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Supporting Information

69451 Weinheim, Germany

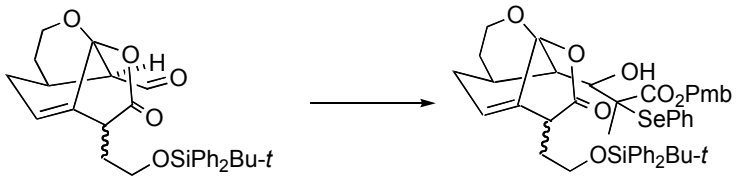
All-Carbon Intramolecular Conjugate Displacement (ICD) Reactions — an Effective Route to Carbocycles

*Bodhuri Prabhudas and Derrick L. J. Clive**

The X-ray data for **25a** has been deposited with the Cambridge Crystallographic Data Centre and assigned the registry number CCDC 653040.

Typical experimental procedures

3-[4-[2-(*tert*-Butyldiphenylsilanyloxy)ethyl]-3-oxo-2,11-dioxatricyclo[6.3.1.$0^{1,5}$]dodec-5-en-12-yl]-3-hydroxy-2-methyl-2-(phenylselanyl)propionic Acid 4-Methoxybenzyl Ester (66).

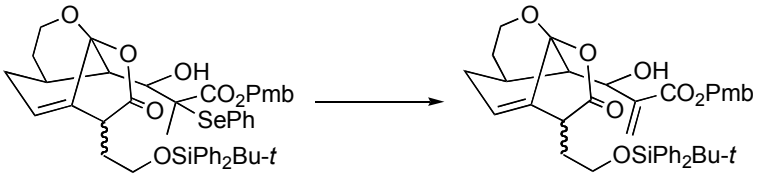


25c **66**

n-BuLi (2.5 M in hexane, 0.2 mL, 0.503 mmol) was added dropwise to a stirred and cooled (-78 °C) solution of *i*-Pr_2NH (56 mg, 0.555 mmol) in THF (3 mL). Stirring was continued for 40 min and a solution of 2-(phenylseleno)propionic acid 4-methoxybenzyl ester (198 mg, 0.567 mmol) in THF (3 mL plus 1 mL as a rinse) was added over 3 min. Stirring was continued for 1 h and a solution of **25c** (90 mg, 0.183 mmol) in THF (3 mL plus 1 mL as a rinse) was added over 2 min. Stirring was continued for 4 h and the mixture was quenched with saturated aqueous NH_4Cl (3 mL). The cooling bath was removed and stirring was continued for 10 min. The mixture was diluted with water (5 mL) and extracted with EtOAc (3 x 5 mL). The combined organic extracts were dried (Na_2SO_4) and evaporated. Flash chromatography of the

residue over silica gel (2 x 16 cm), using 20% EtOAc-hexane, gave **66** (126 mg, 82%) as a viscous oil, which was an inseparable mixture of isomers: FTIR (CH_2Cl_2 cast) 3493, 3071, 2932, 2857, 1792, 1712, 1613, 1588, 1516, 1248, 1111, 742, 703 cm^{-1}; exact mass (electrospray) *m/z* calcd for $C_{46}H_{52}NaO_8{}^{80}SeSi$ 863.24889, found 863.24800.

2-[[4-[2-(*tert*-Butyldiphenylsilanyloxy)ethyl]-3-oxo-2,11-dioxatricyclo[6.3.1.0^{1,5}]dodec-5-en-12-yl]hydroxymethyl]acrylic Acid 4-Methoxybenzyl Ester (67).

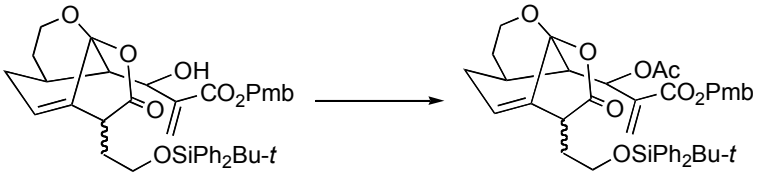


66 **67**

H_2O_2 (30%, 0.18 mL) was added to a stirred and cooled (0 °C) solution of **66** (100 mg, 0.119 mmol) in THF (5 mL) and H_2O (0.5 mL). Stirring was continued for 1 h and the mixture was quenched with saturated aqueous $Na_2S_2O_3$ (2 mL). The ice bath was removed after 5 min and stirring was continued for 5 min. The mixture was diluted with water (5 mL) and extracted with EtOAc (3 x 5 mL). The combined organic extracts were dried (Na_2SO_4) and evaporated. Flash chromatography of the residue over silica gel (2 x 16 cm), using 40% EtOAc-hexane, gave **67** (66 mg, 81%) as a colorless liquid, which was an inseparable (56:44) mixture of diastereomers (epimeric α to the lactone carbonyl): FTIR (CH_2Cl_2 cast) 3502, 3071, 2933, 2857, 1790, 1709, 1614, 1588, 1516, 1249, 1111, 1035, 704 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 1.06–1.08 (two s, 9 H), 1.46–1.54 (m, 0.6 H), 1.66–1.74 (m, 0.4 H), 1.87–2.22 (m, 4 H), 2.48–2.58 (m, 2 H), 2.64–2.71 (m, 1 H), 2.85 (m, 1 H), 3.22–3.33 (m, 1 H), 3.53–3.60 (m, 0.4 H), 3.67–3.79 (m, 1.6 H), 3.81 (s, 3 H), 3.82–3.96 (m, 2 H), 4.05 (t, *J* = 8.8 Hz, 0.6 H), 4.10–4.15 (m, 0.4 H), 5.10–5.19 (m, 2 H), 5.52 (s, 0.56 H), 5.66 (s, 0.44 H), 5.85 (m, 0.44 H), 5.88–5.90 (m, 0.56 H),

6.15 (d, *J* = 0.4 Hz, 0.56 H), 6.22 (d, *J* = 0.4 Hz, 0.44 H), 6.88–6.91 (m, 2 H), 7.33–7.45 (m, 8 H), 7.65–7.70 (m, 4 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 19.20 (s), 19.22 (s), 26.88 (q), 26.89 (q), 28.4 (t), 28.6 (t), 29.0 (d), 29.02 (d), 31.2 (t), 33.71 (t), 33.77 (t), 34.9 (t), 37.2 (d), 39.5 (d), 47.3 (d), 47.6 (d), 55.3 (q), 60.5 (t), 61.3 (t), 62.3 (t), 62.8 (t), 66.6 (t), 66.7 (t), 70.8 (d), 70.9 (d), 102.6 (s), 103.5 (s), 113.91 (d), 113.92 (d), 125.1 (d), 126.3 (s), 127.7 (d), 129.7 (d), 130.04 (d), 130.2 (s), 131.3 (s), 133.38 (s), 133.44 (s), 133.62 (s), 133.66 (s), 135.6 (d), 142.2 (t), 142.3 (t), 159.61 (s), 159.62 (s), 166.5 (s), 166.6 (s), 175.4 (s), 176.1 (s); exact mass (electrospray) *m/z* calcd for $C_{40}H_{46}NaO_8Si$ 705.28542, found 705.28575.

2-[Acetoxy-[4-[2-(*tert*-butyldiphenylsilanyloxy)ethyl]-3-oxo-2,11-dioxatricyclo[6.3.1.0^{1,5}]dodec-5-en-12-yl]methyl]acrylic Acid 4-Methoxybenzyl Ester (20).

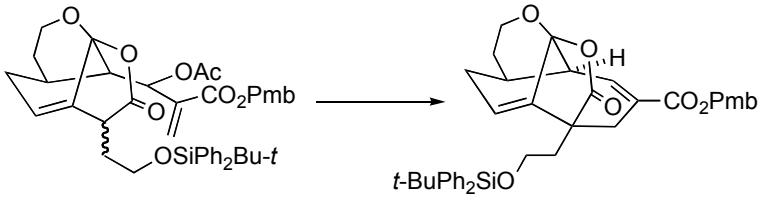


67 **20**

DMAP (1 mg, 0.008 mmol), pyridine (0.09 mL, 1.1 mmol) and AcCl (0.03 mL, 0.44 mL) were added in that order to a stirred and cooled (0 °C) solution of **67** (50 mg, 0.073 mmol) in CH_2Cl_2 (3 mL). Stirring was continued for 1 h and the mixture was diluted with water (10 mL) and 10% HCl (0.5 mL). The aqueous layer was extracted with CH_2Cl_2 (3 x 5 mL) and the combined organic extracts were dried (Na_2SO_4) and evaporated. Flash chromatography of the residue over silica gel (1 x 12 cm), using 20% EtOAc-hexane, gave **20** (47 mg, 89%) as a viscous oil which was an inseparable 53:47 mixture: FTIR (CH_2Cl_2 cast) 2930, 2853, 1793, 1742, 1715, 1614, 1588, 1516, 1246, 1228, 1024, 823, 703 cm^{-1}; ^{1}H NMR ($CDCl_3$, 400 MHz) δ 1.07–1.08 (two s, 9 H), 1.43–1.47

(m, 0.46 H), 1.50–1.55 (m, 0.54 H), 1.66–1.75 (m, 0.56 H), 1.85–2.07 (m, 2.45 H), 2.02–2.03 (two s, 3 H), 2.11–2.24 (m, 1 H), 2.37–2.45 (m, 1 H), 2.56–2.66 (m, 2 H), 3.26–3.33 (m, 1 H), 3.52–3.59 (m, 0.44 H), 3.62–4.01 (m, 3.56 H), 3.80 (s, 3 H), 5.02–5.14 (m, 2 H), 5.53 (d, J = 10.4 Hz, 0.52 H), 5.59 (d, J = 10.0 Hz, 0.48 H), 5.77 (s, 0.52 H), 5.82–5.83 (m, 0.92 H), 5.93–5.95 (m, 0.52 H), 6.30 (s, 0.53 H), 6.34 (s, 0.47 H), 6.86–6.89 (m, 2 H), 7.32–7.45 (m, 8 H), 7.66–7.70 (m, 4 H); ^{13}C NMR ($CDCl_3$, 125 MHz) δ 19.23 (s), 19.25 (s), 20.98 (d), 21.01 (d), 26.9 (q), 28.2 (t), 28.5 (t), 29.3 (q), 29.4 (q), 31.4 (t), 33.5 (t), 34.8 (t), 37.0 (d), 39.3 (d), 47.0 (d), 47.2 (d), 55.3 (q), 60.7 (t), 61.6 (t), 62.1 (t), 62.8 (t), 66.62 (t), 66.66 (t), 69.2 (d), 69.3 (d), 102.0 (s), 102.9 (s), 113.81 (d), 113.84 (d), 124.4 (d), 126.9 (s), 127.1 (d), 127.71 (d), 127.73 (d), 128.0 (s), 128.1 (s), 129.66 (d), 129.69 (d), 130.14 (d), 130.17 (d), 130.4 (s), 131.7 (s), 133.48 (s), 133.56 (s), 133.72 (s), 133.74 (s), 135.57 (d), 135.60 (d), 141.1 (t), 141.2 (t), 159.50 (s), 159.53 (s), 165.0 (s), 165.08 (s), 169.50 (s), 169.51 (s), 175.5 (s), 176.1 (s); exact mass (electrospray) m/z calcd for $C_{42}H_{48}NaO_9Si$ 747.29598 found 747.29579.

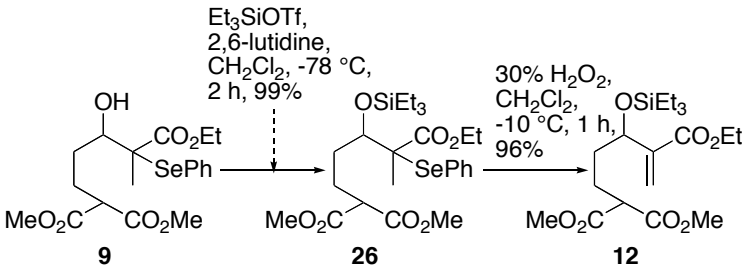
8-[2-(*tert*-Butyldiphenylsilanyloxy)ethyl]-2,3,4,4a,7,8-hexahydro-9-oxo-4,8,10a-[2]propen[1]yl[3]ylidene-9*H*,10a*H*-pyrano[2,3-b]oxocine-5-carboxylic Acid 4-Methoxybenzyl Ester (20a).



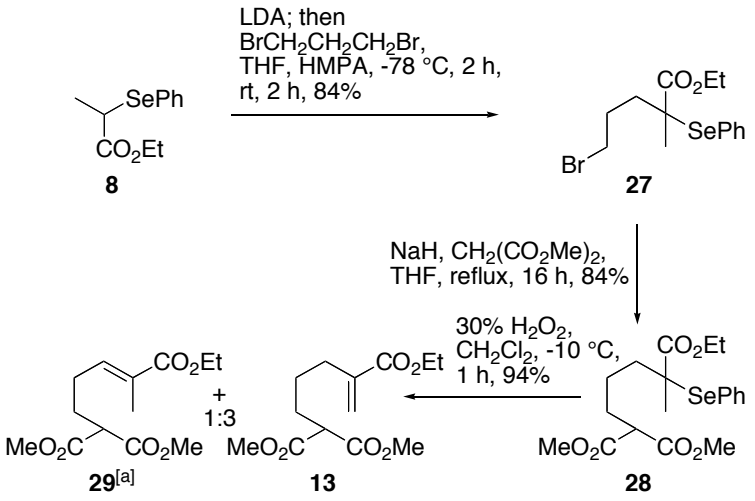
20 **20a**

DBU (0.03 mL, 0.20 mmol) was added to a stirred solution of **20** (25 mg, 0.034 mmol) in MeCN (3 mL). The mixture was refluxed for 1 h, cooled to room temperature and then filtered through a

pad of silica gel (2 x 2 cm) using 50% EtOAc-hexane (60 mL). Evaporation of the filtrate and flash chromatography of the residue over silica gel (0.5 x 8 cm), using 20% EtOAc-hexane, gave **20a** (20 mg, 88%) as a viscous liquid: FTIR (CH_2Cl_2 cast) 2931, 2856, 1787, 1707, 1613, 1588, 1516, 1244, 1113, 704 cm^{-1}; ^1H NMR ($CDCl_3$, 400 MHz) δ 1.02 (s, 9 H), 1.55–1.60 (m, 1 H), 1.88 (ddd, *J* = 14.0, 5.6, 4.4 Hz, 1 H), 2.01 (dddd, *J* = 12.8, 12.8, 5.6, 3.2 Hz, 1 H), 2.12 (dd, *J* = 20.0, 1.6 Hz, 1 H), 2.29 (dt, *J* = 20.0, 6.8 Hz, 1 H), 2.44–2.57 (m, 3 H), 2.91–2.95 (m, 2 H), 3.64–3.70 (m, 1 H), 3.76–3.85 (m, 2 H), 3.82 (s, 3 H), 3.95 (dd, *J* = 12.0, 5.2 Hz, 1 H), 5.04 (d, *J* = 12.0 Hz, 1 H), 5.06 (d, *J* = 12.0 Hz, 1 H), 5.70 (dd, *J* = 6.4, 2.0 Hz, 1 H), 6.8 (ddd, *J* = 5.2, 2.4, 1.6 Hz, 1 H), 6.87–6.91 (m, 2 H), 7.26–7.29 (m, 2 H), 7.35–7.44 (m, 6 H), 7.67–7.71 (m, 4 H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ 18.9 (s), 26.5 (q), 30.5 (d), 30.9 (t), 33.3 (t), 34.2 (t), 47.8 (q), 49.2 (t), 50.0 (s), 55.2 (d), 60.4 (t), 60.6 (t), 66.9 (t), 103.5 (s), 113.9 (d), 126.5 (d), 127.48 (d), 127.50 (d), 127.7 (s), 128.9 (s), 129.42 (d), 129.44 (d), 130.1 (d), 133.4 (s), 133.5 (s), 135.55 (d), 135.58 (d), 136.2 (s), 138.2 (d), 159.6 (s), 167.5 (s), 176.1 (s); exact mass (electrospray) *m/z* calcd for $C_{40}H_{44}NaO_7Si$ 687.27485, found 687.27518.

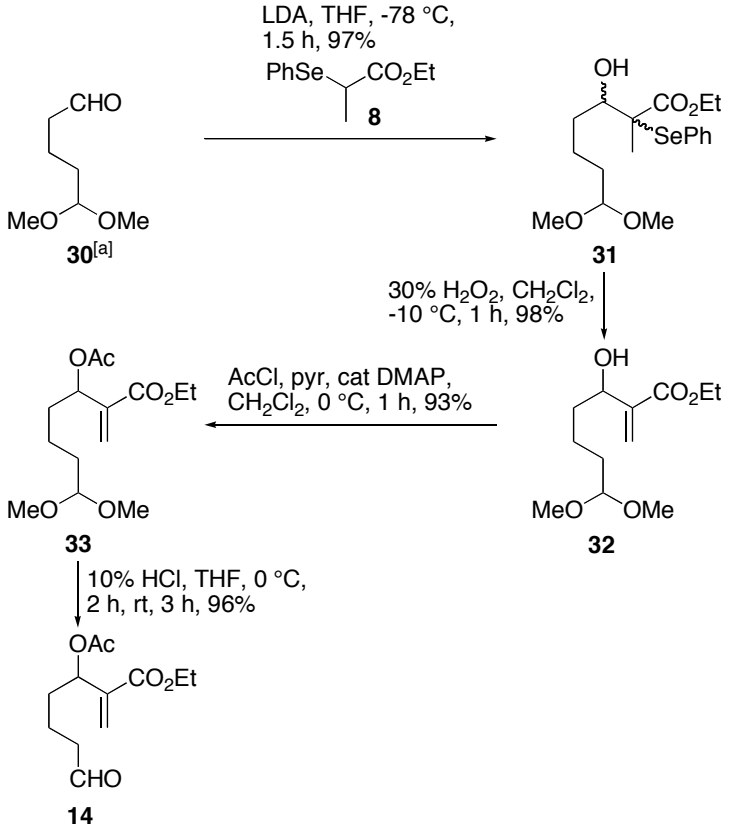


Scheme 6. Preparation of **12**



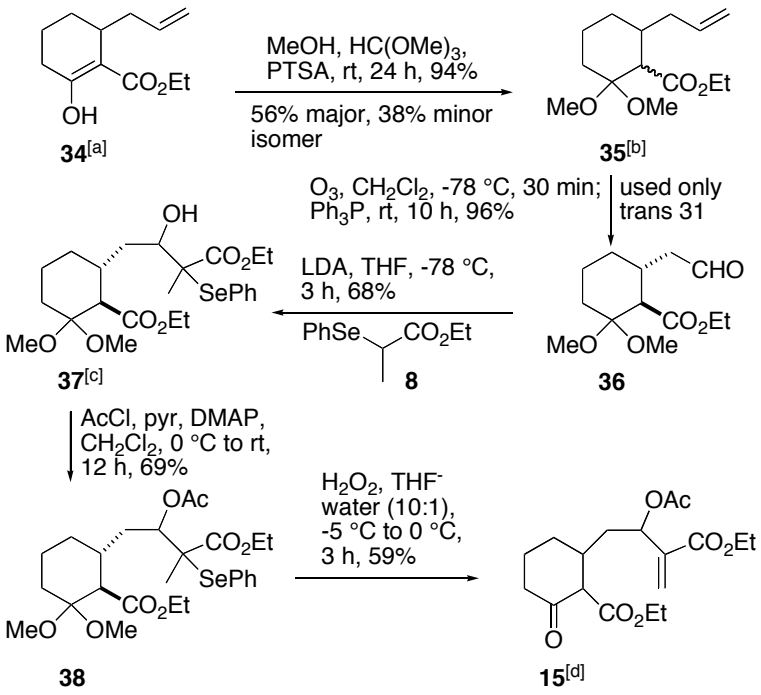
***Scheme* 7.** Preparation of **13**

[a] Compound **29** probably has the *E* geometry shown, based on the chemical shift of the vinyl H (δ 6.7 ppm).



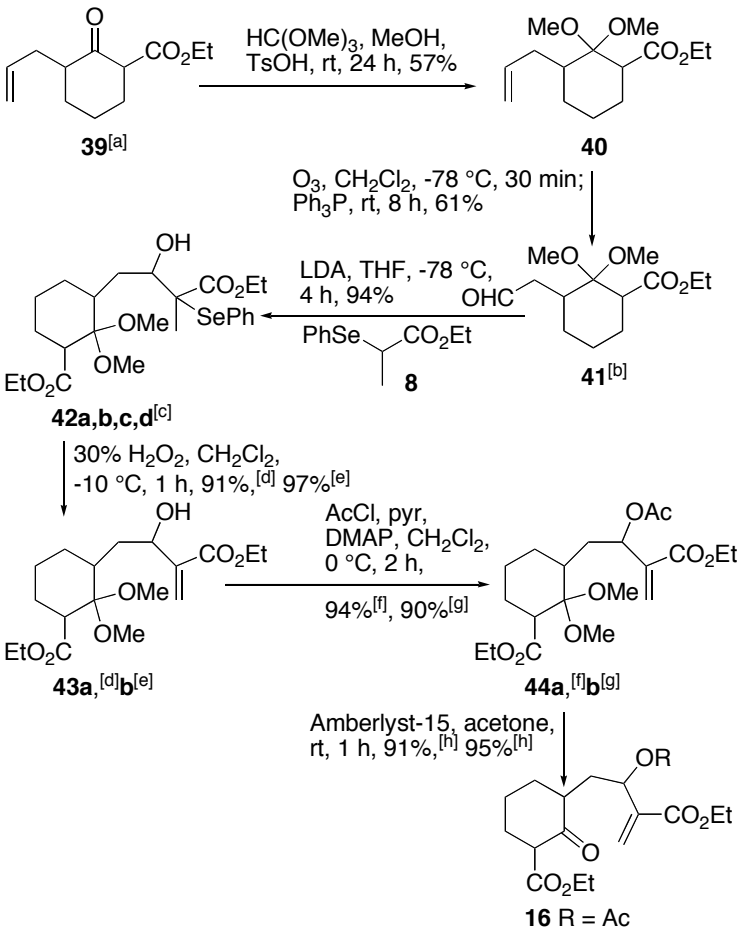
Scheme 8. Preparation of **14**

[a] Compound **30** is known: V. K. Aggarwal, S. Roseblade, J. K. Barrell, R. Alexander, *Org. Lett.* **2002**, *4*, 1227-1229.



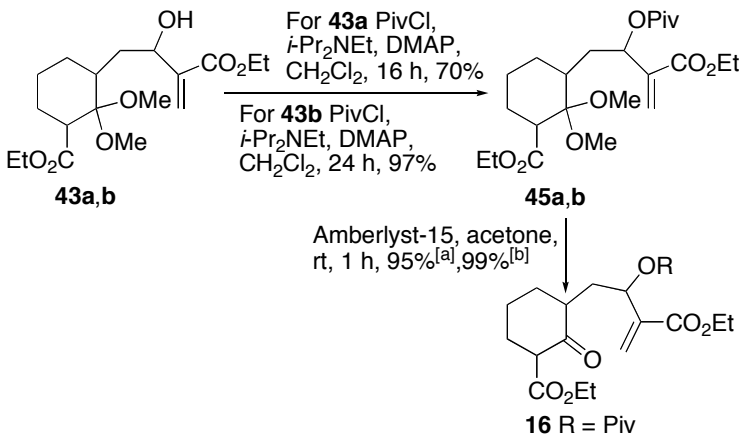
Scheme 9. Preparation of **15**

[a] The methyl ester corresponding to **34** is known: R. Ruel, P. Deslongchamps, *Can. J. Chem.* **1990**, *68*, 1917-1922). [b] Compound **35** is a mixture of two isomers (we assign the trans stereochemistry to the major one by analogy with the corresponding methyl ester: R. Ruel, P. Deslongchamps, *Can. J. Chem.* **1990**, *68*, 1917-1922. [c] Compound **37** is a mixture of four isomers, only one of which was taken on to **38.** [d] Compound **15** is a mixture of isomers.

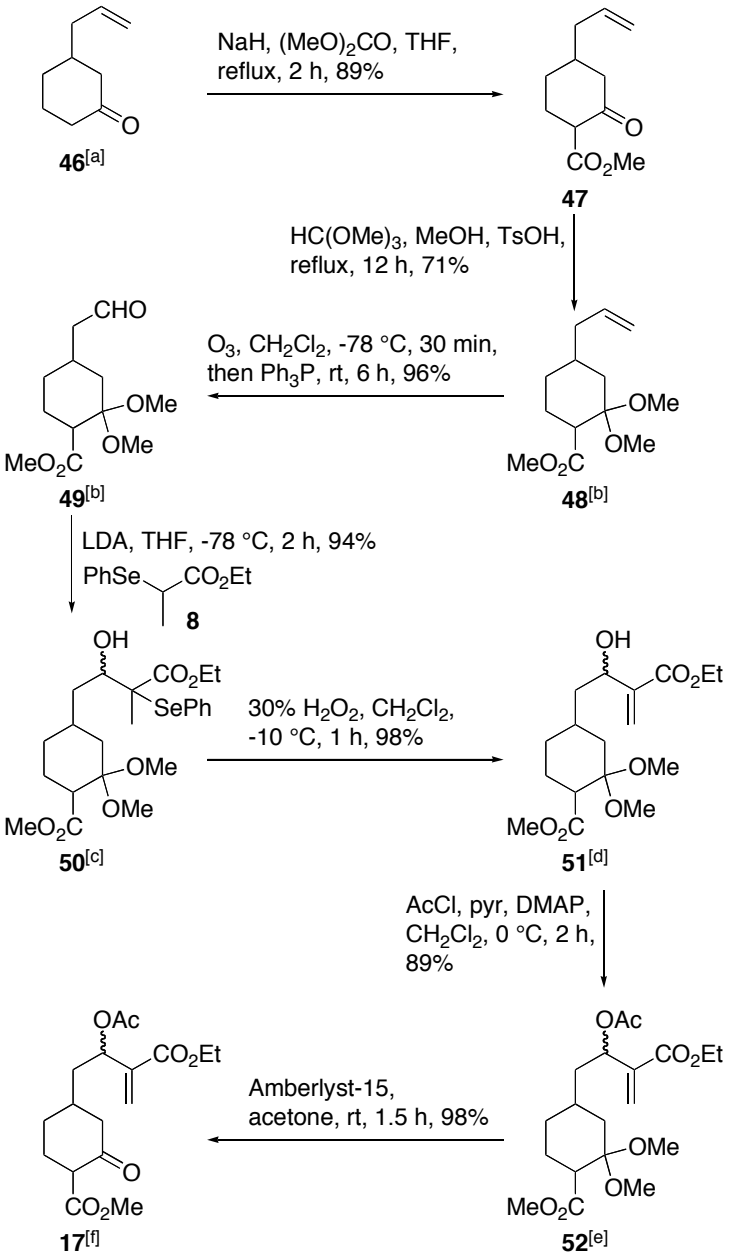


Scheme 10. Preparation of **16,** R = Ac

[a] Compound **39** is known: F. Xue, C. T. Seto, *J. Org. Chem.* **2005,** *70,* 8309-8321. [b] Single isomer. [c] Four isomers separated into fractions: least polar isomer (**42a**); most polar isomer (**42b**); mixture of isomers of intermediate polarity (**42c, 42d**). [d] From **42a.** [e] From **42b;** a 20-min reaction time was used. [f] From **43a.** [g] From **43b.** [h] 91% from **44a,** 95% from **44b.**



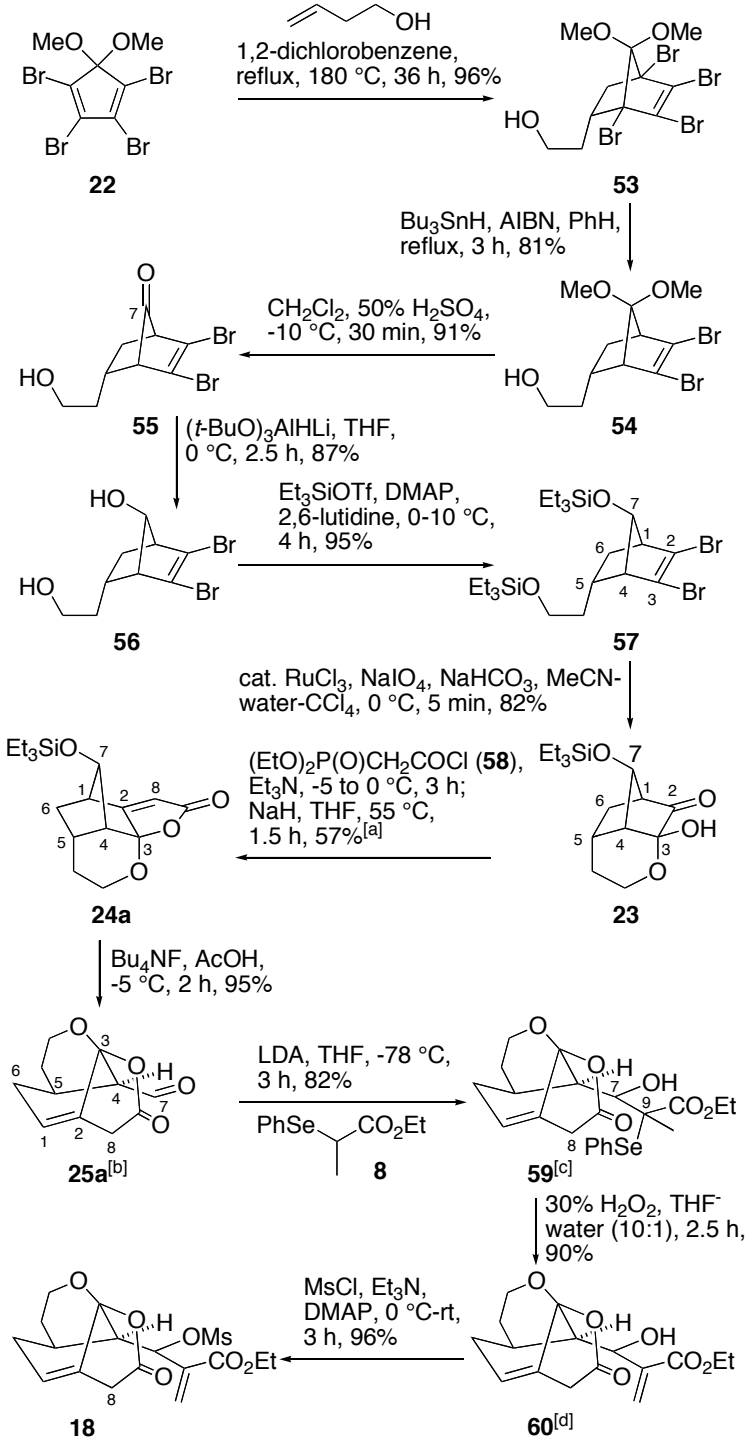
Scheme 11. Preparation of **16,** R = *t*-BuCO
[a] From **45a.** [b] From **45b.**



Scheme 12. Preparation of **17**

[a] Compound **46** is known: A. Hosomi, H. Sakurai, *J. Am. Chem. Soc*. **1977**, *99*, 1673-1675. [b] Single isomer. [c] Inseparable mixture of isomers. [d] Inseparable mixture of two isomers that differ in stereochemistry at the hydroxyl-bearing carbon. [e] Inseparable mixture of two isomers that differ in stereochemistry at the acetoxy-bearing carbon. [f] Mixture of isomers including keto-enol tautomers. Both stereochemistries

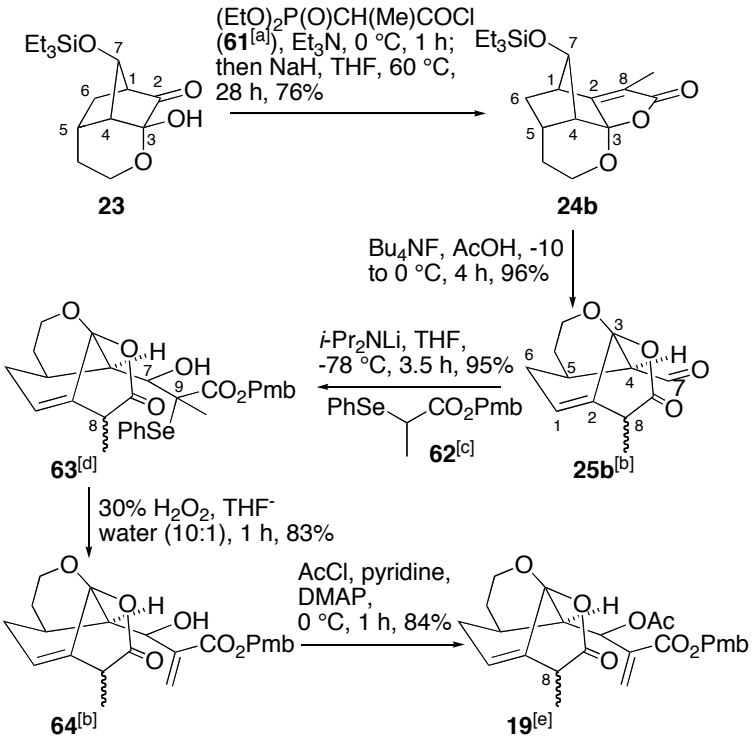
at acetoxy-bearing carbon.



Scheme 13. Preparation of **18**

The tetrachloro analog of **22** has been used in a different route to CP-models: M. M. Bio, J. L. Leighton, *J. Org. Chem.* **2003**, *68*, 1693-1700.

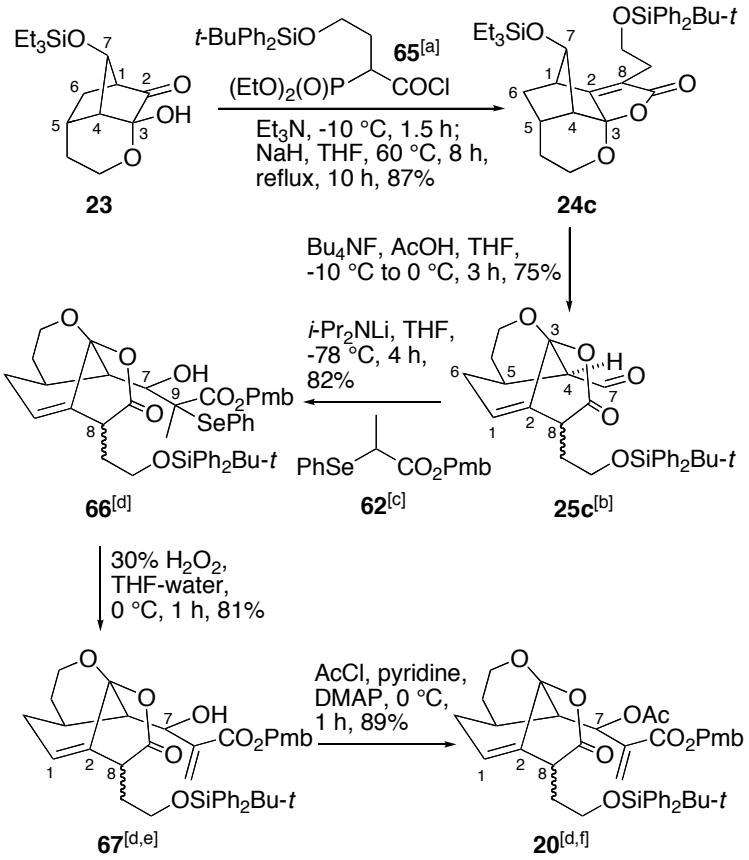
[a] The intermediate phosphonate is very susceptible to hydrolytic reversal to **23**, and so the olefination must be done *in situ* without isolation of the phosphonate; the same protocol was arbitrarily used in making **19** and **20**. [b] Structure of **25a** determined by X-ray analysis. [c] The single stereochemistry at C(7) not determined; both stereochemistries at C(9). [d] Single isomer.



Scheme 14. Preparation of **19**

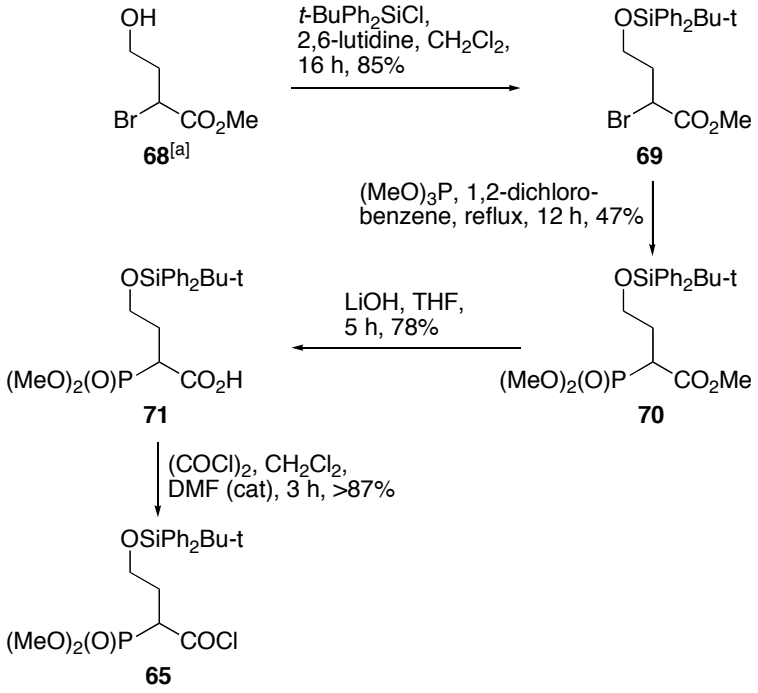
[a] Compound **61** is known: P. Coutrot, A. Ghiribi, *Synthesis* **1986**, 661-664. We used $(COCl)_2$ instead of $SOCl_2$. [b] 85:15 isomer mixture. [c] Preparation of **62:** 2-Bromopropionic acid was esterified with *p*-methoxybenzyl alcohol (DCC, DMAP, CH_2Cl_2, 3 h, 97%) and the bromine was displaced (68%) by treatment with the reagent made from PhSeSePh and $NaBH_4$ in EtOH. [d]

Inseparable 55:29:8:8 isomer mixture. [e] 71:29 isomer mixture.



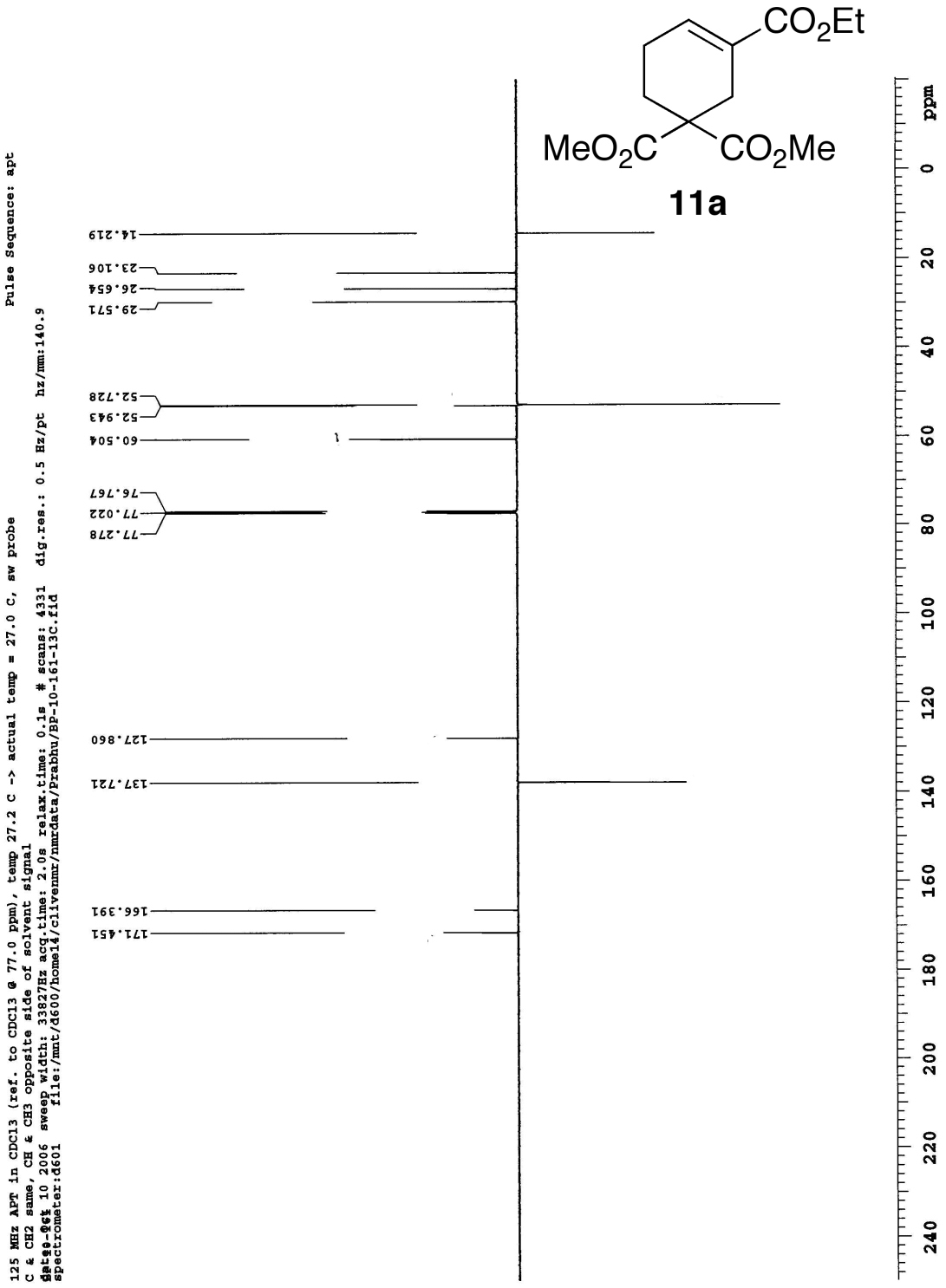
Scheme 15. Preparation of **20**

[a] For preparation of **65**, see Scheme 16. [b] Isomer ratio 60:40; only major isomer characterized. [c] For preparation, see footnote *c* to Scheme 13. [d] The single stereochemistry at C(7) not established. [e] Isomer ratio 56:44. [f] Isomer ratio 53:47.



Scheme 16. Preparation of **65**

[a] Compound **68** is known: A. M. Amat, G. Asensio, M. J. Castello, M. A. Miranda, A. Simon-Fuentes, *Tetrahedron* **1987**, *43*, 905-910.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CO2Me
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77.278
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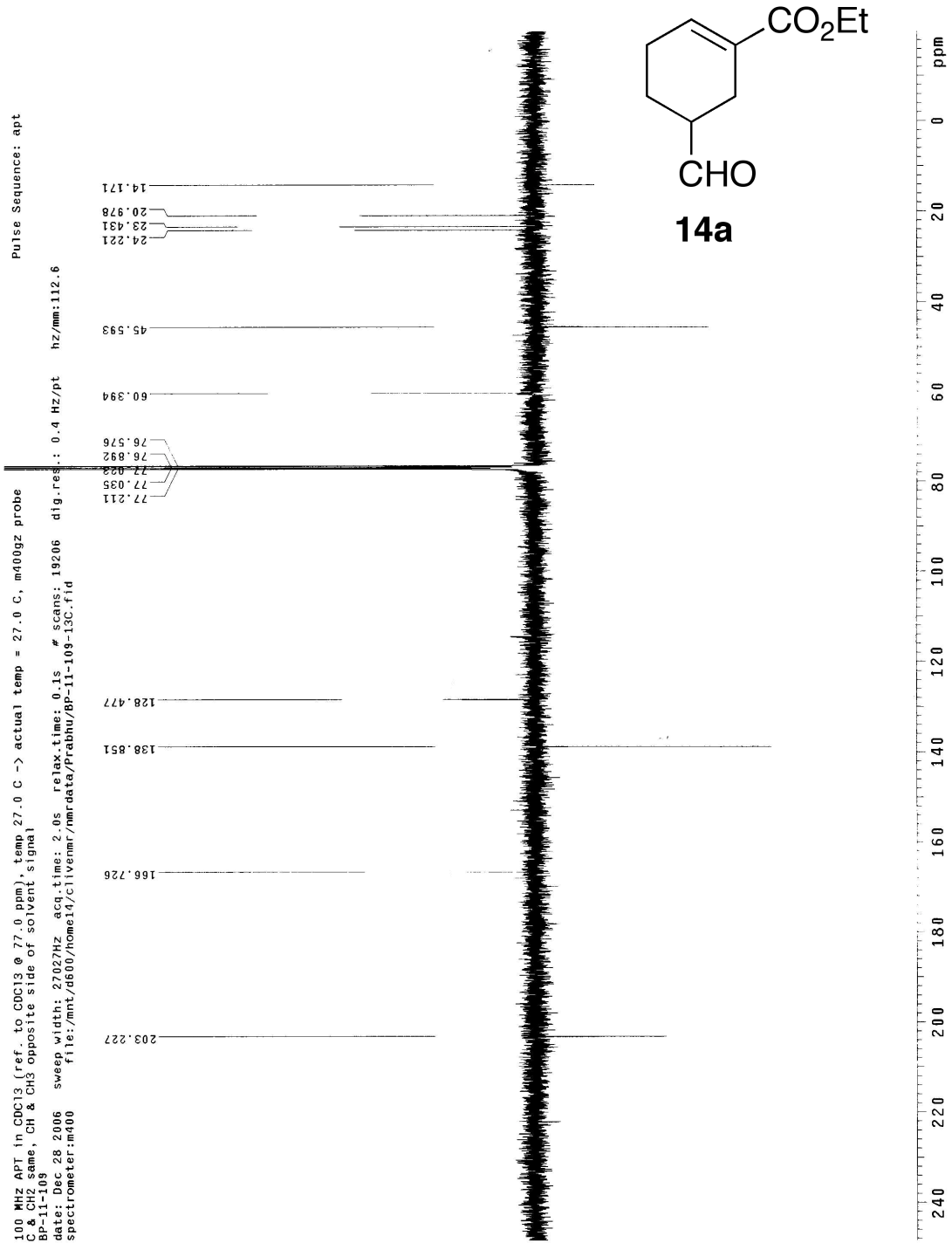
137.721
166.391
171.451
ppm
0
20
40
60
80
100
120
140
160
180
200
220
240
Pulse Sequence: apt
125 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, sw probe
C & CH2 same, CH & CH3 opposite side of solvent signal
date: Oct 10 2006 sweep width: 33827Hz acq.time: 2.0s relax.time: 0.1s # scans: 4331 dig.res.: 0.5 Hz/pt hz/mm:140.9
spectrometer:d601 file:/mnt/d600/home14/clivenmr/nmrdata/Prabhu/BP-10-161-13C.fid


CO2Et
CHO
14a
Pulse Sequence: apt
100 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 C -> actual temp = 27.0 C, m400gz probe
C & CH2 same, CH & CH3 opposite side of solvent signal
BP-11-109
date: Dec 28 2006 sweep width: 27027Hz acq.time: 2.0s relax.time: 0.1s # scans: 19206 dig.res.: 0.4 Hz/pt hz/mm:112.6
spectrometer:m400 file:/mnt/d600/home14/clivenmr/nmrdata/Prabhu/BP-11-109-13C.fid
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45.593
60.394
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77.035
77.211
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203.227
ppm
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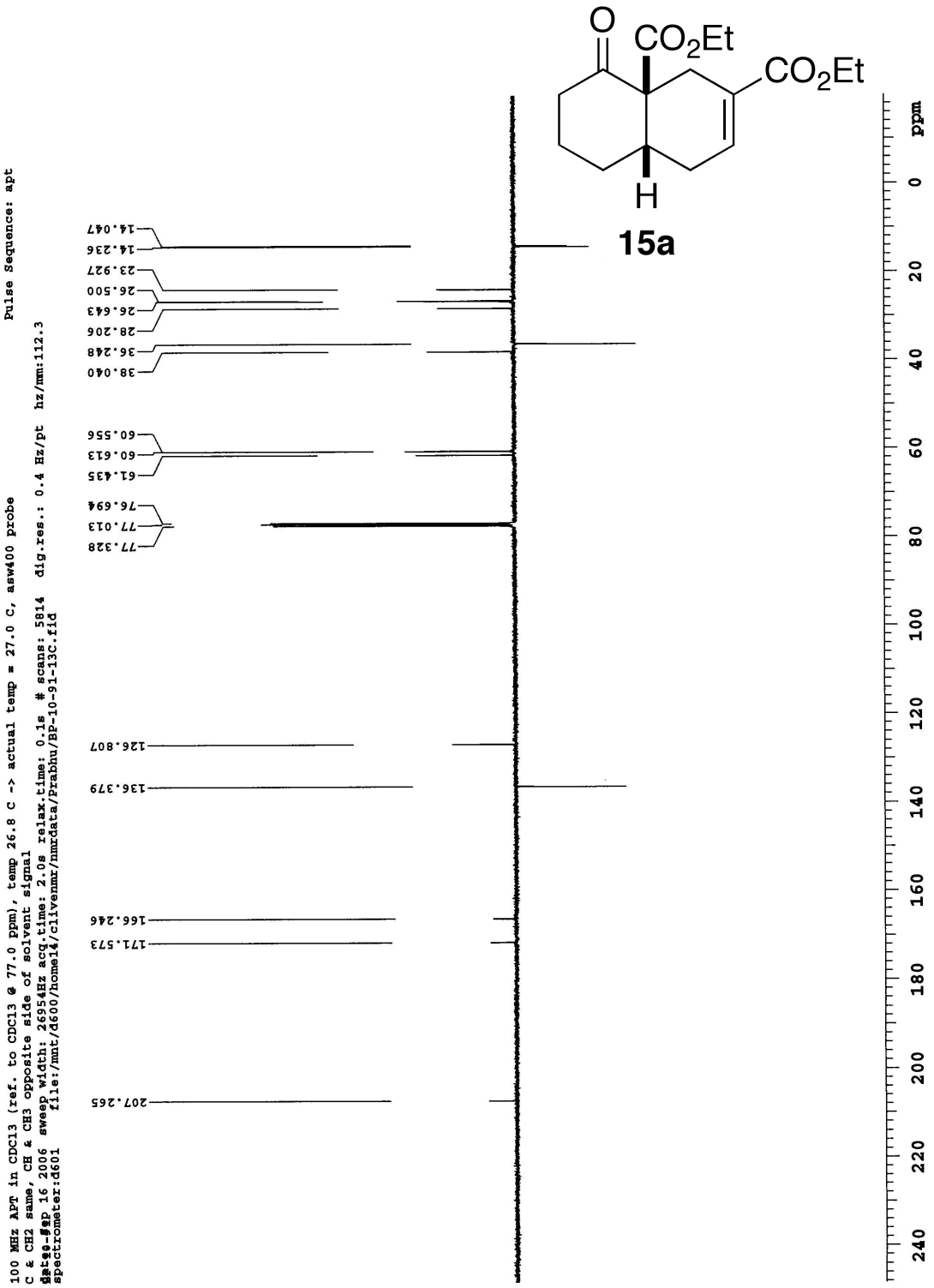
20
40
60
80
100
120
140
160
180
200
220
240


O
CO2Et
CO2Et
H
15a
Pulse Sequence: apt
100 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 26.8 C -> actual temp = 27.0 C, asw400 probe
C & CH2 same, CH & CH3 opposite side of solvent signal
Date_ Sep 16 2006 sweep width: 26954Hz acq.time: 2.0s relax.time: 0.1s # scans: 5814 dig.res.: 0.4 Hz/pt hz/mm:112.3
spectrometer:d601 file:/mnt/d600/home14/clivenmr/nmrdata/Prabhu/BP-10-91-13C.fid
14.047
14.236
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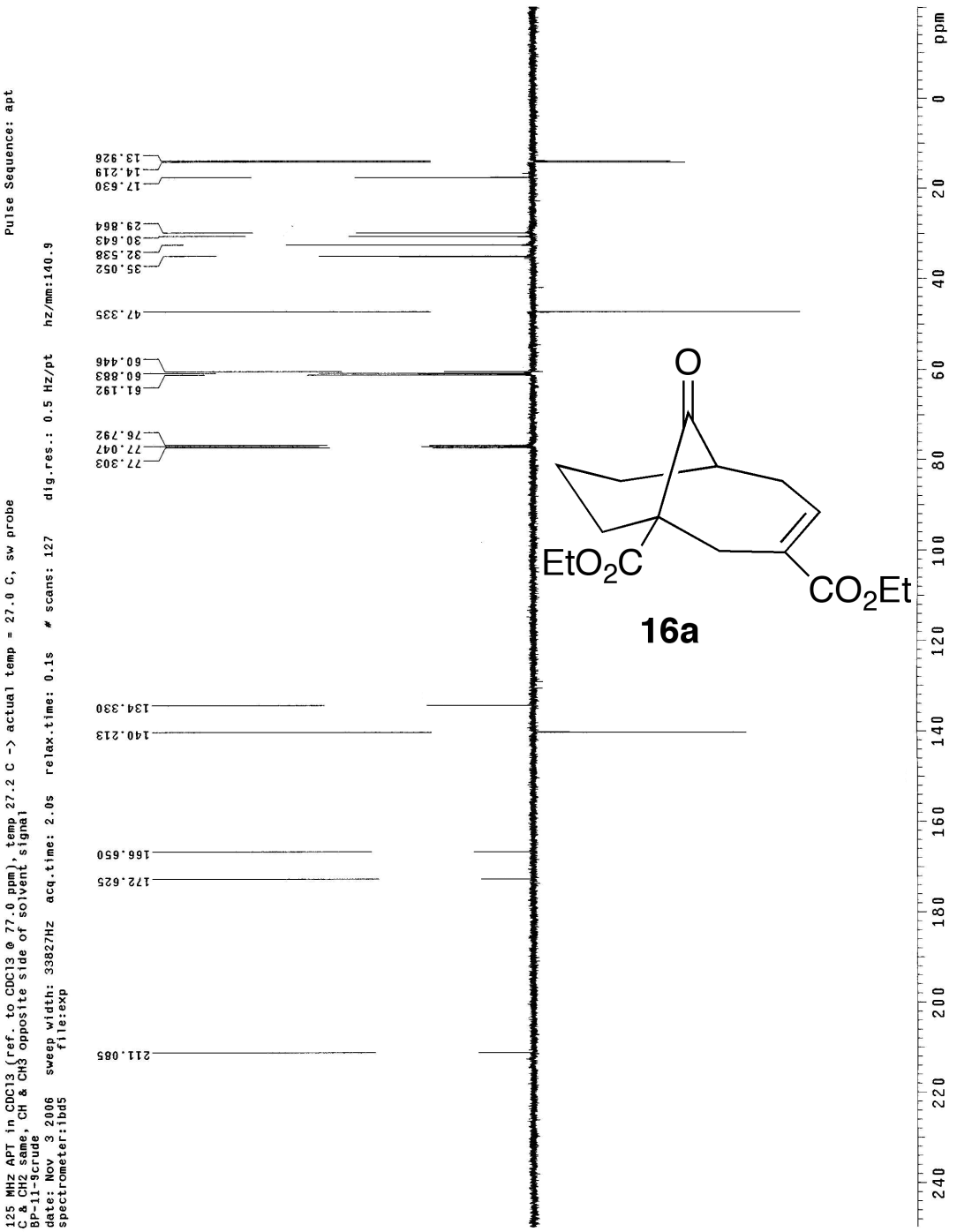
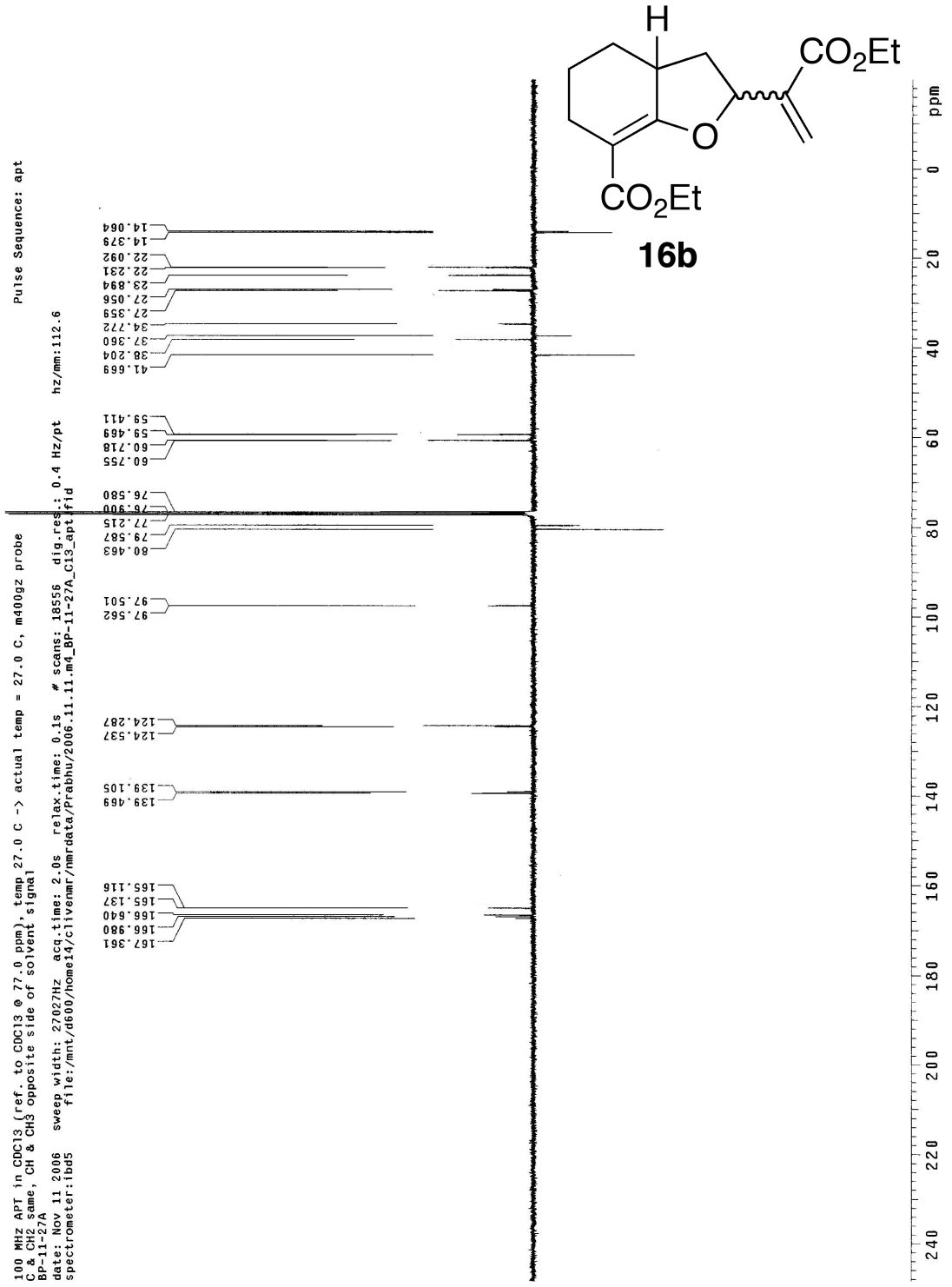
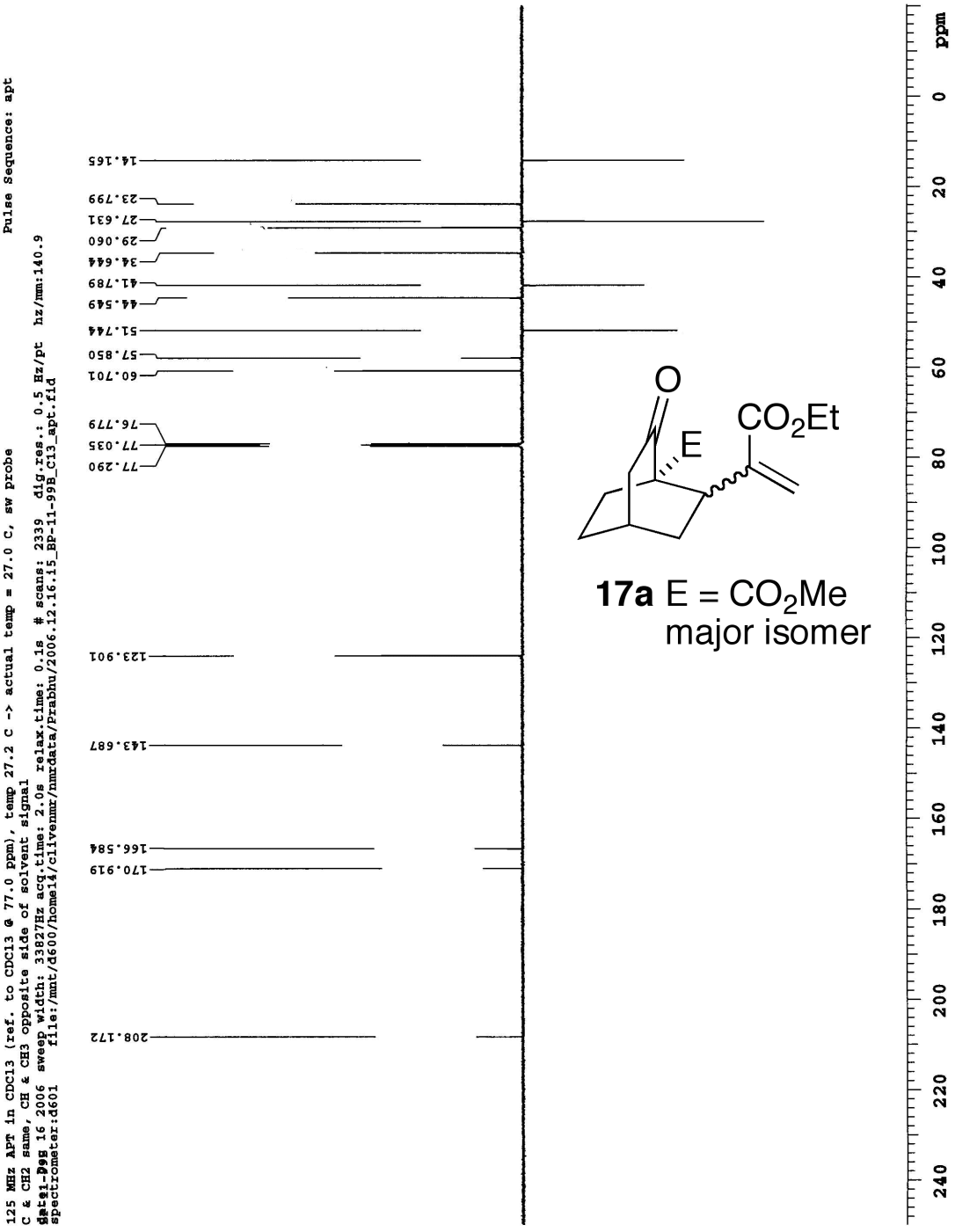
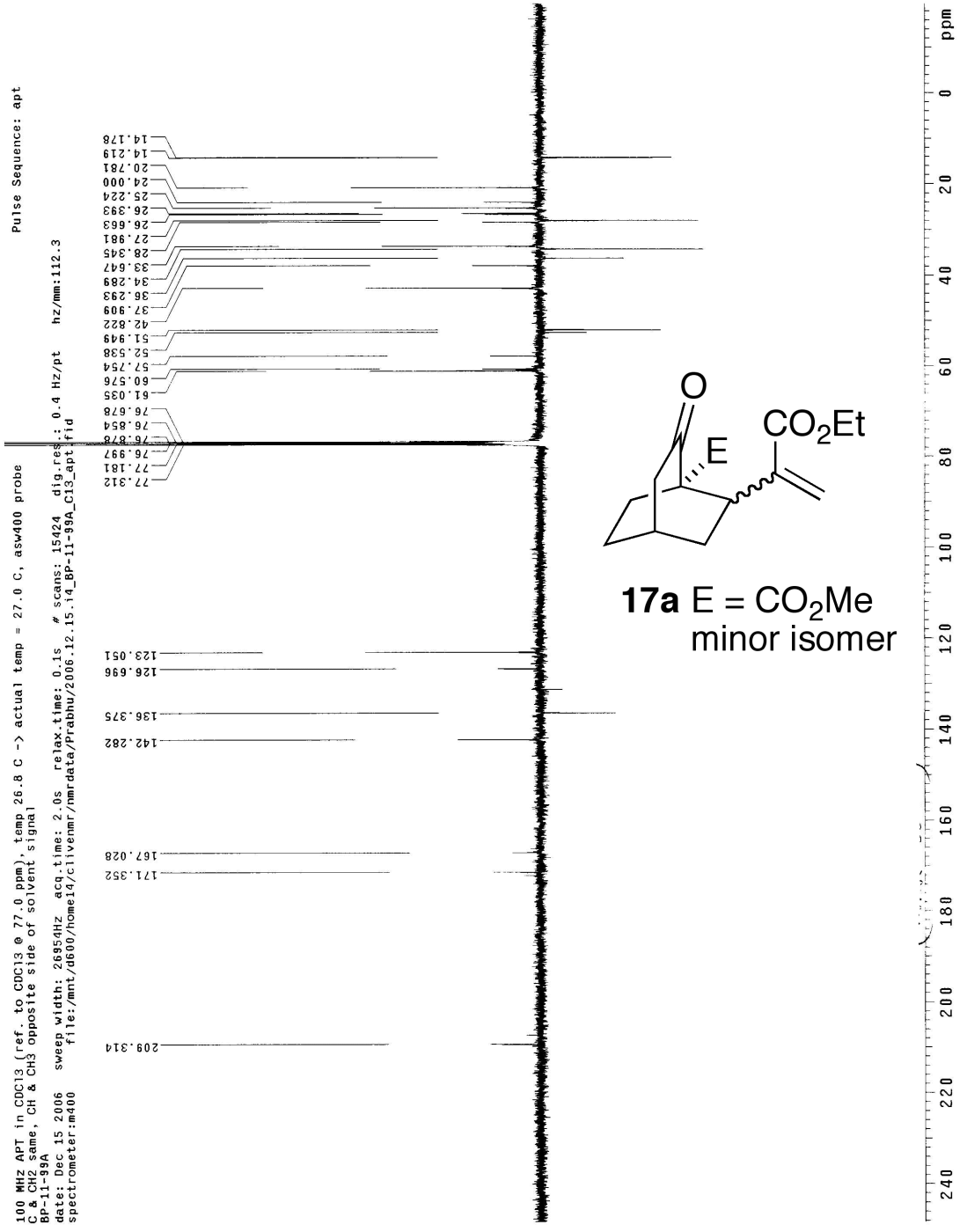
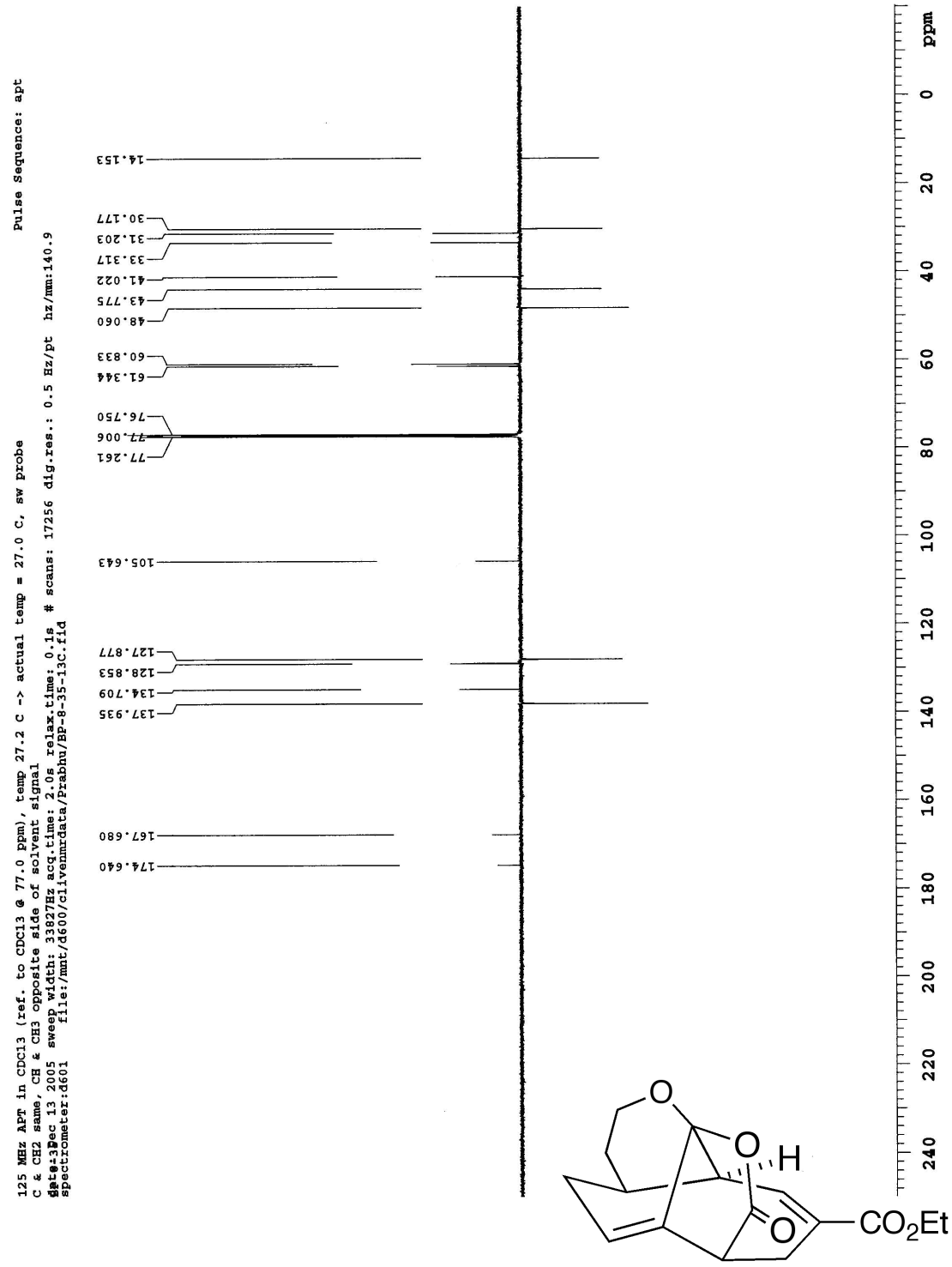
26.500
26.643
28.206
36.248
38.040
60.556
60.613
61.435
76.694
77.013
77.328
126.807
136.379
166.246
171.573
207.265
ppm
0
20
40
60
80
100
120
140
160
180
200
220
240


Pulse Sequence: apt
125 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, sw probe
C & CH2 same, CH & CH3 opposite side of solvent signal
BP-11-9crude
date: Nov 3 2006 sweep width: 33827Hz acq.time: 2.0s relax.time: 0.1s # scans: 127 dig.res.: 0.5 Hz/pt hz/mm:140.9
spectrometer:ibd5 file:exp
13.926
14.219
17.630
29.864
30.643
32.538
35.052
47.335
60.446
60.883
61.192
76.792
77.047
77.303
134.330
140.213
166.650
172.625
211.085
ppm
O
EtO2C
CO2Et
16a

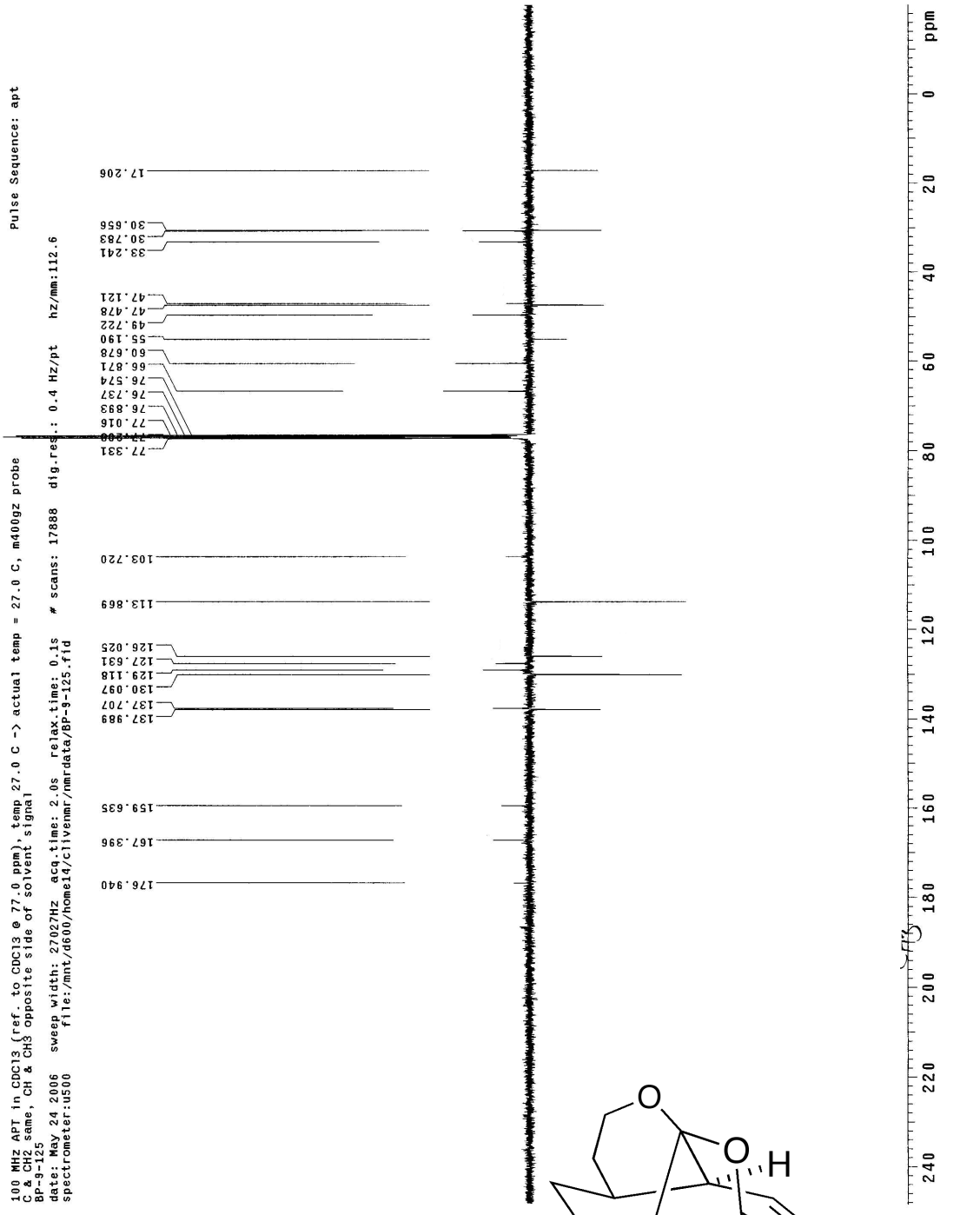

H
CO2Et
O
CO2Et
16b
Pulse Sequence: apt
100 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 C -> actual temp = 27.0 C, m400gz probe
C & CH2 same, CH & CH3 opposite side of solvent signal
BP-11-27A
date: Nov 11 2006 sweep width: 27027Hz acq.time: 2.0s relax.time: 0.1s # scans: 18556 dig.res.: 0.4 Hz/pt
spectrometer:ibd5 file:/mnt/d600/home14/clivenmr/nmrdata/Prabhu/2006.11.11.m4_BP-11-27A_C13_apt.fid
hz/mm:112.6
14.064
14.379
22.092
22.231
23.894
27.056
27.359
34.772
37.360
38.204
41.669
59.411
59.469
60.718
60.755
76.580
76.900
77.215
79.587
80.463
97.501
97.562
124.287
124.537
139.105
139.469
165.116
165.137
166.640
166.980
167.361
ppm


Pulse Sequence: apt
125 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, sw probe
C & CH2 same, CH & CH3 opposite side of solvent signal
acqi-Dgg 16 2006 sweep width: 33827Hz acq.time: 2.0s relax.time: 0.1s # scans: 2339 dig.res.: 0.5 Hz/pt hz/mm:140.9
spectrometer:d601 file:/mnt/d600/home14/clivenmr/nmrdata/Prabhu/2006.12.16.15_BP-11-99B_C13_apt.fid
14.165
23.799
27.631
29.060
34.644
41.789
44.549
51.744
57.850
60.701
76.779
77.035
77.290
123.901
143.687
166.584
170.919
208.172
O
E
CO2Et
17a E = CO2Me
major isomer
ppm
0
20
40
60
80
100
120
140
160
180
200
220
240

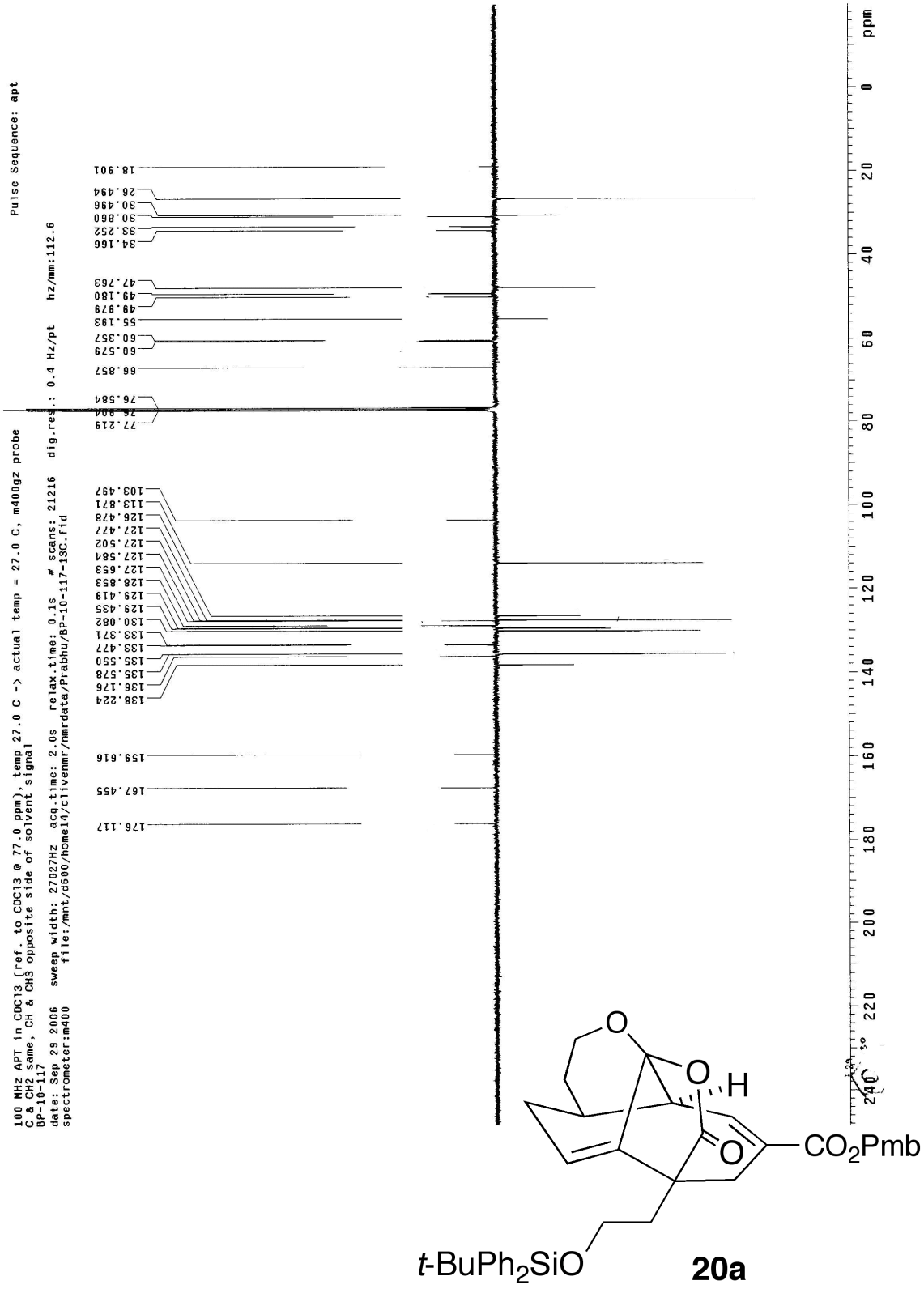

Pulse Sequence: apt
100 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 26.8 C -> actual temp = 27.0 C, asw400 probe
C & CH2 same, CH & CH3 opposite side of solvent signal
BP-11-99A
date: Dec 15 2006 sweep width: 26954Hz acq.time: 2.0s relax.time: 0.1s # scans: 15424 dig.res.: 0.4 Hz/pt hz/mm:112.3
spectrometer:m400 file:/mnt/d600/home14/clivenmr/nmrdata/Prabhu/2006.12.15.14_BP-11-99A_C13_apt.fid
14.178
14.219
20.781
24.000
25.224
26.393
26.663
27.981
28.345
33.647
34.289
36.293
37.909
42.822
51.949
52.538
57.754
60.576
61.035
76.678
76.854
76.878
76.997
77.181
77.312
123.051
126.696
136.375
142.282
167.028
171.352
209.314
O
E
CO2Et
17a E = CO2Me
minor isomer
ppm
0
20
40
60
80
100
120
140
160
180
200
220
240


Pulse Sequence: apt
125 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.2 C -> actual temp = 27.0 C, sw probe
C & CH2 same, CH & CH3 opposite side of solvent signal
spectrometer:d601 file:/mnt/d600/clivenmrdata/Prabhu/BP-8-35-13C.fid
14.153
30.177
31.203
33.317
41.022
43.775
48.060
60.833
61.344
76.750
77.006
77.261
105.643
127.877
128.853
134.709
137.935
167.680
174.640
ppm
O
O
H
O
CO2Et

18a


Pulse Sequence: apt
100 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 C -> actual temp = 27.0 C, m400gz probe
C & CH2 same, CH & CH3 opposite side of solvent signal
BP-9-125
date: May 24 2006 sweep width: 27027Hz acq.time: 2.0s relax.time: 0.1s # scans: 17888 dig.res.: 0.4 Hz/pt hz/mm:112.6
spectrometer:u500 file:/mnt/d600/home14/clivenmr/nmrdata/BP-9-125.fid
17.206
30.656
30.783
33.241
47.121
47.478
49.722
55.190
60.678
66.871
76.574
76.737
76.893
77.016
77.331
103.720
113.869
126.025
127.631
129.118
130.097
137.707
137.989
159.635
167.396
176.940
ppm
O
O
H
O
CO2Pmb
Me

19a


Pulse Sequence: apt
100 MHz APT in CDCl3 (ref. to CDCl3 @ 77.0 ppm), temp 27.0 C -> actual temp = 27.0 C, m400gz probe
C & CH2 same, CH & CH3 opposite side of solvent signal
BP-10-117
date: Sep 29 2006 sweep width: 27027Hz acq.time: 2.0s relax.time: 0.1s # scans: 21216 dig.res.: 0.4 Hz/pt hz/mm:112.6
spectrometer:m400 file:/mnt/d600/home14/clivenmr/nmrdata/Prabhu/BP-10-117-13C.fid
18.901
26.494
30.496
30.860
33.252
34.166
47.763
49.180
49.979
55.193
60.357
60.579
66.857
76.584
77.219
103.497
113.871
126.478
127.477
127.502
127.584
127.653
128.853
129.419
129.435
130.082
133.371
133.477
135.550
135.578
136.176
138.224
159.616
167.455
176.117
ppm
O
O
H
O
CO2Pmb
t-BuPh2SiO
20a