

MS/MS Parameters of Pesticides

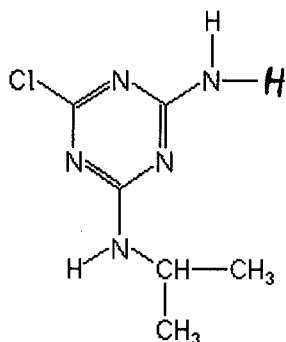
Analyte: Atrazine-desethyl

CAS No.: 6190-65-4

Formula: C₆H₁₀N₅Cl

Molecular mass (lowest isotopes): 187,06 amu

Structure:



Ionisation: ESI +

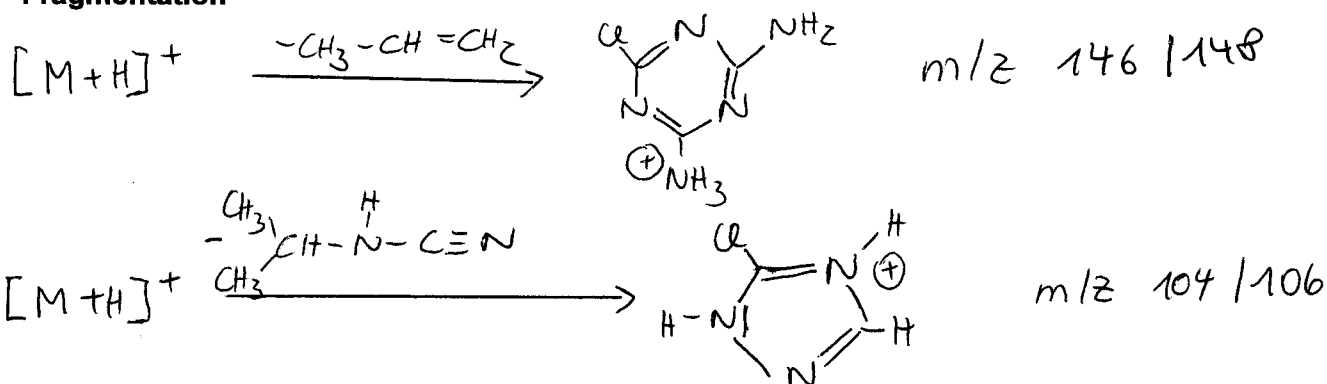
Quasimolecular ion: 188,1 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	188,1 → 104,0	188,1 → 146,0
Declustering potential (DP) ^{*)}	61V	61 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	12 V	10,5 V
Collision cell entrance potential (CEP)	12 V	12 V
Collision energy (CE)	33 V	25 V
Collision cell exit potential (CXP)	6 V	8 V

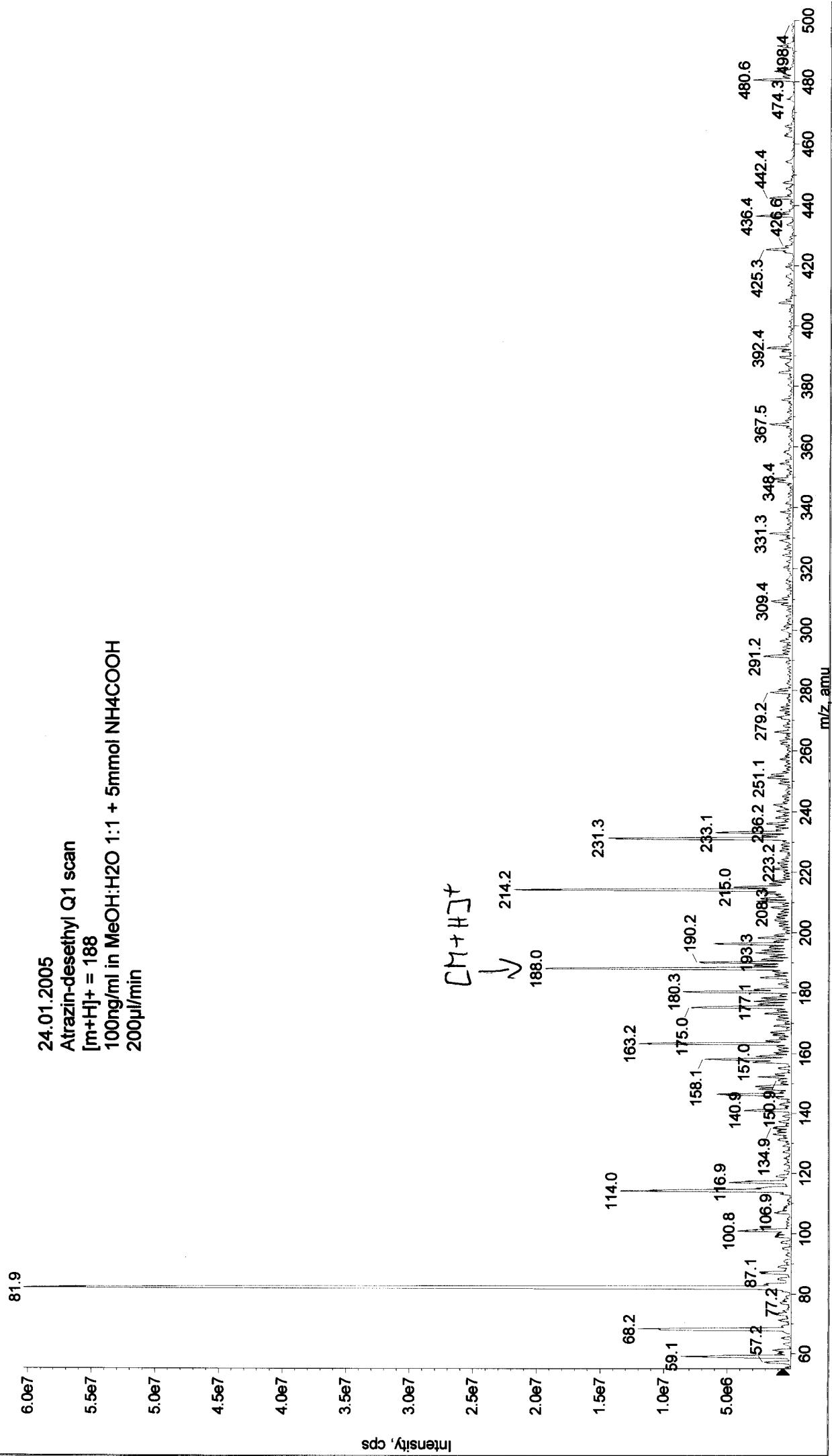
^{*)} For API 3000 and 4000 enhance DP by 20V

Fragmentation

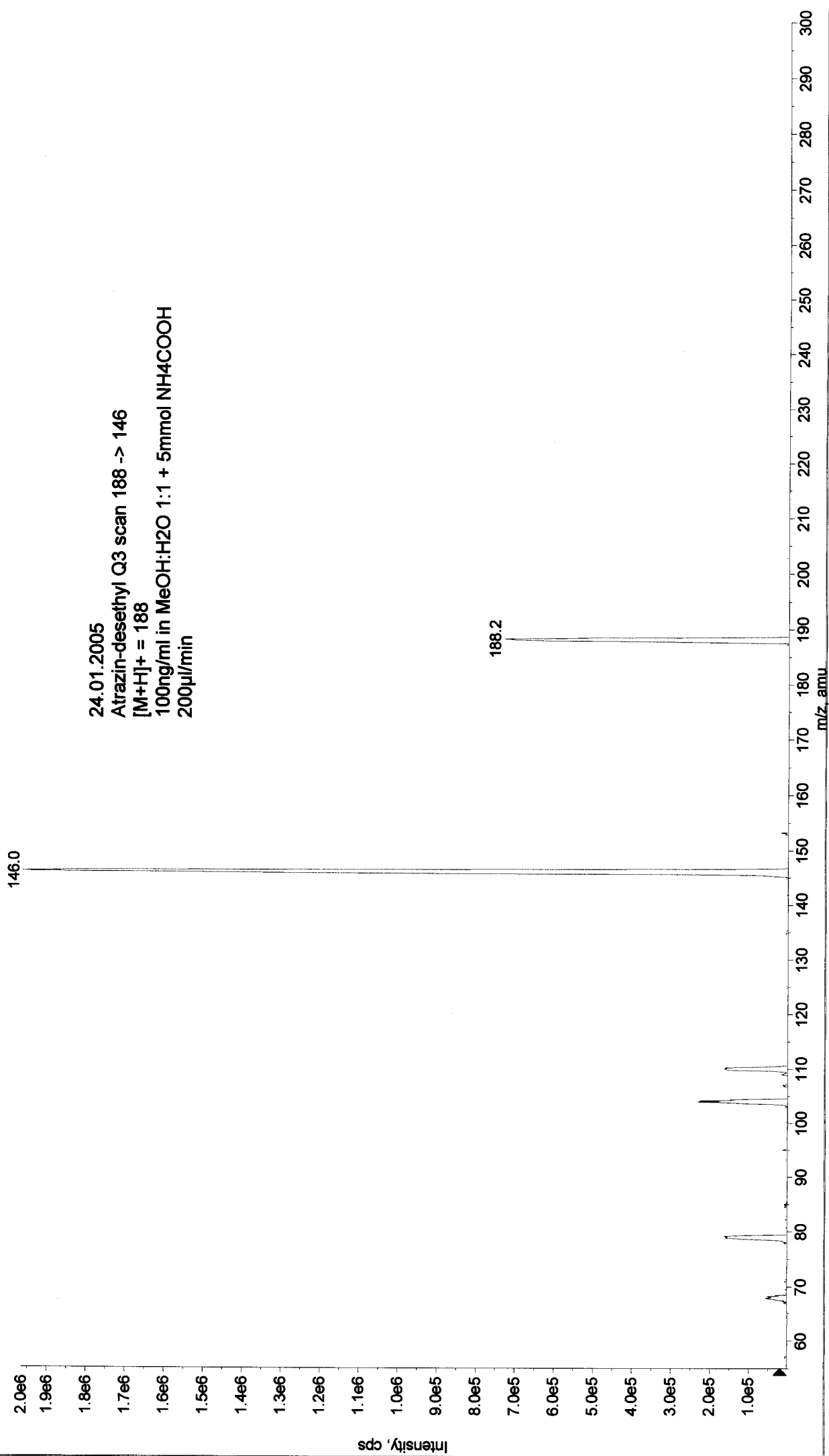


Max. 6.0e7 cps.

+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20050124091614.wiff (Turbo Spray)



+MS2 (188.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050124092858.wiff (Turbo Spray)



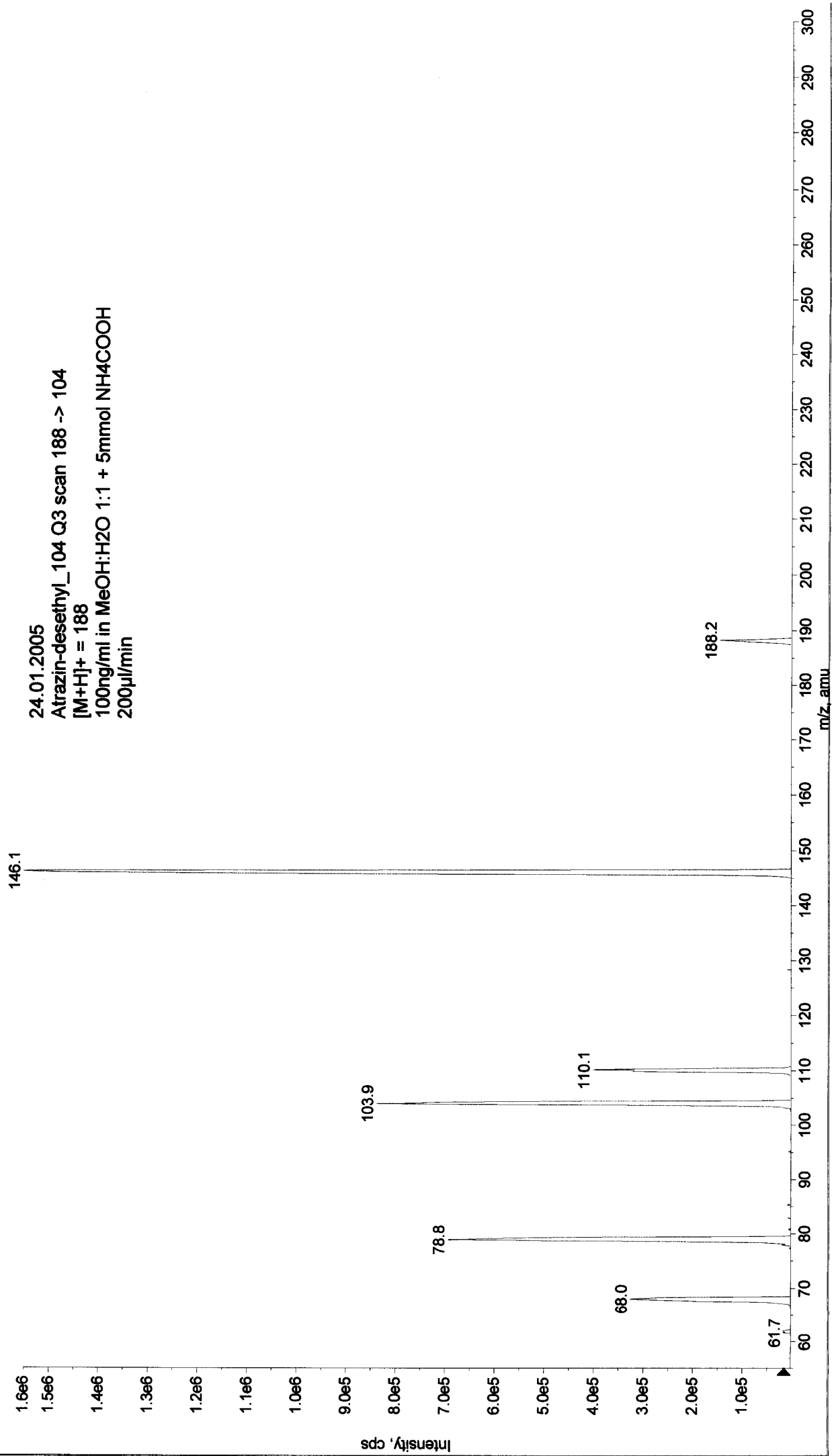
Printing Time: 10:29:27
Printing Date: Monday, January 24, 2005

Acq. Time: 10:28
Acq. Date: Monday, January 24, 2005
Acq. File: MT20050124102809.wiff

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

Max. 1.6e6 cps.

+MS2 (188.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050124102809.wiff (Turbo Spray)



24.01.2005
Atrazin-desethyl_104 Q3 scan 188 -> 104
[M+H]⁺ = 188
100ng/ml in MeOH:H₂O 1:1 + 5mmol NH₄COOH
200µl/min

