Three-Component Solvent-free Synthesis of 1*H*-pyrazol-5-(4*H*)-one-Based Heterocyclic Ketene Aminals Derivatives

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Supporting Information

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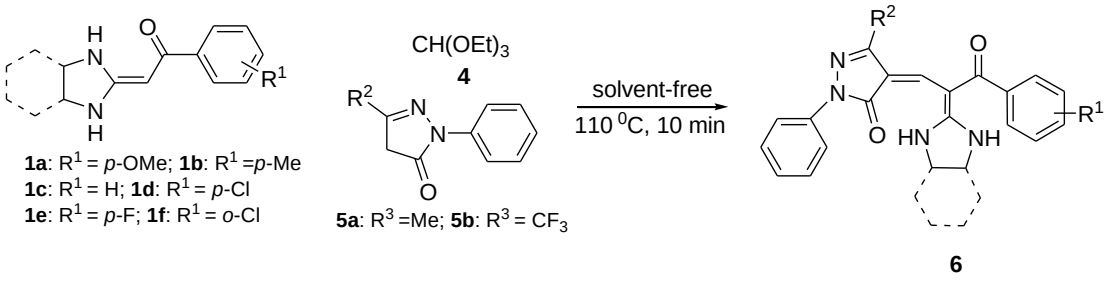
General Information

All compounds were fully characterized by spectroscopic data. The NMR spectra were recorded on the Bruker DRX400 or DRX500, chemical shifts (δ) are expressed in ppm, and J values are given in Hz, DMSO-d_6 and $CDCl_3$ were used as solvent. IR spectra were recorded on a FT-IR Thermo Nicolet Avatar 360 using a KBr pellet. The reactions were monitored by thin-layer chromatography (TLC) using silica gel GF_{254}. The melting points were determined on XT-4A melting point apparatus and are uncorrected. HRMs were performed on a Agilent LC/Msd TOF and Monosiotopic Mass instrument. All chemicals and solvents were used as received without further purification unless otherwise stated. Column chromatography was performed on silica gel (200–300 mesh). The raw material **1**–**3** was synthesized according to the literature.[1]

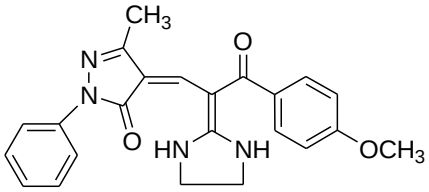
General Procedure for the Preparation of *α,β*-Unsaturated Pyrazolone-Based HKAs Derivative 6 *via* Three-Component Reaction in One-Pot



HKAs **1** (1.0 mmol), triethoxy-methane **4** (2.0 mmol) and 1-phenyl-1*H*-pyrazol-5(4*H*)-one derivatives **5** (1.2 mmol) were charged into a 25 mL round-bottom flask and the mixture was heated to 110°C for about 10 minutes and monitored by TLC. Until the substrate HKA has been used up. Then reaction mixture was cooled to room temperature, filtered and washed by 95% EtOH to give pure product with 85–95% yield. The products were further identified by FTIR, NMR and HRMS, being in good agreement with the assigned structures.

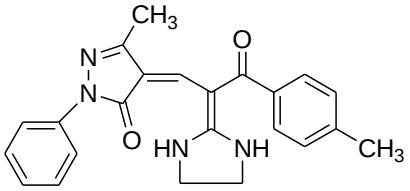
Spectroscopic Data of *α,β*-Unsaturated Pyrazolone-Based HKAs Derivative 6

(*Z*)-4-(2-(Imidazolidin-2-ylidene)-3-(4-methoxyphenyl)-3-oxopropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (6a)



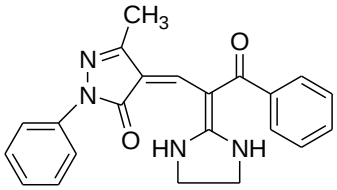
Saffron yellow solid; Mp 204−205.5 °C; IR (KBr): 3307, 2965, 1625, 1593, 1496, 1427, 1392, 1294, 1252, 1176, 1127, 992, 841, 765 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.95 (s, 3H, CH_3), 3.76−3.79 (m, 4H, NCH_2CH_2N), 3.78 (s, 3H, OCH_3), 6.95−6.97 (m, 2H, ArH), 7.00−7.04 (m, 1H, ArH), 7.28−7.32 (m, 2H, ArH), 7.42 (s, 1H, CH), 7.52−7.55 (m, 2H, ArH), 7.89−7.91 (m, 2H, ArH), 9.67 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.3 (CH_3), 43.4 (NCH_2), 43.4 (CH_2N), 55.3 (OCH_3), 113.3, 117.9, 122.9, 128.5, 130.8, 130.8 (=*C*H), 132.7, 139.9, 142.9, 150.4, 161.4 (HN*C*=), 162.8 (CH_3OC=), 165.9 (N*C*=O), 191.8 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{22}N_4O_3$ [M], 402.1692; found, 402.1690.

(*Z*)-4-(2-(Imidazolidin-2-ylidene)-3-oxo-3-*p*-tolylpropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (6b)



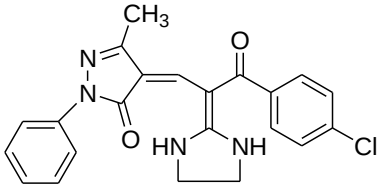
Saffron yellow solid; Mp 238−241 °C; IR (KBr): 3321, 1625, 1593, 1496, 1397, 1257, 1185, 1128, 1048, 990, 763 cm^{-1}; ^{1}H NMR (500 MHz, DMSO-d_6 +$HClO_4$): δ = 2.26 (s, 3H, CH_3), 2.33 (s, 3H, CH_3), 3.82−3.85 (m, 4H, NCH_2CH_2N), 7.27−7.29 (m, 3H, CH and ArH), 7.43−7.49 (m, 5H, ArH), 7.59−7.61 (m, 2H, ArH), 9.72 (br, 2H, NH); ^{13}C NMR (125 MHz, DMSO-d_6 + $HClO_4$): δ = 11.5 (CH_3), 21.4 ($PhCH_3$), 44.4 (NCH_2), 44.4 (CH_2N), 100.8, 114.3, 120.9, 126.7, 129.4, 129.5, 129.5 (=*C*H), 135.2, 135.7, 139.7, 143.3, 150.7, 158.8 (HN*C*=), 165.7 (N*C*=O), 191.8 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{22}N_4O_2$ [M], 386.1743; found, 386.1735.

(*Z*)-4-(2-(Imidazolidin-2-ylidene)-3-oxo-3-phenylpropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (6c)



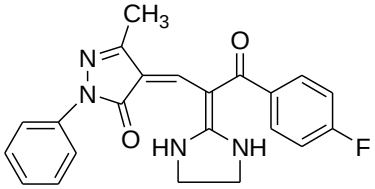
Saffron yellow solid; Mp 231−235 °C; IR (KBr): 3288, 2878, 1623, 1585, 1495, 1428, 1258, 1130, 1037, 994, 751 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.84 (s, 3H, CH_3), 3.87−3.90 (m, 4H, NCH_2CH_2N), 7.18−7.22 (m, 1H, ArH), 7.42−7.55 (m, 7H, ArH), 7.63 (s, 1H, CH), 7.89−7.92 (m, 2H, ArH), 11.34 (br, 2H, NH); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 13.2 (*C*H_3), 43.8 (N*C*H_2), 43.8 (*C*H_2N), 101.5, 106.5, 120.4, 125.0, 128.3, 128.7, 128.7, 130.9, 138.8, 140.8, 147.9, 152.8, 163.5 (HN*C*=), 165.5 (N*C*=O), 198.1 (*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{20}N_4O_2$ [M], 372.1586; found, 372.1590.

(*Z*)-4-(3-(4-Chlorophenyl)-2-(imidazolidin-2-ylidene)-3-oxopropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (6d)



Saffron yellow solid; Mp 233−237 °C; IR (KBr): 3321, 2886, 1631, 1591, 1494, 1428, 1392, 1254, 1182, 1128, 1088, 1044, 993, 823, 763 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 2.27 (s, 3H, CH_3), 3.81−3.86 (m, 4H, NCH_2CH_2N), 7.23−7.26 (m, 1H, ArH), 7.41−7.45 (m, 4H, ArH), 7.47−7.50 (m, 3H, ArH), 7.52 (s, 1H, CH), 7.67−7.69 (m, 2H, ArH), 9.71 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 11.2 (*C*H_3), 44.0 (N*C*H_2), 44.0 (*C*H_2N), 100.9, 112.5, 120.5, 126.2, 128.5, 129.1, 129.2, 130.9, 135.4, 136.5, 137.2, 150.5, 158.6 (HN*C*=), 165.1 (N*C*=O), 190.6 (*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{19}ClN_4O_2$ [M], 406.1197; found, 406.1191.

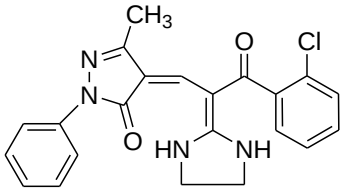
(*Z*)-4-(3-(4-Fluorophenyl)-2-(imidazolidin-2-ylidene)-3-oxopropylidene)-3-methyl-1-*p*henyl-1*H*-pyrazol-5(4*H*)-one (6e)



Saffron yellow solid; Mp 202−204 °C; IR (KBr): 3333, 2900, 1626, 1591, 1496, 1429, 1395, 1338, 1254, 1127, 1044, 993, 841, 765 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.97 (s, 3H, CH_3), 3.74−3.78 (m, 4H, NCH_2CH_2N), 6.99−7.03 (m, 1H, ArH), 7.19−7.24 (m, 2H, ArH), 7.27−7.31 (m, 2H, ArH), 7.41 (s, 1H, CH), 7.57−7.61 (m, 2H, ArH), 7.84−7.86 (m, 2H, ArH), 9.49 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.1 (*C*H_3), 43.4 (N*C*H_2), 43.4 (*C*H_2N), 105.1, 114.8 (d, *J* = 21.5 Hz), 117.8, 123.0, 128.5, 131.0, 137.1, 139.8, 142.9, 150.3, 162.1, 162.7 (HN*C*=), 164.5,

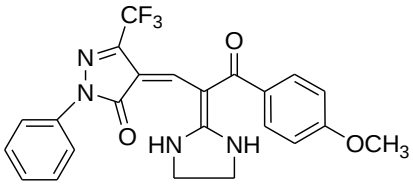
165.8 (N*C*=O), 191.0 (*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{19}FN_4O_2$ [M], 390.1492; found, 390.1492.

(*Z*)-4-(3-(2-Chlorophenyl)-2-(imidazolidin-2-ylidene)-3-oxopropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (6f)



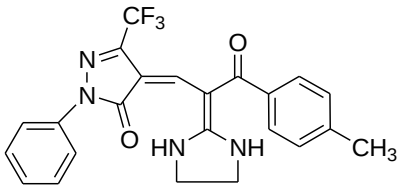
Saffron yellow solid; Mp 204−207 °C; IR (KBr): 3278, 1886, 1625, 1588, 1497, 1434, 1282, 1243, 1133, 1042, 996, 759 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 1.69 (s, 3H, CH_3), 3.80−3.83 (m, 4H, NCH_2CH_2N), 7.04−7.08 (m, 2H, ArH), 7.31−7.35 (m, 3H, CH and ArH), 7.41−7.48 (m, 2H, ArH), 7.53−7.55 (m, 1H, ArH), 7.88−7.89 (m, 2H, ArH), 10.09 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 12.6 (*C*H_3), 43.4 (N*C*H_2), 43.4 (*C*H_2N), 101.4, 105.2, 118.3, 123.6, 127.4, 128.6, 128.6, 129.4, 129.5, 130.6, 139.4, 139.9, 144.6, 150.7, 162.7 (HN*C*=), 164.3 (N*C*=O), 190.9 (*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{19}ClN_4O_2$ [M], 406.1197; found, 406.1191.

(*Z*)-4-(2-(Imidazolidin-2-ylidene)-3-(4-methoxyphenyl)-3-oxopropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (6g)



Saffron yellow solid; Mp 227−230 °C; IR (KBr): 3205, 2965, 1640, 1594, 1500, 1414, 1285, 1112, 1033, 982, 837, 761 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 3.87 (s, 3H, OCH_3), 3.90−3.94 (m, 4H, NCH_2CH_2N), 6.92−6.95 (m, 2H, ArH), 7.24−7.27 (m, 1H, ArH), 7.42−7.46 (m, 2H, ArH), 7.59−7.62 (m, 2H, ArH), 7.81 (s, 1H, CH), 7.89−7.91 (m, 2H, ArH), 11.18 (br, 2H, NH); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 44.0 (N*C*H_2), 44.0 (*C*H_2N), 55.5 (O*C*H_3), 99.6, 105.3, 113.6, 119.5, 121.3, 126.0, 128.8, 128.8, 131.7, 131.9, 131.9, 138.5, 146.9, 162.9 (HN*C*=), 165.5 (N*C*=O), 197.1 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{19}F_3N_4O_3$ [M], 456.1409; found, 456.1407.

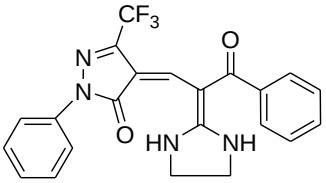
(*Z*)-4-(2-(Imidazolidin-2-ylidene)-3-oxo-3-p-tolylpropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (6h)



Saffron yellow solid; Mp 207−209 °C; IR (KBr): 3292, 1889, 1634, 1531, 1499, 1441,

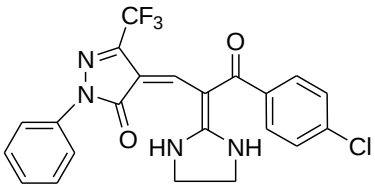
1376, 1278, 1180, 1122, 1040, 972, 766 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 2.42 (s, 3H, CH_3), 3.90−3.94 (m, 4H, NCH_2CH_2N), 7.23−7.27 (m, 3H, ArH), 7.41−7.49 (m, 4H, ArH), 7.83 (s, 1H, CH), 7.88−7.89 (m, 2H, ArH), 11.18 (br, 2H, NH); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 21.6 (Ph*C*H_3), 44.0 (N*C*H_2), 44.0 (*C*H_2N), 99.9, 105.3, 119.2, 121.3, 121.9, 126.1, 128.8, 129.0, 129.4, 136.6, 138.4, 142.6, 147.5, 163.0 (HN*C*=), 165.4 (N*C*=O), 198.3 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{19}F_3N_4O_2$ [M], 440.1460; found, 440.1452.

(*Z*)-4-(2-(Imidazolidin-2-ylidene)-3-oxo-3-phenylpropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (6i)



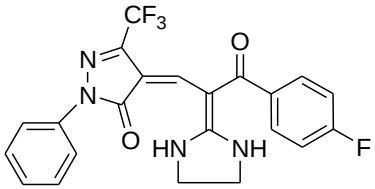
Saffron yellow solid; Mp 233−235 °C; IR (KBr): 3288, 2886, 1632, 1523, 1499, 1437, 1370, 1272, 1183, 1121, 968, 758 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ = 3.91−3.95 (m, 4H, NCH_2CH_2N), 7.24−7.28 (m, 1H, ArH), 7.41−7.47 (m, 4H, ArH), 7.52−7.56 (m, 3H, ArH), 7.82 (s, 1H, CH), 7.87−7.89 (m, 2H, ArH), 11.19 (br, 2H, NH); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 43.9 (N*C*H_2), 43.9 (*C*H_2N), 100.2, 105.0, 119.1, 121.3, 121.8, 126.1, 128.4, 128.8, 128.9, 131.6, 138.4, 139.6, 147.8, 163.5 (HN*C*=), 165.3 (N*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{17}F_3N_4O_2$ [M], 426.1304; found, 426.1296.

(*Z*)-4-(3-(4-Chlorophenyl)-2-(imidazolidin-2-ylidene)-3-oxopropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (6j)



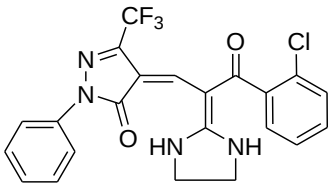
Saffron yellow solid; Mp 230−233 °C; IR (KBr): 3221, 2969, 1640, 1583, 1499, 1403, 1282, 1176, 1114, 982, 836, 757 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 3.80−3.87 (m, 4H, NCH_2CH_2N), 7.14 (m, 1H, ArH), 7.37 (m, 3H, ArH), 7.54 (m, 4H, CH and ArH), 7.89 (m, 2H, ArH), 9.59 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 43.7 (N*C*H_2), 43.7 (*C*H_2N), 106.3, 118.9, 120.0, 122.7, 124.4, 125.4, 128.4, 128.7, 130.2, 135.9, 137.9, 139.3, 141.1, 161.7 (HN*C*=), 166.3 (N*C*=O), 190.3 (*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{16}ClF_3N_4O_2$ [M], 460.0914; found, 460.0915.

(*Z*)-4-(3-(4-Fluorophenyl)-2-(imidazolidin-2-ylidene)-3-oxopropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (6k)



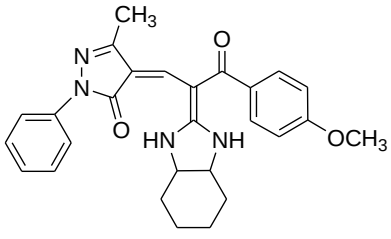
Saffron yellow solid; Mp 237−240 °C; IR (KBr): 3305, 2900, 1633, 1606, 1523, 1500, 1442, 1377, 1274, 1236, 1184, 1123, 1044, 972, 841, 765 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 3.82−3.87 (m, 4H, NCH_2CH_2N), 7.12−7.14 (m, 1H, ArH), 7.28−7.40 (m, 5H, CH and ArH), 7.57−7.62 (m, 2H, ArH), 7.88−7.94 (m, 2H, ArH), 9.61 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 43.7 (NCH_2), 43.7 (CH_2N), 96.7, 106.5, 115.3 (d, J = 23.6 Hz), 118.9, 120.1, 122.8, 124.4, 128.7, 131.1, 135.7, 139.4, 141.1, 161.7, 162 (HN*C*=).4, 166.5 (N*C*=O), 190.4 (*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{16}F_4N_4O_2$ [M], 444.1209; found, 444.1212.

(*Z*)-4-(3-(2-Chlorophenyl)-2-(imidazolidin-2-ylidene)-3-oxopropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (6l)



Saffron yellow solid; Mp 224−226 °C; IR (KBr): 3316, 2893, 1633, 1591, 1431, 1377, 1289, 1249, 1184, 1114, 1044, 971, 826, 757 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 3.86−3.90 (m, 4H, NCH_2CH_2N), 7.10 (s, 1H, CH), 7.11−7.15 (m, 1H, ArH), 7.32−7.40 (m, 3H, ArH), 7.44−7.49 (m, 2H, ArH), 7.54−7.56 (m, 1H, ArH), 7.87−7.89 (m, 2H, ArH), 9.64 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 43.7 (NCH_2), 43.7 (CH_2N), 97.2, 106.9, 119.0, 119.8, 122.5, 124.5, 127.3, 128.6, 128.7, 129.6, 130.9, 138.8, 139.3, 142.2, 161.7 (HN*C*=), 165.2 (N*C*=O), 190.1 (*C*=O); HRMS (EI): *m/z* calcd for $C_{22}H_{16}ClF_3N_4O_2$ [M], 460.0914; found, 460.0912.

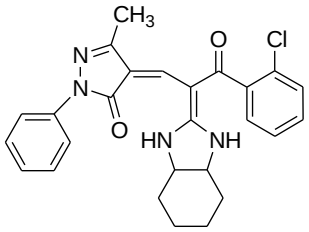
(*Z*)-4-(2-(1*H*-benzo[d]imidazol-2(3*H*,3a*H*,4*H*,5*H*,6*H*,7*H*,7a*H*)-ylidene)-3-(4-methoxyphenyl)-3-oxopropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (6m)



Saffron yellow solid; Mp 206−207.5 °C; IR (KBr): 3264, 2933, 1617, 1583, 1500, 1444, 1388, 1349, 1257, 1171, 1138, 1095, 779 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 1.27−1.30 (m, 2H, CH_2), 1.45−1.49 (m, 2H, CH_2), 1.71−1.75 (m, 2H, CH_2), 2.06−2.11 (m, 2H, CH_2), 2.28 (s, 3H, CH_3), 3.42−3.46 (m, 2H, NCHCHN), 3.82 (s, 3H, OCH_3), 6.96−6.99 (m, 2H, ArH), 7.22−7.26 (m, 1H, ArH), 7.39−7.47 (m, 4H,

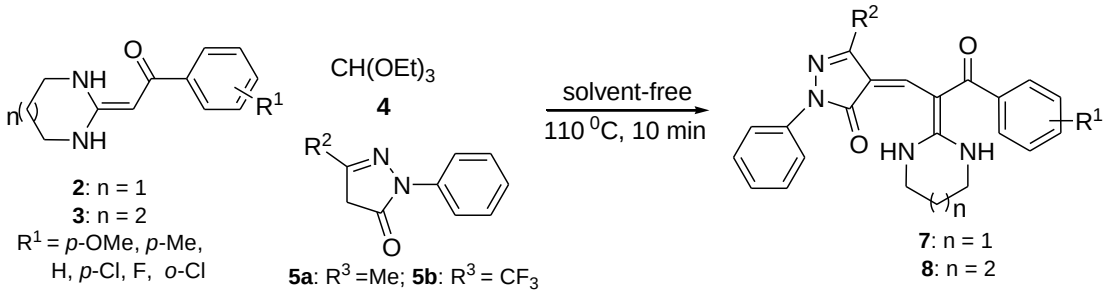
ArH), 7.51 (s, 1H, CH), 7.67−7.69 (m, 2H, ArH), 9.99 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 11.2 (*C*H_3), 23.4 (NCHCH$_2$*C*H$_2$), 23.4 (*C*H$_2$CH$_2$CHN), 28.3 (NCH*C*H$_2$, 28.3 (*C*H$_2$CHN), 55.5 (N*C*H), 55.5 (*C*HN), 64.1, 100.9, 113.7, 120.5, 121.4, 126.2, 129.1, 129.3, 130.3, 131.5, 135.4, 150.4, 158.5, 162.8 (HN*C*=), 166.9 (N*C*=O), 190.5 (*C*=O); HRMS (EI): *m/z* calcd for $C_{27}H_{28}N_4O_3$ [M], 456.2161; found, 456.2157.

(*Z*)-4-(2-(1*H*-benzo[d]imidazol-2(3*H*,3a*H*,4*H*,5*H*,6*H*,7*H*,7a*H*)-ylidene)-3-(2-chlor ophenyl)-3-oxopropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (6n)



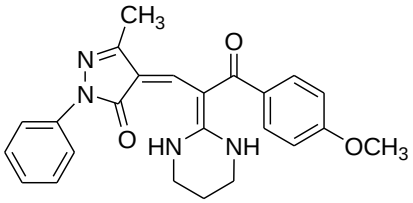
Saffron yellow solid; Mp 204−207.5 °C; IR (KBr): 3283, 2933, 1624, 1583, 1537, 1494, 1437, 1396, 1367, 1277, 1137, 756 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.31−1.34 (m, 2H, CH$_2$), 1.38−1.39 (m, 2H, CH$_2$), 1.57 (m, 2H, CH$_2$), 1.69 (s, 3H, CH$_3$), 1.73 (m, 2H, CH$_2$), 4.11 (m, 2H, NCHCHN), 7.04−7.09 (m, 2H, ArH), 7.31−7.36 (m, 2H, ArH), 7.38 (s, 1H, CH), 7.41−7.47 (m, 2H, ArH), 7.52−7.54 (m, 1H, ArH), 7.86−7.88 (m, 2H, ArH), 10.06 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 12.6 (*C*H$_3$), 19.3 (NCHCH$_2$*C*H$_2$), 19.3 (*C*H$_2$CH$_2$CHN), 25.8 (NCH*C*H$_2$), 25.8 (*C*H$_2$CHN), 54.3 (N*C*H), 54.3 (*C*HN), 101.6, 105.4, 118.2, 123.6, 127.4, 128.6, 128.7, 129.4, 129.5, 130.5, 139.4, 140.0, 144.1, 150.7, 162.7 (HN*C*=), 164.2 (N*C*=O), 191.0 (*C*=O); HRMS (EI): *m/z* calcd for $C_{26}H_{25}ClN_4O_2$ [M], 460.1666; found, 460.1679.

General Procedure for the Preparation of *α,β*-Unsaturated Pyrazolone-Based HKAs Derivative 7−8 *via* Three-Component Reaction in One-Pot



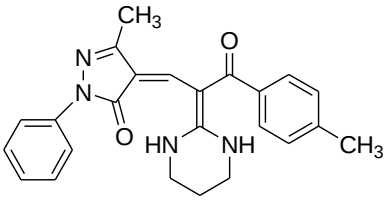
HKAs **2**−**3** (1.0 mmol), triethoxy-methane **4** (2.0 mmol) and 1-phenyl-1*H*-pyrazol-5(4*H*)-one derivatives **5** (1.2 mmol) were charged into a 25 mL round-bottom flask and the mixture was heated to 110°C for about 10 minutes and monitored by TLC. Until the substrate HKA has been used up. Then reaction mixture was cooled to room temperature, filtered and washed by 95% EtOH to give pure product with 89–96% yield. The products were further identified by FTIR, NMR and HRMS, being in good agreement with the assigned structures.

(*Z*)-4-(3-(4-Methoxyphenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (7a)



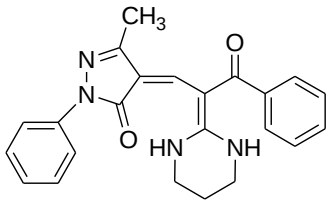
Saffron yellow solid; Mp 224−229 °C; IR (KBr): 3263, 2962, 1635, 1597, 1500, 1461, 1359, 1309, 1265, 1166, 1030, 997, 837, 754 cm^{-1}; ^1H NMR (500 MHz, DMSO-d_6): δ = 1.99 (s, 3H, CH_3), 1.97−2.06 (m, 2H, CH_2), 3.39−3.43 (m, 4H, NCH_2CH_2N), 3.84 (s, 3H, OCH_3), 6.99−7.04 (m, 3H, ArH), 7.27 (s, 1H, CH), 7.31−7.34 (m, 2H, ArH), 7.53−7.55 (m, 2H, ArH), 8.03−8.04 (m, 2H, ArH), 9.03 (br, 2H, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ = 13.6 (CH_3), 17.8 (CH_2), 38.2 (NCH_2), 38.2 (CH_2N), 55.7 (OCH_3), 101.1, 109.9, 113.6, 117.7, 122.4, 128.7, 130.7, 133.2, 141.0, 141.3, 150.0, 161.3, 161.8 (HN*C*=), 163.3 (N*C*=O), 189.8 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{24}N_4O_3$ [M], 416.1848; found, 416.1855.

(*Z*)-3-Methyl-4-(3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)-3-p-tolylpropylidene)-1-phenyl-1*H*-pyrazol-5(4*H*)-one (7b)



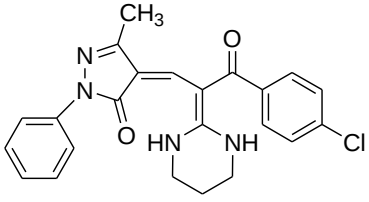
Saffron yellow solid; Mp 249−252 °C; IR (KBr): 3266, 2958, 1635, 1502, 1439, 1352, 1274, 1204, 1142, 1069, 997, 794, 754 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.93 (s, 3H, CH_3), 1.96−1.98 (m, 2H, CH_2), 2.35 (s, 3H, $ArCH_3$), 3.29−3.33 (m, 4H, NCH_2CH_2N), 6.96−6.99 (m, 1H, ArH), 7.22−7.31 (m, 5H, CH and ArH), 7.39−7.42 (m, 2H, ArH), 7.96−7.98 (m, 2H, ArH), 9.00 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.2 (CH_3), 17.4 (CH_2), 21.1 ($PhCH_3$), 37.8 (NCH_2), 37.8 (CH_2N), 100.9, 109.6, 117.4, 122.2, 128.4, 128.4, 128.5, 137.7, 140.2, 140.5, 141.2, 149.7, 161.2 (HN*C*=), 162.8 (N*C*=O), 190.3 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{24}N_4O_2$ [M], 400.1899; found, 400.1906.

(*Z*)-3-Methyl-4-(3-oxo-3-phenyl-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-1-phenyl-1*H*-pyrazol-5(4*H*)-one (7c)



Saffron yellow solid; Mp 257−262 °C; IR (KBr): 3256, 3016, 1632, 1594, 1500, 1442, 1381, 1310, 1269, 1204, 1138, 1066, 990, 946, 758 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.92 (s, 3H, CH_3), 1.95−1.98 (m, 2H, CH_2), 3.30−3.36 (m, 4H, NCH_2CH_2N), 6.96−6.99 (m, 1H, ArH), 7.21 (s, 1H, CH), 7.27−7.31 (m, 2H, ArH), 7.43−7.49 (m, 5H, ArH), 7.98−8.00 (m, 2H, ArH), 9.04 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.1 (CH_3), 17.4 (CH_2), 37.8 (NCH_2), 37.8 (CH_2N), 101.1, 109.4, 117.3, 122.2, 127.9, 128.0, 128.4, 130.1, 140.6, 140.7, 141.2, 149.6, 161.2 (HN*C*=), 162.8 (N*C*=O), 190.3 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{22}N_4O_2$ [M], 386.1743; found, 386.1742.

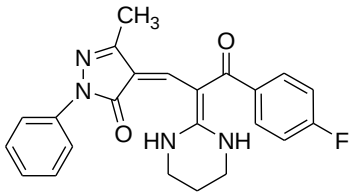
(*Z*)-4-(3-(4-Chlorophenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (7d)



Saffron yellow solid; Mp 265−269 °C; IR (KBr): 3270, 2973, 1634, 1497, 1359, 1271, 1200, 1146, 1088, 997, 834, 747 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.94−1.98 (m, 5H, CH_3 and CH_2), 3.30−3.37 (m, 4H, NCH_2CH_2N), 6.96−7.00 (m, 1H, ArH),

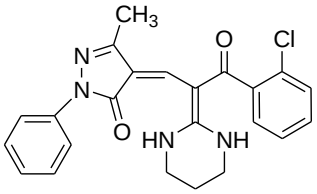
7.21 (s, 1H, CH), 7.27−7.31 (m, 2H, ArH), 7.48−7.54 (m, 4H, ArH), 7.98−7.99 (m, 2H, ArH), 9.05 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.2 (*C*H_3), 17.4 (*C*H_2), 37.8 (N*C*H_2), 37.8 (*C*H_2N), 101.7, 108.9, 117.3, 122.2, 128.1, 128.4, 129.9, 134.7, 139.5, 140.5, 141,0, 149.8, 161.1 (HN*C*=), 162.8 (N*C*=O), 188.6 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{21}ClN_4O_2$ [M], 420.1353; found, 420.1354.

(*Z*)-4-(3-(4-Fluorophenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (7e)



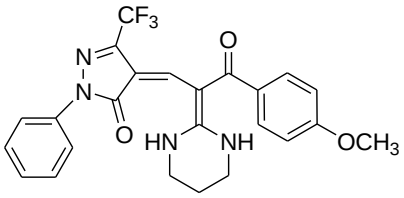
Saffron yellow solid; Mp 263−266 °C; IR (KBr): 3266, 2969, 1635, 1598, 1497, 1359, 1268, 1147, 1073, 997, 845, 754 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.93−1.96 (m, 5H, CH_2 and CH_3), 3.28−3.34 (m, 4H, NCH_2CH_2N), 6.96−7.00 (m, 2H, ArH), 7.20 (s, 1H, CH), 7.26−7.31 (m, 4H, ArH), 7.53−7.56 (m, 2H, ArH), 7.96−7.98 (m, 2H, ArH), 9.03 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.1 (*C*H_3), 17.4 (*C*H_2), 37.8 (N*C*H_2), 37.8 (*C*H_2N), 101.4, 109.1, 114.9 (d, *J* = 21.5 Hz), 117.4, 122.3, 128.4, 130.5, 137.1, 140.4, 141.1, 149.8, 161.1 (HN*C*=), 162.8 (N*C*=O), 163.0 (d, *J* = 245.9 Hz), 188.9 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{21}FN_4O_2$ [M], 404.1649; found, 404.1641.

(*Z*)-4-(3-(2-Chlorophenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (7f)



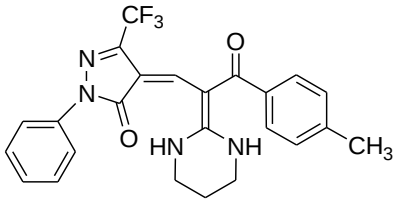
Saffron yellow solid; Mp 252−254.5 °C; IR (KBr): 3299, 2969, 1634, 1584, 1502, 1436, 1356, 1283, 1200, 1149, 1088, 993, 750 cm^{-1}; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 1.83 (s, 3H, CH_3), 1.98−2.04 (m, 2H, CH_2), 3.36−3.44 (m, 4H, NCH_2CH_2N), 6.88 (s, 1H, ACH), 6.99−7.03 (m, 1H, ArH), 7.31−7.36 (m, 3H, ArH), 7.42−7.47 (m, 2H, CH and ArH), 7.53−7.54 (m, 1H, ArH), 8.00−8.02 (m, 2H, ArH), 9.05 (br, 2H, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ = 13.1 (*C*H_3), 17.8 (*C*H_2), 38.3 (N*C*H_2), 38.3 (*C*H_2N), 102.1, 109.9, 117.7, 122.7, 127.2, 128.7, 129.3, 129.8, 130.1, 130.5, 140.5, 140.8, 141.8, 149.7, 160.5 (HN*C*=), 163.2 (N*C*=O), 188.6 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{21}ClN_4O_2$ [M], 420.1353; found, 420.1348.

(*Z*)-4-(3-(4-Methoxyphenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (7g)



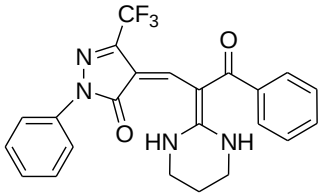
Saffron yellow solid; Mp 291−293 °C; IR (KBr): 3278, 2965, 1641, 1595, 1501, 1465, 1292, 1258, 1172, 1113, 1069, 975, 838, 761 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 1.99−2.01 (m, 2H, CH_2), 3.33−3.37 (m, 4H, NCH_2CH_2N), 3.81 (s, 3H, OCH_3), 7.01−7.03 (m, 2H, ArH), 7.11−7.14 (m, 1H, ArH), 7.33−7.37 (m, 2H, ArH), 7.39 (s, 1H, CH), 7.52−7.54 (m, 2H, ArH), 7.94−7.96 (m, 2H, ArH), 9.19 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 17.3 (CH_2), 37.8 (NCH_2), 37.8 (CH_2N), 55.4 (OCH_3), 95.0, 113.4, 114.3, 118.8, 121.6 (d, J = 268.7 Hz), 124.1, 128.7, 130.7, 139.0, 139.2, 139.6, 139.7, 160.3, 161.5 (HN*C*=), 161.8 (N*C*=O), 190.9 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{21}F_3N_4O_3$ [M], 470.1566; found, 470.1566.

(*Z*)-4-(3-Oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)-3-*p*-tolylpropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (7h)



Saffron yellow solid; Mp 296−298 °C; IR (KBr): 3299, 3013, 1640, 1595, 1499, 1454, 1288, 1179, 1115, 1066, 979, 830, 750 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 1.97−2.01 (m, 2H, CH_2), 2.36 (s, 3H, $ArCH_3$), 3.33−3.37 (m, 4H, NCH_2CH_2N), 7.11−7.14 (m, 1H, ArH), 7.27−7.29 (m, 2H, ArH), 7.34−7.38 (m, 2H, ArH), 7.39 (s, 1H, ArH), 7.43−7.45 (m, 2H, ArH), 7.94−7.96 (m, 2H, ArH), 9.21 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 17.3 (CH_2), 21.1 ($PhCH_3$), 37.8 (NCH_2), 37.8 (CH_2N), 95.1, 114.2, 118.8, 120.2, 122.9, 124.1, 128.5, 128.7, 136.5, 139.3, 139.4, 139.6, 140.9, 160.2 (HN*C*=), 161.8 (N*C*=O), 191.7 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{21}F_3N_4O_2$ [M], 454.1617; found, 454.1613.

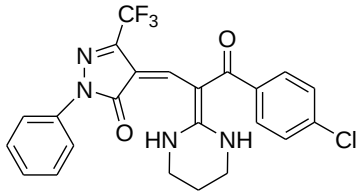
(*Z*)-4-(3-Oxo-3-phenyl-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (7i)



Saffron yellow solid; Mp 276−285 °C; IR (KBr): 3297, 3013, 1640, 1591, 1500, 1288, 1182, 1118, 1073, 986, 834, 696 cm^{-1}; ^1H NMR (400 MHz, DMSO-d_6): δ = 1.97−2.01 (m, 2H, CH_2), 3.33−3.37 (m, 4H, NCH_2CH_2N), 7.11−7.15 (m, 1H, ArH), 7.32 (s, 1H, CH), 7.36−7.39 (m, 2H, ArH), 7.45−7.55 (m, 5H, ArH), 7.93−7.95 (m, 2H, ArH), 9.23

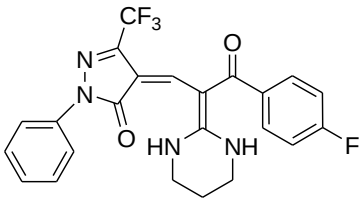
(br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 17.3 (*C*H_2), 37.8 (N*C*H_2), 37.8 (*C*H_2N), 95.3, 114.1, 118.8, 120.2, 122.9, 124.2, 128.1, 128.2, 128.7, 130.8, 139.3, 139.4, 139.7, 160.1 (HN*C*=), 161.8 (N*C*=O), 192.0 (*C*=O); HRMS (EI$^+$): *m/z* calcd for $C_{23}H_{19}F_3N_4O_2$ [M], 440.1460; found, 440.1457.

(*Z*)-4-(3-(4-Chlorophenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (7j)



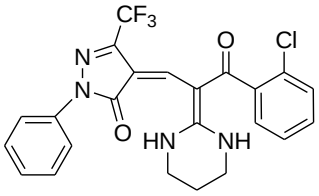
Saffron yellow solid; Mp >300 °C; IR (KBr): 3027, 2581, 1640, 1600, 1499, 1465, 1398, 1291, 1181, 1116, 982, 834, 756 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.96−1.98 (m, 2H, CH_2), 3.32−3.35 (m, 4H, NCH_2CH_2N), 7.11−7.15 (m, 1H, ArH), 7.29 (s, 1H, CH), 7.38−7.39 (m, 2H, ArH), 7.50−7.57 (m, 4H, ArH), 7.91−7.93 (m, 2H, ArH), 9.24 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 17.2 (*C*H_2), 37.8 (N*C*H_2), 37.8 (*C*H_2N), 95.6, 113.6, 118.8, 121.5, 123.0, 124.2, 128.3, 128.7, 130.0, 135.5, 138.2, 139.6, 159.9 (HN*C*=), 161.7 (N*C*=O), 190.5 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{18}ClF_3N_4O_2$ [M], 474.1070; found, 474.1073.

(*Z*)-4-(3-(4-Fluorophenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (7k)



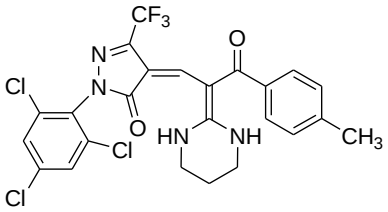
Saffron yellow solid; Mp 284−288.5 °C; IR (KBr): 3263, 3016, 1641, 1595, 1500, 1457, 1399, 1290, 1174, 1116, 1069, 979, 754 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.97−2.02 (m, 2H, CH_2), 3.33−3.36 (m, 4H, NCH_2CH_2N), 7.11−7.15 (m, 1H, ArH), 7.27−7.31 (m, 2H, CH and ArH), 7.32−7.40 (m, 3H, ArH), 7.56−7.60 (m, 2H, ArH), 7.93−7.95 (m, 2H, ArH), 9.24 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 17.3 (*C*H_2), 37.8 (N*C*H_2), 37.8 (*C*H_2N), 95.4, 113.8, 115.1, 115.3, 118.8, 121.5 (d, *J* = 268.7 Hz), 124.2, 128.7, 130.8, 130.9, 135.9, 139.6, 160.1 (HN*C*=), 161.8 (N*C*=O), 163.4 (d, *J* = 247.0 Hz), 190.6 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{18}F_4N_4O_2$ [M], 458.1366; found, 458.1356.

(*Z*)-4-(3-(2-Chlorophenyl)-3-oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)propylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (7l)



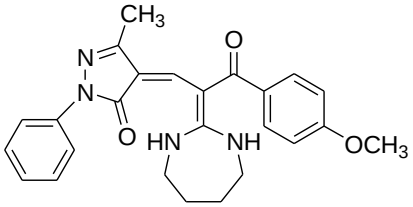
Saffron yellow solid; Mp 283-287 °C; IR (KBr): 3322, 3009, 1641, 1594, 1541, 1504, 1297, 1185, 1119, 1037, 979 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.97−2.02 (m, 2H, CH_2), 3.35−3.39 (m, 4H, NCH_2CH_2N), 6.97−7.00 (s, 1H, CH), 7.13−7.15 (m, 1H, ArH), 7.32−7.39 (m, 3H, ArH), 7.43−7.49 (m, 2H, ArH), 7.52−7.54 (m, 1H, ArH), 7.89−7.92 (m, 2H, ArH), 9.23 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 17.3 (CH_2), 37.8 (NCH_2), 37.8 (CH_2N), 95.8, 114.3, 118.8, 119.9, 122.6, 124.3, 127.0, 128.7, 129.5, 129.7, 130.7, 138.9, 139.5, 139.6, 140.6, 159.1 (HN*C*=), 161.8 (N*C*=O), 190.2 (*C*=O); HRMS (EI): *m/z* calcd for $C_{23}H_{18}ClF_3N_4O_2$ [M], 474.1070; found, 474.1078.

(*Z*)-4-(3-Oxo-2-(tetrahydropyrimidin-2(1*H*)-ylidene)-3-*p*-tolylpropylidene)-1-(2,4, 6-trichlorophenyl)-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (7m)



saffron yellow solid; Mp 286−289 °C; IR (KBr): 3279, 2918, 1633, 1591, 1498, 1345, 1272, 1142, 1091, 993, 747 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.86−1.90 (m, 2H, CH_2), 2.36 (s, 3H, $ArCH_3$), 3.26−3.35 (m, 4H, NCH_2CH_2N), 7.27−7.29 (m, 2H, ArH), 7.35 (s, 1H, CH), 7.42−7.44 (m, 2H, ArH), 7.84 (m, 2H, ArH), 9.23 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 17.3 (CH_2), 21.1 ($PhCH_3$), 37.6 (NCH_2), 37.6 (CH_2N), 93.3, 114.4, 121.4 (d, *J* = 268.8 Hz), 122.7, 128.4, 128.6, 133.9, 134.5, 135.8, 136.5, 139.6, 140.4, 140.8, 160.0 (HN*C*=), 161.8 (N*C*=O), 191.3 (*C*=O); HRMS (TOF ES^+): *m/z* calcd for $C_{24}H_{18}Cl_3F_3N_4O_2$ [$(M+H)^+$], 557.0520; found, 557.0519.

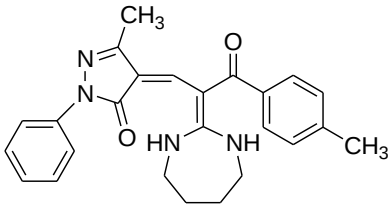
(*Z*)-4-(2-(1,3-Diazepan-2-ylidene)-3-(4-methoxyphenyl)-3-oxopropylidene)-3-met hyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (8a)



Saffron yellow solid; Mp 244−248.5 °C; IR (KBr): 3280, 2924, 1634, 1595, 1501, 1349, 1268, 1162, 1138, 1033, 993, 801, 755 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.74−1.78 (m, 4H, NCH_2CH_2N), 1.97 (s, 3H, CH_3), 3.33−3.36 (m, 4H, NCH_2CH_2N),

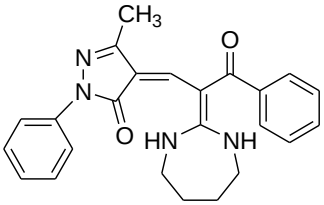
3.78 (s, 3H, OCH_3), 6.97−6.99 (m, 3H, CH and ArH), 7.25−7.31 (m, 3H, ArH), 7.47−7.49 (m, 2H, ArH), 7.94−7.96 (m, 2H, ArH), 8.81 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 13.3 (CH_3), 26.3 (CH_2CH_2), 26.3 (CH_2CH_2), 43.5 (NCH_2), 43.5 (CH_2N), 55.3 (OCH_3), 101.6, 110.9, 113.2, 117.4, 122.4, 128.4, 130.2, 133.1, 140.4, 141.5, 149.9, 160.9 (HN*C*=), 162.9 (N*C*=O), 167.3 (CH_3OC), 190.4 (*C*=O); HRMS (EI): *m/z* calcd for $C_{25}H_{26}N_4O_3$ [M], 430.2005; found, 430.2000.

(*Z*)-4-(2-(1,3-Diazepan-2-ylidene)-3-oxo-3-*p*-tolylpropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (8b)



Saffron yellow solid; Mp 263−265 °C; IR (KBr): 3281, 2922, 1633, 1499, 1352, 1273, 1142, 1001, 790, 750 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.82−1.87 (m, 4H, CH_2CH_2), 2.19 (s, 3H, CH_3), 2.35 (s, 3H, $ArCH_3$), 3.39−3.43 (m, 4H, NCH_2CH_2N), 7.21 (s, 1H, CH), 7.27−7.37 (m, 3H, ArH), 7.46−7.49 (m, 3H, ArH), 7.54−7.57 (m, 3H, ArH), 9.27 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 11.0 (CH_3), 21.1 ($PhCH_3$), 25.9 (CH_2CH_2), 25.9 (CH_2CH_2), 43.6 (NCH_2), 43.6 (CH_2N), 99.8, 120.6, 122.7, 126.4, 129.0, 129.1, 129.3, 135.0, 135.4, 139.0, 142.5, 150.6, 158.5 (HN*C*=), 164.0 (N*C*=O), 192.6 (*C*=O); HRMS (EI): *m/z* calcd for $C_{25}H_{26}N_4O_2$ [M], 414.2056; found, 414.2053.

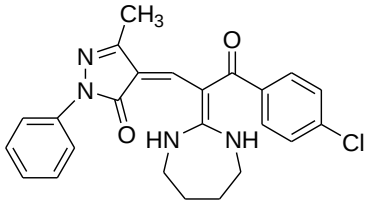
(*Z*)-4-(2-(1,3-Diazepan-2-ylidene)-3-oxo-3-phenylpropylidene)-3-methyl-1-phenyl-1*H*-pyrazol-5(4*H*)-one (8c)



Saffron yellow solid; Mp 223−227 °C; IR (KBr): 3274, 2926, 1633, 1499, 1341, 1268, 1138, 997, 805, 750 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 1.86−1.93 (m, 4H, CH_2CH_2), 1.92 (s, 3H, CH_3), 3.17 (m, 2H, NCH_2), 3.49 (m, 2H, NCH_2), 7.07−7.11 (m, 1H, ArH), 7.26 (s, 1H, CH), 7.31−7.39 (m, 4H, ArH), 7.43−7.46 (m, 1H, ArH), 7.51−7.52 (m, 2H, ArH), 7.76−7.78 (m, 2H, ArH); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 12.9 (CH_3), 26.4 (CH_2CH_2), 26.4 (CH_2CH_2), 44.8 (NCH_2), 44.8 (CH_2N), 104.2, 109.5, 119.9, 124.5, 128.2, 128.6, 128.8, 131.2, 138.8, 140.1, 145.9, 151.5, 162.8 (HN*C*=), 166.6 (N*C*=O), 195.6 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{24}N_4O_2$ [M], 400.1899; found, 400.1908.

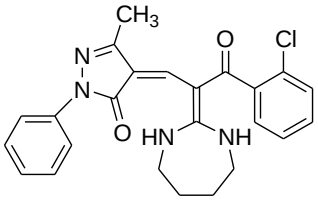
(*Z*)-4-(3-(4-Chlorophenyl)-2-(1,3-diazepan-2-ylidene)-3-oxopropylidene)-3-methy

l-1-phenyl-1*H*-pyrazol-5(4*H*)-one (8d)



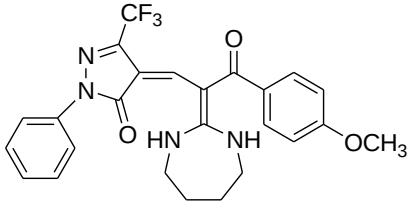
Saffron yellow solid; Mp 275−279 °C; IR (KBr): 3279, 2918, 1633, 1591, 1498, 1345, 1272, 1142, 1091, 933, 837, 747 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.82−1.86 (m, 4H, CH_2CH_2), 2.21 (s, 3H, CH_3), 3.40−3.45 (m, 4H, NCH_2CH_2N), 7.22 (s, 1H, CH), 7.26−7.30 (m, 1H, ArH), 7.46−7.49 (m, 2H, ArH), 7.56−7.58 (m, 4H, ArH), 7.63−7.65 (m, 2H, ArH), 9.29 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 11.1 (CH_3), 25.8 (CH_2CH_2), 26.0 (CH_2CH_2), 43.6 (NCH_2), 43.6 (CH_2N), 99.9, 120.6, 121.9, 126.3, 128.6, 129.3, 130.7, 135.4, 136.6, 136.8, 139.6, 150.8, 158.6 (HN*C*=), 163.9 (N*C*=O), 191.7 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{23}ClN_4O_2$ [M], 434.1510; found, 434.1524.

(*Z*)-4-(3-(2-Chlorophenyl)-2-(1,3-diazepan-2-ylidene)-3-oxopropylidene)-3-methy l-1-phenyl-1*H*-pyrazol-5(4*H*)-one (8e)



Saffron yellow solid; Mp 244−249 °C; IR (KBr): 3317, 2922, 1635, 1581, 1504, 1443, 1349, 1283, 1146, 1055, 993, 750 cm^{-1}; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 1.76−1.96 (m, 7H, CH_3 and CH_2CH_2), 3.38−3.41 (m, 4H, NCH_2CH_2N), 6.99−7.02 (m, 1H, ArH), 7.29−7.32 (m, 2H, ArH), 7.38 (s, 1H, CH), 7.41−7.42 (m, 3H, ArH), 7.49 (m, 1H, ArH), 7.98−7.99 (m, 2H, ArH), 8.83 (br, 2H, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ = 13.2 (CH_3), 26.4 (CH_2CH_2), 26.4 (CH_2CH_2), 43.4 (NCH_2), 43.4 (CH_2N), 102.7, 111.1, 117.7, 122.7, 127.1, 128.1, 128.7, 129.3, 129.7, 130.0, 130.4, 140.7, 141.4, 149.9, 163.3 (HN*C*=), 166.3 (N*C*=O), 188.7 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{23}ClN_4O_2$ [M], 434.1510; found, 434.1502.

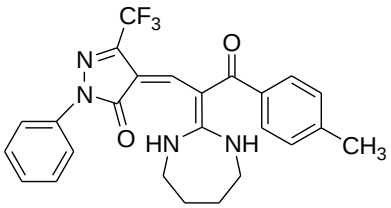
(*Z*)-4-(2-(1,3-Diazepan-2-ylidene)-3-(4-methoxyphenyl)-3-oxopropylidene)-1-phe nyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (8f)



Saffron yellow solid; Mp 288−290.5 °C; IR (KBr): 3305, 2926, 1635, 1595, 1500, 1396, 1289, 1262, 1173, 1115, 1019, 982, 841, 754 cm^{-1}; ^{1}H NMR (400 MHz,

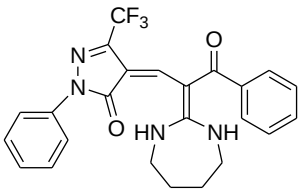
DMSO-d_6): δ = 1.85 (m, 4H, $2CH_2$), 3.44 (m, 4H, $2CH_2$), 3.79 (s, 3H, OCH_3), 7.00−7.02 (m, 2H, ArH), 7.11−7.15 (m, 1H, ArH), 7.32 (s, 1H, CH), 7.36−7.39 (m, 2H, ArH), 7.51−7.53 (m, 2H, ArH), 7.92−7.94 (m, 2H, ArH), 9.025 (s, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 26.2 (CH_2CH_2), 26.2 (CH_2CH_2), 43.2 (NCH_2), 43.2 (CH_2N), 55.4 (OCH_3), 95.3, 113.4, 115.9, 118.8, 120.6 (d, J = 268.7 Hz), 124.2, 128.7, 130.6, 131.6, 139.1, 139.3, 139.7, 161.5, 161.9 (HN*C*=), 165.7 (N*C*=O), 191.6 (*C*=O); HRMS (EI): *m/z* calcd for $C_{25}H_{23}F_3N_4O_3$ [M], 484.1722; found, 484.1727.

(*Z*)-4-(2-(1,3-Diazepan-2-ylidene)-3-oxo-3-p-tolylpropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (8g)



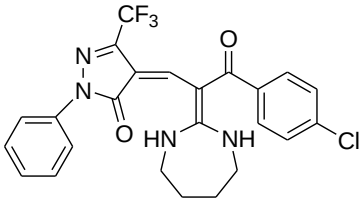
Saffron yellow solid; Mp 298−300 °C; IR (KBr): 3300, 2929, 1636, 1498, 1396, 1285, 1178, 1115, 986, 834, 755 cm^{-1}; ^{1}H NMR (500 MHz, DMSO-d_6): δ = 1.85−1.90 (m, 4H, CH_2CH_2), 2.38 (s, 3H, $ArCH_3$), 3.42−3.48 (m, 4H, NCH_2CH_2N), 7.14−7.17 (m, 1H, ArH), 7.29−7.31 (m, 2H, ArH), 7.37−7.42 (m, 4H, CH and ArH), 7.45−7.47 (m, 1H, ArH), 7.98−7.99 (m, 2H, ArH), 9.08 (br, 2H, NH); ^{13}C NMR (125 MHz, DMSO-d_6): δ = 21.4 (CH_3), 26.6 (CH_2CH_2), 26.6 (CH_2CH_2), 43.6 (NCH_2), 43.6 (CH_2N), 95.8, 116.1, 119.0, 120.9, 123.0, 124.4, 128.7, 128.9, 137.2, 139.6, 140.1, 141.0, 162.0, 162.3 (HN*C*=), 166.1 (N*C*=O), 192.5 (*C*=O); HRMS (EI): *m/z* calcd for $C_{25}H_{23}F_3N_4O_2$ [M], 468.1773; found, 468.1767.

(*Z*)-4-(2-(1,3-Diazepan-2-ylidene)-3-oxo-3-phenylpropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (8h)



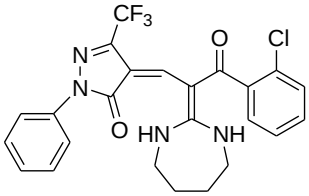
Saffron yellow solid; Mp 267−272 °C; IR (KBr): 3305, 3023, 1640, 1537, 1499, 1396, 1286, 1178, 1116, 986, 827, 689 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.81−1.85 (m, 4H, NCH_2CH_2N), 3.39−3.50 (m, 4H, NCH_2CH_2N), 7.11−7.15 (m, 1H, ArH), 7.32 (s, 1H, CH), 7.36−7.39 (m, 3H, ArH), 7.45−7.54 (m, 4H, ArH), 7.93−7.95 (m, 2H, ArH), 9.08 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 26.2 (CH_2CH_2), 26.2 (CH_2CH_2), 43.2 (NCH_2), 43.2 (CH_2N), 95.6, 115.6, 118.7, 120.2, 124.2, 128.0, 128.1, 128.7, 130.7, 139.5, 139.6, 139.7, 161.9 (HN*C*=), 165.5 (N*C*=O), 192.5 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{21}F_3N_4O2$ [M], 454.1617; found, 454.1611.

(*Z*)-4-(3-(4-Chlorophenyl)-2-(1,3-diazepan-2-ylidene)-3-oxopropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (8i)



Saffron yellow solid; Mp 291−294 °C; IR (KBr): 3300, 3023, 1635, 1591, 1498, 1396, 1288, 1179, 1117, 986, 834, 750 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.81−1.85 (m, 4H, CH_2CH_2), 3.41−3.60 (m, 4H, NCH_2CH_2N), 7.11−7.15 (m, 1H, ArH), 7.29 (s, 1H, CH), 7.36−7.39 (m, 2H, ArH), 7.49−7.52 (m, 2H, ArH), 7.54−7.57 (m, 2H, ArH), 7.90−7.94 (m, 2H, ArH), 9.09 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 26.2 (CH_2CH_2), 26.2 (CH_2CH_2), 43.2 (NCH_2), 43.2 (CH_2N), 95.9, 115.2, 118.8, 121.5 (d, J = 268.8 Hz), 124.3, 128.3, 128.7, 129.9, 135.4, 138.4, 139.3, 139.5, 139.7, 161.9, 165.3(HN*C*=), 165.3 (N*C*=O), 919.1 (*C*=O); HRMS (EI): *m/z* calcd for $C_{24}H_{20}ClF_3N_4O_2$ [M], 488.1227; found, 488.1227.

(*Z*)-4-(3-(2-Chlorophenyl)-2-(1,3-diazepan-2-ylidene)-3-oxopropylidene)-1-phenyl-3-(trifluoromethyl)-1*H*-pyrazol-5(4*H*)-one (8j)



Saffron yellow solid; Mp 298−302 °C; IR (KBr): 3333, 2947, 1640, 1592, 1540, 1500, 1180, 1113, 982, 827, 758 cm^{-1}; ^{1}H NMR (400 MHz, DMSO-d_6): δ = 1.80−1.90 (m, 4H, CH_2CH_2), 3.50−3.55 (m, 4H, NCH_2CH_2N), 7.07 (s, 1H, CH), 7.11−7.15 (m, 1H, ArH), 7.36−7.48 (m, 5H, ArH), 7.51−7.53 (m, 1H, ArH), 7.90−7.92 (m, 2H, ArH), 9.04 (br, 2H, NH); ^{13}C NMR (100 MHz, DMSO-d_6): δ = 26.1 (CH_2CH_2), 26.1 (CH_2CH_2), 43.0 (NCH_2), 43.0 (CH_2N), 95.9, 106.5, 115.8, 118.8, 121.2 (d, J = 268.7 Hz), 124.3, 125.3, 126.9, 128.7, 128.8, 129.5, 129.6, 130.6, 139.1−140.0 (m), 139.3, 161.9 (HN*C*=), 164.4 (N*C*=O), 190.5 (*C*=O); HRMS (TOF ES^+): *m/z* calcd for $C_{24}H_{20}ClF_3N_4O_2$ [$(M+H)^+$], 489.1300; found, 489.1300.

X-ray Structure and Data[2] of 6c

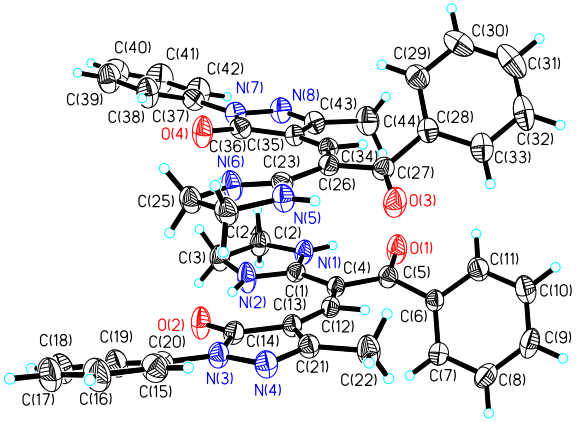


Figure S1 X-Ray crystal structure of **6c**

Table S1 Crystal data and structure refinement for **6c**

Identification code	120910b
Empirical formula	$C_{22}H_{20}N_4O_2$
Formula weight	372.42
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a =21.059(3) A alpha = 90.00 deg. b = 11.2828(16) A beta = 95.888(2) deg. c = 15.679(2) A gamma = 90.00 deg.
Volume	3705.6(9) A^3
Z, Calculated density	8, 1.335 Mg/m^3
Absorption coefficient	0.088 mm^-1
F(000)	1568
Crystal size	0.25 x 0.19 x 0.13 mm
Theta range for data collection	1.94 to 25.00 deg.
Limiting indices	-25<=h<=17, -13<=k<=13, -18<=l<=18
Reflection collected/unique	26082 / 9253 [R(int) = 0.0347]
Completeness to theta = 28.40	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9886 and 0.9783
Refinement method	SHELXL
Data/restraints/parameters	6533 / 0 / 508
Goodness-of-fit on F^2	0.907
Final R indices [I>2sigma(I)]	R1 = 0.1247, wR2 = 0.1373
R indices (all data)	R1 = 0.0525, wR2 = 0.1139
Extinction coefficient	0.0023(4)

Table S2 Bond lengths [A] and angles [deg] for **6c**

N(1)-C(1)	1.323(3)
N(1)-C(2)	1.443(3)
N(1)-H(1)	0.8600
N(2)-C(1)	1.306(3)
N(2)-C(3)	1.446(3)
N(2)-H(2)	0.8600
N(3)-C(14)	1.372(3)
N(3)-N(4)	1.406(3)
N(3)-C(15)	1.416(3)
N(4)-C(21)	1.289(3)
N(5)-C(23)	1.317(3)
N(5)-C(24)	1.444(3)
N(5)-H(5)	0.8600
N(6)-C(23)	1.305(3)
N(6)-C(25)	1.462(3)
N(6)-H(6)	0.8600
N(7)-C(36)	1.375(3)
N(7)-N(8)	1.400(3)
N(7)-C(37)	1.408(3)
N(8)-C(43)	1.296(3)
O(1)-C(5)	1.246(3)
O(2)-C(14)	1.246(3)
O(3)C(27)	1.227(3)
O(4)C(36)	1.253(3)
C(1)-C(4)	1.441(3)
C(2)-C(3)	1.515(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(12)	1.400(3)
C(4)-C(5)	1.450(3)
C(5)-C(6)	1.489(3)
C(6)-C(7)	1.378(3)
C(6)-C(11)	1.380(3)
C(7)-C(8)	1.369(3)
C(7)-H(7)	0.9300
C(8)-C(9)	1.371(4)
C(8)-H(8)	0.9300
C(9)-C(10)	1.357(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.369(4)
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-C(13)	1.392(3)
C(12)-H(12)	0.9300
C(13)-C(21)	1.435(3)
C(13)-C(14)	1.436(3)
C(15)-C(16)	1.374(3)
C(15)-C(20)	1.388(3)
C(16)-C(17)	1.372(4)

C(16)-H(16)	0.9300
C(17)-C(18)	1.371(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.362(4)
C(18)-H(18)	0.9300
C(19)-C(20)	1.366(4)
C(19)-H(19)	0.9300
C(20)-H(20)	0.9300
C(21)-C(22)	1.494(3)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600
C(23)-C(26)	1.442(3)
C(24)-C(25)	1.512(3)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-C(34)	1.400(3)
C(26)-C(27)	1.464(3)
C(27)-C(28)	1.498(4)
C(28)-C(33)	1.377(4)
C(28)-C(29)	1.385(3)
C(29)-C(30)	1.364(4)
C(29)-H(29)	0.9300
C(30)-C(31)	1.369(5)
C(30)-H(30)	0.9300
C(31)-C(32)	1.364(5)
C(31)-H(31)	0.9300
C(32)-C(33)	1.378(4)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-C(35)	1.400(3)
C(34)-H(34)	0.9300
C(35)-C(36)	1.431(3)
C(35)-C(43)	1.442(3)
C(37)-C(38)	1.366(4)
C(37)-C(42)	1.376(3)
C(38)-C(39)	1.372(4)
C(38)-H(38)	0.9300
C(39)-C(40)	1.352(4)
C(39)-H(39)	0.9300
C(40)-C(41)	1.349(4)
C(40)-H (40)	0.9300
C(41)-C(42)	1.384(4)
C(41)-H(41)	0.9300
C(42)-H(42)	0.9300
C(43)-C(44)	1.490(4)
C(44)-H(44A)	0.9600
C(44)-H(44B)	0.9600 .
C(44)-H(44C)	0.9600

Symmetry transformations used to generate equivalent atoms:

Table S3 Torsion angles [deg] for **6c**

C(14)-N(3)-N(4)-C(21)	1.1(3)
C(15)-N(3)-N(4)-C(21)	-169.8(2)
C(36)-N(7)-N(8)-C(43)	0.7(3)
C(37)-N(7)-N(8)-C(43)	176.4(2)
C(3)-N(2)-C(1)-N(1)	-2.6(3)
C(3)-N(2)-C(1)-C(4)	177.8(2)
C(2)-N(1)-C(1)-N(2)	-1.1(3)
C(2)-N(1)-C(1)-C(4)	178.5(2)
C(1)-N(1)-C(2)-C(3)	3.9(3)
C(1)-N(2)-C(3)-C(2)	4.9(3)
N(1)-C(2)-C(3)-N(2)	-5.0(3)
N(2)-C(1)-C(4)-C(12)	-5.0(4)
N(1)-C(1)-C(4)-C(12)	175.6(2)
N(2)-C(1)-C(4)-C(5)	-179.9(2)
N(1)-C(1)-C(4)-C(5)	0.6(4)
C(12)-C(4)-C(5)-O(1)	-162.1(2)
C(1)-C(4)-C(5)-O(1)	13.5(4)
C(12)-C(4)-C(5)-C(6)	18.0(3)
C(1)-C(4)-C(5)-C(6)	-166.5(2)
O(1)-C(5)-C(6)-C(7)	-131.0(3)
C(4)-C(5)-C(6)-C(7)	49.0(4)
O(1)-C(5)-C(6)-C(11)	43.8(3)
C(4)-C(5)-C(6)-C(11)	-136.3(3)
C(11)-C(6)-C(7)-C(8)	0.4(4)
C(5)-C(6)-C(7)-C(8)	175.2(2)
C(6)-C(7)-C(8)-C(9)	0.8(4)
C(7)-C(8)-C(9)-C(10)	-0.7(5)
C(8)-C(9)-C(10)-C(11)	-0.5(5)
C(9)-C(10)-C(11)-C (6)	1.6(4)
C(7)-C(6)-C(11)-C(10)	-1.6(4)
C(5)-C(6)-C(11)-C(10)	-176.6(2)
C(1)-C(4)-C(12)-C(13)	6.4(5)
C(5)-C(4)-C(12)-C(13)	-178.6(3)
C(4)-C(12)-C(13)-C(21)	-179.9(3)
C(4)-C(12)-C(13)-C(14)	1.7(6)
N(4)-N(3)-C(14)-O(2)	179.1(2)
C(15)-N(3)-C(14)-O(2)	-11.2(4)
N(4)-N(3)-C(14)-C(13)	-1.4(3)
C(15)-N(3)-C(14)-C(13)	168.2(2)
C(12)-C(13)-C(14)-O(2)	-1.0(5)
C(21)-C(13)-C(14)-O(2)	-179.5(3)
C(12)-C(13)-C(14)-N(3)	179.6(3)
C(21)-C(13)-C(14)-N(3)	1.1(3)

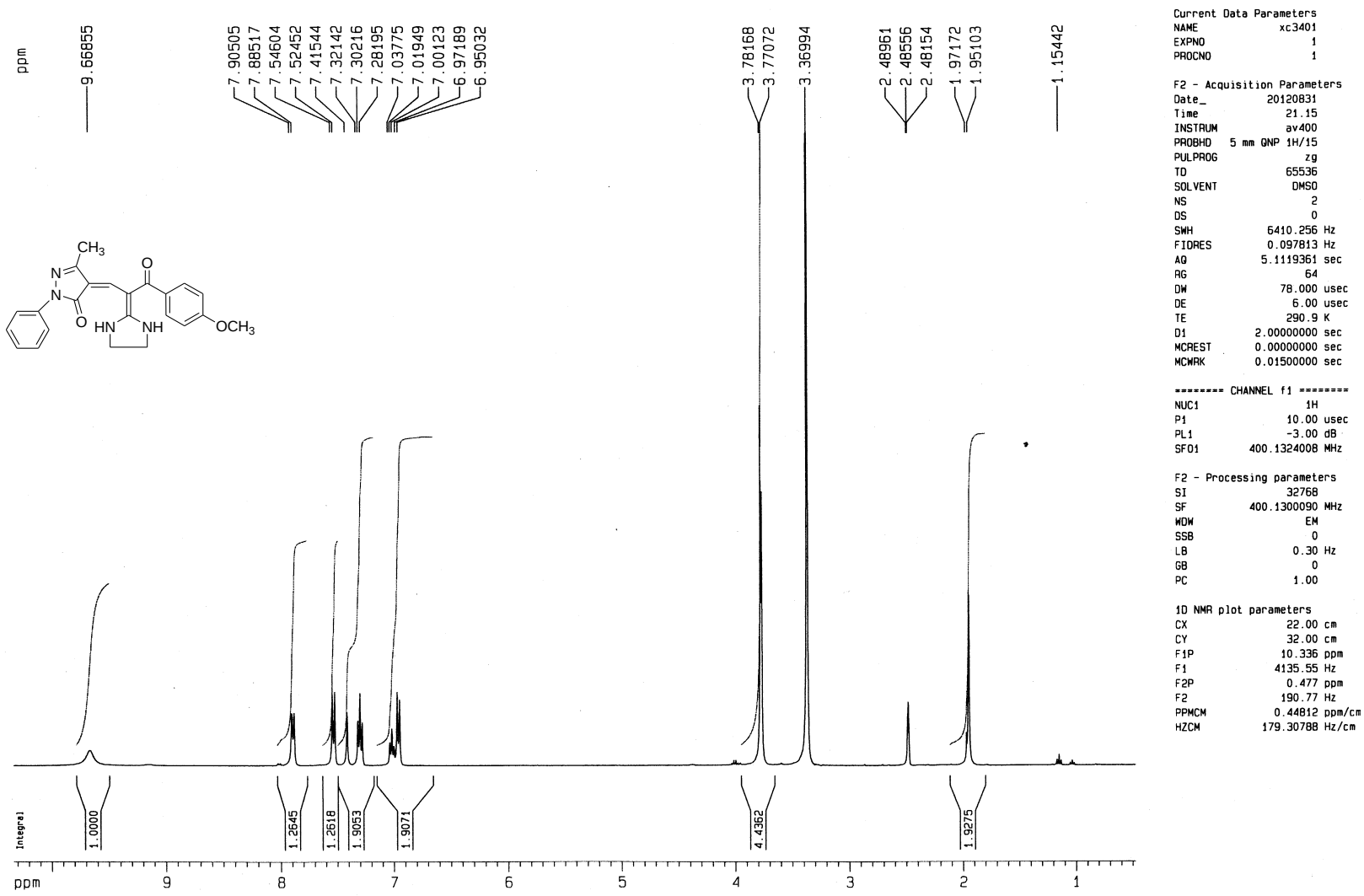
C(14)-N(3)-C(15)-C(16)	21.7(4)
N(4)-N(3)-C(15)-C(16)	-169.2(2)
C(14)-N(3)-C(15)-C(20)	-157.4(3)
N(4)-N(3)-C(15)-C(20)	11.6(3)
C(20)-C(15)-C(16)-C(17)	1.4(4)
N(3)-C(15)-C(16)-C(17)	-177.7(2)
C(15)-C(16)-C(17)-C(18)	-1.5(5)
C(16)-C(17)-C(18)-C(19)	0.4(5)
C(17)-C(18)-C(19)-C(20)	0.9(5)
C(18)-C(19)-C(20)-C(15)	-1.0(5)
C(16)-C(15)-C(20)-C(19)	-0.2(4)
N(3)-C(15)-C(20)-C(19)	179.0(2)
N(3)-N(4)-C(21)-C(13)	-0.4(3)
N(3)-N(4)-C(21)-C(22)	-178.7(2)
C(12)-C(13)-C(21)-N(4)	-179.2(2)
C(14)-C(13)-C(21)-N(4)	-0.4(3)
C(12)-C(13)-C(21)-C(22)	-1.1(4)
C(14)-C(13)-C(21)-C(22)	177.8(3)
C(25)-N(6)-C(23)-N(5)	5.2(3)
C(25)-N(6)-C(23)-C(26)	-173.6(2)
C(24)-N(5)C-(23)-N(6)	-3.1(3)
C(24)-N(5)-C(23)-C(26)	175.7(2)
C(23)N(5)C(24)C(25)	-0.2(3)
C(23)-N(6)-C(25)-C(24)	-5.0(3)
N(5)-C(24)-C(25)-N(6)	2.9(3)
N(6)-C(23)-C(26)-C(34)	1.1(4)
N(5)C(23)C(26)C(34)	-177.5(2)
N(6)-C(23)-C(26)-C(27)	-175.3(2)
N(5)-C(23)-C(26)-C(27)	6.1(4)
C(34)-C(26)-C (27)-O(3)	-151.5(3)
C(23)-C(26)-C(27)-O(3)	25.4(4)
C(34)-C(26)-C(27)-C(28)	31.0(3)
C(23)-C(26)-C(27)-C(28)	-152.1(2)
O(3)-C(27)-C(28)-C(33)	30.5(4)
C(26)-C(27)-C(28)-C(33)	-151.9(2)
O(3)-C(27)-C(28)-C(29)	-143.2(3)
C(26)-C(27)-C(28)-C(29)	34.4(4)
C(33)-C(28)-C(29)-C(30)	1.3(4)
C(27)-C(28)-C(29)-C(30)	175.0(2)
C(28)-C(29)-C(30)-C(31)	0.4(5)
C(29)-C(30)-C(31)-C(32)	-1.3(5)
C(30)-C(31)-C(32)-C(33)	0.7(5)
C(29)-C(28)-C(33)-C(32)	-1.9(4)
C(27)-C(28)-C(33)-C(32)	-175.9(2)

C(31)-C(32)-C(33)-C(28)	1.0(4)
C(23)-C(26)-C(34)-C(35)	8.5(5)
C(27)-C(26)-C(34)-C(35)	-175.0(3)
C(26)-C(34)-C(35)-C(36)	8.1(6)
C(26)-C(34)-C(35)-C(43)	-177.8(3)
N(8)-N(7)-C(36)-O(4)	176.9(2)
C(37)-N(7)-C(36)-O(4)	1.8(4)
N(8)-N(7)-C(36)-C(35)	-1.1(3)
C(37)-N(7)-C(36)-C(35)	-176.2(2)
C(34)-C(35)-C(36)-O(4)	-2.0(5)
C(43)-C(35)-C(36)-O(4)	-176.7(3)
C(34)-C(35)-C(36)-N(7)	175.8(3)
C(43)-C(35)-C(36)-N(7)	1.0(3)
C(36)-N(7)-C(37)-C(38)	6.7(4)
N(8)-N(7)-C(37)-C(38)	-168.2(2)
C(36)-N(7)-C(37)-C(42)	-173.6(3)
N(8)-N(7)-C(37)-C(42)	11.5(4)
C(42)-C(37)-C(38)-C(39)	-1.4(5)
N(7)-C(37)-C(38)-C(39)	178.3(3)
C(37)-C(38)-C(39)-C(40)	1.8(5)
C(38)-C(39)-C(40)-C(41)	-0.4(5)
C(39)-C(40)-C(41)-C(42)	-1.3(6)
C(38)-C(37)-C(42)-C(41)	-0.3(5)
N(7)-C(37)-C(42)-C(41)	-180.0(3)
C(40)-C(41)-C(42)-C(37)	1.6(6)
N(7)-N(8)-C(43)-C(35)	0.1(3)
N(7)-N(8)-C(43)-C (44)	-177.4(2)
C(34)-C(35)-C(43)-N(8)	-176.4(2)
C(36)-C(35)-C(43)-N(8)	-0.7(3)
C(34)-C(35)-C(43)-C(44)	0.8(4)
C(36)-C(35)-C(43)-C(44)	176.5(3)

Table S4 Hydrogen bonds for **6c** [A and deg.]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(6)-H(6)...O(4)	0.86	1.83	2.585(3)	145.1
N(5)-H(5)...O(3)	0.86	2.12	2.675(3)	122.0
N(2)-H(2)...O(2)	0.86	1.74	2.604(3)	178.9
N(1)-H(1)...O(3)	0.86	2.34	3.107(3)	149.3
N(1)-H(1)...O(1)	0.86	1.99	2.586(3)	125.7

^{1}H NMR and ^{13}C NMR Spectra for *α,β*-Unsaturated Pyrazolone-Based HKAs 6-8



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PROCNO 1

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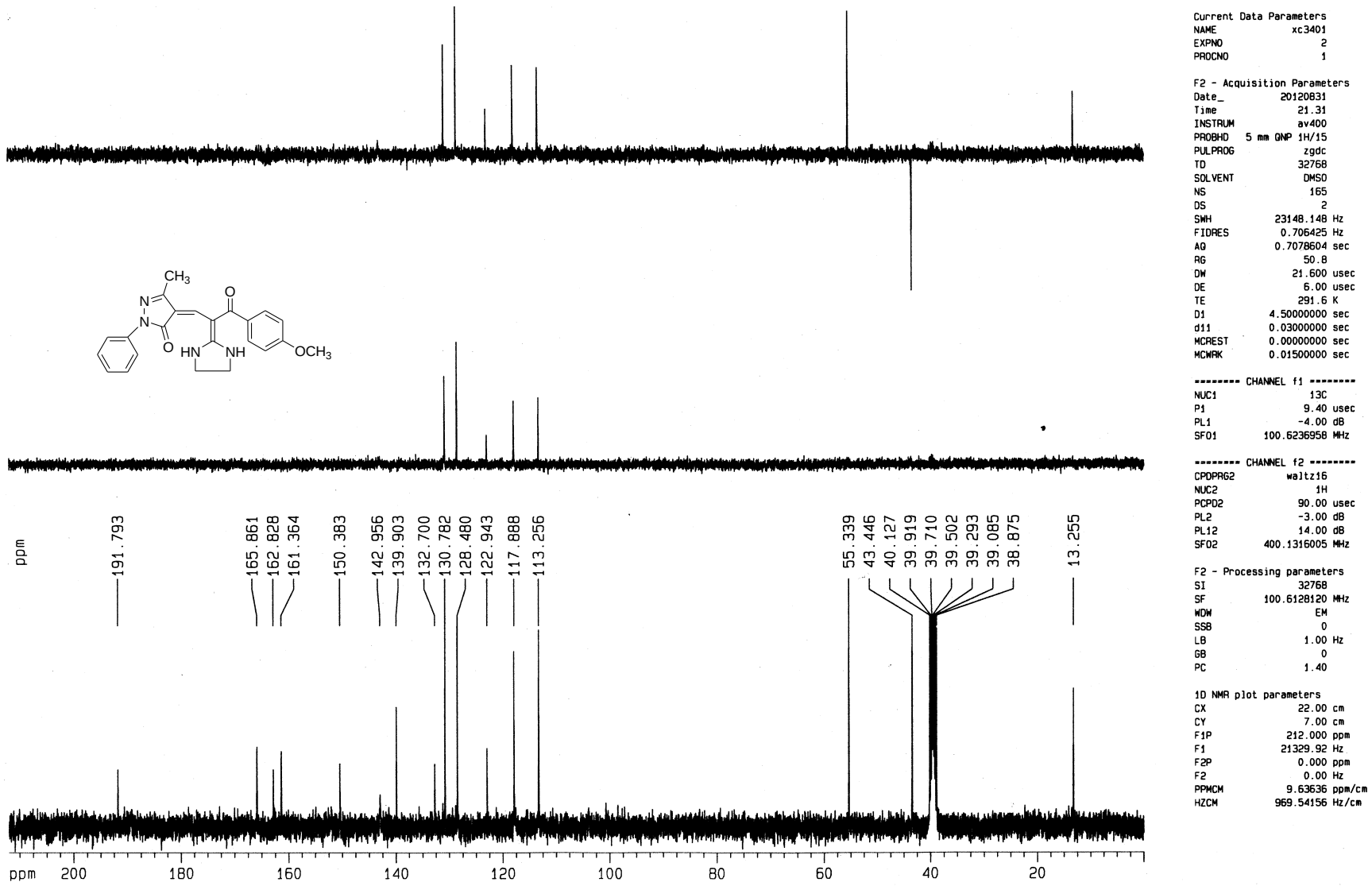
PULPROG zg
TD 65536
SOLVENT DMSO
NS 2
DS 0
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1119361 sec
RG 64
DW 78.000 usec
DE 6.00 usec
TE 290.9 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 32.00 cm
F1P 10.336 ppm
F1 4135.55 Hz
F2P 0.477 ppm
F2 190.77 Hz
PPMCM 0.44812 ppm/cm
HZCM 179.30788 Hz/cm

Figure 1. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6a**



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EXPNO 2
PROCNO 1

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PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 165
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 50.8
DW 21.600 usec
DE 6.00 usec
TE 291.6 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128120 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 7.00 cm
F1P 212.000 ppm
F1 21329.92 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.63636 ppm/cm
HZCM 969.54156 Hz/cm

Figure 2. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6a**

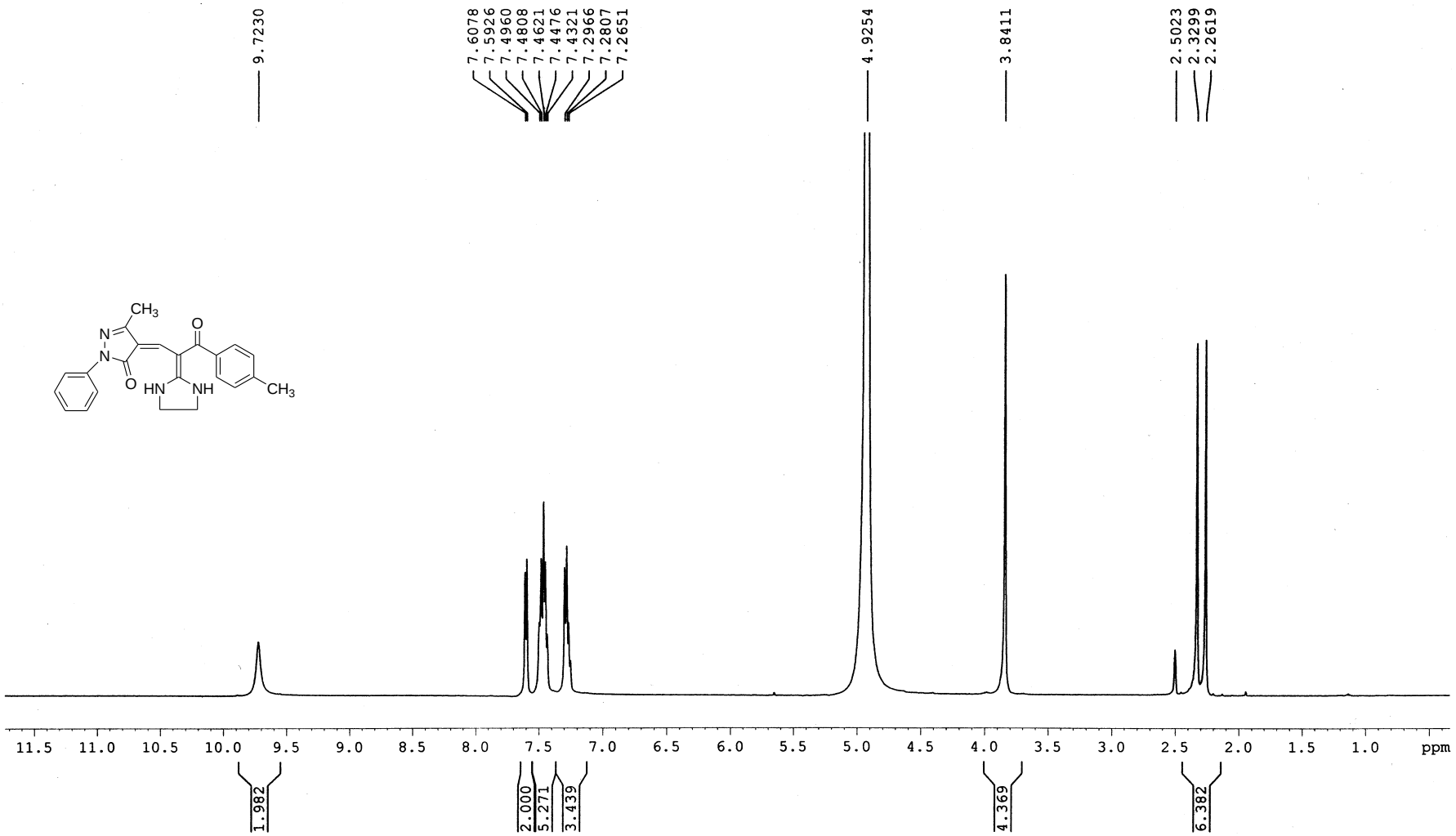


Figure 3. ^{1}H NMR (500 MHz, DMSO-d_6+$HClO_4$) spectra of compound **6b**

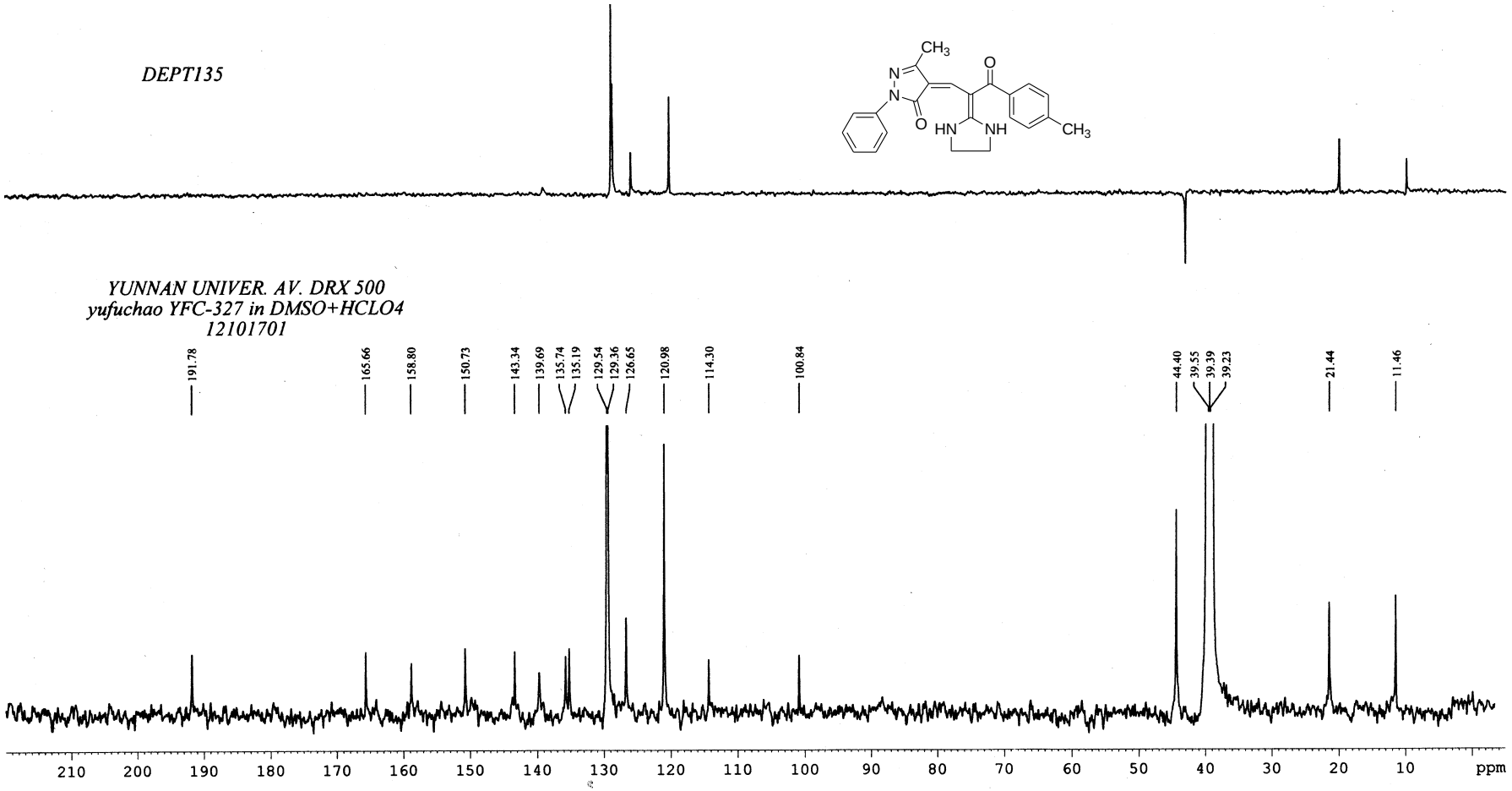
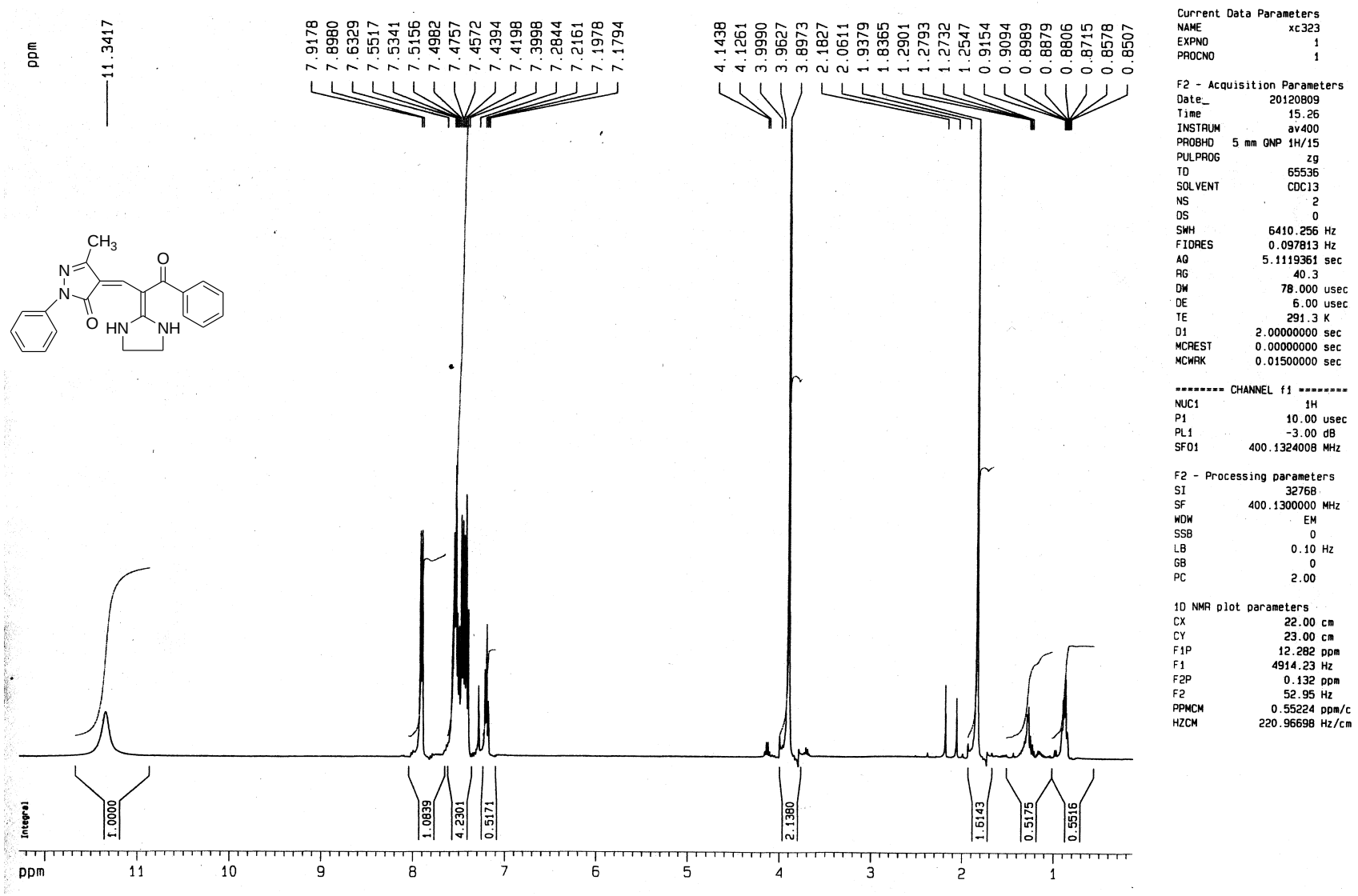


Figure 4. ^{13}C NMR (125 MHz, DMSO-d_6+$HClO_4$) spectra of compound **6b**



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PROCNO	1

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PULPROG	zg
TD	65536
SOLVENT	CDCl3
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	40.3
DW	78.000 usec
DE	6.00 usec
TE	291.3 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

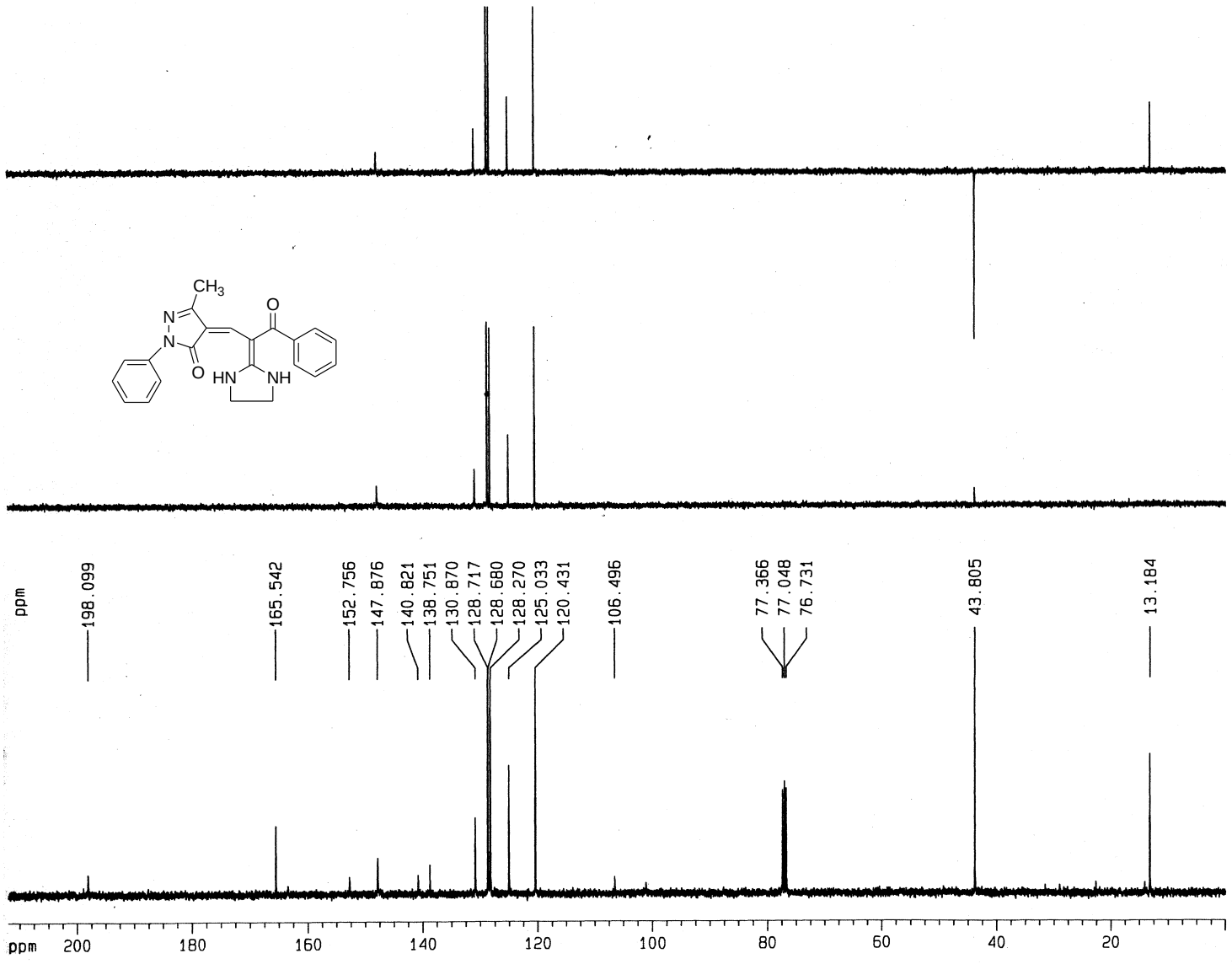
F2 - Processing parameters

SI	32768
SF	400.1300000 MHz
WDW	EM
SSB	0
LB	0.10 Hz
GB	0
PC	2.00

1D NMR plot parameters

CX	22.00 cm
CY	23.00 cm
F1P	12.282 ppm
F1	4914.23 Hz
F2P	0.132 ppm
F2	52.95 Hz
PPMCM	0.55224 ppm/c
HZCM	220.96698 Hz/cm

Figure 5. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of compound **6c**

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EXPNO                    2
PROCNO                   1

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Time                 15.35
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PULPROG              zgdc
TD                   32768
SOLVENT              CDCl3
NS                      98
DS                       2
SWH              23148.148 Hz
FIDRES               0.706425 Hz
AQ                0.7078604 sec
RG                      35.9
DW                   21.600 usec
DE                    6.00 usec
TE                   292.1 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.40 usec
PL1                  -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                90.00 usec
PL2                  -3.00 dB
PL12                 14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6127740 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.00 cm
CY                    7.00 cm
F1P                212.000 ppm
F1               21329.91 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54132 Hz/cm
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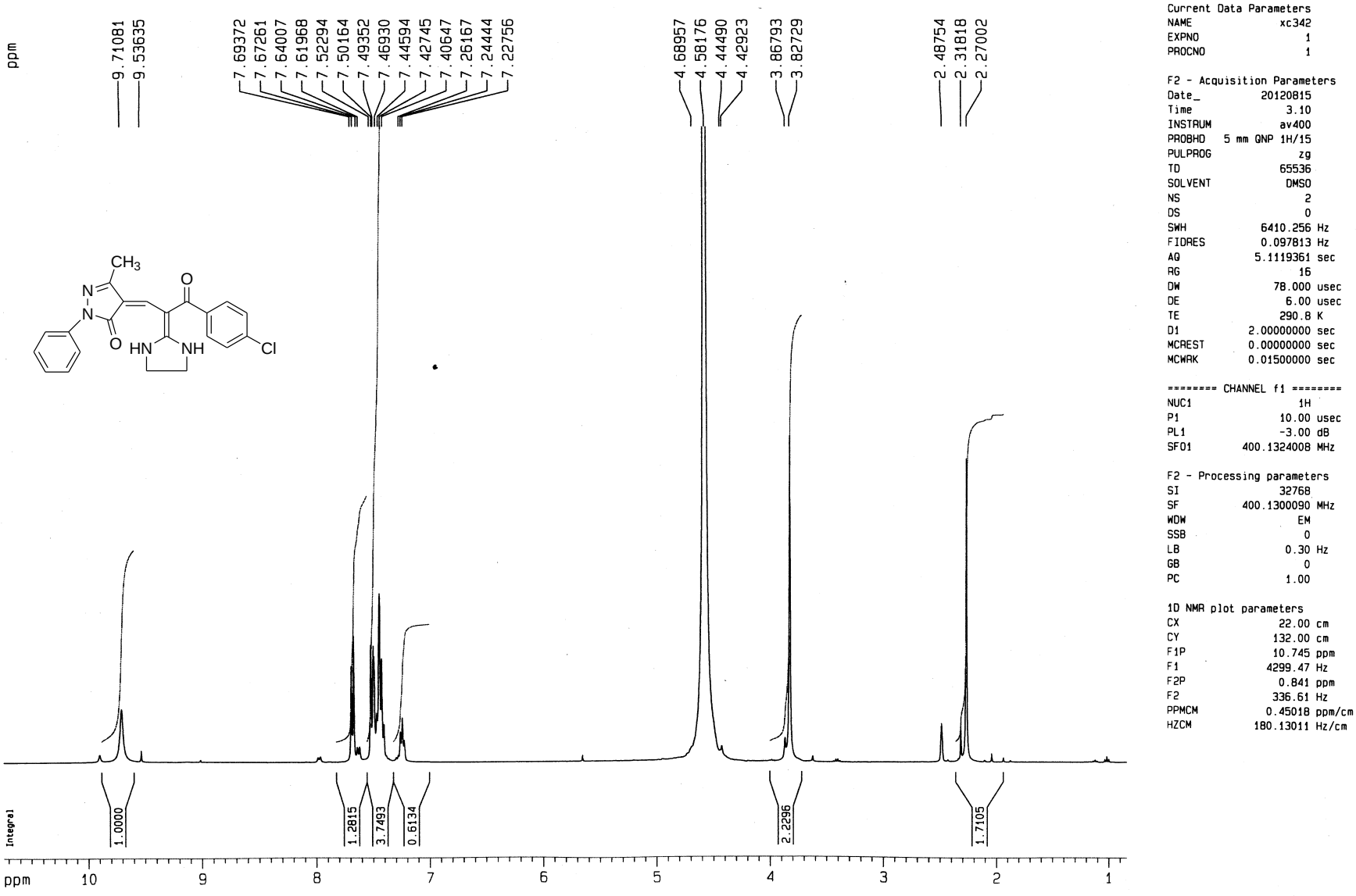
Figure 6. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of compound **6c**



Current Data Parameters

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EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120815
Time	3.10
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	16
DW	78.000 usec
DE	6.00 usec
TE	290.8 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

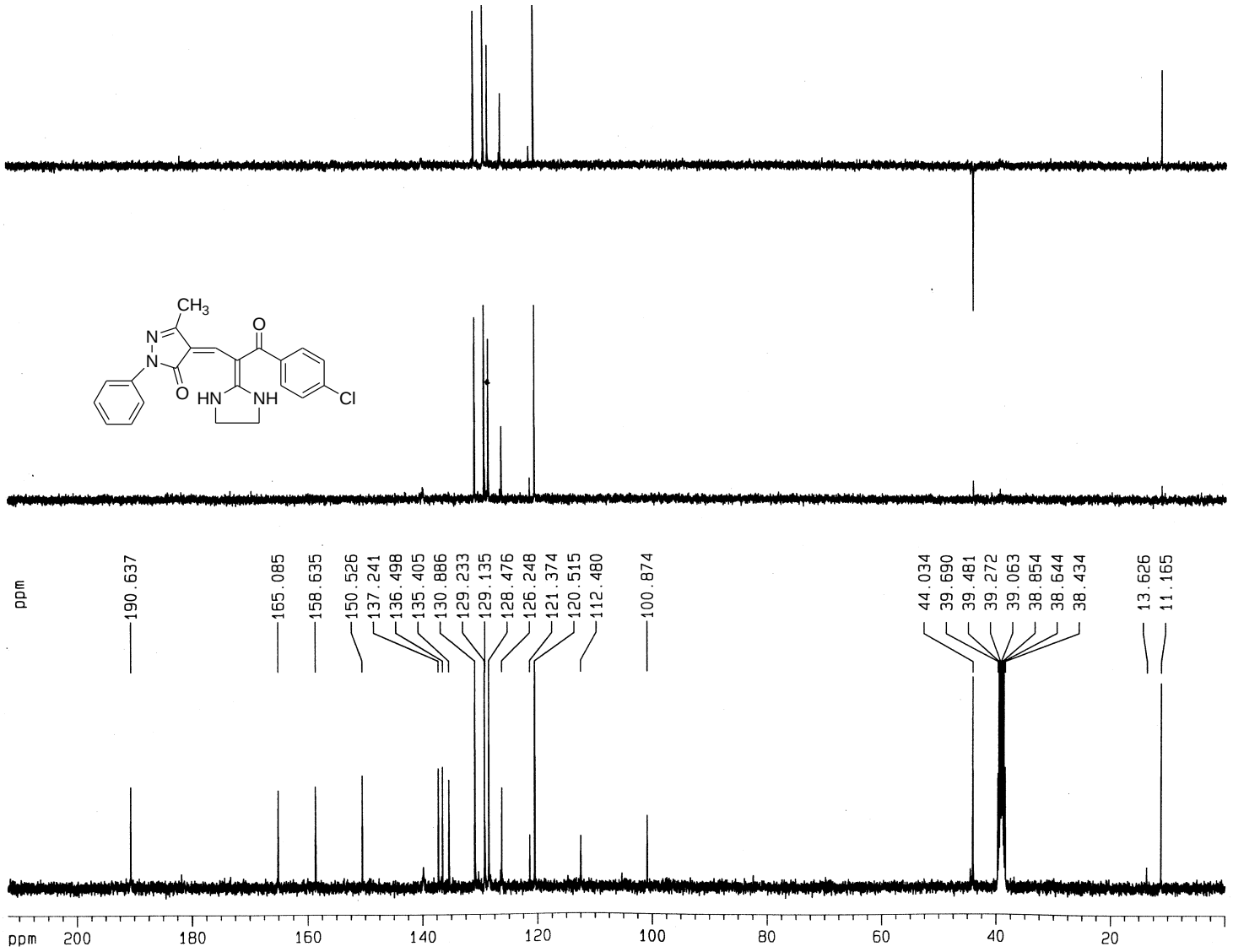
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	132.00 cm
F1P	10.745 ppm
F1	4299.47 Hz
F2P	0.841 ppm
F2	336.61 Hz
PPMCM	0.45018 ppm/cm
HZCM	180.13011 Hz/cm

Figure 7. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6d**

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Current Data Parameters
NAME                 xc342
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20120815
Time                 3.26
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     168
DS                       2
SWH            23148.148 Hz
FIDRES          0.706425 Hz
AQ              0.7078604 sec
RG                     512
DW                21.600 usec
DE                 6.00 usec
TE                 291.6 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.40 usec
PL1                -4.00 dB
SF01          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SF02          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6128120 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.00 cm
CY                 8.00 cm
F1P              212.000 ppm
F1             21329.92 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           9.63636 ppm/cm
HZCM          969.54156 Hz/cm
```

Figure 8. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6d**

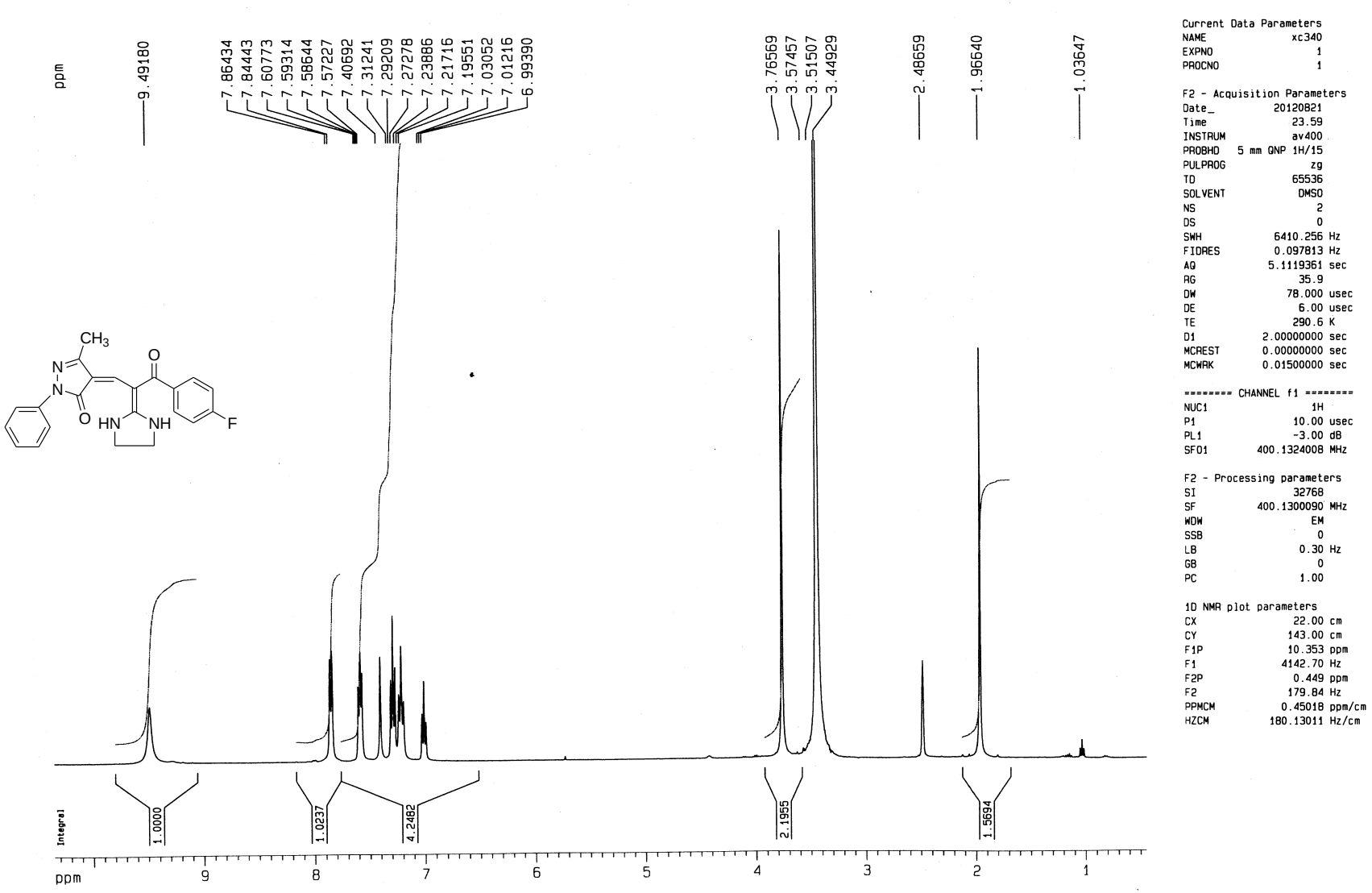
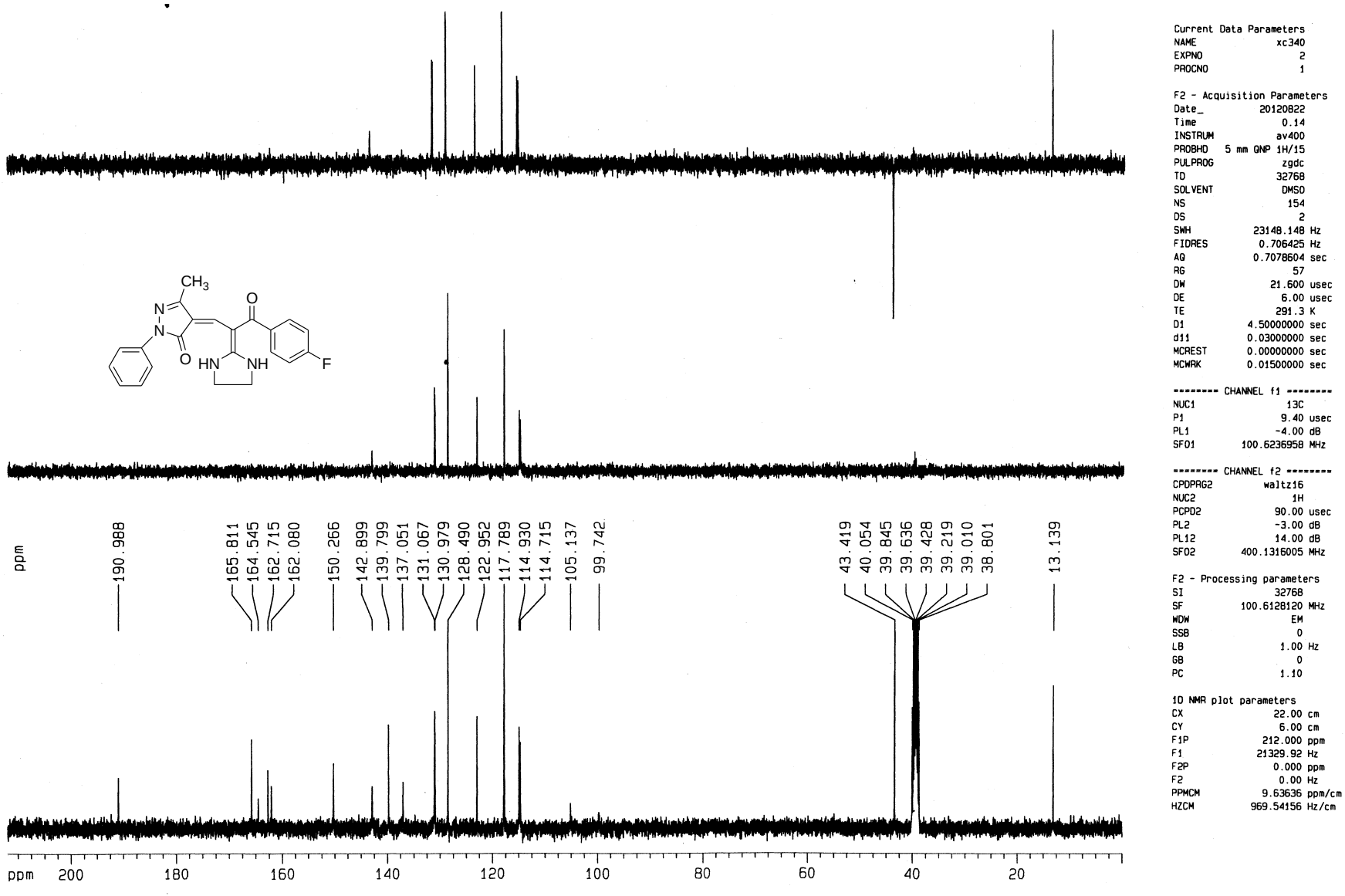


Figure 9. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6e**




```
Current Data Parameters
NAME                  xc340
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120822
Time                  0.14
INSTRUM               av400
PROBHD   5 mm QNP 1H/15
PULPROG                zgdc
TD                    32768
SOLVENT                DMSO
NS                      154
DS                        2
SWH              23148.148 Hz
FIDRES            0.706425 Hz
AQ                0.7078604 sec
RG                       57
DW                  21.600 usec
DE                   6.00 usec
TE                  291.3 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

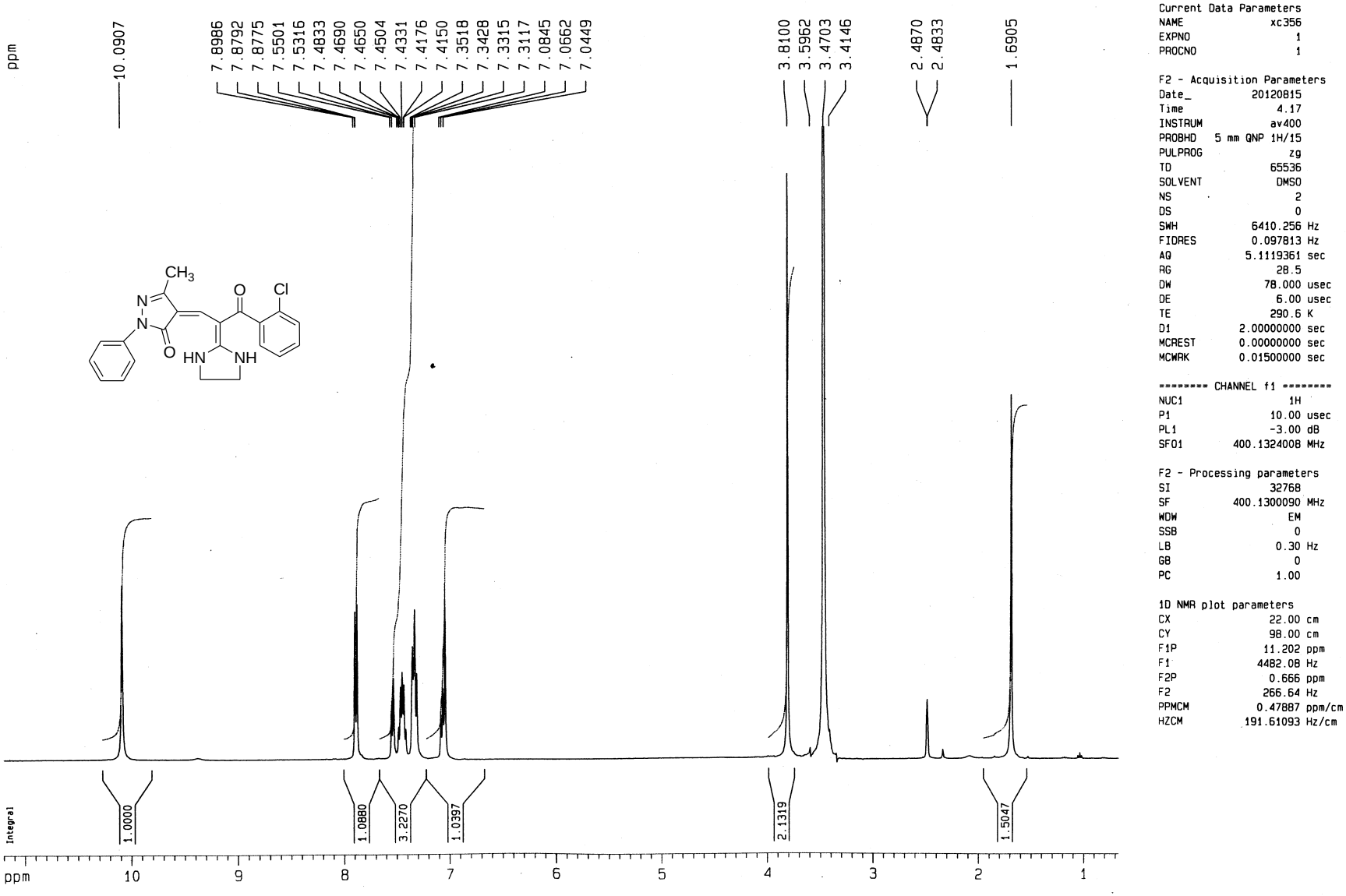
======== CHANNEL f1 ========
NUC1                    13C
P1                   9.40 usec
PL1                 -4.00 dB
SFO1           100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                 -3.00 dB
PL12                14.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6128120 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                     1.10

1D NMR plot parameters
CX                   22.00 cm
CY                    6.00 cm
F1P                212.000 ppm
F1                 21329.92 Hz
F2P                  0.000 ppm
F2                    0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54156 Hz/cm
```

Figure 10. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6e**




```
Current Data Parameters
NAME                  xc356
EXPNO                     1
PROCNO                    1

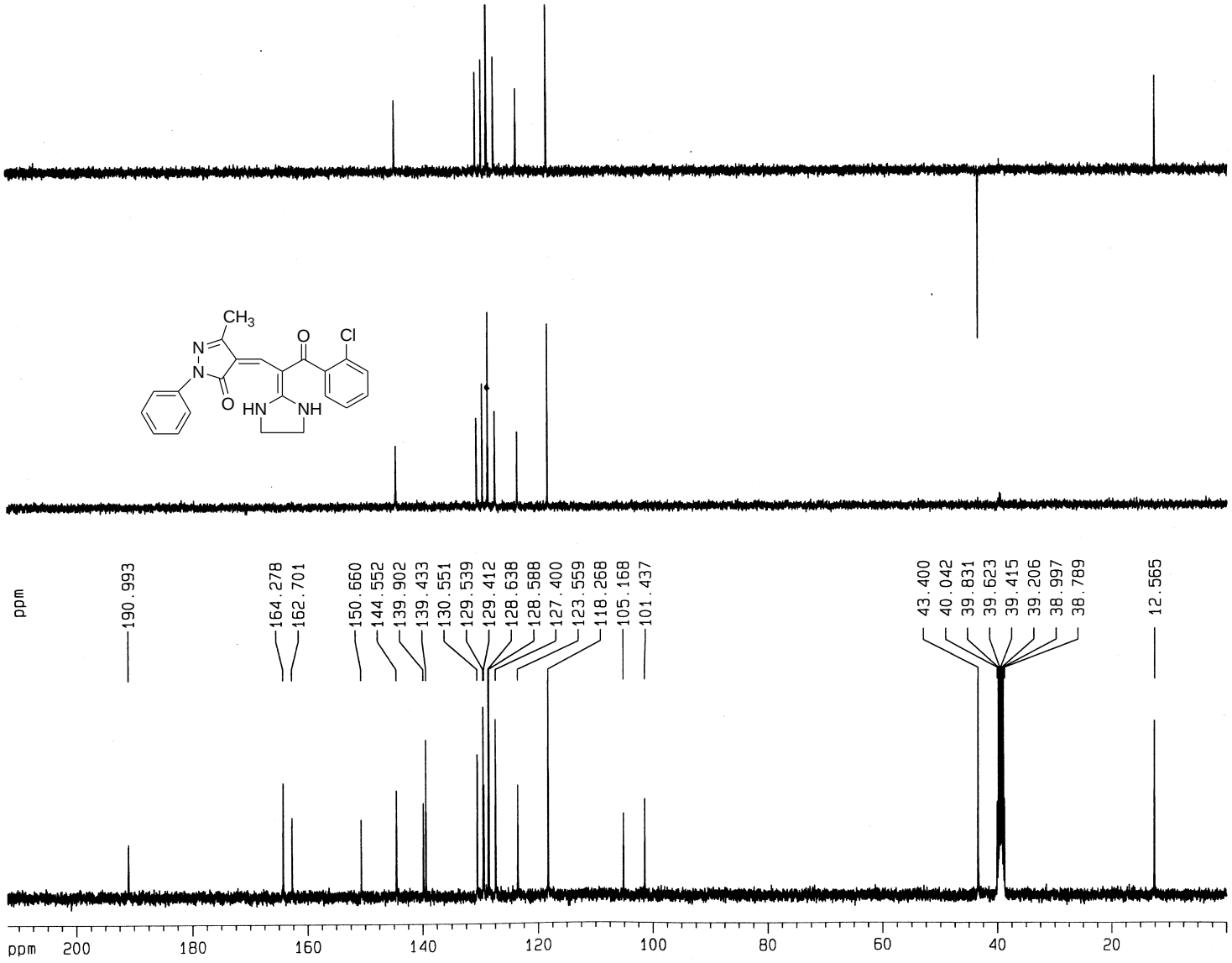
F2 - Acquisition Parameters
Date_              20120815
Time                   4.17
INSTRUM               av400
PROBHD    5 mm QNP 1H/15
PULPROG                zg
TD                    65536
SOLVENT                DMSO
NS                        2
DS                        0
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1119361 sec
RG                     28.5
DW                  78.000 usec
DE                   6.00 usec
TE                   290.6 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                   10.00 usec
PL1                  -3.00 dB
SFO1             400.1324008 MHz

F2 - Processing parameters
SI                        32768
SF               400.1300090 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                    22.00 cm
CY                    98.00 cm
F1P                  11.202 ppm
F1                 4482.08 Hz
F2P                   0.666 ppm
F2                  266.64 Hz
PPMCM              0.47887 ppm/cm
HZCM              191.61093 Hz/cm
```

Figure 11. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6f**




```
Current Data Parameters
NAME                 xc356
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120815
Time                 4.32
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     168
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                   101.6
DW                21.600 usec
DE                 6.00 usec
TE                 291.5 K
D1            4.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

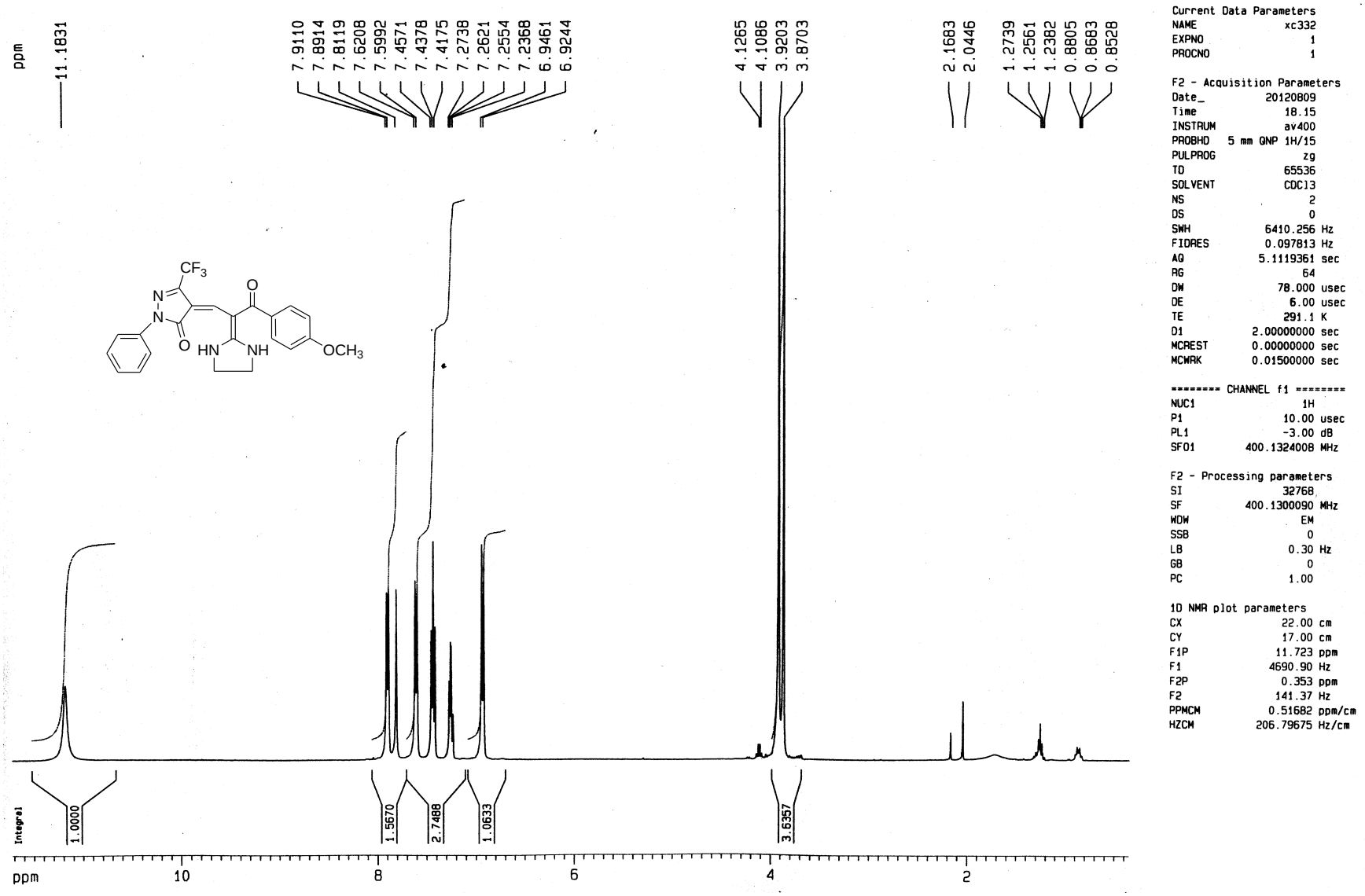
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.40 usec
PL1                -4.00 dB
SFO1         100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6128120 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 2.00

1D NMR plot parameters
CX                22.00 cm
CY                 9.00 cm
F1P              212.000 ppm
F1             21329.92 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           9.63636 ppm/cm
HZCM          969.54156 Hz/cm
```

Figure 12. ^{13}C NMR (100 MHz, DMSO -d_6) spectra of compound **6f**




```
Current Data Parameters
NAME                  xc332
EXPNO                     1
PROCNO                    1

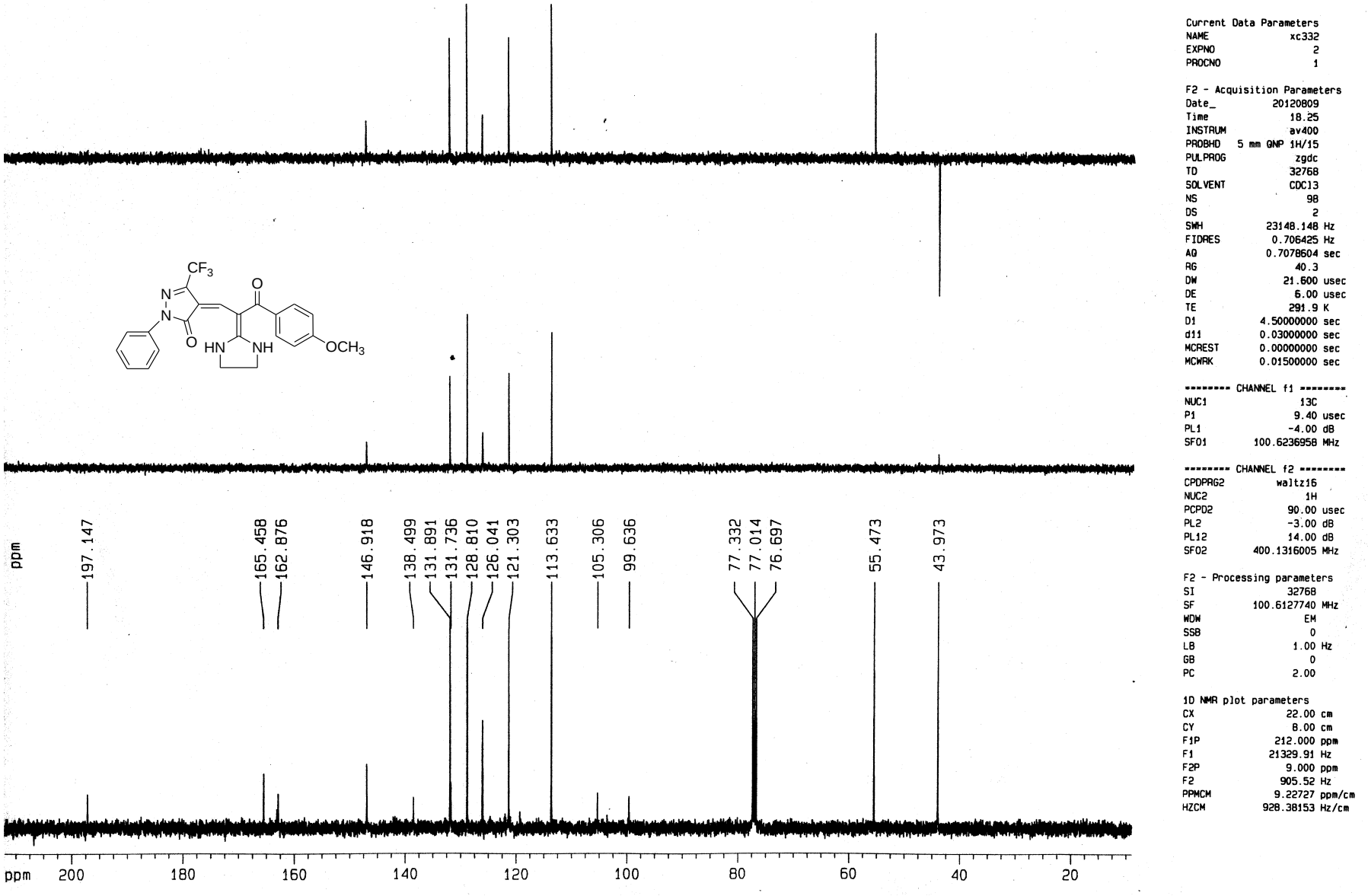
F2 - Acquisition Parameters
Date_              20120809
Time                  18.15
INSTRUM               av400
PROBHD   5 mm QNP 1H/15
PULPROG                  zg
TD                    65536
SOLVENT               CDCl3
NS                        2
DS                        0
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1119361 sec
RG                       64
DW                  78.000 usec
DE                   6.00 usec
TE                   291.1 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                   10.00 usec
PL1                  -3.00 dB
SFO1             400.1324008 MHz

F2 - Processing parameters
SI                       32768
SF               400.1300090 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    22.00 cm
CY                    17.00 cm
F1P                  11.723 ppm
F1                  4690.90 Hz
F2P                   0.353 ppm
F2                  141.37 Hz
PPMCM              0.51682 ppm/cm
HZCM              206.79675 Hz/cm
```

Figure 13. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of compound **6g**



Current Data Parameters
NAME xc332
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120809
Time 18.25
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 98
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 40.3
DW 21.600 usec
DE 6.00 usec
TE 291.9 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

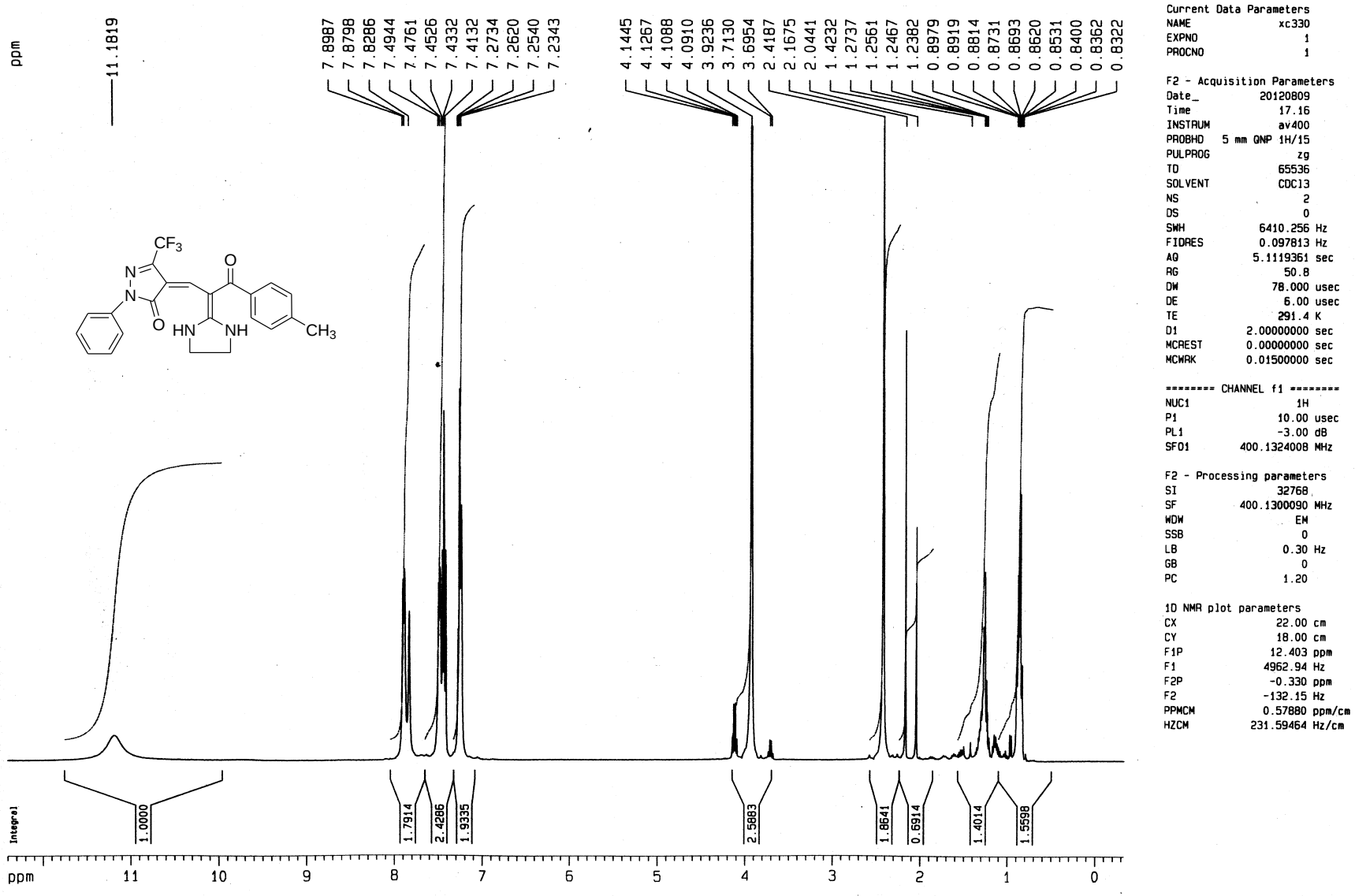
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 212.000 ppm
F1 21329.91 Hz
F2P 9.000 ppm
F2 905.52 Hz
PPMCM 9.22727 ppm/cm
HZCM 928.38153 Hz/cm

Figure 14. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of compound **6g**



Current Data Parameters

NAME	xc330
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120809
Time	17.16
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	CDCl3
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	50.8
DW	78.000 usec
DE	6.00 usec
TE	291.4 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

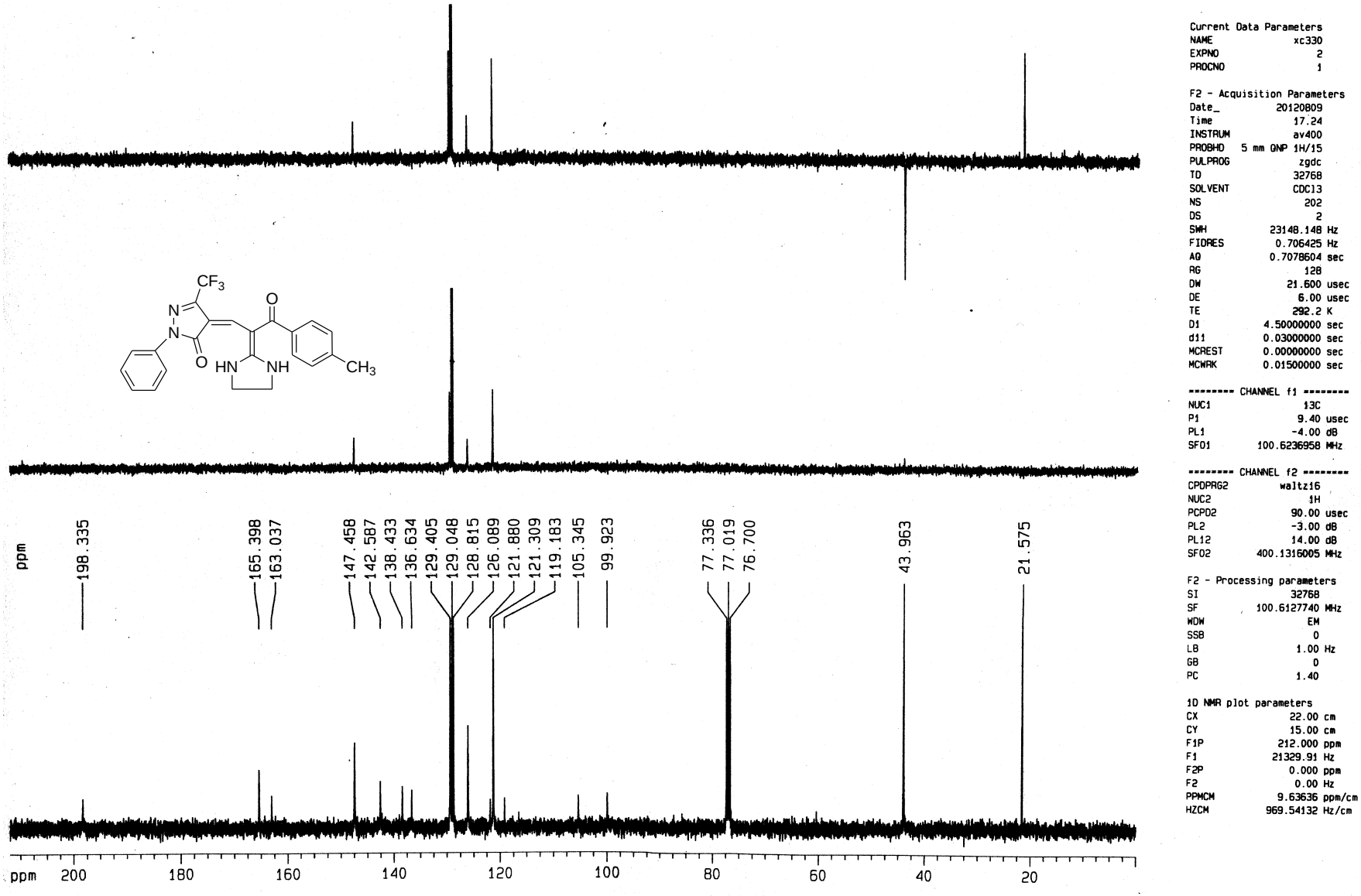
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.20

1D NMR plot parameters

CX	22.00 cm
CY	18.00 cm
F1P	12.403 ppm
F1	4962.94 Hz
F2P	-0.330 ppm
F2	-132.15 Hz
PPMCM	0.57880 ppm/cm
HZCM	231.59464 Hz/cm

Figure 15. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of compound **6h**



Current Data Parameters
NAME xc330
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120809
Time 17.24
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 202
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 128
DW 21.600 usec
DE 6.00 usec
TE 292.2 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

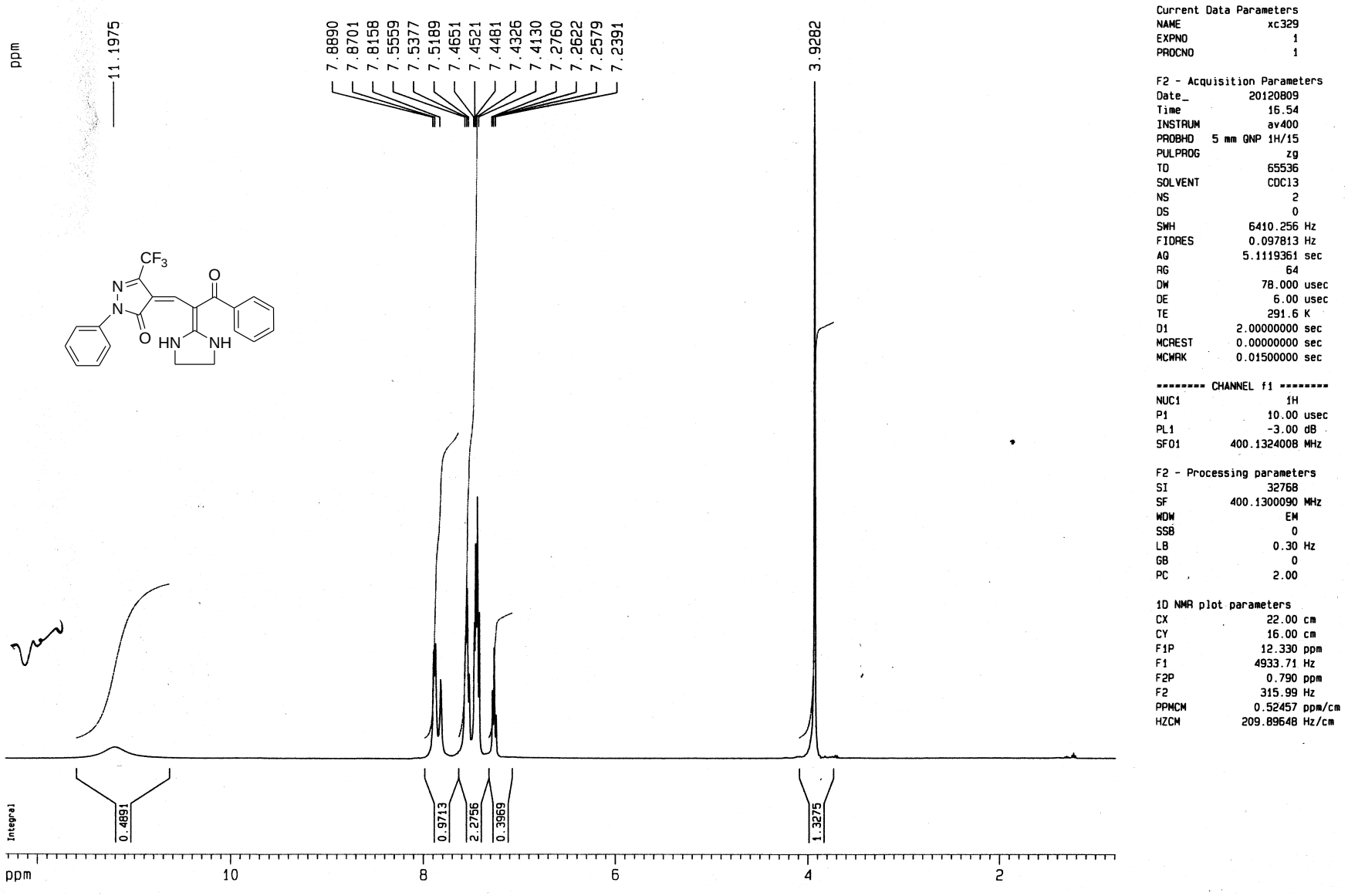
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 15.00 cm
F1P 212.000 ppm
F1 21329.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.63636 ppm/cm
HZCM 969.54132 Hz/cm

Figure 16. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of compound **6h**



Current Data Parameters

NAME	xc329
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120809
Time	16.54
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	CDCl3
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	64
DW	78.000 usec
DE	6.00 usec
TE	291.6 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

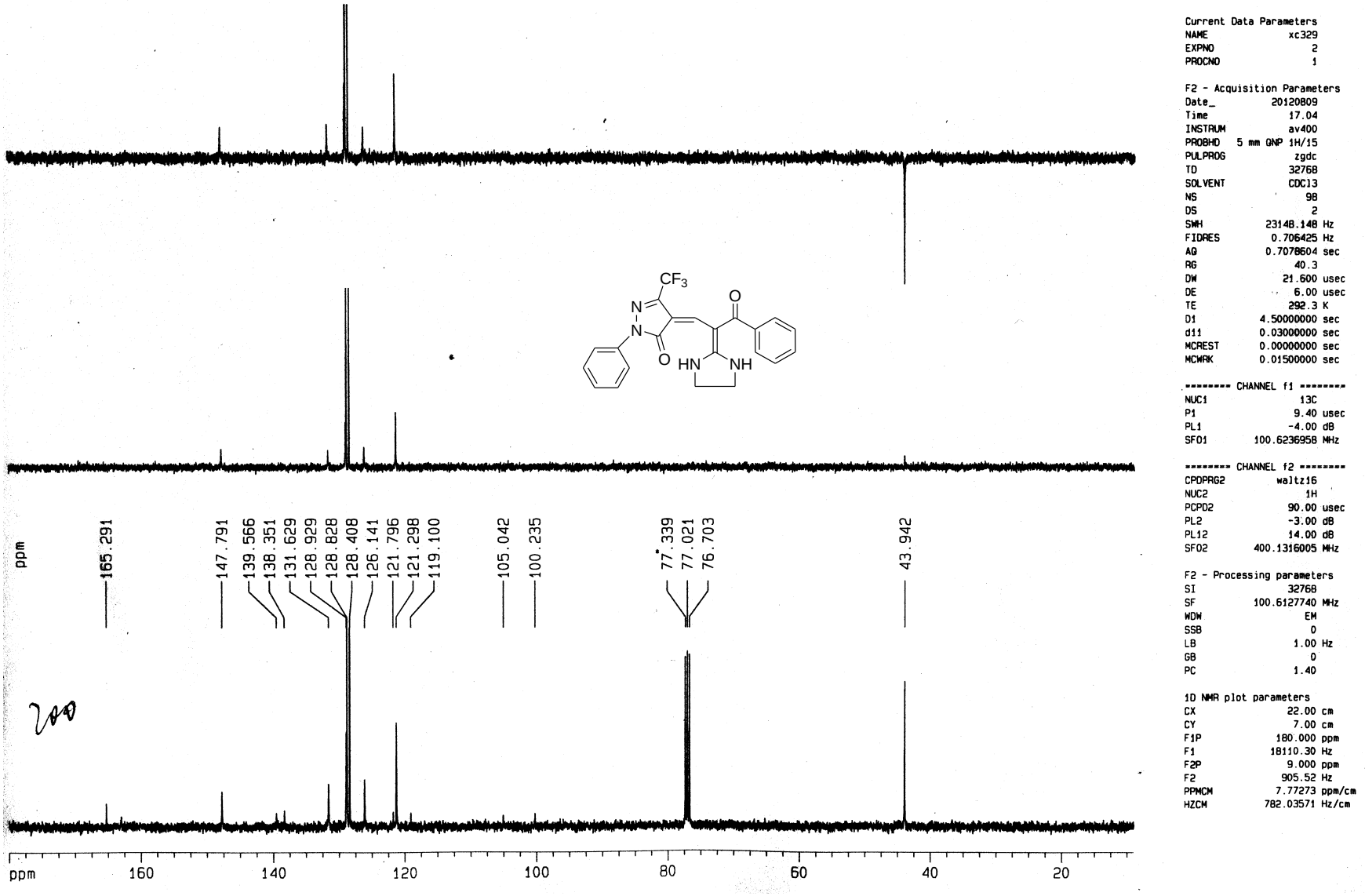
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	2.00

1D NMR plot parameters

CX	22.00 cm
CY	16.00 cm
F1P	12.330 ppm
F1	4933.71 Hz
F2P	0.790 ppm
F2	315.99 Hz
PPMCM	0.52457 ppm/cm
HZCM	209.89648 Hz/cm

Figure 17. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of compound **6i**



Current Data Parameters
NAME xc329
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120809
Time 17.04
INSTRUM av400
PROBHD 5 mm GNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 98
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 40.3
DW 21.600 usec
DE 6.00 usec
TE 292.3 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

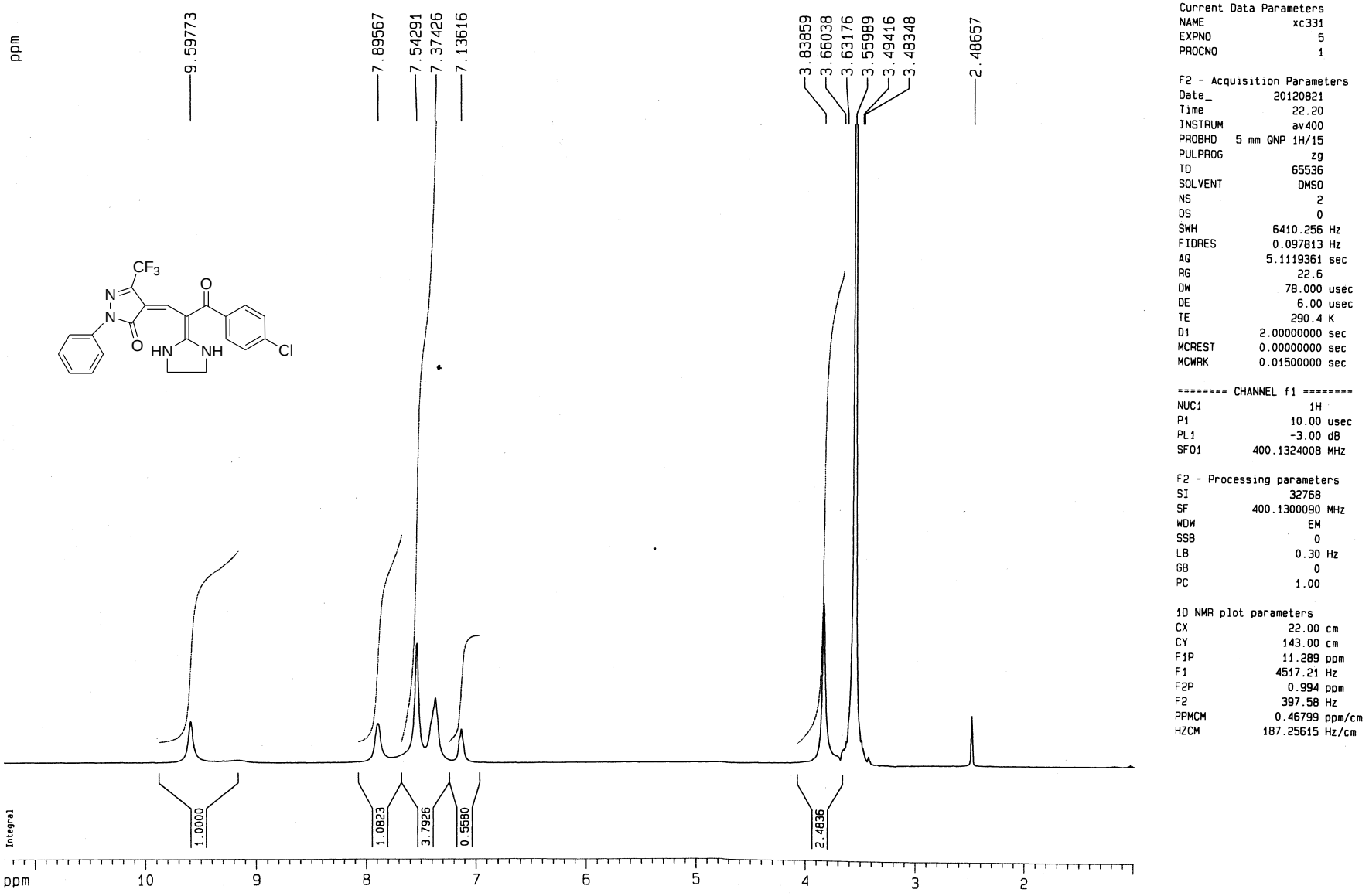
-------- CHANNEL f1 --------
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 7.00 cm
F1P 180.000 ppm
F1 18110.30 Hz
F2P 9.000 ppm
F2 905.52 Hz
PPMCM 7.77273 ppm/cm
HZCM 782.03571 Hz/cm

Figure 18. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of compound **6i**



Current Data Parameters

NAME	xc331
EXPNO	5
PROCNO	1

F2 - Acquisition Parameters

Date_	20120821
Time	22.20
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	22.6
DW	78.000 usec
DE	6.00 usec
TE	290.4 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

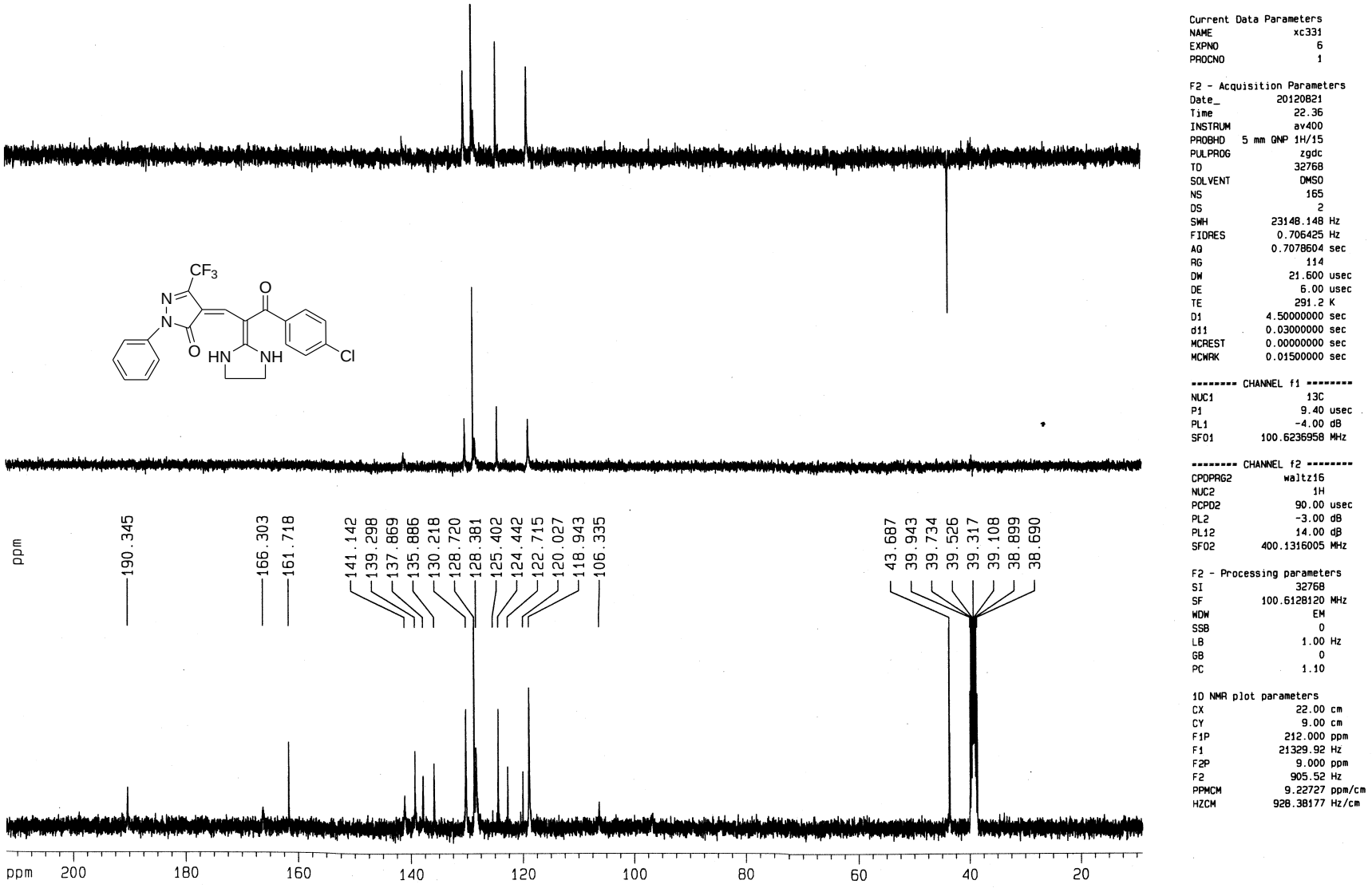
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	143.00 cm
F1P	11.289 ppm
F1	4517.21 Hz
F2P	0.994 ppm
F2	397.58 Hz
PPMCM	0.46799 ppm/cm
HZCM	187.25615 Hz/cm

Figure 19. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6j**




```
Current Data Parameters
NAME                 xc331
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120821
Time                 22.36
INSTRUM              av400
PROBHD   5 mm GNP 1H/15
PULPROG               zgdc
TD                   32768
SOLVENT               DMSO
NS                     165
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                     114
DW                21.600 usec
DE                 6.00 usec
TE                 291.2 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

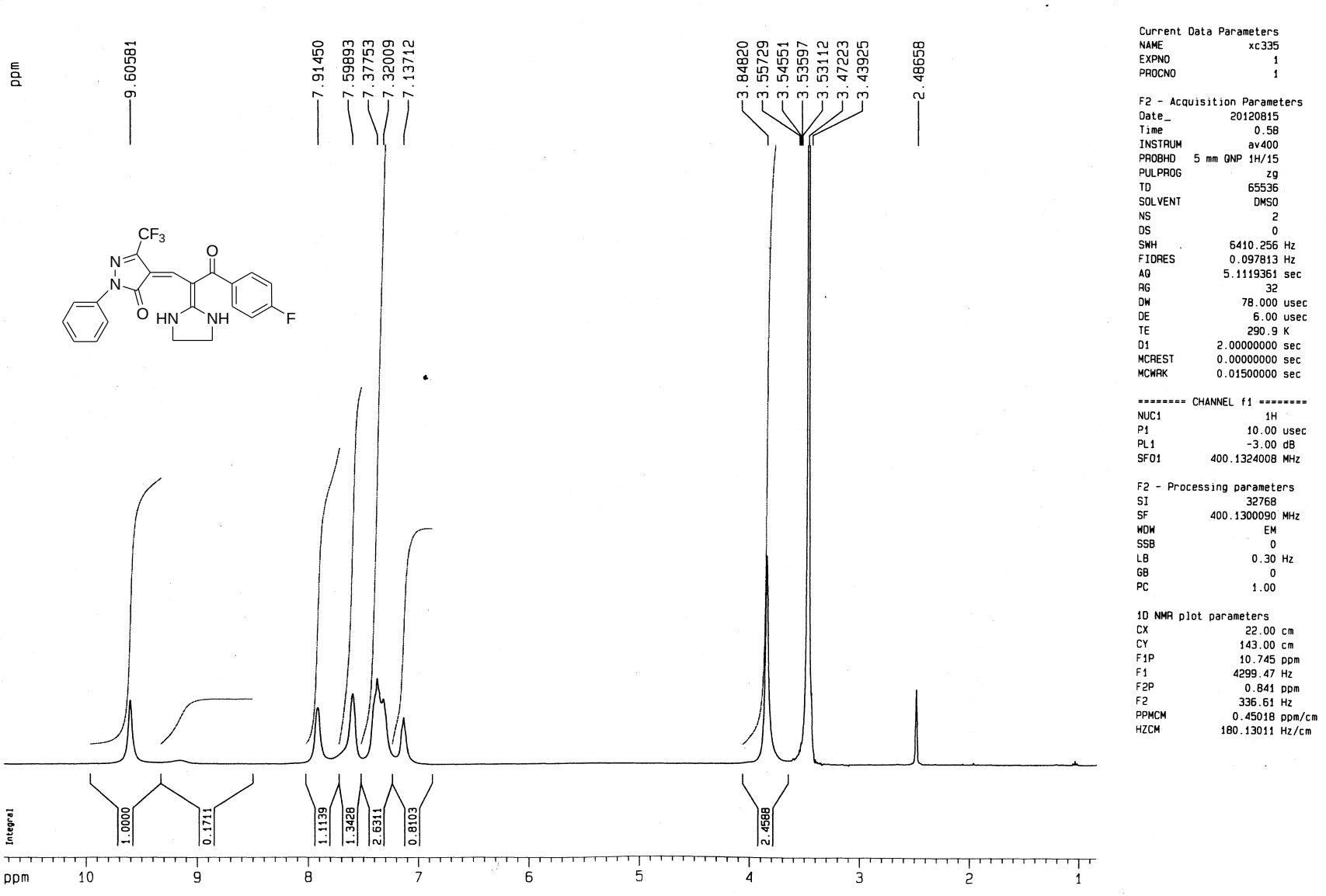
-------- CHANNEL f1 --------
NUC1                   13C
P1                9.40 usec
PL1                -4.00 dB
SFO1         100.6236958 MHz

-------- CHANNEL f2 --------
CPDPRG2            waltz16
NUC2                   1H
PCPD2             90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6128120 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.10

1D NMR plot parameters
CX                  22.00 cm
CY                   9.00 cm
F1P                212.000 ppm
F1               21329.92 Hz
F2P                  9.000 ppm
F2                 905.52 Hz
PPMCM             9.22727 ppm/cm
HZCM            928.38177 Hz/cm
```

Figure 20. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6j**



Current Data Parameters

NAME	xc335
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120815
Time	0.58
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	32
DW	78.000 usec
DE	6.00 usec
TE	290.9 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

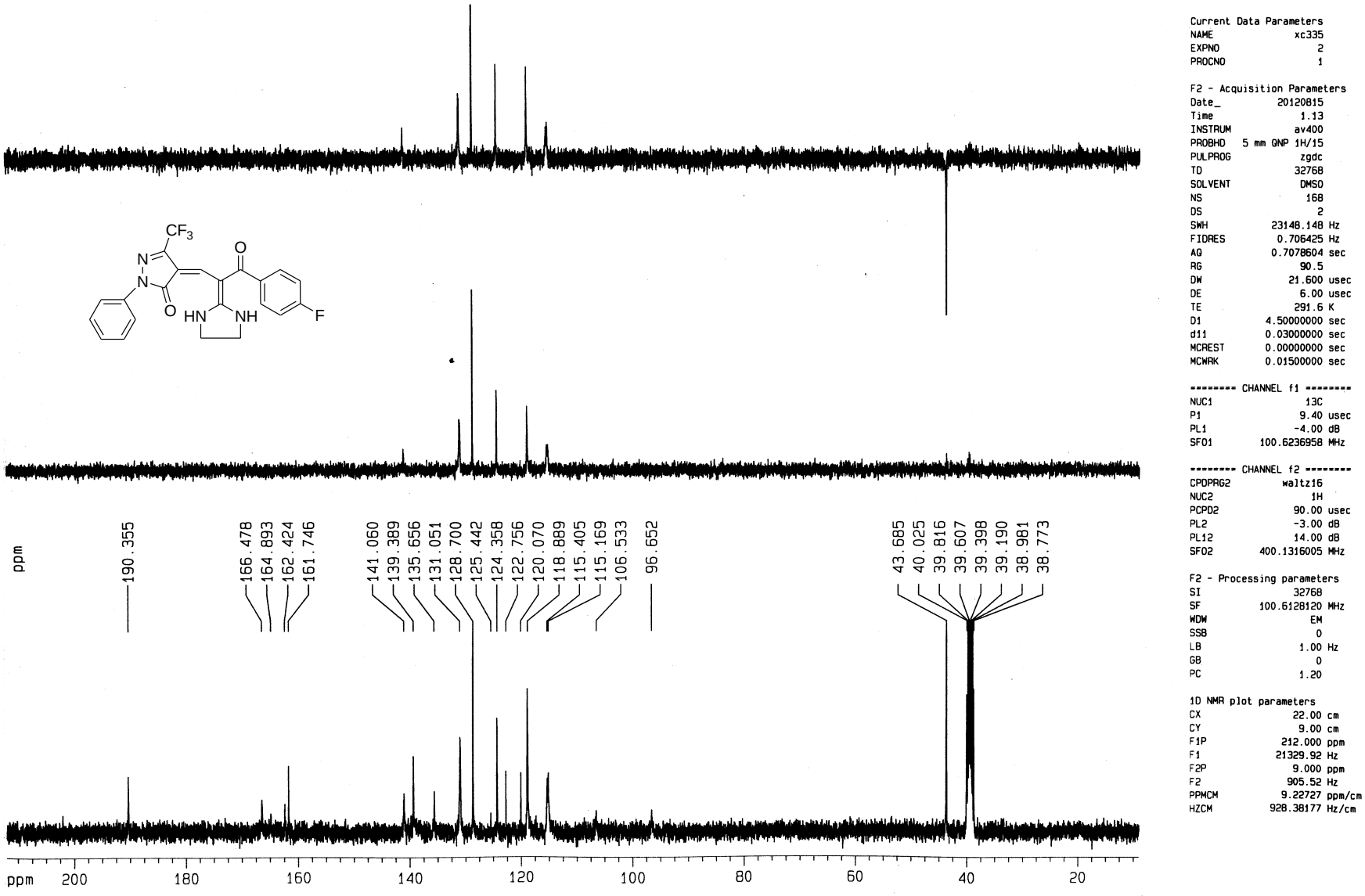
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	143.00 cm
F1P	10.745 ppm
F1	4299.47 Hz
F2P	0.841 ppm
F2	336.61 Hz
PPMCM	0.45018 ppm/cm
HZCM	180.13011 Hz/cm

Figure 21. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6k**




```
Current Data Parameters
NAME                 xc335
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120815
Time                 1.13
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     168
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                    90.5
DW                21.600 usec
DE                 6.00 usec
TE                 291.6 K
D1            4.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

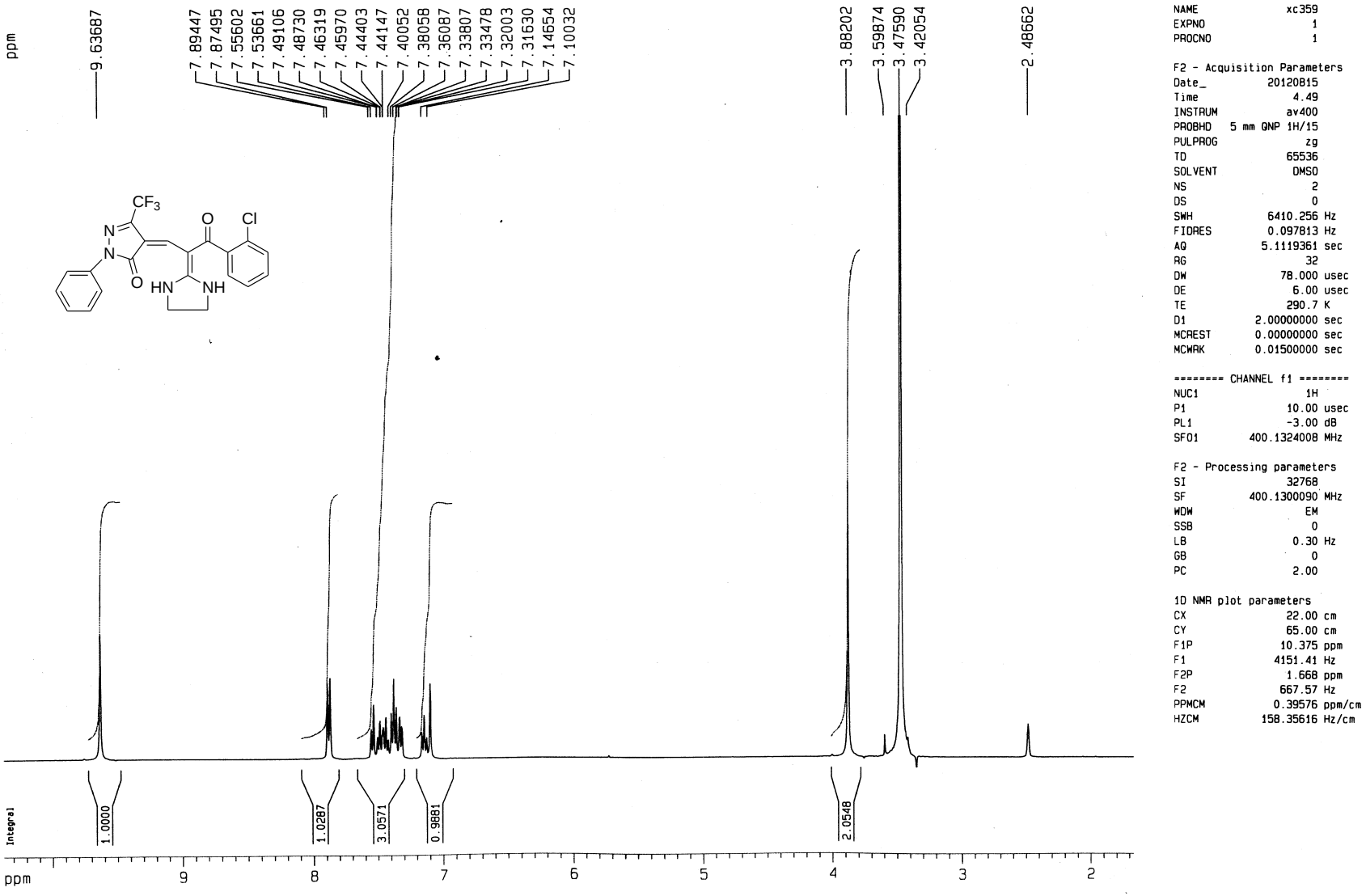
======== CHANNEL f1 ========
NUC1                  13C
P1                 9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6128120 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.20

1D NMR plot parameters
CX                  22.00 cm
CY                   9.00 cm
F1P               212.000 ppm
F1                21329.92 Hz
F2P                 9.000 ppm
F2                 905.52 Hz
PPMCM             9.22727 ppm/cm
HZCM             928.38177 Hz/cm
```

Figure 22. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6k**




```
Current Data Parameters
NAME                 xc359
EXPNO                    1
PROCNO                   1

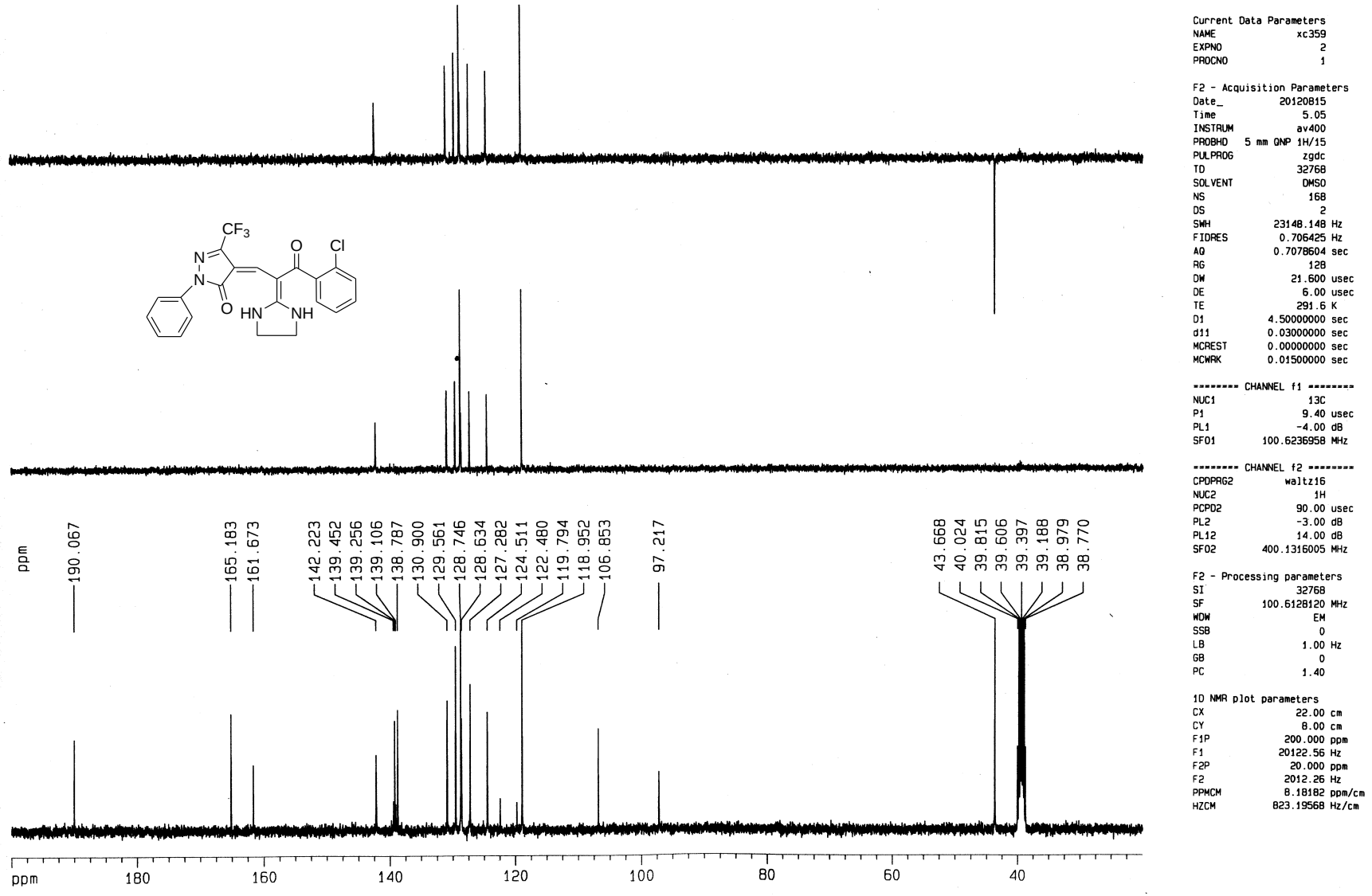
F2 - Acquisition Parameters
Date_             20120815
Time                 4.49
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG                 zg
TD                   65536
SOLVENT               DMSO
NS                       2
DS                       0
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1119361 sec
RG                      32
DW                  78.000 usec
DE                   6.00 usec
TE                  290.7 K
D1              2.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
PL1                  -3.00 dB
SFO1           400.1324008 MHz

F2 - Processing parameters
SI                   32768
SF             400.1300090 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                   22.00 cm
CY                   65.00 cm
F1P                 10.375 ppm
F1                4151.41 Hz
F2P                  1.668 ppm
F2                 667.57 Hz
PPMCM             0.39576 ppm/cm
HZCM            158.35616 Hz/cm
```

Figure 23. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6l**




```
Current Data Parameters
NAME                 xc359
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120815
Time                 5.05
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                    168
DS                      2
SWH             23148.148 Hz
FIDRES          0.706425 Hz
AQ              0.7078604 sec
RG                    128
DW                21.600 usec
DE                 6.00 usec
TE                291.6 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

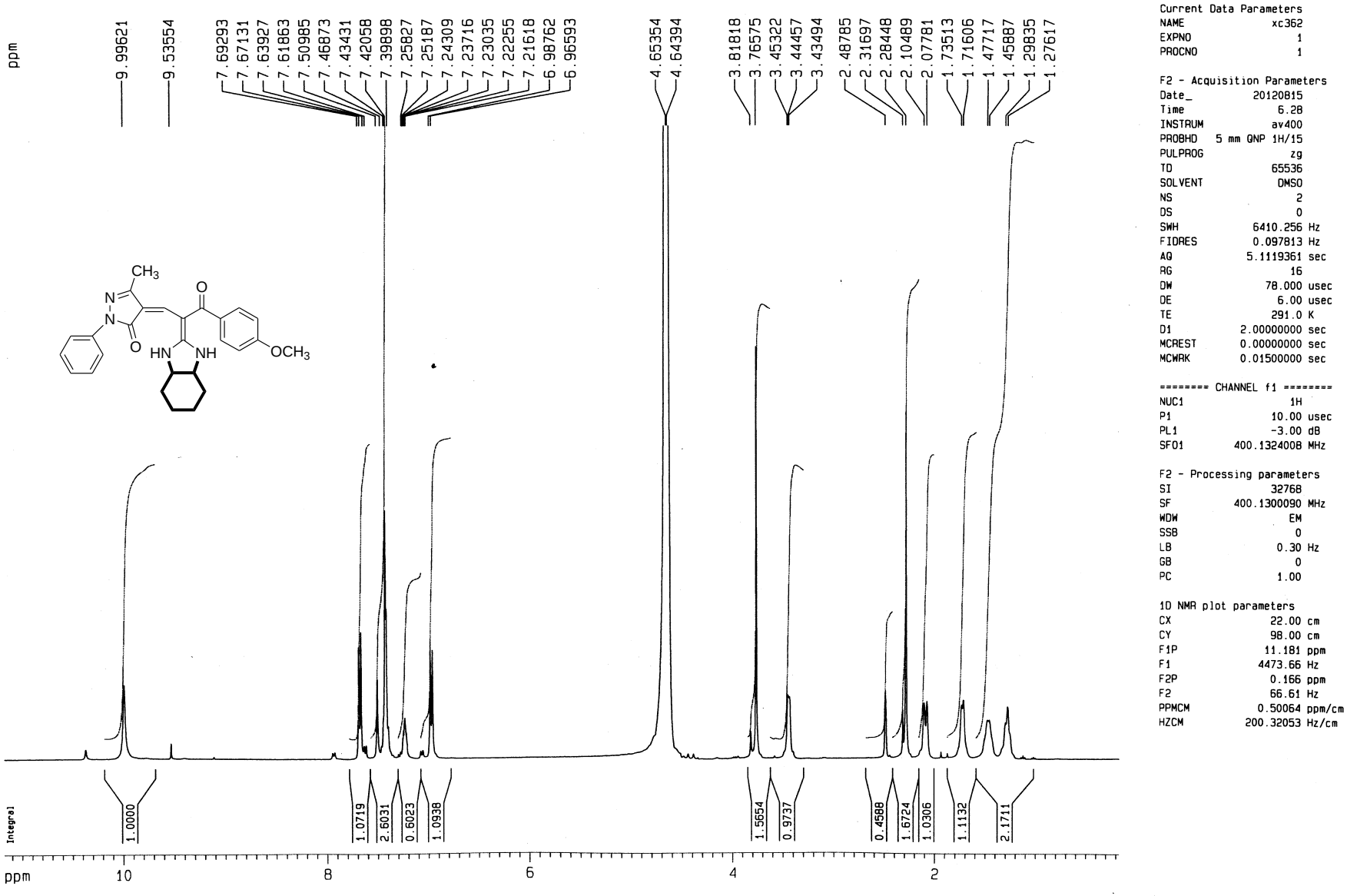
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -3.00 dB
PL12              14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6128120 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  22.00 cm
CY                   8.00 cm
F1P                200.000 ppm
F1               20122.56 Hz
F2P                 20.000 ppm
F2                2012.26 Hz
PPMCM             8.18182 ppm/cm
HZCM            823.19568 Hz/cm
```

Figure 24. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6l**




```
Current Data Parameters
NAME                  xc362
EXPNO                     1
PROCNO                    1

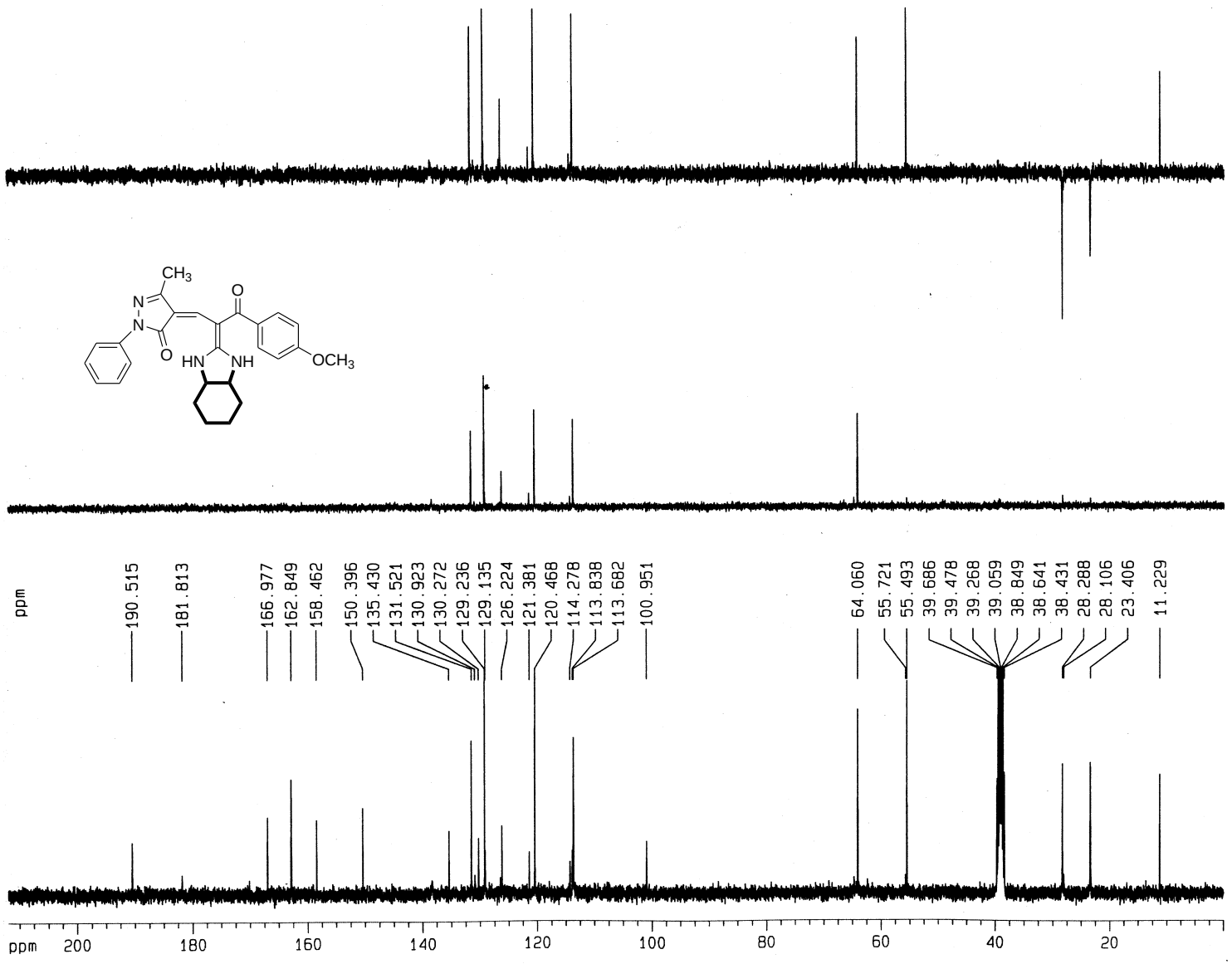
F2 - Acquisition Parameters
Date_              20120815
Time                  6.28
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG                zg
TD                  65536
SOLVENT              DMSO
NS                        2
DS                        0
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1119361 sec
RG                       16
DW                78.000 usec
DE                 6.00 usec
TE                 291.0 K
D1            2.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -3.00 dB
SFO1         400.1324008 MHz

F2 - Processing parameters
SI                    32768
SF           400.1300090 MHz
WDW                   EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                 22.00 cm
CY                 98.00 cm
F1P               11.181 ppm
F1               4473.66 Hz
F2P                0.166 ppm
F2                 66.61 Hz
PPMCM          0.50064 ppm/cm
HZCM          200.32053 Hz/cm
```

Figure 25. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6m**




```
Current Data Parameters
NAME                  xc362
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120815
Time                  6.44
INSTRUM               av400
PROBHD   5 mm QNP 1H/15
PULPROG                zgdc
TD                    32768
SOLVENT                DMSO
NS                      168
DS                        2
SWH               23148.148 Hz
FIDRES            0.706425 Hz
AQ                0.7078604 sec
RG                      128
DW                 21.600 usec
DE                  6.00 usec
TE                  291.7 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

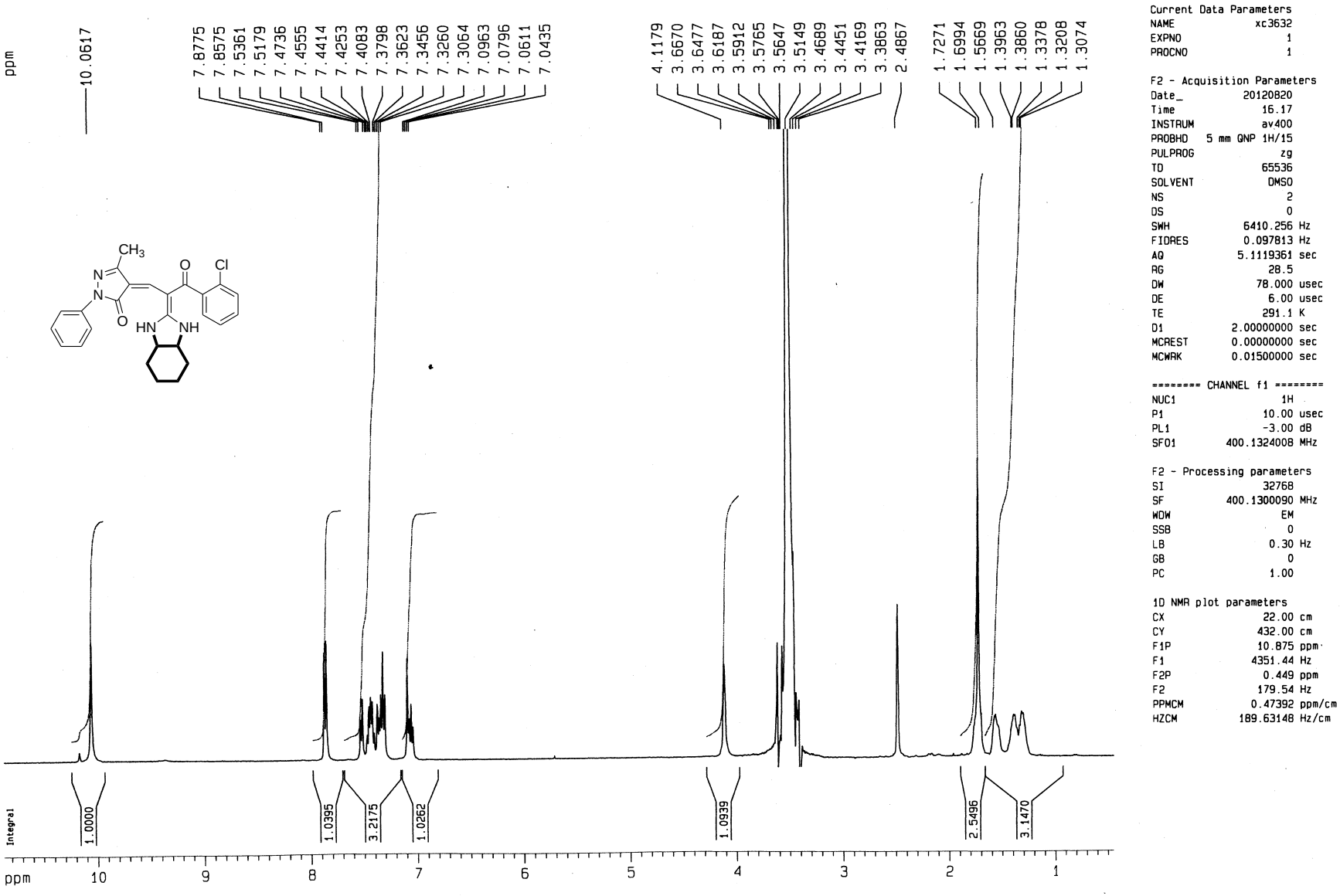
======== CHANNEL f1 ========
NUC1                    13C
P1                   9.40 usec
PL1                 -4.00 dB
SFO1           100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                 -3.00 dB
PL12                14.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6128120 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                    1.40

1D NMR plot parameters
CX                  22.00 cm
CY                   6.00 cm
F1P                212.000 ppm
F1                21329.92 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54156 Hz/cm
```

Figure 26. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6m**



Current Data Parameters
NAME xc3632
EXPNO 1
PROCNO 1

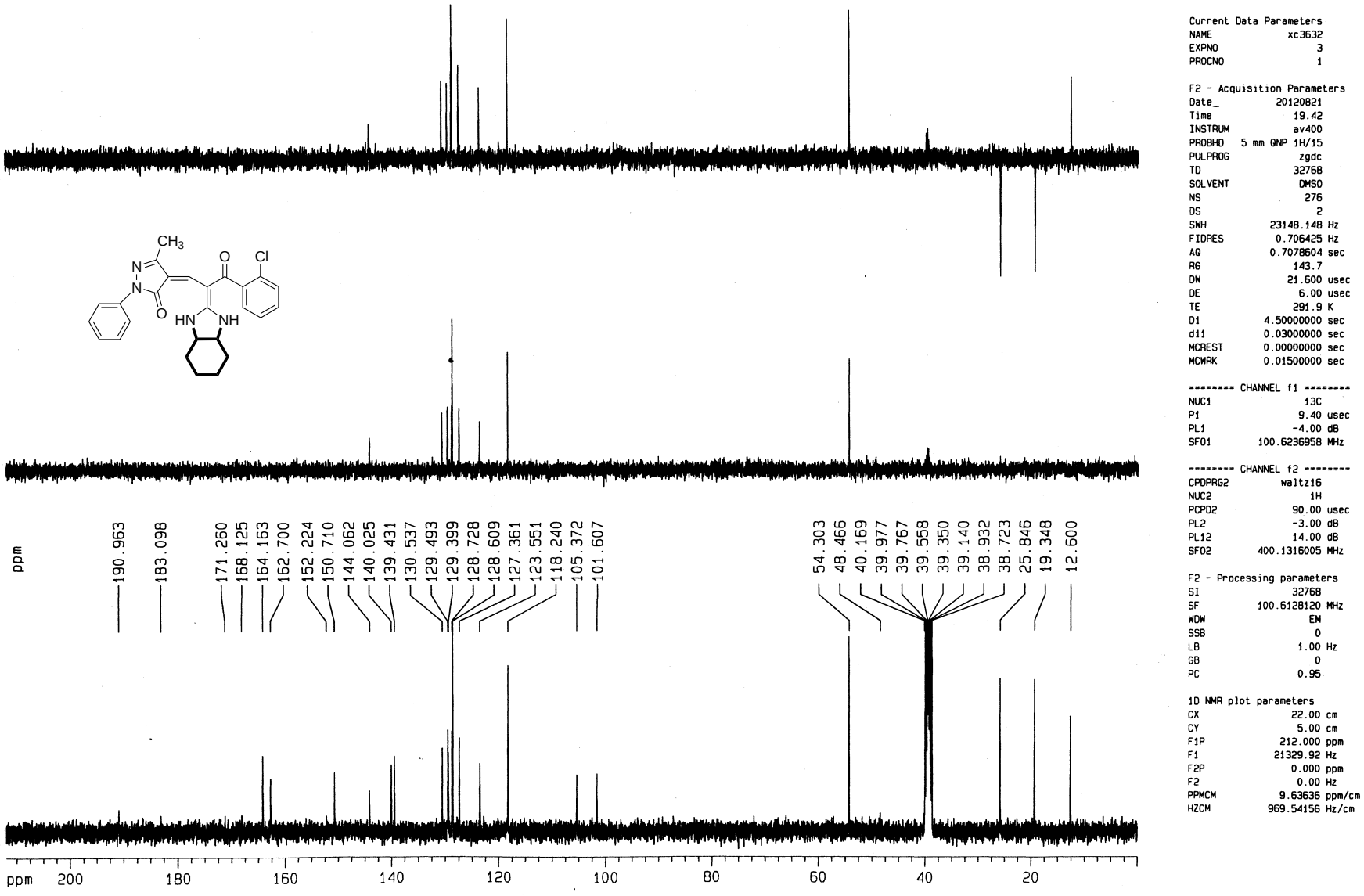
F2 - Acquisition Parameters
Date_ 20120820
Time 16.17
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zg
TD 65536
SOLVENT DMSO
NS 2
DS 0
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1119361 sec
RG 28.5
DW 78.000 usec
DE 6.00 usec
TE 291.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 432.00 cm
F1P 10.875 ppm
F1 4351.44 Hz
F2P 0.449 ppm
F2 179.54 Hz
PPMCM 0.47392 ppm/cm
HZCM 189.63148 Hz/cm

Figure 27. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **6n**




```
Current Data Parameters
NAME                 xc3632
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120821
Time                  19.42
INSTRUM               av400
PROBHD   5 mm QNP 1H/15
PULPROG                zgdc
TD                    32768
SOLVENT                DMSO
NS                      276
DS                        2
SWH               23148.148 Hz
FIDRES            0.706425 Hz
AQ                0.7078604 sec
RG                    143.7
DW                 21.600 usec
DE                  6.00 usec
TE                  291.9 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6128120 MHz
WDW                      EM
SSB                       0
LB                 1.00 Hz
GB                        0
PC                     0.95

1D NMR plot parameters
CX                 22.00 cm
CY                  5.00 cm
F1P               212.000 ppm
F1              21329.92 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM           9.63636 ppm/cm
HZCM          969.54156 Hz/cm
```

Figure 28. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **6n**

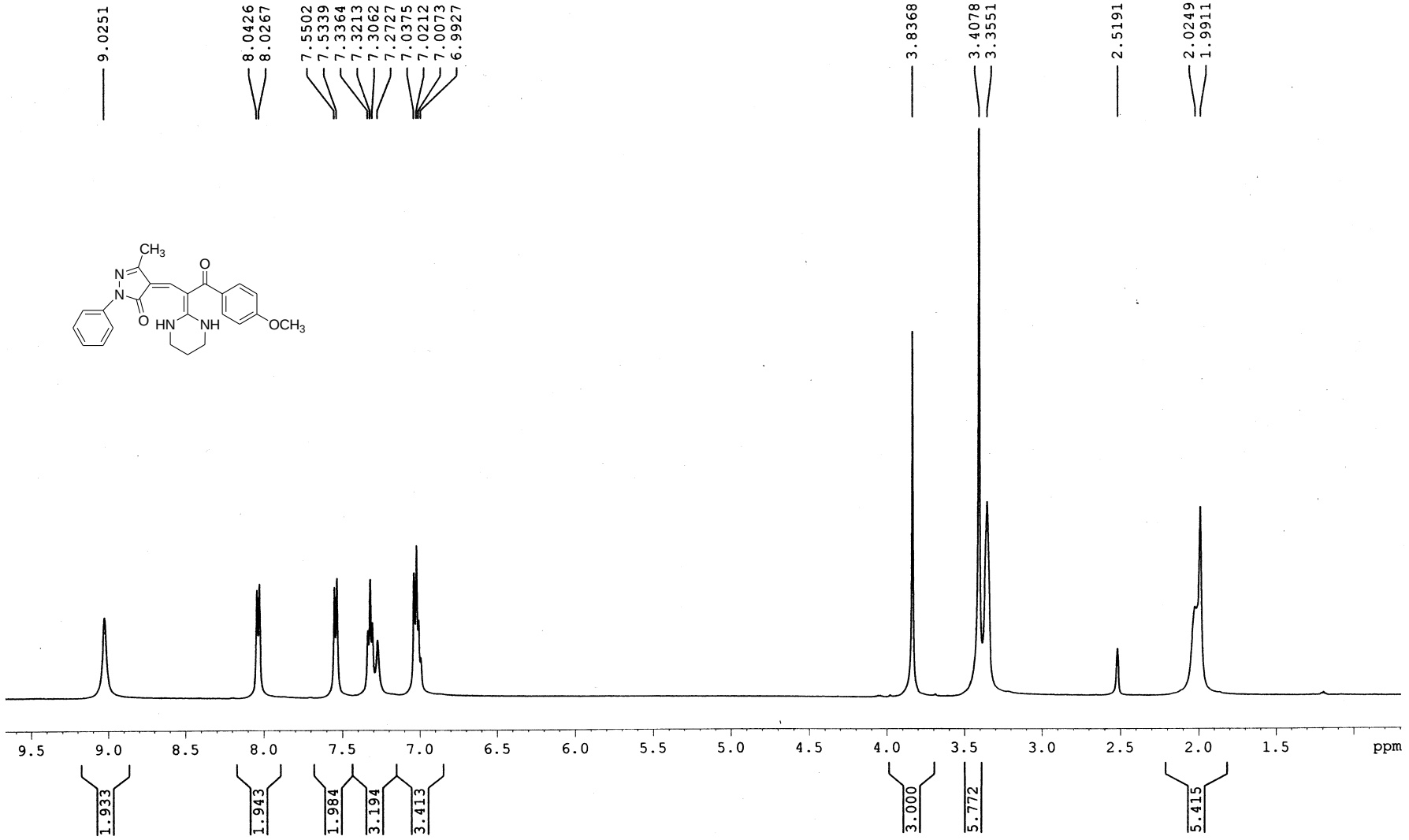


Figure 29. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **7a**

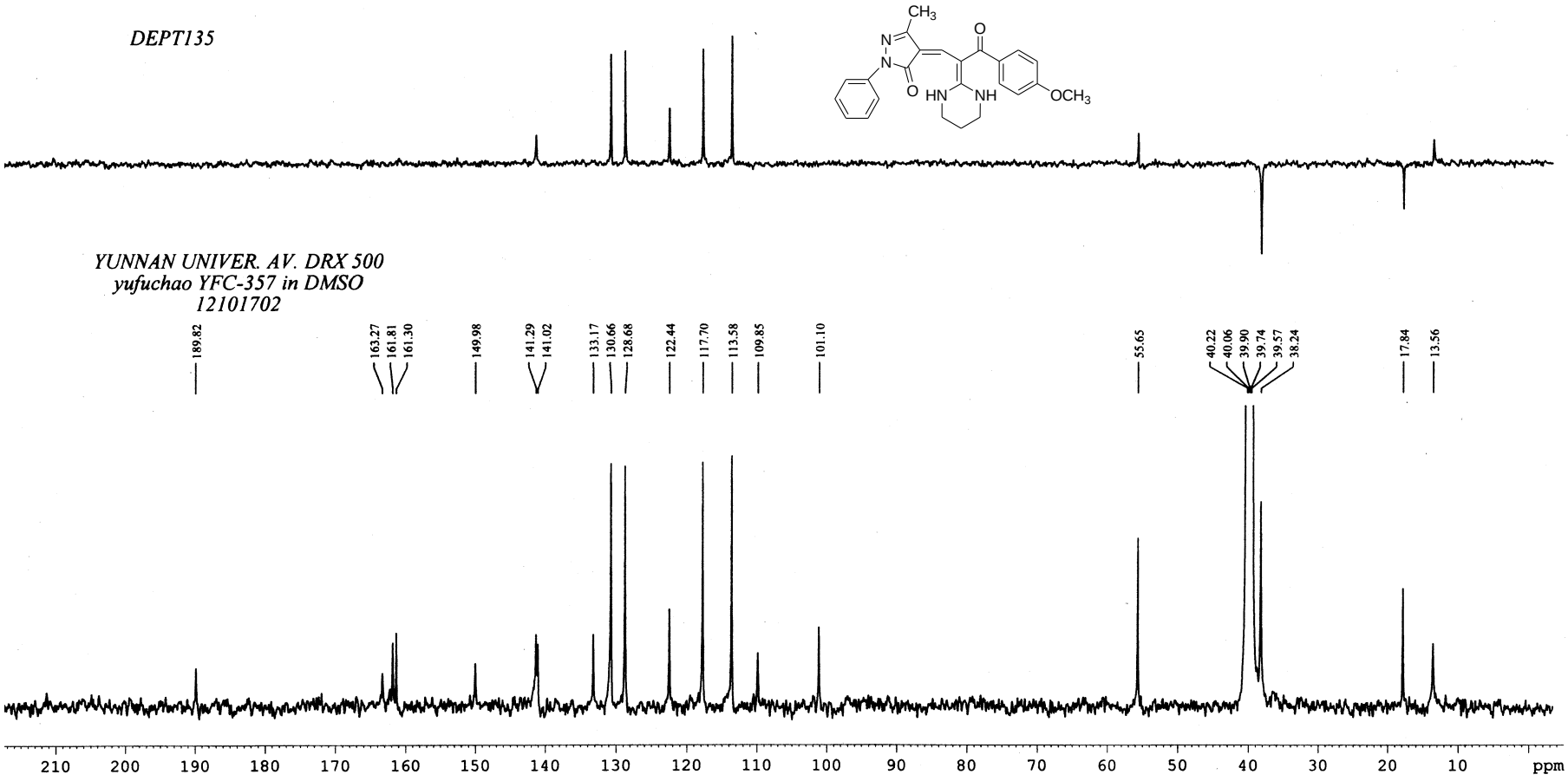
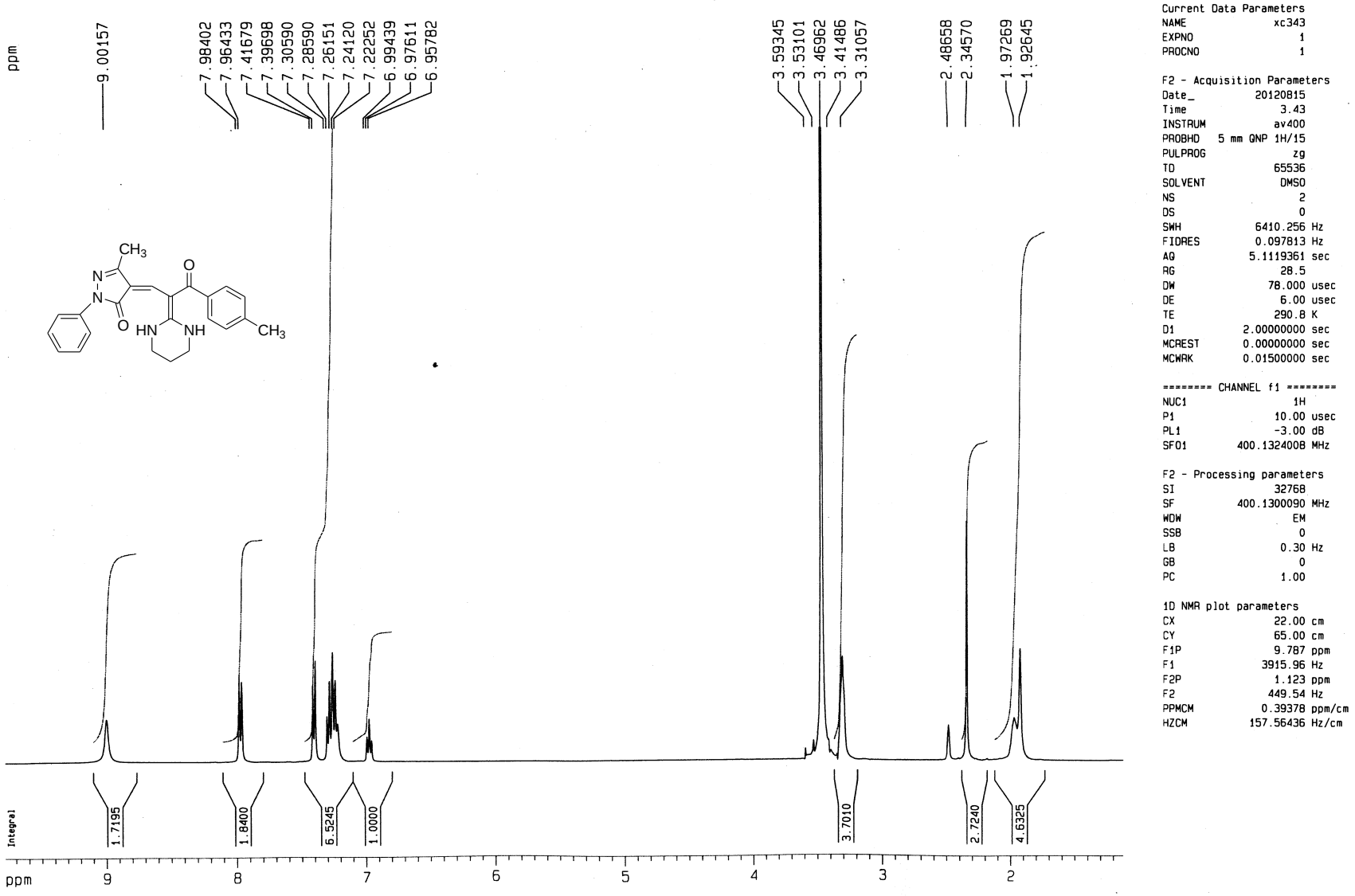


Figure 30. ^{13}C NMR (125 MHz, DMSO-d_6) spectra of compound **7a**




```
Current Data Parameters
NAME                  xc343
EXPNO                     1
PROCNO                    1

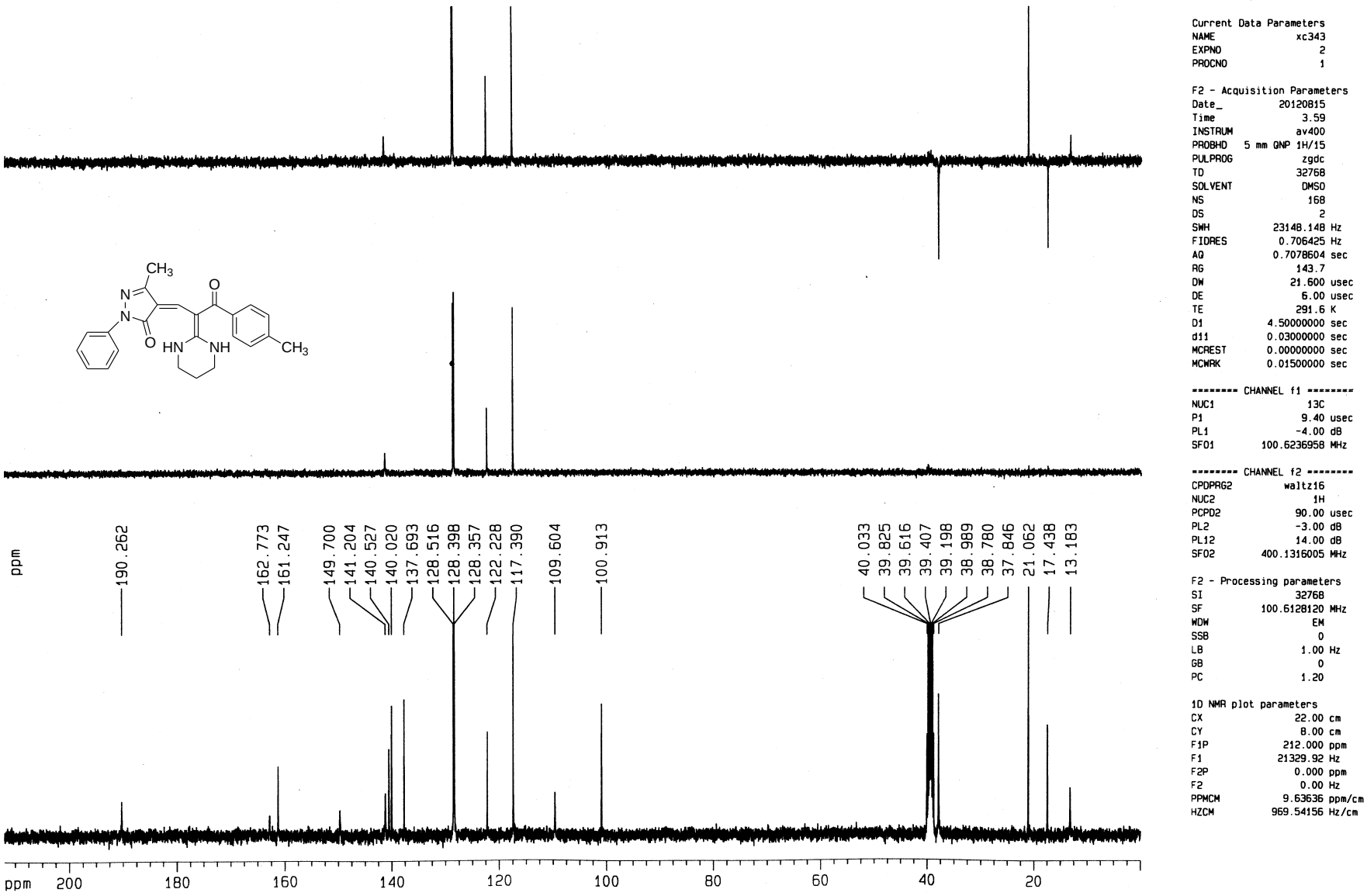
F2 - Acquisition Parameters
Date_              20120815
Time                  3.43
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG                zg
TD                  65536
SOLVENT              DMSO
NS                        2
DS                        0
SWH              6410.256 Hz
FIDRES           0.097813 Hz
AQ               5.1119361 sec
RG                     28.5
DW                78.000 usec
DE                 6.00 usec
TE                 290.8 K
D1               2.00000000 sec
MCREST           0.00000000 sec
MCWRK            0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                 10.00 usec
PL1                -3.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300090 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                 22.00 cm
CY                 65.00 cm
F1P                9.787 ppm
F1               3915.96 Hz
F2P                1.123 ppm
F2                 449.54 Hz
PPMCM           0.39378 ppm/cm
HZCM          157.56436 Hz/cm
```

Figure 31. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7b**




```
Current Data Parameters
NAME                 xc343
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120815
Time                 3.59
INSTRUM              av400
PROBHD   5 mm GNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                    168
DS                      2
SWH           23148.148 Hz
FIDRES        0.706425 Hz
AQ            0.7078604 sec
RG                  143.7
DW                21.600 usec
DE                 6.00 usec
TE                291.6 K
D1           4.50000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

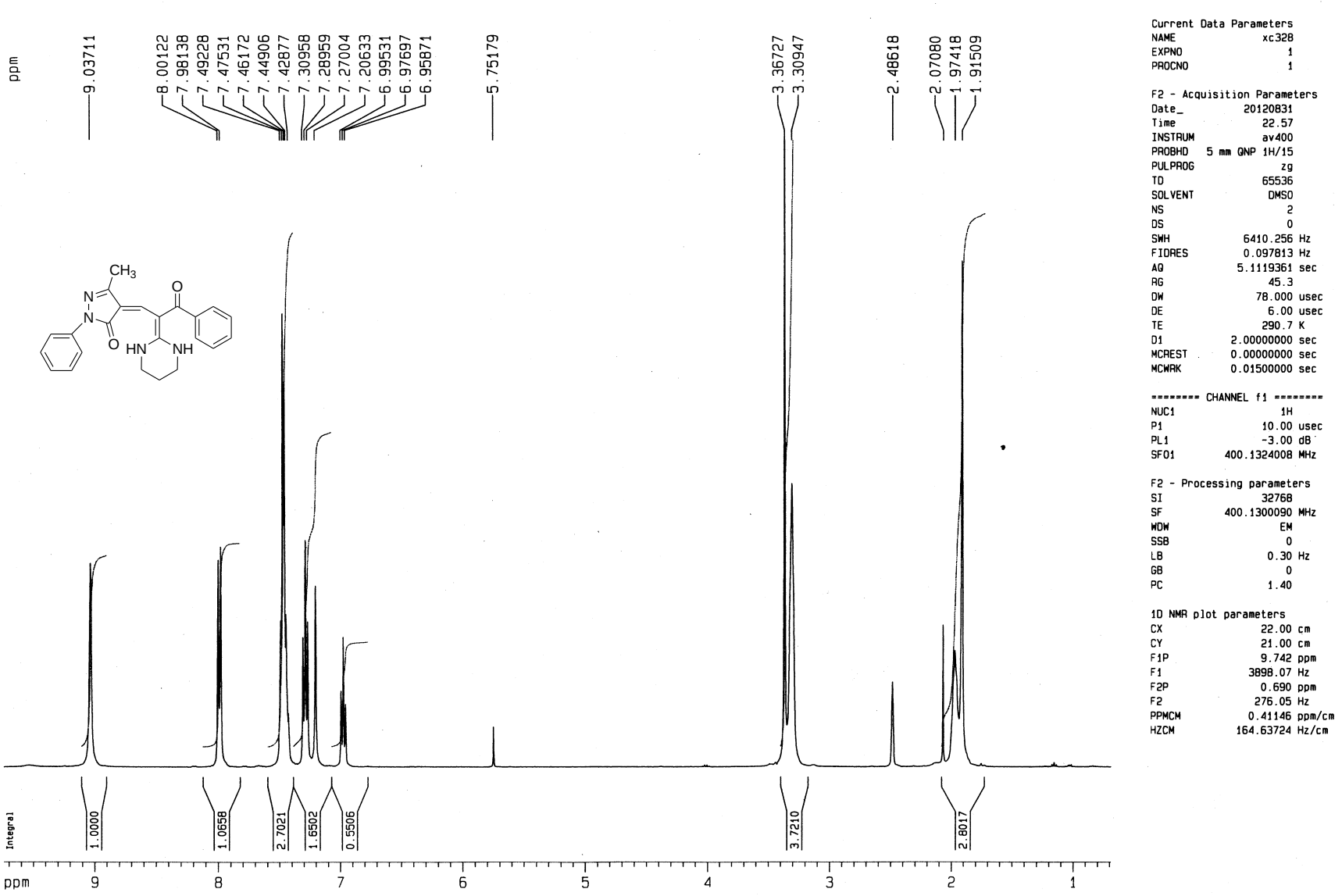
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.40 usec
PL1                -4.00 dB
SFO1         100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -3.00 dB
PL12              14.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6128120 MHz
WDW                    EM
SSB                     0
LB                 1.00 Hz
GB                      0
PC                   1.20

1D NMR plot parameters
CX                 22.00 cm
CY                  8.00 cm
F1P              212.000 ppm
F1             21329.92 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM          9.63636 ppm/cm
HZCM         969.54156 Hz/cm
```

Figure 32. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7b**



Current Data Parameters
NAME xc328
EXPNO 1
PROCNO 1

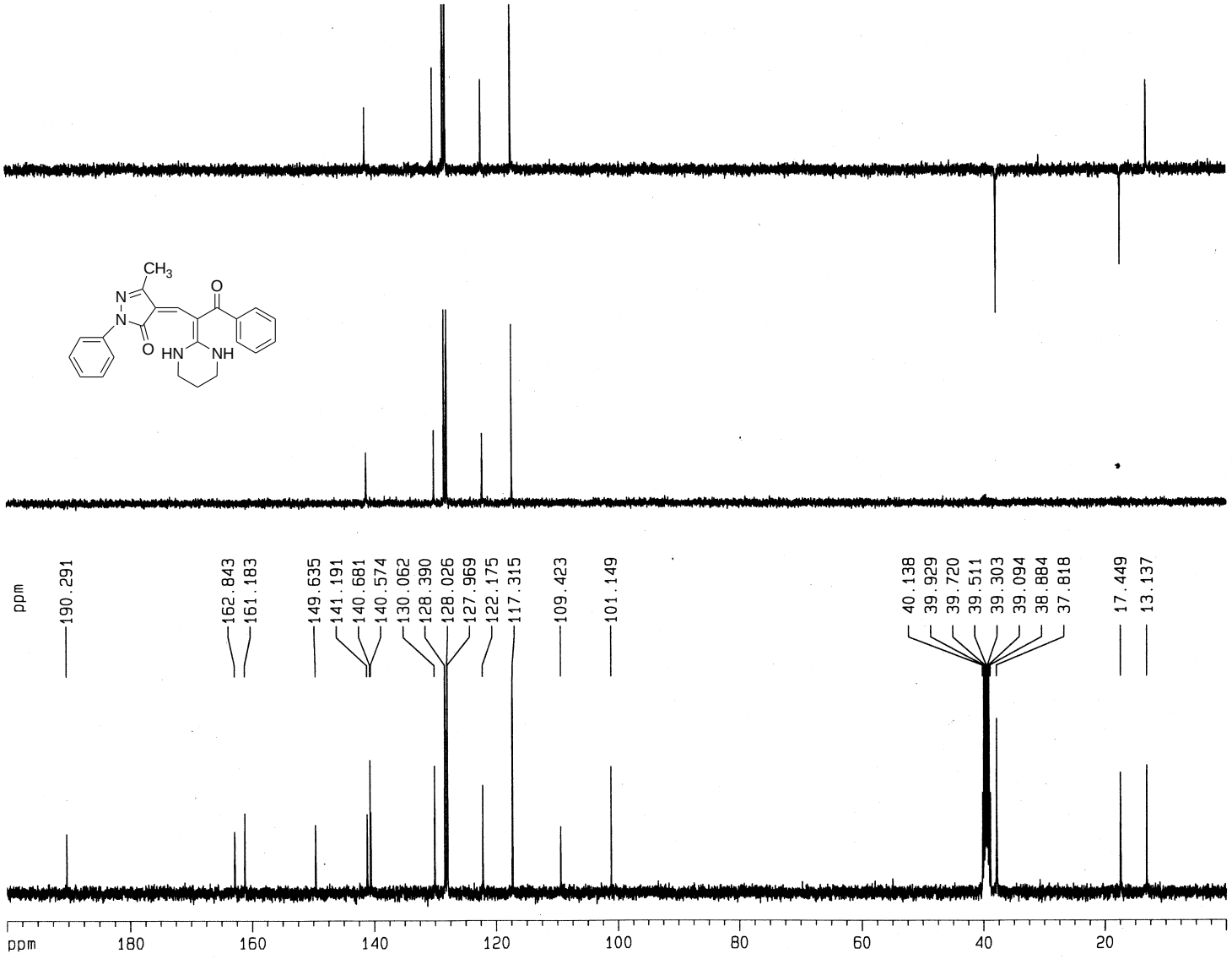
F2 - Acquisition Parameters
Date_ 20120831
Time 22.57
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zg
TD 65536
SOLVENT DMSO
NS 2
DS 0
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1119361 sec
RG 45.3
DW 78.000 usec
DE 6.00 usec
TE 290.7 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 21.00 cm
F1P 9.742 ppm
F1 3898.07 Hz
F2P 0.690 ppm
F2 276.05 Hz
PPMCM 0.41146 ppm/cm
HZCM 164.63724 Hz/cm

Figure 33. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7c**



Current Data Parameters
NAME xc328
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120831
Time 23.12
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 165
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 57
DW 21.600 usec
DE 6.00 usec
TE 291.3 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

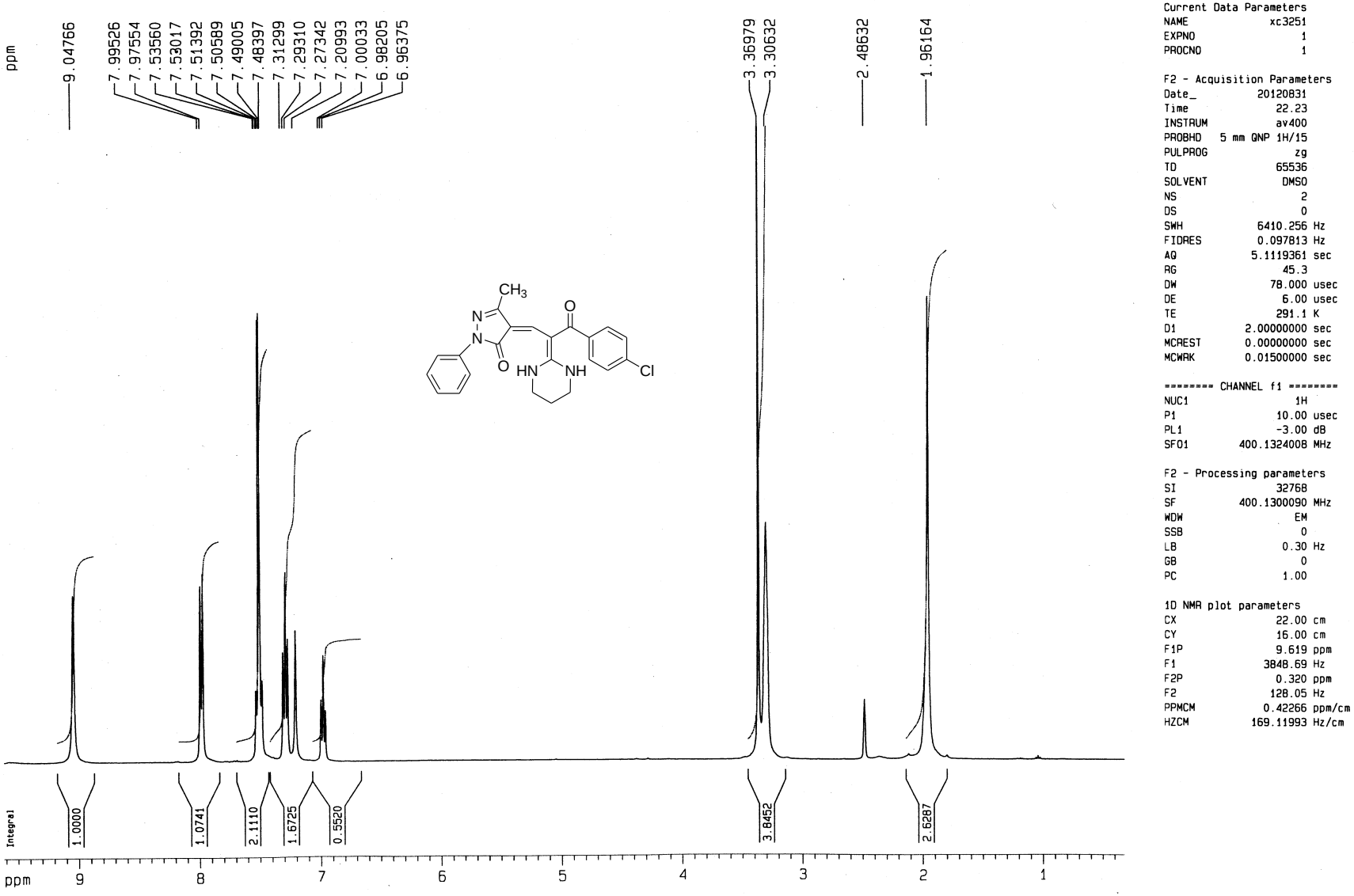
-------- CHANNEL f1 --------
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128120 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 7.00 cm
F1P 200.000 ppm
F1 20122.56 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 9.09091 ppm/cm
HZCM 914.66193 Hz/cm

Figure 34. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7c**



Current Data Parameters

NAME	xc3251
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120831
Time	22.23
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	45.3
DW	78.000 usec
DE	6.00 usec
TE	291.1 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

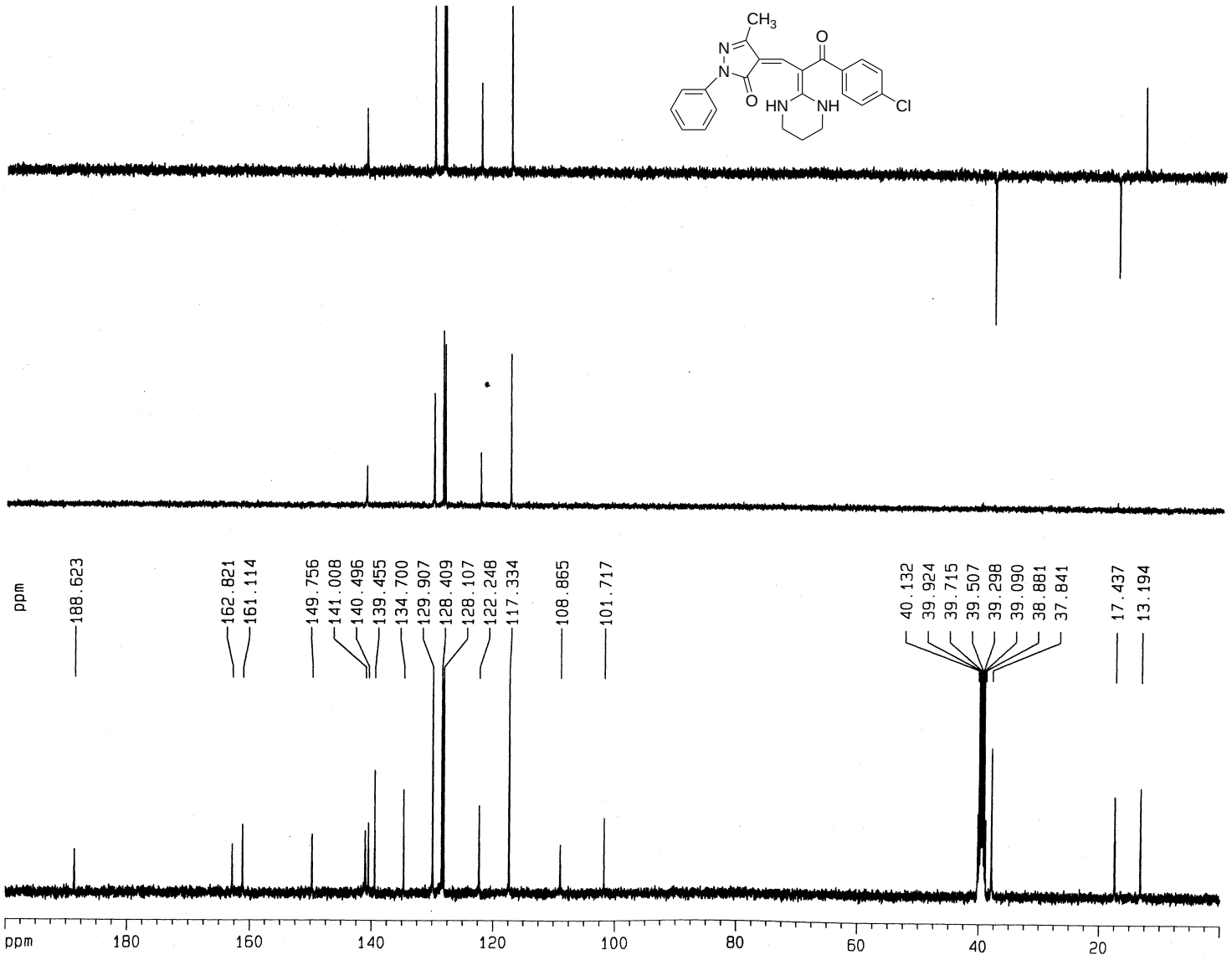
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	16.00 cm
F1P	9.619 ppm
F1	3848.69 Hz
F2P	0.320 ppm
F2	128.05 Hz
PPMCM	0.42266 ppm/cm
HZCM	169.11993 Hz/cm

Figure 35. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7d**



Current Data Parameters
NAME xc3251
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120831
Time 22.39
INSTRUM av400
PROBHD 5 mm GNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 165
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 71.8
DW 21.600 usec
DE 6.00 usec
TE 291.7 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

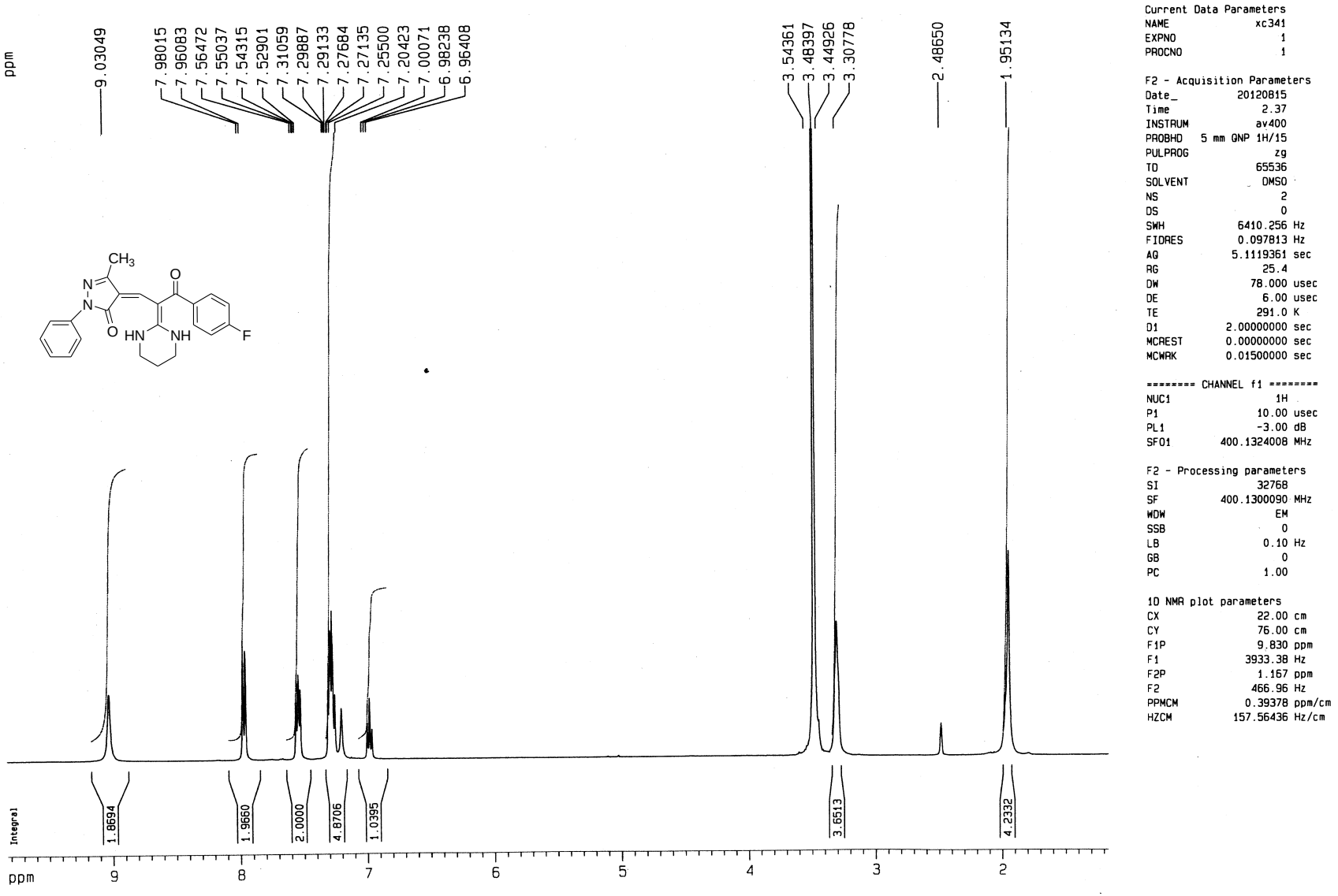
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128120 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 6.00 cm
F1P 200.000 ppm
F1 20122.56 Hz
F2P -0.000 ppm
F2 -0.00 Hz
PPMCM 9.09091 ppm/cm
HZCM 914.66193 Hz/cm

Figure 36. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7d**



Current Data Parameters
NAME xc341
EXPNO 1
PROCNO 1

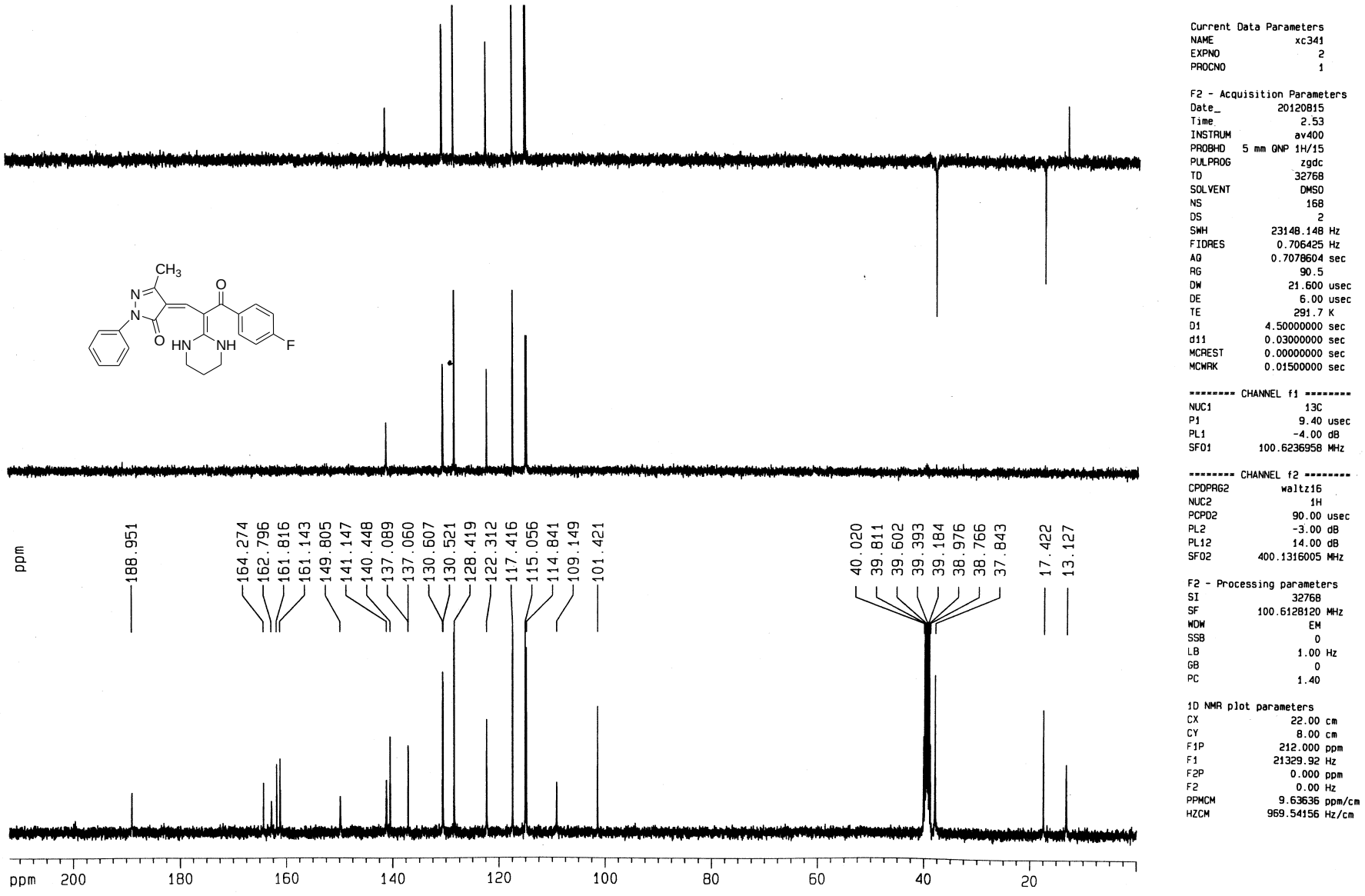
F2 - Acquisition Parameters
Date_ 20120815
Time 2.37
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zg
TD 65536
SOLVENT DMSO
NS 2
DS 0
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1119361 sec
RG 25.4
DW 78.000 usec
DE 6.00 usec
TE 291.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 76.00 cm
F1P 9.830 ppm
F1 3933.38 Hz
F2P 1.167 ppm
F2 466.96 Hz
PPMCM 0.39378 ppm/cm
HZCM 157.56436 Hz/cm

Figure 37. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7e**




```
Current Data Parameters
NAME                 xc341
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120815
Time                 2.53
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                    168
DS                      2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                   90.5
DW                21.600 usec
DE                 6.00 usec
TE                 291.7 K
D1            4.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6128120 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                  1.40

1D NMR plot parameters
CX                 22.00 cm
CY                  8.00 cm
F1P               212.000 ppm
F1              21329.92 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54156 Hz/cm
```

Figure 38. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7e**

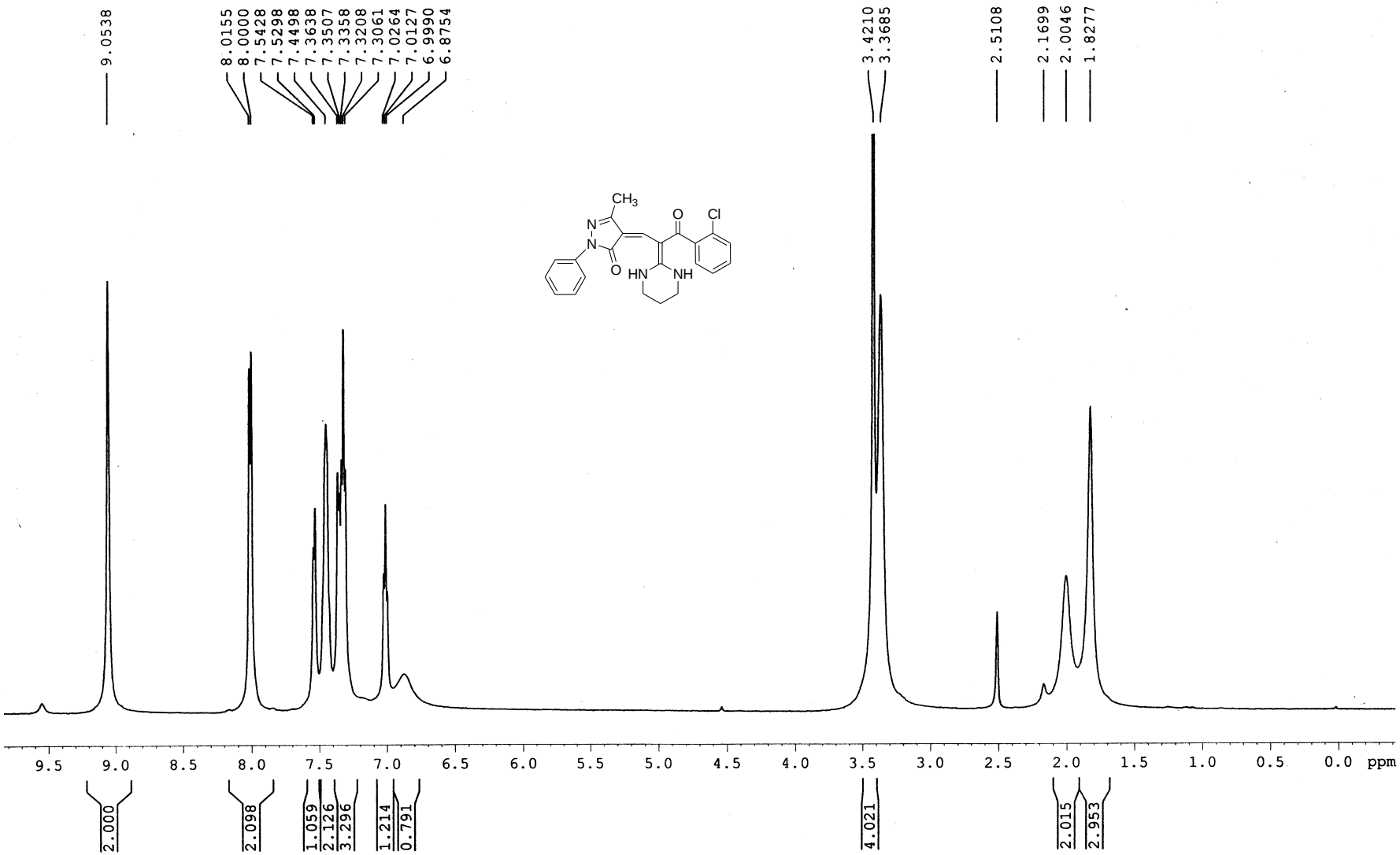


Figure 39. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **7f**

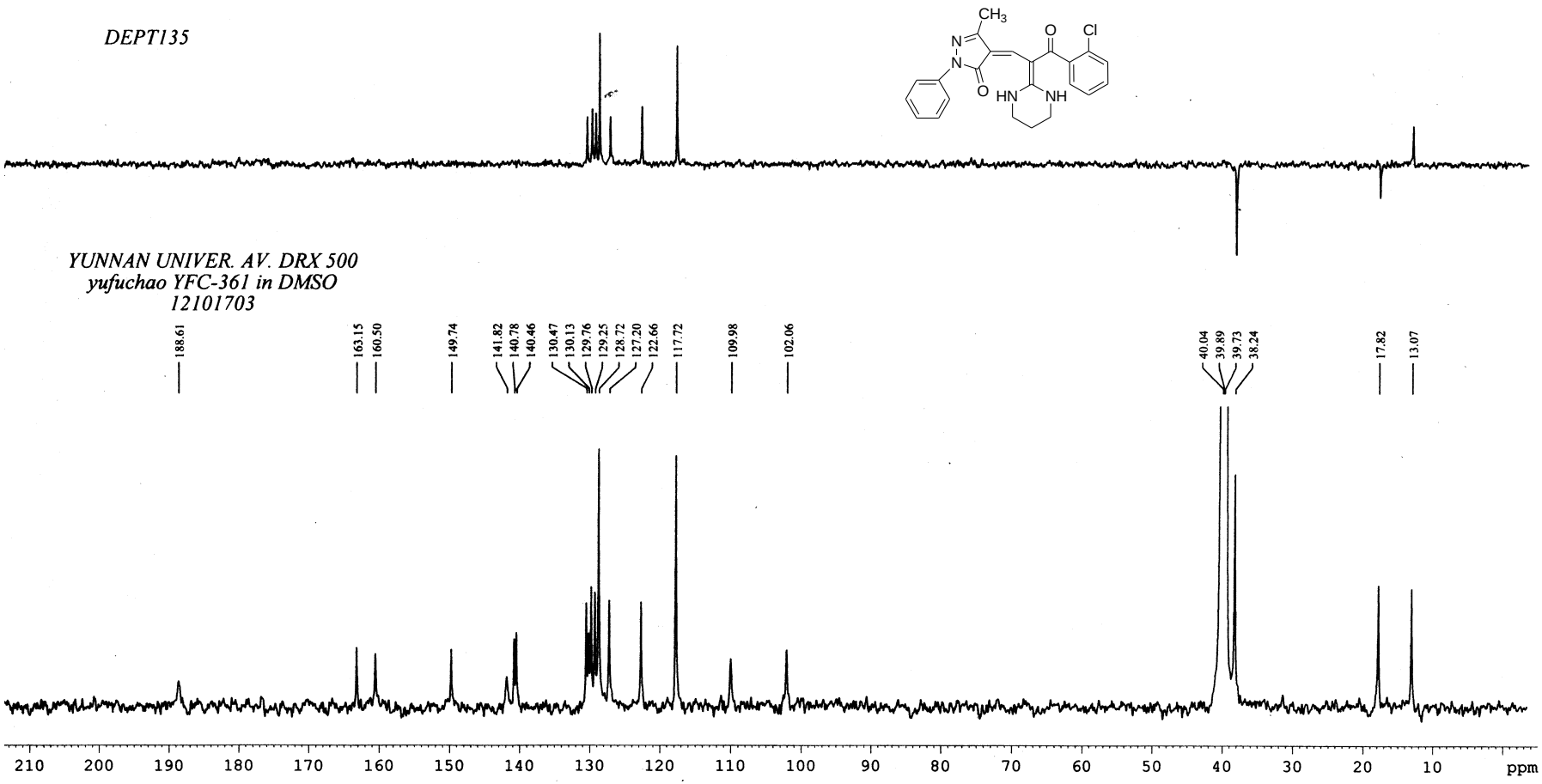
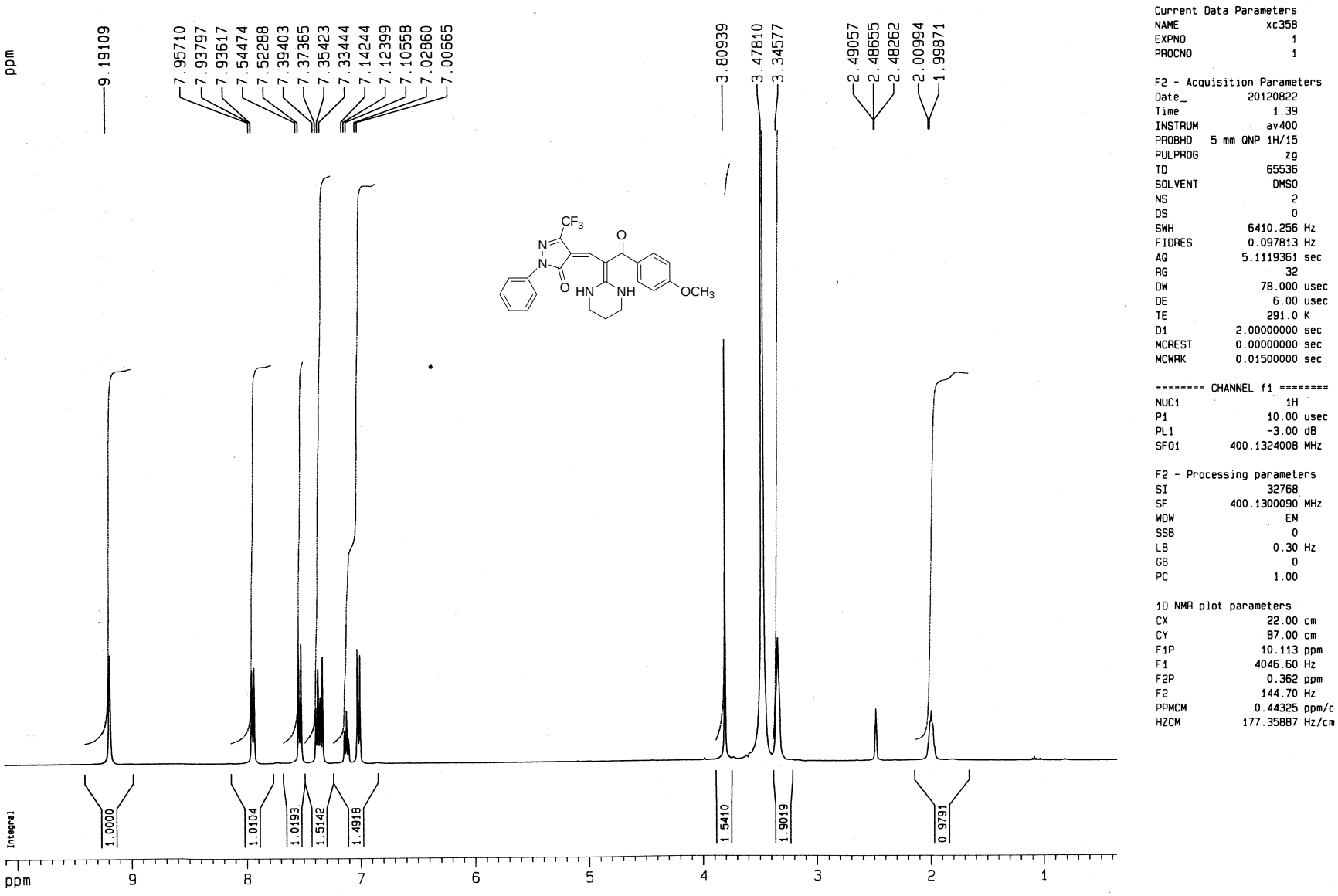


Figure 40. ^{13}C NMR (125 MHz, DMSO -d_6) spectra of compound **7f**



Current Data Parameters
NAME xc358
EXPNO 1
PROCNO 1

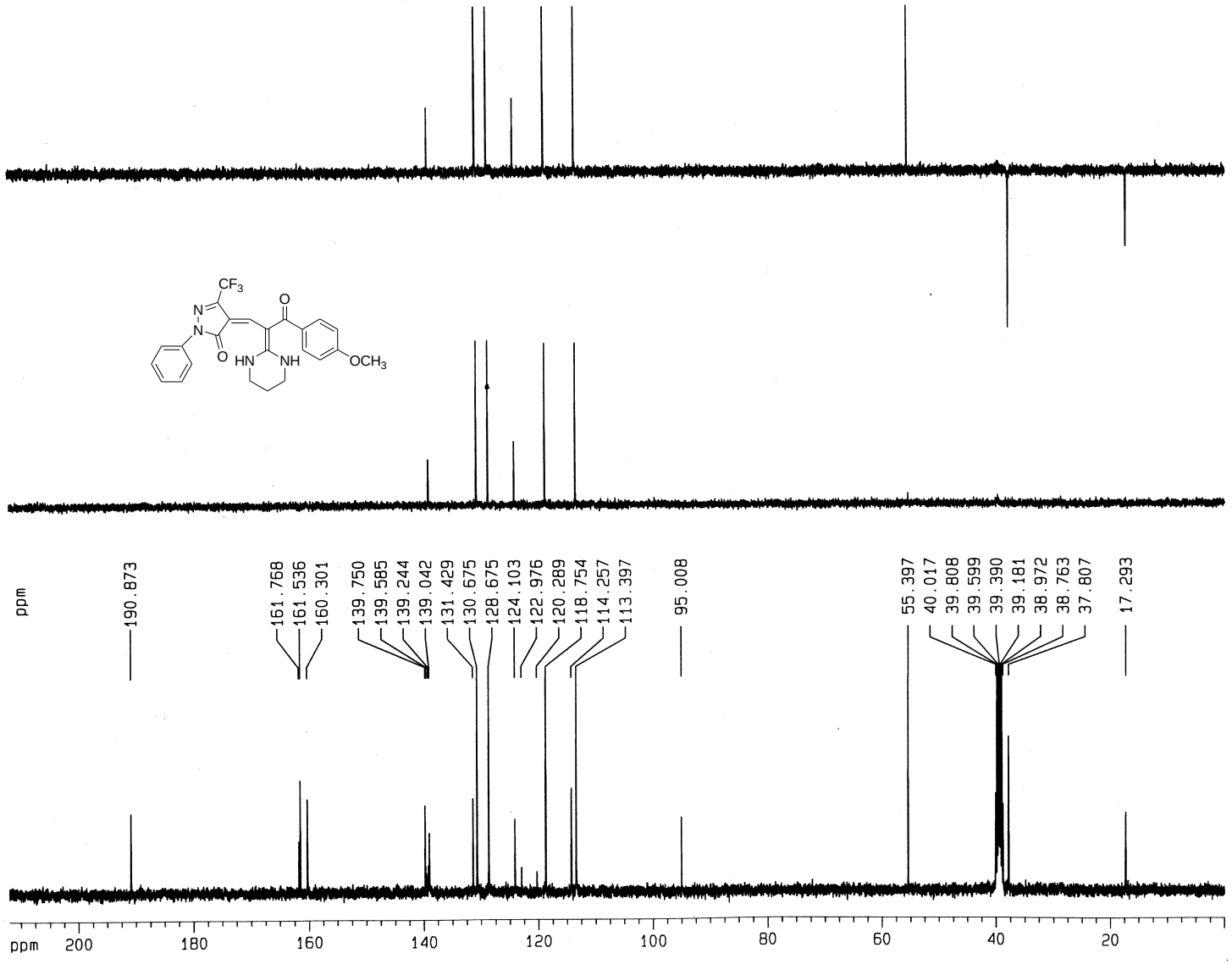
F2 - Acquisition Parameters
Date_ 20120822
Time 1.39
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zg
TD 65536
SOLVENT DMSO
NS 2
DS 0
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1119361 sec
RG 32
DW 78.000 usec
DE 6.00 usec
TE 291.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 87.00 cm
F1P 10.113 ppm
F1 4046.60 Hz
F2P 0.362 ppm
F2 144.70 Hz
PPMCM 0.44325 ppm/c
HZCM 177.35887 Hz/cm

Figure 41. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7g**




```
Current Data Parameters
NAME                 xc358
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120822
Time                 1.54
INSTRUM              av400
PROBHD   5 mm GNP 1H/15
PULPROG              zgdc
TD                   32768
SOLVENT              DMSO
NS                     154
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                     114
DW                21.600 usec
DE                 6.00 usec
TE                 291.7 K
D1            4.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

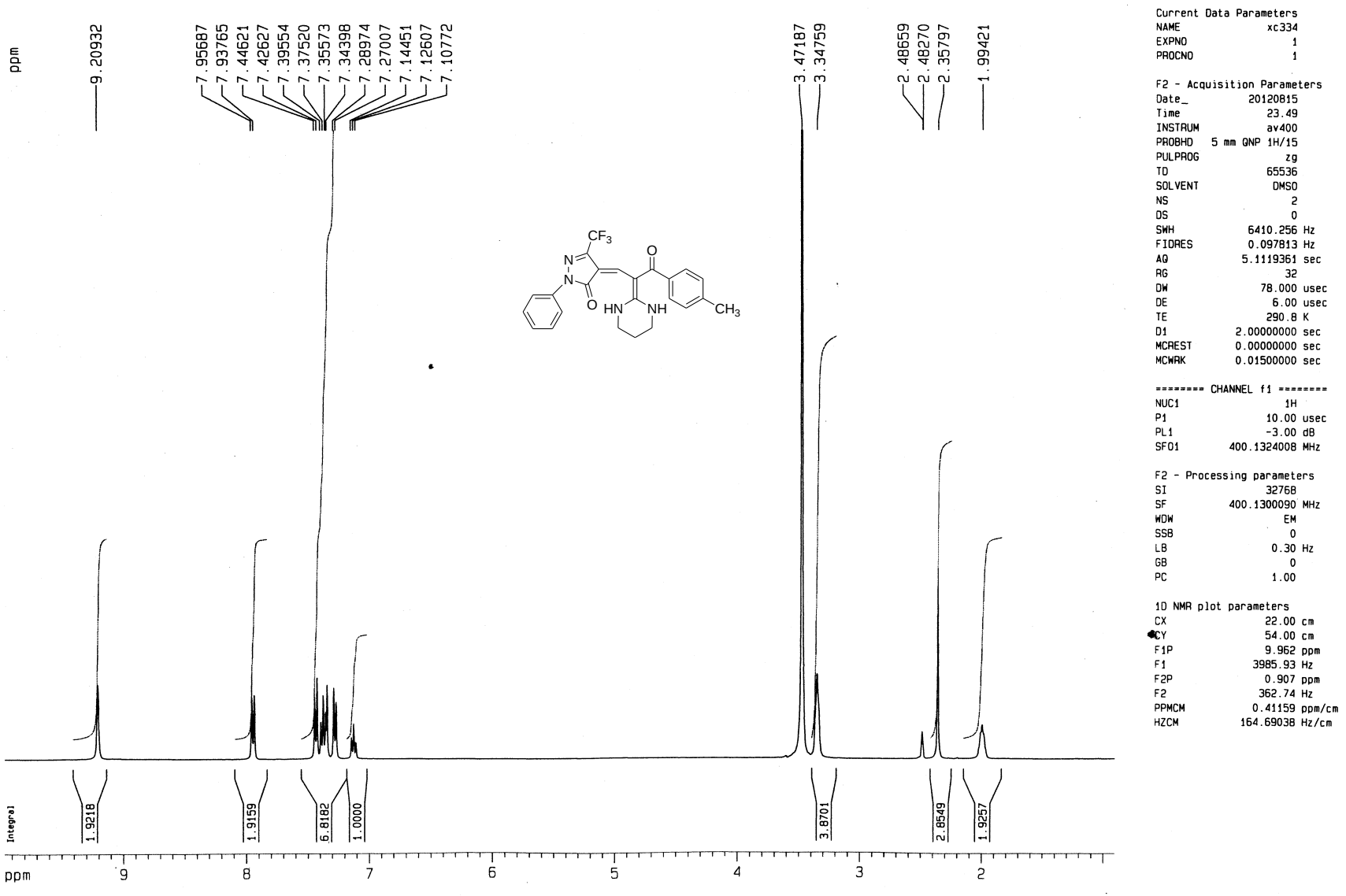
======== CHANNEL f1 ========
NUC1                   13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6128120 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  22.00 cm
CY                   5.00 cm
F1P                212.000 ppm
F1               21329.92 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM              9.63636 ppm/cm
HZCM             969.54156 Hz/cm
```

Figure 42. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7g**



Current Data Parameters

NAME	xc334
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120815
Time	23.49
INSTRUM	av400
PROBHD	5 mm GNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	32
DW	78.000 usec
DE	6.00 usec
TE	290.8 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

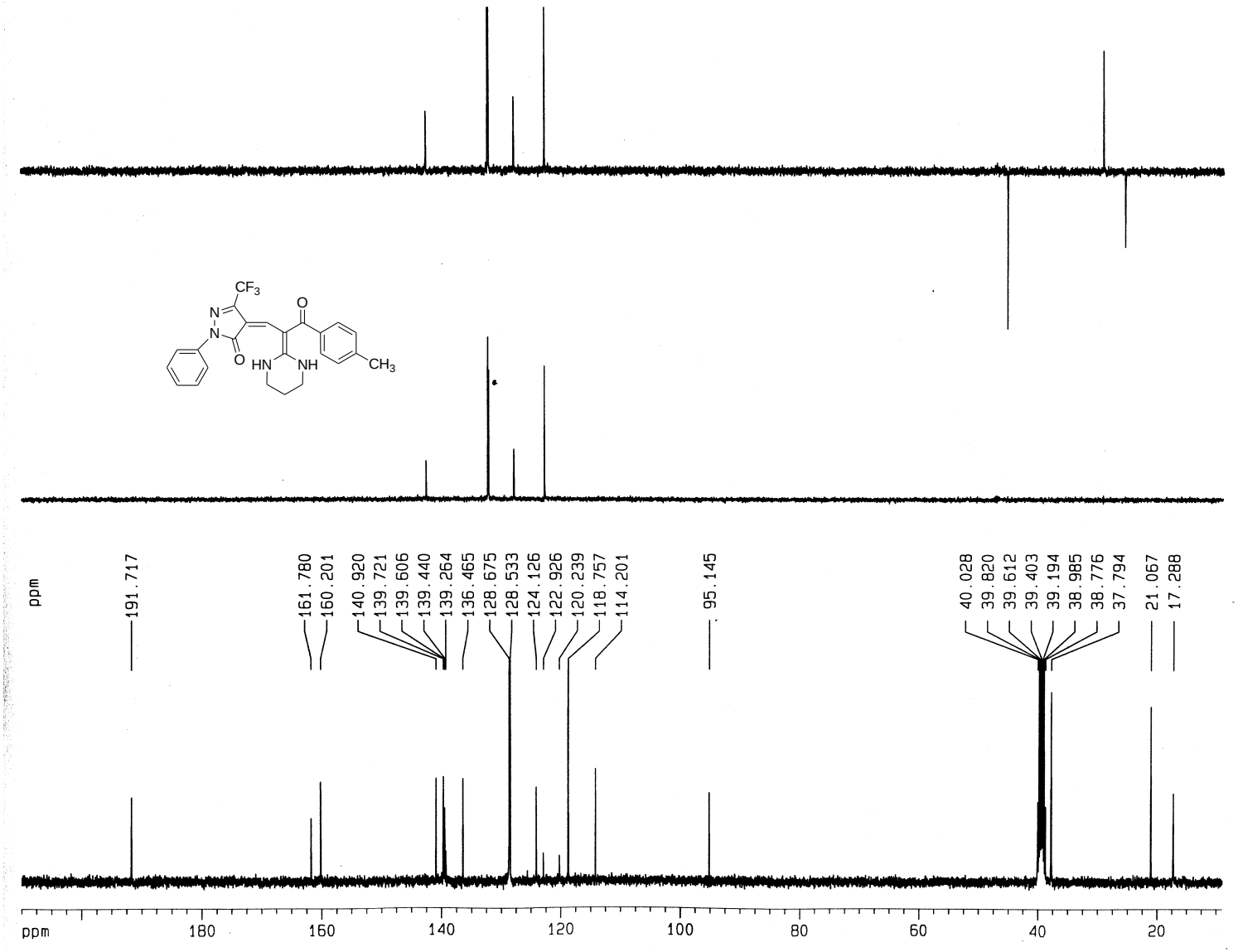
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	54.00 cm
F1P	9.962 ppm
F1	3985.93 Hz
F2P	0.907 ppm
F2	362.74 Hz
PPMCM	0.41159 ppm/cm
HZCM	164.69038 Hz/cm

Figure 43. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7h**



Current Data Parameters
NAME xc334
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120816
Time 0.04
INSTRUM av400
PROBHD 5 mm GNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 168
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 114
DW 21.600 usec
DE 6.00 usec
TE 291.6 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

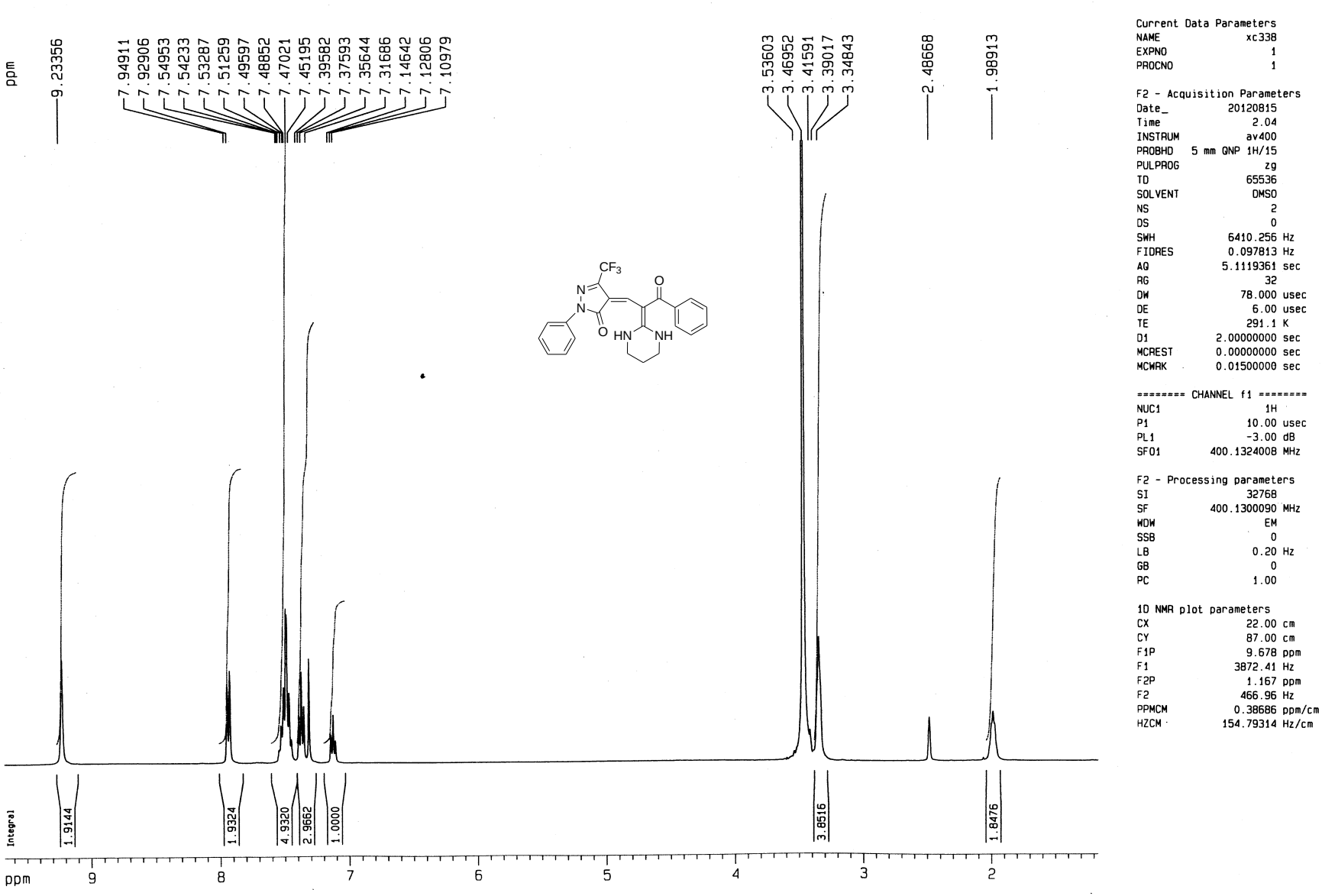
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128120 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.00 cm
CY 8.00 cm
F1P 210.000 ppm
F1 21128.69 Hz
F2P 9.000 ppm
F2 905.52 Hz
PPMCM 9.13636 ppm/cm
HZCM 919.23517 Hz/cm

Figure 44. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7h**




```
Current Data Parameters
NAME                  xc338
EXPNO                     1
PROCNO                    1

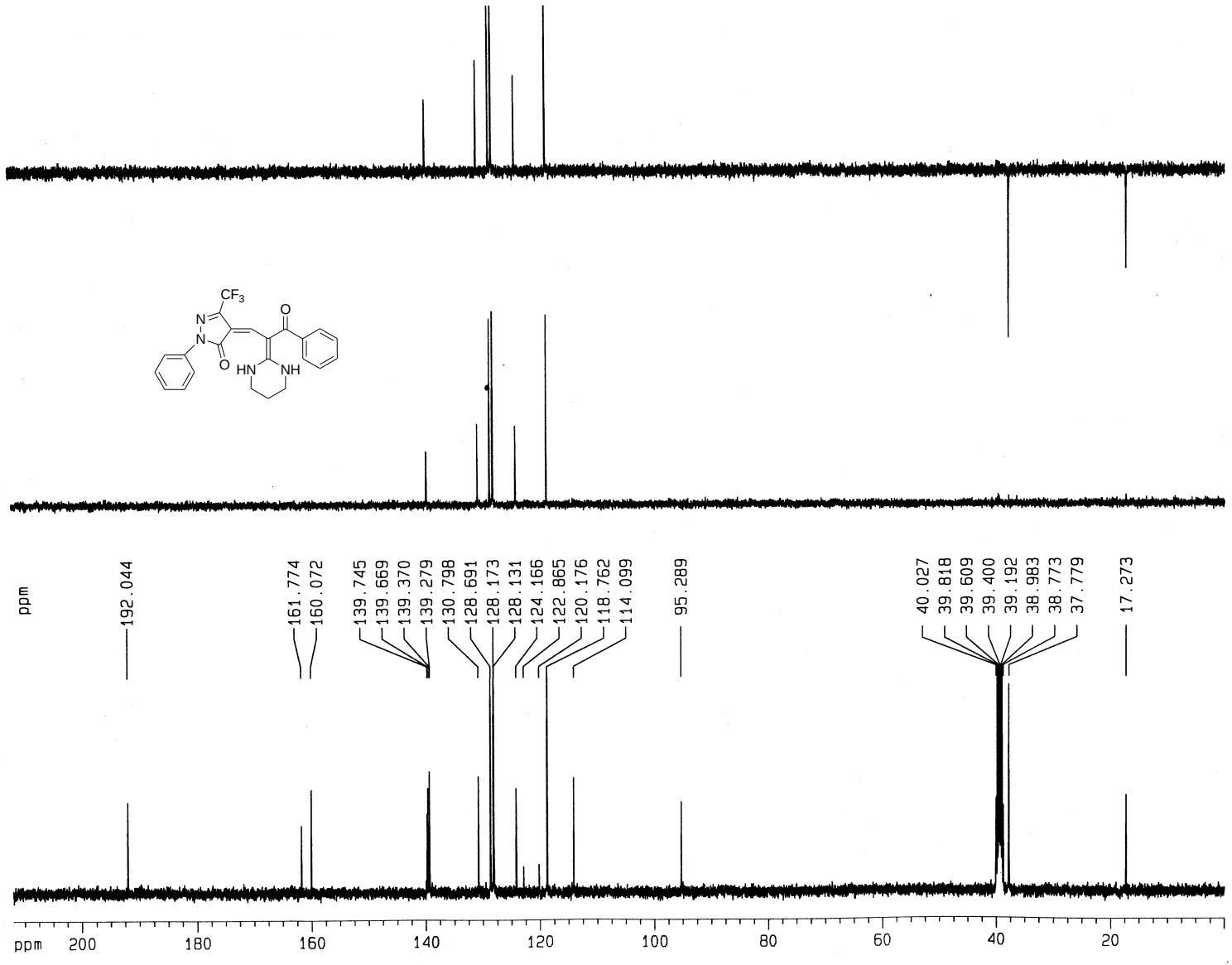
F2 - Acquisition Parameters
Date_              20120815
Time                  2.04
INSTRUM               av400
PROBHD   5 mm QNP 1H/15
PULPROG                zg
TD                    65536
SOLVENT               DMSO
NS                        2
DS                        0
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1119361 sec
RG                       32
DW                  78.000 usec
DE                   6.00 usec
TE                  291.1 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                  10.00 usec
PL1                 -3.00 dB
SFO1           400.1324008 MHz

F2 - Processing parameters
SI                    32768
SF             400.1300090 MHz
WDW                      EM
SSB                       0
LB                   0.20 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                   22.00 cm
CY                   87.00 cm
F1P                  9.678 ppm
F1                 3872.41 Hz
F2P                  1.167 ppm
F2                  466.96 Hz
PPMCM             0.38686 ppm/cm
HZCM            154.79314 Hz/cm
```

Figure 45. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7i**




```
Current Data Parameters
NAME                 xc338
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120815
Time                 2.20
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                    168
DS                      2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                   143.7
DW                21.600 usec
DE                 6.00 usec
TE                 291.8 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

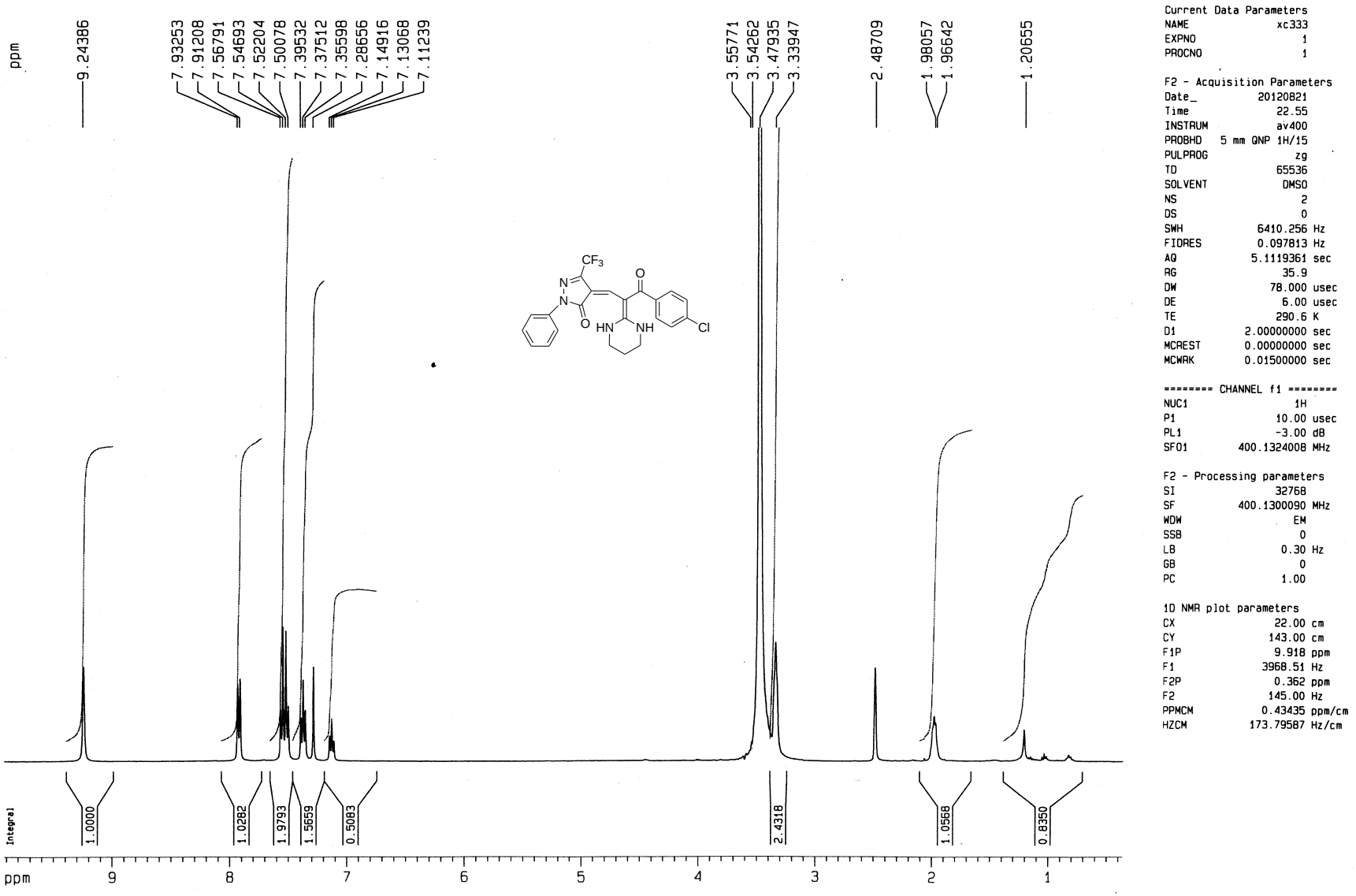
======== CHANNEL f1 ========
NUC1                 13C
P1                 9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6128120 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                22.00 cm
CY                 6.60 cm
F1P              212.000 ppm
F1             21329.92 Hz
F2P              0.000 ppm
F2               0.00 Hz
PPMCM          9.63636 ppm/cm
HZCM           969.54156 Hz/cm
```

Figure 46. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7i**



Current Data Parameters
NAME xc333
EXPNO 1
PROCNO 1

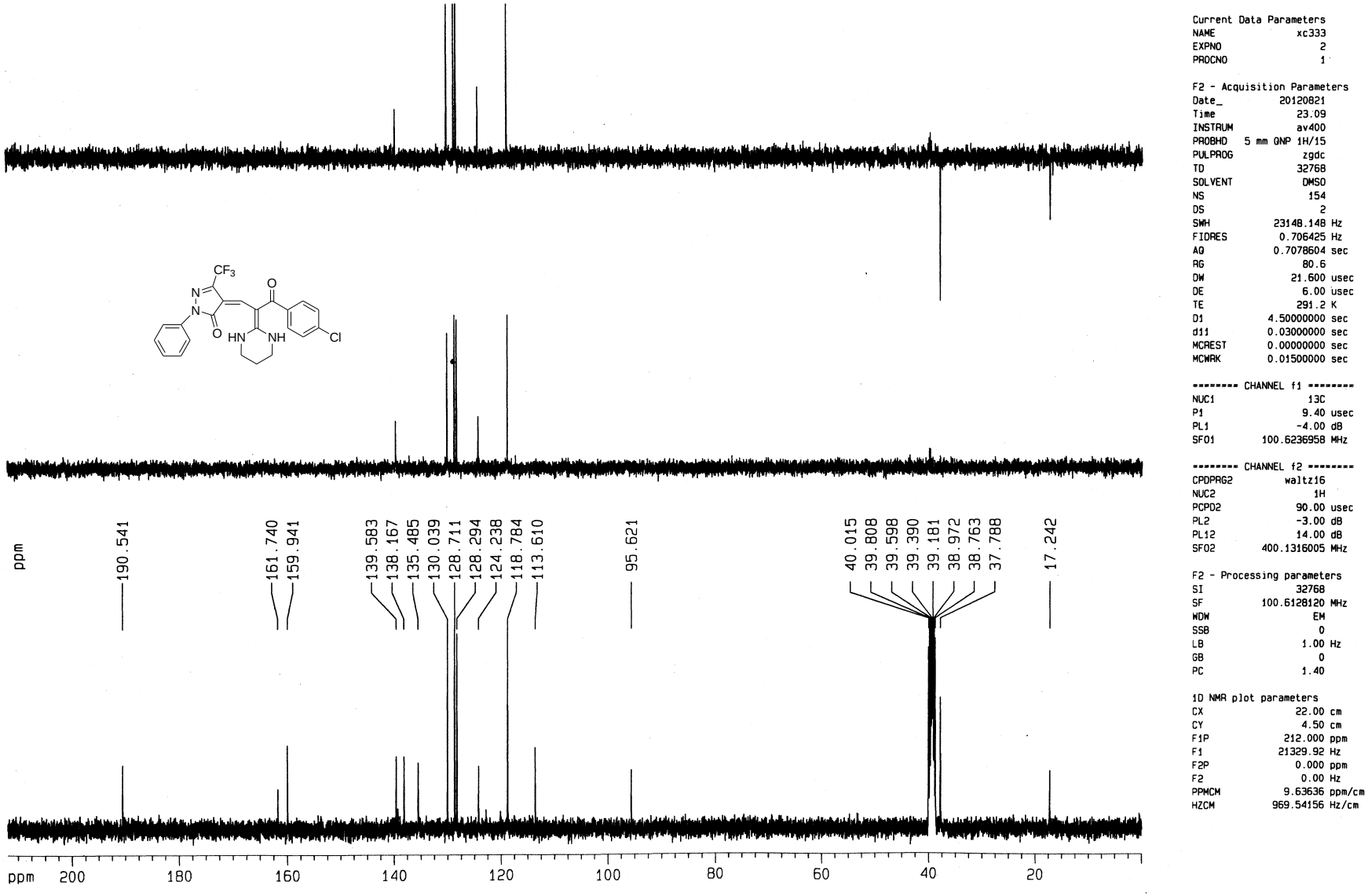
F2 - Acquisition Parameters
Date_ 20120821
Time 22.55
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zg
TD 65536
SOLVENT DMSO
NS 2
DS 0
SWH 6410.256 Hz
FIDRES 0.097813 Hz
AQ 5.1119361 sec
RG 35.9
DW 78.000 usec
DE 6.00 usec
TE 290.6 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 143.00 cm
F1P 9.918 ppm
F1 3968.51 Hz
F2P 0.362 ppm
F2 145.00 Hz
PPMCM 0.43435 ppm/cm
HZCM 173.79587 Hz/cm

Figure 47. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7j**



Current Data Parameters
NAME xc333
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120821
Time 23.09
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 154
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 80.6
DW 21.600 usec
DE 6.00 usec
TE 291.2 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

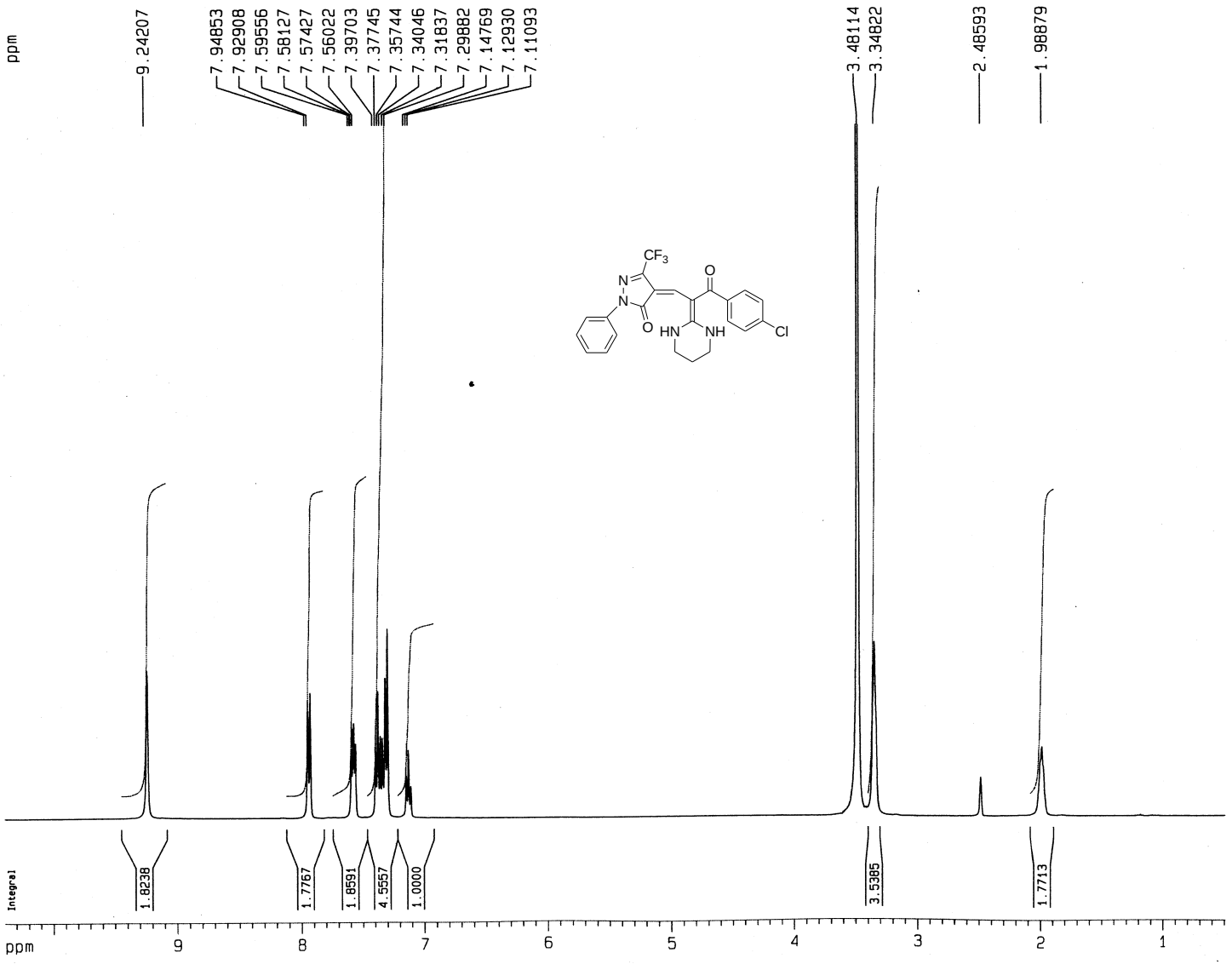
-------- CHANNEL f1 --------
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128120 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 4.50 cm
F1P 212.000 ppm
F1 21329.92 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.63636 ppm/cm
HZCM 969.54156 Hz/cm

Figure 48. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7j**



Current Data Parameters

NAME	xc336
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120815
Time	1.31
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	4
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	28.5
DW	78.000 usec
DE	6.00 usec
TE	291.0 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

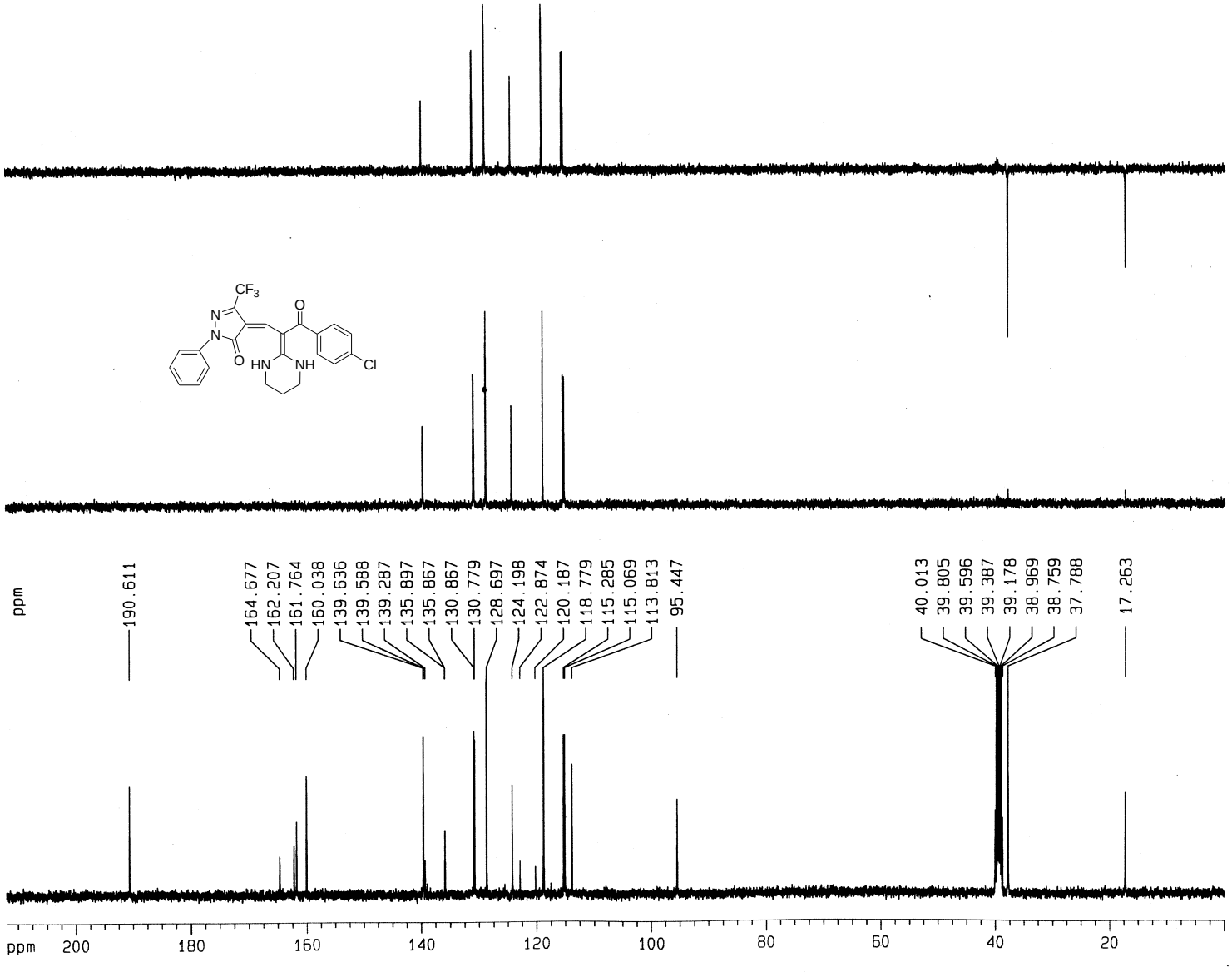
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	87.00 cm
F1P	10.396 ppm
F1	4159.82 Hz
F2P	0.492 ppm
F2	196.96 Hz
PPMCM	0.45018 ppm/cm
HZCM	180.13011 Hz/cm

Figure 49. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7k**



Current Data Parameters
NAME xc336
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120815
Time 1.46
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 168
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 101.6
DW 21.600 usec
DE 6.00 usec
TE 291.7 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128120 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 22.00 cm
CY 6.60 cm
F1P 212.000 ppm
F1 21329.92 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.63636 ppm/cm
HZCM 969.54156 Hz/cm

Figure 50. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7k**

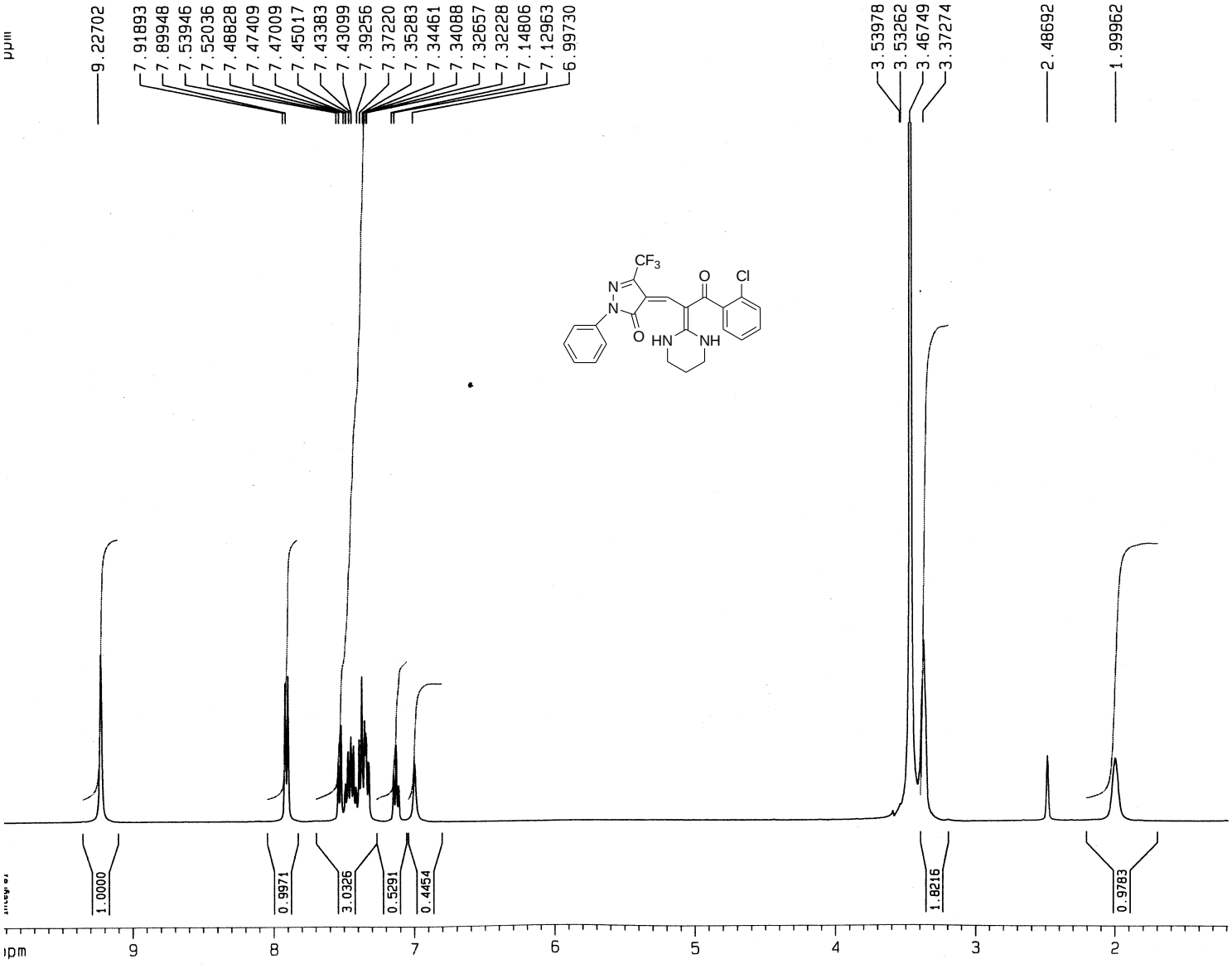
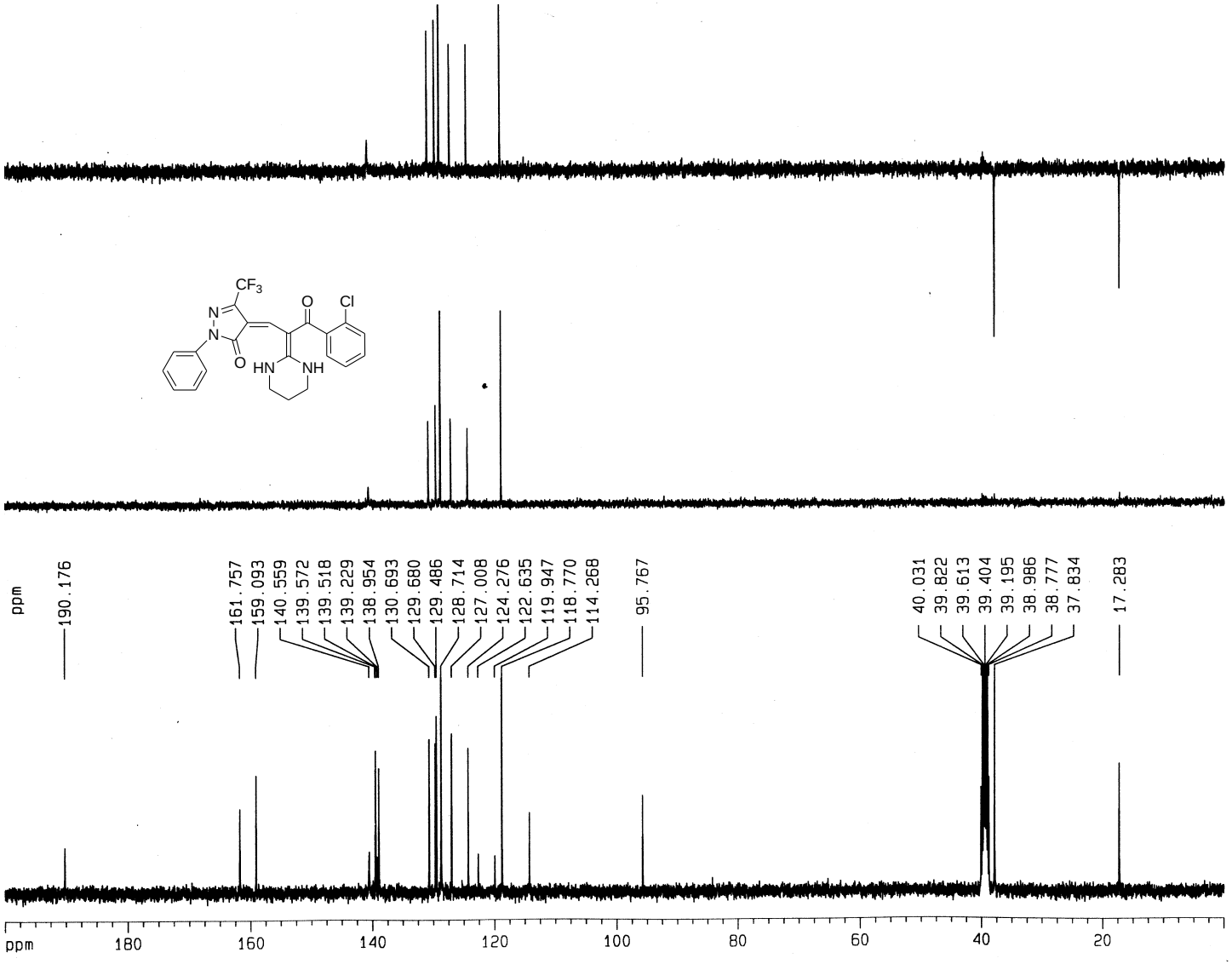


Figure 51. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7l**




```
Current Data Parameters
NAME                 xc360
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20120815
Time                  6.11
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG               zgdc
TD                   32768
SOLVENT               DMSO
NS                     168
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                    90.5
DW                21.600 usec
DE                 6.00 usec
TE                 291.7 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

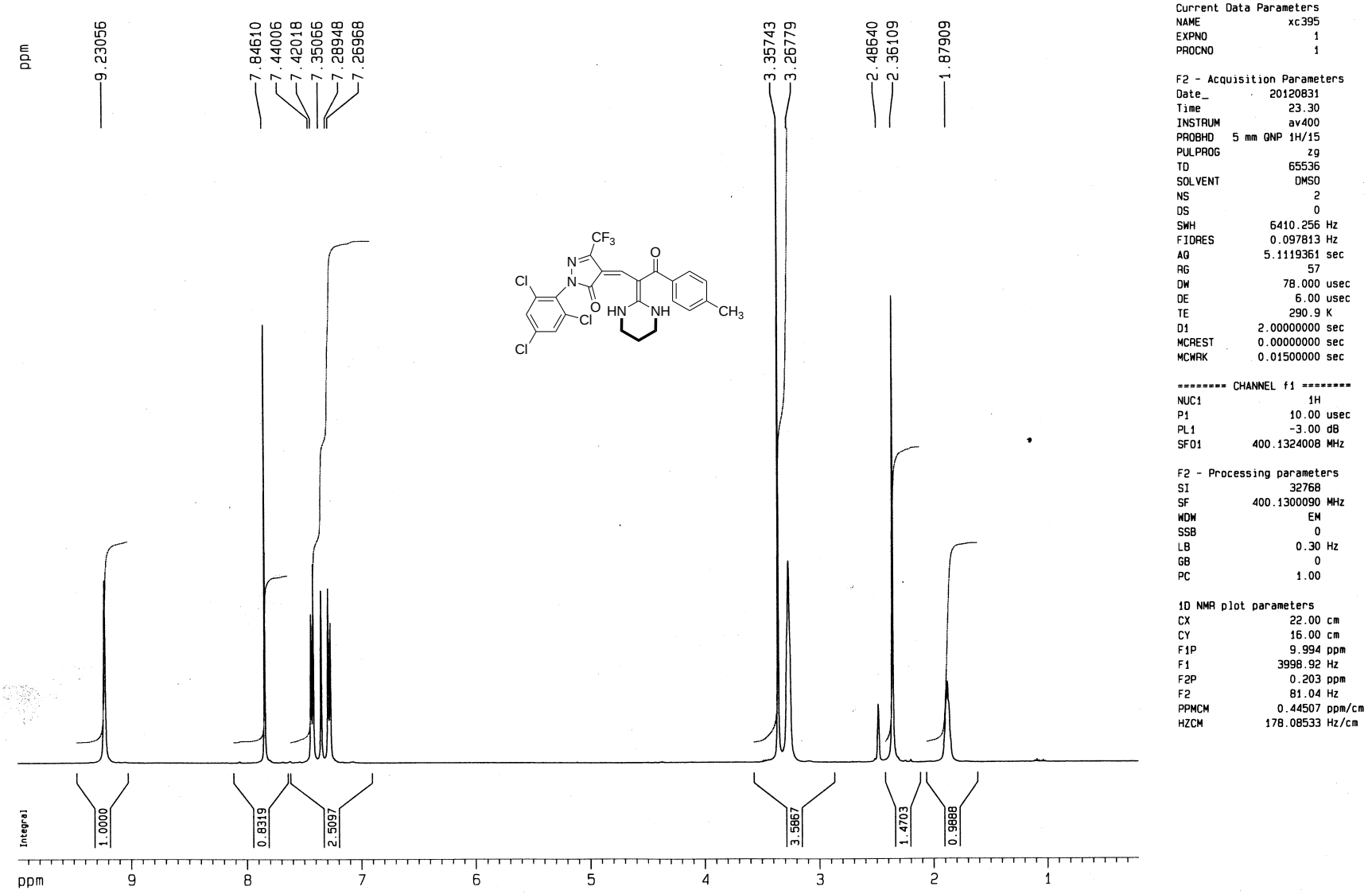
======== CHANNEL f1 ========
NUC1                   13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6128120 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   2.00

1D NMR plot parameters
CX                  22.00 cm
CY                   9.00 cm
F1P                200.000 ppm
F1                20122.56 Hz
F2P                -0.000 ppm
F2                 -0.00 Hz
PPMCM             9.09091 ppm/cm
HZCM             914.66193 Hz/cm
```

Figure 52. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7l**




```
Current Data Parameters
NAME                  xc395
EXPNO                     1
PROCNO                    1

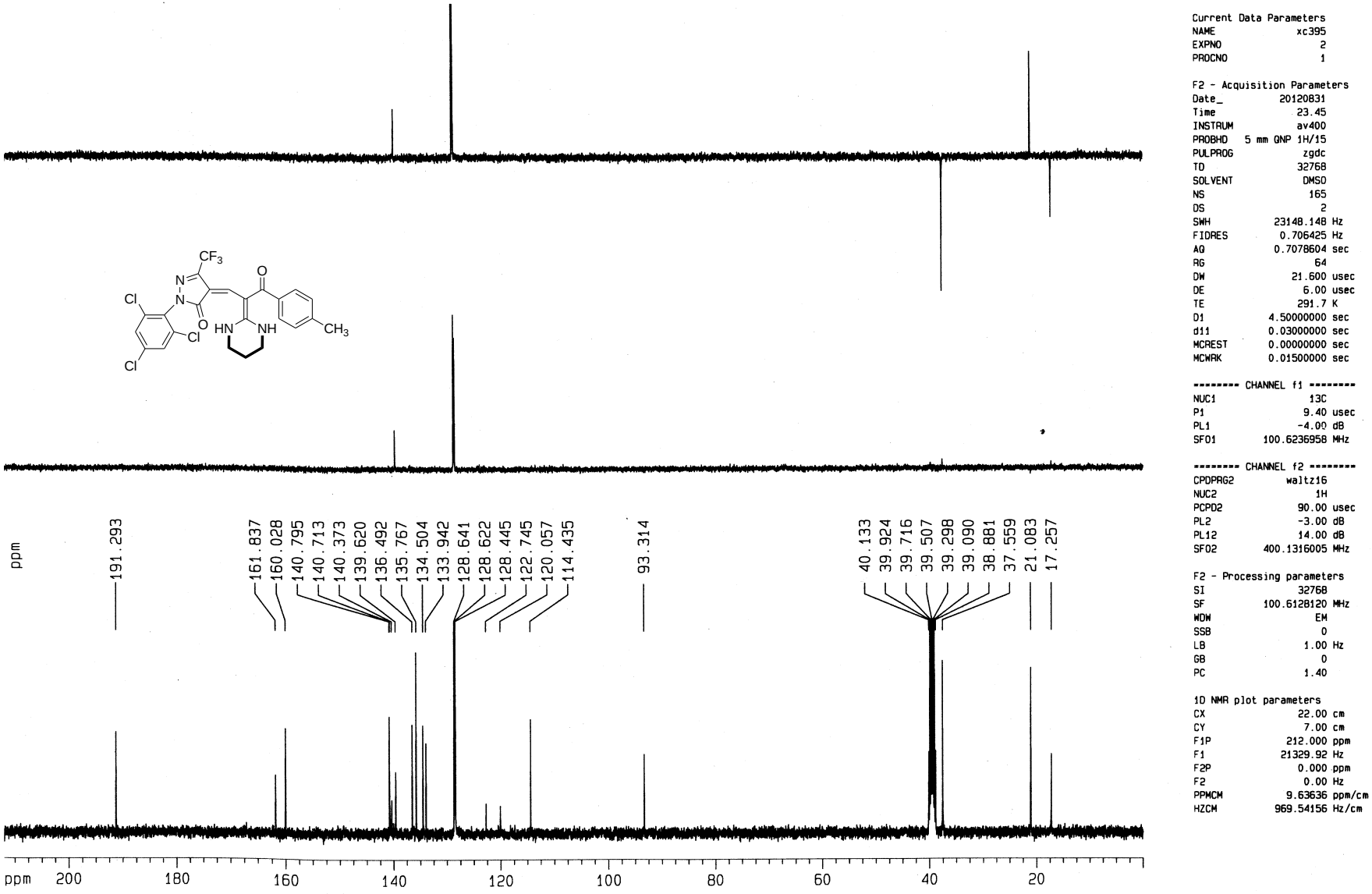
F2 - Acquisition Parameters
Date_              20120831
Time                 23.30
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG                zg
TD                  65536
SOLVENT              DMSO
NS                       2
DS                       0
SWH             6410.256 Hz
FIDRES          0.097813 Hz
AQ              5.1119361 sec
RG                      57
DW                78.000 usec
DE                 6.00 usec
TE                290.9 K
D1             2.00000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -3.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300090 MHz
WDW                   EM
SSB                      0
LB                0.30 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                22.00 cm
CY                16.00 cm
F1P                9.994 ppm
F1              3998.92 Hz
F2P                0.203 ppm
F2                81.04 Hz
PPMCM          0.44507 ppm/cm
HZCM          178.08533 Hz/cm
```

Figure 53. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **7m**




```
Current Data Parameters
NAME                  xc395
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120831
Time                  23.45
INSTRUM               av400
PROBHD   5 mm QNP 1H/15
PULPROG                zgdc
TD                    32768
SOLVENT                DMSO
NS                      165
DS                        2
SWH               23148.148 Hz
FIDRES            0.706425 Hz
AQ                0.7078604 sec
RG                       64
DW                  21.600 usec
DE                   6.00 usec
TE                   291.7 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

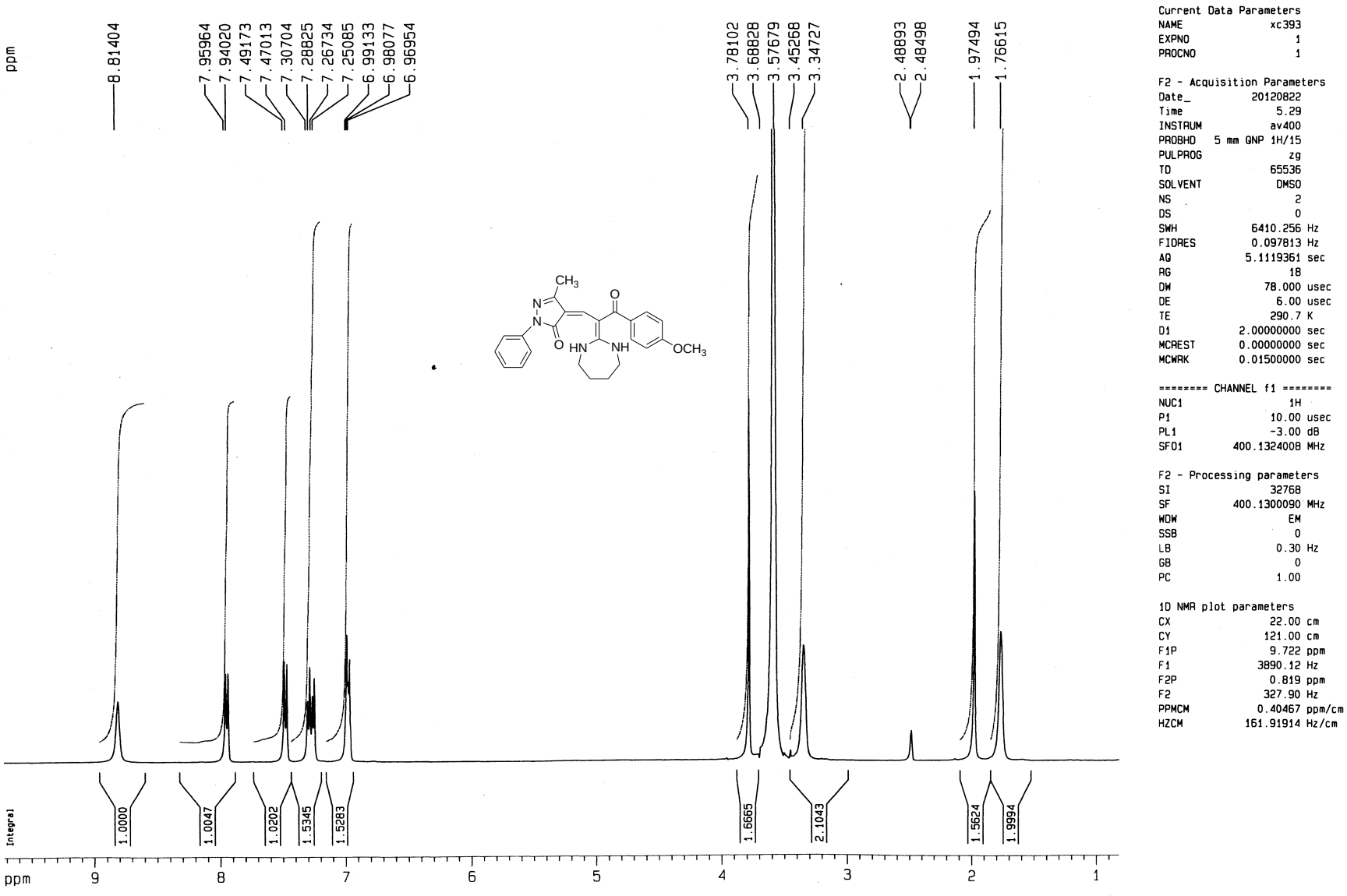
======== CHANNEL f1 ========
NUC1                    13C
P1                    9.40 usec
PL1                  -4.00 dB
SFO1           100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -3.00 dB
PL12                 14.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6128120 MHz
WDW                      EM
SSB                       0
LB                    1.00 Hz
GB                        0
PC                     1.40

1D NMR plot parameters
CX                   22.00 cm
CY                    7.00 cm
F1P                212.000 ppm
F1               21329.92 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54156 Hz/cm
```

Figure 54. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **7m**



Current Data Parameters

NAME	xc393
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120822
Time	5.29
INSTRUM	av400
PROBHD	5 mm GNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	18
DW	78.000 usec
DE	6.00 usec
TE	290.7 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

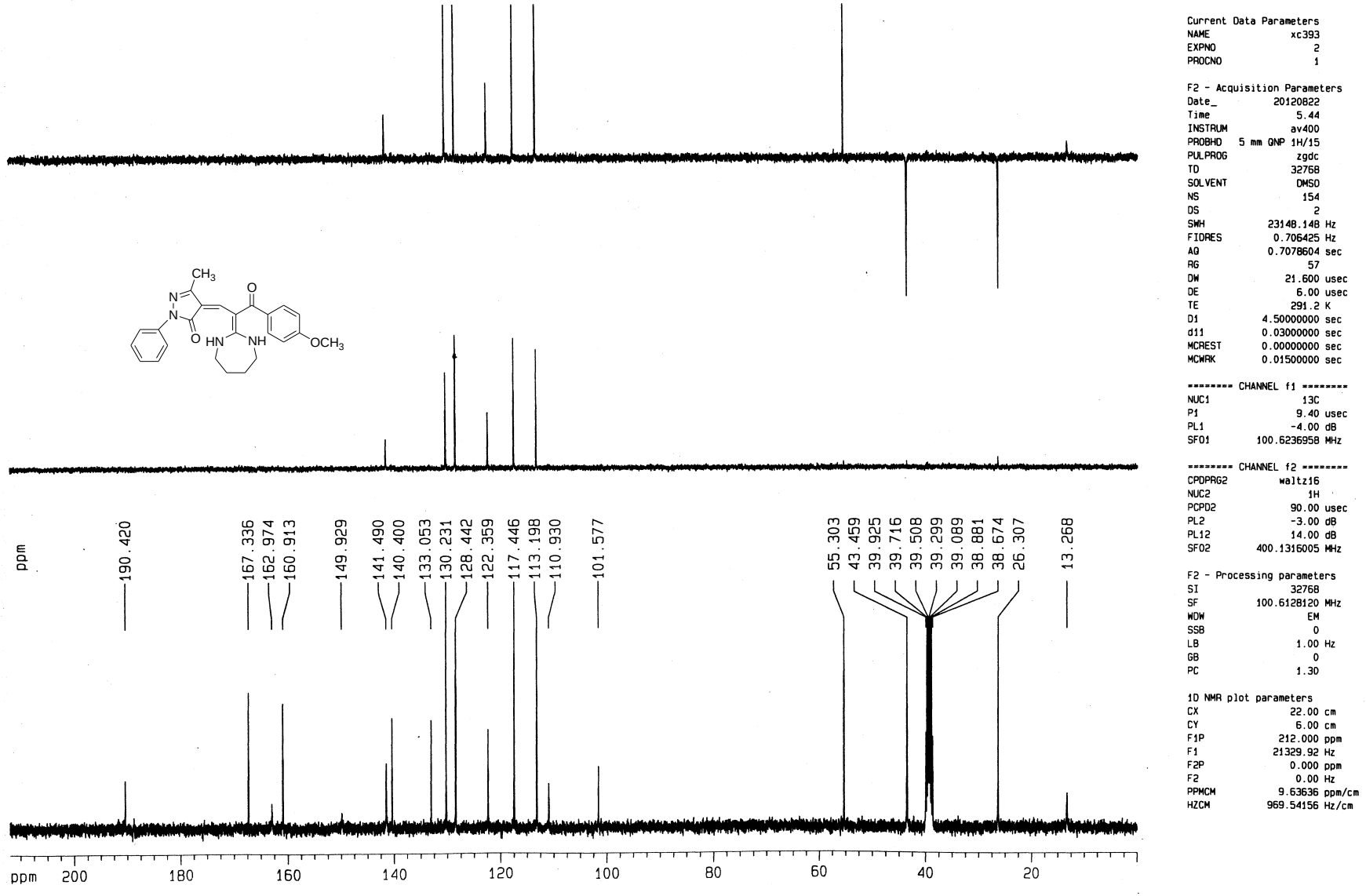
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	121.00 cm
F1P	9.722 ppm
F1	3890.12 Hz
F2P	0.819 ppm
F2	327.90 Hz
PPMCM	0.40467 ppm/cm
HZCM	161.91914 Hz/cm

Figure 55. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **8a**




```
Current Data Parameters
NAME                 xc393
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120822
Time                 5.44
INSTRUM              av400
PROBHD   5 mm GNP 1H/15
PULPROG               zgdc
TD                   32768
SOLVENT               DMSO
NS                     154
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                      57
DW                21.600 usec
DE                 6.00 usec
TE                 291.2 K
D1            4.50000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

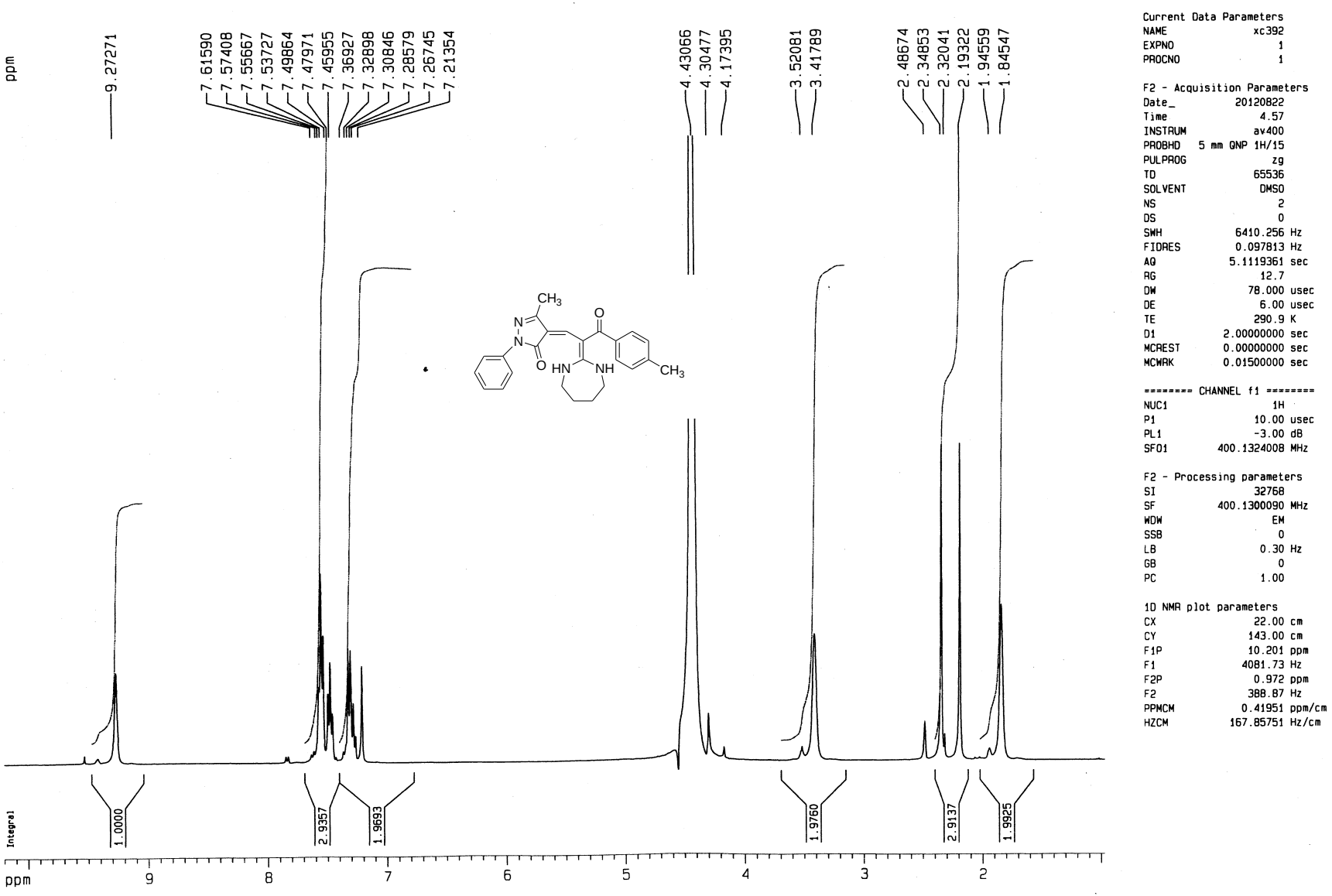
======== CHANNEL f1 ========
NUC1                   13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6128120 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.30

1D NMR plot parameters
CX                  22.00 cm
CY                   6.00 cm
F1P                212.000 ppm
F1               21329.92 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54156 Hz/cm
```

Figure 56. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **8a**



Current Data Parameters

NAME	xc392
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120822
Time	4.57
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	12.7
DW	78.000 usec
DE	6.00 usec
TE	290.9 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

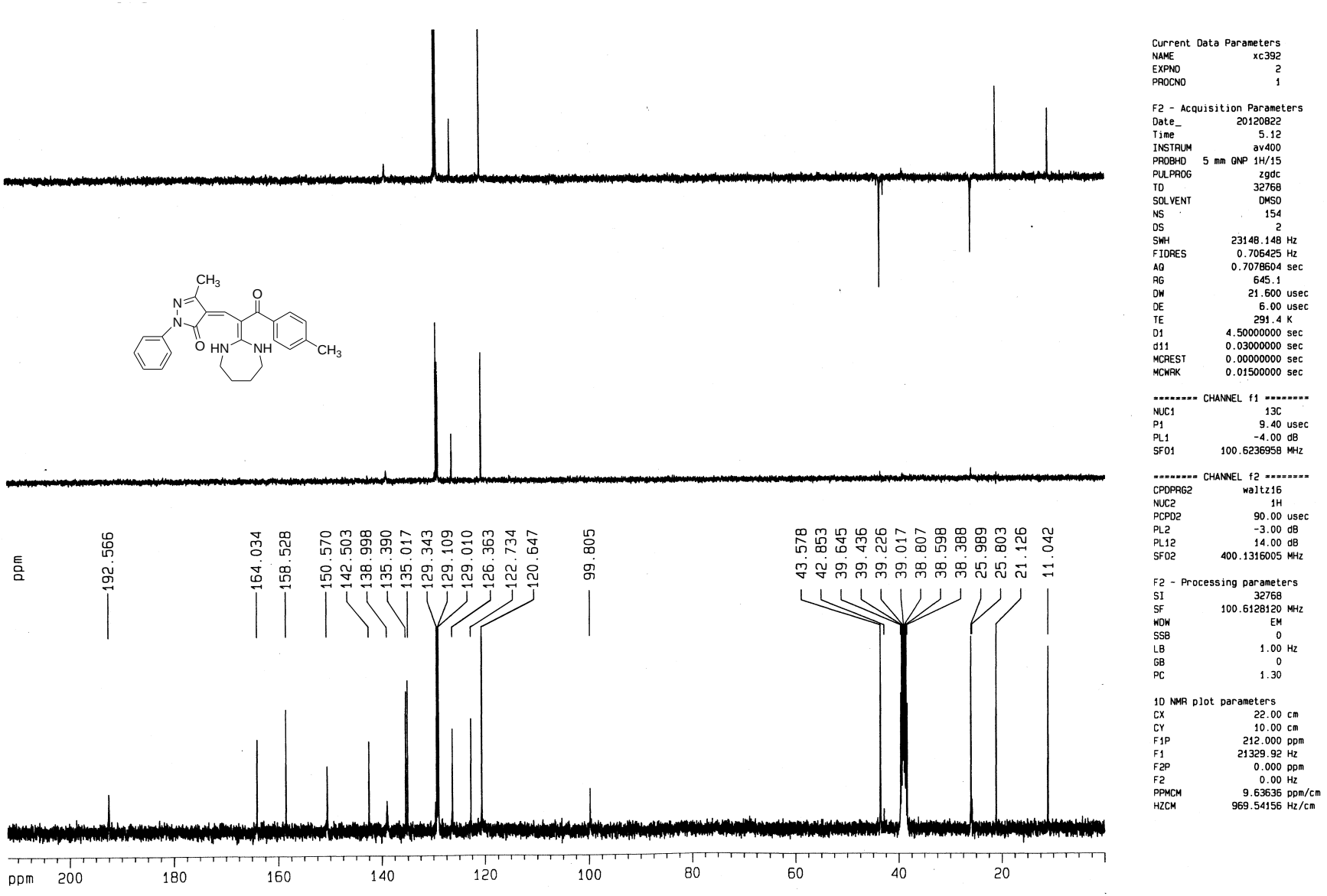
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	143.00 cm
F1P	10.201 ppm
F1	4081.73 Hz
F2P	0.972 ppm
F2	388.87 Hz
PPMCM	0.41951 ppm/cm
HZCM	167.85751 Hz/cm

Figure 57. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **8b**




```
Current Data Parameters
NAME                 xc392
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120822
Time                 5.12
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     154
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                   645.1
DW                 21.600 usec
DE                  6.00 usec
TE                 291.4 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

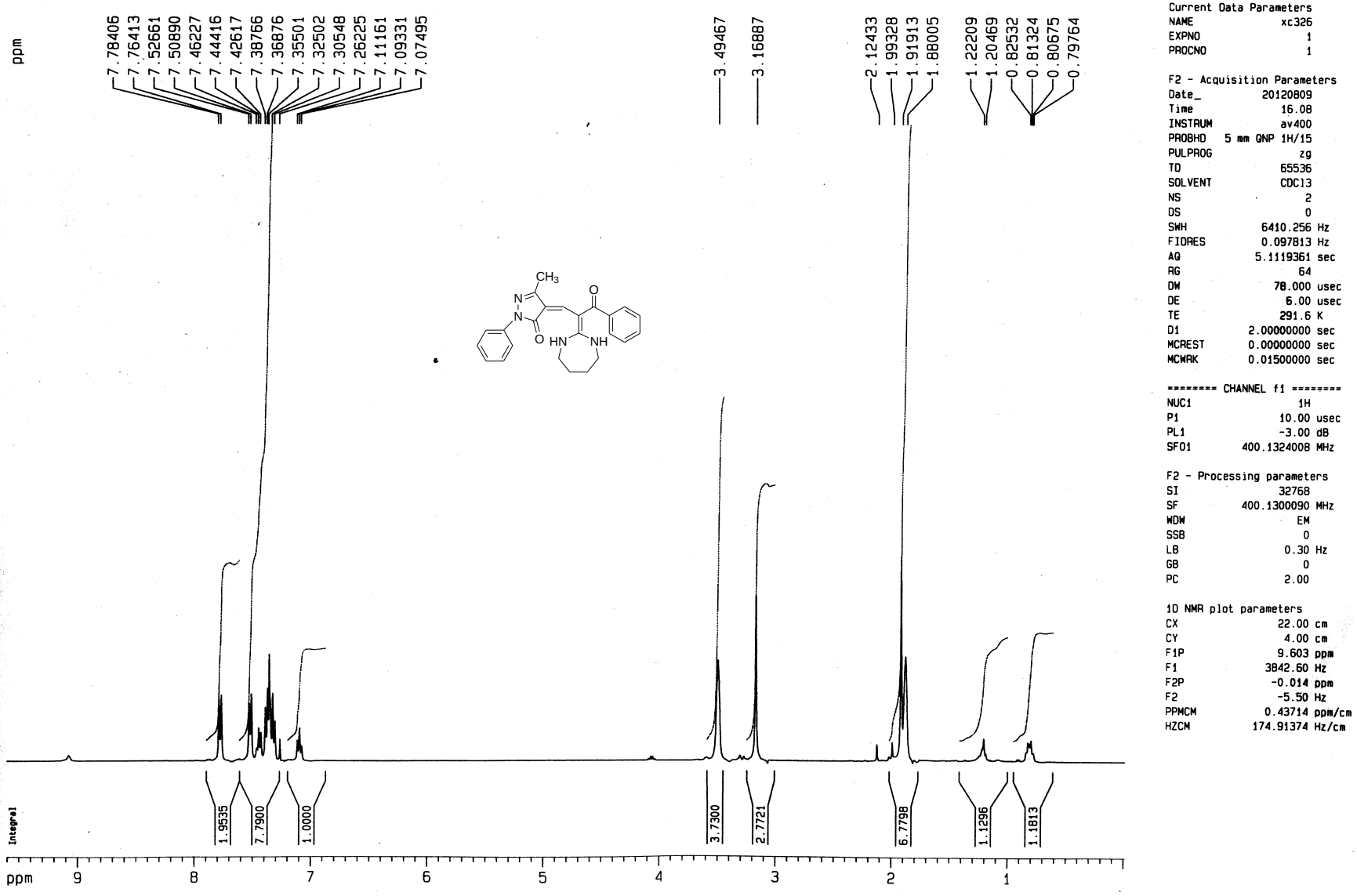
======== CHANNEL f1 ========
NUC1                 13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1           100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF             100.6128120 MHz
WDW                  EM
SSB                  0
LB                  1.00 Hz
GB                   0
PC                  1.30

1D NMR plot parameters
CX                  22.00 cm
CY                  10.00 cm
F1P               212.000 ppm
F1              21329.92 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            9.63636 ppm/cm
HZCM           969.54156 Hz/cm
```

Figure 58. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **8b**




```
Current Data Parameters
NAME                  xc326
EXPNO                     1
PROCNO                    1

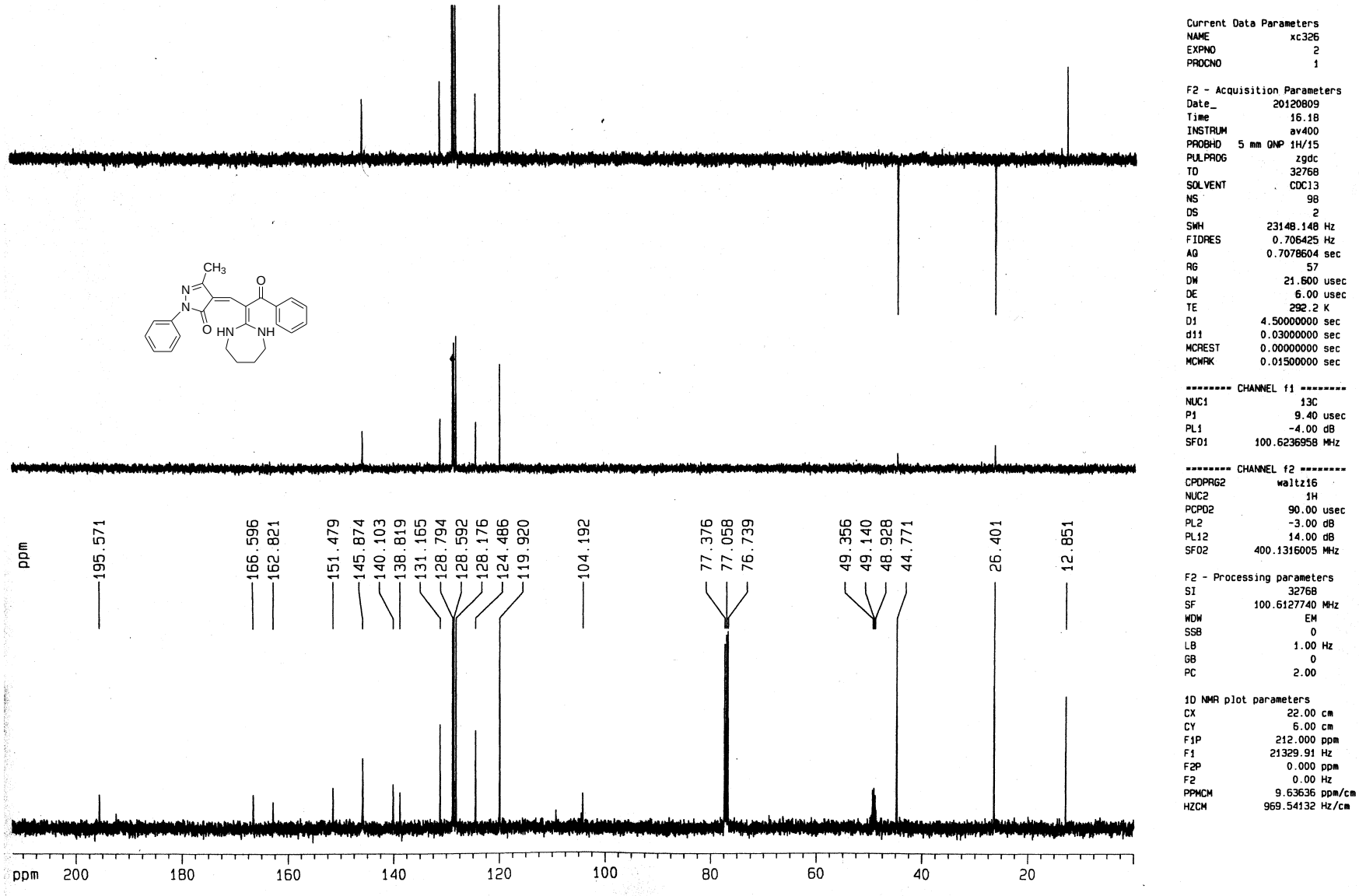
F2 - Acquisition Parameters
Date_              20120809
Time                 16.08
INSTRUM              av400
PROBHD    5 mm QNP 1H/15
PULPROG                zg
TD                   65536
SOLVENT              CDCl3
NS                        2
DS                        0
SWH             6410.256 Hz
FIDRES          0.097813 Hz
AQ              5.1119361 sec
RG                       64
DW                78.000 usec
DE                 6.00 usec
TE                291.6 K
D1              2.00000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                  10.00 usec
PL1                 -3.00 dB
SFO1          400.1324008 MHz

F2 - Processing parameters
SI                    32768
SF              400.1300090 MHz
WDW                      EM
SSB                       0
LB                   0.30 Hz
GB                        0
PC                     2.00

1D NMR plot parameters
CX                   22.00 cm
CY                    4.00 cm
F1P                  9.603 ppm
F1                3842.60 Hz
F2P                -0.014 ppm
F2                 -5.50 Hz
PPMCM            0.43714 ppm/cm
HZCM            174.91374 Hz/cm
```

Figure 59. ^{1}H NMR (400 MHz, $CDCl_3$) spectra of compound **8c**



Current Data Parameters
NAME xc326
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120809
Time 16.18
INSTRUM av400
PROBHD 5 mm QNP 1H/15
PULPROG zgdc
TD 32768
SOLVENT CDCl3
NS 98
DS 2
SWH 23148.148 Hz
FIDRES 0.706425 Hz
AQ 0.7078604 sec
RG 57
DW 21.600 usec
DE 6.00 usec
TE 292.2 K
D1 4.50000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

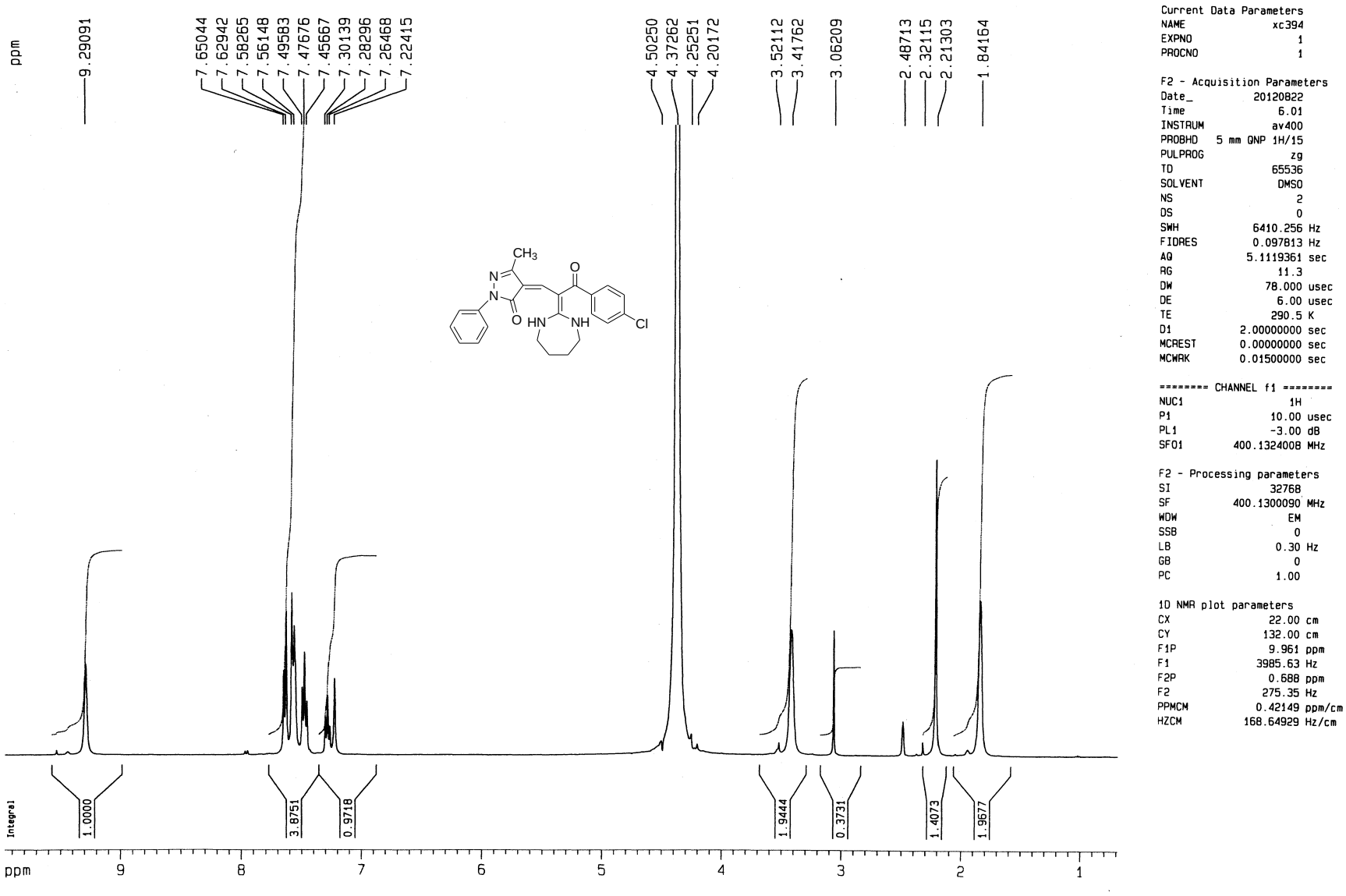
======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 -4.00 dB
SFO1 100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 14.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

1D NMR plot parameters
CX 22.00 cm
CY 6.00 cm
F1P 212.000 ppm
F1 21329.91 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 9.63636 ppm/cm
HZCM 969.54132 Hz/cm

Figure 60. ^{13}C NMR (100 MHz, $CDCl_3$) spectra of compound **8c**



Current Data Parameters

NAME	xc394
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120822
Time	6.01
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	11.3
DW	78.000 usec
DE	6.00 usec
TE	290.5 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

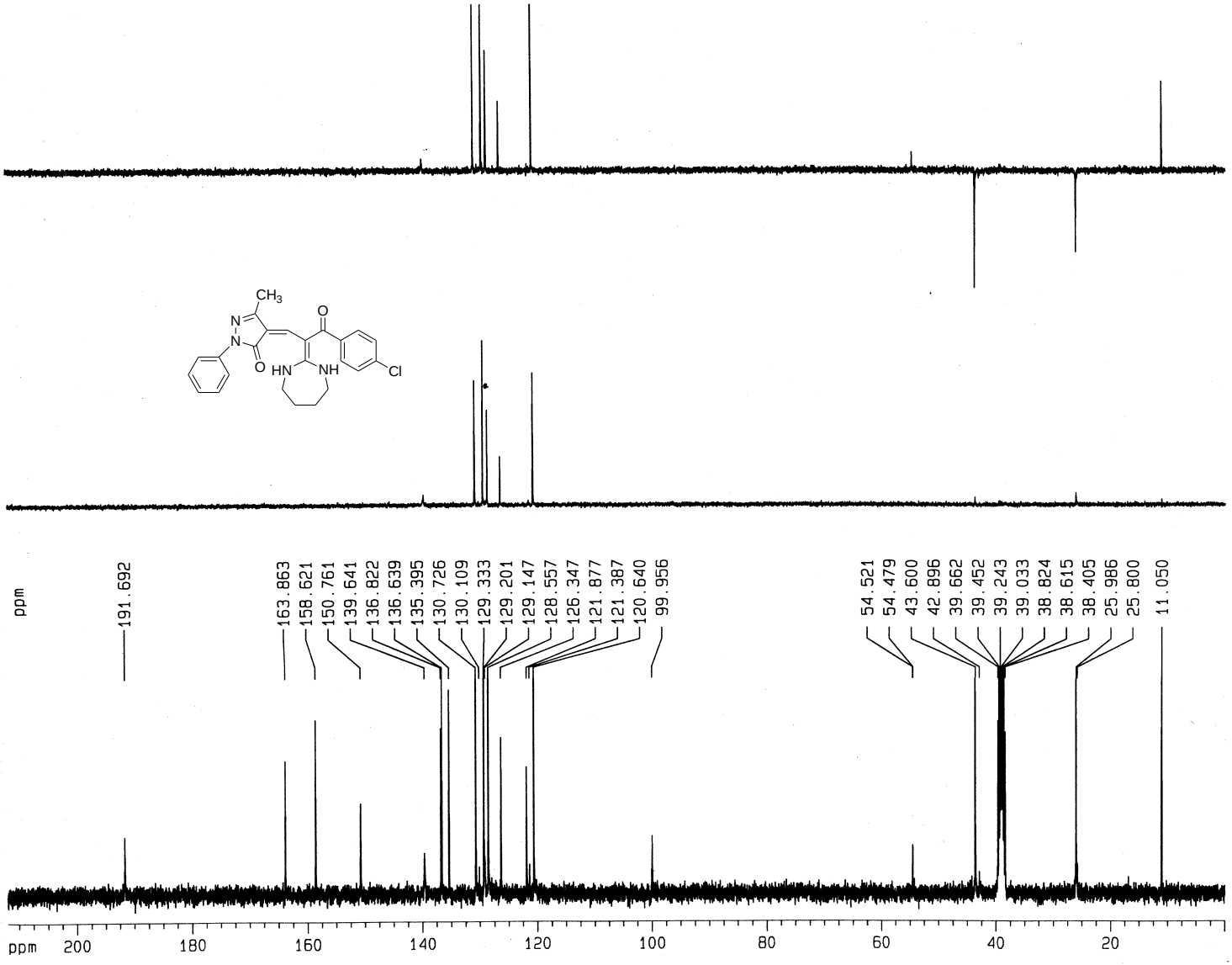
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	132.00 cm
F1P	9.961 ppm
F1	3985.63 Hz
F2P	0.688 ppm
F2	275.35 Hz
PPMCM	0.42149 ppm/cm
HZCM	168.64929 Hz/cm

Figure 61. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **8d**




```
Current Data Parameters
NAME                 xc394
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120822
Time                 6.16
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     154
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                   406.4
DW                21.600 usec
DE                 6.00 usec
TE                 291.0 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6128120 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.30

1D NMR plot parameters
CX                  22.00 cm
CY                  13.00 cm
F1P               212.000 ppm
F1              21329.92 Hz
F2P                0.000 ppm
F2                 0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54156 Hz/cm
```

Figure 62. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **8d**

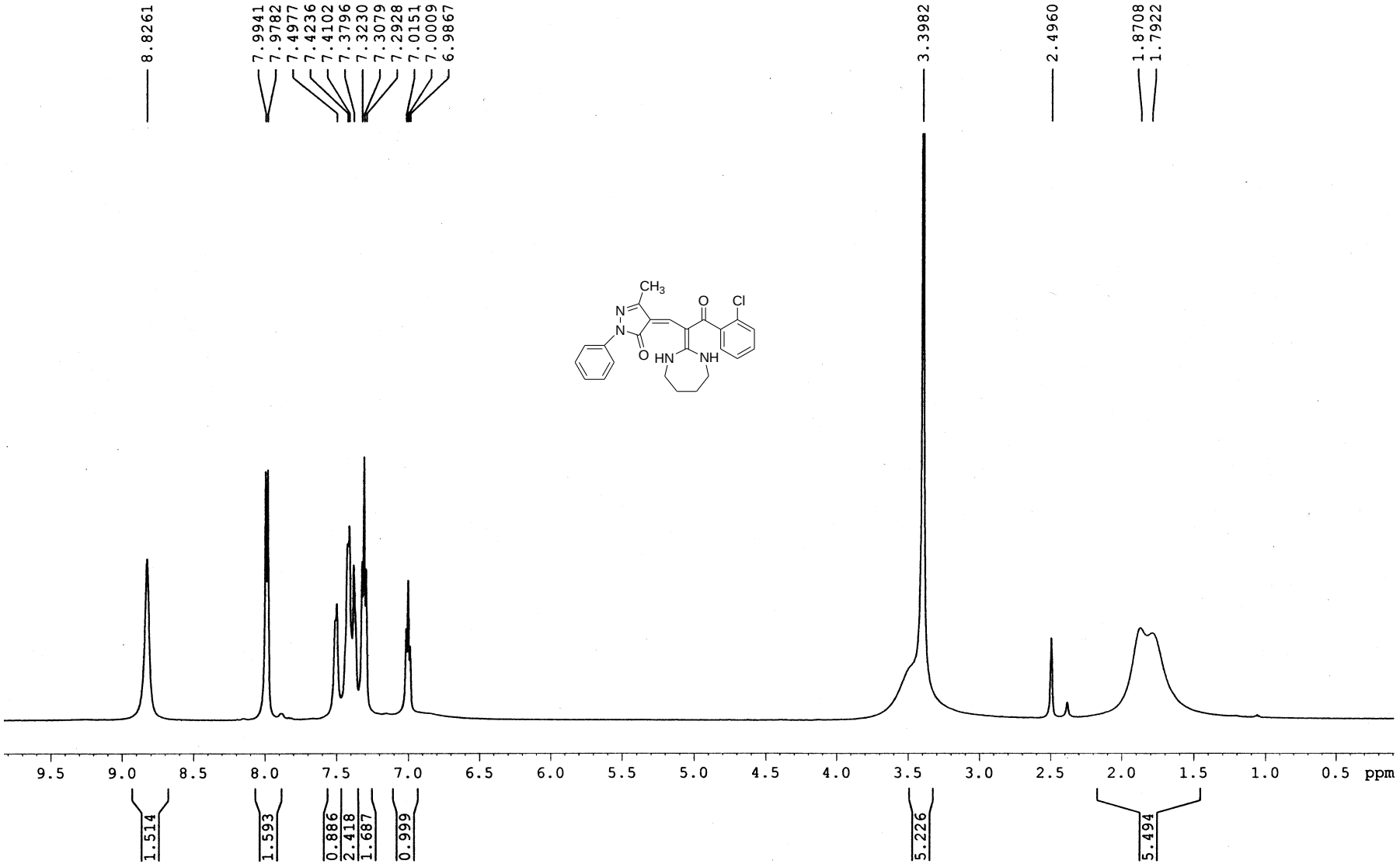


Figure 63. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **8e**

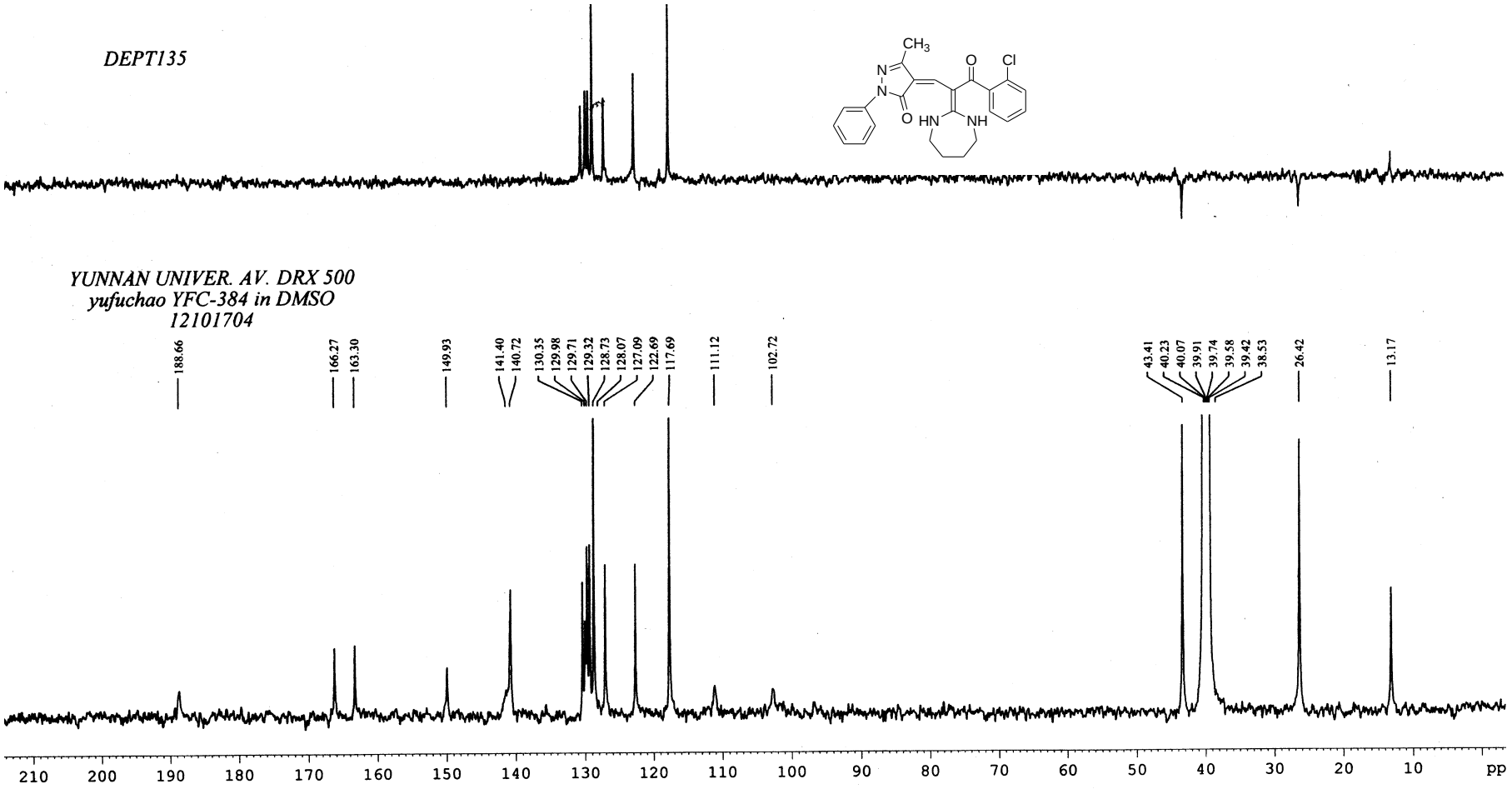
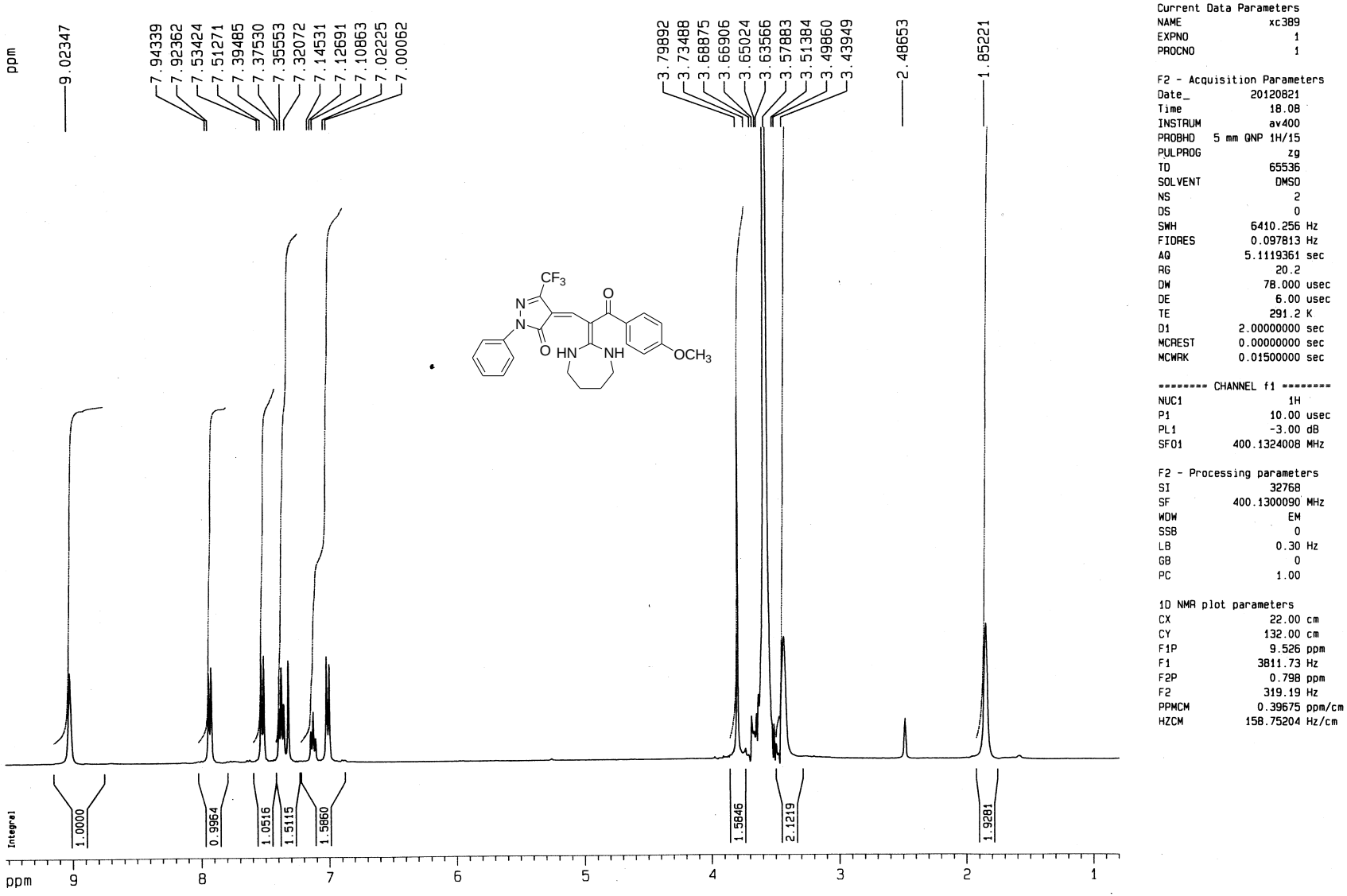


Figure 64. ^{13}C NMR (125 MHz, DMSO-d_6) spectra of compound **8e**




```
Current Data Parameters
NAME                 xc389
EXPNO                    1
PROCNO                   1

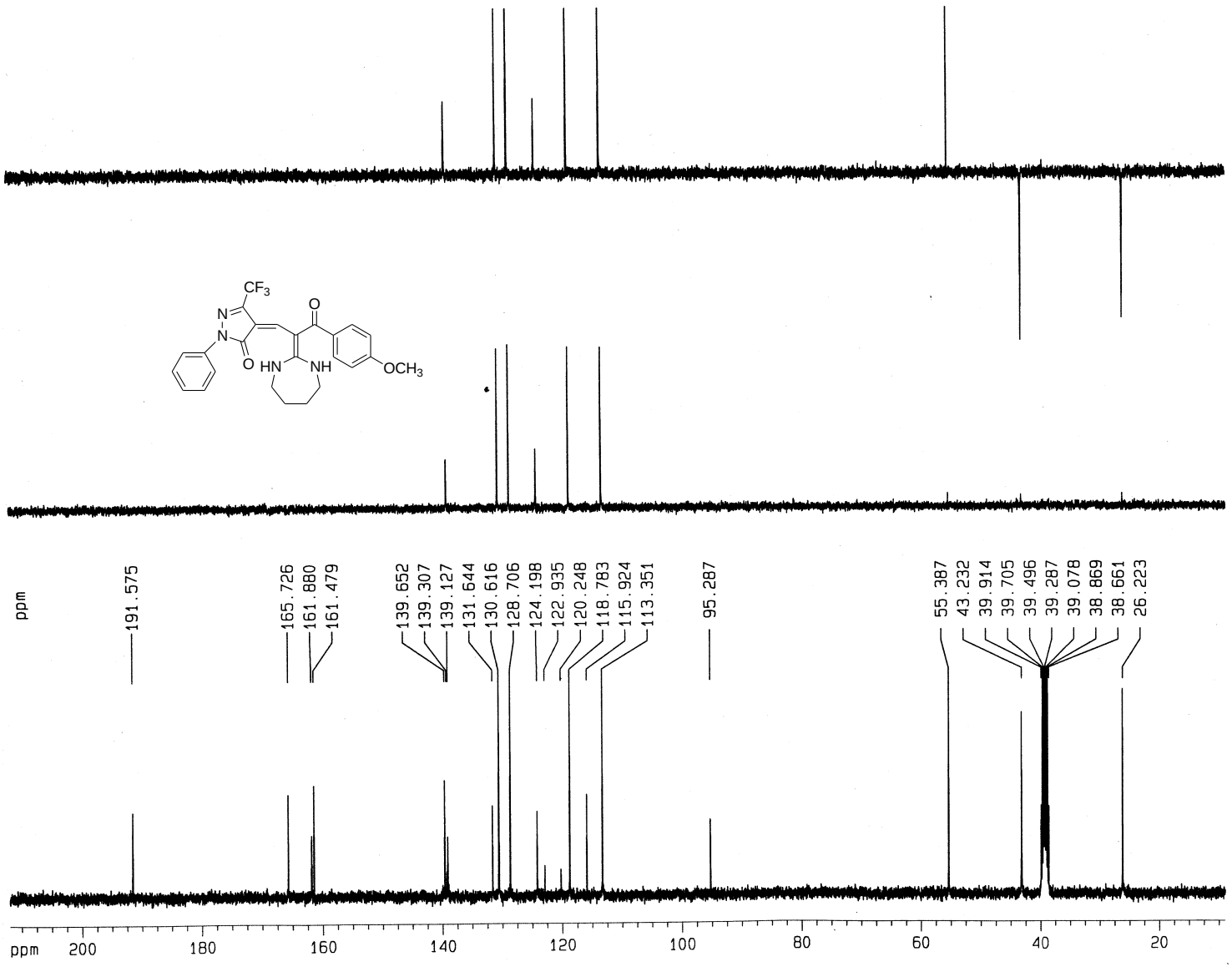
F2 - Acquisition Parameters
Date_             20120821
Time                 18.08
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG                 zg
TD                   65536
SOLVENT               DMSO
NS                       2
DS                       0
SWH               6410.256 Hz
FIDRES            0.097813 Hz
AQ                5.1119361 sec
RG                    20.2
DW                  78.000 usec
DE                   6.00 usec
TE                  291.2 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     1H
P1                   10.00 usec
PL1                  -3.00 dB
SFO1            400.1324008 MHz

F2 - Processing parameters
SI                       32768
SF              400.1300090 MHz
WDW                         EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00

1D NMR plot parameters
CX                   22.00 cm
CY                  132.00 cm
F1P                   9.526 ppm
F1                 3811.73 Hz
F2P                   0.798 ppm
F2                 319.19 Hz
PPMCM             0.39675 ppm/cm
HZCM             158.75204 Hz/cm
```

Figure 65. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **8f**




```
Current Data Parameters
NAME                  xc389
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120821
Time                  18.10
INSTRUM               av400
PROBHD   5 mm QNP 1H/15
PULPROG                zgdc
TD                    32768
SOLVENT                DMSO
NS                      148
DS                        2
SWH               23148.148 Hz
FIDRES            0.706425 Hz
AQ                0.7078604 sec
RG                      114
DW                 21.600 usec
DE                  6.00 usec
TE                  291.4 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                   9.40 usec
PL1                 -4.00 dB
SFO1            100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2               90.00 usec
PL2                 -3.00 dB
PL12                14.00 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF              100.6128120 MHz
WDW                      EM
SSB                       0
LB                   1.00 Hz
GB                        0
PC                     2.00

1D NMR plot parameters
CX                   22.00 cm
CY                    5.00 cm
F1P                212.000 ppm
F1                 21329.92 Hz
F2P                  9.000 ppm
F2                  905.52 Hz
PPMCM             9.22727 ppm/cm
HZCM            928.38177 Hz/cm
```

Figure 66. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **8f**

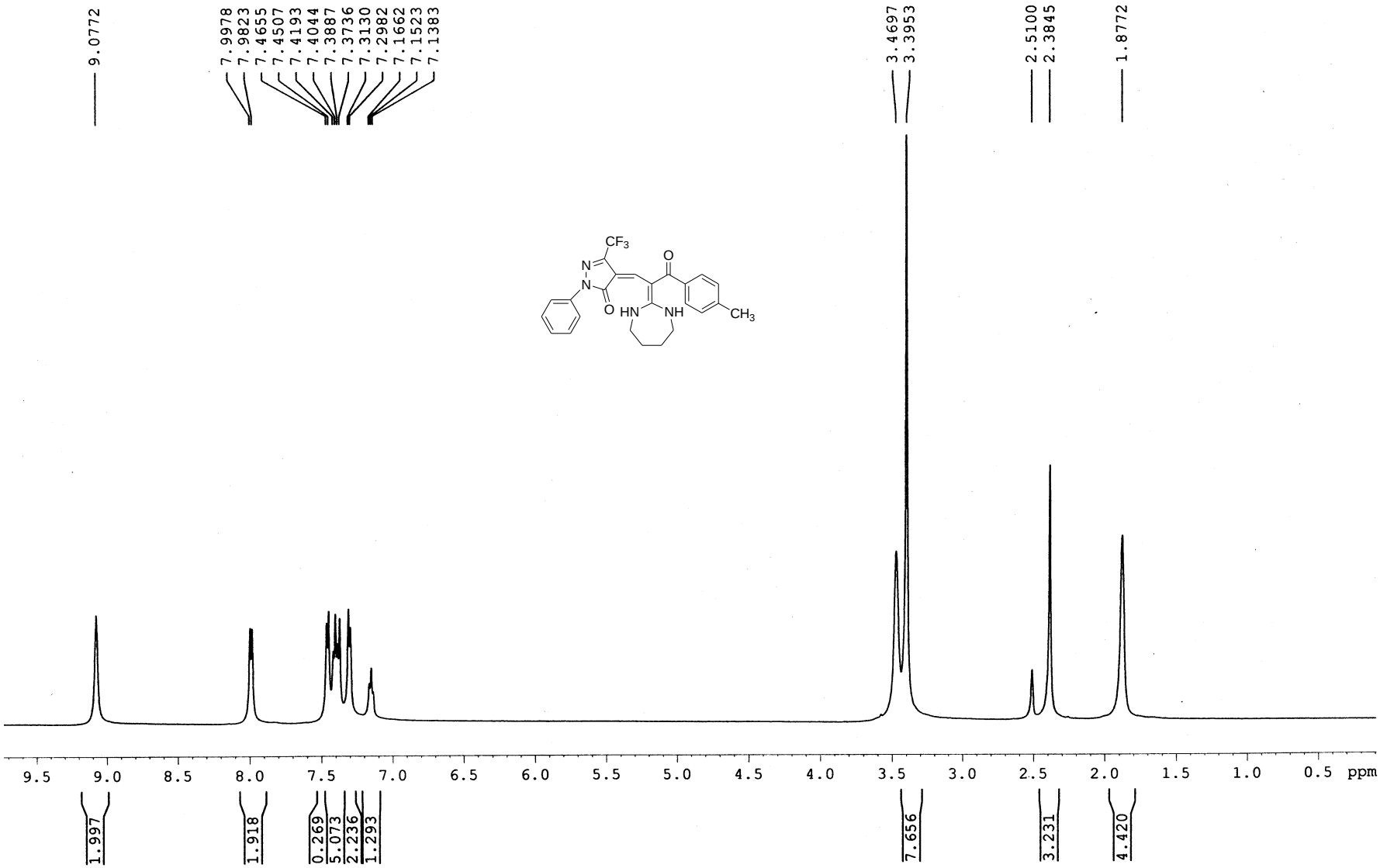


Figure 67. ^{1}H NMR (500 MHz, DMSO-d_6) spectra of compound **8g**

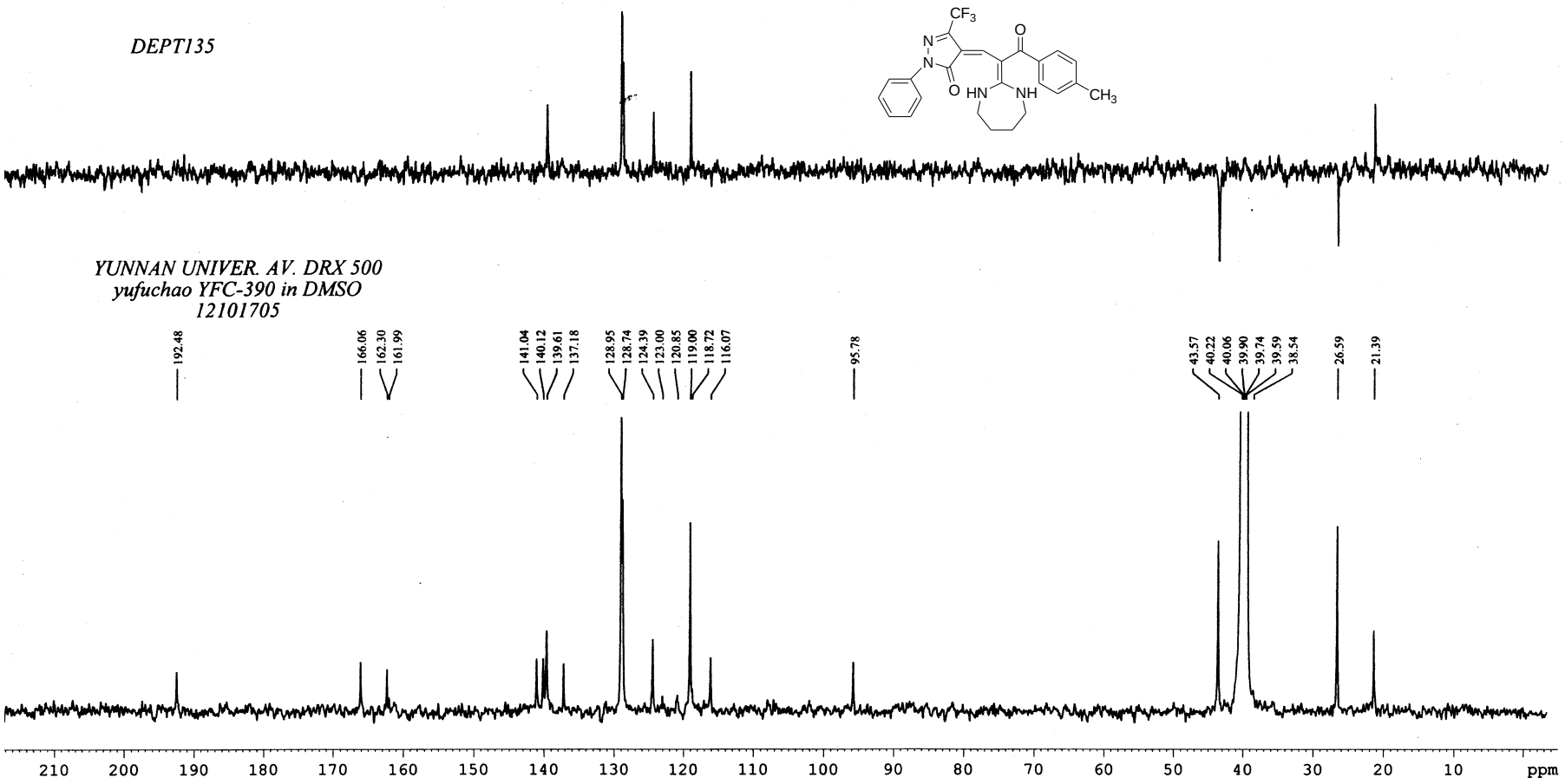
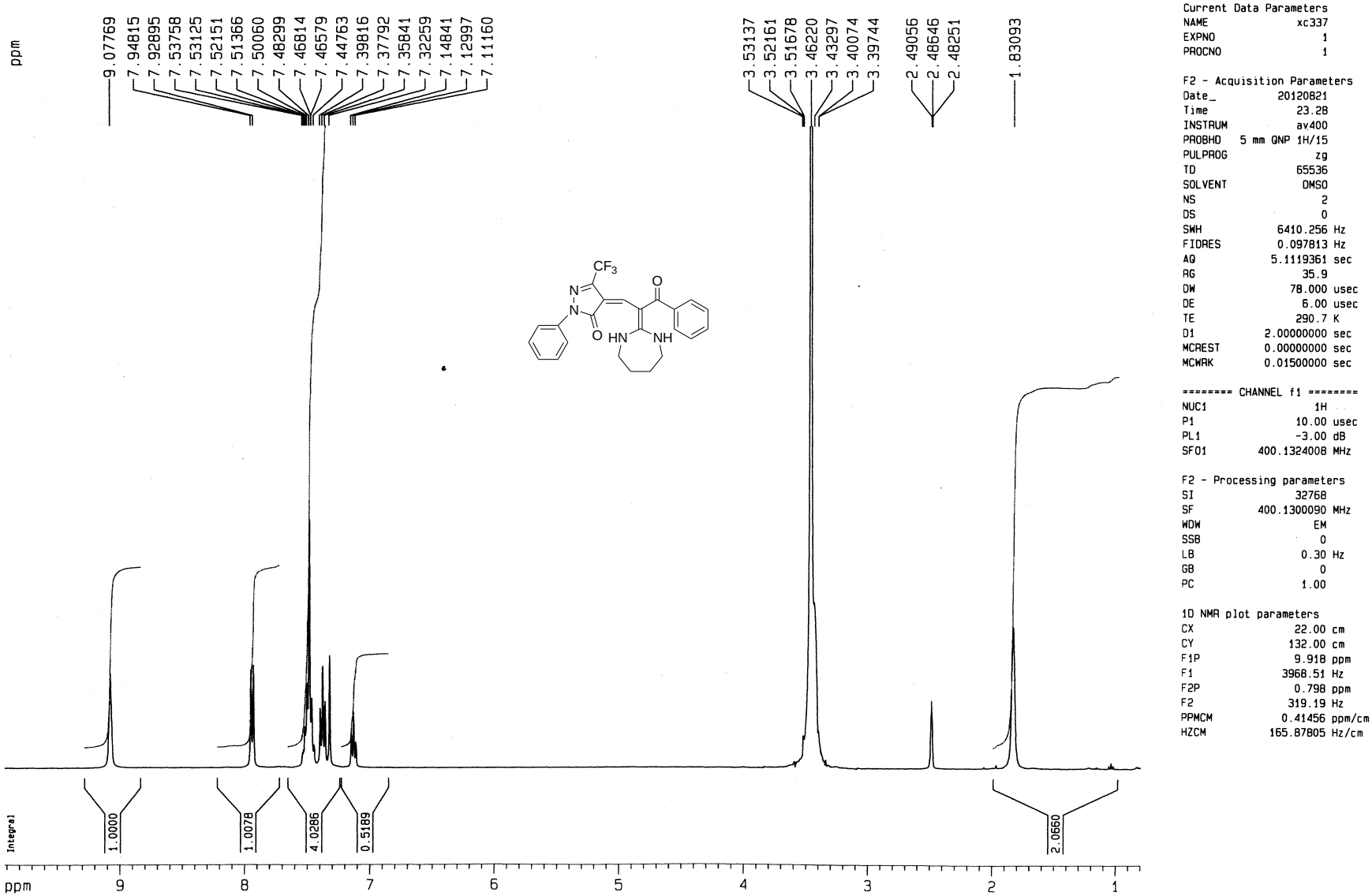


Figure 68. ^{13}C NMR (125 MHz, DMSO-d_6) spectra of compound **8g**



Current Data Parameters

NAME	xc337
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120821
Time	23.28
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	35.9
DW	78.000 usec
DE	6.00 usec
TE	290.7 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

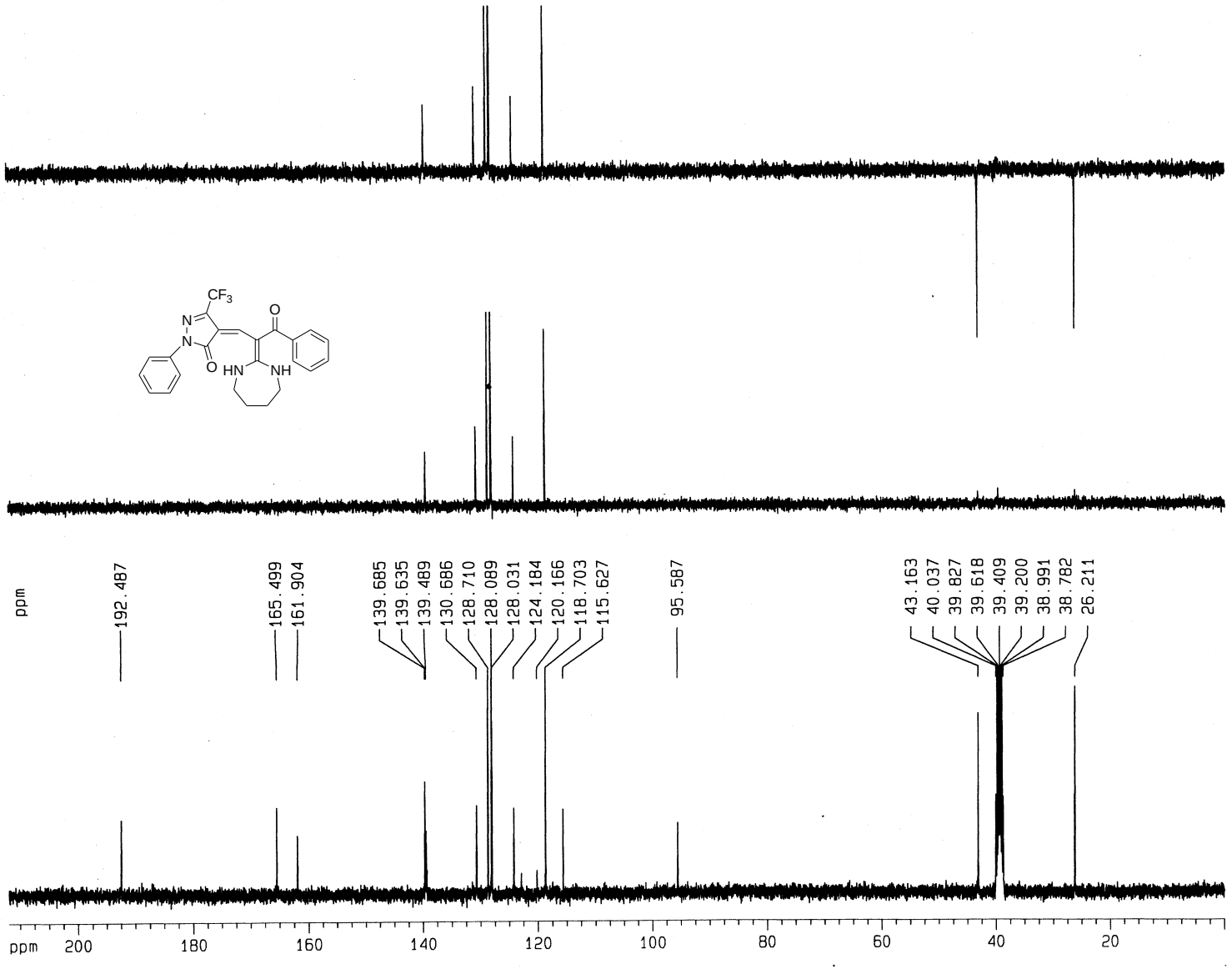
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	132.00 cm
F1P	9.918 ppm
F1	3968.51 Hz
F2P	0.798 ppm
F2	319.19 Hz
PPMCM	0.41456 ppm/cm
HZCM	165.87805 Hz/cm

Figure 69. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **8h**




```
Current Data Parameters
NAME                 xc337
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120821
Time                 23.42
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     154
DS                       2
SWH           23148.148 Hz
FIDRES         0.706425 Hz
AQ             0.7078604 sec
RG                    71.8
DW                21.600 usec
DE                 6.00 usec
TE                291.3 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

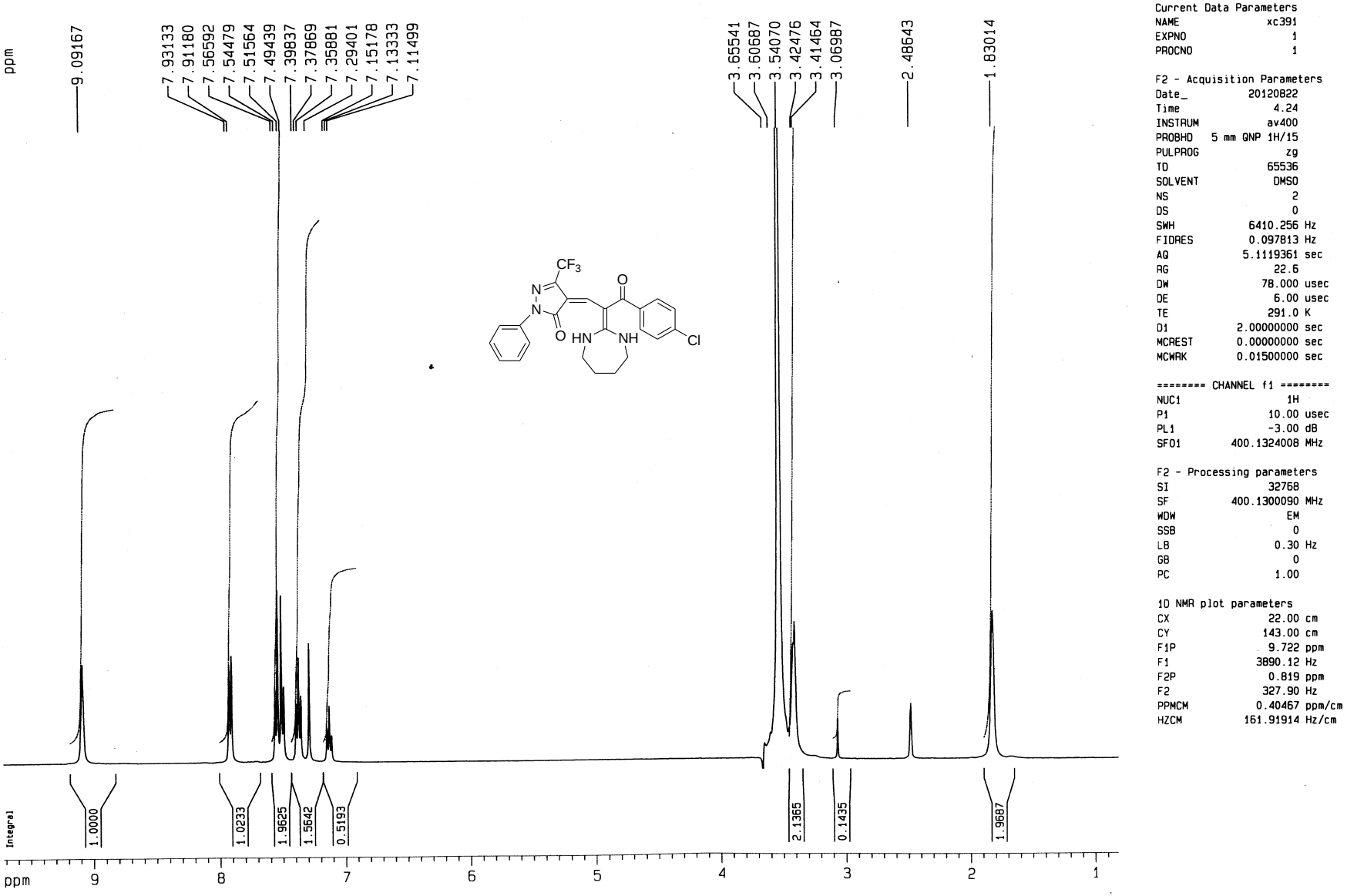
======== CHANNEL f1 ========
NUC1                  13C
P1                 9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF            100.6128120 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    2.00

1D NMR plot parameters
CX                  22.00 cm
CY                   5.00 cm
F1P                212.000 ppm
F1               21329.92 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM           9.63636 ppm/cm
HZCM          969.54156 Hz/cm
```

Figure 70. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **8h**



Current Data Parameters

NAME	xc391
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120822
Time	4.24
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	22.6
DW	78.000 usec
DE	6.00 usec
TE	291.0 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

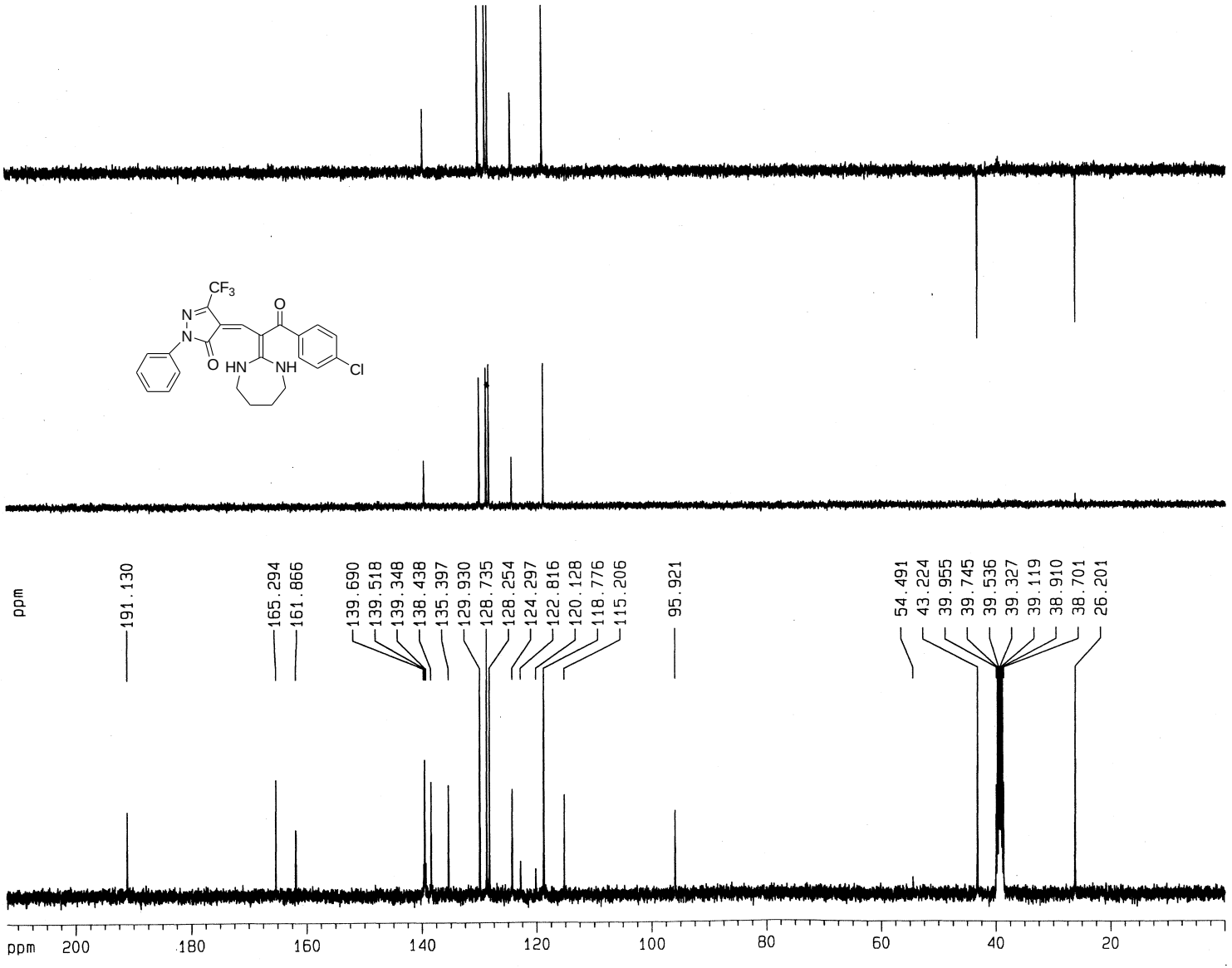
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	143.00 cm
F1P	9.722 ppm
F1	3890.12 Hz
F2P	0.819 ppm
F2	327.90 Hz
PPMCM	0.40467 ppm/cm
HZCM	161.91914 Hz/cm

Figure 71. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **8i**




```
Current Data Parameters
NAME                 xc391
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_              20120822
Time                  4.39
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     154
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                     512
DW                21.600 usec
DE                 6.00 usec
TE                 291.6 K
D1             4.50000000 sec
d11            0.03000000 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

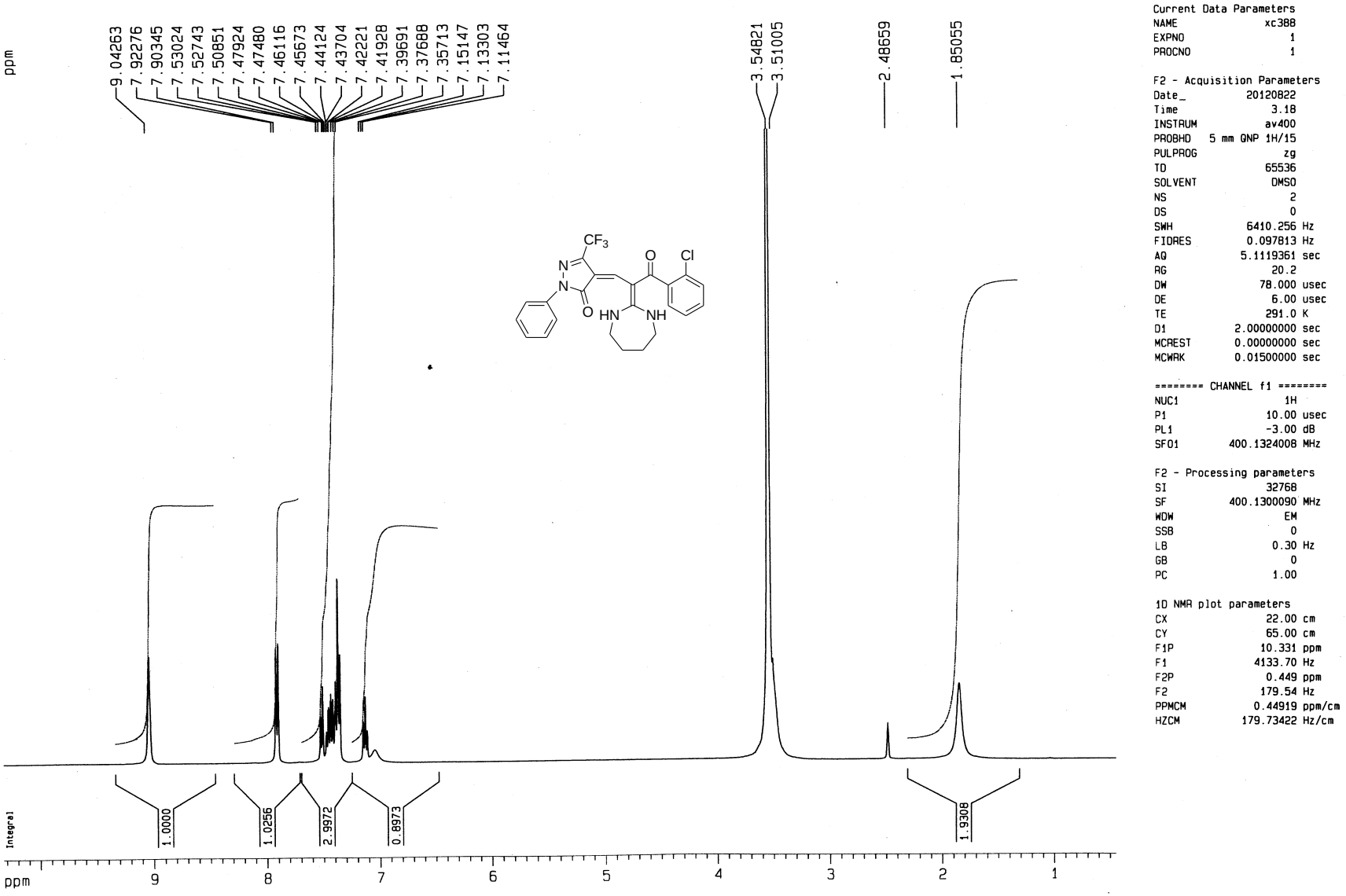
======== CHANNEL f1 ========
NUC1                  13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6128120 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                  22.00 cm
CY                   6.00 cm
F1P                212.000 ppm
F1               21329.92 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM              9.63636 ppm/cm
HZCM             969.54156 Hz/cm
```

Figure 72. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **8i**



Current Data Parameters

NAME	xc388
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20120822
Time	3.18
INSTRUM	av400
PROBHD	5 mm QNP 1H/15
PULPROG	zg
TD	65536
SOLVENT	DMSO
NS	2
DS	0
SWH	6410.256 Hz
FIDRES	0.097813 Hz
AQ	5.1119361 sec
RG	20.2
DW	78.000 usec
DE	6.00 usec
TE	291.0 K
D1	2.00000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

NUC1	1H
P1	10.00 usec
PL1	-3.00 dB
SFO1	400.1324008 MHz

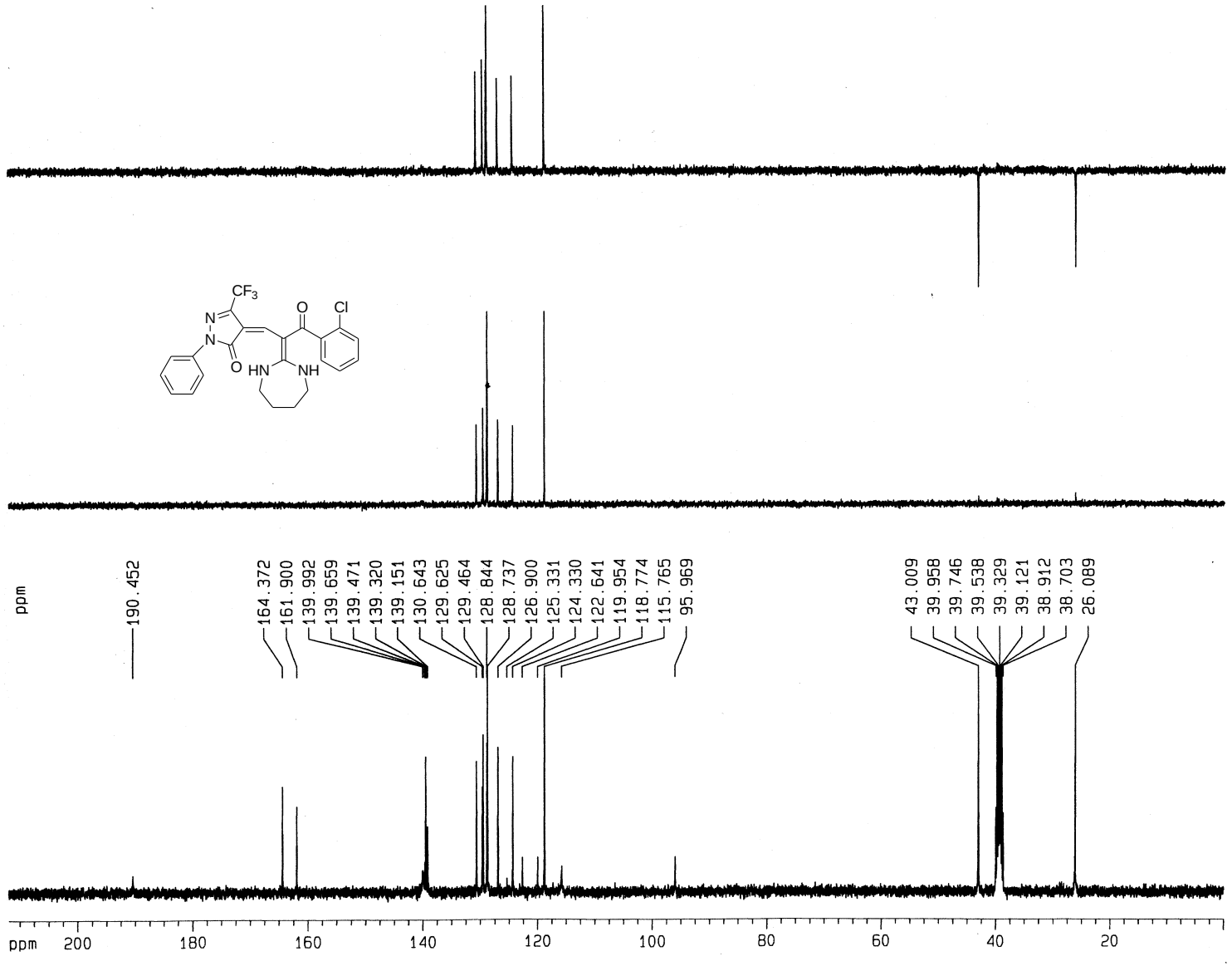
F2 - Processing parameters

SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	22.00 cm
CY	65.00 cm
F1P	10.331 ppm
F1	4133.70 Hz
F2P	0.449 ppm
F2	179.54 Hz
PPMCM	0.44919 ppm/cm
HZCM	179.73422 Hz/cm

Figure 73. ^{1}H NMR (400 MHz, DMSO-d_6) spectra of compound **8j**




```
Current Data Parameters
NAME                 xc388
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20120822
Time                 3.32
INSTRUM              av400
PROBHD   5 mm QNP 1H/15
PULPROG              zgdc
TD                  32768
SOLVENT              DMSO
NS                     154
DS                       2
SWH              23148.148 Hz
FIDRES           0.706425 Hz
AQ               0.7078604 sec
RG                   406.4
DW                  21.600 usec
DE                   6.00 usec
TE                  291.7 K
D1              4.50000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.40 usec
PL1                -4.00 dB
SFO1          100.6236958 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL2                -3.00 dB
PL12               14.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6128120 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.20

1D NMR plot parameters
CX                  22.00 cm
CY                   8.00 cm
F1P                212.000 ppm
F1               21329.92 Hz
F2P                  0.000 ppm
F2                   0.00 Hz
PPMCM             9.63636 ppm/cm
HZCM            969.54156 Hz/cm
```

Figure 74. ^{13}C NMR (100 MHz, DMSO-d_6) spectra of compound **8j**

1. (*a*) Z.-T. Huang, M.-X. Wang, *Synthesis*, 1992, **12**, 1273; (*b*) Z.-J. Li, D. Charles, *Synth. Commun.*, 2001, **31**, 527.
2. CCDC 917318 contain the supplementary crystallographic data for compound **6c**. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.