

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

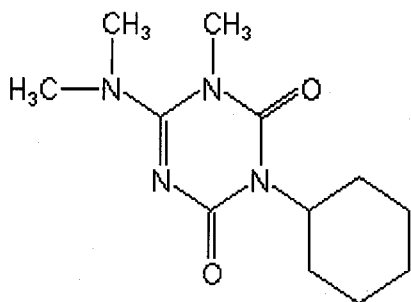
### Analyte: Hexazinone

CAS No.: 51235-04-2

Formula: C<sub>12</sub>H<sub>20</sub>N<sub>4</sub>O<sub>2</sub>

Molecular mass (lowest isotopes): 252,16 amu

Structure:



Ionisation: ESI +

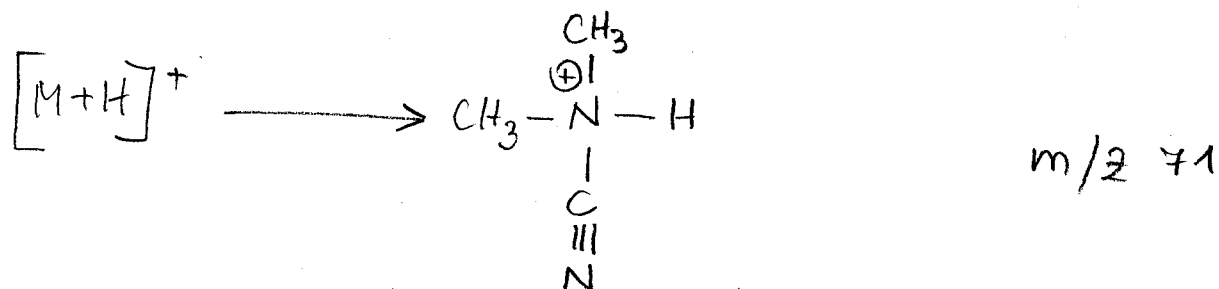
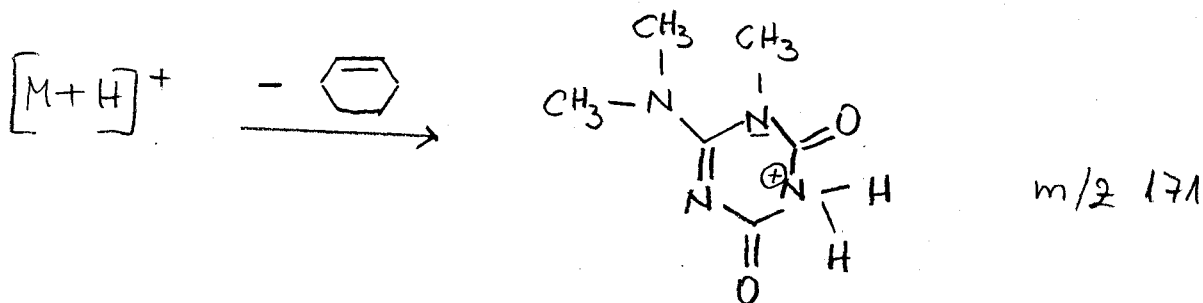
Quasimolecular ion: 253,2 amu = [M+H]<sup>+</sup>

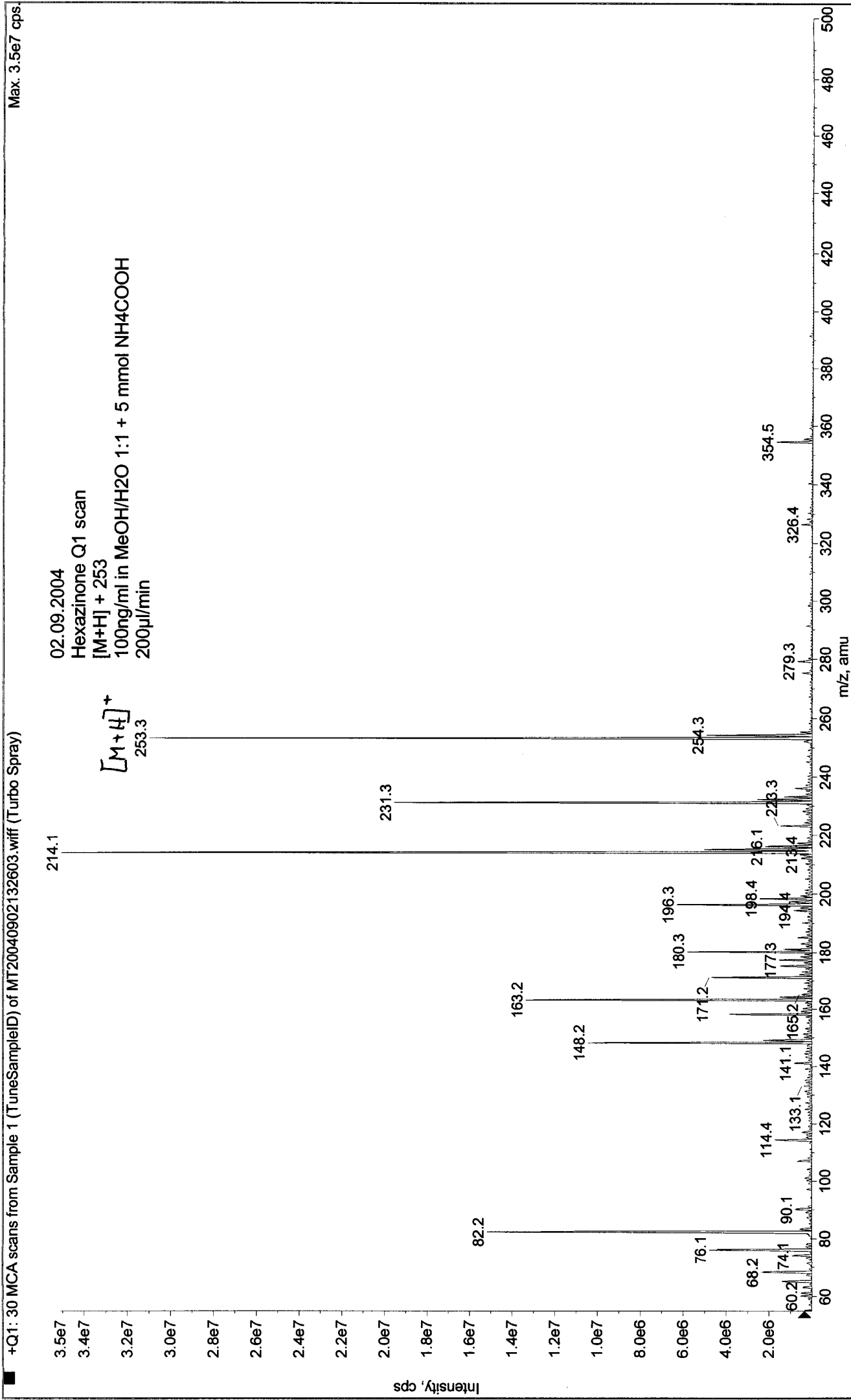
Analyte sensitive parameter set (API 2000)

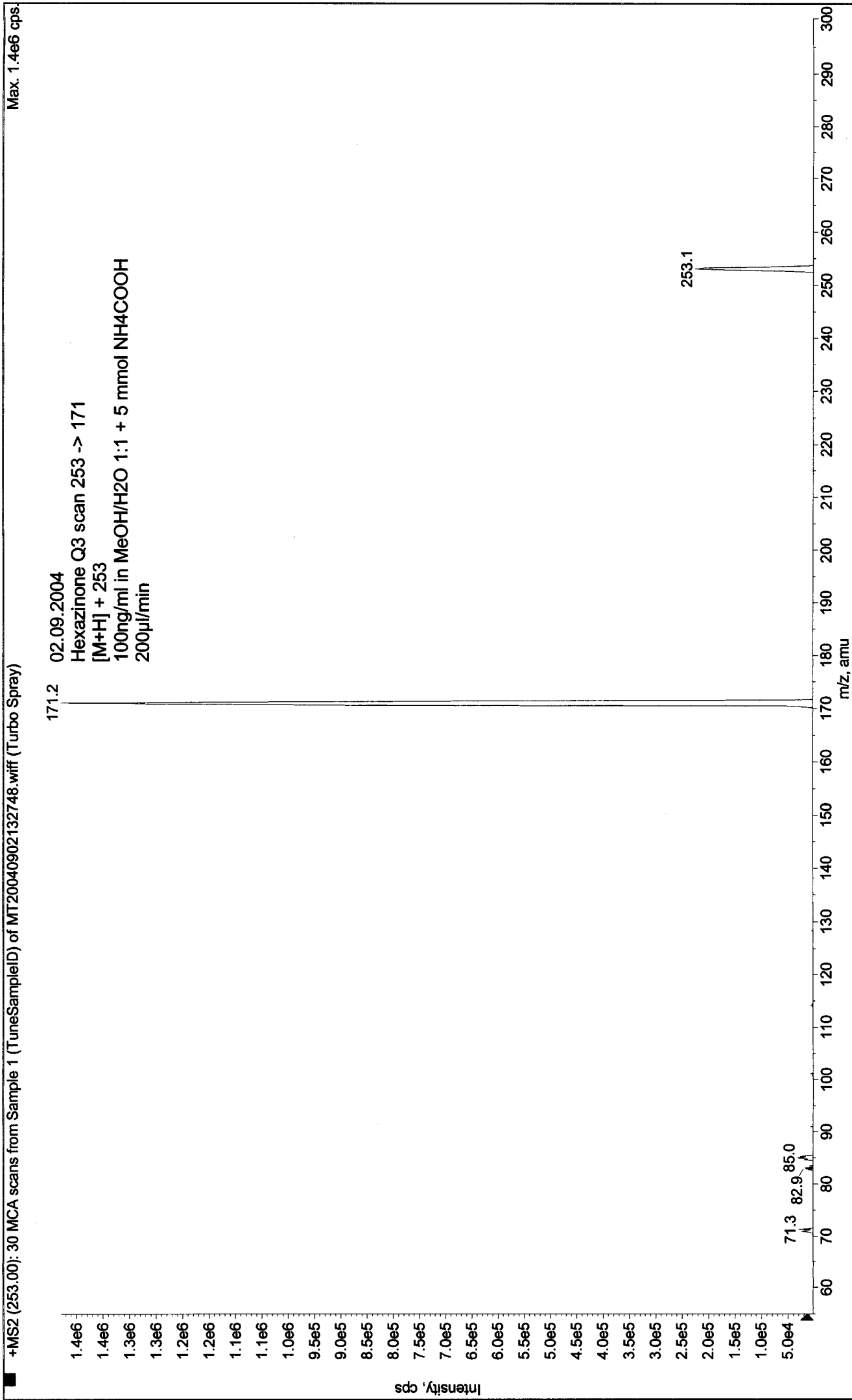
Transition	253,2 → 171,1	253,2 → 71,1
Declustering potential (DP) <sup>*)</sup>	16 V	16 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	10,5 V	11,5 V
Collision cell entrance potential (CEP)	16 V	16 V
Collision energy (CE)	21 V	47 V
Collision cell exit potential (CXP)	8 V	4 V

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

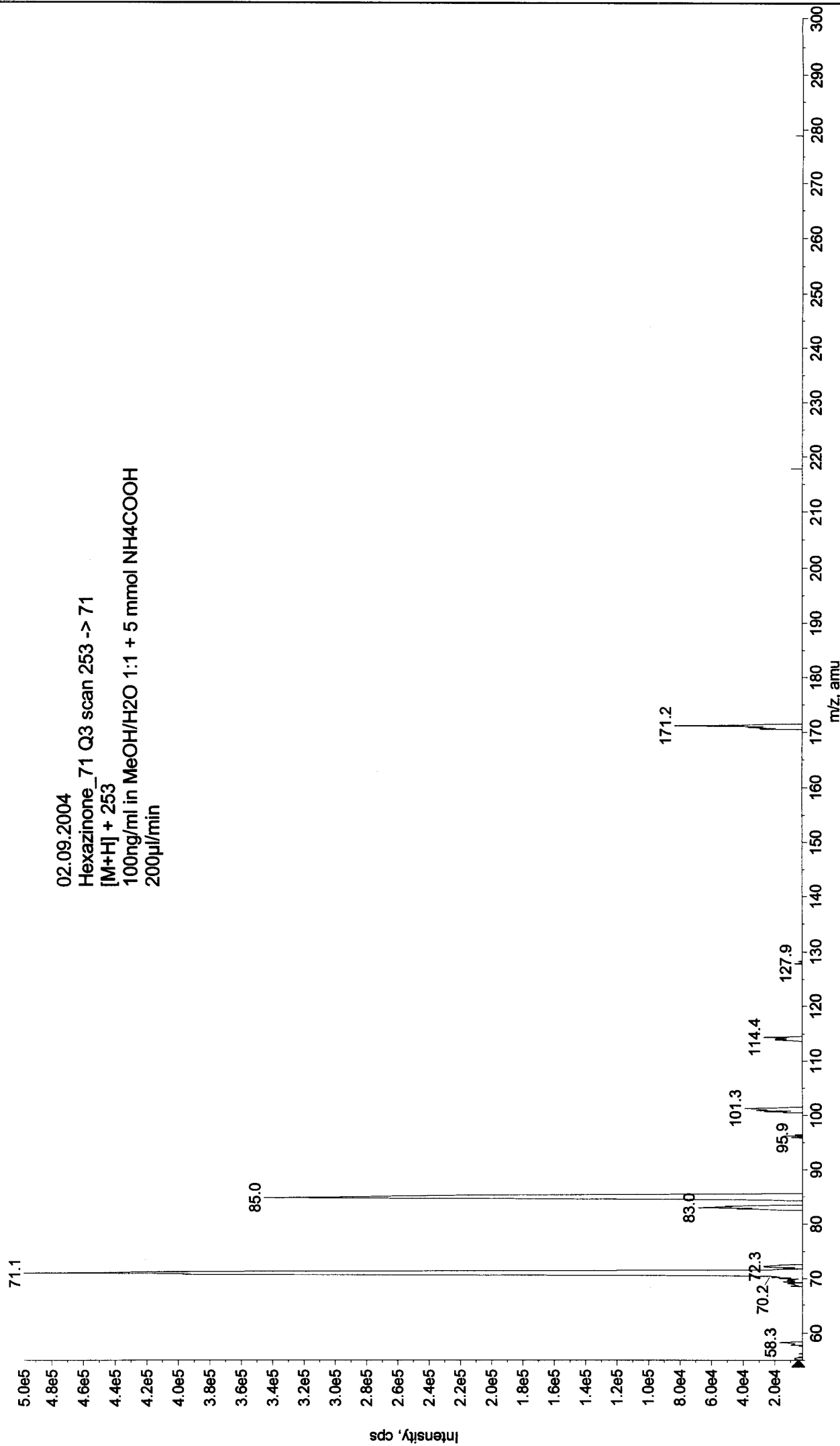
### Fragmentation







+MS2 (253.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040902134304.wiff (Turbo Spray) Max. 5.0e5 cps



02.09.2004  
Hexazinone\_71 Q3 scan 253 -> 71  
[M+H]<sup>+</sup> + 253  
100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5 mmol NH<sub>4</sub>COOH  
200µl/min