Metal complexes of pyridine-fused macrocyclic polyamines targeting the HIV coreceptor CXCR4

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Synthesis of 3,6,9,12,18-pentaazabicyclo[12,3,1]octadeca-1(18),2,12,14,16-pentaene diiodomanganese(II) (2)[37]

A mixture of 0.27 g (2 mmol) of pyridine-2,6-dicarboxaldehyde[38] and 0.49 g (2 mmol) of $Mn(OAc)_2 \bullet 4H_2O$, 30 mL of methanol and two drops of glacial acetic acid were was boiled under reflux in for 0.5 h. The reaction mixture was allowed to cool to 45-50 ^oC and a solution of 0.45 g (2 mmol) of triethylenetetramine hydrate in 15 mL of methanol was added. The color of the solution changed to reddish orange, then dark red upon boiling under reflux for 6 h. The solution was concentrated by rotary evaporation to ca. 20 mL and 2.5 mL of 1.6 M aq. KI solution was added dropwise. The solvent was evaporated further to a volume of ca. 5 mL. The resulting dark precipitate was collected by filtration, washed with 1 mL of cold methanol, then dried overnight in air. A solution of the crude product in 10 mL of methanol was allowed to evaporate slowly at room temperature to yield 0.57 g (53%) of rectangular dark red crystals, mp 270 ^oC (d). The structure was determined by X-ray crystallography. IR (neat, cm^{-1}) 3385 (s), 3256 (m), 3207 (m), 2913 (w), 2864 (w), 1649 (m), 1589 (m), 1461 (m), 1423 (w), 1334 (w), 1277 (m), 1180 (w), 1154 (w), 1109 (w), 1096 (m), 1041 (m), 1014 (w), 941 (m), 914 (s), 824 (s), 808 (s), 663 (w), 640 (s).

Synthesis of 1,2-bis(2-(6-(1-((2-aminoethylamino)ethyl)imidazolidin-2-yl)pyridine-2-yl)imidazolidin-1-yl)ethane bis(dichloromanganese(II)) (4)

A mixture of 0.14 g (1 mmol) of pyridine-2,6-dicarboxaldehyde,[38] 0.19 g (1 mmol) of $Mn(OAc)_2 \bullet 4H_2O$, and 20 mL of methanol was stirred for 0.5 h, then a solution of 0.34 g (1 mmol) of triethylenetetraamine hydrate in 25 mL of methanol was added dropwise by means of a syringe pump over 4 h. The reaction mixture was stirred for 6 h at room temperature, then concentrated by rotary evaporation to a brown viscous oil, which was washed twice with ether (15, 5 mL), then with hexane (5 mL). After evaporation and drying (0.1 mm), 0.43 g of a brown solid was obtained,

which was dissolved in 5 mL of ethanol. Ether was diffused into the ethanolic solution by keeping it in a closed container saturated with ether vapor, resulting in an off-white precipitate, which was washed with 5 mL of ether and 5 mL of acetone. The solid was recrystallized from ethanol to give 25 mg (8.1%) of **4** as white solid, mp 189 ^{o}C (d). Crystals for X-ray crystallography were obtained by slow diffusion of ether into a solution of **4** in methanol.

Synthesis of 3,6,9,12,18-pentaaza-16-methylbicyclo[12.3.1]octadeca-1(18),2,12,14,16-pentaene dichloromanganese(II) (5)

A mixture of 0.97 g (6.5 mmol) of 4-methylpyridine-2,6-dicarboxaldehyde,[38] 1.3 g (6.5 mmol) of $MnCl_2 \bullet 4H_2O$, 60 mL of water and 25 mL of ethanol was stirred at 50 °C for 0.5 h. The resulting solution was cooled to room temperature and stirred as a solution of 1.5 g (6.5 mmol) of triethylenetetraamine hydrate in 40 mL of water was added dropwise over 2.5 h. The reaction mixture was stirred for 0.5 h at room temperature, boiled under reflux for 3 h, then allowed to stand at room temperature overnight. The resulting brown mixture was concentrated to dryness by rotary evaporation (bath temp. 60 °C). The residue was dried at (0.1 mm) to give the Schiff base complex as a reddish brown solid. A solution of this solid in 60 mL of ethanol was stirred as 2 g (53 mmol) of $NaBH_4$ was added in one portion. The resulting suspension was stirred at room temperature for 2 h, then at 45-50 °C for 5 h. The solvent was removed by rotary evaporation, the residue was stirred for 10 h with 75 mL of a 0.5 M solution of LiCl in methanol, then the solvent was again removed by rotary evaporation. The residue was extracted with dichloromethane (3 x 15 mL). The combined extracts were dried (Na_2SO_4), filtered, and concentrated to dryness by rotary evaporation. The residue was dried (0.1 mm) to give 2.18 g (86%) of a glassy brown solid. The crude product was purified by column chromatography, eluting with 99:1-95:5 (v/v) dichloromethane/methanol, yielding 370 mg (15%) of **5** as a white solid. MS (ESI^+) *m/z* 353 (M-Cl, 40%), 159 (M-2Cl(2+),

100%). IR (neat, cm^{-1}) 3270 (w), 3219 (w), 2899 (w), 2857 (m), 1616 (m), 1569 (w), 1467 (w), 1336 (w), 1193 (w), 1121 (m), 1013 (m), 867 (s), 797 (s). Anal. Calcd. for $C_{14}H_{25}Cl_2MnN_5$: C, 43.20; H, 6.47; N, 17.99. Found: C, 43.60; H, 6.75; N, 17.83.

Synthesis of 5,6,7,8,9,10,11,12,14,15,16-undecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine dichloromanganese(II) (10)

A solution of 1.1 g (6.4 mmol) of 6,7-dihydro-8(5*H*)-quinolinone-2-carboxaldehyde[39] and 1.3 g (6.5 mmol) of $MnCl_2 \bullet 4H_2O$ in 75 mL of water and 25 mL of ethanol was stirred at 45-50 °C for 1 h. The resulting pale yellow solution was cooled to room temperature and stirred as a solution of 1.5 g (6.6 mmol) of triethylenetetraamine hydrate in 40 mL of water was added dropwise over 2 h. The reaction mixture was stirred at room temperature for 0.5 h then boiled under reflux for 3 h. The resulting dark brown mixture was cooled to room temperature, filtered, and the filtrate was concentrated to dryness by rotary evaporation (bath temp. 60 °C). The residue was dried at (0.1 mm) overnight to give 2.9 g of a reddish brown solid. The crude product was purified by column chromatography, eluting with 1:99 – 5:95 (v/v) methanol/dichloromethane, yielding 0.83 g (32%) of pure **10**. MS (ESI^+) *m/z* 375 (M-Cl, 10%), 170 (M-2Cl(2+), 100%). IR (neat, cm^{-1}) 3282 (w), 3243 (w), 2906 (w), 2856 (w), 1653 (m), 1584 (w), 1470 (w), 1425 (w), 1333 (w), 1266 (w), 1200 (w), 1115 (s), 1060 (w), 1040 (s), 954 (s), 869 (w), 843 (m), 826 (w), 794 (s), 728 (w). Anal. Calcd. for $C_{16}H_{23}Cl_2MnN_5 \bullet 0.5H_2O$: C, 45.73; H, 5.76; N, 16.67. Found: C, 45.98; H, 5.70; N, 16.03.

Synthesis of 3,4,5,6,7,8,9,10,11,12,13,13a,14,15,16-pentadecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine dichloromanganese(II) (11)

A mixture of 1.2 g (7.1 mmol) of 6,7-dihydro-8(5*H*)-quinolinone-2-carboxaldehyde,[39] 1.4 g (7.2 mmol) of $MnCl_2 \bullet 4H_2O$ and 75 mL of water was stirred at 50 °C for 1 h. The resulting pale yellow solution was allowed to cool to room temperature and stirred as a solution of 1.6 g (6.7 mmol) of

triethylenetetraamine hydrate in 30 mL of water was added dropwise over a period of 50 min. The reaction mixture was stirred at room temperature for 0.5 h then boiled under reflux for 3 h. The resulting brown mixture was cooled to room temperature and concentrated to dryness by rotary evaporation (bath temp. 60 °C). The residue was dried at (0.1 mm) overnight to give 3.10 **10** as a reddish brown solid. A solution of this intermediate in 70 mL of ethanol was stirred as 2.2 g (58 mmol) of $NaBH_4$ was added in one portion. The resulting suspension was stirred at room temperature for 2.5 h, then at 50 °C for 12 h. The solvent was removed by rotary evaporation, then the residue was stirred overnight with 100 mL of a 0.5 M solution of LiCl in methanol, then the solvent was removed by rotary evaporation. A mixture of the residue in 70 mL of water and 10 g (0.2 mole) of NaCl was stirred and filtered, then the filtrate was extracted with dichloromethane (5 x 10 mL). The combined extracts were dried over Na_2SO_4. Filtration, rotary evaporation and drying under vacuum gave 1.65 g (59%) of a light brown solid. The crude product was purified by column chromatography, eluting with 9:1 (v/v) dichloromethane/methanol, yielding 1.2 g (43%) of **11** as a white solid, mp 274-281 °C (dec). A sample for microanalysis was washed with ether and dried under vacuum (0.1 mm) for 16 h at room temperature. MS (ESI+) *m/z* 379 (M-Cl, 100%), 172 (M-2Cl(2+), 98%). IR (neat, cm^{-1}) 3276 (w), 3267 (w), 3237 (w), 2900 (w), 2860 (w), 2845 (w), 1599 (w), 1572 (w), 1475 (w), 1453 (m), 1337 (w), 1228 (w), 1126 (w), 1110 (m), 1070 (w), 1029 (w), 995 (w), 956 (w), 868 (m), 824 (m), 806 (s), 793 (s) 731 (w). Anal. calcd. for $C_{16}H_{27}Cl_2MnN_5$: C, 46.28; H, 6.55; N, 16.86. Found: C, 46.66; H, 6.35; N, 16.73.

Synthesis of 3,4,5,6,7,8,9,10,11,12,13,13a,14,15,16-pentadecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine (12)

A solution of 2.3 g (5.6 mmol) of **11** in 70 mL of 2 M HCl in methanol was stirred for 8 h at room temperature. The solution was evaporated to dryness by rotary evaporation (bath temp. 30-35 °C,

50-100 mm). A mixture the residue and 71 mL of 2 M NaOH in methanol was stirred for 10 h. The mixture was filtered and the filtrate was concentrated to dryness by rotary evaporation. The residual solid was extracted with ether (3 x 25 mL). The combined extracts were dried over Na_2SO_4. Filtration, rotary evaporation and drying under vacuum gave 1.2 g (73%) of **12** as light yellow solid, mp 85-86 ^oC. ^1H NMR ($CDCl_3$, 500 MHz) δ 7.30 (d, J = 8 Hz, 1 H, H18), 6.93 (d, J = 8 Hz, 1 H, H19), 3.86 (m, 2 H, H3), 3.74 (m, 1 H, H13a), 3.03 (m, 1 H, H16), 2.92 (m, 1 H, H16') 2.89-2.68 (m, 12 H, H5,6,8,9,11,12), 2.20 (m, 1 H, H14), 1.99 (m, 1 H, H15), 1.65-1.81 (m, 2 H, H14,15). ^{13}C NMR ($CDCl_3$, 125 MHz) δ 156.7, 155.9, 137.1, 130.2, 120.2, 57.9, 53.3, 49.1, 48.9, 48.52, 48.46, 48.2, 46.6, 29.3, 28.6, 20.2. MS (ESI^+) *m/z* 290 (M+1, 100%). IR (neat, cm^{-1}) 3291 (w), 3264 (w), 3208 (w), 2928 (w), 2879 (w), 2804 (m), 1587 (w), 1569 (w), 1460 (s), 1403 (w), 1326 (w), 1291 (w), 1234 (w), 1129 (m), 1101 (w), 922 (w), 828 (w), 812 (w), 788 (w), 735 (w). Anal. calcd. for $C_{16}H_{27}N_5$: C, 66.40; H, 9.40; N, 24.20. Found: C, 66.13; H, 9.14; N, 24.48.

Synthesis of 3,4,5,6,7,8,9,10,11,12,13,13a,14,15,16-pentadecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine dichlorocopper(II) (13)

To a solution of 47 mg (0.16 mmol) of **12** in 1 mL of absolute ethanol, a solution of 21 mg (0.16 mmol) of $CuCl_2$ in 1 mL of absolute ethanol was added dropwise. The mixture was swirled for 0.5 h at 45-50 ^oC to obtain a deep blue solution, which was concentrated to dryness by rotary evaporation. The residue was dried (0.1 mm) to give 70 mg of a blue solid, which was washed with 5 mL of anhydrous ether. A solution of the residue in 10 mL of dichloromethane was dried (Na_2SO_4), filtered, and concentrated to dryness by rotary evaporation. Drying (0.1 mm) gave 60 mg (91%) of **13** as a blue solid. MS (ESI^+) *m/z* 387 (M-Cl, 20%); 351 (M-H-2Cl, 100%), 176 (M-2Cl(2+), 67%). IR (neat, cm^{-1}) 3363 (br, m), 3091 (br, m), 2915 (m), 2870 (m), 1605 (w), 1578 (w), 1485 (s), 1425 (s), 1342 (m), 1096 (m), 1037 (w), 1013 (w), 968 (s), 947 (m), 881 (w), 848 (m), 809

(m), 791 (w), 773 (w). Anal. calcd. for $C_{16}H_{27}Cl_2CuN_5$: C, 45.34; H, 6.42; N, 16.52. Found: C, 45.53; H, 6.80; N, 16.31.

Synthesis of 3,4,5,6,7,8,9,10,11,12,13,13a,14,15,16-pentadecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine trichloroiron(III) (14)

To a solution of 46 mg (0.15 mmol) of **12** in 1 mL of absolute ethanol, a solution of 24 mg (0.15 mmol) of $FeCl_3$ in 1 mL of absolute ethanol was added dropwise. The resulting mixture was swirled for 0.5 h at 45-50 ^oC, then the solvent was removed by rotary evaporation and the residue was dried (0.1 mm, 8 h). The resulting blue solid was washed with 5 mL of anhydrous ether. A solution of this solid in 10 mL of dichloromethane was dried (Na_2SO_4), filtered, and concentrated to dryness by rotary evaporation. Drying (0.1 mm) gave 60 mg (88%) of **14** as a green solid. MS (ESI^+) *m/z* 379 (M-H-2Cl, 85%), 343 (M-2H-3Cl, 100%). IR (neat, cm^{-1}) 3115 (w), 2912 (w), 2867 (w), 1653 (w), 1602 (w), 1581 (w), 1485 (m), 1449 (s), 1369 (w), 1333 (w), 1288 (w), 1231 (w), 1108 (s), 1055 (m), 1034 (w), 980 (s), 956 (s), 917 (s), 893 (m), 860 (m), 836 (m), 791 (w), 732 (w). Anal. calcd. for $C_{16}H_{27}Cl_3FeN_5$: C, 42.55; H, 6.03; N, 15.51. Found: C, 42.60; H, 6.49; N, 15.39.

Synthesis of 3,4,5,6,7,8,9,10,11,12,13,13a,14,15,16-pentadecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine dichlorozinc(II) (15)

To a solution of 31 mg (0.11 mmol) of **12** in 1 mL of absolute ethanol, a solution of 15 mg (0.11 mmol) of $ZnCl_2$ in 1 mL of absolute ethanol was added dropwise. The resulting mixture was swirled for 0.5 h at 45-50 ^oC, then the solvent was removed by rotary evaporation and residue was dried (0.1 mm) to give a white solid, which was washed with 5 mL of anhydrous ether. A solution of this solid in 10 mL of dichloromethane was dried (Na_2SO_4), filtered, and concentrated to dryness by rotary evaporation. The residue was dried (0.1 mm) to give 42 mg (91%) of **15** as a white solid, mp 132-210 ^oC (dec.). MS (ESI^+) *m/z* 388 (M-Cl, 50%), 352 (M-H-2Cl, 10%), 176.5 (M-2Cl(2+),

100%). IR (neat, cm^{-1}) 3402 (br, w), 3184 (m), 2921 (w), 2867 (w), 1602 (w), 1581 (w), 1449 (s), 1342 (w), 1096 (s), 938 (s), 866 (w), 782 (w), 723 (w). Anal. calcd. for $C_{16}H_{27}Cl_2N_5Zn \bullet 1.5H_2O$: C, 42.44; H, 6.68; N, 15.47. Found: C, 42.50; H, 6.60; N, 15.27.

Synthesis of 2,3,4,6,7,8,9,10,11,12,13,15,16,17-tetradecahydro-1,18-methenodibenzo[b,e]-[1.4.7.10.13]pentaazacyclopentadecine dichloromanganese(II) (16)

A mixture of 1.2 g (5.3 mmol) of 2,3,7,8-tetrahydroacridine-4,5(1*H*,6*H*)-dione,[40] 1.1 g (5.4 mmol) of $MnCl_2 \bullet 4H_2O$, 100 mL of ethanol and 5 mL of water was stirred at 50-55 °C for 0.5 h. The resulting cloudy reddish brown solution was allowed to cool to room temperature and stirred as a solution of 1.15 g (5.0 mmol) of triethylenetetraamine hydrate in 15 mL of ethanol was added dropwise over a period of 2 h by means of a syringe pump. The reaction mixture was stirred at room temperature for 0.5 h and then boiled under reflux for 6 h. The resulting black mixture was cooled to room temperature, filtered and the filtrate was concentrated to dryness by rotary evaporation (bath temp. 60 °C). The residue was dried (0.1 mm) to give crude **16** as a black solid, MS (ESI^+) *m/z* 415 (M-Cl, <10%), 379 (M-H-2Cl, <5%), 190 (M-2Cl(2+), 100%). The product was purified by column chromatography, eluting with 99:1-95:5 (v/v) dichloromethane/methanol, yielding 0.44 g (20%) of **16** as a dark reddish brown solid. IR (neat, cm^{-1}) 3270 (w), 2926 (w), 2900 (w), 2861 (w), 1652 (s), 1566 (w), 1457 (m), 1437 (w), 1348 (w), 1324 (w), 1262 (w), 1227 (s), 1172 (w), 1112 (m), 1074 (w), 1035 (m), 940 (w), 906 (w), 858 (m), 799 (s), 749 (s). Anal. Calcd. for $C_{19}H_{27}Cl_2MnN_5$: C, 50.57; H, 6.03; N, 15.52. Found: C, 50.43; H, 6.40; N, 15.13.

Synthesis of 2,3,4,4a,5,6,7,8,9,10,11,12,13,14,14a,15,16,17-octadecahydro-1,18-methenodibenzo[b,e][1.4.7.10.13]pentaazacyclopentadecine dichloromangan-ese(II) (17)

A mixture of 0.43 g (2.0 mmol) of 2,3,7,8-tetrahydroacridine-4,5(1*H*,6*H*)-dione,[40] 0.41 g (2.1 mmol) of $MnCl_2 \bullet 4H_2O$, 30 mL of ethanol, and 10 mL of water was stirred at 50 °C for 10 min. The resulting cloudy brown solution was allowed to cool to room temperature and stirred as a solution of 0.45 g (2.0 mmol) of triethylenetetraamine hydrate in 5 mL of water was added dropwise over a period of 30 min. The reaction mixture was stirred at room temperature for 0.5 h then boiled under reflux for 5 h. The resulting black mixture was cooled to room temperature and concentrated to dryness by rotary evaporation (bath temp. 60 °C). The residue was dried at (0.1 mm) to give 1 **16** as a black solid. A solution of this intermediate in 25 mL of absolute ethanol was stirred as 0.62 g (16 mmol) of $NaBH_4$ was added in one portion. The resulting suspension was stirred at room temperature for 3 h, then at 40-45 °C for 12 h. An additional 0.30 g (7.9 mmol) portion of $NaBH_4$ was added, then the reaction mixture was stirred for 3 h at 55 °C. The solvent was removed by rotary evaporation, the residue was stirred for 8 h with 20 mL of a 0.5 M solution of LiCl in methanol, then the solvent was removed by rotary evaporation. The residue was powdered and extracted with 20 mL of dichloromethane. After filtration, the residue was further extracted with dichloromethane (2 x 3 mL). The combined dichloromethane extracts were dried over Na_2SO_4, filtered, and concentrated to dryness by rotary evaporation. Drying (0.1 mm) gave 0.65 g (73%) of a yellowish brown solid. The crude product was purified by column chromatography, eluting with 19:1 (v/v) dichloromethane/methanol, yielding 0.26 g (29%) of **17** as a white solid, mp 295-298 °C (dec). A sample for microanalysis and X-ray diffraction was crystallized by diffusing ether into a dichloromethane solution. MS (ESI^+) *m/z* 419 (M-Cl, 100%), 192 (M-2Cl(2+), 55%). IR (neat, cm^-

^{1}) 3234 (w), 2932 (w), 2915 (w), 2854 (w), 1575 (w), 1459 (m), 1452 (m), 1345 (w), 1279 (w), 1249 (w), 1195 (w), 1119 (s), 1081 (w), 1037 (w), 953 (m), 890 (s), 823 (s), 811 (s), 785 (s), 756 (m), 732 (w). Anal. calcd. for $C_{19}H_{31}Cl_2MnN_5$: C, 50.12; H, 6.86; N, 15.38. Found: C, 50.10; H, 6.57; N, 15.24.

Synthesis of 2,3,4,4a,5,6,7,8,9,10,11,12,13,14,14a,15,16,17-octadecahydro-1,18-methenodibenzo[b,e][1.4.7.10.13]pentaazacyclopentadecine (18)

A solution of 0.51 g (1.2 mmol) of **17** in 14.5 mL of 2 M HCl in methanol was stirred for 10 h at room temperature. The solution was evaporated to dryness by rotary evaporation (bath temp. 30-35 °C; 50-100 mm). A solution of 2 M NaOH in methanol (15 mL) was added to the residue and the resulting mixture was stirred for 2.5 h. The mixture was filtered and the filtrate was concentrated to dryness by rotary evaporation. The residue was dried (0.1 mm) for 12 h at room temperature then extracted with ether (4 x 15 mL). The combined extracts were dried over Na_2SO_4, filtered, and concentrated to dryness by rotary evaporation. The residue was dried (0.1 mm) to give 0.27 g (74%) of **18** as a yellowish white solid, mp 155-156 ^{o}C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.04 (s, 1 H, H19), 3.71 (br, 2 H, NH), 3.64 (m, 2 H, H4a,14a), 3.07 (m, 2 H, H9,10), 2.99 (m, 2 H, H6,13), 2.87 (m, 2 H, H7,12), 2.72 (m, 10 H, 2,6',7',9',10',12',13',17), 2.22 (m, 2 H, H4,15), 1.96 (m, 2 H, H3,16), 1.74 (m, 2 H, H3',16'), 1.60 (m, 2 H, H4',15'). ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.0, 137.1, 129.8, 57.7, 49.0, 48.0, 47.0, 29.5, 28.4, 20.6. MS (ESI^+) *m/z* 352 (M+Na, 10%) , 330 (M+H, 100%). IR (neat, cm^{-1}) 3318 (w), 3285 (w), 3202 (w), 2924 (w), 2881 (w), 2808 (m), 1566 (w), 1448 (s), 1420 (m), 1336 (w), 1243 (w), 1139 (m), 1118 (s), 1094 (w), 1049 (w), 926 (m), 866 (w), 848 (w), 783 (m), 730 (m). Anal. calcd. for $C_{19}H_{31}N_5 \bullet 0.25H_2O$: C, 68.33; H, 9.51; N, 20.97. Found: C, 68.25; H, 9.87; N, 20.99.

Synthesis of 2,3,4,4a,5,6,7,8,9,10,11,12,13,14,14a,15,16,17-octadecahydro-1,18-methenodibenzo[b,e][1.4.7.10.13]pentaazacyclopentadecine dichlorocopper(II) (19)

To a solution of 21 mg (0.06 mmol) **8** in 1 mL of absolute ethanol, a solution of 8.4 mg (0.06 mmol) of $CuCl_2$ in 7 mL of absolute ethanol was added dropwise. The mixture was sonicated for 0.5 h to obtain a deep blue solution, which was concentrated to dryness by rotary evaporation. The residue was washed with 2 mL of ether then dissolved in 5 mL of dichloromethane. Filtration, rotary evaporation and drying (0.1 mm) gave 28 mg (97%) of **19** as a blue solid. MS (ESI^+) *m/z* 427 (M-Cl, 20%), 391 (M-H-2Cl, 88%), 196 (M-2Cl(2+), 100%). IR (neat) 3408 (br, w), 3175 (w), 3091 (w), 2909 (m), 2846 (w), 1593 (w), 1479 (m), 1446 (w), 1410 (w), 1339 (w), 1282 (w), 1228 (w), 1084 (s), 1001 (m), 914 (w), 857 (w), 785 (w), 723 (w). Anal. calcd. for $C_{19}H_{31}Cl_2CuN_5 \bullet CH_2Cl_2$: C, 43.77; H, 6.06; N, 12.76. Found: C, 43.18; H, 6.25; N, 13.20.

Synthesis of 2,3,4,4a,5,6,7,8,9,10,11,12,13,14,14a,15,16,17-octadecahydro-1,18-methenodibenzo[b,e][1.4.7.10.13]pentaazacyclopentadecine trichloroiron(III) (20)

To a solution of 27 mg (0.08 mmol) **18** in 1 mL of absolute ethanol, a solution of 13 mg (0.08 mmol) of $FeCl_3$ in 4 mL of absolute ethanol was added dropwise. The mixture was sonicated for 0.5 h to obtain a deep blue solution, which was concentrated to dryness by rotary evaporation. The residue was washed with 2 mL of ether then dissolved in 5 mL of dichloromethane. Filtration, rotary evaporation and drying (0.1 mm) gave 42 mg (100%) of **20** as a light green solid. MS (ESI^+) *m/z* 455 (M-Cl, 80%), 419 (M-H-2Cl, 100%), 383 (M-2H-3Cl, 12%). IR (neat, cm^{-1}) 3357 (br, w), 3217 (br, w), 2929 (w), 2864 (w), 1632 (w), 1584 (w), 1449 (s), 1369 (w), 1336 (w), 1282 (w), 1254 (w), 1207 (w), 1111 (s), 1052 (w), 974 (m), 944 (m), 914 (m) 860 (m), 833 (w), 762 (w), 723 (w). Anal. calcd. for $C_{19}H_{31}Cl_3FeN_5 \bullet H_2O$: C, 44.77; H, 6.53; N, 13.74. Found: C, 44.91; H, 6.67; N, 13.74.

Synthesis of 2,3,4,4a,5,6,7,8,9,10,11,12,13,14,14a,15,16,17-octadecahydro-1,18-methenodibenzo[b,e][1.4.7.10.13]pentaazacyclopentadecine dichlorozinc(II) (21)

To a solution of 33 mg (0.10 mmol) of **18** in 1 mL of absolute ethanol, a solution of 14 mg (0.10 mmol) of $ZnCl_2$ in 3 mL of absolute ethanol was added dropwise. The mixture was sonicated for 0.5 h to obtain a deep blue solution, which was concentrated to dryness by rotary evaporation. The residue was washed with 2 mL of ether then dissolved in 5 mL of dichloromethane. Filtration, rotary evaporation and drying (0.1 mm) gave 46 mg (99%) of **21** as a solid. MS (ESI^+) *m/z* 428 (M-Cl, 100%), 392 (M-H-2Cl, 22%), 196.5 (M-2Cl(2+), 98%). IR (neat, cm^{-1}) 3196 (br, w), 2924 (m), 2861 (w), 1638 (w), 1578 (w), 1455 (s), 1342 (w), 1249 (w), 1192 (w), 1096 (m), 1001 (w), 959 (m), 929 (m), 723 (w). Anal. calcd. for $C_{19}H_{31}Cl_2ZnN_5 \bullet H_2O$: C, 47.17; H, 6.87; N, 14.48. Found: C, 46.77; H, 7.04; N, 14.58

Table 1. Crystallographic data for **2**, **4**, and **17**.

	2 (BJF175)	**4 (BJF224)**	**17 (BJF440)**
Emp. formula	$C_{13}H_{23}I_2MnN_5O_2$	$C_{64}H_{112}Cl_8Mn_4N_{28}O_3$	$C_{39}H_{63}Cl_7Mn_2N_{10}O$
formula weight	590.10	1825.18	1046.02
T (K)	100(2)	100(2)	100(2)
wavelength (Å)	0.71073	0.71073	0.71073
crystal system	Monoclinic	Monoclinic	Monoclinic
space group	P2(1)/c	p2(1)/n	C2/c
a (Å)	7.27960(10)	14.5669(9)	33.9815(7)
b (Å)	27.9338(6)	18.4411(10)	12.1081(3)
c (Å)	10.3113(2)	15.6178(7)	25.8046(5)
α (deg)	90	90	90
β (deg)	106.8240(10)	90.728(2)	117.0730(10)
γ (deg)	90	90	90
volume (Å^3)	2007.03(6)	4195.1(4)	9454.0(4)
Z	4	2	8
D_{calcd} (Mg/m^3)	1.953	1.445	1.470
abs coeff (mm^{-1})	3.748	0.904	0.973
cryst size (mm^3)	0.28 x 0.16 x 0.09	0.31 x 0.13 x 0.07	0.31 x 0.30 x 0.12
θ range (deg)	1.46 to 32.50	1.71 to 25.50	1.35 to 29.94
index ranges	$-10 \le h \le 10$ $-42 \le k \le 41$ $-15 \le l \le 13$	$-16 \le h \le 17$ $-22 \le k \le 17$ $-18 \le l \le 10$	$-47 \le h \le 47$ $-16 \le k \le 17$ $-36 \le l \le 34$
reflns collected	33211	20351	62351
indep reflns	7122 $R_{int} = 0.1177$	7788 $R_{int} = 0.0803$	13557 $R_{int} = 0.0277$
abs corr.	SADABS	SADABS	SADABS
data/restr/para	7122 / 0 / 230	7788 / 0 / 482	13557 / 0 / 565
GOF on F^2	1.118	0.975	1.062
final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.0497$, $wR_2 = 0.1199$	$R_1 = 0.0597$ $wR_2 = 0.1166$	$R_1 = 0.0313$ $wR_2 = 0.0804$
R indices (all data)	$R_1 = 0.0566$, $wR_2 = 0.1233$	$R_1 = 0.1170$ $wR_2 = 0.1351$	$R_1 = 0.0385$ $wR_2 = 0.0843$
CCDC	1062374	1062375	1062376

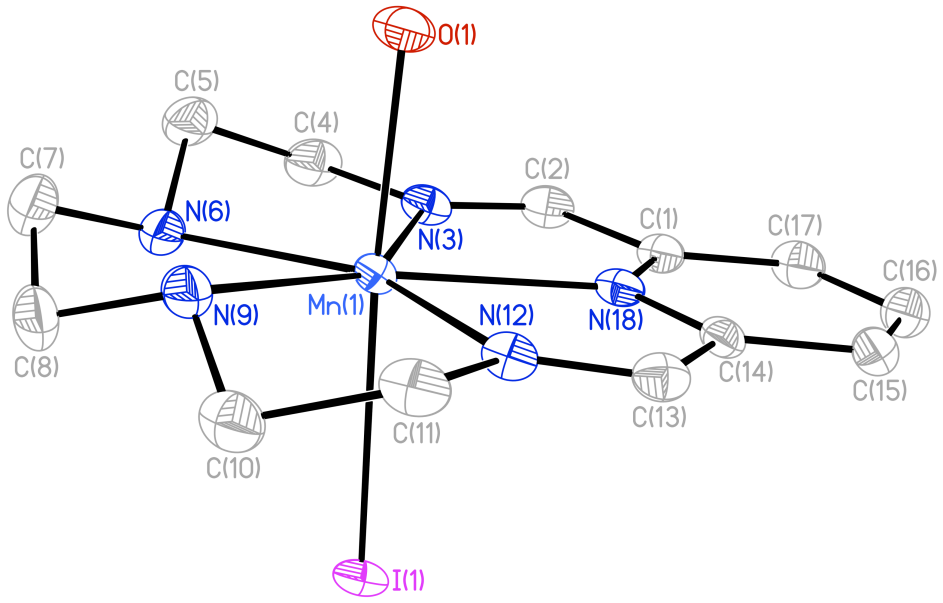


Figure 1. Numbered thermal ellipsoid plot for **2.**

Table 2. Crystal data and structure refinement for **2**.

Identification code	SH11	
Empirical formula	$C_{13}H_{23}I_2MnN_5O_2$	
Formula weight	590.10	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 7.27960(10) Å	α= 90°.
	b = 27.9338(6) Å	β= 106.8240(10)°.
	c = 10.3113(2) Å	γ = 90°.
Volume	2007.03(6) $Å^3$	
Z	4	
Density (calculated)	1.953 Mg/m^3	
Absorption coefficient	3.748 mm^{-1}	
F(000)	1132	
Crystal size	0.28 x 0.16 x 0.09 mm^3	
Theta range for data collection	1.46 to 32.50°.	
Index ranges	-10<=h<=10, -42<=k<=41, -15<=l<=13	
Reflections collected	33211	
Independent reflections	7122 [R(int) = 0.1177]	
Completeness to theta = 32.50°	98.2 %	
Absorption correction	SADABS	
Max. and min. transmission	0.7387 and 0.4244	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7122 / 0 / 230	
Goodness-of-fit on F^2	1.118	
Final R indices [I>2sigma(I)]	R1 = 0.0497, wR2 = 0.1199	
R indices (all data)	R1 = 0.0566, wR2 = 0.1233	
Extinction coefficient	0.00013(19)	
Largest diff. peak and hole	5.535 and -2.566 e.$Å^{-3}$	

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

	x	y	z	U(eq)
Mn(1)	8800(1)	1071(1)	2221(1)	16(1)
I(1)	12741(1)	684(1)	3091(1)	20(1)
I(2)	4287(1)	1856(1)	6569(1)	25(1)
N(3)	8276(5)	809(1)	4198(4)	20(1)
N(6)	9758(6)	1668(1)	3782(5)	25(1)
N(9)	9389(6)	1703(1)	940(5)	25(1)
N(12)	8479(5)	791(1)	73(3)	17(1)
N(18)	7786(5)	302(1)	2018(4)	17(1)
O(1)	5761(5)	1310(1)	1580(4)	26(1)
O(2)	5197(8)	2093(2)	31(4)	39(1)
C(1)	7433(6)	76(1)	3061(4)	18(1)
C(2)	7706(6)	383(2)	4281(4)	21(1)
C(4)	8592(7)	1157(2)	5294(5)	28(1)
C(5)	8542(7)	1660(2)	4697(5)	29(1)
C(7)	9790(8)	2128(2)	3075(6)	33(1)
C(8)	10620(8)	2048(2)	1896(6)	33(1)
C(10)	10164(7)	1522(2)	-130(5)	26(1)
C(11)	8853(6)	1127(2)	-896(5)	24(1)
C(13)	7986(6)	361(2)	-229(4)	19(1)
C(14)	7587(5)	67(1)	860(4)	17(1)
C(15)	7012(6)	-412(2)	687(5)	24(1)
C(16)	6658(7)	-646(2)	1773(5)	26(1)
C(17)	6863(6)	-404(2)	2982(5)	24(1)

Table 4. Bond lengths [Å] and angles [°] for **2**.

Mn(1)-O(1)	2.221(3)	C(1)-C(17)	1.397(6)
Mn(1)-N(18)	2.261(3)	C(1)-C(2)	1.487(6)
Mn(1)-N(6)	2.284(4)	C(2)-H(2A)	0.9500
Mn(1)-N(12)	2.295(4)	C(4)-C(5)	1.529(7)
Mn(1)-N(3)	2.299(4)	C(4)-H(4A)	0.9900
Mn(1)-N(9)	2.320(4)	C(4)-H(4B)	0.9900
Mn(1)-I(1)	2.9521(6)	C(5)-H(5A)	0.9900
N(3)-C(2)	1.272(6)	C(5)-H(5B)	0.9900
N(3)-C(4)	1.458(6)	C(7)-C(8)	1.522(8)
N(6)-C(5)	1.469(7)	C(7)-H(7A)	0.9900
N(6)-C(7)	1.481(7)	C(7)-H(7B)	0.9900
N(6)-H(6)	0.85(7)	C(8)-H(8A)	0.9900
N(9)-C(10)	1.467(7)	C(8)-H(8)	0.9900
N(9)-C(8)	1.481(6)	C(10)-C(11)	1.522(7)
N(9)-H(3N)	0.77(6)	C(10)-H(10A)	0.9900
N(12)-C(13)	1.267(5)	C(10)-H(10B)	0.9900
N(12)-C(11)	1.452(5)	C(11)-H(11A)	0.9900
N(18)-C(14)	1.332(5)	C(11)-H(11B)	0.9900
N(18)-C(1)	1.335(5)	C(13)-C(14)	1.487(6)
O(1)-H(1W)	0.8400	C(13)-H(13A)	0.9500
O(1)-H(2W)	0.89(6)	C(14)-C(15)	1.400(5)
O(2)-H(3W)	0.75(7)	C(15)-C(16)	1.383(7)
O(2)-H(4W)	0.80(10)	C(15)-H(15A)	0.9500

C(16)-C(17)	1.388(7)	N(3)-C(2)-H(2A)	121.7
C(16)-H(16A)	0.9500	C(1)-C(2)-H(2A)	121.7
C(17)-H(17A)	0.9500	N(3)-C(4)-C(5)	108.6(4)
		N(3)-C(4)-H(4A)	110.0
O(1)-Mn(1)-N(18)	89.34(12)	C(5)-C(4)-H(4A)	110.0
O(1)-Mn(1)-N(6)	93.67(14)	N(3)-C(4)-H(4B)	110.0
N(18)-Mn(1)-N(6)	141.68(15)	C(5)-C(4)-H(4B)	110.0
O(1)-Mn(1)-N(12)	90.07(13)	H(4A)-C(4)-H(4B)	108.3
N(18)-Mn(1)-N(12)	69.43(12)	N(6)-C(5)-C(4)	109.0(4)
N(6)-Mn(1)-N(12)	148.60(14)	N(6)-C(5)-H(5A)	109.9
O(1)-Mn(1)-N(3)	87.29(13)	C(4)-C(5)-H(5A)	109.9
N(18)-Mn(1)-N(3)	69.31(13)	N(6)-C(5)-H(5B)	109.9
N(6)-Mn(1)-N(3)	72.69(15)	C(4)-C(5)-H(5B)	109.9
N(12)-Mn(1)-N(3)	138.67(13)	H(5A)-C(5)-H(5B)	108.3
O(1)-Mn(1)-N(9)	86.20(13)	N(6)-C(7)-C(8)	109.4(4)
N(18)-Mn(1)-N(9)	141.32(14)	N(6)-C(7)-H(7A)	109.8
N(6)-Mn(1)-N(9)	76.98(16)	C(8)-C(7)-H(7A)	109.8
N(12)-Mn(1)-N(9)	72.17(14)	N(6)-C(7)-H(7B)	109.8
N(3)-Mn(1)-N(9)	148.47(15)	C(8)-C(7)-H(7B)	109.8
O(1)-Mn(1)-I(1)	175.99(9)	H(7A)-C(7)-H(7B)	108.2
N(18)-Mn(1)-I(1)	86.73(9)	N(9)-C(8)-C(7)	108.9(4)
N(6)-Mn(1)-I(1)	88.94(10)	N(9)-C(8)-H(8A)	109.9
N(12)-Mn(1)-I(1)	89.28(9)	C(7)-C(8)-H(8A)	109.9
N(3)-Mn(1)-I(1)	90.58(9)	N(9)-C(8)-H(8)	109.9
N(9)-Mn(1)-I(1)	97.37(10)	C(7)-C(8)-H(8)	109.9
C(2)-N(3)-C(4)	123.6(4)	H(8A)-C(8)-H(8)	108.3
C(2)-N(3)-Mn(1)	119.9(3)	N(9)-C(10)-C(11)	108.7(4)
C(4)-N(3)-Mn(1)	116.5(3)	N(9)-C(10)-H(10A)	109.9
C(5)-N(6)-C(7)	115.4(4)	C(11)-C(10)-H(10A)	109.9
C(5)-N(6)-Mn(1)	108.8(3)	N(9)-C(10)-H(10B)	109.9
C(7)-N(6)-Mn(1)	109.4(3)	C(11)-C(10)-H(10B)	109.9
C(5)-N(6)-H(6)	107(5)	H(10A)-C(10)-H(10B)	108.3
C(7)-N(6)-H(6)	113(5)	N(12)-C(11)-C(10)	109.0(4)
Mn(1)-N(6)-H(6)	103(5)	N(12)-C(11)-H(11A)	109.9
C(10)-N(9)-C(8)	115.8(4)	C(10)-C(11)-H(11A)	109.9
C(10)-N(9)-Mn(1)	109.9(3)	N(12)-C(11)-H(11B)	109.9
C(8)-N(9)-Mn(1)	107.0(3)	C(10)-C(11)-H(11B)	109.9
C(10)-N(9)-H(3N)	119(4)	H(11A)-C(11)-H(11B)	108.3
C(8)-N(9)-H(3N)	100(4)	N(12)-C(13)-C(14)	116.2(4)
Mn(1)-N(9)-H(3N)	104(4)	N(12)-C(13)-H(13A)	121.9
C(13)-N(12)-C(11)	122.6(4)	C(14)-C(13)-H(13A)	121.9
C(13)-N(12)-Mn(1)	120.2(3)	N(18)-C(14)-C(15)	122.4(4)
C(11)-N(12)-Mn(1)	117.2(3)	N(18)-C(14)-C(13)	114.3(3)
C(14)-N(18)-C(1)	119.5(4)	C(15)-C(14)-C(13)	123.3(4)
C(14)-N(18)-Mn(1)	119.8(3)	C(16)-C(15)-C(14)	117.8(4)
C(1)-N(18)-Mn(1)	120.6(3)	C(16)-C(15)-H(15A)	121.1
Mn(1)-O(1)-H(1W)	109.5	C(14)-C(15)-H(15A)	121.1
Mn(1)-O(1)-H(2W)	121(4)	C(15)-C(16)-C(17)	120.0(4)
H(1W)-O(1)-H(2W)	114.7	C(15)-C(16)-H(16A)	120.0
H(3W)-O(2)-H(4W)	83(7)	C(17)-C(16)-H(16A)	120.0
N(18)-C(1)-C(17)	122.0(4)	C(16)-C(17)-C(1)	118.2(4)
N(18)-C(1)-C(2)	113.5(4)	C(16)-C(17)-H(17A)	120.9
C(17)-C(1)-C(2)	124.5(4)	C(1)-C(17)-H(17A)	120.9
N(3)-C(2)-C(1)	116.7(4)		

Table 5. Torsion angles [°] for **2**.

O(1)-Mn(1)-N(3)-C(2)	90.6(3)	N(6)-Mn(1)-N(18)-C(14)	-171.8(3)
N(18)-Mn(1)-N(3)-C(2)	0.3(3)	N(12)-Mn(1)-N(18)-C(14)	2.8(3)
N(6)-Mn(1)-N(3)-C(2)	-174.7(4)	N(3)-Mn(1)-N(18)-C(14)	-179.6(3)
N(12)-Mn(1)-N(3)-C(2)	3.6(4)	N(9)-Mn(1)-N(18)-C(14)	10.0(4)
N(9)-Mn(1)-N(3)-C(2)	168.8(3)	I(1)-Mn(1)-N(18)-C(14)	-87.7(3)
I(1)-Mn(1)-N(3)-C(2)	-86.0(3)	O(1)-Mn(1)-N(18)-C(1)	-88.7(3)
O(1)-Mn(1)-N(3)-C(4)	-88.1(3)	N(6)-Mn(1)-N(18)-C(1)	6.4(4)
N(18)-Mn(1)-N(3)-C(4)	-178.5(3)	N(12)-Mn(1)-N(18)-C(1)	-179.0(3)
N(6)-Mn(1)-N(3)-C(4)	6.6(3)	N(3)-Mn(1)-N(18)-C(1)	-1.3(3)
N(12)-Mn(1)-N(3)-C(4)	-175.2(3)	N(9)-Mn(1)-N(18)-C(1)	-171.8(3)
N(9)-Mn(1)-N(3)-C(4)	-9.9(4)	I(1)-Mn(1)-N(18)-C(1)	90.5(3)
I(1)-Mn(1)-N(3)-C(4)	95.3(3)	C(14)-N(18)-C(1)-C(17)	0.2(6)
O(1)-Mn(1)-N(6)-C(5)	53.8(3)	Mn(1)-N(18)-C(1)-C(17)	-178.0(3)
N(18)-Mn(1)-N(6)-C(5)	-39.8(4)	C(14)-N(18)-C(1)-C(2)	-179.7(3)
N(12)-Mn(1)-N(6)-C(5)	149.9(3)	Mn(1)-N(18)-C(1)-C(2)	2.1(4)
N(3)-Mn(1)-N(6)-C(5)	-32.2(3)	C(4)-N(3)-C(2)-C(1)	179.3(4)
N(9)-Mn(1)-N(6)-C(5)	139.0(3)	Mn(1)-N(3)-C(2)-C(1)	0.6(5)
I(1)-Mn(1)-N(6)-C(5)	-123.2(3)	N(18)-C(1)-C(2)-N(3)	-1.7(5)
O(1)-Mn(1)-N(6)-C(7)	-73.2(3)	C(17)-C(1)-C(2)-N(3)	178.3(4)
N(18)-Mn(1)-N(6)-C(7)	-166.7(3)	C(2)-N(3)-C(4)-C(5)	-159.5(4)
N(12)-Mn(1)-N(6)-C(7)	23.0(5)	Mn(1)-N(3)-C(4)-C(5)	19.2(5)
N(3)-Mn(1)-N(6)-C(7)	-159.2(3)	C(7)-N(6)-C(5)-C(4)	177.5(4)
N(9)-Mn(1)-N(6)-C(7)	12.1(3)	Mn(1)-N(6)-C(5)-C(4)	54.1(4)
I(1)-Mn(1)-N(6)-C(7)	109.9(3)	N(3)-C(4)-C(5)-N(6)	-47.8(5)
O(1)-Mn(1)-N(9)-C(10)	-120.0(3)	C(5)-N(6)-C(7)-C(8)	-164.3(4)
N(18)-Mn(1)-N(9)-C(10)	-35.8(4)	Mn(1)-N(6)-C(7)-C(8)	-41.2(5)
N(6)-Mn(1)-N(9)-C(10)	145.3(3)	C(10)-N(9)-C(8)-C(7)	-169.7(4)
N(12)-Mn(1)-N(9)-C(10)	-28.7(3)	Mn(1)-N(9)-C(8)-C(7)	-46.8(4)
N(3)-Mn(1)-N(9)-C(10)	161.5(3)	N(6)-C(7)-C(8)-N(9)	60.7(5)
I(1)-Mn(1)-N(9)-C(10)	58.1(3)	C(8)-N(9)-C(10)-C(11)	172.6(4)
O(1)-Mn(1)-N(9)-C(8)	113.5(3)	Mn(1)-N(9)-C(10)-C(11)	51.2(4)
N(18)-Mn(1)-N(9)-C(8)	-162.3(3)	C(13)-N(12)-C(11)-C(10)	-156.6(4)
N(6)-Mn(1)-N(9)-C(8)	18.8(3)	Mn(1)-N(12)-C(11)-C(10)	23.8(4)
N(12)-Mn(1)-N(9)-C(8)	-155.2(3)	N(9)-C(10)-C(11)-N(12)	-48.9(5)
N(3)-Mn(1)-N(9)-C(8)	35.0(4)	C(11)-N(12)-C(13)-C(14)	-177.9(3)
I(1)-Mn(1)-N(9)-C(8)	-68.4(3)	Mn(1)-N(12)-C(13)-C(14)	1.8(5)
O(1)-Mn(1)-N(12)-C(13)	-91.6(3)	C(1)-N(18)-C(14)-C(15)	0.1(6)
N(18)-Mn(1)-N(12)-C(13)	-2.4(3)	Mn(1)-N(18)-C(14)-C(15)	178.4(3)
N(6)-Mn(1)-N(12)-C(13)	171.2(3)	C(1)-N(18)-C(14)-C(13)	178.9(3)
N(3)-Mn(1)-N(12)-C(13)	-5.7(4)	Mn(1)-N(18)-C(14)-C(13)	-2.9(4)
N(9)-Mn(1)-N(12)-C(13)	-177.6(3)	N(12)-C(13)-C(14)-N(18)	0.7(5)
I(1)-Mn(1)-N(12)-C(13)	84.4(3)	N(12)-C(13)-C(14)-C(15)	179.4(4)
O(1)-Mn(1)-N(12)-C(11)	88.0(3)	N(18)-C(14)-C(15)-C(16)	-0.5(6)
N(18)-Mn(1)-N(12)-C(11)	177.3(3)	C(13)-C(14)-C(15)-C(16)	-179.1(4)
N(6)-Mn(1)-N(12)-C(11)	-9.1(4)	C(14)-C(15)-C(16)-C(17)	0.5(7)
N(3)-Mn(1)-N(12)-C(11)	174.0(3)	C(15)-C(16)-C(17)-C(1)	-0.2(7)
N(9)-Mn(1)-N(12)-C(11)	2.1(3)	N(18)-C(1)-C(17)-C(16)	-0.2(6)
I(1)-Mn(1)-N(12)-C(11)	-95.9(3)	C(2)-C(1)-C(17)-C(16)	179.7(4)
O(1)-Mn(1)-N(18)-C(14)	93.1(3)		

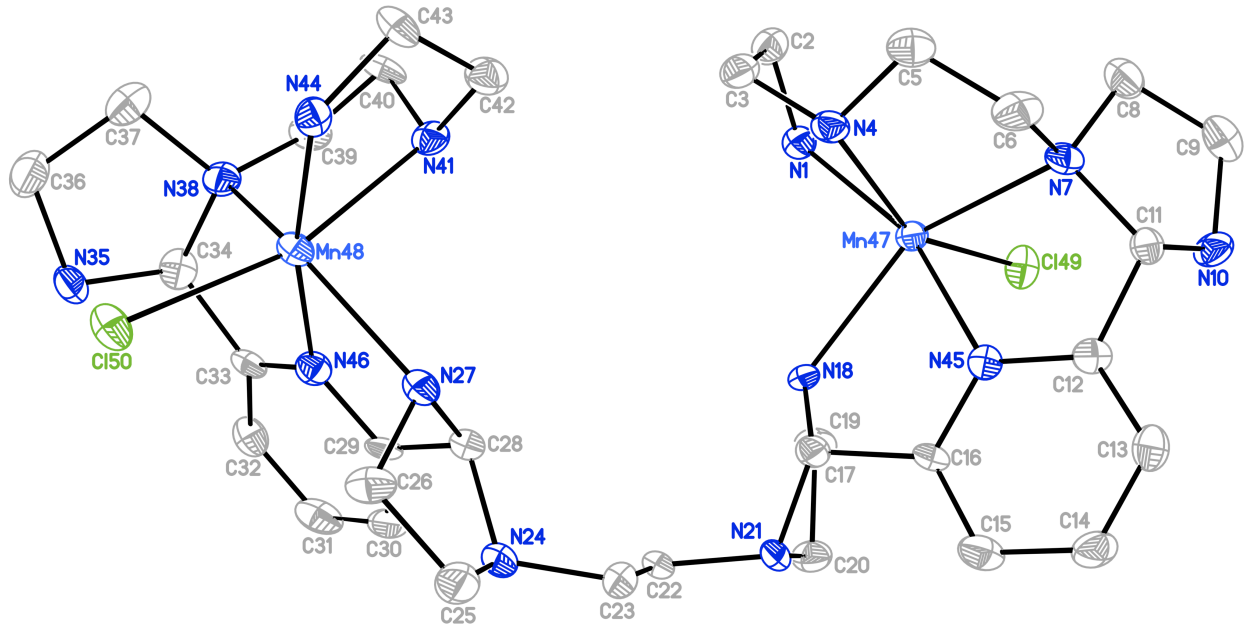


Figure 2. Numbered thermal ellipsoid for **4**.

Table 6. Crystal data and structure refinement for **4**.

Identification code	SH13	
Empirical formula	$C_{32}H_{56}C_{l4}Mn_2N_{14}O_{1.50}$	
Formula weight	912.59	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	p2(1)/n	
Unit cell dimensions	a = 14.5669(9) Å	α= 90°.
	b = 18.4411(10) Å	β= 90.728(2)°.
	c = 15.6178(7) Å	γ = 90°.
Volume	4195.1(4) $Å^3$	
Z	4	
Density (calculated)	1.445 Mg/m^3	
Absorption coefficient	0.904 mm^{-1}	
F(000)	1904	
Crystal size	0.31 x 0.13 x 0.07 mm^3	
Theta range for data collection	1.71 to 25.50°.	
Index ranges	-16<=h<=17, -22<=k<=17, -18<=l<=10	
Reflections collected	20351	
Independent reflections	7788 [R(int) = 0.0803]	
Completeness to theta = 25.50°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9370 and 0.7657	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7788 / 0 / 482	
Goodness-of-fit on F^2	0.975	
Final R indices [I>2sigma(I)]	R1 = 0.0597, wR2 = 0.1166	
R indices (all data)	R1 = 0.1170, wR2 = 0.1351	
Largest diff. peak and hole	1.008 and -0.767 $e.Å^{-3}$	

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(47)	6609(1)	2135(1)	10920(1)	17(1)
Mn(48)	7714(1)	3314(1)	6151(1)	19(1)
Cl(49)	5556(1)	2154(1)	12117(1)	25(1)
Cl(50)	8463(1)	4042(1)	5020(1)	25(1)
Cl(51)	8864(1)	2785(1)	9118(1)	29(1)
Cl(52)	5667(1)	3146(1)	8456(1)	24(1)
N(1)	5529(3)	1752(2)	9957(2)	21(1)
N(4)	7443(3)	1571(2)	9882(2)	20(1)
N(7)	7624(3)	1327(2)	11711(2)	20(1)
N(10)	7406(3)	1622(2)	13147(2)	25(1)
N(18)	6487(3)	3296(2)	10425(2)	19(1)
N(21)	7185(3)	4467(2)	10512(2)	20(1)
N(24)	8070(3)	4872(2)	8307(2)	24(1)
N(27)	8360(3)	3891(2)	7342(2)	21(1)
N(35)	6286(3)	4085(2)	4493(2)	27(1)
N(38)	6294(3)	3104(2)	5420(2)	21(1)
N(41)	7042(2)	2404(2)	6921(2)	20(1)
N(44)	8697(2)	2417(2)	6018(2)	19(1)
N(45)	7747(2)	2771(2)	11560(2)	17(1)
N(46)	6721(3)	4141(2)	6545(2)	20(1)
C(2)	5912(3)	1159(3)	9431(3)	24(1)
C(3)	6852(3)	1388(3)	9139(3)	26(1)
C(5)	7916(3)	928(3)	10233(3)	26(1)
C(6)	8329(3)	1127(3)	11088(3)	29(1)
C(8)	7160(4)	692(3)	12089(3)	32(1)
C(9)	7044(4)	884(3)	13044(3)	31(1)
C(11)	8042(3)	1721(3)	12447(3)	20(1)
C(12)	8195(3)	2510(3)	12253(3)	19(1)
C(13)	8745(3)	2946(3)	12760(3)	31(1)
C(14)	8841(4)	3667(3)	12554(3)	32(1)
C(15)	8403(3)	3933(3)	11829(3)	26(1)
C(16)	7853(3)	3470(3)	11350(3)	17(1)
C(17)	7375(3)	3693(3)	10521(3)	19(1)
C(19)	5799(3)	3797(3)	10807(3)	27(1)
C(20)	6307(3)	4515(3)	10964(3)	25(1)
C(22)	7120(3)	4755(3)	9631(3)	22(1)
C(23)	8077(3)	4788(3)	9247(3)	25(1)
C(25)	9015(4)	4941(3)	7973(3)	31(1)
C(26)	9006(3)	4493(3)	7162(3)	27(1)
C(28)	7646(3)	4250(3)	7842(3)	20(1)
C(29)	6873(3)	4522(3)	7260(3)	20(1)
C(30)	6312(3)	5094(3)	7488(3)	25(1)
C(31)	5592(3)	5282(3)	6948(3)	28(1)
C(32)	5435(3)	4880(3)	6210(3)	24(1)
C(33)	6010(3)	4312(3)	6034(3)	18(1)
C(34)	5873(3)	3820(3)	5265(3)	24(1)
C(36)	6311(4)	3432(3)	3944(3)	34(1)
C(37)	6420(3)	2783(3)	4550(3)	29(1)
C(39)	5726(3)	2655(3)	5990(3)	26(1)
C(40)	6299(3)	2070(3)	6416(3)	24(1)
C(42)	7782(3)	1889(3)	7177(3)	25(1)

C(43)	8395(3)	1740(3)	6429(3)	24(1)
O(1W)	10242(5)	4030(4)	9871(5)	41(2)
O(2W)	8818(2)	1519(2)	4439(2)	31(1)

Table 8. Bond lengths [Å] and angles [°] for **4**.

Mn(47)-N(45)	2.255(4)	N(45)-C(16)	1.340(6)
Mn(47)-N(1)	2.275(4)	N(45)-C(12)	1.345(6)
Mn(47)-N(18)	2.282(4)	N(46)-C(29)	1.335(6)
Mn(47)-N(4)	2.288(4)	N(46)-C(33)	1.337(6)
Mn(47)-N(7)	2.425(4)	C(2)-C(3)	1.509(6)
Mn(47)-Cl(49)	2.4349(13)	C(2)-H(2A)	0.9900
Mn(48)-N(46)	2.195(4)	C(2)-H(2B)	0.9900
Mn(48)-N(44)	2.200(4)	C(3)-H(3A)	0.9900
Mn(48)-N(41)	2.291(4)	C(3)-H(3B)	0.9900
Mn(48)-N(27)	2.330(4)	C(5)-C(6)	1.504(6)
Mn(48)-N(38)	2.381(4)	C(5)-H(5A)	0.9900
Mn(48)-Cl(50)	2.4826(14)	C(5)-H(5B)	0.9900
N(1)-C(2)	1.480(6)	C(6)-H(6A)	0.9900
N(1)-H(1A)	0.9200	C(6)-H(6B)	0.9900
N(1)-H(1B)	0.9200	C(8)-C(9)	1.543(6)
N(4)-C(5)	1.473(6)	C(8)-H(8A)	0.9900
N(4)-C(3)	1.475(6)	C(8)-H(8B)	0.9900
N(4)-H(4A)	0.9300	C(9)-H(9A)	0.9900
N(7)-C(6)	1.470(6)	C(9)-H(9B)	0.9900
N(7)-C(8)	1.480(6)	C(11)-C(12)	1.503(7)
N(7)-C(11)	1.484(6)	C(11)-H(11A)	1.0000
N(10)-C(11)	1.454(6)	C(12)-C(13)	1.379(6)
N(10)-C(9)	1.468(6)	C(13)-C(14)	1.376(7)
N(10)-H(10A)	0.8800	C(13)-H(13A)	0.9500
N(18)-C(17)	1.493(6)	C(14)-C(15)	1.382(6)
N(18)-C(19)	1.493(6)	C(14)-H(14A)	0.9500
N(18)-H(18A)	0.9300	C(15)-C(16)	1.383(6)
N(21)-C(17)	1.455(6)	C(15)-H(15A)	0.9500
N(21)-C(20)	1.471(6)	C(16)-C(17)	1.519(6)
N(21)-C(22)	1.478(5)	C(17)-H(17A)	1.0000
N(24)-C(23)	1.476(5)	C(19)-C(20)	1.536(7)
N(24)-C(25)	1.484(6)	C(19)-H(19A)	0.9900
N(24)-C(28)	1.487(6)	C(19)-H(19B)	0.9900
N(27)-C(28)	1.466(6)	C(20)-H(20A)	0.9900
N(27)-C(26)	1.485(6)	C(20)-H(20B)	0.9900
N(27)-H(27A)	0.9300	C(22)-C(23)	1.525(6)
N(35)-C(34)	1.439(6)	C(22)-H(22A)	0.9900
N(35)-C(36)	1.479(6)	C(22)-H(22B)	0.9900
N(35)-H(35A)	0.8800	C(23)-H(23A)	0.9900
N(38)-C(34)	1.476(6)	C(23)-H(23B)	0.9900
N(38)-C(39)	1.478(6)	C(25)-C(26)	1.513(6)
N(38)-C(37)	1.494(6)	C(25)-H(25A)	0.9900
N(41)-C(40)	1.467(6)	C(25)-H(25B)	0.9900
N(41)-C(42)	1.487(6)	C(26)-H(26A)	0.9900
N(41)-H(41A)	0.9300	C(26)-H(26B)	0.9900
N(44)-C(43)	1.474(6)	C(28)-C(29)	1.523(6)
N(44)-H(44A)	0.9200	C(28)-H(28A)	1.0000
N(44)-H(44B)	0.9200	C(29)-C(30)	1.383(6)

C(30)-C(31)	1.381(7)
C(30)-H(30A)	0.9500
C(31)-C(32)	1.386(7)
C(31)-H(31A)	0.9500
C(32)-C(33)	1.372(6)
C(32)-H(32A)	0.9500
C(33)-C(34)	1.517(6)
C(34)-H(34A)	1.0000
C(36)-C(37)	1.534(7)
C(36)-H(36A)	0.9900
C(36)-H(36B)	0.9900
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(39)-C(40)	1.513(6)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(42)-C(43)	1.505(6)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900

N(45)-Mn(47)-N(1)	162.43(14)
N(45)-Mn(47)-N(18)	73.49(14)
N(1)-Mn(47)-N(18)	90.99(14)
N(45)-Mn(47)-N(4)	99.02(13)
N(1)-Mn(47)-N(4)	76.11(13)
N(18)-Mn(47)-N(4)	103.12(14)
N(45)-Mn(47)-N(7)	69.72(14)
N(1)-Mn(47)-N(7)	123.92(14)
N(18)-Mn(47)-N(7)	142.45(13)
N(4)-Mn(47)-N(7)	75.88(13)
N(45)-Mn(47)-Cl(49)	96.82(9)
N(1)-Mn(47)-Cl(49)	94.28(10)
N(18)-Mn(47)-Cl(49)	101.47(10)
N(4)-Mn(47)-Cl(49)	153.68(11)
N(7)-Mn(47)-Cl(49)	90.21(9)
N(46)-Mn(48)-N(44)	168.86(14)
N(46)-Mn(48)-N(41)	94.27(14)
N(44)-Mn(48)-N(41)	77.40(14)
N(46)-Mn(48)-N(27)	73.75(14)
N(44)-Mn(48)-N(27)	99.34(14)
N(41)-Mn(48)-N(27)	94.97(13)
N(46)-Mn(48)-N(38)	71.13(14)
N(44)-Mn(48)-N(38)	113.20(14)
N(41)-Mn(48)-N(38)	76.01(13)
N(27)-Mn(48)-N(38)	142.82(13)
N(46)-Mn(48)-Cl(50)	96.95(10)
N(44)-Mn(48)-Cl(50)	92.66(10)
N(41)-Mn(48)-Cl(50)	164.59(11)
N(27)-Mn(48)-Cl(50)	98.29(10)
N(38)-Mn(48)-Cl(50)	97.68(10)
C(2)-N(1)-Mn(47)	109.4(3)
C(2)-N(1)-H(1A)	109.8
Mn(47)-N(1)-H(1A)	109.8
C(2)-N(1)-H(1B)	109.8
Mn(47)-N(1)-H(1B)	109.8
H(1A)-N(1)-H(1B)	108.2
C(5)-N(4)-C(3)	112.0(4)
C(5)-N(4)-Mn(47)	110.6(3)
C(3)-N(4)-Mn(47)	110.6(3)
C(5)-N(4)-H(4A)	107.8
C(3)-N(4)-H(4A)	107.8
Mn(47)-N(4)-H(4A)	107.8
C(6)-N(7)-C(8)	113.1(4)
C(6)-N(7)-C(11)	110.6(4)
C(8)-N(7)-C(11)	105.2(4)
C(6)-N(7)-Mn(47)	104.1(3)
C(8)-N(7)-Mn(47)	114.3(3)
C(11)-N(7)-Mn(47)	109.6(3)
C(11)-N(10)-C(9)	105.4(4)
C(11)-N(10)-H(10A)	127.3
C(9)-N(10)-H(10A)	127.3
C(17)-N(18)-C(19)	104.0(4)
C(17)-N(18)-Mn(47)	111.2(3)
C(19)-N(18)-Mn(47)	119.7(3)
C(17)-N(18)-H(18A)	107.1
C(19)-N(18)-H(18A)	107.1
Mn(47)-N(18)-H(18A)	107.1
C(17)-N(21)-C(20)	102.8(4)
C(17)-N(21)-C(22)	111.8(4)
C(20)-N(21)-C(22)	112.3(4)
C(23)-N(24)-C(25)	111.3(4)
C(23)-N(24)-C(28)	113.7(4)
C(25)-N(24)-C(28)	106.0(4)
C(28)-N(27)-C(26)	102.7(4)
C(28)-N(27)-Mn(48)	110.5(3)
C(26)-N(27)-Mn(48)	116.2(3)
C(28)-N(27)-H(27A)	109.1
C(26)-N(27)-H(27A)	109.1
Mn(48)-N(27)-H(27A)	109.1
C(34)-N(35)-C(36)	102.9(4)
C(34)-N(35)-H(35A)	128.5
C(36)-N(35)-H(35A)	128.5
C(34)-N(38)-C(39)	111.4(4)
C(34)-N(38)-C(37)	105.1(4)
C(39)-N(38)-C(37)	113.7(4)
C(34)-N(38)-Mn(48)	106.8(3)
C(39)-N(38)-Mn(48)	107.0(3)
C(37)-N(38)-Mn(48)	112.6(3)
C(40)-N(41)-C(42)	113.8(4)
C(40)-N(41)-Mn(48)	110.0(3)
C(42)-N(41)-Mn(48)	107.2(3)
C(40)-N(41)-H(41A)	108.6
C(42)-N(41)-H(41A)	108.6
Mn(48)-N(41)-H(41A)	108.6
C(43)-N(44)-Mn(48)	113.4(3)
C(43)-N(44)-H(44A)	108.9
Mn(48)-N(44)-H(44A)	108.9
C(43)-N(44)-H(44B)	108.9

Mn(48)-N(44)-H(44B)	108.9	C(13)-C(14)-C(15)	119.2(5)
H(44A)-N(44)-H(44B)	107.7	C(13)-C(14)-H(14A)	120.4
C(16)-N(45)-C(12)	119.0(4)	C(15)-C(14)-H(14A)	120.4
C(16)-N(45)-Mn(47)	118.6(3)	C(14)-C(15)-C(16)	118.8(5)
C(12)-N(45)-Mn(47)	121.1(3)	C(14)-C(15)-H(15A)	120.6
C(29)-N(46)-C(33)	119.6(4)	C(16)-C(15)-H(15A)	120.6
C(29)-N(46)-Mn(48)	119.8(3)	N(45)-C(16)-C(15)	122.0(4)
C(33)-N(46)-Mn(48)	120.3(3)	N(45)-C(16)-C(17)	114.6(4)
N(1)-C(2)-C(3)	108.2(4)	C(15)-C(16)-C(17)	123.3(4)
N(1)-C(2)-H(2A)	110.1	N(21)-C(17)-N(18)	108.3(4)
C(3)-C(2)-H(2A)	110.1	N(21)-C(17)-C(16)	111.0(4)
N(1)-C(2)-H(2B)	110.1	N(18)-C(17)-C(16)	109.9(4)
C(3)-C(2)-H(2B)	110.1	N(21)-C(17)-H(17A)	109.2
H(2A)-C(2)-H(2B)	108.4	N(18)-C(17)-H(17A)	109.2
N(4)-C(3)-C(2)	110.4(4)	C(16)-C(17)-H(17A)	109.2
N(4)-C(3)-H(3A)	109.6	N(18)-C(19)-C(20)	105.8(4)
C(2)-C(3)-H(3A)	109.6	N(18)-C(19)-H(19A)	110.6
N(4)-C(3)-H(3B)	109.6	C(20)-C(19)-H(19A)	110.6
C(2)-C(3)-H(3B)	109.6	N(18)-C(19)-H(19B)	110.6
H(3A)-C(3)-H(3B)	108.1	C(20)-C(19)-H(19B)	110.6
N(4)-C(5)-C(6)	108.2(4)	H(19A)-C(19)-H(19B)	108.7
N(4)-C(5)-H(5A)	110.0	N(21)-C(20)-C(19)	107.0(4)
C(6)-C(5)-H(5A)	110.0	N(21)-C(20)-H(20A)	110.3
N(4)-C(5)-H(5B)	110.0	C(19)-C(20)-H(20A)	110.3
C(6)-C(5)-H(5B)	110.0	N(21)-C(20)-H(20B)	110.3
H(5A)-C(5)-H(5B)	108.4	C(19)-C(20)-H(20B)	110.3
N(7)-C(6)-C(5)	112.0(4)	H(20A)-C(20)-H(20B)	108.6
N(7)-C(6)-H(6A)	109.2	N(21)-C(22)-C(23)	109.4(4)
C(5)-C(6)-H(6A)	109.2	N(21)-C(22)-H(22A)	109.8
N(7)-C(6)-H(6B)	109.2	C(23)-C(22)-H(22A)	109.8
C(5)-C(6)-H(6B)	109.2	N(21)-C(22)-H(22B)	109.8
H(6A)-C(6)-H(6B)	107.9	C(23)-C(22)-H(22B)	109.8
N(7)-C(8)-C(9)	105.1(4)	H(22A)-C(22)-H(22B)	108.2
N(7)-C(8)-H(8A)	110.7	N(24)-C(23)-C(22)	113.6(4)
C(9)-C(8)-H(8A)	110.7	N(24)-C(23)-H(23A)	108.8
N(7)-C(8)-H(8B)	110.7	C(22)-C(23)-H(23A)	108.8
C(9)-C(8)-H(8B)	110.7	N(24)-C(23)-H(23B)	108.8
H(8A)-C(8)-H(8B)	108.8	C(22)-C(23)-H(23B)	108.8
N(10)-C(9)-C(8)	105.9(4)	H(23A)-C(23)-H(23B)	107.7
N(10)-C(9)-H(9A)	110.5	N(24)-C(25)-C(26)	104.4(4)
C(8)-C(9)-H(9A)	110.5	N(24)-C(25)-H(25A)	110.9
N(10)-C(9)-H(9B)	110.5	C(26)-C(25)-H(25A)	110.9
C(8)-C(9)-H(9B)	110.5	N(24)-C(25)-H(25B)	110.9
H(9A)-C(9)-H(9B)	108.7	C(26)-C(25)-H(25B)	110.9
N(10)-C(11)-N(7)	105.2(4)	H(25A)-C(25)-H(25B)	108.9
N(10)-C(11)-C(12)	111.7(4)	N(27)-C(26)-C(25)	104.4(4)
N(7)-C(11)-C(12)	112.2(4)	N(27)-C(26)-H(26A)	110.9
N(10)-C(11)-H(11A)	109.2	C(25)-C(26)-H(26A)	110.9
N(7)-C(11)-H(11A)	109.2	N(27)-C(26)-H(26B)	110.9
C(12)-C(11)-H(11A)	109.2	C(25)-C(26)-H(26B)	110.9
N(45)-C(12)-C(13)	121.7(5)	H(26A)-C(26)-H(26B)	108.9
N(45)-C(12)-C(11)	115.9(4)	N(27)-C(28)-N(24)	108.4(4)
C(13)-C(12)-C(11)	122.4(4)	N(27)-C(28)-C(29)	110.8(4)
C(14)-C(13)-C(12)	119.3(5)	N(24)-C(28)-C(29)	109.7(4)
C(14)-C(13)-H(13A)	120.3	N(27)-C(28)-H(28A)	109.3
C(12)-C(13)-H(13A)	120.3	N(24)-C(28)-H(28A)	109.3

C(29)-C(28)-H(28A)	109.3	N(38)-C(37)-H(37A)	111.0
N(46)-C(29)-C(30)	121.5(5)	C(36)-C(37)-H(37A)	111.0
N(46)-C(29)-C(28)	116.1(4)	N(38)-C(37)-H(37B)	111.0
C(30)-C(29)-C(28)	122.2(4)	C(36)-C(37)-H(37B)	111.0
C(31)-C(30)-C(29)	118.8(5)	H(37A)-C(37)-H(37B)	109.0
C(31)-C(30)-H(30A)	120.6	N(38)-C(39)-C(40)	110.7(4)
C(29)-C(30)-H(30A)	120.6	N(38)-C(39)-H(39A)	109.5
C(30)-C(31)-C(32)	119.3(5)	C(40)-C(39)-H(39A)	109.5
C(30)-C(31)-H(31A)	120.4	N(38)-C(39)-H(39B)	109.5
C(32)-C(31)-H(31A)	120.4	C(40)-C(39)-H(39B)	109.5
C(33)-C(32)-C(31)	118.7(5)	H(39A)-C(39)-H(39B)	108.1
C(33)-C(32)-H(32A)	120.7	N(41)-C(40)-C(39)	109.6(4)
C(31)-C(32)-H(32A)	120.7	N(41)-C(40)-H(40A)	109.7
N(46)-C(33)-C(32)	122.1(4)	C(39)-C(40)-H(40A)	109.7
N(46)-C(33)-C(34)	115.1(4)	N(41)-C(40)-H(40B)	109.7
C(32)-C(33)-C(34)	122.8(4)	C(39)-C(40)-H(40B)	109.7
N(35)-C(34)-N(38)	105.3(4)	H(40A)-C(40)-H(40B)	108.2
N(35)-C(34)-C(33)	114.1(4)	N(41)-C(42)-C(43)	110.1(4)
N(38)-C(34)-C(33)	110.8(4)	N(41)-C(42)-H(42A)	109.6
N(35)-C(34)-H(34A)	108.8	C(43)-C(42)-H(42A)	109.6
N(38)-C(34)-H(34A)	108.8	N(41)-C(42)-H(42B)	109.6
C(33)-C(34)-H(34A)	108.8	C(43)-C(42)-H(42B)	109.6
N(35)-C(36)-C(37)	106.2(4)	H(42A)-C(42)-H(42B)	108.1
N(35)-C(36)-H(36A)	110.5	N(44)-C(43)-C(42)	111.5(4)
C(37)-C(36)-H(36A)	110.5	N(44)-C(43)-H(43A)	109.3
N(35)-C(36)-H(36B)	110.5	C(42)-C(43)-H(43A)	109.3
C(37)-C(36)-H(36B)	110.5	N(44)-C(43)-H(43B)	109.3
H(36A)-C(36)-H(36B)	108.7	C(42)-C(43)-H(43B)	109.3
N(38)-C(37)-C(36)	103.8(4)	H(43A)-C(43)-H(43B)	108.0

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(47)	18(1)	15(1)	17(1)	-1(1)	-1(1)	0(1)
Mn(48)	19(1)	15(1)	22(1)	2(1)	0(1)	2(1)
Cl(49)	19(1)	35(1)	21(1)	2(1)	1(1)	4(1)
Cl(50)	23(1)	24(1)	29(1)	8(1)	4(1)	4(1)
Cl(51)	25(1)	31(1)	29(1)	2(1)	3(1)	-1(1)
Cl(52)	23(1)	26(1)	21(1)	-1(1)	-1(1)	-2(1)
N(1)	23(2)	20(3)	21(2)	-1(2)	-2(2)	0(2)
N(4)	22(2)	16(2)	23(2)	0(2)	2(2)	-4(2)
N(7)	19(2)	15(2)	25(2)	-1(2)	0(2)	3(2)
N(10)	36(2)	23(3)	17(2)	-5(2)	6(2)	-4(2)
N(18)	27(2)	13(2)	17(2)	-3(2)	-6(2)	-2(2)
N(21)	30(2)	13(2)	17(2)	2(2)	0(2)	2(2)
N(24)	31(2)	19(3)	21(2)	3(2)	-1(2)	-9(2)
N(27)	26(2)	16(3)	22(2)	3(2)	-2(2)	1(2)
N(35)	37(3)	19(3)	24(2)	7(2)	5(2)	3(2)
N(38)	22(2)	19(3)	23(2)	-2(2)	1(2)	6(2)
N(41)	21(2)	19(3)	20(2)	-4(2)	6(2)	2(2)
N(44)	17(2)	21(3)	18(2)	1(2)	-3(2)	-3(2)

N(45)	14(2)	18(3)	18(2)	-1(2)	2(2)	3(2)
N(46)	18(2)	19(3)	22(2)	1(2)	0(2)	-2(2)
C(2)	23(3)	26(3)	22(3)	-3(2)	-3(2)	1(2)
C(3)	35(3)	21(3)	21(3)	-4(2)	5(2)	-3(2)
C(5)	22(3)	23(3)	35(3)	-4(2)	2(2)	4(2)
C(6)	22(3)	25(3)	39(3)	-9(3)	-3(3)	11(2)
C(8)	40(3)	22(3)	33(3)	6(3)	-8(3)	-4(3)
C(9)	30(3)	28(4)	34(3)	11(3)	0(3)	0(3)
C(11)	19(3)	19(3)	22(3)	1(2)	-6(2)	4(2)
C(12)	14(2)	19(3)	25(3)	-2(2)	-1(2)	1(2)
C(13)	31(3)	31(4)	30(3)	3(3)	-17(3)	2(3)
C(14)	33(3)	22(3)	40(3)	-5(3)	-20(3)	1(3)
C(15)	25(3)	18(3)	37(3)	2(2)	-2(2)	-3(2)
C(16)	19(2)	10(3)	23(3)	0(2)	1(2)	1(2)
C(17)	22(3)	17(3)	18(2)	1(2)	4(2)	-5(2)
C(19)	24(3)	22(3)	35(3)	-3(2)	-4(2)	2(2)
C(20)	30(3)	18(3)	27(3)	-5(2)	-1(2)	2(2)
C(22)	36(3)	12(3)	19(3)	3(2)	-4(2)	-4(2)
C(23)	34(3)	22(3)	18(3)	0(2)	-4(2)	-6(2)
C(25)	37(3)	30(4)	26(3)	-2(3)	3(3)	-14(3)
C(26)	25(3)	21(3)	34(3)	-5(2)	1(2)	-5(2)
C(28)	27(3)	13(3)	20(3)	1(2)	0(2)	0(2)
C(29)	28(3)	9(3)	24(3)	-1(2)	3(2)	-8(2)
C(30)	32(3)	15(3)	29(3)	-3(2)	5(2)	-4(2)
C(31)	23(3)	16(3)	45(3)	1(3)	14(3)	5(2)
C(32)	21(3)	24(3)	26(3)	6(2)	2(2)	2(2)
C(33)	18(2)	11(3)	25(3)	3(2)	5(2)	-1(2)
C(34)	20(3)	28(3)	24(3)	1(2)	0(2)	4(2)
C(36)	41(3)	37(4)	22(3)	-3(3)	0(3)	8(3)
C(37)	25(3)	35(4)	27(3)	-9(3)	-3(2)	4(3)
C(39)	24(3)	21(3)	32(3)	-1(2)	3(2)	-1(2)
C(40)	24(3)	10(3)	40(3)	5(2)	3(2)	-3(2)
C(42)	27(3)	20(3)	28(3)	0(2)	3(2)	4(2)
C(43)	24(3)	17(3)	32(3)	9(2)	2(2)	3(2)
O(2W)	34(2)	35(2)	22(2)	2(2)	-3(2)	-3(2)

Table 10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(1A)	5019	1589	10241	25
H(1B)	5353	2131	9609	25
H(4A)	7889	1894	9698	24
H(10A)	7267	1938	13547	30
H(18A)	6354	3268	9842	23
H(27A)	8655	3548	7684	25
H(35A)	6477	4526	4377	32
H(41A)	6793	2603	7414	24
H(44A)	8786	2331	5445	23
H(44B)	9251	2555	6255	23
H(2A)	5507	1065	8930	28
H(2B)	5958	709	9774	28

H(3A)	7135	990	8810	31
H(3B)	6795	1815	8758	31
H(5A)	8403	769	9839	32
H(5B)	7474	524	10300	32
H(6A)	8687	711	11313	35
H(6B)	8756	1540	11014	35
H(8A)	7539	250	12026	38
H(8B)	6555	609	11809	38
H(9A)	6388	865	13202	37
H(9B)	7391	540	13411	37
H(11A)	8643	1491	12602	24
H(13A)	9055	2751	13246	37
H(14A)	9204	3979	12905	38
H(15A)	8478	4425	11662	32
H(17A)	7778	3570	10028	23
H(19A)	5568	3598	11352	32
H(19B)	5273	3870	10409	32
H(20A)	5939	4927	10741	30
H(20B)	6417	4589	11585	30
H(22A)	6847	5247	9639	27
H(22B)	6719	4439	9276	27
H(23A)	8416	5200	9506	30
H(23B)	8411	4338	9399	30
H(25A)	9472	4750	8391	37
H(25B)	9163	5454	7848	37
H(26A)	8789	4784	6667	32
H(26B)	9627	4304	7039	32
H(28A)	7392	3899	8265	24
H(30A)	6420	5352	8005	30
H(31A)	5209	5682	7081	34
H(32A)	4939	4997	5834	29
H(34A)	5200	3754	5159	29
H(36A)	6834	3458	3546	40
H(36B)	5736	3389	3603	40
H(37A)	5948	2409	4428	35
H(37B)	7036	2562	4499	35
H(39A)	5221	2429	5654	31
H(39B)	5449	2967	6434	31
H(40A)	5908	1773	6793	29
H(40B)	6561	1748	5975	29
H(42A)	7507	1430	7377	30
H(42B)	8149	2098	7654	30
H(43A)	8940	1464	6629	29
H(43B)	8060	1438	6004	29

Table 11. Torsion angles [°] for **4**.

N(45)-Mn(47)-N(1)-C(2)	96.5(5)	Cl(50)-Mn(48)-N(38)-C(34)	-61.4(3)
N(18)-Mn(47)-N(1)-C(2)	124.0(3)	N(46)-Mn(48)-N(38)-C(39)	-86.1(3)
N(4)-Mn(47)-N(1)-C(2)	20.8(3)	N(44)-Mn(48)-N(38)-C(39)	82.9(3)
N(7)-Mn(47)-N(1)-C(2)	-41.3(3)	N(41)-Mn(48)-N(38)-C(39)	13.5(3)
Cl(49)-Mn(47)-N(1)-C(2)	-134.4(3)	N(27)-Mn(48)-N(38)-C(39)	-66.1(4)
N(45)-Mn(47)-N(4)-C(5)	81.3(3)	Cl(50)-Mn(48)-N(38)-C(39)	179.2(3)
N(1)-Mn(47)-N(4)-C(5)	-115.9(3)	N(46)-Mn(48)-N(38)-C(37)	148.3(3)
N(18)-Mn(47)-N(4)-C(5)	156.4(3)	N(44)-Mn(48)-N(38)-C(37)	-42.7(3)
N(7)-Mn(47)-N(4)-C(5)	15.0(3)	N(41)-Mn(48)-N(38)-C(37)	-112.2(3)
Cl(49)-Mn(47)-N(4)-C(5)	-45.0(4)	N(27)-Mn(48)-N(38)-C(37)	168.3(3)
N(45)-Mn(47)-N(4)-C(3)	-154.0(3)	Cl(50)-Mn(48)-N(38)-C(37)	53.5(3)
N(1)-Mn(47)-N(4)-C(3)	8.8(3)	N(46)-Mn(48)-N(41)-C(40)	85.9(3)
N(18)-Mn(47)-N(4)-C(3)	-79.0(3)	N(44)-Mn(48)-N(41)-C(40)	-101.6(3)
N(7)-Mn(47)-N(4)-C(3)	139.7(3)	N(27)-Mn(48)-N(41)-C(40)	159.9(3)
Cl(49)-Mn(47)-N(4)-C(3)	79.7(4)	N(38)-Mn(48)-N(41)-C(40)	16.5(3)
N(45)-Mn(47)-N(7)-C(6)	-89.5(3)	Cl(50)-Mn(48)-N(41)-C(40)	-50.8(5)
N(1)-Mn(47)-N(7)-C(6)	78.0(3)	N(46)-Mn(48)-N(41)-C(42)	-149.9(3)
N(18)-Mn(47)-N(7)-C(6)	-77.4(3)	N(44)-Mn(48)-N(41)-C(42)	22.6(3)
N(4)-Mn(47)-N(7)-C(6)	15.8(3)	N(27)-Mn(48)-N(41)-C(42)	-75.9(3)
Cl(49)-Mn(47)-N(7)-C(6)	173.3(3)	N(38)-Mn(48)-N(41)-C(42)	140.8(3)
N(45)-Mn(47)-N(7)-C(8)	146.7(3)	Cl(50)-Mn(48)-N(41)-C(42)	73.4(5)
N(1)-Mn(47)-N(7)-C(8)	-45.8(4)	N(46)-Mn(48)-N(44)-C(43)	45.2(9)
N(18)-Mn(47)-N(7)-C(8)	158.8(3)	N(41)-Mn(48)-N(44)-C(43)	2.9(3)
N(4)-Mn(47)-N(7)-C(8)	-108.0(3)	N(27)-Mn(48)-N(44)-C(43)	96.0(3)
Cl(49)-Mn(47)-N(7)-C(8)	49.5(3)	N(38)-Mn(48)-N(44)-C(43)	-65.7(3)
N(45)-Mn(47)-N(7)-C(11)	28.8(3)	Cl(50)-Mn(48)-N(44)-C(43)	-165.2(3)
N(1)-Mn(47)-N(7)-C(11)	-163.7(3)	N(1)-Mn(47)-N(45)-C(16)	26.0(6)
N(18)-Mn(47)-N(7)-C(11)	40.9(4)	N(18)-Mn(47)-N(45)-C(16)	-2.8(3)
N(4)-Mn(47)-N(7)-C(11)	134.2(3)	N(4)-Mn(47)-N(45)-C(16)	98.3(3)
Cl(49)-Mn(47)-N(7)-C(11)	-68.4(3)	N(7)-Mn(47)-N(45)-C(16)	169.5(3)
N(45)-Mn(47)-N(18)-C(17)	22.1(3)	Cl(49)-Mn(47)-N(45)-C(16)	-102.8(3)
N(1)-Mn(47)-N(18)-C(17)	-149.6(3)	N(1)-Mn(47)-N(45)-C(12)	-167.0(4)
N(4)-Mn(47)-N(18)-C(17)	-73.6(3)	N(18)-Mn(47)-N(45)-C(12)	164.2(4)
N(7)-Mn(47)-N(18)-C(17)	10.2(4)	N(4)-Mn(47)-N(45)-C(12)	-94.7(3)
Cl(49)-Mn(47)-N(18)-C(17)	115.9(3)	N(7)-Mn(47)-N(45)-C(12)	-23.5(3)
N(45)-Mn(47)-N(18)-C(19)	-99.3(3)	Cl(49)-Mn(47)-N(45)-C(12)	64.2(3)
N(1)-Mn(47)-N(18)-C(19)	89.0(3)	N(44)-Mn(48)-N(46)-C(29)	47.3(9)
N(4)-Mn(47)-N(18)-C(19)	165.0(3)	N(41)-Mn(48)-N(46)-C(29)	88.5(3)
N(7)-Mn(47)-N(18)-C(19)	-111.2(3)	N(27)-Mn(48)-N(46)-C(29)	-5.5(3)
Cl(49)-Mn(47)-N(18)-C(19)	-5.5(3)	N(38)-Mn(48)-N(46)-C(29)	162.1(4)
N(46)-Mn(48)-N(27)-C(28)	21.1(3)	Cl(50)-Mn(48)-N(46)-C(29)	-102.1(3)
N(44)-Mn(48)-N(27)-C(28)	-150.0(3)	N(44)-Mn(48)-N(46)-C(33)	-138.9(7)
N(41)-Mn(48)-N(27)-C(28)	-71.9(3)	N(41)-Mn(48)-N(46)-C(33)	-97.7(3)
N(38)-Mn(48)-N(27)-C(28)	1.4(4)	N(27)-Mn(48)-N(46)-C(33)	168.3(4)
Cl(50)-Mn(48)-N(27)-C(28)	115.9(3)	N(38)-Mn(48)-N(46)-C(33)	-24.1(3)
N(46)-Mn(48)-N(27)-C(26)	-95.3(3)	Cl(50)-Mn(48)-N(46)-C(33)	71.7(3)
N(44)-Mn(48)-N(27)-C(26)	93.7(3)	Mn(47)-N(1)-C(2)-C(3)	-46.8(4)
N(41)-Mn(48)-N(27)-C(26)	171.7(3)	C(5)-N(4)-C(3)-C(2)	86.9(5)
N(38)-Mn(48)-N(27)-C(26)	-115.0(3)	Mn(47)-N(4)-C(3)-C(2)	-36.9(5)
Cl(50)-Mn(48)-N(27)-C(26)	-0.4(3)	N(1)-C(2)-C(3)-N(4)	56.4(5)
N(46)-Mn(48)-N(38)-C(34)	33.3(3)	C(3)-N(4)-C(5)-C(6)	-167.7(4)
N(44)-Mn(48)-N(38)-C(34)	-157.7(3)	Mn(47)-N(4)-C(5)-C(6)	-43.9(4)
N(41)-Mn(48)-N(38)-C(34)	132.9(3)	C(8)-N(7)-C(6)-C(5)	78.8(5)
N(27)-Mn(48)-N(38)-C(34)	53.3(4)	C(11)-N(7)-C(6)-C(5)	-163.4(4)

Mn(47)-N(7)-C(6)-C(5)	-45.7(5)	C(28)-N(27)-C(26)-C(25)	37.6(5)
N(4)-C(5)-C(6)-N(7)	63.0(5)	Mn(48)-N(27)-C(26)-C(25)	158.2(3)
C(6)-N(7)-C(8)-C(9)	140.0(4)	N(24)-C(25)-C(26)-N(27)	-33.0(5)
C(11)-N(7)-C(8)-C(9)	19.2(5)	C(26)-N(27)-C(28)-N(24)	-28.5(5)
Mn(47)-N(7)-C(8)-C(9)	-101.2(4)	Mn(48)-N(27)-C(28)-N(24)	-153.0(3)
C(11)-N(10)-C(9)-C(8)	-23.6(5)	C(26)-N(27)-C(28)-C(29)	91.9(4)
N(7)-C(8)-C(9)-N(10)	2.5(5)	Mn(48)-N(27)-C(28)-C(29)	-32.6(4)
C(9)-N(10)-C(11)-N(7)	36.2(5)	C(23)-N(24)-C(28)-N(27)	-114.5(4)
C(9)-N(10)-C(11)-C(12)	158.1(4)	C(25)-N(24)-C(28)-N(27)	8.2(5)
C(6)-N(7)-C(11)-N(10)	-156.9(4)	C(23)-N(24)-C(28)-C(29)	124.4(4)
C(8)-N(7)-C(11)-N(10)	-34.5(5)	C(25)-N(24)-C(28)-C(29)	-112.9(4)
Mn(47)-N(7)-C(11)-N(10)	88.8(3)	C(33)-N(46)-C(29)-C(30)	-0.1(7)
C(6)-N(7)-C(11)-C(12)	81.4(5)	Mn(48)-N(46)-C(29)-C(30)	173.7(3)
C(8)-N(7)-C(11)-C(12)	-156.2(4)	C(33)-N(46)-C(29)-C(28)	175.0(4)
Mn(47)-N(7)-C(11)-C(12)	-32.8(4)	Mn(48)-N(46)-C(29)-C(28)	-11.2(5)
C(16)-N(45)-C(12)-C(13)	1.2(7)	N(27)-C(28)-C(29)-N(46)	29.9(6)
Mn(47)-N(45)-C(12)-C(13)	-165.7(4)	N(24)-C(28)-C(29)-N(46)	149.6(4)
C(16)-N(45)-C(12)-C(11)	-180.0(4)	N(27)-C(28)-C(29)-C(30)	-155.0(4)
Mn(47)-N(45)-C(12)-C(11)	13.1(5)	N(24)-C(28)-C(29)-C(30)	-35.4(6)
N(10)-C(11)-C(12)-N(45)	-102.5(4)	N(46)-C(29)-C(30)-C(31)	-1.5(7)
N(7)-C(11)-C(12)-N(45)	15.4(6)	C(28)-C(29)-C(30)-C(31)	-176.3(4)
N(10)-C(11)-C(12)-C(13)	76.4(6)	C(29)-C(30)-C(31)-C(32)	2.0(7)
N(7)-C(11)-C(12)-C(13)	-165.8(4)	C(30)-C(31)-C(32)-C(33)	-0.8(7)
N(45)-C(12)-C(13)-C(14)	0.0(8)	C(29)-N(46)-C(33)-C(32)	1.3(7)
C(11)-C(12)-C(13)-C(14)	-178.8(5)	Mn(48)-N(46)-C(33)-C(32)	-172.5(3)
C(12)-C(13)-C(14)-C(15)	-1.8(8)	C(29)-N(46)-C(33)-C(34)	-176.9(4)
C(13)-C(14)-C(15)-C(16)	2.4(8)	Mn(48)-N(46)-C(33)-C(34)	9.3(5)
C(12)-N(45)-C(16)-C(15)	-0.6(6)	C(31)-C(32)-C(33)-N(46)	-0.8(7)
Mn(47)-N(45)-C(16)-C(15)	166.7(3)	C(31)-C(32)-C(33)-C(34)	177.3(4)
C(12)-N(45)-C(16)-C(17)	175.6(4)	C(36)-N(35)-C(34)-N(38)	41.4(5)
Mn(47)-N(45)-C(16)-C(17)	-17.2(5)	C(36)-N(35)-C(34)-C(33)	163.1(4)
C(14)-C(15)-C(16)-N(45)	-1.2(7)	C(39)-N(38)-C(34)-N(35)	-159.7(4)
C(14)-C(15)-C(16)-C(17)	-177.0(4)	C(37)-N(38)-C(34)-N(35)	-36.1(5)
C(20)-N(21)-C(17)-N(18)	35.9(4)	Mn(48)-N(38)-C(34)-N(35)	83.8(3)
C(22)-N(21)-C(17)-N(18)	-84.9(4)	C(39)-N(38)-C(34)-C(33)	76.5(5)
C(20)-N(21)-C(17)-C(16)	-84.9(4)	C(37)-N(38)-C(34)-C(33)	-159.9(4)
C(22)-N(21)-C(17)-C(16)	154.4(4)	Mn(48)-N(38)-C(34)-C(33)	-40.0(4)
C(19)-N(18)-C(17)-N(21)	-28.5(4)	N(46)-C(33)-C(34)-N(35)	-95.4(5)
Mn(47)-N(18)-C(17)-N(21)	-158.7(3)	C(32)-C(33)-C(34)-N(35)	86.4(6)
C(19)-N(18)-C(17)-C(16)	92.9(4)	N(46)-C(33)-C(34)-N(38)	23.2(6)
Mn(47)-N(18)-C(17)-C(16)	-37.2(4)	C(32)-C(33)-C(34)-N(38)	-155.0(4)
N(45)-C(16)-C(17)-N(21)	156.0(4)	C(34)-N(35)-C(36)-C(37)	-30.8(5)
C(15)-C(16)-C(17)-N(21)	-28.0(6)	C(34)-N(38)-C(37)-C(36)	15.7(5)
N(45)-C(16)-C(17)-N(18)	36.1(5)	C(39)-N(38)-C(37)-C(36)	137.8(4)
C(15)-C(16)-C(17)-N(18)	-147.8(4)	Mn(48)-N(38)-C(37)-C(36)	-100.3(4)
C(17)-N(18)-C(19)-C(20)	9.5(5)	N(35)-C(36)-C(37)-N(38)	9.0(5)
Mn(47)-N(18)-C(19)-C(20)	134.4(3)	C(34)-N(38)-C(39)-C(40)	-158.0(4)
C(17)-N(21)-C(20)-C(19)	-28.7(5)	C(37)-N(38)-C(39)-C(40)	83.4(5)
C(22)-N(21)-C(20)-C(19)	91.7(5)	Mn(48)-N(38)-C(39)-C(40)	-41.7(4)
N(18)-C(19)-C(20)-N(21)	11.9(5)	C(42)-N(41)-C(40)-C(39)	-164.8(4)
C(17)-N(21)-C(22)-C(23)	-72.9(5)	Mn(48)-N(41)-C(40)-C(39)	-44.5(4)
C(20)-N(21)-C(22)-C(23)	172.1(4)	N(38)-C(39)-C(40)-N(41)	59.7(5)
C(25)-N(24)-C(23)-C(22)	176.9(4)	C(40)-N(41)-C(42)-C(43)	77.1(5)
C(28)-N(24)-C(23)-C(22)	-63.4(5)	Mn(48)-N(41)-C(42)-C(43)	-44.8(4)
N(21)-C(22)-C(23)-N(24)	164.0(4)	Mn(48)-N(44)-C(43)-C(42)	-28.4(5)
C(23)-N(24)-C(25)-C(26)	139.4(4)	N(41)-C(42)-C(43)-N(44)	49.7(5)
C(28)-N(24)-C(25)-C(26)	15.3(5)		

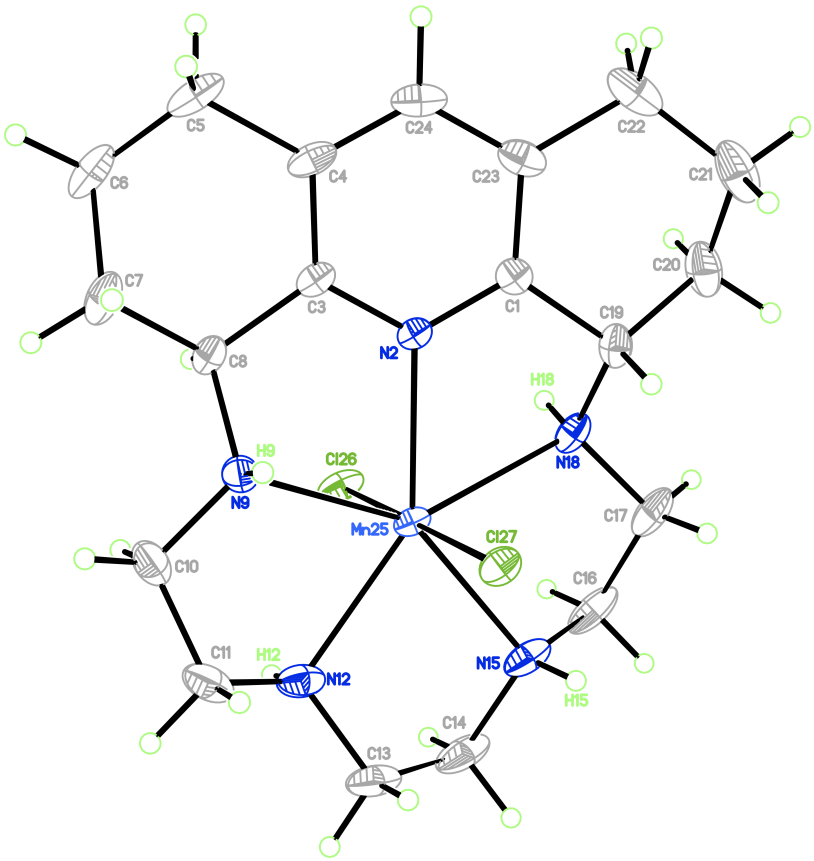


Figure 3. Numbered thermal ellipsoid for **17**.

Table 12. Crystal data and structure refinement for **17**.

Identification code	SH08	
Empirical formula	$C_{19.50}H_{31.50}C_{l3.50}MnN_5O_{0.50}$	
Formula weight	523.01	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 33.9815(7) Å	a= 90°.
	b = 12.1081(3) Å	b= 117.0730(10)°.
	c = 25.8046(5) Å	g = 90°.
Volume	9454.0(4) Å^3	
Z	16	
Density (calculated)	1.470 Mg/m^3	
Absorption coefficient	0.973 mm^{-1}	

F(000)	4352
Crystal size	0.31 x 0.30 x 0.12 mm^3
Theta range for data collection	1.35 to 29.94°.
Index ranges	-47<=h<=47, -16<=k<=17, -36<=l<=34
Reflections collected	62351
Independent reflections	13557 [R(int) = 0.0277]
Completeness to theta = 29.94°	99.0 %
Absorption correction	None
Max. and min. transmission	0.8880 and 0.7510
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	13557 / 0 / 565
Goodness-of-fit on F^2	1.062
Final R indices [I>2sigma(I)]	R1 = 0.0313, wR2 = 0.0804
R indices (all data)	R1 = 0.0385, wR2 = 0.0843
Largest diff. peak and hole	0.839 and -0.719 e.$Å^{-3}$

Table 13. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **17**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mn(25)	1872(1)	4118(1)	3830(1)	16(1)
Mn(52)	678(1)	10354(1)	1444(1)	13(1)
Cl(26)	1679(1)	4056(1)	2752(1)	24(1)
Cl(27)	2078(1)	4143(1)	4929(1)	19(1)
Cl(53)	692(1)	9792(1)	492(1)	19(1)
Cl(54)	758(1)	11000(1)	2454(1)	20(1)
N(2)	2023(1)	5958(1)	3924(1)	14(1)
N(9)	1246(1)	5122(1)	3724(1)	19(1)
N(12)	1311(1)	2841(1)	3591(1)	25(1)
N(15)	2222(1)	2445(1)	4012(1)	24(1)
N(18)	2601(1)	4473(1)	3983(1)	20(1)
N(29)	1026(1)	8731(1)	1801(1)	12(1)
N(36)	154(1)	9001(1)	1390(1)	14(1)
N(39)	-7(1)	11114(1)	876(1)	17(1)

N(42)	812(1)	12231(1)	1381(1)	17(1)
N(45)	1447(1)	10546(1)	1767(1)	13(1)
C(1)	2442(1)	6308(1)	4192(1)	17(1)
C(3)	1689(1)	6685(1)	3730(1)	16(1)
C(4)	1764(1)	7826(1)	3800(1)	21(1)
C(5)	1385(1)	8638(1)	3564(1)	29(1)
C(6)	946(1)	8102(2)	3166(1)	30(1)
C(7)	886(1)	7006(2)	3414(1)	27(1)
C(8)	1232(1)	6178(1)	3436(1)	18(1)
C(10)	845(1)	4440(2)	3455(1)	27(1)
C(11)	956(1)	3277(2)	3705(1)	30(1)
C(13)	1503(1)	1786(1)	3870(1)	32(1)
C(14)	1896(1)	1553(1)	3757(1)	34(1)
C(16)	2571(1)	2485(1)	3827(1)	31(1)
C(17)	2869(1)	3459(2)	4125(1)	29(1)
C(19)	2790(1)	5408(1)	4380(1)	20(1)
C(20)	3225(1)	5870(2)	4436(1)	30(1)
C(21)	3356(1)	6885(2)	4827(1)	36(1)
C(22)	3026(1)	7819(2)	4561(1)	34(1)
C(23)	2550(1)	7427(1)	4287(1)	22(1)
C(24)	2202(1)	8172(1)	4091(1)	25(1)
C(28)	1467(1)	8694(1)	2124(1)	12(1)
C(30)	789(1)	7798(1)	1649(1)	13(1)
C(31)	983(1)	6764(1)	1832(1)	15(1)
C(32)	712(1)	5716(1)	1669(1)	21(1)
C(33)	252(1)	5887(1)	1162(1)	22(1)
C(34)	38(1)	6926(1)	1258(1)	20(1)
C(35)	298(1)	7947(1)	1247(1)	14(1)
C(37)	-297(1)	9341(1)	973(1)	17(1)
C(38)	-343(1)	10588(1)	1003(1)	18(1)
C(40)	13(1)	12325(1)	925(1)	22(1)
C(41)	427(1)	12724(1)	895(1)	21(1)
C(43)	1236(1)	12399(1)	1372(1)	19(1)
C(44)	1587(1)	11705(1)	1853(1)	17(1)
C(46)	1701(1)	9801(1)	2253(1)	13(1)
C(47)	2187(1)	9652(1)	2394(1)	18(1)

C(48)	2404(1)	8778(1)	2867(1)	19(1)
C(49)	2190(1)	7649(1)	2656(1)	18(1)
C(50)	1691(1)	7696(1)	2320(1)	14(1)
C(51)	1440(1)	6733(1)	2173(1)	16(1)
C(1S)	6300(1)	-844(1)	5426(1)	24(1)
Cl(1S)	6589(1)	-269(1)	6129(1)	27(1)
Cl(2S)	5880(1)	80(1)	4967(1)	42(1)
Cl(3S)	6070(1)	-2131(1)	5458(1)	26(1)
O(1S)	0	9575(1)	2500	22(1)
O(2S)	0	2674(2)	2500	75(1)

Table 14. Bond lengths [Å] and angles [°] for **17**.

Mn(25)-N(2)	2.2753(12)
Mn(25)-N(15)	2.2872(13)
Mn(25)-N(12)	2.3095(14)
Mn(25)-N(9)	2.3572(13)
Mn(25)-N(18)	2.3649(13)
Mn(25)-Cl(26)	2.5523(4)
Mn(25)-Cl(27)	2.5949(4)
Mn(52)-N(29)	2.2627(11)
Mn(52)-N(39)	2.3037(12)
Mn(52)-N(42)	2.3374(12)
Mn(52)-N(45)	2.3635(11)
Mn(52)-N(36)	2.3761(12)
Mn(52)-Cl(53)	2.5684(4)
Mn(52)-Cl(54)	2.6141(4)
N(2)-C(3)	1.3386(17)
N(2)-C(1)	1.3396(17)
N(9)-C(10)	1.4692(19)
N(9)-C(8)	1.4702(19)
N(9)-H(9)	0.89(2)
N(12)-C(13)	1.466(2)
N(12)-C(11)	1.467(2)

N(12)-H(12)	0.88(2)
N(15)-C(16)	1.465(2)
N(15)-C(14)	1.471(2)
N(15)-H(15)	0.89(2)
N(18)-C(19)	1.464(2)
N(18)-C(17)	1.4717(19)
N(18)-H(18)	0.87(2)
N(29)-C(30)	1.3381(17)
N(29)-C(28)	1.3431(16)
N(36)-C(35)	1.4726(18)
N(36)-C(37)	1.4761(17)
N(36)-H(36)	0.869(19)
N(39)-C(38)	1.4695(19)
N(39)-C(40)	1.4701(19)
N(39)-H(39)	0.86(2)
N(42)-C(43)	1.4639(18)
N(42)-C(41)	1.4665(18)
N(42)-H(42)	0.878(19)
N(45)-C(46)	1.4652(17)
N(45)-C(44)	1.4659(17)
N(45)-H(45)	0.858(19)
C(1)-C(23)	1.396(2)
C(1)-C(19)	1.515(2)
C(3)-C(4)	1.401(2)
C(3)-C(8)	1.515(2)
C(4)-C(24)	1.393(2)
C(4)-C(5)	1.510(2)
C(5)-C(6)	1.519(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.526(2)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.525(2)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900

C(8)-H(8A)	1.0000
C(10)-C(11)	1.523(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(13)-C(14)	1.516(3)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(16)-C(17)	1.517(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(19)-C(20)	1.525(2)
C(19)-H(19A)	1.0000
C(20)-C(21)	1.523(3)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.521(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.515(2)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.387(2)
C(24)-H(24A)	0.9500
C(28)-C(50)	1.3941(18)
C(28)-C(46)	1.5166(18)
C(30)-C(31)	1.3935(18)
C(30)-C(35)	1.5211(18)
C(31)-C(51)	1.3921(18)
C(31)-C(32)	1.5127(19)
C(32)-C(33)	1.529(2)

C(32)-H(32A)	0.9900
C(32)-H(32B)	0.9900
C(33)-C(34)	1.527(2)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.5267(19)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-H(35A)	1.0000
C(37)-C(38)	1.523(2)
C(37)-H(37A)	0.9900
C(37)-H(37B)	0.9900
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(40)-C(41)	1.522(2)
C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900
C(41)-H(41A)	0.9900
C(41)-H(41B)	0.9900
C(43)-C(44)	1.525(2)
C(43)-H(43A)	0.9900
C(43)-H(43B)	0.9900
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(46)-C(47)	1.5311(18)
C(46)-H(46A)	1.0000
C(47)-C(48)	1.527(2)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.529(2)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(50)	1.5138(18)
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-C(51)	1.3931(18)

C(51)-H(51A)	0.9500
C(1S)-Cl(3S)	1.7609(17)
C(1S)-Cl(1S)	1.7650(17)
C(1S)-Cl(2S)	1.7746(16)
C(1S)-H(1SA)	1.0000

N(2)-Mn(25)-N(15)	140.78(5)
N(2)-Mn(25)-N(12)	143.38(5)
N(15)-Mn(25)-N(12)	75.60(5)
N(2)-Mn(25)-N(9)	69.77(4)
N(15)-Mn(25)-N(9)	147.02(5)
N(12)-Mn(25)-N(9)	73.88(5)
N(2)-Mn(25)-N(18)	68.67(4)
N(15)-Mn(25)-N(18)	73.66(5)
N(12)-Mn(25)-N(18)	147.28(5)
N(9)-Mn(25)-N(18)	138.42(5)
N(2)-Mn(25)-Cl(26)	94.55(3)
N(15)-Mn(25)-Cl(26)	92.85(4)
N(12)-Mn(25)-Cl(26)	85.32(4)
N(9)-Mn(25)-Cl(26)	96.84(4)
N(18)-Mn(25)-Cl(26)	85.26(4)
N(2)-Mn(25)-Cl(27)	86.27(3)
N(15)-Mn(25)-Cl(27)	85.96(4)
N(12)-Mn(25)-Cl(27)	94.56(4)
N(9)-Mn(25)-Cl(27)	84.27(3)
N(18)-Mn(25)-Cl(27)	94.22(4)
Cl(26)-Mn(25)-Cl(27)	178.790(15)
N(29)-Mn(52)-N(39)	142.68(4)
N(29)-Mn(52)-N(42)	142.26(4)
N(39)-Mn(52)-N(42)	74.94(4)
N(29)-Mn(52)-N(45)	69.71(4)
N(39)-Mn(52)-N(45)	145.06(4)
N(42)-Mn(52)-N(45)	73.16(4)
N(29)-Mn(52)-N(36)	70.31(4)
N(39)-Mn(52)-N(36)	74.02(4)
N(42)-Mn(52)-N(36)	146.16(4)

N(45)-Mn(52)-N(36)	140.01(4)
N(29)-Mn(52)-Cl(53)	85.78(3)
N(39)-Mn(52)-Cl(53)	87.19(3)
N(42)-Mn(52)-Cl(53)	95.85(3)
N(45)-Mn(52)-Cl(53)	82.28(3)
N(36)-Mn(52)-Cl(53)	95.77(3)
N(29)-Mn(52)-Cl(54)	93.17(3)
N(39)-Mn(52)-Cl(54)	97.48(3)
N(42)-Mn(52)-Cl(54)	81.03(3)
N(45)-Mn(52)-Cl(54)	91.29(3)
N(36)-Mn(52)-Cl(54)	89.95(3)
Cl(53)-Mn(52)-Cl(54)	173.454(14)
C(3)-N(2)-C(1)	120.46(12)
C(3)-N(2)-Mn(25)	119.50(9)
C(1)-N(2)-Mn(25)	120.00(9)
C(10)-N(9)-C(8)	116.09(12)
C(10)-N(9)-Mn(25)	111.03(10)
C(8)-N(9)-Mn(25)	109.02(8)
C(10)-N(9)-H(9)	111.6(13)
C(8)-N(9)-H(9)	107.1(14)
Mn(25)-N(9)-H(9)	100.9(13)
C(13)-N(12)-C(11)	116.01(14)
C(13)-N(12)-Mn(25)	108.84(11)
C(11)-N(12)-Mn(25)	111.11(10)
C(13)-N(12)-H(12)	106.2(15)
C(11)-N(12)-H(12)	109.6(15)
Mn(25)-N(12)-H(12)	104.4(15)
C(16)-N(15)-C(14)	115.85(14)
C(16)-N(15)-Mn(25)	109.04(10)
C(14)-N(15)-Mn(25)	110.01(10)
C(16)-N(15)-H(15)	105.3(13)
C(14)-N(15)-H(15)	107.1(14)
Mn(25)-N(15)-H(15)	109.2(14)
C(19)-N(18)-C(17)	116.54(13)
C(19)-N(18)-Mn(25)	110.39(9)
C(17)-N(18)-Mn(25)	111.88(10)

C(19)-N(18)-H(18)	107.4(13)
C(17)-N(18)-H(18)	108.7(13)
Mn(25)-N(18)-H(18)	100.6(13)
C(30)-N(29)-C(28)	120.42(11)
C(30)-N(29)-Mn(52)	118.73(8)
C(28)-N(29)-Mn(52)	120.66(9)
C(35)-N(36)-C(37)	114.37(11)
C(35)-N(36)-Mn(52)	106.70(8)
C(37)-N(36)-Mn(52)	110.70(9)
C(35)-N(36)-H(36)	106.9(12)
C(37)-N(36)-H(36)	108.4(12)
Mn(52)-N(36)-H(36)	109.7(12)
C(38)-N(39)-C(40)	115.04(12)
C(38)-N(39)-Mn(52)	110.38(9)
C(40)-N(39)-Mn(52)	110.50(9)
C(38)-N(39)-H(39)	108.3(13)
C(40)-N(39)-H(39)	107.3(13)
Mn(52)-N(39)-H(39)	104.7(13)
C(43)-N(42)-C(41)	115.63(12)
C(43)-N(42)-Mn(52)	111.16(9)
C(41)-N(42)-Mn(52)	109.20(9)
C(43)-N(42)-H(42)	107.1(12)
C(41)-N(42)-H(42)	111.4(12)
Mn(52)-N(42)-H(42)	101.5(12)
C(46)-N(45)-C(44)	115.81(11)
C(46)-N(45)-Mn(52)	111.59(8)
C(44)-N(45)-Mn(52)	112.22(8)
C(46)-N(45)-H(45)	110.0(12)
C(44)-N(45)-H(45)	110.4(12)
Mn(52)-N(45)-H(45)	94.9(11)
N(2)-C(1)-C(23)	122.00(13)
N(2)-C(1)-C(19)	115.39(13)
C(23)-C(1)-C(19)	122.61(13)
N(2)-C(3)-C(4)	121.79(14)
N(2)-C(3)-C(8)	114.99(12)
C(4)-C(3)-C(8)	123.22(13)

C(24)-C(4)-C(3)	116.88(14)
C(24)-C(4)-C(5)	121.83(14)
C(3)-C(4)-C(5)	121.29(15)
C(4)-C(5)-C(6)	112.88(14)
C(4)-C(5)-H(5A)	109.0
C(6)-C(5)-H(5A)	109.0
C(4)-C(5)-H(5B)	109.0
C(6)-C(5)-H(5B)	109.0
H(5A)-C(5)-H(5B)	107.8
C(5)-C(6)-C(7)	111.37(14)
C(5)-C(6)-H(6A)	109.4
C(7)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6B)	109.4
C(7)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(8)-C(7)-C(6)	109.94(13)
C(8)-C(7)-H(7A)	109.7
C(6)-C(7)-H(7A)	109.7
C(8)-C(7)-H(7B)	109.7
C(6)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
N(9)-C(8)-C(3)	107.99(11)
N(9)-C(8)-C(7)	115.95(12)
C(3)-C(8)-C(7)	110.40(13)
N(9)-C(8)-H(8A)	107.4
C(3)-C(8)-H(8A)	107.4
C(7)-C(8)-H(8A)	107.4
N(9)-C(10)-C(11)	108.74(13)
N(9)-C(10)-H(10A)	109.9
C(11)-C(10)-H(10A)	109.9
N(9)-C(10)-H(10B)	109.9
C(11)-C(10)-H(10B)	109.9
H(10A)-C(10)-H(10B)	108.3
N(12)-C(11)-C(10)	108.37(13)
N(12)-C(11)-H(11A)	110.0
C(10)-C(11)-H(11A)	110.0

N(12)-C(11)-H(11B)	110.0
C(10)-C(11)-H(11B)	110.0
H(11A)-C(11)-H(11B)	108.4
N(12)-C(13)-C(14)	107.55(14)
N(12)-C(13)-H(13A)	110.2
C(14)-C(13)-H(13A)	110.2
N(12)-C(13)-H(13B)	110.2
C(14)-C(13)-H(13B)	110.2
H(13A)-C(13)-H(13B)	108.5
N(15)-C(14)-C(13)	109.18(14)
N(15)-C(14)-H(14A)	109.8
C(13)-C(14)-H(14A)	109.8
N(15)-C(14)-H(14B)	109.8
C(13)-C(14)-H(14B)	109.8
H(14A)-C(14)-H(14B)	108.3
N(15)-C(16)-C(17)	108.32(13)
N(15)-C(16)-H(16A)	110.0
C(17)-C(16)-H(16A)	110.0
N(15)-C(16)-H(16B)	110.0
C(17)-C(16)-H(16B)	110.0
H(16A)-C(16)-H(16B)	108.4
N(18)-C(17)-C(16)	109.11(13)
N(18)-C(17)-H(17A)	109.9
C(16)-C(17)-H(17A)	109.9
N(18)-C(17)-H(17B)	109.9
C(16)-C(17)-H(17B)	109.9
H(17A)-C(17)-H(17B)	108.3
N(18)-C(19)-C(1)	107.66(11)
N(18)-C(19)-C(20)	116.43(13)
C(1)-C(19)-C(20)	110.23(14)
N(18)-C(19)-H(19A)	107.4
C(1)-C(19)-H(19A)	107.4
C(20)-C(19)-H(19A)	107.4
C(21)-C(20)-C(19)	109.80(14)
C(21)-C(20)-H(20A)	109.7
C(19)-C(20)-H(20A)	109.7

C(21)-C(20)-H(20B)	109.7
C(19)-C(20)-H(20B)	109.7
H(20A)-C(20)-H(20B)	108.2
C(22)-C(21)-C(20)	111.54(14)
C(22)-C(21)-H(21A)	109.3
C(20)-C(21)-H(21A)	109.3
C(22)-C(21)-H(21B)	109.3
C(20)-C(21)-H(21B)	109.3
H(21A)-C(21)-H(21B)	108.0
C(23)-C(22)-C(21)	112.96(15)
C(23)-C(22)-H(22A)	109.0
C(21)-C(22)-H(22A)	109.0
C(23)-C(22)-H(22B)	109.0
C(21)-C(22)-H(22B)	109.0
H(22A)-C(22)-H(22B)	107.8
C(24)-C(23)-C(1)	117.05(14)
C(24)-C(23)-C(22)	121.21(15)
C(1)-C(23)-C(22)	121.64(15)
C(23)-C(24)-C(4)	121.79(14)
C(23)-C(24)-H(24A)	119.1
C(4)-C(24)-H(24A)	119.1
N(29)-C(28)-C(50)	121.67(12)
N(29)-C(28)-C(46)	115.61(11)
C(50)-C(28)-C(46)	122.71(11)
N(29)-C(30)-C(31)	121.98(12)
N(29)-C(30)-C(35)	115.25(11)
C(31)-C(30)-C(35)	122.73(12)
C(51)-C(31)-C(30)	117.28(12)
C(51)-C(31)-C(32)	121.09(12)
C(30)-C(31)-C(32)	121.63(12)
C(31)-C(32)-C(33)	112.39(12)
C(31)-C(32)-H(32A)	109.1
C(33)-C(32)-H(32A)	109.1
C(31)-C(32)-H(32B)	109.1
C(33)-C(32)-H(32B)	109.1
H(32A)-C(32)-H(32B)	107.9

C(34)-C(33)-C(32)	110.36(12)
C(34)-C(33)-H(33A)	109.6
C(32)-C(33)-H(33A)	109.6
C(34)-C(33)-H(33B)	109.6
C(32)-C(33)-H(33B)	109.6
H(33A)-C(33)-H(33B)	108.1
C(35)-C(34)-C(33)	110.06(11)
C(35)-C(34)-H(34A)	109.6
C(33)-C(34)-H(34A)	109.6
C(35)-C(34)-H(34B)	109.6
C(33)-C(34)-H(34B)	109.6
H(34A)-C(34)-H(34B)	108.2
N(36)-C(35)-C(30)	108.53(11)
N(36)-C(35)-C(34)	115.92(11)
C(30)-C(35)-C(34)	110.80(11)
N(36)-C(35)-H(35A)	107.1
C(30)-C(35)-H(35A)	107.1
C(34)-C(35)-H(35A)	107.1
N(36)-C(37)-C(38)	109.59(11)
N(36)-C(37)-H(37A)	109.8
C(38)-C(37)-H(37A)	109.8
N(36)-C(37)-H(37B)	109.8
C(38)-C(37)-H(37B)	109.8
H(37A)-C(37)-H(37B)	108.2
N(39)-C(38)-C(37)	108.09(11)
N(39)-C(38)-H(38A)	110.1
C(37)-C(38)-H(38A)	110.1
N(39)-C(38)-H(38B)	110.1
C(37)-C(38)-H(38B)	110.1
H(38A)-C(38)-H(38B)	108.4
N(39)-C(40)-C(41)	108.66(12)
N(39)-C(40)-H(40A)	110.0
C(41)-C(40)-H(40A)	110.0
N(39)-C(40)-H(40B)	110.0
C(41)-C(40)-H(40B)	110.0
H(40A)-C(40)-H(40B)	108.3

N(42)-C(41)-C(40)	108.31(12)
N(42)-C(41)-H(41A)	110.0
C(40)-C(41)-H(41A)	110.0
N(42)-C(41)-H(41B)	110.0
C(40)-C(41)-H(41B)	110.0
H(41A)-C(41)-H(41B)	108.4
N(42)-C(43)-C(44)	108.72(12)
N(42)-C(43)-H(43A)	109.9
C(44)-C(43)-H(43A)	109.9
N(42)-C(43)-H(43B)	109.9
C(44)-C(43)-H(43B)	109.9
H(43A)-C(43)-H(43B)	108.3
N(45)-C(44)-C(43)	108.97(11)
N(45)-C(44)-H(44A)	109.9
C(43)-C(44)-H(44A)	109.9
N(45)-C(44)-H(44B)	109.9
C(43)-C(44)-H(44B)	109.9
H(44A)-C(44)-H(44B)	108.3
N(45)-C(46)-C(28)	108.06(10)
N(45)-C(46)-C(47)	115.34(11)
C(28)-C(46)-C(47)	110.44(11)
N(45)-C(46)-H(46A)	107.6
C(28)-C(46)-H(46A)	107.6
C(47)-C(46)-H(46A)	107.6
C(48)-C(47)-C(46)	110.41(11)
C(48)-C(47)-H(47A)	109.6
C(46)-C(47)-H(47A)	109.6
C(48)-C(47)-H(47B)	109.6
C(46)-C(47)-H(47B)	109.6
H(47A)-C(47)-H(47B)	108.1
C(47)-C(48)-C(49)	110.85(12)
C(47)-C(48)-H(48A)	109.5
C(49)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
C(49)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	108.1

C(50)-C(49)-C(48)	113.40(11)
C(50)-C(49)-H(49A)	108.9
C(48)-C(49)-H(49A)	108.9
C(50)-C(49)-H(49B)	108.9
C(48)-C(49)-H(49B)	108.9
H(49A)-C(49)-H(49B)	107.7
C(51)-C(50)-C(28)	117.41(12)
C(51)-C(50)-C(49)	120.81(12)
C(28)-C(50)-C(49)	121.72(12)
C(31)-C(51)-C(50)	121.20(12)
C(31)-C(51)-H(51A)	119.4
C(50)-C(51)-H(51A)	119.4
Cl(3S)-C(1S)-Cl(1S)	110.65(9)
Cl(3S)-C(1S)-Cl(2S)	110.57(9)
Cl(1S)-C(1S)-Cl(2S)	109.92(9)
Cl(3S)-C(1S)-H(1SA)	108.5
Cl(1S)-C(1S)-H(1SA)	108.5
Cl(2S)-C(1S)-H(1SA)	108.5

Symmetry transformations used to generate equivalent atoms:

Table 15. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **17**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mn(25)	21(1)	11(1)	17(1)	2(1)	10(1)	2(1)
Mn(52)	13(1)	12(1)	13(1)	1(1)	5(1)	1(1)
Cl(26)	41(1)	15(1)	16(1)	2(1)	13(1)	4(1)
Cl(27)	24(1)	19(1)	16(1)	3(1)	11(1)	3(1)
Cl(53)	19(1)	23(1)	13(1)	-1(1)	7(1)	1(1)
Cl(54)	21(1)	23(1)	16(1)	-4(1)	9(1)	-4(1)
N(2)	18(1)	14(1)	14(1)	1(1)	10(1)	2(1)
N(9)	19(1)	21(1)	18(1)	3(1)	9(1)	0(1)
N(12)	36(1)	18(1)	17(1)	1(1)	8(1)	-6(1)

N(15)	41(1)	15(1)	16(1)	2(1)	11(1)	8(1)
N(18)	22(1)	22(1)	18(1)	6(1)	12(1)	10(1)
N(29)	13(1)	13(1)	12(1)	0(1)	6(1)	0(1)
N(36)	13(1)	17(1)	12(1)	0(1)	5(1)	2(1)
N(39)	17(1)	18(1)	14(1)	1(1)	7(1)	2(1)
N(42)	19(1)	16(1)	16(1)	1(1)	8(1)	2(1)
N(45)	16(1)	12(1)	12(1)	0(1)	6(1)	-1(1)
C(1)	19(1)	20(1)	13(1)	1(1)	10(1)	-1(1)
C(3)	23(1)	15(1)	14(1)	2(1)	12(1)	4(1)
C(4)	36(1)	14(1)	19(1)	3(1)	18(1)	6(1)
C(5)	50(1)	18(1)	27(1)	7(1)	24(1)	15(1)
C(6)	38(1)	31(1)	26(1)	13(1)	19(1)	22(1)
C(7)	25(1)	34(1)	27(1)	10(1)	16(1)	14(1)
C(8)	18(1)	20(1)	18(1)	4(1)	10(1)	5(1)
C(10)	18(1)	34(1)	28(1)	0(1)	10(1)	-6(1)
C(11)	31(1)	31(1)	28(1)	0(1)	14(1)	-14(1)
C(13)	49(1)	16(1)	19(1)	1(1)	6(1)	-10(1)
C(14)	56(1)	12(1)	21(1)	-1(1)	7(1)	5(1)
C(16)	51(1)	25(1)	22(1)	8(1)	21(1)	23(1)
C(17)	32(1)	33(1)	29(1)	13(1)	20(1)	20(1)
C(19)	16(1)	29(1)	17(1)	3(1)	9(1)	3(1)
C(20)	18(1)	50(1)	24(1)	2(1)	12(1)	-1(1)
C(21)	23(1)	62(1)	23(1)	-5(1)	11(1)	-13(1)
C(22)	36(1)	39(1)	29(1)	-10(1)	17(1)	-20(1)
C(23)	30(1)	22(1)	19(1)	-4(1)	14(1)	-9(1)
C(24)	43(1)	15(1)	24(1)	-2(1)	20(1)	-4(1)
C(28)	13(1)	13(1)	11(1)	0(1)	6(1)	0(1)
C(30)	14(1)	14(1)	12(1)	0(1)	6(1)	0(1)
C(31)	17(1)	14(1)	15(1)	-1(1)	8(1)	-2(1)
C(32)	20(1)	14(1)	26(1)	0(1)	8(1)	-4(1)
C(33)	18(1)	18(1)	27(1)	-5(1)	8(1)	-5(1)
C(34)	15(1)	19(1)	26(1)	-3(1)	9(1)	-4(1)
C(35)	13(1)	15(1)	14(1)	-2(1)	6(1)	-1(1)
C(37)	12(1)	22(1)	17(1)	1(1)	5(1)	1(1)
C(38)	15(1)	23(1)	17(1)	2(1)	7(1)	5(1)
C(40)	20(1)	17(1)	23(1)	2(1)	6(1)	6(1)

C(41)	24(1)	15(1)	21(1)	5(1)	7(1)	4(1)
C(43)	21(1)	14(1)	22(1)	4(1)	11(1)	0(1)
C(44)	18(1)	13(1)	20(1)	0(1)	7(1)	-2(1)
C(46)	13(1)	13(1)	13(1)	0(1)	5(1)	-1(1)
C(47)	13(1)	18(1)	21(1)	3(1)	7(1)	-2(1)
C(48)	14(1)	20(1)	19(1)	2(1)	3(1)	0(1)
C(49)	14(1)	18(1)	19(1)	2(1)	5(1)	2(1)
C(50)	14(1)	15(1)	12(1)	0(1)	5(1)	1(1)
C(51)	18(1)	12(1)	17(1)	1(1)	8(1)	2(1)
C(1S)	23(1)	25(1)	23(1)	3(1)	11(1)	3(1)
Cl(1S)	32(1)	24(1)	27(1)	-5(1)	15(1)	-2(1)
Cl(2S)	40(1)	41(1)	39(1)	16(1)	12(1)	15(1)
Cl(3S)	22(1)	26(1)	26(1)	-2(1)	9(1)	-2(1)
O(1S)	20(1)	25(1)	21(1)	0	10(1)	0
O(2S)	64(2)	60(2)	84(2)	0	18(2)	0

Table 16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for **17**.

	x	y	z	U(eq)
H(9)	1318(7)	5274(17)	4095(9)	30(5)
H(12)	1211(7)	2736(19)	3215(10)	39(6)
H(15)	2362(7)	2331(18)	4395(9)	33(6)
H(18)	2552(6)	4693(16)	3639(9)	25(5)
H(36)	164(6)	8920(15)	1730(8)	20(5)
H(39)	-63(6)	10952(16)	526(9)	23(5)
H(42)	843(6)	12476(15)	1717(8)	18(4)
H(45)	1441(6)	10294(15)	1453(8)	14(4)
H(5A)	1450	9223	3347	35
H(5B)	1360	8992	3894	35
H(6A)	932	7974	2779	36
H(6B)	702	8608	3114	36

H(7A)	918	7123	3810	32
H(7B)	587	6713	3167	32
H(8A)	1166	6008	3025	22
H(10A)	735	4417	3028	32
H(10B)	610	4761	3536	32
H(11A)	1052	3295	4130	36
H(11B)	691	2799	3521	36
H(13A)	1282	1187	3706	38
H(13B)	1599	1830	4294	38
H(14A)	2032	837	3934	41
H(14B)	1798	1509	3333	41
H(16A)	2439	2571	3399	37
H(16B)	2744	1791	3936	37
H(17A)	3019	3344	4552	35
H(17B)	3099	3528	3991	35
H(19A)	2843	5157	4776	24
H(20A)	3458	5301	4603	36
H(20B)	3191	6072	4046	36
H(21A)	3376	6686	5210	43
H(21B)	3652	7138	4891	43
H(22A)	3070	8368	4868	41
H(22B)	3083	8193	4261	41
H(24A)	2264	8938	4157	30
H(32A)	681	5447	2011	25
H(32B)	869	5141	1562	25
H(33A)	275	5958	795	26
H(33B)	64	5238	1127	26
H(34A)	-270	6985	949	24
H(34B)	33	6878	1638	24
H(35A)	264	8017	843	17
H(37A)	-515	8965	1068	21
H(37B)	-357	9124	574	21
H(38A)	-642	10825	716	22
H(38B)	-299	10804	1396	22
H(40A)	22	12553	1299	26
H(40B)	-253	12654	604	26

H(41A)	417	12501	520	26
H(41B)	445	13540	922	26
H(43A)	1319	13190	1435	23
H(43B)	1212	12177	989	23
H(44A)	1873	11780	1842	21
H(44B)	1626	11963	2238	21
H(46A)	1693	10110	2608	16
H(47A)	2207	9424	2039	21
H(47B)	2345	10363	2529	21
H(48A)	2374	8995	3218	23
H(48B)	2723	8733	2976	23
H(49A)	2308	7321	2404	21
H(49B)	2273	7157	2996	21
H(51A)	1582	6042	2308	19
H(1SA)	6512	-957	5262	28

Table 17. Torsion angles [°] for **17**.

N(15)-Mn(25)-N(2)-C(3)	178.07(10)
N(12)-Mn(25)-N(2)-C(3)	-10.35(15)
N(9)-Mn(25)-N(2)-C(3)	-17.71(10)
N(18)-Mn(25)-N(2)-C(3)	161.03(12)
Cl(26)-Mn(25)-N(2)-C(3)	77.92(10)
Cl(27)-Mn(25)-N(2)-C(3)	-102.97(10)
N(15)-Mn(25)-N(2)-C(1)	-4.30(15)
N(12)-Mn(25)-N(2)-C(1)	167.28(10)
N(9)-Mn(25)-N(2)-C(1)	159.92(12)
N(18)-Mn(25)-N(2)-C(1)	-21.35(10)
Cl(26)-Mn(25)-N(2)-C(1)	-104.46(10)
Cl(27)-Mn(25)-N(2)-C(1)	74.66(10)
N(2)-Mn(25)-N(9)-C(10)	163.60(12)
N(15)-Mn(25)-N(9)-C(10)	-34.81(15)
N(12)-Mn(25)-N(9)-C(10)	-11.83(10)
N(18)-Mn(25)-N(9)-C(10)	161.83(10)

Cl(26)-Mn(25)-N(9)-C(10)	71.26(10)
Cl(27)-Mn(25)-N(9)-C(10)	-108.27(10)
N(2)-Mn(25)-N(9)-C(8)	34.49(9)
N(15)-Mn(25)-N(9)-C(8)	-163.93(10)
N(12)-Mn(25)-N(9)-C(8)	-140.95(11)
N(18)-Mn(25)-N(9)-C(8)	32.71(13)
Cl(26)-Mn(25)-N(9)-C(8)	-57.86(10)
Cl(27)-Mn(25)-N(9)-C(8)	122.62(10)
N(2)-Mn(25)-N(12)-C(13)	-155.39(10)
N(15)-Mn(25)-N(12)-C(13)	19.13(11)
N(9)-Mn(25)-N(12)-C(13)	-148.20(12)
N(18)-Mn(25)-N(12)-C(13)	39.59(16)
Cl(26)-Mn(25)-N(12)-C(13)	113.29(11)
Cl(27)-Mn(25)-N(12)-C(13)	-65.51(11)
N(2)-Mn(25)-N(12)-C(11)	-26.45(15)
N(15)-Mn(25)-N(12)-C(11)	148.06(12)
N(9)-Mn(25)-N(12)-C(11)	-19.26(11)
N(18)-Mn(25)-N(12)-C(11)	168.53(10)
Cl(26)-Mn(25)-N(12)-C(11)	-117.78(11)
Cl(27)-Mn(25)-N(12)-C(11)	63.43(11)
N(2)-Mn(25)-N(15)-C(16)	-44.53(14)
N(12)-Mn(25)-N(15)-C(16)	140.64(12)
N(9)-Mn(25)-N(15)-C(16)	163.42(10)
N(18)-Mn(25)-N(15)-C(16)	-28.00(11)
Cl(26)-Mn(25)-N(15)-C(16)	56.22(11)
Cl(27)-Mn(25)-N(15)-C(16)	-123.60(11)
N(2)-Mn(25)-N(15)-C(14)	-172.60(10)
N(12)-Mn(25)-N(15)-C(14)	12.57(11)
N(9)-Mn(25)-N(15)-C(14)	35.35(16)
N(18)-Mn(25)-N(15)-C(14)	-156.07(12)
Cl(26)-Mn(25)-N(15)-C(14)	-71.85(11)
Cl(27)-Mn(25)-N(15)-C(14)	108.33(11)
N(2)-Mn(25)-N(18)-C(19)	35.47(9)
N(15)-Mn(25)-N(18)-C(19)	-133.39(11)
N(12)-Mn(25)-N(18)-C(19)	-154.06(10)
N(9)-Mn(25)-N(18)-C(19)	37.26(13)

Cl(26)-Mn(25)-N(18)-C(19)	132.23(10)
Cl(27)-Mn(25)-N(18)-C(19)	-48.86(10)
N(2)-Mn(25)-N(18)-C(17)	166.99(12)
N(15)-Mn(25)-N(18)-C(17)	-1.87(11)
N(12)-Mn(25)-N(18)-C(17)	-22.53(16)
N(9)-Mn(25)-N(18)-C(17)	168.79(10)
Cl(26)-Mn(25)-N(18)-C(17)	-96.24(11)
Cl(27)-Mn(25)-N(18)-C(17)	82.66(11)
N(39)-Mn(52)-N(29)-C(30)	2.87(14)
N(42)-Mn(52)-N(29)-C(30)	-171.00(9)
N(45)-Mn(52)-N(29)-C(30)	-160.20(11)
N(36)-Mn(52)-N(29)-C(30)	20.78(10)
Cl(53)-Mn(52)-N(29)-C(30)	-76.88(10)
Cl(54)-Mn(52)-N(29)-C(30)	109.59(10)
N(39)-Mn(52)-N(29)-C(28)	177.86(9)
N(42)-Mn(52)-N(29)-C(28)	4.00(14)
N(45)-Mn(52)-N(29)-C(28)	14.79(10)
N(36)-Mn(52)-N(29)-C(28)	-164.22(11)
Cl(53)-Mn(52)-N(29)-C(28)	98.11(10)
Cl(54)-Mn(52)-N(29)-C(28)	-75.42(10)
N(29)-Mn(52)-N(36)-C(35)	-36.43(8)
N(39)-Mn(52)-N(36)-C(35)	132.39(9)
N(42)-Mn(52)-N(36)-C(35)	156.54(9)
N(45)-Mn(52)-N(36)-C(35)	-37.86(12)
Cl(53)-Mn(52)-N(36)-C(35)	46.99(8)
Cl(54)-Mn(52)-N(36)-C(35)	-129.81(8)
N(29)-Mn(52)-N(36)-C(37)	-161.45(10)
N(39)-Mn(52)-N(36)-C(37)	7.37(9)
N(42)-Mn(52)-N(36)-C(37)	31.52(14)
N(45)-Mn(52)-N(36)-C(37)	-162.88(9)
Cl(53)-Mn(52)-N(36)-C(37)	-78.03(9)
Cl(54)-Mn(52)-N(36)-C(37)	105.17(9)
N(29)-Mn(52)-N(39)-C(38)	40.81(13)
N(42)-Mn(52)-N(39)-C(38)	-143.07(10)
N(45)-Mn(52)-N(39)-C(38)	-167.68(9)
N(36)-Mn(52)-N(39)-C(38)	23.28(9)

Cl(53)-Mn(52)-N(39)-C(38)	120.10(9)
Cl(54)-Mn(52)-N(39)-C(38)	-64.51(9)
N(29)-Mn(52)-N(39)-C(40)	169.21(9)
N(42)-Mn(52)-N(39)-C(40)	-14.68(10)
N(45)-Mn(52)-N(39)-C(40)	-39.28(14)
N(36)-Mn(52)-N(39)-C(40)	151.68(11)
Cl(53)-Mn(52)-N(39)-C(40)	-111.50(10)
Cl(54)-Mn(52)-N(39)-C(40)	63.89(10)
N(29)-Mn(52)-N(42)-C(43)	30.40(14)
N(39)-Mn(52)-N(42)-C(43)	-145.76(11)
N(45)-Mn(52)-N(42)-C(43)	19.82(10)
N(36)-Mn(52)-N(42)-C(43)	-169.80(9)
Cl(53)-Mn(52)-N(42)-C(43)	-60.27(10)
Cl(54)-Mn(52)-N(42)-C(43)	113.93(10)
N(29)-Mn(52)-N(42)-C(41)	159.15(9)
N(39)-Mn(52)-N(42)-C(41)	-17.00(10)
N(45)-Mn(52)-N(42)-C(41)	148.57(11)
N(36)-Mn(52)-N(42)-C(41)	-41.04(14)
Cl(53)-Mn(52)-N(42)-C(41)	68.49(10)
Cl(54)-Mn(52)-N(42)-C(41)	-117.31(10)
N(29)-Mn(52)-N(45)-C(46)	-30.53(9)
N(39)-Mn(52)-N(45)-C(46)	167.43(9)
N(42)-Mn(52)-N(45)-C(46)	142.60(10)
N(36)-Mn(52)-N(45)-C(46)	-29.09(12)
Cl(53)-Mn(52)-N(45)-C(46)	-118.87(9)
Cl(54)-Mn(52)-N(45)-C(46)	62.37(9)
N(29)-Mn(52)-N(45)-C(44)	-162.39(11)
N(39)-Mn(52)-N(45)-C(44)	35.57(14)
N(42)-Mn(52)-N(45)-C(44)	10.73(9)
N(36)-Mn(52)-N(45)-C(44)	-160.95(9)
Cl(53)-Mn(52)-N(45)-C(44)	109.27(9)
Cl(54)-Mn(52)-N(45)-C(44)	-69.49(9)
C(3)-N(2)-C(1)-C(23)	1.1(2)
Mn(25)-N(2)-C(1)-C(23)	-176.54(11)
C(3)-N(2)-C(1)-C(19)	-178.83(13)
Mn(25)-N(2)-C(1)-C(19)	3.56(16)

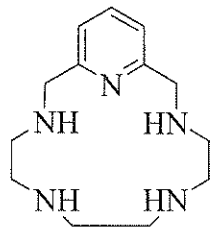
C(1)-N(2)-C(3)-C(4)	-0.4(2)
Mn(25)-N(2)-C(3)-C(4)	177.22(11)
C(1)-N(2)-C(3)-C(8)	179.85(12)
Mn(25)-N(2)-C(3)-C(8)	-2.54(16)
N(2)-C(3)-C(4)-C(24)	-1.1(2)
C(8)-C(3)-C(4)-C(24)	178.64(14)
N(2)-C(3)-C(4)-C(5)	178.25(14)
C(8)-C(3)-C(4)-C(5)	-2.0(2)
C(24)-C(4)-C(5)-C(6)	168.90(15)
C(3)-C(4)-C(5)-C(6)	-10.4(2)
C(4)-C(5)-C(6)-C(7)	43.18(19)
C(5)-C(6)-C(7)-C(8)	-64.98(18)
C(10)-N(9)-C(8)-C(3)	-173.04(13)
Mn(25)-N(9)-C(8)-C(3)	-46.77(13)
C(10)-N(9)-C(8)-C(7)	62.52(19)
Mn(25)-N(9)-C(8)-C(7)	-171.21(11)
N(2)-C(3)-C(8)-N(9)	33.62(17)
C(4)-C(3)-C(8)-N(9)	-146.14(14)
N(2)-C(3)-C(8)-C(7)	161.32(13)
C(4)-C(3)-C(8)-C(7)	-18.4(2)
C(6)-C(7)-C(8)-N(9)	173.55(14)
C(6)-C(7)-C(8)-C(3)	50.36(18)
C(8)-N(9)-C(10)-C(11)	165.25(14)
Mn(25)-N(9)-C(10)-C(11)	40.01(16)
C(13)-N(12)-C(11)-C(10)	171.97(14)
Mn(25)-N(12)-C(11)-C(10)	46.97(15)
N(9)-C(10)-C(11)-N(12)	-58.13(18)
C(11)-N(12)-C(13)-C(14)	-173.31(14)
Mn(25)-N(12)-C(13)-C(14)	-47.16(15)
C(16)-N(15)-C(14)-C(13)	-166.28(14)
Mn(25)-N(15)-C(14)-C(13)	-42.07(16)
N(12)-C(13)-C(14)-N(15)	60.57(17)
C(14)-N(15)-C(16)-C(17)	179.17(13)
Mn(25)-N(15)-C(16)-C(17)	54.46(14)
C(19)-N(18)-C(17)-C(16)	158.73(13)
Mn(25)-N(18)-C(17)-C(16)	30.39(16)

N(15)-C(16)-C(17)-N(18)	-56.53(17)
C(17)-N(18)-C(19)-C(1)	-174.01(13)
Mn(25)-N(18)-C(19)-C(1)	-44.96(13)
C(17)-N(18)-C(19)-C(20)	61.69(19)
Mn(25)-N(18)-C(19)-C(20)	-169.25(11)
N(2)-C(1)-C(19)-N(18)	28.25(17)
C(23)-C(1)-C(19)-N(18)	-151.65(14)
N(2)-C(1)-C(19)-C(20)	156.21(13)
C(23)-C(1)-C(19)-C(20)	-23.7(2)
N(18)-C(19)-C(20)-C(21)	175.76(14)
C(1)-C(19)-C(20)-C(21)	52.79(18)
C(19)-C(20)-C(21)-C(22)	-64.25(19)
C(20)-C(21)-C(22)-C(23)	42.1(2)
N(2)-C(1)-C(23)-C(24)	-0.2(2)
C(19)-C(1)-C(23)-C(24)	179.71(14)
N(2)-C(1)-C(23)-C(22)	-176.70(14)
C(19)-C(1)-C(23)-C(22)	3.2(2)
C(21)-C(22)-C(23)-C(24)	171.46(15)
C(21)-C(22)-C(23)-C(1)	-12.2(2)
C(1)-C(23)-C(24)-C(4)	-1.4(2)
C(22)-C(23)-C(24)-C(4)	175.16(15)
C(3)-C(4)-C(24)-C(23)	2.0(2)
C(5)-C(4)-C(24)-C(23)	-177.36(15)
C(30)-N(29)-C(28)-C(50)	-1.2(2)
Mn(52)-N(29)-C(28)-C(50)	-176.12(10)
C(30)-N(29)-C(28)-C(46)	178.17(12)
Mn(52)-N(29)-C(28)-C(46)	3.26(16)
C(28)-N(29)-C(30)-C(31)	2.2(2)
Mn(52)-N(29)-C(30)-C(31)	177.19(10)
C(28)-N(29)-C(30)-C(35)	-175.69(12)
Mn(52)-N(29)-C(30)-C(35)	-0.68(16)
N(29)-C(30)-C(31)-C(51)	-1.3(2)
C(35)-C(30)-C(31)-C(51)	176.46(13)
N(29)-C(30)-C(31)-C(32)	178.57(13)
C(35)-C(30)-C(31)-C(32)	-3.7(2)
C(51)-C(31)-C(32)-C(33)	-163.36(14)

C(30)-C(31)-C(32)-C(33)	16.8(2)
C(31)-C(32)-C(33)-C(34)	-46.76(18)
C(32)-C(33)-C(34)-C(35)	65.30(17)
C(37)-N(36)-C(35)-C(30)	170.66(11)
Mn(52)-N(36)-C(35)-C(30)	47.90(12)
C(37)-N(36)-C(35)-C(34)	-63.94(16)
Mn(52)-N(36)-C(35)-C(34)	173.31(10)
N(29)-C(30)-C(35)-N(36)	-33.29(16)
C(31)-C(30)-C(35)-N(36)	148.85(13)
N(29)-C(30)-C(35)-C(34)	-161.64(12)
C(31)-C(30)-C(35)-C(34)	20.50(19)
C(33)-C(34)-C(35)-N(36)	-174.41(12)
C(33)-C(34)-C(35)-C(30)	-50.18(16)
C(35)-N(36)-C(37)-C(38)	-156.50(12)
Mn(52)-N(36)-C(37)-C(38)	-35.94(14)
C(40)-N(39)-C(38)-C(37)	-176.22(12)
Mn(52)-N(39)-C(38)-C(37)	-50.34(13)
N(36)-C(37)-C(38)-N(39)	57.82(15)
C(38)-N(39)-C(40)-C(41)	169.43(12)
Mn(52)-N(39)-C(40)-C(41)	43.61(14)
C(43)-N(42)-C(41)-C(40)	171.62(12)
Mn(52)-N(42)-C(41)-C(40)	45.38(14)
N(39)-C(40)-C(41)-N(42)	-60.31(16)
C(41)-N(42)-C(43)-C(44)	-172.09(12)
Mn(52)-N(42)-C(43)-C(44)	-46.86(14)
C(46)-N(45)-C(44)-C(43)	-168.15(12)
Mn(52)-N(45)-C(44)-C(43)	-38.44(14)
N(42)-C(43)-C(44)-N(45)	56.84(16)
C(44)-N(45)-C(46)-C(28)	171.41(11)
Mn(52)-N(45)-C(46)-C(28)	41.39(12)
C(44)-N(45)-C(46)-C(47)	-64.48(16)
Mn(52)-N(45)-C(46)-C(47)	165.50(9)
N(29)-C(28)-C(46)-N(45)	-30.07(16)
C(50)-C(28)-C(46)-N(45)	149.31(13)
N(29)-C(28)-C(46)-C(47)	-157.08(12)
C(50)-C(28)-C(46)-C(47)	22.30(18)

N(45)-C(46)-C(47)-C(48)	-174.59(12)
C(28)-C(46)-C(47)-C(48)	-51.74(16)
C(46)-C(47)-C(48)-C(49)	63.56(16)
C(47)-C(48)-C(49)-C(50)	-42.40(17)
N(29)-C(28)-C(50)-C(51)	-0.6(2)
C(46)-C(28)-C(50)-C(51)	-179.95(13)
N(29)-C(28)-C(50)-C(49)	176.61(13)
C(46)-C(28)-C(50)-C(49)	-2.7(2)
C(48)-C(49)-C(50)-C(51)	-170.15(13)
C(48)-C(49)-C(50)-C(28)	12.7(2)
C(30)-C(31)-C(51)-C(50)	-0.6(2)
C(32)-C(31)-C(51)-C(50)	179.56(14)
C(28)-C(50)-C(51)-C(31)	1.5(2)
C(49)-C(50)-C(51)-C(31)	-175.74(13)

3,6,9,12,18-Pentaazabicyclo-
[12,3,1]octadeca-1(18),14,16-triene

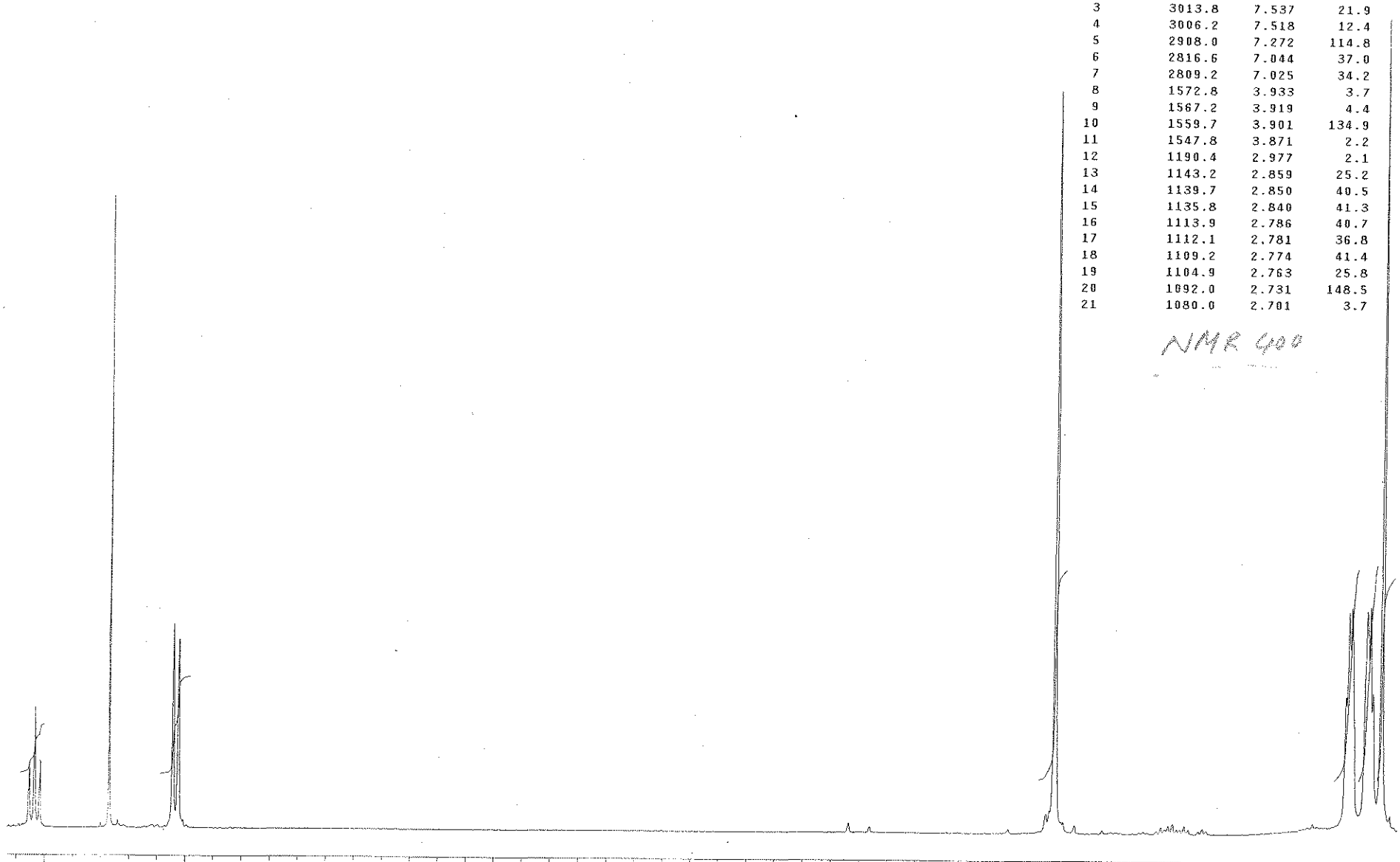


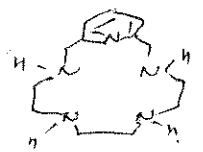
SH05

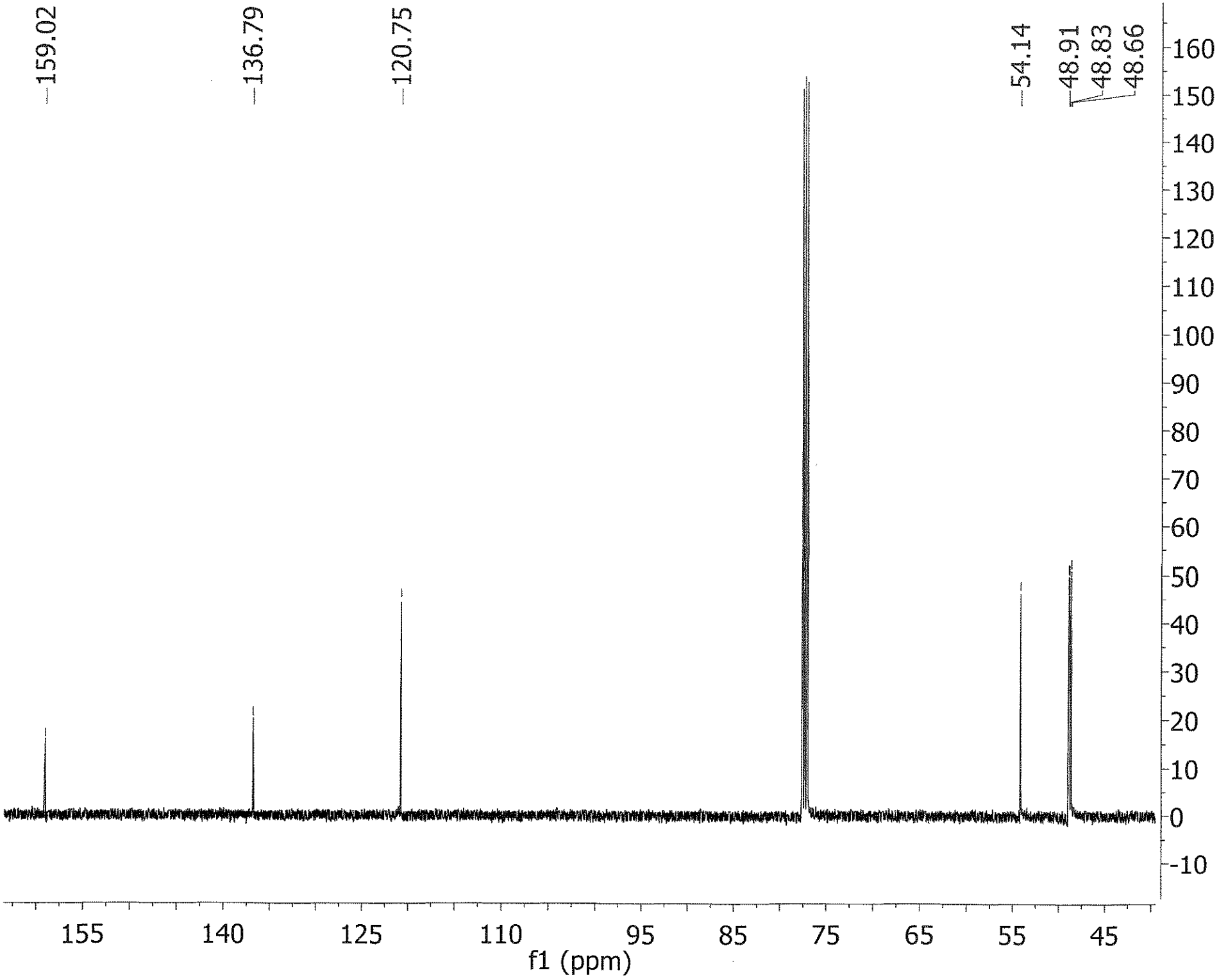
$C_{13}H_{23}N_5$
Exact Mass: 249.2
Mol. Wt.: 249.36
m/e: 249.20 (100.0%), 250.20 (14.3%),
250.19 (1.8%), 251.20 (1.2%)
C, 62.62; H, 9.30; N, 28.09

INDEX	FREQUENCY	PPM	HEIGHT
1	3022.6	7.559	7.0
2	3021.4	7.556	10.9
3	3013.8	7.537	21.9
4	3006.2	7.518	12.4
5	2908.0	7.272	114.8
6	2816.6	7.044	37.0
7	2809.2	7.025	34.2
8	1572.8	3.933	3.7
9	1567.2	3.919	4.4
10	1559.7	3.901	134.9
11	1547.8	3.871	2.2
12	1190.4	2.977	2.1
13	1143.2	2.859	25.2
14	1139.7	2.850	40.5
15	1135.8	2.840	41.3
16	1113.9	2.786	40.7
17	1112.1	2.781	36.8
18	1109.2	2.774	41.4
19	1104.9	2.763	25.8
20	1092.0	2.731	148.5
21	1080.0	2.701	3.7

NMR 400



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136.79
120.75
54.14
48.91
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48.66
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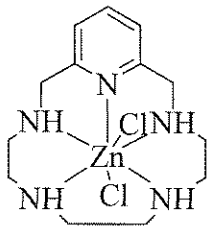
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
155
140
125
110
95
85
75
65
55
45
f1 (ppm)

3,6,9,12,18-Pentaazabicyclo[12,3,1]octadeca-1(18),14,16-triene dichlorozinc (II)



SH20

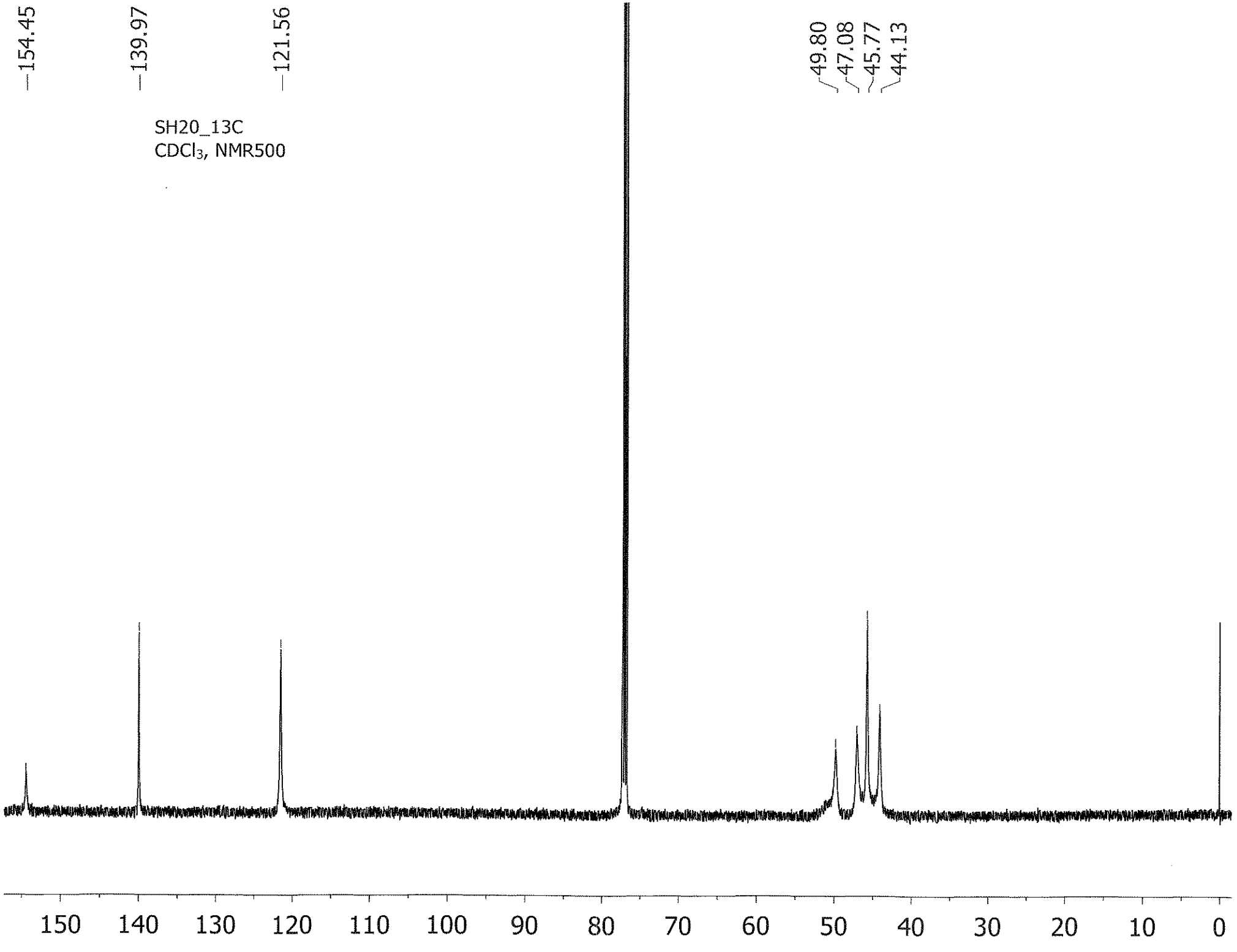
$C_{13}H_{23}Cl_2N_5Zn$

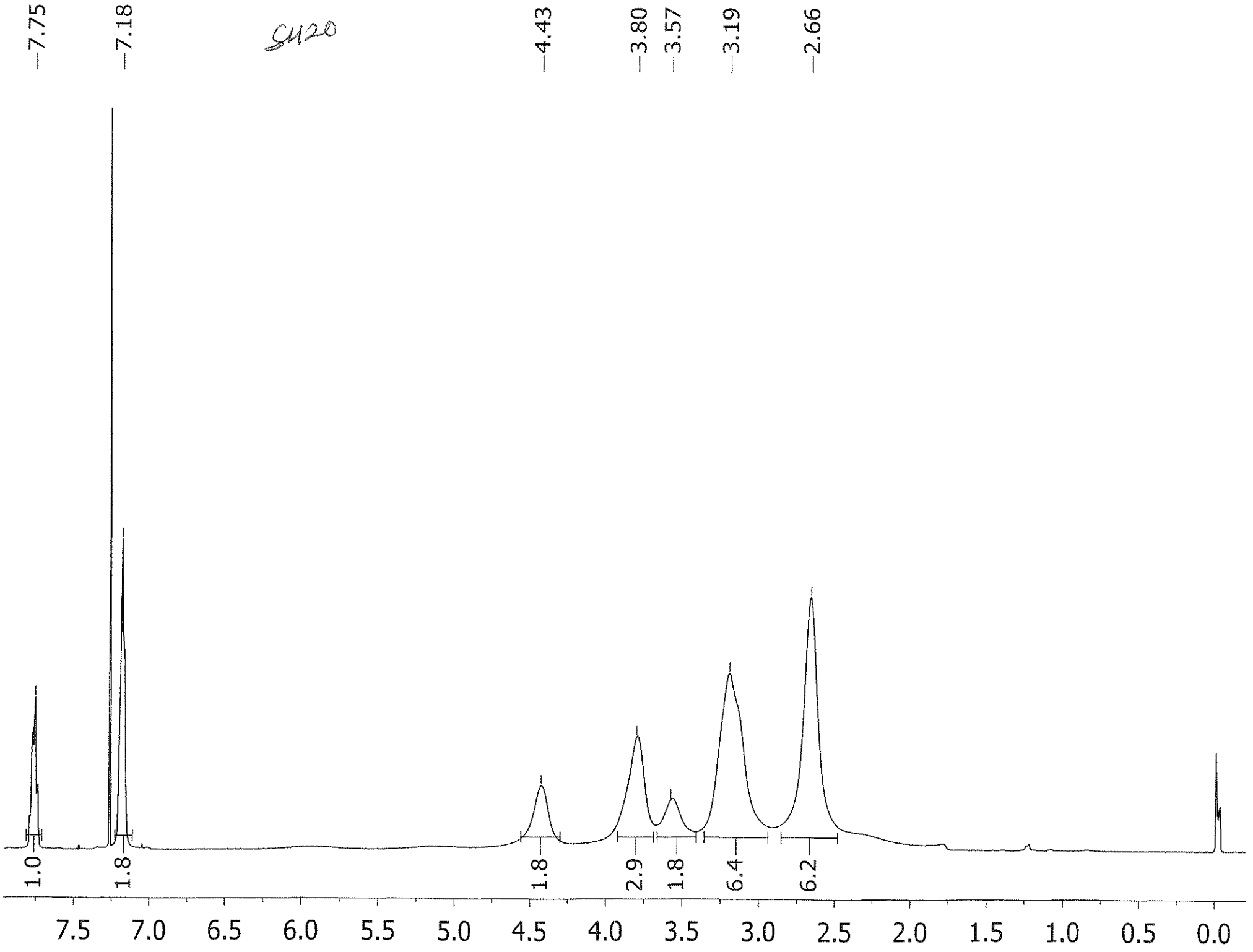
Exact Mass: 383.06

Mol. Wt.: 385.65

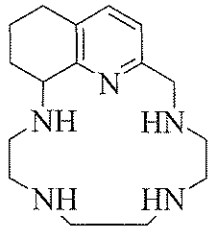
m/e: 385.06 (100.0%), 383.06 (82.3%), 387.06 (71.7%), 389.05 (25.2%), 386.06 (22.8%), 388.06 (14.5%), 384.07 (11.8%), 390.06 (3.8%), 391.05 (3.3%), 389.06 (2.5%), 384.06 (1.5%), 388.05 (1.3%), 390.05 (1.2%), 391.06 (1.1%)

C, 40.49; H, 6.01; Cl, 18.39; N, 18.16; Zn, 16.96


154.45
139.97
121.56
49.80
47.08
45.77
44.13
SH20_13C
CDCl3, NMR500
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


7.75
7.18
SM20
4.43
3.80
3.57
3.19
2.66
1.0
1.8
1.8
2.9
1.8
6.4
6.2
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

3,4,5,6,7,8,9,10,11,12,13,13a,14,15,16-Pentadecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine



SH07

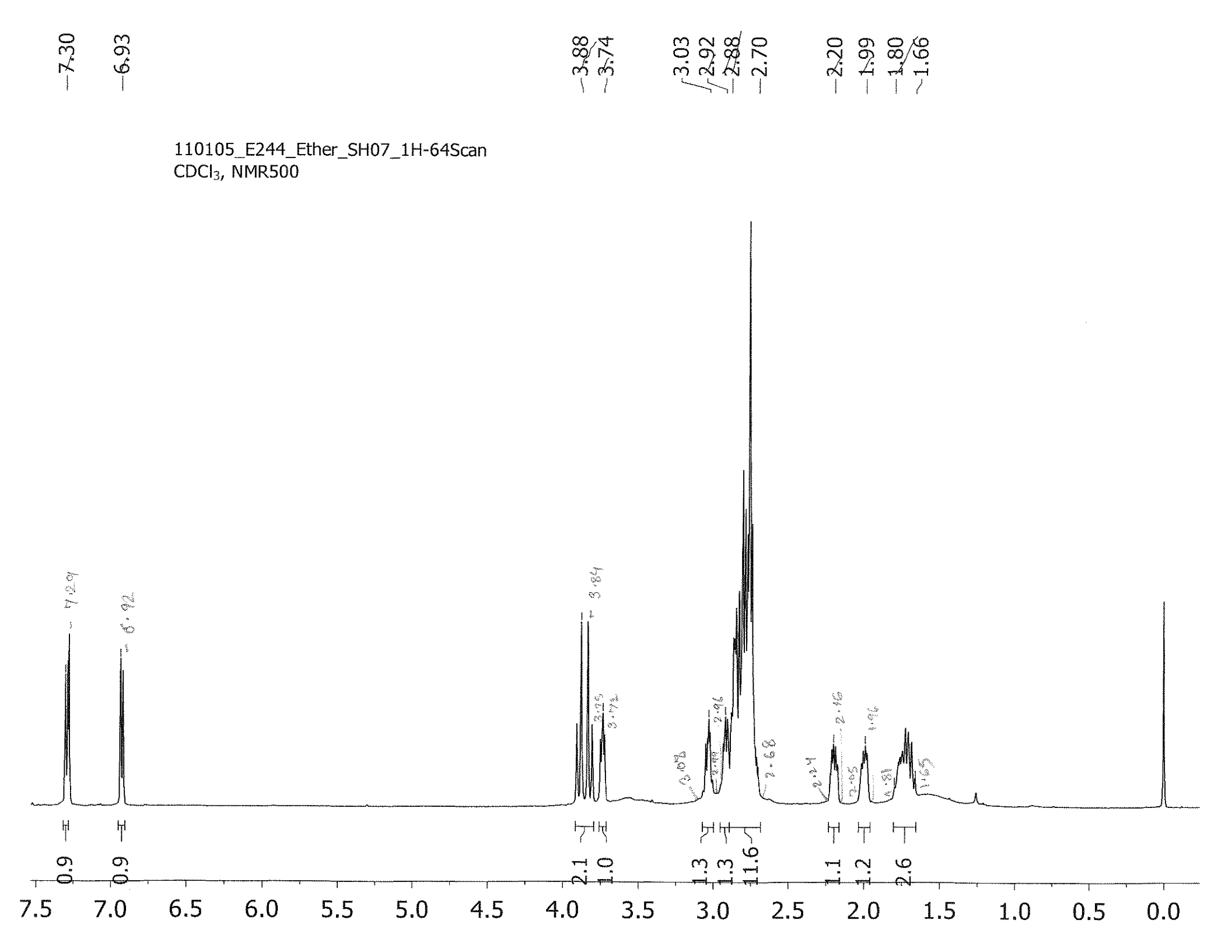
$C_{16}H_{27}N_5$

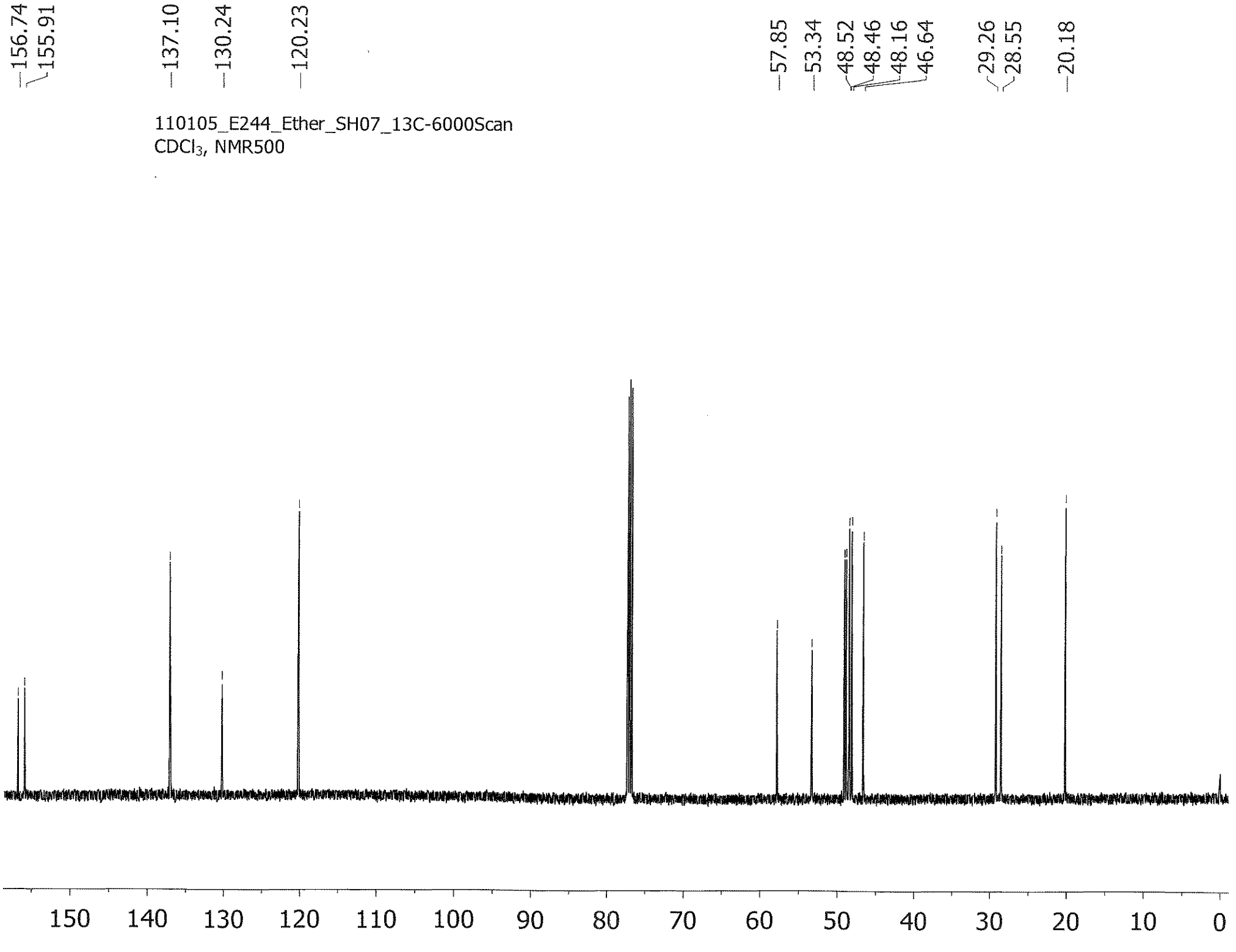
Exact Mass: 289.23

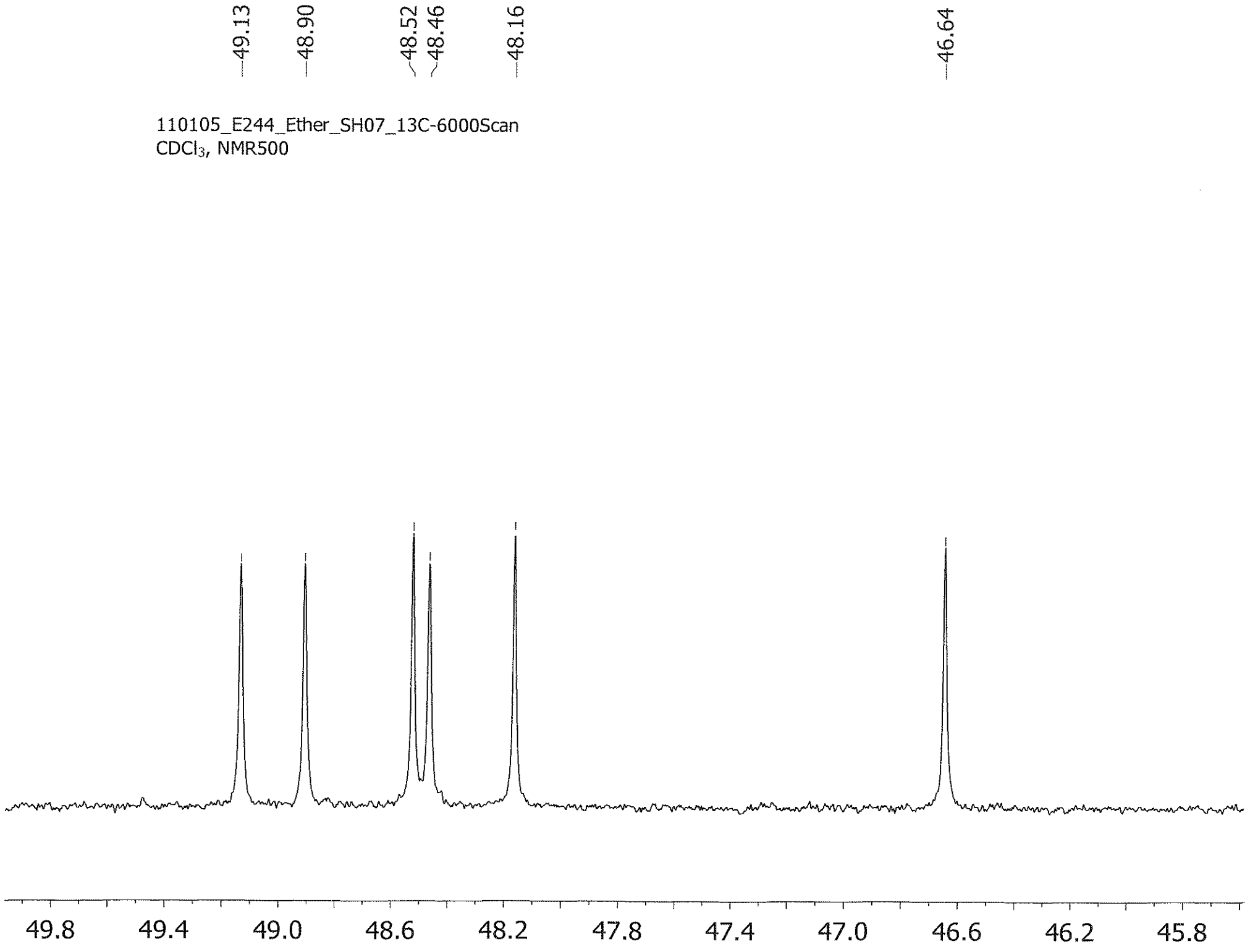
Mol. Wt.: 289.42

m/e: 289.23 (100.0%), 290.23 (17.6%), 290.22 (1.8%), 291.23 (1.7%)

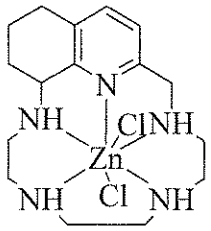
C, 66.40; H, 9.40; N, 24.20


7.30
6.93
3.88
3.74
3.03
2.92
2.88
2.70
2.20
1.99
1.80
1.66
110105_E244_Ether_SH07_1H-64Scan
CDCl3, NMR500
0.9
0.9
2.1
1.0
1.3
1.3
11.6
1.1
1.2
2.6
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


156.74
155.91
137.10
130.24
120.23
57.85
53.34
48.52
48.46
48.16
46.64
29.26
28.55
20.18
110105_E244_Ether_SH07_13C-6000Scan
CDCl3, NMR500
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


49.13
48.90
48.52
48.46
48.16
46.64
110105_E244_Ether_SH07_13C-6000Scan
CDCl3, NMR500
49.8
49.4
49.0
48.6
48.2
47.8
47.4
47.0
46.6
46.2
45.8

3,4,5,6,7,8,9,10,11,12,13,13a,14,15,16-Pentadecahydro-2,17-etheno-1,4,7,10,13-benzopentaazacyclopentadecine dichlorozinc (II)



SH36

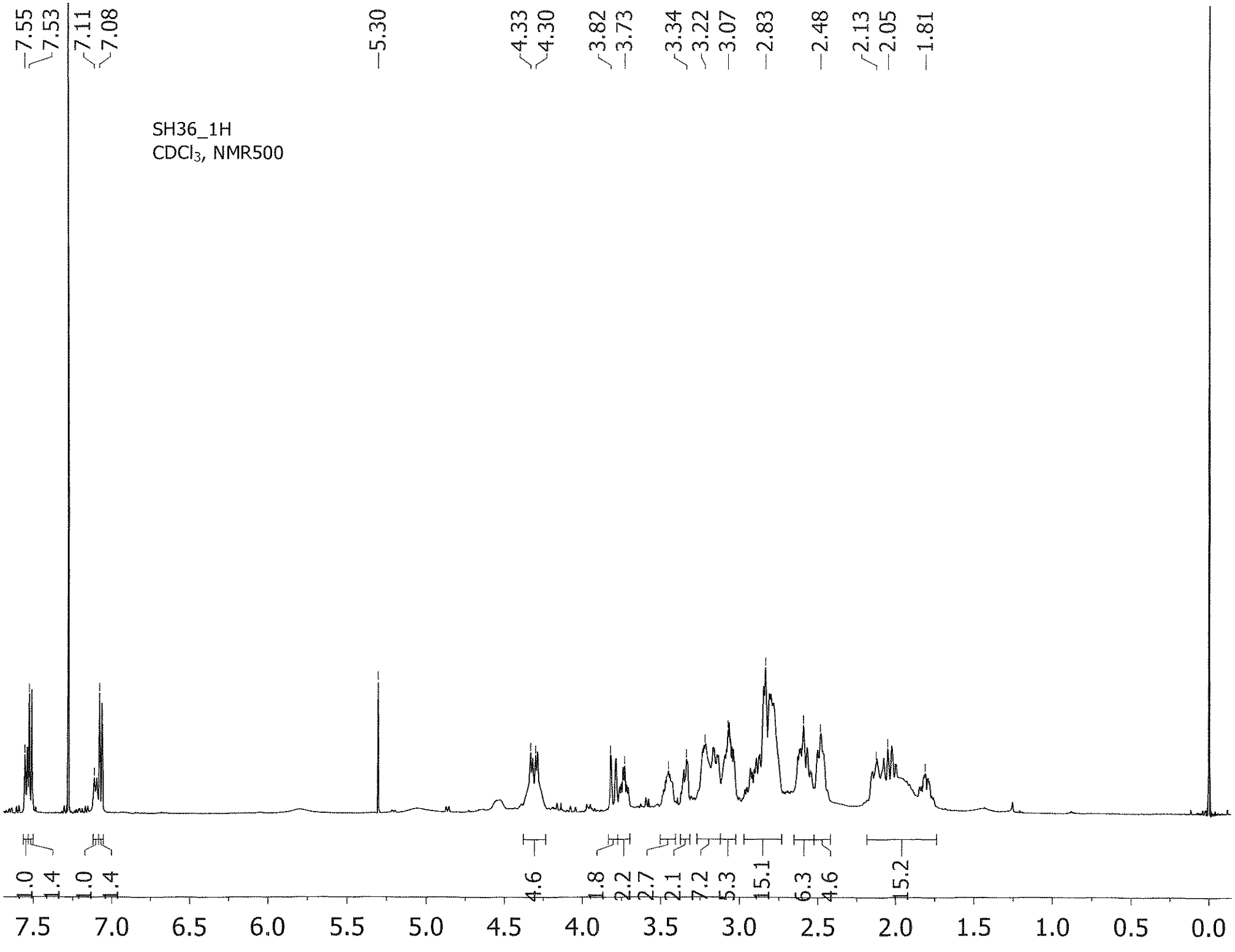
$C_{16}H_{27}Cl_2N_5Zn$

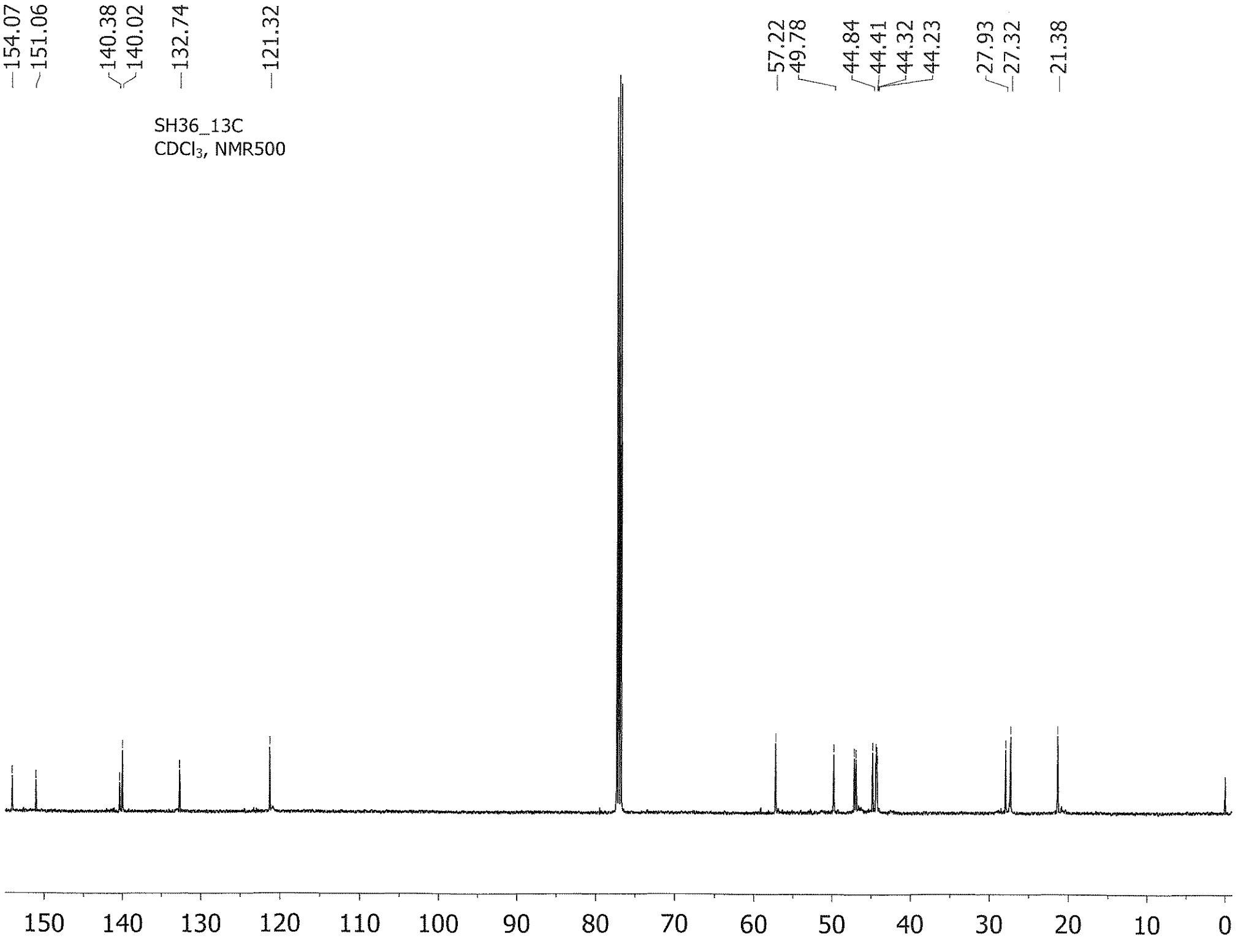
Exact Mass: 423.09

Mol. Wt.: 425.72

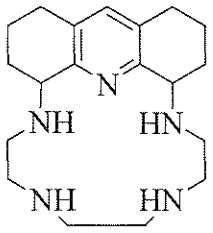
m/e: 425.09 (100.0%), 423.09 (82.2%), 427.09 (71.9%), 426.09 (26.0%), 429.09 (22.9%), 428.09 (17.3%), 424.10 (14.5%), 430.09 (5.4%), 429.08 (4.8%), 431.08 (3.3%), 424.09 (1.5%), 427.10 (1.5%), 431.09 (1.2%), 425.10 (1.2%)

C, 45.14; H, 6.39; Cl, 16.66; N, 16.45; Zn, 15.36


7.55
7.53
7.11
7.08
5.30
4.33
4.30
3.82
3.73
3.34
3.22
3.07
2.83
2.48
2.13
2.05
1.81
SH36_1H
CDCl3, NMR500
1.0
1.4
1.0
1.4
4.6
1.8
2.2
2.7
2.1
7.2
5.3
15.1
6.3
4.6
15.2
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


154.07
151.06
140.38
140.02
132.74
121.32
57.22
49.78
44.84
44.41
44.32
44.23
27.93
27.32
21.38
SH36_13C
CDCl3, NMR500
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

2,3,4,4a,5,6,7,8,9,10,11,12,13,14,14a,15,16,
17-Octaadecahydro-1,18-methenodibenzo
[b,e][1,4,7,10,13]pentaazacyclopentadecine



SH09

$C_{19}H_{31}N_5$
Exact Mass: 329.26
Mol. Wt.: 329.48
m/e: 329.26 (100.0%), 330.26
(20.9%), 331.26 (2.4%), 330.25 (1.8%)
C, 69.26; H, 9.48; N, 21.26

SH09 4th Fraction 5-6 E247 ~~E247~~ E260

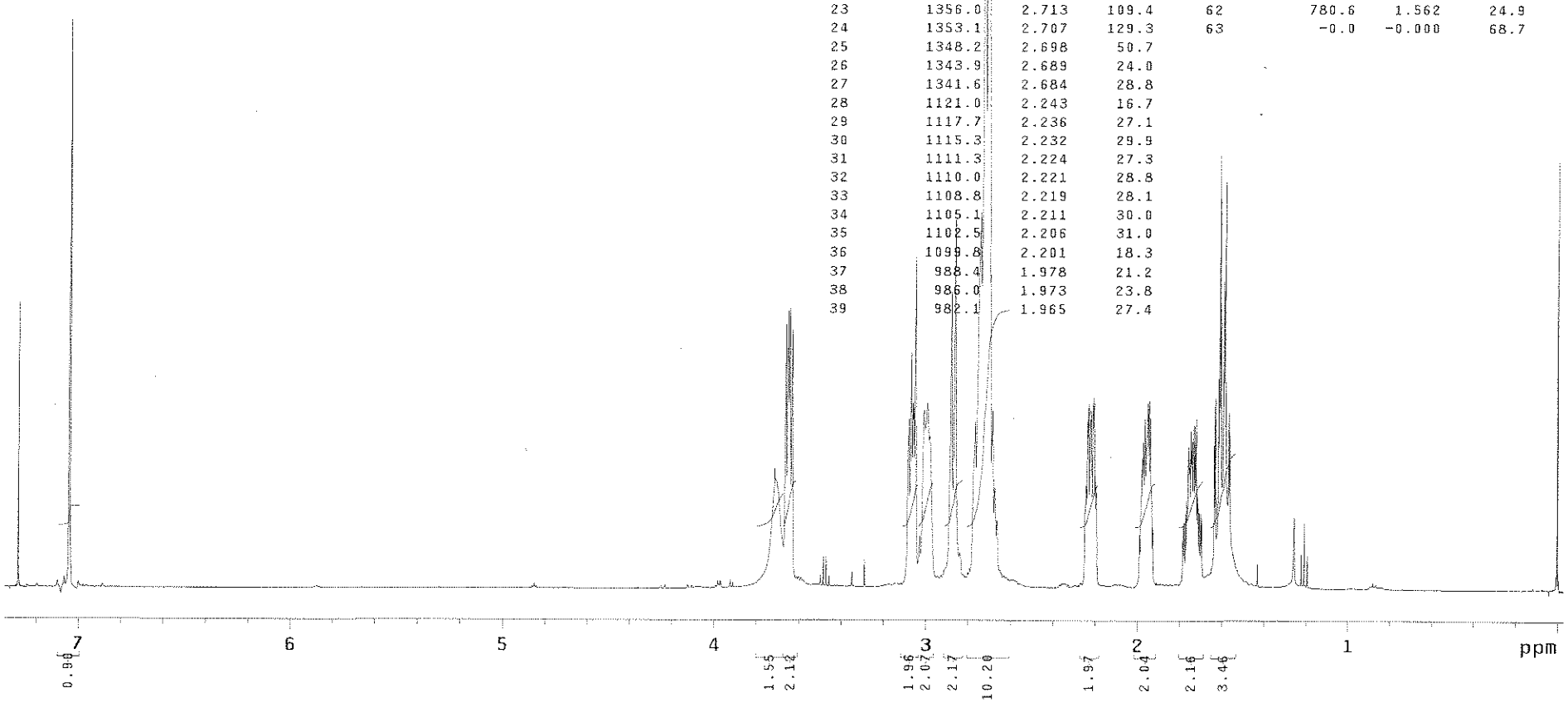
Sample: 110308_E260_SH09_CDCl3_1H
Sample ID: s_20110308_06
File: s_20110308_06/data/cdcl3_01.fid

Pulse Sequence: s2pul

Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: walkup
File: cdcl3_01
VNMRS-500 "nmr500.localdomain"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 2.049 sec
Width 5296.6 Hz
8 repetitions
OBSERVE H1, 499.7811204 MHz
DATA PROCESSING
Resol. enhancement -0.0 Hz
FT size 65536
Total time 0 min, 30 sec

INDEX	FREQUENCY	PPM	HEIGHT	INDEX	FREQUENCY	PPM	HEIGHT
1	3641.1	7.285	37.0	40	978.6	1.958	23.0
2	3640.6	7.284	45.9	41	975.5	1.952	30.1
3	3520.0	7.043	91.4	42	972.3	1.945	30.4
4	1855.9	3.714	19.5	43	969.2	1.939	27.6
5	1830.2	3.662	42.7	44	878.8	1.758	22.9
6	1824.9	3.651	44.8	45	877.2	1.755	19.7
7	1820.9	3.643	45.2	46	875.8	1.752	21.1
8	1815.4	3.632	41.7	47	873.7	1.748	25.6
9	1541.2	3.084	23.6	48	871.1	1.743	22.4
10	1539.3	3.080	27.5	49	869.8	1.740	23.8
11	1533.5	3.068	38.5	50	866.7	1.734	26.5
12	1529.8	3.061	30.0	51	863.8	1.728	26.3
13	1527.8	3.057	29.3	52	860.7	1.722	27.4
14	1523.9	3.049	53.7	53	817.6	1.636	29.5
15	1503.7	3.009	28.9	54	814.8	1.630	31.0
16	1495.5	2.992	30.0	55	808.0	1.617	34.1
17	1489.8	2.981	24.6	56	805.3	1.611	70.0
18	1439.4	2.880	47.8	57	802.5	1.606	46.2
19	1431.0	2.863	59.9	58	795.8	1.592	49.6
20	1382.7	2.767	27.0	59	792.8	1.586	65.4
21	1371.4	2.744	60.5	60	790.3	1.581	31.7
22	1364.4	2.730	151.2	61	783.3	1.567	28.5
23	1356.0	2.713	109.4	62	780.6	1.562	24.9
24	1353.1	2.707	129.3	63	-0.0	-0.000	68.7
25	1348.2	2.698	50.7				
26	1343.9	2.689	24.0				
27	1341.6	2.684	28.8				
28	1121.0	2.243	16.7				
29	1117.7	2.236	27.1				
30	1115.3	2.232	29.9				
31	1111.3	2.224	27.3				
32	1110.0	2.221	28.8				
33	1108.8	2.219	28.1				
34	1105.1	2.211	30.0				
35	1102.5	2.206	31.0				
36	1099.8	2.201	18.3				
37	988.4	1.978	21.2				
38	986.0	1.973	23.8				
39	982.1	1.965	27.4				



SH09 E253

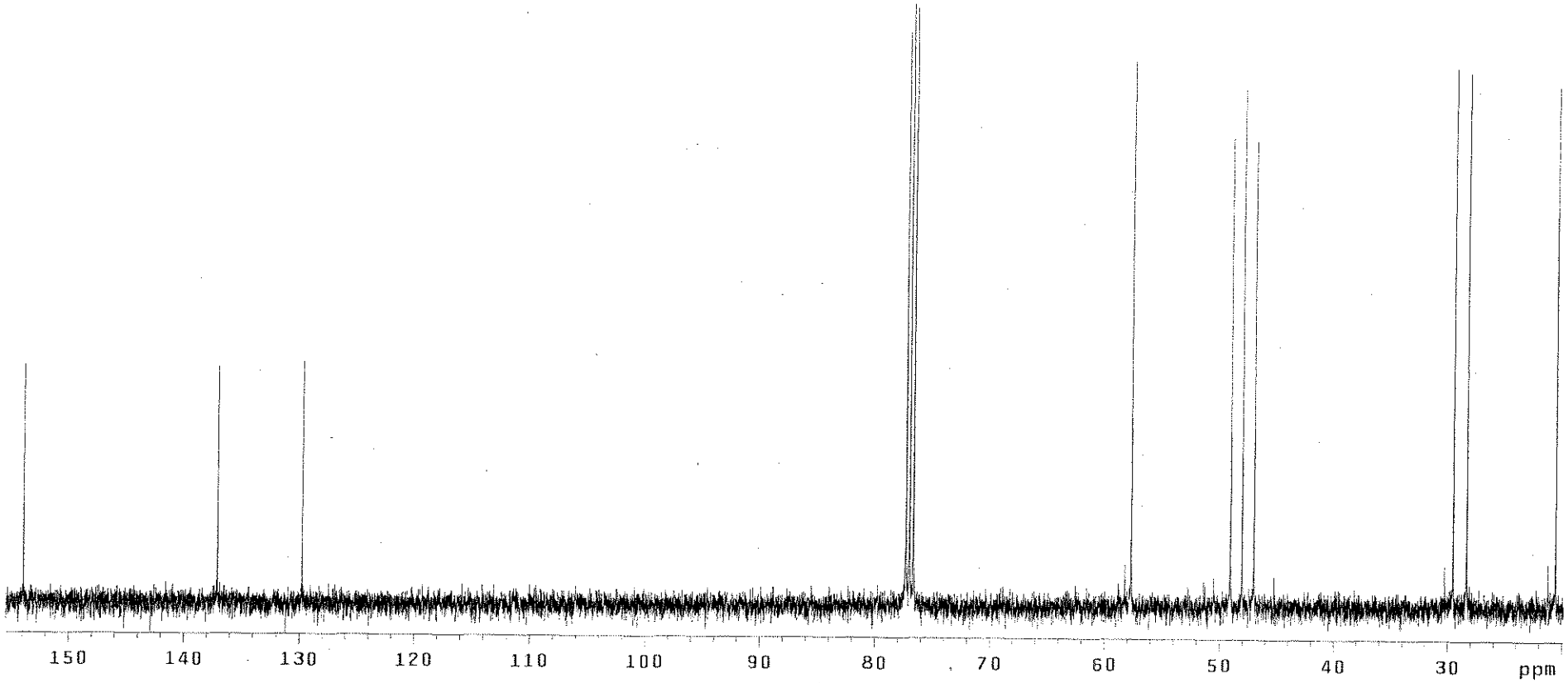
Sample: SH09_E253
Sample ID: s_20110309_01
File: s_20110309_01/data/cdcl3_01.fid

Pulse Sequence: s2pul

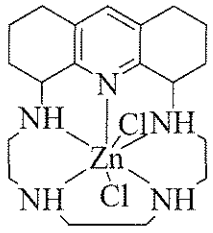
Solvent: cdcl3
Temp. 25.0 C / 298.1 K
Operator: walkup
File: cdcl3_01
VNMRS-400 "nmr400.localdomain"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 24509.8 Hz
256 repetitions
OBSERVE C13, 100.5455532 MHz
DECOUPLE H1, 399.8646885 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 65536
Total time 9 min, 49 sec

INDEX	FREQUENCY	PPM	HEIGHT
1	15480.5	153.965	38.7
2	13786.4	137.116	38.4
3	13048.8	129.780	39.4
4	7774.8	77.327	93.2
5	7742.7	77.007	97.8
6	7710.5	76.687	97.2
7	5802.4	57.709	88.6
8	4931.0	49.043	76.7
9	4830.0	48.038	84.3
10	4725.3	46.997	76.2
11	2970.6	29.544	87.7
12	2850.9	28.354	87.0
13	2067.0	20.558	84.8



2,3,4,4a,5,6,7,8,9,10,11,12,13,14,14a,15
,16,17-Octadecahydro-1,18-
methenodibenzo[b,e][1,4,7,10,13]pentaa
zacyclopentadecine dichlorozinc (II)



SH39

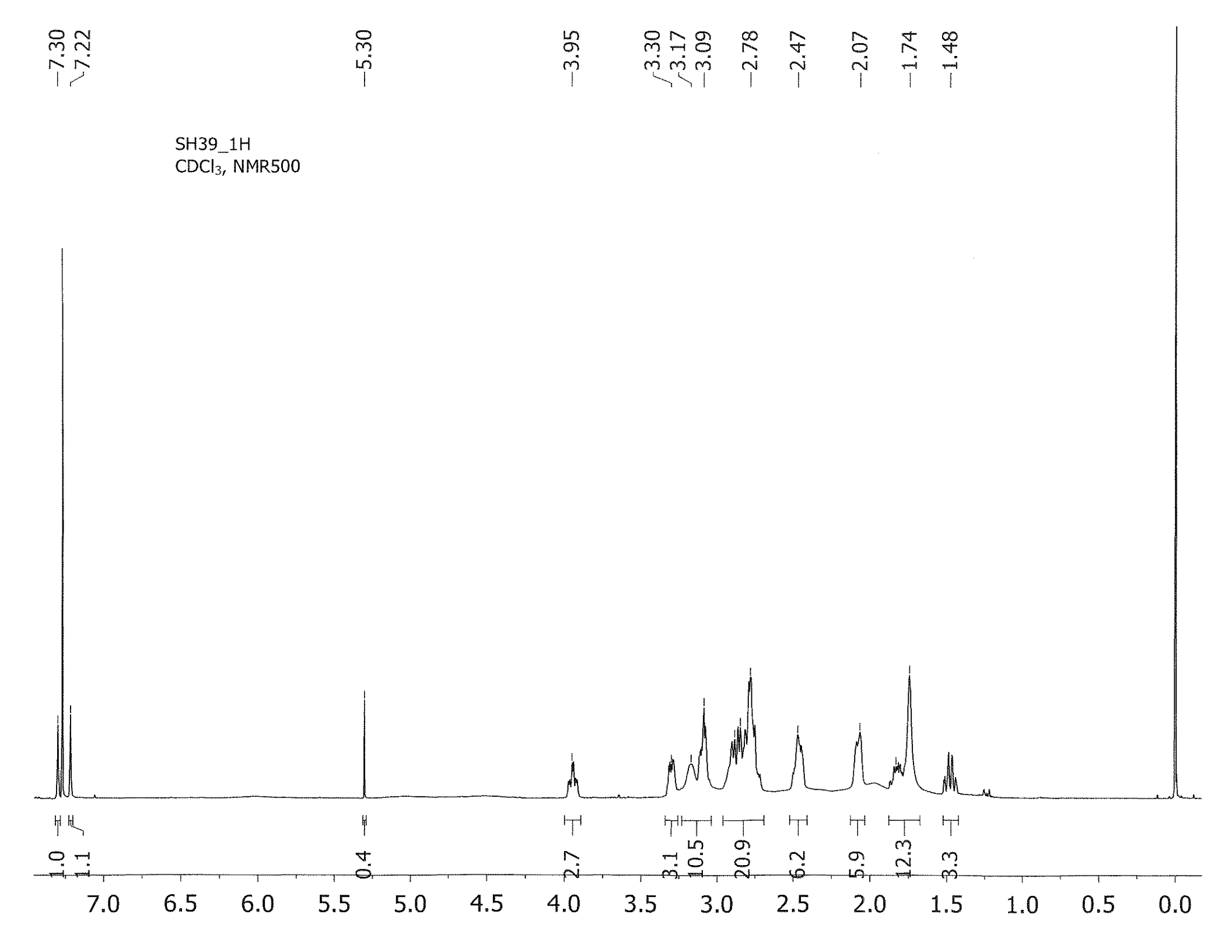
$C_{19}H_{31}Cl_2N_5Zn$

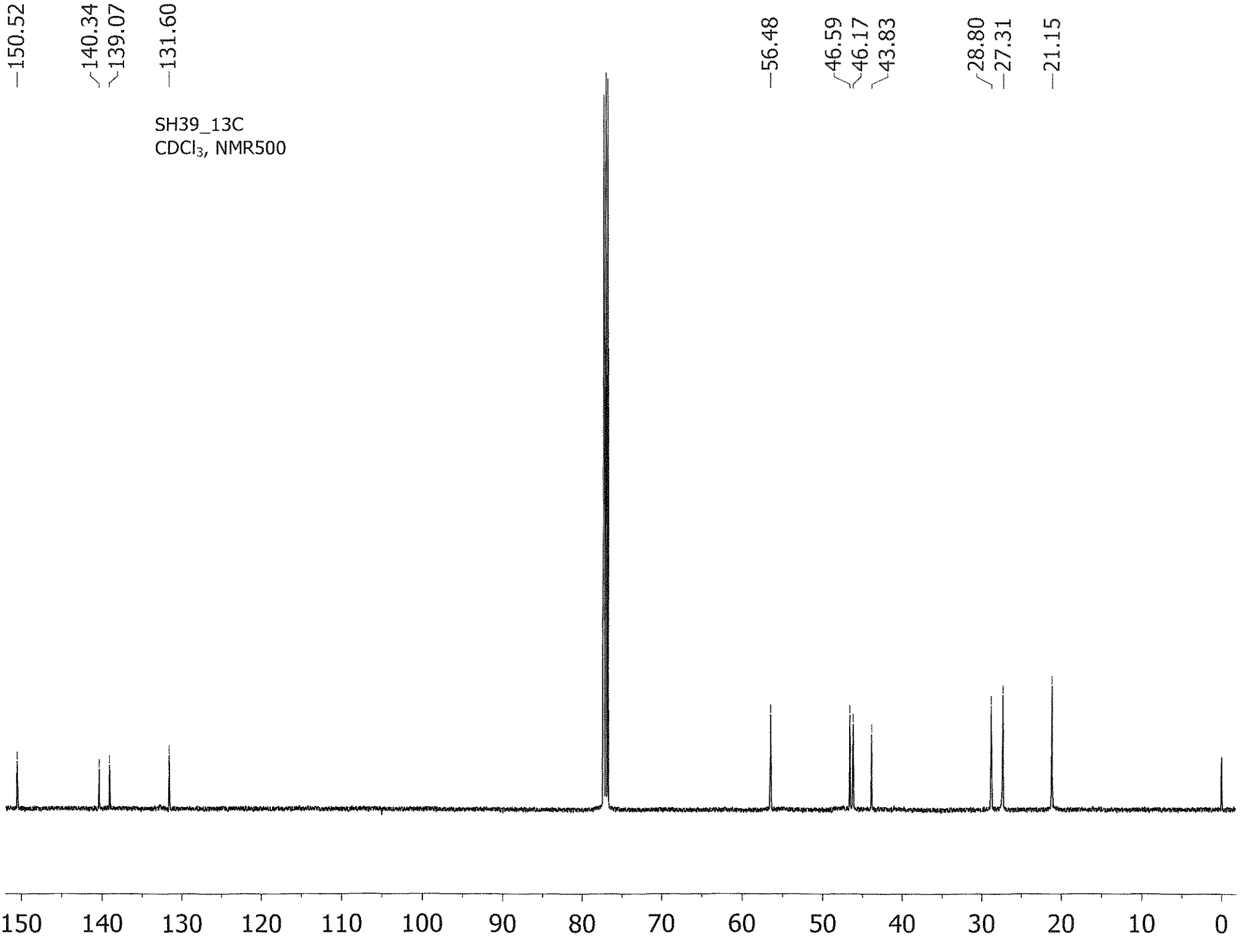
Exact Mass: 463.12

Mol. Wt.: 465.78

m/e: 465.12 (100.0%), 463.12 (82.4%), 467.12 (71.0%), 469.12 (27.5%), 466.13 (21.0%), 468.12 (20.2%), 464.13 (17.2%), 466.12 (8.8%), 470.12 (6.2%), 467.13 (3.5%), 471.11 (3.3%), 465.13 (2.0%), 464.12 (1.5%), 469.13 (1.5%), 471.12 (1.4%)

C, 48.99; H, 6.71; Cl, 15.22; N, 15.04; Zn, 14.04


7.30
7.22
5.30
3.95
3.30
3.17
3.09
2.78
2.47
2.07
1.74
1.48
SH39_1H
CDCl3, NMR500
1.0
1.1
0.4
2.7
3.1
10.5
20.9
6.2
5.9
12.3
3.3
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0


150.52
140.34
139.07
131.60
56.48
46.59
46.17
43.83
28.80
27.31
21.15
SH39_13C
CDCl3, NMR500
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0