

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

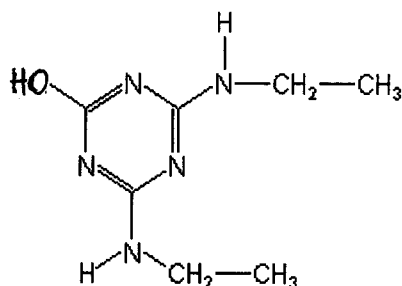
Analyte: Simazine-2-hydroxy

CAS No.: 2599-11-3

Formula: C₇H₁₃N₅O

Molecular mass (lowest isotopes): 183,11 amu

Structure:



Ionisation: ESI +

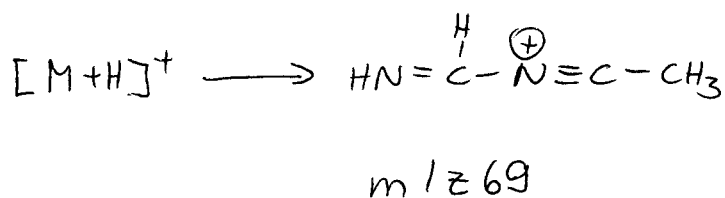
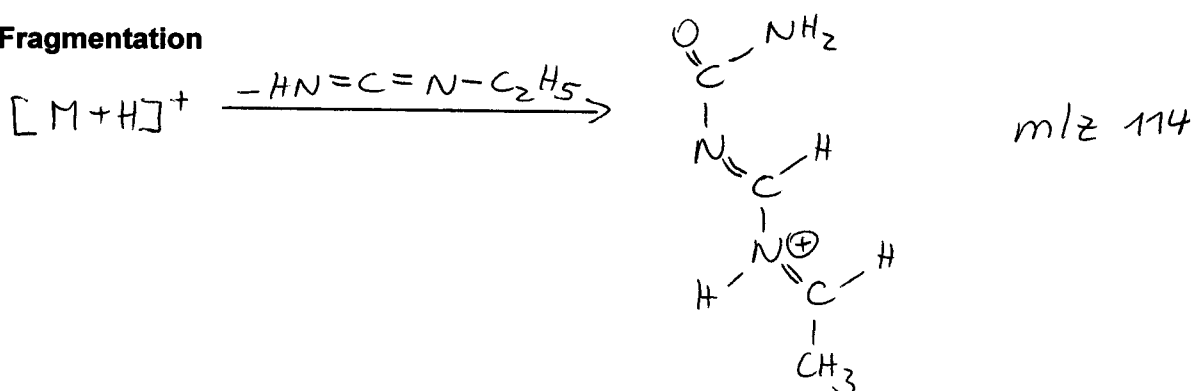
Quasimolecular ion: 184,1 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	184,1 → 69,0	184,1 → 114,1
Declustering potential (DP) ^{*)}	46V	46 V
Focusing potential (FP)	360 V	370 V
Entrance potential (EP)	10,5 V	11 V
Collision cell entrance potential (CEP)	19 V	12 V
Collision energy (CE)	59 V	27 V
Collision cell exit potential (CXP)	6 V	6 V

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

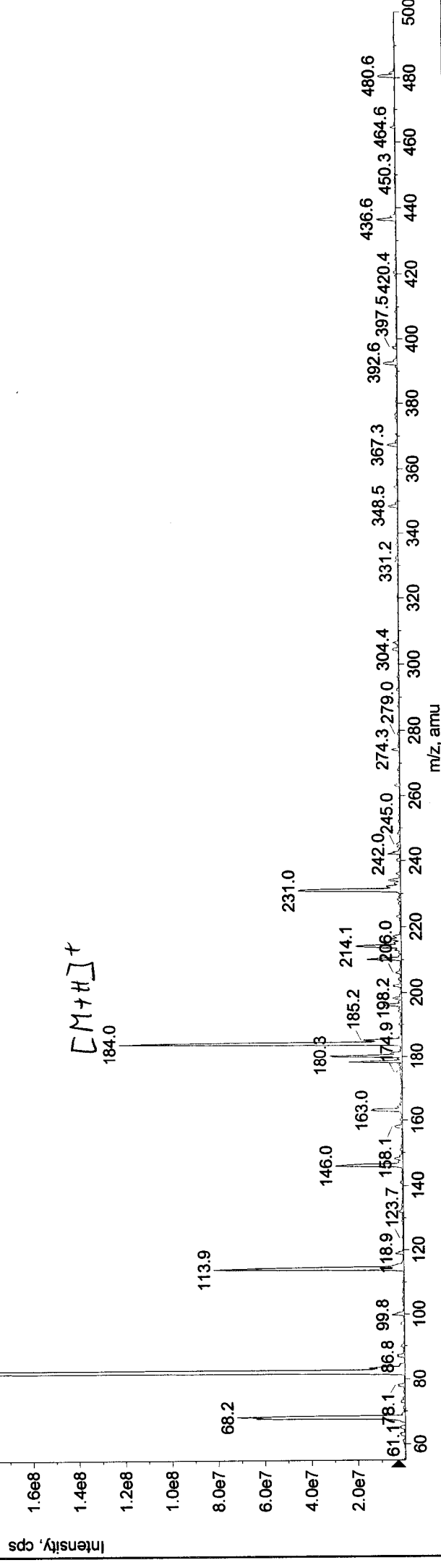
Fragmentation

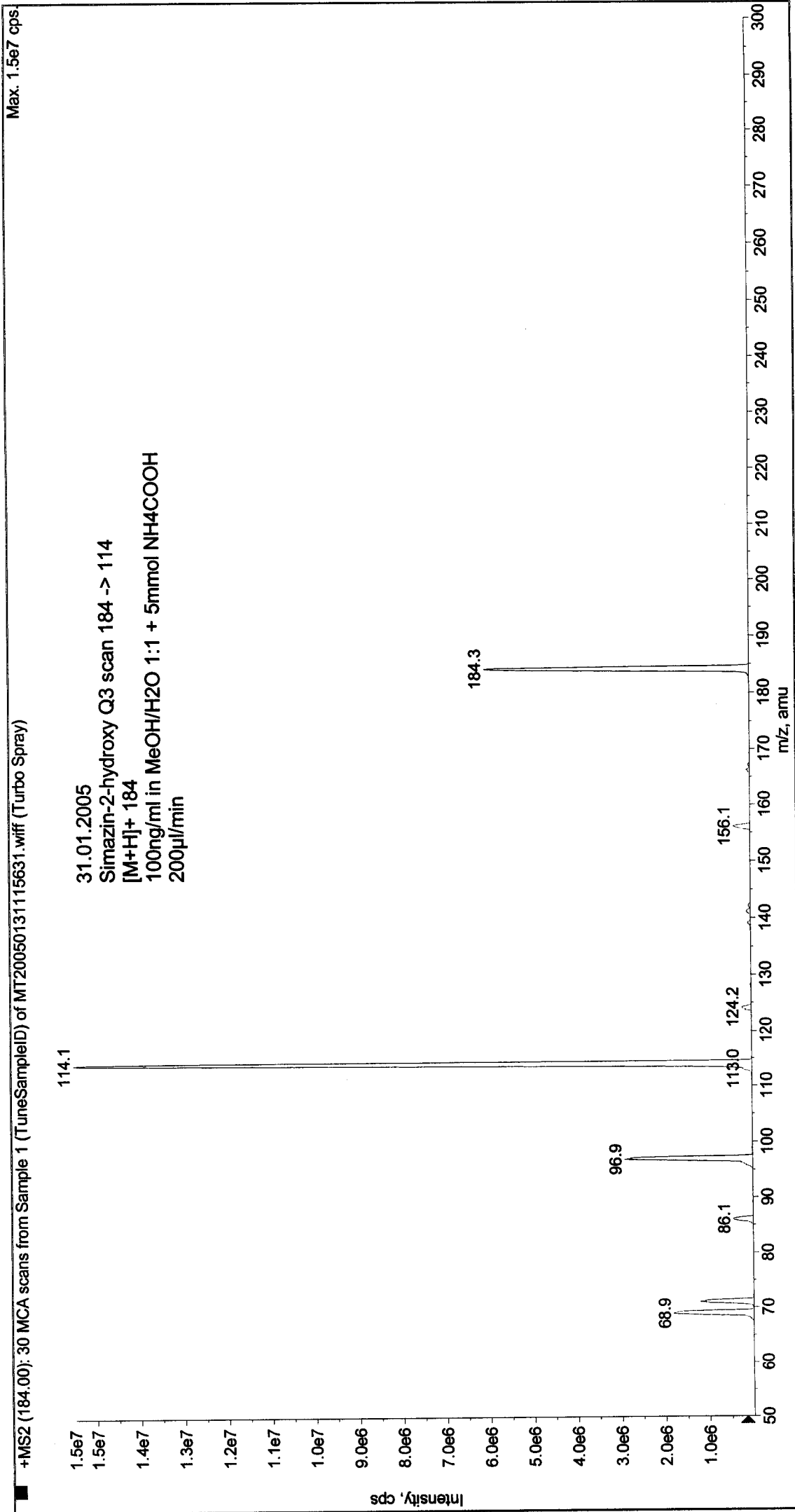


Max. 3.0e8 cps

+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20050131115354.wiff (Turbo Spray)

31.01.2005
Simazin-2-hydroxy Q1 scan
[M+H]⁺ 184
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min





Printing Time: 12:05:22
Printing Date: Monday, January 31, 2005

Acq. Time: 12:04
Acq. Date: Monday, January 31, 2005
Acq. File: MT20050131120411.wiff

Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat

