

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

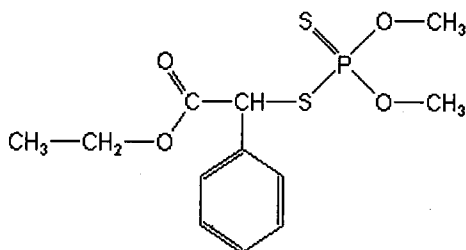
### Analyte: Phenthoate

CAS No.: 2597-03-7

Formula: C<sub>12</sub>H<sub>17</sub>O<sub>4</sub>PS<sub>2</sub>

Molecular mass (lowest isotopes): 320,03 amu

Structure:



Ionisation: ESI +

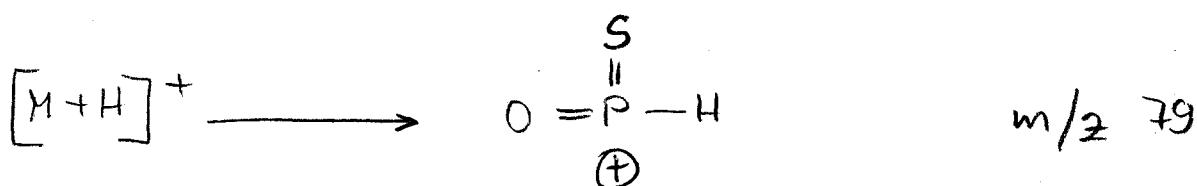
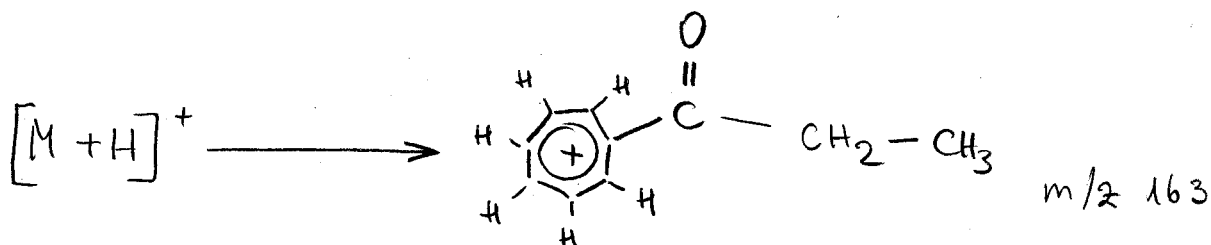
Quasimolecular ion: 321,0 amu = [M+H]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	321,0 → 163,1	321,0 → 79,1
Declustering potential (DP) <sup>*)</sup>	36 V	36 V
Focusing potential (FP)	340 V	370 V
Entrance potential (EP)	11,5 V	11,0 V
Collision cell entrance potential (CEP)	20 V	22 V
Collision energy (CE)	17 V	51 V
Collision cell exit potential (CXP)	8 V	4 V

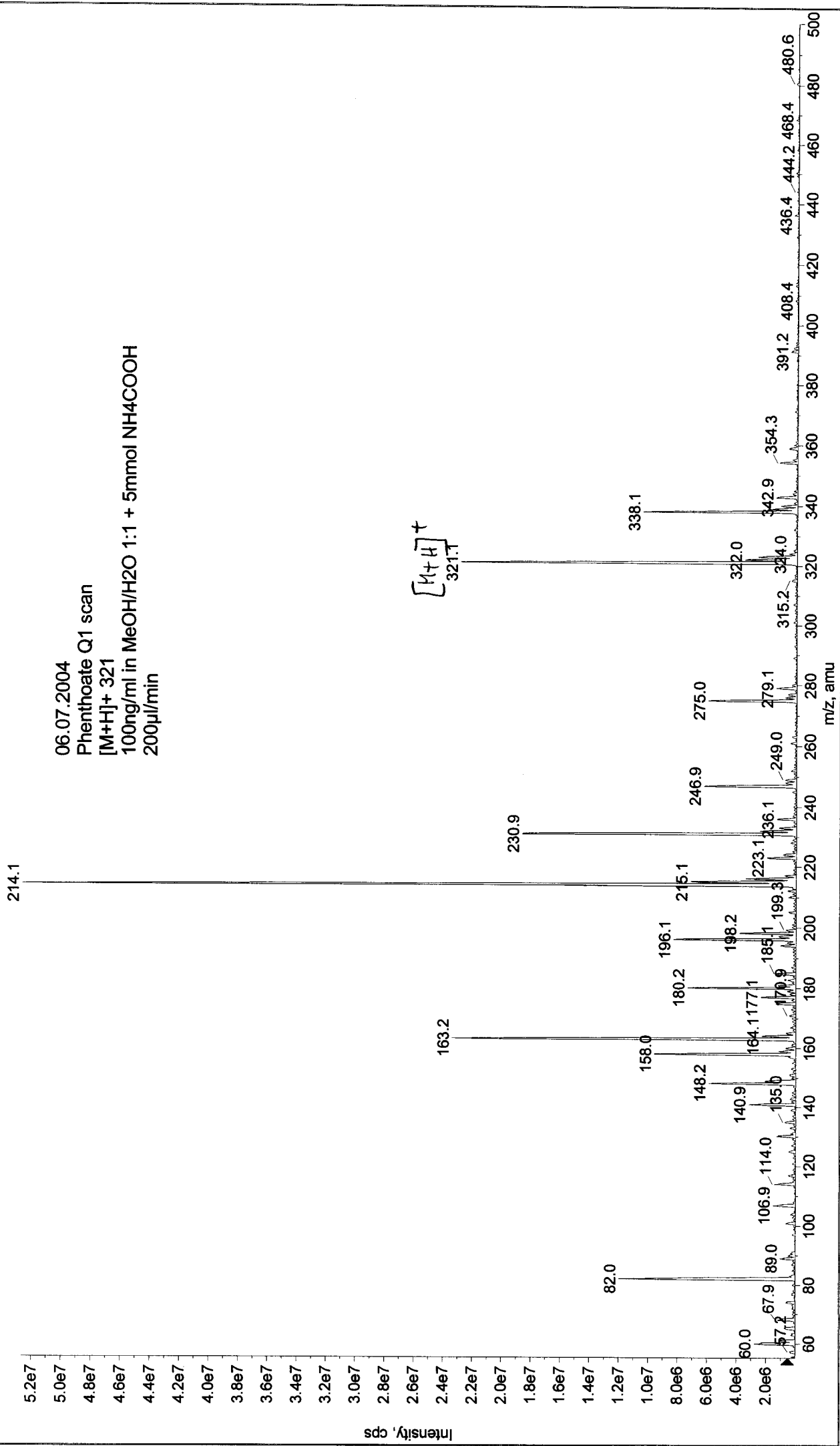
<sup>\*)</sup> For API 3000 and 4000 enhance DP by 20V

### Fragmentation



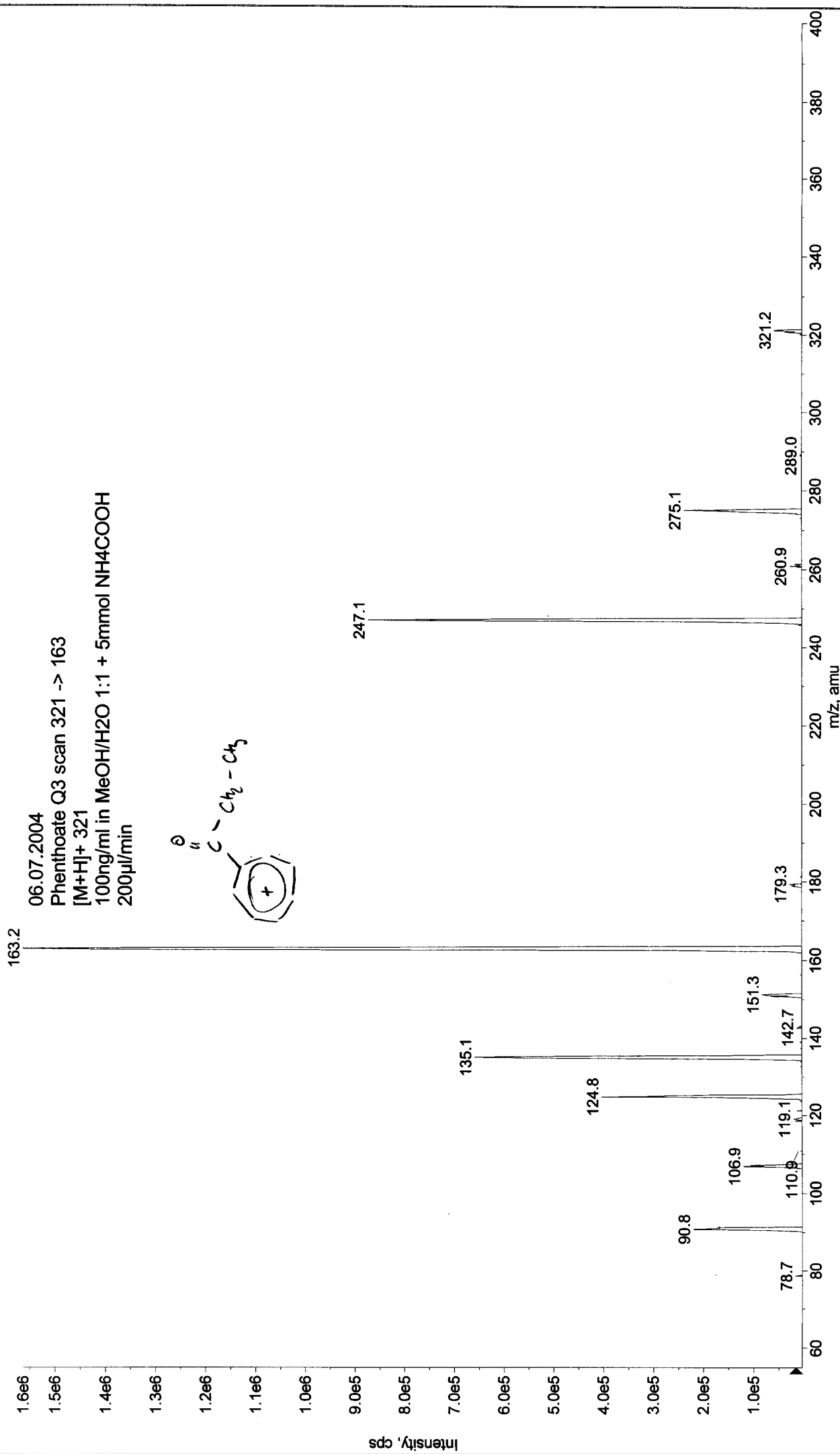
+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20040706141053.wiff (Turbo Spray)

Max. 5.3e7 cps.



+MS2 (321.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040706141329.wiff (Turbo Spray)

Max. 1.6e6 cps



■ +MS2 (323.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20040706141517.wiff (Turbo Spray) Max. 1.7e5 cps

