

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

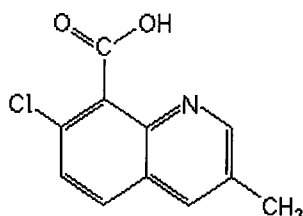
### Analyte: Quinmerac

CAS No.: 90717-03-6

Formula: C<sub>11</sub>H<sub>8</sub>ClNO<sub>2</sub>

Molecular mass (lowest isotopes): 221,02 amu

Structure:



Ionisation: ESI +

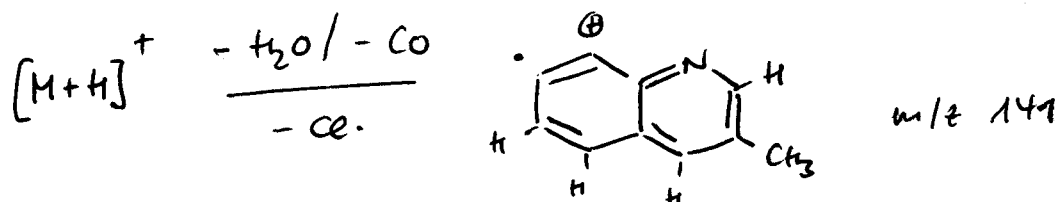
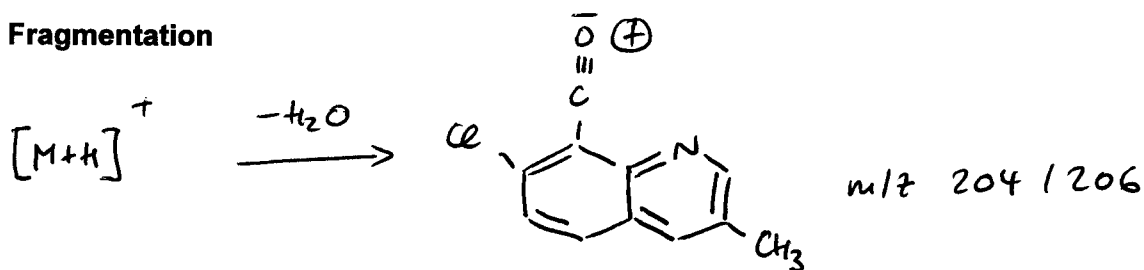
Quasimolecular ion: 222,0 amu = [M+H]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

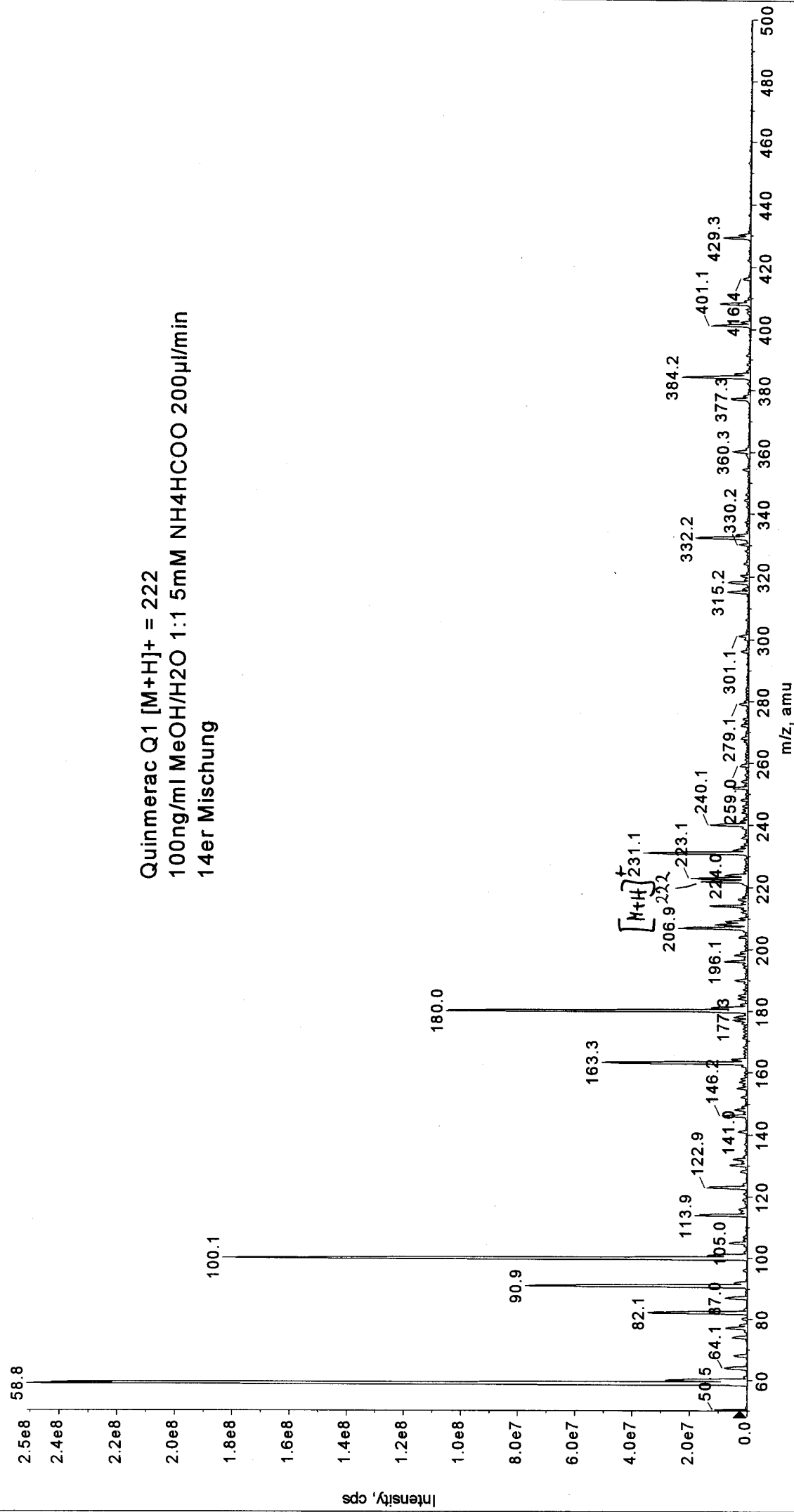
Transition	222,0 → 204,1	222,0 → 141,0
Declustering potential (DP)*)	24 V	24 V
Focusing potential (FP)	340 V	350 V
Entrance potential (EP)	10,0 V	10,0 V
Collision cell entrance potential (CEP)	14 V	14 V
Collision energy (CE)	23 V	43 V
Collision cell exit potential (CXP)	10 V	6 V

\*) For API 3000 and 4000 enhance DP by 20V

### Fragmentation



\*Q1: 30 MCA scans from Sample 1 of MT20020211130753.wiff Max 2.5e8 cps



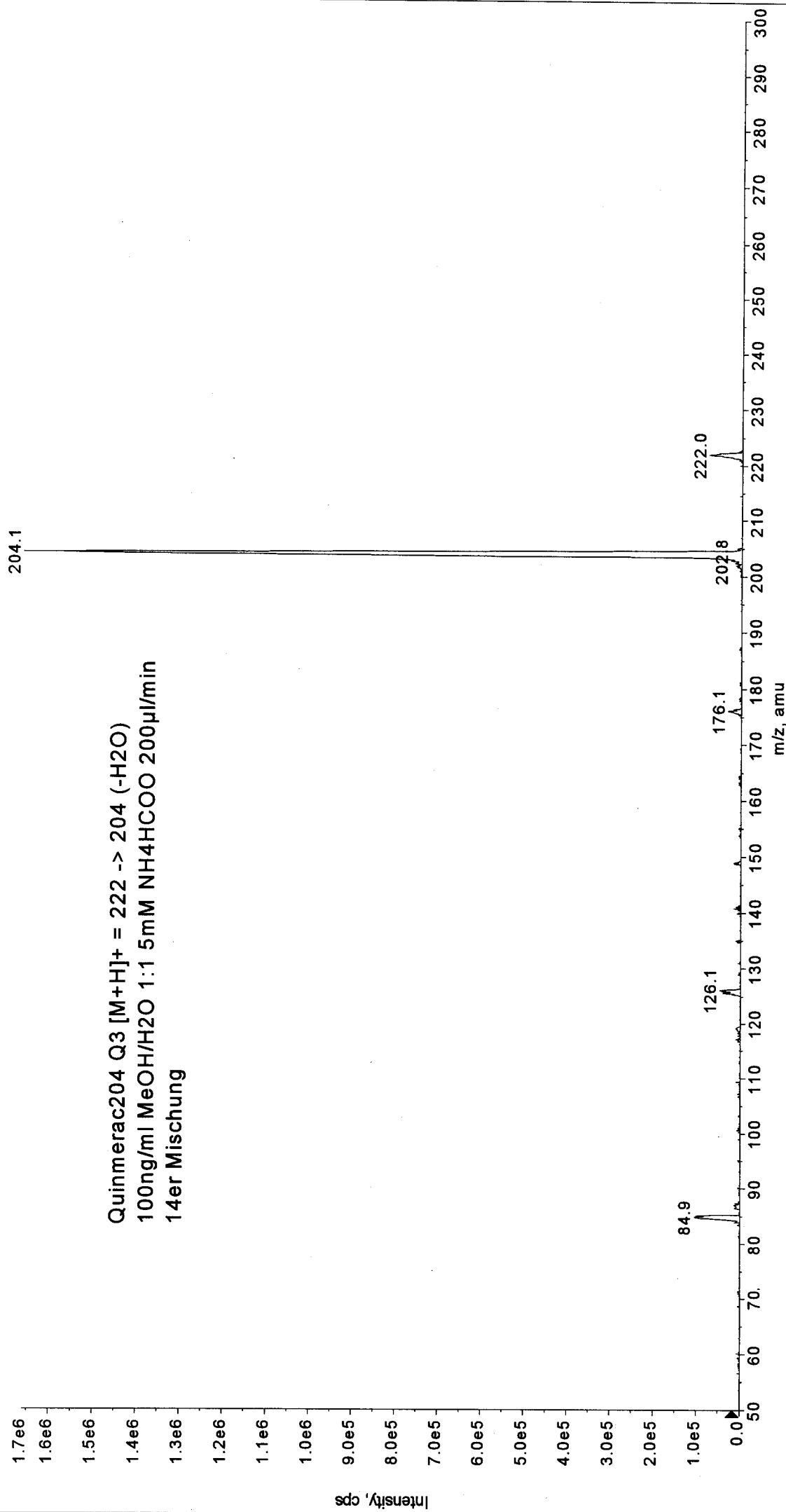
Printing Date: 11 February 2002  
Printing Time: 13:29:34

Acq. Date: Monday, February 11, 2002  
Acq. Time: 13:28  
Acq. File: MT20020211132829.wiff

Sample Comment:  
Sample Name:  
Batch Name: n/a

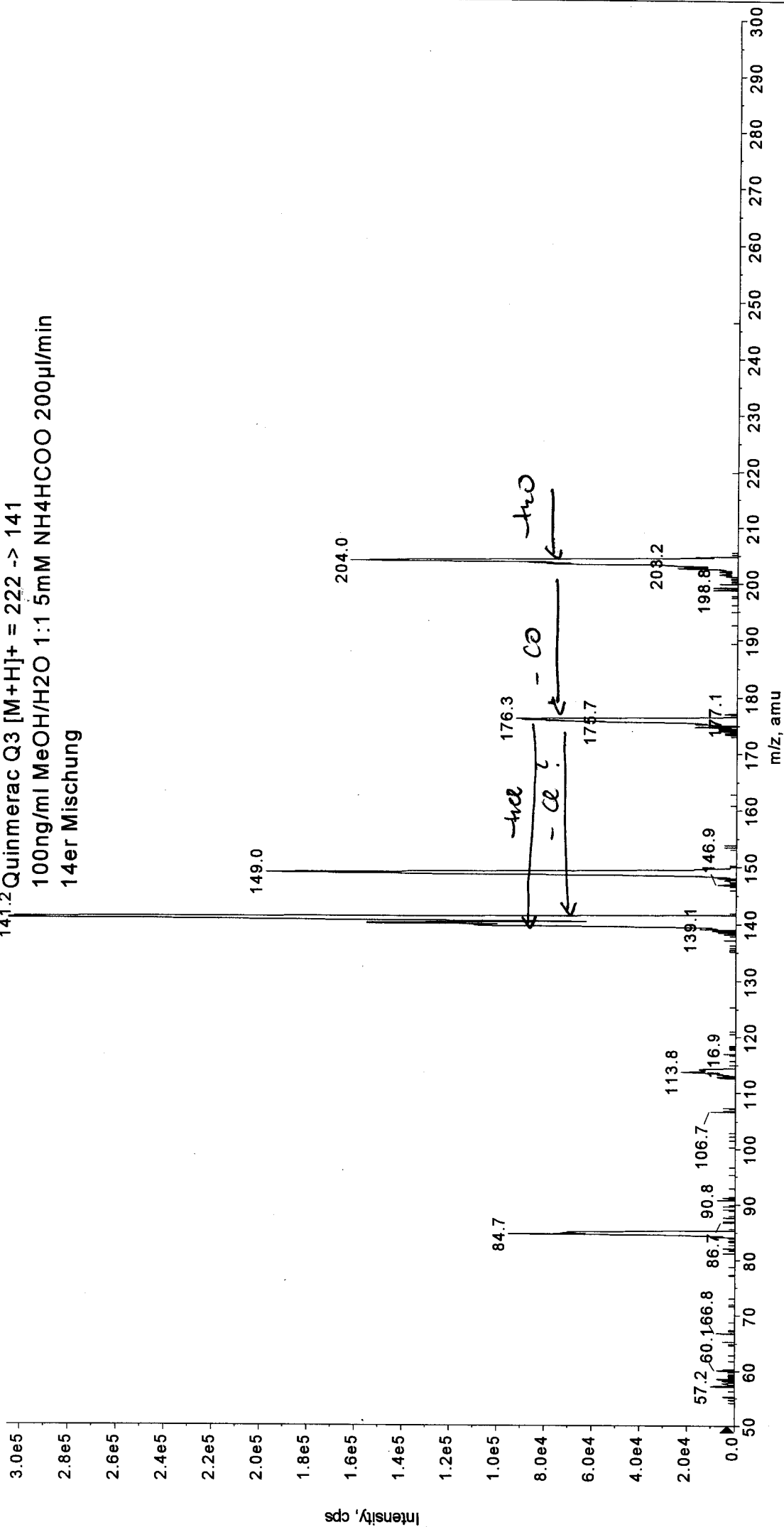
\*Product (222.0): 20 MCA scans from Sample 1 of MT20020211132829.wiff

Max: 1.7e6 cps



\*Product (222.0): 30 MCA scans from Sample 1 of MT20020211131128.wiff Max: 3.1e5 cps

141.2 Quinmerac Q3 [M+H]<sup>+</sup> = 222 -> 141  
100ng/ml MeOH/H<sub>2</sub>O 1:1 5mM NH<sub>4</sub>HCOO 200µl/min  
14er Mischung



Sample Comment:  
Sample Name:  
Batch Name: n/a

Quinmerac140\_CI37\_Q3 [M+H]<sup>+</sup> = 224 -> 140  
100ng/ml MeOH/H<sub>2</sub>O 1:1 5mM NH<sub>4</sub>HCOO 200µl/min  
14er Mischung

Intensity, cps

m/z, amu

m/z, amu	Relative Intensity (cps)
141.1	1.28e5
151.0	7.00e4
178.1	5.00e4
206.2	7.00e4
222.3	2.00e4