

MS/MS Parameters of Pesticides

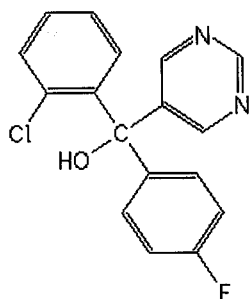
Analyte: Nuarimol

CAS No.: 63284-71-9

Formula: C₁₇H₁₂ClFN₂O

Molecular mass (lowest isotopes): 314,06 amu

Structure:



Ionisation: ESI +

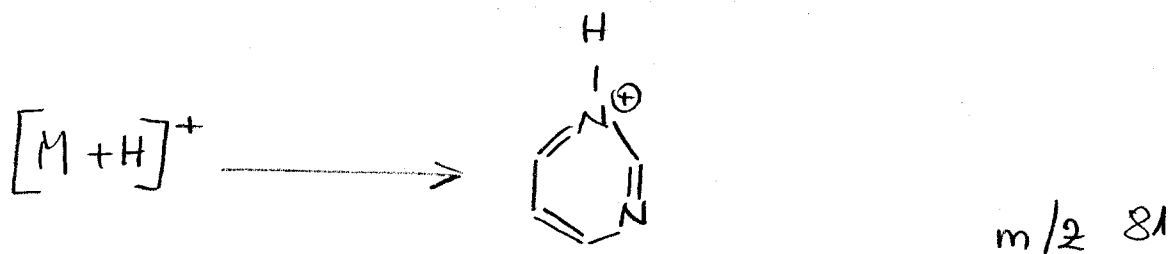
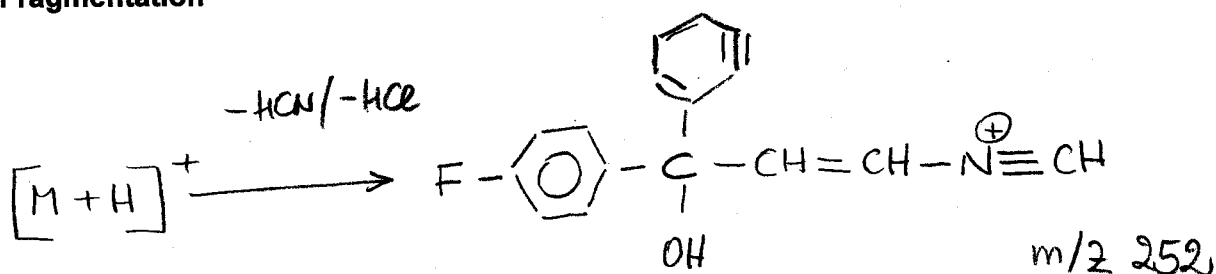
Quasimolecular ion: 315,0 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	315,0 → 81,1	315,0 → 252,1
Declustering potential (DP) ^{*)}	44 V	44 V
Focusing potential (FP)	360 V	370 V
Entrance potential (EP)	12,0 V	12,0 V
Collision cell entrance potential (CEP)	20 V	20 V
Collision energy (CE)	43 V	31 V
Collision cell exit potential (CXP)	4 V	14 V

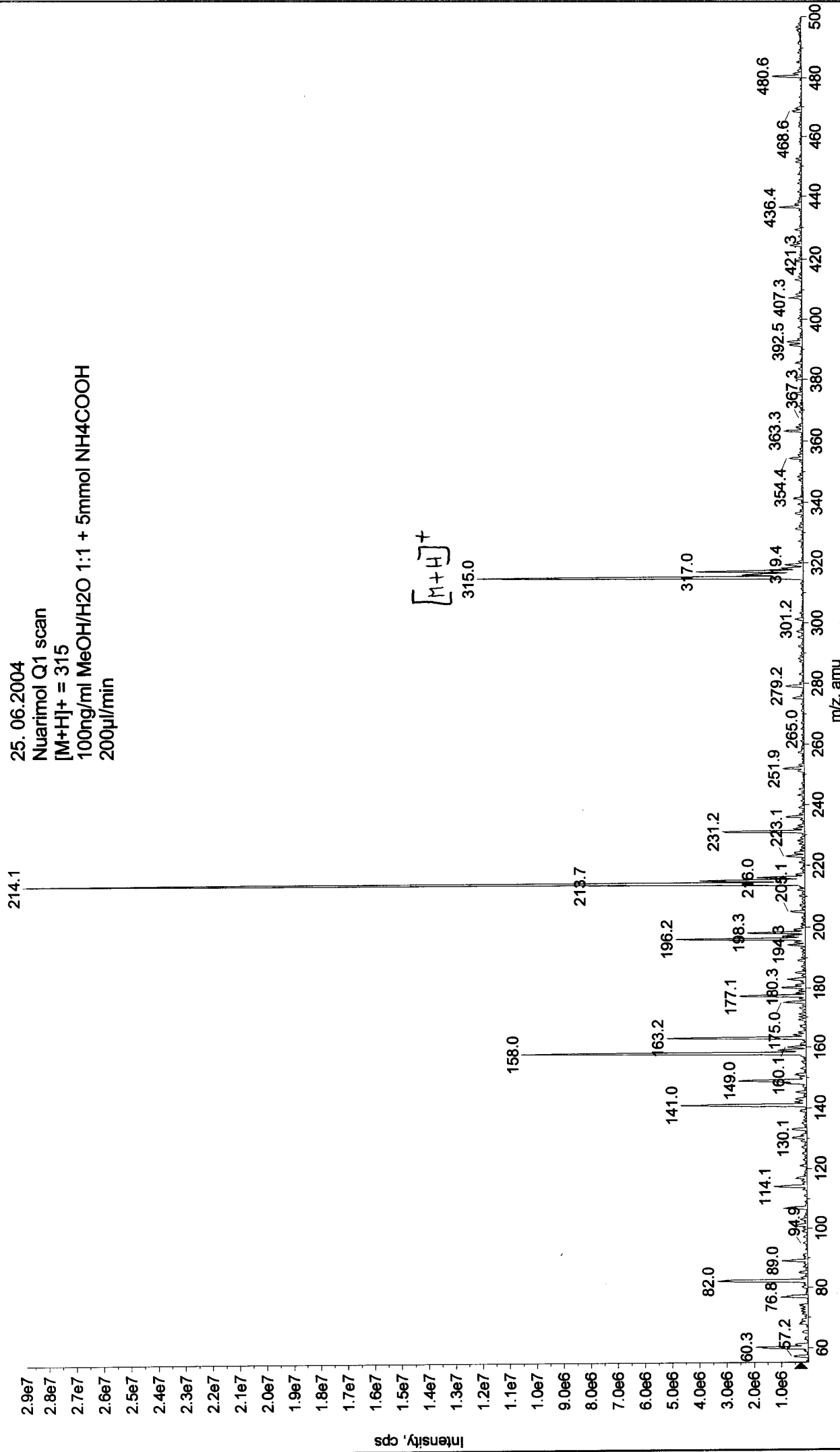
^{*)} For API 3000 and 4000 enhance DP by 20V

Fragmentation



Max. 2.9e7 cps

■ +Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20040625104552.wiff (Turbo Spray)



Printing Time: 10:49:26
Printing Date: Friday, June 25, 2004

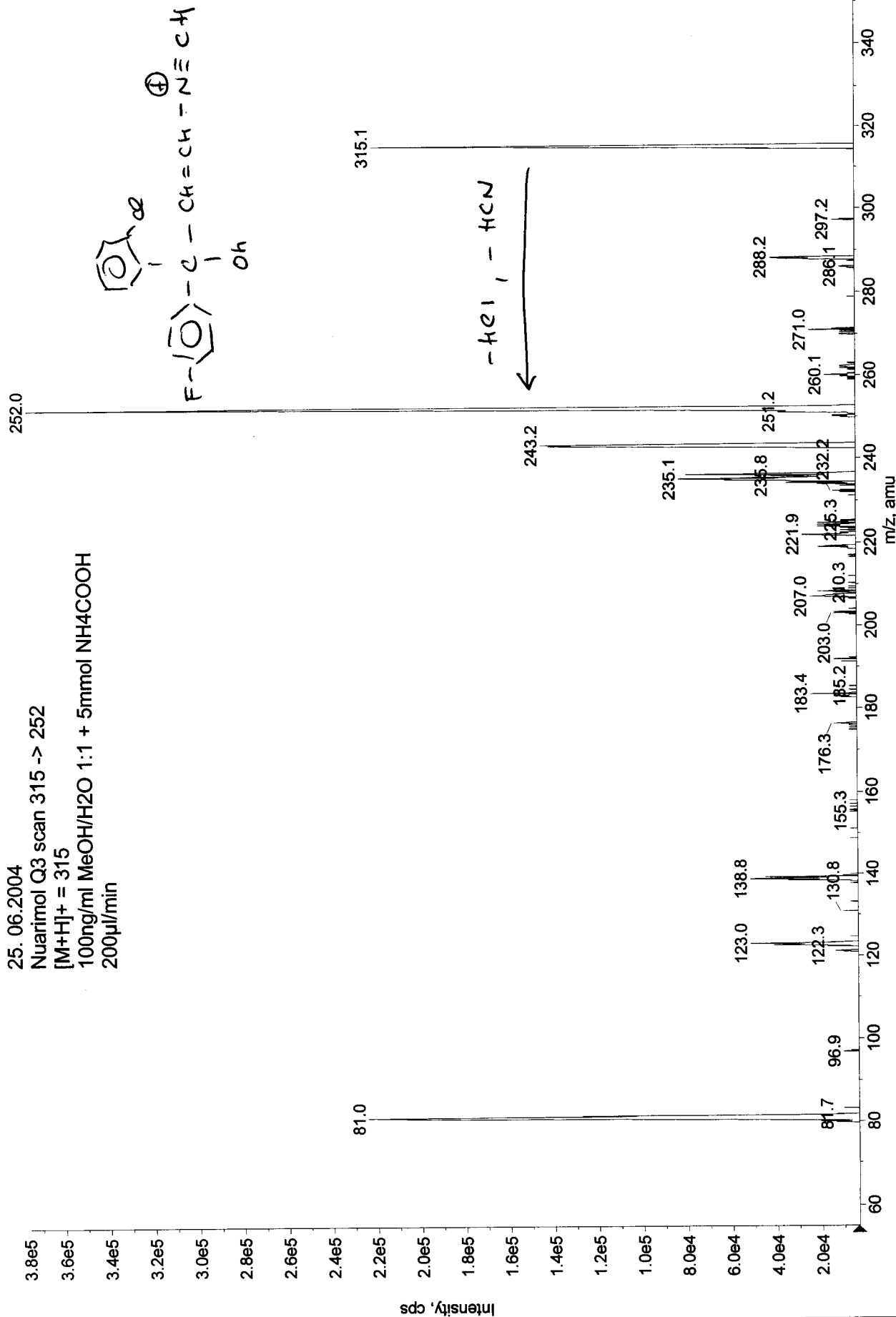
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Acq Date: Friday, June 25, 2004
Acq File: MT20040625104807.wiff

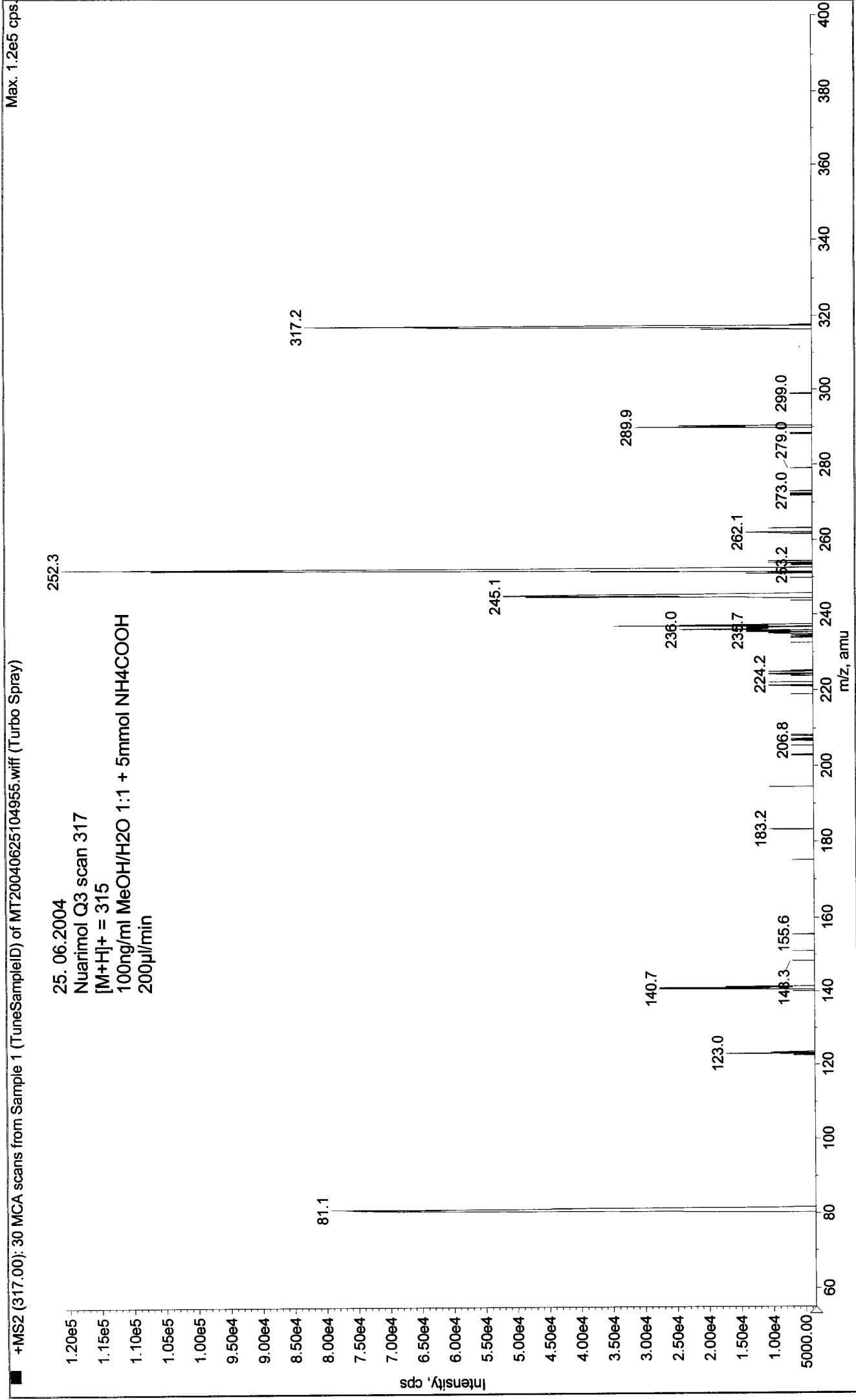
Sample Comment:
Sample Name: TunesSampleID
Batch Name: ManualTune.bat

Max 3.8e5 cps

■ +MS2 (315.00): 30 MCA scans from Sample 1 (TunesSampleID) of MT20040625104807.wiff (Turbo Spray)

25. 06.2004
Nuairimol Q3 scan 315 -> 252
[M+H]⁺ = 315
100ng/ml MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min

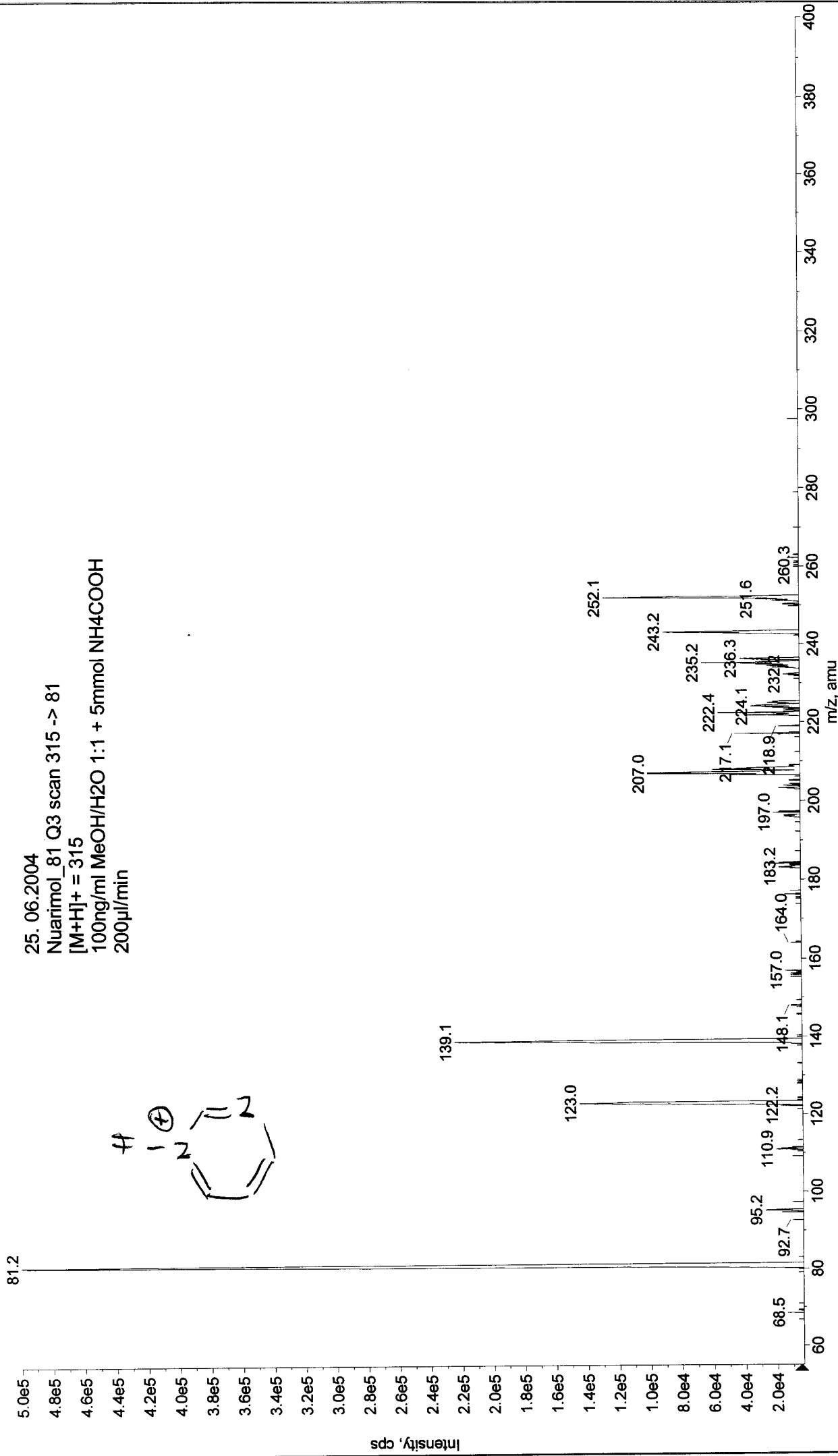




Max. 5.0e5 cps

+MS2 (315.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040625105924.wiff (Turbo Spray)

25. 06.2004
Nuairimol_81 Q3 scan 315 -> 81
[M+H]⁺ = 315
100ng/ml MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min



Printing Time: 11:51:56
Printing Date: Friday, June 25, 2004

Acq Time: 11:01
Acq Date: Friday, June 25, 2004
Acq File: MT20040625110113.wiff

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

Max. 1.9e5 cps

+MS2 (317.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040625110113.wiff (Turbo Spray)

