

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

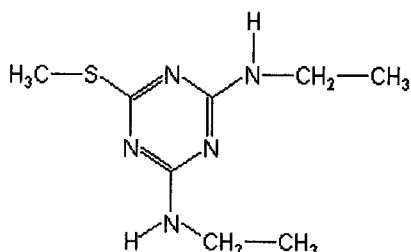
Analyte: Simetryn

CAS No.: 1014-70-6

Formula: C₈H₁₅N₅S

Molecular mass (lowest isotopes): 213,11 amu

Structure:



Ionisation: ESI +

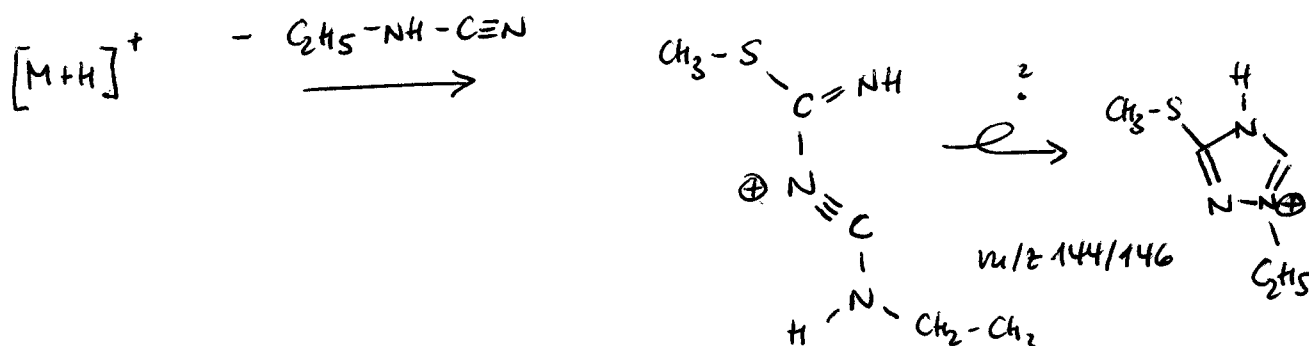
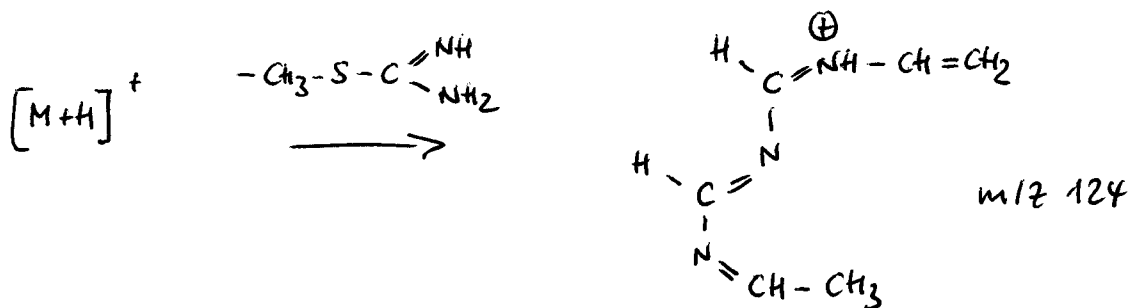
Quasimolecular ion: 214,1 amu = [M+H]⁺

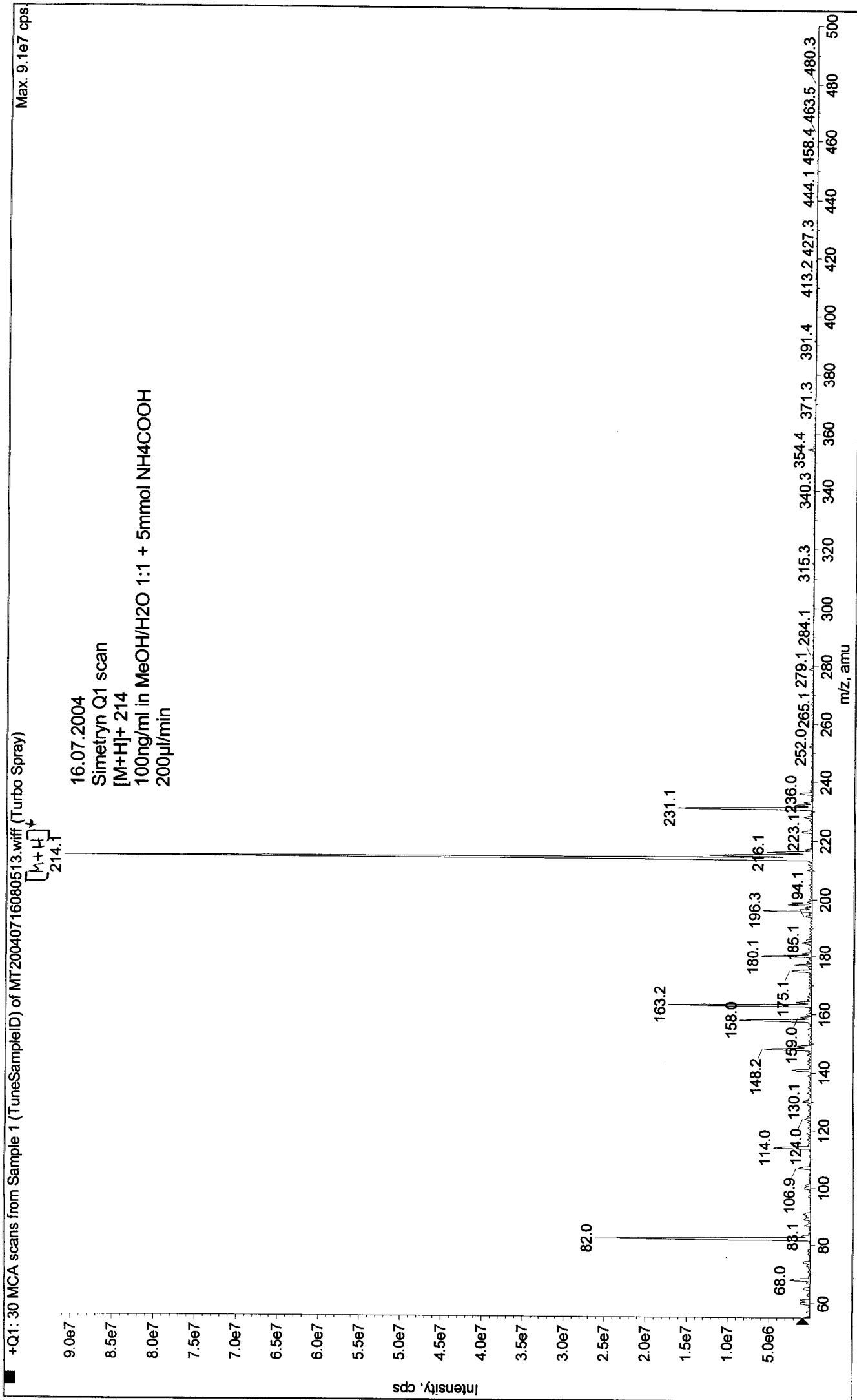
Analyte sensitive parameter set (API 2000)

Transition	214,1 → 124,2	214,1 → 144,0
Declustering potential (DP) ^{*)}	34 V	34 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	10,5 V	9,0 V
Collision cell entrance potential (CEP)	12 V	12 V
Collision energy (CE)	27 V	27 V
Collision cell exit potential (CXP)	6 V	8 V

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

Fragmentation





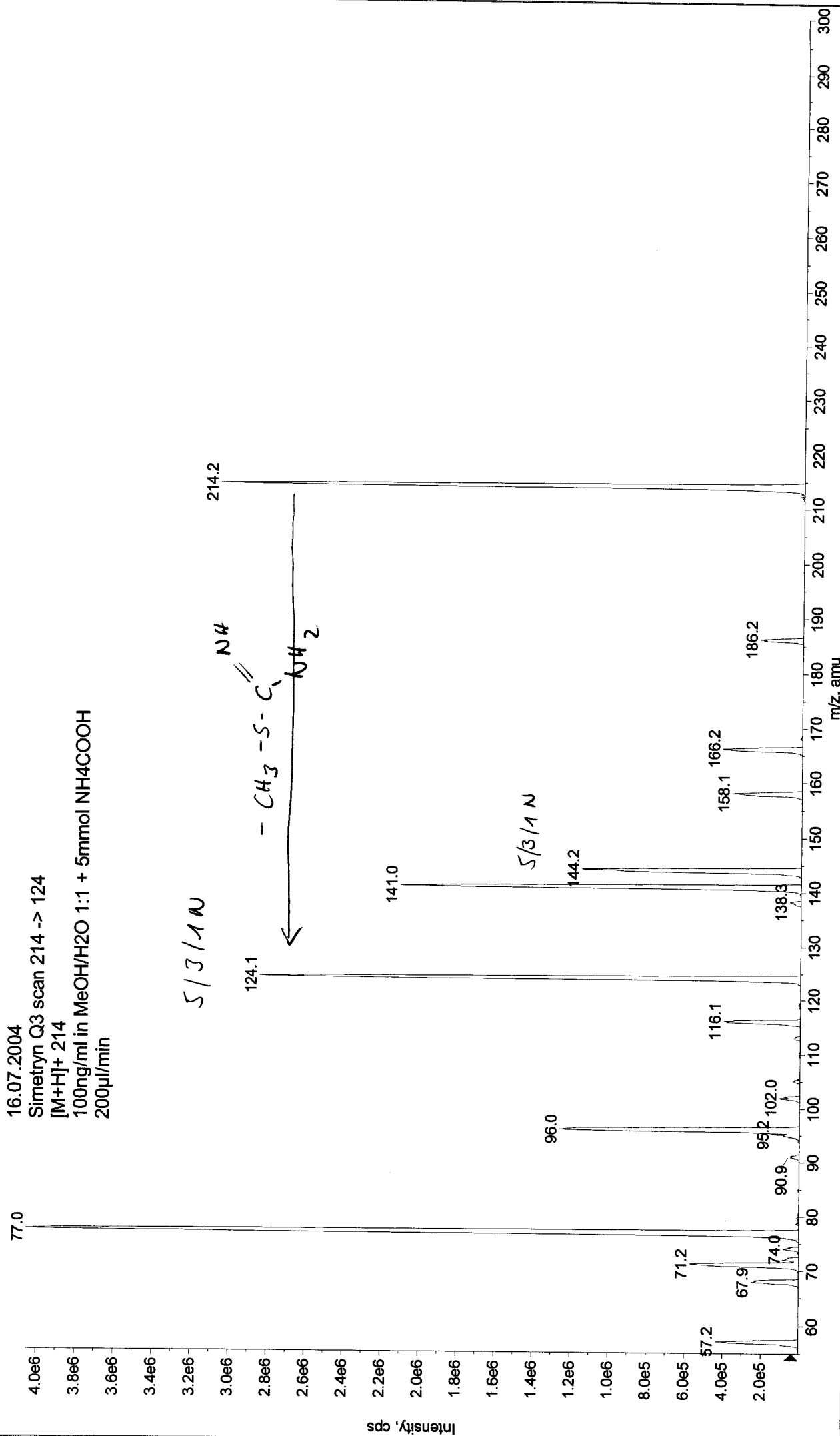
Printing Time: 8:08:13
Printing Date: Friday, July 16, 2004

Acq. Date: Friday, July 16, 2004
Acq. File: MT20040716080708.wiff

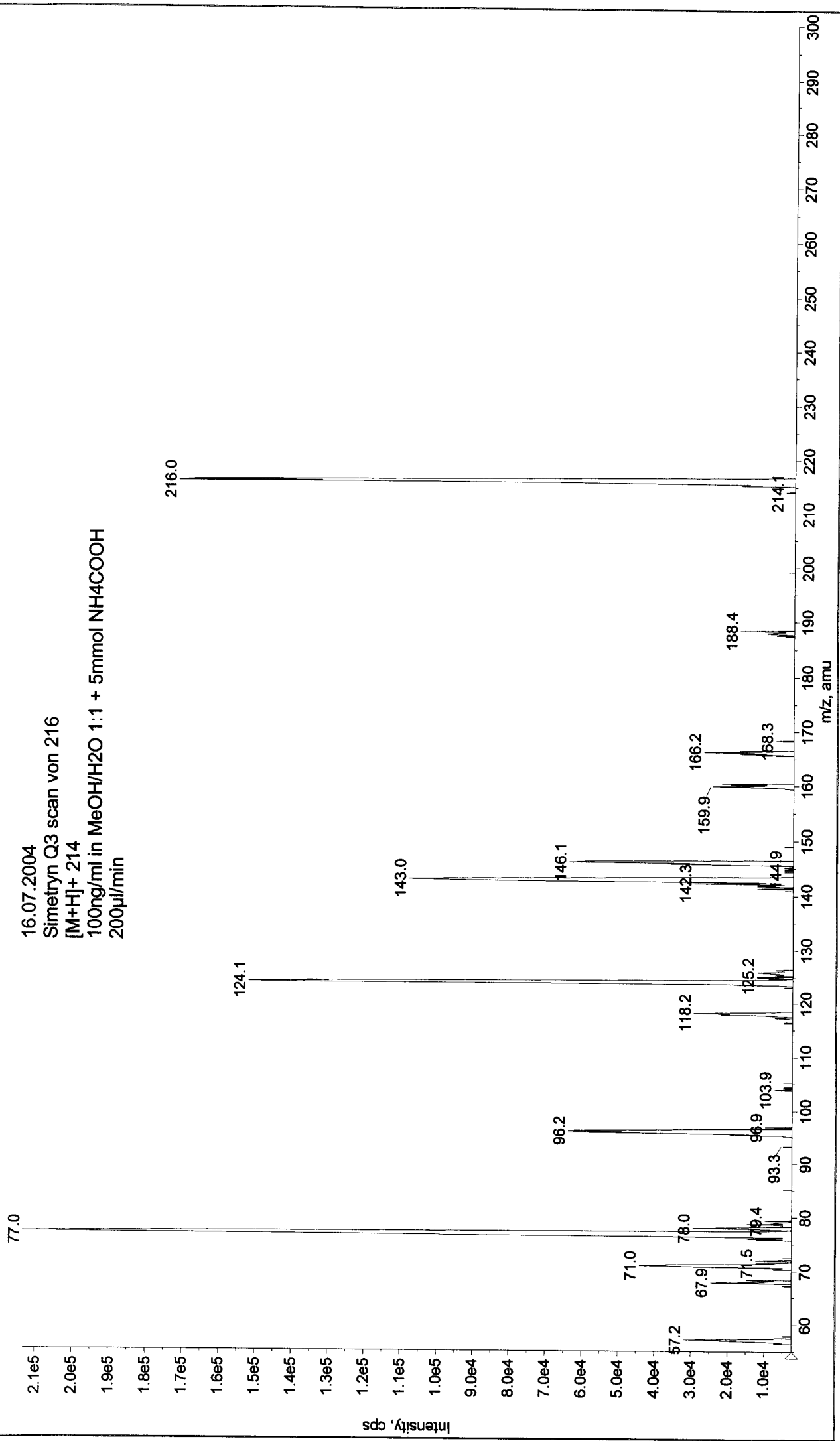
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat

+MS2 (214.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040716080708.wiff (Turbo Spray)

Max. 4.1e6 cps.



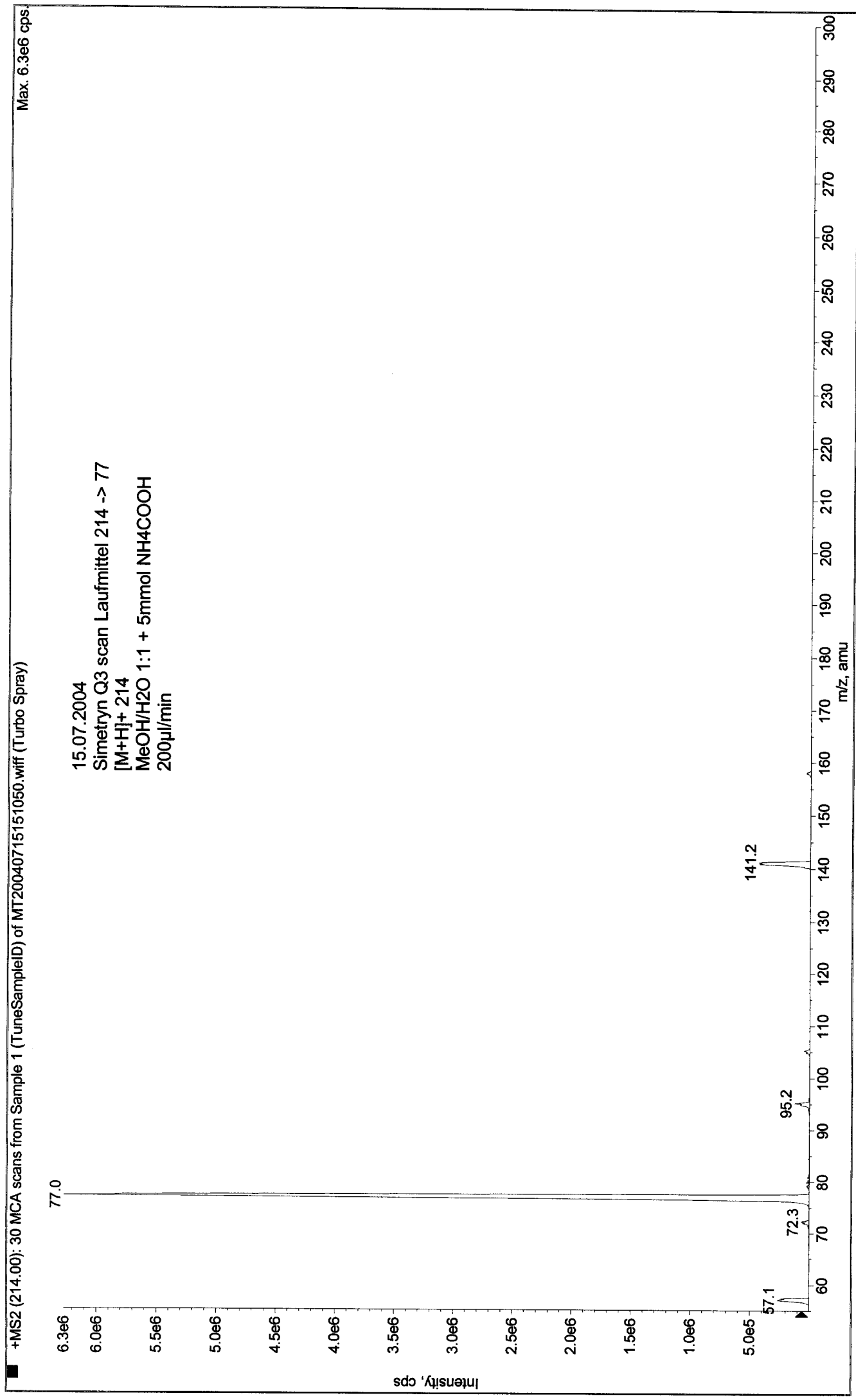
+MS2 (216.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040716080851.wiff (Turbo Spray) Max. 2.1e5 cps.



Printing Time: 15:12:09
Printing Date: Thursday, July 15, 2004

Acq Time: 15:10
Acq Date: Thursday, July 15, 2004
Acq File: MT20040715151050.wiff

Sample Comment:
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Batch Name: ManualTune.bat

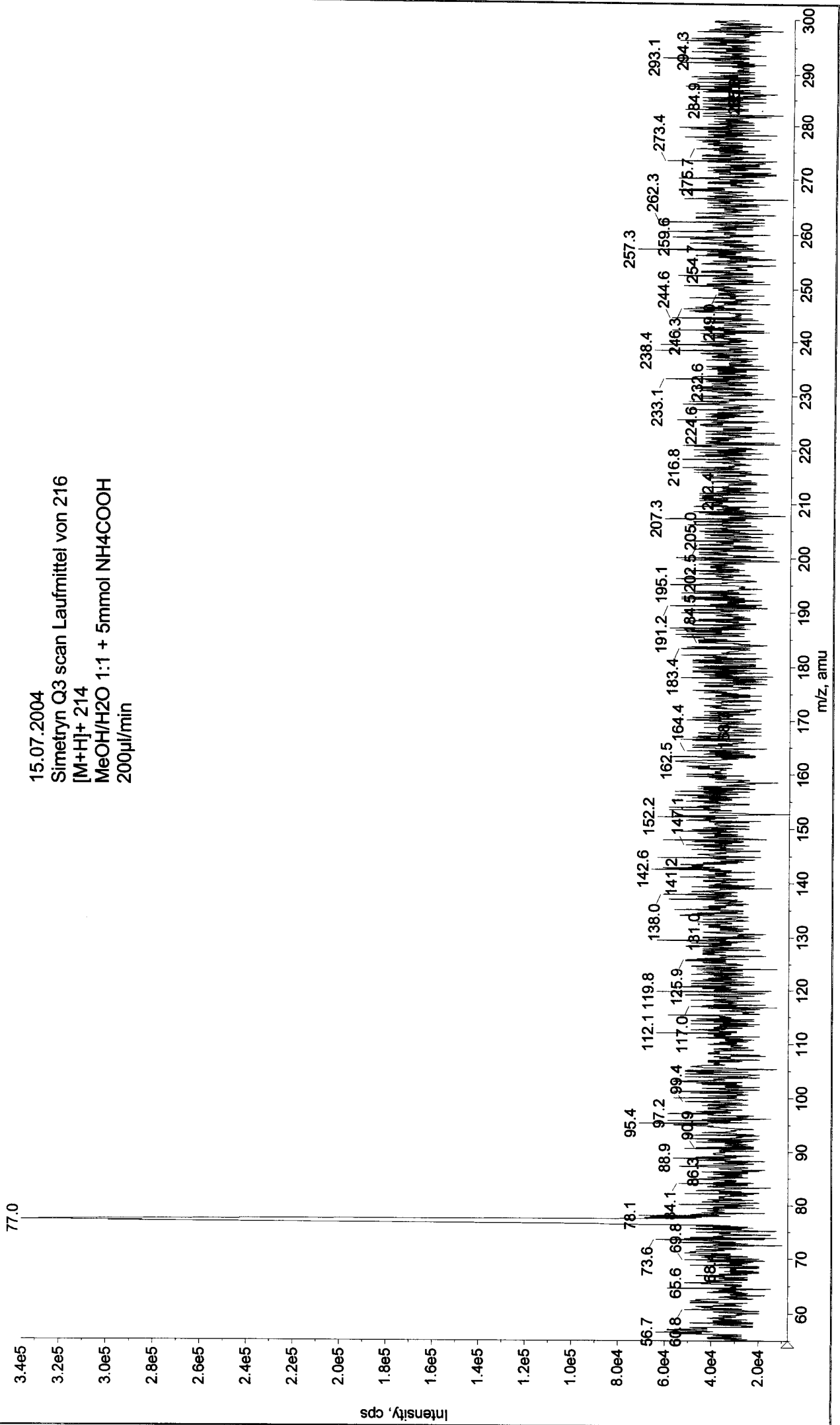


Printing Time: 15:14:12
Printing Date: Thursday, July 15, 2004

Acq Time: 15:13
Acq Date: Thursday, July 15, 2004
Acq File: MT20040715151309.wiff

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

Max. 3.4e5 cps
+MS2 (216.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040715151309.wiff (Turbo Spray)



+MS2 (214.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040716075307.wiff (Turbo Spray) Max. 3.8e6 cps

