

Benzothiazoline: Highly Efficient Reducing Agent for the Enantioselective Organocatalytic Transfer Hydrogenation of Ketimines

Chen Zhu, Takahiko Akiyama*

*Department of Chemistry, Faculty of Science,
Gakushuin University,
Mejiro, Toshima-ku, Tokyo 171-8588, Japan*

takahiko.akiyama@gakushuin.ac.jp

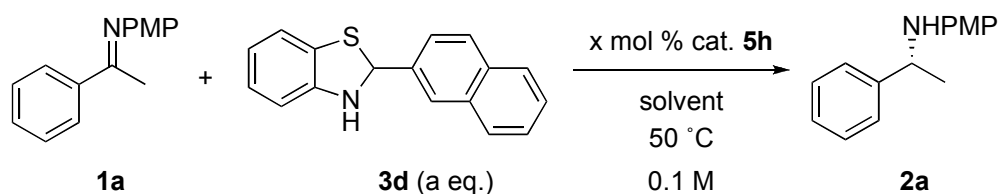
Supporting information

Table of Contents

1. Examination of reaction conditions.	S2
2. General procedure for the preparation of benzothiazolines.	S2-S3
3. General procedure for the transfer hydrogenation.	S3-S7
4. ¹ H NMR, ¹³ C NMR and HPLC spectra	S8-S67

General. NMR spectra were recorded on Unity Inova-400 instrument (Varian Inc., 400 MHz for ¹H, 100 MHz for ¹³C) using CDCl₃ as a solvent. Tetramethylsilane (TMS) (δ = 0) or CHCl₃ (δ = 7.27) served as an internal standard for ¹H NMR, and CDCl₃ was used as an internal standard (δ = 77.0) for ¹³C NMR. Purification of the products was performed by column chromatography on silica gel (Fuji sylisia D60L or PSQ-60B) or preparative TLC on silica gel (Wako gel B-5F). All solvents were purified according to the standard procedures.

1. Examination of reaction conditions.



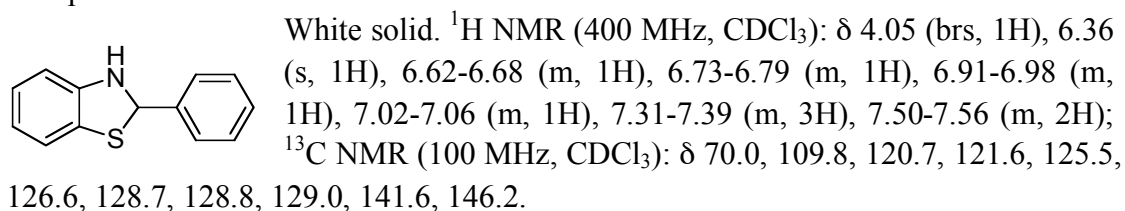
entry	solvent	a eq	x mol %	time (h)	yield (%) ^a	ee (%) ^b
1	toluene	2.0	10	22	89	97
2	benzene	2.0	10	21	85	97
3	mesitylene	2.0	10	21	90	98
4	(CH ₂ Cl) ₂	2.0	10	21	81	92
5	mesitylene	1.4	10	24	92	98
6	mesitylene	1.4	5	24	93	98
7	mesitylene	1.4	2	26	90	98

^a isolated yield. ^b enantiomeric excess determined by chiral HPLC analysis.

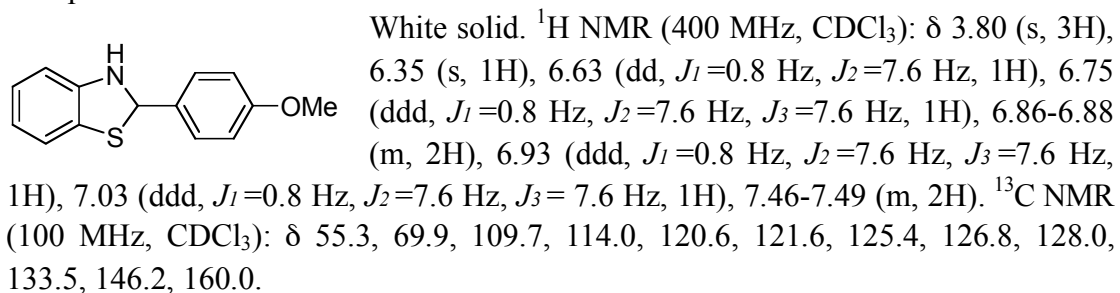
2. General procedure for the preparation of benzothiazolines 3a-3f.

A mixture of 10 mmol of aldehyde and 10.5 mmol of *o*-aminothiophenol in 40 mL of ethanol was stirred under nitrogen for about 3 hours at room temperature, until starting material aldehyde had been consumed monitoring by TLC. The reaction mixture was concentrated. For benzothiazolines **3a-3e**, the products were purified by recrystallization from ethanol while the benzothiazolines **3f** were purified by flash column chromatography.

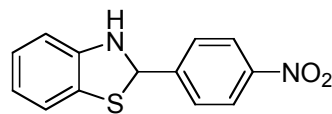
Compound **3a**¹



Compound **3b**¹

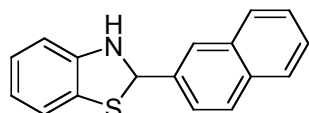


Compound **3e**¹



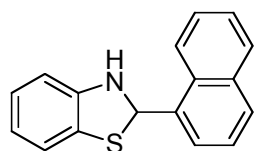
Yellow solid. ¹H NMR (400 MHz, CDCl₃): δ 4.40 (brs, 1H), 6.42 (s, 1H), 6.74 (d, *J* = 7.6 Hz, 1H), 6.80 (dd, *J*₁ = 7.6 Hz, *J*₂ = 7.6 Hz, 1H), 6.98 (dd, *J*₁ = 7.6 Hz, *J*₂ = 7.6 Hz, 1H), 7.03 (d, *J* = 7.6 Hz, 1H), 7.67 (d, *J* = 6.4 Hz, 2H), 8.18 (d, *J* = 6.4 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 68.2, 110.5, 121.4, 121.8, 124.0, 125.9, 127.2, 145.7, 147.8, 149.2.

Compound **3d**²



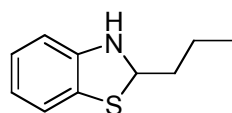
White solid. ¹H NMR (400 MHz, CDCl₃): δ 6.56 (s, 1H), 6.70 (d, *J* = 7.6 Hz, 1H), 6.78 (dd, *J*₁ = 7.6 Hz, *J*₂ = 7.6 Hz, 1H), 6.97 (dd, *J*₁ = 7.6 Hz, *J*₂ = 7.6 Hz, 1H), 7.07 (d, *J* = 7.6 Hz, 1H), 7.48-7.50 (m, 2H), 7.73-7.75 (m, 1H), 7.81-7.88 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 70.2, 109.8, 120.7, 121.7, 124.4, 125.4, 125.6, 126.4, 126.5, 126.6, 127.8, 128.1, 128.9, 133.0, 133.6, 138.8, 146.3.

Compound **3e**³



White solid. ¹H NMR (400 MHz, CDCl₃): δ 4.30 (brs, 1H), 6.70-6.81 (m, 2H), 6.97 (ddd, *J*₁ = 1.2 Hz, *J*₂ = 7.6 Hz, *J*₃ = 7.6 Hz, 1H), 7.05 (s, 1H), 7.04-7.08 (m, 1H), 7.39-7.60 (m, 3H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.84-7.92 (m, 2H), 8.02 (d, *J* = 8.4 Hz, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 66.8, 110.2, 120.8, 122.0, 122.8, 123.8, 125.4, 125.5, 125.9, 126.6, 126.7, 129.0, 130.1, 133.9, 136.5, 146.5.

Compound **3f**⁴

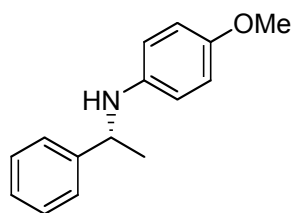


Pale yellow oil. ¹H NMR (400 MHz, CDCl₃): δ 0.96 (t, *J* = 7.6 Hz, 3H), 1.41-1.51 (m, 2H), 1.84-1.92 (m, 2H), 5.28 (t, *J* = 6.8 Hz, 1H), 6.65 (dd, *J*₁ = 1.2 Hz, *J*₂ = 7.6 Hz, 1H), 6.74 (ddd, *J*₁ = 1.2 Hz, *J*₂ = 7.6 Hz, *J*₃ = 7.6 Hz, 1H), 6.90 (ddd, *J*₁ = 0.8 Hz, *J*₂ = 7.6 Hz, *J*₃ = 7.6 Hz, 1H), 7.05-7.07 (m, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 13.7, 19.3, 40.6, 68.5, 110.9, 120.9, 121.9, 125.1, 127.6, 146.5.

2. General procedure for the transfer hydrogenation.

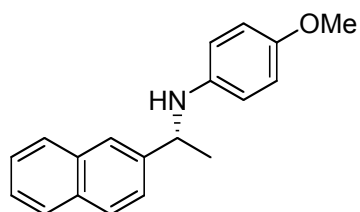
A 10 mL Schlenck flask was charged with 0.1 mmol ketimine, 0.14 mmol benzothiazoline and 0.002 mmol phosphoric acid (2 mol%). After addition of 1 mL mesitylene, the reaction mixture was heated to 50 °C under nitrogen for 20-30 hours and monitored by TLC. Upon completion, the reductive product was purified by flash column chromatography.

Compound **2a**⁵



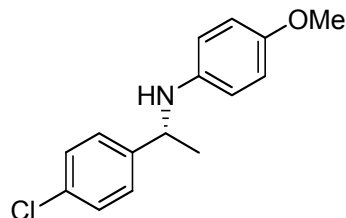
eluted from silica gel using hexane/ethyl acetate 15/1 as eluent. 90% yield, 98% ee; ¹H NMR (400 MHz, CDCl₃): δ 1.50 (d, *J*=6.8 Hz, 3H), 3.69 (s, 3H), 4.41 (q, *J*=6.8 Hz, 1H), 6.45-6.50 (m, 2H), 6.66-6.71 (m, 2H), 7.20-7.24 (m, 1H), 7.29-7.37 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 25.0, 54.3, 55.7, 114.7, 114.8, 125.9, 126.8, 128.6, 141.4, 145.4, 152.0; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 98/2, flow rate = 0.6 mL min⁻¹, major enantiomer: *t*_R = 20.81 min; minor enantiomer: *t*_R = 23.87 min. [α]_D¹⁵ +8.5 (c 0.87, CHCl₃).

Compound **2b**⁵



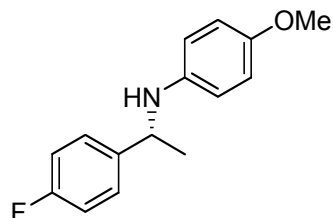
eluted from silica gel using hexane/ethyl acetate 14/1 as eluent. 96% yield, 98% ee; ¹H NMR (400MHz, CDCl₃): δ 1.57 (d, *J*=6.8 Hz, 3H), 3.67 (s, 3H), 4.56 (q, *J*=6.8 Hz, 1H), 6.50-6.56 (m, 2H), 6.65-6.70 (m, 2H), 7.40-7.52 (m, 3H), 7.78-7.82 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 25.1, 54.6, 55.7, 114.8, 124.3, 124.4, 125.5, 125.9, 127.6, 127.8, 128.4, 132.7, 133.6, 141.4, 142.9, 152.0; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 90/10, flow rate = 0.5 mL min⁻¹, major enantiomer: *t*_R = 21.16 min; minor enantiomer: *t*_R = 25.00 min. [α]_D¹⁶ +11.1 (c 1.32, CHCl₃).

Compound **2c**⁵



eluted from silica gel using hexane/ethyl acetate 15/1 as eluent. 90% yield, 97% ee; ¹H NMR (400 MHz, CDCl₃): δ 1.46 (d, *J*=6.8 Hz, 3H), 3.69 (s, 3H), 4.37 (q, *J*=6.8 Hz, 1H), 6.41-6.46 (m, 2H), 6.66-6.71 (m, 2H), 7.22-7.32 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 25.1, 53.8, 55.7, 114.6, 114.7, 127.3, 128.7 132.3, 141.1, 144.0, 152.1; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 97/3, flow rate = 0.5 mL min⁻¹, major enantiomer: *t*_R = 28.08 min; minor enantiomer: *t*_R = 33.44 min. [α]_D¹⁸ +8.9 (c 1.16, CHCl₃).

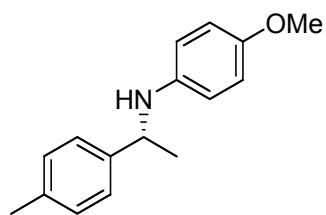
Compound **2d**⁵



eluted from silica gel using hexane/ethyl acetate 15/1 as eluent. 92% yield, 98% ee; ¹H NMR (400 MHz, CDCl₃): δ 1.46 (d, *J*=6.8 Hz, 3H), 3.69 (s, 3H), 4.38 (q, *J*=6.8 Hz, 1H), 6.42-6.46 (m, 2H), 6.67-6.71 (m, 2H), 6.94-7.02 (m, 2H), 7.29-7.35 (m, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 25.2, 53.7, 55.7, 114.6, 114.7, 115.3 (d, *J*_{C-F} =21.0 Hz), 127.3 (d, *J*_{C-F} =8.0 Hz), 141.1 (d, *J*_{C-F} =3.0 Hz), 141.3, 152.0, 161.7 (d, *J*_{C-F} =242.9 Hz); HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 97/3, flow rate = 0.5 mL min⁻¹, major enantiomer: *t*_R = 25.99 min; minor enantiomer: *t*_R =

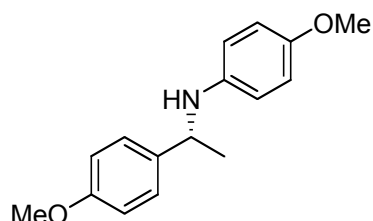
30.07 min. $[\alpha]_D^{18} -23.7$ (c 1.10, CHCl_3).

Compound **2e**⁵



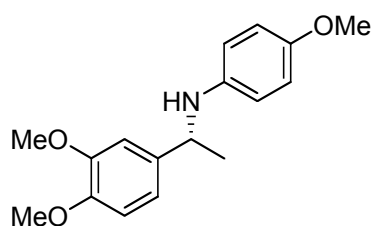
eluted from silica gel using hexane/ethyl acetate 15/1 as eluent. 93% yield, 98% ee; ^1H NMR (400 MHz, CDCl_3): δ 1.47 (d, $J=6.8$ Hz, 3H), 2.31 (s, 3H), 3.68 (s, 3H), 4.37 (q, $J=6.8$ Hz, 1H), 6.42-6.50 (m, 2H), 6.66-6.70 (m, 2H), 7.11 (d, $J=7.6$ Hz, 2H), 7.24 (d, $J=7.6$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 21.0, 25.1, 53.9, 55.7, 114.5, 114.7, 125.8, 129.2, 136.3, 141.6, 142.4, 151.8; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/ 2-propanol = 98/2, flow rate = 0.5 mL min⁻¹, major enantiomer: t_R = 21.75 min; minor enantiomer: t_R = 24.79 min. $[\alpha]_D^{18} + 7.7$ (c 1.05, CHCl_3).

Compound **2f**⁵



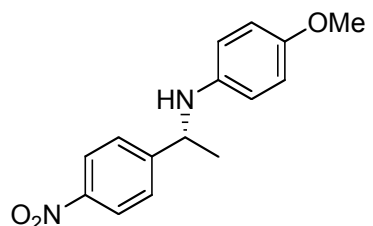
eluted from silica gel using hexane/ethyl acetate 14/1 as eluent. 84% yield, 98% ee; ^1H NMR (400 MHz, CDCl_3): δ 1.46 (d, $J=6.8$ Hz, 3H), 3.68 (s, 3H), 3.77 (s, 3H), 4.36 (q, $J=6.8$ Hz, 1H), 6.45-6.50 (m, 2H), 6.67-6.71 (m, 2H), 6.82-6.86 (m, 2H), 7.25-7.30 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 25.0, 53.6, 55.2, 55.7, 113.9, 114.6, 114.7, 126.9, 137.4, 141.6, 151.8, 158.4; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 95/5, flow rate = 0.5 mL min⁻¹, major enantiomer: t_R = 23.66 min; minor enantiomer: t_R = 26.99 min. $[\alpha]_D^{17} + 24.2$ (c 1.05, CHCl_3).

Compound **2g**⁶



eluted from silica gel using hexane/ethyl acetate 6/1 as eluent. 87% yield, 98% ee; ^1H NMR (400 MHz, CDCl_3): δ 1.48 (d, $J=6.4$ Hz, 3H), 3.69 (s, 3H), 3.85 (s, 3H), 3.87 (s, 3H), 4.34 (q, $J=6.4$ Hz, 1H), 6.47-6.51 (m, 2H), 6.67-6.72 (m, 2H), 6.79-6.83 (m, 1H), 6.88-6.92 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ 25.0, 54.2, 55.7, 55.8, 55.8, 109.1, 111.2, 114.6, 114.7, 117.7, 138.0, 141.5, 147.7, 149.1, 152.0; HPLC conditions: CHIRALPAK[®] AS-H column, hexane/2-propanol = 90/10, flow rate = 0.5 mL min⁻¹, major enantiomer: t_R = 41.73 min; minor enantiomer: t_R = 32.80 min. $[\alpha]_D^{17} -16.0$ (c 0.72, CHCl_3).

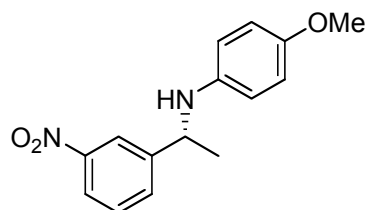
Compound **2h**⁵



eluted from silica gel using hexane/ethyl acetate 8/1 as eluent. 86% yield, 95% ee; ^1H NMR (400 MHz, CDCl_3): δ 1.52 (d, $J=6.8$ Hz, 3H), 3.68 (s, 3H), 4.49 (q, $J=6.8$ Hz, 1H), 6.39-6.43 (m, 2H), 6.67-6.71 (m, 2H), 7.53 (dd, $J_1=2.0$ Hz, $J_2=8.8$ Hz, 2H), 8.16 (dd, $J_1=2.0$ Hz, $J_2=8.8$ Hz, 2H); ^{13}C NMR (100 MHz, CDCl_3): δ

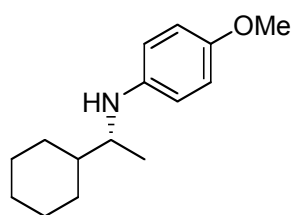
24.9, 54.1, 55.6, 114.6, 114.8, 124.0, 126.7, 140.5, 147.0, 152.3, 153.3; HPLC conditions: CHIRALPAK[®] AD-H column, hexane/2-propanol = 90/10, flow rate = 0.5 mL min⁻¹, major enantiomer: *t*_R = 44.15 min; minor enantiomer: *t*_R = 37.40 min. $[\alpha]_D^{18} + 22.6$ (c 0.92, CHCl₃).

Compound **2i**⁷



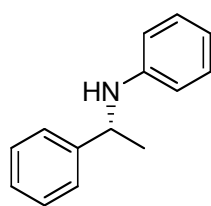
eluted from silica gel using hexane/ethyl acetate 6/1 as eluent. 97% yield, 97% ee; ¹H NMR (400 MHz, CDCl₃): δ 1.53 (d, *J* = 6.8 Hz, 3H), 3.69 (s, 3H), 4.50 (q, *J* = 6.8 Hz, 1H), 6.41-6.45 (m, 2H), 6.67-6.71 (m, 2H), 7.47 (dd, *J*₁ = 8.0 Hz, *J*₂ = 8.0 Hz, 1H), 7.70-7.74 (m, 1H), 8.07-8.10 (m, 1H), 8.24 (s, 1H); ¹³C NMR (100 MHz, CDCl₃): δ 25.0, 53.9, 55.6, 114.6, 114.8, 121.0, 122.0, 129.6, 132.2, 140.6, 148.0, 148.7, 152.3; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 90/10, flow rate = 0.6 mL min⁻¹, major enantiomer: *t*_R = 30.67 min; minor enantiomer: *t*_R = 38.84 min. $[\alpha]_D^{13} - 21.5$ (c 1.31, CHCl₃).

Compound **2j**⁵



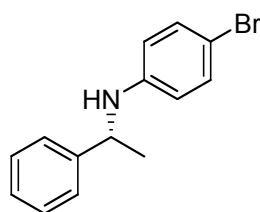
eluted from silica gel using hexane/ethyl acetate 20/1 as eluent. 80% yield, 98% ee; ¹H NMR (400 MHz, CDCl₃): δ 1.02-1.28 (m, 5H), 1.08 (d, *J* = 6.4 Hz, 3H), 1.39-1.47 (m, 1H), 1.65-1.82 (m, 5H), 3.22 (q, *J* = 5.6 Hz, 1H), 3.73 (s, 3H), 6.54 (d, *J* = 8.0 Hz, 2H), 6.76 (d, *J* = 8.0 Hz, 2H); ¹³C NMR (100 MHz, CDCl₃): δ 17.3, 26.3, 26.5, 26.6, 28.2, 29.8, 42.8, 54.1, 55.8, 114.5, 114.9, 142.2, 151.6; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/ 2-propanol = 99/1, flow rate = 0.5 mL min⁻¹, major enantiomer: *t*_R = 14.55 min; minor enantiomer: *t*_R = 16.21 min. $[\alpha]_D^{19} - 19.7$ (c 0.20, CHCl₃).

Compound **2k**⁵



eluted from silica gel using hexane/ethyl acetate 20/1 as eluent. 92% yield, 98% ee; ¹H NMR (400 MHz, CDCl₃): δ 1.50 (d, *J* = 6.8 Hz, 3H), 4.07 (brs, 1H), 4.47 (q, *J* = 6.8 Hz, 1H), 6.50 (d, *J* = 8.4 Hz, 2H), 6.60-6.66 (m, 1H), 7.04-7.12 (m, 2H), 7.18-7.24 (m, 1H), 7.26-7.38 (m, 4H); ¹³C NMR (100 MHz, CDCl₃): δ 24.9, 53.5, 113.3, 117.2, 125.8, 126.8, 128.6, 129.1, 145.1, 147.2; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 98/2, flow rate = 0.5 mL min⁻¹, major enantiomer: *t*_R = 23.79 min; minor enantiomer: *t*_R = 19.43 min. $[\alpha]_D^{18} - 12.0$ (c 0.23, CH₃OH).

Compound **2l**⁷



eluted from silica gel using hexane/ethyl acetate 20/1 as eluent. 93% yield, 97% ee; ¹H NMR (400MHz, CDCl₃): δ 1.43 (d, *J* = 6.8 Hz, 3H), 4.10 (brs, 1H), 4.35 (q, *J* = 6.8 Hz, 1H), 6.28-6.32 (m, 2H), 7.05-7.09 (m, 2H), 7.13-7.18 (m, 1H), 7.20-7.27 (m,

4H); ^{13}C NMR (100 MHz, CDCl_3): δ 24.9, 53.5, 108.9, 114.9, 125.7, 127.0, 128.7, 131.7, 144.5, 146.0; HPLC conditions: CHIRALCELL[®] OD-H column, hexane/2-propanol = 98/2, flow rate = 0.5 mL min⁻¹, major enantiomer: t_{R} = 21.86 min; minor enantiomer: t_{R} = 29.19 min. $[\alpha]_{\text{D}}^{15}$ +7.6 (c 0.53, CHCl_3).

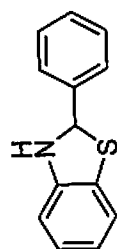
References:

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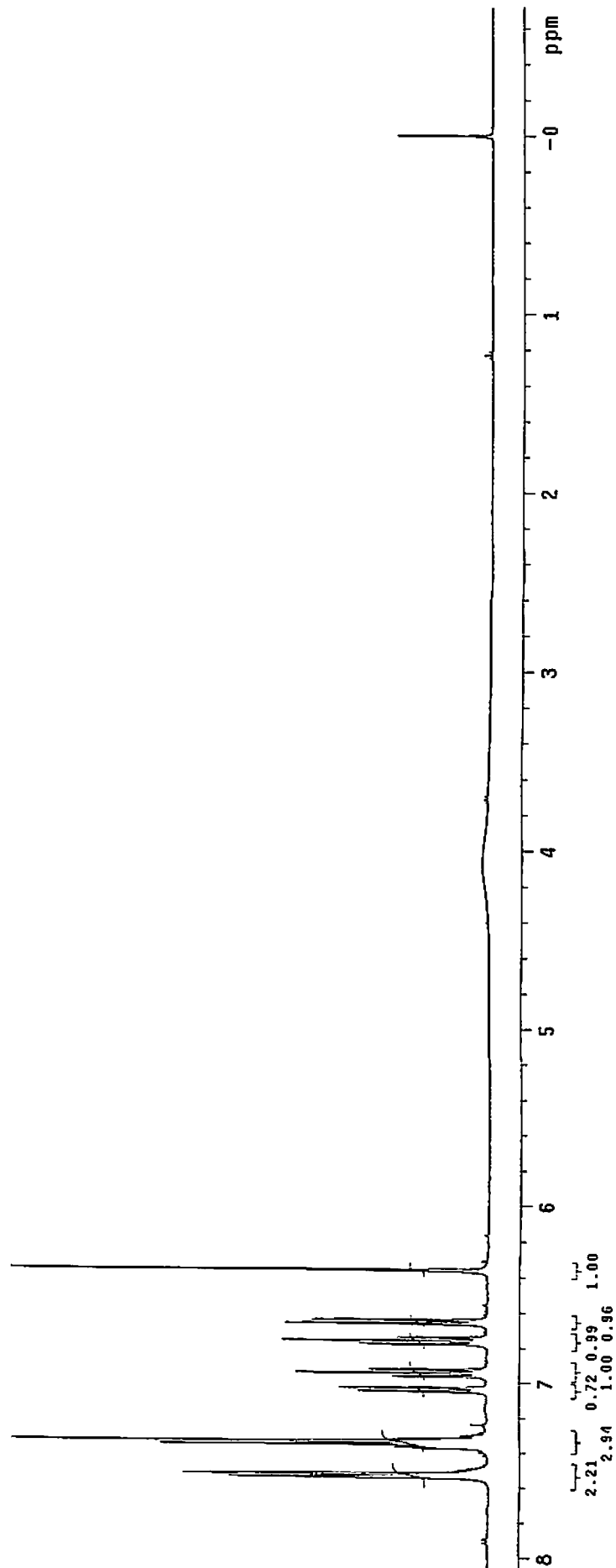
zc2-30

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: ynmr1
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Relax. delay 1.496 sec
Pulse 45.0 degrees
Acq. time 3.504 sec
Width 5999.7 Hz
8 repetitions
OBSERVE H1, 399.9551884 MHz
DATA PROCESSING
F1 size 65536
Total time 0 min, 40 sec



compound 3a



zc2-30

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

608 repetitions

OBSERVE C13, 100.568135 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

Continuously on

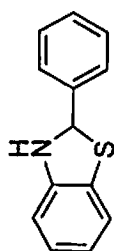
WALTZ-16 modulated

DATA PROCESSING

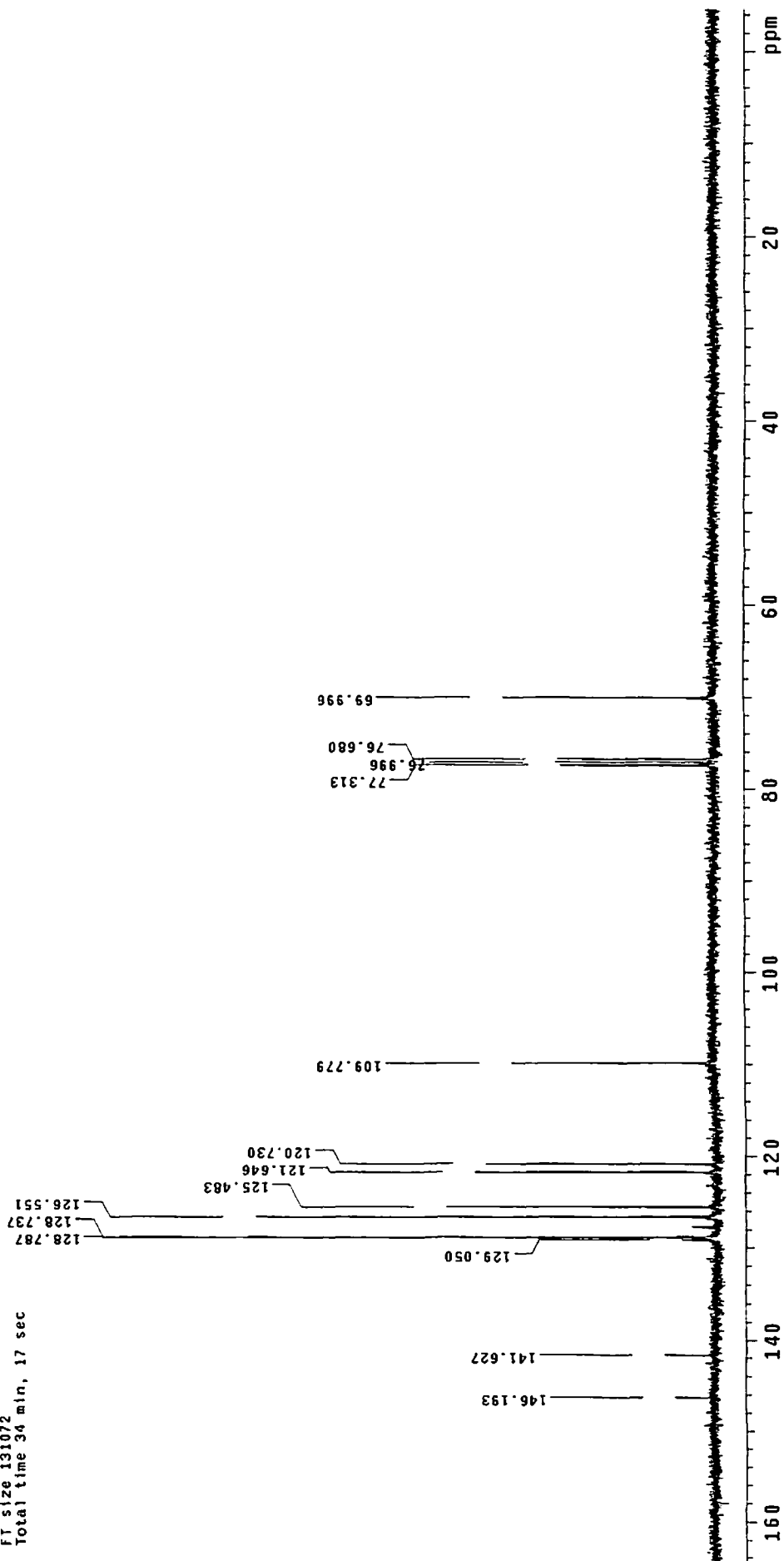
Line broadening 1.0 Hz

FI size 131072

Total time 34 min, 17 sec



Compound 3a



zcl-73

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: ynmr1

INOVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

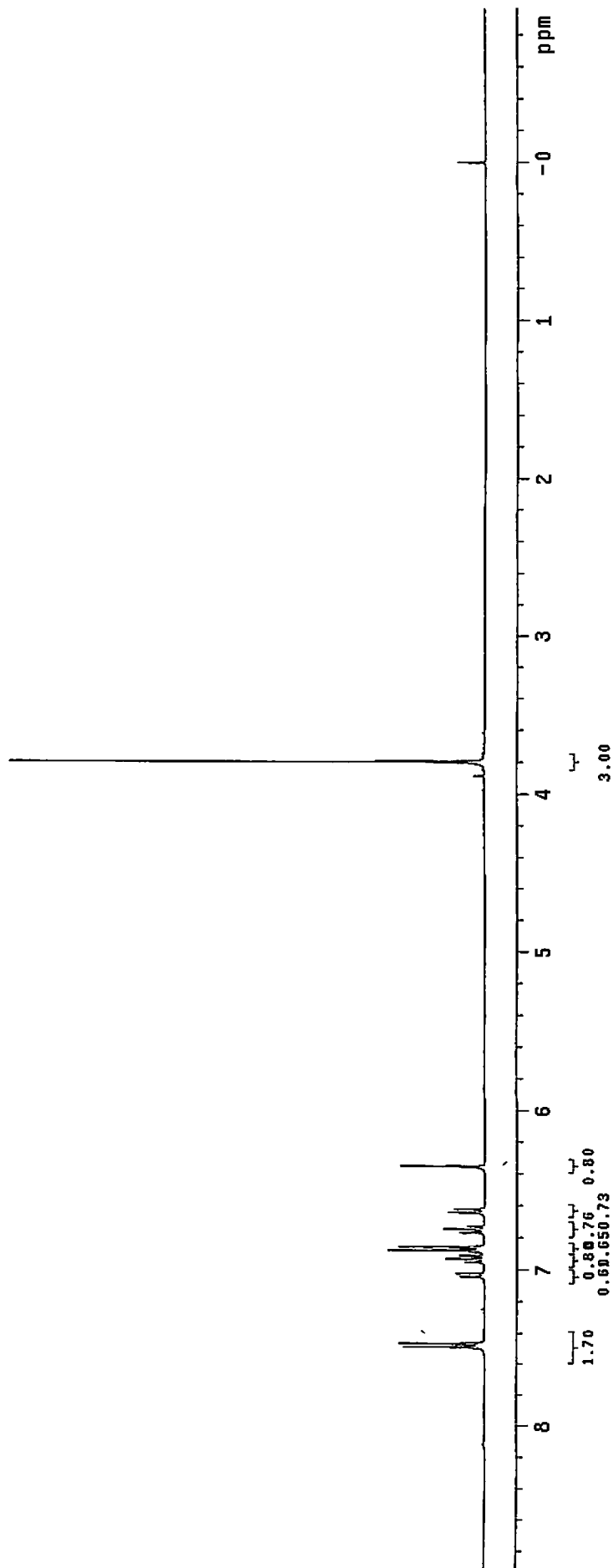
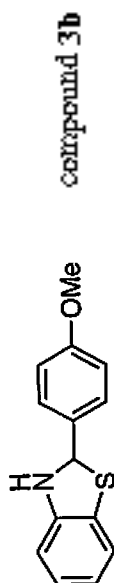
8 repetitions

OBSERVE H1, 399.9551849 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zcl-73

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

616 repetitions

OBSERVE C13, 100.5888120 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

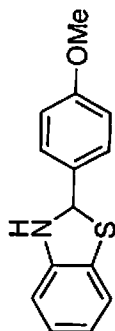
WALTZ-16 modulated

DATA PROCESSING

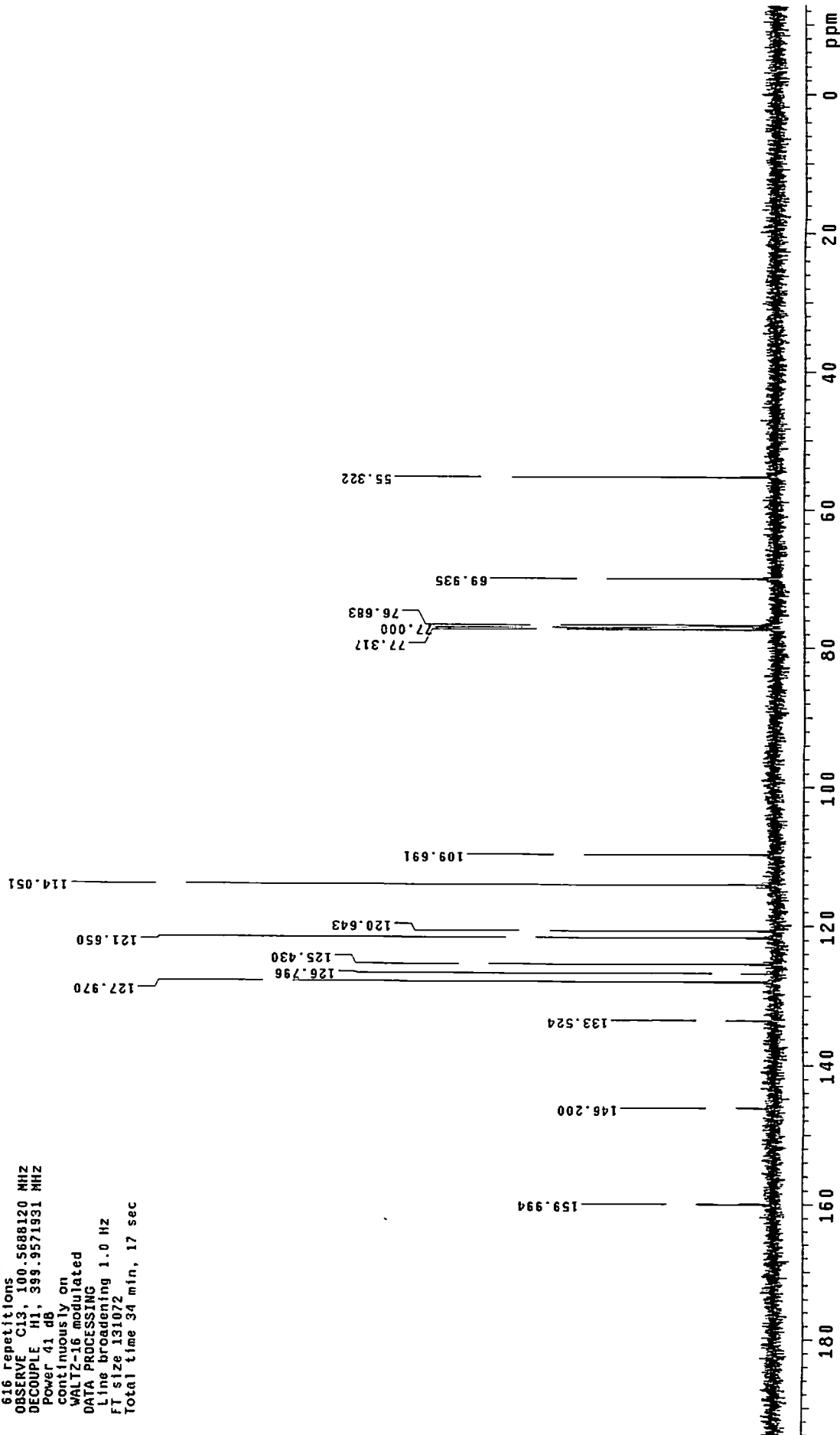
Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



compound 3b



2c2-31

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INDVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

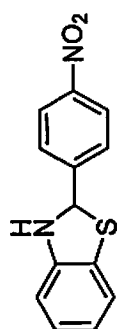
8 repetitions

OBSERVE IN 399.9551818 MHz

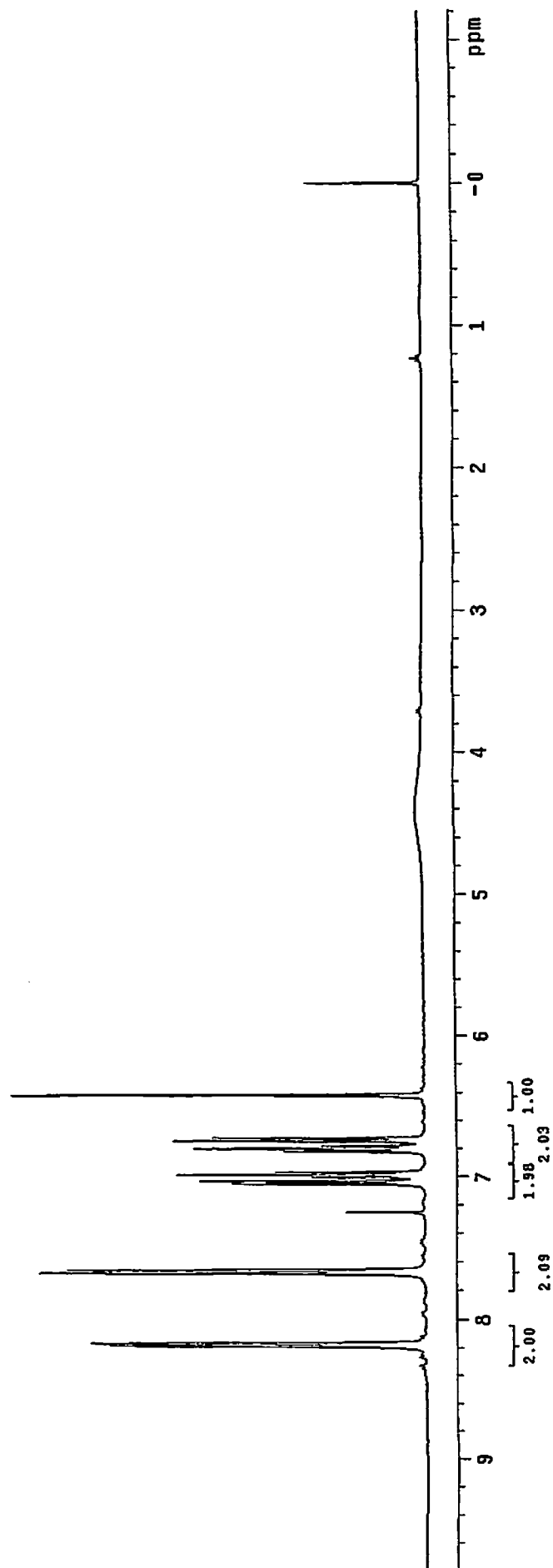
DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec

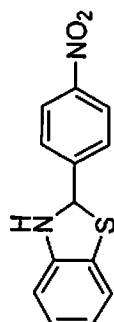


compound 3c



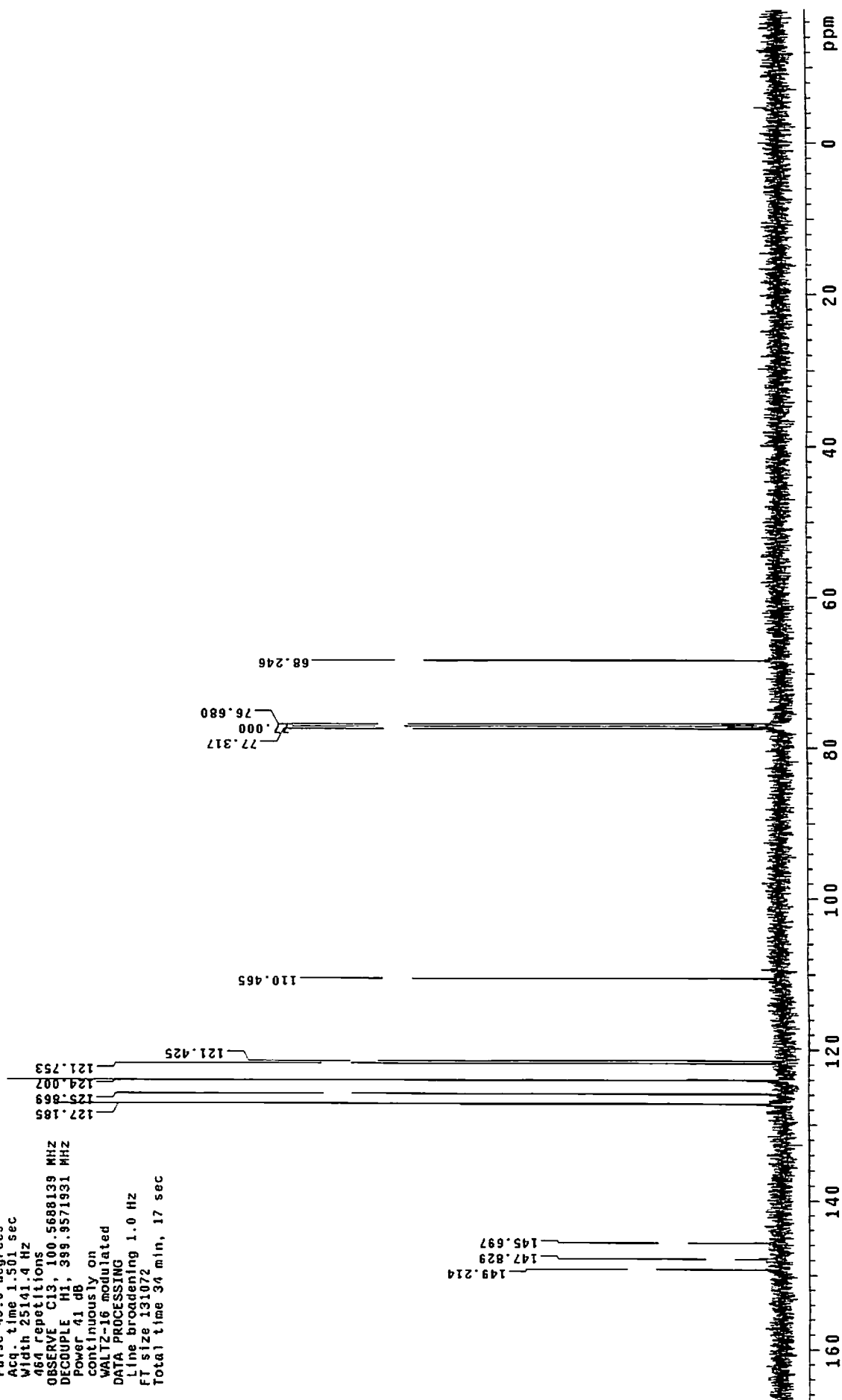
zc2-31

Pulse Sequence: s2pul
Solvent: CDC13
Ambient temperature
User: vnmr1
INQVA-400 "u100"



compound 3c

Relax. delay 0.499 sec
Pulse 45.0 degrees
Acq. time 1.501 sec
Width 25141.4 Hz
464 repetitions
OBSERVE C13, 100.5688139 MHz
DECOUPLE H1, 399.9571931 MHz
Power 41 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min, 17 sec



zc2-98

Pulse Sequence: s2pu1

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "0400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

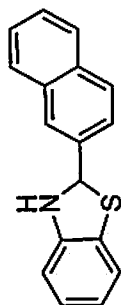
8 repetitions

OBSERVE H1 399.9551825 MHz

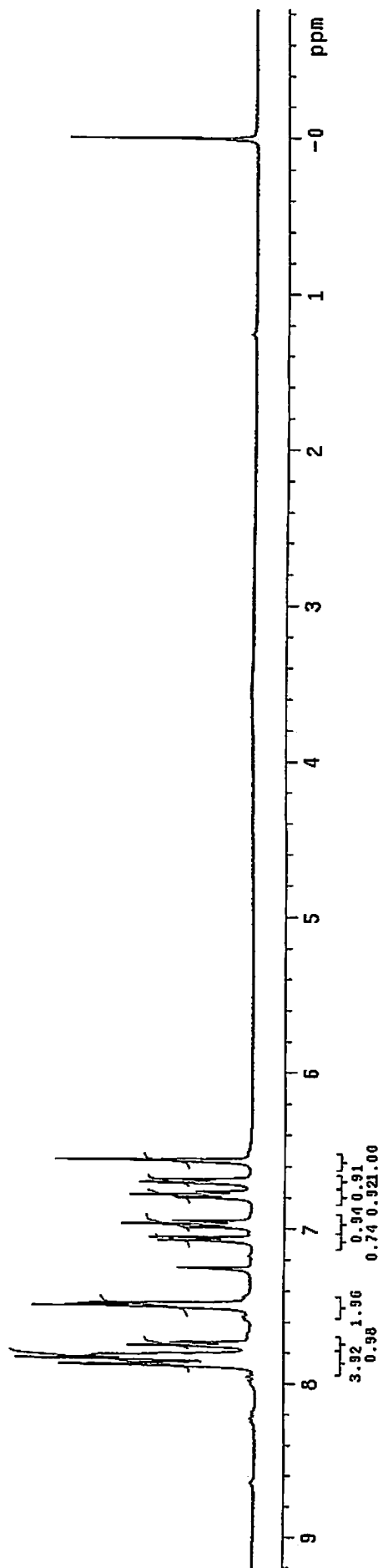
DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



compound 3d



zc2-98

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

480 repetitions

OBSERVE C13, 100.5688143 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

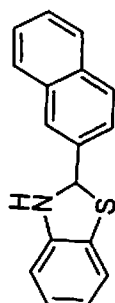
WALTZ-16 modulated

DATA PROCESSING

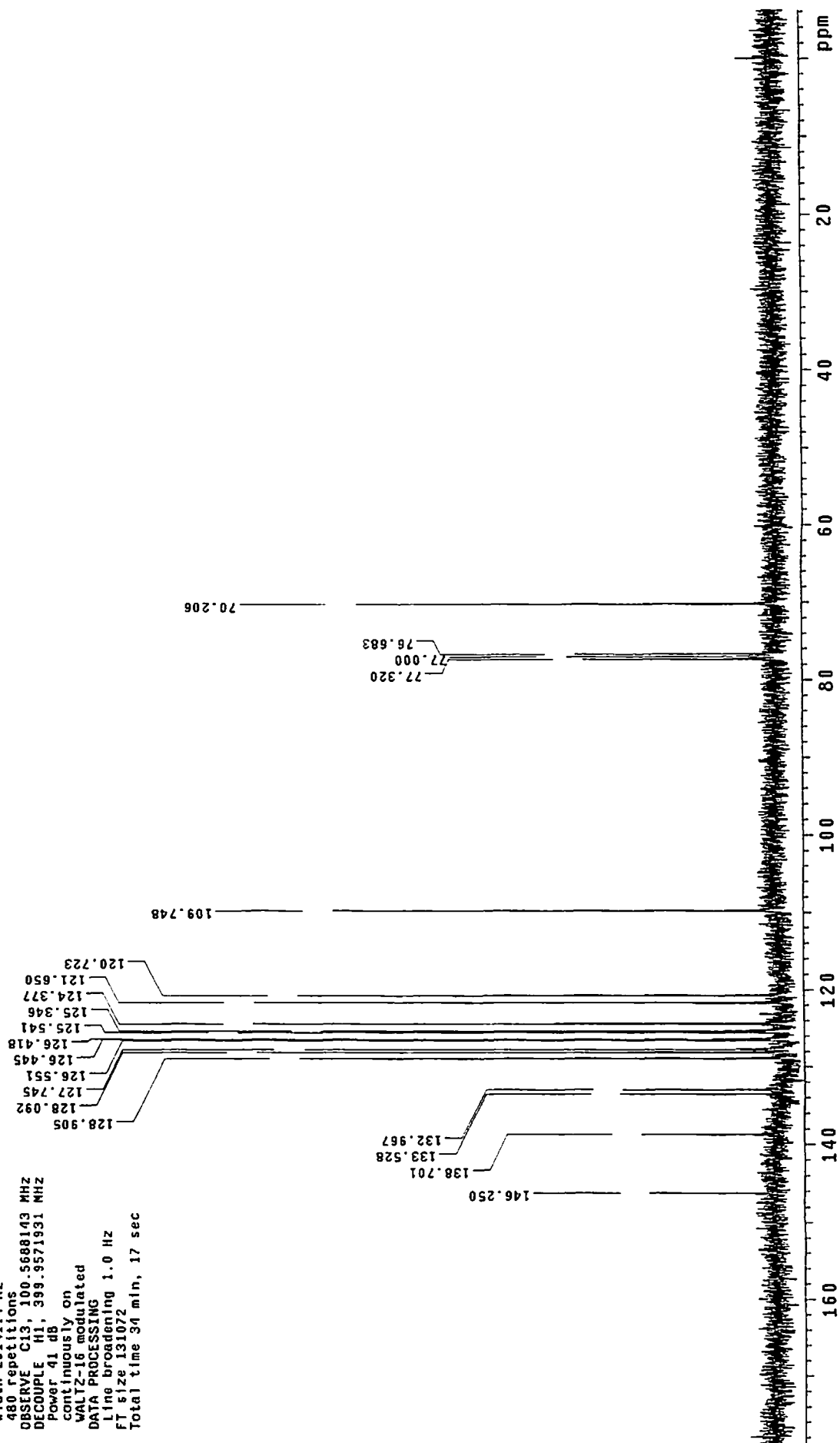
line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



Compound 3d



zc2-99

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: vnmr1

INQVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

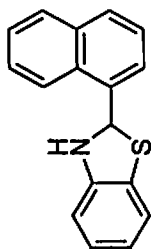
8 repetitions

OBSERVE H1 399.9551933 MHz

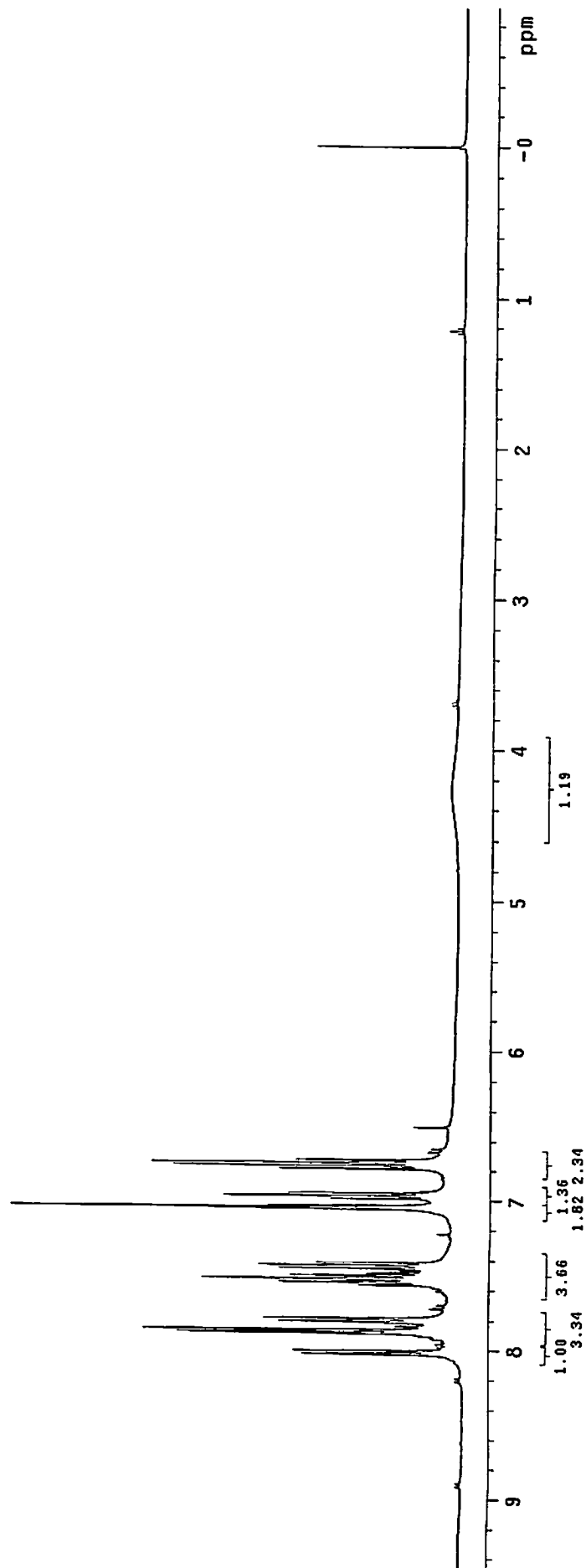
DATA PROCESSING

F1 size 85536

Total time 0 min, 40 sec



compound 3e



zc2-99

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

544 repetitions

OBSERVE C13, 100.5888147 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

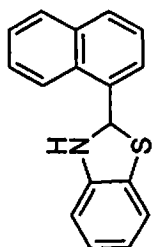
WALTZ-16 modulated

DATA PROCESSING

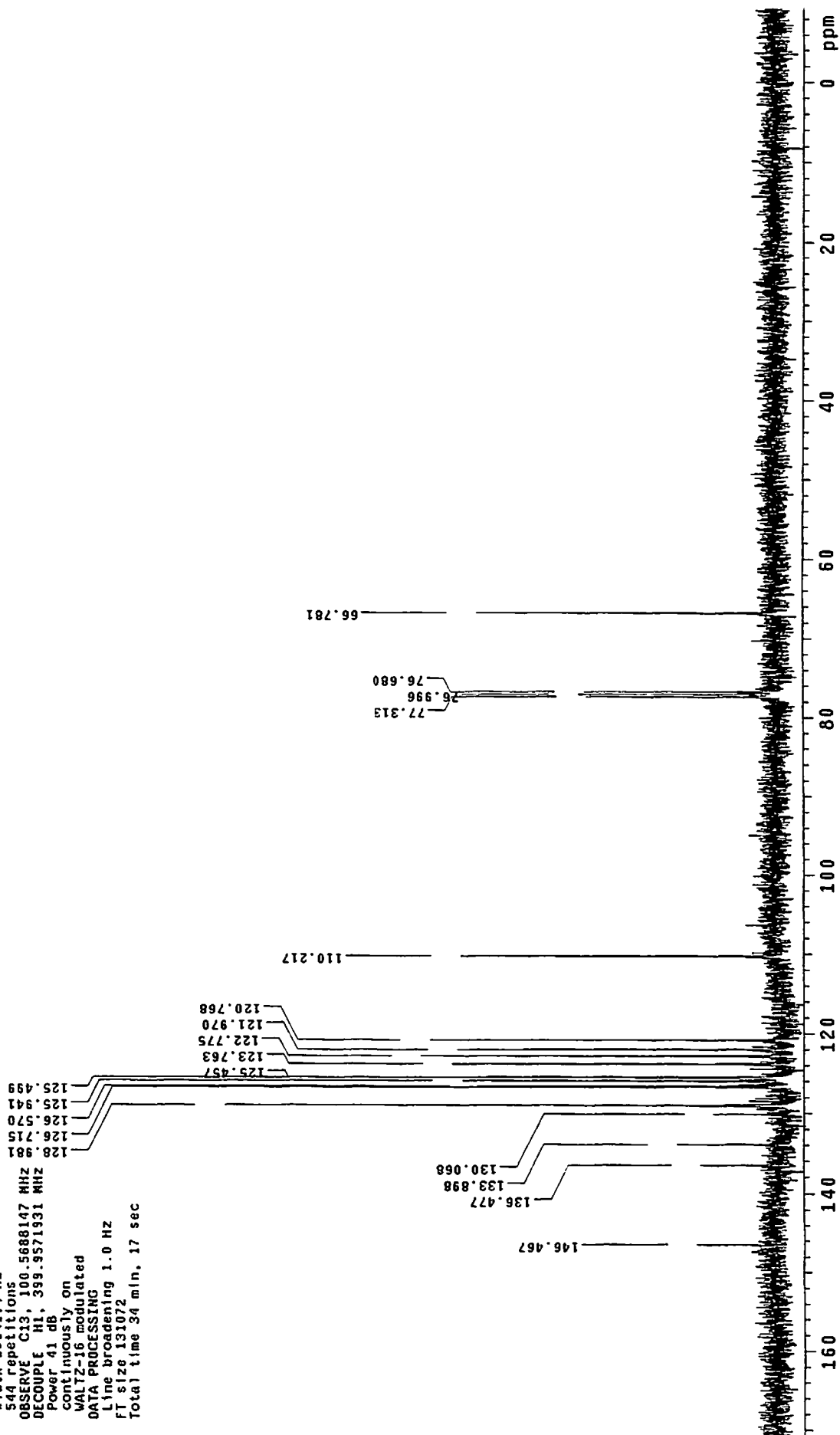
Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



compound 3a



zc2-62

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: vmr1

INOVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5995.7 Hz

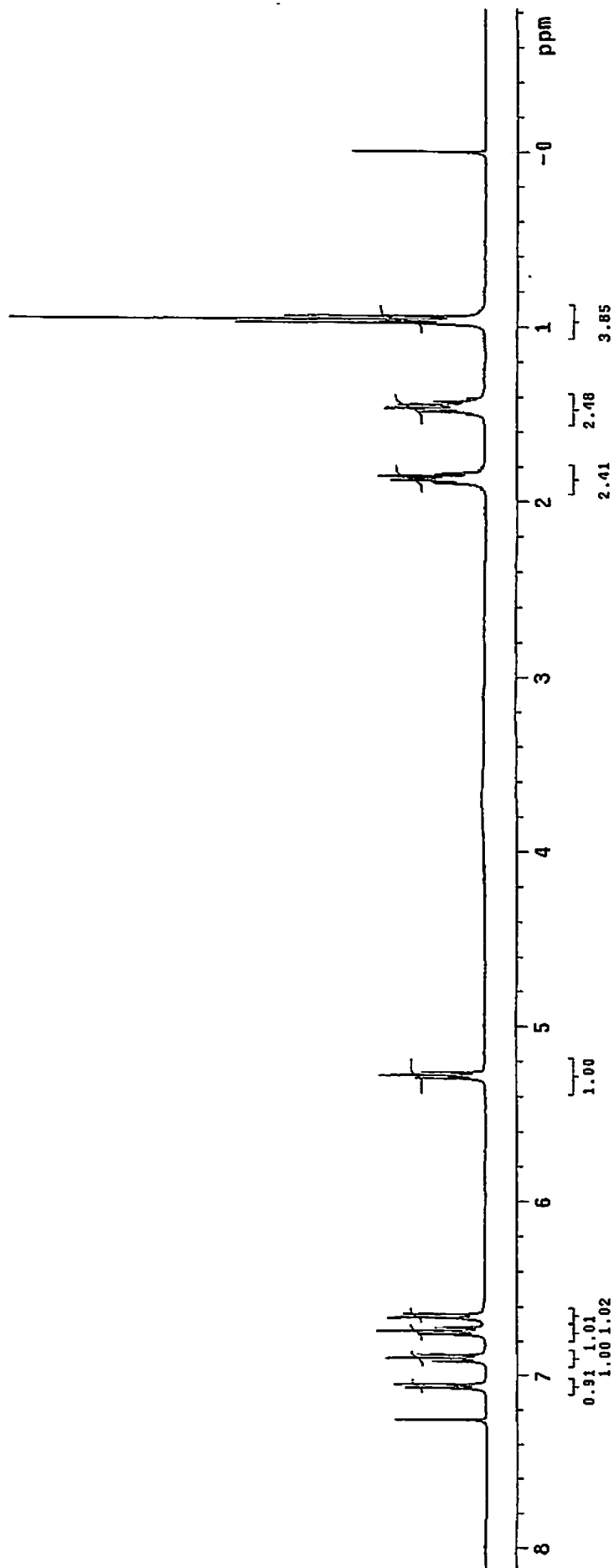
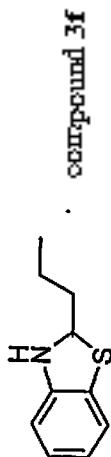
8 repetitions

OBSERVE H1, 399.9551812 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zc2-62

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

568 repetitions

OBSERVE C13, 100.5688128 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

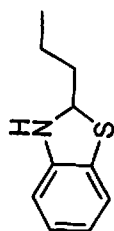
WALTZ-16 modulated

DATA PROCESSING

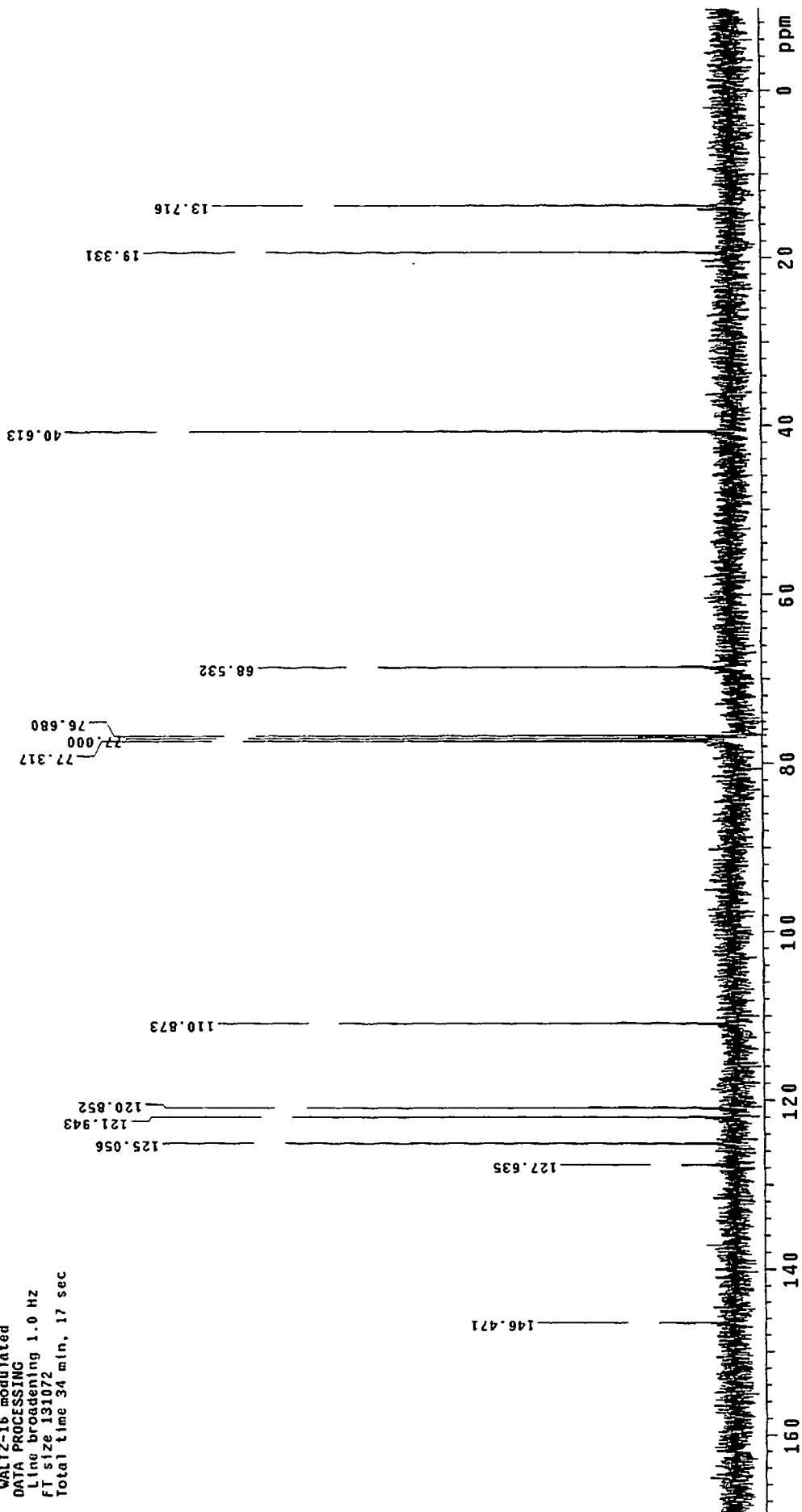
Line broadening 1.0 Hz

FI size 131072

Total time 34 min, 17 sec



compound 3f

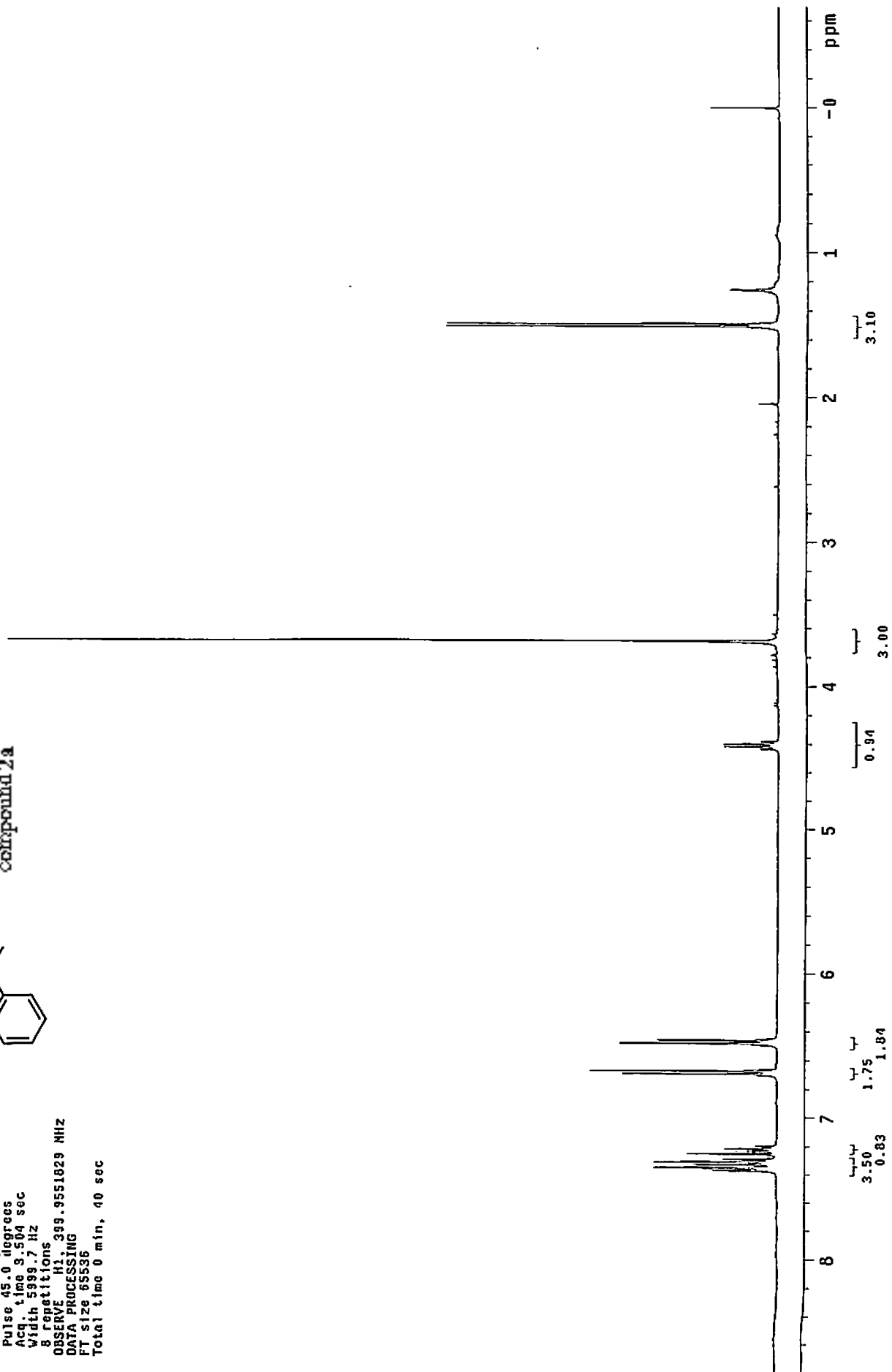
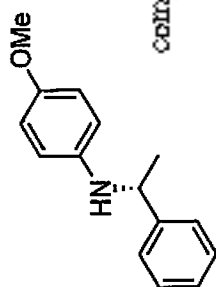


zc3-17

Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: vnmr1
INOVA-400 "uq00"

Relax. delay 1.496 sec
Pulse 45.0 degrees
Acq. time 3.504 sec
Width 5999.7 Hz
8 repetitions

OBSERVE H1 399.9551829 MHz
DATA PROCESSING
FT size 35536
Total time 0 min, 40 sec



zc3-17

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

992 repetitions

OBSERVE C13, 100.5688105 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

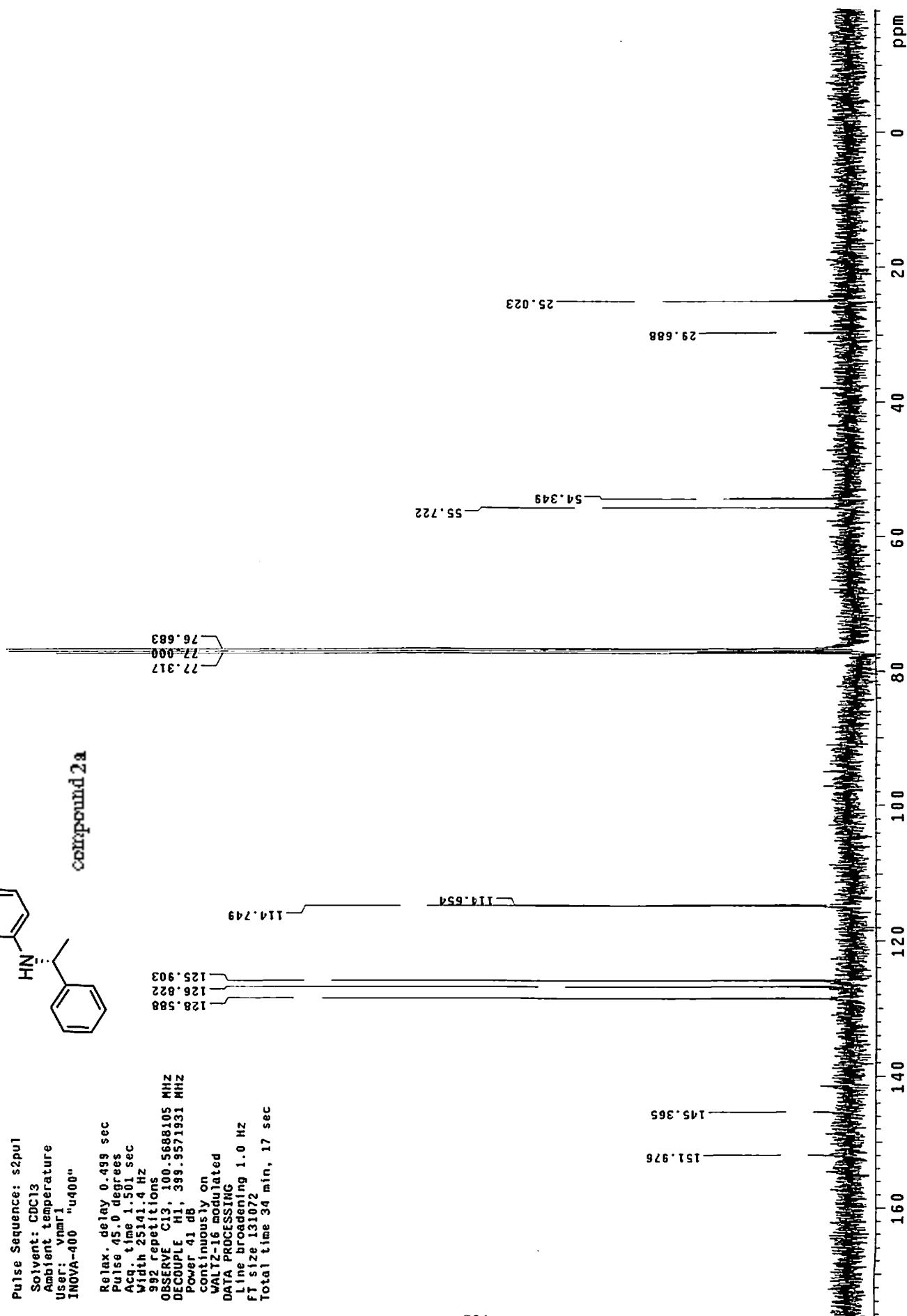
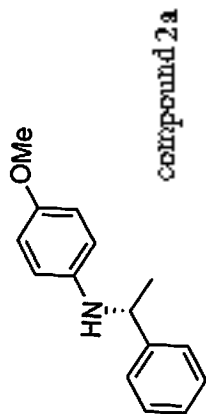
WALTZ-16 modulated

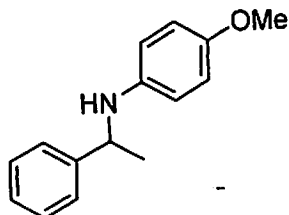
DATA PROCESSING

Line broadening 1.0 Hz

FI size 131072

Total time 34 min, 17 sec

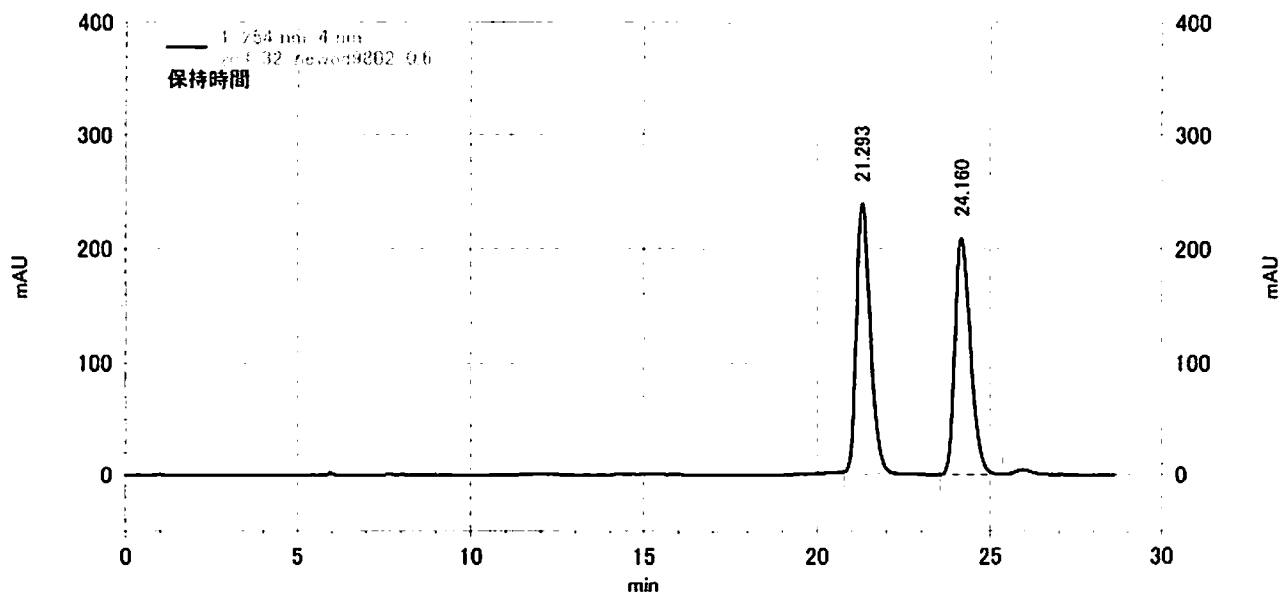




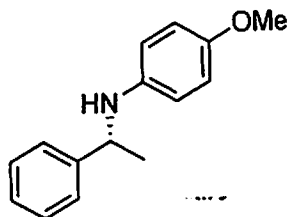
rac- 2a

面積%レポート

データファイル名: D:\データ\chen\zc3-32-newod9802-0.6.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.6ml.met
 ユーザー名: System
 分析日時: 2009/01/14 19:12:17
 印刷日時: 2009/01/26 18:38:33



名前	保持時間	面積	面積%	ピークシンコード
1: 254 nm, 4 nm結果	21.29	26298325	50.083	BB
	24.16	26210780	49.917	BB
トータル		52509105	100.000	

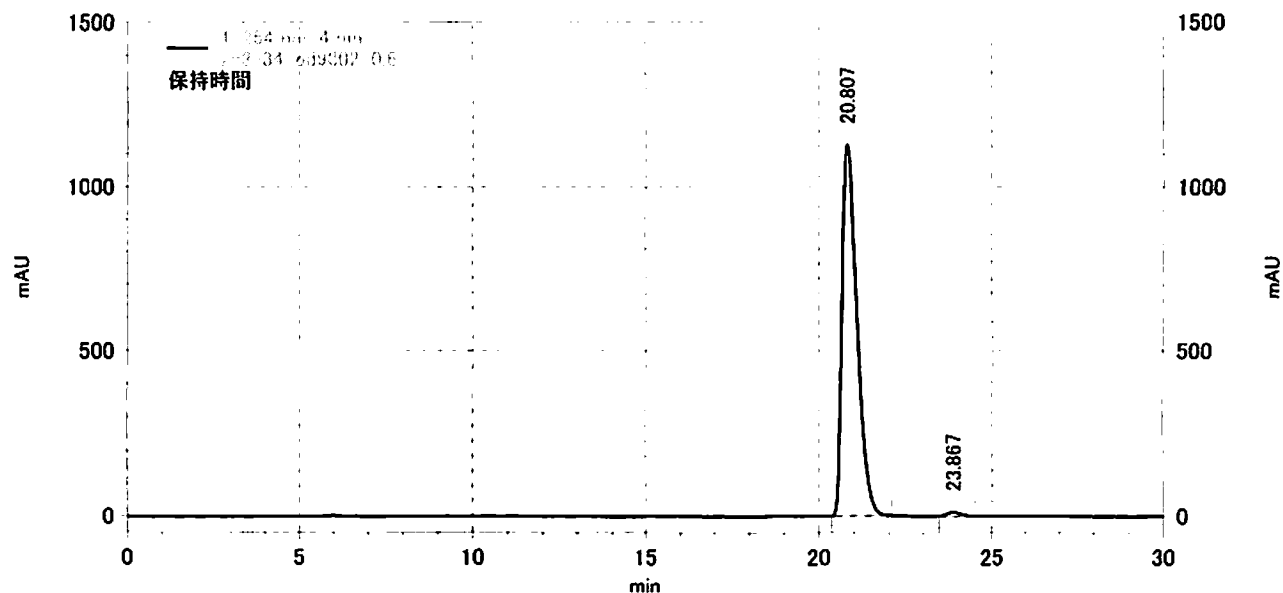


compound 2a

ページ 1/1

面積%レポート

データファイル名: D:\データ\chen\zc3-34-od9802-0.6.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.6ml.met
 ユーザー名: System
 分析日時: 2009/01/16 13:10:53
 印刷日時: 2009/01/26 18:40:02



1: 254 nm, 4
nm結果

名前	保持時間	面積	面積%	ピークコード
	20.81	134538902	99.037	BB
	23.87	1308531	0.963	BI
トータル		135847433	100.000	

zc3-39

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: vnmr1

INDVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.594 sec

Width 5999.7 Hz

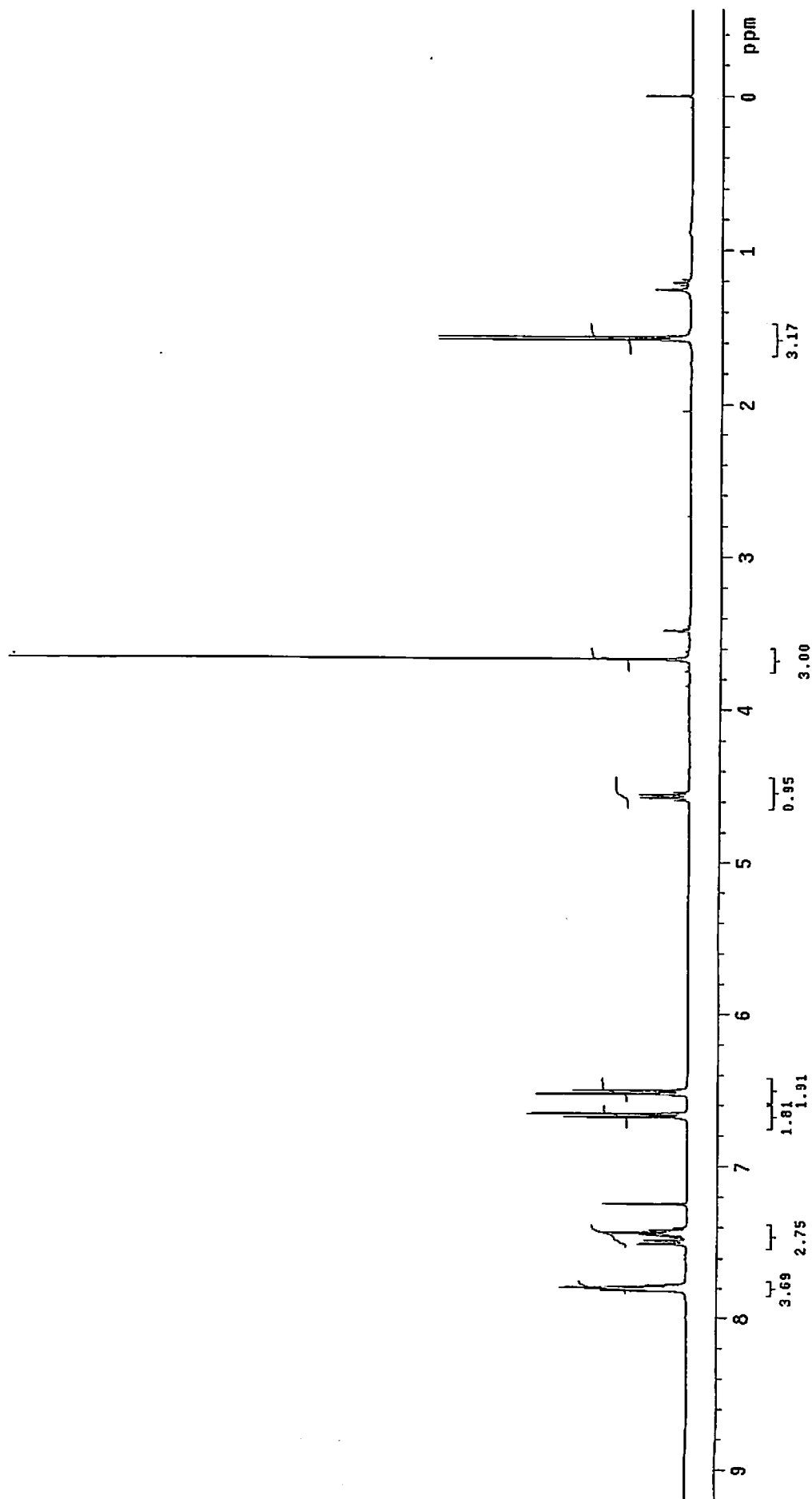
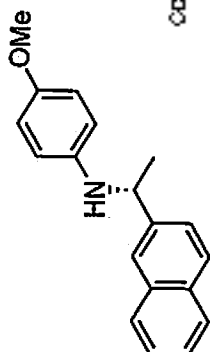
8 repetitions

OBSERVE H1, 399.9551836 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zc3-39

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

608 repetitions

OBSERVE C13, 100.5688112 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

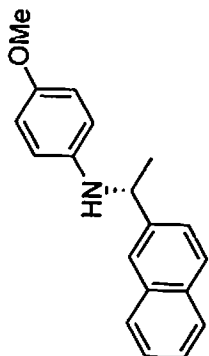
WALTZ-16 modulated

DATA PROCESSING

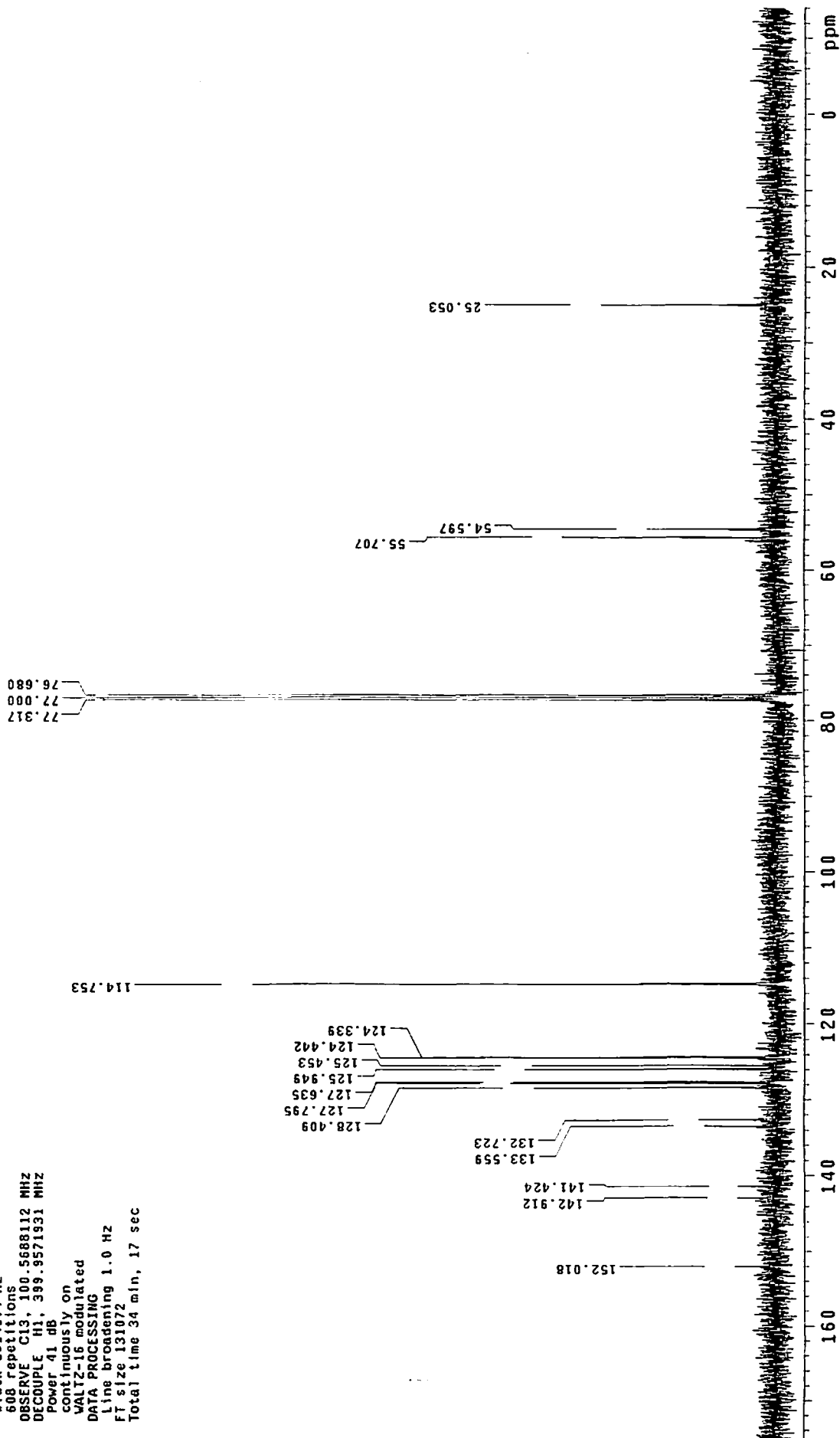
Line broadening 1.0 Hz

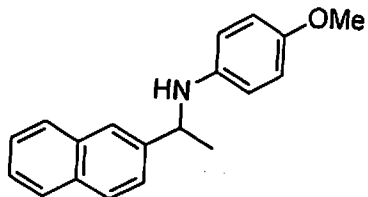
FT size 131072

Total time 34 min, 17 sec



Compound 2b



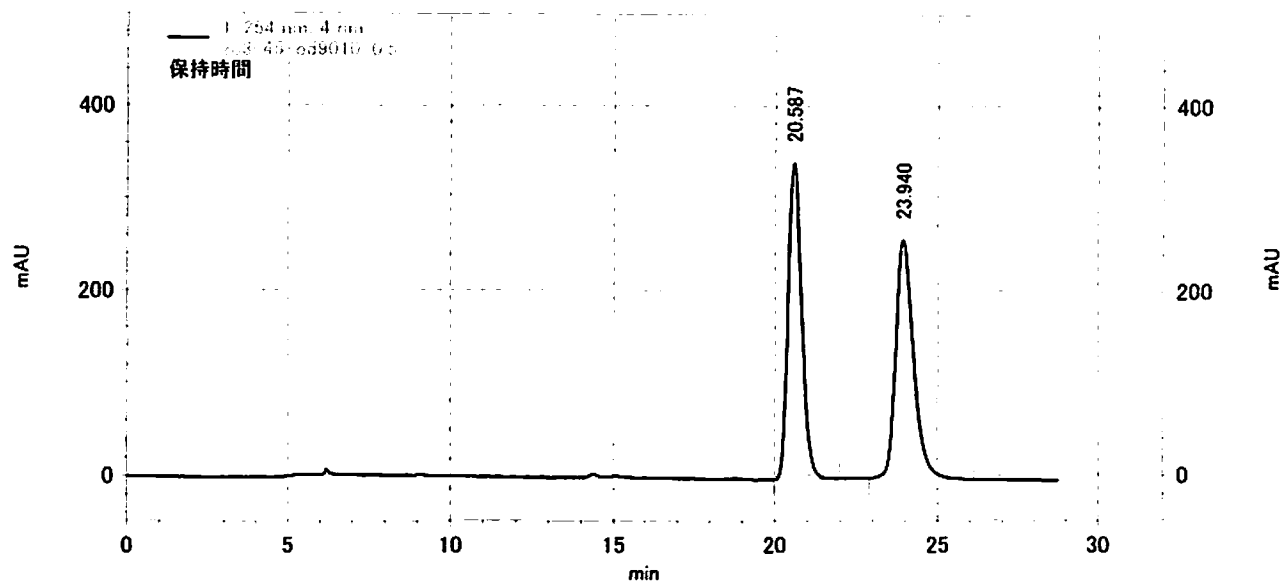


TAC-2b

面積%レポート

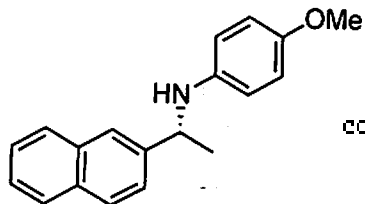
ページ 1/1

データファイル名: D:\データ\chen\zc3-45-od9010-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/19 15:34:34
 印刷日時: 2009/01/26 18:45:31



1: 254 nm, 4 nm
 結果

名前	保持時間	面積	面積%	ピーク番号
	20.59	39252429	49.926	BB
	23.94	39368476	50.074	BB
トータル		78620905	100.000	

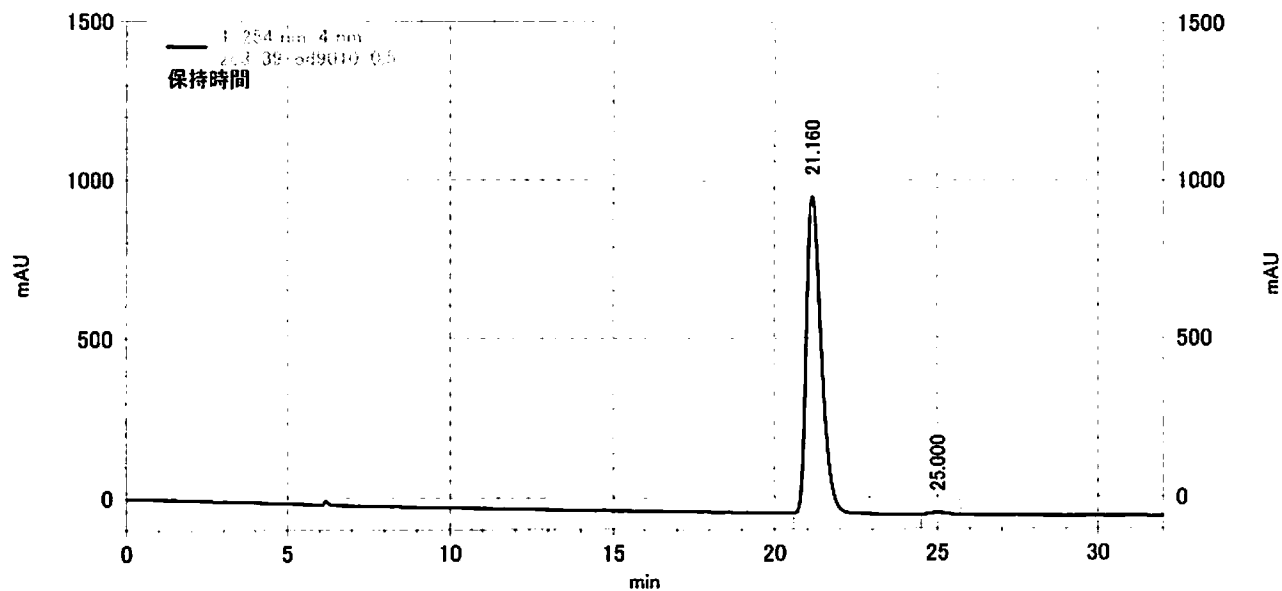


compound 2b

ページ 1/1

面積%レポート

データファイル名: D:\データ\chen\zc3-39-od9010-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/18 14:06:37
 印刷日時: 2009/01/26 18:43:36



1: 254 nm, 4
nm結果

名前	保持時間	面積	面積%	ピークコード
	21.16	126174370	99.107	BB
	25.00	1136334	0.893	BI
トータル		127310704	100.000	

zc3-37

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5989.7 Hz

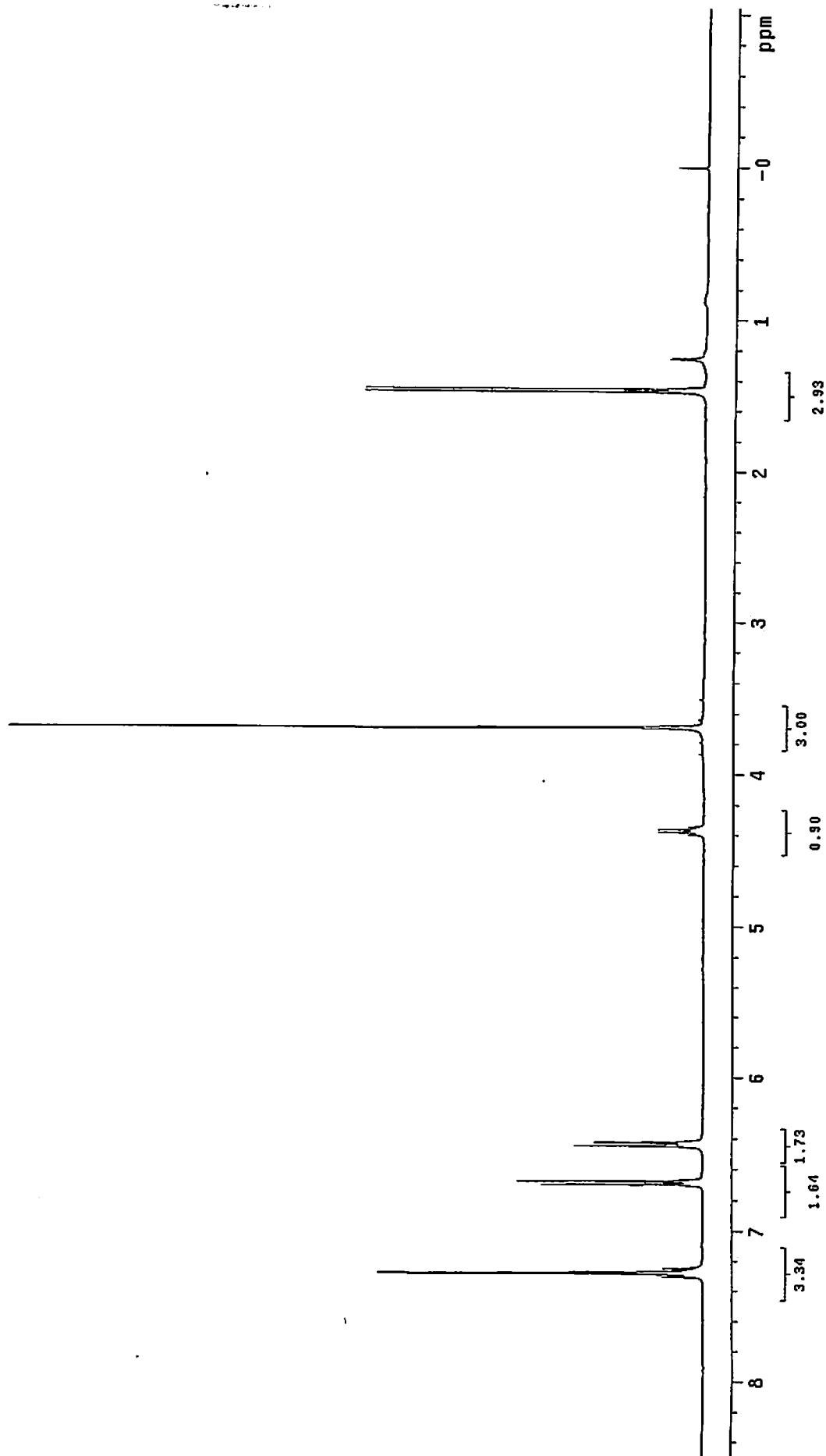
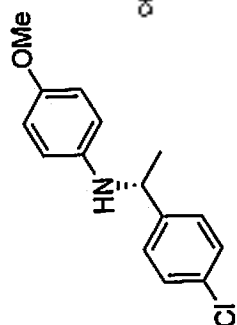
8 repetitions

OBSERVE H1, 399.9551860 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zc3-37

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

240 repetitions

OBSERVE C13, 100.5688135 MHz

DECOUPLE H1, 399.5571931 MHz

Power 41 dB

continuously on

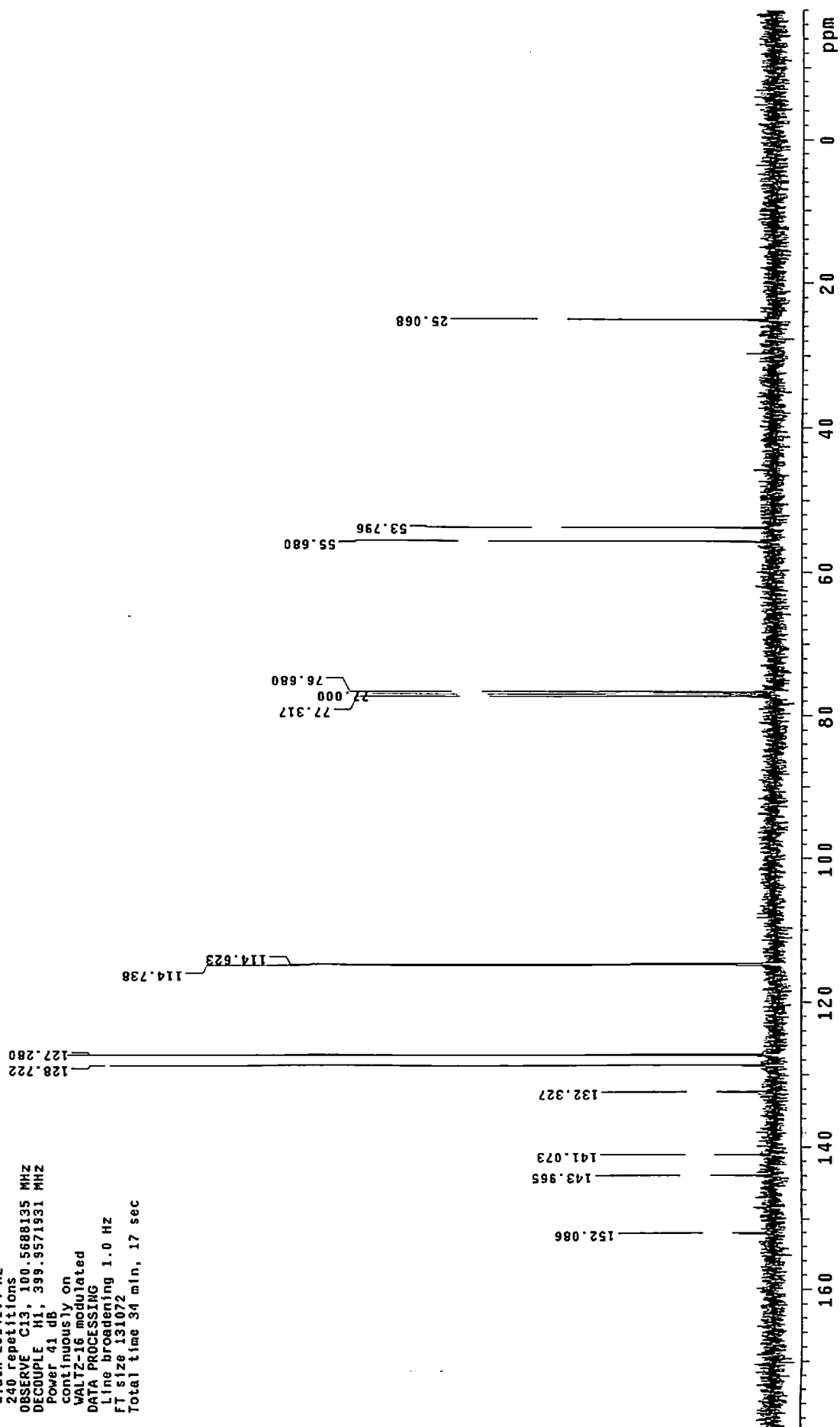
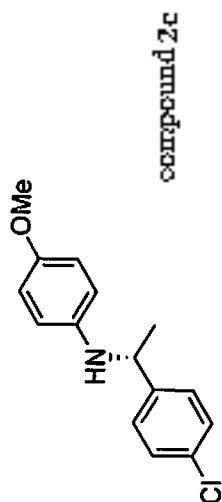
WALTZ-16 modulated

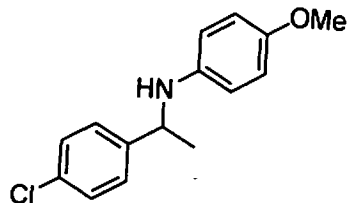
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



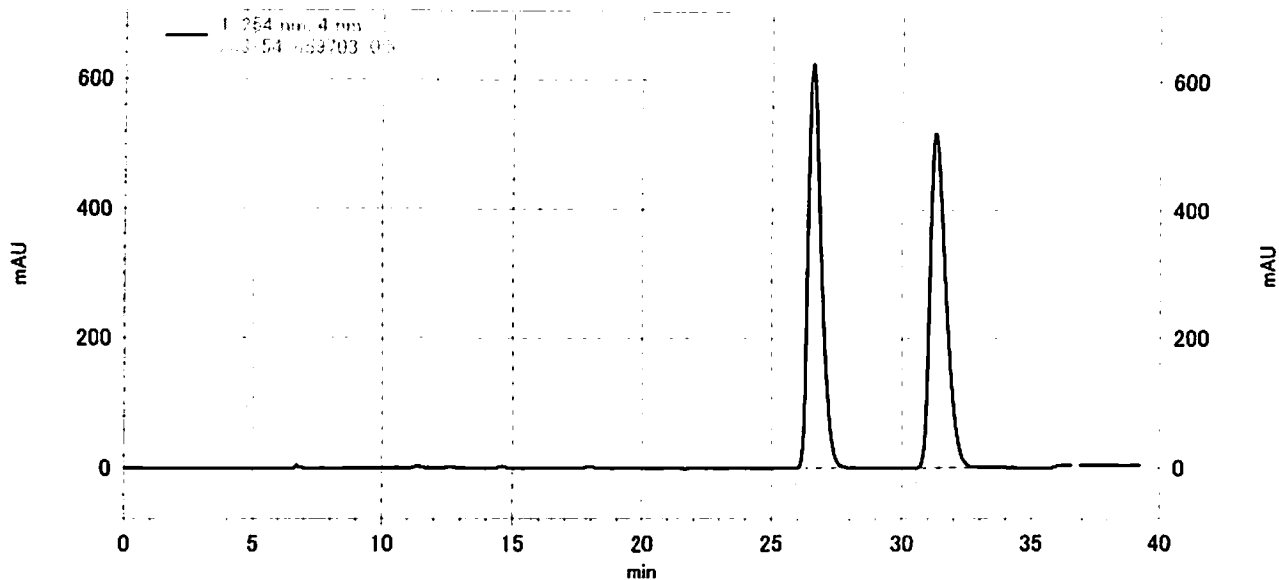


rac-2a

面積%レポート

ページ 1/1

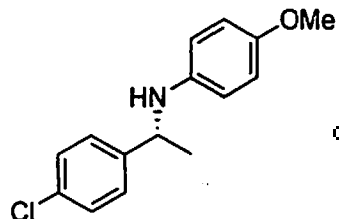
データファイル名: D:\データ\chen\zc3-54-od9703-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/23 15:18:57
 印刷日時: 2009/01/26 11:34:08



1: 254 nm, 4 nm結果

名前	保持時間	面積	面積%	ピークコード
	26.57	87636256	49.947	BB
	31.30	87821236	50.053	BB

トータル		175457492	100.000	
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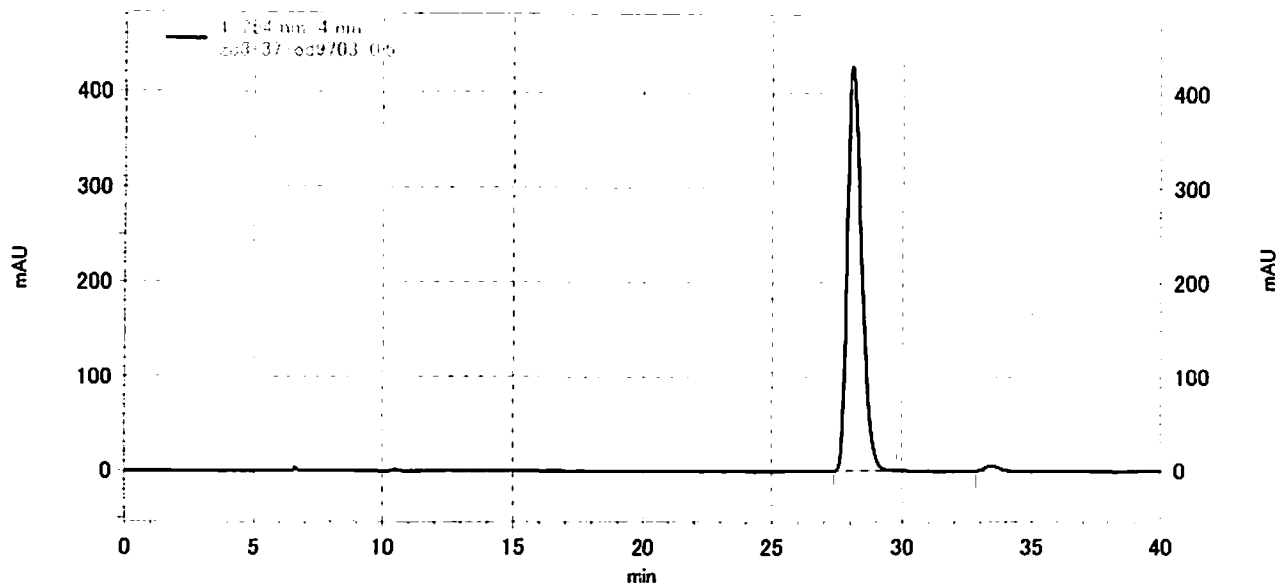


compound 2c

面積%レポート

ページ 1/1

データファイル名: D:\データ\chen\zc3-37-od9703-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.meth
 ユーザー名: System
 分析日時: 2009/01/17 18:02:35
 印刷日時: 2009/01/26 11:35:25



1: 254 nm, 4 nm結果

名前	保持時間	面積	面積%	ベースラインコード
	28.08	65553017	98.591	BB
	33.44	937144	1.409	BB

トータル		66490161	100.000	
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zc3-38

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INQVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

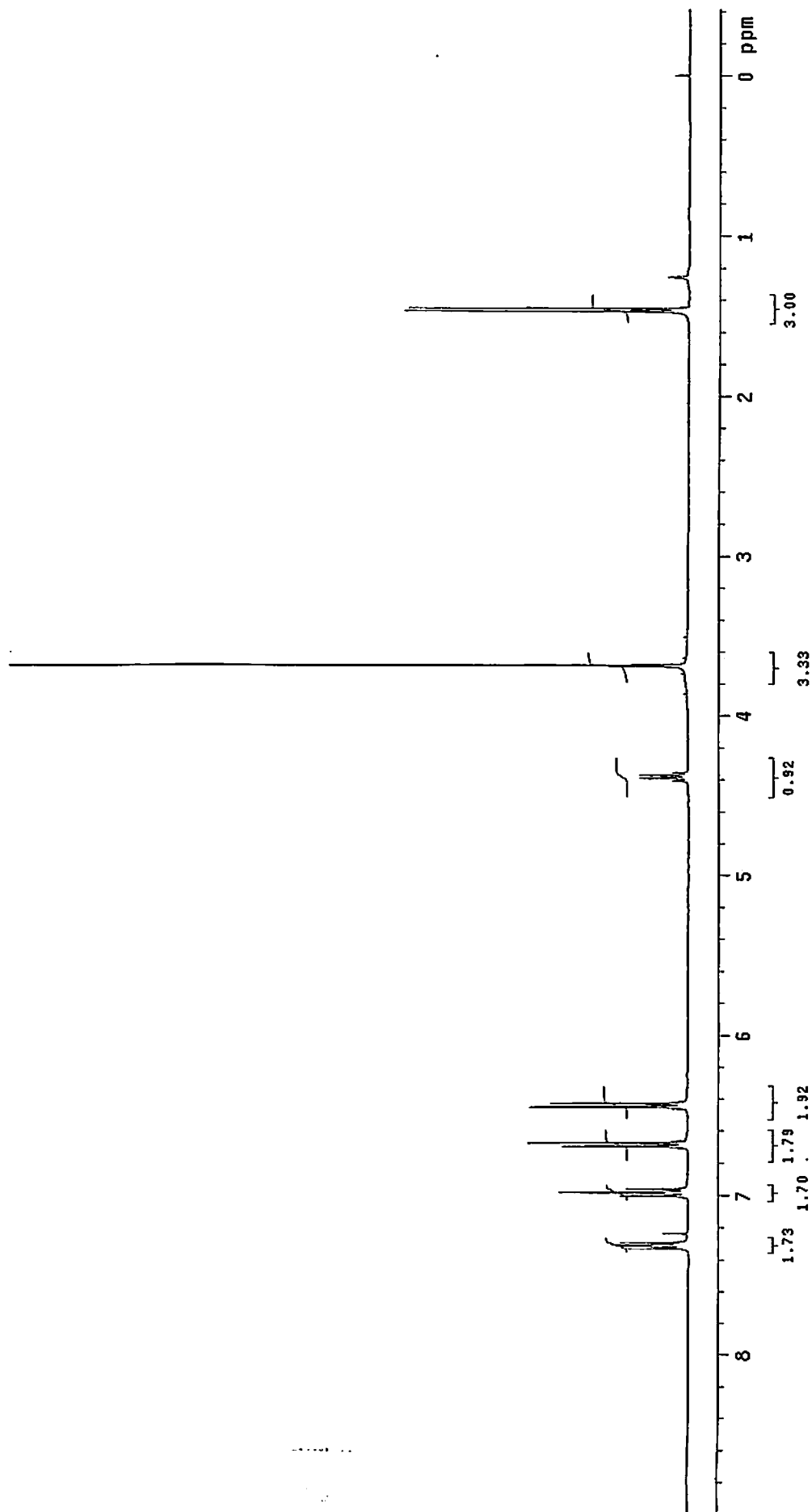
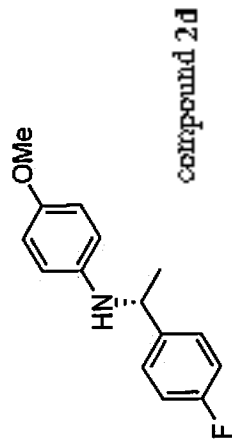
8 repetitions

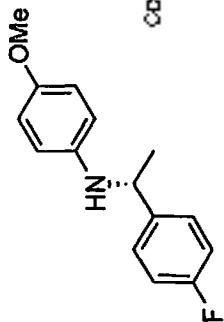
OBSERVE H1, 399.9551880 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec





compound 2d

zc3-38

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

304 repetitions

OBSERVE C13, 100.5688139 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

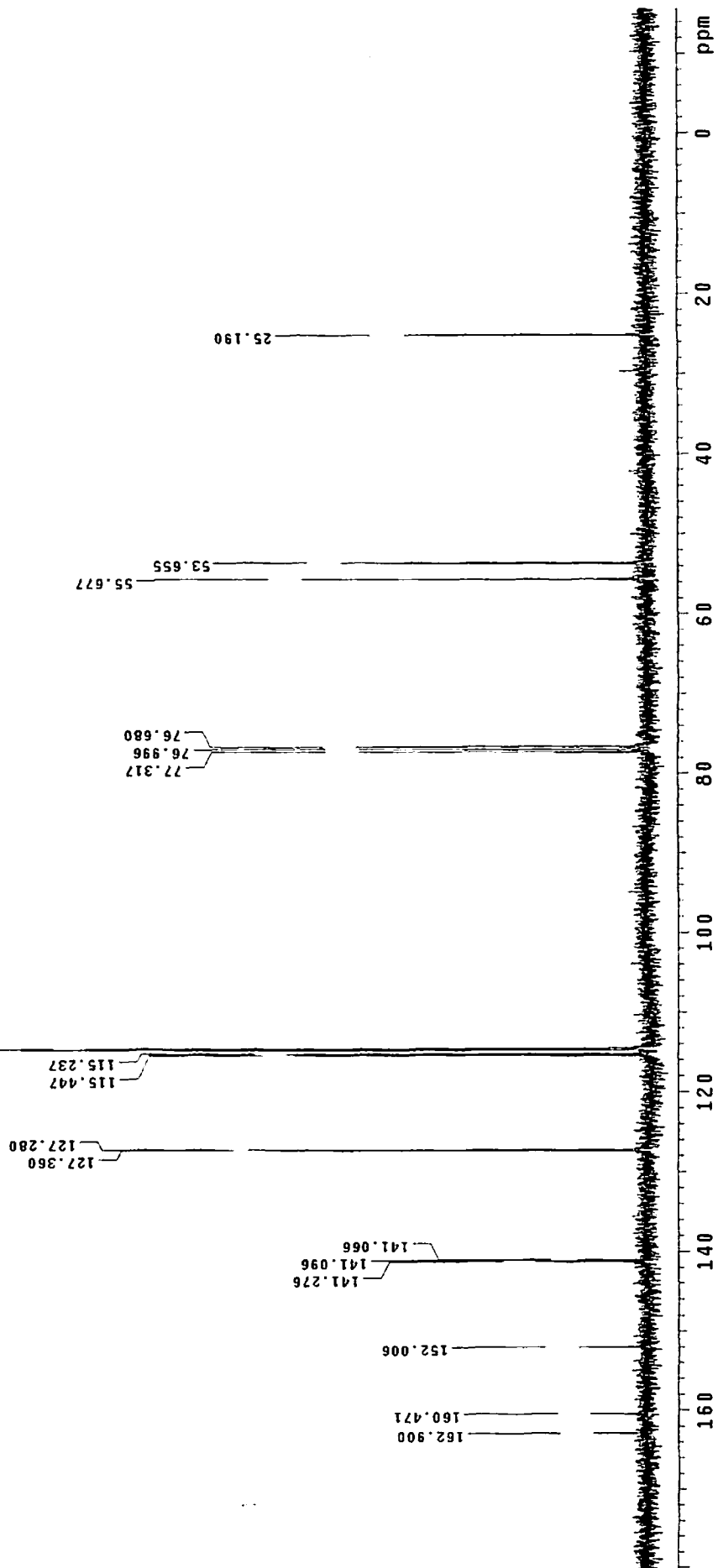
WALTZ-16 modulated

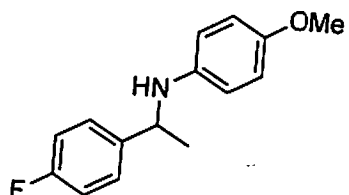
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



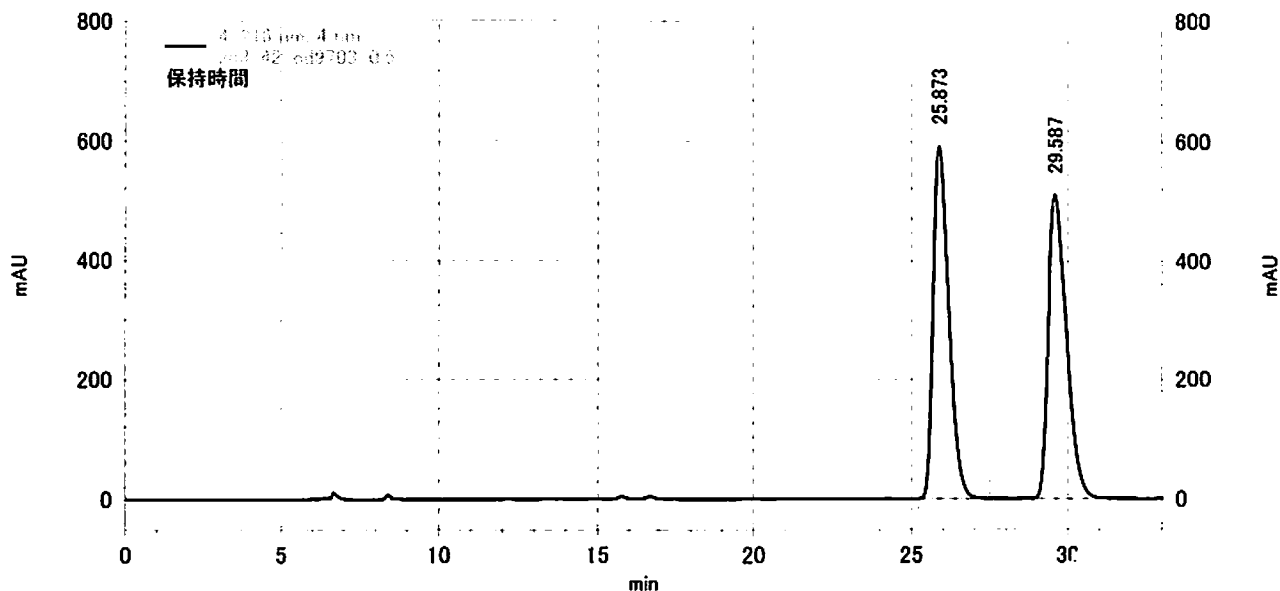


rac-2d

ページ 1/1

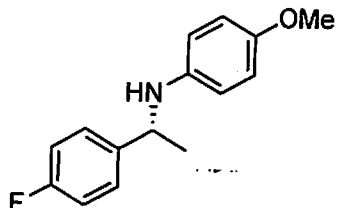
面積%レポート

データファイル名: D:\データ\chen\zc3-42-od9703-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/17 18:51:03
 印刷日時: 2009/01/26 18:29:12



4: 216 nm, 4 nm結果

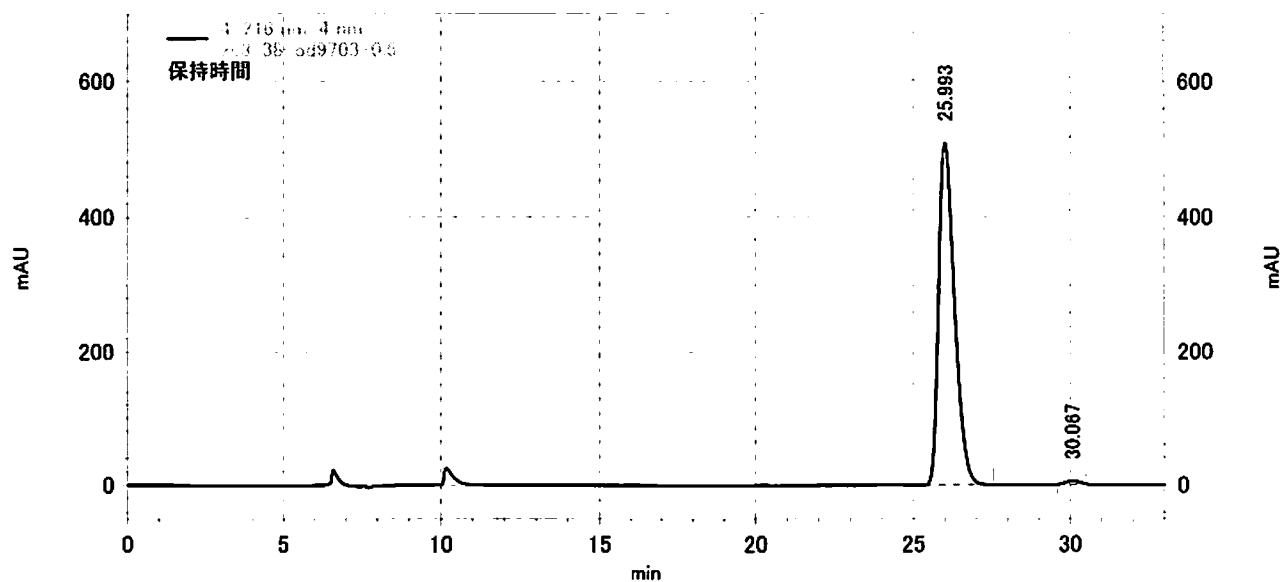
名前	保持時間	面積	面積%	ベースラインコード
	25.87	81459346	49.827	BB
	29.59	82025330	50.173	BB
トータル		163484676	100.000	



compound 2d

面積%レポート

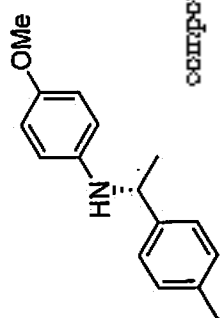
データファイル名: D:\データ\chen\zc3-38-od9703-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/17 19:32:50
 印刷日時: 2009/01/26 18:35:55



4: 216 nm, 4
nm結果

名前	保持時間	面積	面積%	ベースラインコード
	25.99	71286254	99.144	BB
	30.07	615486	0.856	BI

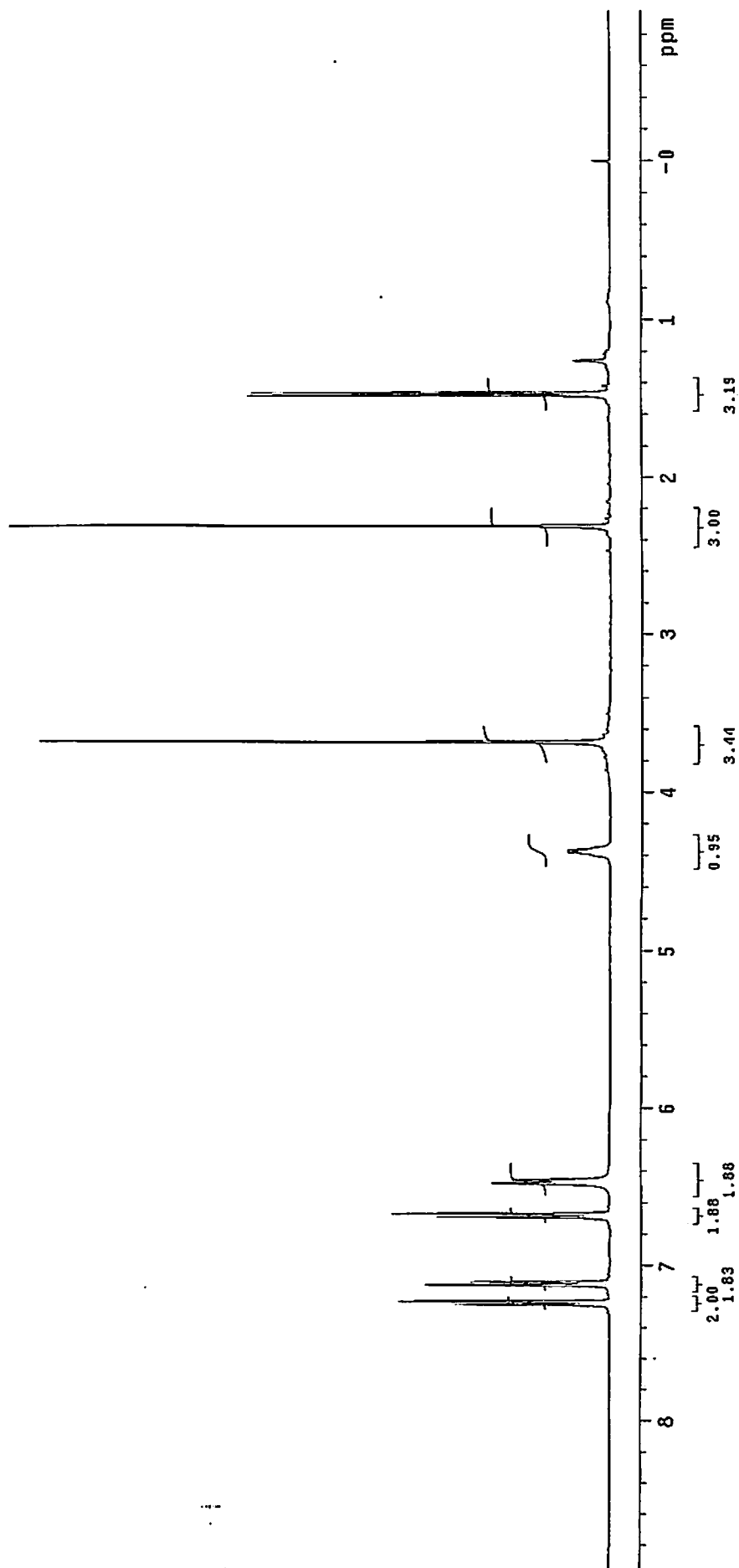
トータル		71901740	100.000	
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2c3-41

Pulse Sequence: s2pu1
 Solvent: CDCl3
 Ambient temperature
 User: Vmwr1
 INOVA-400 "u400"

Relax. delay 1.496 sec
 Pulse 45.0 degrees
 Acq. time 3.504 sec
 Width 5899.7 Hz
 8 repetitions
 OBSERVE H1, 399.9551911 MHZ
 DATA PROCESSING
 FT size 65536
 Total time 0 min, 40 sec



zc3-41

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

280 repetitions

OBSERVE C13, 100.5688151 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

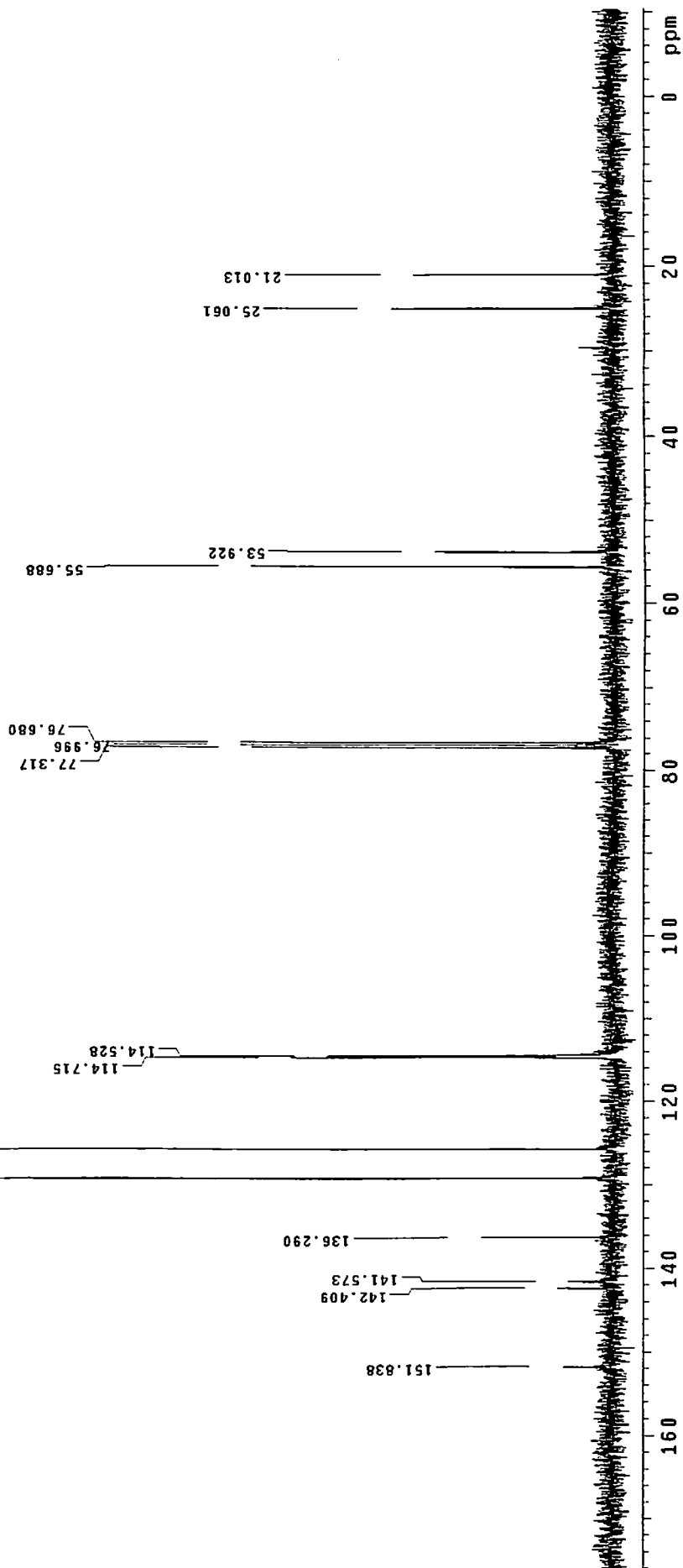
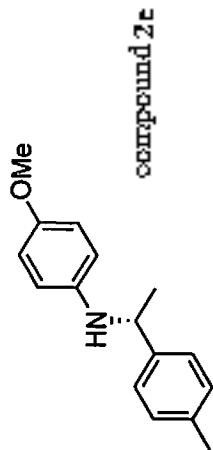
WALTZ-16 modulated

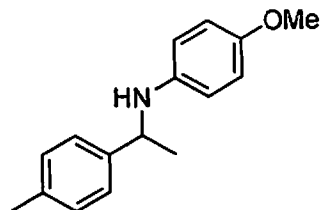
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



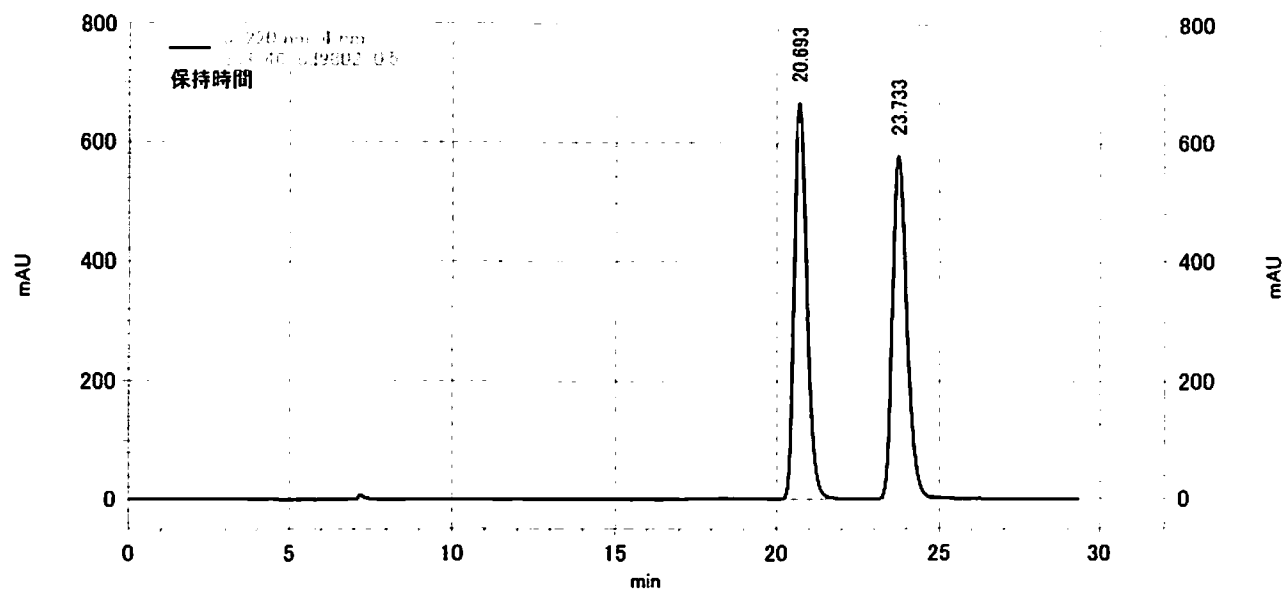


rac-2e

ページ 1/1

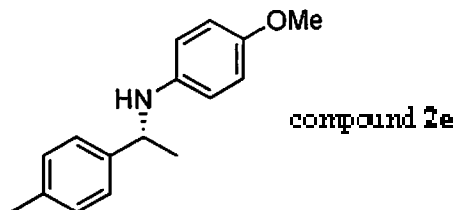
面積%レポート

データファイル名: D:\データ\chen\zc3-46-od9802-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/19 17:58:52
 印刷日時: 2009/01/26 18:52:08



3: 220 nm, 4 nm結果

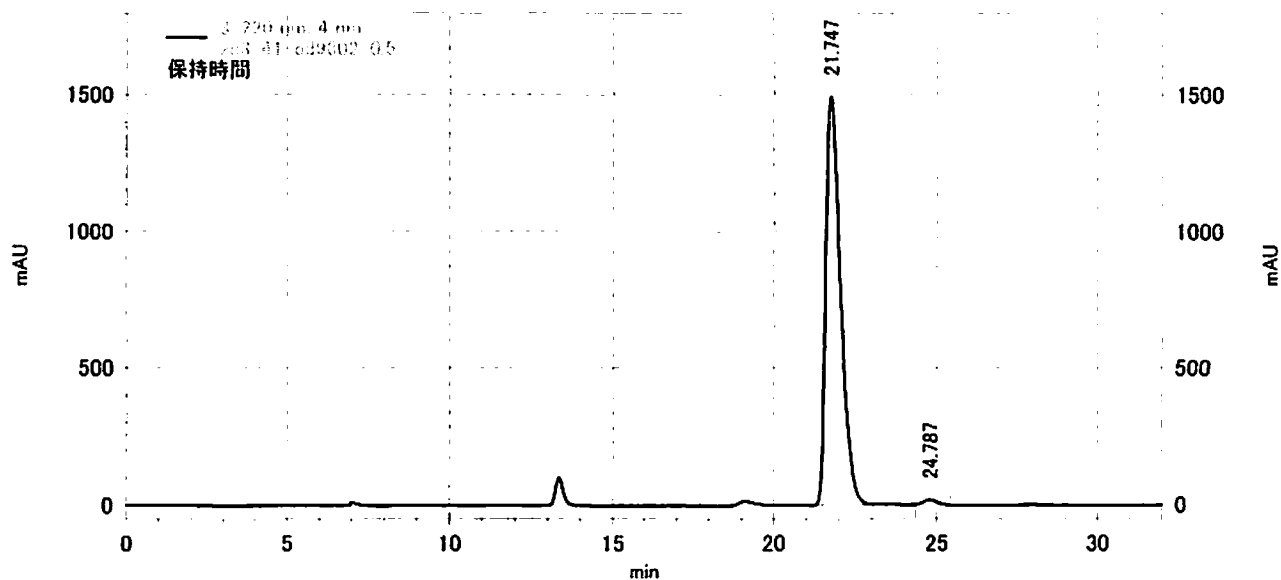
名前	保持時間	面積	面積%	ベースラインコート
	20.69	71265286	50.006	BB
	23.73	71247244	49.994	BB
トータル		142512530	100.000	



ページ 1/1

面積%レポート

データファイル名: D:\データ\chen\zc3-41-od9802-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/19 16:27:33
 印刷日時: 2009/01/26 18:49:59



3: 220 nm, 4
 nm結果

名前	保持時間	面積	面積%	ベースラインコード
	21.75	187497927	98.882	BB
	24.79	2119546	1.118	BI
トータル		189617473	100.000	

zc3-40

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

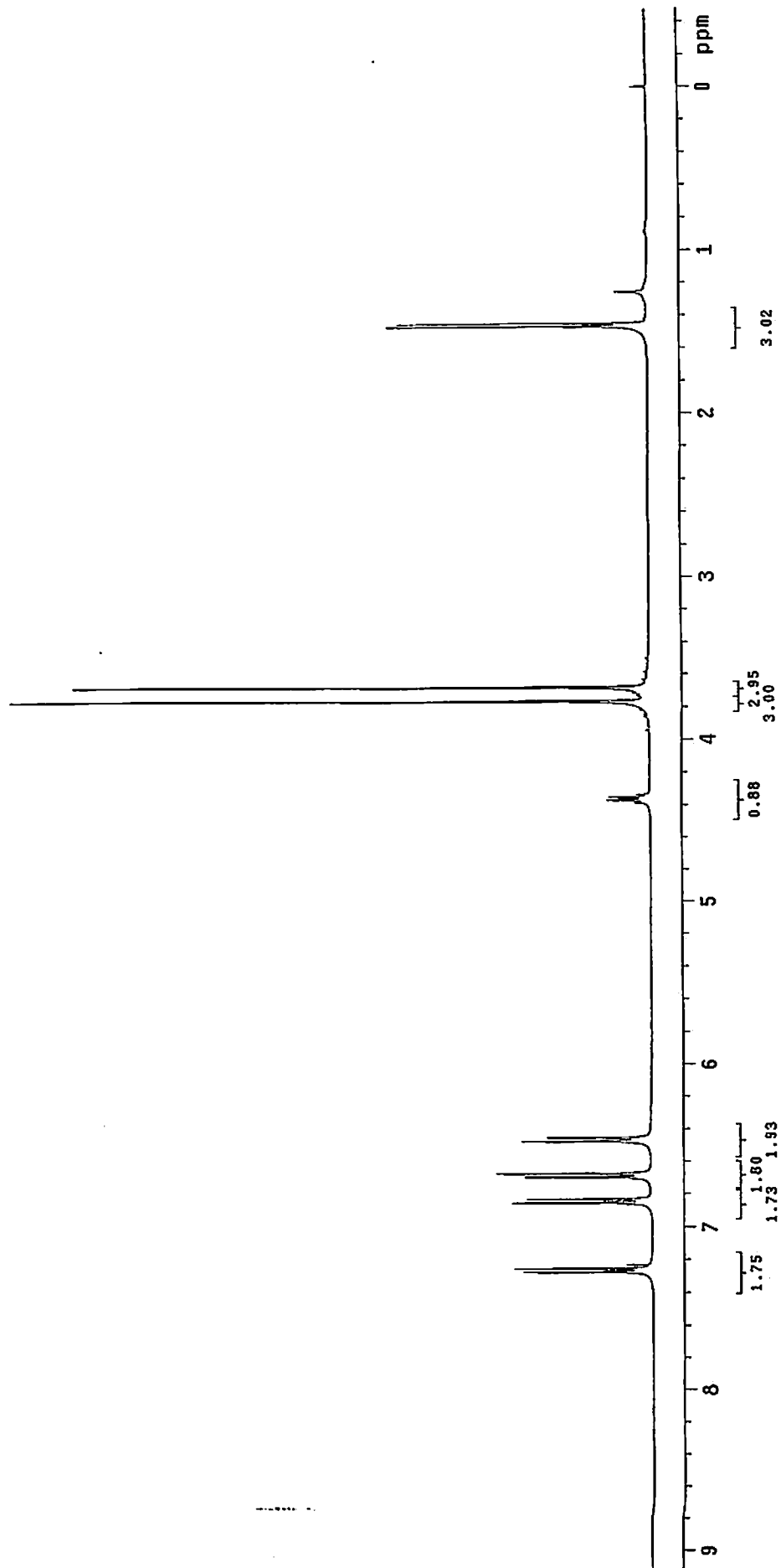
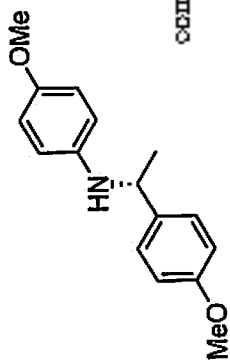
8 repetitions

OBSERVE H1, 399.9551893 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zc3-40

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

200 Repetitions

OBSERVE C13, 100.5688151 MHz

DECUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

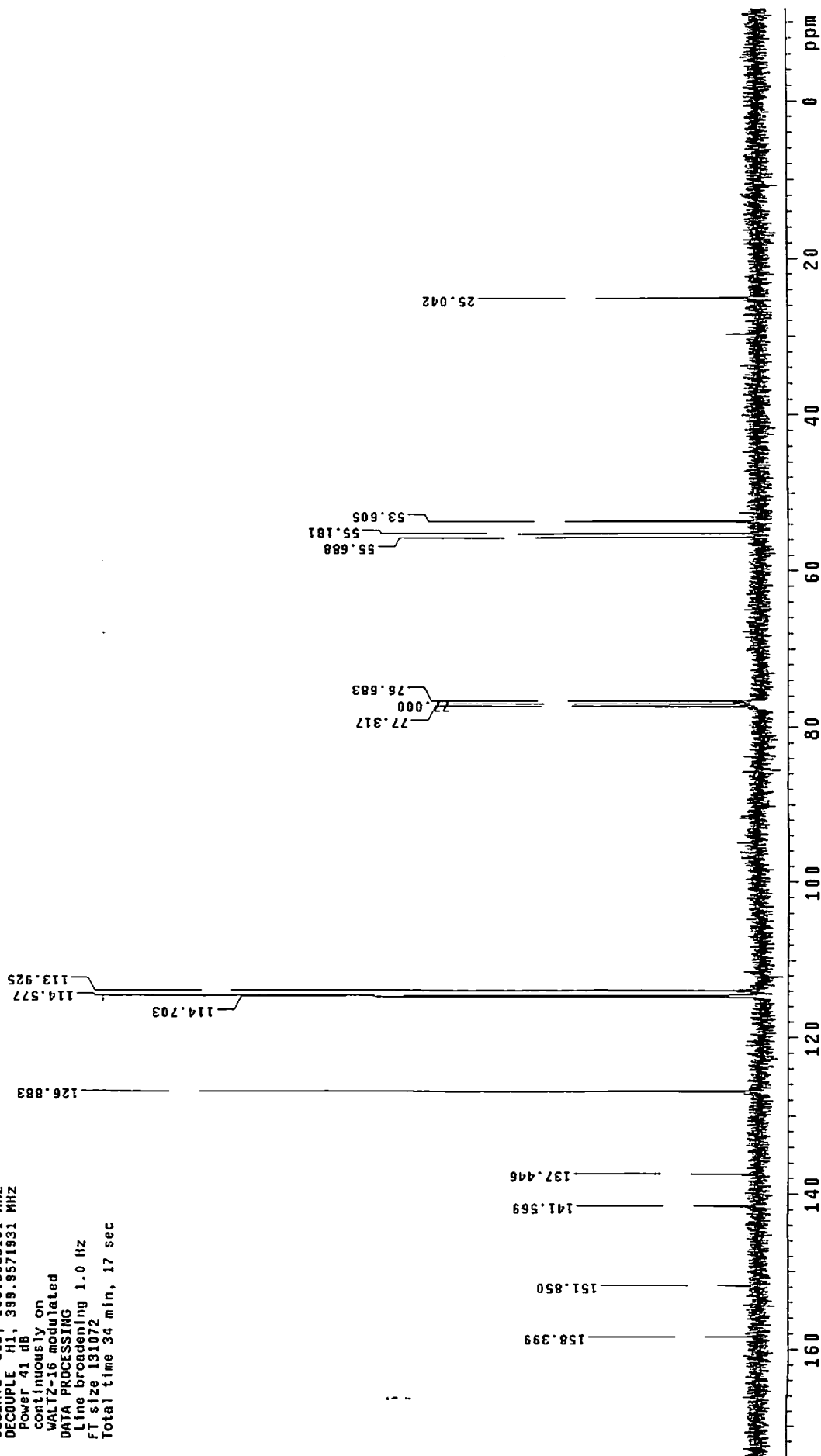
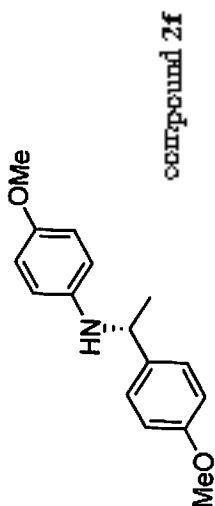
WALTZ-16 modulated

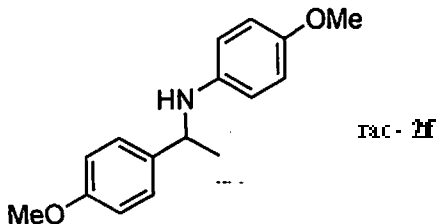
DATA PROCESSING

Line broadening 1.0 Hz

FI size 131072

Total time 34 min, 17 sec

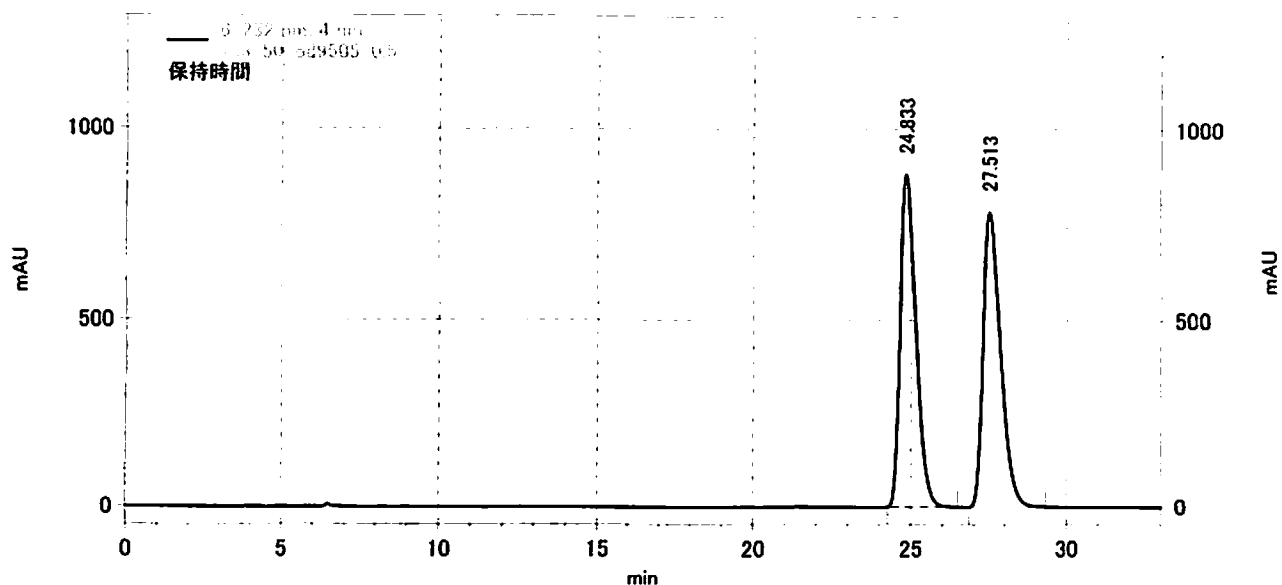




面積%レポート

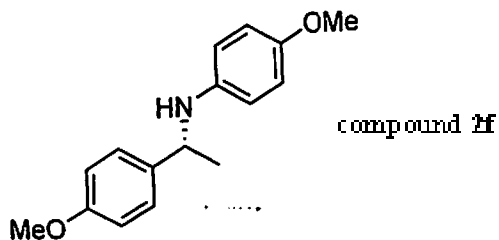
ページ 1/1

データファイル名: D:\データ\chen\zc3-50-od9505-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/20 15:59:21
 印刷日時: 2009/01/26 18:56:19



6: 232 nm, 4 nm
 nm結果

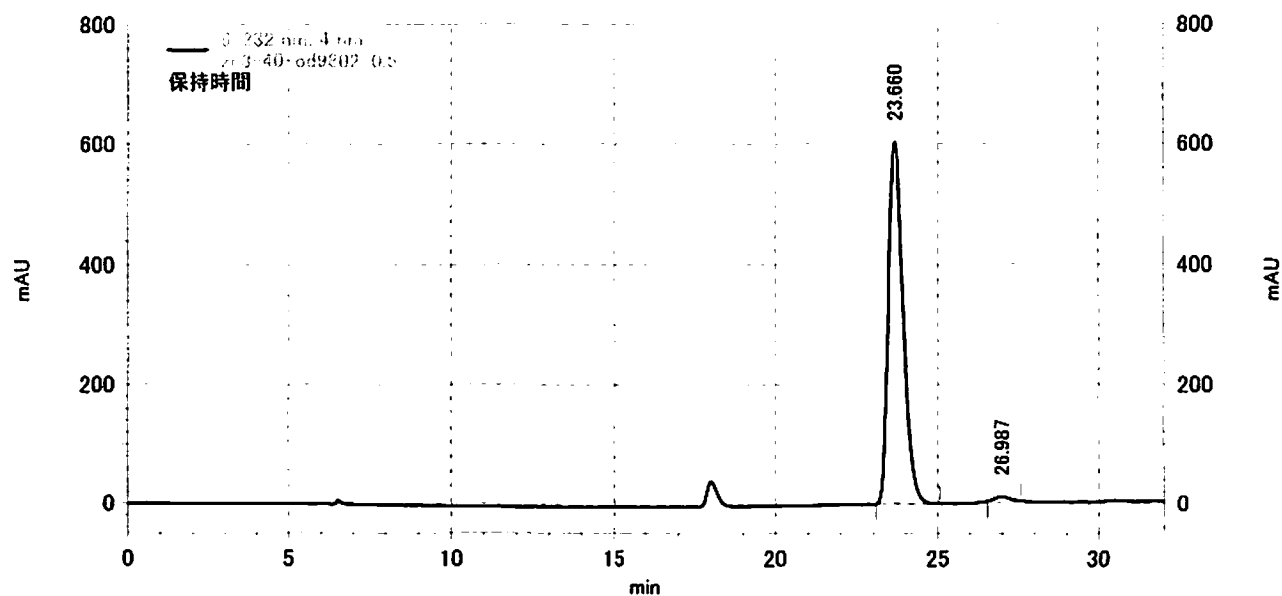
名前	保持時間	面積	面積%	ピークシンコード
	24.83	122533597	50.048	BB
	27.51	122298236	49.952	BB
トータル		244831833	100.000	



ページ 1/1

面積%レポート

データファイル名: D:\データ\chen\zc3-40-od9505-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/19 19:07:49
 印刷日時: 2009/01/26 18:54:42



6: 232 nm, 4 nm

nm結果

名前	保持時間	面積	面積%	ピークインコード
	23.66	76505373	98.775	BB
	26.99	948470	1.225	BI
トータル		77453843	100.000	

zc3-14

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

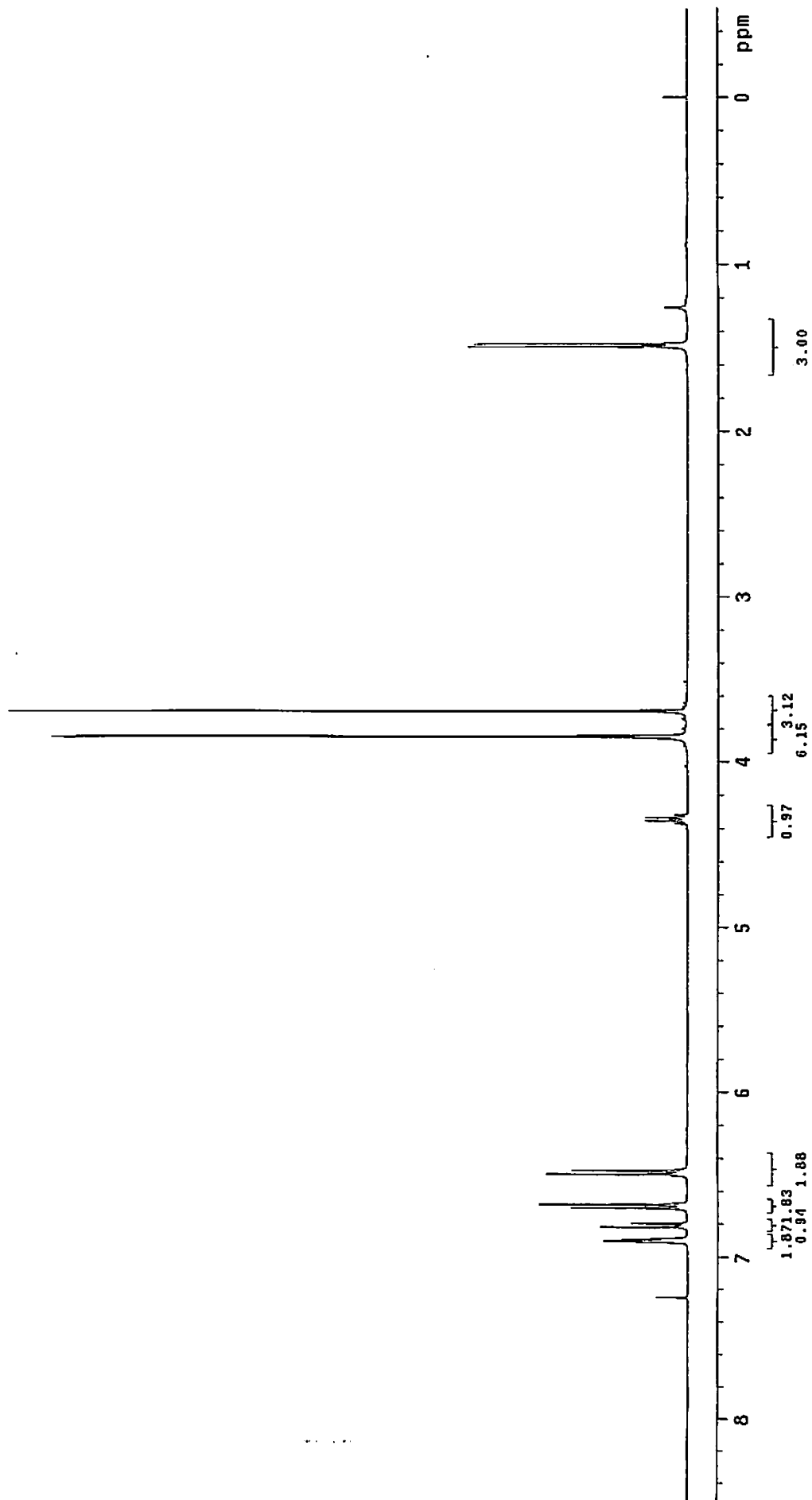
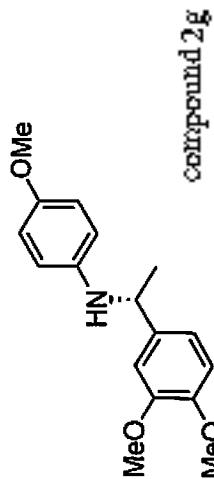
8 repetitions

OBSERVE H1; 399.9551825 MHz

DATA PROCESSING

F1 size 65536

Total time 0 min, 40 sec



zc3-44

Pulse Sequence: s2pul1

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

176 repetitions

OBSERVE C13, 100.5688162 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

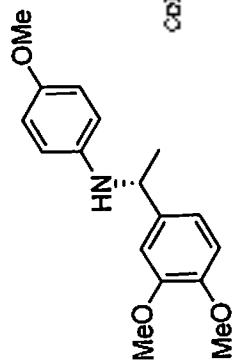
WALTZ-16 modulated

DATA PROCESSING

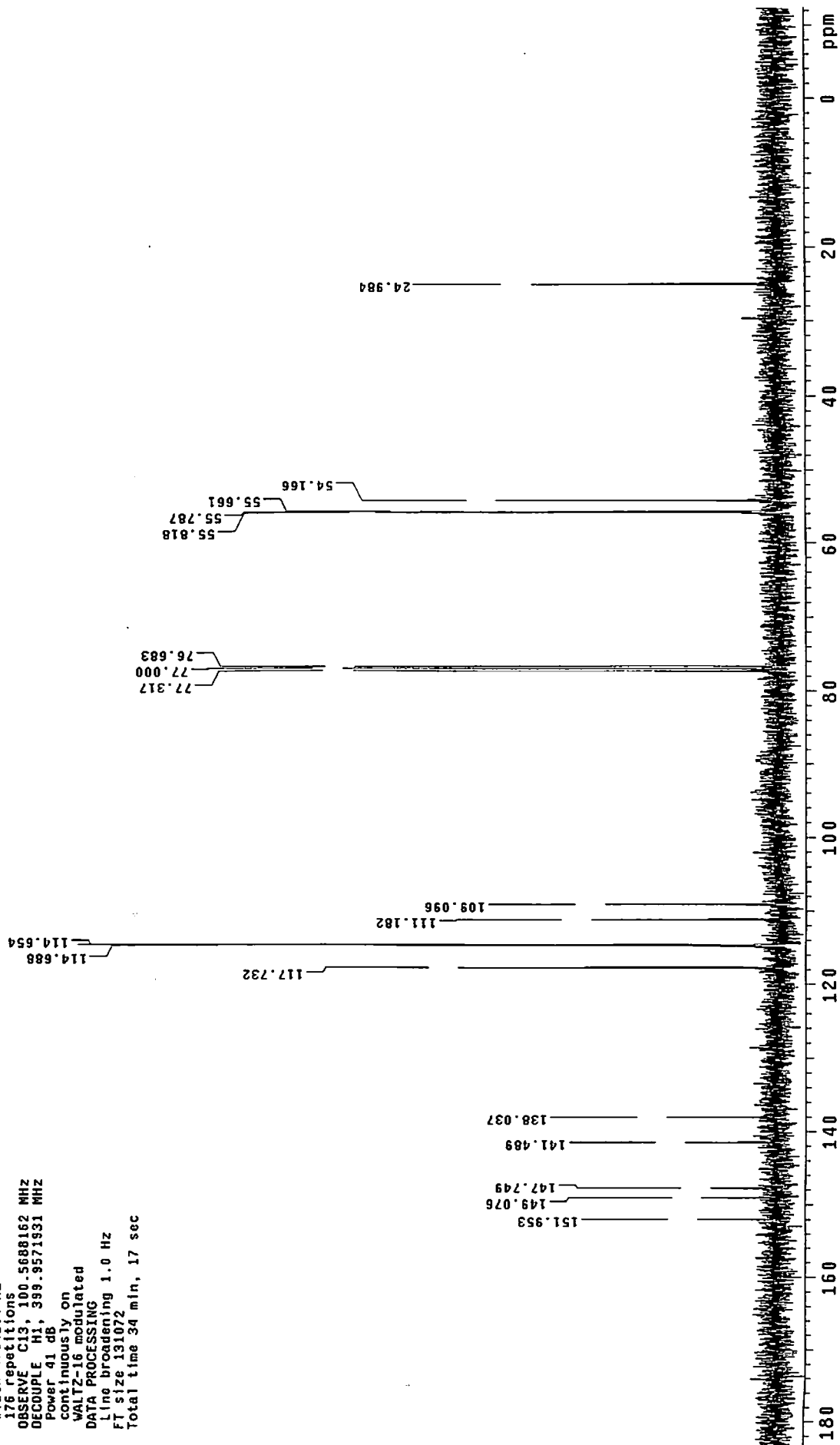
line broadening 1.0 Hz

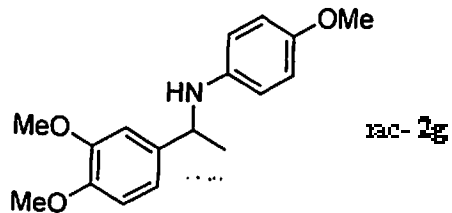
FT size 131072

Total time 34 min, 17 sec



Compound 2g

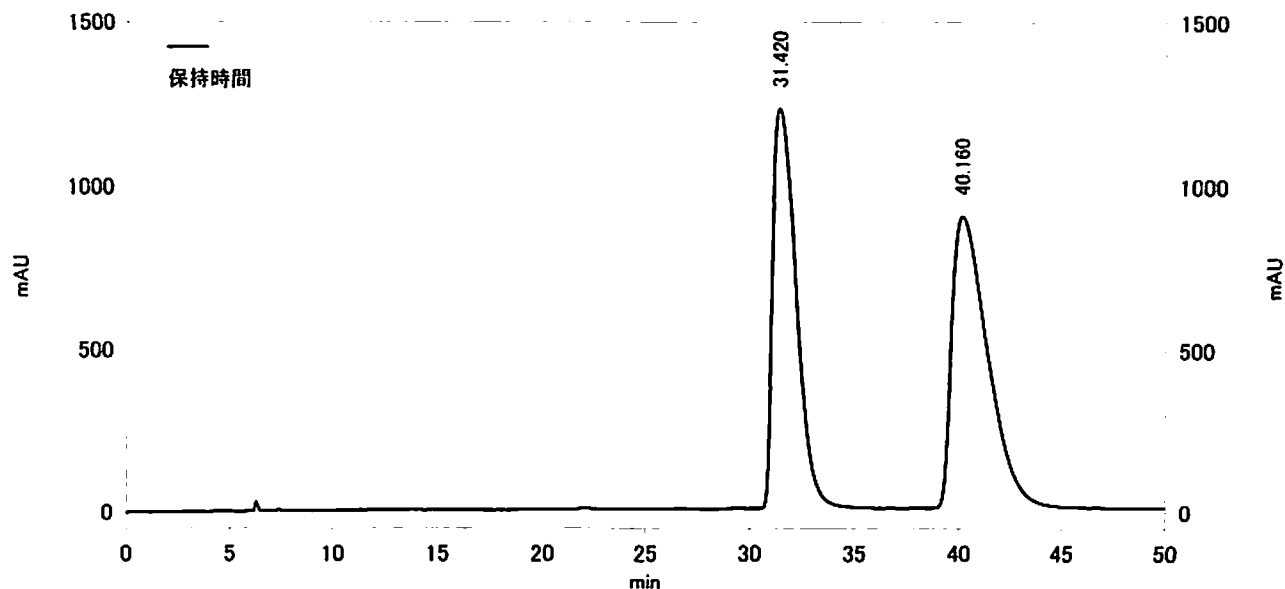




ページ 1/1

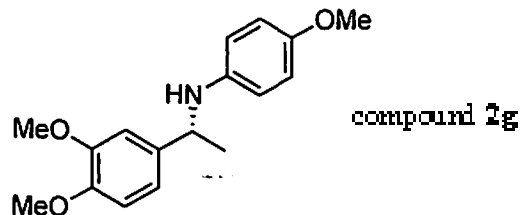
面積%レポート

データファイル名: D:\data\chen\zc3-53-as9010-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen-flow0.50.met
 ユーザー名: System
 分析日時: 2009/01/22 18:15:00
 印刷日時: 2009/01/26 18:15:56



5: 207 nm, 4 nm結果

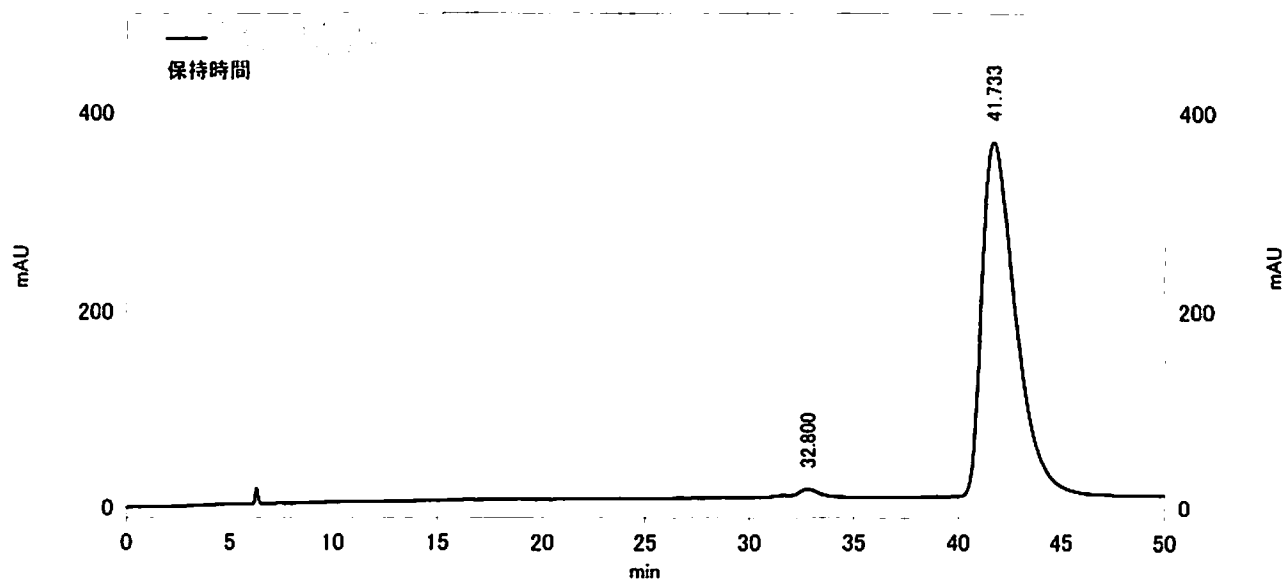
Pk #	名前	保持時間	面積	面積%	ピークコード
1		31.42	375232074	47.149	BB
2		40.16	420619300	52.851	BB
トータル			795851374	100.000	



ページ 1/1

面積%レポート

データファイル名: D:\data\chen\zc3-44-as9010-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen-flow0.50.met
 ユーザー名: System
 分析日時: 2009/01/20 17:52:40
 印刷日時: 2009/01/26 18:12:45



5: 207 nm, 4 nm結果

Pk #	名前	保持時間	面積	面積%	ピークサインコード
1		32.80	1514609	0.923	BB
2		41.73	162610007	99.077	BB
トータル			164124616	100.000	

zc3-43

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

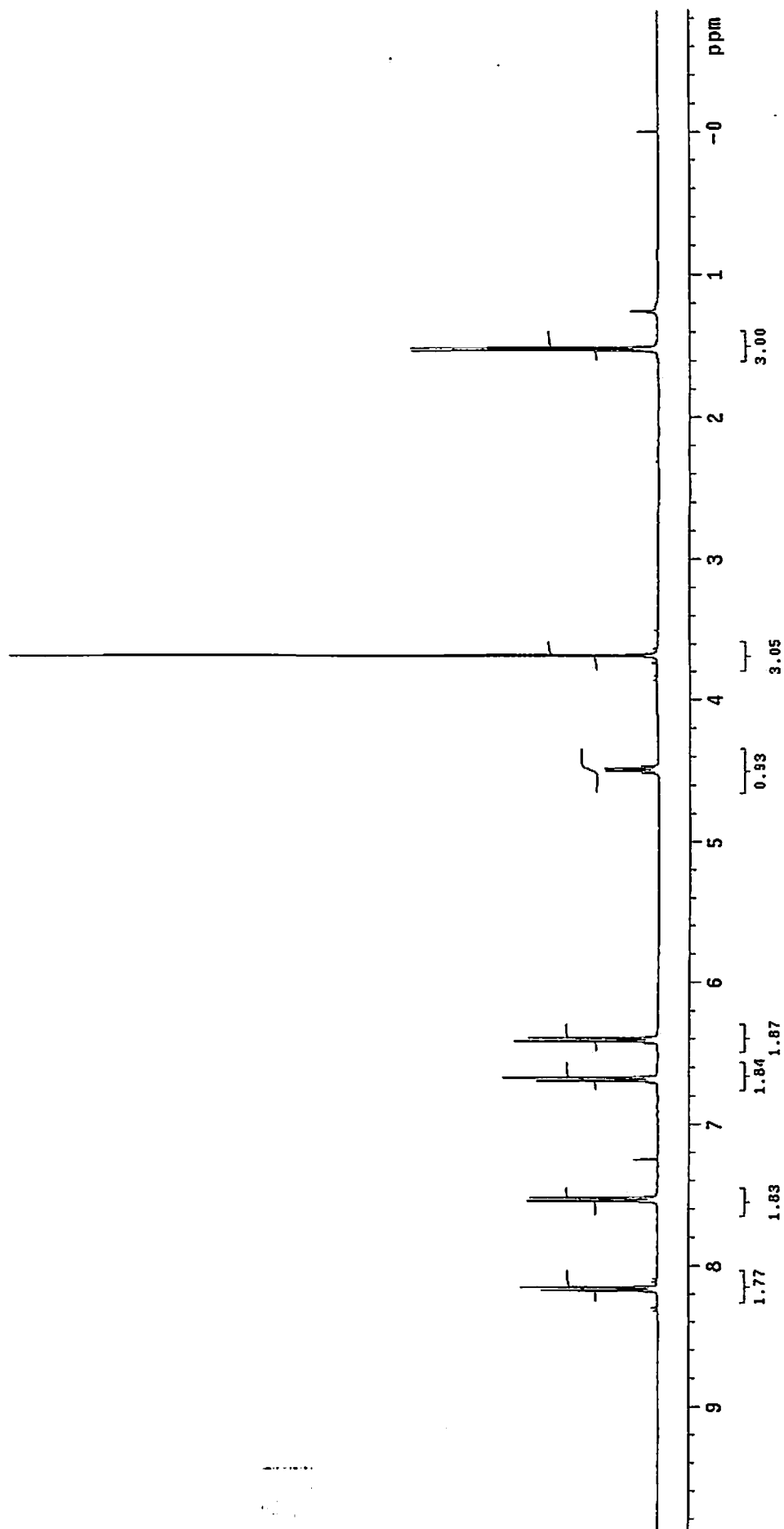
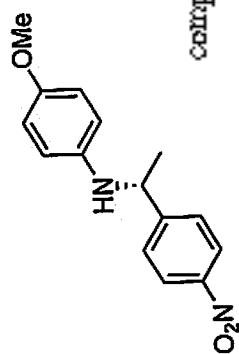
8 repetitions

OBSERVE H1, 399.9551818 MHz

DATA PROCESSING

FT size 85536

Total time 0 min, 40 sec



zc3-43

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INDVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

144 repetitions

OBSERVE C13, 100.568155 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

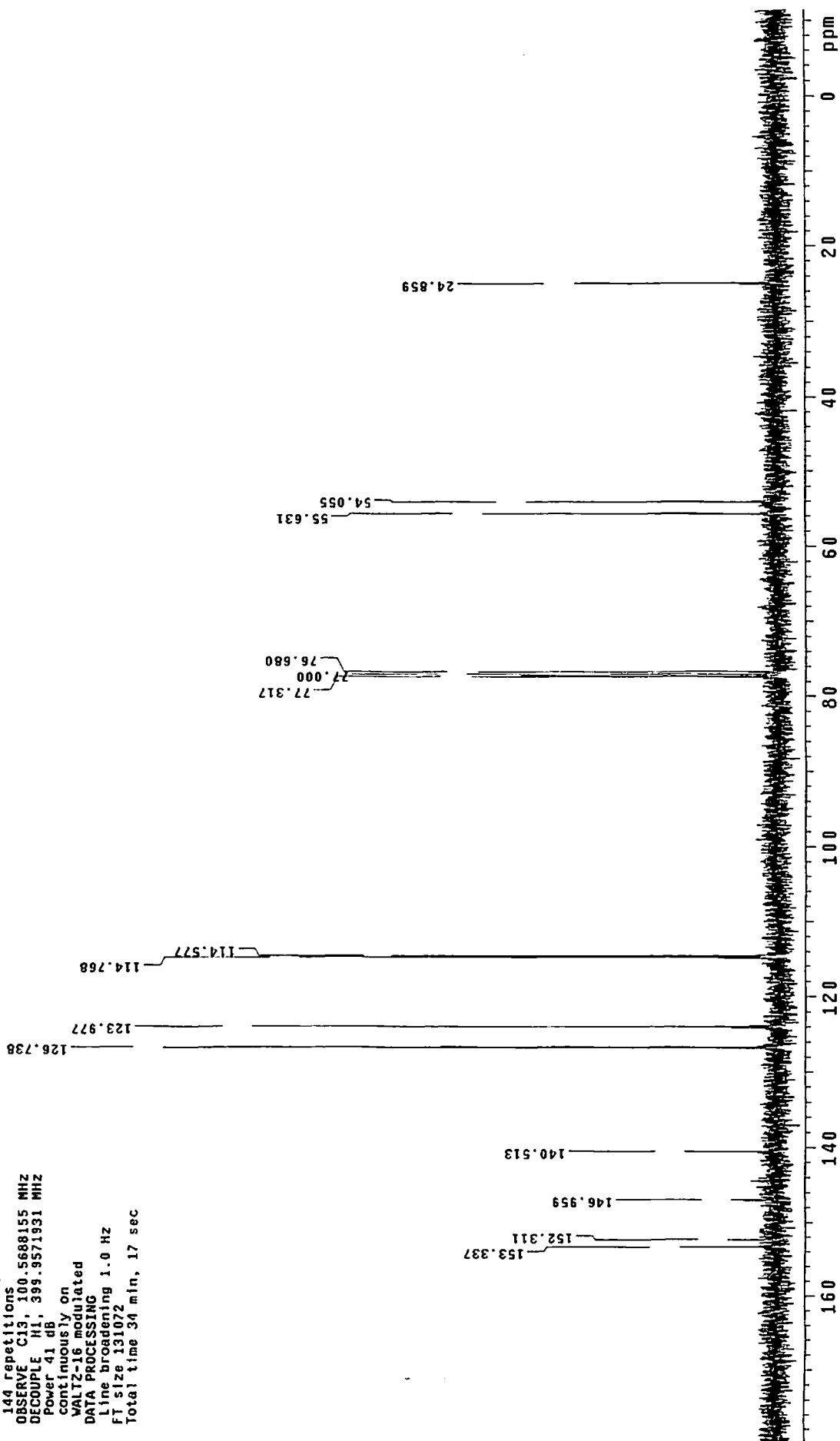
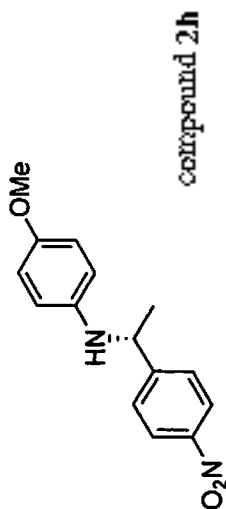
VAL12-16 modulated

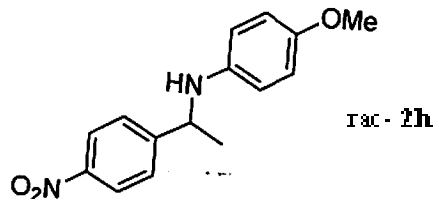
DATA PROCESSING

Line broadening 1.0 Hz

F1 size 131072

Total time 34 min, 17 sec

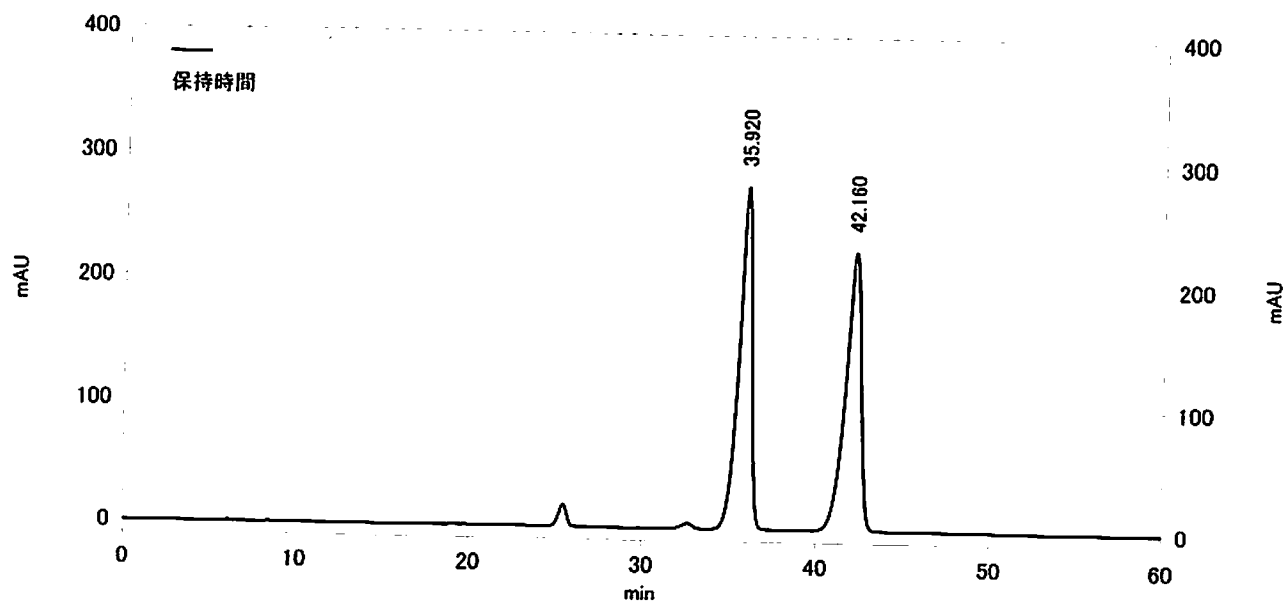




面積%レポート

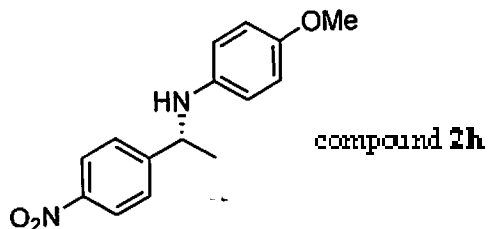
ページ 1/1

データファイル名: D:\data\chen\zc3-52-ad9010-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen-flow0.50.met
 ユーザー名: System
 分析日時: 2009/01/22 18:13:02
 印刷日時: 2009/01/26 18:20:44



4: 280 nm, 4 nm結果

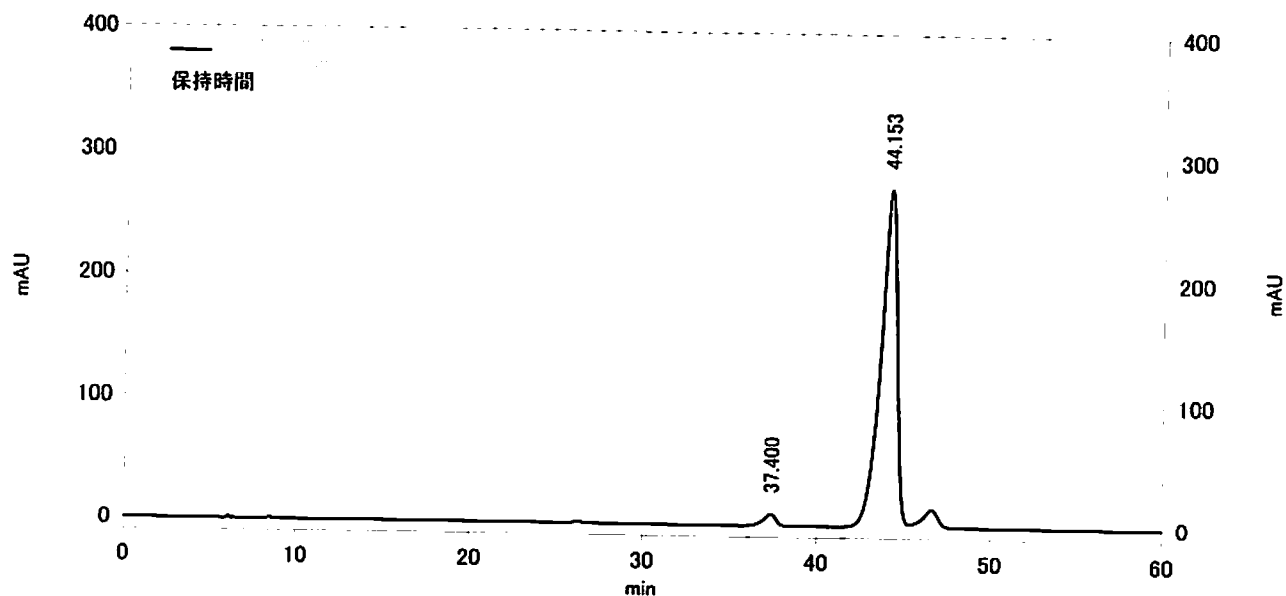
Pk #	名前	保持時間	面積	面積%	ピークサインコード
1		35.92	55391874	50.104	BB
2		42.16	55162609	49.896	BB
トータル			110554483	100.000	



面積%レポート

ページ 1/1

データファイル名: D:\data\chen\zc3-43-ad9010-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen-flow0.50.met
 ユーザー名: System
 分析日時: 2009/01/20 17:55:56
 印刷日時: 2009/01/26 18:21:35



4: 280 nm, 4 nm結果

Pk #	名前	保持時間	面積	面積%	ピークシンコート
1		37.40	1950098	2.716	BB
2		44.15	69862498	97.284	BB
トータル			71812596	100.000	

zc3-47

Pulse Sequence: s2pul

Solvent: CDC13

Ambient temperature

User: vmr1

INOVA-400 "400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 599.7 Hz

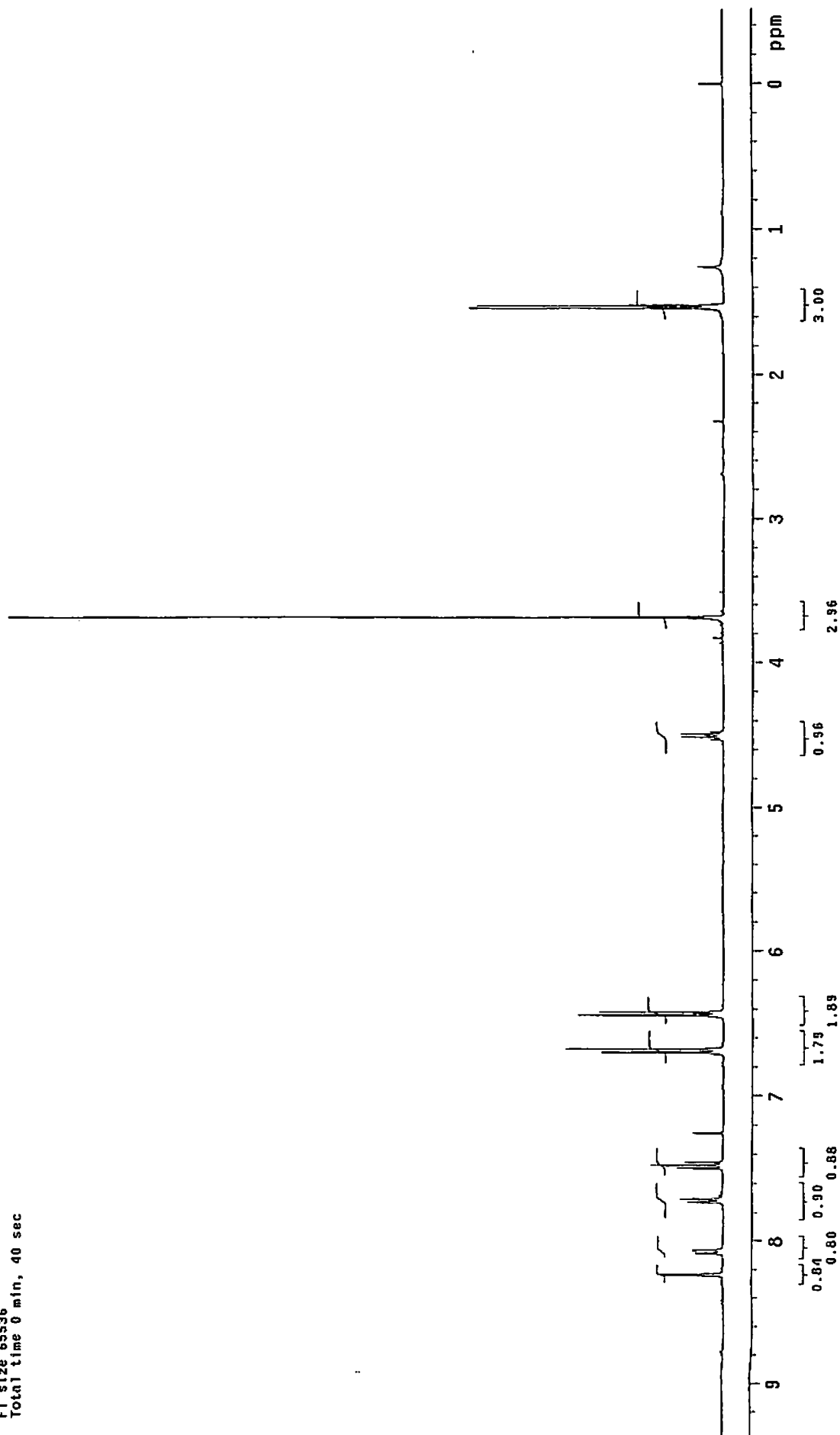
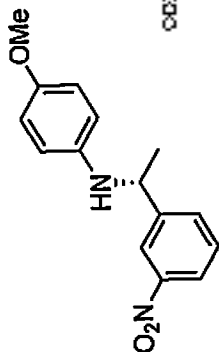
8 repetitions

OBSERVE H1, 399.9551812 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zc3-47

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

208 repetitions

OBSERVE C13, 100.5688139 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

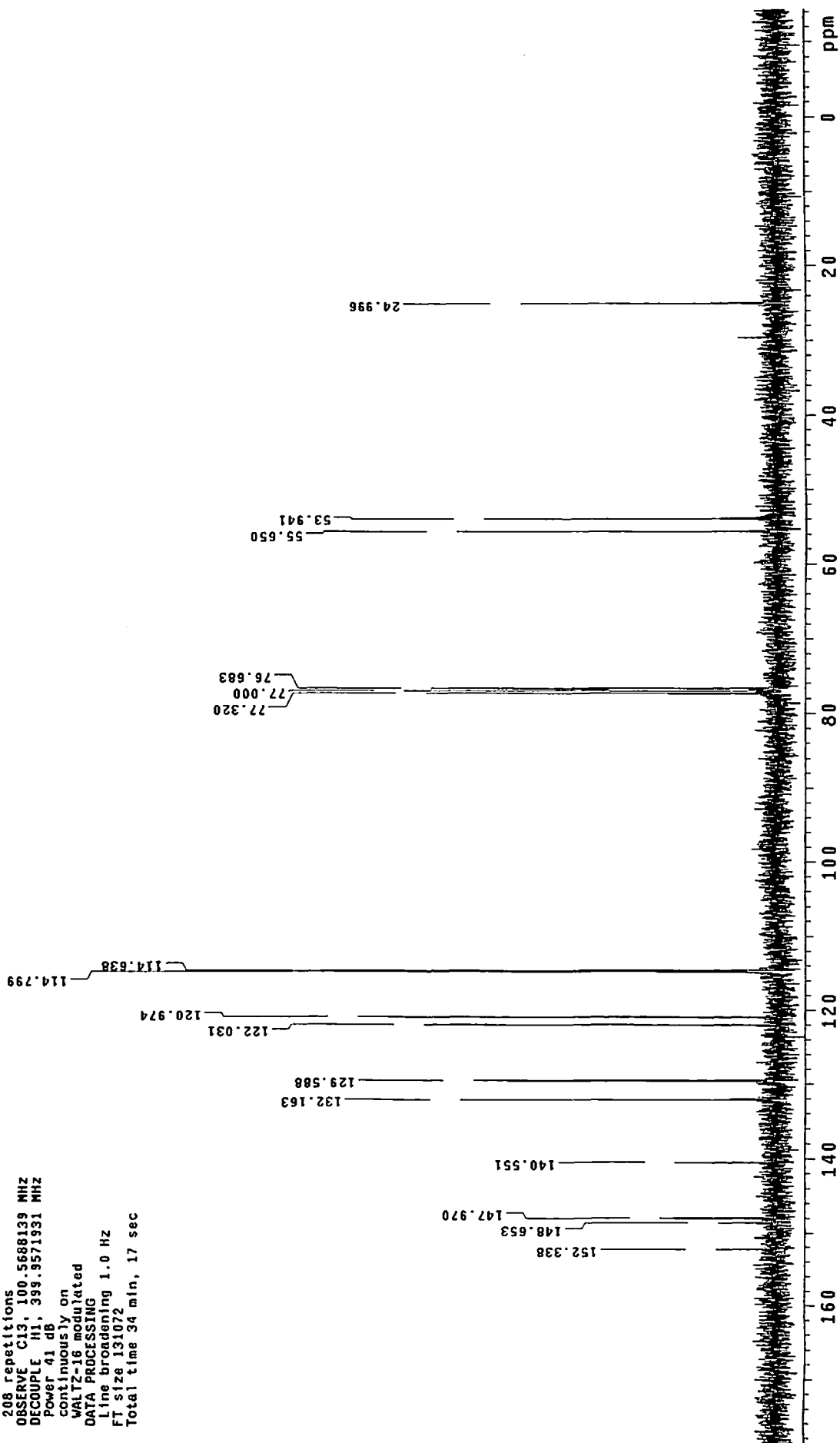
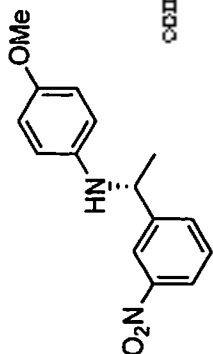
WALTZ-16 modulated

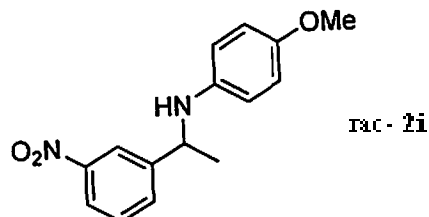
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec

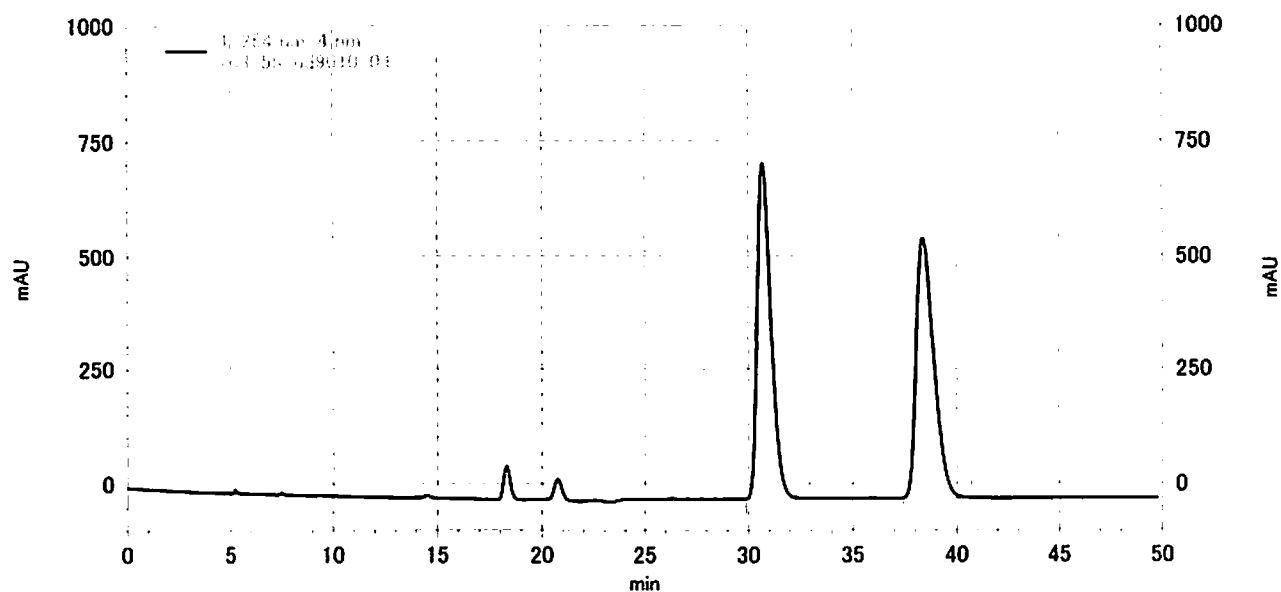




ページ 1/1

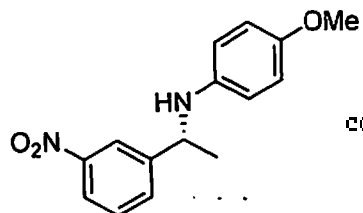
面積%レポート

データファイル名: D:\データ\chen\zc3-55-od9010-0.6.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.6ml.mct
 ユーザー名: System
 分析日時: 2009/01/23 17:42:41
 印刷日時: 2009/01/26 11:20:39



1: 254 nm, 4
nm結果

名前	保持時間	面積	面積%	ピークコード
	30.69	132967839	50.041	BB
	38.38	132751705	49.959	BB
トータル		265719544	100.000	

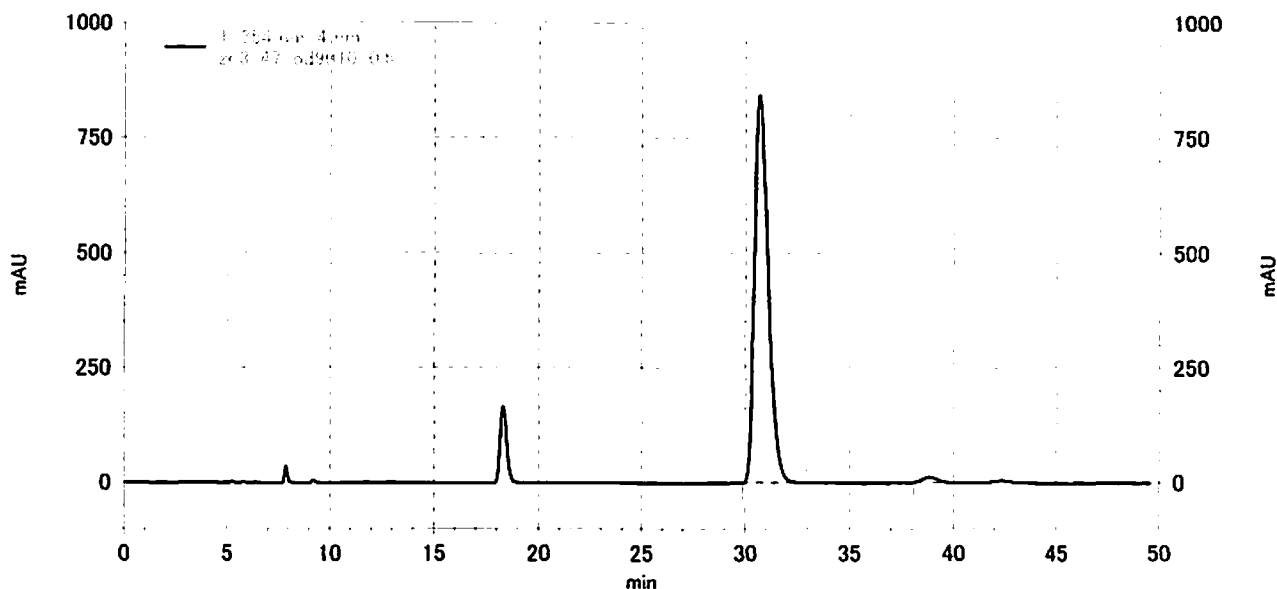


compound 2i

ページ 1/1

面積%レポート

データファイル名: D:\データ\chen\zc3-57-od9010-0.6.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.6ml.met
 ユーザー名: System
 分析日時: 2009/01/23 18:39:03
 印刷日時: 2009/01/26 11:23:20



1: 254 nm, 4
nm結果

名前	保持時間	面積	面積%	ピークコード
	30.67	154776078	98.502	BB
	38.84	2353168	1.498	BI

トータル		157129246	100.000	
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zc3-73

Pulse Sequence: s2pul

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5993.7 Hz

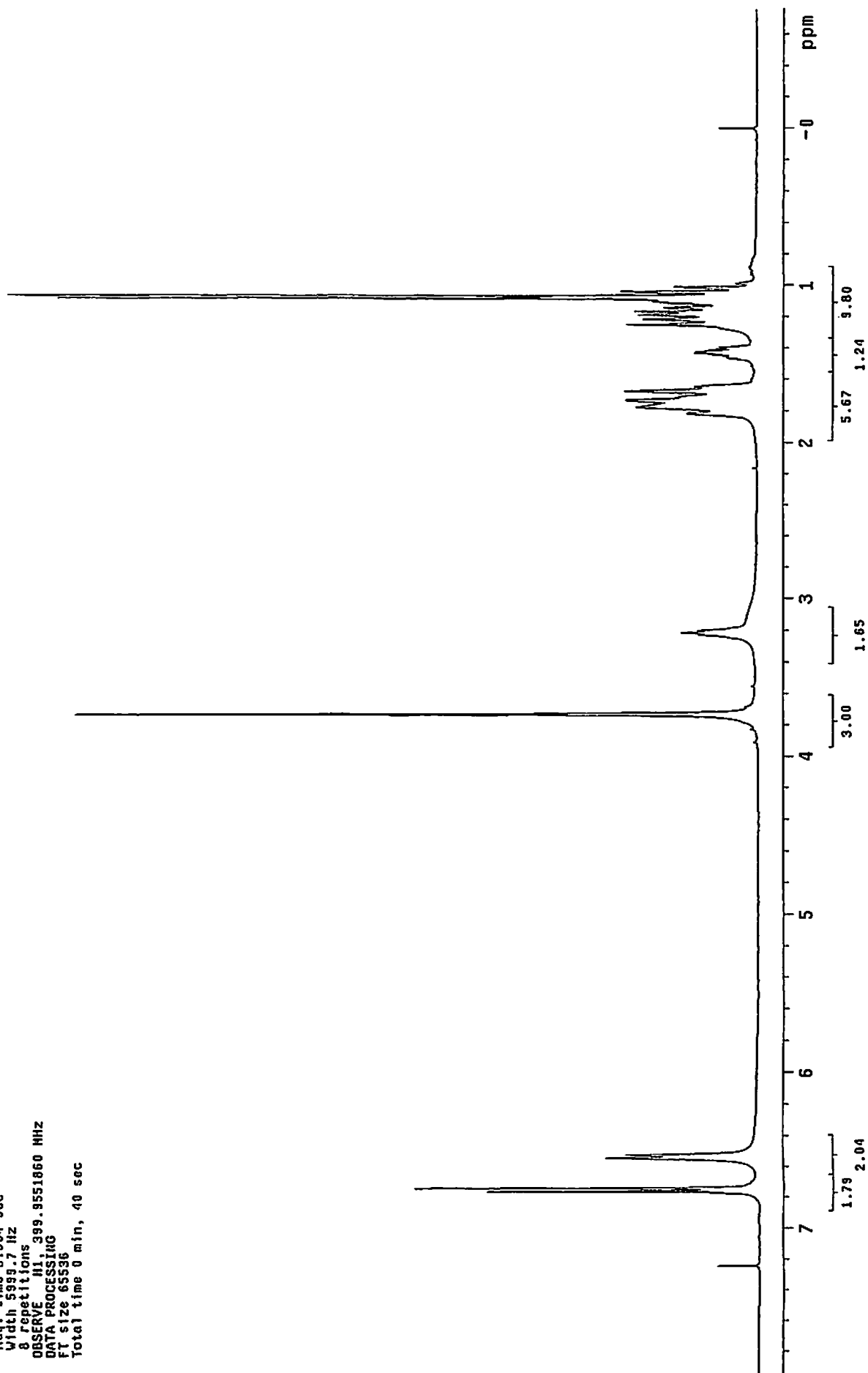
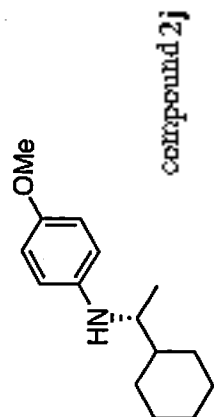
8 repetitions

OBSERVE H1, 399.951860 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zc3-73

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

304 repetitions

OBSERVE C13, 100.5688143 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB

continuously on

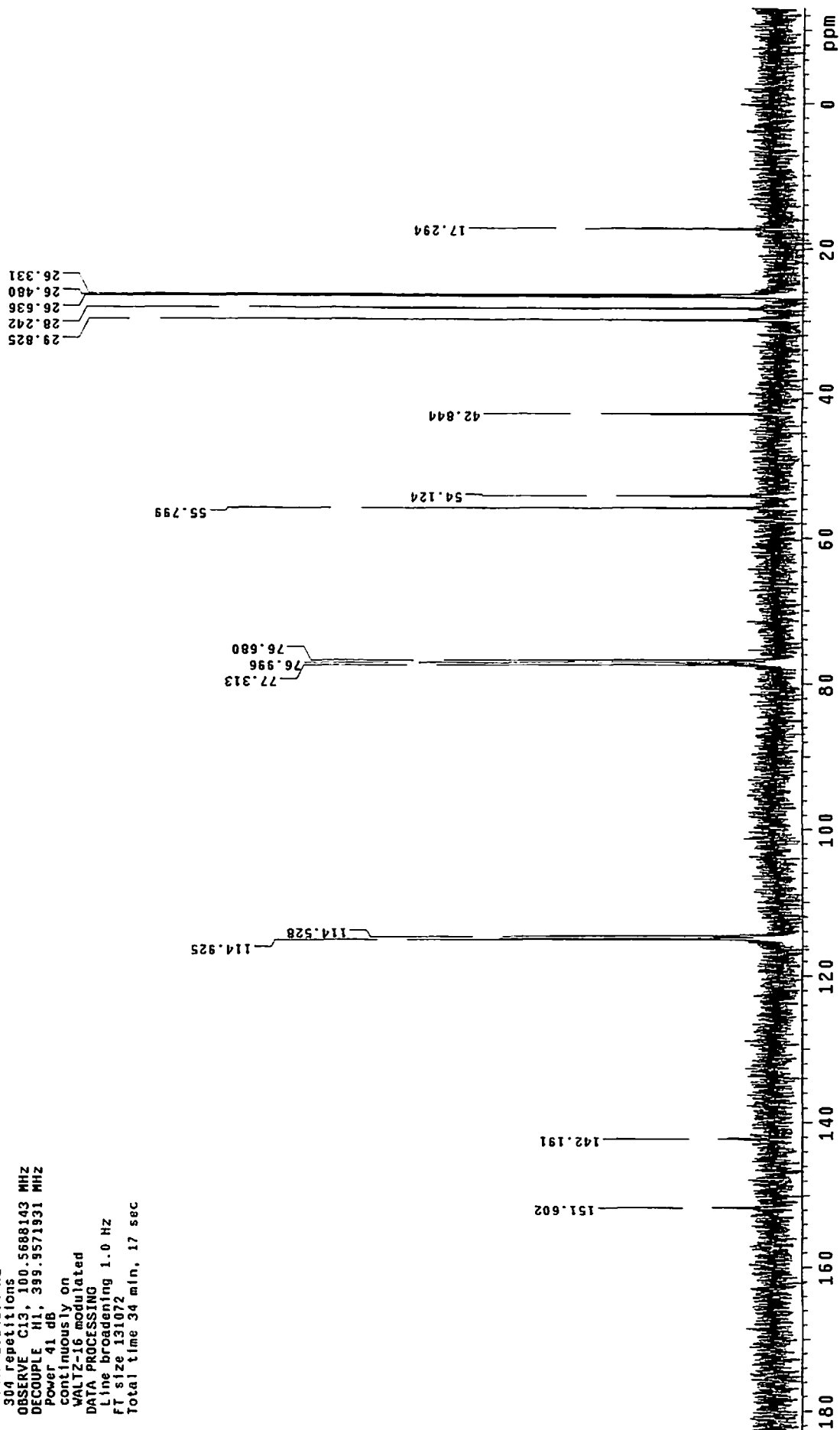
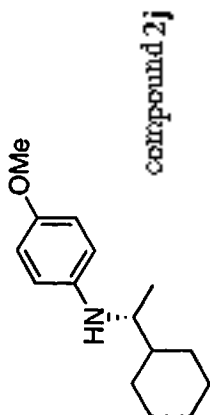
WALTZ-16 modulated

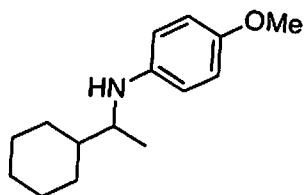
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



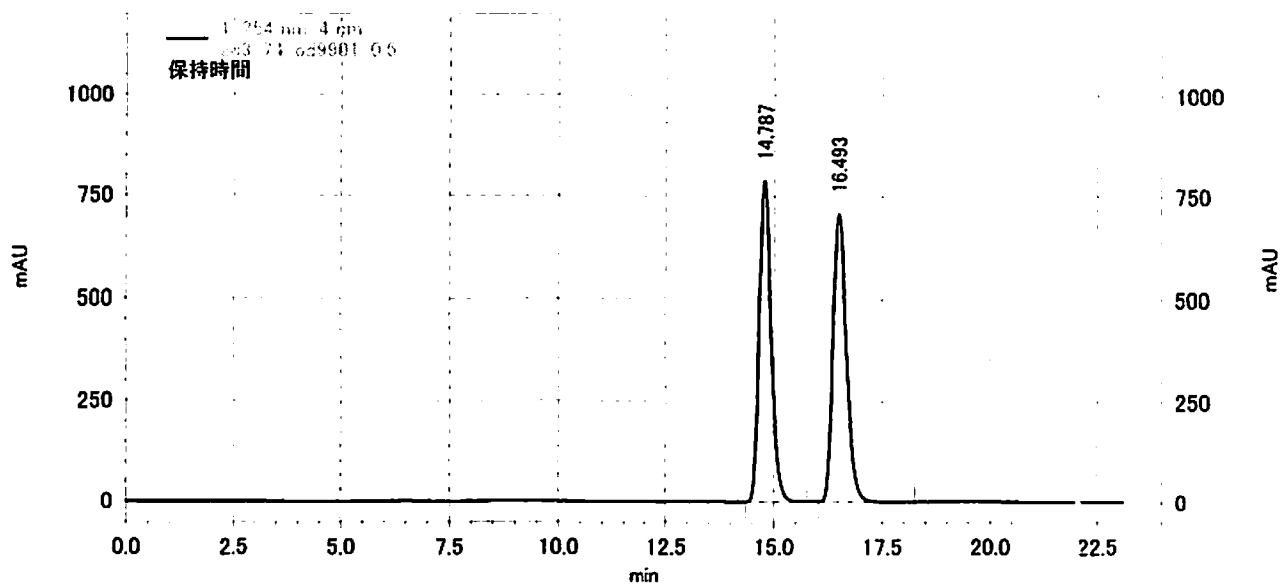


rac-2j

ページ 1/1

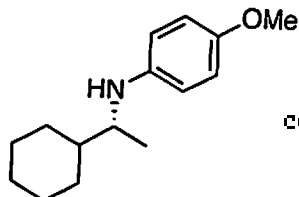
面積%レポート

データファイル名: D:\データ\chen\zc3-74-od9901-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/02/04 9:54:44
 印刷日時: 2009/02/04 10:23:24



1: 254 nm, 4
nm結果

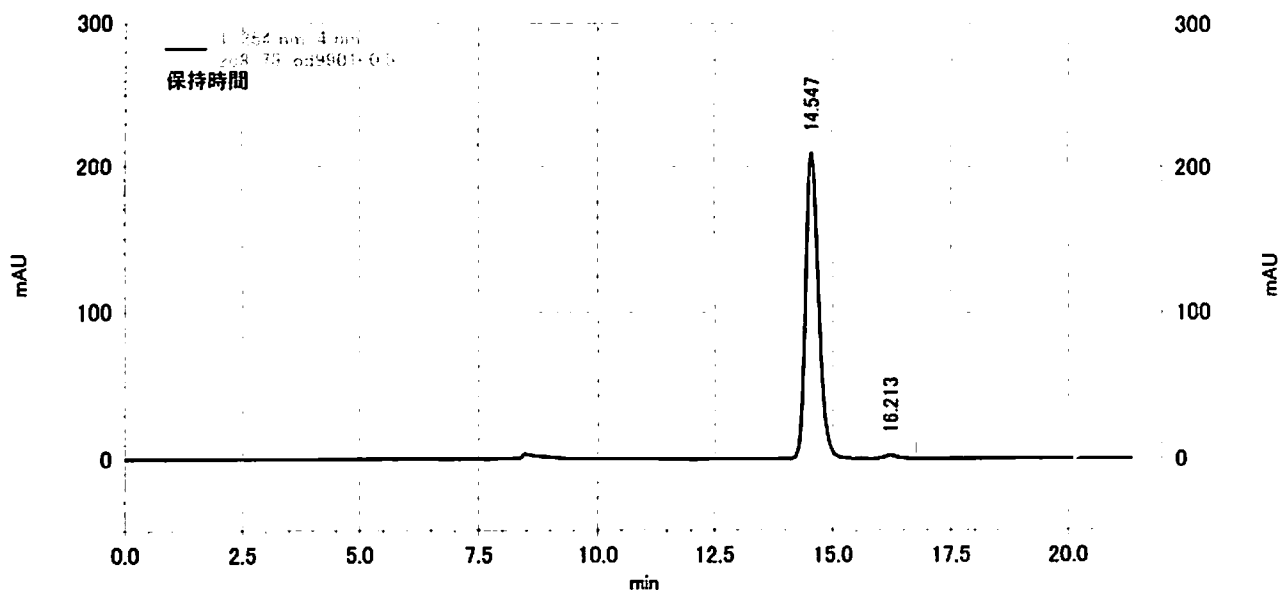
名前	保持時間	面積	面積%	ピークコード
	14.79	60261301	49.809	BB
	16.49	60724186	50.191	BB
トータル		120985487	100.000	



compound 2j

面積%レポート

データファイル名: D:\データ\chen\zc3-73-od9901-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/02/04 12:10:23
 印刷日時: 2009/02/04 12:31:42



1: 254 nm, 4
nm結果

名前	保持時間	面積	面積%	ベースラインコード
	14.55	15854432	98.996	BB
	16.21	160757	1.004	BB
トータル		16015189	100.000	

zc3-49

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: vnmr1

INOVA-400 "u400"

Relax. delay 1.495 sec

Pulse 45.0 degrees

Acq. time 9.504 sec

Width 5999.7 Hz

8 repetitions

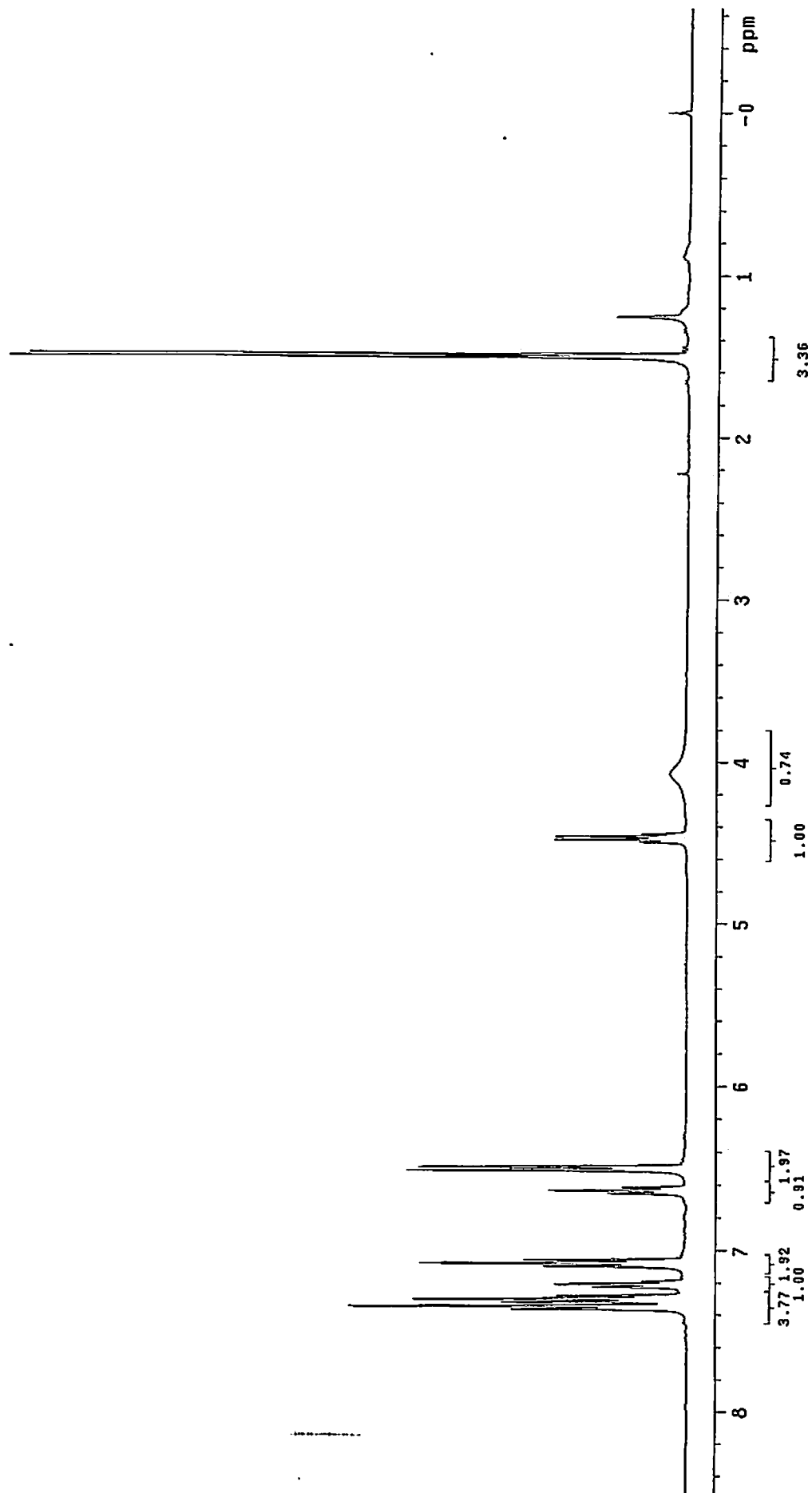
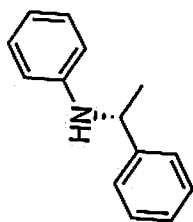
OBSERVE H1, 399.9552001 MHz

DATA PROCESSING

FI size 65536

Total time 0 min, 40 sec

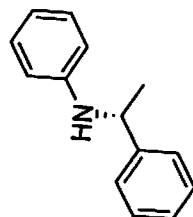
compound 2k



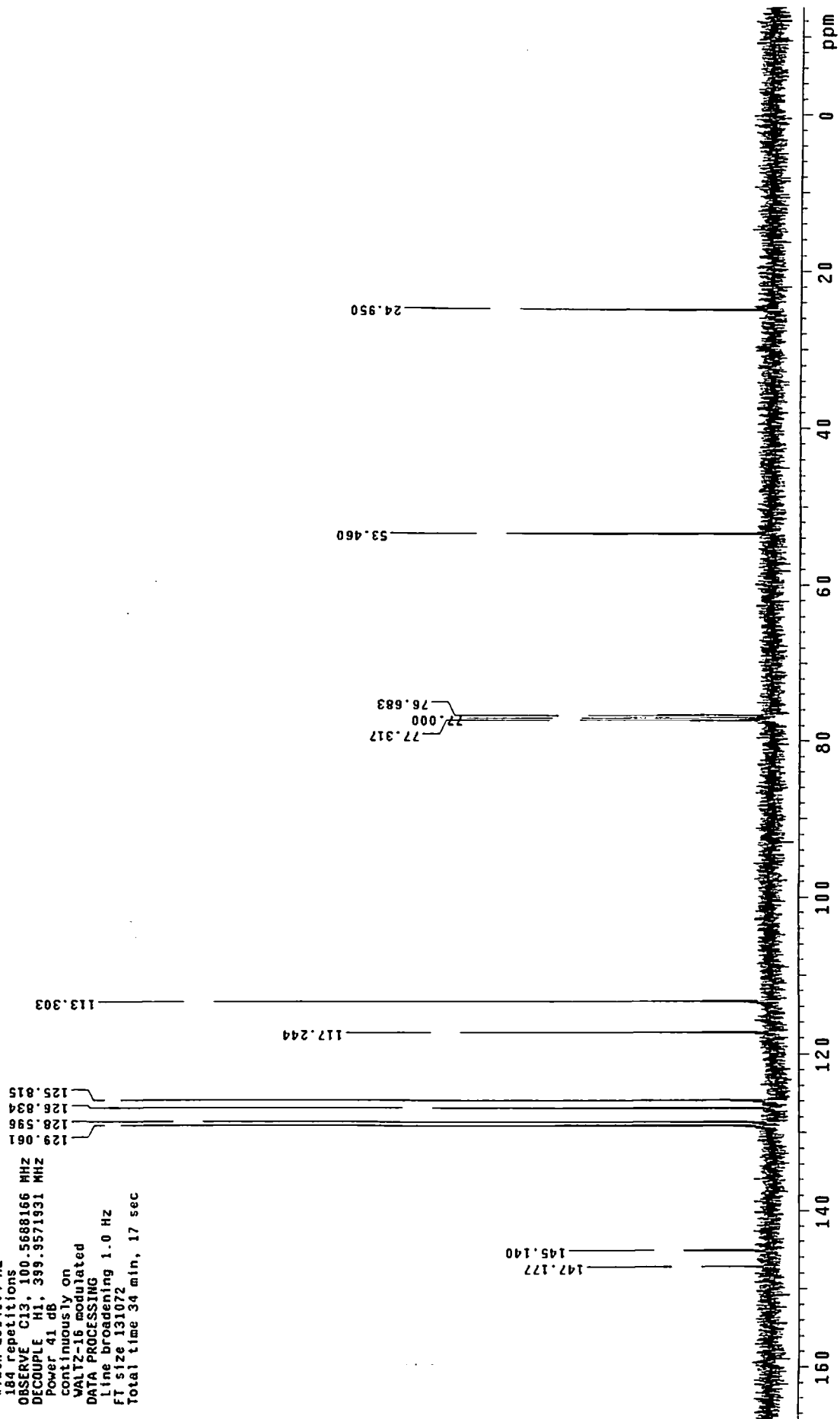
zc3-49

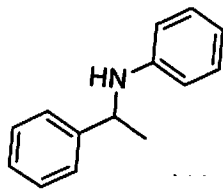
Pulse Sequence: s2pul
Solvent: CDCl3
Ambient temperature
User: vnmr1
INOVA-400 "u400"

Relax. delay 0.499 sec
Pulse 45.0 degrees
Acq. time 1.501 sec
Width 25141.4 Hz
184 repetitions
OBSERVE C13, 100.5688166 MHz
DECOUPLE H1, 399.9571931 MHz
Power 41 dB
Continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 1.0 Hz
FT size 131072
Total time 34 min, 17 sec



compound 2k



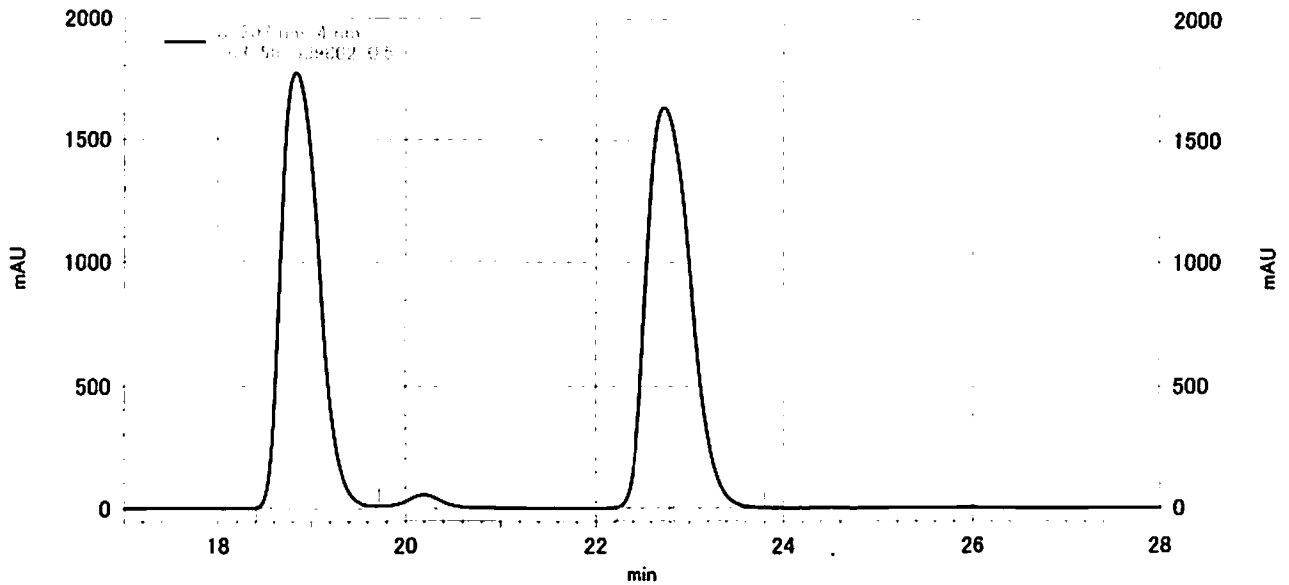


TAC- 2k

ページ 1/1

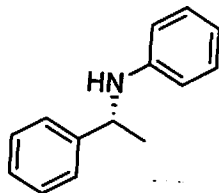
面積%レポート

データファイル名: D:\データ\chen\zc3-56-od9802-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/23 16:30:43
 印刷日時: 2009/01/26 11:27:56



5: 207 nm, 4
nm結果

名前	保持時間	面積	面積%	ベースラインコード
	18.84	195010460	48.196	BI
	22.73	209605169	51.804	BI
トータル		404615629	100.000	

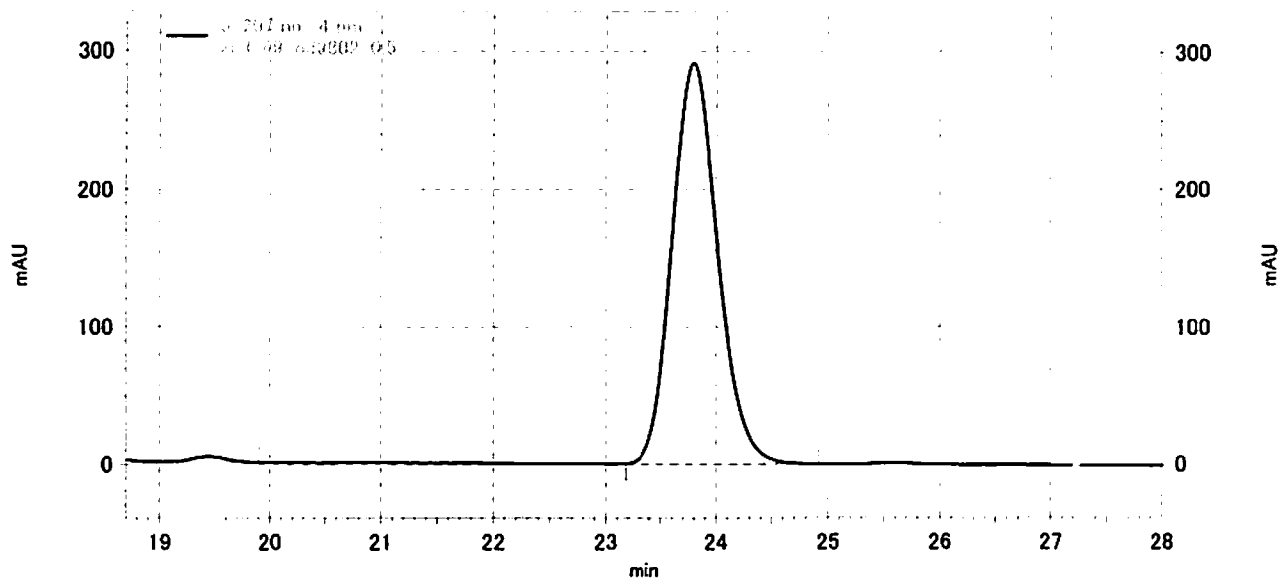


compound 2k

ページ 1/1

面積%レポート

データファイル名: D:\データ\chen\zc3-49-od9802-0.5. dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/21 19:11:59
 印刷日時: 2009/01/26 11:29:54



5: 207 nm, 4 nm
 結果

名前	保持時間	面積	面積%	ベースラインコード
	19.43	296746	0.883	BB
	23.79	33310514	99.117	BB
トータル		33607260	100.000	

zc3-48

Pulse Sequence: s2pu1

Solvent: CDCl3

Ambient temperature

User: vmr1

INOVA-400 "u400"

Relax. delay 1.496 sec

Pulse 45.0 degrees

Acq. time 3.504 sec

Width 5999.7 Hz

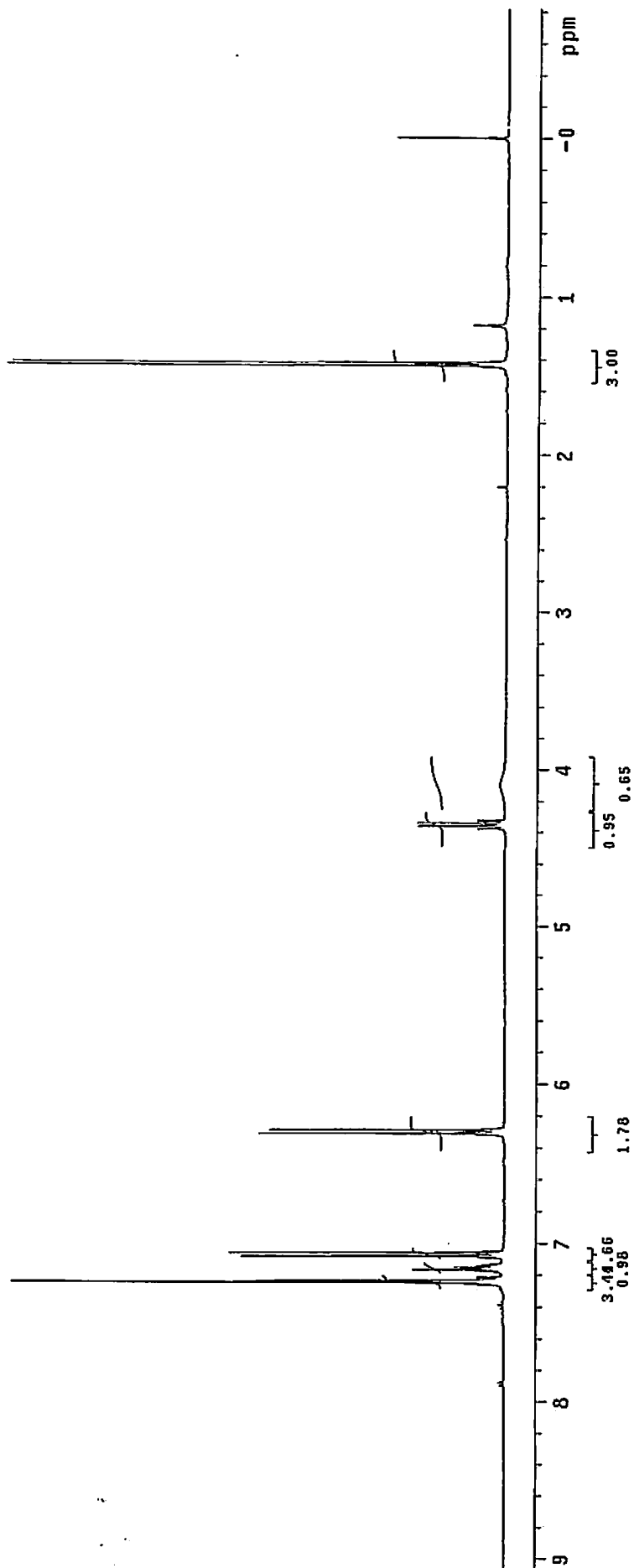
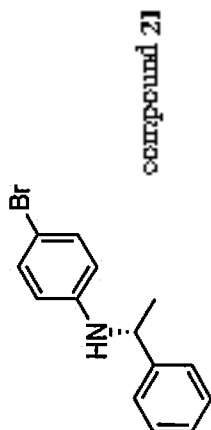
8 repetitions

OBSERVE H1, 399.9552160 MHz

DATA PROCESSING

FT size 65536

Total time 0 min, 40 sec



zc3-48

Pulse Sequence: s2pul

Solvent: CDCl₃

Ambient temperature

User: vmar1

INOVA-400 "q400"

Relax. delay 0.499 sec

Pulse 45.0 degrees

Acq. time 1.501 sec

Width 25141.4 Hz

280 repetitions

OBSERVE C13, 100.5688132 MHz

DECOUPLE H1, 399.9571931 MHz

Power 41 dB,

continuously on

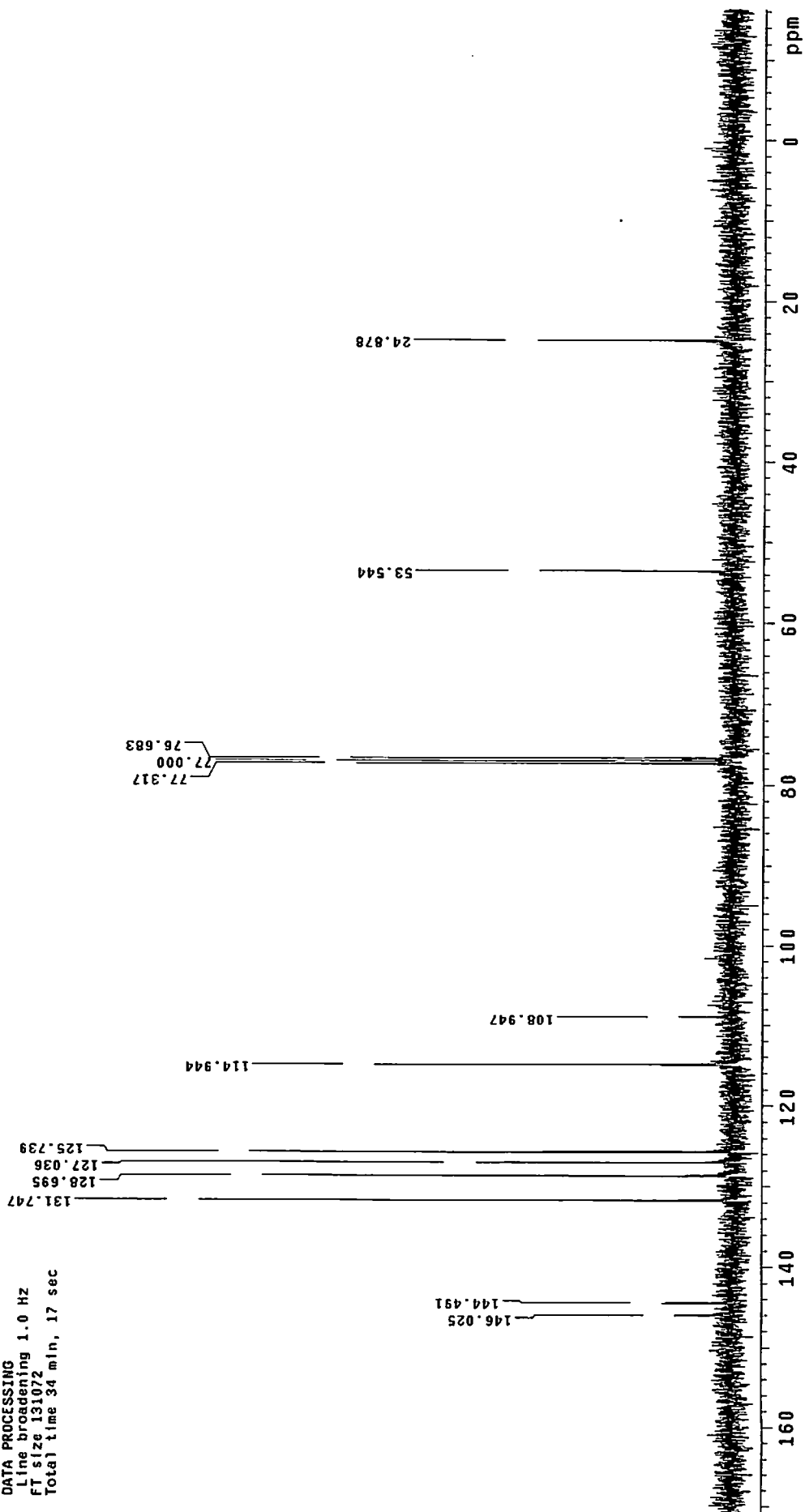
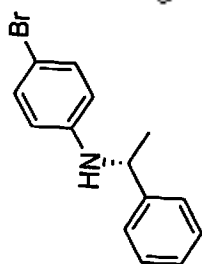
WALTZ-16 modulated

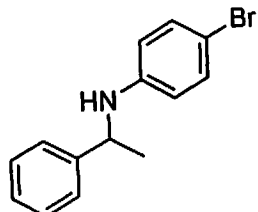
DATA PROCESSING

Line broadening 1.0 Hz

FT size 131072

Total time 34 min, 17 sec



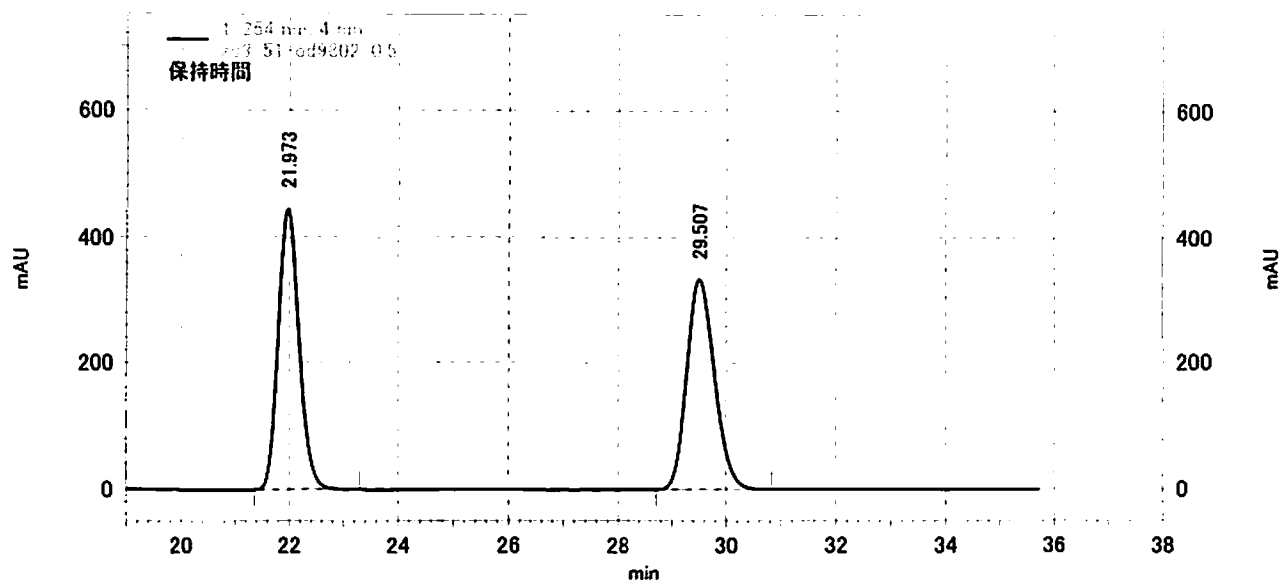


TAC- 21

ページ 1/1

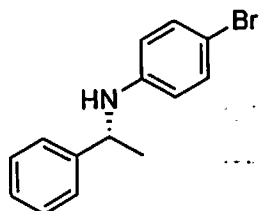
面積%レポート

データファイル名: D:\データ\chen\zc3-51-od9802-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/21 17:44:44
 印刷日時: 2009/01/26 19:00:11



1: 254 nm, 4
 nm結果

名前	保持時間	面積	面積%	ピーク番号
	21.97	47250164	50.043	BB
	29.51	47168462	49.957	BB
トータル		94418626	100.000	

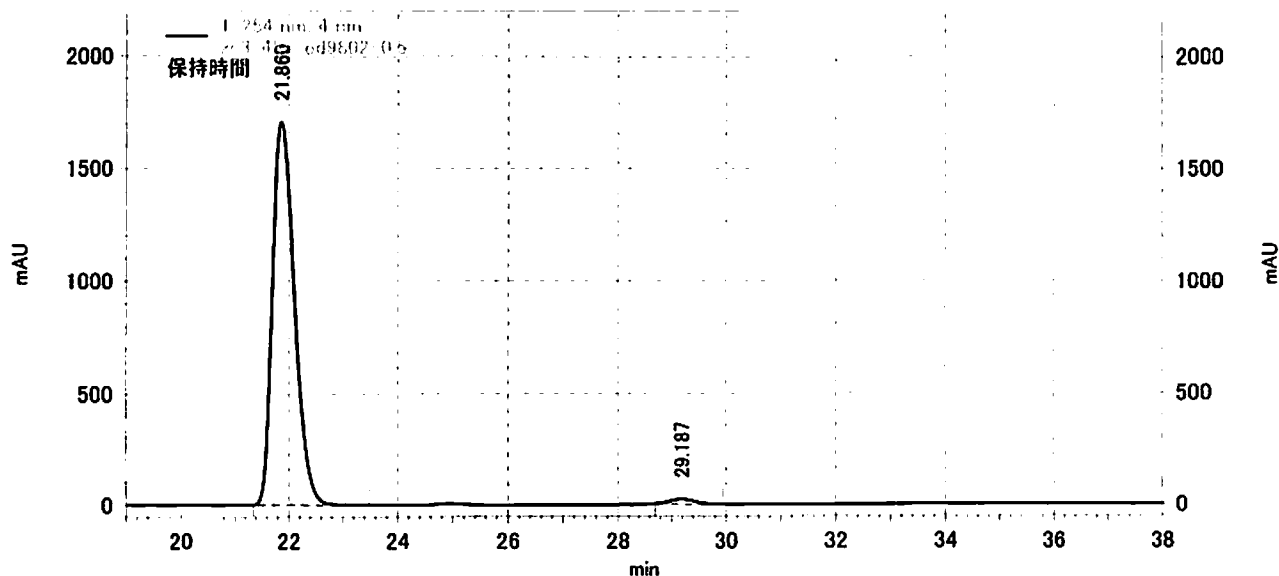


compound 21

ページ 1/1

面積%レポート

データファイル名: D:\データ\chen\zc3-48a-od9802-0.5.dat
 メソッドファイル名: C:\EZChrom Elite\Enterprise\Projects\Default\Method\chen0.5ml.met
 ユーザー名: System
 分析日時: 2009/01/21 18:29:52
 印刷日時: 2009/01/26 18:58:58



1: 254 nm, 4 nm
 結果

名前	保持時間	面積	面積%	ピークコード
	21.86	191776117	98.475	BB
	29.19	2969462	1.525	BB
トータル		194745579	100.000	