

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

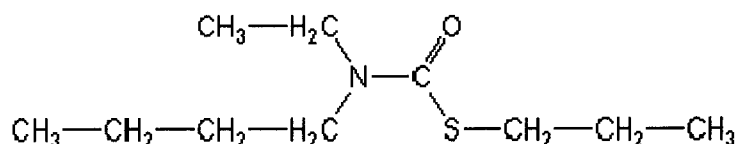
### Analyte: Pebulate

CAS No.: 1114-71-2

Formula: C<sub>10</sub>H<sub>21</sub>NOS

Molecular mass (lowest isotopes): 203,13 amu

Structure:



Ionisation: ESI +

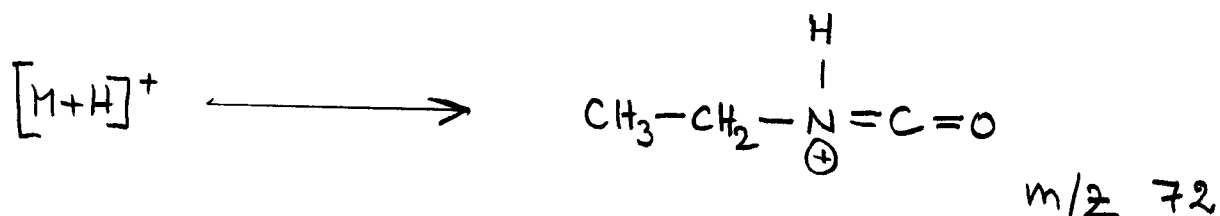
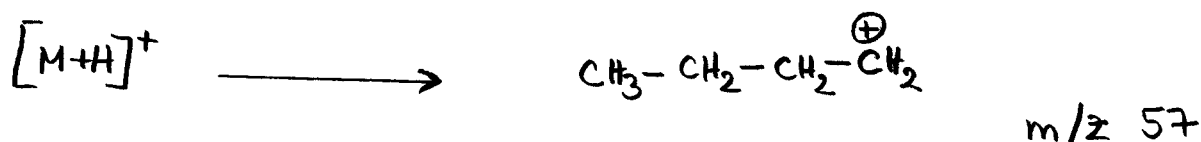
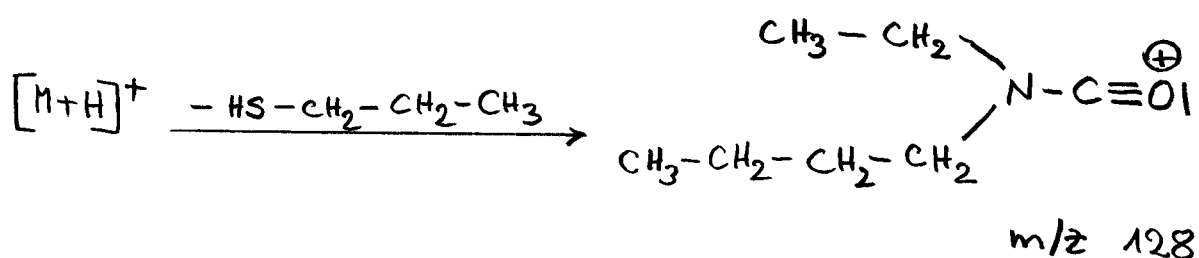
Quasimolecular ion: 204,1 amu = [M+H]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	204,1 → 128,2	204,1 → 57,0
Declustering potential (DP) <sup>*)</sup>	39 V	39 V
Focusing potential (FP)	350 V	360 V
Entrance potential (EP)	10,0 V	9,5 V
Collision cell entrance potential (CEP)	12 V	12 V
Collision energy (CE)	17 V	27 V
Collision cell exit potential (CXP)	6 V	8 V

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

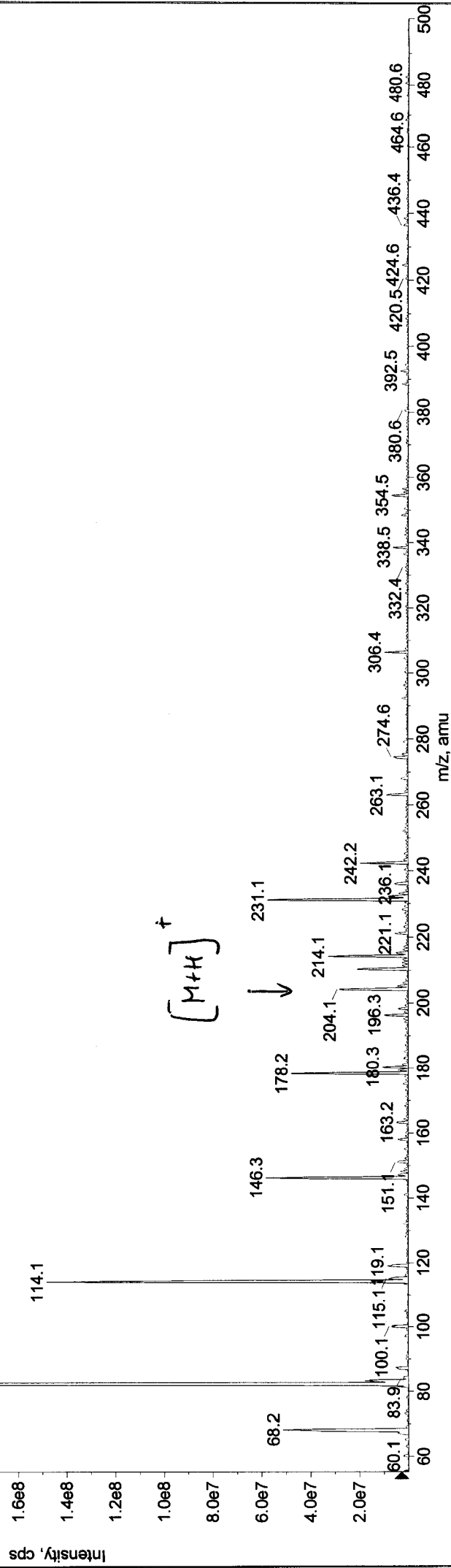
### Fragmentation

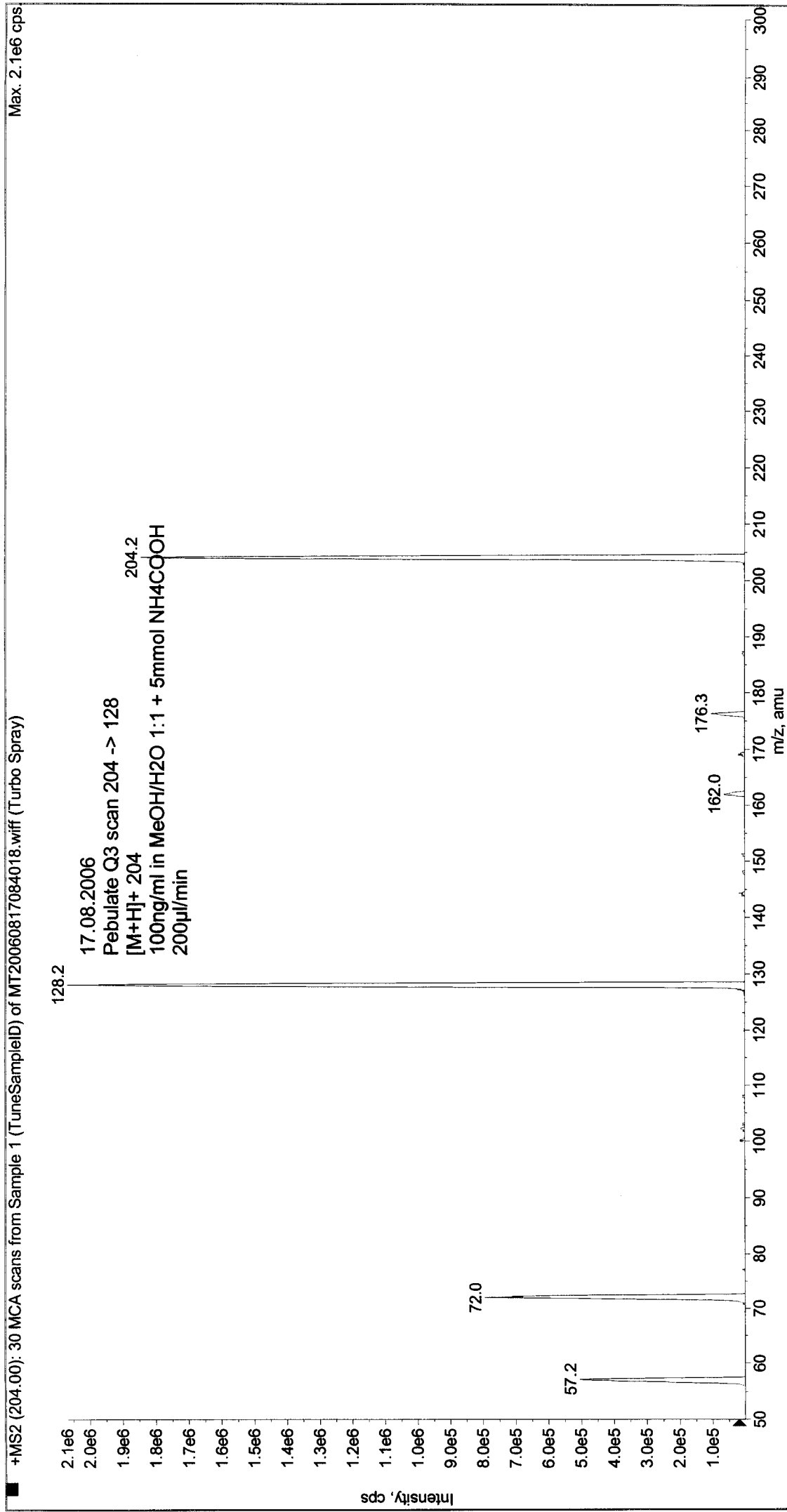


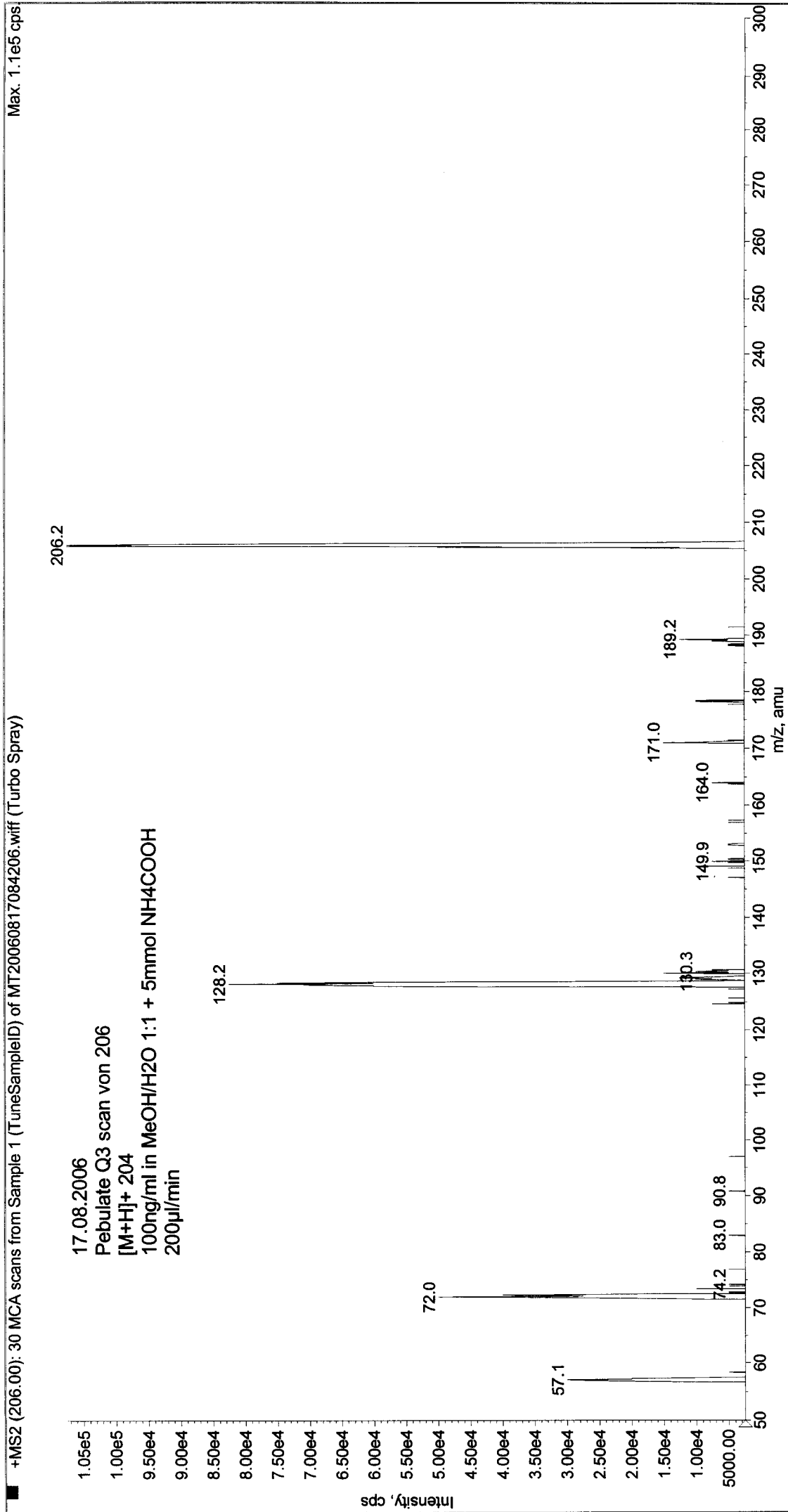
+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060817083753.wiff (Turbo Spray)

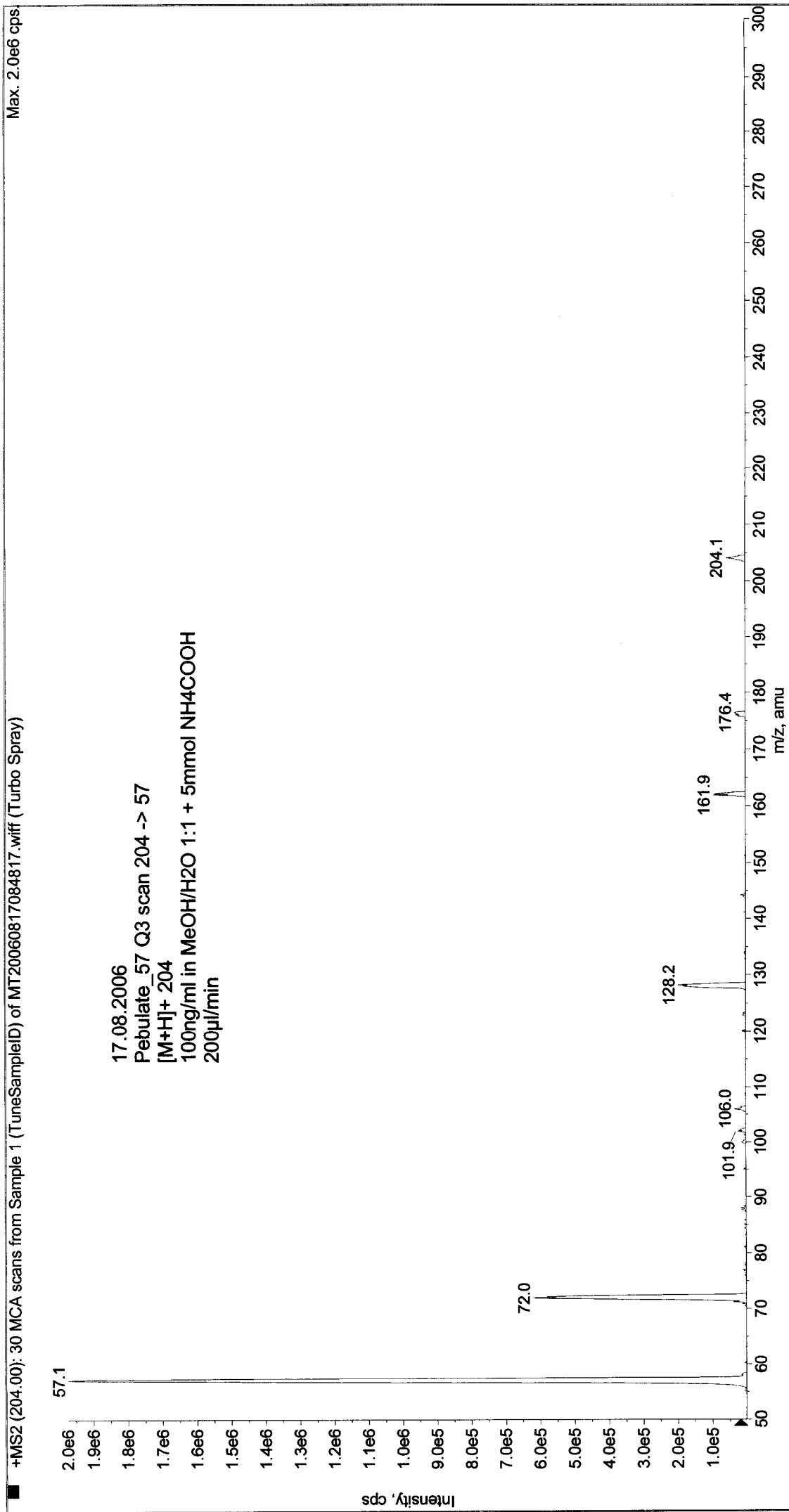
Max. 2.9e8 cps

17.08.2006  
 Pebulate Q1 scan  
 [M+H]<sup>+</sup> 204  
 100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
 200µl/min

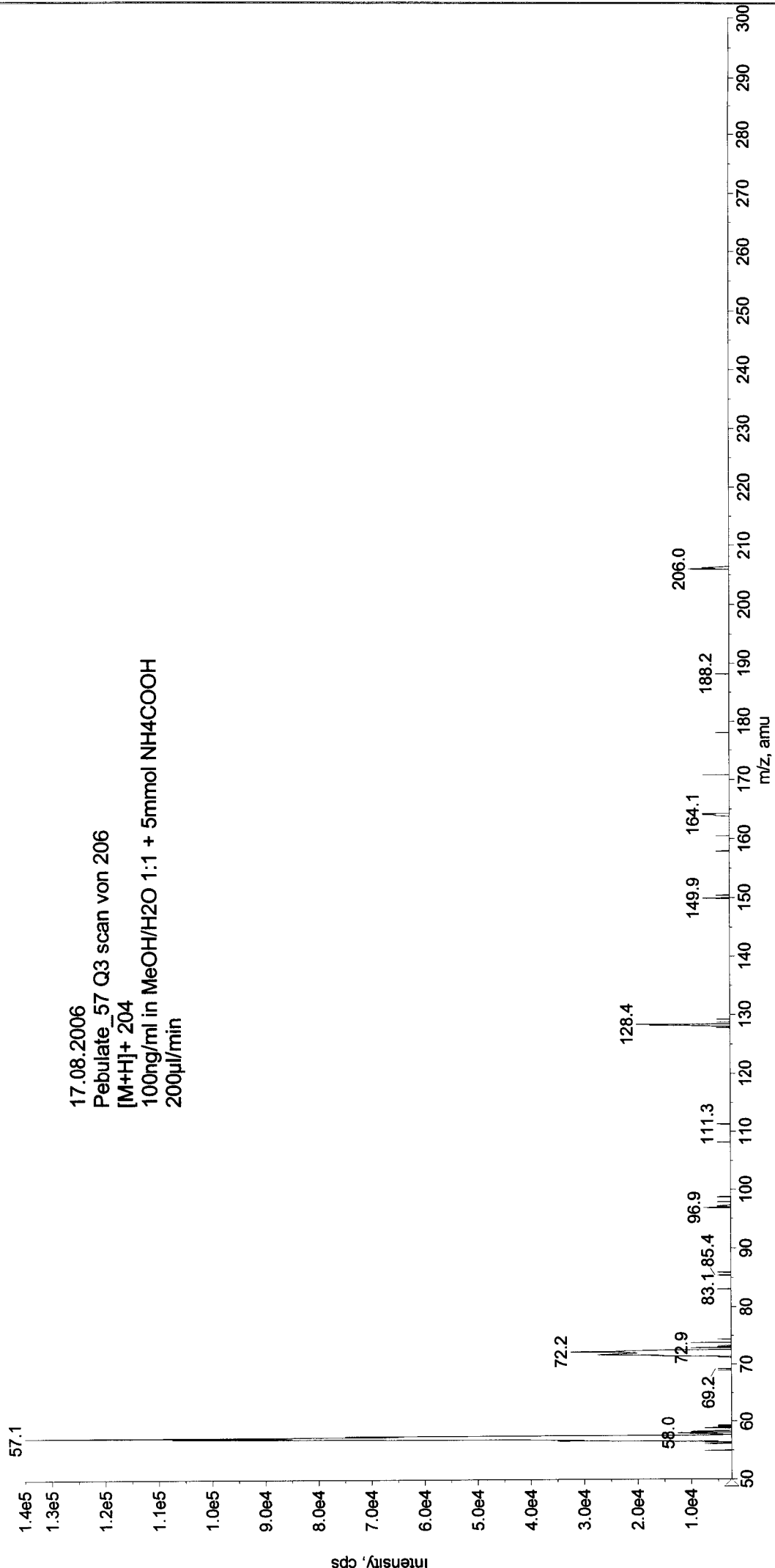








+MS2 (206.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060817084931.wiff (Turbo Spray) Max. 1.4e5 cps



17.08.2006  
 Pebulate\_57 Q3 scan von 206  
 [M+H]<sup>+</sup> + 204  
 100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
 200µl/min