

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

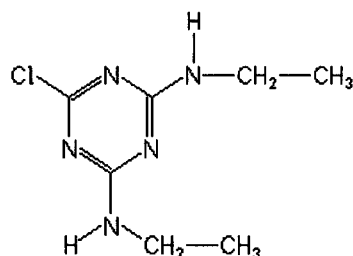
Analyte: Simazine

CAS No.: 122-34-9

Formula: C₇H₁₂ClN₅

Molecular mass (lowest isotopes): 201,08 amu

Structure:



Ionisation: ESI +

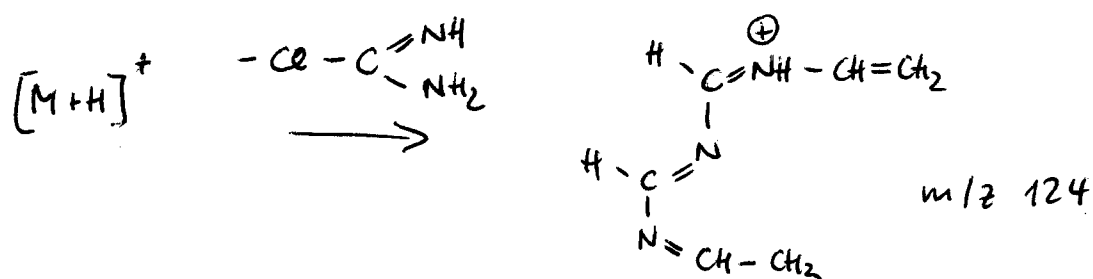
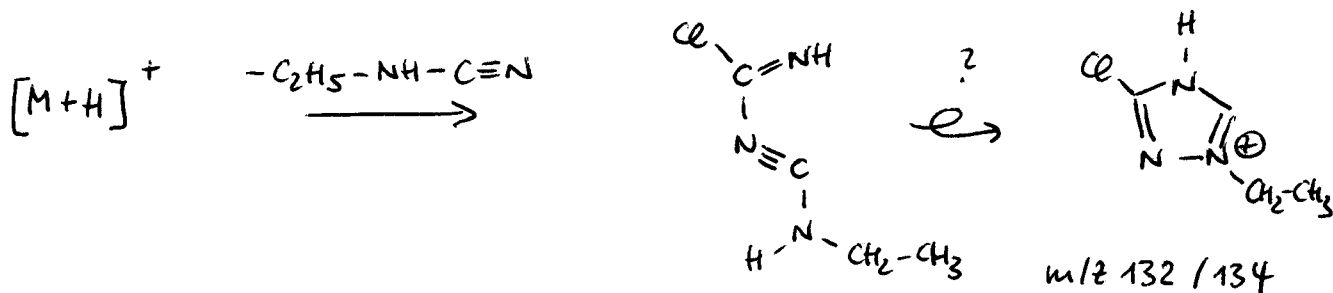
Quasimolecular ion: 202,1 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

Transition	202,1 → 124,2	202,1 → 132,2
Declustering potential (DP) ^{*)}	26 V	26 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	10,0 V	10,0 V
Collision cell entrance potential (CEP)	12 V	14 V
Collision energy (CE)	25 V	27 V
Collision cell exit potential (CXP)	6 V	6 V

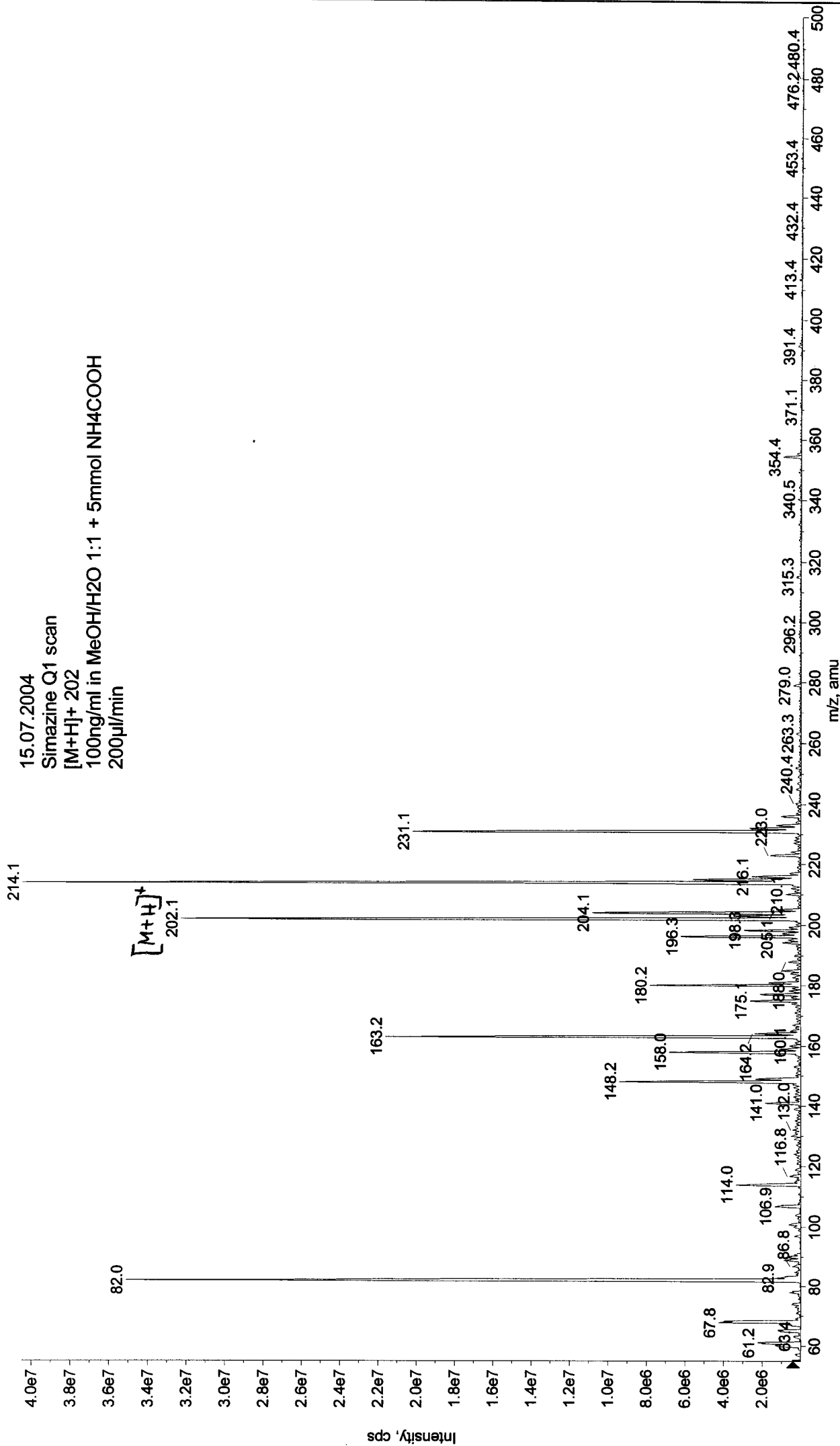
^{*)} For API 3000 and 4000 enhance DP by 20V

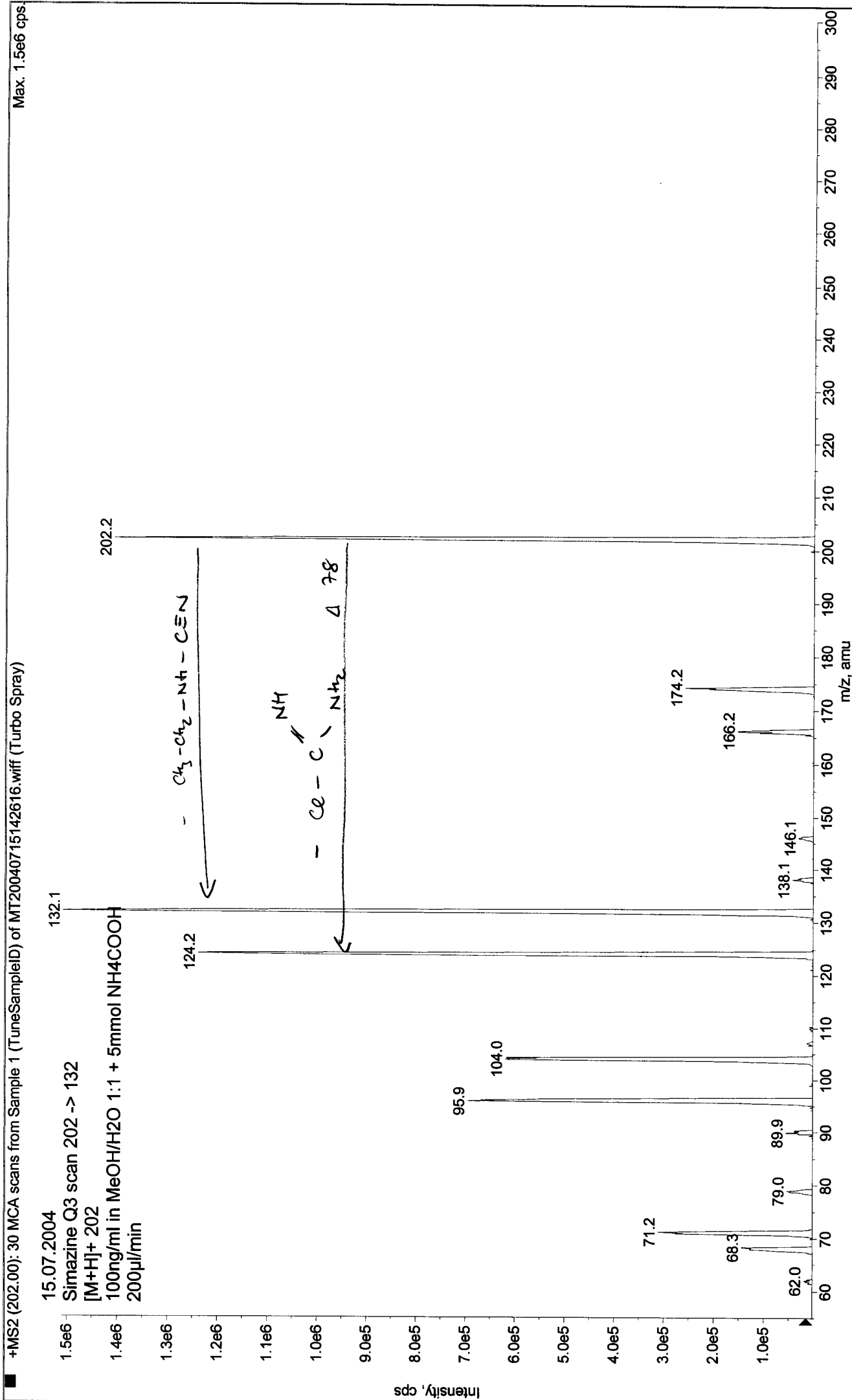
Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20040715142355.wiff (Turbo Spray)

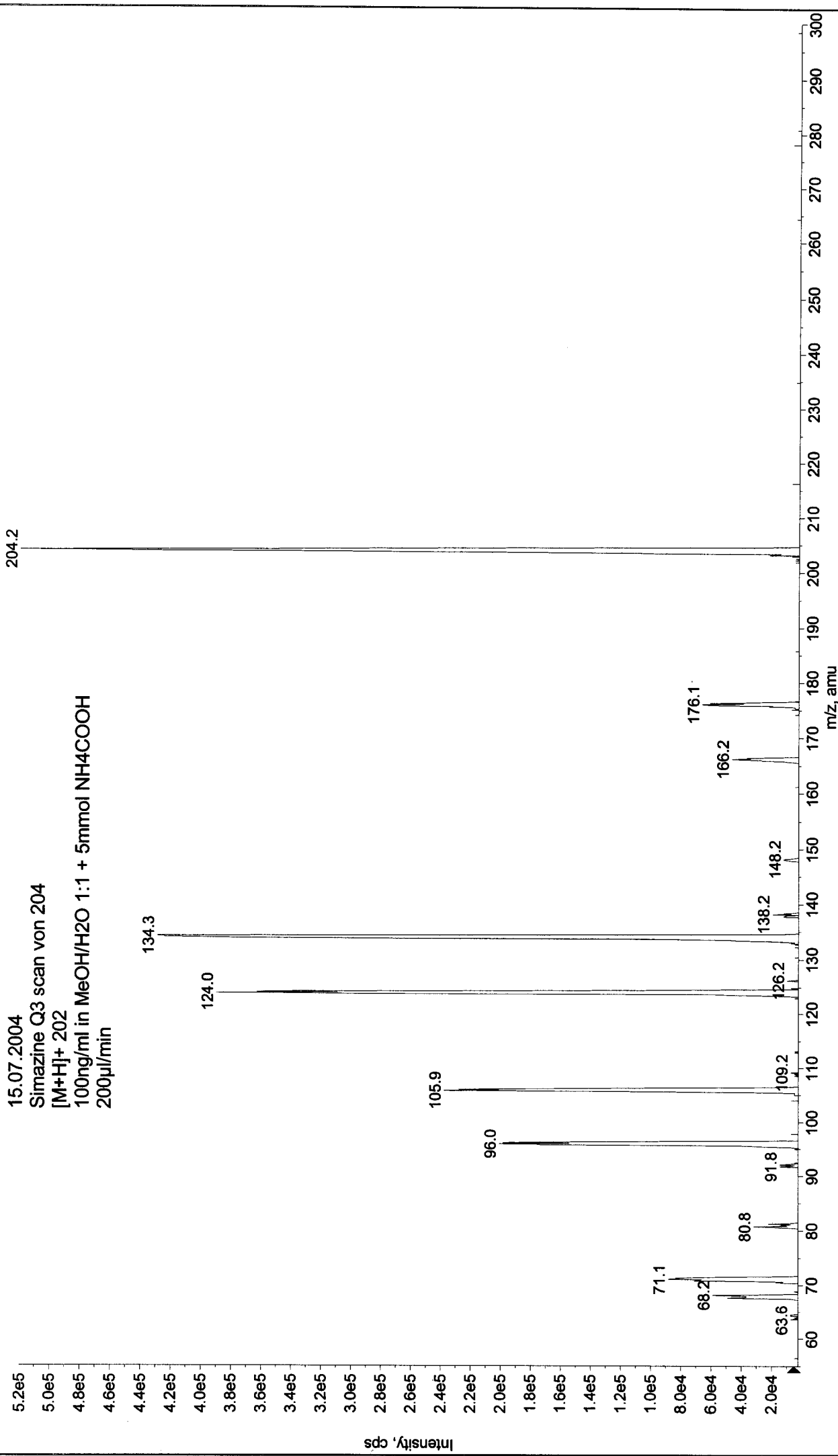
Max. 4.0e7 cps



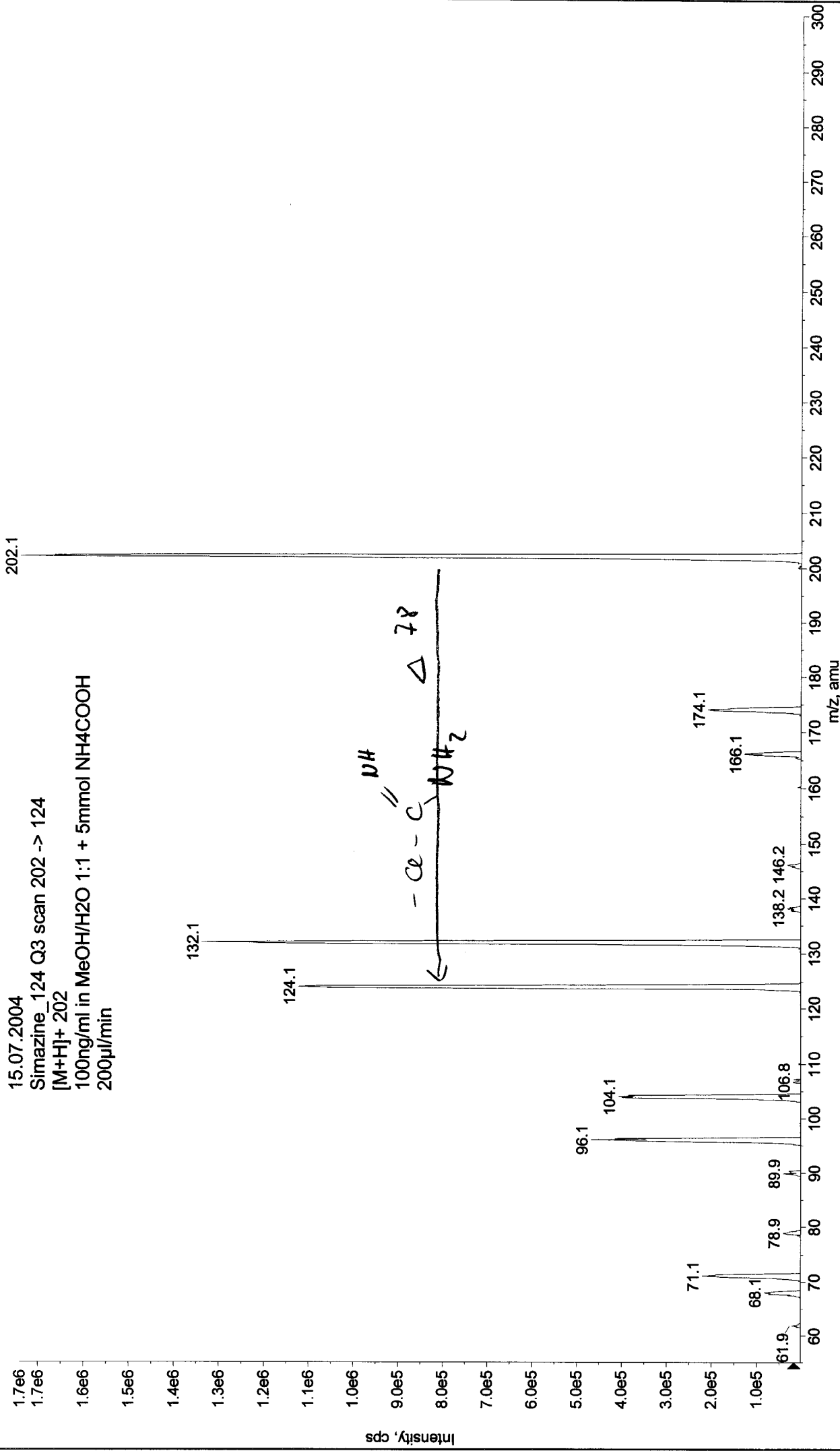


Max. 5.2e5 cps

+MS2 (204.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040715142844.wiff (Turbo Spray)



+MS2 (202.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040716083521.wiff (Turbo Spray) Max. 1.7e6 cps



+MS2 (204.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040716083721.wiff (Turbo Spray) Max. 6.0e5 cps

15.07.2004
Simazine_124 Q3 scan von 204
[M+H]⁺ 202
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min

