

## MS/MS Parameters of Pesticides

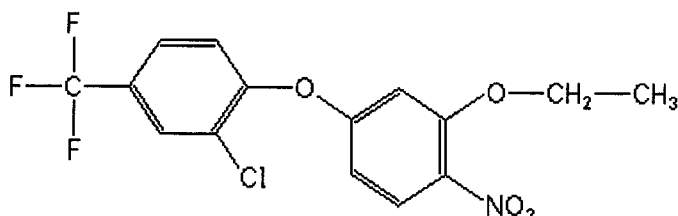
### Analyte: Oxyfluorfen

CAS No.: 42874-03-3

Formula: C<sub>15</sub>H<sub>11</sub>ClF<sub>3</sub>NO<sub>4</sub>

Molecular mass (lowest isotopes): 361,03 amu

Structure:



Ionisation: ESI +

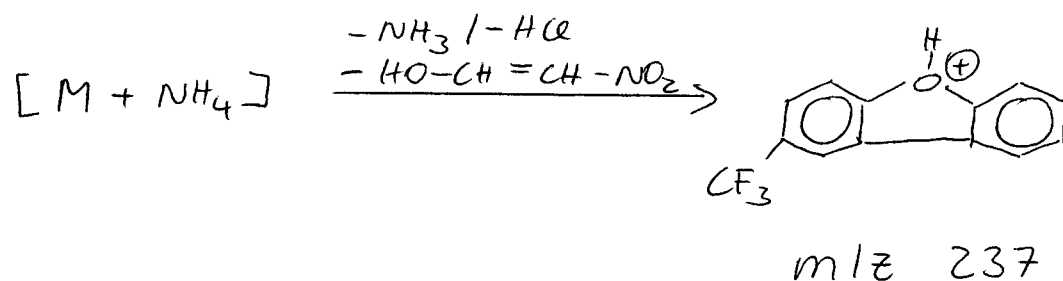
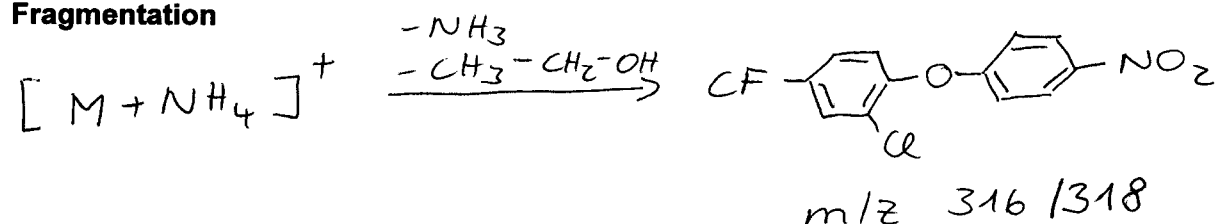
Quasimolecular ion: 379,0 amu = [M+NH<sub>4</sub>]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

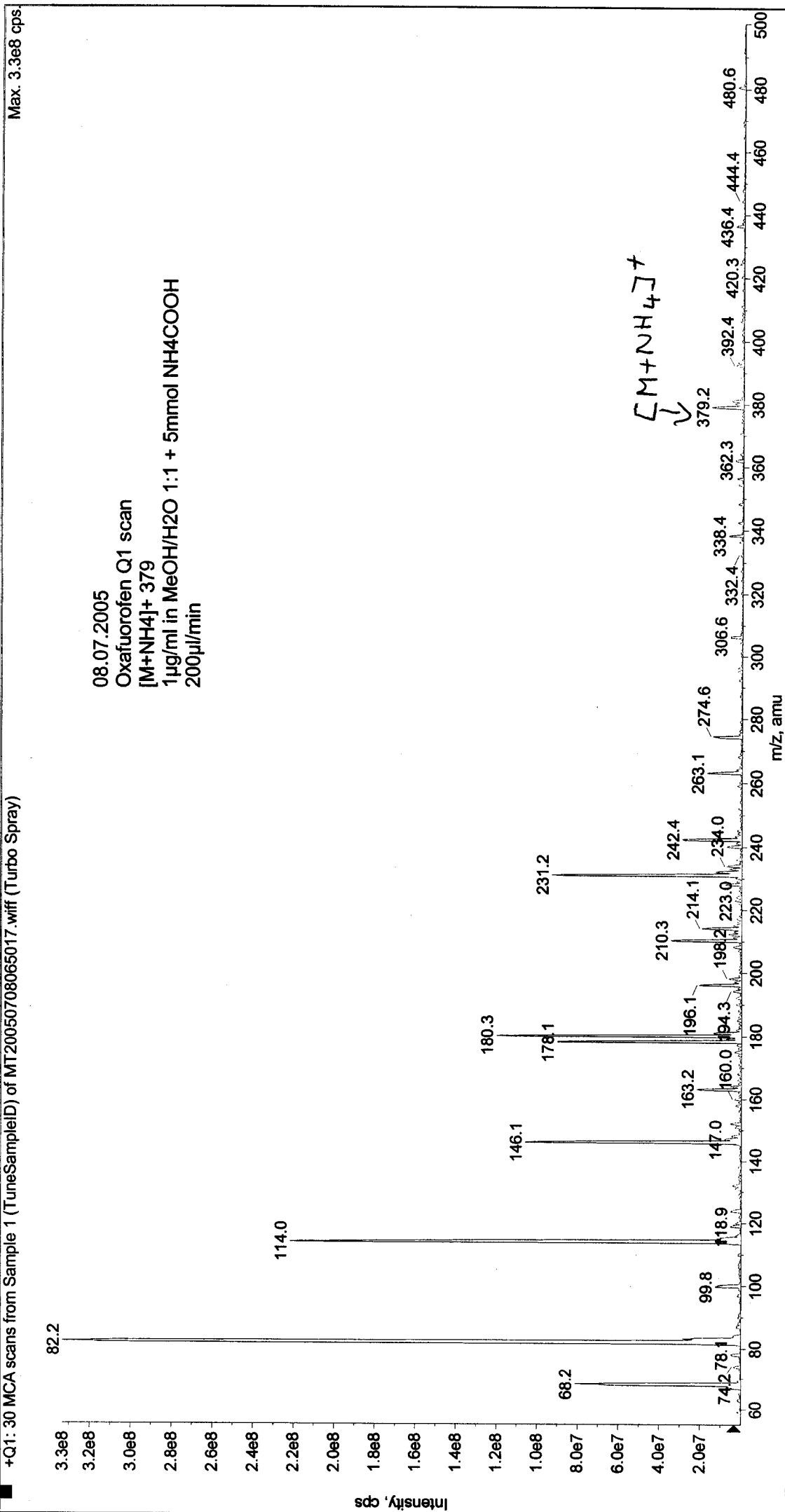
Transition	379,0 → 316,0	379,0 → 237,1
Declustering potential (DP) <sup>*)</sup>	24V	24 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	9,0 V	6,5 V
Collision cell entrance potential (CEP)	20 V	22 V
Collision energy (CE)	23 V	39 V
Collision cell exit potential (CXP)	18 V	12 V

<sup>\*)</sup> For API 3000 and 4000 enhance DP by 20V

### Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20050708065017.wiff (Turbo Spray)



Printing Time: 6:54:43

Printing Date: Friday, July 08, 2005

Acq. Time: 06:53

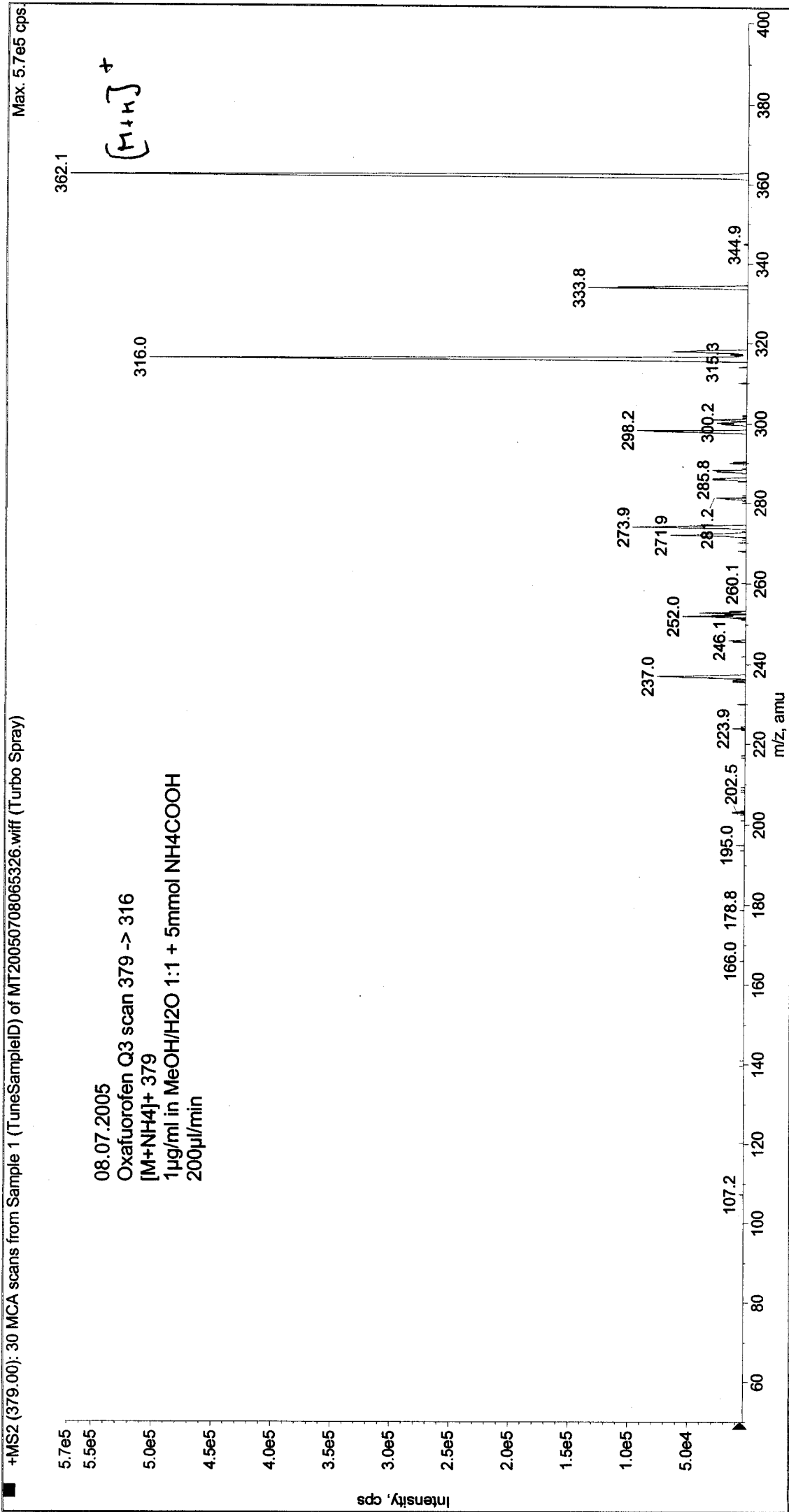
Acq. Date: Friday, July 08, 2005

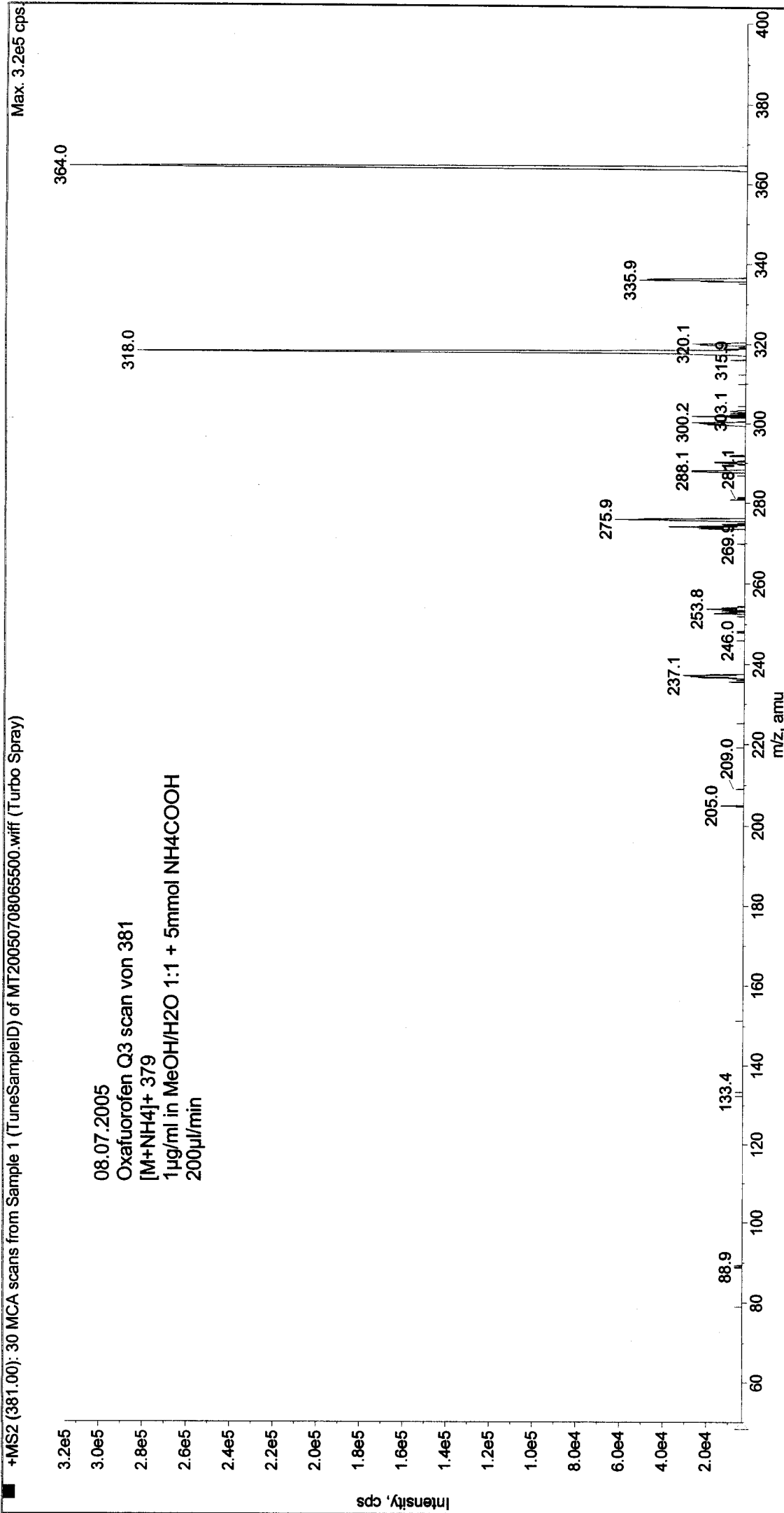
Acq. File: MT20050708065326.wiff

Sample Comment:

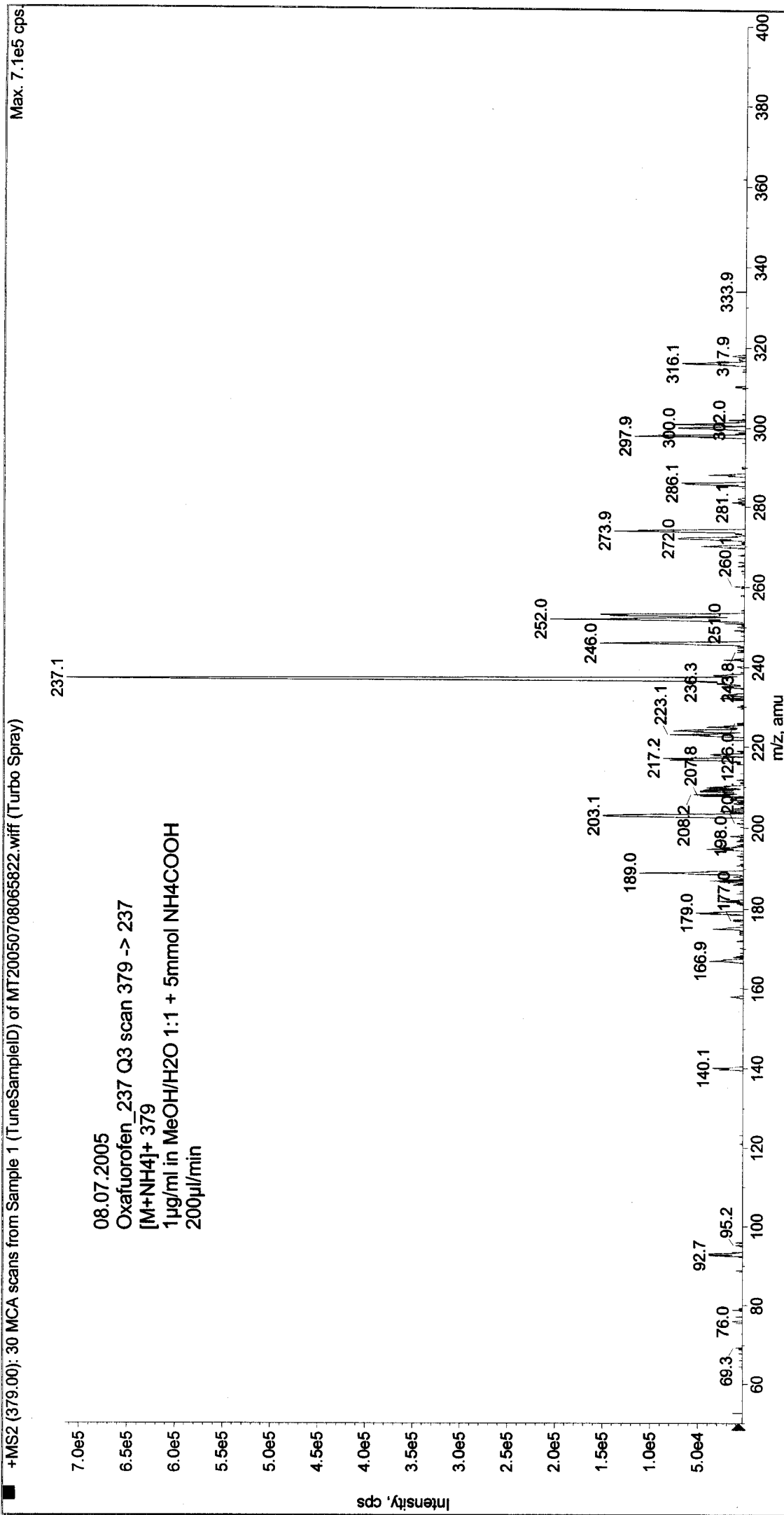
Sample Name: TuneSampleID

Batch Name: ManualTune.bat



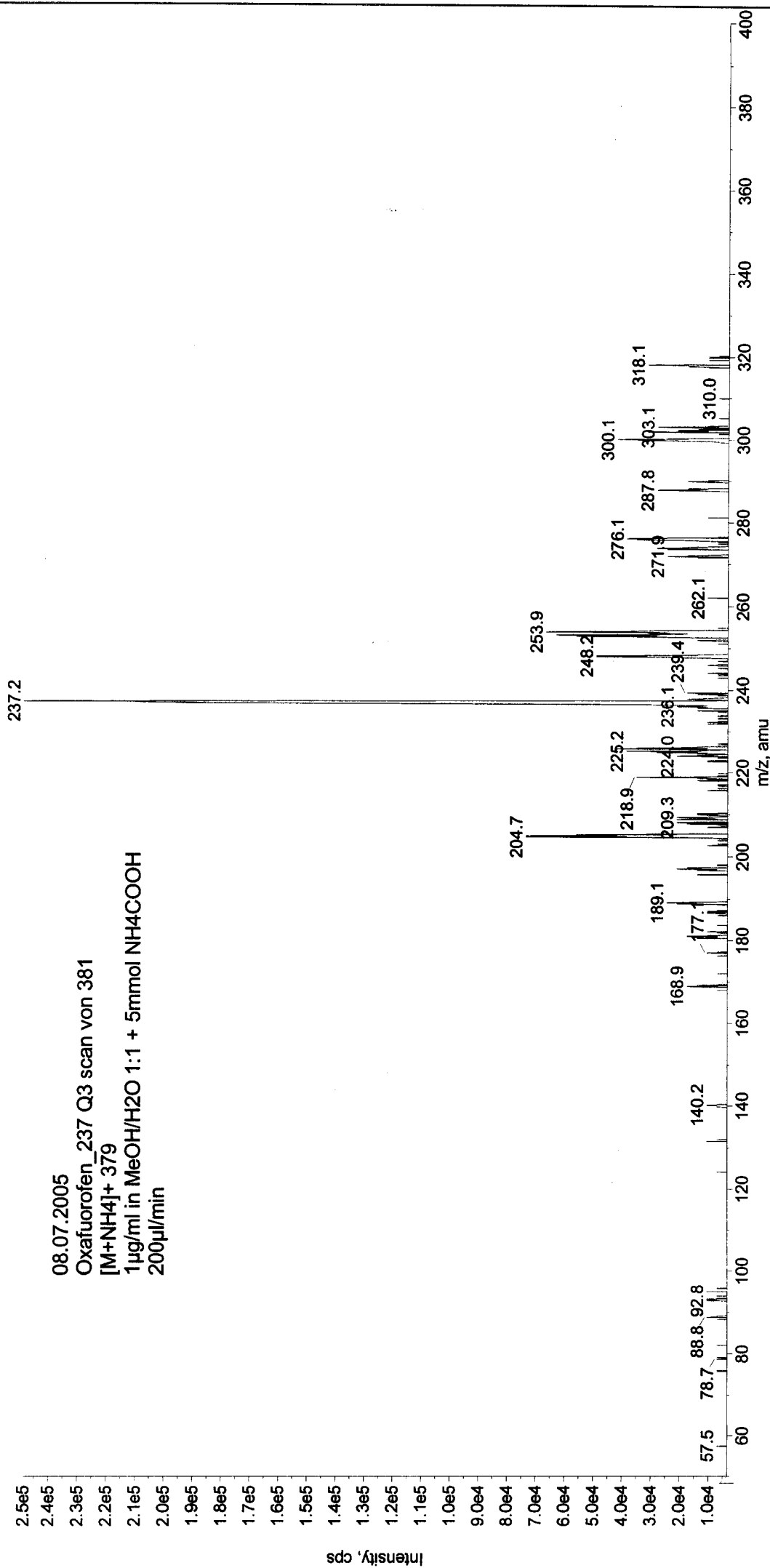


+MS2 (379.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050708065822.wiff (Turbo Spray)



+MS2 (381.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050708065944.wiff (Turbo Spray)

Max. 2.5e5 cps



08.07.2005  
 Oxafurofen\_237 Q3 scan von 381  
 [M+NH4]<sup>+</sup> 379  
 1µg/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
 200µl/min