

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

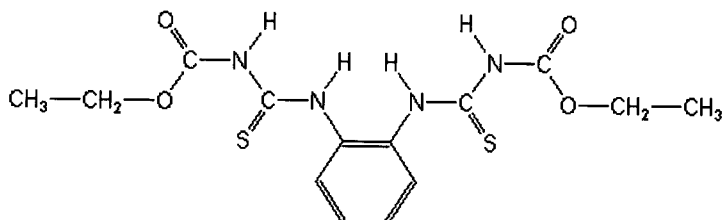
Analyte: Thiophanate (-ethyl)

CAS No.: 23564-06-9

Formula: C₁₄H₁₈N₄O₄S₂

Molecular mass (lowest isotopes): 370,08 amu

Structure:



Ionisation: ESI +

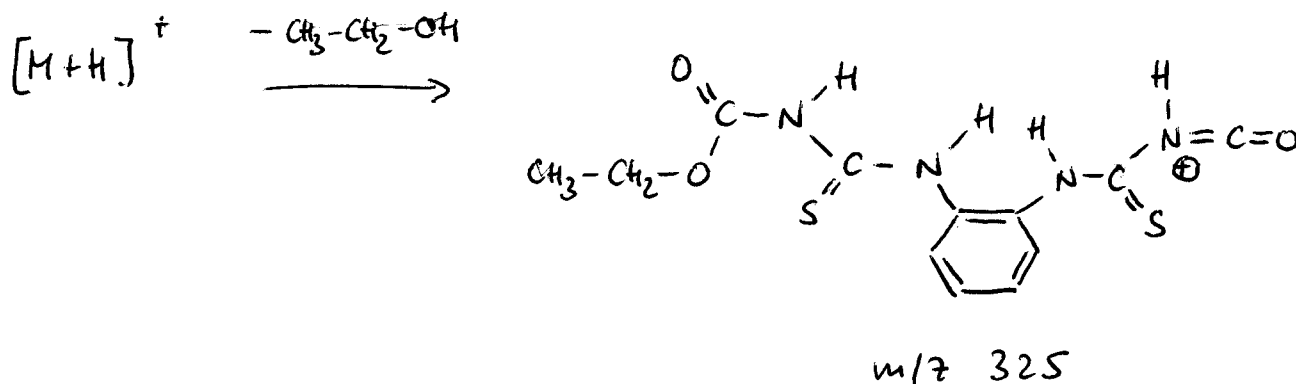
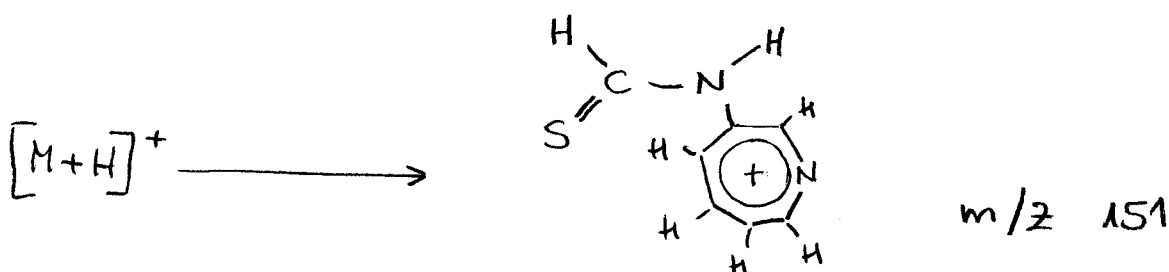
Quasimolecular ion: 371,1 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	371,1 → 151,0	371,1 → 325,1
Declustering potential (DP)*)	41 V	41 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	10,0 V	9,5 V
Collision cell entrance potential (CEP)	22 V	26 V
Collision energy (CE)	27 V	17 V
Collision cell exit potential (CXP)	8 V	18 V

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

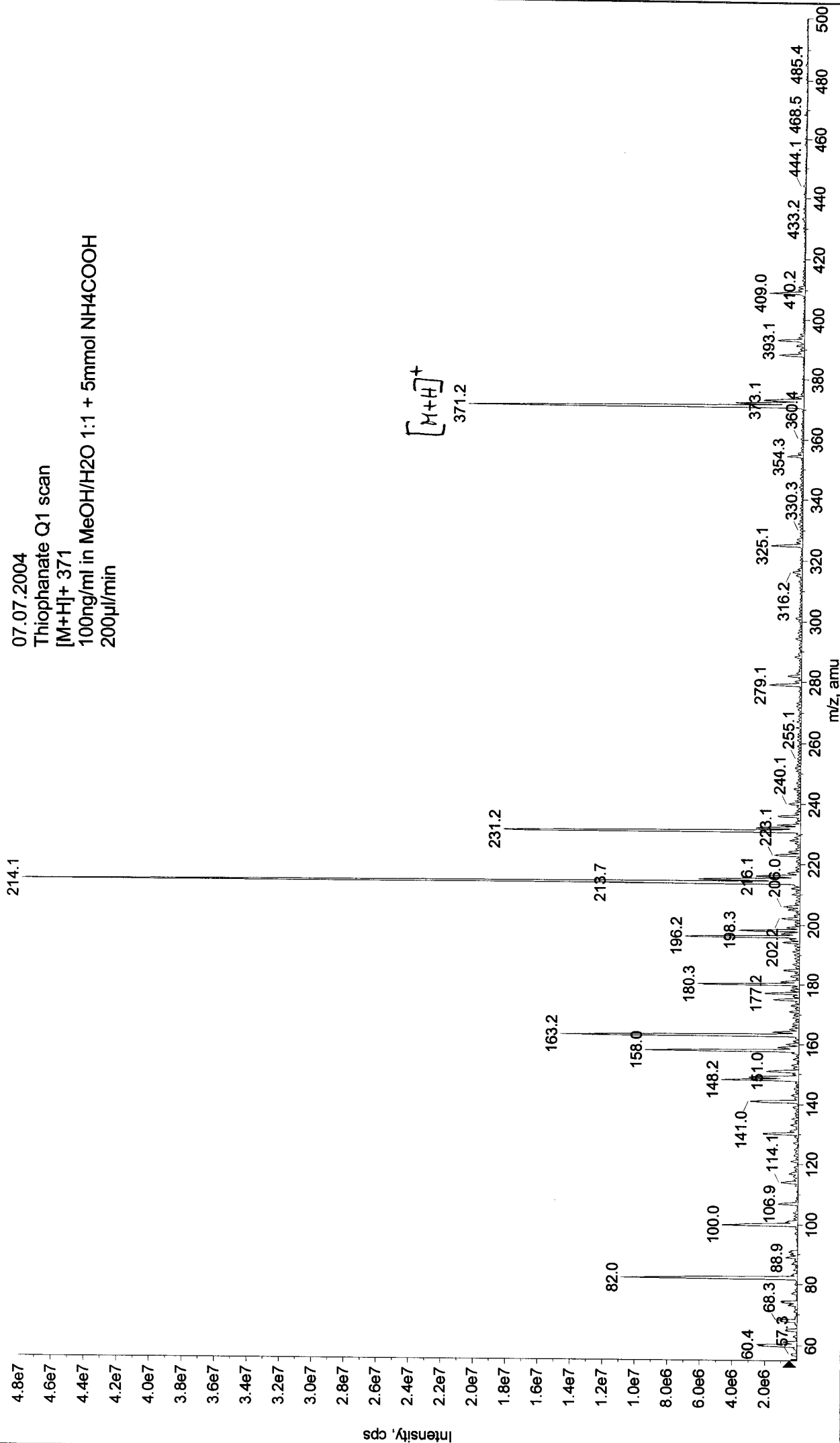
Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20040707083210.wiff (Turbo Spray)

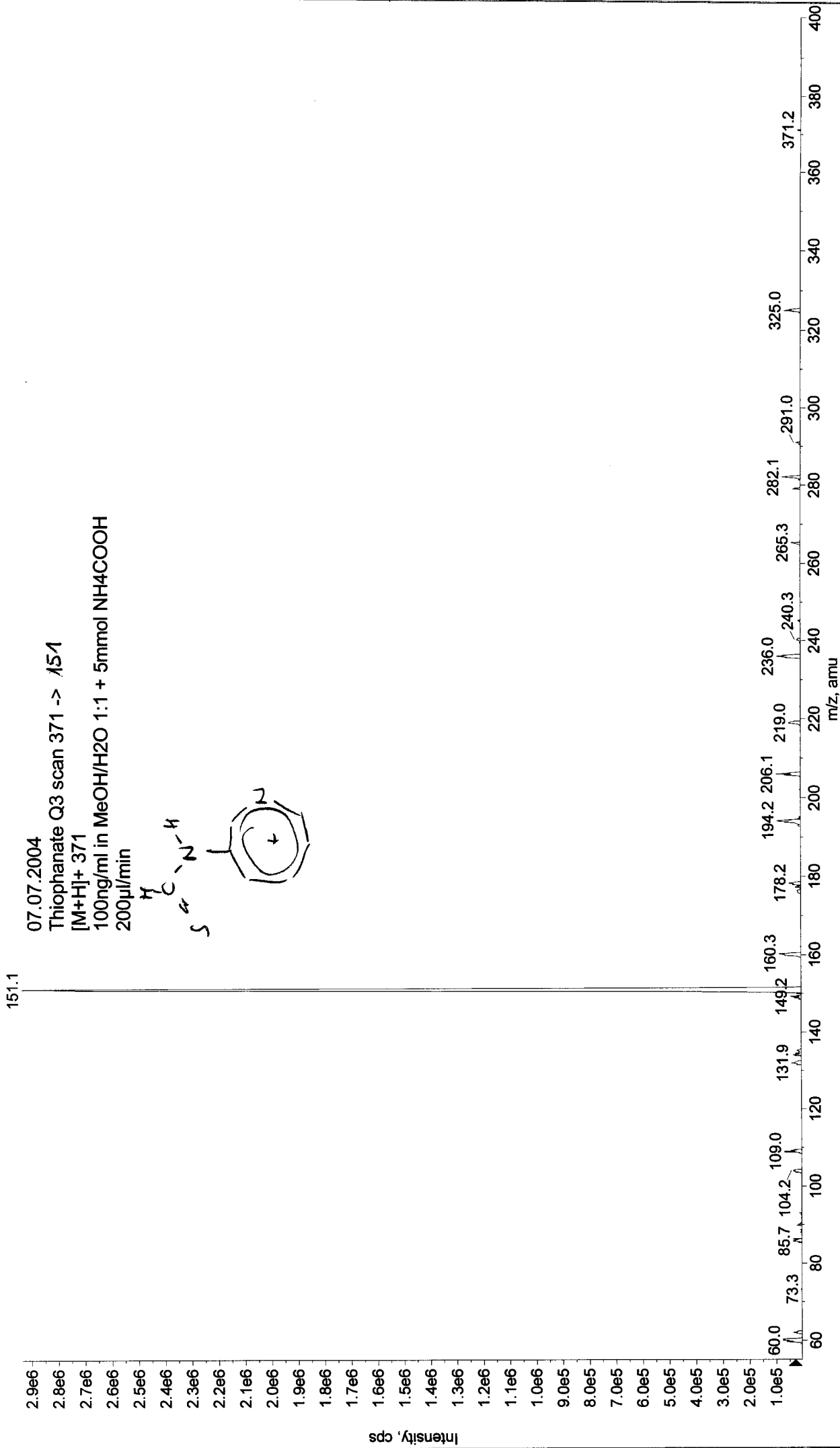
Max. 4.8e7 cps.

07.07.2004
Thiophanate Q1 scan
[M+H]⁺ 371
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min



Max. 2.9e6 cps.

+MS2 (371.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040707083930.wiff (Turbo Spray)



+MS2 (371.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040707084839.wiff (Turbo Spray) Max. 8.4e5 cps

