Supporting Information

The Photochemistry of Polydonor-Substituted Phthalimides. Curtin-Hammett Type Control of Competing Reactions of Potentially Interconverting Zwitterionic Biradical Intermediates

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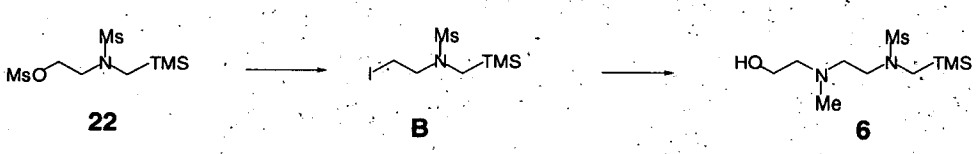

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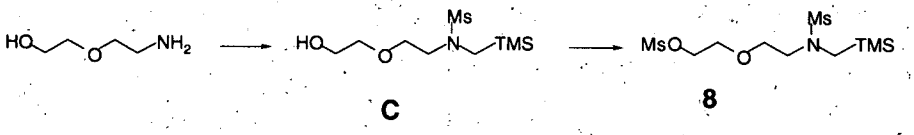

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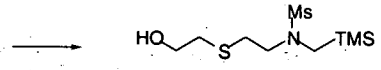

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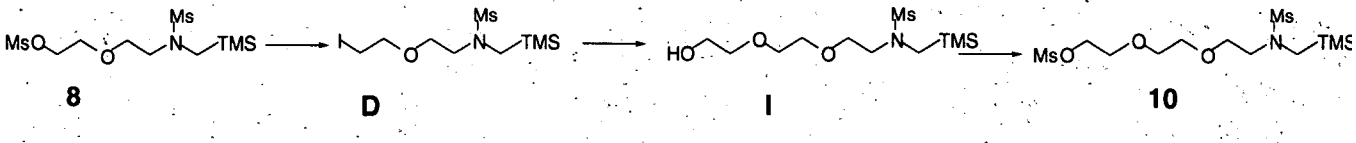

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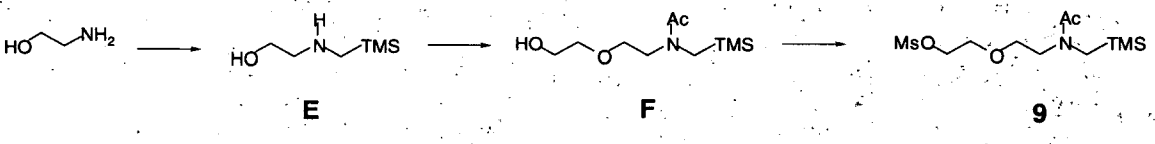

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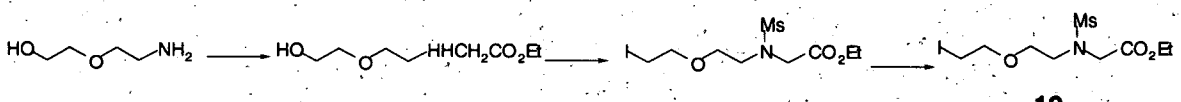

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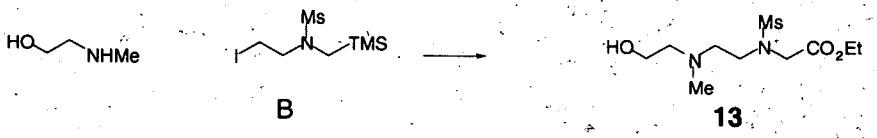

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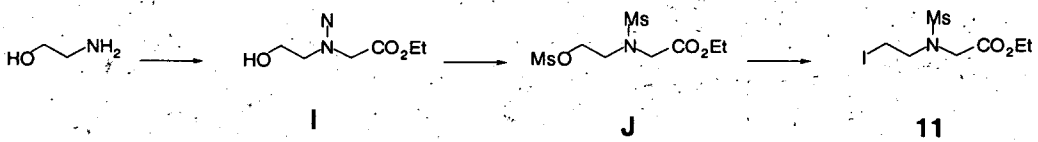


I J 11

Alcohol 6. A solution of sodium iodide (13 g, 87 mmol) and methansulfonate **22***** (4.9 g, 16 mmol) in 50 L acetone at 50 ^{0}C was stirred for 12 h, cooled to room temperature and extracted with ethyl acetate, The extracts were washed with water, dried and concentrated in vacuo to afford a residue which was subjected to column chromatography (silica gel, 1:2 EtAc:hexane) to give iodide **B** (4.8 g, 89%) as a white solid, mp 86-87 ^{0}C (EtAc-hexane). ^{1}H-NMR ($CDCl_3$) 0.13 (s, 9H), 2.69 (s, 2H), 2.82 (s, 3H), 3.22-3.29 (m, 2H), 3.43-3.49 (m, 2H); ^{13}C-NMR ($CDCl_3$) -1.9, 1.2, 35.8, 39.7, 53.

A solution of 2-N-methylaminoethanol (10.9 g, 144 mmol), triethylamine (14.63 g, 144 mmol), and iodide **B** (12 g, 36 mmol) in 150 mL of MeCN at 70-80°C was stirred for 20 h, cooled and filtered through Celite. The filtrate was concentrated in *vacuo* to give a residue that was dissolved in CH_2Cl_2. The CH_2Cl_2 solution was washed with water, dried and concentrated in *vacuo* giving a residue which was subjected to column chromatography (2:1 hexane:EtAc) to give the alcohol **6** (7.52 g, 75%). ^{1}HNMR 0.1 (s, 9H, $SiMe_3$), 2.26 (s, 3H, $NC\underline{H}_3$), 2.54 (t, J=5.3 Hz, 2H, $HOCH_2C\underline{H}_2$) 2.62 (t, J=6.9 Hz, 2H $NC\underline{H}_2CH_2NSO_2CH_3$) 2.83 (s, 3H, $SO_2C\underline{H}_3$), 3.25 (t, J=6.9 Hz, 2H, $NCH_2C\underline{H}_2NSO_2CH_3$), 3.57 (t, J=5.3 Hz, 2H, $HOC\underline{H}_2CH_2$); ^{13}CNMR –1.7 ($SiMe_3$), 36.0 (NCH_3), 38.5 ($N\underline{C}H_2SiMe_3$), 41.9 ($SO_2\underline{C}H_3$), 47.9 ($N\underline{C}H_2CH_2NSO_2CH_3$), 55.4 ($NCH_2\underline{C}H_2NSO_2CH_3$), 58.7 ($HOCH_2\underline{C}H_2$), 59.4 ($HO\underline{C}H_2$); MS(FAB m/z(relative intensity) 283(100) 281(28) 88(36) 73(26); MS(FAB) m/z(relative intensity) 282(2) 203(27) 88(100) 73(72) HRMS (m/z): calcd for $C_{10}H_{26}N_2O_3SiS$ (M+1) 283.1512, found 283.1500.

Alcohol 7. A solution of 2-mercaptoethanol (1.56 g, 20 mmol) and sodium hydroxide (0.8 g, 20 mmol)in 150 mL of MeCN was stirred for 10 min. iodide **1** (1.67g, 5mmol) was added and the resulting mixture was stirred for 16 h at 75-80°C, cooled and filtered through Celite. The filtrate was concentrated in *vacuo* to give a residue that was dissolved in CH_2Cl_2. The CH_2Cl_2 solution was washe

with water, dried and concentrated in *vacuo* giving a residue which wa subjected to column chromatography (2:1 hexane:EtAc) to give the alcohol **7** (1.35 g, 95%). ^{1}H-NMR ($CDCl_3$) 0.096 (s, 9H, $SiMe_3$), 2.64 (s, 2H, CH_2TMS), 2.7 (m, 4H, SCH_2CH_2N), 3.39 (t, 2H, J=7.65 Hz, $HOCH_2CH_2S$), 3.71 (t, 2H, J=7.65 Hz $HOCH_2CH_2S$); ^{13}C-NMR ($CDCl_3$) –1.9 (SiMe3), 35.8 (NCH_3), 29.8, 34.5, 38.9, 50. and 60.7 (CH_2); FT-IR 3150~3650 (br. OH stretching); MS (FAB), m/z (rel intensity) 286 (28), 284 (100); HRMS(FAB) cacld for $C_9H_{23}NO_3S_2Si$ (M+1 286.0967 found 286.0963.

Methansulfonate 8. To a solution of 2-(2-aminoethoxy)ethanol (11 g, 0.1 mol) in 30 mL of MeC was added a solution of tirmethylsilylmethyl iodide (10.7 g, 50 mmol) in 30 mL of MeCN dropwise. Th resulting mixture was stirred for 24 h at 60 ^{0}C, cooled to room temperature and extracted with ethyl ethe The ethereal extracts were washed with 1N sodium hydroxide, dried and concentrated in vacuo to affor alcohol **C**, which was used in the next reaction without purification.

To a solution of **C** in in 100 mL of MeCN containing potassium carbonate (41.4 g, 0.3 mol) at 0 ^{0}(was added a solution of methanesulfonyl chloride (11 g, 96.1 mmol) inin 10 mL of MeCN dropwise. Th resulting mixture was stirred overnight at room temperature and filtered. The filtrate was concentrated an then diluted with ether. The ethereal solution was washed with 0.1N NaOH, dried and concentrated i vacuo to afford a residue which was subjected to column chromatography (2:1 EtAc:Hexane) to afford (7.2 g, 41.4%) as a crystalline solid, mp 46-47 ^{0}C (EtAc-hexane). ^{1}H-NMR 0.12 (s, 9H), 2.72 (s, 2H 2.85 (s, 3H), 3.02 (s, 3H), 3.42 (t, 2H, J=5.5Hz), 3.65 (t, 2H, J= 5.0Hz), 3.73 (t,2H, J=4.6 Hz), 4.33 (t, 2H J=4.5Hz); ^{13}C-NMR -1.8, 36.0, 37.6, 38.1, 48.8, 68.3, 68.5, 68.7. MS (FAB) m/z 348, 332, 270, 252, 20 188, 137, 116, 73. HRMS (FAB) m/z 348.0959 ($C_{10}H_{26}NO_6S_2Si$ required 348.0971).

Methansulfonate 9. A solution of 2-(2-amidoethoxy)ethanol (2.53 mL, 25.22 mmol) and iodomethyltrimethylsilyl (1.80 g, 8.41 mmol) in 60 mL MeCN was stirred for 3h at 60 °C, diluted with water and extracted with CH_2Cl_2. The extracts were dried and concentrated *in vacuo* to afford a residue which was subjected to column chromatography (silica gel. 1:5 MeOH-EA) yielding 1.06 g (73%) of product **E**. ^{1}H NMR 0.04 (s, 9H), 2.06 (s, 2H), 2.79 (t, 2H, J=5.0Hz), 3.55-3.64 (m, 4H), 3.69 (t, 2H J=2.0Hz); ^{13}C-NMR -2.6, 39.9, 53.5, 61.7, 69.4.

A solution of **E** (5.1 g, 29.4 mmol), and triethylamine (12.3 mL, 88.1 mmol), acetylchloride (2.1 mL, 29.37 mmol) in 60 mL MeCN was stirred for 3h at 0 °C, diluted with water and extracted with diethylether. The extracts were dried and concentrated *in vacuo* to afford a residue which was subjected to column chromatography (silica gel, 1:5MeOH-EA) yielding 5.7 g (63%) of alcohol **F**. ^{1}H-NMR (1:2 mixture of two rotamers) rotamer A -0.09 (s, 9H), 1.99 (s, 3H), 2.72 (s, 2H), 3.31-3.50(m, 6H,), 3.59(t 2H, J=4.0Hz); ^{1}H-NMR of rotamer B -0.01 (s, 9H), 1.92 (s, 3H), 2.83 (s, 2H), 3.31-3.50 (m, 6H,), 3.59 (t 2H, J=4.0Hz); ^{13}C-NMR rotamer A –1.3, 14.0, 21.0, 38.5, 50.6, 68.3, 72.6, 169.9; rotamer B –1.7, 21.8 41.1, 47.1, 61.4, 72.3, 170.2.

A solution of alcohol **F** (3.10 g, 14.40 mmol), triethylamine (2.01 ml, 14.4 mmol) and methanesulfonylchloride (1.12 mL, 14.4 mmol) in 150 mL MeCN was stirred for 3h at 0 °C, diluted with water and extracted with diethylether. The extracts were dried and concentrated *in vacuo* to afford residue which was subjected to column chromatography (silica gel. 5:1 EA-hexane) yielding 3.31 g (73% of **9**. ^{1}H-NMR (1:2 mixture of two rotamers) rotamer A 0.03 (s, 9H)$_3$), 2.22 (s, 3H), 2.87 (s, 2H), 3.00 (s 3H), 3.48-3.68 (m, 6H), 4.28 (t, 2H, J=4.0Hz,); rotamer B 0.07 (s, 9H), 2.21 (s, 3H), 2.82 (s, 2H), 3.00 (s 3H), 3.48-3.68 (m, 6H), 4.28 (t, 2H, J=4.0Hz); ^{13}C-NMR rotamer A –1.6, 21.9, 37.5, 38.4, 50.6, 68.6 69.0, 169.8; rotamer B –1.6, 21.9, 41.5, 47.1, 68.4, 68.6, 68.8, 170.1.

Methansulfonate 10. A solution of NaI (2.50 g, 16.7mmol), methansulfonate **8** (1.93 g , 5.5 mmol) in 40 mL of acetone was stirred for 5 h at 60 °C. diluted with water and extracted with $CHCl_3$. Th extracts were dried and concentrated *in vacuo* to afford a residue which was subjected to colum chromatography (silica gel, 1:30 EA-hexane) yielding 1.21 g (58%) of **D**. ^{1}H NMR 0.12 (s, 9H), 2.77 (s 2H), 2.88 (s, 3H), 3.24 (t, 2H, J=6.0Hz), 3.45 (t, 2H, J=6.0Hz), 3.64 (t, 2H, J=6.0Hz), 3.73 (t, 2H J=6.0Hz); ^{13}C-NMR -2.2, 2.4, 36.3, 37.8, 48.6, 67.6, 71.3.

To a solution of ethylene glycol (30 mL) was added Na (0.5 g, 22.7g-at) portionwise over a 12 period with stirring. To this solution was added iodide **D** (1.97 g, 5.25 mmol) in 10 mL THF. Afte stirring for 10 h at 80 °C, the solution was diluted with water and extracted with CH_2Cl_2. The extract were dried and concentrated *in vacuo* to afford a residue which was subjected to column chromatograph (silica gel. 2:1 EA-dichloromethane) yielding 2.94 g (56%) of alcohol **I**. ^{1}H-NMR 0.12 (s, 9H), 2.73 (s 2H), 2.87 (s, 3H), 3.43 (t, 2H, J=6.0Hz), 3.55-3.74 (m, 10H); ^{13}C-NMR -1.7, 36.0, 38.0, 48.9, 61.8, 68.2 70.3 and 70.4, 72.4; MS (CI) m/z (rel. intensity) 314 (0.3), 234 (32), 194 (31); HRMS (CI) m/z 314.146 ($C_{11}H_{28}NO_5SSi$ requires 314.1458).

A solution of alcohol **I** (2.7 g, 8.61 mmol),, triethylamine (1.44 mL, 10.33 mmol) an methanesulfonylchloride (0.67 mL, 8.61 mmol) in 90 mL MeCN was stirred for 3h at 0 °C. diluted wit water and extracted with CH_2Cl_2. The extracts were dried and concentrated *in vacuo* to afford residue which was subjected to column chromatography (silica gel. 5:1 EA-hexane) yielding 1.40 g (43%) of **10** ^{1}H-NMR 0.12 (s, 9H), 2.73 (s, 2H), 2.87 (s, 3H), 3.05 (s, 3H), 3.43 (t, 2H, J=5.4Hz), 3.59-3.63 (m, 6H) 3.74(t, 2H, J=4.6Hz), 4.35(t, 2H, J=4.0Hz); ^{13}C-NMR -1.7, 35.9, 37.6, 37.8, 48.9, 68.0, 68.9, 70.1, 70.5 MS (FAB) m/z (rel. intensity) 392 (90), 376(28), 314 (27), 208 (100), 137(21); HRMS (FAB) m/ 392.1237 ($C_{12}H_{30}NO_7S_2Si$ requires 392.1233).

Iodide 12. A solution of 2-(2-aminoethoxy)ethanol (13.60 mL, 135.0 mmol) anc ethylbromoacetate (5.0 mL, 45.0 mmol) in 60 mL MeCN was stirred for 3h at 60 °C, diluted with wate and extracted with CH_2Cl_2. The extracts were dried and concentrated *in vacuo* to afford a residue whicl was subjected to column chromatography (silica gel, 1:5 EA-MeOH) yielding 2.84 g (52%) of alcohol **G** ^{1}H-NMR 1.17 (t, 3H, J=7.2Hz), 2.82 (t, 2H, J=5.0Hz), 3.42 (s, 2H), 3.55-3.60(m, 4H), 3.72 (t, 2H J=4.8Hz), 4.18(q, 2H, J=7.2Hz,); ^{13}C-NMR 14.0, 48.5, 50.4, 60.5, 61.3, 70.0 and 72.3, 172.1.

A solution of **G** (2.84 g, 14.85 mmol), triethylamine (8.28 mL, 59.4 mmol) anc methanesulfonylchloride (4.60 mL, 59.4 mmol) in 150 mL MeCN was stirred for 4h at 0 °C, diluted witl water and extracted with diethylether. He extracts were dried and concentrated *in vacuo* to afford a residue which was subjected to column chromatography (silica gel,EA-hexane) yielding 1.50 g (29%) o the **H**. ^{13}C-NMR 13.9, 37.3, 39.6, 47.4, 49.2, 60.5, 61.3 , 68.3 and 78.3, 169.7.

A solution of NaI (0.87 g, 5.76 mmol and **H** (1.0 g, 2.88 mmol) in 50 mL acetone was stirred fo 5h at 60 °C, diluted with water and extracted with $CHCl_3$. The extracts were dried and concentrated *i vacuo* to afford a residue which was subjected to column chromatography (silica gel. 1:30 EA-hexane yielding 89 g (68%) of **12**. ^{1}H-NMR 1.23 (t, 3H, J=7.1Hz), 3.02 (s, 2H), 3.22 (t, 2H, J=6.6Hz), 3.45 (t 2H, J=4.8Hz), 3.50-3.72 (m, 4H), 4.17-4.27(m, 4H); ^{13}C-NMR 2.1, 14.0, 39.8, 48.1, 49.8, 48.5, 50.4 61.7, 70.8 and 71.3, 172.1.

Alcohol 13. A solution of 2-(methylamino)ethanol (0.96 mL, 12 mmol) and iodide **B***** (3.9 g 12 mmol) in 60 mL MeCN was stirred for 8h at 60 °C, diluted with water and extracted with CH_2Cl_2. Th extracts were dried and concentrated in vacuo to afford a residue which was subjected to colum chromatography (silica gel, 1:5 MeOH-EA) yielding 2.55 g (75%) of **13**. ^{1}H-NMR 1.26 (t, 3H, J=7Hz) 2.27 (s, 3H), 2.56 (t, 2H, J=5Hz), 2.65 (t, 2H, J=6.6Hz), 3.00 (s, 3H), 3.38 (t, 2H, J=6.6Hz), 3.59 (t, 2H J=5.2Hz), 4.14 (s, 2H), 4.15 (q, 2H, J=7.2Hz); ^{13}C-NMR 14.1, 39.7, 41.7, 45.6, 48.8, 56.4, 58.5, 59.4

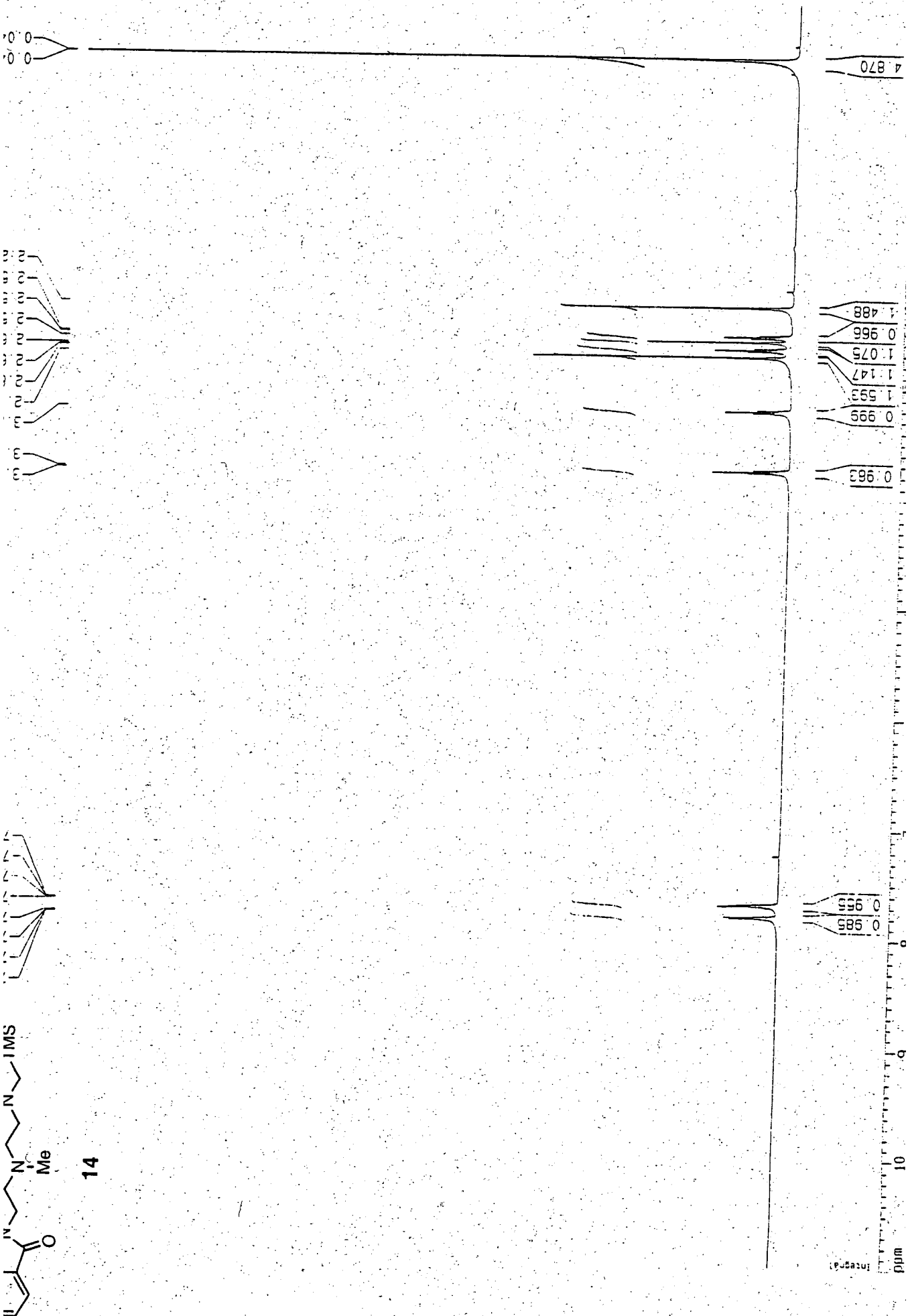
61.6; MS (FAB) m/z(rel. intensity) 283(100), 281 (24), 154 (41), 136(24); HRMS (FAB) m/z 283.133(($C_{10}H_{23}O_5N_2S_1$, requires 283.1328).

Hydroxyester I. To a 0 °C solution of 2-aminoethanol (2.00 g, 32.8 mmol) and K_2CO_3 (22.60 g 164 mmol) in 80 mL of acetonitrile was added a solution of ethyl bromoacetate (5.84 g, 32.8 mmol) in 2(mL of acetonitrile over a 1 h period. The solution was stirred for 1h at 0 °C and filtered. The fitrate wa concentrated *in vacuo* to give a residue which was subjected to column chromatography (silica gel. 1:: Methanol-ethyl acetate) to give **I** 2.07 (43%). ^{1}H-NMR 1.13 (t, 3H, J=7.2Hz), 2.61 (t, 2H, J=5.2Hz), 3.0' (s, 1H), 3.28 (s, 2H), 3.50 (t, 2H, J=5.2Hz), 4.04 (q, 2H, J=7.2Hz); ^{13}C-NMR 13.9, 50.3, 50.9, 60.5, 60.6 172.2; MS (EI), m/z (rel. intensity) 74 (M^+ -CO_2Et, 74), 73 (5), 57 (3), 56 (22); HRMS (EI), m/z 74.058: (M^+ -CO_2Et, C_3H_8NO requires 74.0606)

Bis-Mesylate J. A solution of **I** (5.14 g, 35 mmol), triethylamine (14.6 mL, 105 mmol) in) an(methanesulfonyl chloride (5.42 mL, 70 mmol) in 130 mL of MeCN was stirred for 1 h at roon temperature, diluted with water and extracted with CH_2Cl_2. The CH_2Cl_2 extracts were dried an(concentrated in *vacuo to* afford a residue which was subjected to column chromatography (silica gel chloroform) yielding 450 mg (46%) of **J**. ^{1}H-NMR 1.26 (t, 3H, J=7Hz), 3.02 (s, 3H), 3.03 (s, 3H), 3.59 (t 3H, J=5.2Hz), 4.16 (s, 2H), 4.18 (q, 2H, J=6.8Hz), 4.34 (t, 2H, J=5.4Hz); ^{13}C-NMR 14.1, 37.4, 40.0, 47.5 49.8, 61.8, 68.5, 169.5; MS(FAB), m/z (rel. intensity) 304(M^+, 20), 230(67), 208(100), 152(45), 136(29) 59(33), HRMS(FAB), m/z(rel. intensity) 304.0539 ($C_8H_{18}O_7N_1S_2$, requires 304.0525)

Iodoester 11. A solution of NaI (2.40 g, 16 mmol) and **J** (3.85 g, 13 mmol) in 10 mL acetone wa stirred for 8 h at 60 °C, diluted with water and extracted with CH_2Cl_2. The CH_2Cl_2 extracts were dried an(

concentrated *in vacuo* to afford a residue which was subjected to column chromatography (silica gel. 1: ethyl acetate-hexane) yielding 4.0 g (92%) of **11** (2.40 g, 16 mmol). ^{1}H-NMR ($CDCl_3$) 1.28 (t, 3H, J=7) 3.01(s, 3H), 3.27 (t, 2H, J=6.2Hz), 3.59 (t, 2H, J=8Hz), 4.14 (s, 2H), 4.20 (q, 2H, J=6.8Hz); ^{13}C-NMR 1.4 13.9, 39.6, 48.7, 50.6, 61.5, 169.1; MS(FAB), m/z(rel. intensity) 336(M^+, 100), 262(58), 208(40) 154(87), 136(75), 107(25), 89(35), 77(53), 45(40), 39(30), HRMS(FAB), m/z (rel. intensity) 335.976 ($C_7H_{15}O_4N_1S_1I$, requires 335.9767)



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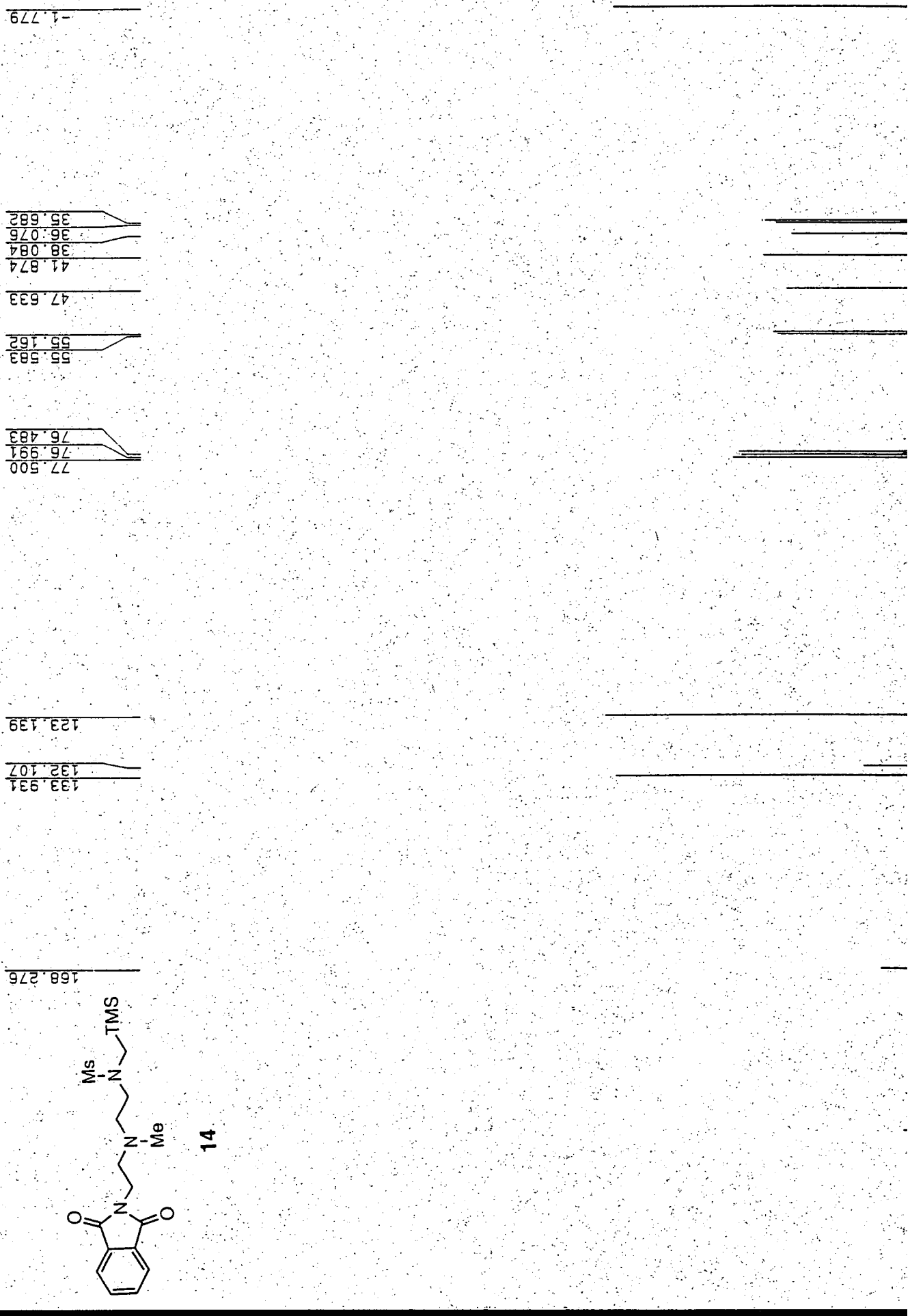

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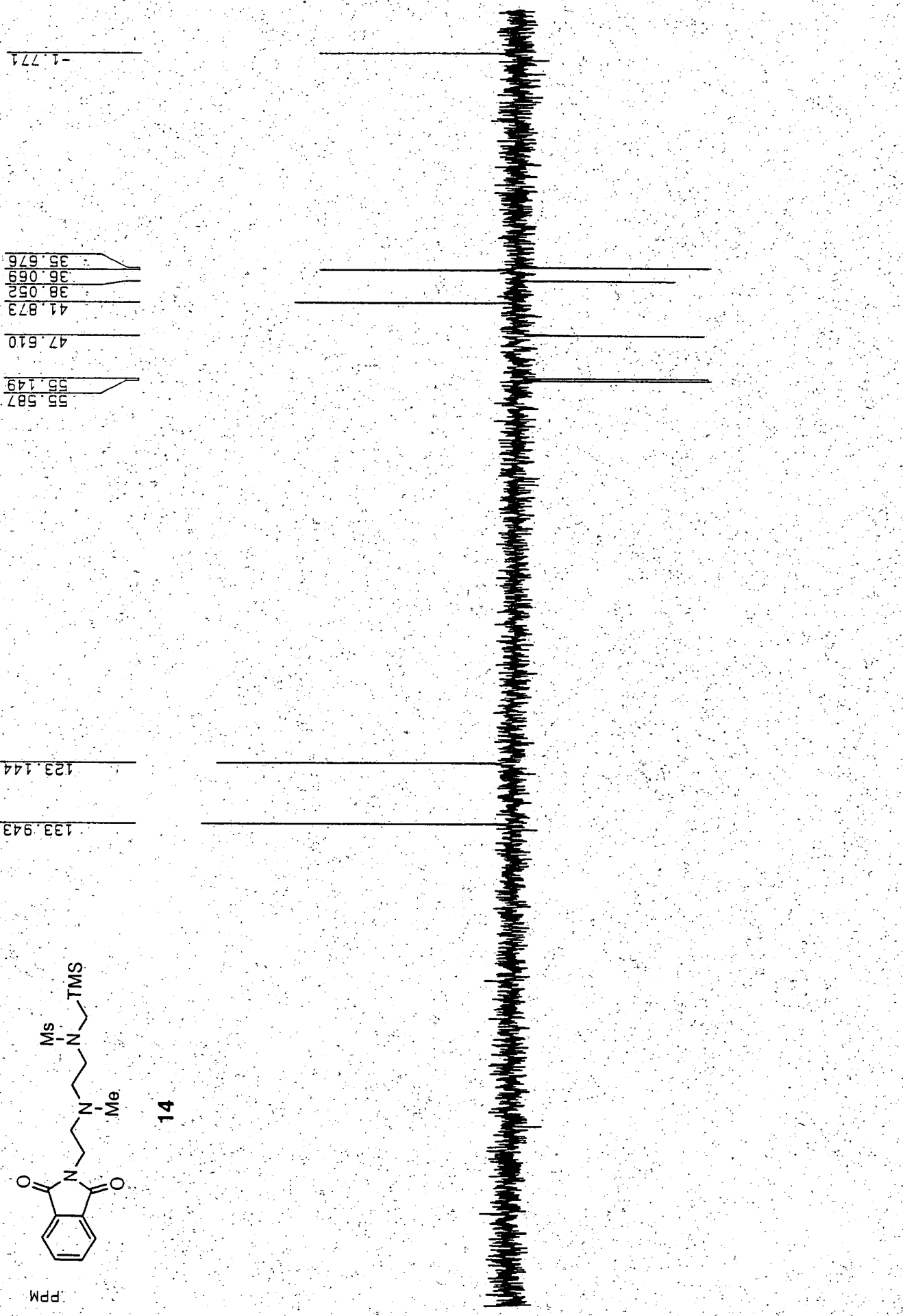

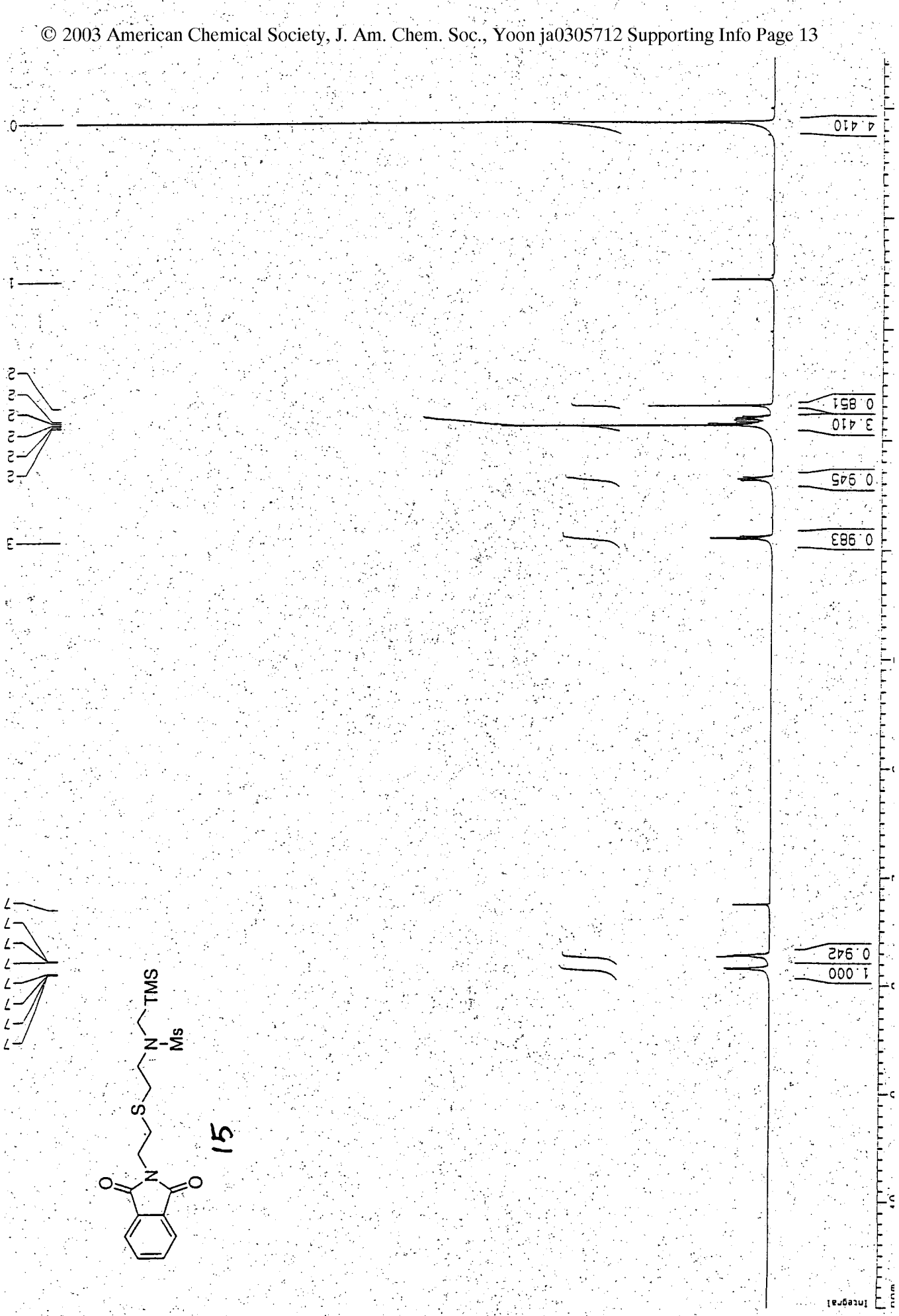

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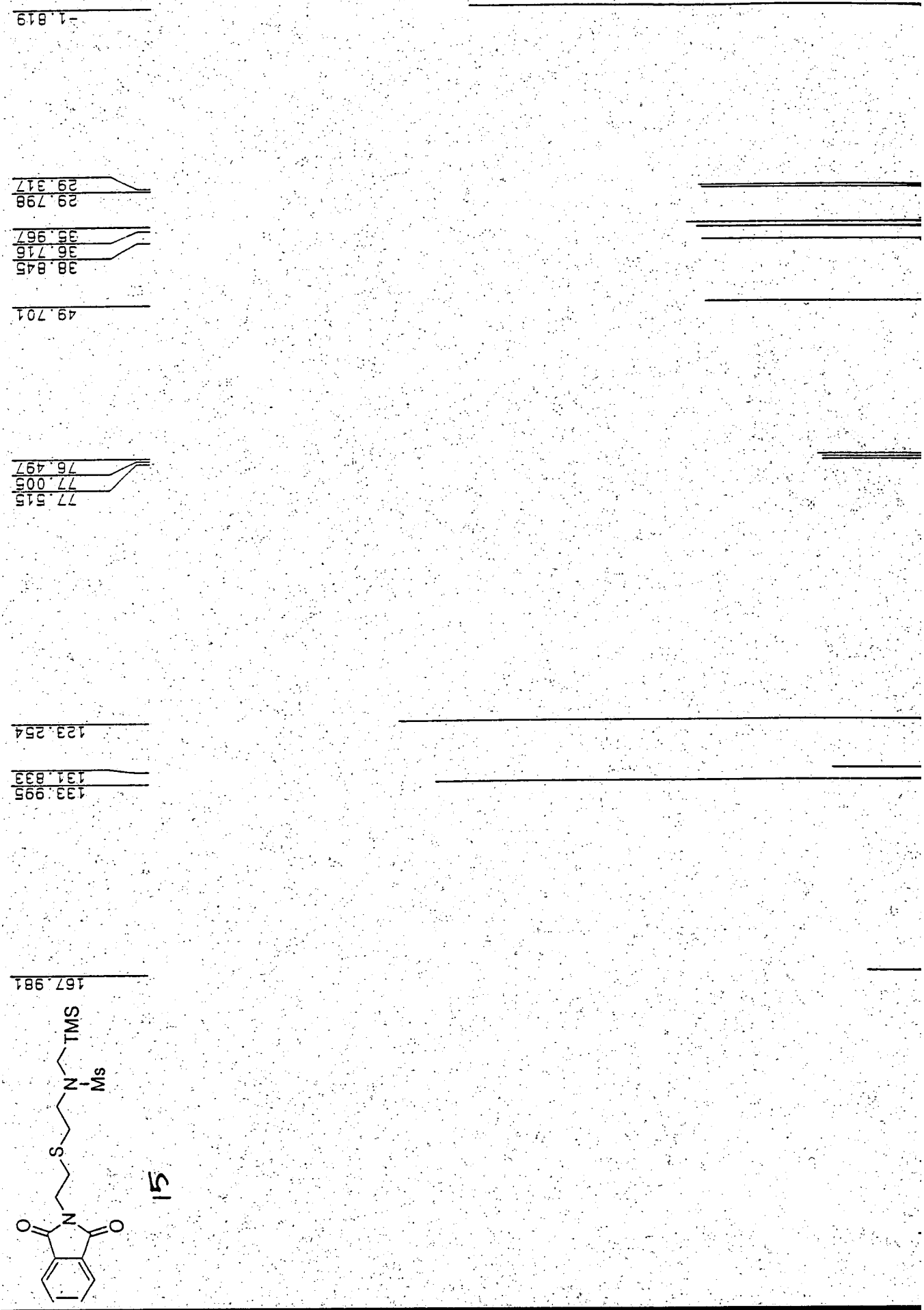

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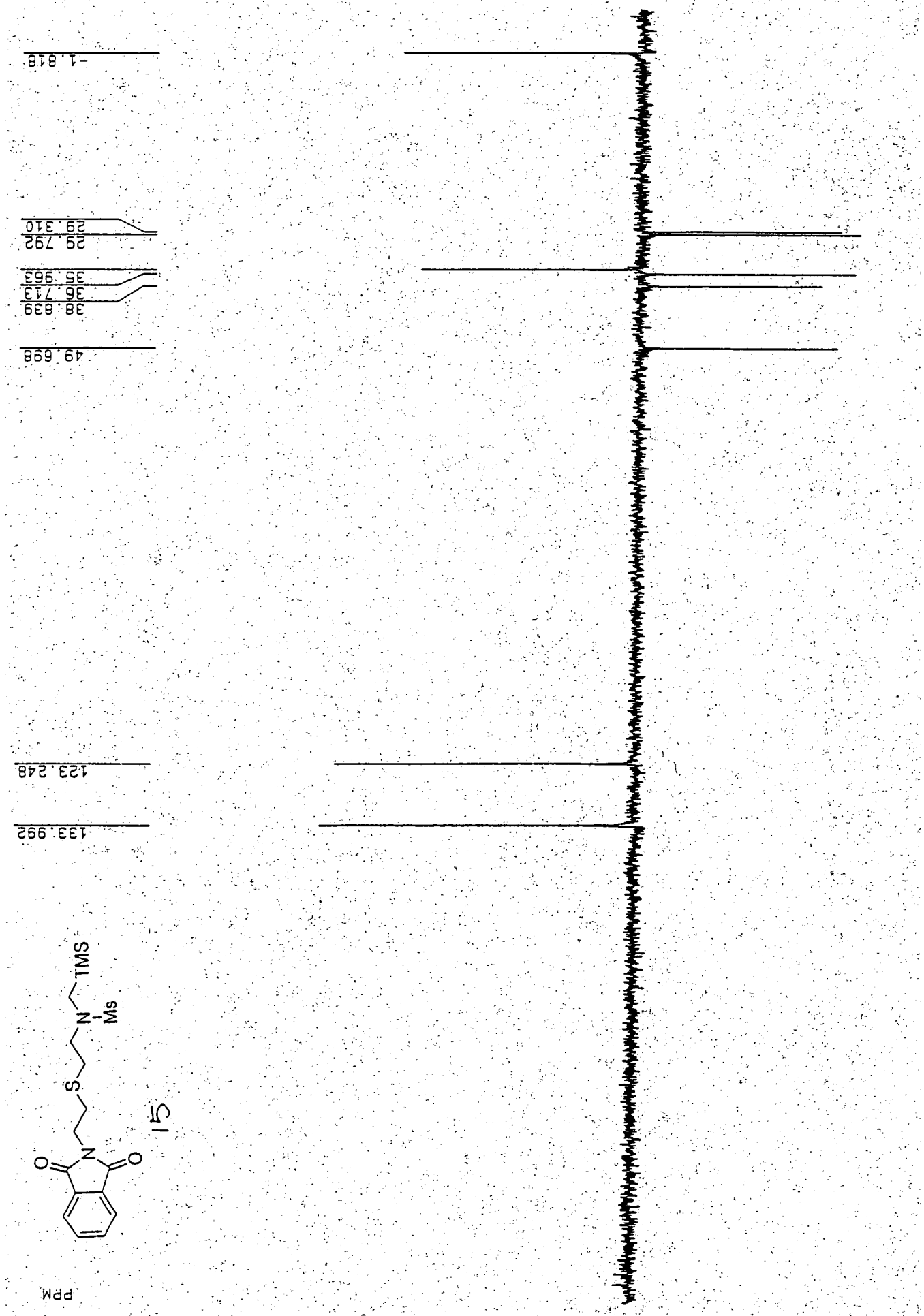

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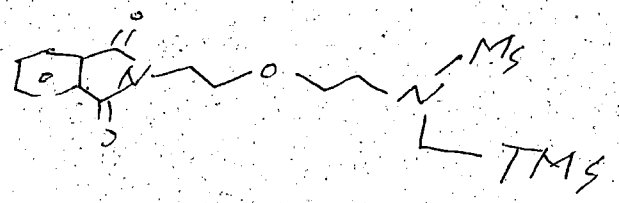

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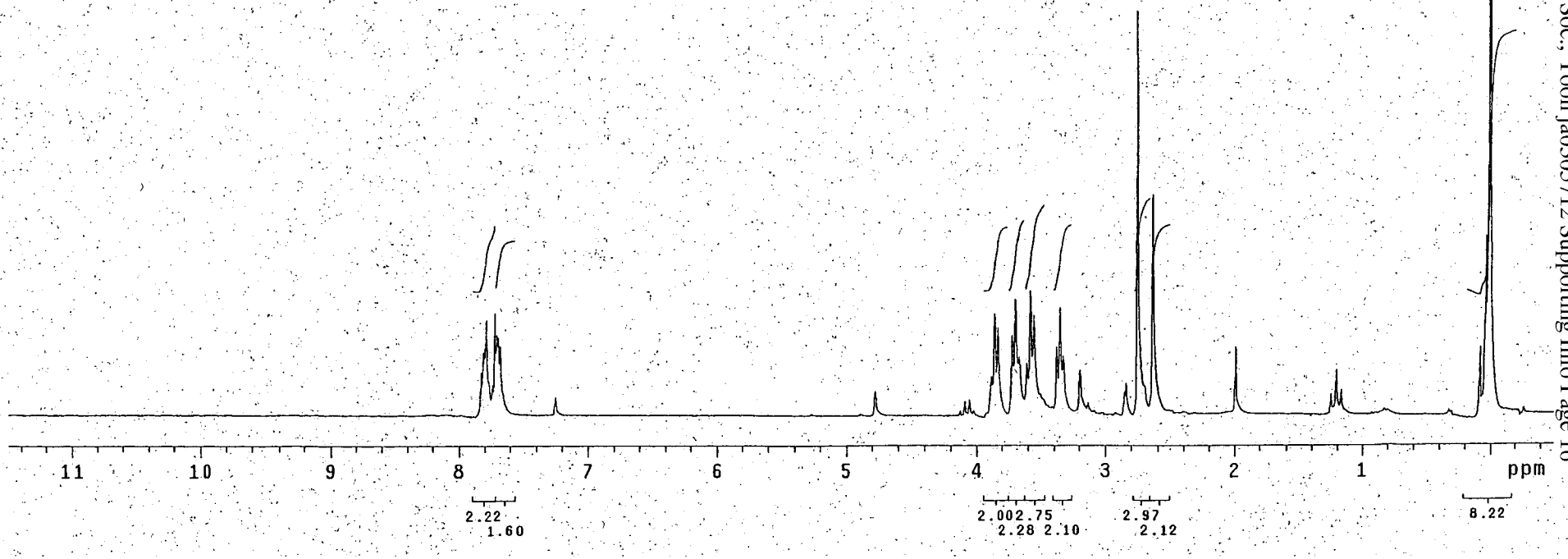

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WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
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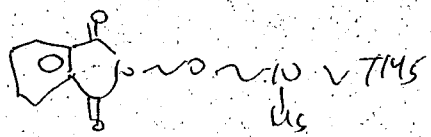
Total time 8 minutes

16



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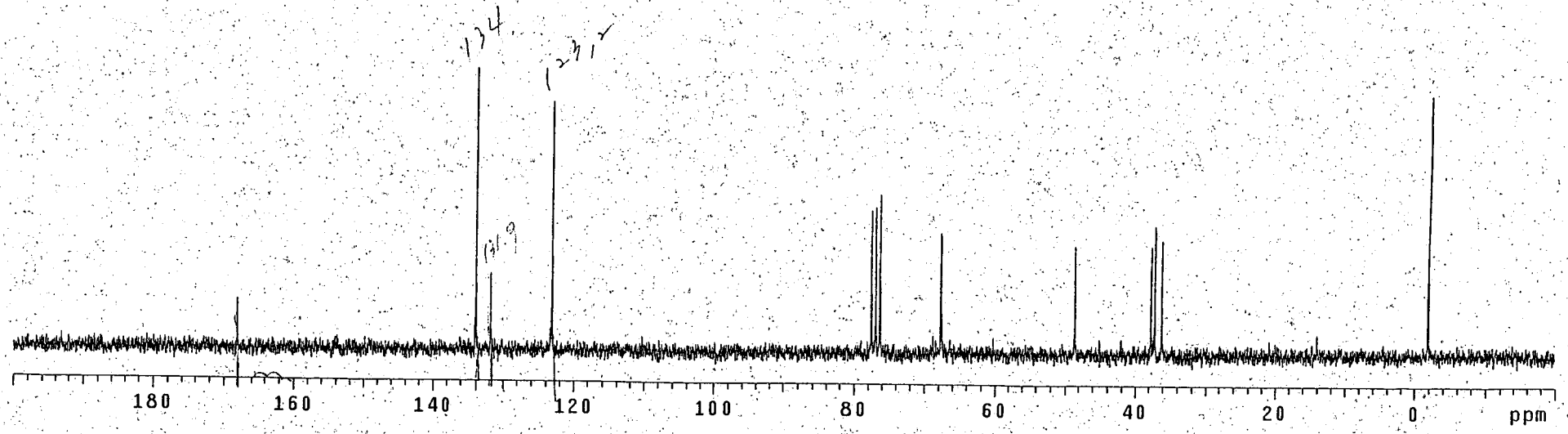
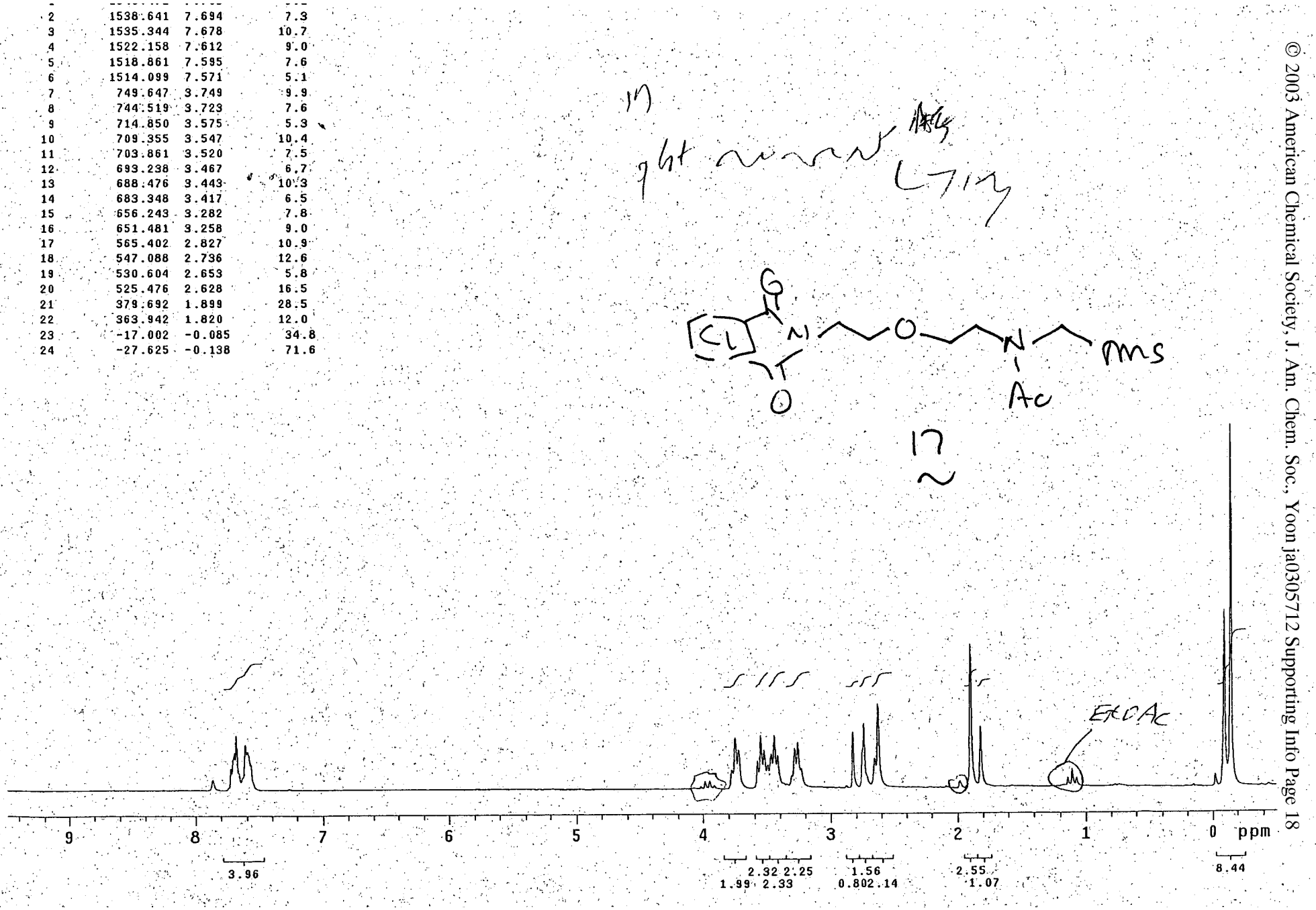


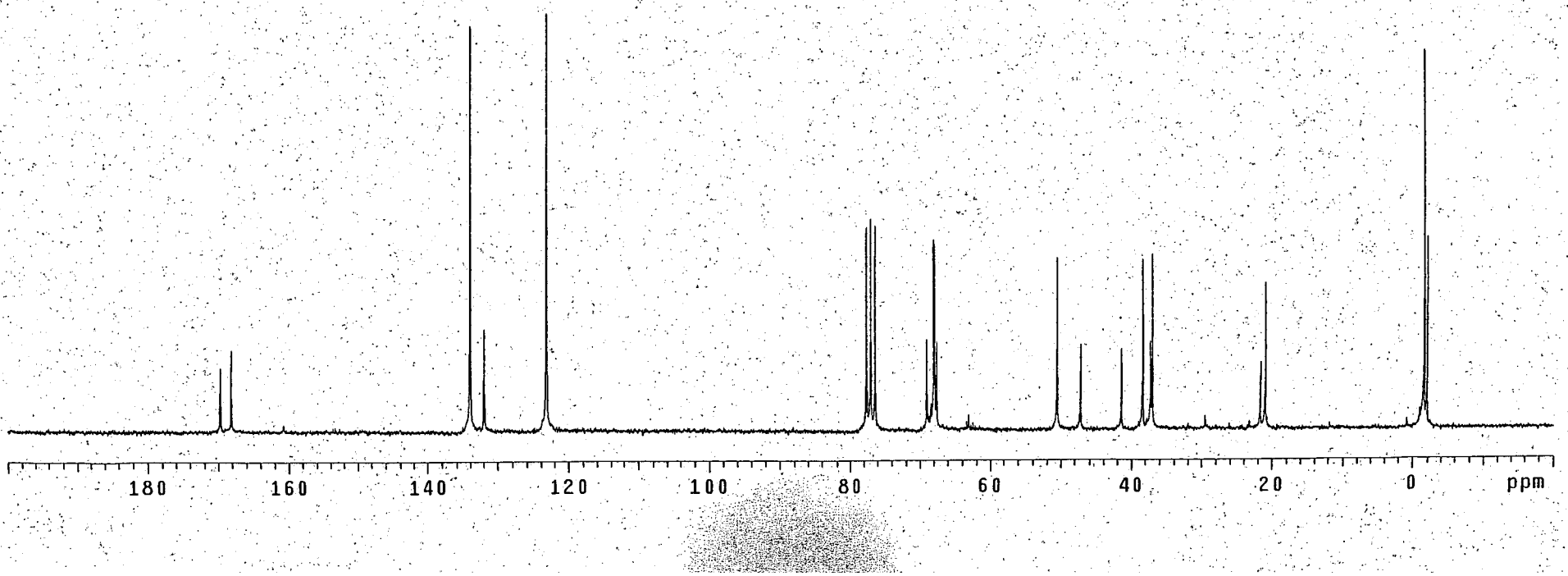
2	1538.641	7.694	7.3
3	1535.344	7.678	10.7
4	1522.158	7.612	9.0
5	1518.861	7.595	7.6
6	1514.099	7.571	5.1
7	749.647	3.749	9.9
8	744.519	3.723	7.6
9	714.850	3.575	5.3
10	709.355	3.547	10.4
11	703.861	3.520	7.5
12	693.238	3.467	6.7
13	688.476	3.443	10.3
14	683.348	3.417	6.5
15	656.243	3.282	7.8
16	651.481	3.258	9.0
17	565.402	2.827	10.9
18	547.088	2.736	12.6
19	530.604	2.653	5.8
20	525.476	2.628	16.5
21	379.692	1.899	28.5
22	363.942	1.820	12.0
23	-17.002	-0.085	34.8
24	-27.625	-0.138	71.6



Ambient temperature
GEMINI-200 "PNU-chem"

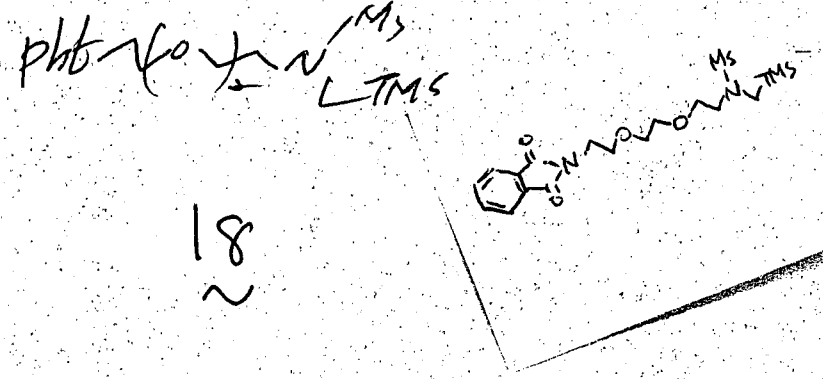
PULSE SEQUENCE
Relax. delay 2.000 sec
Pulse 83.1 degrees
Acq. time 1.497 sec
Width 14992.0 Hz
9724 repetitions
OBSERVE C13, 50.2837695 MHz
DECOUPLE H1, 199.9753237 MHz
Power 30 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 65536
Total time 9.4 hours

17



2	1563.423	7.818	8.9
3	1560.859	7.805	10.0
4	1558.295	7.792	11.8
5	1542.178	7.712	12.7
6	1539.248	7.697	10.9
7	1537.050	7.686	10.0
8	1534.120	7.672	7.8
9	768.935	3.845	13.2
10	763.441	3.818	9.7
11	739.266	3.697	10.6
12	733.771	3.669	14.1
13	728.277	3.642	8.3
14	713.259	3.567	23.5
15	707.765	3.539	26.9
16	702.636	3.514	18.2
17	679.560	3.398	9.8
18	674.432	3.373	12.3
19	564.178	2.821	40.9
20	533.776	2.669	24.4
21	401.544	2.008	25.6
22	250.632	1.253	7.3
23	243.672	1.219	14.1
24	236.346	1.182	7.7
25	13.641	0.068	100.0

10



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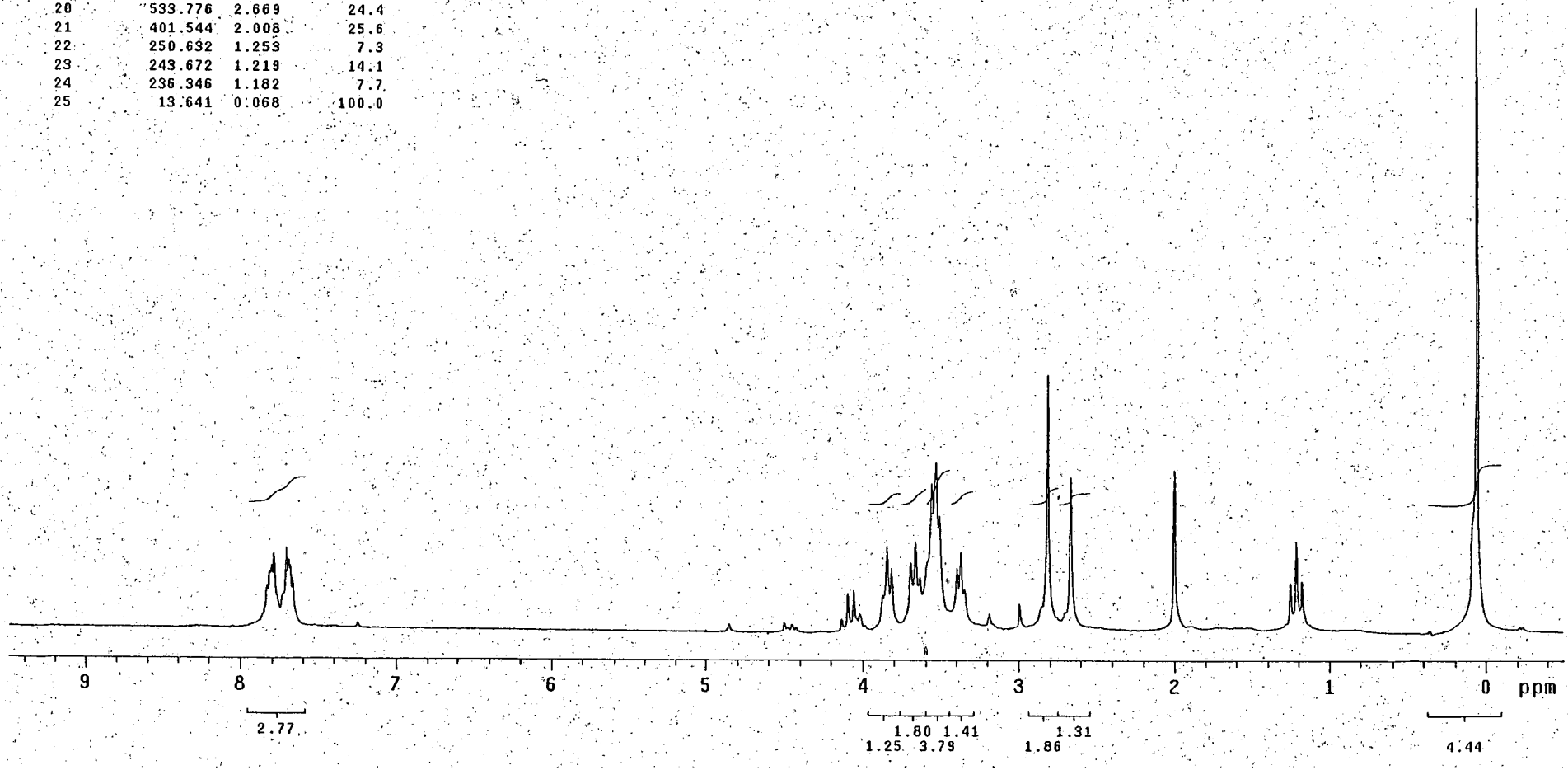
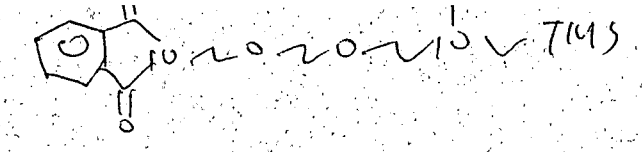


2	6752.321	134.274	10.3
3	6742.256	134.074	29.0
4	6737.680	133.983	26.0
5	6639.311	132.027	6.5
6	6635.650	131.954	5.9
7	6212.889	123.547	9.2
8	6198.706	123.265	39.6
9	3904.175	77.637	79.6
10	3872.148	77.000	81.2
11	3840.121	76.363	78.3
12	3529.913	70.194	12.8
13	3519.847	69.994	12.7
14	3414.157	67.893	29.8
15	3407.752	67.765	13.6
16	2449.219	48.704	19.0
17	1906.127	37.904	10.2
18	1883.708	37.459	11.1
19	1877.302	37.331	13.7
20	1871.354	37.213	12.5
21	1828.346	36.358	13.0
22	1820.568	36.203	12.3
23	-85.974	-1.710	32.4
24	-89.177	-1.773	28.1



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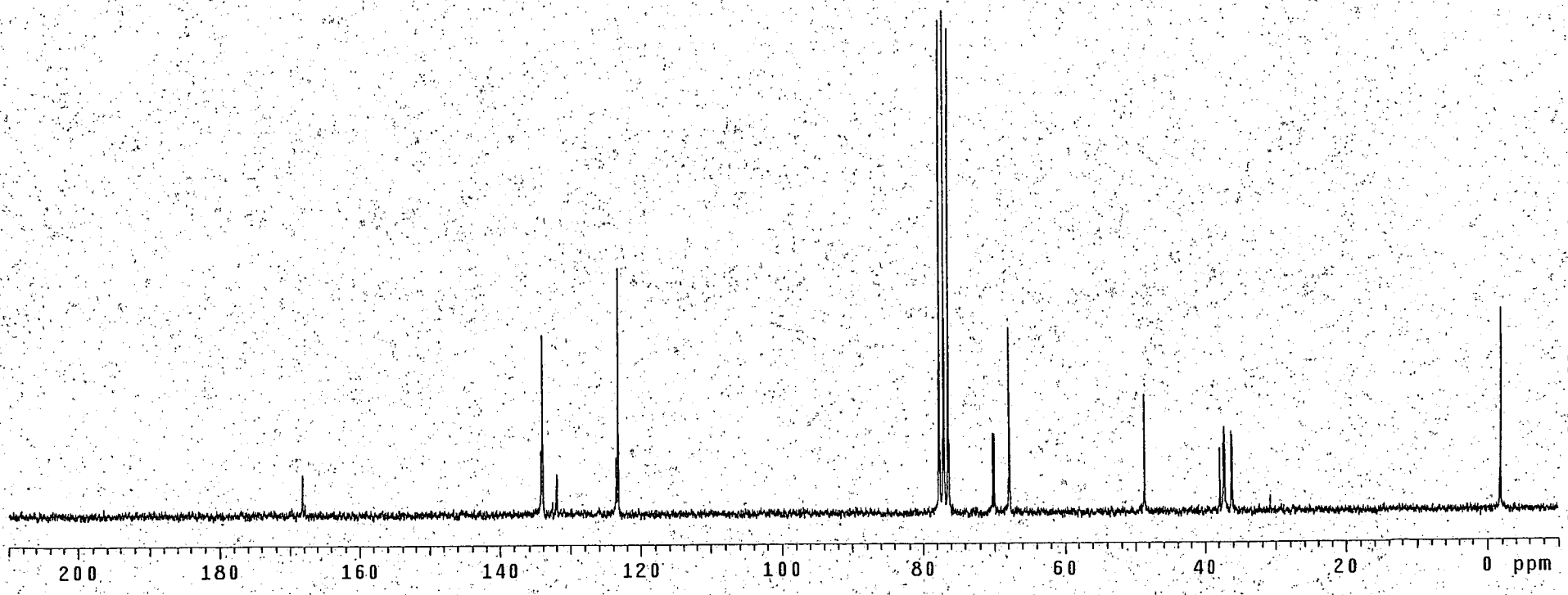
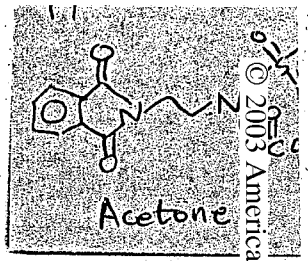
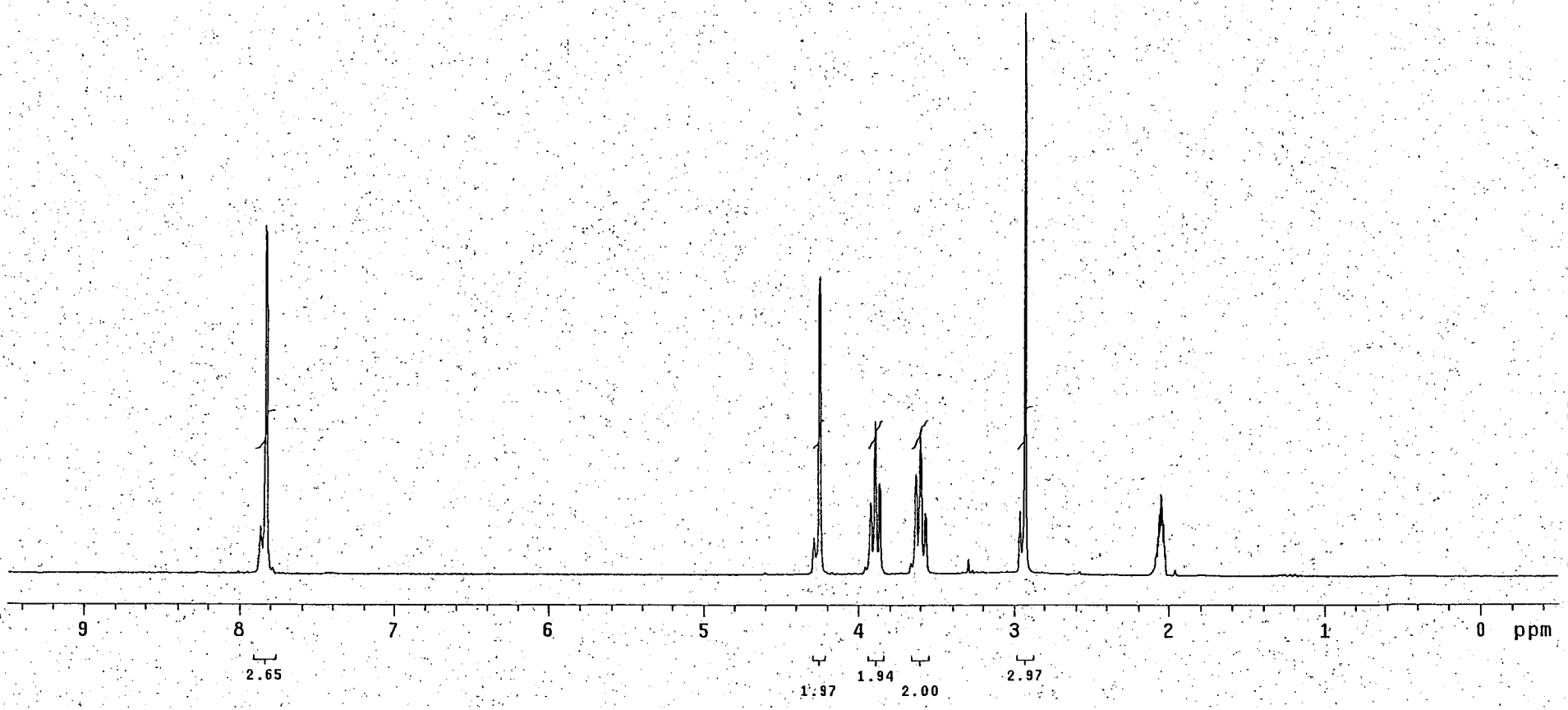


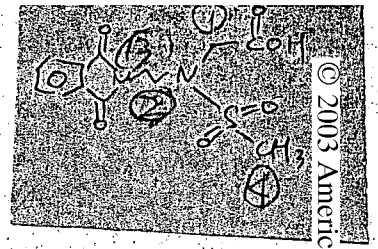
1	1565.367	7.831	55.9
2	1564.888	7.825	55.0
3	850.619	4.254	47.5
4	849.886	4.250	47.8
5	784.686	3.924	11.2
6	783.953	3.920	11.3
7	779.558	3.898	20.9
8	778.459	3.893	24.5
9	776.994	3.885	10.0
10	773.331	3.867	14.3
11	772.598	3.863	14.4
12	725.347	3.627	16.0
13	719.852	3.600	22.1
14	713.991	3.570	9.8
15	592.382	2.962	10.0
16	586.155	2.931	90.3
17	585.057	2.926	87.3
18	411.800	2.059	9.5
19	409.603	2.048	12.6
20	408.137	2.041	12.2



19



1	10215.703	203.154	16.6
2	10195.120	202.744	723.9
3	10174.988	202.344	11.1
4	8438.191	167.805	8.8
5	8315.115	165.358	7.0
6	6607.600	131.401	65.3
7	6531.192	129.882	11.5
8	6047.121	120.255	64.7
9	2230.377	44.354	15.8
10	2141.615	42.589	26.6
11	1820.427	36.202	27.4
12	1631.923	32.453	28.2
13	1385.770	27.558	84.4
14	1366.554	27.176	251.5
15	1346.880	26.785	477.3
16	1327.663	26.402	587.5
17	1308.447	26.020	502.2
18	1289.230	25.638	242.7
19	1269.557	25.247	83.2



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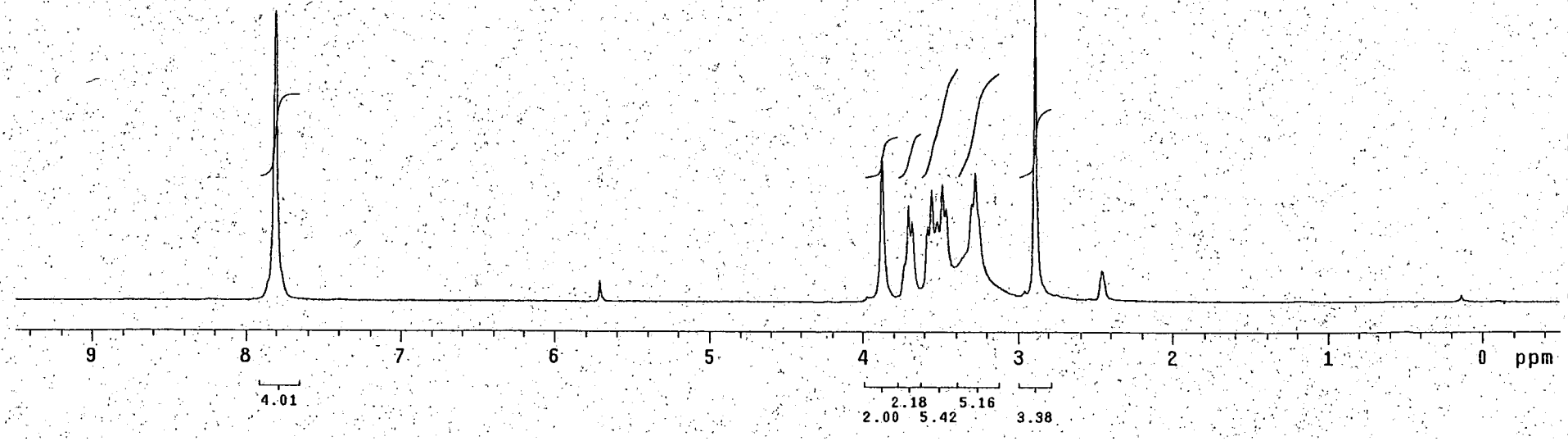
Solvent: DMSO
Ambient temperature
GEMINI-200 "PNU-chem"

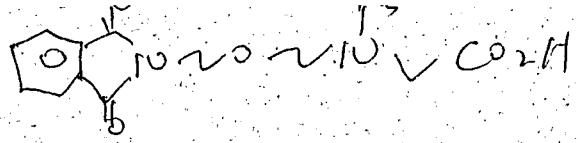
PULSE SEQUENCE
Relax. delay 1.000 sec
Pulse 62.1 degrees
Acq. time 1.994 sec
Width 3000.3 Hz
44 repetitions
OBSERVE H1, 199.9760237 MHz
DATA PROCESSING
FT size 16384
Total time 2 minutes

Pure

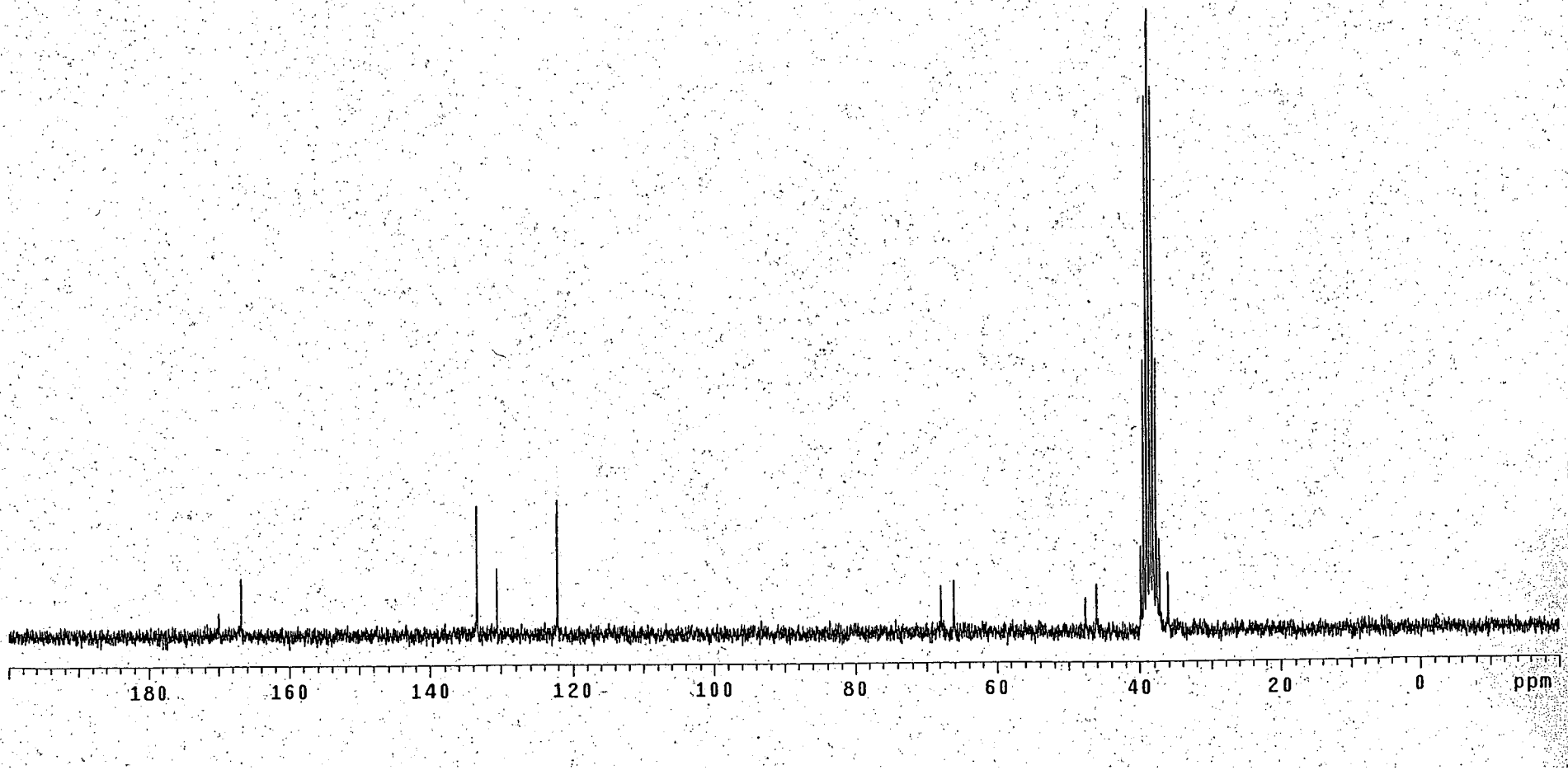
20



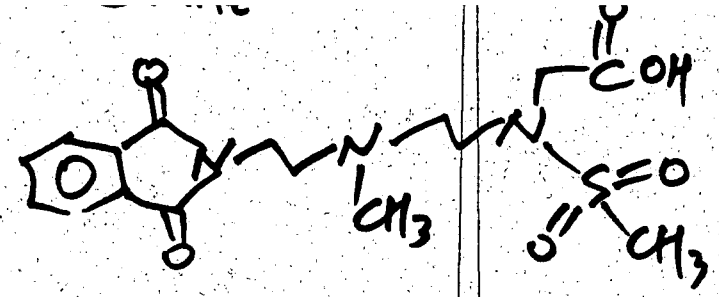
1	8545.697	169.942	3.5
2	8386.018	166.766	9.0
3	6708.700	133.411	20.5
4	6562.289	130.499	10.3
5	6136.325	122.028	21.3
6	3410.341	67.819	7.2
7	3325.240	66.126	8.1
8	2395.532	47.638	5.1
9	2317.751	46.091	7.4
10	1997.935	39.731	13.3
11	1976.888	39.313	43.4
12	1955.842	38.894	86.1
13	1934.795	38.476	100.1
14	1914.206	38.066	87.6
15	1892.702	37.639	43.7
16	1871.656	37.220	14.6
17	1815.379	36.101	9.1



20



5	608.133	3.041	24.2
6	604.470	3.023	19.5
7	564.178	2.821	19.5
8	558.317	2.792	15.4
9	491.652	2.459	8.9
10	406.306	2.032	20.6



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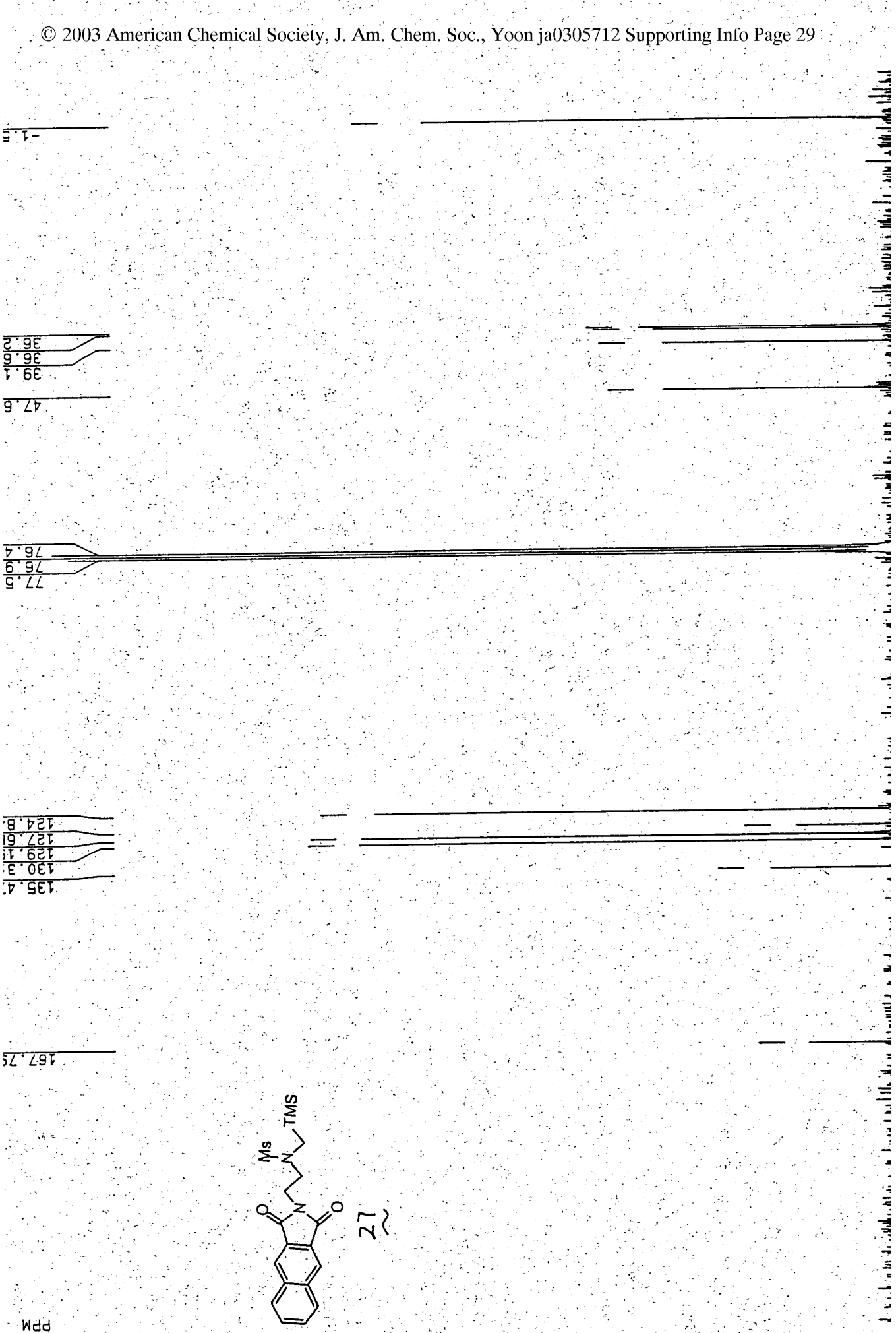

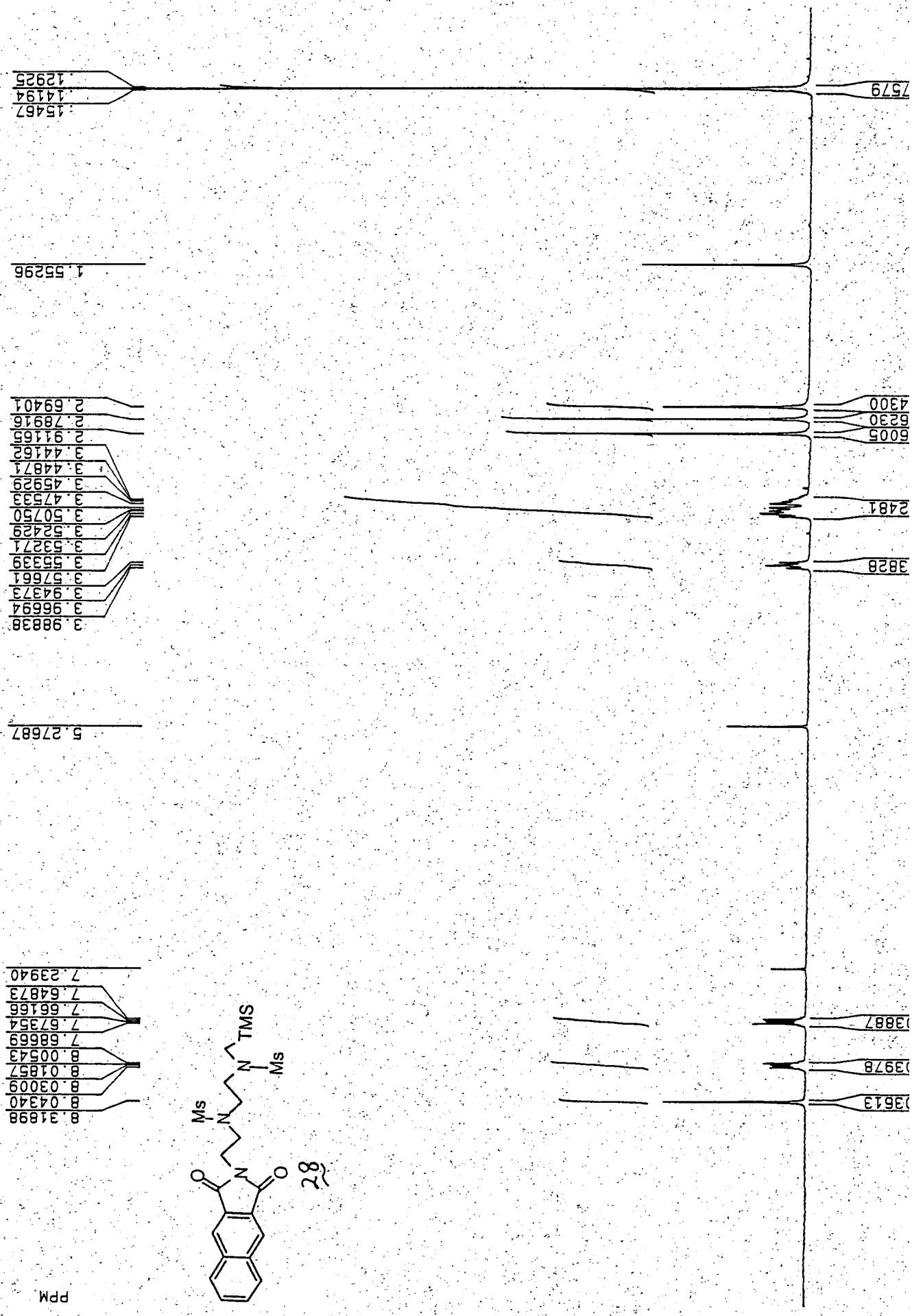

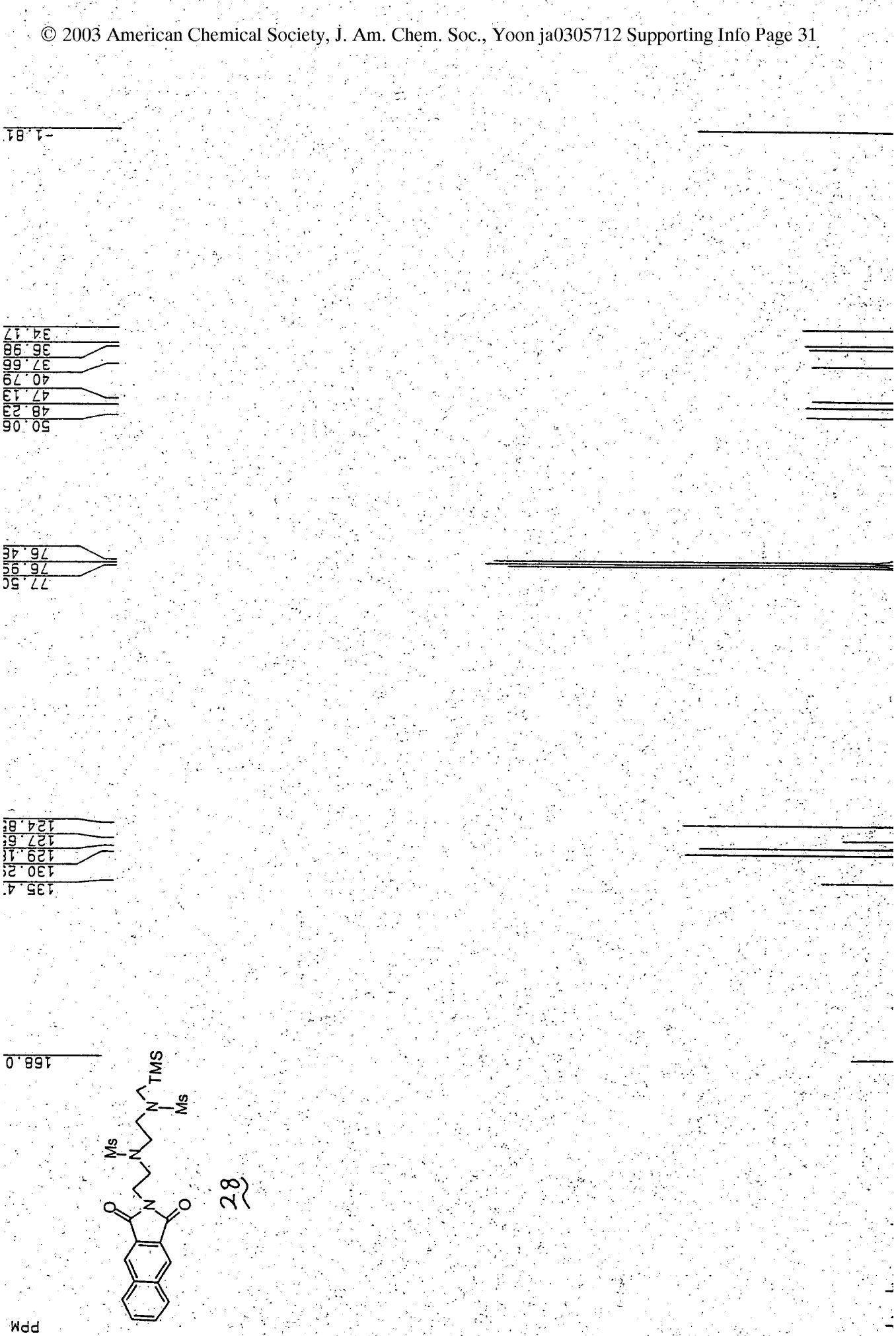

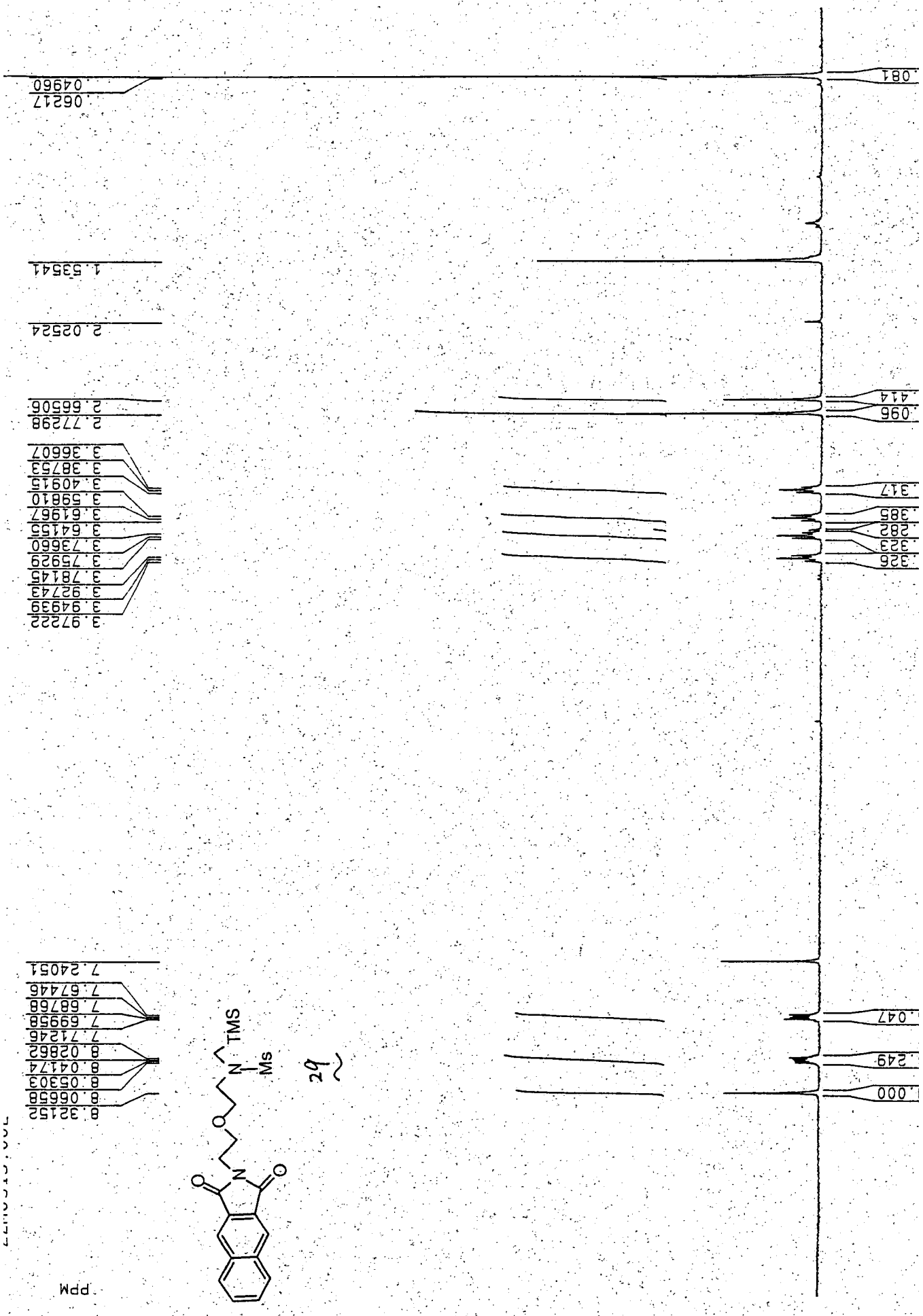

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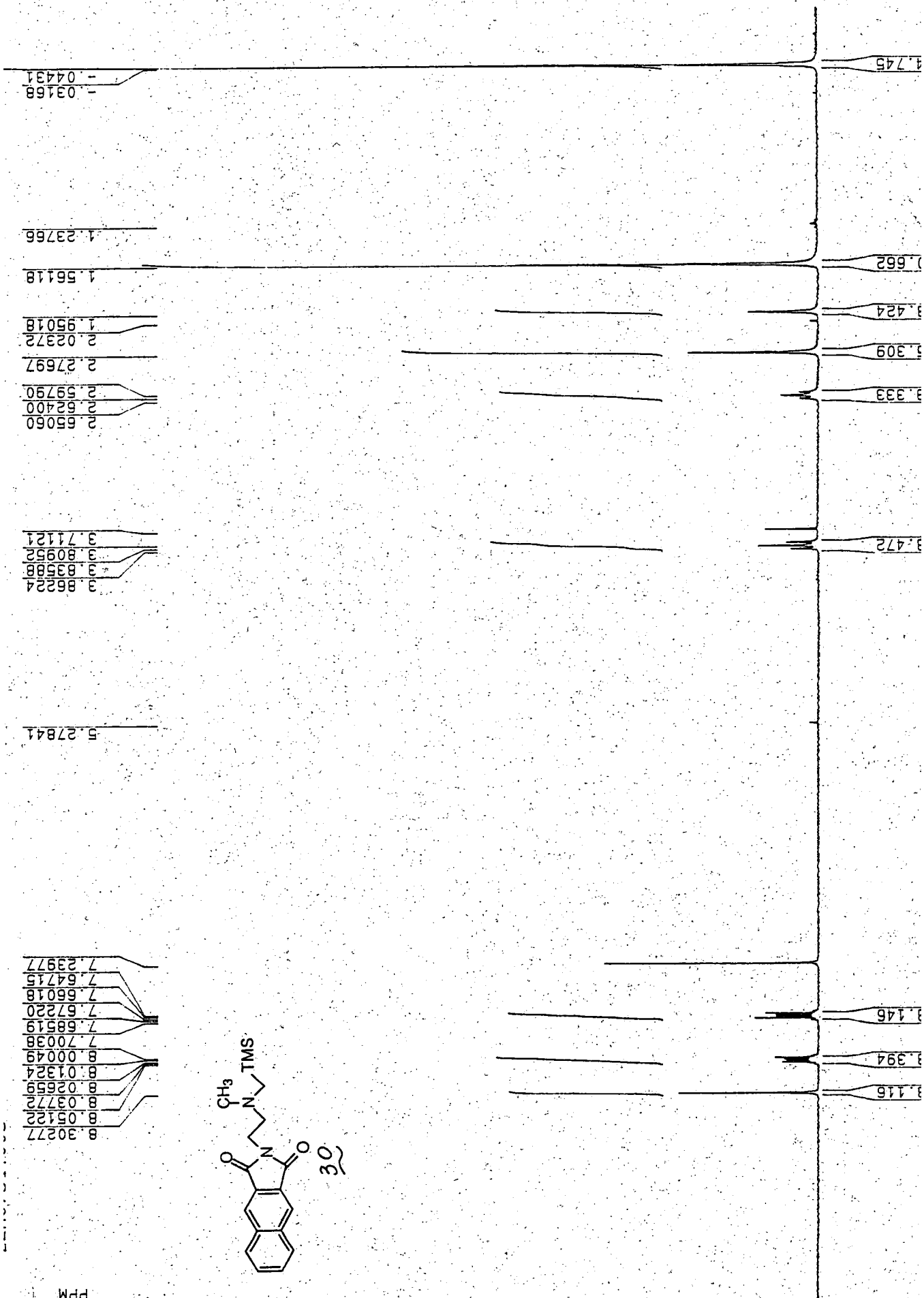
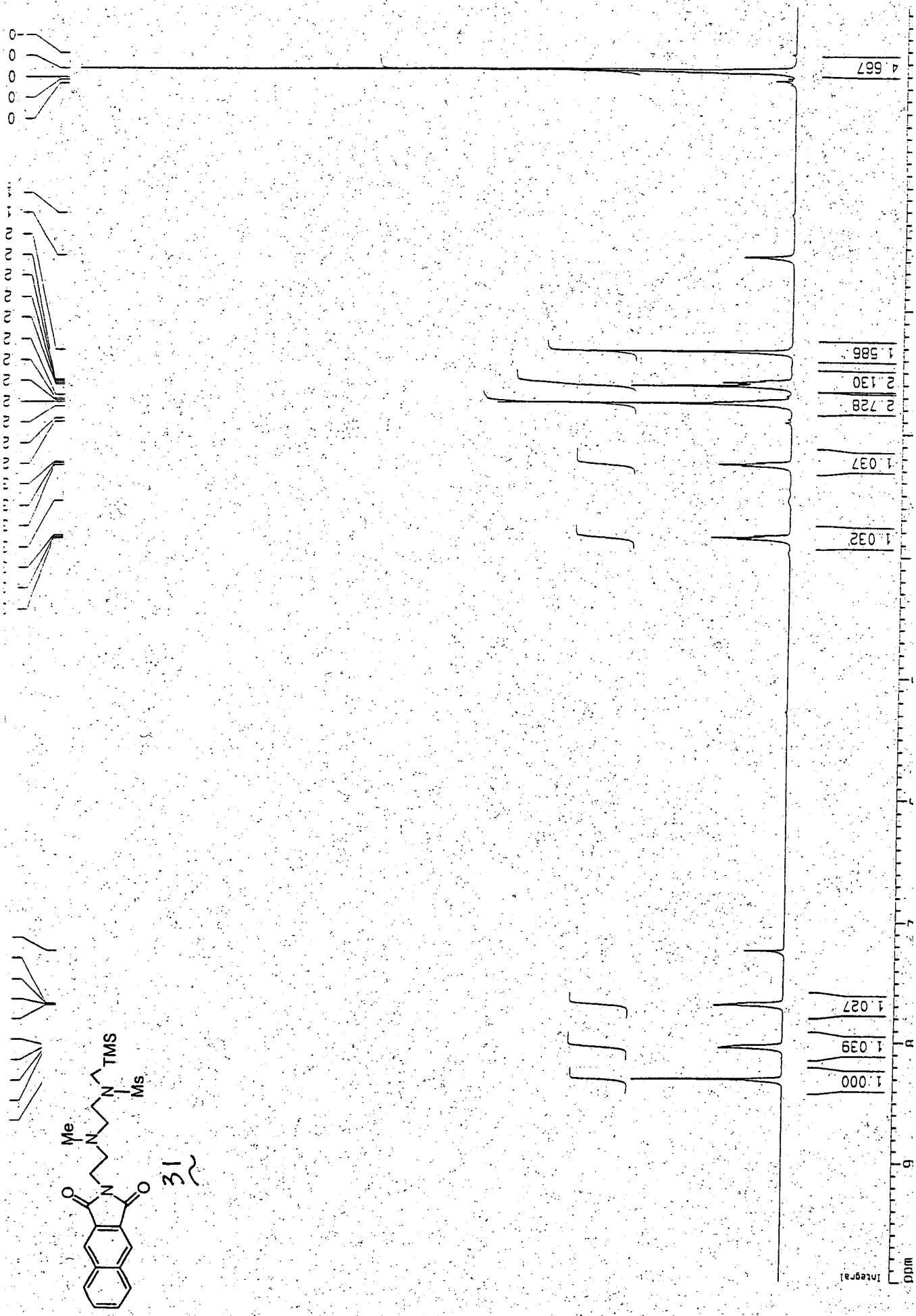
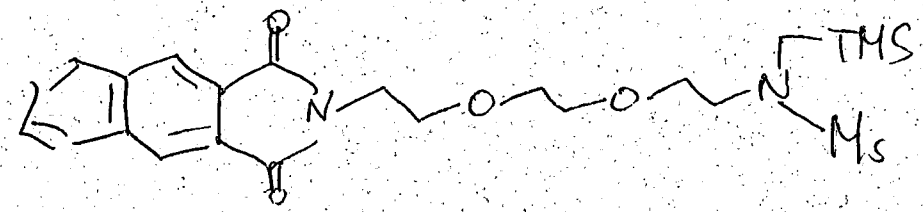




1	1637.154	8.187	34.2
2	1604.448	8.023	9.7
3	1601.518	8.009	9.6
4	1598.587	7.994	11.1
5	1537.050	7.686	14.1
6	1533.754	7.670	10.7
7	1530.823	7.655	10.6
8	1527.527	7.639	10.8
9	783.587	3.918	14.9
10	778.093	3.891	11.3
11	750.987	3.755	11.9
12	745.493	3.728	17.0
13	720.218	3.602	18.0
14	718.021	3.591	20.4
15	712.526	3.563	23.3
16	708.497	3.543	25.7
17	703.003	3.515	17.0
18	677.362	3.387	12.4
19	672.234	3.362	15.7
20	564.178	2.821	67.1
21	532.311	2.662	34.3
22	244.038	1.220	9.6
23	19.501	0.098	15.8
24	11.077	0.055	191.4
25	7.780	0.039	13.2



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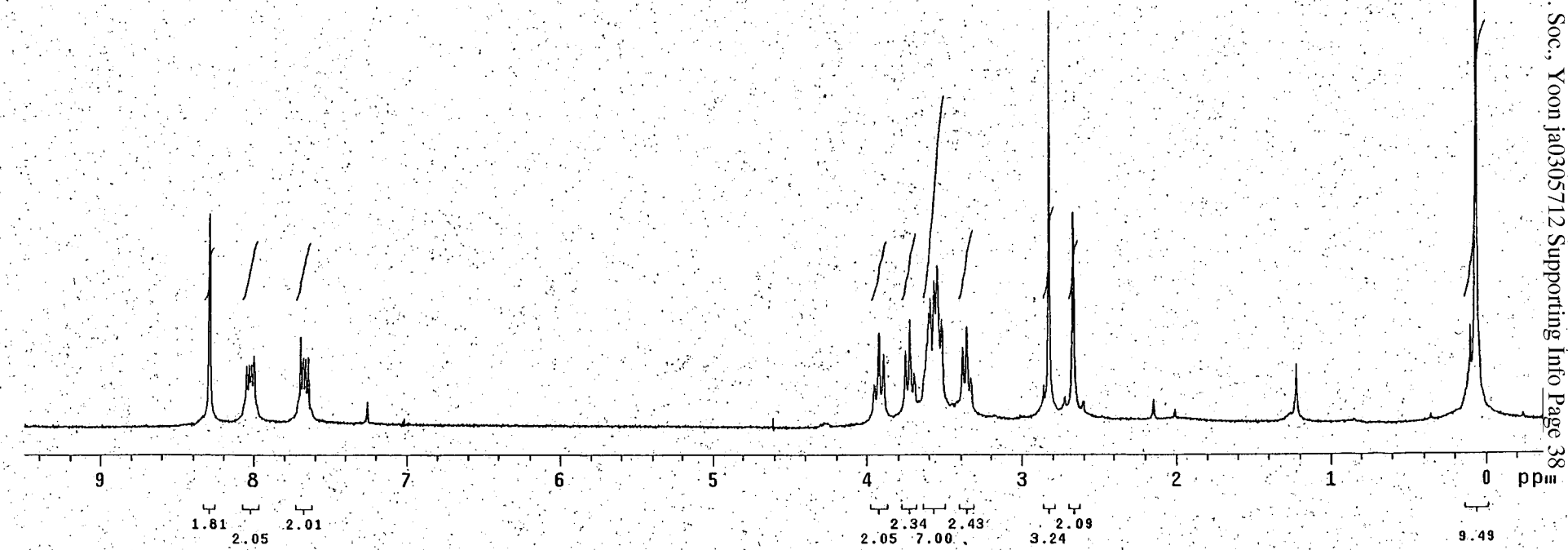

1	8426.855	167.573	12.8
2	6793.003	135.083	24.6
3	6537.700	130.006	45.4
4	6485.541	128.969	38.9
5	6443.905	128.141	-6.3
6	6442.990	128.123	5.6
7	6406.845	127.404	16.8
8	6271.873	124.720	6.0
9	6254.029	124.365	41.7
10	3903.222	77.618	12.4
11	3870.737	76.972	13.6
12	3838.710	76.335	13.8
13	3518.436	69.966	19.6
14	3509.285	69.784	19.8
15	3399.935	67.610	27.4
16	2439.115	48.503	18.8
17	1871.773	37.221	34.1
18	1807.718	35.948	20.8
19	1443.522	28.705	5.9
20	-96.994	-1.929	49.2

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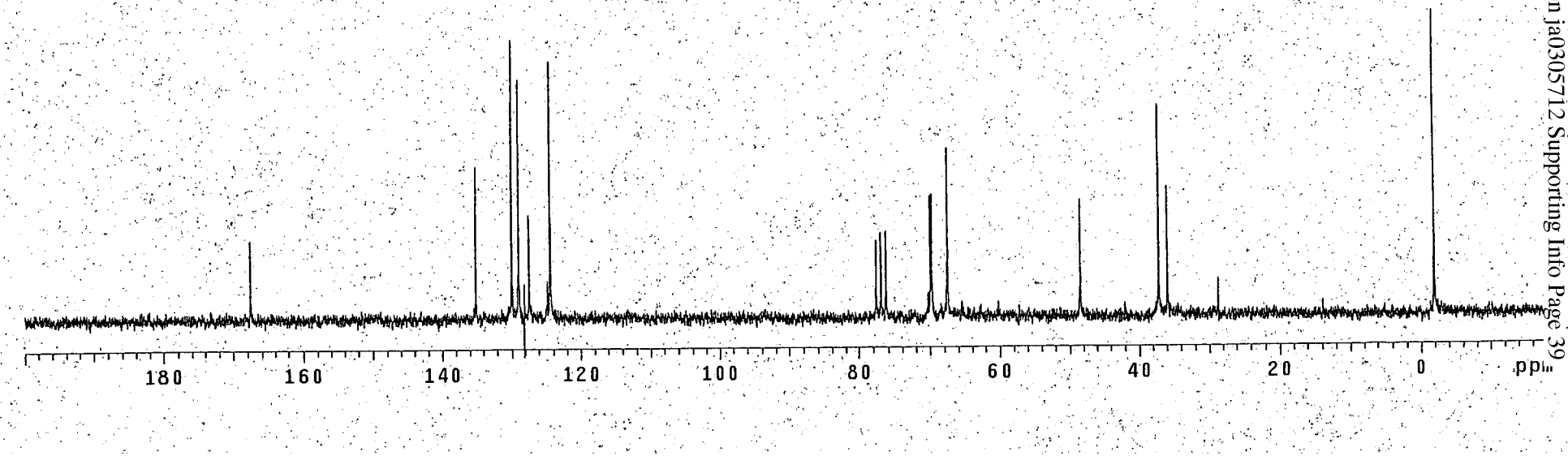
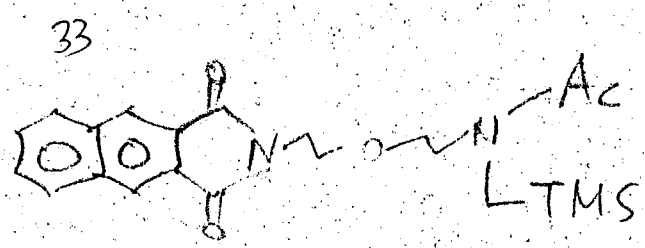


1	1663.421	8.318	38.3
2	1612.506	8.063	10.5
3	1609.210	8.047	9.9
4	1606.279	8.032	9.8
5	1602.983	8.016	13.1
6	1541.079	7.706	16.8
7	1537.783	7.690	11.7
8	1534.852	7.675	11.8
9	1531.556	7.659	13.3
10	1450.972	7.256	11.8
11	789.081	3.946	15.8
12	783.587	3.918	10.4
13	743.295	3.717	16.7
14	737.800	3.689	10.8
15	715.090	3.576	14.7
16	681.391	3.407	9.7
17	676.263	3.382	12.8
18	576.998	2.885	14.3
19	552.090	2.761	29.5
20	430.848	2.154	12.6
21	408.137	2.041	57.6
22	390.189	1.951	28.1
23	5.216	0.026	96.8
24	-3.575	-0.018	180.6



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