BfR

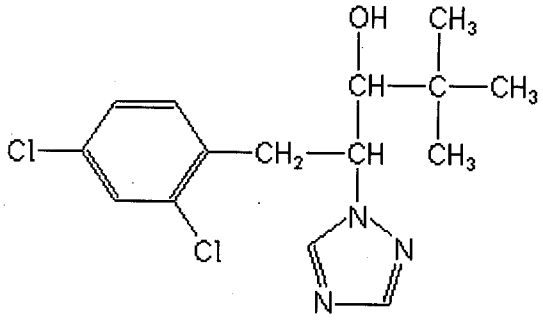
Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

Analyte: Diclobutrazol

CAS No.: 75736-33-3
Formula: C15H19Cl2N3O
Molecular mass (lowest isotopes): 327,09 amu

Structure:



Ionisation: ESI + Quasimolecular ion: 328,1 amu = [M+H]+

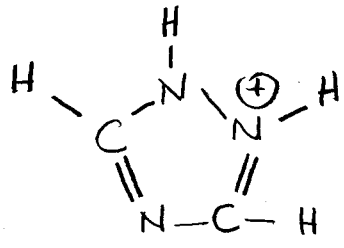
Analyte sensitive parameter set (API 2000)

Transition	328,1 → 70,1	328,1 → 159,9
Declustering potential (DP)*)	19 V	19 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	12,0 V	11,5 V
Collision cell entrance potential (CEP)	20 V	18 V
Collision energy (CE)	39 V	45 V
Collision cell exit potential (CXP)	10 V	8 V

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

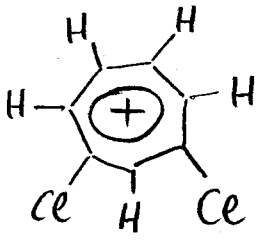
Fragmentation

$[M+H]^+$



m/z 70

$[M+H]^+$

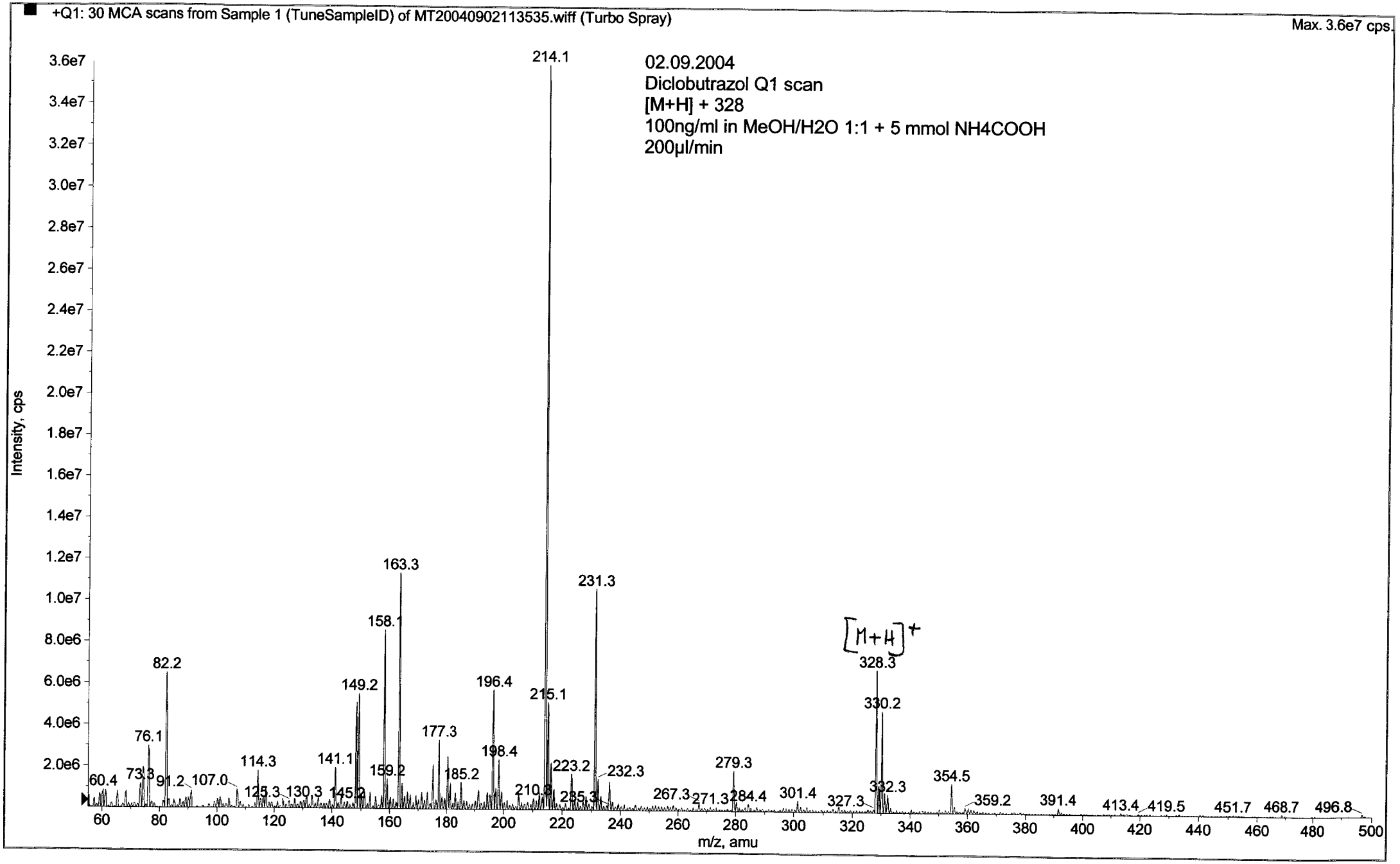


m/z 159

Printing Time: 11:41:10
Printing Date: Thursday, September 02, 2004

Acq. Time: 11:35
Acq. Date: Thursday, September 02, 2004
Acq. File: MT20040902113535.wiff

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



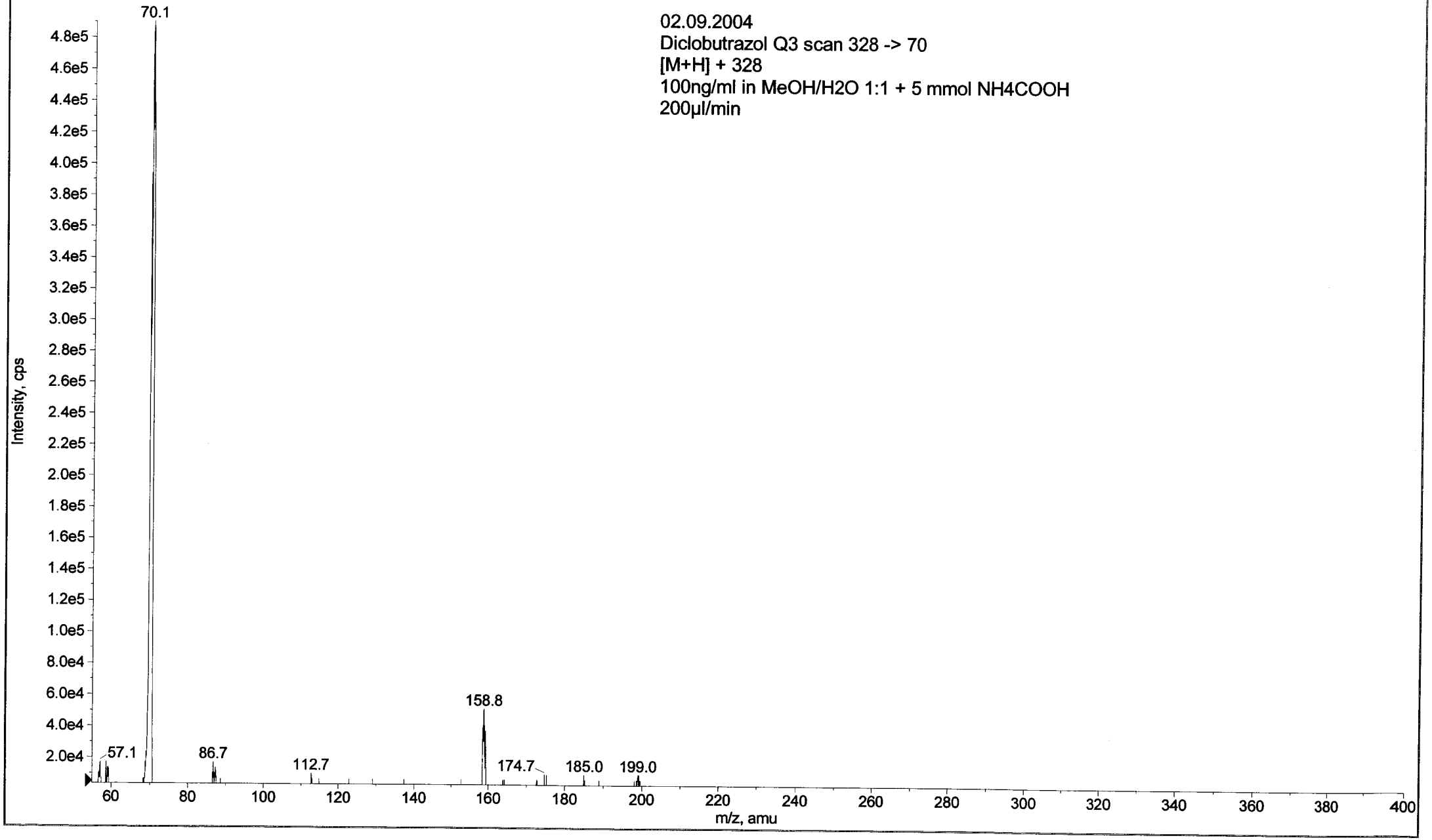
Printing Time: 11:41:49
Printing Date: Thursday, September 02, 2004

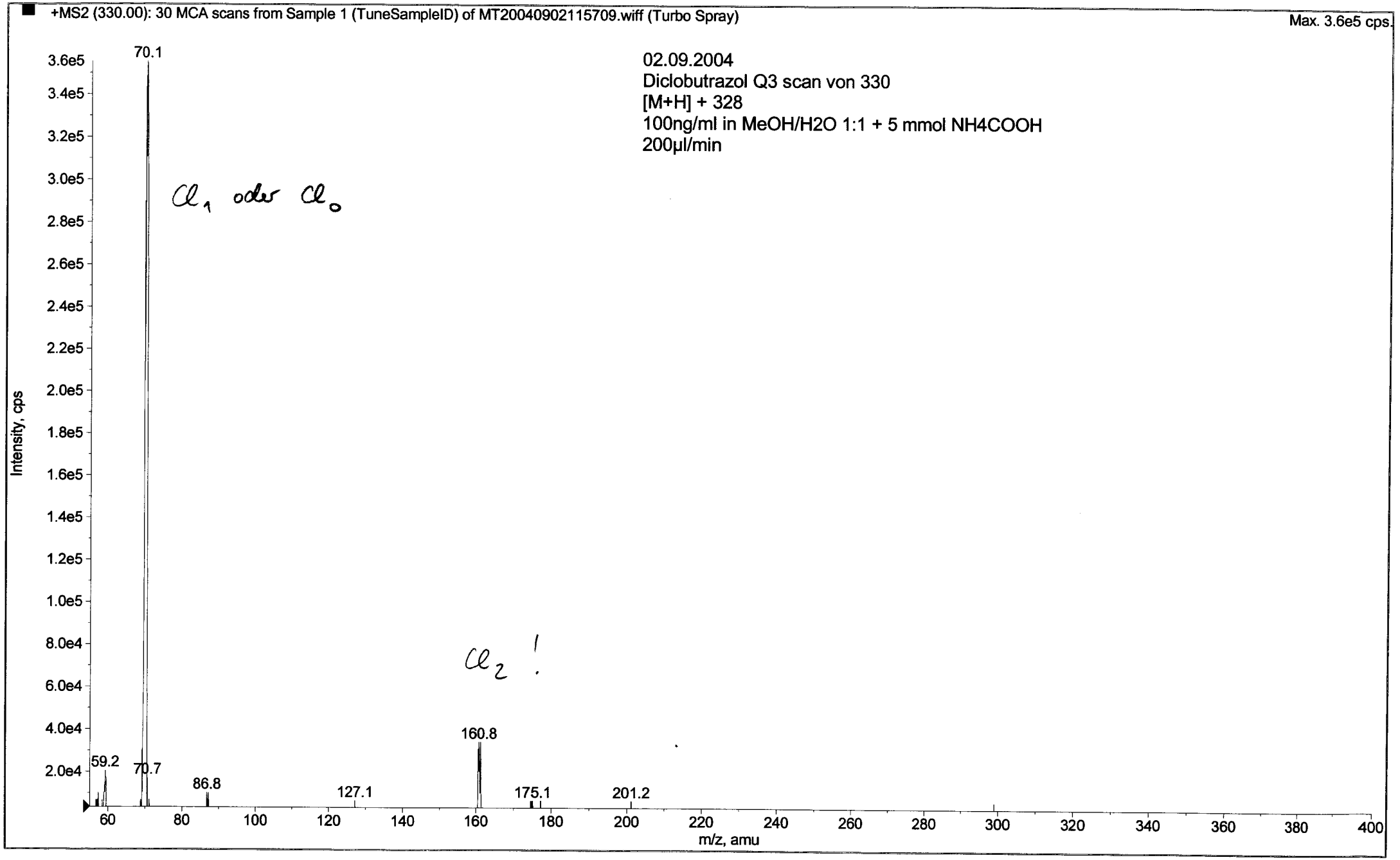
Acq. Time: 11:38
Acq. Date: Thursday, September 02, 2004
Acq. File: MT20040902113800.wiff

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

+MS2 (328.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040902113800.wiff (Turbo Spray)

Max. 4.9e5 cps.




+MS2 (330.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040902115709.wiff (Turbo Spray)
Max. 3.6e5 cps.
02.09.2004
Diclobutrazol Q3 scan von 330
[M+H] + 328
100ng/ml in MeOH/H2O 1:1 + 5 mmol NH4COOH
200µl/min
Cl1 oder Cl0
Cl2 !
Intensity, cps
m/z, amu
70.1
160.8
59.2
70.7
86.8
127.1
175.1
201.2

Printing Time: 11:51:32
Printing Date: Thursday, September 02, 2004

Acq. Time: 11:49
Acq ıte: Thursday, September 02, 2004
Acq. ſile: MT20040902114932.wiff

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

+MS2 (328.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040902114932.wiff (Turbo Spray)

Max. 5.0e5 cps.