

MS/MS Parameters of Pesticides

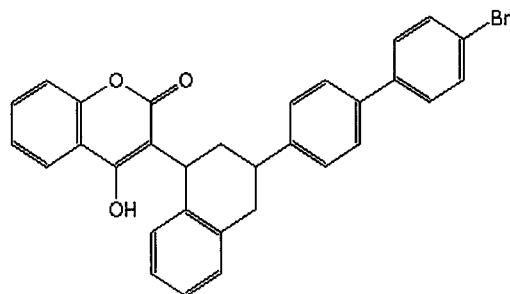
Analyte: Brodifacoum

CAS No.: 56073-10-0

Formula: C₃₁H₂₃BrO₃

Molecular mass (lowest isotopes): 522,08 amu

Structure:



Ionisation: ESI +

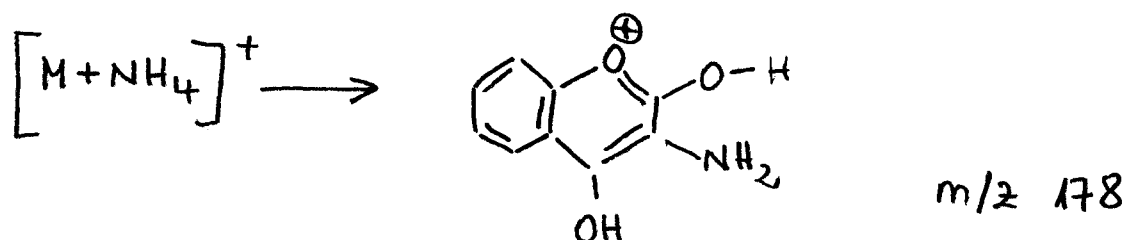
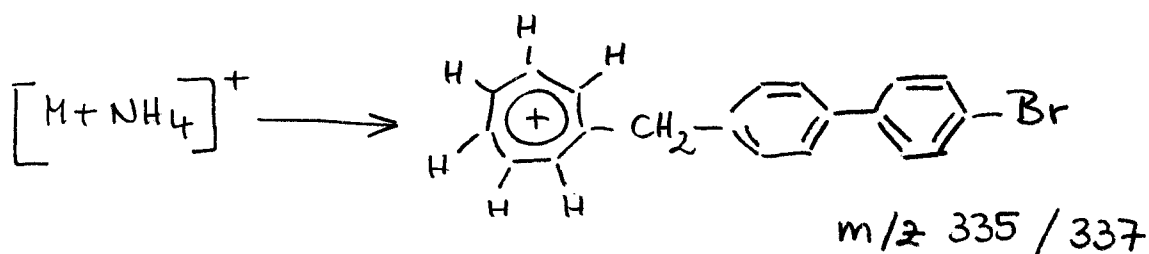
Quasimolecular ion: 540,1 amu = [M+NH₄]⁺

Analyte sensitive parameter set (API 2000)

Transition	540,1 → 335,0	540,1 → 178,1
Declustering potential (DP)*)	36 V	36 V
Focusing potential (FP)	360 V	330 V
Entrance potential (EP)	12,0 V	12 V
Collision cell entrance potential (CEP)	22 V	24,0 V
Collision energy (CE)	33 V	49 V
Collision cell exit potential (CXP)	18 V	10 V

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

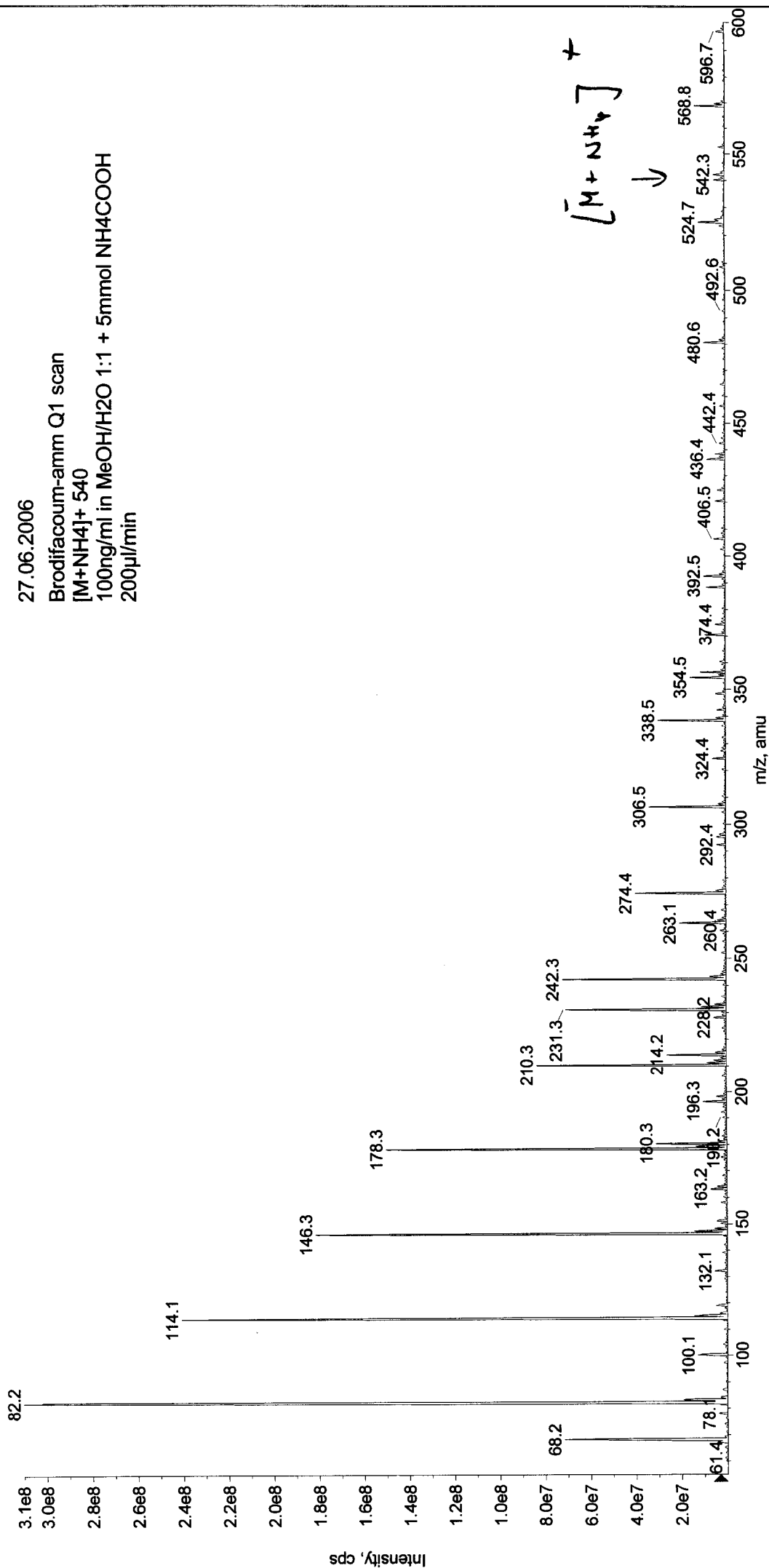
Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20060627143234.wiff (Turbo Spray)

Max. 3.1e8 cps

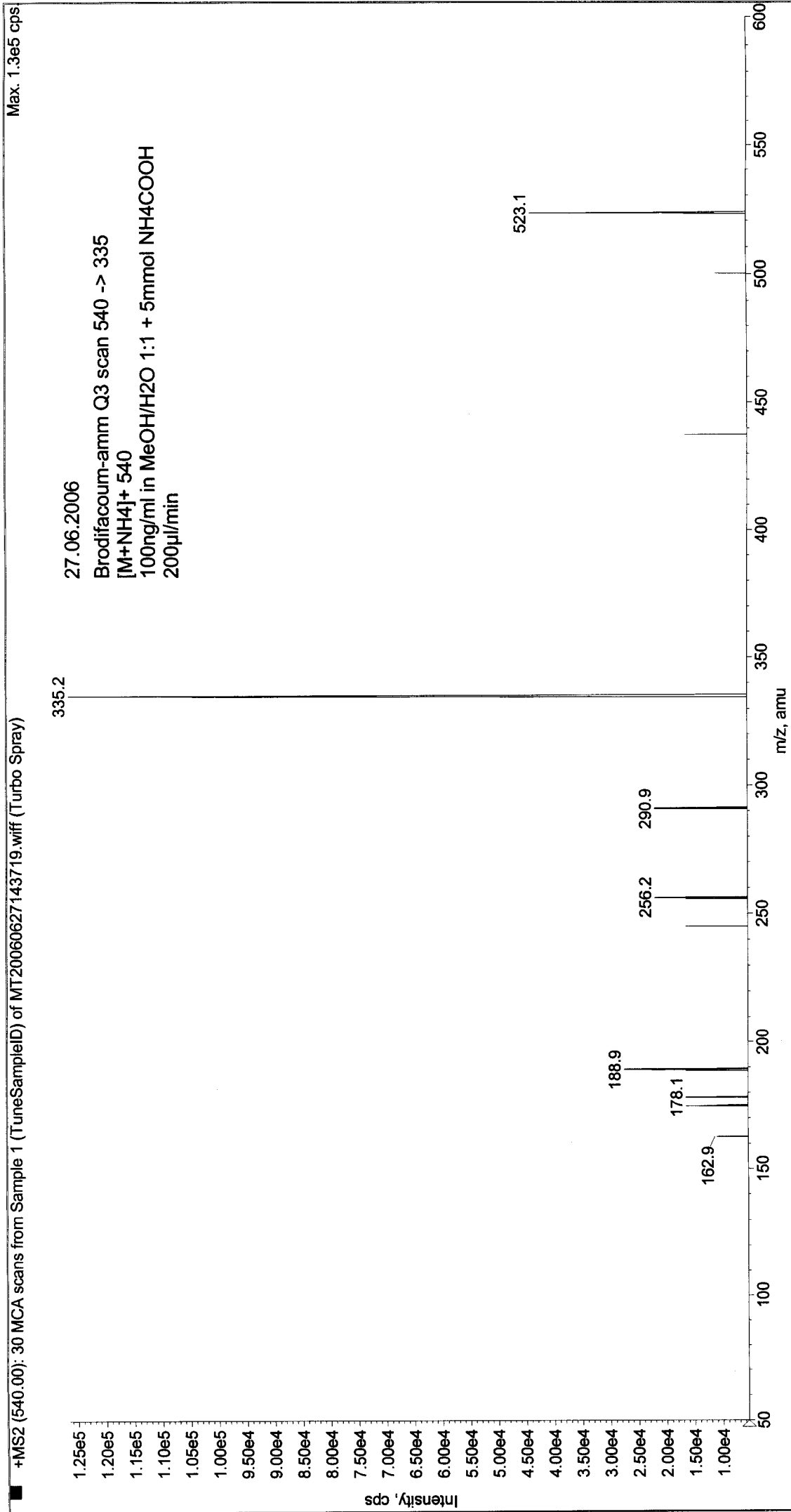
27.06.2006
Brodifacoum-amm Q1 scan
[M+NH4]⁺ 540
100ng/ml in MeOH/H2O 1:1 + 5mmol NH4COOH
200µl/min



Printing Time: 14:38:30
Printing Date: Tuesday, June 27, 2006

Acq. Time: 14:37
Acq. Date: Tuesday, June 27, 2006
Acq. File: MT20060627143719.wiff

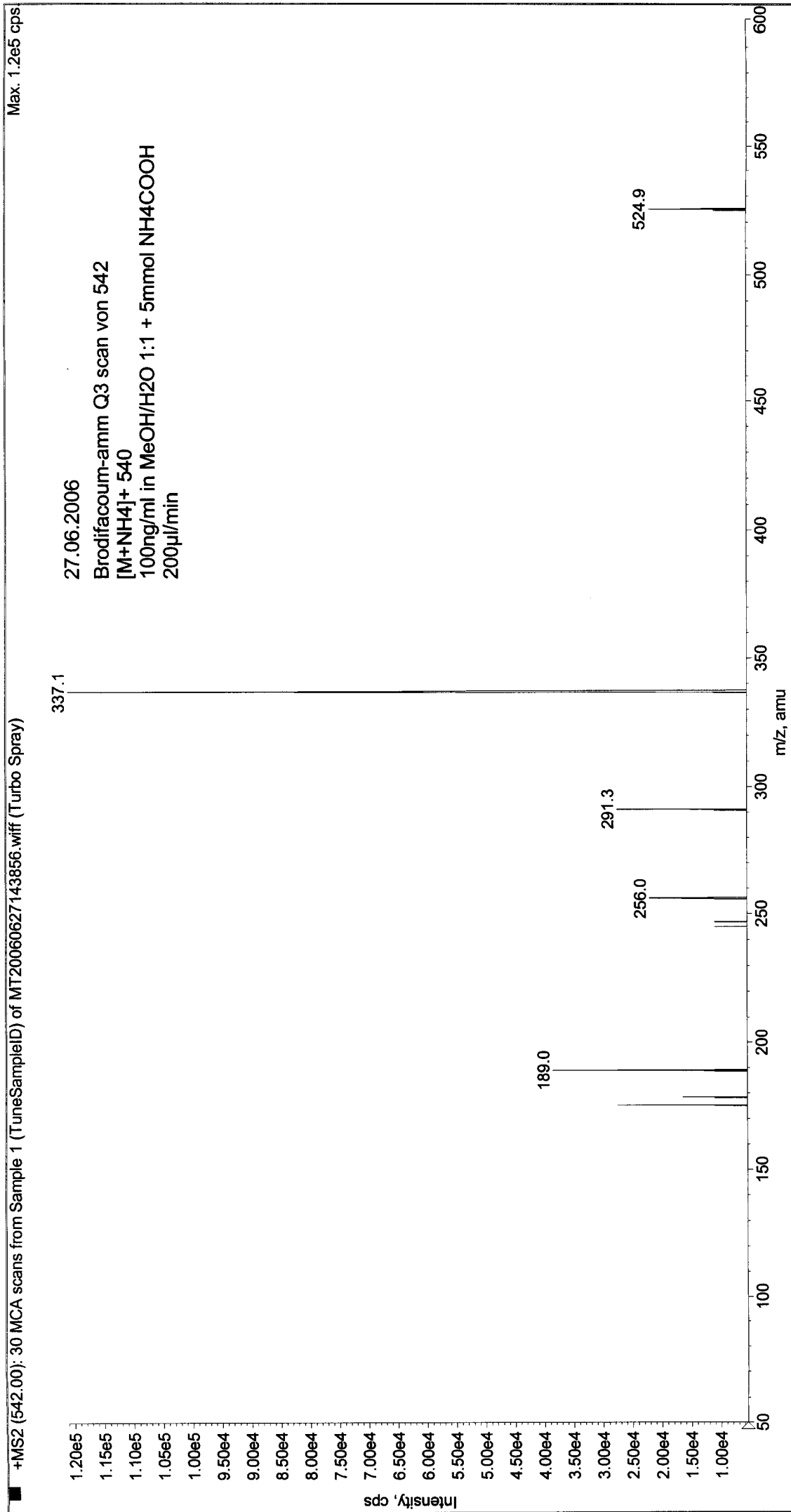
Sample Comment:
Sample Name: TuneSampleID
Batch Name: ManualTune.bat



Printing Time: 14:40:18
Printing Date: Tuesday, June 27, 2006

Acq. Time: 14:38
Acq. Date: Tuesday, June 27, 2006
Acq. File: MT20060627143856.wiff

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



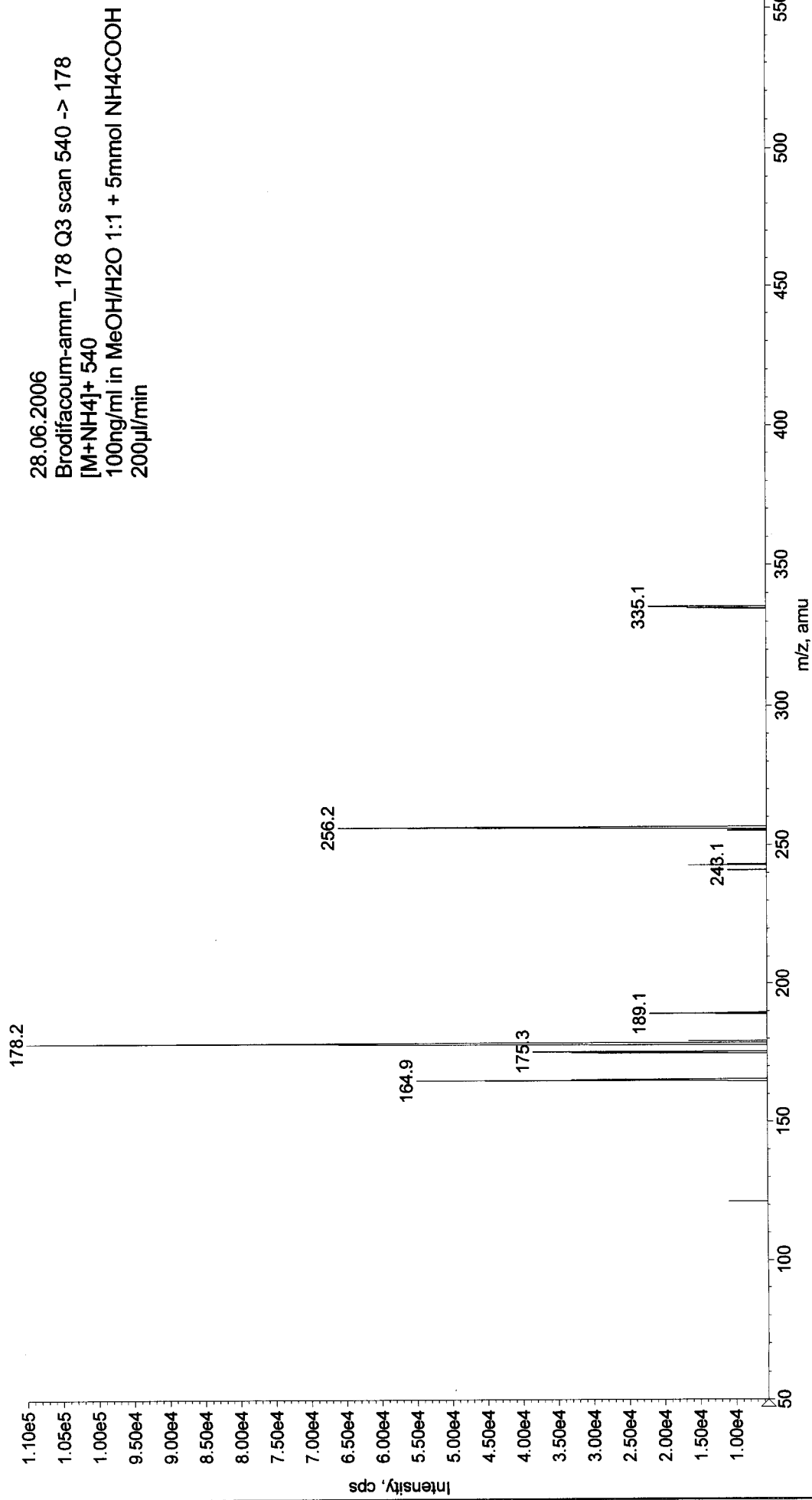
Printing Time: 10:28:27
Printing Date: Wednesday, June 28, 2006

Acq. Time: 10:27
Acq. Date: Wednesday, June 28, 2006
Acq. File: MT20060628102702.wiff

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

■ +MS2 (540.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20060628102702.wiff (Turbo Spray)

Max. 1.1e5 cps



Printing Time: 10:30:09
Printing Date: Wednesday, June 28, 2006

Acq. Time: 10:28
Acq. Date: Wednesday, June 28, 2006
Acq. File: MT20060628102853.wiff

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

