

**BfR**

Risiken erkennen – Gesundheit schützen

## MS/MS Parameters of Pesticides

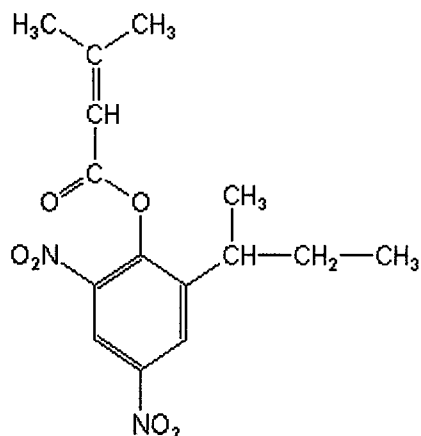
### Analyte: Binapacryl

CAS No.: 485-31-4

Formula: C<sub>15</sub>H<sub>18</sub>N<sub>2</sub>O<sub>6</sub>

Exact molecular mass (lowest isotopes): 322,12 amu

Structure:



Ionisation: ESI +

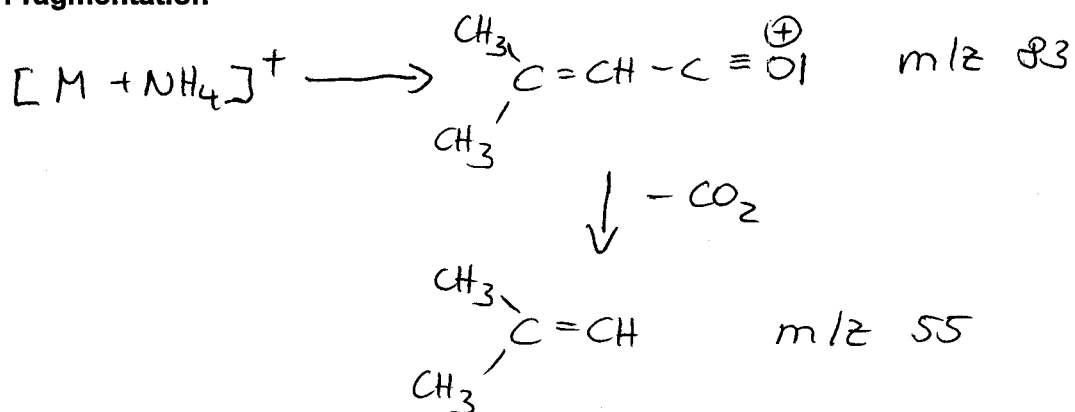
Quasimolecular ion: 340,1 amu = [M+NH<sub>4</sub>]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	340,1 → 83,2	340,1 → 54,9
Declustering potential (DP) <sup>*)</sup>	26V	26 V
Focusing potential (FP)	370 V	370 V
Entrance potential (EP)	10,5 V	11,5 V
Collision cell entrance potential (CEP)	22 V	22 V
Collision energy (CE)	21 V	63 V
Collision cell exit potential (CXP)	4 V	6 V

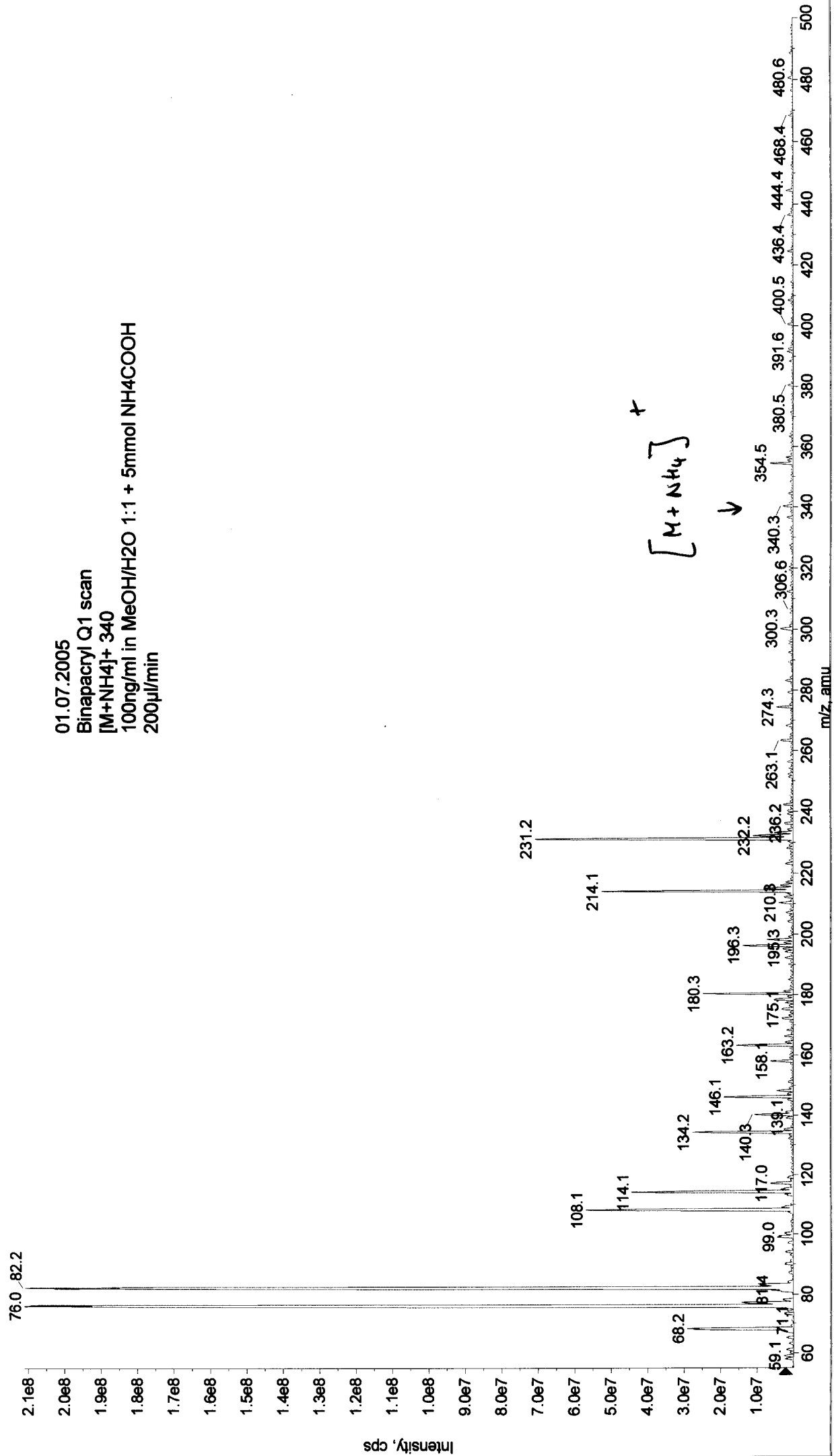
<sup>\*)</sup> For API 3000 and 4000 enhance DP by 20V

### Fragmentation

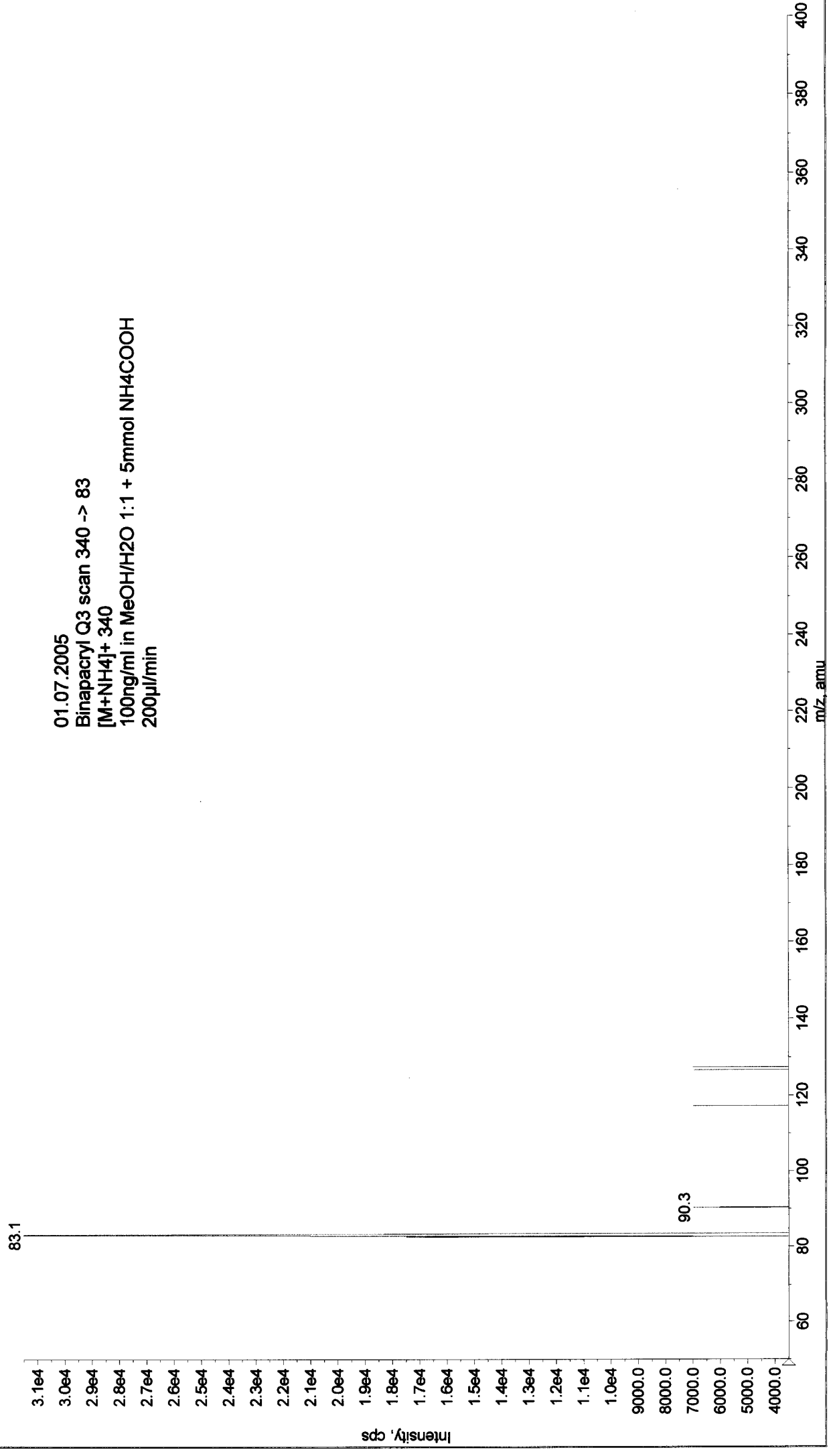


+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20050701090337.wiff (Turbo Spray)

Max. 2.1e8 cps.



■ +MS2 (340.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050701091056.wiff (Turbo Spray)



Printing Time: 9:16:07  
Printing Date: Friday, July 01, 2005

Acq. Time: 09:14  
Acq. Date: Friday, July 01, 2005  
Acq. File: MT20050701091456.wiff

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

Max. 1.1e4 cps.

+MS2 (340.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050701091456.wiff (Turbo Spray)

1.05e4  
55.2

01.07.2005

Binapacryl\_55 Q3 scan 340 -> 55

[M+NH4]<sup>+</sup> 340

100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH

200µl/min

Intensity, cps

60

80

100

120

140

160

180

200

220

240

260

280

300

320

340

360

380

400

m/z, amu