Supporting Information

For

Radical alkylation of \textit{para}-quinone methides with 4-substituted Hantzsch esters/nitriles via organic photoredox catalysis

Qing-Yan Wu,† Qing-Qiang Min,† Gui-Zhen Ao,*† and Feng Liu*,†,§

†Jiangsu Key Laboratory of Neuropsychiatric Diseases and Department of Medicinal Chemistry, College of Pharmaceutical Sciences, Soochow University, 199 Ren-Ai Road, Suzhou, Jiangsu 215123, People’s Republic of China

§Key Laboratory of Organofluorine Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, People’s Republic of China.

E-mail: fliu2@suda.edu.cn, aoguizhen@suda.edu.cn

Table of Contents

1. General remarks S2
2. Typical procedure for synthesis of substituted Hantzsch esters S2
3. Typical experimental procedure S2
4. Fluorescence quenching experiments S3
5. Characterization of the substrates and products S4
6. NMR Spectra for the substrates and products S19
1. General remarks

$^1$H NMR spectra were recorded on 400 or 600 MHz (100 or 150 MHz for $^{13}$C NMR) agilent NMR spectrometer with CDCl$_3$ as the solvent and tetramethylsilane (TMS) as the internal standard. Chemical shifts were reported in parts per million (ppm, $\delta$ scale) downfield from TMS at 0.00 ppm and referenced to the CDCl$_3$ at 7.26 ppm (for $^1$H NMR) or 77.16 ppm (for $^{13}$C NMR). HRMS was recorded on a GCT PremierTM (CI) Mass Spectrometer. Infrared (FT-IR) spectra were recorded on a Varian 1000FT-IR, $\nu_{\text{max}}$ in cm$^{-1}$. Melting points were measured using SGW, X-4B and values are uncorrected. All commercially available reagents and solvents were used as received unless otherwise specified. The substrates we are readily prepared according to known methods (Org. Lett. 2015, 17, 3390–3393; J. Am. Chem. Soc. 2016, 138, 12312–12315).

2. Typical procedure for synthesis of substituted Hantzsch esters

To a flask charged with ethyl acetoacetate (2.6 mL, 20 mmol), the cyclohexylformaldehyde (10 mmol) and ethanol (20 mL) was added ammonia aqueous solution (1.5 mL, 25%, 20 mmol). The mixture was heated at 70 ºC for about 8 hours. The reaction was allowed to cool to room temperature. The solution was concentrated under reduced pressure. A mixture of water and CH$_2$Cl$_2$ were added to the concentrated residue and the layers were separated. The aqueous layer was extracted with CH$_2$Cl$_2$ for 3 times. The combined organic layers were washed with brine, dried (MgSO$_4$), and filtered. The filtrate was concentrated under reduced pressure. The residue was purified by chromatography on silica gel to obtain 2a as a light yellow solid (3.56 g, 53% yield).

3. Typical experimental procedure
To a suspension of 1a (58.8 mg, 0.2 mmol), 2a (134.1 mg, 0.4 mmol) and N-methyl-9-mesityl acridinium perchlorate (4.1 mg, 0.01 mmol) in acetone (without dehydration, 2 mL) was added KH₂PO₄ (54.4 mg, 0.4 mmol) at rt. The resulting mixture was stirred upon 22W blue LEDs irradiation under argon balloon. After the reaction was finished, the solvent was removed under reduced pressure and the residue was purified by flash column chromatography on silica gel to give 3a as a white solid (57.5 mg, 76% yield).

**Reaction setup:**

![Figure S1](image_url). Photographs of the 22w blue light strip and reaction vessel.

4. **Fluorescence quenching experiments**

Emission intensities were recorded using LS55 Luminescence Spectrometer for all experiments. All Mes-Acr⁺ solutions were excited at 450 nm and the emission intensity was collected at 490-570 nm. In a typical experiment, the DMSO solution of Mes-Acr⁺ (0.02 mM) was added the appropriate amount of quencher in a screw-top 1.0 cm quartz cuvette. After degassing with nitrogen for 10 min, the emission spectra of the samples were collected.
5. Characterization of the substrates and products

\[ \text{4-Benzylidene-2,6-di-tert-butycyclohexa-2,5-dien-1-one (1a):} \]
\[ ^1\text{H NMR (600 MHz, CDCl}_3\text{)} \delta 7.54 (d, J = 2.2 \text{ Hz, 1H}), 7.48 - 7.43 (m, 4H), 7.41 - 7.37 (m, 1H), 7.19 (s, 1H), 7.03 (d, J = 2.3 \text{ Hz, 1H}), 1.35 (s, 9H), 1.32 (s, 9H); ^{13}\text{C NMR (150 MHz, CDCl}_3\text{)} \delta 186.6, 149.5, 147.9, 142.6, 136.0, 135.2, 132.1, 130.4, 129.2, 128.9, 127.9, 35.6, 35.1, 29.67, 29.65. \]

\[ \text{2,6-Di-tert-butyl-4-(4-chlorobenzylidene)cyclohexa-2,5-dien-1-one (1b):} \]
\[ ^1\text{H NMR (400 MHz, CDCl}_3\text{)} \delta 7.46 - 7.40 (m, 3H), 7.38 (d, J = 8.3 \text{ Hz, 2H}), 7.11 (s, 1H), 6.99 (s, 1H), 1.33 (s, 9H), 1.30 (s, 9H); ^{13}\text{C NMR (150 MHz, CDCl}_3\text{)} \delta 186.7, 149.9, 148.2, 140.8, 135.3, 135.0, 134.5, 132.5, 131.6, 129.2, 127.4, 35.6, 35.2, 29.68, 29.65. \]

\[ \text{4-(4-Bromobenzylidene)-2,6-di-tert-butycyclohexa-2,5-dien-1-one (1c):} \]
\[ ^1\text{H NMR (400 MHz, CDCl}_3\text{)} \delta 7.56 (d, J = 8.0 \text{ Hz, 2H}), 7.43 (s, 1H), 7.30 (d, J = 8.0 \text{ Hz, 2H}), 7.07 (s, 1H), 6.98 (s, 1H), 1.32 (s, 9H), 1.29 (s, 9H); ^{13}\text{C NMR (150 MHz, CDCl}_3\text{)} \delta 186.6, 149.8, 148.2, 140.7, 134.9, 134.9, 132.5, 132.1, 131.8, 127.3, 123.6, 35.6, 35.1, 29.7, 29.6. \]
2,6-Di-tert-butyl-4-(4-methylbenzylidene)cyclohexa-2,5-dien-1-one (1d): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.56 (s, 1H), 7.37 (d, $J$ = 7.7 Hz, 2H), 7.25 (d, $J$ = 7.6 Hz, 2H), 7.16 (s, 1H), 7.01 (s, 1H), 2.40 (s, 3H), 1.34 (s, 9H), 1.31 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 186.6, 149.2, 147.6, 143.0, 139.7, 135.4, 133.3, 131.5, 130.5, 129.7, 128.0, 35.6, 35.1, 29.69, 29.65, 21.6.

5-((3,5-Di-tert-butyl-4-oxocyclohexa-2,5-dien-1-ylidene)methyl)benzonitrile (1e): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.73 (d, $J$ = 8.0 Hz, 2H), 7.53 (d, $J$ = 8.0 Hz, 2H), 7.35 (s, 1H), 7.11 (s, 1H), 7.00 (s, 1H), 1.32 (s, 9H), 1.28 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 186.5, 150.6, 149.0, 140.5, 139.0, 134.6, 134.1, 132.5, 130.7, 126.8, 118.6, 112.2, 35.7, 35.3, 29.62, 29.59.

Methyl 4-((3,5-di-tert-butyl-4-oxocyclohexa-2,5-dien-1-ylidene)methyl)benzoate (1f): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.11 (d, $J$ = 7.6 Hz, 2H), 7.51 (d, $J$ = 7.6 Hz, 2H), 7.45 (s, 1H), 7.17 (s, 1H), 7.01 (s, 1H), 3.95 (s, 3H), 1.33 (s, 9H), 1.29 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 186.7, 166.7, 150.1, 148.6, 140.6, 140.5, 134.9, 133.5, 130.3, 130.0, 127.5, 52.5, 35.7, 35.2, 29.67, 29.65.
2,6-Di-tert-butyl-4-(2-chlorobenzylidene)cyclohexa-2,5-dien-1-one (1g): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.51 – 7.45 (m, 1H), 7.44 – 7.38 (m, 1H), 7.38 – 7.32 (m, 2H), 7.32 – 7.28 (m, 2H), 7.07 (s, 1H), 1.34 (s, 9H), 1.27 (s, 9H); $^{13}$C NMR (151 MHz, CDCl$_3$) $\delta$ 186.7, 149.8, 148.4, 138.7, 135.0, 134.8, 134.2, 133.0, 132.3, 130.1, 127.8, 126.8, 35.6, 35.2, 29.6.

4-(2-Bromobenzylidene)-2,6-di-tert-butylcyclohexa-2,5-dien-1-one (1h): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.69 (d, $J = 7.9$ Hz, 1H), 7.44 – 7.36 (m, 2H), 7.31 – 7.21 (m, 3H), 7.08 (s, 1H), 1.35 (s, 9H), 1.27 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 186.7, 149.8, 148.4, 140.9, 136.0, 134.7, 133.4, 132.7, 132.4, 130.4, 127.8, 127.4, 125.2, 35.6, 35.3, 29.6.

2,6-Di-tert-butyl-4-(3-chlorobenzylidene)cyclohexa-2,5-dien-1-one (1i): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.43 (d, $J = 3.4$ Hz, 2H), 7.39 – 7.28 (m, 3H), 7.08 (s, 1H), 6.99 (s, 1H), 1.33 (s, 9H), 1.30 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 186.6, 150.0, 148.4, 140.2, 137.7, 134.9, 134.8, 133.0, 130.2, 130.1, 129.0, 128.4, 127.4, 35.6, 35.2, 29.63.
2,6-Di-tert-butyl-4-(3-methoxybenzylidene)cyclohexa-2,5-dien-1-one (1j): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.56 (s, 1H), 7.36 (t, $J = 7.8$ Hz, 1H), 7.16 (s, 1H), 7.05 (d, $J = 7.5$ Hz, 1H), 7.01 (s, 1H), 6.99 (s, 1H), 6.95 (d, $J = 8.2$ Hz, 1H), 3.85 (s, 3H), 1.34 (s, 9H), 1.31 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 186.7, 159.9, 149.5, 148.0, 142.5, 137.3, 135.2, 132.2, 129.9, 128.0, 123.1, 115.4, 115.3, 55.4, 35.6, 35.1, 29.71, 29.65.

4-Benzylidene-2,6-dimethylcyclohexa-2,5-dien-1-one (1k): $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.48 (s, 1H), 7.42 – 7.39 (m, 4H), 7.38 – 7.34 (m, 1H), 7.09 (s, 1H), 6.98 (s, 1H), 2.03 (s, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 186.9, 142.6, 138.7, 137.2, 135.3, 131.4, 131.1, 130.2, 129.1, 128.5, 16.7, 16.0.

Diethyl 4-cyclohexyl-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (2a): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 5.97 (s, 1H), 4.26 – 4.04 (m, 4H), 3.89 (d, $J = 5.6$ Hz, 1H), 2.27 (s, 6H), 1.68 – 1.58 (m, 2H), 1.52 (d, $J = 11.8$ Hz, 3H), 1.27 (t, $J = 7.1$ Hz, 6H), 1.21 – 1.13 (m, 1H), 1.12 – 0.99 (m, 3H), 0.96 – 0.83 (m, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 168.8, 144.5, 102.1, 59.7, 45.9, 38.6, 29.0, 26.9, 26.8, 19.6, 14.5.
Diethyl 4-isopropyl-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (2b): $^1$H NMR (400 MHz, CDCl$_3$) δ 5.89 (s, 1H), 4.24 – 4.06 (m, 4H), 3.89 (d, $J = 5.2$ Hz, 1H), 2.28 (s, 6H), 1.61 – 1.51 (m, 1H), 1.27 (t, $J = 7.0$ Hz, 6H), 0.72 (d, $J = 6.8$ Hz, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ 168.9, 144.8, 101.7, 59.6, 38.9, 35.6, 19.4, 18.6, 14.5.

![Chemical structure of 2b](image)

4-(Tert-butyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarbonitrile (2c): $^1$H NMR (400 MHz, CDCl$_3$) δ 6.17 (s, 1H), 2.89 (s, 1H), 2.19 (s, 6H), 0.96 (s, 9H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 148.9, 120.8, 81.3, 46.5, 41.0, 26.2, 18.5.

![Chemical structure of 2c](image)

Diethyl 4-benzyl-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (2d): $^1$H NMR (400 MHz, CDCl$_3$) δ 7.18 – 7.08 (m, 3H), 7.01 (d, $J = 6.8$ Hz, 2H), 5.86 (s, 1H), 4.18 (t, $J = 5.3$ Hz, 1H), 4.09 – 3.94 (m, 4H), 2.56 (d, $J = 5.5$ Hz, 2H), 2.16 (s, 6H), 1.21 (t, $J = 7.1$ Hz, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 168.0, 145.8, 139.3, 130.1, 127.3, 125.6, 101.7, 59.6, 42.4, 35.5, 19.1, 14.4.

![Chemical structure of 2d](image)

Diethyl 4-(4-chlorobenzyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (2e): $^1$H NMR (400 MHz, CDCl$_3$) δ 7.09 (d, $J = 7.9$ Hz, 2H), 6.90 (d, $J = 7.9$ Hz, 2H), 5.66 (s, 1H), 4.13 (t, $J = 5.0$ Hz, 1H), 4.08 – 3.98 (m, 4H), 2.50 (d, $J = 5.1$ Hz, 2H), 2.12 (s, 6H), 1.20 (t, $J = 7.0$ Hz, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) δ 167.9, 145.9, 137.9, 131.6, 131.4, 127.3, 101.4, 59.8, 41.6, 35.4, 19.2, 14.4.
Diethyl 4-(4-bromobenzyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarboxylate (2f): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.29 (d, $J$ = 8.1 Hz, 2H), 6.89 (d, $J$ = 8.1 Hz, 2H), 5.59 (s, 1H), 4.17 (t, $J$ = 5.2 Hz, 1H), 4.15 – 4.00 (m, 4H), 2.53 (d, $J$ = 5.2 Hz, 2H), 2.17 (s, 6H), 1.25 (t, $J$ = 7.1 Hz, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 167.8, 145.8, 138.4, 131.9, 130.3, 119.7, 101.5, 59.8, 41.7, 35.4, 19.3, 14.5.

Diethyl 2,6-dimethyl-4-(thiophen-2-ylmethyl)-1,4-dihydropyridine-3,5-dicarboxylate (2g): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.08 (d, $J$ = 4.9 Hz, 1H), 6.86 – 6.82 (m, 1H), 6.62 (d, $J$ = 2.0 Hz, 1H), 5.42 (s, 1H), 4.19 (t, $J$ = 4.8 Hz, 1H), 4.11 (q, $J$ = 7.0 Hz, 4H), 2.81 (d, $J$ = 5.0 Hz, 2H), 2.20 (s, 6H), 1.26 (t, $J$ = 7.0 Hz, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 167.8, 145.8, 141.5, 126.33, 126.27, 123.9, 101.6, 59.8, 36.2, 35.8, 19.6, 14.5.

Diethyl 2,6-dimethyl-4-(1-phenylethyl)-1,4-dihydropyridine-3,5-dicarboxylate (2h): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.20 – 7.14 (m, 2H), 7.13 – 7.05 (m, 3H), 5.92 (s, 1H), 4.26 (d, $J$ = 5.0 Hz, 1H), 4.06 – 3.94 (m, 3H), 3.90 – 3.80 (m, 1H), 2.78 – 2.68 (m, 1H), 2.19 (s, 6H), 1.29 – 1.22 (m, 3H), 1.20 – 1.12 (m, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 168.5, 168.5, 145.6, 145.3, 144.2, 128.5, 127.2, 125.8, 100.8, 100.7, 59.59, 59.56, 46.0, 40.1, 19.1, 19.0, 15.4, 14.4, 14.3.
4-Benzhydryl-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarbonitrile (2i): $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.35 – 7.32 (m, 4H), 7.32 – 7.27 (m, 5H), 7.26 – 7.22 (m, 2H), 3.99 (d, $J = 7.9$ Hz, 1H), 3.92 (d, $J = 7.9$ Hz, 1H), 1.89 (s, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 148.7, 139.4, 129.2, 128.4, 127.1, 118.9, 81.7, 58.4, 40.7, 18.0.

2,6-Dimethyl-4-(2-phenylpropan-2-yl)-1,4-dihydropyridine-3,5-dicarbonitrile (2j): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.34 – 7.20 (m, 6H), 3.29 (s, 1H), 2.00 (s, 6H), 1.38 (s, 6H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 149.6, 144.5, 127.9, 126.9, 126.6, 119.8, 79.9, 47.5, 46.6, 24.3, 18.0.

4-(1-Benzycyclohexyl)-2,6-dimethyl-1,4-dihydropyridine-3,5-dicarbonitrile (2k): $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.44 (s, 1H), 7.26 – 7.18 (m, 3H), 7.06 (d, $J = 6.9$ Hz, 2H), 3.79 (s, 1H), 2.37 (s, 2H), 2.21 (s, 6H), 2.10 – 2.05 (m, 2H), 1.81 – 1.73 (m, 2H), 1.66 – 1.52 (m, 4H), 1.13 – 1.02 (m, 2H).

2,6-Di-tert-butyl-4-(cyclohexyl(phenyl)methyl)phenol (3a): White solid; m.p. 130-134 °C; 76% yield (58 mg); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.30 – 7.19 (m, 4H),
7.15 – 7.07 (m, 1H), 7.03 (s, 2H), 4.95 (s, 1H), 3.35 (d, J = 10.6 Hz, 1H), 2.07 – 1.93 (m, 1H), 1.72 – 1.57 (m, 4H), 1.40 (s, 18H), 1.29 – 1.07 (m, 4H), 0.90 – 0.73 (m, 2H);

\(^{13}\)C NMR (150 MHz, CDCl3) δ 151.9, 145.5, 135.5, 153.0, 128.4, 128.3, 125.7, 124.6, 59.7, 42.0, 34.5, 32.4, 32.3, 30.6, 26.8, 26.6, 26.5; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3619, 2921, 2849, 1433, 751; HRMS (CI) calcd C\(_{27}H_{38}O\) [M]+: 378.2923, found: 378.2928.

\begin{image}
\centering
\includegraphics[width=0.2\textwidth]{image1}
\end{image}

**2,6-Di-tert-butyl-4-((4-chlorophenyl)(cyclohexyl)methyl)phenol (3b):** White solid; m.p. 130-132 ℃; 74% yield (61 mg); \(^1\)H NMR (400 MHz, CDCl3) δ 7.25 – 7.15 (m, 4H), 7.00 (s, 2H), 5.00 (s, 1H), 3.35 (d, J = 10.7 Hz, 1H), 2.03 – 1.91 (m, 1H), 1.73 – 1.58 (m, 4H), 1.24 – 1.10 (m, 4H), 1.41 (s, 18H), 0.89 – 0.75 (m, 2H); \(^{13}\)C NMR (150 MHz, CDCl3) δ 152.0, 144.0, 135.7, 134.4, 131.4, 129.6, 128.5, 124.5, 58.9, 41.9, 34.5, 32.3, 32.2, 30.5, 26.7, 26.53, 26.48; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3631, 2917, 2847, 1435, 768; HRMS (CI) calcd C\(_{27}H_{37}ClO\) [M]+: 412.2533, found: 412.2530.

\begin{image}
\centering
\includegraphics[width=0.2\textwidth]{image2}
\end{image}

**4-((4-Bromophenyl)(cyclohexyl)methyl)-2,6-di-tert-butylphenol (3c):** White solid; m.p. 113-115 ℃; 80% yield (73 mg); \(^1\)H NMR (400 MHz, CDCl3) δ 7.36 (d, J = 7.9 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 6.99 (s, 2H), 4.99 (s, 1H), 3.33 (d, J = 10.7 Hz, 1H), 2.04 – 1.89 (m, 1H), 1.72 – 1.60 (m, 4H), 1.40 (s, 18H), 1.24 – 1.10 (m, 4H), 0.88 – 0.74 (m, 2H); \(^{13}\)C NMR (150 MHz, CDCl3) δ 152.0, 144.6, 135.7, 134.3, 131.5, 130.0, 124.4, 119.4, 59.0, 41.8, 34.5, 32.3, 32.2, 30.5, 26.7, 26.51, 26.47; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3640, 2920, 2851, 1434, 833; HRMS (CI) calcd C\(_{27}H_{37}BrO\) [M]+: 456.2028, found: 456.2027.

\begin{image}
\centering
\includegraphics[width=0.2\textwidth]{image3}
\end{image}
2,6-Di-tert-butyl-4-(cyclohexyl(p-tolyl)methyl)phenol (3d): White solid; m.p. 148-151 °C; 66% yield (52 mg); $^1$H NMR (400 MHz, CDCl₃) δ 7.17 (d, $J = 7.7$ Hz, 2H), 7.07 (d, $J = 7.6$ Hz, 2H), 7.04 (s, 2H), 4.95 (s, 1H), 3.32 (d, $J = 10.7$ Hz, 1H), 2.29 (s, 3H), 2.09 – 1.90 (m, 1H), 1.71 – 1.60 (m, 4H), 1.61 (s, 1H), 1.28 – 1.08 (m, 4H), 0.88 – 0.75 (m, 2H); $^{13}$C NMR (150 MHz, CDCl₃) δ 151.8, 142.6, 135.5, 135.1, 135.1, 129.1, 128.1, 124.5, 59.3, 42.0, 34.4, 32.4, 32.3, 30.6, 26.8, 26.61, 26.56, 21.1; FT-IR (thin film, KBr): ν (cm$^{-1}$) 3628, 2917, 2850, 1434, 770; HRMS (CI) calcd C$_{28}$H$_{40}$O [M]$^+$: 392.3079, found: 392.3078.

![Image of 2,6-Di-tert-butyl-4-(cyclohexyl(p-tolyl)methyl)phenol (3d)]

4-(Cyclohexyl(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)benzonitrile (3e): White solid; m.p. 106-108 °C; 53% yield (43 mg); 70% yield (66 mg); $^1$H NMR (400 MHz, CDCl₃) δ 7.54 (d, $J = 7.4$ Hz, 2H), 7.37 (d, $J = 7.4$ Hz, 2H), 6.98 (s, 2H), 5.04 (s, 1H), 3.44 (d, $J = 10.6$ Hz, 1H), 2.09 – 1.93 (m, 1H), 1.73 – 1.57 (m, 4H), 1.41 (s, 1H), 1.29 – 1.10 (m, 4H), 0.92 – 0.76 (m, 2H); $^{13}$C NMR (150 MHz, CDCl₃) δ 152.3, 151.2, 136.0, 133.4, 132.4, 129.0, 124.5, 119.3, 109.6, 59.6, 41.6, 34.5, 32.2, 32.0, 30.5, 26.6, 26.42, 26.37; FT-IR (thin film, KBr): ν (cm$^{-1}$) 3628, 2927, 2229, 1434, 749; HRMS (CI) calcd C$_{28}$H$_{38}$NO [M + H]$^+$: 404.2953, found: 404.2958.

![Image of 4-(Cyclohexyl(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)benzonitrile (3e)]

Methyl 4-(cyclohexyl(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)benzoate (3f): White solid; m.p. 165-168 °C; 49% yield (43 mg); $^1$H NMR (400 MHz, CDCl₃) δ 7.93 (d, $J = 8.0$ Hz, 2H), 7.34 (d, $J = 8.0$ Hz, 2H), 7.02 (s, 2H), 5.00 (s, 1H), 3.88 (s, 3H), 3.44 (d, $J = 10.7$ Hz, 1H), 2.09 – 1.98 (m, 1H), 1.72 – 1.58 (m, 4H), 1.40 (s, 1H), 1.25 – 1.10 (m, 4H), 0.90 – 0.80 (m, 2H); $^{13}$C NMR (150 MHz, CDCl₃) δ 167.3, 152.1, 151.1, 135.7, 134.0, 129.9, 128.3, 127.7, 124.6, 59.6, 52.1, 41.8, 34.5, 32.3, 32.1, 30.5, 26.7, 26.5, 26.4; FT-IR (thin film, KBr): ν (cm$^{-1}$) 3626, 2923, 1716, 1260, 711; HRMS (CI) calcd C$_{29}$H$_{41}$O$_3$ [M + H]$^+$: 437.3056, found: 437.3060.

![Image of Methyl 4-(cyclohexyl(3,5-di-tert-butyl-4-hydroxyphenyl)methyl)benzoate (3f)]
2,6-Di-tert-butyl-4-((2-chlorophenyl)(cyclohexyl)methyl)phenol (3g): White solid; m.p. 175-178 °C; 69% yield (57 mg); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.43 (d, $J = 7.6$ Hz, 1H), 7.30 (d, $J = 7.9$ Hz, 1H), 7.21 (t, $J = 7.4$ Hz, 1H), 7.10 (s, 2H), 7.05 (t, $J = 7.4$ Hz, 1H), 4.99 (s, 1H), 4.10 (d, $J = 11.1$ Hz, 1H), 2.11 – 2.00 (m, 1H), 1.71 – 1.59 (m, 4H), 1.41 (s, 18H), 1.27 – 1.13 (m, 4H), 0.95 – 0.85 (m, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 152.0, 142.8, 135.5, 134.6, 133.6, 129.7, 128.4, 127.0, 126.7, 124.9, 53.3, 41.8, 34.5, 32.0, 31.6, 30.5, 26.7, 26.5; FT-IR (thin film, KBr): $\nu$ (cm$^{-1}$) 3640, 2920, 2851, 1435, 746; HRMS (CI) calcd C$_{27}$H$_{37}$ClO $[M+]$: 412.2533, found: 412.2518.

4-((2-Bromophenyl)(cyclohexyl)methyl)-2,6-di-tert-butylphenol (3h): White solid; m.p. 182-184 °C; 84% yield (77 mg); $^1$H NMR (600 MHz, CDCl$_3$) $\delta$ 7.49 (d, $J = 8.0$ Hz, 1H), 7.41 (d, $J = 9.0$ Hz, 1H), 7.28 – 7.21 (m, 1H), 7.13 (s, 2H), 6.96 (t, $J = 7.6$ Hz, 1H), 4.97 (s, 1H), 4.09 (d, $J = 11.1$ Hz, 1H), 2.09 – 1.99 (m, 1H), 1.72 – 1.60 (m, 4H), 1.40 (s, 18H), 1.24 – 1.13 (m, 4H), 0.96 – 0.85 (m, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 152.0, 144.5, 135.5, 133.6, 133.0, 128.5, 127.7, 127.1, 126.0, 124.9, 56.1, 42.1, 34.5, 32.0, 31.6, 30.6, 26.7, 26.5; FT-IR (thin film, KBr): $\nu$ (cm$^{-1}$) 3638, 2919, 2850, 1435, 745; HRMS (Cl) calcd C$_{27}$H$_{37}$BrO $[M+]$: 456.2028, found: 456.2029.

2,6-Di-tert-butyl-4-((3-chlorophenyl)(cyclohexyl)methyl)phenol (3i): White solid; m.p. 158-160 °C; 61% yield (50 mg); $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.25 – 7.22 (m, 1H), 7.19 – 7.14 (m, 2H), 7.12 – 7.07 (m, 1H), 7.00 (s, 2H), 5.00 (s, 1H), 3.33 (d, $J = 10.8$ Hz, 1H), 2.03 – 1.91 (m, 1H), 1.73 – 1.59 (m, 4H), 1.41 (s, 18H), 1.29 – 1.09 (m, 4H), 0.89 – 0.73 (m, 2H); $^{13}$C NMR (150 MHz, CDCl$_3$) $\delta$ 152.1, 147.6, 135.7, 134.2,
134.1, 129.7, 128.5, 126.3, 125.9, 124.5, 59.4, 41.9, 34.5, 32.3, 32.1, 30.5, 26.7, 26.50, 26.46; FT-IR (thin film, KBr): ν (cm⁻¹) 3629, 2918, 2846, 1436, 693; HRMS (CI) calcd C₂₇H₃₇ClO [M]+: 412.2533, found: 412.2538.

2,6-Di-tert-butyl-4-(cyclohexyl(3-methoxyphenyl)methyl)phenol (3j): White solid; m.p. 170-173 °C; 76% yield (62 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.18 (t, J = 7.8 Hz, 1H), 7.06 (s, 2H), 6.90 (d, J = 7.5 Hz, 1H), 6.84 (s, 1H), 6.69 (d, J = 6.9 Hz, 1H), 4.98 (s, 1H), 3.79 (s, 3H), 3.33 (d, J = 10.8 Hz, 1H), 2.06 – 1.95 (m, 1H), 1.74 – 1.62 (m, 4H), 1.42 (s, 18H), 1.29 – 1.14 (m, 4H), 0.91 – 0.78 (m, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 159.6, 151.9, 147.2, 135.5, 134.8, 129.3, 124.6, 120.7, 114.4, 110.7, 59.7, 55.2, 42.0, 34.5, 32.4, 32.2, 30.6, 26.8, 26.6, 26.5; FT-IR (thin film, KBr): ν (cm⁻¹) 3614, 2917, 1433, 1234, 703; HRMS (CI) calcd C₂₈H₄₀O₂ [M]+: 408.3028, found: 408.3020.

4-(cyclohexyl(phenyl)methyl)-2,6-dimethylphenol (3k): Colorless oil; 29% yield (17 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.25 (m, 4H), 7.12 (m, 1H), 6.86 (s, 2H), 4.42 (s, 1H), 3.32 (d, J = 10.8 Hz, 1H), 2.19 (s, 6H), 2.09 – 1.96 (m, 1H), 1.72 – 1.60 (m, 4H), 1.30 – 1.10 (m, 4H), 0.92 – 0.78 (m, 2H); ¹³C NMR (150 MHz, CDCl₃) δ 150.4, 145.3, 136.3, 128.5, 128.2, 128.1, 125.8, 122.9, 59.0, 41.4, 32.3, 32.3, 26.7, 26.5, 16.3.
4-(1-(4-Bromophenyl)-2-methylpropyl)-2,6-di-tert-butylphenol (4a): White solid; m.p. 102-107 °C; 52% yield (43 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.38 (d, \(J = 7.7\) Hz, 2H), 7.17 (d, \(J = 7.7\) Hz, 2H), 7.02 (s, 2H), 5.01 (s, 1H), 3.27 (d, \(J = 10.6\) Hz, 1H), 2.41 – 2.33 (m, 1H), 1.42 (s, 18H), 0.89 – 0.80 (m, 6H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 152.1, 145.0, 135.7, 134.8, 131.5, 129.9, 124.4, 119.5, 60.3, 34.5, 32.4, 30.5, 22.0; FT-IR thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3630, 2921, 2866, 1434, 787; HRMS (CI) calcd C\(_{24}\)H\(_{33}\)BrO \([M]^+\): 416.1715, found: 416.1707.

\[\text{\includegraphics[width=0.2\textwidth]{image}}\]

4-(1-(4-Bromophenyl)-2,2-dimethylpropyl)-2,6-di-tert-butylphenol (4b): White solid; m.p. 138-139 °C; 70% yield (60 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.41 (d, \(J = 8.2\) Hz, 2H), 7.33 (d, \(J = 8.3\) Hz, 2H), 7.17 (s, 2H), 5.05 (s, 1H), 3.58 (s, 1H), 1.45 (s, 18H), 0.99 (s, 9H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 152.2, 143.2, 135.1, 133.0, 131.6, 131.1, 126.3, 119.8, 63.8, 35.2, 34.4, 30.5, 29.3; FT-IR thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3629, 2921, 2868, 1236, 778; HRMS (CI) calcd C\(_{25}\)H\(_{35}\)BrO \([M]^+\): 430.1871, found: 430.1863.

\[\text{\includegraphics[width=0.2\textwidth]{image}}\]

4-(1-(4-Bromophenyl)-2-phenylethyl)-2,6-di-tert-butylphenol (4c): White solid; m.p. 108-110 °C; 46% yield (43 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.35 (d, \(J = 8.0\) Hz, 2H), 7.21 – 7.11 (m, 3H), 7.06 (d, \(J = 8.0\) Hz, 2H), 6.95 (d, \(J = 7.0\) Hz, 2H), 6.92 (s, 2H), 5.06 (s, 1H), 4.08 (t, \(J = 7.6\) Hz, 1H), 3.26 (d, \(J = 7.6\) Hz, 2H), 1.38 (s, 18H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\) 152.3, 143.9, 140.4, 135.7, 134.7, 131.4, 130.0, 129.3, 128.2, 126.0, 124.5, 119.8, 52.8, 42.8, 34.5, 30.4; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3624, 2919, 1766, 1432, 698; HRMS (CI) calcd C\(_{28}\)H\(_{33}\)BrO \([M]^+\): 464.1715, found: 464.1698.

\[\text{\includegraphics[width=0.2\textwidth]{image}}\]
4-(1-(4-Bromophenyl)-2-(4-chlorophenyl)ethyl)-2,6-di-tert-butylphenol (4d): White solid; m.p. 94-98 °C; 51% yield (51 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.36 (d, \(J = 8.2\) Hz, 2H), 7.13 (d, \(J = 8.1\) Hz, 2H), 7.04 (d, \(J = 8.2\) Hz, 2H), 6.90 (s, 2H), 6.87 (d, \(J = 8.1\) Hz, 2H), 5.07 (s, 1H), 4.02 (t, \(J = 7.8\) Hz, 1H), 3.22 (d, \(J = 7.8\) Hz, 2H), 1.38 (s, 18H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 152.4, 143.6, 138.9, 135.8, 134.3, 131.8, 131.5, 130.6, 130.0, 128.3, 124.4, 120.0, 52.7, 42.1, 34.5, 30.4; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3635, 2956, 1435, 1010, 809; HRMS (CI) calcd C\(_{28}\)H\(_{33}\)Cl\(_7\)BrO \([M + H]^+\): 499.1403, found: 499.1379.

4-(1,2-Bis(4-bromophenyl)ethyl)-2,6-di-tert-butylphenol (4e): White solid; m.p. 77-80 °C; 63% yield (68 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.36 (d, \(J = 8.2\) Hz, 2H), 7.29 (d, \(J = 8.1\) Hz, 2H), 7.04 (d, \(J = 8.2\) Hz, 2H), 6.90 (s, 2H), 6.81 (d, \(J = 8.1\) Hz, 2H), 5.07 (s, 1H), 4.03 (t, \(J = 7.8\) Hz, 1H), 3.21 (d, \(J = 7.8\) Hz, 2H), 1.38 (s, 18H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 152.4, 143.5, 139.4, 135.8, 134.2, 131.5, 131.2, 131.0, 129.9, 124.4, 120.0, 119.9, 52.7, 42.2, 34.5, 30.4; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3633, 2956, 2919, 1435, 1010; HRMS (CI) calcd C\(_{28}\)H\(_{33}\)Br\(_2\)O \([M + H]^+\): 543.0898, found: 543.0925.

4-(1-(4-Bromophenyl)-2-(thiophen-2-yl)ethyl)-2,6-di-tert-butylphenol (4f): White solid; m.p. 84-86 °C; 51% yield (48 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.39 (d, \(J = 8.2\) Hz, 2H), 7.13 (d, \(J = 8.2\) Hz, 2H), 7.05 (d, \(J = 5.0\) Hz, 1H), 6.99 (s, 2H), 6.84 – 6.79 (m, 1H), 6.59 (d, \(J = 2.3\) Hz, 1H), 5.09 (s, 1H), 4.13 (t, \(J = 7.7\) Hz, 1H), 3.50 (d, \(J = 6.9\) Hz, 2H), 1.41 (s, 18H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 152.5, 143.6, 142.9,
135.9, 134.2, 131.5, 129.9, 126.6, 125.6, 124.4, 123.6, 120.1, 53.0, 36.9, 34.5, 30.5; FT-IR (thin film, KBr): ν (cm⁻¹) 3636, 2956, 1434, 1010, 717; HRMS (CI) calcd C₂₆H₃₁⁷⁹BrOS [M⁺]: 470.1279, found: 470.1270.

4-(1-(4-Bromophenyl)-2-phenylpropyl)-2,6-di-tert-butylphenol (4g): White solid; two isomers (1.7 : 1); m.p. 100-102 °C; 50% yield (48 mg); ¹H NMR (400 MHz, CDCl₃) δ 7.46 (d, J = 8.1 Hz, 0.74H), 7.29 (d, J = 8.2 Hz, 0.74H), 7.22 – 7.04 (m, 6.75H), 7.02 – 6.97 (m, 2.04H), 6.72 (s, 0.74H), 5.06 (s, 0.63H), 4.87 (s, 0.37H), 3.92 (d, J = 11.2 Hz, 0.63H), 3.85 (d, J = 11.0 Hz, 0.37H), 3.49 – 3.34 (m, 1H), 1.45 (s, 11.34H), 1.27 (s, 6.66H), 1.21 (d, J = 6.9 Hz, 1.11H), 1.18 (d, J = 6.8 Hz, 1.89H); ¹³C NMR (150 MHz, CDCl₃) δ 152.3/151.7, 146.0/145.9, 143.9/143.6, 135.9/135.1, 134.0/133.6, 131.6/131.1, 130.3/130.0, 128.3/128.0, 127.9/127.8, 126.0/125.9, 124.9/124.7, 119.9/119.3, 59.4/58.9, 45.4/44.9, 34.5/34.3, 30.6/30.4, 22.1/21.3; FT-IR (thin film, KBr): ν (cm⁻¹) 3637, 2957, 1435, 1009, 698; HRMS (CI) calcd C₂₉H₃₆⁷⁹BrO [M + H]⁺: 479.1950, found: 479.1953.

4-(1-(4-Bromophenyl)-2,2-diphenylethyl)-2,6-di-tert-butylphenol (4h): White solid; m.p. 138-141 °C; 42% yield (45 mg); ¹H NMR (600 MHz, CDCl₃) δ 7.25 (d, J = 3.6 Hz, 2H), 7.20 (d, J = 7.7 Hz, 2H), 7.14 (t, J = 7.6 Hz, 2H), 7.09 (d, J = 8.2 Hz, 2H), 7.07 – 7.02 (m, 3H), 7.01 – 6.95 (m, 3H), 6.70 (s, 2H), 4.89 (s, 1H), 4.59 (d, J = 12.0 Hz, 1H), 4.52 (d, J = 12.0 Hz, 1H), 1.25 (s, 18H); ¹³C NMR (151 MHz, CDCl₃) δ 151.8, 143.9, 143.1, 143.0, 135.3, 133.3, 131.3, 130.5, 128.7, 128.6, 128.4, 128.1, 126.1, 125.9, 125.3, 119.5, 57.4, 55.9, 34.3, 30.3; FT-IR (thin film, KBr): ν (cm⁻¹) 3359, 2920, 2851, 1470, 743; HRMS (CI) calcd C₃₄H₃₈⁷⁹BrO [M + H]⁺: 541.2106, found: 541.2116.
4-(1-(4-Bromophenyl)-2-methyl-2-phenylpropyl)-2,6-di-tert-butylphenol (4i):
White solid; m.p. 69-72 °C; 78% yield (77 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.33 (d, \(J = 8.1\) Hz, 2H), 7.25 – 7.19 (m, 3H), 7.08 – 7.01 (m, 4H), 6.83 (s, 2H), 5.03 (s, 1H), 3.97 (s, 1H), 1.39 (s, 3H), 1.38 (s, 3H), 1.36 (s, 18H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 152.3, 147.0, 142.2, 134.7, 132.0, 131.7, 130.8, 128.0, 127.4, 126.9, 126.0, 120.0, 64.4, 42.3, 34.4, 30.4, 29.2, 28.4; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3639, 2957, 1436, 1009, 700; HRMS (CI) calcd C\(_{30}\)H\(_{38}\)BrO [M + H]\(^+\): 493.2106, found: 493.2087.

4-((1-Benzylcyclohexyl)(4-bromophenyl)methyl)-2,6-di-tert-butylphenol (4j):
White solid; m.p. 101-104 °C; 43% yield (47 mg); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\) 7.40 (d, \(J = 8.1\) Hz, 2H), 7.30 (d, \(J = 8.2\) Hz, 2H), 7.24 – 7.15 (m, 5H), 6.94 (d, \(J = 6.2\) Hz, 2H), 5.07 (s, 1H), 4.03 (s, 1H), 2.95 (d, \(J = 13.3\) Hz, 1H), 2.83 (d, \(J = 13.2\) Hz, 1H), 1.71 – 1.55 (m, 4H), 1.44 (s, 18H), 1.40 – 1.18 (m, 6H); \(^{13}\)C NMR (150 MHz, CDCl\(_3\)) \(\delta\) 152.2, 142.3, 138.9, 135.2, 132.5, 132.3, 131.5, 131.0, 127.6, 127.1, 125.9, 119.8, 56.4, 41.2, 34.5, 32.5, 32.4, 30.6, 25.8, 22.1, 22.0; FT-IR (thin film, KBr): \(\nu\) (cm\(^{-1}\)) 3638, 2924, 2862, 1436, 702; HRMS (CI) calcd C\(_{34}\)H\(_{44}\)BrO [M + H]\(^+\): 547.2576, found: 547.2575.
5. NMR Spectra for the substrates and products

$^1$H NMR of 1a

$^{13}$C NMR of 1a
$^1$H NMR of 1b

$^{13}$C NMR of 1b
$^1$H NMR of 1c

$^{13}$C NMR of 1c
$^1$H NMR of 1d

$^{13}$C NMR of 1d
$^1$H NMR of 1e

$^{13}$C NMR of 1e
$^1$H NMR of $1f$

$^{13}$C NMR of $1f$
$^1$H NMR of $^{13}$C NMR of $^{13}$C NMR of 1g
$^1$H NMR of 1h

$^{13}$C NMR of 1h
$^1$H NMR of 1i

$^{13}$C NMR of 1i
$^1$H NMR of 1j
$^{13}$C NMR of 1j

$^1$H NMR of 1k
$^{13}C$ NMR of 1k

$^1H$ NMR of 2a

$^{13}C$ NMR of 2a
$^1$H NMR of 2b

$^{13}$C NMR of 2b
$^1$H NMR of 2c

$^{13}$C NMR of 2c
$^1$H NMR of 2d

$^{13}$C NMR of 2d
$^1$H NMR of 2e

$^{13}$C NMR of 2e
$^1$H NMR of 2f

$^{13}$C NMR of 2f
$^{1}H$ NMR of $2g$

$^{13}C$ NMR of $2g$
$^1$H NMR of 2h

$^{13}$C NMR of 2h
$^1$H NMR of 2i

$^{13}$C NMR of 2i
$^1$H NMR of 2j

$^{13}$C NMR of 2j
$^1$H NMR of 2k
$^1$H NMR of 3a

$^{13}$C NMR of 3a
$^1$H NMR of 3b

$^{13}$C NMR of 3b
\(^1\)H NMR of 3c

\[^{13}\text{C} \text{ NMR of 3c}\]
$^1$H NMR of 3d

$^{13}$C NMR of 3d
$^1$H NMR of $3e$

$^{13}$C NMR of $3e$
$^1$H NMR of $3g$

$^{13}$C NMR of $3g$
$^1$H NMR of 3h

$^{13}$C NMR of 3h
$^1$H NMR of 3i

$^{13}$C NMR of 3i
$^1$H NMR of 3j

$^{13}$C NMR of 3j
$^1$H NMR of 3k

$^{13}$C NMR of 3k
$^1$H NMR of 4a

$^{13}$C NMR of 4a
$^1$H NMR of 4b

$^{13}$C NMR of 4b
$^1$H NMR of 4c

$^{13}$C NMR of 4c
$^1$H NMR of $4d$

$^{13}$C NMR of $4d$
$^1$H NMR of 4e

$^{13}$C NMR of 4e
$^{1}H$ NMR of 4f

$^{13}C$ NMR of 4f
$^1$H NMR of 4g

$^{13}$C NMR of 4g
$^1$H NMR of 4h

$^{13}$C NMR of 4h
$^1$H NMR of 4i

$^{13}$C NMR of 4i