Supporting Information

Lewis Acid-catalyzed Cycloaddition of Methylene cyclopropanes with Salicylaldehydes

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S1
General Remarks. $^1$H and $^{13}$C NMR spectra were recorded on a Bruker AM-400 spectrometer for solution in CDCl$_3$ with tetramethylsilane (TMS) as an internal standard; $J$-values are in Hz. Mass spectra were recorded by EI methods, and HRMS was measured on a Finnigan MA$^+$ mass spectrometer. The employed solvents were dry up by the standard procedures. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC with Huanghai GF$_{254}$ silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

General Procedure for this Reaction.

Preparation of the products 3a: Under an argon atmosphere, to a solution of salicylaldehyde 1a (30 mg, 0.25 mmol) and CH(OEt)$_3$ (44 mg, 0.3 mmol) in 1,2-dichloroethane (DCE) Sc(OTf)$_3$ (15 mg, 0.03 mmol) was added, the reaction mixture was stirred at room temperature (20 °C) for 0.5 h. The diphenylmethylenecyclopropane 2a (42 mg, 0.2 mmol) was added for 24 h at room temperature (monitored by TLC plates). Then the solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO$_2$) to give the corresponding products 3a (53 mg, 78%) as a white solid.

Preparation of the products 5a: Under an argon atmosphere, to a solution of salicylaldehyde 1a (30 mg, 0.25 mmol) and CH(OEt)$_3$ (44 mg, 0.3 mmol) in 1,2-dichloroethane (DCE) Sc(OTf)$_3$ (15 mg, 0.03 mmol) was added, the reaction mixture was stirred at room temperature (20 °C) for 0.5 h. The diphenylmethylenecyclopropane 2a (42 mg, 0.2 mmol) was added for 10 h at 60 °C (monitored by TLC plates). Then the solvent was removed under reduced pressure and the residue was purified by a flash column chromatography (SiO$_2$) to give the corresponding products 5a (63 mg, 84%) as a white solid.
Compound 3a: A white solid, m.p. 112-114 °C; IR (CH₂Cl₂): ν 3060, 2975, 2865, 1664, 1607, 1486, 1447, 1377, 1240, 1109, 936, 847, 760 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.14 (3H, t, J = 6.8 Hz, CH₃), 2.17 (2H, td, J = 6.8, 1.2 Hz, CH₂), 3.31-3.38 (4H, m, CH₂), 6.57 (1H, s, =CH), 6.78-6.81 (2H, m, ArH), 6.96-7.03 (2H, m, ArH), 7.24-7.30 (6H, m, ArH), 7.37-7.40 (4H, m, ArH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 15.1, 34.3, 66.1, 68.5, 86.3, 116.4, 121.2, 122.0, 122.7, 125.9, 127.8, 128.5, 128.6, 135.8, 143.0, 151.9; MS (EI) m/z (%): 356 (96.54) [M⁺], 310 (94.81), 279 (40.45), 233 (100.00), 219 (35.99), 165 (14.66), 107 (8.70), 91 (16.63); HRMS (EI) Calcd. for C₂₅H₂₄O₂ (M⁺) requires 356.1776, Found: 356.1777.
**Compound 3b:** A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3060, 2974, 2865, 2800, 1601, 1583, 1480, 1414, 1263, 1227, 1082, 814, 756, 701 cm$^{-1}$; $^{1}$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.14 (3H, t, $J$ = 7.2 Hz, CH$_3$), 2.14-2.18 (5H, m, CH$_2$, CH$_3$), 3.30-3.39 (4H, m, CH$_2$), 6.52 (1H, s, =CH), 6.69 (1H, d, $J$ = 7.8 Hz, ArH), 6.79-6.82 (2H, m, ArH), 7.24-7.31 (6H, m, ArH), 7.36-7.39 (4H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 20.6, 34.3, 66.1, 68.6, 86.1, 116.1, 122.1, 122.5, 126.3, 127.7, 128.6, 129.1, 130.3, 135.8, 143.1, 149.7; MS (EI) $m/z$ (%): 370 (100.00) [M$^+$], 324 (71.58), 309 (40.21), 297 (39.35), 247 (76.97), 233 (37.70), 165 (17.74), 71 (29.28); HRMS (EI) Calcd. for C$_{26}$H$_{26}$O$_2$ (M$^+$) requires 370.1933, Found: 370.1934.
**Compound 3c**: A colorless oil; IR (CH<sub>2</sub>Cl<sub>2</sub>): ν 3062, 2973, 2866, 1613, 1578, 1519, 1481, 1343, 1266, 1248, 1107, 1090, 980, 908, 832, 751, 701 cm<sup>-1</sup>; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, TMS): δ 1.17 (3H, t, <i>J</i> = 7.2 Hz, CH<sub>3</sub>), 2.17 (2H, td, <i>J</i> = 5.2, 1.2 Hz, CH<sub>2</sub>), 3.32-3.43 (4H, m, CH<sub>2</sub>), 6.66 (1H, s, =CH), 6.86 (1H, d, <i>J</i> = 8.0 Hz, ArH), 7.31-7.37 (10H, m, ArH), 7.92-7.95 (2H, m, ArH); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>, TMS): δ 15.1, 34.2, 66.3, 67.9, 87.9, 116.7, 120.5, 121.6, 122.7, 124.6, 128.0, 128.3, 128.6, 138.6, 141.8, 157.4; MS (EI) <i>m/z</i> (%): 401 (31.93) [M<sup>+</sup>], 355 (100.00), 338 (31.04), 328 (26.77), 278 (68.15), 218 (15.32), 165 (15.48), 59 (27.53); HRMS (EI) Calcd. for C<sub>25</sub>H<sub>23</sub>O<sub>4</sub>N (M<sup>+</sup>) requires 401.1627, Found: 401.1620.
**Compound 3d**: A colorless oil, m.p. 116-118 °C; IR (CH$_2$Cl$_2$): $\nu$ 3059, 2973, 2864, 1477, 1446, 1224, 1107, 986, 899, 812, 755, 728, 700 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.15 (3H, t, $J = 6.9$ Hz, CH$_3$), 2.15 (2H, t, $J = 6.6$ Hz, CH$_2$), 3.32-3.41 (4H, m, CH$_2$), 6.52 (1H, s, =CH), 6.88 (1H, d, $J = 9.6$ Hz, ArH), 7.07-7.11 (2H, m, ArH), 7.26-7.37 (10H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 34.3, 53.4, 66.2, 68.2, 107.6, 113.3, 118.2, 120.9, 127.8, 128.0, 128.3, 128.6, 131.1, 137.6, 142.4, 151.0; MS (EI) m/z (%): 434 (60.52) [M$^+$], 388 (94.07), 309 (100.00), 296 (94.45), 252 (37.43), 218 (55.84), 165 (38.69), 91 (33.41); HRMS (EI) Calcd. for C$_{25}$H$_{23}$O$_2$Br (M$^+$) requires 434.0881, Found: 434.0874.
**Compound 3e**: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3060, 2974, 2865, 2800, 1956, 1601, 1583, 1480, 1446, 1263, 1227, 1108, 987, 903, 885, 757 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.15 (3H, t, $J = 7.2$ Hz, CH$_3$), 2.15 (2H, td, $J = 7.2$, 1.6 Hz, CH$_2$), 3.32-3.40 (4H, m, CH$_2$), 6.52 (1H, s, =CH), 6.71-6.73 (1H, m, ArH), 6.93-6.96 (2H, m, ArH), 7.24-7.37 (10H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 34.3, 66.2, 68.2, 86.6, 117.7, 121.0, 124.1, 125.4, 125.9, 127.8, 127.9, 128.1, 128.6, 137.6, 142.4, 150.4; MS (EI) $m/z$ (%): 390 (5.11) [M$^+$], 370 (4.79), 309 (8.95), 267 (9.13), 203 (8.70), 155 (10.31), 85 (56.27), 57 (100.00); HRMS (EI) Calcd. for C$_{25}$H$_{23}$O$_2$Cl (M$^+$) requires 390.1387, Found: 390.1395.
**Compound 3f:** A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3060, 2974, 2865, 2800, 1601, 1583, 1480, 1414, 1263, 1227, 1082, 814, 756, 701 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.13 (3H, t, $J = 6.8$ Hz, CH$_3$), 2.14-2.18 (2H, m, CH$_2$), 2.16 (3H, s, CH$_3$), 3.27-3.37 (4H, m, CH$_2$), 6.55 (1H, s, =CH), 6.70 (1H, t, $J = 8.0$ Hz, ArH), 6.82-6.88 (2H, m, ArH), 7.25-7.31 (6H, m, ArH), 7.37-7.41 (4H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 20.6, 34.3, 66.1, 68.6, 86.1, 116.1, 122.1, 122.5, 126.3 127.7, 128.6, 129.1, 130.3, 135.8, 143.1, 149.7; MS (EI) $m/z$ (%): 370 (100.00) [M$^+$], 324 (71.58), 309 (40.21), 297 (39.35), 247 (76.97), 233 (37.70), 165 (17.74), 71 (29.28); HRMS (EI) Calcd. for C$_{26}$H$_{26}$O$_2$ (M$^+$) requires 370.1933, Found: 370.1934.
**Compound 3g** having some acetophenone: A colorless oil; IR (CH₂Cl₂): ν 3059, 2975, 2866, 2801, 1686, 1578, 1486, 1374,1245, 1109, 1027, 930, 753, 699 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.17 (3H, t, J = 6.8 Hz, CH₃), 1.82 (3H, s, CH₃), 2.14-2.20 (1H, m, CH₂), 2.24-2.30 (3H, m, CH₂), 3.39-3.46 (3H, m, CH₂), 3.45-3.54 (1H, m, CH₂), 6.33 (1H, s, =CH), 6.76 (1H, d, J = 8.0 Hz, ArH), 6.80-6.84 (1H, m, ArH), 6.96 (1H, d, J = 8.4 Hz, ArH), 7.02-7.07 (1H, m, ArH), 7.31 (3H, t, J = 7.2 Hz, ArH), 7.53 (2H, d, J = 7.2 Hz, ArH); having some acetophenone ¹H NMR (400 MHz, CDCl₃, TMS): δ 2.59 (3H, s, CH₃), 7.24 (2H, t, J = 7.2 Hz, ArH), 7.45 (1H, t, J = 7.2 Hz, ArH), 7.94 (2H, d, J = 8.4 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 15.1, 24.3, 26.5, 32.2, 66.1, 68.8, 81.9, 115.9, 119.8, 120.9, 121.9, 125.8, 126.5, 127.7, 128.1, 128.2, 128.5, 133.0, 137.3, 143.6, 151.7; MS (EI) m/z (%): 294 (38.13) [M⁺], 279 (100.00), 235 (24.21), 217 (28.84), 173 (6.43), 141 (8.21), 91 (15.67), 43 (16.63); HRMS (EI) Calcd. for C₂₀H₂₂O₂ (M⁺) requires 294.1620, Found: 294.1621.
**Compound 3h:** A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3422, 2974, 2866, 2801, 1906, 1774, 1741, 1593, 1492, 1378, 997, 835, 737, 703 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.17 (3H, t, $J$ = 7.2 Hz, CH$_3$), 2.22-2.27 (2H, m, CH$_2$), 3.41 (2H, q, $J$ = 7.2 Hz, CH$_2$), 3.51 (2H, t, $J$ = 7.2 Hz, CH$_2$), 5.74 (1H, s, CH), 6.44 (1H, s, =CH), 6.67 (1H, d, $J$ = 8.0 Hz, ArH), 6.82-6.86 (1H, m, ArH), 6.98-7.06 (2H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 33.6, 66.3, 68.6, 79.1, 115.8, 120.7, 121.2, 121.8, 126.0, 128.7, 128.8, 129.2, 133.4, 134.5, 137.5, 151.3; MS (EI) m/z (%): 314 (9.44) [M$^+$], 139 (100.00), 113 (12.26), 111 (20.14), 85 (17.00), 71 (19.69), 57 (31.44), 43 (15.16); HRMS (EI) Calcd. for C$_{19}$H$_{19}$O$_2$Cl (M$^+$) requires 314.1074, Found: 314.1070.
**Compound 3i**: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3024, 2956, 2870, 1606, 1580, 1488, 1378, 1246, 1224, 1112, 1030, 925, 871, 749 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 0.86 (6H, t, $J = 7.2$ Hz, CH$_3$), 1.22-1.36 (9H, m, CH$_2$), 1.43-1.50 (2H, m, CH$_2$), 1.64-1.74 (4H, m, CH$_2$), 2.31-2.35 (2H, m, CH$_2$), 3.54 (2H, q, $J = 7.2$ Hz, CH$_2$), 3.66 (2H, t, $J = 6.0$ Hz, CH$_2$), 6.17 (1H, s, =CH), 6.67 (1H, d, $J = 8.0$ Hz, ArH), 6.72-6.76 (1H, m, ArH), 6.83-6.85 (1H, m, ArH), 6.99-7.03 (1H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 14.0, 15.2, 23.0, 25.7, 30.9, 38.9, 66.4, 69.1, 84.8, 114.7, 119.9, 120.3, 121.1, 125.6, 128.3, 135.8, 153.3; MS (EI) $m/z$ (%): 316 (3.60) [M$^+$], 259 (100.00), 213 (5.20), 171 (6.63), 145 (5.50), 131 (6.57), 71 (5.08), 41 (7.37); HRMS (EI) Calcd. for C$_{21}$H$_{32}$O$_2$ (M$^+$) requires 316.2402, Found: 316.2405.
**Compound 3j:** A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3024, 2930, 2861, 1665, 1577, 1486, 1455, 1273, 1111, 956, 931, 852, 752, 736 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.23 (3H, t, $J$ = 7.2 Hz, CH$_3$), 1.46-1.54 (5H, m, CH$_2$), 1.72-1.80 (3H, m, CH$_2$), 1.91-1.95 (2H, m, CH$_2$), 2.38-2.42 (2H, m, CH$_2$), 3.53 (2H, q, $J$ = 7.2 Hz, CH$_2$), 3.63 (2H, t, $J$ = 7.2 Hz, CH$_2$), 6.12 (1H, s, =CH), 6.82-6.85 (2H, m, ArH), 6.93 (1H, d, $J$ = 7.6 Hz, ArH), 7.05-7.09 (1H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.2, 21.2, 25.3, 31.5, 32.6, 66.3, 69.3, 78.7, 116.1, 119.4, 120.8, 123.3, 125.6, 128.1, 139.3, 151.6; MS (EI) m/z (%): 272 (88.15) [M$^+$], 243 (100.00), 229 (87.92), 201 (81.09), 185 (83.82), 131 (31.24), 84 (38.45), 49 (50.19); HRMS (EI) Calcd. for C$_{18}$H$_{24}$O$_2$ (M$^+$) requires 272.1776, Found: 272.1772.
**Compound 3k** (a diastereoisomeric mixture, ratio = 2:1): A colorless oil; IR (CH₂Cl₂): ν 3058, 2930, 2866, 1577, 1455, 1375, 1224, 1111, 948, 754, 699 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.17 (2H, t, J = 7.2 Hz, CH₃), 1.25 (1H, t, J = 7.2 Hz, CH₃), 1.69-1.84 (4H, m, CH₂), 2.03-2.07 (3H, m, CH₂), 2.26-2.33 (3H, m, CH), 2.43-2.47 (0.66H, m, CH), 2.50-2.54 (0.33H, m, CH), 3.43 (1.32H, q, J = 7.2 Hz, CH₂), 3.50 (1.32H, t, J = 7.2 Hz, CH₂), 3.55 (0.66H, q, J = 7.2 Hz, CH₂), 3.66 (0.66H, t, J = 7.2 Hz, CH₂), 6.11 (0.66H, s, =CH), 6.18 (0.33H, s, =CH), 6.83-6.97 (3H, m, ArH), 7.08-7.10 (1H, m, ArH), 7.19-7.21 (1H, m, ArH), 7.23-7.38 (4H, m, ArH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 15.1, 15.2, 25.0, 28.7, 28.8, 30.3, 31.6, 31.7, 32.9, 35.5, 43.3, 66.2, 66.3, 69.0, 69.3, 78.0, 78.5, 116.1, 116.2, 119.5, 119.9, 120.9, 121.0, 123.3, 125.6, 125.7, 126.0, 126.8, 127.2, 128.20, 128.24, 128.3, 138.3, 138.8, 139.0, 143.8, 147.1, 151.5, 151.7; MS (EI) m/z (%): 348 (11.59) [M⁺], 229 (100.00), 183 (13.41), 172 (12.68), 128 (6.84), 115 (6.35), 107 (3.18), 91 (8.05); HRMS (EI) Calcd. for C₂₄H₂₈O₂ (M⁺) requires 348.2089, Found: 348.2085.
**Compound 3l (a diastereoisomeric mixture, ratio = 1.6:1.4):** A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3037, 2933, 2865, 1609, 1512, 1486, 1555, 1253, 1181, 1110, 948, 836, 753, 737 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.18 (1.6H, t, $J$ = 7.2 Hz, CH$_3$), 1.25 (1.4H, t, $J$ = 7.2 Hz, CH$_3$), 1.68-1.82 (4H, m, CH$_2$), 1.99-2.10 (3H, m, CH$_2$), 2.26-2.33 (2H, m, CH$_2$), 2.43-2.48 (1.47H, m, CH$_2$), 3.05 (0.53H, s, CH$_2$), 3.43-3.58 (3H, m, CH$_2$), 3.66 (1H, t, $J$ = 7.2 Hz, CH$_2$), 3.79 (1.4H, s, OCH$_3$), 3.80 (1.6H, s, OCH$_3$), 6.10 (0.53H, s, =CH), 6.17 (0.47H, s, =CH), 6.84-6.90 (4H, m, ArH), 6.94-6.97 (1H, m, ArH), 7.10 (1H, t, $J$ = 8.8 Hz, ArH), 7.20 (1H, d, $J$ = 8.8 Hz, ArH), 7.27 (1H, d, $J$ = 7.6 Hz, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 15.2, 25.1, 28.5, 29.0, 31.5, 31.6, 32.9, 34.7, 42.4, 55.2, 66.3, 66.4, 69.0, 69.3, 78.0, 78.6, 113.7, 116.1, 116.2, 119.4, 119.8, 120.9, 121.0, 123.2, 123.3, 125.6, 125.7, 127.6, 128.12, 128.19, 128.2, 135.6, 138.8, 139.0, 139.3, 151.5, 151.7, 157.4, 157.8; MS (EI) $m/z$ (%): 378 (14.00) [M$^+$], 229 (100.00), 183 (10.38), 172 (12.20), 134 (7.10), 121 (5.66), 107 (2.47), 91 (5.01); HRMS (EI) Calcd. for C$_{25}$H$_{30}$O$_3$ (M$^+$) requires 378.2195, Found: 378.2192.
Compound 3m: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 2957, 2864, 1659, 1589, 1495, 1467, 1271, 1227, 1114, 996, 887, 813, 732 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 0.85 (3H, t, $J$ = 7.2 Hz, CH$_3$), 1.21-1.28 (9H, m, CH$_2$, CH$_3$), 1.43-1.50 (2H, m, CH$_2$), 1.65-1.70 (2H, m, CH$_2$), 2.21 (3H, s, CH$_3$), 2.33 (2H, t, $J$ = 7.5 Hz, CH$_2$), 3.54 (2H, q, $J$ = 7.2 Hz, CH$_2$), 3.66 (2H, t, $J$ = 7.5 Hz, CH$_2$), 6.13 (1H, s, =CH), 6.57 (1H, d, $J$ = 7.8 Hz, ArH), 6.66 (1H, s, ArH), 6.81 (1H, d, $J$ = 8.1 Hz, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 14.1, 15.2, 20.5, 23.0, 25.7, 30.8, 38.8, 66.4, 69.1, 84.5, 114.4, 119.7, 120.3, 126.2, 128.7, 133.4, 135.8, 151.0; MS (EI) $m/z$ (%): 330 (4.92) [M$^+$], 273 (100.00), 227 (4.14), 185 (5.62), 159 (3.79), 145 (5.62), 121 (4.34), 71 (6.62); HRMS (EI) Calcd. for C$_{22}$H$_{34}$O$_2$ (M$^+$) requires 330.2559, Found: 330.2557.
**Compound 3n**: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3011, 2929, 2861, 1657, 1590, 1493, 1447, 1282, 1236, 1109, 959, 931, 815 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.23 (3H, t, $J$ = 7.2 Hz, CH$_3$), 1.47-1.53 (5H, m, CH$_2$), 1.73-1.79 (3H, m, CH$_2$), 1.90-1.94 (2H, m, CH$_2$), 2.24 (3H, s, CH$_3$), 2.37-2.41 (2H, m, CH$_2$), 3.53 (2H, q, $J$ = 7.2 Hz, CH$_2$), 3.62 (2H, t, $J$ = 7.2 Hz, CH$_2$), 6.08 (1H, s, =CH), 6.75 (1H, s, ArH), 6.86-6.90 (2H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.2, 21.2, 25.3, 31.5, 32.5, 66.3, 69.3, 78.5, 115.8, 119.5, 126.1, 128.5, 129.9, 138.0, 149.4; MS (El) $m/z$ (%): 286 (94.83) [M$^+$], 257 (100.00), 243 (95.93), 215 (80.44), 199 (67.79), 185 (19.32), 84 (41.21), 49 (52.30); HRMS (El) Calcd. for C$_{19}$H$_{26}$O$_2$ (M$^+$) requires 286.1933, Found: 286.1935.
Compound 4a: A colorless oil; IR (CH₂Cl₂): ν 3014, 2974, 2862, 1730, 1671, 1597, 1494, 1376, 1112, 1031, 863, 810, 768, 695 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.18 (3H, t, J = 7.2 Hz, CH₃), 2.01 (3H, s, CH₃), 2.21-2.24 (2H, m, CH₂), 2.31 (3H, s, CH₃), 3.41-3.47 (4H, m, CH₂), 6.24 (1H, t, J = 7.2 Hz, =CH), 6.90 (1H, s, ArH), 6.98-7.04 (2H, m, ArH), 7.18-7.26 (5H, m, ArH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 15.2, 19.1, 21.0, 30.4, 66.0, 70.0, 119.8, 125.3, 126.2, 126.8, 127.9, 128.2, 129.9, 130.5, 133.2, 139.0, 142.3; MS (EI) m/z (%): 280 (27.92) [M⁺], 236 (20.10), 221 (100.00), 206 (18.42), 193 (27.50), 143 (29.20), 115 (52.04), 59 (10.17); HRMS (EI) Calcd. for C₂₀H₂₄O (M⁺) requires 280.1827, Found: 280.1838.
**Compound 4b:** This is a known compound; a colorless oil; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.18 (3H, t, $J = 7.2$ Hz, CH$_3$), 2.28 (3H, s, CH$_3$), 2.30 (3H, s, CH$_3$), 2.39 (2H, q, $J = 6.8$ Hz, CH$_2$), 3.42-3.49 (4H, m, CH$_2$), 6.05 (1H, t, $J = 7.2$ Hz, =CH), 7.04-7.08 (4H, m, ArH), 7.11-7.16 (4H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.2, 30.5, 55.2, 55.3, 66.1, 70.4, 113.4, 113.5, 123.8, 128.4, 131.0, 132.5, 135.7, 142.2, 158.5, 158.7. Their spectroscopic data are consistent with those reported in the literature.[1]
**Compound 4c**: This is a known compound; a colorless oil; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.19 (3H, t, $J = 7.2$ Hz, CH$_3$), 2.39 (2H, q, $J = 7.2$ Hz, CH$_2$), 3.44-3.50 (4H, m, CH$_2$), 3.78 (3H, s, OCH$_3$), 3.83 (3H, s, OCH$_3$), 5.97 (1H, t, $J = 7.2$ Hz, =CH), 6.79 (2H, d, $J = 8.8$ Hz, ArH), 6.89 (2H, d, $J = 8.8$ Hz, ArH), 7.10 (2H, d, $J = 8.8$ Hz, ArH), 7.15 (2H, d, $J = 8.8$ Hz, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.2, 30.5, 55.2, 55.3, 66.1, 70.4, 113.4, 113.5, 123.8, 128.4, 131.0, 132.5, 135.7, 142.2, 158.5, 158.7. Their spectroscopic data are consistent with those reported in the literature.$[1]$
**Compound 4d**: This is a known compound; A colorless oil; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.20 (3H, t, $J = 6.9$ Hz, CH$_3$), 2.37 (2H, q, $J = 7.2$ Hz, CH$_2$), 3.43-3.51 (4H, m, CH$_2$), 6.12 (1H, t, $J = 7.2$ Hz, =CH), 7.10-7.14 (4H, m, ArH), 7.22 (2H, d, $J = 8.4$ Hz, ArH), 7.35 (2H, d, $J = 8.4$ Hz, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.2, 30.5, 66.2, 69.9, 127.1, 128.1, 128.2, 128.4, 128.5, 128.7, 129.9, 131.2, 133.0, 133.1, 137.9, 140.6, 140.9. Their spectroscopic data are consistent with those reported in the literature.$^{[1]}$
**Compound 4e:** This is a known compound; A colorless oil; $^1$H NMR (400 MHz, CDCl$_3$, TMS): δ 1.17-1.21 (3H, m, CH$_3$), 2.36-2.42 (2H, m, CH$_2$), 3.43-3.51 (4H, m, CH$_2$), 6.09-6.15 (1H, m, =CH), 7.12-7.26 (5H, m, ArH), 7.29-7.38 (4H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): δ 15.2, 30.4, 30.5, 66.1, 66.2, 70.0, 70.1, 126.4, 126.5, 127.1, 127.2, 127.3, 128.1, 128.2, 128.3, 128.4, 128.5, 129.8, 131.3, 132.7, 132.9, 138.4, 139.5, 141.1, 142.0, 142.1.

Their spectroscopic data are consistent with those reported in the literature.$^{[1]}$
**Compound 3o**: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3024, 2972, 2926, 2867, 1644, 1607, 1575, 1485, 1455, 1243, 1108, 1030, 986, 934, 886, 849, 761, 703 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.15 (3H, t, $J = 7.2$ Hz, CH$_3$), 2.02-2.08 (1H, m, CH$_2$), 2.20-2.26 (1H, m, CH$_2$), 2.20 (3H, s, CH$_3$), 2.22 (3H, s, CH$_3$), 3.25-3.29 (1H, m, CH$_2$), 3.34-3.46 (3H, m, CH$_2$), 6.57 (1H, s, =CH), 6.80 (2H, d, $J = 6.8$ Hz, ArH), 6.87 (1H, s, ArH), 6.95-7.02 (6H, m, ArH), 7.22-7.27 (2H, m, ArH), 7.49-7.54 (1H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.2, 21.1, 21.3, 34.4, 66.1, 68.5, 86.9, 115.9, 121.1, 122.0, 122.8, 125.9, 127.4, 127.6, 127.8, 128.1, 128.4, 128.7, 130.4, 132.2, 133.9, 135.7, 135.8, 139.3, 143.2, 152.0; MS (EI) $m/z$ (%): 384 (80.40) [M$^+$], 338 (69.43), 323 (100.00), 279 (21.48), 233 (55.77), 219 (31.92), 107 (21.10), 91 (22.76); HRMS (EI) Calcd. for C$_{27}$H$_{28}$O$_2$ (M$^+$) requires 384.2089, Found: 384.2092.
**Compound 3p:** A colorless oil; IR (CH₂Cl₂): ν 2922, 2851, 1686, 1604, 1512, 1459, 1375, 1265, 1017, 834 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.14 (3H, t, J = 7.2 Hz, CH₃), 2.15 (2H, t, J = 7.2 Hz, CH₂), 2.31 (6H, s, CH₃), 3.33-3.38 (4H, m, CH₂), 6.53 (1H, s, =CH), 6.76-6.80 (2H, m, ArH), 6.95-7.00 (2H, m, ArH), 7.08 (4H, d, J = 8.0 Hz, ArH), 7.26 (4H, d, J = 8.0 Hz, ArH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 15.1, 21.0, 34.2, 66.1, 68.6, 86.1, 116.4, 121.1, 121.7, 122.8, 125.8, 126.3, 128.3, 128.4, 128.5, 128.6, 128.7, 128.8, 129.3, 136.2, 137.3, 140.1, 152.0; MS (EI) m/z (%): 384 (100.00) [M⁺], 323 (81.82), 311 (68.21), 293 (34.83), 247 (61.92), 178 (13.18), 119 (16.49), 71 (12.48); HRMS (EI) Calcd. for C₂₇H₂₈O₂ (M⁺) requires 384.2089, Found: 384.2090.
**Compound 3q:** A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3061, 3036, 2973, 2865, 1903, 1813, 1606, 1578, 1488, 1455, 1233, 1093, 991, 933, 829, 701 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.15 (3H, t, $J = 7.2$ Hz, CH$_3$), 2.13 (2H, t, $J = 6.8$ Hz, CH$_2$), 3.33-3.41 (4H, m, CH$_2$), 6.57 (1H, s, =CH), 6.77-6.83 (2H, m, ArH), 6.97-7.02 (2H, m, ArH), 7.24-7.36 (9H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 34.2, 66.2, 68.3, 85.8, 116.4, 121.4, 122.2, 122.6, 125.9, 127.8, 127.9, 128.0, 128.5, 128.7, 130.1, 133.7, 135.3, 141.5, 142.6, 151.7; MS (EI) m/z (%): 390 (10.05) [M$^+$$]$, 344 (9.45), 309 (11.98), 267 (11.03), 233 (14.69), 99 (24.49), 71 (70.31), 57 (100.00); HRMS (EI) Calcd. for C$_{25}$H$_{23}$O$_2$Cl (M$^+$) requires 390.1387, Found: 390.1381.
**Compound 3r**: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3024, 2972, 2926, 2867, 1644, 1607, 1575, 1485, 1455, 1243, 1108, 1030, 986, 934, 886, 849, 761, 703 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.17 (3H, t, $J$ = 7.2 Hz, CH$_3$), 2.10 (2H, t, $J$ = 7.2 Hz, CH$_2$), 3.37-3.44 (4H, m, CH$_2$), 6.58 (1H, s, =CH), 6.76-6.85 (2H, m, ArH), 6.98-7.06 (2H, m, ArH), 7.25-7.32 (8H, m, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 34.1, 66.3, 68.1, 85.3, 116.4, 121.6, 122.3, 122.5, 126.0, 128.1, 128.9, 129.9, 133.9, 134.8, 141.1, 151.4; MS (EI) m/z (%): 424 (74.51) [M$^+$], 378 (58.33), 343 (100.00), 267 (93.53), 218 (19.39), 131 (12.08), 107 (8.66), 59 (18.65); HRMS (EI) Calcd. for C$_{25}$H$_{22}$O$_2$Cl$_2$ (M$^+$) requires 424.0997, Found: 424.0993.
**Compound 3s:** A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3026, 2925, 2856, 1607, 1511, 1485, 1456, 1377, 1231, 1108, 1012, 991, 822, 753 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.15 (3H, t, $J = 7.2$ Hz, CH$_3$), 2.13 (2H, t, $J = 7.2$ Hz, CH$_2$), 2.31 (3H, s, CH$_3$), 3.35-3.39 (4H, m, CH$_2$), 6.55 (1H, s, =CH), 6.78 (2H, t, $J = 8.0$ Hz, ArH), 6.96-7.01 (2H, m, ArH), 7.09 (2H, d, $J = 8.4$ Hz, ArH), 7.22-7.28 (4H, m, ArH), 7.40 (2H, d, $J = 8.4$ Hz, ArH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 15.1, 21.0, 29.3, 34.2, 66.2, 68.3, 85.7, 116.4, 121.3, 121.9, 122.0, 122.6, 125.9, 128.4, 128.6, 128.7, 130.4, 130.9, 135.4, 137.6, 139.5, 142.3, 151.7; MS (EI) $m/z$ (%): 448 (98.32) [M$^+$], 404 (61.66), 323 (80.36), 247 (88.64), 233 (26.22), 189 (11.93), 131 (13.10), 59 (15.05); HRMS (EI) Calcd. for C$_{26}$H$_{25}$O$_2$Br (M$^+$) requires 448.1038, Found: 448.1033.
Compound 5a: A white solid, m.p. 104-106 °C; IR (CH2Cl2): ν 3297, 3065, 2970, 2925, 2864, 1738, 1596, 1487, 1454, 1364, 1217, 1097, 774, 754, 702 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.35 (3H, t, J = 6.8 Hz, CH₃), 2.20-2.28 (1H, m, CH₂), 2.61-2.65 (1H, m, CH₂), 3.47-3.52 (1H, m, CH₂), 3.55-3.65 (2H, m, CH₂), 3.72-3.75 (1H, m, CH₂), 5.15 (1H, s, CH), 6.38-6.40 (1H, m, ArH), 6.71 (1H, t, J = 8.0 Hz, ArH), 7.02 (1H, d, J = 7.6 Hz, ArH), 7.10-7.26 (4H, m, ArH), 7.39 (4H, d, J = 7.6 Hz, ArH), 7.46 (2H, t, J = 7.6 Hz, ArH), 8.10 (1H, s, OH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 14.7, 27.0, 52.1, 67.3, 72.3, 117.8, 119.9, 120.8, 124.4, 125.2, 126.0, 126.7, 127.4, 128.1, 128.3, 129.2, 146.0, 147.2, 148.0, 155.3; MS (EI) m/z (%): 356 (18.76) [M⁺], 310 (100.00), 297 (19.64), 277 (7.85), 203 (27.16), 191 (4.69), 84 (23.55), 71 (14.54); HRMS (EI) Calcd. for C₂₅H₂₄O₂ (M⁺) requires 356.1776, Found: 356.1772.
**Compound 5b**: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3390, 3059, 3026, 2925, 2867, 1715, 1661, 1596, 1498, 1448, 1269, 1105, 928, 811, 765, 702 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.33 (3H, t, $J$ = 6.8 Hz, CH$_3$), 2.07 (3H, s, CH$_3$), 2.20-2.29 (1H, m, CH$_2$), 2.61-2.65 (1H, m, CH$_2$), 3.46-3.51 (1H, m, CH$_2$), 3.55-3.61 (2H, m, CH$_2$), 3.71-3.73 (1H, m, CH$_2$), 5.12 (1H, s, CH), 6.17 (1H, s, ArH), 6.92 (2H, s, ArH), 7.17-7.30 (4H, m, ArH), 7.36-7.48 (5H, m, ArH), 7.89 (1H, s, OH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 14.7, 20.5, 27.0, 52.1, 67.2, 72.3, 117.5, 119.8, 124.4, 125.1, 125.6, 126.6, 127.4, 128.3, 128.5, 128.8, 129.2, 129.9, 135.0, 139.3, 146.0, 147.3, 148.0, 153.0; MS (EI) $m/z$ (%): 370 (3.46) [M$^+$], 338 (63.73), 324 (13.36), 233 (35.36), 218 (8.80), 189 (7.05), 105 (100.00), 77 (77.55); HRMS (EI) Calcd. for C$_{26}$H$_{26}$O$_2$ (M$^+$) requires 370.1933, Found: 370.1931.
Compound 5c: A colorless oil; IR (CH$_2$Cl$_2$): $\nu$ 3379, 3063, 2926, 2870, 1714, 1661, 1470, 1449, 1272, 1108, 932, 810, 764, 702 cm$^{-1}$; $^1$H NMR (400 MHz, CDCl$_3$, TMS): $\delta$ 1.34 (3H, t, $J = 7.2$ Hz, CH$_3$), 2.16-2.24 (1H, m, CH$_2$), 2.61-2.66 (1H, m, CH$_2$), 3.46-3.52 (1H, m, CH$_2$), 3.56-3.65 (2H, m, CH$_2$), 3.73-3.79 (1H, m, CH$_2$), 5.07 (1H, s, CH), 6.47 (1H, d, $J = 2.4$ Hz, ArH), 6.91 (1H, d, $J = 8.4$ Hz, ArH), 7.20-7.32 (5H, m, ArH), 7.36-7.38 (2H, m, ArH), 7.43-7.46 (3H, m, ArH), 8.31 (1H, s, OH); $^{13}$C NMR (100 MHz, CDCl$_3$, TMS): $\delta$ 14.7, 26.9, 52.1, 67.4, 72.4, 119.3, 120.1, 124.3, 125.4, 125.5, 127.0, 127.5, 127.8, 127.9, 128.1, 128.5, 128.6, 129.1, 134.6, 139.8, 145.9, 146.4, 147.1, 154.1. MS (EI) m/z (%): 448 (15.34) [M$^+$], 401 (100.00), 372 (39.56), 298 (20.09), 294 (30.08), 218 (71.37), 105 (91.75), 77 (40.73); HRMS (EI) Calcd. for C$_{26}$H$_{25}$O$_2$Br (M$^+$) requires 448.1038, Found: 448.1034.
**Compound 5d**: A colorless oil; IR (CH₂Cl₂): ν 3375, 2974, 2870, 1715, 1663, 1596, 1474, 1449, 1287, 1110, 927, 807, 765, 704, 639 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.34 (3H, t, J = 7.2 Hz, CH₃), 2.17-2.20 (1H, m, CH₂), 2.61-2.65 (1H, m, CH₂), 3.46-3.51 (1H, m, CH₂), 3.55-3.62 (2H, m, CH₂), 3.73-3.75 (1H, m, CH₂), 5.08 (1H, s, CH), 6.34 (1H, s, ArH), 6.95 (1H, d, J = 8.4 Hz, ArH), 7.07 (1H, d, J = 8.4 Hz, ArH), 7.19-7.31 (4H, m, ArH), 7.37-7.48 (5H, m, ArH), 8.30 (1H, s, OH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 14.7, 26.9, 52.1, 67.4, 72.4, 119.3, 120.1, 124.3, 125.4, 125.5, 127.0, 127.5, 127.8, 127.9, 128.1, 128.6, 129.1, 134.6, 139.8, 145.9, 146.4, 147.1, 154.1; MS (EI) m/z (%): 390 (3.69) [M⁺], 358 (75.52), 344 (18.09), 309 (12.50), 253 (36.14), 218 (27.00), 189 (9.53), 105 (100.00); HRMS (EI) Calcd. for C₂₅H₂₃O₂Cl (M⁺) requires 390.1387, Found: 390.1384.
**Compound 5e**: A colorless oil; IR (CH₂Cl₂): ν 3354, 3065, 2973, 2928, 2870, 1714, 1669, 1587, 1487, 1455, 1399, 1286, 1246, 1091, 1014, 929, 751 cm⁻¹; ¹H NMR (400 MHz, CDCl₃, TMS): δ 1.34 (3H, t, J = 7.2 Hz, CH₃), 2.21-2.28 (1H, m, CH₂), 2.55-2.59 (1H, m, CH₂), 3.42-3.49 (1H, m, CH₂), 3.55-3.64 (2H, m, CH₂), 3.70-3.74 (1H, m, CH₂), 5.13 (1H, s, CH), 6.36 (1H, d, J = 7.6 Hz, ArH), 6.73 (1H, t, J = 7.2 Hz, ArH), 7.02 (1H, d, J = 8.4 Hz, ArH), 7.08-7.17 (2H, m, ArH), 7.24-7.31 (5H, m, ArH), 7.41-7.45 (2H, m, ArH), 7.88 (1H, s, OH); ¹³C NMR (100 MHz, CDCl₃, TMS): δ 14.7, 27.0, 52.1, 67.2, 72.3, 117.5, 119.8, 124.4, 125.1, 125.6, 126.6, 127.4, 128.3, 128.5, 128.8, 129.2, 129.9, 135.0, 139.3, 146.0, 147.3, 148.0, 153.0. MS (EI) m/z (%): 424 (11.27) [M⁺], 392 (91.16), 378 (31.61), 338 (64.77), 253 (74.71), 218 (54.53), 139 (98.35), 59 (100.00); HRMS (EI) Calcd. for C₂₅H₂₂O₂Cl₂ (M⁺) requires 424.0997, Found: 424.1001.
Reference:

The crystal data of 3a have been deposited in CCDC with number 760083. Empirical Formula: C_{25}H_{24}O_2; Formula Weight: 356.44; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.402 x 0.307 x 0.231 mm; Crystal System: Monoclinic; Lattice Type: Primitive; Lattice Parameters: a = 9.4459(9)Å, b = 11.0752(10)Å, c = 18.8988(18)Å, α = 90°, β = 100.572(2)°, γ = 90°, V = 1943.5(3)Å³; Space group: P2(1)/n; Z = 4; D_{calc} = 1.218 g/cm³; F_{000} = 760; Diffractometer: Rigaku AFC7R; Residuals: R; Rw: 0.0479, 0.1174.
Table 1. Crystal data and structure refinement for cd29665.

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Table 2. Atomic coordinates ($x \times 10^4$) and equivalent isotropic displacement parameters ($\text{Å}^2 \times 10^3$) for cd29665. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized $U_{ij}$ tensor.

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Symmetry transformations used to generate equivalent atoms:
Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd29665. The anisotropic displacement factor exponent takes the form: 
\[-2 \pi^2 \left( h^2 a^* a^* U11 + \ldots + 2 h k a^* b^* U12 \right)\]

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S66
Table 5. Hydrogen coordinates (x 10^-4) and isotropic displacement parameters (Å^2 x 10^-3) for cd29665.

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Table 6. Torsion angles [deg] for cd29665.

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Symmetry transformations used to generate equivalent atoms:
Table 7. Hydrogen bonds for od29665 [Å and deg.].

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<th>d(H...A)</th>
<th>d(D...A)</th>
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The crystal data of 5a have been deposited in CCDC with number 739822. Empirical Formula: C$_{25}$H$_{24}$O$_2$; Formula Weight: 356.44; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.401 x 0.311 x 0.269 mm; Crystal System: Monoclinic; Lattice Type: Primitive; Lattice Parameters: a = 15.829(2)Å, b = 7.5020(12)Å, c = 16.492(3)Å, α = 90°, β = 95.853(3)°, γ = 90°, V = 1948.2(5)Å$^3$; Space group: P2(1)/n; Z = 4; $D_{calc}$ = 1.215 g/cm$^3$; $F_{000}$ = 760; Diffractometer: Rigaku AFC7R; Residuals: R; Rw: 0.0593, 0.1714.
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<th><strong>Table 1. Crystal data and structure refinement for cd29352.</strong></th>
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<td><strong>Wavelength</strong></td>
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<td><strong>Crystal system, space group</strong></td>
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<tr>
<td><strong>Volume</strong></td>
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<td><strong>Z, Calculated density</strong></td>
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<td><strong>Absorption coefficient</strong></td>
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<td><strong>F(000)</strong></td>
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<td><strong>Crystal size</strong></td>
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<td><strong>Theta range for data collection</strong></td>
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<td><strong>Limiting indices</strong></td>
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<td><strong>Reflections collected / unique</strong></td>
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<td><strong>Goodness-of-fit on F²</strong></td>
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<td><strong>Final R indices [I&gt;2sigma(I)]</strong></td>
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<td><strong>Largest diff. peak and hole</strong></td>
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Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for cad3952.

*U(eq)* is defined as one third of the trace of the orthogonalized U_{ij} tensor.

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Table 3. Bond lengths [Å] and angles [deg] for cd29352.

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C(24)→C(25)→H(25C) 109.5

Symmetry transformations used to generate equivalent atoms:
Table 4. Anisotropic displacement parameters (Å² × 10⁻³) for cd29352. The anisotropic displacement factor exponent takes the form: -2 π² u | h² a⁺² U11 + ... + 2 h k a⁺ b⁺ U12 |

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Table 5. Hydrogen coordinates ($x \times 10^4$) and isotropic displacement parameters (A$^2 \times 10^3$) for cd29352.

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Symmetry transformations used to generate equivalent atoms:
Table 7. Hydrogen bonds for cd29352 [Å and deg.].

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Symmetry transformations used to generate equivalent atoms: