SUPPORTING INFORMATION

FOR

Lewis Acid Mediated Reactions of Aldehydes with Styrene Derivatives: Synthesis of 1,3-Dihalo-1,3-diarylpropanes and 3-Chloro-1,3-diarylpropanols

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1,3-Dichloro-1-(4-fluorophenyl)-3-phenylpropane (1b): Colorless oil; ^1H NMR: δ 7.36–7.28 (m, 7H), 7.05–6.97 (m, 2H), 5.20 (dd, $J = 7.7, 7.6$ Hz, 0.5H), 5.17 (dd, $J = 6.7, 6.4$ Hz, 0.5H), 4.80–4.71 (m, 1H), 2.96–2.87 (m, 0.5H), 2.68–2.56 (m, 1.5H). ^{13}C NMR: δ 164.5, 160.6, 140.6, 139.9, 136.6, 135.9, 128.8, 128.7, 128.6, 127.0, 126.9, 116.0, 115.9, 115.6, 115.5, 60.6, 59.9, 59.3, 49.6, 49.5. Anal. Calcd for $\text{C}_{15}\text{H}_{13}\text{Cl}_2\text{F}$: C, 63.62; H, 4.63. Found: C, 63.77; H, 4.73.

1,3-Dichloro-1-(4-chlorophenyl)-3-phenylpropane (1c): Colorless oil; ^1H NMR: δ 7.37–7.20 (m, 9H), 5.20–5.13 (m, 1H), 4.78–4.70 (m, 1H), 2.98–2.86 (m, 0.5H), 2.67–2.56 (m, 1.5H). ^{13}C NMR: δ 140.5, 139.9, 139.3, 138.6, 134.6, 134.4, 129.0, 128.8, 128.7, 128.5, 128.4, 127.0, 126.9, 60.6, 59.9, 59.8, 59.2, 49.5, 49.4. Anal. Calcd for $\text{C}_{15}\text{H}_{13}\text{Cl}_3$: C, 60.13; H, 4.37. Found: C, 60.36; H, 4.45.

1,3-Dichloro-1-(4-bromophenyl)-3-phenylpropane (1d): Colorless oil; ^1H NMR: δ 7.47–7.20 (m, 9H), 5.20–5.11 (m, 1.5H), 4.76–4.70 (m, 0.5H), 2.97–2.85 (m, 0.25H), 2.66–2.54 (m, 1.75H). ^{13}C NMR: δ 140.5, 139.8, 139.7, 139.0, 131.9, 128.8, 128.7, 128.6, 126.9, 122.7, 122.5, 60.5, 59.8, 59.2, 49.4, 49.3. Anal. Calcd for $\text{C}_{15}\text{H}_{13}\text{BrCl}_2$: C, 52.36; H, 3.81. Found: C, 52.52; H, 3.88.

1,3-Dichloro-1-(2-fluorophenyl)-3-phenylpropane (1e): Colorless oil; ^1H NMR: δ 7.47–6.99 (m, 9H), 5.57 (dd, $J = 8.5, 8.3$ Hz, 0.6H), 5.23 (dd, $J = 9.0, 8.8$ Hz, 0.6H), 5.03 (dd, $J = 8.5, 8.4$ Hz, 0.4H), 4.91 (dd, $J = 9.0, 8.7$ Hz, 0.4H), 3.01–2.89 (m, 0.4H), 2.83–2.75 (m, 1.6H). ^{13}C NMR: δ 161.7, 161.5, 157.7, 157.6, 140.7, 139.7, 130.4, 130.3, 130.2, 128.8, 128.6, 128.0, 127.8, 127.3, 126.9, 124.6, 124.5, 116.0, 115.7, 60.6, 59.8,

53.8, 53.3, 53.2, 48.3, 48.1. Anal. Calcd for C₁₅H₁₃Cl₂F: C, 63.62; H, 4.63. Found: C, 63.65; H, 4.62.

1,3-Dichloro-1-(2-chlorophenyl)-3-phenylpropane (1f): Colorless oil; ¹H NMR: δ 7.54–7.20 (m, 9H), 5.81 (dd, J = 10.3, 10.2 Hz, 0.6H), 5.26 (dd, J = 10.4, 10.2 Hz, 0.6H), 5.11 (dd, J = 9.2, 9.1 Hz, 0.4H), 5.01 (dd, J = 8.5, 8.4 Hz, 0.4H), 2.83–2.45 (m, 2H). ¹³C–NMR: δ 140.7, 139.4, 138.0, 137.6, 132.4, 129.7, 129.5, 128.8, 128.7, 128.5, 127.4, 127.3, 127.2, 126.9, 60.6, 59.7, 56.8, 56.2, 48.5, 48.4. Anal. Calcd for C₁₅H₁₃Cl₃: C, 60.13; H, 4.37. Found: C, 60.55; H, 4.39.

1,3-Dichloro-1-(2-bromophenyl)-3-phenylpropane (1g): Colorless oil; ¹H NMR: δ 7.56–7.09 (m, 9H), 5.79 (dd, J = 10.5, 10.4 Hz, 0.6H), 5.26 (dd, J = 10.6, 10.4 Hz, 0.6H), 5.09–5.00 (m, 0.8H), 2.80–2.41 (m, 2H). ¹³C NMR: δ 140.7, 139.7, 139.3, 132.9, 129.8, 128.8, 128.6, 128.5, 128.1, 128.0, 127.3, 126.9, 122.7, 122.6, 60.6, 59.6, 59.4, 58.8, 48.6. Anal. Calcd for C₁₅H₁₃BrCl₂: C, 52.36; H, 3.81. Found: C, 52.39; H, 3.91.

1,3-Dichloro-1-(3-bromophenyl)-3-phenylpropane (1h): Colorless oil; ¹H NMR: δ 7.53–7.17 (m, 9H), 5.22–5.13 (m, 1H), 4.82–4.65 (m, 1H), 2.98–2.86 (m, 0.5H), 2.69–2.58 (m, 1.5H). ¹³C NMR: δ 142.9, 142.3, 140.5, 139.8, 131.9, 131.7, 130.4, 130.1, 128.9, 128.8, 128.7, 127.0, 126.9, 125.7, 122.8, 122.7, 60.6, 59.8, 59.7, 59.0, 49.6, 49.3. Anal. Calcd for C₁₅H₁₃BrCl₂: C, 52.36; H, 3.81. Found: C, 52.58; H, 3.89.

1,3-Dichloro-1-(*p*-tolyl)-3-phenylpropane (1i): Colorless oil; ¹H NMR: δ 7.36–7.14 (m, 9H), 5.21–5.14 (m, 0.8H), 4.81–4.74 (m, 1.2H), 3.02–2.90 (m, 0.6H), 2.72–2.61 (m, 1.4H), 2.34 (s, 3H). ¹³C NMR: δ 140.8, 140.2, 138.7, 138.6, 137.8, 137.1, 129.5, 129.4, 128.8, 128.7, 128.6, 127.0, 126.9, 60.7, 60.2, 60.1, 49.5, 49.4, 21.2. Anal. Calcd for C₁₆H₁₆Cl₂: C, 68.83; H, 5.78. Found: C, 69.23; H, 5.88.

1,3-Dichloro-1-(*o*-tolyl)-3-phenylpropane (1j): Colorless oil; ^1H NMR: δ 7.44–7.10 (m, 9H), 5.53–5.48 (m, 0.5H), 5.27–5.22 (m, 0.5H), 5.98 (dd, $J = 8.7, 8.4$ Hz, 0.5H), 4.88 (dd, $J = 7.6, 7.4$ Hz, 0.5 H), 3.01–2.89 (m, 0.5H), 2.74–2.60 (m, 1.5H), 2.34 (s, 1.5H), 2.16 (s, 1.5H). ^{13}C NMR: δ 140.7, 140.2, 138.6, 138.0, 135.4, 135.1, 130.7, 130.6, 128.7, 128.5, 128.4, 128.3, 127.0, 126.9, 126.7, 126.6, 126.5, 126.4, 60.9, 60.0, 56.9, 56.1, 48.6, 48.5, 18.9, 18.8. Anal. Calcd for $\text{C}_{16}\text{H}_{16}\text{Cl}_2$: C, 68.83; H, 5.78. Found: C, 69.31; H, 5.79.

1,3-Dichloro-1-(4-cyanophenyl)-3-phenylpropane (1k): Colorless oil; ^1H NMR: δ 7.68–7.34 (m, 9H), 5.28–5.19 (m, 1.2H), 4.79–4.73 (m, 0.8H), 3.00–2.88 (m, 0.4H), 2.70–2.53 (m, 1.6H). ^{13}C NMR: δ 145.8, 145.1, 140.3, 139.6, 132.7, 129.0, 128.9, 128.8, 127.9, 127.8, 127.0, 126.9, 118.2, 112.7, 112.5, 60.4, 59.6, 59.5, 58.7, 49.5, 49.3. Anal. Calcd for $\text{C}_{16}\text{H}_{13}\text{NCl}_2$: C, 66.22; H, 4.52; N, 4.83. Found: C, 66.42; H, 4.52; N, 4.79.

1,3-Dichloro-1-(4-nitrophenyl)-3-phenylpropane (1l): Pale-yellow oil; ^1H NMR: δ 8.21–7.23 (m, 9H), 5.33–5.21 (m, 1H), 4.85–4.74 (m, 1H), 3.01–2.89 (m, 0.5H), 2.72–2.60 (m, 1.5H). ^{13}C NMR: δ 147.8, 147.7, 147.4, 146.8, 140.2, 139.4, 128.9, 128.8, 128.7, 128.0, 127.9, 126.9, 126.8, 124.0, 60.3, 59.5, 59.1, 58.3, 49.3, 49.2. Anal. Calcd for $\text{C}_{15}\text{H}_{13}\text{NO}_2\text{Cl}_2$: C, 58.08; H, 4.22; N, 4.52. Found: C, 58.33; H, 4.33; N, 4.42.

1,3-Dichloro-1,3-di(4-fluorophenyl)propane (1m): Colorless crystals; m.p. 48–49 °C, ^1H NMR: δ 7.38–7.30 (m, 4H), 7.07–7.00 (m, 4H), 5.18 (t, $J = 7.0$ Hz, 1H), 4.75 (t, $J = 7.4$ Hz, 1H), 2.99–2.87 (m, 0.5H), 2.65–2.54 (m, 1.5H). ^{13}C NMR: δ 164.7, 164.6, 160.6, 136.6, 135.8, 128.9, 128.8, 128.7, 116.0, 115.9, 115.7, 115.6, 59.9, 59.2, 49.8, 49.6. Anal. Calcd for $\text{C}_{15}\text{H}_{12}\text{Cl}_2\text{F}_2$: C, 59.82; H, 4.02. Found: C, 60.03; H, 4.08.

1,3-Dichloro-1-(4-fluorophenyl)-3-(4-chlorophenyl)propane (1n): Colorless crystals; m.p. 43–44 °C, ^1H NMR: δ 7.38–7.24 (m, 6H), 7.08–7.01 (m, 2H), 5.20–5.13 (m, 1.2H), 4.76–4.70 (m, 0.8H), 2.98–2.85 (m, 0.4H), 2.64–2.53 (m, 1.6H). ^{13}C NMR: δ 164.7, 164.6, 160.6, 159.8, 139.1, 138.4, 136.5, 135.8, 134.6, 134.5, 129.1, 129.0, 128.9, 128.8, 128.7, 128.4, 116.0, 115.9, 115.7, 115.6, 59.8, 59.1, 49.6, 49.5. Anal. Calcd for $\text{C}_{15}\text{H}_{12}\text{Cl}_3\text{F}$: C, 56.72; H, 3.81. Found: C, 56.86; H, 3.81.

1,3-Dichloro-1-(4-fluorophenyl)-3-(4-bromophenyl)propane (1o): Colorless crystals; m.p. 49–50 °C, ^1H NMR: δ 7.50–7.00 (m, 8H), 5.20–5.12 (m, 1H), 4.76–4.69 (m, 1H), 2.97–2.85 (m, 0.5H), 2.64–2.53 (m, 1.5H). ^{13}C NMR: δ 164.6, 160.7, 160.6, 160.2, 139.6, 138.9, 136.5, 135.8, 132.0, 131.9, 128.9, 128.7, 122.8, 122.6, 116.0, 115.9, 115.7, 115.6, 59.8, 59.1, 49.6, 49.4. Anal. Calcd for $\text{C}_{15}\text{H}_{12}\text{Cl}_3\text{FBr}$: C, 49.70; H, 3.34. Found: C, 49.97; H, 3.36.

1,3-Dichloro-1-(4-fluorophenyl)-3-(2-fluorophenyl)propane (1p): Colorless oil; ^1H NMR: δ 7.48–7.00 (m, 8H), 5.57–5.52 (m, 0.6H), 5.25–5.19 (m, 0.6H), 5.01–4.89 (m, 0.8H), 2.99–2.87 (m, 0.4H), 2.79–2.62 (m, 1.6H). ^{13}C NMR: δ 164.7, 164.6, 161.5, 160.8, 160.6, 157.6, 136.7, 135.6, 130.5, 130.4, 130.3, 129.0, 128.8, 128.7, 128.6, 127.9, 127.6, 127.2, 124.6, 116.1, 115.9, 115.7, 115.6, 59.8, 59.0, 53.8, 53.2, 48.4, 48.2. Anal. Calcd for $\text{C}_{15}\text{H}_{12}\text{Cl}_2\text{F}_2$: C, 59.82; H, 4.02. Found: C, 59.99; H, 3.95.

1,3-Dichloro-1-(4-fluorophenyl)-3-(2-chlorophenyl)propane (1q): Colorless oil; ^1H NMR: δ 7.58–6.98 (m, 8H), 5.82–5.77 (m, 0.6H), 5.27–5.22 (m, 0.6H), 5.08–5.00 (m, 0.8H), 2.87–2.44 (m, 2H). ^{13}C NMR: δ 164.7, 164.5, 160.8, 160.6, 137.9, 136.7, 135.3, 132.5, 132.3, 129.7, 129.6, 129.2, 129.1, 128.8, 128.7, 128.5, 127.5, 127.4, 115.9, 115.8,

115.6, 115.5, 59.8, 58.8, 56.7, 56.1, 48.6. HRMS for $C_{15}H_{12}Cl_3F$ 315.9989. Found: 315.9976.

1,3-Dichloro-1-(4-fluorophenyl)-3-(2-bromophenyl)propane (1r): Colorless oil; 1H NMR: δ 7.59–6.98 (m, 8H), 5.79–5.74 (m, 0.5H), 5.28–5.22 (m, 0.5H), 5.09–4.98 (m, 1H), 2.82–2.40 (m, 2H). ^{13}C NMR: δ 164.7, 164.5, 160.8, 160.5, 139.6, 139.3, 136.7, 136.6, 135.2, 133.0, 129.9, 129.3, 129.2, 128.8, 128.7, 128.1, 128.0, 122.7, 122.5, 115.9, 115.6, 115.5, 59.8, 59.3, 58.8, 58.7, 48.7. Anal. Calcd for $C_{15}H_{12}Cl_3FBr$: C, 49.70; H, 3.34. Found: C, 49.60; H, 3.36.

1,3-Dichloro-1-(4-fluorophenyl)-3-(*p*-tolyl)propane (1s): Colorless oil; 1H NMR: δ 7.38–6.88 (m, 8H), 5.19–5.12 (m, 1H), 4.79–4.71 (m, 1H), 2.99–2.86 (m, 0.5H), 2.67–2.55 (m, 1.5H), 2.32 (s, 3H). ^{13}C NMR: δ 164.5, 160.6, 138.7, 137.7, 136.9, 136.7, 136.1, 136.0, 129.5, 129.4, 128.9, 128.8, 128.7, 126.9, 115.9, 115.8, 115.6, 115.5, 60.6, 59.9, 59.4, 49.6, 49.5, 21.1. Anal. Calcd for $C_{16}H_{15}Cl_2F$: C, 64.66; H, 5.09. Found: C, 64.69; H, 5.14.

1,3-Dichloro-1-(4-fluorophenyl)-3-(*o*-tolyl)propane (1t): Colorless oil; 1H NMR: δ 7.44–6.96 (m, 8H), 5.52–5.47 (m, 0.5H), 5.27–5.21 (m, 0.5H), 4.99–4.85 (m, 1H), 3.00–2.88 (m, 0.5H), 2.71–2.60 (m, 1.5H), 2.36 (s, 1.5H), 2.19 (s, 1.5H). ^{13}C NMR: δ 164.6, 164.5, 160.7, 160.6, 138.5, 137.9, 136.8, 136.7, 136.0, 135.4, 135.2, 130.8, 130.7, 128.9, 128.8, 128.7, 128.5, 128.4, 126.8, 126.5, 126.4, 115.9, 115.8, 115.6, 115.5, 60.2, 59.3, 56.9, 56.0, 48.8, 48.6, 19.0, 18.8. Anal. Calcd for $C_{16}H_{15}Cl_2F$: C, 64.66; H, 5.09. Found: C, 64.92; H, 5.04.

1,3-Dichloro-1-(4-fluorophenyl)-3-(4-nitrophenyl)propane (1u): Yellow crystals; m.p. 70–71 °C. 1H NMR: δ 8.21 (d, J = 8.7 Hz, 2H), 7.58 (d, J = 8.7 Hz, 2H), 7.40–7.34

(m, 2H), 7.09–7.01 (m, 2H), 5.34–5.22 (m, 1.2H), 4.84–4.75 (m, 0.8H), 3.01–2.89 (m, 0.4H), 2.70–2.54 (m, 1.6H). ^{13}C NMR: δ 164.7, 164.6, 160.7, 160.6, 147.9, 147.8, 147.4, 146.7, 136.2, 136.1, 135.4, 128.9, 128.8, 128.6, 128.1, 127.9, 124.0, 116.1, 115.9, 115.7, 115.6, 59.6, 59.1, 58.8, 58.2, 49.4, 49.2. Anal. Calcd for $\text{C}_{15}\text{H}_{13}\text{Cl}_2\text{FNO}_2$: C, 54.90; H, 3.69; N, 4.27. Found: C, 54.63; H, 3.68; N, 4.06.

1,3-Dichloro-1-(4-chlorophenyl)-3-(*p*-tolyl)propane (1v): White solid; m.p. 46–47 °C. ^1H NMR: δ 7.30–7.11 (m, 8H), 5.14 (t, $J = 7.0$ Hz, 1H), 4.72 (t, $J = 7.4$ Hz, 1H), 2.96–2.84 (m, 0.5H), 2.64–2.53 (m, 1.5H), 2.31 (s, 3H). ^{13}C NMR: δ 139.2, 138.7, 138.6, 138.5, 137.6, 136.9, 134.4, 134.3, 129.5, 128.9, 128.4, 128.3, 126.9, 126.8, 60.5, 59.9, 59.8, 59.2, 49.4, 49.3, 21.1. Anal. Calcd for $\text{C}_{16}\text{H}_{15}\text{Cl}_3$: C, 61.27; H, 4.82. Found: C, 61.48; H, 4.90.

1,3-Dichloro-1-(4-bromophenyl)-3-(*p*-tolyl)propane (1w): White solid; m.p. 54–56 °C. ^1H NMR: δ 7.45 (d, $J = 8.3$ Hz, 2H), 7.26–7.17 (m, 4H), 7.13 (d, $J = 8.2$ Hz, 2H), 5.16–5.10 (m, 1H), 4.75–4.69 (m, 1H), 2.96–2.84 (m, 0.5H), 2.65–2.53 (m, 1.5H), 2.32 (s, 3H). ^{13}C NMR: δ 139.7, 139.1, 138.7, 138.6, 137.5, 136.9, 131.9, 131.8, 129.5, 129.4, 128.7, 128.6, 127.6, 126.9, 126.8, 123.9, 122.6, 122.5, 60.5, 59.9, 59.2, 49.4, 49.2, 21.1. Anal. Calcd for $\text{C}_{16}\text{H}_{15}\text{Cl}_3\text{Br}$: C, 53.66; H, 4.22. Found: C, 53.90; H, 4.19.

1,3-Dichloro-1-(2-fluorophenyl)-3-(*p*-tolyl)propane (1x): Colorless oil; ^1H NMR: δ 7.47–6.99 (m, 8H), 5.55 (t, $J = 7.2$ Hz, 0.5H), 5.20 (t, $J = 6.7$ Hz, 0.5H), 5.01 (dd, $J = 8.7$, 8.4 Hz, 0.5H), 4.91 (t, $J = 7.2$ Hz, 0.5H), 3.00–2.88 (m, 0.5H), 2.82–2.73 (m, 0.5H), 2.67 (t, $J = 7.0$ Hz, 1H), 2.35 (s, 1.5H), 2.33 (s, 1.5H). ^{13}C NMR: δ 161.5, 157.6, 138.7, 138.5, 137.8, 136.7, 130.4, 130.2, 130.1, 129.5, 129.4, 127.2, 127.0, 126.8, 124.6, 116.0, 115.7,

60.6, 59.8, 53.9, 59.2, 53.4, 48.2, 47.9, 21.1. Anal. Calcd for $C_{16}H_{15}FCl_2$: C, 64.66; H, 5.09. Found: C, 64.69; H, 5.14.

1,3-Dichloro-1-(2-chlorophenyl)-3-(*p*-tolyl)propane (1y): Colorless oil; 1H NMR: δ 7.58–7.14 (m, 8H), 5.81 (dd, $J = 10.3, 10.1$ Hz, 0.6H), 5.24 (dd, $J = 10.4, 10.3$ Hz, 0.6H), 5.12 (dd, $J = 9.1, 8.9$ Hz, 0.4H), 5.01 (dd, $J = 8.7, 8.5$ Hz, 0.4H), 2.84–2.47 (m, 2H), 2.36 (s, 1.2H), 2.24 (s, 1.8H). ^{13}C NMR: δ 138.8, 138.5, 138.2, 137.9, 136.5, 132.6, 129.8, 129.5, 129.4, 128.5, 127.5, 127.4, 127.2, 126.9, 60.6, 59.7, 56.9, 56.3, 48.5, 48.3, 21.1. Anal. Calcd for $C_{16}H_{15}Cl_3$: C, 61.27; H, 4.82. Found: C, 61.47; H, 4.85.

1,3-Dichloro-1-(2-bromophenyl)-3-(*p*-tolyl)propane (1z): Colorless oil; 1H NMR: δ 7.59–7.09 (m, 8H), 5.79 (dd, $J = 10.5, 10.3$ Hz, 0.6H), 5.24 (dd, $J = 10.6, 10.3$ Hz, 0.6H), 5.10–4.99 (m, 0.8H), 2.80–2.42 (m, 2H), 2.32 (s, 3H). ^{13}C NMR: δ 139.8, 139.5, 138.7, 138.4, 137.8, 136.4, 132.9, 129.8, 129.4, 128.7, 128.1, 128.0, 127.3, 126.8, 122.7, 122.6, 60.6, 59.7, 58.9, 48.6, 48.4, 21.1. Anal. Calcd for $C_{16}H_{15}Cl_2Br$: C, 53.66; H, 4.22. Found: C, 53.84; H, 4.23.

1,3-Dichloro-1,3-di(*p*-tolyl)propane (1aa): Colorless oil; 1H NMR: δ 7.25–7.11 (m, 8H), 5.14 (t, $J = 6.8$ Hz, 1H), 4.76 (t, $J = 7.3$ Hz, 1H), 2.99–2.88 (m, 0.5H), 2.69–2.61 (m, 1.5H), 2.32 (s, 6H). ^{13}C NMR: δ 138.6, 138.4, 137.8, 137.2, 129.5, 126.9, 60.7, 60.2, 49.4, 49.3, 21.1. Anal. Calcd for $C_{17}H_{18}Cl_2$: C, 69.63; H, 6.19. Found: C, 69.78; H, 6.22.

1,3-Dichloro-1-(*o*-tolyl)-3-(*p*-tolyl)propane (1ab): Colorless oil; 1H NMR: δ 7.46–7.09 (m, 8H), 5.49 (t, $J = 7.2$ Hz, 0.5H), 5.23 (t, $J = 7.2$ Hz, 0.5H), 5.00 (dd, $J = 8.7, 8.3$ Hz, 0.5H), 4.88 (t, $J = 7.4$ Hz, 0.5H), 3.02–2.89 (m, 0.5H), 2.76–2.62 (m, 1.5H), 2.36 (s, 1.5H), 2.33 (s, 1.5H), 2.32 (s, 1.5H), 2.21 (s, 1.5H). ^{13}C NMR: δ 138.7, 138.5, 138.1, 137.9, 137.1, 135.6, 135.2, 130.7, 130.6, 129.5, 129.4, 128.4, 128.3, 126.9, 126.8, 126.7,

126.6, 126.5, 126.4, 60.9, 60.1, 57.1, 56.2, 48.6, 48.4, 21.1, 19.0. Anal. Calcd for $C_{17}H_{18}Cl_2$: C, 69.63; H, 6.19. Found: C, 69.78; H, 6.18.

1,3-Dichloro-1-(4-nitrophenyl)-3-(*p*-tolyl)propane (1ac): Yellow oil; 1H NMR: δ 8.19 (d, $J = 8.5$ Hz, 2H), 7.55 (d, $J = 8.5$ Hz, 2H), 7.28–7.15 (m, 4H), 5.31–5.26 (m, 0.5H), 5.22–5.16 (m, 0.5H), 4.83–4.73 (m, 1H), 3.00–2.88 (m, 0.5H), 2.70–2.59 (m, 1.5H), 2.34 (s, 3H). ^{13}C NMR: δ 147.8, 147.7, 147.5, 146.9, 138.9, 138.7, 137.3, 136.5, 129.6, 129.5, 128.0, 127.9, 126.9, 126.8, 123.9, 60.3, 59.6, 59.1, 58.4, 49.3, 49.1, 21.1. Anal. Calcd for $C_{16}H_{15}Cl_2NO_2$: C, 59.28; H, 4.66; N, 4.32. Found: C, 58.88; H, 4.65; N, 4.32.

1,3-Dichloro-1-(4-cyanophenyl)-3-(*p*-tolyl)propane (1ad): Colorless oil; 1H NMR: δ 7.68–7.12 (m, 8H), 5.26–5.15 (m, 1H), 4.75 (t, $J = 7.5$ Hz, 1H), 2.99–2.87 (m, 0.5H), 2.68–2.57 (m, 1.5H), 2.35 (s, 3H). ^{13}C NMR: δ 145.8, 145.2, 139.0, 138.8, 137.4, 136.6, 132.6, 129.6, 129.5, 127.9, 127.8, 126.9, 126.8, 118.2, 112.5, 60.3, 59.6, 59.5, 58.8, 49.4, 49.2, 21.1. Anal. Calcd for $C_{17}H_{15}Cl_2N$: C, 67.12; H, 4.97; N, 4.60. Found: C, 67.14; H, 5.02; N, 4.51.

1,3-Dibromo-1-(4-fluorophenyl)-3-phenylpropane (1af): Colorless oil; 1H NMR: δ 7.34–7.25 (m, 7H), 7.03–6.96 (m, 2H), 5.16 (t, $J = 7.1$ Hz, 1H), 4.83 (m, 1H), 3.24–3.11 (m, 0.5H), 2.90–2.78 (m, 1.5H). ^{13}C NMR: δ 164.4, 160.5, 140.7, 140.1, 136.9, 136.2, 129.3, 129.1, 128.9, 128.7, 127.4, 116.0, 115.7, 52.8, 52.0, 51.6, 50.6, 49.3, 49.1. Anal. Calcd for $C_{15}H_{13}Br_2F$: C, 48.42; H, 3.52. Found: C, 48.48; H, 3.51.

1,3-Dibromo-1-(*p*-tolyl)-3-phenylpropane (1ag): Colorless oil; 1H NMR: δ 7.31–7.10 (m, 9H), 5.15 (t, $J = 7.0$ Hz, 1H), 4.90–4.81 (m, 1H), 3.25–3.13 (m, 0.5H), 2.93–2.81 (m, 1.5H), 2.31 (s, 3H). ^{13}C NMR: δ 140.9, 140.4, 138.7, 138.6, 137.9, 137.3, 129.5, 128.8,

128.6, 127.3, 127.2, 53.0, 52.9, 52.0, 51.9, 49.2, 49.0, 21.2. Anal. Calcd for C₁₆H₁₆Br₂: C, 52.21; H, 4.38. Found: C, 52.31; H, 4.34.

1,3-Dibromo-1-(*p*-tolyl)-3-(4-fluorophenyl)propane (1ah): Colorless oil; ¹H NMR: δ 7.36–6.98 (m, 8H), 5.18–5.11 (m, 1H), 4.88–4.81 (m, 1H), 3.24–3.12 (m, 0.5H), 2.91–2.78 (m, 1.5H), 2.34 (s, 3H). ¹³C NMR: δ 164.5, 160.6, 138.9, 137.3, 136.9, 136.4, 129.6, 129.3, 129.2, 127.3, 116.0, 115.7, 52.9, 52.0, 51.8, 50.9, 49.3, 49.2, 21.2. Anal. Calcd for C₁₆H₁₅Br₂F: C, 49.77; H, 3.92. Found: C, 49.55; H, 3.92.

1,3-Dibromo-1-(*p*-tolyl)-3-(4-chlorophenyl)propane (1ai): Colorless oil; ¹H NMR: δ 7.31–7.11 (m, 8H), 5.14–5.08 (m, 1H), 4.85–4.79 (m, 1H), 3.22–3.09 (m, 0.5H), 2.89–2.76 (m, 1.5H), 2.32 (s, 3H). ¹³C NMR: δ 139.4, 138.9, 138.8, 137.7, 137.1, 134.4, 134.3, 129.6, 129.0, 128.7, 127.2, 52.8, 51.7, 50.6, 49.0, 48.9, 21.1. Anal. Calcd for C₁₆H₁₅Br₂Cl: C, 47.74; H, 3.76. Found: C, 48.20; H, 3.80.

1,3-Dibromo-1-(*p*-tolyl)-3-(4-bromophenyl)propane (1aj): Colorless oil; ¹H NMR: δ 7.47 (d, *J* = 8.2 Hz, 2H), 7.26–7.22 (m, 4H), 7.14 (d, *J* = 8.2 Hz, 2H), 5.10 (dd, *J* = 11.7, 10.7 Hz, 1H), 4.81 (d, *J* = 7.4 Hz, 1H), 3.22–3.10 (m, 0.5H), 2.90–2.77 (m, 1.5H), 2.34 (s, 3H). ¹³C NMR: δ 140.0, 139.4, 138.9, 138.8, 137.8, 137.2, 132.1, 129.6, 129.1, 127.2, 122.7, 52.8, 51.7, 50.7, 49.1, 48.9, 21.2. Anal. Calcd for C₁₆H₁₅Br₃: C, 42.99; H, 3.38. Found: C, 42.99; H, 3.77.

1,3-Dibromo-1,3-di(*p*-tolyl)propane (1ak): Colorless oil; ¹H NMR: δ 7.25 (d, *J* = 7.9 Hz, 4H), 7.14 (d, *J* = 7.9 Hz, 4H), 5.13 (t, *J* = 7.2 Hz, 1H), 4.86 (t, 7.5 Hz, 1H), 3.22–3.13 (m, 0.5H), 2.95–2.81 (m, 1.5H), 2.33 (s, 6H). ¹³C NMR: δ 138.7, 138.0, 137.5, 129.6, 127.3, 53.1, 52.1, 49.1, 21.2. Anal. Calcd for C₁₇H₁₈Br₂: C, 53.42; H, 4.75. Found: C, 53.74; H, 4.80.

1,3-Dibromo-1,3-di(4-fluorophenyl)propane (1al): Colorless crystals; m.p. 74–75 °C. ¹H NMR (*R,R/S,S*-isomers): δ 7.38–7.31 (m, 4H), 7.09–7.00 (m, 4H), 5.17 (t, J = 7.2 Hz, 2H), 2.86 (t, J = 7.2 Hz, 2H). ¹³C NMR: δ 164.6, 136.8, 129.3, 116.1, 115.7, 51.9, 49.4. ¹H NMR (*R,S/S,R*-isomers): δ 7.37–7.32 (m, 4H), 7.06–6.99 (m, 4H), 4.83 (t, J = 7.4 Hz, 2H), 3.23–3.10 (m, 1H), 2.88–2.76 (m, 1H). ¹³C NMR (*R,S/S,R*-isomers): δ 160.6, 136.1, 129.1, 116.1, 115.7, 50.6, 49.5. Anal. Calcd for C₁₅H₁₂Br₂F₂: C, 46.19; H, 3.10. Found: C, 46.15; H, 3.11.

1,3-Dibromo-1-(4-fluorophenyl)-3-(2-fluorophenyl)propane (1am): Colorless oil; ¹H NMR: δ 7.40–6.96 (m, 8H), 5.49 (dd, J = 8.8, 8.7 Hz, 0.5H), 5.20 (dd, J = 8.8, 8.7 Hz, 0.5H), 5.08–4.94 (m, 1H), 3.24 (m, 0.5H), 2.98–2.81 (m, 1.5H). ¹³C NMR: δ 164.5, 164.4, 161.5, 160.6, 160.5, 157.5, 136.8, 135.9, 135.8, 130.5, 130.4, 129.3, 129.2, 129.1, 128.9, 128.0, 127.8, 127.4, 124.7, 124.6, 116.2, 116.0, 115.9, 115.7, 115.6, 51.9, 50.3, 48.0, 47.9, 44.9, 44.8, 43.8. Anal. Calcd for C₁₅H₁₂Br₂F₂: C, 46.19; H, 3.10. Found: C, 46.31; H, 3.19.

1,3-Dibromo-1-(4-fluorophenyl)-3-(4-bromophenyl)propane (1an): Colorless crystals; m.p. 68–69 °C. ¹H NMR: δ 7.46 (d, J = 8.3 Hz, 2H), 7.38–7.31 (m, 2H), 7.23 (d, J = 8.3 Hz, 2H), 7.06–6.99 (m, 2H), 5.21–5.10 (m, 1H), 4.89–4.68 (m, 1H), 3.21–3.08 (m, 0.5H), 2.86–2.74 (m, 1.5H). ¹³C NMR: δ 164.5, 160.6, 160.5, 139.8, 139.2, 136.7, 132.1, 129.2, 129.1, 129.0, 122.8, 122.7, 116.1, 115.7, 51.8, 51.7, 50.5, 50.4, 49.2, 49.0. Anal. Calcd for C₁₅H₁₂Br₃F: C, 39.95; H, 2.68. Found: C, 40.15; H, 2.73.

1,3-Dibromo-1-(4-fluorophenyl)-3-(3-bromophenyl)propane (1ao): Colorless oil; ¹H NMR: δ 7.52–6.98 (m, 8H), 5.21–5.10 (m, 1H), 4.86 (t, J = 7.5 Hz, 0.5H), 4.72 (t, J = 7.1 Hz, 0.5H), 3.20–3.09 (m, 0.5H), 2.86–2.75 (m, 1.5H). ¹³C NMR: δ 164.5, 160.5,

143.0, 142.3, 136.7, 131.9, 131.8, 130.4, 129.2, 129.1, 126.0, 125.9, 125.8, 116.1, 116.0, 115.7, 51.9, 51.5, 50.4, 50.1, 49.1, 49.0. Anal. Calcd for C₁₅H₁₂Br₃F: C, 39.95; H, 2.68. Found: C, 39.82; H, 2.72.

1,3-Diiodo-1-(4-fluorophenyl)-3-phenylpropane (1aq): Yellow oil; ¹H NMR: δ 7.37–7.26 (m, 7H), 7.01–6.95 (m, 2H), 5.12–5.05 (m, 1H), 4.96 (dd, *J* = 7.9, 7.8 Hz, 1H), 3.31–3.18 (m, 0.5H), 2.97 (t, *J* = 7.6 Hz, 1H), 2.76–2.65 (m, 0.5H). ¹³C NMR: δ 164.1, 160.1, 142.2, 141.9, 138.3, 138.0, 129.0, 128.4, 127.3, 127.2, 116.0, 115.7, 51.9, 51.6, 30.9, 30.6, 30.0, 29.6. HRMS calcd for C₁₅H₁₃FI₂ 465.9091. Found 465.9088.

1,4-Di[1',3'-dichloro-3'-(*p*-tolyl)propyl]benzene (7b): Colorless oil; ¹H NMR: δ 7.60–7.15 (m, 12H), 5.20–5.14 (m, 2H), 4.83–4.71 (m, 2H), 3.00–2.88 (m, 1H), 2.68–2.60 (m, 3H), 2.34 (s, 6H). ¹³C NMR: δ 141.3, 141.2, 140.7, 140.6, 138.7, 138.6, 137.7, 136.9, 129.5, 127.5, 126.9, 126.8, 60.6, 60.2, 59.9, 59.6, 49.5, 49.2, 21.1. Anal. Calcd for C₂₆H₂₆Cl₄: C, 65.02; H, 5.46. Found: C, 65.38; H, 5.38.

1,4-Di[1',3'-dichloro-3'-(4-fluorophenylpropyl)]benzene (7c): Colorless crystals; m.p. 142–143 °C. ¹H NMR (*R,R,S,S/S,S,R,R*-isomers): δ 7.40–7.34 (m, 8H), 7.09–7.02 (m, 4H), 5.21 (t, *J* = 6.7 Hz, 4H), 2.62 (t, *J* = 6.7 Hz, 4H). ¹³C NMR (*R,R,S,S/S,S,R,R*-isomers): δ 164.6, 160.7, 141.2, 136.6, 128.8, 128.7, 127.5, 116.0, 115.6, 60.0, 59.8, 49.7. ¹H NMR (*R,S,S,R/S,R,R,S*-isomers): δ 7.38–7.34 (m, 8H), 7.06–7.00 (m, 4H), 4.83–4.69 (m, 4H), 2.99–2.87 (m, 2H), 2.67–2.57 (m, 2H). ¹³C NMR (*R,S,S,R/S,R,R,S*-isomers): δ 164.5, 160.6, 141.1, 140.6, 140.4, 135.7, 128.9, 127.5, 115.9, 115.5, 59.3, 59.1, 49.3. Anal. Calcd for C₂₄H₂₀Cl₄F₂: C, 59.04; H, 4.13. Found: C, 59.24; H, 4.28.

1,1,1-Tribromo-4-chloro-4-(*p*-tolyl)butan-2-ol (9b): Wax; ¹H NMR (*2R,4R/2S,4S*-isomers): δ 7.33 (d, *J* = 7.8 Hz, 2H), 7.18 (d, *J* = 7.8 Hz, 2H), 5.24 (dd, *J* = 11.7, 11.6 Hz,

1H), 4.45 (dd, $J = 9.8, 9.7$ Hz, 1H), 3.02–2.88 (m, 1H), 2.36 (s, 3H), 2.26–2.16 (m, 1H). ^{13}C NMR (2*R*,4*R*/2*S*,4*S*-isomers): δ 138.5, 136.2, 129.4, 126.8, 81.8, 60.1, 53.5, 42.6, 21.2. ^1H NMR (2*R*,4*S*/2*S*,4*R*-isomers): δ 7.32 (d, $J = 7.7$ Hz, 2H), 7.17 (d, $J = 7.7$ Hz, 2H), 5.16 (dd, $J = 11.4, 11.2$ Hz, 1H), 3.52 (dd, $J = 9.8, 9.6$ Hz, 1H), 3.11–2.98 (m, 1H), 2.62–2.50 (m, 1H), 2.37 (s, 3H). ^{13}C NMR (2*R*,4*S*/2*S*,4*R*-isomers): δ 139.7, 129.0, 128.8, 127.3, 81.5, 59.1, 53.3, 42.3, 21.2. Anal. Calcd for $\text{C}_{11}\text{H}_{12}\text{Br}_3\text{ClO}$: C, 30.35; H, 2.78. Found: C, 30.27; H, 2.82.

1,1,1-Tribromo-4-bromo-4-(p-tolyl)butan-2-ol (9c): Wax; ^1H NMR (2*R*,4*R*/2*S*,4*S*-isomers): δ 7.33 (d, $J = 7.6$ Hz, 2H), 7.18 (d, $J = 7.6$ Hz, 2H), 5.31 (dd, $J = 12.0, 11.8$ Hz, 1H), 4.45 (dd, $J = 9.6, 9.5$ Hz, 1H), 3.12–3.05 (m, 1H), 2.33 (s, 3H), 2.27–2.03 (m, 1H). ^{13}C NMR (2*R*,4*R*/2*S*,4*S*-isomers): δ 138.5, 136.9, 129.6, 127.4, 82.7, 53.3, 52.3, 42.1, 21.2. ^1H NMR (2*R*,4*S*/2*S*,4*R*-isomers): δ 7.32 (d, $J = 7.6$ Hz, 2H), 7.17 (d, $J = 7.6$ Hz, 2H), 5.25 (dd, $J = 11.8, 11.7$ Hz, 1H), 3.50 (dd, $J = 9.7, 9.6$ Hz, 1H), 3.22–3.08 (m, 1H), 2.71–2.60 (m, 1H), 2.33 (s, 3H). ^{13}C NMR (2*R*,4*S*/2*S*,4*R*-isomers): δ 138.8, 136.5, 129.4, 127.1, 81.6, 53.0, 49.4, 42.5, 21.2. HRMS for $\text{C}_{11}\text{H}_{12}\text{Br}_4\text{O}$ 475.7622. Found: 475.7609.

1,3-Dichloro-1-(4-fluorophenyl)-2-methyl-3-phenylpropane (10b): White solid; m.p. 76–77 °C. ^1H NMR (three pairs of diastereomers): δ 7.47–7.28 (m, 7H), 7.09–6.97 (m, 2H), 5.89 (s, 0.5H) 5.03 (d, $J = 7.0$ Hz, 0.2H), 4.96–4.90 (m, 0.5H), 4.72 (d, $J = 6.3$ Hz, 0.8H), 2.86–2.77 (m, 0.2H), 2.55–2.46 (m, 0.8H), 1.20 (d, $J = 6.5$ Hz, 1.2H), 0.73 (d, $J = 7.0$ Hz, 0.3H), 0.64 (d, $J = 6.7$ Hz, 1.5H). ^{13}C NMR (three pairs of diastereomers): δ 164.5, 164.3, 164.1, 160.5, 160.4, 160.2, 139.9, 139.8, 138.1, 135.9, 135.8, 133.9, 129.8, 129.7, 129.4, 129.3, 129.0, 128.9, 128.7, 128.5, 128.3, 127.9, 127.8, 127.6, 127.2, 115.8, 115.7,

115.5, 115.4, 115.1, 115.0, 66.5, 65.9, 64.7, 63.9, 49.9, 49.5, 49.1, 11.9, 10.8. Anal. Calcd for C₁₆H₁₅Cl₂F: C, 64.66; H, 5.09. Found: C, 64.56; H, 5.11.

1,3-Dichloro-1-(4-bromophenyl)-2-methyl-3-phenylpropane (10c): White solid; m.p. 78–80 °C. ¹H NMR (1*R*,2*S*,3*R*/1*S*,2*R*,3*S*-isomers): δ 7.48 (d, *J* = 8.4 Hz, 2H), 7.35–7.27 (m, 5H), 7.22 (d, *J* = 8.4 Hz, 2H), 4.70 (d, *J* = 6.4 Hz, 2H), 2.54–2.46 (m, 1H), 1.20 (d, *J* = 6.4 Hz, 3H). ¹³C NMR (1*R*,2*S*,3*R*/1*S*,2*R*,3*S*-isomers): δ 139.7, 138.9, 131.7, 128.9, 128.6, 128.3, 127.2, 122.2, 65.8, 65.1, 49.8, 10.9. ¹H NMR (other two pairs of diastereomers): δ 7.50–7.20 (m, 9H), 5.87 (s, 0.9H), 5.02 (d, *J* = 6.9 Hz, 0.2H), 4.97–4.88 (m, 0.9H), 2.85–2.77 (m, 0.2H), 2.54–2.42 (m, 0.8H), 0.72 (d, *J* = 6.9 Hz, 0.3H), 0.63 (d, *J* = 6.6 Hz, 2.7H). ¹³C NMR (other two pairs of diastereomers): δ 139.8, 139.0, 131.9, 131.5, 131.4, 129.7, 129.3, 128.7, 128.5, 128.4, 128.3, 127.9, 127.6, 122.4, 121.7, 66.4, 65.6, 64.7, 63.7, 49.2, 48.9, 11.9, 10.7. Anal. Calcd for C₁₆H₁₅Cl₂Br: C, 53.66; H, 4.22. Found: C, 53.27; H, 4.27.

1,3-Dichloro-1-(4-chlorophenyl)-2,3-diphenylpropane (10d): Wax; ¹H NMR (three pairs of diastereomers): δ 7.25–6.96 (m, 14H), 6.80–6.77 (m, 0.6H), 6.57–6.55 (m, 0.4H), 6.03 (d, *J* = 3.3 Hz, 0.2H), 5.59–5.47 (m, 0.8H), 4.04–3.99 (m, 0.5H), 3.65–3.59 (m, 0.5H). ¹³C NMR (three pairs of diastereomers): δ 139.1, 138.0, 137.7, 136.4, 134.1, 133.8, 133.7, 131.0, 130.3, 129.8, 129.3, 128.5, 128.4, 128.3, 128.2, 128.0, 127.9, 127.6, 127.5, 127.1, 64.4, 63.7, 63.3, 62.5, 60.8, 60.5. HRMS for C₂₁H₁₇Cl₃ 374.0396. Found: 374.0388.

1,3-Dichloro-1-(4-bromophenyl)-2,3-diphenylpropane (10e): Wax; ¹H NMR (three pairs of diastereomers): δ 7.35–6.97 (m, 14H), 6.79–6.77 (m, 0.7H), 6.57–6.55 (m, 0.3H), 6.04–6.02 (m, 0.3H), 5.61–5.46 (m, 0.7H), 4.05–3.97 (m, 0.4H), 3.64–3.59 (m, 0.6H). ¹³C

NMR (three pairs of diastereomers): δ 139.2, 139.0, 138.5, 137.7, 134.1, 133.6, 131.4, 131.1, 130.9, 130.3, 130.0, 129.5, 129.3, 129.2, 128.5, 128.3, 128.2, 128.1, 128.0, 127.9, 127.5, 127.4, 127.1, 122.3, 122.0, 64.5, 64.3, 63.8, 63.7, 63.2, 62.5, 60.7, 60.4. Anal. Calcd for $C_{21}H_{17}Cl_2Br$: C, 60.03; H, 4.08. Found: C, 60.26; H, 4.12.

3-Chloro-1-(4-fluorophenyl)-3-phenylpropanol (6b): white solid; m.p 75–76 °C. 1H NMR (*R,R/S,S*-isomers): δ 7.26–7.04 (m, 7H), 7.05–6.98 (m, 2H), 5.21 (dd, $J = 9.8, 9.7$ Hz, 1H), 5.03 (dd, $J = 8.8, 8.6$ Hz, 1H), 2.34–2.28 (m, 2H), 2.15 (s, 1H). ^{13}C NMR (*R,R/S,S*-isomers): δ 164.2, 160.3, 141.5, 139.7, 128.7, 128.4, 127.5, 127.4, 126.9, 115.6, 115.3, 70.7, 60.5, 48.9. Anal. Calcd for $C_{15}H_{14}FCIO$: C, 68.06; H, 5.33. Found: C, 68.26; H, 5.25.

3-Chloro-1-(4-chlorophenyl)-3-phenylpropanol (6c): white solid; m.p. 81–82 °C. 1H NMR (*R,R/S,S*-isomers): δ 7.39–7.22 (m, 9H), 5.21 (dd, $J = 10.0, 9.7$ Hz, 1H), 5.02 (dd, $J = 8.9, 8.6$ Hz, 1H), 2.35–2.14 (m, 3H). ^{13}C NMR (*R,R/S,S*-isomers): δ 142.4, 141.4, 133.4, 128.7, 128.4, 127.1, 126.9, 70.7, 60.4, 48.8. Anal. Calcd for $C_{15}H_{14}OCl_2$: C, 64.07; H, 5.02. Found: C, 64.02; H, 5.13.

3-Chloro-1-(4-bromophenyl)-3-phenylpropanol (6d): white solid; m.p. 86–87 °C. 1H NMR (*R,R/S,S*-isomers): δ 7.42 (d, $J = 8.4$ Hz, 2H), 7.31–7.23 (m, 5H), 7.17 (d, $J = 8.4$ Hz, 2H), 5.18 (dd, $J = 10.1, 10.0$ Hz, 1H), 4.97 (dd, $J = 9.2, 8.8$ Hz, 1H), 2.45 (s, 1H), 2.33–2.20 (m, 2H). ^{13}C NMR (*R,R/S,S*-isomers): δ 142.7, 141.1, 131.5, 128.5, 128.2, 127.3, 126.7, 121.4, 70.5, 60.2, 48.5. Anal. Calcd for $C_{15}H_{14}OBrCl$: C, 55.33; H, 4.33. Found: C, 55.32; H, 4.32.

3-Chloro-1-(*p*-tolyl)-3-phenylpropanol (6e): Colorless oil; 1H NMR (*R,R/S,S*-isomers): δ 7.40–7.07 (m, 9H), 5.20 (dd, $J = 8.9, 8.7$ Hz, 1H), 4.97 (dd, $J = 8.0, 7.9$ Hz,

1H), 2.37–2.30 (m, 5H), 2.16 (s, 1H). ¹³C NMR (*R,R/S,S*-isomers): δ 141.7, 140.9, 137.6, 129.3, 128.6, 128.2, 127.0, 125.7, 71.2, 60.6, 48.7, 21.1. Anal. Calcd for C₁₆H₁₇OCl: C, 73.70; H, 6.57. Found: C, 73.45; H, 6.64.

3-Chloro-1-(*o*-tolyl)-3-phenylpropanol (6f): Colorless oil; ¹H NMR (*R,R/S,S*-isomers): δ 7.42–7.13 (m, 9H), 5.35–5.29 (m, 2H), 2.35 (s, 3H), 2.30–2.08 (m, 3H). ¹³C NMR (*R,R/S,S*-isomers): δ 141.7, 134.2, 130.4, 128.6, 128.2, 127.4, 126.9, 126.3, 124.9, 67.8, 61.0, 47.8, 18.9. Anal. Calcd for C₁₆H₁₇OCl: C, 73.70; H, 6.57. Found: C, 73.85; H, 6.78.

3-Chloro-1-(2-fluorophenyl)-3-phenylpropanol (6g): Colorless oil; ¹H NMR (*R,R/S,S*-isomers): δ 7.42–7.00 (m, 9H), 5.37 (d, *J* = 9.3 Hz, 1H), 5.25 (dd, *J* = 10.6, 3.5 Hz, 1H), 2.43–2.30 (m, 3H). ¹³C NMR (*R,R/S,S*-isomers): δ 161.6, 157.7, 141.6, 129.2, 129.1, 128.6, 128.3, 127.2, 127.1, 126.9, 124.4, 115.6, 115.3, 65.7, 60.4, 47.3. HRMS for C₁₅H₁₄FCIO 264.0717. Found: 264.0723.

3-Chloro-1-(4-nitrophenyl)-3-phenylpropanol (6h): Yellow solid; m.p. 50–51 °C. ¹H NMR (*R,R/S,S*-isomers): δ 8.18 (d, *J* = 8.6 Hz, 2H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.41–7.24 (m, 5H), 5.30–5.21 (m, 2H), 2.45 (s, 1H), 2.32–2.19 (m, 2H). ¹³C NMR (*R,R/S,S*-isomers): δ 151.3, 147.4, 141.1, 128.6, 128.5, 126.9, 126.4, 123.8, 70.6, 60.3, 48.9. Anal. Calcd for C₁₅H₁₄NO₃Cl: C, 61.76; H, 4.84; N, 4.80. Found: C, 61.84; H, 4.84; N, 4.55.

3-Chloro-1-(4-cyanophenyl)-3-phenylpropanol (6i): a pale-yellow solid; m.p. 54–55 °C. ¹H NMR (*R,R/S,S*-isomers): δ 7.60–7.26 (m, 9H), 5.26 (dd, *J* = 10.7, 10.6 Hz, 1H), 5.15 (d, *J* = 9.6 Hz, 1H), 2.94 (s, 1H), 2.40–2.15 (m, 2H). ¹³C NMR (*R,R/S,S*-isomers): δ 149.5, 141.1, 132.3, 128.9, 128.4, 126.8, 126.3, 118.6, 111.0, 70.4, 60.2, 48.8. Anal. Calcd for C₁₆H₁₄NOCl: C, 72.72; H, 5.19; N, 5.15. Found: C, 70.63; H, 5.34; N, 4.95.

3-Chloro-1-(4-carboxyphenyl)-3-phenylpropanol (6j): Yellow solid; m.p. 43–44.5 °C. ^1H NMR (*R,R/S,S*-isomers): δ 9.97 (s, 1H), 7.85 (d, J = 8.1 Hz, 2H), 7.65 (d, J = 8.1 Hz, 2H), 7.56–7.06 (m, 5H), 5.28 (dd, J = 10.4, 10.3 Hz, 1H), 5.18 (dd, J = 9.6, 9.5 Hz, 1H), 2.95 (s, 1H), 2.44–2.21 (m, 2H). ^{13}C NMR (*R,R/S,S*-isomers): δ 191.8, 150.9, 141.5, 135.8, 130.5, 130.0, 128.7, 127.1, 126.2, 70.9, 60.4, 48.9. Anal. Calcd for $\text{C}_{16}\text{H}_{15}\text{O}_2\text{Cl}$: C, 69.95; H, 5.50. Found: C, 69.82; H, 5.45.

3-Chloro-1-(4-nitrophenyl)-3-(4-chlorophenyl)propanol (6k): Solid; m.p. 53–55 °C. ^1H NMR (*R,R/S,S*-isomers): δ 8.15 (d, J = 8.7 Hz, 2H), 7.54 (d, J = 8.7 Hz, 2H), 7.35–7.26 (m, 4H), 5.29–5.20 (m, 2H), 2.70 (s, 1H), 2.39–2.14 (m, 2H). ^{13}C NMR (*R,R/S,S*-isomers): δ 151.3, 147.1, 139.6, 134.1, 128.8, 128.2, 126.3, 123.7, 70.3, 59.3, 48.6. Anal. Calcd for $\text{C}_{15}\text{H}_{13}\text{NO}_3\text{Cl}_2$: C, 55.23; H, 4.02; N, 4.29. Found: C, 55.51; H, 4.34; N, 4.51.

3-Chloro-1-(4-chlorophenyl)-3-(4-chlorophenyl)propanol (6l): Solid; m.p. 74–76 °C. ^1H NMR (*R,R/S,S*-isomers): δ 7.32–7.24 (m, 8H), 5.17 (dd, J = 9.8, 9.7 Hz, 1H), 5.00 (dd, J = 8.8, 8.7 Hz, 1H), 2.46 (s, 1H), 2.35–2.14 (m, 2H). ^{13}C NMR (*R,R/S,S*-isomers): δ 142.2, 139.9, 134.1, 133.6, 128.9, 128.8, 128.3, 127.1, 70.6, 59.5, 48.7. Anal. Calcd for $\text{C}_{15}\text{H}_{13}\text{OCl}_3$: C, 57.08; H, 4.15. Found: C, 57.33; H, 4.34.

3-Chloro-1-(4-nitrophenyl)-3-(*p*-tolyl)propanol (6m): Yellow Solid; m.p. 61–63 °C. ^1H NMR (*R,R/S,S*-isomers): δ 8.16 (d, J = 8.6 Hz, 2H), 7.54–7.12 (m, 6H), 5.27–5.18 (m, 2H), 2.68 (s, 1H), 2.63–2.12 (m, 5H). ^{13}C NMR (*R,R/S,S*-isomers): δ 151.3, 147.1, 138.2, 138.0, 129.3, 126.7, 126.4, 123.6, 70.4, 59.7, 48.6, 20.9. Anal. Calcd for $\text{C}_{16}\text{H}_{16}\text{NO}_3\text{Cl}$: C, 62.85; H, 5.27; N, 4.58. Found: C, 62.54; H, 5.34; N, 4.37.

3-Chloro-1-phenyl-3-(*p*-tolyl)propanol (6n): Wax; ^1H NMR (*R,R/S,S*-isomers): δ 7.32–7.10 (m, 9H), 5.18 (dd, $J = 9.8, 9.7$ Hz, 1H), 4.98 (dd, $J = 9.0, 8.9$ Hz, 1H), 2.58 (s, 1H), 2.37–2.24 (m, 5H). ^{13}C NMR (*R,R/S,S*-isomers): δ 143.9, 138.6, 138.1, 129.3, 128.5, 127.7, 126.8, 125.9, 71.3, 60.5, 48.7, 21.1. HRMS for $\text{C}_{16}\text{H}_{17}\text{OCl}$ 260.0968. Found: 260.0971.

3-Chloro-1-(4-cyanophenyl)-3-(*p*-tolyl)propanol (6o): Yellow solid; m.p. 63–66 °C. ^1H NMR (*R,R/S,S*-isomers): δ 7.58 (d, $J = 8.2$ Hz, 2H), 7.47 (d, $J = 8.2$ Hz, 2H), 7.27–7.12 (m, 4H), 5.23 (dd, $J = 10.6, 10.5$ Hz, 1H), 5.13 (dd, $J = 9.7, 9.6$ Hz, 1H), 2.85 (s, 1H), 2.36–2.20 (m, 5H). ^{13}C NMR (*R,R/S,S*-isomers): δ 149.6, 138.3, 132.3, 129.3, 127.4, 126.7, 126.4, 118.6, 110.9, 70.5, 60.3, 48.7, 21.0. Anal. Calcd for $\text{C}_{17}\text{H}_{16}\text{NOCl}$: C, 71.45; H, 5.64. Found: C, 71.74; H, 5.77.

3-Chloro-1-(3-pyridinyl)-3-(4-fluorophenyl)propanol (11b): yellow oil; ^1H NMR (*R,R/S,S*-isomers): δ 9.30 (s, 1H), 9.16 (s, 1H), 8.27 (t, $J = 10.0$ Hz, 1H), 7.81 (t, $J = 7.5$ Hz, 1H), 7.43–7.35 (m, 2H), 7.09–6.89 (m, 2H), 5.41–5.27 (m, 1H), 5.07 (t, $J = 7.8$ Hz, 0.5 H), 4.68 (t, $J = 8.5, 0.5$ H), 2.84 (s, 1H), 2.78–2.67 (m, 0.5 H), 2.48–2.24 (m, 1.5H). ^{13}C NMR (*R,R/S,S*-isomers): δ 164.6, 164.4, 160.6, 160.5, 143.8, 143.7, 143.3, 142.7, 142.4, 142.2, 141.6, 141.4, 136.4, 135.8, 127.0, 126.8, 126.0, 116.1, 115.9, 115.8, 115.5, 68.8, 68.2, 58.9, 58.5, 46.6, 46.3. HRMS for $\text{C}_{14}\text{H}_{13}\text{ClFNO}$ 265.0670. Found: 265.0667.

3-Chloro-3-(4-chlorophenyl)-1-(3-pyridinyl)propanol (11c): yellow solid; m.p. 97–98 °C. ^1H NMR (*R,R/S,S*-isomers): δ 9.36 (s, 1H), 9.24 (s, 1H), 8.38 (s, 1H), 7.76 (t, $J = 8.0$ Hz, 1H), 7.42–7.22 (m, 4H), 5.74 (dd, $J = 10.1, 9.8$ Hz, 1H), 5.34 (t, $J = 9.0$ Hz, 1H), 2.88 (s, 1H), 2.43–2.27 (m, 2H). ^{13}C NMR (*R,R/S,S*-isomers): δ 145.6, 144.5, 138.3,

137.8, 136.3, 131.2, 128.9, 127.1, 123.2, 69.2, 54.9, 46.8. Anal. Calcd for C₁₄H₁₃Cl₂NO: C, 59.59; H, 4.64; N, 4.96. Found: C, 59.80; H, 4.47; N, 5.11.

3-Chloro-3-(2-chlorophenyl)-1-(3-pyridinyl)propanol (11d): yellow solid; m.p. 128–129 °C. ¹H NMR (*R,R/S,S*-isomers): δ 9.34 (s, 1H), 9.24 (s, 1H), 8.34 (t, *J* = 8.0 Hz, 1H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.60 (d, *J* = 10.0 Hz, 1H), 7.39–7.25 (m, 3H), 5.83 (dd, *J* = 8.5, 8.2 Hz, 1H), 5.42 (t, *J* = 7.4 Hz, 1H), 2.78 (s, 1H), 2.39–2.33 (m, 2H). ¹³C NMR (*R,R/S,S*-isomers): δ 143.6, 143.5, 142.2, 142.1, 141.5, 137.5, 132.2, 129.7, 128.5, 127.8, 127.6, 125.9, 68.1, 55.9, 47.3. Anal. Calcd for C₁₄H₁₃Cl₂NO: C, 59.59; H, 4.64; N, 4.96. Found: C, 59.76; H, 4.62; N, 5.02.

3-Chloro-1-(3-pyridinyl)-3-(*p*-tolyl)propanol (11e): yellow oil; ¹H NMR (*R,R/S,S*-isomers): δ 9.28 (s, 1H), 9.17 (s, 1H), 8.25 (t, *J* = 7.7 Hz, 1H), 7.76 (t, *J* = 7.3 Hz, 1H), 7.30–7.03 (m, 4H), 5.34 (d, *J* = 7.5 Hz, 1H), 5.21 (dd, *J* = 7.8, 7.5 Hz, 1H), 2.74–2.68 (m, 2H), 2.47–2.25 (m, 2H). ¹³C NMR (*R,R/S,S*-isomers): δ 143.7, 143.4, 142.3, 138.7, 137.5, 136.7, 129.5, 127.3, 126.8, 126.0, 68.4, 59.8, 48.5, 21.1. Anal. Calcd for C₁₅H₁₆ClNO: C, 68.83; H, 6.16; N, 5.35. Found: C, 68.93; H, 6.42; N, 5.48.

3-Chloro-1-(4-chlorophenyl)-2-methyl-3-phenylpropanol (12b): Colorless oil; ¹H NMR (*R,R,R/S,S,S*-isomers): δ 7.32–7.18 (m, 9H), 5.50 (d, *J* = 2.1 Hz, 1H), 4.98 (d, *J* = 10.4 Hz, 1H), 2.39 (s, 1H), 0.58 (d, *J* = 6.9 Hz, 3H). ¹³C NMR (*R,R,R/S,S,S*-isomers): δ 141.8, 140.5, 132.6, 128.6, 128.3, 127.4, 126.9, 71.9, 66.5, 48.0, 9.9. Anal. Calcd for C₁₆H₁₆Cl₂O: C, 65.10; H, 5.46. Found: C, 64.88; H, 5.40.

3-Chloro-2-methyl-1-(4-methylphenyl)-3-phenylpropanol (12c): Colorless oil; ¹H NMR (*R,R,R/S,S,S*-isomers): δ 7.37–7.14 (m, 9H), 5.51 (s, 1H), 5.00 (d, *J* = 10.3 Hz, 1H), 2.35–2.28 (m, 4H), 2.15 (bs, 1H), 0.53 (d, *J* = 7.0 Hz, 3H). ¹³C NMR (*R,R,R/S,S,S*-

isomers): δ 140.9, 140.5, 136.6, 128.9, 128.6, 128.2, 126.9, 125.5, 72.4, 66.6, 48.1, 21.1, 10.0. HRMS for $C_{17}H_{19}ClO$ 274.1124. Found: 274.1129.

3-Chloro-2-methyl-1-(4-nitrophenyl)-3-phenylpropanol (12d): Yellow crystals; m.p. 121–122 °C. 1H NMR (*R,R,R/S,S,S*-isomers): δ 8.17 (d, J = 8.6 Hz, 2H), 7.57 (d, J = 8.6 Hz, 2H), 7.43–7.24 (m, 5H), 5.69 (s, 1H), 5.05 (d, J = 10.4 Hz, 1H), 2.84 (bs, 1H), 2.46–2.34 (m, 1H), 0.49 (d, J = 6.9 Hz, 3H). ^{13}C NMR (*R,R,R/S,S,S*-isomers): δ 151.3, 146.7, 128.6, 128.2, 127.4, 126.3, 123.3, 71.8, 66.3, 47.9, 9.8. Anal. Calcd for $C_{16}H_{16}ClNO_3$: C, 62.85; H, 5.27; N, 4.58. Found: C, 62.65; H, 5.11; N, 4.55.

3-Chloro-1-(4-cyanophenyl)-2-methyl-3-phenylpropanol (12e): Colorless crystals; m.p. 153–154 °C. 1H NMR (*R,R,R/S,S,S*-isomers): δ 7.65 (d, J = 8.4 Hz, 2H), 7.52 (d, J = 8.4 Hz, 2H), 7.39–7.31 (m, 5H), 5.65 (s, 1H), 5.02 (d, J = 10.3 Hz, 1H), 2.40–2.30 (m, 1H), 1.87 (bs, 1H), 0.49 (d, J = 6.9 Hz, 3H). ^{13}C NMR (*R,R,R/S,S,S*-isomers): δ 149.1, 140.3, 132.1, 128.7, 128.5, 127.5, 126.3, 118.8, 110.7, 71.9, 66.4, 48.1, 9.9. Anal. Calcd for $C_{17}H_{16}ClNO$: C, 71.45; H, 5.64; N, 4.90. Found: C, 71.17; H, 5.63; N, 4.84.

3-Chloro-1-(2-fluorophenyl)-2-methyl-3-phenylpropanol (12f): Colorless oil; 1H NMR (*R,R,R/S,S,S*-isomers): δ 7.50–7.14 (m, 7H), 7.04–6.95 (m, 2H), 5.52 (s, 1H), 5.00 (d, J = 10.3 Hz, 1H), 2.53 (s, 1H), 2.37–2.20 (m, 1H), 0.50 (d, J = 7.1 Hz, 3H). ^{13}C NMR (*R,R,R/S,S,S*-isomers): δ 163.7, 159.8, 140.6, 139.1, 128.6, 128.1, 127.5, 127.1, 127.0, 115.3, 114.8, 71.9, 64.8, 48.1, 9.9. Anal. Calcd for $C_{16}H_{16}FCIO$: C, 68.94; H, 5.79. Found: C, 68.85; H, 5.62.

Figure 1. X-ray derived structure of compound 1 a1

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Figure 2. X-ray derived structure of compound **7a**

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Figure 3. X-ray derived structure of compound **10a**

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 H12 H 0.1185 -0.0227 -0.0694 1.000 4 e ? d Uiso -1.20000

C10 C 0.2511 0.3209 -0.0539 1.000 4 e ? d Uani ?
 H10 H 0.2923 0.1808 -0.0548 1.000 4 e ? d Uiso -1.20000
 C14 C -0.0744 0.2140 -0.1807 1.000 4 e ? d Uani ?
 H14 H -0.1454 0.1888 -0.2070 1.000 4 e ? d Uiso -1.20000
 C2 C 0.3964 0.5872 0.1776 1.000 4 e ? d Uani ?
 H2 H 0.4305 0.6942 0.1553 1.000 4 e ? d Uiso -1.20000
 C6 C 0.3035 0.2353 0.1780 1.000 4 e ? d Uani ?
 H6 H 0.2747 0.1047 0.1560 1.000 4 e ? d Uiso -1.20000
 C15 C -0.0213 0.4145 -0.1852 1.000 4 e ? d Uani ?
 H15 H -0.0563 0.5244 -0.2150 1.000 4 e ? d Uiso -1.20000
 C16 C 0.0844 0.4537 -0.1453 1.000 4 e ? d Uani ?
 H16 H 0.1195 0.5900 -0.1486 1.000 4 e ? d Uiso -1.20000
 C9 C 0.1801 0.5773 0.0293 1.000 4 e ? d Uani ?
 H9A H 0.2242 0.7040 0.0218 1.000 4 e ? d Uiso -1.50000
 H9B H 0.1667 0.5835 0.0745 1.000 4 e ? d Uiso -1.50000
 H9C H 0.1101 0.5798 -0.0030 1.000 4 e ? d Uiso -1.50000
 C4 C 0.3401 0.4625 0.2784 1.000 4 e ? d Uani ?
 H4 H 0.3357 0.4855 0.3235 1.000 4 e ? d Uiso -1.20000
 C13 C -0.0223 0.0526 -0.1376 1.000 4 e ? d Uani ?
 H13 H -0.0580 -0.0832 -0.1346 1.000 4 e ? d Uiso -1.20000
 C3 C 0.3895 0.6207 0.2447 1.000 4 e ? d Uani ?
 H3 H 0.4184 0.7508 0.2671 1.000 4 e ? d Uiso -1.20000
 C5 C 0.2970 0.2689 0.2450 1.000 4 e ? d Uani ?
 H5 H 0.2637 0.1616 0.2677 1.000 4 e ? d Uiso -1.20000

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_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

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 Cl2 0.07030 0.12207 0.05433 -0.03947 0.01800 0.00819
 C8 0.04015 0.05092 0.03765 -0.00308 0.00757 0.00226
 C7 0.03824 0.04972 0.04656 -0.00435 0.00842 0.00167
 C1 0.03820 0.04830 0.04197 -0.00214 0.00057 0.00217
 C11 0.04970 0.05225 0.03700 -0.00154 0.01052 -0.00637
 C12 0.06385 0.05022 0.06600 -0.00212 -0.00160 0.00100
 C10 0.04763 0.05863 0.04244 -0.00504 0.01114 -0.00307
 C14 0.05045 0.07867 0.05337 -0.00056 0.00322 -0.01635
 C2 0.05435 0.05098 0.05501 -0.00790 -0.00213 0.00268
 C6 0.05233 0.05700 0.04843 -0.01082 0.00611 0.00209
 C15 0.06135 0.07709 0.04561 0.01244 0.00693 0.00553

C16 0.06356 0.05578 0.04768 -0.00298 0.01294 0.00231
 C9 0.05843 0.07241 0.04454 0.01513 0.00321 -0.00367
 C4 0.06744 0.08860 0.04030 0.00518 0.00022 -0.00434
 C13 0.06161 0.06193 0.08069 -0.01376 0.00268 -0.01087
 C3 0.06897 0.06405 0.05527 -0.00189 -0.00943 -0.01159
 C5 0.06339 0.07651 0.04996 -0.00746 0.01072 0.00874

Figure 4. X-ray derived structure of compound **12e**

CIF data of compound **12e**:

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 _audit_update_record05-06-16
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 _cell_length_c26.4386(20)
 _cell_angle_alpha90.000
 _cell_angle_beta95.945(1)
 _cell_angle_gamma90.000
 _cell_volume3020.1(5)
 _symmetry_int_tables_number15

_symmetry_space_group_name_H-M'C 1 2/c 1'
 _symmetry_space_group_name_Hall'-C_2yc'

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 _atom_type_oxidation_number
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 O?1.200
 H?1.200
 C?1.200
 N?1.200

loop_
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 _atom_site_type_symbol
 _atom_site_fract_x
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 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_Wyckoff_symbol
 _atom_site_attached_hydrogens
 _atom_site_calc_flag
 _atom_site_thermal_displace_type
 _atom_site_u_iso_or_equiv
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 O O 0.0690 0.3633 0.4447 1.000 8 f ? d Uani ?
 H0 H 0.1106 0.3715 0.4488 1.000 8 f ? d Uiso -1.50000
 C5 C -0.0232 0.0984 0.4327 1.000 8 f ? d Uani ?
 C9 C 0.0568 0.1468 0.3648 1.000 8 f ? d Uani ?
 H9 H 0.0360 0.0051 0.3502 1.000 8 f ? d Uiso -1.20000
 C10 C 0.1313 0.1509 0.3539 1.000 8 f ? d Uani ?
 H10 H 0.1521 0.2908 0.3693 1.000 8 f ? d Uiso -1.20000
 C2 C -0.1578 0.0070 0.4477 1.000 8 f ? d Uani ?
 C1 C -0.2281 -0.0348 0.4536 1.000 8 f ? d Uani ?
 N N -0.2845 -0.0666 0.4574 1.000 8 f ? d Uani ?
 C8 C 0.0495 0.1479 0.4226 1.000 8 f ? d Uani ?
 H8 H 0.0790 0.0281 0.4389 1.000 8 f ? d Uiso -1.20000
 C3 C -0.1287 0.2165 0.4628 1.000 8 f ? d Uani ?
 H3 H -0.1540 0.3269 0.4780 1.000 8 f ? d Uiso -1.20000
 C6 C -0.0521 -0.1133 0.4194 1.000 8 f ? d Uani ?
 H6 H -0.0260 -0.2262 0.4057 1.000 8 f ? d Uiso -1.20000
 C4 C -0.0616 0.2608 0.4551 1.000 8 f ? d Uani ?
 H4 H -0.0423 0.4016 0.4652 1.000 8 f ? d Uiso -1.20000
 C11 C 0.1420 0.1526 0.2982 1.000 8 f ? d Uani ?

C7 C -0.1194 -0.1593 0.4262 1.000 8 f ? d Uani ?
 H7 H -0.1386 -0.3007 0.4164 1.000 8 f ? d Uiso -1.20000
 C16 C 0.1759 0.3332 0.2781 1.000 8 f ? d Uani ?
 H16 H 0.1921 0.4536 0.2992 1.000 8 f ? d Uiso -1.20000
 C12 C 0.1182 -0.0258 0.2660 1.000 8 f ? d Uani ?
 H12 H 0.0954 -0.1494 0.2787 1.000 8 f ? d Uiso -1.20000
 C14 C 0.1624 0.1628 0.1959 1.000 8 f ? d Uani ?
 H14 H 0.1690 0.1666 0.1616 1.000 8 f ? d Uiso -1.20000
 C13 C 0.1286 -0.0195 0.2151 1.000 8 f ? d Uani ?
 H13 H 0.1126 -0.1391 0.1937 1.000 8 f ? d Uiso -1.20000
 C15 C 0.1862 0.3385 0.2274 1.000 8 f ? d Uani ?
 H15 H 0.2093 0.4612 0.2145 1.000 8 f ? d Uiso -1.20000
 C17 C 0.0195 0.3523 0.3384 1.000 8 f ? d Uani ?
 H17A H 0.0430 0.4920 0.3487 1.000 8 f ? d Uiso -1.50000
 H17B H -0.0261 0.3588 0.3477 1.000 8 f ? d Uiso -1.50000
 H17C H 0.0183 0.3348 0.3022 1.000 8 f ? d Uiso -1.50000

loop_

_atom_site_aniso_label

_atom_site_aniso_U_11

_atom_site_aniso_U_22

_atom_site_aniso_U_33

_atom_site_aniso_U_12

_atom_site_aniso_U_13

_atom_site_aniso_U_23

Cl1 0.06222 0.09542 0.06473 0.03441 0.01487 0.01099
 O 0.03958 0.09741 0.06564 -0.01886 0.01557 -0.03312
 C5 0.03500 0.05300 0.03668 0.00063 0.00726 0.00216
 C9 0.03470 0.04920 0.04199 -0.00160 0.00767 -0.00387
 C10 0.03589 0.05508 0.04796 0.00238 0.01044 -0.00402
 C2 0.03681 0.05335 0.04213 -0.00237 0.00816 0.00752
 C1 0.04047 0.05791 0.05017 -0.00311 0.00582 0.00475
 N 0.03987 0.07635 0.07405 -0.00892 0.00959 0.00018
 C8 0.03292 0.06614 0.04230 0.00095 0.00814 -0.00166
 C3 0.03971 0.05971 0.05178 -0.00050 0.01410 -0.00803
 C6 0.04847 0.04823 0.06457 0.00409 0.02080 -0.00067
 C4 0.04053 0.05502 0.05167 -0.00650 0.01136 -0.01017
 Cl1 0.03792 0.05495 0.05119 0.00196 0.01238 -0.00423
 C7 0.05120 0.04401 0.06571 -0.00608 0.01421 0.00169
 C16 0.05155 0.06573 0.06619 -0.00628 0.02078 -0.00370
 C12 0.06291 0.06114 0.05619 -0.00256 0.01212 -0.00682
 C14 0.07246 0.10042 0.05082 0.01853 0.02240 0.00736
 C13 0.07880 0.08236 0.05546 0.00697 0.01021 -0.01499
 C15 0.06690 0.08455 0.07152 -0.00186 0.03026 0.01276
 C17 0.04665 0.06887 0.05587 0.00989 0.01200 0.00593