Supporting Information

Selective Approach toward Multi-functionalized Lactams by Lewis Acid-Promoted PhSe Group Transfer Radical Cyclization

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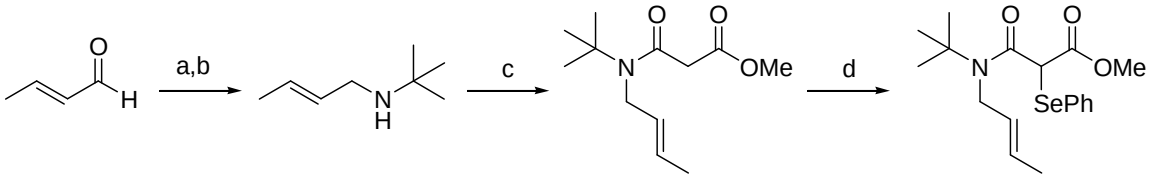
General methods:

All reagents and solvents for reactions were of analytical grade and were dried and distilled if necessary. Flash column chromatography was performed on silica gel 60 (230−400 mesh ASTM) using ethyl acetate/*n*-hexane as eluting solvents. A 320 nm, 125W high-pressure mercury lamp was used as the UV source. The reactions were carried out in Pyrex glass flasks. NMR spectra were recorded at a 400 MHz or a 500 MHz NMR spectrometer. IR spectra were recorded at a Fourier transform infrared spectrometer as a thin film unless otherwise noted. Mass spectra were recorded at a mass spectrometer for both low resolution and high resolution mass spectra.

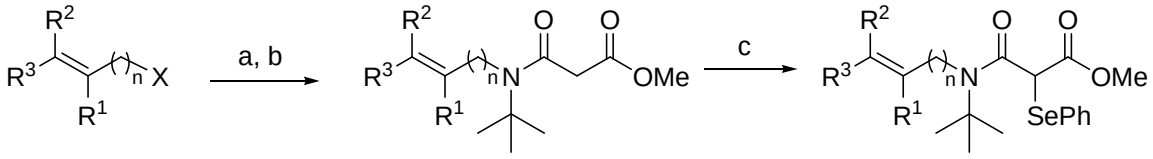
Preparation of substrates 1a–h

The substrates were prepared according to the standard procedures shown in Schemes S1−S4.



4a **1a**

Scheme S1. Synthesis of Cyclization Precursor **1a.** *Reagents and conditions*: (a) *t*-butyl amine, $MgSO_4$, CH_2Cl_2, reflux; (b) $NaBH_4$, MeOH, 0°C~rt; 70% (two steps); (c) potassium 3-methoxy-3-oxopropanoate, EDCI•HCl, HOBt, CH_2Cl_2, rt, 80%; (d) NaH, THF, 0°C, then PhSeCl, −78 ~ 0°C, 60%.

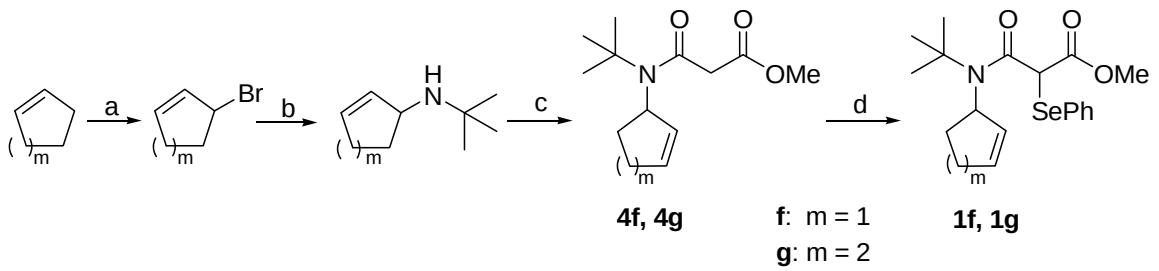


X = Br or Cl
n = 1 or 2

4 **1**

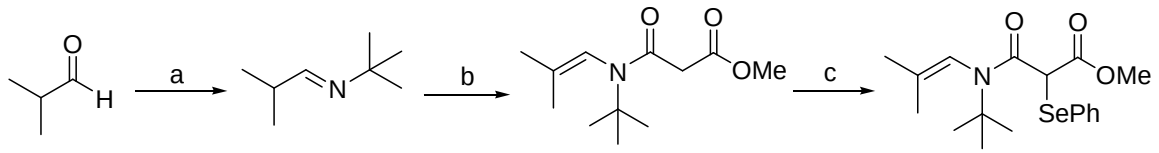
b : R^1, R^2, R^3 = H (n=1)
c : R^1= Me, R^2, R^3 = H (n=1)
d : R^1= H, R^2, R^3 = Me (n=1)
e : R^1, R^2, R^3 = H (n=2)

Scheme S2. Synthesis of **1b–e**. *Reagents and conditions*: (a) *t*-butyl amine, Et_2O, rt, overnight; (b) potassium 3-methoxy-3-oxopropanoate, EDCI•HCl, HOBt, CH_2Cl_2, rt, overnight, 30–57% (two steps); (c) NaH, THF, 0°C, then PhSeCl, −78 ~ 0°C, 5h, 30–60%.



4f, 4g **f**: m = 1 **g**: m = 2 **1f, 1g**

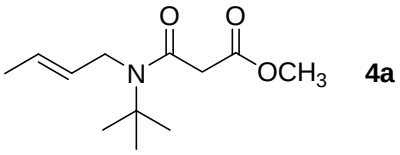
Scheme S3. Synthesis of **1f**–**g**. *Reagents and conditions*: (a) NBS, AIBN, reflux, 1h; (b) *t*-butyl amine, Et_2O, rt, overnight, 72% (two steps) (m=1); *t*-butyl amine, K_2CO_3, CH_3CN, rt, overnight, 80% (two steps) (m=2); (c) potassium 3-methoxy-3-oxopropanoate, EDCI•HCl, HOBt, CH_2Cl_2, rt, overnight, 51% (m=1), 69% (m=2); (d) NaH, THF, 0°C, then PhSeCl, –78 ~ 0°C, 5h, 55% (m=1), 68% (m=2).



4h **1h**

Scheme S4. Synthesis of **1h**. *Reagents and conditions*: (a) *t*-butyl amine, $MgSO_4$, CH_2Cl_2, rt, 6h; (b) methyl malonyl chloride, Et_3N, CH_2Cl_2, rt, overnight, 10% (two steps); (c) NaH, THF, 0°C, then PhSeCl, –78 ~ 0°C, 5h, 36%.

(*E*)-Methyl 3-(but-2-enyl(*t*-butyl)amino)-3-oxopropanoate (4a).

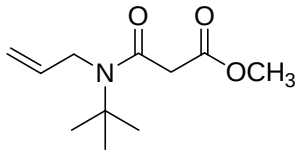


4a

(*E*)-*N*-*tert*-butylbut-2-en-1-amine (1.90 g, 15.0 mmol), potassium 3-methoxy-3-oxopropanoate (2.34 g, 15.0 mmol), EDCI•HCl (3.74 g, 19.5 mmol) and HOBt (3.04 g, 22.5 mmol) were dissolved in CH_2Cl_2 (150 mL) at 0°C. The reaction mixture was stirred at room temperature overnight, and the white precipitate was filtered off. The organic layer was washed sequentially with saturated $NaHCO_3$ solution (100 mL) and dilute hydrochloric acid (100 mL). It was then dried over anhydrous Na_2SO_4 and concentrated. The crude product was purified by flash column chromatography to give **4a** (2.73 g, 80%) as a light yellow oil. Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.37; ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.63–5.58 (m, 1H), 5.44–5.41 (m, 0.9 × 1H), 5.36–5.33 (m, 0.1 × 1H), 3.95 (d, *J* = 4.6 Hz, 0.1 × 2H), 3.86–3.85 (m, 0.9 × 2H), 3.74 (s, 3H), 3.43 (s, 2H), 1.72 (dd, *J* = 6.4, 1.5 Hz, 0.9 × 3H), 1.64 (dd, *J* = 6.9, 1.2 Hz, 0.1 × 3H), 1.44 (s, 9H); ^{13}C

NMR (100 MHz, $CDCl_3$) δ 168.9, 167.1, 128.1, 127.3, 57.9, 52.3, 47.2, 43.7, 28.7, 17.8; IR (neat) 2960, 1745, 1651 cm^{-1}; LRMS for $C_{12}H_{21}NO_3$ (EI, 20 eV) *m/z* 228 (M^++1, 6), 227 (M^+, 41), 170 (100); HRMS (EI) for $C_{12}H_{21}NO_3$ (M^+): calcd 227.1521, found 227.1517.

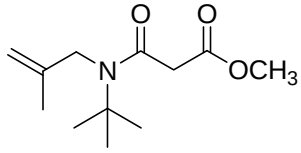
Methyl 3-(allyl(*t*-butyl)amino)-3-oxopropanoate (4b).



4b

Yield 74%; A light yellow oil; Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.39; ^1H NMR (400 MHz, $CDCl_3$) δ 5.85 (ddt, *J* = 17.1, 10.2, 3.9 Hz, 1H), 5.27–5.23 (m, 2H), 3.94 (dt, *J* = 3.9, 2.0 Hz, 2H), 3.74 (s, 3H), 3.42 (s, 2H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 167.2, 135.3, 116.3, 58.0, 52.4, 47.8, 43.6, 28.6; IR (neat) 2960, 1746, 1654 cm^{-1}; LRMS for $C_{11}H_{19}NO_3$ (EI, 20 eV) *m/z* 214 (M^++1, 3), 213 (M^+, 17), 157 (100); HRMS (EI) for $C_{11}H_{19}NO_3$ (M^+): calcd 213.1365, found 213.1370.

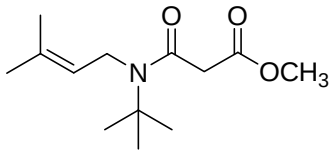
Methyl 3-(*t*-butyl(2-methylallyl)amino)-3-oxopropanoate (4c).



4c

Yield 37% (two steps); A light yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.36; ^1H NMR (400 MHz, $CDCl_3$) δ 5.00 (s, 1H), 4.96 (s, 1H), 3.76 (s, 2H), 3.74 (s, 3H), 3.37 (s, 2H), 1.72 (s, 3H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 167.4, 142.2, 111.0, 58.0, 52.3, 50.9, 43.4, 28.3, 20.1; IR (neat) 2924, 1746, 1655 cm^{-1}; LRMS for $C_{12}H_{21}NO_3$ (EI, 20 eV) *m/z* 227 (M^+, 13), 170 (18), 112 (100); HRMS (EI) for $C_{12}H_{21}NO_3$ (M^+): calcd 227.1521, found 227.1518.

Methyl 3-(*t*-butyl(3-methylbut-2-enyl)amino)-3-oxopropanoate (4d).

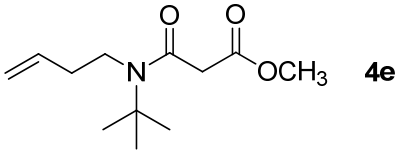


4d

Yield 60%; A light yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.47; ^1H NMR (400 MHz, $CDCl_3$) δ 5.05 (t, br, 1H), 3.85 (d, *J* = 5.4 Hz, 2H), 3.73 (s, 3H),

3.40 (s, 2H), 1.71 (s, 3H), 1.60 (s, 3H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 166.8, 133.8, 122.8, 57.9, 52.3, 44.3, 43.9, 28.9, 25.6, 17.9; IR (neat) 2925, 1746, 1652 cm^{-1}; LRMS for $C_{13}H_{23}NO_3$ (EI, 20 eV) *m/z* 242 (M^++1, 5), 241 (M^+, 39), 185 (37), 184 (100); HRMS (EI) for $C_{13}H_{23}NO_3$ (M^+): calcd 241.1678, found 241.1679.

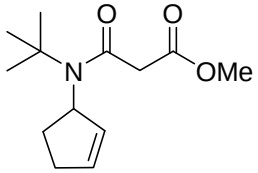
Methyl 3-(but-3-enyl(*t*-butyl)amino)-3-oxopropanoate (4e).



4e

Yield 75%; A light yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.42; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.73 (ddt, *J* = 17.2, 10.3, 6.9 Hz, 1H), 5.13–5.08 (m, 2H), 3.75 (s, 3H), 3.46 (s, 2H), 3.33–3.29 (m, 2H), 2.35–2.29 (m, 2H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 166.6, 133.9, 117.5, 57.8, 52.4, 45.4, 43.8, 36.1, 28.9; IR (neat) 2966, 1746, 1651 cm^{-1}; LRMS for $C_{12}H_{21}NO_3$ (EI, 20 eV) *m/z* 228 (M^++1, 7), 130 (41), 86 (100); HRMS (EI) for $C_{12}H_{21}NO_3$ (M^+): calcd 227.1521, found 227.1518.

Methyl 3-(*t*-butyl(cyclopent-2-enyl)amino)-3-oxopropanoate (4f).

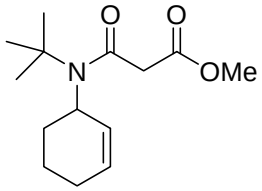


4f

A solution of 3-bromocyclopent-1-ene (4.4 g, 30.0 mmol) and *t*-butyl amine (9.5 mL, 90.0 mmol) in Et_2O (40 mL) was stirred at room temperature overnight. Then the mixture was neutralized by saturated $NaHCO_3$ solution and the aqueous layer was extracted with Et_2O (30 mL × 3). The organic phase was dried with anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified on a silical gel column eluted with petroleum ether/EtOAc (2:1 with 5% of triethylamine) to give pure *N*-*tert*-butylcyclopent-2-enamine (3.02 g, 72%) as a light yellow oil. This secondary amine (3.02 g, 21.7 mmol), potassium 3-methoxy-3-oxopropanoate (4.06 g, 26.0 mmol), EDCI•HCl (6.49 g, 33.8 mmol), and HOBt (5.28 g, 39.1 mmol) were dissolved in CH_2Cl_2 (150 mL) at 0°C. The mixture was stirred at room temperature overnight. The white precipitate was filtered off. The organic layer was washed sequentially with saturated $NaHCO_3$ solution (100 mL) and dilute hydrochloric acid (100 mL). It was then dried over anhydrous Na_2SO_4 and concentrated. The crude product was purified by flash column chromatography to give **4f** (2.64 g, 51%)

as a light yellow oil. Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.41; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.81–5.77 (m, 1H), 5.73–5.70 (m, 1H), 4.87–4.80 (m, 1H), 3.72 (s, 3H), 3.44 (d, J_{AB} = 15.6 Hz, 1H), 3.35 (d, J_{AB} = 15.6 Hz, 1H), 2.59–2.50 (m, 1H), 2.45–2.33 (m, 2H), 1.85–1.75 (m, 1H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 168.4, 134.2, 131.2, 62.0, 59.1, 52.2, 45.1, 31.4, 31.3, 29.4; IR (neat) 2981, 1739, 1594 cm^{-1}; LRMS for $C_{13}H_{21}NO_3$ (EI, 20 eV) *m/z* 239 (M^+, 10), 82 (100); HRMS (EI) for $C_{13}H_{21}NO_3$ (M^+): calcd 239.1521, found 239.1520.

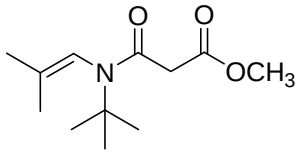
Methyl 3-(*t*-butyl(cyclohex-2-enyl)amino)-3-oxopropanoate (4g).



4g

To a stirred solution of 3-bromocyclohex-1-ene (8.06 g, 50.1 mmol) and *t*-butyl amine (14.2 mL, 134 mmol) in CH_3CN (100 mL) was added K_2CO_3 at room temperature, and the mixture was further stirred overnight. Then the mixture was diluted with water and extracted with EtOAc. The organic phase was dried with anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified on a silica gel column eluted with petroleum ether/EtOAc (2:1 with 5% of triethylamine) to give pure *N*-*tert*-butyl-*N*-(cyclohex-2-enyl)amine (6.09 g, 80%) as a light yellow oil. This amine (3.0 g, 17.9 mmol), potassium 3-methoxy-3-oxopropanoate (2.8 g, 17.9 mmol), EDCI•HCl (4.46 g, 23.2 mmol), and HOBt (3.63 g, 26.9 mmol) were dissolved in CH_2Cl_2 (150 mL) at 0°C. The mixture was stirred at room temperature overnight. The white precipitate was filtered off. The organic layer was washed sequentially with saturated $NaHCO_3$ solution (100 mL) and dilute hydrochloric acid (100 mL). It was then dried over anhydrous Na_2SO_4 and concentrated. The crude product was purified by flash column chromatography to give **4g** (3.4 g, 69%) as a light yellow oil. Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.47; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.80–5.60 (m, 2H), 4.40–4.28 (m, 1H), 3.72 (s, 3H), 3.54 (d, J_{AB} = 15.1 Hz, 1H), 3.50 (d, J_{AB} = 15.1 Hz, 1H), 2.04–1.99 (m, 3H), 1.91–1.88 (m, 1H), 1.82–1.63 (m, 2H), 1.47 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 168.3, 131.8, 128.4, 59.2, 52.8, 52.2, 44.8, 31.2, 29.4, 24.0, 22.7; IR (neat) 2951, 1743, 1638 cm^{-1}; LRMS for $C_{14}H_{23}NO_3$ (EI, 20 eV) *m/z* 253 (M^+, 39), 138 (100); HRMS (EI) for $C_{14}H_{23}NO_3$ (M^+): calcd 253.1678, found 253.1675.

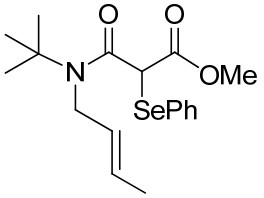
Methyl 3-(*t*-butyl(2-methylprop-1-enyl)amino)-3-oxopropanoate (4h).



4h

The isobutyraldehyde (2.74 mL, 30.0 mmol, freshly distilled) and *t*-butyl amine (3.17 mL, 30.0 mmol) were stirred in CH_2Cl_2 (100 mL) at room temperature in presence of excess anhydrous $MgSO_4$ for 6 hours. $MgSO_4$ was filtered off, and triethylamine (21.0 mL, 151 mmol) was added. Then, a solution of methyl 3-chloro-3-oxopropanoate (30 mmol) in CH_2Cl_2 (50 mL) was added dropwise and the reaction mixture stirred overnight at room temperature. The solvent was removed under reduced pressure to give an oily residue, which was subsequently purified on a silical gel column eluted with petroleum ether/EtOAc to give pure **4h** (0.679 g, 10%) as a light yellow oil. Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.50; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.76 (s, 1H), 3.72 (s, 3H), 3.34 (d, J_{AB} = 15.6 Hz, 1H), 3.19 (d, J_{AB} = 15.6 Hz, 1H), 1.74 (s, 3H), 1.66 (s, 3H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.7, 166.8, 137.6, 123.5, 58.6, 52.2, 44.3, 28.4, 21.7, 17.7; IR (neat) 2975, 1746, 1655 cm^{-1}; LRMS for $C_{12}H_{21}NO_3$ (EI, 20 eV) *m/z* 228 (M^++1, 8), 227 (M^+, 51), 171 (100); HRMS (EI) for $C_{12}H_{21}NO_3$ (M^+): calcd 227.1521, found 227.1520.

(*E*)-Methyl 3-(but-2-enyl(*t*-butyl)amino)-3-oxo-2-(phenylseleno)propanoate (1a).

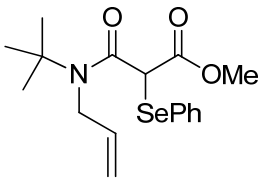


1a

To a stirred suspension of NaH (548 mg, 60% mineral oil dispersion, 13.7 mmol) in THF (20 mL) was added THF (50 mL) solution of **4a** (2.594 g, 11.4 mmol) slowly at 0°C. After 20 min, phenylselenyl chloride (2.183 g, 11.4 mmol) was added in one portion at –78°C. The reaction was stirred and the temperature was allowed to rise to room temperature for 4 h, then quenched with water. After removal of solvent, the residue was extracted with Et_2O, washed with water, dried over anhydrous Na_2SO_4, and concentrated. The crude product was purified by pre-cooled column chromatography to give **1a** (2.614 g, 60%) as a yellow oil. Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.44; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 6.4 Hz, 2H), 7.35–7.27 (m, 3H), 5.58–5.44 (m, 1H), 5.40–5.22 (m, 1H), 4.69 (s, 1H), 3.90 (d, J_{AB} = 18.6 Hz, 1H), 3.78 (d, J_{AB} = 18.6 Hz, 1H), 3.71 (s, 3H),

1.66 (d, J = 6.4 Hz, 3H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 166.9, 135.7, 129.1, 128.7, 128.6, 128.0, 127.5, 58.4, 53.1, 50.4, 47.1, 28.6, 17.8; IR (neat) 2961, 1734, 1649 cm^{-1}; LRMS for $C_{18}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 384 (M^++1, 4), 383 (M^+, 22), 154 (100); HRMS (EI) for $C_{18}H_{25}NO_3Se$ (M^+): calcd 383.1000, found 383.0995.

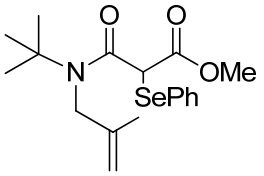
Methyl 3-(allyl(*t*-butyl)amino)-3-oxo-2-(phenylseleno)propanoate (1b).



1b

Yield 62%; A light yellow oil; Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.51; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, J = 7.3 Hz, 0.1 × 2H), 7.64 (d, J = 7.1 Hz, 0.9 × 2H), 7.44–7.26 (m, 3H), 5.85–5.73 (m, 1H), 5.22 (d, J = 17.6 Hz, 1H), 5.20 (d, J = 8.3 Hz, 1H), 4.64 (s, 1H), 3.99 (d, J_{AB} = 19.3 Hz, 1H), 3.86 (d, J_{AB} = 19.3 Hz, 1H), 3.71 (s, 0.9 × 3H), 3.56 (s, 0.1 × 3H), 1.43 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.5, 166.9, 137.5, 135.8, 135.3, 130.1, 129.1, 128.9, 128.8, 128.4, 116.4, 58.5, 53.1, 50.2, 47.7, 28.5; IR (neat) 2958, 1732, 1651, 742, 693 cm^{-1}; LRMS for $C_{17}H_{23}NO_3Se$ (EI, 20 eV) *m/z* 369 (M^+, 26), 212 (15), 157 (12), 149 (100); HRMS (EI) for $C_{17}H_{23}NO_3Se$ (M^+): calcd 369.0843, found 369.0854.

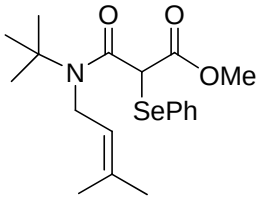
Methyl 3-(*t*-butyl(2-methylallyl)amino)-3-oxo-2-(phenylseleno)propanoate (1c).



1c

Yield 30%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.64; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 6.8 Hz, 2H), 7.35–7.27 (m, 3H), 4.96 (s, 2H), 4.54 (s, 1H), 3.79 (d, J_{AB} = 19.6 Hz, 1H), 3.66 (d, J_{AB} = 19.6 Hz, 1H), 3.72 (s, 3H), 1.62 (s, 3H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 167.2, 142.2, 135.7, 129.1, 128.8, 128.6, 111.3, 58.5, 53.1, 50.9, 50.1, 28.3, 20.1; IR (neat) 2966, 1735, 1650 cm^{-1}; LRMS for $C_{18}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 383 (M^+, 27), 226 (20), 149 (100); HRMS (EI) for $C_{18}H_{25}NO_3Se$ (M^+): calcd 383.1000, found 383.1002.

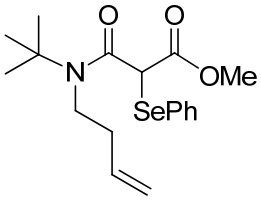
Methyl 3-(*tert*-butyl(3-methylbut-2-enyl)amino)-3-oxo-2-(phenylseleno)propanoate (1d).



1d

Yield 47%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.63; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64–7.62 (m, 2H), 7.33–7.27 (m, 3H), 4.96 (t, *J* = 6.0 Hz, 1H), 4.70 (s, 1H), 3.90–3.84 (m, 2H), 3.71 (s, 3H), 1.66 (s, 3H), 1.50 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 166.5, 135.7, 134.0, 129.1, 128.7, 128.6, 122.7, 58.4, 53.0, 50.7, 44.4, 28.7, 25.6, 17.9; LRMS for $C_{19}H_{27}NO_3Se$ (EI, 20 eV) *m/z* 397 (M^+, 19), 240 (30), 157 (15), 149 (100); HRMS (EI) for $C_{19}H_{27}NO_3Se$ (M^+): calcd 397.1156, found 397.1149.

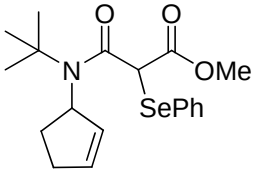
Methyl 3-(but-3-enyl(*t*-butyl)amino)-3-oxo-2-(phenylseleno)propanoate (1e).



1e

Yield 54%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.50; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 6.8 Hz, 2H), 7.36–7.28 (m, 3H), 5.64 (ddt, *J* = 17.1, 10.2, 6.8 Hz, 1H), 5.04–4.98 (m, 2H), 4.73 (s, 1H), 3.71 (s, 3H), 3.34–3.20 (m, 2H), 2.24 (q, *J* = 6.8 Hz, 2H), 1.43 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 166.4, 135.8, 133.7, 129.2, 128.9, 128.4, 117.6, 58.2, 53.1, 50.6, 45.3, 36.2, 28.8; IR (neat) 2925, 1736, 1642 cm^{-1}; LRMS for $C_{18}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 383 (M^+, 21), 149 (100); HRMS (EI) for $C_{18}H_{25}NO_3Se$ (M^+): calcd 383.1000, found 383.1031.

Methyl 3-(*t*-butyl(cyclopent-2-enyl)amino)-3-oxo-2-(phenylseleno)propanoate (1f).

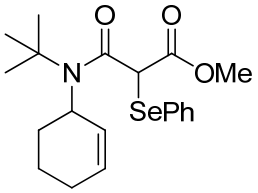


1f

Yield 55%; A yellow oil; two separable diastereomeric mixture; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_{f1} = 0.59; R_{f2} = 0.55; Diastereomer 1: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66–7.63 (m, 2H), 7.32–7.27 (m, 3H), 5.66 (br, 2H), 4.81–4.77 (m, 1H), 4.54 (s, 1H), 3.72 (s, 3H), 2.32–2.19 (m, 2H), 2.13–2.05 (m, 1H), 1.67–1.57 (m, 1H), 1.46 (s, 9H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 169.0, 134.9, 134.0, 132.0, 130.1, 129.1, 128.5, 62.1, 59.1, 52.9, 50.4, 31.5, 31.1, 29.1; IR (neat) 2955, 1736, 1643, 1579, 1476 cm^{-1}; LRMS for $C_{19}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 395 (M^+, 43), 149 (100); HRMS (EI) for $C_{19}H_{25}NO_3Se$ (M^+): calcd 395.1000, found 395.1006; Diastereomer 2: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63–7.60 (m, 2H), 7.31–7.25 (m, 3H), 5.61–5.59 (m, 1H), 5.52–5.50 (m, 1H), 4.88 (s, 1H), 4.82–4.73 (m, 1H), 3.72 (s, 3H), 2.47–2.25 (m, 3H), 1.83–1.74 (m, 1H), 1.46 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 169.0, 135.1, 134.0, 132.2, 129.3, 129.0, 128.3, 62.3, 59.3, 53.0, 50.7, 31.4, 31.2, 29.1; IR (neat) 2952, 1735, 1644, 1478 cm^{-1}; LRMS for $C_{19}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 395 (M^+, 38), 149 (100); HRMS (EI) for $C_{19}H_{25}NO_3Se$ (M^+): calcd 395.1000, found 395.0994.

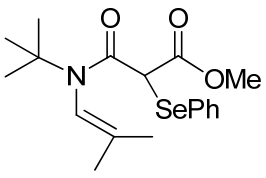
Methyl 3-(*t*-butyl(cyclohex-2-enyl)amino)-3-oxo-2-(phenylseleno)propanoate (1g).



1g

Yield 68%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.61; ^{1}H NMR (400 MHz, $CDCl_3$) (diastereomer ratio 0.77/0.23) δ 7.74–7.62 (m, 2H), 7.30–7.27 (m, 3H), 5.63–5.58 (m, 0.77 × 2H), 5.53–5.37 (m, 0.23 × 2H), 5.03 (s, 0.23 × 1H), 4.83 (s, 0.77 × 1H), 4.35–4.20 (m, 1H), 3.72 (s, 3H), 1.94–1.52 (m, 6H), 1.47 (s, 0.77 × 9H), 1.45 (s, 0.23 × 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 169.0, 137.5, 134.8, 134.6, 131.6, 131.5, 129.5, 129.2, 128.9, 128.3, 128.2, 59.4, 59.3, 53.2, 53.1, 52.9 (2), 50.4, 31.4, 29.3, 29.0, 24.1, 23.8, 22.8, 22.6; IR (neat) 2951, 1736, 1633 cm^{-1}; LRMS for $C_{20}H_{27}NO_3Se$ (EI, 20 eV) *m/z* 409 (M^+, 22), 252 (32), 164 (100), 157 (95); HRMS (EI) for $C_{20}H_{27}NO_3Se$ (M^+): calcd 409.1156, found 409.1154.

Methyl 3-(*tert*-butyl(2-methylprop-1-enyl)amino)-3-oxo-2-(phenylseleno)propanoate (1h).

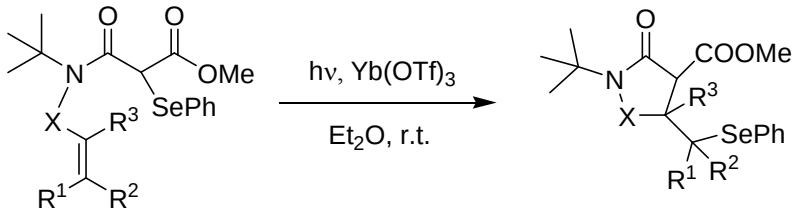


1h

Yield 36%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.63; ^{1}H NMR (500 MHz, $CDCl_3$) (rotamer ratio 1/1) δ 7.65–7.60 (m, 2H), 7.33–7.27 (m, 3H),

5.59 (s, 0.5 × 1H), 5.36 (s, 0.5 × 1H), 4.70 (s, 0.5 × 1H), 4.61 (s, 0.5 × 1H), 3.70 (s, 0.5 × 3H), 3.57 (s, 0.5 × 3H), 1.64 (d, J = 1.0 Hz, 0.5 × 3H), 1.62 (d, J = 0.9 Hz, 0.5 × 3H), 1.60 (d, J = 0.8 Hz, 0.5 × 3H), 1.58 (d, J = 1.0 Hz, 0.5 × 3H), 1.39 (s, 0.5 × 9H), 1.33 (s, 0.5 × 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.3, 168.9, 166.8, 165.8, 138.9, 138.4, 135.8(2), 131.6, 129.1, 129.0, 128.7, 128.6, 128.4, 123.5, 123.0, 59.2, 59.1, 52.9, 52.6, 52.4, 49.9, 28.3, 28.2, 21.8, 21.7, 17.8; IR (neat) 2974, 1733, 1647 cm^{-1}; LRMS for $C_{18}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 226 (M^+ – SePh, 60), 170 (49), 157 (4), 138 (100); HRMS (EI) for $C_{18}H_{25}NO_3Se$ (M^+): calcd 383.1000, found 383.1026.

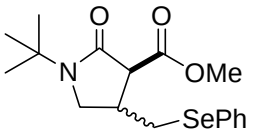
General Procedure for the Group Transfer Radical Cyclization.



R^1, R^2, R^3 = H, CH_3; X = CH_2, $(CH_2)_2$
or
R^2, R^3 = H; R^1, X = -$(CH_2)_3$-, -$(CH_2)_4$-

7 examples
81–95% yield

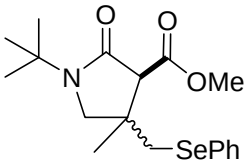
Methyl 1-*t*-butyl-2-oxo-4-(phenylselenomethyl)pyrrolidine-3-carboxylate (2b).



2b

Yield 85%; A yellow oil; Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.33; ^{1}H NMR (400 MHz, $CDCl_3$) (diastereomer ratio 13.4/1) δ 7.52–7.50 (m, 2H), 7.30–7.26 (m, 3H), 3.76 (s, 0.93 × 3H), 3.72 (s, 0.07 × 3H), 3.66 (dd, J = 9.9, 7.6 Hz, 0.93 × 1H), 3.58 (dd, J = 9.2, 7.8 Hz, 0.07 × 1H), 3.41 (d, J = 8.7 Hz, 0.07 × 1H), 3.33 (t, J = 9.2 Hz, 0.07 × 1H), 3.27 (d, J = 8.0 Hz, 0.93 × 1H), 3.11 (dd, J = 9.9, 6.7 Hz, 0.93 × 1H), 3.07–3.02 (m, 1H), 2.95–2.87 (m, 2H), 1.37 (s, 0.07 × 9H), 1.36 (s, 0.93 × 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 168.8, 133.4, 133.2, 129.4, 129.2, 127.7, 127.6, 56.6, 54.9, 54.8, 52.7, 52.3, 50.7, 49.8, 36.1, 35.9, 31.0, 27.6; IR (neat) 2972, 1740, 1689, 740, 692 cm^{-1}; LRMS for $C_{17}H_{23}NO_3Se$ (EI, 20 eV) *m/z* 369 (M^+, 100), 212 (95); HRMS (EI) for $C_{17}H_{23}NO_3Se$ (M^+): calcd 369.0843, found 369.0855.

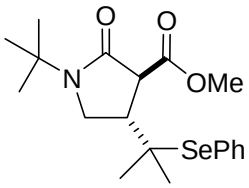
Methyl 1-*t*-butyl-4-methyl-2-oxo-4-(phenylselenomethyl)pyrrolidine-3-carboxylate (2c).



2c

Yield 95%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.51; ^{1}H NMR (400 MHz, $CDCl_3$) (diastereomer ratio 0.7/0.3) δ 7.55–7.50 (m, 2H), 7.29–7.25 (m, 3H), 3.71 (s, 0.7 × 3H), 3.68 (s, 0.3 × 3H), 3.50 (d, *J* = 9.6 Hz, 0.3 × 1H), 3.41 (d, *J* = 10.1 Hz, 0.7 × 1H), 3.28 (d, *J* = 9.6 Hz, 0.7 × 1H), 3.25 (s, 0.7 × 1H), 3.15–3.08 (m, 0.3 × 1H + 2H), 3.03 (d, *J* = 12.4 Hz, 0.3 × 1H), 1.34 (s, 0.3 × 9H), 1.28 (s, 0.3 × 3H and 0.7 × 9H), 1.13 (s, 0.7 × 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 169.5, 169.4, 169.3, 133.2, 133.1, 130.6, 130.5, 129.4, 129.3, 127.5, 127.4, 61.9, 60.9, 56.3, 55.2, 54.5(2), 52.3, 52.1, 40.7, 40.4, 35.6, 27.5(2), 26.2, 21.0; IR (neat) 2970, 1737, 1691 cm^{-1}; LRMS for $C_{18}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 383 (M^+, 98), 226 (100), 212 (28); HRMS (EI) for $C_{18}H_{25}NO_3Se$ (M^+): calcd 383.1000, found 383.1006.

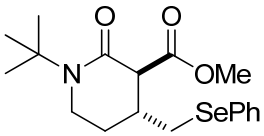
Methyl *trans*-1-*tert*-butyl-2-oxo-4-(2-(phenylseleno)propan-2-yl)pyrrolidine-3-carboxylate (2d).



2d

Yield 95%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.53; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 6.8 Hz, 2H), 7.41–7.29 (m, 3H), 3.76 (s, 3H), 3.60 (t, *J* = 9.3 Hz, 1H), 3.57 (d, *J* = 8.3 Hz, 1H), 3.39 (dd, *J* = 9.8, 7.3 Hz, 1H), 2.88–2.82 (m, 1H), 1.40 (s, 9H), 1.35 (s, 3H), 1.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 169.0, 138.4, 129.1, 129.0, 126.5, 54.9, 53.5, 52.7, 48.4, 47.0, 45.7, 28.4, 27.7, 27.0; IR (neat) 2963, 1741, 1689 cm^{-1}; LRMS for $C_{19}H_{27}NO_3Se$ (EI, 20 eV) *m/z* 397 (M^+, 7), 240 (75), 184 (100); HRMS (EI) for $C_{19}H_{27}NO_3Se$ (M^+): calcd 397.1156, found 397.1172.

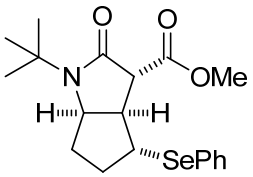
Methyl *trans*-1-*t*-butyl-2-oxo-4-(phenylselenomethyl)piperidine-3-carboxylate (2e).



2e

Yield 83%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.44; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49–7.46 (m, 2H), 7.29–7.25 (m, 3H), 3.71 (s, 3H), 3.42 (dt, *J* = 11.9, 4.7 Hz, 1H), 3.27 (d, *J* = 10.6 Hz, 1H), 3.27–3.21 (m, 1H), 3.05 (dd, *J* = 12.8, 4.1 Hz, 1H), 2.69 (dd, *J* = 12.7, 8.3 Hz, 1H), 2.43–2.34 (m, 1H), 2.16 (dq, *J* = 13.4, 4.2 Hz, 1H), 1.54–1.46 (m, 1H), 1.41 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 166.4, 132.6, 130.1, 129.3, 127.2, 58.0, 57.7, 52.4, 42.9, 36.4, 32.5, 28.4, 28.2; IR (neat) 2955, 1740, 1644 cm^{-1}; LRMS for $C_{18}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 384 (M^++1, 9), 383 (M^+, 46), 226 (64), 170 (100); HRMS (EI) for $C_{18}H_{25}NO_3Se$ (M^+): calcd 383.1000, found 383.0992.

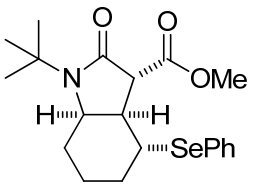
Methyl *cis*-1-*tert*-butyl-2-oxo-*cis*-4-(phenylseleno)-octahydrocyclopenta[*b*]pyrrole-*cis*-3-carboxylate (2f).



2f

Yield 81%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.33; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.51 (m, 2H), 7.31–7.26 (m, 3H), 4.33 (td, *J* = 8.0, 5.0 Hz, 1H), 3.69 (s, 3H), 3.50–3.46 (m, 1H), 3.20 (d, *J* = 6.9 Hz, 1H), 3.03 (ddd, *J* = 8.0, 6.9, 4.1 Hz, 1H), 2.31–2.15 (m, 2H), 1.79–1.65 (m, 2H), 1.41 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 168.4, 134.8, 129.3, 128.6, 128.0, 61.6, 55.9, 55.2, 52.7, 47.2, 46.3, 34.4, 32.0, 28.2; IR (neat) 2961, 1740, 1685, 1578cm^{-1}; LRMS for $C_{19}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 395 (M^+, 58), 150 (100); HRMS (EI) for $C_{19}H_{25}NO_3Se$ (M^+): calcd 395.1000, found 395.0999.

Methyl *cis*-1-*tert*-butyl-2-oxo-*cis*-4-(phenylseleno)-octahydro-*1H*-indole-*cis*-3-carboxylate (2g).

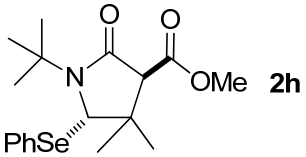


2g

Yield 84%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.29;

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.51 (m, 2H), 7.31–7.27 (m, 3H), 3.95 (dt, *J* = 11.5, 6.0 Hz, 1H), 3.72–3.67 (m, 4H), 3.43 (d, *J* = 12.8 Hz, 1H), 2.99 (dd, *J* = 12.8, 6.4 Hz, 1H), 2.20–2.16 (m, 1H), 1.91–1.86 (m, 1H), 1.83–1.75 (m, 1H), 1.72–1.57 (m, 2H), 1.41 (s, 9H), 1.24–1.14 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 168.5, 133.9, 129.6, 129.3, 127.7, 54.9, 53.8, 52.7, 52.6, 42.9, 41.6, 31.6, 28.3, 26.1, 19.5; IR (neat) 2974, 1744, 1675 cm^{-1}; LRMS for $C_{20}H_{27}NO_3Se$ (EI, 20 eV) *m/z* 410 (M^++1, 6), 409 (M^+, 36), 252 (27), 164 (100), 157 (6); HRMS (EI) for $C_{20}H_{27}NO_3Se$ (M^+): calcd 409.1156, found 409.1157.

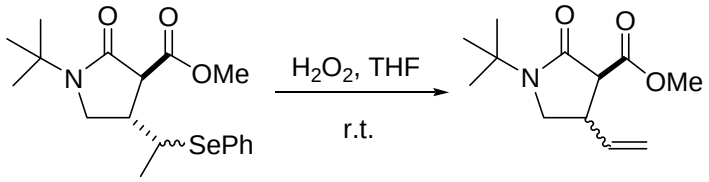
Methyl *trans*-1-*t*-butyl-4,4-dimethyl-2-oxo-5-(phenylseleno)pyrrolidine-3- carboxylate (2h).



2h

Yield 65%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.57; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.57–7.54 (m, 2H), 7.31–7.29 (m, 3H), 4.86 (s, 1H), 3.74 (s, 3H), 3.50 (s, 1H), 1.58 (s, 9H), 1.27 (s, 3H), 1.20 (s, 3H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.2, 168.5, 134.4, 129.8, 129.6, 128.0, 76.4, 57.8, 55.9, 52.1, 44.5, 27.6, 25.2, 24.1; IR (neat) 2971, 1753, 1701 cm^{-1}; LRMS for $C_{18}H_{25}NO_3Se$ (EI, 20 eV) *m/z* 226 ($C_{12}H_{20}NO_3$, M^+–SePh, 58), 170 (100); HRMS (EI) for $C_{18}H_{25}NO_3Se$: calcd 226.1443 ($C_{12}H_{20}NO_3$, M^+–SePh), found 226.1446.

General Procedure for the oxidative elimination of phenylseleno-group.

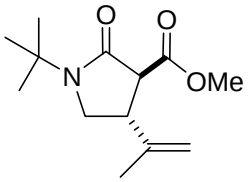


2a **3a**

Methyl *trans*-1-*t*-butyl-2-oxo-4-vinylpyrrolidine-3-carboxylate (3a). H_2O_2 (0.12 mL, 1.06 mmol, 30% wt in H_2O) was added to a solution of **2a** (223 mg, 0.58 mmol) in THF (25 mL) at 0°C. The solution was then stirred overnight at room temperature. After removal of the solvent, the mixture was diluted with CH_2Cl_2 (30 mL), washed with water and brine, dried over anhydrous Na_2SO_4, and concentrated. The crude residue was purified by flash column chromatography to provide **3a** (121 mg, 92%) as colorless oil. Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.52; ^{1}H NMR (400 MHz, $CDCl_3$)

(diastereomer ratio: 9:1) δ 5.76 (ddd, J = 17.1, 10.3, 6.8 Hz, 1H), 5.18 (d, J = 17.1 Hz, 1H), 5.12 (d, J = 10.3 Hz, 1H), 3.78 (s, 0.9 × 3H), 3.70 (s, 0.1 × 3H), 3.66 (dd, J = 9.5, 7.6 Hz, 0.9 × 1H), 3.53 (d, J = 8.8 Hz, 0.1 × 2H), 3.42 (d, J = 8.8 Hz, 0.1 × 1H), 3.31–3.27 (m, 0.9 × 2H), 3.18–3.12 (m, 1H), 1.42 (s, 0.1 × 9H), 1.40 (s, 0.89 × 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.0, 169.1, 136.4, 134.0, 118.6, 117.3, 55.8, 55.4, 54.7, 54.6, 52.6, 52.0, 49.6, 49.1, 40.1, 39.7, 27.6; IR (neat) 2975, 1743, 1691 cm^{-1}; LRMS for $C_{12}H_{19}NO_3$ (EI, 20 eV) *m/z* 226 (M^++1, 6), 225 (M^+, 44), 210 (100); HRMS (EI) for $C_{12}H_{19}NO_3$ (M^+): calcd 225.1365, found 225.1364.

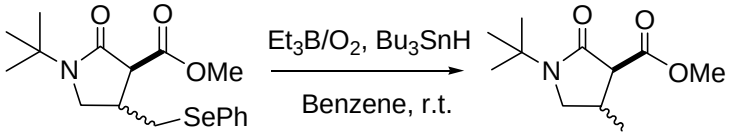
Methyl *trans*-1-*t*-butyl-2-oxo-4-(prop-1-en-2-yl)pyrrolidine-3-carboxylate (3d).



3d

Yield 92%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.51; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.85 (s, 1H), 4.82 (s, 1H), 3.79 (s, 3H), 3.67 (t, J = 8.8 Hz, 1H), 3.40 (d, J = 9.6 Hz, 1H), 3.29 (q, J = 8.8 Hz, 1H), 3.20 (t, J = 8.8 Hz, 1H), 1.74 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.5, 169.3, 142.8, 112.2, 54.8, 54.6, 52.6, 48.4, 42.5, 27.7, 20.4; IR (neat) 2972, 1743, 1691 cm^{-1}; LRMS for $C_{13}H_{21}NO_3$ (EI, 20 eV) *m/z* 241 (M^++2, 51), 226 (100), 198 (48); HRMS (EI) for $C_{13}H_{21}NO_3$ (M^+): calcd 239.1521, found 239.1522.

General Procedure for the reductive dephenylselenation.

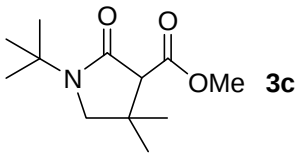


2b **3b**

Methyl *trans*-1-*t*-butyl-4-methyl-2-oxopyrrolidine-3-carboxylate (3b). To a stirred solution of **2b** (111 mg, 0.30 mmol) in dry benzene (10 mL) was added Bu_3SnH (0.16 mL, 0.60 mmol) at room temperature. Et_3B (1 M *n*-hexane solution, 0.29 mL, 0.29 mmol) and oxygen gas (7 mL) were added via syringe. The reaction was finished 3.5 h later. After removal of benzene, the residue was diluted with Et_2O. DBU (48 μl, 0.32 mmol) was added followed by I_2/Et_2O solution till the light yellow color persisted. The precipitate was

filtered off, and the filtrate was concentrated. The crude product was purified by column chromatography to give **3b** (53 mg, 82%) as a white solid. M.p. 65–66 °C; Analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.30; ^{1}H NMR (400 MHz, $CDCl_3$) (diastereomer ratio 0.95/0.05) δ 3.78 (s, 0.95 × 3H), 3.72 (s, 0.05 × 3H), 3.65 (dd, *J* = 9.3, 7.8 Hz, 0.95 × 1H), 3.52 (dd, *J* = 9.3, 7.3 Hz, 0.05 × 1H), 3.34 (d, *J* = 9.3 Hz, 0.05 × 1H), 3.23 (t, *J* = 9.1 Hz, 0.05 × 1H), 3.03 (d, *J* = 8.3 Hz, 0.95 × 1H), 2.97 (dd, *J* = 9.3, 7.8 Hz, 0.95 × 1H), 2.74–2.63 (m, 1H), 1.41 (s, 0.05 × 9H), 1.39 (s, 0.95 × 9H), 1.13 (d, *J* = 6.8 Hz, 0.95 × 3H), 1.05 (d, *J* = 6.8 Hz, 0.05 × 3H); ^{13}C NMR (100 MHz, $CDCl_3$) (major diastereomer) δ 170.6, 169.7, 58.1, 54.5, 52.5, 51.4, 30.9, 27.7, 18.3; IR (neat) 2926, 1742, 1690 cm^{-1}; LRMS for $C_{11}H_{19}NO_3$ (EI, 20 eV) *m/z* 213 (M^+, 62), 198 (100); HRMS (EI) for $C_{11}H_{19}NO_3$ (M^+): calcd 213.1365, found 213.1371.

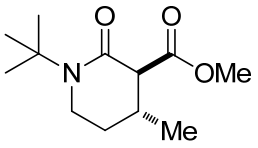
Methyl 1-*t*-butyl-4,4-dimethyl-2-oxopyrrolidine-3-carboxylate (3c).



3c

Yield 87%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.45; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.72 (s, 3H), 3.38 (d, *J* = 9.3 Hz, 1H), 3.11 (d, *J* = 9.3 Hz, 1H), 2.99 (s, 1H), 1.41 (s, 9H), 1.21 (s, 3H), 1.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 169.8, 62.1, 57.9, 54.2, 51.9, 35.7, 28.7, 27.6, 22.6; IR (neat) 2964, 1739, 1690 cm^{-1}; LRMS for $C_{12}H_{21}NO_3$ (EI, 20 eV) *m/z* 227 (M^+, 57), 212 (100), 170 (3); HRMS (EI) for $C_{12}H_{21}NO_3$ (M^+): calcd 227.1521, found 227.1530.

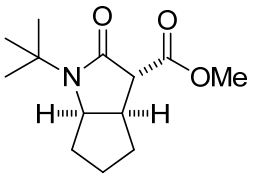
Methyl *trans*-1-*t*-butyl-4-methyl-2-oxopiperidine-3-carboxylate (3e).



3e

Yield 81%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.40; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.74 (s, 3H), 3.45–3.38 (m, 1H), 3.26 (td, *J* = 11.6, 4.4 Hz, 1H), 2.98 (d, *J* = 11.0 Hz, 1H), 2.21–2.15 (m, 1H), 1.89 (dq, *J* = 13.7, 3.9 Hz, 1H), 1.46–1.35 (m, 10H), 0.97 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 167.0, 59.6, 57.8, 52.2, 43.2, 31.0, 30.8, 28.1, 20.1; IR (neat) 2958, 1743, 1643 cm^{-1}; LRMS for $C_{12}H_{21}NO_3$ (EI, 20 eV) *m/z* 228 (M^++1, 15), 227 (M^+, 100), 212 (87); HRMS (EI) for $C_{12}H_{21}NO_3$ (M^+): calcd 227.1521, found 227.1549.

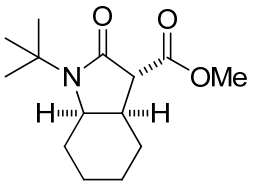
Methyl *cis*-1-*t*-butyl-2-oxo-octahydrocyclopenta[*b*]pyrrole-*cis*-3-carboxylate (3f).



3f

Yield 60%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.33; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.18 (td, *J* = 7.8, 4.1 Hz, 1H), 3.77 (s, 3H), 3.19 (d, *J* = 6.9 Hz, 1H), 3.03 (qd, *J* = 7.8, 3.6 Hz, 1H), 1.92–1.50 (m, 6H), 1.42 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 169.3, 62.4, 56.7, 54.9, 52.6, 40.0, 35.3, 31.9, 28.2, 24.6; IR (neat) 2960, 1741, 1683 cm^{-1}; LRMS for $C_{13}H_{21}NO_3$ (EI, 20 eV) *m/z* 239 (M^+, 48), 224 (100); HRMS (EI) for $C_{13}H_{21}NO_3$ (M^+): calcd 239.1521, found 239.1524.

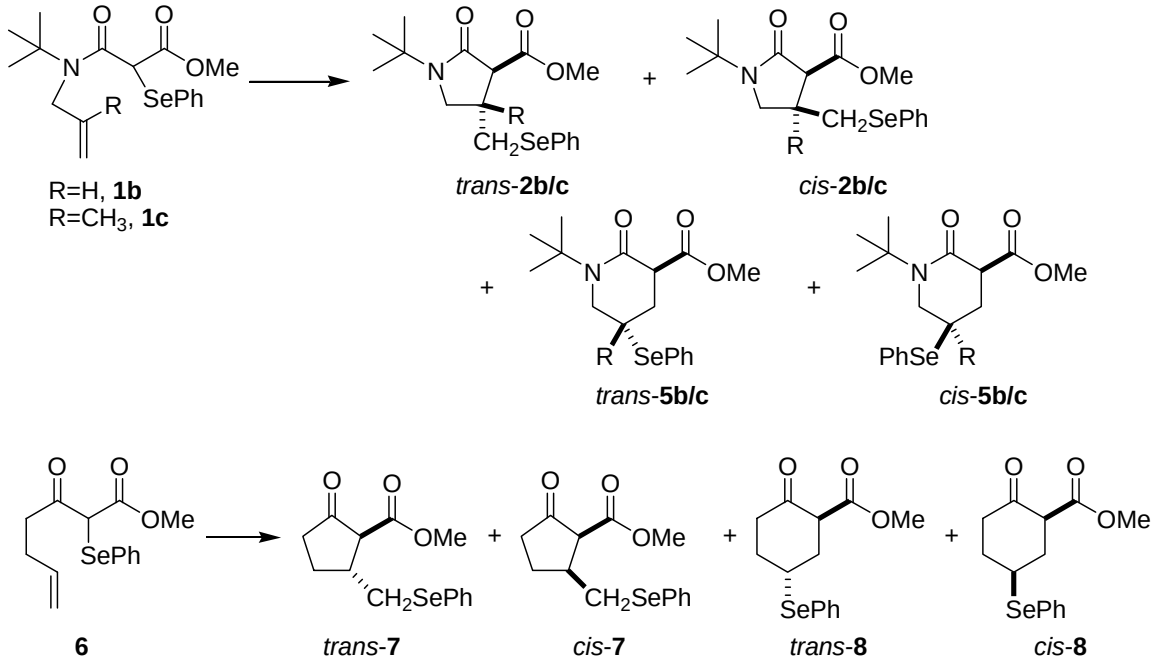
Methyl *cis*-1-*t*-butyl-2-oxo-octahydro-*1H*-indole-*cis*-3-carboxylate (3g).



3g

Yield 81%; A yellow oil; analytical TLC (silica gel 60), 50% EtOAc in *n*-hexane, R_f = 0.44; ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.79 (s, 3H), 3.65–3.59 (m, 1H), 3.46 (d, *J* = 13.3 Hz, 1H), 2.82–2.76 (m, 1H), 2.14–2.10 (m, 1H), 1.76–1.72 (m, 2H), 1.60–1.56 (m, 2H), 1.41 (s, 9H), 1.30–1.11 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.7, 169.6, 56.4, 54.6, 52.5, 51.6, 37.3, 31.8, 28.3, 25.4, 23.2, 20.4; IR (neat) 2945, 1740, 1688 cm^{-1}; LRMS for $C_{14}H_{23}NO_3$ (EI, 20 eV) *m/z* 254 (M^++1, 9), 253 (M^+, 63), 238 (100), 196 (7); HRMS (EI) for $C_{14}H_{23}NO_3$ (M^+): calcd 253.1678, found 253.1681.

Table S1. Energies and Cartesian coordinates for **2b/c, 5b/c, 7, and 8**



trans-**2b**

E = -3341.50076157 a.u.

C	0	-1.894574	-1.010863	0.612193
C	0	-0.783041	-0.960384	-0.455179
C	0	-0.998442	0.413789	-1.126300
N	0	-1.604630	1.235968	-0.070636
C	0	-2.211540	0.481814	0.894988
C	0	0.600606	-1.077629	0.194674
C	0	-1.839942	2.707167	-0.200519
O	0	-2.901548	0.871999	1.825722
C	0	-3.162360	-1.671064	0.099010
O	0	-3.828898	-2.290016	1.088589
C	0	-5.089975	-2.872586	0.714595
O	0	-3.540237	-1.629007	-1.054487
H	0	-0.910118	-1.757418	-1.193925
H	0	-1.669184	0.322098	-1.989225
H	0	-0.047303	0.830717	-1.462812
H	0	-1.596949	-1.486617	1.549845
C	0	-1.409842	3.405463	1.104291
C	0	-0.996034	3.264970	-1.358737
C	0	-3.334471	2.956474	-0.485516
H	0	-3.525226	4.030576	-0.591469
H	0	-3.639303	2.463124	-1.415700

H	0	-3.949520	2.573057	0.331749
H	0	-1.566303	4.486344	1.012293
H	0	-1.986422	3.036672	1.953486
H	0	-0.345486	3.230336	1.299369
H	0	-1.170692	4.343267	-1.431038
H	0	0.075859	3.112088	-1.192310
H	0	-1.266577	2.820771	-2.322215
H	0	-5.487136	-3.315720	1.627838
H	0	-5.766486	-2.103163	0.334092
H	0	-4.946503	-3.635530	-0.055051
H	0	0.680728	-1.999617	0.774986
Se	0	2.022429	-1.111317	-1.195216
H	0	0.809057	-0.223880	0.844592
C	0	3.469128	-0.437788	-0.113012
C	0	3.728169	0.936359	-0.067363
C	0	4.785287	1.423459	0.703130
C	0	5.588699	0.539792	1.426781
C	0	5.335862	-0.832573	1.377102
C	0	4.279462	-1.322093	0.606918
H	0	3.104159	1.616885	-0.638776
H	0	4.982216	2.491790	0.735401
H	0	6.412636	0.919533	2.024933
H	0	5.961316	-1.523569	1.936062
H	0	4.080579	-2.388400	0.558766

cis-**2b**

E = -3341.50166810 a.u.

C	0	1.323556	0.989156	0.944539
C	0	0.160923	0.318878	0.173139
C	0	0.867986	-0.770255	-0.655956
N	0	2.019166	-1.140891	0.173458
C	0	2.363910	-0.156424	1.058320
C	0	-0.736016	1.239609	-0.646242
C	0	2.922912	-2.294180	-0.127372
O	0	3.330015	-0.129185	1.807156
C	0	1.993093	2.128496	0.196771
O	0	2.240017	3.174298	1.005795
C	0	2.940731	4.274342	0.397943
O	0	2.290033	2.101384	-0.982092
H	0	3.914557	3.945804	0.026529
H	0	2.361413	4.685564	-0.432866

H	0	-0.455282	-0.186558	0.926742
H	0	-1.227404	1.990566	-0.022143
H	0	-0.168824	1.747899	-1.429039
H	0	1.187715	-0.374902	-1.629456
H	0	0.205798	-1.617909	-0.834932
H	0	1.049303	1.328753	1.944646
H	0	3.060234	5.014916	1.188779
Se	0	-2.149014	0.265350	-1.641068
C	0	2.249892	-3.226321	-1.148555
C	0	4.244732	-1.758828	-0.713307
C	0	3.182438	-3.086319	1.168823
C	0	-3.305897	-0.154626	-0.157042
C	0	-4.174080	0.820852	0.347541
C	0	-5.029607	0.517094	1.406909
C	0	-5.034880	-0.767391	1.956300
C	0	-4.182796	-1.747093	1.444185
C	0	-3.318626	-1.442158	0.390043
H	0	-4.177675	1.811707	-0.097169
H	0	-5.698401	1.280134	1.796345
H	0	-5.705966	-1.004918	2.777279
H	0	-4.187390	-2.749064	1.865103
H	0	-2.655674	-2.201601	-0.013180
H	0	3.831145	-3.943346	0.953865
H	0	3.664512	-2.458657	1.919370
H	0	2.240429	-3.466050	1.580837
H	0	4.916104	-2.591072	-0.954080
H	0	4.059840	-1.191757	-1.632803
H	0	4.745293	-1.105231	0.004546
H	0	2.924183	-4.063912	-1.353910
H	0	1.311829	-3.642477	-0.765192
H	0	2.046438	-2.724545	-2.100283

trans-**5b**

E = -3341.49545529 a.u.

C	0	3.500204	1.013774	-0.713471
C	0	3.088331	-0.253431	-0.286498
C	0	3.982947	-1.074691	0.409861
C	0	5.273288	-0.624620	0.691726
C	0	5.679487	0.643689	0.270329
C	0	4.793896	1.460165	-0.435116
Se	0	1.309336	-0.883076	-0.684513

C	0	0.476467	-0.415300	1.075651
C	0	0.023767	1.034318	1.141521
C	0	-1.066279	1.287739	0.094717
C	0	-2.117548	0.164285	-0.080477
N	0	-1.759478	-1.126247	0.251779
C	0	-0.712559	-1.344057	1.268797
C	0	-1.818153	2.577959	0.390190
O	0	-2.235633	2.888975	1.485362
O	0	-3.183732	0.462227	-0.609927
C	0	-2.717911	-2.253470	-0.074564
C	0	-3.005949	-2.245619	-1.590685
O	0	-1.943506	3.344020	-0.707976
C	0	-2.701450	4.551908	-0.528897
C	0	-2.076039	-3.615048	0.252516
C	0	-4.014348	-2.101482	0.745066
H	0	1.230440	-0.632353	1.836896
H	0	-0.383298	1.238348	2.140830
H	0	0.864058	1.720670	0.988030
H	0	-0.598802	1.367632	-0.893052
H	0	-1.121576	-1.202654	2.282889
H	0	-0.359341	-2.368599	1.193964
H	0	-4.695135	-2.932344	0.525657
H	0	-3.798535	-2.121037	1.820267
H	0	-4.517917	-1.164134	0.504959
H	0	-2.752450	-4.400468	-0.098281
H	0	-1.117984	-3.747462	-0.263010
H	0	-1.928822	-3.774191	1.325770
H	0	-3.629674	-3.109788	-1.845296
H	0	-3.522899	-1.338371	-1.898656
H	0	-2.066758	-2.324503	-2.150211
H	0	-2.697927	5.045609	-1.501011
H	0	-3.723142	4.314876	-0.221604
H	0	-2.238256	5.188546	0.229774
H	0	3.665189	-2.064690	0.723935
H	0	5.962449	-1.266472	1.234198
H	0	6.685871	0.991992	0.486484
H	0	5.107753	2.445614	-0.768987
H	0	2.809727	1.643602	-1.266213

cis-**5b**
E = -3341.49324103 a.u.

C	0	0.086747	0.677613	-0.594959
C	0	0.291881	-0.727512	-0.041451
C	0	-0.970616	-1.549180	-0.241482
C	0	-2.114643	-0.864170	0.515918
C	0	-2.200628	0.675458	0.365874
N	0	-1.077102	1.371812	-0.003307
Se	0	1.810155	-1.599933	-0.982295
C	0	-3.463039	-1.430780	0.082246
O	0	-3.790858	-1.593605	-1.073182
O	0	-3.271075	1.204917	0.658363
C	0	-1.177141	2.879519	-0.148521
C	0	-1.584573	3.502022	1.202632
O	0	-4.230375	-1.753396	1.137894
C	0	-5.543661	-2.240902	0.813860
C	0	0.184613	3.485000	-0.538131
C	0	-2.194851	3.225622	-1.254607
H	0	-1.228428	-1.600488	-1.306315
H	0	-0.836577	-2.577013	0.113288
H	0	-2.003942	-1.038065	1.592774
H	0	-0.016716	0.616502	-1.688245
H	0	0.982472	1.260244	-0.388597
H	0	0.562121	-0.684997	1.018546
H	0	0.056811	4.569347	-0.613333
H	0	0.956020	3.300328	0.217599
H	0	0.548504	3.134155	-1.509049
H	0	-1.598953	4.594119	1.109687
H	0	-2.570515	3.163543	1.517018
H	0	-0.855086	3.238267	1.977188
H	0	-2.254370	4.313301	-1.377600
H	0	-1.883707	2.795812	-2.214305
H	0	-3.186719	2.847753	-1.005119
H	0	-6.016529	-2.463264	1.770731
H	0	-6.107838	-1.476001	0.274396
H	0	-5.478078	-3.140416	0.196051
C	0	3.258140	-0.741393	-0.042589
C	0	3.967433	0.303179	-0.645232
C	0	5.033872	0.903763	0.027690
C	0	5.392290	0.465201	1.303522
C	0	4.689552	-0.582204	1.904118
C	0	3.630494	-1.190953	1.229807
H	0	3.682939	0.639021	-1.637787

H	0	5.581715	1.714654	-0.444957
H	0	6.221116	0.934068	1.826956
H	0	4.971531	-0.932246	2.893576
H	0	3.091901	-2.018604	1.681916

trans-**2c**

E = -3380.81425836 a.u.

C	0	3.508649	0.690754	-0.319287
C	0	3.233318	-0.644614	-0.005352
C	0	3.974571	-1.290460	0.990030
C	0	4.973268	-0.599188	1.678015
C	0	5.241422	0.735664	1.368302
C	0	4.510795	1.378973	0.367362
Se	0	1.864173	-1.608927	-0.964933
C	0	0.371318	-1.305244	0.319956
C	0	-0.978629	-1.031587	-0.378725
C	0	-0.917175	0.292206	-1.176923
N	0	-1.149032	1.333094	-0.168201
C	0	-1.820387	0.852705	0.921249
C	0	-1.996714	-0.674755	0.747285
C	0	-1.370053	-2.223598	-1.261682
C	0	-3.446455	-0.924082	0.368485
O	0	-3.997053	-0.452251	-0.606351
O	0	-2.245902	1.485118	1.877978
C	0	-0.986318	2.796298	-0.427766
C	0	-0.204132	3.431627	0.738495
O	0	-4.056870	-1.735428	1.252805
C	0	-5.448986	-1.992796	0.994363
C	0	-0.192265	3.005299	-1.727663
C	0	-2.379808	3.440918	-0.567156
H	0	-1.695101	0.312994	-1.950116
H	0	0.060578	0.399256	-1.650183
H	0	-1.786269	-1.178350	1.693191
H	0	-2.281535	4.512832	-0.773982
H	0	-2.937759	2.981672	-1.390946
H	0	-2.953625	3.314548	0.353462
H	0	-0.073417	4.504381	0.554871
H	0	-0.736131	3.298307	1.681508
H	0	0.789088	2.976206	0.827088
H	0	-0.077013	4.080534	-1.898287
H	0	0.810479	2.568261	-1.667356

H	0	-0.704282	2.584517	-2.599230
H	0	-5.779405	-2.643344	1.804229
H	0	-6.014567	-1.057788	0.994316
H	0	-5.574141	-2.486105	0.026874
H	0	0.295347	-2.197108	0.946639
H	0	0.677160	-0.458643	0.937559
H	0	2.941707	1.184821	-1.102501
H	0	4.719931	2.416244	0.119513
H	0	6.020936	1.271948	1.902683
H	0	5.543254	-1.104973	2.452864
H	0	3.766896	-2.330947	1.220371
H	0	-0.627923	-2.373144	-2.055069
H	0	-1.418306	-3.147231	-0.672583
H	0	-2.340463	-2.065263	-1.739191

cis-**2c**

E = -3380.81340803 a.u.

C	0	-3.969222	-1.461105	0.417394
C	0	-3.521283	-0.314597	-0.247094
C	0	-4.235988	0.882239	-0.119115
C	0	-5.365509	0.939536	0.697685
C	0	-5.807131	-0.205146	1.365756
C	0	-5.112513	-1.406528	1.217379
Se	0	-1.992957	-0.420792	-1.416970
C	0	-0.736475	0.829407	-0.510986
C	0	0.312609	0.131263	0.365074
C	0	1.425050	1.083109	0.900418
C	0	2.664615	0.158770	1.002674
N	0	2.423004	-0.966318	0.264902
C	0	1.141756	-0.899698	-0.443745
C	0	1.806470	2.215248	-0.037457
O	0	2.098205	2.075192	-1.209482
C	0	3.495633	-1.961154	-0.049231
C	0	4.052980	-2.540520	1.265557
O	0	3.678538	0.443915	1.623871
C	0	2.906431	-3.109751	-0.884545
C	0	4.609833	-1.260352	-0.851890
O	0	1.801177	3.404044	0.593209
C	0	2.215034	4.527949	-0.204792
H	0	3.235988	4.381594	-0.565830
H	0	1.548045	4.655941	-1.061355

C	0	-0.358175	-0.560269	1.564784
H	0	-1.343302	1.532926	0.065735
H	0	-0.265432	1.364321	-1.336314
H	0	1.282403	-0.562779	-1.479525
H	0	0.641696	-1.869638	-0.463647
H	0	1.195324	1.496819	1.884000
H	0	2.160885	5.390965	0.458881
H	0	-3.910608	1.763116	-0.665044
H	0	-5.909886	1.874767	0.799031
H	0	-6.692767	-0.161510	1.993770
H	0	-5.453452	-2.301836	1.730537
H	0	-3.419569	-2.391370	0.309273
H	0	4.828147	-3.282181	1.041193
H	0	4.485395	-1.754239	1.885510
H	0	3.258041	-3.038508	1.832609
H	0	5.400565	-1.976300	-1.103635
H	0	4.212874	-0.844789	-1.784958
H	0	5.049166	-0.447886	-0.268827
H	0	3.704135	-3.826002	-1.106220
H	0	2.119574	-3.646975	-0.343751
H	0	2.499338	-2.762169	-1.839665
H	0	-1.096617	-1.285978	1.213196
H	0	0.377622	-1.083972	2.183813
H	0	-0.876114	0.171219	2.195905

trans-**5c**

E = -3380.81340803 a.u.

C	0	-0.997668	-1.372842	1.201071
C	0	0.329075	-0.611431	1.177920
C	0	0.044626	0.884447	1.244975
C	0	-0.905242	1.318915	0.126017
C	0	-2.070664	0.355050	-0.196032
N	0	-1.934716	-0.973735	0.136777
Se	0	1.151595	-1.124983	-0.600417
C	0	2.917659	-0.373934	-0.411636
C	0	3.171178	0.946182	-0.805138
C	0	4.460067	1.473939	-0.706853
C	0	5.505859	0.683639	-0.226286
C	0	5.261624	-0.638002	0.152286
C	0	3.972925	-1.166000	0.058438
C	0	1.218690	-1.082356	2.326233

C	0	-1.511788	2.682828	0.425747
O	0	-1.410158	3.514464	-0.626790
C	0	-2.019345	4.804031	-0.449184
O	0	-3.021832	0.808057	-0.827010
C	0	-3.002903	-1.948570	-0.317893
C	0	-4.348890	-1.605330	0.350714
O	0	-2.006371	2.992244	1.488781
C	0	-3.105294	-1.894974	-1.856867
C	0	-2.620136	-3.392303	0.059219
H	0	-0.420984	1.108029	2.214686
H	0	0.974685	1.463075	1.197247
H	0	-0.350590	1.375645	-0.816233
H	0	-1.458205	-1.232963	2.193424
H	0	-0.778145	-2.432163	1.091002
H	0	-5.116645	-2.320163	0.032023
H	0	-4.265838	-1.667568	1.442657
H	0	-4.672127	-0.599854	0.079448
H	0	-3.386742	-4.058910	-0.347617
H	0	-1.659969	-3.690821	-0.376703
H	0	-2.588880	-3.560174	1.140832
H	0	-3.805144	-2.664034	-2.202766
H	0	-3.453642	-0.923063	-2.202767
H	0	-2.124327	-2.096924	-2.302119
H	0	-1.838839	5.342987	-1.379661
H	0	-3.091959	4.693839	-0.270718
H	0	-1.568209	5.330150	0.396432
H	0	3.779988	-2.194887	0.346158
H	0	6.073890	-1.260189	0.518711
H	0	6.509569	1.093812	-0.154367
H	0	4.646968	2.500064	-1.012180
H	0	2.363034	1.555711	-1.197866
H	0	1.384897	-2.163816	2.282612
H	0	2.193798	-0.588108	2.297842
H	0	0.750452	-0.841963	3.290449

cis-**5c**

E = -3380.81340803 a.u.

C	0	3.990725	-1.069938	0.968119
C	0	3.248542	-0.741563	-0.173548
C	0	3.696586	0.284595	-1.015251
C	0	4.858498	0.992624	-0.702892

C	0	5.585094	0.673288	0.446014
C	0	5.152171	-0.360502	1.278853
Se	0	1.683825	-1.765236	-0.641667
C	0	0.216473	-0.751015	0.296591
C	0	0.097661	0.625882	-0.362666
N	0	-1.089481	1.388450	0.083762
C	0	-2.279591	0.747215	0.320357
C	0	-2.280462	-0.791169	0.503169
C	0	-1.051657	-1.540625	-0.029374
C	0	-3.550300	-1.314960	-0.161910
O	0	-4.500241	-1.609813	0.742474
C	0	-5.752802	-2.053057	0.192786
O	0	-3.354444	1.324953	0.470886
C	0	-1.106972	2.895868	-0.097748
C	0	-1.973604	3.259096	-1.321136
O	0	-3.678269	-1.466882	-1.357644
C	0	-1.643347	3.561994	1.185873
C	0	0.314413	3.439115	-0.336262
H	0	-1.153251	-1.649827	-1.115434
H	0	-1.008424	-2.549555	0.398036
H	0	-2.382645	-0.943503	1.582788
H	0	0.079321	0.496766	-1.453583
H	0	0.988849	1.200360	-0.118872
C	0	0.509643	-0.675923	1.795969
H	0	0.242304	4.526878	-0.434247
H	0	0.988464	3.232166	0.502343
H	0	0.768693	3.061086	-1.257631
H	0	-1.605696	4.651591	1.072809
H	0	-2.671340	3.265854	1.388750
H	0	-1.018886	3.289480	2.044730
H	0	-1.973715	4.345639	-1.466202
H	0	-1.569600	2.798575	-2.230658
H	0	-3.002309	2.924899	-1.184621
H	0	-6.392269	-2.257129	1.051883
H	0	-6.187966	-1.270368	-0.433642
H	0	-5.611249	-2.955494	-0.407767
H	0	3.137172	0.518507	-1.915919
H	0	5.198382	1.788528	-1.360250
H	0	6.491247	1.222582	0.686835
H	0	5.720740	-0.619808	2.167991
H	0	3.657680	-1.884104	1.604161

H	0	0.531378	-1.678802	2.234640
H	0	1.477536	-0.202033	1.986726
H	0	-0.250895	-0.085024	2.320072

trans-**7**

E = -3168.18824973 a.u.

C	0	2.422350	-0.059147	0.515753
C	0	1.228938	-0.718267	-0.203235
C	0	1.283377	-2.191306	0.269512
C	0	2.780434	-2.522716	0.319413
C	0	3.474927	-1.199150	0.639541
C	0	-0.096419	-0.008374	0.051762
O	0	4.636102	-1.047067	0.932876
C	0	2.998305	1.152347	-0.187489
O	0	3.592626	1.983902	0.686533
C	0	4.257085	3.119606	0.104913
O	0	2.954803	1.339558	-1.385215
H	0	3.066603	-3.293684	1.041279
H	0	4.683923	3.668104	0.944632
H	0	5.042873	2.790572	-0.579540
H	0	3.543717	3.742331	-0.441332
H	0	-0.378556	-0.057982	1.107629
H	0	-0.050064	1.036391	-0.264195
H	0	1.444319	-0.679868	-1.279522
H	0	0.713263	-2.856758	-0.383335
H	0	0.841049	-2.269622	1.271858
H	0	2.159824	0.221143	1.545625
H	0	3.150081	-2.850682	-0.662587
Se	0	-1.548085	-0.880569	-0.991476
C	0	-3.034497	0.002398	-0.138151
C	0	-3.619648	-0.561258	1.001043
C	0	-4.706115	0.065844	1.613069
C	0	-5.215414	1.254622	1.086052
C	0	-4.637136	1.815449	-0.054459
C	0	-3.548907	1.191020	-0.666918
H	0	-3.223209	-1.490625	1.399145
H	0	-5.156733	-0.376593	2.497649
H	0	-6.063596	1.740603	1.560811
H	0	-5.032965	2.738517	-0.469770
H	0	-3.097581	1.619946	-1.556558

cis-**7**

E = -3168.18381068 a.u.

C	0	3.260409	1.487293	-0.283643
C	0	2.818459	0.162760	-0.201047
C	0	3.364455	-0.693314	0.761461
C	0	4.340868	-0.224076	1.641730
C	0	4.776226	1.100301	1.561847
C	0	4.236109	1.954752	0.598557
Se	0	1.484380	-0.497546	-1.426270
C	0	-0.124327	0.000002	-0.362349
C	0	-1.316449	-0.850361	-0.823076
C	0	-2.673236	-0.476782	-0.160719
C	0	-2.685381	-1.279426	1.164697
C	0	-1.675488	-2.420652	1.032748
C	0	-1.160316	-2.343038	-0.413356
C	0	-3.012787	0.981799	0.056020
O	0	-2.292872	1.799915	0.588402
O	0	-3.385172	-1.042394	2.120287
O	0	-4.251904	1.260523	-0.397881
C	0	-4.702063	2.607161	-0.167003
H	0	-2.143026	-3.373202	1.301931
H	0	-5.712177	2.650251	-0.574690
H	0	-4.707258	2.827562	0.903311
H	0	-4.049535	3.321545	-0.675873
H	0	-1.399819	-0.759998	-1.912553
H	0	-0.305931	1.061940	-0.510328
H	0	0.122739	-0.167475	0.688753
H	0	-0.122122	-2.666741	-0.521984
H	0	-1.776355	-2.970900	-1.067987
H	0	-3.472418	-0.923271	-0.768552
H	0	-0.878674	-2.245005	1.767335
H	0	3.024657	-1.723331	0.813331
H	0	4.761858	-0.893244	2.387561
H	0	5.537036	1.464874	2.246834
H	0	4.573873	2.985578	0.532015
H	0	2.838948	2.145116	-1.037569

trans-**8**

E = -3168.19281508a.u.

C	0	-0.167696	-0.047577	0.981179
C	0	1.249717	-0.618379	1.095318

C	0	2.215211	-0.043754	0.032093
C	0	2.158817	1.497605	0.013086
C	0	0.757139	2.072513	-0.078635
C	0	-0.163429	1.483569	1.008877
C	0	3.643040	-0.506637	0.270342
O	0	4.339599	-0.528874	-0.880988
C	0	5.732821	-0.859026	-0.750878
O	0	3.158496	2.184141	0.075166
Se	0	-1.001120	-0.751765	-0.701785
O	0	4.101078	-0.811109	1.349708
H	0	6.134935	-0.831979	-1.763862
H	0	6.237360	-0.125967	-0.116498
H	0	5.852329	-1.854138	-0.314352
H	0	-0.786047	-0.440947	1.792357
C	0	-2.836819	-0.339261	-0.285132
H	0	1.655379	-0.382728	2.086605
H	0	1.225222	-1.709966	1.012597
H	0	1.904195	-0.375546	-0.968429
H	0	0.820027	3.161992	-0.014915
H	0	0.337976	1.797900	-1.056826
H	0	0.182756	1.810570	2.000579
H	0	-1.179303	1.873682	0.885363
C	0	-3.458388	0.777732	-0.853932
C	0	-4.796541	1.055839	-0.566024
C	0	-5.515760	0.222717	0.292378
C	0	-4.898593	-0.896036	0.857211
C	0	-3.564716	-1.181300	0.563991
H	0	-2.896225	1.421917	-1.523135
H	0	-5.274465	1.924348	-1.011377
H	0	-6.556425	0.440633	0.516629
H	0	-5.457505	-1.551942	1.519390
H	0	-3.084334	-2.059101	0.986234

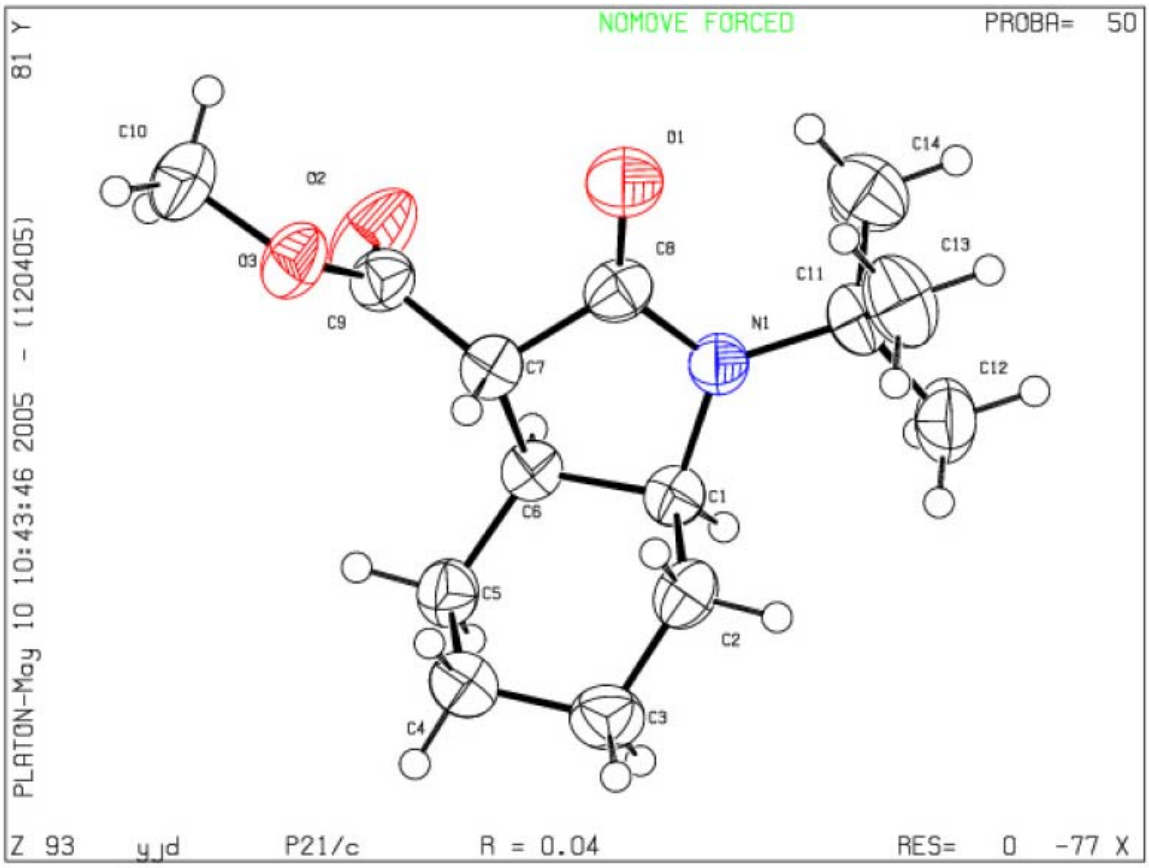
cis-**8**

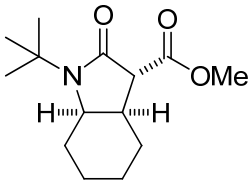
E = -3168.19616763 a.u.

C	0	0.074641	0.005980	-0.020252
C	0	-1.275401	-0.710122	-0.127470
C	0	-2.424311	0.157563	0.438916
C	0	-2.419476	1.562596	-0.195911
C	0	-1.071215	2.262784	-0.164974
C	0	0.044436	1.357847	-0.734537

C	0	-3.779293	-0.500273	0.229495
O	0	-4.655564	-0.104334	1.171876
C	0	-5.998675	-0.590395	1.004332
O	0	-3.412380	2.056219	-0.689733
Se	0	1.465838	-1.193201	-0.797005
O	0	-4.043092	-1.272040	-0.665408
H	0	-6.565791	-0.173875	1.837077
H	0	-6.407683	-0.248727	0.050297
H	0	-6.017893	-1.683088	1.032346
H	0	-1.502826	-0.941738	-1.174942
H	0	-1.242406	-1.667272	0.403251
H	0	-2.272323	0.304393	1.517548
H	0	-1.156086	3.201249	-0.720419
H	0	-0.838718	2.510538	0.881727
H	0	-0.126420	1.192374	-1.805687
H	0	1.011618	1.863101	-0.641498
H	0	0.347717	0.137275	1.033119
C	0	3.020593	-0.368125	-0.012054
C	0	3.814745	0.501670	-0.767468
C	0	4.957267	1.074118	-0.203848
C	0	5.308764	0.781471	1.115024
C	0	4.521076	-0.091680	1.869194
C	0	3.383967	-0.671547	1.305395
H	0	3.536029	0.723521	-1.793060
H	0	5.570418	1.748606	-0.795668
H	0	6.197697	1.227499	1.552891
H	0	4.796707	-0.329107	2.893346
H	0	2.777066	-1.365999	1.878923

Figure S1. Perspective view of the structure of **3g**, showing the crystallographic labeling.





3g

Table S2. Crystal data and structure refinement for compound **3g**.

Identification code	**3g**
Empirical formula	C14 H23 N O3
Formula weight	253.33
Temperature	295(2) K
Wavelength	0.71073 Agst
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a = 9.847(4)Agst alpha = 90deg
	b = 12.586(2)Agst beta = 99.81(2)deg
	c = 11.541(3)Agst gamma = 90deg
Volume	1409.4(7) Agst@3
Z	4
Density (calculated)	1.194 Mg/m@3
Absorption coefficient	0.083 mm@-1
F(000)	552
Crystal size	0.40 x 0.40 x 0.30 mm
Theta range for data collection	2.41 to 25.18 deg.
Index ranges	0<=h<=11; -1<=k<=15; -13<=l<=13
Reflections collected	2941
Independent reflections	2526 [R(int) = 0.0424]
Reflections observed (>2sigma)	1329
Data Completeness	0.999
Max. and min. transmission	0.9755 and 0.9676
Refinement method	Full-matrix least-squares on F@2
Data / restraints / parameters	2526 / 0 / 168
Goodness-of-fit on F@2	1.057
Final R indices [I>2sigma(I)]	R~1 = 0.0430 wR~2 = 0.0914
R indices (all data)	R~1 = 0.1213 wR~2 = 0.1130
Largest diff. peak and hole	0.137 and -0.165 e.Agst@-3

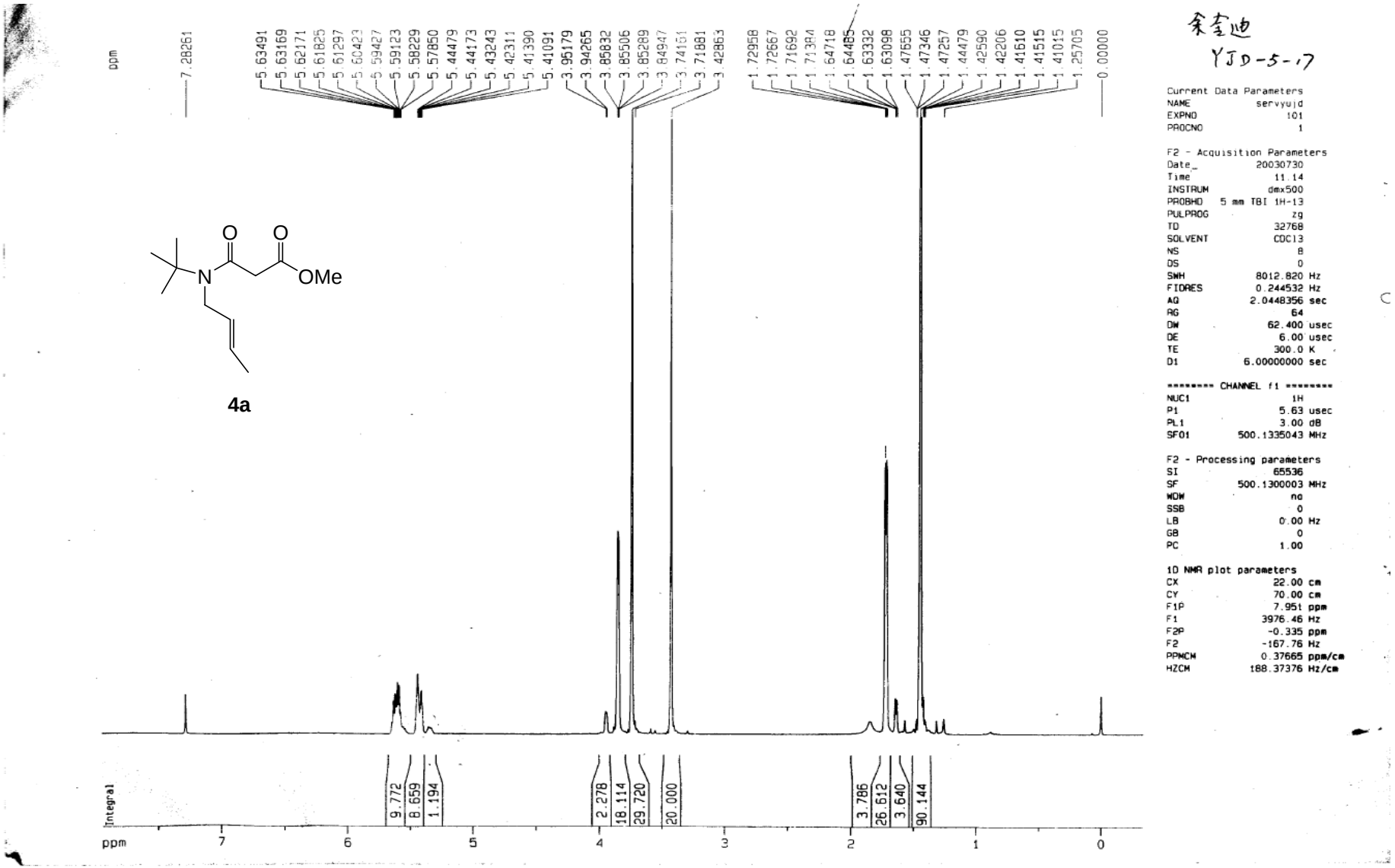
Table S3. Atomic coordinates (x 10@4) and equivalent isotropic displacement parameters (Agst@2 x 10@3) for YJD.U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
N(1)	7184(2)	5313(2)	-1423(2)	41(1)
O(1)	8111(2)	6642(2)	-153(2)	65(1)
O(2)	6350(2)	5424(2)	1838(2)	75(1)
O(3)	8589(2)	5309(2)	2528(1)	55(1)
C(1)	7045(2)	4150(2)	-1359(2)	38(1)
C(2)	8304(2)	3562(2)	-1650(2)	47(1)
C(3)	8335(3)	2408(2)	-1261(2)	55(1)
C(4)	8349(3)	2332(2)	51(2)	54(1)
C(5)	7080(3)	2856(2)	366(2)	48(1)
C(6)	6880(2)	3996(2)	-75(2)	38(1)
C(7)	7851(2)	4838(2)	549(2)	41(1)
C(8)	7735(2)	5727(2)	-366(2)	45(1)
C(9)	7492(3)	5224(2)	1685(2)	44(1)
C(10)	8347(3)	5641(2)	3671(2)	68(1)
C(11)	6914(2)	5957(2)	-2523(2)	47(1)
C(12)	6200(3)	5275(2)	-3546(2)	66(1)
C(13)	8276(3)	6374(3)	-2808(3)	69(1)
C(14)	5945(3)	6861(2)	-2347(3)	67(1)

Table S4. Bond lengths [Agst] and angles [deg] for **3g**.

N(1)-C(8)	1.352(3)	N(1)-C(1)	1.473(3)
N(1)-C(11)	1.492(3)	O(1)-C(8)	1.222(3)
O(2)-C(9)	1.194(3)	O(3)-C(9)	1.329(3)
O(3)-C(10)	1.442(3)	C(1)-C(6)	1.530(3)
C(1)-C(2)	1.530(3)	C(1)-H(1)	0.9800
C(2)-C(3)	1.519(3)	C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700	C(3)-C(4)	1.514(3)
C(3)-H(3A)	0.9700	C(3)-H(3B)	0.9700
C(4)-C(5)	1.511(3)	C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700	C(5)-C(6)	1.524(3)
C(5)-H(5A)	0.9700	C(5)-H(5B)	0.9700
C(6)-C(7)	1.524(3)	C(6)-H(6)	0.9800
C(7)-C(9)	1.496(3)	C(7)-C(8)	1.529(3)
C(7)-H(7)	0.9800	C(10)-H(10A)	0.9599
C(10)-H(10B)	0.9599	C(10)-H(10C)	0.9599
C(11)-C(14)	1.521(3)	C(11)-C(13)	1.527(3)
C(11)-C(12)	1.531(3)	C(12)-H(12A)	0.9599
C(12)-H(12B)	0.9599	C(12)-H(12C)	0.9599
C(13)-H(13A)	0.9599	C(13)-H(13B)	0.9599
C(13)-H(13C)	0.9599	C(14)-H(14A)	0.9599
C(14)-H(14B)	0.9599	C(14)-H(14C)	0.9599
C(8)-N(1)-C(1)	111.34(19)	C(8)-N(1)-C(11)	123.0(2)
C(1)-N(1)-C(11)	125.35(19)	C(9)-O(3)-C(10)	116.9(2)
N(1)-C(1)-C(6)	101.60(18)	N(1)-C(1)-C(2)	112.54(19)
C(6)-C(1)-C(2)	111.99(19)	N(1)-C(1)-H(1)	110.1
C(6)-C(1)-H(1)	110.1	C(2)-C(1)-H(1)	110.1
C(3)-C(2)-C(1)	111.9(2)	C(3)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2A)	109.2	C(3)-C(2)-H(2B)	109.2
C(1)-C(2)-H(2B)	109.2	H(2A)-C(2)-H(2B)	107.9
C(4)-C(3)-C(2)	110.6(2)	C(4)-C(3)-H(3A)	109.5

C(2)-C(3)-H(3A)	109.5	C(4)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3B)	109.5	H(3A)-C(3)-H(3B)	108.1
C(5)-C(4)-C(3)	110.3(2)	C(5)-C(4)-H(4A)	109.6
C(3)-C(4)-H(4A)	109.6	C(5)-C(4)-H(4B)	109.6
C(3)-C(4)-H(4B)	109.6	H(4A)-C(4)-H(4B)	108.1
C(4)-C(5)-C(6)	113.3(2)	C(4)-C(5)-H(5A)	108.9
C(6)-C(5)-H(5A)	108.9	C(4)-C(5)-H(5B)	108.9
C(6)-C(5)-H(5B)	108.9	H(5A)-C(5)-H(5B)	107.7
C(7)-C(6)-C(5)	117.50(19)	C(7)-C(6)-C(1)	102.01(18)
C(5)-C(6)-C(1)	114.50(19)	C(7)-C(6)-H(6)	107.4
C(5)-C(6)-H(6)	107.4	C(1)-C(6)-H(6)	107.4
C(9)-C(7)-C(6)	114.66(19)	C(9)-C(7)-C(8)	111.5(2)
C(6)-C(7)-C(8)	102.44(18)	C(9)-C(7)-H(7)	109.3
C(6)-C(7)-H(7)	109.3	C(8)-C(7)-H(7)	109.3
O(1)-C(8)-N(1)	127.3(2)	O(1)-C(8)-C(7)	124.5(2)
N(1)-C(8)-C(7)	108.2(2)	O(2)-C(9)-O(3)	122.9(2)
O(2)-C(9)-C(7)	124.5(2)	O(3)-C(9)-C(7)	112.6(2)
O(3)-C(10)-H(10A)	109.5	O(3)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5	O(3)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5
N(1)-C(11)-C(14)	108.6(2)	N(1)-C(11)-C(13)	109.55(19)
C(14)-C(11)-C(13)	111.5(2)	N(1)-C(11)-C(12)	110.0(2)
C(14)-C(11)-C(12)	107.9(2)	C(13)-C(11)-C(12)	109.4(2)
C(11)-C(12)-H(12A)	109.5	C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5	C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5	H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5	C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5	C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5	H(13B)-C(13)-H(13C)	109.5
C(11)-C(14)-H(14A)	109.5	C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5	C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5	H(14B)-C(14)-H(14C)	109.5



余奎池

YJD-5-17

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PROCNO 1

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PROBHD 5 mm TBI 1H-13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0448356 sec
RG 64
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

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P1 5.63 usec
PL1 3.00 dB
SF01 500.1335043 MHz

F2 - Processing parameters
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SF 500.1300003 MHz
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SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
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CY 70.00 cm
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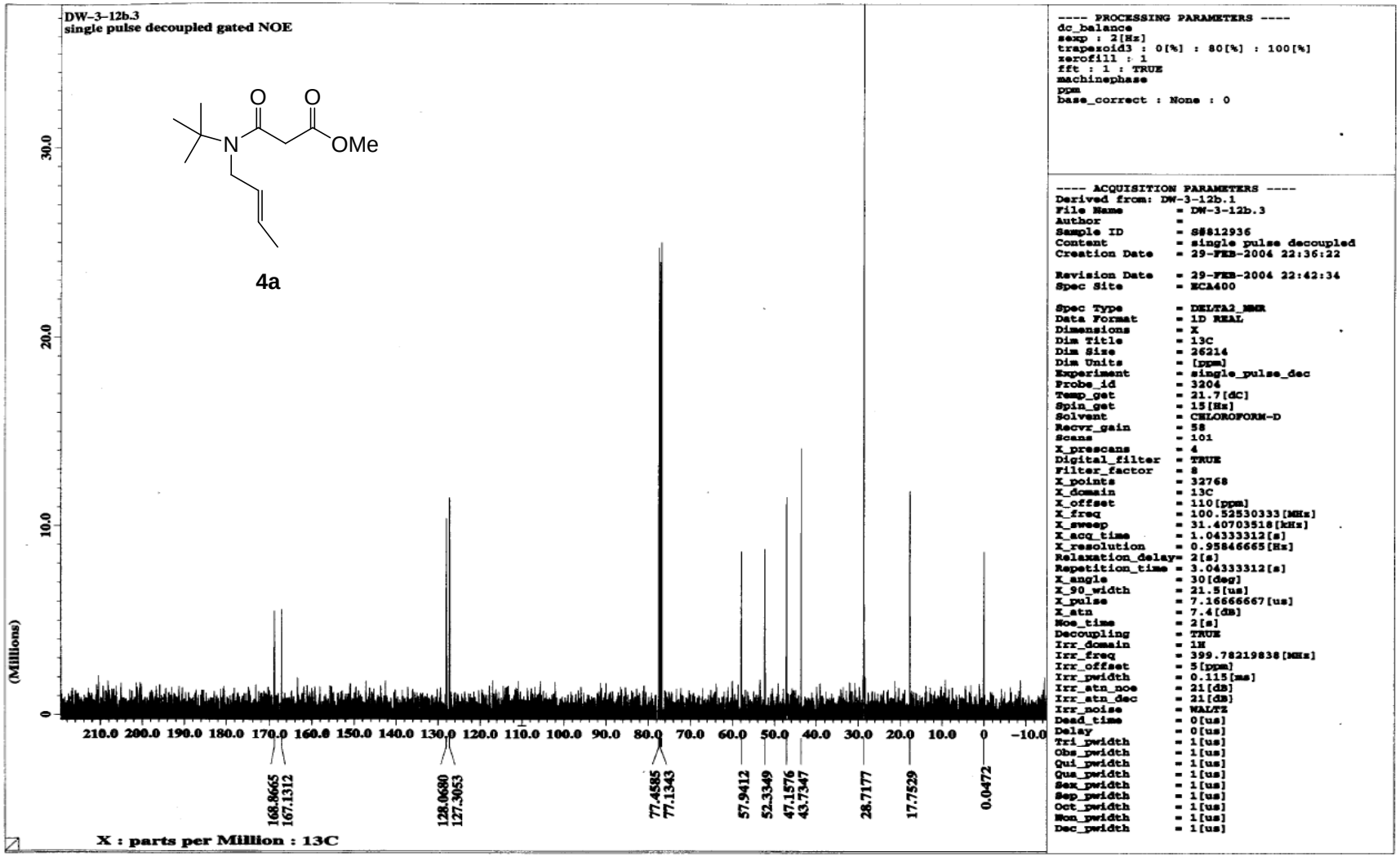
F2P -0.335 ppm
F2 -167.76 Hz
PPMCM 0.37665 ppm/cm
HZCM 188.37376 Hz/cm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O
N
OMe
4a
30.0
20.0
10.0
0
(Millions)
210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
168.8665
167.1312
128.0680
127.3053
77.4585
77.1343
57.9412
52.3349
47.1576
43.7347
28.7177
17.7529
0.0472
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zerofill : 1
fft : 1 : TRUE
machinephase
ppm
base_correct : None : 0
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Content = single pulse decoupled
Creation Date = 29-FEB-2004 22:36:22
Revision Date = 29-FEB-2004 22:42:34
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Spin_get = 15[Hz]
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Recvr_gain = 58
Scans = 101
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
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X_resolution = 0.95846665[Hz]
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Repetition_time = 3.04333312[s]
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X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
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Decoupling = TRUE
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Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
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Irr_atn_noe = 21[dB]
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Tri_pwidth = 1[us]
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Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
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Non_pwidth = 1[us]
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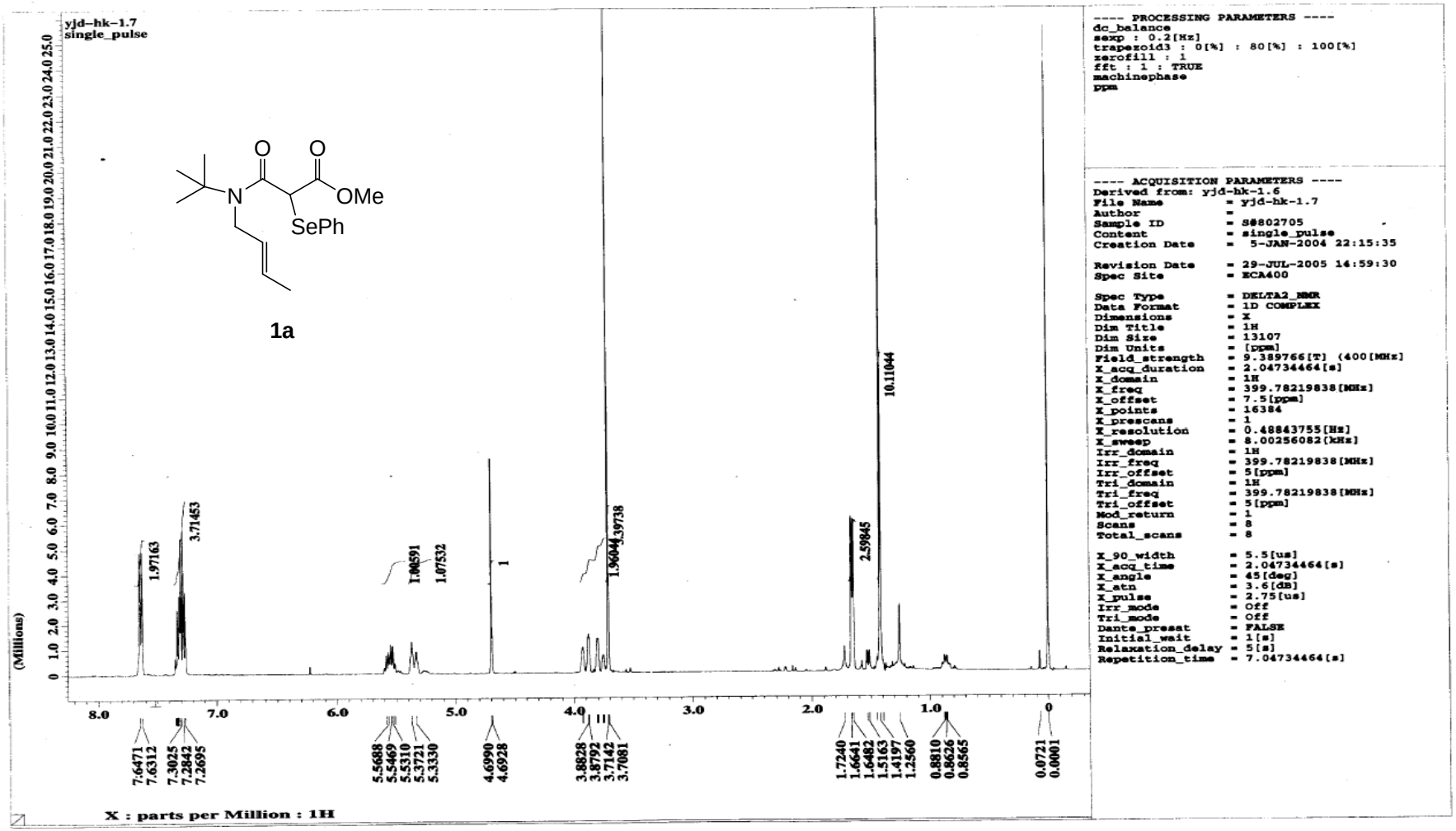
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O
O
N
OMe
SePh
1a
(Millions)
X : parts per Million : 1H
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fft : 1 : TRUE
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ppm
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Sample ID = S#802705
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Creation Date = 5-JAN-2004 22:15:35
Revision Date = 29-JUL-2005 14:59:30
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X_sweep = 8.00256082[kHz]
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Irr_offset = 5[ppm]
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Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
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Total_scans = 8
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X_acq_time = 2.04734464[s]
X_angle = 45[deg]
X_atn = 3.6[dB]
X_pulse = 2.75[us]
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Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
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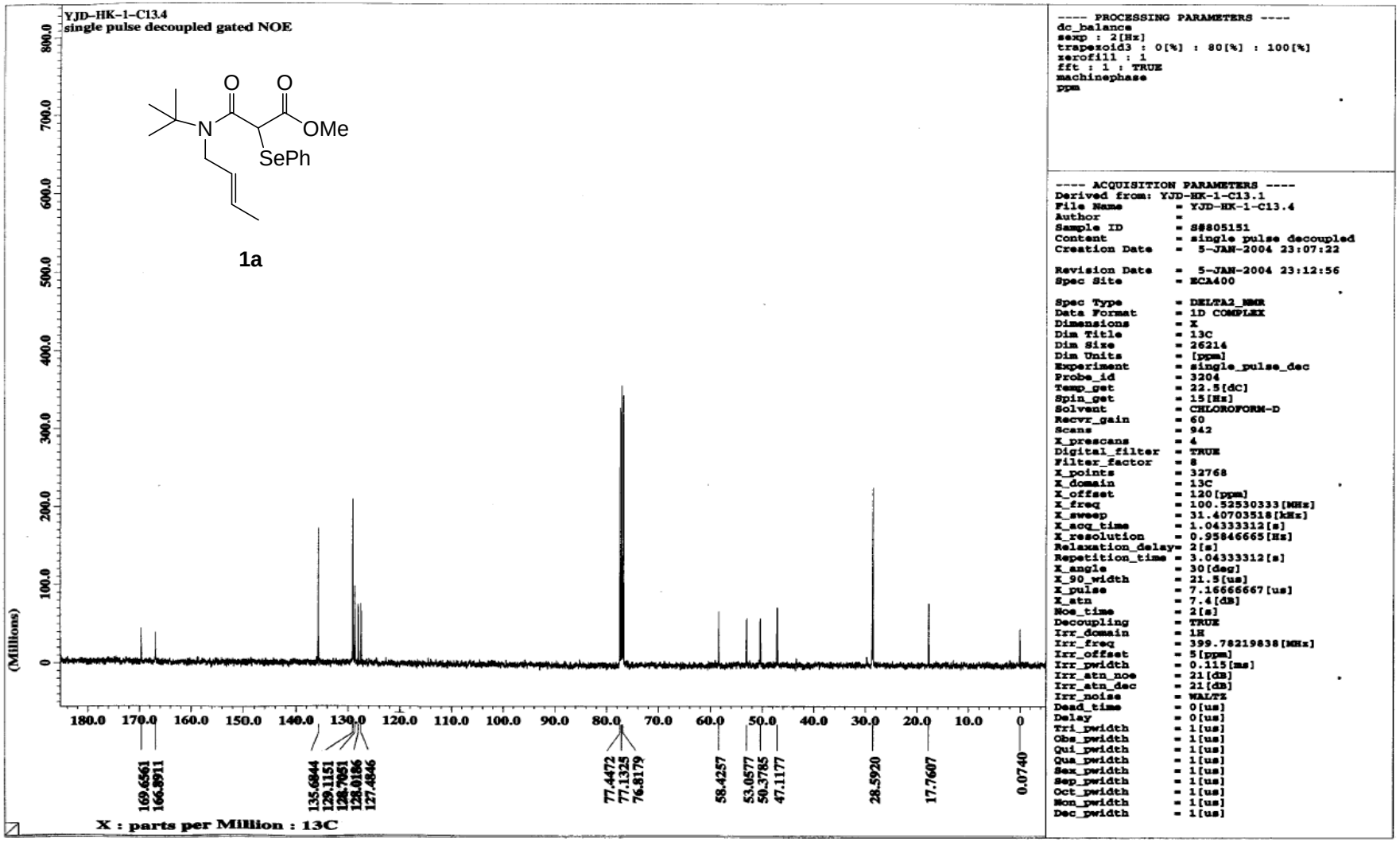
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single pulse decoupled gated NOE
O
O
N
OMe
SePh
1a
(Millions)
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700.0
600.0
500.0
400.0
300.0
200.0
100.0
0
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.6561
166.8911
135.6944
129.1151
128.7651
128.0186
127.4846
77.4472
77.1325
76.8179
58.4257
53.0577
50.3785
47.1177
28.5920
17.7607
0.0740
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
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trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
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Revision Date = 5-JAN-2004 23:12:56
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Spin_get = 15[Hz]
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Recvr_gain = 60
Scans = 942
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
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X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
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Repetition_time = 3.04333312[s]
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X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
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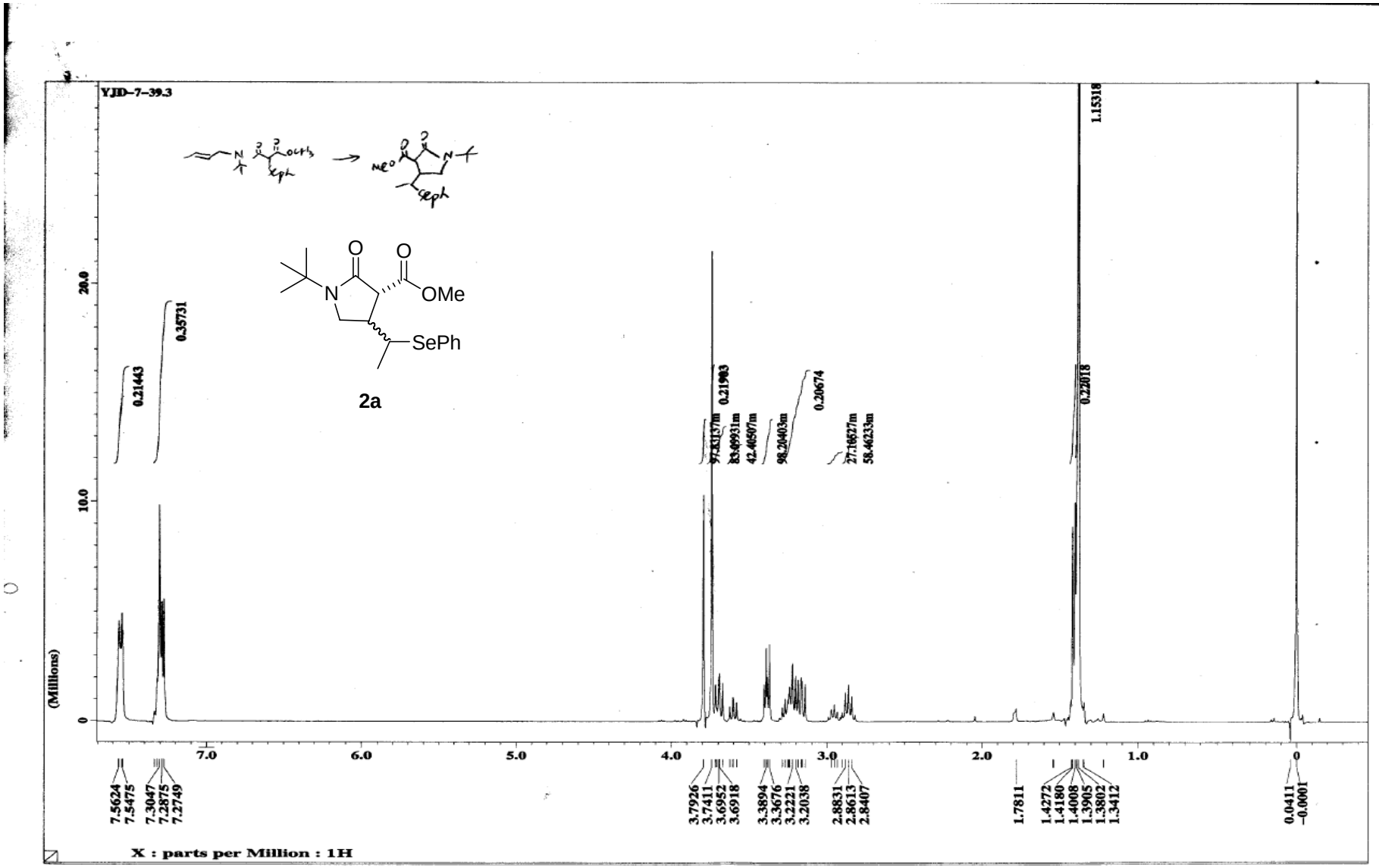
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]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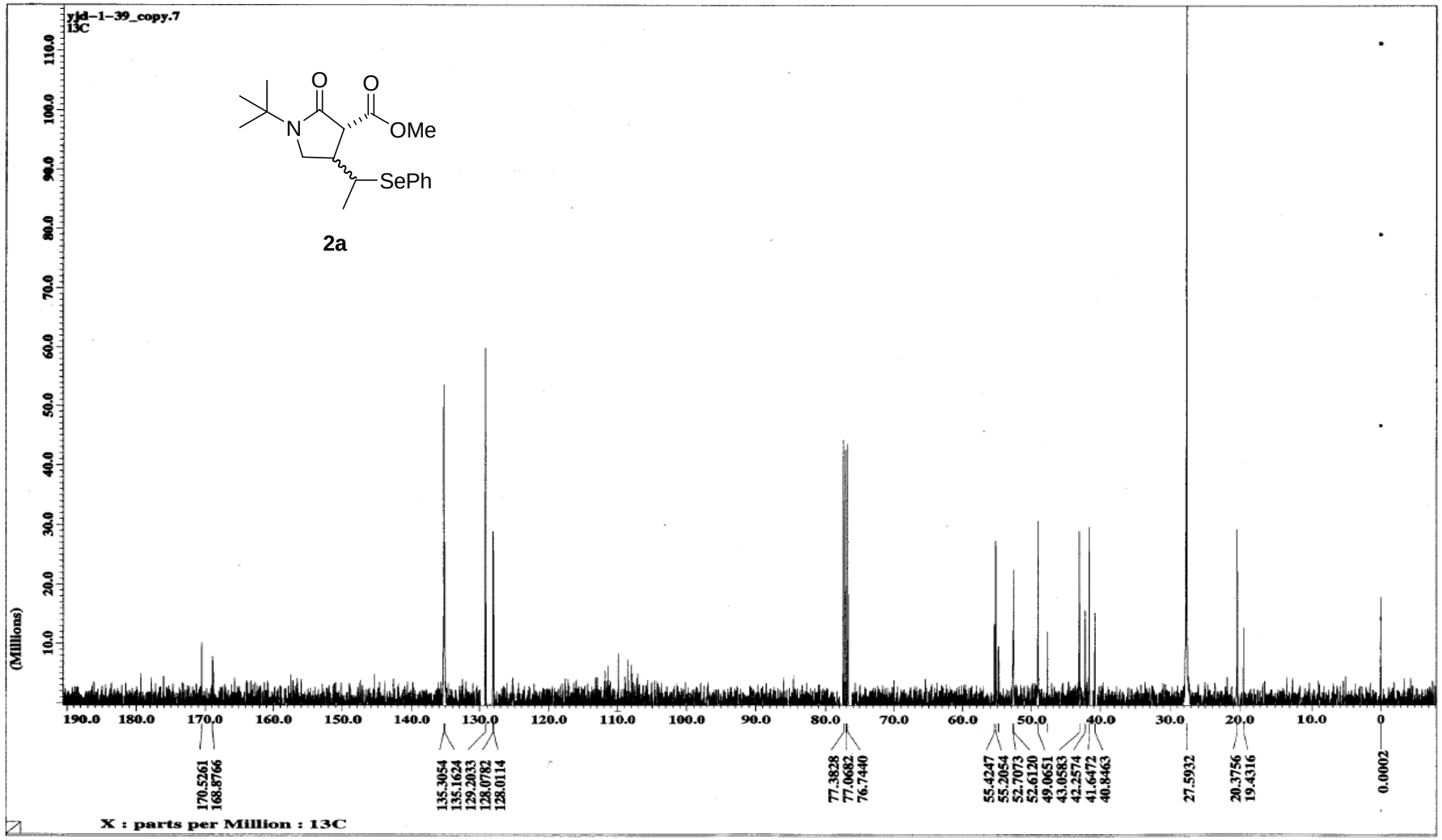
SePh
2a
(Millions)
X : parts per Million : 1H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O
O
N
OMe
SePh
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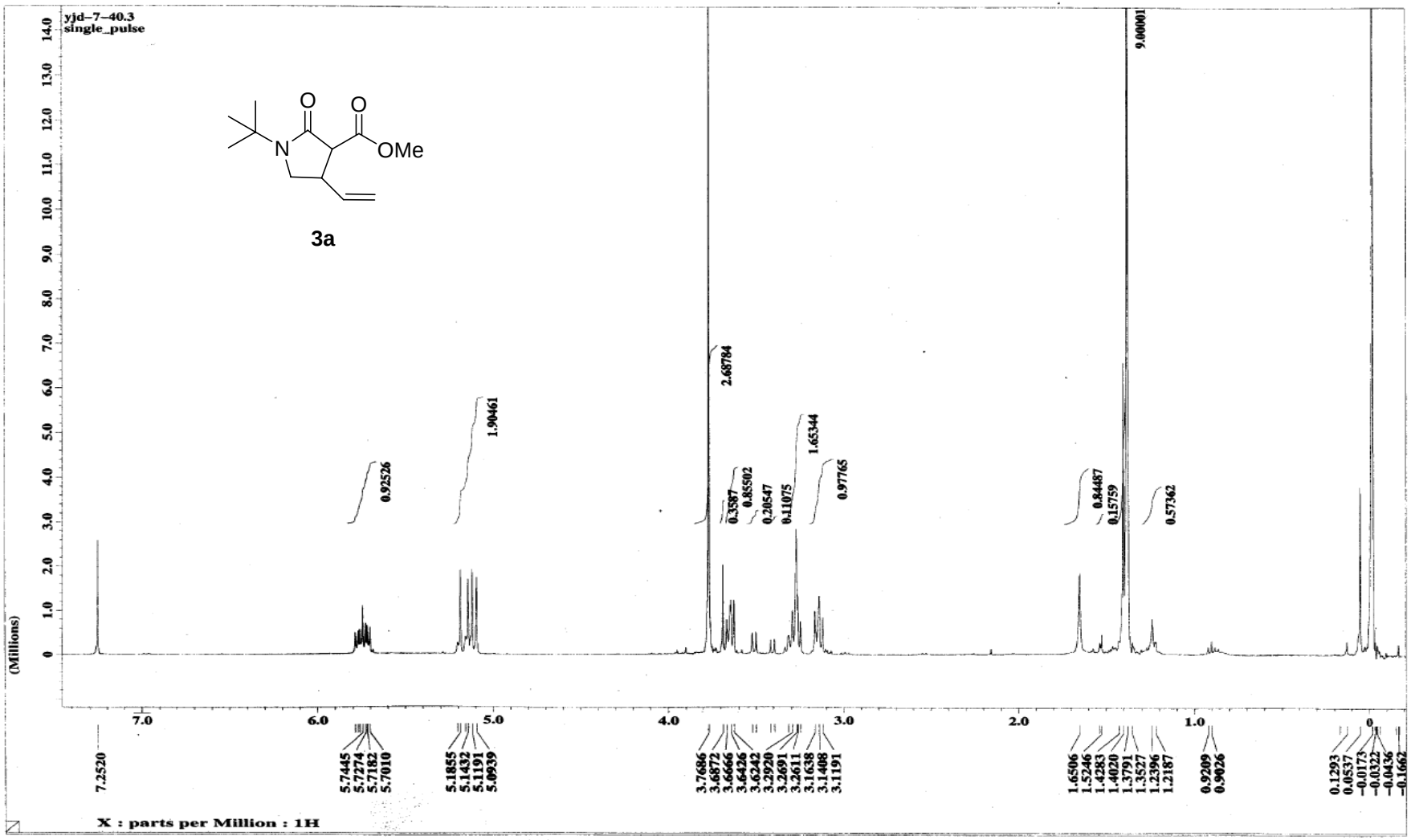
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single_pulse
O
O
N
OMe
3a
(Millions)
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1.2396
1.2187
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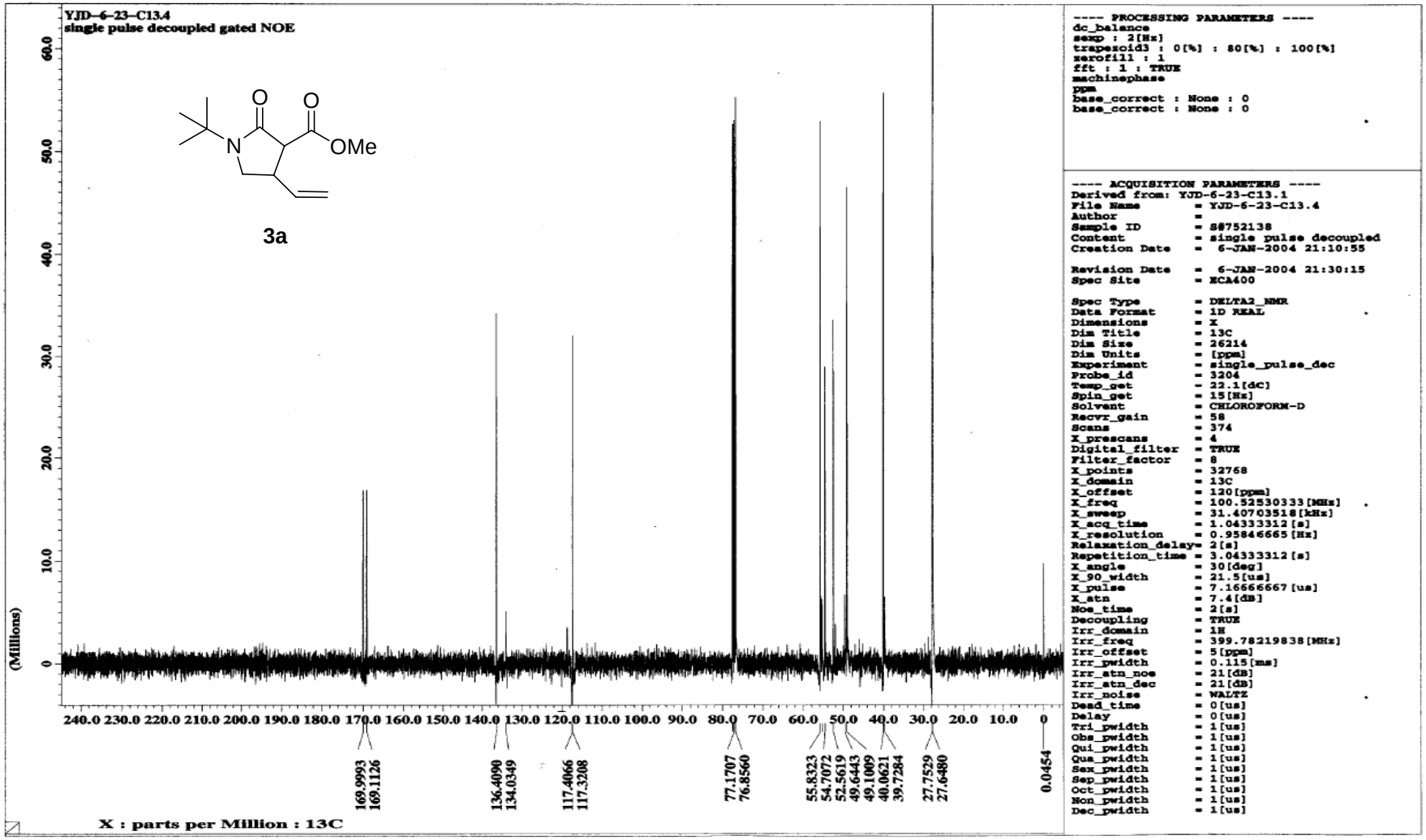
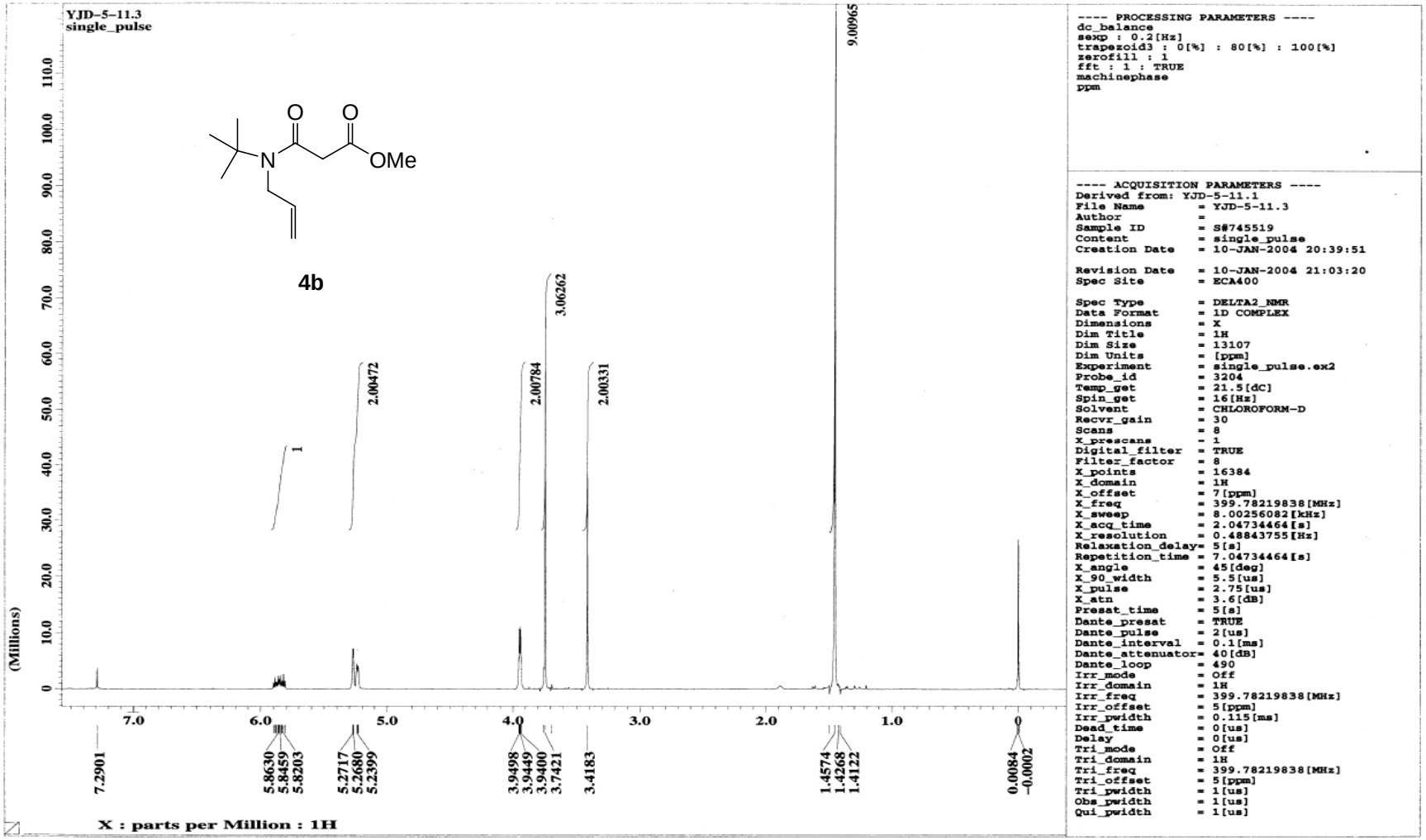
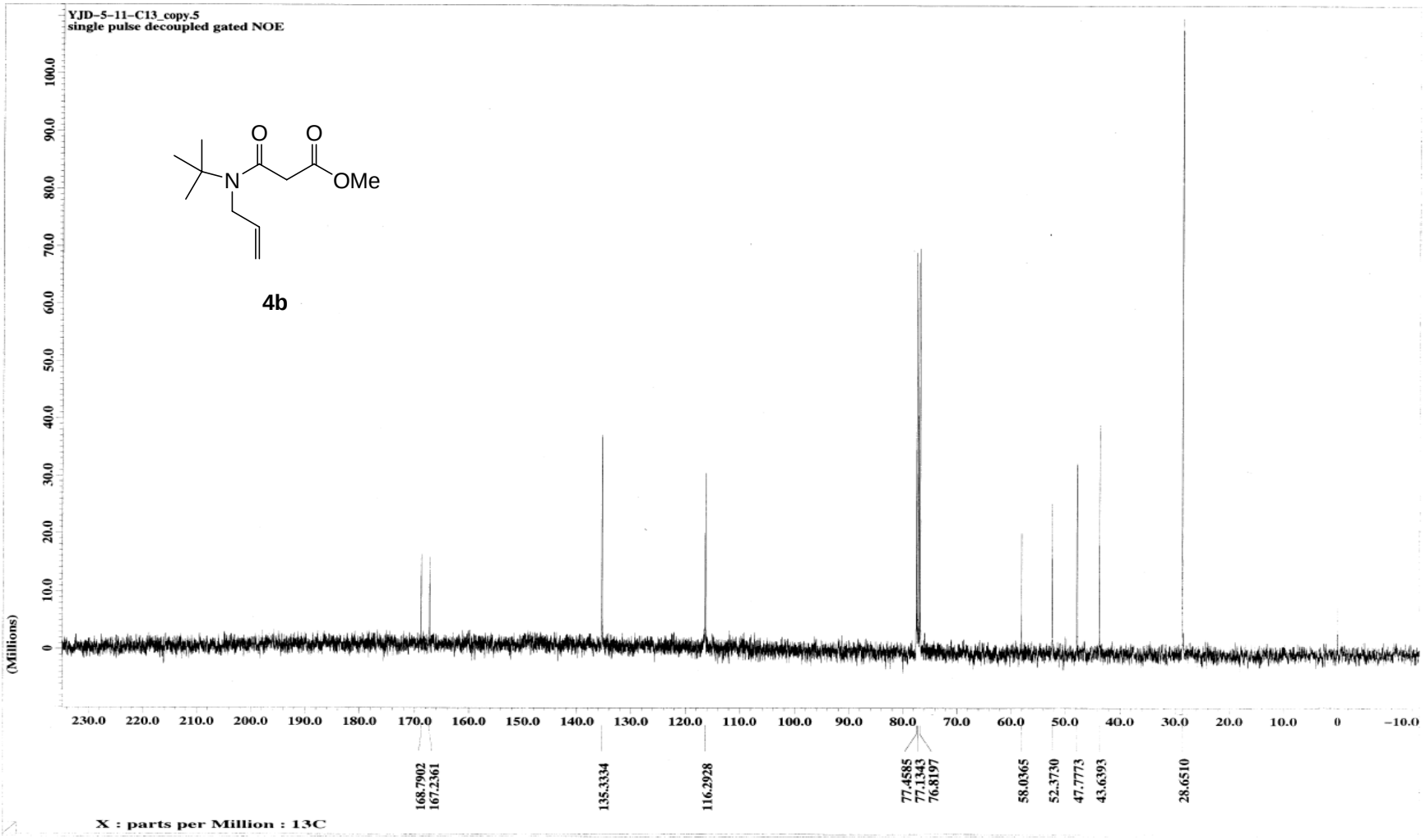
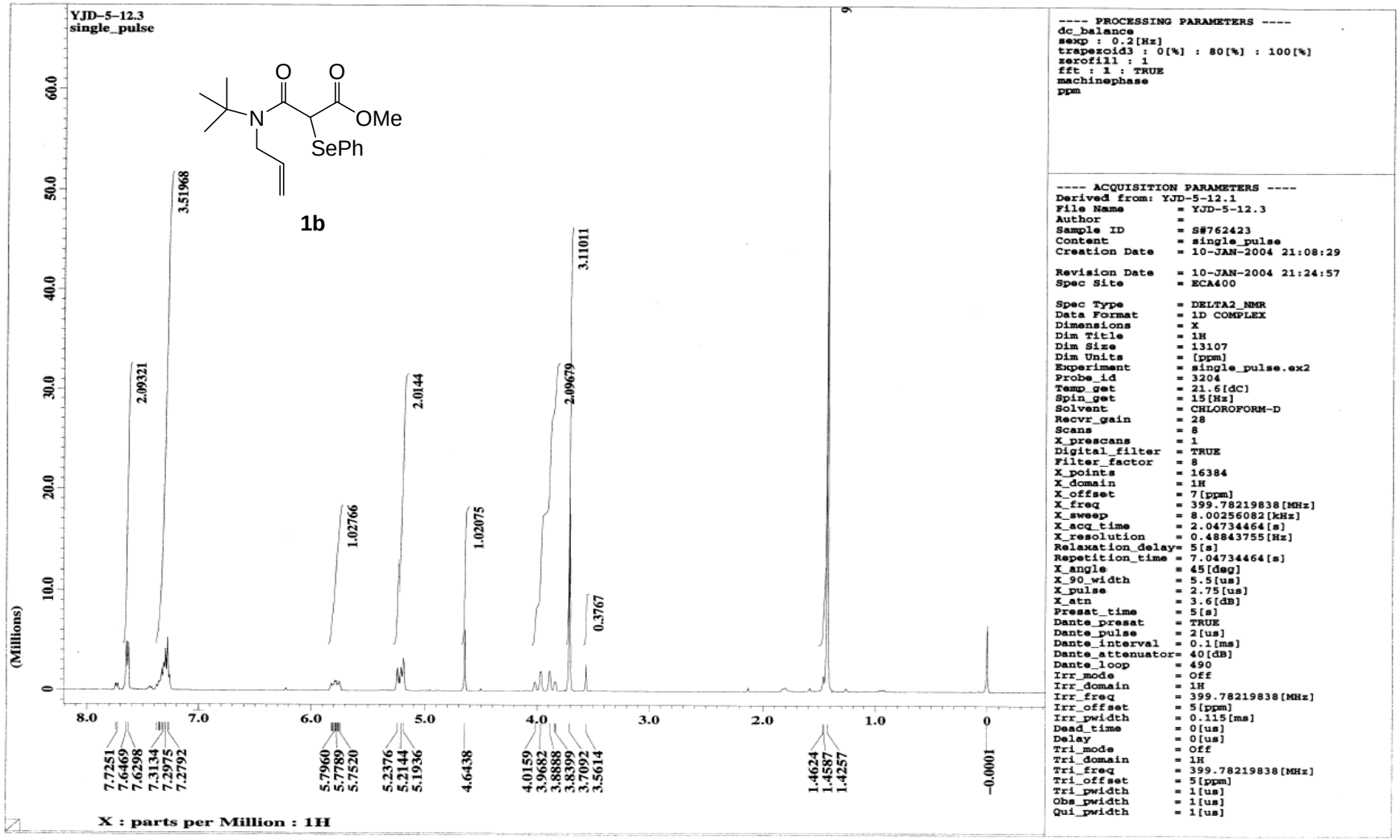
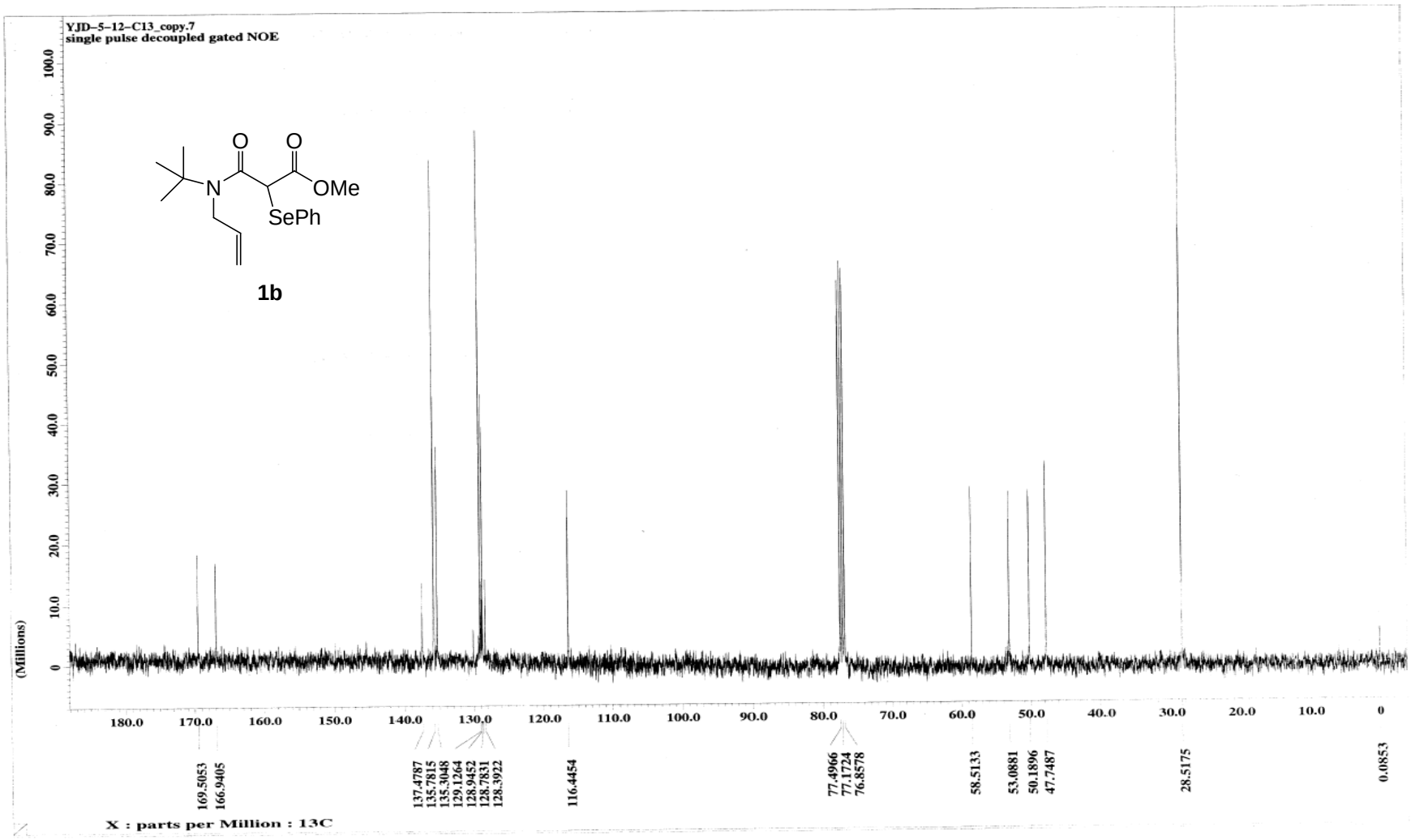
0.15759
0.57362
9.00001

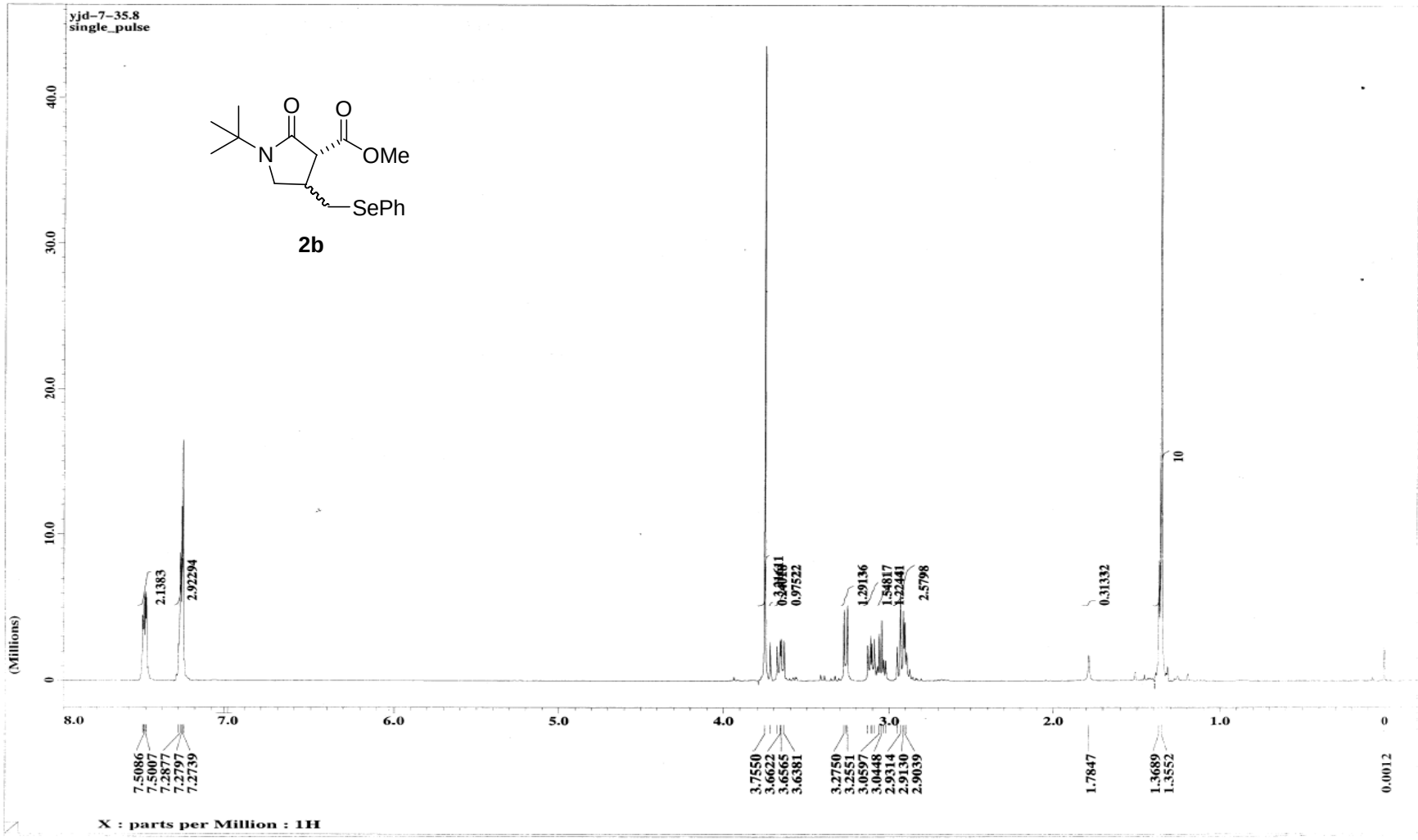

YJD–6–23–C13.4
single pulse decoupled gated NOE
O
O
N
OMe
3a
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
240.0 230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
169.9993
169.1126
136.4090
134.0349
117.4066
117.3208
77.1707
76.8560
55.8323
54.7072
52.5619
49.6443
49.1009
40.0621
39.7284
27.7529
27.6480
0.0454
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
base_correct : None : 0
base_correct : None : 0
---- ACQUISITION PARAMETERS ----
Derived from: YJD-6-23-C13.1
File Name = YJD-6-23-C13.4
Author =
Sample ID = S#752138
Content = single pulse decoupled
Creation Date = 6-JAN-2004 21:10:55
Revision Date = 6-JAN-2004 21:30:15
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D REAL
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 22.1[dC]
Spin_get = 15[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 58
Scans = 374
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 120[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

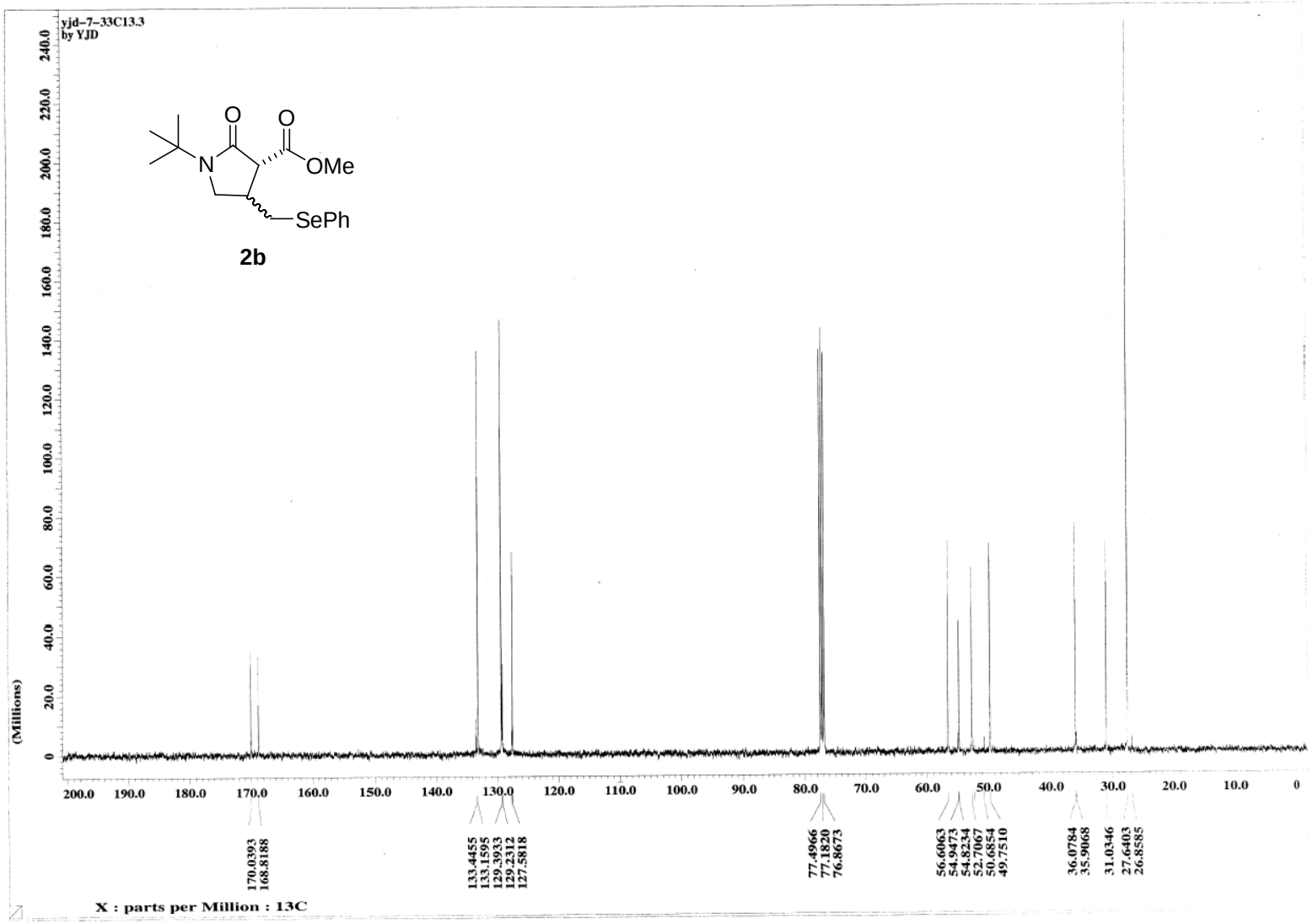

YJD-5-11.3
single_pulse
4b
(Millions)
X : parts per Million : 1H
1
2.00472
2.00784
3.06262
2.00331
9.00965
7.2901
5.8630
5.8459
5.8203
5.2717
5.2680
5.2399
3.9498
3.9449
3.9400
3.7421
3.4183
1.4574
1.4268
1.4122
0.0084
-0.0002
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-5-11.1
File Name = YJD-5-11.3
Author =
Sample ID = S#745519
Content = single_pulse
Creation Date = 10-JAN-2004 20:39:51
Revision Date = 10-JAN-2004 21:03:20
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 21.5[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 30
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay= 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Presat_time = 5[s]
Dante_presat = TRUE
Dante_pulse = 2[us]
Dante_interval = 0.1[ms]
Dante_attenuator= 40[dB]
Dante_loop = 490
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]

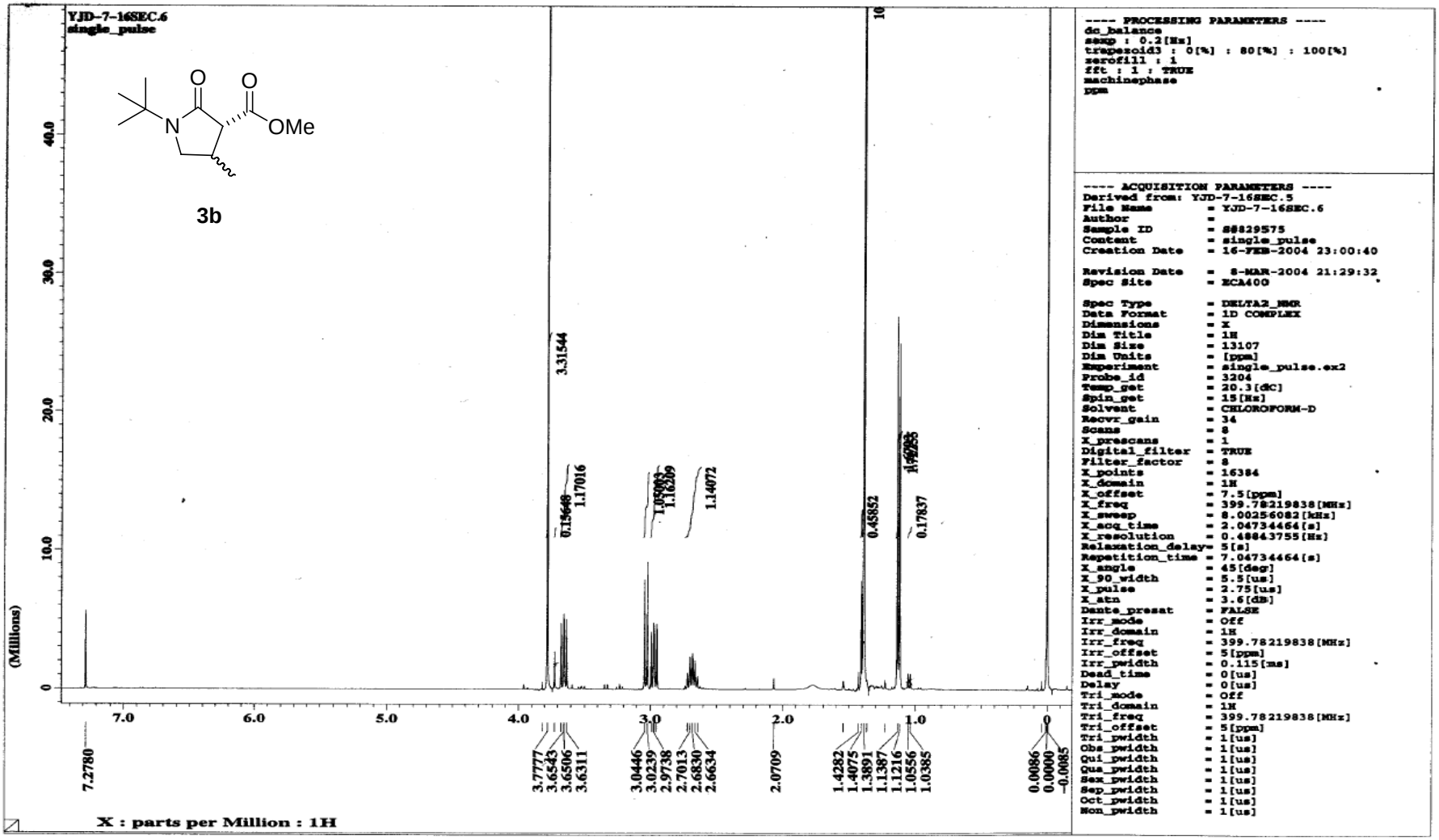

YJD-5-11-C13_copy.5
single pulse decoupled gated NOE
O
O
N
OMe
4b
(Millions)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
168.7902
167.2361
135.3334
116.2928
77.4585
77.1343
76.8197
58.0365
52.3730
47.7773
43.6393
28.6510
X : parts per Million : 13C

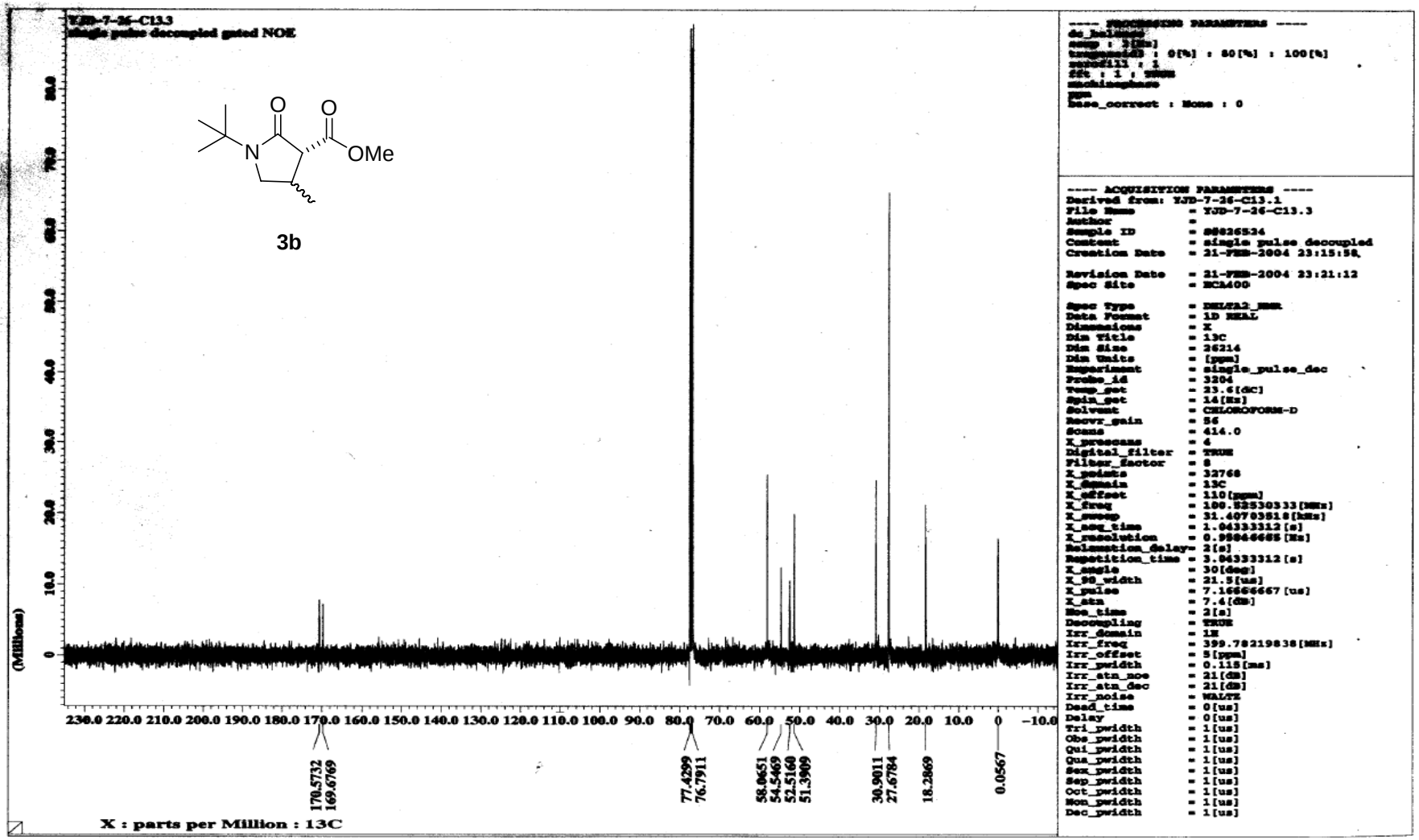

YJD-5-12.3
single_pulse
O
O
N
OMe
SePh
1b
3.51968
2.09321
2.0144
1.02766
1.02075
2.09679
3.11011
0.3767
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.7251
7.6469
7.6298
7.3134
7.2975
7.2792
5.7960
5.7789
5.7520
5.2376
5.2144
5.1936
4.6438
4.0159
3.9682
3.8888
3.8399
3.7092
3.5614
1.4624
1.4587
1.4257
-0.0001
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-5-12.1
File Name = YJD-5-12.3
Author =
Sample ID = S#762423
Content = single_pulse
Creation Date = 10-JAN-2004 21:08:29
Revision Date = 10-JAN-2004 21:24:57
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 21.6[dC]
Spin_get = 15[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 28
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay= 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Presat_time = 5[s]
Dante_presat = TRUE
Dante_pulse = 2[us]
Dante_interval = 0.1[ms]
Dante_attenuator= 40[dB]
Dante_loop = 490
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]

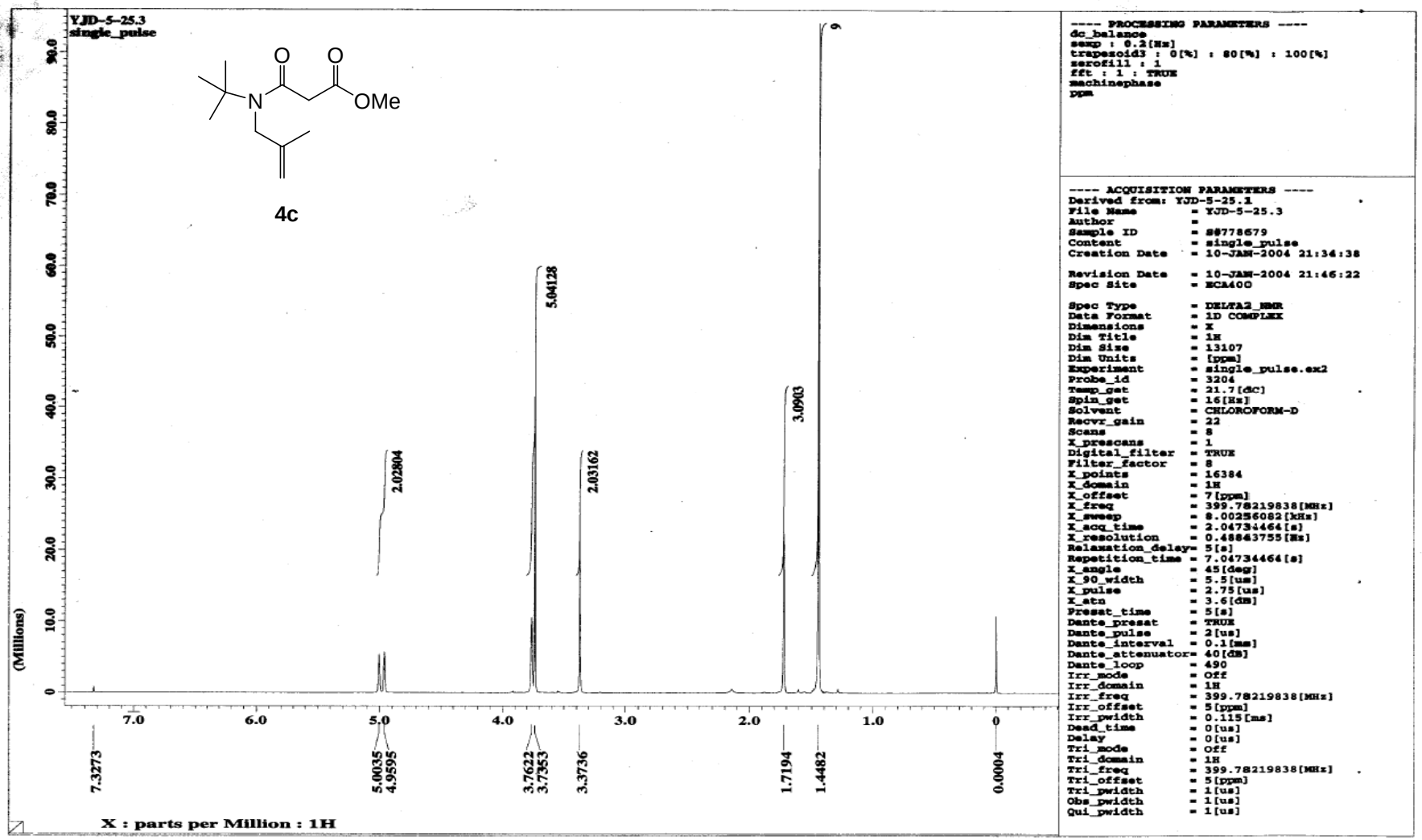

YJD–5–12–C13_copy.7
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1b
(Millions)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.5053
166.9405
137.4787
135.7815
135.3048
129.1264
128.9452
128.7831
128.3922
116.4454
77.4966
77.1724
76.8578
58.5133
53.0881
50.1896
47.7487
28.5175
0.0853
X : parts per Million : 13C

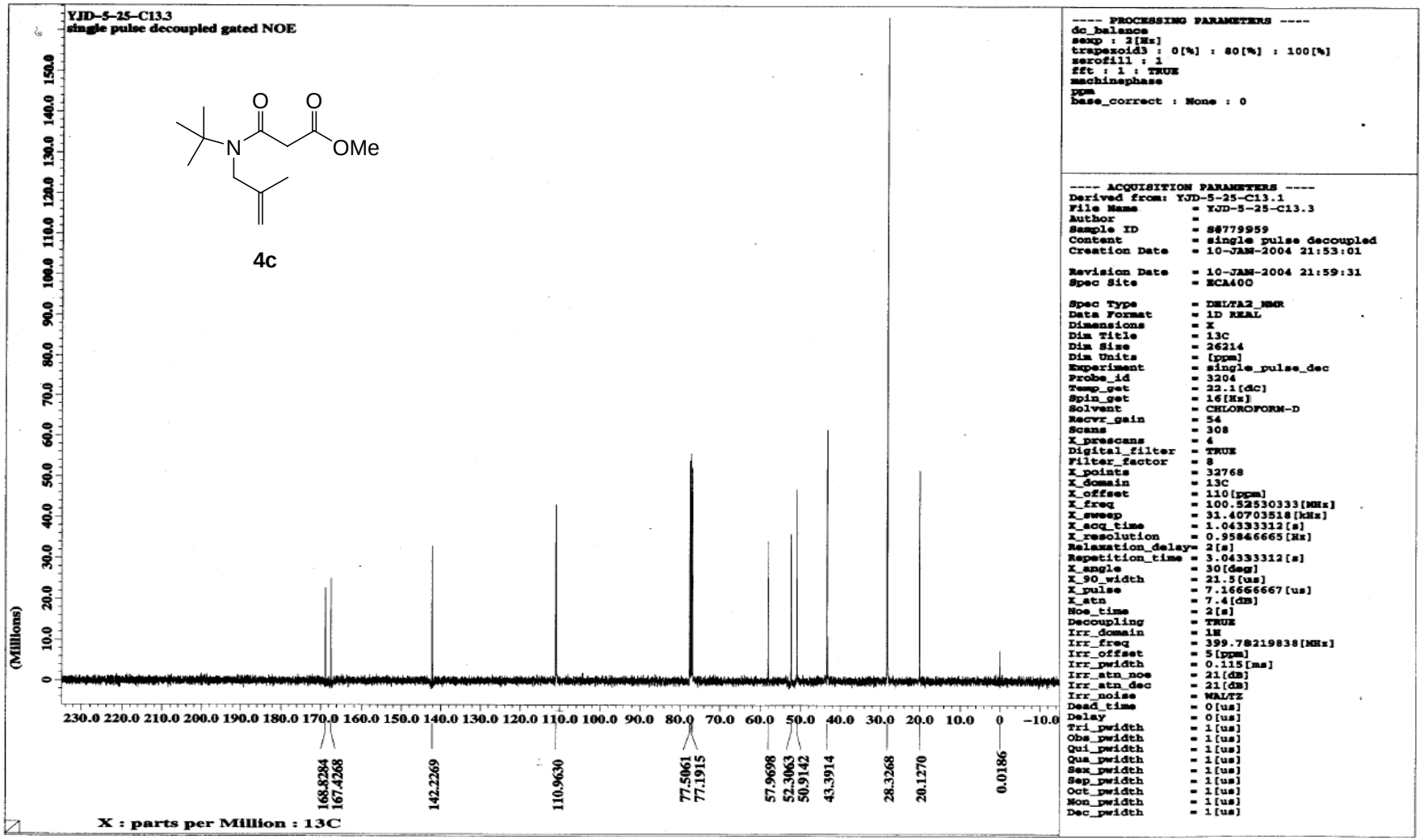

yjd-7-35.8
single_pulse
O
O
N
OMe
SePh
2b
(Millions)
40.0
30.0
20.0
10.0
0
2.1383
2.92294
0.97522
1.29136
1.54817
1.32441
2.5798
0.31332
10
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5086
7.5007
7.2877
7.2797
7.2739
3.7550
3.6622
3.6565
3.6381
3.2750
3.2551
3.0597
3.0448
2.9314
2.9130
2.9039
1.7847
1.3689
1.3552
0.0012
X : parts per Million : 1H

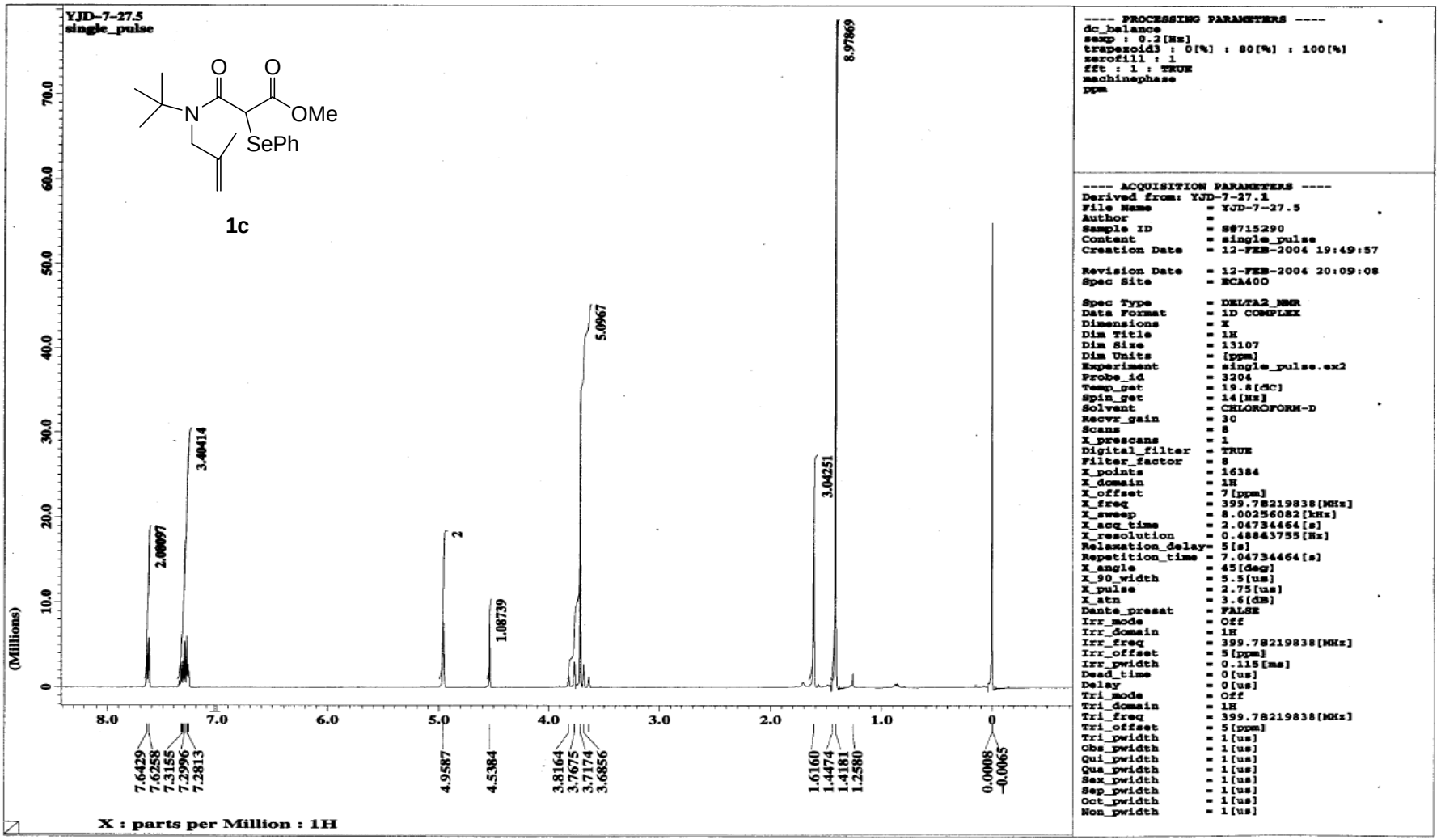

yjd-7-33C13.3
by YJD
O
O
N
OMe
SePh
2b
(Millions)
240.0
220.0
200.0
180.0
160.0
140.0
120.0
100.0
80.0
60.0
40.0
20.0
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
170.0393
168.8188
133.4455
133.1595
129.3933
129.2312
127.5818
77.4966
77.1820
76.8673
56.6063
54.9473
54.8234
52.7067
50.6854
49.7510
36.0784
35.9068
31.0346
27.6403
26.8585
X : parts per Million : 13C

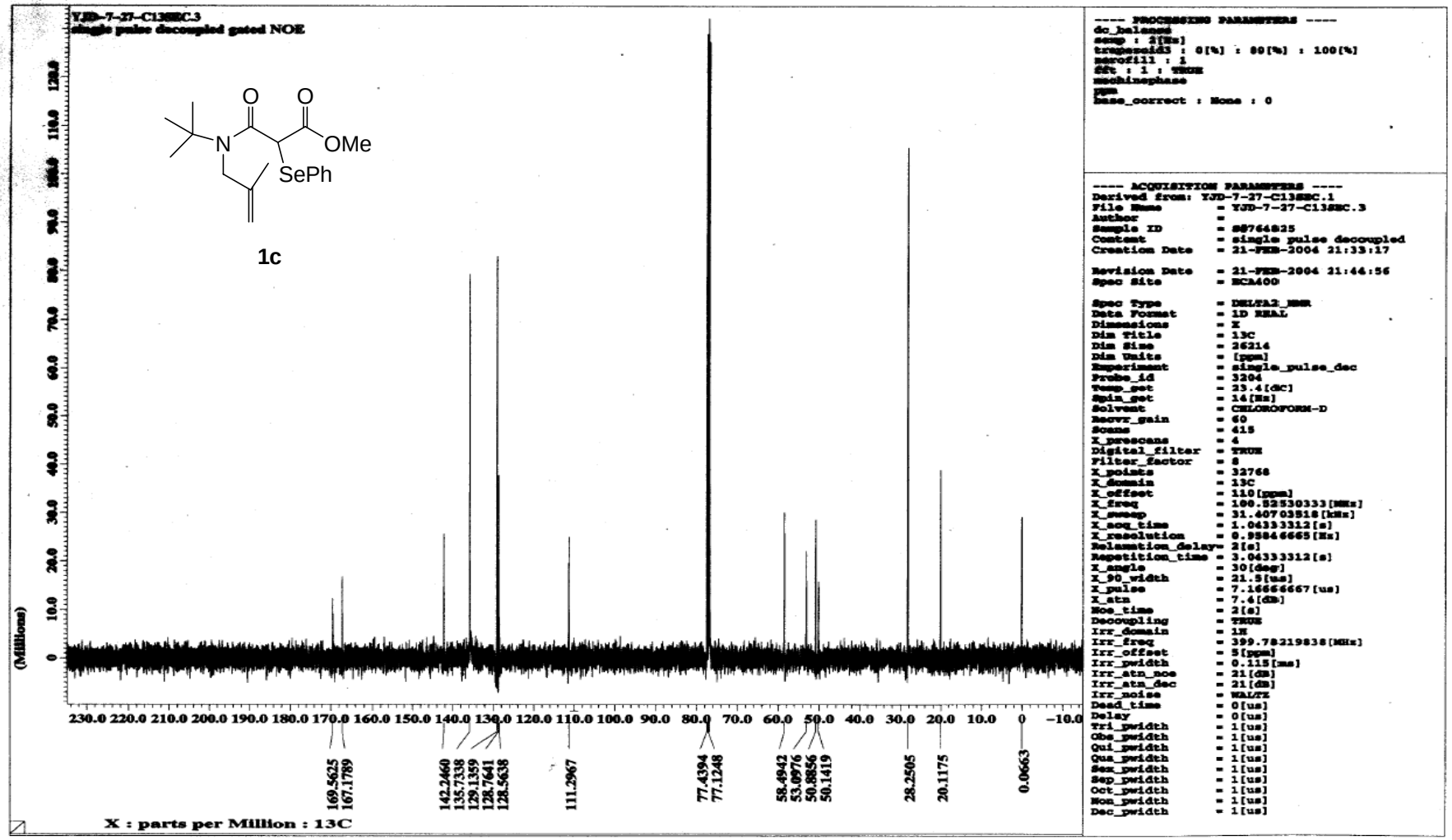

YJD-7-16SEC.6
single_pulse
O
O
N
OMe
3b
(Millions)
40.0
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
3.31544
1.17016
0.15648
1.14072
0.45852
0.17837
7.2780
3.7777
3.6543
3.6506
3.6311
3.0446
3.0239
2.9738
2.7013
2.6830
2.6634
2.0709
1.4282
1.4075
1.3891
1.1387
1.1216
1.0556
1.0385
0.0086
0.0000
-0.0085
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
smsp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-16SEC.5
File Name = YJD-7-16SEC.6
Author =
Sample ID = S#829575
Content = single_pulse
Creation Date = 16-FEB-2004 23:00:40
Revision Date = 8-MAR-2004 21:29:32
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 20.3[dC]
Spin_get = 15[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 34
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7.5[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay= 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_presat = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

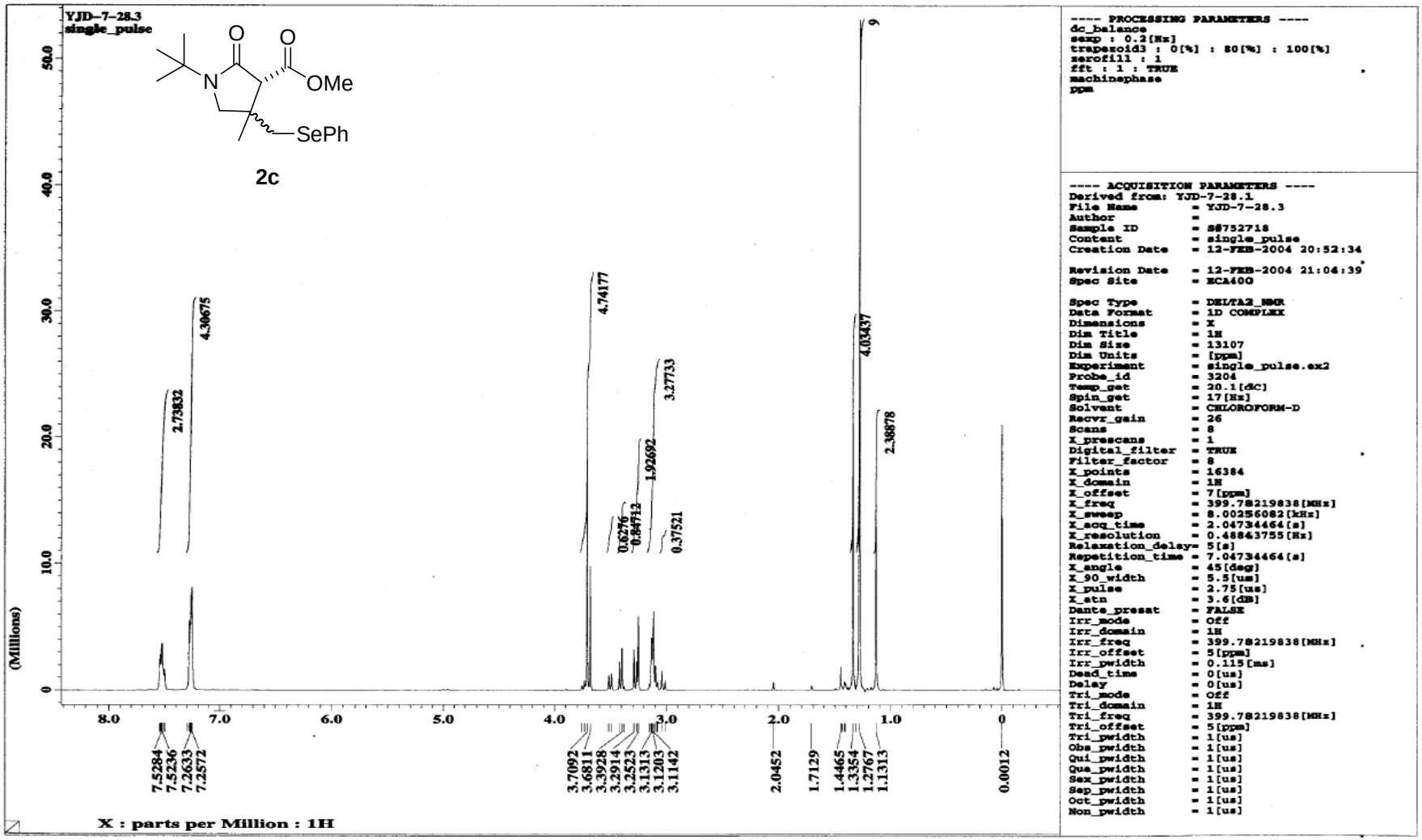

YJD-7-26-C13.3
single pulse decoupled gated NOE
O
O
N
OMe
3b
(Millions)
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
170.5732
169.6769
77.4299
76.7911
58.0651
54.5469
52.5160
51.3909
30.9011
27.6784
18.2869
0.0567
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
Base_correct : None : 0
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-26-C13.1
File Name = YJD-7-26-C13.3
Author =
Sample ID = 00026534
Content = single pulse decoupled
Creation Date = 21-FEB-2004 23:15:58
Revision Date = 21-FEB-2004 23:21:12
Spec Site = NCA400
Spec Type = DELTA2_NMR
Data Format = 1D REAL
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 23.6[dC]
Spin_get = 14[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 56
Scans = 414.0
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 110[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846685[Hz]
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

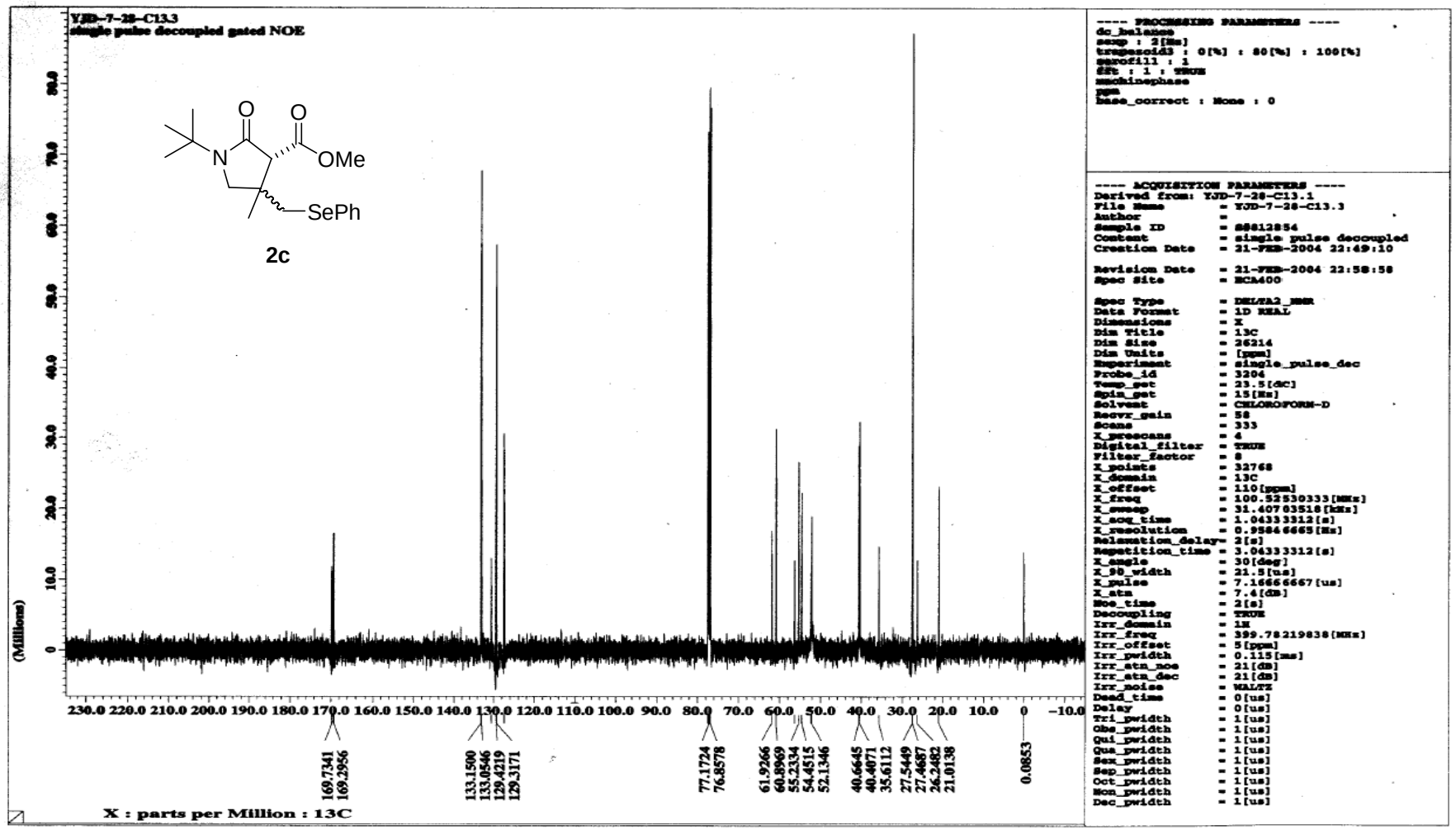

YJD-5-25.3
single_pulse
O
O
N
OMe
4c
(Millions)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
2.02804
5.04128
2.03162
3.0903
9
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.3273
5.0035
4.9595
3.7622
3.7353
3.3736
1.7194
1.4482
0.0004
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-5-25.1
File Name = YJD-5-25.3
Author =
Sample ID = S#778679
Content = single_pulse
Creation Date = 10-JAN-2004 21:34:38
Revision Date = 10-JAN-2004 21:46:22
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 21.7[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 22
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay= 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Presat_time = 5[s]
Dante_presat = TRUE
Dante_pulse = 2[us]
Dante_interval = 0.1[ms]
Dante_attenuator= 40[dB]
Dante_loop = 490
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]

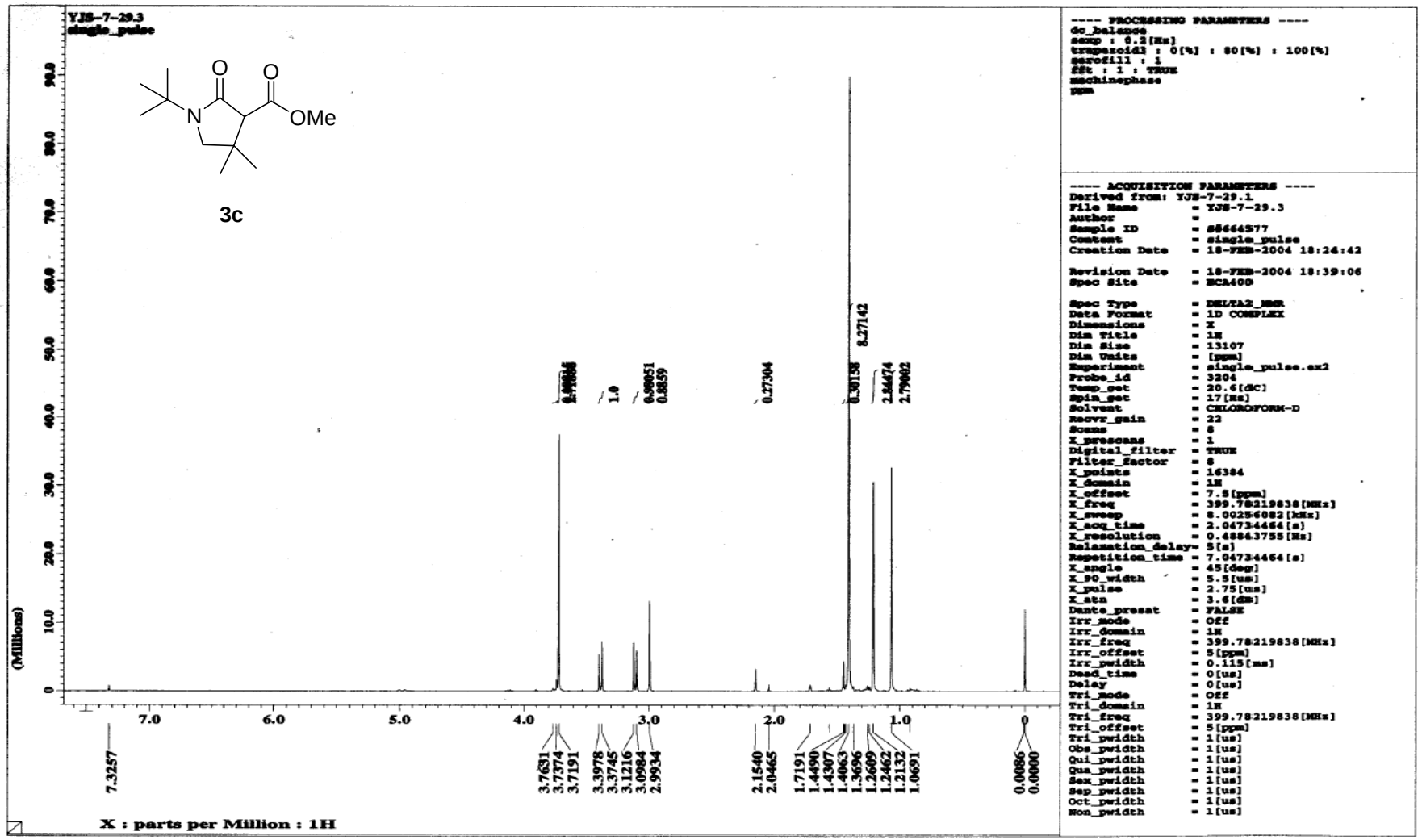

YJD-5-25-C13.3
single pulse decoupled gated NOE
O
O
N
OMe
4c
(Millions)
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
168.8284
167.4268
142.2269
110.9630
77.5061
77.1915
57.9698
52.3063
50.9142
43.3914
28.3268
20.1270
0.0186
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
base_correct : None : 0
---- ACQUISITION PARAMETERS ----
Derived from: YJD-5-25-C13.1
File Name = YJD-5-25-C13.3
Author =
Sample ID = S#779959
Content = single pulse decoupled
Creation Date = 10-JAN-2004 21:53:01
Revision Date = 10-JAN-2004 21:59:31
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D REAL
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 22.1[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 54
Scans = 308
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 110[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay= 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

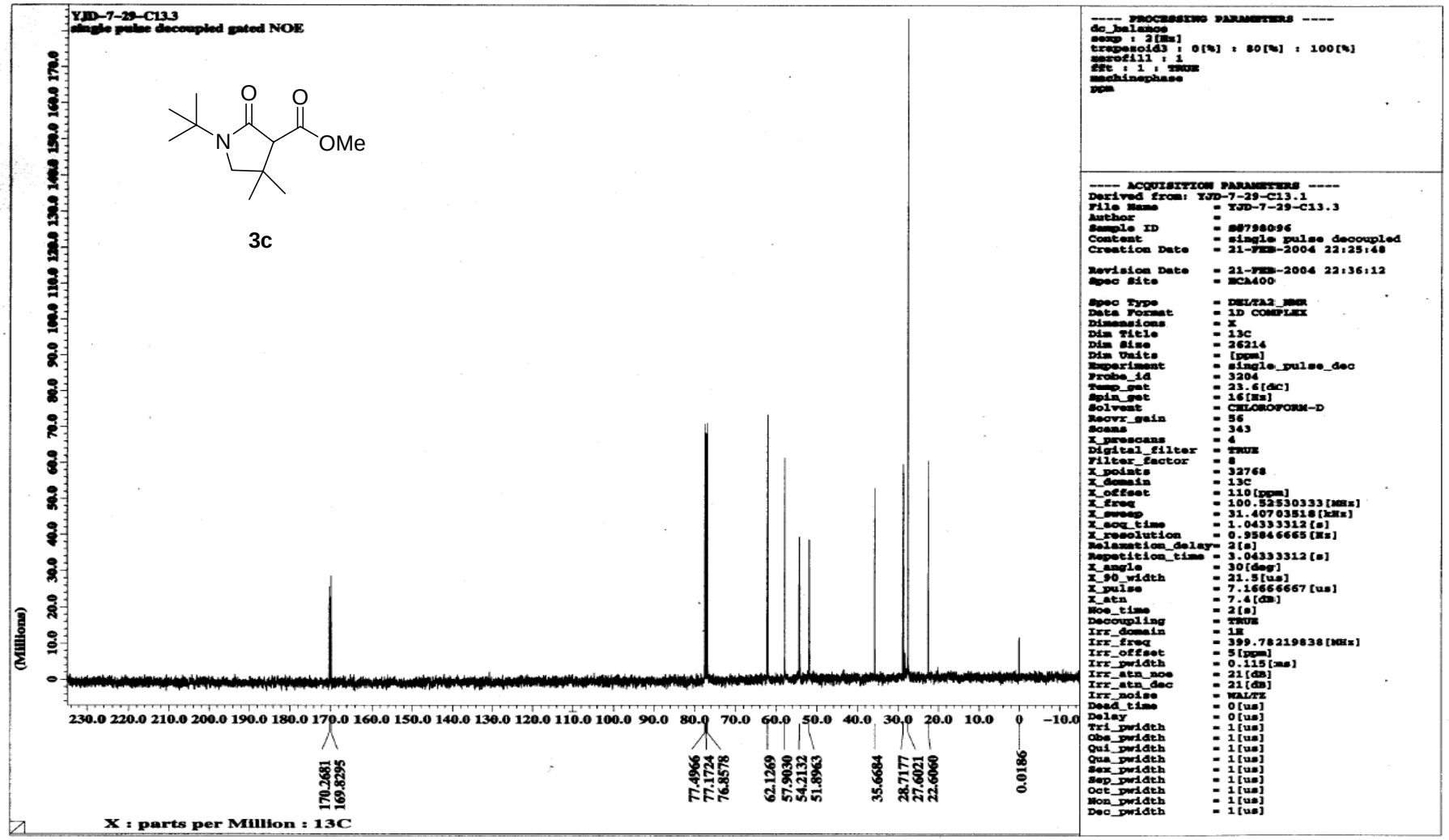

YJD-7-27.5
single_pulse
O
O
N
OMe
SePh
1c
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
2.00097
3.40414
2
1.08739
5.09967
3.04251
8.97869
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6429
7.6258
7.3155
7.2996
7.2813
4.9587
4.5384
3.8164
3.7675
3.7174
3.6856
1.6160
1.4474
1.4181
1.2580
0.0008
-0.0065
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-27.1
File Name = YJD-7-27.5
Author =
Sample ID = S#715290
Content = single_pulse
Creation Date = 12-FEB-2004 19:49:57
Revision Date = 12-FEB-2004 20:09:08
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 19.8[dC]
Spin_get = 14[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 30
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48863755[Hz]
Relaxation_delay = 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_presat = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

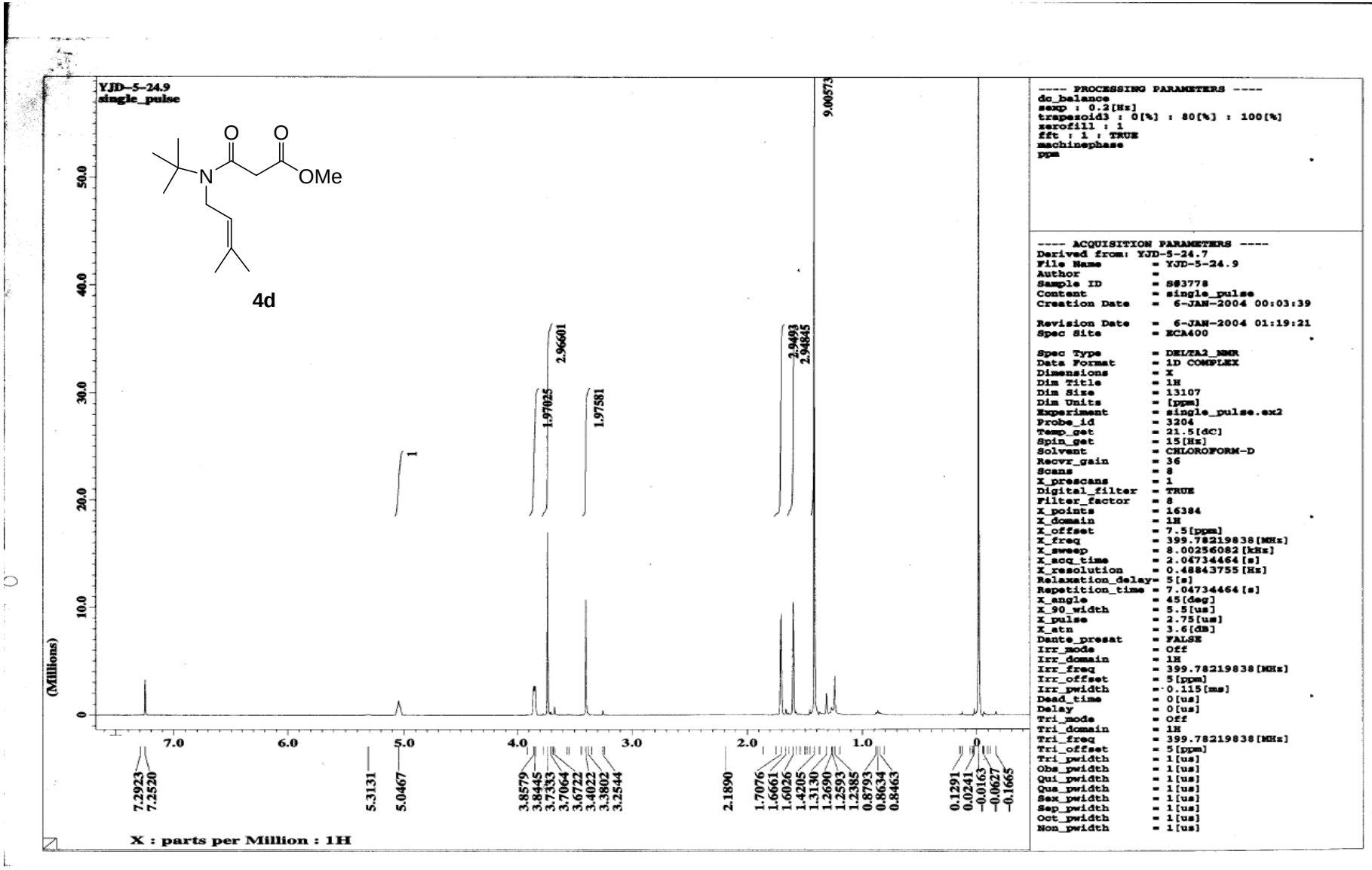

YJD-7-27-C13EC.3
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1c
(Millions)
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 −10.0
169.5625
167.1789
142.2460
135.7338
129.1359
128.7641
128.5638
111.2967
77.4394
77.1248
58.4942
53.0976
50.8856
50.1419
28.2505
20.1175
0.0663
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
manphasephase
ppm
base_correct : None : 0
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-27-C13EC.1
File Name = YJD-7-27-C13EC.3
Author =
Sample ID = s8764825
Content = single pulse decoupled
Creation Date = 21-FEB-2004 21:33:17
Revision Date = 21-FEB-2004 21:44:56
Spec Site = NCA400
Spec Type = DELTA2_NMR
Data Format = 1D REAL
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 23.4[dC]
Spin_get = 14[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 60
Scans = 416
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 110[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Che_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

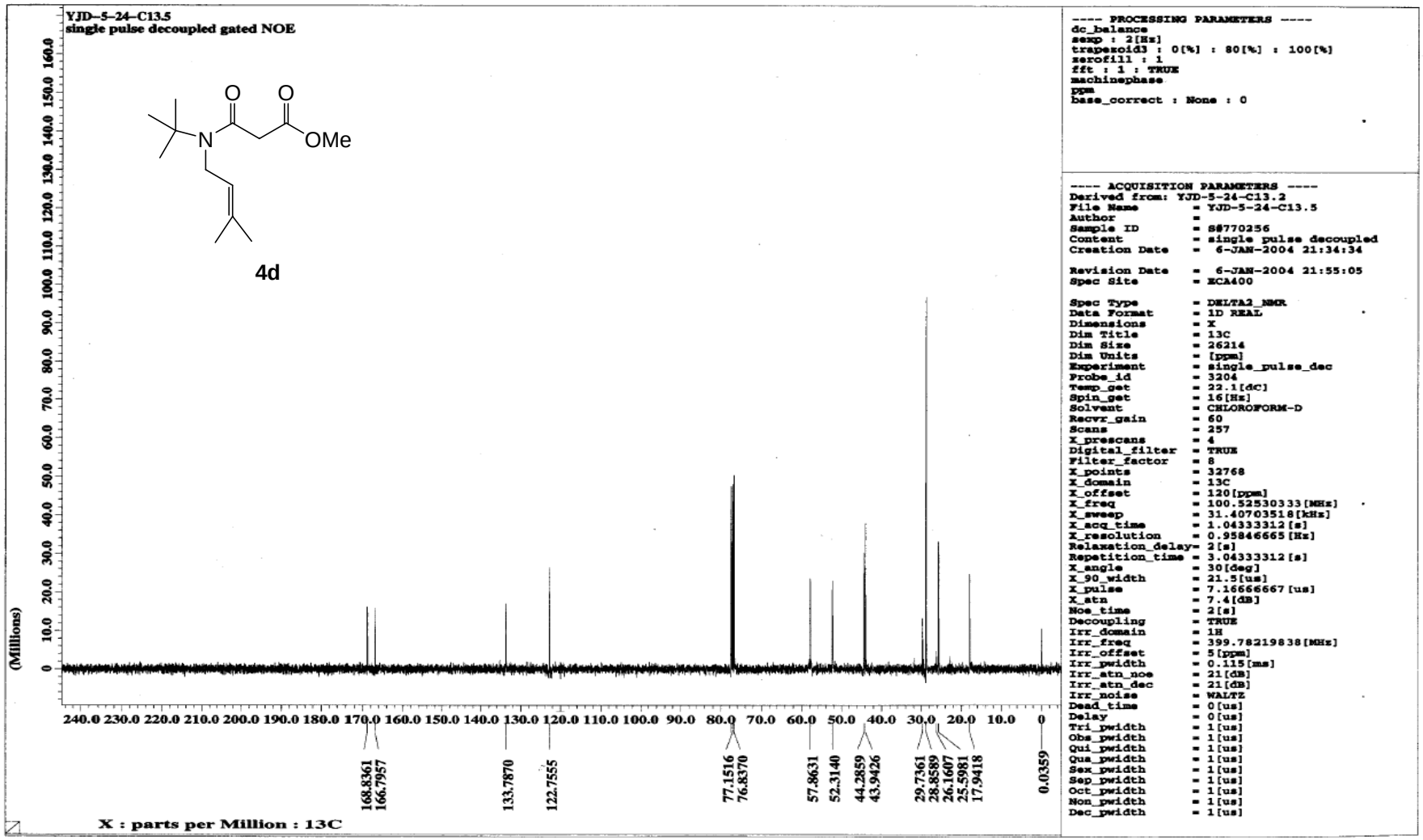

YJD-7-28.3
single_pulse
OMe
SePh
2c
(Millions)
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-28.1
File Name = YJD-7-28.3
Author =
Sample ID = S#752718
Content = single_pulse
Creation Date = 12-FEB-2004 20:52:34
Revision Date = 12-FEB-2004 21:04:39
Spec Site = NCA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 20.1[dC]
Spin_get = 17[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 26
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay= 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_presat = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

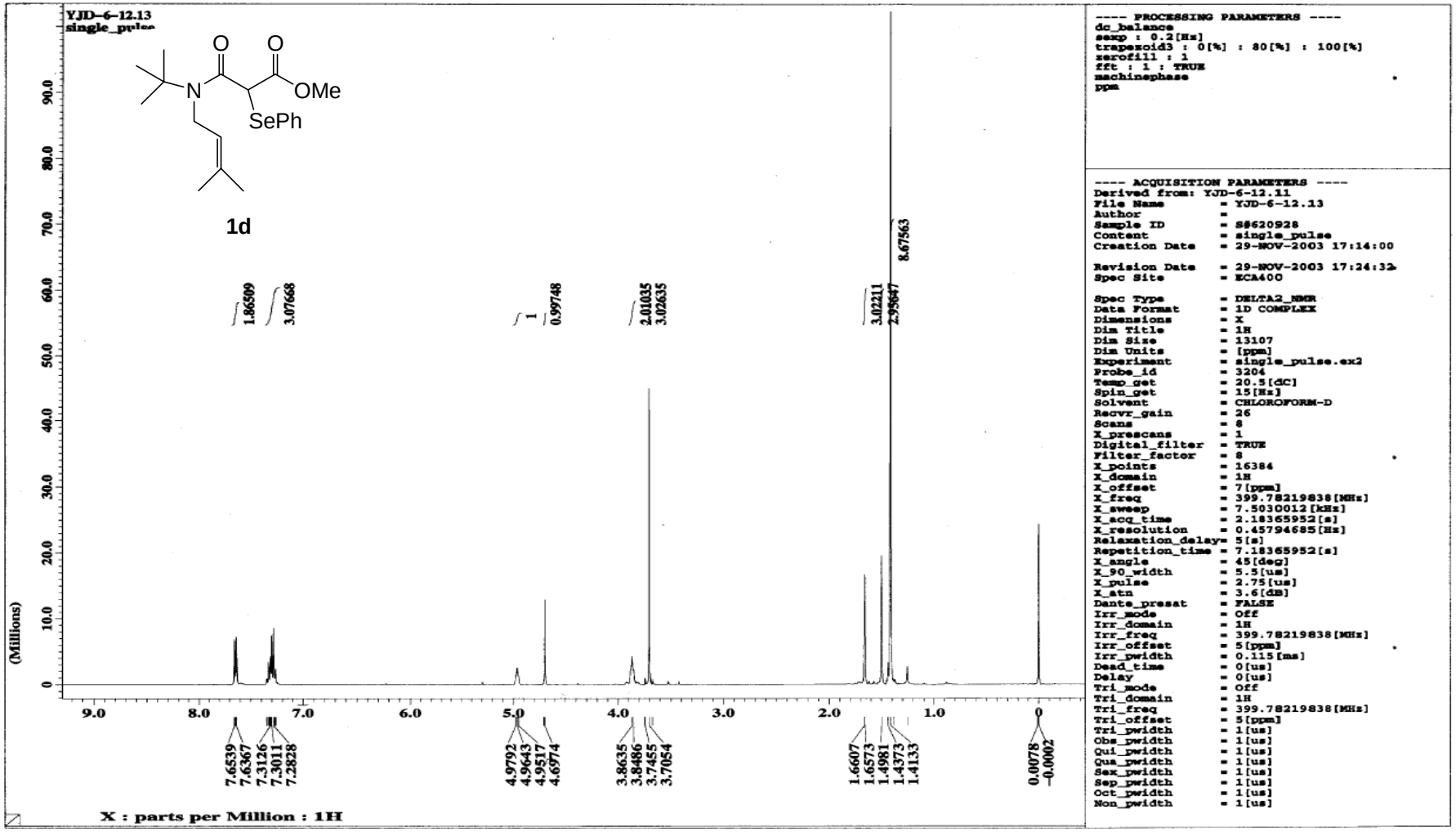

YJD-7-28-C13.3
single pulse decoupled gated NOE
O
O
N
OMe
SePh
2c
(Millions)
X : parts per Million : 13C
169.7341
169.2956
133.1500
133.0546
129.4219
129.3171
77.1724
76.8578
61.9266
60.8969
55.2334
54.4515
52.1346
40.6645
40.4671
35.6112
27.5449
27.4687
26.2482
21.0138
0.0853
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
gaussfill : 1
fft : 1 : TRUE
machinephase
ppm
base_correct : None : 0
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-28-C13.1
File Name = YJD-7-28-C13.3
Author =
Sample ID = 88812854
Content = single pulse decoupled
Creation Date = 21-FEB-2004 22:49:10
Revision Date = 21-FEB-2004 22:58:58
Spec Site = NCA400
Spec Type = DEL/EA2_NMR
Data Format = 1D REAL
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 23.5[dC]
Spin_get = 15[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 58
Scans = 333
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 110[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Noa_pwidth = 1[us]
Dec_pwidth = 1[us]

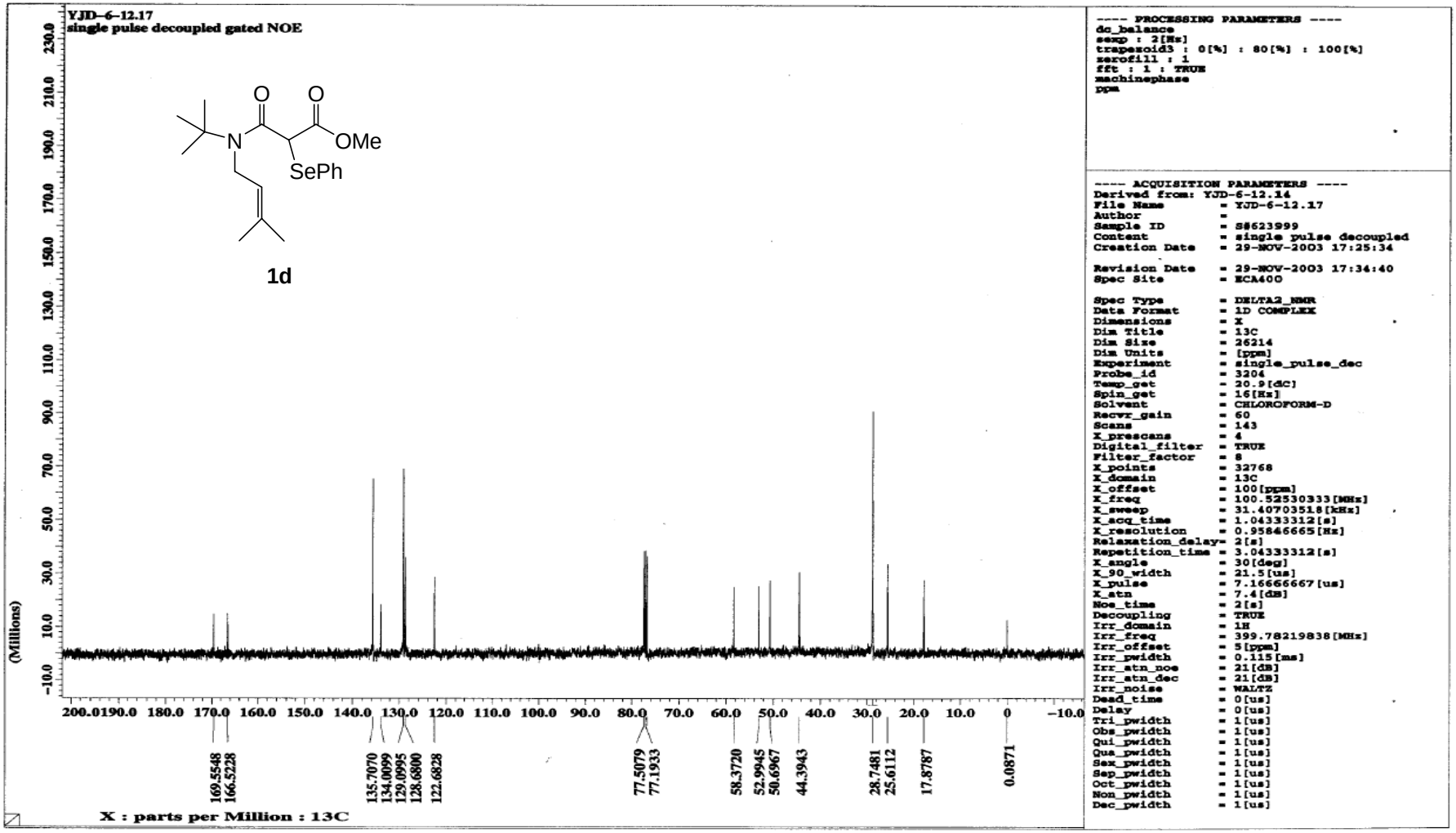

YJS-7-29.3
single_pulse
O
O
N
OMe
3c
(Millions)
50.0
40.0
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.0
0.98051
0.88559
0.27304
8.27142
2.84474
2.79002
7.3257
3.7631
3.7374
3.7191
3.3978
3.3745
3.1216
3.0984
2.9934
2.1540
2.0465
1.7191
1.4490
1.4307
1.4063
1.3696
1.2609
1.2462
1.2132
1.0691
0.0086
0.0000
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid1 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJS-7-29.1
File Name = YJS-7-29.3
Author =
Sample ID = S#664577
Content = single_pulse
Creation Date = 18-FEB-2004 18:24:42
Revision Date = 18-FEB-2004 18:39:06
Spec Site = BCA400
Spec Type = DEL/TA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_set = 20.6[dC]
Spin_set = 17[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 22
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7.5[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay = 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_presat = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Hex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

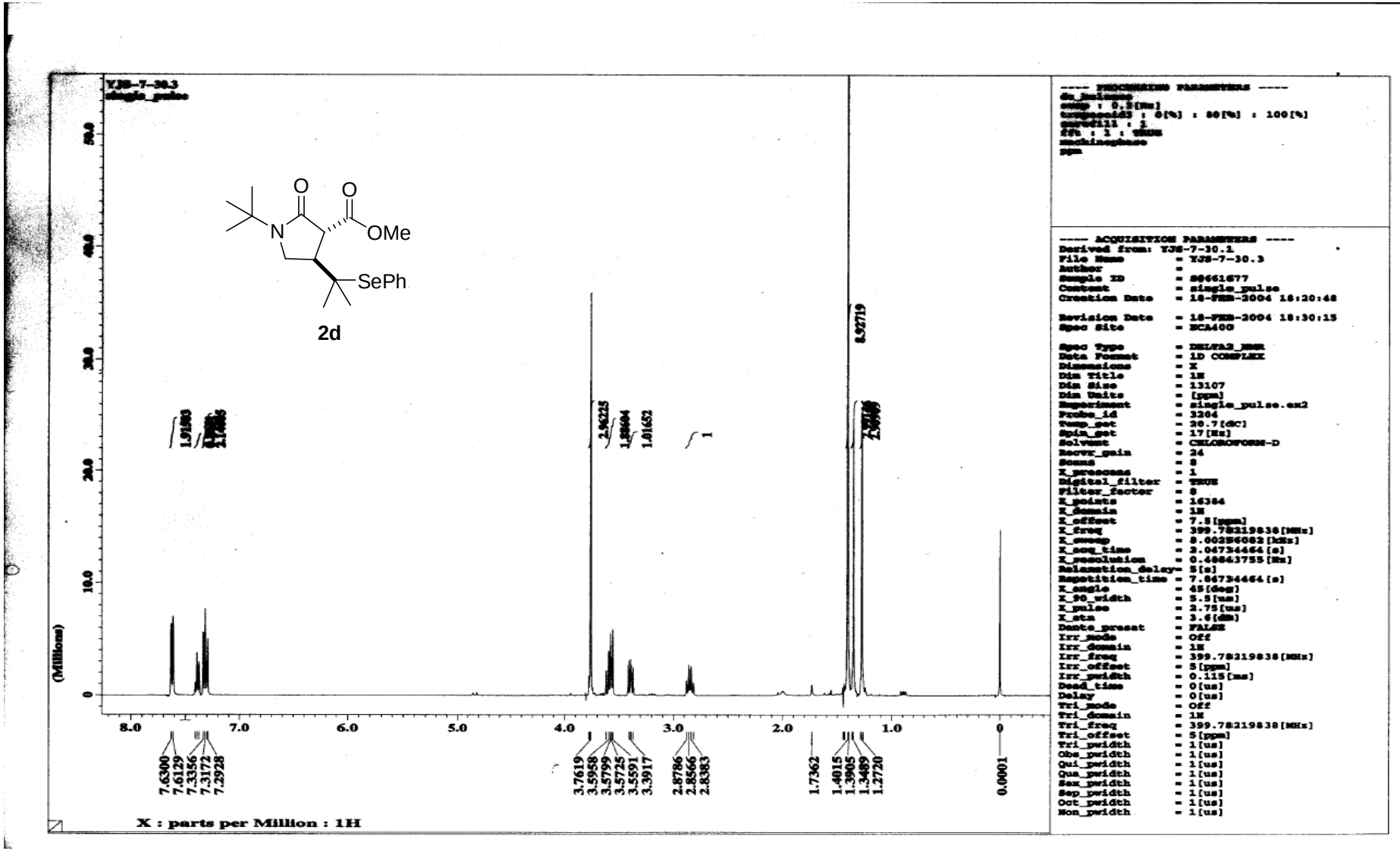

YJD-7-29-C13.3
single pulse decoupled gated NOE
O
O
N
OMe
3c
(Millions)
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
80.0
90.0
100.0
110.0
120.0
130.0
140.0
150.0
160.0
170.0
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
170.2681
169.8295
77.4966
77.1724
76.8578
62.1269
57.9030
54.2132
51.8963
35.6684
28.7177
27.6021
22.6060
0.0186
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-29-C13.1
File Name = YJD-7-29-C13.3
Author =
Sample ID = 98798096
Content = single pulse decoupled
Creation Date = 21-FEB-2004 22:25:48
Revision Date = 21-FEB-2004 22:36:12
Spec Site = NCA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 21.6[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 56
Scans = 343
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 110[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay= 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

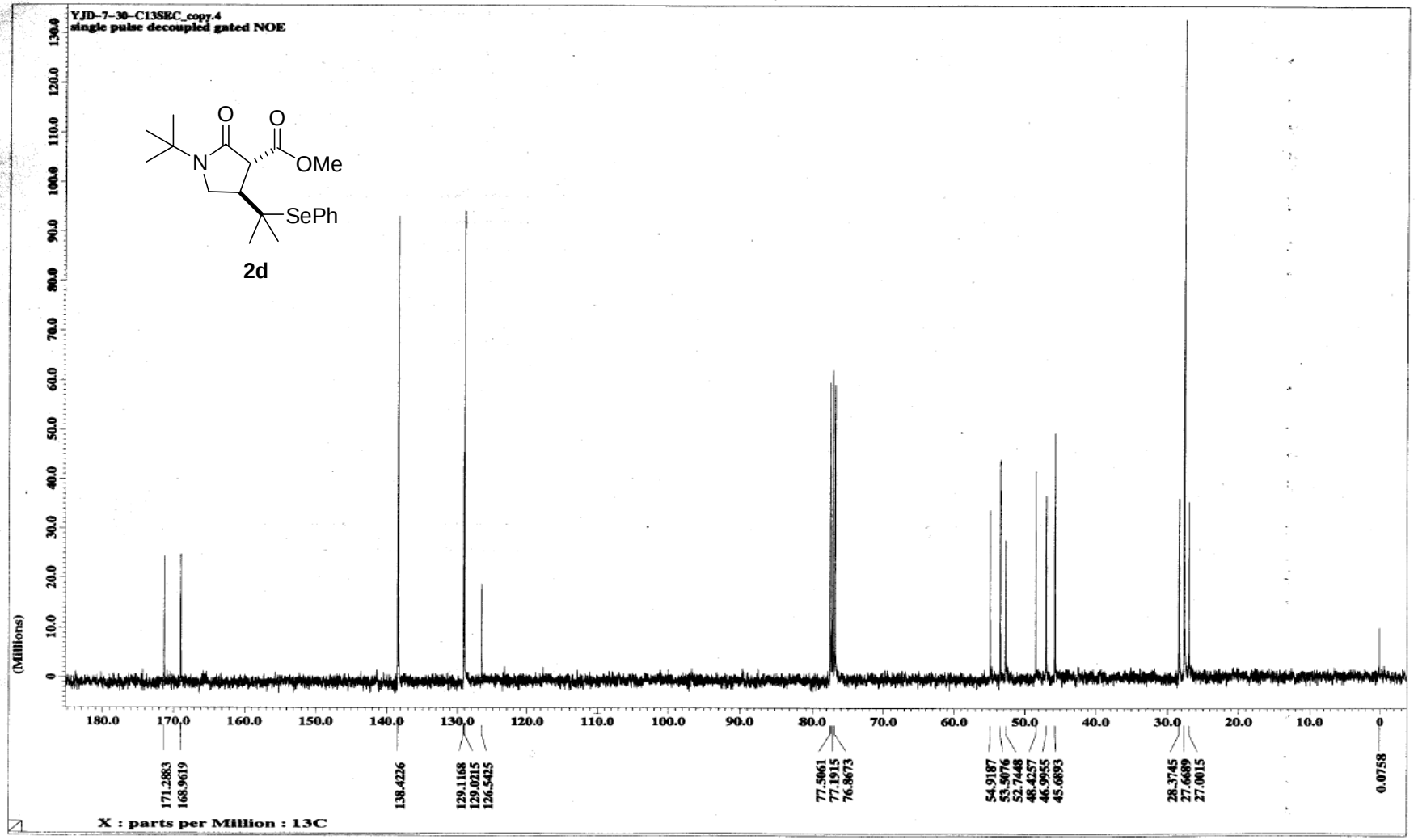

YJD-5-24.9
single_pulse
4d
(Millions)
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-5-24.7
File Name = YJD-5-24.9
Author =
Sample ID = S#3778
Content = single_pulse
Creation Date = 6-JAN-2004 00:03:39
Revision Date = 6-JAN-2004 01:19:21
Spec Site = ECA400
Spec Type = DEL/TA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 21.5[dC]
Spin_get = 15[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 36
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7.5[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay= 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_presat = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

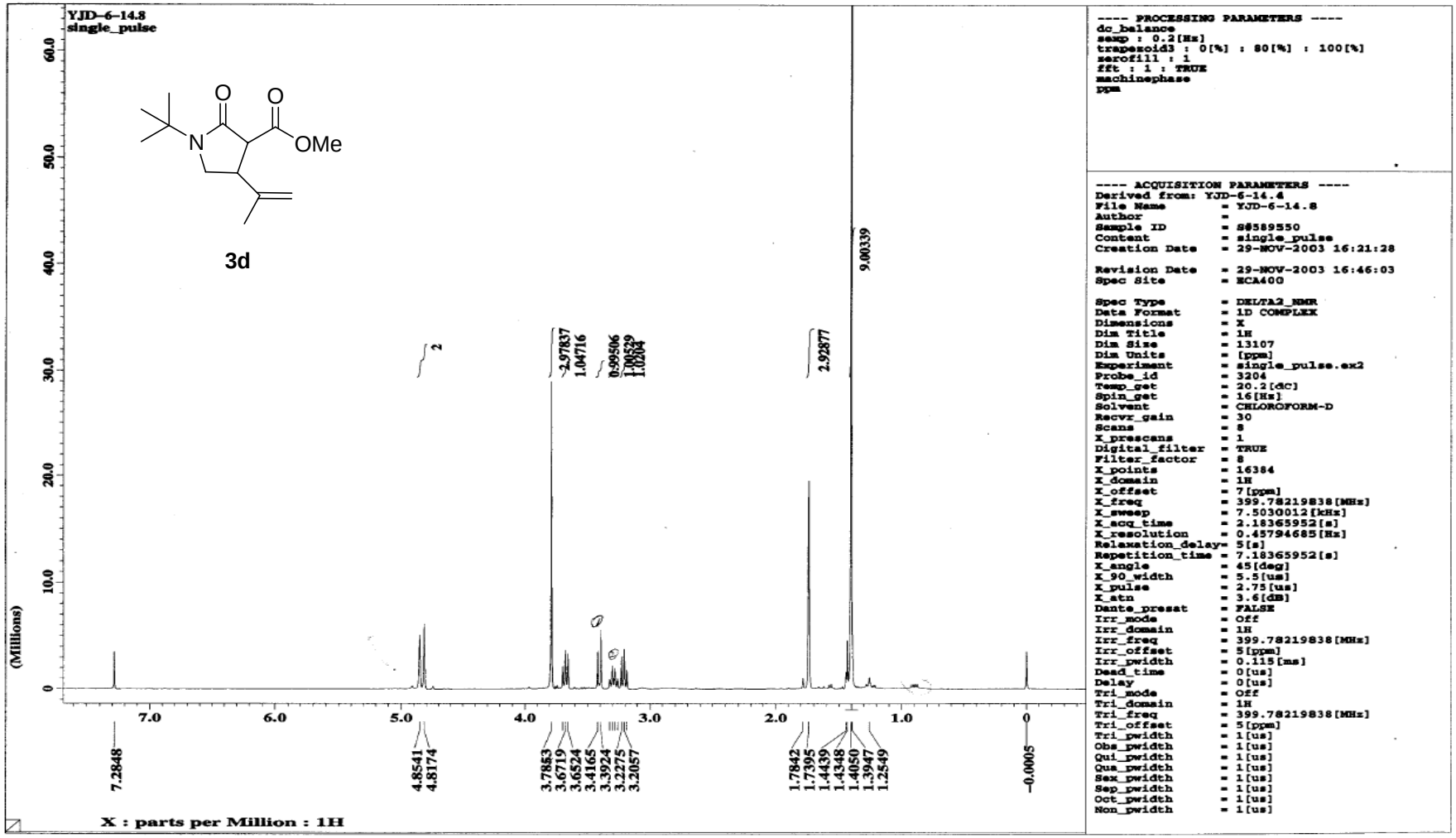

YJD-5-24-C13.5
single pulse decoupled gated NOE
O
O
N
OMe
4d
(Millions)
240.0 230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
168.8361
166.7957
133.7870
122.7555
77.1516
76.8370
57.8631
52.3140
44.2859
43.9426
29.7361
28.8589
26.1607
25.5981
17.9418
0.0359
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
base_correct : None : 0
---- ACQUISITION PARAMETERS ----
Derived from: YJD-5-24-C13.2
File Name = YJD-5-24-C13.5
Author =
Sample ID = S#770256
Content = single pulse decoupled
Creation Date = 6-JAN-2004 21:34:34
Revision Date = 6-JAN-2004 21:55:05
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D REAL
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 22.1[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 60
Scans = 257
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 120[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

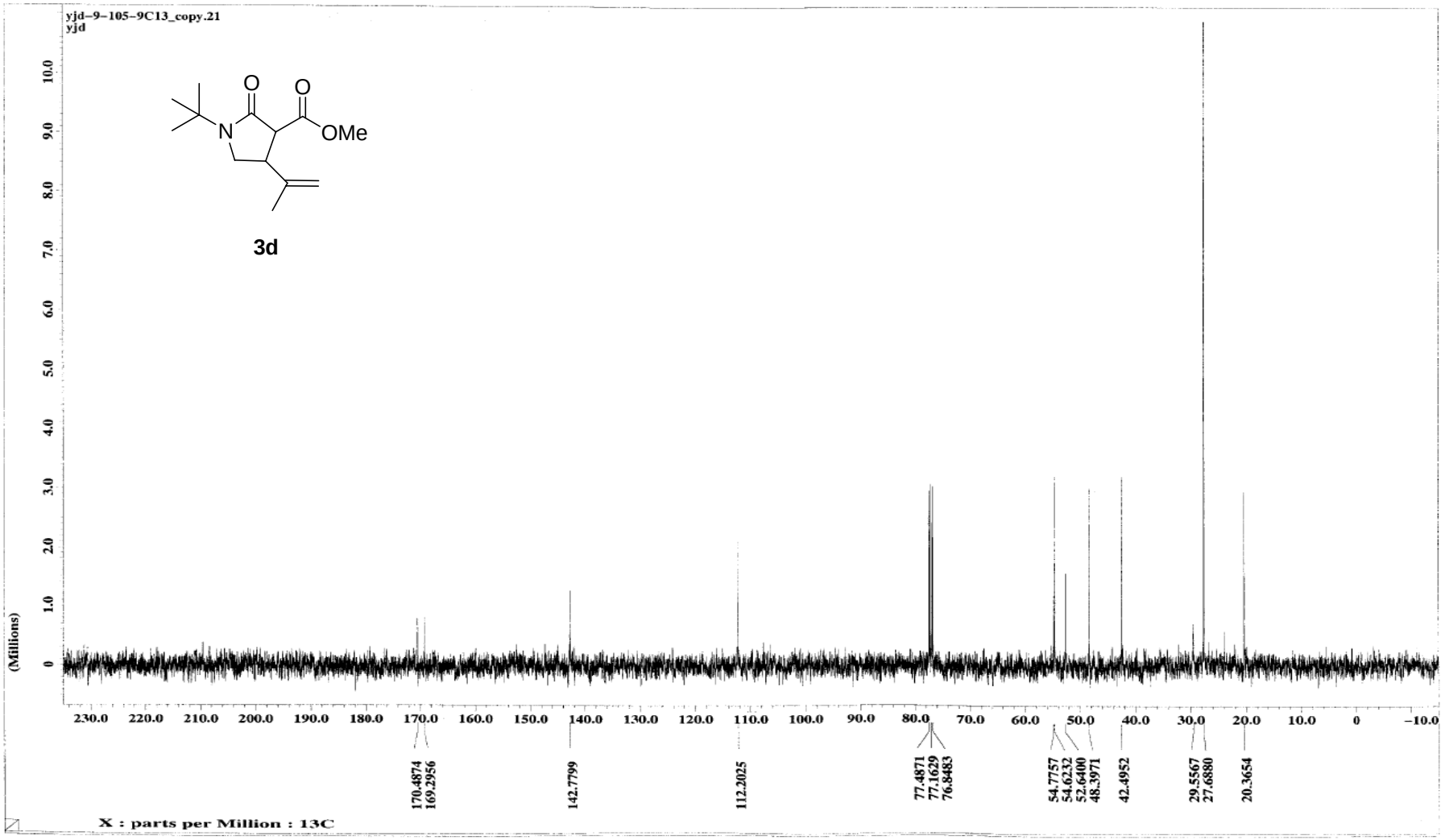

YJD-6-12.13
single_pulse
O
O
N
OMe
SePh
1d
1.86509
3.07668
1
0.99748
2.01035
3.02635
3.02211
2.95647
8.67563
(Millions)
X : parts per Million : 1H
7.6539
7.6367
7.3126
7.3011
7.2828
4.9792
4.9643
4.9517
4.6974
3.8635
3.8486
3.7455
3.7054
1.6607
1.6573
1.4981
1.4373
1.4133
0.0078
-0.0002
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-6-12.11
File Name = YJD-6-12.13
Author =
Sample ID = S#620928
Content = single_pulse
Creation Date = 29-NOV-2003 17:14:00
Revision Date = 29-NOV-2003 17:24:32
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 20.5[dC]
Spin_get = 15[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 26
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 7.5030012[kHz]
X_acq_time = 2.18365952[s]
X_resolution = 0.45794685[Hz]
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_presat = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

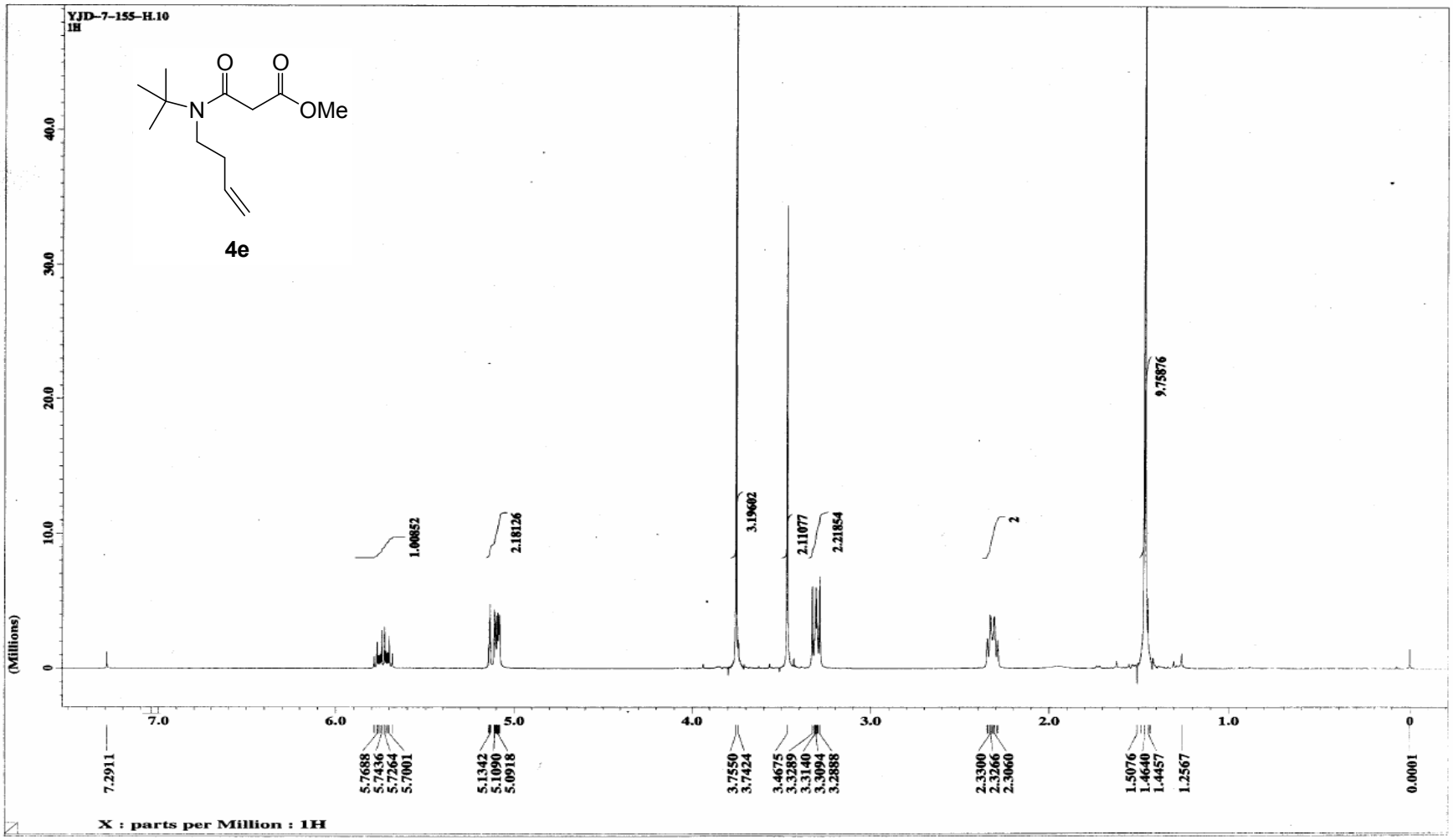

YJD-6-12.17
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1d
(Millions)
X : parts per Million : 13C
169.5548
166.5228
135.7070
134.0099
129.0995
128.6800
122.6828
77.5079
77.1933
58.3720
52.9945
50.6967
44.3943
28.7481
25.6112
17.8787
0.0871
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-6-12.14
File Name = YJD-6-12.17
Author =
Sample ID = S#623999
Content = single pulse decoupled
Creation Date = 29-NOV-2003 17:25:34
Revision Date = 29-NOV-2003 17:34:40
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 3204
Temp_get = 20.9[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 60
Scans = 143
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 100[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay= 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 21.5[us]
X_pulse = 7.16666667[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 21[dB]
Irr_atn_dec = 21[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

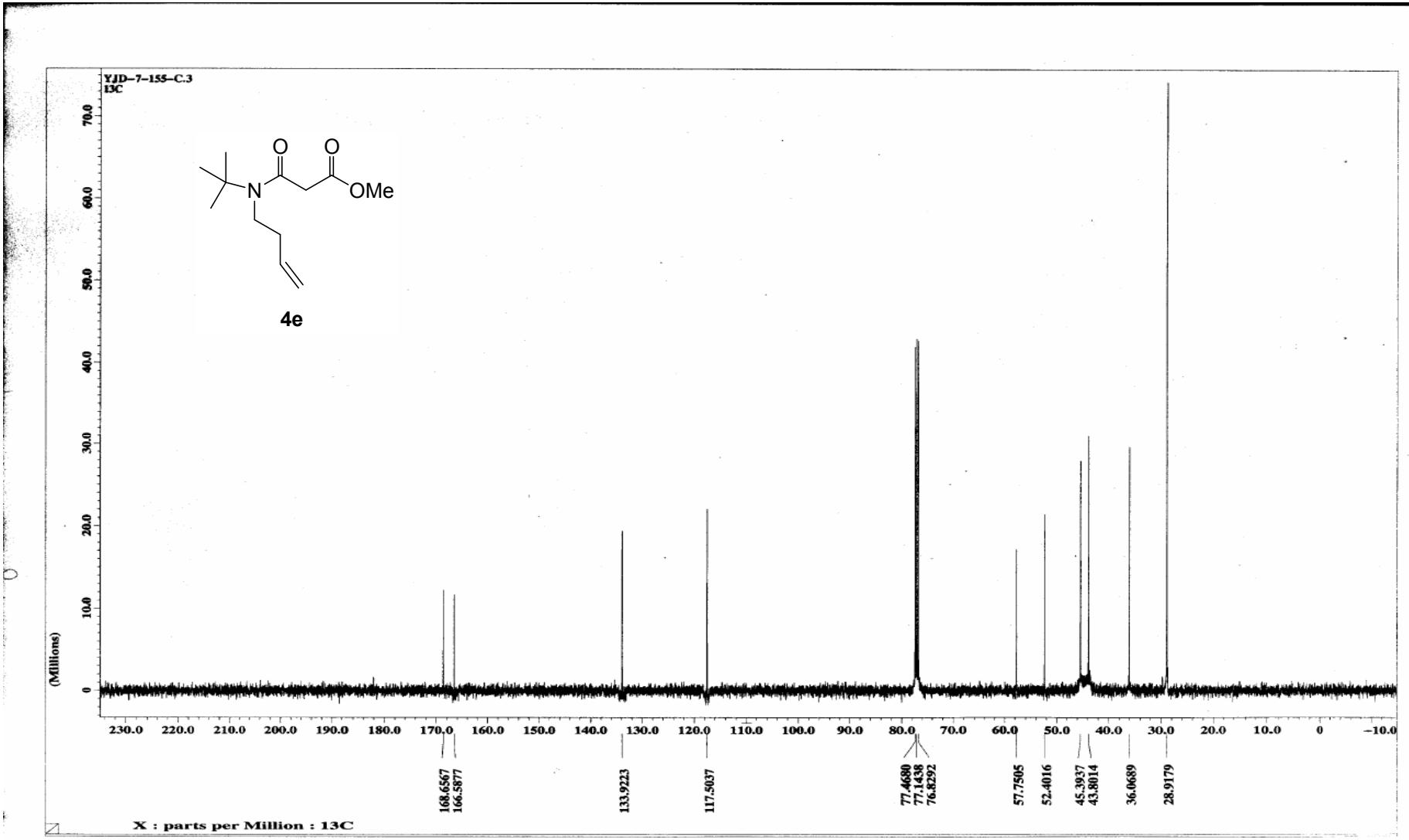

YJS-7-30.3
single_pulse
O
O
N
OMe
SePh
2d
(Millions)
8.92719
2.86225
1.88604
1.01652
1
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6300
7.6129
7.3356
7.3172
7.2928
3.7619
3.5958
3.5799
3.5725
3.5591
3.3917
2.8786
2.8566
2.8383
1.7362
1.4015
1.3905
1.3489
1.2720
0.0001
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_baseline
emsp : 0.3[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJS-7-30.1
File Name = YJS-7-30.3
Author =
Sample ID = 80661677
Content = single_pulse
Creation Date = 18-FEB-2004 18:20:48
Revision Date = 18-FEB-2004 18:30:15
Spec Site = BCA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
X_Title = 1H
X_Size = 13107
X_Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 20.7[dC]
Spin_get = 17[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 24
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 3
X_points = 16384
X_Domain = 1H
X_offset = 7.5[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 8.00256082[kHz]
X_acq_time = 2.04734464[s]
X_resolution = 0.48843755[Hz]
Relaxation_delay= 5[s]
Repetition_time = 7.04734464[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_preset = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

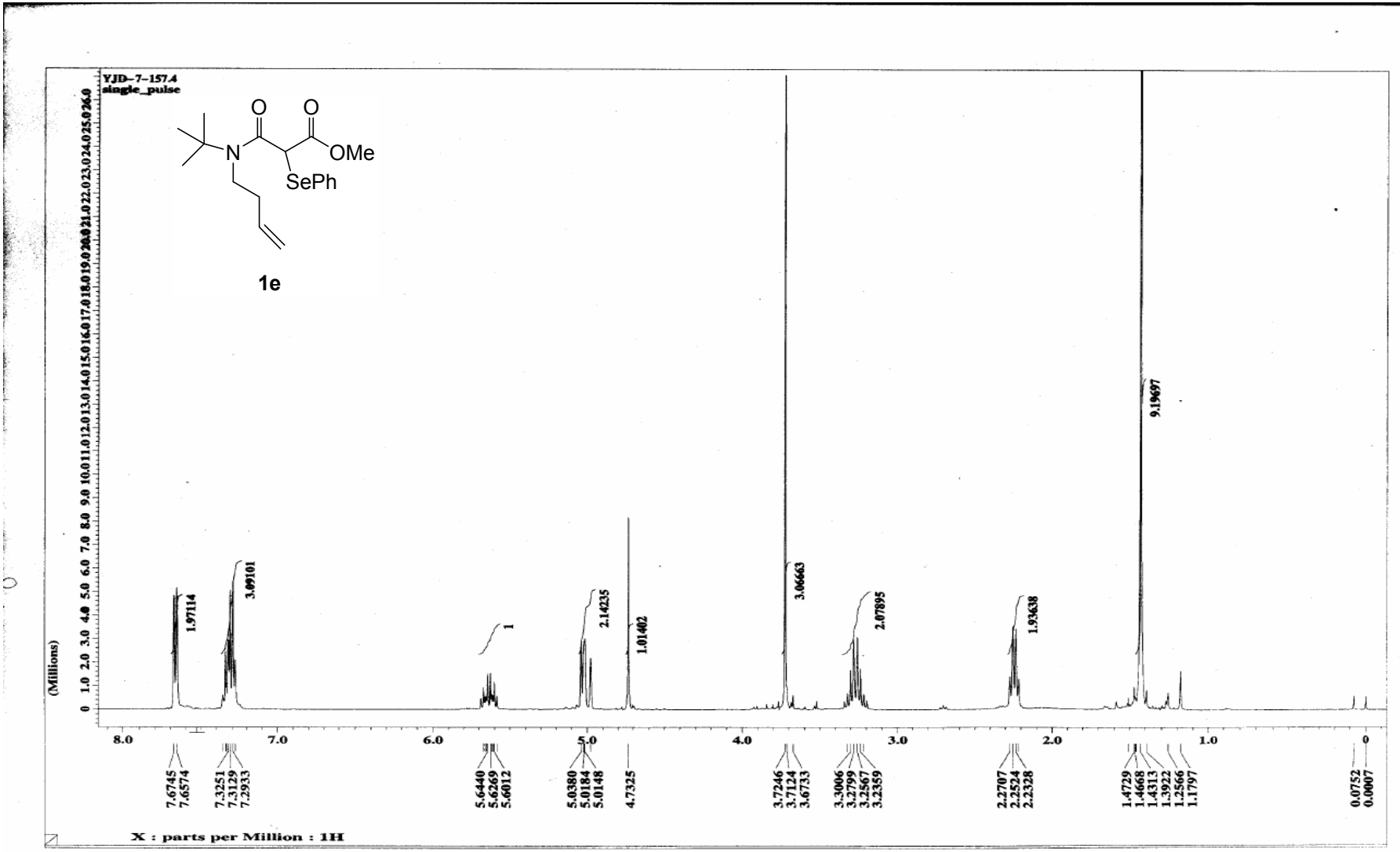

YJD-7-30-C13SEC_copy.4
single pulse decoupled gated NOE
O
O
N
OMe
SePh
2d
(Millions)
X : parts per Million : 13C
171.2883
168.9619
138.4226
129.1168
129.0215
126.5425
77.5061
77.1915
76.8673
54.9187
53.5976
52.7448
48.4257
46.9955
45.6893
28.3745
27.6689
27.0015
0.0758

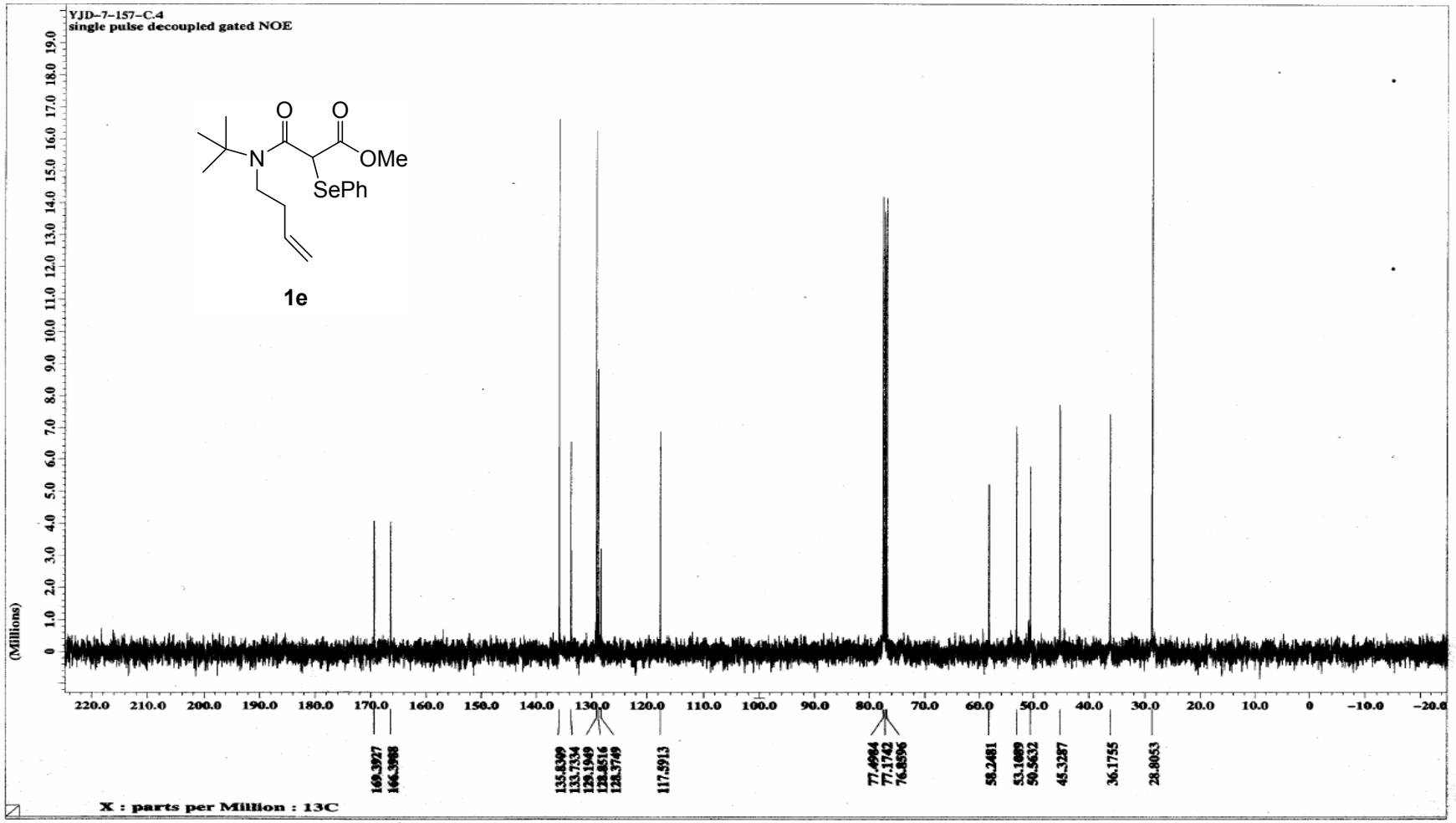

YJD-6-14.8
single_pulse
O
O
N
OMe
3d
(Millions)
60.0
50.0
40.0
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
2
2.97837
1.04716
0.99506
1.00529
1.02004
2.92877
9.00339
7.2848
4.8541
4.8174
3.7853
3.6719
3.6524
3.4165
3.3924
3.2275
3.2057
1.7842
1.7395
1.4439
1.4348
1.4050
1.3947
1.2549
-0.0005
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-6-14.4
File Name = YJD-6-14.8
Author =
Sample ID = S0589550
Content = single_pulse
Creation Date = 29-NOV-2003 16:21:28
Revision Date = 29-NOV-2003 16:46:03
Spec Site = NCA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Experiment = single_pulse.ex2
Probe_id = 3204
Temp_get = 20.2[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 30
Scans = 8
X_prescans = 1
Digital_filter = TRUE
Filter_factor = 8
X_points = 16384
X_domain = 1H
X_offset = 7[ppm]
X_freq = 399.78219838[MHz]
X_sweep = 7.5030012[kHz]
X_acq_time = 2.18365952[s]
X_resolution = 0.45794685[Hz]
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]
X_angle = 45[deg]
X_90_width = 5.5[us]
X_pulse = 2.75[us]
X_atn = 3.6[dB]
Dante_presat = FALSE
Irr_mode = Off
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Dead_time = 0[us]
Delay = 0[us]
Tri_mode = Off
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Sex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]

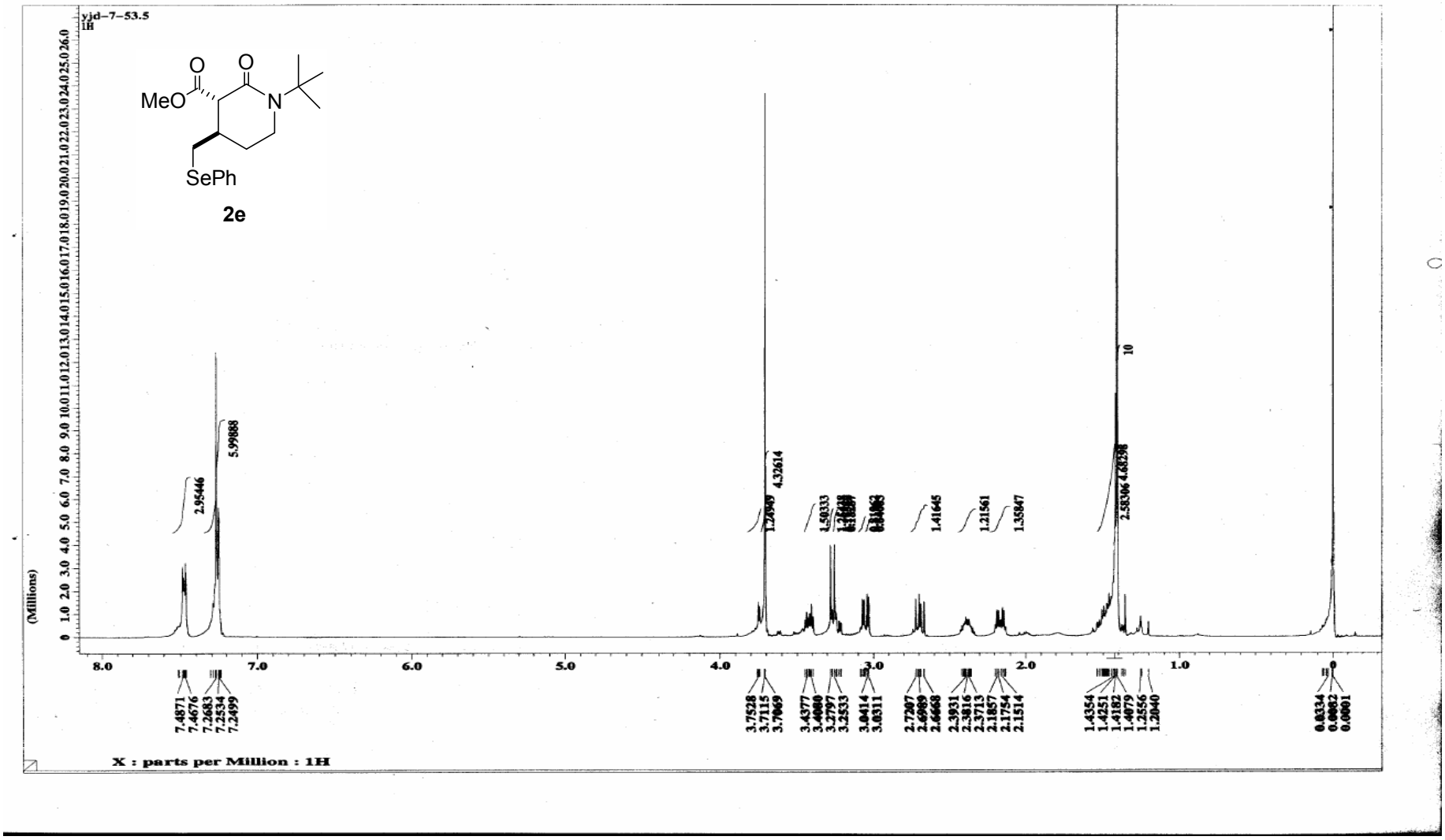

yjd--9--105--9C13_copy.21
yjd
O
O
N
OMe
3d
(Millions)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
230.0
220.0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
170.4874
169.2956
142.7799
112.2025
77.4871
77.1629
76.8483
54.7757
54.6232
52.6400
48.3971
42.4952
29.5567
27.6880
20.3654
X : parts per Million : 13C

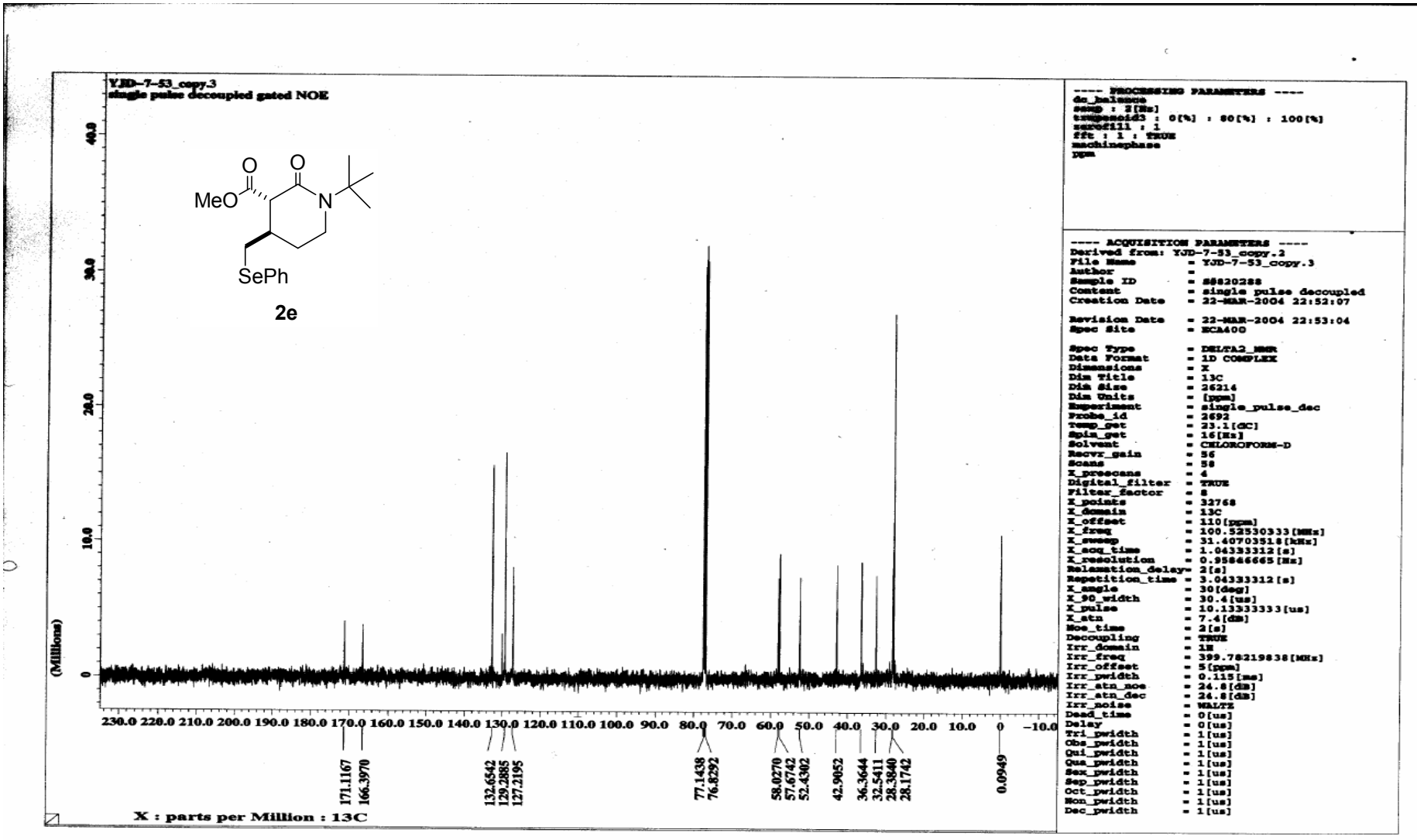

YJD-7-155-H.10
1H
O
O
N
OMe
4e
(Millions)
40.0
30.0
20.0
10.0
0
1.00852
2.18126
3.19602
2.11077
2.21854
2
9.75876
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2911
5.7688
5.7436
5.7264
5.7001
5.1342
5.1090
5.0918
3.7550
3.7424
3.4675
3.3289
3.3140
3.3094
3.2888
2.3300
2.3266
2.3060
1.5076
1.4640
1.4457
1.2567
0.0001
X : parts per Million : 1H

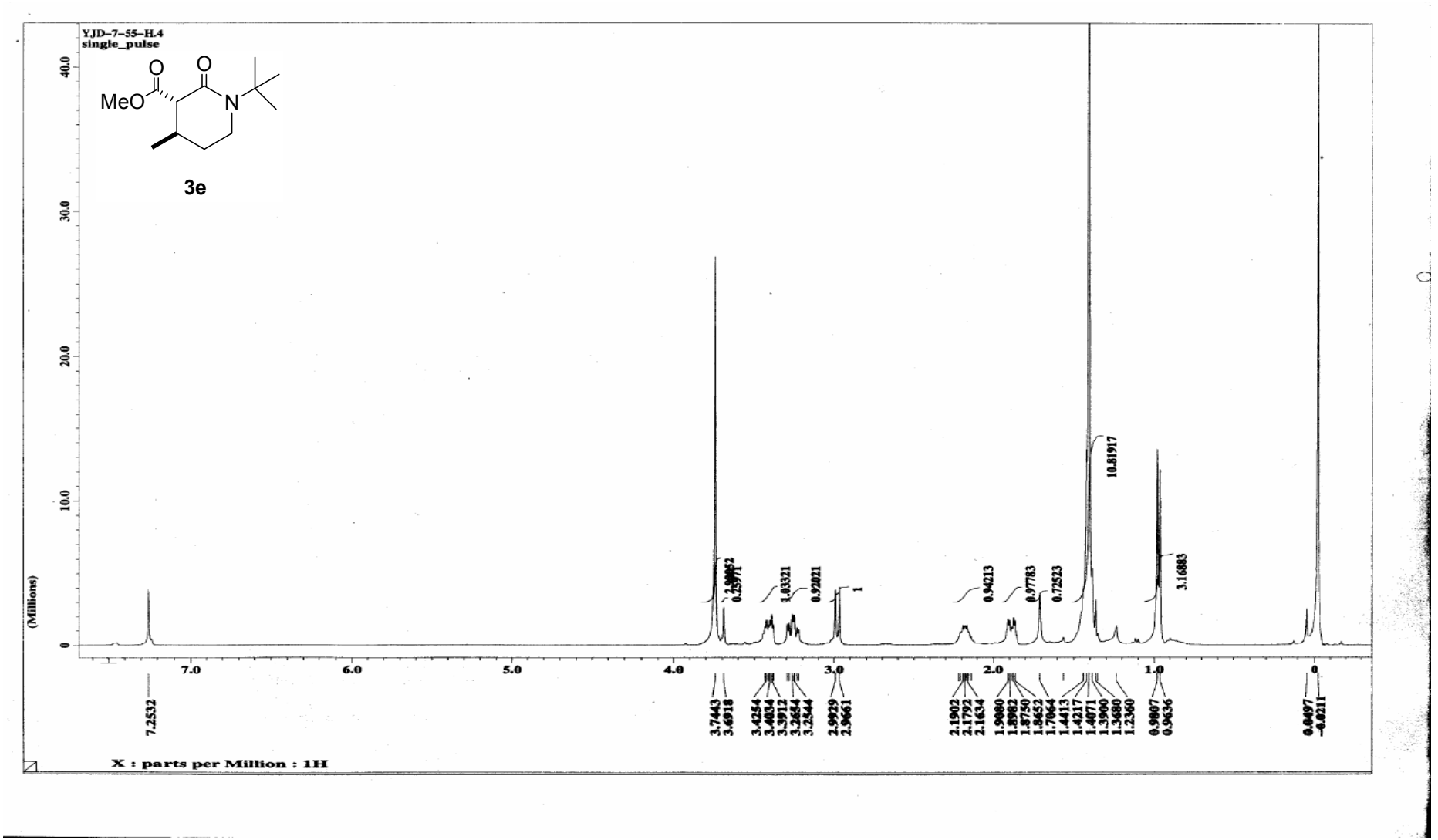

YJD-7-155-C.3
13C
O
O
N
OMe
4e
(Millions)
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
168.6567
166.5877
133.9223
117.5037
77.4680
77.1438
76.8292
57.7505
52.4016
45.3937
43.8014
36.0689
28.9179
X : parts per Million : 13C

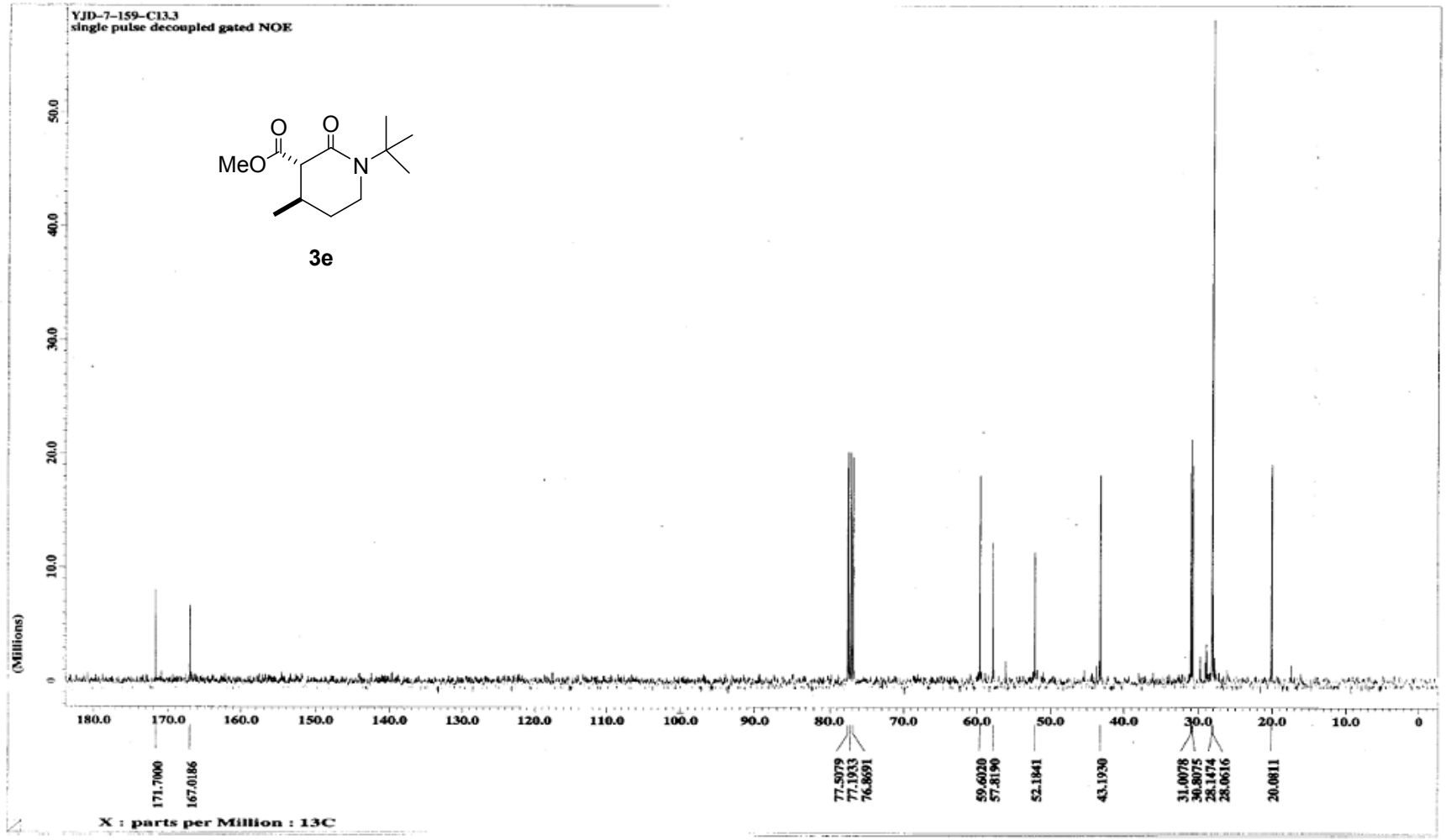

YJD-7-157.4
single_pulse
O
O
N
OMe
SePh
1e
(Millions)
9.19697
3.09101
3.06663
2.14235
2.07895
1.97114
1.93638
1.01402
1
7.6745
7.6574
7.3251
7.3129
7.2933
5.6440
5.6269
5.6012
5.0380
5.0184
5.0148
4.7325
3.7246
3.7124
3.6733
3.3006
3.2799
3.2567
3.2359
2.2707
2.2524
2.2328
1.4729
1.4668
1.4313
1.3922
1.2566
1.1797
0.0752
0.0007
X : parts per Million : 1H

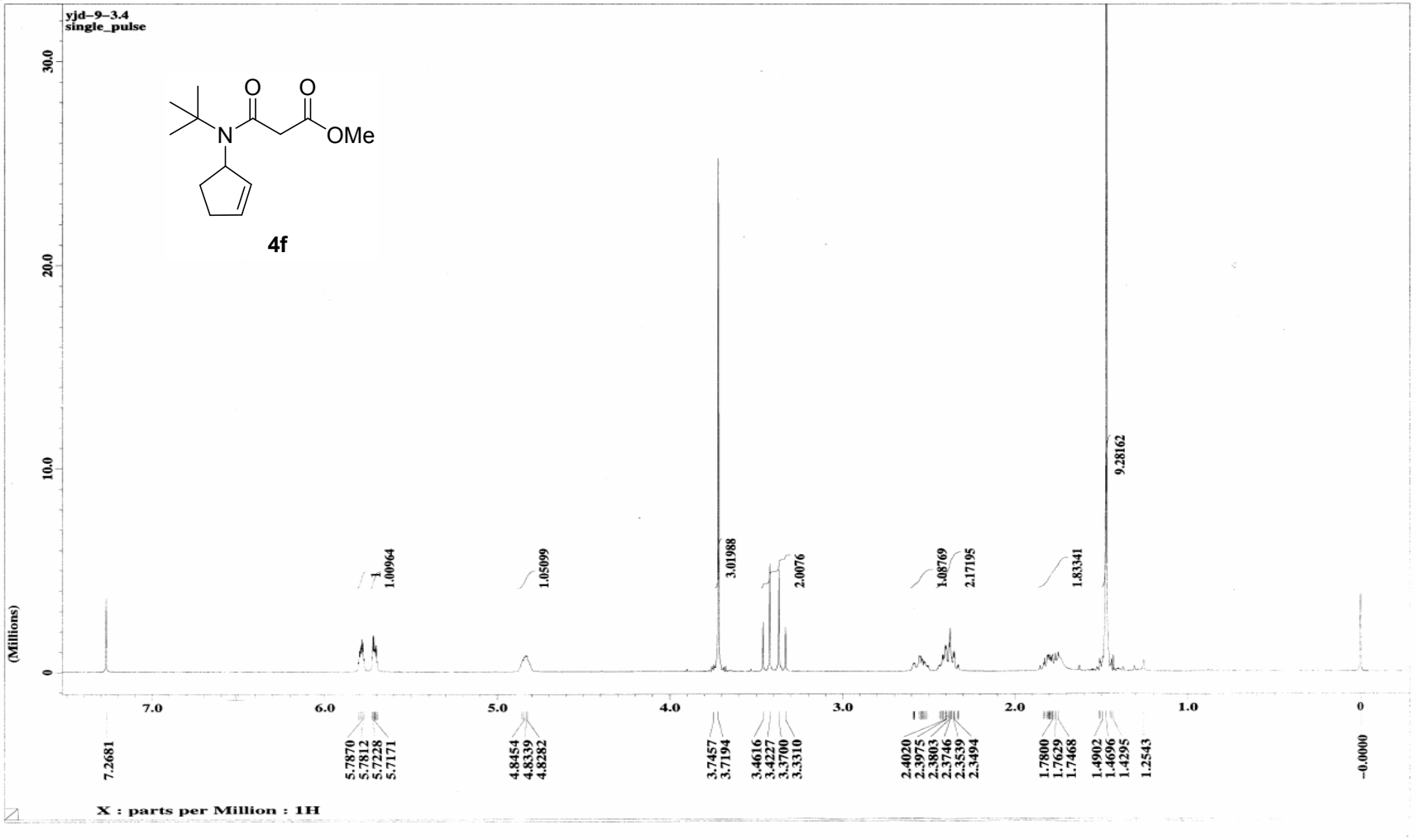

YJD-7-157-C.4
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1e
(Millions)
X : parts per Million : 13C
169.3927
166.5988
135.8349
133.7334
129.1949
128.8516
128.3749
117.5913
77.4984
77.1742
76.8596
58.2481
53.1689
50.5632
45.3287
36.1755
28.8053

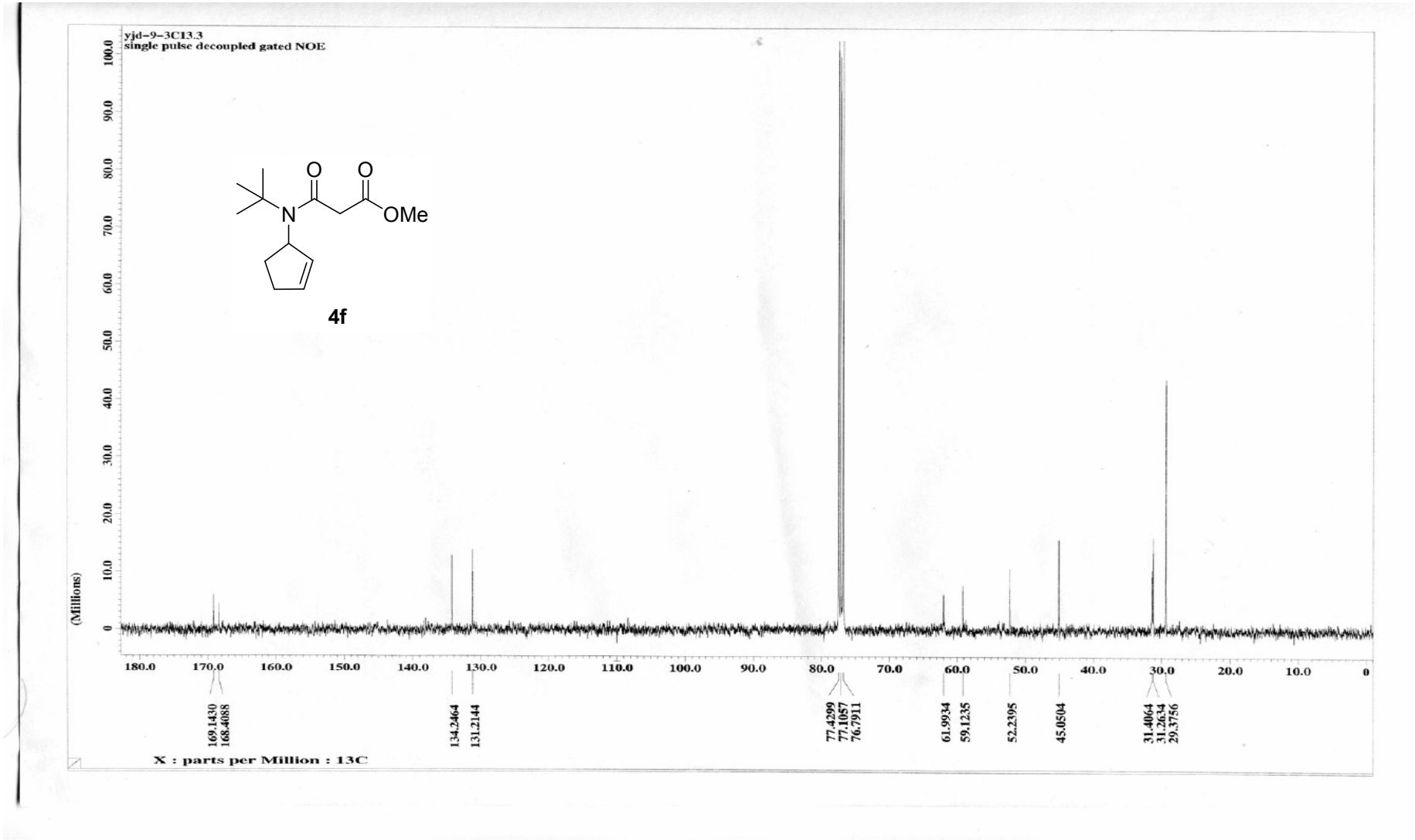

yjd-7-53.5
1H
MeO
O
O
N
SePh
2e
(Millions)
X : parts per Million : 1H

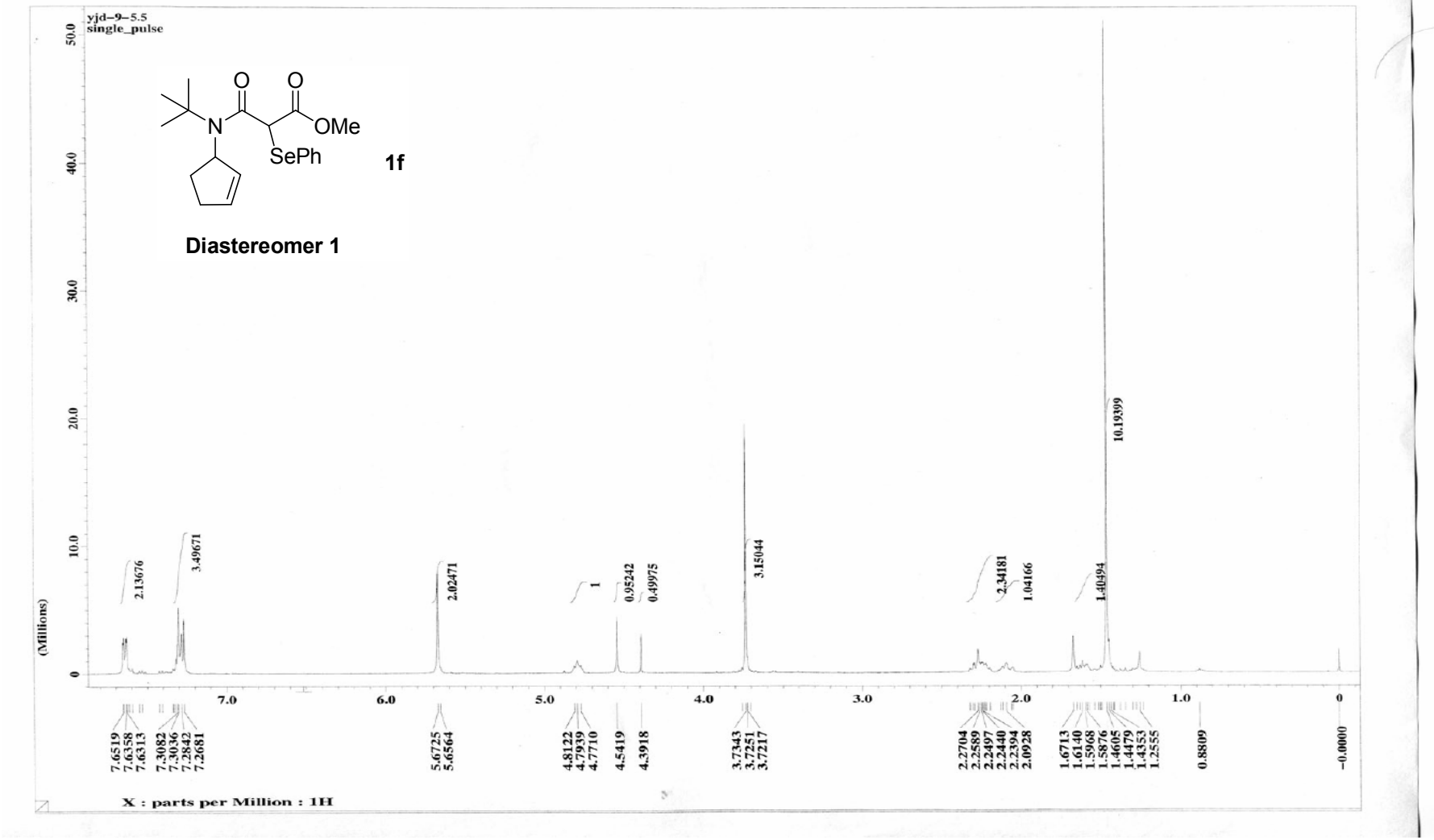

YJD-7-53_copy.3
single pulse decoupled gated NOE
MeO
O
O
N
SePh
2e
(Millions)
40.0
30.0
20.0
10.0
0
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
171.1167
166.3970
132.6542
129.2885
127.2195
77.1438
76.8292
58.0270
57.6742
52.4302
42.9052
36.3644
32.5411
28.3840
28.1742
0.0949
X : parts per Million : 13C
---- PROCESSING PARAMETERS ----
dc_balance
sweep : 2[Hz]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: YJD-7-53_copy.2
File Name = YJD-7-53_copy.3
Author =
Sample ID = S$820288
Content = single pulse decoupled
Creation Date = 22-MAR-2004 22:52:07
Revision Date = 22-MAR-2004 22:53:04
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 13C
Dim Size = 26214
Dim Units = [ppm]
Experiment = single_pulse_dec
Probe_id = 2692
Temp_get = 23.1[dC]
Spin_get = 16[Hz]
Solvent = CHLOROFORM-D
Recvr_gain = 56
Scans = 58
X_prescans = 4
Digital_filter = TRUE
Filter_factor = 8
X_points = 32768
X_domain = 13C
X_offset = 110[ppm]
X_freq = 100.52530333[MHz]
X_sweep = 31.40703518[kHz]
X_acq_time = 1.04333312[s]
X_resolution = 0.95846665[Hz]
Relaxation_delay = 2[s]
Repetition_time = 3.04333312[s]
X_angle = 30[deg]
X_90_width = 30.4[us]
X_pulse = 10.13333333[us]
X_atn = 7.4[dB]
Noe_time = 2[s]
Decoupling = TRUE
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Irr_pwidth = 0.115[ms]
Irr_atn_noe = 24.8[dB]
Irr_atn_dec = 24.8[dB]
Irr_noise = WALTZ
Dead_time = 0[us]
Delay = 0[us]
Tri_pwidth = 1[us]
Obs_pwidth = 1[us]
Qui_pwidth = 1[us]
Qua_pwidth = 1[us]
Hex_pwidth = 1[us]
Sep_pwidth = 1[us]
Oct_pwidth = 1[us]
Non_pwidth = 1[us]
Dec_pwidth = 1[us]

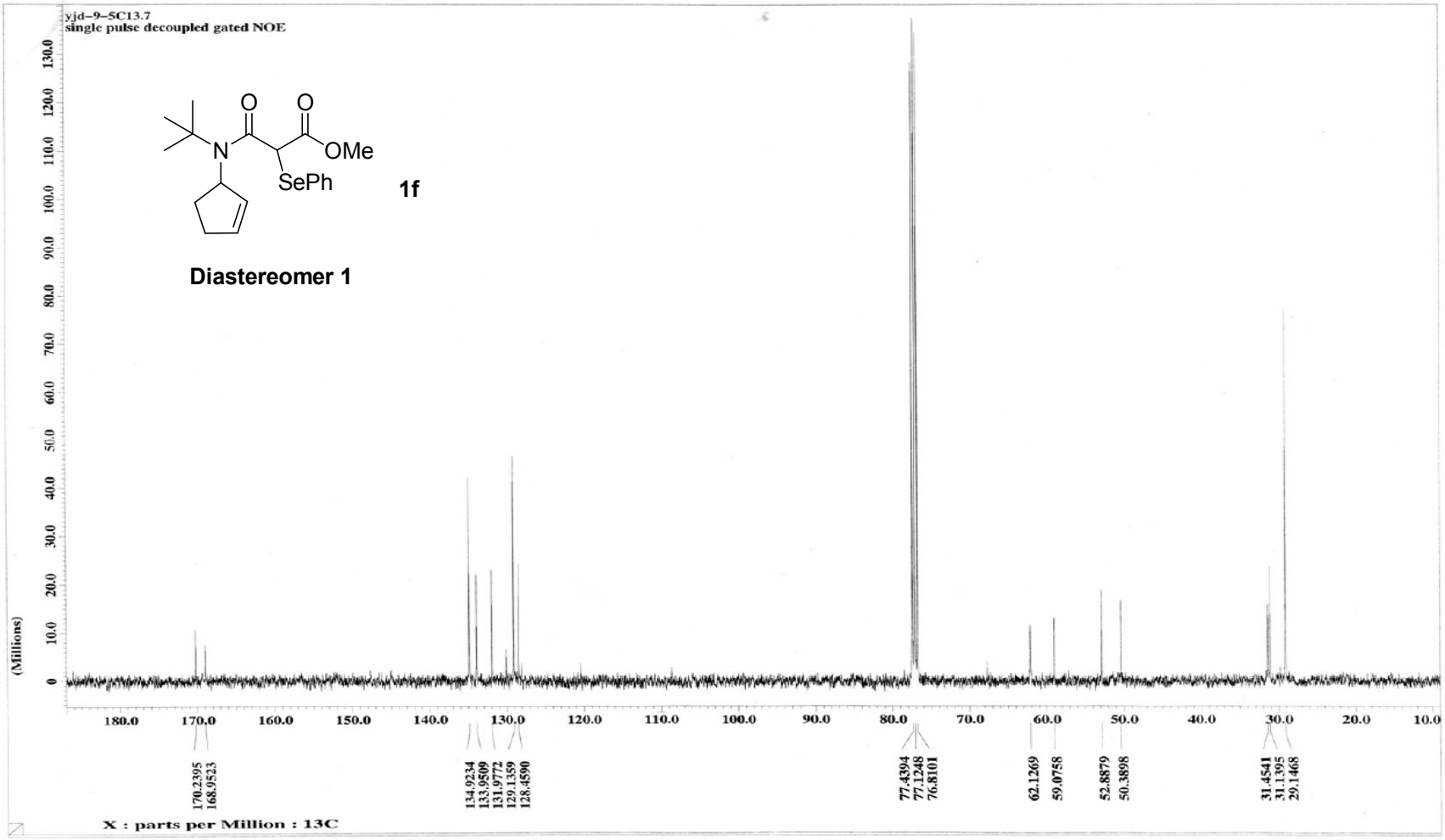

YJD-7-55-H4
single_pulse
MeO
O
O
N
3e
(Millions)
40.0
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2532
3.7443
3.6918
3.4254
3.4034
3.3912
3.2654
3.2544
2.9929
2.9661
2.1902
2.1792
2.1634
1.9060
1.8982
1.8750
1.8652
1.7064
1.4413
1.4217
1.4071
1.3900
1.3680
1.2360
0.9807
0.9636
0.8497
-0.0211
0.83321
0.92021
1
0.94213
0.97783
0.72523
10.81917
3.16883
X : parts per Million : 1H

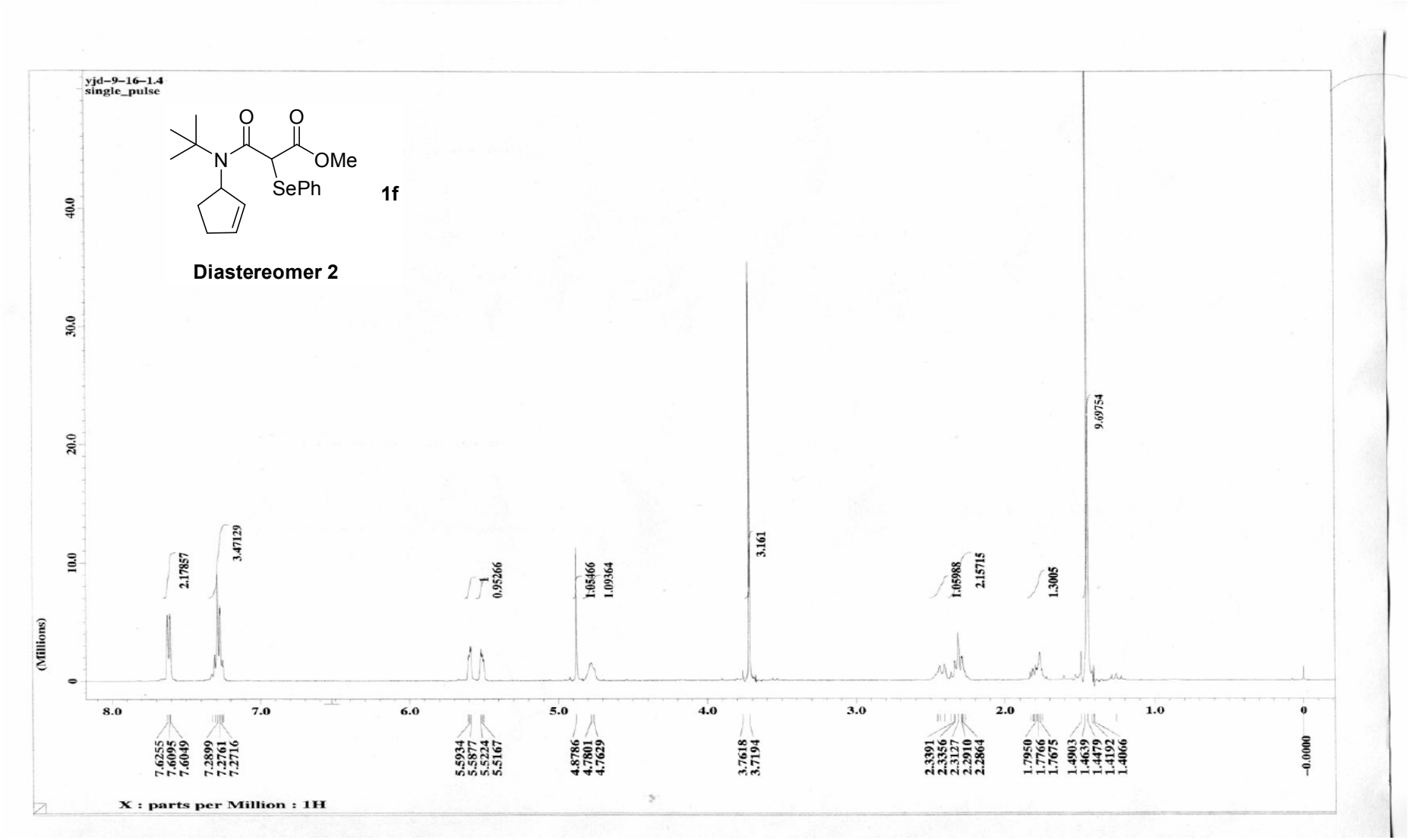

YJD-7-159-C13.3
single pulse decoupled gated NOE
MeO
O
O
N
3e
(Millions)
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.7000
167.0186
77.5079
77.1933
76.8691
59.6020
57.8190
52.1841
43.1930
31.0078
30.8075
28.1474
28.0616
20.0811
X : parts per Million : 13C

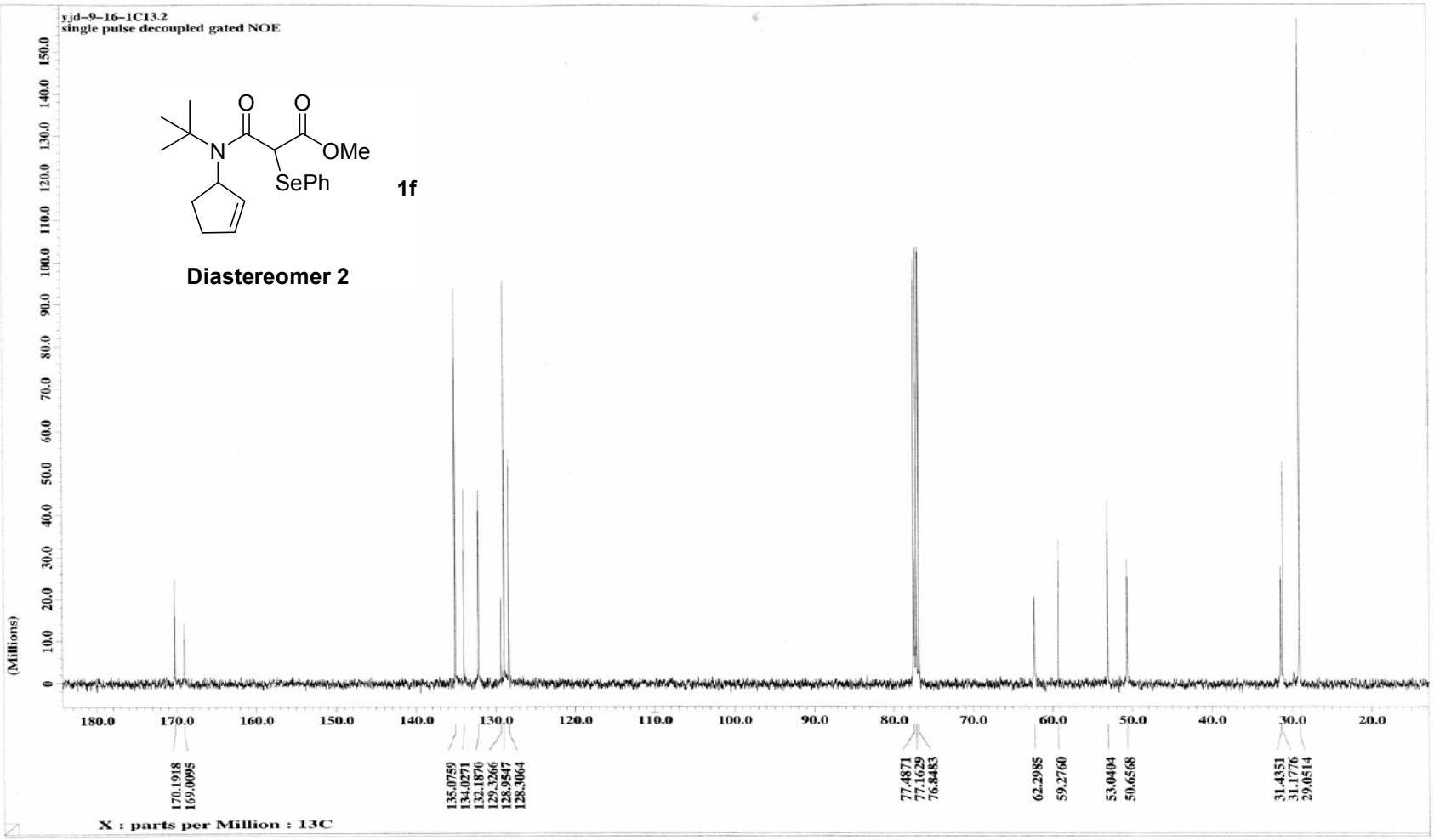

yjd-9-3.4
single_pulse
4f
(Millions)
X : parts per Million : 1H
1.00964
1.05099
3.01988
2.0076
1.08769
2.17195
1.83341
9.28162
7.2681
5.7870
5.7812
5.7228
5.7171
4.8454
4.8339
4.8282
3.7457
3.7194
3.4616
3.4227
3.3700
3.3310
2.4020
2.3975
2.3803
2.3746
2.3539
2.3494
1.7800
1.7629
1.7468
1.4902
1.4696
1.4295
1.2543
-0.0000

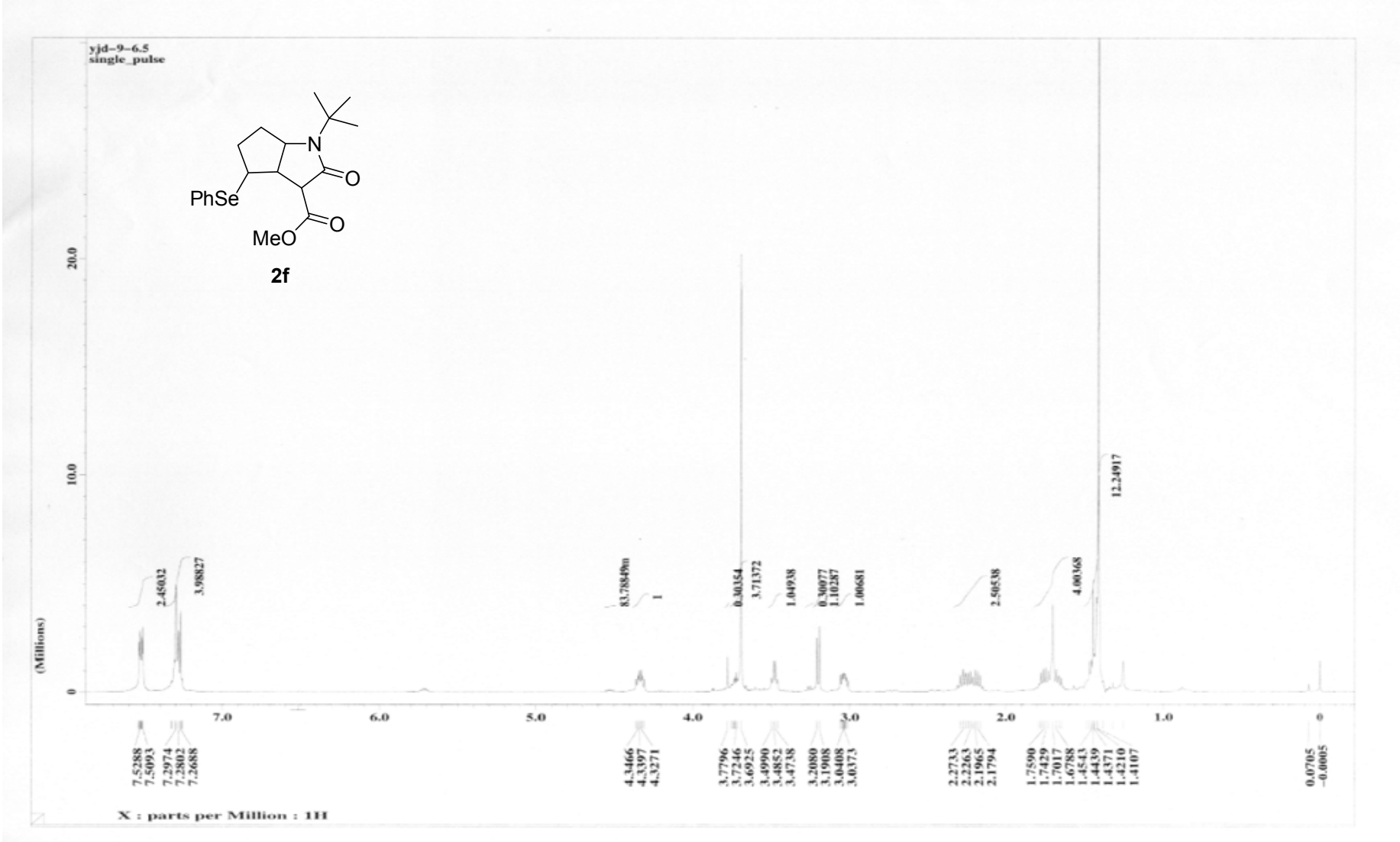

yjd-9-3C13.3
single pulse decoupled gated NOE
O
O
N
OMe
4f
(Millions)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
169.1430
168.4088
134.2464
131.2144
77.4299
77.1057
76.7911
61.9934
59.1235
52.2395
45.0504
31.4064
31.2634
29.3756
X : parts per Million : 13C

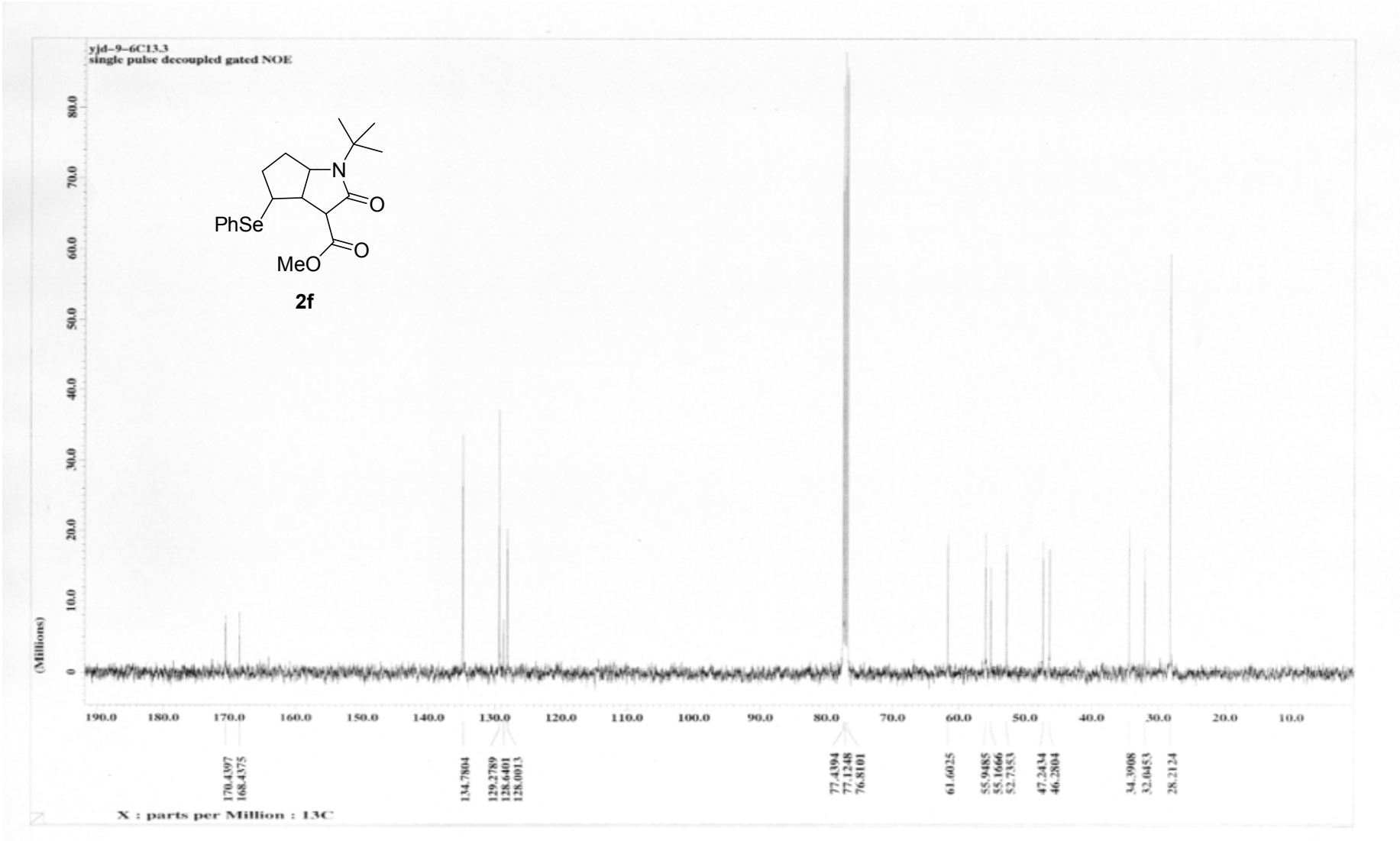

yjd-9-5.5
single_pulse
O
O
N
OMe
SePh
1f
Diastereomer 1
(Millions)
50.0
40.0
30.0
20.0
10.0
0
2.13676
3.49671
2.02471
1
0.95242
0.49975
3.15044
2.34181
1.04166
1.40494
10.19399
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6519
7.6358
7.6313
7.3082
7.3036
7.2842
7.2681
5.6725
5.6564
4.8122
4.7939
4.7710
4.5419
4.3918
3.7343
3.7251
3.7217
2.2704
2.2589
2.2497
2.2440
2.2394
2.0928
1.6713
1.6140
1.5968
1.5876
1.4605
1.4479
1.4353
1.2555
0.8809
-0.0000
X : parts per Million : 1H

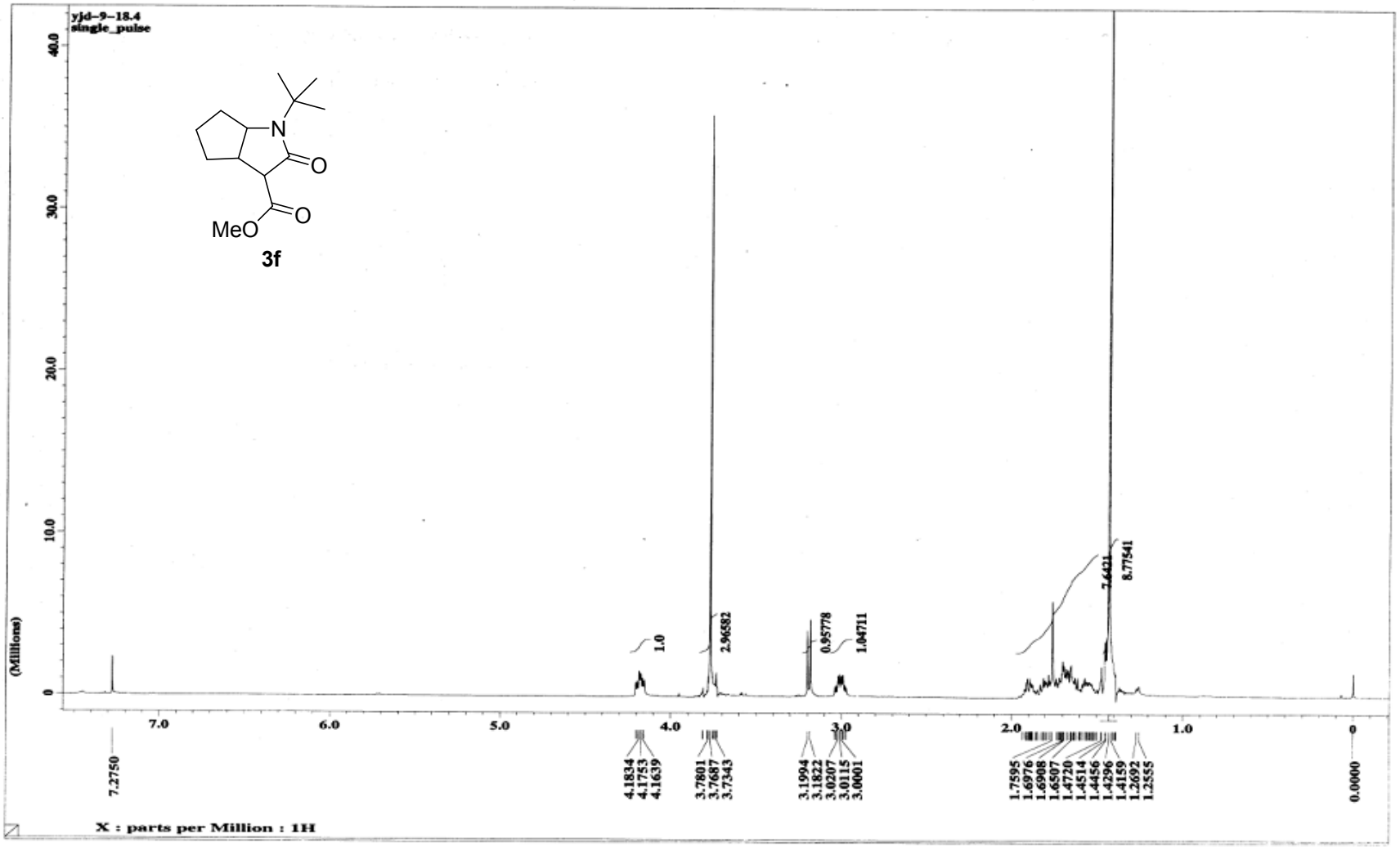

yjd-9-5C13.7
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1f
Diastereomer 1
(Millions)
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.2395
168.9523
134.9234
133.9509
131.9772
129.1359
128.4590
77.4394
77.1248
76.8101
62.1269
59.0758
52.8879
50.3898
31.4541
31.1395
29.1468
X : parts per Million : 13C

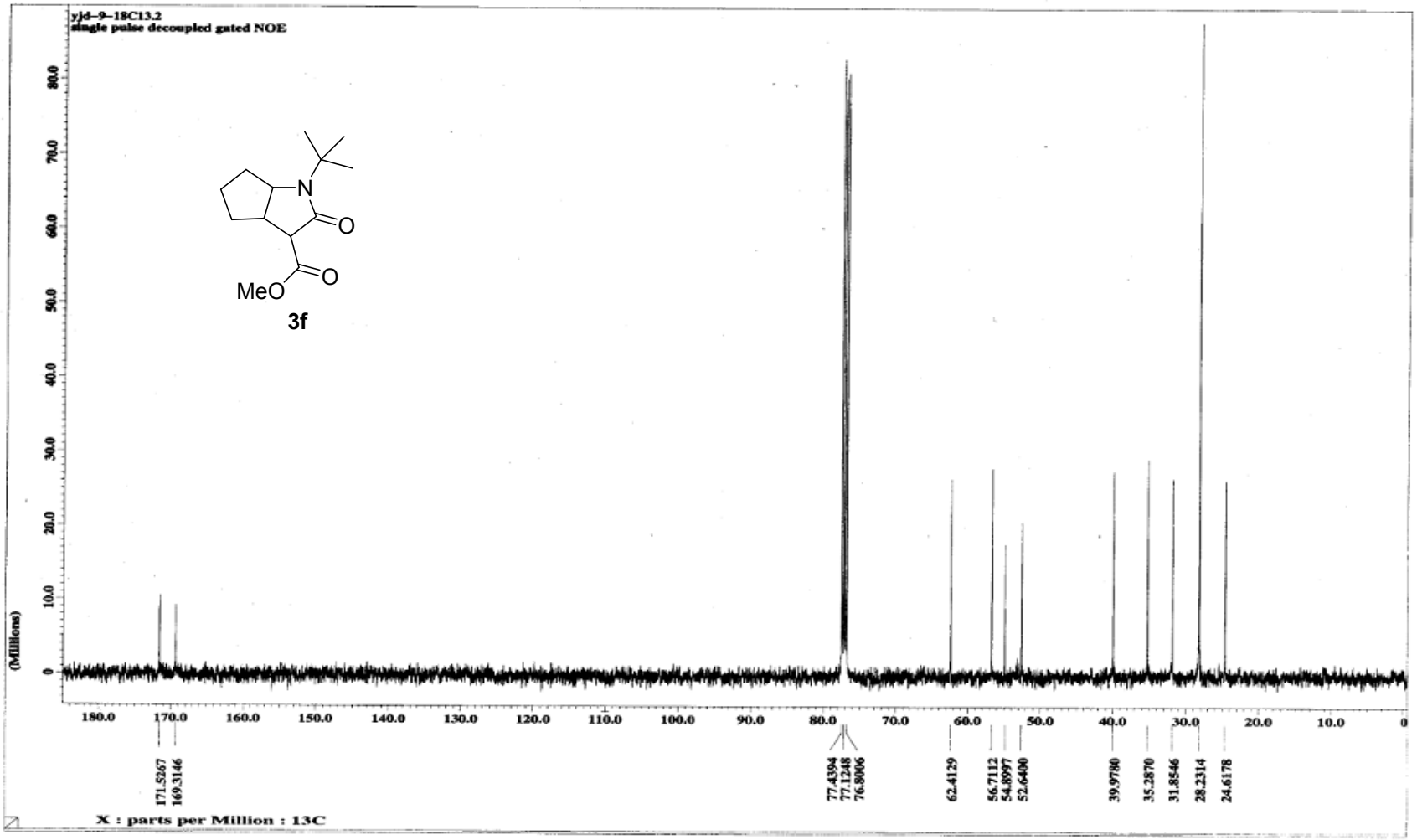

yjd-9-16-1.4
single_pulse
O
O
N
OMe
SePh
1f
Diastereomer 2
(Millions)
40.0
30.0
20.0
10.0
0
2.17857
3.47129
0.95266
1.05466
1.09364
3.161
1.05988
2.15715
1.3005
9.69754
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.6255
7.6095
7.6049
7.2899
7.2761
7.2716
5.5934
5.5877
5.5224
5.5167
4.8786
4.7801
4.7629
3.7618
3.7194
2.3391
2.3356
2.3127
2.2910
2.2864
1.7950
1.7766
1.7675
1.4903
1.4639
1.4479
1.4192
1.4066
-0.0000
X : parts per Million : 1H

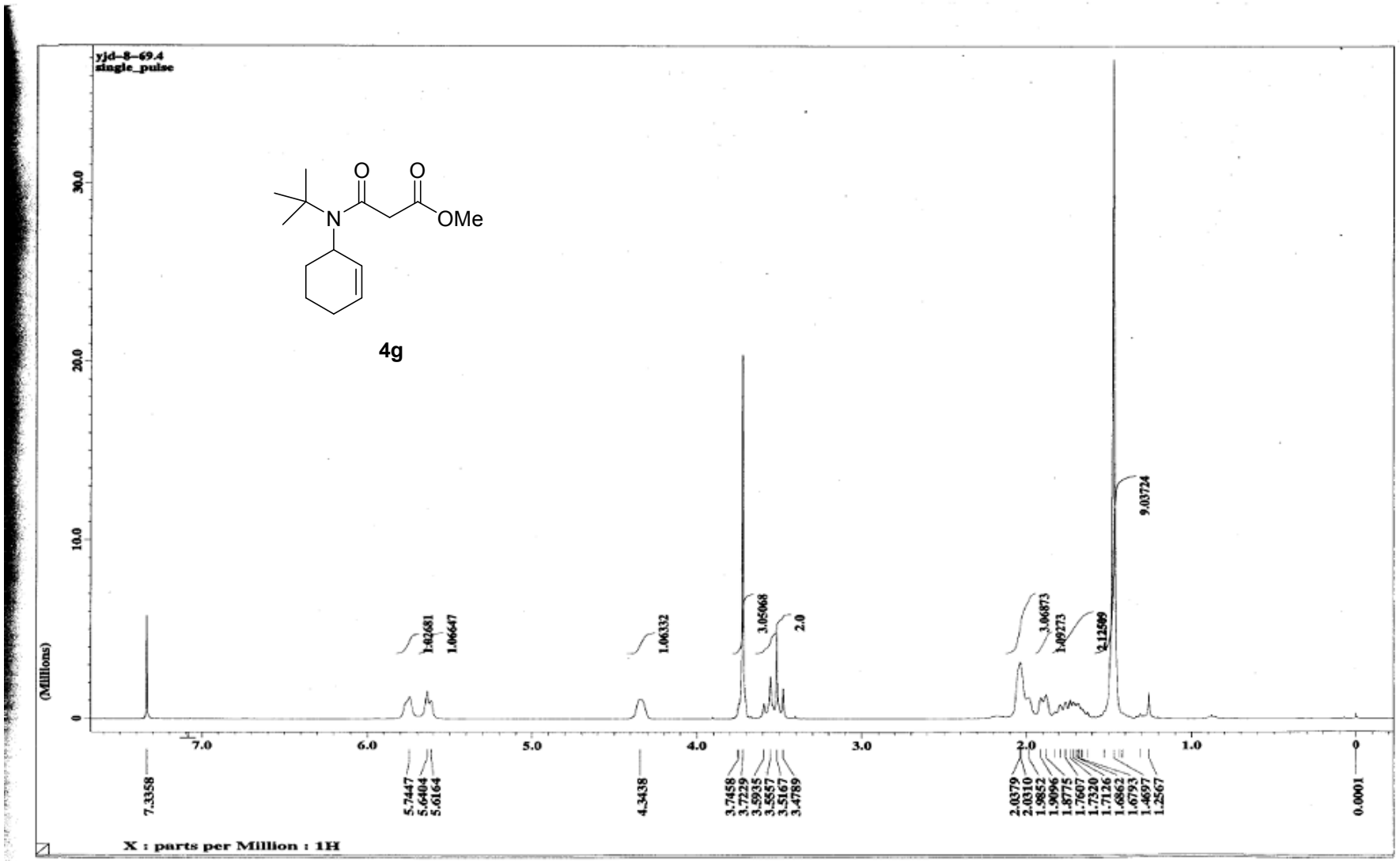

yjd-9-16-1C13.2
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1f
Diastereomer 2
(Millions)
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
170.1918
169.0095
135.0759
134.0271
132.1870
129.3266
128.9547
128.3064
77.4871
77.1629
76.8483
62.2985
59.2760
53.0404
50.6568
31.4351
31.1776
29.0514
X : parts per Million : 13C

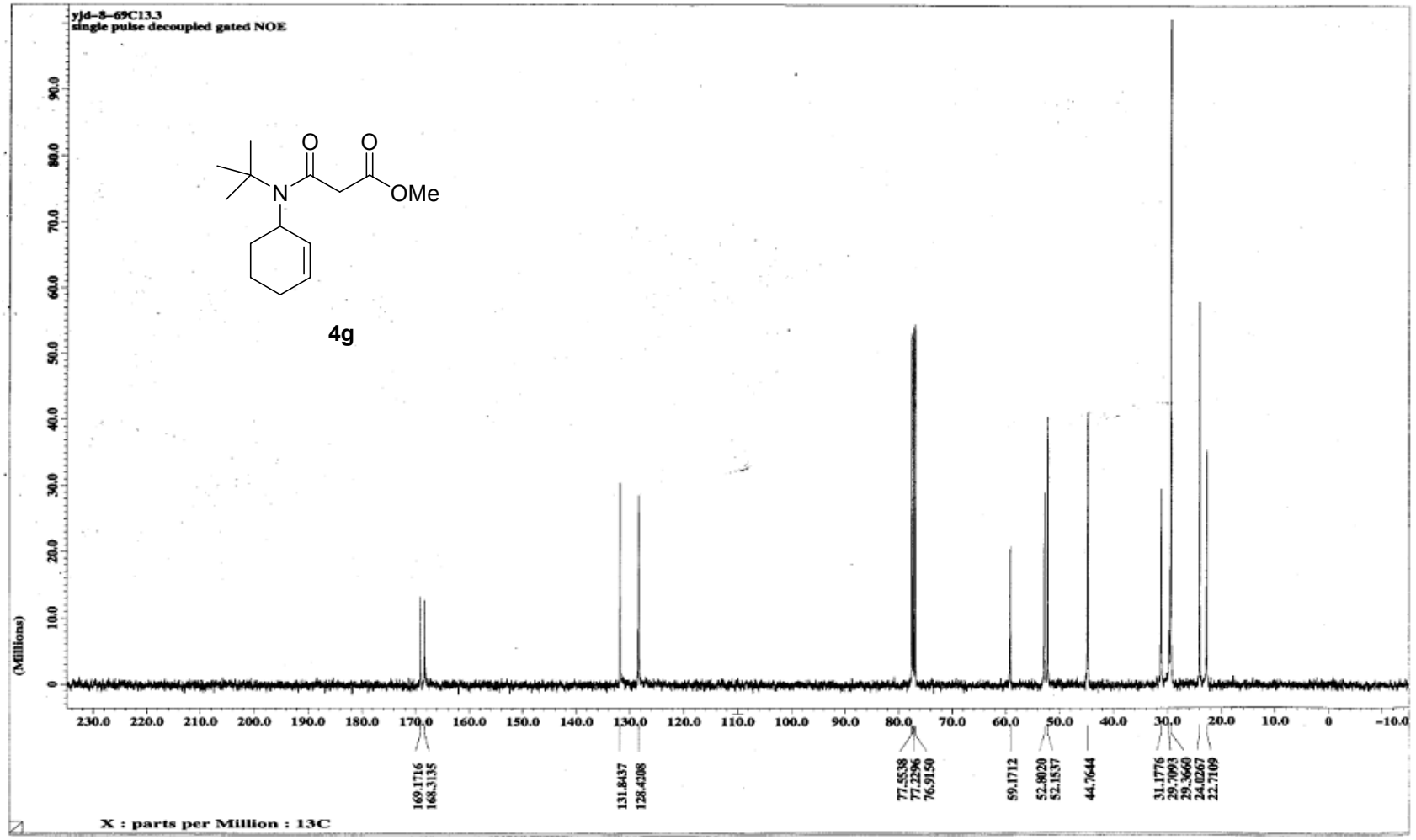

yjd-9-6.5
single_pulse
PhSe
N
O
O
MeO
O
2f
(Millions)
20.0
10.0
0
2.45032
3.98827
83.78849m
1
0.30354
3.71372
1.04938
0.30977
1.10287
1.00681
2.50538
4.00368
12.24917
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5288
7.5093
7.2974
7.2802
7.2688
4.3466
4.3397
4.3271
3.7796
3.7246
3.6925
3.4990
3.4852
3.4738
3.2080
3.1908
3.0408
3.0373
2.2733
2.2263
2.1965
2.1794
1.7590
1.7429
1.7017
1.6788
1.4543
1.4439
1.4371
1.4210
1.4107
0.0705
-0.0005
X : parts per Million : 1H

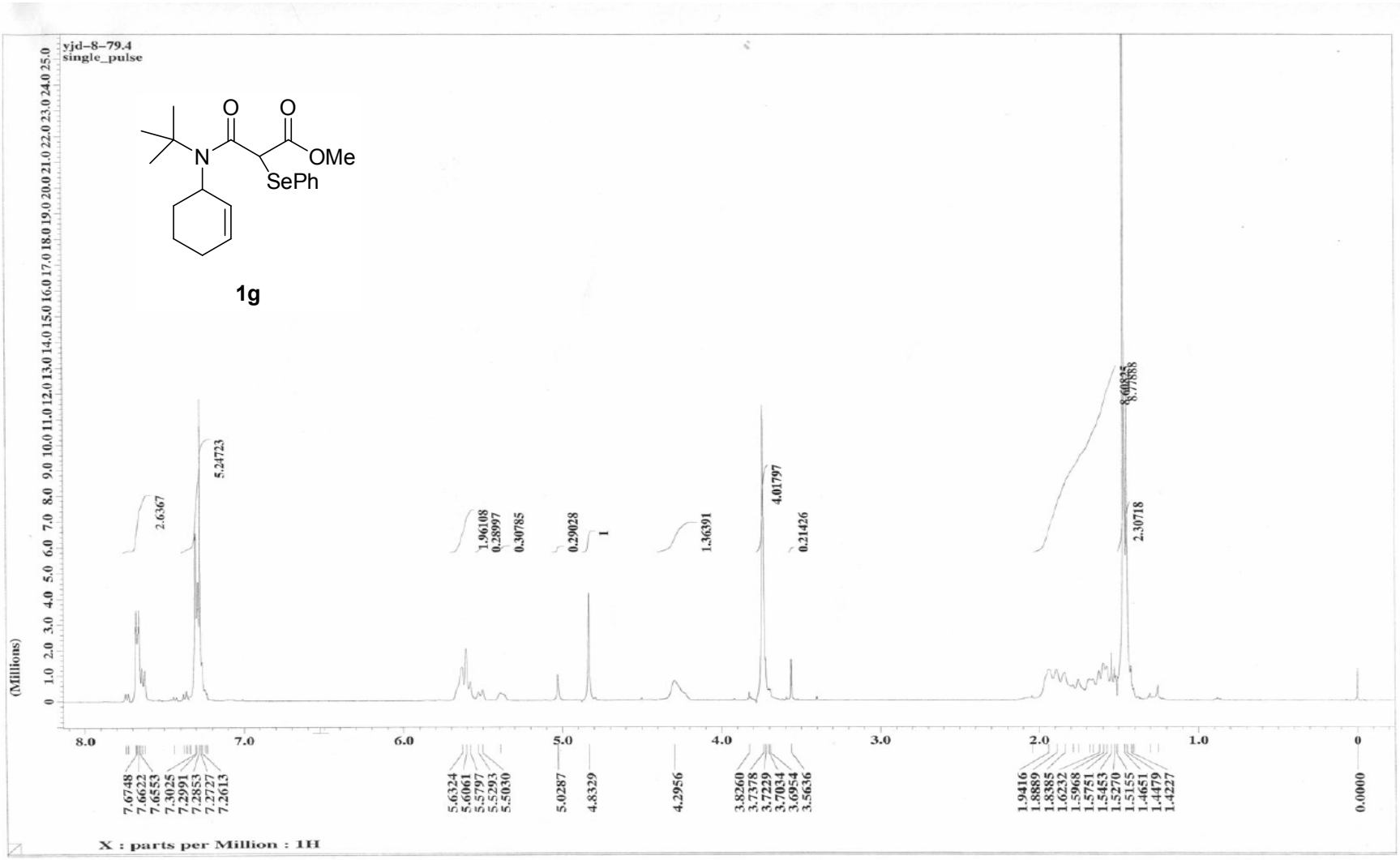

yjd-9-6C13.3
single pulse decoupled gated NOE
PhSe
N
O
O
MeO
O
2f
(Millions)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
170.4397
168.4375
134.7804
129.2789
128.6401
128.0013
77.4394
77.1248
76.8101
61.6025
55.9485
55.1666
52.7353
47.2434
46.2804
34.3908
32.0453
28.2124
X : parts per Million : 13C

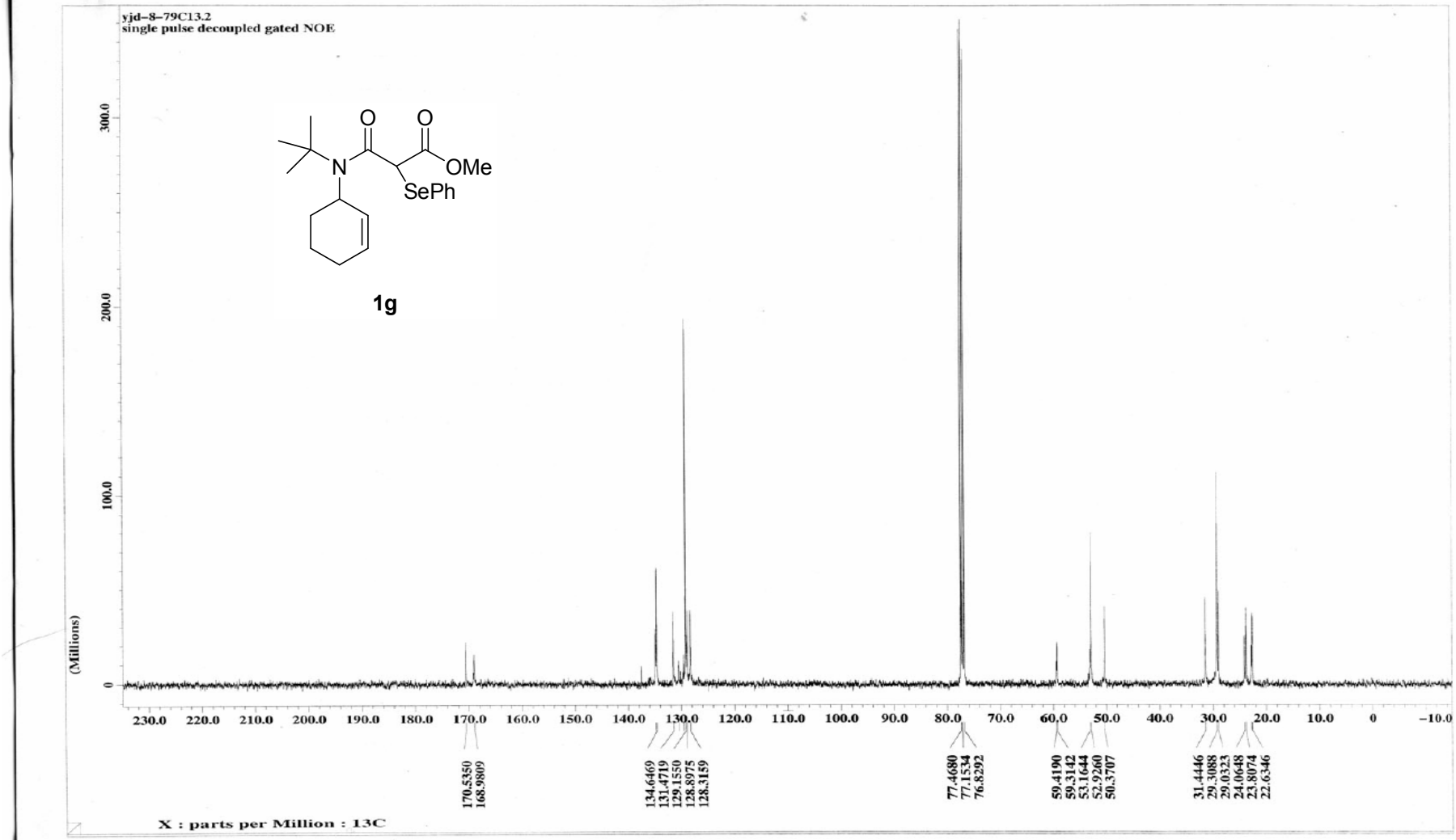

yjd-9-18.4
single_pulse
N
O
O
MeO
3f
(Millions)
40.0
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.0
2.96582
0.85778
1.04711
7.6421
8.77541
7.2750
4.1834
4.1753
4.1639
3.7801
3.7687
3.7343
3.1994
3.1822
3.0207
3.0115
3.0001
1.7595
1.6976
1.6908
1.6507
1.4720
1.4514
1.4456
1.4296
1.4159
1.2692
1.2555
0.0000
X : parts per Million : 1H

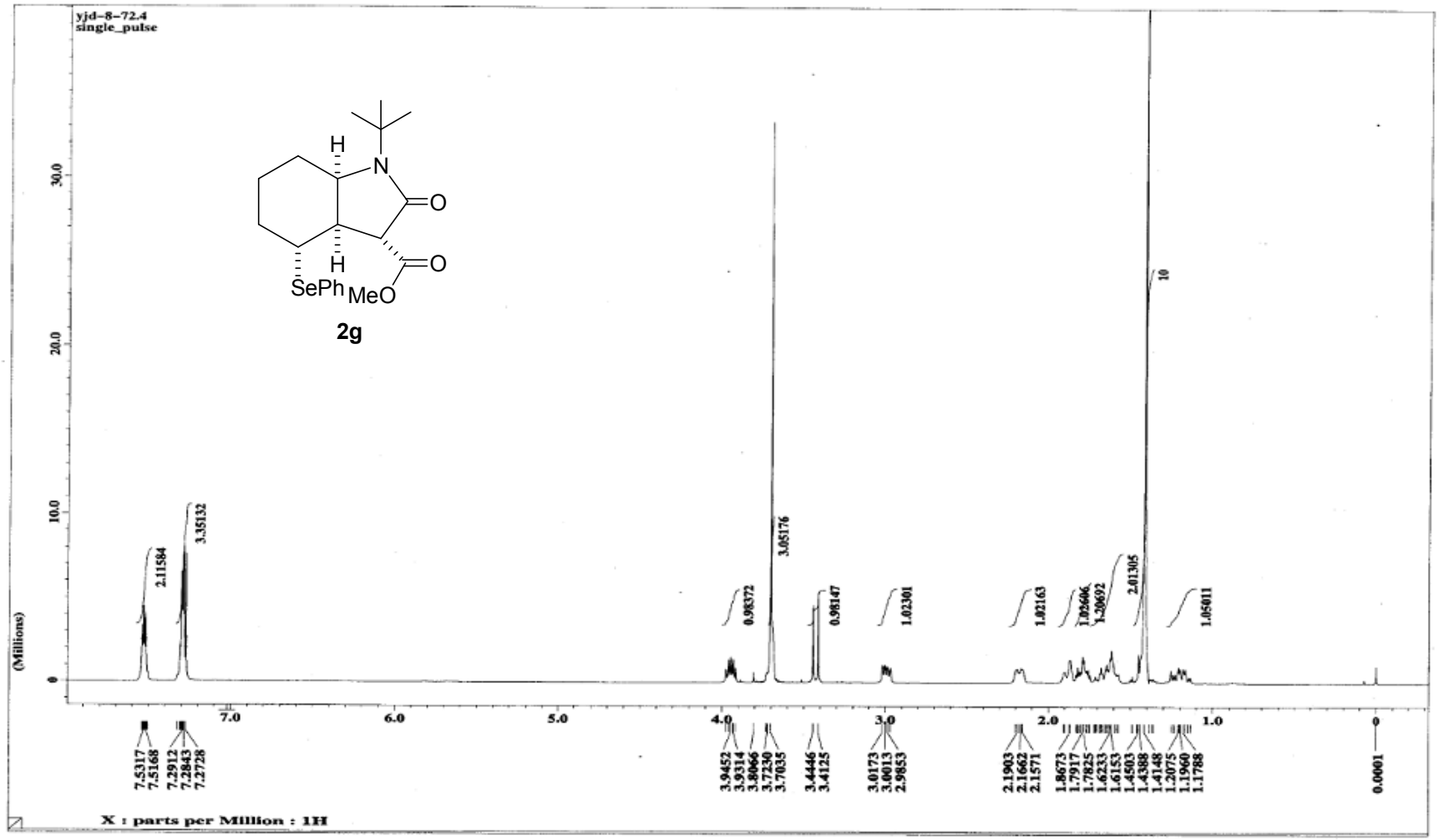

yjd-9-18C13.2
single pulse decoupled gated NOE
N
O
O
MeO
3f
(Millions)
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
171.5267
169.3146
77.4394
77.1248
76.8006
62.4129
56.7112
54.8997
52.6400
39.9780
35.2870
31.8546
28.2314
24.6178
X : parts per Million : 13C

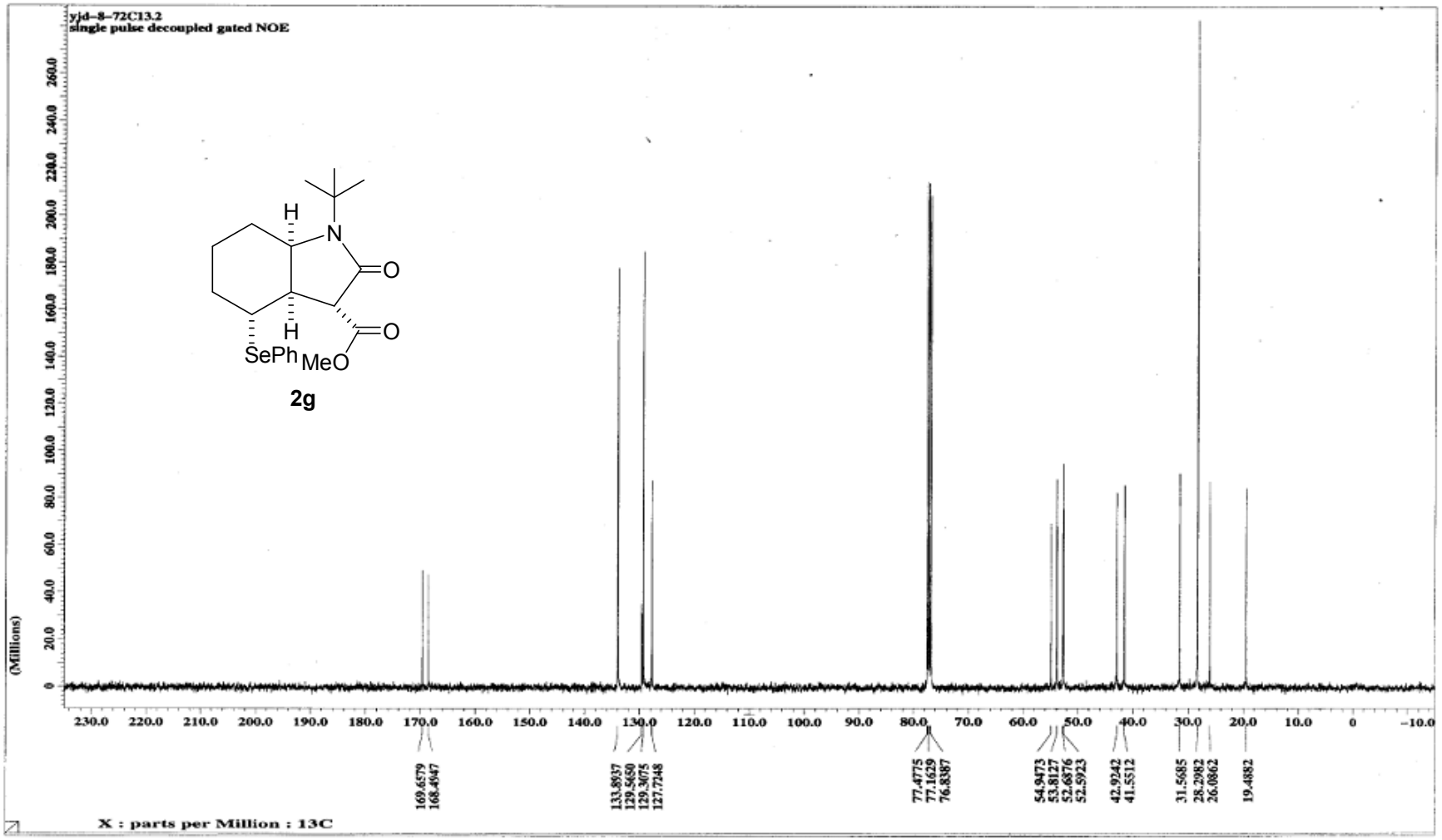

yjd-8-69.4
single_pulse
O
O
N
OMe
4g
(Millions)
30.0
20.0
10.0
0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
1.02681
1.06647
1.06332
3.05068
2.0
3.06873
1.09273
2.12589
9.03724
7.3358
5.7447
5.6404
5.6164
4.3438
3.7458
3.7229
3.5935
3.5557
3.5167
3.4789
2.0379
2.0310
1.9852
1.9096
1.8775
1.7607
1.7320
1.7126
1.6862
1.6793
1.4697
1.2567
0.0001
X : parts per Million : 1H


yjd-8-69C13.3
single pulse decoupled gated NOE
O
O
N
OMe
4g
(Millions)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
169.1716
168.3135
131.8437
128.4208
77.5538
77.2296
76.9150
59.1712
52.8020
52.1537
44.7644
31.1776
29.7093
29.3660
24.0267
22.7109
X : parts per Million : 13C

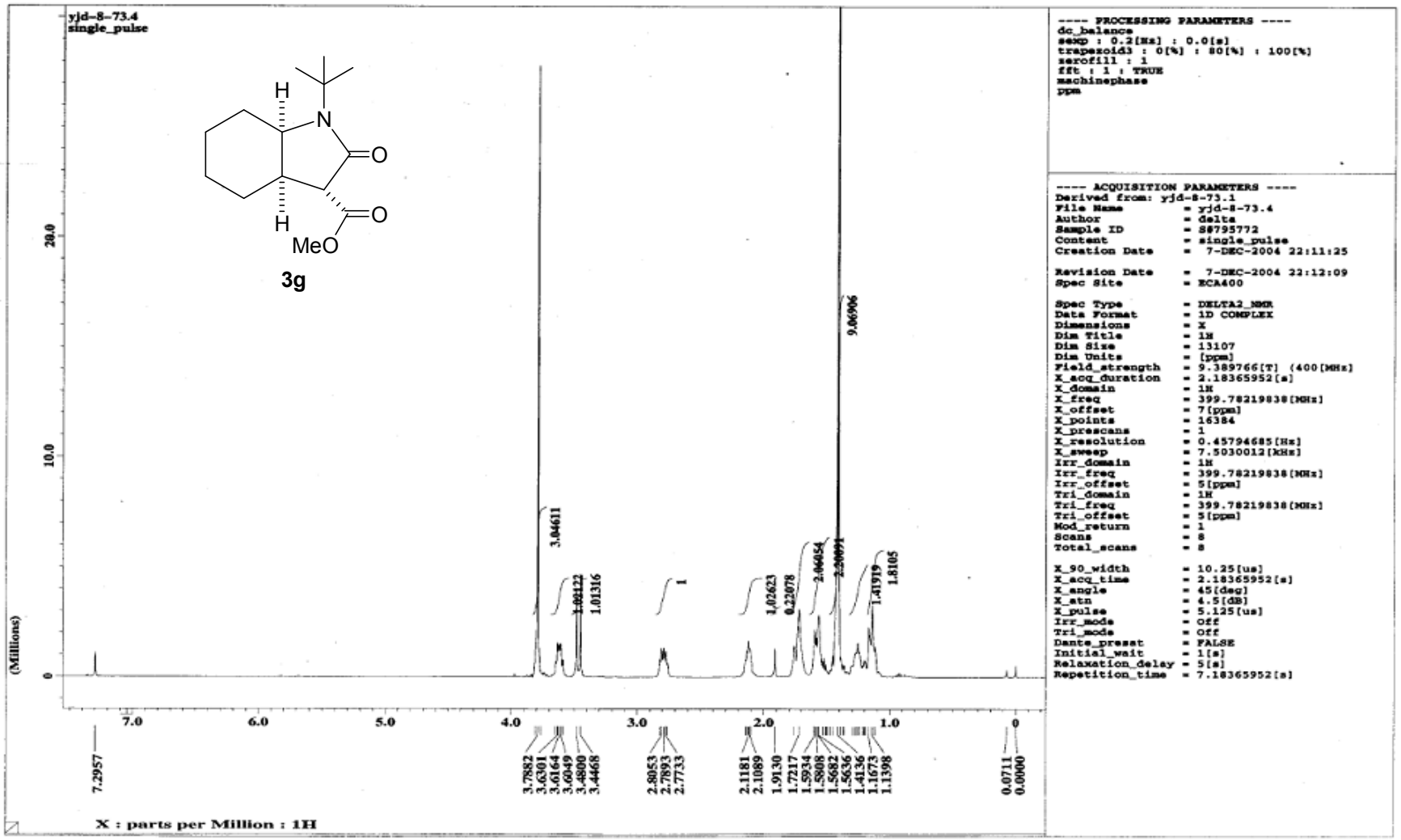

yjd-8-79.4
single_pulse
O
O
N
OMe
SePh
1g
(Millions)
X : parts per Million : 1H

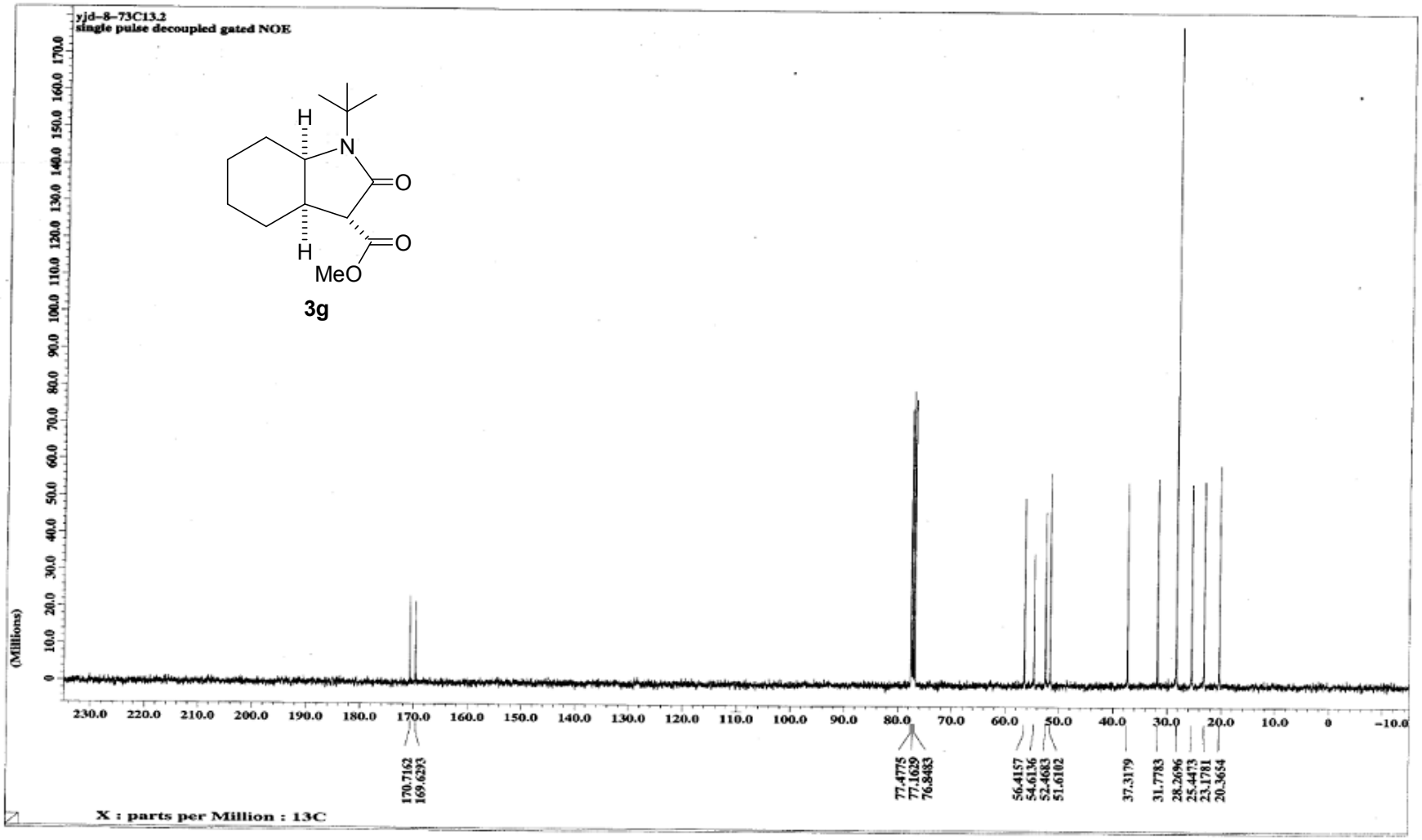

yjd-8-79C13.2
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1g
300.0
200.0
100.0
0
(Millions)
230.0 220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
170.5350
168.9809
134.6469
131.4719
129.1550
128.8975
128.3159
77.4680
77.1534
76.8292
59.4190
59.3142
53.1644
52.9260
50.3707
31.4446
29.3088
29.0323
24.0648
23.8074
22.6346
X : parts per Million : 13C

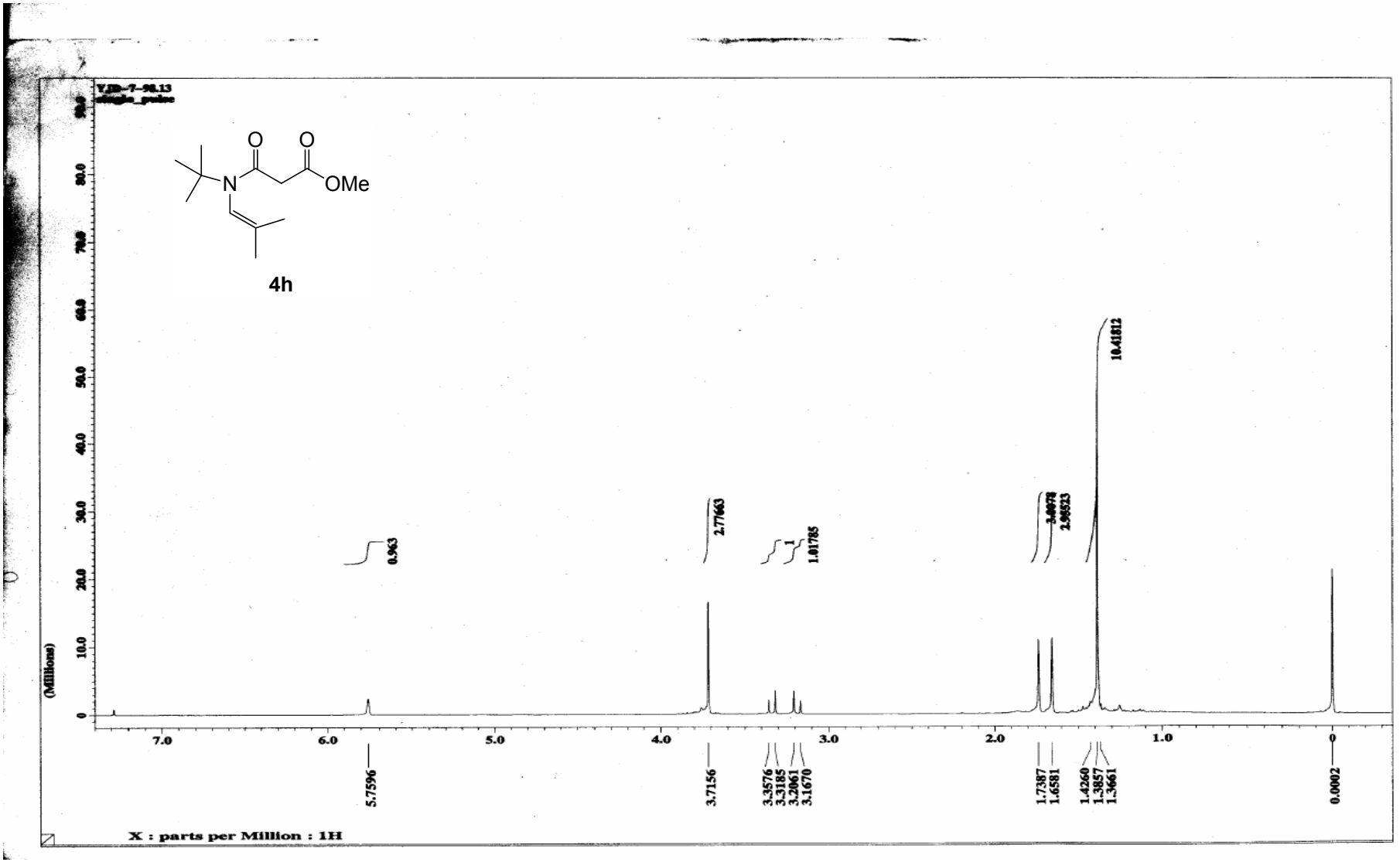

yjd-8-72.4
single_pulse
H
N
O
O
H
SePh
MeO
2g
(Millions)
30.0
20.0
10.0
0
2.11584
3.35132
0.98372
3.05176
0.98147
1.02301
1.02163
1.02606
1.20692
2.01305
10
1.05011
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5317
7.5168
7.2912
7.2843
7.2728
3.9452
3.9314
3.8066
3.7230
3.7035
3.4446
3.4125
3.0173
3.0013
2.9853
2.1903
2.1662
2.1571
1.8673
1.7917
1.7825
1.6233
1.6153
1.4503
1.4388
1.4148
1.2075
1.1960
1.1788
0.0001
X : parts per Million : 1H

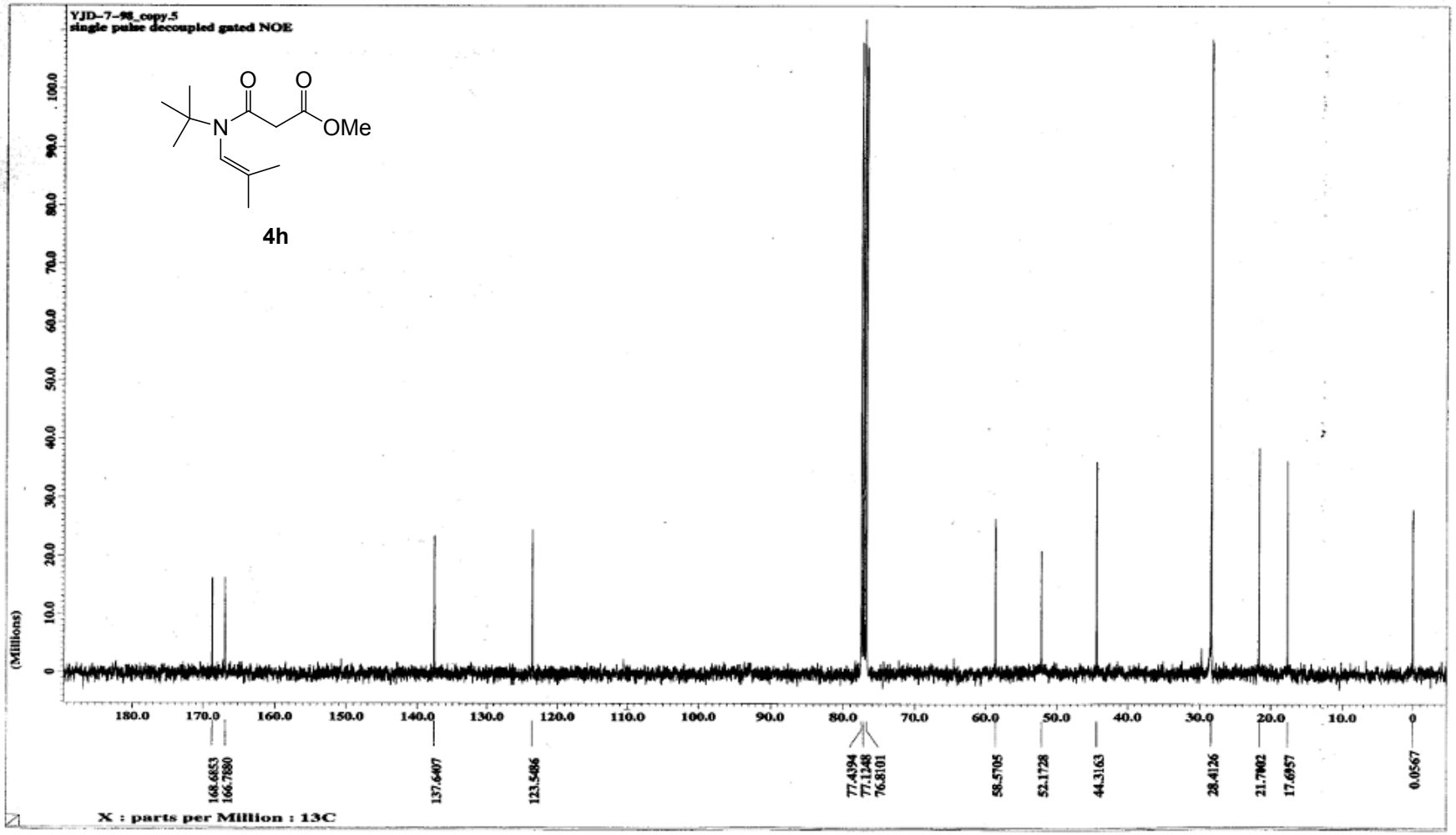

yjd-8-72C13.2
single pulse decoupled gated NOE
(Millions)
X : parts per Million : 13C
169.6579
168.4947
133.8937
129.5650
129.3075
127.7248
77.4775
77.1629
76.8387
54.9473
53.8127
52.6876
52.5923
42.9242
41.5512
31.5685
28.2982
26.0862
19.4882

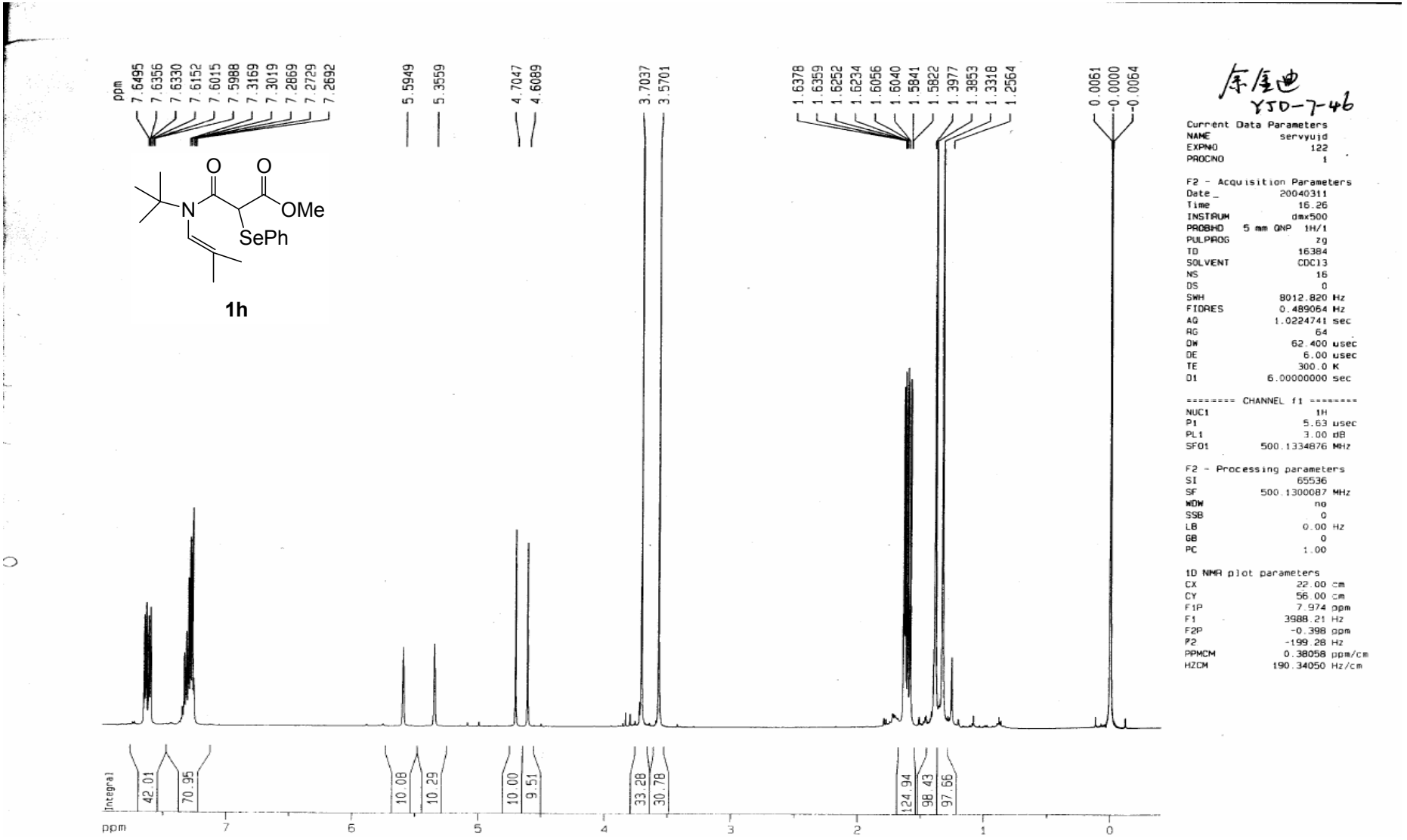
2g


yjd-8-73.4
single_pulse
H
N
O
O
H
MeO
3g
(Millions)
20.0
10.0
0
9.06906
3.84611
1.01316
1
1.02623
0.22078
2.06054
2.20691
1.41919
1.8105
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.2957
3.7882
3.6301
3.6164
3.6049
3.4800
3.4468
2.8053
2.7893
2.7733
2.1181
2.1089
1.9130
1.7217
1.5934
1.5808
1.5682
1.5636
1.4136
1.1673
1.1398
0.0711
0.0000
X : parts per Million : 1H
---- PROCESSING PARAMETERS ----
dc_balance
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE
machinephase
ppm
---- ACQUISITION PARAMETERS ----
Derived from: yjd-8-73.1
File Name = yjd-8-73.4
Author = delta
Sample ID = S0795772
Content = single_pulse
Creation Date = 7-DEC-2004 22:11:25
Revision Date = 7-DEC-2004 22:12:09
Spec Site = ECA400
Spec Type = DELTA2_NMR
Data Format = 1D COMPLEX
Dimensions = X
Dim Title = 1H
Dim Size = 13107
Dim Units = [ppm]
Field_strength = 9.389766[T] (400[MHz]
X_acq_duration = 2.18365952[s]
X_domain = 1H
X_freq = 399.78219838[MHz]
X_offset = 7[ppm]
X_points = 16384
X_prescans = 1
X_resolution = 0.45794685[Hz]
X_sweep = 7.5030012[kHz]
Irr_domain = 1H
Irr_freq = 399.78219838[MHz]
Irr_offset = 5[ppm]
Tri_domain = 1H
Tri_freq = 399.78219838[MHz]
Tri_offset = 5[ppm]
Mod_return = 1
Scans = 8
Total_scans = 8
X_90_width = 10.25[us]
X_acq_time = 2.18365952[s]
X_angle = 45[deg]
X_atn = 4.5[dB]
X_pulse = 5.125[us]
Irr_mode = Off
Tri_mode = Off
Dante_presat = FALSE
Initial_wait = 1[s]
Relaxation_delay = 5[s]
Repetition_time = 7.18365952[s]


yjd-8-73C13.2
single pulse decoupled gated NOE
H
N
O
O
H
MeO
3g
(Millions)
170.7162
169.6293
77.4775
77.1629
76.8483
56.4157
54.6136
52.4683
51.6102
37.3179
31.7783
28.2696
25.4473
23.1781
20.3654
X : parts per Million : 13C


O
O
N
OMe
4h
(Millions)
0.963
2.77663
1
1.01785
10.41812
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
5.7596
3.7156
3.3576
3.3185
3.2061
3.1670
1.7387
1.6581
1.4260
1.3857
1.3661
0.0002
X : parts per Million : 1H


YJD-7-98_copy.5
single pulse decoupled gated NOE
O
O
N
OMe
4h
(Millions)
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
168.6853
166.7880
137.6407
123.5486
77.4394
77.1248
76.8101
58.5705
52.1728
44.3163
28.4126
21.7902
17.6957
0.0567
X : parts per Million : 13C



康佳迪
YSD-7-46

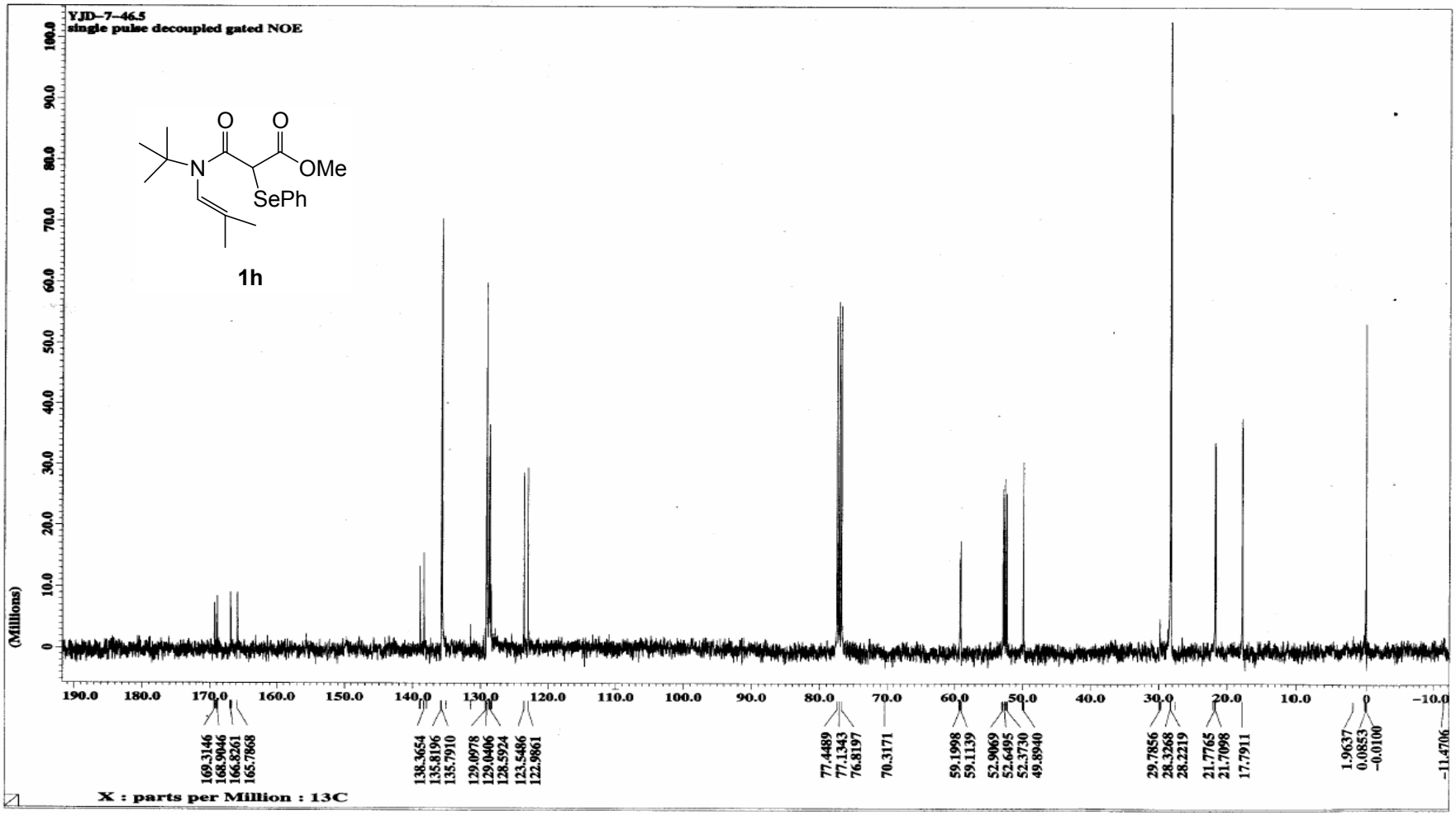
Current Data Parameters
NAME servyujd
EXPNO 122
PROCNO 1

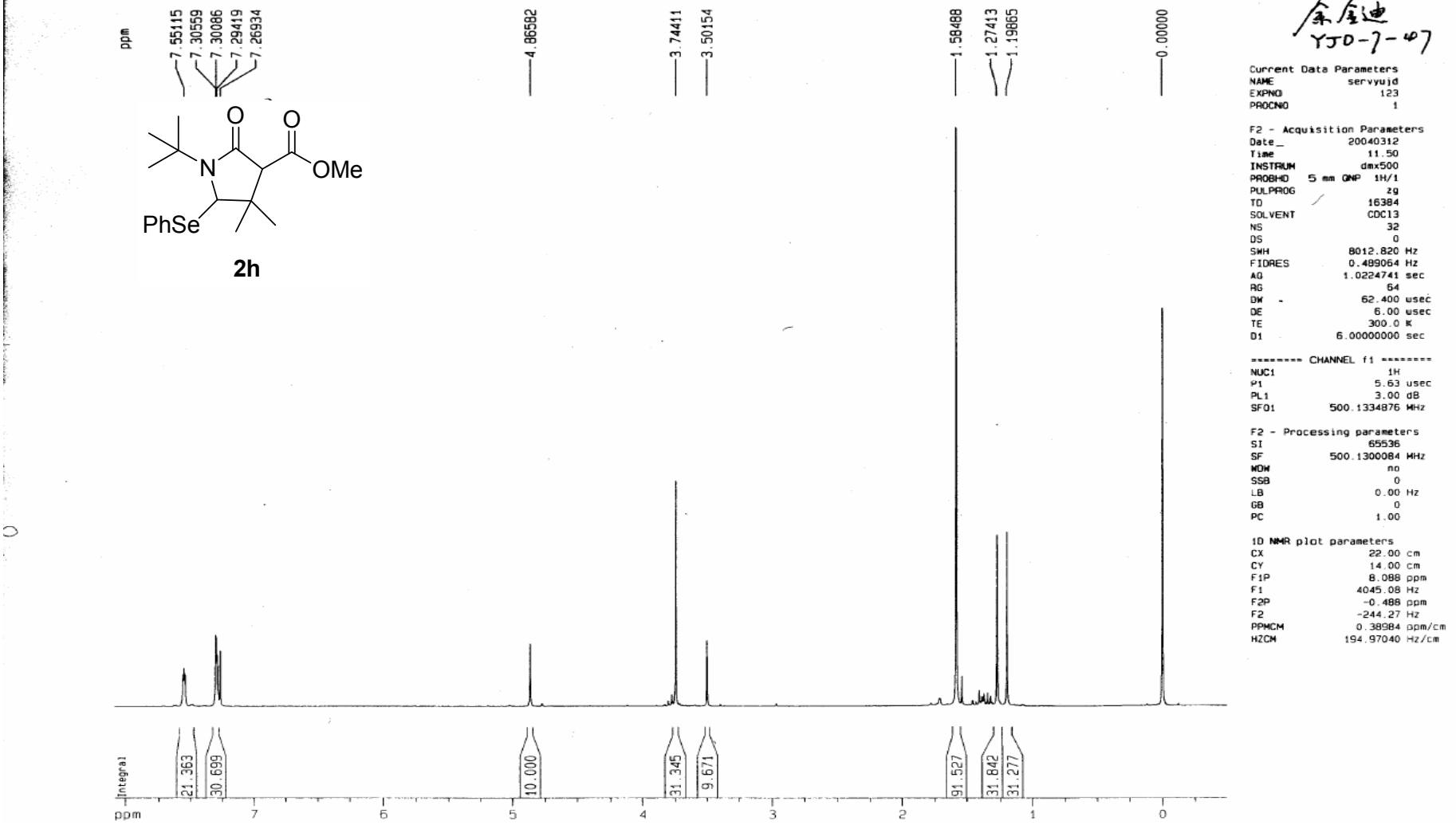
F2 - Acquisition Parameters
Date_ 20040311
Time 16.26
INSTRUM dmx500
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 16
DS 0
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0224741 sec
RG 64
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 5.63 usec
PL1 3.00 dB
SFO1 500.1334876 MHz

F2 - Processing parameters
SI 65536
SF 500.1300087 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 22.00 cm
CY 56.00 cm
F1P 7.974 ppm
F1 3988.21 Hz
F2P -0.398 ppm
F2 -199.28 Hz
PPMCM 0.38058 ppm/cm
HZCM 190.34050 Hz/cm


YJD-7-46.5
single pulse decoupled gated NOE
O
O
N
OMe
SePh
1h
(Millions)
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
169.3146
168.9046
166.8261
165.7868
138.3654
135.8196
135.7910
129.0978
129.0406
128.5924
123.5486
122.9861
77.4489
77.1343
76.8197
70.3171
59.1998
59.1139
52.9069
52.6495
52.3730
49.8940
29.7856
28.3268
28.2219
21.7765
21.7098
17.7911
1.9637
0.0853
-0.0100
-11.4706
X : parts per Million : 13C



余金迪
YJD-7-107

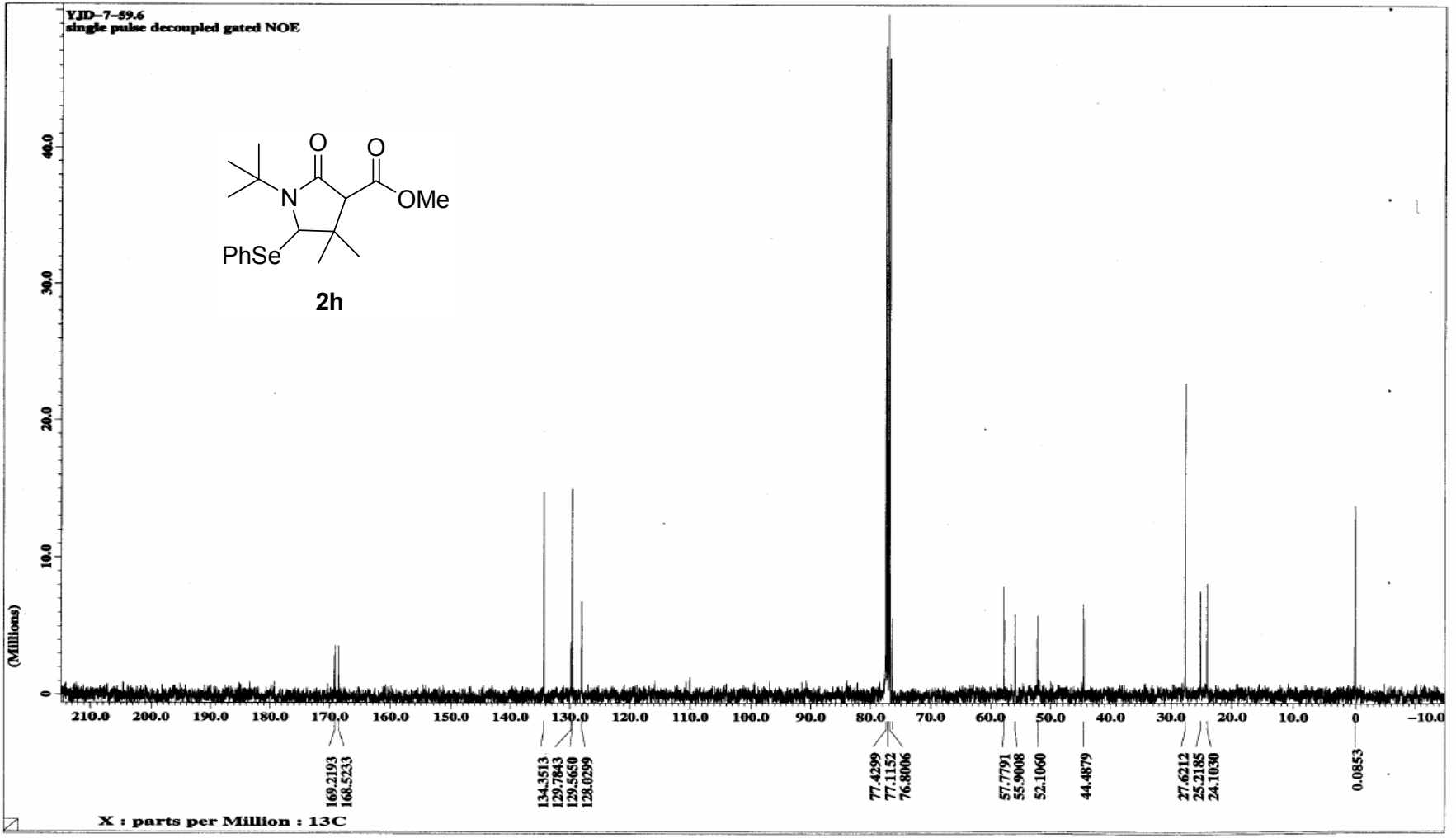
Current Data Parameters
NAME servyujd
EXPNO 123
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040312
Time 11.50
INSTRUM dmx500
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 16384
SOLVENT CDCl3
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0224741 sec
RG 64
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 6.00000000 sec

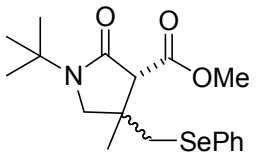
======== CHANNEL f1 ========
NUC1 1H
P1 5.63 usec
PL1 3.00 dB
SFO1 500.1334876 MHz

F2 - Processing parameters
SI 65536
SF 500.1300084 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

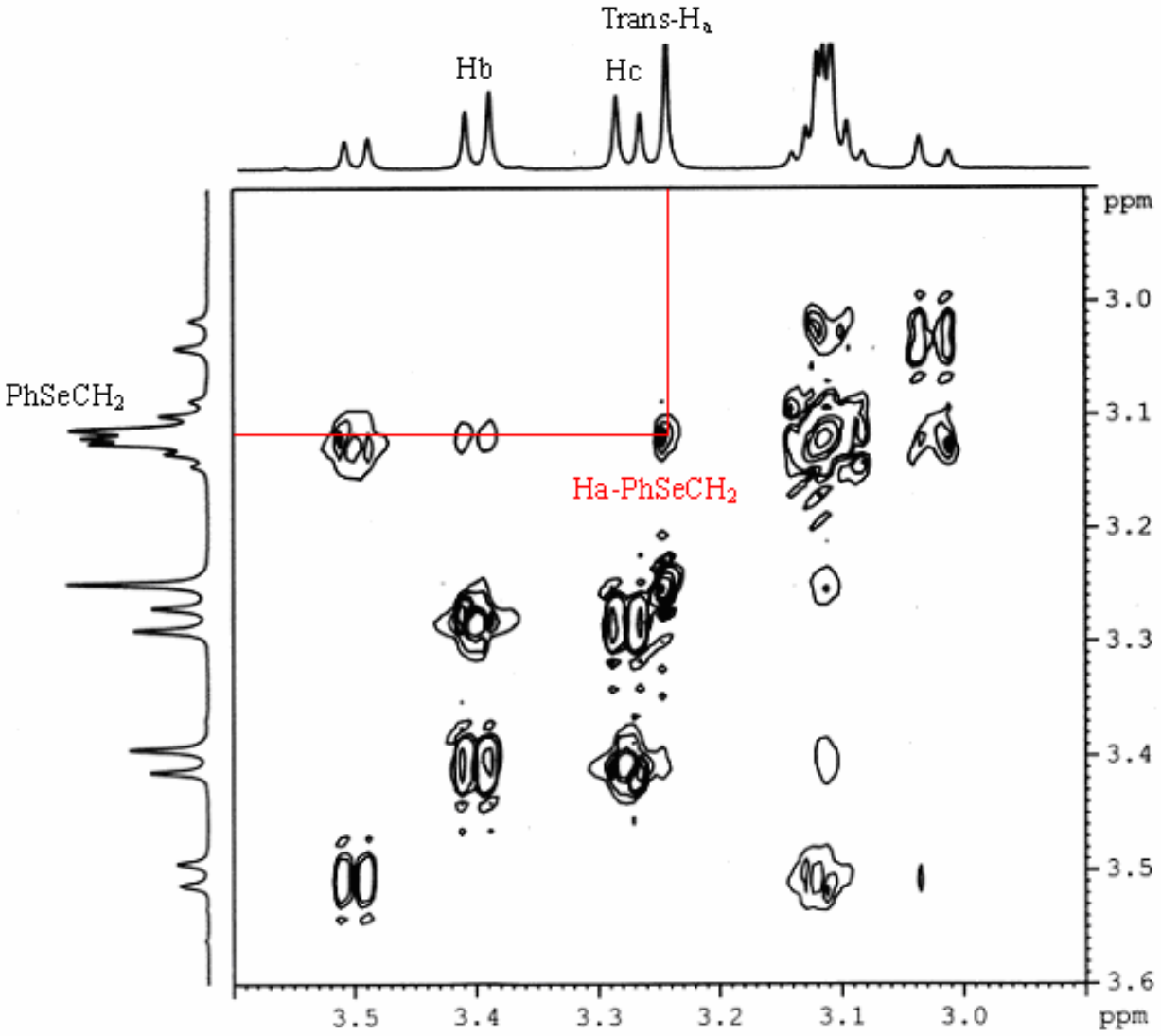
1D NMR plot parameters
CX 22.00 cm
CY 14.00 cm
F1P 8.088 ppm
F1 4045.08 Hz
F2P -0.488 ppm
F2 -244.27 Hz
PPMCM 0.38984 ppm/cm
HZCM 194.97040 Hz/cm

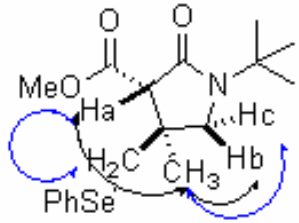

YJD--7--59.6
single pulse decoupled gated NOE
O
O
N
OMe
PhSe
2h
(Millions)
40.0
30.0
20.0
10.0
0
210.0
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
169.2193
168.5233
134.3513
129.7843
129.5650
128.0299
77.4299
77.1152
76.8006
57.7791
55.9008
52.1060
44.4879
27.6212
25.2185
24.1030
0.0853
X : parts per Million : 13C

NOESY spectra of 2c, 3d, 2f, 3g, 2h



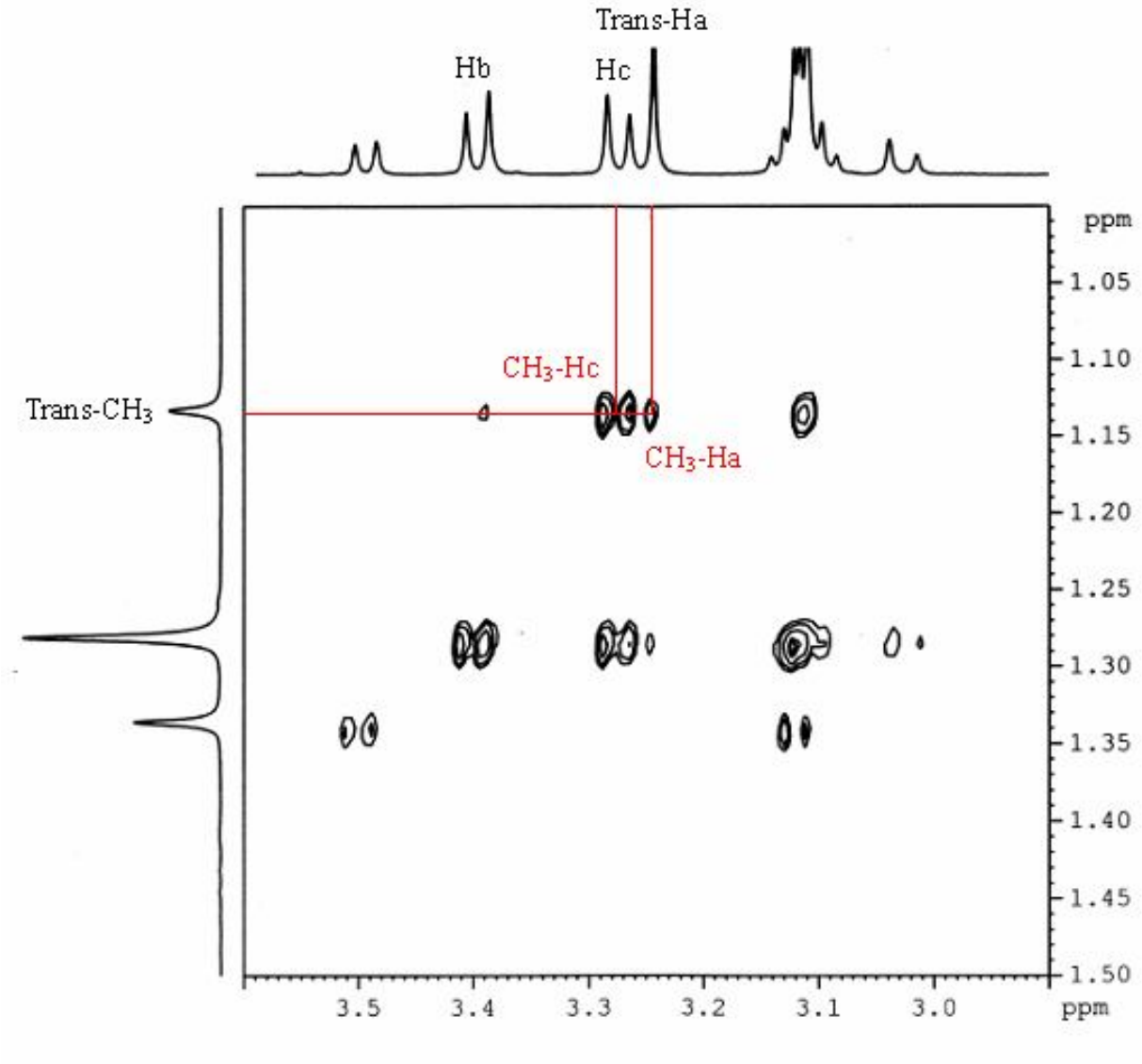
2c

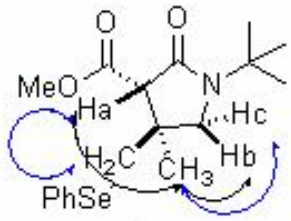




2c

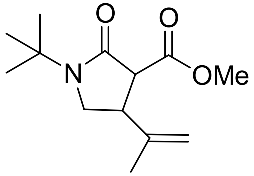
Ha-PhSeCH$_2$: strong NOE
CH$_3$-Hc: strong NOE
Ha-CH$_3$: weak NOE
CH$_3$-Hb: weak NOE



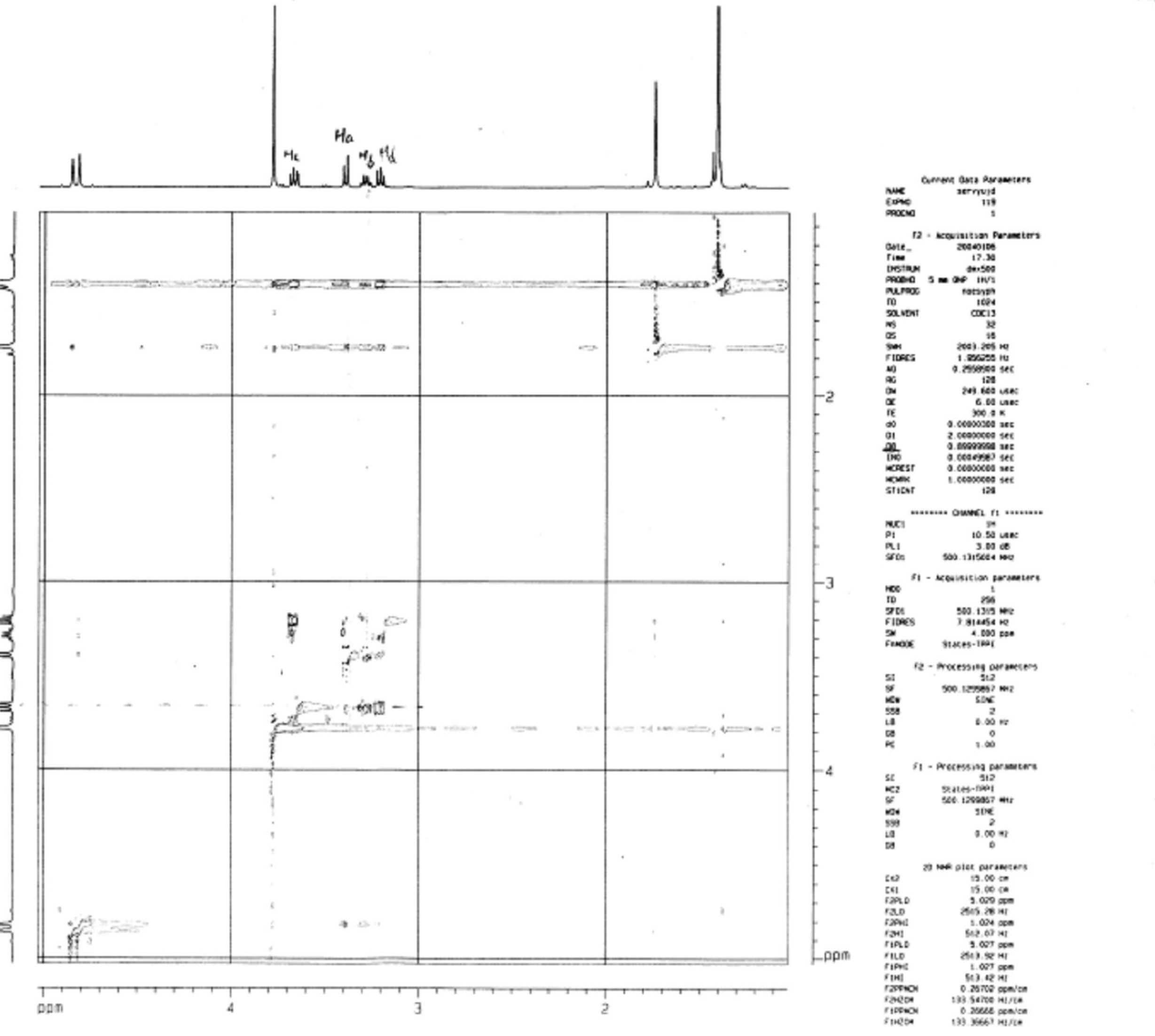


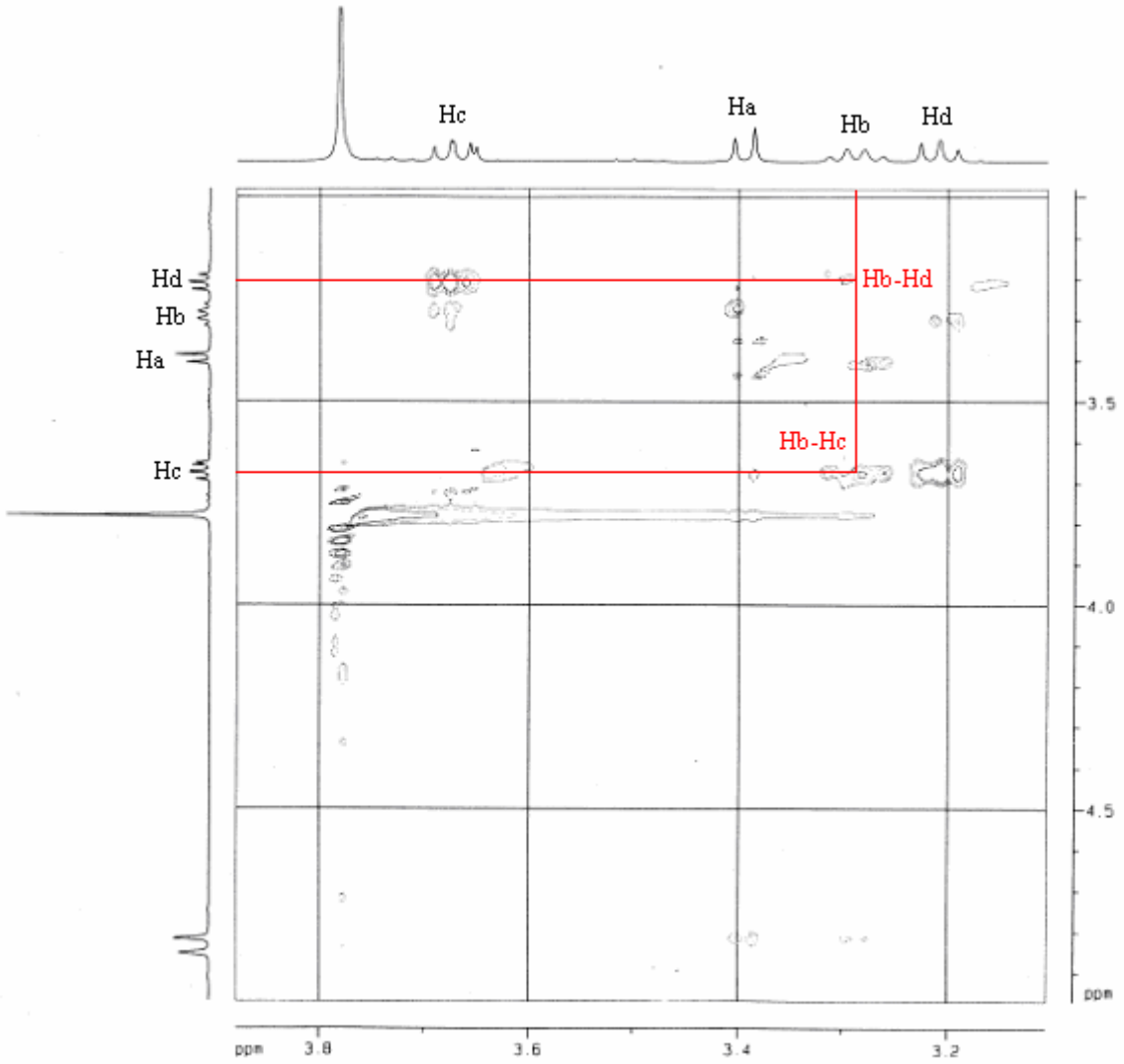
2c

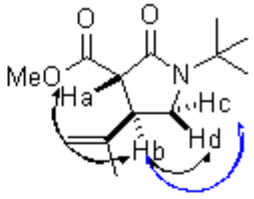
Ha-PhSeCH_2: strong NOE
CH_3-Hc: strong NOE
Ha-CH_3: weak NOE
CH_3-Hb: weak NOE


O
O
N
OMe

3d

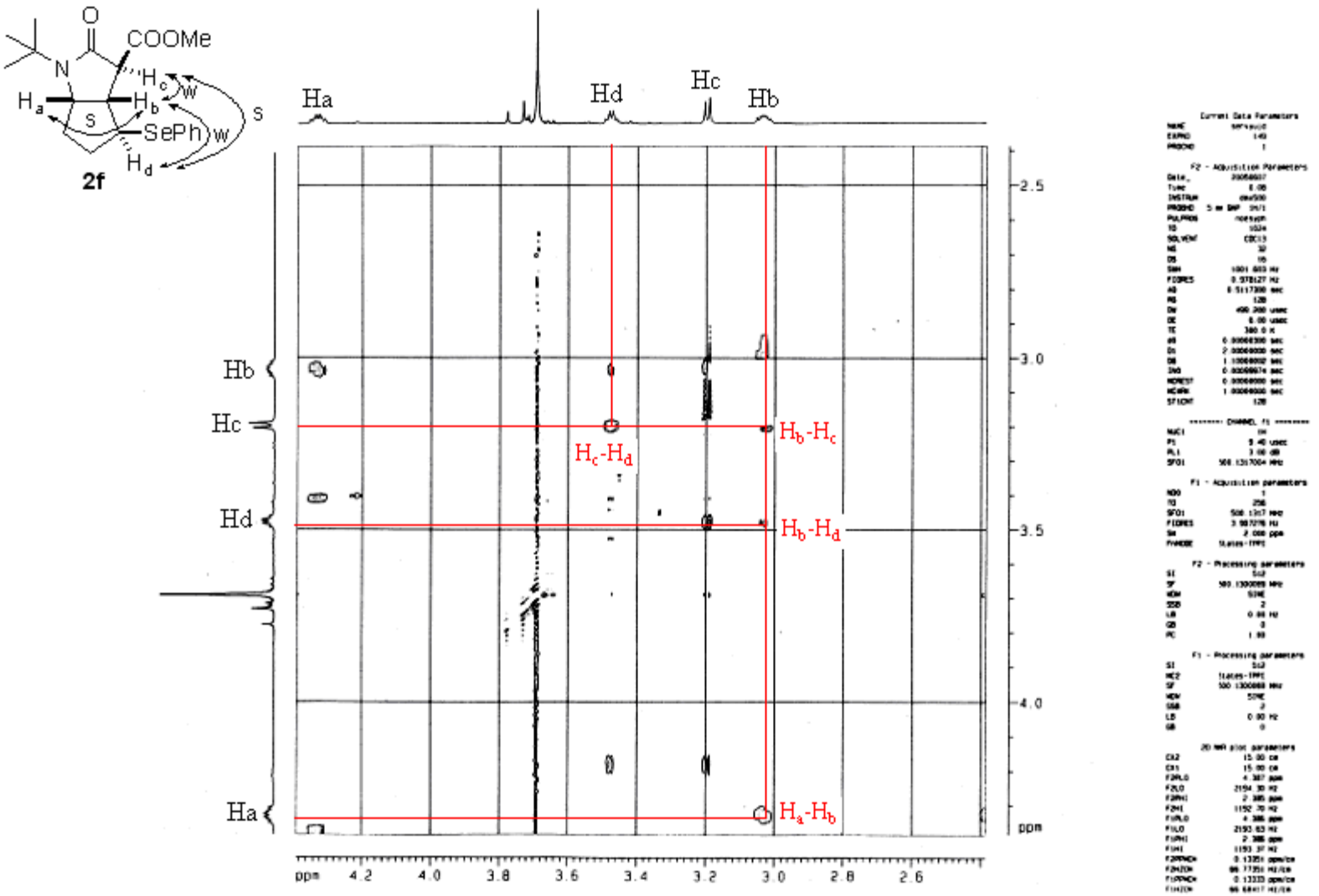

Current Data Parameters
EXPNO 119
PROCNO 1
F2 - Acquisition Parameters
Time 17.30
TD 1024
SOLVENT CDCl3
NS 32
DS 16
RG 128
DE 6.00 usec
TE 300.0 K
STIME 128
CHANNEL f1
P1 10.50 usec
PL1 3.00 dB
F1 - Acquisition parameters
TD 256
SW 4.000 ppm
F2 - Processing parameters
SI 512
SSB 2
LB 0.00 Hz
GB 0
PC 1.00
F1 - Processing parameters
SI 512
SSB 2
LB 0.00 Hz
GB 0
2D NMR plot parameters
CX2 15.00 cm
CX1 15.00 cm
F2PLO 5.029 ppm
F2PHI 1.024 ppm
F1PLO 5.027 ppm
F1PHI 1.027 ppm
ppm
4
3
2
ppm

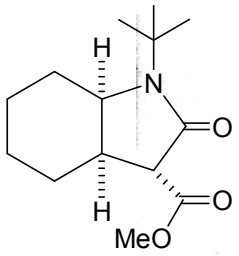




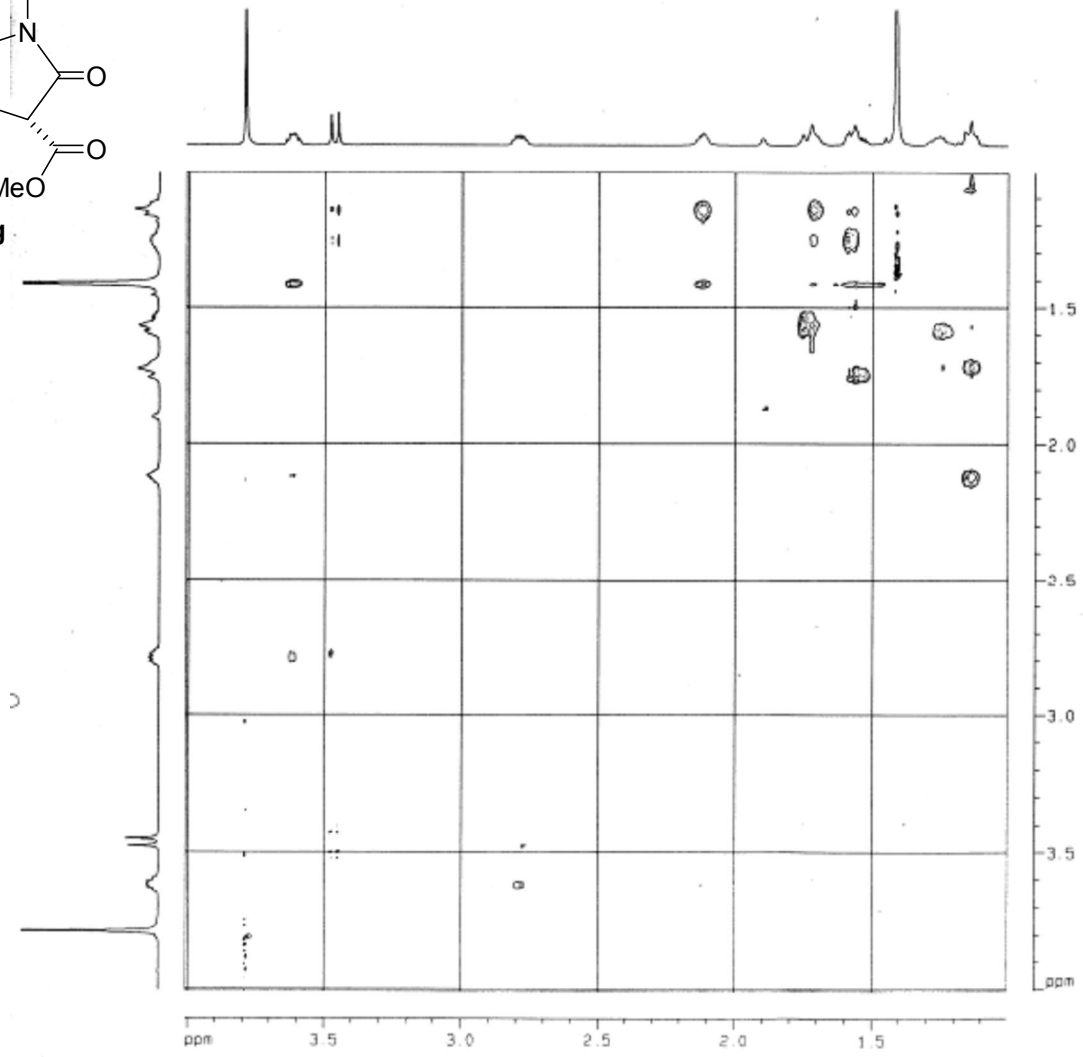
3d

Hb-Hc: strong NOE
Hb-Hd: weak NOE
Ha-Hb: weak NOE


O
COOMe
N
Ha
Hb
Hc
Hd
SePh
s
w
2f
Ha
Hd
Hc
Hb
Hb
Hc
Hd
Ha
Hc-Hd
Hb-Hc
Hb-Hd
Ha-Hb
2.5
3.0
3.5
4.0
ppm
ppm 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6



3g



Current Data Parameters
NAME
EXPNO 142
PROCNO 1

F2 - Acquisition Parameters
Date_ 20041220
Time 16.54
INSTRUM dmx500
PROBHD 5 mm BNP SH/1
PULPROG noesygpph
TD 1024
SOLVENT CDCl3
NS 32
DS 16
SWH 1502.404 Hz
FIDRES 1.467191 Hz
AQ 0.3415700 sec
RG 32
DW 332.800 usec
DE 6.00 usec
TE 300.0 K
d0 0.00003300 sec
D1 2.00000000 sec
D8 0.89999998 sec
D9 0.00666545 sec
MCREST 0.00000000 sec
MCWRK 1.00000000 sec
ST1CNT 0

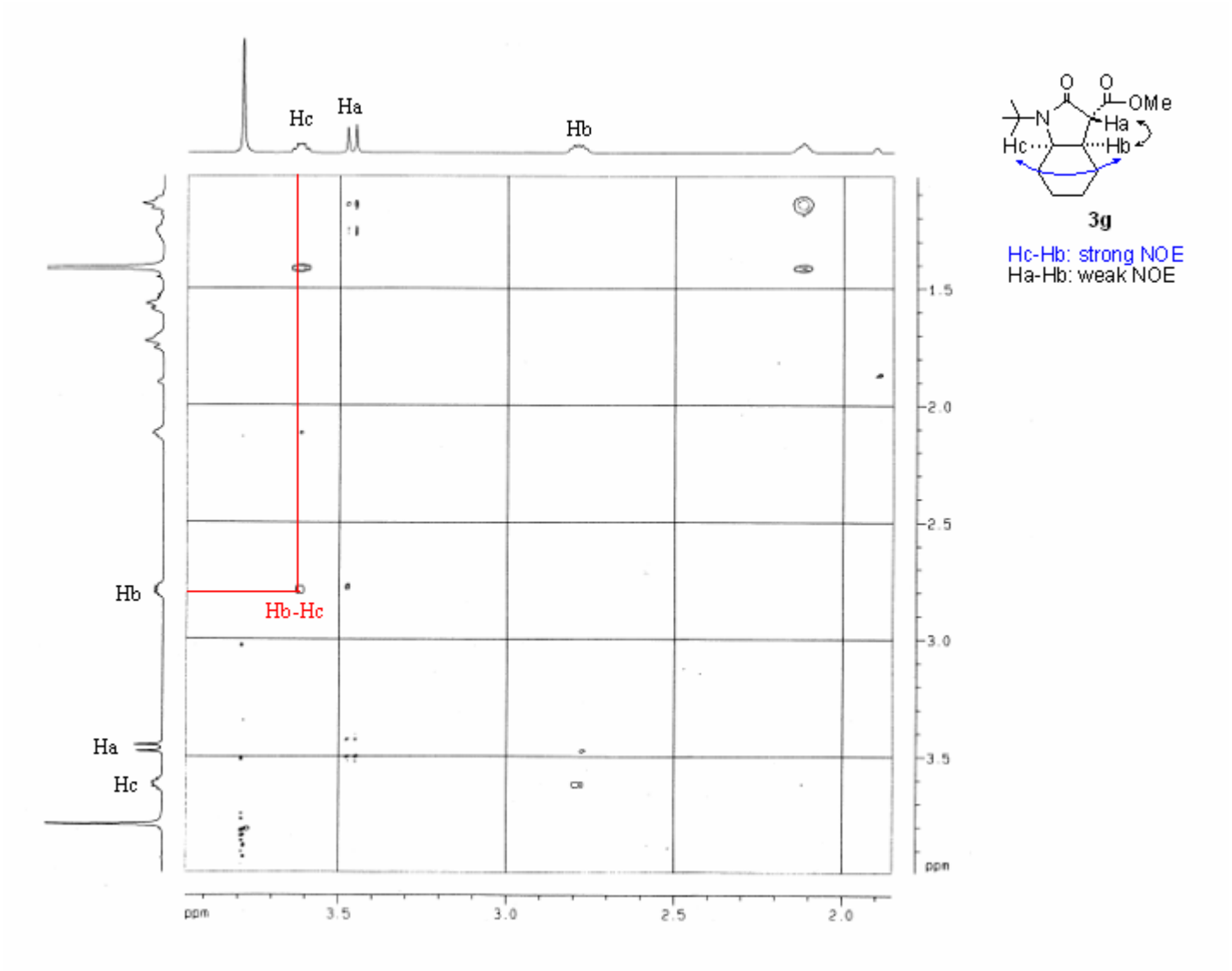
======== CHANNEL f1 ========
NUC1 1H
P1 9.40 usec
PL1 3.00 dB
SFO1 500.1302503 MHz

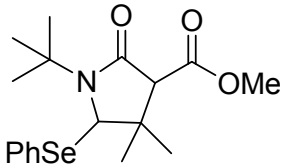
F1 - Acquisition parameters
NUC 1
TD 256
SFO1 500.1313 MHz
FIDRES 5.860950 Hz
SW 3.000 ppm
FnMODE States-TPPI

F2 - Processing parameters
SI 512
SF 500.1299985 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00

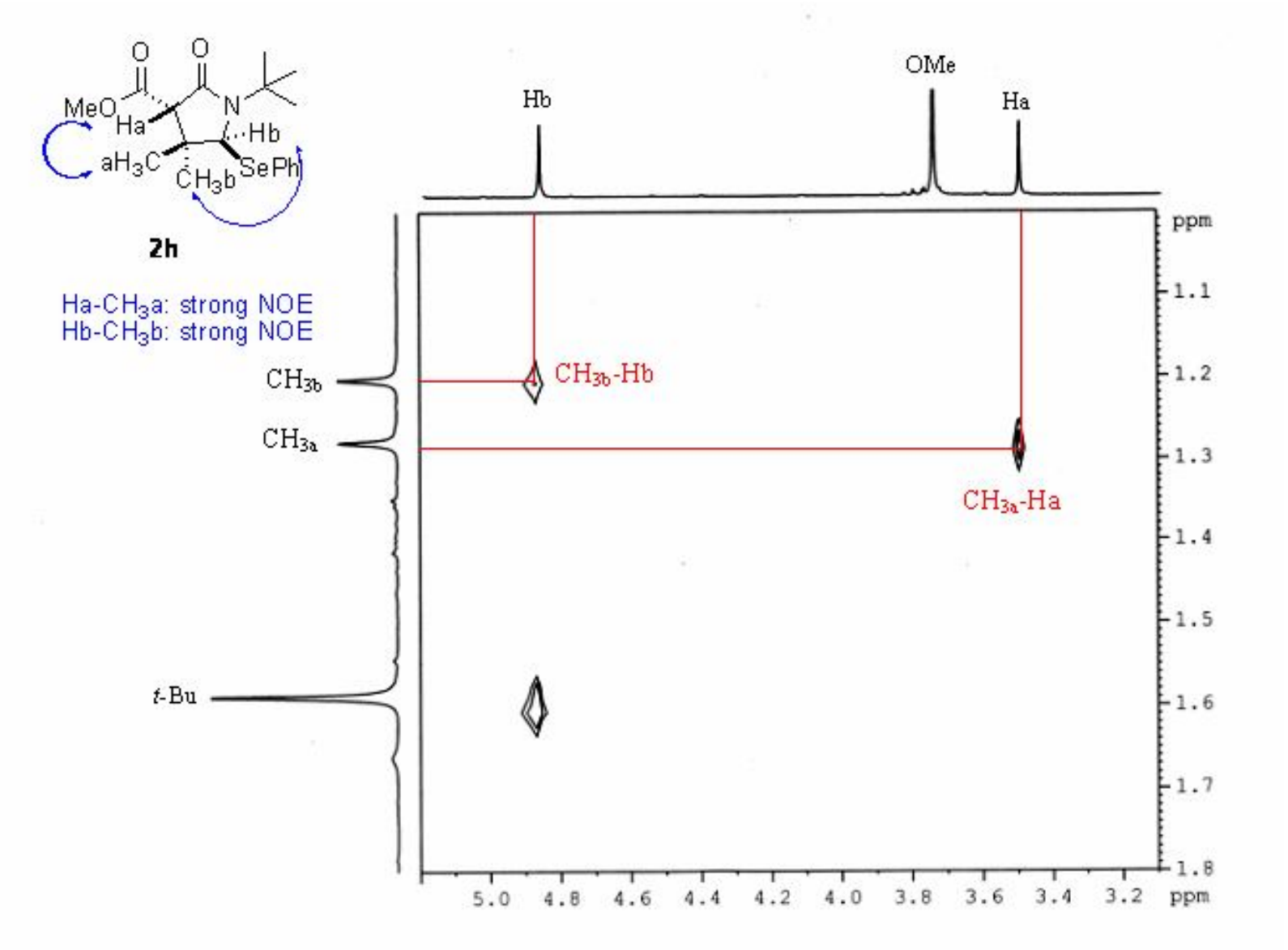
F1 - Processing parameters
SI 512
MC2 States-TPPI
SF 500.1299985 MHz
WDW SINE
SSB 2
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 15.00 cm
CY1 15.00 cm
F2PLO 4.009 ppm
F2LO 2005.05 Hz
F2PH1 1.005 ppm
F2H1 502.65 Hz
F1PLO 4.007 ppm
F1LO 2004.05 Hz
F1PH1 1.007 ppm
F1H1 503.64 Hz
F2PPHZ 0.20027 ppm/cm
F2HZCM 100.15029 Hz/cm
F1PPHZ 0.20008 ppm/cm
F1HZCM 100.03686 Hz/cm


Hc
Ha
Hb
Hb
Hb-Hc
Ha
Hc
1.5
2.0
2.5
3.0
3.5
ppm
ppm
3.5
3.0
2.5
2.0
O
O
OMe
N
Ha
Hc
Hb
3g
Hc-Hb: strong NOE
Ha-Hb: weak NOE



2h


2h
Ha-CH3a: strong NOE
Hb-CH3b: strong NOE
Hb
OMe
Ha
CH3b-Hb
CH3a-Ha
CH3b
CH3a
t-Bu
ppm
1.1
1.2
1.3
1.4
1.5
1.6
1.7
1.8
5.0
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
3.2
ppm