

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

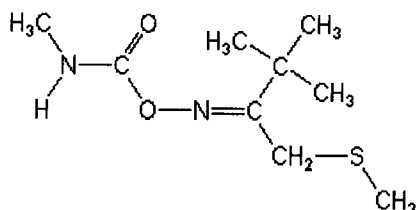
### Analyte: Thiofanox

CAS No.: 39196-18-4

Formula: C<sub>9</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>S

Molecular mass (lowest isotopes): 218,11 amu

Structure:



Ionisation: ESI +

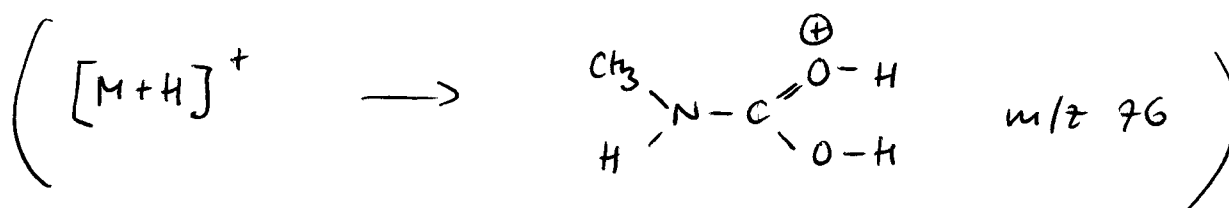
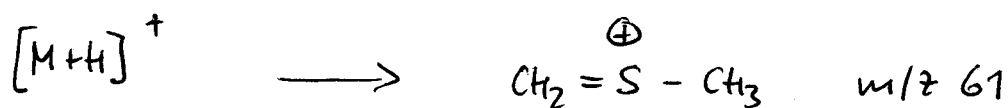
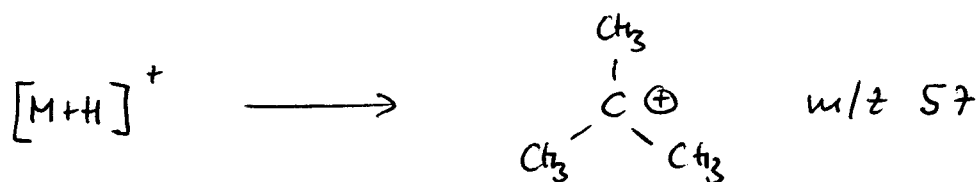
Quasimolecular ion: 219,1 amu = [M+H]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

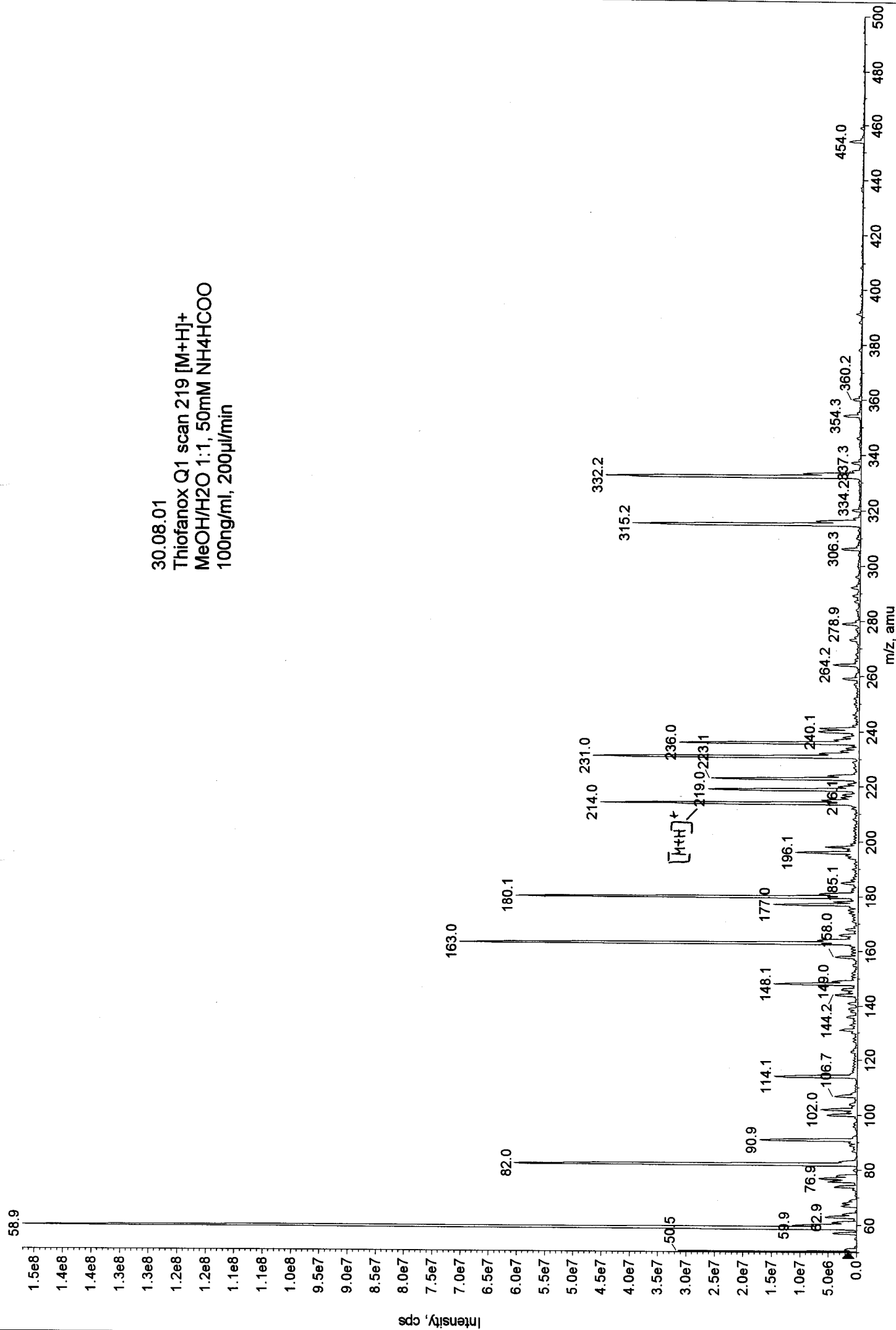
Transition	219,1 → 57,0	219,1 → 60,9
Declustering potential (DP) <sup>*)</sup>	14 V	14 V
Focusing potential (FP)	350 V	360 V
Entrance potential (EP)	9,0 V	9,0 V
Collision cell entrance potential (CEP)	14 V	14 V
Collision energy (CE)	17 V	15 V
Collision cell exit potential (CXP)	8 V	8 V

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

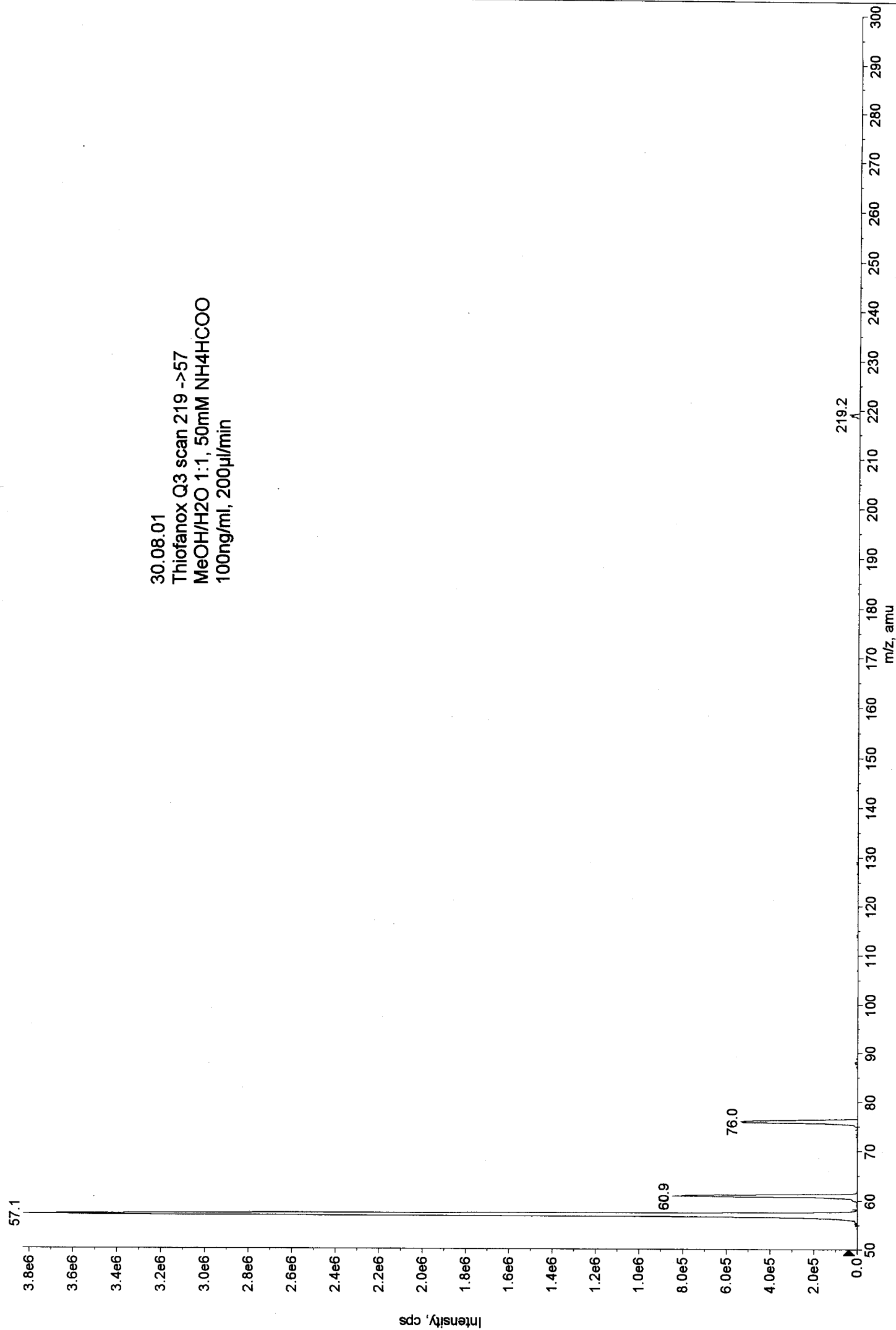
### Fragmentation



30.08.01  
Thiofanox Q1 scan 219 [M+H]<sup>+</sup>  
MeOH/H<sub>2</sub>O 1:1, 50mM NH<sub>4</sub>HCOO  
100ng/ml, 200µl/min



30.08.01  
Thiofanox Q3 scan 219 ->57  
MeOH/H2O 1:1, 50mM NH4HCOO  
100ng/ml, 200µl/min



30.08.01  
Thiofanox61 Q3 scan 219 ->61  
MeOH/H2O 1:1, 50mM NH4HCOO  
100ng/ml, 200µl/min

