Supporting Information (Part-A)

Novel Syntheses of Tetrahydrobenzodiazepines and Dihydropyrazines via Isocyanide-based Multicomponent Reactions of Diamines

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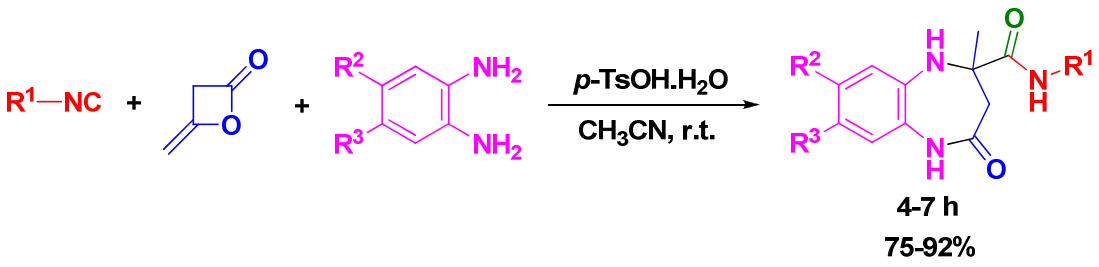


Table 1. Detailed list of CONTENTS of the supporting information **4a-n**

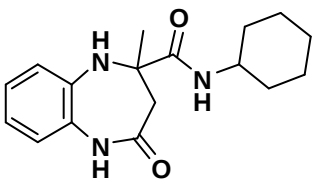
EXPERIMENTAL PROCEDURES

General

Melting points were measured on an Electrothermal 9200 apparatus. Mass spectra were recorded on a Finnigan-MAT 8430 mass spectrometer operating at an ionization potential of 70 eV. IR spectra were recorded on a Shimadzu IR-470 spectrometer. ^{1}H NMR Spectra were recorded on a Bruker DRX-300 Avance spectrometer 300.13 MHz; chemical shifts (δ scale) are reported in parts per million (ppm). ^{1}H NMR Spectra are reported in order: number of protons, multiplicity and approximate coupling constant (*J* value) in hertz (Hz); signals were characterized as s (singlet), d (doublet), t (triplet), m (multiplet), br s (broad signal) and Ar (aryl). The ^{13}C NMR spectra were recorded at 75.47 MHz; chemical shifts (δ scale) are reported in parts per million (ppm). The elemental analyses were performed with an Elementar Analysensysteme GmbH VarioEL. All the products are new compounds, which were characterized by IR, ^{1}H NMR and ^{13}C NMR spectra and Mass spectral data.

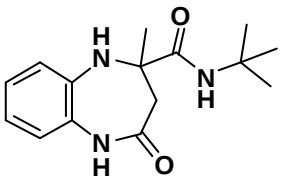
Compounds Characterization Data

_N_-Cyclohexyl-2-methyl-4-oxo-2,3,4,5-tetrahydro-1_H_-benzo[_b_][1,4]diazepine-2-carboxamide (4a).



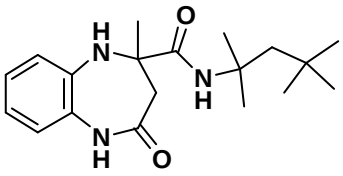
Colorless crystals; mp 263–265°C. IR (KBr) cm^{-1}: 3347, 3295, 3200, 3139, 3087, 2926, 2851, 1675, 1634, 1597, 1526, 1449, 1376. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.00-1.70 (13H, m, 5CH_2 of cyclohexyl and CH_3), 2.39 (2H, br s, CH_2), 3.52 (1H, m, CH of cyclohexyl), 5.34 (1H, br s, NH), 6.85 (2H, br s, H-Ar), 6.95 (2H, br s, H-Ar), 7.64 (1H, br s, NH-CO), 9.55 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 24.9, 25.0, 25.6, 26.6, 32.6, 32.8, 43.4, 48.2, 67.7, 121.9, 122.0, 122.6, 125.0, 131.3, 138.7, 170.4, 173.2. MS *m/z*: 302 (M^++1, 30), 175 (100), 133 (85), 55 (14), 41 (23). Anal. Calcd for $C_{17}H_{23}N_3O_2$: C, 67.75; H, 7.69; N, 13.94; found C, 67.65; H, 7.74; N, 13.84.

***N*-*tert*-Butyl-2,3,4,5-tetrahydro-2-methyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4b).**



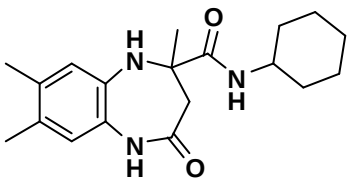
Yellow crystals; mp 246–247°C. IR (KBr) cm^{-1}: 3348, 3289, 3196, 3128, 3075, 2970, 2917, 2870, 1674, 1648, 1600, 1523, 1467, 1374. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.25 (9H, m, $3CH_3$), 1.30 (3H, br s, CH_3), 2.37 (2H, m, CH_2), 5.40 (1H, br s, NH), 6.87 (2H, br s, H-Ar), 6.96 (2H, br s, H-Ar), 7.40 (1H, br s, NH-CO), 9.58 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 26.2, 28.8, 43.5, 50.5, 68.2, 122.0, 122.2, 122.6, 125.1, 131.5, 138.6, 170.5, 173.5. MS *m/z*: 276 (M^++1, 5), 175 (85), 133 (100), 41 (25). Anal. Calcd for $C_{15}H_{21}N_3O_2$: C, 65.43; H, 7.69; N, 15.26; found C, 65.33; H, 7.59; N, 15.35.

2,3,4,5-Tetrahydro-2-methyl-*N*-(2,4,4-trimethylpentan-2-yl)-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4c).



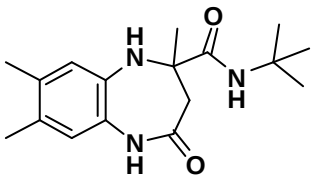
Brown crystals; mp 192–194°C. IR (KBr) cm^{-1}: 3357, 3310, 3196, 3075, 2962, 2891, 2860, 1672, 1603, 1507, 1393, 1319. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 0.95 (9H, br s, $3CH_3$), 1.4 (6H, br s, CH_3), 1.64 (1H, AB_q, J = 14.6 Hz, CH_2), 2.30-2.50 (5H, m, CH_3 and CH_2), 3.98 (1H, br s, NH), 6.80-7.30 (4H, br s, H-Ar), 7.48 (1H, br s, NH-CO), 9.60 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 21.2, 25.0, 26.0, 28.5, 29.2, 31.7, 31.8, 43.4, 52.1, 54.5, 68.2, 122.0, 122.4, 122.7, 125.0, 128.5, 131.3, 170.3, 172.8. MS *m/z*: 175 (100), 133 (70), 57 (15), 41 (18). Anal. Calcd for $C_{19}H_{29}N_3O_2$: C, 68.85; H, 8.82; N, 12.68; found C, 68.78; H, 8.72; N, 12.58.

***N*-Cyclohexyl-2,3,4,5-tetrahydro-2,7,8-trimethyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4d).**



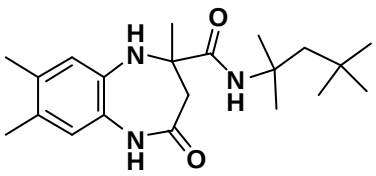
Colorless crystals; mp 248–249°C. IR (KBr) cm^{-1}: 3353, 3308, 3210, 2930, 2855, 1684, 1636, 1518, 1454, 1374, 1314. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.00-1.70 (16H, m, $5CH_2$ of cyclohexyl and CH_3), 2.09 (6H, br s, $2CH_3$), 2.33 (2H, AB_q, J = 12.8, CH_2), 3.53 (1H, m, CH of cyclohexyl), 5.10 (1H, br s, NH), 6.63 (1H, br s, H-Ar), 6.74 (1H, br s, H-Ar), 7.63 (1H, d, J = 8.2, NH-CO), 9.41 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 19.0, 19.3, 25.0, 25.6, 25.4, 32.6, 32.8, 43.2, 48.1, 67.9, 122.9, 123.8, 129.2, 129.8, 132.6, 136.3, 170.6, 173.4. MS *m/z*: 330 (M^++1, 9), 203 (100), 161 (84), 55 (16), 41 (25). Anal. Calcd for $C_{19}H_{27}N_3O_2$: C, 69.27; H, 8.26; N, 12.76; found C, 69.18; H, 8.20; N, 12.66.

***N*-*tert*-Butyl-2,3,4,5-tetrahydro-2,7,8-trimethyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4e).**

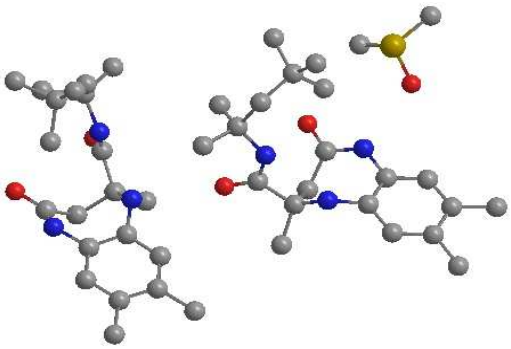


Colorless crystals; mp 268–269°C. IR (KBr) cm^{-1}: 3337, 3296, 3178, 3070, 2962, 2962, 2854, 1671, 1509, 1520, 1455, 1380, 1320. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.25 (9H, m, $3CH_3$), 1.28 (3H, br s, CH_3), 2.10 (6H, br s, $2CH_3$), 2.34 (2H, AB_q, J = 12.8 Hz, CH_2), 5.15 (1H, br s, NH), 6.64 (1H, br s, H-Ar), 6.73 (1H, br s, H-Ar), 7.42 (1H, br s, NH-CO), 9.43 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 19.0, 19.3, 26.0, 28.8, 43.5, 50.5, 68.4, 123.0, 123.8, 129.3, 130.0, 132.7, 136.2, 170.6, 173.7. MS *m/z*: 304 (M^++1, 14), 203 (100), 161 (84), 57 (20), 41 (26). Anal. Calcd for $C_{17}H_{25}N_3O_2$: C, 67.30; H, 8.31; N, 13.85; found C, 67.25; H, 8.22; N, 13.67.

2,3,4,5-Tetrahydro-2,7,8-trimethyl-*N*-(2,4,4-trimethylpentan-2-yl)-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4f).

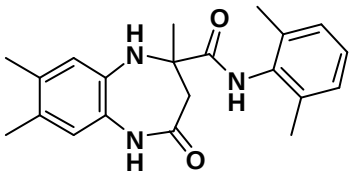


Colorless crystals; mp 205–207°C. IR (KBr) cm^{-1}: 3353, 3296, 3183, 3075, 2957, 2855, 1668, 1510, 1518, 1437, 1391, 1226. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 0.94 (9H, br s, $3CH_3$), 1.27 (3H, br s, CH_3), 1.31 (6H, br s, $2CH_3$), 1.62 (2H, AB_q, J = 14.7 Hz, CH_2), 2.09 (3H, br s, CH_3), 2.10 (3H, br s, CH_3), 2.30 (2H, AB_q, J = 12.9 Hz, CH_2), 5.10 (1H, br s, NH), 6.63 (1H, br s, H-Ar), 6.77 (1H, br s, H-Ar), 7.20 (1H, br s, NH-CO), 9.43 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 19.0, 19.3, 26.0, 28.4, 29.2, 31.7, 31.8, 43.5, 52.4, 54.4, 68.4, 123.0, 123.8, 129.0, 129.8, 132.6, 136.1, 170.4, 173.1. MS *m/z*: 360 (M^++1, 6), 203 (100), 161 (82), 57 (22), 41 (25). Anal. Calcd for $C_{21}H_{33}N_3O_2$: C, 70.16; H, 9.25; N, 11.69; found C, 70.10; H, 9.15; N, 11.60.



ORTEP diagram for **4f**; summary of data: The Cambridge Crystallographic Data Centre (CCDC) no.: 735911; unit cell parameters: a 27.1869(6) b 10.2149(2) c 34.7688(9) beta 106.095(1); space group C2/c.

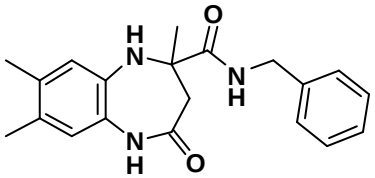
2,3,4,5-Tetrahydro-2,7,8-trimethyl-*N*-(2,6-dimethylphenyl)-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4g).



Dark white crystals; mp 261–263°C. IR (KBr) cm^{-1}: 3363, 3285, 3270, 3183, 2963, 2916, 1670, 1506, 1389. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.48 (3H, br s, CH_3), 2.11 (12H, m, $4CH_3$), 2.48 (1H, d, J = 12.8 Hz, CH_2), 2.58 (1H, d, J = 12.9 Hz, CH_2), 5.26 (1H, br s, NH), 6.68 (1H, br s, H-Ar), 6.85 (1H, br s, H-Ar), 7.04 (3H, br s, H-Ar), 9.28 (1H, br s, NH-CO), 9.53 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 18.5, 19.0, 19.3, 27.1, 43.3, 68.1, 122.9, 123.9, 126.8, 128.0, 128.8, 129.6, 132.6, 135.5, 135.7,

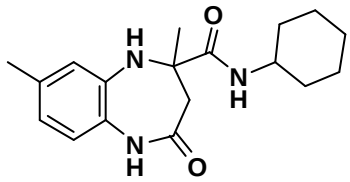
136.2, 170.6, 173.1. MS *m/z*: 352 (M^++1, 9), 203 (100), 161 (75), 120 (20), 91 (20). Anal. Calcd for $C_{21}H_{25}N_3O_2$: C, 71.77; H, 7.17; N, 11.96; found C, 71.67; H, 7.10; N, 11.92.

***N*-Benzyl-2,3,4,5-tetrahydro-2,7,8-trimethyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4h).**



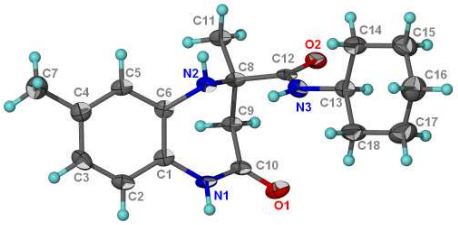
Brown powder; mp 192–194°C. IR (KBr) cm^{-1}: 3354, 3285, 3212, 3028, 2965, 2854, 1681, 1635, 1517, 1450, 1374. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.37 (3H, br s, CH_3), 2.09 (6H, br s, $2CH_3$), 2.44 (2H, AB_q, J = 12.7 Hz, CH_2), 4.30 (2H, m, CH_2), 5.13 (1H, br s, NH), 6.66 (1H, d, J = 8.0 Hz, H-Ar), 6.76 (2H, m, H-Ar), 7.27 (5H, m, H-Ar), 8.45 (1H, m, NH-CO), 9.47 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 19.0, 19.3, 26.8, 42.9, 43.3, 68.0, 122.9, 123.9, 127.1, 127.5, 128.6, 129.0, 129.7, 132.6, 136.2, 139.8, 170.6, 174.6. MS *m/z*: 337 (M^+, 15), 320 (17), 304 (30), 203 (100), 161 (80), 91 (85), 65 (25), 39 (25). Anal. Calcd for $C_{20}H_{23}N_3O_2$: C, 71.19; H, 6.87; N, 12.45; found C, 71.10; H, 6.78; N, 12.35.

***N*-Cyclohexyl-2,3,4,5-tetrahydro-2,8-dimethyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4i).**



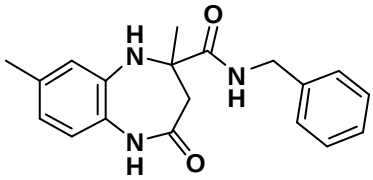
Light yellow crystals; mp 264–265°C. IR (KBr) cm^{-1}: 3359, 3301, 3201, 3112, 2928, 2849, 1674, 1636, 1524, 1488, 1451, 1375. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.00-1.70 (13H, m, $5CH_2$ of cyclohexyl and CH_3), 2.19 (3H, br s, CH_3), 2.42 (2H, m, CH_2), 3.51 (1H, m, CH of cyclohexyl), 5.26 (1H, br s, NH), 6.50-6.80 (3H, m, H-Ar), 7.63 (1H, d, J = 6.3, NH-CO), 9.46 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 20.9, 24.9, 25.0, 25.6, 26.6, 32.6, 32.8, 43.3, 48.2, 67.6, 121.9, 122.6, 122.9, 128.7, 134.1, 138.4,

170.6, 173.3. MS *m/z*: 316 (M^++1, 8), 189 (100), 147 (80), 41 (25). Anal. Calcd for $C_{18}H_{25}N_3O_2$: C, 68.54; H, 7.99; N, 13.32; found C, 68.44; H, 7.87; N, 13.22.



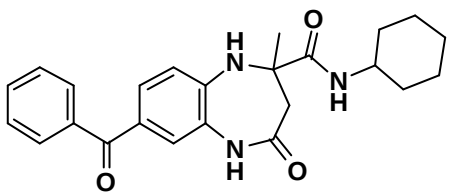
ORTEP diagram for **4i;** summary of data: The Cambridge Crystallographic Data Centre (CCDC) no.: 735910; unit cell parameters: a 5.7118(2) b 25.8049(10) c 11.8905(6) beta 94.801(3); space group P21/n.

***N*-Benzyl-2,3,4,5-tetrahydro-2,7,8-trimethyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4j).**



Brown crystals; mp 183–185°C. IR (KBr) cm^{-1}: 3306, 3263, 3029, 2942, 1676, 1631, 1524, 1452, 1355. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.38 (3H, br s, CH_3), 2.18 (3H, br s, CH_3), 2.50 (2H, AB_q, J = 13.0 Hz, CH_2), 4.30 (2H, ABX, J = 15.2, 5.7, 6.2 Hz, CH_2), 5.31 (1H, br s, NH), 6.67 (1H, d, J = 8.0 Hz, H-Ar), 6.77 (2H, m, H-Ar), 7.10-7.35 (5H, m, H-Ar), 8.47 (1H, dd, J = 5.9, 5.9 Hz, NH-CO), 9.51 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 20.9, 27.1, 42.9, 43.4, 67.6, 121.9, 122.4, 122.9, 127.0, 127.5, 128.4, 128.6, 134.0, 138.5, 139.8, 170.4, 174.5. MS *m/z*: 324 (M^++1, 14), 189 (100), 147 (82), 121 (12), 91 (45). Anal. Calcd for $C_{19}H_{21}N_3O_2$: C, 70.57; H, 6.55; N, 12.99; found C, 70.50; H, 6.52; N, 12.89.

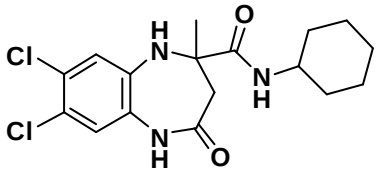
7-Benzoyl-*N*-cyclohexyl-2-methyl-4-oxo-2,3,4,5-tetrahydro-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4k).



Light yellow powder; mp 189–191°C. IR (KBr) cm^{-1}: 3290, 3286, 3064, 2986, 2933, 2865, 1680, 1634,

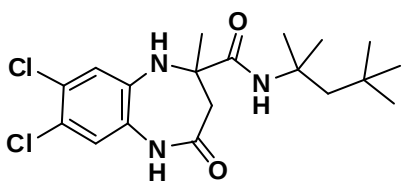
1530, 1470, 1425, 1318. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.00-1.70 (13H, m, 5CH_2 of cyclohexyl and CH_3), 2.61 (2H, br s, CH_2), 3.52 (1H, m, CH of cyclohexyl), 6.35 (1H, br s, NH), 7.01 (1H, d, J = 8.2, H-Ar), 6.30-7.70 (8H, m, H-Ar and NH-CO), 9.68 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 25.1, 25.6, 27.6, 31.1, 32.5, 32.7, 44.5, 48.4, 65.1, 120.5, 124.5, 127.1, 127.3, 128.2, 128.8, 129.6, 132.2, 138.4, 143.2, 170.2, 172.5, 194.2. MS *m/z*: 406 (M^++1, 1), 280 (25), 279 (100), 237 (86), 105 (35), 77 (40), 55 (18), 41 (25). Anal. Calcd for $C_{24}H_{27}N_3O_3$: C, 71.09; H, 6.71; N, 10.36; found C, 71.00; H, 6.61; N, 10.26.

7,8-Dichloro-*N*-cyclohexyl-2,3,4,5-tetrahydro-2-methyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4l).



White powder; mp 262–264°C. IR (KBr) cm^{-1}: 3364, 3270, 3185, 3070, 2933, 2854, 1677, 1670, 1598, 1521, 1485, 1456, 1388. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.00-2.20 (15H, m, 5CH_2 of cyclohexyl, CH_2 and CH_3), 3.48 (1H, m, CH of cyclohexyl), 5.78 (1H, br s, NH), 7.01 (1H, br s, H-Ar), 7.15 (1H, br s, H-Ar), 7.57 (1H, br s, NH-CO), 9.68 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 25.0, 25.1, 25.6, 26.9, 32.5, 32.7, 43.7, 48.3, 66.4, 121.9, 122.7, 125.8, 130.2, 139.0, 170.1, 172.6. MS *m/z*: 372 (M^+, ^{37}Cl, 4), 370 (M^+, ^{35}Cl, 8), 243 (100), 201 (100), 55 (20), 41 (25). Anal. Calcd for $C_{17}H_{21}Cl_2N_3O_2$: C, 55.14; H, 5.72; N, 11.35; found C, 55.10; H, 5.62; N, 11.25.

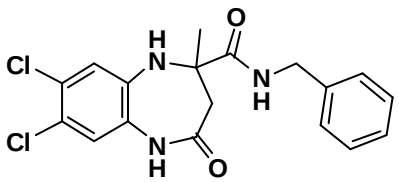
7,8-Dichloro-2,3,4,5-tetrahydro-2-methyl-*N*-(2,4,4-trimethylpentan-2-yl)-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4m).



Violet powder; mp 248–250°C. IR (KBr) cm^{-1}: 3363, 3327, 3188, 3139, 3060, 2947, 2865, 1680, 1495, 1394,

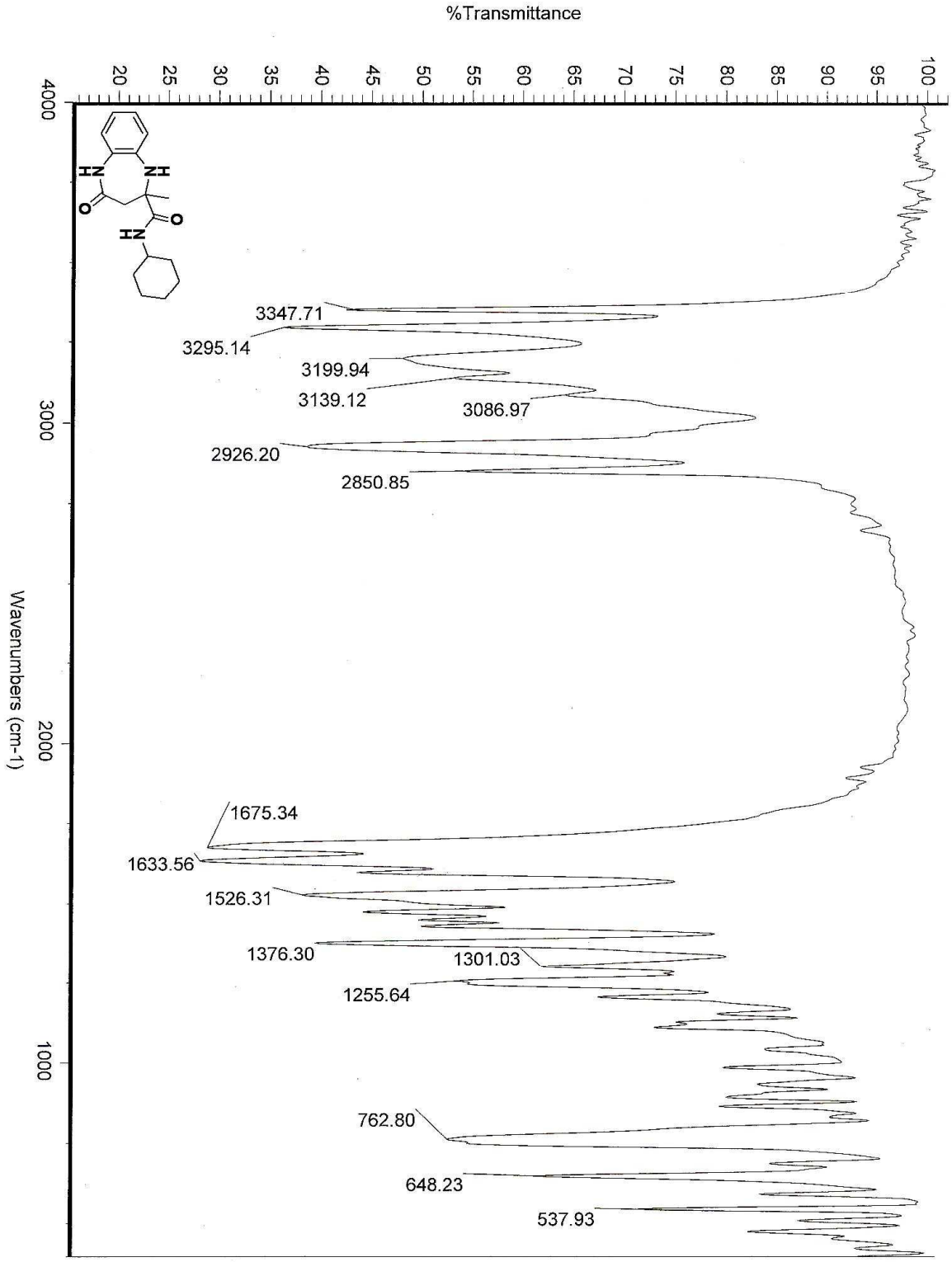
1376. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 0.91 (9H, br s, 3CH_3), 1.27 (6H, br s, 2CH_3), 1.32 (3H, br s, CH_3), 1.61 (2H, AB_q, J = 14.8 Hz, CH_2), 2.07 (1H, m, CH_2), 2.26 (1H, m, CH_2), 5.80 (1H, br s, NH), 7.04 (1H, br s, H-Ar), 7.18 (1H, br s, H-Ar), 7.21 (1H, br s, NH-CO), 9.73 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 26.6, 28.6, 29.3, 31.7, 43.8, 51.9, 54.6, 66.8, 122.2, 122.6, 122.7, 125.8, 130.2, 138.7, 170.2, 172.4. MS *m/z*: 402 (M^++1, ^{37}Cl, 1), 400 (M^++1, ^{35}Cl, 2), 243 (86), 201 (100), 165 (18), 97 (20), 57 (28), 41 (32). Anal. Calcd for $C_{19}H_{27}Cl_2N_3O_2$: C, 57.00; H, 6.80; N, 10.50; found C, 57.10; H, 6.72; N, 10.40.

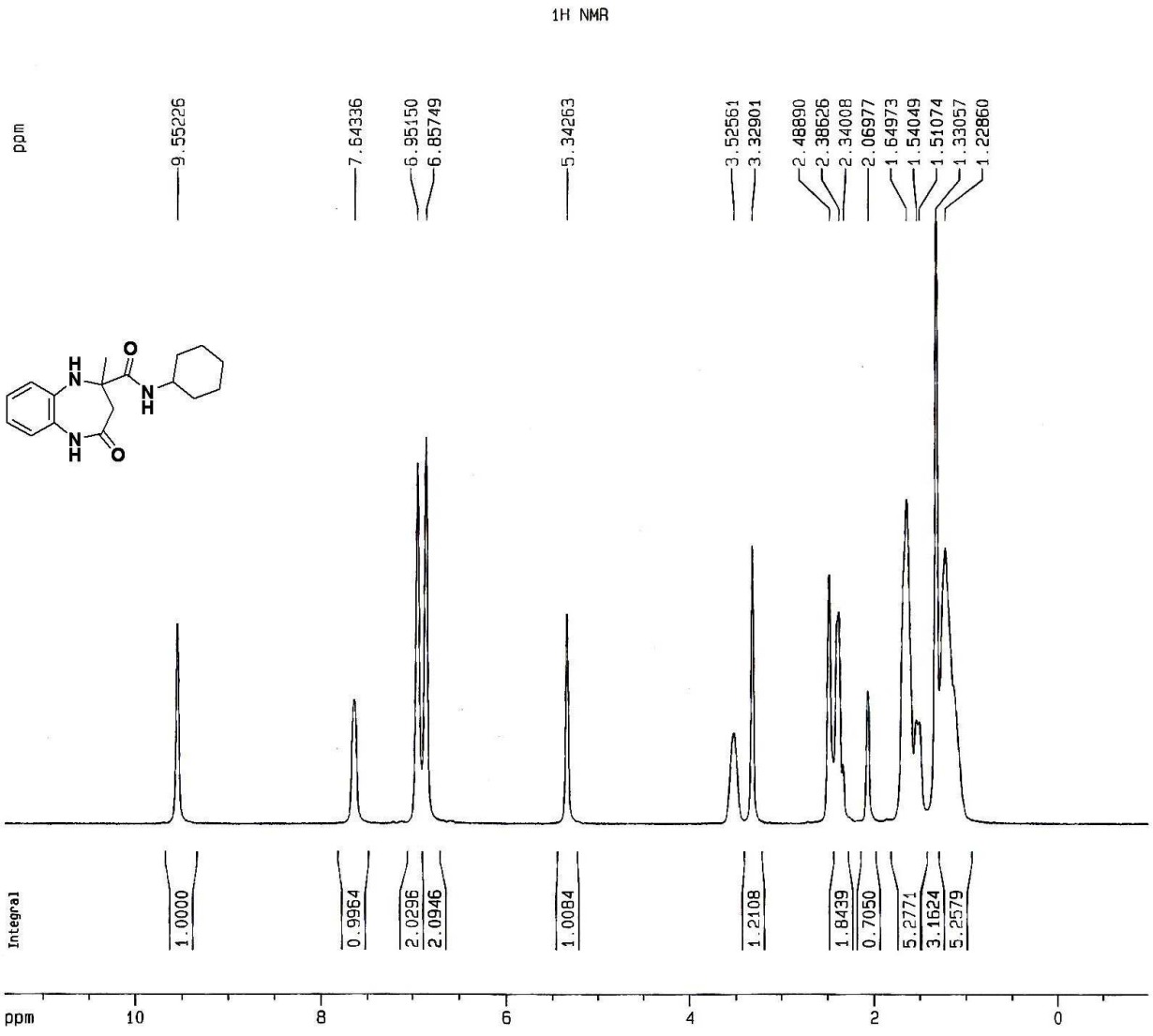
***N*-Benzyl-7,8-dichloro-2,3,4,5-tetrahydro-2-methyl-4-oxo-1*H*-benzo[*b*][1,4]diazepine-2-carboxamide (4n).**



Violet powder; mp 246–247°C. IR (KBr) cm^{-1}: 3332, 3214, 3086, 3009, 1668, 1621, 1493, 1390. ^{1}H NMR (300.13 MHz, DMSO-d_6) δ: 1.41 (3H, br s, CH_3), 2.40-2.65 (2H, m, CH_2), 4.28 (2H, ABX, J = 15.0, 6.1, 5.5 Hz, CH_2), 5.92 (1H, br s, NH), 7.07 (1H, br s, H-Ar), 7.00-7.30 (6H, m, H-Ar), 8.50 (1H, m, NH-CO), 9.75 (1H, br s, NH-CO). ^{13}C NMR (75.47 MHz, DMSO-d_6) δ: 27.4, 42.9, 44.0, 66.2, 121.6, 122.5, 122.6, 125.8, 127.0, 127.4, 128.6, 129.6, 138.8, 139.9, 170.2, 173.9. MS *m/z*: 380 (M^++1, ^{37}Cl, 1), 378 (M^++1, ^{35}Cl, 2), 243 (82), 201 (100), 91 (70), 65 (20), 41 (20). Anal. Calcd for $C_{18}H_{17}Cl_2N_3O_2$: C, 57.16; H, 4.53; N, 11.11; found C, 57.05; H, 4.44; N, 11.01.

IR of **4a**


%Transmittance
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
4000
3000
2000
1000
Wavenumbers (cm-1)
3347.71
3295.14
3199.94
3139.12
3086.97
2926.20
2850.85
1675.34
1633.56
1526.31
1376.30
1301.03
1255.64
762.80
648.23
537.93



Current Data Parameters
NAME Maleki-PHD
EXPNO 398
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090518
Time 15.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
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P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz

F2 - Processing parameters
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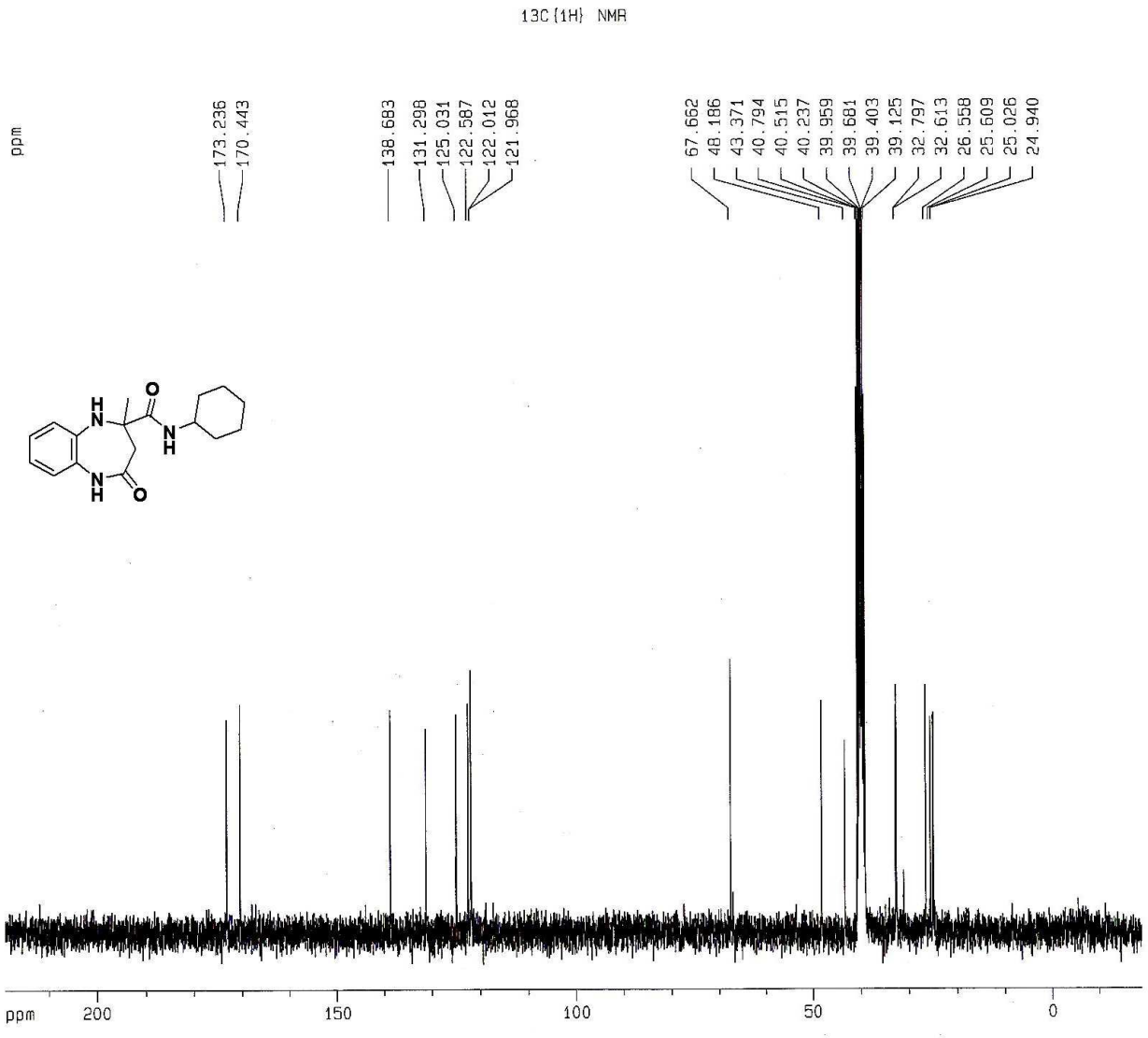
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 11.44 cm
F1P 11.413 ppm
F1 3425.51 Hz
F2P -0.998 ppm
F2 -299.52 Hz
PPMCM 0.62057 ppm/cm
HZCM 186.25162 Hz/cm

^{1}H NMR of **4a**

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Current Data Parameters
NAME          Maleki-PHD
EXPNO                399
PROCNO                 1

F2 - Acquisition Parameters
Date_          20090518
Time              16.27
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PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                1024
DS                   2
SWH          17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                2048
DW              27.800 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                8.75 usec
PL1              -2.00 dB
SF01         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            87.00 usec
PL2              -2.00 dB
PL12             12.00 dB
PL13             18.00 dB
SF02        300.1312005 MHz

F2 - Processing parameters
SI                 65536
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40

1D NMR plot parameters
CX                20.00 cm
CY                65.99 cm
F1P             219.155 ppm
F1            16539.10 Hz
F2P             -19.167 ppm
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HZCM          899.28058 Hz/cm
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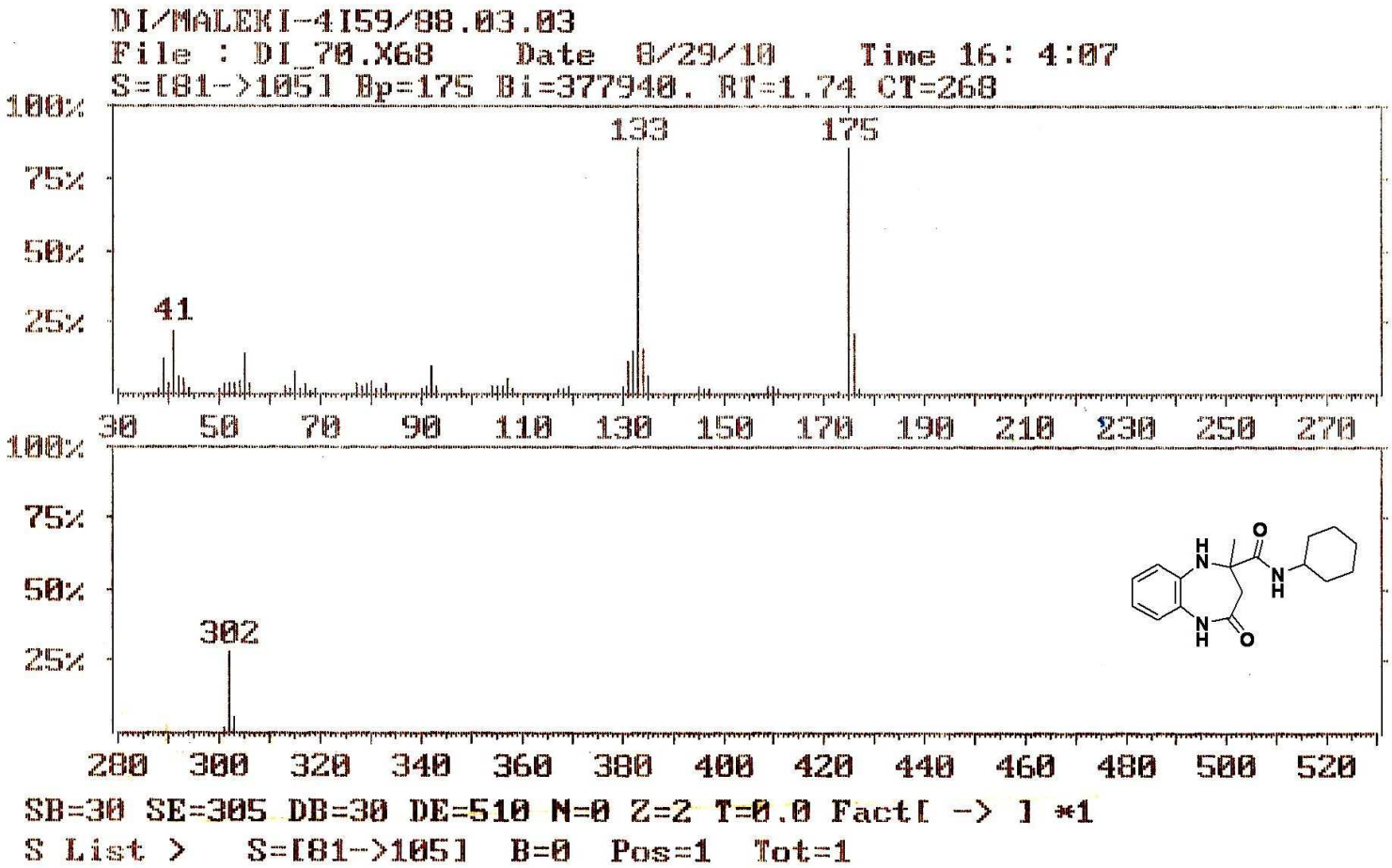
^{13}C NMR of **4a**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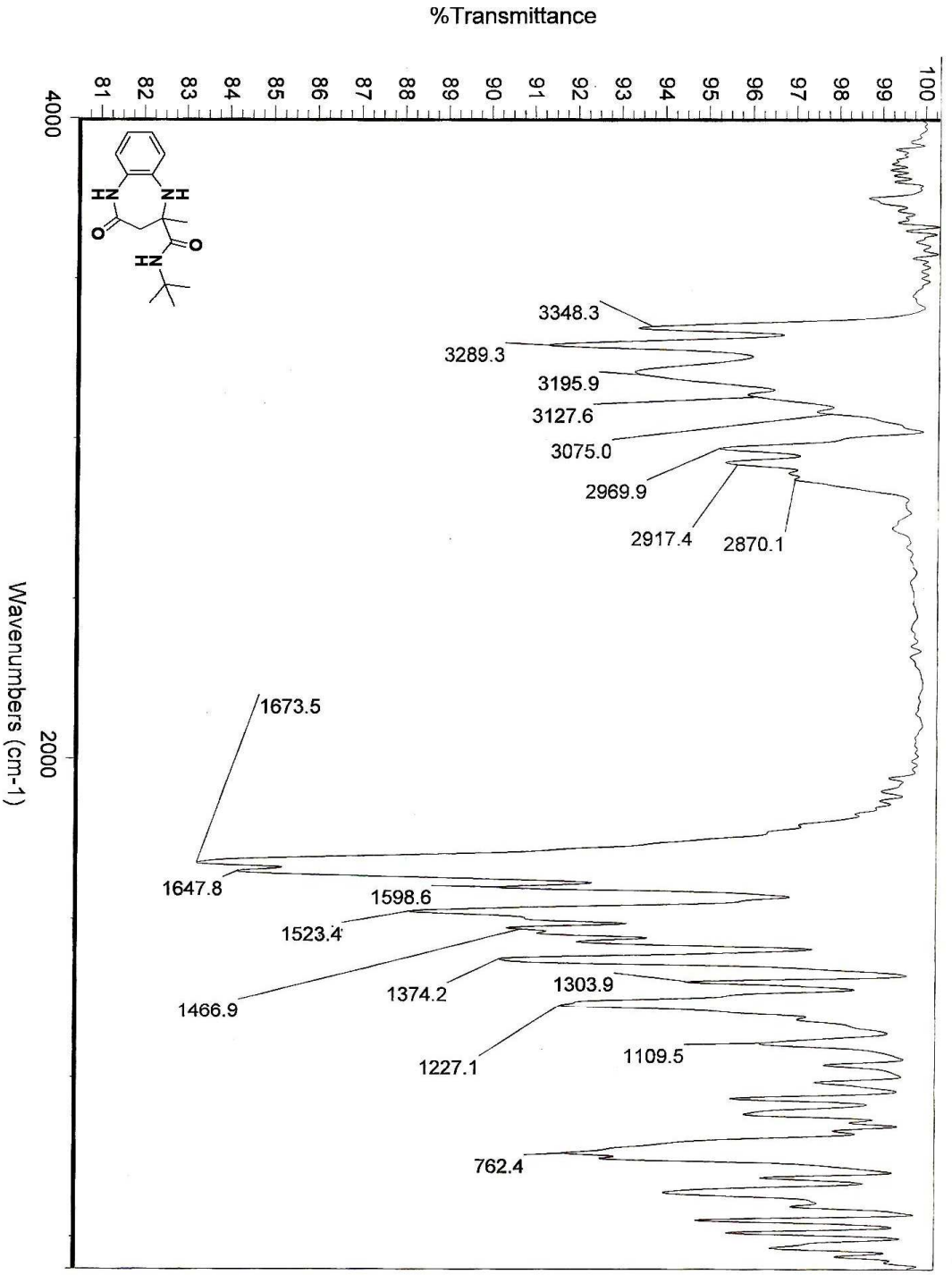
75%
50%
25%
133
175
41
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
302
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=305 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[81->105] B=0 Pos=1 Tot=1

Mass of **4a**

IR of **4b**


%Transmittance
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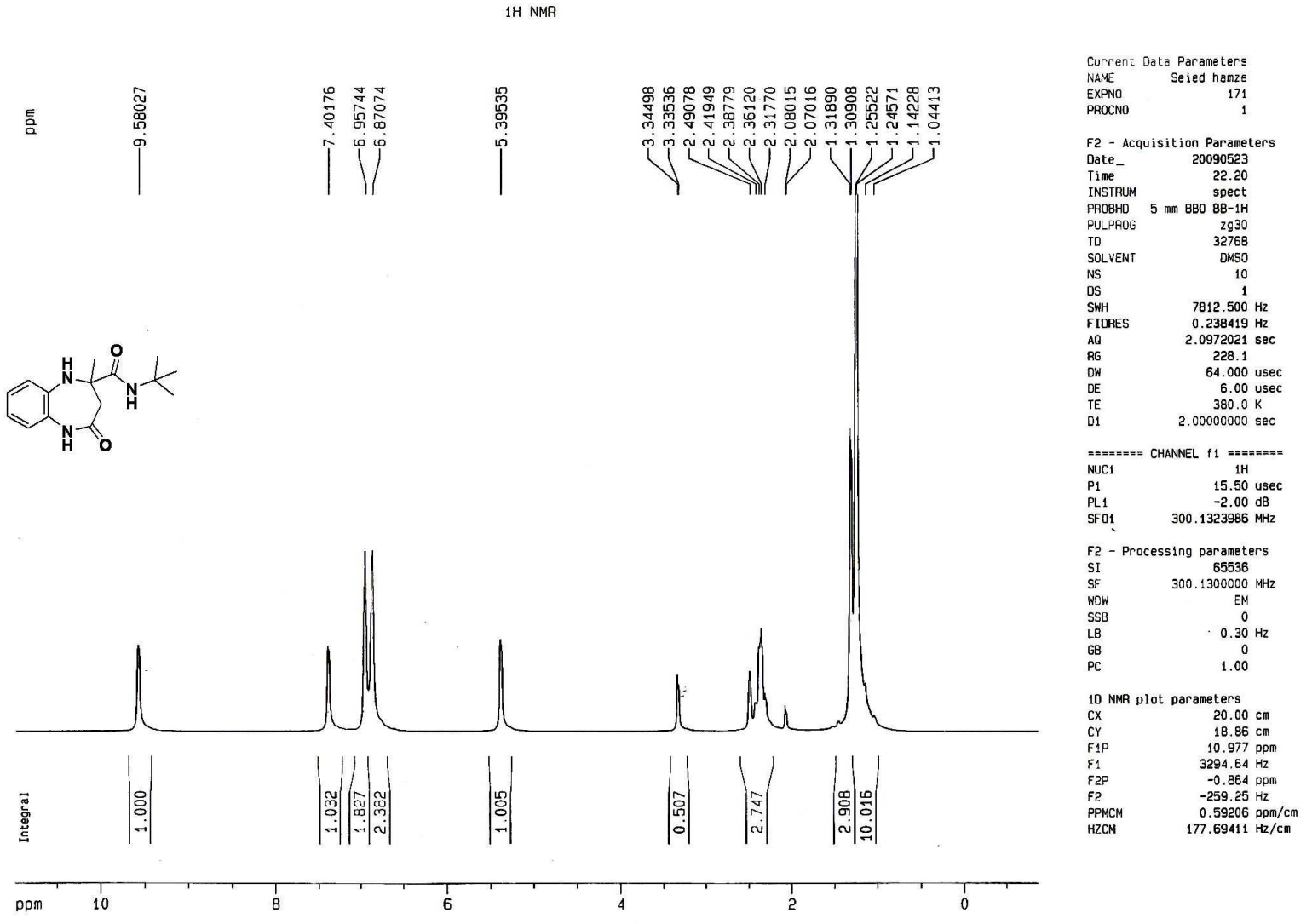
82
83
84
85
86
87
88
89
90
91
92
93
94
95
96
97
98
99
100
4000
2000
Wavenumbers (cm-1)
3348.3
3289.3
3195.9
3127.6
3075.0
2969.9
2917.4
2870.1
1673.5
1647.8
1598.6
1523.4
1466.9
1374.2
1303.9
1227.1
1109.5
762.4



Current Data Parameters

NAME	Seied hamze
EXPNO	171
PROCNO	1

F2 - Acquisition Parameters

Date_	20090523
Time	22.20
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	10
DS	1
SWH	7812.500 Hz
FIDRES	0.238419 Hz
AQ	2.0972021 sec
RG	228.1
DW	64.000 usec
DE	6.00 usec
TE	380.0 K
D1	2.00000000 sec

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NUC1	1H
P1	15.50 usec
PL1	-2.00 dB
SFO1	300.1323986 MHz

F2 - Processing parameters

SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	18.86 cm
F1P	10.977 ppm
F1	3294.64 Hz
F2P	-0.864 ppm
F2	-259.25 Hz
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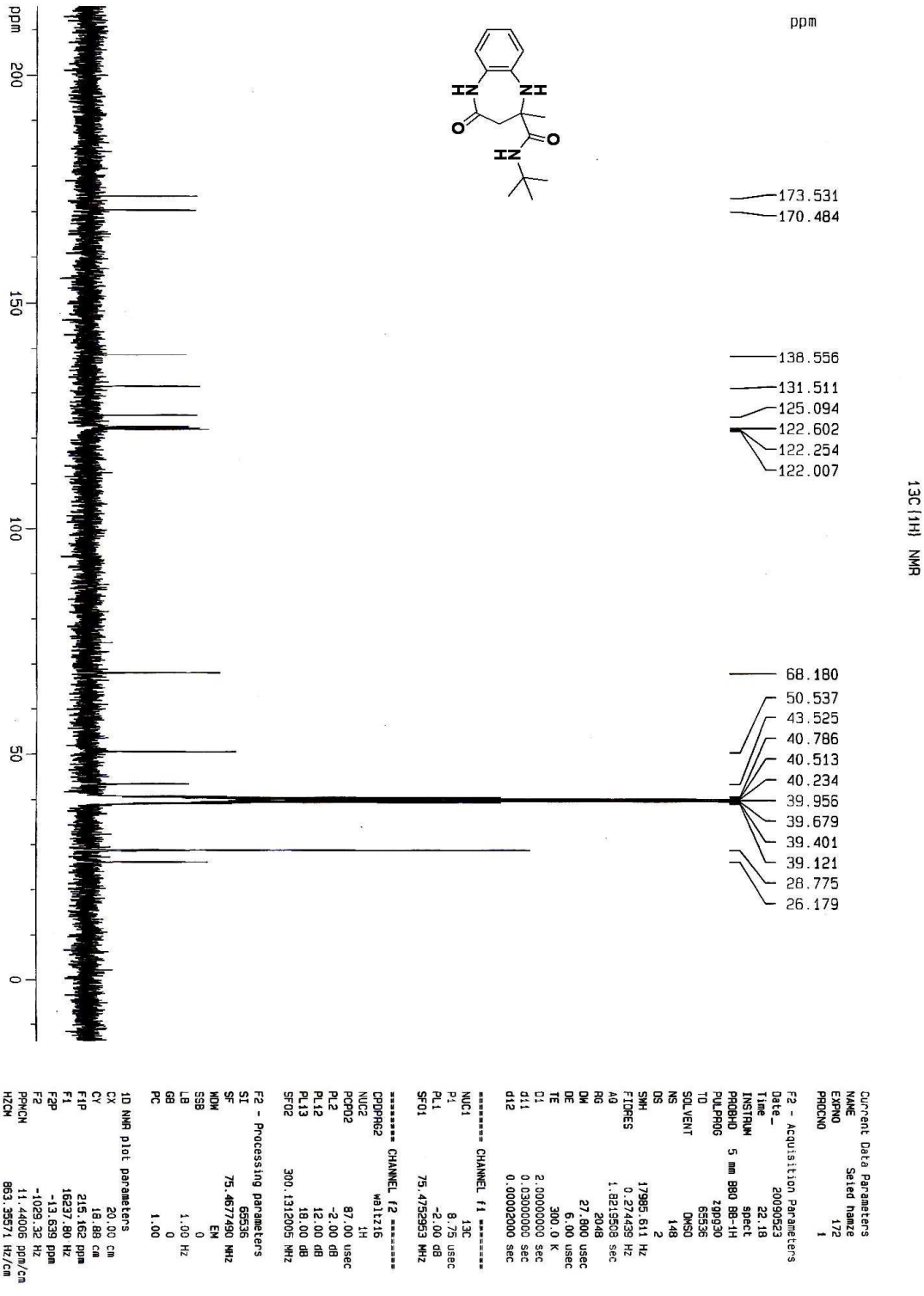
HZCM	177.69411 Hz/cm

^{1}H NMR of **4b**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68.180
50.537
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40.786
40.513
40.234
39.956
39.679
39.401
39.121
28.775
26.179
13C{1H} NMR
Current Data Parameters
NAME Seied hamza
EXPNO 172
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090523
Time 22.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
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DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
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NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752993 MHz
======== CHANNEL f2 ========
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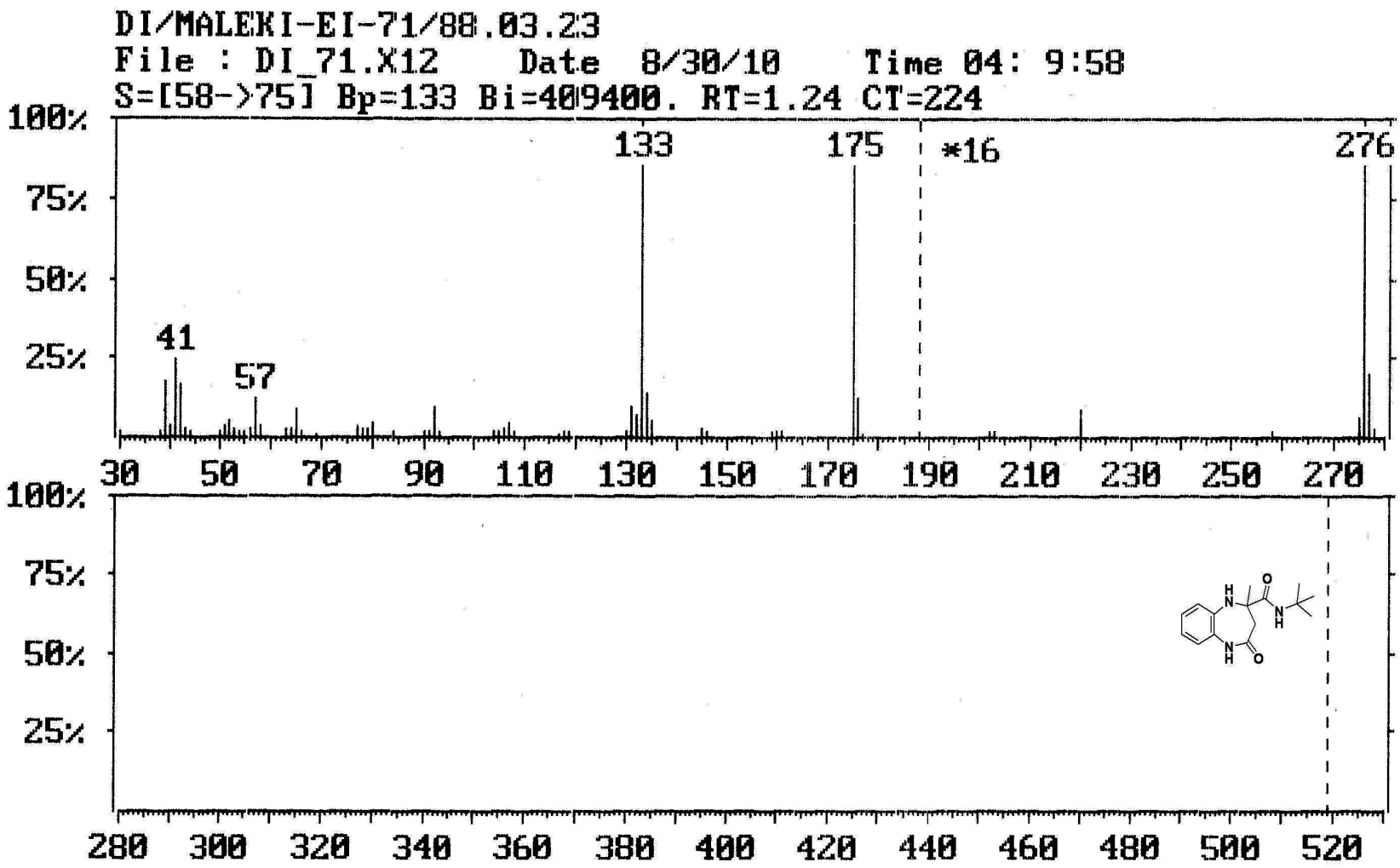
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 18.88 cm
F1P 215.162 ppm
F1 16237.80 Hz
F2P -13.639 ppm
F2 -1029.32 Hz
PPMCM 11.44006 ppm/cm
HZCM 863.35571 Hz/cm

^{13}C NMR of **4b**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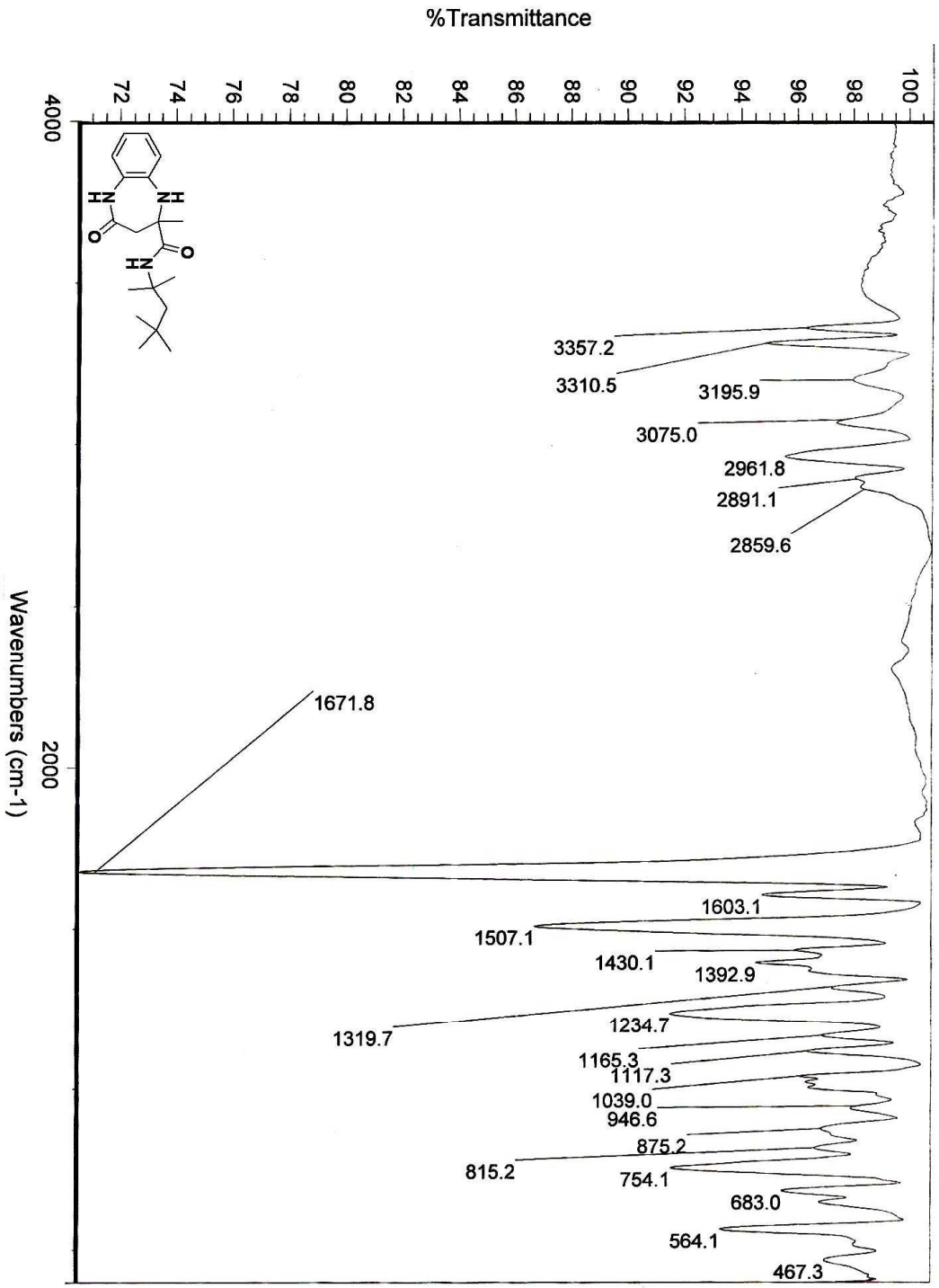
100%
75%
50%
25%
133
175
*16
276
41
57
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 Fact[188->519] *16
S List > S=[58->75] B=0 Pos=1 Tot=1

Mass of **4b**

IR of **4c**


%Transmittance
72
74
76
78
80
82
84
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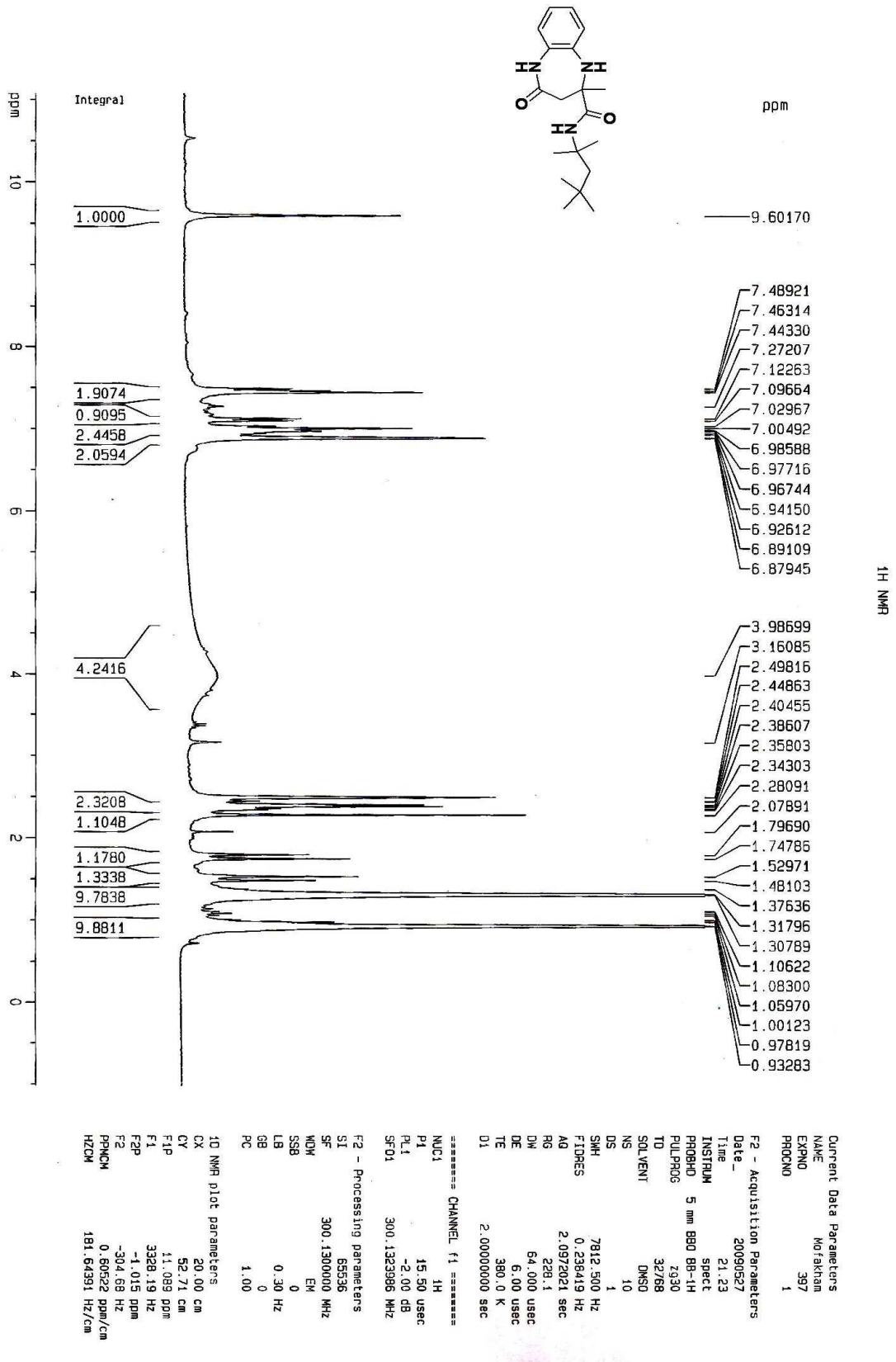
98
100
4000
2000
Wavenumbers (cm-1)
3357.2
3310.5
3195.9
3075.0
2961.8
2891.1
2859.6
1671.8
1603.1
1507.1
1430.1
1392.9
1319.7
1234.7
1165.3
1117.3
1039.0
946.6
875.2
815.2
754.1
683.0
564.1
467.3

^{1}H NMR of **4c**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1.1048
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1.3338
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9.8811
9.60170
7.48921
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7.44330
7.27207
7.12263
7.09664
7.02967
7.00492
6.98588
6.97716
6.96744
6.94150
6.92612
6.89109
6.87945
3.98699
3.16085
2.49816
2.44863
2.40455
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2.35803
2.34303
2.28091
2.07891
1.79690
1.74786
1.52971
1.48103
1.37636
1.31796
1.30789
1.10622
1.08300
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1H NMR
Current Data Parameters
NAME Mofakham
EXPNO 397
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090527
Time 21.23
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PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
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P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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CY 52.71 cm
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F2P -1.015 ppm
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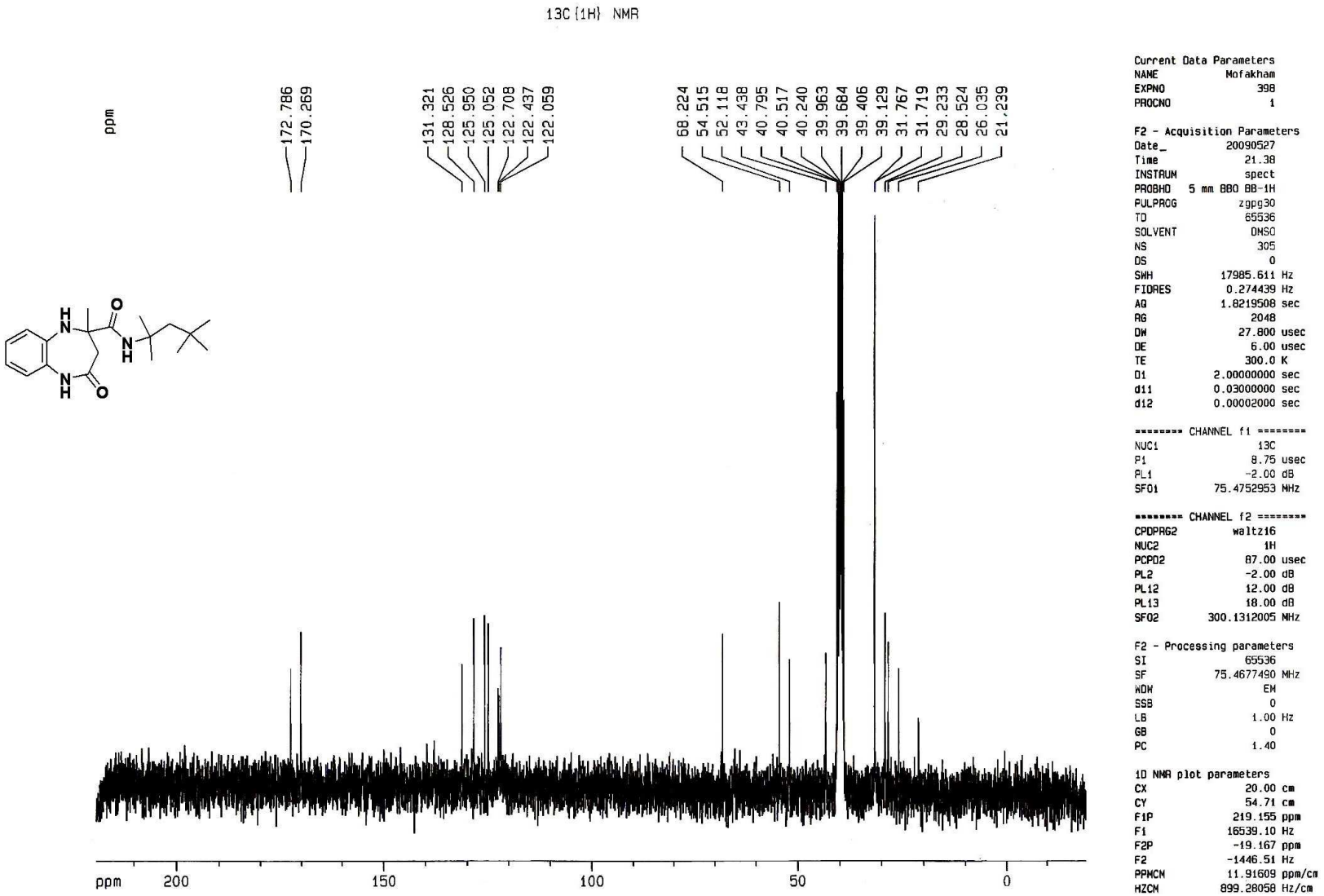

Current Data Parameters

NAME	Mofakham
EXPNO	398
PROCNO	1

F2 - Acquisition Parameters

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SOLVENT	DMSO
NS	305
DS	0
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2048
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

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

NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	87.00 usec
PL2	-2.00 dB
PL12	12.00 dB
PL13	18.00 dB
SFO2	300.1312005 MHz

F2 - Processing parameters

SI	65536
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

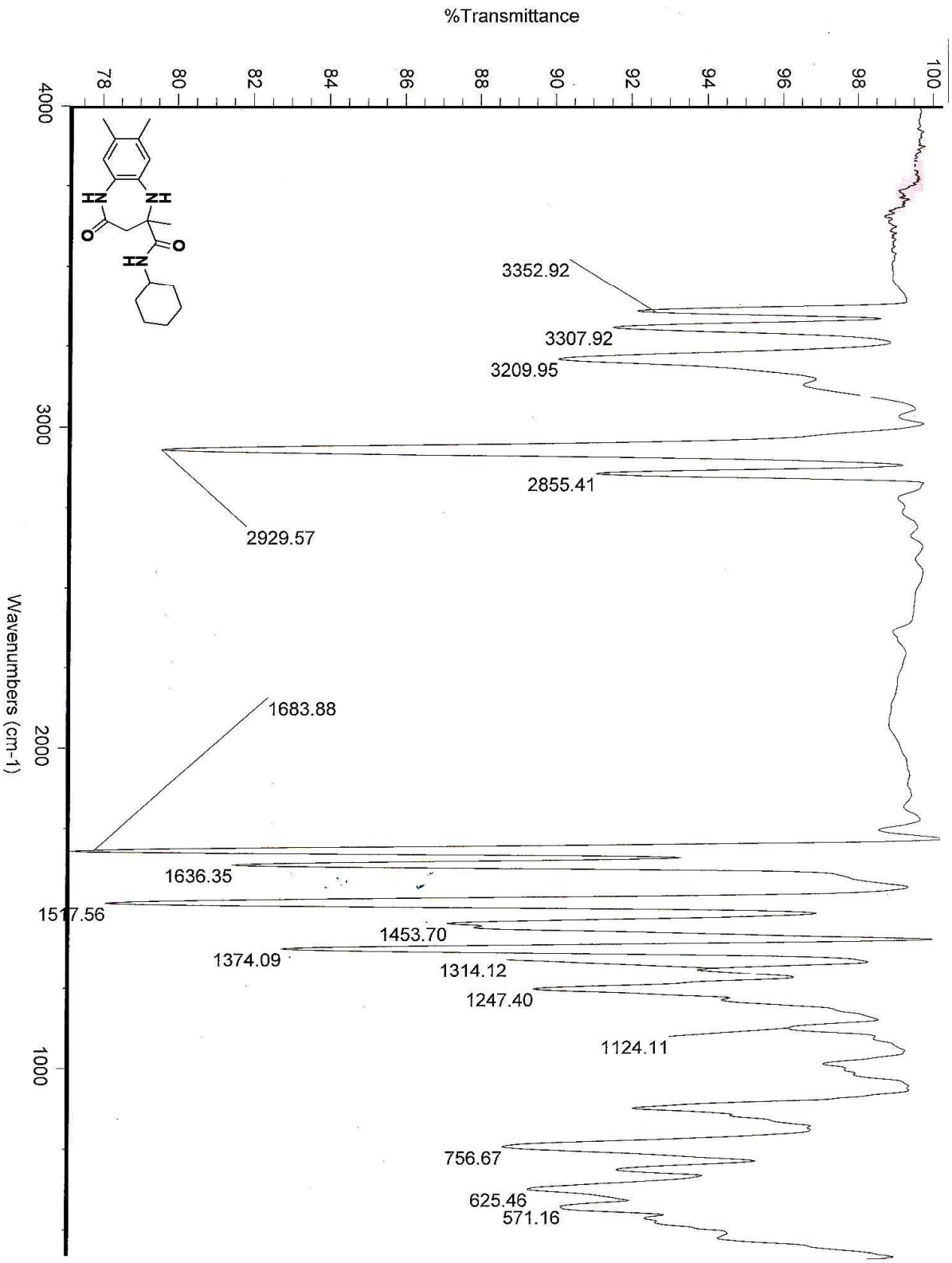
1D NMR plot parameters

CX	20.00 cm
CY	54.71 cm
F1P	219.155 ppm
F1	16539.10 Hz
F2P	-19.167 ppm
F2	-1446.51 Hz
PPMCM	11.91609 ppm/cm
HZCM	899.28058 Hz/cm

^{13}C NMR of **4c**

Mass of **4c**

IR of **4d**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92
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98
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4000
3000
2000
1000
Wavenumbers (cm-1)
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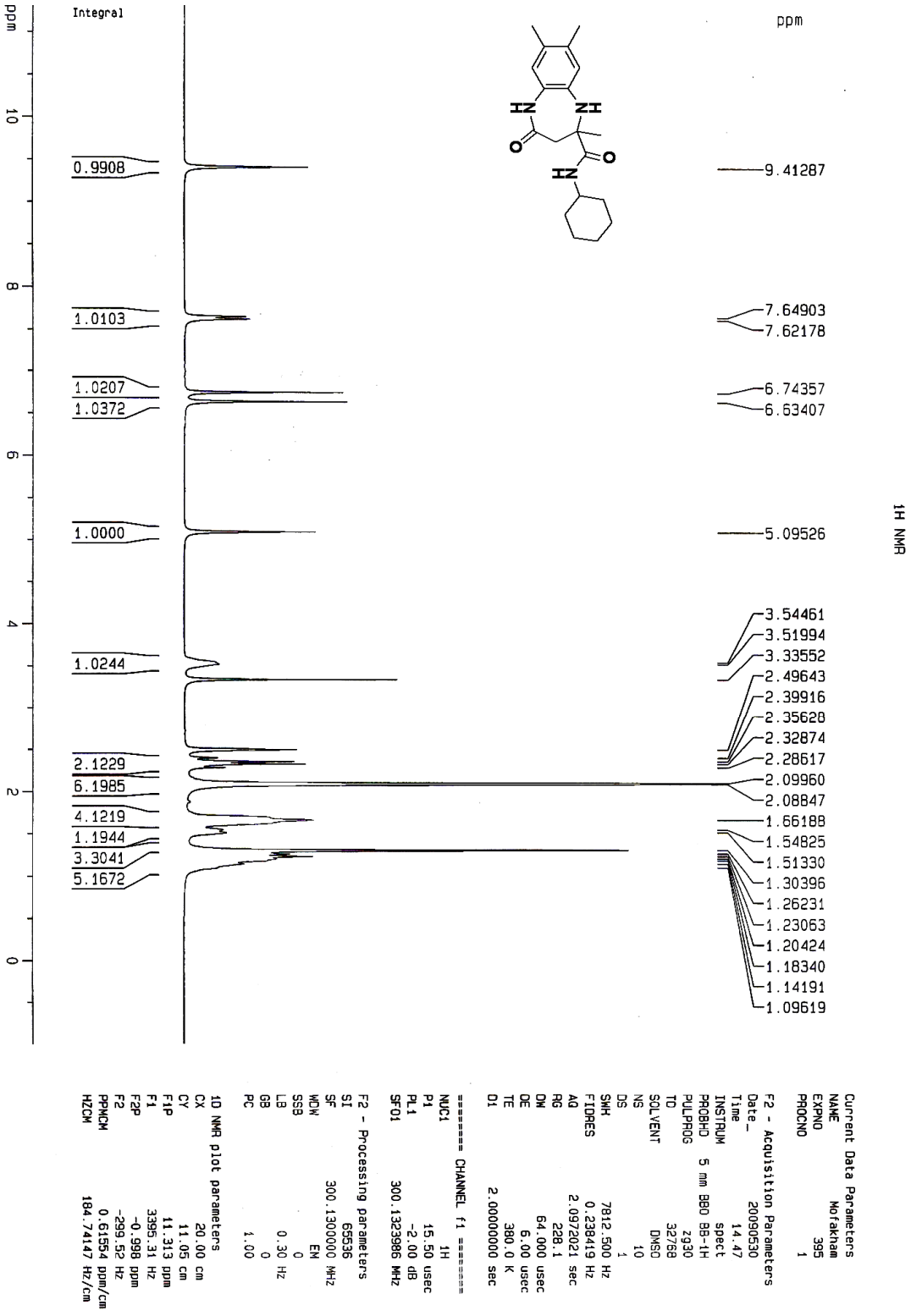
3307.92
3209.95
2855.41
2929.57
1683.88
1636.35
1517.56
1453.70
1374.09
1314.12
1247.40
1124.11
756.67
625.46
571.16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3.51994
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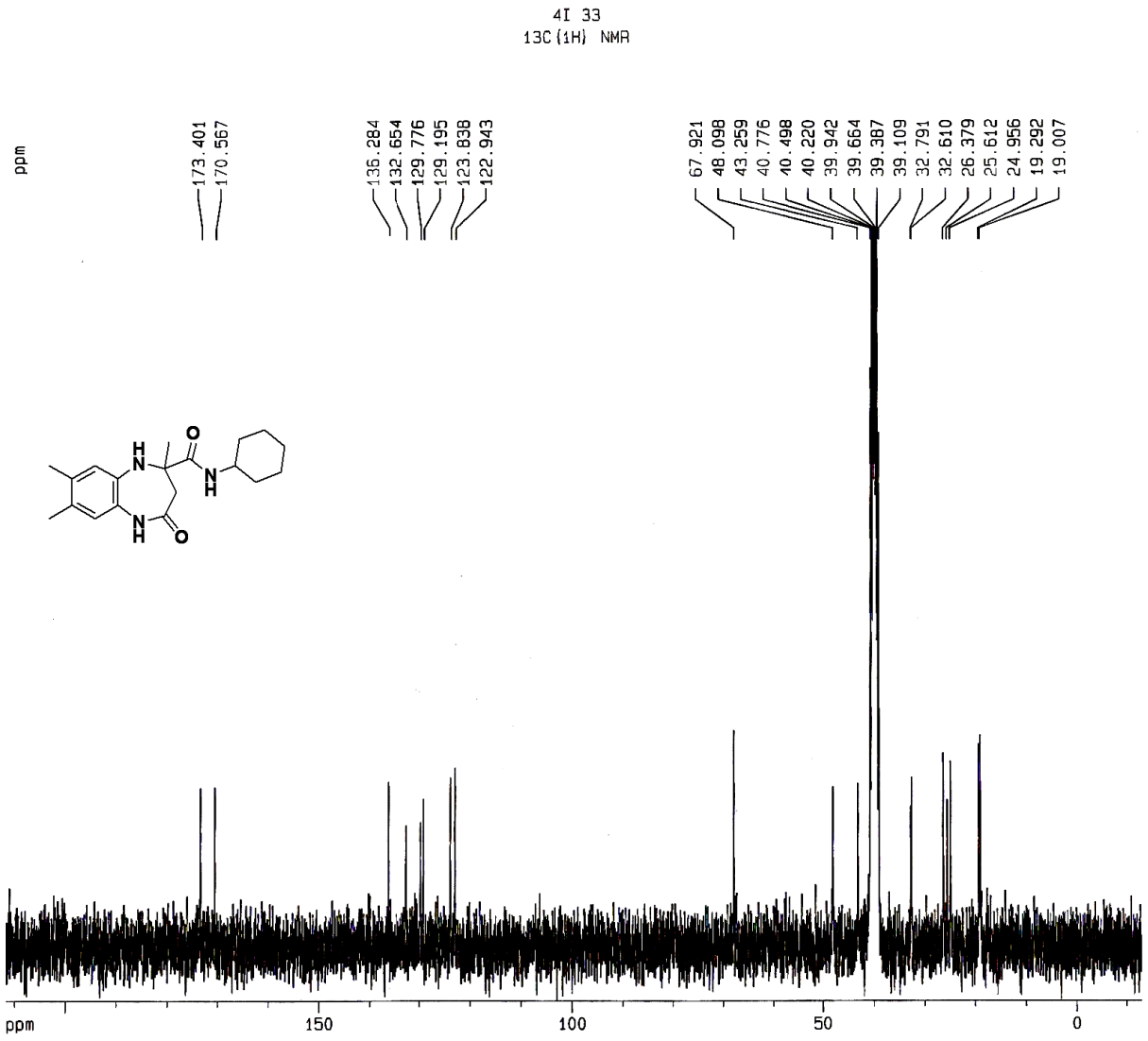
2.49643
2.39916
2.35628
2.32874
2.28617
2.09960
2.08847
1.66188
1.54825
1.51330
1.30396
1.26231
1.23063
1.20424
1.18340
1.14191
1.09619
0.9908
1.0103
1.0207
1.0372
1.0000
1.0244
2.1229
6.1985
4.1219
1.1944
3.3041
5.1672
Current Data Parameters
NAME Mofakham
EXPNO 395
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090530
Time 14.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 11.05 cm
F1P 11.313 ppm
F1 3395.31 Hz
F2P -0.998 ppm
F2 -299.52 Hz
PPMCM 0.61554 ppm/cm
HZCM 184.74147 Hz/cm

^{1}H NMR of **4d**

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Current Data Parameters
NAME          Seied hamze
EXPNO                 156
PROCNO                  1

F2 - Acquisition Parameters
Date_           20090513
Time               20.39
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   501
DS                     2
SWH            17985.611 Hz
FIDRES         0.274439 Hz
AQ             1.8219508 sec
RG                  2048
DW                27.800 use
DE                 6.00 use
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
d12            0.00002000 sec

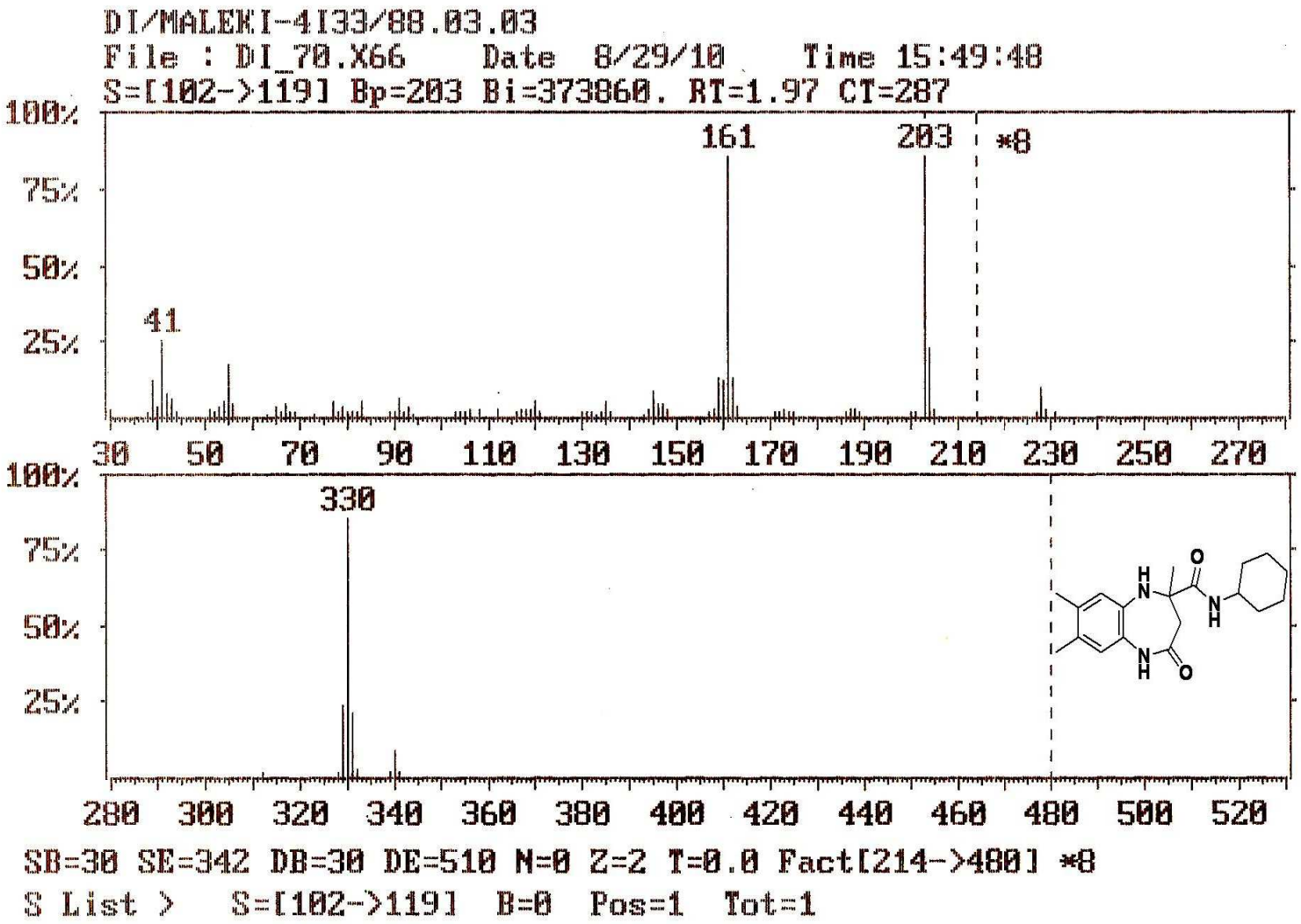
======== CHANNEL f1 ========
NUC1                 13C
P1                  8.75 usec
PL1                -2.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              87.00 usec
PL2                -2.00 dB
PL12               12.00 dB
PL13               18.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                  65536
SF            75.4677490 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00

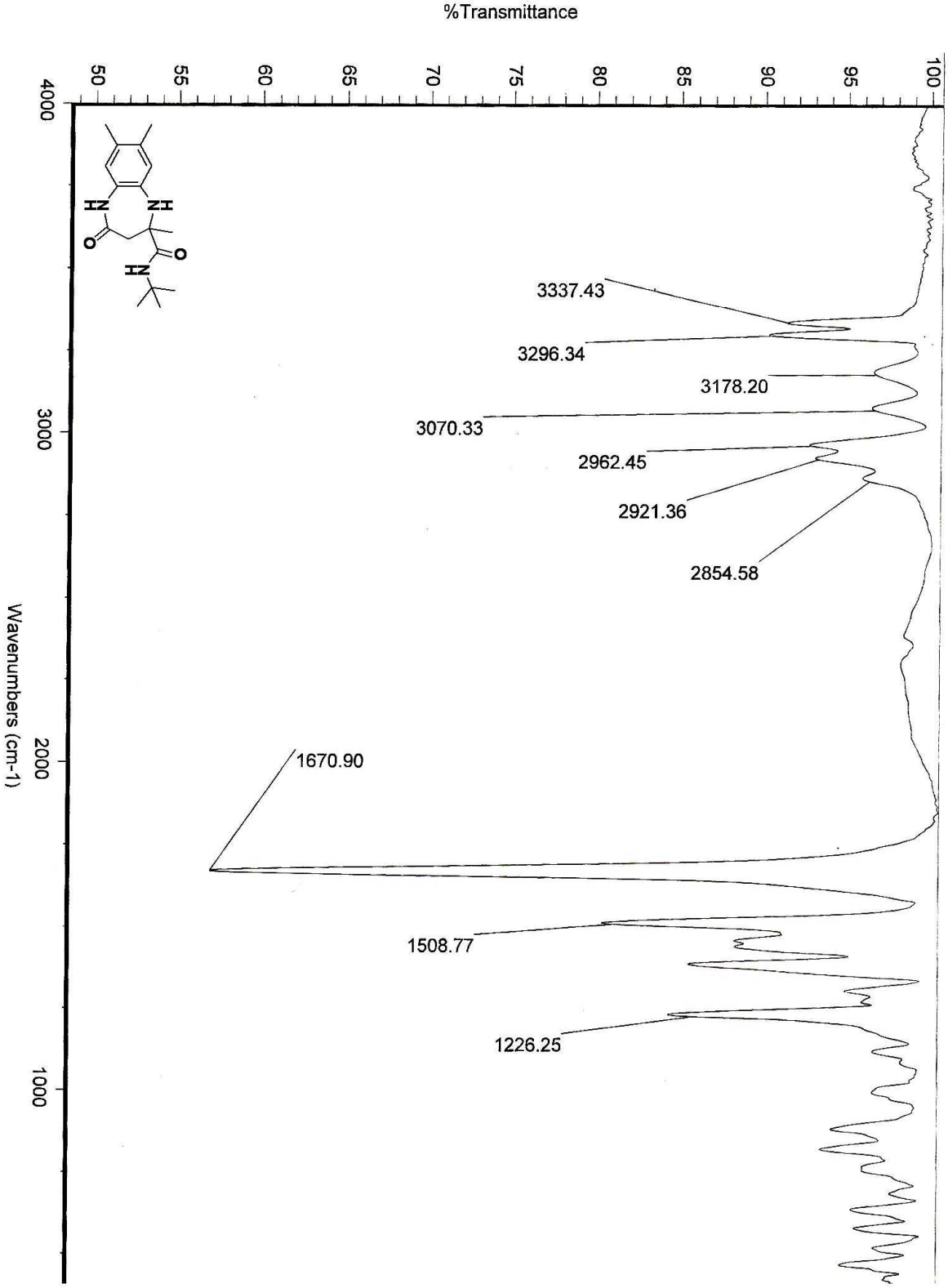
1D NMR plot parameters
CX                 20.00 cm
CY                 63.42 cm
F1P               211.784 ppm
F1              15982.85 Hz
F2P               -13.025 ppm
F2              -982.96 Hz
PPMCM           11.24044 ppm/cm
HZCM          848.29041 Hz/cm
```

^{13}C NMR of **4d**

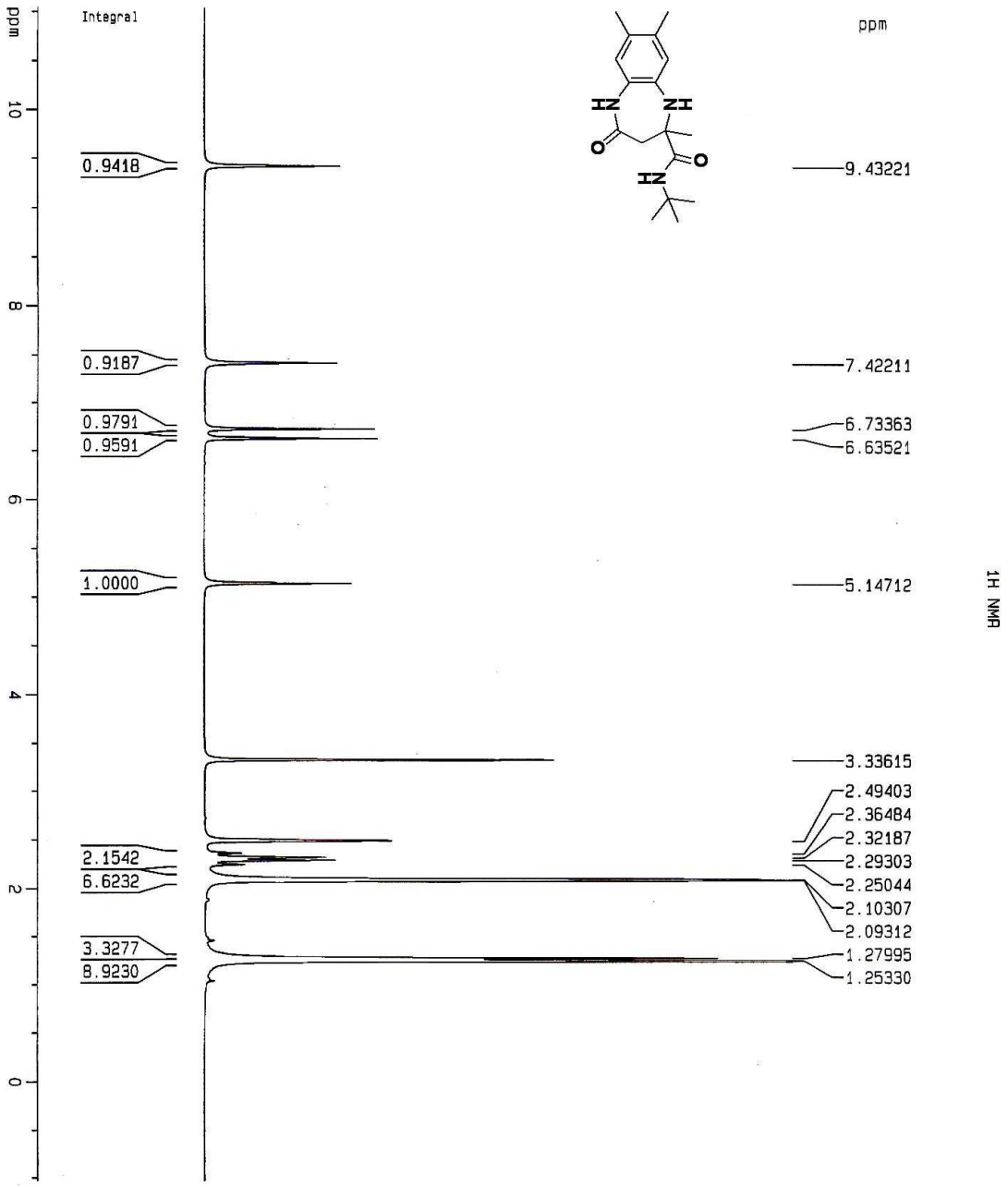

DI/MALEKI-4133/88.03.03
File : DI_70.X66 Date 8/29/10 Time 15:49:48
S=[102->119] Bp=203 Bi=373860. RT=1.97 CT=287
100%
75%
50%
25%
41
161
203
*8
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
330
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=342 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[214->480] *8
S List > S=[102->119] B=0 Pos=1 Tot=1

Mass of **4d**

IR of **4e**


%Transmittance
50
55
60
65
70
75
80
85
90
95
100
4000
3000
2000
1000
Wavenumbers (cm-1)
3337.43
3296.34
3178.20
3070.33
2962.45
2921.36
2854.58
1670.90
1508.77
1226.25

^{1}H NMR of **4e**



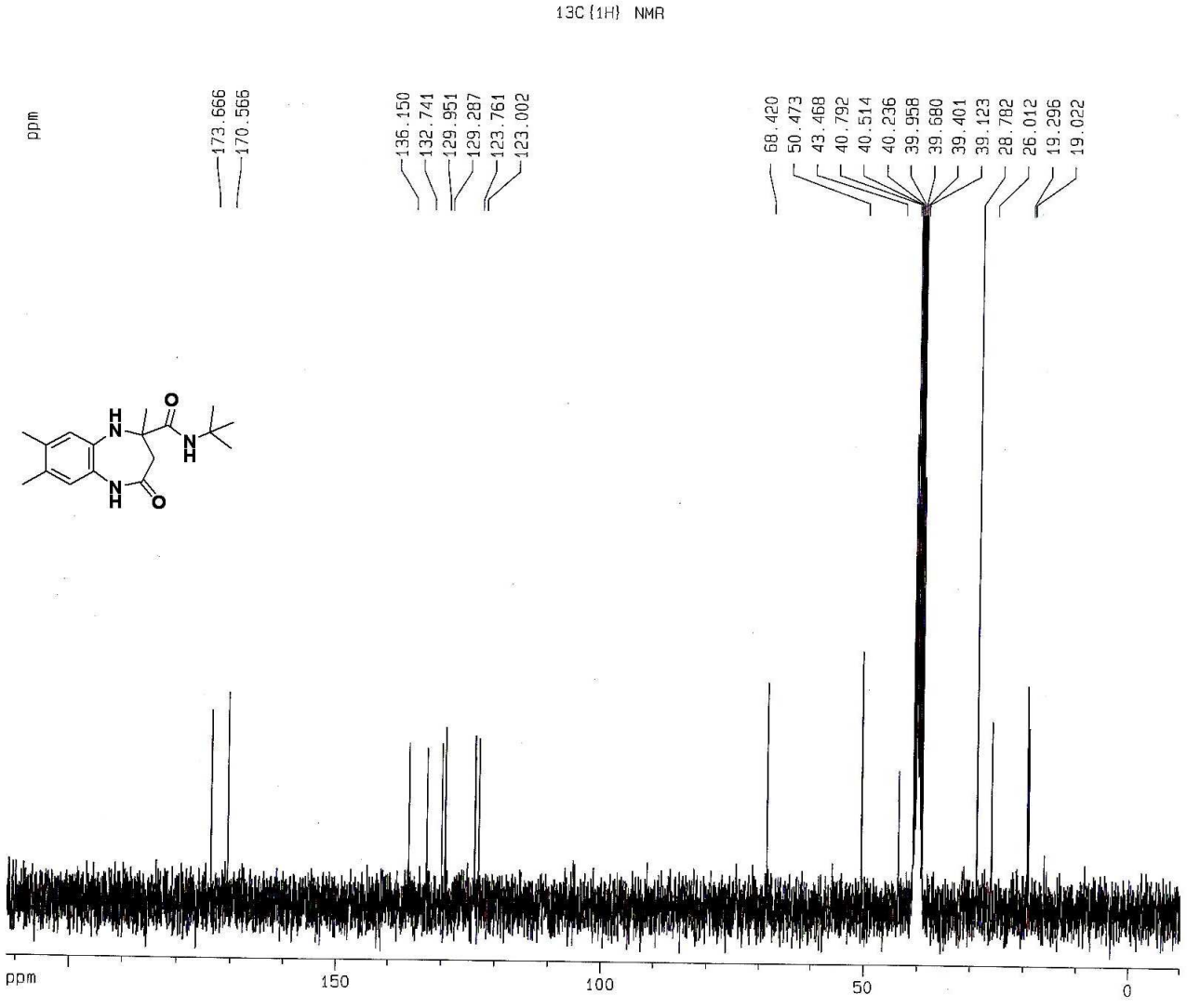
Current Data Parameters
NAME Mofakham
EXPNO 392
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090519
Time 22.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 28.54 cm
F1P 11.044 ppm
F1 3314.77 Hz
F2P -1.032 ppm
F2 -309.58 Hz
PPMCM 0.60360 ppm/cm
HZCM 181.21777 Hz/cm



Current Data Parameters

NAME	Mofakham
EXPNO	393
PROCNO	1

F2 - Acquisition Parameters

Date_	20090519
Time	23.03
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	201
DS	2
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2048
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

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

NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	87.00 usec
PL2	-2.00 dB
PL12	12.00 dB
PL13	18.00 dB
SFO2	300.1312005 MHz

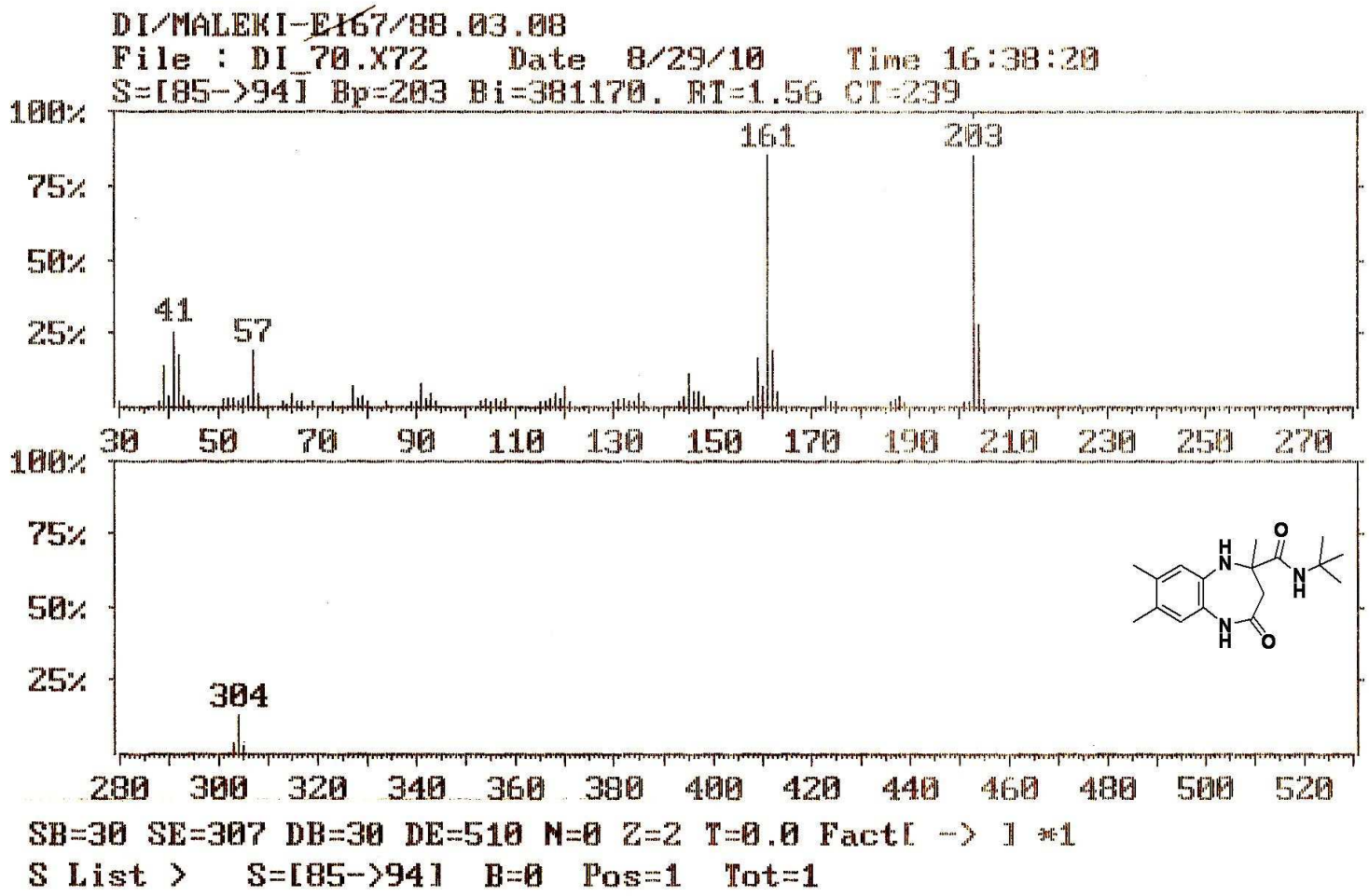
F2 - Processing parameters

SI	65536
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

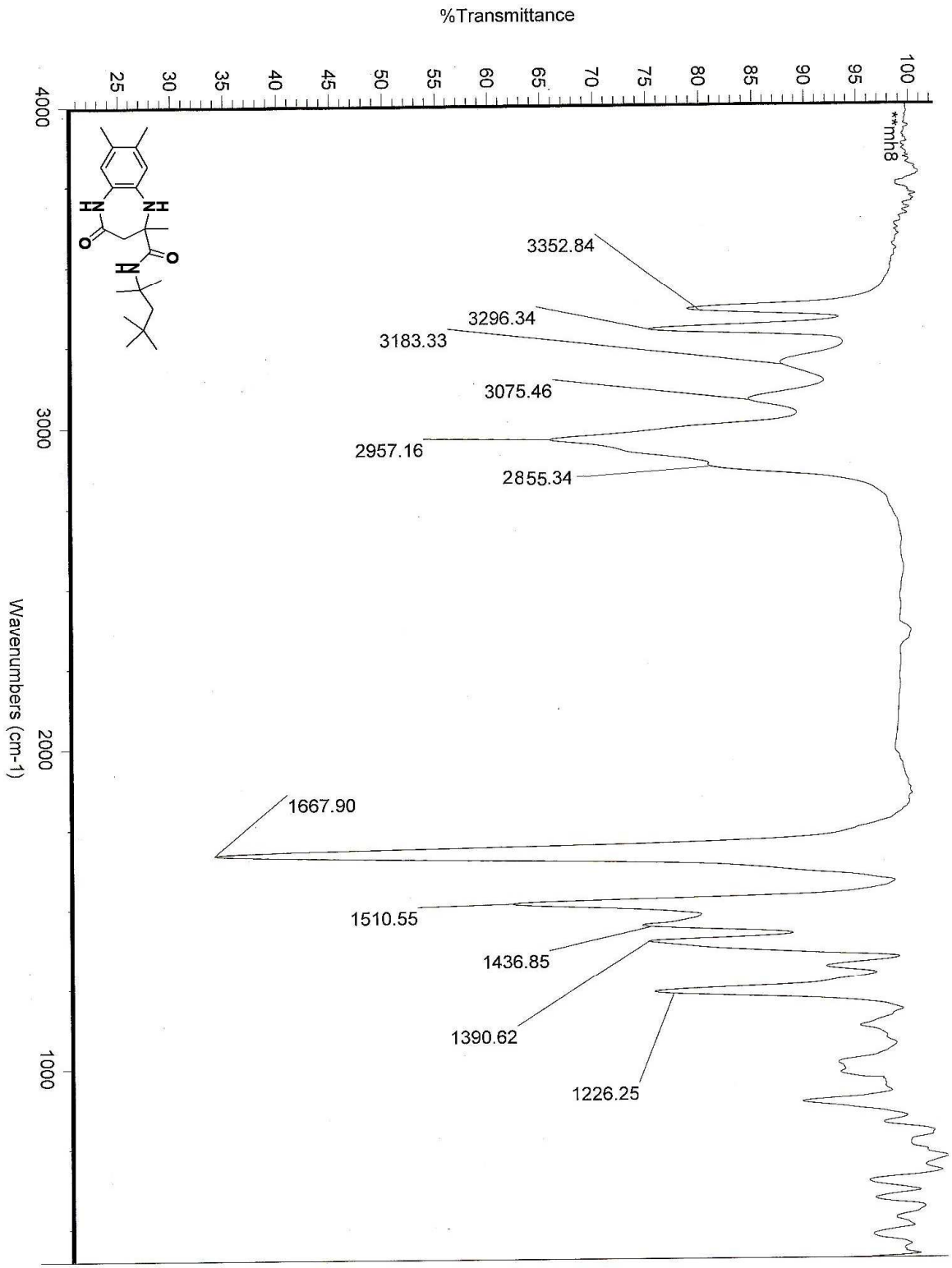
1D NMR plot parameters

CX	20.00 cm
CY	59.58 cm
F1P	211.603 ppm
F1	15969.20 Hz
F2P	-10.126 ppm
F2	-764.18 Hz
PPMCM	11.08644 ppm/cm
HZCM	836.66901 Hz/cm

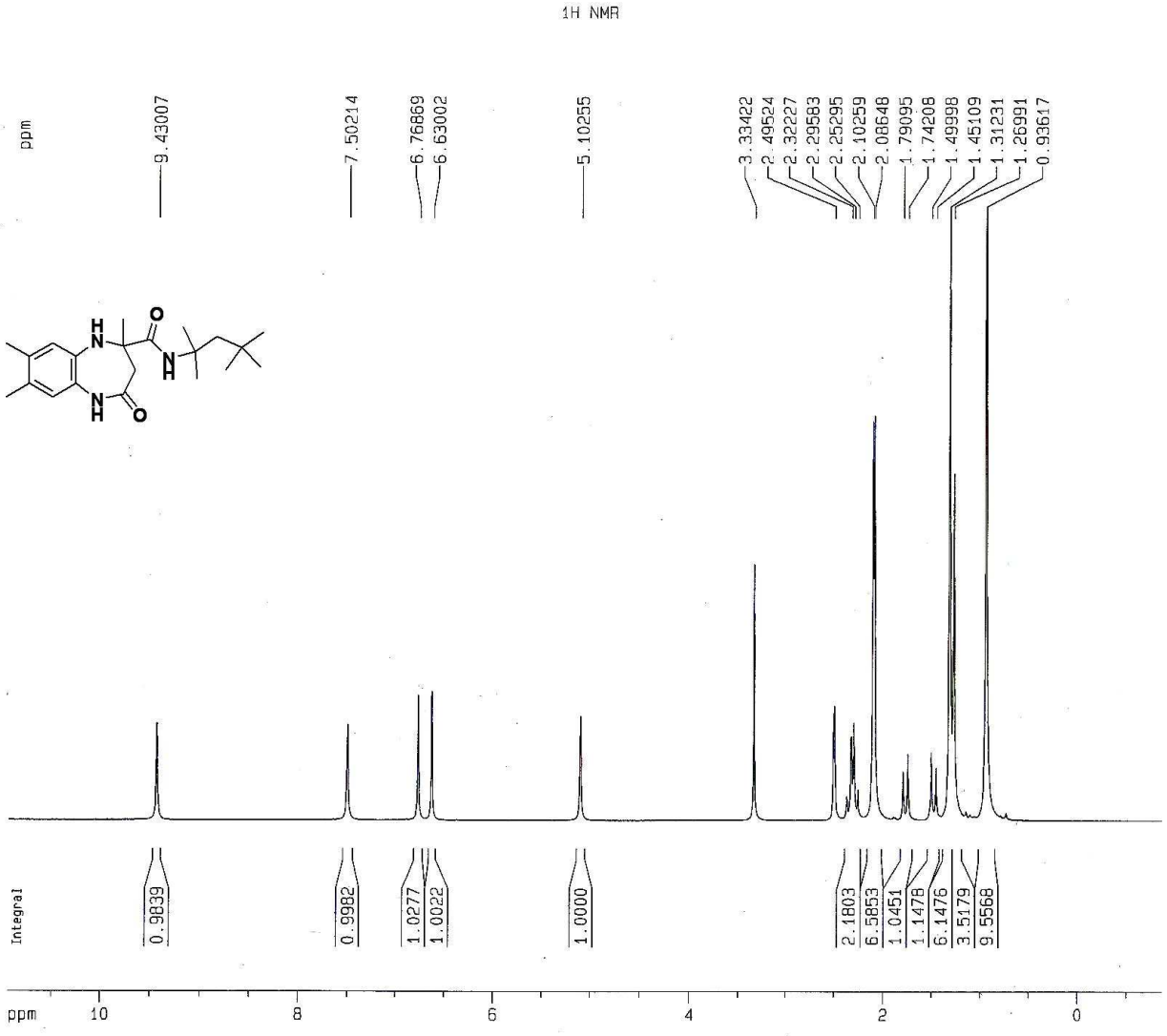
^{13}C NMR of **4e**


DI/MALEKI-E167/88.03.08
File : DI_70.X72 Date 8/29/10 Time 16:38:20
S=[85->94] Bp=203 Bi=381170. RT=1.56 CT=239
100%
75%
50%
25%
41
57
161
203
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
304
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=307 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[85->94] B=0 Pos=1 Tot=1

Mass of **4e**


%Transmittance
Wavenumbers (cm-1)
**mh8
3352.84
3296.34
3183.33
3075.46
2957.16
2855.34
1667.90
1510.55
1436.85
1390.62
1226.25

IR of **4f**



Current Data Parameters

NAME	Mofakham
EXPNO	384
PROCNO	1

F2 - Acquisition Parameters

Date_	20090519
Time	20.22
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	10
DS	1
SWH	7812.500 Hz
FIDRES	0.238419 Hz
AQ	2.0972021 sec
RG	228.1
DW	64.000 usec
DE	6.00 usec
TE	380.0 K
D1	2.00000000 sec

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

NUC1	1H
P1	15.50 usec
PL1	-2.00 dB
SFO1	300.1323986 MHz

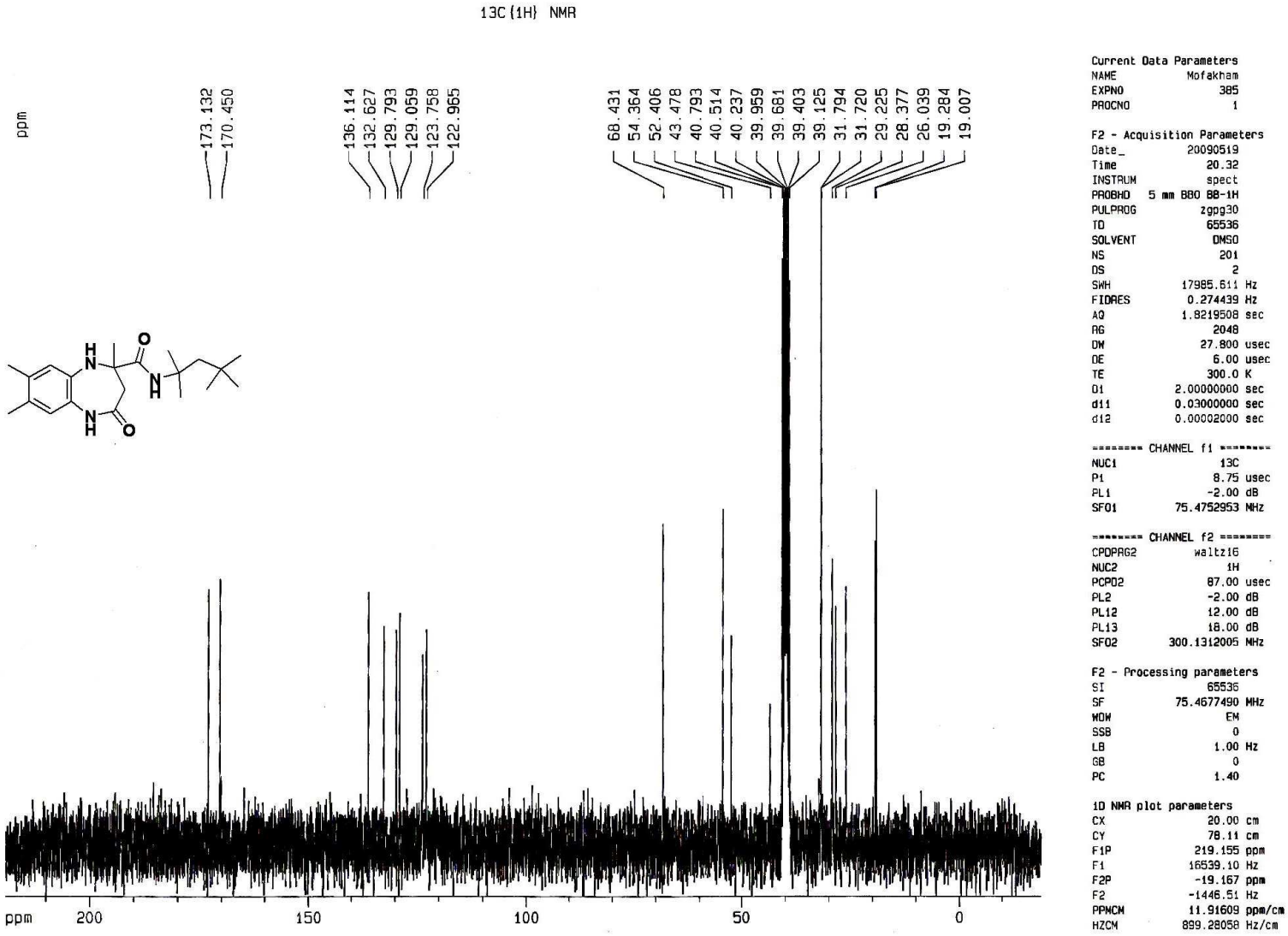
F2 - Processing parameters

SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	19.55 cm
F1P	10.944 ppm
F1	3284.57 Hz
F2P	-0.864 ppm
F2	-259.25 Hz
PPMCM	0.59038 ppm/c…
HZCM	177.19073 Hz/cm

^{1}H NMR of **4f**



Current Data Parameters

NAME	Mofakham
EXPNO	385
PROCNO	1

F2 - Acquisition Parameters

Date_	20090519
Time	20.32
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	201
DS	2
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2048
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

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

NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	87.00 usec
PL2	-2.00 dB
PL12	12.00 dB
PL13	18.00 dB
SFO2	300.1312005 MHz

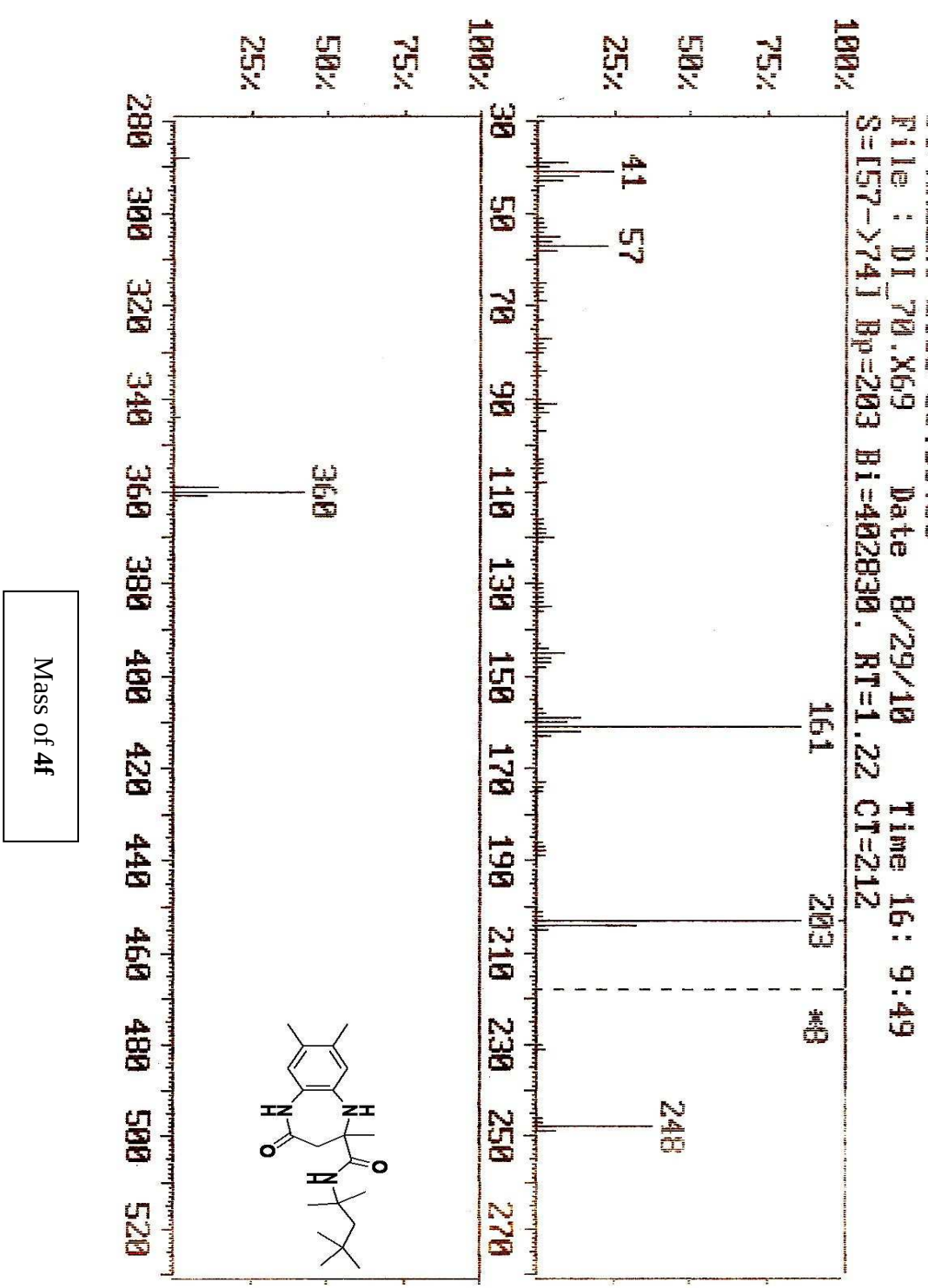
F2 - Processing parameters

SI	65536
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

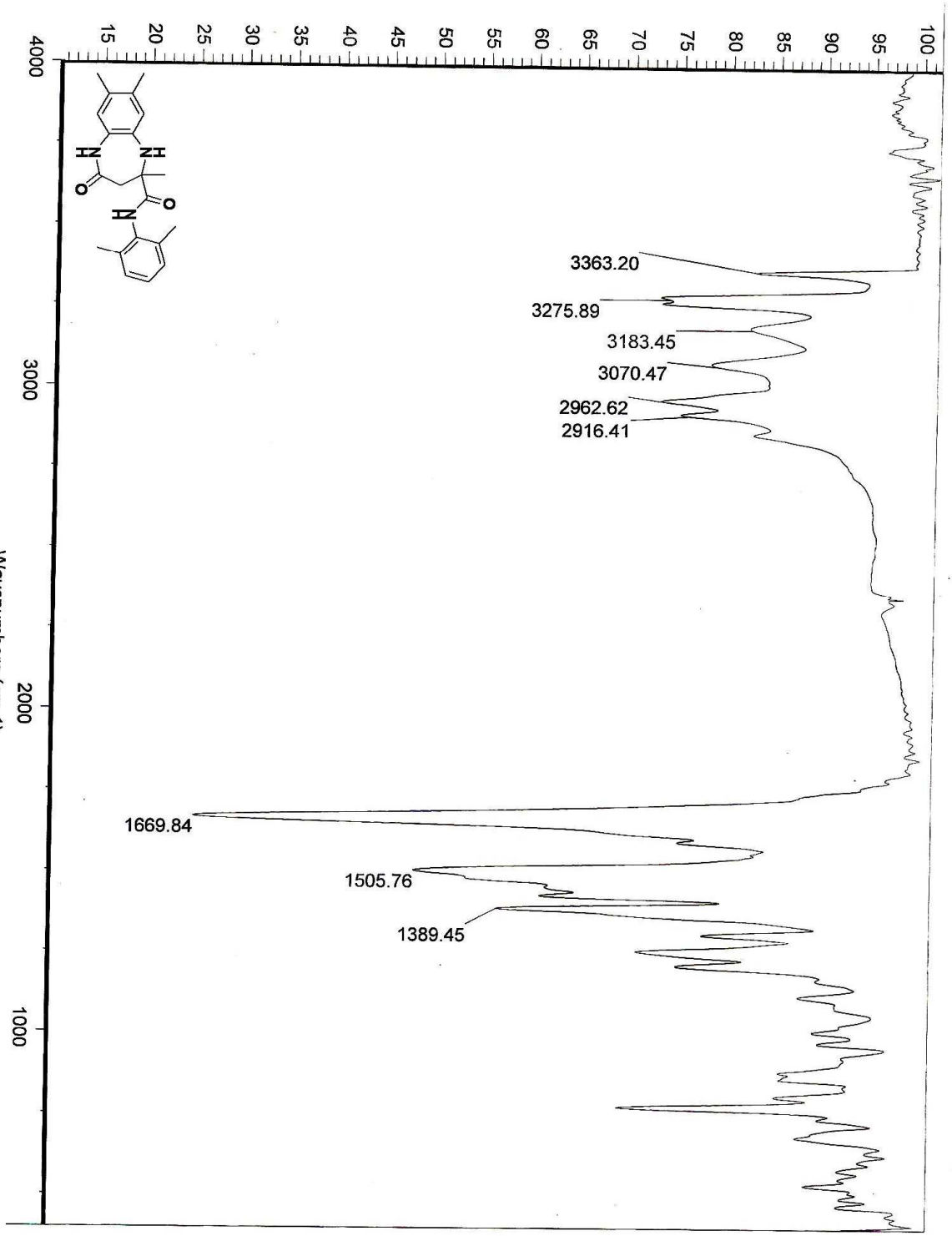
CX	20.00 cm
CY	78.11 cm
F1P	219.155 ppm
F1	16539.10 Hz
F2P	-19.167 ppm
F2	-1446.51 Hz
PPMCM	11.91609 ppm/cm
HZCM	899.28058 Hz/cm

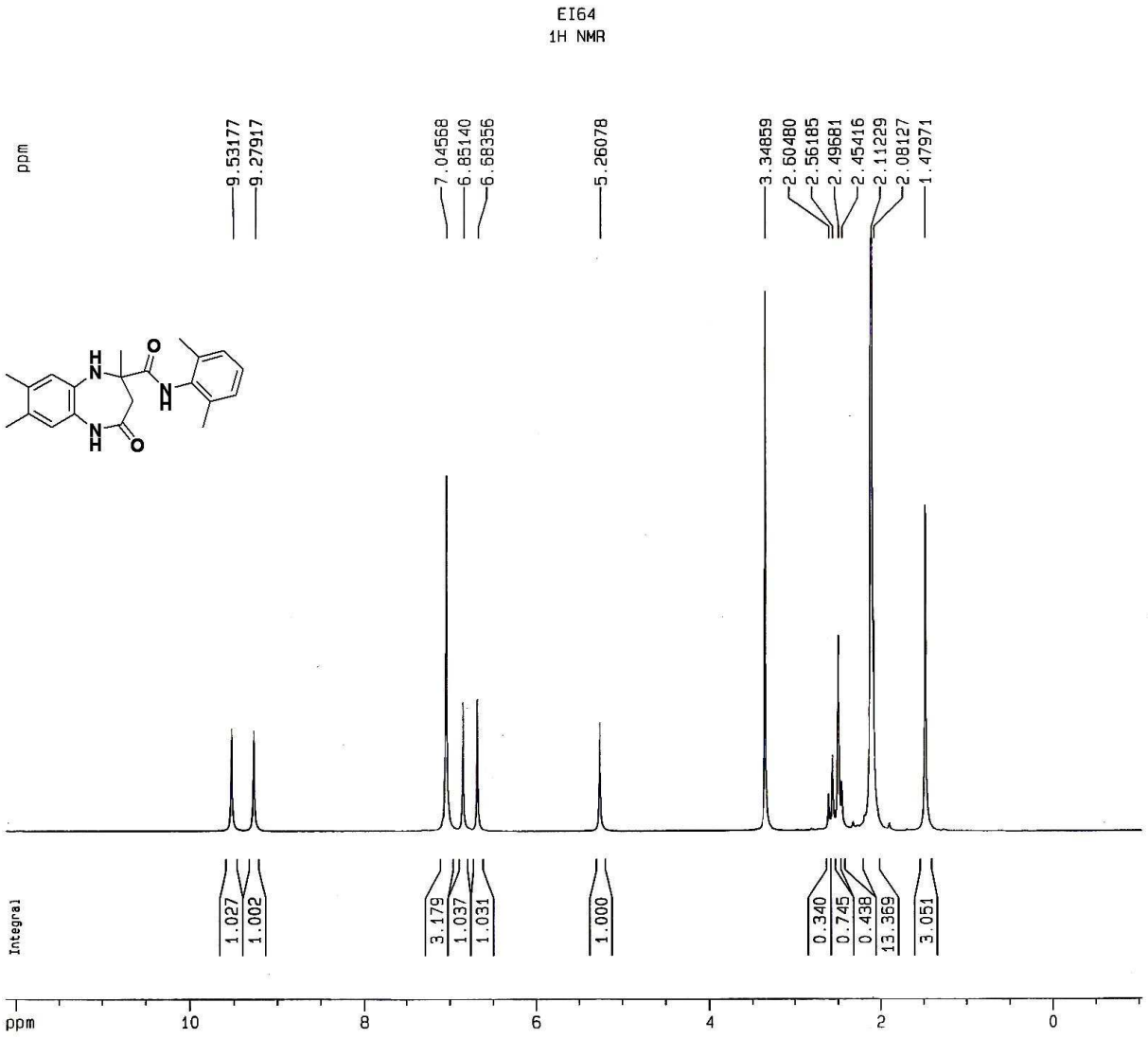
^{13}C NMR of **4f**


DI/MALEKI-EI63/88,03,03
File : DI_70.X69 Date 8/26/10 Time 16: 9:49
S=157-<741> Bp=203 Bi=402830, RT=1.22 CT=212
100%
75%
50%
25%
41
57
191
203
248
360
30 50 70 90 110 130 150 170 190 210 230 250 270
280 300 320 340 360 380 400 420 440 460 480 500 520
O
N
H
O
N
H
O
N
H

Mass of **4f**

IR of **4g**


3363.20
3275.89
3183.45
3070.47
2962.62
2916.41
1669.84
1505.76
1389.45
Wavenumbers (cm-1)
4000
3000
2000
1000



Current Data Parameters
NAME Mofakham
EXPNO 386
PROCNO 1

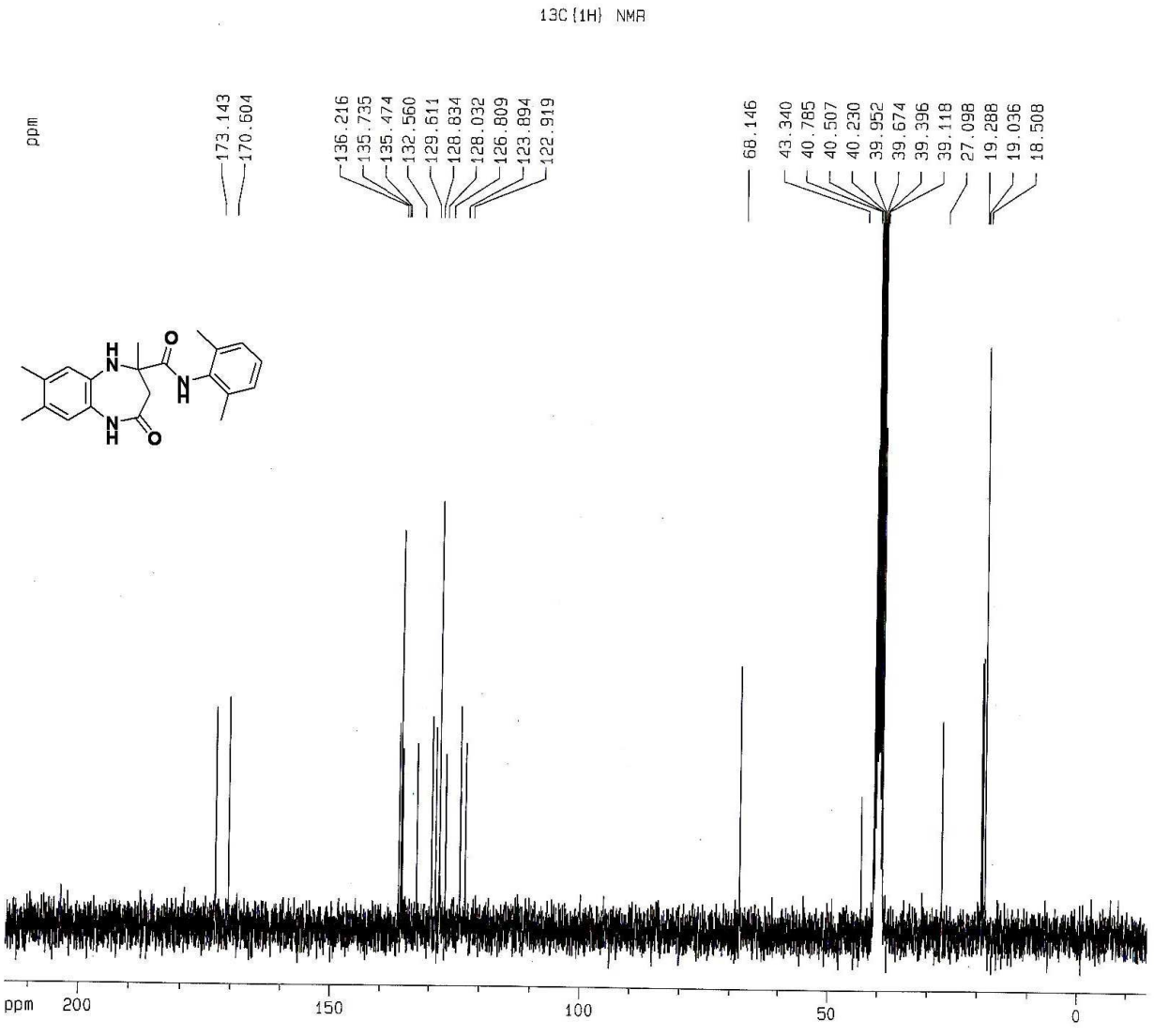
F2 - Acquisition Parameters
Date_ 20090519
Time 20.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 20.53 cm
F1P 12.118 ppm
F1 3636.94 Hz
F2P -1.032 ppm
F2 -309.58 Hz
PPMCM 0.65747 ppm/cm
HZCM 197.32603 Hz/cm

^{1}H NMR of **4g**



Current Data Parameters

NAME	Mofakham
EXPNO	387
PROCNO	1

F2 - Acquisition Parameters

Date_	20090519
Time	20.58
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	373
DS	2
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2048
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

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

NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	87.00 usec
PL2	-2.00 dB
PL12	12.00 dB
PL13	18.00 dB
SFO2	300.1312005 MHz

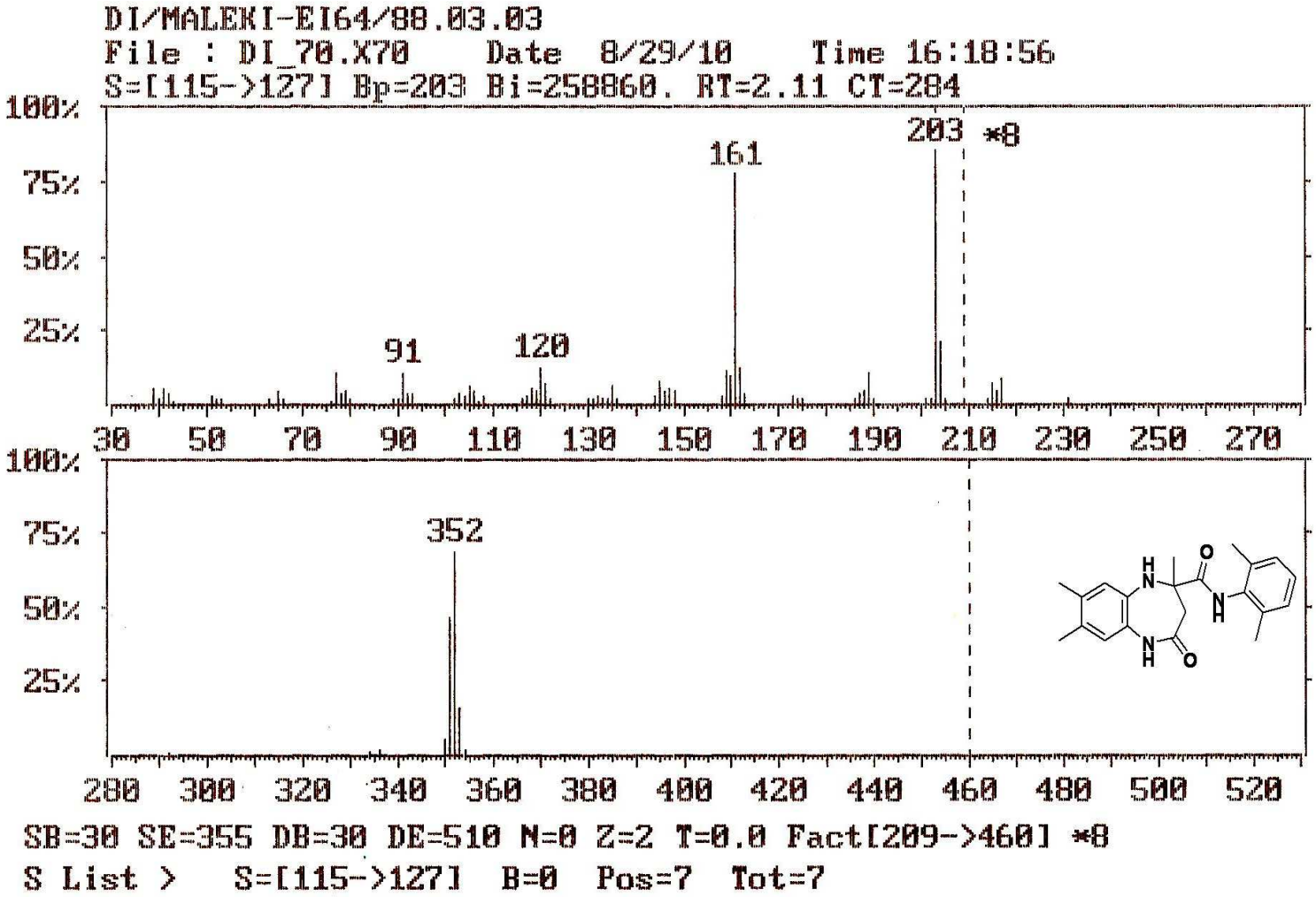
F2 - Processing parameters

SI	65536
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

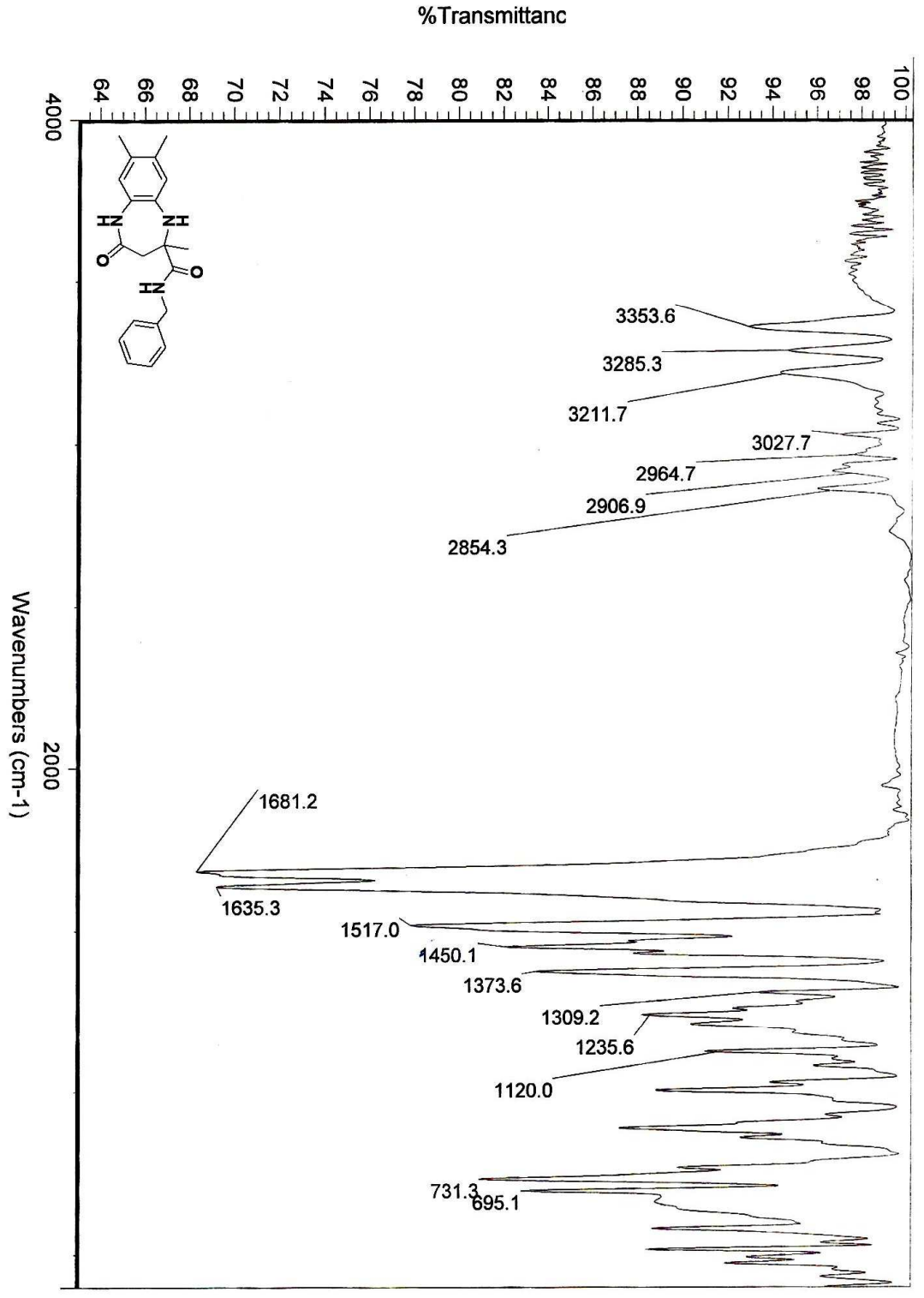
CX	20.00 cm
CY	61.30 cm
F1P	214.548 ppm
F1	16191.44 Hz
F2P	-14.253 ppm
F2	-1075.67 Hz
PPMCM	11.44006 ppm/cm
HZCM	863.35571 Hz/cm

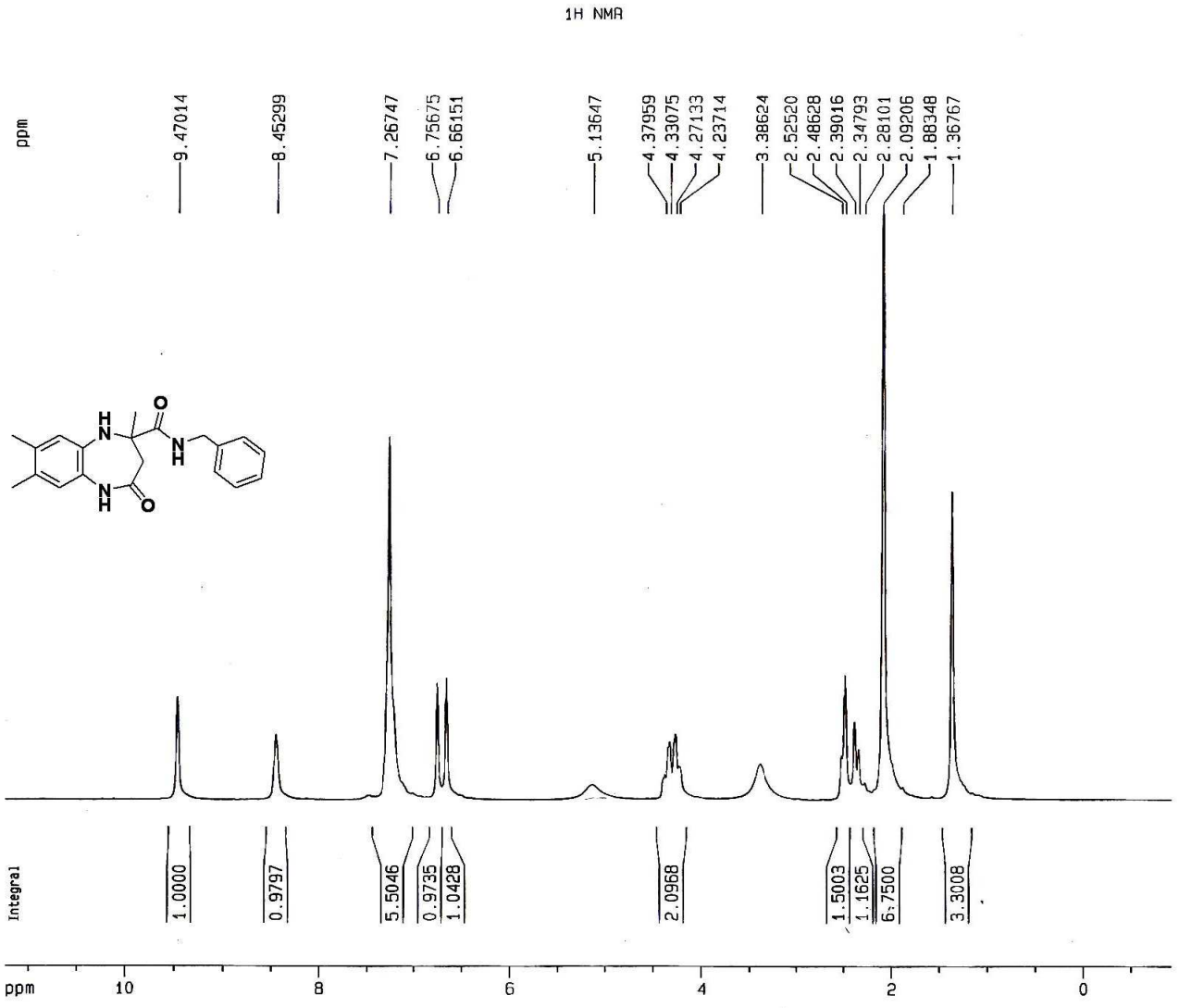
^{13}C NMR of **4g**


DI/MALEKI-EI64/88.03.03
File : DI_70.X70 Date 8/29/10 Time 16:18:56
S=[115->127] Bp=203 Bi=258860. RT=2.11 CT=284
100%
75%
50%
25%
91
120
161
203
*8
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
352
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=355 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[209->460] *8
S List > S=[115->127] B=0 Pos=7 Tot=7

Mass of **4g**

IR of **4h**


%Transmittanc
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
4000
2000
Wavenumbers (cm-1)
3353.6
3285.3
3211.7
3027.7
2964.7
2906.9
2854.3
1681.2
1635.3
1517.0
1450.1
1373.6
1309.2
1235.6
1120.0
731.3
695.1



Current Data Parameters

NAME	Seied hamze
EXPNO	165
PROCNO	1

F2 - Acquisition Parameters

Date_	20090523
Time	14.54
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	10
DS	1
SWH	7812.500 Hz
FIDRES	0.238419 Hz
AQ	2.0972021 se
RG	228.1
DW	64.000 usec
DE	6.00 usec
TE	360.0 K
D1	2.00000000 sec

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

NUC1	1H
P1	15.50 usec
PL1	-2.00 dB
SFO1	300.1323986 MHz

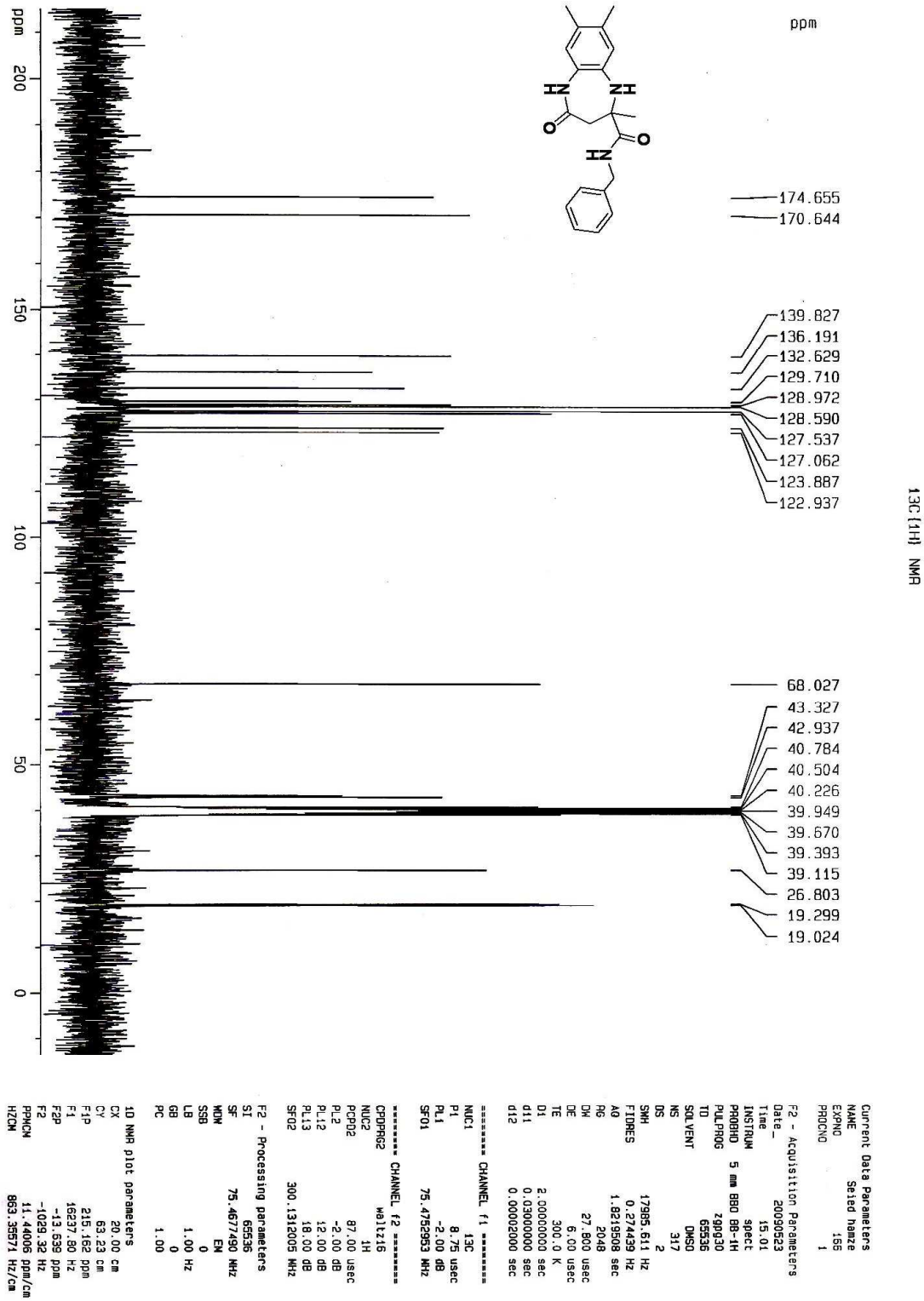
F2 - Processing parameters

SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

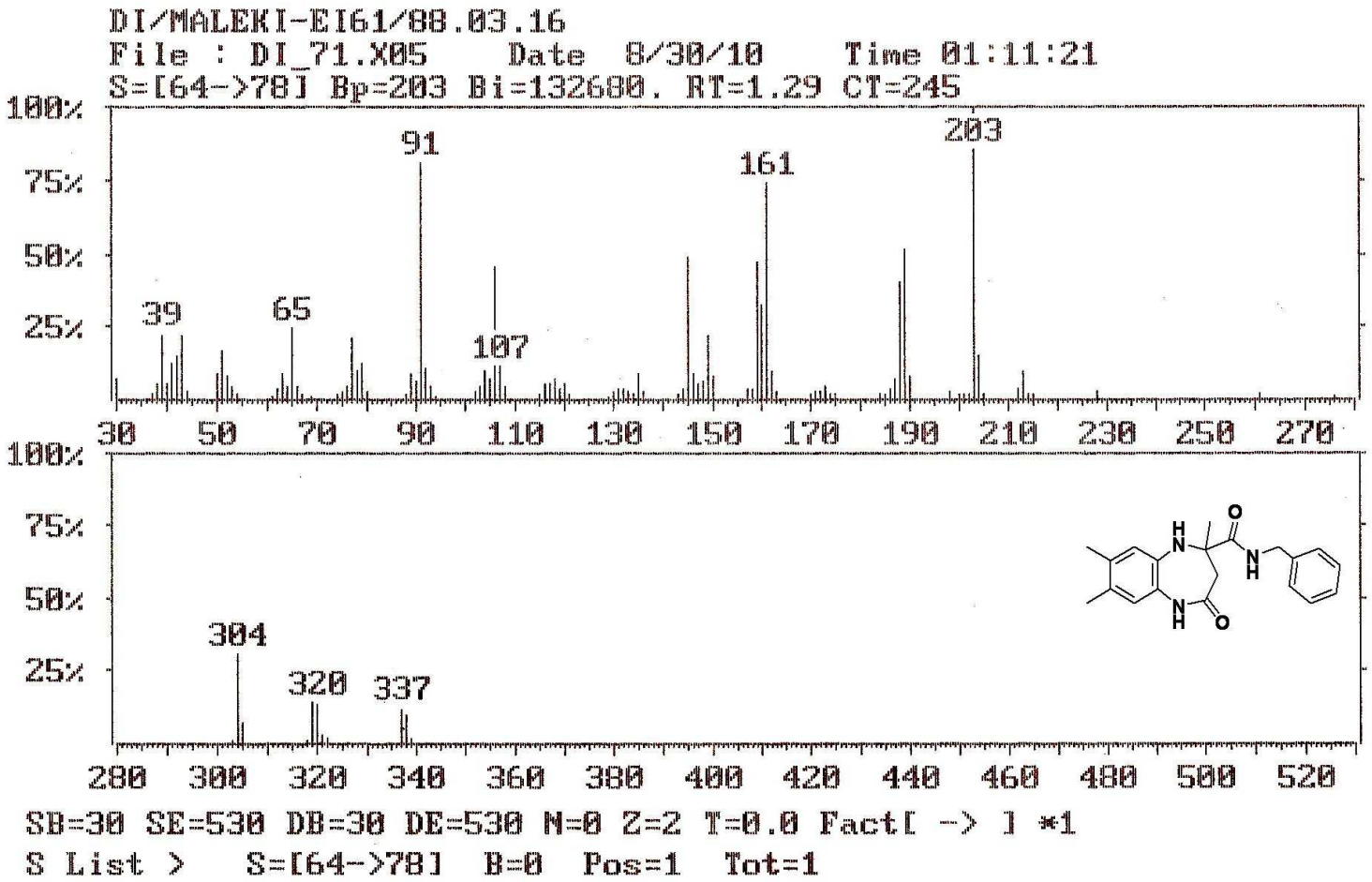
1D NMR plot parameters

CX	20.00 cm
CY	11.82 cm
F1P	11.246 ppm
F1	3375.18 Hz
F2P	-0.931 ppm
F2	-279.38 Hz
PPMCM	0.60883 ppm/cm
HZCM	182.72794 Hz/cm

^{1}H NMR of **4h**

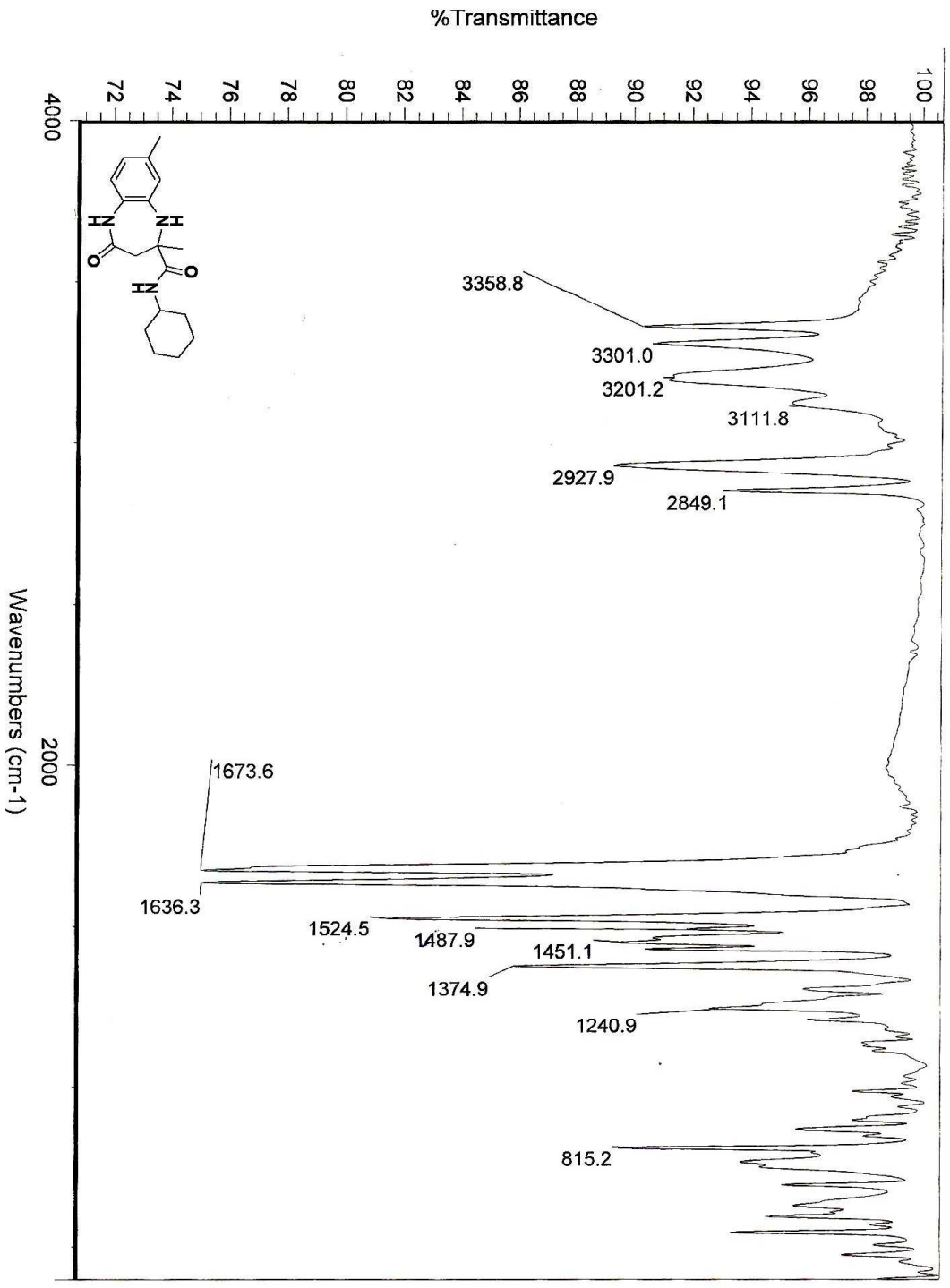

ppm
200
150
100
50
0
174.655
170.644
139.827
136.191
132.629
129.710
128.972
128.590
127.537
127.062
123.887
122.937
68.027
43.327
42.937
40.784
40.504
40.226
39.949
39.670
39.393
39.115
26.803
19.299
19.024
13C {1H} NMR

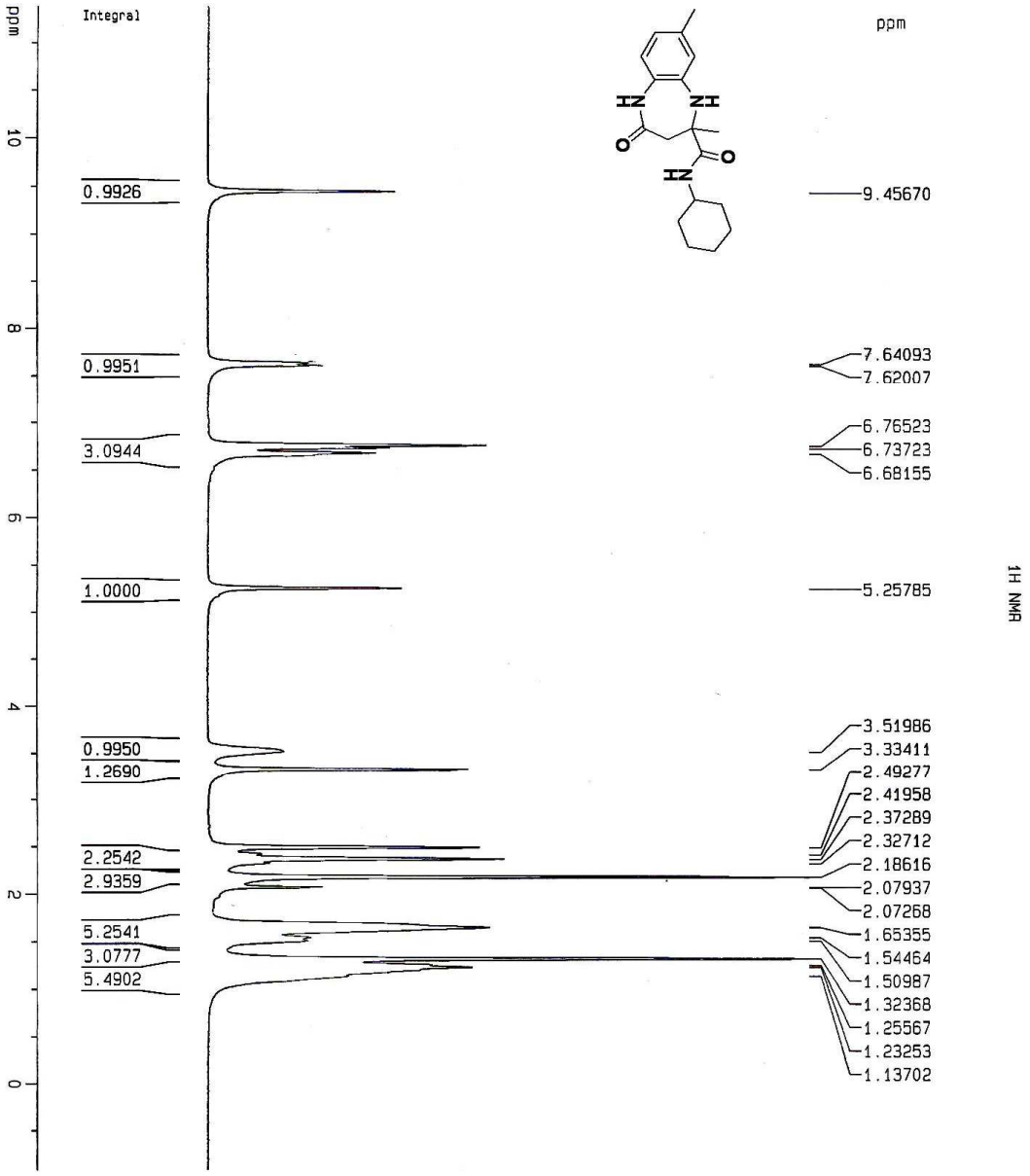
^{13}C NMR of **4h**


DI/MALEKI-EI61/88.03.16
File : DI_71.X05 Date 8/30/10 Time 01:11:21
S=[64->78] Bp=203 Bi=132680. RT=1.29 CT=245
100%
75%
50%
25%
91
161
203
39
65
107
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
304
320
337
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=530 DB=30 DE=530 M=0 Z=2 T=0.0 Fact[->] *1
S List > S=[64->78] B=0 Pos=1 Tot=1

Mass of **4h**

IR of **4i**


%Transmittance
72
74
76
78
80
82
84
86
88
90
92
94
96
98
100
4000
2000
Wavenumbers (cm-1)
3358.8
3301.0
3201.2
3111.8
2927.9
2849.1
1673.6
1636.3
1524.5
1487.9
1451.1
1374.9
1240.9
815.2




```
Current Data Parameters
NAME                  Seied hamze
EXPNO                         169
PROCNO                          1

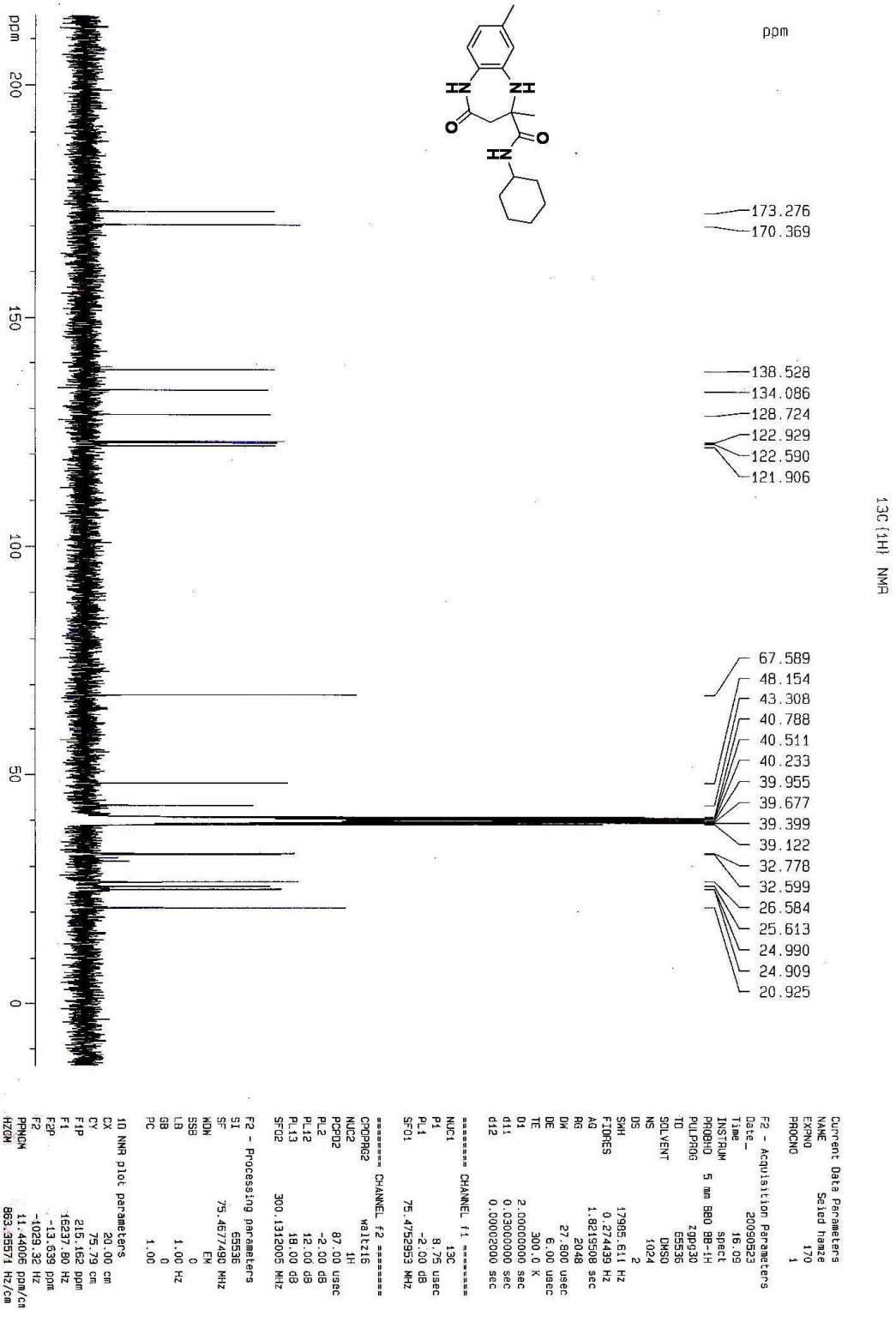
F2 - Acquisition Parameters
Date_              20090523
Time                   16.06
INSTRUM                spect
PROBHD  5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                        10
DS                         1
SWH                7812.500 Hz
FIDRES             0.238419 Hz
AQ                 2.0972021 sec
RG                     228.1
DW                64.000 usec
DE                 6.00 usec
TE                 380.0 K
D1                 2.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     15.50 usec
PL1                    -2.00 dB
SFO1          300.1323986 MHz

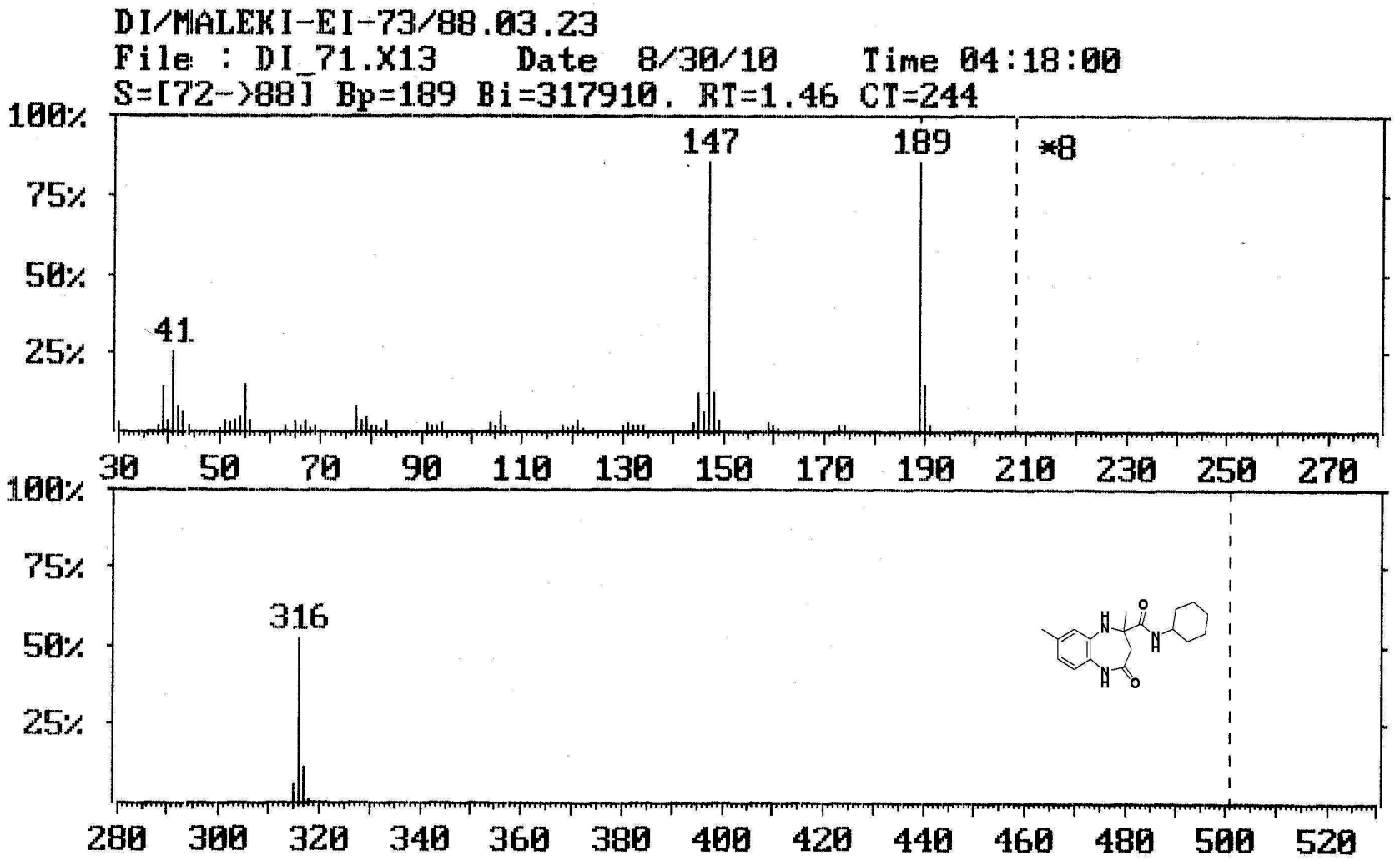
F2 - Processing parameters
SI                        65536
SF            300.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
CY                     10.80 cm
F1P                   11.380 ppm
F1                   3415.45 Hz
F2P                   -0.931 ppm
F2                   -279.38 Hz
PPMCM                0.61554 ppm/cm
HZCM                 184.74147 Hz/cm
```


^{1}H NMR of **4i**

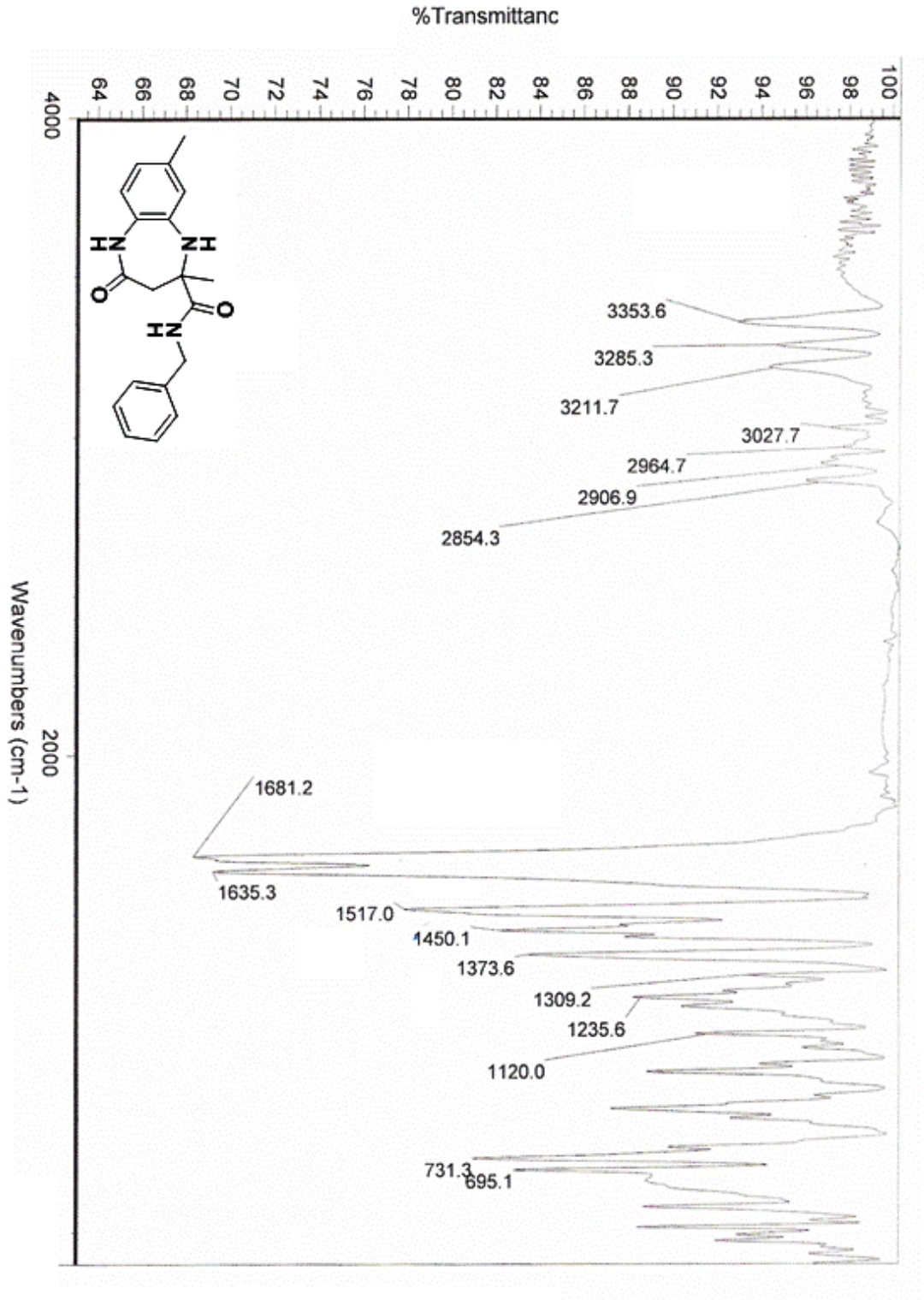

13C{1H} NMA
ppm
173.276
170.369
138.528
134.086
128.724
122.929
122.590
121.906
67.589
48.154
43.308
40.788
40.511
40.233
39.955
39.677
39.399
39.122
32.778
32.599
26.584
25.613
24.990
24.909
20.925
ppm 200 150 100 50 0
Current Data Parameters
NAME Saied hamze
EXPNO 170
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090523
Time 16.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 75.79 cm
F1P 215.162 ppm
F1 16237.80 Hz
F2P -13.639 ppm
F2 -1029.32 Hz
PPMCM 11.44006 ppm/cm
HZCM 863.35571 Hz/cm

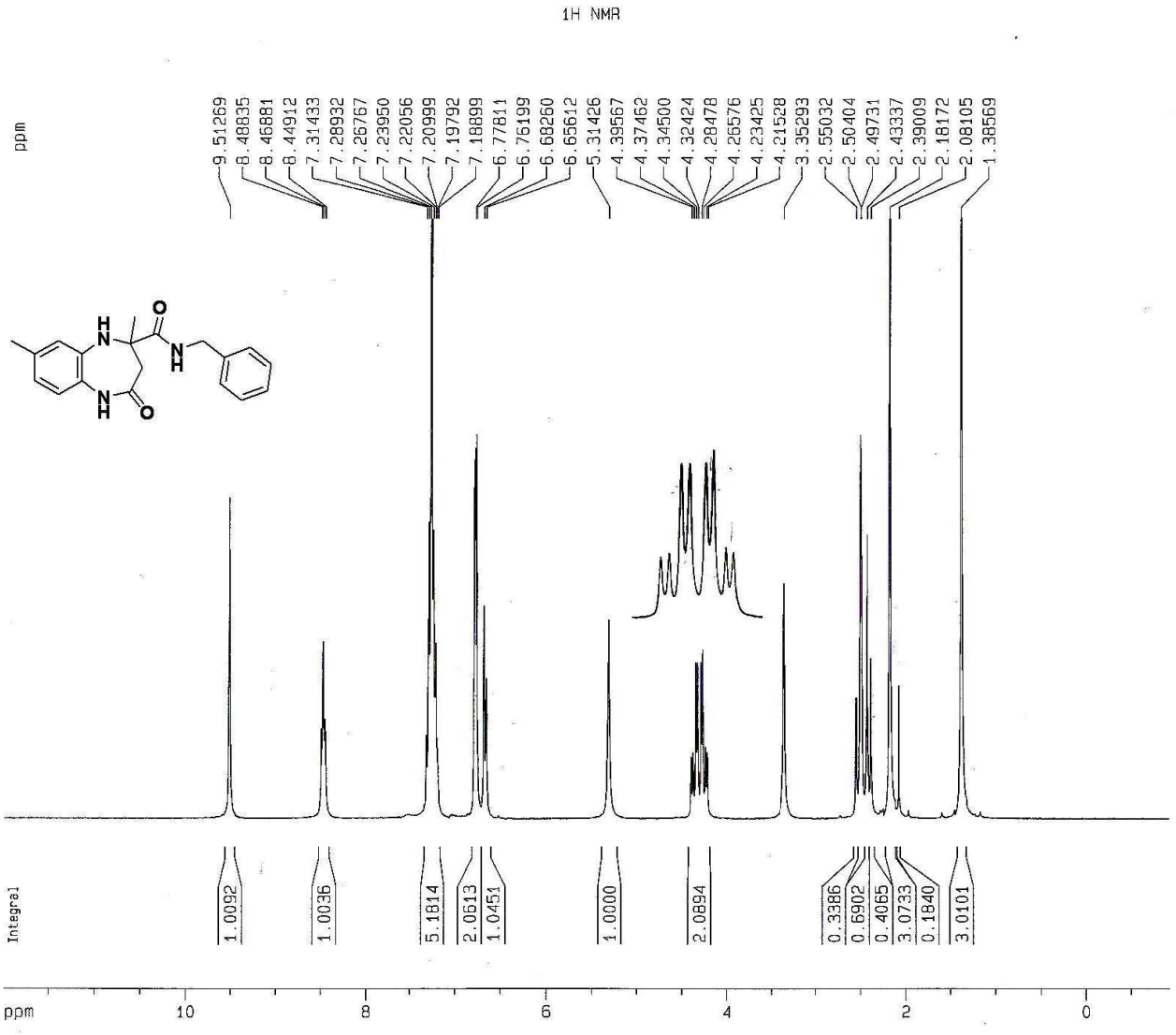
^{13}C NMR of **4i**


DI/MALEKI-EI-73/88.03.23
File : DI_71.X13 Date 8/30/10 Time 04:18:00
S=[72->88] Bp=189 Bi=317910. RT=1.46 CT=244
100%
75%
50%
25%
41
147
189
*8
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
316
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=318 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[208->501] *8
S List > S=[72->88] B=0 Pos=1 Tot=1

Mass of **4i**

IR of **4j**


%Transmittanc
100
98
96
94
92
90
88
86
84
82
80
78
76
74
72
70
68
66
64
4000
2000
Wavenumbers (cm-1)
3353.6
3285.3
3211.7
3027.7
2964.7
2906.9
2854.3
1681.2
1635.3
1517.0
1450.1
1373.6
1309.2
1235.6
1120.0
731.3
695.1




```
Current Data Parameters
NAME                  Mofakham
EXPNO                      388
PROCNO                       1

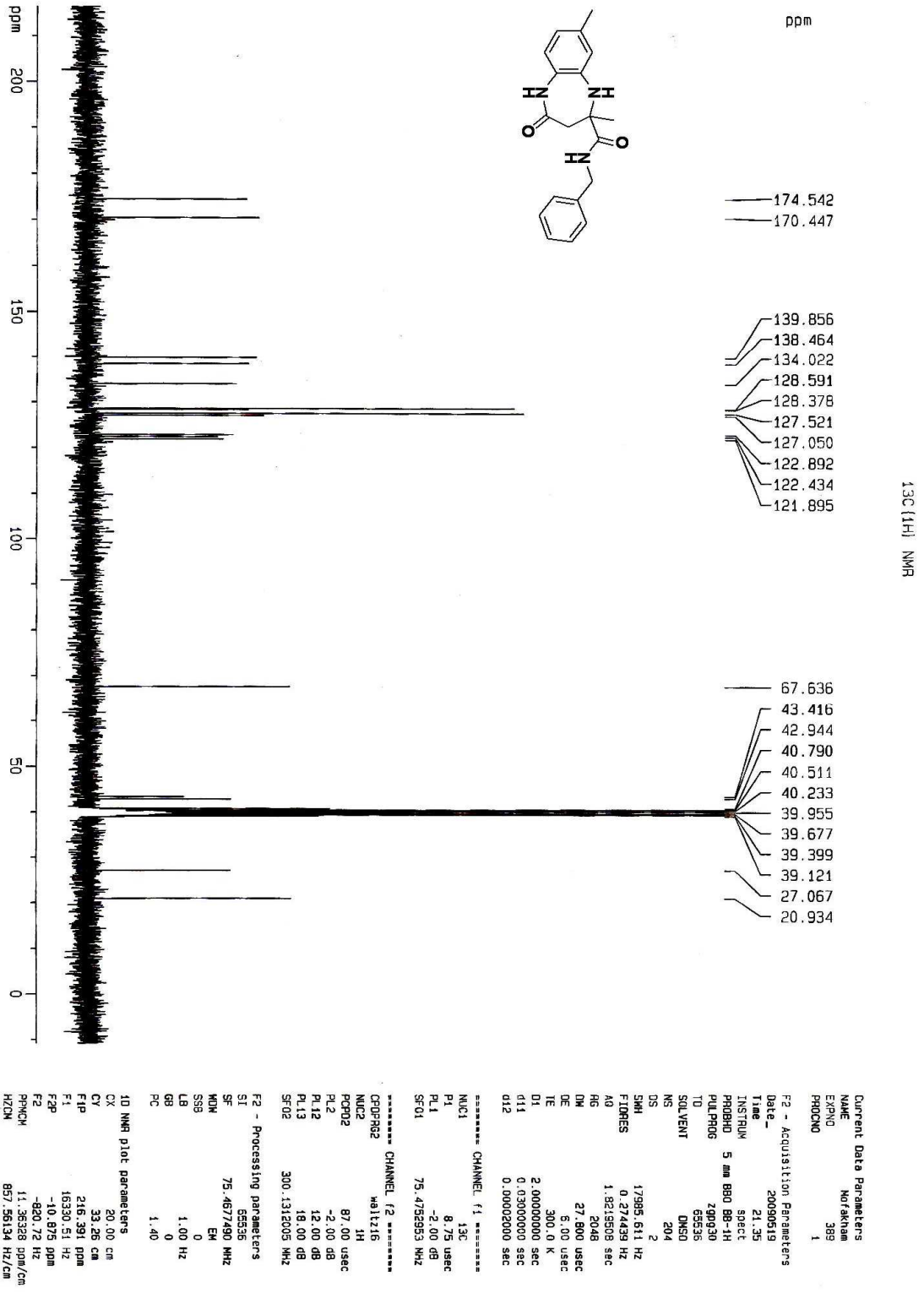
F2 - Acquisition Parameters
Date_                 20090519
Time                     21.25
INSTRUM                  spect
PROBHD    5 mm BBO BB-1H
PULPROG                   zg30
TD                       32768
SOLVENT                   DMSO
NS                          10
DS                           1
SWH                  7812.500 Hz
FIDRES               0.238419 Hz
AQ                   2.0972021 sec
RG                       228.1
DW                      64.000 usec
DE                       6.00 usec
TE                      380.0 K
D1                   2.00000000 sec

======== CHANNEL f1 ========
NUC1                        1H
P1                       15.50 usec
PL1                      -2.00 dB
SFO1              300.1323986 MHz

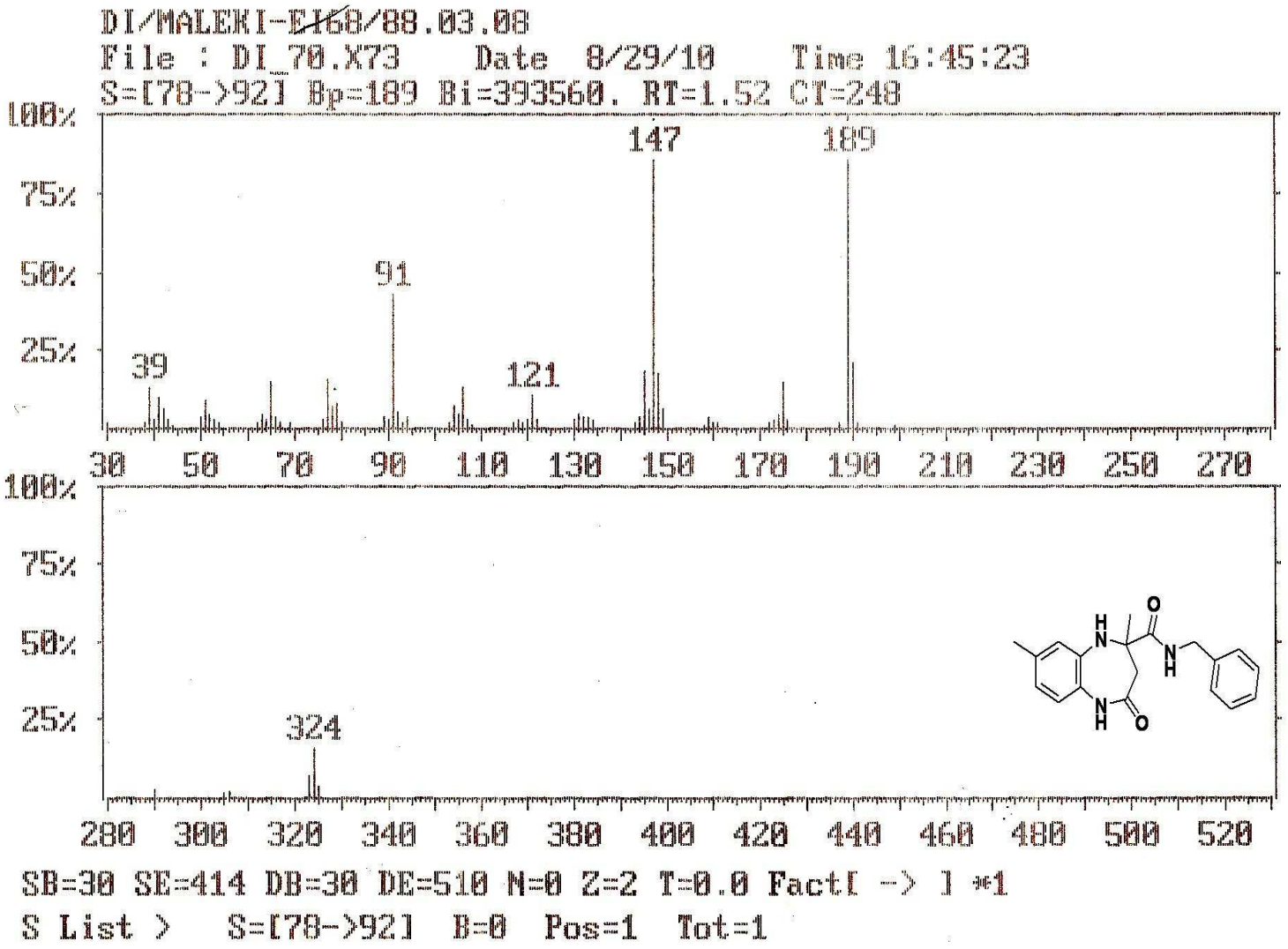
F2 - Processing parameters
SI                       65536
SF                300.1300000 MHz
WDW                         EM
SSB                          0
LB                       0.30 Hz
GB                           0
PC                        1.00

1D NMR plot parameters
CX                       20.00 cm
CY                       22.72 cm
F1P                     11.984 ppm
F1                     3596.67 Hz
F2P                     -0.931 ppm
F2                     -279.38 Hz
PPMCM                  0.64573 ppm/cm
HZCM                 193.80235 Hz/cm
```

^{1}H NMR of **4j**

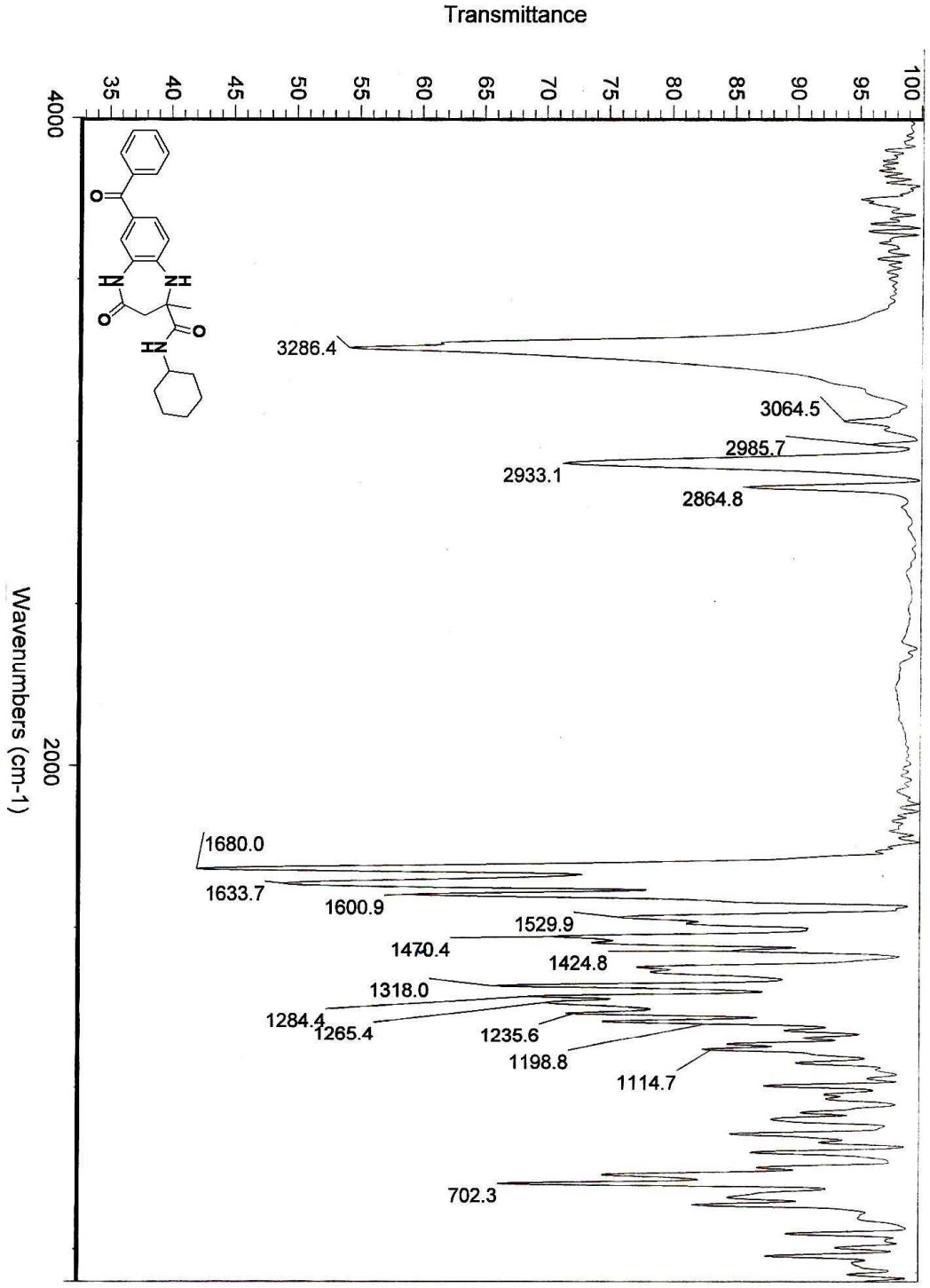

ppm
174.542
170.447
139.856
138.464
134.022
128.591
128.378
127.521
127.050
122.892
122.434
121.895
67.636
43.416
42.944
40.790
40.511
40.233
39.955
39.677
39.399
39.121
27.067
20.934
13C{1H} NMR
Current Data Parameters
NAME Nafakham
EXPNO 389
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090519
Time 21.35
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 204
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.821508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SF01 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 33.26 cm
F1P 216.391 ppm
F1 16330.51 Hz
F2P -10.875 ppm
F2 -820.72 Hz
PPMCM 11.36328 ppm/cm
HZCM 857.56134 Hz/cm
ppm
200
150
100
50
0

^{13}C NMR of **4j**

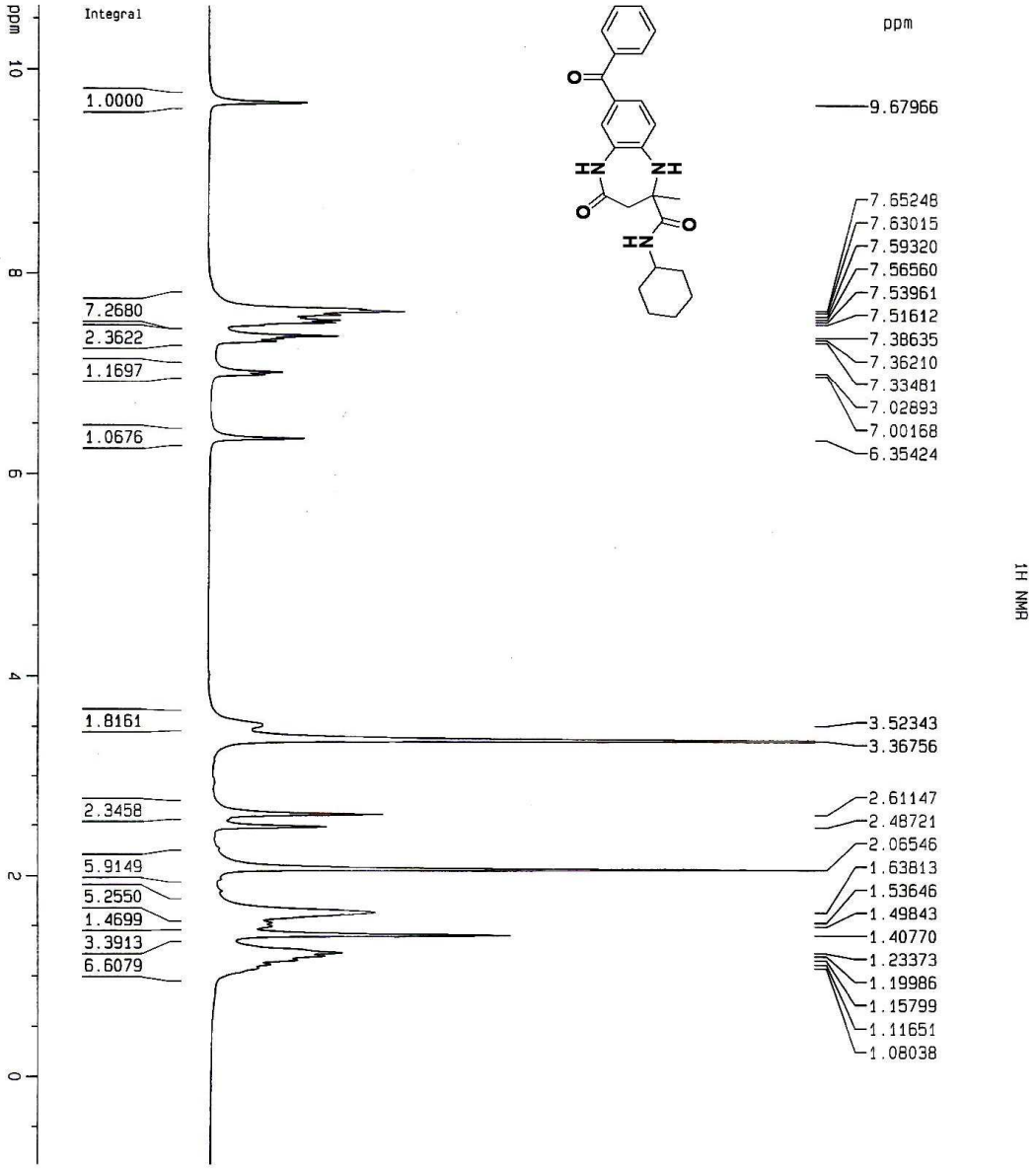

DI/MALEKI-E168/08.03.08
File : DI_70.X73 Date 8/29/10 Time 16:45:23
S=[78->92] Bp=189 Bi=393560. RT=1.52 CT=248
100%
75%
50%
25%
147
189
91
39
121
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
324
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=414 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[->] *1
S List > S=[78->92] B=0 Pos=1 Tot=1

Mass of **4j**

IR of **4k**


Transmittance
100
95
90
85
80
75
70
65
60
55
50
45
40
35
4000
2000
Wavenumbers (cm-1)
3286.4
3064.5
2985.7
2933.1
2864.8
1680.0
1633.7
1600.9
1529.9
1470.4
1424.8
1318.0
1284.4
1265.4
1235.6
1198.8
1114.7
702.3

^{1}H NMR of **4k**




```
Current Data Parameters
NAME                  Mofakham
EXPNO                      413
PROCNO                       1

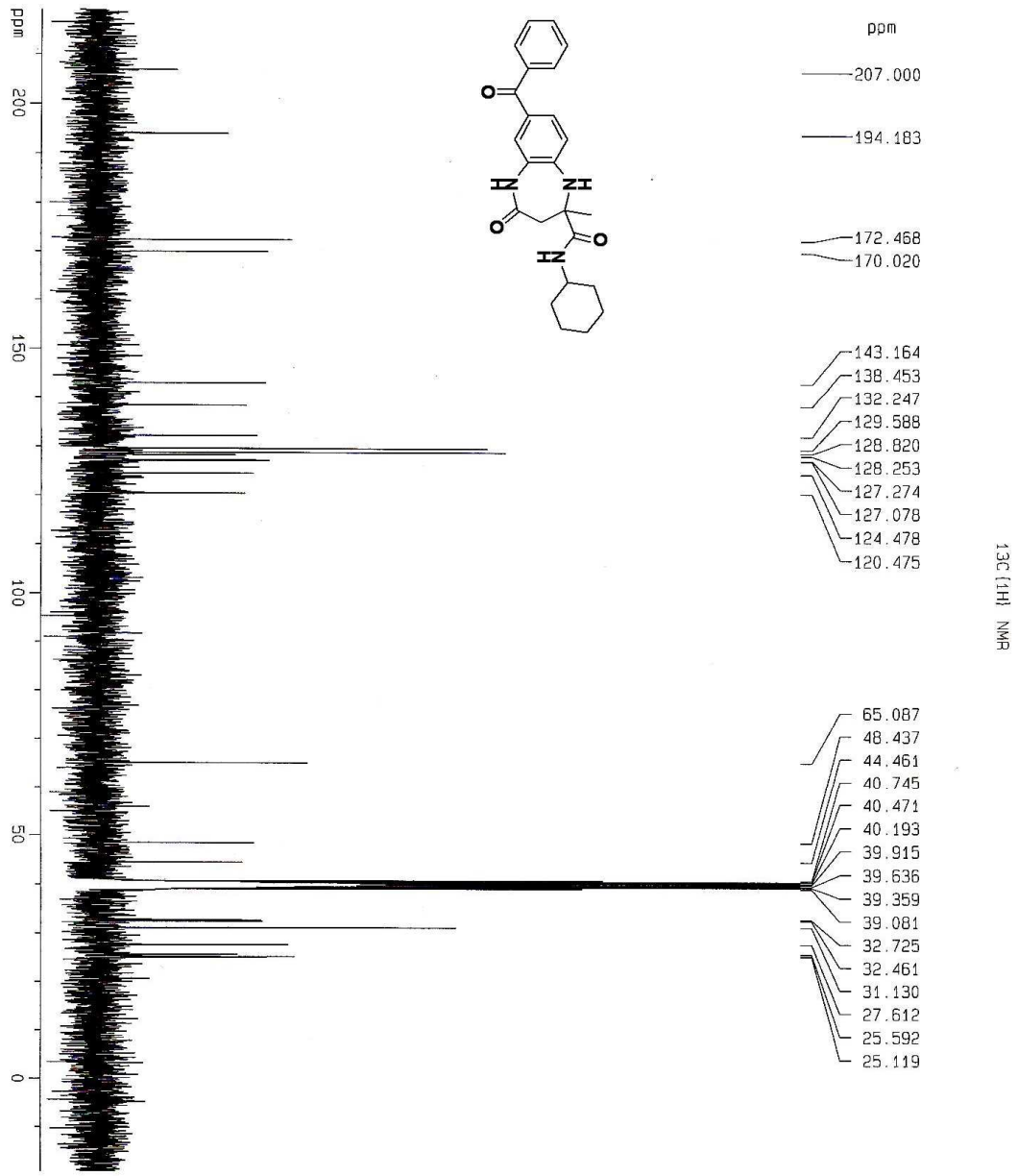
F2 - Acquisition Parameters
Date_              20090609
Time                   18.13
INSTRUM                spect
PROBHD  5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT               DMSO
NS                       10
DS                        1
SWH                7812.500 Hz
FIDRES             0.238419 Hz
AQ                 2.0972021 sec
RG                     228.1
DW                  64.000 usec
DE                   6.00 usec
TE                  380.0 K
D1                 2.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.50 usec
PL1                    -2.00 dB
SFO1          300.1323986 MHz

F2 - Processing parameters
SI                       65536
SF            300.1300000 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                      17.72 cm
F1P                   10.630 ppm
F1                  3190.42 Hz
F2P                   -0.875 ppm
F2                  -262.66 Hz
PPMCM                 0.57526 ppm/cm
HZCM                172.65373 Hz/cm
```

^{13}C NMR of **4k**



Current Data Parameters
NAME Mofakham
EXPNO 414
PROCNO 1

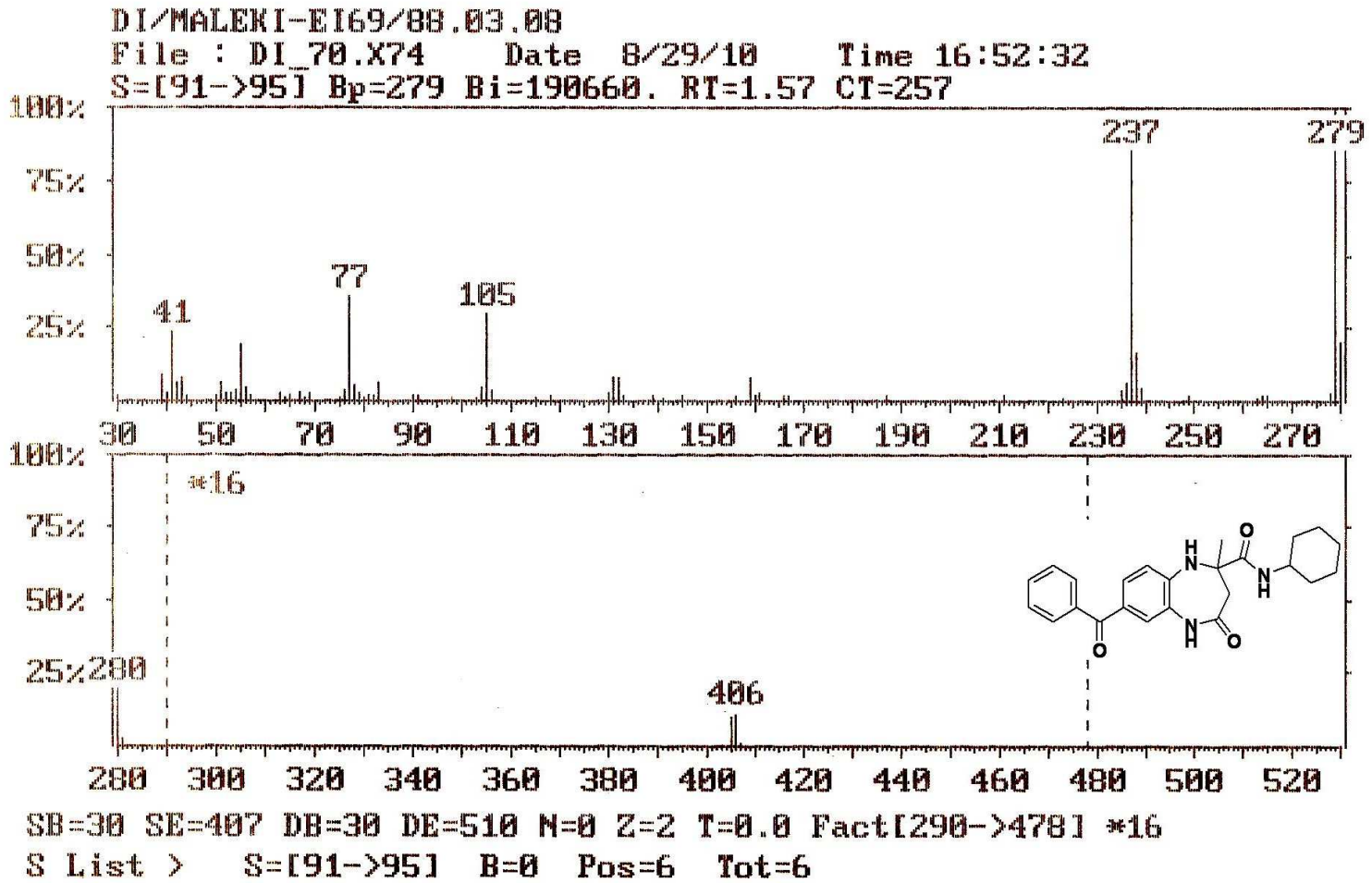
F2 - Acquisition Parameters
Date_ 20090609
Time 18.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 257
DS 0
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

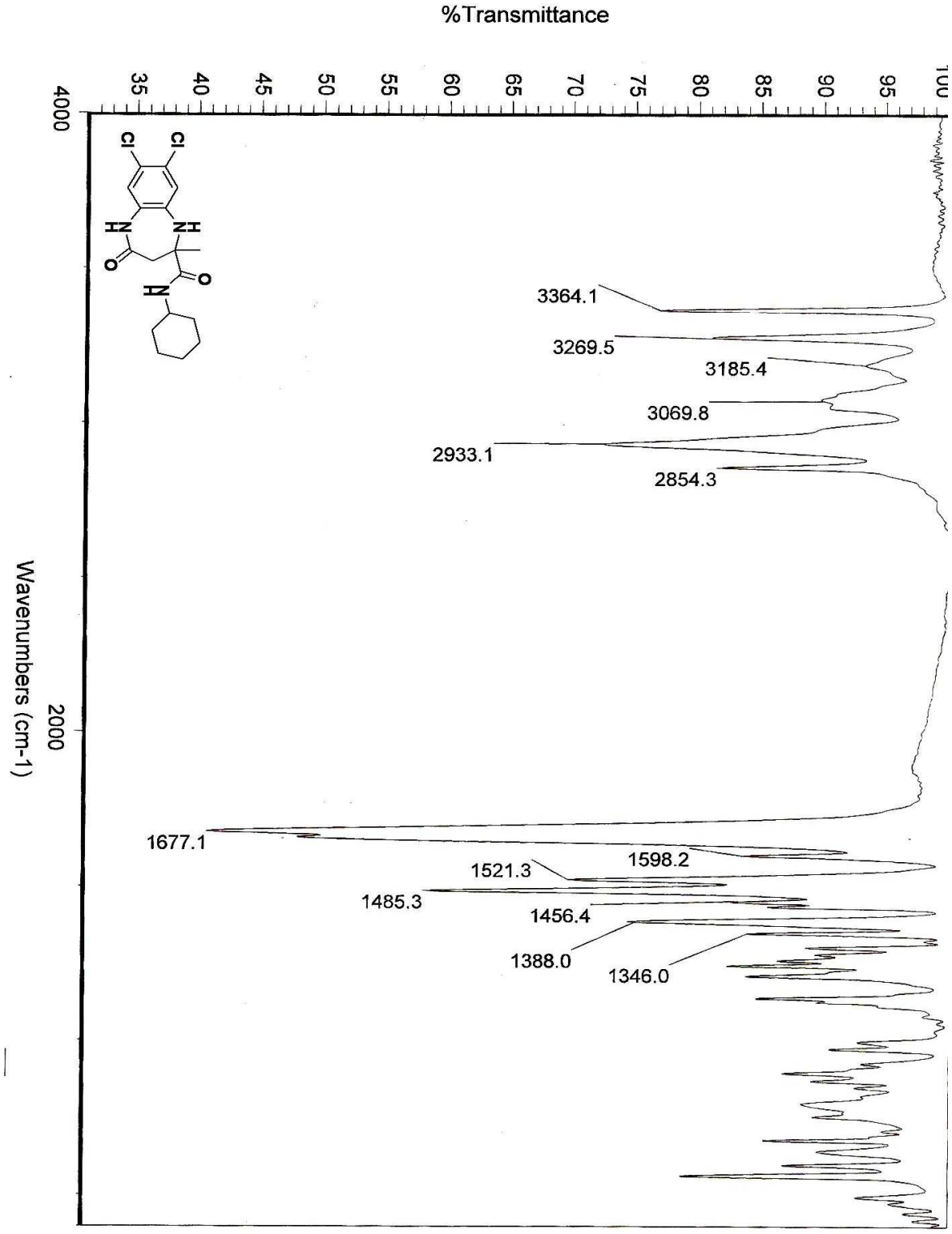
======== CHANNEL f2 ========
CPDPRG2 waltz15
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

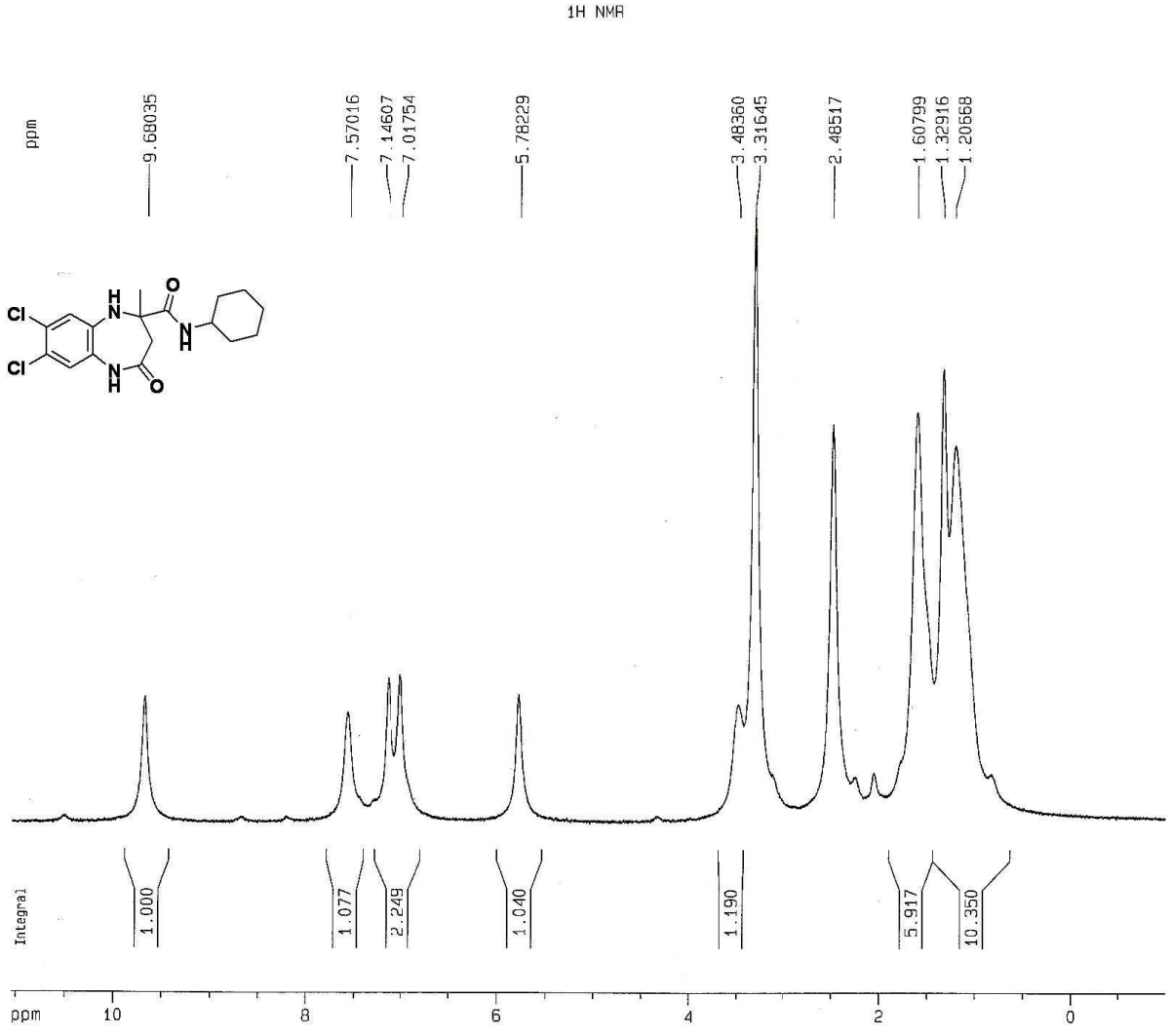
1D NMR plot parameters
CX 20.00 cm
CY 60.99 cm
F1P 219.155 ppm
F1 16539.11 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm


DI/MALEKI-EI69/88.03.08
File : DI_70.X74 Date 8/29/10 Time 16:52:32
S=[91->95] Bp=279 Bi=190660. RT=1.57 CT=257
100%
75%
50%
25%
41
77
105
237
279
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
*16
280
406
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=407 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[290->478] *16
S List > S=[91->95] B=0 Pos=6 Tot=6

Mass of **4k**


%Transmittance
35
40
45
50
55
60
65
70
75
80
85
90
95
100
4000
2000
Wavenumbers (cm-1)
Cl
Cl
N
H
N
H
O
O
N
H
O
3364.1
3269.5
3185.4
3069.8
2933.1
2854.3
1677.1
1598.2
1521.3
1485.3
1456.4
1388.0
1346.0

IR of **4l**



Current Data Parameters
NAME Maleki-PHD
EXPNO 404
PROCNO 1

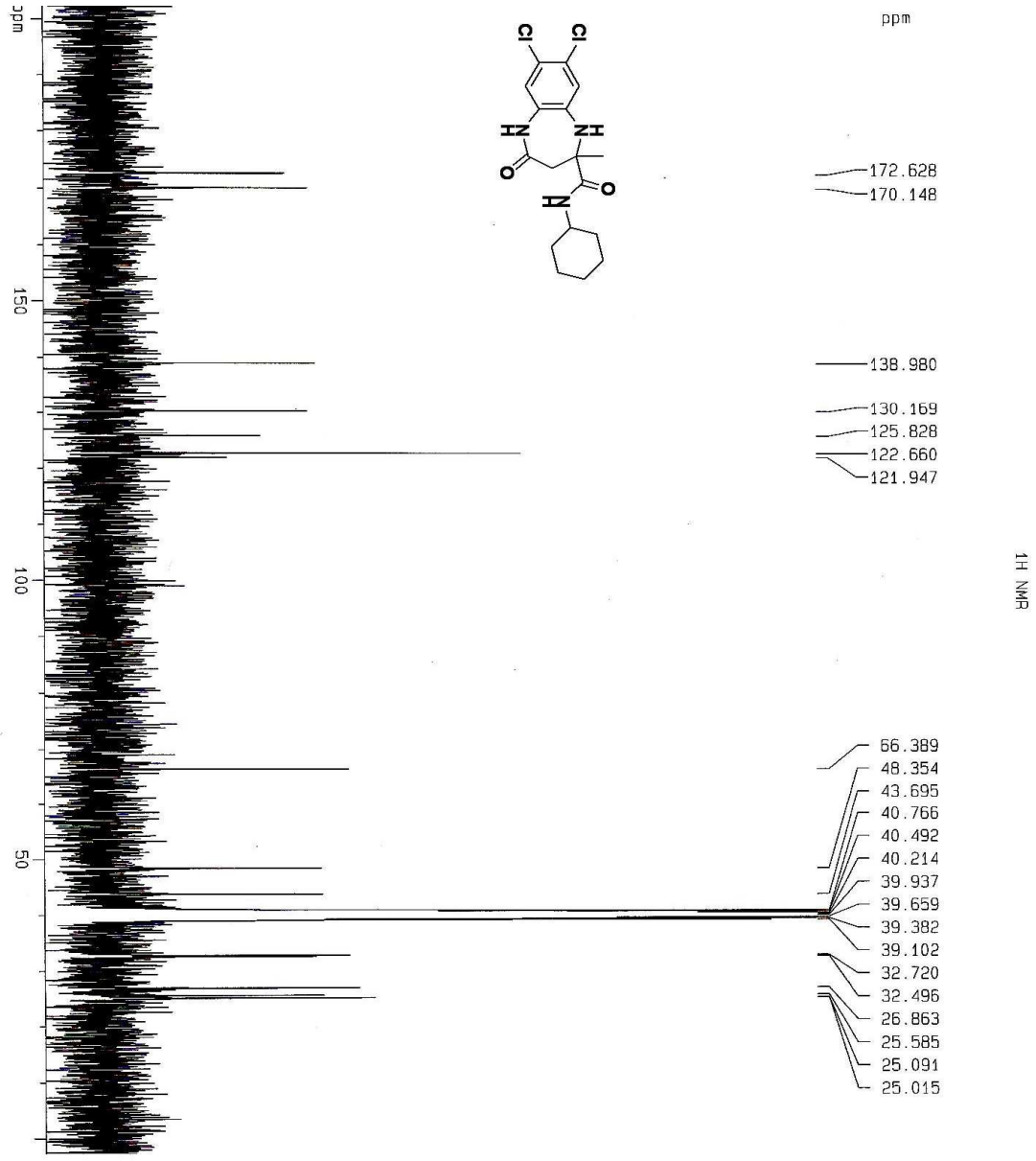
F2 - Acquisition Parameters
Date_ 20090520
Time 12.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 10.65 cm
F1P 11.044 ppm
F1 3314.77 Hz
F2P -0.998 ppm
F2 -299.52 Hz
PPMCM 0.60212 ppm/cm
HZCM 180.71439 Hz/cm

^{1}H NMR of **4l**



^{13}C NMR of **41**

1H NMR

Current Data Parameters
NAME Maleki-PhD
EXPNO 405
PROCNO 1

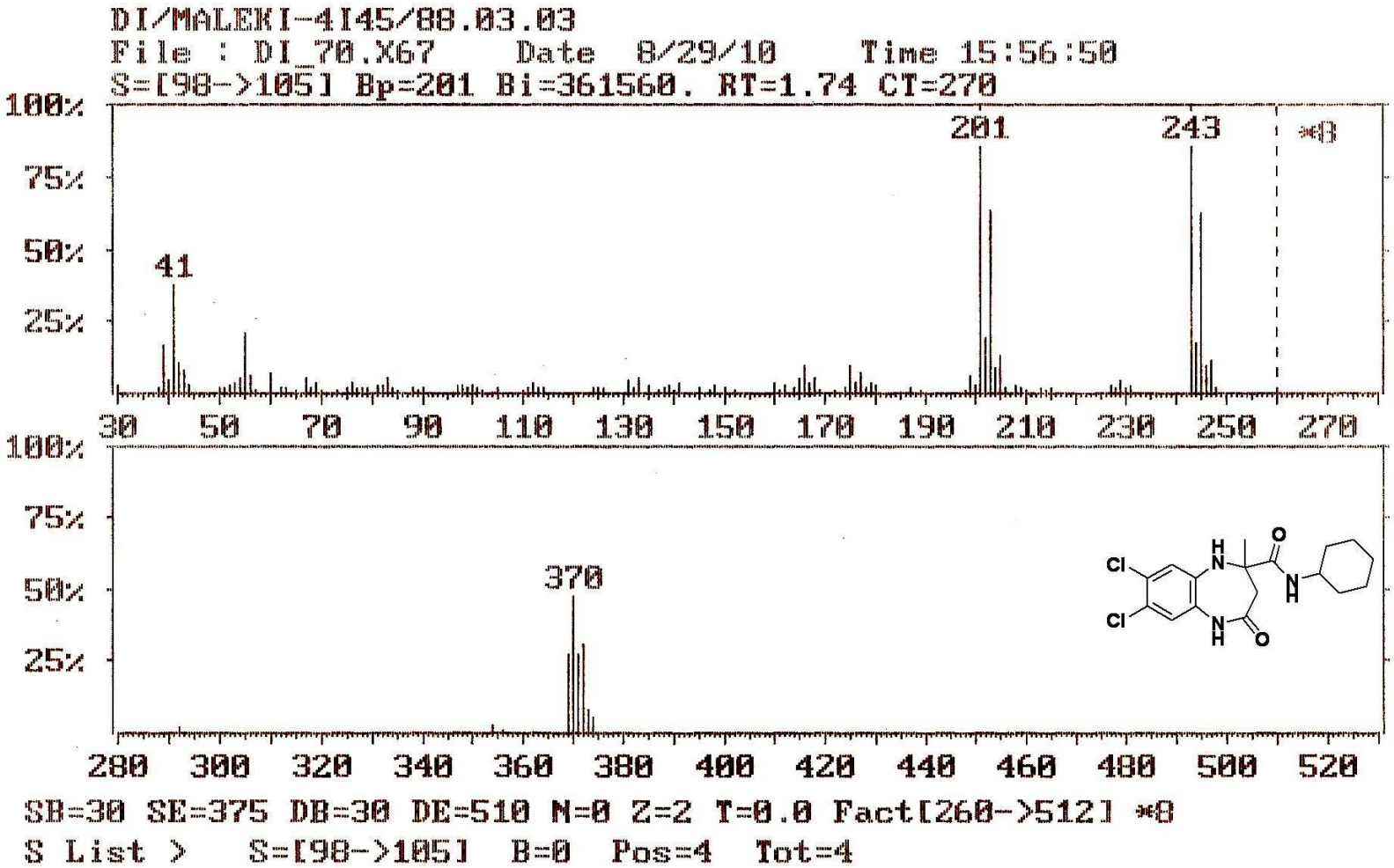
F2 - Acquisition Parameters
Date_ 20090520
Time 12.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 60
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 8.75 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz

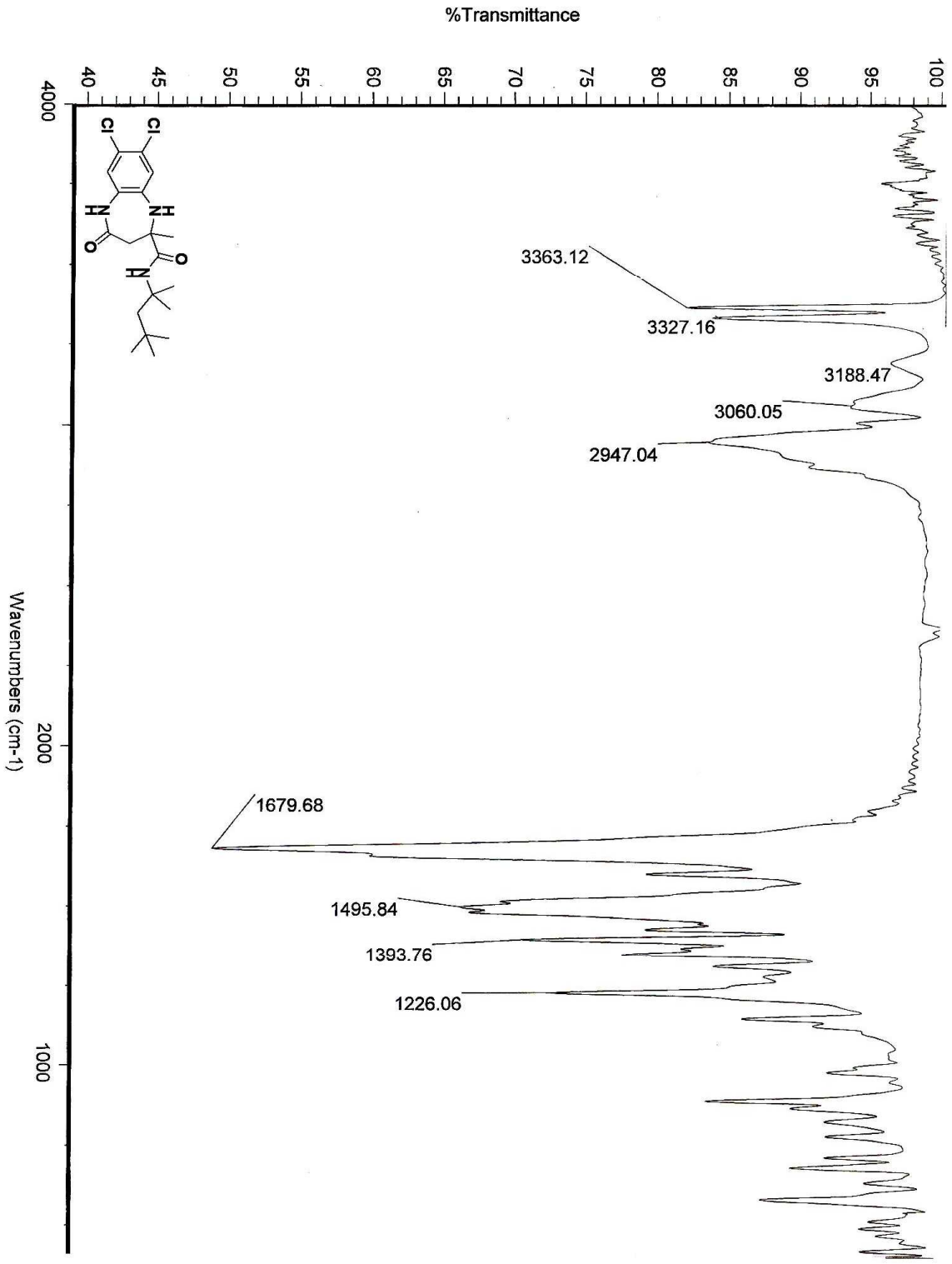
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 81.26 cm
F1P 202.719 ppm
F1 15298.72 Hz
F2P -2.731 ppm
F2 -206.12 Hz
PPMCM 10.27249 ppm/cm
HZCM 775.24176 Hz/cm

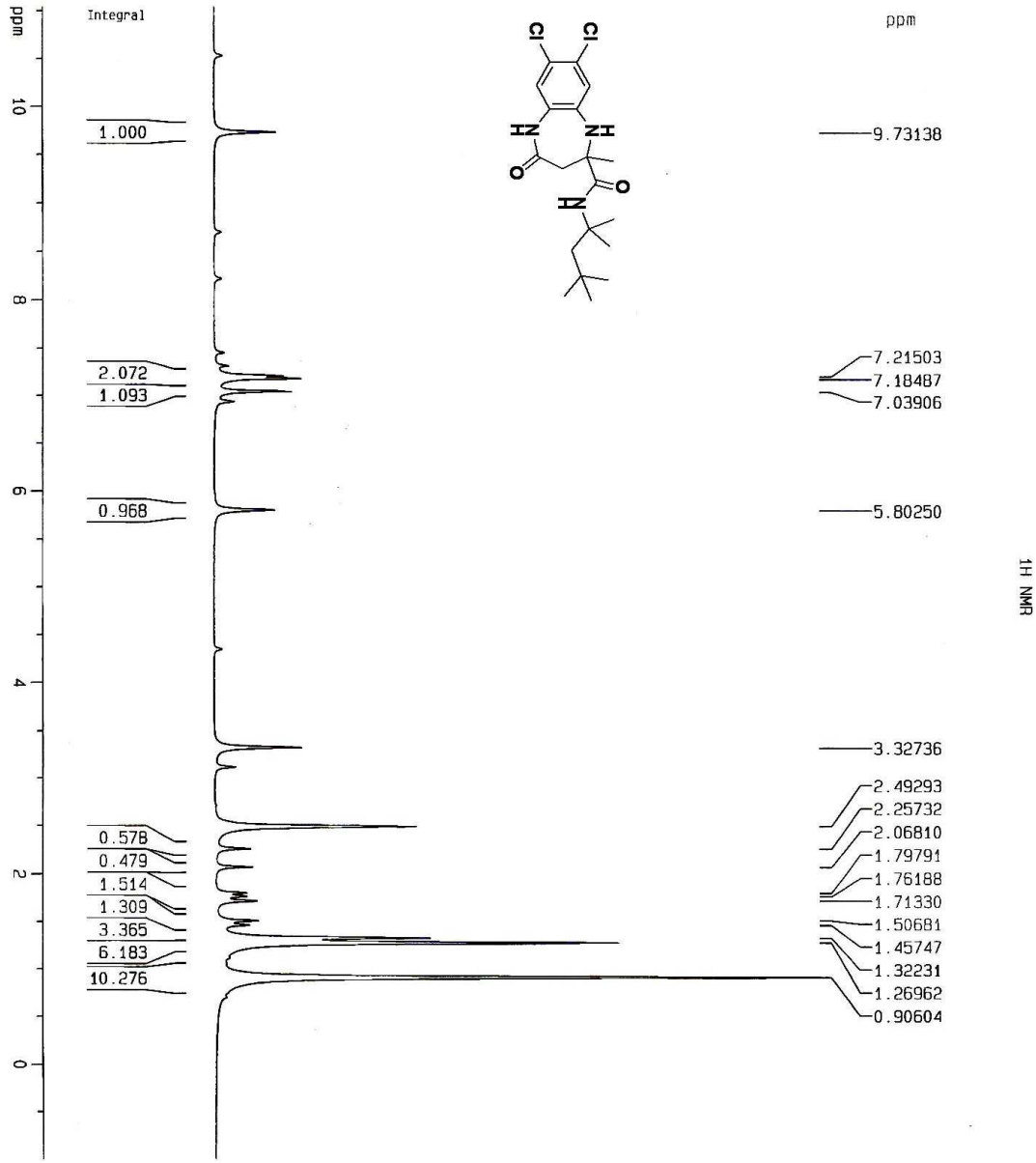

DI/MALEKI-4I45/88.03.03
File : DI_70.X67 Date 8/29/10 Time 15:56:50
S=[98->105] Bp=201 Bi=361560. RT=1.74 CI=270
100%
75%
50%
25%
41
201
243
370
30 50 70 90 110 130 150 170 190 210 230 250 270
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=375 DB=30 DE=510 N=0 Z=2 T=0.0 Fact[260->512]
S List > S=[98->105] B=0 Pos=4 Tot=4
Cl
Cl
H
N
O
N
H
O

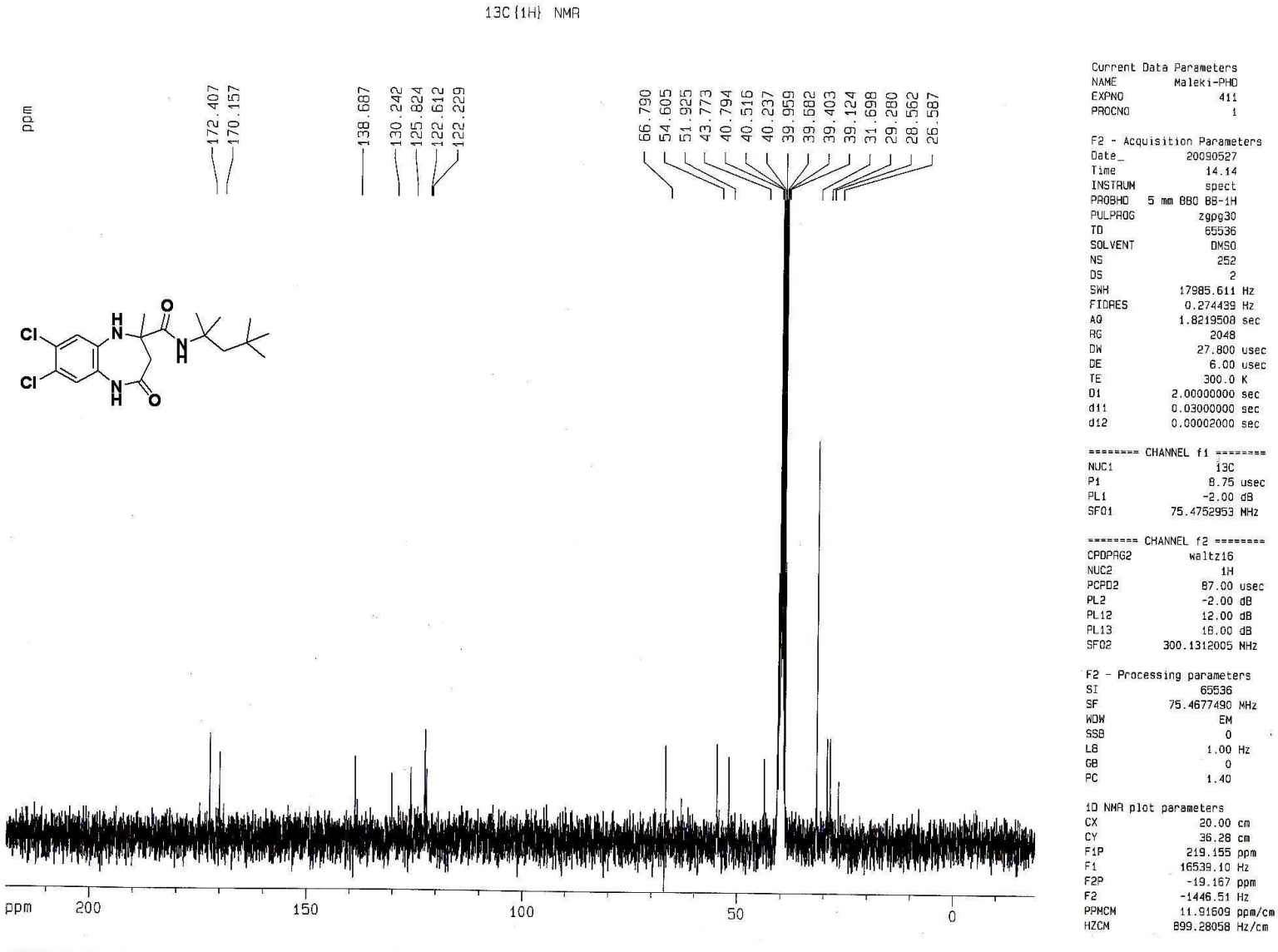
Mass of **4l**

IR of **4m**


%Transmittance
100
95
90
85
80
75
70
65
60
55
50
45
40
4000
2000
1000
Wavenumbers (cm-1)
3363.12
3327.16
3188.47
3060.05
2947.04
1679.68
1495.84
1393.76
1226.06

^{1}H NMR of **4m**


Integral
ppm
1.000
2.072
1.093
0.968
0.578
0.479
1.514
1.309
3.365
6.183
10.276
9.73138
7.21503
7.18487
7.03906
5.80250
3.32736
2.49293
2.25732
2.06810
1.79791
1.76188
1.71330
1.50681
1.45747
1.32231
1.26962
0.90604
Cl
Cl
N
H
O
1H NMR
Current Data Parameters
NAME Maleki-PhD
EXPNO 410
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090527
Time 13.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.65 cm
F1P 11.044 ppm
F1 3314.77 Hz
F2P -0.998 ppm
F2 -299.52 Hz
PPMCM 0.60212 ppm/cm
HZCM 180.71439 Hz/cm



Current Data Parameters

NAME	Maleki-PHD
EXPNO	411
PROCNO	1

F2 - Acquisition Parameters

Date_	20090527
Time	14.14
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	252
DS	2
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	2048
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
d12	0.00002000 sec

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

NUC1	13C
P1	8.75 usec
PL1	-2.00 dB
SFO1	75.4752953 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	87.00 usec
PL2	-2.00 dB
PL12	12.00 dB
PL13	18.00 dB
SFO2	300.1312005 MHz

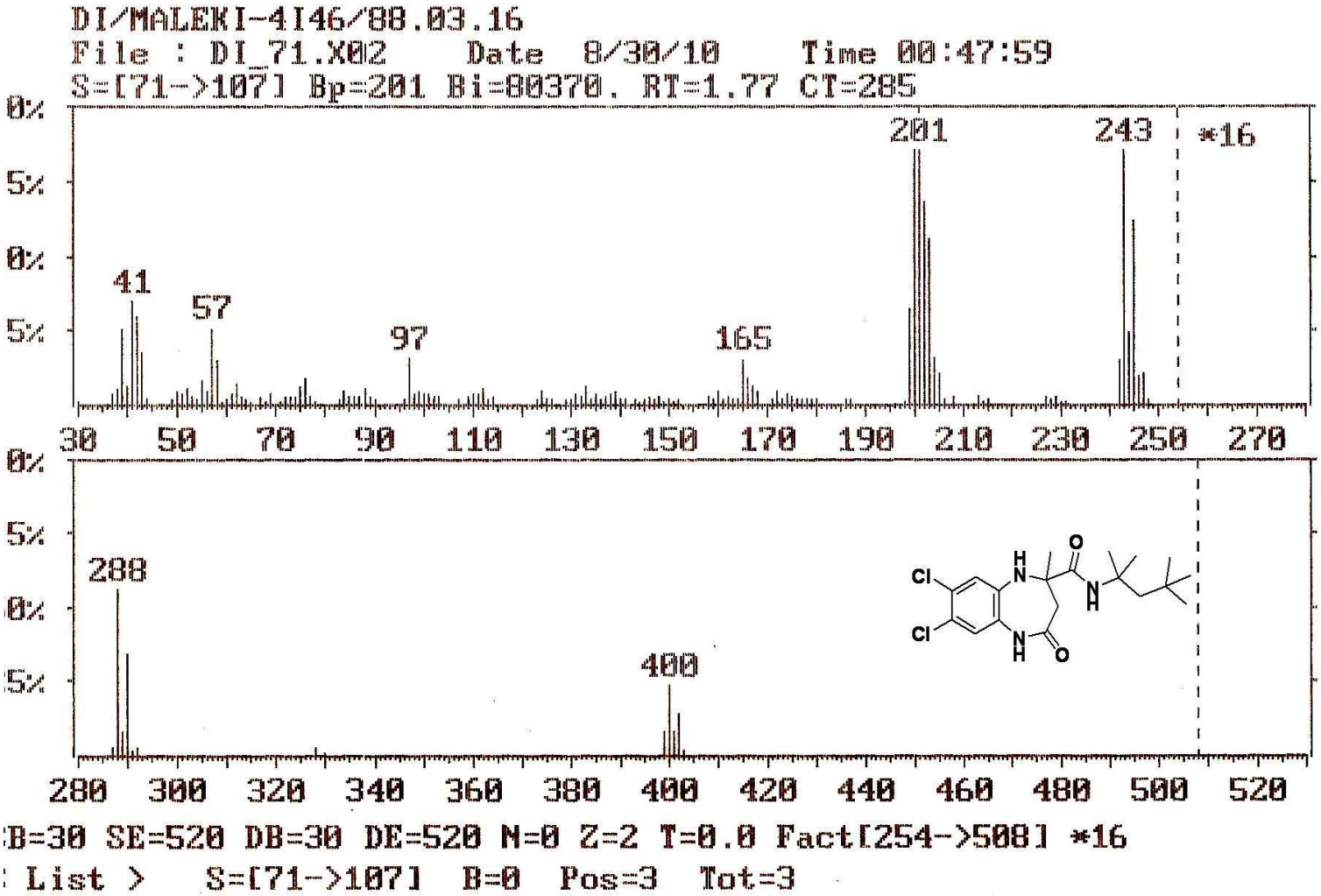
F2 - Processing parameters

SI	65536
SF	75.4677490 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

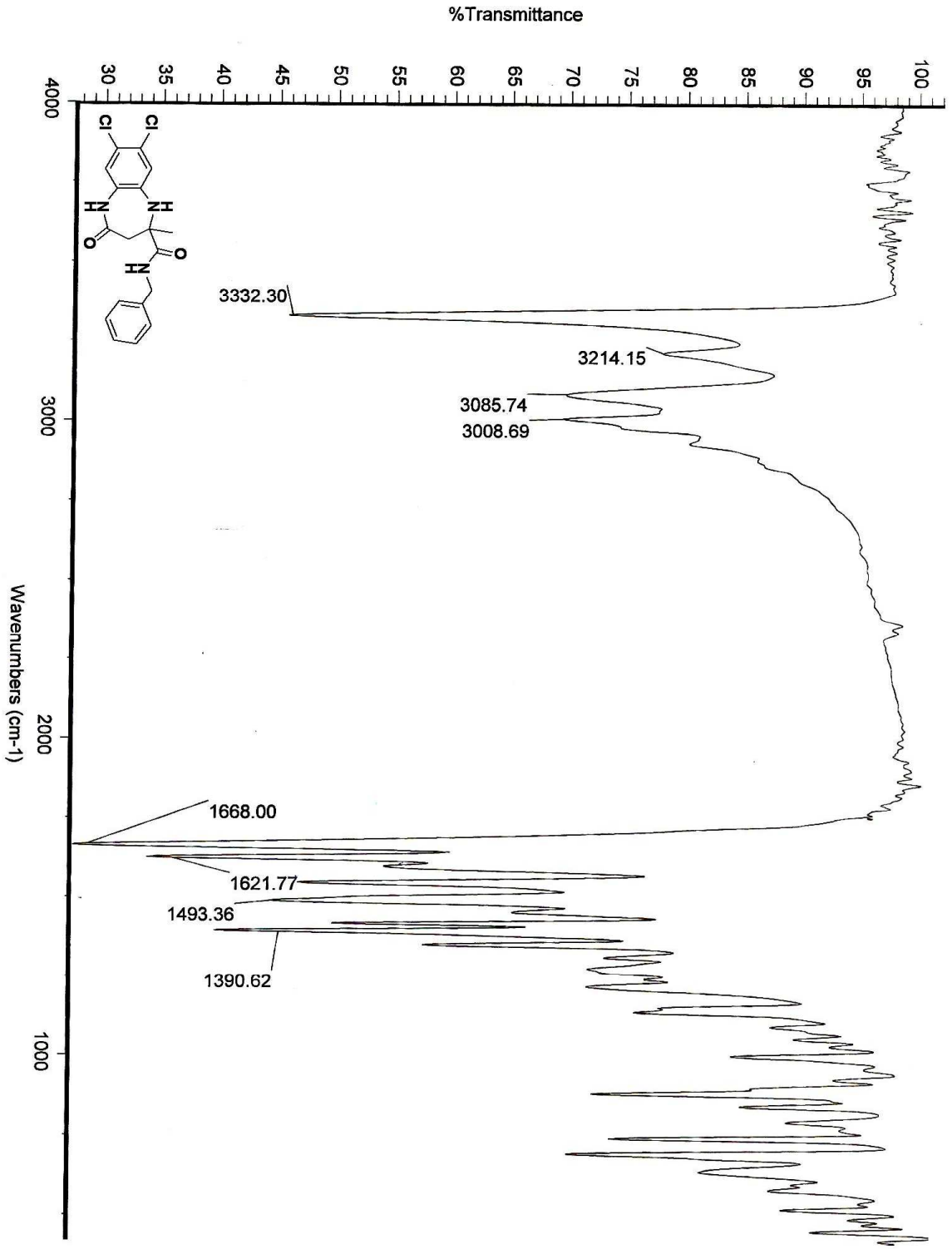
CX	20.00 cm
CY	36.28 cm
F1P	219.155 ppm
F1	16539.10 Hz
F2P	-19.167 ppm
F2	-1446.51 Hz
PPMCM	11.91609 ppm/cm
HZCM	899.28058 Hz/cm

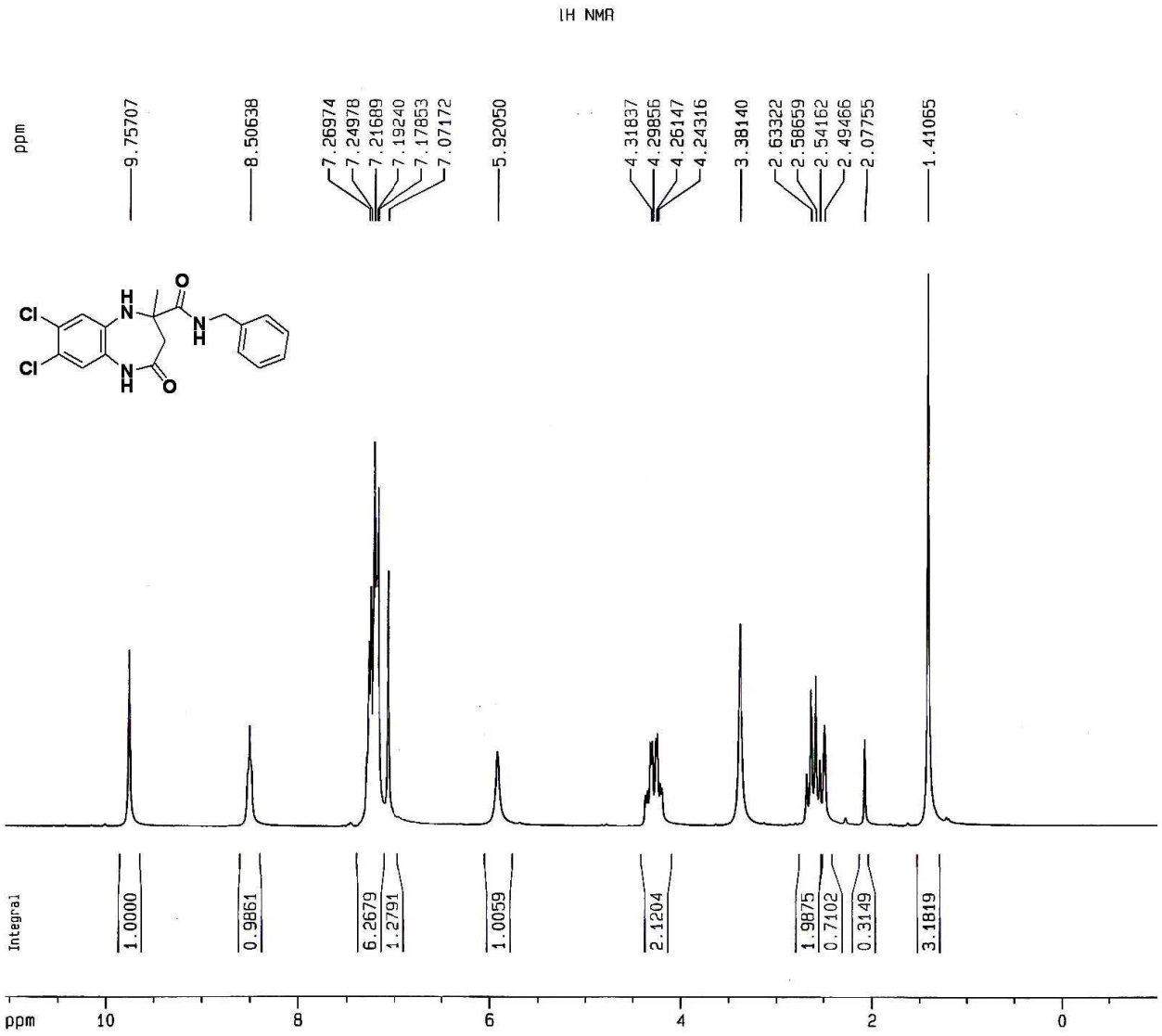
^{13}C NMR of **4m**


DI/MALEKI-4I46/88.03.16
File : DI_71.X02 Date 8/30/10 Time 00:47:59
S=[71->107] Bp=201 Bi=80370. RT=1.77 CT=285
201
243
*16
41
57
97
165
288
400
Cl
Cl
H
N
O
N
H
H
N
O
B=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 Fact[254->508] *16
List > S=[71->107] B=0 Pos=3 Tot=3

Mass of **4m**

IR of **4n**


%Transmittance
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
4000
3000
2000
1000
Wavenumbers (cm-1)
Cl
Cl
N
H
O
N
H
O
HN
3332.30
3214.15
3085.74
3008.69
1668.00
1621.77
1493.36
1390.62



Current Data Parameters
NAME Maleki-PHD
EXPNO 408
PROCNO 1

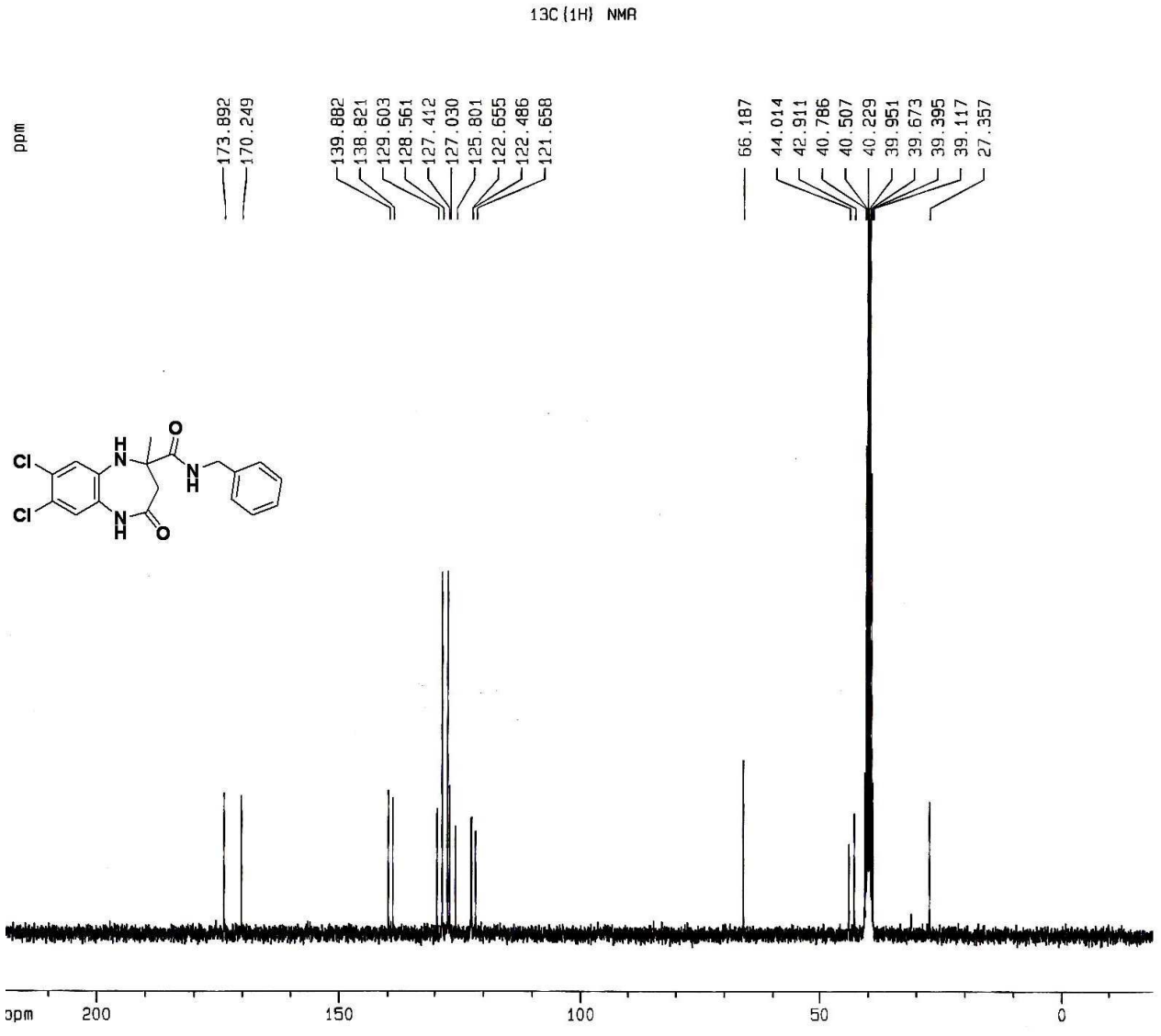
F2 - Acquisition Parameters
Date_ 20090527
Time 13.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 9.60 cm
F1P 11.044 ppm
F1 3314.77 Hz
F2P -0.998 ppm
F2 -299.52 Hz
PPMCM 0.60212 ppm/cm
HZCM 180.71439 Hz/cm

^{1}H NMR of **4n**

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Current Data Parameters
NAME          Maleki-PHD
EXPNO               409
PROCNO                1

F2 - Acquisition Parameters
Date_          20090527
Time              13.47
INSTRUM           spect
PROBHD  5 mm BBO BB-1H
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                 507
DS                   2
SWH           17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                2048
DW              27.800 usec
DE               6.00 usec
TE              300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
d12           0.00002000 sec

======== CHANNEL f1 ========
NUC1               13C
P1               8.75 usec
PL1             -2.00 dB
SF01         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2           87.00 usec
PL2             -2.00 dB
PL12            12.00 dB
PL13            18.00 dB
SF02        300.1312005 MHz

F2 - Processing parameters
SI                65536
SF           75.4677490 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                19.37 cm
F1P             219.155 ppm
F1              16539.10 Hz
F2P             -19.167 ppm
F2              -1446.51 Hz
PPMCM          11.91609 ppm/cm
HZCM          899.28058 Hz/cm
```
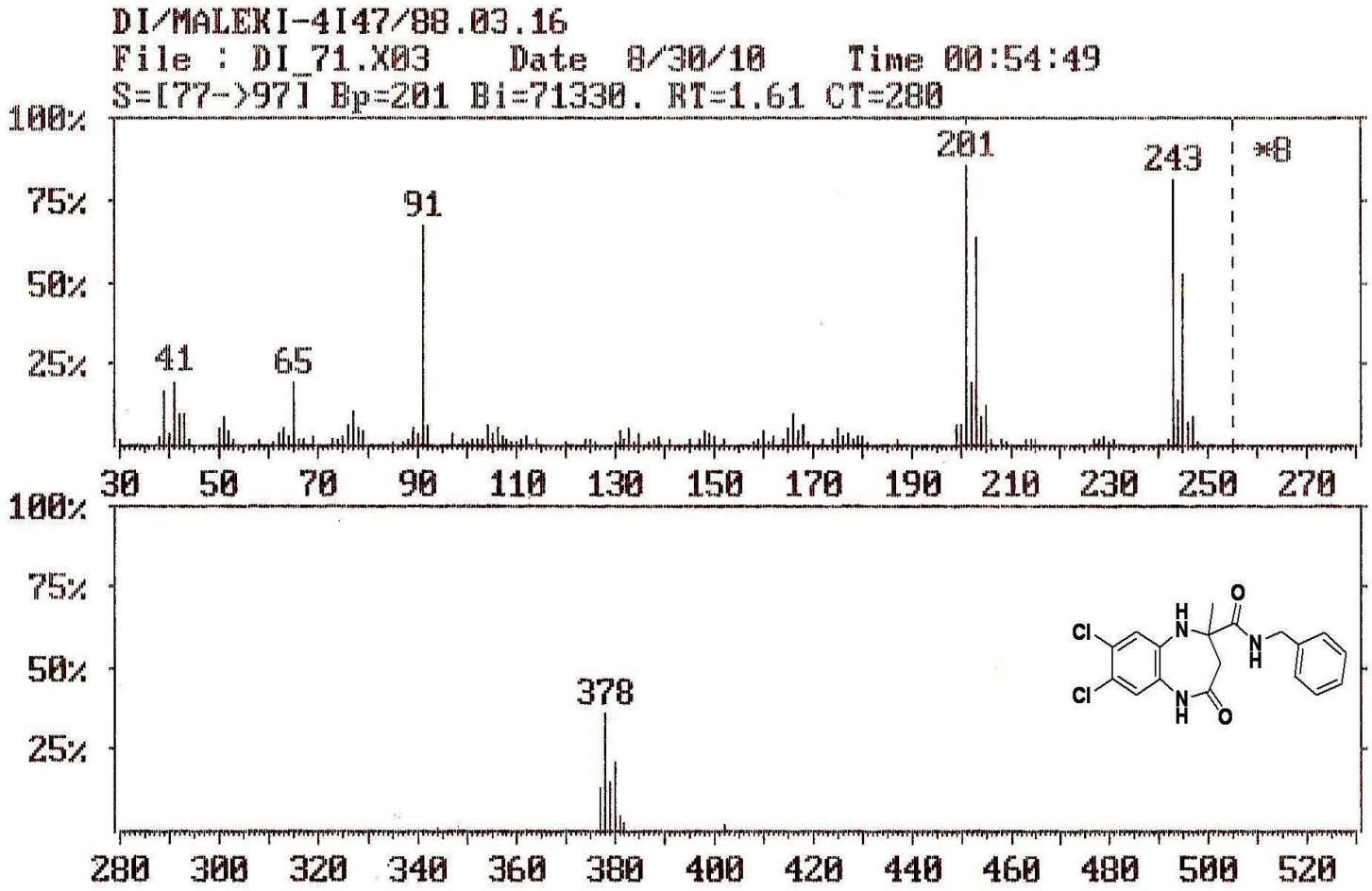

^{13}C NMR of **4n**


DI/MALEKI-4I47/88.03.16
File : DI_71.X03 Date 8/30/10 Time 00:54:49
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100%
75%
50%
25%
41
65
91
201
243
*8
30 50 70 90 110 130 150 170 190 210 230 250 270
100%
75%
50%
25%
378
Cl
Cl
H
N
O
N
H
N
H
O
280 300 320 340 360 380 400 420 440 460 480 500 520
SB=30 SE=520 DB=30 DE=520 N=0 Z=2 T=0.0 Fact[255->522] *8
S List > S=[77->97] B=0 Pos=2 Tot=2

Mass of **4n**