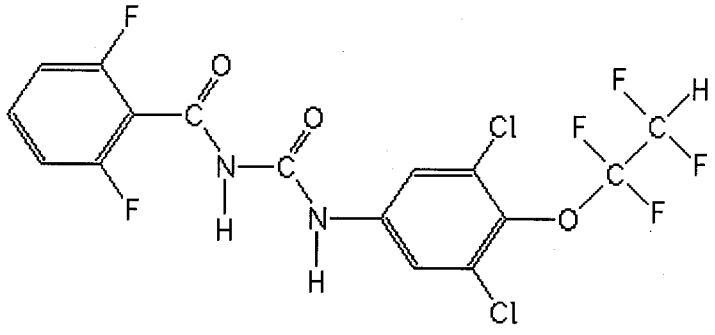
Risiken erkennen – Gesundheit schützen

MS/MS Parameters of Pesticides

Analyte: Hexaflumuron

CAS No.: 86479-06-3
Formula: C16H8Cl2F6N2O3
Molecular mass (lowest isotopes): 459,98 amu

Structure:



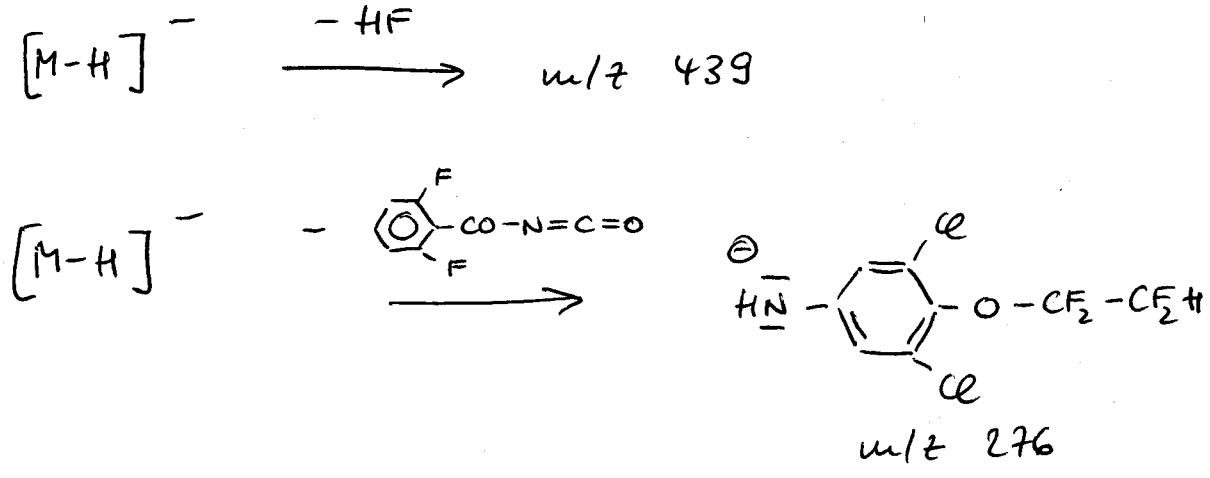
Ionisation: ESI - Quasimolecular ion: 459,0 amu = [M-H]-

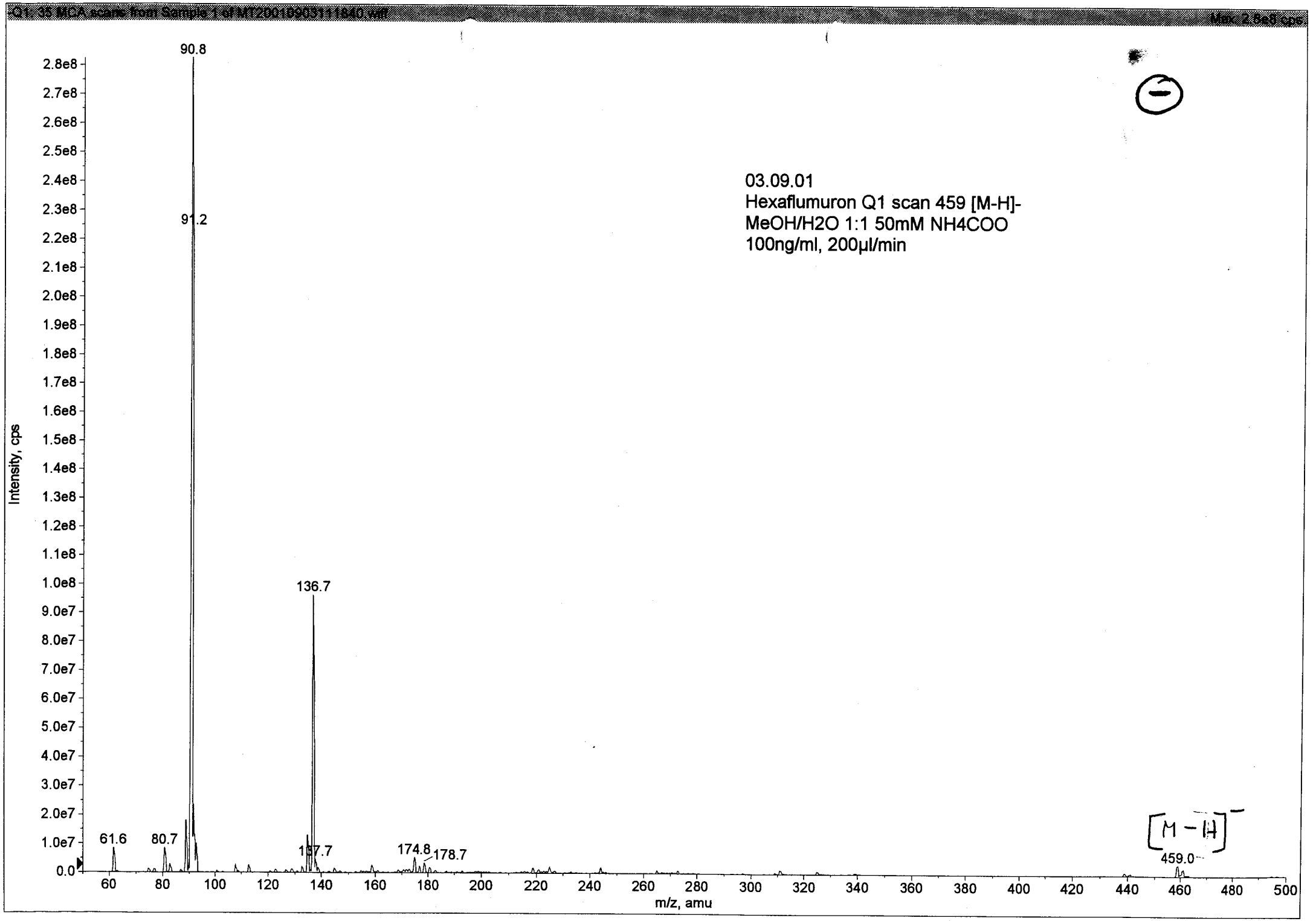
Analyte sensitive parameter set (API 2000)

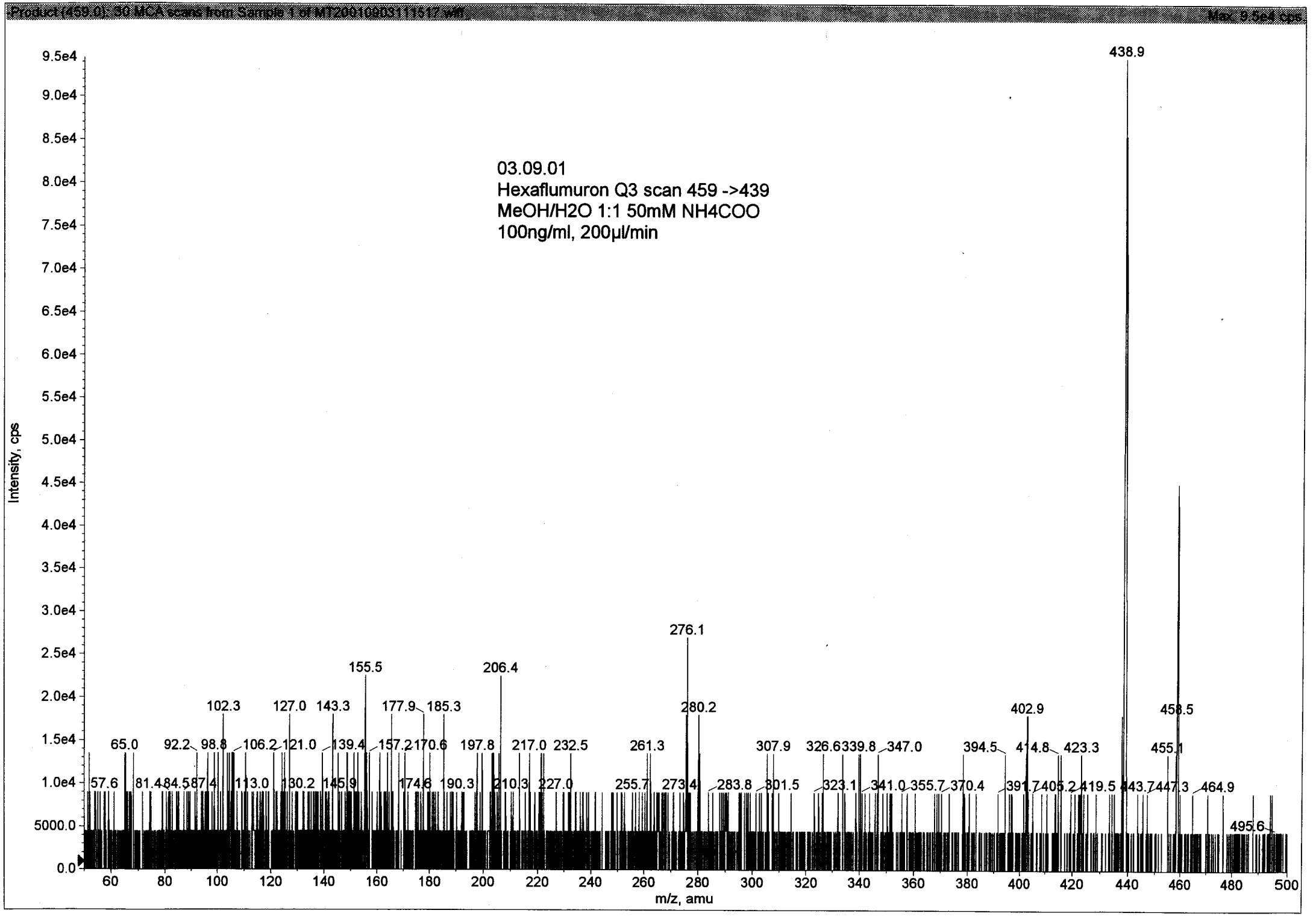
Transition	459,0 → 438,8	459,0 → 275,9
Declustering potential (DP)*)	-11V	-11 V
Focusing potential (FP)	-350 V	-350 V
Entrance potential (EP)	- 9,5 V	-10,0 V
Collision cell entrance potential (CEP)	-20 V	-38 V
Collision energy (CE)	-14 V	-22 V
Collision cell exit potential (CXP)	-26 V	-16 V

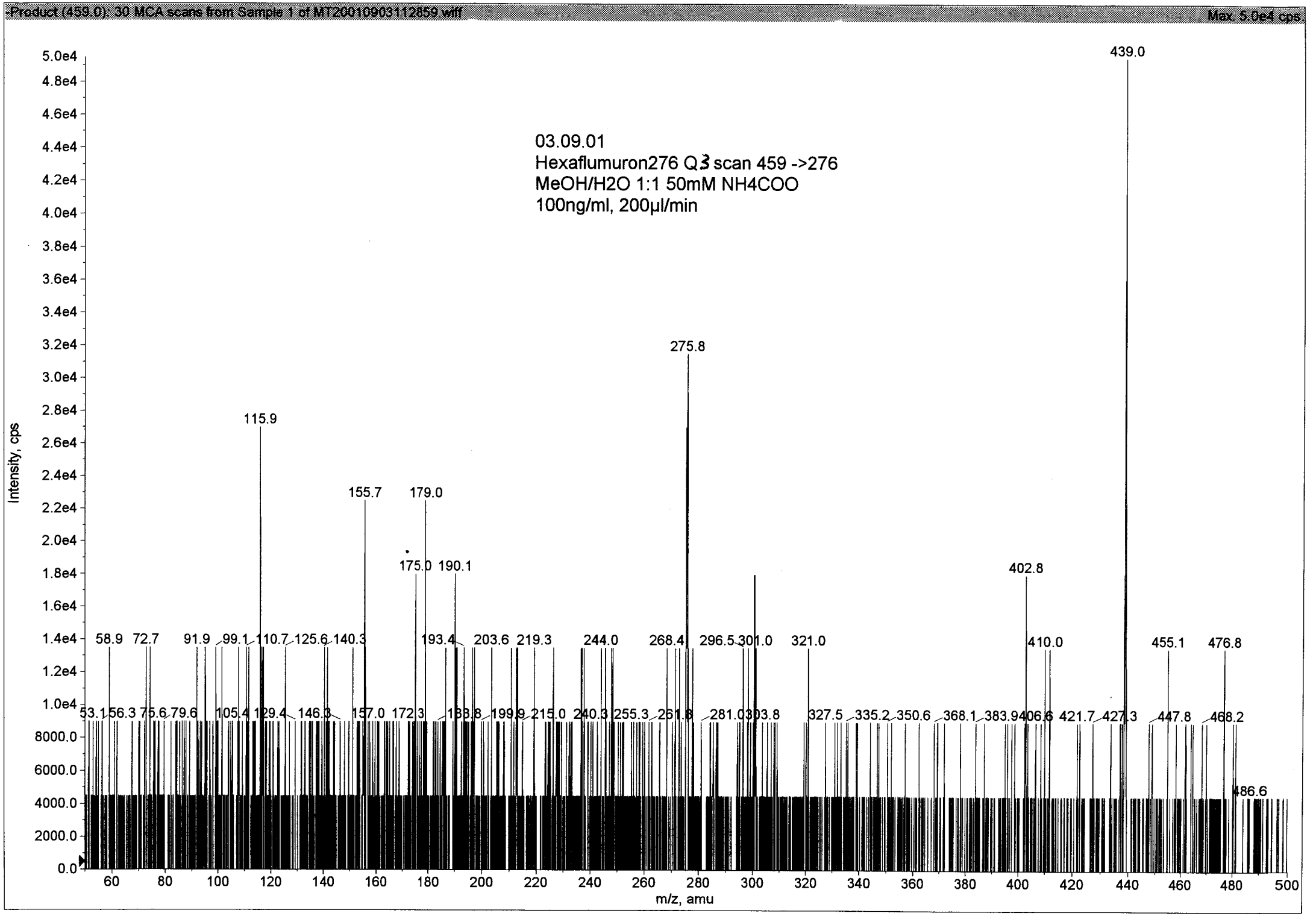
*) For API 3000 and 4000 enhance DP by 20V

Fragmentation




Q1: 35 MCA scans from Sample 1 of MT20010903111840.wiff
Max. 2.8e8 cps
90.8
91.2
136.7
61.6
80.7
157.7
174.8
178.7
459.0
Intensity, cps
m/z, amu
03.09.01
Hexaflumuron Q1 scan 459 [M-H]-
MeOH/H2O 1:1 50mM NH4COO
100ng/ml, 200µl/min
[M-H]-


Product (459.0): 30 MCA scans from Sample 1 of MT20010903111517.wiff
Max. 9.5e4 cps
03.09.01
Hexaflumuron Q3 scan 459 ->439
MeOH/H2O 1:1 50mM NH4COO
100ng/ml, 200µl/min
Intensity, cps
m/z, amu
438.9
276.1
155.5
206.4
280.2
458.5
402.9
102.3
127.0
143.3
177.9
185.3
65.0
92.2
98.8
106.2
121.0
139.4
157.2
170.6
197.8
217.0
232.5
261.3
307.9
326.6
339.8
347.0
394.5
414.8
423.3
455.1
57.6
81.4
84.5
87.4
113.0
130.2
145.9
174.6
190.3
210.3
227.0
255.7
273.4
283.8
301.5
323.1
341.0
355.7
370.4
391.7
405.2
419.5
443.7
447.3
464.9
495.6


Product (459.0): 30 MCA scans from Sample 1 of MT20010903112859.wiff
Max. 5.0e4 cps
03.09.01
Hexaflumuron276 Q3 scan 459 ->276
MeOH/H2O 1:1 50mM NH4COO
100ng/ml, 200µl/min
Intensity, cps
m/z, amu
439.0
275.8
115.9
155.7
179.0
175.0
190.1
402.8
410.0
455.1
476.8
486.6
58.9
72.7
91.9
99.1
110.7
125.6
140.3
193.4
203.6
219.3
244.0
268.4
296.5
301.0
321.0
53.1
56.3
75.6
79.6
105.4
129.4
146.3
157.0
172.3
188.8
199.9
215.0
240.3
255.3
261.8
281.0
303.8
327.5
335.2
350.6
368.1
383.9
406.6
421.7
427.3
447.8
468.2