

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

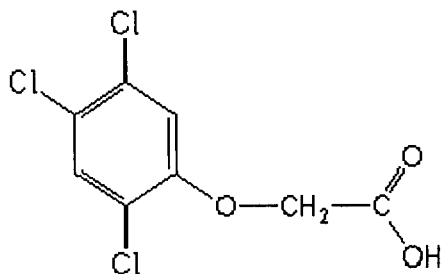
### Analyte: 2,4,5-T

CAS No.: 93-76-5

Formula: C<sub>8</sub>H<sub>5</sub>Cl<sub>3</sub>O<sub>3</sub>

Molecular mass (lowest isotopes): 253,93 amu

Structure:



Ionisation: ESI -

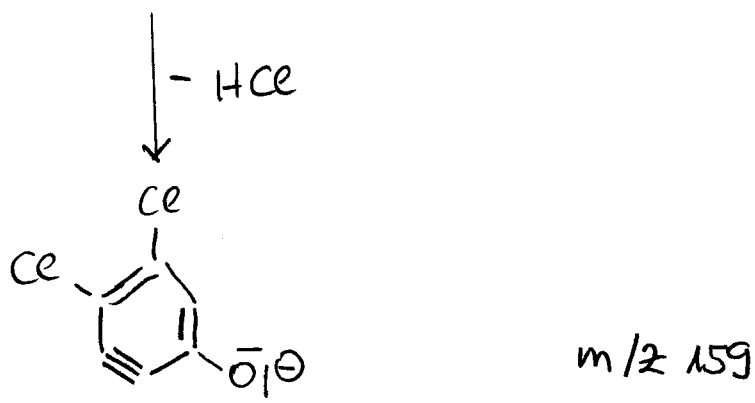
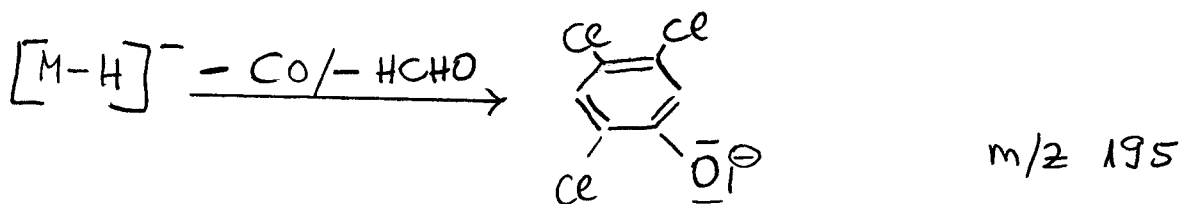
Quasimolecular ion: 252,93 amu = [M-H]<sup>-</sup>

Analyte sensitive parameter set (API 2000)

Transition	252,9 → 195,0	252,9 → 159,0
Declustering potential (DP) <sup>*)</sup>	-61 V	-61 V
Focusing potential (FP)	-330 V	-330 V
Entrance potential (EP)	-10 V	-9 V
Collision cell entrance potential (CEP)	-22 V	-24 V
Collision energy (CE)	-16 V	-34 V
Collision cell exit potential (CXP)	-12 V	-10 V

<sup>\*)</sup> For API 3000 and 4000 enhance DP by 20V

### Fragmentation



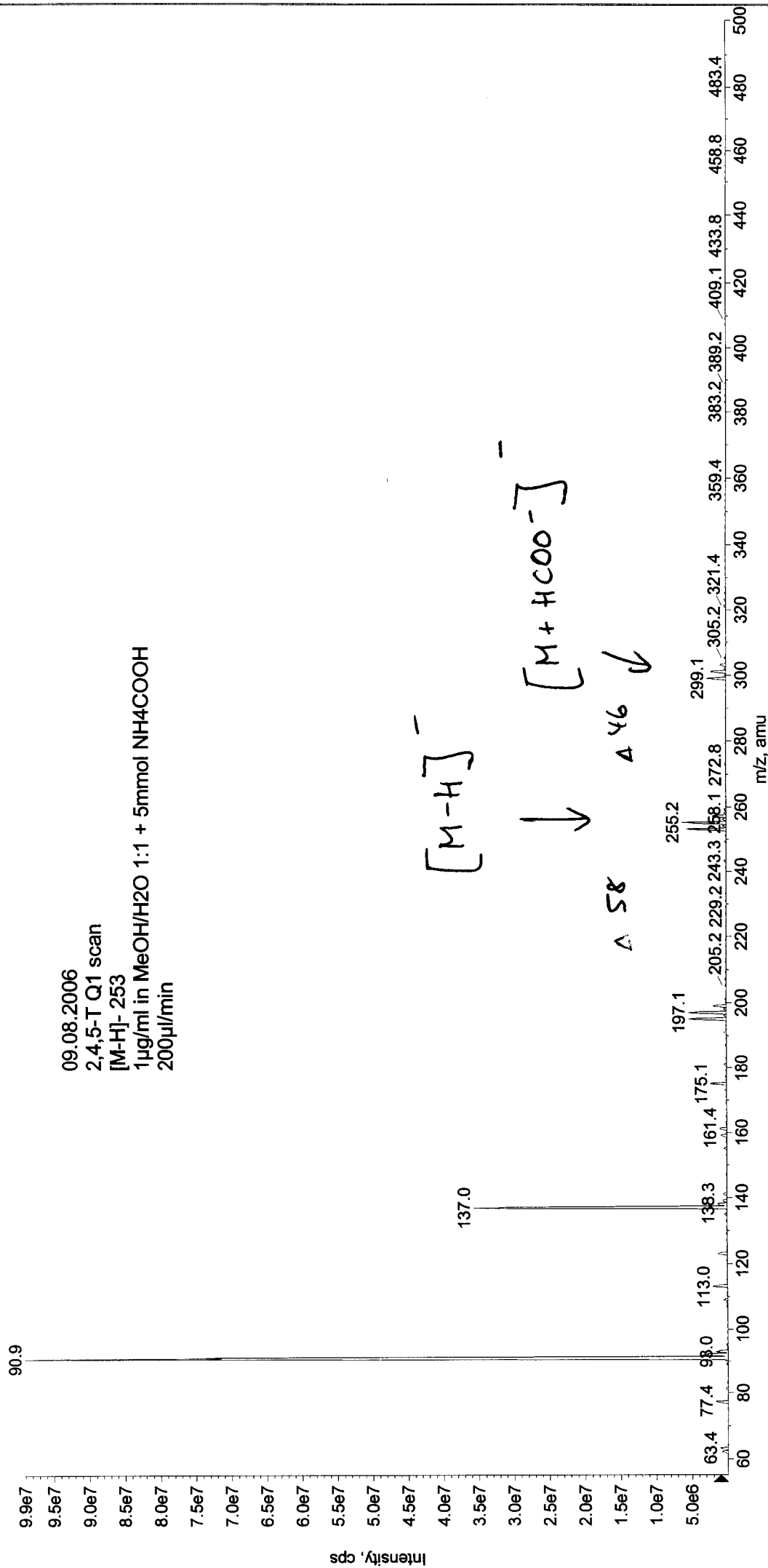
Printing Time: 11:46:28  
Printing Date: Wednesday, August 09, 2006

Acq. Time: 11:43  
Acq. Date: Wednesday, August 09, 2006  
Acq. File: MT20060809114348.wiff

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

■ -Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060809114348.wiff (Turbo Spray)

Max. 9.9e7 cps



Printing Time: 11:48:40

Printing Date: Wednesday, August 09, 2006

Acq. Time: 11:47

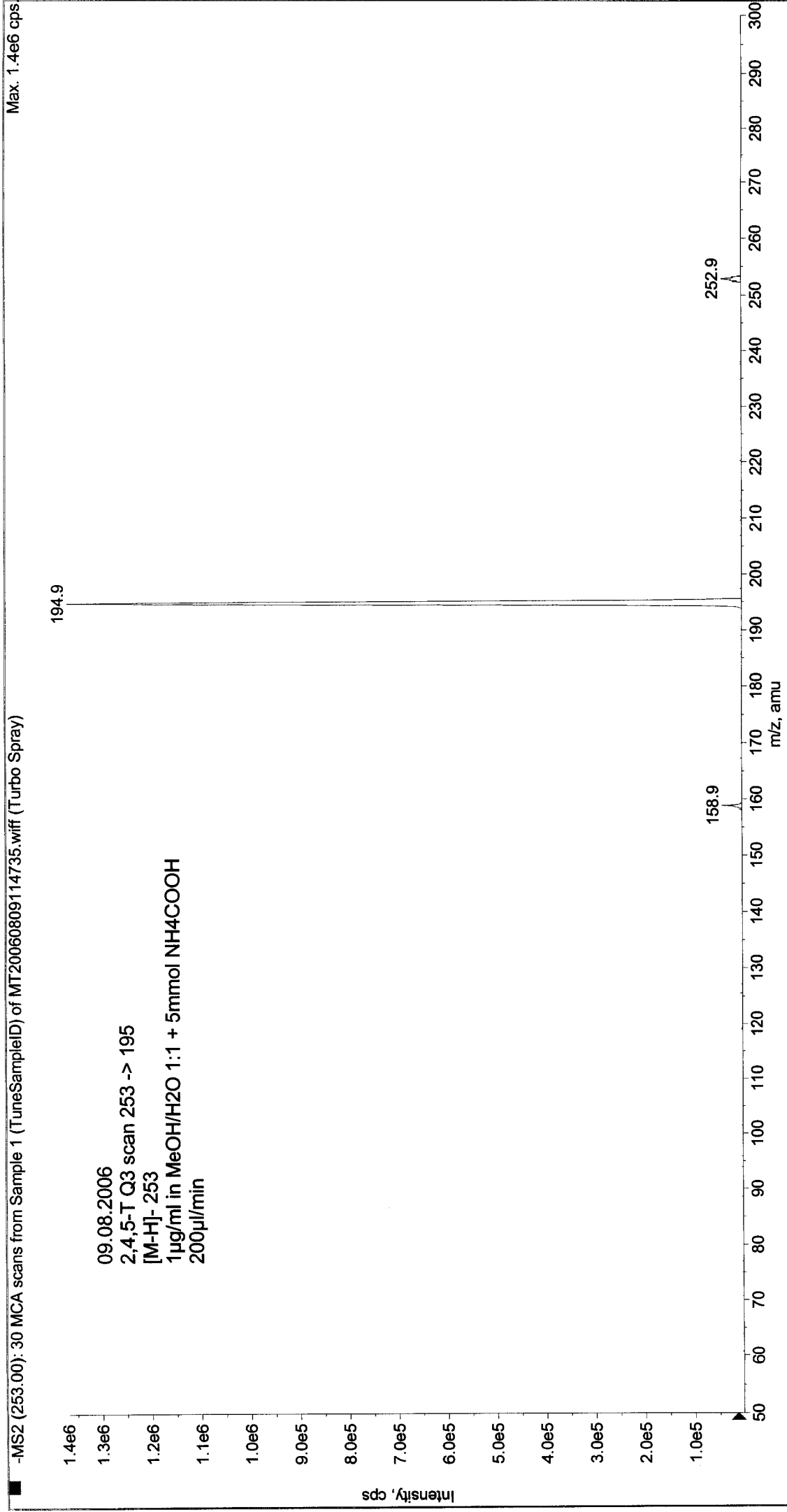
Acq. Date: Wednesday, August 09, 2006

Acq. File: MT20060809114735.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat



Printing Time: 11:49:59

Printing Date: Wednesday, August 09, 2006

Acq. Time: 11:48

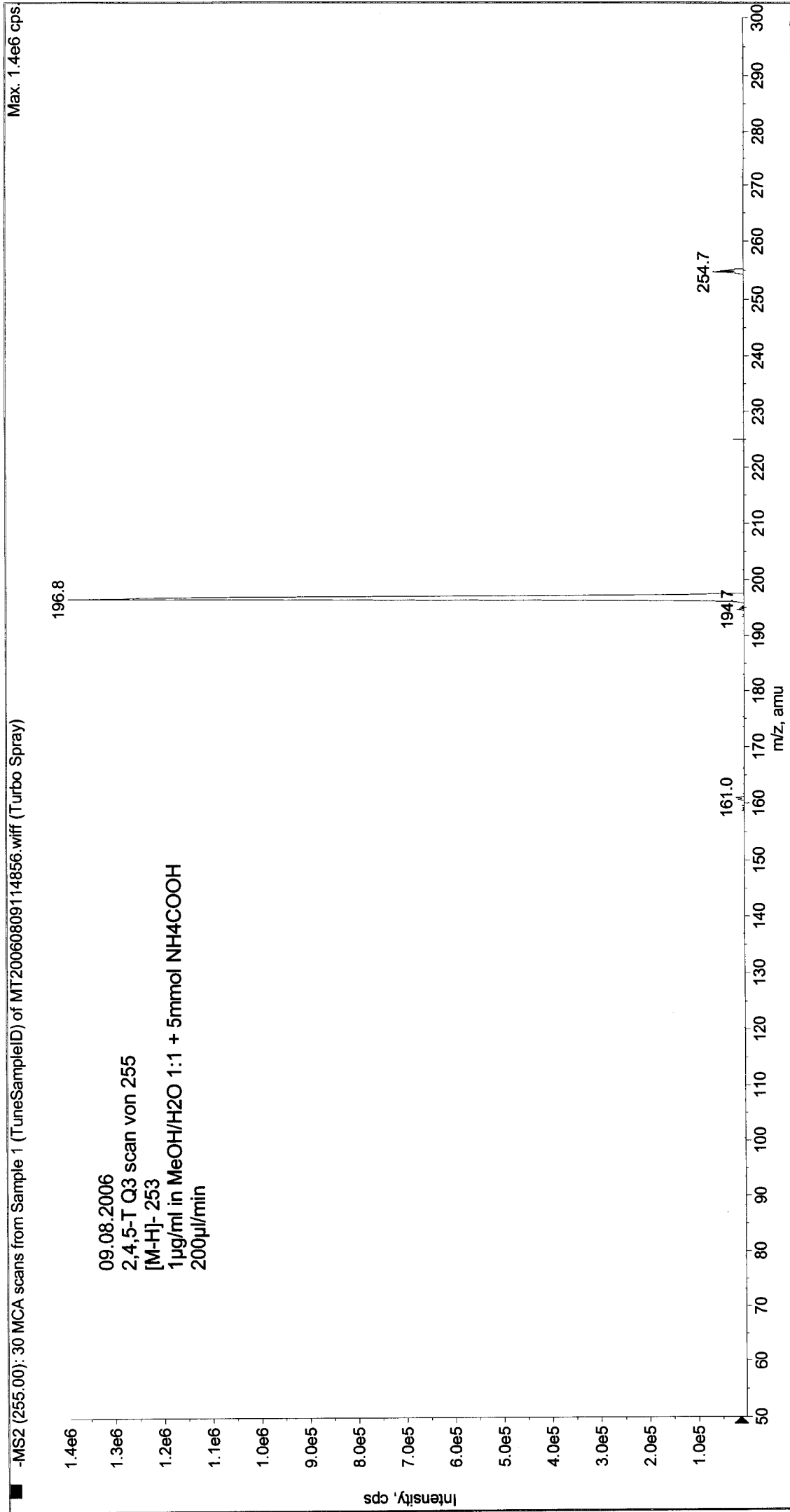
Acq. Date: Wednesday, August 09, 2006

Acq. File: MT20060809114856.wiff

Sample Comment:

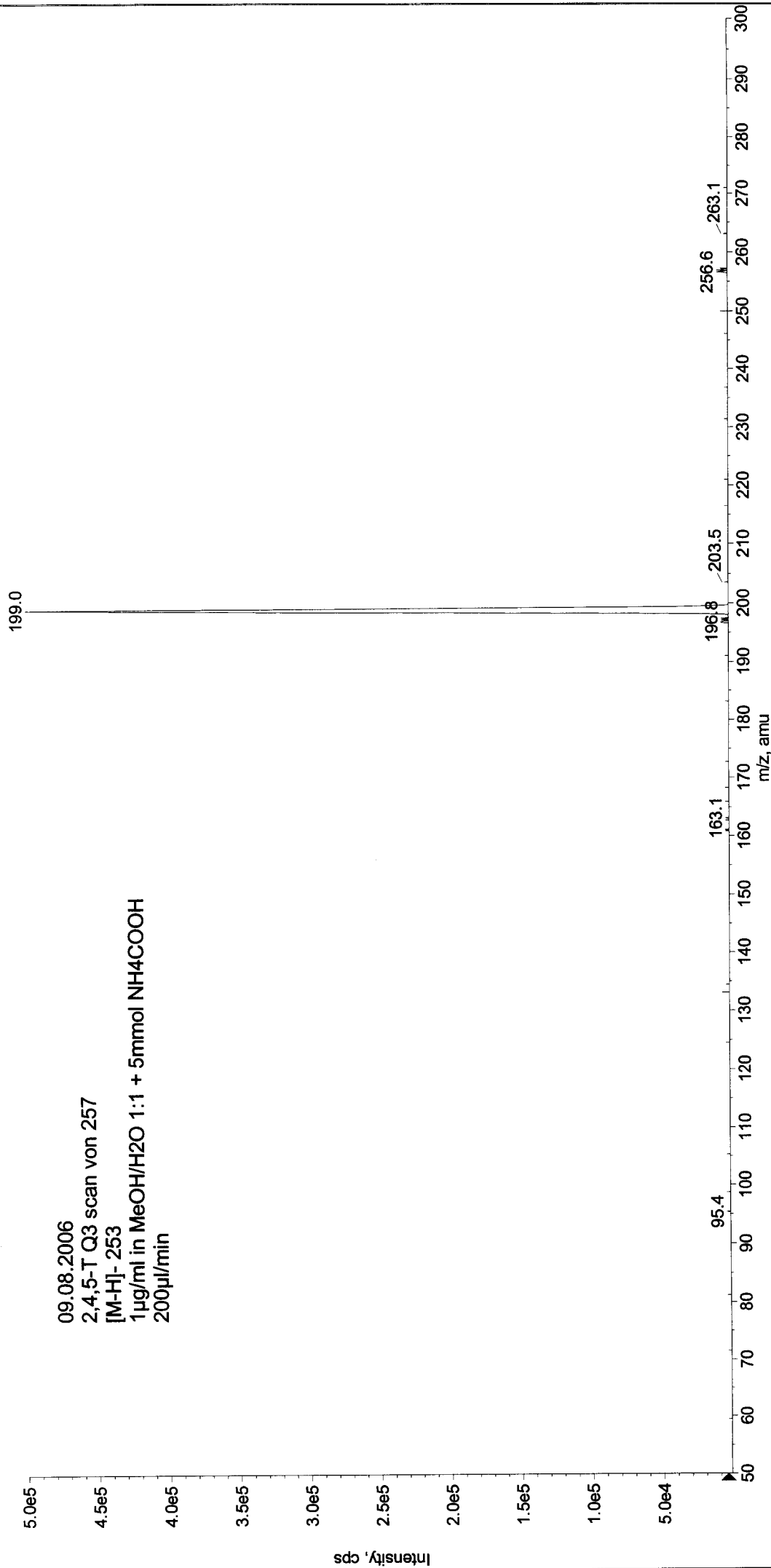
Sample Name: TuneSampleID

Batch Name: ManualTune.bat



Max. 5.0e5 cps

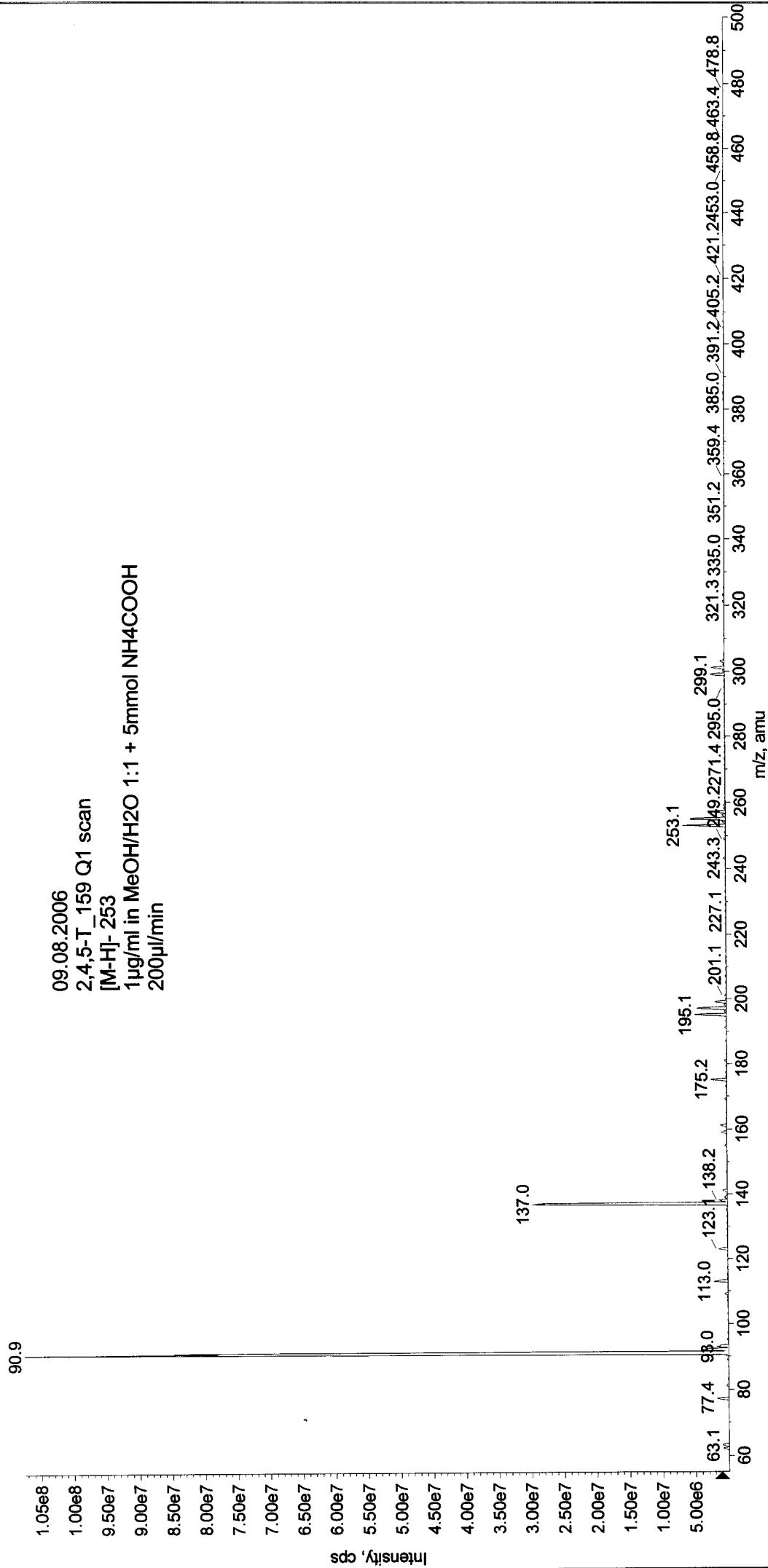
-MS2 (257.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060809115013.wiff (Turbo Spray)



09.08.2006  
2,4,5-T Q3 scan von 257  
[M-H]<sup>-</sup> 253  
1 µg/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
200 µl/min

Max. 1.1e8 cps

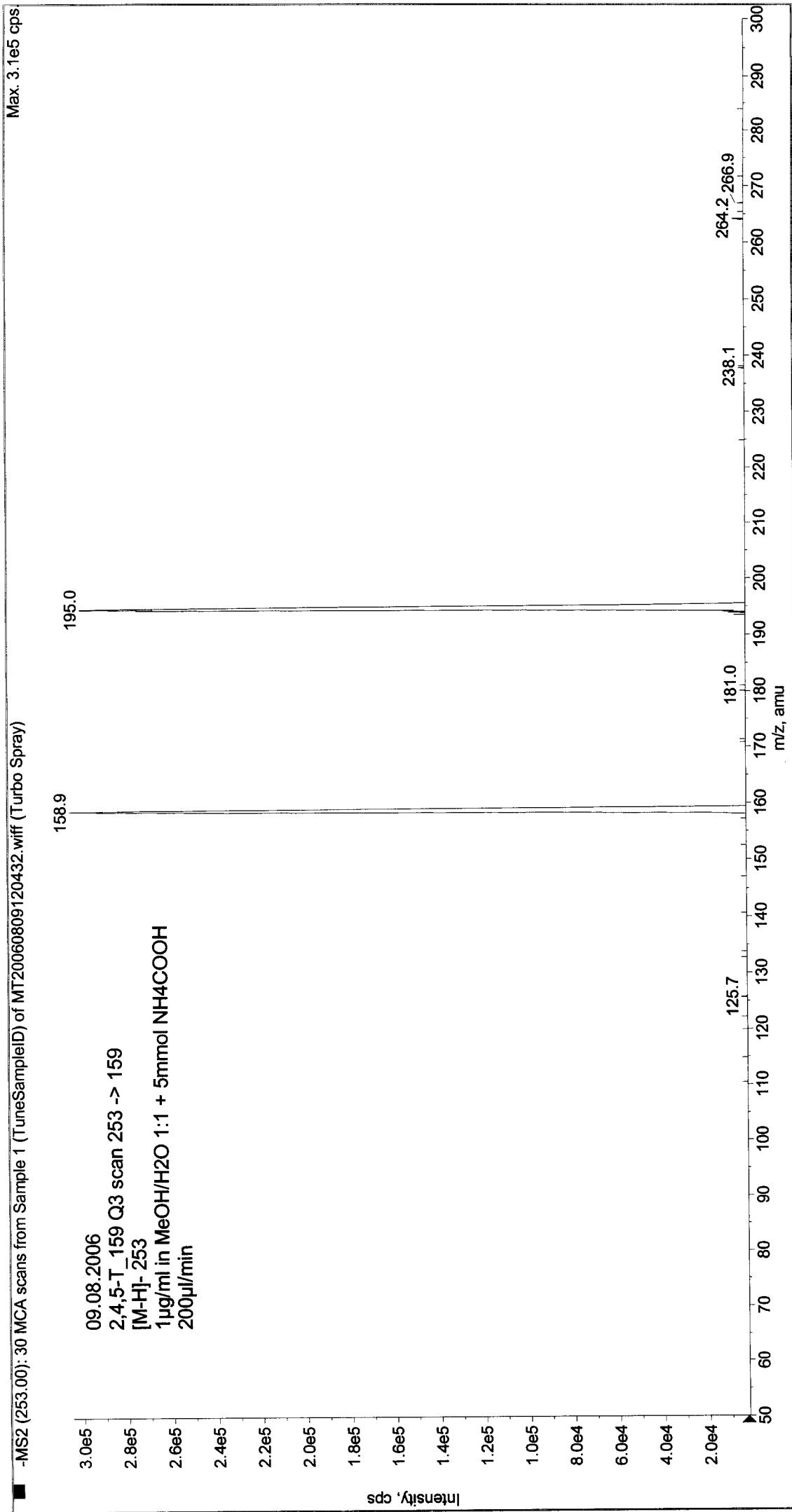
-Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060809120220.wiff (Turbo Spray)



Printing Time: 12:05:46  
Printing Date: Wednesday, August 09, 2006

Acq. Time: 12:04  
Acq. Date: Wednesday, August 09, 2006  
Acq. File: MT20060809120432.wiff

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



Printing Time: 12:07:13

Printing Date: Wednesday, August 09, 2006

Acq. Time: 12:06

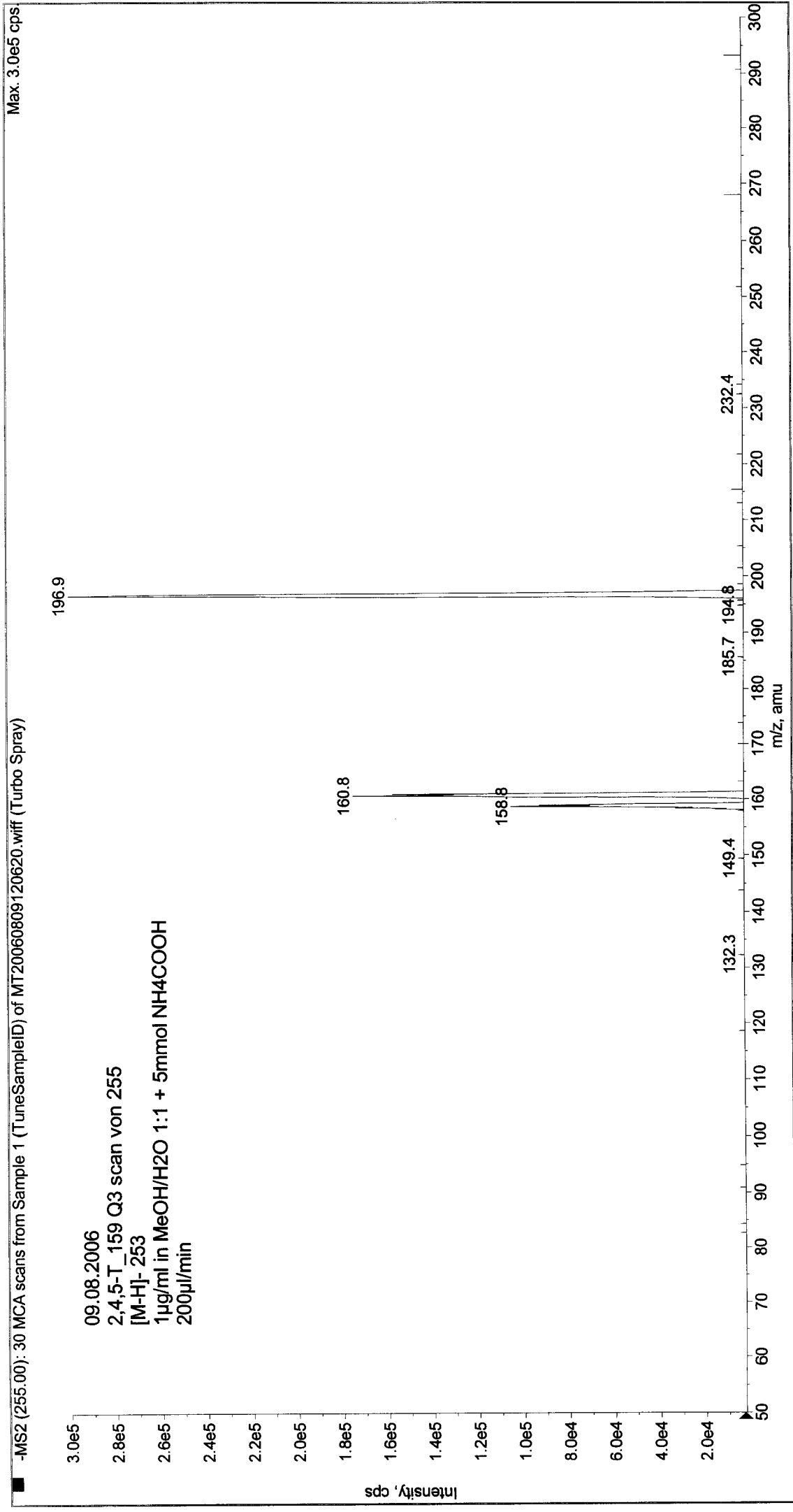
Acq. Date: Wednesday, August 09, 2006

Acq. File: MT20060809120620.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat





Printing Time: 12:08:11

Printing Date: Wednesday, August 09, 2006

Acq. Time: 12:07

Acq. Date: Wednesday, August 09, 2006

Acq. File: MT20060809120724.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat

