

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

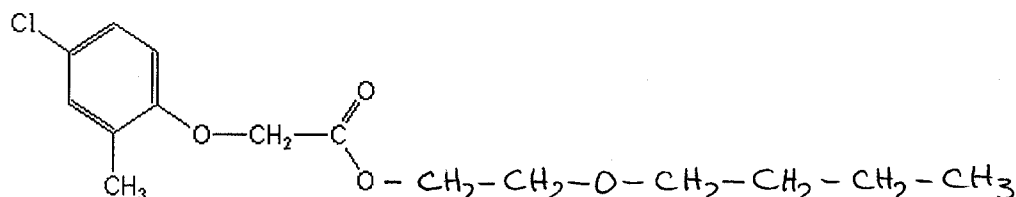
Analyte: MCPA-butotyl

CAS No.: 19480-43-4

Formula: C₁₅H₂₁ClO₄

Molecular mass (lowest isotopes): 300,11 amu

Structure:



Ionisation: ESI +

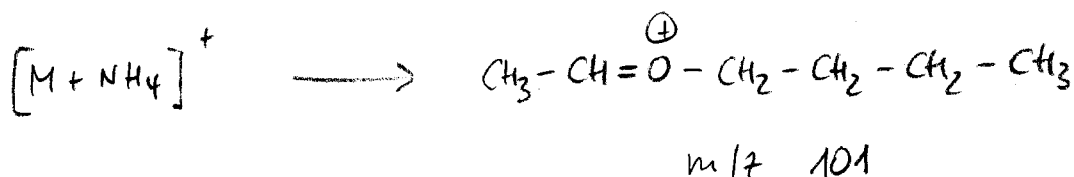
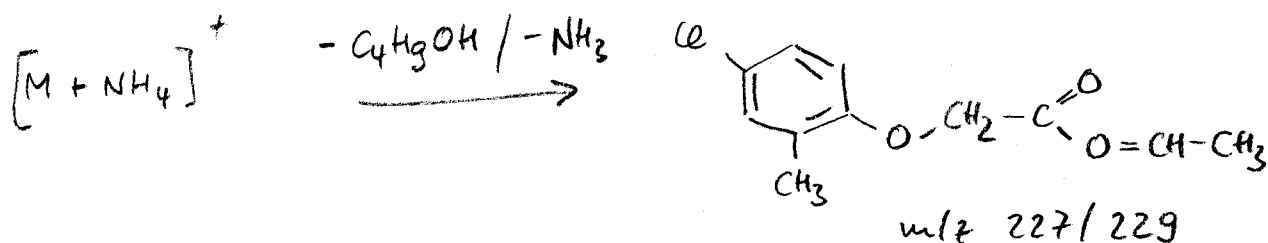
Quasimolecular ion: 318,1 amu = [M+NH₄]⁺

Analyte sensitive parameter set (API 2000)

Transition	318,1 → 227,0	318,1 → 101,2
Declustering potential (DP) ^{*)}	9 V	9 V
Focusing potential (FP)	350 V	370 V
Entrance potential (EP)	5,0 V	12,0 V
Collision cell entrance potential (CEP)	20 V	20 V
Collision energy (CE)	17 V	19 V
Collision cell exit potential (CXP)	12 V	4 V

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

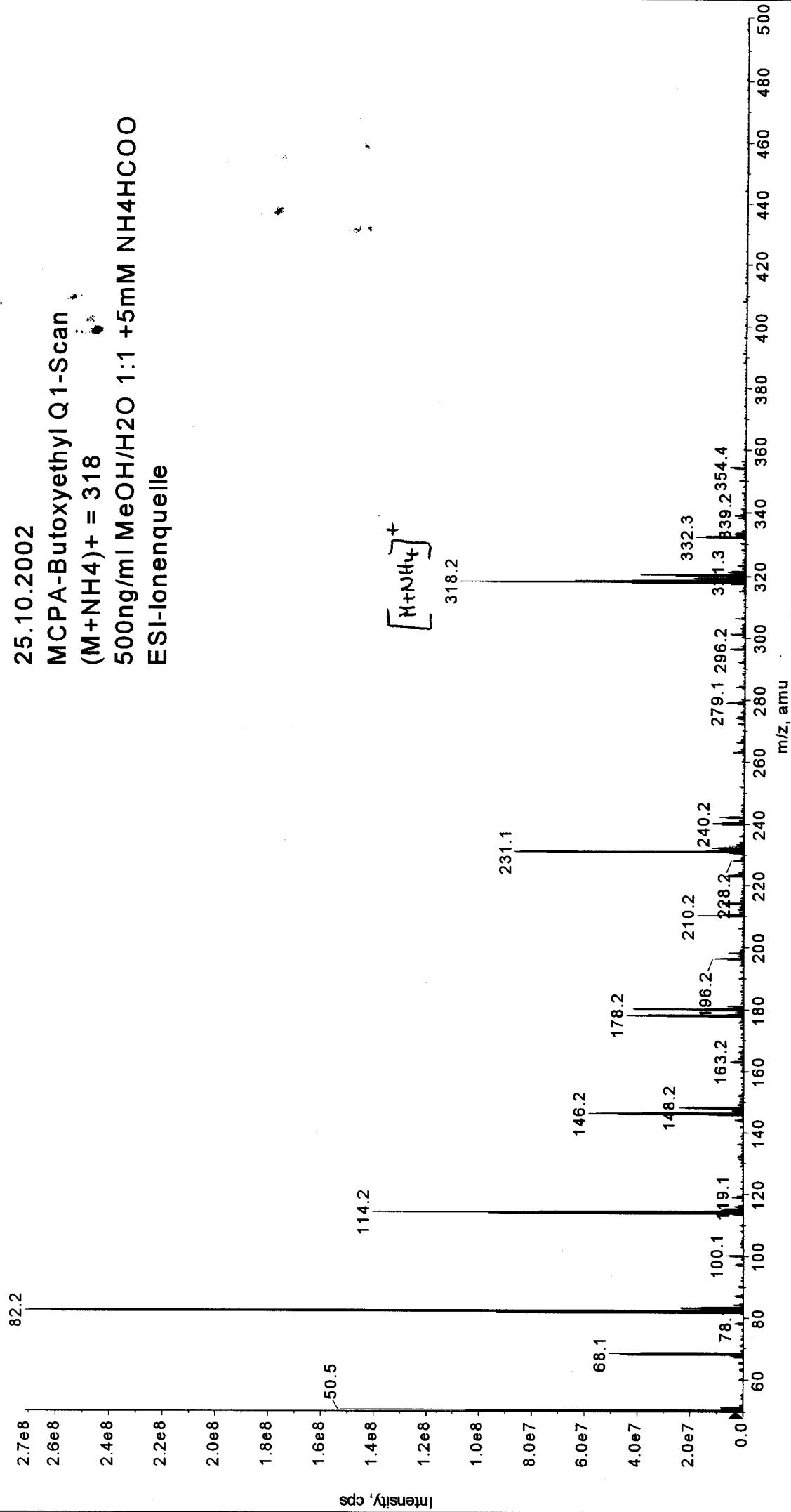
Fragmentation



■ +Q1: 30 MCA scans from MT20021025111057.wiff

Max. 2.7e8 cps

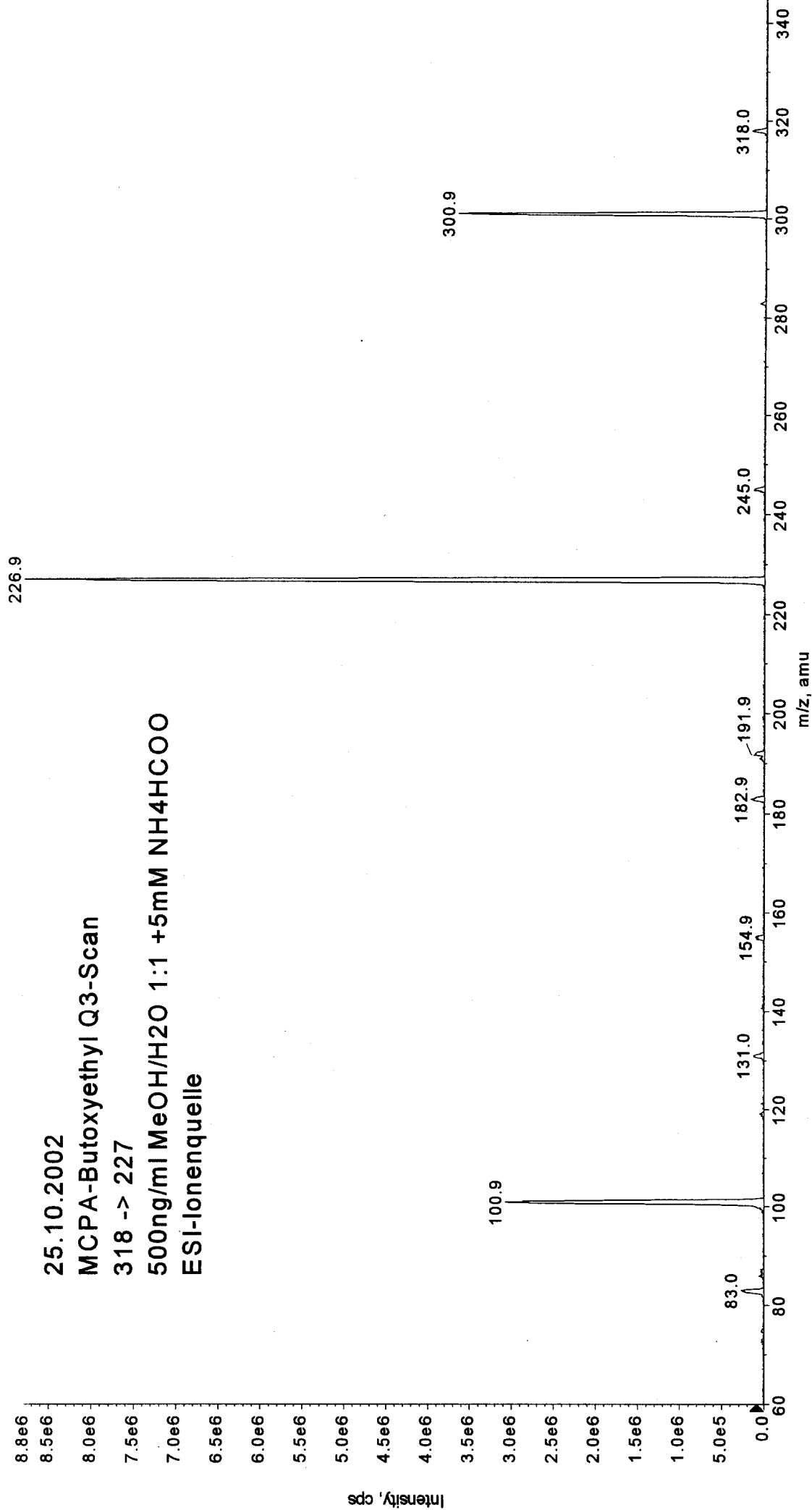
25.10.2002
MCPA-Butoxyethyl Q1-Scan
(M+NH₄)⁺ = 318
500ng/ml MeOH/H₂O 1:1 +5mM NH₄HCOO
ESI-Ionenquelle



■ +Product (318.0): 30 MCA scans from MT20021025111355.wiff

Max. 8.8e6 cps

25.10.2002
MCPA-Butoxyethyl Q3-Scan
318 -> 227
500ng/ml MeOH/H2O 1:1 +5mM NH4HCOO
ESI-Ionenquelle



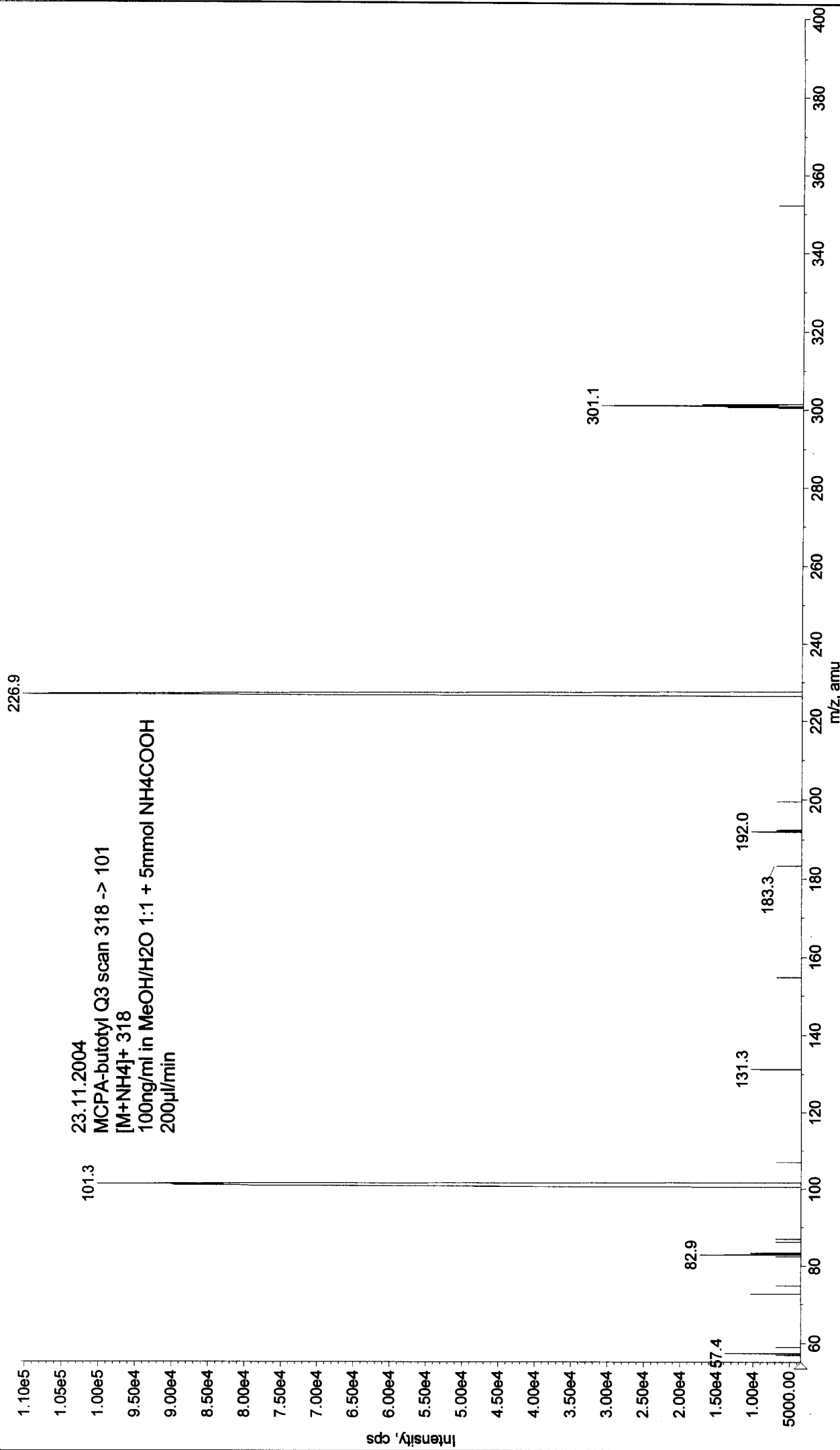
Printing Time: 15:11:25
Printing Date: Tuesday, November 23, 2004

Acq. Time: 15:10
Acq. Date: Tuesday, November 23, 2004
Acq. File: MT20041123151010.wiff

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

Max. 1.1e5 cps

+MS2 (318.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20041123151010.wiff (Turbo Spray)



■ +MS2 (320.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20041123151141.wiff (Turbo Spray) Max. 4.5e4 cps

