

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

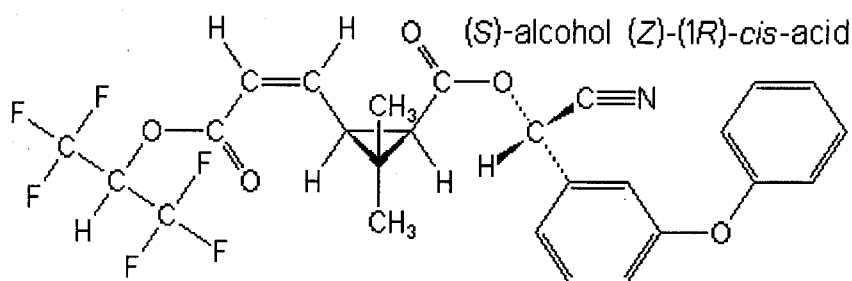
### Analyte: Acrinathrin

CAS No.: 101007-06-1

Formula: C<sub>26</sub>H<sub>21</sub>F<sub>6</sub>NO<sub>5</sub>

Molecular mass (lowest isotopes): 541,13 amu

Structure:



Ionisation: ESI +

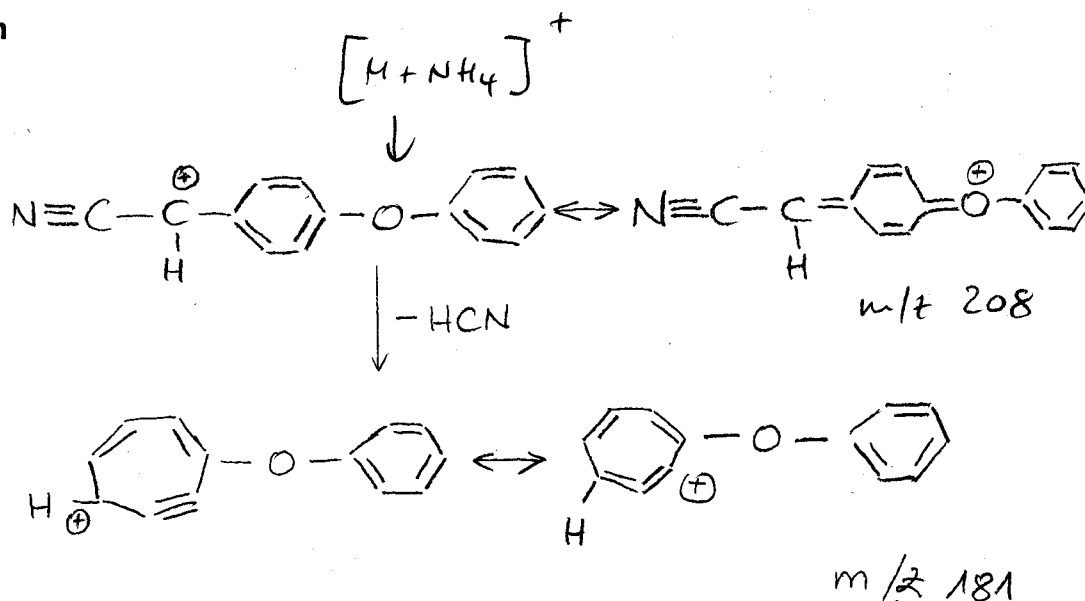
Quasimolecular ion: 559,1 amu = [M+NH<sub>4</sub>]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	559,1 → 208,1	559,1 → 181,1
Declustering potential (DP) <sup>*)</sup>	24V	24 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	11,5 V	11,0 V
Collision cell entrance potential (CEP)	24 V	24 V
Collision energy (CE)	23 V	43 V
Collision cell exit potential (CXP)	10 V	10 V

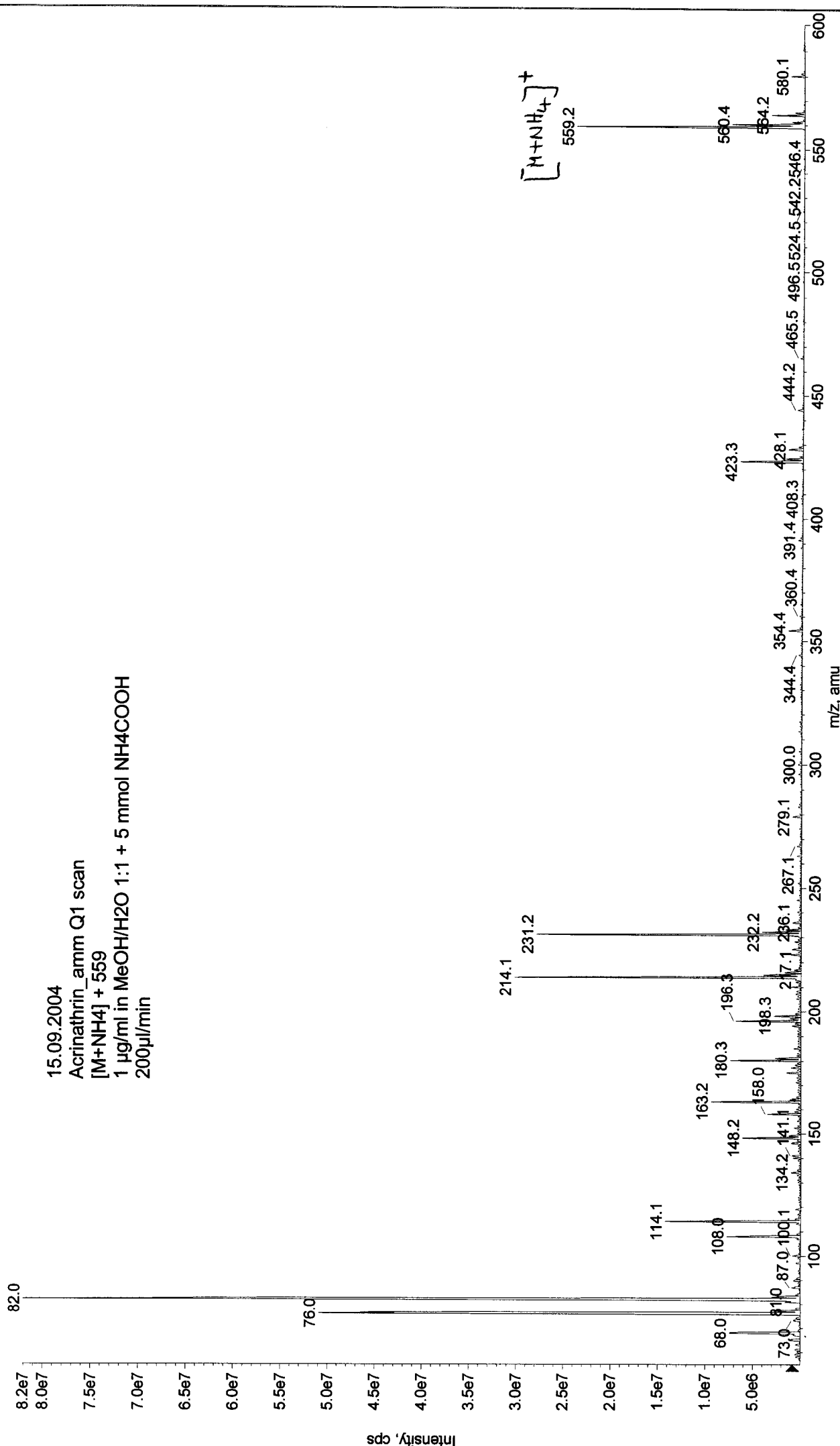
<sup>\*)</sup> For API 3000 and 4000 enhance DP by 20V

### Fragmentation



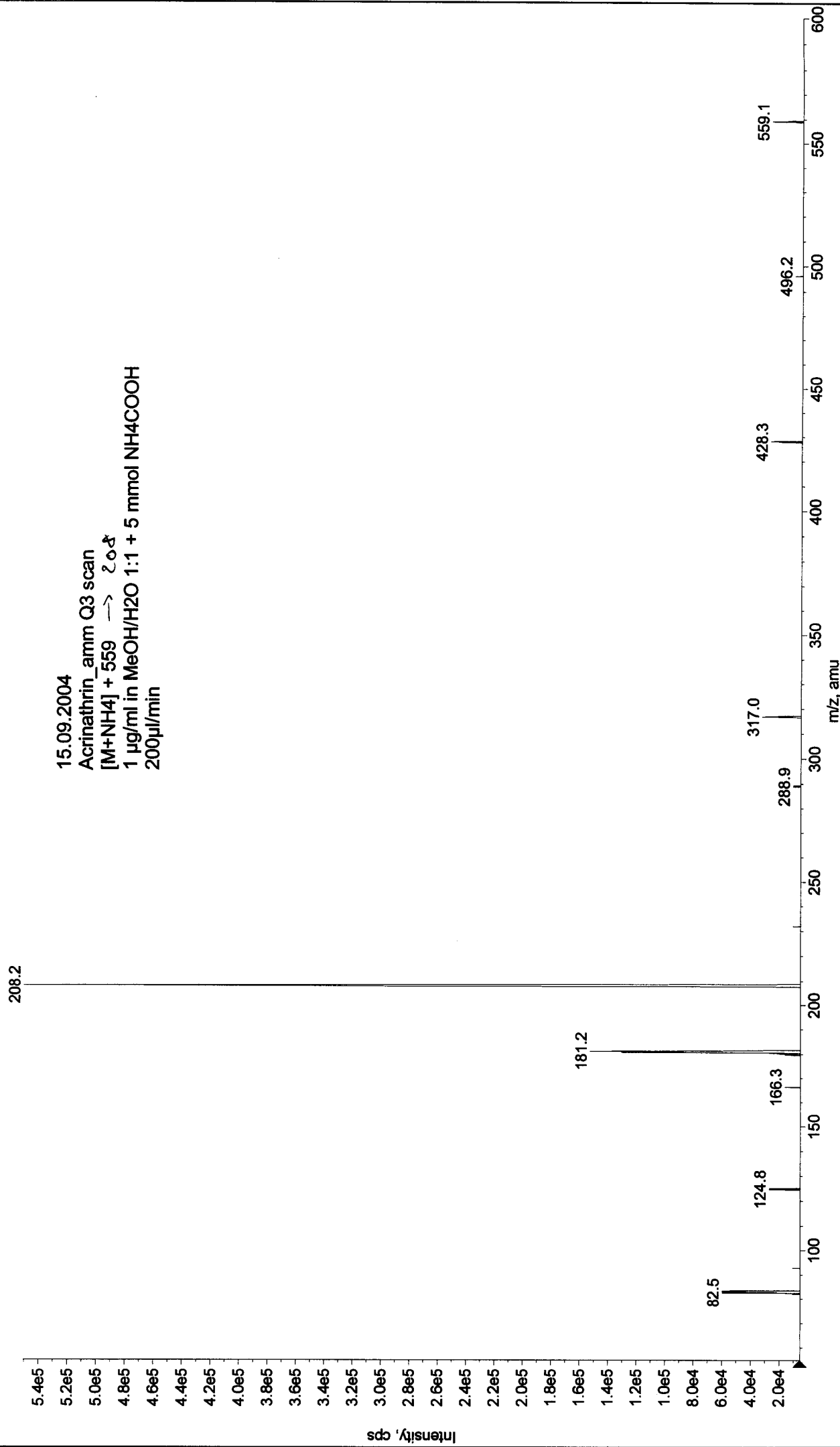
+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20040915132958.wiff (Turbo Spray)

Max. 8.2e7 cps



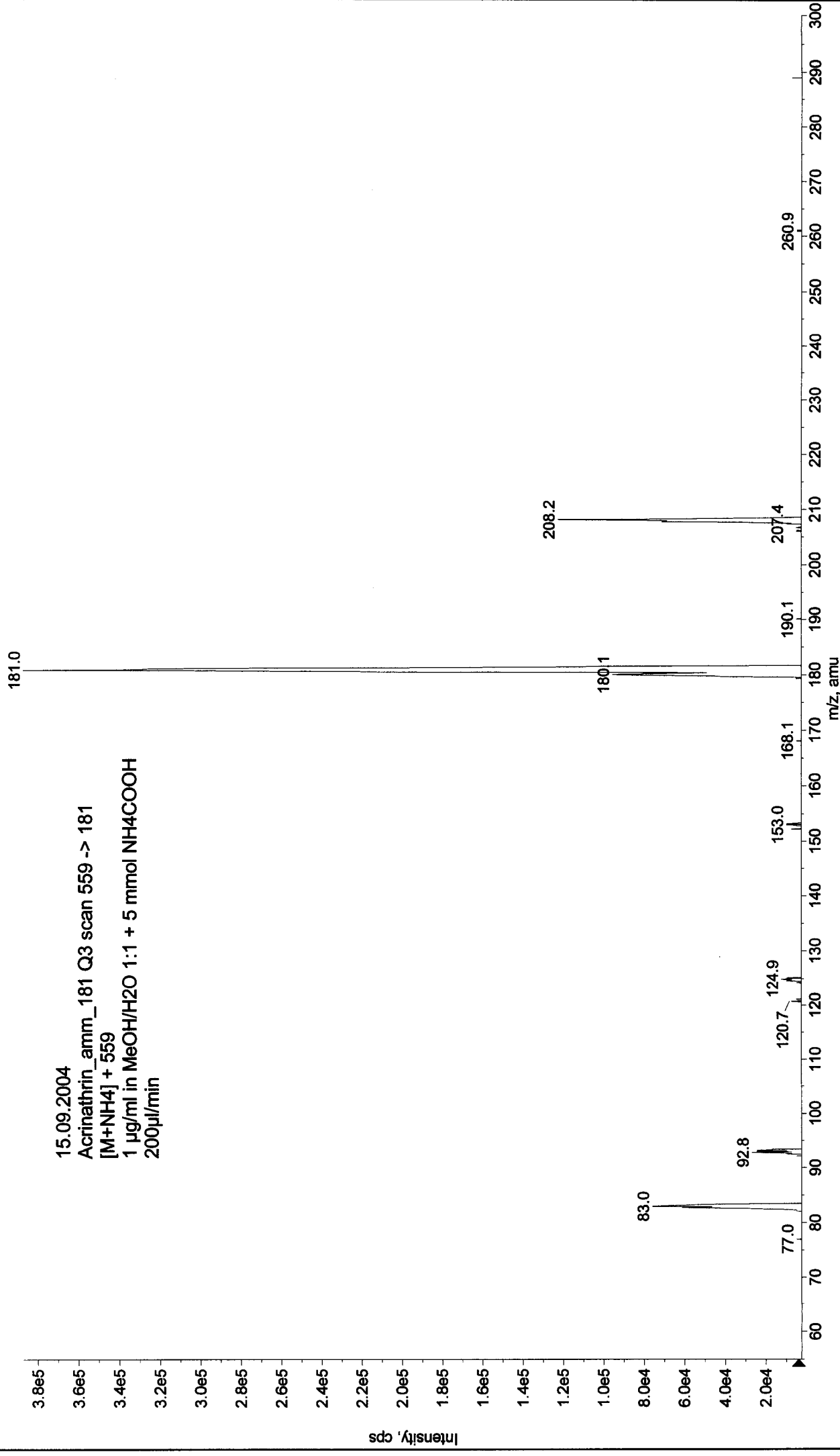
Max. 5.5e5 cps

+MS2 (559.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040915134622.wiff (Turbo Spray)



Max. 3.9e5 cps

+MS2 (559.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040915133957.wiff (Turbo Spray)



15.09.2004  
Acrinathrin\_amm\_181 Q3 scan 559 -> 181  
[M+NH4]<sup>+</sup> + 559  
1 µg/ml in MeOH/H<sub>2</sub>O 1:1 + 5 mmol NH<sub>4</sub>COOH  
200 µl/min