Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Design of CID-Cleavable Protein Cross-linkers: Identical Mass Modifications for Simpler Sequence Analysis

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Supporting Information

Contents:

General Methods

^{1}H NMR and ^{13}C NMR spectra were recorded at ambient temperature at 500 MHz and 125 MHz, respectively, on a Bruker DRX500 NMR instrument. ^{1}H and ^{13}C NMR data is reported as follows: chemical shifts are reported in ppm on a δ scale and referenced to internal tetramethylsilane or residual solvent (TMS: δ 0.00; $CHCl_3$: δ 7.27(^{1}H), 77.23 (^{13}C)), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, qu = quintet, m = multiplet), coupling constants (Hz), and integration. Infrared (IR) spectra were obtained using a FT-IR spectrometer. Accurate mass spectra were acquired on a Waters LCT Premier quadrupole time-of-flight spectrometer and were obtained by peak matching. Gas chromatography/mass spectrometry (GC/MS) was performed with a Thermo-Finnigan Trace Mass Spectrometer Plus quadrupole system with a fused silica capillary column (30 m x 0.32 mm x 0.25 mm) wall-coated with DB-5 (J & W Scientific) using electron ionization (70 eV) or a Waters GCT Premier orthogonal acceleration time-of-flight spectrometer using chemical ionization. Melting points are uncorrected and were obtained using a Büchi 510 melting point apparatus. Analytical thin layer chromatography was performed on EMD Chemicals Inc. silica gel 60 F_{254} plates. Liquid chromatography was performed using forced flow (flash chromatography) of the indicated solvent system on Sorbent Technologies silica gel (SiO_2) 60 (230–400 mesh). Unless otherwise noted, all reactions were carried out under an atmosphere of argon in flame-dried glassware. Solvents were distilled from CaH_2 or filtered through alumina before use.[1]

General procedure 1: Ester Hydrolysis

Starting ester was dissolved in 2:1 or 4:1 THF:H_2O, depending on solubility. The mixture was cooled to 0 °C and lithium hydroxide (98%, 5 equiv.) dissolved in minimal

H_2O was added slowly. The reaction was monitored by thin layer chromatography, while stirring vigorously. Upon completion, the mixture was diluted with diethyl ether and water before the layers were separated. Diethyl ether was added to the resulting aqueous layer, followed by addition of HCl to pH 1. The layers were separated and the aqueous layer was extracted with diethyl ether (2x). Organics were combined, washed with brine, dried over Na_2SO_4, filtered and evaporated *in vacuo*.

General procedure 2: TBAF-Promoted Michael Additions

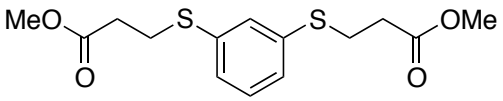
Acrylic acid (0.28 mmol), thiophenol (0.51 mmol), and THF (1 mL) were combined in a round bottom flask to which TBAF•$3H_2O$ (0.06 mmol) was added at rt. The flask was fitted with a cold-water condenser and the mixture was heated to 50° C for 16 h. The mixture was cooled to rt, evaporated *in vacuo*, diluted with EtOAc and washed with 1N HCl (2x). The organic layer was washed with brine, dried over Na_2SO_4, filtered, and evaporated *in vacuo* to yield the crude product. In some cases, this reaction was run neat.[2]

General procedure 3: NHS Ester Preparation

Crude diacid (0.08 mmol) was dissolved in dry dichloromethane (0.62 mL) in a flame dried round bottom flask under argon. NHS•TFA (0.41 mmol) was added before a slow addition of triethylamine (0.49 mmol) at 0° C. The mixture was left to warm slowly overnight while stirring under argon. After 16 h, the mixture was diluted with dichloromethane and washed with water (2x). The organic layer was dried with Na_2SO_4, filtered, and evaporated *in vacuo*.

General procedure 4: *m*-CPBA-Oxidation to Sulfoxide

Di-NHS ester (0.026 mmol) was dissolved in $CDCl_3$ (1 mL) and *m*-CPBA (77% w/w, 0.026 mmol) was added slowly while monitoring by LRMS ESI + and ^1H NMR. When this reaction was run on larger scale than 30 mg starting material, the solution was cooled in an ice bath prior to *m*-CPBA addition. Once the reaction was complete, the solution was diluted with dichloromethane (2 mL) and washed with 10% sodium bicarbonate solution (3 x 2 mL). The organic layer was dried over Na_2SO_4, filtered, and evaporated *in vacuo* to afford the product.

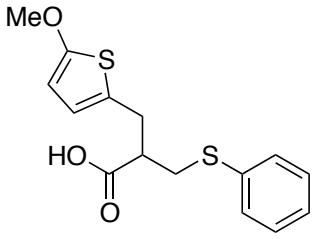


33

Dimethyl 3,3'-(1,3-phenylenebis(sulfanediyl))dipropanoate (33): 1,3-benzenedithiol (0.500 g, 3.52 mmol) and methyl acrylate (0.632 mL, 7.02 mmol) were dissolved in THF (6 mL), and Et_3N (0.980 mL, 7.03 mmol) was added to the solution. After 5 h, the reaction mixture was partitioned between H_2O (10 mL) and EtOAc (10 mL). The EtOAc layer was collected, washed with brine (10 mL), dried over $MgSO_4$, filtered, and concentrated under reduced pressure. The crude oil was purified by silica gel chromatography (5:1 hexanes:EtOAc) to afford 0.550 g (50%) of the sulfide as a clear, colorless oil: ^1H (500 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.29–7.22 (m, 3H), 3.73 (s, 6H), 3.22 (t, *J* = 7.5 Hz, 4H), 2.69 (t, *J* = 7.5 Hz, 4H); ^{13}C (125 MHz, $CDCl_3$) δ 172.2, 136.6, 130.5, 129.6, 127.0, 52.0, 34.2, 28.8; IR (neat) 2997, 2951, 2846, 1739, 1570 cm^{-1}; Accurate Mass (ES+/MeOH) m/*z* calcd for $C_{14}H_{18}O_4S_2Na$ $[M+Na]^+$ 337.0544, found 337.0547.

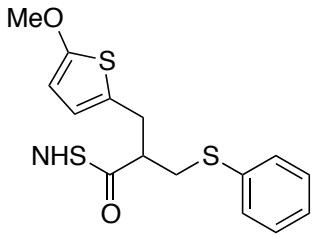
Bis(2,5-dioxopyrrolidin-1-yl) 3,3'-(1,3-phenylenedisulfinyl)dipropanoate (2). Bis(2,5-dioxopyrrolidin-1-yl) 3,3'-(1,3-phenylenebis(sulfanediyl))dipropanoate (0.110 g, 0.229 mmol) was dissolved in $CHCl_3$ (7 mL), and the reaction mixture was cooled to 0°C.

A solution of *m*-CPBA (0.105 g, 0.457 mmol) in $CHCl_3$ (2 mL) was added drop–wise, and the reaction mixture was stirred for 10 min. The reaction mixture was then partitioned between $CHCl_3$ (10 mL) and saturated aqueous $NaHCO_3$ (10 mL). The $CHCl_3$ layer was collected, dried over $MgSO_4$, filtered, and concentrated to afford 0.080 g (75%) of sulfoxide **2** as a white solid: ^{1}H (500 MHz, $CDCl_3$) δ 7.93–7.90 (m, 1H), 7.80–7,78 (m, 3H), 3.46–3.38 (m, 2H), 3.17–3.10 (m, 4H), 2.82 (brs, 10H); ^{13}C (125 MHz, $CDCl_3$) δ 169.0, 167.0, 144.6, 144.5, 131.0, 127.1, 120.3, 49.7, 49.5, 25.7, 22.9, 22.7; IR (KBr) 2943, 2935, 1786, 1736, 1427 cm^{-1}; Accurate Mass (ES+/MeOH) m/*z* calcd for $C_{20}H_{20}N_{20}O_{10}S_2Na$ $[M+Na]^+$ 535.0457, found 535.0457.



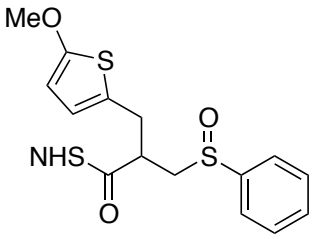
31

3-(5-methoxythiophen-2-yl)-2-((phenylthio)methyl)propanoic acid (31). Acrylic acid **29** (0.073 g, 0.25 mmol) and thiophenol (0.039 mL, 0.38 mmol) were subjected to general procedure 2 without solvent. The crude product was purified by flash column chromatography (30% EtOAc/hexanes) to yield desired product (0.018 g, 23%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (d, *J* = 7.9, 2H), 7.29 (t, *J* = 7.6, 2H), 7.22 (t, *J* = 7.6, 1H), 6.42 (d, *J* = 3.6, 1H), 5.99 (d, *J* = 3.8, 1H), 3.84 (s, 3H), 3.23 (dd, *J* = 7.7, 13.7, 1H), 3.16–3.04 (m, 3H), 2.88 (quintet, *J* = 6.8, 1H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 179.2, 165.3, 135.2, 130.5, 129.3, 127.0, 126.0, 123.8, 103.4, 60.4, 47.0, 34.6, 31.6; cm^{-1}; Accurate Mass ES- *m / z* calcd for $C_{15}H_{15}O_3S_2$ $(M-H)^-$ 307.0463, found 307.0466.



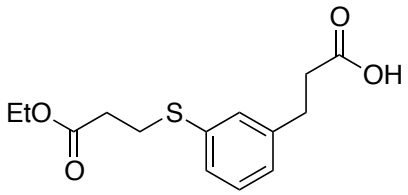
40

NHS ester 40. Carboxylic acid **31** (0.018 g, 0.058 mmol) was combined with dry DMF (0.3 mL), NHS (0.013 g, 0.12 mmol), pyridine (0.019 mL, 0.23 mmol), and, lastly, trifluoroacetic anhydride (0.016 mL, 0.12 mmol). After 2.5 h stirring at rt, the mixture was diluted with dichloromethane and 1M HCl. After the layers were separated, the organic layer was washed with 1 M HCl (2x) and dilute $NaHCO_3$ solution (2x). The organic layer was dried with Na_2SO_4, filtered, and evaporated *in vacuo*. This procedure is adapted from a published procedure.[3] The crude product was purified by flash column chromatography (2% EtOAc/CH_2Cl_2) to yield desired product (0.015 g, 63%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26-7.20 (m, 3H), 7.07 (d, *J* = 6.5, 1H), 4.15 (q, *J* = 7.2, 2H), 3.17 (t, *J* = 7.4, 2H), 3.04 (t, *J* = 7.5, 2H), 2.92 (t, *J* = 7.7, 2H), 2.85 (s, 4H), 2.62 (t, *J* = 7.4, 2H), 1.26 (t, *J* = 7.1, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.0, 169.3, 168.0, 140.2, 136.0, 129.9, 129.5, 128.4, 126.7, 60.9, 34.6, 32.7, 30.5, 29.1, 25.8, 14.4; IR (liquid) 2928, 1814, 1784, 1737, 1591 cm^{-1}; Accurate Mass ES+ *m / z* calcd for $C_{19}H_{19}O_5S_2NNa$ $(M+Na)^+$ 428.0602, found 428.0591.



10

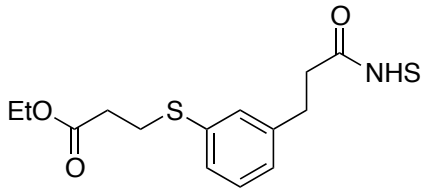
Sulfoxide 10. NHS ester **40** (0.012 g, 0.03 mmol) was subjected to general procedure 4. The crude product was purified by flash column chromatography (10–20% EtOAc/CH_2Cl_2) to yield desired product as a mixture of diastereomers (0.003 g, 26%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.68–7.63 (m, 2H), 7.53 (m, 3H), 6.61 (d, *J* = 3.8, 0.6H), 6.49 (d, *J* = 3.7, 0.5H), 6.04 (d, *J* = 3.8, 0.6H), 5.98 (d, *J* = 3.8, 0.5H), 3.86 (s, 1.8H), 3.84 (s, 1.3H), 3.60–3.53 (m, 0.5H), 3.47–3.40 (m, 0.6H), 3.39 (s, 0.6H), 3.38 (s, 0.5H), 3.30–3.24 (m, 1.5H), 3.10 (dd, *J* = 7.2, 15.3, 0.5H), 3.03 (dd, *J* = 8.0, 13.2, 0.6H), 2.96 (dd, *J* = 4.0, 13.4, 0.5H), 2.87 (s, 2.1H), 2.84 (s, 2.3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 168.7, 168.6, 168.3, 165.7, 165.6, 143.5, 143.0, 131.6, 131.4, 129.6, 129.5, 125.3, 124.8, 124.2, 124.0, 123.5, 123.2, 103.6, 103.5, 60.2, 60.2, 57.8, 56.6, 39.5, 39.0, 32.5, 31.0, 29.8, 25.7, 25.6; IR (thin film) 2924, 1810, 1782, 1739, 1507, cm^{-1}; Accurate Mass ES+ *m / z* calcd for $C_{19}H_{19}NO_6S_2Na$ $(M+Na)^+$ 444.0551, found 444.0548.



32

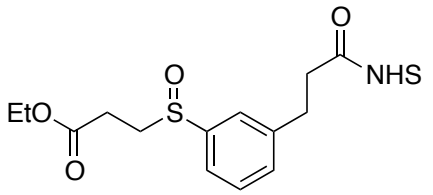
3-(3-((3-Ethoxy-3-oxopropyl)thio)phenyl)propanoic acid (32). Carboxylic acid **15** (0.10 g, 0.55 mmol) was combined with ethyl acrylate (0.088 mL, 0.82 mmol) in ethanol (5.5 mL) in a scintillation vial. Triethylamine (0.15 mL, 1.1 mmol) was added and the mixture was capped and stirred 14 days. The solvent was removed and the crude product was purified by flash column chromatography (50% EtOAc/hexanes) to yield desired product (0.022 g, 14%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.23 (br s, 3H), 7.07 (d, *J* = 6.7, 1H), 4.16 (q, *J* = 7.2, 2H), 3.17 (t, *J* = 7.3, 2H), 2.95 (t, *J* = 7.6, 2H), 2.68 (t, *J* = 7.6, 2H), 2.61 (t, *J* = 7.5, 2H), 1.25 (t, *J* = 7.2, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 177.7, 172.2, 141.3, 135.6, 130.0, 129.4, 128.2, 126.8, 61.1, 35.5, 34.7, 30.7, 29.2, 14.4; IR

(thin film) 3200, 2982, 2661, 2361, 1732 cm^{-1}; Accurate Mass ES- *m / z* calcd for $C_{14}H_{17}O_4S$ $(M-H)^-$ 281.0847, found 281.0844.



41

NHS ester 41. Carboxylic acid **32** (0.022 g, 0.078 mmol) was combined with dry DMF (0.4 mL), NHS (0.018 g, 0.16 mmol), pyridine (0.025 mL, 0.31 mmol), and, lastly, trifluoroacetic anhydride (0.022 mL, 0.16 mmol). After 2.5 h stirring at rt, the mixture was diluted with dichloromethane and 1M HCl. After the layers were separated, the organic layer was washed with 1 M HCl (2x) and dilute $NaHCO_3$ solution (2x). The organic layer was dried with Na_2SO_4, filtered, and evaporated *in vacuo*. This procedure is adapted from a published procedure.[3] The crude product was purified by flash column chromatography (10% EtOAc/CH_2Cl_2) to yield desired product (0.009 g, 30%). ^1H NMR (500 MHz, $CDCl_3$) δ 7.40 (d, *J* = 7.4, 2H), 7.31 (t, *J* = 7.5, 2H), 7.26 (t, *J* = 7.3, 1H), 6.50 (d, *J* = 3.7, 1H), 6.00 (d, *J* = 3.7, 1H), 3.85 (s, 3H), 3.33–3.05 (m, 5H), 2.84 (s, 4H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.1, 169.0, 165.5, 134.6, 131.1, 129.4, 127.3, 124.7, 124.6, 103.6, 60.4, 44.9, 34.7, 31.4, 25.8; IR (liquid) 3057, 2944, 1810, 1737, 1562 cm^{-1}; Accurate Mass ES+ *m / z* calcd for $C_{18}H_{21}O_6SNNa$ $(M+Na)^+$ 402.0987, found 402.0979.

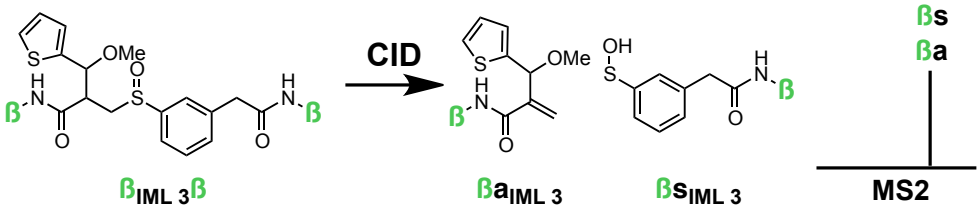


11

Sulfoxide 11. NHS ester **41** (0.007 g, 0.02 mmol) was subjected to general procedure 4 to yield desired product (0.005 g, 60%). ^1H NMR (500 MHz, $CDCl_3$) δ 7.54–7.46 (m,

3H), 7.39 (d, *J* = 3.8, 1H), 4.18–4.07 (m, 2H), 3.28–3.20 (m, 1H), 3.15 (t, *J* = 7.5, 2H), 3.00–2.93 (m, 3H), 2.90–2.79 (m, 5H), 2.56–2.45 (m, 1H), 1.25 (t, *J* = 7.0, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.5, 169.2, 167.8, 143.7, 140.8, 131.4, 129.9, 124.0, 122.8, 61.3, 51.3, 32.6, 30.6, 26.4, 25.8, 14.4; IR (thin film) 2930, 2360, 1813, 1783, 1737 cm^{-1}; Accurate Mass ES+ *m / z* calcd for $C_{18}H_{21}NO_7SNa$ $(M+Na)^+$ 418.0937, found 418.0917.

IML 2 MS Data:



ß$_{IML\ 3}$ß ßa$_{IML\ 3}$ ßs$_{IML\ 3}$

Figure 1. Expected fragmentation of IML 3 in single peptide crosslinking

Initial testing of IML 3 with synthetic peptide Ac-IR7 in the MS instrument showed significant loss of the methoxy group during CID (Figure 2). The MS^2 spectrum shows three peaks representing the IML 3-modified peptides. The first peak, *m/z* 496.73, represents a doubly charged IML 3-modified peptide that has lost a methoxy substituent during CID fragmentation (Figure 2, top left). This peak could only represent the alkene half of the linker, since it contains a labile methoxy in the benzylic position. When this peak was subjected to further CID, sequence data was acquired (Figure 2, top right). Similarly, the MS^2 peak with *m/z* 1024.48 represents a singly charged ion with the expected half IML modification. This peak could represent either the sulfenic acid-modified or the alkene-modified peptide, or it could represent a mixture of the two. Further CID of the *m/z* 1024.48 peak results in sequence data acquisition as well (Figure 2, lower right). The third peak in MS^2, with *m/z* 595.75, represents a dead end-modified peptide that has lost the methoxy substituent during the first CID and has not undergone sulfoxide elimination. This dead end could be linked to the peptide on either end, so it is assumed the peak represents a mixture of both possible peptide linkages. When the *m/z*

595.75 peak is subjected to CID, the result is the expected products of sulfoxide fragmentation of the two differently-linked dead ends: one peak is the sulfenic acid modified peptide (1^+ with *m/z* 1024.48), and one is the alkene-modified peptide without a methoxy substituent (2^+ with *m/z* 496.73) (Figure 2, lower left). This data strongly supports the notion that the *m/z* 595.75 peak represents a mixture of both dead ends. With sulfoxide fragmentation occurring between MS^2 and MS^3, sequence data could not be gathered for the *m/z* 595.75 peptides.

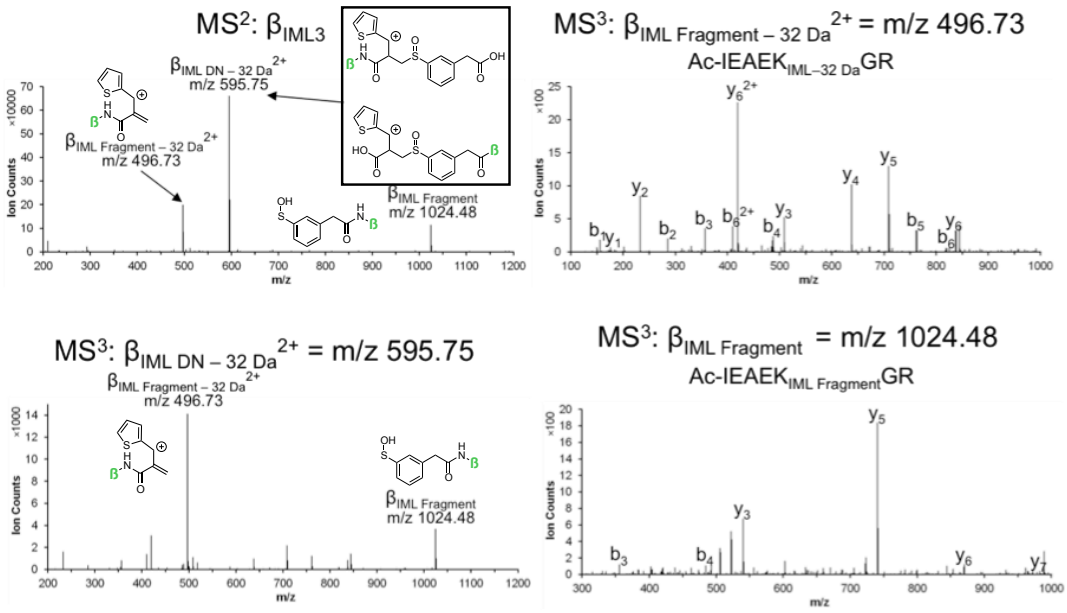
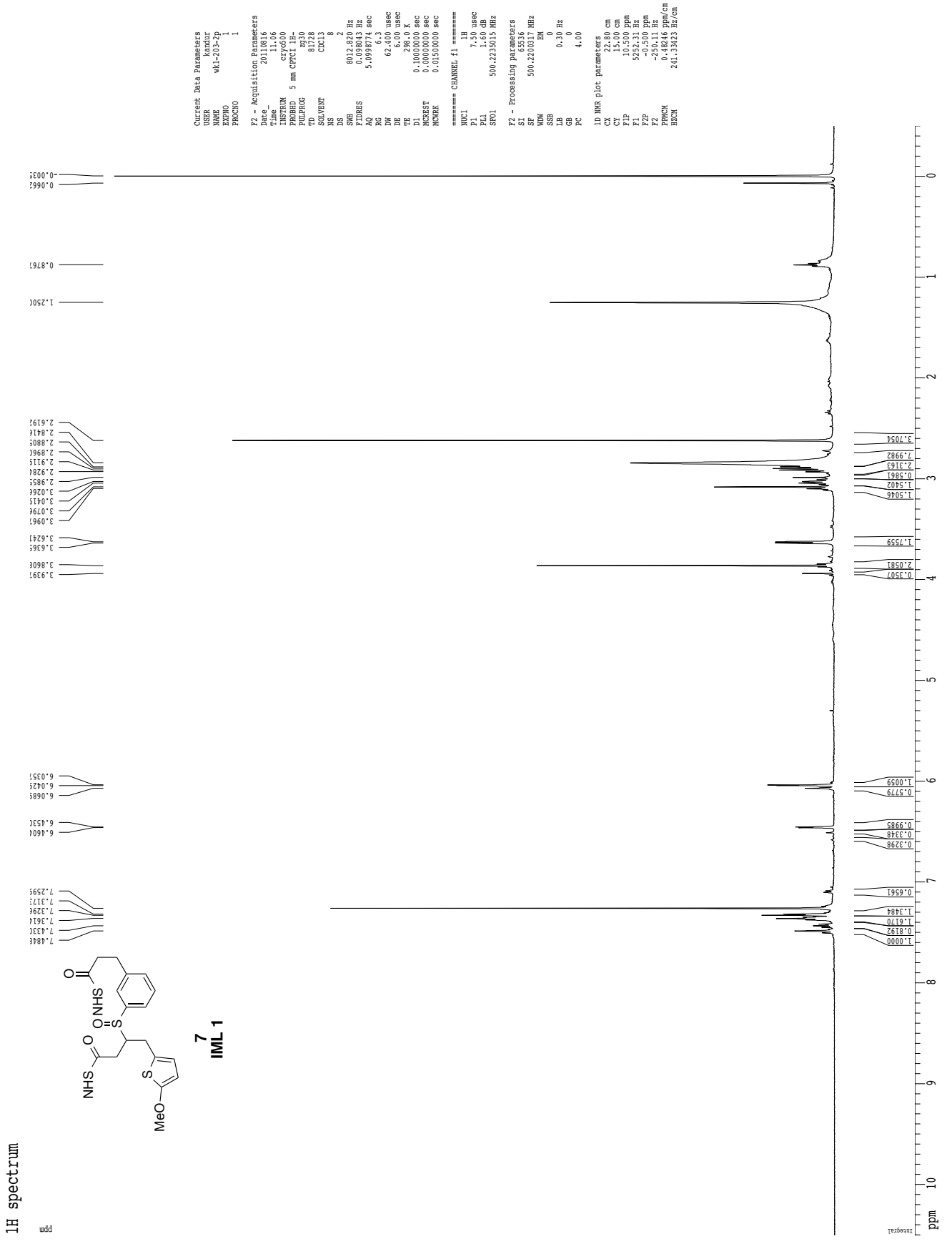


Figure 2. IML 2 Methoxy-loss in MS

References:

1. A. B. Pangborn, M. A. Giardello, R. H. Grubbs, R. K. Rosen, and F. J. Timmers, *Organometallics*, 1996, **15**, 1518–1520.
2. S. Gao, C. Tseng, C. H. Tsai, and C.-F. Yao, *Tetrahedron*, 2008, **64**, 1955–1961.
3. N. M. Leonard and J. Brunckova, *J. Org. Chem.*, 2011, **76**, 9169–9174.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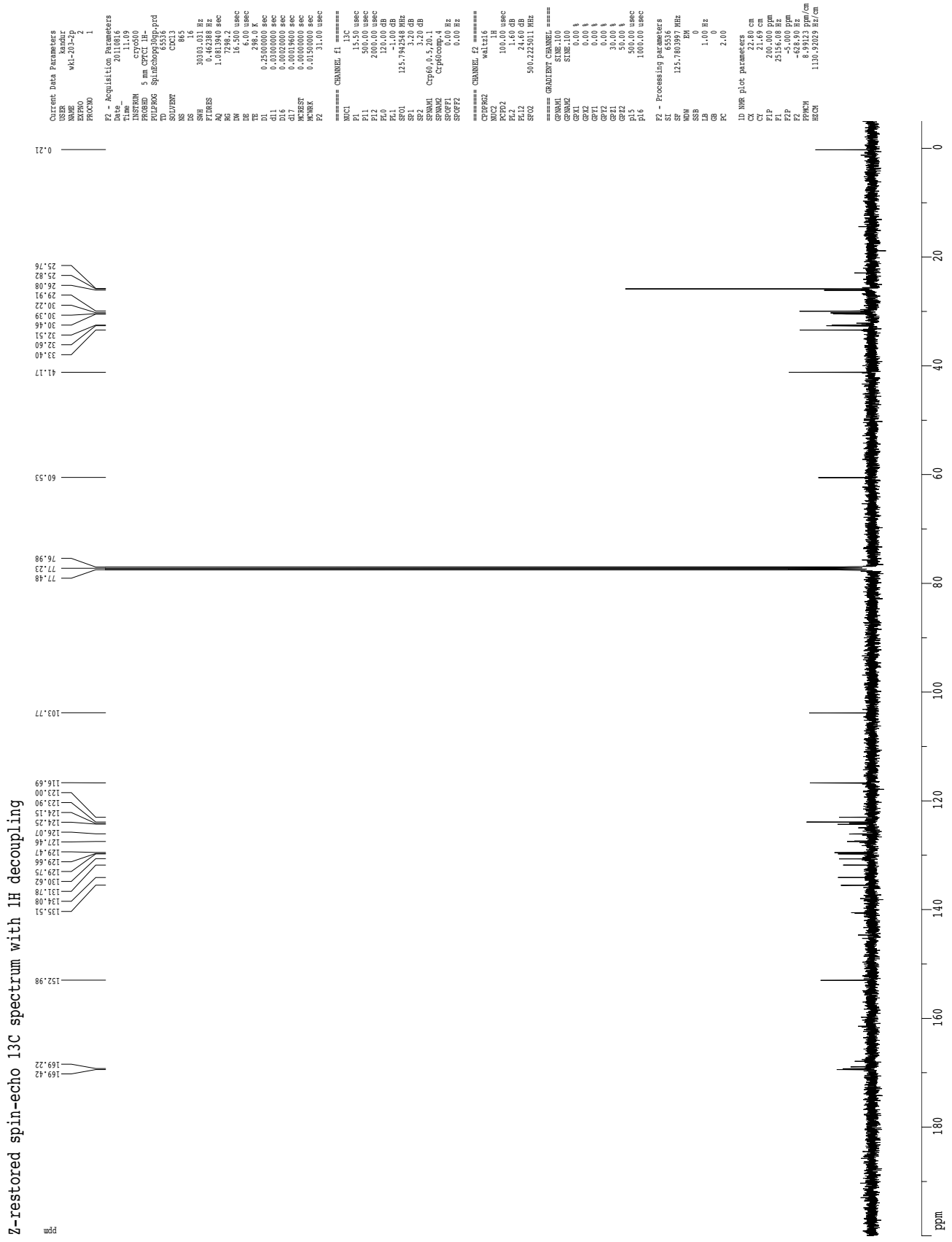
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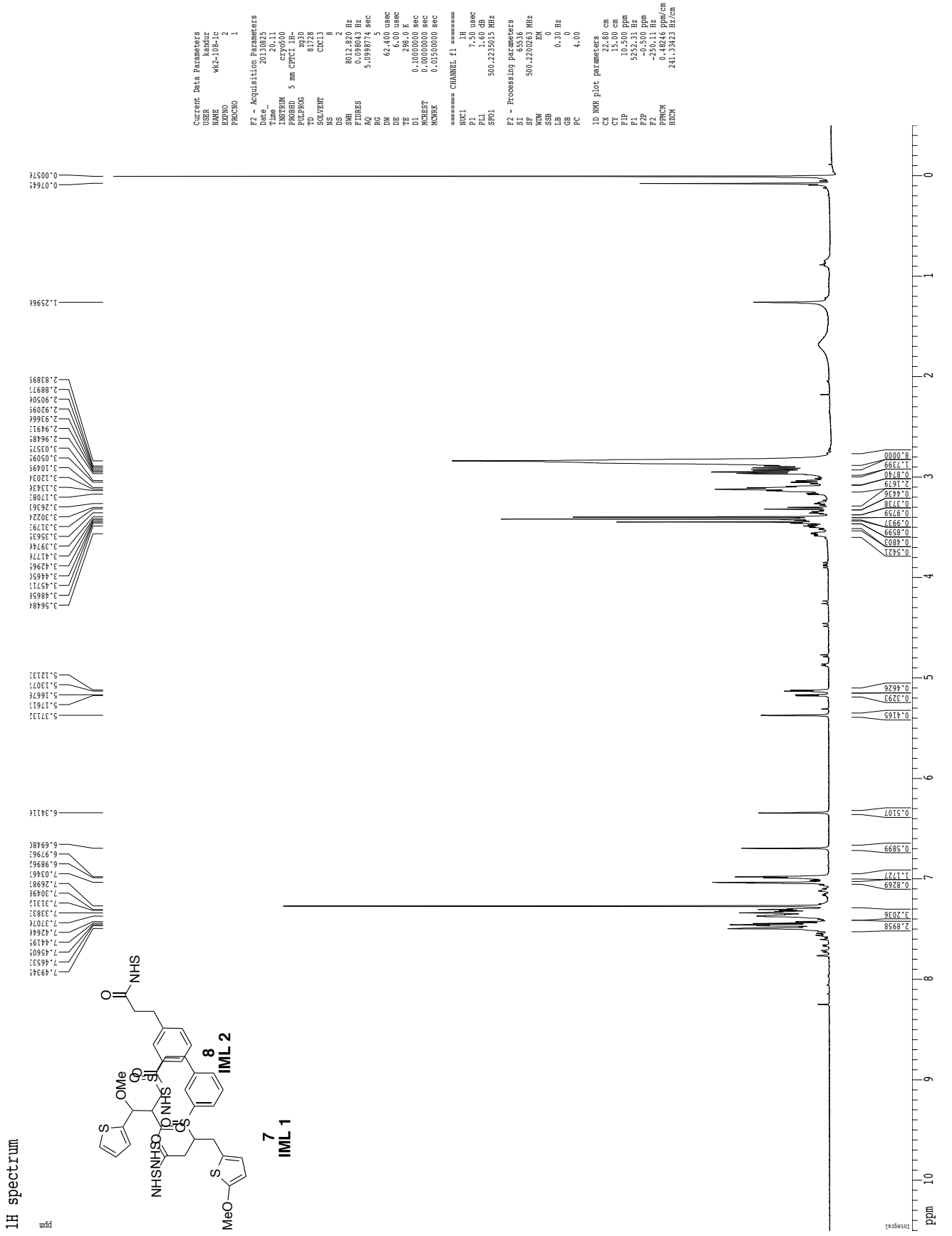
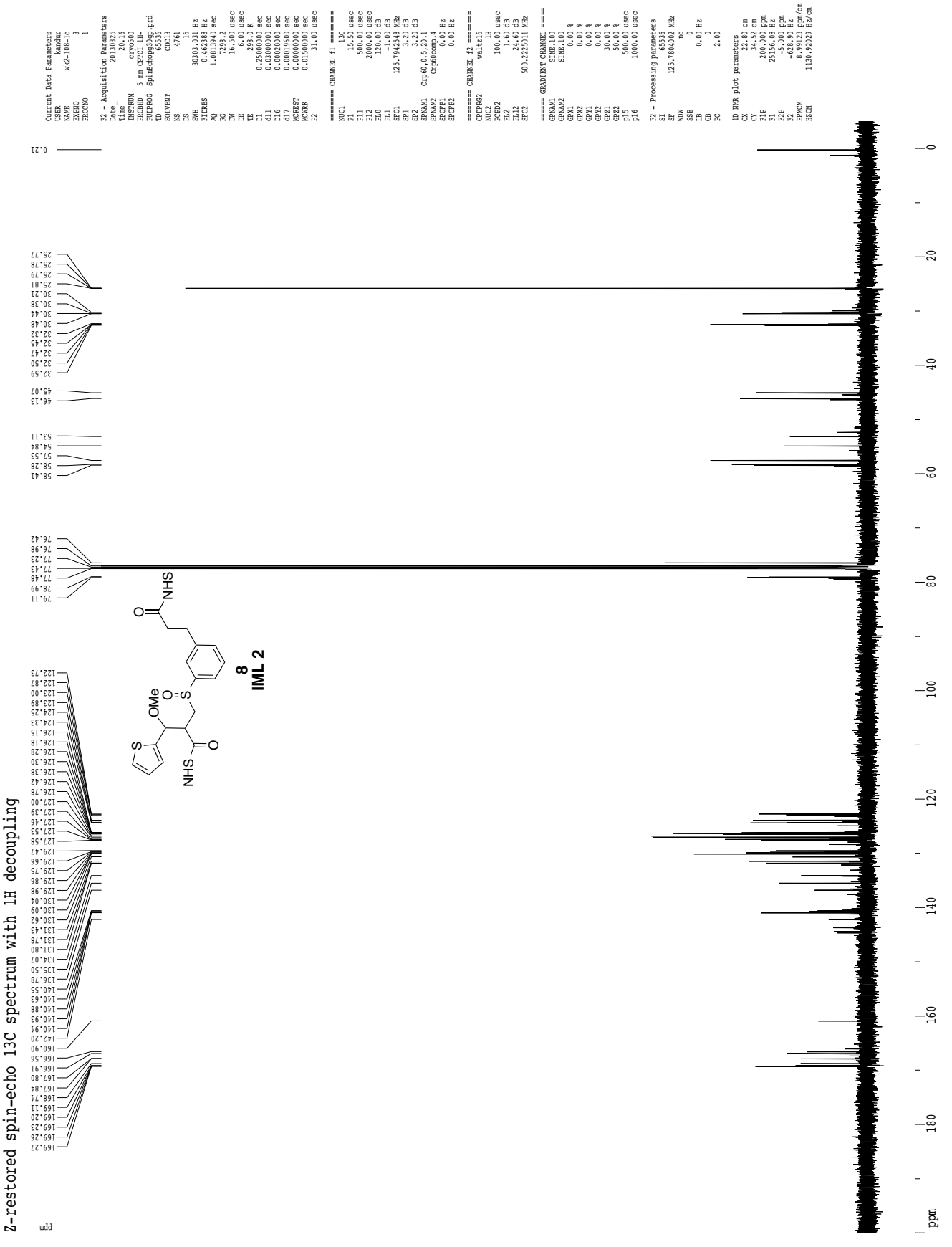
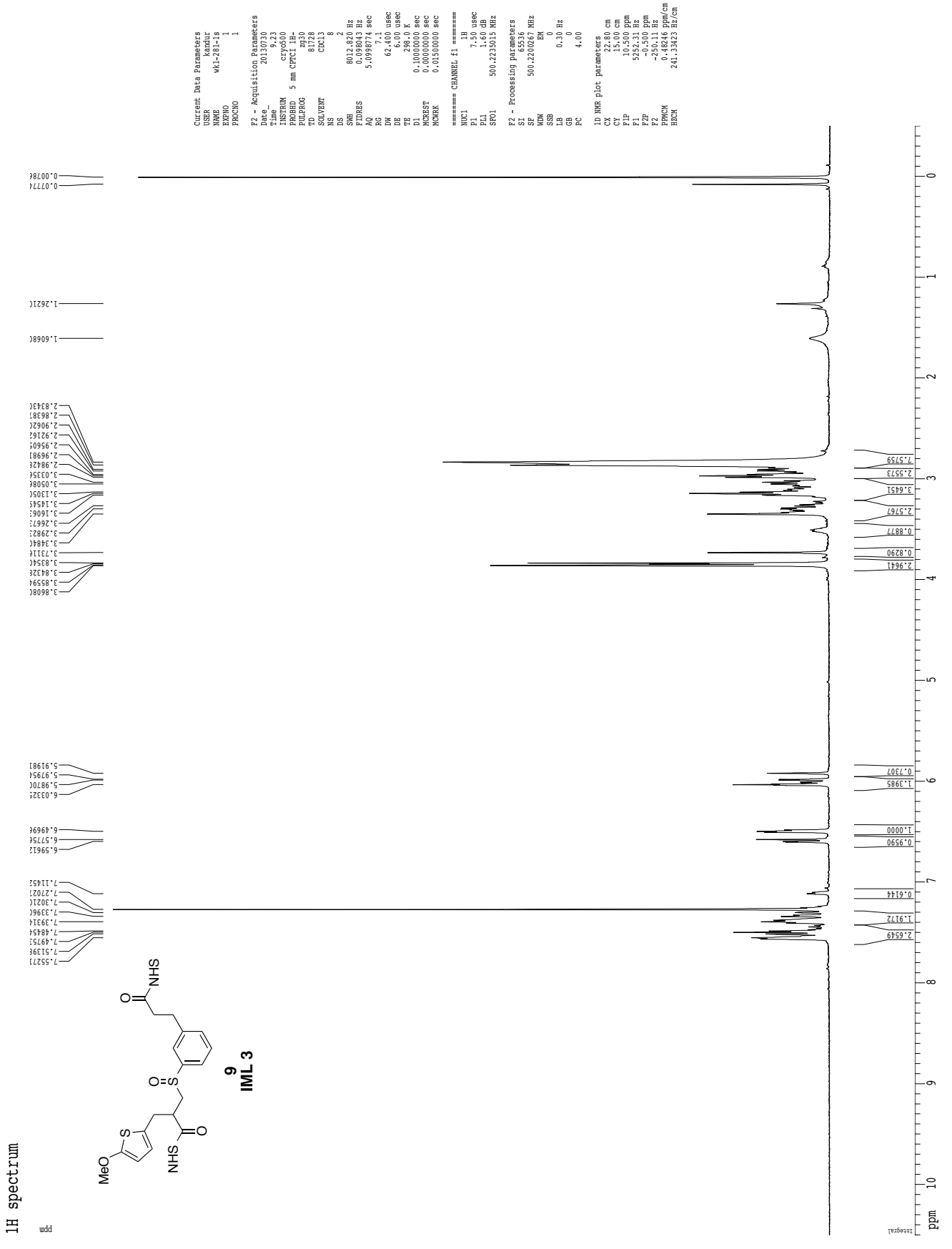
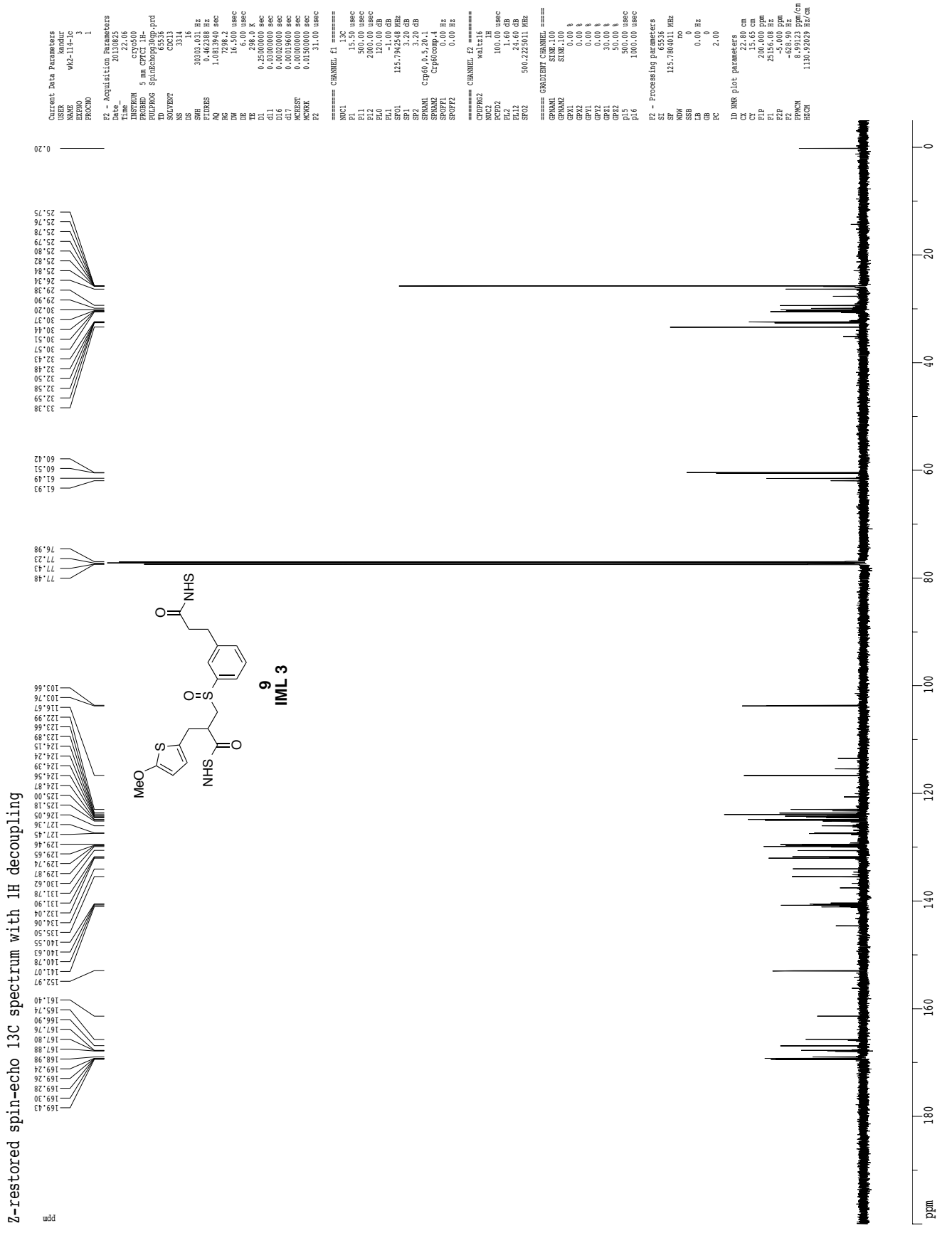
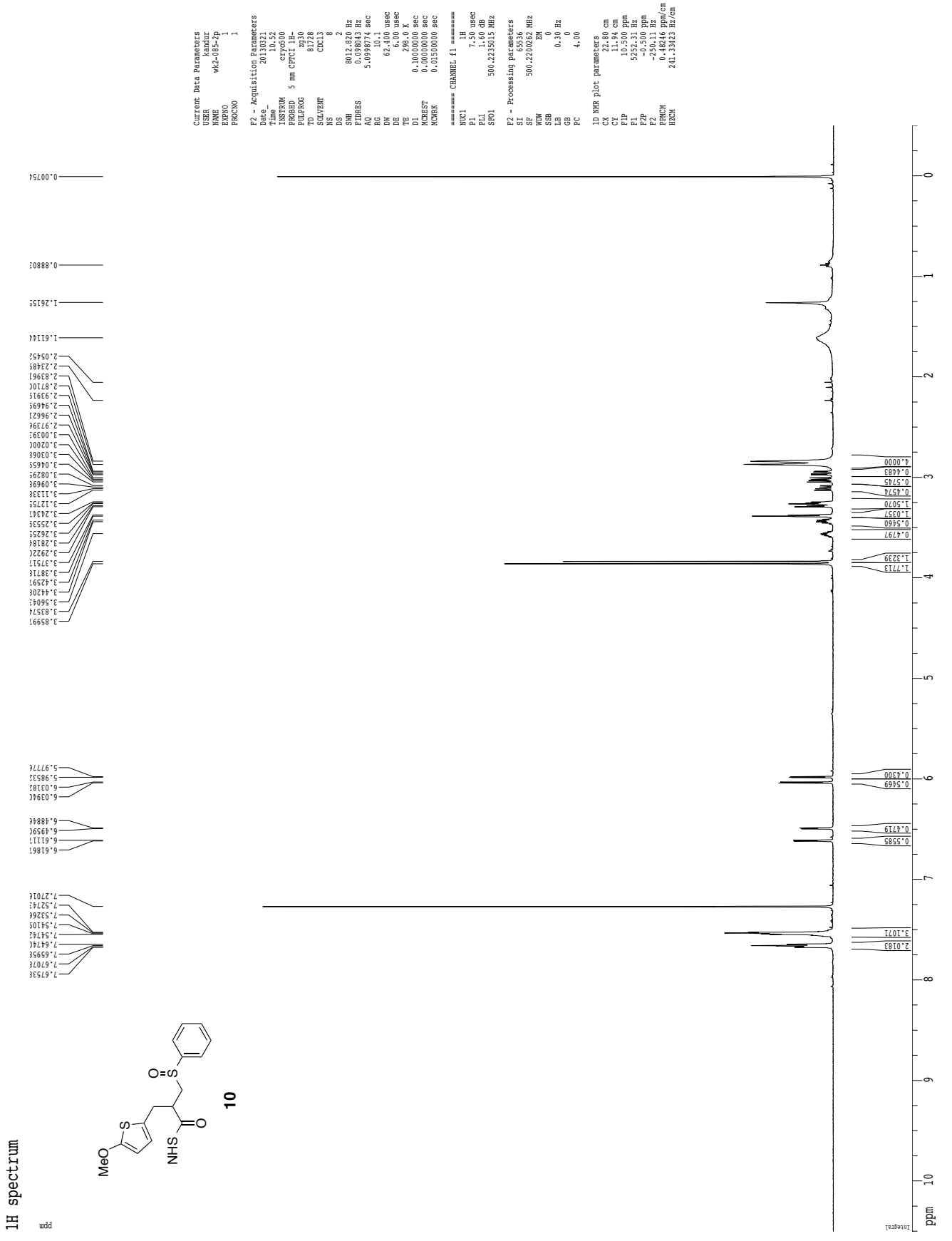
SF 125.7803997 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 21.69 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -62.000 ppm
F2 -7800.92 Hz
PPMCM 8.95123 ppm/cm
HZCM 1130.92029 Hz/cm
0.21
25.76
25.82
26.08
29.91
30.22
30.39
30.46
32.51
32.60
33.40
41.17
60.53
76.98
77.23
77.48
103.77
116.69
123.00
123.90
124.15
124.25
126.07
127.46
129.47
129.66
129.75
130.62
131.78
134.08
135.51
152.98
169.22
169.42
ppm
0
20
40
60
80
100
120
140
160
180

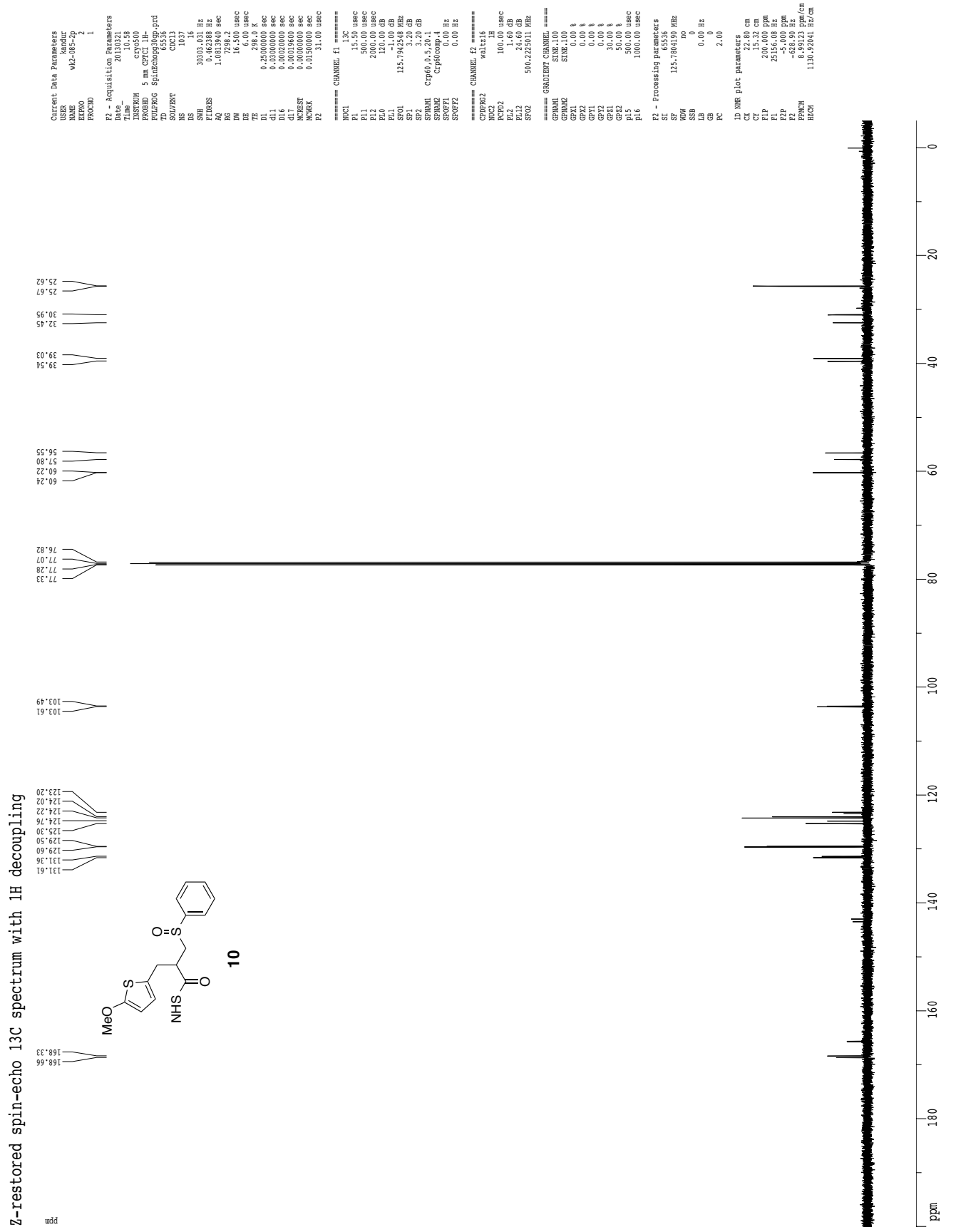

1H spectrum
Current Data Parameters
USER kandur
NAME wk2-108-1c
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130825
Time_ 20.11
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200263 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.00574
0.07645
1.25966
2.83895
2.88977
2.90506
2.92095
2.93666
2.94913
2.96485
3.03575
3.05095
3.10495
3.12034
3.13436
3.17083
3.26361
3.30224
3.31795
3.35635
3.39746
3.41774
3.42965
3.44656
3.45717
3.48656
3.56484
5.12133
5.13077
5.16676
5.17617
5.37132
6.34114
6.69486
6.97965
6.98962
7.03467
7.26983
7.30496
7.31312
7.33831
7.37074
7.42644
7.44195
7.45605
7.46531
7.49345
8.0000
1.7399
0.8740
2.1679
0.4436
0.3738
0.9759
0.9937
0.8599
0.4803
0.5421
0.4626
0.3293
0.4165
0.5107
0.5899
1.1727
0.8269
3.2036
2.8958
ppm
integral
7
IML 1
8
IML 2
OMe
NHS
NHSNHS
MeO

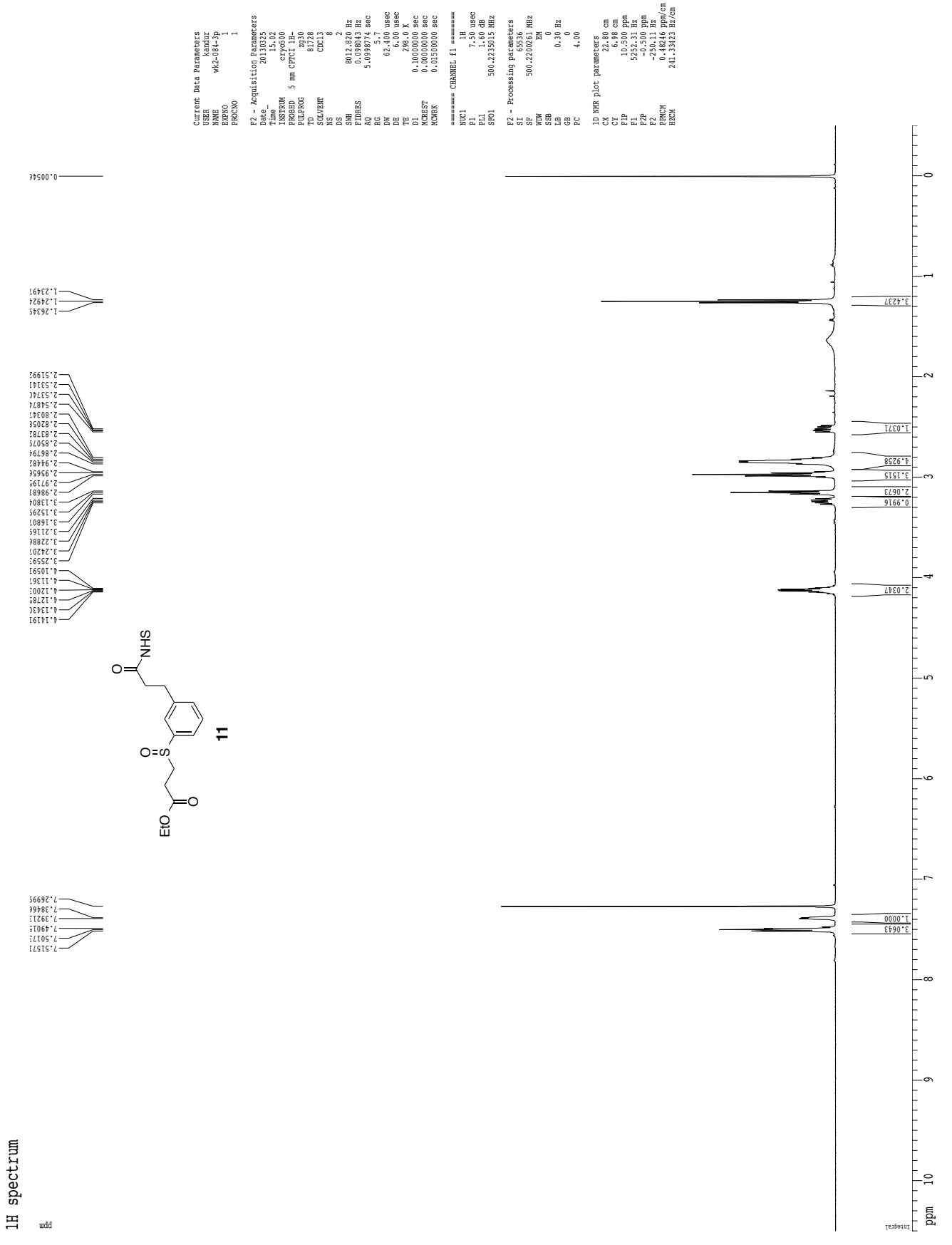

Z-restored spin-echo 13C spectrum with 1H decoupling
8
IML 2
NHS
OMe
S
O
ppm


1H spectrum
9
IML 3
MeO
NHS
NHS

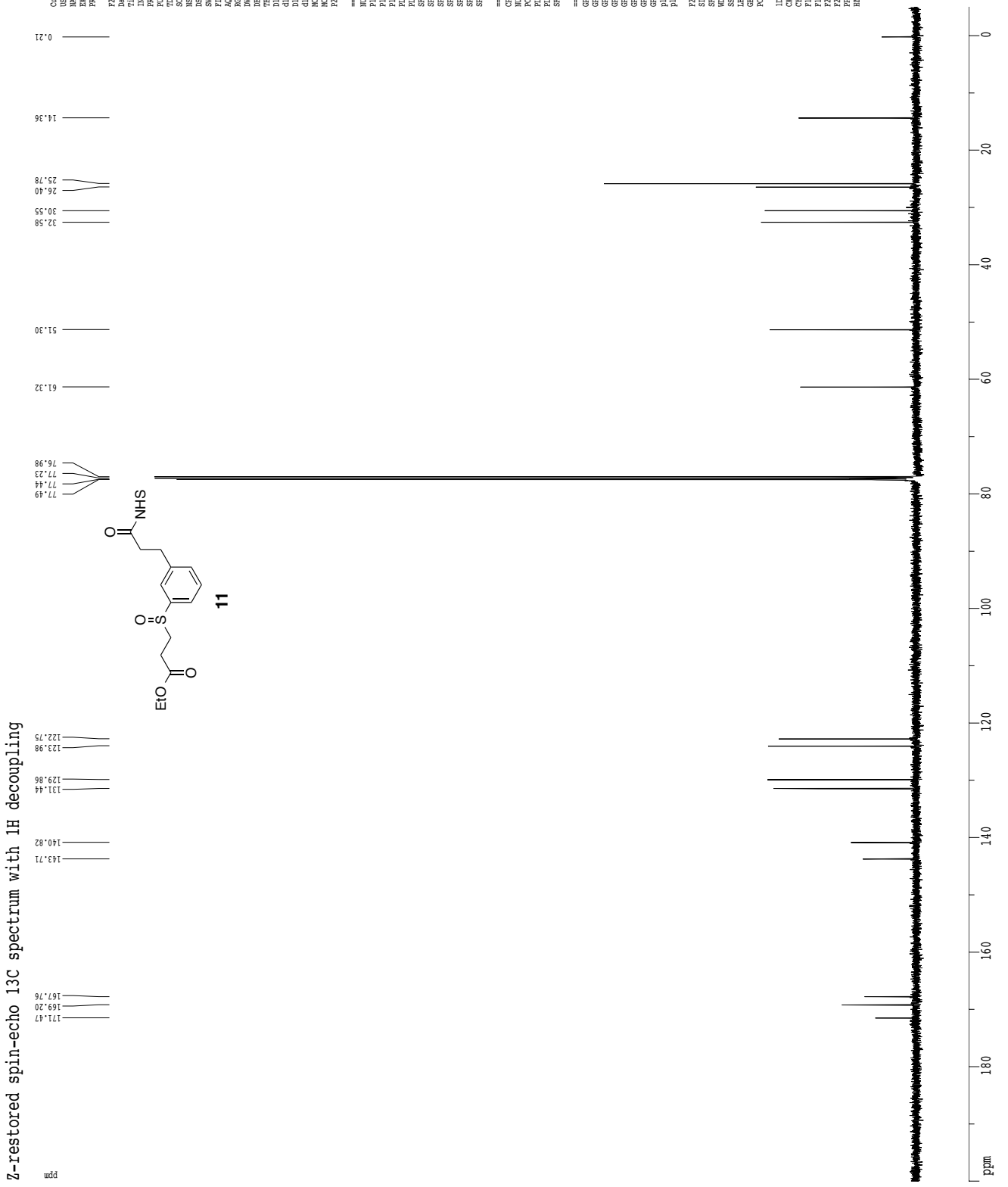

Z-restored spin-echo 13C spectrum with 1H decoupling
9
IML 3
MeO
NHS
O
S
ppm

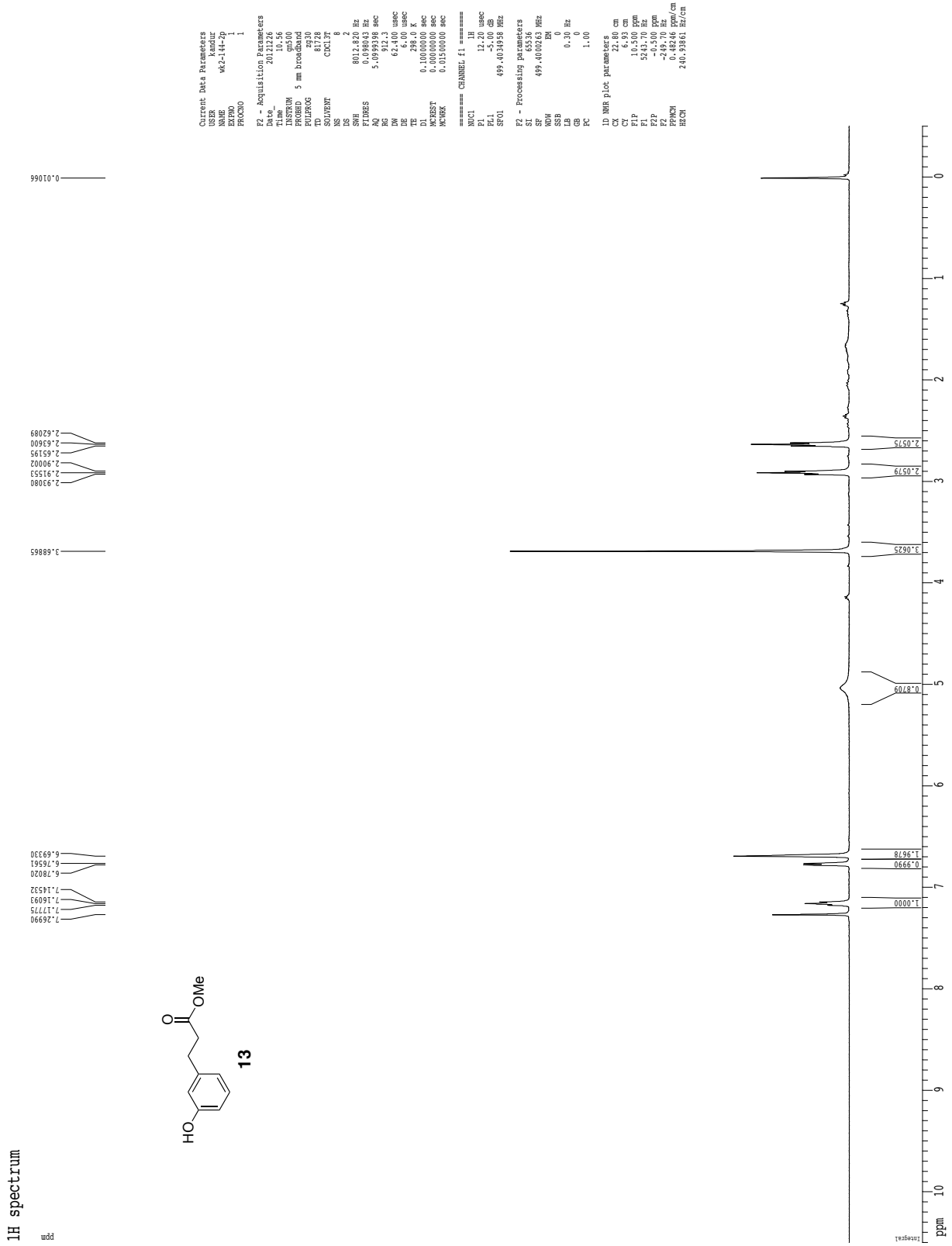

1H spectrum
Current Data Parameters
USER kandur
NAME wk2-085-2p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130321
Time_ 10.52
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998674 sec
RG 10.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200262 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 11.94 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.00754
0.88801
1.26155
1.61144
2.05452
2.23485
2.89961
2.87100
2.93915
2.94695
2.96621
2.97396
3.00391
3.02000
3.03066
3.04655
3.08295
3.09696
3.11338
3.12759
3.24341
3.25535
3.26295
3.28184
3.29220
3.37517
3.38718
3.42597
3.44208
3.56043
3.83574
3.85997
5.97774
5.98532
6.03982
6.03182
6.48844
6.49590
6.61117
6.61867
7.27014
7.52742
7.53266
7.54105
7.54742
7.64744
7.65956
7.67076
7.67536
4.0000
0.4483
0.5745
0.4574
1.5070
1.0357
0.5460
0.4797
1.3239
1.7713
0.4300
0.5469
0.4719
0.5585
3.1071
2.0183
integral
ppm
MeO
S
NHS
O=S
O
O
10

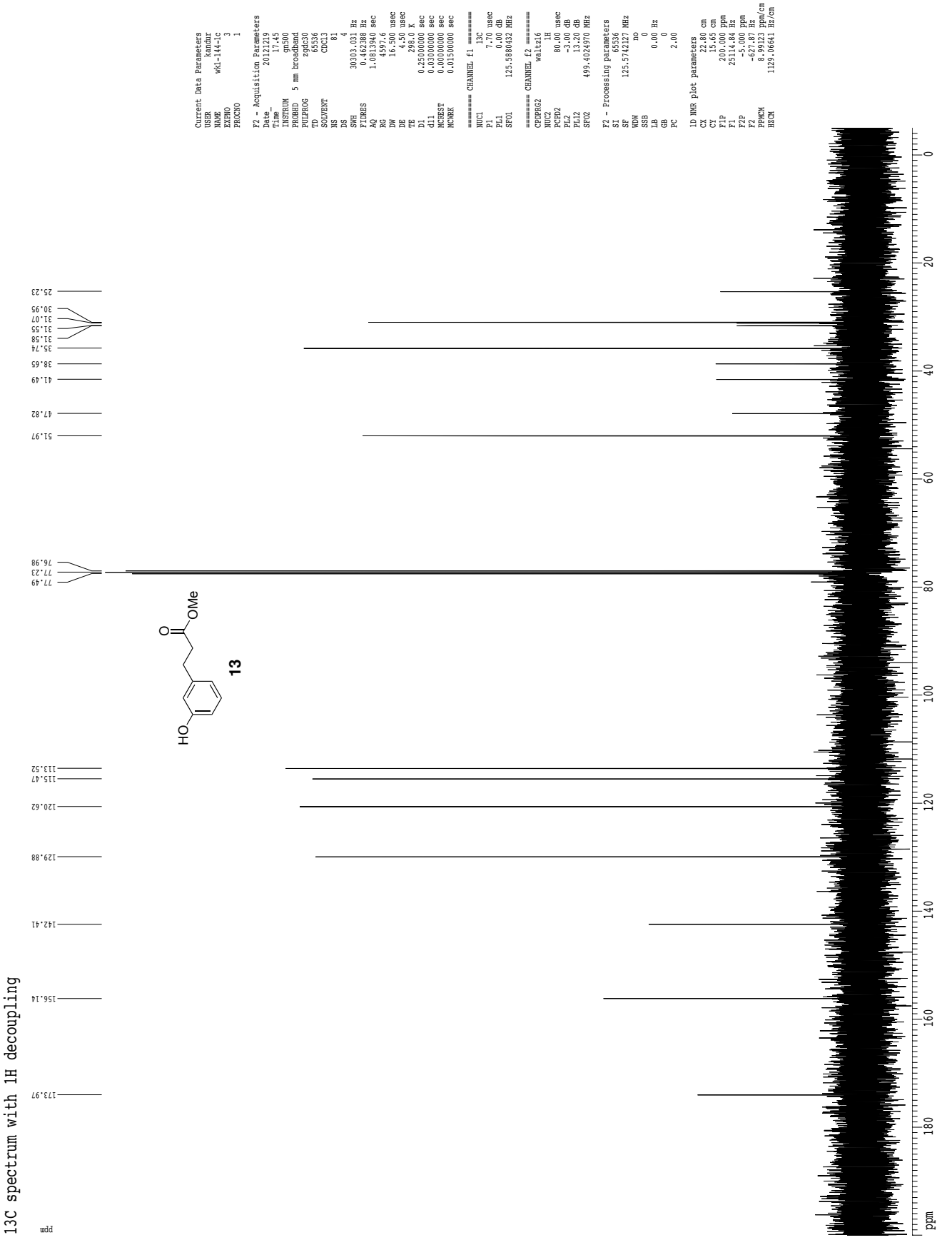

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
MeO
S
NHS
O=S
O
O
10
168.66
168.33
133.61
133.36
129.60
129.50
125.30
124.76
124.22
124.02
123.20
103.61
103.49
77.33
77.28
77.07
76.82
60.24
60.22
57.80
56.55
39.94
39.03
32.45
30.95
25.67
25.62
0
20
40
60
80
100
120
140
160
180
ppm

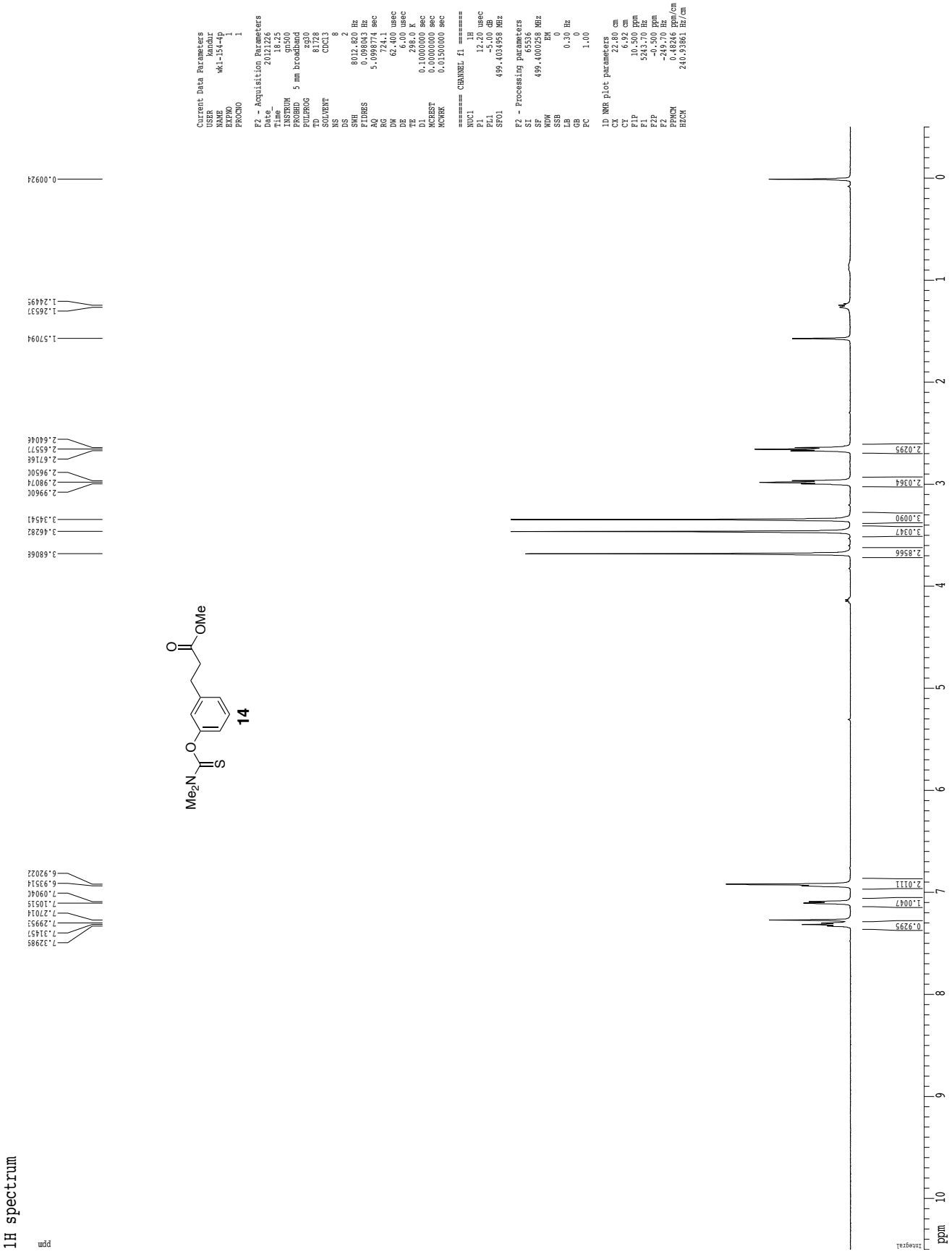

1H spectrum
Current Data Parameters
USER kandur
NAME wk2-084-3p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130325
Time_ 15.02
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 5.7
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200261 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.98 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.0054
1.2345
1.2492
1.2349
2.5199
2.5314
2.5374
2.5487
2.8034
2.8205
2.8378
2.8507
2.8679
2.9448
2.9565
2.9719
2.9868
3.1380
3.1529
3.1680
3.2116
3.2288
3.2420
3.2559
4.1059
4.1136
4.1200
4.1278
4.1343
4.1419
7.2699
7.3846
7.3921
7.4901
7.5017
7.5157
3.4237
1.0371
4.9258
3.1515
2.0673
0.9916
2.0347
1.0000
3.0643
11
NHS
O
O
O=S
O
EtO
ppm
Integral

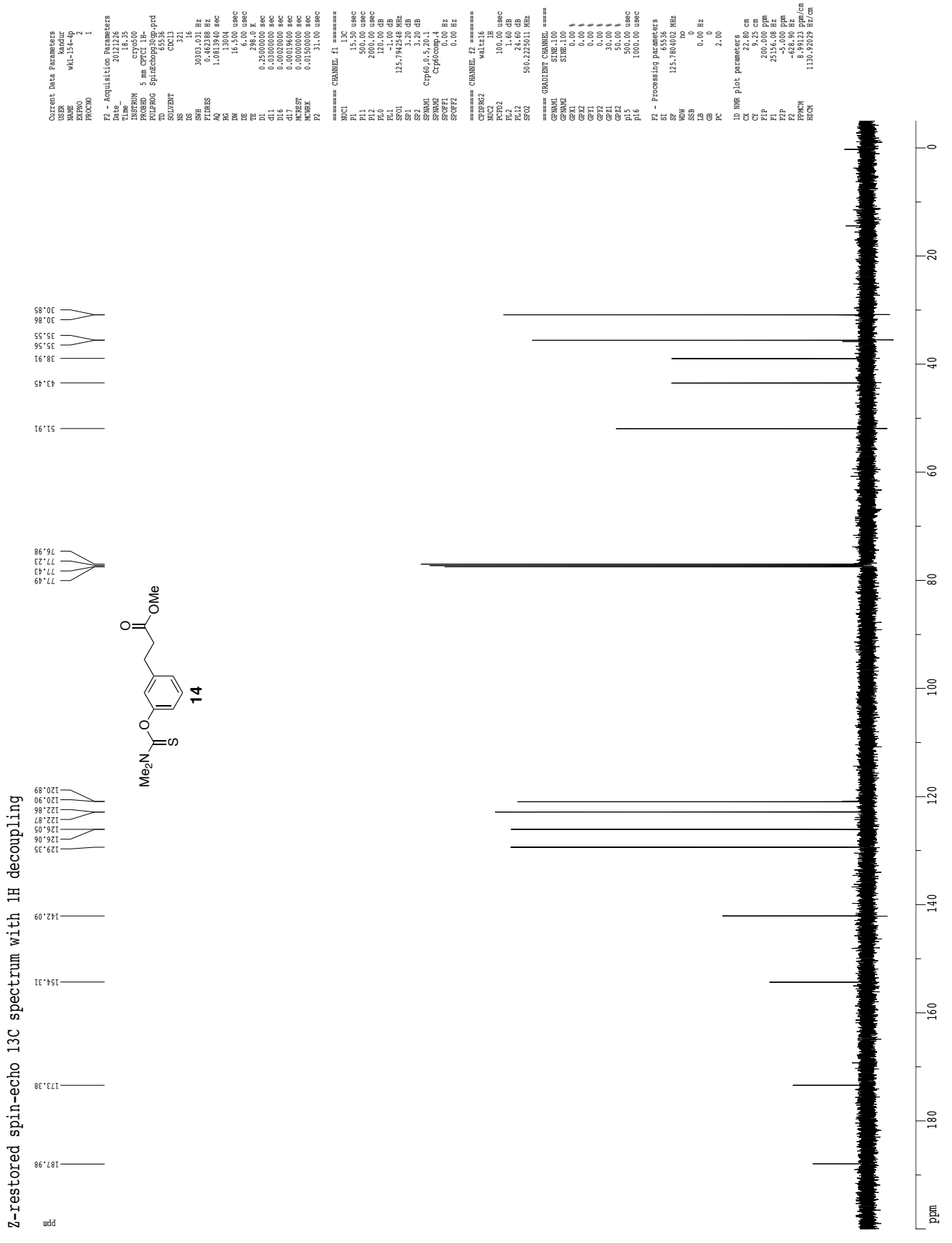
Z-restored spin-echo 13C spectrum with 1H decoupling

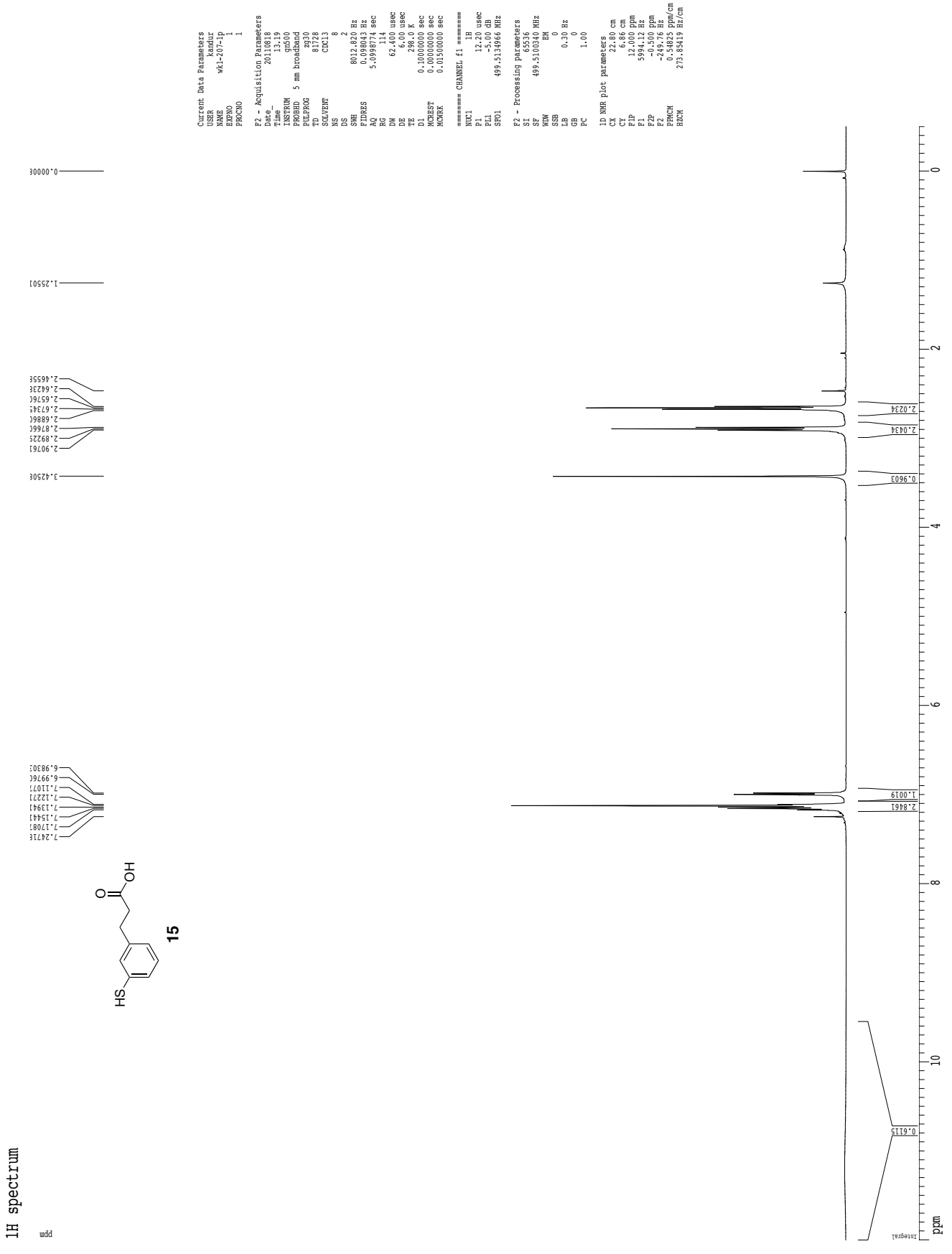


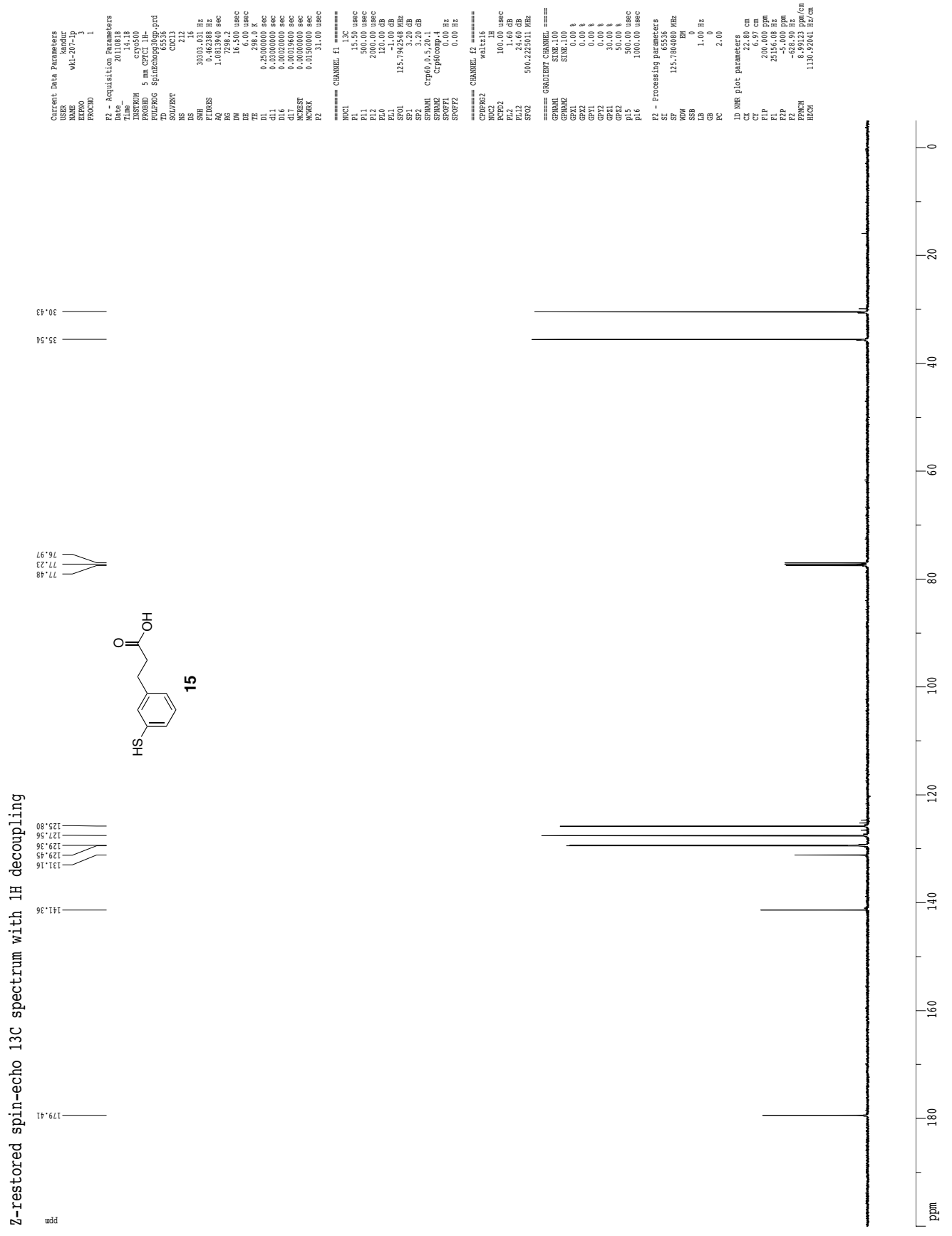

1H spectrum
ppm
Integral
13
O
OMe
HO
Current Data Parameters
USER kandur
NAME wk2-144-2p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121226
Time_ 10.56
INSTRUM gm500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3rr
NS 2
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 912.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -3.00 dB
SFO1 499.4034936 MHz
F2 - Processing parameters
SI 65536
SF 499.4000263 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 6.93 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.500 ppm
F2 -249.70 Hz
PPMCM 0.46146 ppm/cm
HZCM 240.93861 Hz/cm
0.01066
2.62089
2.63600
2.65195
2.90002
2.91553
2.93080
3.68865
6.69330
6.76561
6.78020
7.14532
7.16093
7.17775
7.26990
2.0575
2.0579
3.0625
0.8709
1.9678
0.9990
1.0000

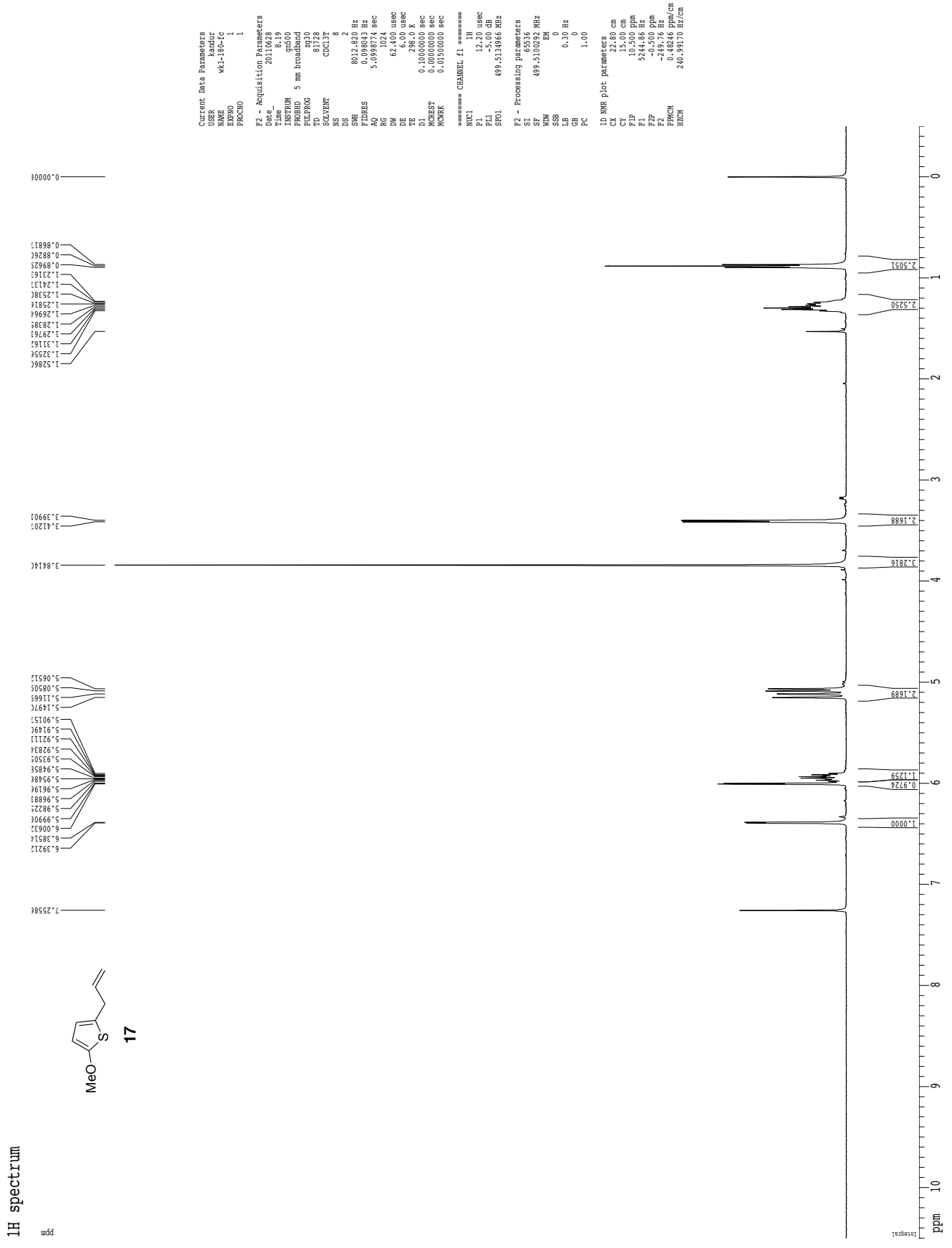

13C spectrum with 1H decoupling
Current Data Parameters
USER kandur
NAME wk1-144-1c
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121219
Time 17.45
INSTRUM dpx500
PROBHD 5 mm broadband
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 81
DS 4
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.08139940 sec
RG 4597.6
DW 16.500 usec
DE 4.50 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 7.70 usec
PL1 0.00 dB
SFO1 125.5880432 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 13.20 dB
SFO2 499.4024970 MHz
F2 - Processing parameters
SI 65536
SF 125.5742127 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25114.84 Hz
F2P -5.000 ppm
F2 -627.87 Hz
PPMCM 8.99123 ppm/cm
HZCM 1129.06641 Hz/cm
25.23
30.95
31.07
31.55
31.58
35.74
38.65
41.49
47.82
51.97
76.98
77.49
77.23
113.52
115.47
120.62
129.88
142.41
156.14
173.97
O
OMe
HO
13
ppm
0
20
40
60
80
100
120
140
160
180

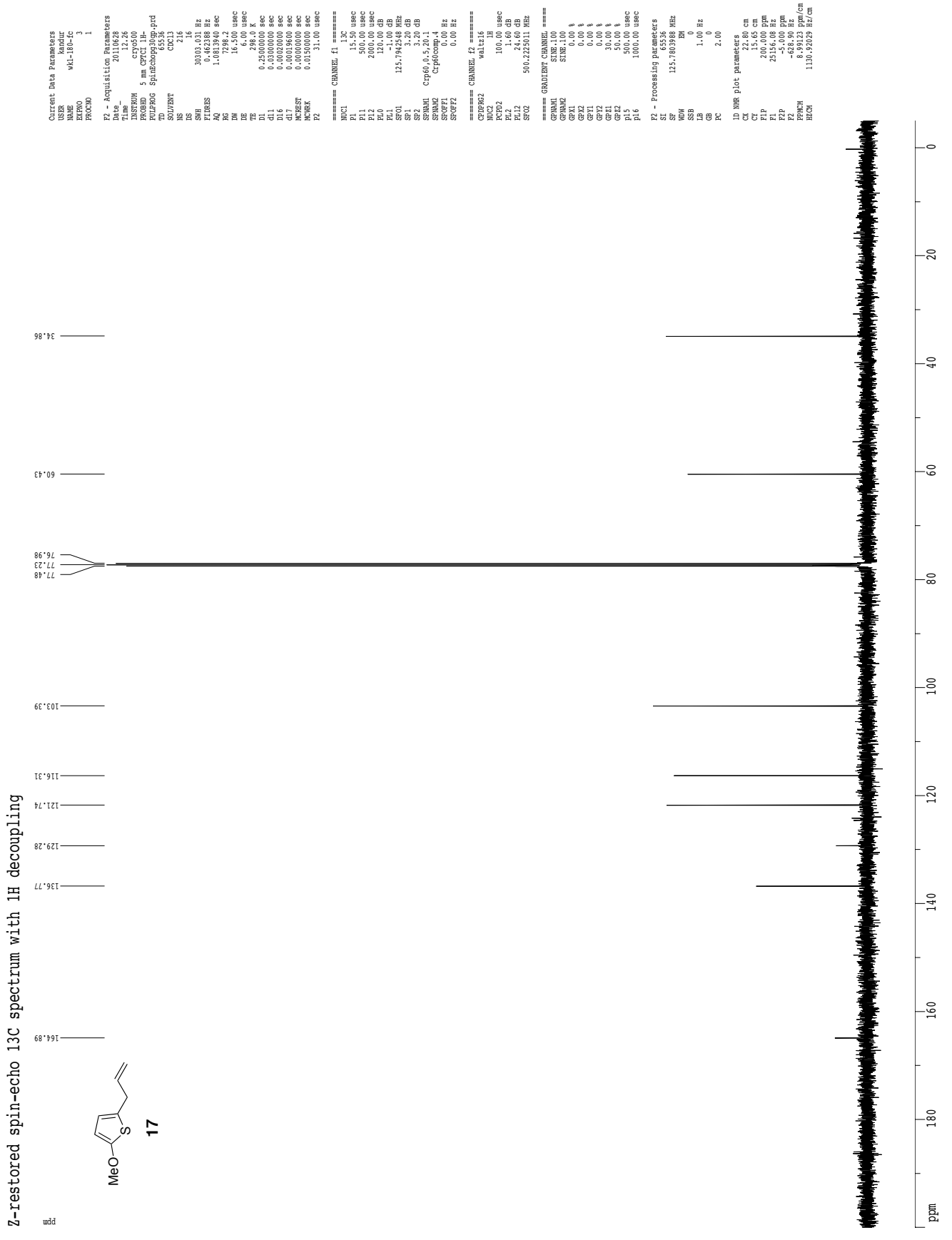

1H spectrum
ppm
Integral
Current Data Parameters
USER Kandur
NAME wk1-154-4p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121226
Time 18.25
INSTRUM spn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 724.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.4034958 MHz
F2 - Processing parameters
SI 65536
SF 499.4000258 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 6.92 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.500 ppm
F2 -249.70 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.93861 Hz/cm
0.00924
1.24495
1.26537
1.57094
2.64046
2.65577
2.67168
2.96500
2.98074
2.99600
3.34541
3.46282
3.68068
6.92022
6.93514
7.09040
7.10515
7.27014
7.29953
7.31457
7.32989
2.0295
2.0364
3.0090
3.0347
2.8566
2.0111
1.0047
0.9295
14
O
OMe
O
O
S
Me2N

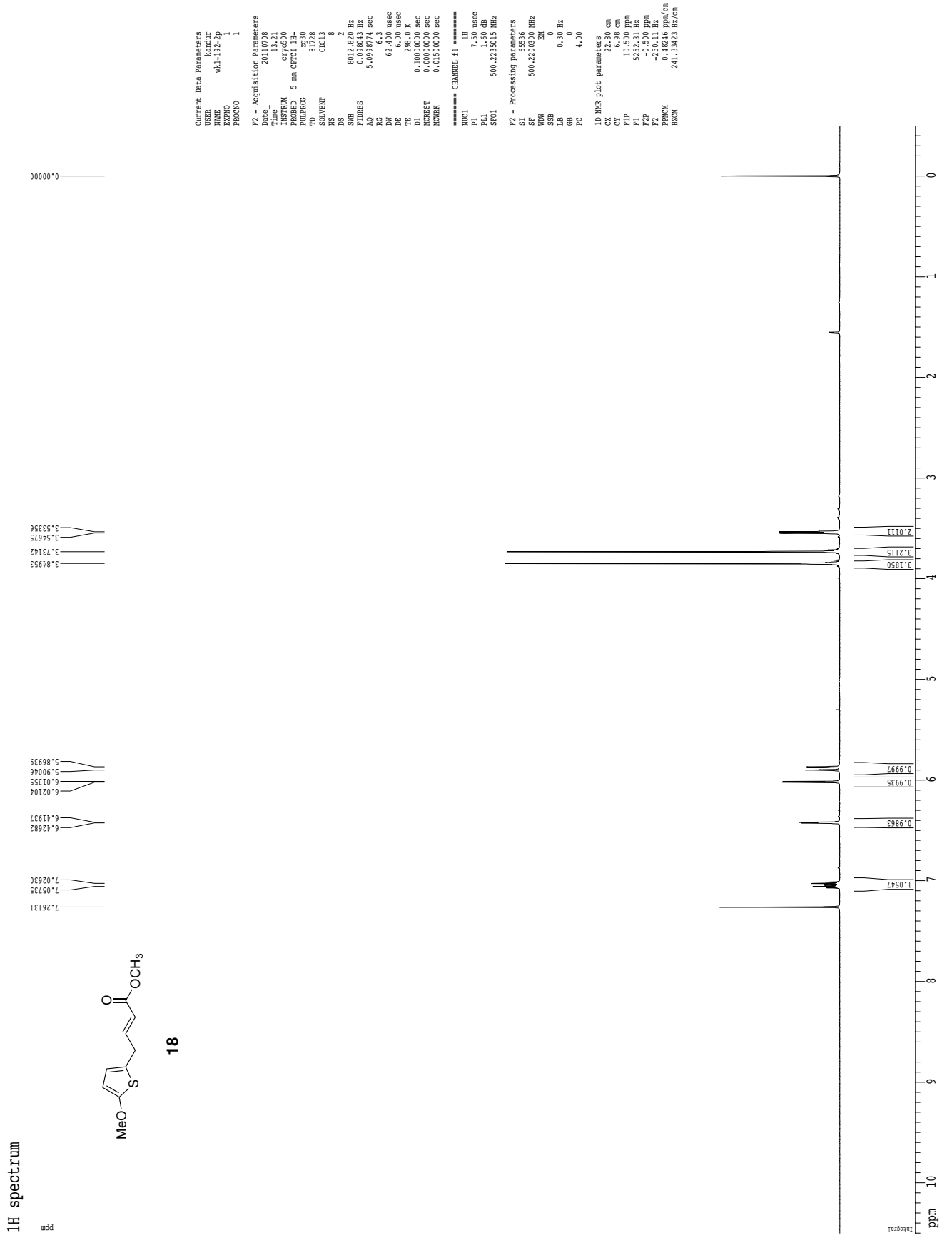

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
187.98
173.38
154.31
142.09
129.35
126.06
126.05
122.87
122.86
120.90
120.89
76.98
77.49
77.43
77.23
51.91
43.45
38.91
35.56
35.55
30.86
30.85
Me2N
O
S
O
OMe
14
Current Data Parameters
USER kandur
NAME wkl-154-4p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121226
Time_ 18.35
INSTRUM cryo500
PROBHD 5 mm CPPCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 321
DS 16
SWH 30303.031 Hz
FIDRES 0.462318 Hz
AQ 1.081940 sec
RG 13004
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00100000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======= CHANNEL f1 =======
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7904218 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======= CHANNEL f2 =======
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7804002 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 9.25 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
0
20
40
60
80
100
120
140
160
180
ppm


1H spectrum
Current Data Parameters
USER kandur
NAME wk1-207-1p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110818
Time_ 13.19
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 114
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.5134966 MHz
F2 - Processing parameters
SI 65536
SF 499.5100340 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 6.86 cm
F1P 12.000 ppm
F1 5994.12 Hz
F2P -0.500 ppm
F2 -249.76 Hz
PPMCM 0.54825 ppm/cm
HZCM 273.85419 Hz/cm
0.00000
1.25501
2.46556
2.64236
2.65760
2.67345
2.68866
2.87666
2.89225
2.90761
3.42506
6.98305
6.99760
7.11071
7.12271
7.13941
7.15441
7.17087
7.24716
2.0234
2.0434
0.9603
1.0019
2.8461
0.6115
integral
ppm
0
2
4
6
8
10
HS
O
OH
15

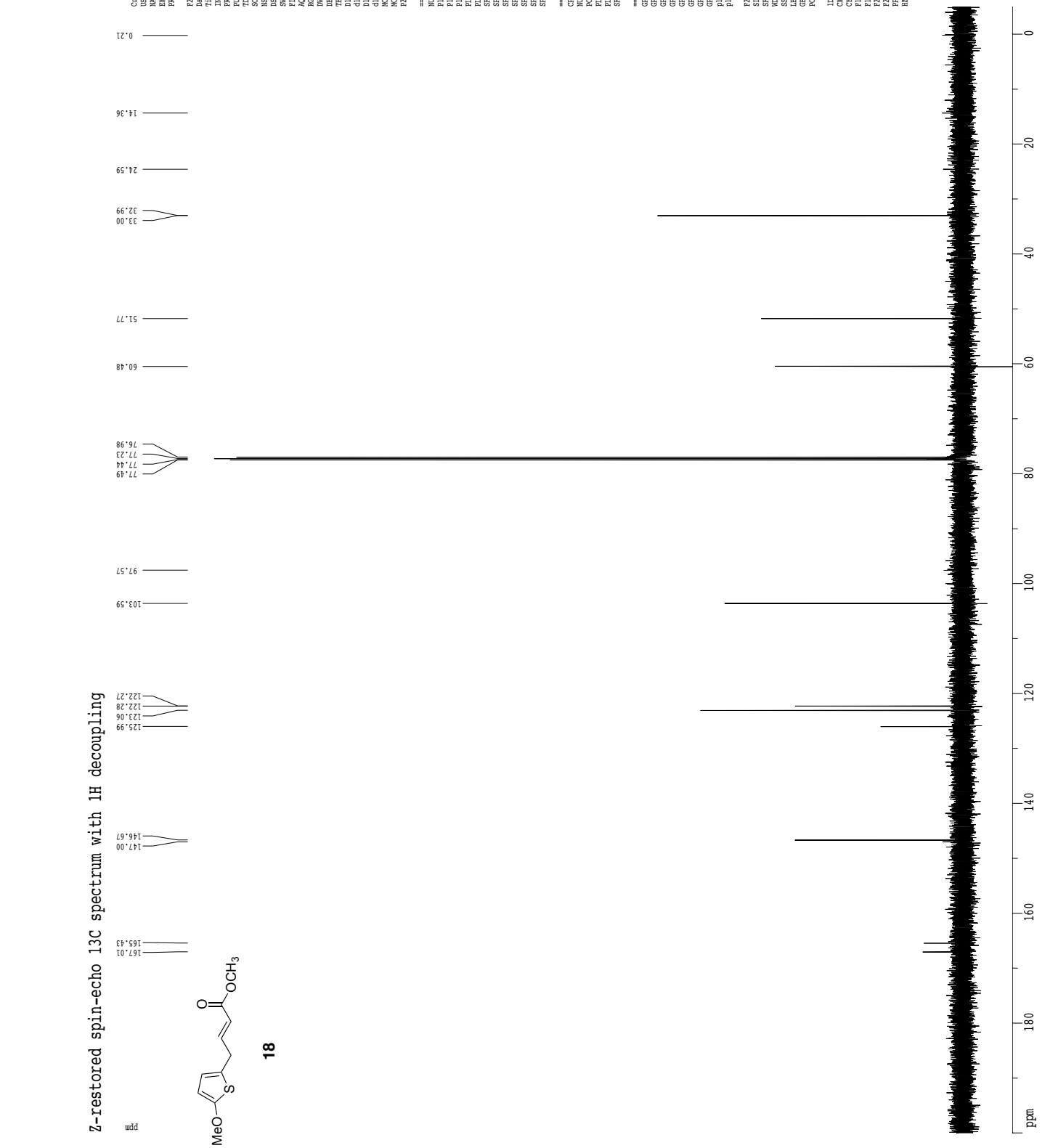

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
179.41
141.36
131.16
129.45
129.36
127.56
125.80
77.48
77.23
76.97
30.43
35.54
OH
O
HS
15
Current Data Parameters
USER kandur
NAME wk1-207-1p
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110818
Time_ 14.18
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 212
DS 16
SWH 30303.031 Hz
FIDRES 0.462386 Hz
AQ 1.081394D sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00180000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7904248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7804088 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 6.97 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92041 Hz/cm
ppm
0
20
40
60
80
100
120
140
160
180


Current Data Parameters
USER Kandur
NAME wk1-180-1c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110628
Time_ 8.19
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 1024
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.5134966 MHz
F2 - Processing parameters
SI 65536
SF 499.5100292 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.500 ppm
F1 5244.66 Hz
F2P -0.500 ppm
F2 -249.76 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.99170 Hz/cm
0.00000
0.86817
0.88276
0.89625
1.23163
1.24137
1.25380
1.25814
1.26964
1.28385
1.29761
1.31162
1.32556
1.52866
3.39901
3.41207
3.84146
5.06512
5.08505
5.11665
5.14976
5.90157
5.91496
5.92111
5.92834
5.93505
5.94856
5.95486
5.96196
5.96881
5.98225
5.99906
6.00632
6.38514
6.39212
7.25586
2.5051
2.5250
2.1688
3.2816
2.1689
1.1259
0.9724
1.0000
MeO
S
17
1H spectrum
ppm
Integral

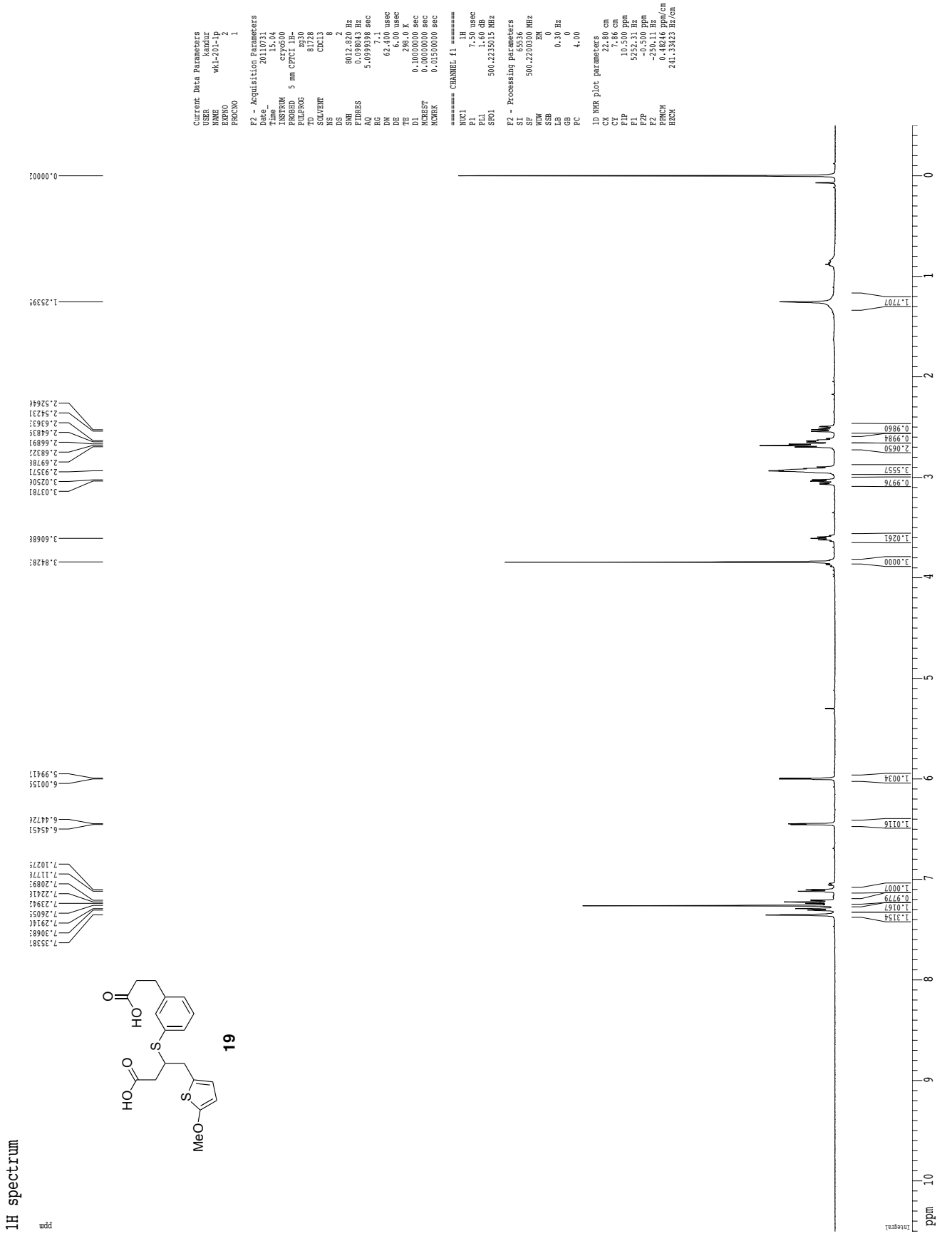

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
MeO
S
17
164.89
136.77
129.28
121.74
116.31
103.39
77.48
77.23
76.98
60.43
34.86
Current Data Parameters
USER kandur
NAME wk1-186-fc
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110628
Time 12.26
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 216
DS 16
SWH 30303.031 Hz
FIDRES 0.462386 Hz
AQ 1.081394O sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00100000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7941248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7803988 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
ppm
0
20
40
60
80
100
120
140
160
180

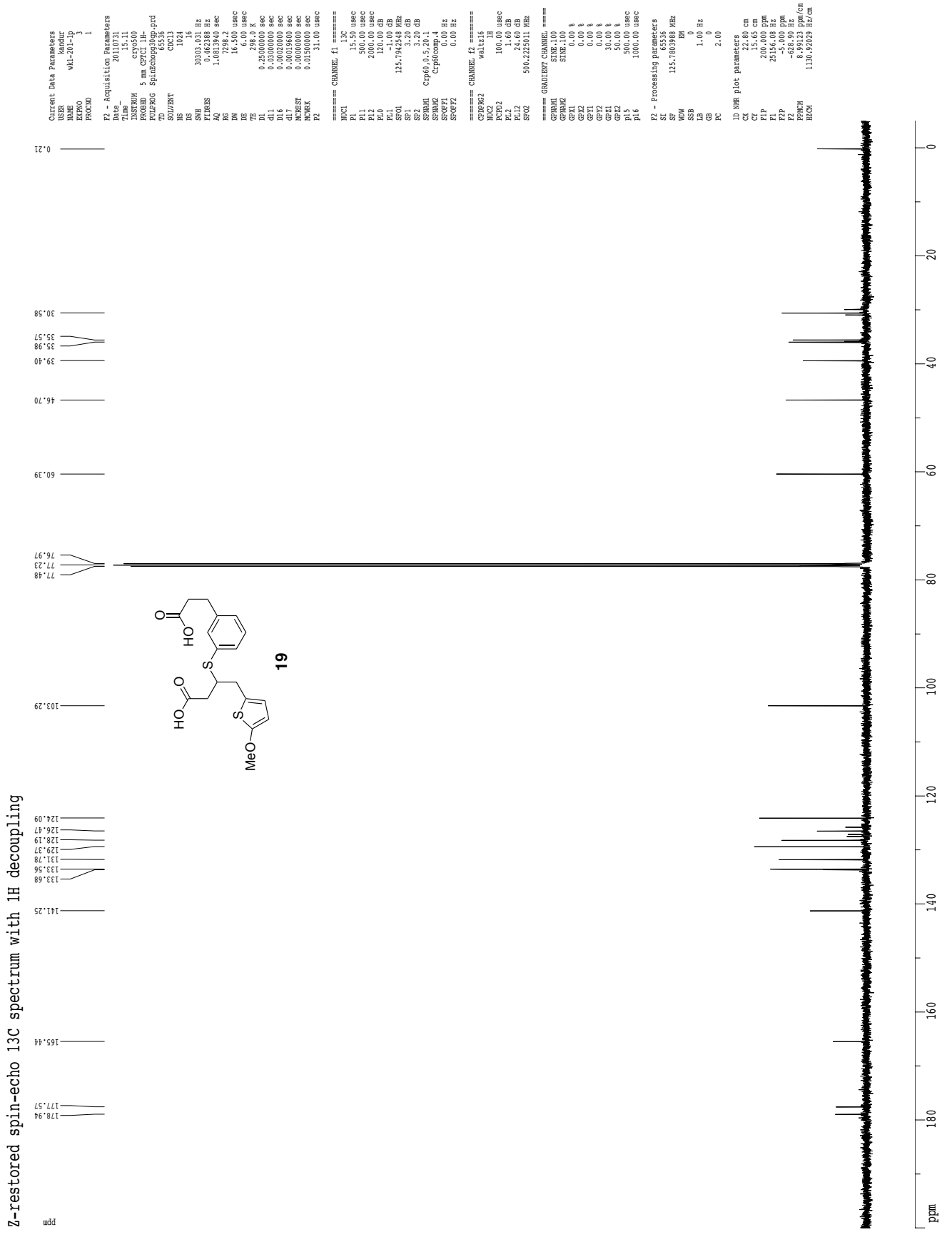

1H spectrum
ppm
integral
Current Data Parameters
USER kandur
NAME wk1-192-2p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110708
Time_ 13.21
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 6.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200300 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.98 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
7.26131
7.05735
7.02636
6.42682
6.41937
6.02104
6.01355
5.90046
5.86935
3.84955
3.73142
3.54675
3.53356
1.0547
0.9863
0.9935
0.9997
3.1850
3.2115
2.0111
MeO
S
O
OCH3
18

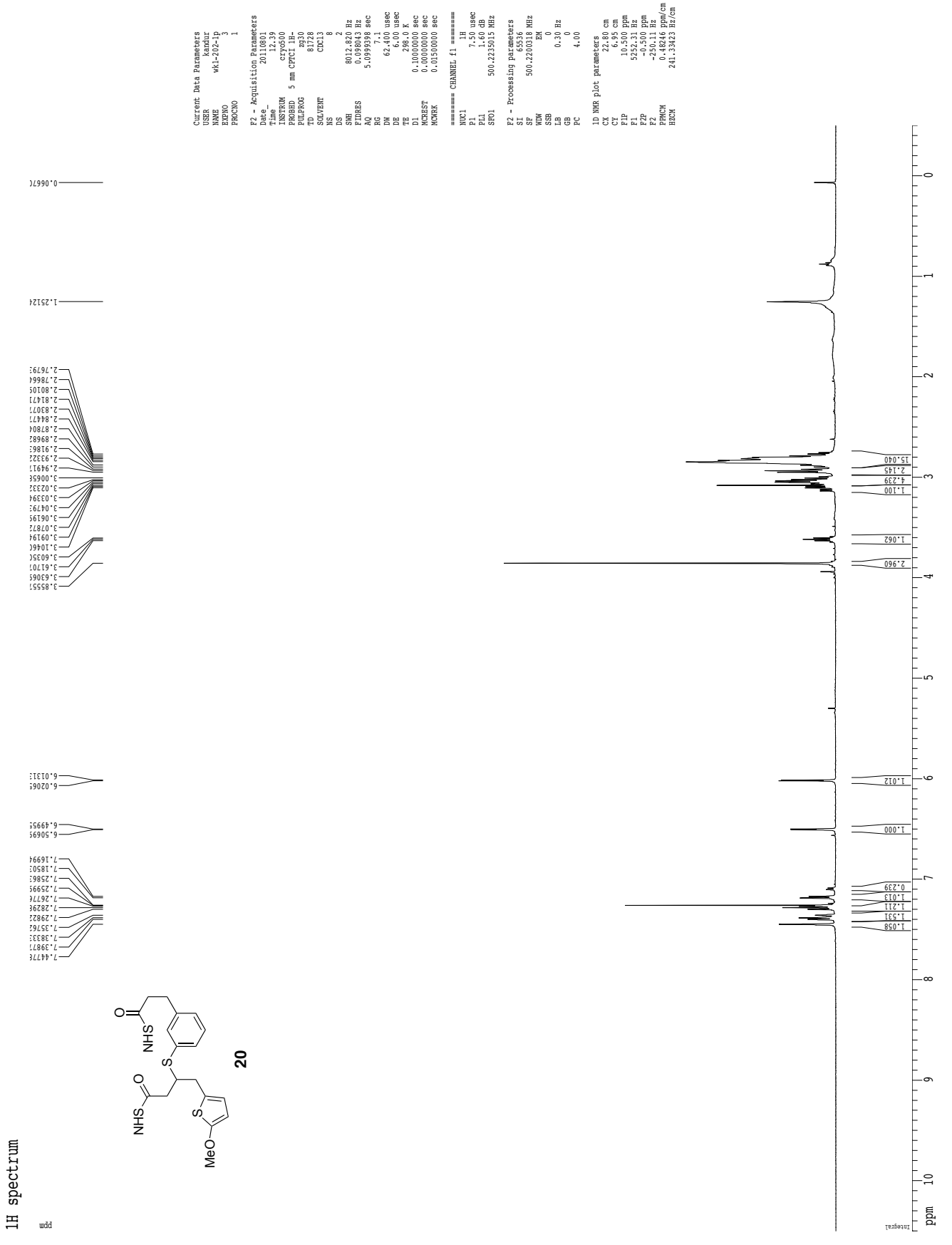
Z-restored spin-echo 13C spectrum with 1H decoupling



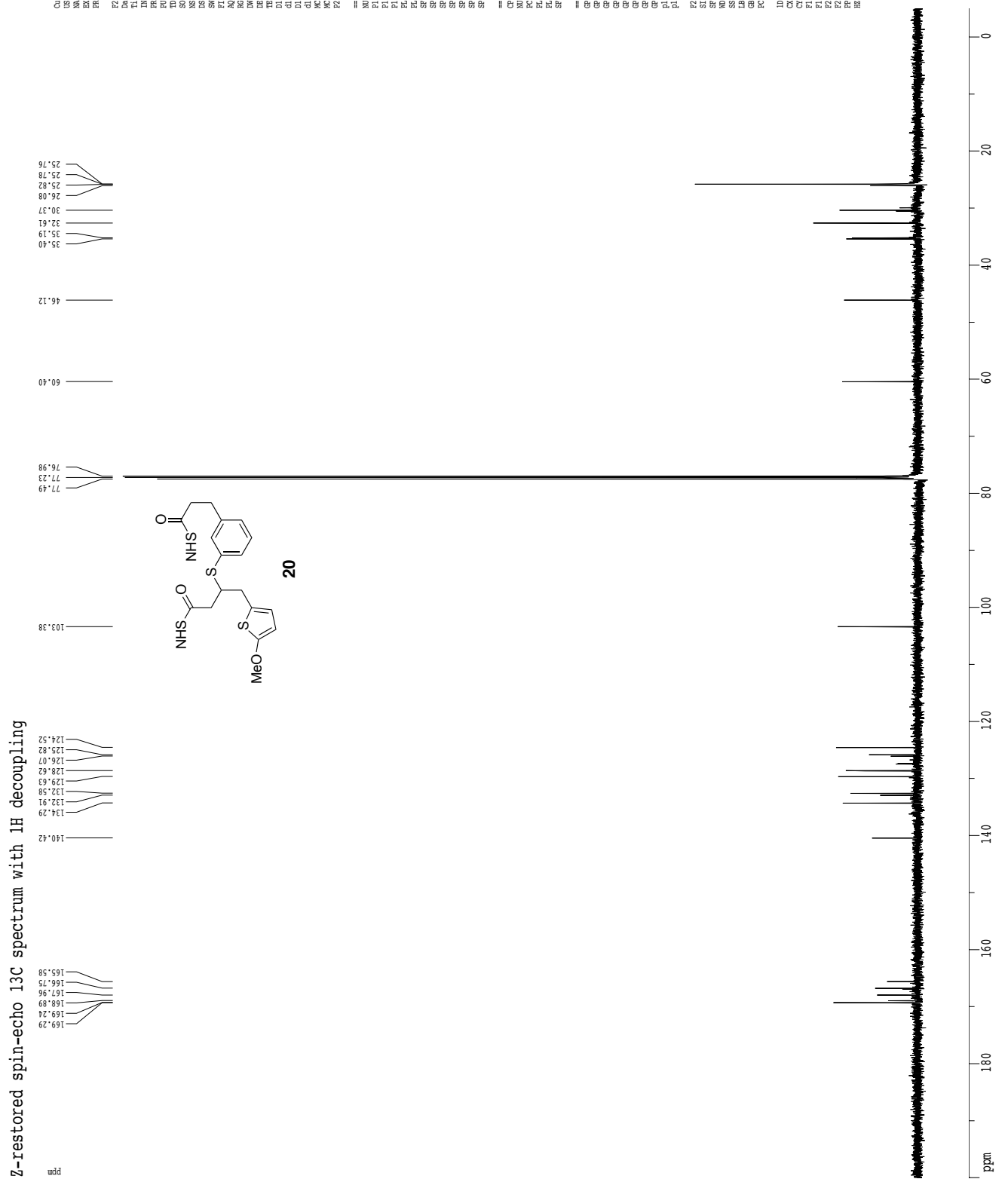
18

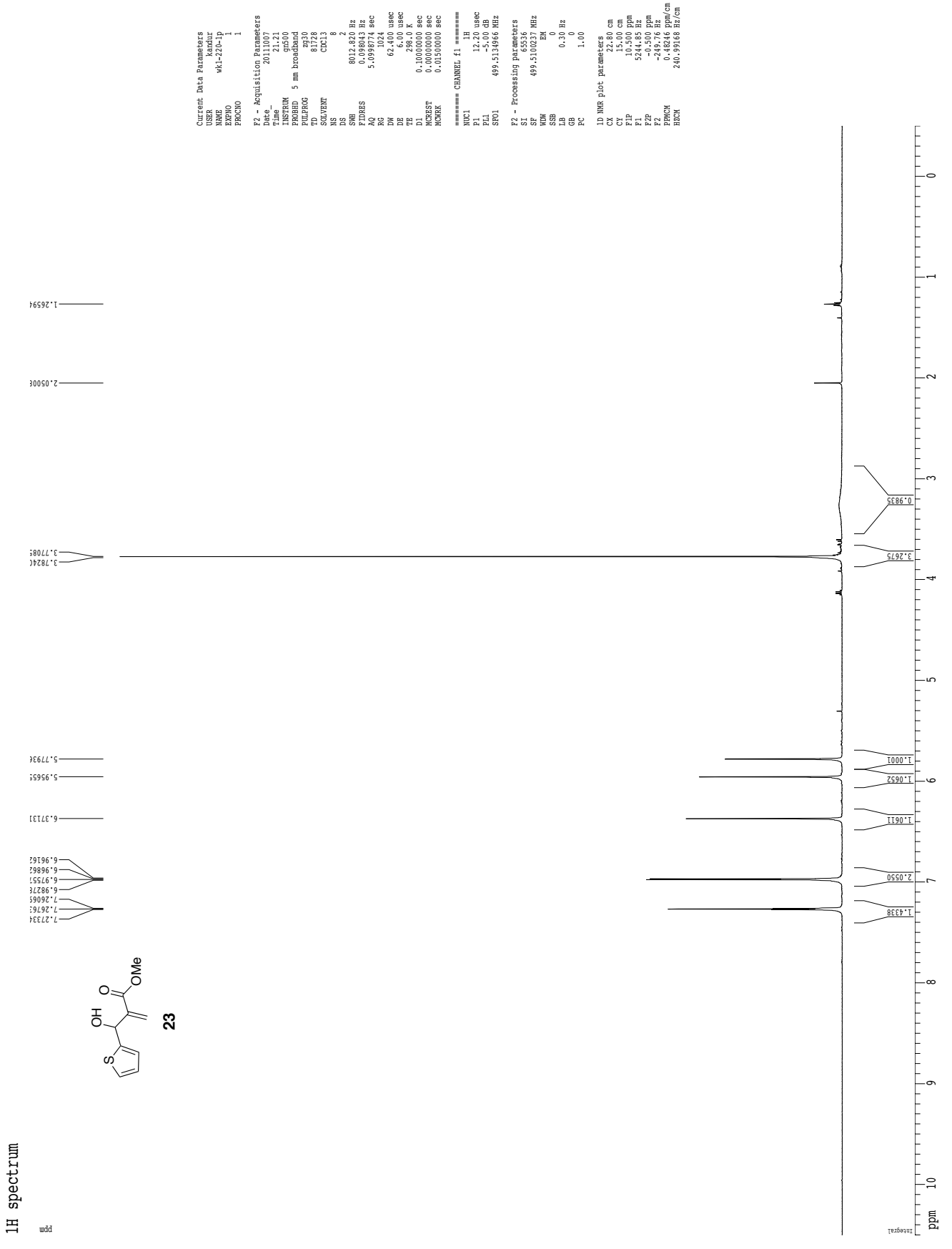

1H spectrum
Current Data Parameters
USER kandur
NAME wkl-201-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110731
Time_ 15.04
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 7.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200300 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 7.86 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.00002
1.25395
2.52644
2.54231
2.56331
2.64835
2.66891
2.68321
2.69788
2.93571
3.02506
3.03781
3.60686
3.84283
5.99417
6.00159
6.44724
6.45451
7.10275
7.11776
7.20895
7.22418
7.23942
7.26055
7.29140
7.30683
7.35381
1.7707
0.9860
0.9984
2.0650
3.5557
0.9976
1.0261
3.0000
1.0034
1.0116
1.0007
0.9779
1.0167
1.3154
integral
ppm
19
HO
O
O
HO
S
S
MeO

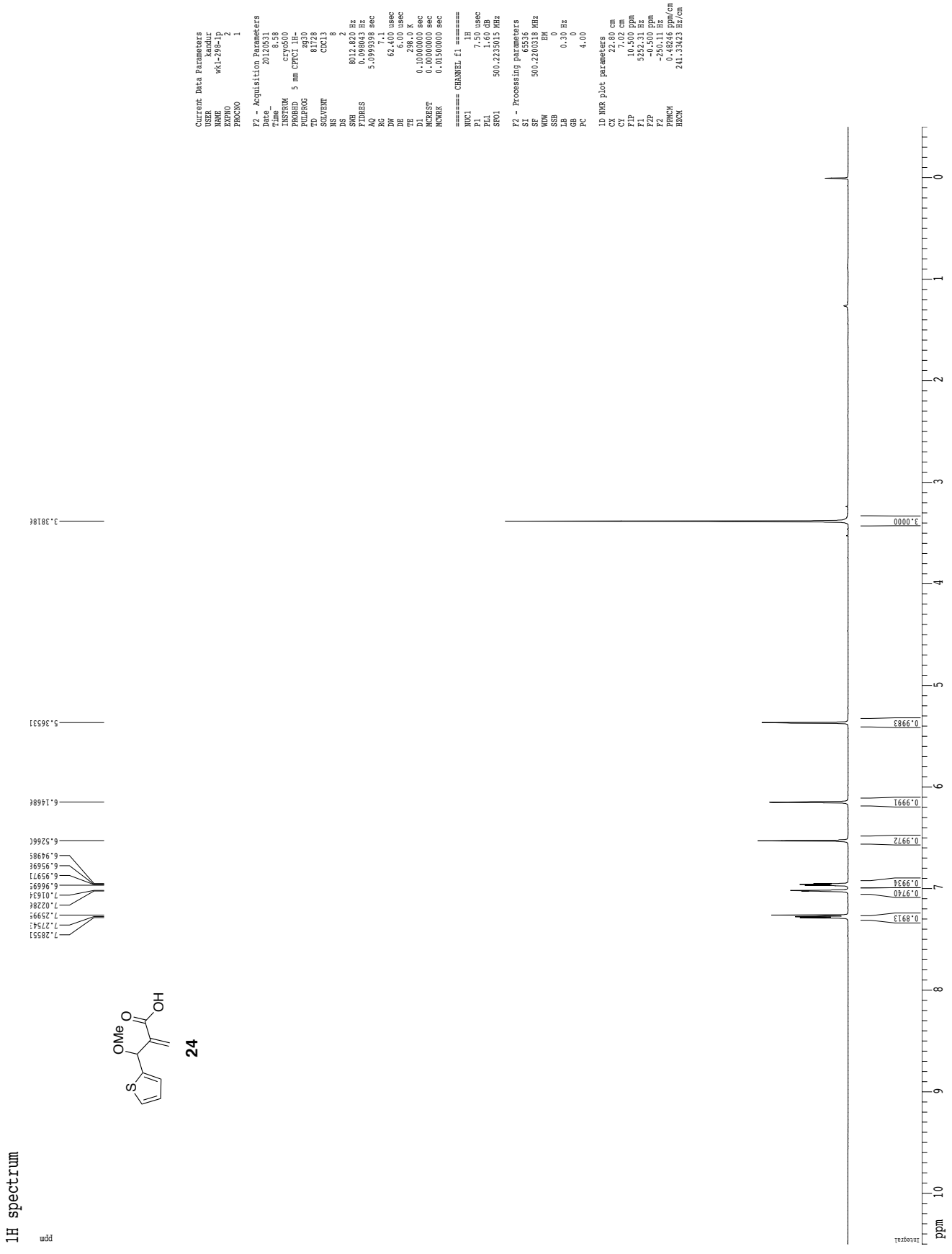

Z-restored spin-echo 13C spectrum with 1H decoupling
Current Data Parameters
USER kandur
NAME wk1-201-1p
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110731
Time 15.11
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 1024
DS 16
SWH 30303.031 Hz
FIDRES 0.462386 Hz
AQ 1.081394 sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00160000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7941248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7803988 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
0.21
30.58
35.57
35.98
39.40
46.70
60.39
76.97
77.23
77.48
103.29
124.09
126.47
128.19
129.37
131.78
133.56
133.68
141.25
165.44
177.57
178.94
ppm
0
20
40
60
80
100
120
140
160
180
ppm
O
HO
S
O
HO
S
MeO
19

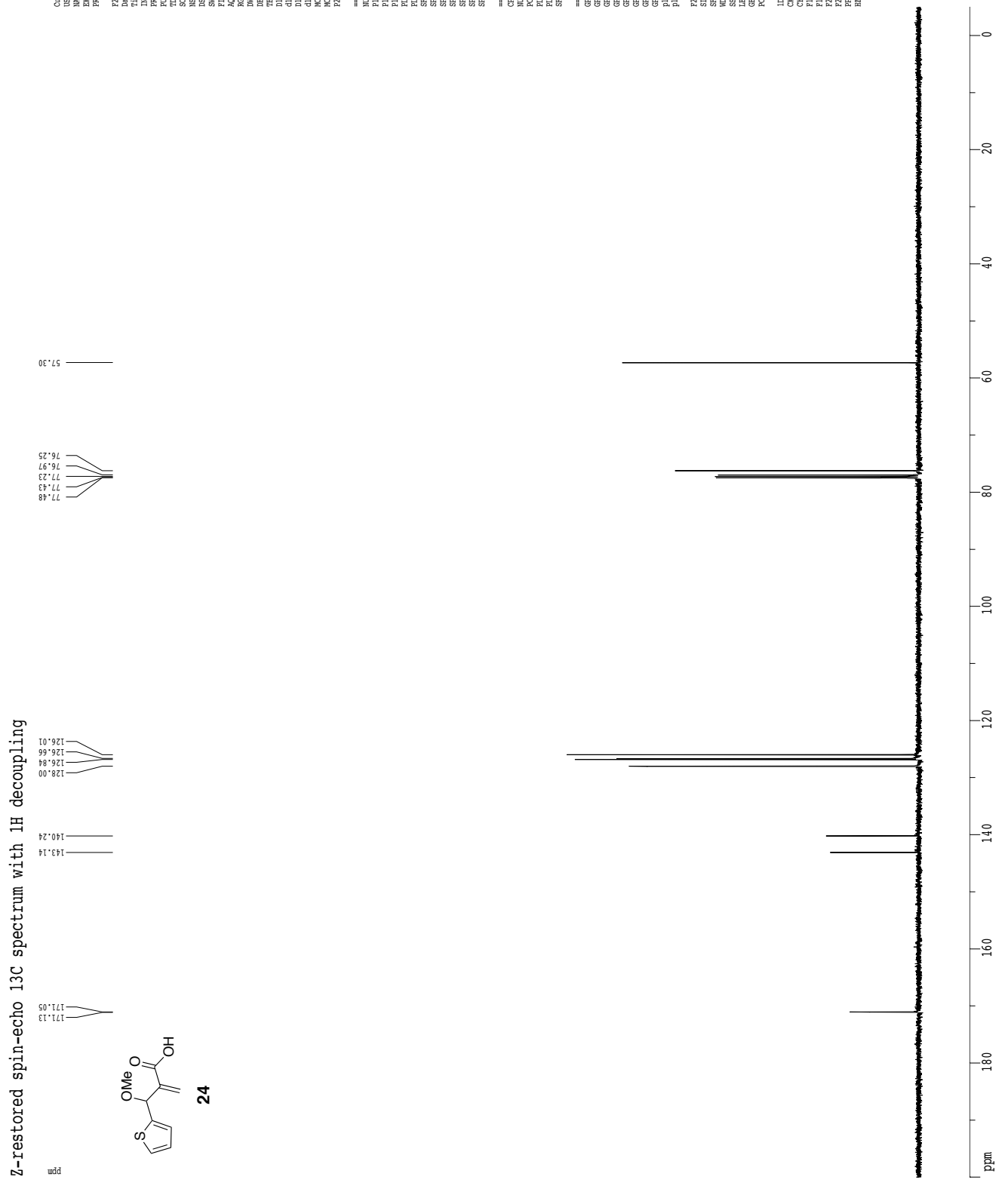

1H spectrum
Current Data Parameters
USER kandur
NAME wk1-202-1p
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110801
Time_ 12.39
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 7.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200318 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.95 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.06670
1.25124
2.76793
2.78664
2.80105
2.81471
2.83071
2.84471
2.87804
2.89682
2.91865
2.93322
2.94917
3.00656
3.02332
3.03394
3.04792
3.06195
3.07872
3.09194
3.10466
3.60356
3.61707
3.63065
3.85551
6.01313
6.02065
6.49955
6.50695
7.16994
7.18503
7.25864
7.25995
7.26776
7.28296
7.29822
7.35762
7.38337
7.39871
7.44776
15.040
2.145
4.239
1.100
1.062
2.960
1.012
1.000
0.239
1.013
1.211
1.531
1.058
integral
ppm
NHS
O
S
NHS
O
S
MeO
20

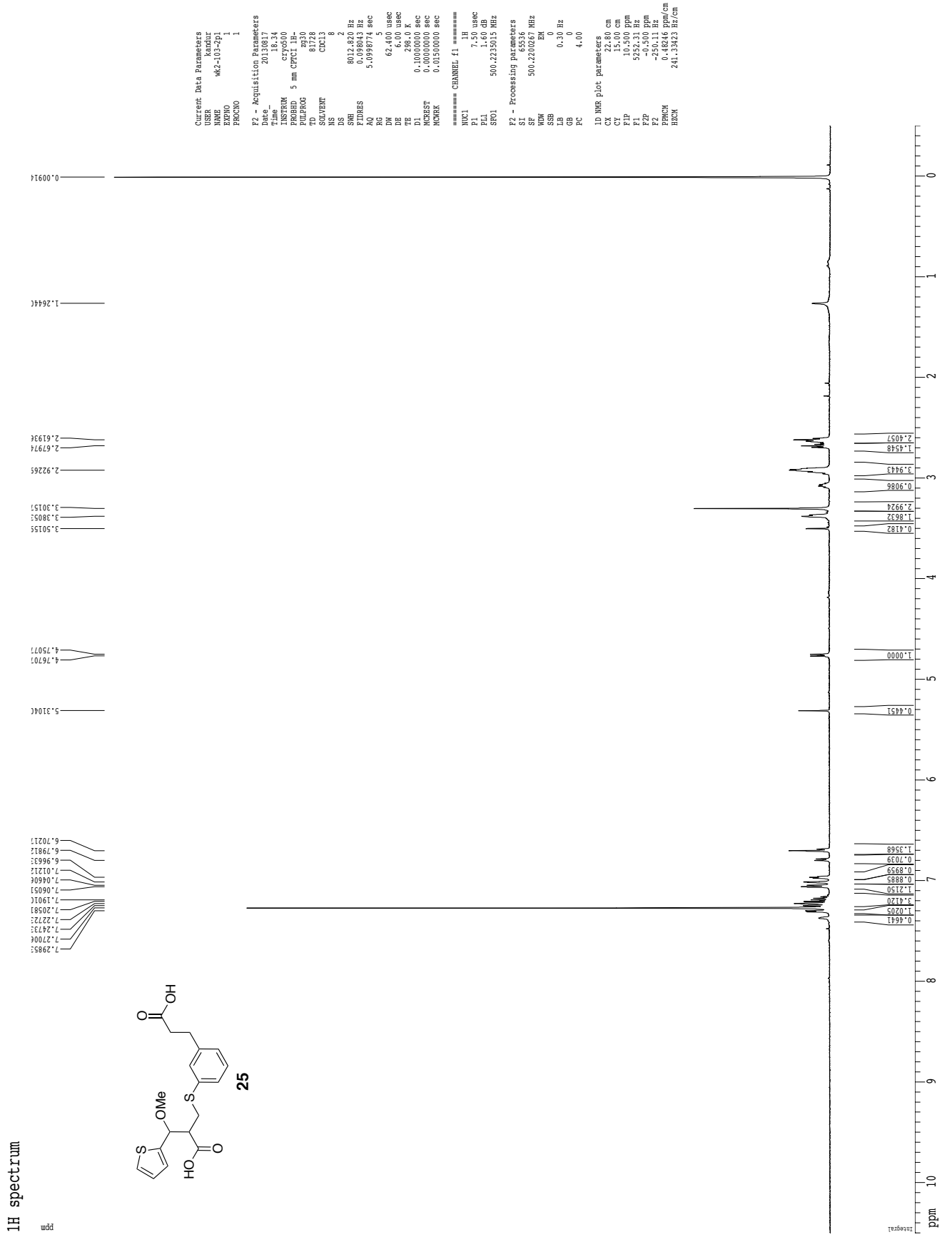
Z-restored spin-echo 13C spectrum with 1H decoupling



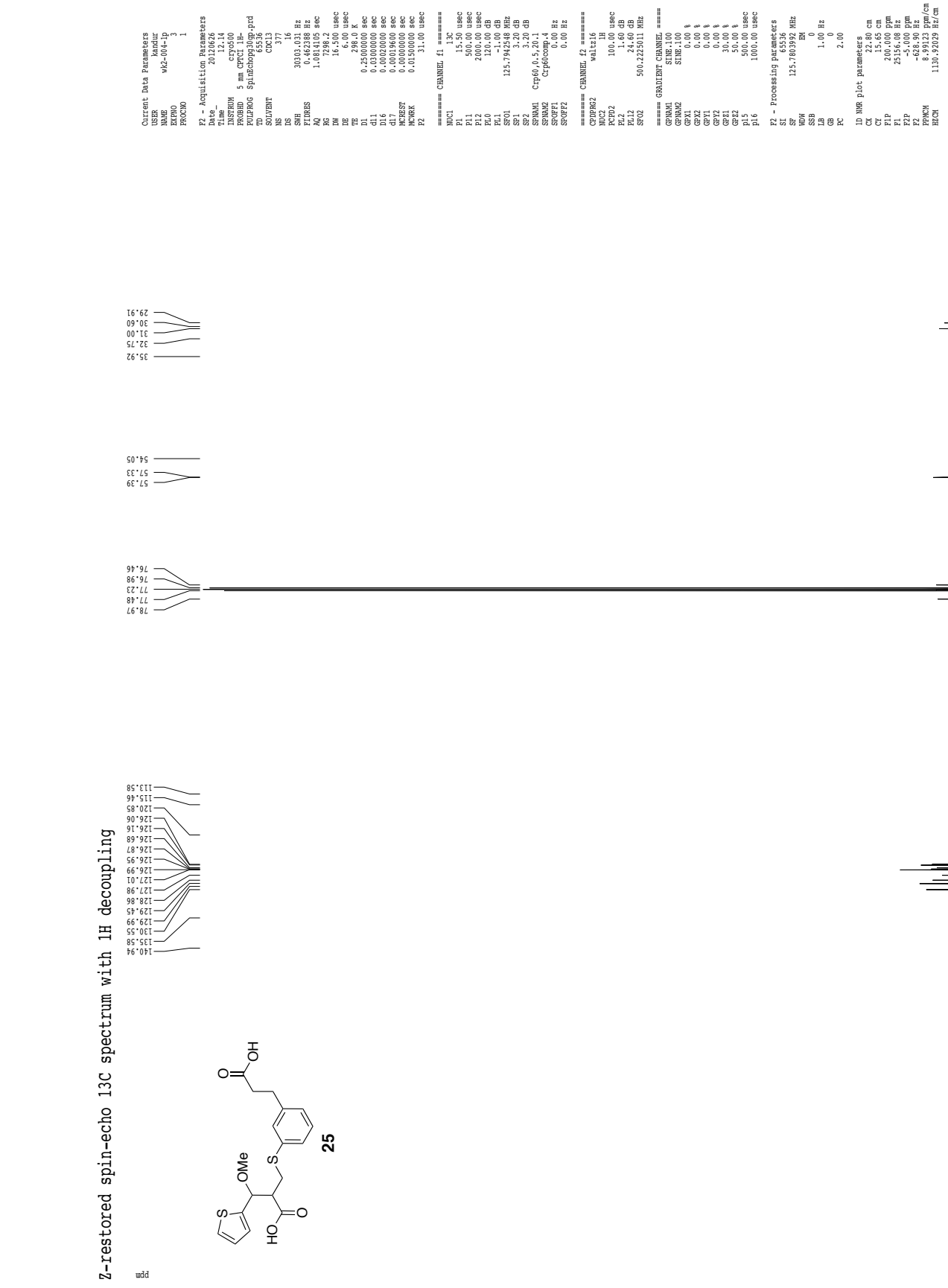

1H spectrum
Current Data Parameters
USER kandur
NAME wk1-220-1p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111007
Time_ 21.21
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 1024
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.5134966 MHz
F2 - Processing parameters
SI 65536
SF 499.5100237 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.500 ppm
F1 5244.65 Hz
F2P -0.500 ppm
F2 -249.76 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.99168 Hz/cm
1.26594
2.05006
3.76244
3.77085
5.77934
5.95659
6.37131
6.96162
6.98862
6.97551
6.98276
7.26065
7.26763
7.27334
0.9835
3.2675
1.0001
1.0652
1.0611
2.0550
1.4338
integral
ppm
OH
O
OMe
S
23

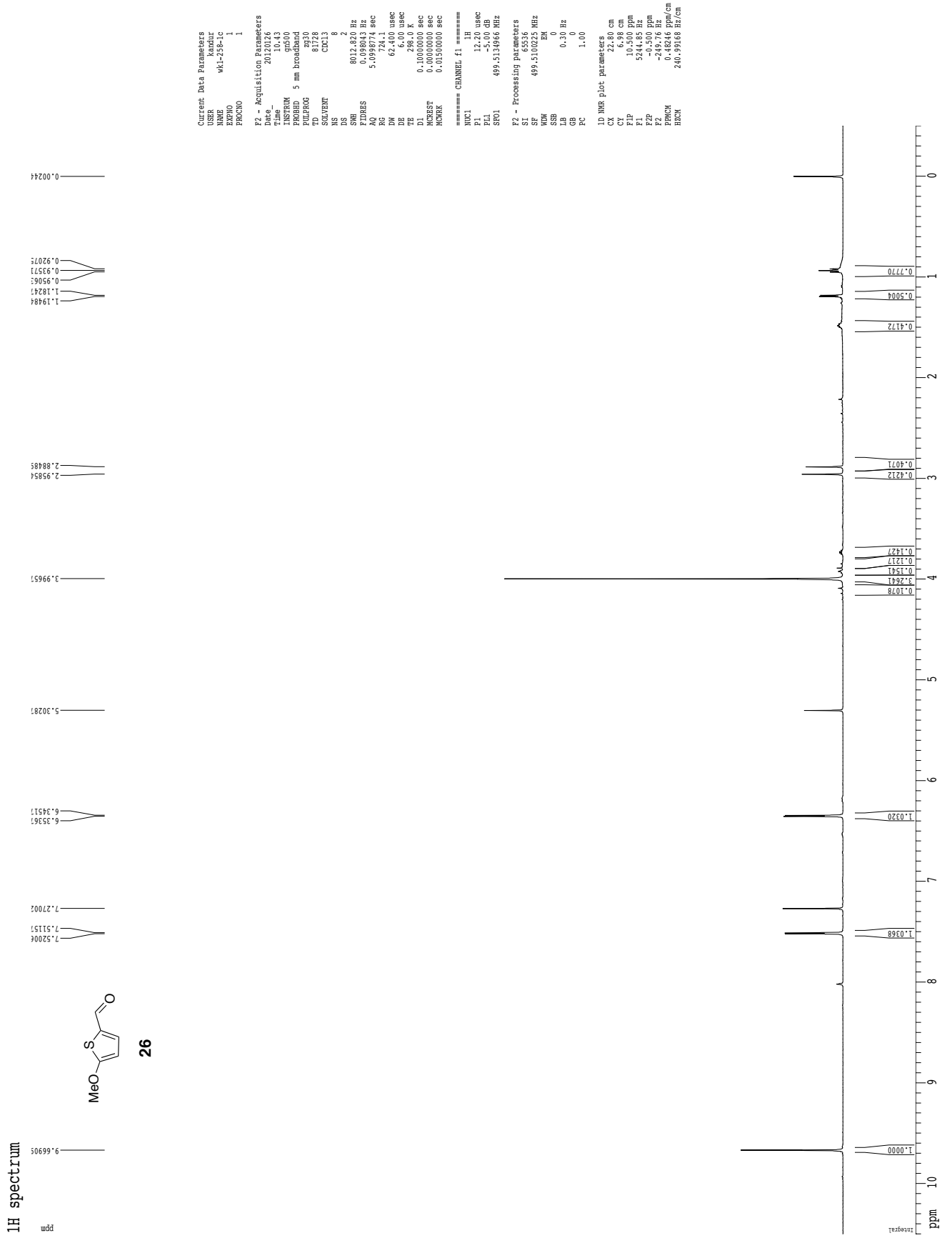

1H spectrum
ppm
Current Data Parameters
USER kandur
NAME wk1-298-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time_ 8.58
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 7.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200318 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 7.02 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
7.2855
7.2754
7.2599
7.0228
7.0163
6.9669
6.9597
6.9498
6.5266
6.1468
5.3653
3.8188
integral
0.8913
0.9740
0.9934
0.9972
0.9991
0.9983
3.0000
OMe
O
OH
S
24

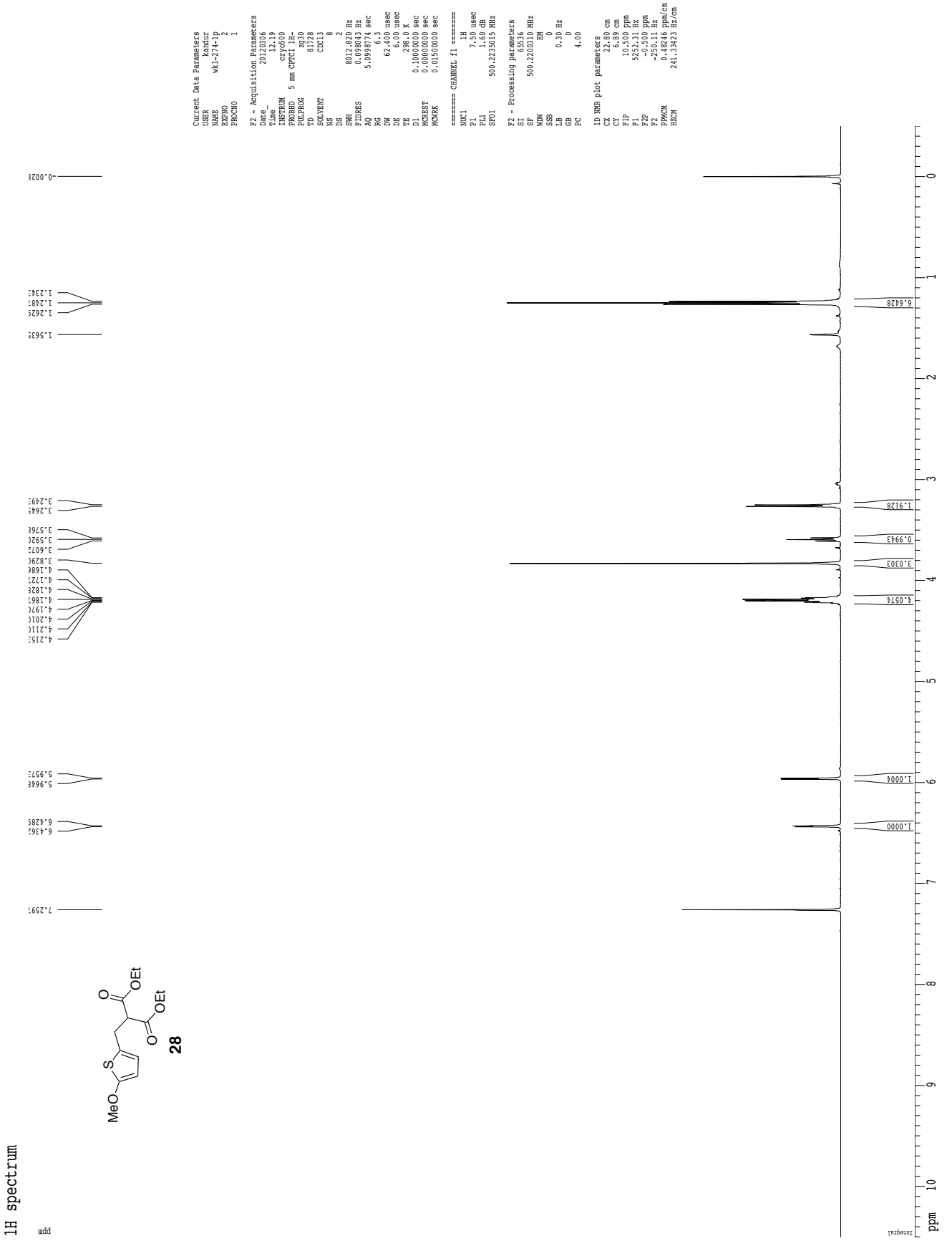

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
171.13
171.05
143.14
140.24
128.00
126.84
126.66
126.01
77.48
77.43
77.23
76.97
76.25
57.30
OMe
O
OH
S
24
Current Data Parameters
USER kandur
NAME wk1-296-1p
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120531
Time_ 9.01
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 135
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0814105 sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00001600 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7794248 MHz
SP1 3.20 dB
SP2 3.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7804020 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 6.85 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
0
20
40
60
80
100
120
140
160
180
ppm


1H spectrum
Current Data Parameters
USER kandur
NAME wk2-103-2p1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130817
Time_ 18.34
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200267 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.00914
1.26446
2.61934
2.61974
2.92265
3.30157
3.38053
3.50155
4.75071
4.76701
5.31046
6.70217
6.79812
6.96631
7.01211
7.04606
7.06051
7.19011
7.20581
7.22723
7.24731
7.27006
7.29853
2.40571
1.45481
3.94431
0.90861
2.99241
1.86321
0.41821
1.00001
0.44511
1.35681
0.70391
0.89591
0.88851
1.21501
3.41201
1.02051
0.46411
O
OH
S
OMe
S
HO
O
25
integral
ppm
0
1
2
3
4
5
6
7
8
9
10

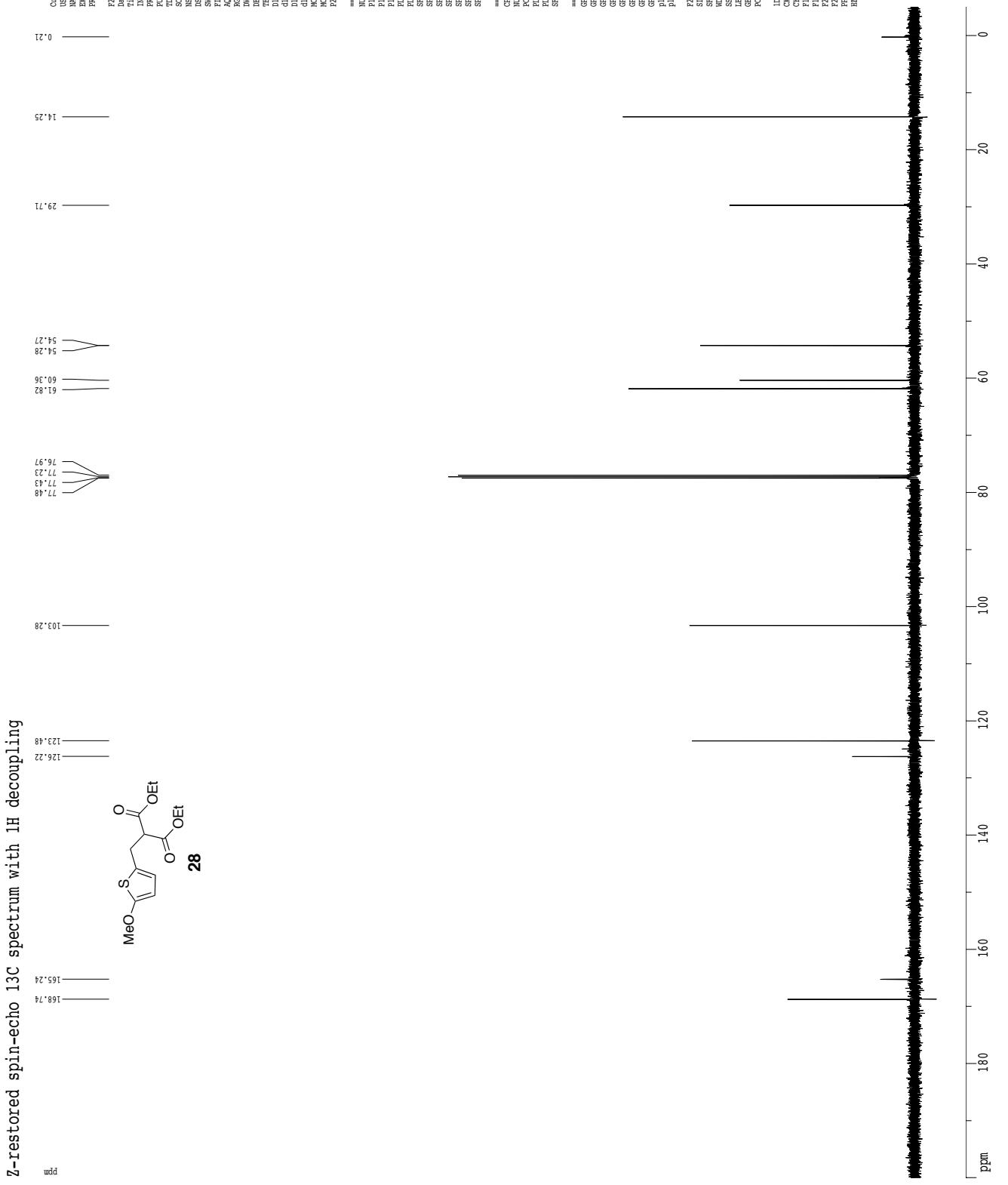
Z-restored spin-echo 13C spectrum with 1H decoupling

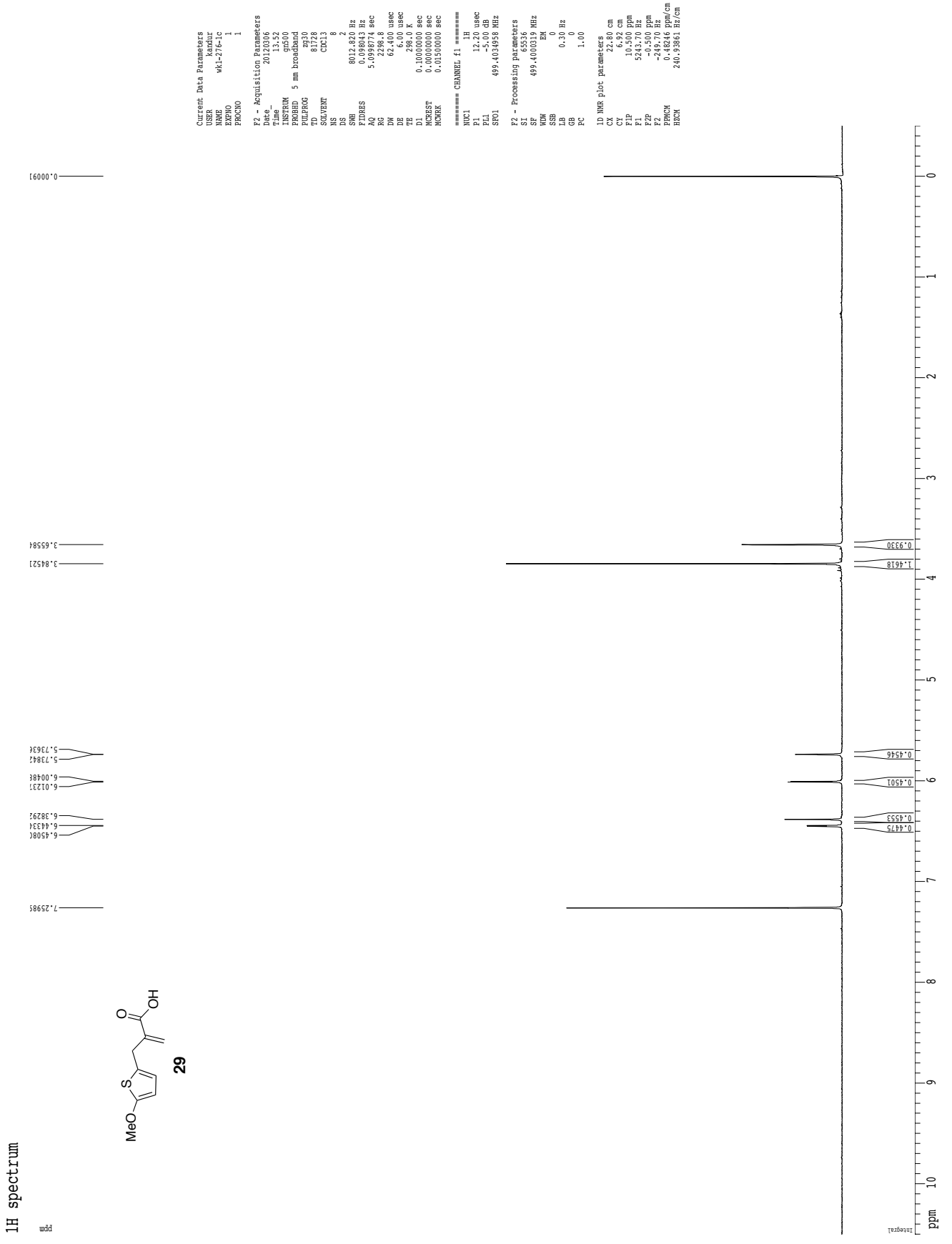



1H spectrum
ppm
integral
Current Data Parameters
USER Kandur
NAME wk1-256-1c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120126
Time_ 10.43
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 724.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.5134966 MHz
F2 - Processing parameters
SI 65536
SF 499.5100225 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 6.98 cm
F1P 10.500 ppm
F1 5244.65 Hz
F2P -0.500 ppm
F2 -249.76 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.99168 Hz/cm
9.66905
7.52006
7.51157
7.27002
6.35361
6.34517
5.30287
3.99657
2.98854
2.88485
1.94984
1.82471
0.95063
0.93571
0.92075
0.00244
1.0000
1.0368
1.0320
0.1078
3.2641
0.1541
0.1217
0.1427
0.4212
0.4071
0.4172
0.5004
0.7770
MeO
S
O
26

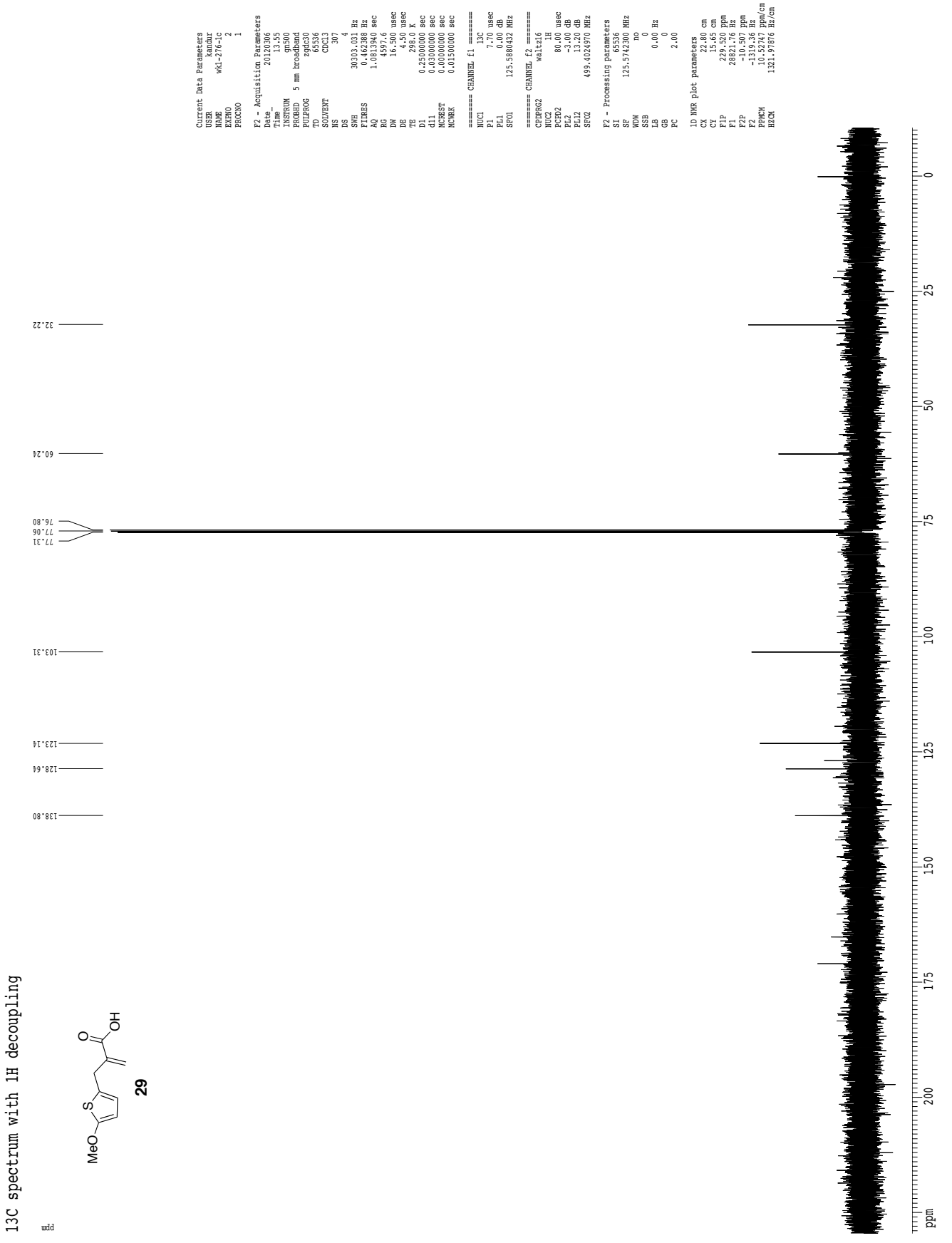

1H spectrum
ppm
Integral
Current Data Parameters
USER kandur
NAME wk1-274-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120306
Time_ 12.19
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 6.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200310 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.89 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
7.2597
6.4362
6.4285
5.9648
5.9572
4.2153
4.2114
4.2014
4.1970
4.1861
4.1826
4.1727
4.1688
3.8296
3.6072
3.5920
3.5766
3.2649
3.2491
1.5635
1.2673
1.2481
1.2341
-0.0026
6.4428
1.9128
0.9943
3.0303
4.0574
1.0004
1.0000
MeO
S
O
OEt
O
OEt
28

Z-restored spin-echo 13C spectrum with 1H decoupling

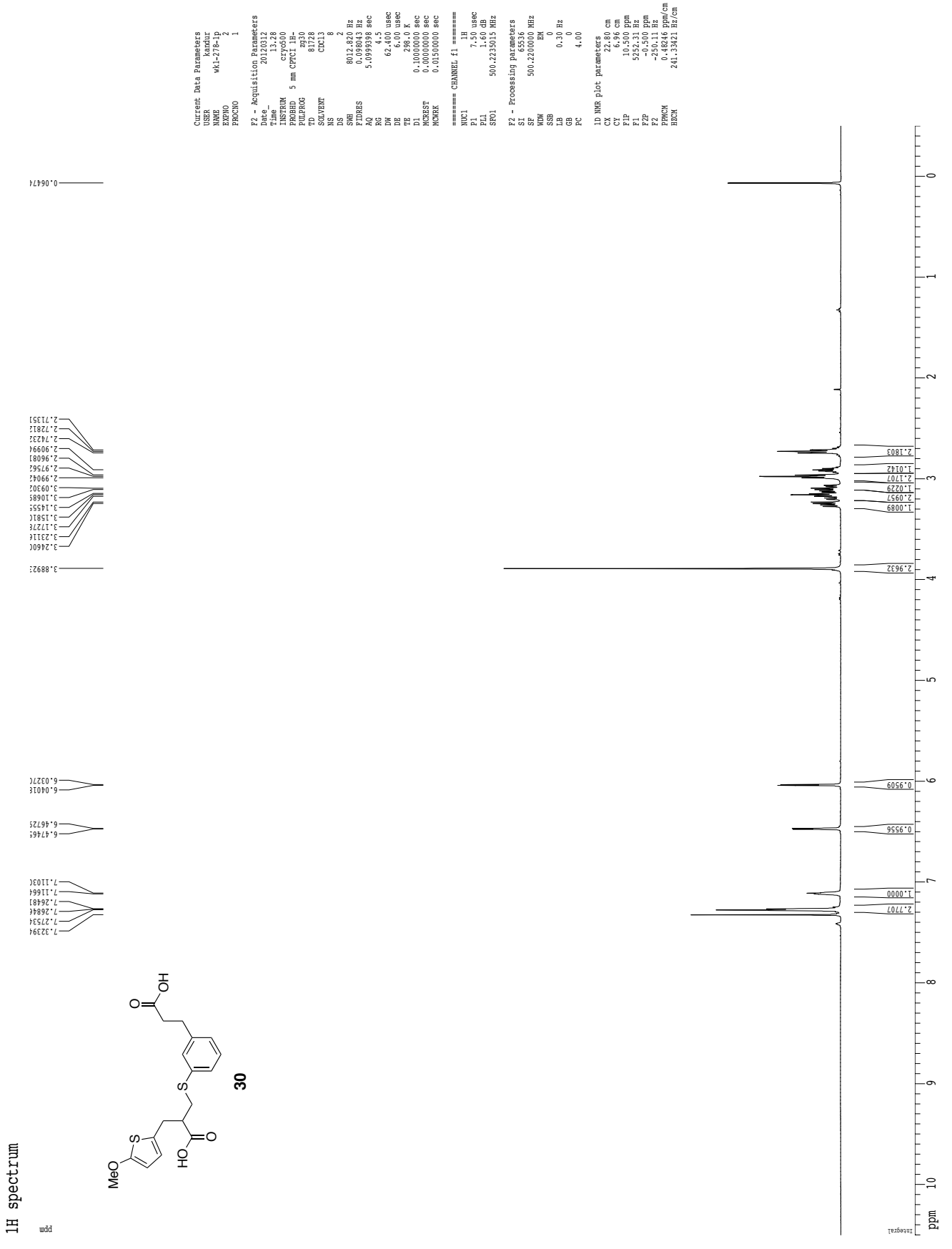


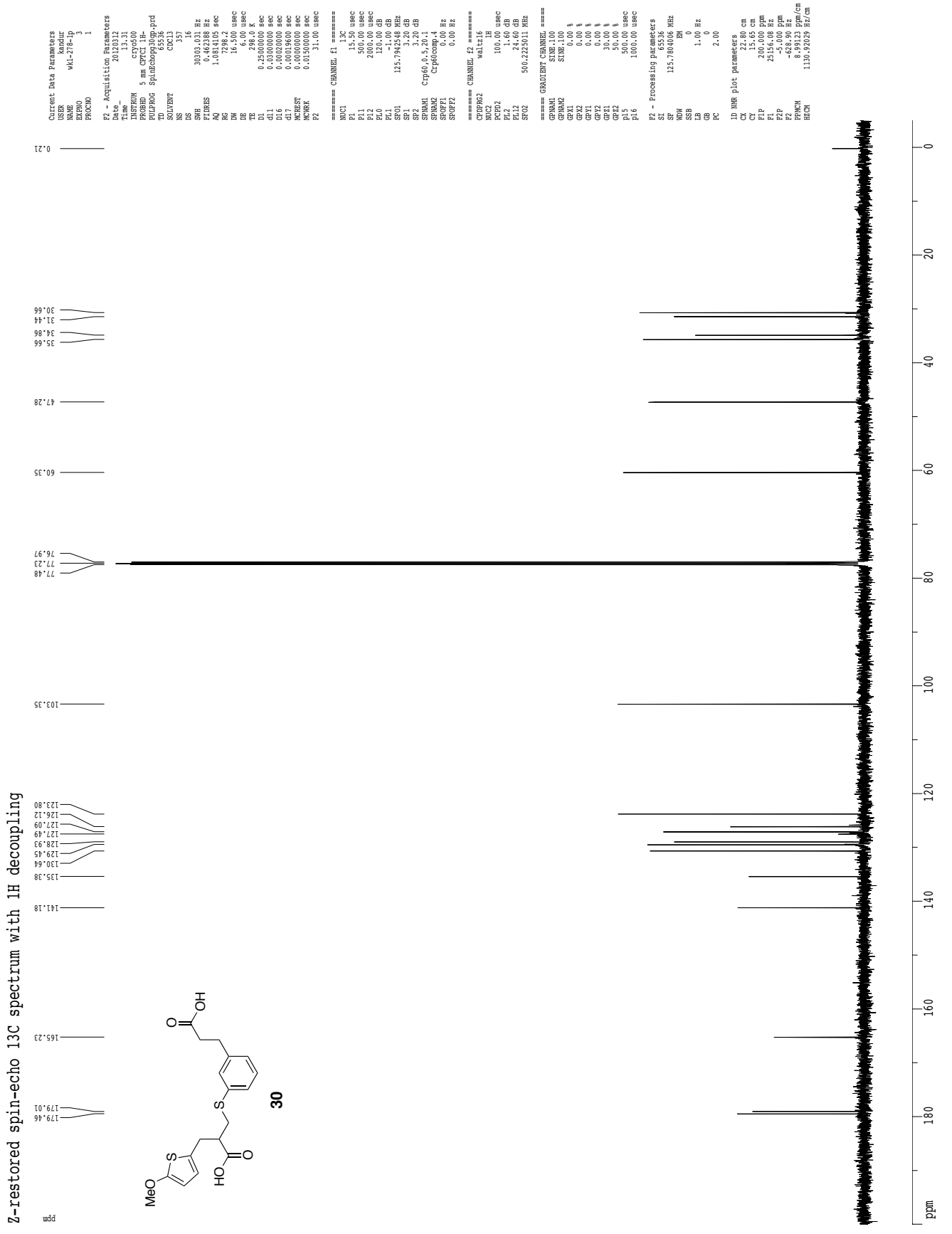

Current Data Parameters
USER Kandur
NAME wk1-276-1c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120306
Time_ 13.52
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 2298.8
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.4034958 MHz
F2 - Processing parameters
SI 65536
SF 499.4000319 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 6.92 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.500 ppm
F2 -249.70 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.93861 Hz/cm
0.00091
3.65584
3.84521
7.25985
6.45086
6.44334
6.38292
6.01237
6.00488
5.78842
5.76364
0.9330
1.4618
0.4546
0.4501
0.4553
0.4475
ppm
integral
1H spectrum
ppm
MeO
S
O
OH
29

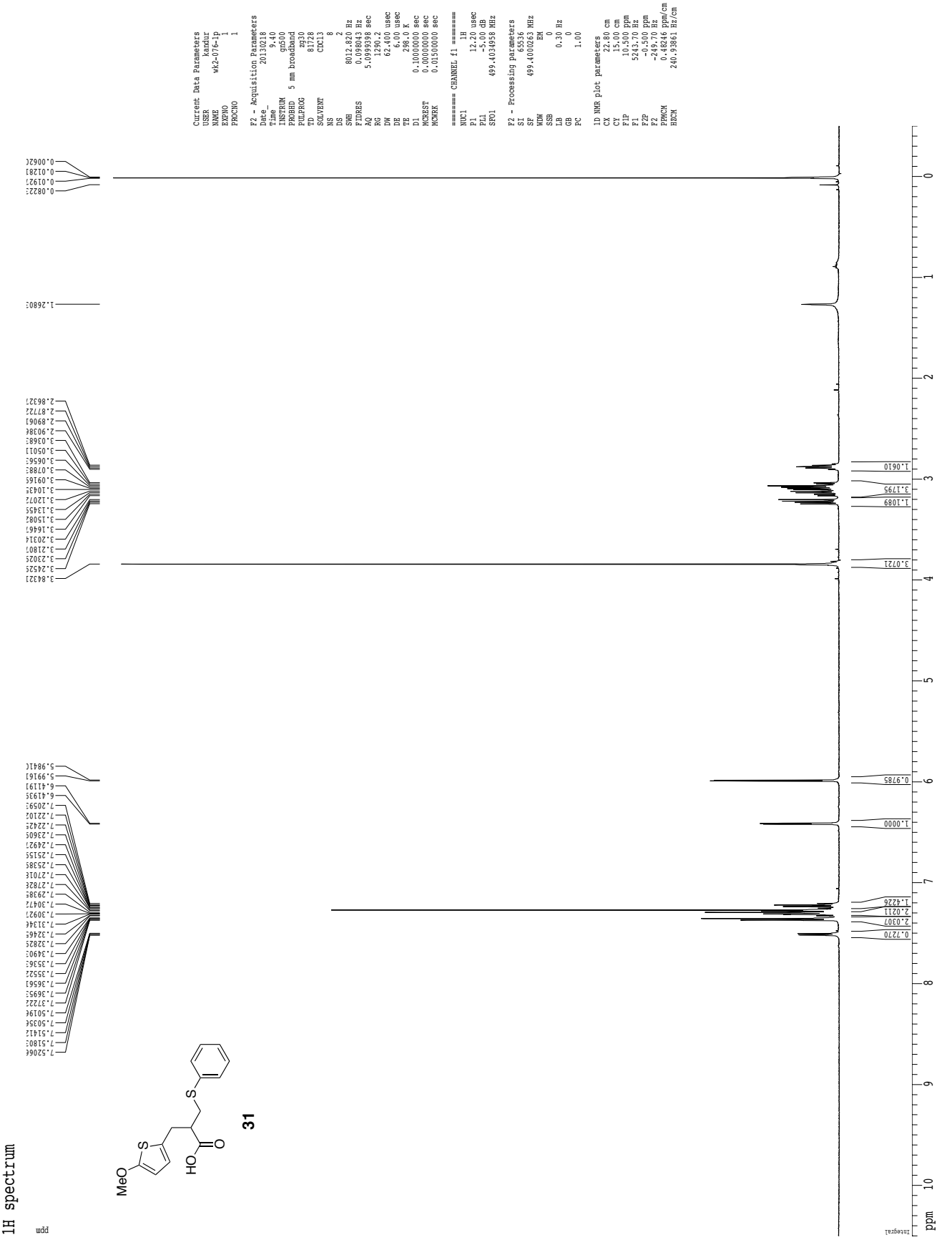
13C spectrum with 1H decoupling

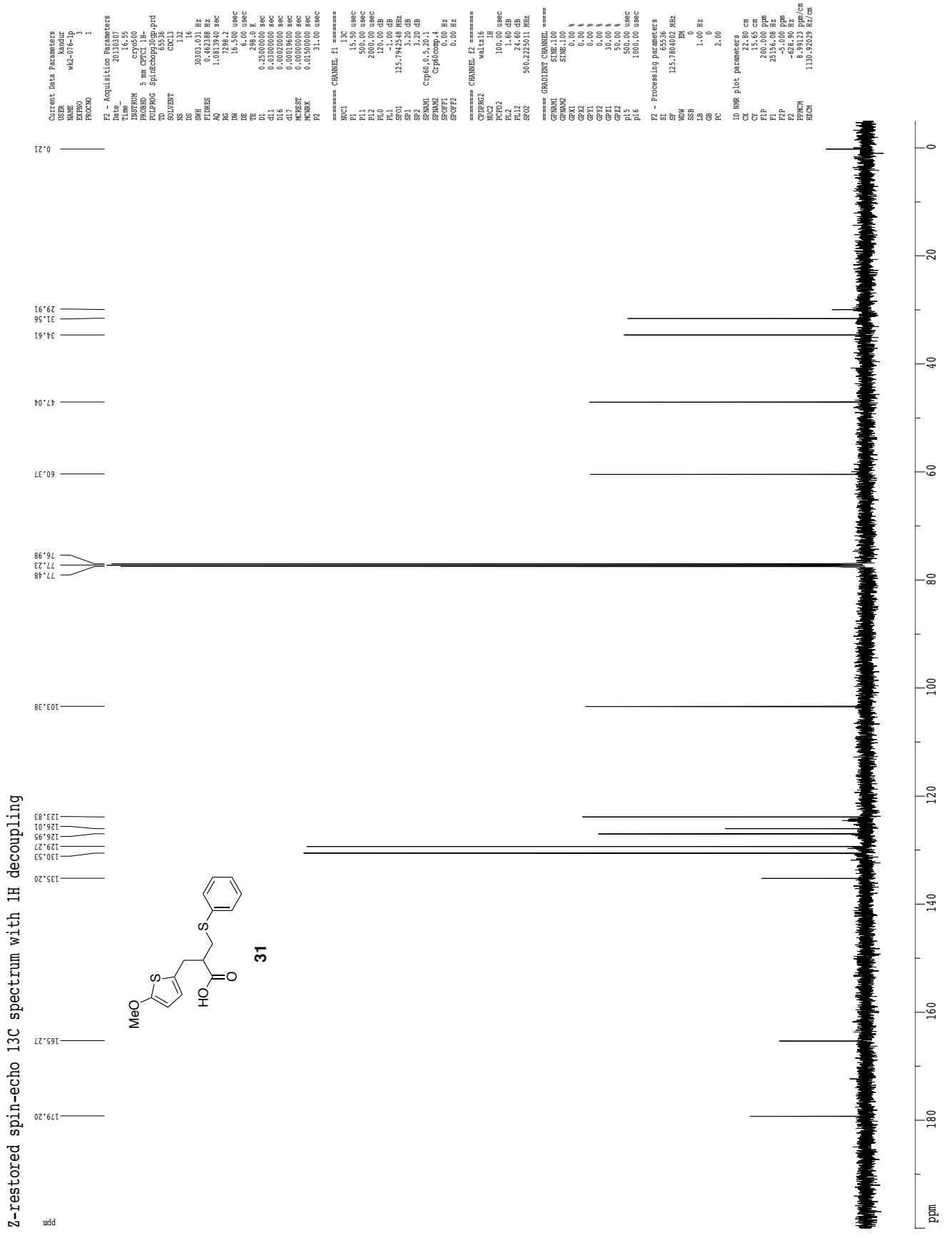


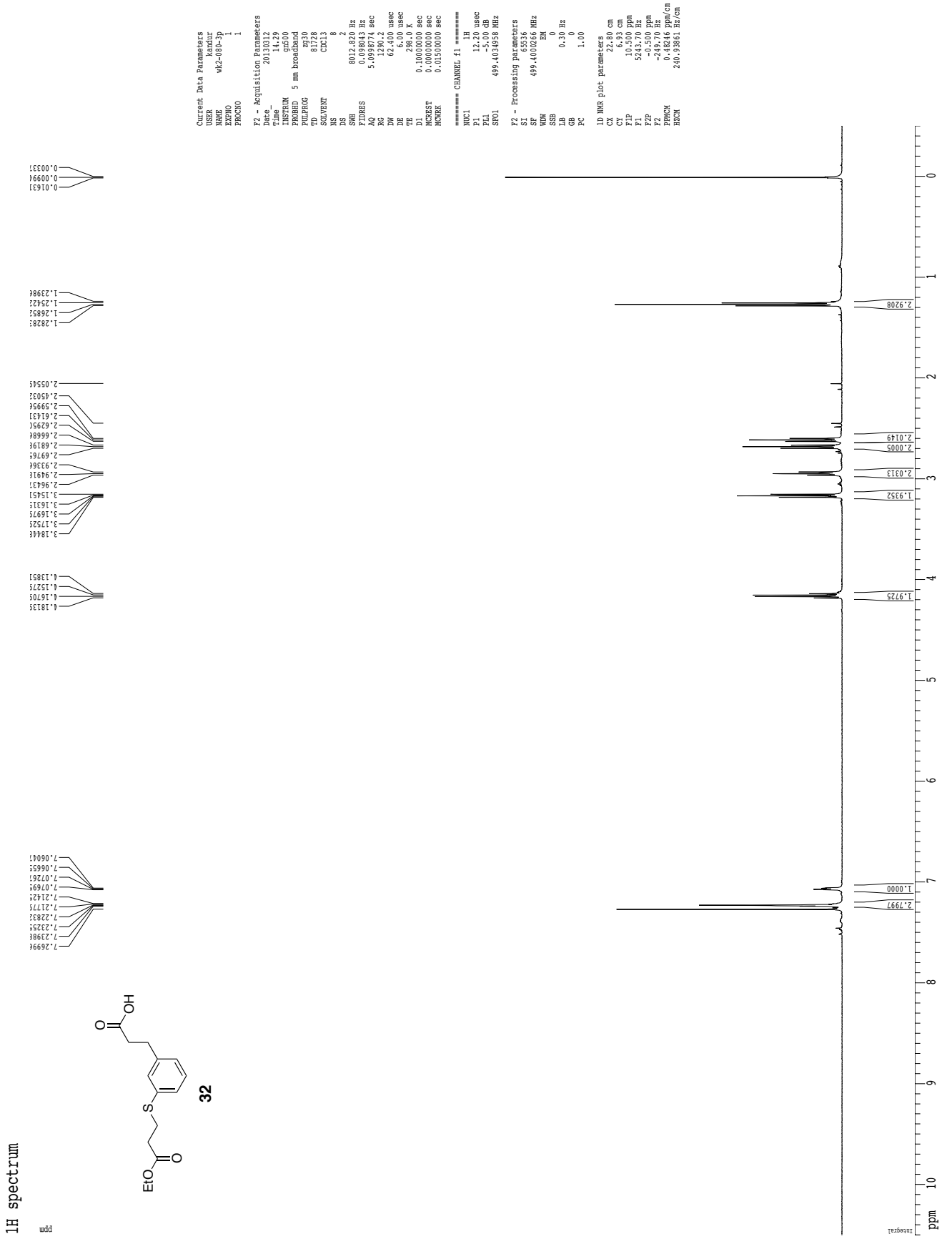
29

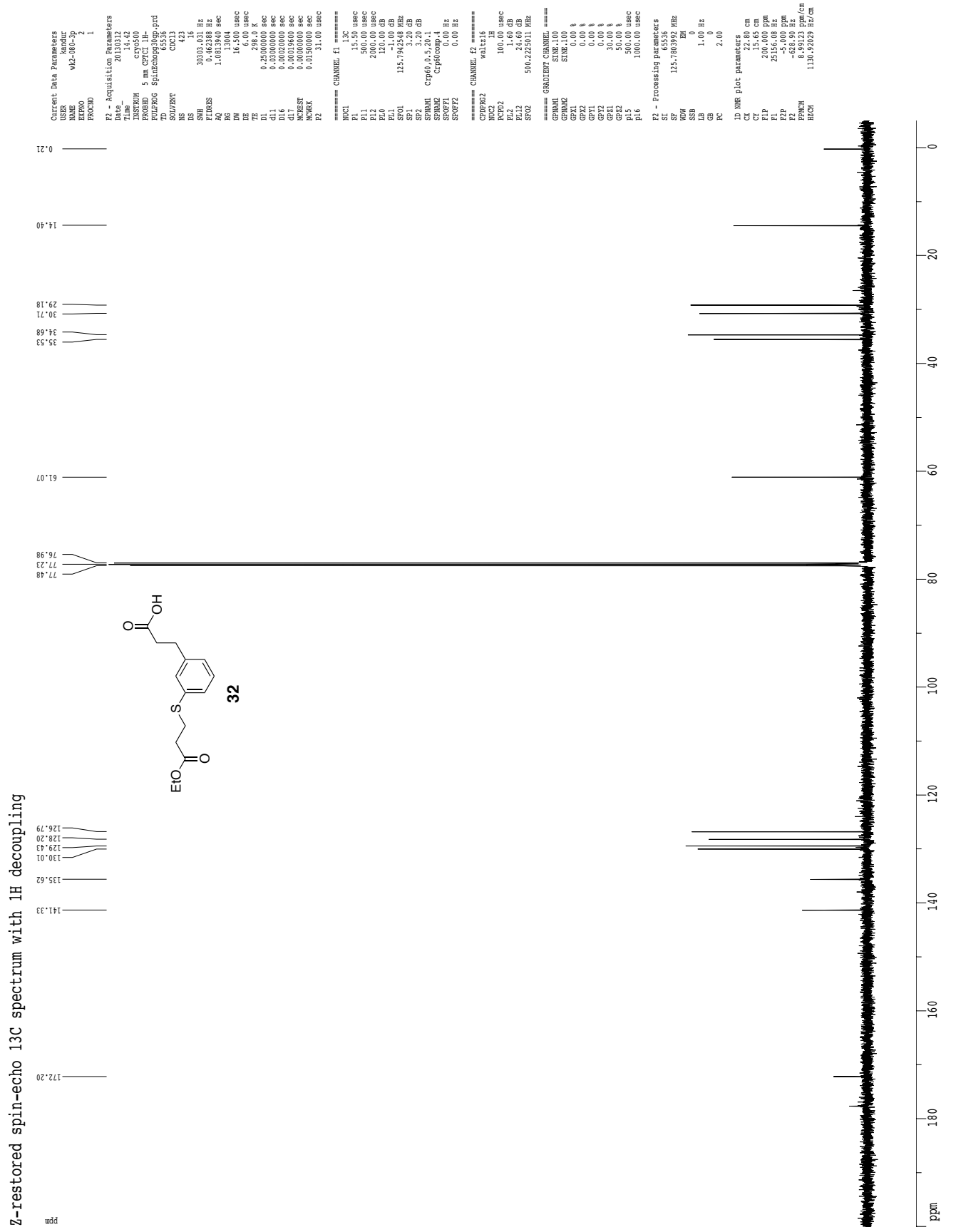

1H spectrum
Current Data Parameters
USER kandur
NAME wk1-278-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120312
Time_ 13.28
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 4.5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.96 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33421 Hz/cm
0.06474
2.71351
2.72812
2.74232
2.90994
2.96083
2.97562
2.99042
3.09302
3.10685
3.14555
3.15811
3.17276
3.23114
3.24600
3.88923
6.03270
6.04018
6.46725
6.47465
7.11003
7.11664
7.26481
7.26846
7.27534
7.32394
0.95509
0.95556
1.00000
2.77077
2.96321
1.00895
2.09573
1.02293
2.11707
1.01842
2.18033
MeO
S
S
HO
O
O
OH
O
30
ppm
Integral

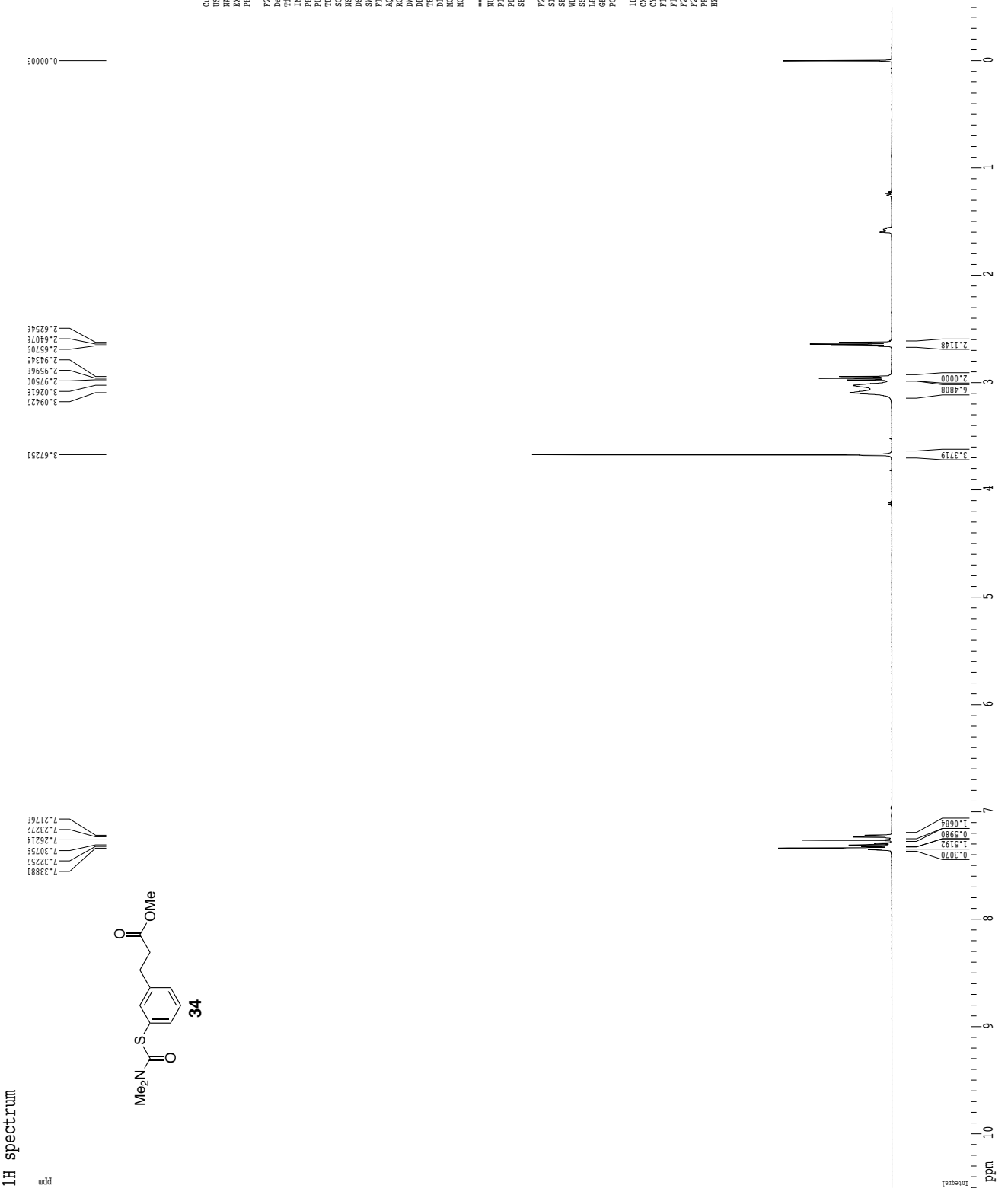

Z-restored spin-echo 13C spectrum with 1H decoupling
30
MeO
OH
HO
ppm

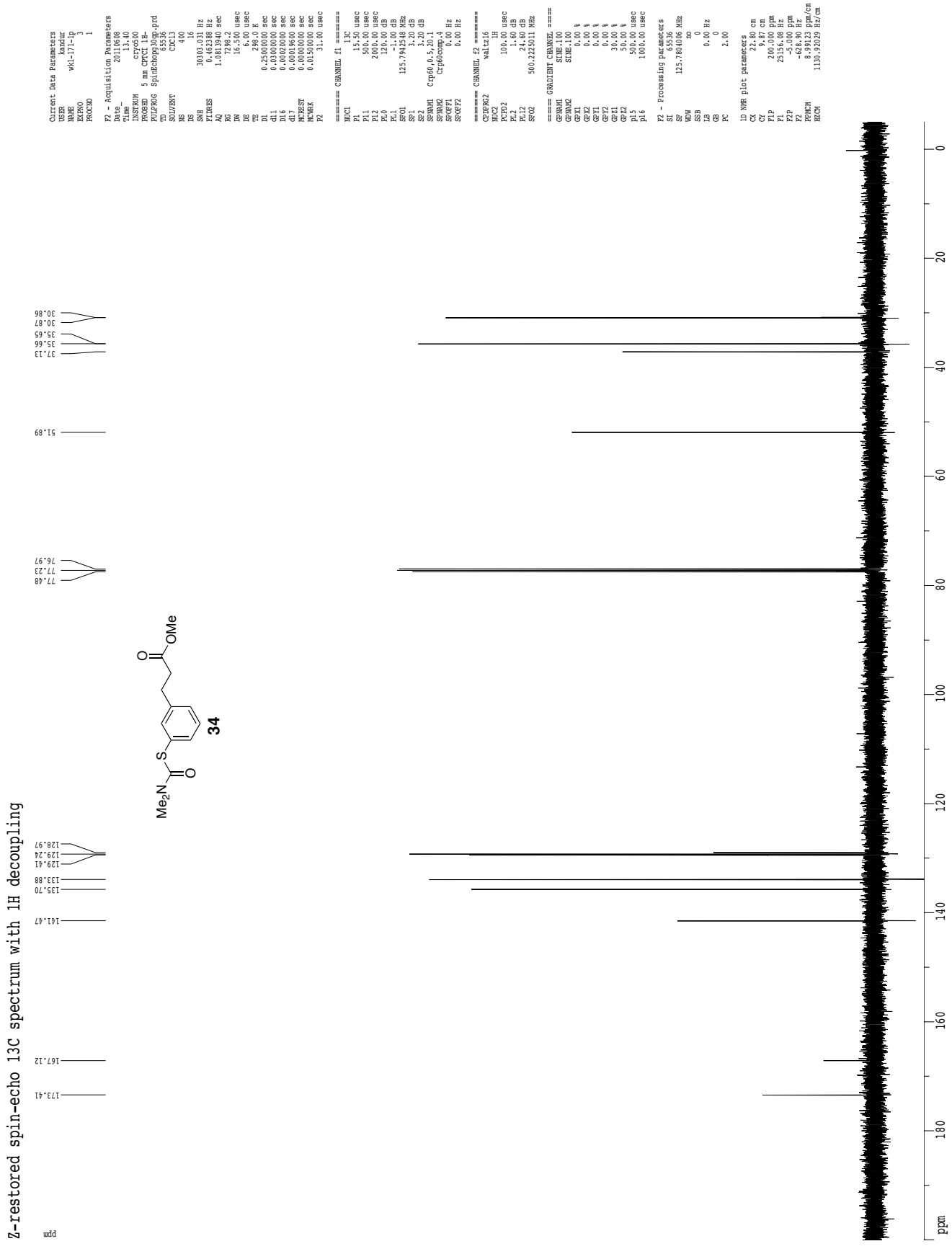

1H spectrum
Current Data Parameters
USER kandur
NAME wk2-076-1p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130218
Time_ 9.40
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 1290.2
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.4034958 MHz
F2 - Processing parameters
SI 65536
SF 499.4000263 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 15.00 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.500 ppm
F2 -249.70 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.93861 Hz/cm
MeO
S
S
HO
O
31
ppm
integral

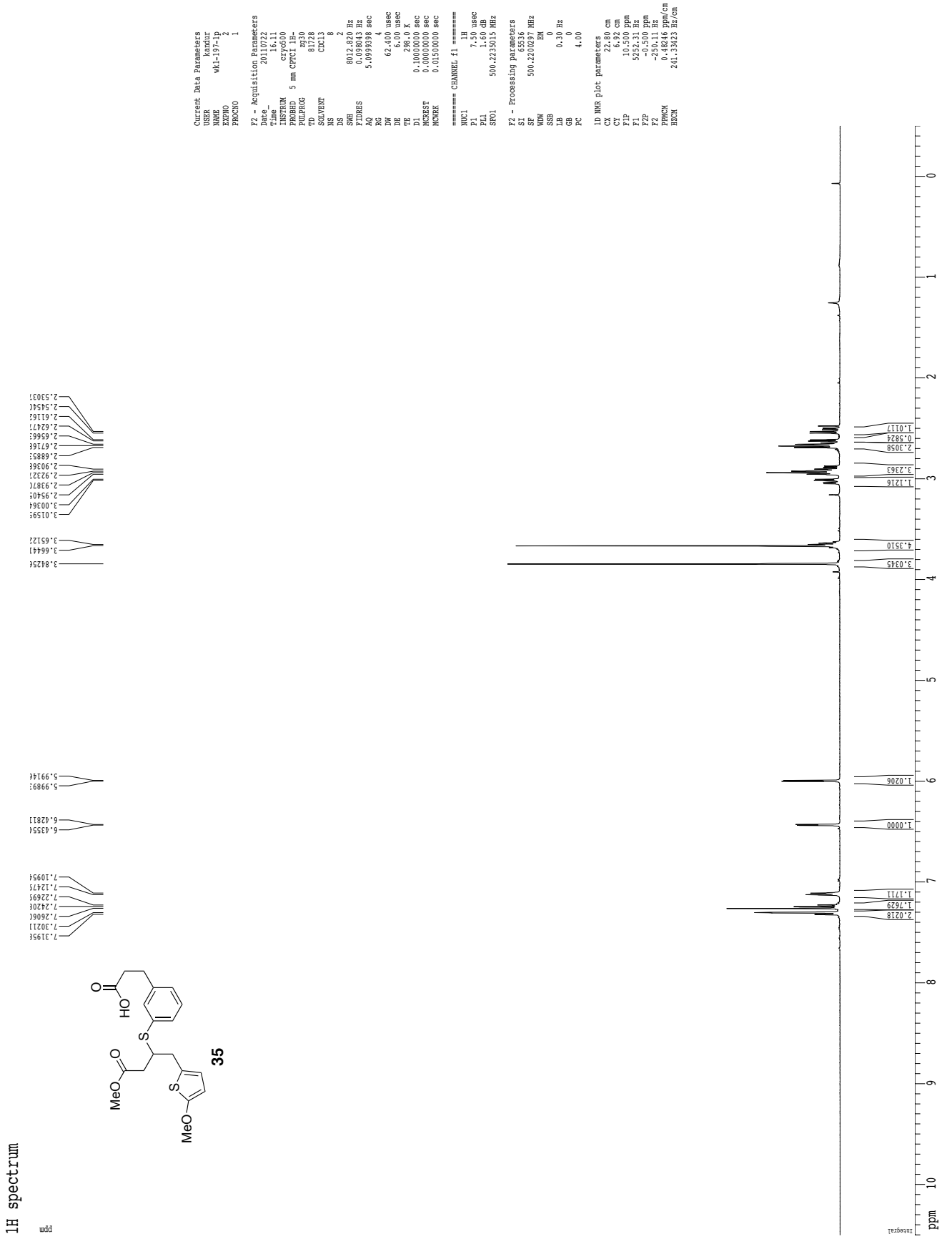

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
0.21
29.91
31.56
34.61
47.04
60.37
76.98
77.23
77.48
103.38
123.83
126.01
126.95
129.27
130.53
135.20
165.27
179.20
MeO
S
S
HO
O
31
ppm

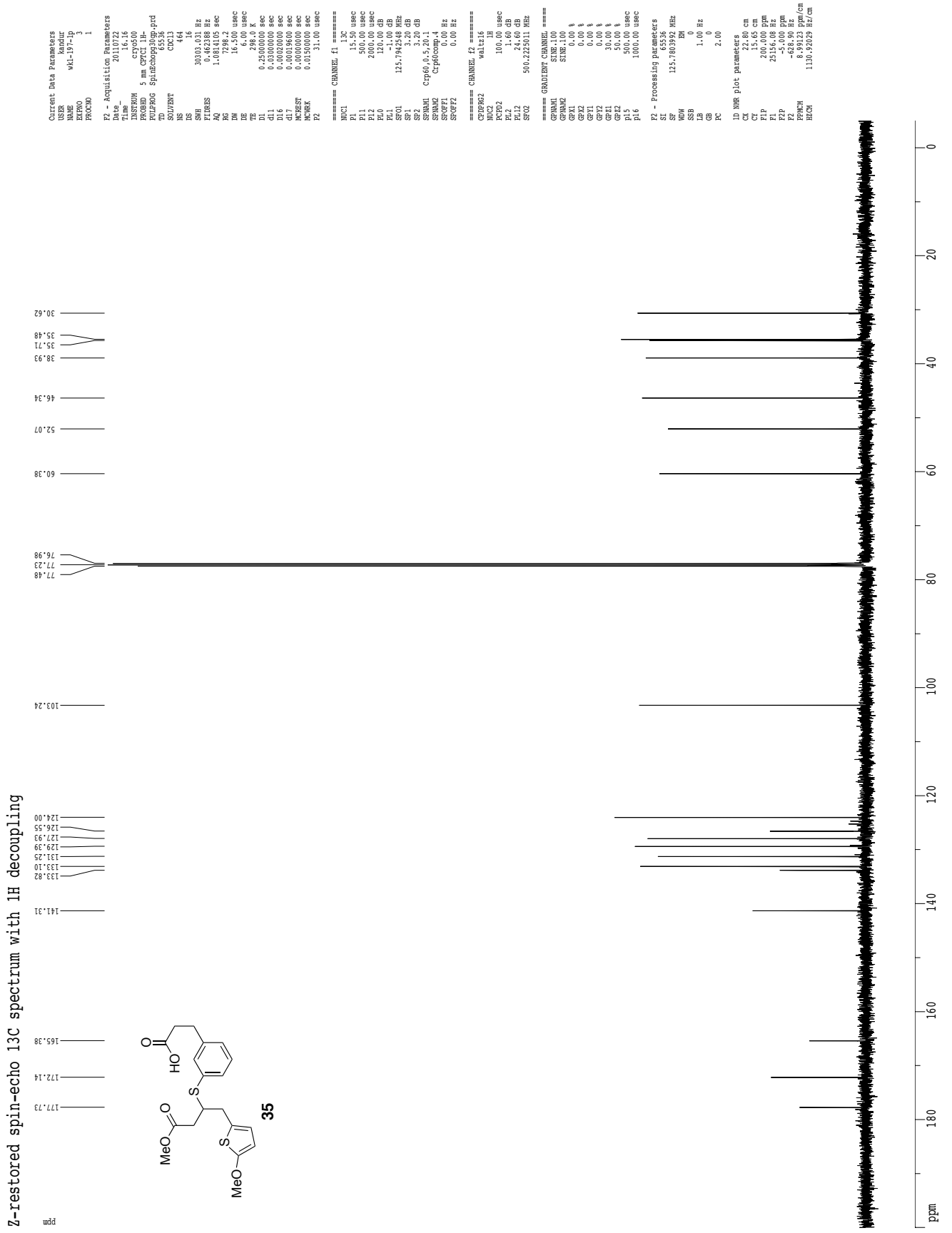

1H spectrum
ppm
integral
Current Data Parameters
USER kandur
NAME wk2-080-3p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130312
Time_ 14.29
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 1290.2
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.4034958 MHz
F2 - Processing parameters
SI 65536
SF 499.4000266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 6.93 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.500 ppm
F2 -249.70 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.93861 Hz/cm
0.0163
0.0099
0.0033
1.2398
1.2542
1.2685
1.2828
2.0554
2.4503
2.5996
2.6143
2.6296
2.6668
2.6819
2.6976
2.9336
2.9491
2.9643
3.1545
3.1631
3.1697
3.1752
3.1844
4.1385
4.1527
4.1670
4.1813
7.0604
7.0665
7.0726
7.0769
7.2142
7.2177
7.2283
7.2325
7.2398
7.2699
2.9208
2.0149
2.0005
2.0313
1.9352
1.9725
1.0000
2.7997
O
OH
S
O
EtO
O
32

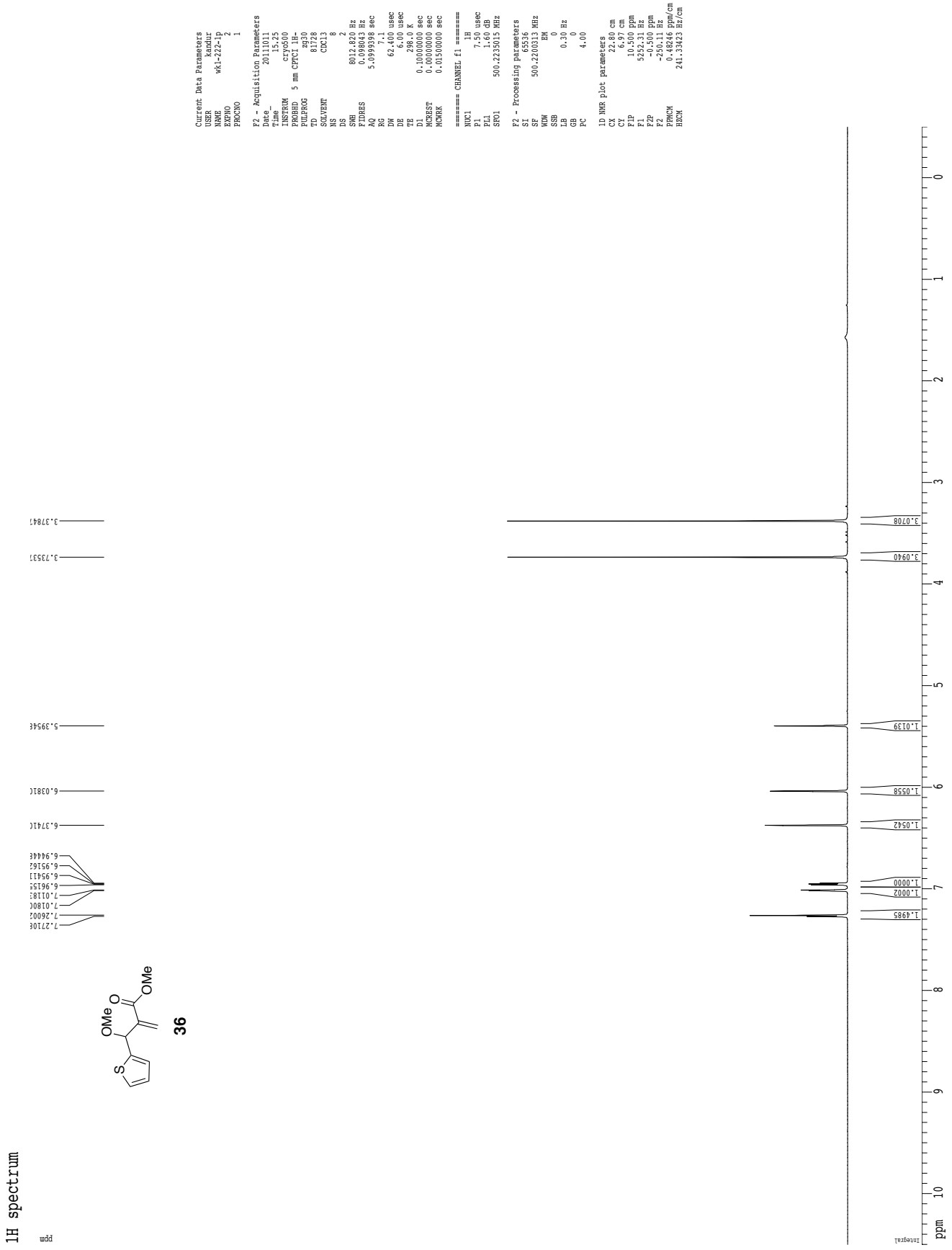

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
Current Data Parameters
USER kandur
NAME wk2-086-3p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130312
Time_ 14.42
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchopg30gp.prd
TD 65536
SOLVENT CDCl3
NS 423
DS 16
SWH 30303.031 Hz
FIDRES 0.462386 Hz
AQ 1.081940 sec
RG 13004
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00180000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7941248 MHz
SP1 3.20 dB
SP2 Crp60,0.5,20.1
SPNAM1 Crp60comp.4
SPNAM2
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7803992 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
0.21
14.40
29.18
30.71
34.68
35.53
61.07
76.98
77.23
77.48
126.79
128.20
129.43
130.01
135.62
141.33
172.20
EtO
O
S
O
OH
O
32
0
20
40
60
80
100
120
140
160
180
ppm

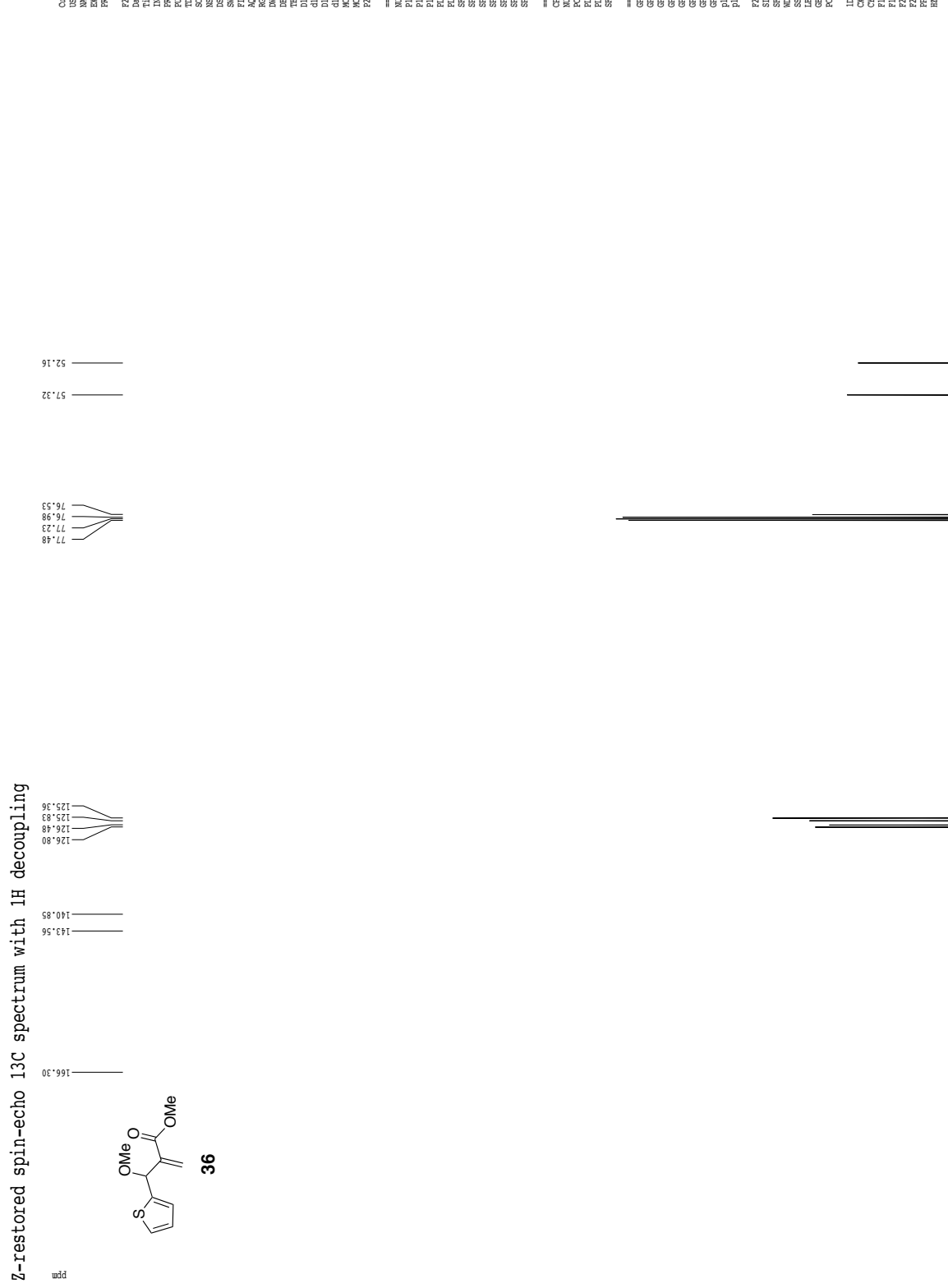

1H spectrum
ppm
integral
Current Data Parameters
USER kandur
NAME wk1-171-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110608
Time_ 13.33
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200313 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.97 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.00001
2.62946
2.64076
2.65705
2.94345
2.99566
2.97506
3.02618
3.09427
3.67251
7.21766
7.23272
7.26214
7.30755
7.32251
7.33881
2.1149
2.0000
6.4808
3.3719
1.0684
0.5980
1.5192
0.3070
O
OMe
S
O
Me2N
34

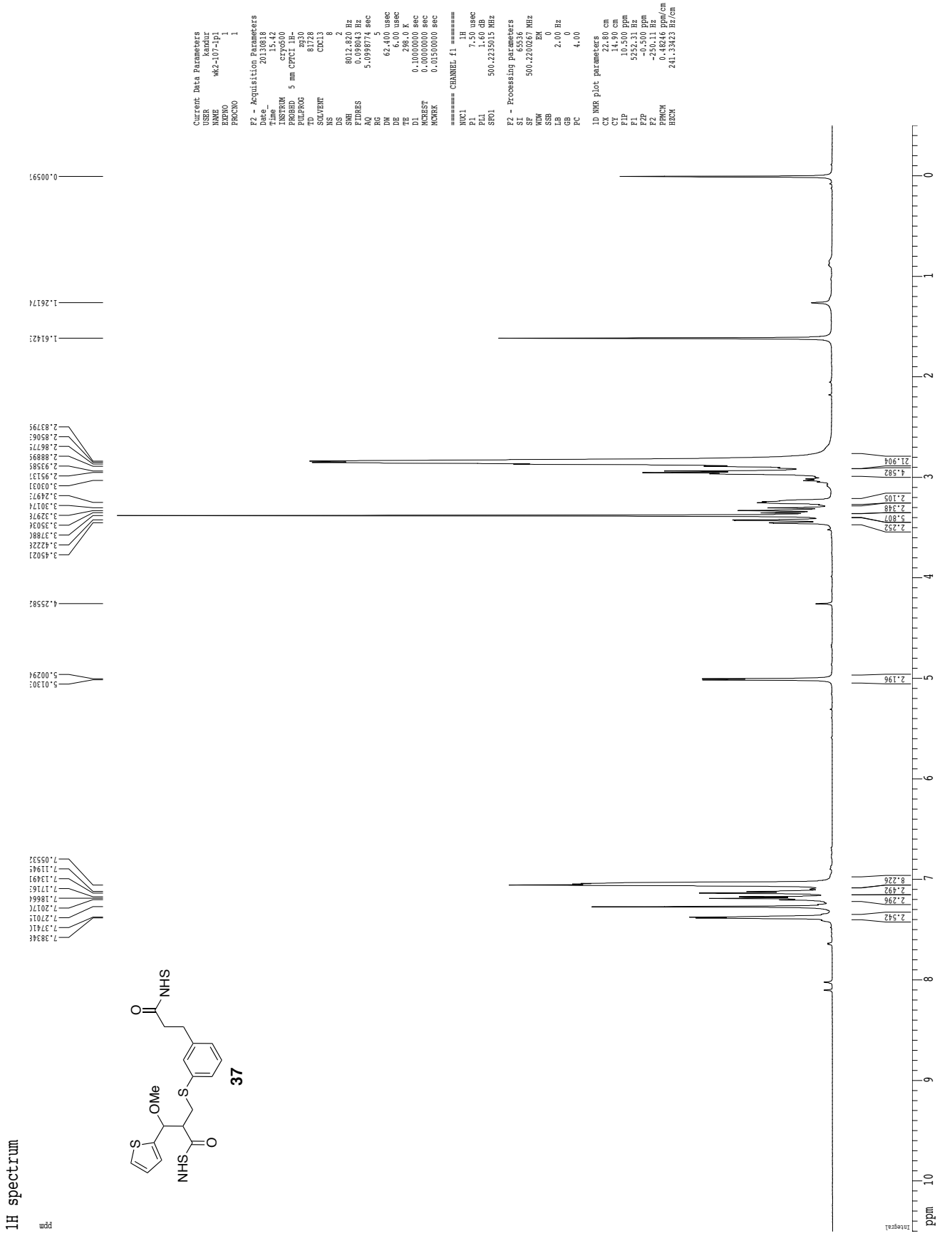

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
Me2N
S
O
OMe
34
Current Data Parameters
F2 - Acquisition Parameters
F2 - Processing parameters
1D NMR plot parameters
77.48
77.23
76.97
51.89
37.13
35.66
35.65
30.87
30.86
173.41
167.12
141.47
135.70
133.88
129.41
129.24
128.97
ppm

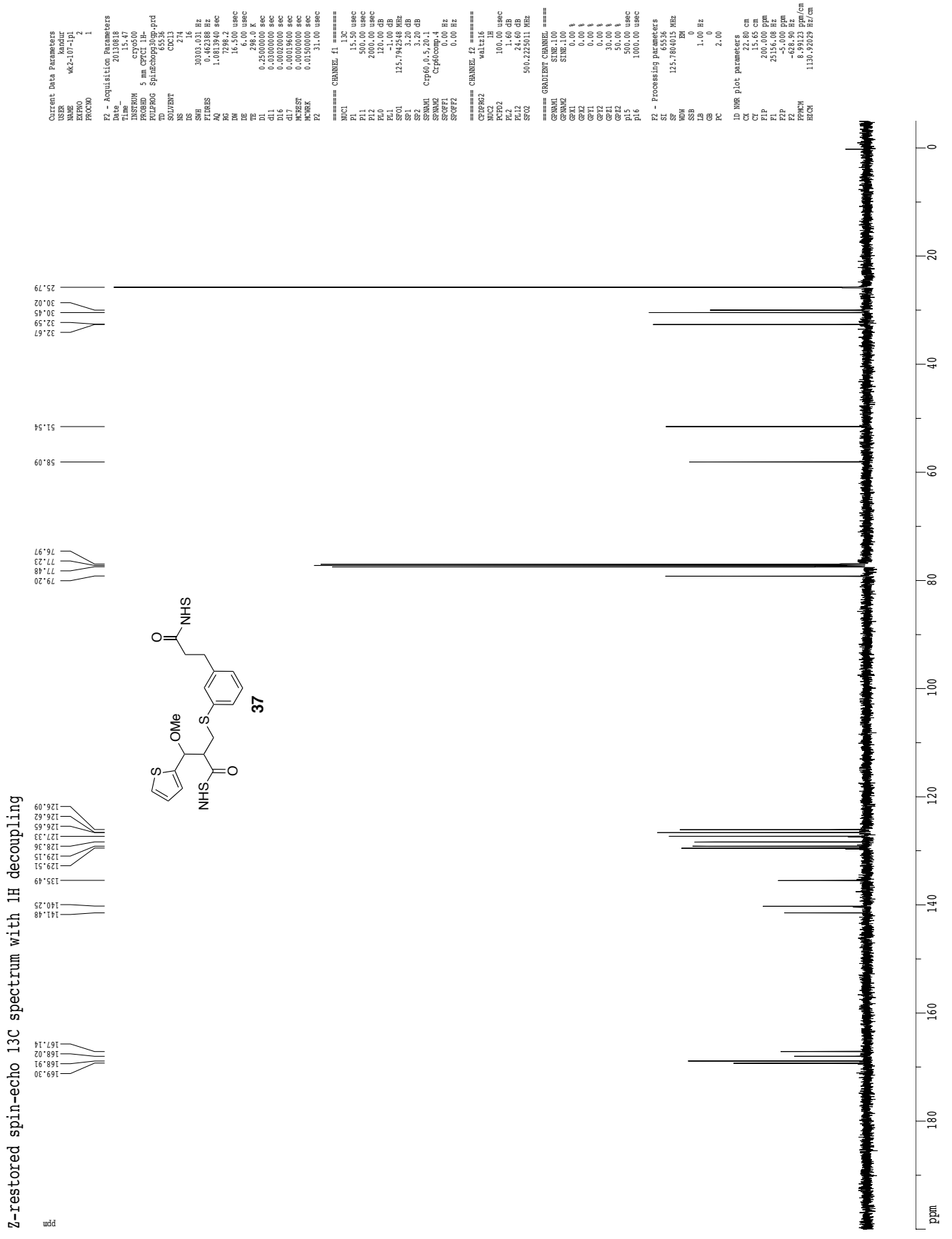

1H spectrum
Current Data Parameters
USER kandur
NAME wk1-197-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110722
Time_ 16.11
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 4
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200297 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.92 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
7.3195d
7.3021
7.2606t
7.2420d
7.2269
7.1247s
7.1095d
6.4281
6.4355d
5.9914d
5.9989s
3.8425d
3.6644
3.6512
3.0159s
3.0036d
2.9405t
2.9387d
2.9232
2.9036d
2.6885
2.6716d
2.6566
2.6247
2.6116
2.5454d
2.5303
2.0218
1.7629
1.1711
1.0000
1.0206
4.3510
3.0345
1.1216
3.2363
2.3058
0.3824
1.0117
integral
ppm
MeO
MeO
HO
O
O
S
S
35

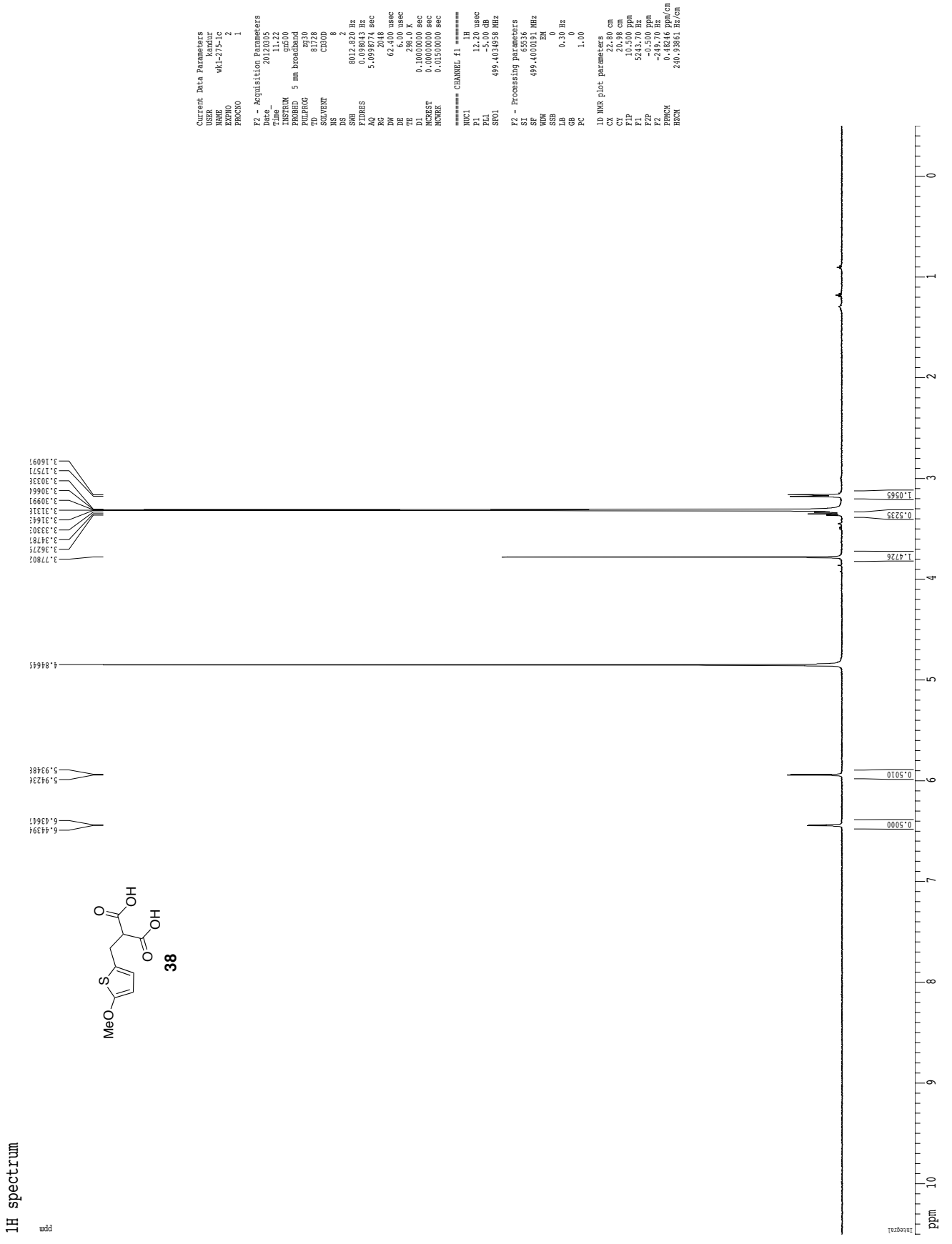

Z-restored spin-echo 13C spectrum with 1H decoupling
35
MeO
MeO
HO
O
O
S
S
ppm
30.62
35.48
35.71
38.93
46.34
52.07
60.38
76.98
77.23
77.48
103.24
124.00
126.55
127.93
129.39
131.25
133.10
133.82
141.31
165.38
172.14
177.73
Current Data Parameters
USER kandur
NAME wk1-197-1p
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110722
Time_ 16.16
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 464
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0814105 sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00180000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7794248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7803992 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
0
20
40
60
80
100
120
140
160
180
ppm

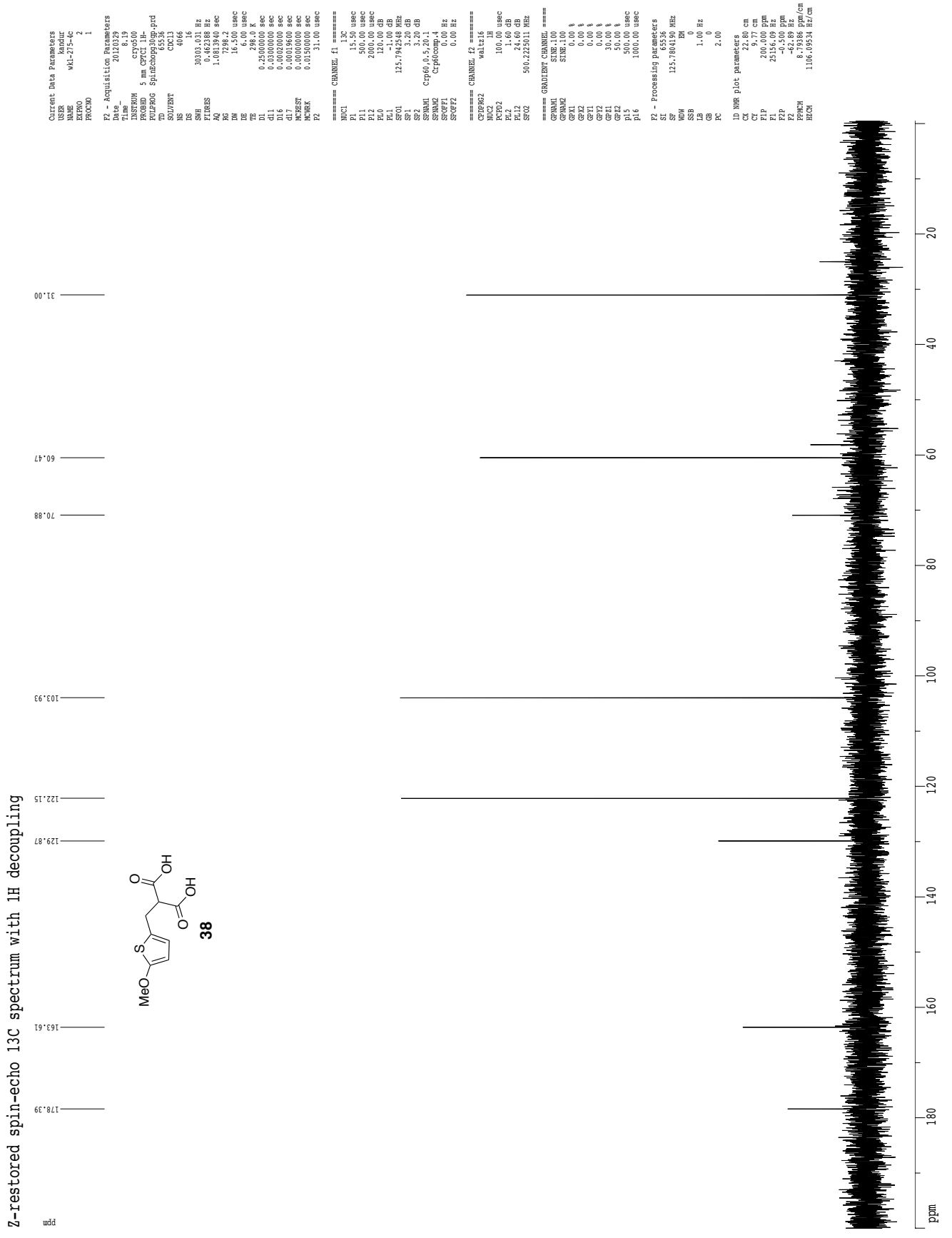

1H spectrum
Current Data Parameters
USER kandur
NAME wk1-222-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111011
Time_ 15.25
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 7.1
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200313 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 6.97 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
7.2710
7.2600
7.0180
7.0118
6.9615
6.9541
6.9516
6.9444
6.0381
6.3741
5.3954
3.7953
3.7844
1.4985
1.0002
1.0000
1.0558
1.0542
1.0139
3.0940
3.0708
OMe
O
OMe
S
36
ppm
Integral

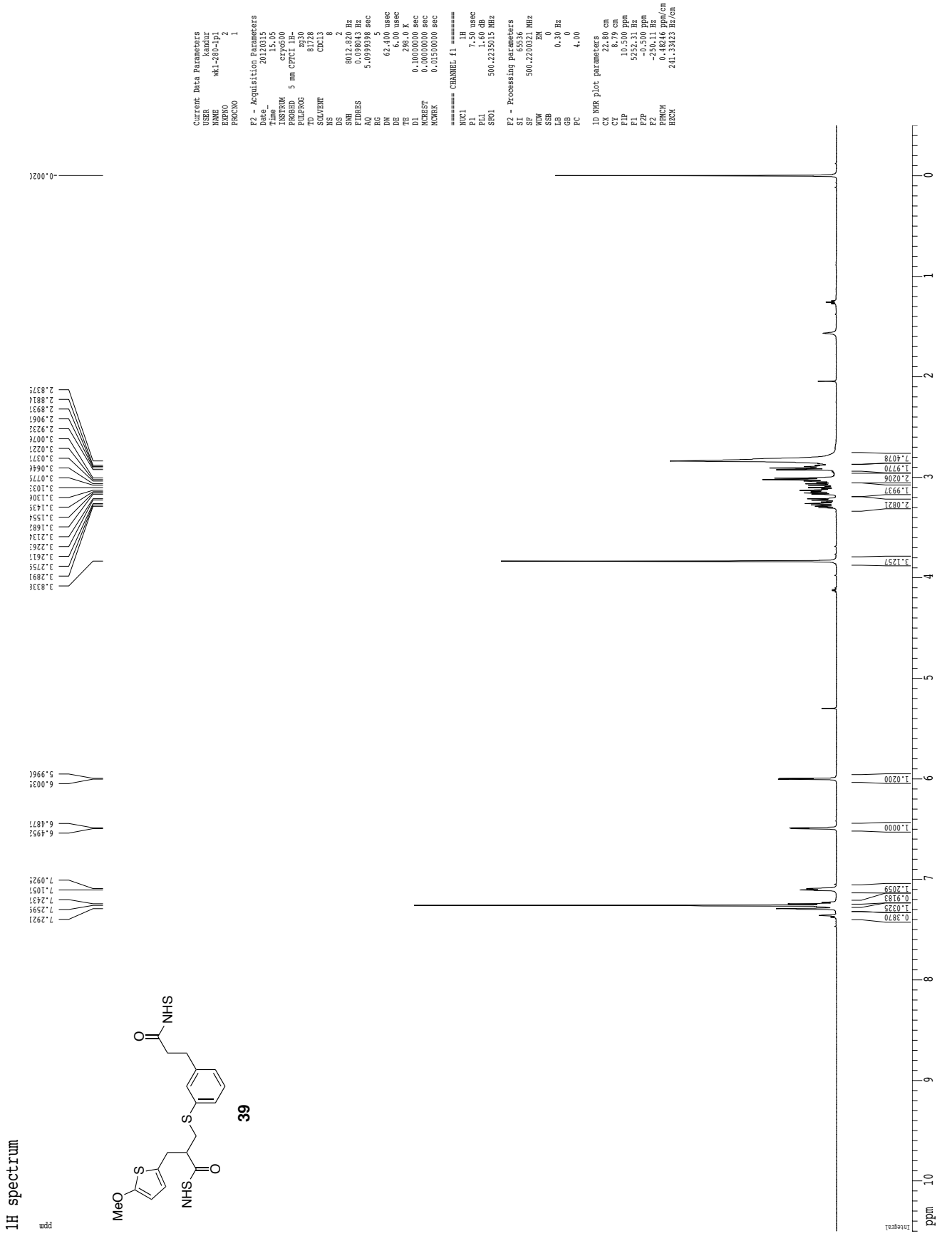

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
166.30
143.56
140.85
126.80
126.48
125.83
125.36
77.48
77.23
76.98
76.53
57.32
52.16
OMe
O
OMe
S
36
Current Data Parameters
USER kandur
NAME wkl-222-1p
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111011
Time 15.28
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 370
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0814105 sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00100000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7743248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7803997 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 6.92 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
ppm
0
20
40
60
80
100
120
140
160
180


1H spectrum
Current Data Parameters
USER kandur
NAME wk2-107-1p1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130818
Time_ 15.42
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======= CHANNEL f1 =======
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200267 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 14.90 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
0.00597
1.26174
1.61423
2.83795
2.85063
2.86775
2.88895
2.95585
2.99513
3.03033
3.24972
3.30174
3.32976
3.35036
3.37886
3.42226
3.45021
4.25582
5.00294
5.01303
7.05532
7.11945
7.13491
7.17163
7.18664
7.20176
7.27015
7.37416
7.38346
21.904
4.582
2.105
2.348
5.807
2.252
2.196
8.226
2.492
2.296
2.542
ppm
Integral
OMe
S
NHS
O
37

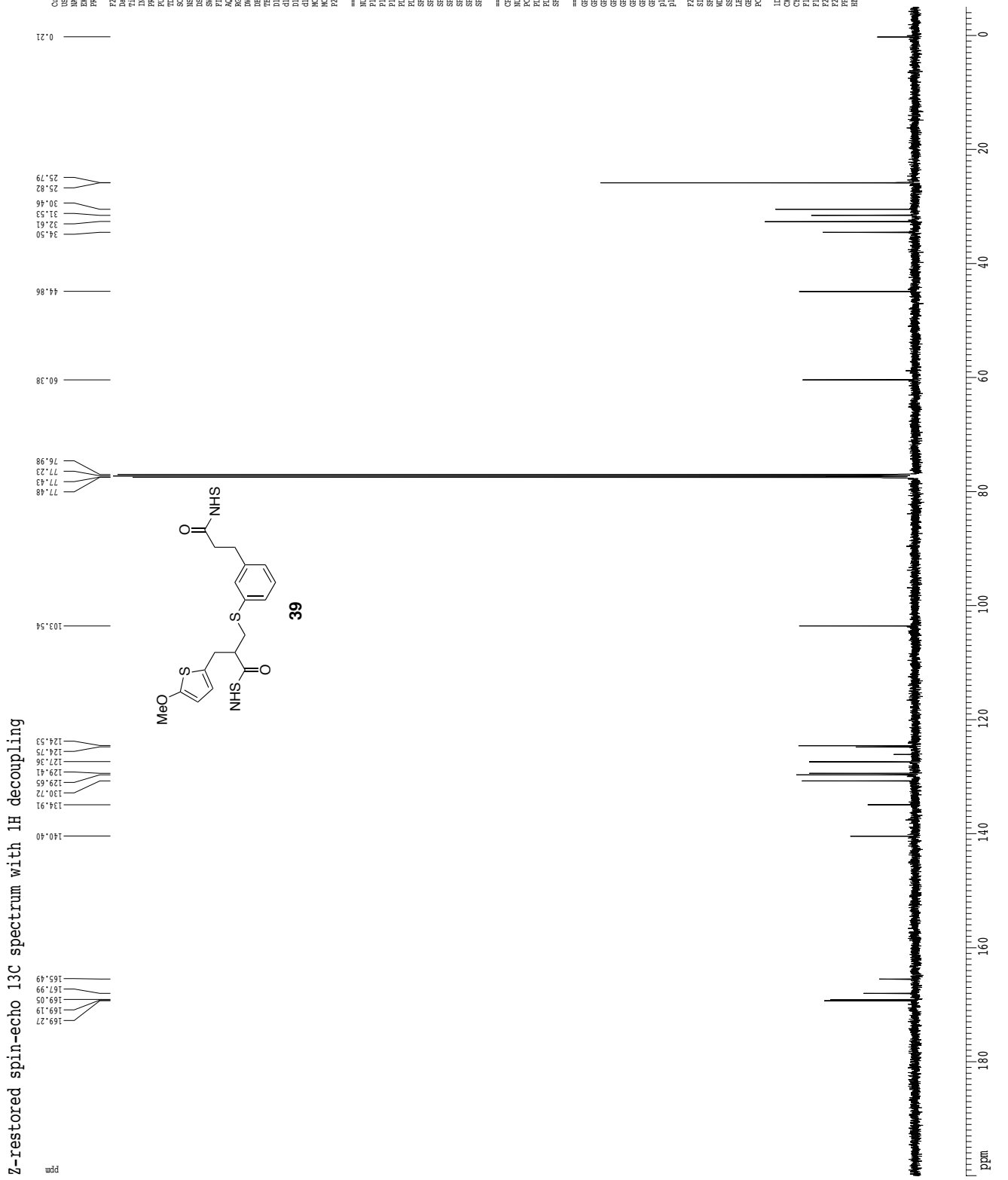

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
169.30
168.91
168.02
167.14
141.48
140.25
135.49
129.51
129.15
128.36
127.33
126.65
126.62
126.09
79.20
77.48
77.23
76.97
58.09
51.94
32.67
32.59
30.45
30.02
25.79
Current Data Parameters
USER kandur
NAME wk2-107-1p1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130818
Time_ 15.47
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 274
DS 16
SWH 30303.031 Hz
FIDRES 0.462318 Hz
AQ 1.0813940 sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00150000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7941248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7804015 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
0
20
40
60
80
100
120
140
160
180
ppm
S
OMe
S
O
NHS
O
NHS
37

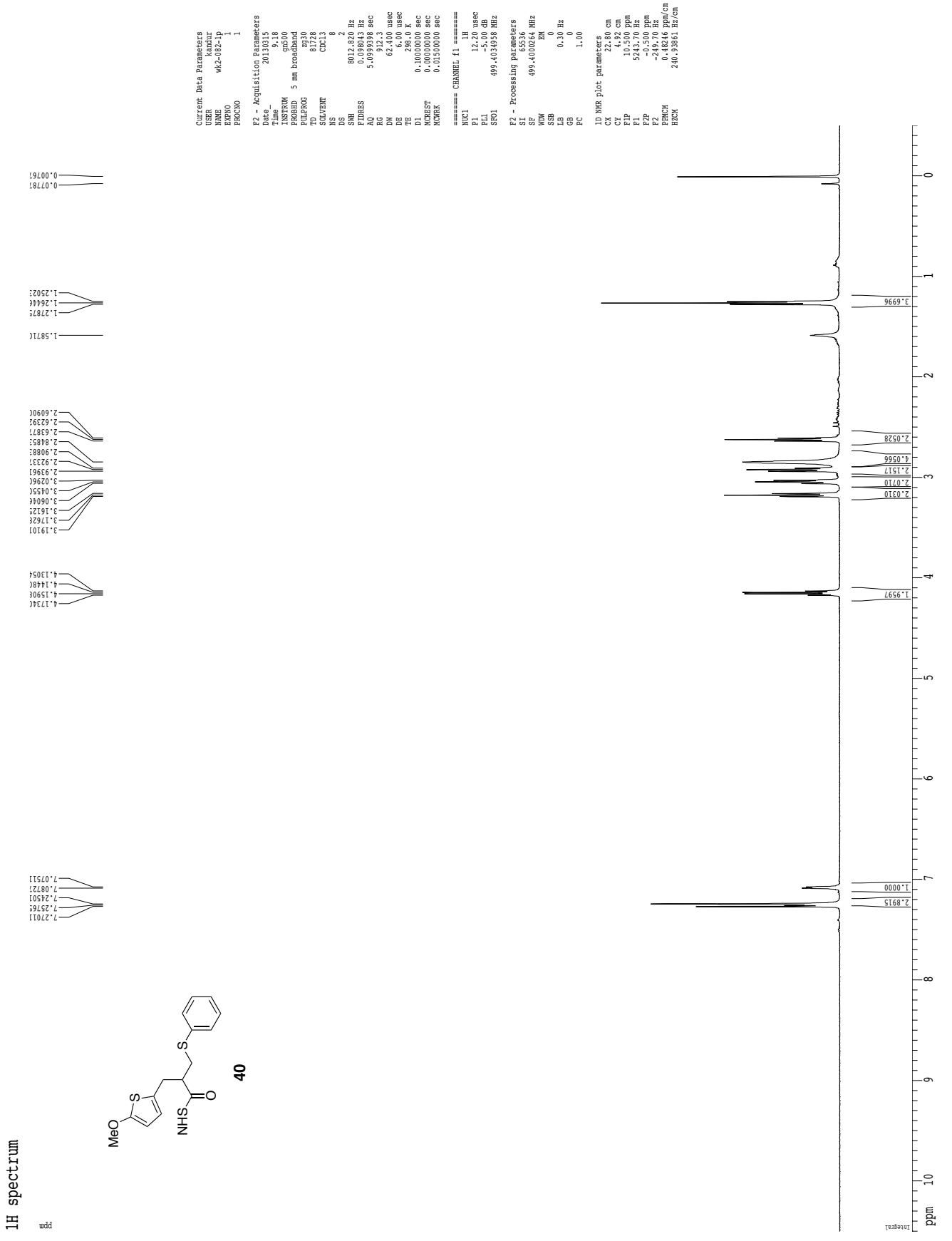

Current Data Parameters
USER Kandur
NAME wk1-275-1c
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120305
Time_ 11.22
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CD3OD
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 2048
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.4034958 MHz
F2 - Processing parameters
SI 65536
SF 499.4000191 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 20.98 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.500 ppm
F2 -249.70 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.93861 Hz/cm
3.77802
3.36275
3.34781
3.33302
3.31316
3.31641
3.30991
3.30664
3.30336
3.17571
3.16097
4.84645
5.93486
5.92236
6.44394
6.43647
1.4726
0.5235
1.0565
0.5010
0.5000
integral
ppm
1H spectrum
O
OH
O
OH
S
MeO
38

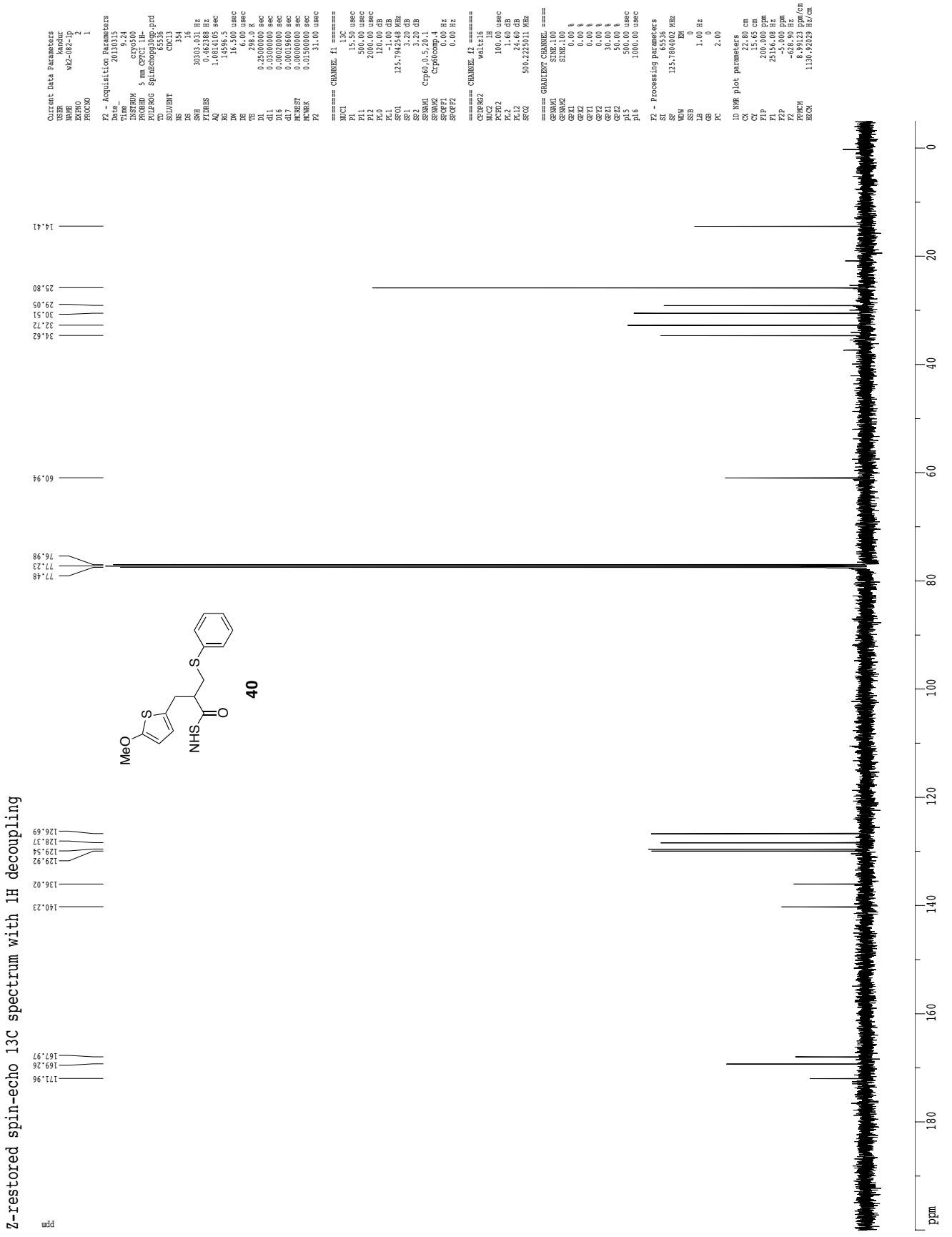

Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
178.39
163.61
129.87
122.15
103.93
70.88
60.47
31.00
MeO
S
O
OH
O
OH
38
Current Data Parameters
USER kandur
NAME wk1-275-4c
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120329
Time_ 8.19
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 4066
DS 16
SWH 30303.031 Hz
FIDRES 0.462386 Hz
AQ 1.081394O sec
RG 7298.2
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00100000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 1.10 dB
SFO1 125.7904218 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7804190 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 9.77 cm
F1P 200.000 ppm
F1 25156.09 Hz
F2P -0.500 ppm
F2 -62.89 Hz
PPMCM 8.79360 ppm/cm
HZCM 1106.09534 Hz/cm
ppm
20
40
60
80
100
120
140
160
180

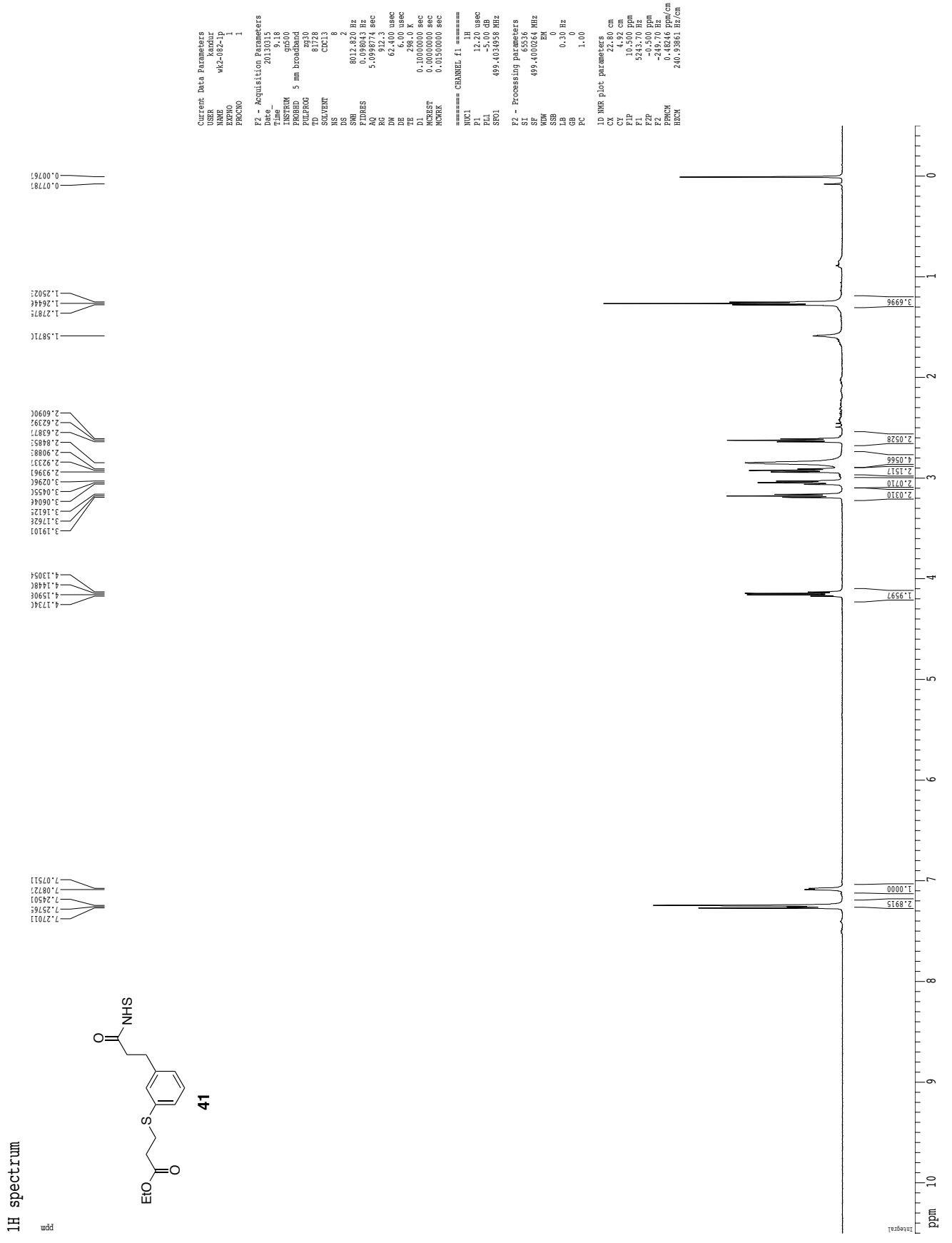

1H spectrum
Current Data Parameters
USER kandur
NAME wk1-280-1p1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120315
Time_ 15.05
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 5
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.50 usec
PL1 1.60 dB
SFO1 500.2235015 MHz
F2 - Processing parameters
SI 65536
SF 500.2200321 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1D NMR plot parameters
CX 22.80 cm
CY 8.79 cm
F1P 10.500 ppm
F1 5252.31 Hz
F2P -0.500 ppm
F2 -250.11 Hz
PPMCM 0.48246 ppm/cm
HZCM 241.33423 Hz/cm
7.4078
1.9770
2.0206
1.9937
2.0821
3.1257
1.0200
1.0000
1.2059
0.9183
1.0325
0.3870
integral
ppm
MeO
S
NHS
O
S
NHS
O
39

Z-restored spin-echo 13C spectrum with 1H decoupling




1H spectrum
Current Data Parameters
USER kandur
NAME wk2-082-1p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130315
Time_ 9.18
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0999398 sec
RG 912.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.4034958 MHz
F2 - Processing parameters
SI 65536
SF 499.4000264 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 4.92 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.500 ppm
F2 -249.70 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.93861 Hz/cm
0.00761
0.07781
1.25021
1.26446
1.27875
1.58710
2.60900
2.62392
2.63871
2.84853
2.90883
2.92331
2.99361
3.02966
3.04556
3.06044
3.16125
3.17626
3.19101
4.13054
4.14486
4.15906
4.17346
7.07511
7.08721
7.24501
7.25765
7.27011
3.6996
2.0528
4.0566
2.1517
2.0710
2.0310
1.9597
1.0000
2.8915
MeO
S
S
NHS
O
40
ppm
integral


Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
MeO
S
S
NHS
O
40
Current Data Parameters
USER kandur
NAME wk2-062-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130315
Time_ 9.24
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 354
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0814105 sec
RG 14596.5
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00150000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7904248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
p15 500.00 usec
p16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7804002 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
14.41
25.80
29.05
30.51
32.72
34.62
60.94
76.98
77.23
77.48
126.69
128.37
129.54
129.92
136.02
140.23
167.97
169.26
171.96
0
20
40
60
80
100
120
140
160
180
ppm


1H spectrum
41
NHS
O
S
EtO
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Current Data Parameters
USER kandur
NAME wk2-082-1p
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130315
Time_ 9.18
INSTRUM qn500
PROBHD 5 mm broadband
PULPROG zg30
TD 81728
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.098043 Hz
AQ 5.0998774 sec
RG 912.3
DW 62.400 usec
DE 6.00 usec
TE 298.0 K
D1 0.10000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.20 usec
PL1 -5.00 dB
SFO1 499.4034958 MHz
F2 - Processing parameters
SI 65536
SF 499.4000264 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 22.80 cm
CY 4.92 cm
F1P 10.500 ppm
F1 5243.70 Hz
F2P -0.570 ppm
F2 -249.70 Hz
PPMCM 0.48246 ppm/cm
HZCM 240.93861 Hz/cm
0.00761
0.07781
1.25021
1.26446
1.27875
1.58710
2.60900
2.62392
2.63871
2.84853
2.90883
2.92331
2.99961
3.02966
3.04556
3.06044
3.16125
3.17626
3.19101
4.13054
4.14486
4.15906
4.17340
7.07511
7.08721
7.24501
7.25765
7.27011
3.6996
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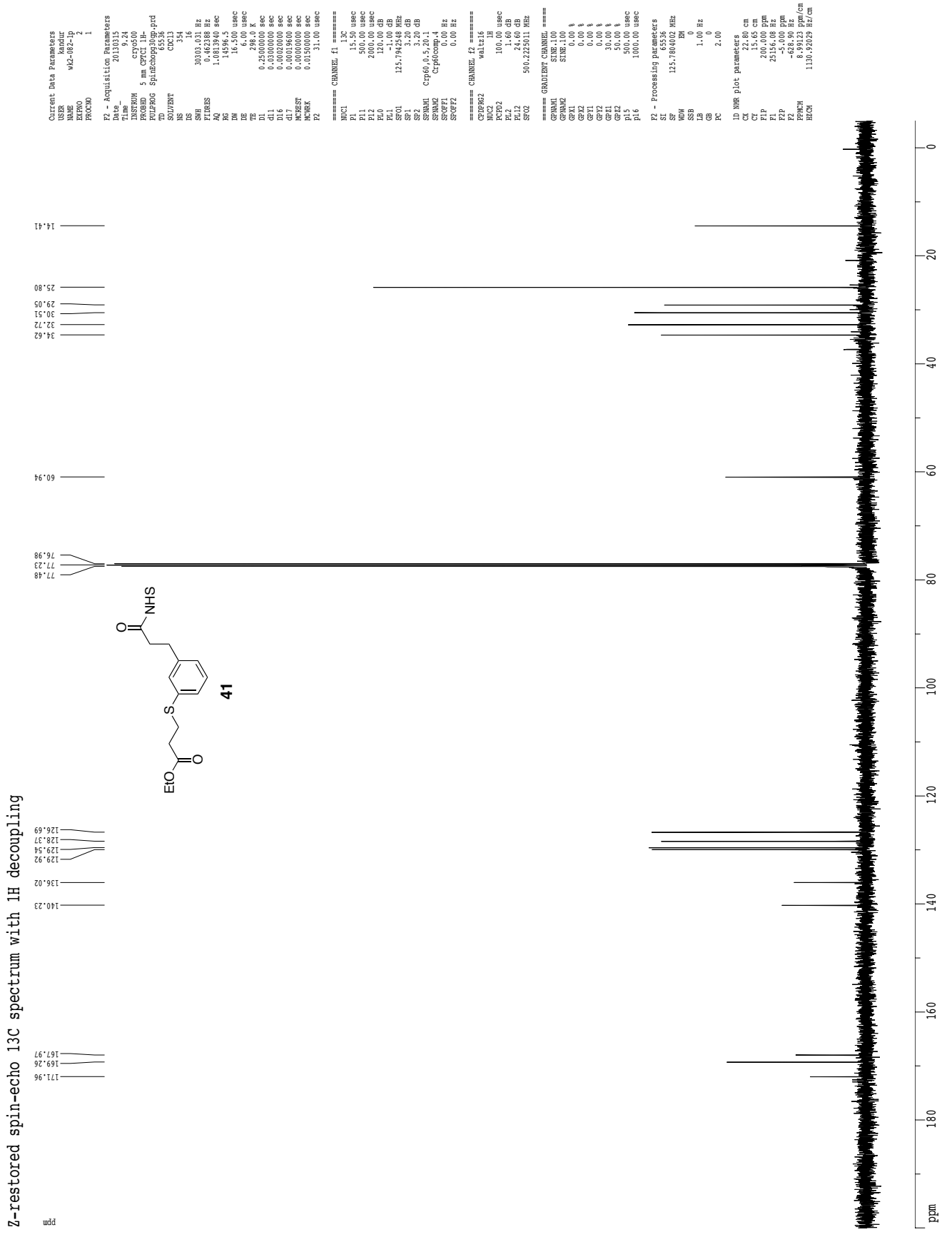
4.0566
2.1517
2.0710
2.0310
1.9597
1.0000
2.8915
ppm
Integral


Z-restored spin-echo 13C spectrum with 1H decoupling
ppm
Current Data Parameters
USER kandur
NAME wk2-062-1p
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130315
Time_ 9.24
INSTRUM cryo500
PROBHD 5 mm CPTCI 1H-
PULPROG SpinEchop30gp.prd
TD 65536
SOLVENT CDCl3
NS 354
DS 16
SWH 30303.031 Hz
FIDRES 0.462318 Hz
AQ 1.081940 sec
RG 14596.5
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00180000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
P2 31.00 usec
======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 -1.00 dB
SFO1 125.7794248 MHz
SP1 3.20 dB
SP2 1.20 dB
SPNAM1 Crp60,0.5,20.1
SPNAM2 Crp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 24.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPX1 0.00 %
GPX2 0.00 %
GPY1 0.00 %
GPY2 0.00 %
GPZ1 30.00 %
GPZ2 50.00 %
P15 500.00 usec
P16 1000.00 usec
F2 - Processing parameters
SI 65536
SF 125.7804002 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 22.80 cm
CY 15.65 cm
F1P 200.000 ppm
F1 25156.08 Hz
F2P -5.000 ppm
F2 -628.90 Hz
PPMCM 8.99123 ppm/cm
HZCM 1130.92029 Hz/cm
14.41
25.80
29.05
30.51
32.72
34.62
60.94
76.98
77.23
77.48
126.69
128.37
129.54
129.92
136.02
140.23
167.97
169.26
171.96
NHS
O
O
S
EtO
O
41
0
20
40
60
80
100
120
140
160
180
ppm