

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

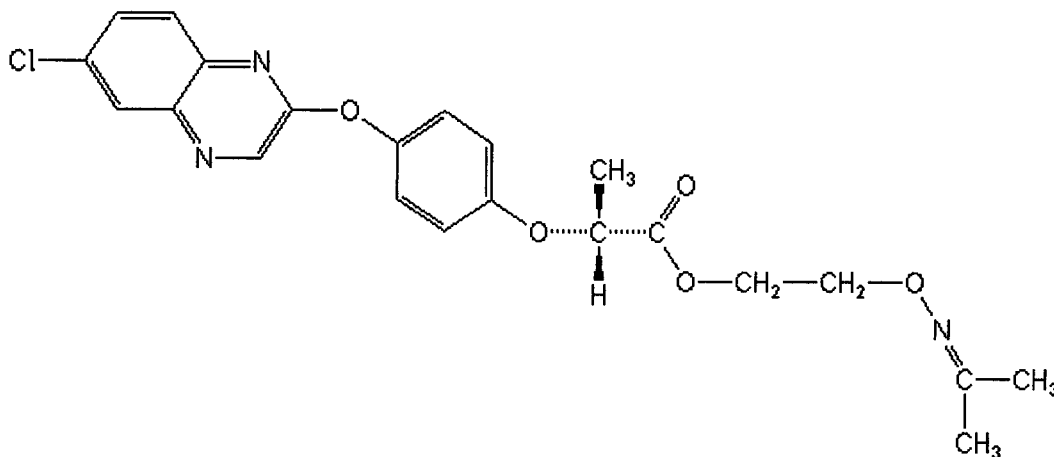
Analyte: Propaquizafop

CAS No.: 111479-05-1

Formula: C₂₂H₂₂ClN₃O₅

Molecular mass (lowest isotopes): 443,13 amu

Structure:



Ionisation: ESI +

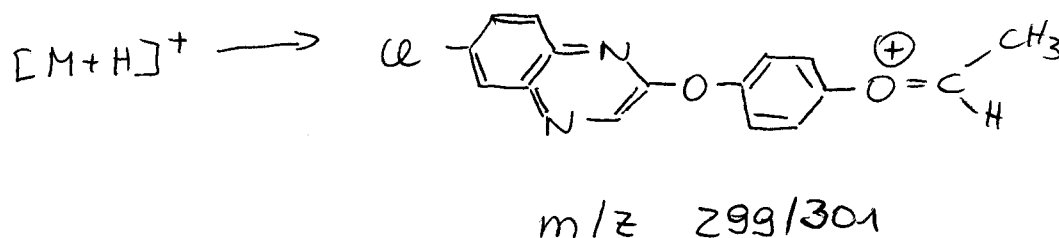
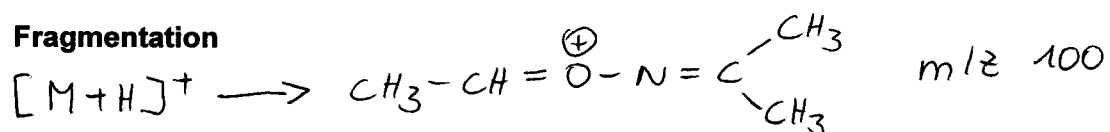
Quasimolecular ion: 444,1 amu = [M+H]⁺

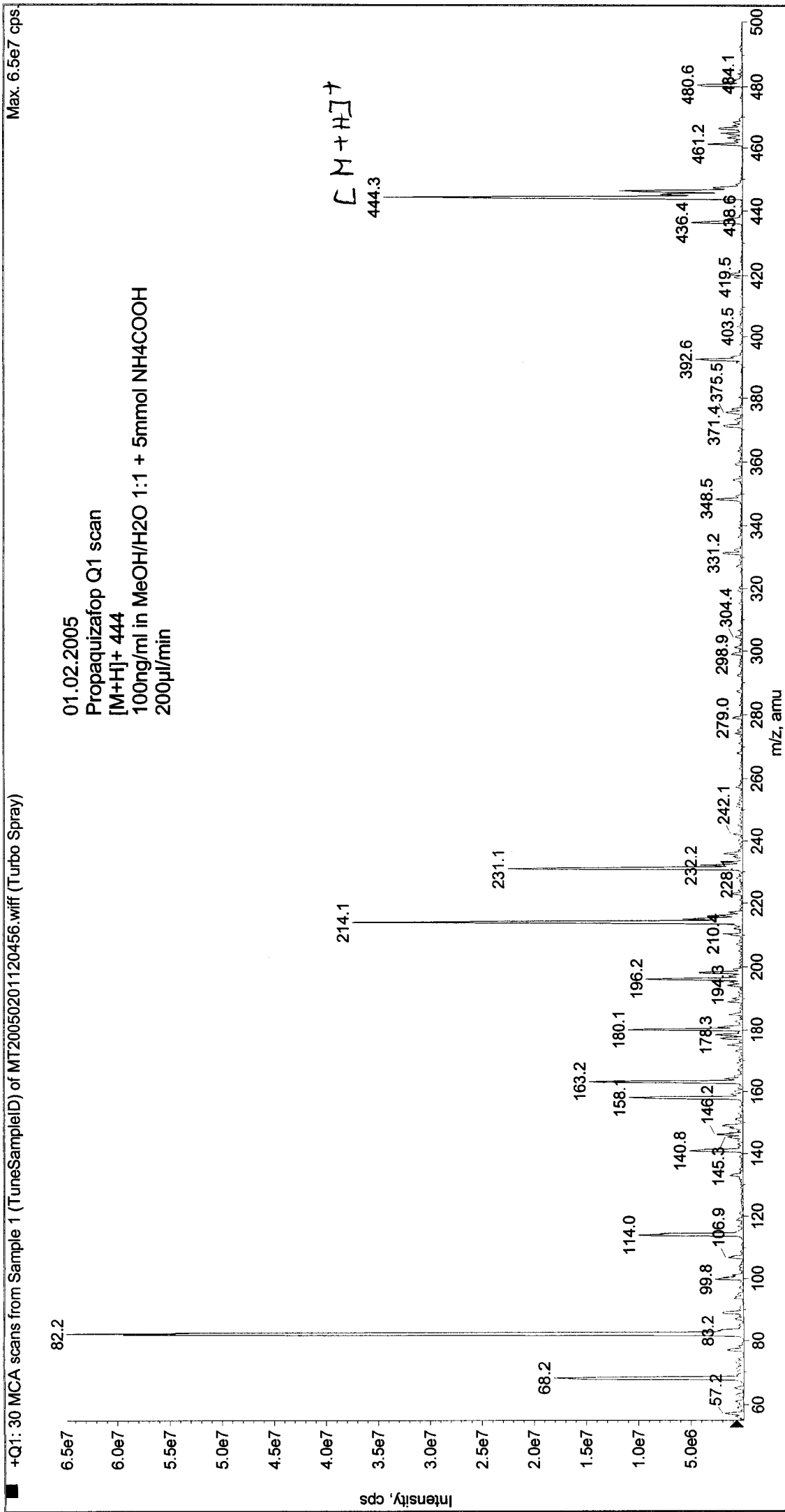
Analyte sensitive parameter set (API 2000)

Transition	444,1 → 299,1	444,1 → 100,0
Declustering potential (DP) ^{*)}	79V	79 V
Focusing potential (FP)	370 V	360 V
Entrance potential (EP)	9,5 V	9,5 V
Collision cell entrance potential (CEP)	20 V	20 V
Collision energy (CE)	31 V	27 V
Collision cell exit potential (CXP)	16 V	6 V

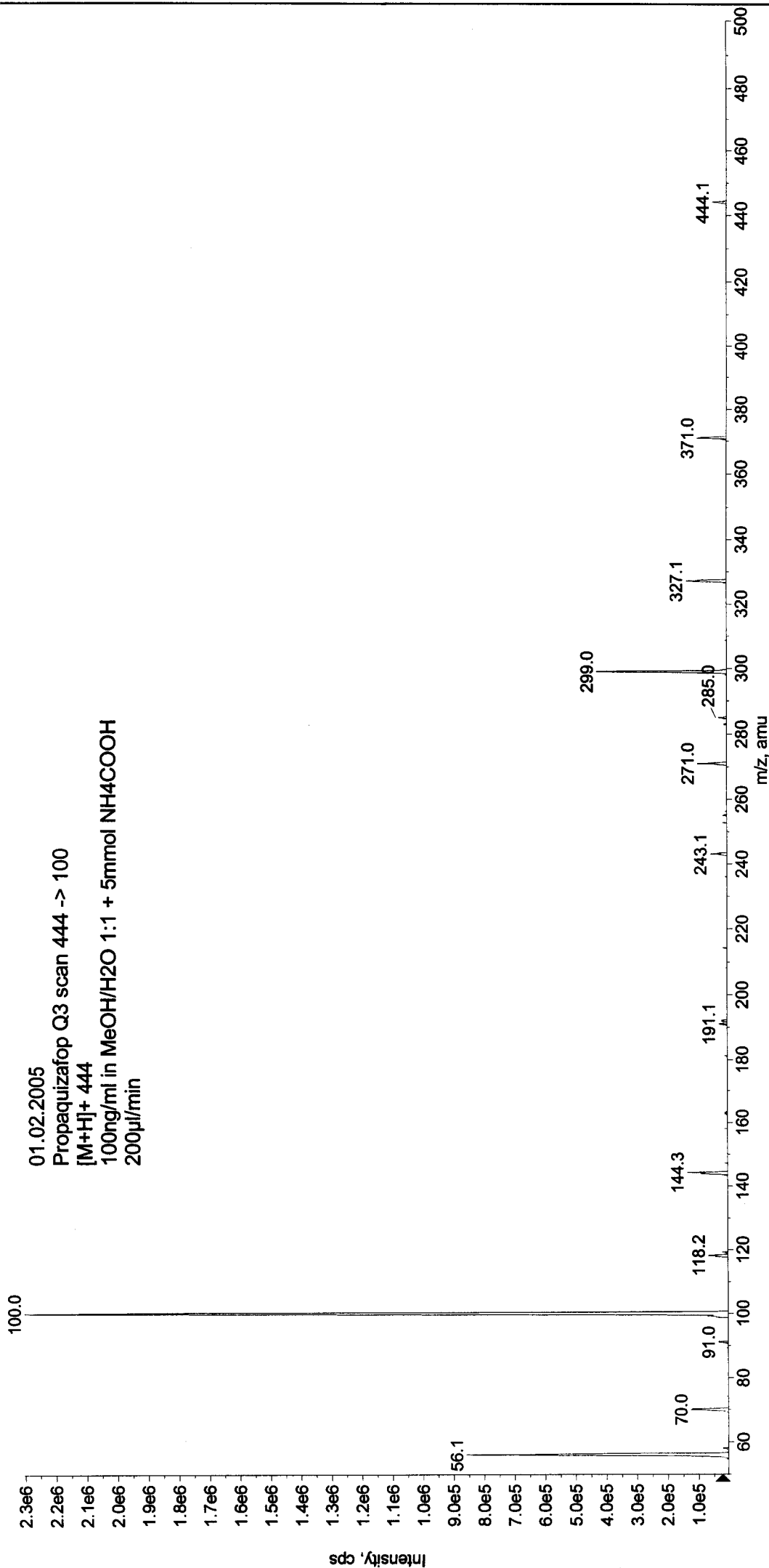
^{*)} For API 3000 and 4000 enhance DP by 20V

Fragmentation





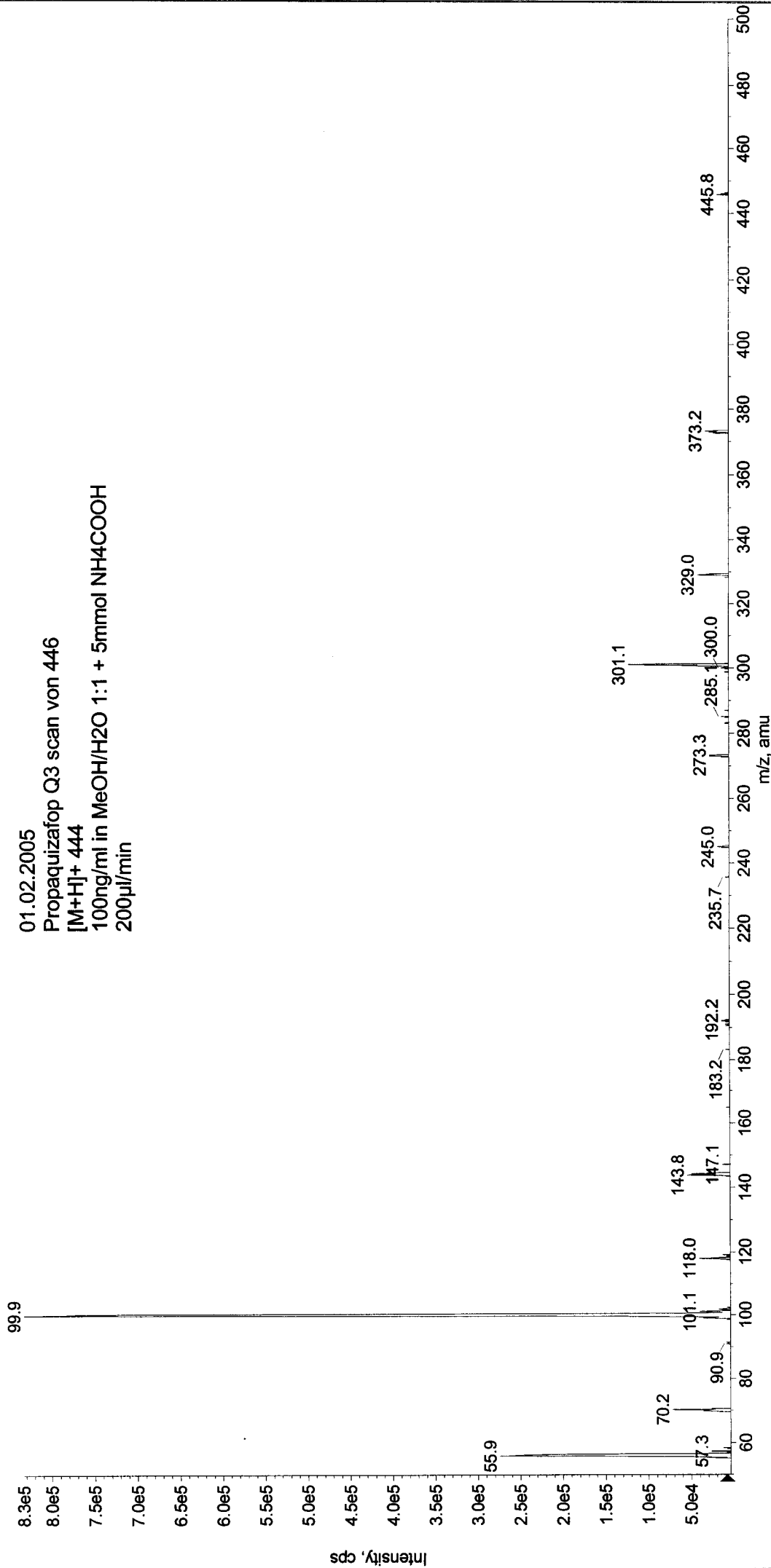
■ +MS2 (444.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050201120721.wiff (Turbo Spray) Max. 2.3e6 cps.



Max. 8.3e5 cps

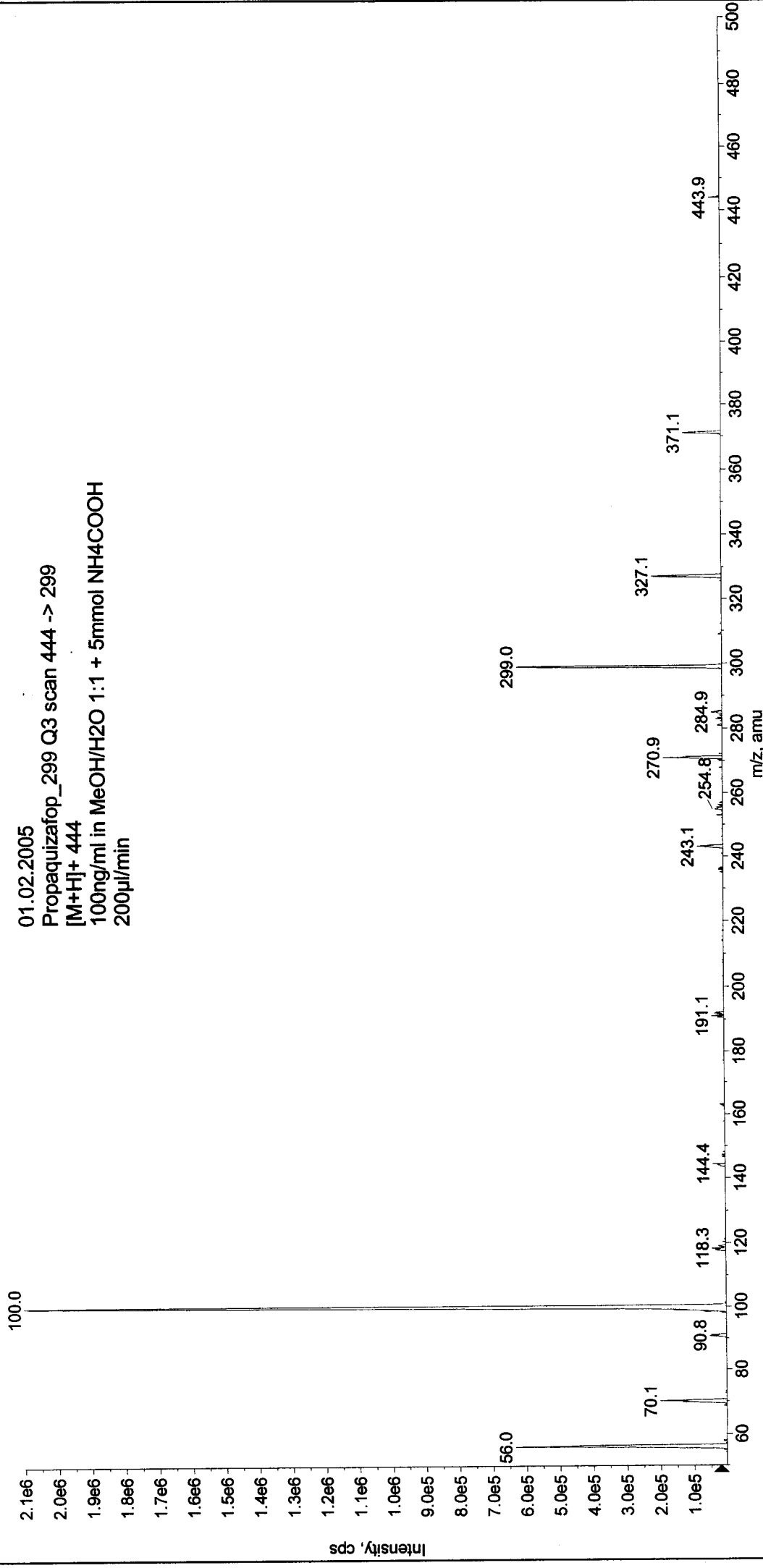
+MS2 (446.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050201132550.wiff (Turbo Spray)

01.02.2005
Propaquizafop Q3 scan von 446
[M+H]⁺ 444
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min



Max. 2.1e6 cps

■ +MS2 (444.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050201132352.wiff (Turbo Spray)



Max. 6.3e5 cps

■ +MS2 (446.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050201132214.wiff (Turbo Spray)

01.02.2005
Propaquizafop_299 Q3 scan von 446
[M+H]⁺ 444
100ng/ml in MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min

