

boscalid

STATUS: ISO 1750 (provisionally approved)

IUPAC: 2-chloro-*N*-(4'-chlorobiphenyl-2-yl)nicotinamide

CAS: 2-chloro-*N*-(4'-chloro[1,1'-biphenyl]-2-yl)-3-pyridinecarboxamide

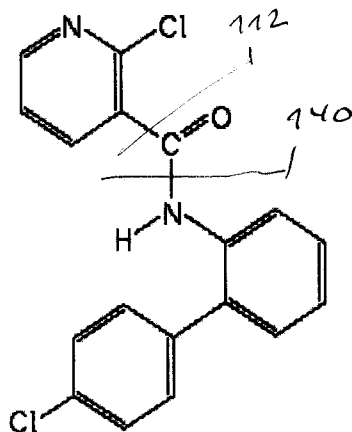
REG. NO.: 188425-85-6

FORMULA: $C_{18}H_{12}Cl_2N_2O$ 342.03

ACTIVITY: fungicides (anilide fungicides; pyridine fungicides)

NOTES: The name "nicobifen" was provisionally approved for this substance, but was replaced at the request of the sponsor.

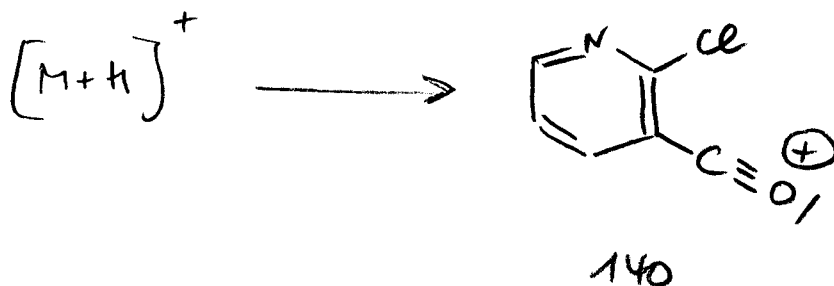
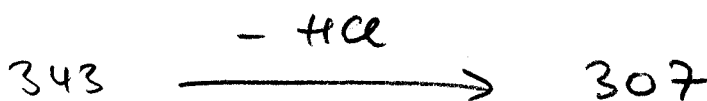
STRUCTURE:



$[M+H]^+$ 343

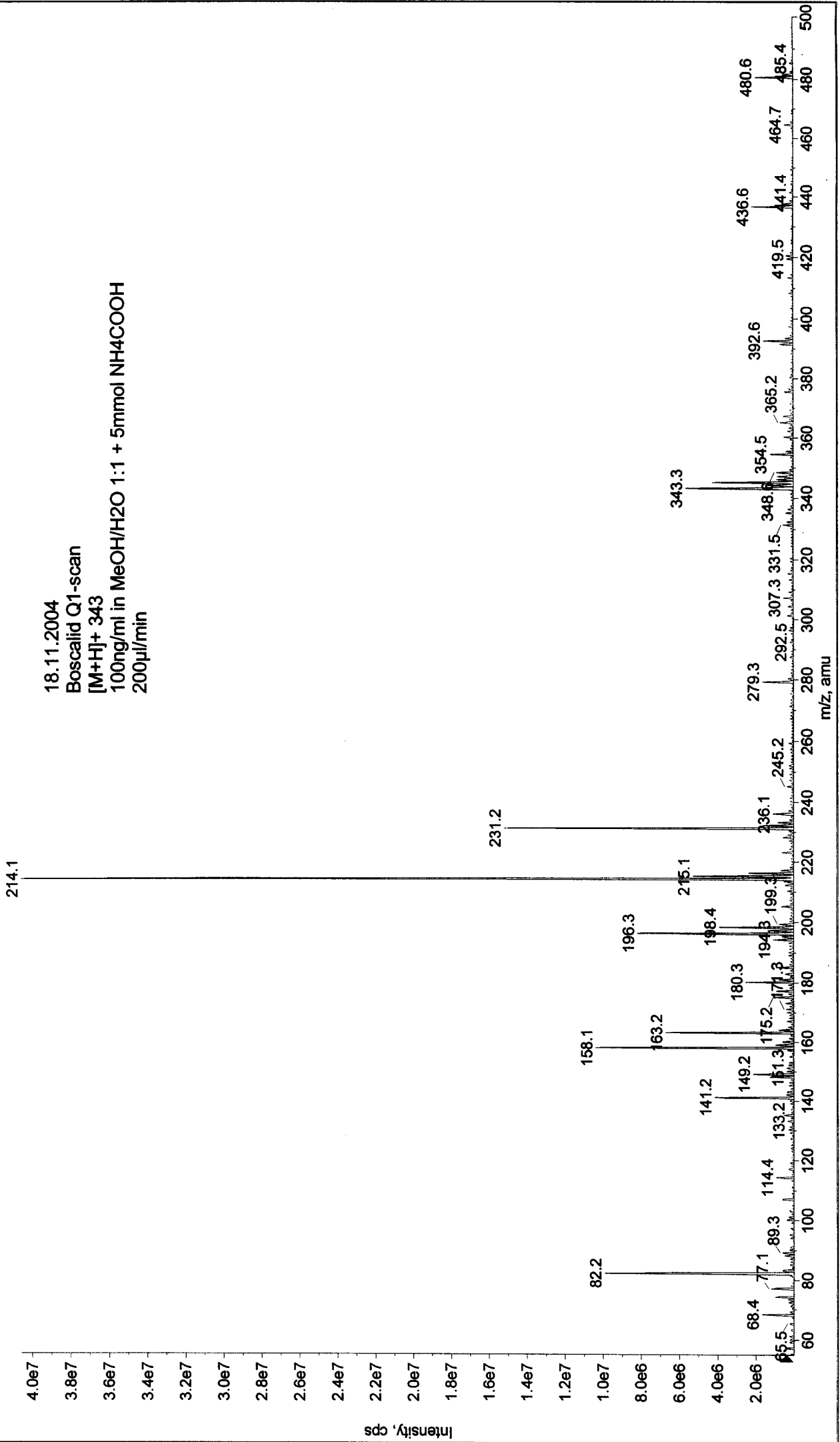
343 \rightarrow 307 Δ 36 -HCl !

343 \rightarrow 140 mit Chlor !



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20041118090904.wiff (Turbo Spray)

Max. 4.1e7 cps



Printing Time: 9:28:26

Printing Date: Thursday, November 18, 2004

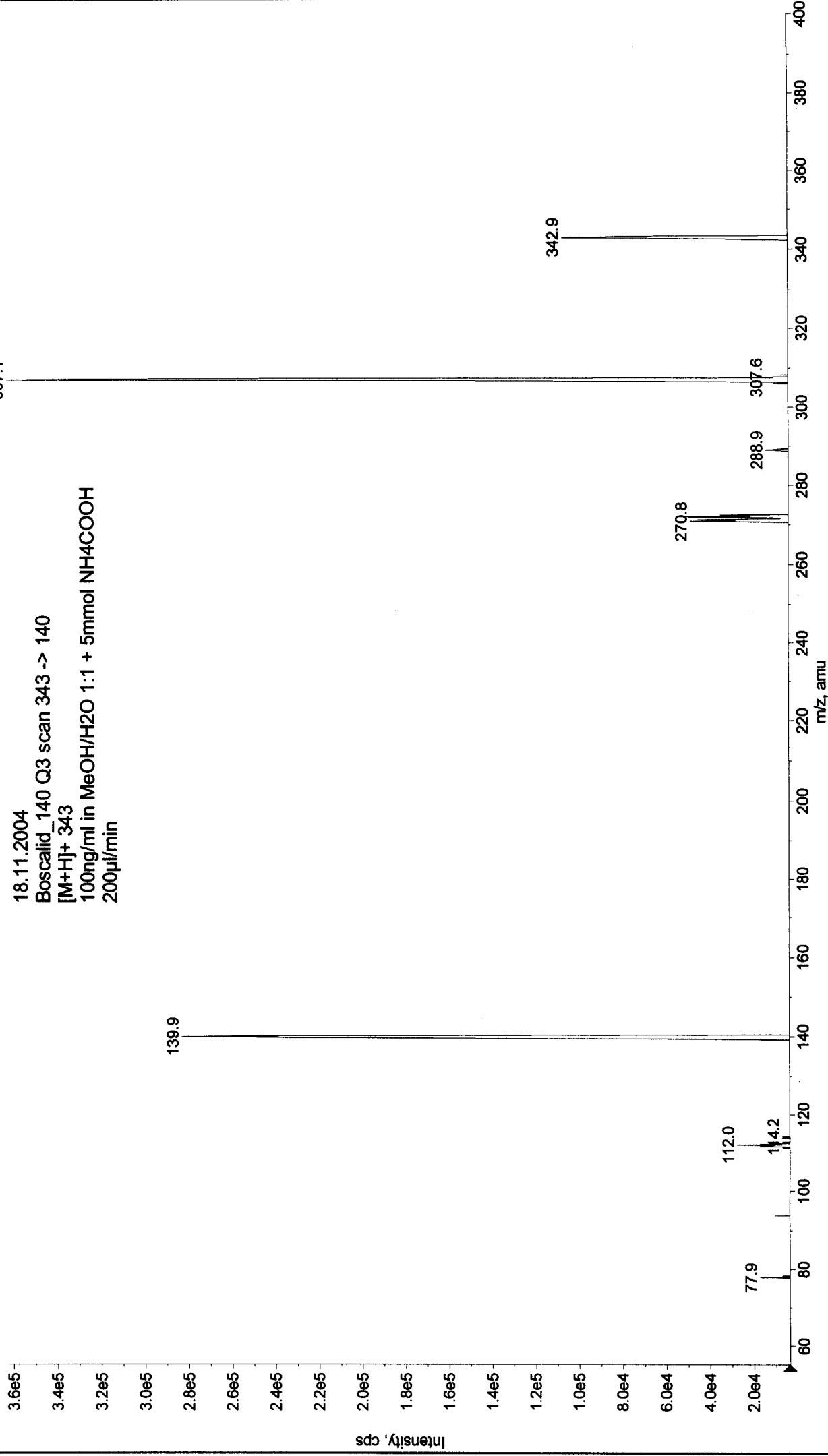
Acq. Time: 09:26

Acq. Date: Thursday, November 18, 2004

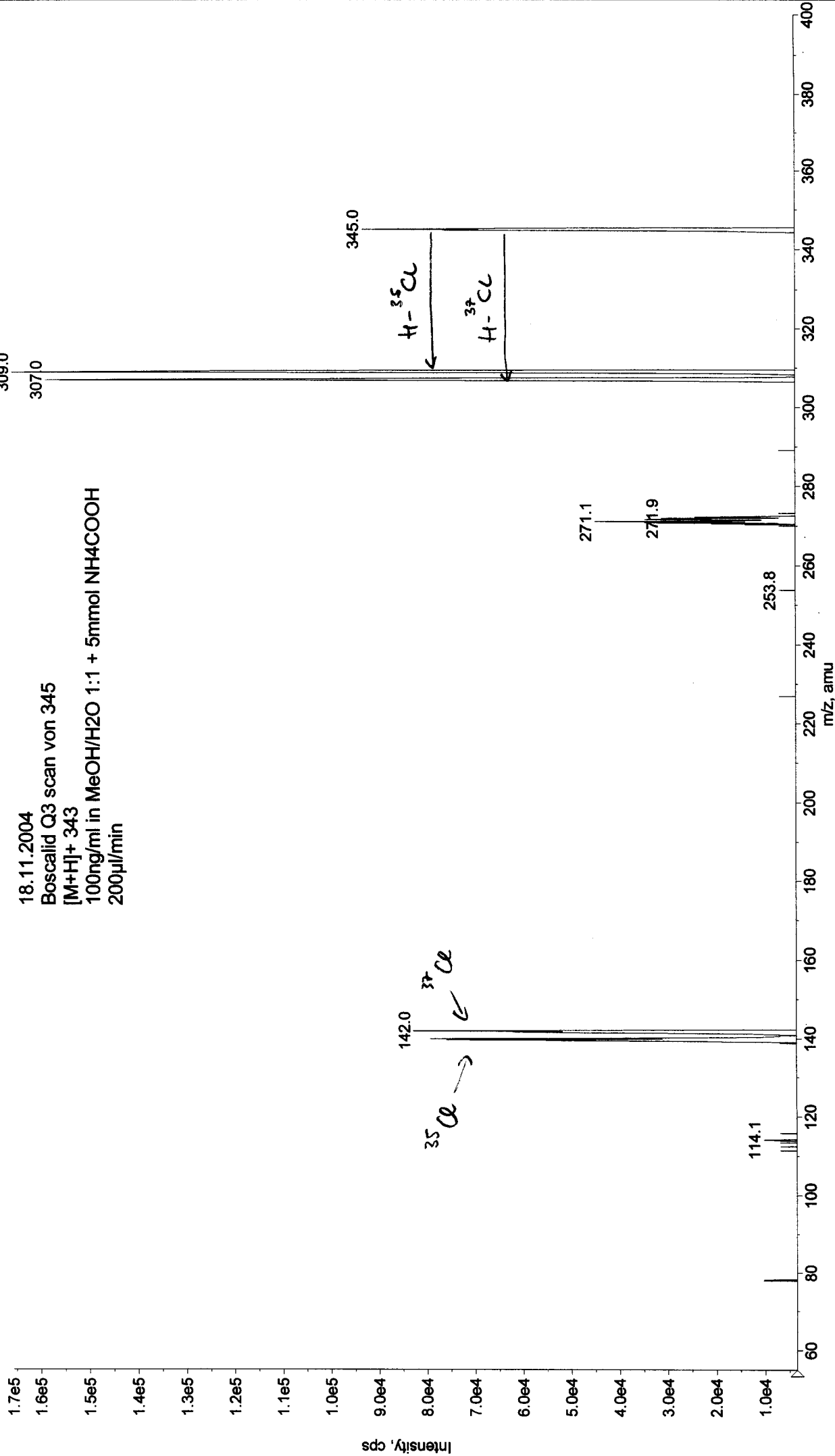
Acq. File: MT20041118092633.wiff

Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat

+MS2 (343.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20041118092633.wiff (Turbo Spray) Max. 3.6e5 cps.



+MS2 (345.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20041118092928.wiff (Turbo Spray) Max. 1.7e5 cps



State Parameter Editor

Mass Spectrometer Method Properties

Ion Source: Turbo Spray
 Temperature Reached
 Curtain Gas (CUR) 50.0
 Collision Gas (CAD) 5
 IonSpray Voltage (IS) 5500.0
 Temperature (TEM) 350.0
 Ion Source Gas 1 (GS1) 60.0
 Ion Source Gas 2 (GS2) 60.0
 Interface Heater (ihe) On

 Declustering Potential (DP) 71.0
 Focusing Potential (FP) 370.0
 Entrance Potential (EP) 10.0
 Collision Energy (CE) 27.0
 Collision Cell Exit Potential (CXP) 18.0

 Q1 Resolution: Unit
 Q3 Resolution: Unit
 Ion Energy 1 (IE1) 0.8
 Ion Energy 3 (IE3) 1.0

 Deflector (DF) -150.0
 CEM (CEM) 2400.0

Period 1:
 Scans in Period: 1935
 Relative Start Time: 0.00 msec
 Experiments in Period: 1

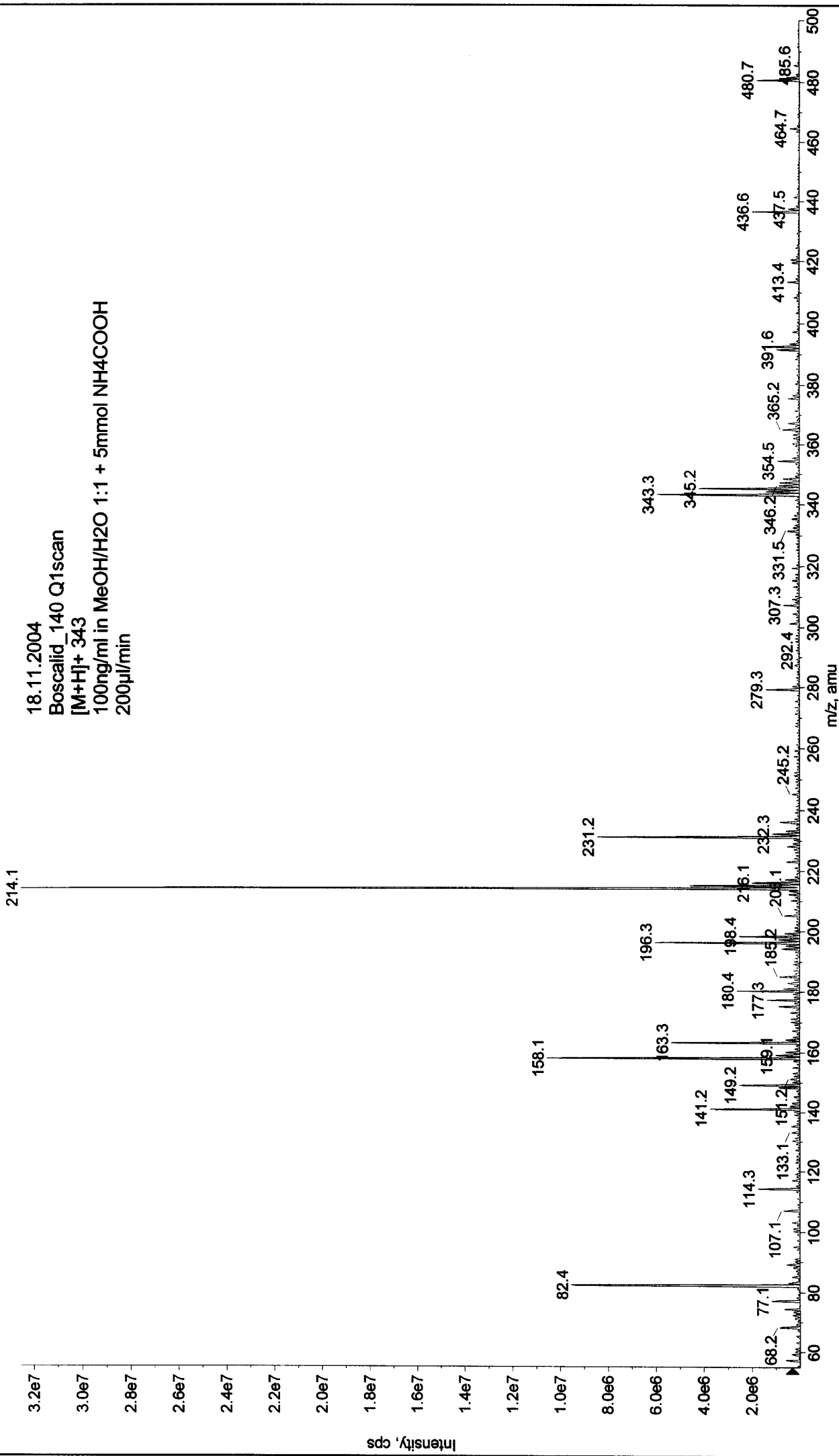
 Period 1 Experiment 1:
 Scan Type: MFM (MFM)
 Polarity: Positive
 Scan Mode: N/A
 Ion Source: Turbo Spray
 Resolution Q1: Unit
 Resolution Q3: Unit
 Intensity Thres.: 0.00 cps
 Settling Time: 0.0000 msec
 MR Pause: 5.0000 msec
 MCA: No
 Step Size: 0.00 amu

Q1 Mass (amu)	Q3 Mass (amu)	Dwell (msec)	Param	Start	Stop
343.16	307.00	150.00			

 Parameter Table (Period 1 Experiment 1):
 CUR: 50.00
 IS: 5500.00
 TEM: 350.00
 GS1: 60.00
 GS2: 60.00
 ihe: ON
 CAD: 5.00
 DF: 71.00
 FP: 370.00
 EP: 10.00
 CEF: 20.00
 CE: 27.00
 CXP: 18.00

Printing Time: 9:24:07
Printing Date: Thursday, November 18, 2004
Acq. Time: 09:22
Acq. File: MT20041118092251.wiff
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat

+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20041118092251.wiff (Turbo Spray) Max. 3.3e7 cps



Printing Time: 9:17:36

Printing Date: Thursday, November 18, 2004

Acq. Time: 09:16

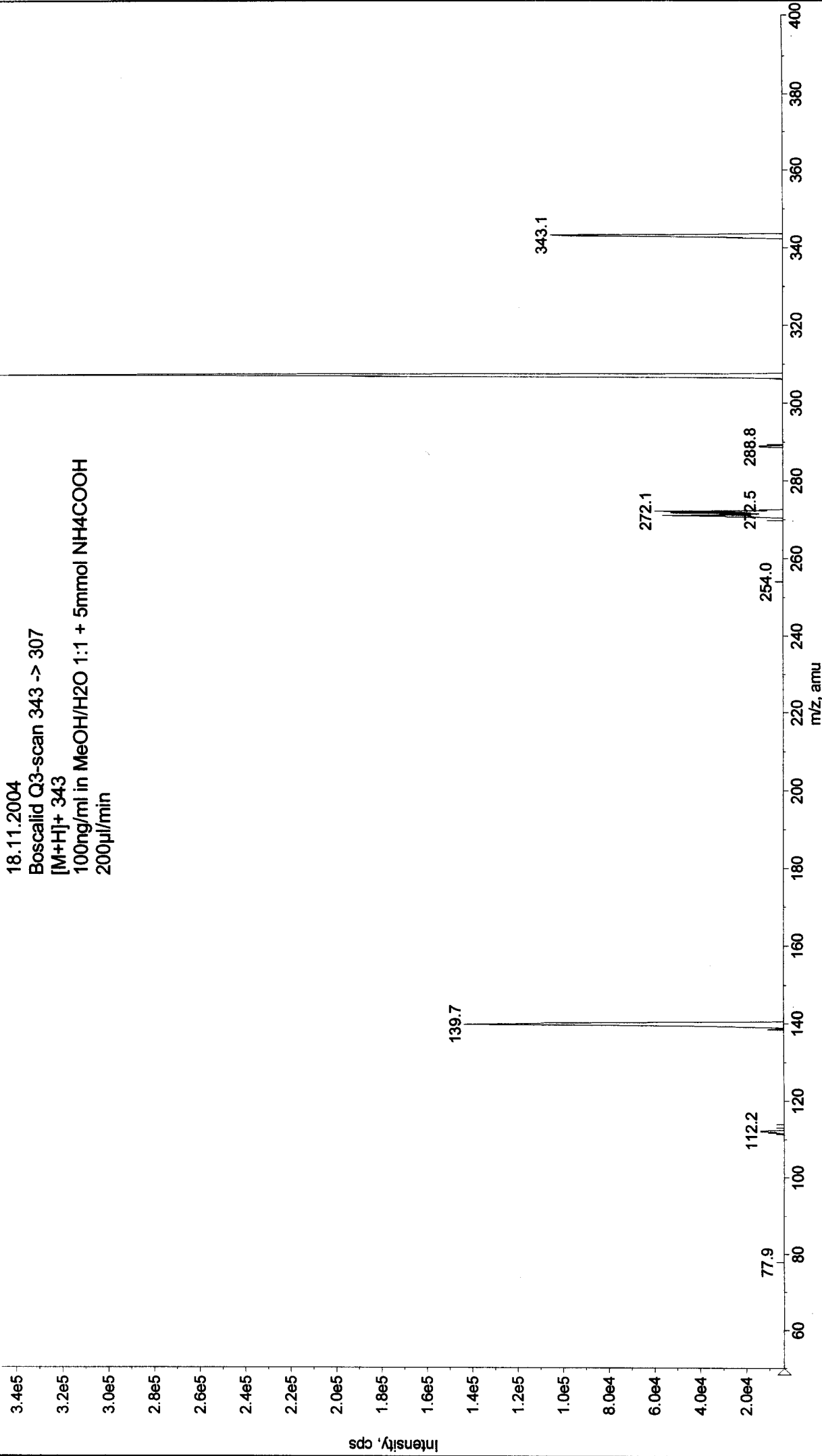
Acq. Date: Thursday, November 18, 2004

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat

+MS2 (343.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20041118091607.wiff (Turbo Spray) Max. 3.5e5 cps



State Parameter Editor

Mass Spectrometer Method Properties

Ion Source: Turbo Spray
 Temperature Reached
 Curtain Gas (CUR) 50.0
 Collision Gas (CAD) 5
 IonSpray Voltage (IS) 5500.0
 Temperature (TEM) 350.0
 Ion Source Gas 1 (GS1) 60.0
 Ion Source Gas 2 (GS2) 60.0
 Interface Heater (ihe) On

 Declustering Potential (DP) 76.0
 Focusing Potential (FP) 310.0
 Entrance Potential (EP) 11.0
 Collision Energy (CE) 27.0
 Collision Cell Exit Potential (CXP) 8.0

 Q1 Resolution: Unit
 Resolution: Unit
 Ion Energy 1 (IE1) 0.8
 Ion Energy 3 (IE3) 1.0

 Deflector (DF) -150.0
 CEM (CEM) 2400.0

Period 1:
 Scans in Period: 1935
 Relative Start Time: 0.00 msec
 Experiments in Period: 1

 Period 1 Experiment 1:
 Scan Type: MFM (MFM)
 Polarity: Positive
 Scan Mode: N/A
 Ion Source: Turbo Spray
 Resolution Q1: Unit
 Resolution Q3: Unit
 Intensity Thres.: 0.00 cps
 Settling Time: 0.0000 msec
 MR Pause: 5.0000 msec
 MCA: No
 Step Size: 0.00 amu

Q1 Mass (amu)	Q3 Mass (amu)	Dwell (msec)	Param	Start	Stop
343.16	139.9C	150.0C			

 Parameter Table (Period 1 Experiment 1):
 CUR: 50.00
 CAD: 5.00
 IS: 5500.00
 TEM: 350.00
 GS1: 60.00
 GS2: 60.00
 ihe: ON
 DF: 76.00
 FP: 310.00
 EP: 11.00
 CEF: 20.00
 CE: 27.00
 CXP: 8.00