

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

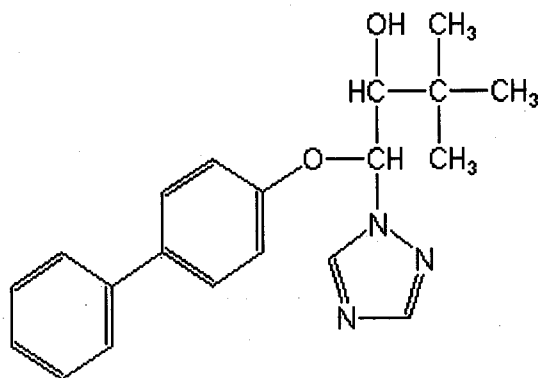
Analyte: Bitertanol

CAS No.: 55179-31-2

Formula: C₂₀H₂₃N₃O₂

Molecular mass (lowest isotopes): 337,18 amu

Structure:



Ionisation: ESI +

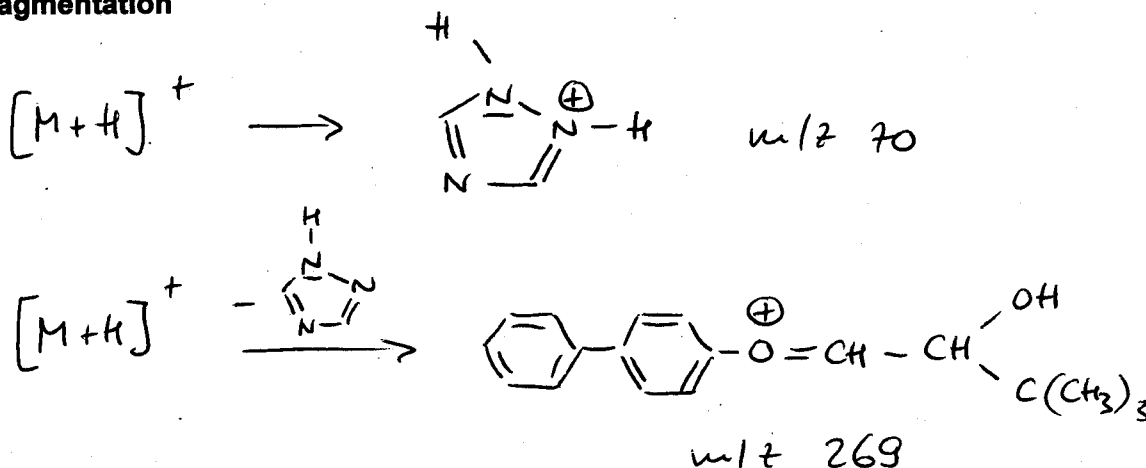
Quasimolecular ion: 338,2 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

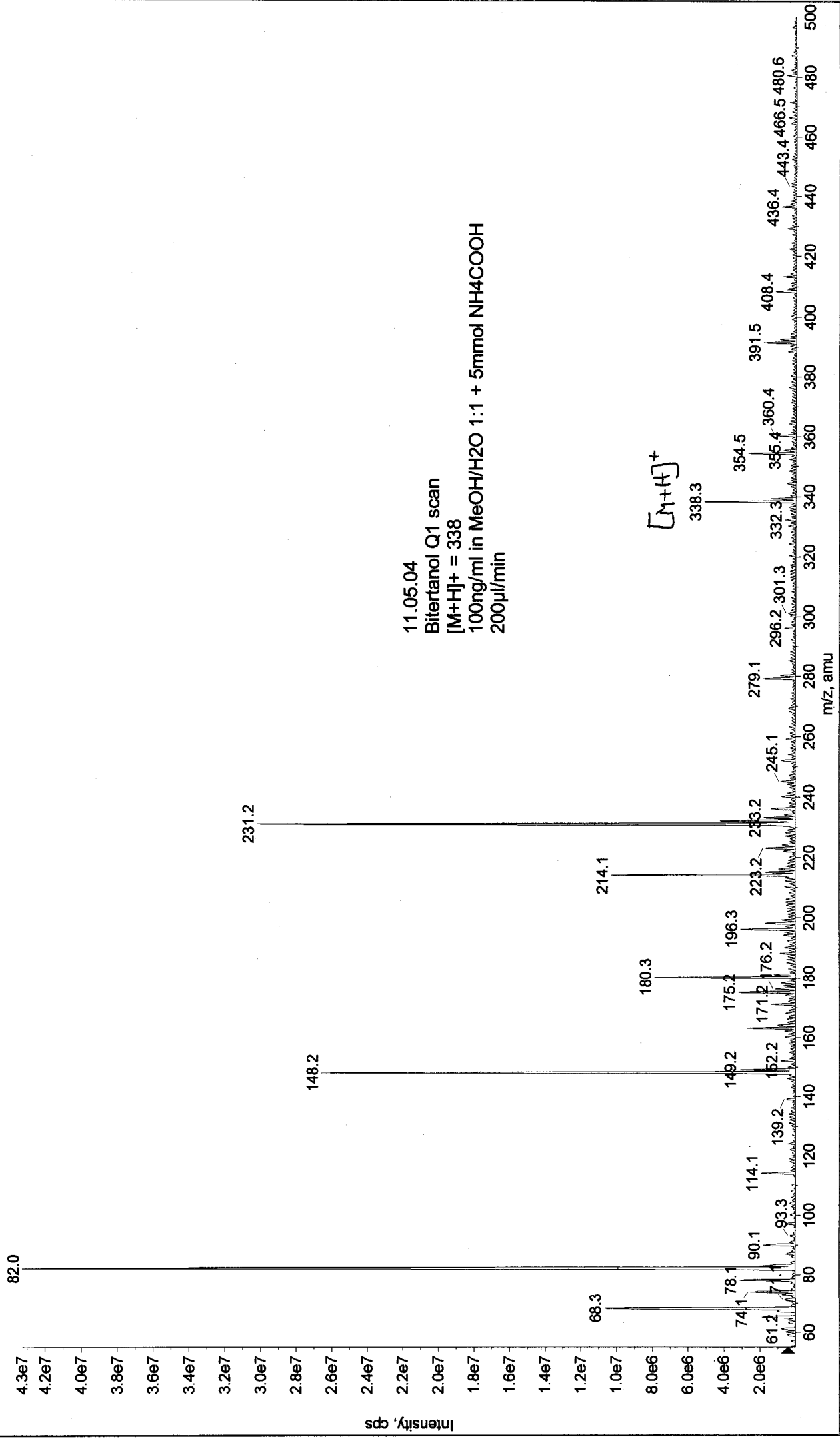
Transition	338,2 → 70,0	338,2 → 269,2
Declustering potential (DP) ^{*)}	1 V	1 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	8,5 V	8,5 V
Collision cell entrance potential (CEP)	20 V	22 V
Collision energy (CE)	25 V	15 V
Collision cell exit potential (CXP)	10 V	14 V

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

Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20040511090434.wiff (Turbo Spray)



11.05.04
 Bitertanol Q1 scan
 $[M+H]^+ = 338$
 100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
 200µl/min

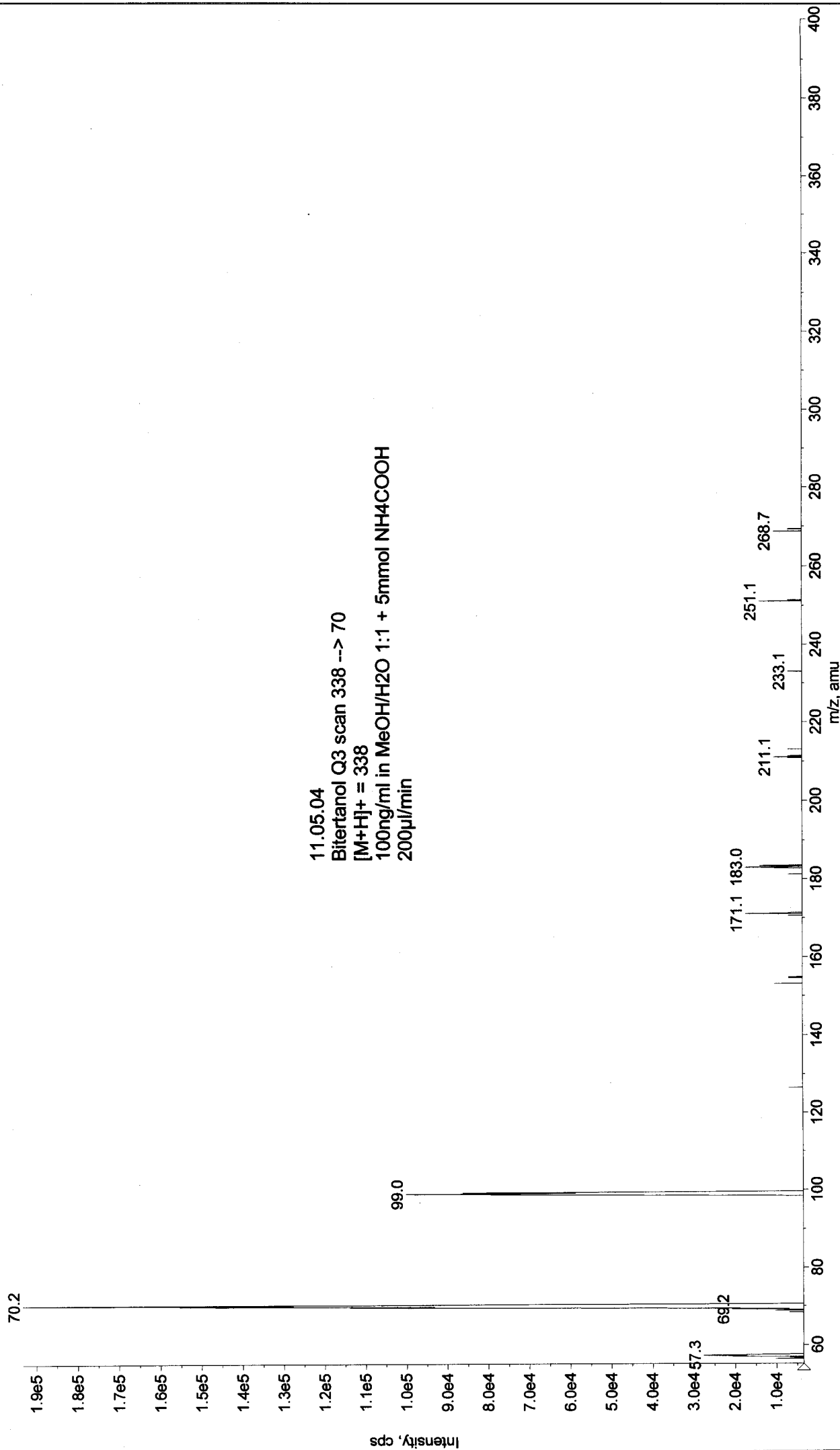
Printing Time: 9:27:45
Printing Date: Tuesday, May 11, 2004

Acq Time: 09:14
Acq Date: Tuesday, May 11, 2004
Acq File: MT20040511091440.wiff

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

Max. 1.9e5 cps

■ +MS2 (338.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040511091440.wiff (Turbo Spray)



Printing Time: 11:05:12
Printing Date: Tuesday, May 11, 2004

Acq. Time: 11:03
Acq. Date: Tuesday, May 11, 2004
Acq. File: MT20040511110324.wiff

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

