

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

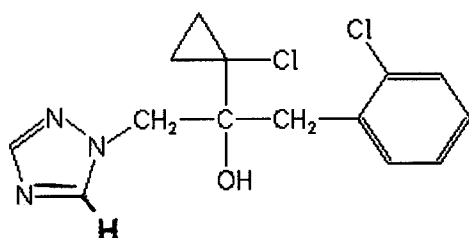
Analyte: Prothioconazole, Desthiometabolit (JAU 6476-desthio)

CAS No.: not available

Formula: C₁₄H₁₅Cl₂N₃O

Molecular mass (lowest isotopes): 311,06 amu

Structure:



Ionisation: ESI +

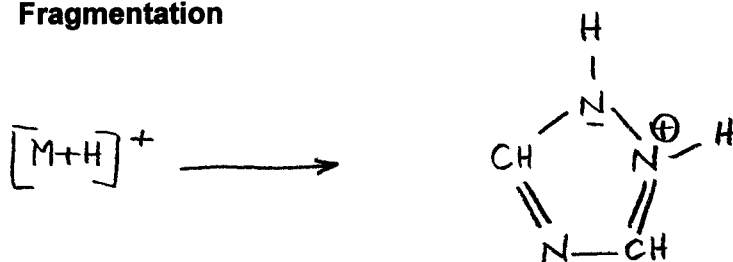
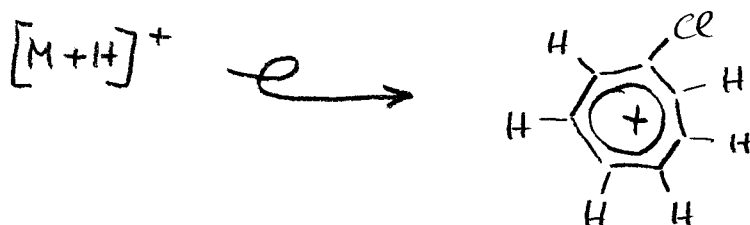
Quasimolecular ion: 312,1 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	312,1 → 70,1	312,1 → 125,0
Declustering potential (DP) ^{*)}	49 V	49 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	11,5 V	12,0 V
Collision cell entrance potential (CEP)	22 V	20 V
Collision energy (CE)	43 V	43 V
Collision cell exit potential (CXP)	10 V	6 V

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

Fragmentation

 m/z 70 m/z 125/127

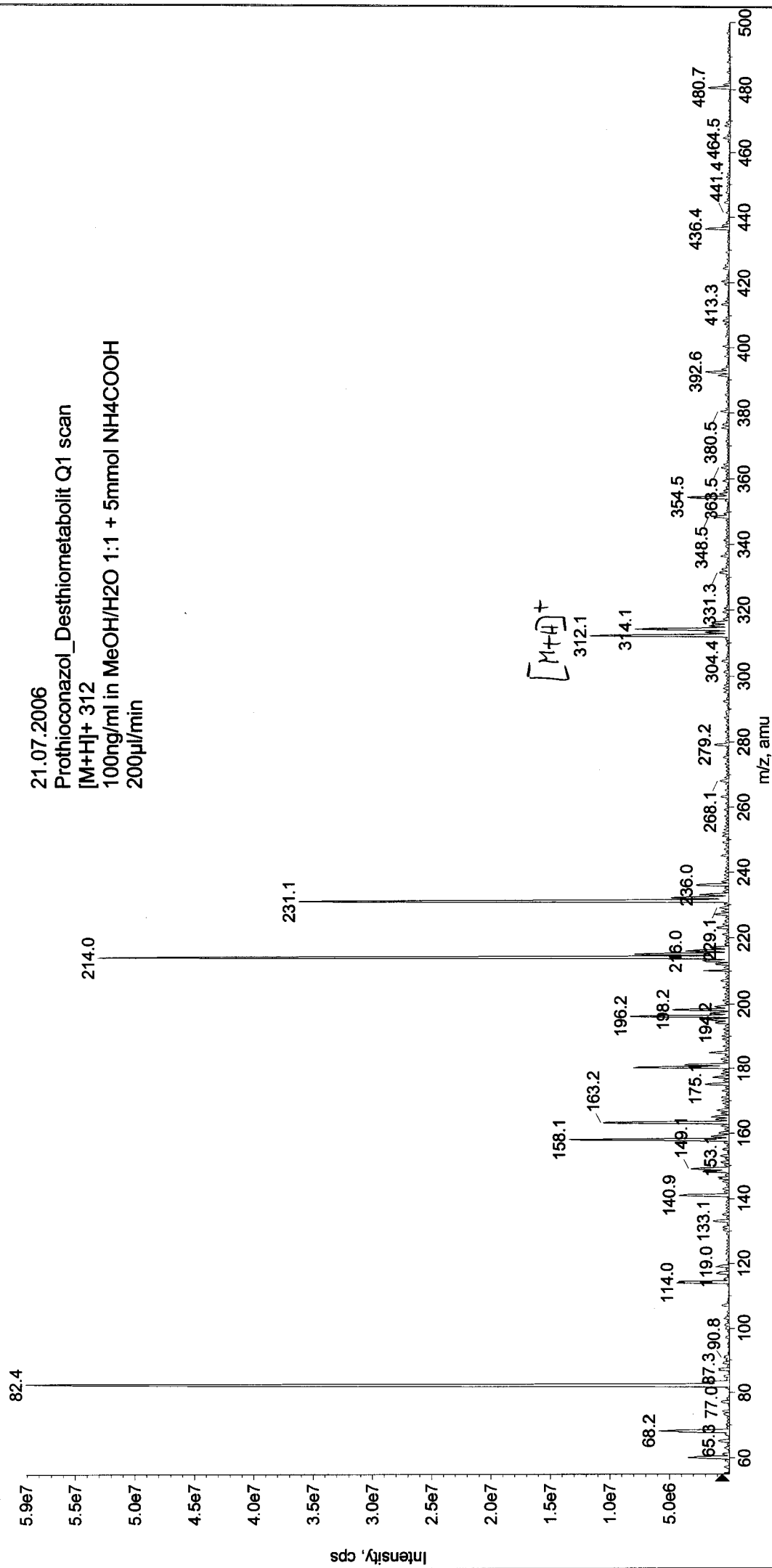
Printing Time: 12:31:48
Printing Date: Friday, July 21, 2006

Acq. Time: 12:30
Acq. Date: Friday, July 21, 2006
Acq. File: MT20060721123003.wiff

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

+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060721123003.wiff (Turbo Spray)

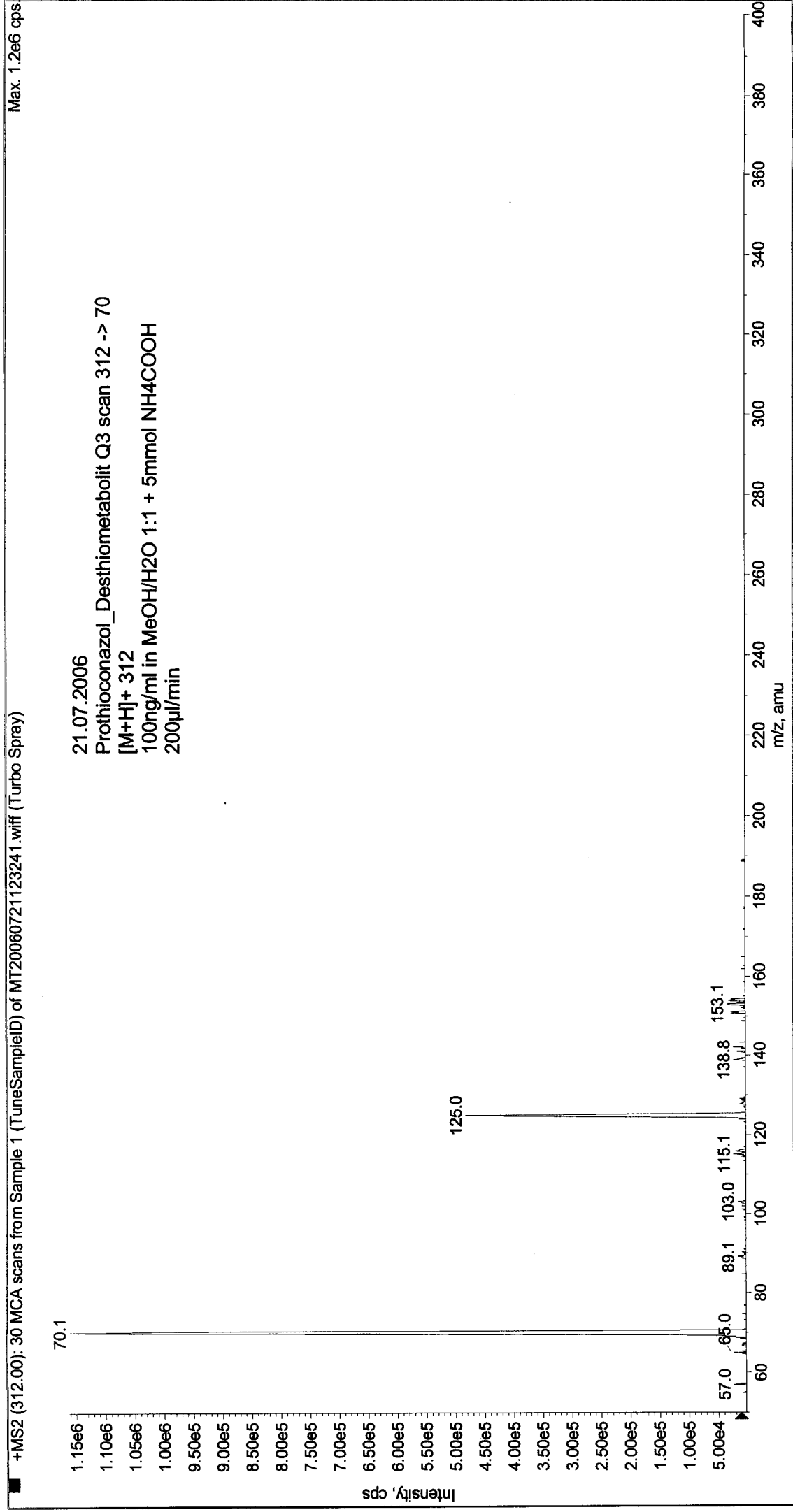
Max. 5.9e7 cps



Printing Time: 12:33:48
Printing Date: Friday, July 21, 2006

Acq. Time: 12:32
Acq. Date: Friday, July 21, 2006
Acq. File: MT20060721123241.wiff

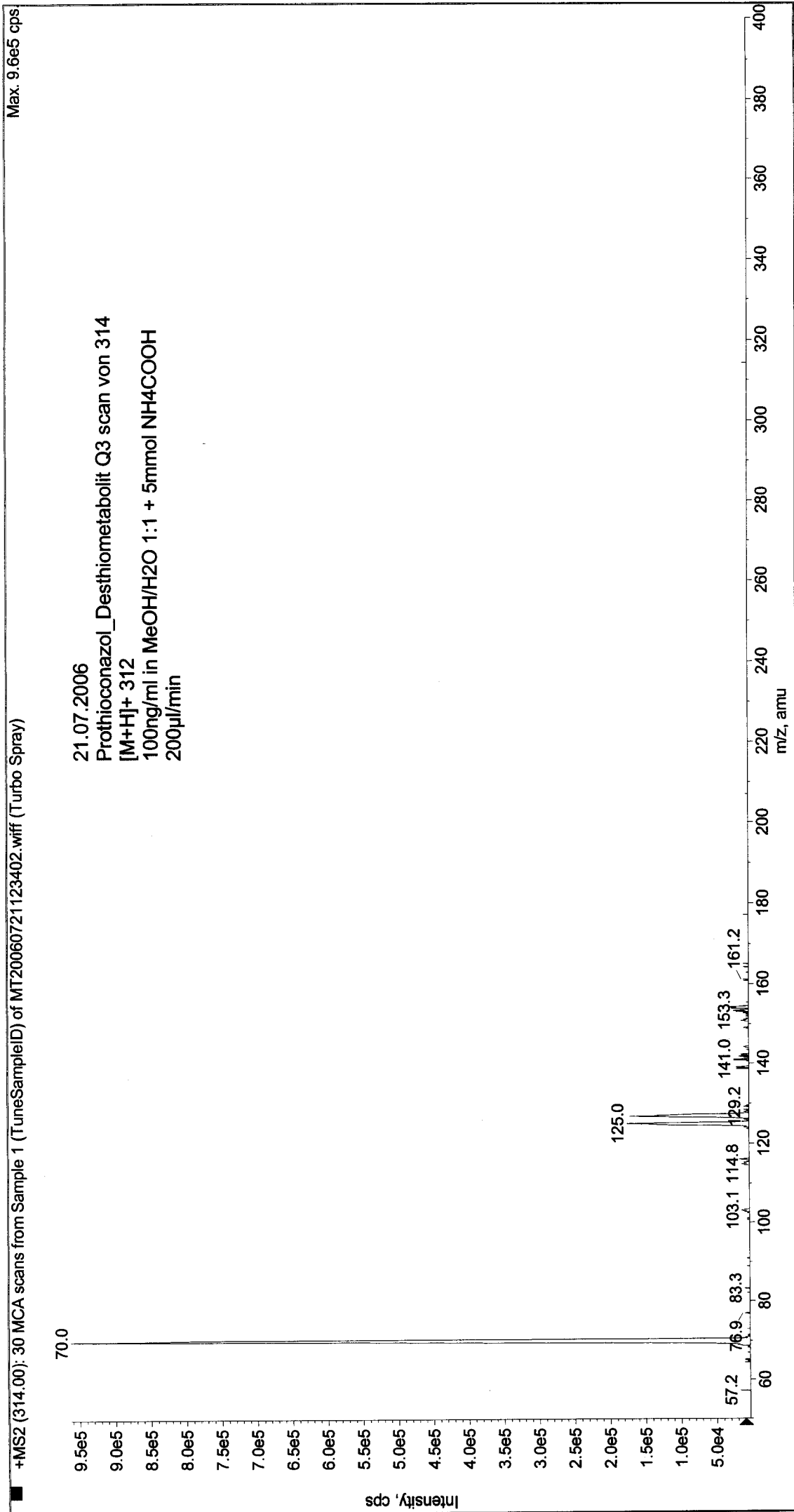
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat



Printing Time: 12:34:58
Printing Date: Friday, July 21, 2006

Acq. Time: 12:34
Acq. Date: Friday, July 21, 2006
Acq. File: MT20060721123402.wiff

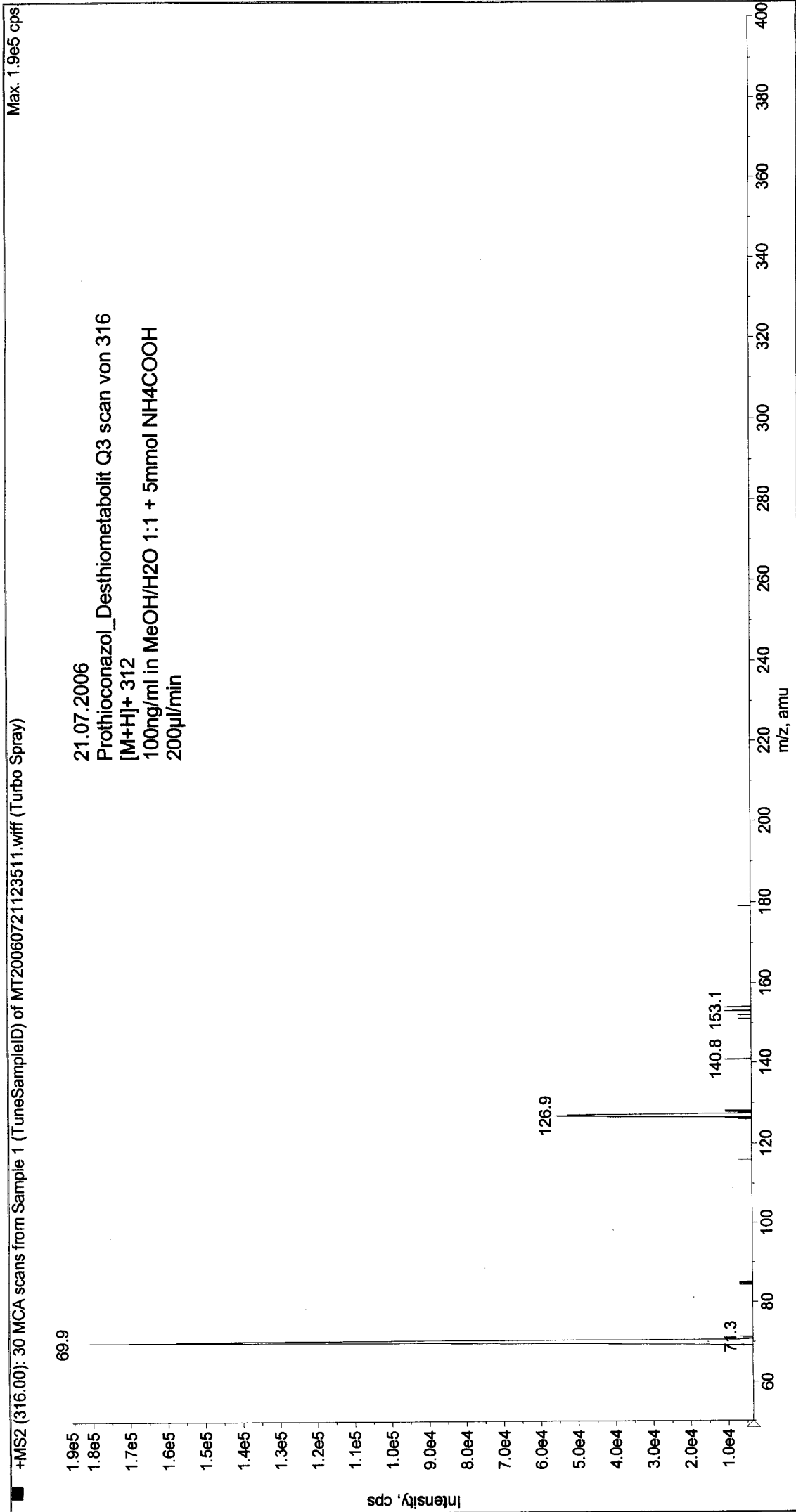
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat



Printing Time: 12:36:05
Printing Date: Friday, July 21, 2006

Acq. Time: 12:35
Acq. Date: Friday, July 21, 2006
Acq. File: MT20060721123511.wiff

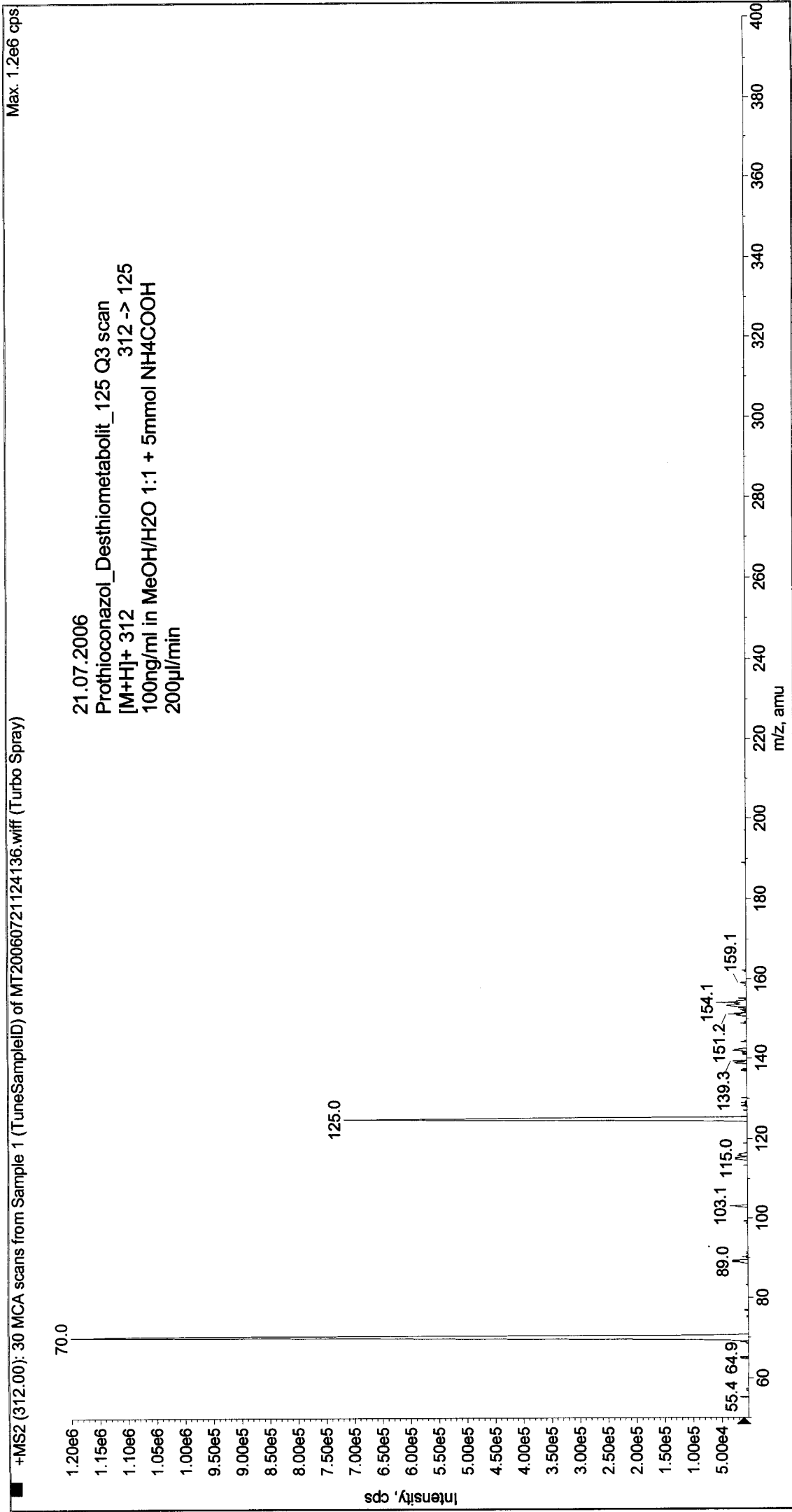
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat



Printing Time: 12:43:53
Printing Date: Friday, July 21, 2006

Acq. Time: 12:41
Acq. Date: Friday, July 21, 2006
Acq. File: MT20060721124136.wiff

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



Printing Time: 12:45:37
Printing Date: Friday, July 21, 2006

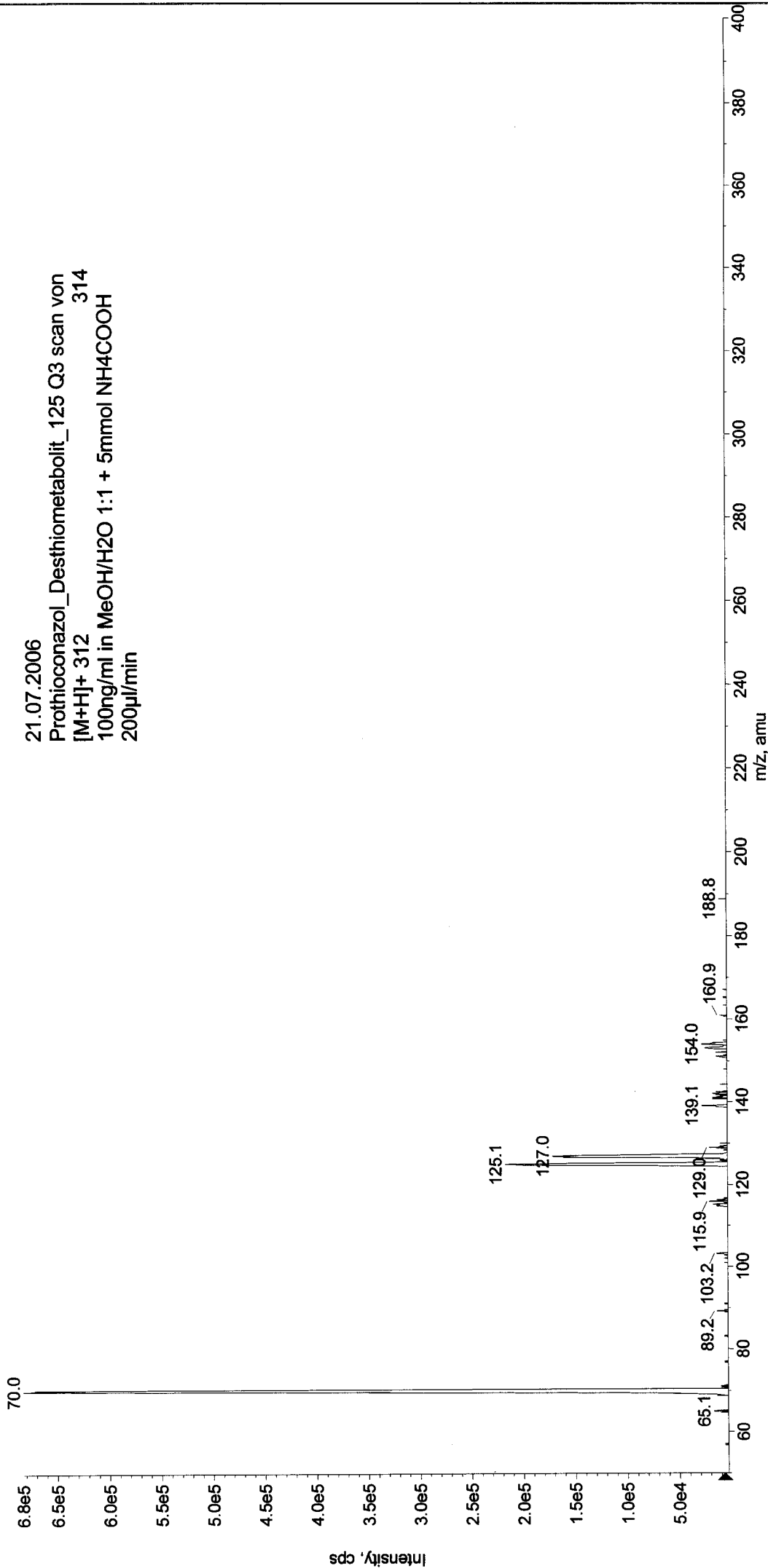
Acq. ime: 12:44
Acq. Date: Friday, July 21, 2006
Acq. File: MT20060721124415.wiff

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

Max. 6.8e5 cps

■ +MS2 (314.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060721124415.wiff (Turbo Spray)

21.07.2006
Prothioconazol_Desthiometabolit_125 Q3 scan von
[M+H]⁺ 312
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min



Printing Time: 12:46:45
Printing Date: Friday, July 21, 2006

Acq. Time: 12:45
Acq. Date: Friday, July 21, 2006
Acq. File: MT20060721124548.wiff

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

