

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

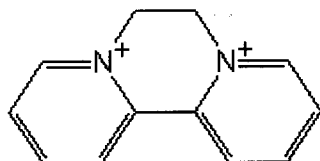
Analyte: Diquat

CAS No.: 2764-72-9

Formula: C₁₂H₁₂N₂

Molecular mass (lowest isotopes): 184,10 amu

Structure:



Ionisation: ESI +

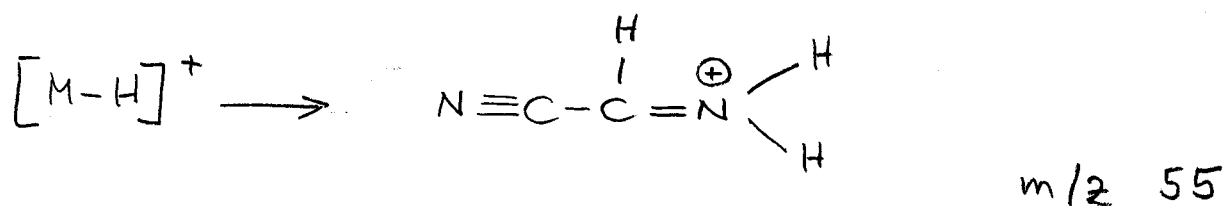
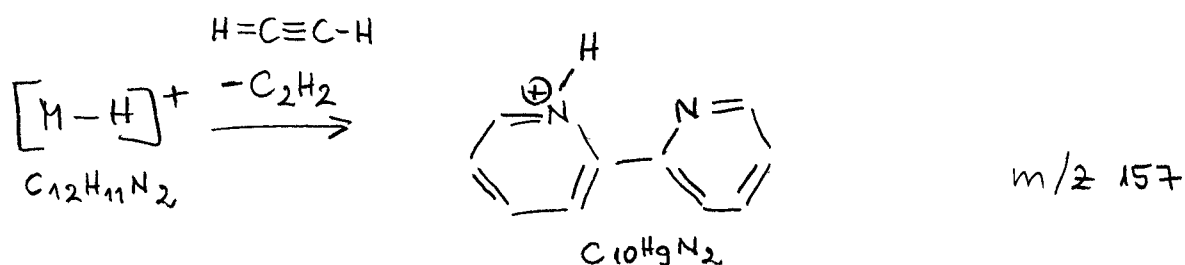
Quasimolecular ion: 183,1 amu = [M-H]⁺

Analyte sensitive parameter set (API 2000)

Transition	183,1 → 157,1	183,1 → 55,1
Declustering potential (DP) ^{*)}	9 V	9 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	12,0 V	10,5 V
Collision cell entrance potential (CEP)	12 V	12 V
Collision energy (CE)	31 V	13 V
Collision cell exit potential (CXP)	8 V	8 V

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

Fragmentation



Printing Time: 14:34:08

Printing Date: Monday, April 10, 2006

Acq. Time: 14:30

Acq. Date: Monday, April 10, 2006

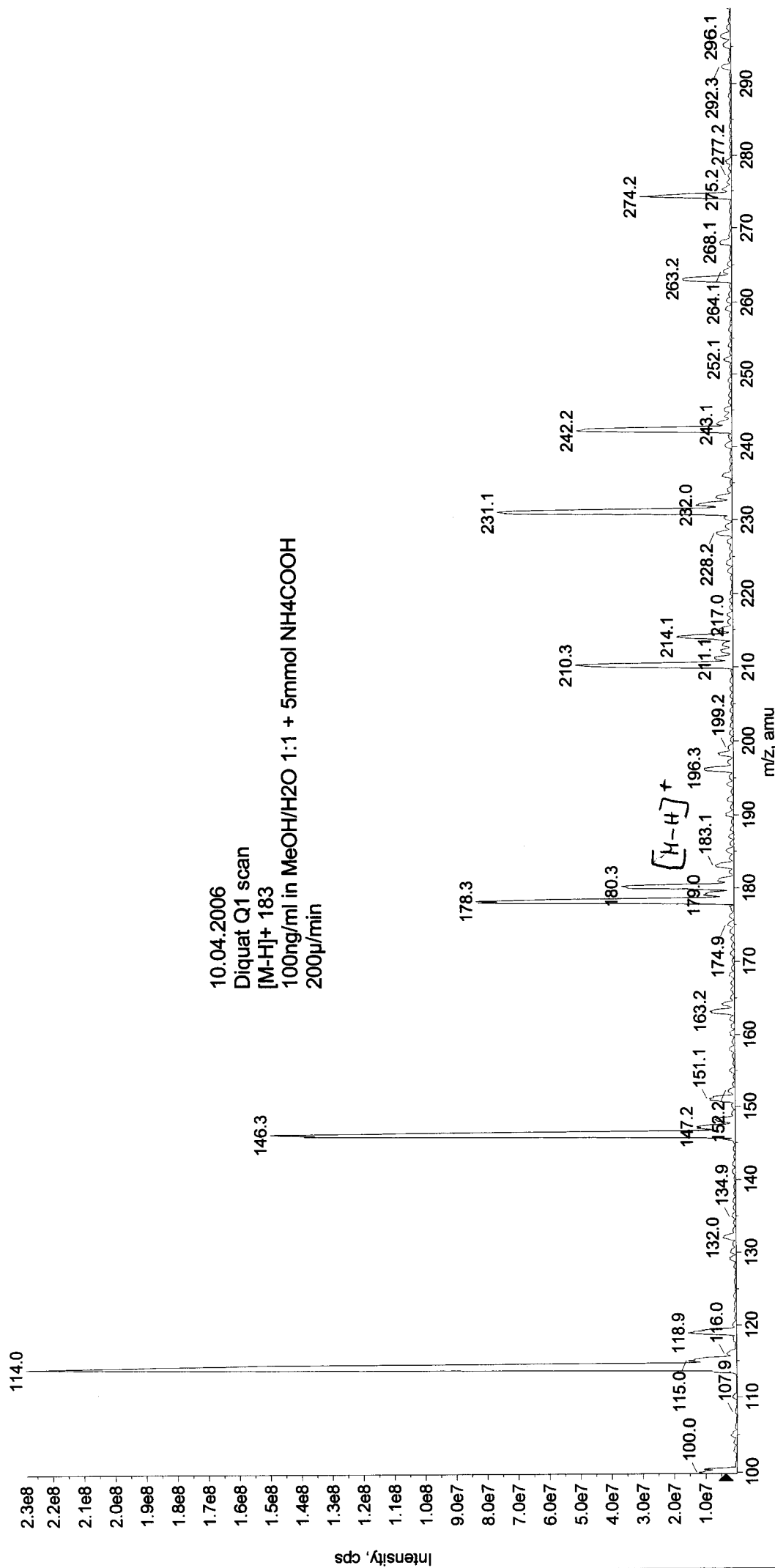
Acq. File: MT20060410143034.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat

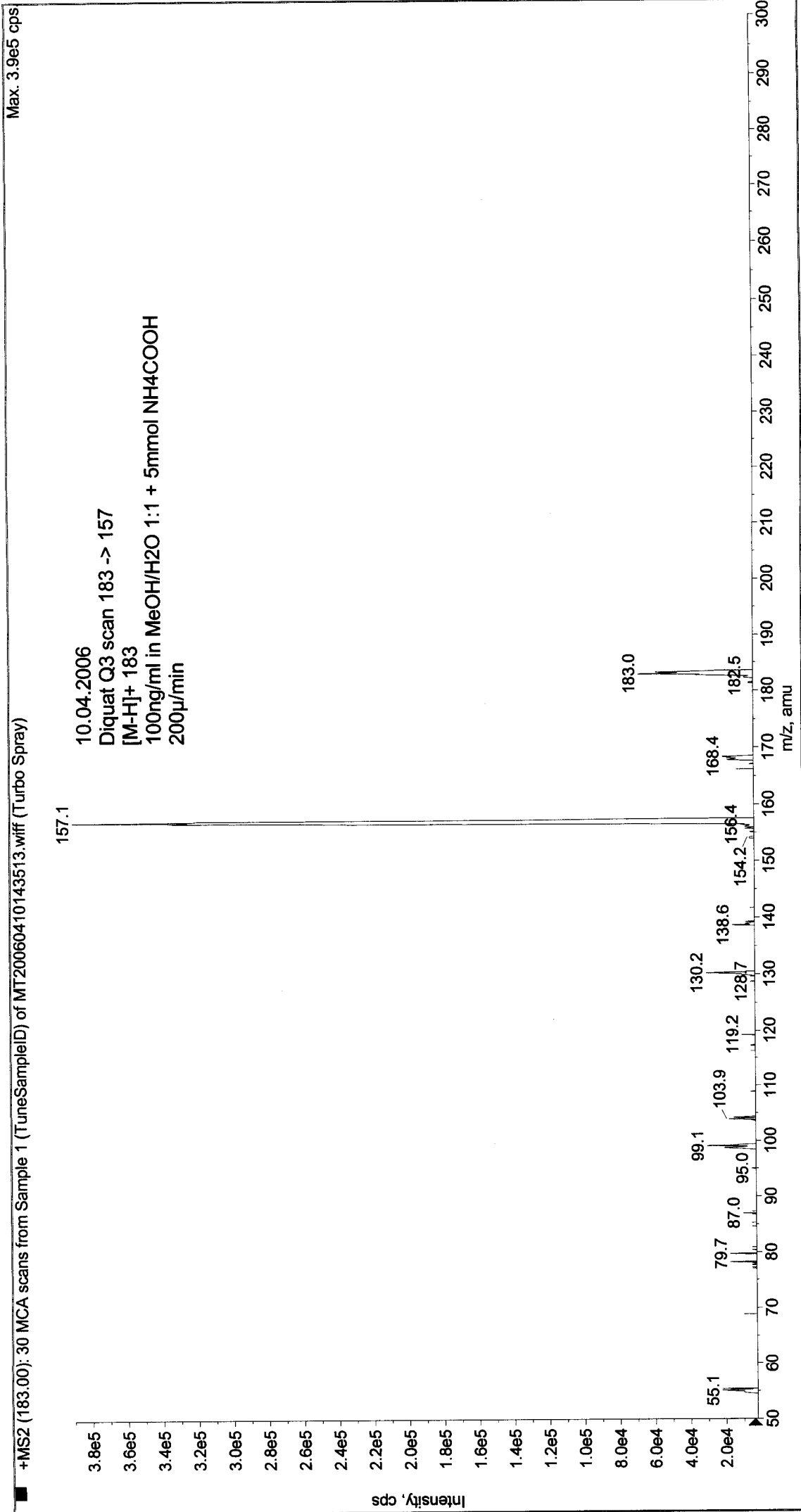
+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060410143034.wiff (Turbo Spray) Max. 3.5e8 cps



Printing Time: 14:36:34
Printing Date: Monday, April 10, 2006

Acq. Time: 14:35
Acq. Date: Monday, April 10, 2006
Acq. File: MT20060410143513.wiff

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



Printing Time: 14:50:38

Printing Date: Monday, April 10, 2006

Acq. Time: 14:49

Acq. Date: Monday, April 10, 2006

Acq. File: MT20060410144925.wiff

Sample Comment:

Sample Name: TuneSampleID

Batch Name: ManualTune.bat

Max. 4.3e5 cps

+MS2 (183.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060410144925.wiff (Turbo Spray)

