

Supporting Information

Phosphine-Catalyzed Annulation of Ethyl (Arylimino)acetates: Synthesis of Highly Functionalized Oxoimidazolidines

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Experimental Section

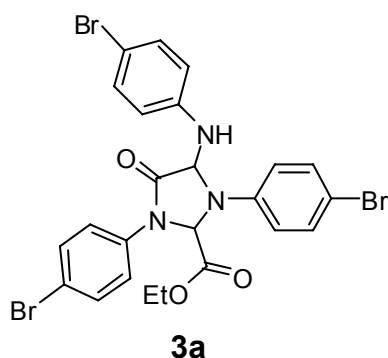
General Remarks. ¹H NMR and ¹³C NMR spectra were recorded for a solution in CDCl₃ with tetramethylsilane (TMS) as internal standard and *J*-values are in Hz. Mass spectra were recorded with a HP-5989 instrument. Organic solvents used were dried by standard methods when necessary. Commercially obtained reagents were used without further purification. All reactions were monitored by TLC with Huanghai GF254 silica gel coated plates. Flash column chromatography was carried out using silica gel at increased pressure. Reaction experiments were performed under argon atmosphere using standard Schlenk techniques.

General Reaction Procedure.

To a mixture of the corresponding ethyl (arylimino)acetate **1** (0.6 mmol), methyl vinyl ketone (63.0 mg, 0.9 mmol, 79 μ L), PPh₂Me (36.0mg, 0.18 mmol, 34 μ L), and 4 $\text{\AA}$ molecular sieves (120 mg, 200 mg/mmol of **1**) was added CH₃CN (1.5 mL) and the solution was stirred under argon atmosphere at 20 $^{\circ}$ C for the required time indicated in the Tables. After the reaction solution was filtered and concentrated under reduced pressure, the residue was purified by

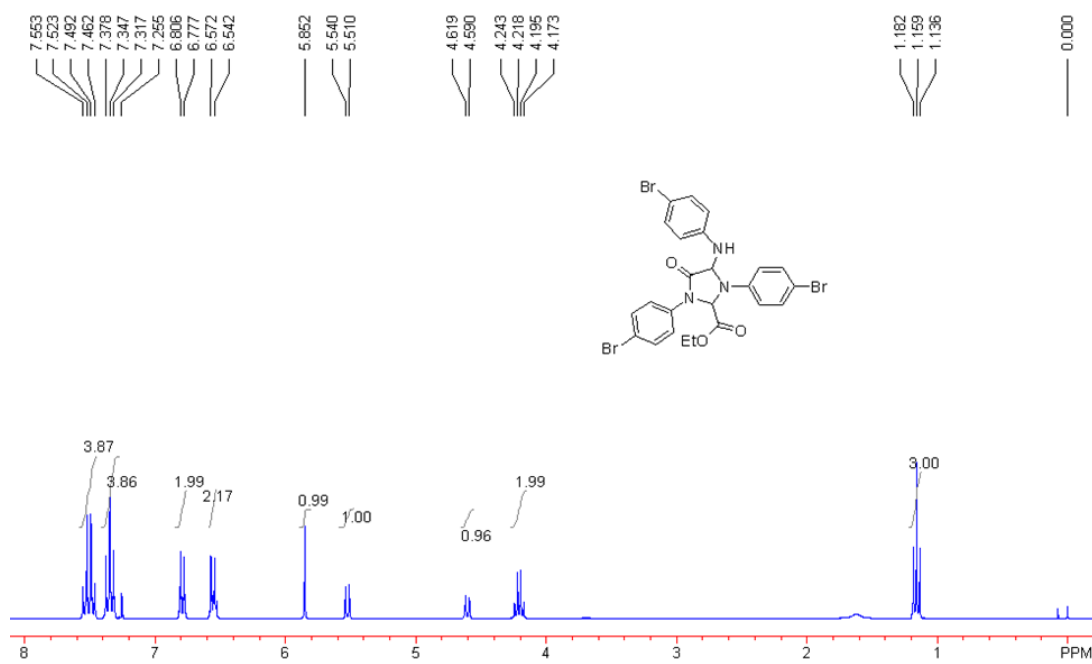
flash chromatography on silica gel (eluent: EtOAc/petroleum ether = 1/10) to afford the corresponding pure product.

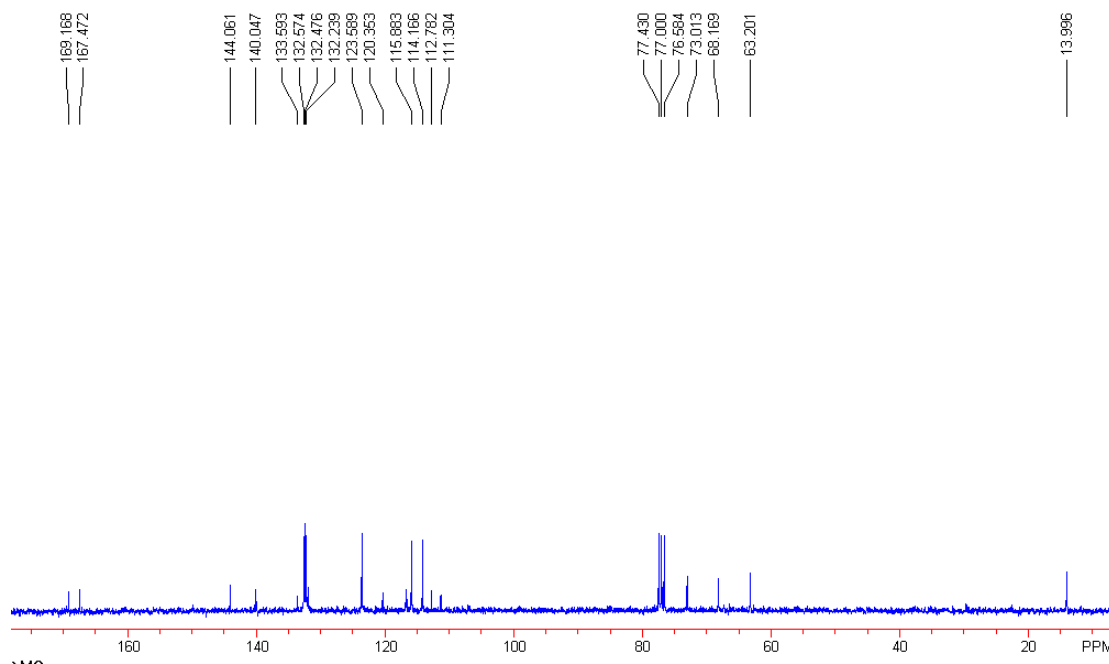
Compound 3a



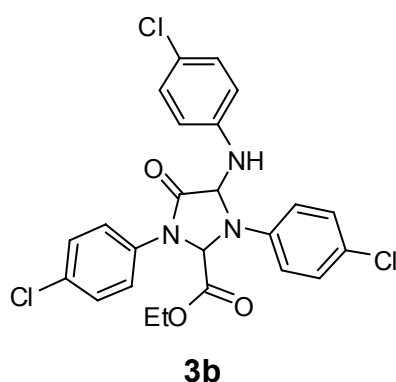
A white solid. Mp. 104-105 °C. IR (CH₂Cl₂) ν 2921, 2869, 1731 (C=O), 1590, 1492, 1372, 1286, 1200, 1071, 1010, 809 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.16 (t, J = 7.2 Hz, 3 H, CH₃), 4.20 (q, J = 7.2 Hz, 2H, CH₂), 4.61 (d, J = 8.7 Hz, 1H, NH), 5.53 (d, J = 8.7 Hz, 1H, CH), 5.85 (s, 1H, CH), 6.56 (d, J = 8.7 Hz, 2H, ArH), 6.80 (d, J = 8.7 Hz, 2H, ArH). 7.35 (t, J = 8.4 Hz, 4H, ArH), 7.51 (q, J = 8.7 Hz, 4H, ArH). ¹³C

NMR (CDCl₃, 75 MHz) δ 14.0, 63.2, 68.2, 73.0, 111.3, 112.8, 114.2, 115.9, 120.4, 123.6, 132.2, 132.5, 132.6, 133.6, 140.0, 144.1, 167.5, 169.2. HRMS (EI) m/z [M^+] Calcd. for C₂₄H₂₀Br₃N₃O₃ requires 634.9055, Found: 634.9055. Anal. Calcd for C₂₄H₂₀Br₃N₃O₃: C, 45.17, H, 3.16, N, 6.58. Found: C, 45.30, H, 3.34, N, 6.43.



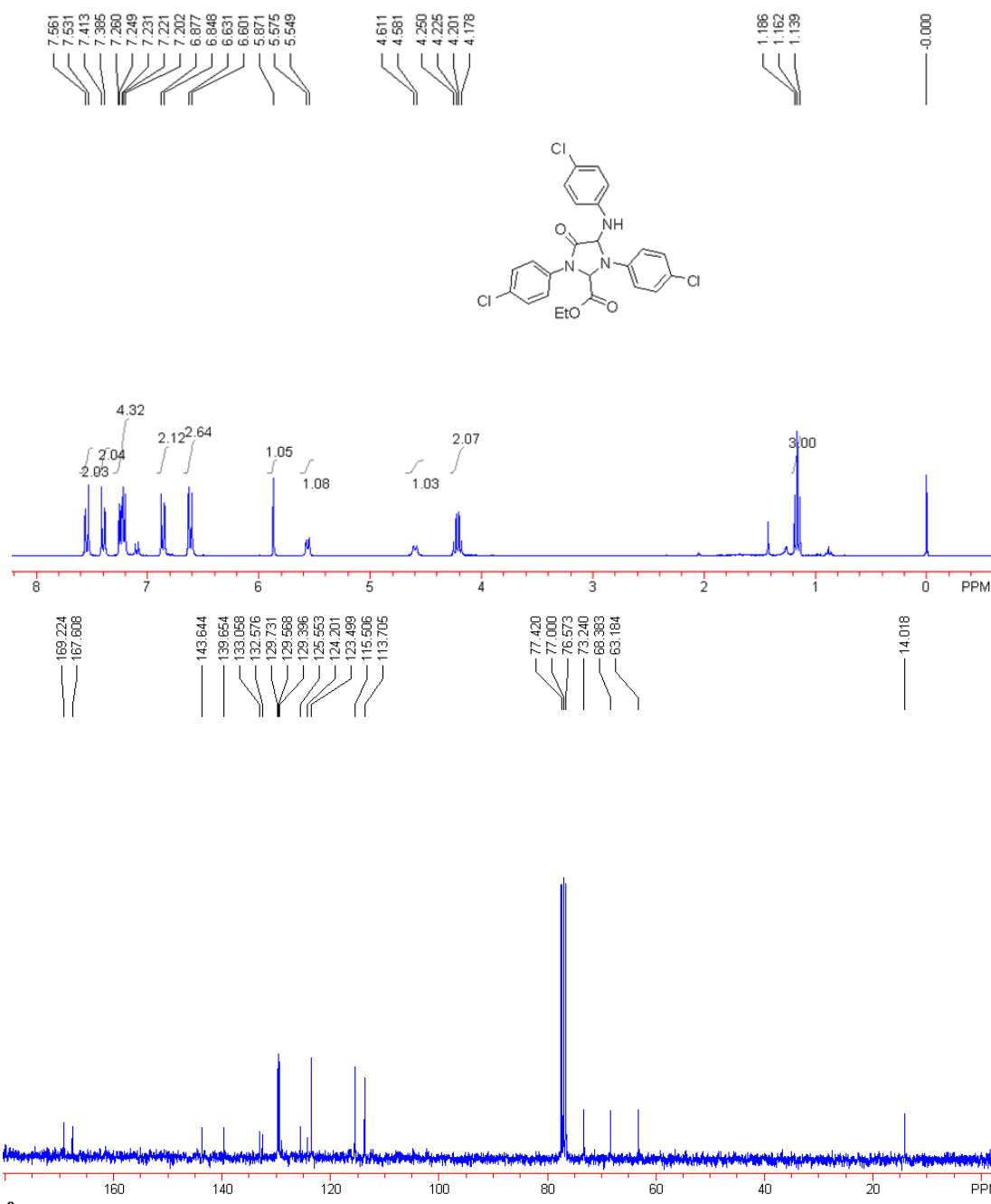


Compound **3b**

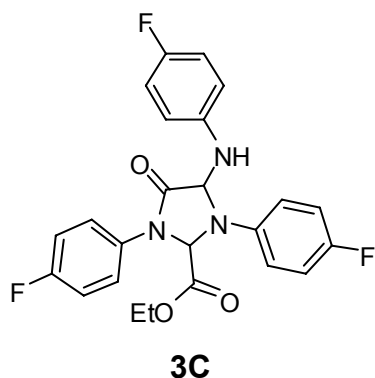


A colorless oil. IR (CH₂Cl₂) ν 2924, 2856, 1732 (C=O), 1677, 1598 1495, 1373, 1287, 1200, 1094, 1013, 813 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.16 (t, J = 7.2 Hz, 3H, CH₃), 4.21 (q, J = 7.2 Hz, 2H, CH₂), 4.59 (d, J = 8.7 Hz, 1H, NH), 5.57 (d, J = 8.7 Hz, 1H, CH), 5.87 (s, 1H, CH), 6.62 (d, J = 8.7 Hz, 2H, ArH), 6.86 (d, J = 8.7 Hz, 2H, ArH), 7.20-7.27 (m, 4H, ArH), 7.40 (d, J = 8.7 Hz, 2H, ArH), 7.54 (d, J = 8.7

Hz, 2H, ArH). ¹³C NMR (CDCl₃, 75 MHz) δ 14.0, 63.2, 68.4, 73.2, 113.7, 115.5, 123.5, 124.2, 125.6, 129.4, 129.6, 129.8, 132.6, 133.1, 139.7, 143.6, 167.6, 169.2. MS (ESI) m/e 526.0 (M⁺+Na). HRMS (ESI) m/z [M⁺+Na] Calcd. for C₂₄H₂₀Cl₃N₃O₃Na requires 526.0468, Found: 526.0487.

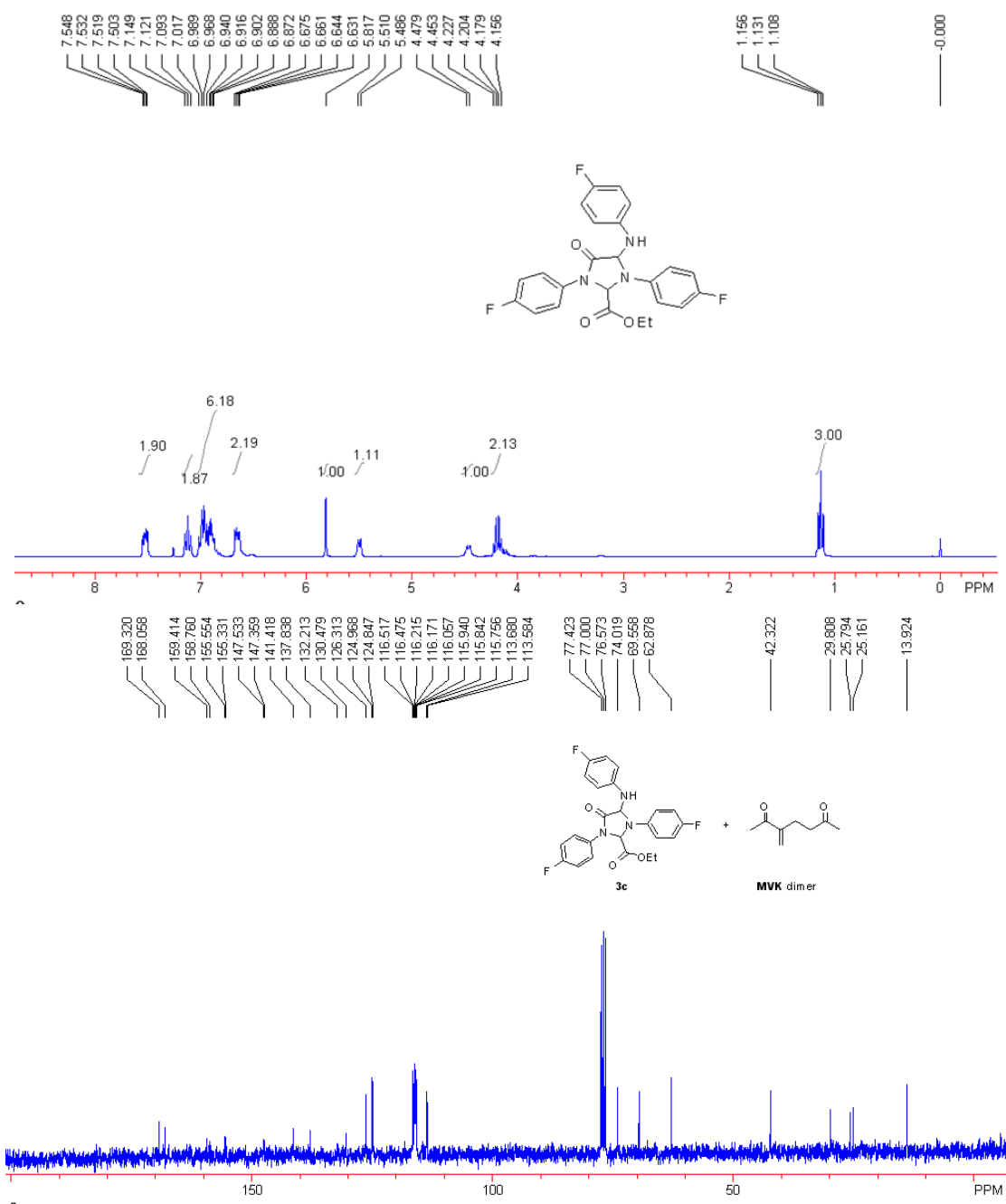


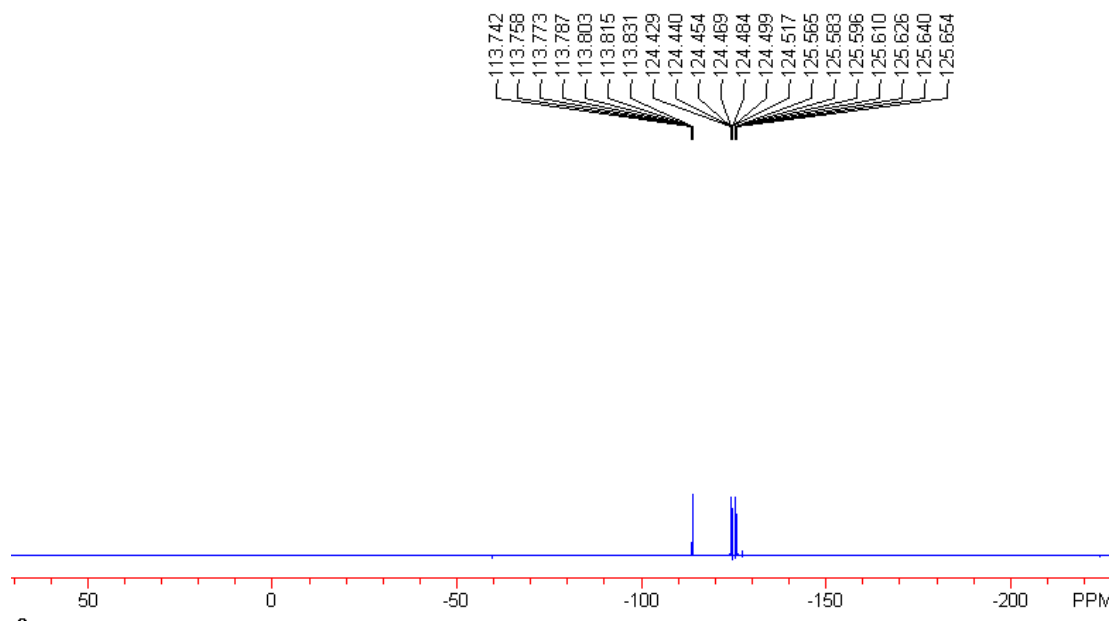
Compound 3c



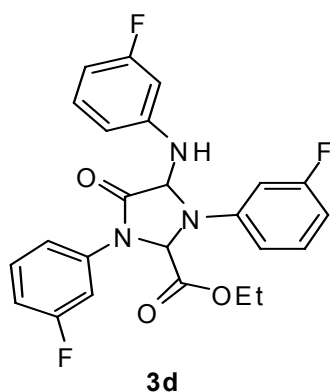
A colorless oil. IR (CH₂Cl₂) ν 2983, 2935, 1732 (C=O), 1614, 1510, 1399, 1372, 1233, 1163, 1094, 1015, 821 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.13 (t, J = 7.2 Hz, 3H, CH₃), 4.19 (q, J = 7.2 Hz, 2H, CH₂), 4.47 (d, J = 8.4 Hz, 1H, NH), 5.50 (d, J = 8.4 Hz, 1H, CH), 5.82 (s, 1H, CH), 6.62-6.68 (m, 2H, ArH), 6.82-7.03 (m, 6H, ArH), 7.12 (t, J = 8.7 Hz, 2H, ArH),

7.48-7.56 (m, 2H, ArH); ^{13}C NMR (CDCl_3 , 75 MHz) δ 13.9, 62.9, 69.6, 74.0, 113.6, 113.7, 115.8, 115.9, 116.1, 116.17, 116.21, 116.47, 116.52, 124.8, 124.9, 126.3, 130.5, 132.2, 137.8, 141.4, 147.4, 147.5, 155.3, 155.6, 128.8, 159.4, 168.1, 169.3. ^{19}F NMR (CDCl_3 , 282 MHz) δ -113.787 (m), -124.469 (m), -125.610 (m). MS (EI) m/e (%) 455 (M^+ , 2.67), 409 ($\text{M}^+ - 46$, 2.67), 345 ($\text{M}^+ - 110$, 100), 316 ($\text{M}^+ - 139$, 11.09), 243 ($\text{M}^+ - 213$, 6.62), 196 ($\text{M}^+ - 259$, 24.85), 122 ($\text{M}^+ - 333$, 82.48), 95 ($\text{M}^+ - 360$, 27.02). HRMS (EI) m/z [M^+] Calcd. for $\text{C}_{24}\text{H}_{20}\text{N}_3\text{O}_3\text{F}_3$ requires 455.1457, Found: 455.1458.



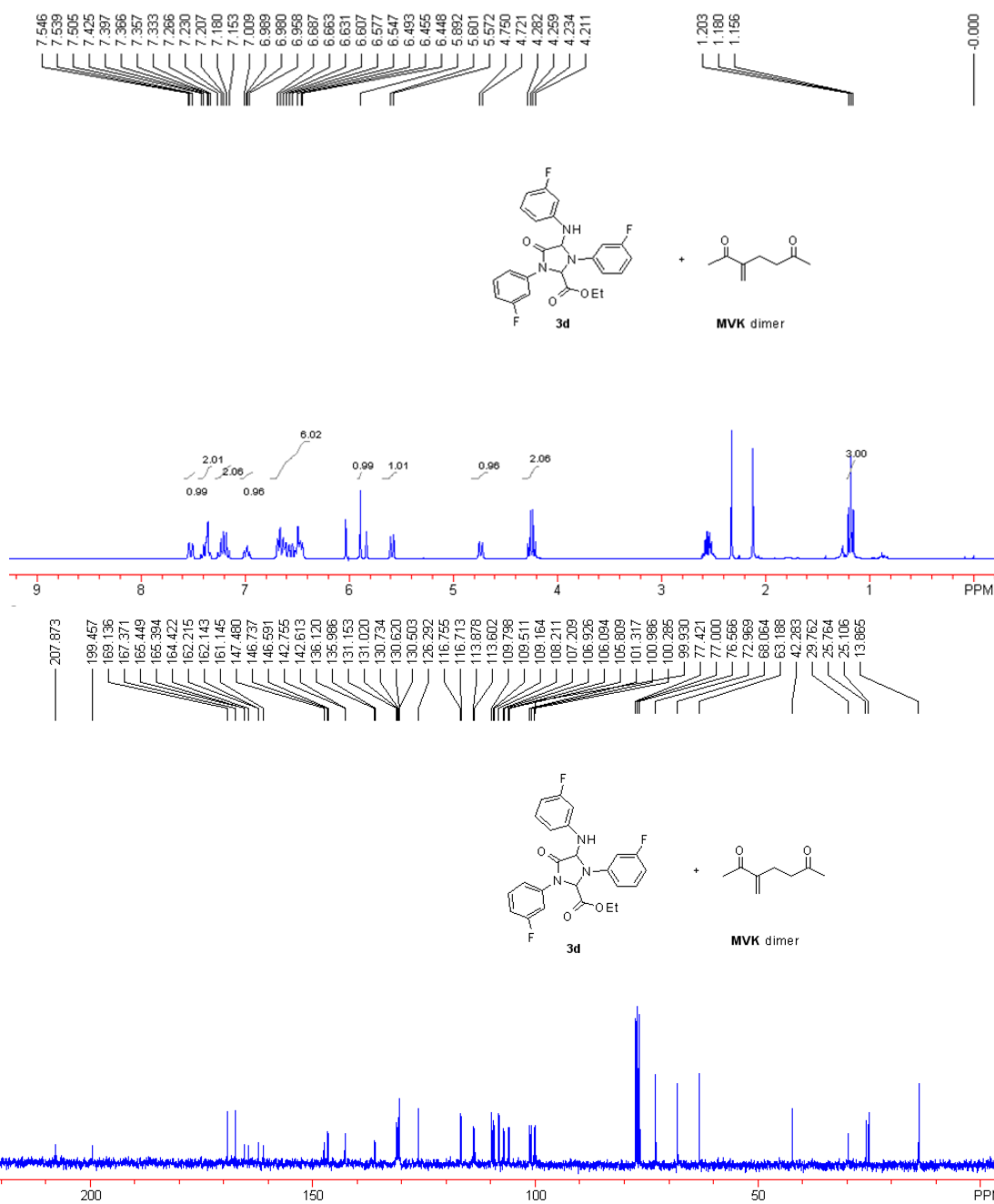


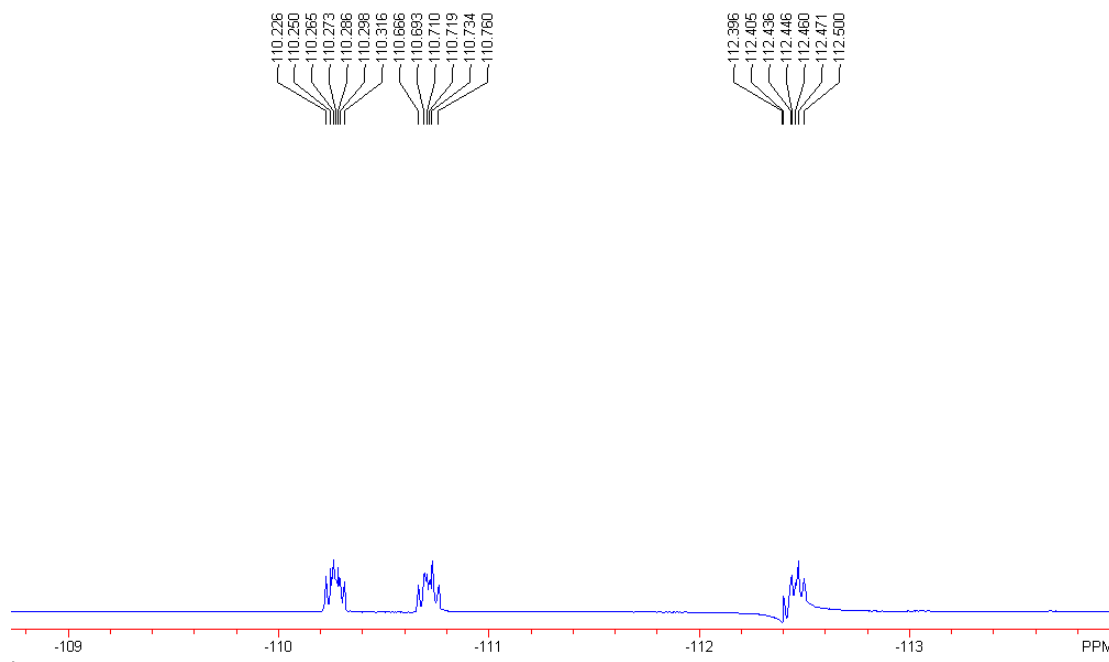
Compound **3d**



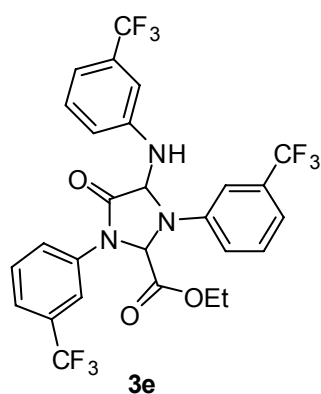
A colorless oil. IR (CH₂Cl₂) ν 2975, 2933, 1736 (C=O), 1612, 1591, 1494, 1375, 1269, 1200 1165, 1152, 764 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.18 (t, J = 7.2 Hz, 3H, CH₃), 4.24 (q, J = 7.2 Hz, 2H, CH₂), 4.73 (d, J = 8.7 Hz, 1H, NH), 5.58 (d, J = 8.7 Hz, 1H, CH), 5.89 (s, 1H, CH), 6.43-6.69 (m, 6H, ArH), 6.92-7.01 (m, 1H, ArH), 7.14-7.27 (m, 2H, ArH), 7.34-7.43 (m, 2H, ArH), 7.49-7.55 (m, 1H, ArH); ¹³C NMR (CDCl₃, 75 MHz) δ

13.9, 63.2, 68.1, 76.6, 99.9, 100.3, 100.9, 101.3, 105.8, 106.1, 106.9, 107.2, 108.18, 108.22, 109.2, 109.5, 109.77, 109.80, 113.6, 113.9, 116.72, 116.78, 130.6, 130.7, 131.0, 131.2, 135.9, 136.1, 142.6, 142.8, 146.6, 146.7, 162.1, 162.2, 164.4, 165.4, 167.4, 169.1. ¹⁹F NMR (CDCl₃, 282 MHz) δ -110.273 (m), -110.710 (m), -112.460 (m). MS (EI) m/e (%) 455 (M⁺, 2.33), 409 (M⁺-46, 4.68), 345 (M⁺-110, 100), 316 (M⁺-139, 13.34), 243 (M⁺-213, 6.68), 196 (M⁺-259, 28.85), 122 (M⁺-333, 83.68), 95 (M⁺-360, 22.56). HRMS (ESI) m/z [M⁺] Calcd. for C₂₄H₂₀N₃O₃F₃ requires 455.1457, Found: 455.1449.



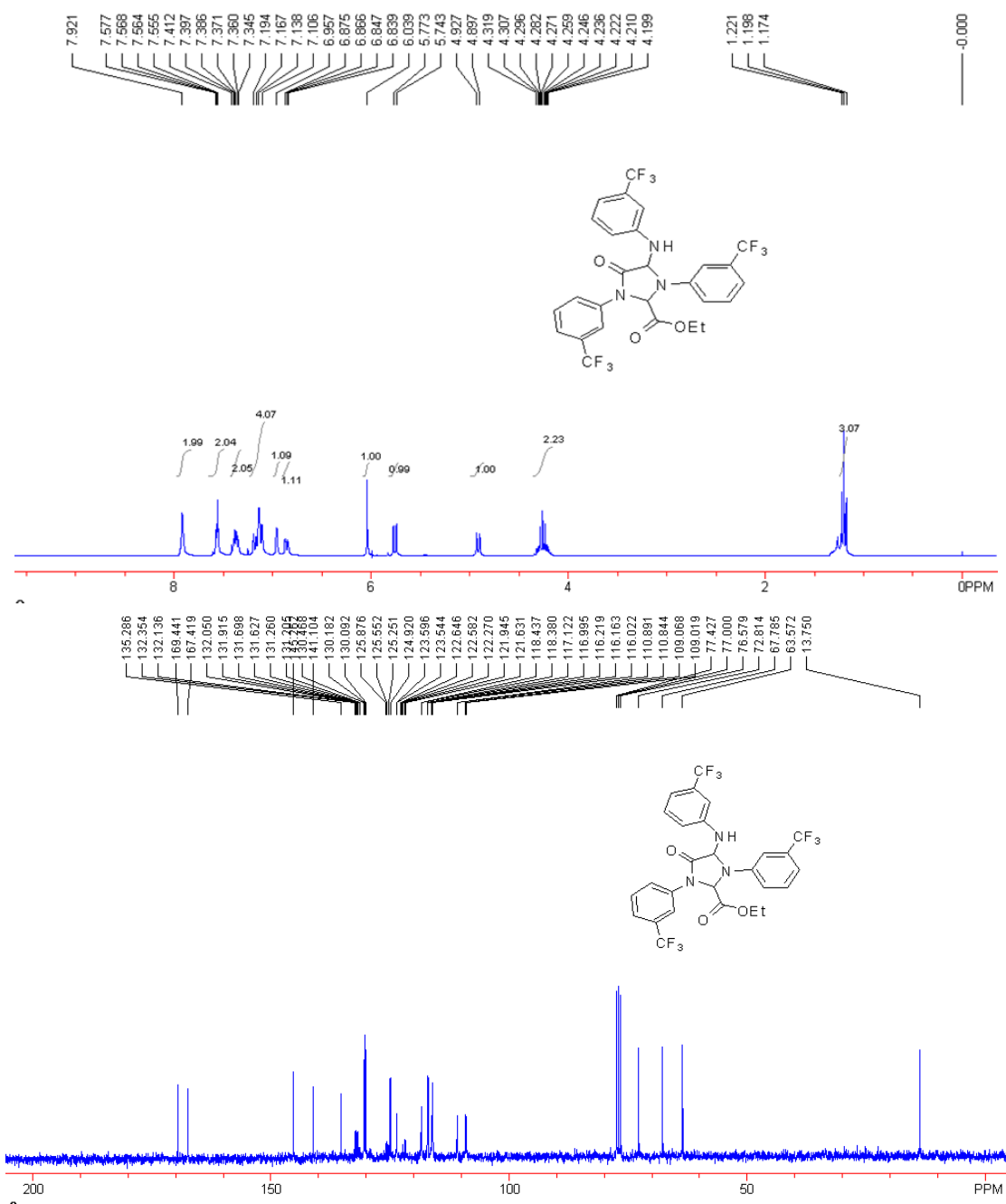


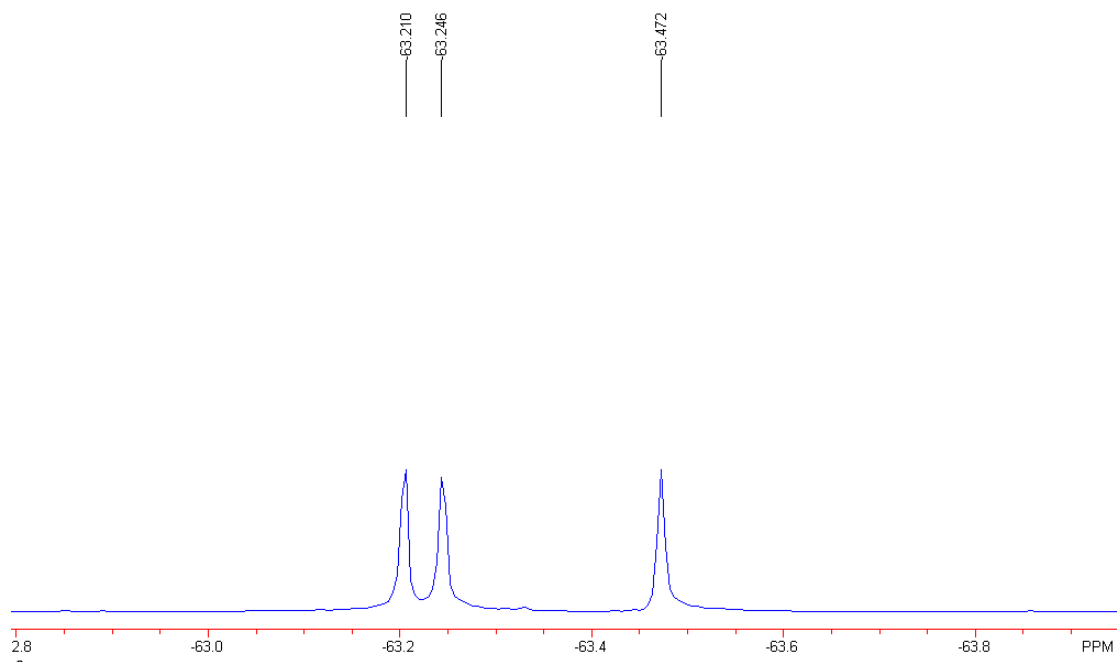
Compound 3e



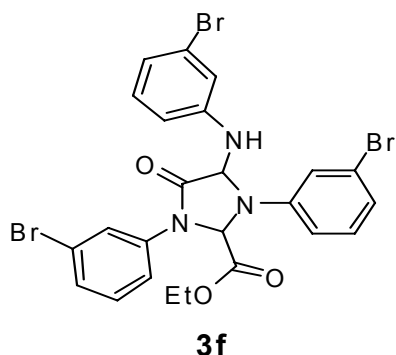
A colorless oil. IR (CH₂Cl₂) ν 2975, 2933, 1736 (C=O), 1612, 1591, 1494, 1375, 1269, 1200 1165, 1152, 764 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.20 (t, J = 7.2 Hz, 3H, CH₃), 4.20-4.32 (m, 2H, CH₂), 4.95 (d, J = 9.0 Hz, 1H, NH), 5.76 (d, J = 9.0 Hz, 1H, CH), 6.04 (s, 1H, CH), 6.85 (dd, J = 2.4 Hz, 8.4 Hz, 1H, ArH), 6.96 (s, 1H, ArH), 7.09-7.20 (m, 4H, ArH), 7.33-7.43 (m, 2H, ArH), 7.54-7.59 (m, 2H, ArH), 7.92 (s, 2H, ArH); ¹³C NMR (CDCl₃, 75

MHz) δ 13.7, 63.6, 67.8, 72.8, 109.0, 109.1, 110.85, 110.89, 110.60, 116.17, 116.20, 117.0, 117.07, 117.12, 118.38, 118.44, 121.6, 121.9, 122.3, 123.55, 123.60, 124.9, 125.3, 125.6, 125.9, 130.1, 130.2, 130.5, 131.6, 131.7, 131.9, 132.0, 132.1, 132.4, 135.3, 141.1, 145.1, 167.4, 169.5. ¹⁹F NMR (CDCl₃, 282 MHz) δ -63.21 (s), -63.25 (s), -63.47 (s). MS (ESI) m/e (%) 628 (M⁺+Na). HRMS (ESI) m/z [M⁺+Na] Calcd. for C₂₇H₂₀N₃O₃F₉Na requires 628.1259, Found: 628.1242.

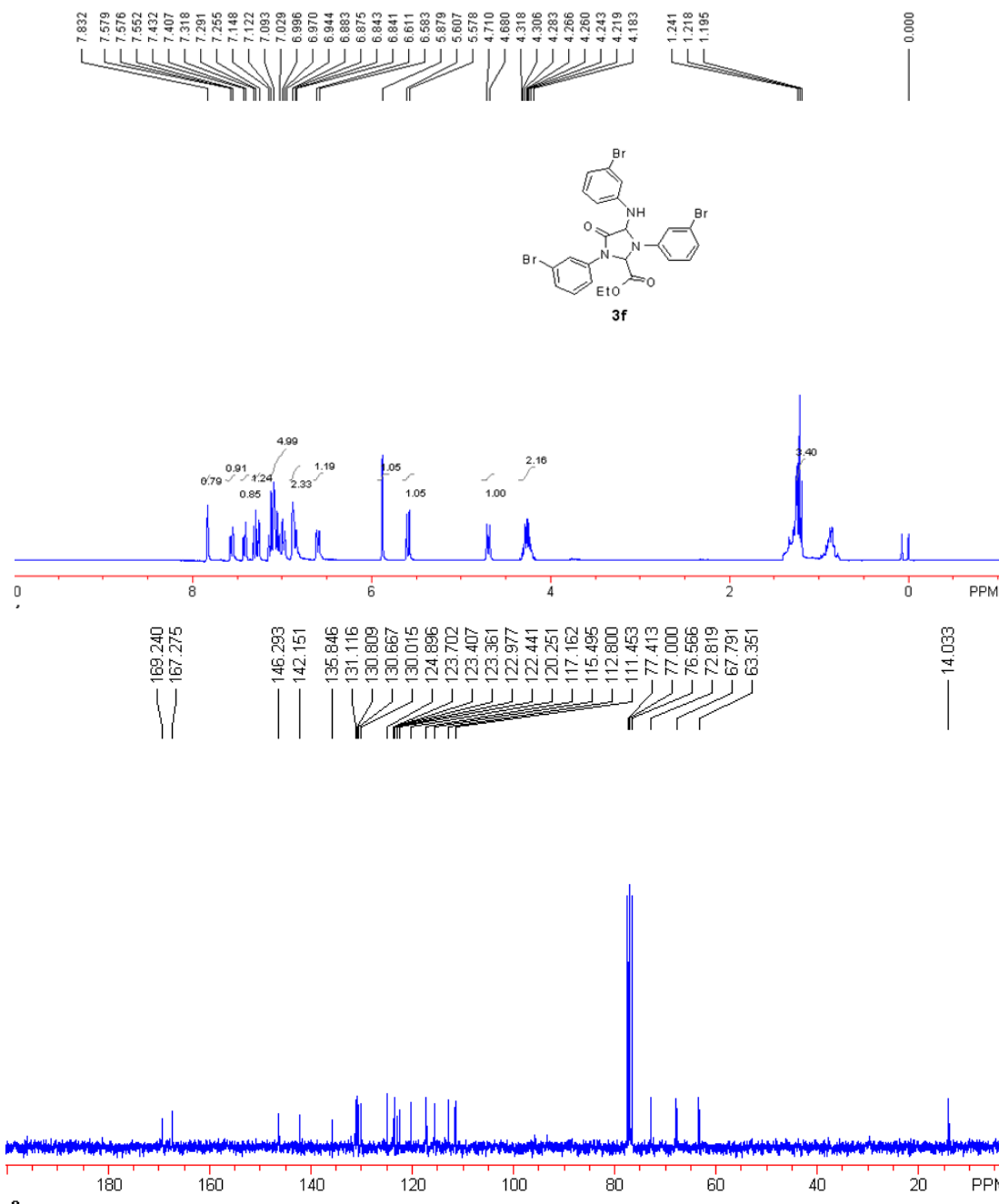




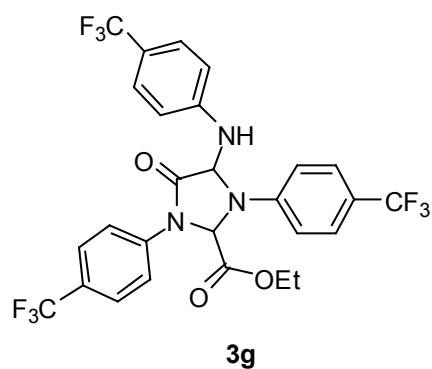
Compound **3f**



A colorless oil. IR (CH₂Cl₂) ν 2926, 2855, 1736 (C=O), 1592, 1481, 1373, 1274, 1201, 1069, 1015, 842 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.22 (t, J = 7.2 Hz, 3H, CH₃), 4.20-4.33 (m, 2H, CH₂), 4.70 (d, J = 8.7 Hz, 1H, NH), 5.58 (d, J = 8.7 Hz, 1H, CH), 5.88 (s, 1H, CH), 6.56 (d, J = 8.7 Hz, 2H, ArH), 6.60 (d, J = 9.0 Hz, 1H, ArH), 6.82 (d, J = 9.0 Hz, 1H, ArH), 6.88 (s, 1H, ArH), 6.96-7.16 (m, 5H, ArH), 7.29 (t, J = 8.7 Hz, 1H, ArH), 7.42 (d, J = 8.7 Hz, 1H, ArH), 7.56 (d, J = 8.7 Hz, 1H, ArH), 7.83 (s, 1H, ArH). ¹³C NMR (CDCl₃, 75 MHz) δ 14.0, 63.4, 67.8, 72.8, 111.5, 112.8, 115.5, 117.2, 120.3, 122.4, 122.9, 123.36, 123.40, 123.7, 124.9, 130.0, 130.7, 130.8, 131.1, 135.8, 142.2, 146.3, 167.3, 169.2. HRMS (EI) m/z [M⁺] Calcd. for C₂₄H₂₀Br₃N₃O₃ requires 634.9055, Found: 634.9031.

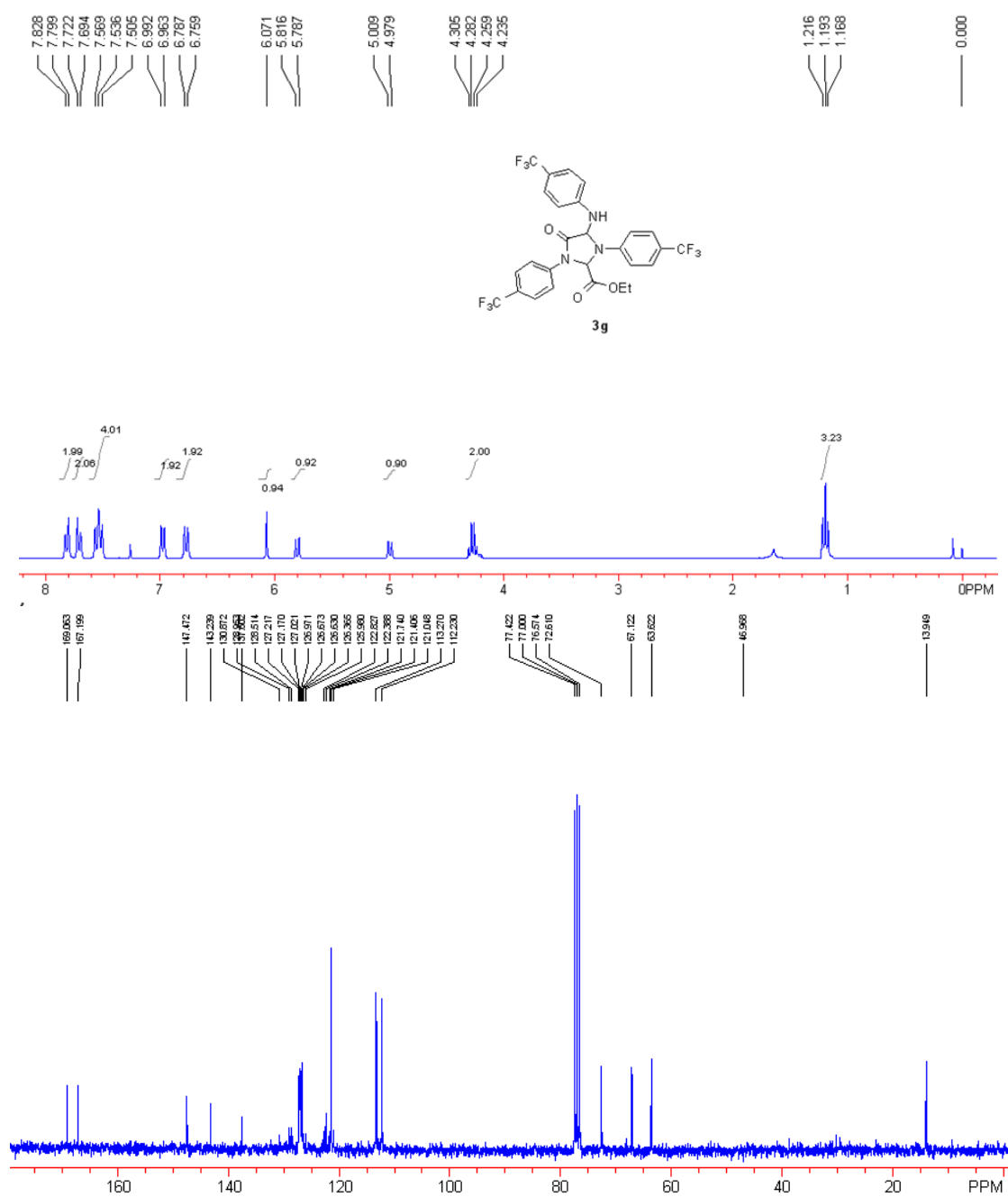


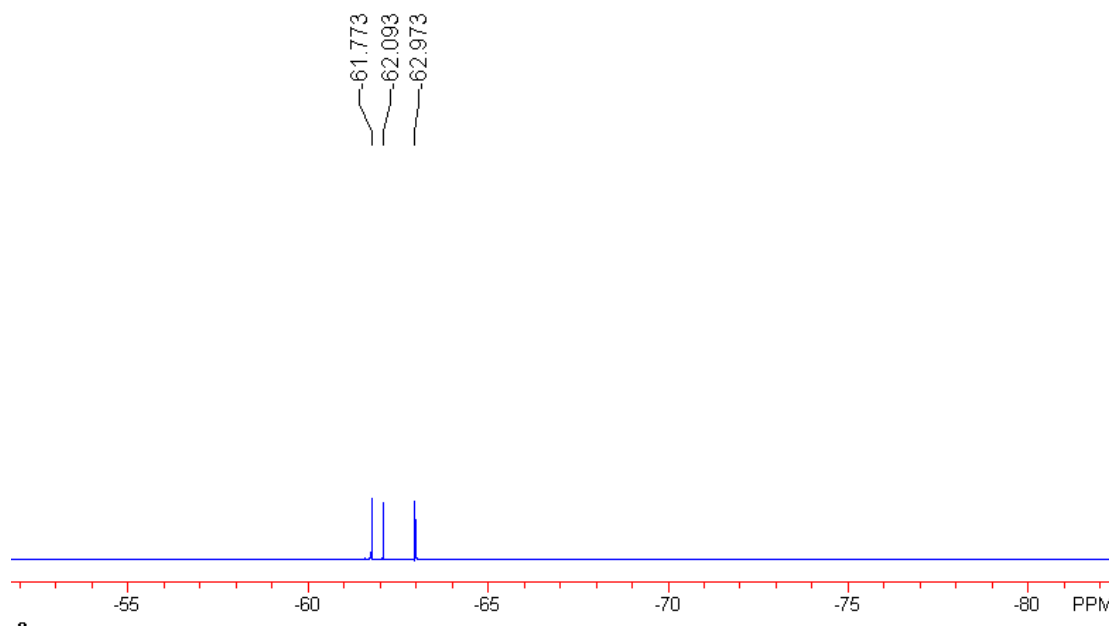
Compound **3g**



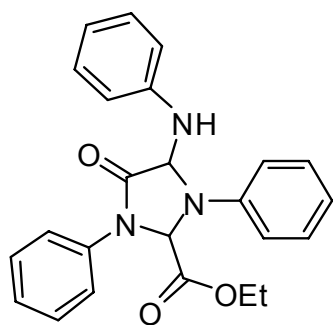
A colorless oil. IR (CH₂Cl₂) ν 2926, 2846, 1740 (C=O), 1616, 1524, 1481, 1326, 1277, 1203 1168, 1056, 843 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.20 (t, *J* = 7.2 Hz, 3H, CH₃), 4.27 (q, 2H, CH₂), 4.99 (d, *J* = 9.0 Hz, 1H, NH), 5.79 (d, *J* = 9.0 Hz, 1H, CH), 6.07 (s, 1H, CH), 6.77 (d, *J* = 9.0 Hz, 2H, ArH), 6.97

(d, $J = 9.0$ Hz, 2H, ArH), 7.54 (t, $J = 9.0$ Hz, 4H, ArH), 7.71 (d, 2H, $J = 8.7$ Hz, ArH), 7.80 (m, $J = 8.7$ Hz, 2H, ArH); ^{13}C NMR (CDCl_3 , 75 MHz) δ 13.9, 63.6, 67.1, 72.6, 112.2, 113.3, 116.4, 120.9, 121.1, 121.4, 121.7, 121.9, 122.4, 122.77, 122.83, 123.3, 125.4, 125.9, 126.4, 126.6, 126.7, 126.9, 127.0, 127.17, 127.21, 128.1, 128.5, 128.7, 128.9, 129.4, 129.6, 130.9, 132.3, 167.2, 169.1; ^{19}F NMR (CDCl_3 , 282 MHz) δ -61.77 (s), -62.09 (s), -62.97 (s). MS (ESI) m/e (%) 628 ($\text{M}^+ + \text{Na}$). HRMS (ESI) m/z [$\text{M}^+ + \text{Na}$] Calcd. for $\text{C}_{27}\text{H}_{20}\text{N}_3\text{O}_3\text{F}_9$ requires 605.1361. Found: 605.1368.



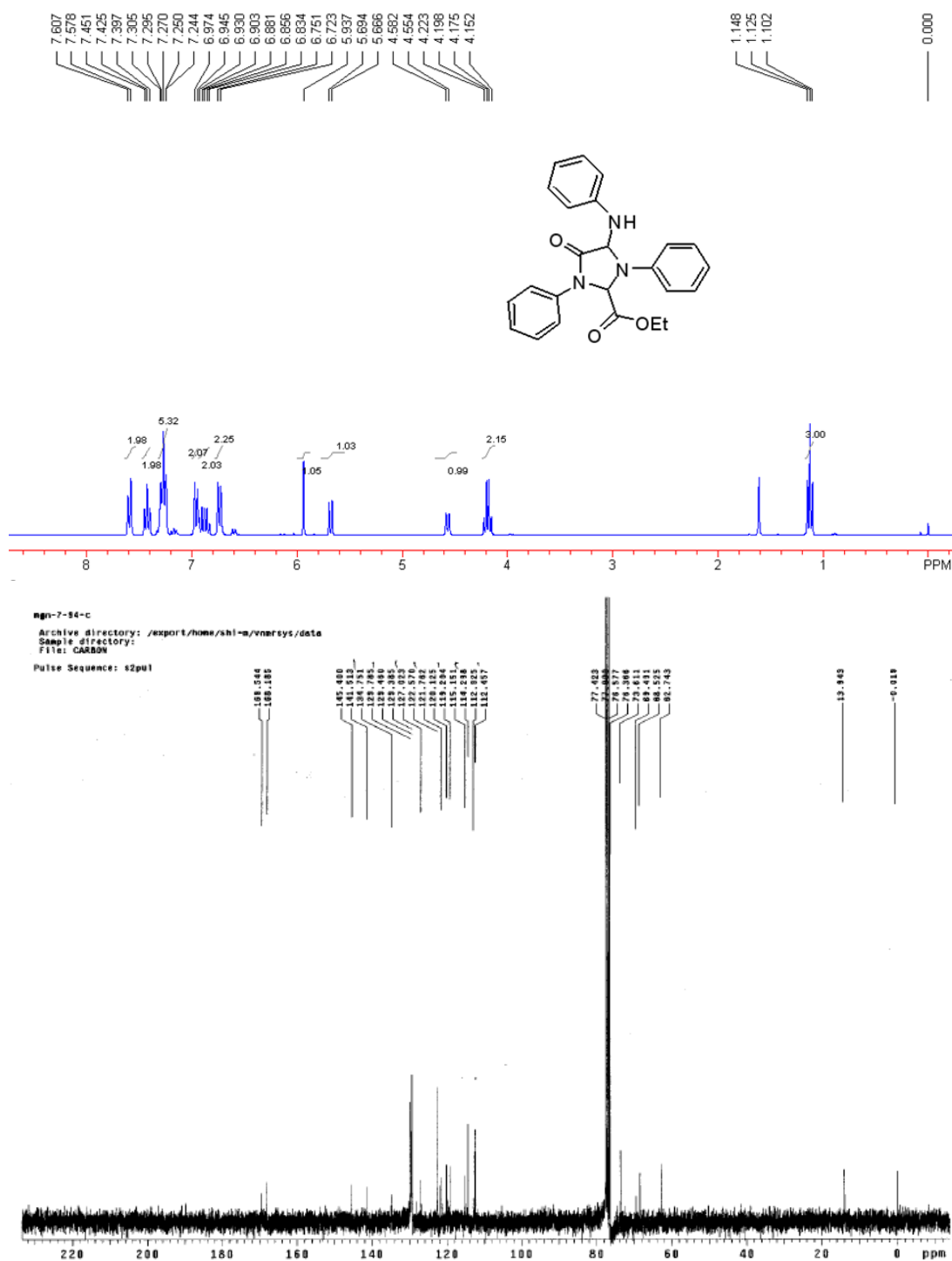


Compound **3h**

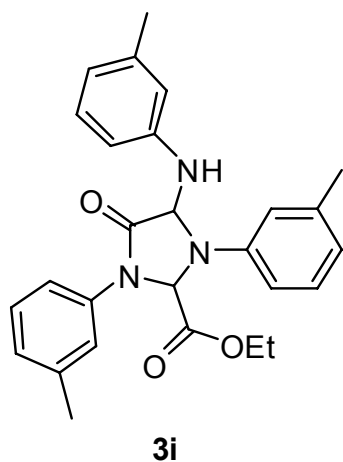


3h

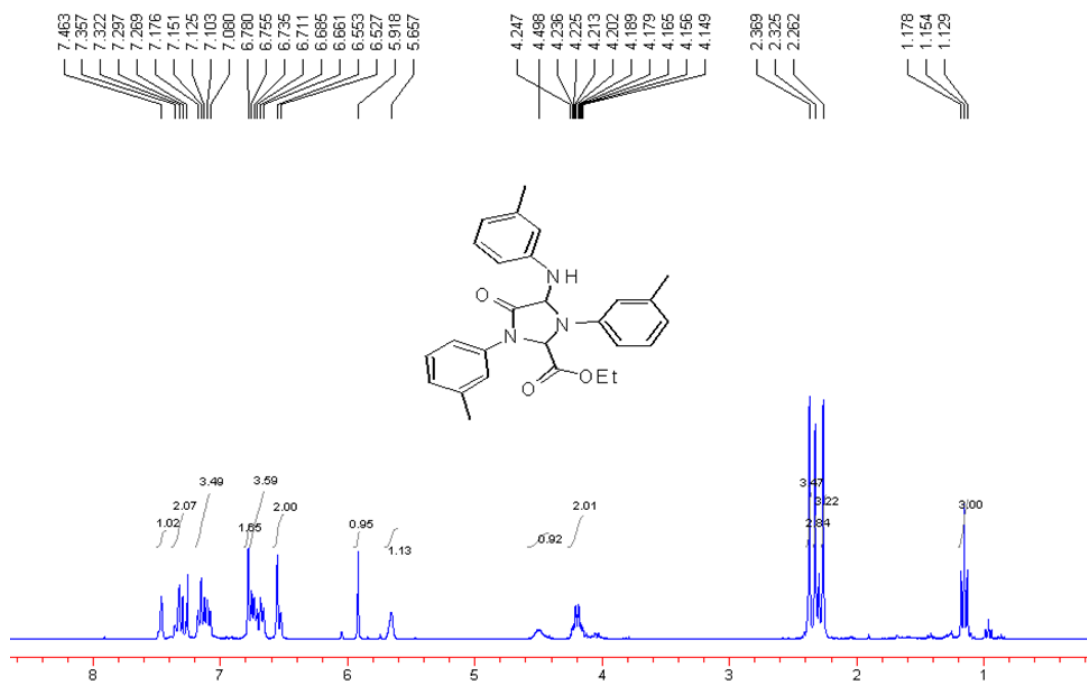
A white solid. Mp 70-72 °C. IR (CH₂Cl₂) ν 2920, 2868, 1731 (C=O), 1599, 1500, 1398, 1262, 1198, 1096, 1020, 749 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.13 (t, J = 7.2 Hz, 3H, CH₃), 4.18 (q, J = 7.2 Hz, 2H, CH₂), 4.57 (d, J = 8.7 Hz, 1H, NH), 5.68 (d, J = 8.7 Hz, 1H, CH), 5.94 (s, 1H, CH), 6.73 (d, J = 8.7 Hz, 2H, ArH), 6.80-6.94 (m, 2H, ArH). 6.95 (d, J = 8.7 Hz, 2H, ArH), 7.22-7.34 (m, 5H, ArH), 7.42 (t, J = 8.7 Hz, 2H, ArH), 7.60 (d, J = 8.7 Hz, 2H, ArH). ¹³C NMR (CDCl₃, 75 MHz) δ 13.9, 62.7, 68.5, 73.6, 112.5, 114.3, 119.2, 120.1, 122.6, 127.0, 129.4, 129.5, 129.8, 134.8, 141.5, 145.4, 168.2, 169.5. MS (EI) m/e (%) 401 (M⁺, 9.87), 309 (M⁺-92, 100), 280 (M⁺-121, 5.71), 237 (M⁺-164, 8.08), 178 (M⁺-223, 21.38), 104 (M⁺-297, 38.02), 93 (M⁺-308, 27.40), 77 (M⁺-324, 19.94). HRMS (EI) m/z [M⁺] Calcd. for C₂₄H₂₃N₃O₃ requires 401.1739, Found: 401.1720. Anal. Calcd for C₂₄H₂₃N₃O₃: C, 70.80, H, 5.77, N, 10.74. Found: C, 71.25, H, 5.65, N, 10.11.

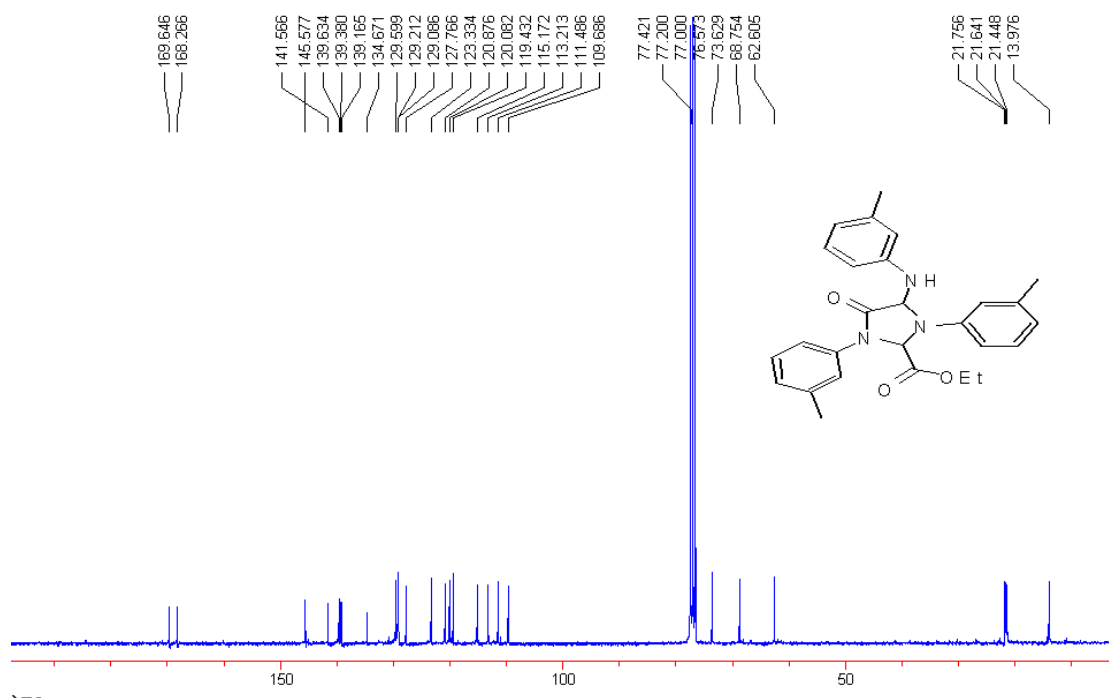


Compound **3i**

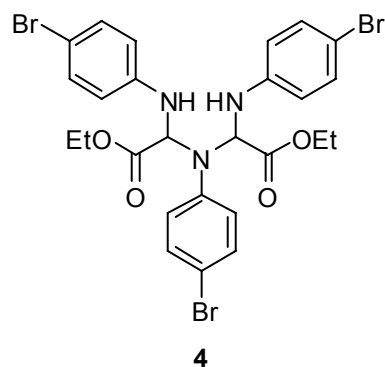


A colorless oil. IR (CH₂Cl₂) ν 2985, 2920, 1732 (C=O), 1606, 1589, 1494, 1370, 1288, 1197, 1096, 1018, 770 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 1.15 (t, J = 7.2 Hz, 3H, CH₃), 2.26 (s, 3H, CH₃), 2.33 (s, 3H, CH₃), 2.37 (s, 3H, CH₃), 4.13-4.24 (m, 2H, CH₂), 4.49 (brs, 1H, NH), 5.65 (s, 1H, CH), 5.92 (s, 1H, CH), 6.52-6.56 (m, 2H, ArH), 6.64-6.80 (m, 4H, ArH), 7.06-7.20 (m, 3H, ArH), 7.27-7.38 (m, 2H, ArH), 7.46 (s, 1H, ArH); ¹³C NMR (CDCl₃, 75 MHz) δ 14.0, 21.4, 21.6, 21.7, 62.6, 68.7, 73.6, 109.7, 111.5, 113.2, 115.2, 119.4, 120.1, 120.9, 123.3, 127.8, 129.1, 129.2, 129.6, 134.7, 139.2, 139.4, 139.6, 141.6, 145.6, 168.3, 169.6. MS (EI) m/e (%) 443 (M⁺, 11.26), 337 (M⁺-106, 100), 308 (M⁺-135, 5.09), 265 (M⁺-178, 8.61), 192 (M⁺-251, 13.81), 118 (M⁺-325, 23.87), 107 (M⁺-336, 16.92), 91 (M⁺-352, 14.31). HRMS (EI) m/z [M⁺] Calcd. for C₂₇H₂₉N₃O₃ requires 443.2209, Found: 443.2203.

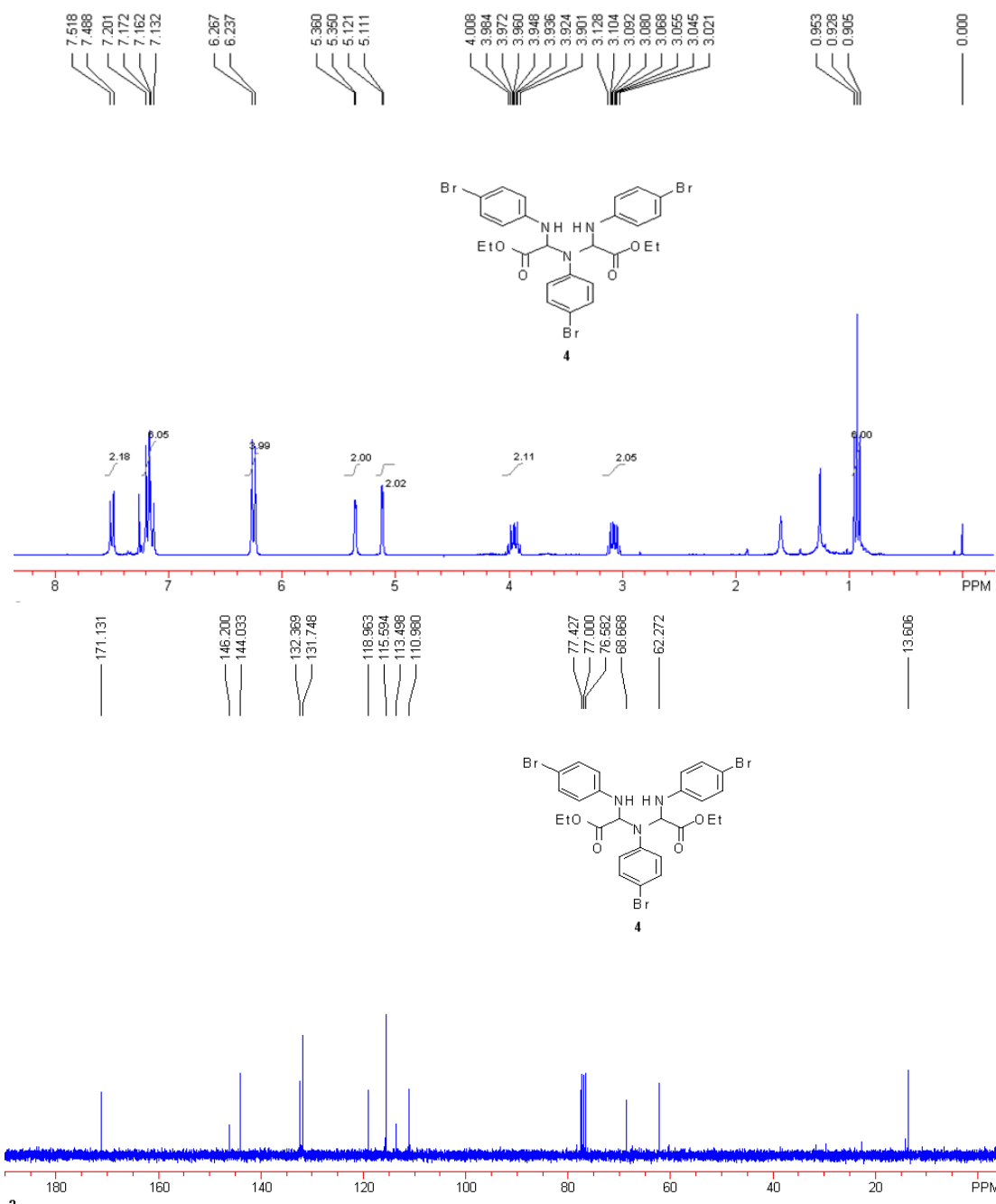




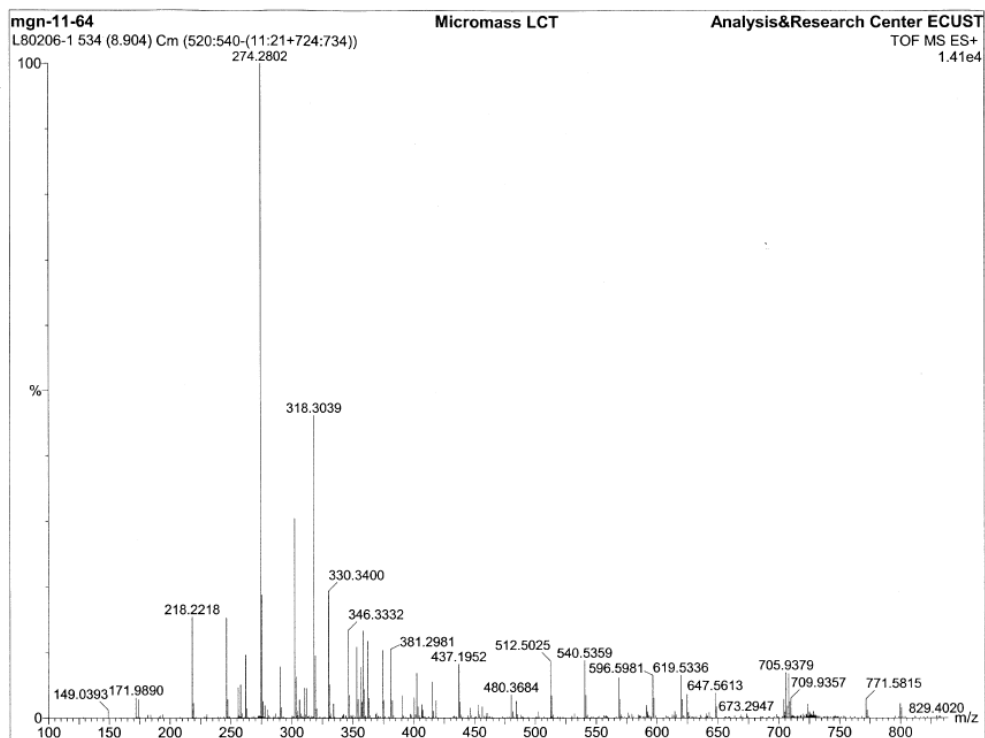
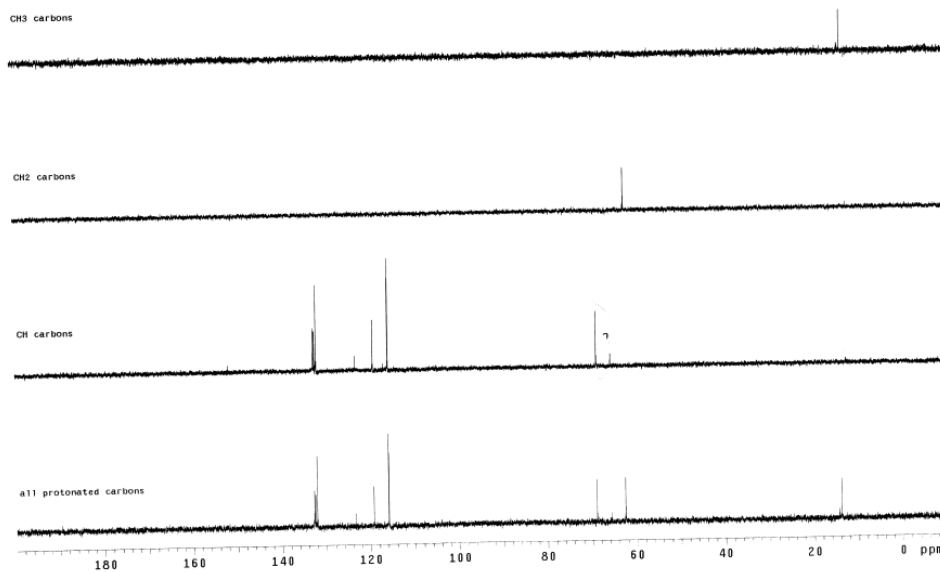
Compound 4



A white solid. Mp 73-74 °C. IR (CH₂Cl₂) ν 2934, 2868, 1734 (C=O), 15939, 1508, 1398, 1262, 1198, 1096, 1020, 749 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz, TMS) δ 0.93 (t, J = 7.2 Hz, 3H, CH₃), 3.07 (dq, J = 7.2 Hz, 10.8 Hz, 2H, CH₂), 3.95 (dq, J = 7.2 Hz, 10.8 Hz, 2H, CH₂), 5.11 (d, J = 3.0 Hz, 2H, NH), 5.35 (d, J = 3.0 Hz, 2H, CH), 6.24 (d, J = 9.0 Hz, 4H, ArH), 7.13 (d, J = 9.0 Hz, 2H, ArH), 7.18 (d, J = 9.0 Hz, 4H, ArH), 7.49 (d, J = 9.0 Hz, 2H, ArH). ¹³C NMR (CDCl₃, 75 MHz) δ 13.6, 62.3, 68.7, 110.9, 113.5, 115.6, 118.9, 131.7, 132.4, 144.0, 146.2, 171.1. HRMS (ESI) m/z [M^+] Calcd. for C₂₆H₂₆N₃O₄Br₃Na requires 703.9371, Found: 703.9381.



MGN-6-21-D-Dept



Elemental Composition Report

Page 1

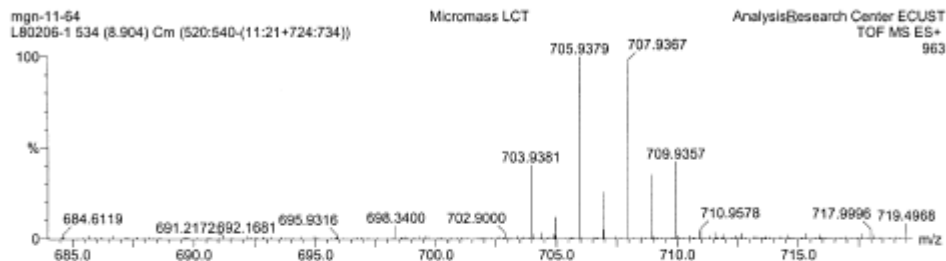
Multiple Mass Analysis: 4 mass(es) processed

Tolerance = 5.0 mDa / DBE: min = -20.0, max = 100.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

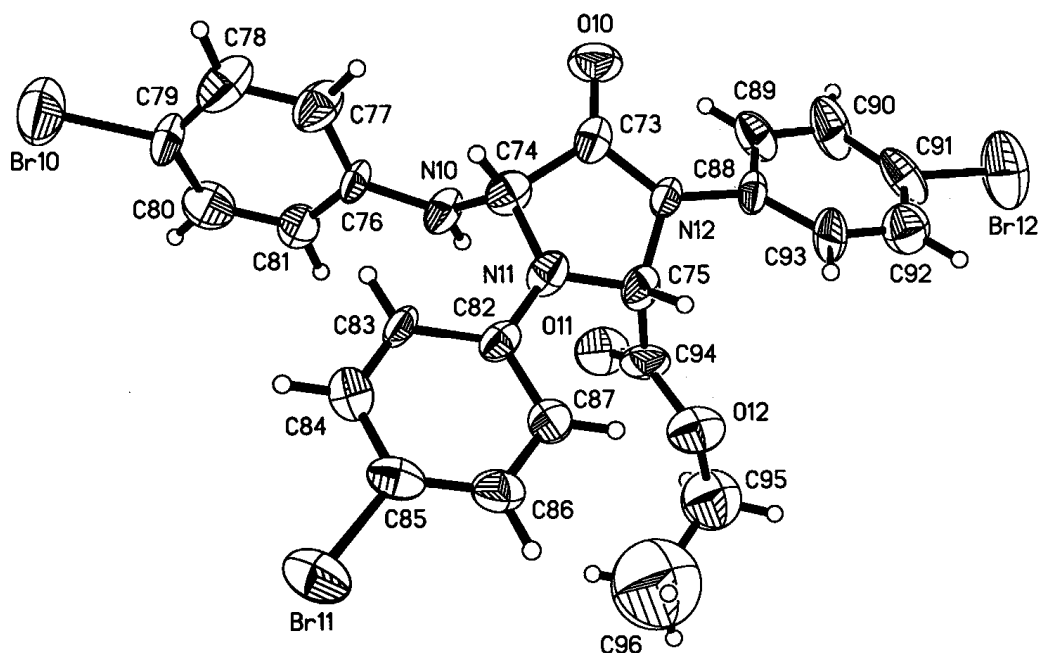
Monoisotopic Mass, Odd and Even Electron Ions

52 formula(e) evaluated with 4 results within limits (up to 50 closest results for each mass)



Minimum: 40.00
Maximum: 100.00

Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
703.9381	40.37	703.9371	1.0	1.4	13.5	n/a	12C26 1H26 14N3 16O4 23Na 79Br3
705.9379	100.00	705.9351	2.8	4.0	13.5	n/a	12C26 1H26 14N3 16O4 23Na 79Br2 81Br
707.9367	97.88	707.9330	3.7	5.2	13.5	n/a	12C26 1H26 14N3 16O4 23Na 79Br 81Br2
709.9357	42.27	709.9310	4.7	6.7	13.5	n/a	12C26 1H26 14N3 16O4 23Na 81Br3



The crystal data of **3a** have been deposited in CCDC with number CD26131. Empirical Formula: $C_{24.25}H_{20.50}Br_3Cl_{0.50}N_3O_3$; Formula Weight: 659.39; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.291 x 0.126 x 0.044 mm; Crystal System: Triclinic; Lattice Type: Primitive; Lattice Parameters: $a = 13.9165(14)\text{\AA}$, $b = 19.129(2)\text{\AA}$, $c = 19.595(2)\text{\AA}$, $\alpha = 90.901(3)^\circ$, $\beta = 98.503(2)^\circ$, $\gamma = 90.942(2)^\circ$, $V = 5157.5(9)\text{\AA}^3$; Space group: P-1; $Z = 8$; $D_{calc} = 1.698\text{ g/cm}^3$; $F_{000} = 2596$; Diffractometer: Rigaku AFC7R; Residuals: R ; R_w : 0.0691, 0.1475.

Table 1. Crystal data and structure refinement for cd26131.

Identification code	cd26131
Empirical formula	C ₂₄ H ₂₅ Br ₃ ClO ₅ N ₃ O ₃
Formula weight	659.39
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 13.9165(14) Å alpha = 90.901(3) deg. b = 19.129(2) Å beta = 98.503(2) deg. c = 19.595(2) Å gamma = 90.942(2) deg.
Volume	5157.5(9) Å ³
Z, Calculated density	8, 1.698 Mg/m ³
Absorption coefficient	4.776 mm ⁻¹
F(000)	2596
Crystal size	0.291 x 0.126 x 0.044 mm
Theta range for data collection	1.68 to 25.50 deg.
Limiting indices	-16<=h<=16, -22<=k<=23, -20<=l<=23
Reflections collected / unique	27508 / 18902 [R(int) = 0.1779]
Completeness to theta = 25.50	98.6 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.78936
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	18902 / 4 / 1205
Goodness-of-fit on F ²	0.648
Final R indices [I>2sigma(I)]	R1 = 0.0691, wR2 = 0.1475
R indices (all data)	R1 = 0.2501, wR2 = 0.1895
Largest diff. peak and hole	0.825 and -0.564 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd26131. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Br(1)	13755(1)	5593(1)	1236(1)	111(1)
Br(2)	12906(1)	10383(1)	864(1)	108(1)
Br(3)	3667(1)	7723(1)	328(1)	115(1)
Br(4)	-4687(1)	5367(1)	3013(1)	129(1)
Br(5)	-3323(1)	10233(1)	4359(1)	127(1)
Br(6)	5554(1)	7289(1)	4372(1)	148(1)
Br(7)	-4165(1)	360(1)	1111(1)	125(1)
Br(8)	-3655(1)	5296(1)	627(1)	100(1)
Br(9)	5672(1)	2962(1)	1560(1)	142(1)
Br(10)	14227(1)	583(1)	3288(1)	136(1)
Br(11)	13635(1)	5095(1)	4687(1)	104(1)
Br(12)	4206(1)	2822(1)	3362(1)	136(1)
O(1)	8478(5)	6709(4)	687(4)	83(3)
O(2)	8318(7)	8347(5)	2215(5)	107(3)
O(3)	8390(6)	9428(5)	1828(4)	82(3)
O(4)	695(6)	6382(5)	4295(5)	94(3)
O(5)	616(6)	8208(4)	2935(4)	94(3)
O(6)	1384(6)	9095(5)	3526(4)	93(3)
O(7)	893(6)	1794(5)	660(4)	85(3)
O(8)	973(6)	3439(5)	2249(5)	91(3)
O(9)	1422(6)	4433(5)	1862(4)	97(3)
O(10)	8889(6)	1543(4)	4145(4)	89(3)
O(11)	8965(6)	3309(5)	2738(4)	95(3)
O(12)	8661(6)	4301(5)	3273(4)	88(3)
N(1)	10255(6)	7287(5)	1635(4)	61(3)
N(2)	9605(7)	8336(5)	1117(4)	65(3)
N(3)	8086(6)	7845(5)	853(4)	53(2)
N(4)	-996(7)	7123(5)	3400(5)	71(3)
N(5)	-270(7)	8061(5)	4171(4)	62(3)
N(6)	1189(8)	7535(5)	4242(4)	66(3)
N(7)	-694(6)	2331(4)	1456(5)	60(3)
N(8)	-239(7)	3368(5)	888(4)	64(3)
N(9)	1300(7)	2942(4)	906(4)	55(3)
N(10)	10530(6)	2140(5)	3402(5)	65(3)
N(11)	10151(7)	3115(5)	4098(4)	65(3)
N(12)	8589(6)	2692(5)	4013(4)	60(3)
Cl(1)	5566(5)	9035(4)	2599(4)	277(3)
Cl(2)	4643(5)	7780(4)	2363(4)	263(3)
C(1)	8691(8)	7317(7)	832(5)	55(3)
C(2)	9709(8)	7595(6)	1028(6)	57(3)
C(3)	8605(8)	8498(6)	1062(6)	54(3)
C(4)	10998(8)	6864(5)	1578(6)	49(3)
C(5)	10992(9)	6371(7)	1049(6)	72(4)
C(6)	11805(11)	5988(6)	951(6)	73(4)
C(7)	12641(9)	6075(7)	1390(7)	69(4)
C(8)	12695(8)	6513(7)	1951(7)	83(4)
C(9)	11885(10)	6896(6)	2028(6)	75(4)
C(10)	10373(8)	8805(6)	1032(5)	52(3)
C(11)	11271(8)	8584(6)	1032(5)	55(3)
C(12)	12036(8)	9051(7)	980(6)	70(4)
C(13)	11812(9)	9770(7)	929(6)	67(3)
C(14)	10906(10)	9995(6)	906(6)	72(4)
C(15)	10156(7)	9520(6)	970(5)	63(3)
C(16)	7036(8)	7837(6)	728(5)	55(3)
C(17)	6506(10)	7206(6)	728(6)	83(4)
C(18)	5545(10)	7165(8)	610(8)	108(5)
C(19)	5050(9)	7770(8)	480(6)	77(4)
C(20)	5497(9)	8405(7)	462(6)	90(4)
C(21)	6485(9)	8422(6)	592(6)	71(4)
C(22)	8372(8)	8774(8)	1758(7)	75(4)
C(23)	8314(10)	9753(7)	2492(6)	106(5)

C(24)	9054(11)	10294(7)	2652(7)	112(6)
C(25)	567(10)	6996(8)	4235(6)	78(4)
C(26)	-476(9)	7309(6)	4068(6)	68(3)
C(27)	737(8)	8202(6)	4157(6)	65(3)
C(28)	-1818(8)	6713(6)	3306(7)	59(3)
C(29)	-2022(9)	6233(7)	3778(6)	80(4)
C(30)	-2839(10)	5828(6)	3686(6)	77(4)
C(31)	-3511(9)	5885(9)	3114(8)	101(5)
C(32)	-3329(10)	6332(8)	2620(8)	103(5)
C(33)	-2515(10)	6773(7)	2718(7)	101(5)
C(34)	-968(8)	8561(6)	4209(5)	51(3)
C(35)	-1950(9)	8371(7)	4173(5)	70(4)
C(36)	-2648(9)	8898(9)	4234(6)	81(4)
C(37)	-2387(9)	9560(7)	4310(6)	66(3)
C(38)	-1415(11)	9772(7)	4351(6)	80(4)
C(39)	-703(9)	9272(7)	4303(5)	75(4)
C(40)	2240(11)	7479(8)	4276(6)	72(4)
C(41)	2609(12)	6922(8)	3945(6)	85(4)
C(42)	3615(12)	6917(8)	4011(7)	89(4)
C(43)	4215(10)	7388(11)	4338(8)	104(6)
C(44)	3835(12)	7988(9)	4651(7)	103(5)
C(45)	2876(10)	8000(7)	4609(6)	84(4)
C(46)	898(8)	8504(7)	3439(7)	72(4)
C(47)	1686(12)	9395(9)	2869(9)	125(7)
C(48)	2652(13)	9059(11)	2811(8)	127(10)
C(49)	698(9)	2388(8)	799(6)	64(4)
C(50)	-311(8)	2602(5)	853(5)	54(3)
C(51)	788(7)	3567(6)	1030(6)	61(3)
C(52)	-1455(8)	1843(6)	1393(6)	62(3)
C(53)	-1568(7)	1339(6)	889(6)	59(3)
C(54)	-2370(10)	885(6)	824(7)	83(4)
C(55)	-3089(9)	943(7)	1230(8)	77(4)
C(56)	-2944(8)	1435(7)	1758(7)	77(4)
C(57)	-2148(9)	1904(6)	1834(6)	64(3)
C(58)	-1017(9)	3824(6)	836(5)	56(3)
C(59)	-1948(9)	3558(6)	745(5)	63(3)
C(60)	-2707(8)	4004(7)	677(5)	67(3)
C(61)	-2610(8)	4693(7)	684(6)	66(3)
C(62)	-1649(10)	4963(6)	784(5)	74(4)
C(63)	-862(8)	4543(6)	852(5)	59(3)
C(64)	2322(9)	2923(7)	1005(6)	60(3)
C(65)	2799(11)	2332(8)	1167(6)	83(4)
C(66)	3781(13)	2337(7)	1289(7)	97(5)
C(67)	4293(8)	2944(10)	1302(6)	84(4)
C(68)	3820(11)	3563(8)	1132(7)	102(5)
C(69)	2821(10)	3545(7)	982(7)	97(5)
C(70)	1085(8)	3807(8)	1791(7)	67(4)
C(71)	1714(10)	4763(9)	2557(7)	121(7)
C(72)	2752(13)	4552(11)	2711(10)	131(10)
C(73)	9165(8)	2132(7)	4074(6)	61(3)
C(74)	10197(8)	2385(6)	4021(6)	66(3)
C(75)	9178(8)	3340(6)	3971(6)	62(3)
C(76)	11321(8)	1741(6)	3384(7)	56(3)
C(77)	11744(10)	1322(7)	3914(6)	93(4)
C(78)	12574(12)	967(7)	3865(8)	103(5)
C(79)	13044(8)	1029(7)	3289(10)	89(5)
C(80)	12588(12)	1393(9)	2770(7)	107(5)
C(81)	11753(10)	1748(7)	2818(7)	81(4)
C(82)	10952(8)	3601(6)	4230(5)	56(3)
C(83)	11888(8)	3340(6)	4278(5)	57(3)
C(84)	12655(8)	3810(7)	4427(5)	70(4)
C(85)	12548(9)	4515(7)	4521(5)	67(3)
C(86)	11600(10)	4753(6)	4438(6)	75(4)
C(87)	10793(8)	4306(6)	4308(5)	61(3)
C(88)	7559(8)	2753(7)	3882(5)	56(3)
C(89)	7028(10)	2162(7)	3572(6)	80(4)
C(90)	6043(12)	2169(9)	3434(7)	109(6)
C(91)	5588(9)	2772(10)	3584(6)	91(5)
C(92)	6101(11)	3335(7)	3916(7)	91(4)
C(93)	7066(8)	3306(7)	4058(6)	81(4)
C(94)	8881(9)	3652(7)	3213(8)	74(4)
C(95)	8303(10)	4669(8)	2618(8)	119(6)

C(96)	9190(14)	5194(13)	2585(12)	125(13)
C(97)	5824(11)	8159(8)	2505(9)	153(9)

Table 3. Bond lengths [Å] and angles [deg] for cd26131.

Br(1)-C(7)	1.876(11)
Br(2)-C(13)	1.927(11)
Br(3)-C(19)	1.905(12)
Br(4)-C(31)	1.882(13)
Br(5)-C(37)	1.857(11)
Br(6)-C(43)	1.867(15)
Br(7)-C(55)	1.836(12)
Br(8)-C(61)	1.863(12)
Br(9)-C(67)	1.909(11)
Br(10)-C(79)	1.868(12)
Br(11)-C(85)	1.847(11)
Br(12)-C(91)	1.912(13)
O(1)-C(1)	1.215(12)
O(2)-C(22)	1.231(13)
O(3)-C(22)	1.255(14)
O(3)-C(23)	1.451(12)
O(4)-C(25)	1.197(15)
O(5)-C(46)	1.144(11)
O(6)-C(46)	1.305(12)
O(6)-C(47)	1.529(16)
O(7)-C(49)	1.209(12)
O(8)-C(70)	1.177(12)
O(9)-C(70)	1.276(13)
O(9)-C(71)	1.490(14)
O(10)-C(73)	1.201(13)
O(11)-C(94)	1.151(13)
O(12)-C(94)	1.290(13)
O(12)-C(95)	1.499(15)
N(1)-C(4)	1.341(11)
N(1)-C(2)	1.452(12)
N(1)-H(1)	0.8600
N(2)-C(10)	1.413(12)
N(2)-C(3)	1.421(12)
N(2)-C(2)	1.439(12)
N(3)-C(1)	1.330(12)
N(3)-C(16)	1.444(11)
N(3)-C(3)	1.455(12)
N(4)-C(28)	1.364(11)
N(4)-C(26)	1.436(11)
N(4)-H(4)	0.8600
N(5)-C(34)	1.382(12)
N(5)-C(27)	1.428(11)
N(5)-C(26)	1.467(12)
N(6)-C(25)	1.334(13)
N(6)-C(27)	1.433(13)
N(6)-C(40)	1.460(14)
N(7)-C(52)	1.391(12)
N(7)-C(50)	1.464(11)
N(7)-H(7)	0.8600
N(8)-C(58)	1.396(12)
N(8)-C(51)	1.458(11)
N(8)-C(50)	1.465(12)
N(9)-C(49)	1.334(14)
N(9)-C(64)	1.408(12)
N(9)-C(51)	1.438(11)
N(10)-C(76)	1.355(11)
N(10)-C(74)	1.435(12)
N(10)-H(10)	0.8600
N(11)-C(74)	1.406(13)
N(11)-C(75)	1.416(11)
N(11)-C(82)	1.430(12)
N(12)-C(73)	1.345(13)
N(12)-C(88)	1.426(12)
N(12)-C(75)	1.484(12)
Cl(1)-C(97)	1.734(13)
Cl(2)-C(97)	1.767(14)
C(1)-C(2)	1.498(13)
C(2)-H(2)	0.9800

C(3)-C(22)	1.535(16)
C(3)-H(3)	0.9800
C(4)-C(5)	1.389(13)
C(4)-C(9)	1.407(13)
C(5)-C(6)	1.393(15)
C(5)-H(5)	0.9300
C(6)-C(7)	1.348(13)
C(6)-H(6)	0.9300
C(7)-C(8)	1.364(14)
C(8)-C(9)	1.381(14)
C(8)-H(8)	0.9300
C(9)-H(9)	0.9300
C(10)-C(11)	1.326(12)
C(10)-C(15)	1.410(13)
C(11)-C(12)	1.395(13)
C(11)-H(11)	0.9300
C(12)-C(13)	1.418(14)
C(12)-H(12)	0.9300
C(13)-C(14)	1.333(13)
C(14)-C(15)	1.395(13)
C(14)-H(14)	0.9300
C(15)-H(15)	0.9300
C(16)-C(21)	1.376(13)
C(16)-C(17)	1.403(14)
C(17)-C(18)	1.324(13)
C(17)-H(17)	0.9300
C(18)-C(19)	1.366(16)
C(18)-H(18)	0.9300
C(19)-C(20)	1.358(15)
C(20)-C(21)	1.361(13)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(23)-C(24)	1.445(14)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(25)-C(26)	1.570(16)
C(26)-H(26)	0.9800
C(27)-C(46)	1.574(15)
C(27)-H(27)	0.9800
C(28)-C(29)	1.369(14)
C(28)-C(33)	1.400(14)
C(29)-C(30)	1.353(13)
C(29)-H(29)	0.9300
C(30)-C(31)	1.357(14)
C(30)-H(30)	0.9300
C(31)-C(32)	1.351(16)
C(32)-C(33)	1.389(15)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-C(35)	1.400(12)
C(34)-C(39)	1.405(14)
C(35)-C(36)	1.428(15)
C(35)-H(35)	0.9300
C(36)-C(37)	1.313(15)
C(36)-H(36)	0.9300
C(37)-C(38)	1.396(14)
C(38)-C(39)	1.400(14)
C(38)-H(38)	0.9300
C(39)-H(39)	0.9300
C(40)-C(41)	1.384(15)
C(40)-C(45)	1.408(15)
C(41)-C(42)	1.386(15)
C(41)-H(41)	0.9300
C(42)-C(43)	1.311(16)
C(42)-H(42)	0.9300
C(43)-C(44)	1.437(19)
C(44)-C(45)	1.325(15)
C(44)-H(44)	0.9300
C(45)-H(45)	0.9300

C(47)-C(48)	1.52(2)
C(47)-H(47A)	0.9700
C(47)-H(47B)	0.9700
C(48)-H(48A)	0.9600
C(48)-H(48B)	0.9600
C(48)-H(48C)	0.9600
C(49)-C(50)	1.489(14)
C(50)-H(50)	0.9800
C(51)-C(70)	1.547(14)
C(51)-H(51)	0.9800
C(52)-C(53)	1.360(13)
C(52)-C(57)	1.392(13)
C(53)-C(54)	1.391(13)
C(53)-H(53)	0.9300
C(54)-C(55)	1.373(15)
C(54)-H(54)	0.9300
C(55)-C(56)	1.378(15)
C(56)-C(57)	1.402(13)
C(56)-H(56)	0.9300
C(57)-H(57)	0.9300
C(58)-C(59)	1.369(12)
C(58)-C(63)	1.388(14)
C(59)-C(60)	1.361(13)
C(59)-H(59)	0.9300
C(60)-C(61)	1.322(14)
C(60)-H(60)	0.9300
C(61)-C(62)	1.411(13)
C(62)-C(63)	1.361(13)
C(62)-H(62)	0.9300
C(63)-H(63)	0.9300
C(64)-C(65)	1.338(15)
C(64)-C(69)	1.372(14)
C(65)-C(66)	1.352(14)
C(65)-H(65)	0.9300
C(66)-C(67)	1.350(16)
C(66)-H(66)	0.9300
C(67)-C(68)	1.387(16)
C(68)-C(69)	1.377(14)
C(68)-H(68)	0.9300
C(69)-H(69)	0.9300
C(71)-C(72)	1.495(14)
C(71)-H(71A)	0.9700
C(71)-H(71B)	0.9700
C(72)-H(72A)	0.9600
C(72)-H(72B)	0.9600
C(72)-H(72C)	0.9600
C(73)-C(74)	1.527(14)
C(74)-H(74)	0.9800
C(75)-C(94)	1.608(16)
C(75)-H(75)	0.9800
C(76)-C(81)	1.339(14)
C(76)-C(77)	1.386(15)
C(77)-C(78)	1.365(15)
C(77)-H(77)	0.9300
C(78)-C(79)	1.391(16)
C(78)-H(78)	0.9300
C(79)-C(80)	1.330(16)
C(80)-C(81)	1.370(17)
C(80)-H(80)	0.9300
C(81)-H(81)	0.9300
C(82)-C(87)	1.379(13)
C(82)-C(83)	1.394(12)
C(83)-C(84)	1.379(13)
C(83)-H(83)	0.9300
C(84)-C(85)	1.372(14)
C(84)-H(84)	0.9300
C(85)-C(86)	1.390(14)
C(86)-C(87)	1.390(13)
C(86)-H(86)	0.9300
C(87)-H(87)	0.9300
C(88)-C(93)	1.338(14)
C(88)-C(89)	1.417(14)

C(89)-C(90)	1.358(14)
C(89)-H(89)	0.9300
C(90)-C(91)	1.373(17)
C(90)-H(90)	0.9300
C(91)-C(92)	1.381(15)
C(92)-C(93)	1.333(13)
C(92)-H(92)	0.9300
C(93)-H(93)	0.9300
C(95)-C(96)	1.589(15)
C(95)-H(95A)	0.9700
C(95)-H(95B)	0.9700
C(96)-H(96A)	0.9600
C(96)-H(96B)	0.9600
C(96)-H(96C)	0.9600
C(97)-H(97A)	0.9700
C(97)-H(97B)	0.9700
C(22)-O(3)-C(23)	120.5(11)
C(46)-O(6)-C(47)	114.8(10)
C(70)-O(9)-C(71)	121.6(11)
C(94)-O(12)-C(95)	116.5(11)
C(4)-N(1)-C(2)	120.6(9)
C(4)-N(1)-H(1)	119.7
C(2)-N(1)-H(1)	119.7
C(10)-N(2)-C(3)	126.4(10)
C(10)-N(2)-C(2)	120.6(10)
C(3)-N(2)-C(2)	109.8(8)
C(1)-N(3)-C(16)	129.1(10)
C(1)-N(3)-C(3)	111.7(9)
C(16)-N(3)-C(3)	119.2(9)
C(28)-N(4)-C(26)	123.2(10)
C(28)-N(4)-H(4)	118.4
C(26)-N(4)-H(4)	118.4
C(34)-N(5)-C(27)	125.3(9)
C(34)-N(5)-C(26)	124.6(10)
C(27)-N(5)-C(26)	109.8(9)
C(25)-N(6)-C(27)	114.3(11)
C(25)-N(6)-C(40)	125.1(12)
C(27)-N(6)-C(40)	120.4(10)
C(52)-N(7)-C(50)	122.0(9)
C(52)-N(7)-H(7)	119.0
C(50)-N(7)-H(7)	119.0
C(58)-N(8)-C(51)	126.0(9)
C(58)-N(8)-C(50)	125.9(9)
C(51)-N(8)-C(50)	108.0(9)
C(49)-N(9)-C(64)	125.8(10)
C(49)-N(9)-C(51)	111.4(10)
C(64)-N(9)-C(51)	121.9(9)
C(76)-N(10)-C(74)	124.8(10)
C(76)-N(10)-H(10)	117.6
C(74)-N(10)-H(10)	117.6
C(74)-N(11)-C(75)	111.0(9)
C(74)-N(11)-C(82)	127.1(10)
C(75)-N(11)-C(82)	121.7(10)
C(73)-N(12)-C(88)	131.8(10)
C(73)-N(12)-C(75)	110.3(9)
C(88)-N(12)-C(75)	117.1(10)
O(1)-C(1)-N(3)	127.2(11)
O(1)-C(1)-C(2)	124.5(11)
N(3)-C(1)-C(2)	108.3(11)
N(2)-C(2)-N(1)	111.8(9)
N(2)-C(2)-C(1)	104.6(10)
N(1)-C(2)-C(1)	115.3(9)
N(2)-C(2)-H(2)	108.3
N(1)-C(2)-H(2)	108.3
C(1)-C(2)-H(2)	108.3
N(2)-C(3)-N(3)	105.2(9)
N(2)-C(3)-C(22)	110.2(9)
N(3)-C(3)-C(22)	111.8(10)
N(2)-C(3)-H(3)	109.8
N(3)-C(3)-H(3)	109.8
C(22)-C(3)-H(3)	109.8

N(1)-C(4)-C(5)	123.7(12)
N(1)-C(4)-C(9)	123.4(12)
C(5)-C(4)-C(9)	112.8(10)
C(4)-C(5)-C(6)	123.2(11)
C(4)-C(5)-H(5)	118.4
C(6)-C(5)-H(5)	118.4
C(7)-C(6)-C(5)	120.0(12)
C(7)-C(6)-H(6)	120.0
C(5)-C(6)-H(6)	120.0
C(6)-C(7)-C(8)	120.9(11)
C(6)-C(7)-Br(1)	120.2(12)
C(8)-C(7)-Br(1)	118.9(11)
C(7)-C(8)-C(9)	117.7(11)
C(7)-C(8)-H(8)	121.1
C(9)-C(8)-H(8)	121.1
C(8)-C(9)-C(4)	125.2(11)
C(8)-C(9)-H(9)	117.4
C(4)-C(9)-H(9)	117.4
C(11)-C(10)-C(15)	121.0(11)
C(11)-C(10)-N(2)	121.4(11)
C(15)-C(10)-N(2)	117.6(9)
C(10)-C(11)-C(12)	121.3(11)
C(10)-C(11)-H(11)	119.4
C(12)-C(11)-H(11)	119.4
C(11)-C(12)-C(13)	117.1(9)
C(11)-C(12)-H(12)	121.4
C(13)-C(12)-H(12)	121.4
C(14)-C(13)-C(12)	122.1(11)
C(14)-C(13)-Br(2)	123.2(11)
C(12)-C(13)-Br(2)	114.7(10)
C(13)-C(14)-C(15)	119.7(12)
C(13)-C(14)-H(14)	120.1
C(15)-C(14)-H(14)	120.1
C(14)-C(15)-C(10)	118.6(10)
C(14)-C(15)-H(15)	120.7
C(10)-C(15)-H(15)	120.7
C(21)-C(16)-C(17)	115.2(10)
C(21)-C(16)-N(3)	124.1(11)
C(17)-C(16)-N(3)	120.7(11)
C(18)-C(17)-C(16)	123.5(12)
C(18)-C(17)-H(17)	118.3
C(16)-C(17)-H(17)	118.3
C(17)-C(18)-C(19)	117.8(12)
C(17)-C(18)-H(18)	121.1
C(19)-C(18)-H(18)	121.1
C(20)-C(19)-C(18)	123.2(12)
C(20)-C(19)-Br(3)	118.5(12)
C(18)-C(19)-Br(3)	118.3(11)
C(19)-C(20)-C(21)	116.9(12)
C(19)-C(20)-H(20)	121.5
C(21)-C(20)-H(20)	121.5
C(20)-C(21)-C(16)	123.4(11)
C(20)-C(21)-H(21)	118.3
C(16)-C(21)-H(21)	118.3
O(2)-C(22)-O(3)	126.4(14)
O(2)-C(22)-C(3)	117.6(14)
O(3)-C(22)-C(3)	115.2(12)
C(24)-C(23)-O(3)	110.0(12)
C(24)-C(23)-H(23A)	109.7
O(3)-C(23)-H(23A)	109.7
C(24)-C(23)-H(23B)	109.7
O(3)-C(23)-H(23B)	109.7
H(23A)-C(23)-H(23B)	108.2
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(4)-C(25)-N(6)	131.5(15)
O(4)-C(25)-C(26)	122.3(11)
N(6)-C(25)-C(26)	106.0(13)

N(4)-C(26)-N(5)	114.1(9)
N(4)-C(26)-C(25)	115.2(10)
N(5)-C(26)-C(25)	101.9(10)
N(4)-C(26)-H(26)	108.5
N(5)-C(26)-H(26)	108.5
C(25)-C(26)-H(26)	108.5
N(5)-C(27)-N(6)	104.9(9)
N(5)-C(27)-C(46)	110.7(9)
N(6)-C(27)-C(46)	109.0(10)
N(5)-C(27)-H(27)	110.7
N(6)-C(27)-H(27)	110.7
C(46)-C(27)-H(27)	110.7
N(4)-C(28)-C(29)	122.8(12)
N(4)-C(28)-C(33)	121.0(12)
C(29)-C(28)-C(33)	116.2(11)
C(30)-C(29)-C(28)	122.7(11)
C(30)-C(29)-H(29)	118.6
C(28)-C(29)-H(29)	118.6
C(29)-C(30)-C(31)	121.0(12)
C(29)-C(30)-H(30)	119.5
C(31)-C(30)-H(30)	119.5
C(32)-C(31)-C(30)	118.6(12)
C(32)-C(31)-Br(4)	120.3(11)
C(30)-C(31)-Br(4)	121.1(12)
C(31)-C(32)-C(33)	121.1(12)
C(31)-C(32)-H(32)	119.5
C(33)-C(32)-H(32)	119.5
C(32)-C(33)-C(28)	120.1(12)
C(32)-C(33)-H(33)	119.9
C(28)-C(33)-H(33)	119.9
N(5)-C(34)-C(35)	120.9(11)
N(5)-C(34)-C(39)	120.7(11)
C(35)-C(34)-C(39)	118.4(11)
C(34)-C(35)-C(36)	119.5(11)
C(34)-C(35)-H(35)	120.2
C(36)-C(35)-H(35)	120.2
C(37)-C(36)-C(35)	121.1(12)
C(37)-C(36)-H(36)	119.4
C(35)-C(36)-H(36)	119.4
C(36)-C(37)-C(38)	121.2(12)
C(36)-C(37)-Br(5)	119.8(12)
C(38)-C(37)-Br(5)	119.1(11)
C(37)-C(38)-C(39)	119.7(12)
C(37)-C(38)-H(38)	120.2
C(39)-C(38)-H(38)	120.2
C(38)-C(39)-C(34)	120.2(12)
C(38)-C(39)-H(39)	119.9
C(34)-C(39)-H(39)	119.9
C(41)-C(40)-C(45)	119.8(14)
C(41)-C(40)-N(6)	119.1(13)
C(45)-C(40)-N(6)	121.0(14)
C(40)-C(41)-C(42)	114.5(13)
C(40)-C(41)-H(41)	122.8
C(42)-C(41)-H(41)	122.8
C(43)-C(42)-C(41)	126.2(15)
C(43)-C(42)-H(42)	116.9
C(41)-C(42)-H(42)	116.9
C(42)-C(43)-C(44)	119.6(16)
C(42)-C(43)-Br(6)	119.9(18)
C(44)-C(43)-Br(6)	120.5(14)
C(45)-C(44)-C(43)	115.6(14)
C(45)-C(44)-H(44)	122.2
C(43)-C(44)-H(44)	122.2
C(44)-C(45)-C(40)	124.2(14)
C(44)-C(45)-H(45)	117.9
C(40)-C(45)-H(45)	117.9
O(5)-C(46)-O(6)	128.8(13)
O(5)-C(46)-C(27)	121.0(11)
O(6)-C(46)-C(27)	110.3(10)
C(48)-C(47)-O(6)	104.6(14)
C(48)-C(47)-H(47A)	110.8
O(6)-C(47)-H(47A)	110.8

C(48)-C(47)-H(47B)	110.8
O(6)-C(47)-H(47B)	110.8
H(47A)-C(47)-H(47B)	108.9
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
O(7)-C(49)-N(9)	127.8(12)
O(7)-C(49)-C(50)	122.3(12)
N(9)-C(49)-C(50)	109.9(11)
N(7)-C(50)-N(8)	110.7(8)
N(7)-C(50)-C(49)	114.3(9)
N(8)-C(50)-C(49)	103.5(10)
N(7)-C(50)-H(50)	109.4
N(8)-C(50)-H(50)	109.4
C(49)-C(50)-H(50)	109.4
N(9)-C(51)-N(8)	105.1(9)
N(9)-C(51)-C(70)	109.1(9)
N(8)-C(51)-C(70)	111.5(9)
N(9)-C(51)-H(51)	110.3
N(8)-C(51)-H(51)	110.3
C(70)-C(51)-H(51)	110.3
C(53)-C(52)-N(7)	121.8(12)
C(53)-C(52)-C(57)	119.5(10)
N(7)-C(52)-C(57)	118.6(12)
C(52)-C(53)-C(54)	119.7(11)
C(52)-C(53)-H(53)	120.1
C(54)-C(53)-H(53)	120.1
C(55)-C(54)-C(53)	122.7(12)
C(55)-C(54)-H(54)	118.7
C(53)-C(54)-H(54)	118.7
C(54)-C(55)-C(56)	116.9(11)
C(54)-C(55)-Br(7)	121.9(12)
C(56)-C(55)-Br(7)	121.2(11)
C(55)-C(56)-C(57)	121.5(11)
C(55)-C(56)-H(56)	119.2
C(57)-C(56)-H(56)	119.2
C(52)-C(57)-C(56)	119.4(11)
C(52)-C(57)-H(57)	120.3
C(56)-C(57)-H(57)	120.3
C(59)-C(58)-C(63)	119.6(11)
C(59)-C(58)-N(8)	119.5(11)
C(63)-C(58)-N(8)	120.9(11)
C(60)-C(59)-C(58)	119.4(11)
C(60)-C(59)-H(59)	120.3
C(58)-C(59)-H(59)	120.3
C(61)-C(60)-C(59)	124.1(11)
C(61)-C(60)-H(60)	117.9
C(59)-C(60)-H(60)	117.9
C(60)-C(61)-C(62)	116.1(11)
C(60)-C(61)-Br(8)	123.5(10)
C(62)-C(61)-Br(8)	120.3(10)
C(63)-C(62)-C(61)	122.5(11)
C(63)-C(62)-H(62)	118.8
C(61)-C(62)-H(62)	118.8
C(62)-C(63)-C(58)	118.3(11)
C(62)-C(63)-H(63)	120.8
C(58)-C(63)-H(63)	120.8
C(65)-C(64)-C(69)	120.6(12)
C(65)-C(64)-N(9)	121.6(12)
C(69)-C(64)-N(9)	117.6(12)
C(64)-C(65)-C(66)	120.3(13)
C(64)-C(65)-H(65)	119.9
C(66)-C(65)-H(65)	119.9
C(67)-C(66)-C(65)	120.7(14)
C(67)-C(66)-H(66)	119.7
C(65)-C(66)-H(66)	119.7
C(66)-C(67)-C(68)	120.1(12)
C(66)-C(67)-Br(9)	120.7(14)
C(68)-C(67)-Br(9)	119.2(13)

C(69)-C(68)-C(67)	118.4(13)
C(69)-C(68)-H(68)	120.8
C(67)-C(68)-H(68)	120.8
C(64)-C(69)-C(68)	119.8(13)
C(64)-C(69)-H(69)	120.1
C(68)-C(69)-H(69)	120.1
O(8)-C(70)-O(9)	124.8(14)
O(8)-C(70)-C(51)	121.3(13)
O(9)-C(70)-C(51)	113.9(12)
O(9)-C(71)-C(72)	101.0(14)
O(9)-C(71)-H(71A)	111.6
C(72)-C(71)-H(71A)	111.6
O(9)-C(71)-H(71B)	111.6
C(72)-C(71)-H(71B)	111.6
H(71A)-C(71)-H(71B)	109.4
C(71)-C(72)-H(72A)	109.5
C(71)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(71)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
O(10)-C(73)-N(12)	124.7(12)
O(10)-C(73)-C(74)	127.6(11)
N(12)-C(73)-C(74)	107.7(11)
N(11)-C(74)-N(10)	115.6(10)
N(11)-C(74)-C(73)	103.6(10)
N(10)-C(74)-C(73)	112.7(9)
N(11)-C(74)-H(74)	108.2
N(10)-C(74)-H(74)	108.2
C(73)-C(74)-H(74)	108.2
N(11)-C(75)-N(12)	104.2(9)
N(11)-C(75)-C(94)	113.4(9)
N(12)-C(75)-C(94)	107.8(9)
N(11)-C(75)-H(75)	110.4
N(12)-C(75)-H(75)	110.4
C(94)-C(75)-H(75)	110.4
C(81)-C(76)-N(10)	118.5(13)
C(81)-C(76)-C(77)	116.0(11)
N(10)-C(76)-C(77)	125.5(13)
C(78)-C(77)-C(76)	121.5(13)
C(78)-C(77)-H(77)	119.3
C(76)-C(77)-H(77)	119.3
C(77)-C(78)-C(79)	120.9(13)
C(77)-C(78)-H(78)	119.5
C(79)-C(78)-H(78)	119.5
C(80)-C(79)-C(78)	116.3(13)
C(80)-C(79)-Br(10)	125.1(16)
C(78)-C(79)-Br(10)	118.6(14)
C(79)-C(80)-C(81)	122.5(14)
C(79)-C(80)-H(80)	118.8
C(81)-C(80)-H(80)	118.8
C(76)-C(81)-C(80)	122.5(13)
C(76)-C(81)-H(81)	118.7
C(80)-C(81)-H(81)	118.7
C(87)-C(82)-C(83)	121.5(10)
C(87)-C(82)-N(11)	120.5(10)
C(83)-C(82)-N(11)	118.0(11)
C(84)-C(83)-C(82)	117.6(11)
C(84)-C(83)-H(83)	121.2
C(82)-C(83)-H(83)	121.2
C(85)-C(84)-C(83)	123.9(11)
C(85)-C(84)-H(84)	118.1
C(83)-C(84)-H(84)	118.1
C(84)-C(85)-C(86)	116.3(11)
C(84)-C(85)-Br(11)	119.7(11)
C(86)-C(85)-Br(11)	123.9(11)
C(85)-C(86)-C(87)	122.8(12)
C(85)-C(86)-H(86)	118.6
C(87)-C(86)-H(86)	118.6
C(82)-C(87)-C(86)	117.9(11)
C(82)-C(87)-H(87)	121.0
C(86)-C(87)-H(87)	121.0

C(93)-C(88)-C(89)	118.5(11)
C(93)-C(88)-N(12)	125.0(12)
C(89)-C(88)-N(12)	116.4(12)
C(90)-C(89)-C(88)	120.6(12)
C(90)-C(89)-H(89)	119.7
C(88)-C(89)-H(89)	119.7
C(89)-C(90)-C(91)	117.8(13)
C(89)-C(90)-H(90)	121.1
C(91)-C(90)-H(90)	121.1
C(90)-C(91)-C(92)	121.5(13)
C(90)-C(91)-Br(12)	119.3(13)
C(92)-C(91)-Br(12)	119.1(14)
C(93)-C(92)-C(91)	119.1(13)
C(93)-C(92)-H(92)	120.5
C(91)-C(92)-H(92)	120.5
C(92)-C(93)-C(88)	122.3(12)
C(92)-C(93)-H(93)	118.9
C(88)-C(93)-H(93)	118.9
O(11)-C(94)-O(12)	131.8(15)
O(11)-C(94)-C(75)	119.0(13)
O(12)-C(94)-C(75)	108.9(12)
O(12)-C(95)-C(96)	100.2(13)
O(12)-C(95)-H(95A)	111.7
C(96)-C(95)-H(95A)	111.7
O(12)-C(95)-H(95B)	111.7
C(96)-C(95)-H(95B)	111.7
H(95A)-C(95)-H(95B)	109.5
C(95)-C(96)-H(96A)	109.5
C(95)-C(96)-H(96B)	109.5
H(96A)-C(96)-H(96B)	109.5
C(95)-C(96)-H(96C)	109.5
H(96A)-C(96)-H(96C)	109.5
H(96B)-C(96)-H(96C)	109.5
Cl(1)-C(97)-Cl(2)	101.2(9)
Cl(1)-C(97)-H(97A)	111.5
Cl(2)-C(97)-H(97A)	111.5
Cl(1)-C(97)-H(97B)	111.5
Cl(2)-C(97)-H(97B)	111.5
H(97A)-C(97)-H(97B)	109.4

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd26131. 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
Br (1)	110(1)	115(1)	111(1)	20(1)	18(1)	39(1)
Br (2)	112(1)	84(1)	138(1)	-14(1)	54(1)	-39(1)
Br (3)	77(1)	110(1)	150(2)	-29(1)	-6(1)	6(1)
Br (4)	115(1)	232(2)	148(2)	32(2)	-16(1)	-74(1)
Br (5)	112(1)	93(1)	170(2)	-5(1)	3(1)	34(1)
Br (6)	96(1)	183(2)	168(2)	52(1)	25(1)	29(1)
Br (7)	112(1)	114(1)	145(2)	10(1)	9(1)	-49(1)
Br (8)	87(1)	79(1)	136(1)	8(1)	18(1)	19(1)
Br (9)	76(1)	180(2)	178(2)	81(1)	36(1)	15(1)
Br (10)	102(1)	128(2)	303(3)	12(2)	47(1)	33(1)
Br (11)	102(1)	104(1)	101(1)	11(1)	8(1)	-37(1)
Br (12)	81(1)	222(2)	163(2)	-59(2)	24(1)	-9(1)
O (1)	100(6)	42(5)	107(7)	-5(5)	15(5)	-11(5)
O (2)	187(9)	68(7)	68(7)	3(5)	29(6)	-5(6)
O (3)	150(7)	47(6)	57(7)	3(5)	39(5)	-8(5)
O (4)	123(7)	48(6)	117(8)	4(6)	33(5)	-21(5)
O (5)	123(7)	89(7)	64(7)	-12(5)	0(5)	-50(6)
O (6)	125(7)	94(7)	57(6)	1(5)	10(5)	-43(6)
O (7)	107(7)	73(7)	77(7)	9(5)	19(5)	-10(6)
O (8)	116(7)	81(7)	77(7)	15(5)	19(6)	-16(5)
O (9)	133(7)	85(7)	68(7)	0(6)	6(5)	-52(6)
O (10)	105(7)	56(6)	107(8)	9(5)	20(5)	-15(5)
O (11)	141(8)	85(8)	64(7)	-14(6)	31(6)	4(6)
O (12)	127(7)	88(7)	47(6)	8(5)	5(5)	3(6)
N (1)	73(6)	74(7)	45(7)	13(5)	33(5)	20(6)
N (2)	65(7)	65(8)	67(7)	7(6)	19(5)	-19(6)
N (3)	59(7)	41(6)	64(7)	14(5)	21(5)	16(5)
N (4)	95(7)	68(7)	49(7)	7(6)	6(6)	-27(6)
N (5)	63(7)	45(7)	77(8)	-9(5)	10(5)	10(5)
N (6)	82(8)	42(7)	72(8)	1(5)	13(6)	-1(6)
N (7)	70(6)	53(6)	54(7)	13(5)	-5(5)	-4(5)
N (8)	56(7)	69(8)	64(7)	11(6)	0(5)	-14(6)
N (9)	56(7)	29(6)	81(8)	-5(5)	12(5)	2(5)
N (10)	69(6)	73(7)	53(7)	2(6)	2(5)	31(5)
N (11)	58(7)	58(7)	74(8)	-5(6)	-4(5)	11(6)
N (12)	46(6)	45(6)	92(8)	0(5)	18(5)	14(5)
Cl (1)	278(8)	238(9)	311(10)	48(7)	25(6)	12(7)
Cl (2)	224(6)	278(9)	287(9)	25(6)	41(6)	-63(6)
C (1)	56(8)	75(10)	35(8)	10(7)	10(6)	10(8)
C (2)	80(9)	48(8)	44(8)	6(6)	10(7)	-12(6)
C (3)	73(9)	57(8)	34(8)	3(6)	14(6)	-7(7)
C (4)	56(8)	35(7)	55(9)	7(6)	6(7)	20(6)
C (5)	87(10)	74(10)	54(10)	3(8)	7(7)	-12(8)
C (6)	126(12)	57(9)	36(9)	2(7)	10(9)	-7(9)
C (7)	81(10)	71(9)	55(9)	-9(8)	10(8)	13(7)
C (8)	79(10)	74(10)	85(12)	41(9)	-29(8)	23(8)
C (9)	92(10)	60(9)	70(10)	-2(7)	0(8)	7(8)
C (10)	41(7)	56(8)	57(8)	-4(6)	3(6)	31(6)
C (11)	61(8)	53(8)	47(8)	8(6)	-1(6)	-7(7)
C (12)	53(8)	81(10)	82(10)	-9(8)	24(7)	33(7)
C (13)	65(9)	78(10)	58(9)	-1(7)	5(7)	-15(8)
C (14)	86(10)	61(9)	70(10)	0(7)	15(8)	1(8)
C (15)	46(7)	55(8)	92(10)	2(7)	21(6)	19(6)
C (16)	58(8)	66(9)	44(8)	-2(7)	16(6)	11(7)
C (17)	90(10)	30(8)	129(13)	-5(7)	16(9)	1(7)
C (18)	64(10)	75(12)	189(17)	-21(11)	32(10)	-20(9)
C (19)	83(10)	67(10)	83(10)	-30(8)	20(8)	-10(9)
C (20)	67(10)	95(12)	106(12)	31(9)	2(8)	25(8)
C (21)	76(9)	38(8)	103(11)	21(7)	20(8)	18(7)
C (22)	77(9)	77(11)	64(12)	33(10)	-12(8)	-20(8)
C (23)	116(14)	80(11)	54(10)	-16(9)	25(9)	13(10)
C (24)	142(17)	56(10)	88(12)	-8(9)	-8(11)	-19(11)

C(25)	106(12)	76(11)	52(9)	-11(8)	13(8)	-50(11)
C(26)	102(11)	52(9)	49(9)	1(7)	10(8)	-25(8)
C(27)	70(9)	57(9)	65(10)	-21(7)	1(7)	-16(7)
C(28)	62(8)	43(7)	75(11)	17(7)	21(8)	14(6)
C(29)	82(10)	96(11)	55(10)	6(8)	-11(7)	-26(8)
C(30)	99(10)	79(10)	53(10)	7(7)	14(8)	-12(8)
C(31)	76(10)	158(15)	62(11)	34(10)	-12(9)	-24(9)
C(32)	109(12)	109(13)	77(12)	10(10)	-31(9)	-20(10)
C(33)	113(11)	97(11)	80(11)	46(9)	-28(9)	-11(9)
C(34)	49(8)	64(9)	38(7)	0(6)	0(6)	8(7)
C(35)	72(9)	80(10)	56(9)	4(7)	7(7)	-23(8)
C(36)	84(10)	97(12)	61(10)	4(9)	4(7)	-7(10)
C(37)	73(9)	64(10)	58(9)	0(7)	-1(7)	12(7)
C(38)	118(12)	66(10)	58(9)	4(7)	17(8)	12(9)
C(39)	103(10)	61(10)	55(9)	6(7)	1(7)	-22(9)
C(40)	102(12)	87(11)	27(8)	18(8)	5(8)	-12(10)
C(41)	130(14)	76(11)	46(9)	3(8)	-1(9)	4(10)
C(42)	81(11)	93(12)	96(12)	29(9)	15(9)	54(9)
C(43)	84(12)	147(17)	73(12)	55(11)	-14(9)	-43(12)
C(44)	90(13)	119(15)	99(13)	1(11)	16(10)	-22(11)
C(45)	69(10)	102(12)	78(11)	6(9)	7(8)	-15(9)
C(46)	88(9)	73(10)	45(10)	-8(8)	-13(8)	-45(8)
C(47)	117(16)	108(16)	104(18)	17(13)	43(14)	-38(14)
C(48)	120(20)	170(30)	49(13)	17(14)	51(14)	-60(20)
C(49)	72(10)	60(10)	61(9)	18(8)	9(7)	29(9)
C(50)	87(9)	35(7)	36(8)	2(6)	-2(6)	0(6)
C(51)	47(8)	68(9)	66(10)	16(7)	-3(6)	22(6)
C(52)	65(9)	58(9)	60(9)	3(7)	0(7)	-11(7)
C(53)	64(8)	49(8)	64(9)	1(7)	6(6)	-1(6)
C(54)	111(11)	32(8)	96(12)	-26(7)	-17(9)	1(8)
C(55)	73(10)	60(9)	94(12)	2(8)	3(8)	13(7)
C(56)	56(8)	86(10)	92(11)	-2(9)	24(7)	-7(7)
C(57)	64(8)	55(8)	70(10)	-1(7)	2(7)	27(7)
C(58)	66(9)	57(9)	44(8)	12(7)	8(6)	-1(7)
C(59)	64(8)	47(8)	73(9)	7(6)	-3(7)	-20(7)
C(60)	78(9)	54(9)	66(9)	7(7)	0(7)	-1(8)
C(61)	74(9)	63(10)	64(9)	-1(7)	22(7)	-6(7)
C(62)	100(10)	65(9)	57(9)	10(7)	8(8)	8(9)
C(63)	54(8)	67(9)	58(9)	20(7)	13(6)	0(7)
C(64)	56(9)	52(9)	69(9)	4(7)	1(7)	1(8)
C(65)	79(10)	99(13)	72(10)	8(9)	20(8)	-21(10)
C(66)	129(14)	71(11)	97(12)	19(9)	33(10)	-1(10)
C(67)	55(8)	127(14)	82(11)	35(10)	43(7)	11(9)
C(68)	110(13)	87(12)	118(13)	43(10)	40(10)	-5(10)
C(69)	59(9)	105(13)	127(13)	29(9)	14(8)	-24(8)
C(70)	60(8)	80(11)	61(11)	33(9)	4(7)	-6(7)
C(71)	135(16)	150(19)	81(13)	-1(13)	7(11)	-83(14)
C(73)	58(9)	71(10)	52(9)	-5(8)	3(6)	18(8)
C(74)	82(10)	53(9)	61(9)	-15(7)	9(7)	4(7)
C(75)	72(9)	52(8)	65(10)	-19(7)	21(7)	11(7)
C(76)	54(8)	55(8)	62(10)	-3(7)	12(7)	30(6)
C(77)	119(12)	99(11)	64(11)	13(9)	16(9)	45(9)
C(78)	128(14)	96(12)	78(12)	0(10)	-9(10)	46(10)
C(79)	59(9)	84(10)	126(15)	9(11)	16(10)	37(7)
C(80)	122(14)	128(14)	82(13)	37(10)	45(10)	16(11)
C(81)	78(10)	85(10)	83(12)	16(9)	22(9)	18(8)
C(82)	70(9)	48(8)	50(8)	-1(6)	10(6)	16(7)
C(83)	60(8)	46(7)	68(9)	4(6)	17(6)	30(7)
C(84)	60(8)	85(11)	63(9)	-10(8)	9(6)	-2(8)
C(85)	94(10)	68(10)	37(8)	2(7)	11(7)	-20(8)
C(86)	88(10)	69(9)	70(10)	17(7)	18(8)	-4(9)
C(87)	59(8)	69(9)	54(9)	9(7)	3(6)	3(7)
C(88)	43(8)	81(10)	46(8)	12(7)	12(6)	28(7)
C(89)	79(10)	99(11)	68(10)	-19(8)	37(8)	-19(9)
C(90)	101(13)	131(15)	107(13)	-62(11)	61(10)	-24(11)
C(91)	80(10)	150(15)	45(9)	-17(10)	28(7)	-37(11)
C(92)	95(12)	96(12)	86(11)	-6(9)	21(9)	4(9)
C(93)	30(8)	106(12)	106(11)	0(9)	5(7)	15(7)
C(94)	92(10)	35(9)	95(15)	-5(9)	17(9)	-18(8)
C(97)	240(20)	160(20)	161(19)	-31(15)	-18(15)	73(18)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for cd26131.

	x	y	z	U(eq)
H(1)	10100	7378	2036	74
H(4)	-779	7277	3041	85
H(7)	-440	2478	1861	72
H(10)	10204	2255	3014	78
H(2)	10063	7515	638	69
H(3)	8442	8849	707	65
H(5)	10419	6293	746	86
H(6)	11770	5671	582	88
H(8)	13259	6552	2272	100
H(9)	11929	7200	2407	90
H(11)	11393	8108	1066	66
H(12)	12666	8897	978	84
H(14)	10776	10468	846	86
H(15)	9525	9672	972	76
H(17)	6848	6796	816	100
H(18)	5218	6738	615	130
H(20)	5143	8809	367	107
H(21)	6805	8853	588	85
H(23A)	7676	9954	2480	127
H(23B)	8392	9403	2847	127
H(24A)	9684	10095	2658	138
H(24B)	9009	10498	3097	138
H(24C)	8961	10648	2309	138
H(26)	-862	7154	4419	82
H(27)	1003	8525	4533	78
H(29)	-1580	6183	4179	96
H(30)	-2941	5506	4020	92
H(32)	-3755	6346	2208	124
H(33)	-2433	7109	2393	121
H(35)	-2146	7904	4110	83
H(36)	-3298	8770	4220	98
H(38)	-1240	10243	4410	96
H(39)	-55	9410	4334	89
H(41)	2215	6578	3699	102
H(42)	3889	6545	3804	106
H(44)	4236	8344	4869	123
H(45)	2606	8377	4813	100
H(47A)	1208	9276	2471	134
H(47B)	1760	9900	2907	134
H(48A)	3075	9111	3243	138
H(48B)	2944	9281	2455	138
H(48C)	2546	8570	2699	138
H(50)	-743	2455	433	65
H(51)	936	3936	718	73
H(53)	-1112	1297	589	71
H(54)	-2420	529	492	100
H(56)	-3385	1457	2071	93
H(57)	-2085	2251	2175	76
H(59)	-2060	3077	729	75
H(60)	-3332	3812	622	81
H(62)	-1550	5445	805	89
H(63)	-235	4733	907	71
H(65)	2452	1917	1196	99
H(66)	4106	1919	1364	117
H(68)	4168	3981	1119	123
H(69)	2485	3953	866	117
H(71A)	1332	4579	2892	131
H(71B)	1657	5268	2542	131
H(72A)	2792	4055	2647	141
H(72B)	3006	4679	3179	141
H(72C)	3124	4785	2404	141
H(74)	10633	2208	4417	79
H(75)	9056	3681	4325	75

H (77)	11455	1283	4310	112
H (78)	12829	678	4222	123
H (80)	12846	1408	2358	129
H (81)	11475	2005	2442	97
H (83)	11992	2866	4211	68
H (84)	13282	3639	4467	84
H (86)	11501	5231	4472	90
H (87)	10167	4477	4274	73
H (89)	7357	1766	3462	96
H (90)	5688	1779	3245	131
H (92)	5778	3728	4039	110
H (93)	7409	3683	4287	97
H (95A)	7707	4916	2648	137
H (95B)	8203	4349	2224	137
H (96A)	9396	5401	3033	138
H (96B)	8992	5555	2261	138
H (96C)	9720	4944	2439	138
H (97A)	6205	7982	2919	232
H (97B)	6165	8078	2115	232

Table 6. Torsion angles [deg] for cd26131.

C(16)-N(3)-C(1)-O(1)	1.5(18)
C(3)-N(3)-C(1)-O(1)	178.7(11)
C(16)-N(3)-C(1)-C(2)	-177.9(9)
C(3)-N(3)-C(1)-C(2)	-0.6(12)
C(10)-N(2)-C(2)-N(1)	80.0(12)
C(3)-N(2)-C(2)-N(1)	-119.0(10)
C(10)-N(2)-C(2)-C(1)	-154.6(9)
C(3)-N(2)-C(2)-C(1)	6.4(11)
C(4)-N(1)-C(2)-N(2)	-130.7(10)
C(4)-N(1)-C(2)-C(1)	110.0(12)
O(1)-C(1)-C(2)-N(2)	177.2(10)
N(3)-C(1)-C(2)-N(2)	-3.5(11)
O(1)-C(1)-C(2)-N(1)	-59.7(15)
N(3)-C(1)-C(2)-N(1)	119.7(10)
C(10)-N(2)-C(3)-N(3)	152.9(9)
C(2)-N(2)-C(3)-N(3)	-6.8(11)
C(10)-N(2)-C(3)-C(22)	-86.4(13)
C(2)-N(2)-C(3)-C(22)	113.9(11)
C(1)-N(3)-C(3)-N(2)	4.6(12)
C(16)-N(3)-C(3)-N(2)	-177.9(8)
C(1)-N(3)-C(3)-C(22)	-115.0(11)
C(16)-N(3)-C(3)-C(22)	62.5(12)
C(2)-N(1)-C(4)-C(5)	-39.3(15)
C(2)-N(1)-C(4)-C(9)	137.3(10)
N(1)-C(4)-C(5)-C(6)	172.7(11)
C(9)-C(4)-C(5)-C(6)	-4.3(16)
C(4)-C(5)-C(6)-C(7)	1.6(18)
C(5)-C(6)-C(7)-C(8)	3.0(18)
C(5)-C(6)-C(7)-Br(1)	-177.0(9)
C(6)-C(7)-C(8)-C(9)	-4.2(18)
Br(1)-C(7)-C(8)-C(9)	175.8(9)
C(7)-C(8)-C(9)-C(4)	1.1(18)
N(1)-C(4)-C(9)-C(8)	-174.1(11)
C(5)-C(4)-C(9)-C(8)	2.9(16)
C(3)-N(2)-C(10)-C(11)	-173.7(10)
C(2)-N(2)-C(10)-C(11)	-16.0(15)
C(3)-N(2)-C(10)-C(15)	8.2(15)
C(2)-N(2)-C(10)-C(15)	165.9(9)
C(15)-C(10)-C(11)-C(12)	1.0(16)
N(2)-C(10)-C(11)-C(12)	-177.0(9)
C(10)-C(11)-C(12)-C(13)	0.1(16)
C(11)-C(12)-C(13)-C(14)	-2.5(17)
C(11)-C(12)-C(13)-Br(2)	179.7(8)
C(12)-C(13)-C(14)-C(15)	3.6(17)
Br(2)-C(13)-C(14)-C(15)	-178.7(8)
C(13)-C(14)-C(15)-C(10)	-2.4(17)
C(11)-C(10)-C(15)-C(14)	0.2(16)
N(2)-C(10)-C(15)-C(14)	178.2(9)
C(1)-N(3)-C(16)-C(21)	-162.9(11)
C(3)-N(3)-C(16)-C(21)	20.1(14)
C(1)-N(3)-C(16)-C(17)	16.1(16)
C(3)-N(3)-C(16)-C(17)	-160.9(10)
C(21)-C(16)-C(17)-C(18)	-0.2(18)
N(3)-C(16)-C(17)-C(18)	-179.3(11)
C(16)-C(17)-C(18)-C(19)	0(2)
C(17)-C(18)-C(19)-C(20)	0(2)
C(17)-C(18)-C(19)-Br(3)	-178.7(10)
C(18)-C(19)-C(20)-C(21)	-1(2)
Br(3)-C(19)-C(20)-C(21)	178.3(9)
C(19)-C(20)-C(21)-C(16)	0.8(19)
C(17)-C(16)-C(21)-C(20)	-0.3(17)
N(3)-C(16)-C(21)-C(20)	178.8(10)
C(23)-O(3)-C(22)-O(2)	-2.0(19)
C(23)-O(3)-C(22)-C(3)	-171.6(10)
N(2)-C(3)-C(22)-O(2)	-75.4(13)
N(3)-C(3)-C(22)-O(2)	41.2(15)
N(2)-C(3)-C(22)-O(3)	95.1(12)
N(3)-C(3)-C(22)-O(3)	-148.3(10)

C(22)-O(3)-C(23)-C(24)	132.6(12)
C(27)-N(6)-C(25)-O(4)	-179.5(14)
C(40)-N(6)-C(25)-O(4)	5(2)
C(27)-N(6)-C(25)-C(26)	4.7(13)
C(40)-N(6)-C(25)-C(26)	-170.6(9)
C(28)-N(4)-C(26)-N(5)	-129.2(11)
C(28)-N(4)-C(26)-C(25)	113.5(12)
C(34)-N(5)-C(26)-N(4)	67.5(14)
C(27)-N(5)-C(26)-N(4)	-106.7(11)
C(34)-N(5)-C(26)-C(25)	-167.8(9)
C(27)-N(5)-C(26)-C(25)	18.1(11)
O(4)-C(25)-C(26)-N(4)	-65.9(16)
N(6)-C(25)-C(26)-N(4)	110.4(10)
O(4)-C(25)-C(26)-N(5)	170.1(12)
N(6)-C(25)-C(26)-N(5)	-13.6(12)
C(34)-N(5)-C(27)-N(6)	170.0(9)
C(26)-N(5)-C(27)-N(6)	-16.0(12)
C(34)-N(5)-C(27)-C(46)	-72.5(12)
C(26)-N(5)-C(27)-C(46)	101.5(11)
C(25)-N(6)-C(27)-N(5)	6.6(13)
C(40)-N(6)-C(27)-N(5)	-177.9(9)
C(25)-N(6)-C(27)-C(46)	-112.0(11)
C(40)-N(6)-C(27)-C(46)	63.5(12)
C(26)-N(4)-C(28)-C(29)	-25.8(17)
C(26)-N(4)-C(28)-C(33)	152.8(12)
N(4)-C(28)-C(29)-C(30)	179.8(11)
C(33)-C(28)-C(29)-C(30)	1.0(18)
C(28)-C(29)-C(30)-C(31)	-1(2)
C(29)-C(30)-C(31)-C(32)	3(2)
C(29)-C(30)-C(31)-Br(4)	-175.7(10)
C(30)-C(31)-C(32)-C(33)	-6(2)
Br(4)-C(31)-C(32)-C(33)	173.0(11)
C(31)-C(32)-C(33)-C(28)	6(2)
N(4)-C(28)-C(33)-C(32)	177.5(12)
C(29)-C(28)-C(33)-C(32)	-3.7(19)
C(27)-N(5)-C(34)-C(35)	175.6(10)
C(26)-N(5)-C(34)-C(35)	2.4(15)
C(27)-N(5)-C(34)-C(39)	-6.2(16)
C(26)-N(5)-C(34)-C(39)	-179.4(10)
N(5)-C(34)-C(35)-C(36)	178.1(10)
C(39)-C(34)-C(35)-C(36)	-0.1(15)
C(34)-C(35)-C(36)-C(37)	1.3(18)
C(35)-C(36)-C(37)-C(38)	-1.6(19)
C(35)-C(36)-C(37)-Br(5)	178.0(8)
C(36)-C(37)-C(38)-C(39)	0.7(18)
Br(5)-C(37)-C(38)-C(39)	-178.9(8)
C(37)-C(38)-C(39)-C(34)	0.5(17)
N(5)-C(34)-C(39)-C(38)	-179.0(10)
C(35)-C(34)-C(39)-C(38)	-0.8(16)
C(25)-N(6)-C(40)-C(41)	34.9(16)
C(27)-N(6)-C(40)-C(41)	-140.0(12)
C(25)-N(6)-C(40)-C(45)	-148.4(12)
C(27)-N(6)-C(40)-C(45)	36.7(15)
C(45)-C(40)-C(41)-C(42)	3.4(17)
N(6)-C(40)-C(41)-C(42)	-179.9(9)
C(40)-C(41)-C(42)-C(43)	-1(2)
C(41)-C(42)-C(43)-C(44)	-2(2)
C(41)-C(42)-C(43)-Br(6)	179.8(10)
C(42)-C(43)-C(44)-C(45)	3(2)
Br(6)-C(43)-C(44)-C(45)	-178.7(9)
C(43)-C(44)-C(45)-C(40)	-1(2)
C(41)-C(40)-C(45)-C(44)	-2.3(19)
N(6)-C(40)-C(45)-C(44)	-179.0(12)
C(47)-O(6)-C(46)-O(5)	-6(2)
C(47)-O(6)-C(46)-C(27)	173.2(11)
N(5)-C(27)-C(46)-O(5)	-55.0(16)
N(6)-C(27)-C(46)-O(5)	59.9(15)
N(5)-C(27)-C(46)-O(6)	125.9(10)
N(6)-C(27)-C(46)-O(6)	-119.2(11)
C(46)-O(6)-C(47)-C(48)	-87.1(15)
C(64)-N(9)-C(49)-O(7)	-13(2)
C(51)-N(9)-C(49)-O(7)	177.4(11)

C(64)-N(9)-C(49)-C(50)	169.2(9)
C(51)-N(9)-C(49)-C(50)	-0.6(13)
C(52)-N(7)-C(50)-N(8)	130.8(10)
C(52)-N(7)-C(50)-C(49)	-112.8(12)
C(58)-N(8)-C(50)-N(7)	-67.6(12)
C(51)-N(8)-C(50)-N(7)	108.8(10)
C(58)-N(8)-C(50)-C(49)	169.5(10)
C(51)-N(8)-C(50)-C(49)	-14.1(11)
O(7)-C(49)-C(50)-N(7)	70.5(14)
N(9)-C(49)-C(50)-N(7)	-111.3(10)
O(7)-C(49)-C(50)-N(8)	-169.0(11)
N(9)-C(49)-C(50)-N(8)	9.2(12)
C(49)-N(9)-C(51)-N(8)	-8.3(12)
C(64)-N(9)-C(51)-N(8)	-178.6(9)
C(49)-N(9)-C(51)-C(70)	111.3(10)
C(64)-N(9)-C(51)-C(70)	-58.9(13)
C(58)-N(8)-C(51)-N(9)	-169.6(9)
C(50)-N(8)-C(51)-N(9)	14.0(11)
C(58)-N(8)-C(51)-C(70)	72.3(13)
C(50)-N(8)-C(51)-C(70)	-104.1(10)
C(50)-N(7)-C(52)-C(53)	34.3(15)
C(50)-N(7)-C(52)-C(57)	-141.7(10)
N(7)-C(52)-C(53)-C(54)	-176.6(10)
C(57)-C(52)-C(53)-C(54)	-0.6(16)
C(52)-C(53)-C(54)-C(55)	3.1(18)
C(53)-C(54)-C(55)-C(56)	-5.8(19)
C(53)-C(54)-C(55)-Br(7)	177.4(8)
C(54)-C(55)-C(56)-C(57)	6.2(19)
Br(7)-C(55)-C(56)-C(57)	-177.0(8)
C(53)-C(52)-C(57)-C(56)	1.1(17)
N(7)-C(52)-C(57)-C(56)	177.2(9)
C(55)-C(56)-C(57)-C(52)	-4.0(17)
C(51)-N(8)-C(58)-C(59)	-175.7(10)
C(50)-N(8)-C(58)-C(59)	0.1(16)
C(51)-N(8)-C(58)-C(63)	6.5(16)
C(50)-N(8)-C(58)-C(63)	-177.7(10)
C(63)-C(58)-C(59)-C(60)	-0.6(16)
N(8)-C(58)-C(59)-C(60)	-178.4(10)
C(58)-C(59)-C(60)-C(61)	0.9(18)
C(59)-C(60)-C(61)-C(62)	-1.4(18)
C(59)-C(60)-C(61)-Br(8)	-177.4(9)
C(60)-C(61)-C(62)-C(63)	1.7(17)
Br(8)-C(61)-C(62)-C(63)	177.8(8)
C(61)-C(62)-C(63)-C(58)	-1.4(17)
C(59)-C(58)-C(63)-C(62)	0.9(16)
N(8)-C(58)-C(63)-C(62)	178.6(9)
C(49)-N(9)-C(64)-C(65)	-16.5(18)
C(51)-N(9)-C(64)-C(65)	152.3(11)
C(49)-N(9)-C(64)-C(69)	168.5(12)
C(51)-N(9)-C(64)-C(69)	-22.8(16)
C(69)-C(64)-C(65)-C(66)	-2(2)
N(9)-C(64)-C(65)-C(66)	-177.1(11)
C(64)-C(65)-C(66)-C(67)	5(2)
C(65)-C(66)-C(67)-C(68)	-6(2)
C(65)-C(66)-C(67)-Br(9)	174.1(9)
C(66)-C(67)-C(68)-C(69)	3(2)
Br(9)-C(67)-C(68)-C(69)	-176.7(10)
C(65)-C(64)-C(69)-C(68)	0(2)
N(9)-C(64)-C(69)-C(68)	174.7(11)
C(67)-C(68)-C(69)-C(64)	0(2)
C(71)-O(9)-C(70)-O(8)	0(2)
C(71)-O(9)-C(70)-C(51)	177.9(10)
N(9)-C(51)-C(70)-O(8)	-58.2(15)
N(8)-C(51)-C(70)-O(8)	57.5(15)
N(9)-C(51)-C(70)-O(9)	123.8(11)
N(8)-C(51)-C(70)-O(9)	-120.5(11)
C(70)-O(9)-C(71)-C(72)	88.7(16)
C(88)-N(12)-C(73)-O(10)	-14(2)
C(75)-N(12)-C(73)-O(10)	177.1(12)
C(88)-N(12)-C(73)-C(74)	165.0(10)
C(75)-N(12)-C(73)-C(74)	-4.2(12)
C(75)-N(11)-C(74)-N(10)	105.0(11)

C(82)-N(11)-C(74)-N(10)	-69.9(14)
C(75)-N(11)-C(74)-C(73)	-18.7(12)
C(82)-N(11)-C(74)-C(73)	166.3(10)
C(76)-N(10)-C(74)-N(11)	120.8(12)
C(76)-N(10)-C(74)-C(73)	-120.4(12)
O(10)-C(73)-C(74)-N(11)	-167.5(12)
N(12)-C(73)-C(74)-N(11)	13.8(12)
O(10)-C(73)-C(74)-N(10)	66.8(16)
N(12)-C(73)-C(74)-N(10)	-111.9(11)
C(74)-N(11)-C(75)-N(12)	16.5(12)
C(82)-N(11)-C(75)-N(12)	-168.2(9)
C(74)-N(11)-C(75)-C(94)	-100.4(11)
C(82)-N(11)-C(75)-C(94)	74.9(12)
C(73)-N(12)-C(75)-N(11)	-7.0(12)
C(88)-N(12)-C(75)-N(11)	-177.9(8)
C(73)-N(12)-C(75)-C(94)	113.7(10)
C(88)-N(12)-C(75)-C(94)	-57.2(12)
C(74)-N(10)-C(76)-C(81)	-156.9(11)
C(74)-N(10)-C(76)-C(77)	22.2(18)
C(81)-C(76)-C(77)-C(78)	2.8(19)
N(10)-C(76)-C(77)-C(78)	-176.3(12)
C(76)-C(77)-C(78)-C(79)	2(2)
C(77)-C(78)-C(79)-C(80)	-7(2)
C(77)-C(78)-C(79)-Br(10)	175.3(10)
C(78)-C(79)-C(80)-C(81)	6(2)
Br(10)-C(79)-C(80)-C(81)	-175.5(10)
N(10)-C(76)-C(81)-C(80)	176.1(12)
C(77)-C(76)-C(81)-C(80)	-3(2)
C(79)-C(80)-C(81)-C(76)	-2(2)
C(74)-N(11)-C(82)-C(87)	-178.7(10)
C(75)-N(11)-C(82)-C(87)	6.8(15)
C(74)-N(11)-C(82)-C(83)	1.2(16)
C(75)-N(11)-C(82)-C(83)	-173.3(9)
C(87)-C(82)-C(83)-C(84)	1.9(15)
N(11)-C(82)-C(83)-C(84)	-177.9(10)
C(82)-C(83)-C(84)-C(85)	-0.9(17)
C(83)-C(84)-C(85)-C(86)	-1.7(17)
C(83)-C(84)-C(85)-Br(11)	-177.7(9)
C(84)-C(85)-C(86)-C(87)	3.6(17)
Br(11)-C(85)-C(86)-C(87)	179.4(8)
C(83)-C(82)-C(87)-C(86)	-0.2(16)
N(11)-C(82)-C(87)-C(86)	179.6(10)
C(85)-C(86)-C(87)-C(82)	-2.7(17)
C(73)-N(12)-C(88)-C(93)	156.1(12)
C(75)-N(12)-C(88)-C(93)	-35.3(15)
C(73)-N(12)-C(88)-C(89)	-20.5(16)
C(75)-N(12)-C(88)-C(89)	148.1(10)
C(93)-C(88)-C(89)-C(90)	2.5(18)
N(12)-C(88)-C(89)-C(90)	179.3(11)
C(88)-C(89)-C(90)-C(91)	2(2)
C(89)-C(90)-C(91)-C(92)	-5(2)
C(89)-C(90)-C(91)-Br(12)	177.2(9)
C(90)-C(91)-C(92)-C(93)	4(2)
Br(12)-C(91)-C(92)-C(93)	-178.6(9)
C(91)-C(92)-C(93)-C(88)	1(2)
C(89)-C(88)-C(93)-C(92)	-4.0(18)
N(12)-C(88)-C(93)-C(92)	179.5(11)
C(95)-O(12)-C(94)-O(11)	10(2)
C(95)-O(12)-C(94)-C(75)	-176.3(9)
N(11)-C(75)-C(94)-O(11)	56.9(15)
N(12)-C(75)-C(94)-O(11)	-57.9(14)
N(11)-C(75)-C(94)-O(12)	-117.5(11)
N(12)-C(75)-C(94)-O(12)	127.7(10)
C(94)-O(12)-C(95)-C(96)	-111.2(14)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd26131 [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(5)#1	0.86	2.38	3.048(12)	135.4
N(4)-H(4)...O(5)	0.86	2.65	3.268(11)	130.3
N(7)-H(7)...O(8)	0.86	2.69	3.310(11)	130.4
N(1)-H(1)...O(2)	0.86	3.18	3.698(12)	121.3
N(4)-H(4)...O(5)	0.86	2.65	3.268(11)	130.3
N(10)-H(10)...O(11)	0.86	2.68	3.295(13)	129.1
N(7)-H(7)...O(11)#2	0.86	2.56	3.206(12)	132.7

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z #2 x-1,y,z