

## MS/MS Parameters of Pesticides

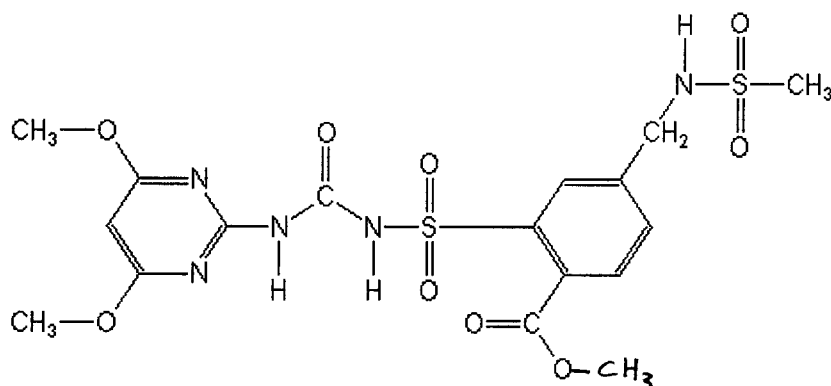
### Analyte: Mesosulfuron-methyl

CAS No.: 208465-21-8

Formula: C<sub>17</sub>H<sub>21</sub>N<sub>5</sub>O<sub>9</sub>S<sub>2</sub>

Molecular mass (lowest isotopes): 503,08 amu

Structure:



Ionisation: ESI +

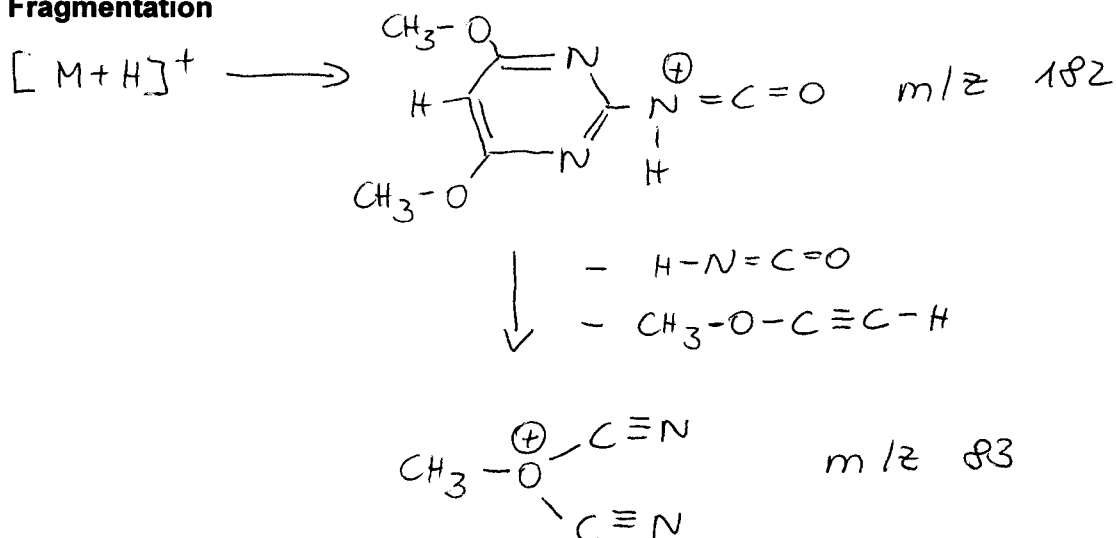
Quasimolecular ion: 504,1 amu = [M+H]<sup>+</sup>

Analyte sensitive parameter set (API 2000)

Transition	504,1 → 182,1	504,1 → 83,0
Declustering potential (DP) <sup>*)</sup>	61V	61 V
Focusing potential (FP)	360 V	320 V
Entrance potential (EP)	12 V	11 V
Collision cell entrance potential (CEP)	22 V	22 V
Collision energy (CE)	33 V	75 V
Collision cell exit potential (CXP)	10 V	4 V

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

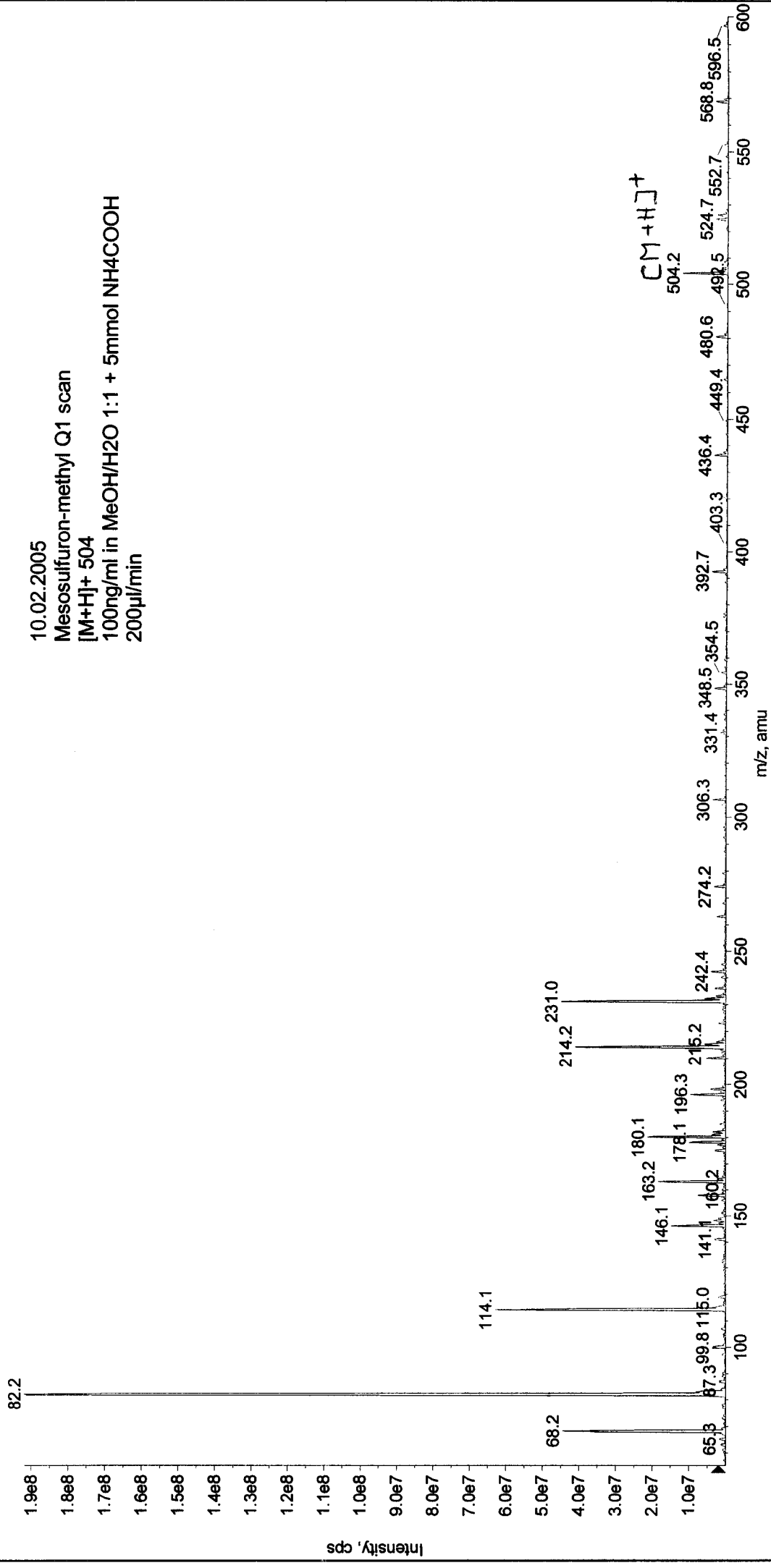
### Fragmentation



+Q1: 30 MCA scans from Sample 1 (TuneSampleID) of MT20050210133552.wiff (Turbo Spray)

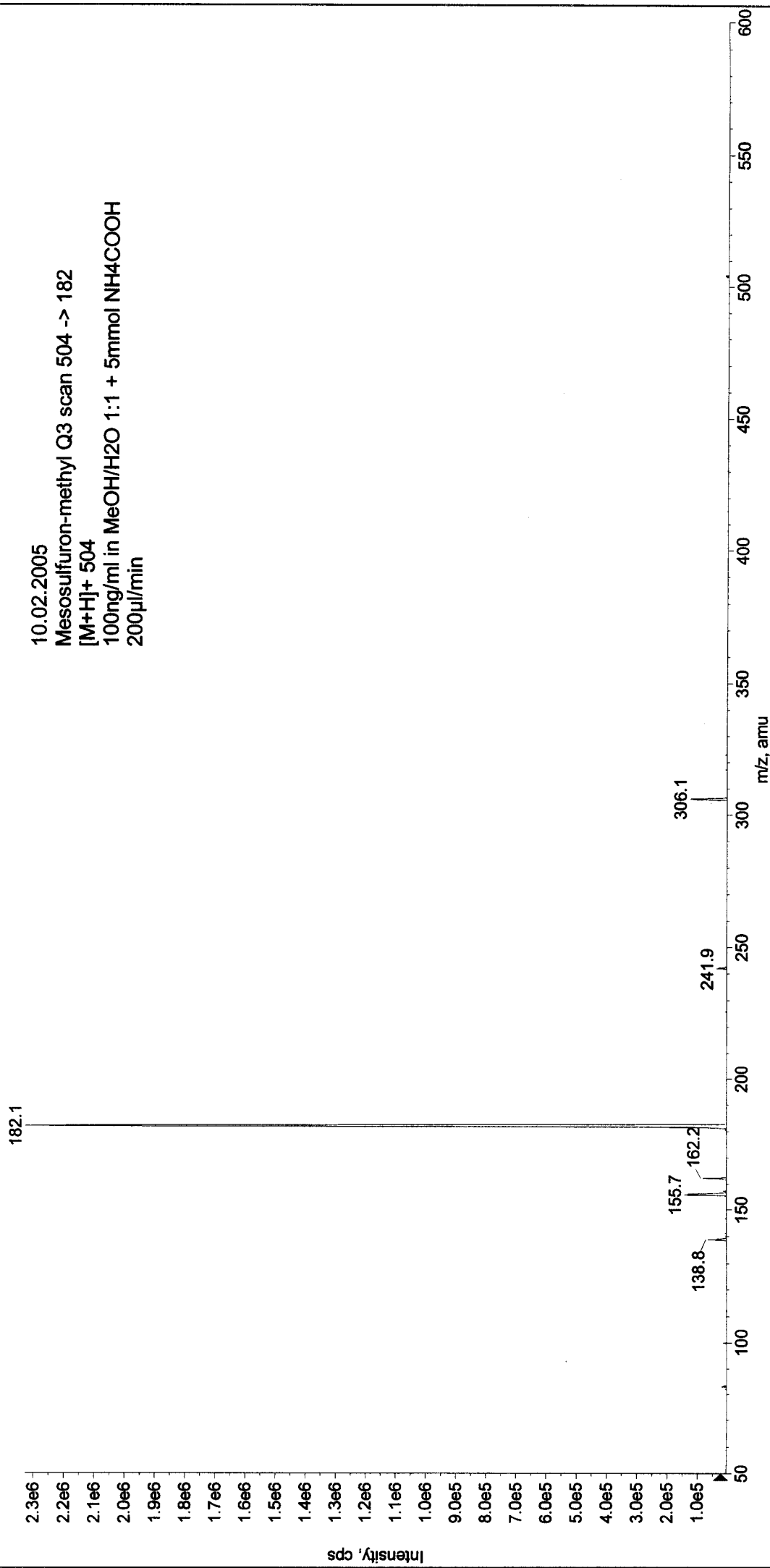
Max. 1.9e8 cps

10.02.2005  
 Mesosulfuron-methyl Q1 scan  
 [M+H]<sup>+</sup> 504  
 100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
 200µl/min



+MS2 (504.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050210133807.wiff (Turbo Spray)

Max. 2.3e6 cps



Printing Time: 13:41:07

Printing Date: Thursday, February 10, 2005

Acq. Time: 13:40

Acq. Date: Thursday, February 10, 2005

Acq. File: MT20050210134009.wiff

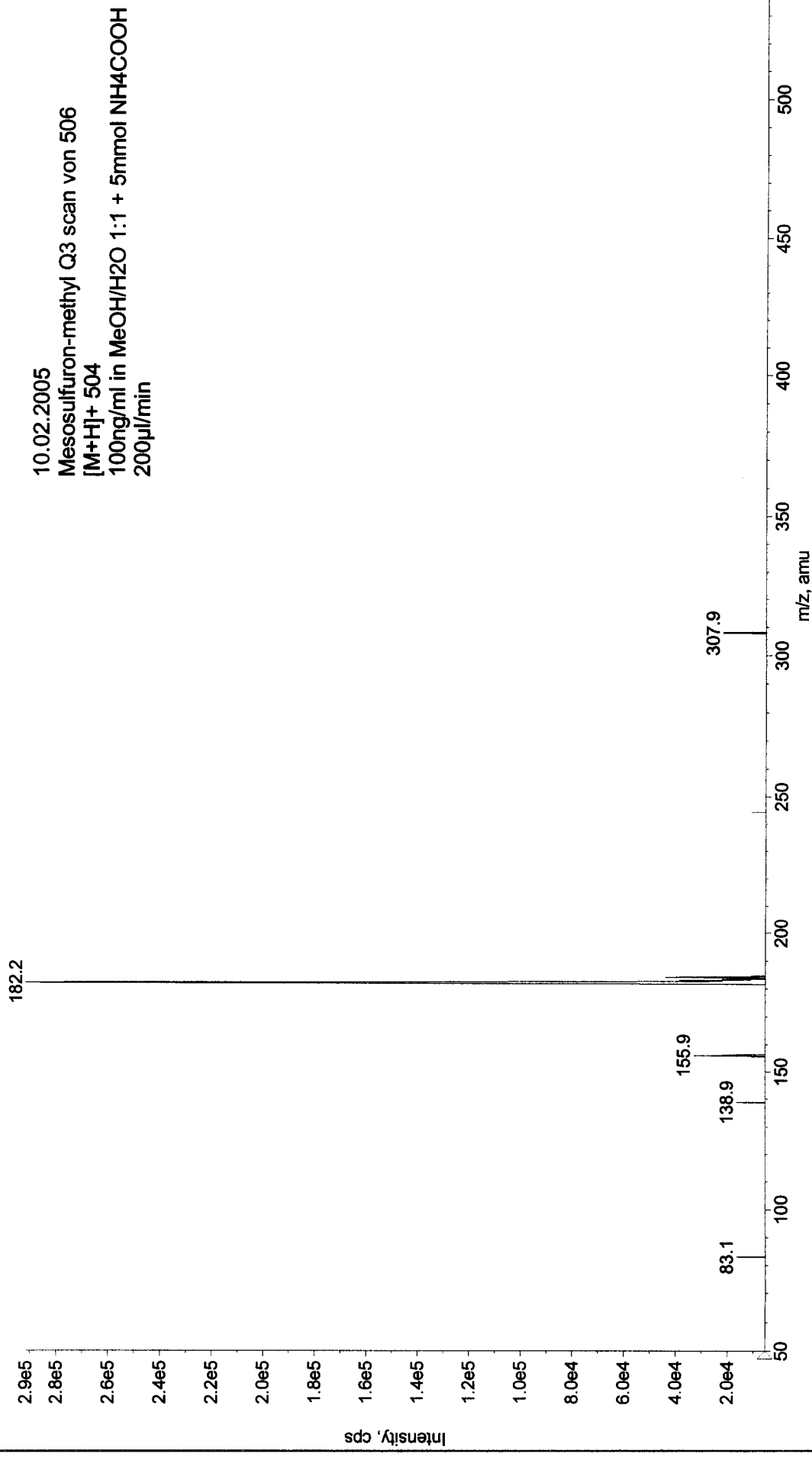
Sample Comment:

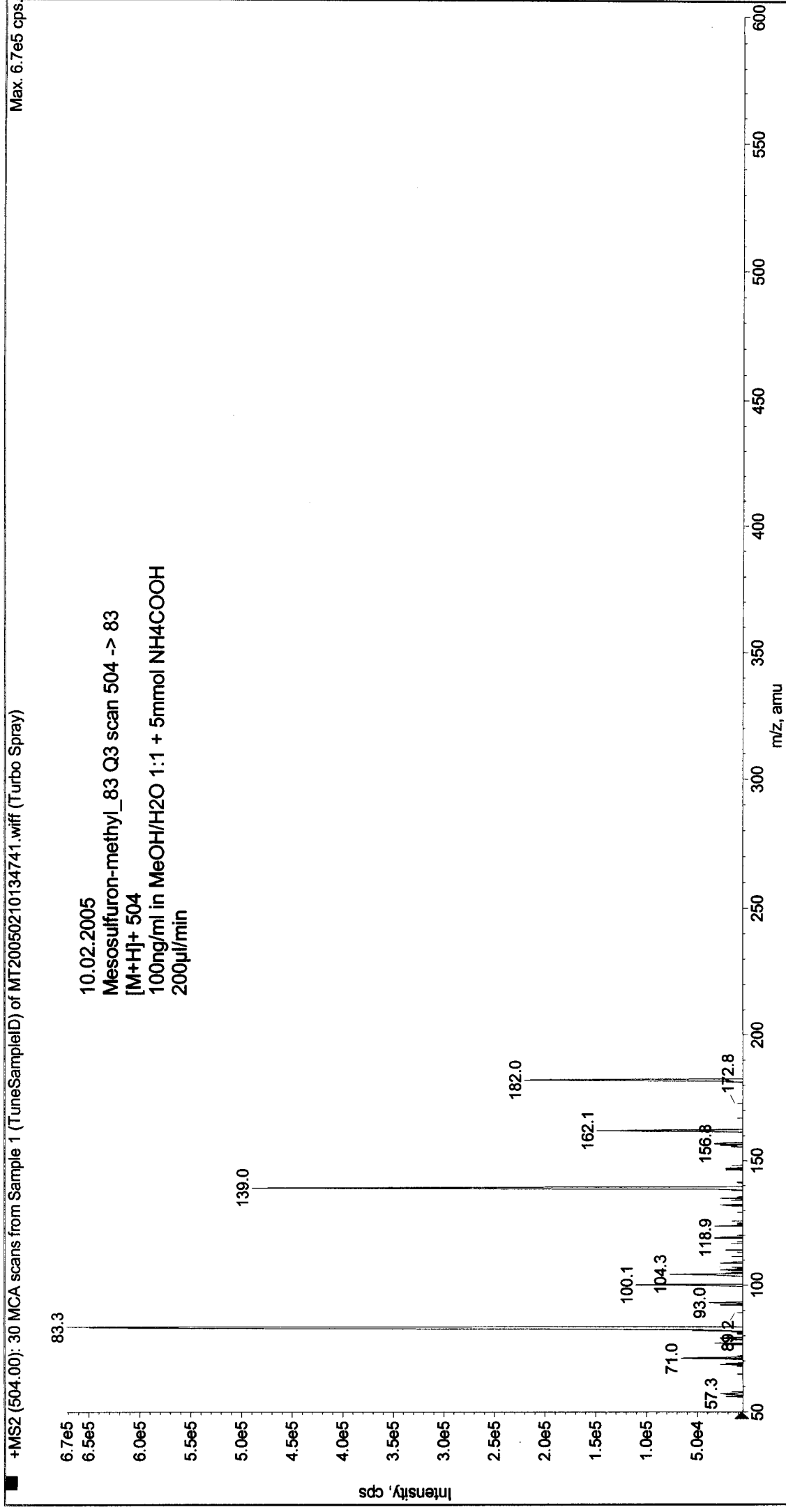
Sample Name: TuneSampleID

Batch Name: ManualTune.bat

■ +MS2 (506.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050210134009.wiff (Turbo Spray)

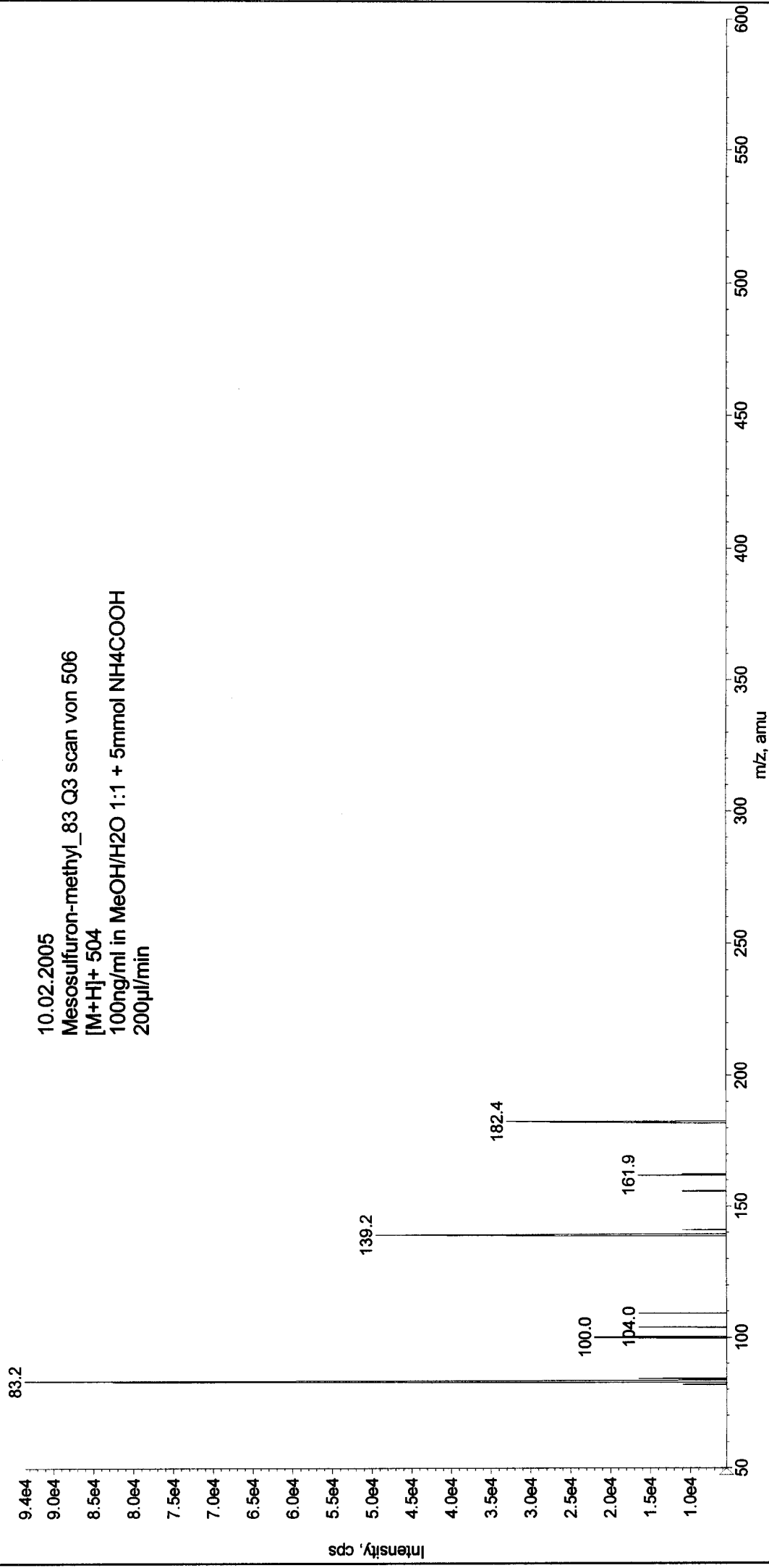
Max. 2.9e5 cps





Max. 9.4e4 cps

+MS2 (506.00): 30 MCA scans from Sample 1 (TuneSampleID) of MT20050210134916.wiff (Turbo Spray)



10.02.2005  
 Mesosulfuron-methyl\_83 Q3 scan von 506  
 [M+H]<sup>+</sup> 504  
 100ng/ml in MeOH/H<sub>2</sub>O 1:1 + 5mmol NH<sub>4</sub>COOH  
 200µl/min