

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

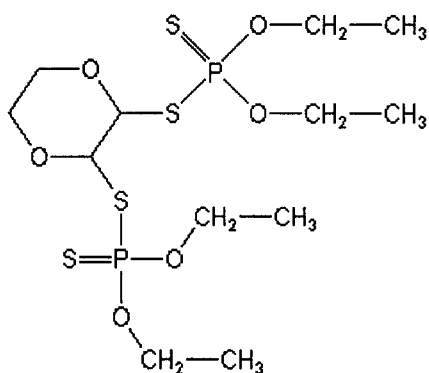
### Analyte: Dioxathion

CAS No.: 78-34-2

Formula: C<sub>12</sub>H<sub>26</sub>O<sub>6</sub>P<sub>2</sub>S<sub>4</sub>

Molecular mass (lowest isotopes): 456,01 amu

Structure:



Ionisation: ESI +

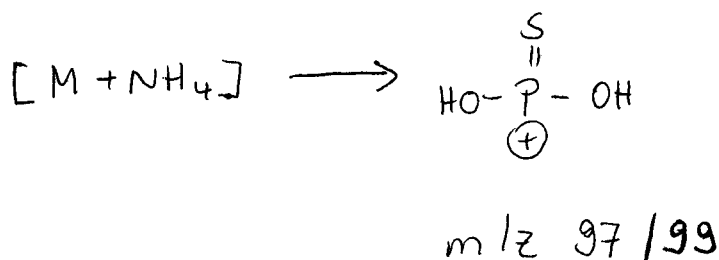
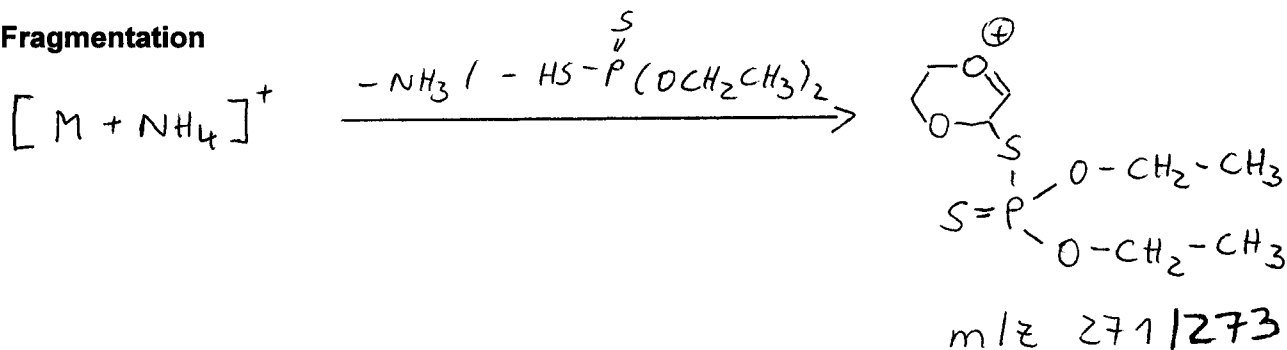
Quasimolecular ion: 474,0 amu = [M+NH<sub>4</sub>]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	474,0 → 271,0	474,0 → 97,1
Declustering potential (DP)*)	26V	26 V
Focusing potential (FP)	360 V	360 V
Entrance potential (EP)	6,5 V	11,5 V
Collision cell entrance potential (CEP)	20 V	20 V
Collision energy (CE)	19 V	61 V
Collision cell exit potential (CXP)	14 V	4 V

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

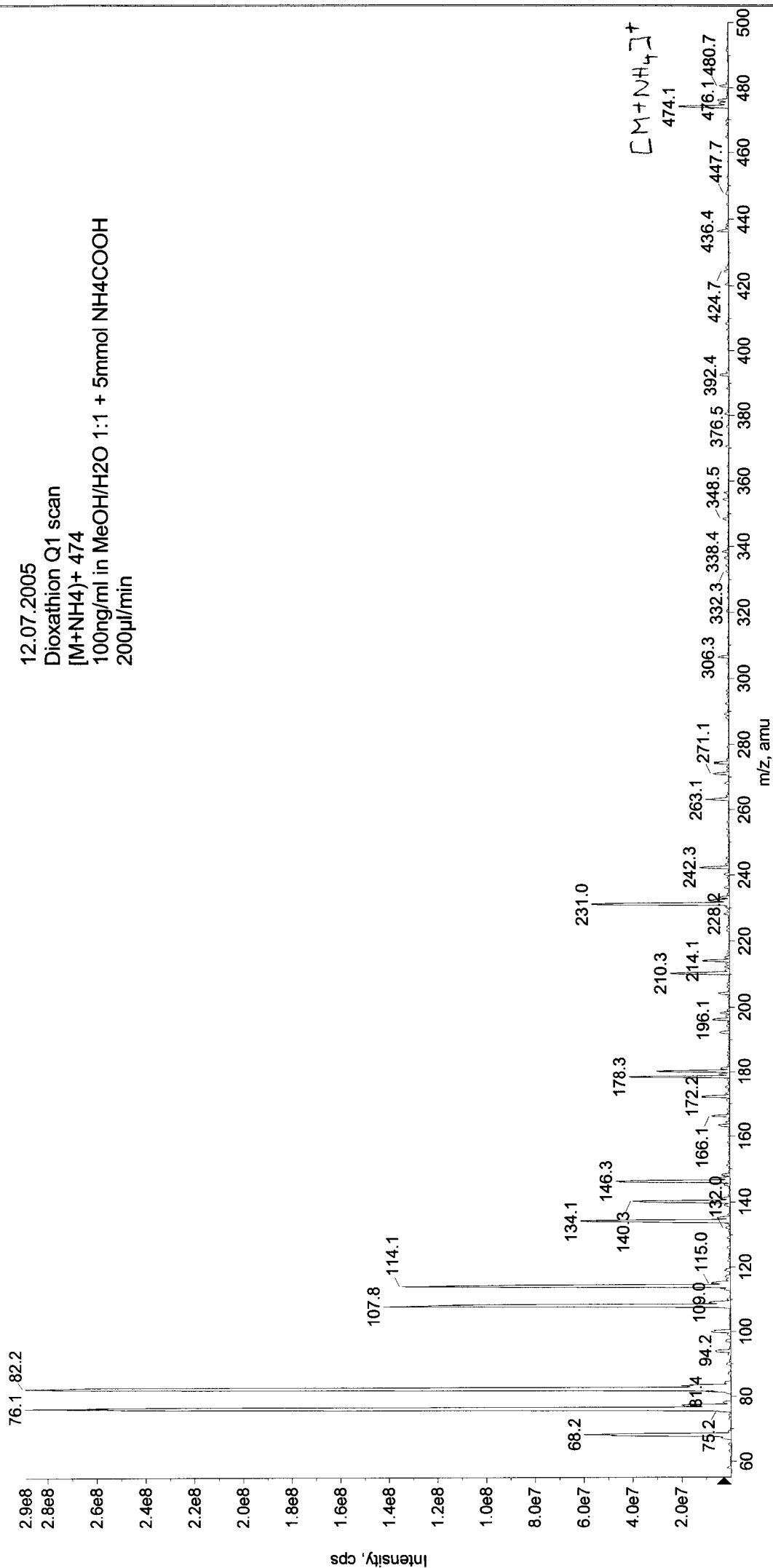
### Fragmentation

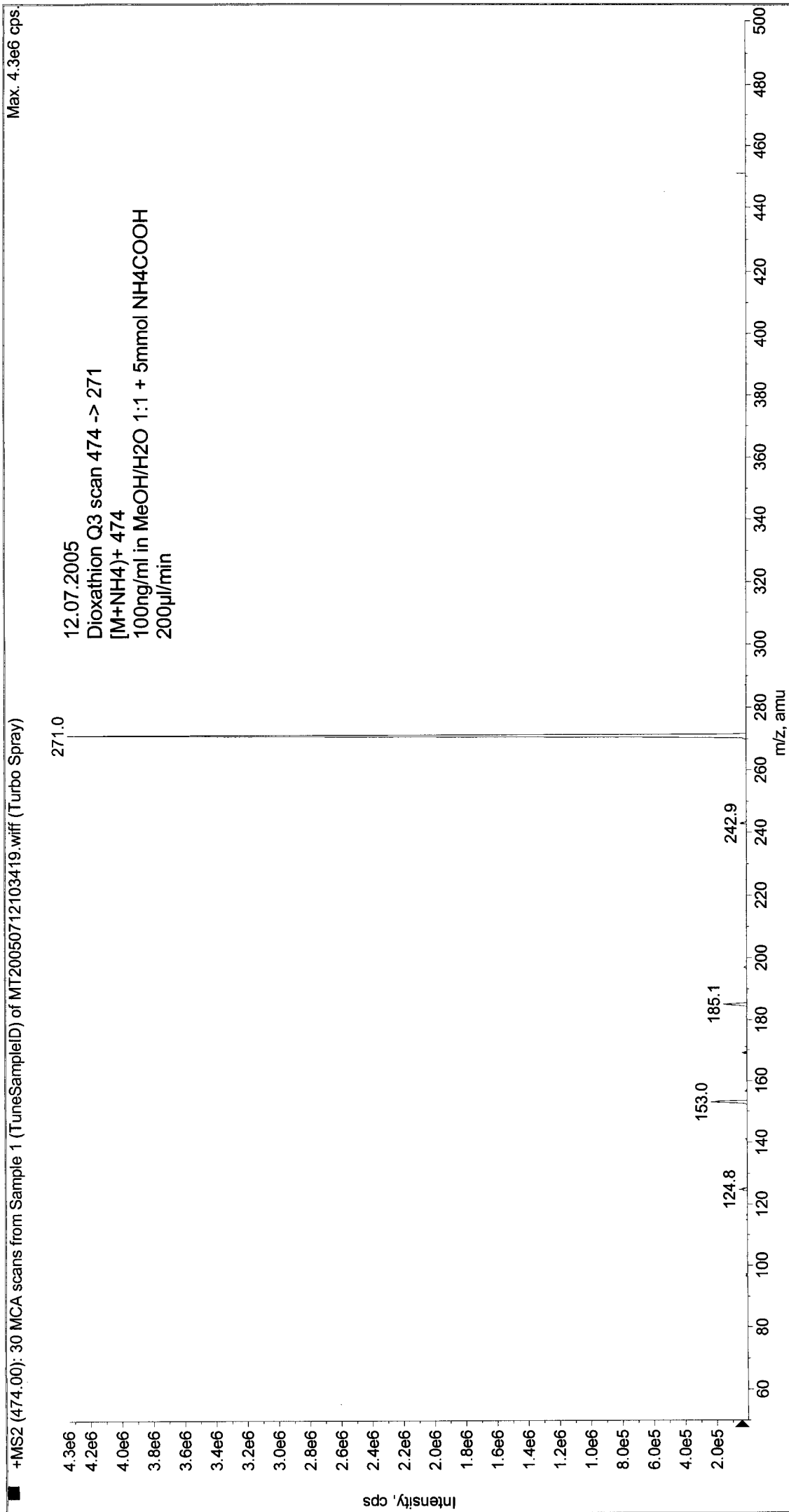


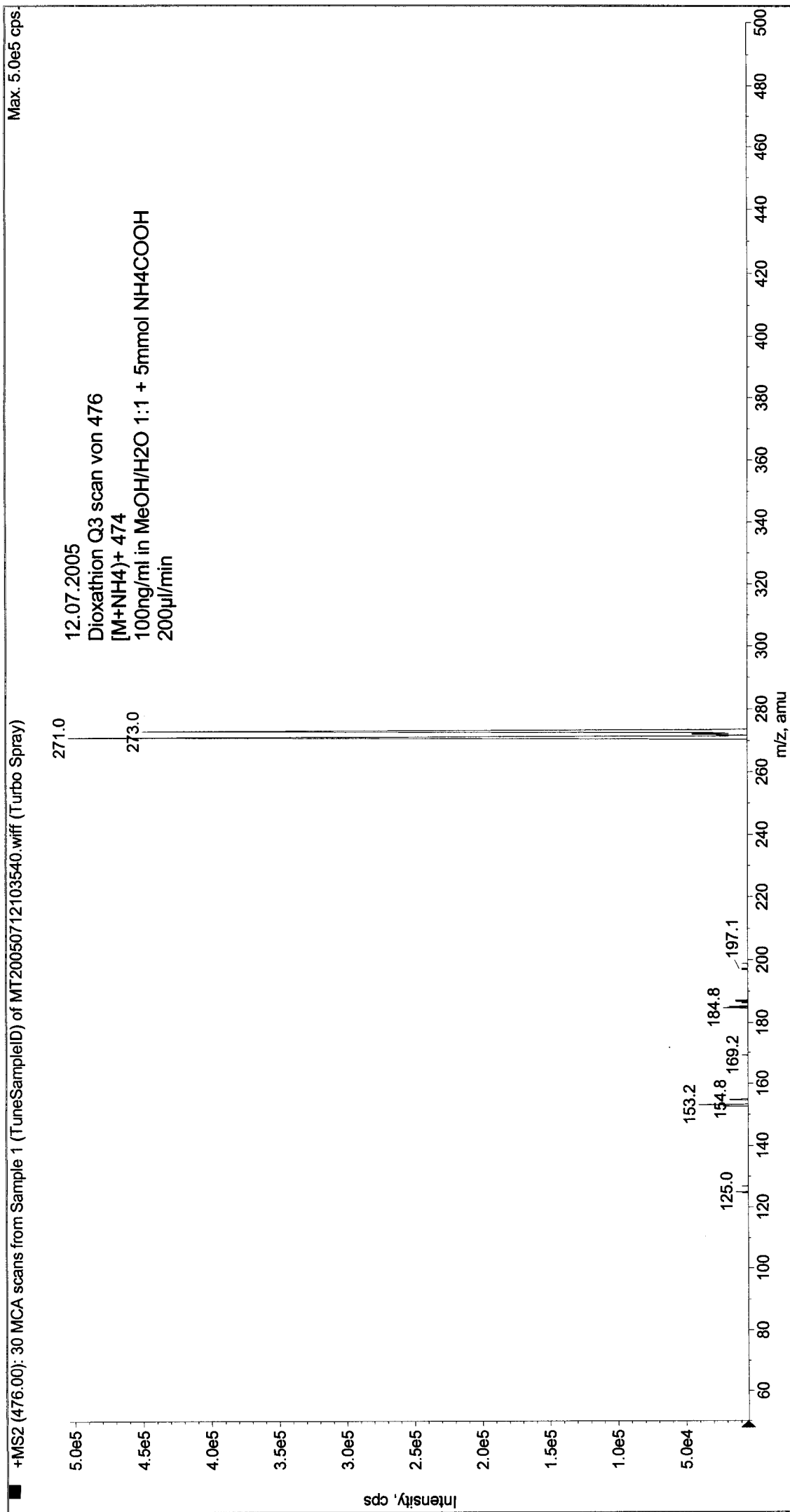
+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20050712103052.wiff (Turbo Spray)

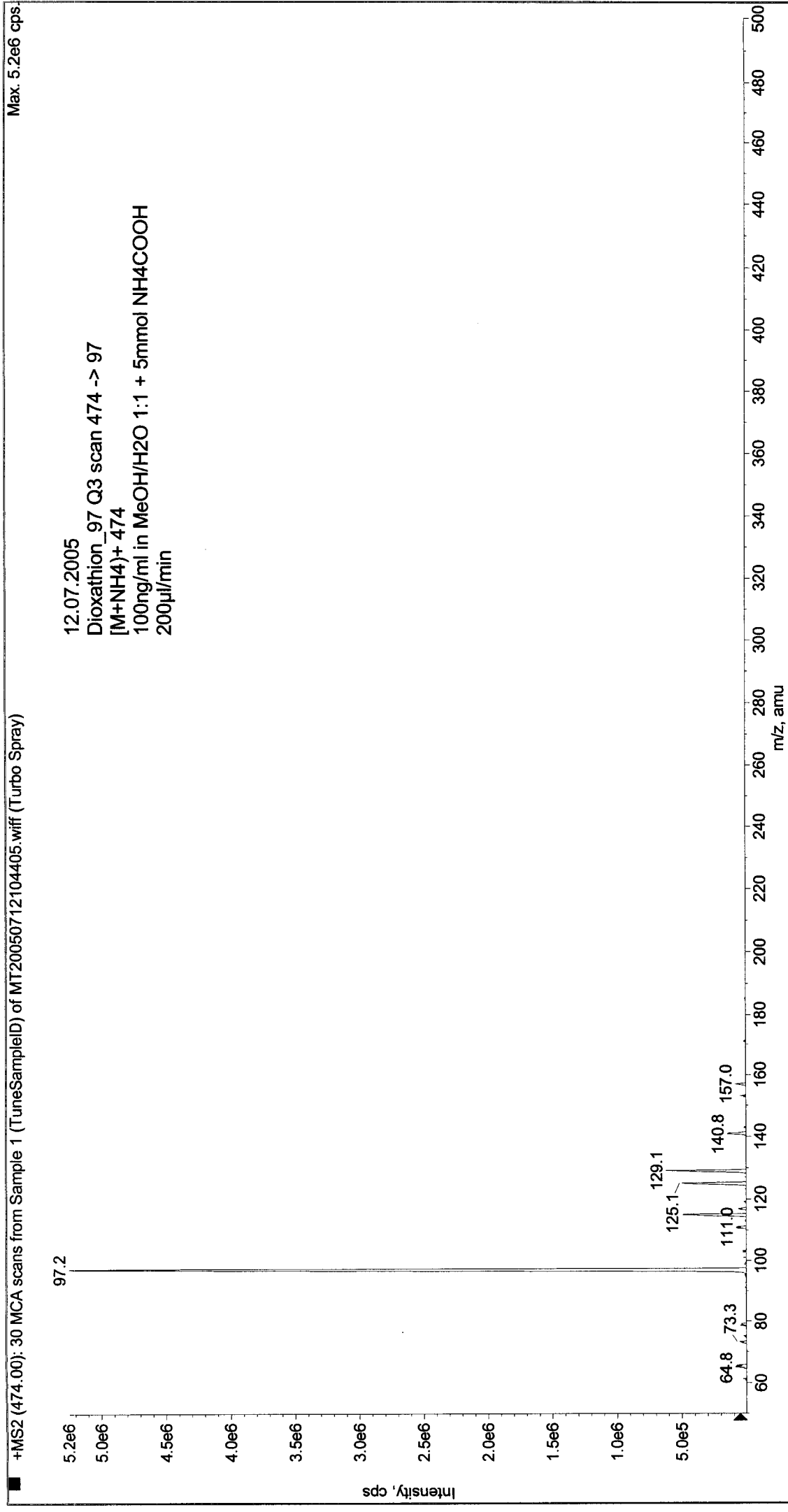
Max. 2.9e8 cps

12.07.2005  
Dioxathion Q1 scan  
[M+NH<sub>4</sub>]<sup>+</sup> 474  
100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
200µl/min









■ +MS2 (476.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050712104521.wiff (Turbo Spray)

Max. 6.9e5 cps.

