

## Supporting Information

### Triflic Imide-Catalyzed Cycloaddition and Friedel-Crafts Reaction of Diarylvinyldenecyclopropanes and Ethyl 5,5-Diarylpenta-2,3,4-trienoate

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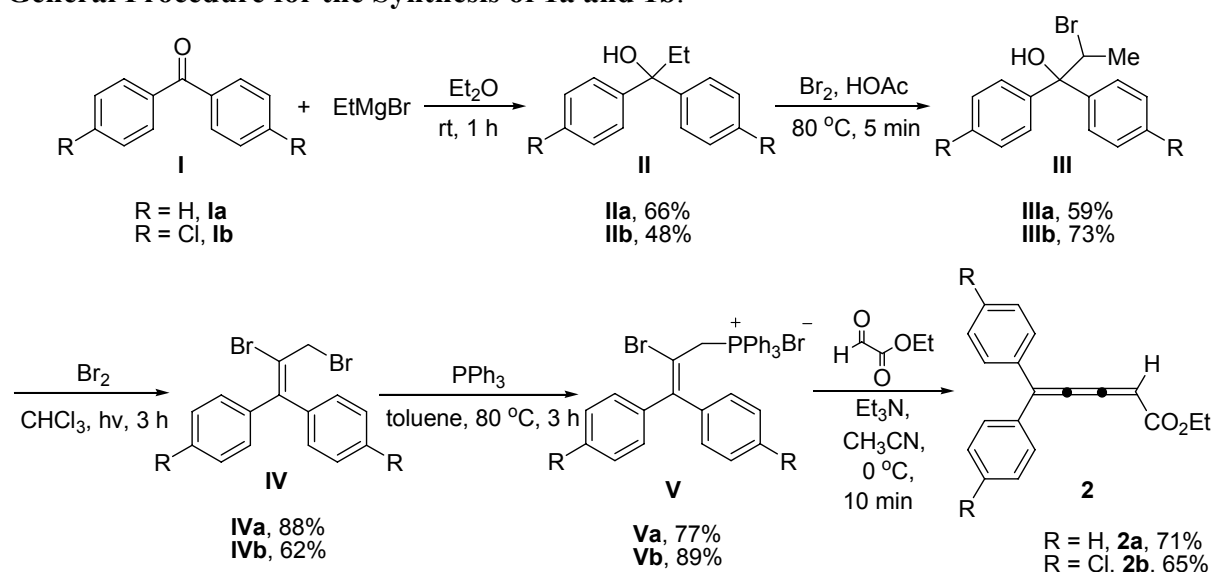
[Mshi@mail.sioc.ac.cn](mailto:Mshi@mail.sioc.ac.cn). Fax 86-21-64166128

#### Content

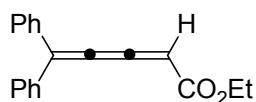
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**General remarks.**  $^1\text{H-NMR}$  spectra were recorded on a 300 MHz spectrometer in  $\text{CDCl}_3$  using tetramethylsilane as the internal standard. Infrared spectra were measured on a spectrometer. Mass spectra were recorded by EI method, and HRMS was measured on Kratos Analytical Concept mass spectrometer (EI), and IonSpec 4.7 Tesla FFMS (MALDI). Satisfactory CHN microanalyses were obtained with an analyzer. Melting points are uncorrected. All reactions were monitored by TLC with silica gel coated plates. Flash Column Chromatography was carried out using 300-400 mesh silica gel at increased pressure.

### General Procedure for the Synthesis of **1a** and **1b**.

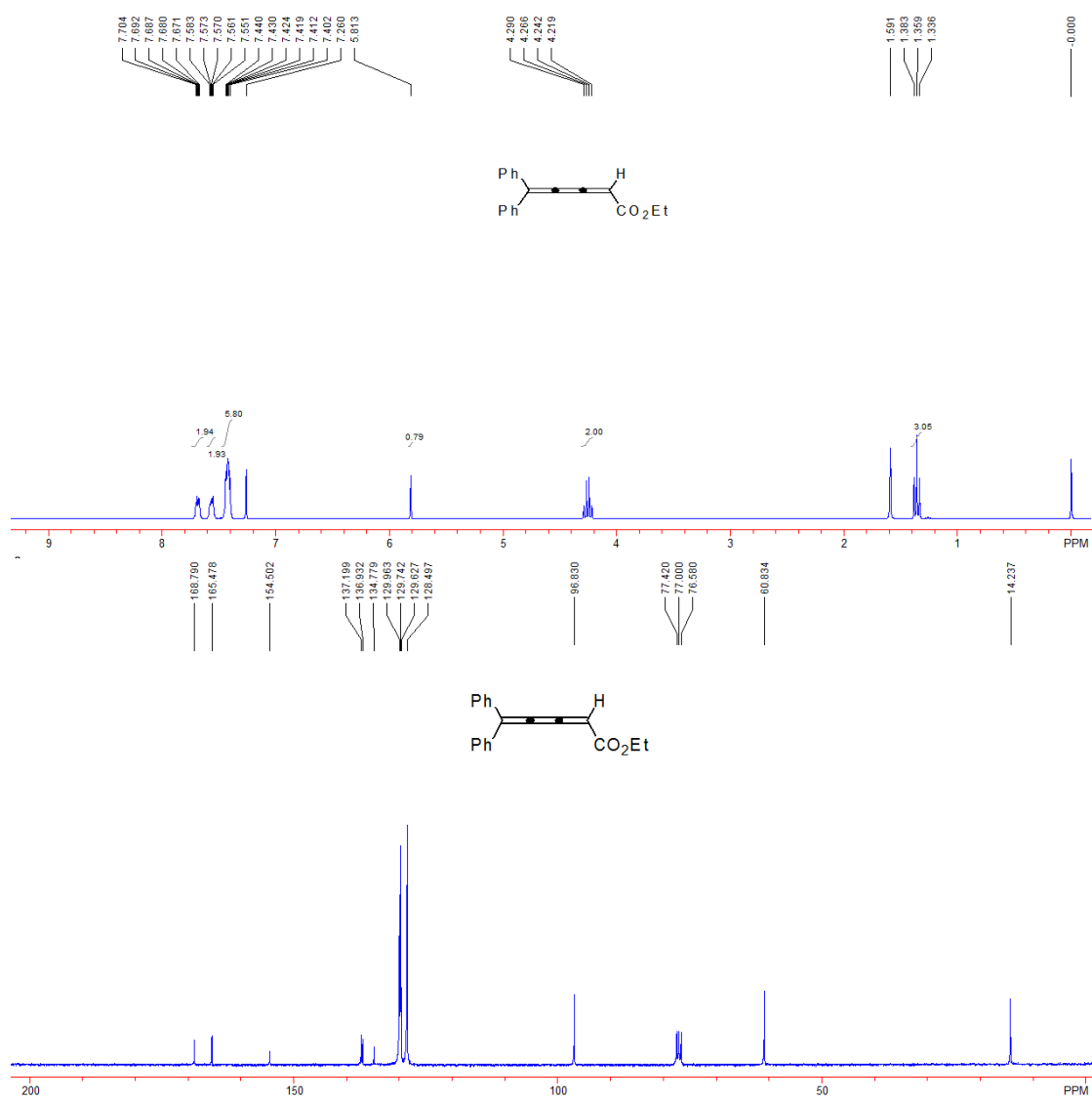


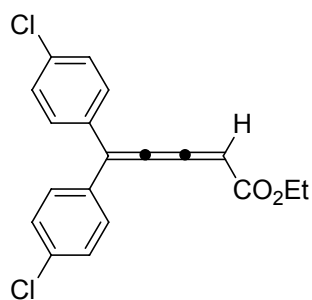
According to the previous literature,<sup>1</sup> the compound **Va** was synthesized starting from **1a**. In a 25 mL of RB flask, **Va** (1.0 g, 1.63 mmol) was dissolved in 10 mL of  $\text{CH}_3\text{CN}$  and the solution was cooled to 0 °C. Ethyl glyoxylate (449 mg of its 50% solution in toluene, 2.45 mmol) was added at 0 °C, then  $\text{Et}_3\text{N}$  (329 mg, 3.26 mmol) was added dropwise. The mixture was stirred at 0 °C for 5 minutes and the mixture was purified by flash column chromatography ( $\text{SiO}_2$ , eluent: Petroleum ether) without removal of the solvent. The solvent was removed under reduced pressure from the collected eluents without heating to yield the corresponding product **2a** (320 mg, 71%) as a yellow powder. Using the similar procedure, compound **2b** could be synthesized.



**ethyl 5,5-diphenylpenta-2,3,4-trienoate 2a.**

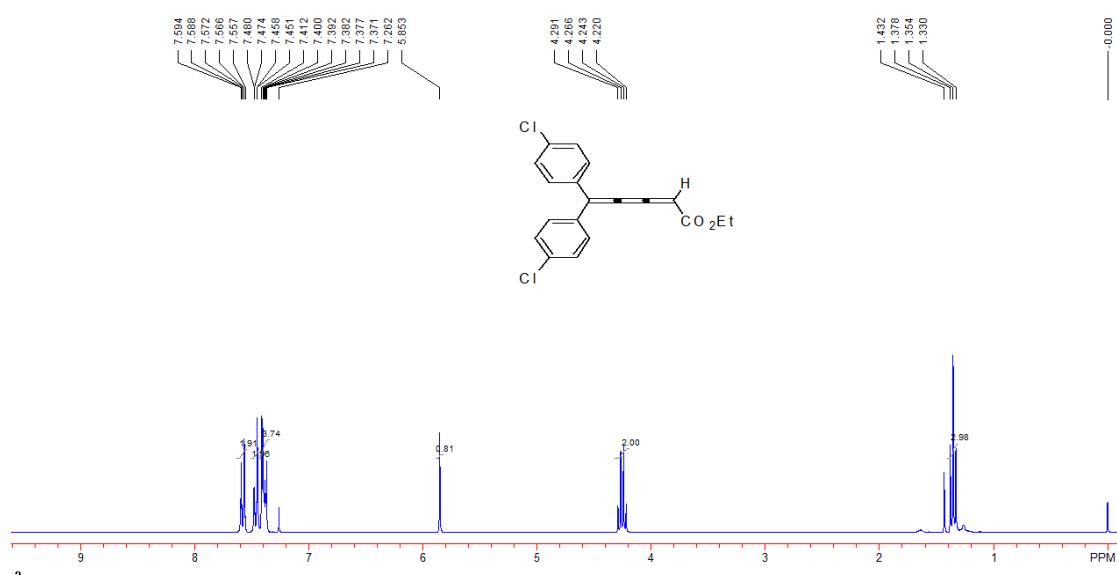
A yellow solid, Mp: 83-85 °C. <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 1.36 (t, 3H, *J* = 7.2 Hz), 4.25 (q, 2H, *J* = 7.2 Hz), 5.81 (s, 1H), 7.40-7.44 (m, 6H), 7.55-7.58 (m, 2H), 7.67-7.70 (m, 2H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, TMS) δ 14.2, 60.8, 96.8, 128.5, 129.6, 129.7, 130.0, 134.8, 136.9, 137.2, 154.5, 165.5, 168.8; IR (CH<sub>2</sub>Cl<sub>2</sub>): ν 3056, 2980, 2925, 2359, 2341, 2053, 1733, 1699, 1489, 1446, 1365, 1329, 1243, 1185, 1150, 757, 692 cm<sup>-1</sup>; MS (EI) *m/z* (%): 276 [M<sup>+</sup>] (73.2), 202 (100.0), 204 (78.0), 203 (73.5), 276 (73.2), 231 (25.7), 201 (25.1), 200 (21.5), 101 (17.8); HRMS (EI) Calcd. for C<sub>19</sub>H<sub>16</sub>O<sub>2</sub> (M<sup>+</sup>) requires 276.1150, Found: 276.1153.

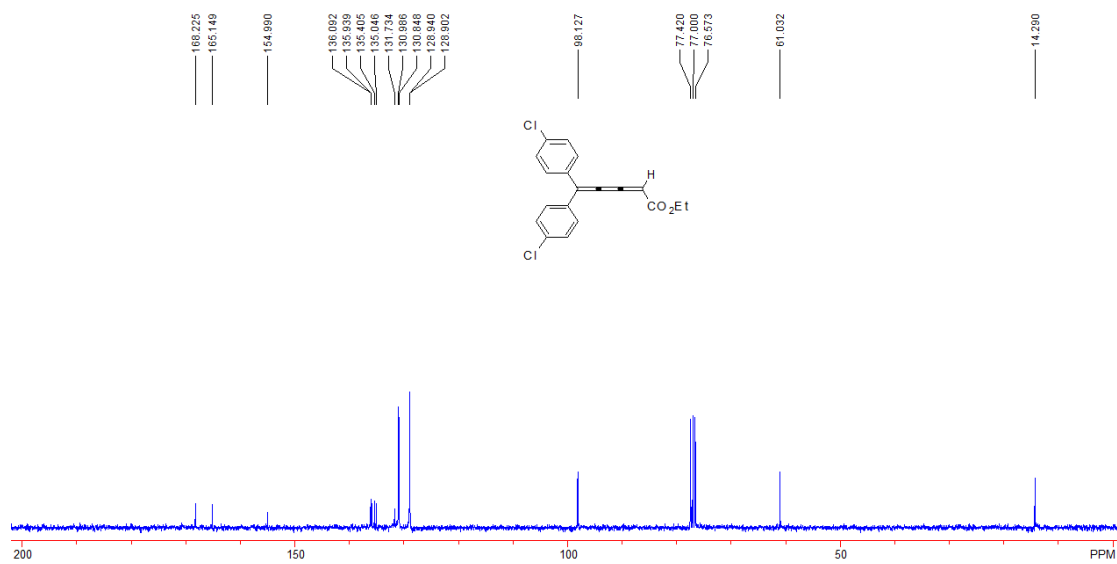




**ethyl 5,5-bis(4-chlorophenyl)penta-2,3,4-trienoate 2b.**

A yellow solid, Mp: 87-89 °C.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, TMS)  $\delta$  1.36 (t, 3H,  $J = 6.9$  Hz), 4.25 (q, 2H,  $J = 6.9$  Hz), 5.85 (s, 1H), 7.37-7.41 (m, 4H), 7.45-7.48 (m, 2H), 7.56-7.59 (m, 2H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, TMS)  $\delta$  14.3, 61.0, 98.1, 128.90, 128.94, 130.8, 131.0, 131.7, 135.0, 135.4, 135.9, 136.1, 155.0, 165.1, 168.2; IR ( $\text{CH}_2\text{Cl}_2$ ):  $\nu$  3053, 2980, 2359, 2341, 2053, 1702, 1585, 1488, 1405, 1366, 1322, 1300, 1244, 1189, 1152, 1092, 1012, 833, 749  $\text{cm}^{-1}$ ; MS (EI)  $m/z$  (%): 344 [ $\text{M}^+$ ] (8.0), 57 (100.0), 91 (63.4), 56 (49.5), 131 (43.6), 92 (39.7), 77 (29.8), 128 (29.3), 55 (27.4); HRMS (EI) Calcd. for  $\text{C}_{19}\text{H}_{14}\text{Cl}_2\text{O}_2$  ( $\text{M}^+$ ) requires 344.0371, Found: 344.0369.

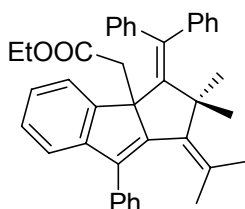




### General procedure for the cycloaddition of diarylvinylenecyclopropanes **1** with ethyl 5,5-diarylpenta-2,3,4-trienoate **2**.

**Procedure A:** Diarylvinylenecyclopropanes (VDCPs) **1** (0.18 mmol) and ethyl 5,5-diarylpenta-2,3,4-trienoate **2** (0.22 mmol, 1.2 equiv) were dissolved in CH<sub>2</sub>Cl<sub>2</sub> (3 mL), then Tf<sub>2</sub>NH (2 mg, 4 mol %) was added. The mixture was stirred for 4 to 5 days at room temperature (25 °C). The solvent was removed in vacuo, and the residue was purified by flash column chromatography on silica gel column with petroleum ether-EtOAc (50:1) as an eluent.

**Procedure B:** Diarylvinylenecyclopropanes (VDCPs) **1** (0.18 mmol) and ethyl 5,5-diarylpenta-2,3,4-trienoate **2** (0.22 mmol, 1.2 equiv) were dissolved in CH<sub>2</sub>Cl<sub>2</sub> (3 mL), and then Tf<sub>2</sub>NH (2 mg, 4 mol %) was added at 40 °C. The mixture was stirred for several hours at this temperature till the substrates were consumed. The solvent was removed in vacuo, and the residue was purified by flash column chromatography on silica gel column with petroleum ether-EtOAc (50:1) as an eluent.

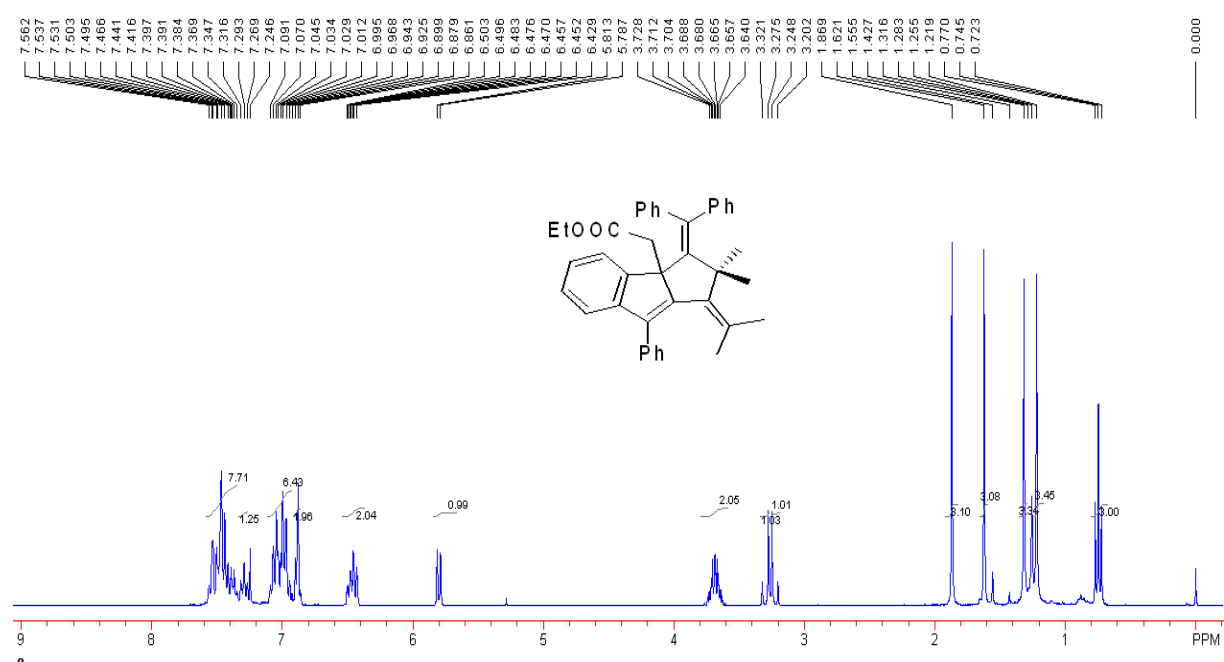


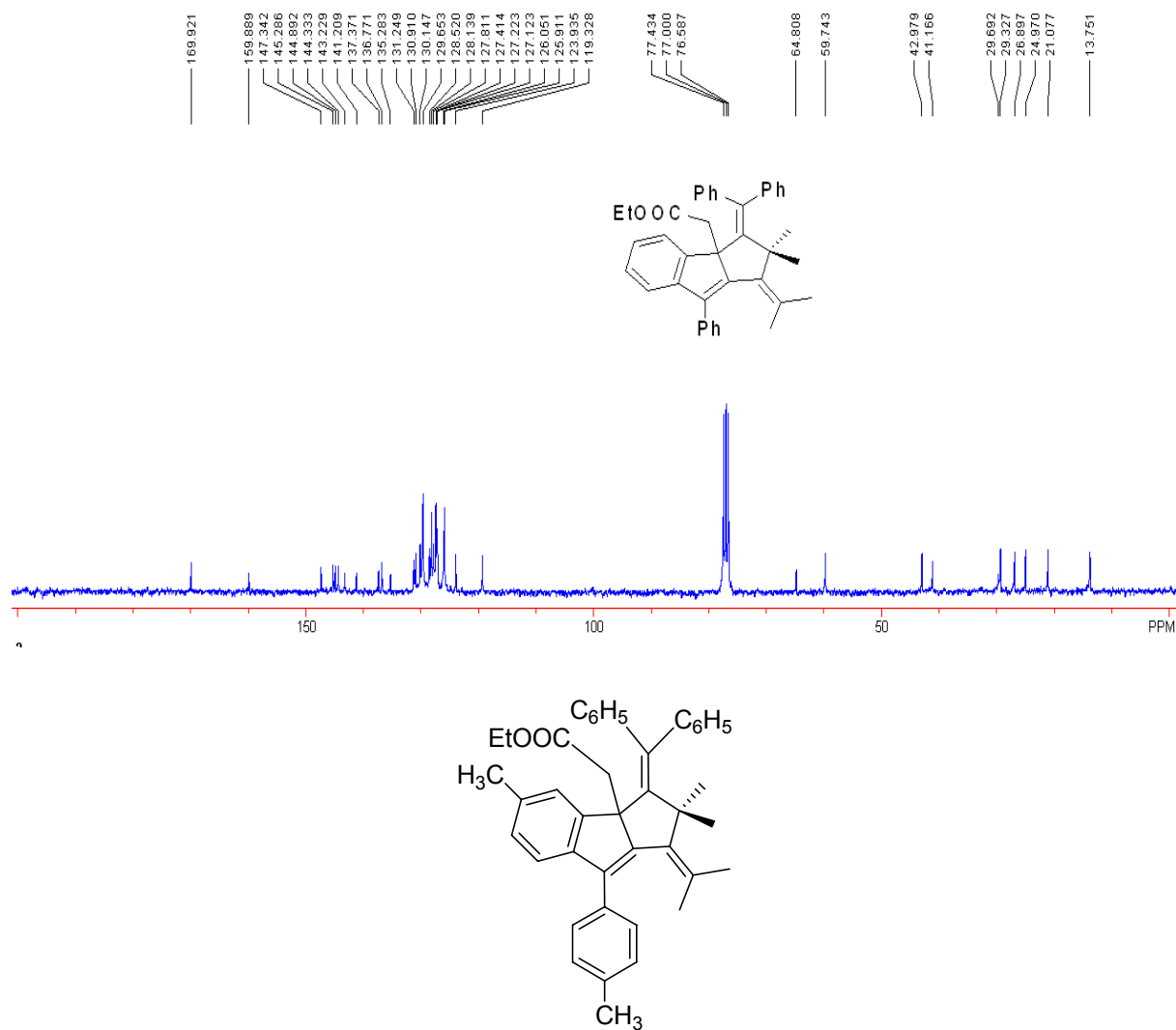
ethyl

### 2-(3-(diphenylmethylene)-2,2-dimethyl-8-phenyl-1-(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate **3a**.

A white solid, Mp: 210-212 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 0.75 (t, *J* = 6.9 Hz, 3H,

CH<sub>3</sub>), 1.22 (s, 3H, CH<sub>3</sub>), 1.32 (s, 3H, CH<sub>3</sub>), 1.62 (s, 3H, CH<sub>3</sub>), 1.87 (s, 3H, CH<sub>3</sub>), 3.22 (d, *J* = 13.5 Hz, 1H), 3.30 (d, *J* = 13.5 Hz, 1H), 3.61-3.76 (m, 2H, CH<sub>2</sub>), 5.80 (d, *J* = 7.8 Hz, 1H, Ar), 6.43-6.50 (m, 2H, Ar), 6.86-6.90 (m, 2H, Ar), 6.94-7.09 (m, 6H, Ar), 7.27-7.32 (m, 1H, Ar), 7.37-7.56 (m, 7H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, TMS) δ 13.7, 21.1, 25.0, 26.9, 29.3, 41.2, 43.0, 59.7, 64.8, 119.3, 123.9, 125.9, 126.0, 127.1, 127.2, 127.4, 127.8, 128.1, 128.5, 129.7, 130.1, 130.9, 131.2, 135.3, 136.8, 137.4, 141.2, 143.2, 144.3, 144.9, 145.3, 147.3, 159.9, 169.9. IR (CH<sub>2</sub>Cl<sub>2</sub>) ν 3057, 3021, 2976, 2931, 2903, 2867, 1950, 1630, 1597, 1491, 1462, 1442, 1386, 1366, 1310, 1266, 1169, 1114, 1094, 1031, 779, 761, 701, 608, 597 cm<sup>-1</sup>. MS (%) *m/e* 550 (M<sup>+</sup>, 100), 535 (17), 463 (85), 462 (43), 448 (26), 447 (53), 372 (19), 230 (15), 215 (14). Anal. calcd. for C<sub>40</sub>H<sub>38</sub>O<sub>2</sub>: C, 87.23%; H, 6.95%. Found: C, 86.91%; H, 7.00%.



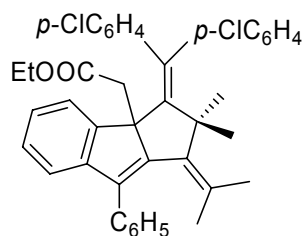
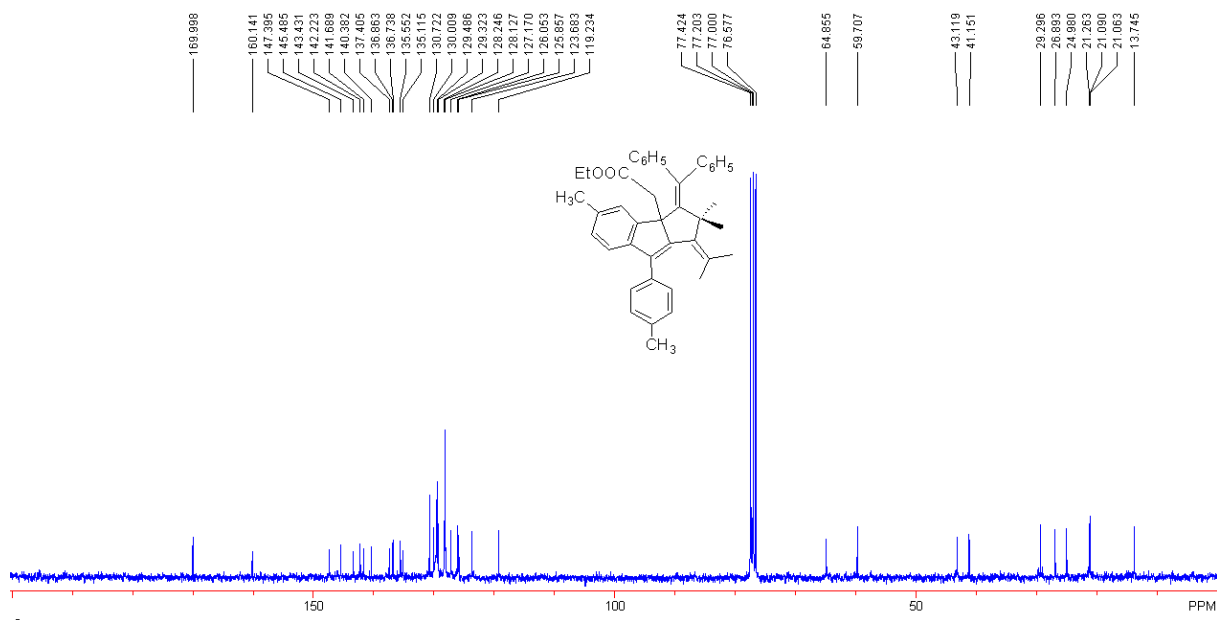
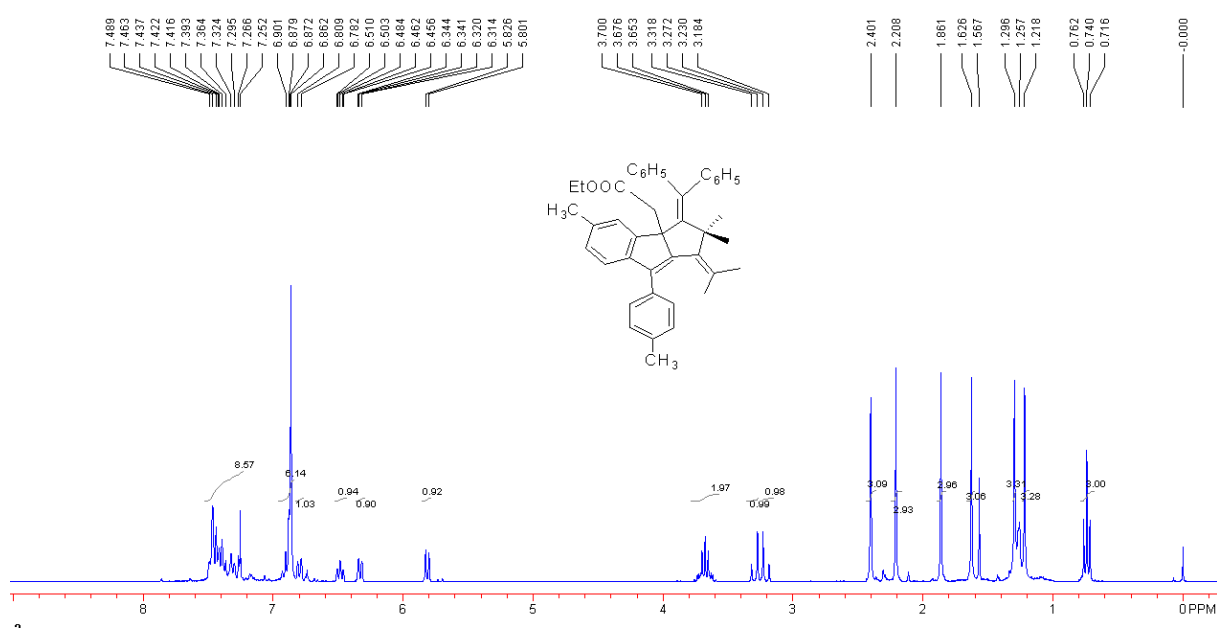


ethyl

**2-(3-(diphenylmethylene)-2,2,5-trimethyl-1-(propan-2-ylidene)-8-*p*-tolyl-1,2,3,3a-tetrahydrocyclopenta[*a*]inden-3a-yl)acetate 3b.**

A white solid, Mp: 150-152 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 0.74 (t, *J* = 6.9 Hz, 3H, CH<sub>3</sub>), 1.22 (s, 3H, CH<sub>3</sub>), 1.30 (s, 3H, CH<sub>3</sub>), 1.63 (s, 3H, CH<sub>3</sub>), 1.86 (s, 3H, CH<sub>3</sub>), 2.21 (s, 3H, CH<sub>3</sub>), 2.40 (s, 3H, CH<sub>3</sub>), 3.21 (d, *J* = 13.8 Hz, 1H), 3.29 (d, *J* = 13.8 Hz, 1H), 3.62-3.74 (m, 2H, CH<sub>2</sub>), 5.81 (d, *J* = 7.5 Hz, 1H, Ar), 6.33 (dd, *J* = 7.5, 1.8 Hz, 1H, Ar), 6.48 (dt, *J* = 7.2, 1.8 Hz, 1H, Ar), 6.79 (d, *J* = 7.5 Hz, 1H, Ar), 6.86-6.93 (m, 6H, Ar), 7.29-7.49 (m, 7H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, TMS) δ 13.7, 21.06, 21.09, 21.3, 25.0, 26.9, 29.3, 41.2, 43.1, 59.7, 64.9, 119.2, 123.7, 125.9, 126.1, 127.2, 128.1, 128.2, 129.3, 129.5, 130.0, 130.7, 135.1, 135.6, 136.7, 136.9, 137.4, 140.4, 141.7, 142.2, 143.4, 145.5, 147.4, 160.1, 170.0. IR (CH<sub>2</sub>Cl<sub>2</sub>) ν 3021, 2975, 2927, 2866, 1731, 1597, 1508, 1492, 1461, 1443, 1366, 1306, 1266, 1213, 1166, 1114, 1094, 1036, 819, 747, 702, 549 cm<sup>-1</sup>. MS (%) *m/e* 578 (M<sup>+</sup>, 40), 491 (45), 475 (36), 461 (29), 386 (21), 305 (17), 238 (53), 230 (100), 215 (78), 105 (68). HRMS (EI) for C<sub>42</sub>H<sub>42</sub>O<sub>2</sub>:

578.3185; Found: 578.3188.



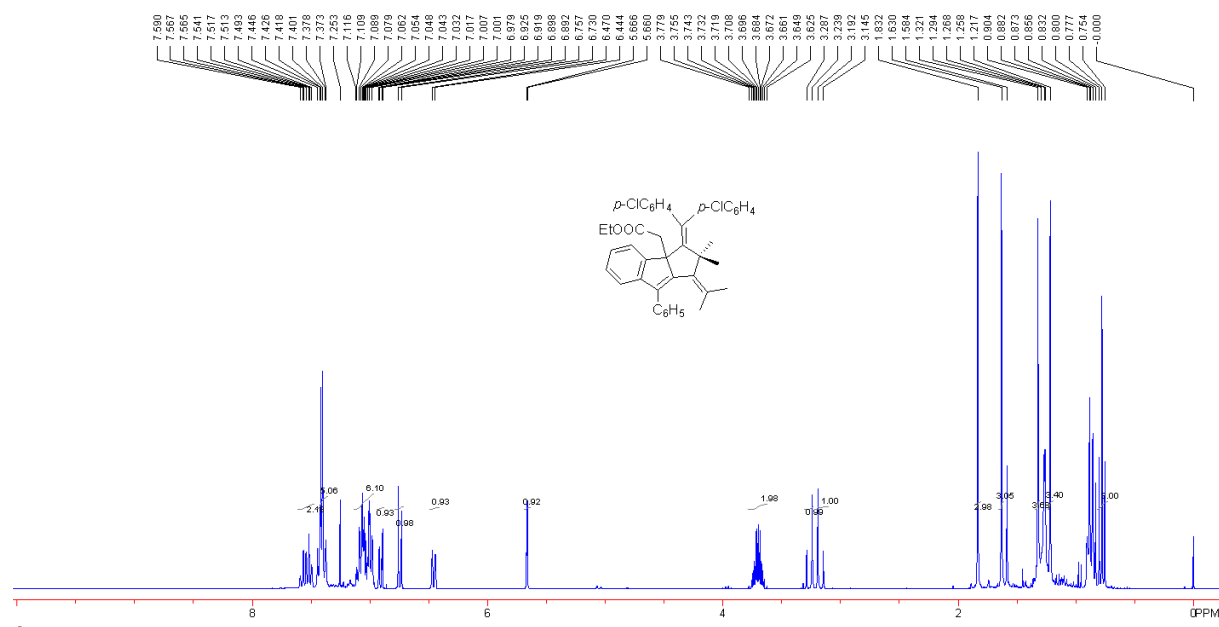
ethyl

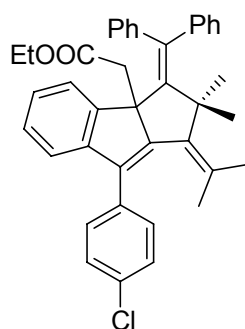
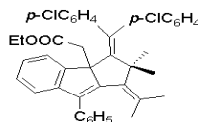
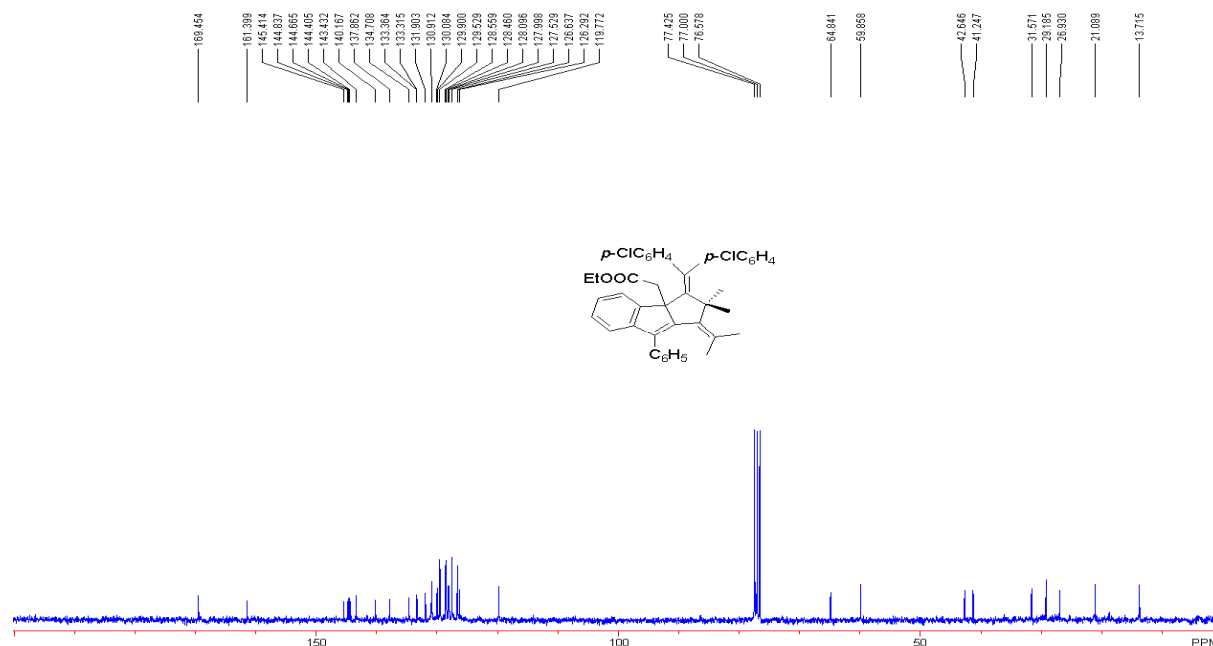
**2-(3-(bis(4-chlorophenyl)methylene)-2,2-dimethyl-8-phenyl-1-(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate 3c.**

A white solid, Mp: 150-152 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, TMS) δ 0.78 (t, *J* = 7.2 Hz, 3H,



CH<sub>3</sub>), 1.22 (s, 3H, CH<sub>3</sub>), 1.32 (s, 3H, CH<sub>3</sub>), 1.63 (s, 3H, CH<sub>3</sub>), 1.83 (s, 3H, CH<sub>3</sub>), 3.17 (d, *J* = 14.1 Hz, 1H), 3.26 (d, *J* = 14.1 Hz, 1H), 3.65-3.75 (m, 2H, CH<sub>2</sub>), 5.67 (d, *J* = 2.8 Hz, 1H, Ar), 6.45 (d, *J* = 7.8 Hz, 1H, Ar), 6.74 (d, *J* = 7.8 Hz, 1H, Ar), 6.90 (dd, *J* = 2.4 Hz, *J* = 8.1 Hz, 1H, Ar), 6.98-7.09 (m, 6H, Ar), 7.37-7.45 (m, 5H, Ar), 7.49-7.59 (m, 2H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS) δ 13.7, 21.1, 26.9, 29.2, 31.6, 41.2, 42.6, 59.8, 64.8, 119.8, 126.3, 126.6, 127.5, 128.0, 128.1, 128.5, 128.6, 129.5, 129.9, 130.1, 130.9, 131.9, 133.3, 133.4, 134.7, 137.9, 140.2, 143.4, 144.4, 144.7, 144.8, 145.4, 161.4, 169.5. IR (CH<sub>2</sub>Cl<sub>2</sub>) ν 3078, 3057, 3018, 2976, 2931, 2904, 2855, 1731, 1637, 1595, 1570, 1489, 1458, 1442, 1412, 1397, 1366, 1309, 1277, 1260, 1198, 1164, 1120, 1090, 1059, 1031, 1016, 987, 912, 850, 824, 763, 763, 742, 699, 677, 650, 631, 593 cm<sup>-1</sup>. MS (%) *m/e* 618 (M<sup>+</sup>, 28), 531 (38), 277 (38), 263 (72), 233 (46), 207 (61), 167 (90), 91 (100). HRMS (EI) for C<sub>40</sub>H<sub>36</sub>O<sub>2</sub>Cl<sub>2</sub>: 618.2092; Found: 618.2091.



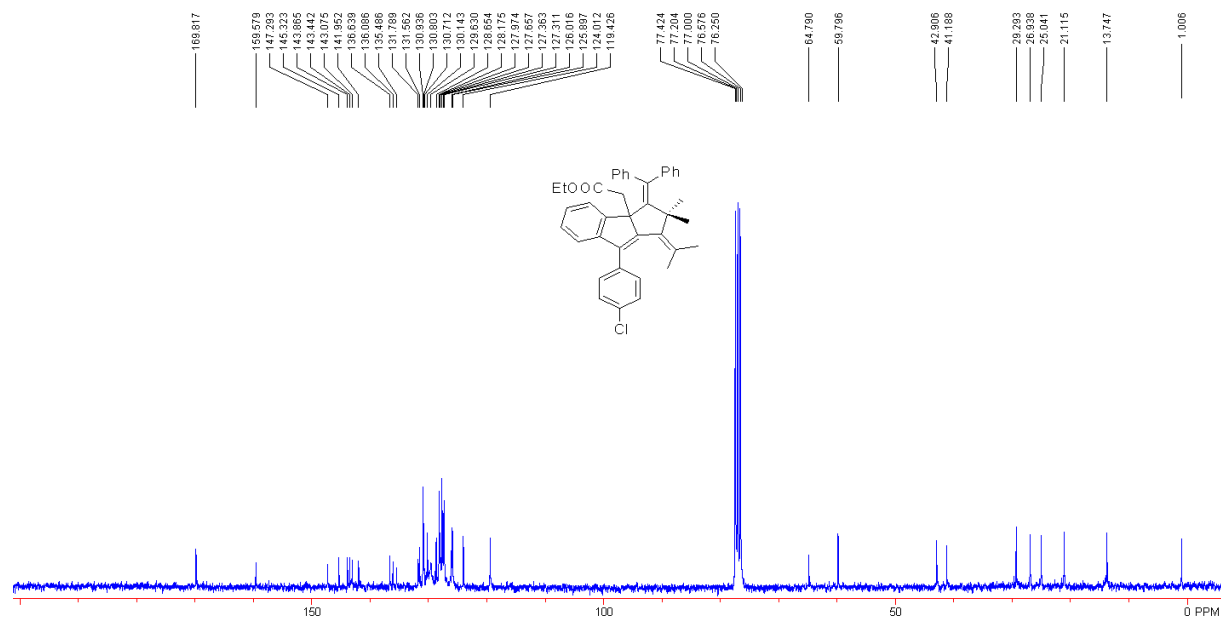
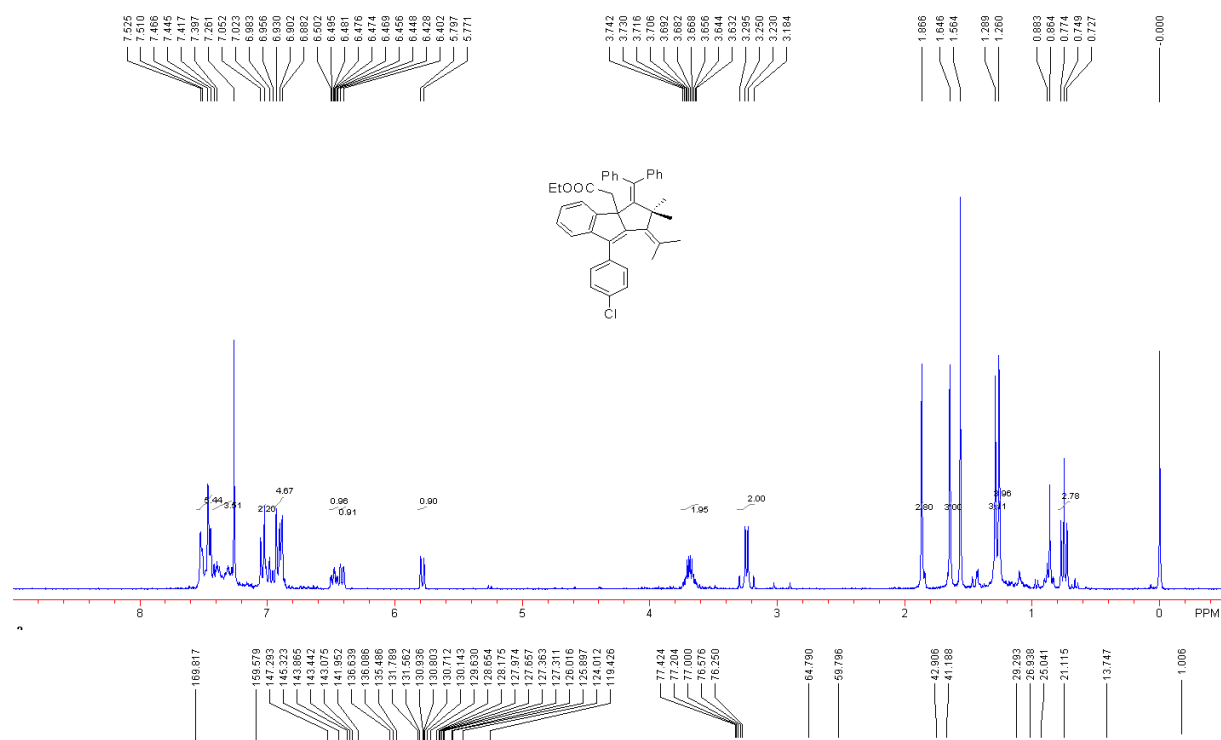


ethyl

**2-(8-(4-chlorophenyl)-2,2-dimethyl-1,3-di(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate 3f.**

A light yellow oil.  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 300 MHz, TMS)  $\delta$  0.75 (t,  $J = 7.2$  Hz, 3H,  $\text{CH}_3$ ), 1.26 (s, 3H,  $\text{CH}_3$ ), 1.29 (s, 3H,  $\text{CH}_3$ ), 1.65 (s, 3H,  $\text{CH}_3$ ), 1.87 (s, 3H,  $\text{CH}_3$ ), 3.21 (d,  $J = 13.8$  Hz, 1H), 3.28 (d,  $J = 13.8$  Hz, 1H), 3.61-3.74 (m, 2H,  $\text{CH}_2$ ), 5.79 (d,  $J = 7.5$  Hz, 1H, Ar), 6.41 (d,  $J = 7.5$  Hz, 1H, Ar), 6.45-6.50 (m, 1H, Ar), 6.88-6.90 (m, 4H, Ar), 6.93-7.02 (m, 3H, Ar), 7.13-7.17 (m, 1H, Ar), 7.28-7.33 (m, 2H, Ar), 7.37-7.40 (m, 1H, Ar), 7.44-7.47 (m, 3H, Ar), 7.50-7.52 (m, 2H, Ar).  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz, TMS)  $\delta$  13.7, 21.1, 25.0, 26.9, 29.3, 41.2, 42.9, 59.8, 64.8, 119.4, 124.0, 125.9, 126.0, 127.3, 127.4, 127.7, 128.0, 128.2, 128.7, 129.6, 130.1, 130.8, 130.9, 131.6, 131.8, 135.5, 136.1, 136.6, 142.0, 143.1, 143.4, 143.9, 145.3, 147.3, 159.6, 169.8. IR ( $\text{CH}_2\text{Cl}_2$ )  $\nu$  3058, 2970, 2929, 2871, 1730, 1596, 1489, 1461, 1443, 1394, 1367, 1304, 1264, 1214, 1166, 1118, 1090, 1071, 1035, 1014, 825, 749, 703, 681  $\text{cm}^{-1}$ . MS (%)  $m/e$  584 ( $\text{M}^+$ , 15), 497 (15), 341 (21), 252 (41), 133 (51), 105 (86), 71 (90), 57 (100).

HRMS (EI) for  $C_{40}H_{37}O_2Cl$ : 584.2482; Found: 584.2490.

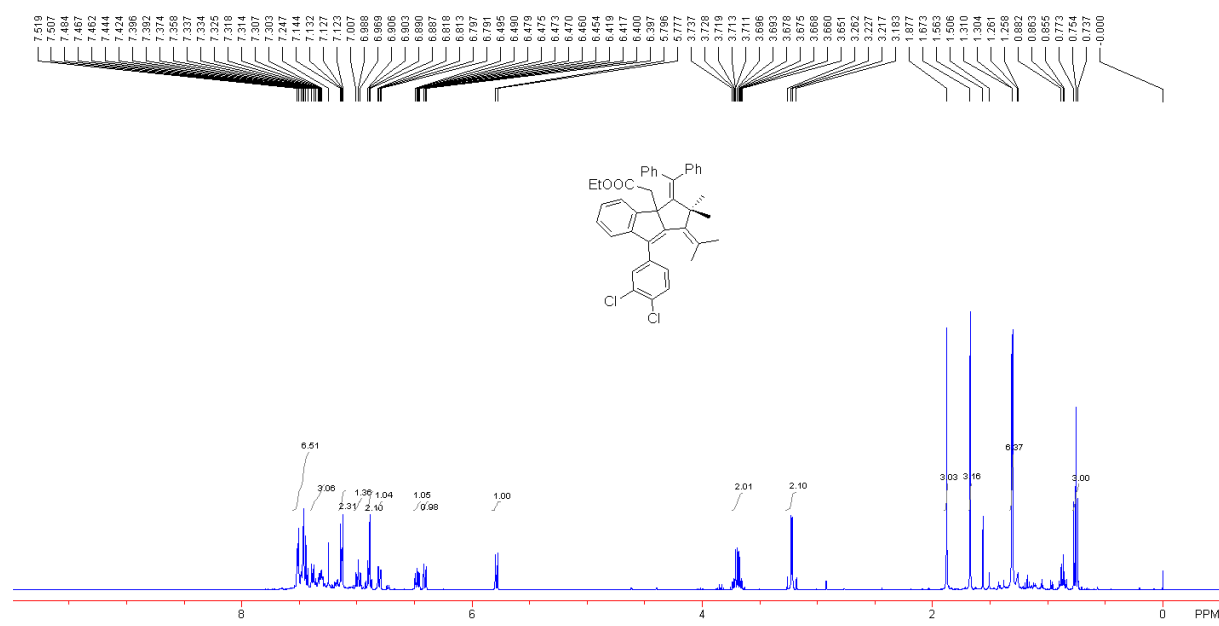


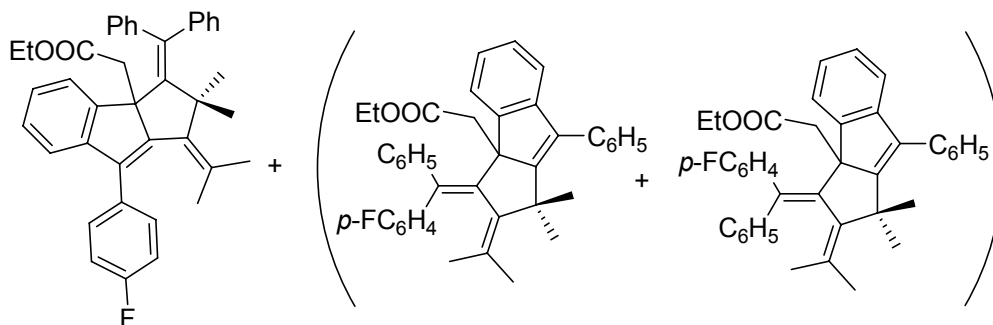
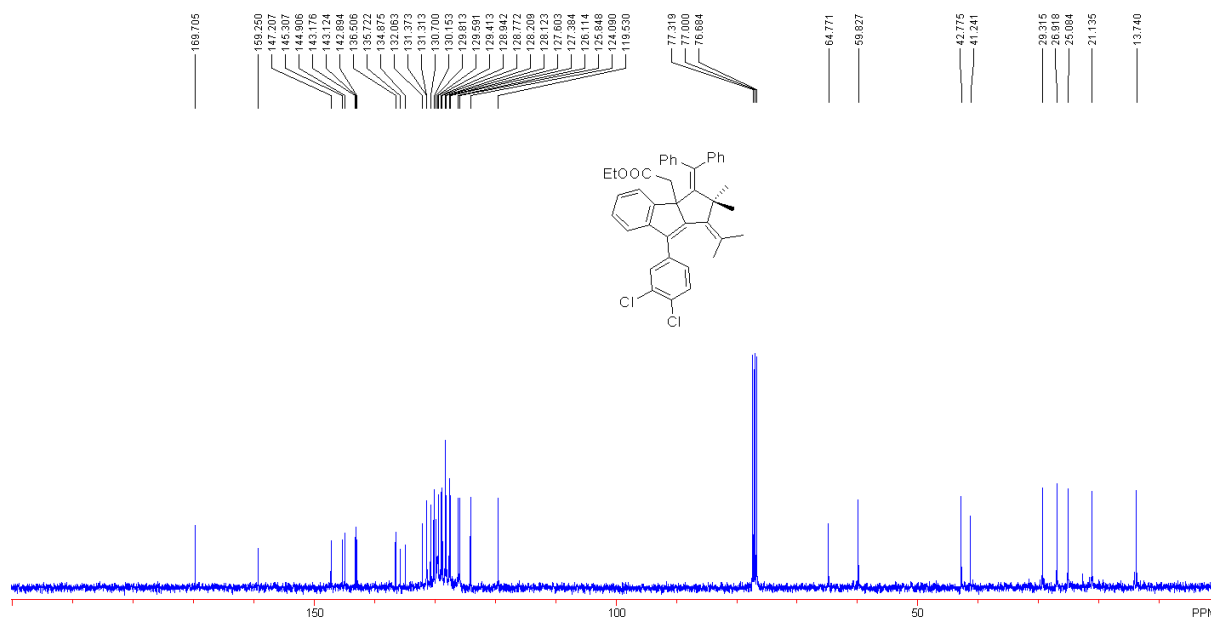
ethyl

2-(8-(3,4-dichlorophenyl)-2,2-dimethyl-1,3-di(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclo

**penta[a]inden-3a-yl)acetate 3g.**

A white solid, Mp: 95-97 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz, TMS) δ 0.76 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>), 1.31 (s, 3H, CH<sub>3</sub>), 1.31 (s, 3H, CH<sub>3</sub>), 1.67 (s, 3H, CH<sub>3</sub>), 1.88 (s, 3H, CH<sub>3</sub>), 3.20 (d, *J* = 13.6 Hz, 1H), 3.24 (d, *J* = 13.6 Hz, 1H), 3.63-3.76 (m, 2H, CH<sub>2</sub>), 5.79 (d, *J* = 7.6 Hz, 1H, Ar), 6.40 (dd, *J* = 7.6, 1.2 Hz, 1H, Ar), 6.47 (dt, *J* = 6.4, 2.0 Hz, 1H, Ar), 6.80 (dd, *J* = 2.0 Hz, *J* = 8.1 Hz, 1H, Ar), 6.87-6.91 (m, 1H, Ar), 6.99 (t, *J* = 7.8 Hz, 1H, Ar), 7.12-7.15 (m, 2H, Ar), 7.29-7.40 (m, 3H, Ar), 7.43-7.49 (m, 4H, Ar), 7.51 (d, *J* = 4.8 Hz, 2H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS) δ 13.7, 21.1, 25.1, 26.9, 29.3, 41.2, 42.8, 59.8, 64.8, 119.5, 124.1, 125.8, 126.1, 127.4, 127.6, 128.1, 128.2, 128.8, 128.9, 129.4, 129.8, 130.2, 130.7, 131.3, 131.4, 132.1, 134.9, 135.7, 136.5, 142.9, 143.1, 143.2, 144.9, 145.3, 147.2, 159.3, 169.7. IR (CH<sub>2</sub>Cl<sub>2</sub>) ν 3059, 2976, 2932, 1730, 1598, 1504, 1464, 1443, 1366, 1308, 1265, 1222, 1156, 1093, 1034, 1015, 836, 778, 703, 599, 531 cm<sup>-1</sup>. MS (%) *m/e* 618 (M<sup>+</sup>, 100), 532 (50), 531 (79), 515 (41), 341 (29), 230 (79), 215 (73), 91 (33). HRMS (EI) for C<sub>40</sub>H<sub>36</sub>O<sub>2</sub>Cl<sub>2</sub>: 618.2092; Found: 618.2086.





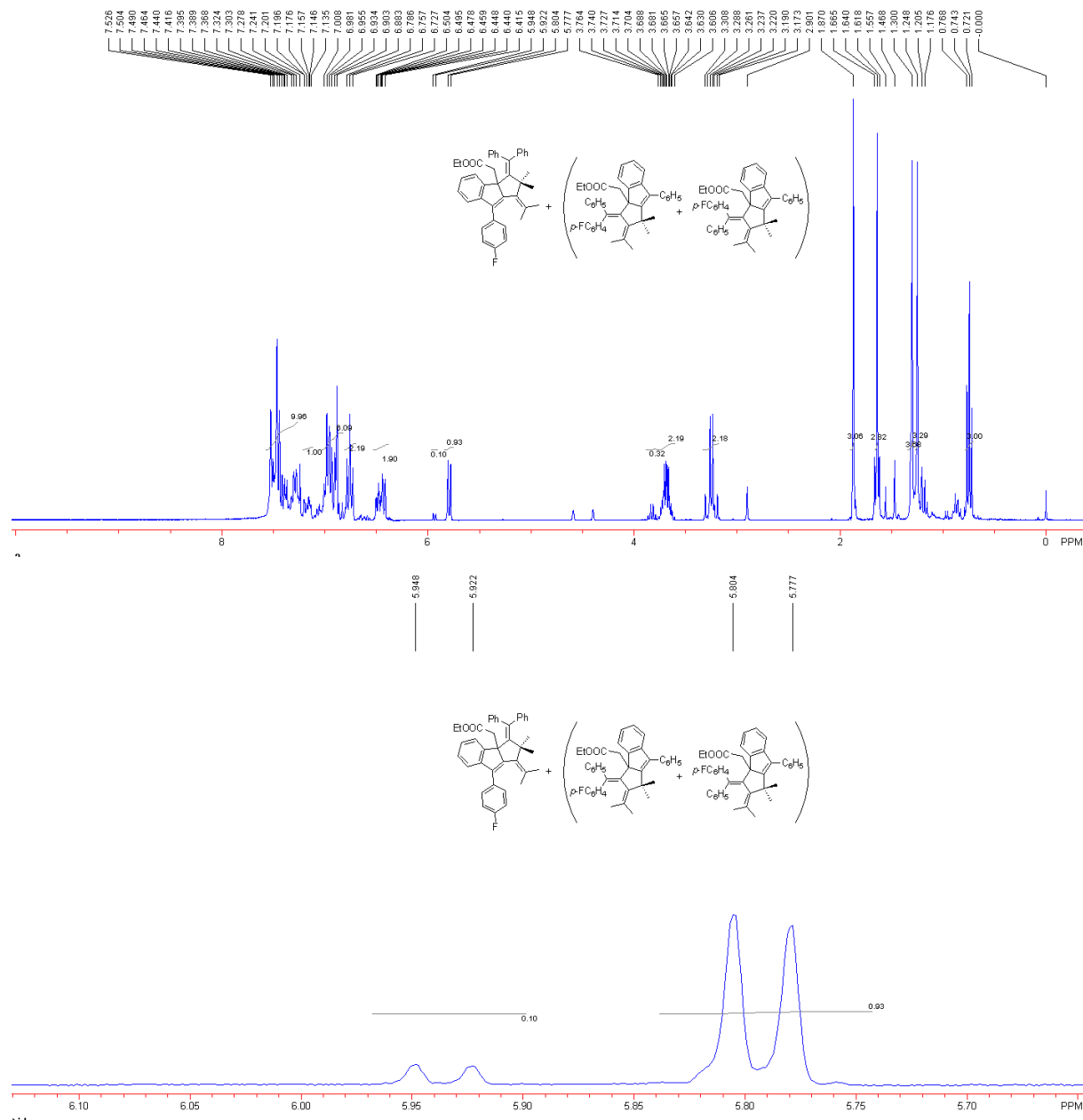
The ratio of **3h** : **4h** = 9 : 1

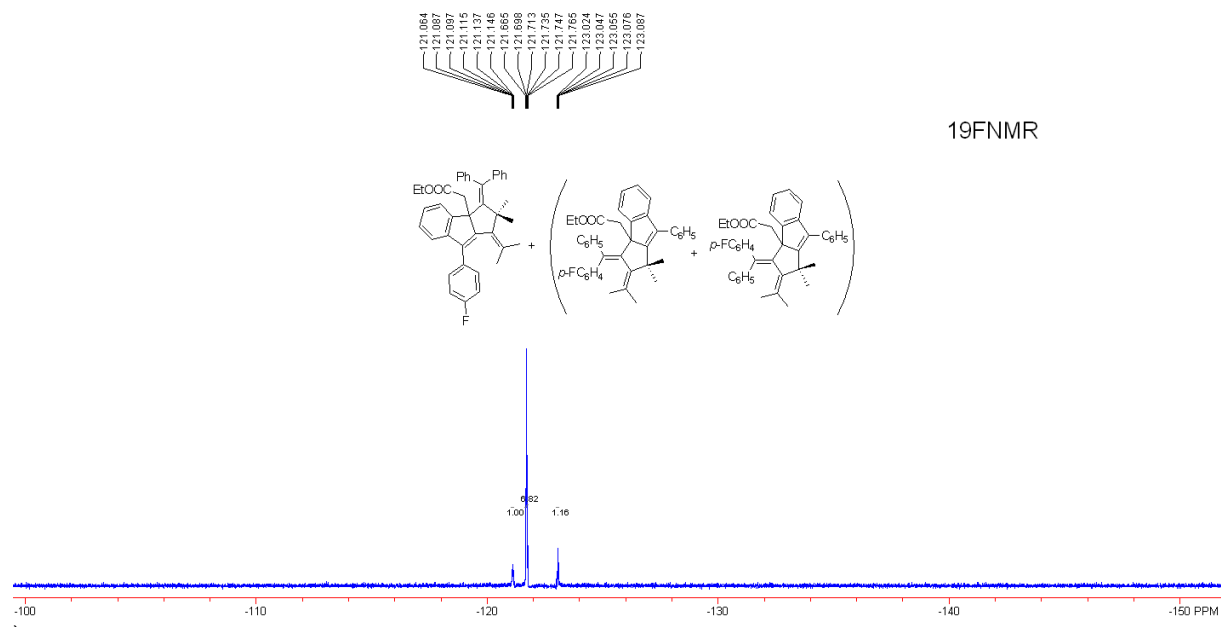
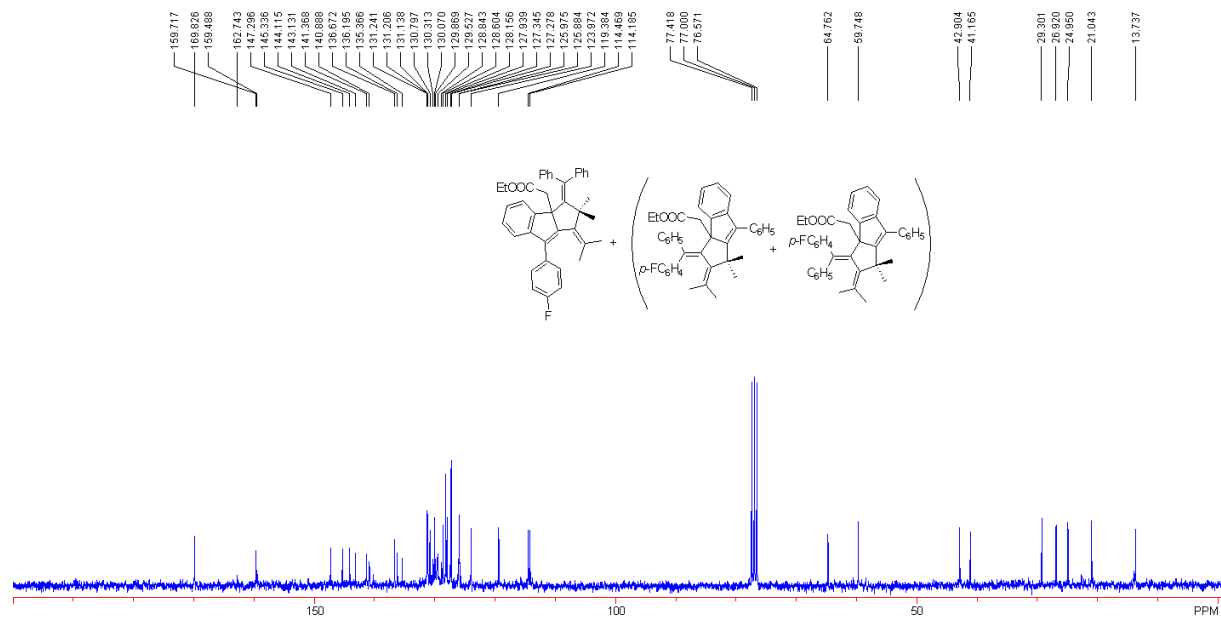
ethyl

**2-(3-(diphenylmethylene)-8-(4-fluorophenyl)-2,2-dimethyl-1-(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate** **3h** and ethyl **2-(3-((4-fluorophenyl)(phenyl)methylene)-1,1-dimethyl-8-phenyl-2-(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate** **4h**

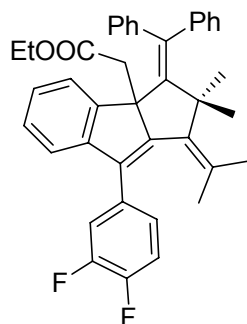
A white solid, Mp: 90-92 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 0.74 (t, *J* = 6.9 Hz, 3H, CH<sub>3</sub>), 1.25 (s, 3H, CH<sub>3</sub>), 1.30 (s, 3H, CH<sub>3</sub>), 1.64 (m, 3H, CH<sub>3</sub>), 1.87 (s, 3H, CH<sub>3</sub>), 3.17-3.31 (m, 2H, CH<sub>2</sub>), 3.63-3.74 (m, 2H, CH<sub>2</sub>), 5.79 (d, *J* = 7.8 Hz, 1H, Ar), 5.93 (d, *J* = 7.8 Hz, 0.1H, Ar), 6.42-6.50 (m, 2H, Ar), 6.76 (t, *J* = 8.7 Hz, 2H, Ar), 6.88-7.01 (m, 6H, Ar), 7.14-7.20 (m, 1H, Ar), 7.30-7.53 (m, 6H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, TMS) δ 13.7, 21.0, 25.0, 26.9, 29.3, 41.2, 42.9, 59.7, 64.8, 114.3 (d, *J*<sub>C-F</sub> = 21.3 Hz), 119.4, 124.0, 125.9 (d, *J*<sub>C-F</sub> = 6.8 Hz), 127.3, 128.2, 128.6, 128.8, 129.5, 129.9, 130.1, 130.3, 130.8, 131.1, 131.2 (d, *J*<sub>C-F</sub> = 2.6 Hz), 135.4, 136.2, 136.7, 140.9, 141.4, 143.1, 144.1, 145.3, 147.3, 159.7, 161.1 (d, *J*<sub>C-F</sub> = 244.1 Hz), 169.8. <sup>19</sup>F NMR (CDCl<sub>3</sub>, 282 MHz, CFCl<sub>3</sub>) δ -123.1, -121.7, -121.1. IR (CH<sub>2</sub>Cl<sub>2</sub>) ν 3056,

2973, 2931, 1730, 1598, 1581, 1505, 1490, 1443, 1391, 1367, 1306, 1268, 1223, 1188, 1157, 1117, 1090, 1035, 920, 866, 839, 779, 750, 702, 613  $\text{cm}^{-1}$ . MS (%)  $m/e$  568 ( $M^+$ , 36), 481 (42), 451 (57), 341 (40), 229 (100), 215 (67), 165 (17), 91 (19). HRMS (EI) for  $\text{C}_{40}\text{H}_{37}\text{O}_2\text{F}$ : 568.2778; Found: 568.2790.





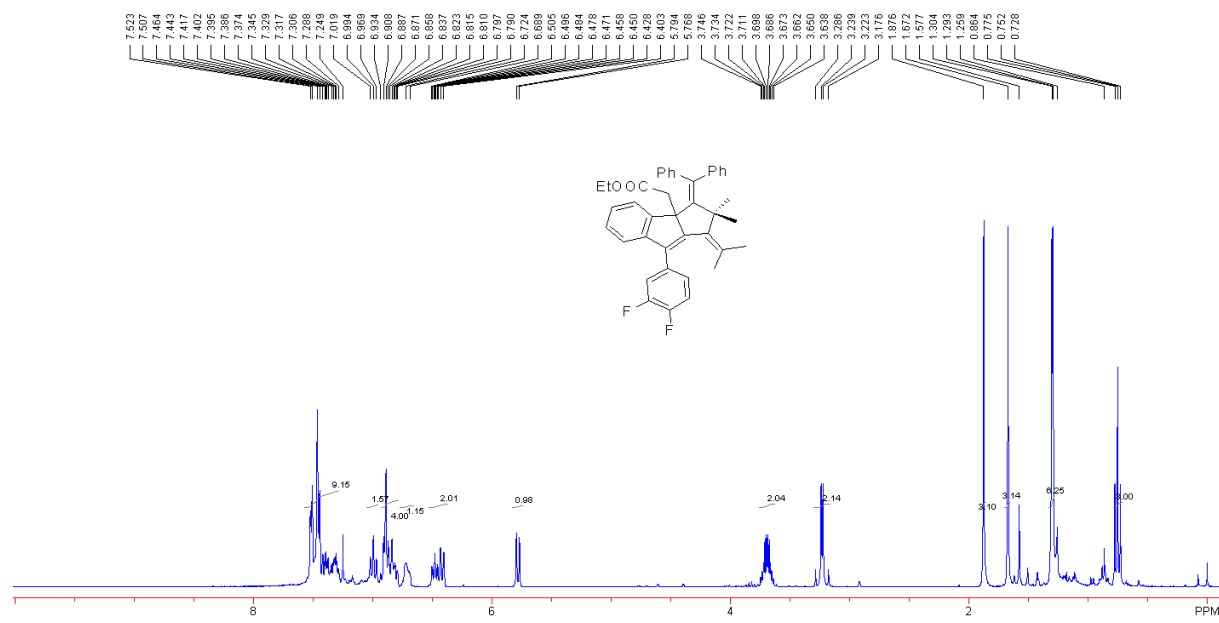
<sup>19</sup>F NMR



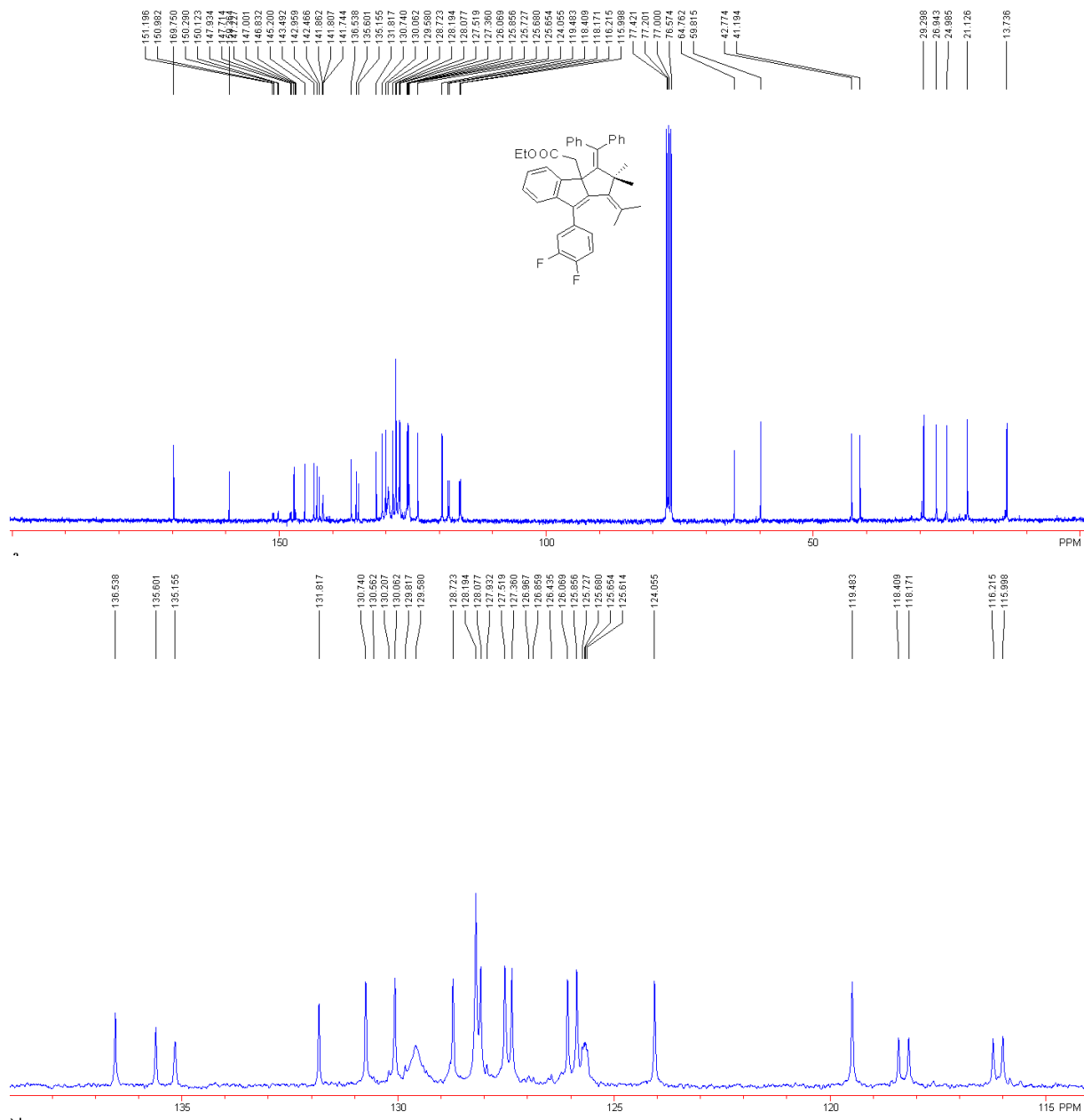
ethyl

**2-(8-(3,4-difluorophenyl)-2,2-dimethyl-1,3-di(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate 3i.**

A white solid, Mp: 100-102 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 0.75 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>), 1.29 (s, 3H, CH<sub>3</sub>), 1.30 (s, 3H, CH<sub>3</sub>), 1.67 (s, 3H, CH<sub>3</sub>), 1.88 (s, 3H, CH<sub>3</sub>), 3.20 (d, *J* = 13.8 Hz, 1H), 3.26 (d, *J* = 13.8 Hz, 1H), 3.64-3.75 (m, 2H, CH<sub>2</sub>), 5.78 (d, *J* = 7.5 Hz, 1H, Ar), 6.41 (d, *J* = 7.6 Hz, 1H, Ar), 6.45-6.51 (m, 1H, Ar), 6.69-6.72 (m, 1H, Ar), 6.79-6.91 (m, 4H, Ar), 6.99 (t, *J* = 7.5 Hz, 1H, Ar), 7.31-7.42 (m, 3H, Ar), 7.44-7.47 (m, 3H, Ar), 7.52 (d, *J* = 4.5 Hz, 2H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, TMS) δ 13.7, 21.1, 25.0, 26.9, 29.3, 41.2, 42.8, 59.8, 64.8, 116.1 (d, *J*<sub>C-F</sub> = 16.3 Hz), 118.3 (d, *J*<sub>C-F</sub> = 16.3 Hz), 119.5, 124.1, 125.7 (dd, *J*<sub>C-F</sub> = 3.0 Hz, *J*<sub>C-F</sub> = 3.5 Hz), 125.9, 126.1, 127.5 (d, *J*<sub>C-F</sub> = 11.9 Hz), 128.1, 128.2, 128.7, 129.6, 130.1, 130.7, 131.8, 135.2, 135.6, 136.5, 141.8 (dd, *J*<sub>C-F</sub> = 4.5 Hz, *J*<sub>C-F</sub> = 4.7 Hz), 142.5, 143.2 (d, *J*<sub>C-F</sub> = 40.0 Hz), 145.2, 147.2, 148.6 (dd, *J*<sub>C-F</sub> = 12.6 Hz, *J*<sub>C-F</sub> = 246.7 Hz), 149.5 (dd, *J*<sub>C-F</sub> = 12.6 Hz, *J*<sub>C-F</sub> = 244.9 Hz), 159.4, 169.8. <sup>19</sup>F NMR (CDCl<sub>3</sub>, 282 MHz, CFCl<sub>3</sub>) δ -144.6, -146.2. IR (CH<sub>2</sub>Cl<sub>2</sub>) ν 3058, 2976, 2928, 2855, 2360, 2342, 1731, 1599, 1511, 1492, 1459, 1443, 1367, 1299, 1267, 1204, 1171, 1113, 1094, 1072, 1034, 880, 821, 749, 702, 669, 598 cm<sup>-1</sup>. MS (%) *m/e* 586 (M<sup>+</sup>, 40), 499 (35), 483 (36), 341 (31), 242 (52), 230 (100), 215 (90), 203 (83). HRMS (EI) for C<sub>40</sub>H<sub>36</sub>O<sub>2</sub>F<sub>2</sub>Na: 609.2558; Found: 609.2576.





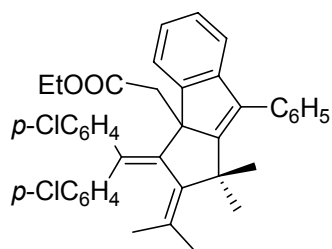
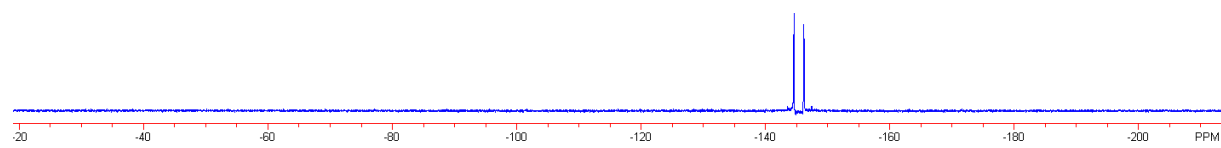
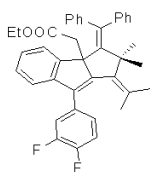
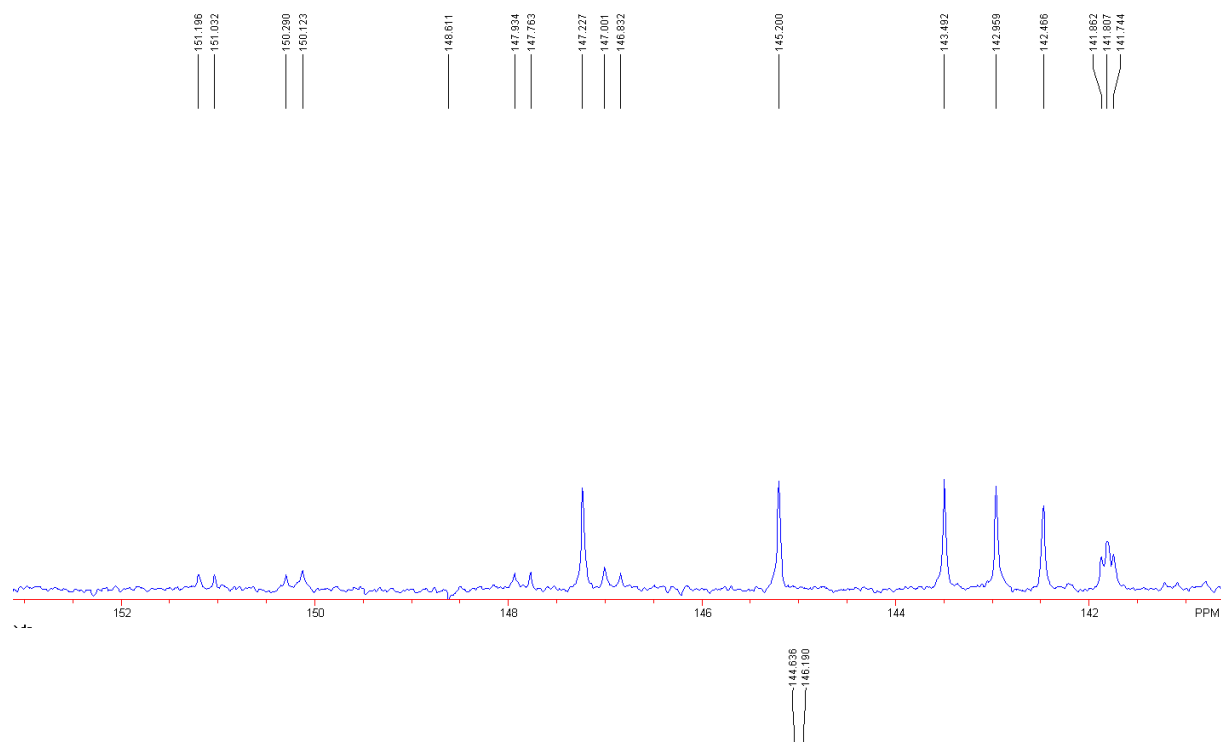


151.196  
150.982  
149.750  
150.290  
150.123  
147.934  
147.577  
147.577  
147.001  
146.832  
145.200  
143.492  
142.959  
141.982  
141.807  
141.744  
136.538  
135.601  
135.195  
135.195  
130.740  
130.740  
130.062  
128.817  
128.590  
128.723  
128.194  
128.077  
127.960  
127.960  
126.069  
125.856  
125.727  
125.680  
125.654  
125.654  
119.483  
119.483  
118.409  
118.171  
116.215  
115.998  
77.421  
77.000  
77.000  
76.574  
64.762  
59.815  
42.774  
41.194

29.298  
26.943  
24.985  
21.126  
13.736

136.538  
135.601  
135.155  
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130.740  
130.562  
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128.194  
128.077  
127.960  
127.519  
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125.654  
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116.215  
115.998

135  
130  
125  
120  
115 PPM

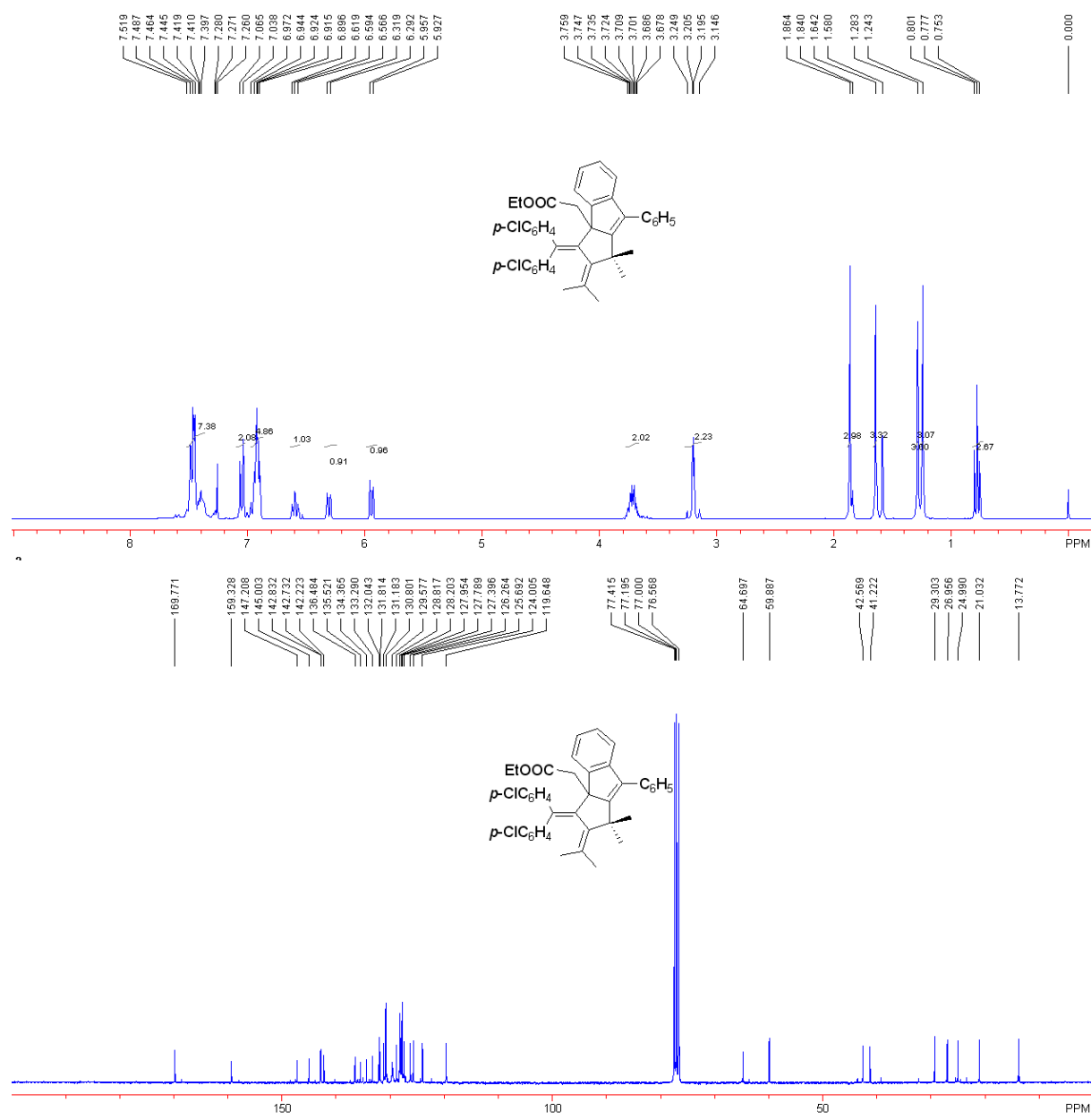


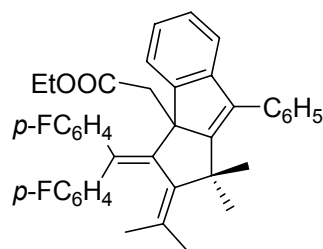
ethyl

**2-(3-(bis(4-chlorophenyl)methylene)-1,1-dimethyl-8-phenyl-2-(propan-2-ylidene)-1,2,3,3-a-tetrahydrocyclopenta[a]inden-3a-yl)acetate 4c.**

A white solid, Mp: 152-154 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 0.77 (t, *J* = 6.9 Hz, 3H, CH<sub>3</sub>), 1.24 (s, 3H, CH<sub>3</sub>), 1.29 (s, 3H, CH<sub>3</sub>), 1.64 (s, 3H, CH<sub>3</sub>), 1.87 (s, 3H, CH<sub>3</sub>), 3.17 (d, *J* =

13.8 Hz, 1H), 3.23 (d,  $J = 13.8$  Hz, 1H), 3.66-3.77 (m, 2H, CH<sub>2</sub>), 5.94 (d,  $J = 7.8$  Hz, 1H, Ar), 6.31 (d,  $J = 8.7$  Hz, 1H, Ar), 6.62 (dt,  $J = 7.5, 1.8$  Hz, 1H, Ar), 6.90-6.94 (m, 5H, Ar), 7.05 (d,  $J = 8.7$  Hz, 2H, Ar), 7.37-7.49 (m, 7H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, TMS)  $\delta$  13.8, 21.0, 25.0, 26.9, 29.3, 41.2, 42.6, 59.9, 64.7, 119.6, 124.0, 125.7, 126.3, 127.4, 127.8, 127.9, 128.2, 128.8, 129.6, 130.8, 131.2, 131.8, 132.0, 133.3, 134.3, 135.5, 136.4, 142.2, 142.7, 142.8, 145.0, 147.2, 159.3, 169.7. IR (CH<sub>2</sub>Cl<sub>2</sub>)  $\nu$  2974, 2930, 1731, 1488, 1463, 1442, 1396, 1366, 1310, 1264, 1215, 1167, 1115, 1091, 1034, 1015, 826, 803, 778, 750, 702, 690 cm<sup>-1</sup>. MS (%)  $m/e$  618 (M<sup>+</sup>, 16), 531 (15), 406 (11), 339 (11), 229 (66), 215 (75), 202 (27), 141 (30), 84 (100). HRMS (EI) for C<sub>40</sub>H<sub>36</sub>O<sub>2</sub>Cl<sub>2</sub>: 618.2092; Found: 618.2086.

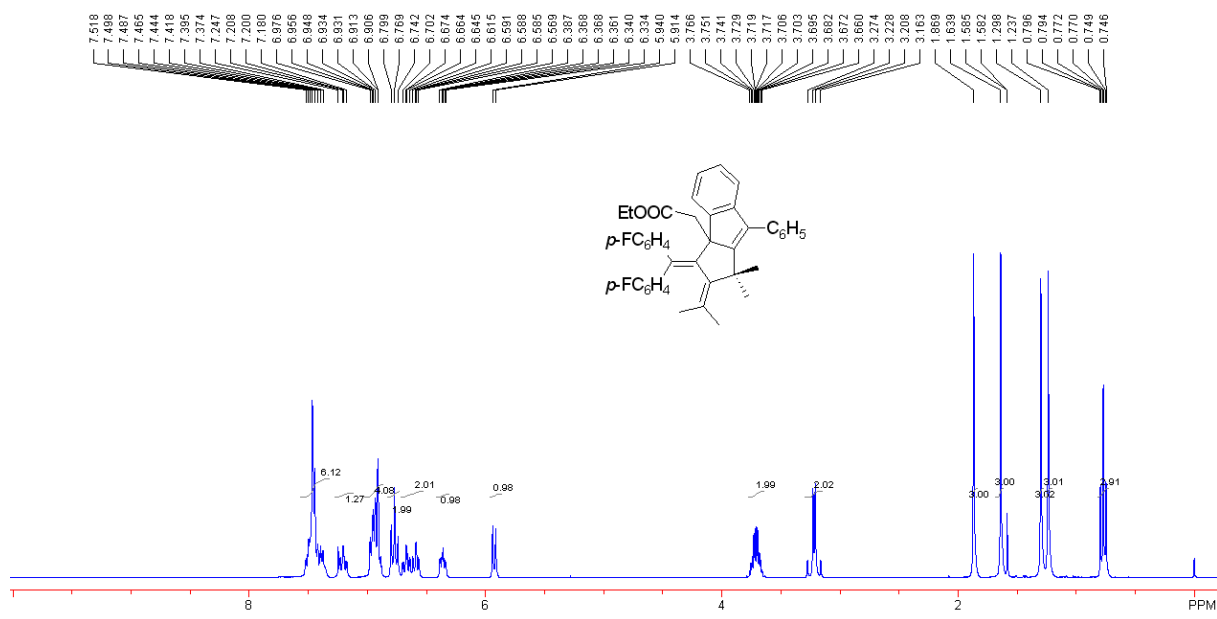


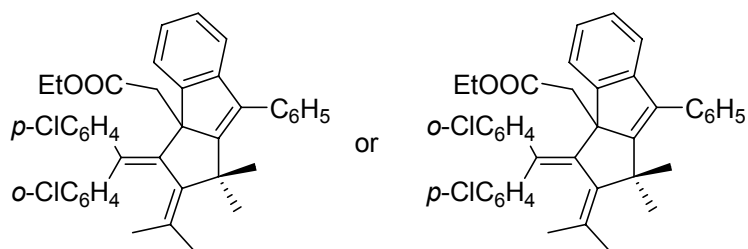
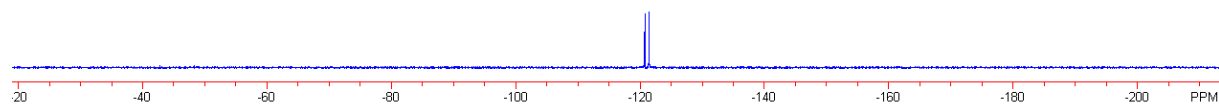
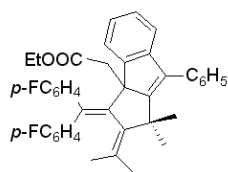
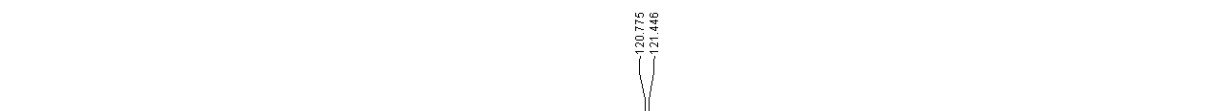
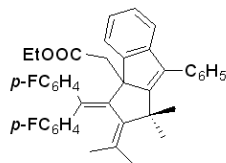
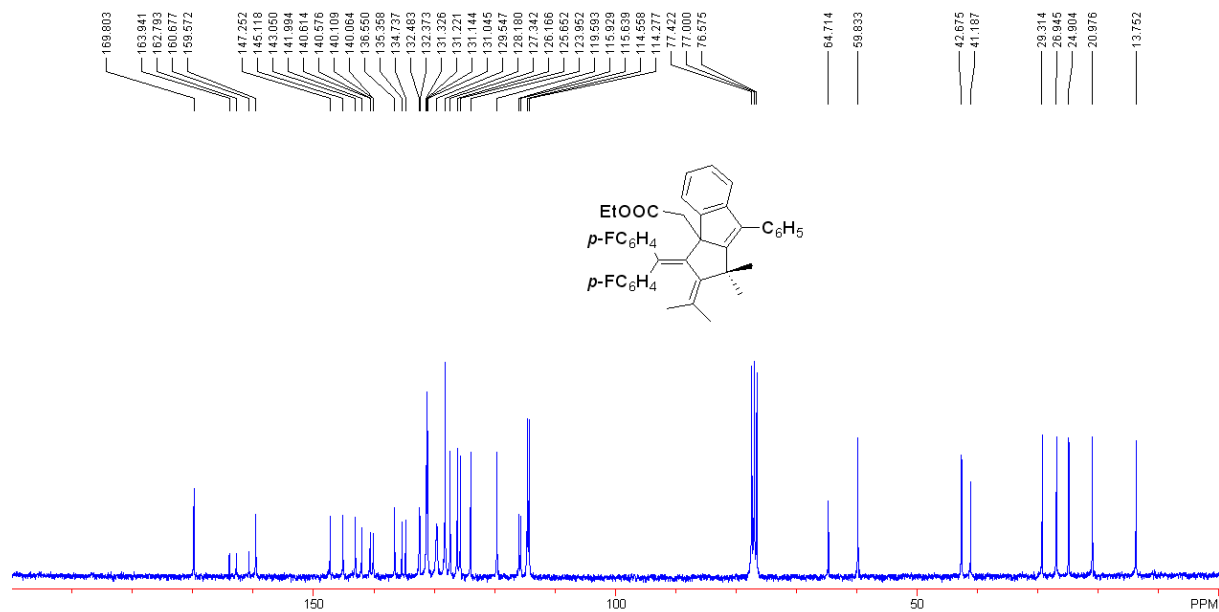


ethyl

**2-(3-(bis(4-fluorophenyl)methylene)-1,1-dimethyl-8-phenyl-2-(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate 4d.**

A white solid, Mp: 190-192 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 0.77 (t, *J* = 6.9 Hz, 3H, CH<sub>3</sub>), 1.23 (s, 3H, CH<sub>3</sub>), 1.30 (s, 3H, CH<sub>3</sub>), 1.64 (s, 3H, CH<sub>3</sub>), 1.87 (s, 3H, CH<sub>3</sub>), 3.17 (d, *J* = 13.8 Hz, 1H), 3.25 (d, *J* = 13.8 Hz, 1H), 3.66-3.76 (m, 2H, CH<sub>2</sub>), 5.92 (d, *J* = 7.8 Hz, 1H, Ar), 6.33-6.39 (m, 1H, Ar), 6.56-6.61 (m, 1H, Ar), 6.63-6.70 (m, 1H, Ar), 6.77 (t, *J* = 8.7 Hz, 2H, Ar), 6.89-6.98 (m, 4H, Ar), 7.17-7.24 (m, 1H, Ar), 7.35-7.52 (m, 6H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 75 MHz, TMS) δ 13.8, 21.0, 24.9, 26.9, 29.3, 41.2, 42.7, 59.8, 64.7, 114.4 (d, *J*<sub>C-F</sub> = 21.1 Hz), 115.8 (d, *J*<sub>C-F</sub> = 21.8 Hz), 119.6, 124.0, 125.7, 126.2, 127.4, 128.2, 129.5, 131.1 (d, *J*<sub>C-F</sub> = 7.4 Hz), 131.2, 131.3, 132.4 (d, *J*<sub>C-F</sub> = 8.3 Hz), 134.7, 135.4, 136.5, 140.1 (d, *J*<sub>C-F</sub> = 3.4 Hz), 140.6 (d, *J*<sub>C-F</sub> = 2.9 Hz), 142.0, 143.1, 145.1, 147.3, 159.5, 161.2 (d, *J*<sub>C-F</sub> = 241.6 Hz), 162.3 (d, *J*<sub>C-F</sub> = 244.8 Hz), 169.8. <sup>19</sup>F NMR (CDCl<sub>3</sub>, 282 MHz, CFCl<sub>3</sub>) δ -115.6, -116.2. IR (CH<sub>2</sub>Cl<sub>2</sub>) ν 3061, 2977, 2932, 1887, 1731, 1599, 1504, 1464, 1443, 1403, 1387, 1367, 1309, 1266, 1224, 1156, 1115, 1093, 1059, 1034, 1015, 982, 939, 911, 836, 777, 749, 739, 703, 676, 600, 584, 548 cm<sup>-1</sup>. MS (%) *m/e* 586 (M<sup>+</sup>, 57), 499 (48), 483 (28), 390 (30), 309 (31), 242 (78), 230 (100), 215 (99), 109 (39). HRMS (EI) for C<sub>40</sub>H<sub>36</sub>O<sub>2</sub>F<sub>2</sub>: 586.2683; Found: 586.2684.

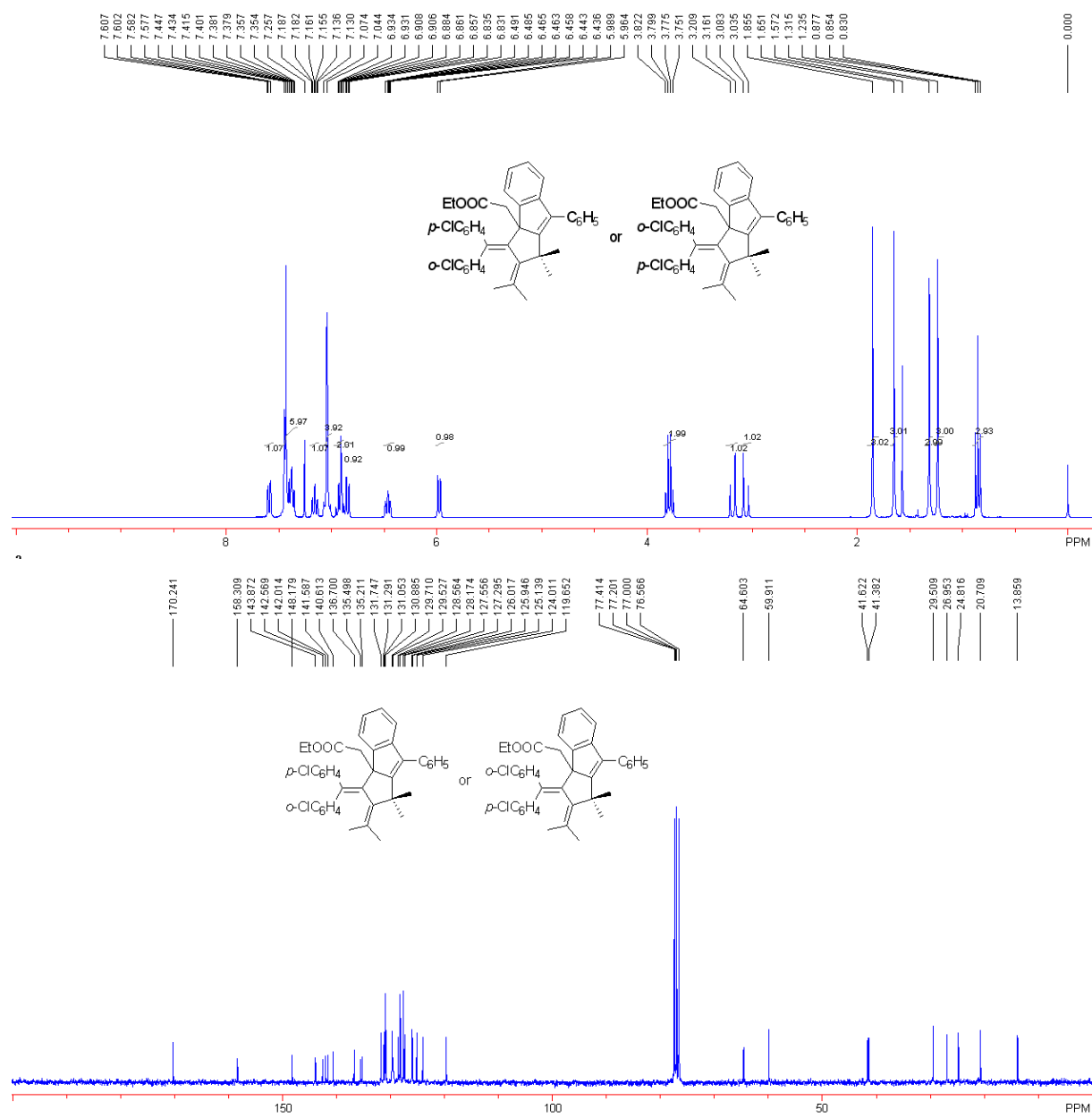




**(E)** or **(Z)-ethyl**  
**2-(3-((2-chlorophenyl)(4-chlorophenyl)methylene)-1,1-dimethyl-8-phenyl-2-(propan-2-ylidene)-1,2,3,3a-tetrahydrocyclopenta[a]inden-3a-yl)acetate 4e.**

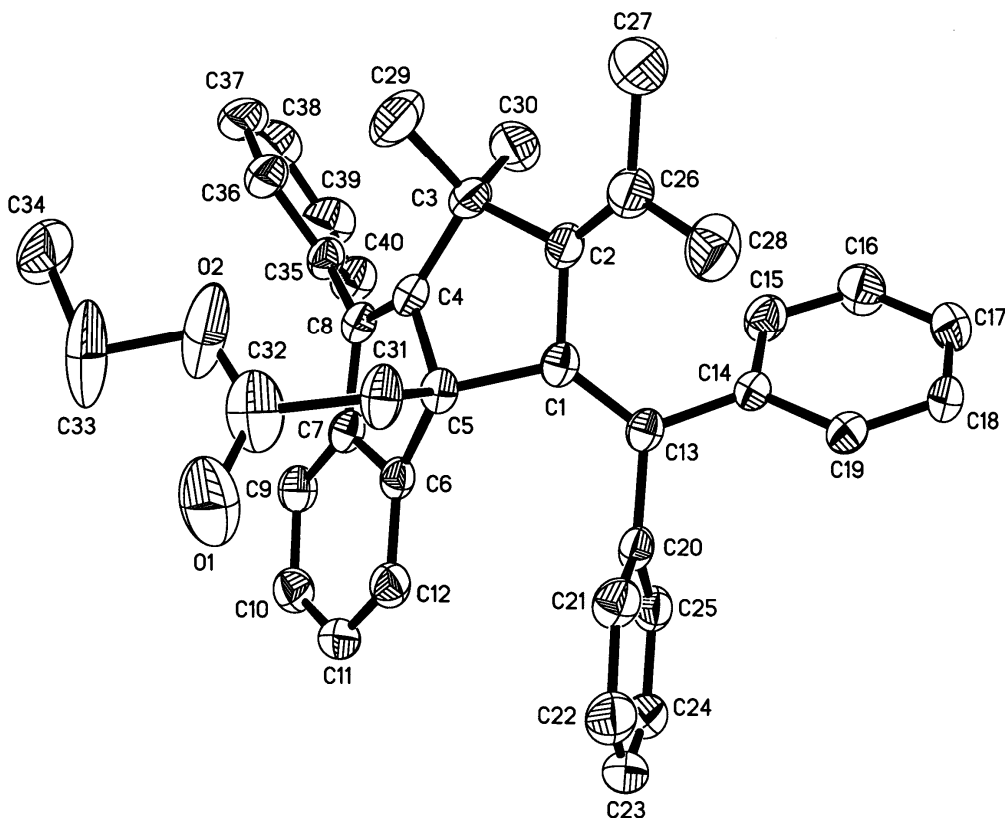
A white solid, Mp: 164-166 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz, TMS) δ 0.85 (t, *J* = 7.2 Hz, 3H, CH<sub>3</sub>), 1.24 (s, 3H, CH<sub>3</sub>), 1.32 (s, 3H, CH<sub>3</sub>), 1.65 (s, 3H, CH<sub>3</sub>), 1.86 (s, 3H, CH<sub>3</sub>), 3.06 (d, *J* =

14.1 Hz, 1H), 3.18 (d,  $J = 14.1$  Hz, 1H), 3.79 (q,  $J = 7.2$  Hz, 2H, CH<sub>2</sub>), 5.98 (d,  $J = 7.5$  Hz, 1H, Ar), 6.46 (dt,  $J = 7.8, 1.8$  Hz, 1H, Ar), 6.85 (dd,  $J = 7.8, 1.2$  Hz, 1H, Ar), 6.88-6.96 (m, 2H, Ar), 7.01-7.07 (m, 4H, Ar), 7.16 (dt,  $J = 1.5$  Hz,  $J = 7.5$  Hz, 1H, Ar), 7.35-7.45 (m, 6H, Ar), 7.59 (dd,  $J = 1.5$  Hz,  $J = 7.5$  Hz, 1H, Ar). <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz, TMS)  $\delta$  13.9, 20.7, 24.8, 27.0, 29.5, 41.4, 41.6, 59.9, 64.6, 119.7, 124.0, 125.1, 125.9, 126.0, 127.3, 127.6, 128.2, 128.6, 129.5, 129.7, 130.9, 131.1, 131.3, 131.7, 135.2, 135.5, 136.7, 140.6, 141.6, 142.0, 142.6, 143.9, 148.2, 158.3, 170.2. IR (CH<sub>2</sub>Cl<sub>2</sub>)  $\nu$  2976, 2927, 2854, 2359, 2340, 1731, 1699, 1683, 1668, 1652, 1594, 1558, 1539, 1506, 1488, 1471, 1456, 1384, 1367, 1307, 1275, 1261, 1169, 1118, 1093, 1034, 750, 703 cm<sup>-1</sup>. MS (%)  $m/e$  618 (M<sup>+</sup>, 22), 531 (28), 515 (23), 341 (21), 259 (28), 229 (87), 215 (100), 117 (63). HRMS (EI) for C<sub>40</sub>H<sub>36</sub>O<sub>2</sub>Cl<sub>2</sub>Na: 641.1989; Found: 641.1985.



## Reference

- 1) N. R. Browne, R. F. C. Brown, F. W. Eastwood, G. D. Fallon, *Aust. J. Chem.* 1987, **40**, 1675-1686.



The crystal data of **3a** have been deposited in CCDC with number 689419. Empirical Formula:  $C_{40}H_{38}O_2$ ; Formula Weight: 550.70; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.265 x 0.234 x 0.175 mm; Crystal System: Triclinic; Lattice Type: Primitive; Lattice Parameters:  $a = 10.8855(10)\text{\AA}$ ,  $b = 12.0229(11)\text{\AA}$ ,  $c = 13.1337(12)\text{\AA}$ ,  $\alpha = 88.141(2)^\circ$ ,  $\beta = 75.077(2)^\circ$ ,  $\gamma = 73.626(2)^\circ$ ,  $V = 1592.0(3)\text{\AA}^3$ ; Space group: P-1;  $Z = 2$ ;  $D_{calc} = 1.149\text{ g/cm}^3$ ;  $F_{000} = 588$ ; Diffractometer: Rigaku AFC7R; Residuals: R;  $R_w = 0.0757, 0.1628$ .



Table 1. Crystal data and structure refinement for cd28246.

Identification code	cd28246
Empirical formula	C <sub>40</sub> H <sub>38</sub> O <sub>2</sub>
Formula weight	550.70
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 10.8855(10) Å    alpha = 88.141(2) deg. b = 12.0229(11) Å    beta = 75.077(2) deg. c = 13.1337(12) Å    gamma = 73.626(2) deg.
Volume	1592.0(3) Å <sup>3</sup>
Z, Calculated density	2, 1.149 Mg/m <sup>3</sup>
Absorption coefficient	0.069 mm <sup>-1</sup>
F(000)	588
Crystal size	0.265 x 0.234 x 0.175 mm
Theta range for data collection	1.61 to 25.50 deg.
Limiting indices	-10 ≤ h ≤ 13, -14 ≤ k ≤ 14, -14 ≤ l ≤ 15
Reflections collected / unique	8447 / 5832 [R(int) = 0.0489]
Completeness to theta = 25.50	98.5 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.75212
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	5832 / 2 / 395
Goodness-of-fit on F <sup>2</sup>	0.941
Final R indices [I > 2σ(I)]	R1 = 0.0757, wR2 = 0.1628
R indices (all data)	R1 = 0.1545, wR2 = 0.1982
Largest diff. peak and hole	0.309 and -0.206 e.Å <sup>-3</sup>

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd28246. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	12306(4)	-152(4)	-137(3)	112(2)
O(2)	11995(4)	1721(4)	-112(3)	115(2)
C(1)	8587(3)	1843(3)	2598(2)	43(1)
C(2)	7985(4)	3008(3)	2229(3)	54(1)
C(3)	9059(4)	3671(3)	1997(3)	59(1)
C(4)	10263(4)	2727(3)	2075(2)	44(1)
C(5)	10074(3)	1519(3)	1995(2)	43(1)
C(6)	11196(3)	765(3)	2423(2)	43(1)
C(7)	11969(4)	1467(3)	2597(2)	45(1)
C(8)	11344(4)	2674(3)	2414(2)	44(1)
C(9)	13132(4)	971(3)	2888(3)	56(1)
C(10)	13543(4)	-222(3)	2982(3)	65(1)
C(11)	12794(4)	-899(3)	2794(3)	62(1)
C(12)	11655(4)	-429(3)	2499(3)	55(1)
C(13)	7959(3)	1262(3)	3358(2)	42(1)
C(14)	6664(3)	1811(3)	4105(2)	43(1)
C(15)	6428(4)	2856(3)	4660(3)	61(1)
C(16)	5246(5)	3321(3)	5390(3)	74(1)
C(17)	4256(4)	2781(3)	5579(3)	73(1)
C(18)	4472(4)	1766(3)	5064(3)	59(1)
C(19)	5654(4)	1285(3)	4354(3)	53(1)
C(20)	8504(3)	-7(3)	3491(3)	45(1)
C(21)	8581(4)	-803(3)	2723(3)	58(1)
C(22)	9041(4)	-1976(4)	2838(4)	75(1)
C(23)	9436(4)	-2370(3)	3721(4)	78(1)
C(24)	9359(4)	-1613(4)	4500(3)	70(1)
C(25)	8871(4)	-433(3)	4397(3)	54(1)
C(26)	6837(4)	3317(4)	1980(3)	69(1)
C(27)	6212(5)	4522(4)	1647(4)	114(2)
C(28)	5969(4)	2546(4)	1985(3)	86(1)
C(29)	9280(5)	4176(4)	892(4)	106(2)
C(30)	8677(5)	4643(3)	2863(4)	94(2)
C(31)	10233(4)	1078(3)	856(3)	64(1)
C(32)	11635(6)	852(6)	153(4)	100(2)
C(33)	13408(7)	1430(7)	-728(6)	118(3)
C(35)	11828(4)	3661(3)	2626(3)	51(1)
C(36)	12068(4)	4449(3)	1867(3)	65(1)
C(37)	12453(5)	5402(3)	2091(5)	85(1)
C(38)	12621(5)	5548(4)	3058(5)	89(2)
C(39)	12438(5)	4752(4)	3815(4)	85(1)
C(40)	12049(4)	3816(3)	3596(3)	67(1)
C(34)	13650(30)	2549(15)	-1000(30)	113(15)
C(34')	14148(10)	1880(20)	-232(12)	117(9)

Table 3. Bond lengths [Å] and angles [deg] for cd28246.

O(1)-C(32)	1.235 (6)
O(2)-C(32)	1.227 (6)
O(2)-C(33)	1.489 (7)
C(1)-C(13)	1.351 (4)
C(1)-C(2)	1.492 (4)
C(1)-C(5)	1.551 (5)
C(2)-C(26)	1.321 (5)
C(2)-C(3)	1.557 (5)
C(3)-C(4)	1.496 (5)
C(3)-C(29)	1.543 (5)
C(3)-C(30)	1.548 (5)
C(4)-C(8)	1.346 (4)
C(4)-C(5)	1.534 (4)
C(5)-C(6)	1.524 (5)
C(5)-C(31)	1.554 (4)
C(6)-C(12)	1.390 (4)
C(6)-C(7)	1.409 (4)
C(7)-C(9)	1.383 (5)
C(7)-C(8)	1.460 (4)
C(8)-C(35)	1.487 (4)
C(9)-C(10)	1.388 (5)
C(9)-H(9)	0.9300
C(10)-C(11)	1.372 (5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.359 (5)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.480 (4)
C(13)-C(20)	1.495 (4)
C(14)-C(19)	1.381 (4)
C(14)-C(15)	1.399 (4)
C(15)-C(16)	1.372 (5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.375 (5)
C(16)-H(16)	0.9300
C(17)-C(18)	1.346 (5)
C(17)-H(17)	0.9300
C(18)-C(19)	1.363 (5)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-C(21)	1.384 (4)
C(20)-C(25)	1.388 (5)
C(21)-C(22)	1.375 (5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.365 (6)
C(22)-H(22)	0.9300
C(23)-C(24)	1.361 (5)
C(23)-H(23)	0.9300
C(24)-C(25)	1.383 (5)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(26)-C(28)	1.497 (5)
C(26)-C(27)	1.521 (5)
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-C(32)	1.520 (6)
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700

C(33)-C(34')	1.380(9)
C(33)-C(34)	1.456(13)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(33)-H(33C)	0.9600
C(33)-H(33D)	0.9600
C(35)-C(36)	1.380(5)
C(35)-C(40)	1.383(5)
C(36)-C(37)	1.389(5)
C(36)-H(36)	0.9300
C(37)-C(38)	1.353(6)
C(37)-H(37)	0.9300
C(38)-C(39)	1.374(6)
C(38)-H(38)	0.9300
C(39)-C(40)	1.371(5)
C(39)-H(39)	0.9300
C(40)-H(40)	0.9300
C(34)-H(33C)	1.1701
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(34')-H(34D)	0.9600
C(34')-H(34E)	0.9600
C(34')-H(34F)	0.9600
C(32)-O(2)-C(33)	112.2(6)
C(13)-C(1)-C(2)	125.9(3)
C(13)-C(1)-C(5)	128.6(3)
C(2)-C(1)-C(5)	105.3(3)
C(26)-C(2)-C(1)	124.8(3)
C(26)-C(2)-C(3)	127.0(3)
C(1)-C(2)-C(3)	107.3(3)
C(4)-C(3)-C(29)	110.4(3)
C(4)-C(3)-C(30)	111.7(3)
C(29)-C(3)-C(30)	110.6(3)
C(4)-C(3)-C(2)	101.4(3)
C(29)-C(3)-C(2)	113.6(3)
C(30)-C(3)-C(2)	109.0(3)
C(8)-C(4)-C(3)	135.0(3)
C(8)-C(4)-C(5)	111.3(3)
C(3)-C(4)-C(5)	111.9(3)
C(6)-C(5)-C(4)	101.7(3)
C(6)-C(5)-C(31)	109.4(3)
C(4)-C(5)-C(31)	114.7(3)
C(6)-C(5)-C(1)	124.5(3)
C(4)-C(5)-C(1)	96.9(2)
C(31)-C(5)-C(1)	109.0(3)
C(12)-C(6)-C(7)	118.9(3)
C(12)-C(6)-C(5)	132.1(3)
C(7)-C(6)-C(5)	108.1(3)
C(9)-C(7)-C(6)	119.9(3)
C(9)-C(7)-C(8)	130.4(3)
C(6)-C(7)-C(8)	109.7(3)
C(4)-C(8)-C(7)	108.9(3)
C(4)-C(8)-C(35)	127.3(3)
C(7)-C(8)-C(35)	123.8(3)
C(7)-C(9)-C(10)	119.6(4)
C(7)-C(9)-H(9)	120.2
C(10)-C(9)-H(9)	120.2
C(11)-C(10)-C(9)	120.0(4)
C(11)-C(10)-H(10)	120.0
C(9)-C(10)-H(10)	120.0
C(12)-C(11)-C(10)	121.2(4)
C(12)-C(11)-H(11)	119.4
C(10)-C(11)-H(11)	119.4
C(11)-C(12)-C(6)	120.2(3)
C(11)-C(12)-H(12)	119.9
C(6)-C(12)-H(12)	119.9
C(1)-C(13)-C(14)	123.2(3)
C(1)-C(13)-C(20)	122.4(3)
C(14)-C(13)-C(20)	114.4(3)
C(19)-C(14)-C(15)	116.0(3)

C(19)-C(14)-C(13)	122.2(3)
C(15)-C(14)-C(13)	121.6(3)
C(16)-C(15)-C(14)	120.8(3)
C(16)-C(15)-H(15)	119.6
C(14)-C(15)-H(15)	119.6
C(15)-C(16)-C(17)	120.7(4)
C(15)-C(16)-H(16)	119.6
C(17)-C(16)-H(16)	119.6
C(18)-C(17)-C(16)	119.3(4)
C(18)-C(17)-H(17)	120.3
C(16)-C(17)-H(17)	120.3
C(17)-C(18)-C(19)	120.3(4)
C(17)-C(18)-H(18)	119.8
C(19)-C(18)-H(18)	119.8
C(18)-C(19)-C(14)	122.8(3)
C(18)-C(19)-H(19)	118.6
C(14)-C(19)-H(19)	118.6
C(21)-C(20)-C(25)	117.8(3)
C(21)-C(20)-C(13)	119.9(3)
C(25)-C(20)-C(13)	122.2(3)
C(22)-C(21)-C(20)	121.2(4)
C(22)-C(21)-H(21)	119.4
C(20)-C(21)-H(21)	119.4
C(23)-C(22)-C(21)	119.8(4)
C(23)-C(22)-H(22)	120.1
C(21)-C(22)-H(22)	120.1
C(24)-C(23)-C(22)	120.7(4)
C(24)-C(23)-H(23)	119.7
C(22)-C(23)-H(23)	119.7
C(23)-C(24)-C(25)	119.7(4)
C(23)-C(24)-H(24)	120.2
C(25)-C(24)-H(24)	120.2
C(24)-C(25)-C(20)	120.8(3)
C(24)-C(25)-H(25)	119.6
C(20)-C(25)-H(25)	119.6
C(2)-C(26)-C(28)	125.5(4)
C(2)-C(26)-C(27)	124.1(4)
C(28)-C(26)-C(27)	110.3(4)
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(3)-C(29)-H(29A)	109.5
C(3)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(3)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(3)-C(30)-H(30A)	109.5
C(3)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(3)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(5)	113.7(3)
C(32)-C(31)-H(31A)	108.8
C(5)-C(31)-H(31A)	108.8
C(32)-C(31)-H(31B)	108.8
C(5)-C(31)-H(31B)	108.8
H(31A)-C(31)-H(31B)	107.7
O(1)-C(32)-O(2)	124.7(6)
O(1)-C(32)-C(31)	120.0(6)
O(2)-C(32)-C(31)	115.3(6)
C(34')-C(33)-C(34)	58.6(12)

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C(34')-C(33)-O(2)	111.3(6)
C(34)-C(33)-O(2)	104.5(12)
C(34')-C(33)-H(33A)	53.7
C(34)-C(33)-H(33A)	110.9
O(2)-C(33)-H(33A)	110.9
C(34')-C(33)-H(33B)	137.9
C(34)-C(33)-H(33B)	110.8
O(2)-C(33)-H(33B)	110.8
H(33A)-C(33)-H(33B)	108.9
C(34')-C(33)-H(33C)	106.6
C(34)-C(33)-H(33C)	53.3
O(2)-C(33)-H(33C)	108.8
H(33A)-C(33)-H(33C)	140.1
H(33B)-C(33)-H(33C)	59.7
C(34')-C(33)-H(33D)	111.8
C(34)-C(33)-H(33D)	146.2
O(2)-C(33)-H(33D)	108.8
H(33A)-C(33)-H(33D)	61.4
H(33B)-C(33)-H(33D)	51.8
H(33C)-C(33)-H(33D)	109.4
C(36)-C(35)-C(40)	118.0(3)
C(36)-C(35)-C(8)	121.3(3)
C(40)-C(35)-C(8)	120.8(3)
C(35)-C(36)-C(37)	120.8(4)
C(35)-C(36)-H(36)	119.6
C(37)-C(36)-H(36)	119.6
C(38)-C(37)-C(36)	119.7(4)
C(38)-C(37)-H(37)	120.1
C(36)-C(37)-H(37)	120.1
C(37)-C(38)-C(39)	120.6(4)
C(37)-C(38)-H(38)	119.7
C(39)-C(38)-H(38)	119.7
C(38)-C(39)-C(40)	119.6(4)
C(38)-C(39)-H(39)	120.2
C(40)-C(39)-H(39)	120.2
C(39)-C(40)-C(35)	121.2(4)
C(39)-C(40)-H(40)	119.4
C(35)-C(40)-H(40)	119.4
C(33)-C(34)-H(33C)	41.1
C(33)-C(34)-H(34A)	109.4
H(33C)-C(34)-H(34A)	143.5
C(33)-C(34)-H(34B)	109.5
H(33C)-C(34)-H(34B)	74.5
C(33)-C(34)-H(34C)	109.5
H(33C)-C(34)-H(34C)	102.5
C(33)-C(34')-H(34D)	109.5
C(33)-C(34')-H(34E)	109.5
H(34D)-C(34')-H(34E)	109.5
C(33)-C(34')-H(34F)	109.5
H(34D)-C(34')-H(34F)	109.5
H(34E)-C(34')-H(34F)	109.5

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{Å}^2 \times 10^3$ ) for cd28246. The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
O(1)	117(4)	161(4)	105(3)	-42(3)	10(3)	-37(3)
O(2)	125(4)	175(4)	97(3)	-40(3)	48(3)	-118(4)
C(1)	43(2)	52(2)	40(2)	-1(2)	-11(2)	-22(2)
C(2)	45(3)	63(2)	52(2)	15(2)	-8(2)	-21(2)
C(3)	52(3)	54(2)	74(3)	23(2)	-14(2)	-23(2)
C(4)	45(2)	50(2)	39(2)	7(2)	-7(2)	-23(2)
C(5)	44(2)	51(2)	38(2)	-5(2)	-7(2)	-21(2)
C(6)	44(2)	47(2)	36(2)	-5(2)	0(2)	-18(2)
C(7)	47(2)	54(2)	36(2)	2(2)	-8(2)	-22(2)
C(8)	47(2)	51(2)	38(2)	0(2)	-5(2)	-24(2)
C(9)	48(3)	70(3)	55(2)	-2(2)	-13(2)	-25(2)
C(10)	49(3)	70(3)	70(3)	11(2)	-11(2)	-11(2)
C(11)	53(3)	49(2)	78(3)	4(2)	-6(2)	-13(2)
C(12)	49(3)	53(2)	64(3)	-6(2)	-4(2)	-22(2)
C(13)	42(2)	49(2)	39(2)	0(2)	-10(2)	-21(2)
C(14)	40(2)	42(2)	47(2)	4(2)	-9(2)	-16(2)
C(15)	64(3)	57(2)	63(3)	-6(2)	-4(2)	-28(2)
C(16)	74(3)	61(3)	77(3)	-21(2)	-1(3)	-19(2)
C(17)	53(3)	65(3)	82(3)	-2(2)	8(2)	-9(2)
C(18)	42(3)	63(3)	68(3)	14(2)	-2(2)	-20(2)
C(19)	50(3)	44(2)	65(2)	4(2)	-9(2)	-20(2)
C(20)	41(2)	51(2)	46(2)	-2(2)	-2(2)	-22(2)
C(21)	67(3)	57(2)	54(2)	-8(2)	-10(2)	-30(2)
C(22)	76(3)	58(3)	88(3)	-18(2)	-1(3)	-32(3)
C(23)	65(3)	44(2)	105(4)	-1(3)	8(3)	-13(2)
C(24)	60(3)	62(3)	77(3)	19(2)	-5(2)	-13(2)
C(25)	51(3)	58(2)	49(2)	-1(2)	-2(2)	-19(2)
C(26)	53(3)	81(3)	73(3)	28(2)	-19(2)	-21(3)
C(27)	68(4)	122(4)	152(5)	57(4)	-38(4)	-25(3)
C(28)	68(3)	122(4)	88(3)	25(3)	-38(3)	-44(3)
C(29)	77(4)	135(4)	118(4)	80(3)	-31(3)	-51(3)
C(30)	69(3)	52(3)	154(5)	-8(3)	-6(3)	-23(2)
C(31)	59(3)	97(3)	42(2)	-13(2)	-3(2)	-39(2)
C(32)	108(5)	151(6)	43(3)	-39(3)	-13(3)	-44(4)
C(33)	74(5)	183(10)	88(5)	-38(5)	42(4)	-69(6)
C(35)	48(2)	52(2)	55(2)	1(2)	-8(2)	-25(2)
C(36)	63(3)	61(3)	76(3)	13(2)	-14(2)	-30(2)
C(37)	76(4)	58(3)	127(4)	23(3)	-23(3)	-34(3)
C(38)	76(4)	61(3)	139(5)	-13(3)	-27(3)	-30(3)
C(39)	95(4)	75(3)	100(4)	-8(3)	-36(3)	-38(3)
C(40)	79(3)	62(3)	70(3)	-4(2)	-19(2)	-37(2)
C(34)	130(20)	78(14)	150(30)	0(12)	25(19)	-64(15)
C(34')	69(7)	210(20)	112(11)	-68(13)	4(6)	-72(10)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd28246.

	x	y	z	U (eq)
H(9)	13635	1433	3020	68
H(10)	14328	-562	3172	78
H(11)	13071	-1696	2871	75
H(12)	11180	-907	2347	66
H(15)	7081	3240	4532	74
H(16)	5112	4009	5761	88
H(17)	3446	3113	6058	88
H(18)	3811	1391	5193	71
H(19)	5787	573	4024	63
H(21)	8317	-539	2117	69
H(22)	9083	-2499	2316	89
H(23)	9761	-3163	3792	93
H(24)	9633	-1888	5099	84
H(25)	8787	81	4941	65
H(27A)	6690	5043	1769	130
H(27B)	5305	4795	2051	130
H(27C)	6244	4491	911	130
H(28A)	6463	1752	2018	119
H(28B)	5670	2641	1353	119
H(28C)	5218	2751	2588	119
H(29A)	10118	4347	708	130
H(29B)	8582	4875	895	130
H(29C)	9277	3620	384	130
H(30A)	8636	4304	3538	132
H(30B)	7828	5165	2864	132
H(30C)	9331	5061	2722	132
H(31A)	9974	367	891	77
H(31B)	9635	1650	538	77
H(33A)	13988	1007	-308	141
H(33B)	13553	964	-1360	141
H(33C)	13456	1782	-1398	141
H(33D)	13750	602	-837	141
H(36)	11970	4342	1197	78
H(37)	12595	5936	1578	102
H(38)	12863	6194	3212	107
H(39)	12577	4847	4472	102
H(40)	11931	3276	4109	80
H(34A)	13350	3046	-370	134
H(34B)	13169	2898	-1500	134
H(34C)	14577	2441	-1292	134
H(34D)	14875	2035	-750	136
H(34E)	14483	1331	248	136
H(34F)	13599	2589	152	136



Table 6. Torsion angles [deg] for cd28246.

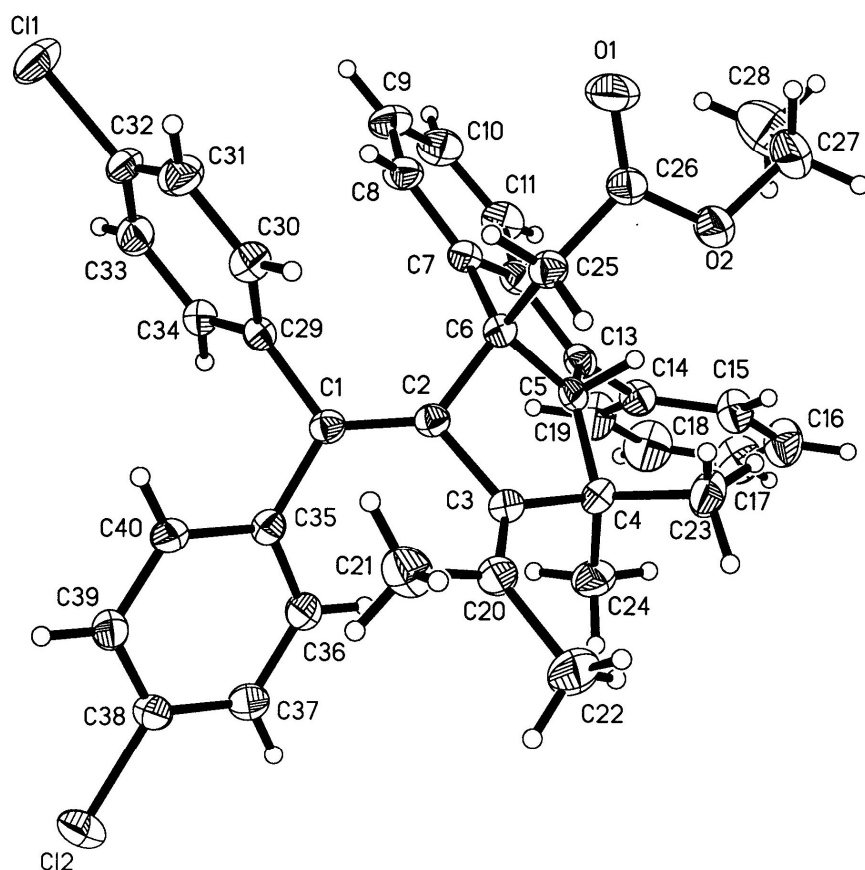
C(13)-C(1)-C(2)-C(26)	-47.9(5)
C(5)-C(1)-C(2)-C(26)	136.7(4)
C(13)-C(1)-C(2)-C(3)	142.5(3)
C(5)-C(1)-C(2)-C(3)	-32.9(3)
C(26)-C(2)-C(3)-C(4)	-159.5(4)
C(1)-C(2)-C(3)-C(4)	9.8(4)
C(26)-C(2)-C(3)-C(29)	-41.2(6)
C(1)-C(2)-C(3)-C(29)	128.2(3)
C(26)-C(2)-C(3)-C(30)	82.6(5)
C(1)-C(2)-C(3)-C(30)	-108.1(4)
C(29)-C(3)-C(4)-C(8)	93.9(5)
C(30)-C(3)-C(4)-C(8)	-29.6(5)
C(2)-C(3)-C(4)-C(8)	-145.5(4)
C(29)-C(3)-C(4)-C(5)	-103.1(3)
C(30)-C(3)-C(4)-C(5)	133.4(3)
C(2)-C(3)-C(4)-C(5)	17.5(4)
C(8)-C(4)-C(5)-C(6)	3.7(3)
C(3)-C(4)-C(5)-C(6)	-163.4(3)
C(8)-C(4)-C(5)-C(31)	-114.2(3)
C(3)-C(4)-C(5)-C(31)	78.6(4)
C(8)-C(4)-C(5)-C(1)	131.2(3)
C(3)-C(4)-C(5)-C(1)	-36.0(3)
C(13)-C(1)-C(5)-C(6)	-25.7(5)
C(2)-C(1)-C(5)-C(6)	149.6(3)
C(13)-C(1)-C(5)-C(4)	-135.0(3)
C(2)-C(1)-C(5)-C(4)	40.3(3)
C(13)-C(1)-C(5)-C(31)	105.9(4)
C(2)-C(1)-C(5)-C(31)	-78.9(3)
C(4)-C(5)-C(6)-C(12)	-174.6(3)
C(31)-C(5)-C(6)-C(12)	-52.9(5)
C(1)-C(5)-C(6)-C(12)	78.5(5)
C(4)-C(5)-C(6)-C(7)	-5.7(3)
C(31)-C(5)-C(6)-C(7)	116.0(3)
C(1)-C(5)-C(6)-C(7)	-112.6(3)
C(12)-C(6)-C(7)-C(9)	-3.0(5)
C(5)-C(6)-C(7)-C(9)	-173.6(3)
C(12)-C(6)-C(7)-C(8)	176.5(3)
C(5)-C(6)-C(7)-C(8)	5.9(3)
C(3)-C(4)-C(8)-C(7)	162.7(4)
C(5)-C(4)-C(8)-C(7)	-0.4(4)
C(3)-C(4)-C(8)-C(35)	-14.7(6)
C(5)-C(4)-C(8)-C(35)	-177.7(3)
C(9)-C(7)-C(8)-C(4)	175.9(4)
C(6)-C(7)-C(8)-C(4)	-3.5(4)
C(9)-C(7)-C(8)-C(35)	-6.6(5)
C(6)-C(7)-C(8)-C(35)	173.9(3)
C(6)-C(7)-C(9)-C(10)	1.5(5)
C(8)-C(7)-C(9)-C(10)	-177.9(3)
C(7)-C(9)-C(10)-C(11)	-0.5(5)
C(9)-C(10)-C(11)-C(12)	1.1(6)
C(10)-C(11)-C(12)-C(6)	-2.7(6)
C(7)-C(6)-C(12)-C(11)	3.6(5)
C(5)-C(6)-C(12)-C(11)	171.5(4)
C(2)-C(1)-C(13)-C(14)	-14.5(5)
C(5)-C(1)-C(13)-C(14)	159.9(3)
C(2)-C(1)-C(13)-C(20)	163.6(3)
C(5)-C(1)-C(13)-C(20)	-22.1(5)
C(1)-C(13)-C(14)-C(19)	135.6(4)
C(20)-C(13)-C(14)-C(19)	-42.6(4)
C(1)-C(13)-C(14)-C(15)	-49.2(5)
C(20)-C(13)-C(14)-C(15)	132.6(3)
C(19)-C(14)-C(15)-C(16)	-1.1(6)
C(13)-C(14)-C(15)-C(16)	-176.6(4)
C(14)-C(15)-C(16)-C(17)	-1.2(7)
C(15)-C(16)-C(17)-C(18)	2.1(7)
C(16)-C(17)-C(18)-C(19)	-0.7(6)
C(17)-C(18)-C(19)-C(14)	-1.7(6)
C(15)-C(14)-C(19)-C(18)	2.6(5)

C(13)-C(14)-C(19)-C(18)	178.0(3)
C(1)-C(13)-C(20)-C(21)	-67.0(4)
C(14)-C(13)-C(20)-C(21)	111.3(3)
C(1)-C(13)-C(20)-C(25)	117.0(4)
C(14)-C(13)-C(20)-C(25)	-64.8(4)
C(25)-C(20)-C(21)-C(22)	-1.8(5)
C(13)-C(20)-C(21)-C(22)	-178.1(3)
C(20)-C(21)-C(22)-C(23)	-0.3(6)
C(21)-C(22)-C(23)-C(24)	1.1(7)
C(22)-C(23)-C(24)-C(25)	0.2(6)
C(23)-C(24)-C(25)-C(20)	-2.4(6)
C(21)-C(20)-C(25)-C(24)	3.2(5)
C(13)-C(20)-C(25)-C(24)	179.3(3)
C(1)-C(2)-C(26)-C(28)	-2.5(7)
C(3)-C(2)-C(26)-C(28)	165.1(4)
C(1)-C(2)-C(26)-C(27)	177.4(4)
C(3)-C(2)-C(26)-C(27)	-15.0(7)
C(6)-C(5)-C(31)-C(32)	-46.8(5)
C(4)-C(5)-C(31)-C(32)	66.7(5)
C(1)-C(5)-C(31)-C(32)	174.0(4)
C(33)-O(2)-C(32)-O(1)	-6.9(9)
C(33)-O(2)-C(32)-C(31)	175.5(5)
C(5)-C(31)-C(32)-O(1)	111.1(5)
C(5)-C(31)-C(32)-O(2)	-71.2(6)
C(32)-O(2)-C(33)-C(34')	-119.9(14)
C(32)-O(2)-C(33)-C(34)	179(2)
C(4)-C(8)-C(35)-C(36)	-54.8(5)
C(7)-C(8)-C(35)-C(36)	128.2(4)
C(4)-C(8)-C(35)-C(40)	125.1(4)
C(7)-C(8)-C(35)-C(40)	-51.9(5)
C(40)-C(35)-C(36)-C(37)	-3.2(6)
C(8)-C(35)-C(36)-C(37)	176.6(4)
C(35)-C(36)-C(37)-C(38)	1.3(7)
C(36)-C(37)-C(38)-C(39)	1.2(7)
C(37)-C(38)-C(39)-C(40)	-1.7(7)
C(38)-C(39)-C(40)-C(35)	-0.4(7)
C(36)-C(35)-C(40)-C(39)	2.8(6)
C(8)-C(35)-C(40)-C(39)	-177.1(4)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd28246 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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The crystal data of **4c** have been deposited in CCDC with number 700829. Empirical Formula:  $C_{41}H_{39}Cl_4O_2$ ; Formula Weight: 705.52; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.465 x 0.414 x 0.270 mm; Crystal System: Monoclinic; Lattice Type: Primitive; Lattice Parameters:  $a = 11.0910(8)\text{\AA}$ ,  $b = 12.2148(8)\text{\AA}$ ,  $c = 27.0216(19)\text{\AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 99.3620(10)^\circ$ ,  $\gamma = 90^\circ$ ,  $V = 3612.0(4)\text{\AA}^3$ ; Space group:  $P2(1)/n$ ;  $Z = 4$ ;  $D_{calc} = 1.297\text{ g/cm}^3$ ;  $F_{000} = 1476$ ; Diffractometer: Rigaku AFC7R; Residuals:  $R$ ;  $R_w$ : 0.0602, 0.1556.

Table 1. Crystal data and structure refinement for cd28383.

Identification code	cd28383
Empirical formula	C41 H39 Cl4 O2
Formula weight	705.52
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 11.0910(8) Å    alpha = 90 deg. b = 12.2148(8) Å    beta = 99.3620(10) deg. c = 27.0216(19) Å    gamma = 90 deg.
Volume	3612.0(4) Å <sup>3</sup>
Z, Calculated density	4, 1.297 Mg/m <sup>3</sup>
Absorption coefficient	0.362 mm <sup>-1</sup>
F(000)	1476
Crystal size	0.465 x 0.414 x 0.270 mm
Theta range for data collection	1.83 to 26.00 deg.
Limiting indices	-11<=h<=13, -14<=k<=15, -33<=l<=25
Reflections collected / unique	19458 / 7099 [R(int) = 0.0362]
Completeness to theta = 26.00	100.0 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.7680
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	7099 / 0 / 429
Goodness-of-fit on F <sup>2</sup>	0.983
Final R indices [I>2sigma(I)]	R1 = 0.0602, wR2 = 0.1556
R indices (all data)	R1 = 0.0969, wR2 = 0.1737
Largest diff. peak and hole	0.497 and -0.641 e.Å <sup>-3</sup>

Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd28383. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U (eq)
C1(1)	4088(1)	3442(1)	3937(1)	82(1)
C1(2)	-1713(1)	6396(1)	1104(1)	71(1)
C1(3)	10364(2)	701(3)	3670(1)	229(1)
C1(4)	9537(2)	1265(2)	2665(1)	233(1)
O(1)	5380(2)	-530(2)	2025(1)	89(1)
O(2)	5121(2)	-348(2)	1202(1)	61(1)
C(1)	2303(2)	3129(2)	1725(1)	34(1)
C(2)	2689(2)	2389(2)	1417(1)	33(1)
C(3)	2070(2)	2076(2)	906(1)	39(1)
C(4)	3062(2)	1921(2)	569(1)	42(1)
C(5)	4205(2)	1982(2)	964(1)	35(1)
C(6)	3923(2)	1784(2)	1490(1)	34(1)
C(7)	5066(2)	2226(2)	1816(1)	36(1)
C(8)	5433(2)	2228(2)	2327(1)	44(1)
C(9)	6567(3)	2644(3)	2524(1)	56(1)
C(10)	7355(3)	3011(3)	2215(1)	57(1)
C(11)	7037(3)	2953(2)	1702(1)	51(1)
C(12)	5883(2)	2561(2)	1500(1)	38(1)
C(13)	5319(2)	2415(2)	973(1)	38(1)
C(14)	5947(3)	2727(2)	552(1)	43(1)
C(15)	6087(3)	1994(2)	176(1)	52(1)
C(16)	6686(3)	2281(3)	-214(1)	68(1)
C(17)	7168(4)	3304(3)	-234(2)	75(1)
C(18)	7067(4)	4037(3)	136(2)	81(1)
C(19)	6450(3)	3758(3)	531(1)	66(1)
C(20)	870(3)	1869(2)	778(1)	48(1)
C(21)	-4(3)	1859(3)	1145(1)	62(1)
C(22)	247(3)	1615(3)	251(1)	78(1)
C(23)	2988(3)	801(3)	292(1)	62(1)
C(24)	3035(3)	2864(3)	192(1)	60(1)
C(25)	3723(2)	563(2)	1625(1)	40(1)
C(26)	4821(3)	-158(2)	1648(1)	45(1)
C(27)	6204(4)	-1019(3)	1187(2)	77(1)
C(28)	7308(4)	-354(4)	1259(2)	108(2)
C(29)	2807(2)	3194(2)	2270(1)	35(1)
C(30)	2616(3)	2343(2)	2589(1)	46(1)
C(31)	3001(3)	2403(3)	3098(1)	54(1)
C(32)	3604(3)	3332(3)	3290(1)	50(1)
C(33)	3806(3)	4185(3)	2989(1)	50(1)
C(34)	3394(2)	4119(2)	2480(1)	41(1)
C(35)	1307(2)	3941(2)	1562(1)	35(1)
C(36)	1187(3)	4480(2)	1103(1)	44(1)
C(37)	268(3)	5227(2)	963(1)	49(1)
C(38)	-541(2)	5459(2)	1285(1)	44(1)
C(39)	-432(2)	4973(2)	1744(1)	43(1)
C(40)	496(2)	4215(2)	1881(1)	40(1)
C(41)	9293(6)	497(5)	3155(3)	192(4)

Table 3. Bond lengths [Å] and angles [deg] for cd28383.

C1(1)-C(32)	1.749(3)
C1(2)-C(38)	1.741(3)
C1(3)-C(41)	1.695(9)
C1(4)-C(41)	1.679(8)
O(1)-C(26)	1.193(3)
O(2)-C(26)	1.320(3)
O(2)-C(27)	1.460(4)
C(1)-C(2)	1.343(3)
C(1)-C(29)	1.491(3)
C(1)-C(35)	1.497(3)
C(2)-C(3)	1.489(3)
C(2)-C(6)	1.540(3)
C(3)-C(20)	1.343(4)
C(3)-C(4)	1.551(4)
C(4)-C(5)	1.520(4)
C(4)-C(24)	1.535(4)
C(4)-C(23)	1.554(4)
C(5)-C(13)	1.340(4)
C(5)-C(6)	1.524(3)
C(5)-H(5)	0.9800
C(6)-C(7)	1.520(3)
C(6)-C(25)	1.559(4)
C(7)-C(8)	1.374(4)
C(7)-C(12)	1.404(4)
C(8)-C(9)	1.380(4)
C(8)-H(8)	0.9300
C(9)-C(10)	1.379(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.374(4)
C(10)-H(10)	0.9300
C(11)-C(12)	1.393(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.468(4)
C(13)-C(14)	1.478(4)
C(14)-C(19)	1.382(4)
C(14)-C(15)	1.383(4)
C(15)-C(16)	1.378(4)
C(15)-H(15)	0.9300
C(16)-C(17)	1.364(5)
C(16)-H(16)	0.9300
C(17)-C(18)	1.360(5)
C(17)-H(17)	0.9300
C(18)-C(19)	1.400(5)
C(18)-H(18)	0.9300
C(19)-H(19)	0.9300
C(20)-C(21)	1.497(4)
C(20)-C(22)	1.509(4)
C(21)-H(21A)	0.9600
C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-H(23A)	0.9600
C(23)-H(23B)	0.9600
C(23)-H(23C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.497(4)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(27)-C(28)	1.456(6)
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600

C(29)-C(34)	1.380(4)
C(29)-C(30)	1.388(4)
C(30)-C(31)	1.374(4)
C(30)-H(30)	0.9300
C(31)-C(32)	1.375(4)
C(31)-H(31)	0.9300
C(32)-C(33)	1.363(4)
C(33)-C(34)	1.379(4)
C(33)-H(33)	0.9300
C(34)-H(34)	0.9300
C(35)-C(40)	1.384(4)
C(35)-C(36)	1.392(4)
C(36)-C(37)	1.374(4)
C(36)-H(36)	0.9300
C(37)-C(38)	1.377(4)
C(37)-H(37)	0.9300
C(38)-C(39)	1.363(4)
C(39)-C(40)	1.389(4)
C(39)-H(39)	0.9300
C(40)-H(40)	0.9300
C(41)-H(41A)	0.9700
C(41)-H(41B)	0.9700
C(26)-O(2)-C(27)	117.1(2)
C(2)-C(1)-C(29)	122.7(2)
C(2)-C(1)-C(35)	123.9(2)
C(29)-C(1)-C(35)	113.3(2)
C(1)-C(2)-C(3)	126.9(2)
C(1)-C(2)-C(6)	127.6(2)
C(3)-C(2)-C(6)	105.2(2)
C(20)-C(3)-C(2)	125.2(2)
C(20)-C(3)-C(4)	126.4(2)
C(2)-C(3)-C(4)	108.2(2)
C(5)-C(4)-C(24)	110.7(2)
C(5)-C(4)-C(3)	99.9(2)
C(24)-C(4)-C(3)	111.1(2)
C(5)-C(4)-C(23)	110.7(2)
C(24)-C(4)-C(23)	110.3(2)
C(3)-C(4)-C(23)	113.8(2)
C(13)-C(5)-C(4)	133.9(2)
C(13)-C(5)-C(6)	111.9(2)
C(4)-C(5)-C(6)	111.9(2)
C(13)-C(5)-H(5)	94.9
C(4)-C(5)-H(5)	94.9
C(6)-C(5)-H(5)	94.9
C(7)-C(6)-C(5)	101.9(2)
C(7)-C(6)-C(2)	122.9(2)
C(5)-C(6)-C(2)	96.78(19)
C(7)-C(6)-C(25)	109.9(2)
C(5)-C(6)-C(25)	115.4(2)
C(2)-C(6)-C(25)	109.35(19)
C(8)-C(7)-C(12)	119.7(2)
C(8)-C(7)-C(6)	131.7(2)
C(12)-C(7)-C(6)	108.1(2)
C(7)-C(8)-C(9)	119.4(3)
C(7)-C(8)-H(8)	120.3
C(9)-C(8)-H(8)	120.3
C(10)-C(9)-C(8)	120.9(3)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(11)-C(10)-C(9)	120.6(3)
C(11)-C(10)-H(10)	119.7
C(9)-C(10)-H(10)	119.7
C(10)-C(11)-C(12)	118.9(3)
C(10)-C(11)-H(11)	120.6
C(12)-C(11)-H(11)	120.6
C(11)-C(12)-C(7)	120.3(3)
C(11)-C(12)-C(13)	129.9(3)
C(7)-C(12)-C(13)	109.8(2)
C(5)-C(13)-C(12)	108.2(2)
C(5)-C(13)-C(14)	129.4(2)
C(12)-C(13)-C(14)	122.4(2)

C(19)-C(14)-C(15)	117.7(3)
C(19)-C(14)-C(13)	120.7(3)
C(15)-C(14)-C(13)	121.5(2)
C(16)-C(15)-C(14)	121.5(3)
C(16)-C(15)-H(15)	119.2
C(14)-C(15)-H(15)	119.3
C(17)-C(16)-C(15)	120.3(3)
C(17)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(18)-C(17)-C(16)	119.6(3)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(17)-C(18)-C(19)	120.6(3)
C(17)-C(18)-H(18)	119.7
C(19)-C(18)-H(18)	119.7
C(14)-C(19)-C(18)	120.3(3)
C(14)-C(19)-H(19)	119.9
C(18)-C(19)-H(19)	119.9
C(3)-C(20)-C(21)	123.5(3)
C(3)-C(20)-C(22)	124.3(3)
C(21)-C(20)-C(22)	112.2(3)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(4)-C(23)-H(23A)	109.5
C(4)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(4)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(4)-C(24)-H(24A)	109.5
C(4)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(4)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(6)	115.2(2)
C(26)-C(25)-H(25A)	108.5
C(6)-C(25)-H(25A)	108.5
C(26)-C(25)-H(25B)	108.5
C(6)-C(25)-H(25B)	108.5
H(25A)-C(25)-H(25B)	107.5
O(1)-C(26)-O(2)	122.6(3)
O(1)-C(26)-C(25)	124.4(3)
O(2)-C(26)-C(25)	113.0(2)
C(28)-C(27)-O(2)	111.2(3)
C(28)-C(27)-H(27A)	109.4
O(2)-C(27)-H(27A)	109.4
C(28)-C(27)-H(27B)	109.4
O(2)-C(27)-H(27B)	109.4
H(27A)-C(27)-H(27B)	108.0
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(34)-C(29)-C(30)	117.8(2)
C(34)-C(29)-C(1)	121.8(2)
C(30)-C(29)-C(1)	120.2(2)
C(31)-C(30)-C(29)	121.9(3)
C(31)-C(30)-H(30)	119.1
C(29)-C(30)-H(30)	119.1



C (30)-C (31)-C (32)	118.4 (3)
C (30)-C (31)-H (31)	120.8
C (32)-C (31)-H (31)	120.8
C (33)-C (32)-C (31)	121.5 (3)
C (33)-C (32)-Cl (1)	119.0 (2)
C (31)-C (32)-Cl (1)	119.5 (2)
C (32)-C (33)-C (34)	119.4 (3)
C (32)-C (33)-H (33)	120.3
C (34)-C (33)-H (33)	120.3
C (33)-C (34)-C (29)	121.0 (3)
C (33)-C (34)-H (34)	119.5
C (29)-C (34)-H (34)	119.5
C (40)-C (35)-C (36)	117.6 (2)
C (40)-C (35)-C (1)	120.0 (2)
C (36)-C (35)-C (1)	122.3 (2)
C (37)-C (36)-C (35)	121.2 (3)
C (37)-C (36)-H (36)	119.4
C (35)-C (36)-H (36)	119.4
C (36)-C (37)-C (38)	119.6 (3)
C (36)-C (37)-H (37)	120.2
C (38)-C (37)-H (37)	120.2
C (39)-C (38)-C (37)	121.0 (3)
C (39)-C (38)-Cl (2)	119.5 (2)
C (37)-C (38)-Cl (2)	119.5 (2)
C (38)-C (39)-C (40)	119.0 (3)
C (38)-C (39)-H (39)	120.5
C (40)-C (39)-H (39)	120.5
C (35)-C (40)-C (39)	121.5 (3)
C (35)-C (40)-H (40)	119.2
C (39)-C (40)-H (40)	119.2
Cl (4)-C (41)-Cl (3)	112.6 (3)
Cl (4)-C (41)-H (41A)	109.1
Cl (3)-C (41)-H (41A)	109.1
Cl (4)-C (41)-H (41B)	109.1
Cl (3)-C (41)-H (41B)	109.1
H (41A)-C (41)-H (41B)	107.8

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd28383.  
 The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
C1(1)	88(1)	125(1)	31(1)	-7(1)	-2(1)	16(1)
C1(2)	66(1)	75(1)	70(1)	12(1)	3(1)	34(1)
C1(3)	176(2)	311(3)	202(2)	-56(2)	37(2)	-107(2)
C1(4)	147(2)	172(2)	387(4)	114(2)	69(2)	95(1)
O(1)	102(2)	112(2)	54(2)	30(1)	17(1)	58(2)
O(2)	66(1)	70(2)	51(1)	3(1)	16(1)	26(1)
C(1)	33(1)	37(1)	32(1)	3(1)	6(1)	-1(1)
C(2)	30(1)	36(1)	32(1)	2(1)	5(1)	-1(1)
C(3)	40(2)	41(2)	33(2)	0(1)	1(1)	6(1)
C(4)	48(2)	47(2)	30(2)	-5(1)	3(1)	4(1)
C(5)	44(2)	24(1)	36(1)	-1(1)	7(1)	7(1)
C(6)	33(1)	34(1)	33(1)	0(1)	4(1)	0(1)
C(7)	34(1)	37(1)	37(2)	2(1)	3(1)	4(1)
C(8)	36(2)	54(2)	40(2)	6(1)	2(1)	5(1)
C(9)	46(2)	73(2)	44(2)	0(2)	-10(1)	8(2)
C(10)	37(2)	65(2)	65(2)	1(2)	-6(2)	-5(1)
C(11)	37(2)	52(2)	63(2)	5(2)	7(1)	-9(1)
C(12)	39(2)	32(1)	43(2)	1(1)	6(1)	1(1)
C(13)	44(2)	30(1)	42(2)	3(1)	11(1)	3(1)
C(14)	46(2)	40(2)	45(2)	6(1)	12(1)	-1(1)
C(15)	62(2)	46(2)	54(2)	3(1)	27(2)	-2(2)
C(16)	80(2)	72(2)	60(2)	0(2)	35(2)	1(2)
C(17)	84(3)	84(3)	65(2)	17(2)	39(2)	-7(2)
C(18)	105(3)	62(2)	81(3)	17(2)	33(2)	-22(2)
C(19)	93(3)	48(2)	62(2)	4(2)	30(2)	-11(2)
C(20)	41(2)	50(2)	48(2)	-10(1)	-4(1)	3(1)
C(21)	39(2)	62(2)	82(2)	-10(2)	5(2)	-7(2)
C(22)	56(2)	100(3)	69(3)	-26(2)	-18(2)	1(2)
C(23)	64(2)	70(2)	50(2)	-25(2)	1(2)	3(2)
C(24)	66(2)	75(2)	38(2)	13(2)	8(2)	14(2)
C(25)	42(2)	42(2)	37(2)	4(1)	8(1)	-1(1)
C(26)	54(2)	41(2)	41(2)	8(1)	10(1)	4(1)
C(27)	83(3)	77(3)	75(3)	-4(2)	24(2)	33(2)
C(28)	67(3)	106(4)	156(5)	20(3)	34(3)	20(3)
C(29)	30(1)	40(2)	35(1)	-1(1)	6(1)	5(1)
C(30)	46(2)	49(2)	42(2)	1(1)	7(1)	-2(1)
C(31)	55(2)	68(2)	39(2)	10(2)	11(1)	3(2)
C(32)	44(2)	78(2)	27(2)	-4(2)	1(1)	16(2)
C(33)	46(2)	56(2)	47(2)	-12(2)	1(1)	4(1)
C(34)	43(2)	41(2)	38(2)	-4(1)	5(1)	5(1)
C(35)	36(1)	38(1)	33(1)	-2(1)	5(1)	-3(1)
C(36)	47(2)	47(2)	38(2)	3(1)	10(1)	6(1)
C(37)	59(2)	49(2)	39(2)	10(1)	6(1)	9(1)
C(38)	42(2)	44(2)	45(2)	-1(1)	0(1)	8(1)
C(39)	41(2)	48(2)	42(2)	-5(1)	8(1)	3(1)
C(40)	41(2)	45(2)	33(1)	4(1)	4(1)	3(1)
C(41)	137(5)	129(5)	348(11)	-20(6)	157(7)	-55(4)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd28383.

	x	y	z	U (eq)
H(5)	4462	1228	914	42
H(8)	4922	1952	2538	53
H(9)	6802	2676	2870	67
H(10)	8109	3301	2355	69
H(11)	7583	3171	1494	61
H(15)	5770	1291	186	63
H(16)	6762	1775	-464	82
H(17)	7563	3500	-499	90
H(18)	7412	4729	127	97
H(19)	6378	4268	780	79
H(21A)	445	1859	1481	92
H(21B)	-504	1214	1095	92
H(21C)	-514	2497	1096	92
H(22A)	790	1783	19	117
H(22B)	-481	2048	174	117
H(22C)	37	852	227	117
H(23A)	3764	639	195	93
H(23B)	2371	836	-1	93
H(23C)	2784	237	512	93
H(24A)	3206	3541	369	90
H(24B)	2241	2901	-12	90
H(24C)	3641	2738	-19	90
H(25A)	3450	539	1948	48
H(25B)	3072	265	1379	48
H(27A)	6267	-1572	1447	92
H(27B)	6124	-1390	866	92
H(28A)	7260	175	993	162
H(28B)	8006	-816	1255	162
H(28C)	7384	18	1575	162
H(30)	2217	1715	2454	55
H(31)	2857	1830	3307	64
H(33)	4219	4805	3125	60
H(34)	3512	4709	2276	49
H(36)	1738	4332	886	53
H(37)	194	5574	653	59
H(39)	-971	5145	1962	52
H(40)	575	3884	2194	48
H(41A)	9293	-269	3061	230
H(41B)	8494	669	3236	230

Table 6. Torsion angles [deg] for cd28383.

C(29)-C(1)-C(2)-C(3)	164.5(2)
C(35)-C(1)-C(2)-C(3)	-13.5(4)
C(29)-C(1)-C(2)-C(6)	-23.1(4)
C(35)-C(1)-C(2)-C(6)	158.9(2)
C(1)-C(2)-C(3)-C(20)	-45.2(4)
C(6)-C(2)-C(3)-C(20)	141.1(3)
C(1)-C(2)-C(3)-C(4)	140.5(3)
C(6)-C(2)-C(3)-C(4)	-33.3(3)
C(20)-C(3)-C(4)-C(5)	-165.0(3)
C(2)-C(3)-C(4)-C(5)	9.3(3)
C(20)-C(3)-C(4)-C(24)	78.1(4)
C(2)-C(3)-C(4)-C(24)	-107.6(2)
C(20)-C(3)-C(4)-C(23)	-47.0(4)
C(2)-C(3)-C(4)-C(23)	127.3(2)
C(24)-C(4)-C(5)-C(13)	-25.2(4)
C(3)-C(4)-C(5)-C(13)	-142.3(3)
C(23)-C(4)-C(5)-C(13)	97.5(3)
C(24)-C(4)-C(5)-C(6)	135.8(2)
C(3)-C(4)-C(5)-C(6)	18.7(3)
C(23)-C(4)-C(5)-C(6)	-101.6(3)
C(13)-C(5)-C(6)-C(7)	2.2(3)
C(4)-C(5)-C(6)-C(7)	-163.1(2)
C(13)-C(5)-C(6)-C(2)	127.9(2)
C(4)-C(5)-C(6)-C(2)	-37.4(2)
C(13)-C(5)-C(6)-C(25)	-116.9(2)
C(4)-C(5)-C(6)-C(25)	77.8(3)
C(1)-C(2)-C(6)-C(7)	-23.6(4)
C(3)-C(2)-C(6)-C(7)	150.0(2)
C(1)-C(2)-C(6)-C(5)	-132.5(3)
C(3)-C(2)-C(6)-C(5)	41.2(2)
C(1)-C(2)-C(6)-C(25)	107.5(3)
C(3)-C(2)-C(6)-C(25)	-78.8(2)
C(5)-C(6)-C(7)-C(8)	-175.1(3)
C(2)-C(6)-C(7)-C(8)	78.7(4)
C(25)-C(6)-C(7)-C(8)	-52.2(4)
C(5)-C(6)-C(7)-C(12)	-2.9(3)
C(2)-C(6)-C(7)-C(12)	-109.2(3)
C(25)-C(6)-C(7)-C(12)	120.0(2)
C(12)-C(7)-C(8)-C(9)	5.2(4)
C(6)-C(7)-C(8)-C(9)	176.6(3)
C(7)-C(8)-C(9)-C(10)	-2.9(4)
C(8)-C(9)-C(10)-C(11)	-1.2(5)
C(9)-C(10)-C(11)-C(12)	2.8(5)
C(10)-C(11)-C(12)-C(7)	-0.4(4)
C(10)-C(11)-C(12)-C(13)	-179.9(3)
C(8)-C(7)-C(12)-C(11)	-3.6(4)
C(6)-C(7)-C(12)-C(11)	-176.8(2)
C(8)-C(7)-C(12)-C(13)	176.0(2)
C(6)-C(7)-C(12)-C(13)	2.8(3)
C(4)-C(5)-C(13)-C(12)	160.3(3)
C(6)-C(5)-C(13)-C(12)	-0.7(3)
C(4)-C(5)-C(13)-C(14)	-19.3(5)
C(6)-C(5)-C(13)-C(14)	179.8(2)
C(11)-C(12)-C(13)-C(5)	178.2(3)
C(7)-C(12)-C(13)-C(5)	-1.3(3)
C(11)-C(12)-C(13)-C(14)	-2.2(4)
C(7)-C(12)-C(13)-C(14)	178.3(2)
C(5)-C(13)-C(14)-C(19)	128.3(3)
C(12)-C(13)-C(14)-C(19)	-51.2(4)
C(5)-C(13)-C(14)-C(15)	-53.8(4)
C(12)-C(13)-C(14)-C(15)	126.7(3)
C(19)-C(14)-C(15)-C(16)	-1.2(5)
C(13)-C(14)-C(15)-C(16)	-179.2(3)
C(14)-C(15)-C(16)-C(17)	0.5(5)
C(15)-C(16)-C(17)-C(18)	0.8(6)
C(16)-C(17)-C(18)-C(19)	-1.5(6)
C(15)-C(14)-C(19)-C(18)	0.5(5)
C(13)-C(14)-C(19)-C(18)	178.5(3)

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C(17)-C(18)-C(19)-C(14)	0.8(6)
C(2)-C(3)-C(20)-C(21)	-3.8(5)
C(4)-C(3)-C(20)-C(21)	169.5(3)
C(2)-C(3)-C(20)-C(22)	176.4(3)
C(4)-C(3)-C(20)-C(22)	-10.3(5)
C(7)-C(6)-C(25)-C(26)	-49.1(3)
C(5)-C(6)-C(25)-C(26)	65.4(3)
C(2)-C(6)-C(25)-C(26)	173.1(2)
C(27)-O(2)-C(26)-O(1)	-1.8(5)
C(27)-O(2)-C(26)-C(25)	178.3(3)
C(6)-C(25)-C(26)-O(1)	109.5(3)
C(6)-C(25)-C(26)-O(2)	-70.5(3)
C(26)-O(2)-C(27)-C(28)	-86.3(4)
C(2)-C(1)-C(29)-C(34)	118.8(3)
C(35)-C(1)-C(29)-C(34)	-63.0(3)
C(2)-C(1)-C(29)-C(30)	-66.0(3)
C(35)-C(1)-C(29)-C(30)	112.2(3)
C(34)-C(29)-C(30)-C(31)	-0.5(4)
C(1)-C(29)-C(30)-C(31)	-175.9(3)
C(29)-C(30)-C(31)-C(32)	-0.8(4)
C(30)-C(31)-C(32)-C(33)	0.9(5)
C(30)-C(31)-C(32)-C1(1)	179.2(2)
C(31)-C(32)-C(33)-C(34)	0.3(4)
C1(1)-C(32)-C(33)-C(34)	-178.0(2)
C(32)-C(33)-C(34)-C(29)	-1.7(4)
C(30)-C(29)-C(34)-C(33)	1.7(4)
C(1)-C(29)-C(34)-C(33)	177.1(2)
C(2)-C(1)-C(35)-C(40)	142.9(3)
C(29)-C(1)-C(35)-C(40)	-35.3(3)
C(2)-C(1)-C(35)-C(36)	-40.0(4)
C(29)-C(1)-C(35)-C(36)	141.9(3)
C(40)-C(35)-C(36)-C(37)	-2.4(4)
C(1)-C(35)-C(36)-C(37)	-179.6(3)
C(35)-C(36)-C(37)-C(38)	0.8(4)
C(36)-C(37)-C(38)-C(39)	1.2(4)
C(36)-C(37)-C(38)-C1(2)	-179.3(2)
C(37)-C(38)-C(39)-C(40)	-1.4(4)
C1(2)-C(38)-C(39)-C(40)	179.1(2)
C(36)-C(35)-C(40)-C(39)	2.1(4)
C(1)-C(35)-C(40)-C(39)	179.4(2)
C(38)-C(39)-C(40)-C(35)	-0.3(4)

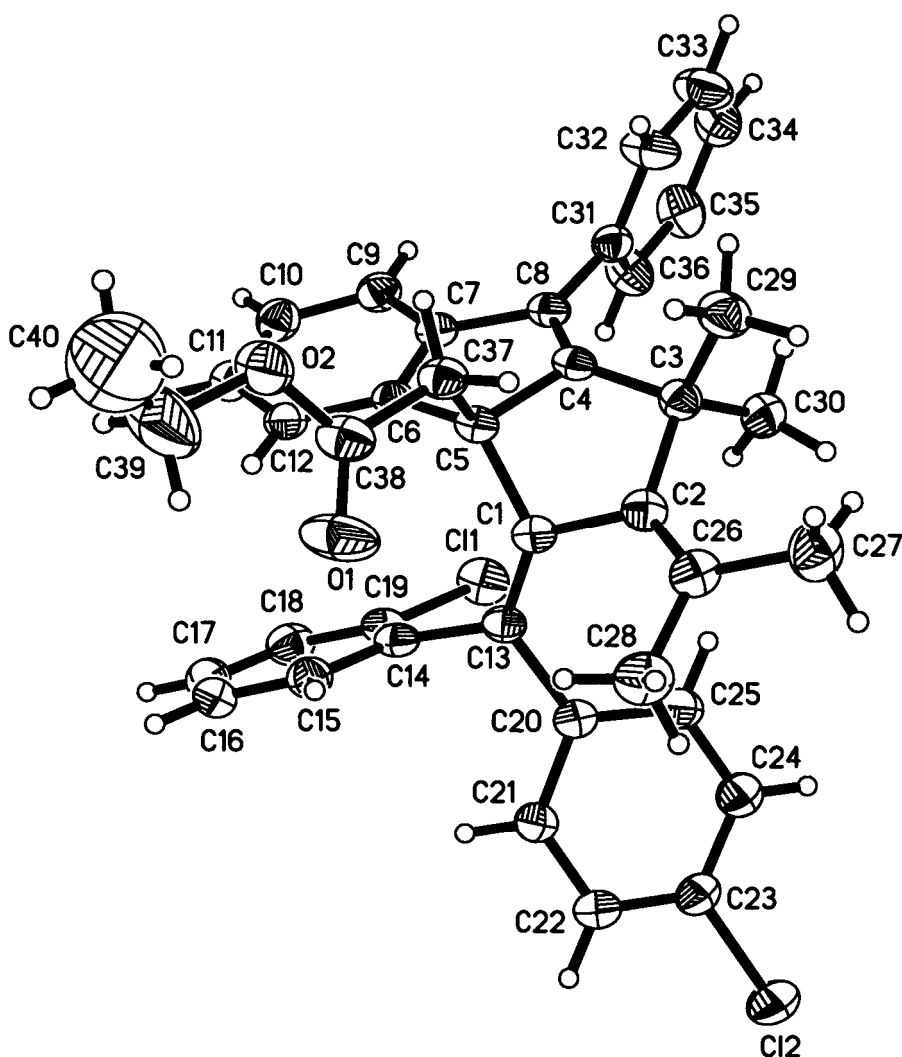
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Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd28383 [A and deg.].

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D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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The crystal data of **4e** have been deposited in CCDC with number 719328. Empirical Formula:  $C_{43}H_{42}Cl_2O_2$ ; Formula Weight: 661.67; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.471 x 0.425 x 0.360 mm; Crystal System: Triclinic; Lattice Type: Primitive; Lattice Parameters:  $a = 9.7469(12)\text{\AA}$ ,  $b = 11.6130(14)\text{\AA}$ ,  $c = 15.7201(18)\text{\AA}$ ,  $\alpha = 90.102(2)^\circ$ ,  $\beta = 93.697(3)^\circ$ ,  $\gamma = 100.409(2)^\circ$ ,  $V = 1746.3(4)\text{\AA}^3$ ; Space group: P-1;  $Z = 2$ ;  $D_{calc} = 1.258\text{ g/cm}^3$ ;  $F_{000} = 700$ ; Diffractometer: Rigaku AFC7R; Residuals: R;  $R_w = 0.0733, 0.1969$ .

Table 1. Crystal data and structure refinement for cd2931.

Identification code	cd2931
Empirical formula	C43 H42 Cl2 O2
Formula weight	661.67
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 9.7469(12) Å    alpha = 90.102(2) deg. b = 11.6130(14) Å    beta = 93.697(3) deg. c = 15.7201(18) Å    gamma = 100.409(2) deg.
Volume	1746.3(4) Å <sup>3</sup>
Z, Calculated density	2, 1.258 Mg/m <sup>3</sup>
Absorption coefficient	0.222 mm <sup>-1</sup>
F(000)	700
Crystal size	0.471 x 0.425 x 0.360 mm
Theta range for data collection	1.78 to 26.00 deg.
Limiting indices	-12<=h<=8, -14<=k<=14, -19<=l<=17
Reflections collected / unique	9592 / 6727 [R(int) = 0.0800]
Completeness to theta = 26.00	98.2 %
Absorption correction	Empirical
Max. and min. transmission	1.0000 and 0.8254
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	6727 / 5 / 409
Goodness-of-fit on F <sup>2</sup>	0.956
Final R indices [I>2sigma(I)]	R1 = 0.0733, wR2 = 0.1969
R indices (all data)	R1 = 0.1097, wR2 = 0.2209
Largest diff. peak and hole	0.826 and -0.340 e.Å <sup>-3</sup>



Table 2. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd2931.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.

	x	y	z	U(eq)
C1(1)	-442(1)	7180(1)	3580(1)	65(1)
C1(2)	-733(2)	12031(1)	1226(1)	89(1)
O(1)	2709(4)	5494(4)	807(2)	102(1)
O(2)	3725(4)	4067(3)	1298(2)	92(1)
C(1)	2577(4)	7366(3)	2241(2)	43(1)
C(2)	3865(4)	8299(3)	2289(2)	47(1)
C(3)	4663(4)	8183(3)	3159(2)	48(1)
C(4)	3891(4)	6999(3)	3426(2)	43(1)
C(5)	3068(4)	6305(3)	2669(2)	42(1)
C(6)	2109(4)	5347(3)	3109(2)	40(1)
C(7)	2404(4)	5474(3)	3988(2)	44(1)
C(8)	3515(4)	6519(3)	4178(2)	43(1)
C(9)	1718(4)	4682(3)	4548(2)	51(1)
C(10)	738(4)	3756(3)	4207(3)	56(1)
C(11)	469(4)	3587(3)	3348(3)	54(1)
C(12)	1173(4)	4384(3)	2780(2)	48(1)
C(13)	1260(4)	7501(3)	2031(2)	41(1)
C(14)	34(4)	6518(3)	1993(2)	44(1)
C(15)	-335(4)	5813(3)	1276(2)	54(1)
C(16)	-1523(5)	4955(4)	1229(3)	63(1)
C(17)	-2372(5)	4775(4)	1909(3)	67(1)
C(18)	-2040(4)	5452(4)	2619(3)	60(1)
C(19)	-853(4)	6334(3)	2662(2)	47(1)
C(20)	831(4)	8651(3)	1817(2)	44(1)
C(21)	-181(4)	8724(3)	1167(2)	54(1)
C(22)	-649(4)	9749(4)	978(3)	60(1)
C(23)	-115(5)	10728(3)	1446(3)	58(1)
C(24)	873(5)	10707(4)	2108(3)	67(1)
C(25)	1337(5)	9675(4)	2286(3)	59(1)
C(26)	4270(4)	9005(4)	1641(2)	55(1)
C(27)	5543(5)	9993(4)	1711(3)	77(1)
C(28)	3511(5)	8928(4)	775(2)	69(1)
C(29)	6233(4)	8173(4)	3121(3)	67(1)
C(30)	4464(5)	9146(3)	3791(2)	60(1)
C(31)	4043(4)	6871(3)	5057(2)	46(1)
C(32)	5380(5)	6808(4)	5355(3)	72(1)
C(33)	5830(6)	7088(5)	6191(3)	84(2)
C(34)	4967(6)	7439(4)	6740(3)	73(1)
C(35)	3631(5)	7498(4)	6461(3)	74(1)
C(36)	3164(5)	7218(4)	5632(3)	64(1)
C(37)	4086(4)	5772(3)	2135(2)	52(1)
C(38)	3407(5)	5118(4)	1349(3)	62(1)
C(39)	3108(9)	3374(8)	557(5)	170(4)
C(40)	4025(13)	2794(10)	184(7)	171(5)
C(41)	1235(9)	609(7)	4669(5)	141(3)
C(42)	1384(8)	-293(6)	5166(5)	122(2)
C(43)	509(10)	-458(8)	5731(5)	150(3)

Table 3. Bond lengths [Å] and angles [deg] for cd2931.

C1(1)-C(19)	1.728(4)
C1(2)-C(23)	1.753(4)
O(1)-C(38)	1.190(5)
O(2)-C(38)	1.315(5)
O(2)-C(39)	1.449(6)
C(1)-C(13)	1.342(5)
C(1)-C(2)	1.501(5)
C(1)-C(5)	1.541(5)
C(2)-C(26)	1.343(5)
C(2)-C(3)	1.548(5)
C(3)-C(4)	1.517(5)
C(3)-C(29)	1.537(5)
C(3)-C(30)	1.540(5)
C(4)-C(8)	1.352(5)
C(4)-C(5)	1.533(5)
C(5)-C(6)	1.516(5)
C(5)-C(37)	1.549(5)
C(6)-C(12)	1.386(5)
C(6)-C(7)	1.395(5)
C(7)-C(9)	1.388(5)
C(7)-C(8)	1.490(5)
C(8)-C(31)	1.472(5)
C(9)-C(10)	1.384(6)
C(9)-H(9)	0.9300
C(10)-C(11)	1.367(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.406(5)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.493(5)
C(13)-C(20)	1.502(5)
C(14)-C(15)	1.381(5)
C(14)-C(19)	1.397(5)
C(15)-C(16)	1.383(6)
C(15)-H(15)	0.9300
C(16)-C(17)	1.387(6)
C(16)-H(16)	0.9300
C(17)-C(18)	1.352(6)
C(17)-H(17)	0.9300
C(18)-C(19)	1.398(5)
C(18)-H(18)	0.9300
C(20)-C(21)	1.387(5)
C(20)-C(25)	1.393(5)
C(21)-C(22)	1.375(5)
C(21)-H(21)	0.9300
C(22)-C(23)	1.356(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.375(6)
C(24)-C(25)	1.378(5)
C(24)-H(24)	0.9300
C(25)-H(25)	0.9300
C(26)-C(28)	1.501(6)
C(26)-C(27)	1.528(6)
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600
C(31)-C(32)	1.370(6)
C(31)-C(36)	1.392(5)
C(32)-C(33)	1.378(6)

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C(32)-H(32)	0.9300
C(33)-C(34)	1.354(7)
C(33)-H(33)	0.9300
C(34)-C(35)	1.360(7)
C(34)-H(34)	0.9300
C(35)-C(36)	1.372(6)
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300
C(37)-C(38)	1.500(6)
C(37)-H(37A)	0.9700
C(37)-H(37B)	0.9700
C(39)-C(40)	1.372(11)
C(39)-H(39A)	0.9700
C(39)-H(39B)	0.9700
C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600
C(41)-C(42)	1.332(9)
C(42)-C(43)	1.262(9)
C(38)-O(2)-C(39)	115.4(4)
C(13)-C(1)-C(2)	127.2(3)
C(13)-C(1)-C(5)	127.7(3)
C(2)-C(1)-C(5)	103.9(3)
C(26)-C(2)-C(1)	124.0(3)
C(26)-C(2)-C(3)	128.3(4)
C(1)-C(2)-C(3)	107.4(3)
C(4)-C(3)-C(29)	110.8(3)
C(4)-C(3)-C(30)	110.5(3)
C(29)-C(3)-C(30)	109.2(3)
C(4)-C(3)-C(2)	99.8(3)
C(29)-C(3)-C(2)	115.3(3)
C(30)-C(3)-C(2)	111.1(3)
C(8)-C(4)-C(3)	134.7(3)
C(8)-C(4)-C(5)	111.7(3)
C(3)-C(4)-C(5)	111.8(3)
C(6)-C(5)-C(4)	102.1(3)
C(6)-C(5)-C(1)	123.8(3)
C(4)-C(5)-C(1)	95.6(3)
C(6)-C(5)-C(37)	110.5(3)
C(4)-C(5)-C(37)	109.3(3)
C(1)-C(5)-C(37)	112.9(3)
C(12)-C(6)-C(7)	120.0(3)
C(12)-C(6)-C(5)	131.0(3)
C(7)-C(6)-C(5)	108.7(3)
C(9)-C(7)-C(6)	121.1(3)
C(9)-C(7)-C(8)	129.0(3)
C(6)-C(7)-C(8)	109.9(3)
C(4)-C(8)-C(31)	130.4(3)
C(4)-C(8)-C(7)	107.5(3)
C(31)-C(8)-C(7)	122.1(3)
C(10)-C(9)-C(7)	117.9(3)
C(10)-C(9)-H(9)	121.0
C(7)-C(9)-H(9)	121.0
C(11)-C(10)-C(9)	122.1(4)
C(11)-C(10)-H(10)	119.0
C(9)-C(10)-H(10)	119.0
C(10)-C(11)-C(12)	120.0(4)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(6)-C(12)-C(11)	118.8(3)
C(6)-C(12)-H(12)	120.6
C(11)-C(12)-H(12)	120.6
C(1)-C(13)-C(14)	123.7(3)
C(1)-C(13)-C(20)	124.6(3)
C(14)-C(13)-C(20)	111.7(3)
C(15)-C(14)-C(19)	117.1(4)
C(15)-C(14)-C(13)	121.9(3)
C(19)-C(14)-C(13)	120.8(3)
C(14)-C(15)-C(16)	121.3(4)
C(14)-C(15)-H(15)	119.3
C(16)-C(15)-H(15)	119.3

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C(15)-C(16)-C(17)	120.4(4)
C(15)-C(16)-H(16)	119.8
C(17)-C(16)-H(16)	119.8
C(18)-C(17)-C(16)	119.7(4)
C(18)-C(17)-H(17)	120.2
C(16)-C(17)-H(17)	120.2
C(17)-C(18)-C(19)	120.0(4)
C(17)-C(18)-H(18)	120.0
C(19)-C(18)-H(18)	120.0
C(14)-C(19)-C(18)	121.5(4)
C(14)-C(19)-C1(1)	119.3(3)
C(18)-C(19)-C1(1)	119.1(3)
C(21)-C(20)-C(25)	116.2(3)
C(21)-C(20)-C(13)	120.9(3)
C(25)-C(20)-C(13)	122.8(3)
C(22)-C(21)-C(20)	122.6(4)
C(22)-C(21)-H(21)	118.7
C(20)-C(21)-H(21)	118.7
C(23)-C(22)-C(21)	119.2(4)
C(23)-C(22)-H(22)	120.4
C(21)-C(22)-H(22)	120.4
C(22)-C(23)-C(24)	121.0(4)
C(22)-C(23)-C1(2)	119.6(3)
C(24)-C(23)-C1(2)	119.4(3)
C(23)-C(24)-C(25)	119.1(4)
C(23)-C(24)-H(24)	120.5
C(25)-C(24)-H(24)	120.5
C(24)-C(25)-C(20)	122.0(4)
C(24)-C(25)-H(25)	119.0
C(20)-C(25)-H(25)	119.0
C(2)-C(26)-C(28)	123.9(4)
C(2)-C(26)-C(27)	123.5(4)
C(28)-C(26)-C(27)	112.6(3)
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(3)-C(29)-H(29A)	109.5
C(3)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(3)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(3)-C(30)-H(30A)	109.5
C(3)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(3)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(32)-C(31)-C(36)	117.4(4)
C(32)-C(31)-C(8)	121.9(3)
C(36)-C(31)-C(8)	120.6(4)
C(31)-C(32)-C(33)	120.9(4)
C(31)-C(32)-H(32)	119.6
C(33)-C(32)-H(32)	119.6
C(34)-C(33)-C(32)	120.9(5)
C(34)-C(33)-H(33)	119.5
C(32)-C(33)-H(33)	119.5
C(33)-C(34)-C(35)	119.3(4)
C(33)-C(34)-H(34)	120.4
C(35)-C(34)-H(34)	120.4
C(34)-C(35)-C(36)	120.6(4)
C(34)-C(35)-H(35)	119.7
C(36)-C(35)-H(35)	119.7

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C(35)-C(36)-C(31)	120.9(4)
C(35)-C(36)-H(36)	119.5
C(31)-C(36)-H(36)	119.5
C(38)-C(37)-C(5)	114.2(3)
C(38)-C(37)-H(37A)	108.7
C(5)-C(37)-H(37A)	108.7
C(38)-C(37)-H(37B)	108.7
C(5)-C(37)-H(37B)	108.7
H(37A)-C(37)-H(37B)	107.6
O(1)-C(38)-O(2)	122.4(4)
O(1)-C(38)-C(37)	125.6(4)
O(2)-C(38)-C(37)	111.9(4)
C(40)-C(39)-O(2)	113.3(7)
C(40)-C(39)-H(39A)	108.9
O(2)-C(39)-H(39A)	108.9
C(40)-C(39)-H(39B)	108.9
O(2)-C(39)-H(39B)	108.9
H(39A)-C(39)-H(39B)	107.7
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
C(42)-C(41)-C(43)#1	109.6(7)
C(43)-C(42)-C(41)	112.8(8)
C(42)-C(43)-C(41)#1	114.1(7)

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Symmetry transformations used to generate equivalent atoms:  
#1 -x, -y, -z+1

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd2931.  
 The anisotropic displacement factor exponent takes the form:  
 $-2 \pi^2 [ h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12} ]$

	U11	U22	U33	U23	U13	U12
C1(1)	67(1)	82(1)	49(1)	-2(1)	12(1)	20(1)
C1(2)	108(1)	57(1)	107(1)	3(1)	-26(1)	37(1)
O(1)	121(3)	152(3)	50(2)	-21(2)	-21(2)	82(3)
O(2)	104(3)	91(2)	88(2)	-43(2)	-30(2)	50(2)
C(1)	44(2)	49(2)	39(2)	3(2)	4(2)	15(2)
C(2)	41(2)	54(2)	47(2)	2(2)	8(2)	12(2)
C(3)	41(2)	50(2)	53(2)	4(2)	2(2)	9(2)
C(4)	36(2)	52(2)	44(2)	1(2)	-3(2)	16(2)
C(5)	39(2)	51(2)	38(2)	2(2)	1(2)	13(2)
C(6)	40(2)	42(2)	42(2)	1(2)	-2(2)	18(2)
C(7)	44(2)	46(2)	43(2)	3(2)	0(2)	17(2)
C(8)	44(2)	49(2)	40(2)	-1(2)	-2(2)	18(2)
C(9)	60(3)	54(2)	41(2)	6(2)	4(2)	15(2)
C(10)	59(3)	53(2)	56(2)	10(2)	6(2)	8(2)
C(11)	52(2)	45(2)	62(3)	4(2)	-5(2)	6(2)
C(12)	53(2)	49(2)	45(2)	-1(2)	-5(2)	18(2)
C(13)	43(2)	50(2)	33(2)	3(2)	3(2)	13(2)
C(14)	43(2)	50(2)	43(2)	5(2)	-2(2)	20(2)
C(15)	64(3)	53(2)	46(2)	-3(2)	-3(2)	21(2)
C(16)	68(3)	54(2)	65(3)	-4(2)	-21(2)	14(2)
C(17)	52(3)	54(3)	92(3)	12(2)	-11(2)	4(2)
C(18)	45(2)	64(3)	72(3)	15(2)	7(2)	12(2)
C(19)	41(2)	54(2)	47(2)	7(2)	2(2)	16(2)
C(20)	44(2)	48(2)	43(2)	6(2)	5(2)	13(2)
C(21)	57(3)	50(2)	55(2)	-2(2)	-9(2)	14(2)
C(22)	60(3)	56(3)	64(3)	8(2)	-11(2)	17(2)
C(23)	66(3)	47(2)	64(3)	3(2)	-3(2)	19(2)
C(24)	73(3)	54(2)	77(3)	-5(2)	-12(2)	22(2)
C(25)	65(3)	60(3)	54(2)	-1(2)	-8(2)	21(2)
C(26)	53(2)	60(2)	55(2)	9(2)	14(2)	14(2)
C(27)	74(3)	76(3)	78(3)	12(2)	17(3)	-2(3)
C(28)	71(3)	85(3)	52(2)	17(2)	18(2)	14(2)
C(29)	47(3)	77(3)	77(3)	11(2)	1(2)	10(2)
C(30)	68(3)	53(2)	58(2)	4(2)	-3(2)	9(2)
C(31)	53(2)	44(2)	40(2)	4(2)	-2(2)	11(2)
C(32)	69(3)	100(4)	55(3)	-10(2)	-11(2)	44(3)
C(33)	86(4)	103(4)	67(3)	-11(3)	-28(3)	39(3)
C(34)	98(4)	69(3)	47(2)	-3(2)	-11(3)	10(3)
C(35)	78(3)	85(3)	56(3)	-12(2)	11(2)	6(3)
C(36)	59(3)	82(3)	51(2)	-11(2)	5(2)	10(2)
C(37)	51(2)	60(2)	47(2)	-3(2)	3(2)	24(2)
C(38)	58(3)	85(3)	51(2)	-7(2)	4(2)	33(2)
C(39)	148(7)	201(8)	174(7)	-125(7)	-70(6)	97(6)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for cd2931.

	x	y	z	U(eq)
H(9)	1910	4770	5134	61
H(10)	247	3232	4575	68
H(11)	-180	2946	3138	65
H(12)	1013	4266	2194	58
H(15)	226	5919	816	64
H(16)	-1754	4494	738	75
H(17)	-3166	4192	1876	81
H(18)	-2602	5331	3079	72
H(21)	-557	8055	846	65
H(22)	-1324	9769	535	72
H(24)	1223	11380	2432	81
H(25)	2009	9663	2732	71
H(27A)	5811	10173	2302	116
H(27B)	5313	10675	1434	116
H(27C)	6303	9751	1443	116
H(28A)	2866	8198	717	103
H(28B)	4173	8973	345	103
H(28C)	3007	9564	711	103
H(29A)	6595	7920	3657	101
H(29B)	6715	8947	3004	101
H(29C)	6369	7645	2676	101
H(30A)	3489	9076	3885	90
H(30B)	4801	9900	3559	90
H(30C)	4978	9060	4322	90
H(32)	5991	6574	4988	86
H(33)	6739	7035	6382	101
H(34)	5284	7637	7301	87
H(35)	3030	7730	6836	88
H(36)	2247	7261	5451	77
H(37A)	4816	6398	1968	62
H(37B)	4528	5244	2491	62
H(39A)	2317	2807	724	204
H(39B)	2759	3885	140	204
H(40A)	4757	3352	-43	281
H(40B)	3538	2297	-269	281
H(40C)	4423	2327	602	281

Table 6. Torsion angles [deg] for cd2931.

C(13)-C(1)-C(2)-C(26)	-55.7(5)
C(5)-C(1)-C(2)-C(26)	136.1(4)
C(13)-C(1)-C(2)-C(3)	130.3(4)
C(5)-C(1)-C(2)-C(3)	-37.9(3)
C(26)-C(2)-C(3)-C(4)	-161.2(4)
C(1)-C(2)-C(3)-C(4)	12.6(3)
C(26)-C(2)-C(3)-C(29)	-42.5(5)
C(1)-C(2)-C(3)-C(29)	131.2(3)
C(26)-C(2)-C(3)-C(30)	82.3(5)
C(1)-C(2)-C(3)-C(30)	-104.0(3)
C(29)-C(3)-C(4)-C(8)	93.1(5)
C(30)-C(3)-C(4)-C(8)	-28.0(6)
C(2)-C(3)-C(4)-C(8)	-145.0(4)
C(29)-C(3)-C(4)-C(5)	-104.2(4)
C(30)-C(3)-C(4)-C(5)	134.7(3)
C(2)-C(3)-C(4)-C(5)	17.7(4)
C(8)-C(4)-C(5)-C(6)	1.4(4)
C(3)-C(4)-C(5)-C(6)	-165.4(3)
C(8)-C(4)-C(5)-C(1)	127.8(3)
C(3)-C(4)-C(5)-C(1)	-39.1(3)
C(8)-C(4)-C(5)-C(37)	-115.6(3)
C(3)-C(4)-C(5)-C(37)	77.6(3)
C(13)-C(1)-C(5)-C(6)	-14.9(5)
C(2)-C(1)-C(5)-C(6)	153.3(3)
C(13)-C(1)-C(5)-C(4)	-123.5(4)
C(2)-C(1)-C(5)-C(4)	44.6(3)
C(13)-C(1)-C(5)-C(37)	122.8(4)
C(2)-C(1)-C(5)-C(37)	-69.1(3)
C(4)-C(5)-C(6)-C(12)	-174.7(3)
C(1)-C(5)-C(6)-C(12)	79.9(5)
C(37)-C(5)-C(6)-C(12)	-58.6(5)
C(4)-C(5)-C(6)-C(7)	-1.9(3)
C(1)-C(5)-C(6)-C(7)	-107.2(4)
C(37)-C(5)-C(6)-C(7)	114.3(3)
C(12)-C(6)-C(7)-C(9)	-3.5(5)
C(5)-C(6)-C(7)-C(9)	-177.3(3)
C(12)-C(6)-C(7)-C(8)	175.5(3)
C(5)-C(6)-C(7)-C(8)	1.8(4)
C(3)-C(4)-C(8)-C(31)	-18.7(7)
C(5)-C(4)-C(8)-C(31)	178.5(3)
C(3)-C(4)-C(8)-C(7)	162.3(4)
C(5)-C(4)-C(8)-C(7)	-0.4(4)
C(9)-C(7)-C(8)-C(4)	178.1(4)
C(6)-C(7)-C(8)-C(4)	-0.9(4)
C(9)-C(7)-C(8)-C(31)	-0.9(6)
C(6)-C(7)-C(8)-C(31)	-179.9(3)
C(6)-C(7)-C(9)-C(10)	0.5(5)
C(8)-C(7)-C(9)-C(10)	-178.4(3)
C(7)-C(9)-C(10)-C(11)	2.1(6)
C(9)-C(10)-C(11)-C(12)	-1.5(6)
C(7)-C(6)-C(12)-C(11)	4.0(5)
C(5)-C(6)-C(12)-C(11)	176.2(3)
C(10)-C(11)-C(12)-C(6)	-1.5(5)
C(2)-C(1)-C(13)-C(14)	179.5(3)
C(5)-C(1)-C(13)-C(14)	-15.0(5)
C(2)-C(1)-C(13)-C(20)	-1.3(5)
C(5)-C(1)-C(13)-C(20)	164.2(3)
C(1)-C(13)-C(14)-C(15)	-84.8(4)
C(20)-C(13)-C(14)-C(15)	95.9(4)
C(1)-C(13)-C(14)-C(19)	100.3(4)
C(20)-C(13)-C(14)-C(19)	-79.0(4)
C(19)-C(14)-C(15)-C(16)	-0.7(5)
C(13)-C(14)-C(15)-C(16)	-175.9(3)
C(14)-C(15)-C(16)-C(17)	-0.4(6)
C(15)-C(16)-C(17)-C(18)	0.5(6)
C(16)-C(17)-C(18)-C(19)	0.5(6)
C(15)-C(14)-C(19)-C(18)	1.8(5)
C(13)-C(14)-C(19)-C(18)	177.0(3)



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C(15)-C(14)-C(19)-C1(1)	179.6(3)
C(13)-C(14)-C(19)-C1(1)	-5.3(5)
C(17)-C(18)-C(19)-C(14)	-1.8(6)
C(17)-C(18)-C(19)-C1(1)	-179.5(3)
C(1)-C(13)-C(20)-C(21)	140.7(4)
C(14)-C(13)-C(20)-C(21)	-40.1(4)
C(1)-C(13)-C(20)-C(25)	-43.9(5)
C(14)-C(13)-C(20)-C(25)	135.4(4)
C(25)-C(20)-C(21)-C(22)	1.1(6)
C(13)-C(20)-C(21)-C(22)	176.9(4)
C(20)-C(21)-C(22)-C(23)	-0.4(6)
C(21)-C(22)-C(23)-C(24)	-0.7(7)
C(21)-C(22)-C(23)-C1(2)	-178.6(3)
C(22)-C(23)-C(24)-C(25)	1.1(7)
C1(2)-C(23)-C(24)-C(25)	179.0(3)
C(23)-C(24)-C(25)-C(20)	-0.3(7)
C(21)-C(20)-C(25)-C(24)	-0.7(6)
C(13)-C(20)-C(25)-C(24)	-176.4(4)
C(1)-C(2)-C(26)-C(28)	-2.0(6)
C(3)-C(2)-C(26)-C(28)	170.8(4)
C(1)-C(2)-C(26)-C(27)	176.8(4)
C(3)-C(2)-C(26)-C(27)	-10.5(6)
C(4)-C(8)-C(31)-C(32)	-66.4(5)
C(7)-C(8)-C(31)-C(32)	112.4(4)
C(4)-C(8)-C(31)-C(36)	117.3(5)
C(7)-C(8)-C(31)-C(36)	-63.9(5)
C(36)-C(31)-C(32)-C(33)	-0.4(7)
C(8)-C(31)-C(32)-C(33)	-176.8(4)
C(31)-C(32)-C(33)-C(34)	-0.4(8)
C(32)-C(33)-C(34)-C(35)	1.0(8)
C(33)-C(34)-C(35)-C(36)	-0.7(7)
C(34)-C(35)-C(36)-C(31)	-0.2(7)
C(32)-C(31)-C(36)-C(35)	0.7(6)
C(8)-C(31)-C(36)-C(35)	177.2(4)
C(6)-C(5)-C(37)-C(38)	71.2(4)
C(4)-C(5)-C(37)-C(38)	-177.2(3)
C(1)-C(5)-C(37)-C(38)	-72.1(4)
C(39)-O(2)-C(38)-O(1)	-3.0(8)
C(39)-O(2)-C(38)-C(37)	179.9(5)
C(5)-C(37)-C(38)-O(1)	53.8(6)
C(5)-C(37)-C(38)-O(2)	-129.3(4)
C(38)-O(2)-C(39)-C(40)	136.7(9)
C(43)#1-C(41)-C(42)-C(43)	-51.7(10)
C(41)-C(42)-C(43)-C(41)#1	54.1(10)

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Symmetry transformations used to generate equivalent atoms:  
#1 -x,-y,-z+1

Table 7. Hydrogen bonds for cd2931 [A and deg.].

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D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
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