

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

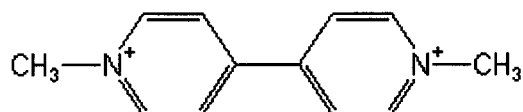
Analyte: Paraquat

CAS No.: 4685-14-7

Formula: C₁₂H₁₄N₂

Molecular mass (lowest isotopes): 186,115 amu

Structure:



Ionisation: ESI +

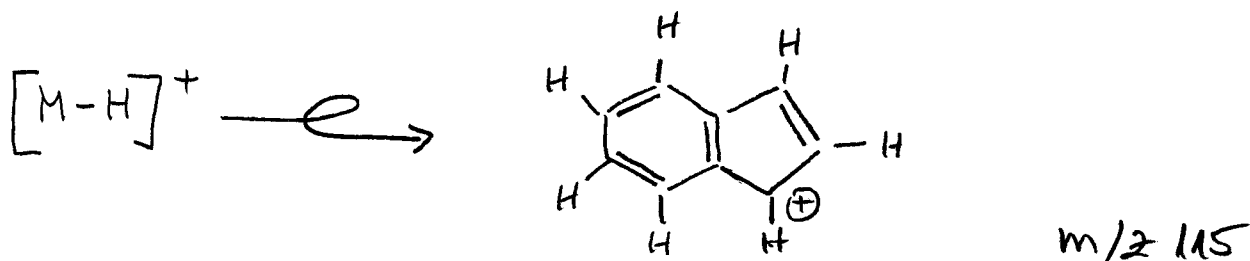
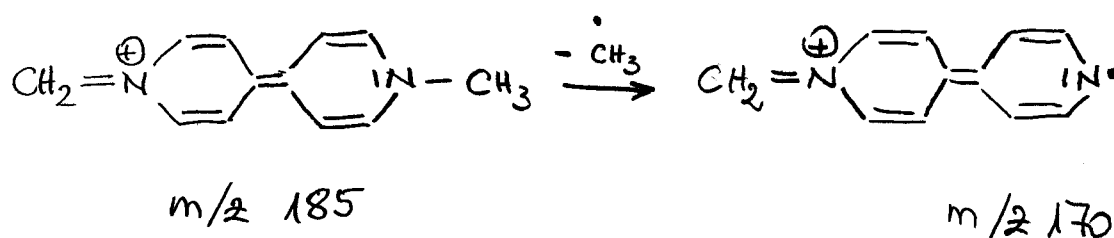
Quasimolecular ion: 185,1 amu = [M-H]⁺

Analyte sensitive parameter set (API 2000)

Transition	185,1 → 170,0	185,1 → 115,0
Declustering potential (DP) ^{*)}	94 V	94 V
Focusing potential (FP)	360 V	370 V
Entrance potential (EP)	10,5 V	11,0 V
Collision cell entrance potential (CEP)	16 V	12 V
Collision energy (CE)	27 V	57 V
Collision cell exit potential (CXP)	8 V	6 V

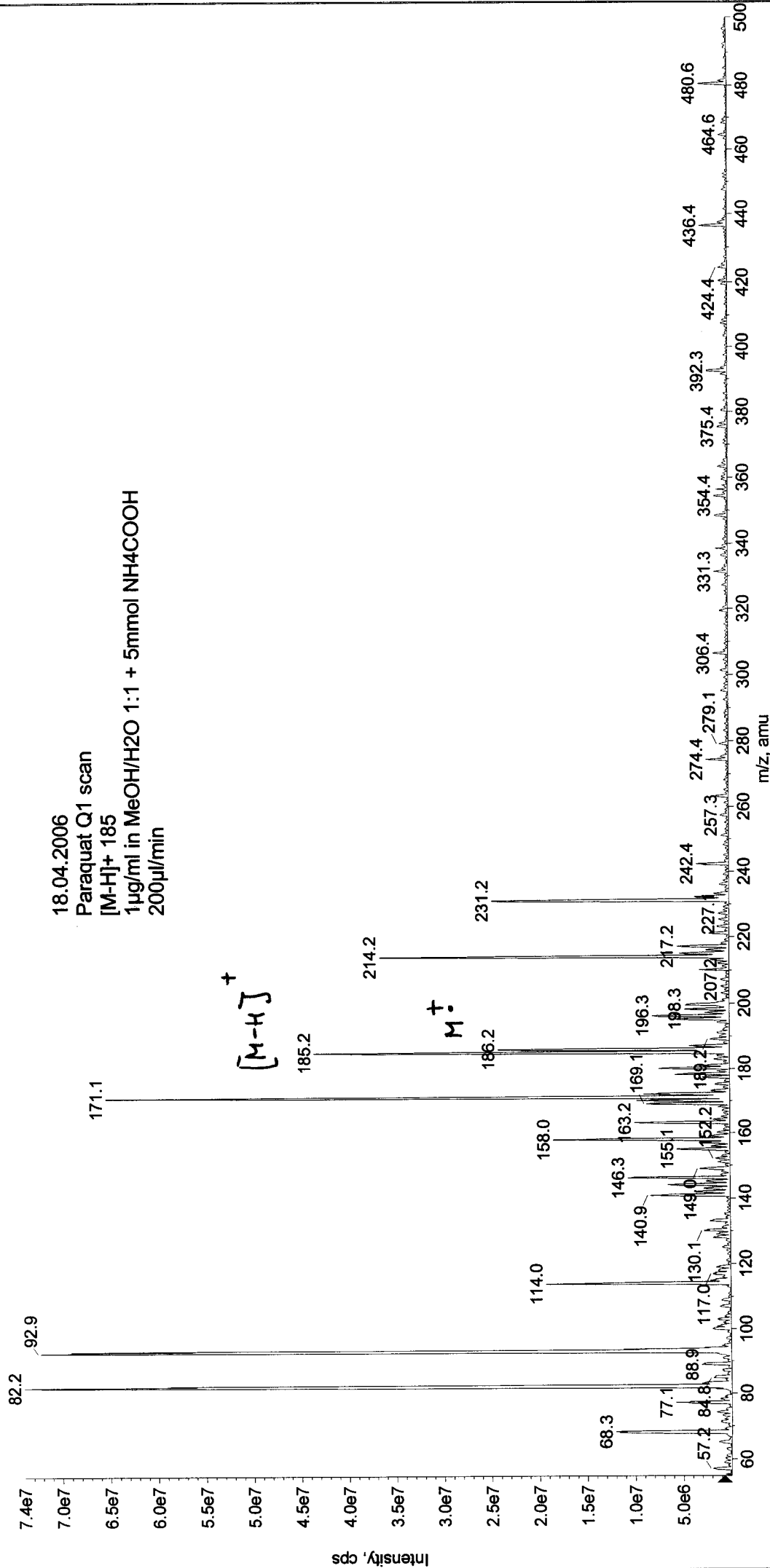
^{*)} For API 3000 and 4000 enhance DP by 20V

Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060418122338.wiff (Turbo Spray)

Max. 7.4e7 cps



Printing Time: 11:25:46
Printing Date: Tuesday, April 18, 2006

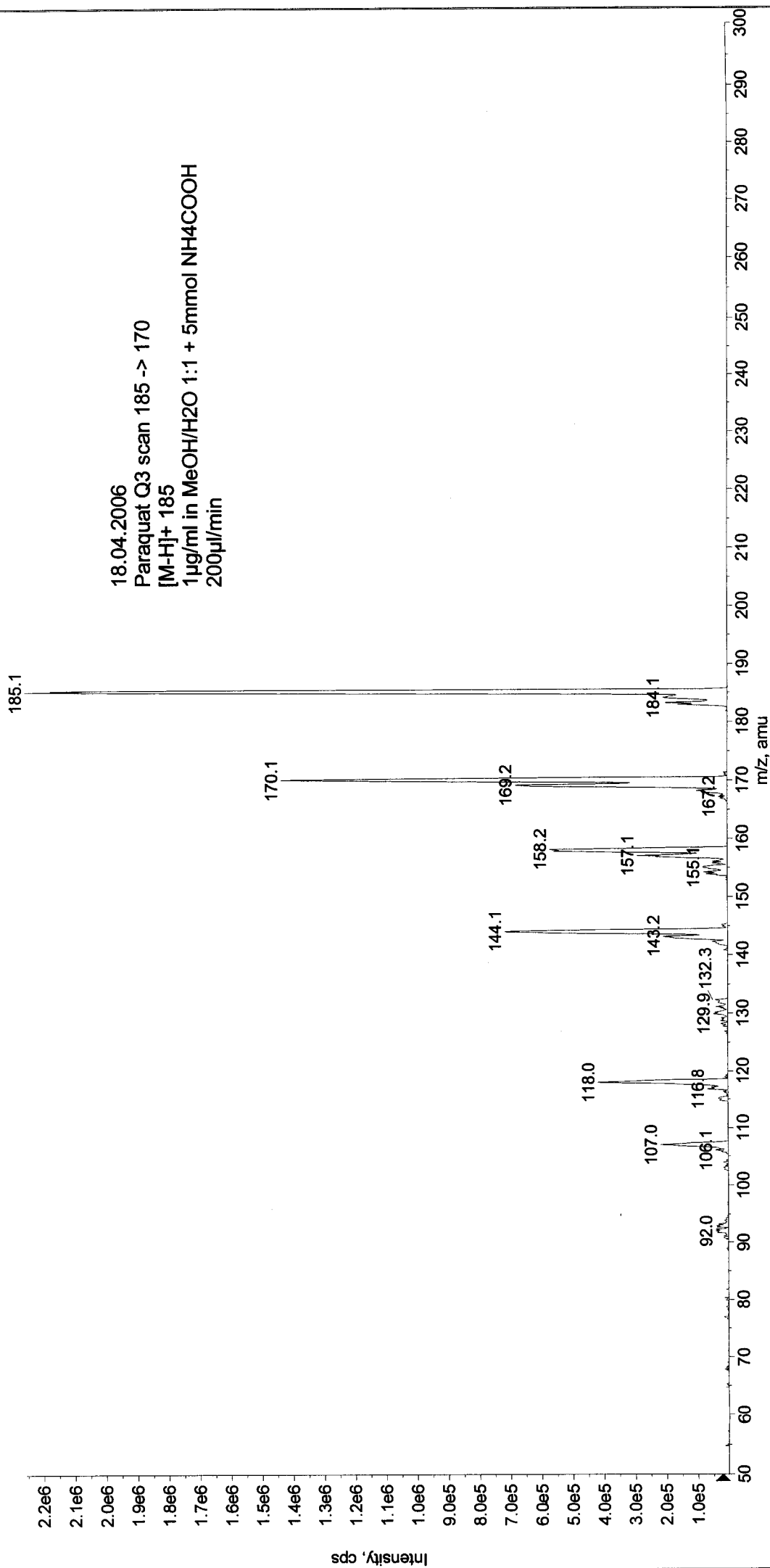
Acq. Time: 11:24
Acq. Date: Tuesday, April 18, 2006
Acq. File: MT20060418112425.wiff

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

18.04.2006
Paraquat Q3 scan 185 -> 170
[M-H]⁺ 185
1 µg/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200 µl/min

Max. 2.3e6 cps

+MS2 (185.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060418112425.wiff (Turbo Spray)



Sample Comment:

Sample Name: TunesSampleID

Batch Name: ManualTune.bat

