

MS/MS Parameters of Pesticides

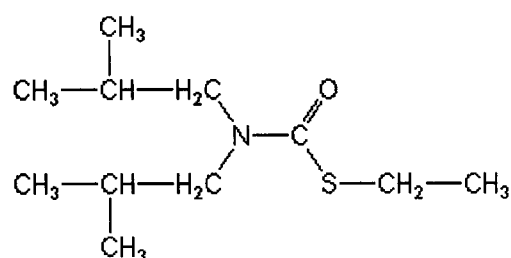
Analyte: Butylate

CAS No.: 2008-41-5

Formula: C₁₁H₂₃NOS

Molecular mass (lowest isotopes): 217,15 amu

Structure:



Ionisation: ESI +

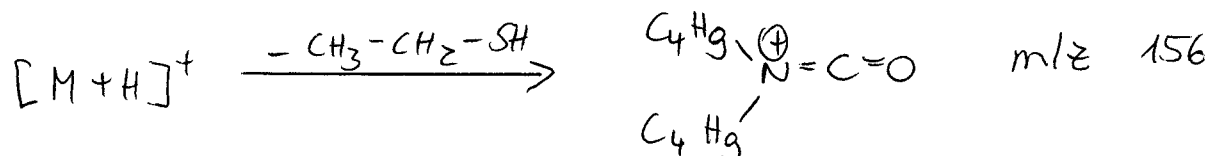
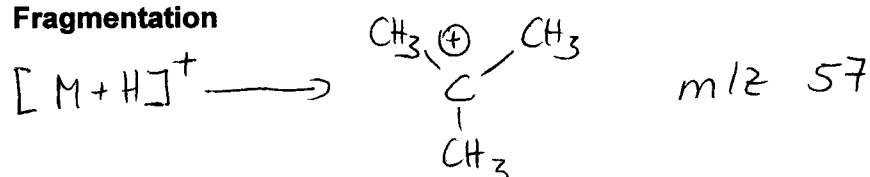
Quasimolecular ion: 218,2 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	218,2 → 57,1	218,2 → 156,2
Declustering potential (DP) ^{*)}	64V	64 V
Focusing potential (FP)	60 V	330 V
Entrance potential (EP)	12 V	12 V
Collision cell entrance potential (CEP)	12 V	12 V
Collision energy (CE)	29 V	17 V
Collision cell exit potential (CXP)	8 V	8 V

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

Fragmentation

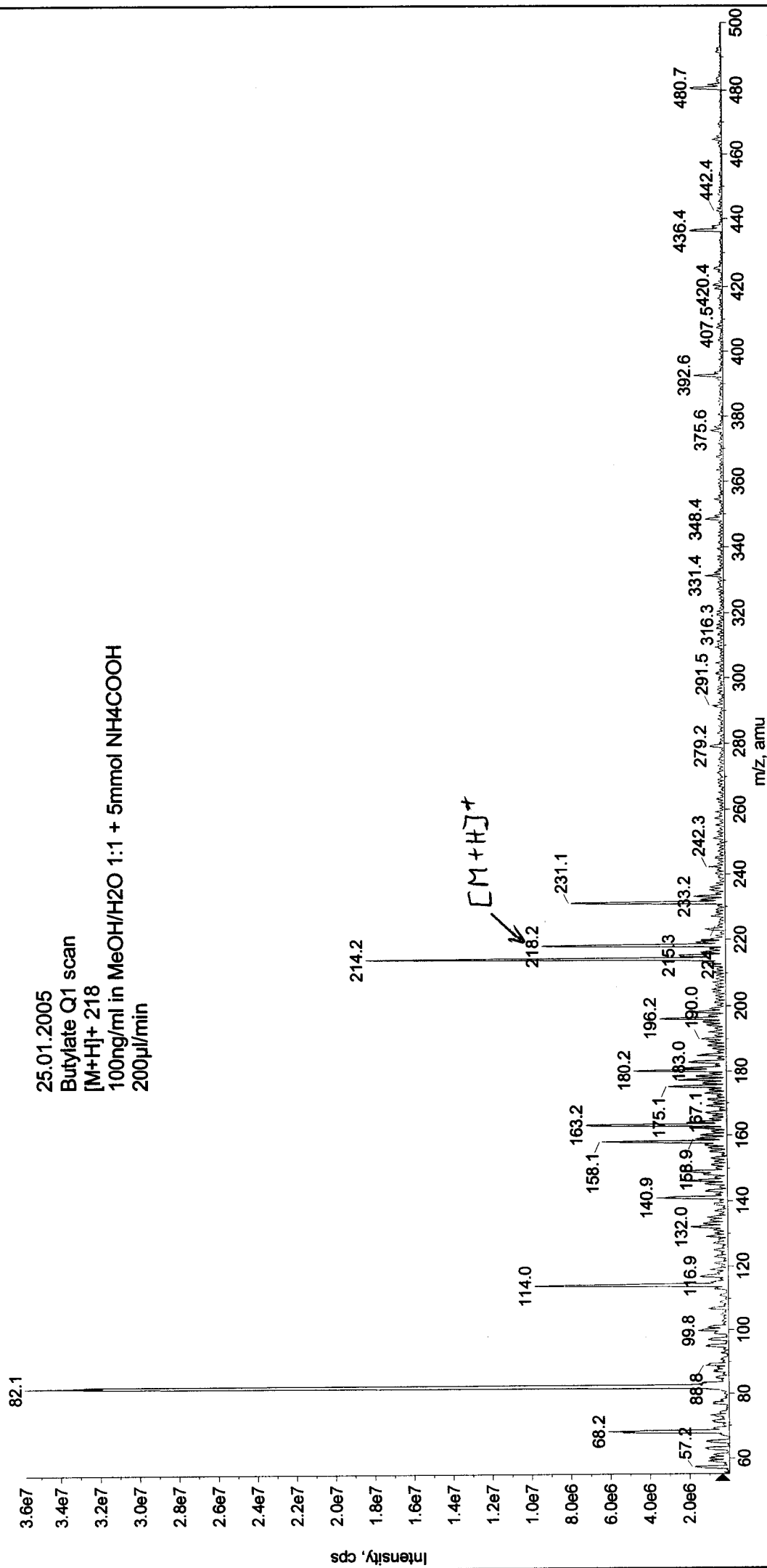


Printing Time: 10:35:56
Printing Date: Tuesday, January 25, 2005

Acq. time: 10:32
Acq. date: Tuesday, January 25, 2005
Acq. File: MT20050125103238.wiff

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

	Max. 3.6e7 cps.
+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20050125103238.wiff (Turbo Spray)	



Printing Time: 10:38:19

Printing Date: Tuesday, January 25, 2005

Acq. Time: 10:37

Acq. Date: Tuesday, January 25, 2005

Acq. File: MT20050125103706.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat

Max. 6.8e5 cps

■ +MS2 (218.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050125103706.wiff (Turbo Spray)

57.2

6.8e5

6.5e5

6.0e5

5.5e5

5.0e5

4.5e5

4.0e5

3.5e5

3.0e5

2.5e5

2.0e5

1.5e5

1.0e5

5.0e4

Intensity, cps

25.01.2005

Butylate Q3 scan 218 -> 57

[M+H]⁺ 218

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

200µl/min

100.0

89.1

86.0

62.7

162.3

156.2

134.1

122.7

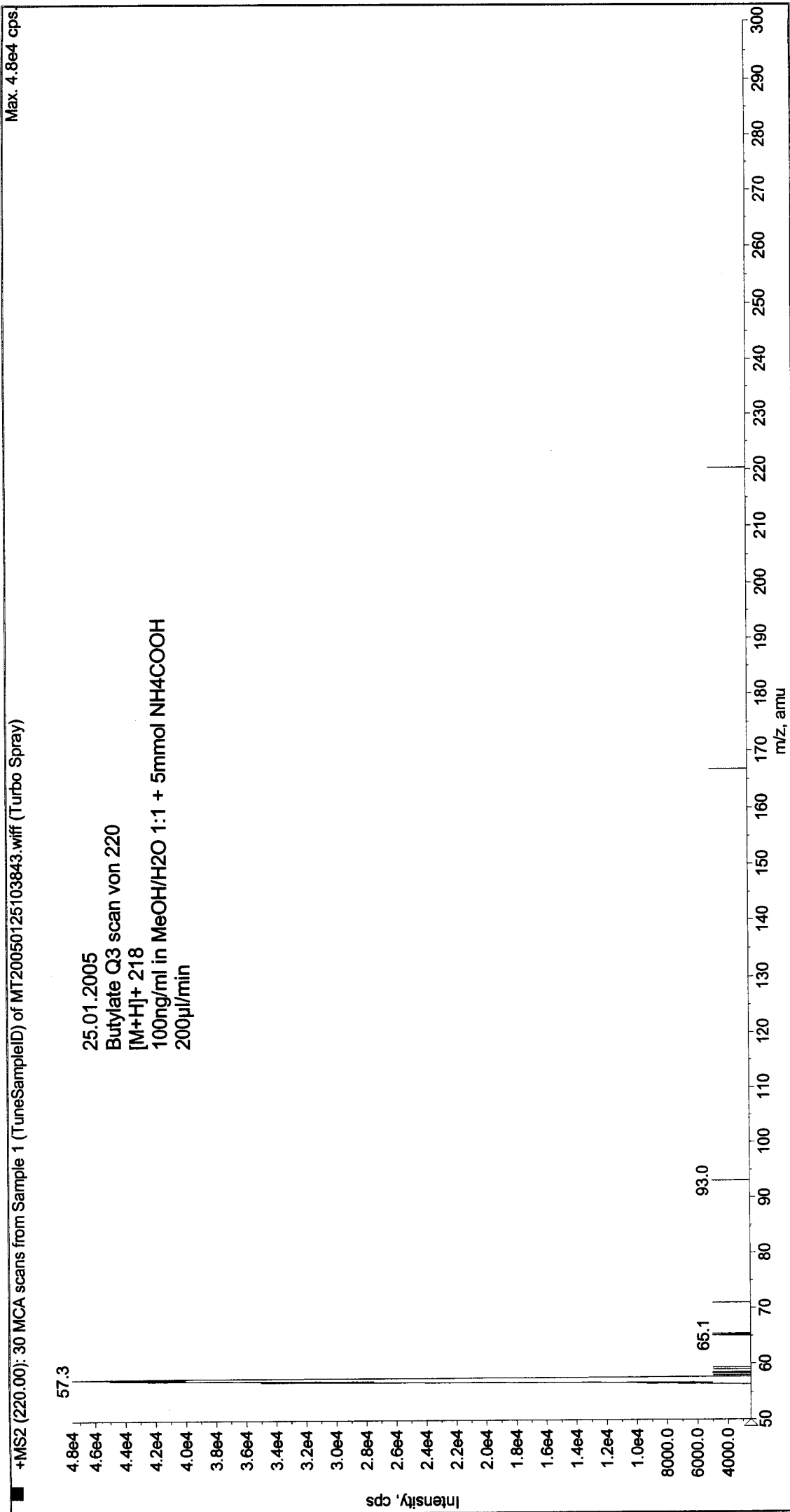
218.2

m/z, amu

Printing Time: 10:39:40
Printing Date: Tuesday, January 25, 2005

Acq. Time: 10:38
Acq. Date: Tuesday, January 25, 2005
Acq. File: MT20050125103843.wiff

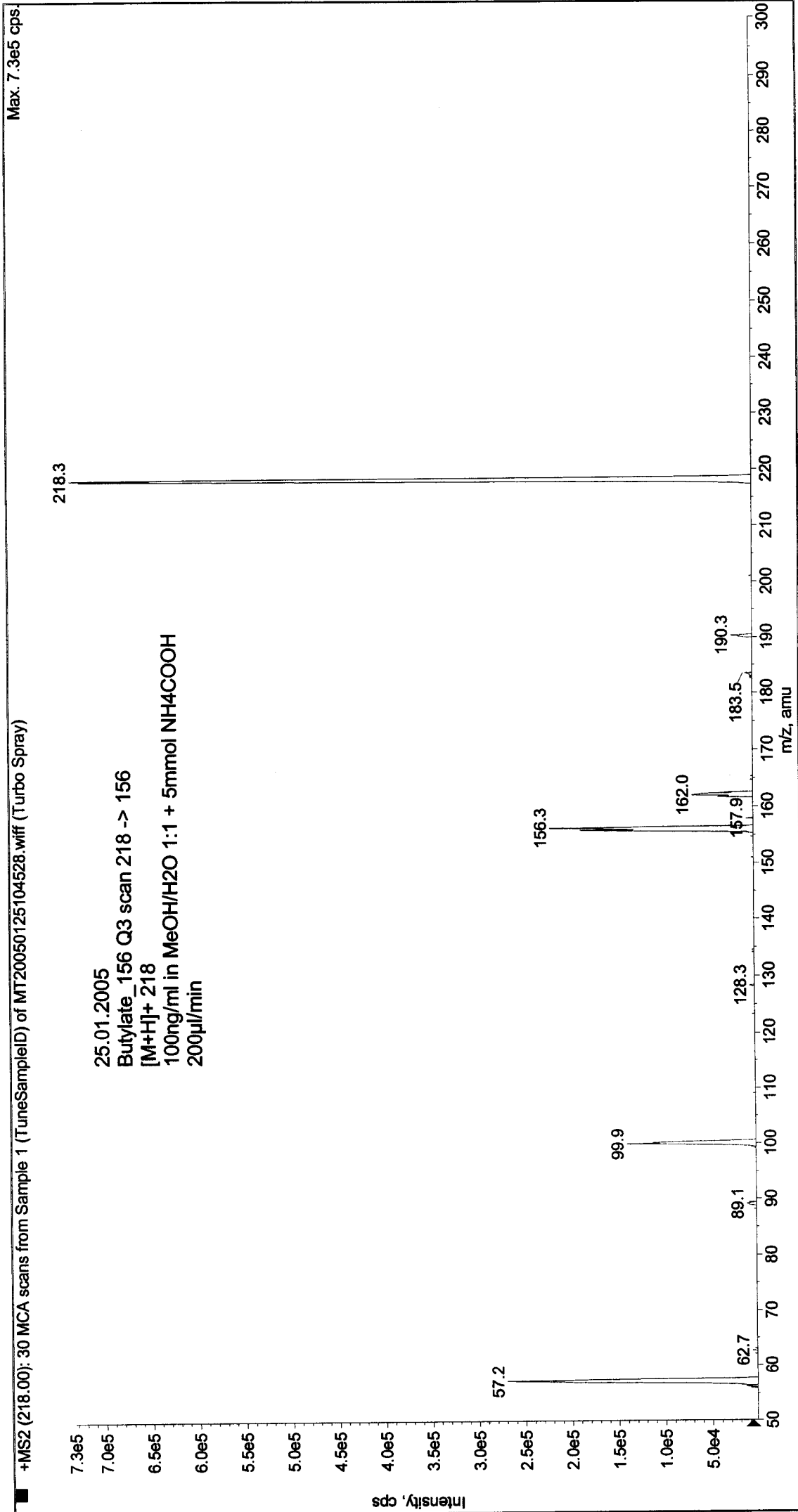
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Sample Name: TuneSampleID
Batch Name: ManualTune.bat



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Printing Date: Tuesday, January 25, 2005

Acq. Time: 10:45
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Acq. File: MT20050125104528.wiff

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



Printing Time: 10:48:16

Printing Date: Tuesday, January 25, 2005

Acq. Time: 10:46

Acq. Date: Tuesday, January 25, 2005

Acq. File: MT20050125104658.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat

