

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

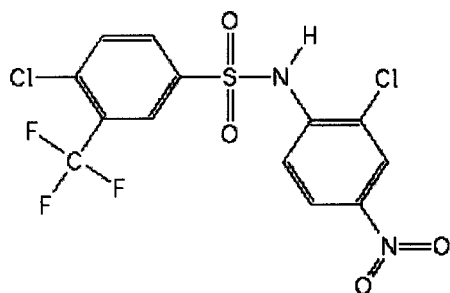
Analyte: Flusulfamide

CAS No.: 106917-52-6

Formula: C₁₃H₇Cl₂F₃N₂O₄S

Molecular mass (lowest isotopes): 413,95 amu

Structure:



Ionisation: ESI -

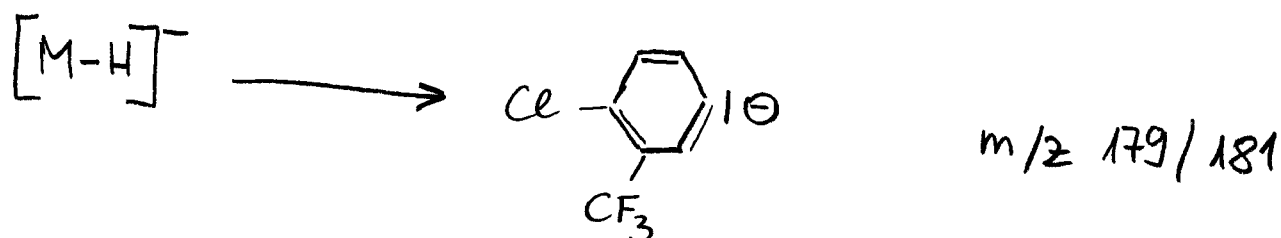
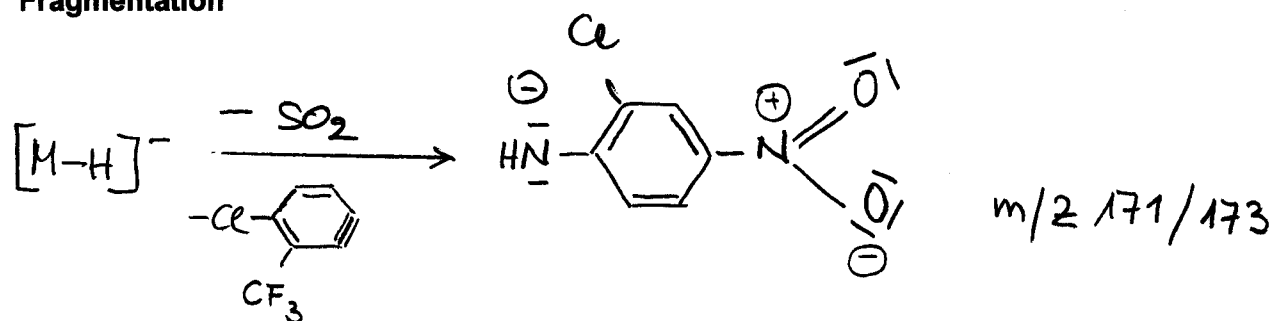
Quasimolecular ion: 412,95 amu = [M-H]⁻

Analyte sensitive parameter set (API 2000)

Transition	413,0 → 171,0	413,0 → 178,9
Declustering potential (DP) ^{*)}	-64 V	-64 V
Focusing potential (FP)	-310 V	-340 V
Entrance potential (EP)	-10 V	-10 V
Collision cell entrance potential (CEP)	-22 V	-22 V
Collision energy (CE)	-46 V	-44 V
Collision cell exit potential (CXP)	-12 V	-12 V

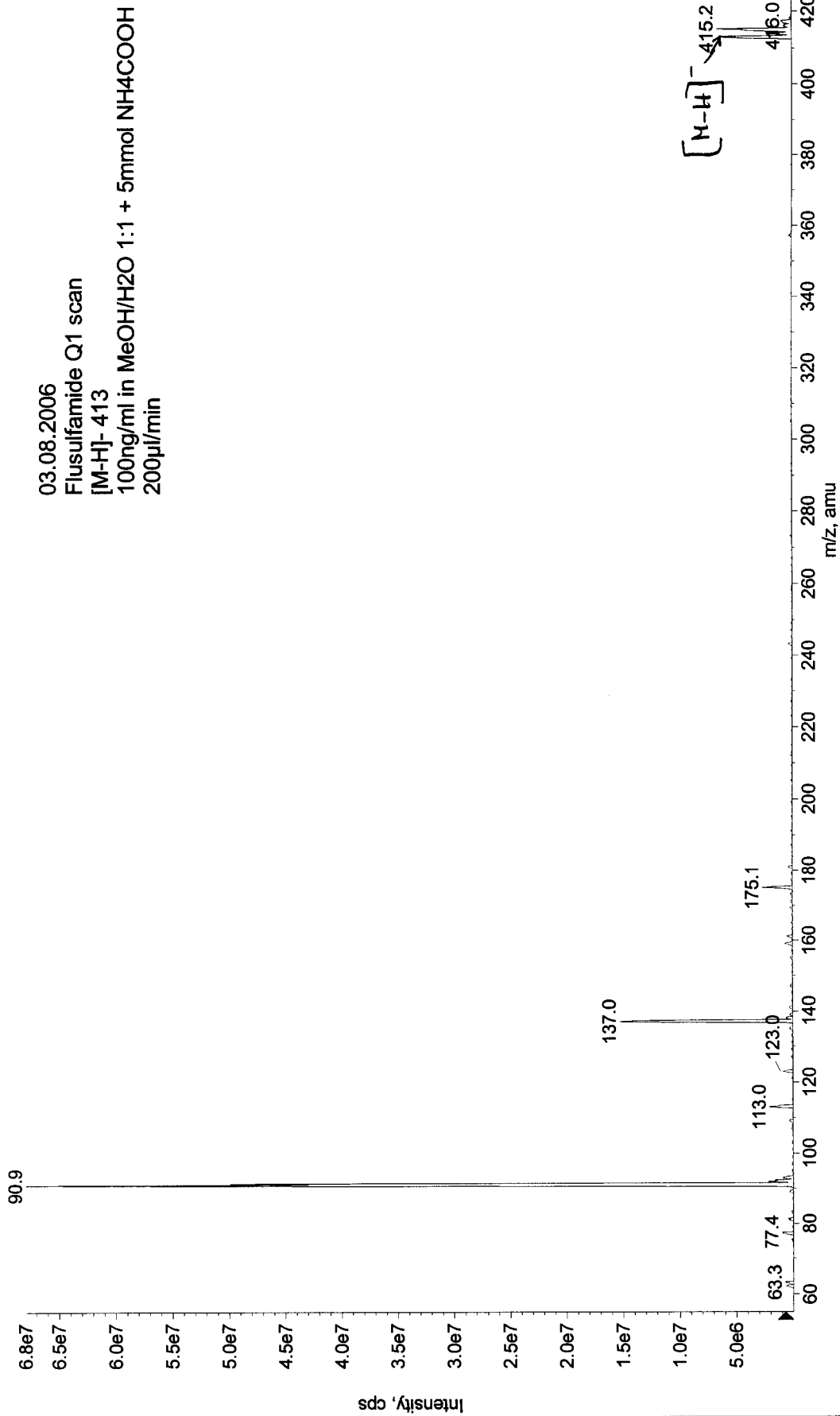
^{*)} For API 3000 and 4000 enhance DP by 20V

Fragmentation



-Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060803135132.wiff (Turbo Spray)

Max. 6.8e7 cps



Max. 3.3e5 cps

03.08.2006

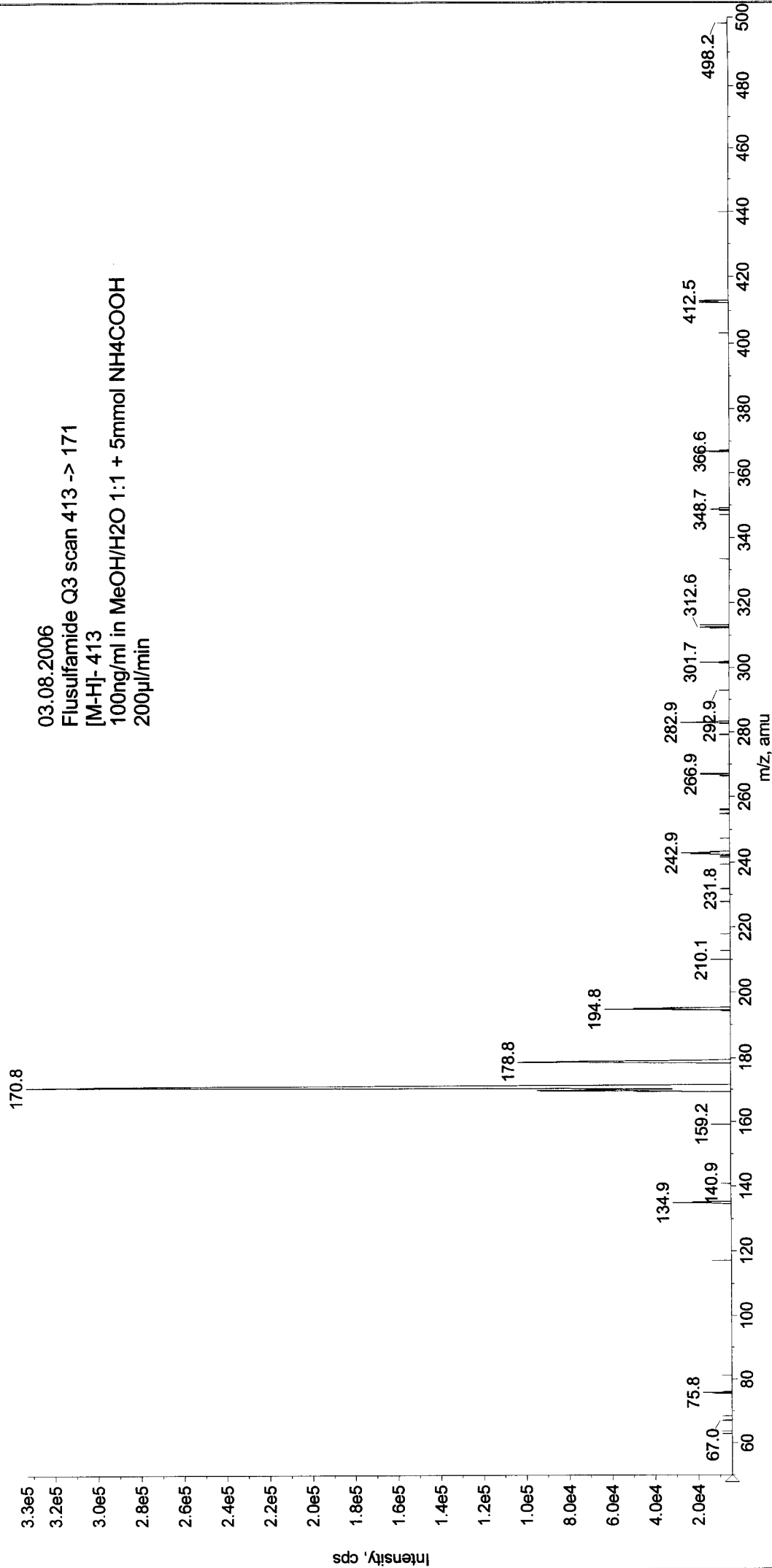
Flusulfamide Q3 scan 413 -> 171

[M-H]⁻ 413

100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH

200µl/min

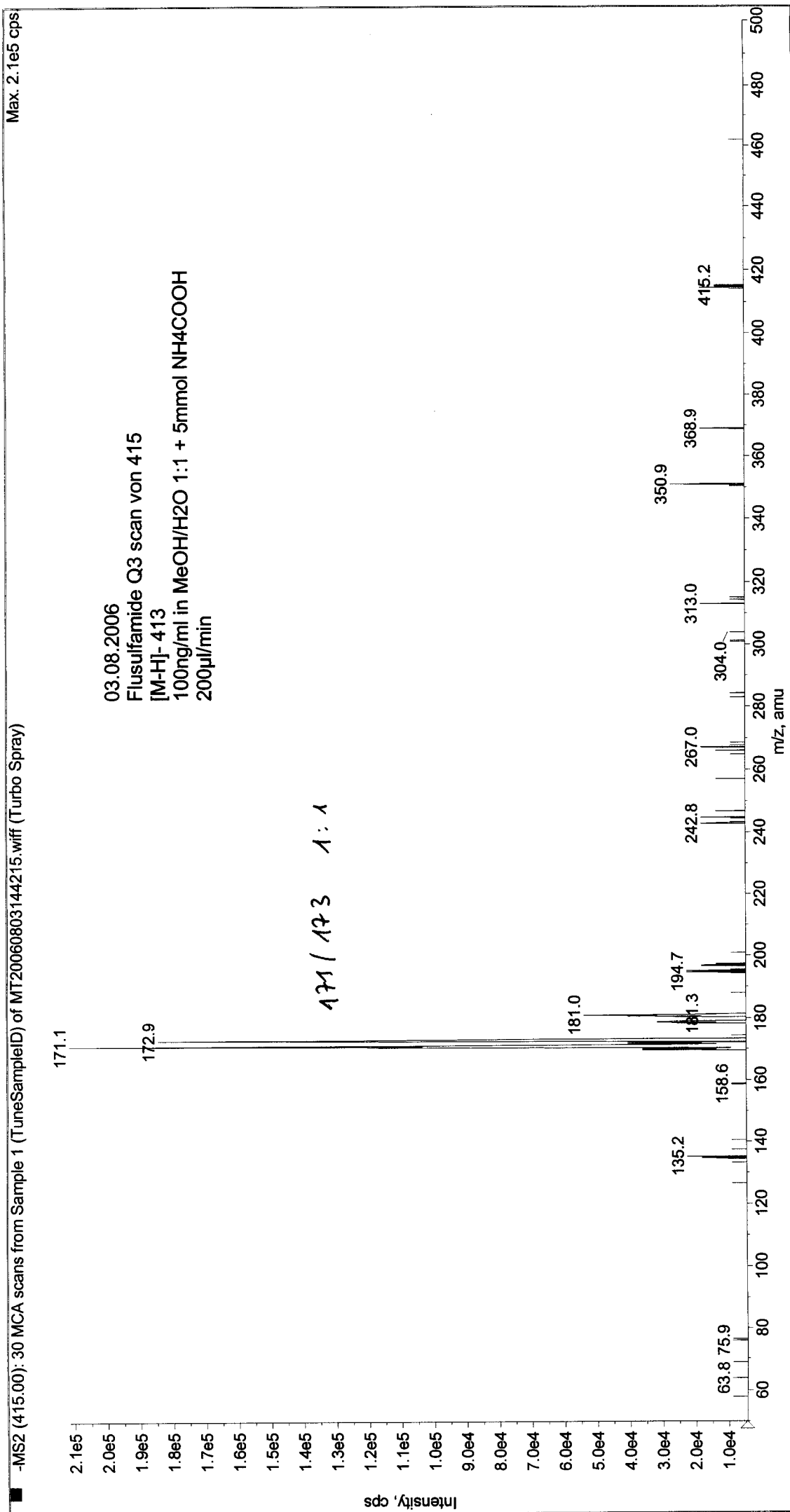
-MS2 (413.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060803134422.wiff (Turbo Spray)



Printing Time: 14:43:14
Printing Date: Thursday, August 03, 2006

Acq Time: 14:42
Acq. Date: Thursday, August 03, 2006
Acq. File: MT20060803144215.wiff

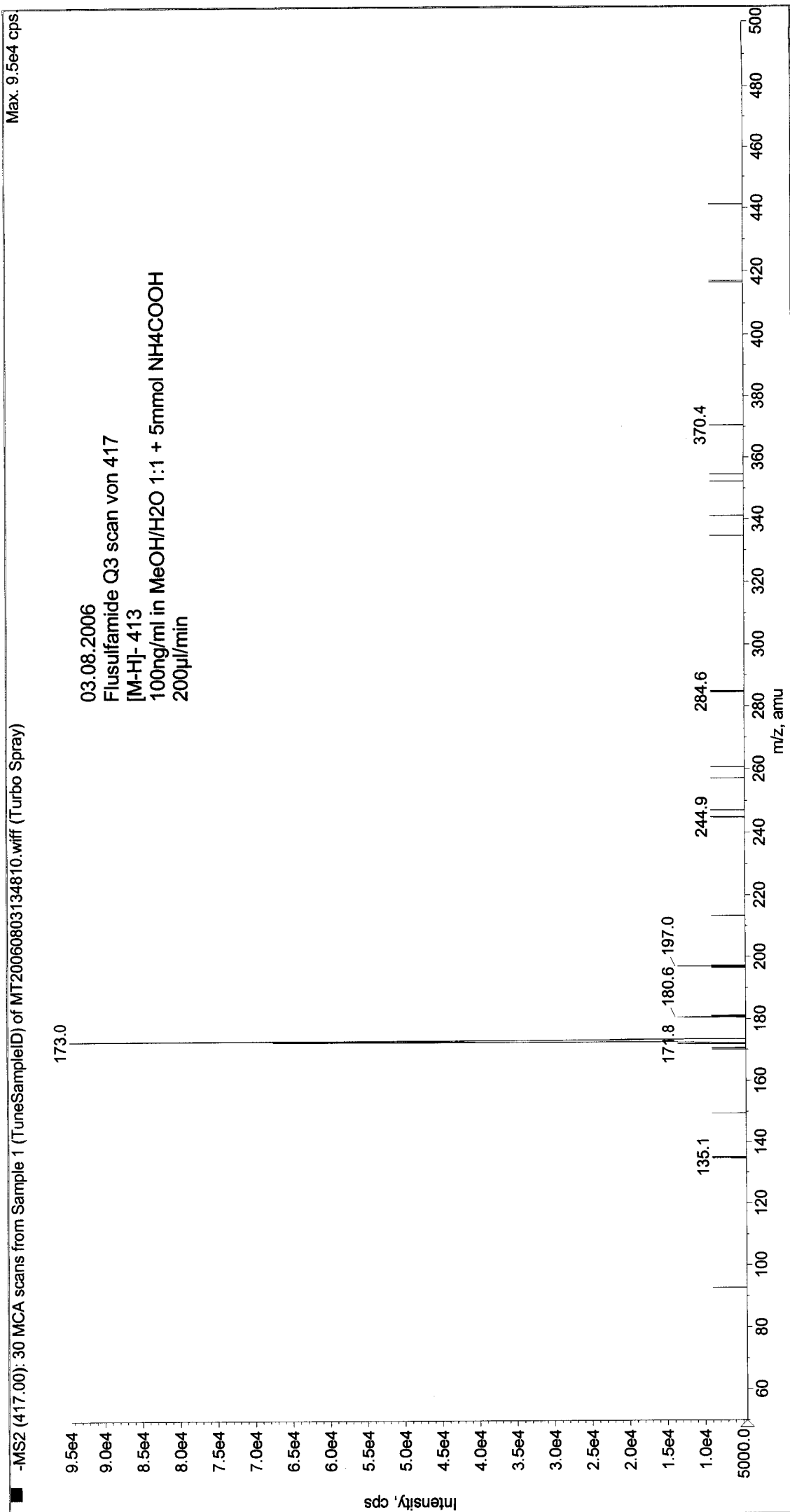
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat



Printing Time: 13:48:59
Printing Date: Thursday, August 03, 2006

Acq. Time: 13:48
Acq. Date: Thursday, August 03, 2006
Acq. File: MT20060803134810.wiff

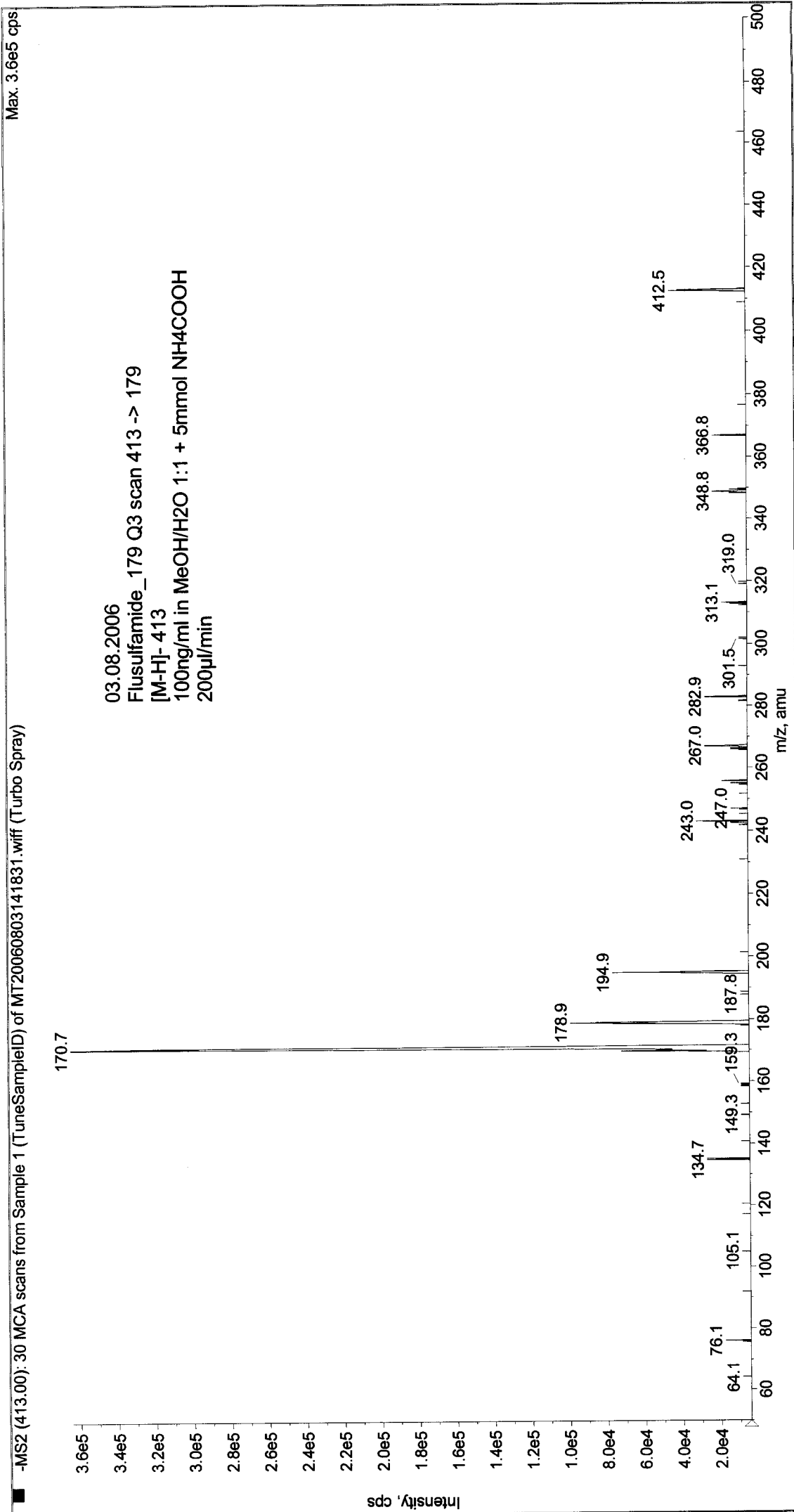
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat



Printing Time: 14:19:43
Printing Date: Thursday, August 03, 2006

Acq Time: 14:18
Acq. Date: Thursday, August 03, 2006
Acq. File: MT20060803141831.wiff

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

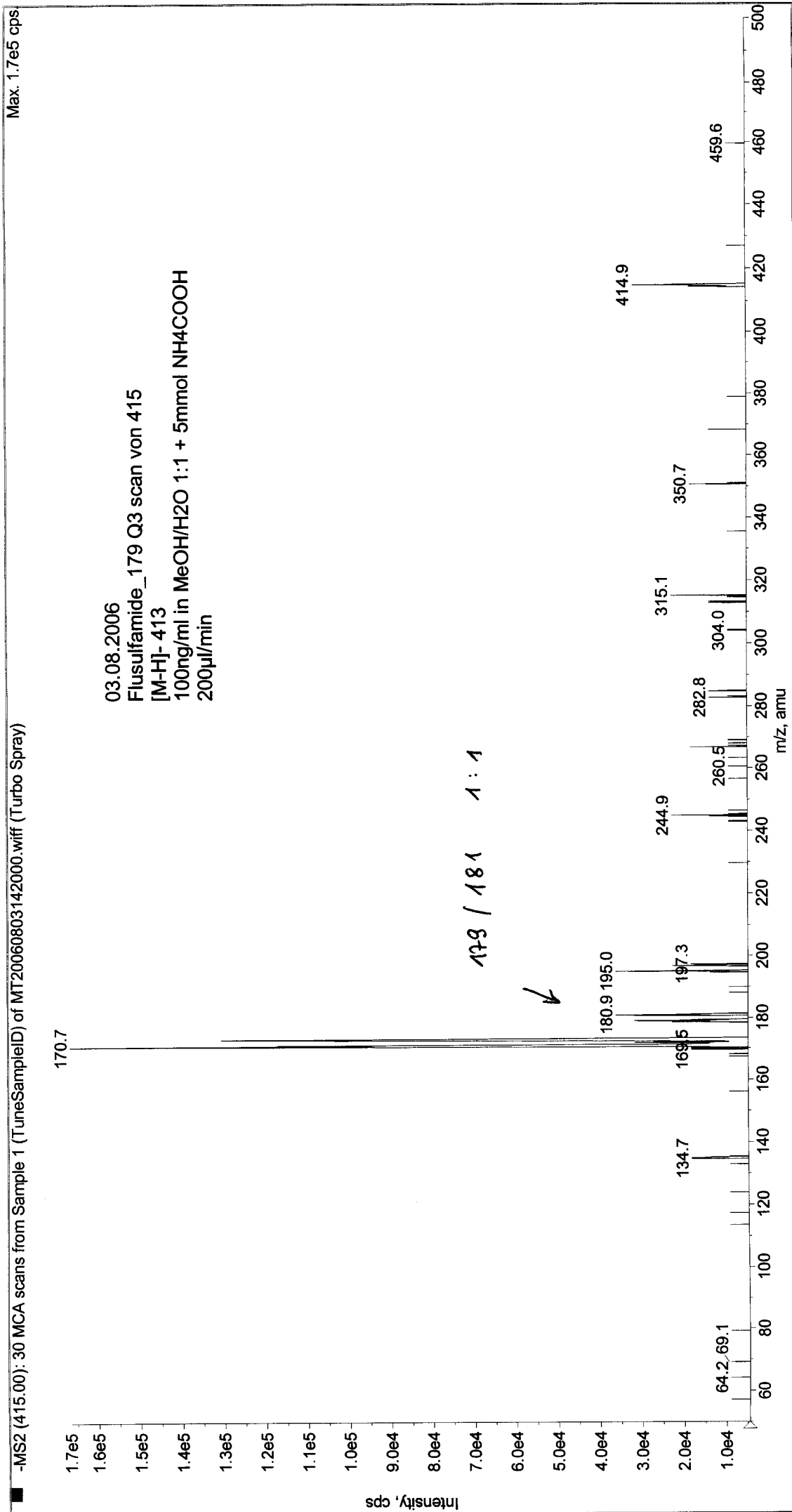


Printing Time: 14:20:55
Printing Date: Thursday, August 03, 2006

Acq Time: 14:20
Acq Date: Thursday, August 03, 2006
Acq File: MT20060803142000.wiff

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

■ -MS2 (415.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060803142000.wiff (Turbo Spray)



Printing Time: 14:35:02
Printing Date: Thursday, August 03, 2006

Acq. Time: 14:22
Acq. Date: Thursday, August 03, 2006
Acq. File: MT20060803142231.wiff

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

