

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

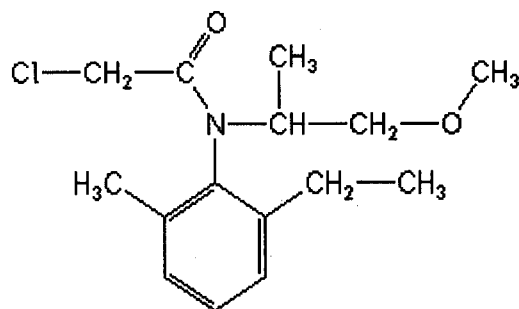
Analyte: Metolachlor

CAS No.: 51218-45-2

Formula: C₁₅H₂₂ClNO₂

Molecular mass (lowest isotopes): 283,13 amu

Structure:



Ionisation: ESI +

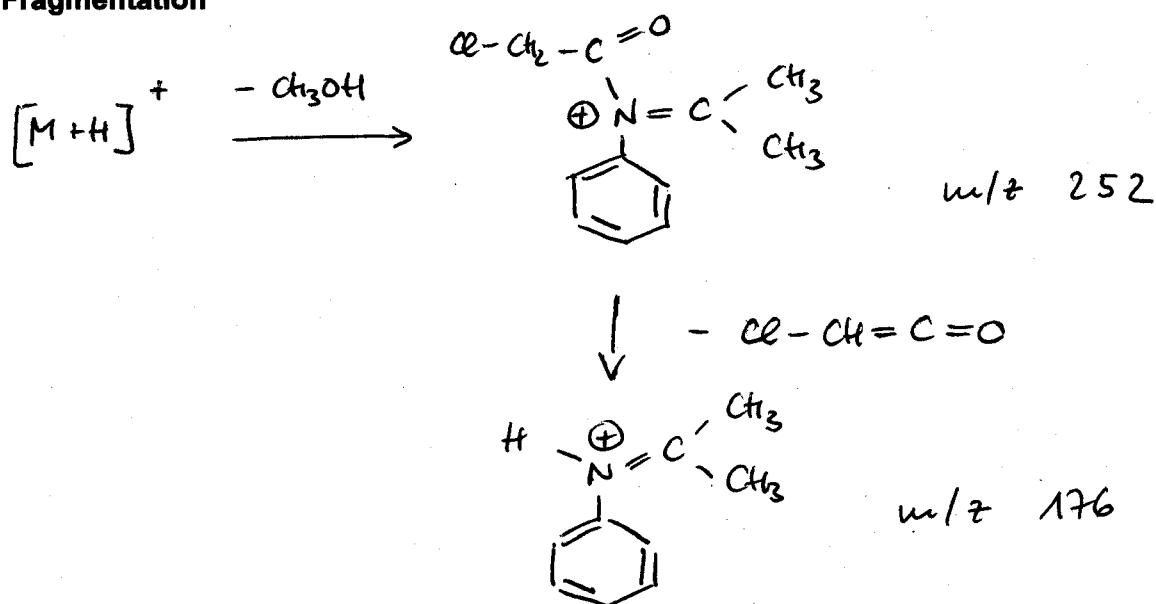
Quasimolecular ion: 284,1 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

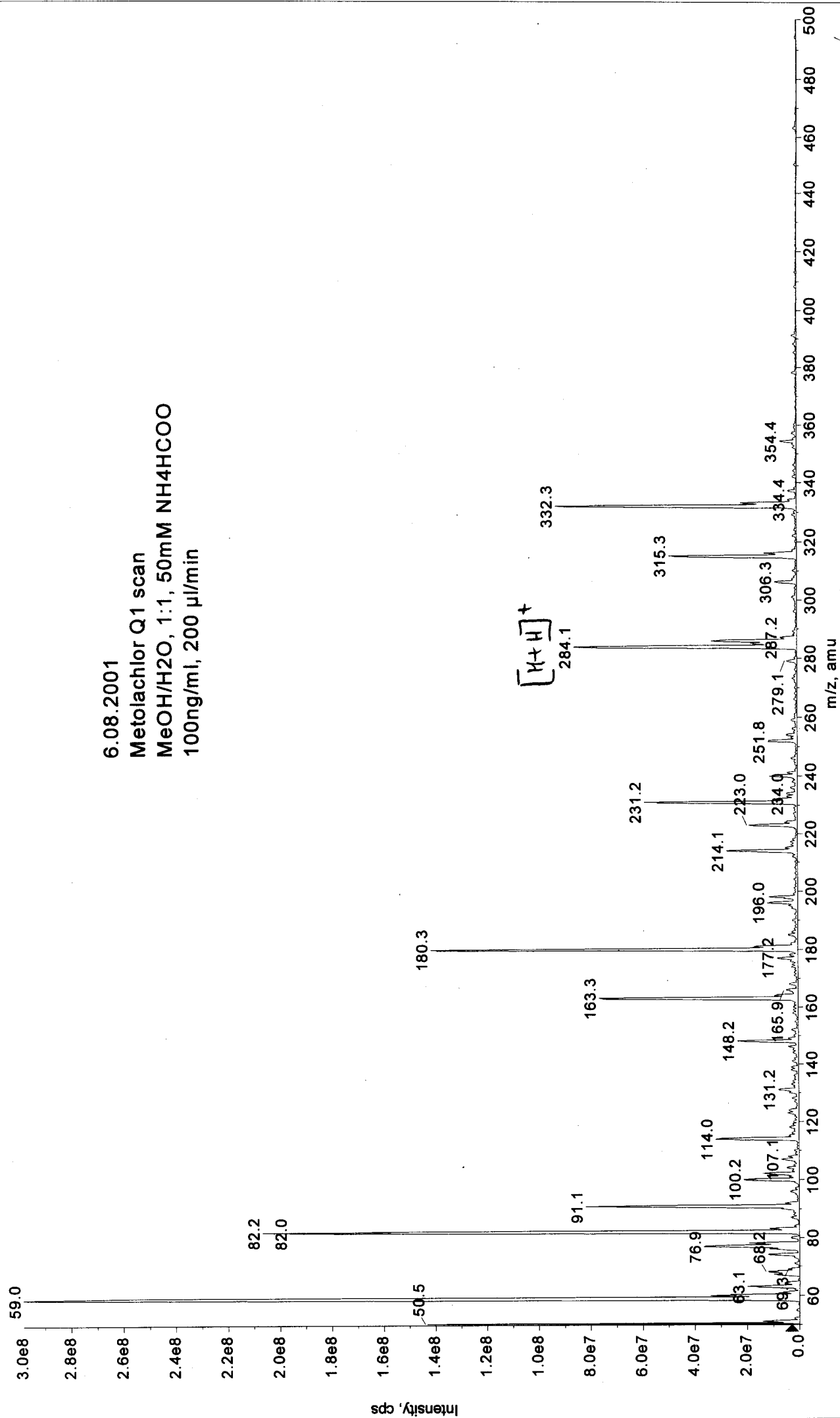
Transition	284,1 → 251,9	284,1 → 176,1
Declustering potential (DP) ^{*)}	14 V	14 V
Focusing potential (FP)	360 V	350 V
Entrance potential (EP)	6,0 V	7,5 V
Collision cell entrance potential (CEP)	14 V	14 V
Collision energy (CE)	19 V	35 V
Collision cell exit potential (CXP)	14 V	8 V

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

Fragmentation



6.08.2001
Metolachlor Q1 scan
MeOH/H₂O, 1:1, 50mM NH₄HCOO
100ng/ml, 200 µl/min



251.9

6.08.2001
Metolachlor Q3 scan 284 -> 252
MeOH/H₂O, 1:1, 50mM NH₄HCOO
100ng/ml, 200 µl/min

284.0

176.0

Intensity, cps
1.27e7
1.20e7
1.10e7
1.00e7
9.00e6
8.00e6
7.00e6
6.00e6
5.00e6
4.00e6
3.00e6
2.00e6
1.00e6
0.00

m/z, amu
50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300

6.08.2001
Metolachlor176 Q3 scan 284 -> 176
MeOH/H2O, 1:1, 50mM NH4HCOO
100ng/ml, 200 µl/min

