

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

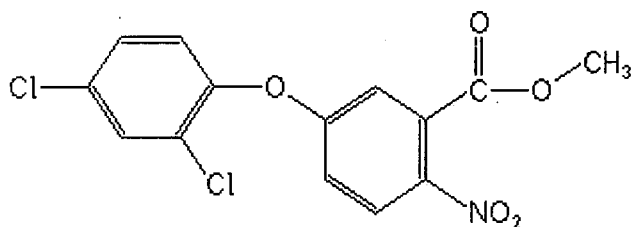
Analyte: Bifenox

CAS No.: 42576-02-3

Formula: C₁₄H₉Cl₂NO₅

Molecular mass (lowest isotopes): 340,99 amu

Structure:



Ionisation: ESI +

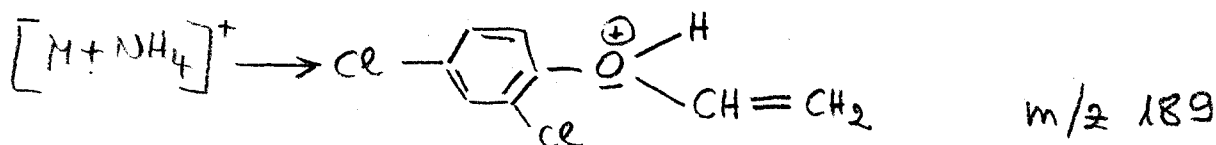
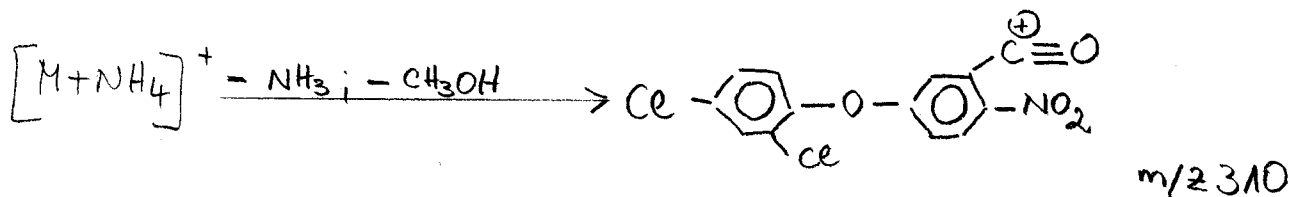
Quasimolecular ion: 358,9 amu = [M+NH₄]⁺

Analyte sensitive parameter set (API 2000)

| Transition | 358,9 → 309,9 | 358,9 → 189,1 |
|---|---------------|---------------|
| Declustering potential (DP) ^{*)} | 4 V | 4 V |
| Focusing potential (FP) | 370 V | 370 V |
| Entrance potential (EP) | 8,0 V | 7,0 V |
| Collision cell entrance potential (CEP) | 24 V | 22 V |
| Collision energy (CE) | 17 V | 35 V |
| Collision cell exit potential (CXP) | 18 V | 10 V |

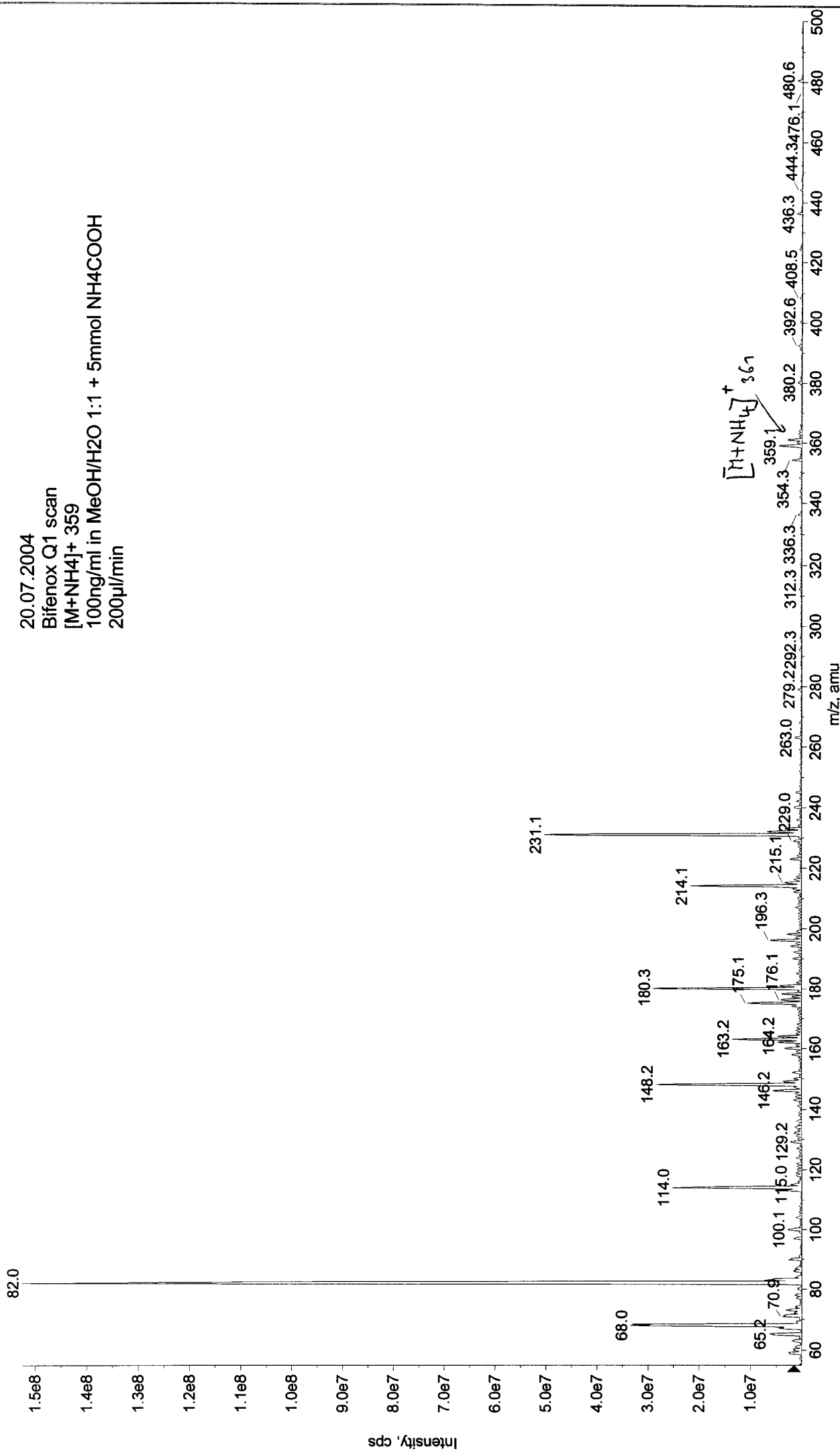
^{*)} For API 3000 and 4000 enhance DP by 20V

Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20040720151128.wiff (Turbo Spray) Max. 1.5e8 cps

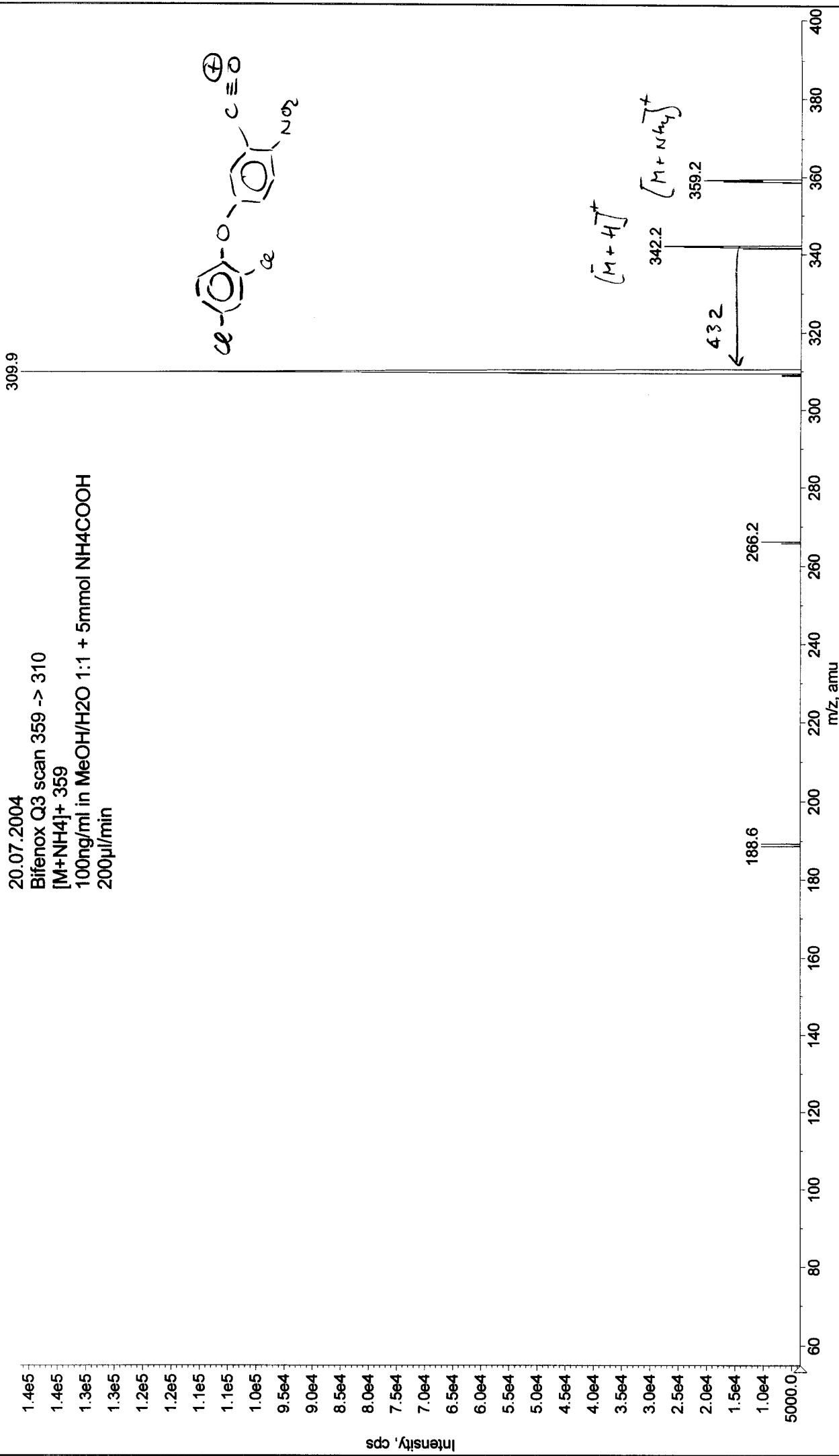
20.07.2004
Bifenox Q1 scan
[M+NH4]⁺ 359
100ng/ml in MeOH/H2O 1:1 + 5mmol NH4COOH
200µl/min



+MS2 (359.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040720151510.wiff (Turbo Spray)

Max. 1.4e5 cps

20.07.2004
Bifenox Q3 scan 359 -> 310
[M+NH4]⁺ 359
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min



Max. 3.8e4 cps.

■ +MS2 (359.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040721105045.wiff (Turbo Spray)

