

MS/MS Parameters of Pesticides

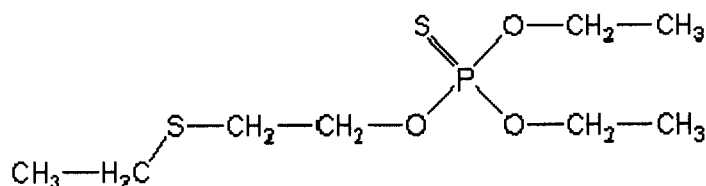
Analyte: Demeton-O

CAS No.: 298-03-3

Formula: C₈H₁₉O₃PS₂

Molecular mass (lowest isotopes): 258,05 amu

Structure:



Ionisation: ESI +

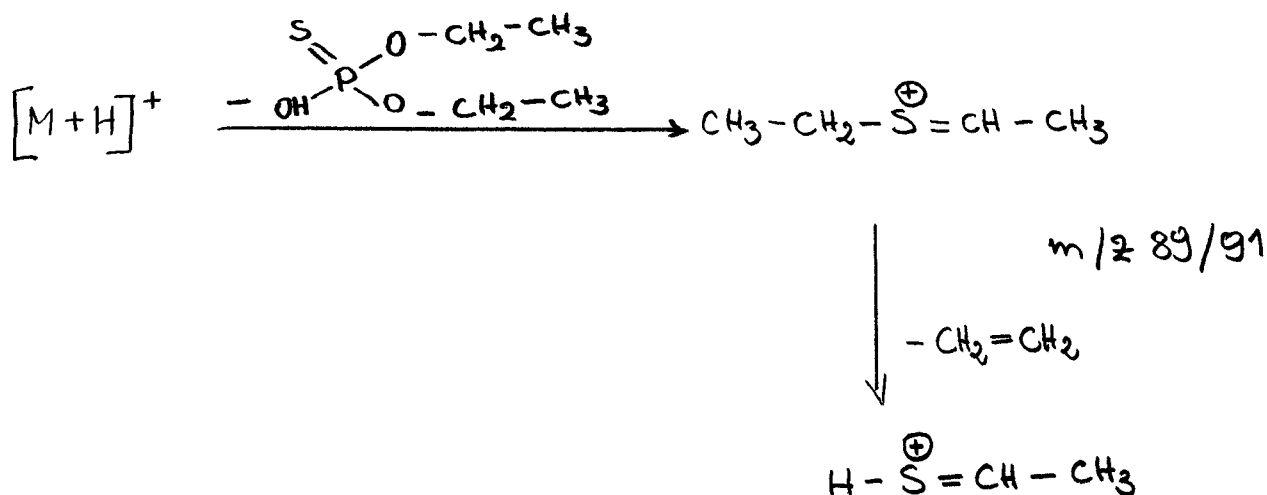
Quasimolecular ion: 259,1 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

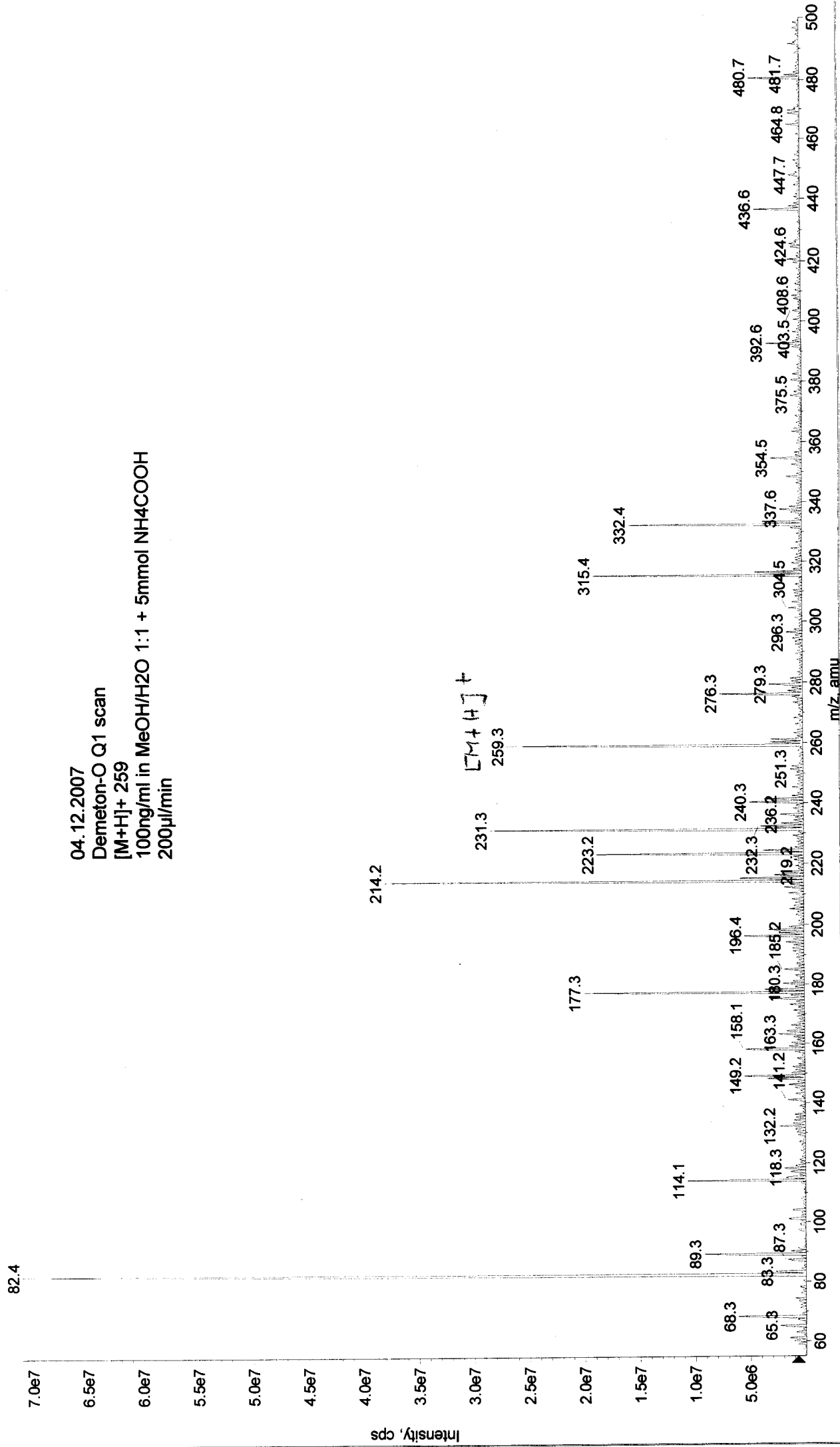
Transition	259,1 → 89,0	259,1 → 60,9
Declustering potential (DP) ^{*)}	16 V	16 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	12 V	11,5 V
Collision cell entrance potential (CEP)	18 V	18 V
Collision energy (CE)	19 V	47 V
Collision cell exit potential (CXP)	6 V	6 V

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

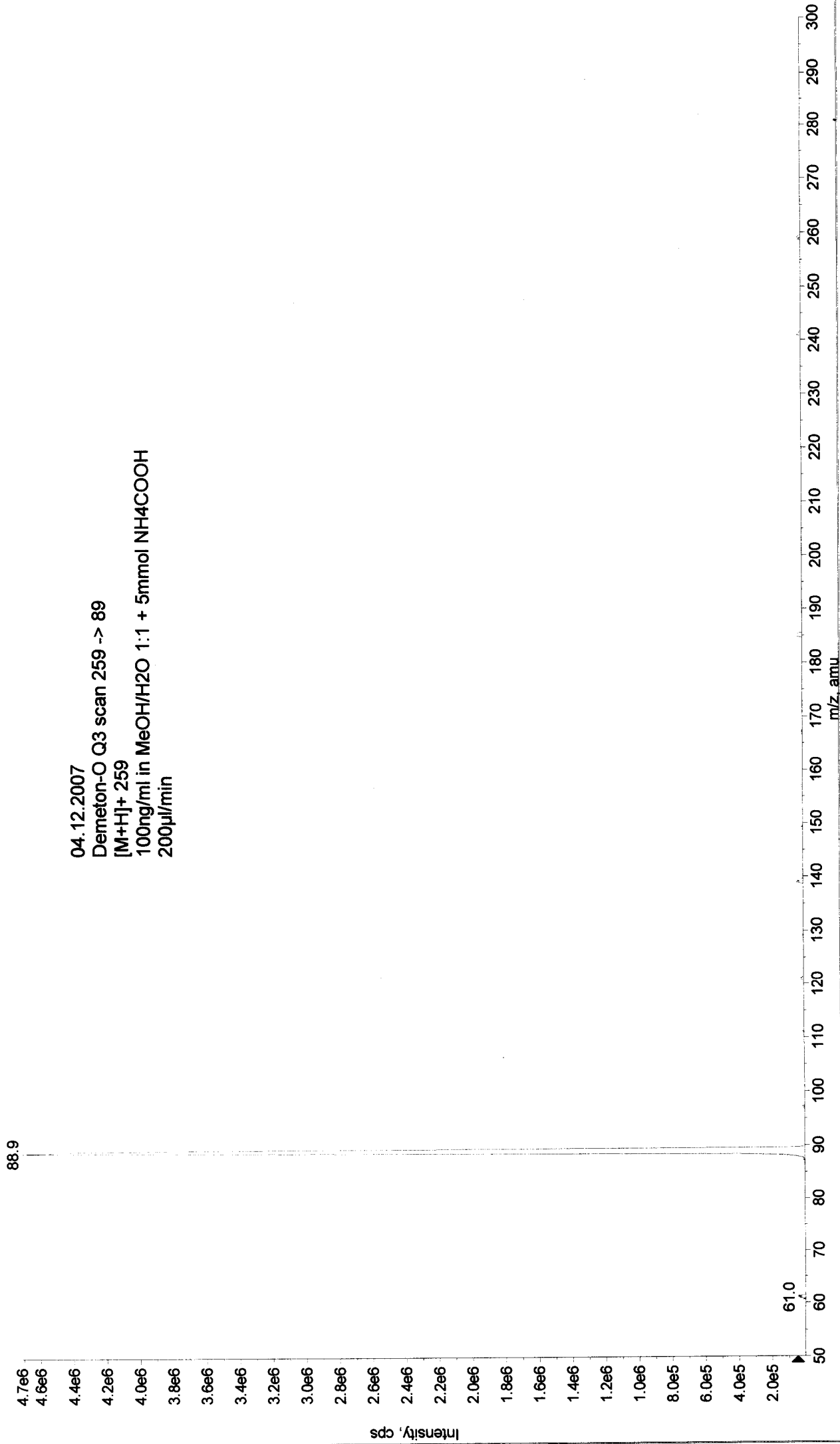
Fragmentation



■ +Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20071204142310.wiff (Turbo Spray)

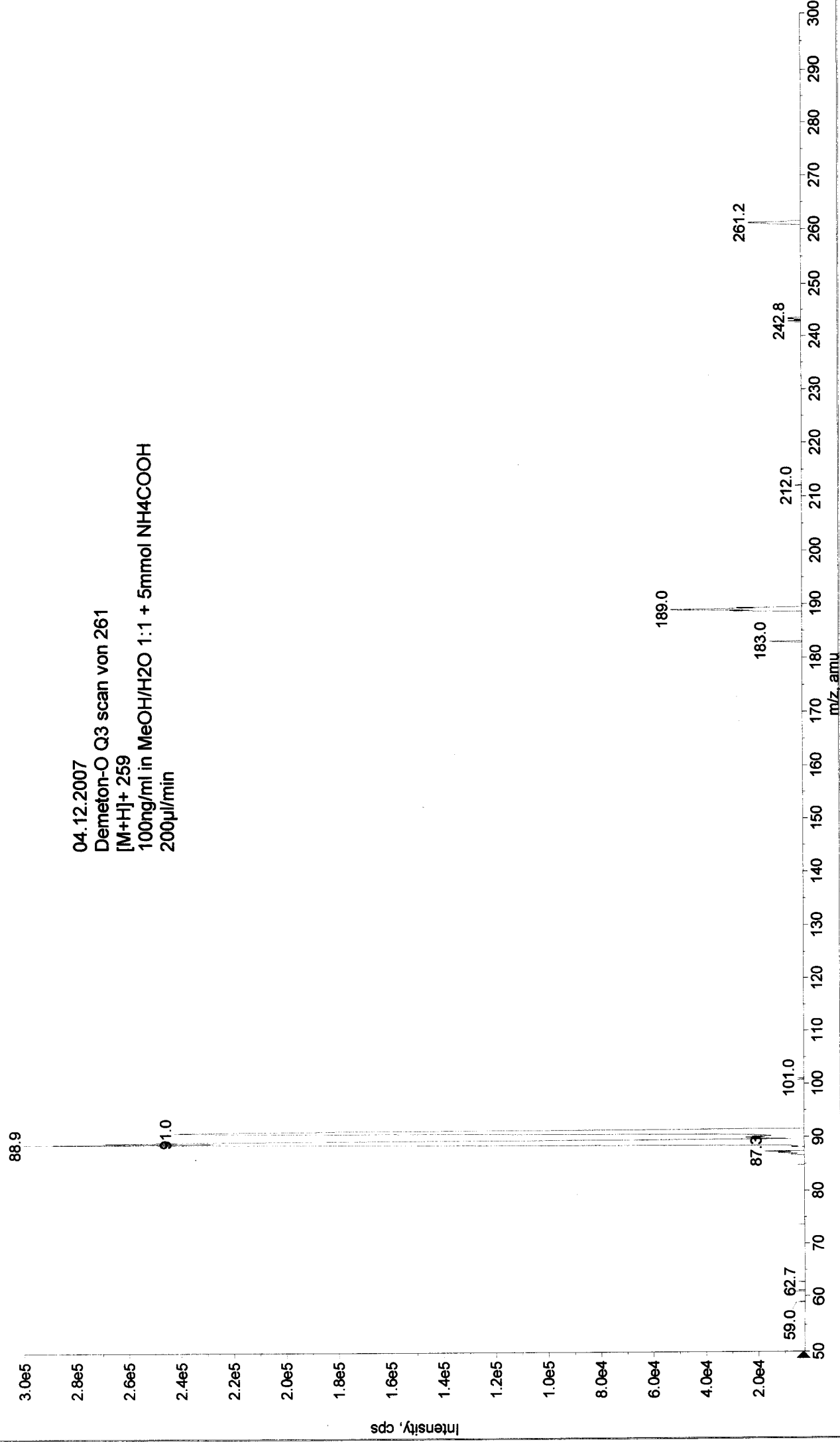


■ +MS2 (259.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071204142627.wiff (Turbo Spray)



■ +MS2 (261.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071204142803.wiff (Turbo Spray)

Max. 3.0e5 cps.



■ +Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20071204143347.wiff (Turbo Spray)

Max. 1.3e8 cps.

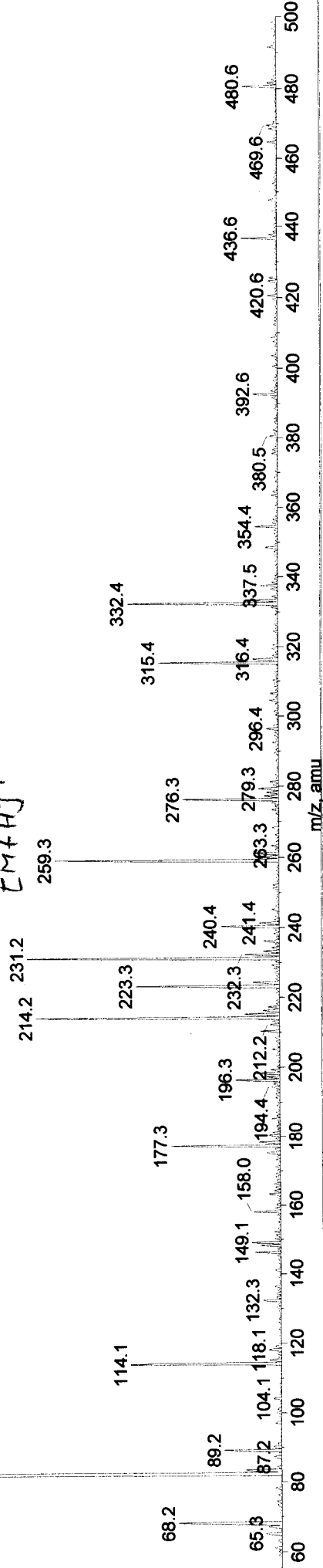
82.4

1.33e8
1.30e8
1.25e8
1.20e8
1.15e8
1.10e8
1.05e8
1.00e8
9.50e7
9.00e7
8.50e7
8.00e7
7.50e7
7.00e7
6.50e7
6.00e7
5.50e7
5.00e7
4.50e7
4.00e7
3.50e7
3.00e7
2.50e7
2.00e7
1.50e7
1.00e7
5.00e6

04.12.2007
Demeton-O_61 Q1 scan
[M+H]⁺ 259
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min

Intensity, cps

$[M+H]^+$



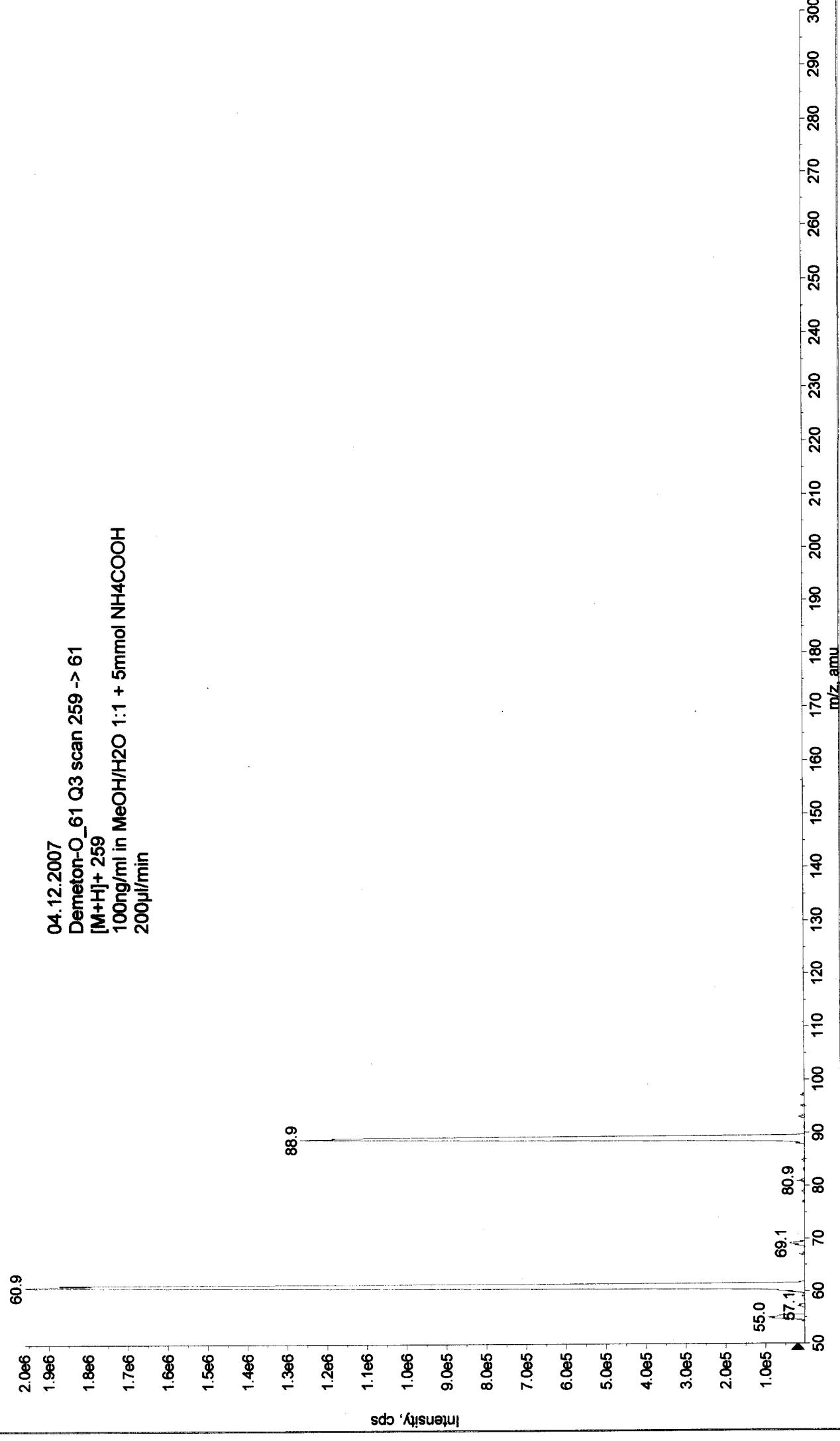
Batch Name: ManualTune.bat
Sample Name: TuneSampleID
Sample Comment:

Acq. File: MT20071204143625.wiff
Acq. Date: Tuesday, December 04, 2007
Acq. Time: 14:36

Printing Time: 02:43:42 PM
Printing Date: Tuesday, December 04, 2007

Max. 2.0e6 cps.

+MS2 (259.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071204143625.wiff (Turbo Spray)



■ +MS2 (261.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071204144402.wiff (Turbo Spray)

