Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Palladium Catalyzed Synthesis and Physical Properties of Indolo[2,3-*b*]quinoxalines

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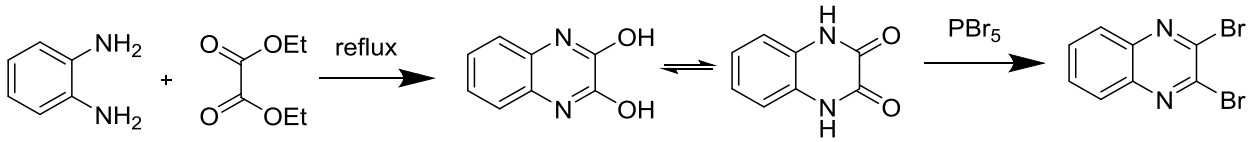
Supporting Information

Content List:

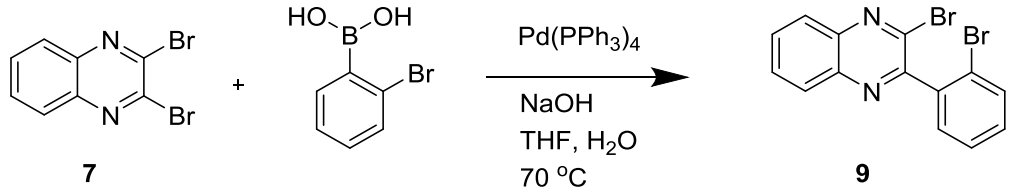
Experimental Section

Synthesis of 2,3-dibromoquinoxaline



2,3-Dibromoquinoxaline was synthesized in 94% of overall yield using Li's procedure by reflux of 1,2-phenylenediamine with diethyl oxalate, to give 1,4-dihydroquinoxaline-2,3-dione, and subsequent reaction with PBr_5.[1] M.p. 179-180 ºC. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.08 – 8.01 (m, 2H), 7.86 – 7.78 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 141.42, 140.97, 131.49, 128.57; IR (ATR, cm^{-1}): ν =3097 (m), 3034 (m), 1564 (m), 1549 (s), 1514 (s), 1479 (m), 1254 (s), 1169 (s), 1126 (m), 1107 (s), 1072 (m), 1059 (m), 957 (vs), 901 (m), 883 (m), 868 (s), 769 (vs), 692 (m), 677 (m), 621 (m), 582 (s); GC-MS (EI, 70 eV): m/z (%) = 288 (96), 209 (95), 128 (61), 102 (100), 75 (98), 50 (59); HRMS (EI): calcd. for $C_8H_4N_2Br_2$ ($[M]^+$): 285.87357; found: 285.87325; calcd. for $C_8H_4N_2Br_1{}^{81}Br_1$ ($[M]^+$): 287.87153; found: 287.87137; calcd. for $C_8H_4N_2{}^{81}Br_2$ ($[M]^+$): 289.86948; found: 289.86935.

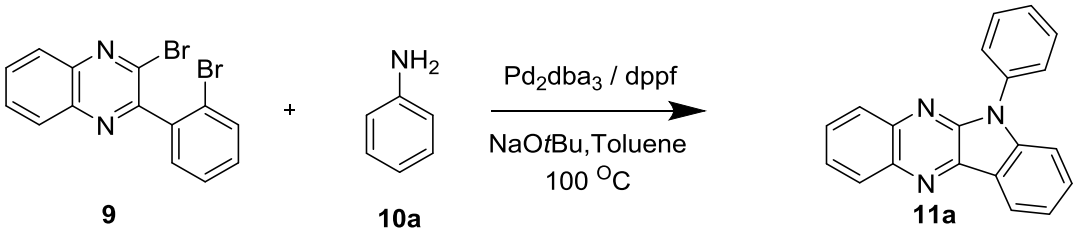
General procedure for the preparation of 2-bromo-3-(2-bromophenyl)quinoxaline(9).



2,3-Dibromoquinoxaline **7** (1 g, 3.5 mmol), 2-bromophenyl boronic acid (837 mg, 4.2 mmol), $Pd(PPh_3)_4$ (100 mg, 87 µmol) and sodium hydroxide (417 mg, 10.4 mmol) were added to a 500 mL Schlenk flask. The mixture was back-filled several times with Argon. To the mixture 70 mL THF and 10 mL distilled water were added, then, back-filled several times. The reaction was heated at 70 ºC for 4h. The solvent was evaporated *in vacuo*. The residue was extracted with

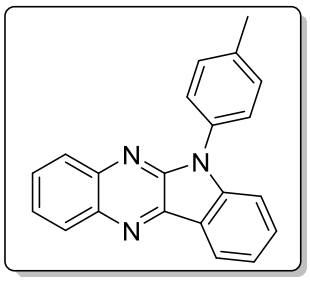
dichloromethane and water. The organic layer was dried over $MgSO_4$, filtered and the solvent was evaporated *in vacuo*. The yellow residue was purified by column chromatography (silica gel, Heptane/ethylacetate 10:1) to yield 2-bromo-3-(2-bromophenyl)quinoxaline **9** (1.1 g, 87 %) as white solid. M.p. 127-129 ºC; ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.20 – 8.07 (m, 2H), 7.90 – 7.79 (m, 2H), 7.73 (dd, *J* = 7.9, 0.8 Hz, 1H), 7.55 – 7.35 (m, 3H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 154.95, 142.47, 140.67, 140.11, 139.38, 132.99, 131.46, 131.01, 130.84, 130.49, 129.58, 128.57, 127.76, 122.83; IR (ATR, cm^{-1}): ν =3059 (w), 1610 (w), 1556 (m), 1535 (w), 1477 (m), 1433 (m), 1385 (w), 1333 (m), 1290 (m), 1273 (w), 1252 (m), 1236 (w), 1213 (w), 1167 (w), 1147 (m), 1132 (m), 1084, 1041, 1024 (m), 999 (w), 970, 955 (m), 943 (m), 885 (m), 870 (w), 862 (w), 752 (vs), 727, 715, 710, 690 (m), 652 (m), 638 (m), 613 (m), 588, 571 (m), 557 (m); GC-MS (EI, 70 eV): m/z (%) = 364 (32), 285 (100), 102 (48), 75 (28), 50 (14); HRMS (EI): calcd. for $C_{14}H_8N_2Br_2$ ($[M]^+$): 361.90488; found: 361.90467;calcd. for $C_{14}H_8N_2Br_1{}^{81}Br_1$ ($[M]^+$): 363.90283; found: 363.90277; calcd. for $C_{14}H_8N_2{}^{81}Br_2$ ($[M]^+$):365.90078; found: 365.90082.

General procedure A for double C-N coupling with aniline derivatives,exemplified by the synthesis of6-phenyl-6*H*-indolo[2,3-*b*]quinoxaline(11a)

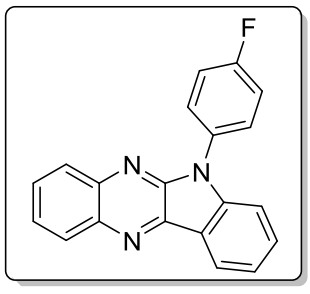


Aniline **10a** (75 µL, 0.82 mmol) was added to a pressure tube charged with **9** (100 mg, 0.28 mmol), $Pd_2(dba)_3$ (12 mg, 14 µmol), ligand dppf (15mg, 27 µmol) and sodium *tert*-butoxide (79 mg, 0.82 mmol) under Argon. The mixture was back-filled with Argon several times. The mixture was dissolved in anhydrous Toluene (10 mL) and heated at 100 ºC for 7 h. After cooling, the reaction mixture was diluted with dichloromethane (20mL) and filtered through a celite pad, washing with dichloromethane (40 mL). The filtrate was reduced *in vacuo*. The product was separated via flashchromatography (silica gel, heptanes/ethylacetate 5:1) to yield 6-phenyl-6*H*-

indolo[2,3-*b*]quinoxaline **11a** (67 mg, 83%) as a yellow solid; m.p. 238-239 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.56 (d, *J* = 7.7 Hz, 1H), 8.40 – 8.29 (m, 1H), 8.14 – 8.06 (m, 1H), 7.84 – 7.59 (m, 7H), 7.59 – 7.38 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.00, 144.90, 140.72, 140.08, 139.69, 135.50, 131.25, 129.92, 129.24, 128.99, 128.38, 128.13, 127.27, 126.71, 122.94, 122.02, 119.83, 110.75; IR (ATR, cm^{-1}): ν =3053 (m), 1608 (m), 1597 (m), 1581 (m), 1500, 1483 (m), 1470 (m), 1458, 1402, 1390, 1354 (m), 1336 (m), 1317 (m), 1304 (m), 1252 (m), 1227 (m), 1205, 1174 (m), 1147 (m), 1132 (m), 1126 (m), 1099 (m), 1072 (m), 1041 (m), 1024 (m), 1014 (m), 1007 (m), 955 (m), 924 (m), 779 (m), 766 (m), 748 (vs), 719 (m), 694, 687, 648, 590, 567 (m); GC-MS (EI, 70 eV): m/z (%) = 295 (100), 147 (9), 90 (6), 77 (6); HRMS (ESI): calcd. for $C_{20}H_{14}N_3$ ($[M + H]^+$): 296.11822; found: 296.11835.

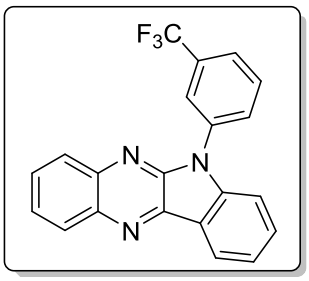


6-(p-Tolyl)-6H-indolo[2,3-b]quinoxaline **11b** was prepared following general procedure A using compound **9** (100 mg, 0.28 mmol) and toluidine (88 mg, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11b** (73 mg, 86%) as a yellow solid; m.p. 216-217 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 – 8.43 (m, 1H), 8.29 – 8.22 (m, 1H), 8.05 – 7.99 (m, 1H), 7.68 – 7.57 (m, 2H), 7.57 – 7.49 (m, 3H), 7.45 – 7.31 (m, 4H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.01, 144.99, 140.66, 140.06, 139.62, 138.04, 132.68, 131.06, 130.45, 129.17, 128.79, 128.27, 127.02, 126.46, 122.72, 121.73, 119.68, 110.62, 21.35; IR (ATR, cm^{-1}): ν =3057 (w), 3034 (w), 2918 (w), 1606 (m), 1585 (m), 1514, 1485 (m), 1470 (m), 1460, 1404, 1354 (m), 1335 (m), 1317, 1304 (m), 1255 (m), 1227 (m), 1221 (m), 1205, 1182 (m), 1169 (m), 1130 (m), 1122 (m), 1099 (m), 1043 (m), 1016 (m), 955 (m), 924 (m), 816 (m), 764, 750 (vs), 721 (m), 710 (m), 673 (w), 633 (m), 602, 579, 567 (m), 559 (m); GC-MS (EI, 70 eV): m/z (%) = 309 (100), 293 (8), 154 (7), 90 (5); HRMS (EI): calcd. for $C_{21}H_{15}N_3$ ($[M]^+$): 309.12605; found: 309.12523.



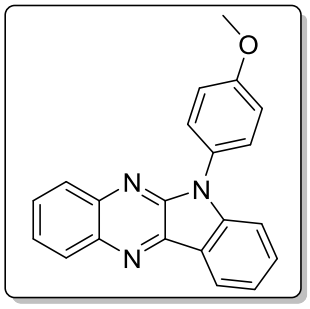
6-(4-Fluorophenyl)-6H-indolo[2,3-b]quinoxaline **11c** was prepared following general procedure A using compound **9** (100 mg, 0.28 mmol) and 4-fluoroaniline (78 µL, 0.82 mmol). The product was

purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11c** (69 mg, 80 %) as a yellow solid; m.p. 219-220 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.55 (d, *J* = 7.8 Hz, 1H), 8.37 – 8.30 (m, 1H), 8.12 – 8.04 (m, 1H), 7.78 – 7.61 (m, 5H), 7.50 – 7.41 (m, 2H), 7.41 – 7.30 (m, 2H); ^{19}F NMR (282 MHz, $CDCl_3$) δ -113.01; ^{13}C NMR (75 MHz, $CDCl_3$) δ 162.08 (d, *J* = 247.9 Hz), 146.07, 144.90, 140.70, 140.01 (d, *J* = 18.0 Hz), 131.43 (d, *J* = 3.2 Hz), 131.32, 129.38, 129.18 (d, *J* = 8.4 Hz), 129.12, 128.32, 126.81, 122.98, 122.15, 119.92, 116.99 (d, *J* = 22.9 Hz), 110.52; IR (ATR, cm^{-1}): ν =3057 (m), 1608 (m), 1579 (m), 1574 (m), 1514, 1485, 1471 (m), 1460, 1402, 1356 (m), 1335 (m), 1313, 1292 (m), 1259 (m), 1223, 1203, 1171 (m), 1151 (m), 1130 (m), 1122, 1099, 1043 (m), 1012 (m), 1007 (m), 949 (m), 924 (m), 872 (m), 831, 812 (m), 800 (m), 764, 748 (vs), 723 (m), 710, 673 (m), 638 (m), 629 (m), 602, 579, 567 (m), 557 (m), 548 (m); GC-MS (EI, 70 eV): m/z (%) = 313 (100), 156 (12), 75 (7); HRMS (EI): calcd. for $C_{20}H_{12}N_3F_1$ ($[M]^+$): 313.10098; found: 313.10007.

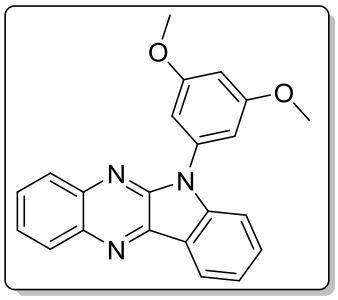


6-(3-(Trifluoromethyl)phenyl)-6H-indolo[2,3-b]quinoxaline **11d** was prepared following general procedure A using compound **9** (100 mg, 0.28 mmol) and 3-(trifluoromethyl)aniline (103 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11d** (90 mg, 90 %) as a yellow solid; m.p. 201-202 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.46 (ddd, *J* = 7.7, 1.2, 0.7 Hz, 1H), 8.29 – 8.19 (m, 1H), 8.03 – 7.95 (m, 2H), 7.92 (ddd, *J* = 3.7, 3.0, 1.9 Hz, 1H), 7.76 – 7.53 (m, 5H), 7.48 – 7.33 (m, 2H); ^{19}F NMR (282 MHz, $CDCl_3$) δ -62.58; ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.55, 144.00, 140.39, 140.07, 136.11, 132.31 (q, *J* = 33.0 Hz), 131.25, 130.40, 130.32, 130.31, 129.33, 129.11, 128.23, 126.90, 124.49 (q, *J* = 3.7 Hz), 123.85 (q, *J* = 3.9 Hz), 122.92, 123.74 (q, *J* = 272.5 Hz),122.41, 120.16, 110.31; IR (ATR, cm^{-1}): ν =3051 (w), 3028 (w), 1608 (w), 1597 (w), 1579 (w), 1574 (w), 1495 (m), 1464 (m), 1446 (m), 1406, 1356 (m), 1329, 1308 (m), 1279 (w), 1250 (m), 1230 (m), 1205 (m), 1167, 1134 (m), 1126 (m), 1113, 1105, 1095, 1068, 1045 (m), 1011 (m), 987 (w), 976 (w), 958 (m), 943 (m), 924 (w), 904 (m), 874 (w), 860 (w), 854 (w), 802 (m), 795 (m), 768 (m), 748 (vs), 719 (m), 700, 671, 656 (m), 631 (w), 615 (w), 588 (m), 567 (w), 546 (w); GC-MS (EI, 70 eV): m/z (%) = 363 (100), 294 (9);

HRMS (ESI): calcd. for $C_{21}H_{12}F_3N_3$ ($[M + H]^+$): 364.10561; found: 364.10566; calcd. for $C_{37}H_{37}N_5Na$ ($[M + Na]^+$): 574.29412; found: 574.2944.

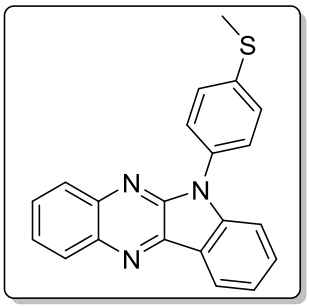


6-(4-Methoxyphenyl)-6H-indolo[2,3-b]quinoxaline **11e** was prepared following general procedure A using compound **9** (100 mg, 0.28 mmol) and p-anisidine (101 mg, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 3:1) to yield **11e** (88 mg, 98 %) as a yellow solid; m.p. 226-228 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.57 (d, *J* = 7.6 Hz, 1H), 8.35 (d, *J* = 8.9 Hz, 1H), 8.15 – 8.05 (m, 1H), 7.80 – 7.55 (m, 5H), 7.44 (t, *J* = 8.3 Hz, 2H), 7.21 – 7.13 (m, 2H), 3.94 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.42, 145.47, 140.85, 139.42, 131.35, 129.13, 129.00, 128.72, 128.38, 128.02, 126.67, 123.02, 121.87, 119.53, 115.27, 113.39, 110.68, 55.77; IR (ATR, cm^{-1}): ν =3076 (w), 3053 (m), 3022 (m), 2956 (m), 2933 (m), 2912 (m), 2839 (m), 1606 (m), 1585 (m), 1578 (m), 1512, 1506, 1487 (m), 1464, 1446, 1406, 1356 (m), 1336 (m), 1313 (m), 1296, 1244, 1230, 1205, 1178, 1167, 1136, 1128, 1103, 1041 (m), 1026, 1009 (m), 968 (m), 955 (m), 939 (m), 924 (m), 870 (m), 852 (m), 829, 820, 804 (m), 795 (m), 768, 748 (vs), 723, 715, 669 (m), 642 (m), 629 (m), 602, 579, 569, 550; GC-MS (EI, 70 eV): m/z (%) = 325 (100), 310 (39), 282 (18), 141 (8); HRMS (ESI): calcd. for $C_{21}H_{15}N_3O$ ($[M + H]^+$): 326.12879; found: 326.12858.

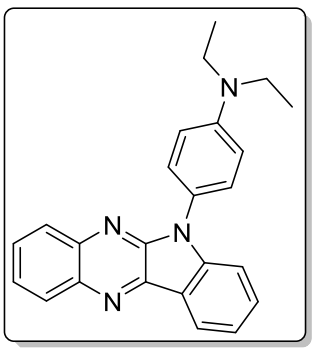


6-(3,5-Dimethoxyphenyl)-6H-indolo[2,3-b]quinoxaline **11f** was prepared following general procedure A using compound **9** (100 mg, 0.28 mmol) and 3,5-dimethoxyaniline (126 mg, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 2:1) to yield **11f** (93 mg, 95 %) as a yellow solid; m.p. 188-189 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.45 (d, *J* = 7.6 Hz, 1H), 8.28 – 8.20 (m, 1H), 8.07 – 8.00 (m, 1H), 7.71 – 7.47 (m, 4H), 7.35 (ddd, *J* = 8.1, 6.9, 1.3 Hz, 1H), 6.81 (d, *J* = 2.3 Hz, 2H), 6.54 (t, *J* = 2.3 Hz, 1H), 3.79 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.59, 145.81, 144.67, 140.60, 140.16, 139.77, 136.91, 131.08, 129.25, 128.83, 128.35, 126.55, 122.66, 121.86, 119.84, 110.92, 105.51, 100.33, 55.66; IR (ATR, cm^{-1}): ν =2993 (w), 2956 (w), 2926 (w), 1606 (m), 1591 (m), 1508 (w), 1491 (m), 1458, 1427 (m), 1404 (m),

1363 (w), 1325 (m), 1298 (m), 1257 (m), 1242 (m), 1207 (m), 1194, 1153, 1134 (m), 1124 (m), 1107 (m), 1066 (m), 1051 (m), 1039 (m), 1014 (m), 1003 (m), 993 (m), 953 (m), 933 (m), 912 (m), 877 (m), 860 (m), 847, 818 (m), 791 (m), 768, 735 (vs), 721, 688, 667 (m), 640 (m), 631 (m), 617 (m), 607 (m), 600 (m), 584, 577 (m), 565 (m), 534 (m); GC-MS (EI, 70 eV): m/z (%) =355 (100), 325 (13), 268 (12); HRMS (EI): calcd. for $C_{22}H_{17}O_2N_3$ ($[M]^+$): 355.13153; found: 355.13066.

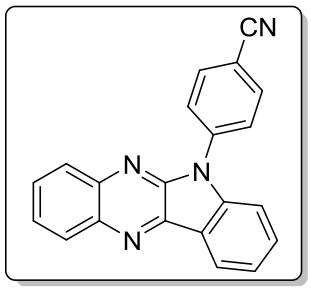


6-(4-(Methylthio)phenyl)-6H-indolo[2,3-b]quinoxaline **11g** was prepared following general procedure A using compound **9** (100 mg, 0.28 mmol) and 4-(methylthio)aniline (103 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 3:1) to yield **11g** (88 mg, 94 %) as a white solid; m.p. 249-250ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 (d, *J* = 7.4 Hz, 1H), 8.28 – 8.20 (m, 1H), 8.06 – 7.98 (m, 1H), 7.72 – 7.53 (m, 5H), 7.51 – 7.30 (m, 4H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.88, 144.73, 140.58, 140.17, 139.82, 138.69, 132.30, 131.09, 129.28, 128.89, 128.23, 127.62, 127.52, 126.56, 122.73, 121.91, 119.85, 110.56, 15.92; IR (ATR, cm^{-1}): ν =2955 (m), 2920, 2850 (m), 1608 (m), 1579 (m), 1498, 1483 (m), 1460, 1431 (m), 1402, 1352 (m), 1335 (m), 1311, 1296 (m), 1252 (m), 1230 (m), 1203, 1184 (m), 1132 (m), 1124 (m), 1115 (m), 1103, 1090, 1041 (m), 1012 (m), 1003 (m), 984 (m), 970 (m), 955 (m), 937 (m), 922 (m), 904 (w), 870 (m), 854 (w), 833 (m), 816, 768 (vs), 748 (vs), 719, 702, 661 (m), 634 (m), 625 (m), 590, 567, 548 (m); GC-MS (EI, 70 eV): m/z (%) = 341 (100), 326 (36), 294 (20), 102 (6); HRMS (ESI): calcd. for $C_{24}H_{22}N_4$ ($[M + H]^+$): 367.19172; found: 367.19173.



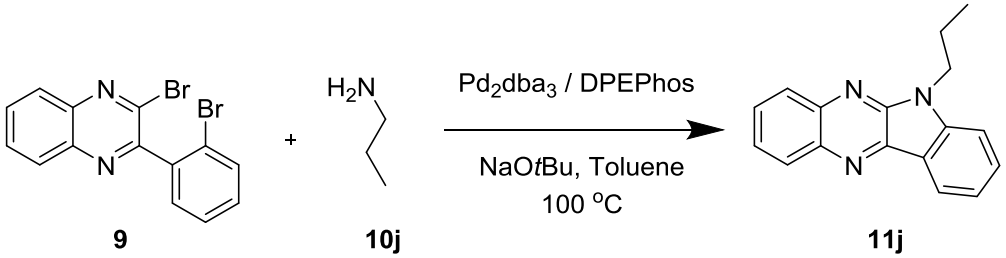
5,7-Bis(4-(N,N-diethylamino)phenyl)-6H-indolo[2,3-b]quinoxaline **11h** was prepared following general procedure A using compound **9**(100 mg, 0.28 mmol) and N^1,N^1-diethylbenzene-1,4-diamine (137 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, Heptane/ethylacetate 3:1) to yield **11h** (76 mg, 75 %) as a yellow solid; m.p. 228-229 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 –

8.39 (m, 1H), 8.26 – 8.19 (m, 1H), 8.05 – 8.00 (m, 1H), 7.70 – 7.50 (m, 3H), 7.45 – 7.27 (m, 4H), 6.84 – 6.73 (m, 2H), 3.37 (q, *J* = 7.1 Hz, 4H), 1.17 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.61, 146.39, 145.80, 140.82, 140.23, 139.58, 130.90, 129.22, 128.57, 128.39, 128.29, 126.09, 122.55, 122.47, 121.29, 119.45, 112.09, 110.74, 44.55, 12.69; IR (ATR, cm^{-1}): ν =2970 (w), 2926 (w), 2866 (w), 1626 (w), 1608 (m), 1578 (w), 1522, 1489 (m), 1462 (m), 1446 (m), 1429 (w), 1404 (m), 1371 (m), 1352 (m), 1333 (m), 1315 (m), 1279 (m), 1259 (m), 1228 (m), 1203, 1194, 1169 (m), 1157 (m), 1149 (m), 1134 (m), 1122 (m), 1101 (m), 1080 (m), 1041 (m), 1014 (m), 1003 (m), 978 (m), 953 (m), 924 (m), 864 (m), 849 (m), 814, 798, 758, 735 (vs), 723, 712, 667 (m), 640 (m), 631 (m), 596, 575, 563 (m), 548 (m), 532 (m); GC-MS (EI, 70 eV): m/z (%) = 366 (67), 351 (100), 322 (28), 294 (14), 243 (35), 194 (13), 165 (22); HRMS (ESI): calcd. for $C_{24}H_{22}N_4$ ($[M + H]^+$): 367.18780; found: 367.19184.



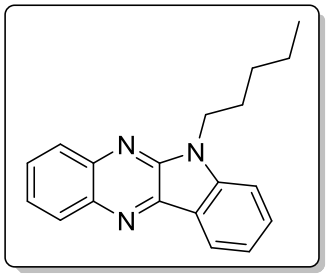
5,7-Bis(4-cyanophenyl)-6H-indolo[2,3-b]quinoxaline **11i** was prepared following general procedure A using compound **9** (100 mg, 0.28 mmol) and 4-aminobenzonitrile (97 mg, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 3:1) to yield **11i** (73 mg, 83 %) as a yellow solid; m.p. 272-273 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.47 (d, *J* = 7.7 Hz, 1H), 8.28 – 8.21 (m, 1H), 8.03 – 7.97 (m, 1H), 7.96 – 7.85 (m, 4H), 7.74 – 7.51 (m, 4H), 7.46 – 7.38 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.27, 143.33, 140.25, 140.17, 140.11, 139.68, 133.65, 131.31, 129.34, 129.32, 128.20, 127.20, 127.02, 123.06, 122.85, 120.49, 118.40, 110.91, 110.52; IR (ATR, cm^{-1}): ν =2922 (m), 2852 (m), 2227 (m), 1601 (s), 1583 (m), 1506 (s), 1485 (m), 1456 (s), 1400 (s), 1354 (m), 1319 (s), 1304 (m), 1257 (m), 1238 (m), 1228 (m), 1219 (m), 1198 (s), 1169 (m), 1151 (m), 1136 (m), 1124 (s), 1103 (s), 1043 (m), 1014 (m), 955 (m), 949 (m), 922 (m), 837 (s), 823 (m), 769 (m), 758 (s), 746 (vs), 725 (m), 715 (m), 698 (m), 669 (m), 631 (m), 598 (s), 571 (m), 555 (s), 538 (s); GC-MS (EI, 70 eV): m/z (%) = 320 (100), 160 (9), 102 (7); HRMS (EI): calcd. for $C_{21}H_{12}N_4$ ($[M]^+$): 320.10565; found: 320.10491.

General procedure B for double C-N coupling with chain amine derivatives, exemplified by *6-propyl-6H-indolo[2,3-b]quinoxaline* 11j

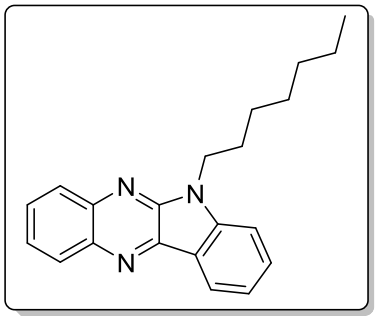


9 **10j** **11j**

To a pressure tube charged with **9** (100 mg, 0.28 mmol), $Pd_2(dba)_3$ (13 mg, 14 µmol), ligand DPEPhos (15 mg, 27 µmol) and sodium tert-butoxide (79 mg, 0.82 mmol) under Argon. The mixture was back-filled with Argon several times. The mixture was dissolved in anhydrous toluene (10 mL). n-propylamine (68 µL, 0.82 mmol) was added to the mixture and heated at 100 ºC for 7 h. After cooling, the reaction mixture was diluted with dichloromethane (20 mL) and filtered through a celite pad, washing with dichloromethane (40 mL). The filtrate was reduced *in vacuo*. The product was separated via flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11j** (69 mg, 80%) as a yellow solid; m.p. 99-100 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.7 Hz, 1H), 8.31 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.14 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.82 – 7.60 (m, 3H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.44 – 7.33 (m, 1H), 4.58 – 4.37 (m, 2H), 2.13 – 1.90 (m, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 145.88, 144.70, 140.80, 140.09, 139.28, 131.08, 129.41, 128.84, 127.94, 126.05, 122.94, 120.90, 119.54, 109.68, 43.21, 21.96, 11.75; IR (ATR, cm^{-1}): ν =3057 (w), 2970 (m), 2951 (m), 2929 (w), 2870 (m), 1610 (m), 1581 (m), 1574 (m), 1487 (s), 1464 (s), 1435 (m), 1406 (s), 1394 (m), 1369 (m), 1358 (s), 1348 (s), 1321 (s), 1294 (m), 1265 (w), 1257 (m), 1242 (m), 1232 (m), 1203 (s), 1182 (m), 1155 (m), 1113 (s), 1070 (m), 1034 (w), 1014 (m), 1003 (m), 951 (w), 939 (m), 893 (m), 883 (w), 870 (m), 850 (m), 768 (m), 746 (vs), 727 (s), 698 (s), 642 (m), 617 (m), 586 (s), 569 (m), 534 (m);GC-MS (EI, 70 eV): m/z (%) = 261 (46), 232 (73), 219 (100), 102 (11), 90 (10), 77 (7); HRMS (ESI): calcd. for $C_{17}H_{16}N_3$ ($[M + H]^+$): 262.13387; found: 262.13391.

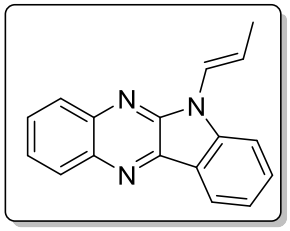


6-Pentyl-6H-indolo[2,3-b]quinoxaline **11k** was prepared following general procedure B using compound **9** (100 mg, 0.28mmol) and n-pentylamine (96 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11k** (74 mg, 93 %) as a yellow solid; m.p. 90-91 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.6 Hz, 1H), 8.22 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.06 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.73 – 7.53 (m, 3H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.35 – 7.25 (m, 1H), 4.45 – 4.34 (m, 2H), 1.94 – 1.77 (m, 2H), 1.33 (m, 4H), 0.81 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 145.65, 144.46, 140.66, 140.03, 139.23, 130.87, 129.31, 128.63, 127.82, 125.83, 122.72, 120.69, 119.47, 109.48, 41.44, 29.16, 28.15, 22.39, 13.94; IR (ATR, cm^{-1}): ν =2964 (w), 2953 (w), 2931 (w), 2870 (w), 1608 (m), 1579 (m), 1491 (m), 1466 (s), 1441 (w), 1406 (s), 1379 (m), 1358 (m), 1323 (m), 1304 (m), 1246 (s), 1234 (m), 1200 (s), 1163 (m), 1153 (m), 1130 (m), 1115 (s), 1070 (m), 1051 (w), 1036 (w), 1014 (m), 1003 (m), 976 (w), 945 (w), 928 (m), 897 (w), 872 (w), 860 (w), 850 (m), 837 (w), 764 (s), 752 (s), 742 (vs), 729 (s), 717 (s), 692 (s), 665 (m), 640 (m), 629 (w), 613 (m), 606 (m), 586 (s), 571 (s), 555 (m), 534 (m); GC-MS (EI, 70 eV): m/z (%) = 289 (52), 260 (6), 246 (11), 2332 (80), 219 (100), 129 (11), 90 (10), 77 (9); HRMS (EI): calcd. for $C_{19}H_{19}N_3$ ($[M]^+$): 289.15735; found: 289.15720.

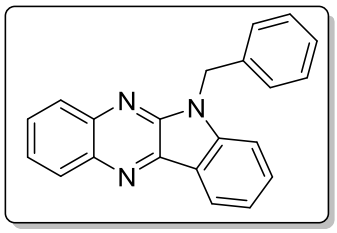


6-Heptyl-6H-indolo[2,3-b]quinoxaline **11k** was prepared following general procedure B using compound **9** (100 mg, 0.28mmol) and n-heptylamine (122 µL, 0.82mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11j** (74 mg, 85 %) as a yellow solid; m.p. 66-68 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.7 Hz, 1H), 8.32 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.81 – 7.64 (m, 3H), 7.47 (d, *J* = 8.2 Hz, 1H), 7.42 – 7.32 (m, 1H), 4.58 – 4.40 (m, 2H), 2.03 – 1.85 (m, 2H), 1.51 – 1.16 (m, 8H), 0.86 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.81, 144.67, 140.78, 139.89, 139.05, 131.16, 129.26, 128.86, 127.95, 126.10, 123.05, 120.92, 119.43, 109.67, 41.63, 31.85, 29.11, 28.60, 27.16, 22.73, 14.18; IR (ATR, cm^{-1}): ν =2951 (m), 2922 (m), 2870 (m), 2850 (m), 1606 (m), 1581 (m), 1487 (s), 1464 (s), 1435 (m), 1408 (s), 1394 (m), 1369 (s), 1358

(s), 1346 (m), 1321 (s), 1304 (m), 1250 (m), 1240 (m), 1232 (m), 1203 (m), 1188 (m), 1176 (m), 1161 (m), 1149 (m), 1113 (s), 1070 (m), 1014 (m), 999 (m), 945 (m), 764 (s), 748 (vs), 721 (s), 698 (s), 642 (m), 615 (m), 586 (s), 569 (m), 534 (m); GC-MS (EI, 70 eV): m/z (%) = 317 (41), 233 (100), 219 (96), 102 (6); HRMS (ESI): calcd. for $C_{21}H_{24}N_3$ ($[M + H]^+$): 318.19647; found: 318.19666.

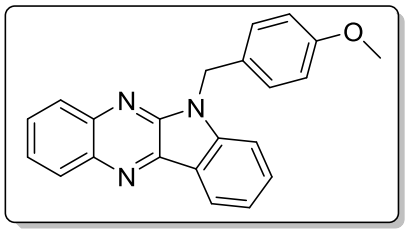


6-(Prop-1-en-1-yl)-6H-indolo[2,3-b]quinoxaline **11m** was prepared following general procedure B using compound **9** (100 mg, 0.28mmol) and allylamine (62 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11m** (52 mg, 73 %) as a yellow solid; m.p. 142-143 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.50 (d, *J* = 7.6 Hz, 1H), 8.32 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.17 (dt, *J* = 12.4, 6.4 Hz, 1H), 7.83 – 7.63 (m, 3H), 7.42 (ddd, *J* = 10.8, 9.2, 8.0 Hz, 2H), 6.92 – 6.79 (m, 1H), 6.27 – 6.07 (m, 1H), 1.76 (dd, *J* = 7.0, 1.8 Hz, 3H);^{13}C NMR (63 MHz, $CDCl_3$) δ 144.21, 140.60, 140.21, 139.48, 131.09, 129.27, 128.90, 128.23, 128.10, 126.42, 122.66, 121.60, 121.15, 119.85, 110.89, 14.18;IR (ATR, cm^{-1}): ν =3055 (m), 3045 (m), 2978 (m), 2931 (m), 2912 (m), 2852 (m), 1662 (m), 1628 (m), 1606 (m), 1581 (m), 1574 (m), 1485 (s), 1462 (s), 1435 (m), 1427 (m), 1408 (vs), 1392 (s), 1358 (m), 1348 (m), 1335 (m), 1315 (s), 1265 (m), 1254 (s), 1234 (m), 1225 (m), 1209 (s), 1201 (s), 1178 (m), 1149 (m), 1138 (m), 1117 (s), 1093 (s), 1059 (m), 1034 (m), 1024 (m), 1016 (m), 1003 (m), 974 (m), 951 (m), 918 (m), 766 (s), 758 (s), 746 (vs), 735 (vs), 714 (s), 640 (m), 627 (s), 596 (s), 569 (m), 557 (m), 536 (s);GC-MS (EI, 70 eV): m/z (%) = 259 (100, 244 (29), 232 (22), 219 (42); HRMS (ESI): calcd. for $C_{17}H_{14}N_3$ ($[M + H]^+$): 260.11822; found: 260.11817.

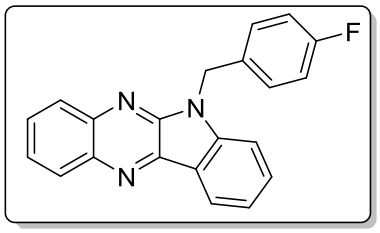


6-Benzyl-6H-indolo[2,3-b]quinoxaline **11n** was prepared following general procedure B using compound **9** (100 mg, 0.28 mmol) and benzylamine (90 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 4:1) to yield **11n** (80 mg, 94 %) as a yellow solid; m.p. 181-182 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.42 (d, *J* = 7.5 Hz, 1H), 8.25 (dd, *J* = 8.2, 1.3 Hz, 1H), 8.06 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.65 (dtd, *J* = 16.6, 6.9, 1.5 Hz, 2H), 7.57 – 7.47 (m, 1H), 7.36 – 7.08 (m, 7H), 5.63 (s,

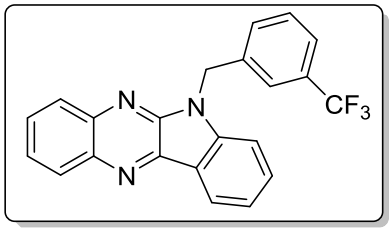
2H);^{13}C NMR (75 MHz, $CDCl_3$) δ 145.96, 144.44, 140.81, 140.01, 139.50, 136.62, 131.21, 129.38, 128.99, 128.94, 128.04, 127.82, 127.34, 126.32, 122.95, 121.32, 119.72, 110.29, 45.16; IR (ATR, cm^{-1}): ν =3059 (m), 3026 (w), 1610 (m), 1581 (m), 1574 (m), 1485 (s), 1466 (s), 1452 (m), 1433 (m), 1406 (s), 1394 (s), 1358 (m), 1346 (s), 1321 (s), 1306 (m), 1269 (m), 1259 (m), 1234 (m), 1196 (s), 1151 (m), 1134 (m), 1126 (m), 1113 (s), 1078 (m), 1066 (m), 1034 (m), 1026 (m), 1016 (m), 1007 (m), 985 (m), 918 (m), 895 (m), 854 (m), 766 (s), 746 (vs), 725 (s), 700 (vs), 685 (s), 650 (m), 615 (m), 592 (s), 575 (s), 555 (m), 534 (m); GC-MS (EI, 70 eV): m/z (%) = 309 (100), 266 (7), 251 (7), 232 (14), 207 (7), 91 (43), 84 (17), 66 (15), 49 (8); HRMS (ESI): calcd. for $C_{21}H_{16}N_3$ ($[M + H]^+$): 310.13387; found: 310.13398; calcd. for $C_{21}H_{16}N_3Na$ ($[M + Na]^+$): 332.11582; found: 332.11606.



6-(4-Methoxybenzyl)-6H-indolo[2,3-b]quinoxaline **11o** was prepared following general procedure B using compound **9** (100 mg, 0.28 mmol) and 4-methoxybenzylamine (108 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 2:1) to yield **11o** (86 mg, 92 %) as a yellow solid; m.p.129-130 ºC;^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.2 Hz, 1H), 8.23 (dd, *J* = 8.2, 1.3 Hz, 1H), 8.07 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.81 – 7.47 (m, 3H), 7.45 – 7.00 (m, 7H), 4.46 (t, *J* = 7.2 Hz, 2H), 2.84 – 2.57 (m, 2H), 2.24 (dt, *J* = 14.7, 7.5 Hz, 2H);^{13}C NMR (63 MHz, $CDCl_3$) δ 145.68, 144.33, 141.01, 140.61, 140.01, 139.25, 130.92, 129.31, 128.72, 128.39, 128.35, 127.79, 126.06, 125.94, 122.77, 120.82, 119.51, 109.44, 41.01, 33.21, 29.73;IR (ATR, cm^{-1}): ν =2929 (w), 1612 (w), 1583 (m), 1489 (m), 1470 (m), 1443 (w), 1410 (m), 1369 (m), 1360 (m), 1350 (m), 1325 (m), 1308 (w), 1282 (w), 1267 (w), 1244 (w), 1232 (w), 1207 (m), 1174 (m), 1161 (w), 1140 (w), 1128 (w), 1115 (m), 1088 (w), 1076 (w), 1070 (w), 1039 (w), 1032 (w), 1016 (w), 1005 (w), 987 (w), 976 (w), 951 (w), 935 (w), 928 (w), 758 (m), 737 (vs), 721 (m), 702 (s), 679 (m), 636 (w), 629 (w), 606 (m), 594 (m), 577 (m), 565 (m), 546 (w), 532 (m); GC-MS (EI, 70 eV): m/z (%) = 339 (37), 121 (100), 90 (12); HRMS (ESI): calcd. for $C_{22}H_{17}N_3O_1$ ($[M + H]^+$): 340.14444; found: 340.14427.

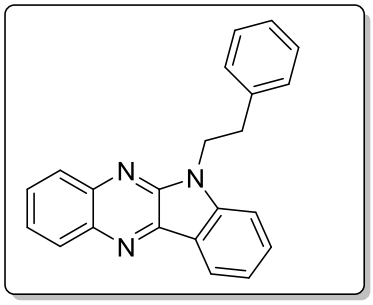


6-(4-Fluorobenzyl)-6H-indolo[2,3-b]quinoxaline **11p** was prepared following general procedure B using compound **9** (100 mg, 0.28 mmol)and 4-fluorobenzylamine (94 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ ethylacetate 4:1) to yield **11p** (78 mg, 87 %) as a yellow solid; m.p. 176-177 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.40 (d, *J* = 7.7 Hz, 1H), 8.24 (dd, *J* = 8.3, 1.5 Hz, 1H), 8.05 (dd, *J* = 8.4, 1.3 Hz, 1H), 7.72 – 7.48 (m, 3H), 7.26 (ddd, *J* = 7.5, 6.8, 1.3 Hz, 4H), 6.94 – 6.83 (m, 2H), 5.57 (s, 2H); ^{19}F NMR (282 MHz, $CDCl_3$) δ -114.59;^{13}C NMR (75 MHz, $CDCl_3$) δ 162.30 (d, *J* = 246.1 Hz), 145.70, 144.08, 140.63, 140.01, 139.59, 132.30 (d, *J* = 3.2 Hz), 131.05, 129.39, 129.00 (d, *J* = 8.2 Hz), 128.92, 127.88, 126.23, 122.82, 121.29, 119.74, 115.74 (d, *J* = 21.6 Hz), 109.97, 44.36; IR (ATR, cm^{-1}): ν =3057 (w), 3045 (w), 1632 (w), 1610 (m), 1581 (m), 1508 (s), 1489 (m), 1468 (s), 1443 (w), 1435 (w), 1406 (s), 1363 (m), 1344 (m), 1325 (m), 1309 (w), 1300 (w), 1267 (w), 1240 (m), 1230 (w), 1217 (s), 1200 (s), 1171 (w), 1157 (m), 1140 (w), 1126 (w), 1117 (m), 1097 (m), 1066 (w), 1039 (w), 1016 (w), 1007 (w), 984 (w), 955 (w), 939 (w), 858 (m), 850 (m), 825 (m), 768 (m), 762 (s), 746 (vs), 729 (m), 721 (m), 712 (m), 690 (m), 640 (m), 631 (w), 617 (m), 592 (m), 571 (m), 557 (w), 534 (w); GC-MS (EI, 70 eV): m/z (%) = 327 (100), 232 (11), 218 (8), 109 (79), 90 (14); HRMS (EI): calcd. for $C_{21}H_{14}N_3F_1$ ($[M]^+$): 327.11663; found: 327.11625.

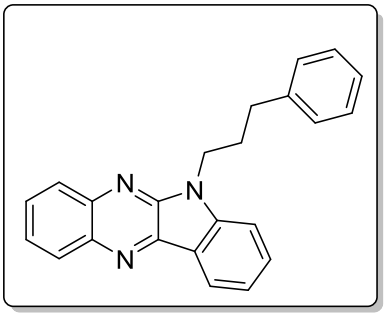


6-(3-(Trifluoromethyl)benzyl)-6H-indolo[2,3-b]quinoxaline **11q** was prepared following general procedure B using compound **9** (100 mg, 0.28 mmol) and trifluoromethylbenzylamine (118 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 4:1) to yield **11q** (87 mg, 84 %) as a yellow solid; m.p. 161-162 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.44 – 8.38 (m, 1H), 8.28 – 8.21 (m, 1H), 8.07 – 8.01 (m, 1H), 7.72 – 7.40 (m, 5H), 7.40 – 7.19 (m, 4H), 5.65 (s, 2H);^{19}F NMR (282 MHz, $CDCl_3$) δ -114.59; ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.69, 143.97, 140.60, 139.99, 139.71, 137.63, 131.22 (q, *J* = 32.4 Hz), 131.15, 130.48, 129.43, 129.00, 127.89, 126.35, 124.68 (q, *J* = 3.7 Hz), 124.12 (q, *J* = 3.8 Hz), 123.93 (q, *J* = 272.4 Hz), 122.89, 121.48, 119.84, 109.79, 44.67; IR (ATR, cm^{-1}): ν =3064 (w), 1612 (m), 1587 (m), 1489 (m), 1468 (s), 1452 (w),

1435 (w), 1410 (s), 1358 (w), 1338 (s), 1325 (s), 1275 (m), 1267 (w), 1244 (m), 1196 (s), 1163 (m), 1151 (s), 1111 (s), 1099 (vs), 1074 (s), 1043 (m), 1009 (m), 989 (m), 978 (w), 951 (w), 941 (w), 933 (w), 914 (m), 891 (w), 864 (w), 852 (w), 804 (m), 766 (m), 746 (vs), 729 (m), 721 (m), 704 (s), 698 (s), 675 (w), 661 (m), 648 (m), 629 (m), 607 (m), 600 (m), 592 (m), 575 (m), 552 (m), 534 (w); GC-MS (EI, 70 eV): m/z (%) = 377 (100), 232 (25), 218 (11), 159 (27), 90 (19); HRMS (EI): calcd. for $C_{22}H_{14}N_3F_3$ ($[M]^+$): 377.11343; found: 377.11287.

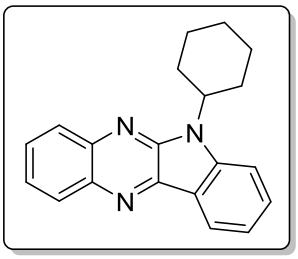


6-Phenethyl-6H-indolo[2,3-b]quinoxaline **11r** was prepared following general procedure B using compound **9** (100 mg, 0.28 mmol)and phenylethylamine (104 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11r** (79 mg, 89 %) as a yellow solid; m.p. 155-156 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.7 Hz, 1H), 8.23 (dd, *J* = 8.2, 1.3 Hz, 1H), 8.07 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.74 – 7.49 (m, 3H), 7.35 – 7.04 (m, 7H), 4.69 – 4.56 (m, 2H), 3.22 – 3.09 (m, 2H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 145.46, 144.32, 140.63, 140.05, 139.31, 138.46, 130.86, 129.31, 128.86, 128.69, 128.58, 127.86, 126.65, 125.97, 122.71, 120.80, 119.42, 109.35, 43.11, 34.74; IR (ATR, cm^{-1}): ν =3055 (w), 2933 (w), 1610 (m), 1581 (m), 1487 (m), 1466 (s), 1439 (m), 1410 (s), 1394 (m), 1360 (m), 1344 (m), 1321 (m), 1286 (w), 1259 (w), 1244 (m), 1205 (m), 1184 (m), 1176 (m), 1151 (m), 1138 (m), 1117 (s), 1066 (m), 1039 (m), 1032 (m), 1014 (m), 999 (m), 982 (w), 947 (w), 930 (w), 868 (w), 766 (s), 756 (s), 742 (vs), 725 (m), 704 (s), 692 (s), 640 (m), 619 (w), 594 (s), 571 (m), 559 (m), 532 (m); GC-MS (EI, 70 eV): m/z (%) = 323 (16), 232 (100), 219 (61), 129 (10), 102 (10), 91 (9); HRMS (EI): calcd. for $C_{22}H_{17}N_3$ ($[M]^+$): 323.14170; found: 323.14153.



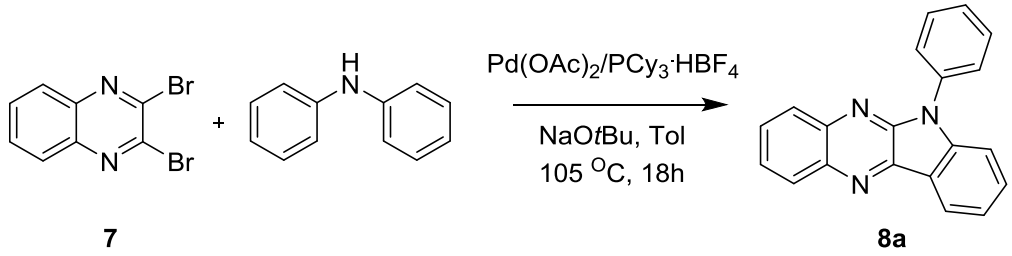
6-(3-Phenylpropyl)-6H-indolo[2,3-b]quinoxaline **11s** was prepared following general procedure B using compound **9** (100 mg, 0.28 mmol) and phenylpropylamine (117 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11s** (84 mg, 91 %) as a yellow

solid; m.p. 180-181 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.41 (d, *J* = 7.7 Hz, 1H), 8.25 (dd, *J* = 8.3, 1.3 Hz, 1H), 8.08 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.77 – 7.49 (m, 3H), 7.36 – 7.19 (m, 4H), 6.78 – 6.71 (m, 2H), 5.58 (s, 2H), 3.67 (s, 3H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.11, 145.77, 144.26, 140.67, 140.05, 139.47, 130.95, 129.33, 128.77, 128.62, 128.59, 127.88, 126.06, 122.69, 121.06, 119.66, 114.15, 110.14, 55.22, 44.49; IR (ATR, cm^{-1}): ν =3055 (w), 2955 (w), 2931 (w), 2837 (w), 1610 (m), 1581 (m), 1514 (s), 1489 (m), 1466 (s), 1439 (m), 1423 (w), 1408 (s), 1398 (m), 1365 (m), 1344 (m), 1327 (m), 1304 (m), 1271 (m), 1246 (s), 1196 (s), 1184 (s), 1157 (w), 1142 (m), 1115 (s), 1066 (m), 1032 (s), 1005 (m), 984 (w), 953 (w), 933 (w), 858 (w), 835 (m), 820 (m), 802 (w), 762 (s), 742 (vs), 721 (m), 714 (m), 685 (s), 650 (m), 633 (m), 615 (m), 590 (s), 571 (m), 557 (w), 540 (m); GC-MS (EI, 70 eV): m/z (%) = 337 (35), 233 (100); HRMS (ESI): calcd. for ($[M + H]^+$): 338.16517; found: 338.16549; calcd. for $C_{23}H_{19}N_3Na$ ($[M + Na]^+$): 360.14712; found: 360.14751.



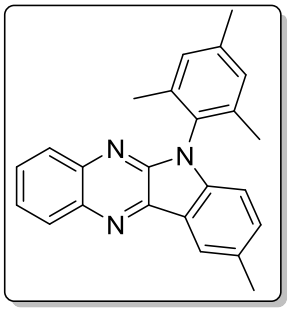
6-Cyclohexyl-6H-indolo[2,3-b]quinoxaline **11t** was prepared following general procedure B using compound **9** (100 mg, 0.28 mmol) and cyclohexylamine (90 µL, 0.82 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **11t** (61 mg, 74 %) as a yellow solid; m.p. 215-216 ºC; ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.52 (d, *J* = 7.7 Hz, 1H), 8.30 (dd, *J* = 8.2, 1.2 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.2 Hz, 1H), 7.81 – 7.57 (m, 4H), 7.36 (ddd, *J* = 8.0, 4.8, 3.4 Hz, 1H), 4.97 (ddd, *J* = 12.4, 8.8, 3.8 Hz, 1H), 2.59 (tt, *J* = 12.4, 6.1 Hz, 2H), 2.23 – 0.59 (m, 8H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 145.68, 144.03, 140.60, 140.05, 139.06, 130.76, 129.29, 128.70, 128.05, 126.02, 122.96, 120.53, 119.96, 111.27, 54.09, 30.38, 26.40, 25.71; IR (ATR, cm^{-1}): ν =2931 (m), 2854 (m), 1608 (w), 1579 (m), 1574 (m), 1485 (m), 1460 (m), 1435 (w), 1404 (s), 1383 (m), 1346 (m), 1327 (m), 1321 (m), 1298 (m), 1263 (w), 1252 (w), 1234 (m), 1205 (s), 1124 (m), 1117 (s), 1090 (w), 1066 (m), 1043 (m), 1009 (m), 980 (w), 945 (m), 889 (m), 862 (w), 850 (w), 804 (w), 764 (m), 746 (vs), 717 (m), 696 (w), 638 (m), 592 (s), 569 (m), 540 (w); GC-MS (EI, 70 eV): m/z (%) = 301 (20), 219 (100); HRMS (EI): calcd. for $C_{20}H_{19}N_3$ ($[M]^+$): 301.15735; found: 301.15679.

General procedure C for C-N coupling/C-H bond activation, exemplified by: *6-phenyl-6H-indolo[2,3-b]quinoxaline* 8a

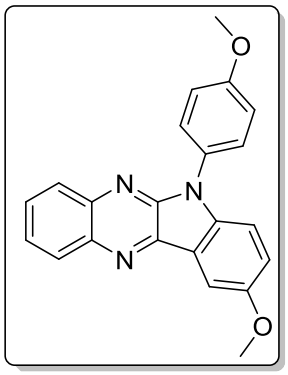


7 **8a**

To a pressure tube charged with 2,3-dibromoquinoxaline **7** (100 mg, 0.35 mmol), $Pd(OAc)_2$ (3 mg, 14 µmol), ligand $PCy_3 \cdot HBF_4$ (11 mg, 29 µmol) and sodium *tert*-butoxide (83 mg, 0.87mmol) under Argon. The mixture was back-filled with Argon several times. The mixture was dissolved in anhydrous Toluene (10 mL). Diphenylamine (49 mg, 0.29mmol) was added to the mixture and heated at 105 ºC for 18 h. After cooling, the reaction mixture was diluted with dichloromethane (20 mL) and filtered through a celite pad, washing with dichloromethane (40 mL). The filtrate was reduced *in vacuo*. The product was separated via flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **8a** (77 mg, 90%) as a yellow solid; m.p. 230-231ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.49 – 8.41 (m, 1H), 8.27 – 8.20 (m, 1H), 8.03 – 7.97 (m, 1H), 7.70 – 7.51 (m, 7H), 7.48 – 7.39 (m, 2H), 7.39 – 7.31 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.86, 144.74, 140.60, 140.18, 139.82, 135.43, 131.03, 129.80, 129.27, 128.83, 128.26, 127.99, 127.16, 126.51, 122.70, 121.86, 119.86, 110.62; IR (ATR, cm^{-1}): ν =3054 (w), 1608 (w), 1597 (w), 1581 (m), 1571 (w), 1501 (m), 1483 (m), 1470 (m), 1458 (m), 1451 (m), 1403 (s), 1390 (m), 1354 (w), 1336 (w), 1318 (m), 1303 (m), 1252 (m), 1226 (m), 1219 (m), 1205 (s), 1174 (m), 1166 (m), 1133 (m), 1126 (m), 1100 (m), 1073 (w), 1042 (w), 1025 (w), 1015 (w), 1007 (w), 954 (w), 949 (w), 780 (m), 766 (m), 758 (m), 748 (vs), 719 (w), 694 (s), 687 (s), 649 (m), 590 (s), 485 (m), 451 (s), 428 (w); GC-MS (EI, 70 eV): m/z (%) = 295 (100), 147 (10); HRMS (EI): calcd. for $C_{20}H_{13}N_3$ ($[M]^+$):295.11040; found: 295.10963.



6-Mesityl-9-methyl-6H-indolo[2,3-b]quinoxaline **8b** was prepared following general procedure C using compound **7** (100 mg, 0.35 mmol) and 2,4,6-trimethyl-*N*-(p-tolyl)aniline (65 mg, 0.29 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 5:1) to yield **8b** (48 mg, 47 %) as a yellow solid; m.p.175-176 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 – 8.20 (m, 2H), 8.03 – 7.94 (m, 1H), 7.65 – 7.53 (m, 2H), 7.36 – 7.30 (m, 1H), 7.02 (s, 2H), 6.81 (d, *J* = 8.3 Hz, 1H), 2.48 (s, 3H), 2.33 (s, 3H), 1.82 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.80, 142.90, 141.03, 139.92, 139.52, 139.07, 137.45, 132.42, 131.04, 130.35, 129.65, 129.30, 128.58, 128.23, 126.08, 122.74, 119.66, 110.07, 21.30, 21.29, 17.88; IR (ATR, cm^{-1}): ν =3019 (w), 2944 (w), 2913 (w), 2855 (w), 1609 (w), 1587 (w), 1577 (w), 1483 (s), 1471 (m), 1454 (m), 1441 (m), 1394 (m), 1386 (m), 1377 (m), 1361 (w), 1349 (m), 1326 (w), 1316 (m), 1303 (m), 1289 (m), 1251 (m), 1237 (m), 1206 (m), 1197 (m), 1179 (m), 1143 (w), 1130 (m), 1124 (m), 1112 (m), 1044 (m), 1032 (w), 1015 (w), 960 (w), 949 (w), 912 (m), 884 (m), 863 (w), 852 (m), 815 (w), 806 (s), 773 (w), 755 (vs), 749 (s), 728 (m), 719 (m), 678 (w), 670 (w), 656 (w), 642 (w), 630 (m), 603 (w), 596 (m), 586 (m), 571 (m), 565 (m), 549 (w), 540 (w), 522 (w), 516 (w), 512 (w), 508 (w), 498 (w), 485 (m), 472 (w), 449 (vs), 428 (m), 422 (m), 409 (w), 400 (w), 396 (w), 393 (w), 389 (w), 380 (w); GC-MS (EI, 70 eV): m/z (%) = 351 (100), 336 (20), 320 (7), 160 (11), 119 (7); HRMS (EI): calcd. for $C_{24}H_{21}N_3$ ($[M]^+$): 351.17300; found: 351.17195.

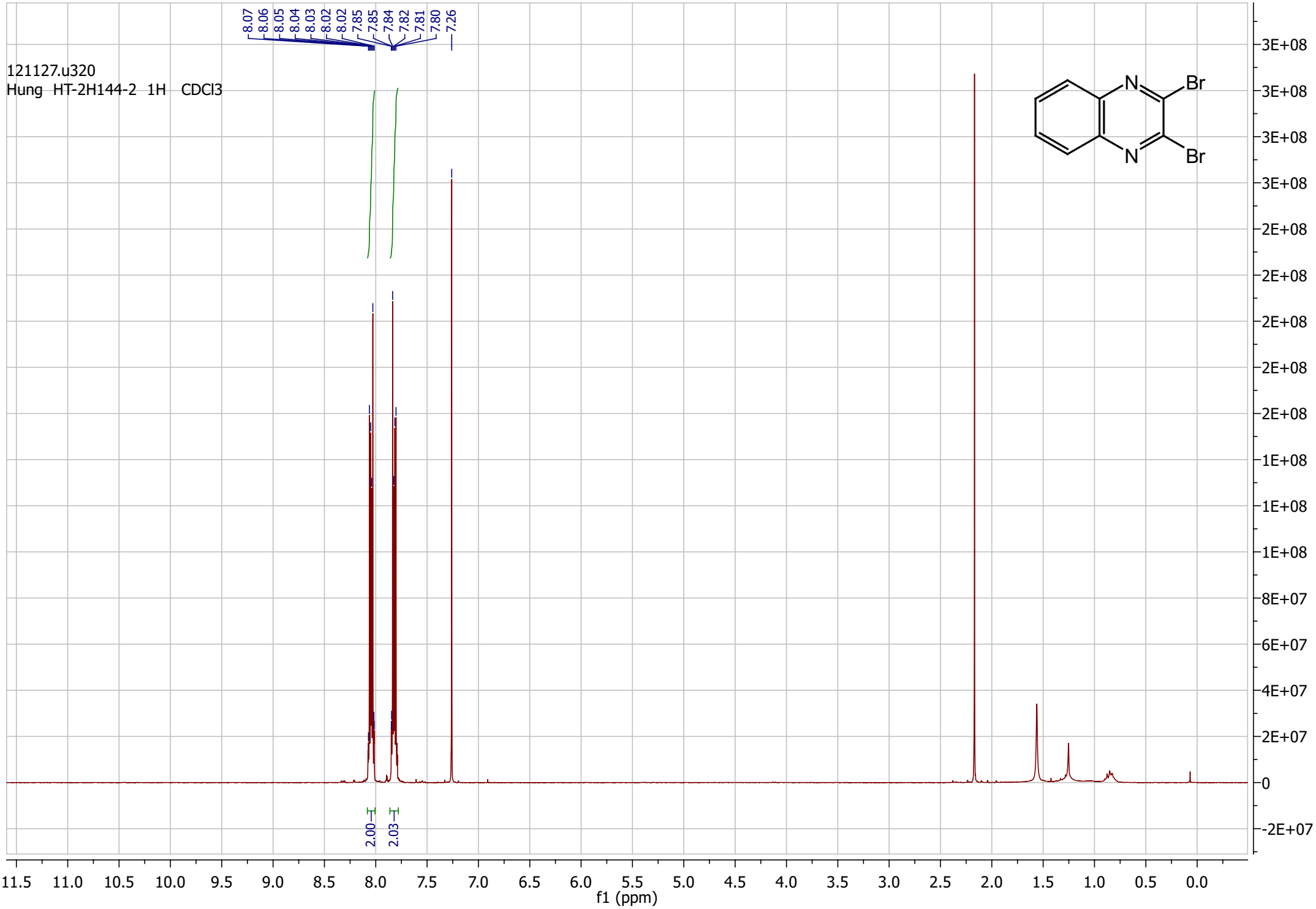


9-Methoxy-6-(4-methoxyphenyl)-6H-indolo[2,3-b]quinoxaline **8c** was prepared following general procedure C using compound **7** (100 mg, 0.35 mmol) and bis(4-methoxyphenyl)amine (66 mg, 0.29 mmol). The product was purified by flash chromatography (silica gel, heptanes/ethylacetate 1:1) to yield **8c** (56 mg, 54 %) as a yellow solid; m.p.163-164 ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.26 – 8.20 (m, 2H), 8.03 – 7.98 (m, 2H), 7.93 (d, *J* = 2.5 Hz, 2H), 7.62 (tt, *J* = 6.8, 5.1 Hz, 4H), 7.56 – 7.49 (m, 4H), 7.30 (d, *J* = 8.9 Hz, 2H), 7.17 (dd, *J* = 8.6, 2.9 Hz, 3H), 7.11 – 7.04 (m, 4H), 3.91 (s, 6H), 3.85 (s, 6H); ^{13}C NMR (63 MHz, $CDCl_3$) δ 159.05, 155.31, 146.25, 140.69, 139.95, 139.84, 139.43, 129.13, 128.70, 128.36, 128.20, 128.16, 126.24, 120.47, 119.88, 115.04,

111.51, 104.45, 56.12, 55.59; IR (ATR, cm^{-1}): ν =3054 (w), 3017 (w), 2993 (w), 2837 (m), 1614 (w), 1572 (w), 1512 (s), 1487 (vs), 1473 (s), 1466 (s), 1458 (s), 1454 (s), 1438 (s), 1420 (m), 1395 (s), 1388 (s), 1293 (s), 1247 (s), 1197 (vs), 1185 (s), 1174 (vs), 1164 (s), 1138 (m), 1126 (s), 1107 (m), 1040 (s), 1031 (s), 1024 (s), 954 (m), 925 (m), 888 (m), 827 (vs), 809 (s), 802 (m), 793 (s), 764 (s), 756 (vs), 751 (s), 719 (m), 712 (m), 652 (m), 635 (m), 631 (m), 624 (m), 603 (s), 590 (s), 561 (m), 555 (m), 549 (m), 525 (m), 518 (m), 489 (m), 455 (s), 435 (m), 419 (m); GC-MS (EI, 70 eV): m/z (%) = 355 (100), 340 (76), 269 (12), 178 (7); HRMS (EI): calcd. for $C_{22}H_{17}O_2N_3$ ($[M]^+$): 355.13153; found: 355.13112.

References

(1) Li, J. J.; Carson, K. G.; Trivedi, B. K.; Yue, W. S.; Ye, Q.; Glynn, R. a; Miller, S. R.; Connor, D. T.; Roth, B. D.; Luly, J. R.; Low, J. E.; Heilig, D. J.; Yang, W.; Qin, S.; Hunt, S. *Bioorg. Med. Chem.***2003**, *11*, 3777–3790.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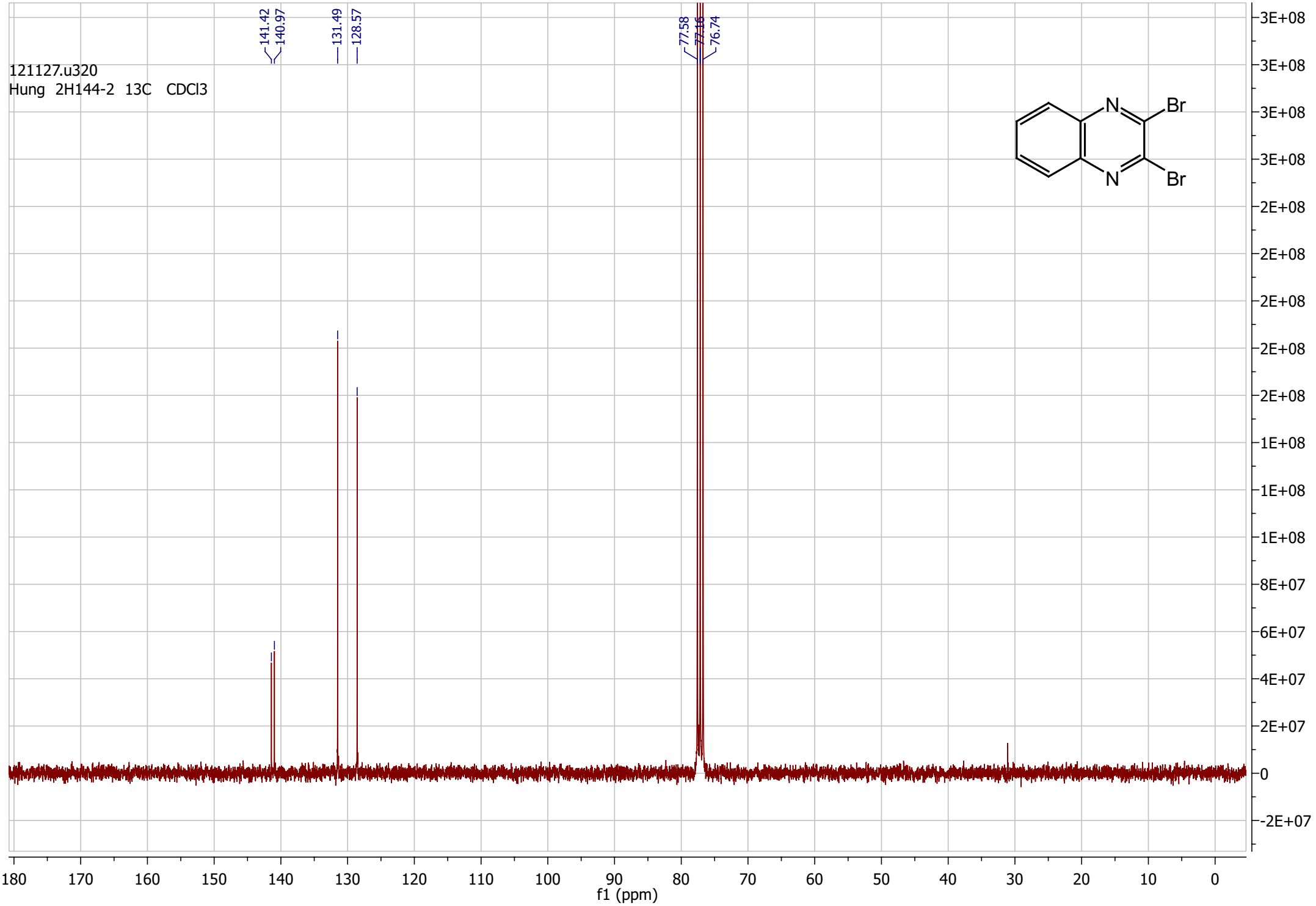
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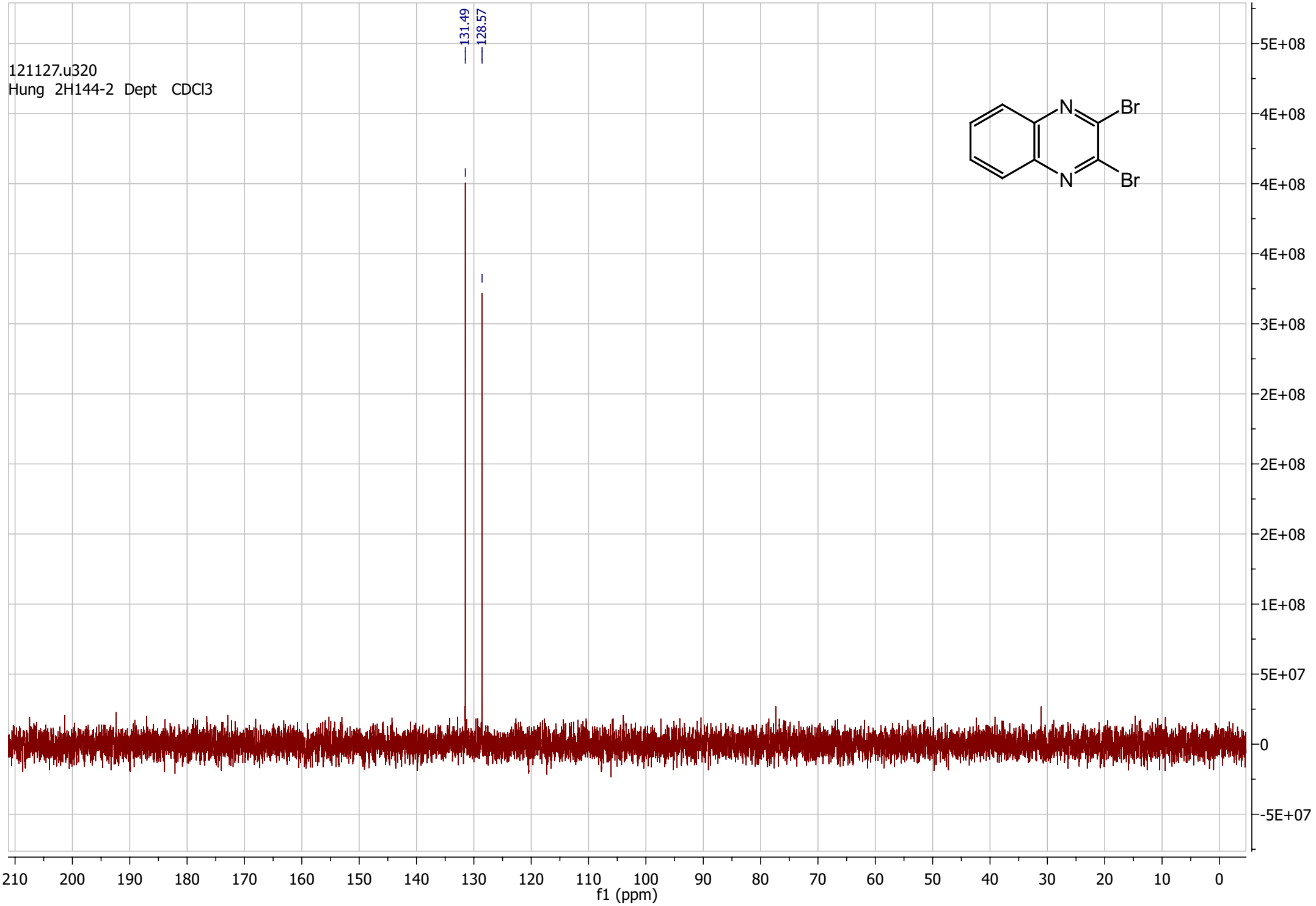
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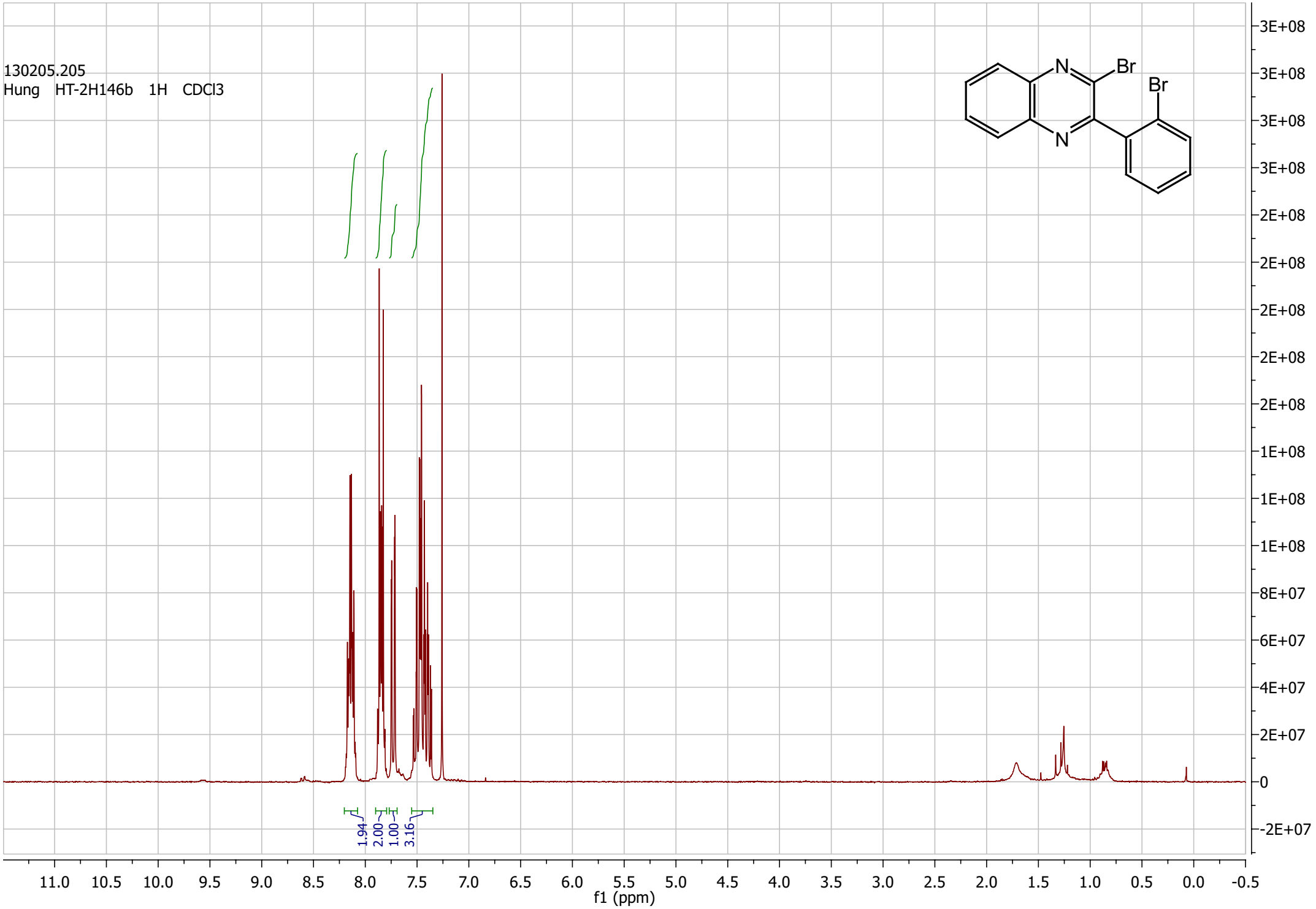
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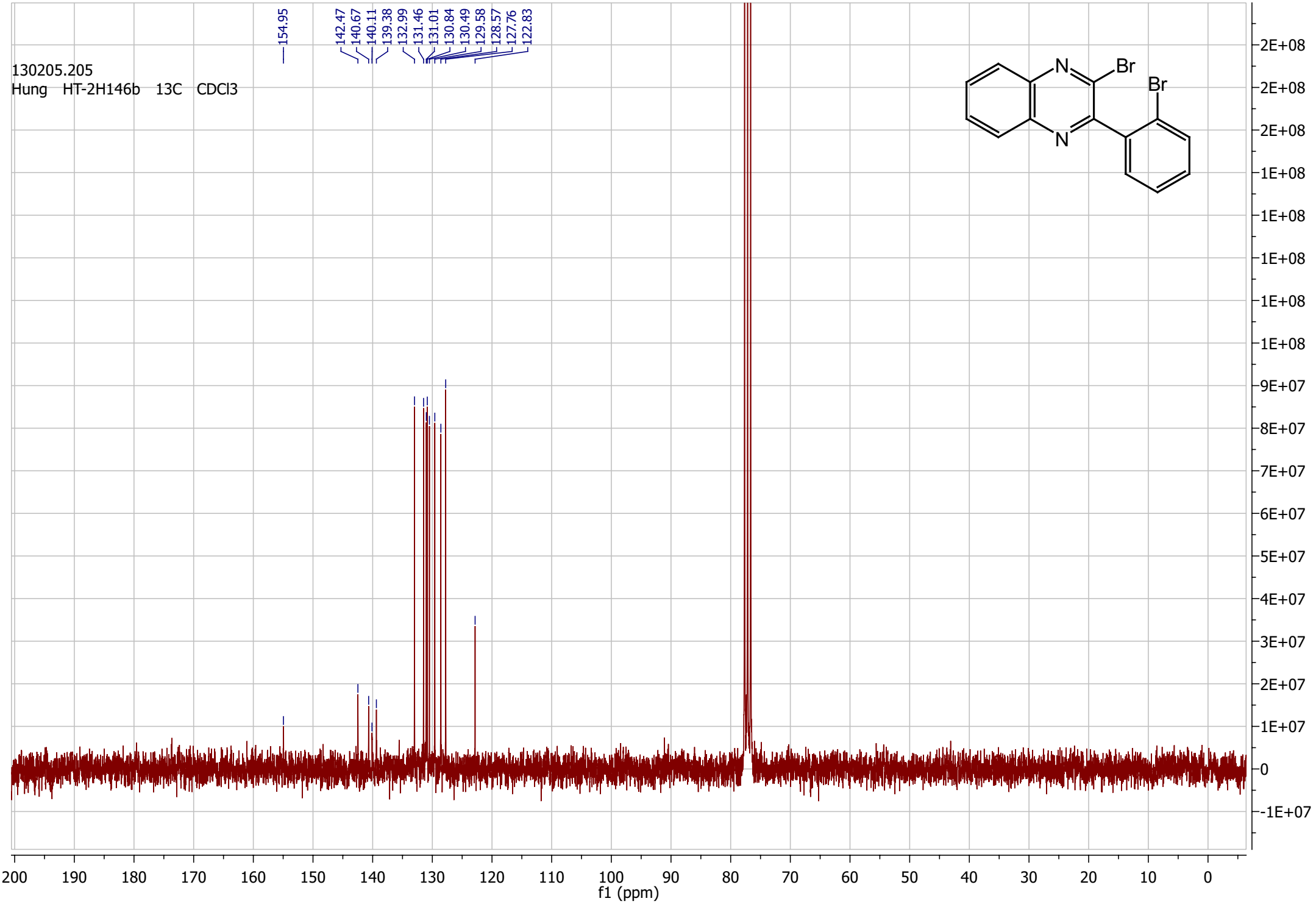
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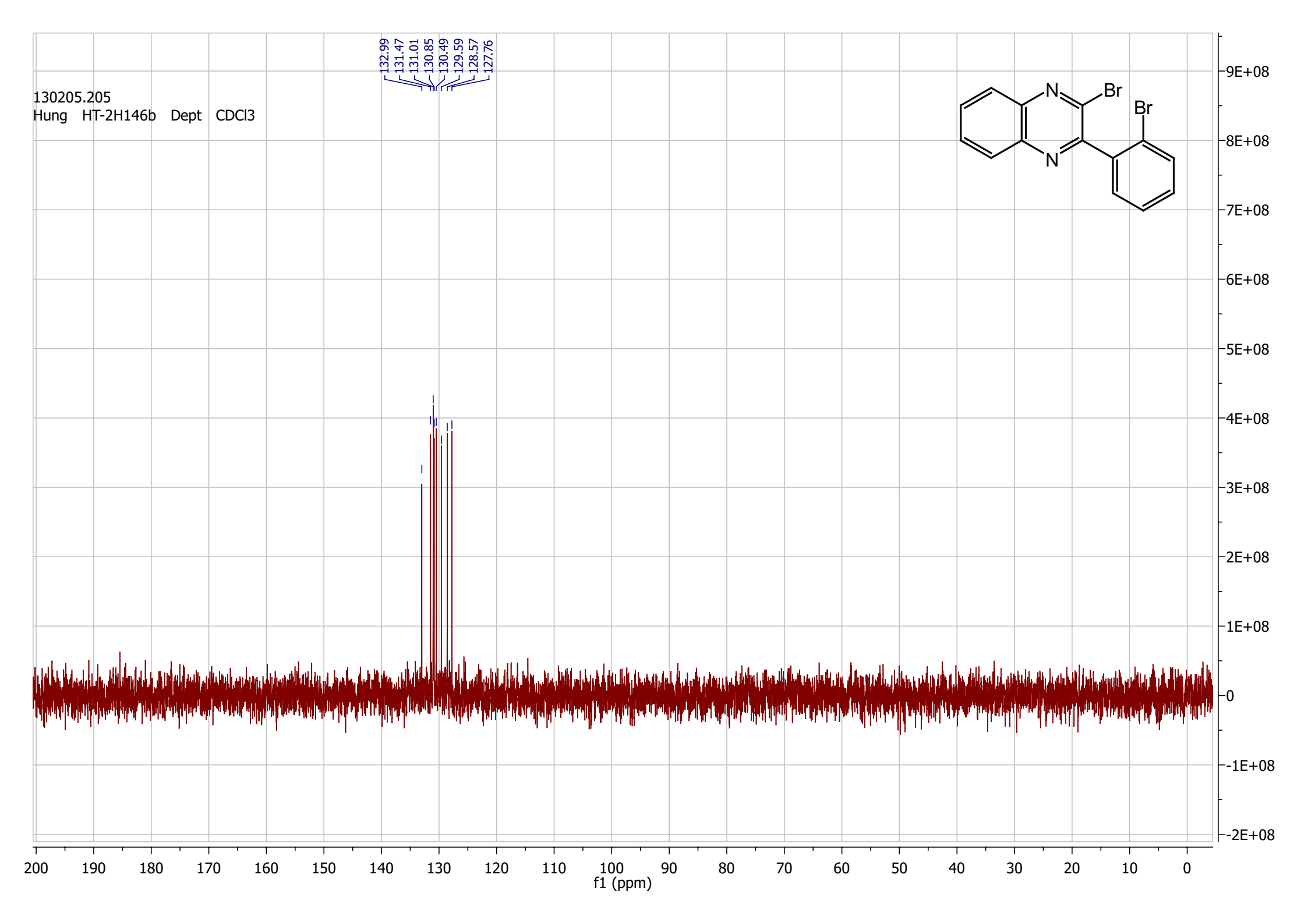
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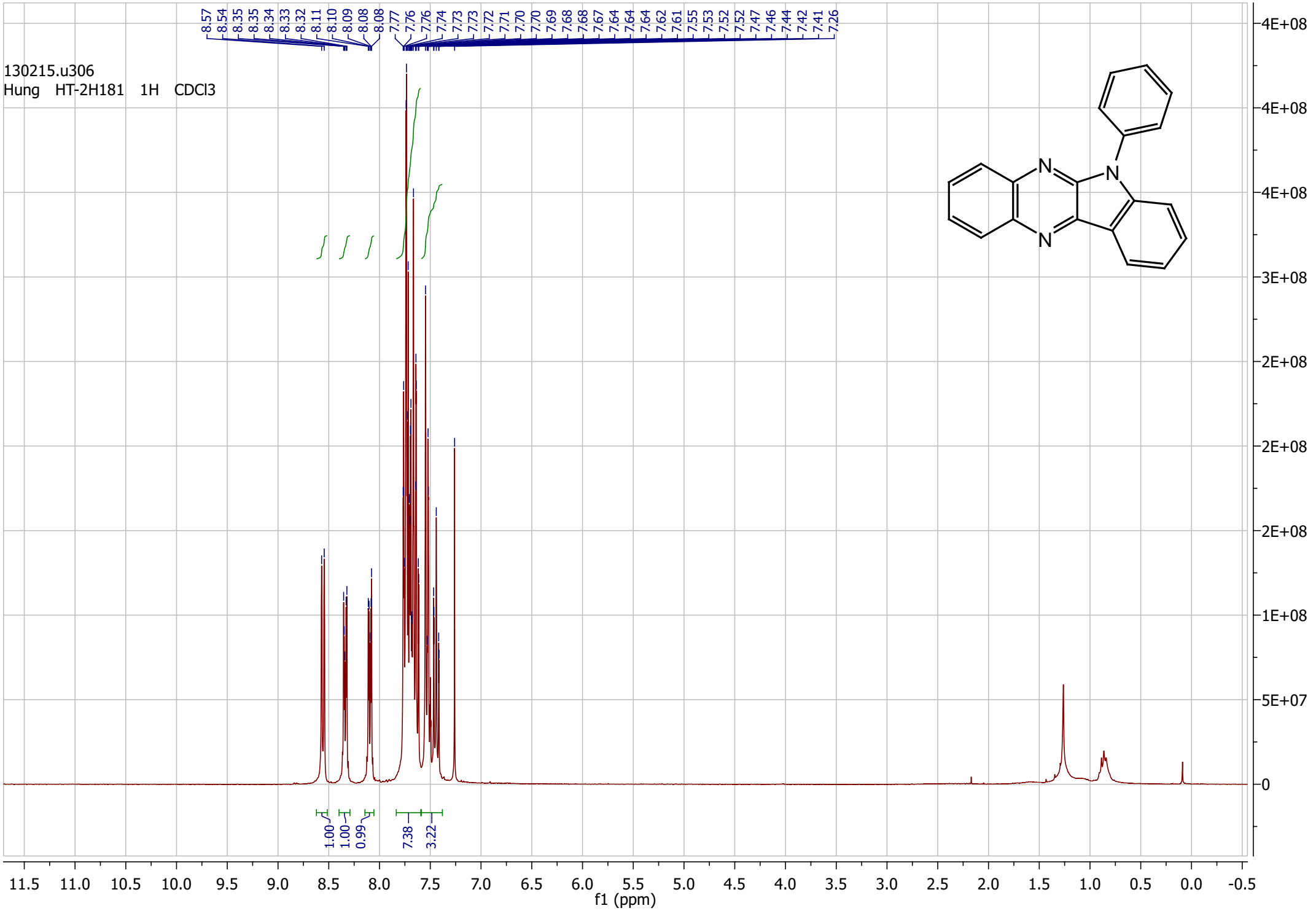
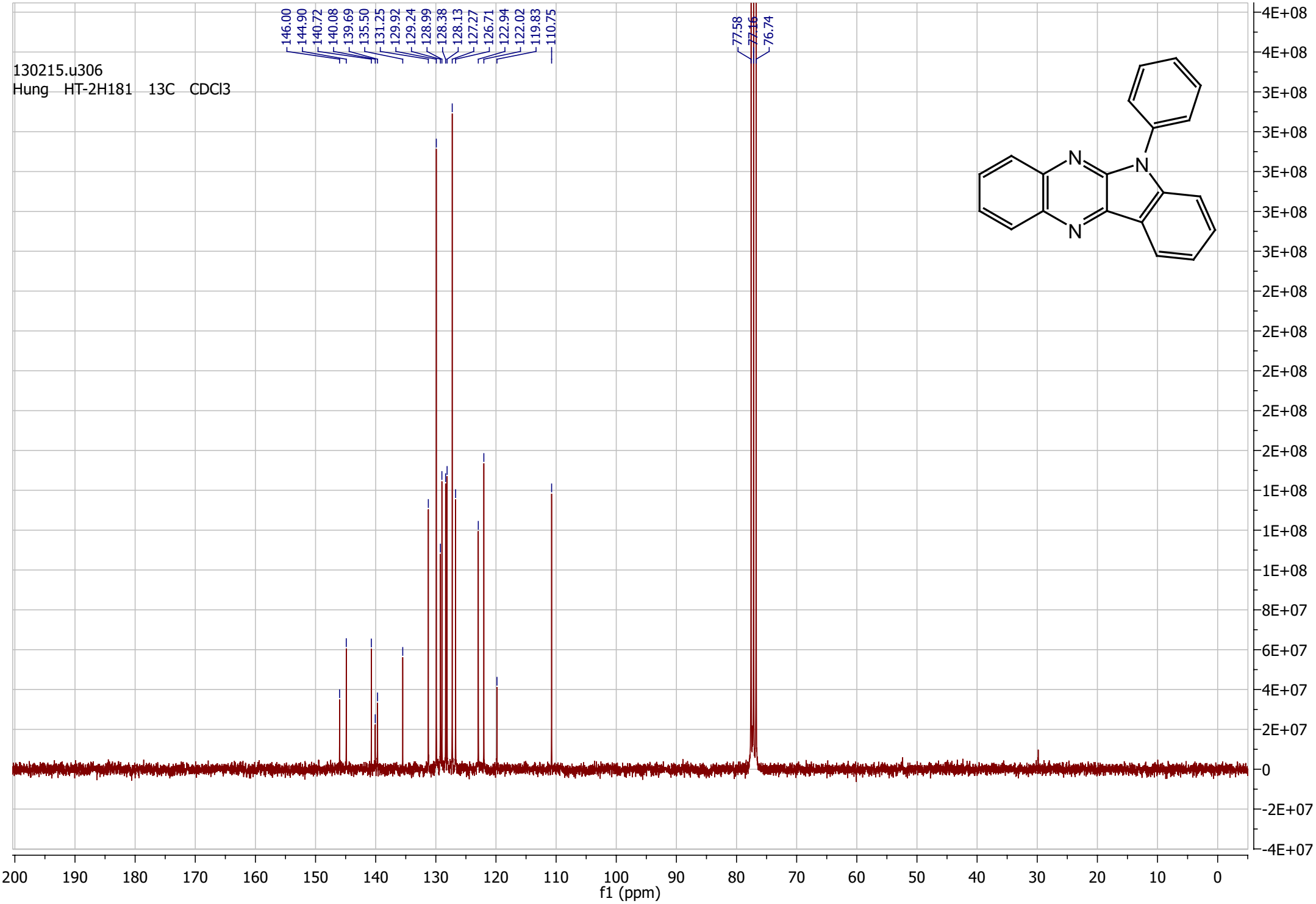
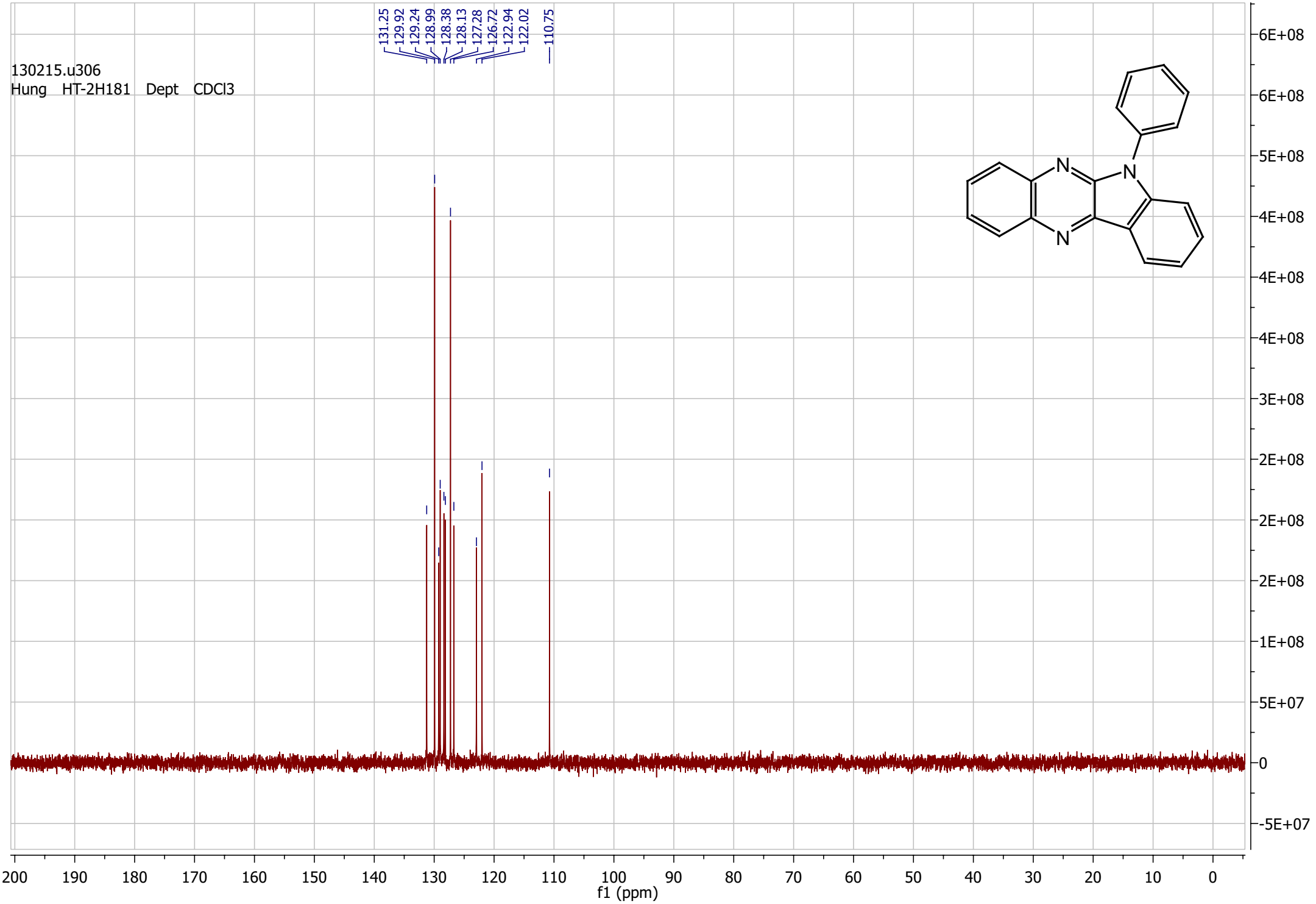
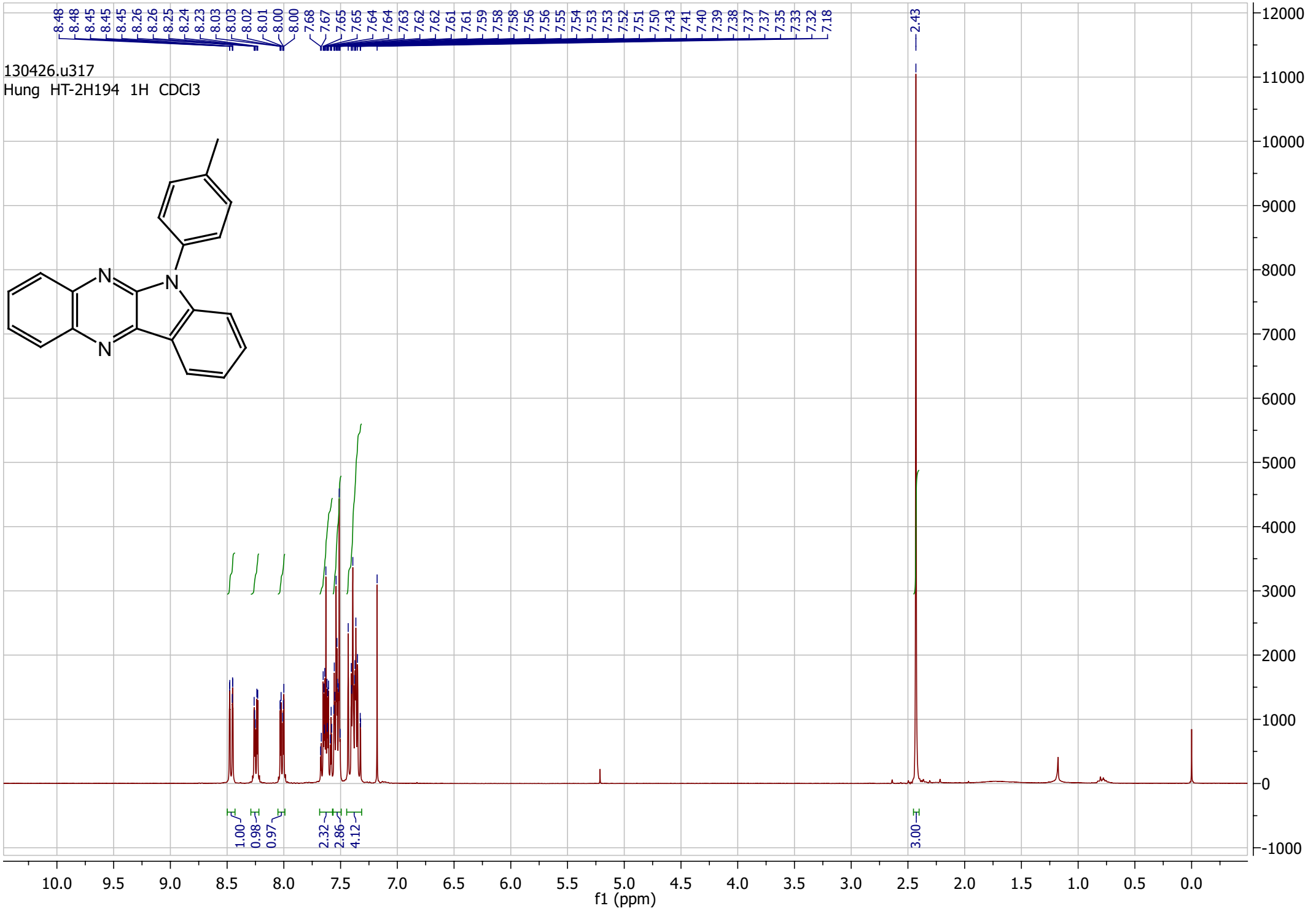
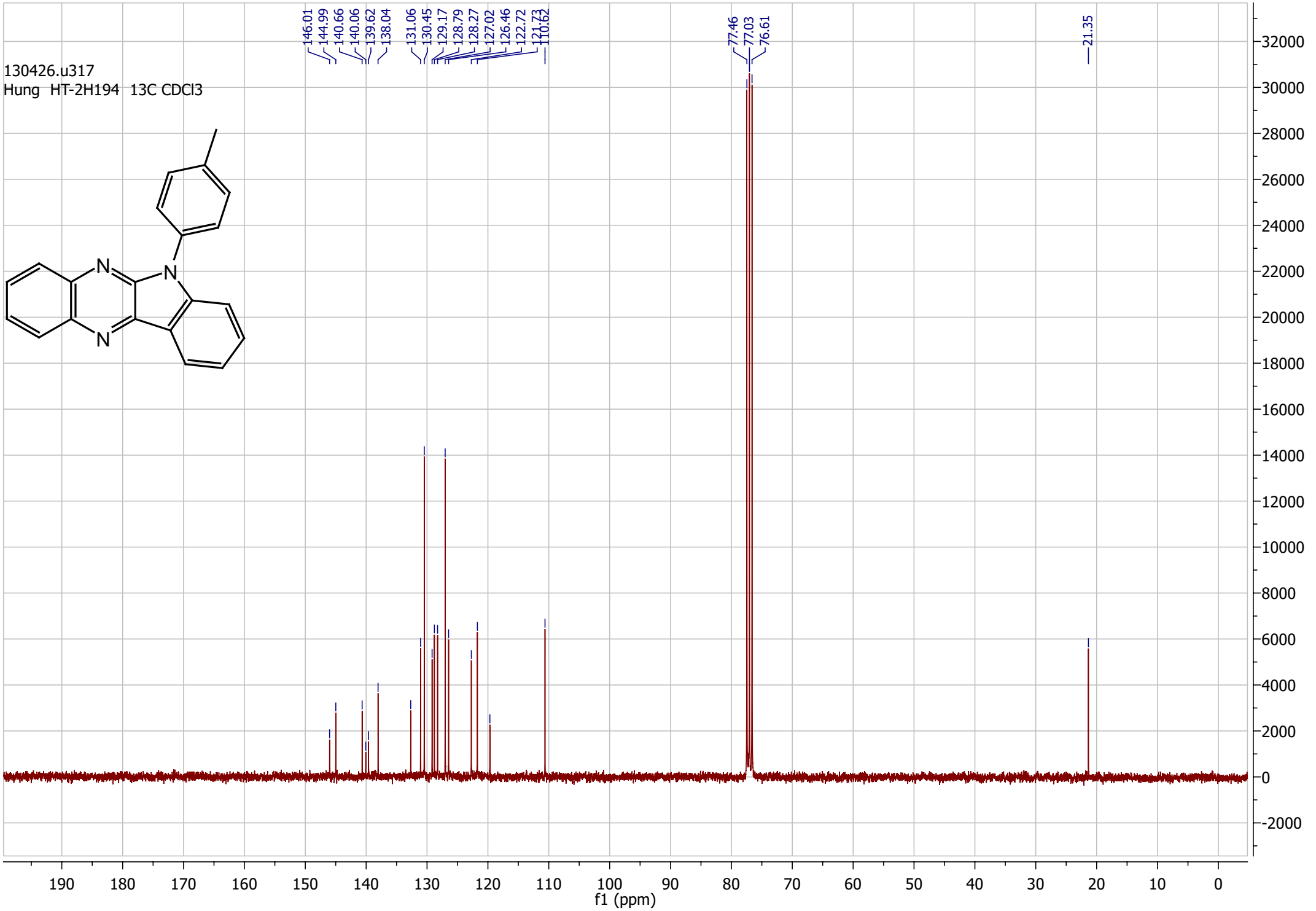
f1 (ppm)

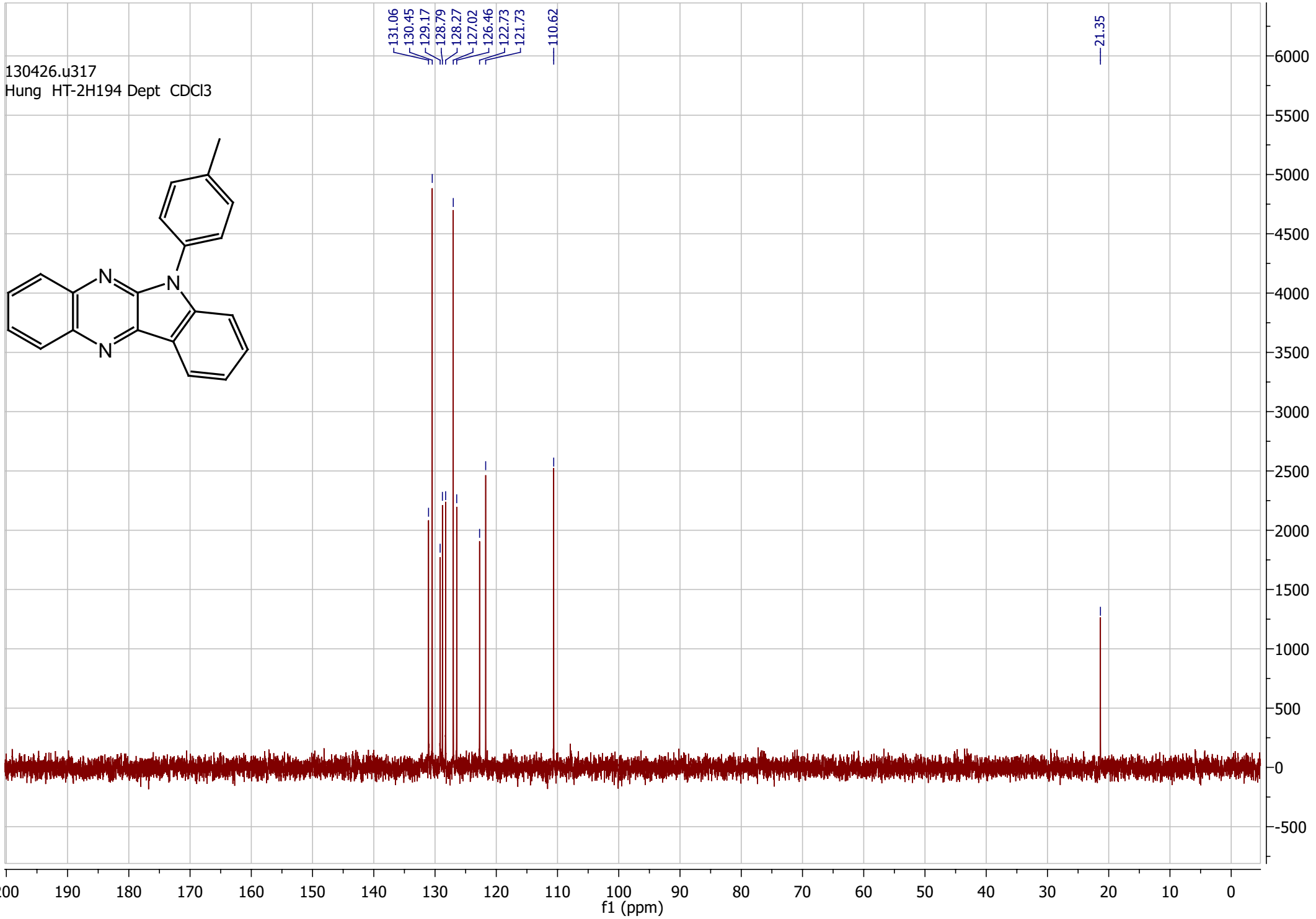

130215.u306
Hung HT-2H181 1H CDCl3
8.57 8.54 8.35 8.35 8.34 8.33 8.32 8.11 8.10 8.09 8.08 8.08 7.77 7.76 7.76 7.74 7.73 7.73 7.72 7.71 7.70 7.70 7.69 7.68 7.68 7.67 7.64 7.64 7.64 7.62 7.61 7.55 7.53 7.52 7.52 7.47 7.46 7.44 7.42 7.41 7.26
1.00 1.00 0.99 7.38 3.22
N
N
N
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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 -0.5
f1 (ppm)

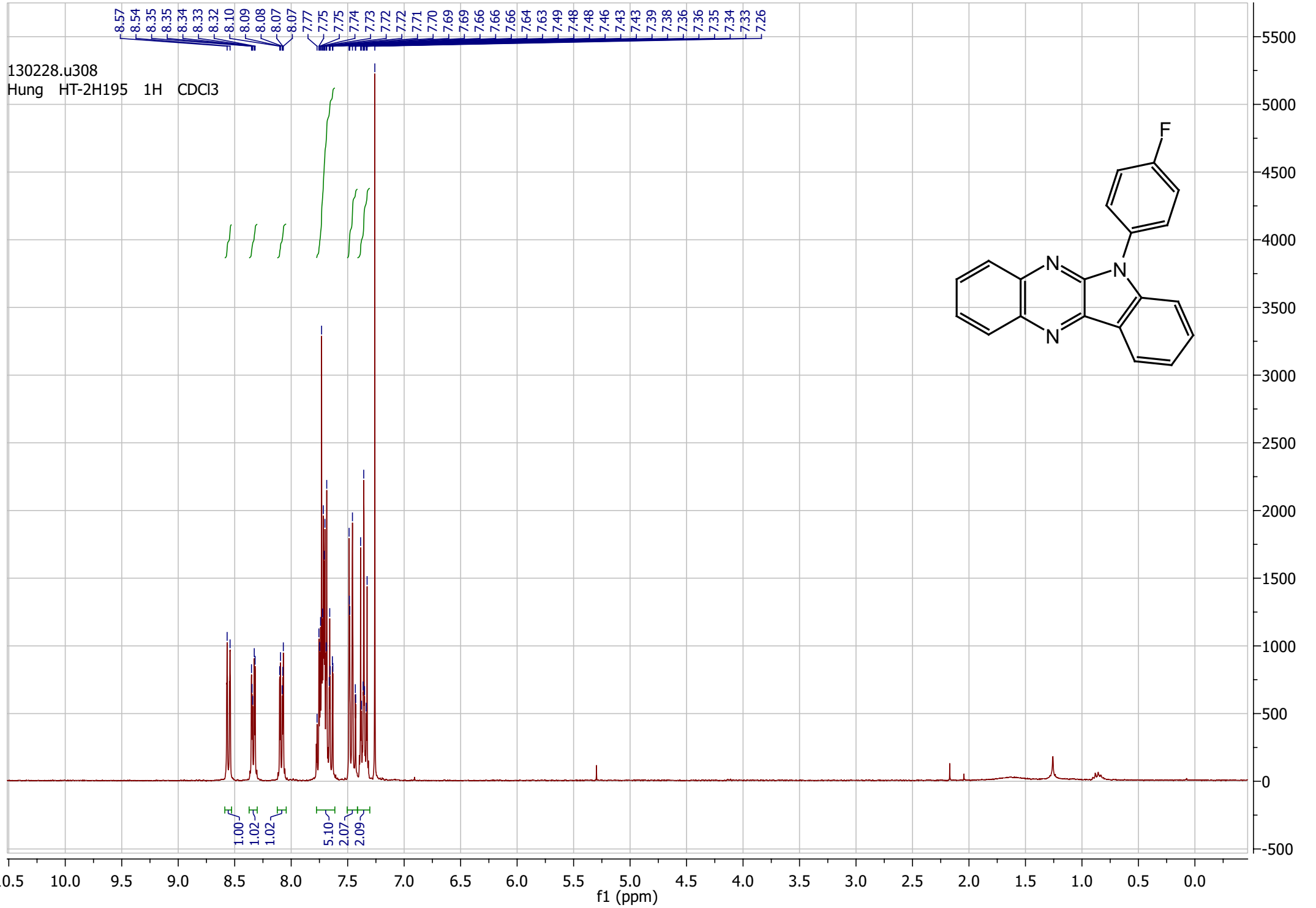

130215.u306
Hung HT-2H181 13C CDCl3
146.00
144.90
140.72
140.08
139.69
135.50
131.25
129.92
129.24
128.99
128.38
128.13
127.27
126.71
122.94
122.02
119.83
110.75
77.58
77.16
76.74
N
N
N
4E+08
4E+08
3E+08
3E+08
3E+08
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
-4E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

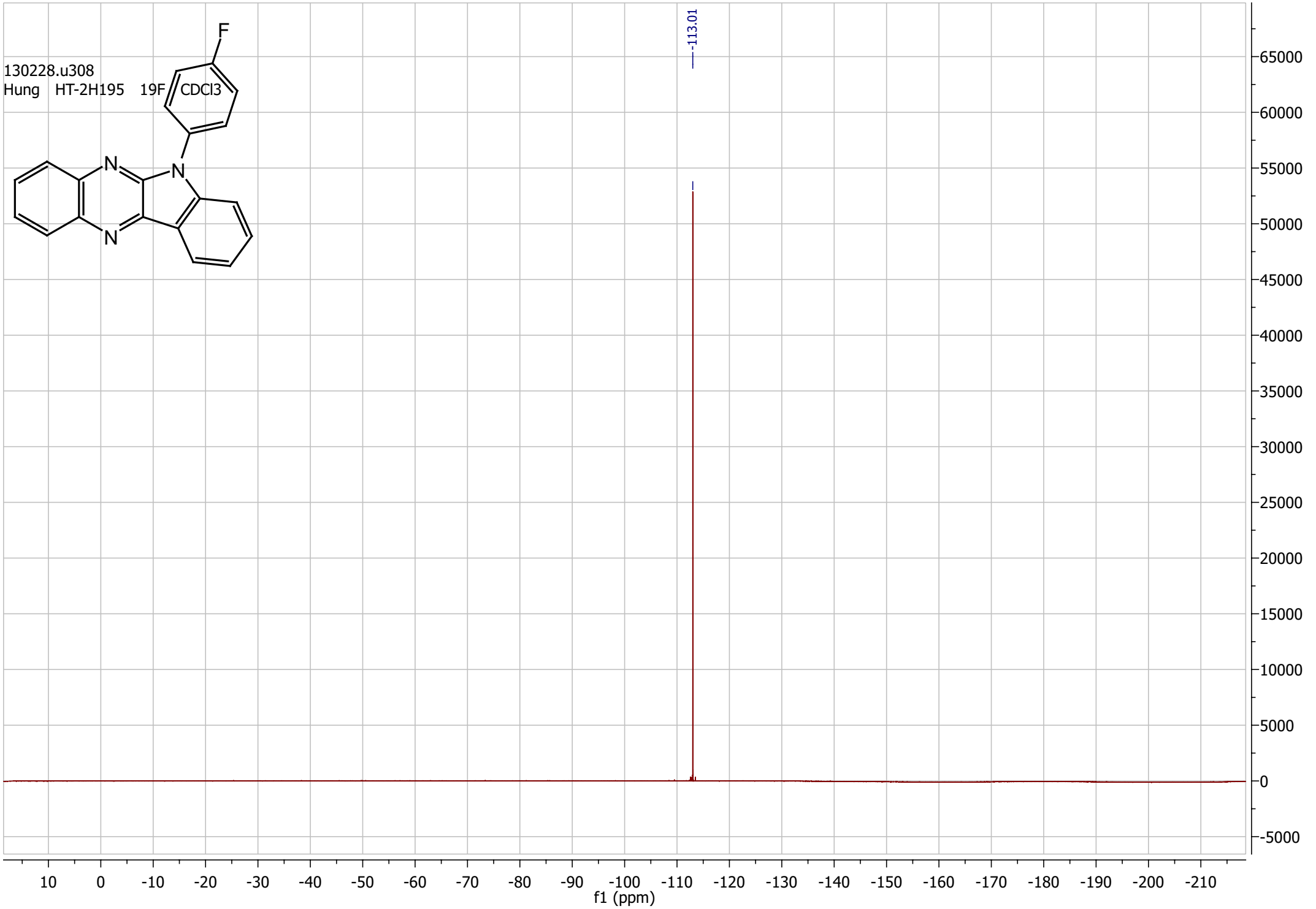

131.25
129.92
129.24
128.99
128.38
128.13
127.28
126.72
122.94
122.02
110.75
130215.u306
Hung HT-2H181 Dept CDCl3
N
N
N
6E+08
6E+08
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

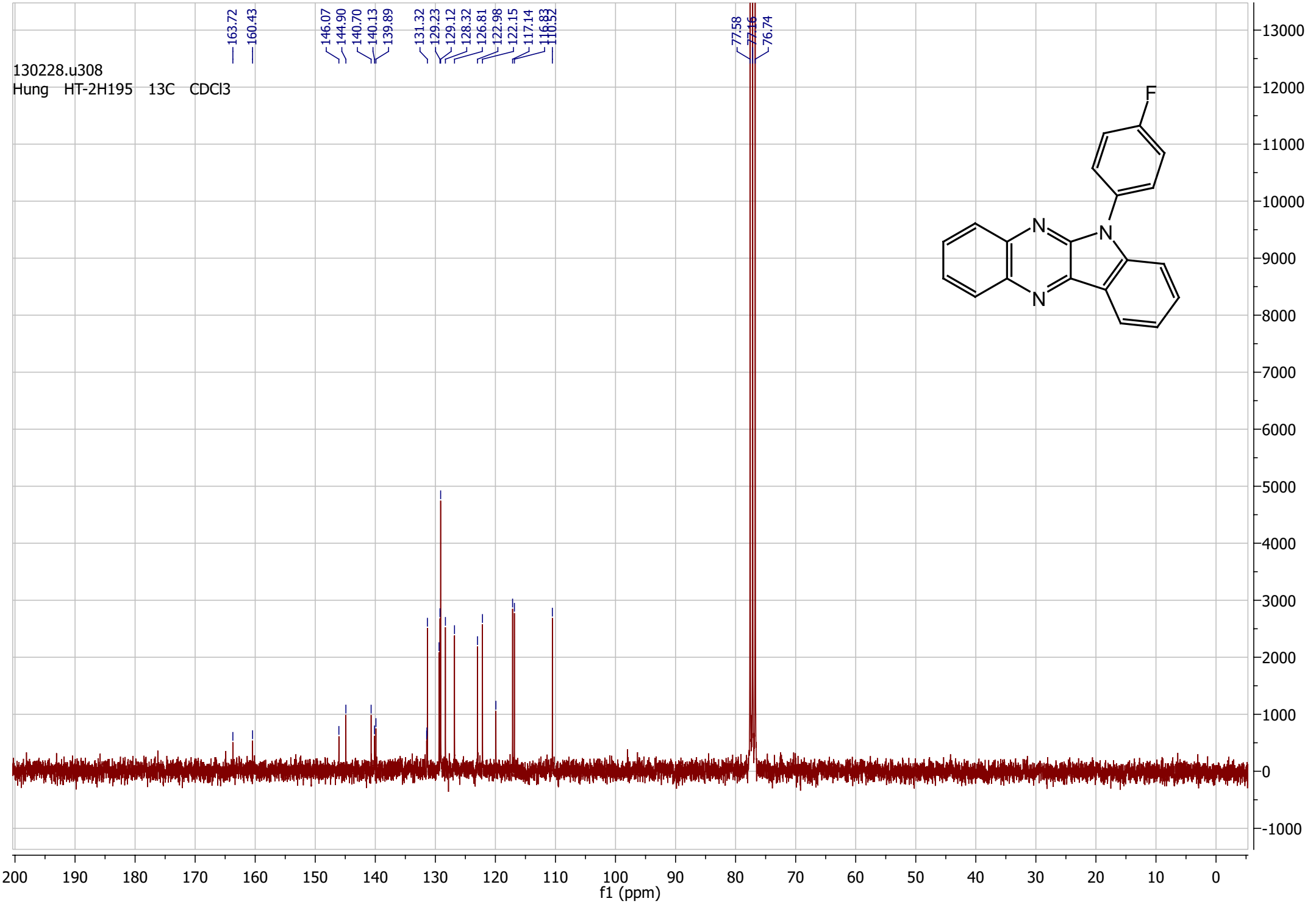

130426.u317
Hung HT-2H194 1H CDCl3
8.48 8.48 8.45 8.45 8.45 8.26 8.26 8.25 8.24 8.23 8.03 8.03 8.02 8.01 8.00 8.00
7.68 7.67 7.65 7.65 7.64 7.64 7.63 7.62 7.62 7.61 7.61 7.59 7.58 7.58 7.56 7.56 7.55 7.54 7.53 7.53 7.52 7.51 7.50 7.43 7.41 7.40 7.39 7.38 7.37 7.37 7.35 7.33 7.32 7.18
2.43
N
N
N
1.00
0.98
0.97
2.32
2.86
4.12
3.00
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)

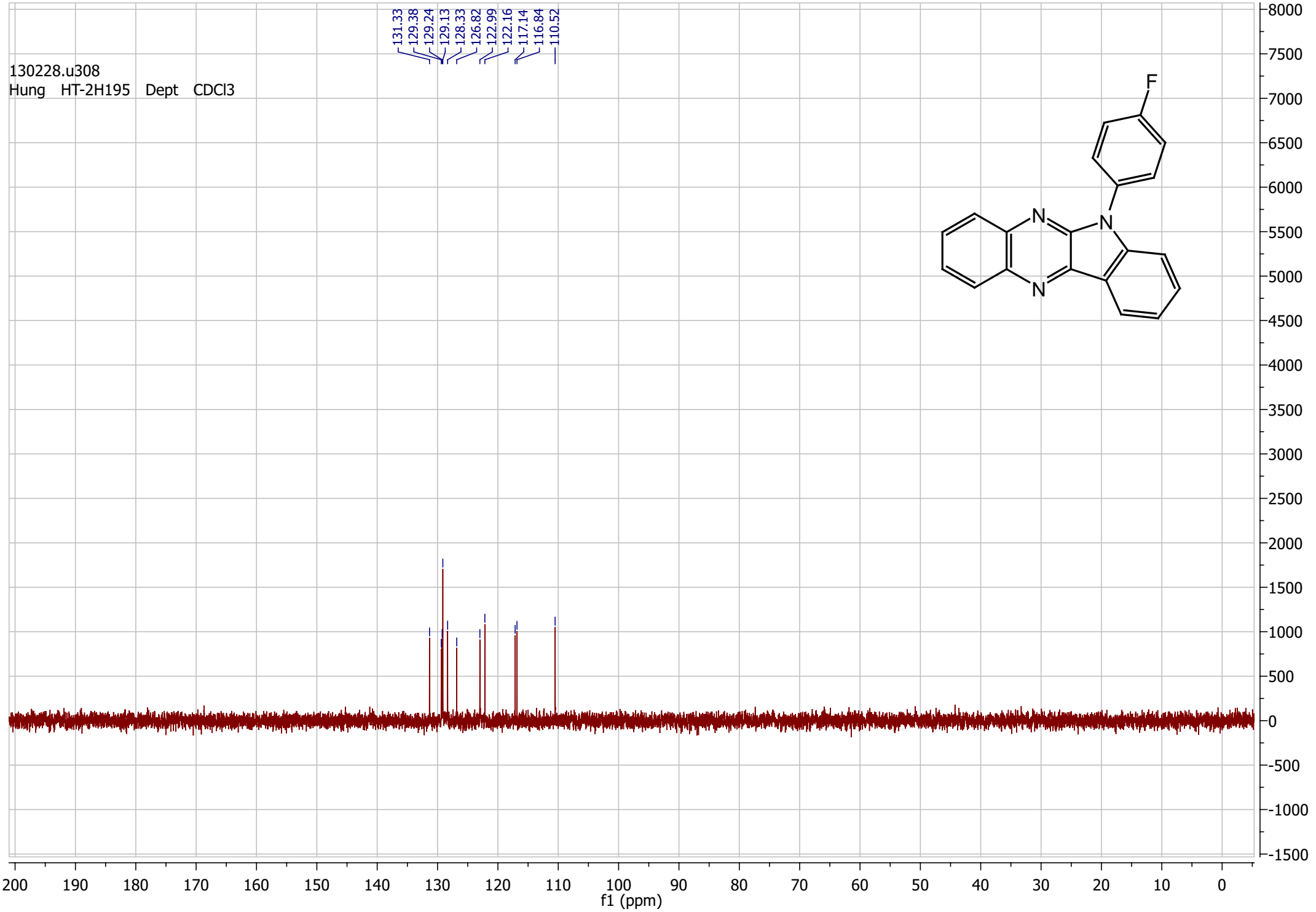

130426.u317
Hung HT-2H194 13C CDCl3
146.01
144.99
140.66
140.06
139.62
138.04
131.06
130.45
129.17
128.79
128.27
127.02
126.46
122.72
121.73
110.62
77.46
77.03
76.61
21.35
N
N
N
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

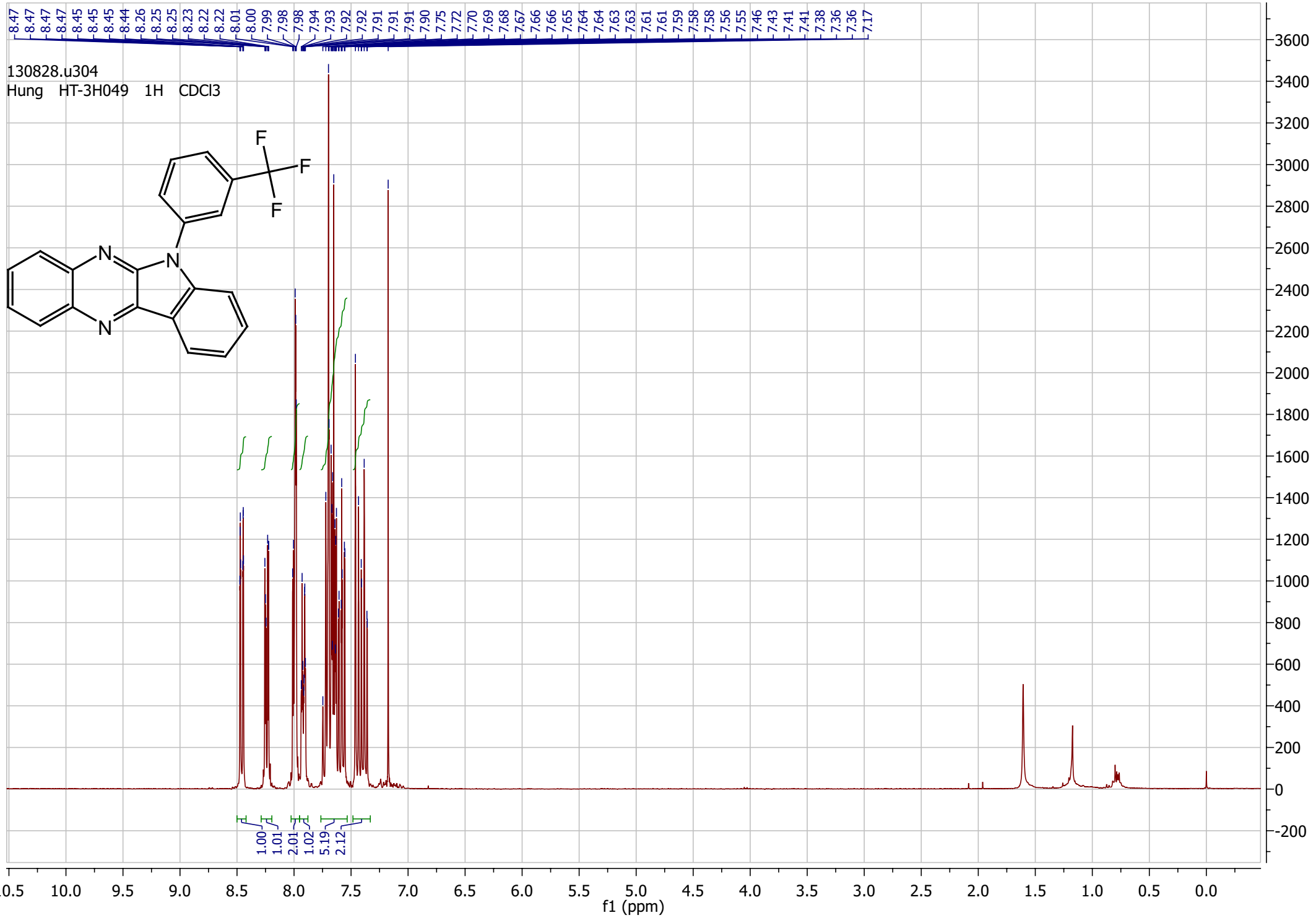

131.06
130.45
129.17
128.79
128.27
127.02
126.46
122.73
121.73
110.62
21.35
130426.u317
Hung HT-2H194 Dept CDCl3
N
N
N
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

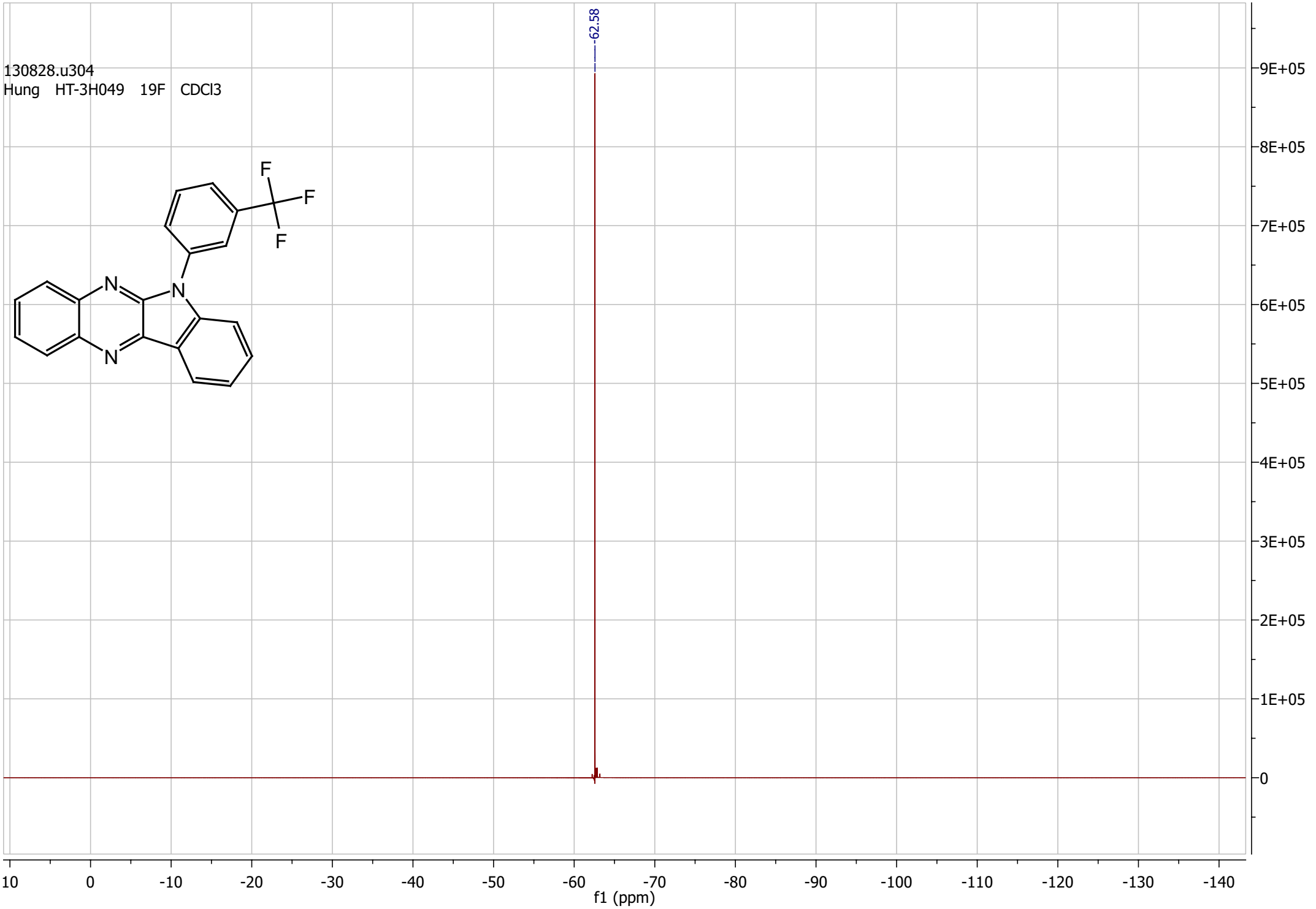

130228.u308
Hung HT-2H195 1H CDCl3
8.57 8.54 8.35 8.35 8.34 8.33 8.32 8.10 8.09 8.08 8.07 8.07 7.77 7.75 7.75 7.74 7.73 7.72 7.72 7.71 7.70 7.69 7.69 7.66 7.66 7.66 7.64 7.63 7.49 7.48 7.48 7.46 7.43 7.43 7.39 7.38 7.36 7.36 7.35 7.34 7.33 7.26
1.00 1.02 1.02 5.10 2.07 2.09
F
N
N
N
f1 (ppm)

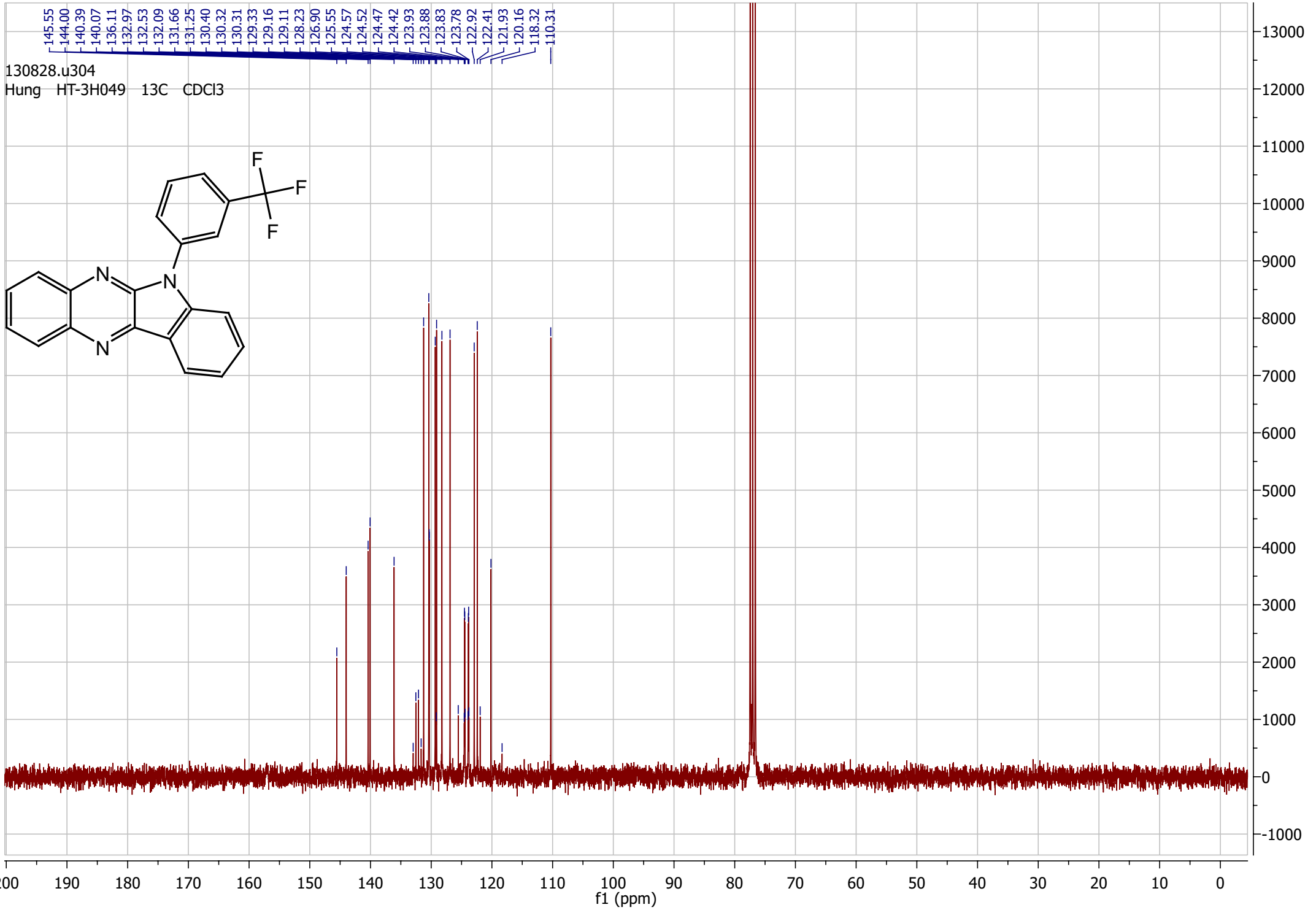

130228.u308
Hung HT-2H195 19F CDCl3
F
N
N
N
-113.01
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

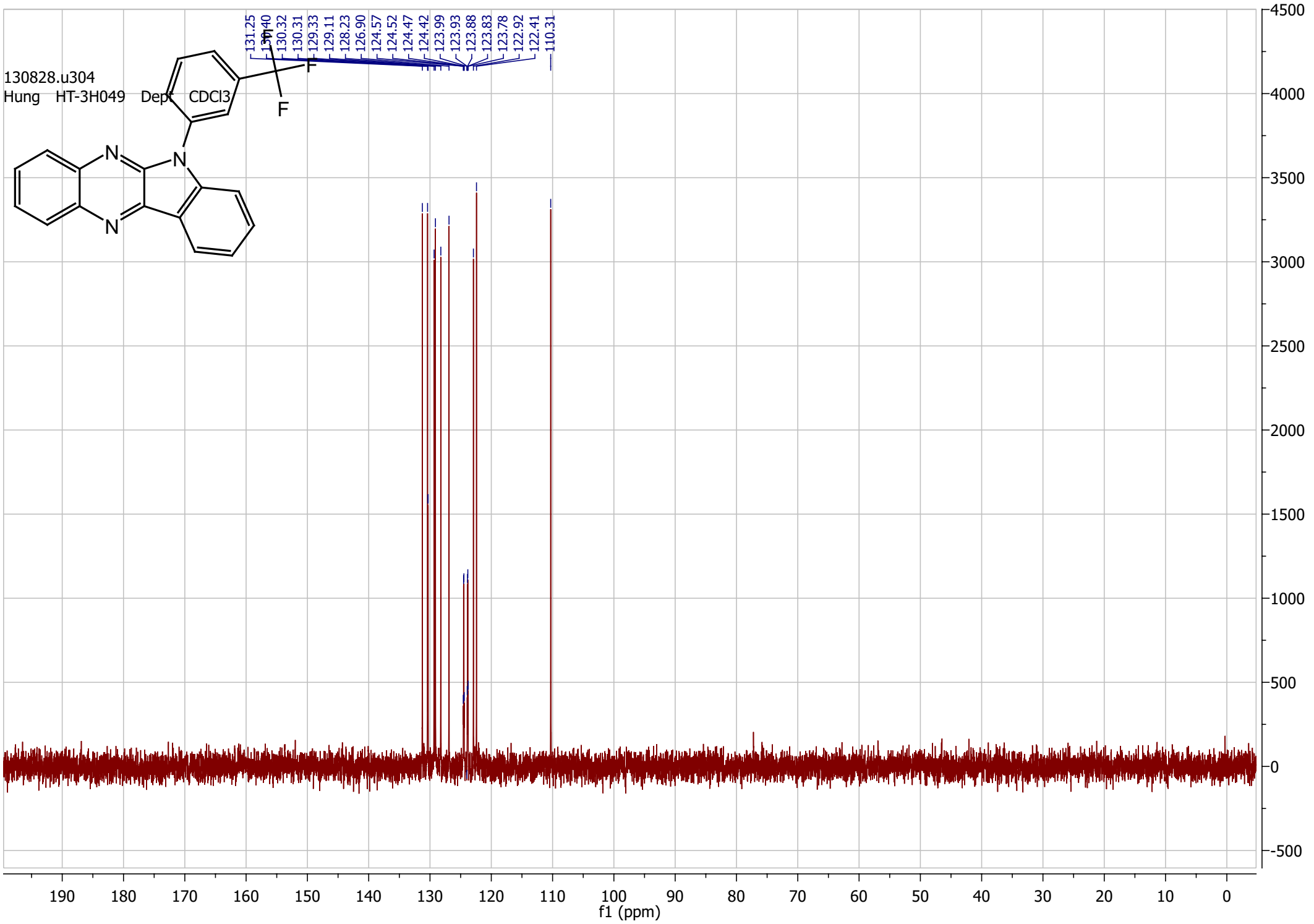

130228.u308
Hung HT-2H195 13C CDCl3
163.72
160.43
146.07
144.90
140.70
140.13
139.89
131.32
129.23
129.12
128.32
126.81
122.98
122.15
117.14
116.83
110.52
77.58
77.16
76.74
F
N
N
N
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

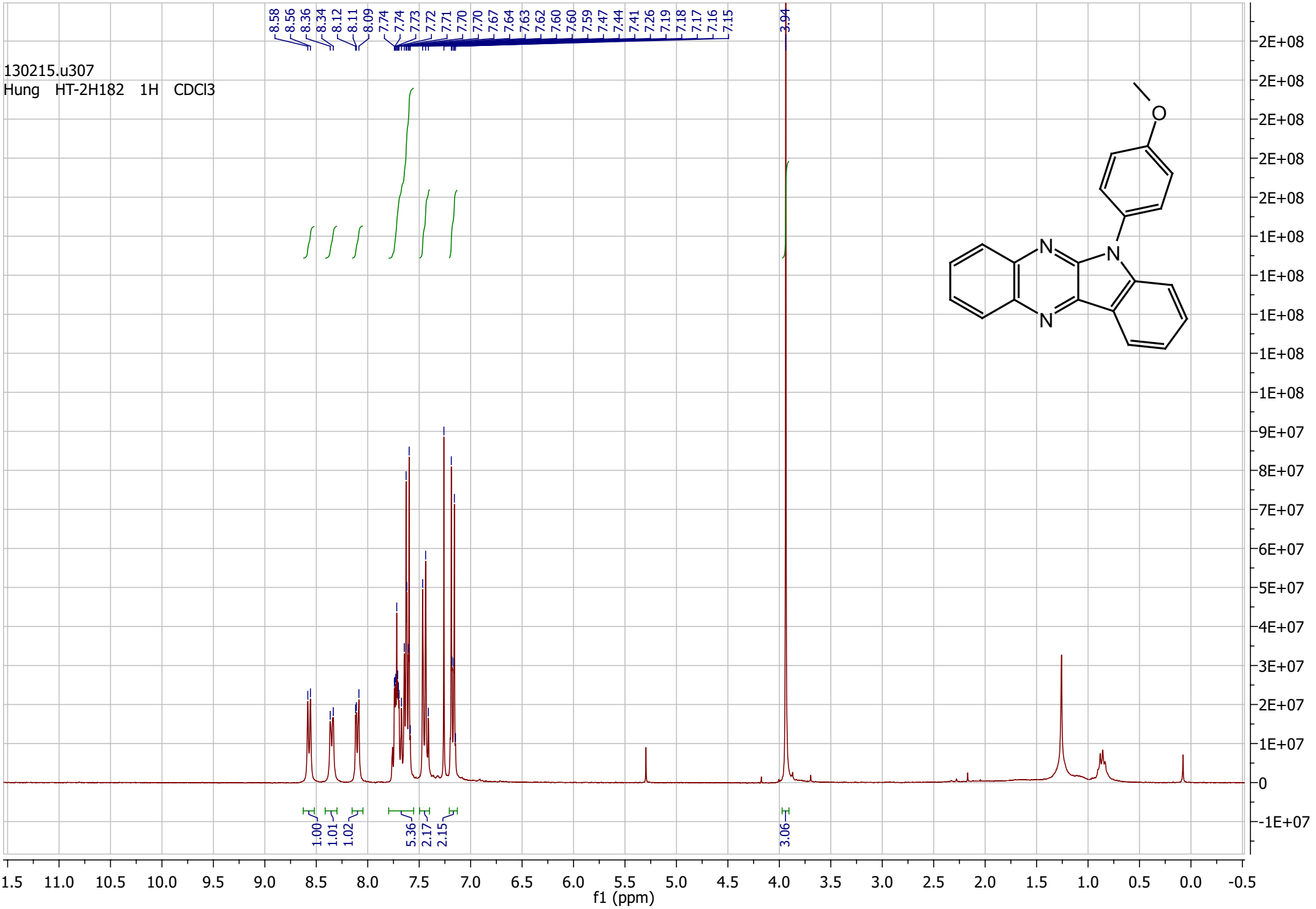

131.33
129.38
129.24
129.13
128.33
126.82
122.99
122.16
117.14
116.84
110.52
130228.u308
Hung HT-2H195 Dept CDCl3
F
N
N
N
8000
7500
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

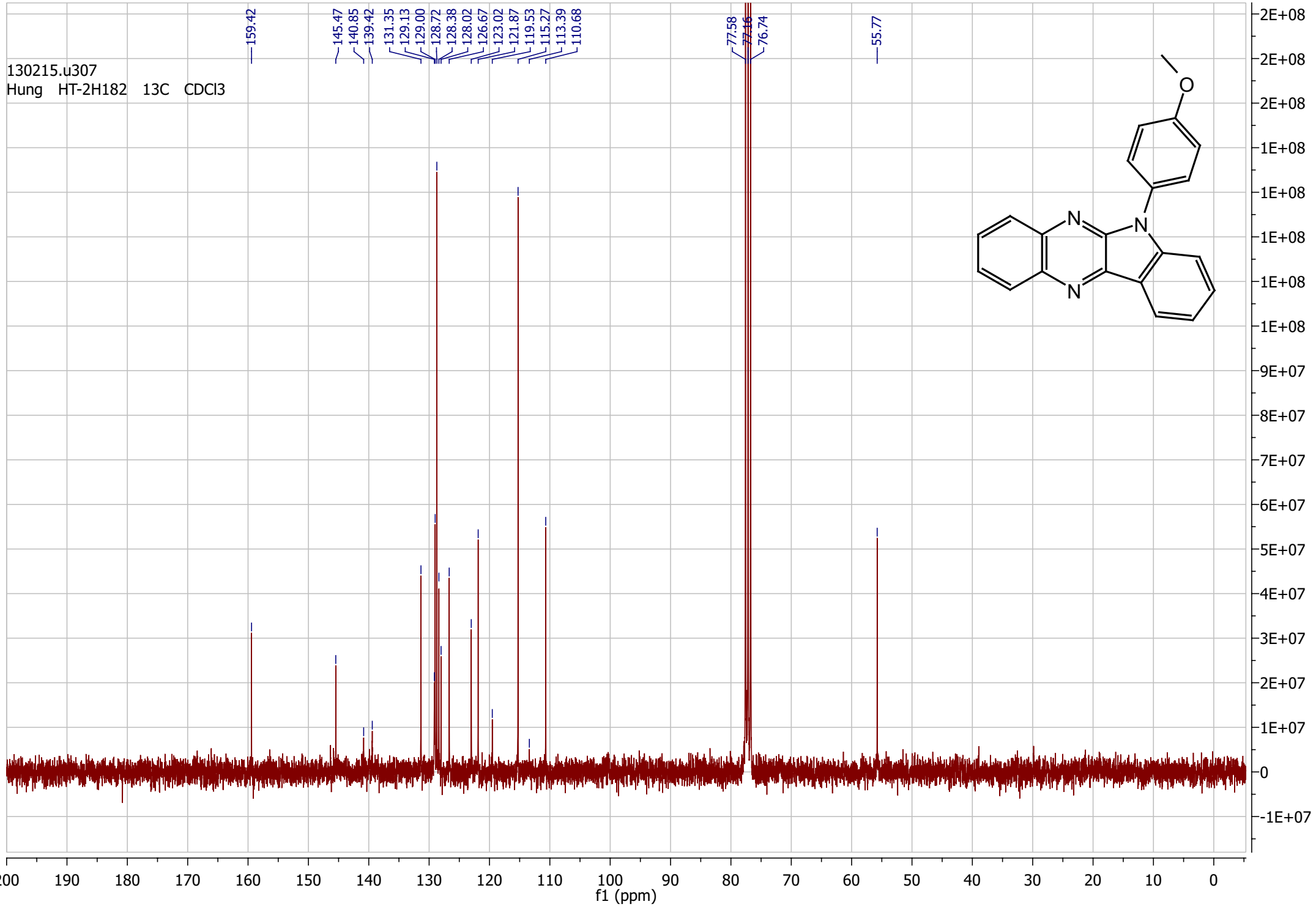

8.47 8.47 8.47 8.45 8.45 8.45 8.44 8.26 8.25 8.25 8.23 8.22 8.22 8.01 8.00 7.99 7.98 7.98 7.94 7.93 7.92 7.92 7.91 7.91 7.91 7.90 7.75 7.72 7.70 7.69 7.68 7.67 7.66 7.66 7.65 7.64 7.64 7.63 7.63 7.61 7.61 7.59 7.58 7.58 7.56 7.55 7.46 7.43 7.41 7.41 7.38 7.36 7.36 7.17
130828.u304
Hung HT-3H049 1H CDCl3
F
F
F
N
N
N
1.00
1.01
2.01
1.02
5.19
2.12
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
10.5 10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)

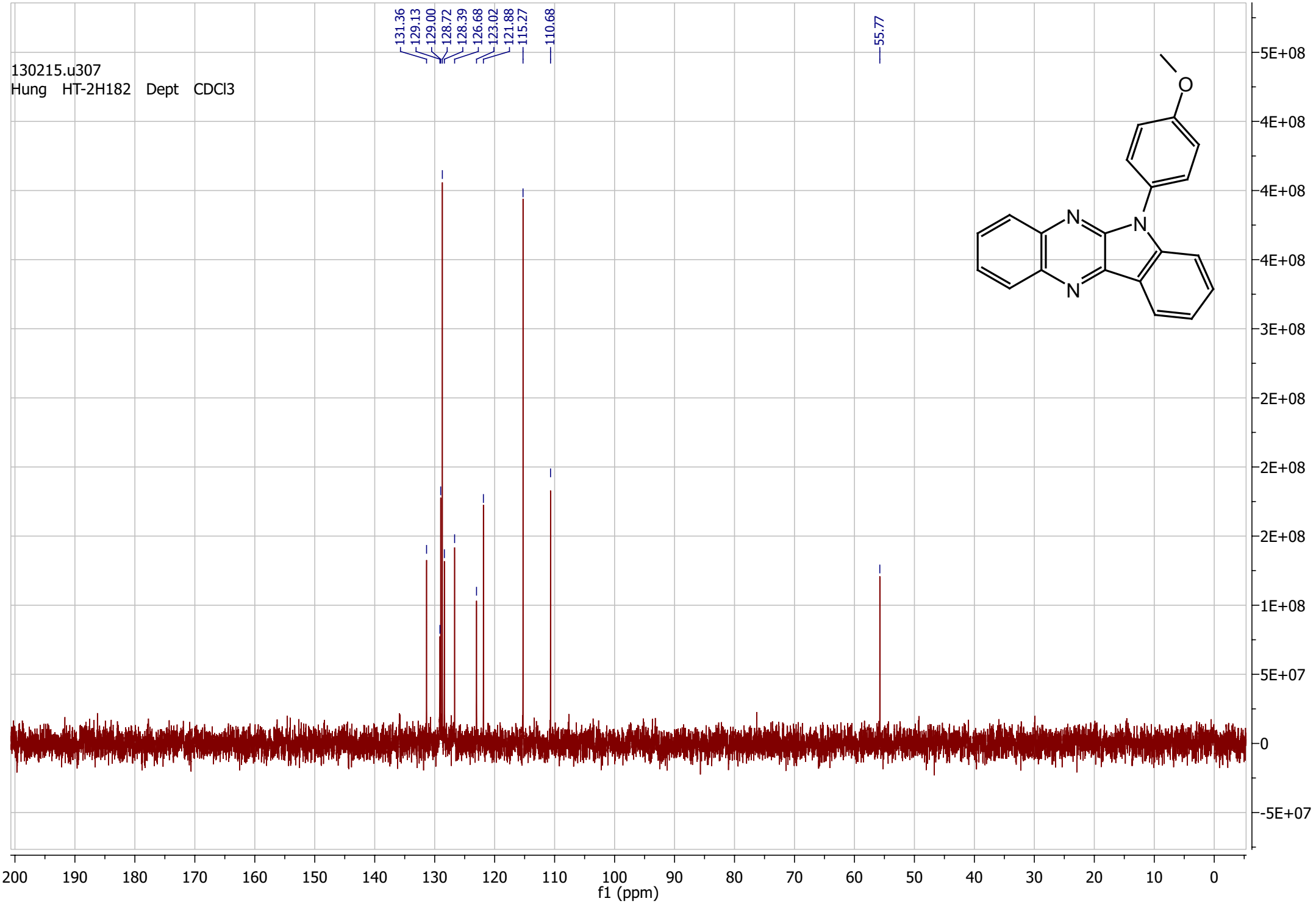

130828.u304
Hung HT-3H049 19F CDCl3
-62.58
F
F
F
N
N
N
9E+05
8E+05
7E+05
6E+05
5E+05
4E+05
3E+05
2E+05
1E+05
0
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

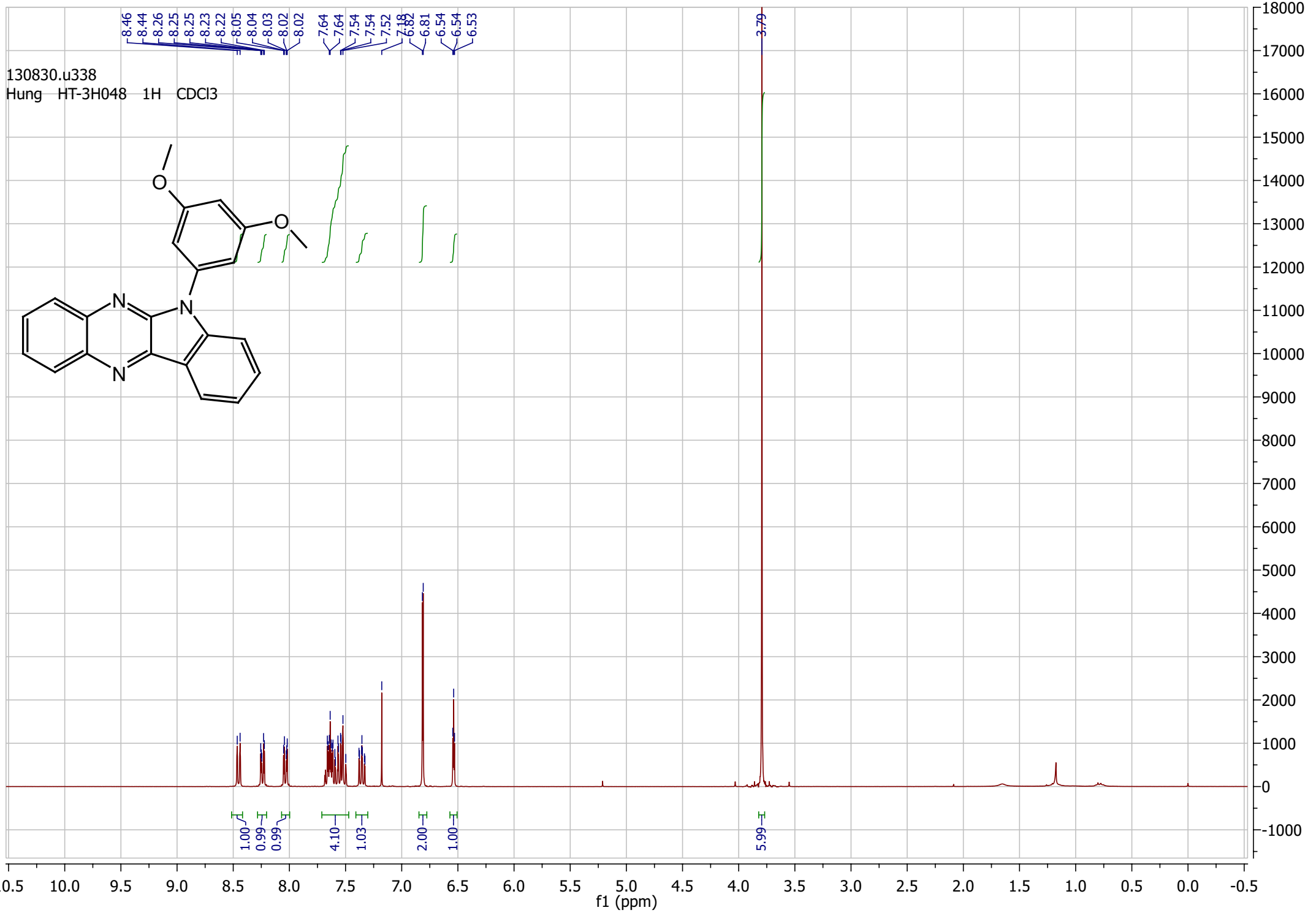

145.55
144.00
140.39
140.07
136.11
132.97
132.53
132.09
131.66
131.25
130.40
130.32
130.31
129.33
129.16
129.11
128.23
126.90
125.55
124.57
124.52
124.47
124.42
123.93
123.88
123.83
123.78
122.92
122.41
121.93
120.16
118.32
110.31
130828.u304
Hung HT-3H049 13C CDCl3
F
F
F
N
N
N
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

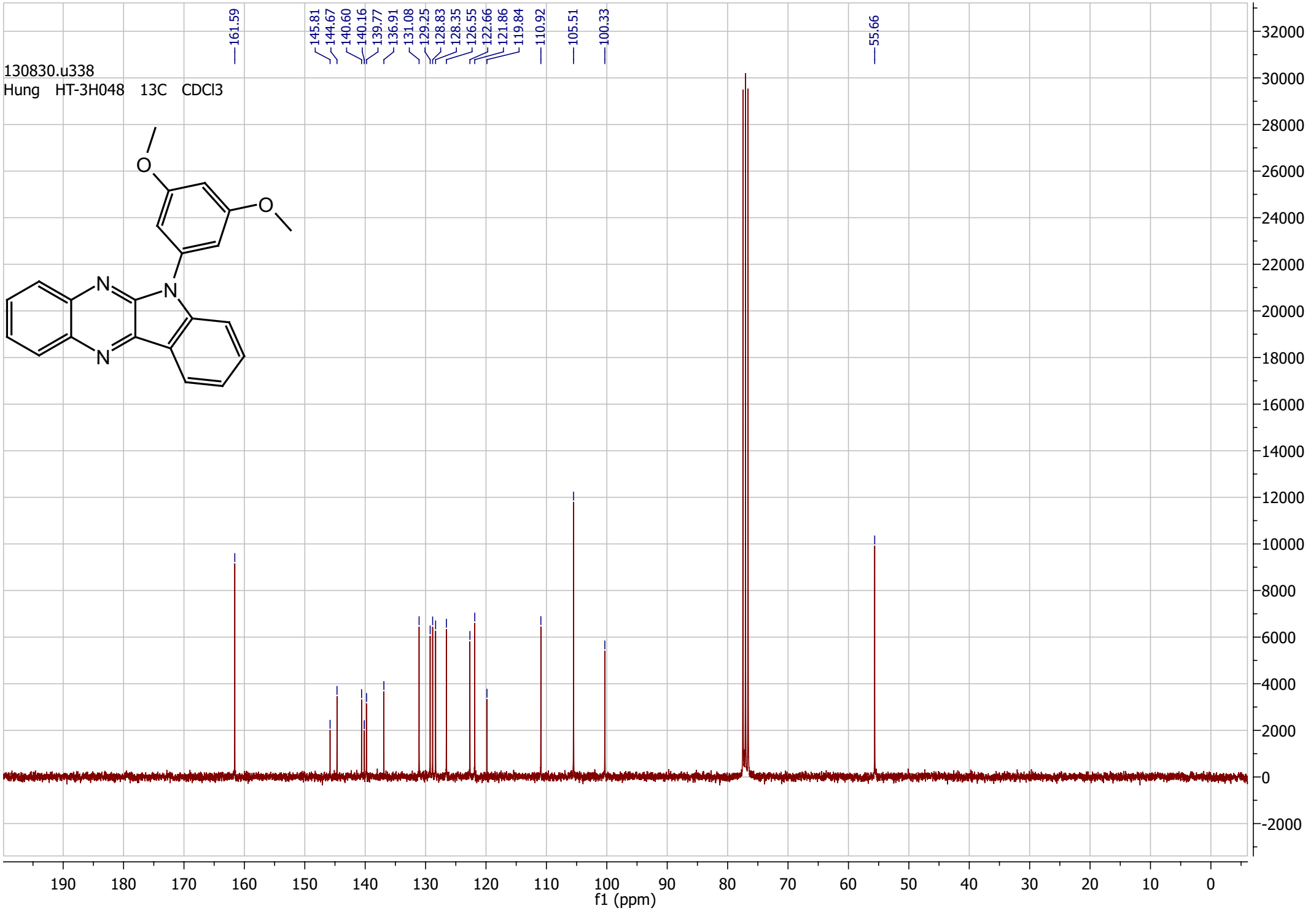

130828.u304
Hung HT-3H049 Dept CDCl3
131.25
130.40
130.32
130.31
129.33
129.11
128.23
126.90
124.57
124.52
124.47
124.42
123.99
123.93
123.88
123.83
123.78
122.92
122.41
110.31
F
F
N
N
N
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

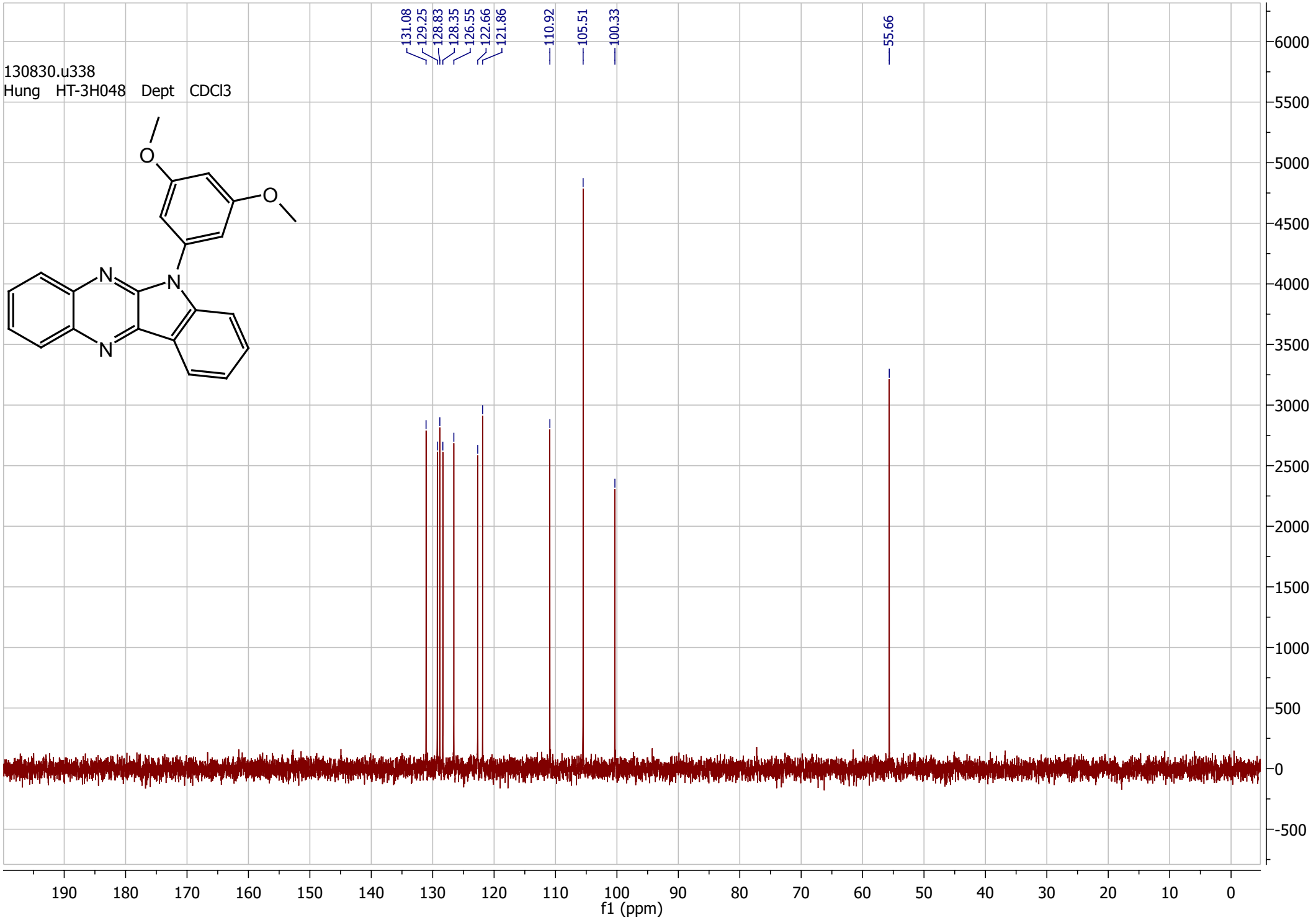

130215.u307
Hung HT-2H182 1H CDCl3
8.58
8.56
8.36
8.34
8.12
8.11
8.09
7.74
7.74
7.73
7.72
7.71
7.70
7.70
7.67
7.64
7.63
7.62
7.60
7.60
7.59
7.47
7.44
7.41
7.26
7.19
7.18
7.17
7.16
7.15
3.94
O
N
N
N
1.00
1.01
1.02
5.36
2.17
2.15
3.06
f1 (ppm)

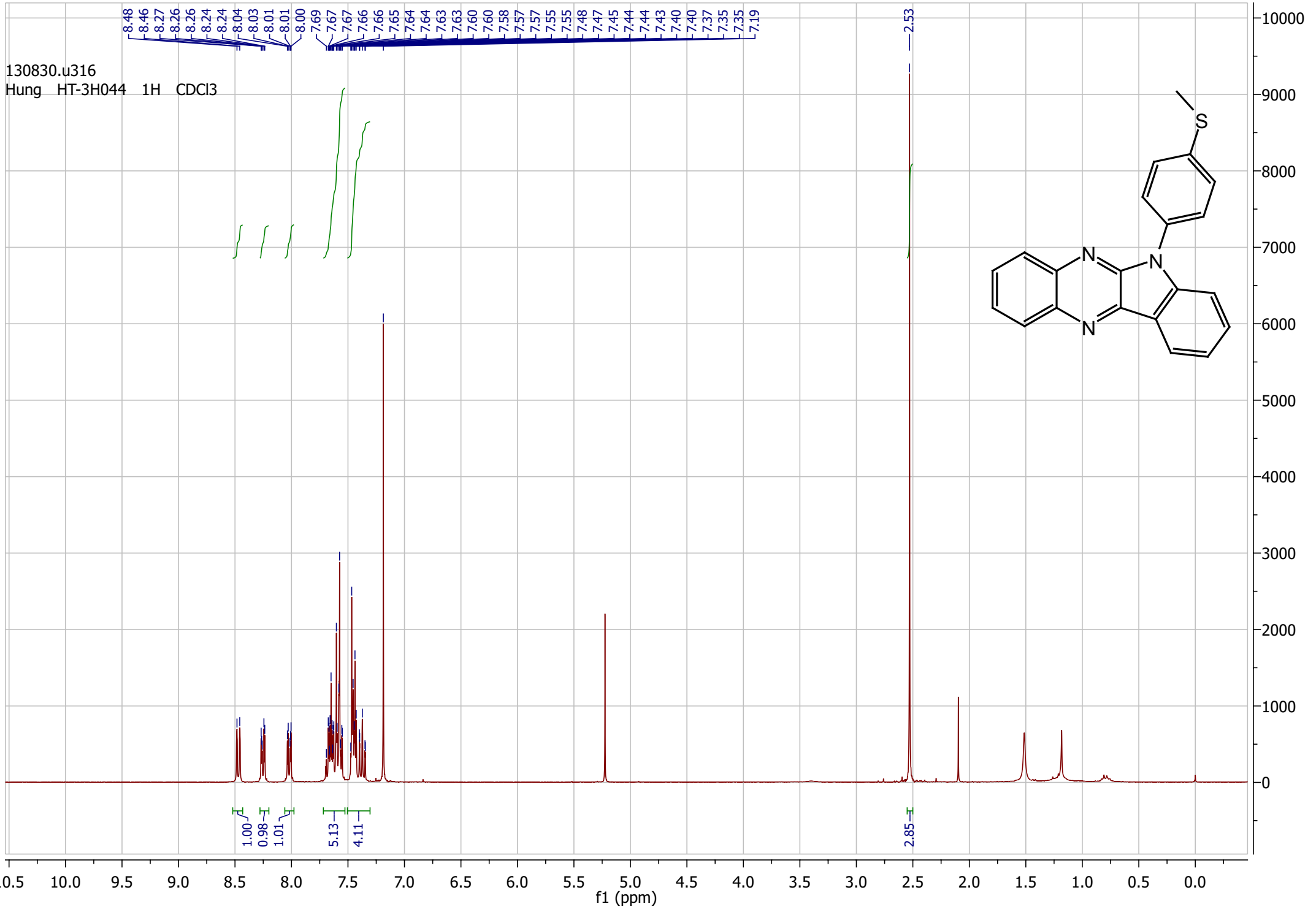

130215.u307
Hung HT-2H182 13C CDCl3
159.42
145.47
140.85
139.42
131.35
129.13
129.00
128.72
128.38
128.02
126.67
123.02
121.87
119.53
115.27
113.39
110.68
77.58
77.16
76.74
55.77
O
N
N
N
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
1E+08
1E+08
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
-1E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

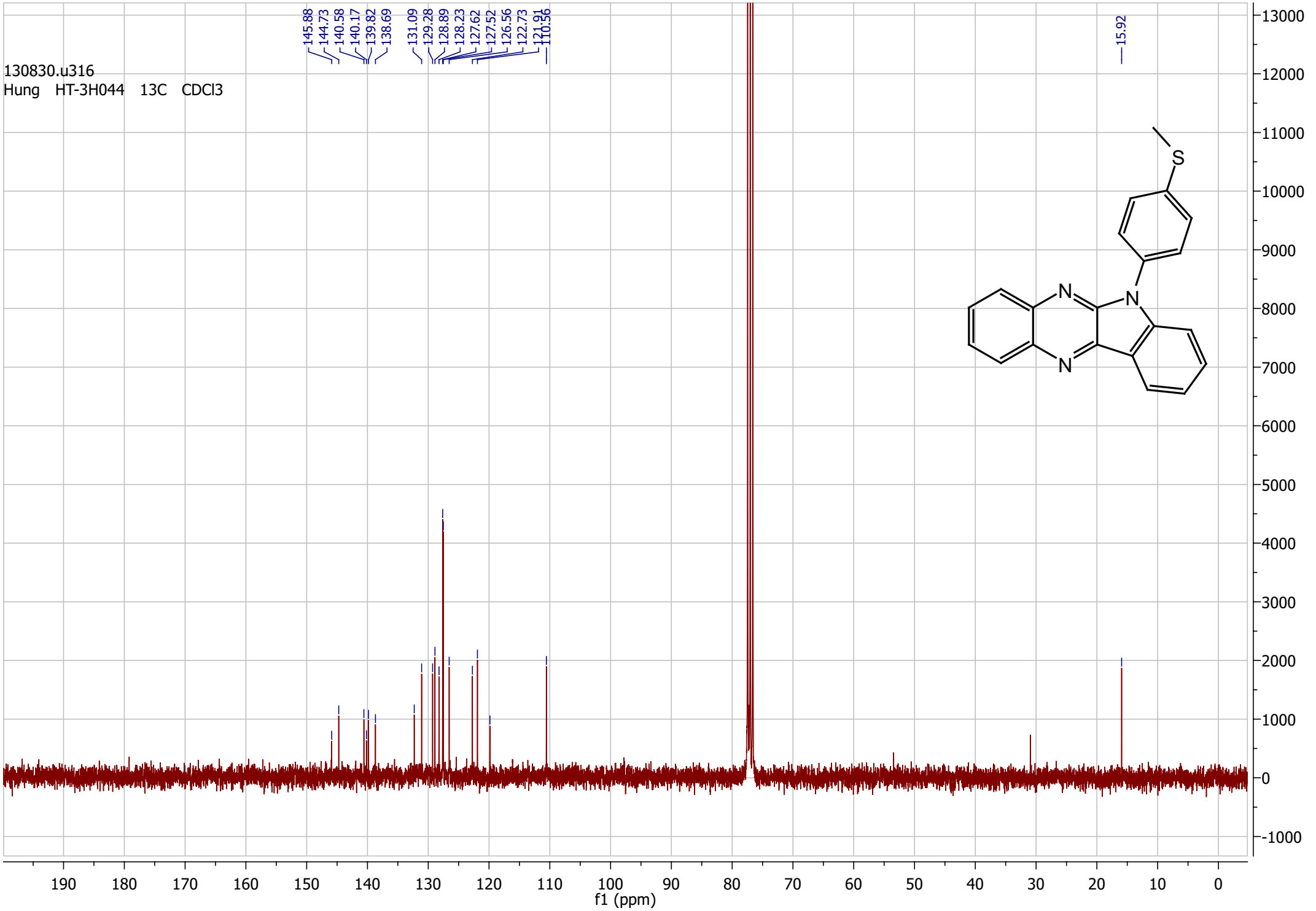

130215.u307
Hung HT-2H182 Dept CDCl3
131.36
129.13
129.00
128.72
128.39
126.68
123.02
121.88
115.27
110.68
55.77
O
N
N
N
5E+08
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

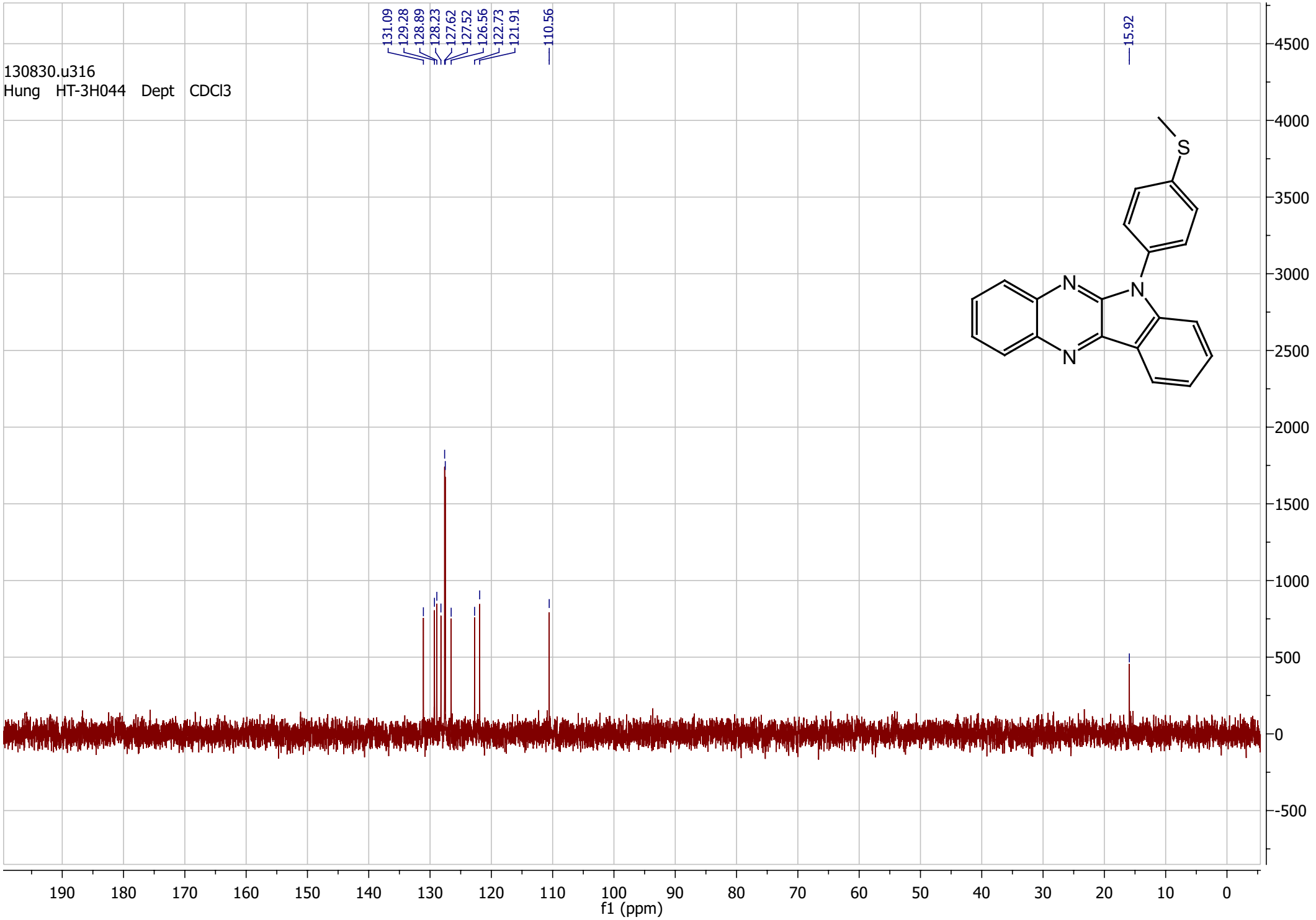

130830.u338
Hung HT-3H048 1H CDCl3
8.46
8.44
8.26
8.25
8.25
8.23
8.22
8.05
8.04
8.03
8.02
8.02
7.64
7.64
7.54
7.54
7.52
7.18
6.82
6.81
6.54
6.54
6.53
3.79
O
O
N
N
N
1.00
0.99
0.99
4.10
1.03
2.00
1.00
5.99
f1 (ppm)

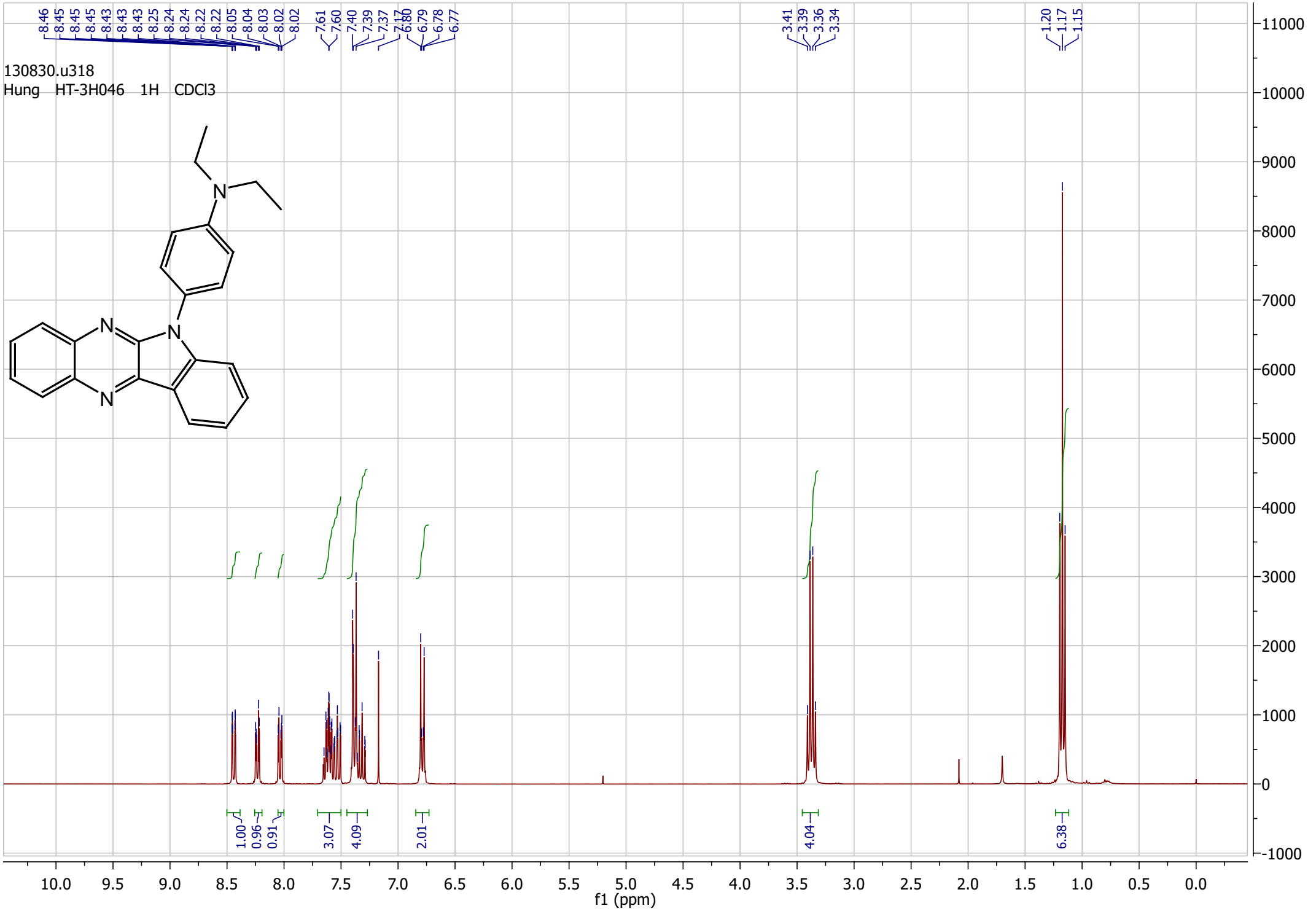

130830.u338
Hung HT-3H048 13C CDCl3
161.59
145.81
144.67
140.60
140.16
139.77
136.91
131.08
129.25
128.83
128.35
126.55
122.66
121.86
119.84
110.92
105.51
100.33
55.66
O
O
N
N
N
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

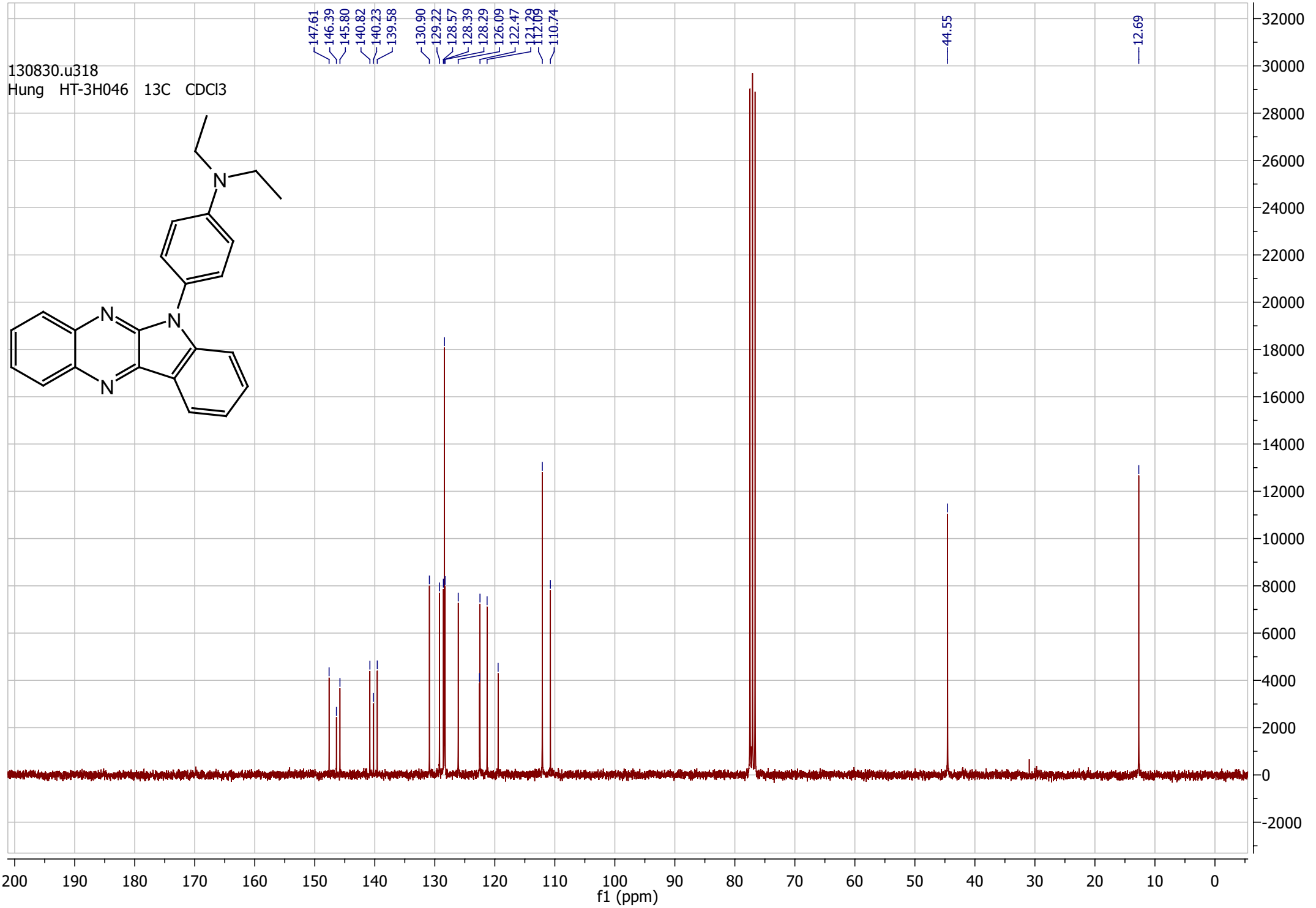

131.08
129.25
128.83
128.35
126.55
122.66
121.86
110.92
105.51
100.33
55.66
130830.u338
Hung HT-3H048 Dept CDCl3
O
O
N
N
N
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

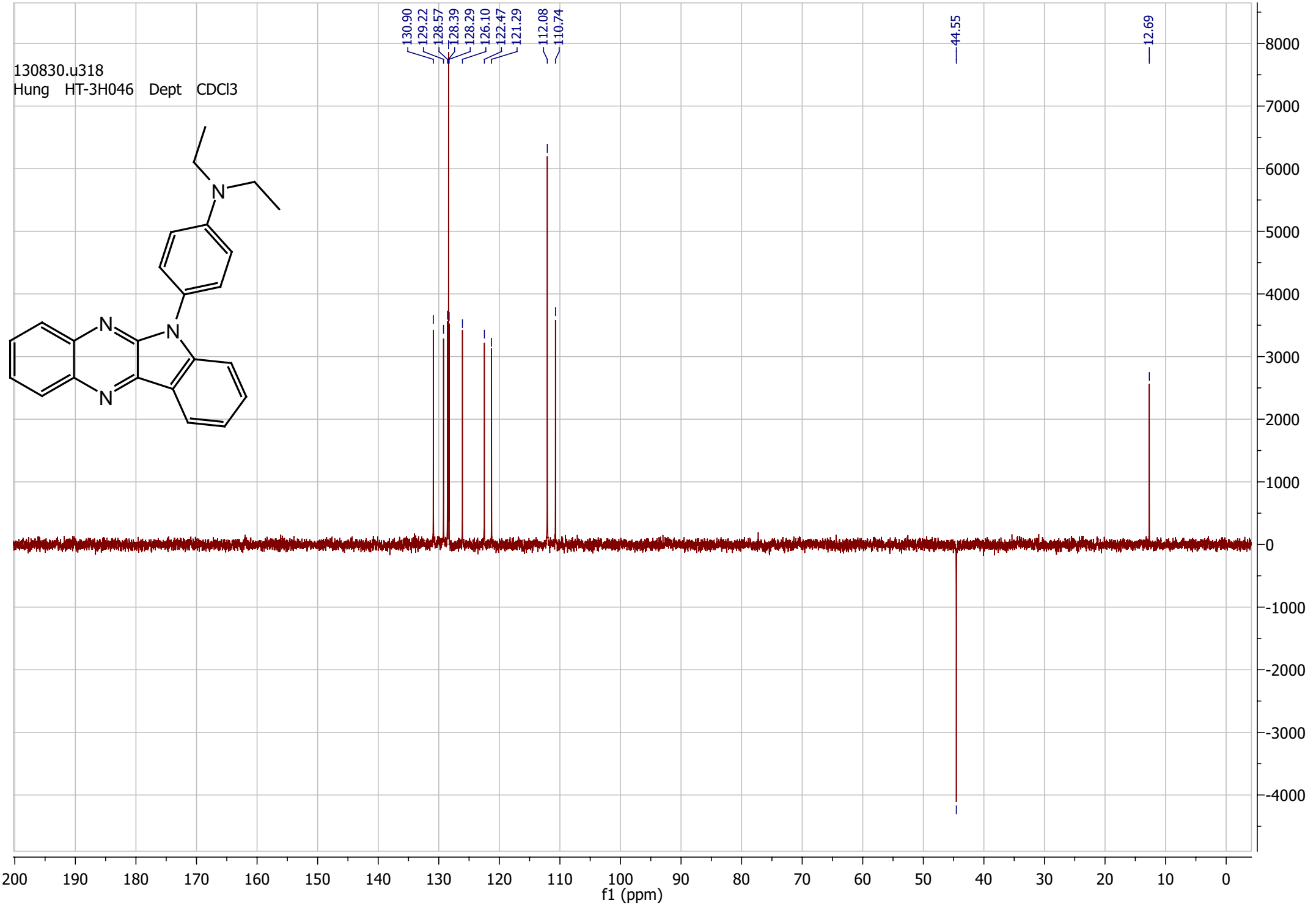

130830.u316
Hung HT-3H044 1H CDCl3
8.48 8.46 8.27 8.26 8.26 8.24 8.24 8.04 8.03 8.01 8.01 8.00 7.69 7.67 7.67 7.66 7.66 7.65 7.64 7.64 7.63 7.63 7.60 7.60 7.58 7.57 7.57 7.55 7.55 7.48 7.47 7.45 7.44 7.44 7.43 7.40 7.40 7.37 7.35 7.35 7.19
2.53
1.00 0.98 1.01 5.13 4.11 2.85
S
N
N
N
10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0
10.5 10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)

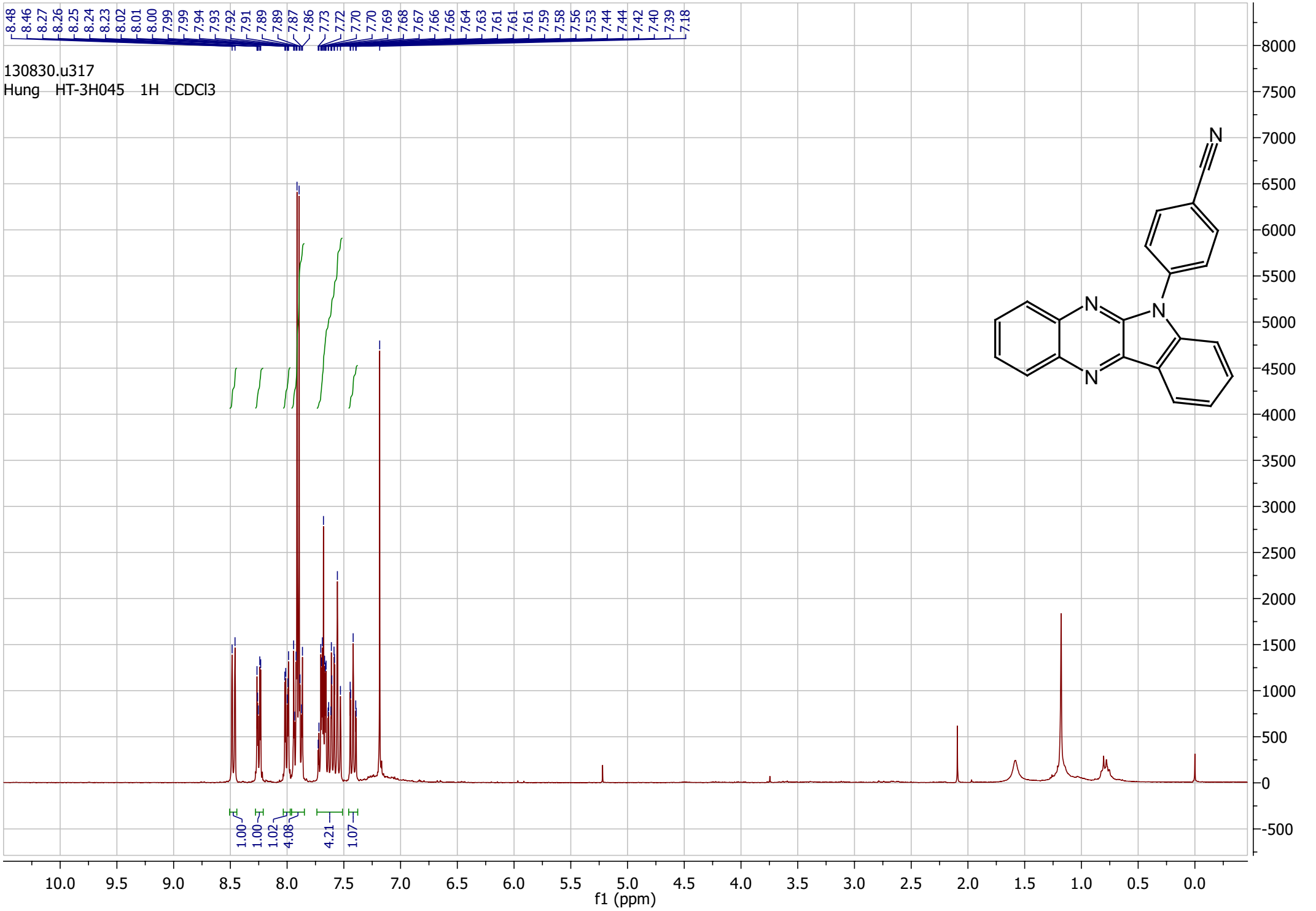

130830.u316
Hung HT-3H044 13C CDCl3
145.88
144.73
140.58
140.17
139.82
138.69
131.09
129.28
128.89
128.23
127.62
127.52
126.56
122.73
121.91
110.56
15.92
S
N
N
N
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

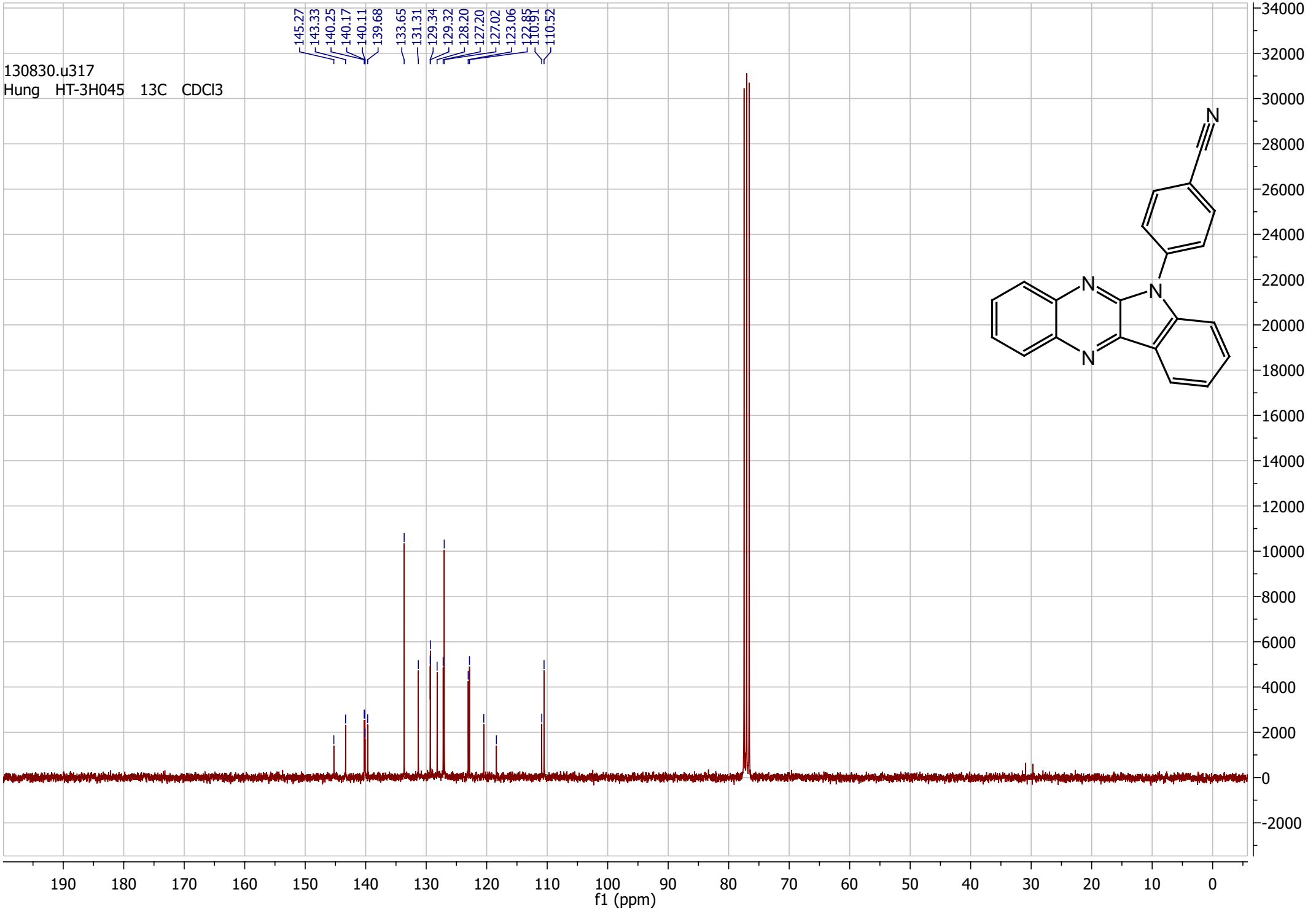

131.09
129.28
128.89
128.23
127.62
127.52
126.56
122.73
121.91
110.56
15.92
130830.u316
Hung HT-3H044 Dept CDCl3
S
N
N
N
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

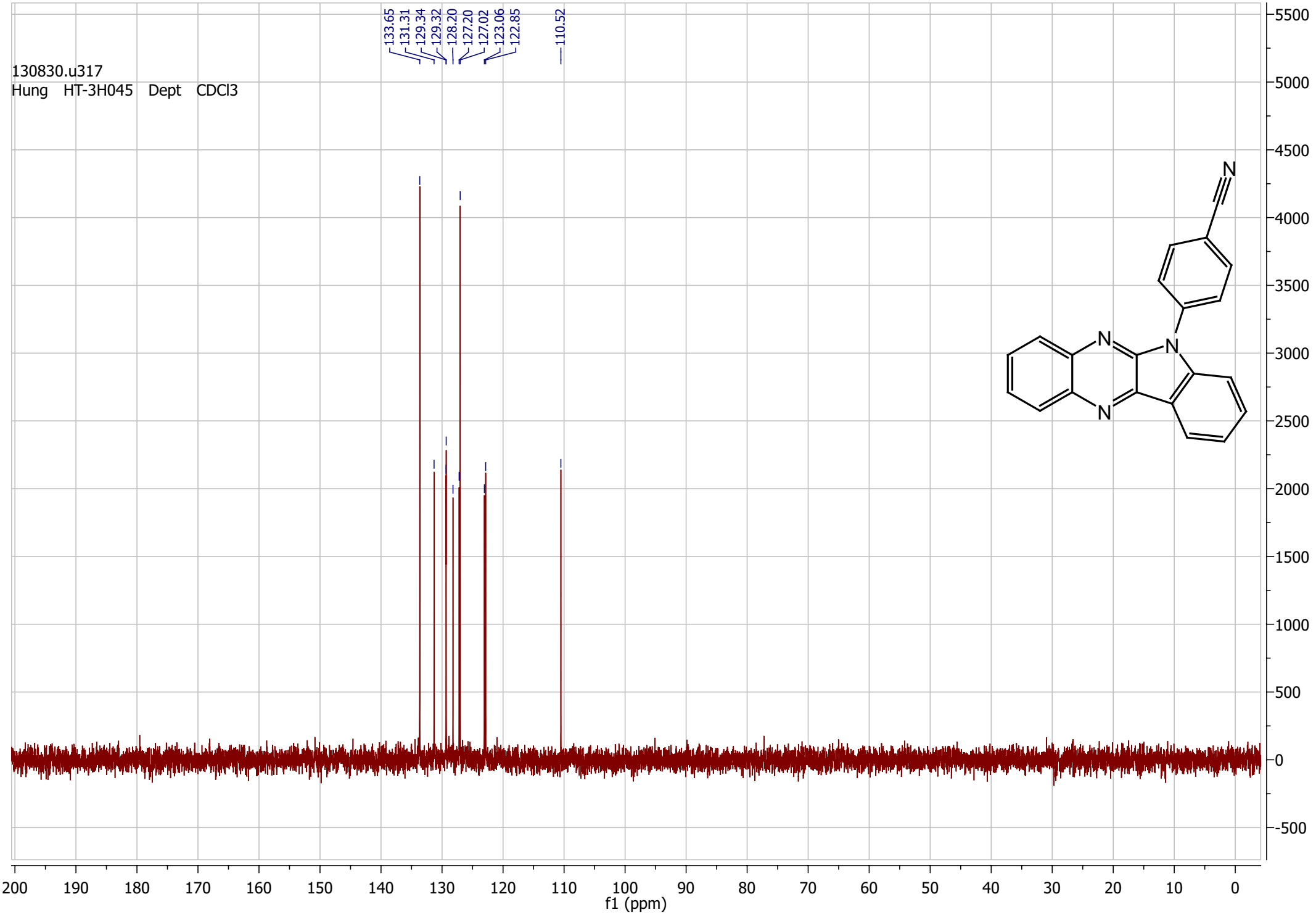

130830.u318
Hung HT-3H046 1H CDCl3
8.46
8.45
8.45
8.45
8.43
8.43
8.43
8.25
8.24
8.24
8.22
8.22
8.05
8.04
8.03
8.02
8.02
7.61
7.60
7.40
7.39
7.37
7.17
6.80
6.79
6.78
6.77
3.41
3.39
3.36
3.34
1.20
1.17
1.15
N
N
N
N
1.00
0.96
0.91
3.07
4.09
2.01
4.04
6.38
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
10.0
9.5
9.0
8.5
8.0
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
f1 (ppm)

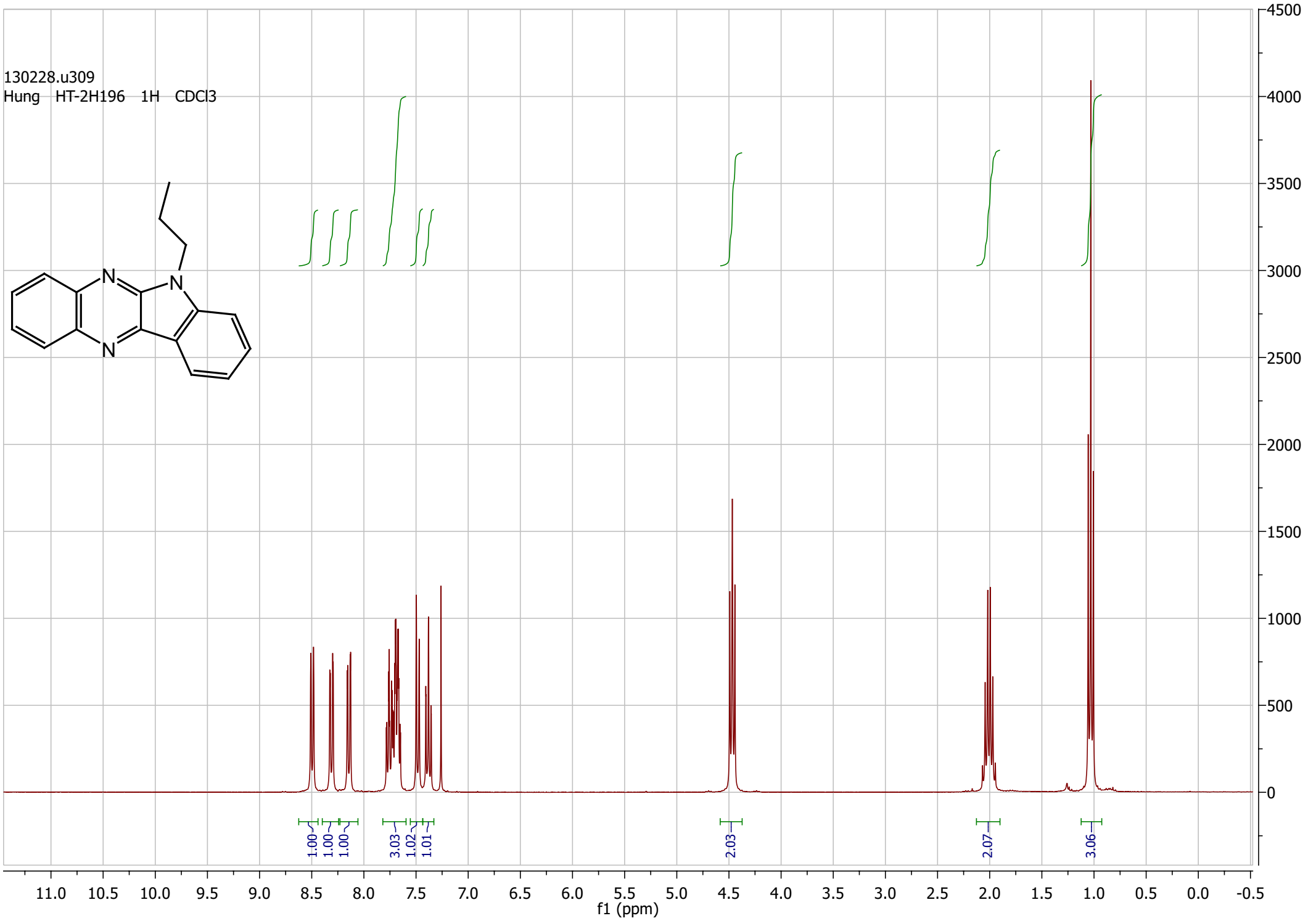

147.61
146.39
145.80
140.82
140.23
139.58
130.90
129.22
128.57
128.39
128.29
126.09
122.47
121.28
112.09
110.74
44.55
12.69
130830.u318
Hung HT-3H046 13C CDCl3
N
N
N
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

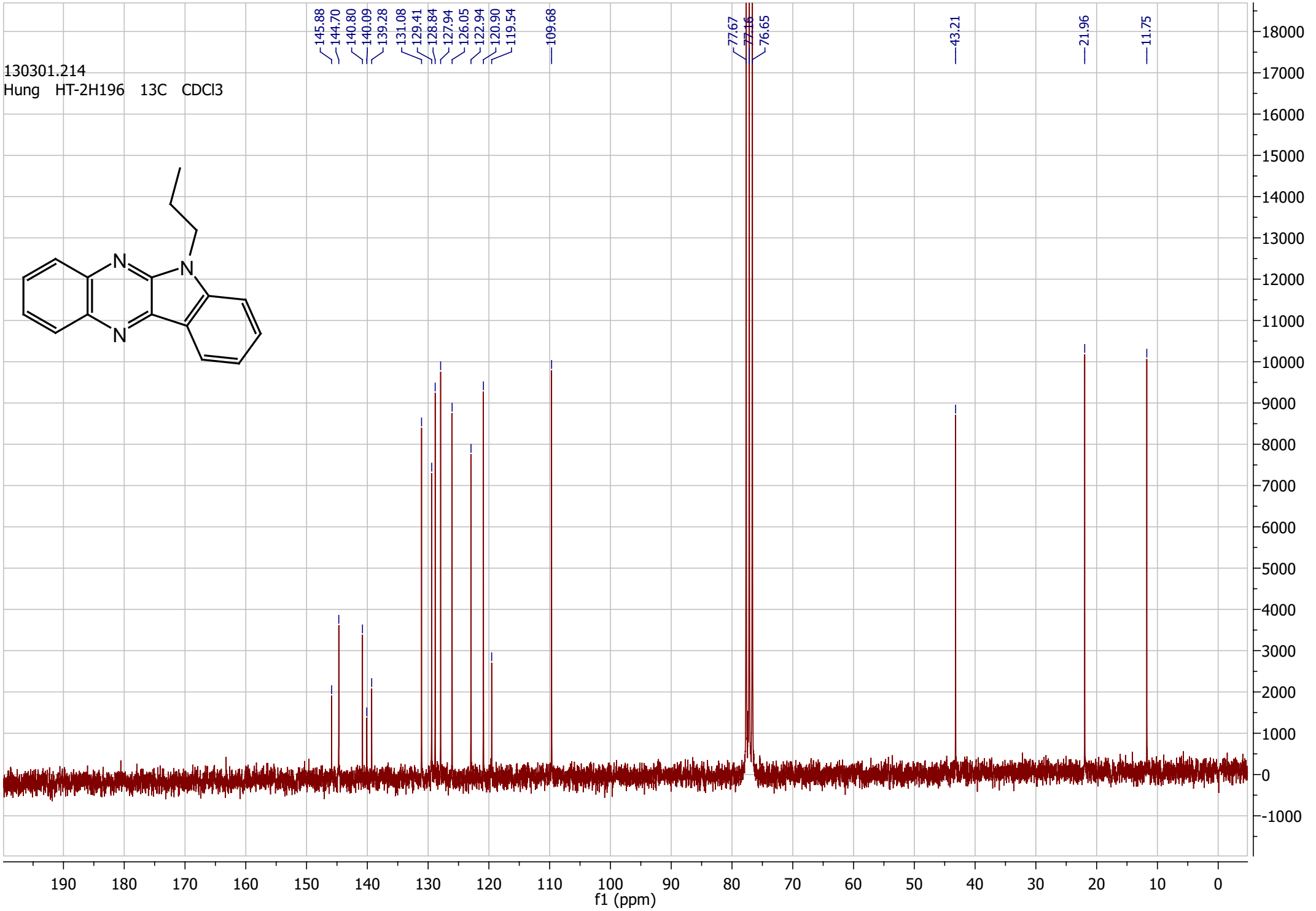

130830.u318
Hung HT-3H046 Dept CDCl3
130.90
129.22
128.57
128.39
128.29
126.10
122.47
121.29
112.08
110.74
44.55
12.69
N
N
N
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

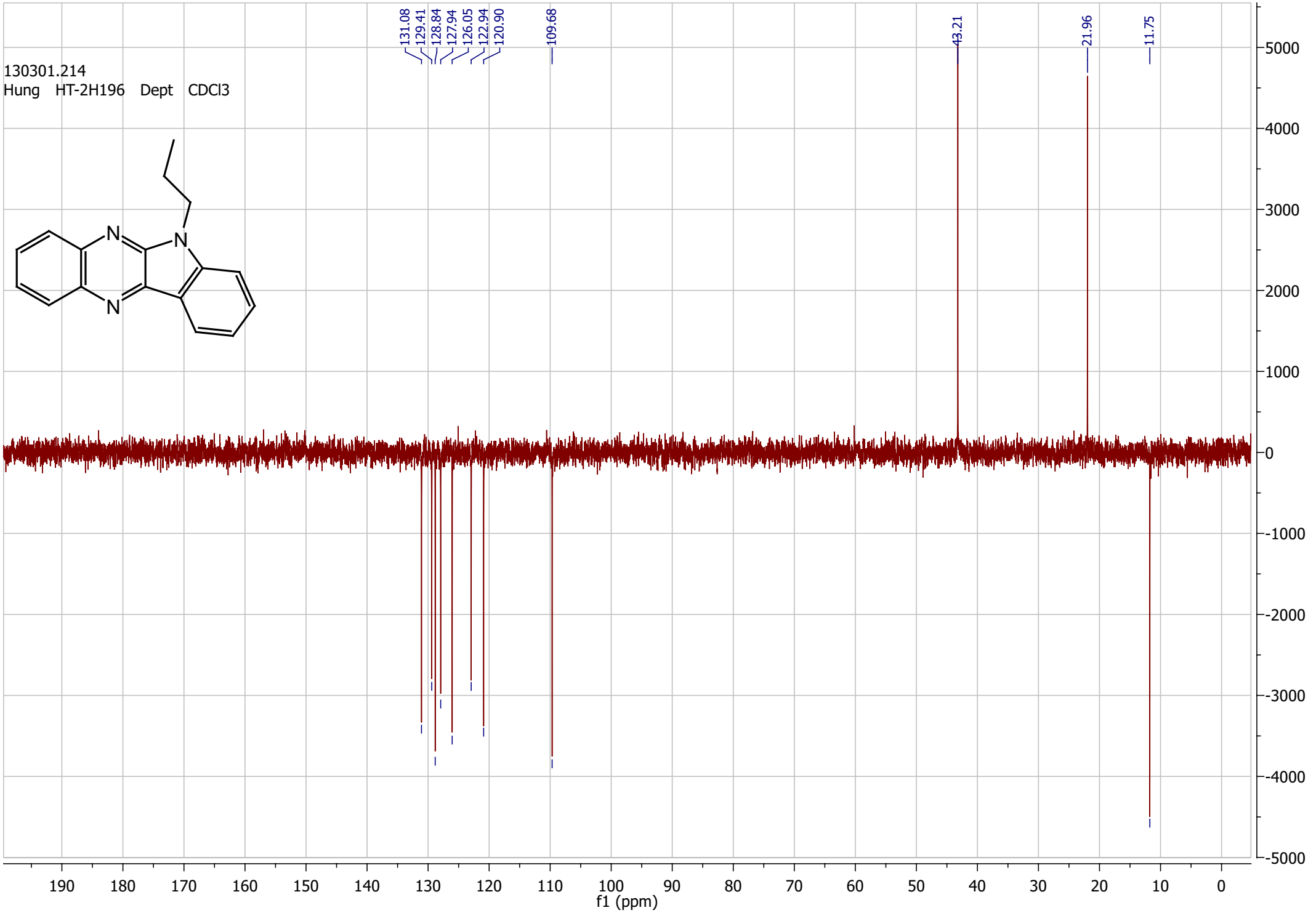

8.48 8.46 8.27 8.26 8.25 8.24 8.23 8.02 8.01 8.00 7.99 7.99 7.94 7.93 7.92 7.91 7.89 7.89 7.87 7.86 7.73 7.72 7.70 7.70 7.69 7.68 7.67 7.66 7.66 7.64 7.63 7.61 7.61 7.61 7.59 7.58 7.56 7.53 7.44 7.44 7.42 7.40 7.39 7.18
130830.u317
Hung HT-3H045 1H CDCl3
N
N
N
1.00 1.00 1.02 4.08 4.21 1.07
8000 7500 7000 6500 6000 5500 5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0 -500
10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)

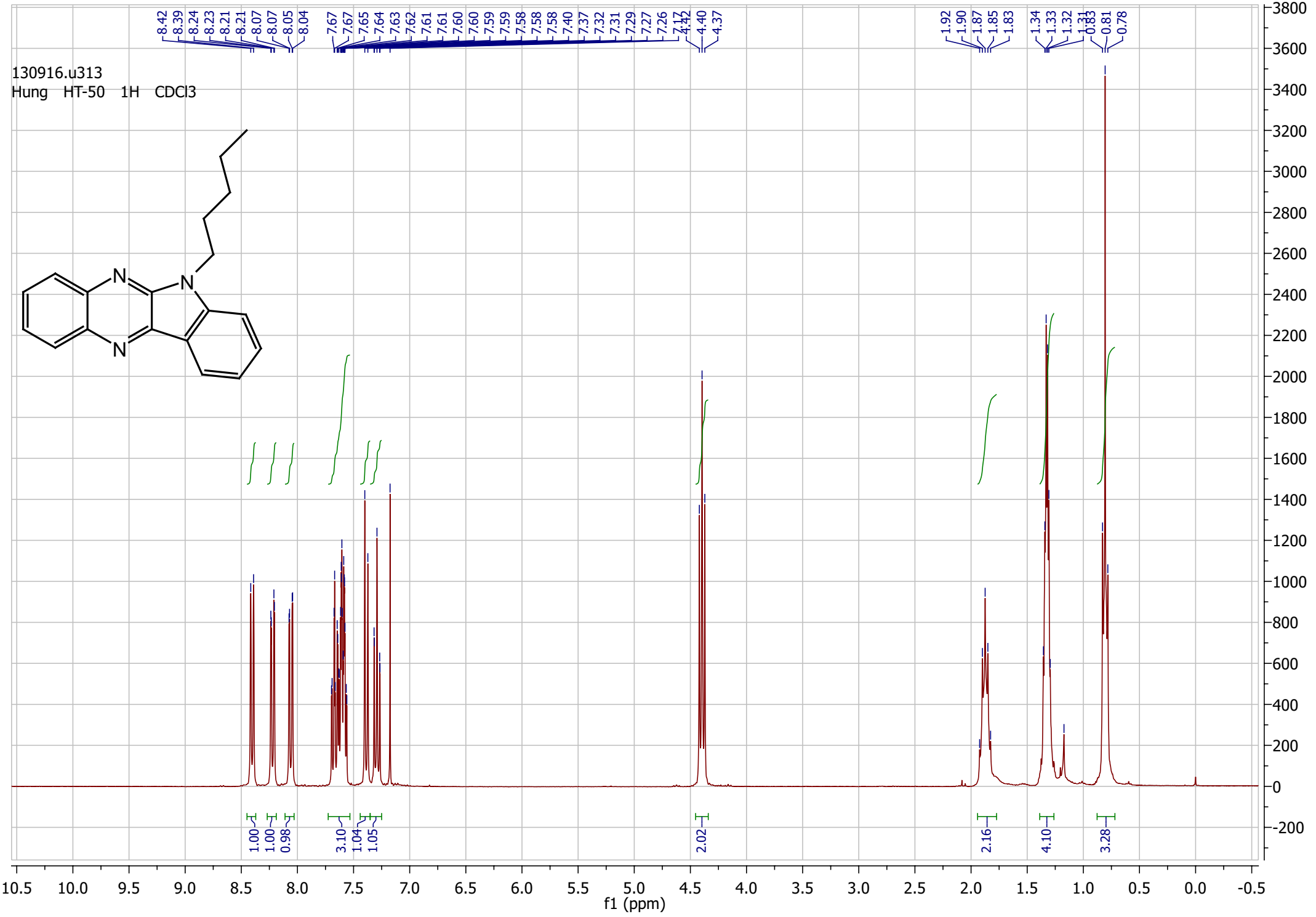

145.27
143.33
140.25
140.17
140.11
139.68
133.65
131.31
129.34
129.32
128.20
127.20
127.02
123.06
122.85
110.91
110.52
130830.u317
Hung HT-3H045 13C CDCl3
N
N
N
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

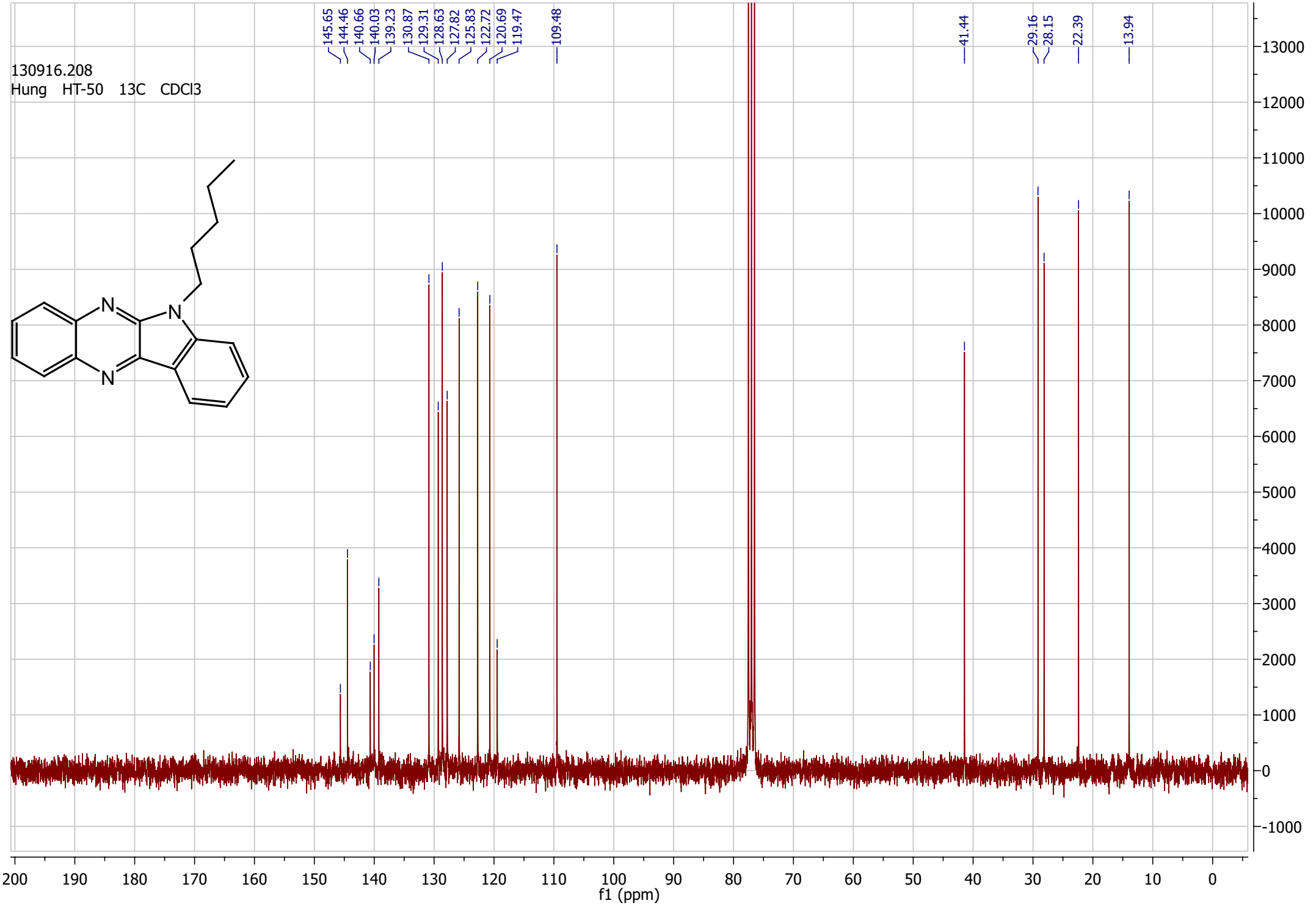

133.65
131.31
129.34
129.32
128.20
127.20
127.02
123.06
122.85
110.52
130830.u317
Hung HT-3H045 Dept CDCl3
N
N
N
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

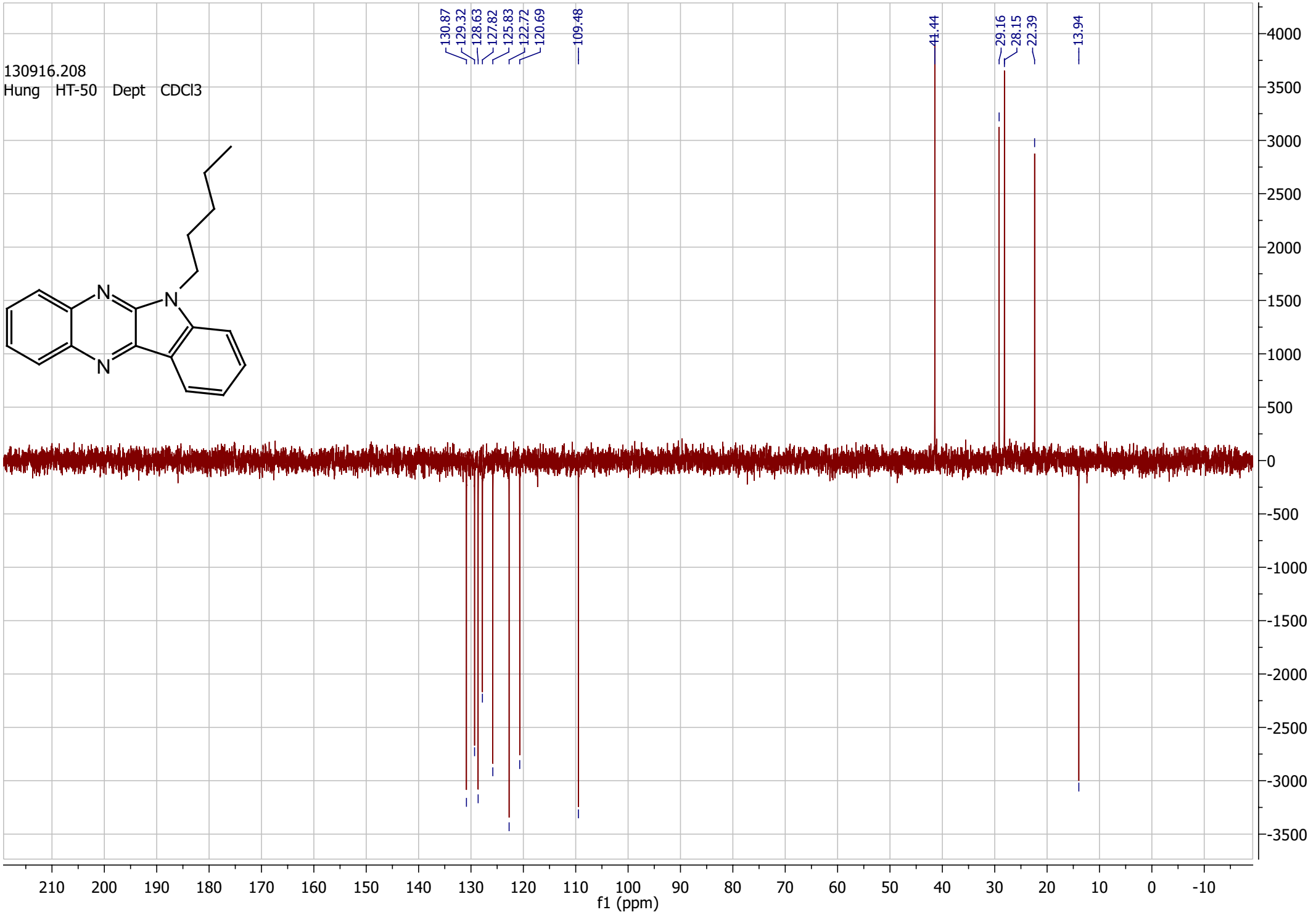

130228.u309
Hung HT-2H196 1H CDCl3
N
N
N
1.00
1.00
1.00
3.03
1.02
1.01
2.03
2.07
3.06
f1 (ppm)

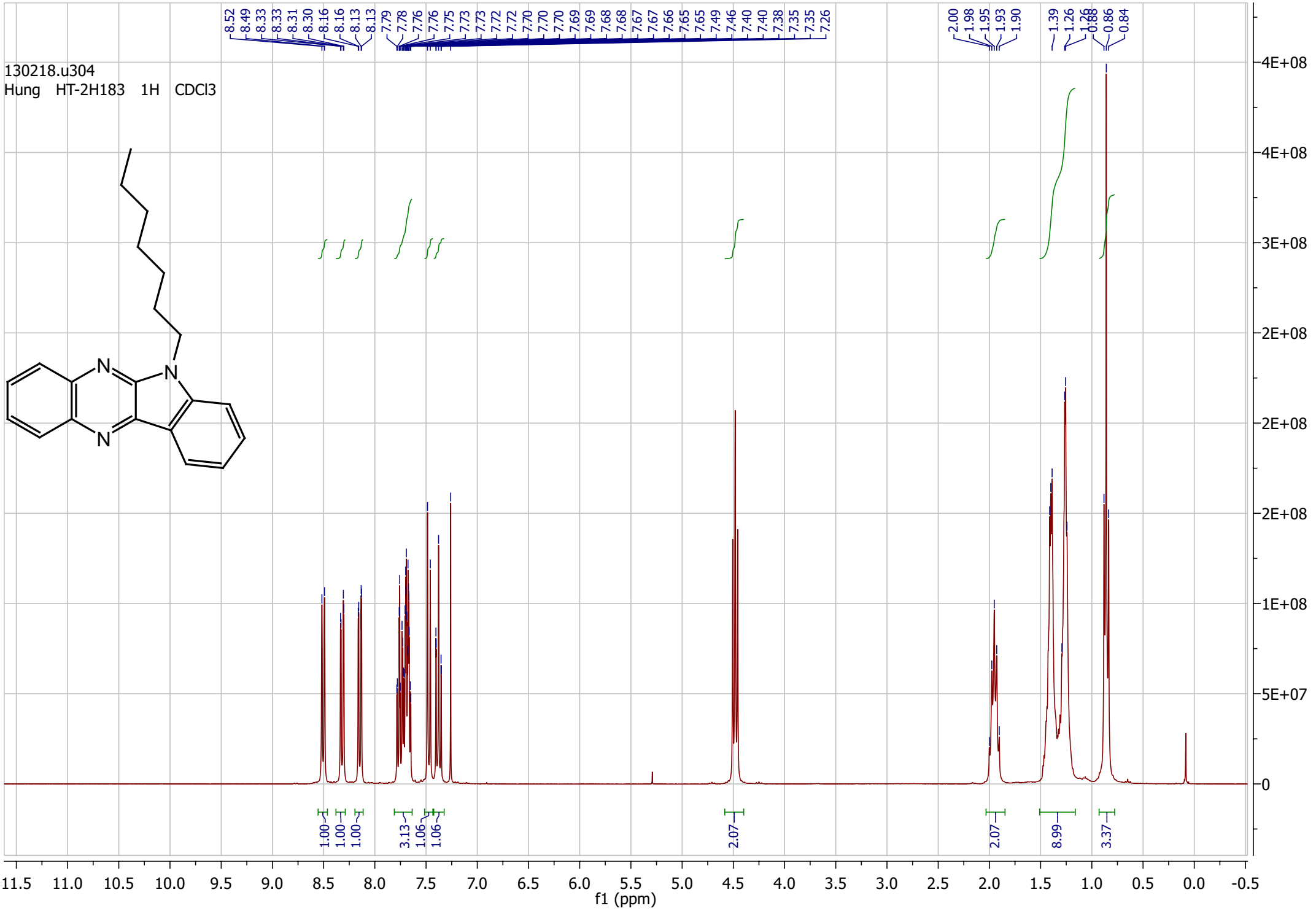

130301.214
Hung HT-2H196 13C CDCl3
145.88
144.70
140.80
140.09
139.28
131.08
129.41
128.84
127.94
126.05
122.94
120.90
119.54
109.68
77.67
77.16
76.65
43.21
21.96
11.75
N
N
f1 (ppm)

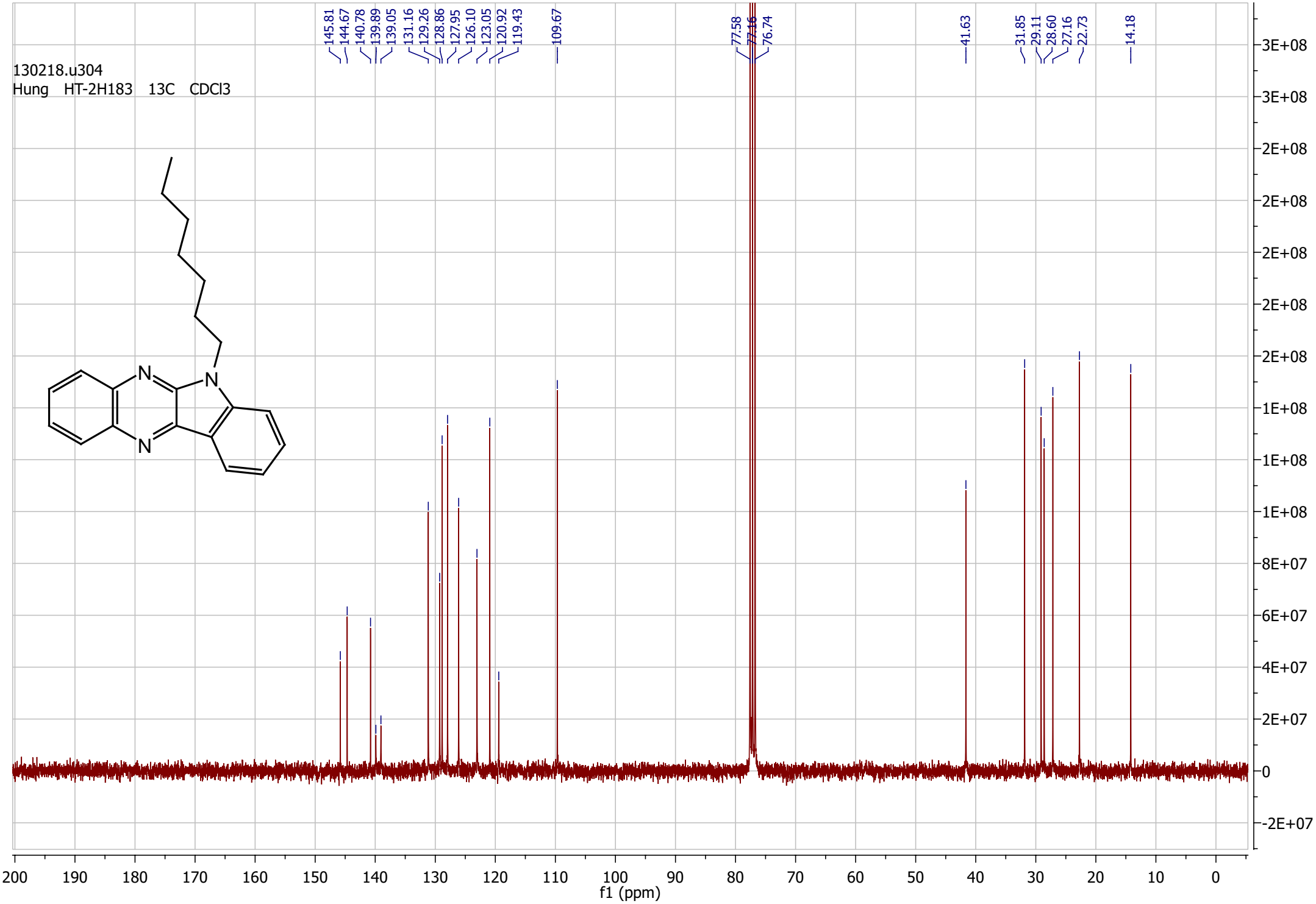

130301.214
Hung HT-2H196 Dept CDCl3
131.08
129.41
128.84
127.94
126.05
122.94
120.90
109.68
43.21
21.96
11.75
N
N
N
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
-5000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

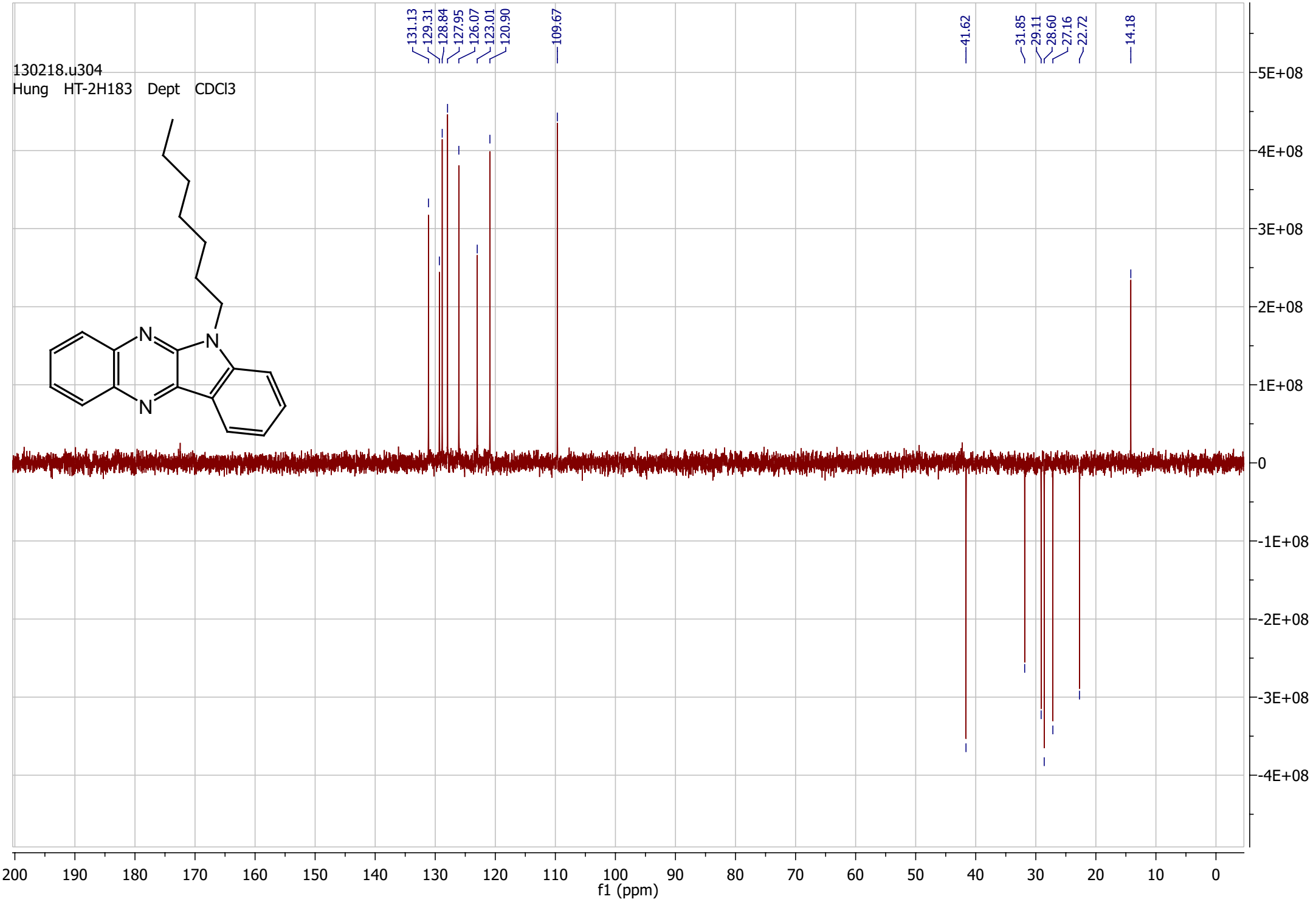

130916.u313
Hung HT-50 1H CDCl3
8.42 8.39 8.24 8.23 8.21 8.21 8.07 8.07 8.05 8.04
7.67 7.67 7.65 7.64 7.63 7.62 7.61 7.61 7.60 7.60 7.59 7.59 7.58 7.58 7.58 7.40 7.37 7.32 7.31 7.29 7.27 7.26 7.17 4.42 4.40 4.37
1.92 1.90 1.87 1.85 1.83
1.34 1.33 1.32 1.31 0.83 0.81 0.78
1.00 1.00 0.98 3.10 1.04 1.05 2.02 2.16 4.10 3.28
f1 (ppm)

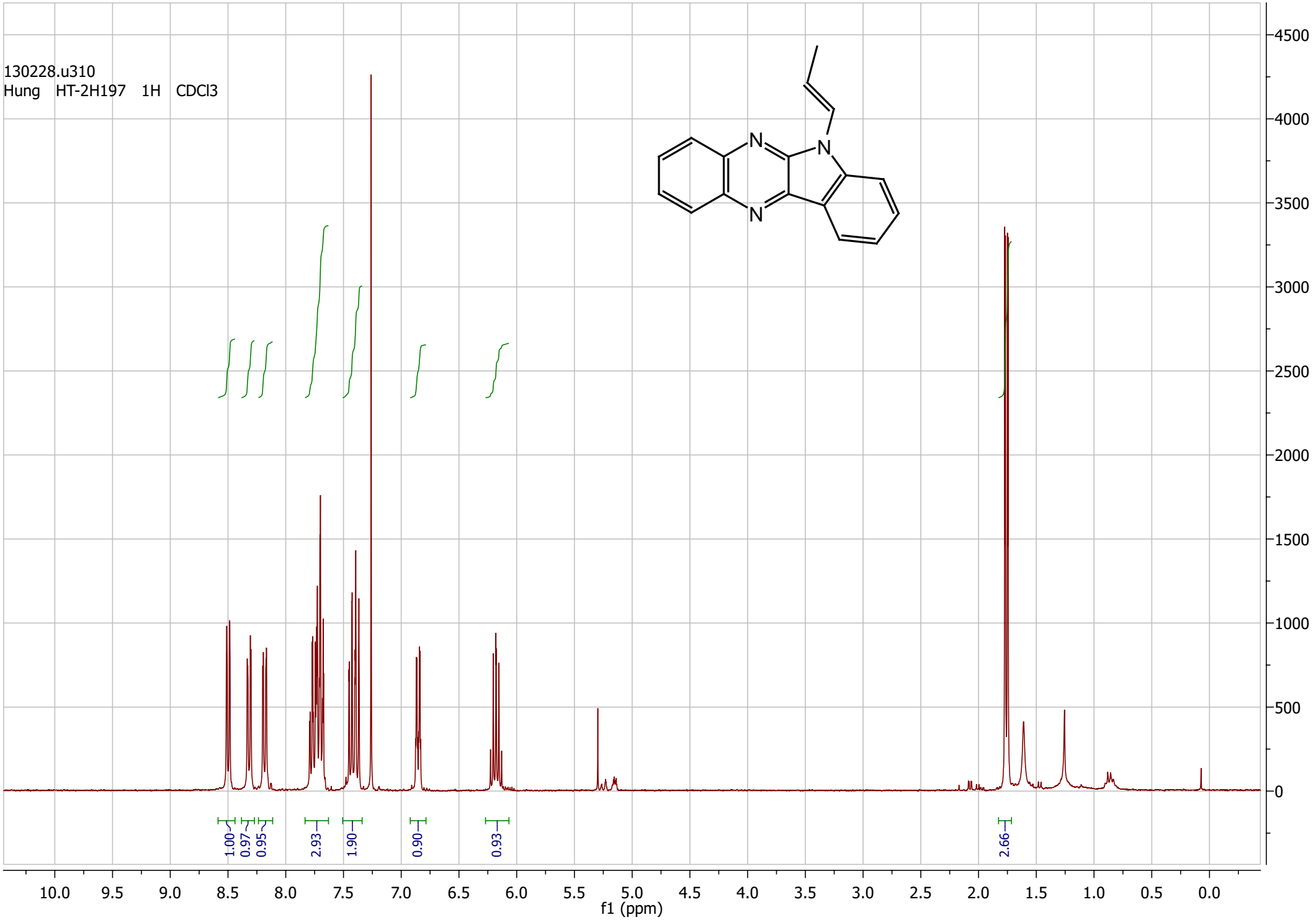

145.65
144.46
140.66
140.03
139.23
130.87
129.31
128.63
127.82
125.83
122.72
120.69
119.47
109.48
41.44
29.16
28.15
22.39
13.94
130916.208
Hung HT-50 13C CDCl3
N
N
N
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

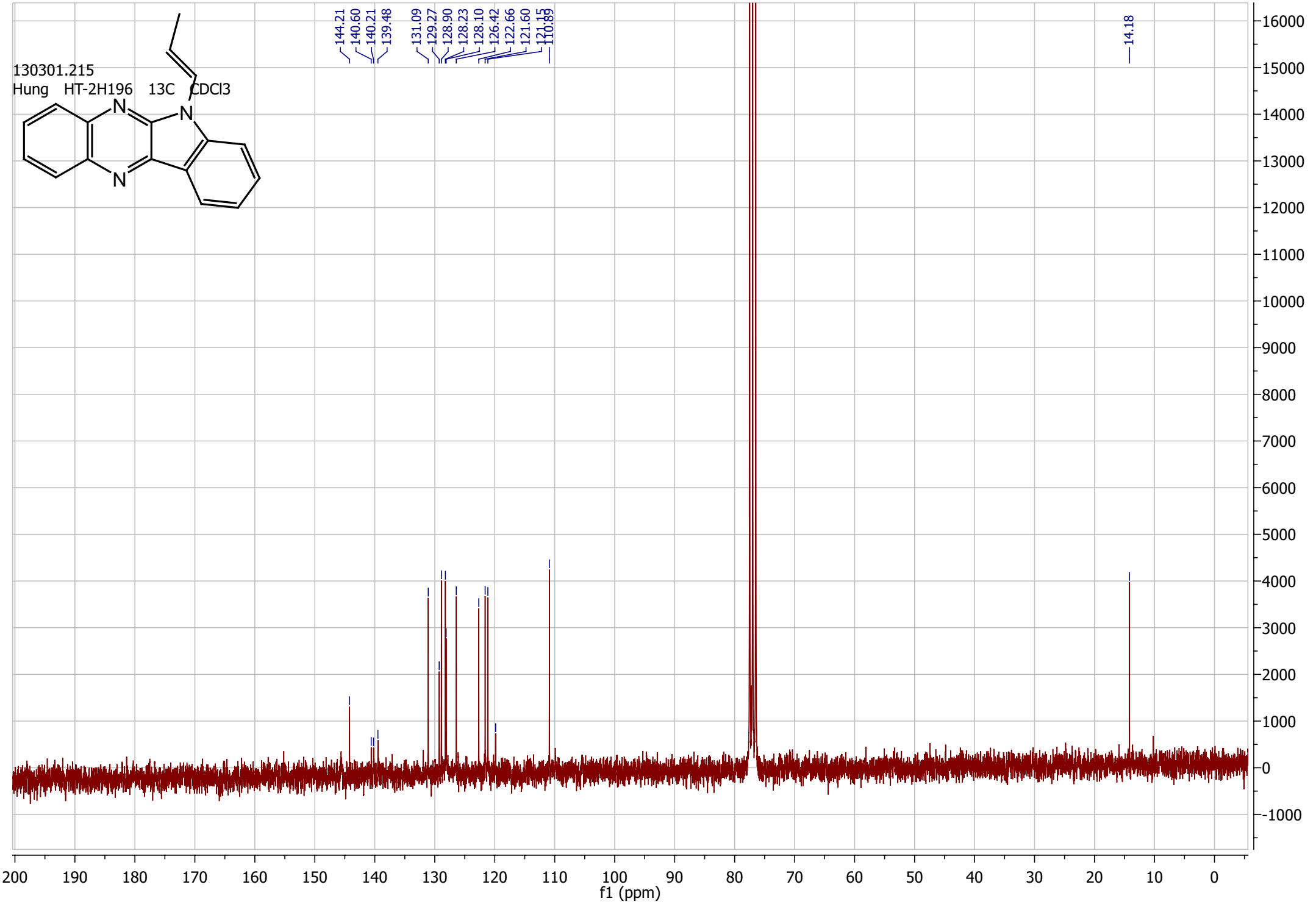

130916.208
Hung HT-50 Dept CDCl3
130.87
129.32
128.63
127.82
125.83
122.72
120.69
109.48
41.44
29.16
28.15
22.39
13.94
N
N
N
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
-3000
-3500
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

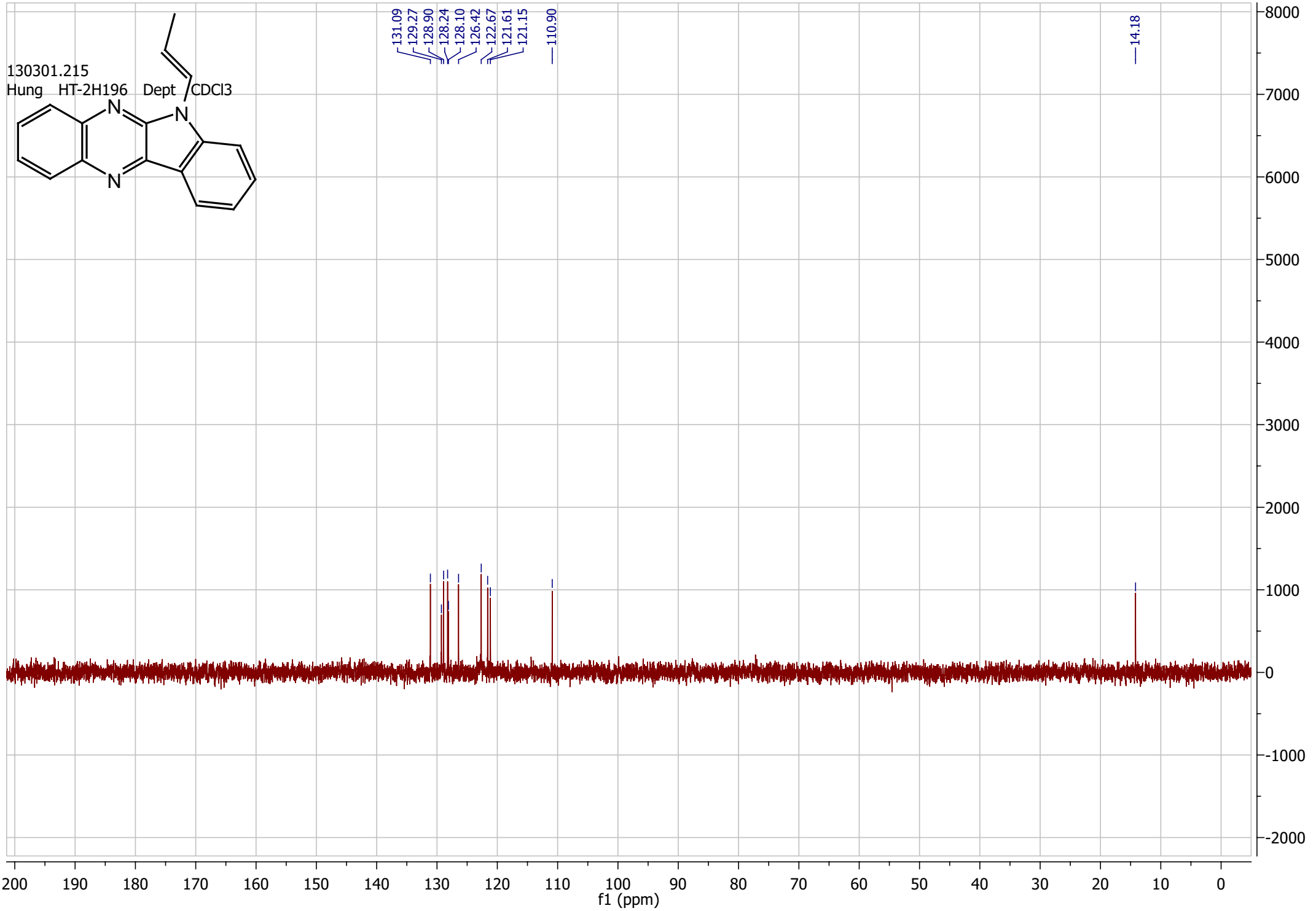

130218.u304
Hung HT-2H183 1H CDCl3
8.52 8.49 8.33 8.33 8.31 8.30 8.16 8.16 8.13 8.13
7.79 7.78 7.76 7.76 7.75 7.73 7.73 7.72 7.72 7.70 7.70 7.70 7.69 7.69 7.68 7.68 7.67 7.67 7.66 7.65 7.65 7.49 7.46 7.40 7.40 7.38 7.35 7.35 7.26
2.00 1.98 1.95 1.93 1.90
1.39 1.26 1.26 0.88 0.86 0.84
N
N
N
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00 1.00 1.00 3.13 1.06 1.06 2.07 2.07 8.99 3.37
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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 -0.5
f1 (ppm)

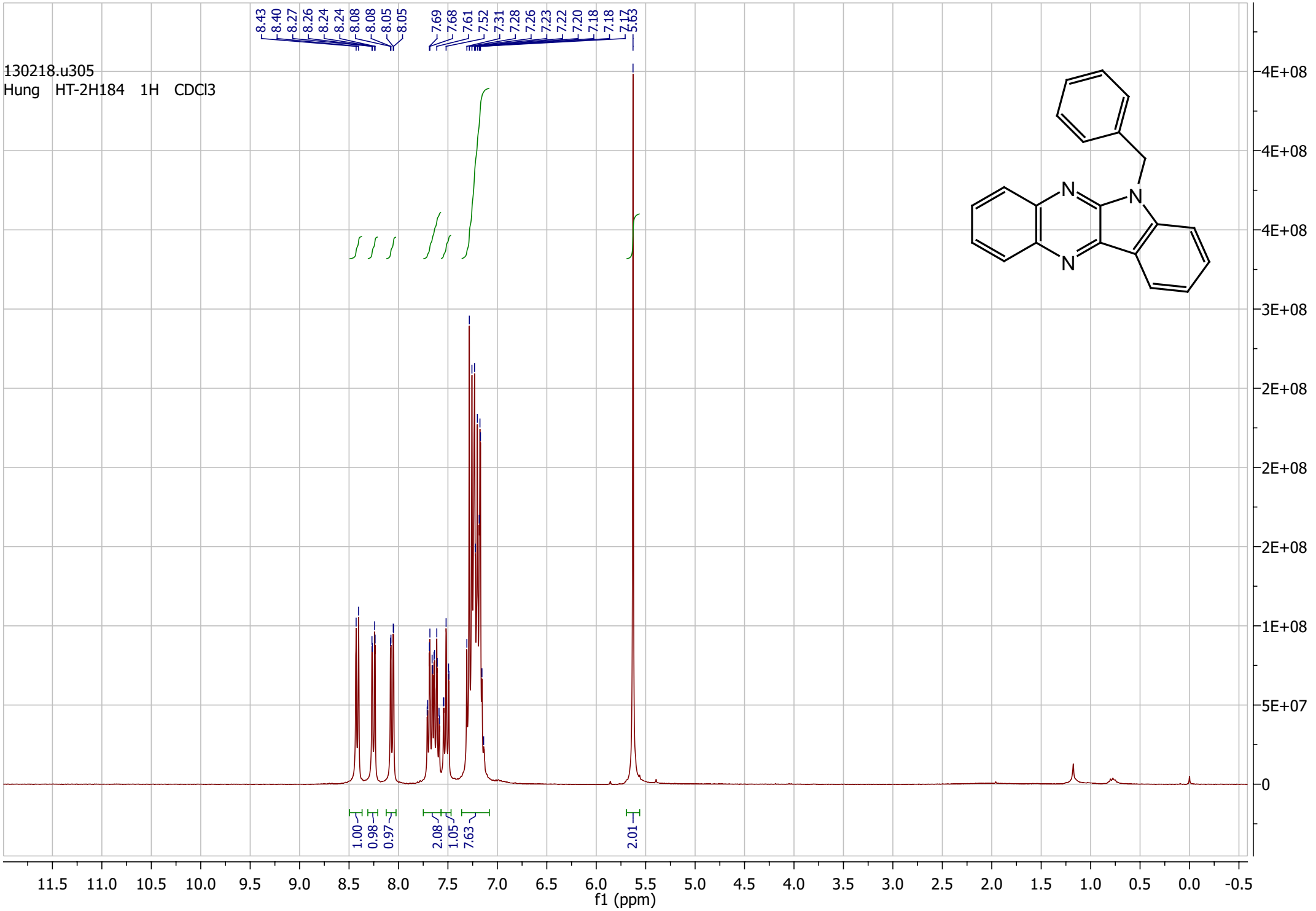

130218.u304
Hung HT-2H183 13C CDCl3
145.81
144.67
140.78
139.89
139.05
131.16
129.26
128.86
127.95
126.10
123.05
120.92
119.43
109.67
77.58
77.16
76.74
41.63
31.85
29.11
28.60
27.16
22.73
14.18
N
N
N
3E+08
3E+08
2E+08
2E+08
2E+08
2E+08
2E+08
1E+08
1E+08
1E+08
8E+07
6E+07
4E+07
2E+07
0
-2E+07
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

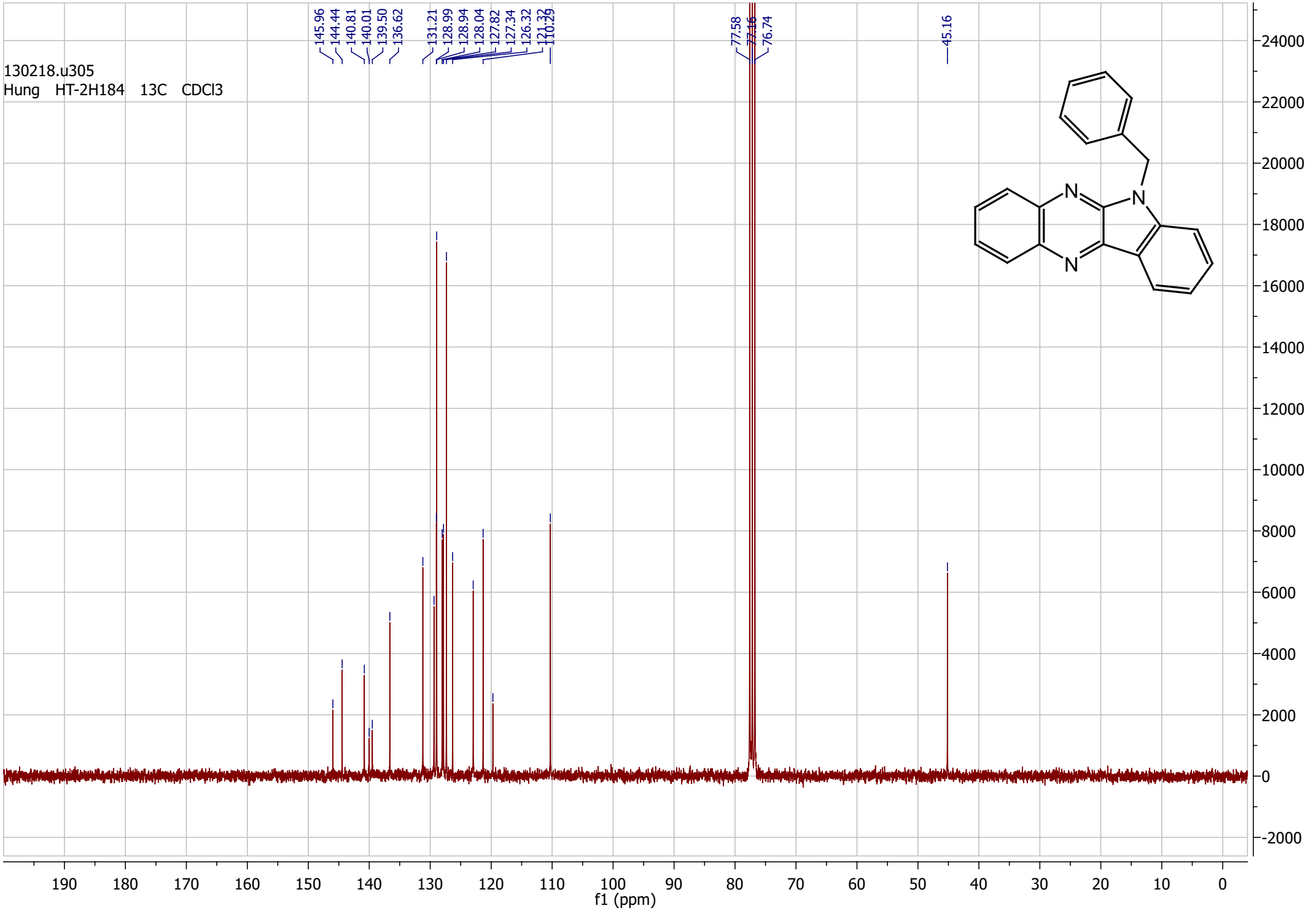

130218.u304
Hung HT-2H183 Dept CDCl3
131.13
129.31
128.84
127.95
126.07
123.01
120.90
109.67
41.62
31.85
29.11
28.60
27.16
22.72
14.18
N
N
N
5E+08
4E+08
3E+08
2E+08
1E+08
0
-1E+08
-2E+08
-3E+08
-4E+08
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

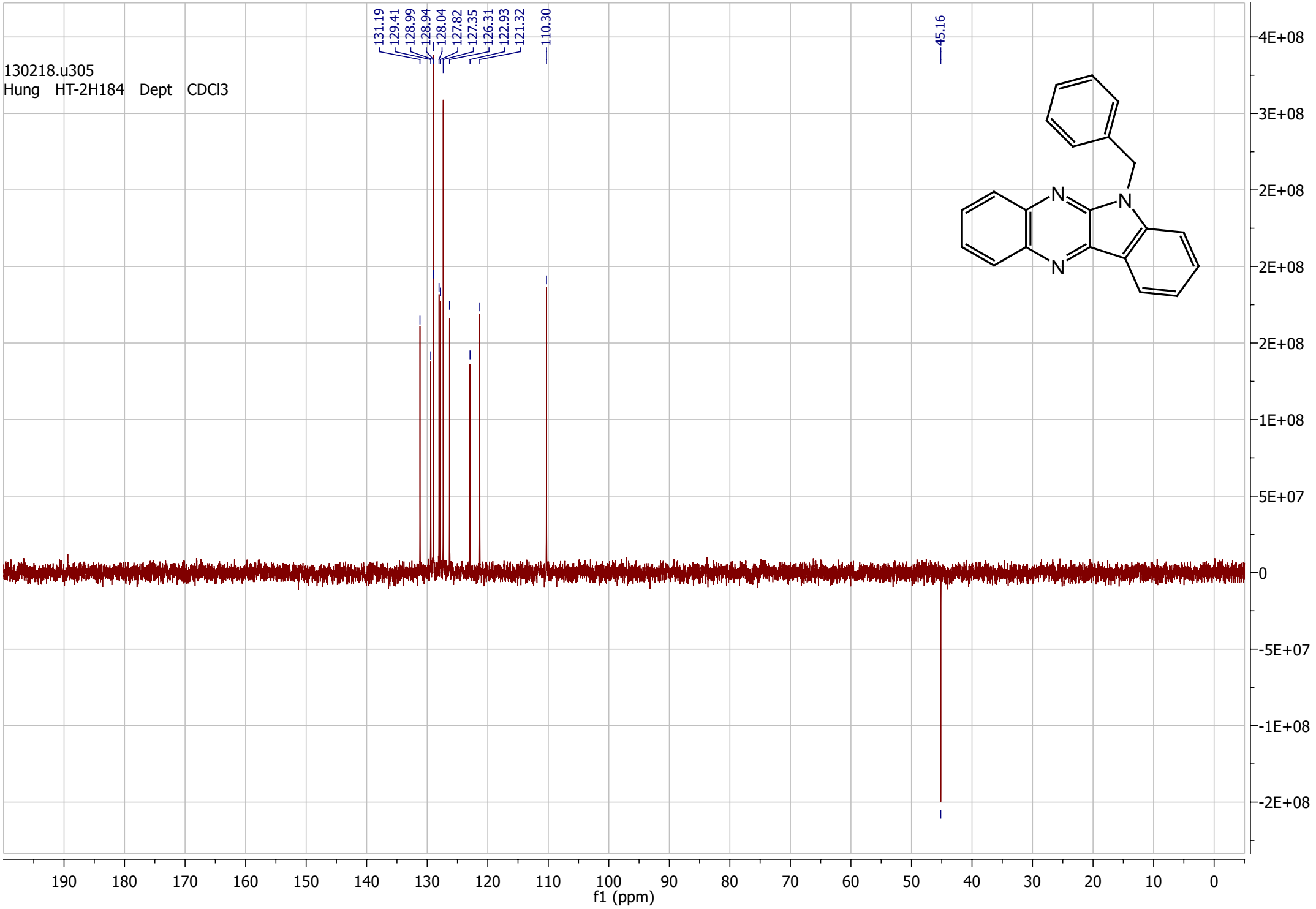

130228.u310
Hung HT-2H197 1H CDCl3
N
N
N
1.00
0.97
0.95
2.93
1.90
0.90
0.93
2.66
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)
4500
4000
3500
3000
2500
2000
1500
1000
500
0

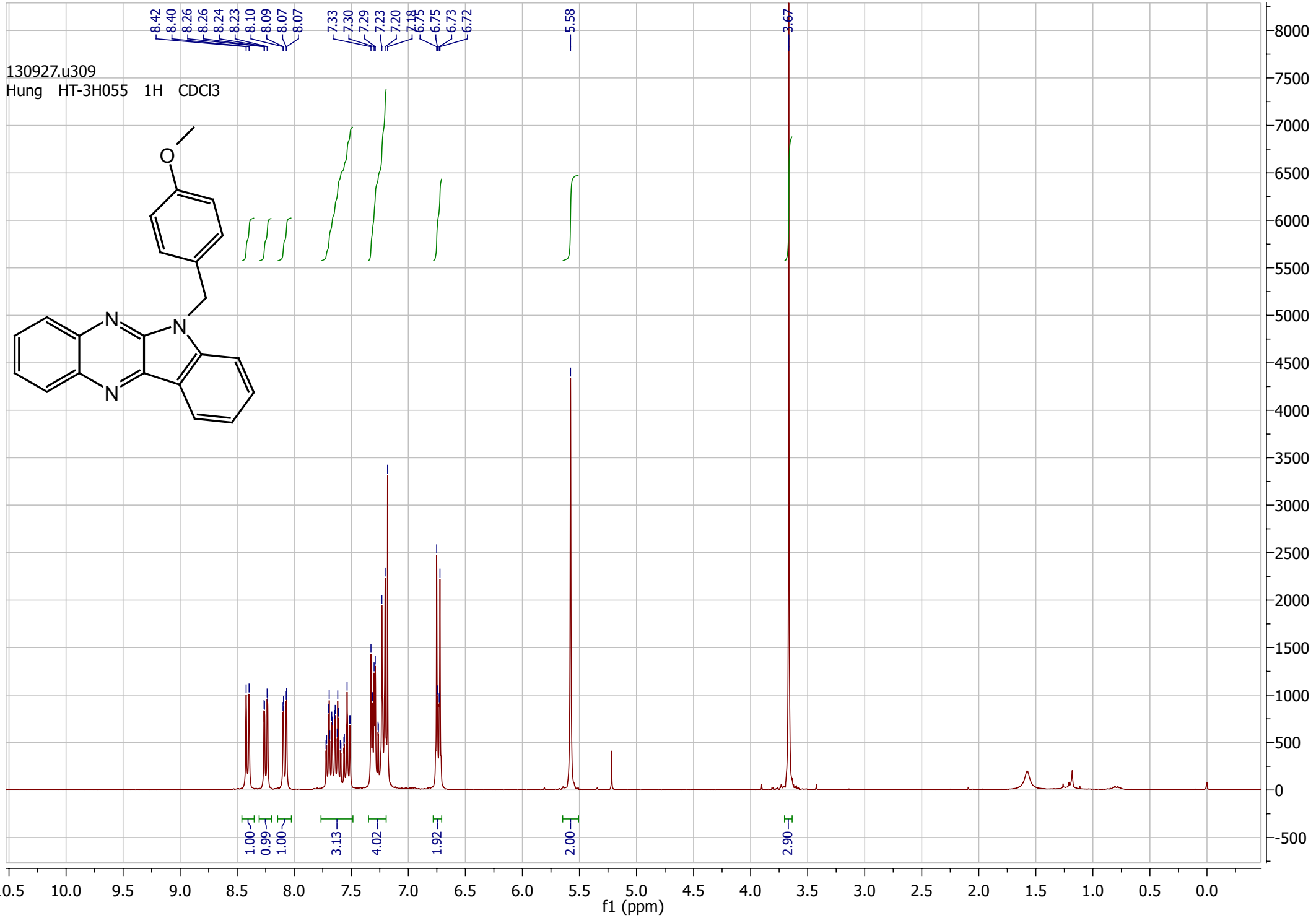

130301.215
Hung HT-2H196 13C CDCl3
144.21
140.60
140.21
139.48
131.09
129.27
128.90
128.23
128.10
126.42
122.66
121.60
121.15
110.89
14.18
f1 (ppm)

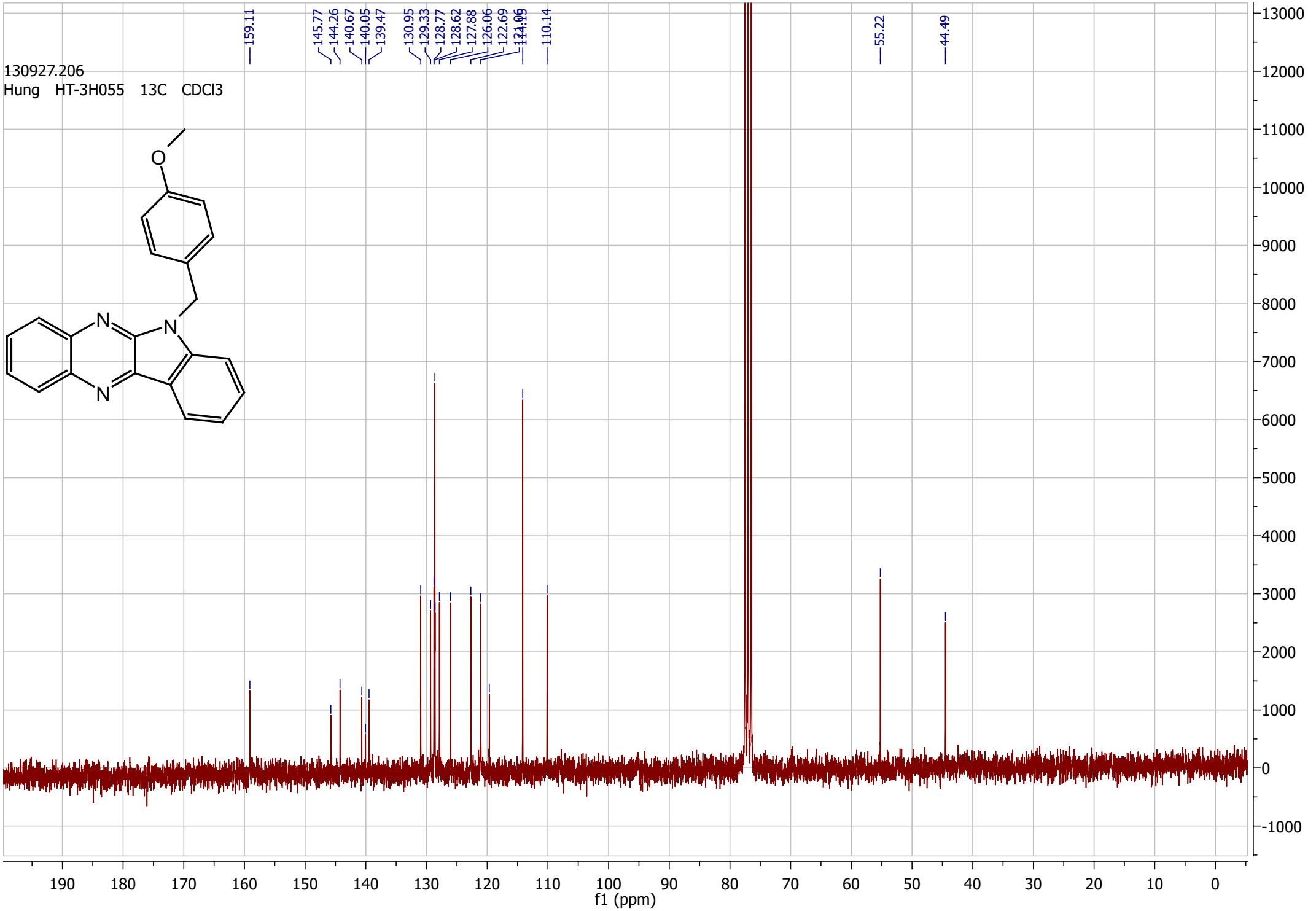

130301.215
Hung HT-2H196 Dept CDCl3
131.09
129.27
128.90
128.24
128.10
126.42
122.67
121.61
121.15
110.90
14.18
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

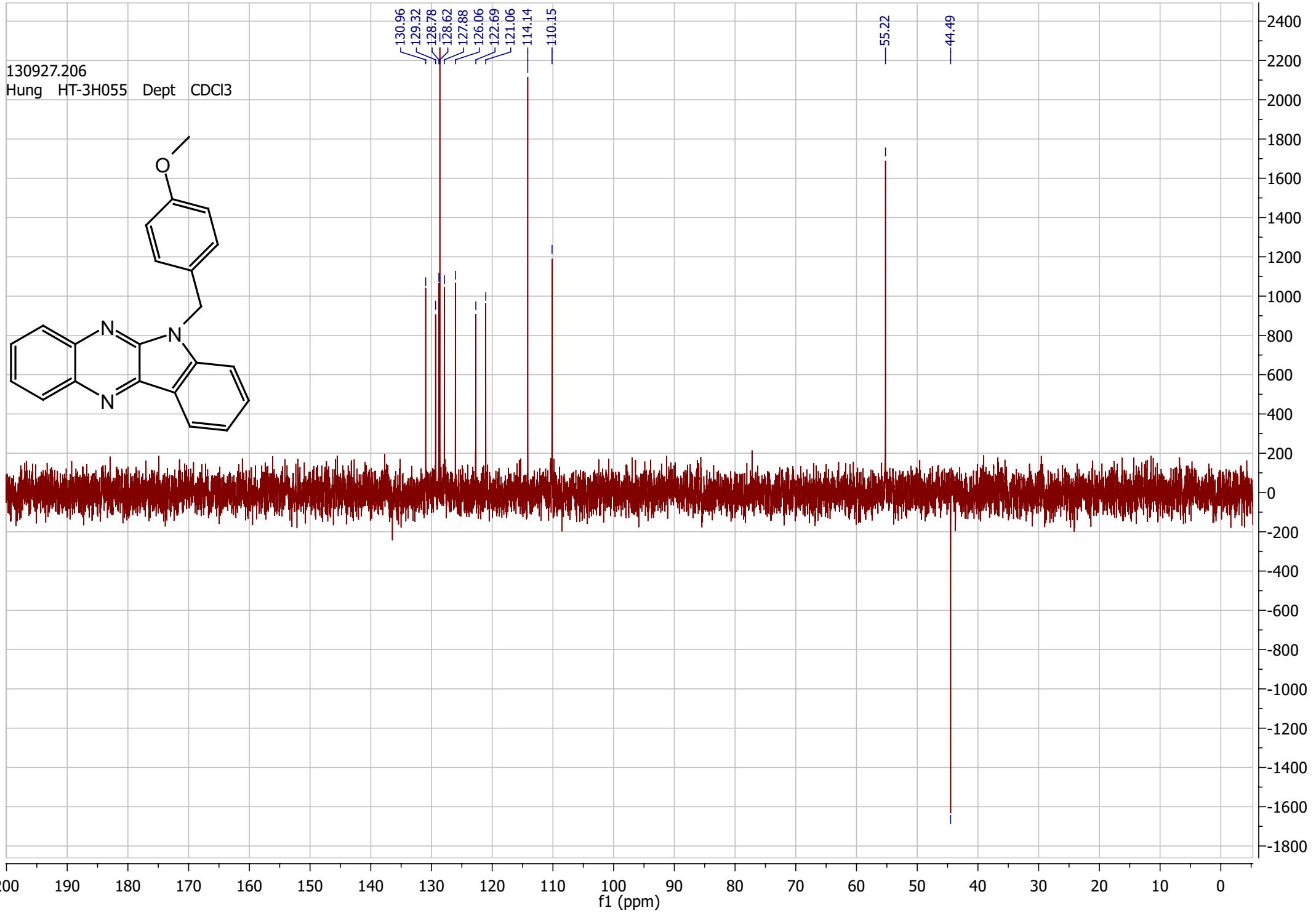

130218.u305
Hung HT-2H184 1H CDCl3
8.43
8.40
8.27
8.26
8.24
8.24
8.08
8.08
8.05
8.05
7.69
7.68
7.61
7.52
7.31
7.28
7.26
7.23
7.22
7.20
7.18
7.17
5.63
N
N
N
4E+08
4E+08
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
1.00
0.98
0.97
2.08
1.05
7.63
2.01
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

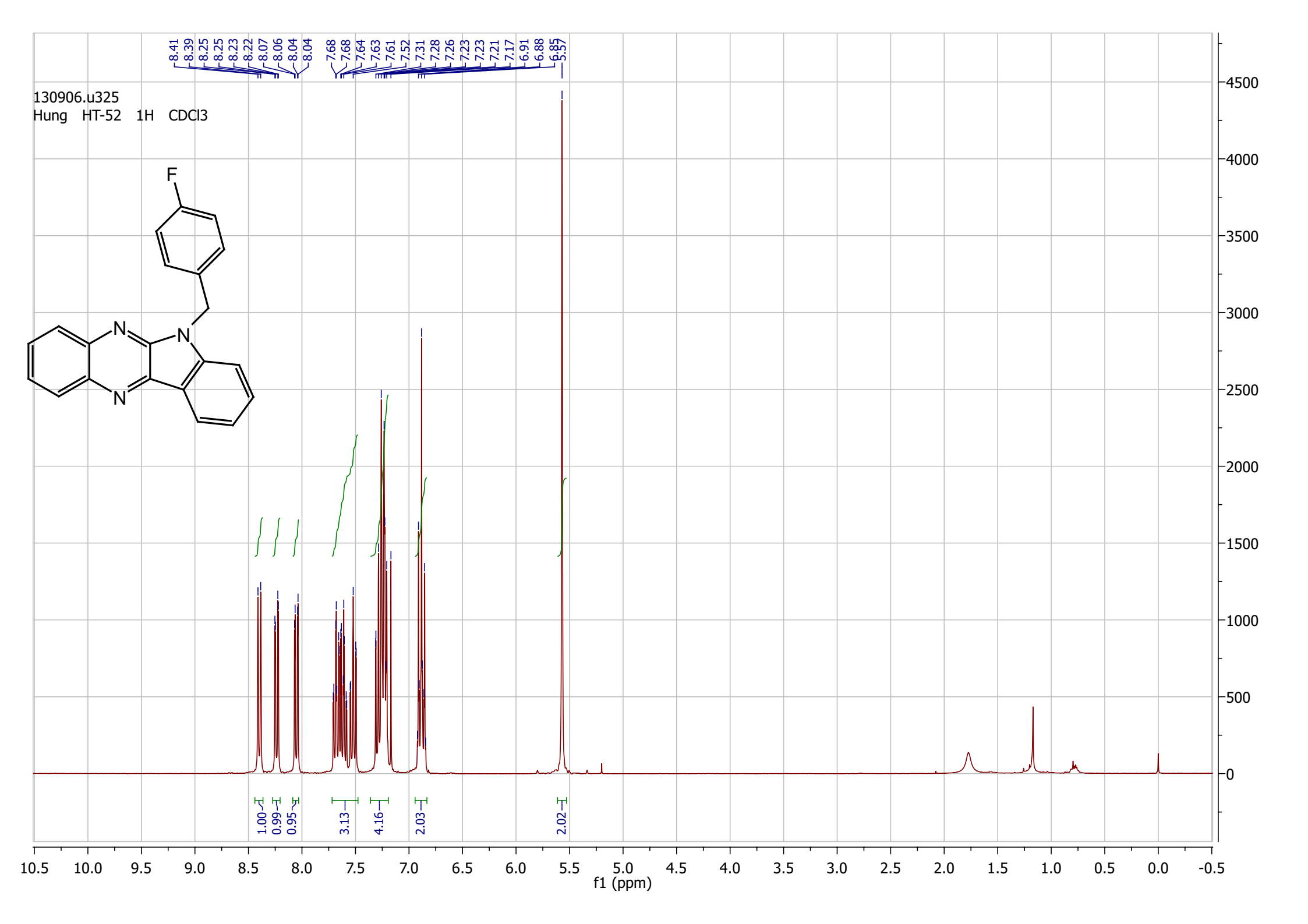

130218.u305
Hung HT-2H184 13C CDCl3
145.96
144.44
140.81
140.01
139.50
136.62
131.21
128.99
128.94
128.04
127.82
127.34
126.32
121.32
110.29
77.58
77.16
76.74
45.16
N
N
N
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

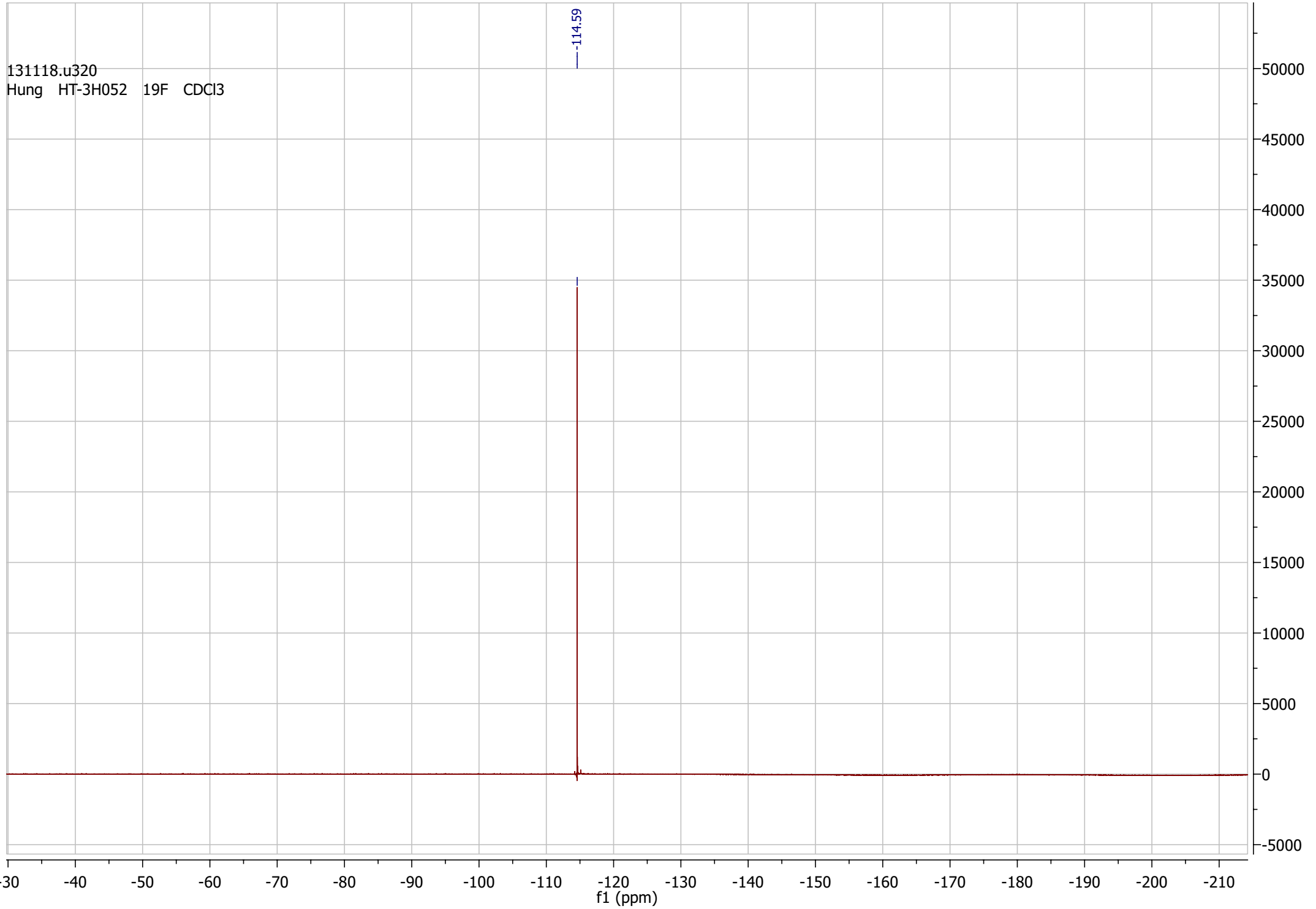

130218.u305
Hung HT-2H184 Dept CDCl3
131.19
129.41
128.99
128.94
128.04
127.82
127.35
126.31
122.93
121.32
110.30
45.16
N
N
N
4E+08
3E+08
2E+08
2E+08
2E+08
1E+08
5E+07
0
-5E+07
-1E+08
-2E+08
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

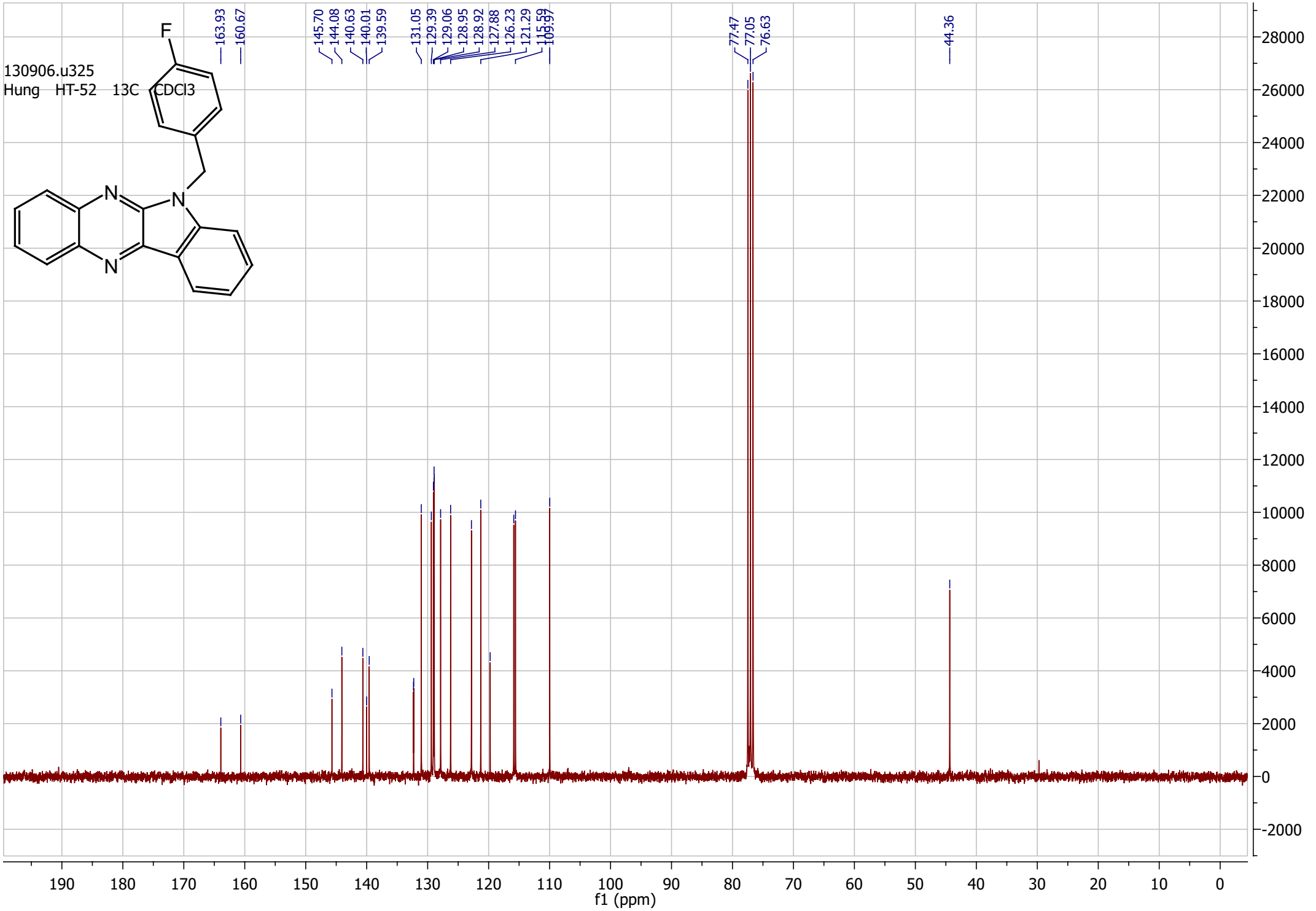

130927.u309
Hung HT-3H055 1H CDCl3
8.42
8.40
8.26
8.26
8.24
8.23
8.10
8.09
8.07
8.07
7.33
7.30
7.29
7.23
7.20
7.18
6.75
6.75
6.73
6.72
5.58
3.67
O
N
N
N
1.00
0.99
1.00
3.13
4.02
1.92
2.00
2.90
f1 (ppm)

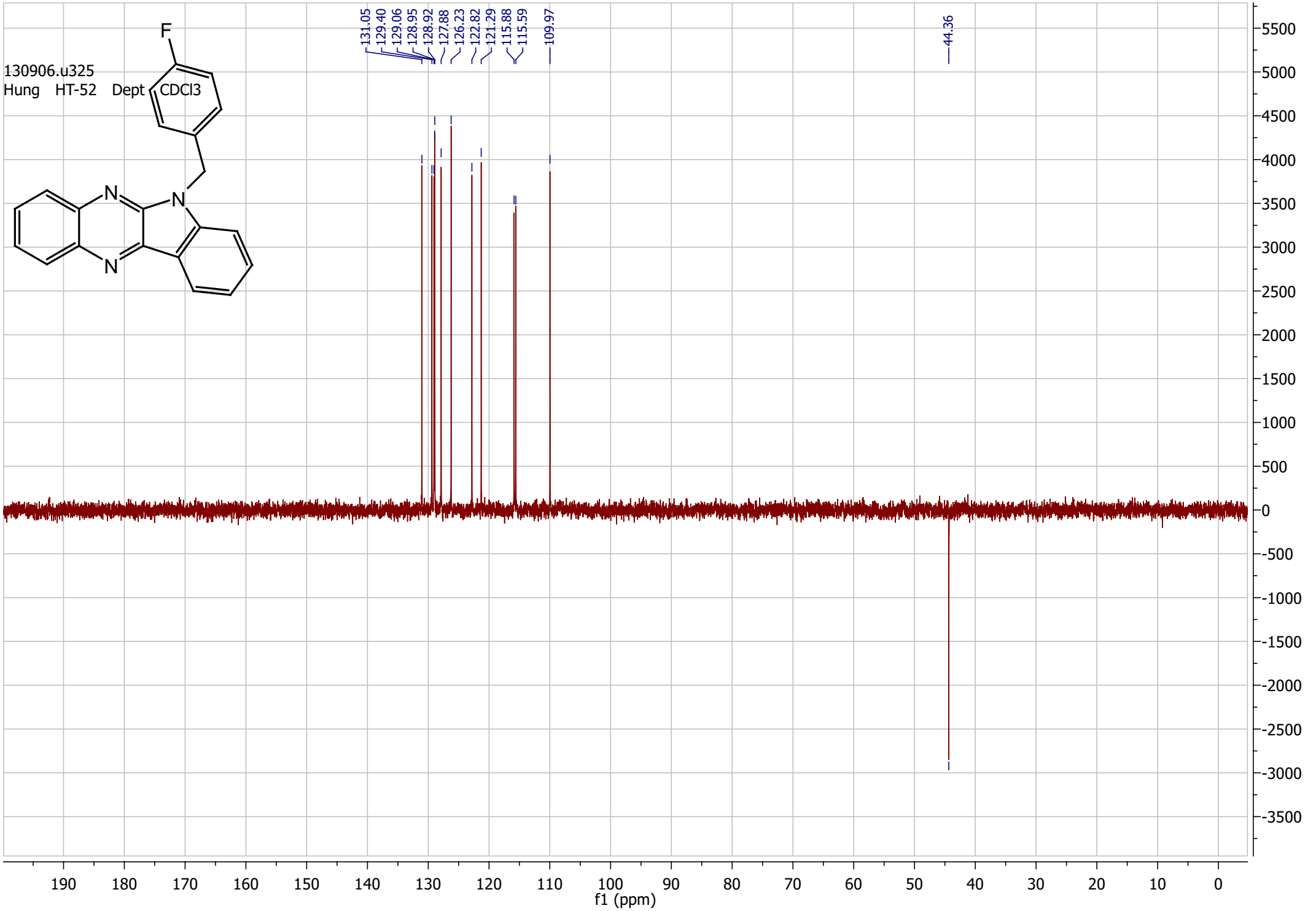

130927.206
Hung HT-3H055 13C CDCl3
159.11
145.77
144.26
140.67
140.05
139.47
130.95
129.33
128.77
128.62
127.88
126.06
122.69
110.14
55.22
44.49
O
N
N
N
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

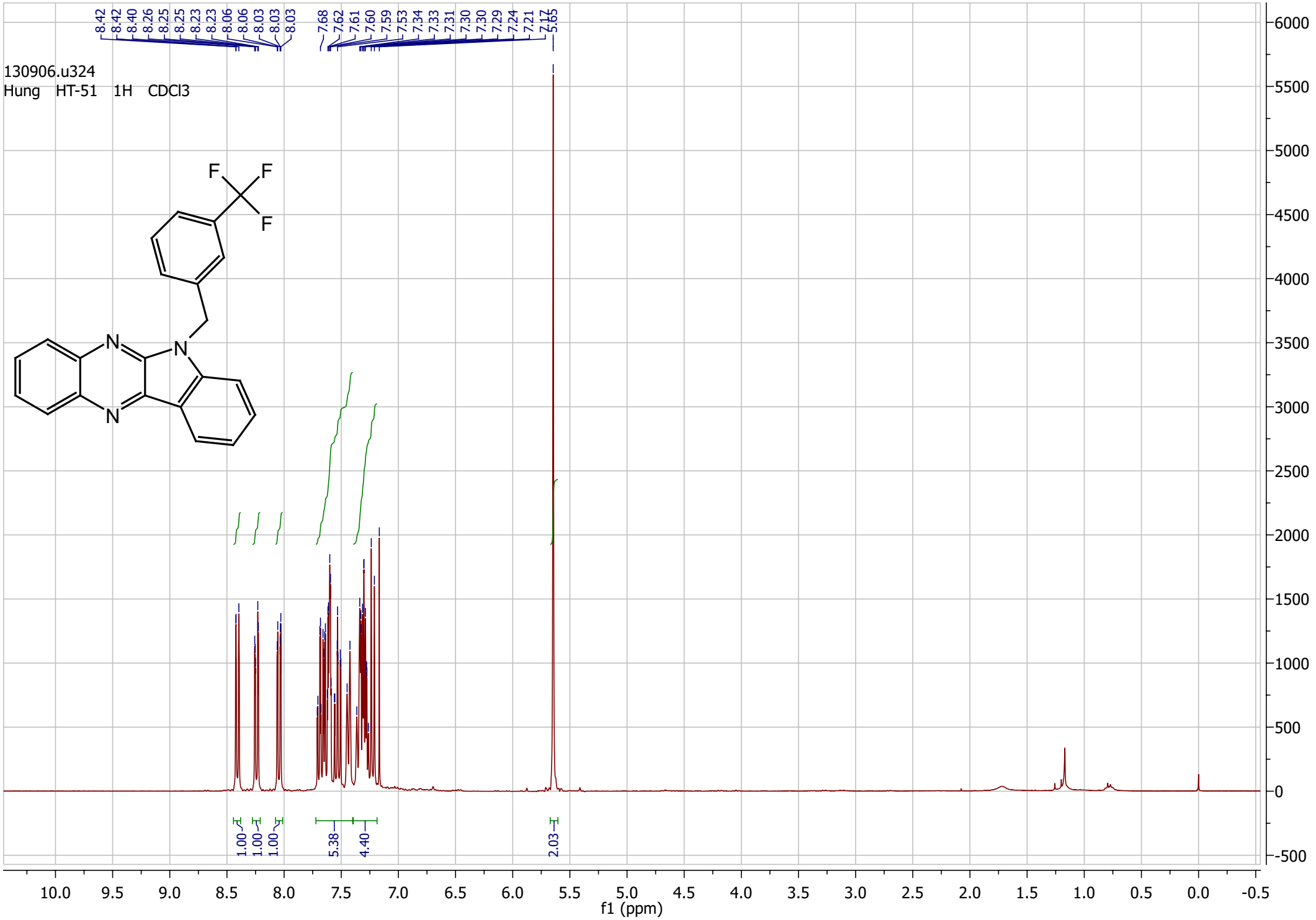

130927.206
Hung HT-3H055 Dept CDCl3
130.96
129.32
128.78
128.62
127.88
126.06
122.69
121.06
114.14
110.15
55.22
44.49
O
N
N
N
2400
2200
2000
1800
1600
1400
1200
1000
800
600
400
200
0
-200
-400
-600
-800
-1000
-1200
-1400
-1600
-1800
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

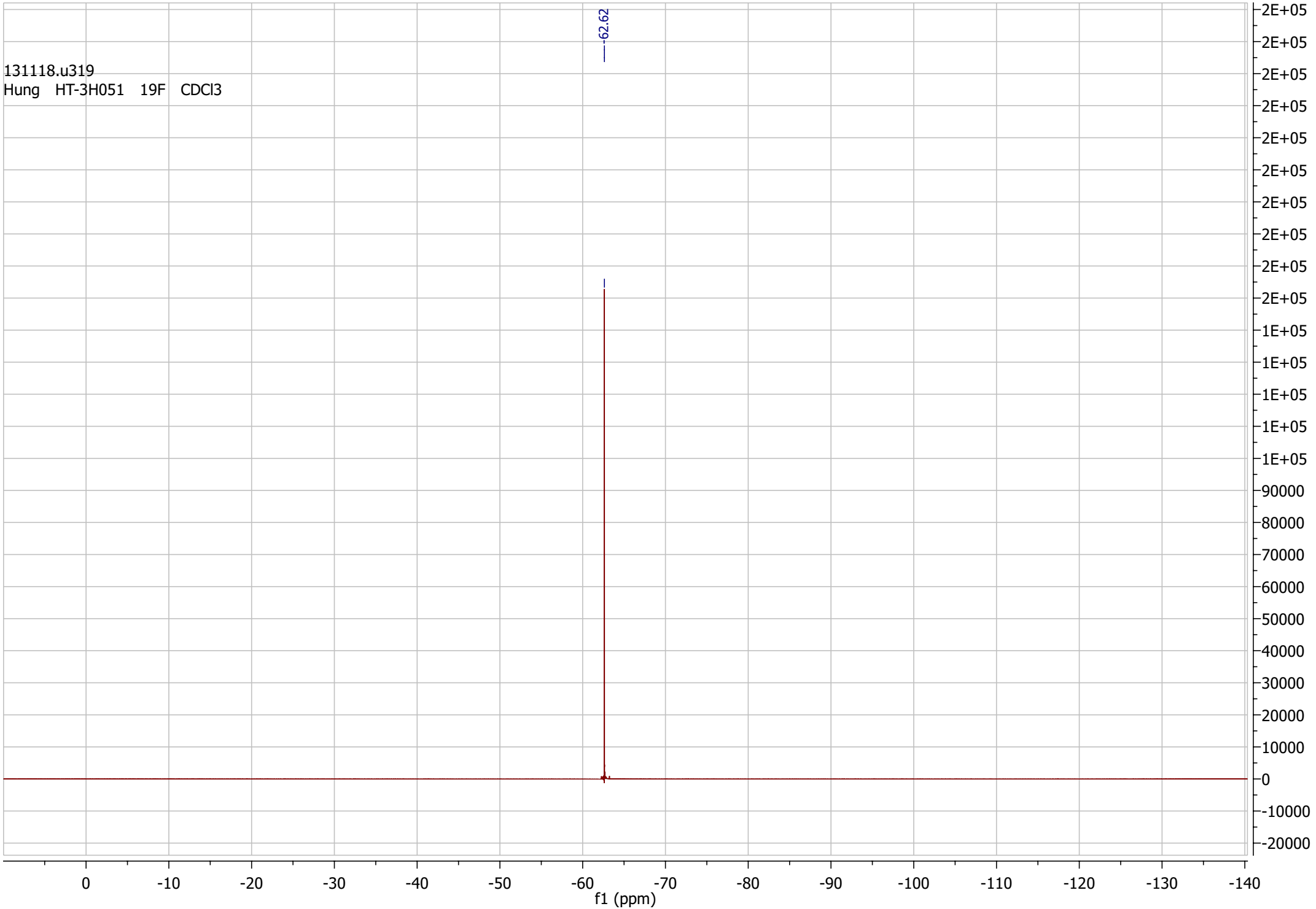

130906.u325
Hung HT-52 1H CDCl3
8.41
8.39
8.25
8.25
8.23
8.22
8.07
8.06
8.04
8.04
7.68
7.68
7.64
7.63
7.61
7.52
7.31
7.28
7.26
7.23
7.23
7.21
7.17
6.91
6.88
6.85
5.57
F
N
N
N
1.00
0.99
0.95
3.13
4.16
2.03
2.02
f1 (ppm)

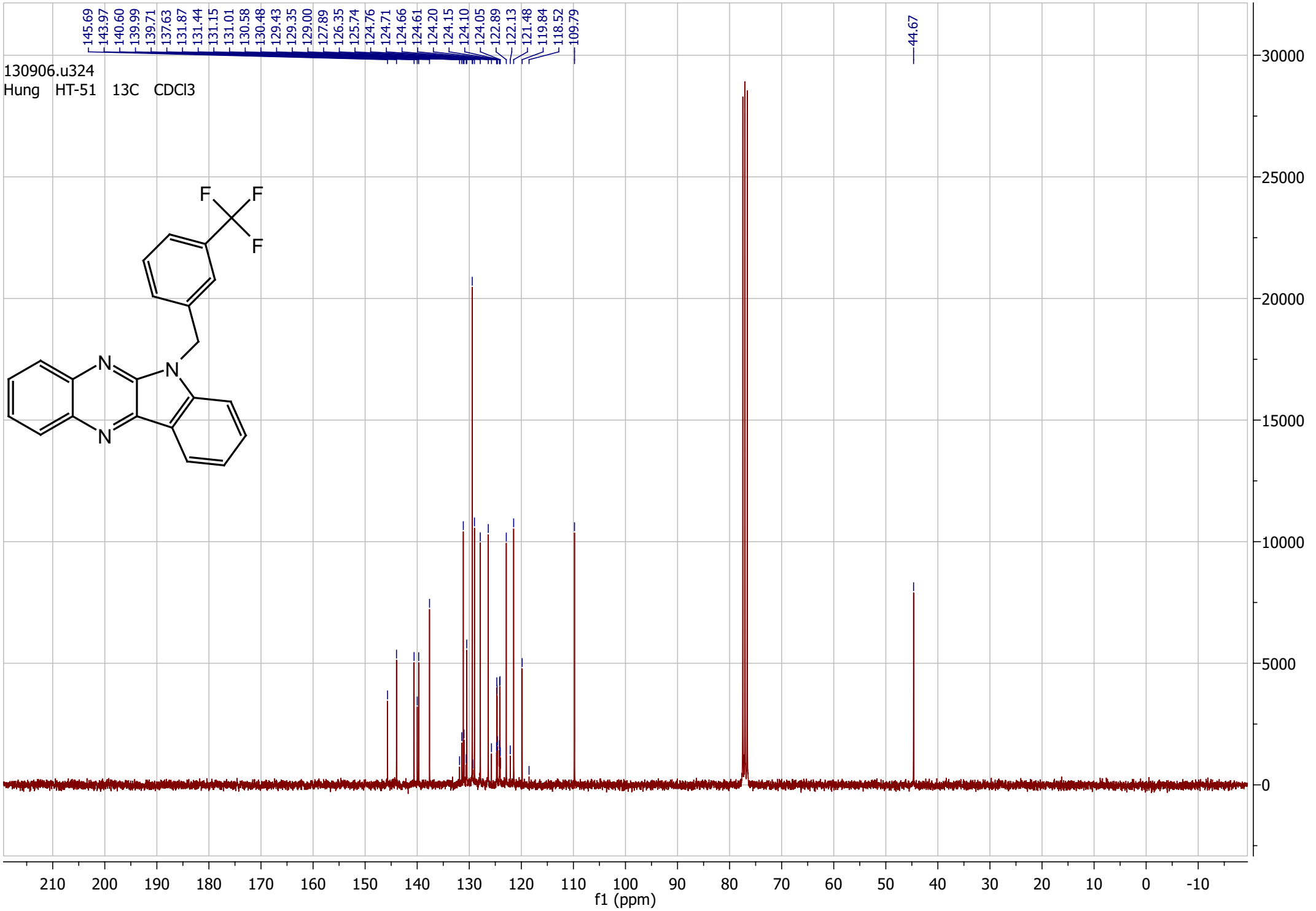

131118.u320
Hung HT-3H052 19F CDCl3
-114.59
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
-5000
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)

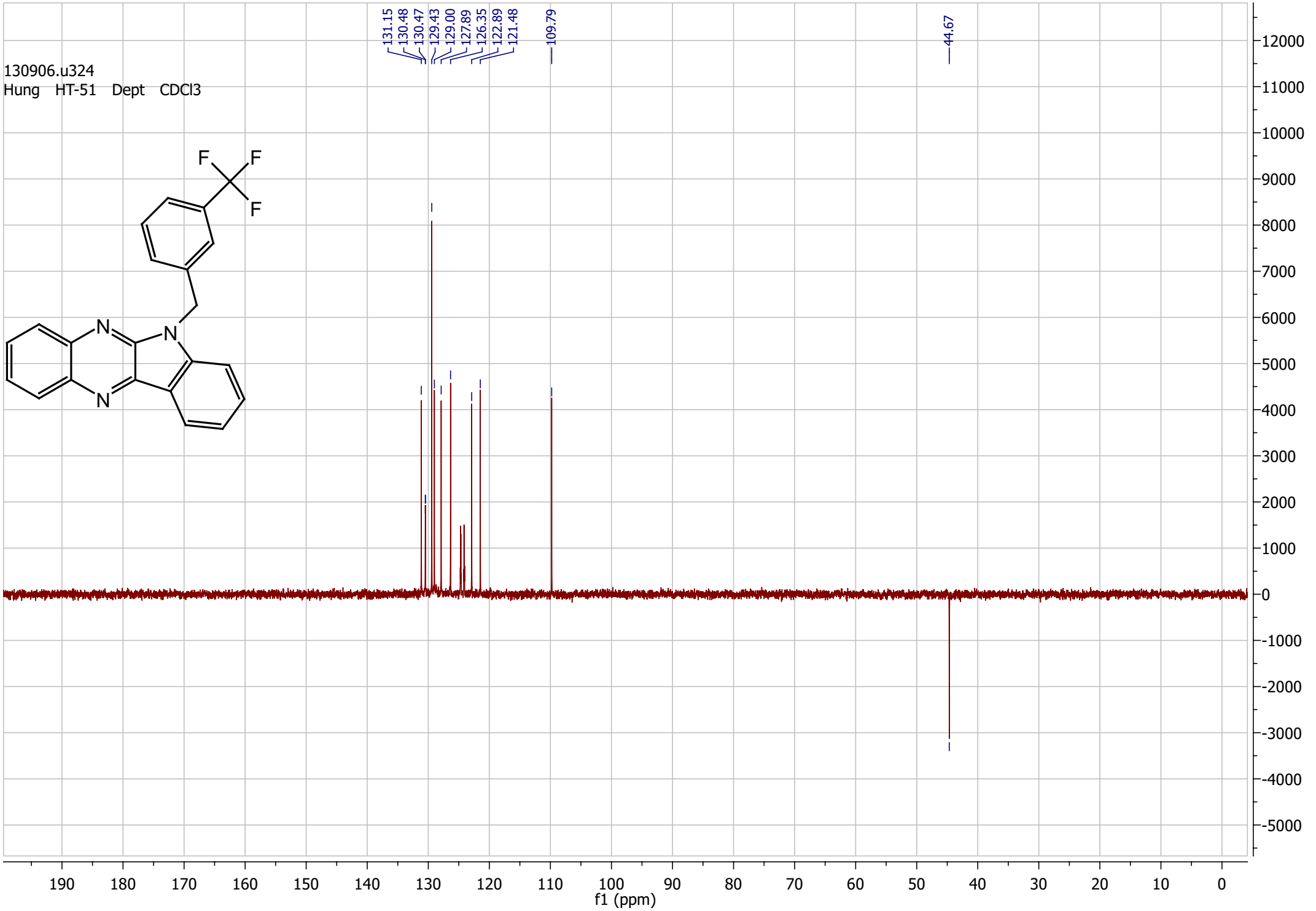

130906.u325
Hung HT-52 13C CDCl3
F
N
N
N
163.93
160.67
145.70
144.08
140.63
140.01
139.59
131.05
129.39
129.06
128.95
128.92
127.88
126.23
121.29
115.59
109.97
77.47
77.05
76.63
44.36
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

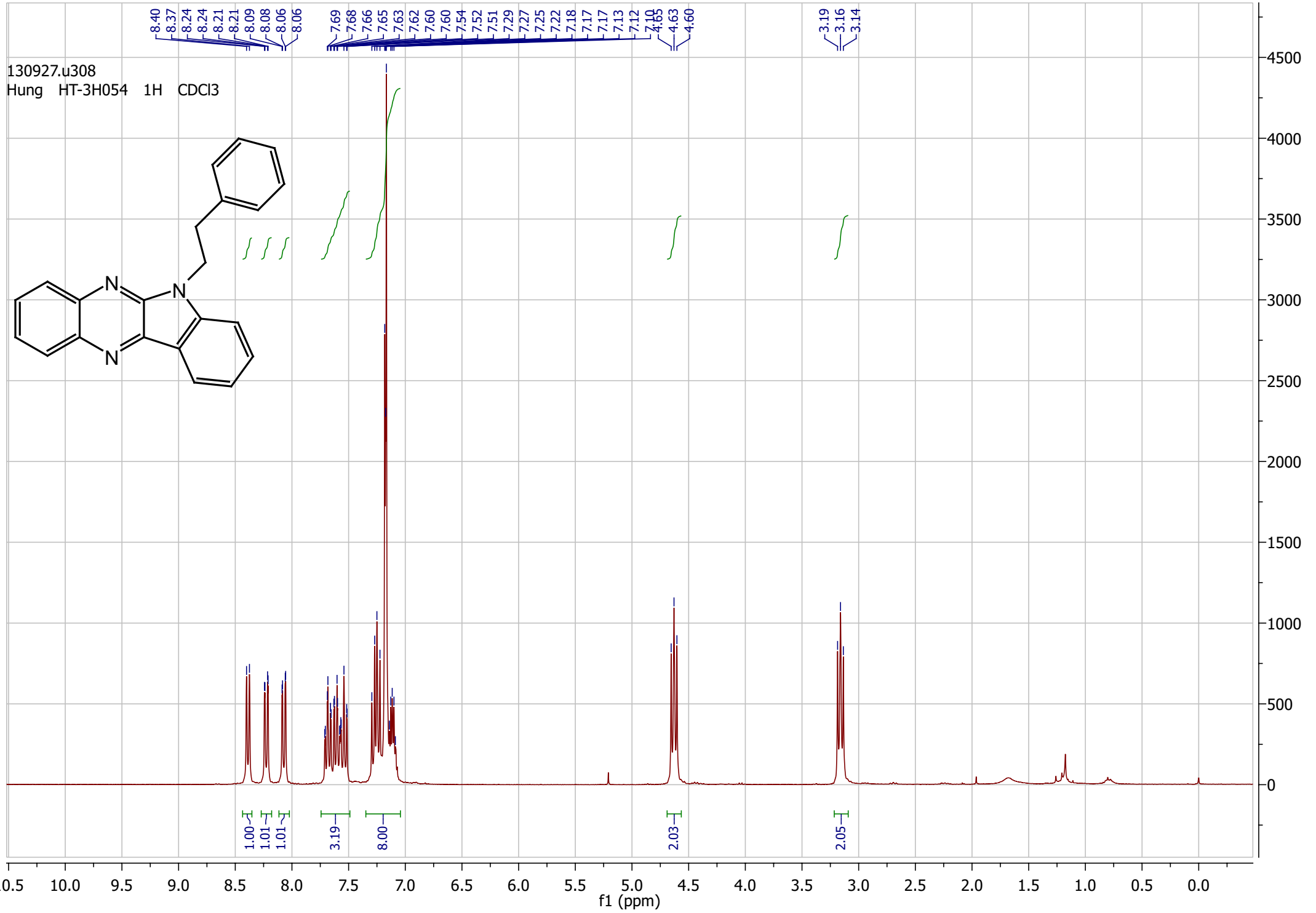

130906.u325
Hung HT-52 Dept CDCl3
F
N
N
N
131.05
129.40
129.06
128.95
128.92
127.88
126.23
122.82
121.29
115.88
115.59
109.97
44.36
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
-3000
-3500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

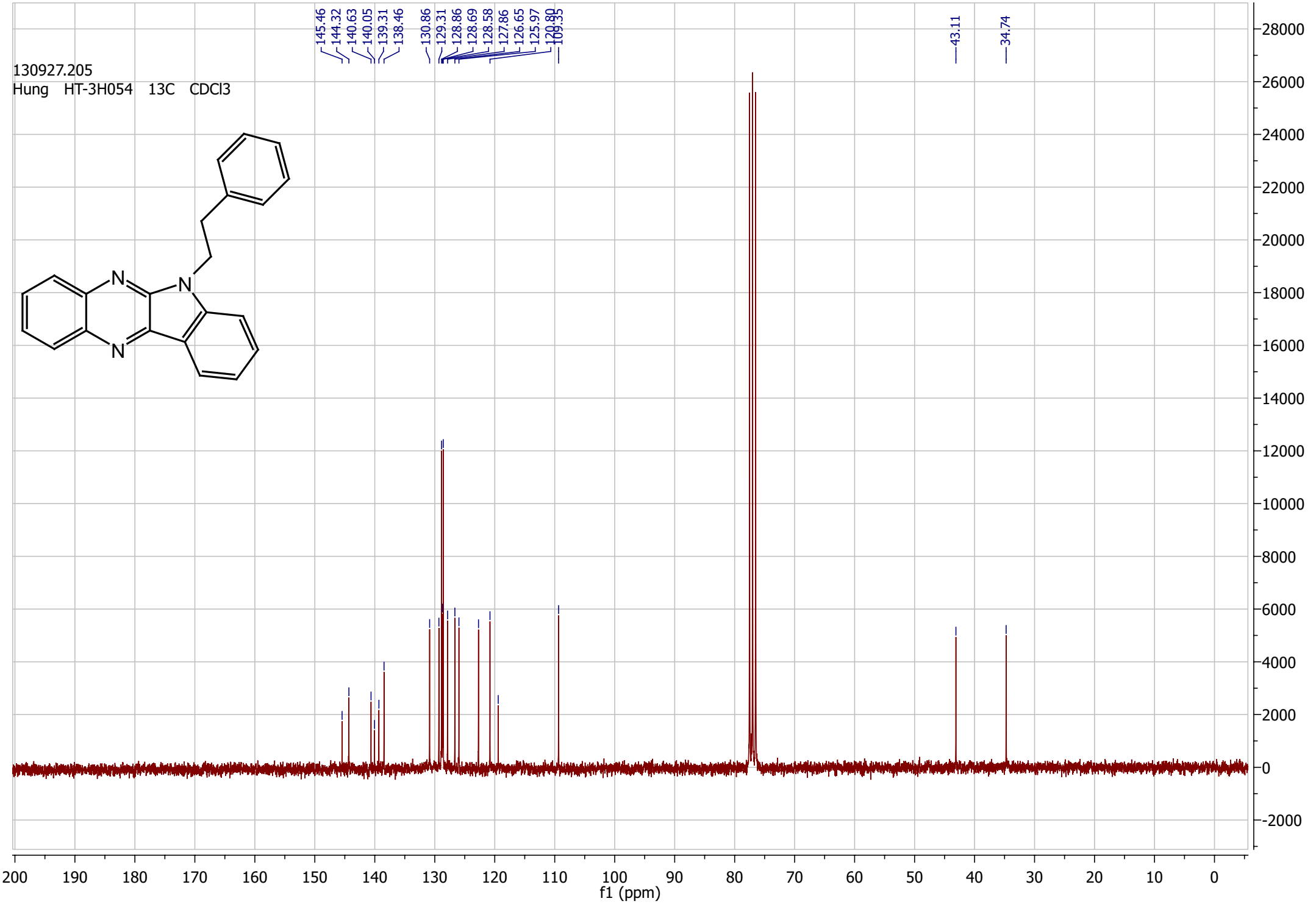

8.42
8.42
8.40
8.26
8.25
8.25
8.23
8.23
8.06
8.06
8.03
8.03
8.03
7.68
7.62
7.61
7.60
7.59
7.53
7.34
7.33
7.31
7.30
7.30
7.29
7.24
7.21
7.17
5.65
130906.u324
Hung HT-51 1H CDCl3
F
F
F
N
N
N
1.00
1.00
1.00
5.38
4.40
2.03
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
10.0
9.5
9.0
8.5
8.0
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
-0.5
f1 (ppm)

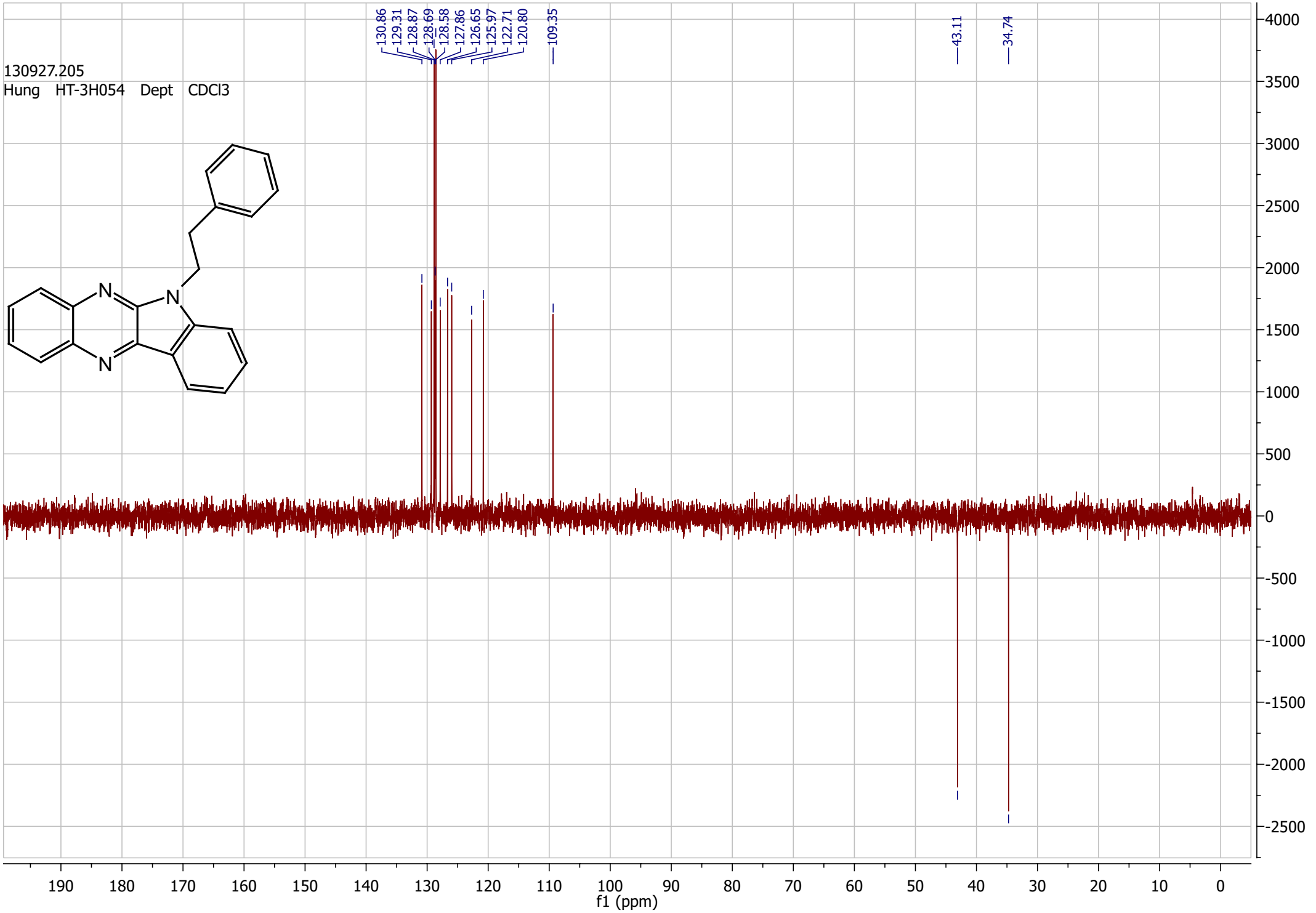

131118.u319
Hung HT-3H051 19F CDCl3
-62.62
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
2E+05
1E+05
1E+05
1E+05
1E+05
1E+05
1E+05
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
-10000
-20000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
f1 (ppm)

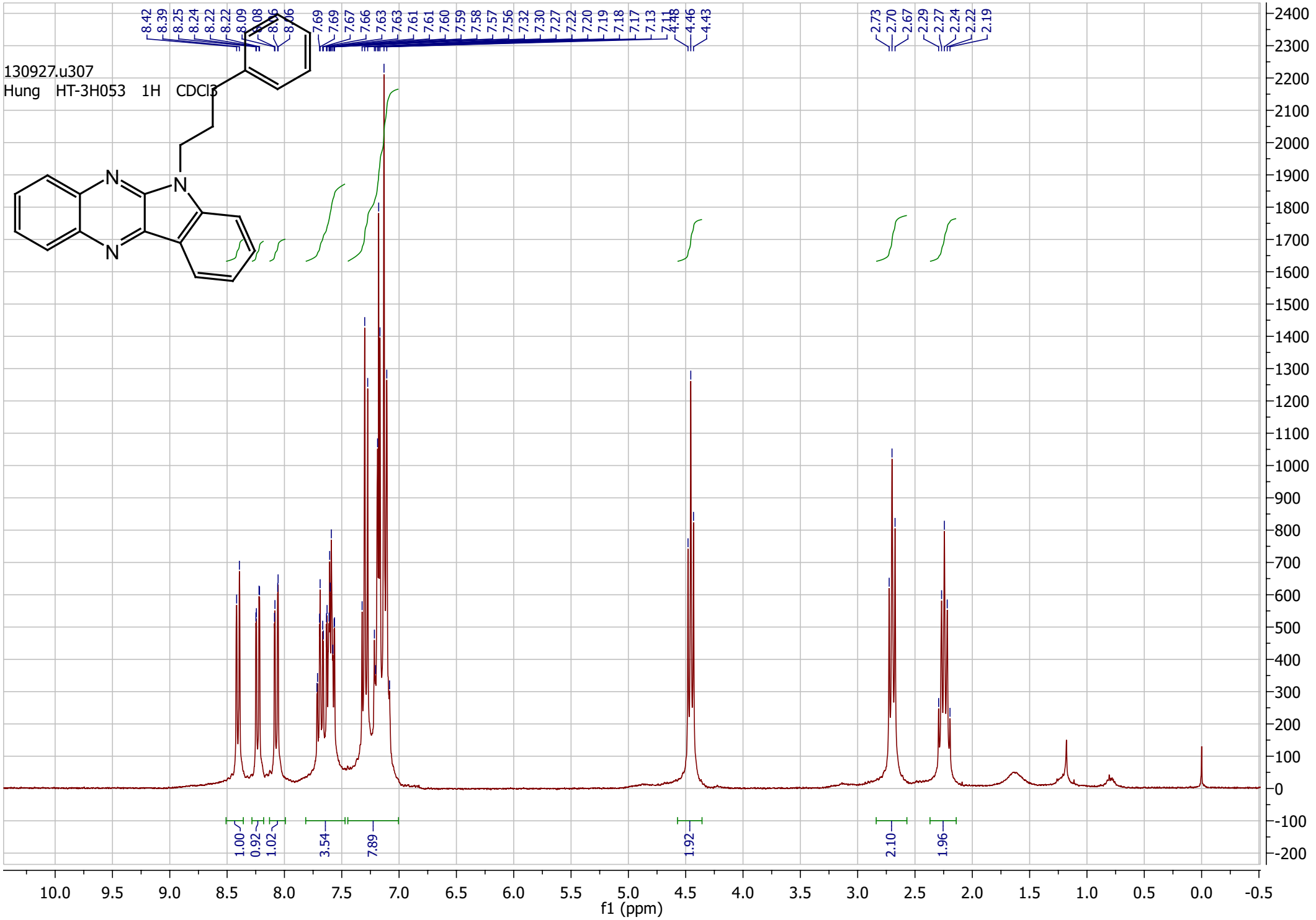

145.69
143.97
140.60
139.99
139.71
137.63
131.87
131.44
131.15
131.01
130.58
130.48
129.43
129.35
129.00
127.89
126.35
125.74
124.76
124.71
124.66
124.61
124.20
124.15
124.10
124.05
122.89
122.13
121.48
119.84
118.52
109.79
44.67
130906.u324
Hung HT-51 13C CDCl3
F
F
F
N
N
N
30000
25000
20000
15000
10000
5000
0
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

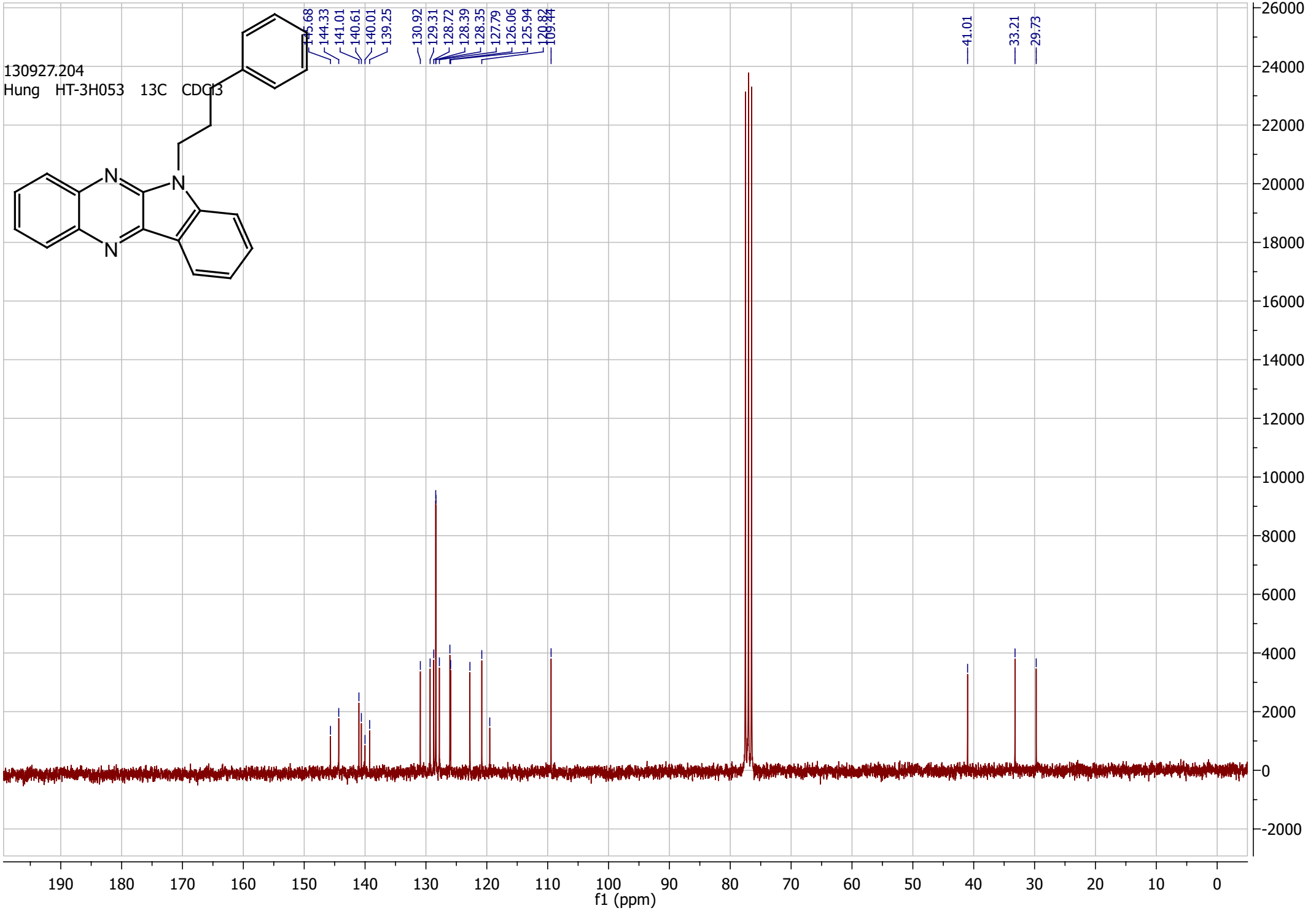

131.15
130.48
130.47
129.43
129.00
127.89
126.35
122.89
121.48
109.79
44.67
130906.u324
Hung HT-51 Dept CDCl3
F
F
F
N
N
N
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
-5000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

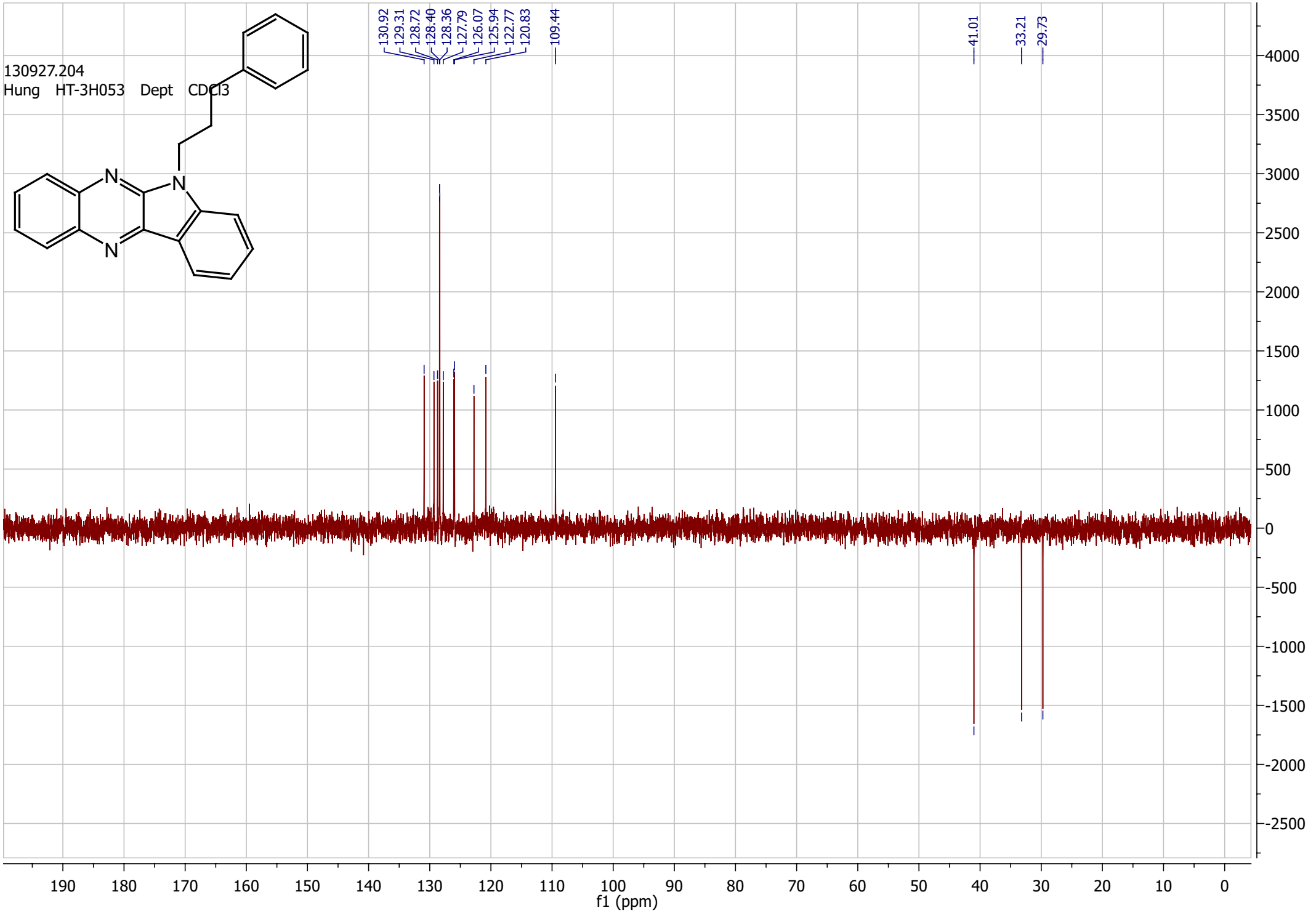

130927.u308
Hung HT-3H054 1H CDCl3
8.40
8.37
8.24
8.24
8.21
8.21
8.09
8.08
8.06
8.06
7.69
7.68
7.66
7.65
7.63
7.62
7.60
7.60
7.54
7.52
7.51
7.29
7.27
7.25
7.22
7.18
7.17
7.17
7.13
7.12
7.10
4.65
4.63
4.60
3.19
3.16
3.14
N
N
N
1.00
1.01
1.01
3.19
8.00
2.03
2.05
4500
4000
3500
3000
2500
2000
1500
1000
500
0
10.5
10.0
9.5
9.0
8.5
8.0
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
f1 (ppm)

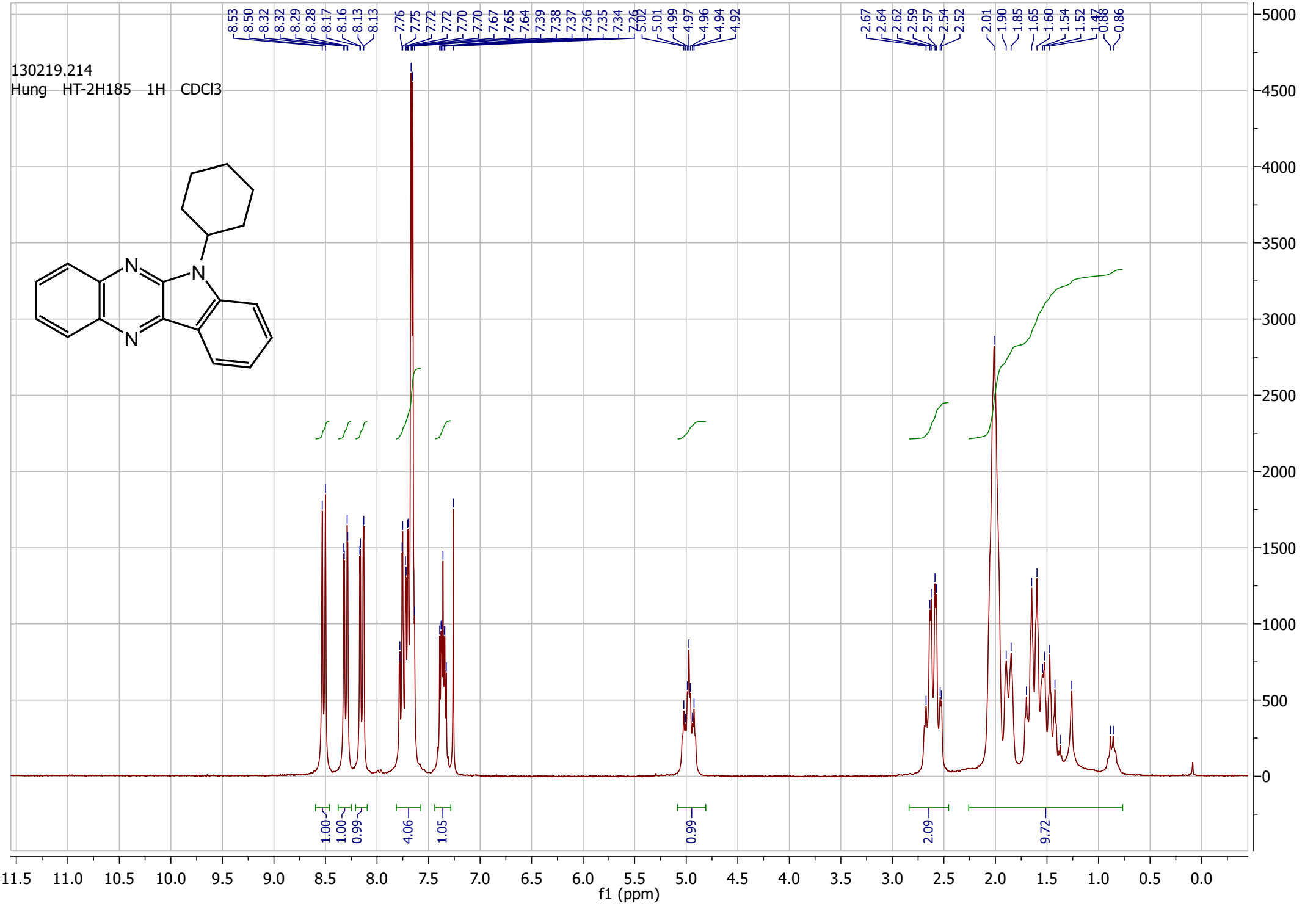

145.46
144.32
140.63
140.05
139.31
138.46
130.86
129.31
128.86
128.69
128.58
127.86
126.65
125.97
120.80
109.35
43.11
34.74
130927.205
Hung HT-3H054 13C CDCl3
N
N
N
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

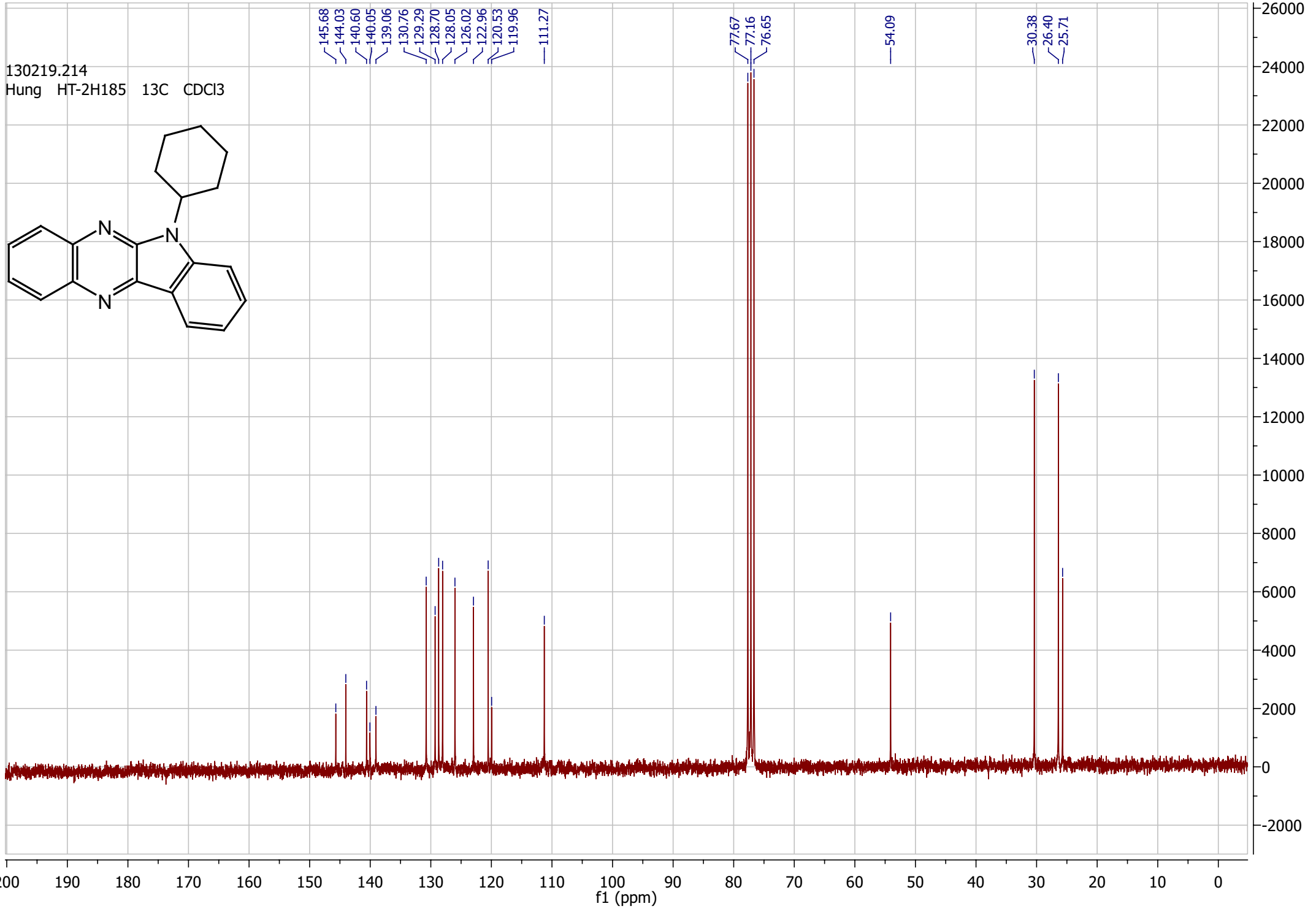

130927.205
Hung HT-3H054 Dept CDCl3
130.86
129.31
128.87
128.69
128.58
127.86
126.65
125.97
122.71
120.80
109.35
43.11
34.74
N
N
N
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

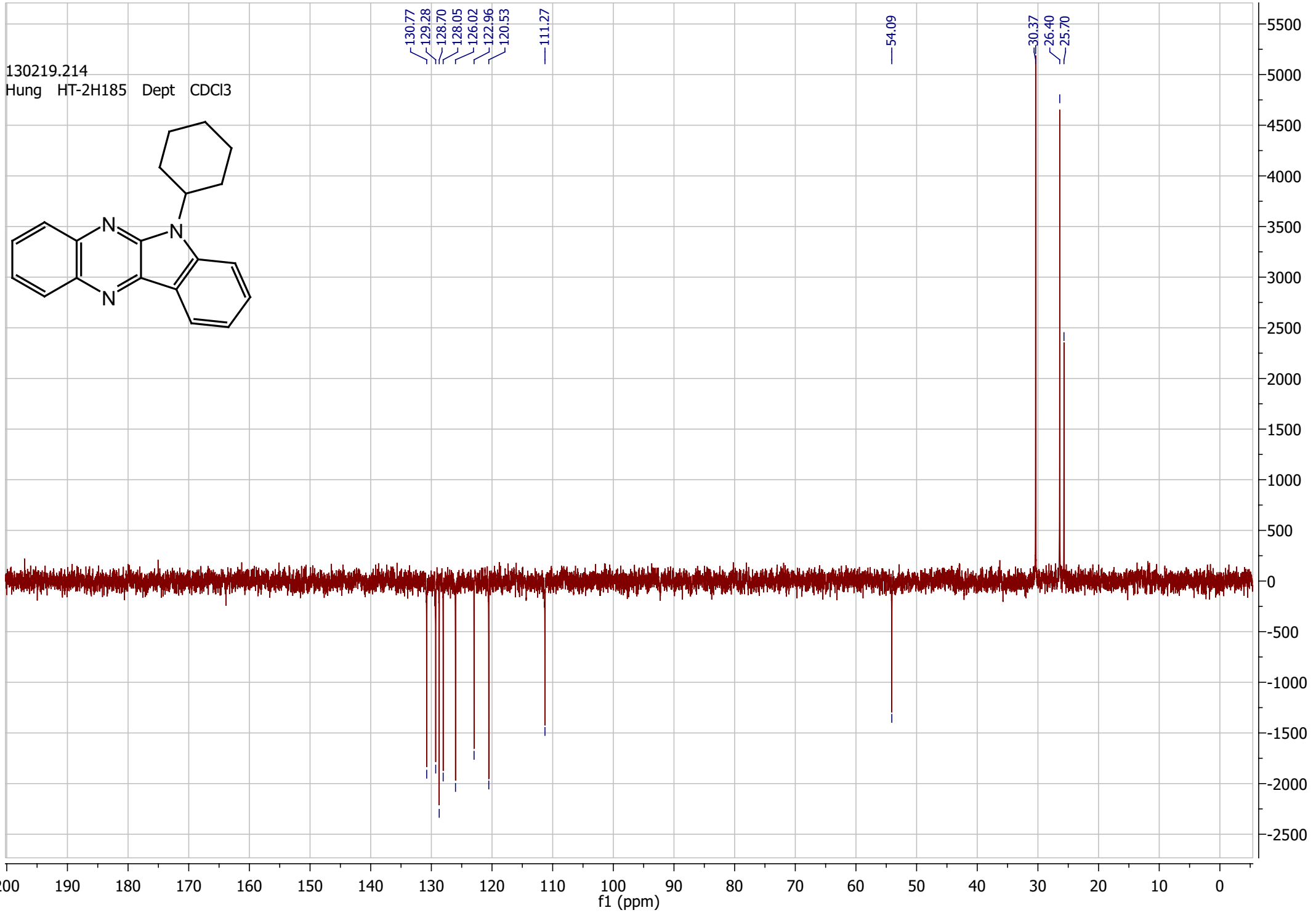

130927.u307
Hung HT-3H053 1H CDCl3
8.42 8.39 8.25 8.24 8.22 8.22 8.09 8.08 8.06 8.06 7.69 7.69 7.67 7.66 7.63 7.63 7.61 7.61 7.60 7.59 7.58 7.57 7.56 7.32 7.30 7.27 7.22 7.20 7.19 7.18 7.17 7.13 7.11 4.48 4.46 4.43 2.73 2.70 2.67 2.29 2.27 2.24 2.22 2.19
1.00 0.92 1.02 3.54 7.89 1.92 2.10 1.96
f1 (ppm)

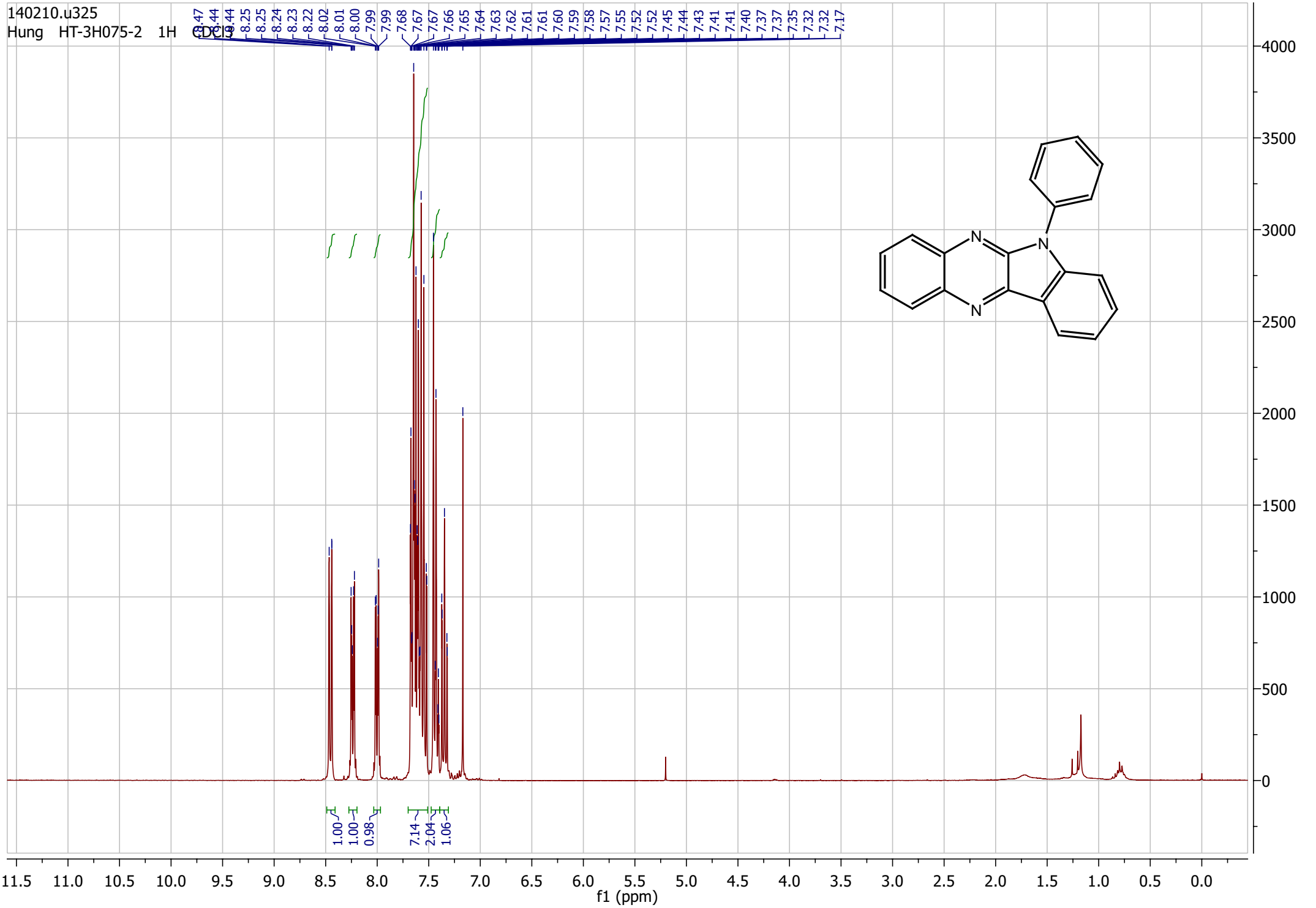

130927.204
Hung HT-3H053 13C CDCl3
145.68
144.33
141.01
140.61
140.01
139.25
130.92
129.31
128.72
128.39
128.35
127.79
126.06
125.94
120.82
109.44
41.01
33.21
29.73
N
N
N
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

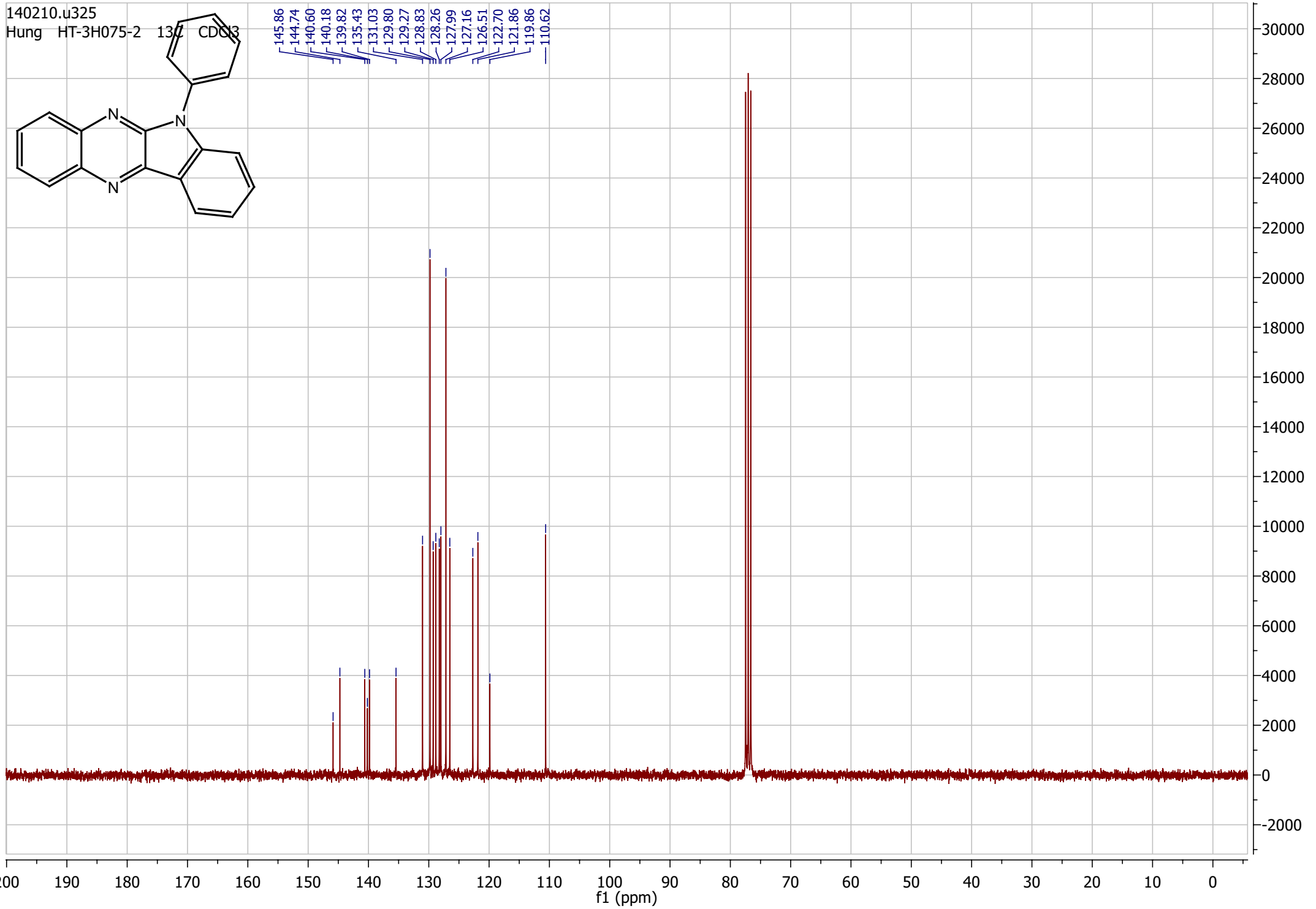

130927.204
Hung HT-3H053 Dept CDCl3
130.92
129.31
128.72
128.40
128.36
127.79
126.07
125.94
122.77
120.83
109.44
41.01
33.21
29.73
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

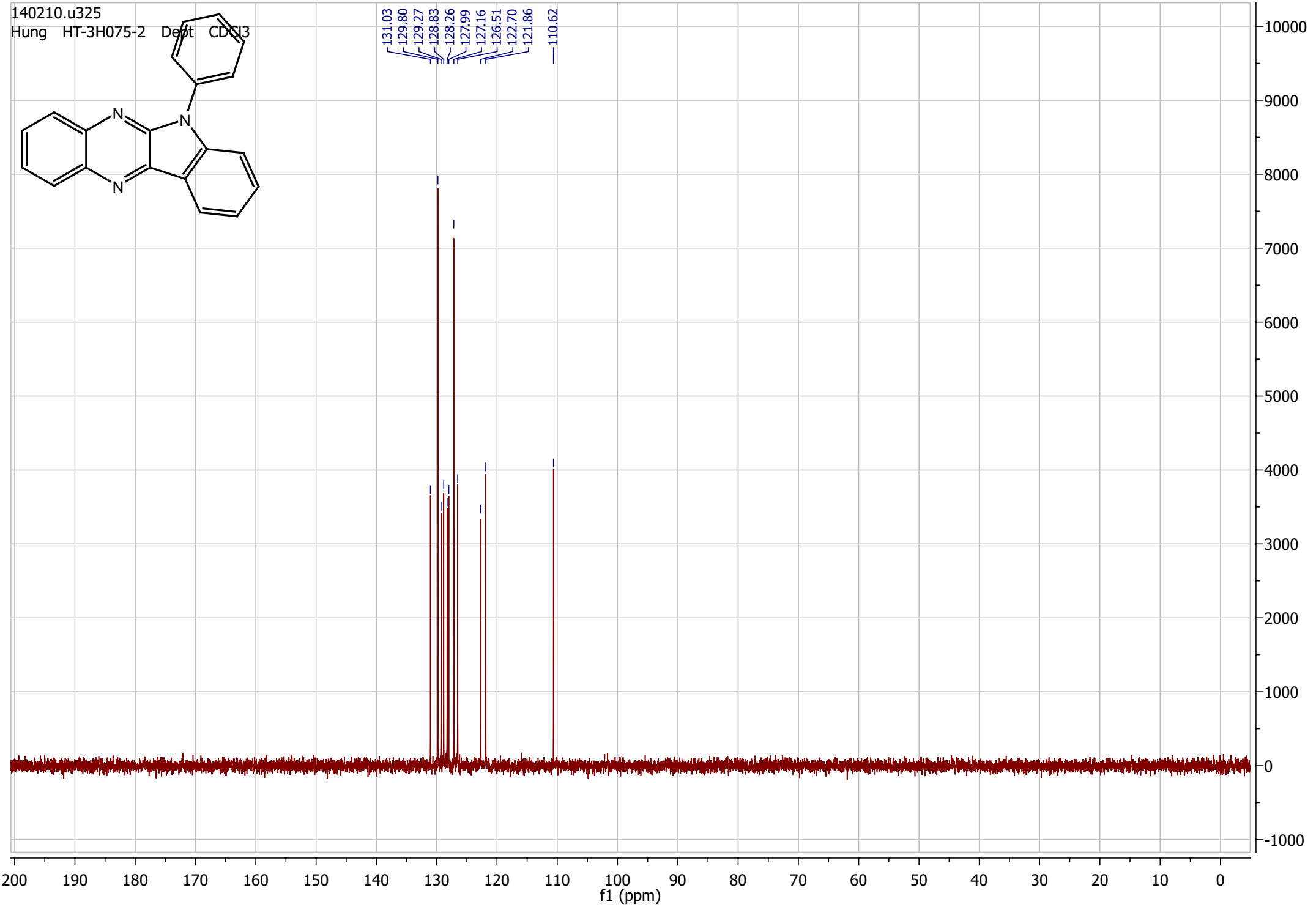

130219.214
Hung HT-2H185 1H CDCl3
8.53 8.50 8.32 8.32 8.29 8.28 8.17 8.16 8.13 8.13
7.76 7.75 7.72 7.72 7.70 7.70 7.67 7.65 7.64 7.39 7.38 7.37 7.36 7.35 7.34 7.26
5.02 5.01 4.99 4.97 4.96 4.94 4.92
2.67 2.64 2.62 2.59 2.57 2.54 2.52
2.01 1.90 1.85 1.65 1.60 1.54 1.52 1.47 0.88 0.86
N
N
N
1.00 1.00 0.99 4.06 1.05 0.99 2.09 9.72
5000 4500 4000 3500 3000 2500 2000 1500 1000 500 0
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)

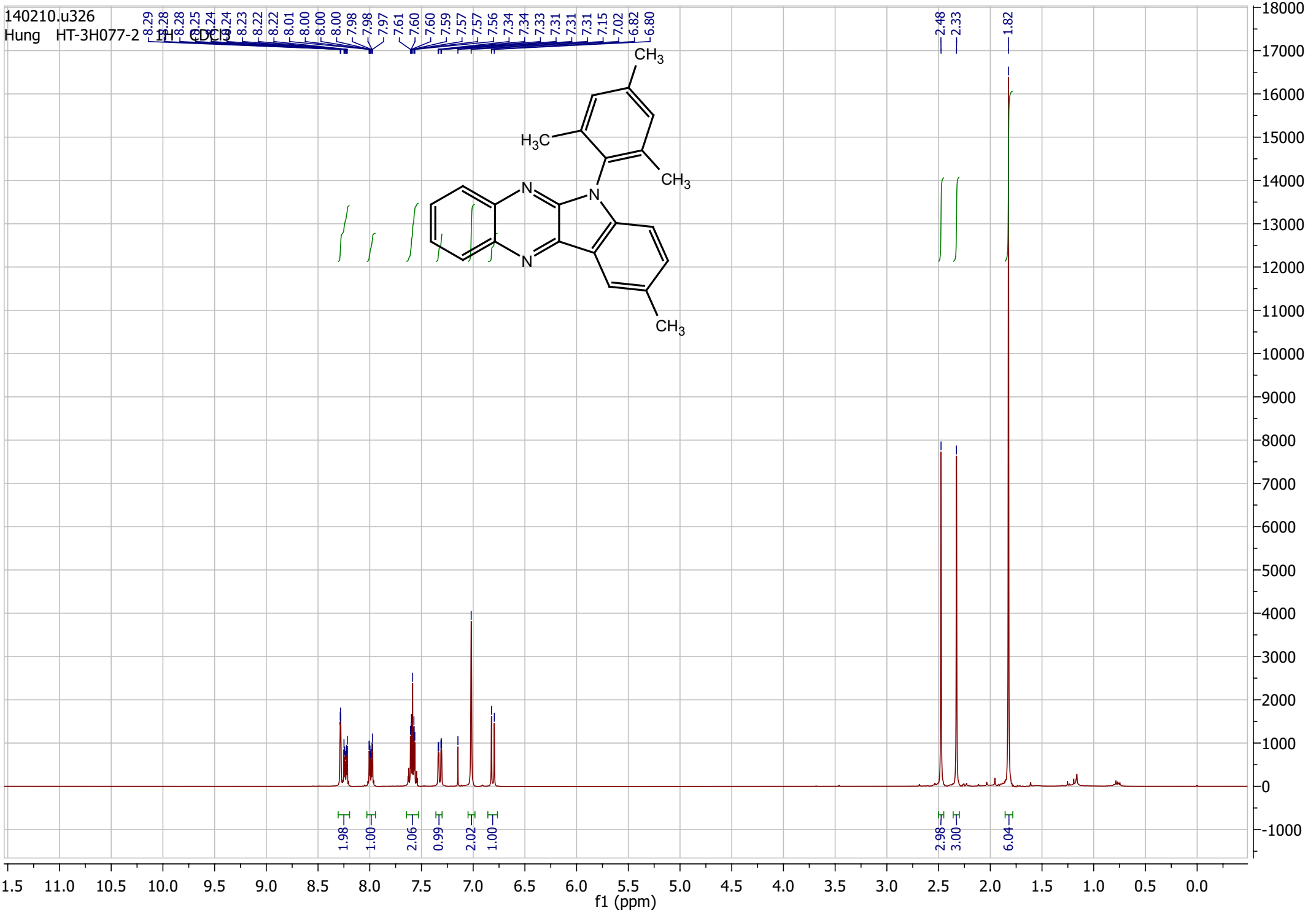

130219.214
Hung HT-2H185 13C CDCl3
145.68
144.03
140.60
140.05
139.06
130.76
129.29
128.70
128.05
126.02
122.96
120.53
119.96
111.27
77.67
77.16
76.65
54.09
30.38
26.40
25.71
N
N
N
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

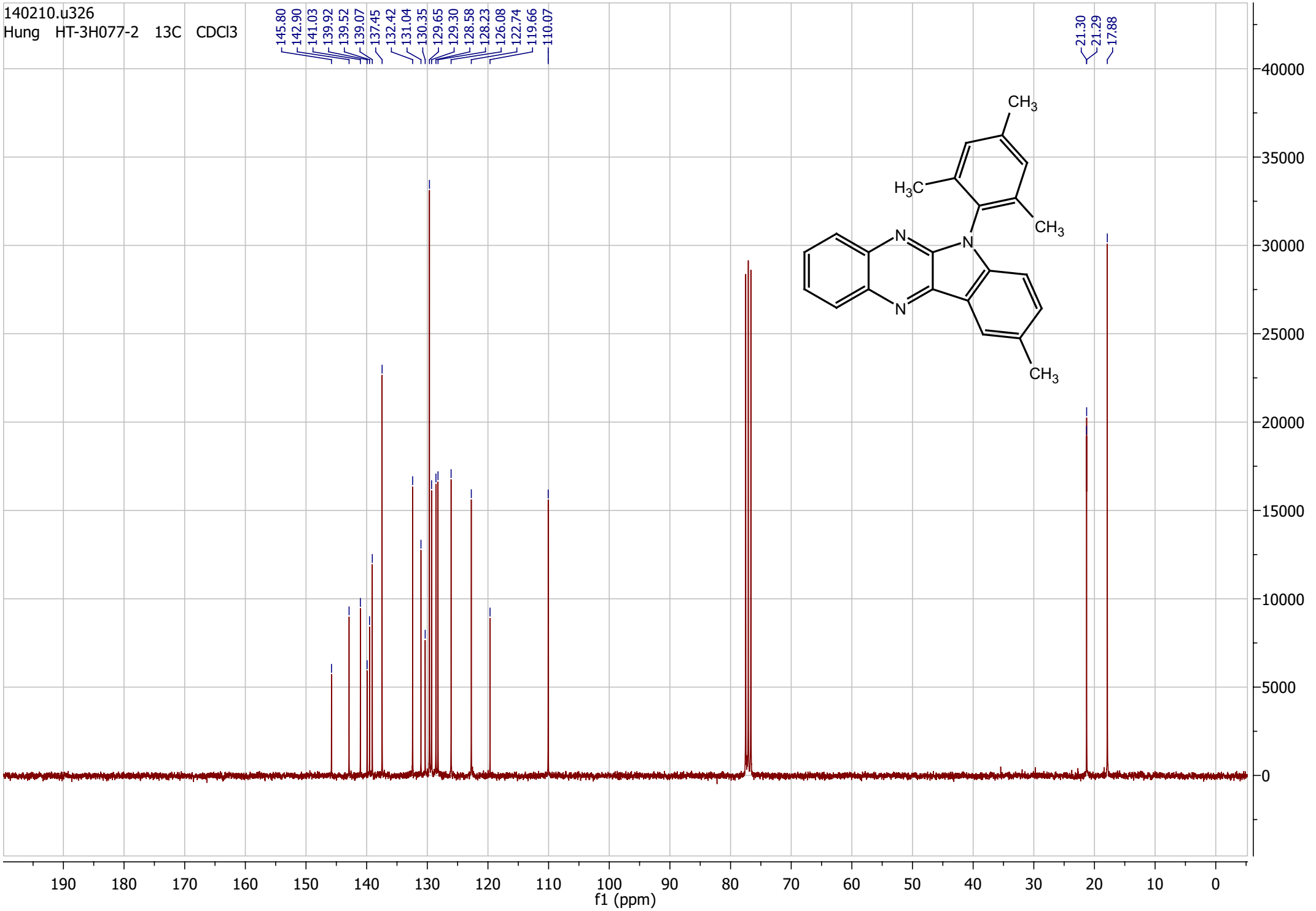

130219.214
Hung HT-2H185 Dept CDCl3
130.77
129.28
128.70
128.05
126.02
122.96
120.53
111.27
54.09
30.37
26.40
25.70
N
N
N
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


140210.u325
Hung HT-3H075-2 1H CDCl3
8.47 8.44 8.44 8.25 8.25 8.24 8.23 8.22 8.02 8.01 8.00 7.99 7.99 7.68 7.67 7.67 7.66 7.65 7.64 7.63 7.62 7.61 7.61 7.60 7.59 7.58 7.57 7.55 7.52 7.52 7.45 7.44 7.43 7.41 7.41 7.40 7.37 7.37 7.35 7.32 7.32 7.17
N
N
N
1.00 1.00 0.98 7.14 2.04 1.06
4000 3500 3000 2500 2000 1500 1000 500 0
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)

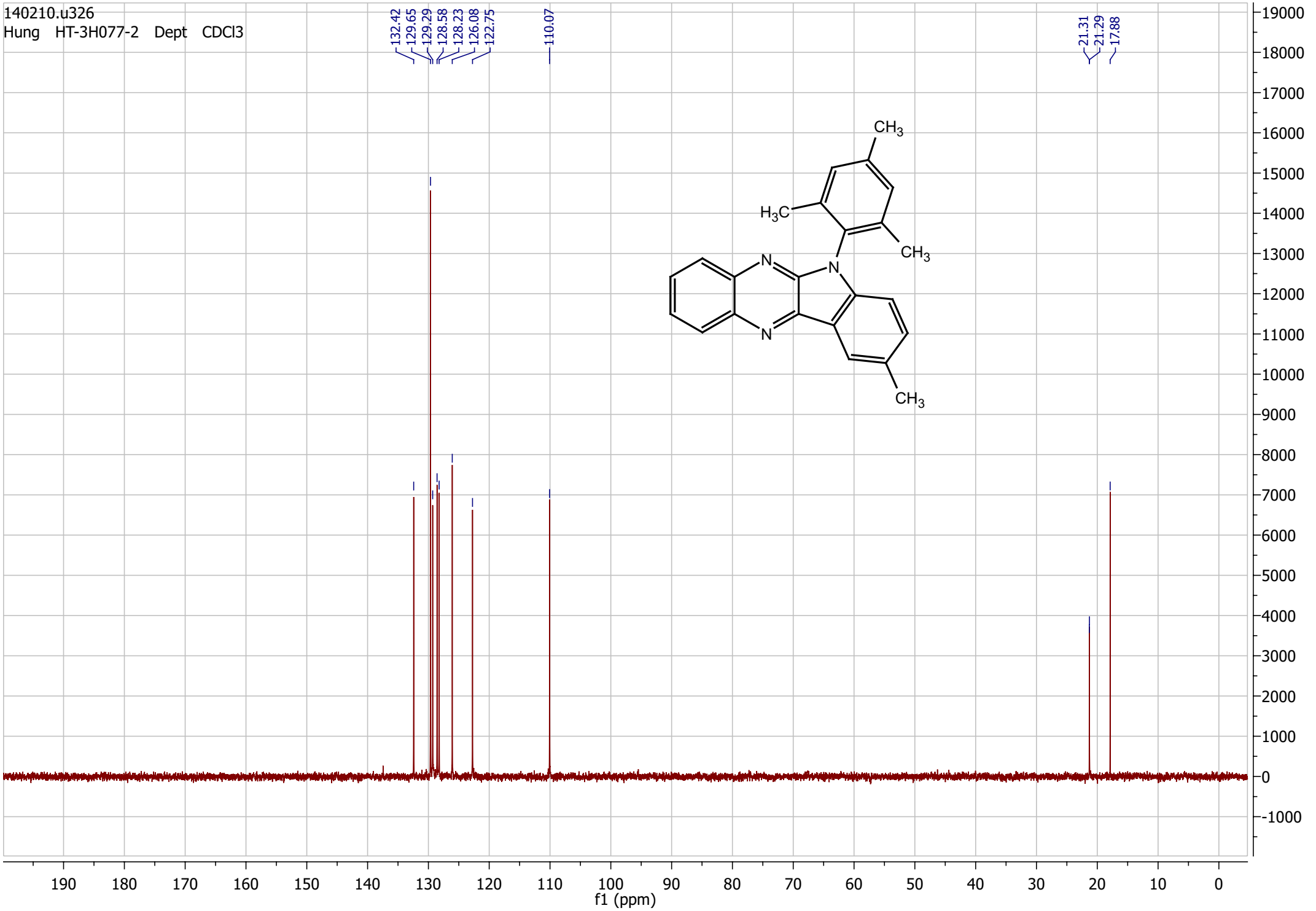

140210.u325
Hung HT-3H075-2 13C CDCl3
145.86
144.74
140.60
140.18
139.82
135.43
131.03
129.80
129.27
128.83
128.26
127.99
127.16
126.51
122.70
121.86
119.86
110.62
N
N
N
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
-2000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

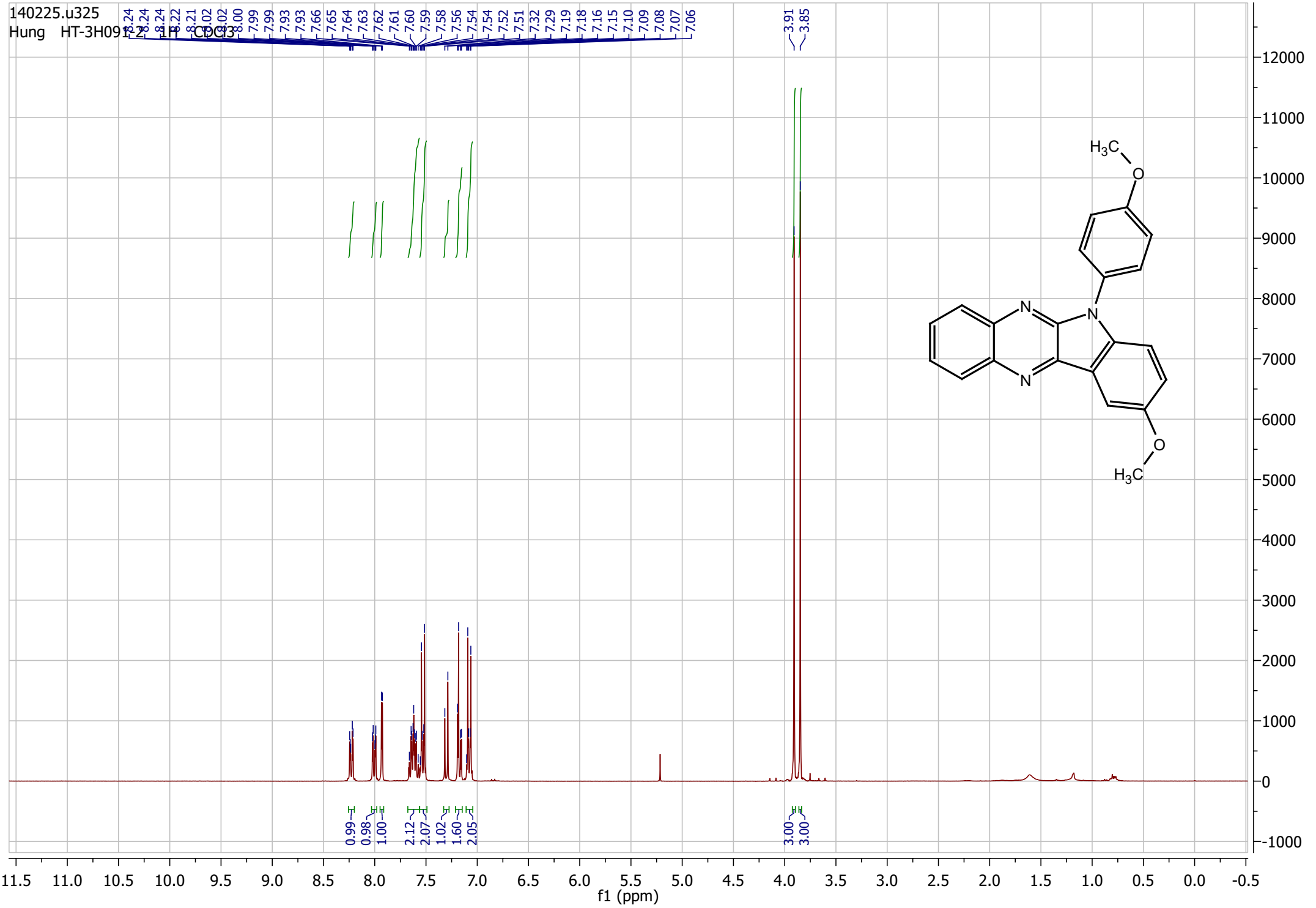

140210.u325
Hung HT-3H075-2 Dept CDCl3
131.03
129.80
129.27
128.83
128.26
127.99
127.16
126.51
122.70
121.86
110.62
N
N
N
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

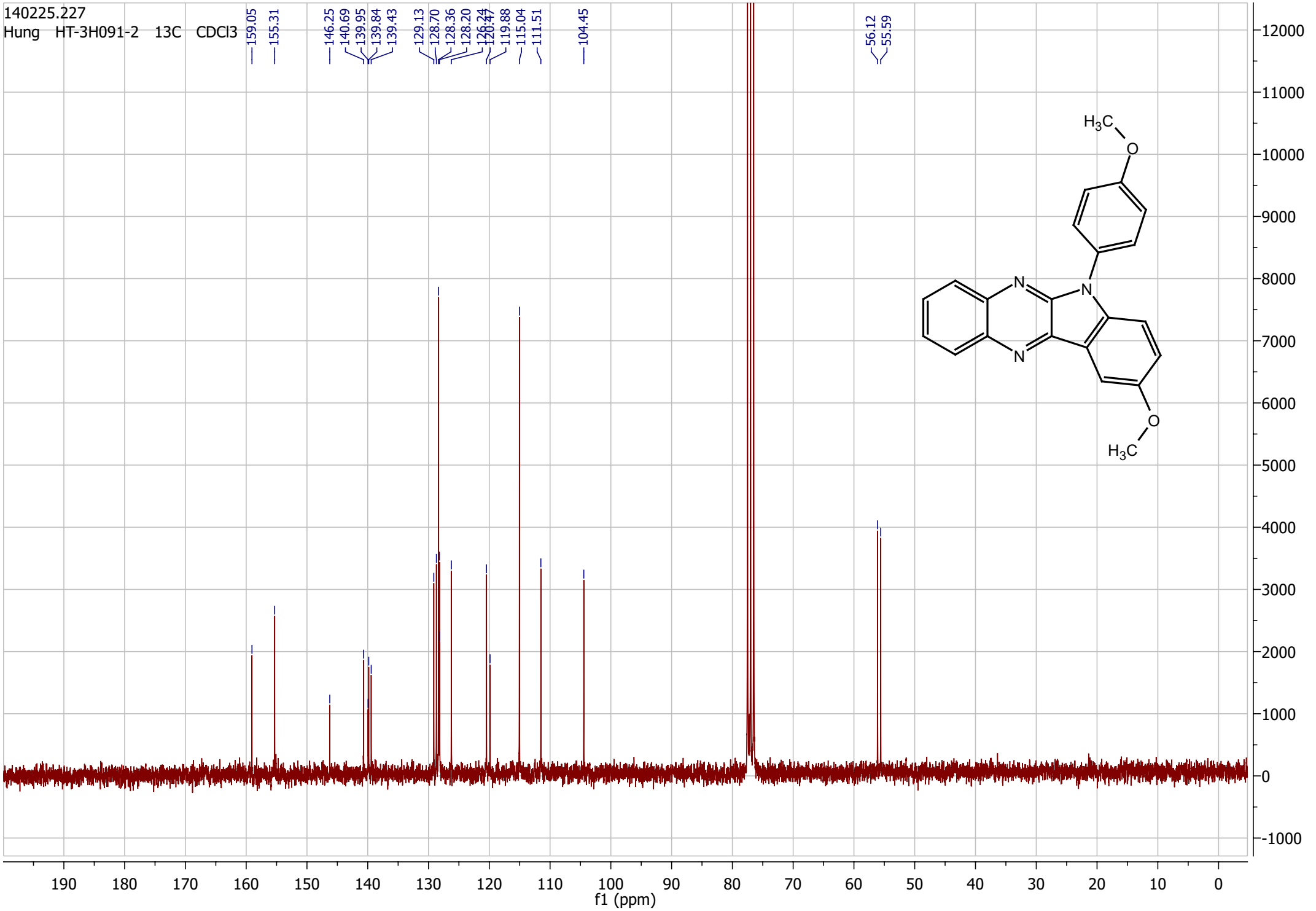

140210.u326
Hung HT-3H077-2 1H CDCl3
8.29 8.28 8.28 8.25 8.24 8.24 8.23 8.22 8.22 8.01 8.00 8.00 8.00 7.98 7.98 7.97 7.61 7.60 7.60 7.59 7.57 7.57 7.56 7.34 7.34 7.33 7.31 7.31 7.31 7.15 7.02 6.82 6.80
2.48 2.33 1.82
CH3
H3C
CH3
N
N
N
CH3
1.98 1.00 2.06 0.99 2.02 1.00
2.98 3.00 6.04
18000 17000 16000 15000 14000 13000 12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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
f1 (ppm)

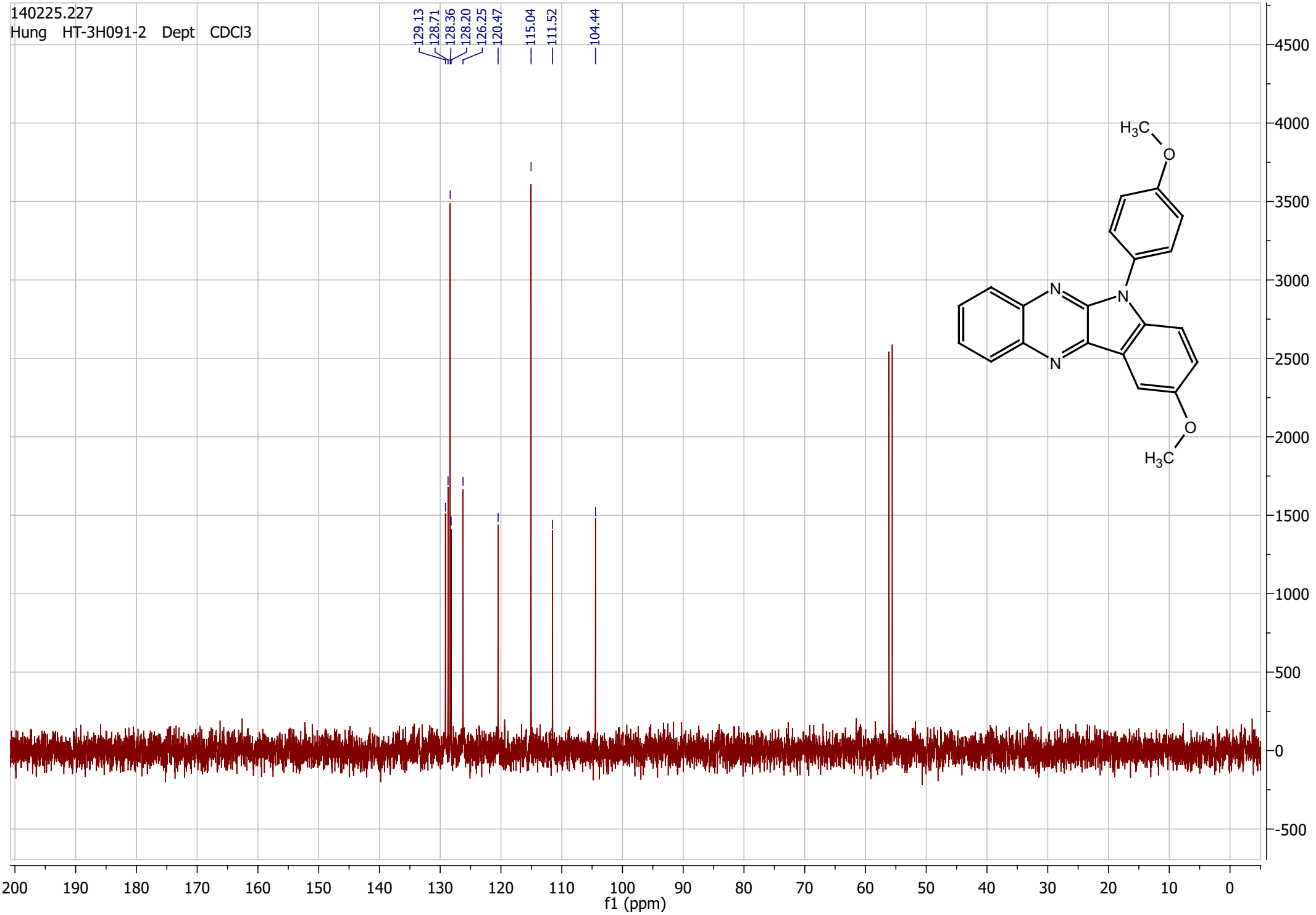

140210.u326
Hung HT-3H077-2 13C CDCl3
145.80
142.90
141.03
139.92
139.52
139.07
137.45
132.42
131.04
130.35
129.65
129.30
128.58
128.23
126.08
122.74
119.66
110.07
21.30
21.29
17.88
CH3
H3C
CH3
CH3
N
N
N
40000
35000
30000
25000
20000
15000
10000
5000
0
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

140210.u326
Hung HT-3H077-2 Dept CDCl3




140225.u325
Hung HT-3H0912-2 1H CDCl3
8.24 8.24 8.24 8.22 8.21 8.02 8.02 8.00 7.99 7.99 7.93 7.93 7.66 7.65 7.64 7.63 7.62 7.61 7.60 7.59 7.58 7.56 7.54 7.54 7.52 7.51 7.32 7.29 7.19 7.18 7.16 7.15 7.10 7.09 7.08 7.07 7.06
3.91 3.85
0.99 0.98 1.00 2.12 2.07 1.02 1.60 2.05 3.00 3.00
H3C O O CH3
N N N
12000 11000 10000 9000 8000 7000 6000 5000 4000 3000 2000 1000 0 -1000
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 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 -0.5
f1 (ppm)


140225.227
Hung HT-3H091-2 13C CDCl3
159.05
155.31
146.25
140.69
139.95
139.84
139.43
129.13
128.70
128.36
128.20
126.24
120.47
119.88
115.04
111.51
104.45
56.12
55.59
H3C
O
N
N
N
O
H3C
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


140225.227
Hung HT-3H091-2 Dept CDCl3
129.13
128.71
128.36
128.20
126.25
120.47
115.04
111.52
104.44
H3C
O
N
N
N
O
H3C
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)