

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

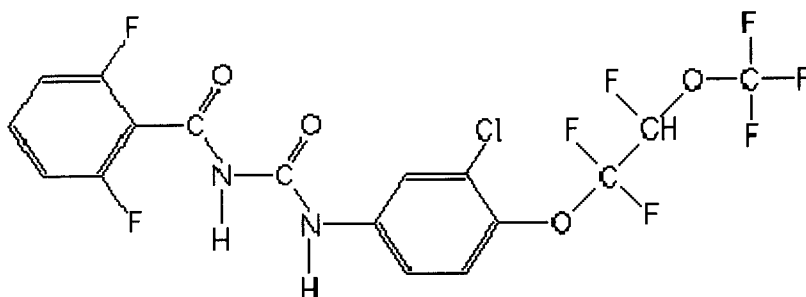
### Analyte: Novaluron

CAS No.: 116714-46-6

Formula: C<sub>17</sub>H<sub>9</sub>ClF<sub>8</sub>N<sub>2</sub>O<sub>4</sub>

Molecular mass (lowest isotopes): 492,01 amu

Structure:



Ionisation: ESI +

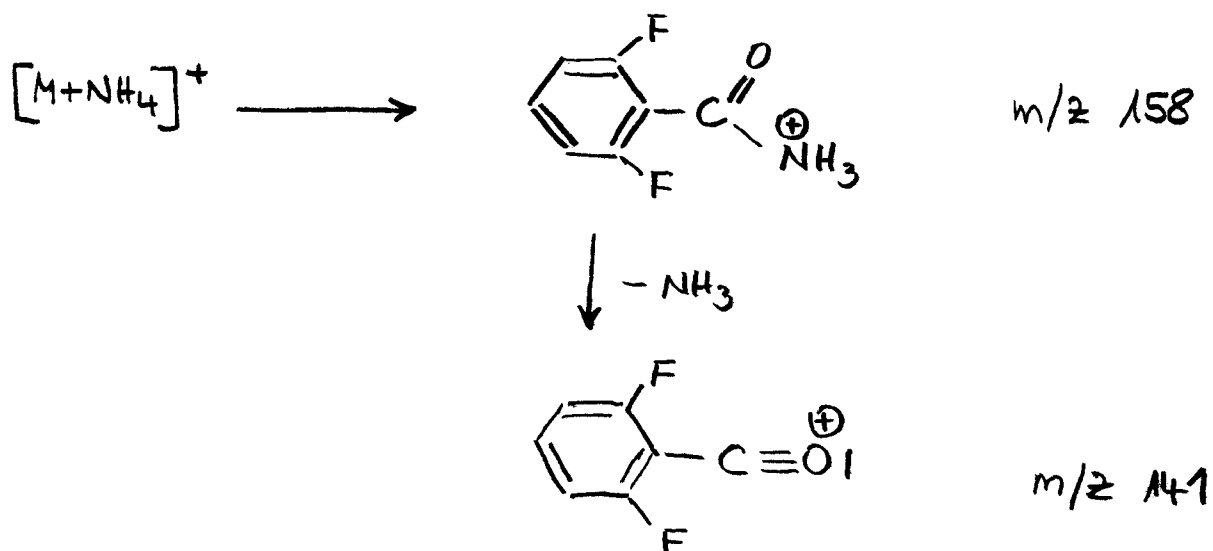
Quasimolecular ion: 510,0 amu = [M+NH<sub>4</sub>]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	510,0 → 158,0	510,0 → 140,9
Declustering potential (DP) <sup>*)</sup>	11 V	11 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	11,5 V	11,0 V
Collision cell entrance potential (CEP)	22 V	24 V
Collision energy (CE)	31 V	63 V
Collision cell exit potential (CXP)	8 V	8 V

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

### Fragmentation



Printing Time: 13:20:44  
Printing Date: Friday, August 11, 2006

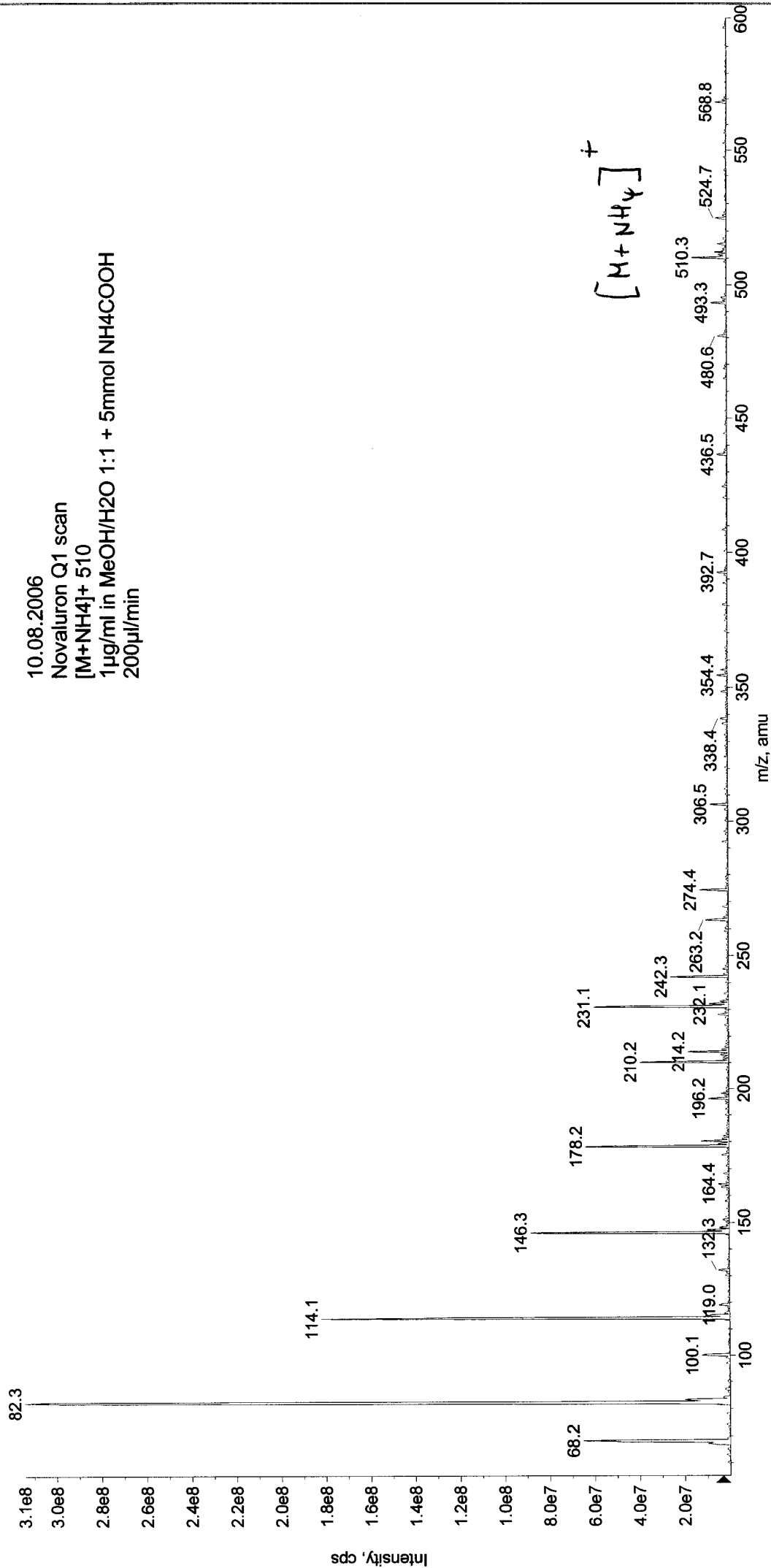
Acq. Time: 13:19  
Acq. Date: Friday, August 11, 2006  
Acq. File: MT20060811131938.wiff

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

+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060811131938.wiff (Turbo Spray)

Max. 3.1e8 cps

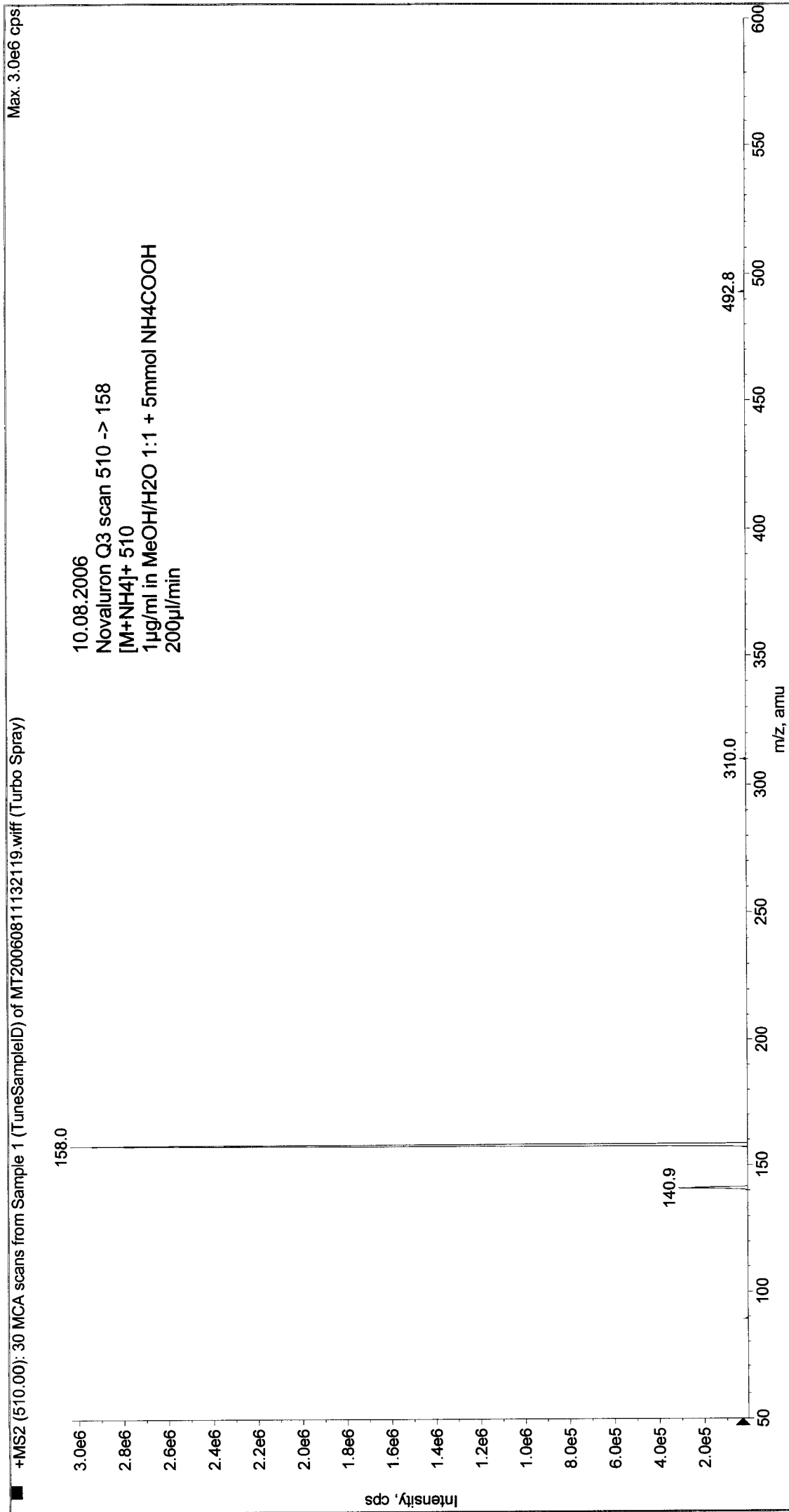
10.08.2006  
Novaluron Q1 scan  
[M+NH<sub>4</sub>]<sup>+</sup> 510  
1 µg/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
200 µl/min



Printing Time: 13:22:25  
Printing Date: Friday, August 11, 2006

Acq. Time: 13:21  
Acq. Date: Friday, August 11, 2006  
Acq. File: MT20060811132119.wiff

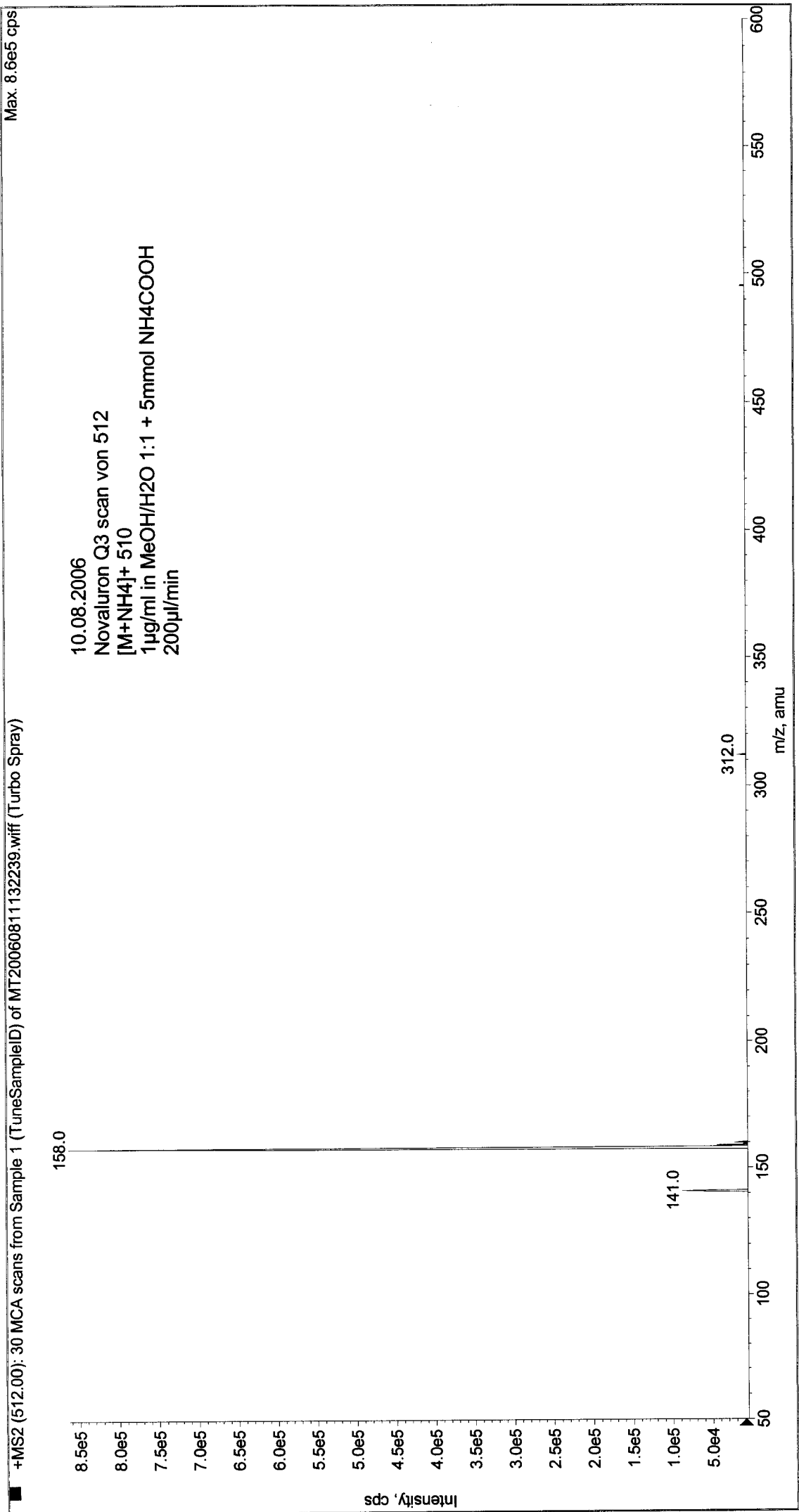
Sample Comment:  
Sample Name: TuneSampleID  
Batch Name: ManualTune.bat



Printing Time: 13:23:33  
Printing Date: Friday, August 11, 2006

Acq. Time: 13:22  
Acq. Date: Friday, August 11, 2006  
Acq. File: MT20060811132239.wiff

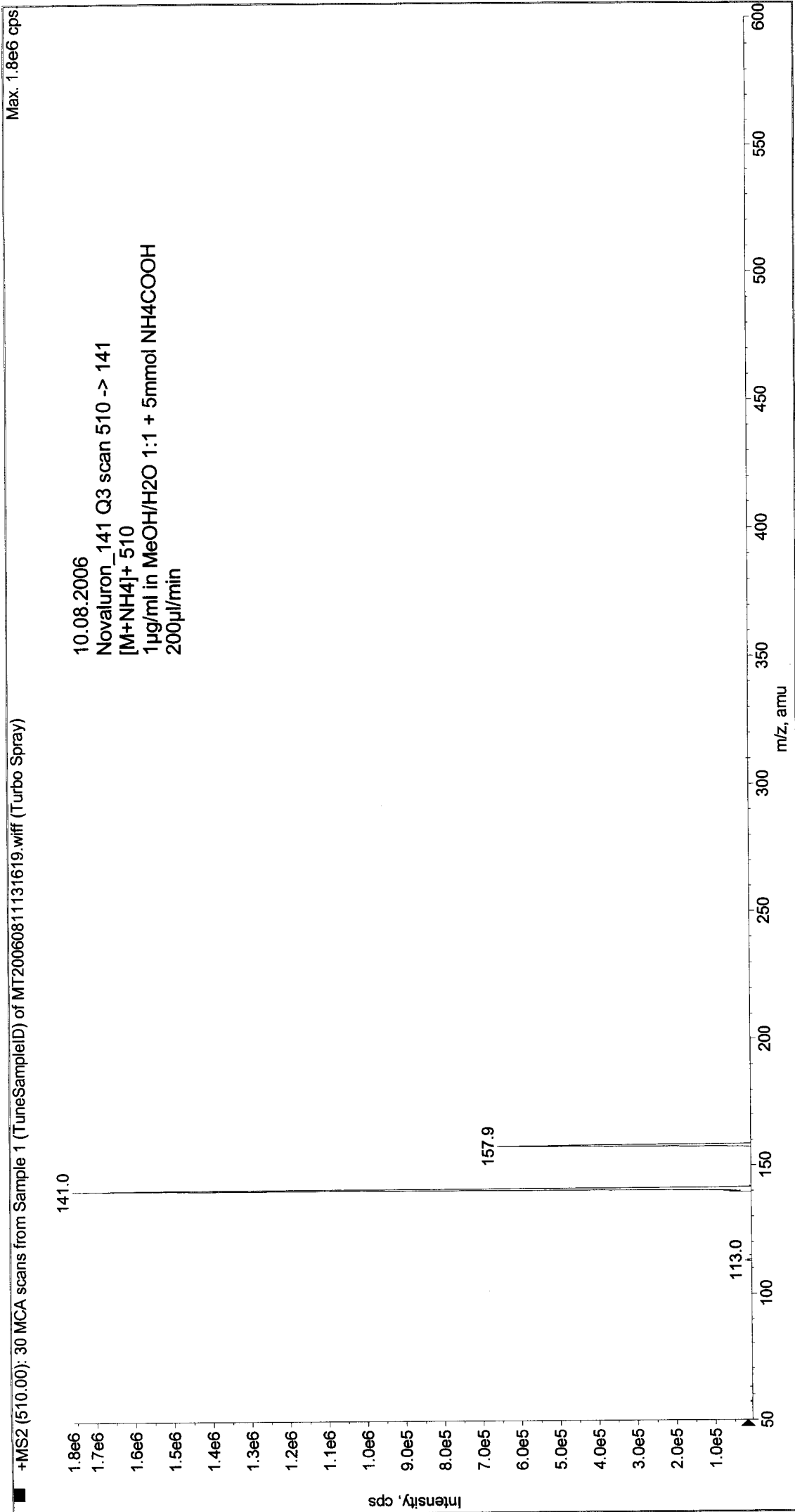
Sample Comment:  
Sample Name: TuneSampleID  
Batch Name: ManualTune.bat



Printing Time: 13:17:26  
Printing Date: Friday, August 11, 2006

Acq. Time: 13:16  
Acq. Date: Friday, August 11, 2006  
Acq. File: MT20060811131619.wiff

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



Printing Time: 13:19:00  
Printing Date: Friday, August 11, 2006

Acq. Time: 13:17  
Acq. Date: Friday, August 11, 2006  
Acq. File: MT20060811131746.wiff

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

