

**BfR**

Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

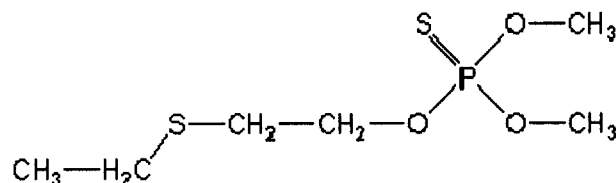
Analyte: Demeton-O-methyl

CAS No.: 867-27-6

Formula: C₆H₁₅O₃PS₂

Molecular mass (lowest isotopes): 230,02 amu

Structure:



Ionisation: ESI +

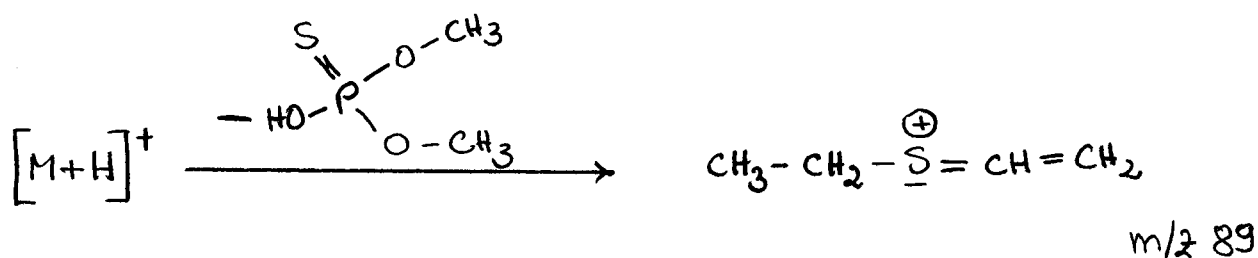
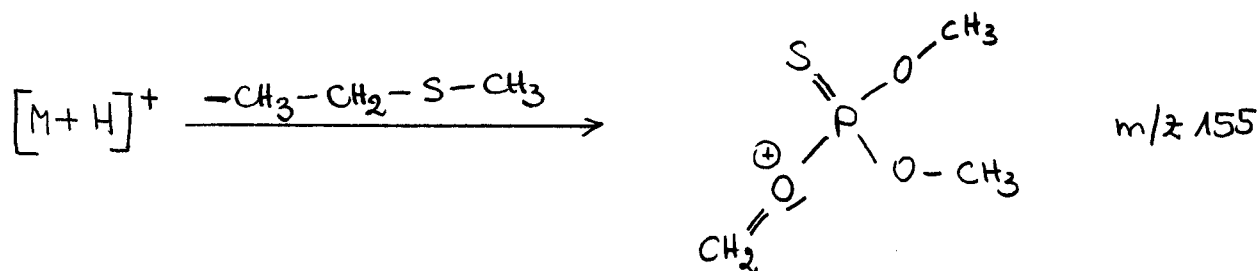
Quasimolecular ion: 231,0 amu = [M+H]⁺

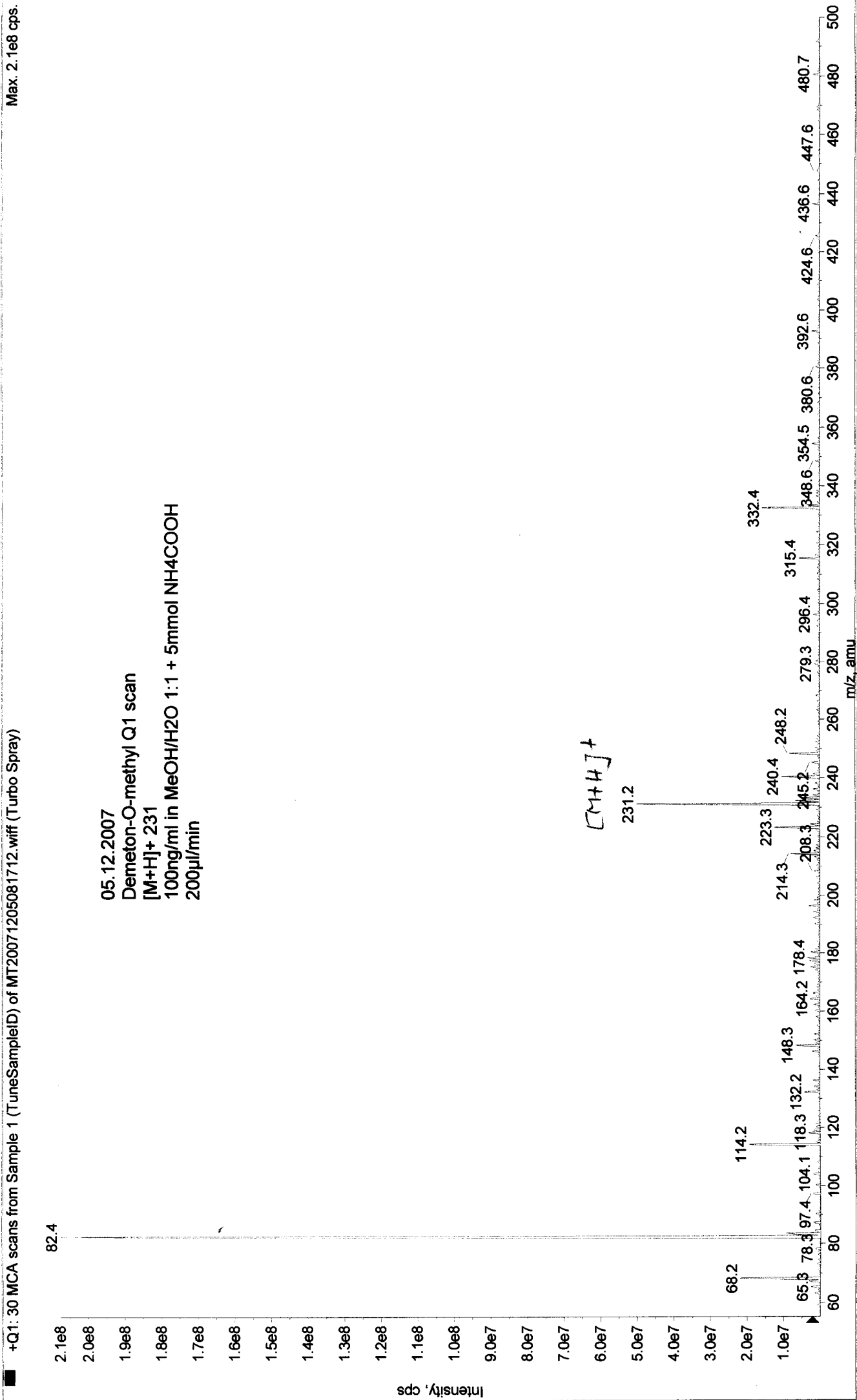
Analyte sensitive parameter set (API 2000)

Transition	231,0 → 155,0	231,0 → 89,1
Declustering potential (DP) ^{*)}	3,5 V	3,5 V
Focusing potential (FP)	360 V	360 V
Entrance potential (EP)	8 V	8 V
Collision cell entrance potential (CEP)	16 V	16 V
Collision energy (CE)	17 V	17 V
Collision cell exit potential (CXP)	8 V	4 V

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

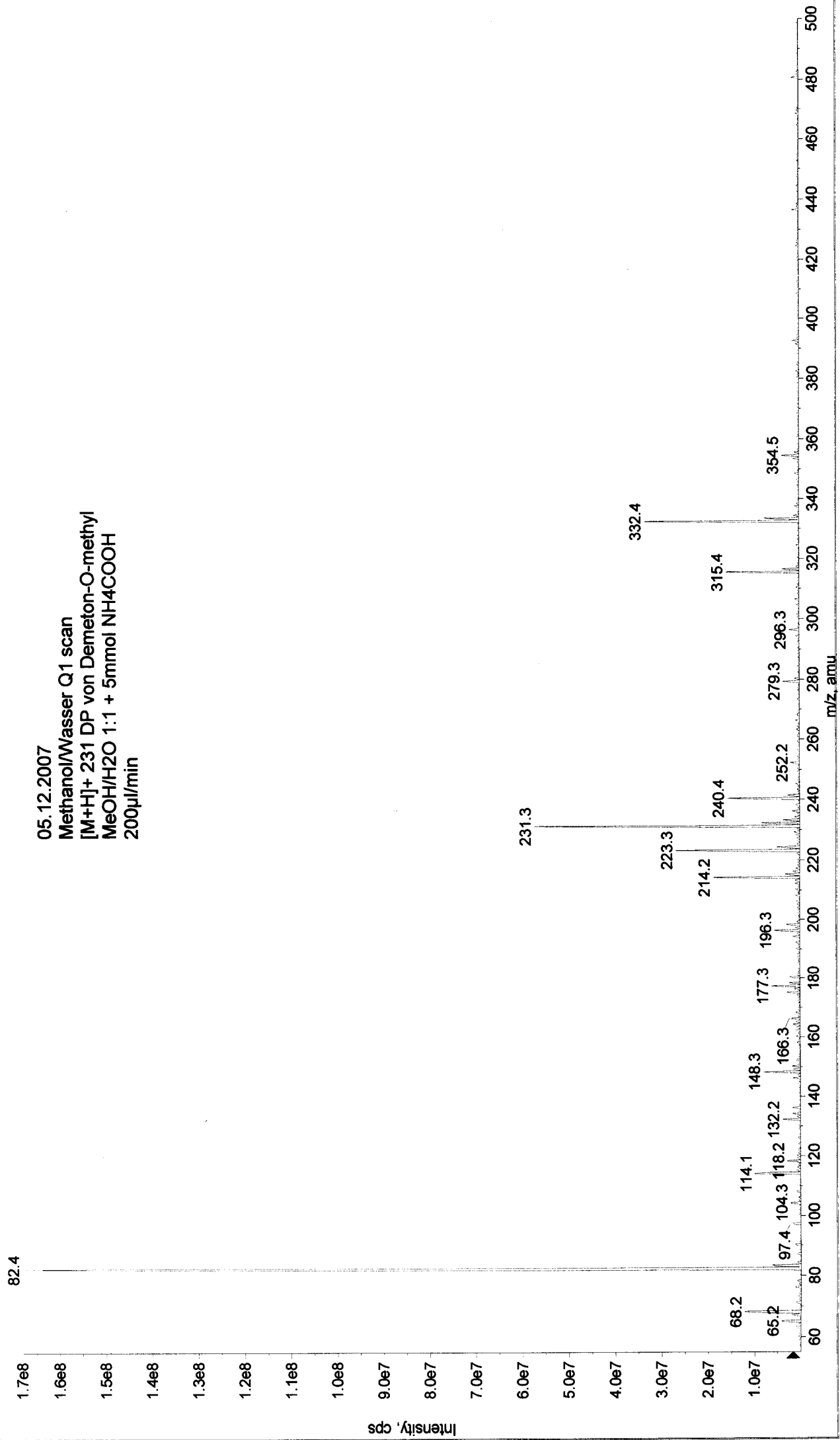
Fragmentation



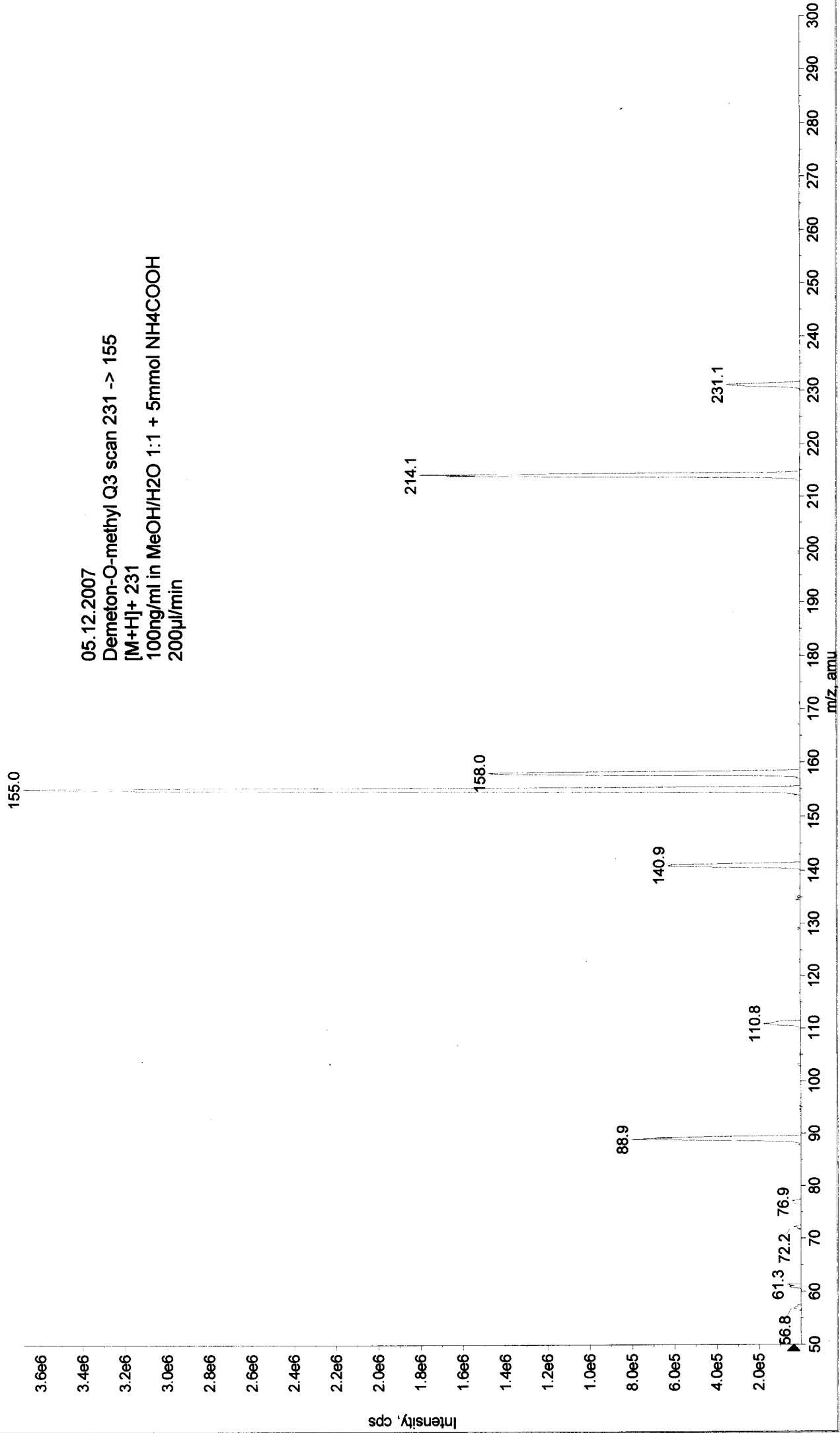


■ +Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205110808.wiff (Turbo Spray)

Max. 1.7e8 cps.

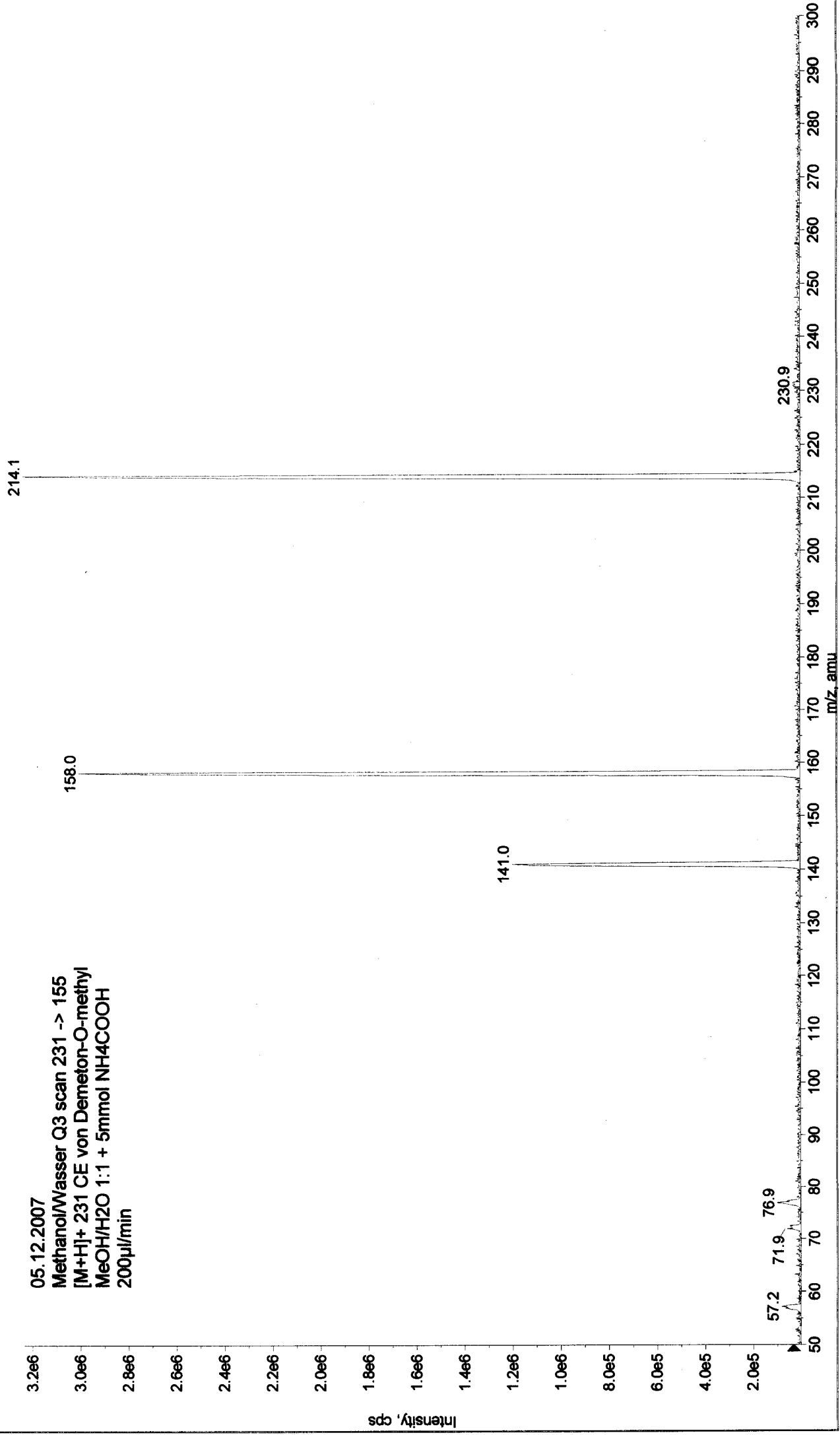


■ +MS2 (231.10): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205082133.wiff (Turbo Spray)

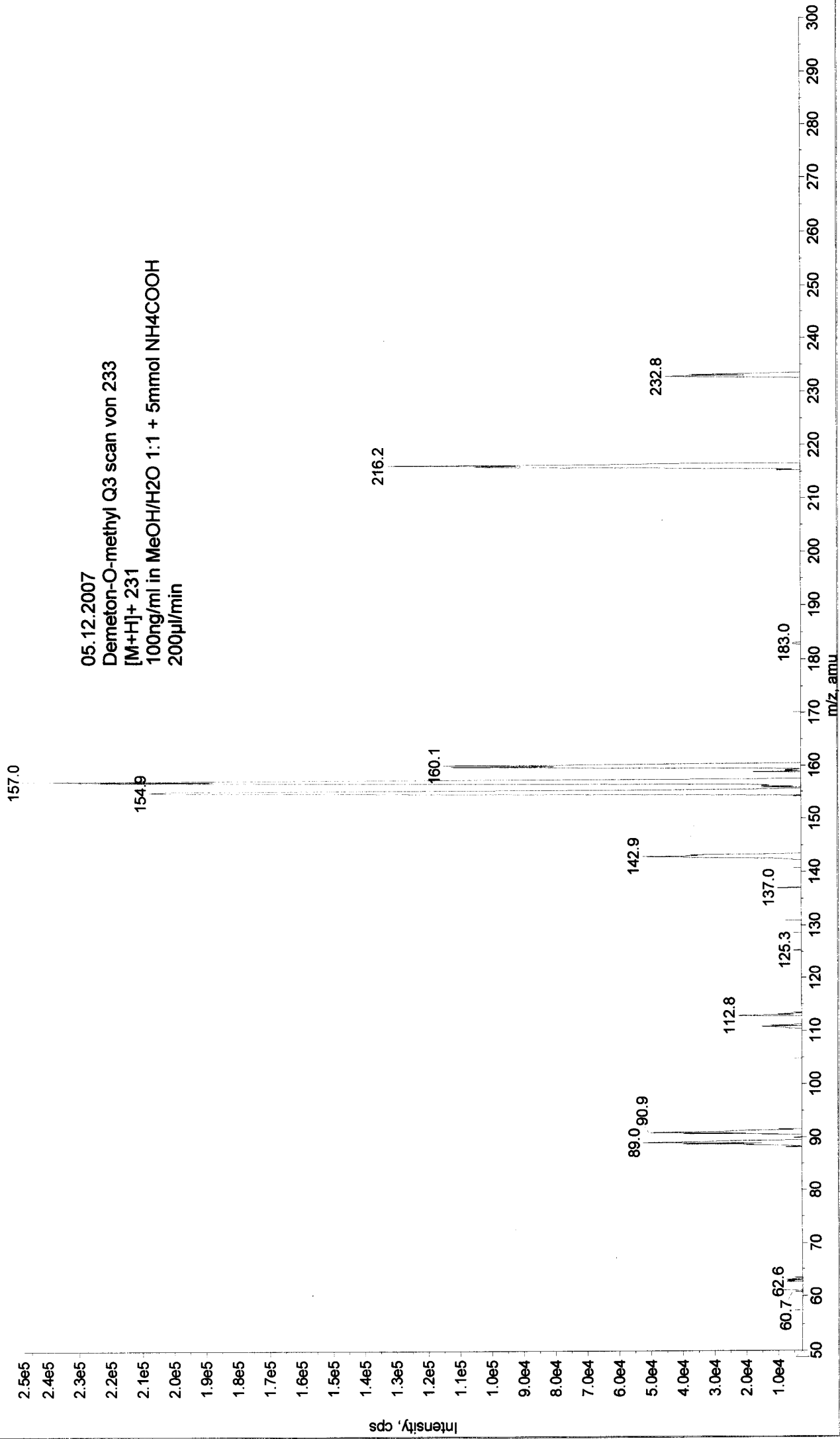


■ +MS2 (231.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205105933.wiff (Turbo Spray)

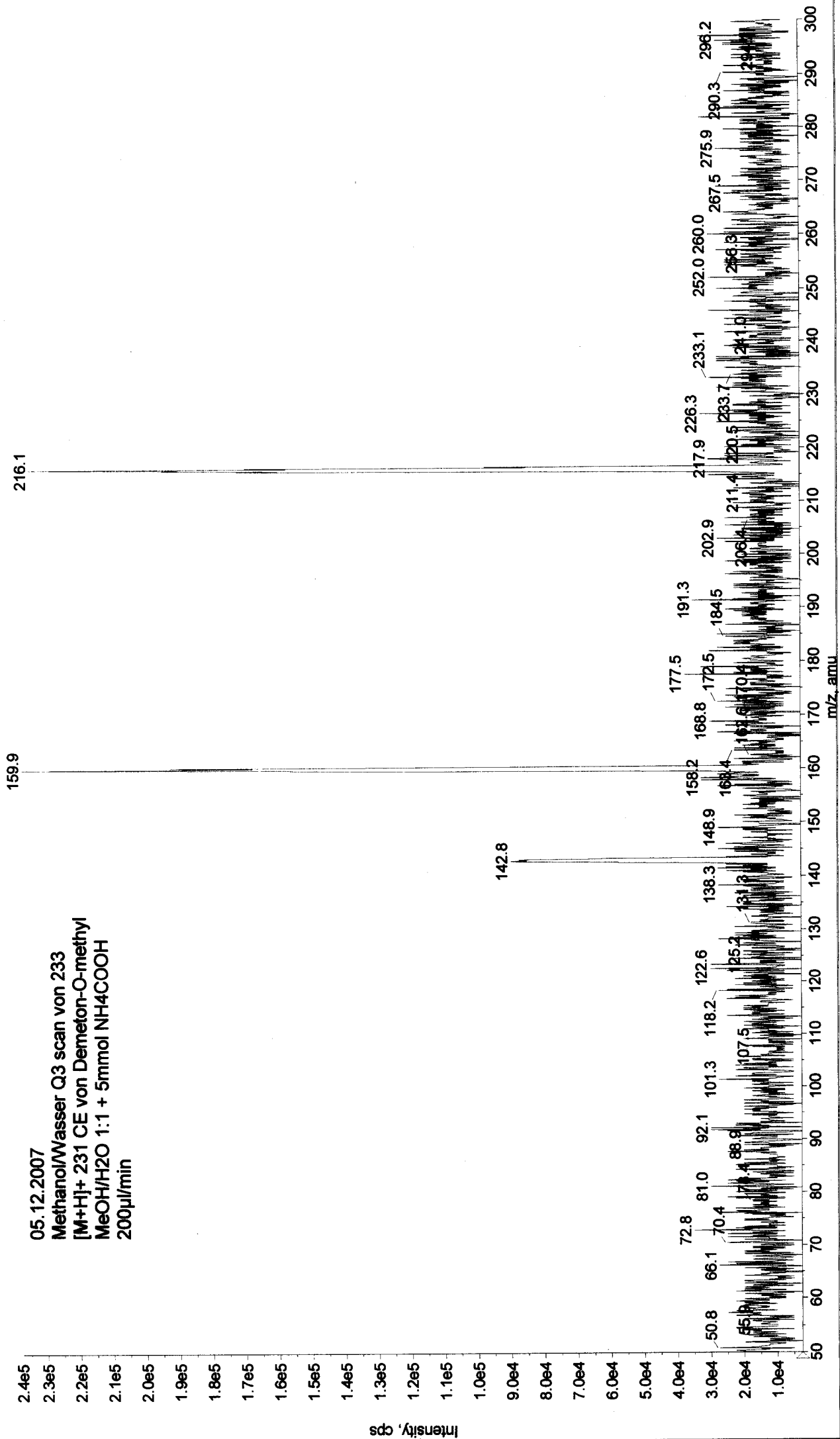
05.12.2007
Methanol/Wasser Q3 scan 231 -> 155
[M+H]⁺ 231 CE von Demeton-O-methyl
MeOH/H₂O 1:1 + 5mmol NH₄COOH
200µl/min



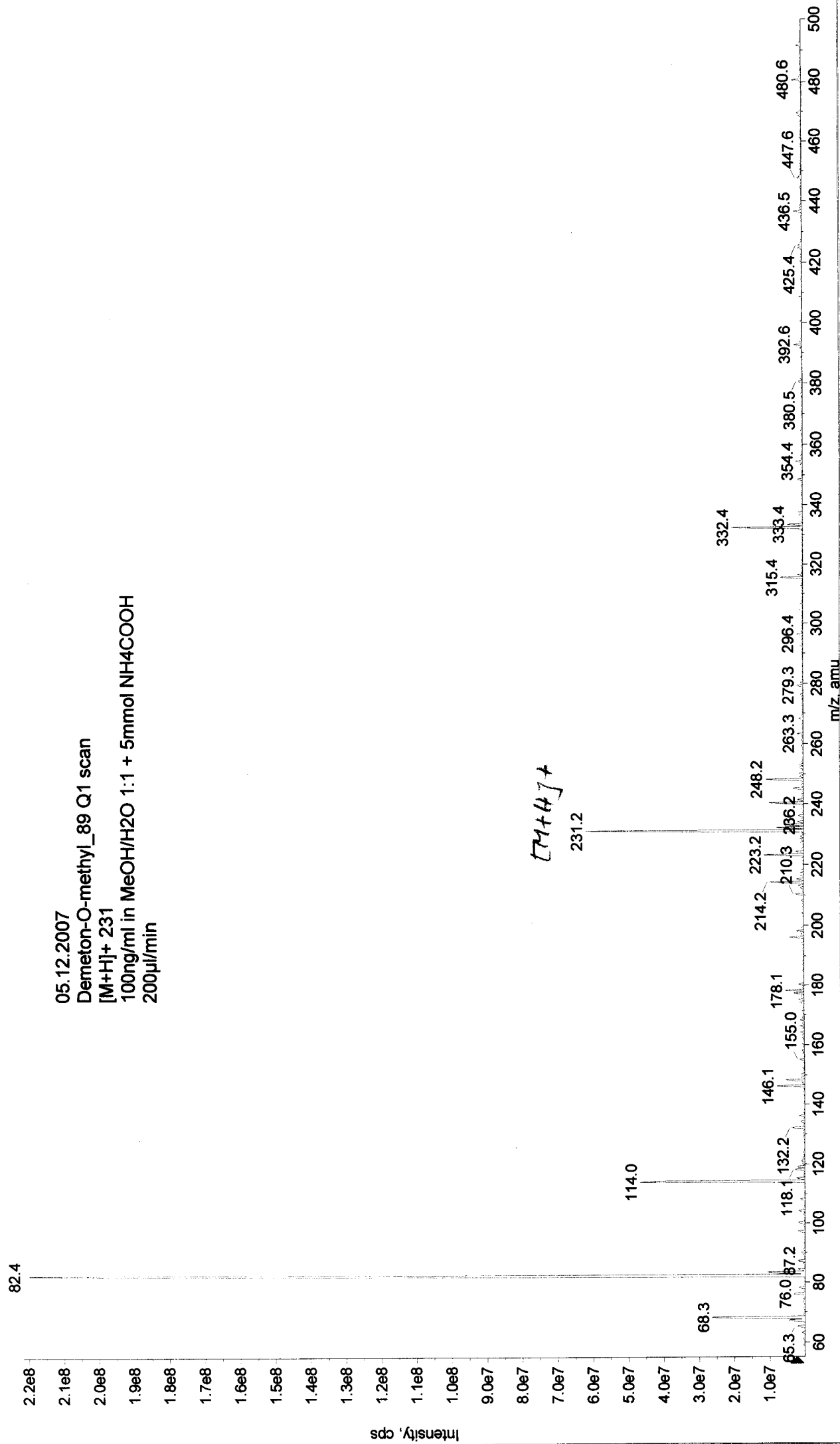
■ +MS2 (233.10): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205082505.wiff (Turbo Spray)

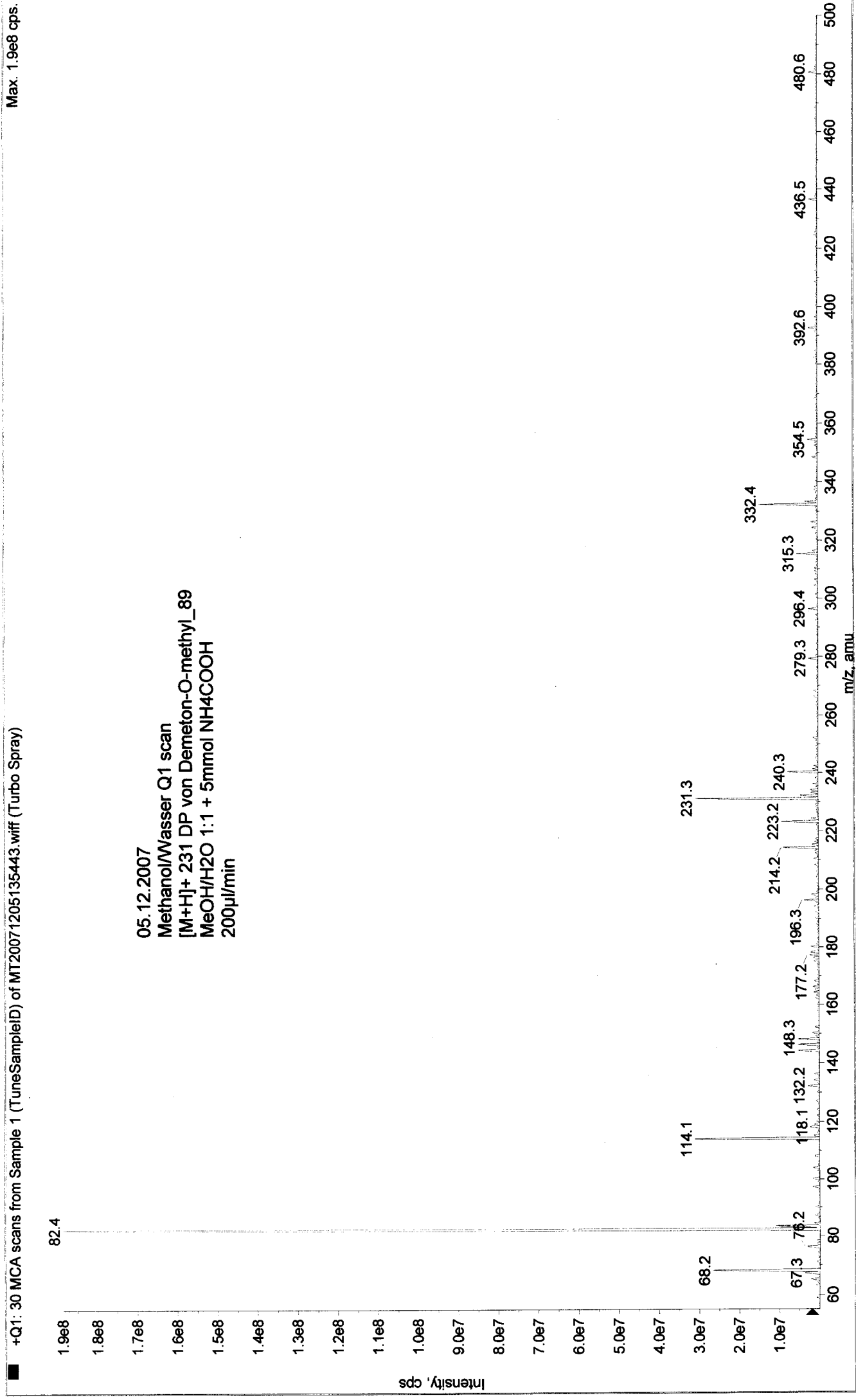


■ +MS2 (233.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205111558.wiff (Turbo Spray)

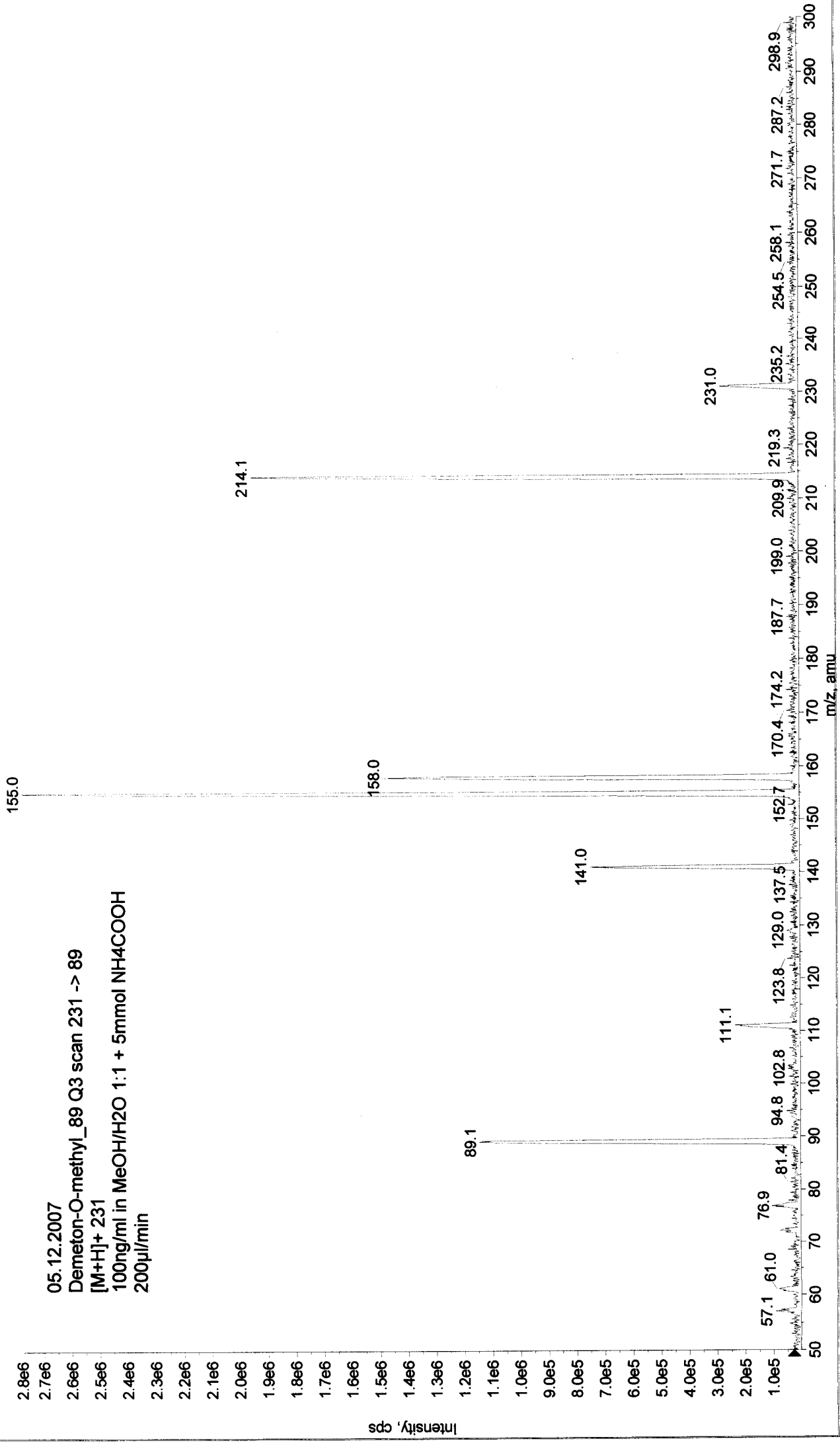


Max. 2.2e8 cps.



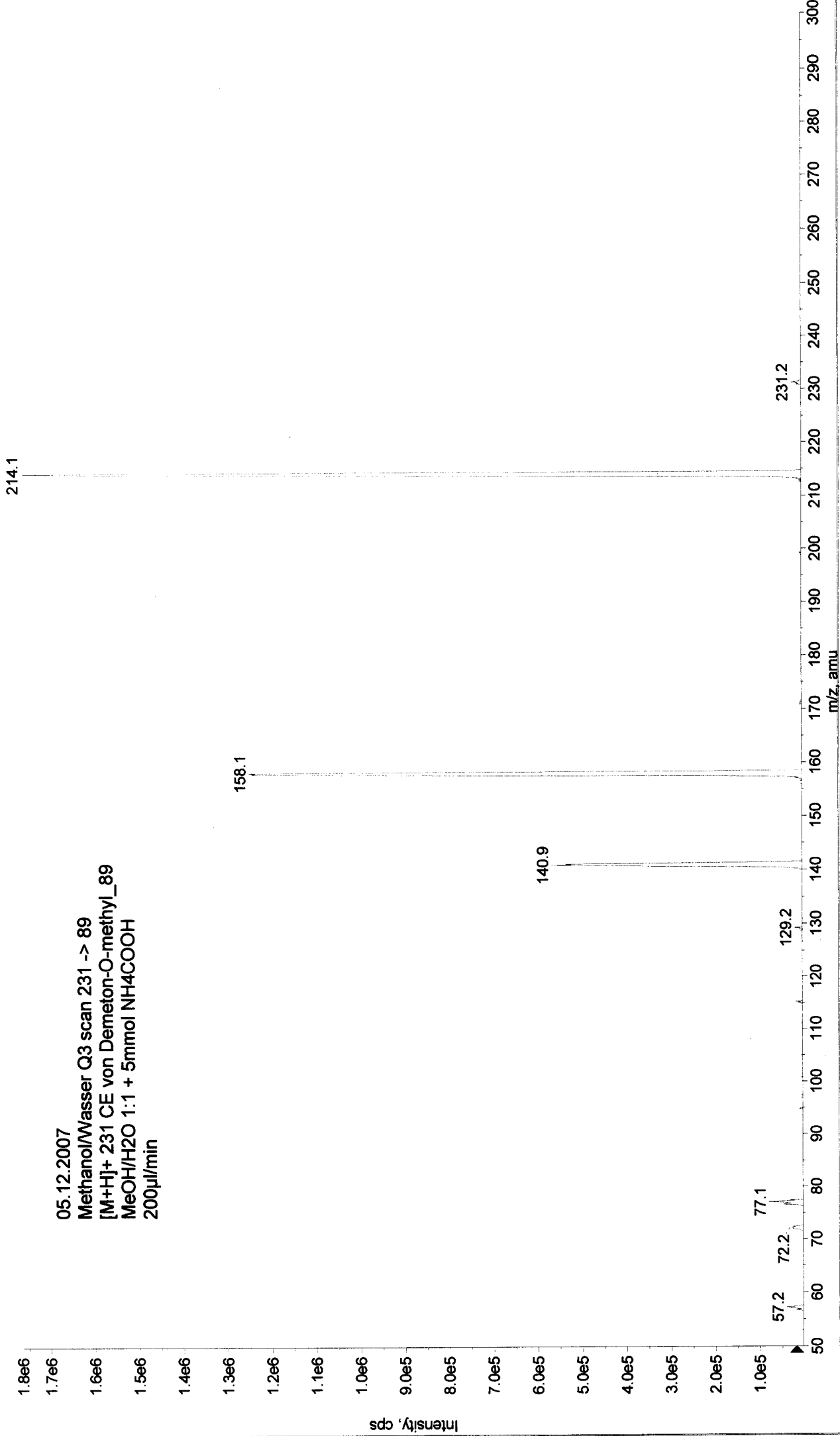


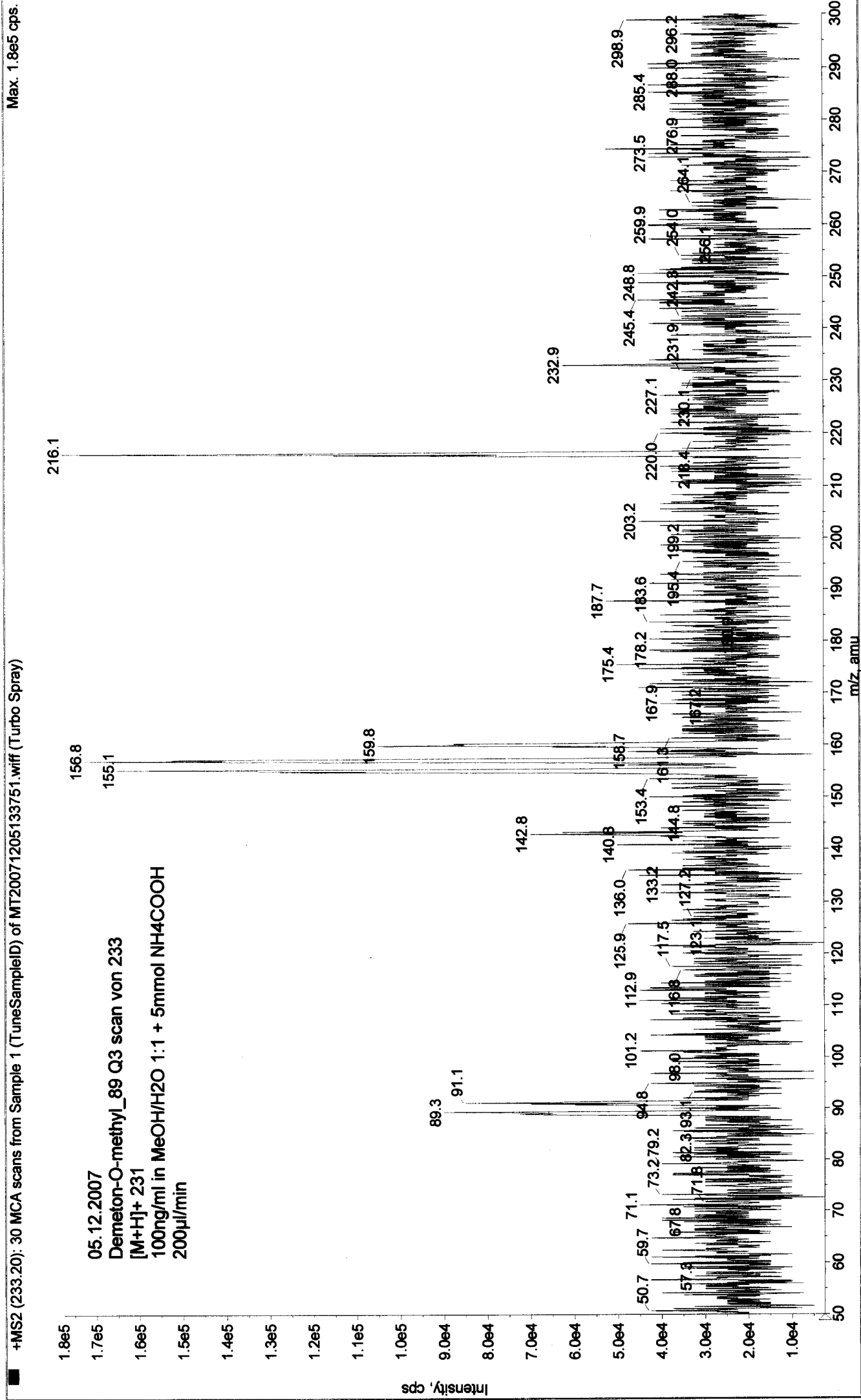
+MS2 (231.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205133616.wiff (Turbo Spray)



■ +MS2 (231.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205135745.wiff (Turbo Spray)

Max. 1.8e6 cps.





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Batch Name: ManualTune.bat
Sample Name: TuneSampleID
Sample Comment:
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+MS2 (233.20): 30 MCA scans from Sample 1 (TuneSampleID) of MT20071205135945 wiff (Turbo Spray)

