

MS/MS Parameters of Pesticides

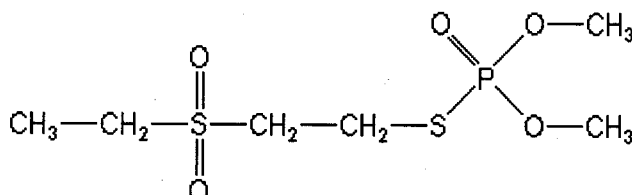
Analyte: Demeton-S-methyl-sulfon

CAS No.: 17040-19-6

Formula: C₆H₁₅O₅PS₂

Molecular mass (lowest isotopes): 262,01 amu

Structure:



Ionisation: ESI +

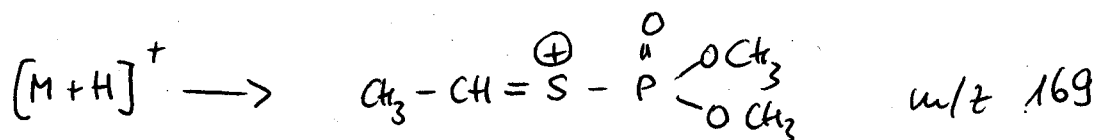
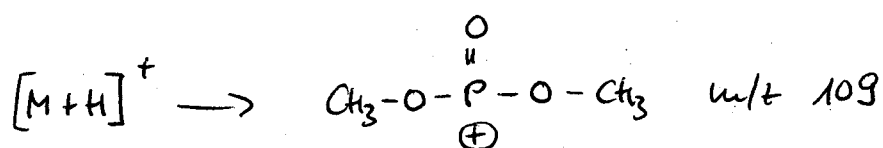
Quasimolecular ion: 263,0 amu = [M+H]⁺

Analyte sensitive parameter set (API 2000)

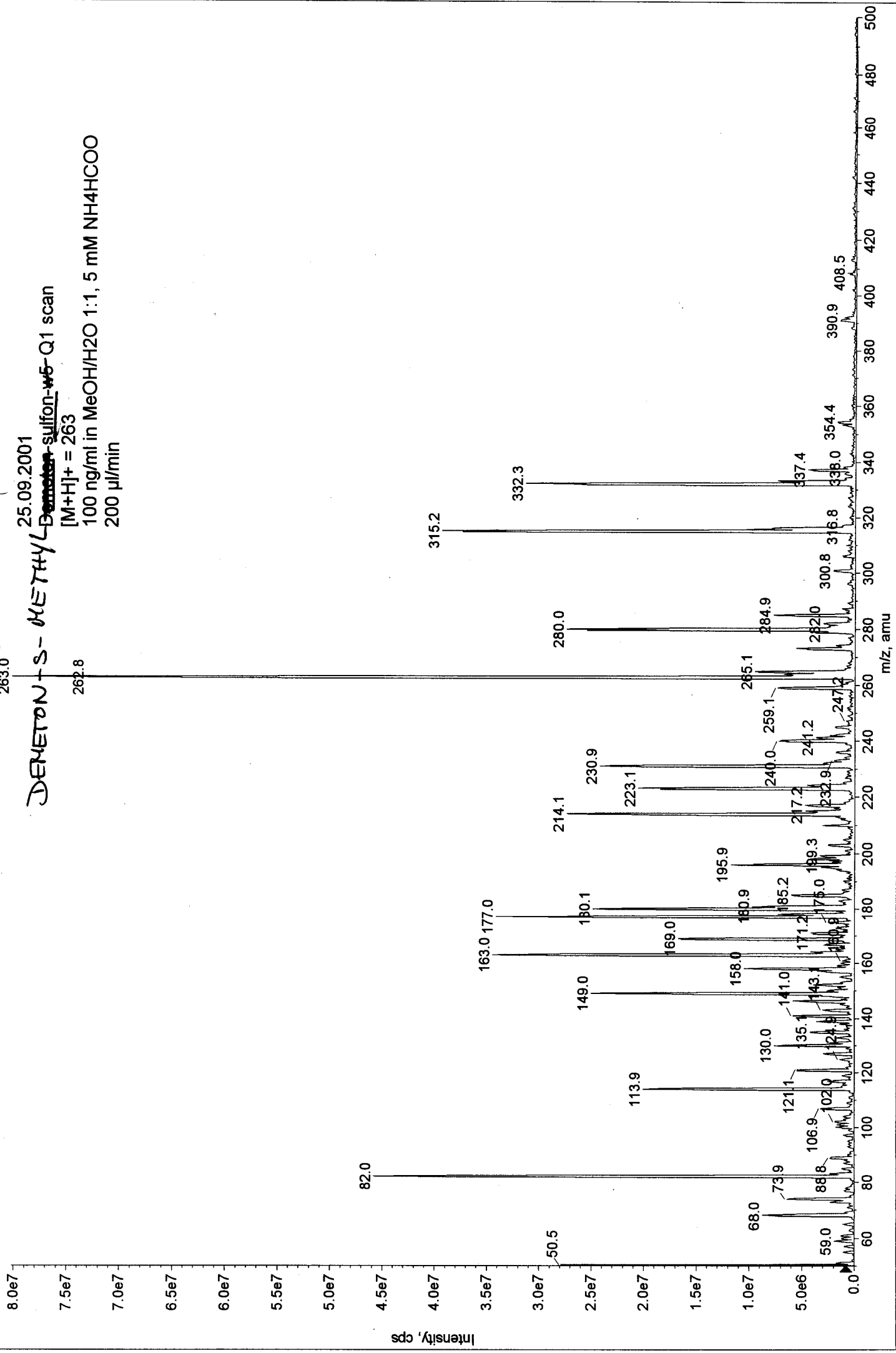
Transition	263,0 → 108,9	263,0 → 169,0
Declustering potential (DP) ^{*)}	69 V	69 V
Focusing potential (FP)	360 V	370 V
Entrance potential (EP)	12,0 V	12,0 V
Collision cell entrance potential (CEP)	18 V	20 V
Collision energy (CE)	37 V	21 V
Collision cell exit potential (CXP)	6 V	8 V

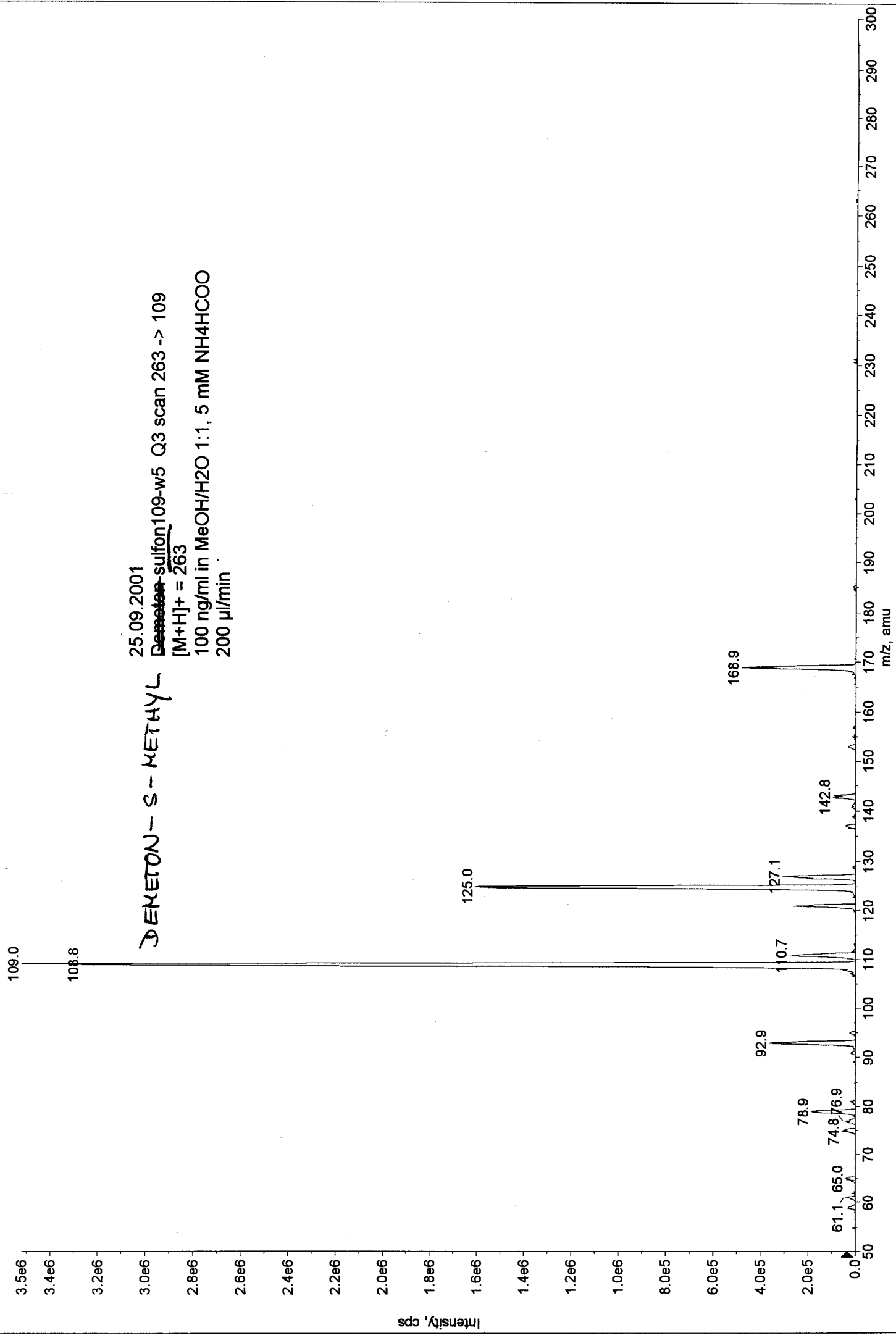
^{*)} For API 3000 and 4000 enhance DP by 20V

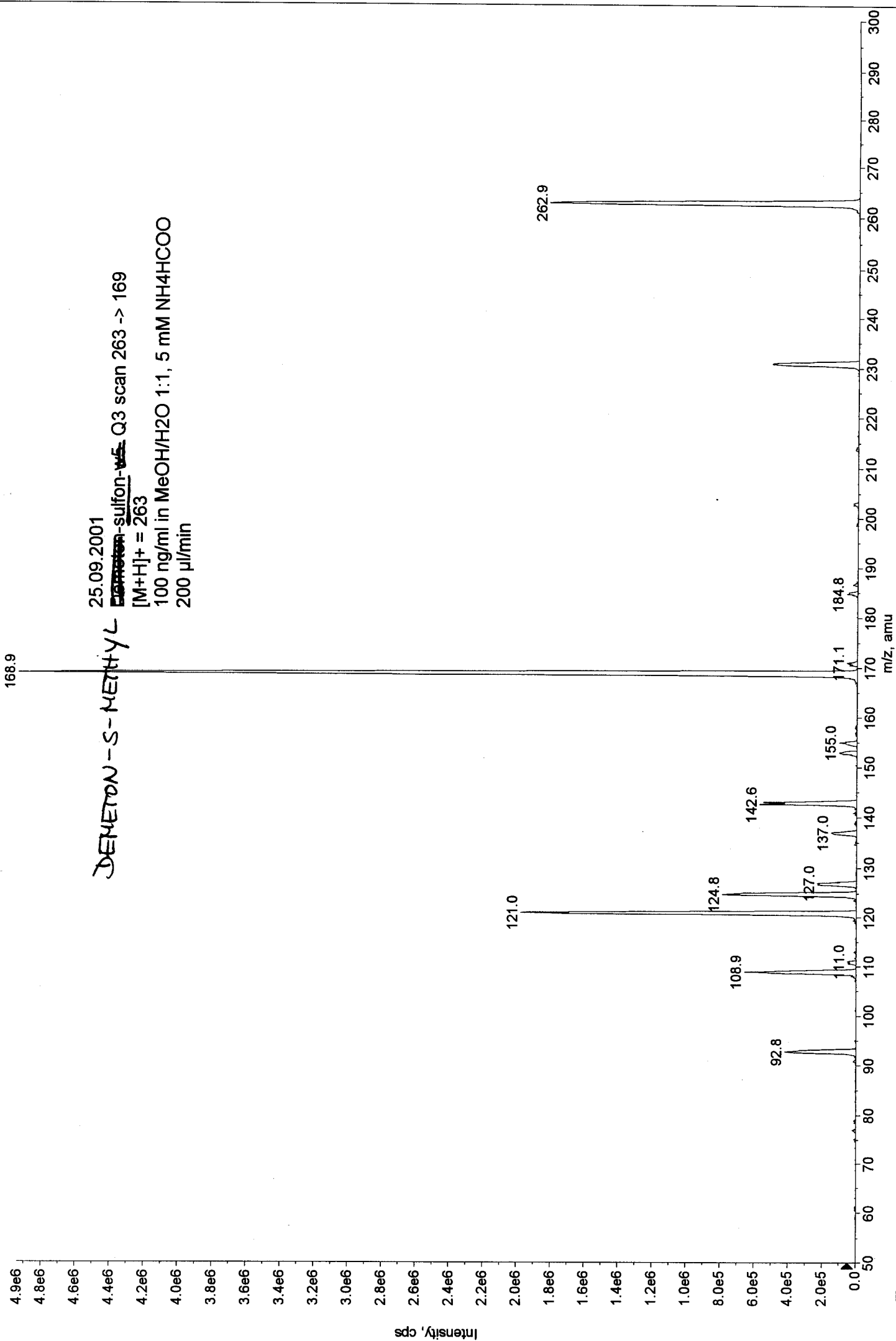
Fragmentation



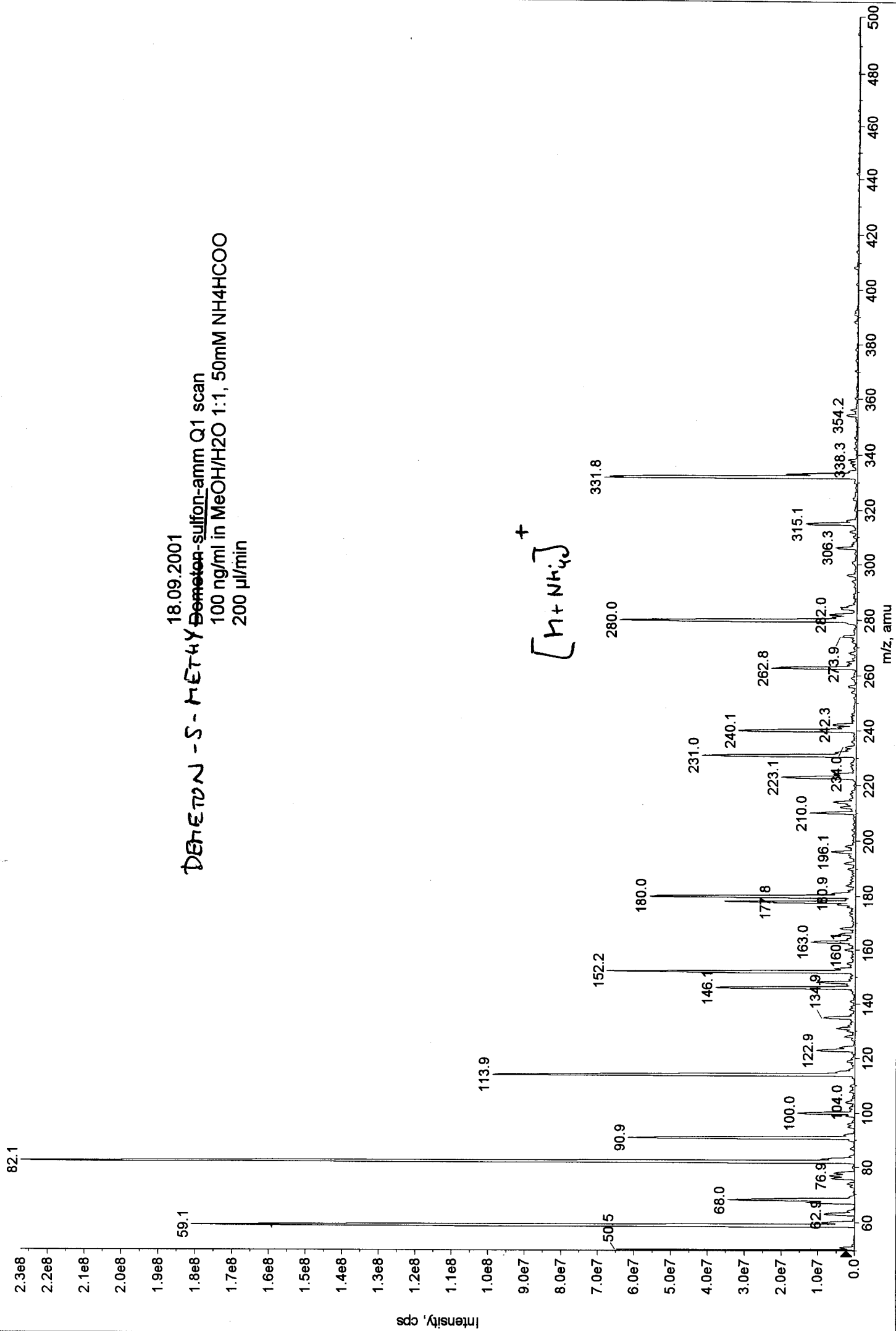
25.09.2001
DEMETON-S-METHYL
~~Demeton-sulfon-w5~~-Q1 scan
[M+H]⁺ = 263
100 ng/ml in MeOH/H₂O 1:1, 5 mM NH₄HCOO
200 µl/min



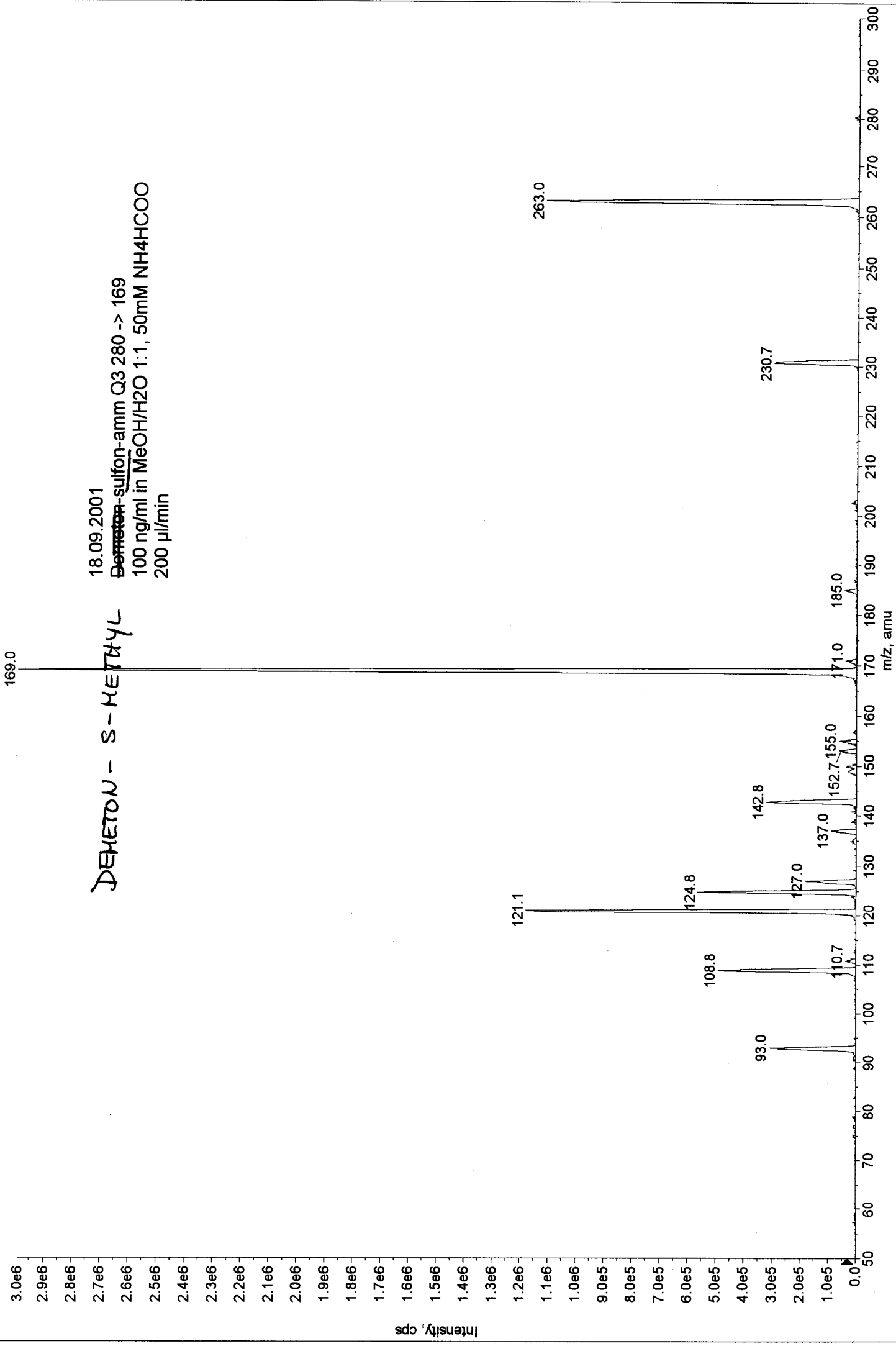




18.09.2001
Demeton-sulfon-amm Q1 scan
100 ng/ml in MeOH/H2O 1:1, 50mM NH4HCOO
200 µl/min



$[M + NH_4]^+$



DEKETON - S-METHYL

18.09.2001
~~Demeton~~-sulfon-amm Q3 280 -> 169
100 ng/ml in MeOH/H2O 1:1, 50mM NH4HCOO
200 µl/min