

MS/MS Parameters of Pesticides

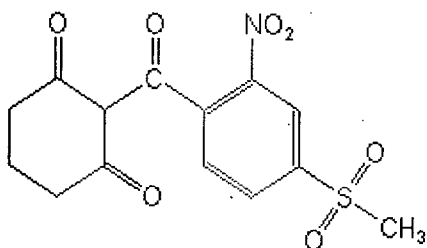
Analyte: Mesotrione

CAS No.: 104206-82-8

Formula: C₁₄H₁₃NO₇S

Molecular mass (lowest isotopes): 339,04 amu

Structure:



Ionisation: ESI +

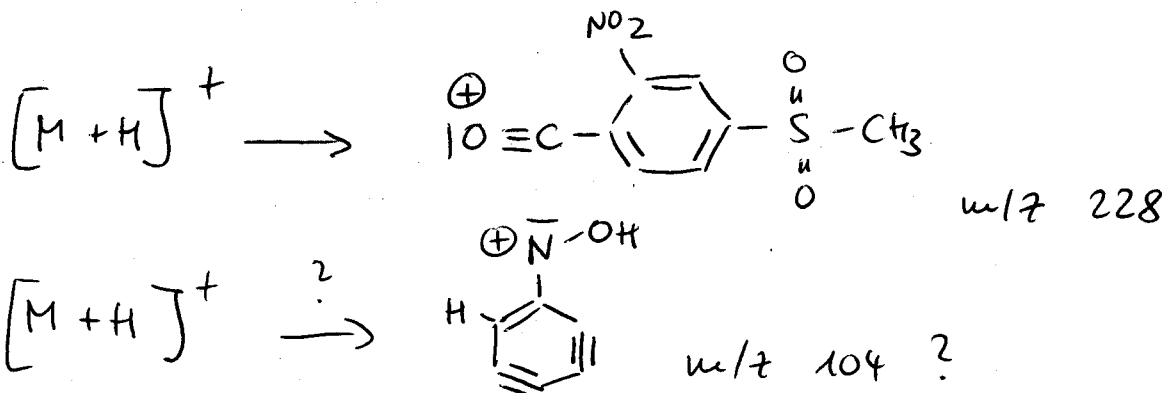
Quasimolecular ion: 357,1 amu = [M+NH₄]⁺

Analyte sensitive parameter set (API 2000)

Transition	357,1 → 227,8	357,1 → 104,1
Declustering potential (DP) ^{*)}	16V	16 V
Focusing potential (FP)	360 V	370 V
Entrance potential (EP)	7,0 V	11,5 V
Collision cell entrance potential (CEP)	24 V	22 V
Collision energy (CE)	29 V	49 V
Collision cell exit potential (CXP)	12 V	4 V

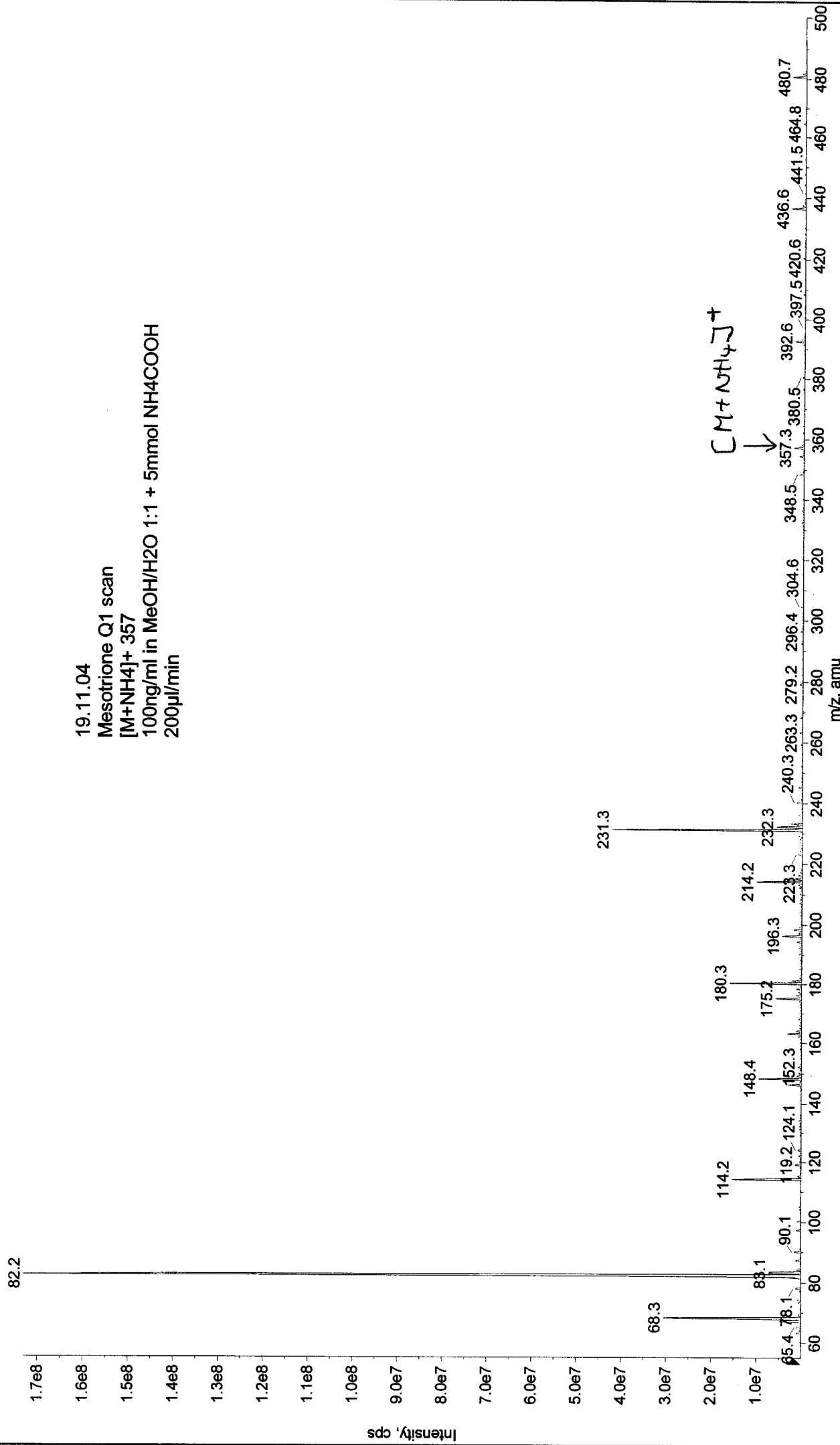
^{*)} For API 3000 and 4000 enhance DP by 20V

Fragmentation



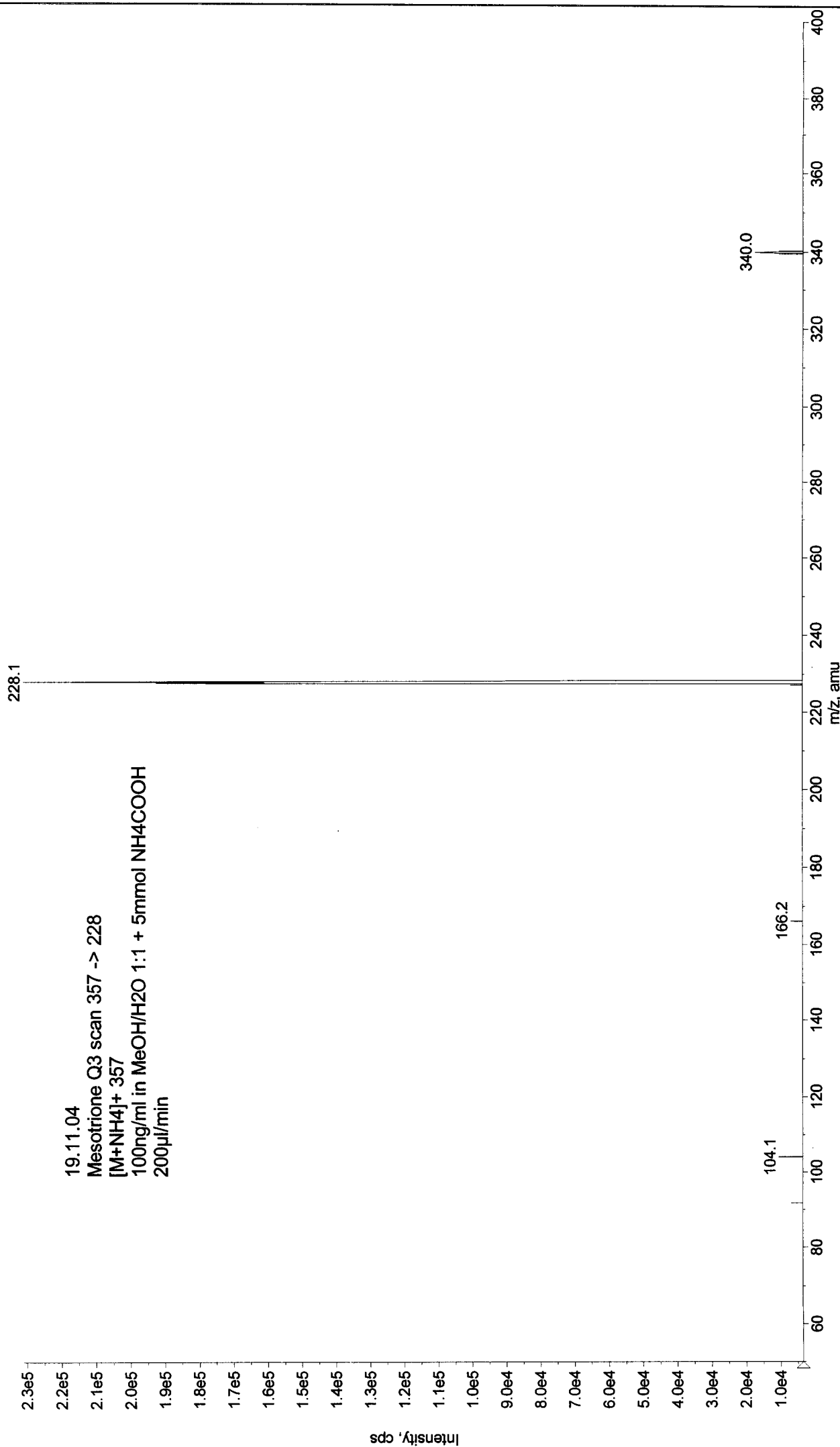
+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20041119091252.wiff (Turbo Spray)

Max. 1.7e8 cps



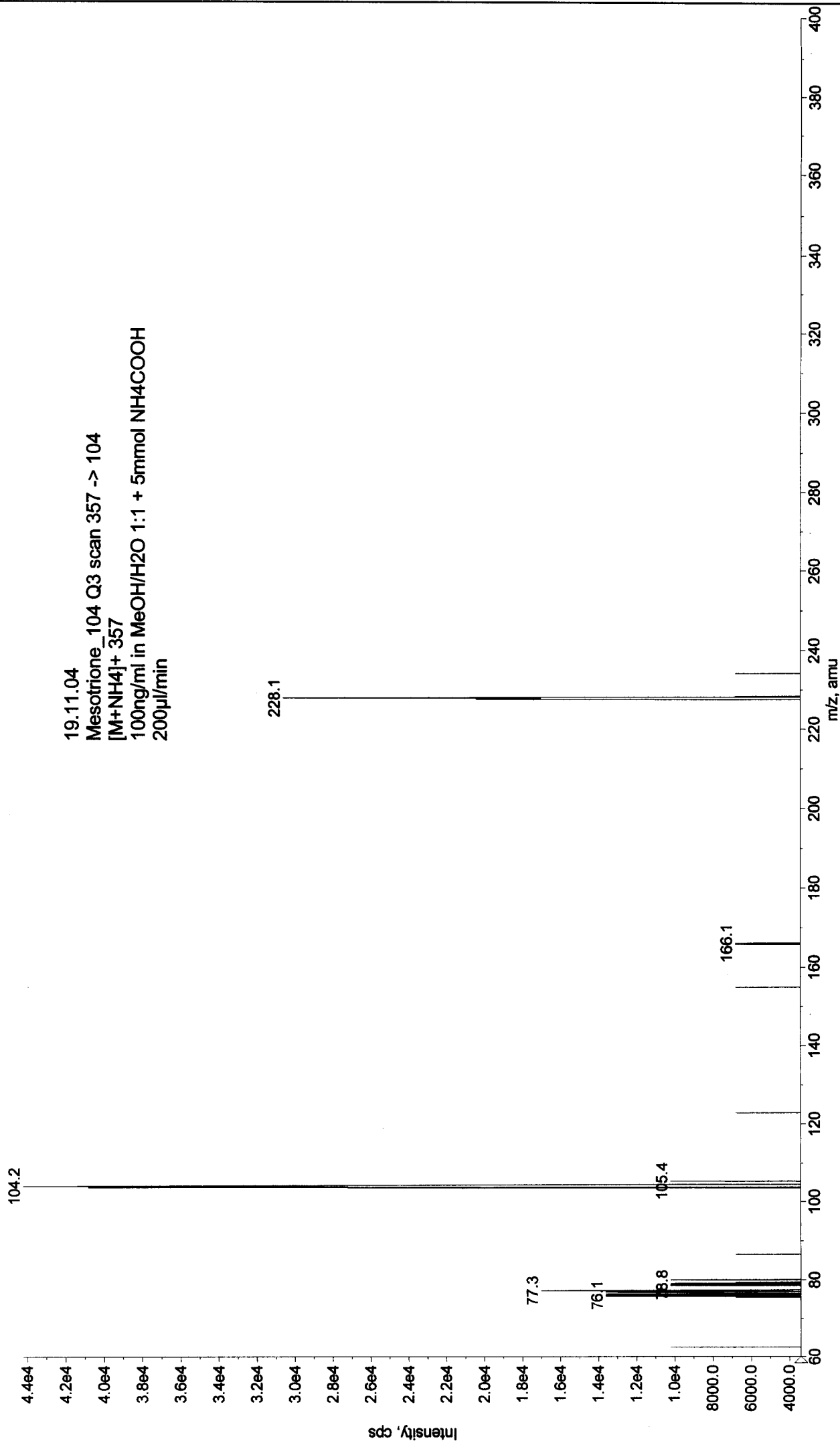
19.11.04
Mesotrione Q1 scan
[M+NH4]⁺ 357
100ng/ml in MeOH/H2O 1:1 + 5mmol NH4COOH
200μl/min

+MS2 (357.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20041119092046.wiff (Turbo Spray) Max. 2.3e5 cps



Max. 4.4e4 cps

+MS2 (357.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20041122110901.wiff (Turbo Spray)



19.11.04
Mesotrione_104 Q3 scan 357 -> 104
[M+NH4]⁺ 357
100ng/ml in MeOH/H2O 1:1 + 5mmol NH4COOH
200µl/min