biphenyl](image)
2-Methoxynaphthalene (2g, 2g')$^8$: $^1$H NMR (CDCl$_3$, 500 MHz): δ 7.31 (t, $J$ = 7.5 Hz, 2H), 6.96 (t, $J$ = 7.5 Hz, 1H), 6.93 (d, $J$ = 7.8 Hz, 2H), 3.82 (s, 3H).

\[
\text{\includegraphics[width=0.3\textwidth]{naphthalene.png}}
\]

2-Methoxynaphthalene (2h)$^9$: $^1$H NMR (CDCl$_3$, 500 MHz): δ 7.81-7.73 (m, 3H), 7.45 (t, $J$ = 7.8 Hz, 1H), 7.35 (t, $J$ = 7.6 Hz, 1H), 7.18-7.14 (m, 2H), 3.94 (s, 3H).

\[
\text{\includegraphics[width=0.3\textwidth]{naphthalene2.png}}
\]
4-Methoxy-1,1'-biphenyl (2i). $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.58-7.51 (m, 4H), 7.42 (t, $J$=7.5 Hz, 2H), 7.31 (t, $J$=7.5 Hz, 1H), 6.99 (t, $J$=7.7 Hz, 2H), 3.86 (s, 3H).

4-Butoxy-1,1'-biphenyl (2j). $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.57 (d, $J$=7.7 Hz 2H), 7.53 (d, $J$=7.7 Hz, 2H) 7.43 (t, $J$=7.5 Hz, 2H), 7.31 (t, $J$=7.5 Hz, 1H), 6.99 (d, $J$=7.7 Hz, 2H), 4.02 (t, $J$=6.5 Hz, 2H), 1.85-1.77 (m, 2H), 1.58-1.49 (m, 2H), 1.01 (t, $J$=7.4 Hz, 3H).
4-Methyl-diphenyl ether (2k)\textsuperscript{11}: \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): δ 7.33 (t, $J$ =7.3 Hz, 2H), 7.16 (d, $J$ =7.5 Hz, 2H), 7.08 (t, $J$ =7.3 Hz, 1H), 7.00 (d, $J$ =7.5 Hz, 2H), 6.94 (d, $J$ =7.5 Hz, 2H), 2.35 (s, 3H).

4-Fluoro-1,1'-biphenyl (2l)\textsuperscript{12}: \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): δ 7.62-7.51 (m, 4H), 7.47-7.40 (m, 2H), 7.35 (t, $J$ =7.5 Hz, 1H), 7.13 (t, $J$ =8.6 Hz, 2H).
4-(Trifluoromethyl)-1,1'-biphenyl (2m): $^1$H NMR (CDCl$_3$, 500 MHz): δ 7.70 (s, 4H), 7.60 (d, $J$ =7.5 Hz, 2H), 7.48 (t, $J$ =7.5 Hz, 2H), 7.41 (t, $J$ =7.5 Hz, 1H).

4-Amino-1,1'-biphenyl (2n): $^1$H NMR (DMSO-$d_6$, 500 MHz): δ 7.52 (d, $J$ =7.8 Hz, 2H), 7.38-7.32 (m, 4H), 7.21 (t, $J$ =7.5 Hz, 1H), 6.64 (d, $J$ =7.8 Hz, 2H), 5.21 (br, 2H).
N-phenylbenzamide (2o): $^1$H NMR (DMSO-$d_6$, 500 MHz): δ 10.24 (br, 1H), 7.95 (d, $J=7.8$ Hz, 2H), 7.78 (d, $J=7.8$ Hz, 2H), 7.59 (t, $J=7.2$ Hz, 1H), 7.53 (t, $J=7.3$ Hz, 2H), 7.35 (t, $J=7.7$ Hz, 2H), 7.10 (t, $J=7.4$ Hz, 1H).

E-N-cyclohexyl-1-phenylmethanimine (2p): $^1$H NMR (DMSO-$d_6$, 500 MHz): δ 8.36 (s, 1H), 7.75-7.67 (m, 2H), 7.47-7.39 (m, 3H), 3.25-3.17 (m, 1H), 1.81-1.72 (m, 2H), 1.70-1.58 (m, 3H), 1.53-1.42 (m, 2H), 1.39-1.28 (m, 2H), 1.27-1.16 (m, 1H).
2-Phenyl-1,3-dioxolane (2r) $^1$H NMR (DMSO-$d_6$, 500 MHz): δ 7.46-7.37 (m, 5H), 5.72 (s, 1H), 4.08-4.00 (m, 2H), 3.98-3.90 (m, 2H).

2-Methyl-2-phenyl-1,3-dioxolane (2s) $^1$H NMR (DMSO-$d_6$, 500 MHz): δ 7.41 (d, $J$ =7.2 Hz, 2H), 7.35 (t, $J$ =7.2 Hz, 2H), 7.30 (t, $J$ =7.3 Hz, 1H), 4.01-3.93 (m, 2H), 3.71-3.63 (m, 2H), 1.54 (s, 3H).
8-Phenyl-1,4-dioxaspiro[4,5]decan (2t) $^1$H NMR (DMSO-$d_6$, 500 MHz): $\delta$ 7.27 (d, $J = 7.3$ Hz, 2H), 7.21 (t, $J = 7.5$ Hz, 2H), 7.17 (t, $J = 7.2$ Hz, 1H), 3.91-3.85 (m, 4H), 2.60-2.52 (m, 1H), 1.79-1.56 (m, 8H).

7-Phenyl-1-heptene (2u) $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.32-7.25 (m, 2H), 7.22-7.16 (m, 3H), 5.87-5.77 (m, 1H), 5.04-4.92 (m, 2H), 2.61 (t, $J = 7.7$ Hz, 2H), 2.06 (q, $J = 7.2$ Hz, 2H), 1.67-1.60 (m, 2H), 1.47-1.33 (m, 4H).
2-Methyl-6-phenylpyridine (4a): $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.98 (d, $J=7.5$ Hz, 2H), 7.63 (t, $J=7.7$ Hz, 1H), 7.51 (d, $J=7.8$ Hz, 1H), 7.46 (t, $J=7.4$ Hz, 2H), 7.39 (t, $J=7.4$ Hz, 1H), 7.10 (d, $J=7.5$ Hz, 1H), 2.63 (s, 3H).

1-Phenyl-indole (4b): $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.69 (d, $J=7.8$ Hz, 1H), 7.57 (d, $J=8.2$ Hz, 1H), 7.54-7.48 (m, 4H), 7.38-7.32 (m, 2H), 7.25-7.15 (m, 2H), 6.68 (d, $J=3.2$ Hz, 1H).
1-Benzyl-indole (4c, 4c')\textsuperscript{21}: \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): \(\delta 7.65\) (d, \(J = 7.8\) Hz, 1H), 7.31-7.22 (m, 4H), 7.19-7.08 (m, 5H), 6.55 (d, \(J = 3.2\) Hz, 1H), 5.32 (s, 2H).

![1-Benzyl-indole](image)

Quinoline (4d)\textsuperscript{22}: \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): \(\delta 8.90\) (d, \(J = 4.2\) Hz, 1H), 8.11 (t, \(J = 7.4\) Hz, 2H), 7.78 (t, \(J = 8.1\) Hz, 1H), 7.69 (t, \(J = 7.7\) Hz, 1H), 7.51 (t, \(J = 7.5\) Hz, 1H), 7.35 (dd, \(J_1 = 8.4\) Hz, \(J_2 = 4.2\) Hz, 1H).

![Quinoline](image)
Hexadec-1-ene\textsuperscript{23}. \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): δ 5.87-5.76 (m, 1H), 5.03-4.89 (m, 2H), 2.04 (q, \textit{J} = 7.5 Hz, 2H), 1.41-1.10 (m, 24H), 0.87 (t, \textit{J} = 7.0 Hz, 3H).

2-Methylnaphthalene (4f)\textsuperscript{24}. \textsuperscript{1}H NMR (CDCl\textsubscript{3}, 500 MHz): δ 7.84-7.73 (m, 3H), 7.63 (s, 1H), 7.48-7.39 (m, 2H), 7.34 (t, \textit{J} = 8.2 Hz, 1H), 2.53 (s, 3H).

\textit{(E)}-2-(prop-1-en-1-yl)naphthalene\textsuperscript{25}: 7.71-7.65 (m, 0.4H), 7.60-7.56 (m, 0.3H), 7.34 (t, \textit{J} = 8.2 Hz, 0.7H), 6.58 (d, \textit{J} = 15.7 Hz, 0.2H), 6.43-6.34 (m, 0.2H), 1.96 (d, \textit{J} = 6.6 Hz, 0.6H).

2-Propylnaphthalene\textsuperscript{25}: 7.84-7.73 (m, 2.8H), 7.63 (s, 0.7H), 7.48-7.39 (m, 1.8H), 2.77 (t, \textit{J} = 7.7 Hz, 1.5H), 1.79-1.70 (m, 1.5H), 0.99 (t, \textit{J} = 7.3 Hz, 2.3H).
1-Ethynaphthalene (4g): $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 8.08 (d, $J$ = 8.2 Hz, 1H), 7.87 (d, $J$ = 8.2 Hz, 1H), 7.72 (d, $J$ = 8.0 Hz, 1H), 7.55-7.47 (m, 2H), 7.43 (t, $J$ = 7.7 Hz, 1H), 7.36 (d, $J$ = 7.0 Hz, 1H), 3.14 (q, $J$ = 7.5 Hz, 2H), 1.40 (t, $J$ = 7.5 Hz, 3H).
(E)-1,2-diphenylethene (4h): $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.54 (d, $J$ = 7.5 Hz, 4H), 7.38 (t, $J$ = 7.5 Hz, 4H), 7.28 (t, $J$ = 7.5 Hz, 2H), 7.13 (s, 2H).

1,2-Diphenylethane: 7.30-7.26 (m, 0.35H), 7.22-7.20 (m, 0.4H), 2.94 (s, 0.3H).

1,1,2-Triphenylethene (4i): $^1$H NMR (CDCl$_3$, 500 MHz): $\delta$ 7.36-7.28 (m, 8H), 7.24-7.20 (m, 2H), 7.16-7.09 (m, 3H), 7.04 (d, $J$ = 7.2 Hz, 2H), 6.98 (s, 1H).
4-Methyl-1,1'-biphenyl-4'-d (2e-d): $^1$H NMR (CDCl$_3$, 400 MHz): δ 7.58 (d, $J$ = 7.5 Hz, 2H), 7.50 (d, $J$ = 7.5 Hz, 2H), 7.43 (d, $J$ = 7.5 Hz, 2H), 7.27-7.24 (m, 2H), 2.40 (s, 3H).

![2e-d (89% D)](image)

4-Methoxy-1,1'-biphenyl-4'-d (2i-d) $^1$H NMR (CDCl$_3$, 500 MHz): δ 7.58-7.51 (m, 4H), 7.42 (t, $J$ = 7.5 Hz, 2H), 6.99 (t, $J$ = 7.7 Hz, 2H), 3.86 (s, 3H).

![2i-d (83% D)](image)
4-Butyl-1,1'-biphenyl-4'-d (2f-d) \( ^1\)H NMR (CDCl\(_3\), 500 MHz): \( \delta \) 7.60 (d, \( J = 7.8 \) Hz, 2H), 7.53 (d, \( J = 7.5 \) Hz, 2H), 7.44 (t, \( J = 7.5 \) Hz, 2H), 7.27 (d, \( J = 7.8 \) Hz, 2H), 2.67 (t, \( J = 7.6 \) Hz, 2H), 1.69-1.62 (m, 2H), 1.45-1.36 (m, 2H), 0.97 (t, \( J = 7.3 \) Hz, 3H).

Benzophenone (2q)
\(^1\)H NMR (CDCl\(_3\), 500 MHz): \( \delta \) 7.81 (d, \( J = 7.5 \) Hz, 4H), 7.59 (t, \( J = 7.5 \) Hz, 2H), 7.49 (t, \( J = 7.5 \) Hz, 4H).
Complex I: $^1$H NMR (C$_6$D$_6$, 500 MHz): δ 8.25 (s, 1H), 7.89-7.70 (m, 2H), 7.40-7.30 (m, 1H), 7.10-6.91 (m, 5H), 2.08-1.99 (m, 2H), 1.91-1.79 (m, 2H), 1.79-0.25 (m, 44H)

$^{31}$P NMR (C$_6$D$_6$, 202 MHz): δ 59.6 (d, $J_{pp} = 60.6$ Hz, 1P), 52.9 (d, $J_{pp} = 60.6$ Hz, 1P).
8. Reference


