

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

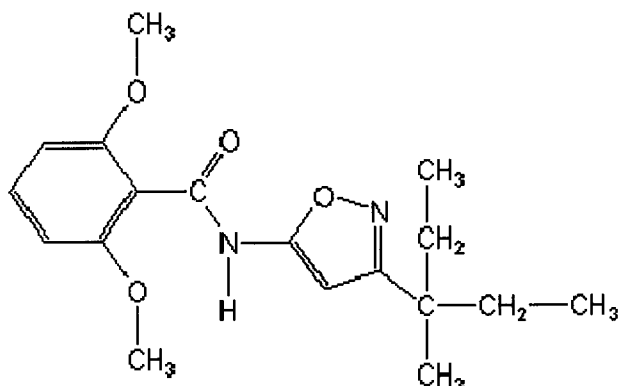
### Analyte: Isoxaben

CAS No.: 82558-50-7

Formula: C<sub>18</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>

Molecular mass (lowest isotopes): 332,17 amu

Structure:



Ionisation: ESI +

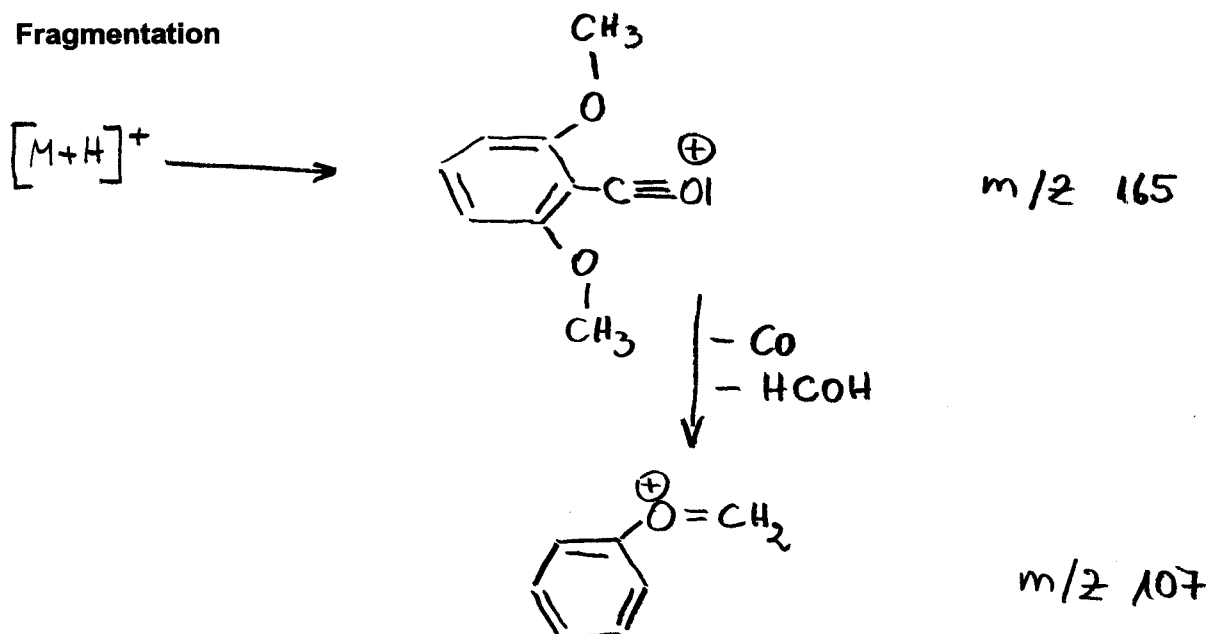
Quasimolecular ion: 333,2 amu = [M+H]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	333,2 → 165,1	333,2 → 107,0
Declustering potential (DP) <sup>*)</sup>	51 V	51 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	10,0 V	12,0 V
Collision cell entrance potential (CEP)	22 V	20 V
Collision energy (CE)	25 V	79 V
Collision cell exit potential (CXP)	8 V	6 V

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

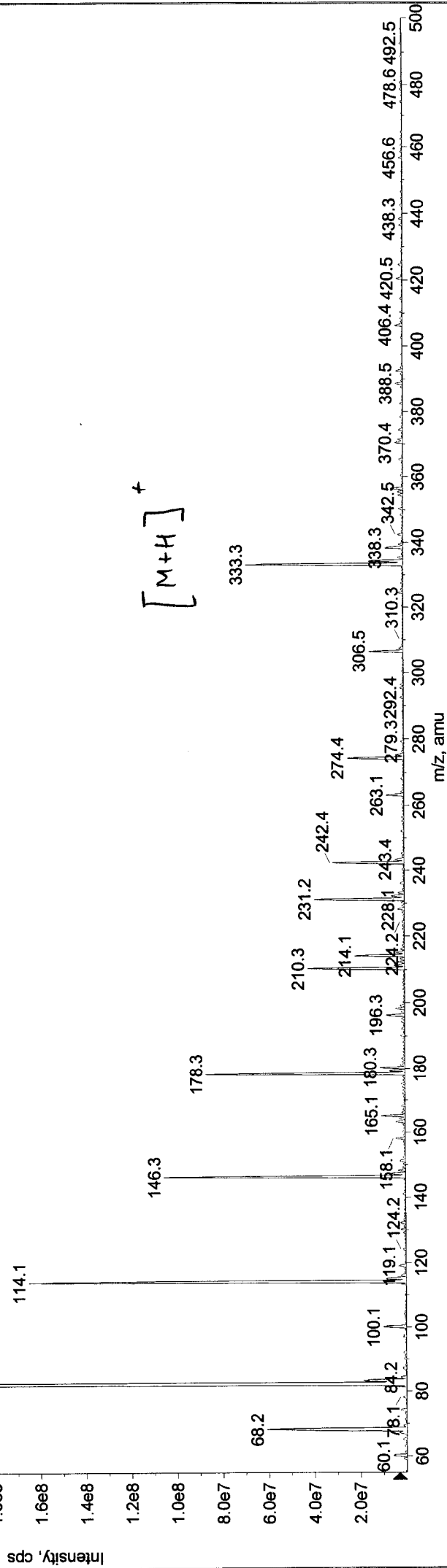
### Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060830140253.wiff (Turbo Spray)

Max. 3.1e8 cps

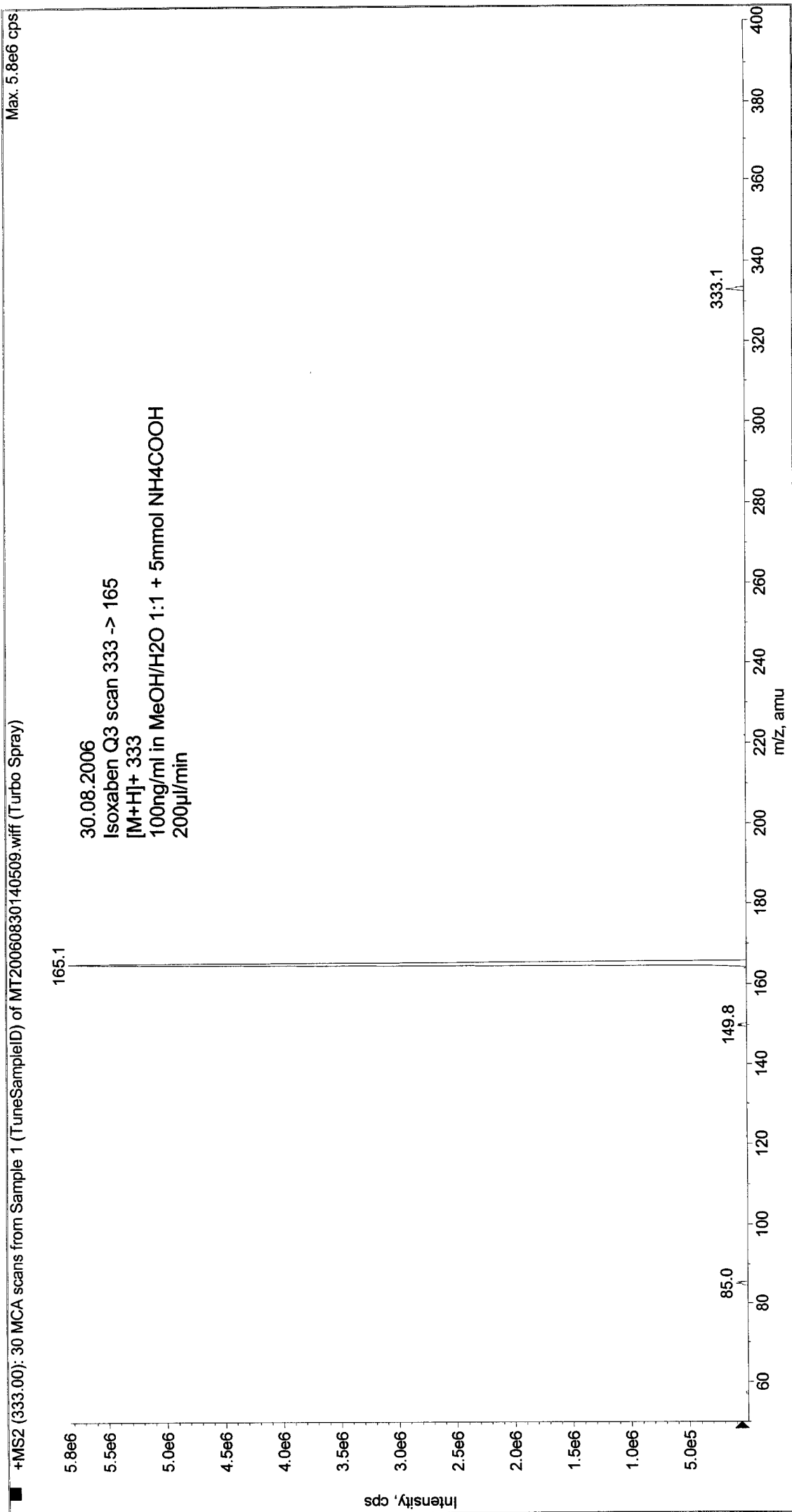
30.08.2006  
Isoxaben Q1 scan  
[M+H]<sup>+</sup> 333  
100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
200µl/min



Printing Time: 14:06:19  
Printing Date: Wednesday, August 30, 2006

Acq Time: 14:05  
Acq. Date: Wednesday, August 30, 2006  
Acq. File: MT20060830140509.wiff

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



Printing Time: 14:12:54  
Printing Date: Wednesday, August 30, 2006

Acq Time: 14:11  
Acq. Date: Wednesday, August 30, 2006  
Acq. File: MT20060830141136.wiff

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

