Supporting Information for the Paper:

Unexpected Reaction Pathways Leading to Thiodiglycol During the Degradation of Long-Chain Sulfur Mustards

Esther Gómez-Caballero,[b] Roberto Martínez-Álvarez,*,[a] Miguel A. Sierra*[a]

[a] *Departamento de Química Orgánica, Facultad de Química and Centro de Innovación en Química Avanzada (ORFEO-CINQA), Universidad Complutense, 28040 Madrid, Spain.*

[b] Laboratorio de Verificación de Armas Químicas (*LAVEMA), Área de Defensa Química. Departamento NBQM, Subdirección General de Sistemas Terrestres. INTA-Campus La Marañosa. M-301, km 10.5, 28330, Madrid, Spain.*

Page S2 Composition of the commercial decontamination agents**.**

Page S3 ^{1}H NMR and GC-MS copies of compounds **7** and **8**

Page S16 GC Experimental Data for decontamination mixtures

Page S23 MS Data of degradation products

Page S26 Cartesian Coordinates and Energies (in Hartree) of all optimized species and imaginary frequencies values for TSs

Page S34 Full GC data for degradation mixtures of compounds **7b-d**

Composition of the commercial decontamination agents:

The following commercial decontamination agents were used in this work:

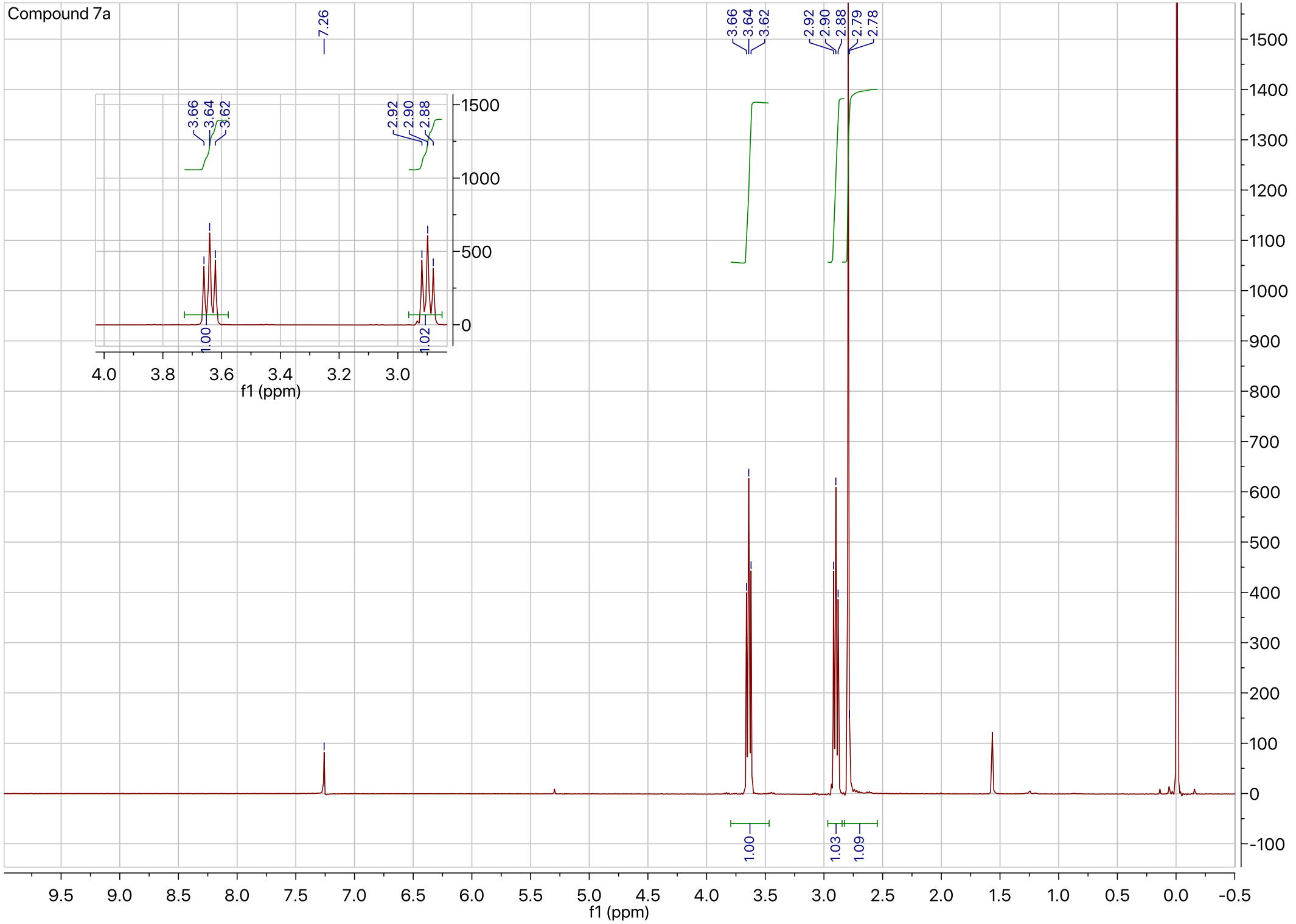
RM21: Neutral decontaminant for the decontamination of sensitive equipment and persons. It is a mixture of amines, alkyldimethyl *N*-oxides, 2-propanol and no-ionic tensioactive agents, commercialized by Kärcher Futuretech GmbH. http://www.karcher-futuretech.com/futuretech_en/products_/CBRN_Protection__Systems/Decontamination_and_Cleaning_Agents/Decontamination_Agents/Decontamination_agents_Persons/62912110.htm (Accessed June 28, 2018).

RM31: Strongly alkaline (NaOH, pH 13.5) liquid recommended for removal of greases and oils. This decontaminant solution is commercialized by Kärcher Futuretech GmbH. https://www.kaercher.com/int/professional/cleaning-and-care-products/reinigungsmittel-professional/high-pressure/pressurepro-oil-and-grease-cleaner-extra-rm-31-62950690.html (Accessed June 28).

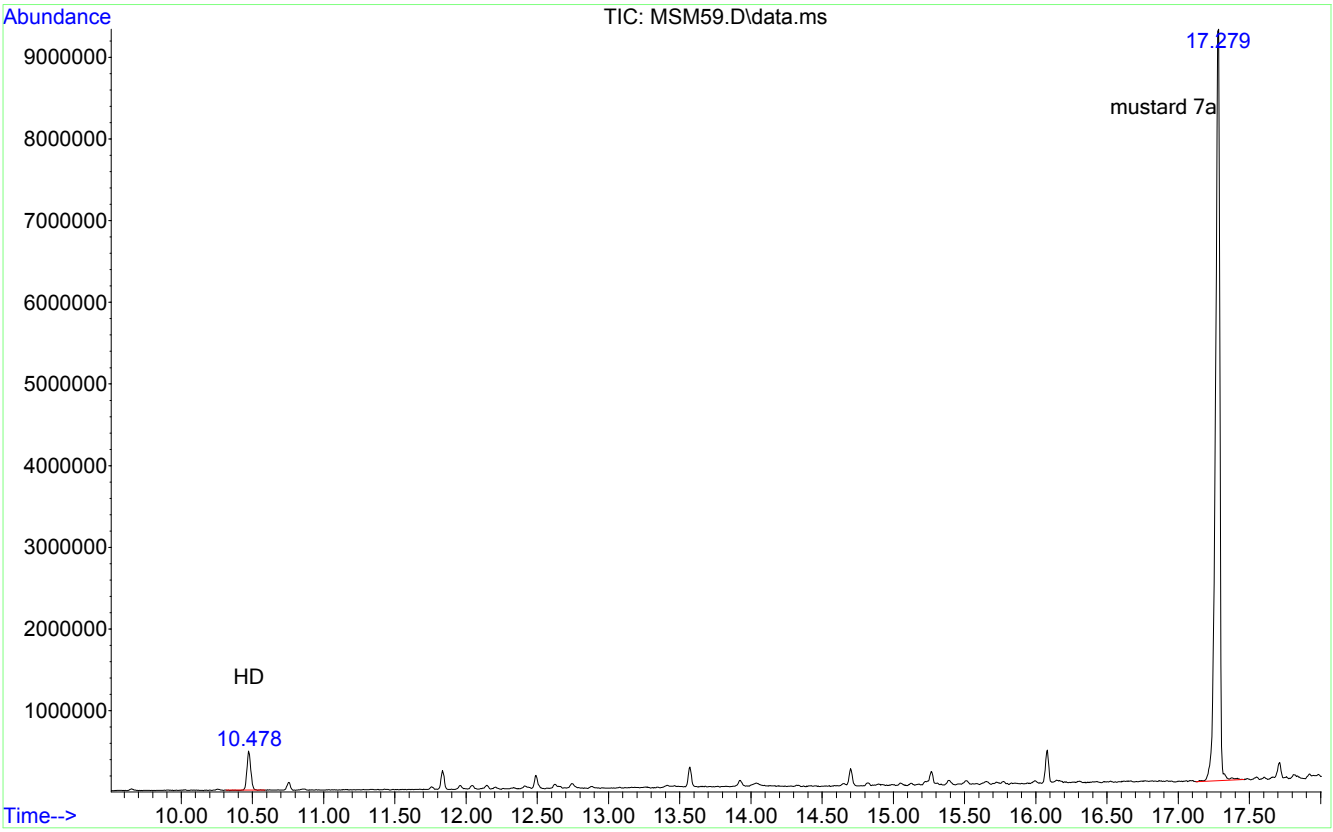
BX24: Commercialized as a white solid with a strong chlorine odor by Cristianini S.p.a. Indicated to decontaminate hardware and vehicles. Contains silicates, phosphates, surfactants and oxidants. When solved for use the composition is 88% water and 12% Fi-Clor. http://www.cristanini.it/eng/products/cbrn-decontamination /decontamination-of-vehicles-materials-terrains-platforms-and-aircrafts/products/bx-24. (Accessed June 28, 2018).

BX29: Neutral decontaminant for persons containing amphoteric detergents (54%), amide (6%) and sodium sulfate laurilether (40 %). Liquid Decontaminant used in the decontamination of personnel. The sample used in this work was obtained from Cristianini S.p.a. http://www.cristanini.it/eng/products/cbrn-decontamination/personnel-decontamination/decontamination-of-people/bx-29-decontaminant-product-for-people (Accessed June 28, 2018).

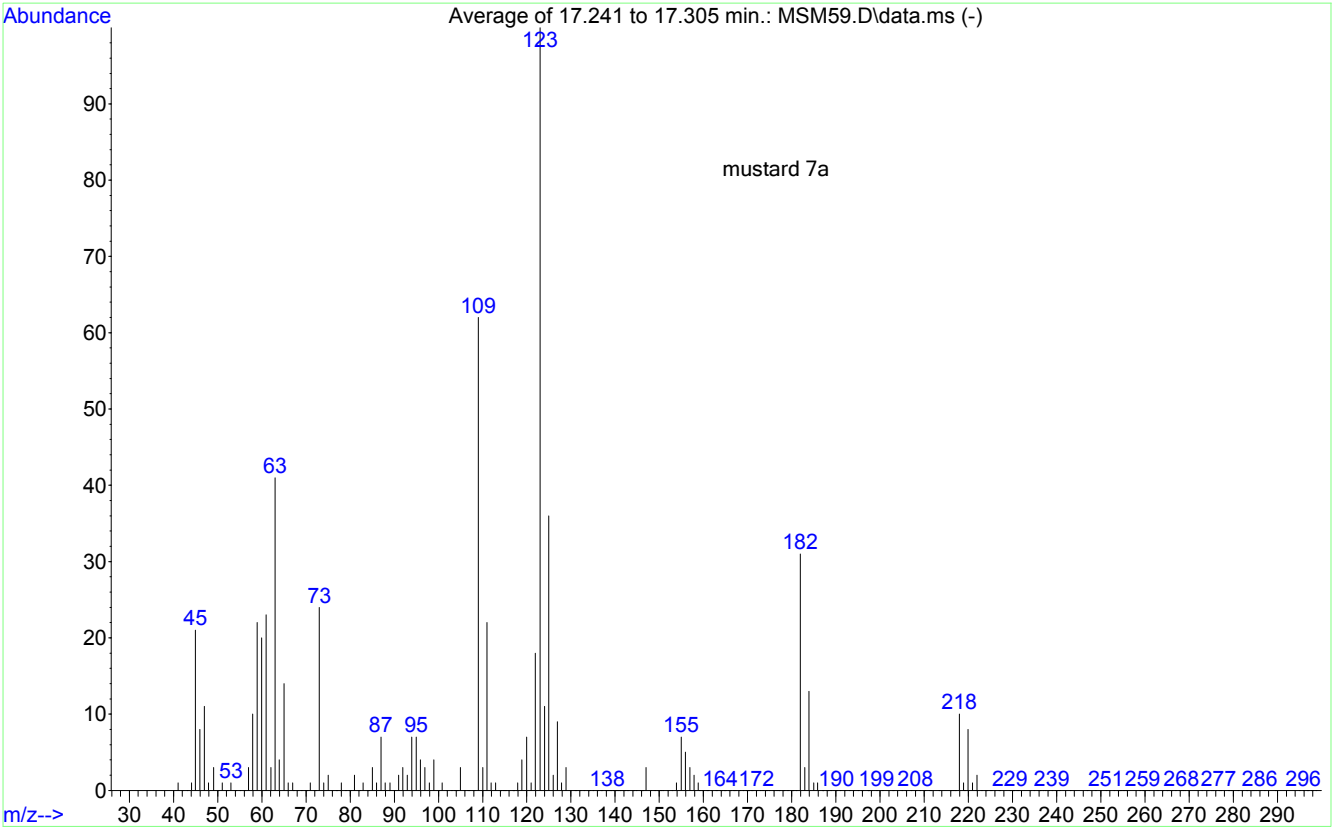
BX40: Powder, it is dissolved instantly in water prior to use. Used in the decontamination of airplanes and helicopters. It contains 2-butoxyethanol (5-15%) and sodium metasilicate (< 5%), together with sodium phosphate, surface active agents (anionic), and 5–15% glycoether. The pH of the working solution is ≈ 13. http://www.pointtrading.com/uploads/product_pdf/up%20984%20-%20msds%20_%20bx40.pdf (Accessed June 28, 2018).

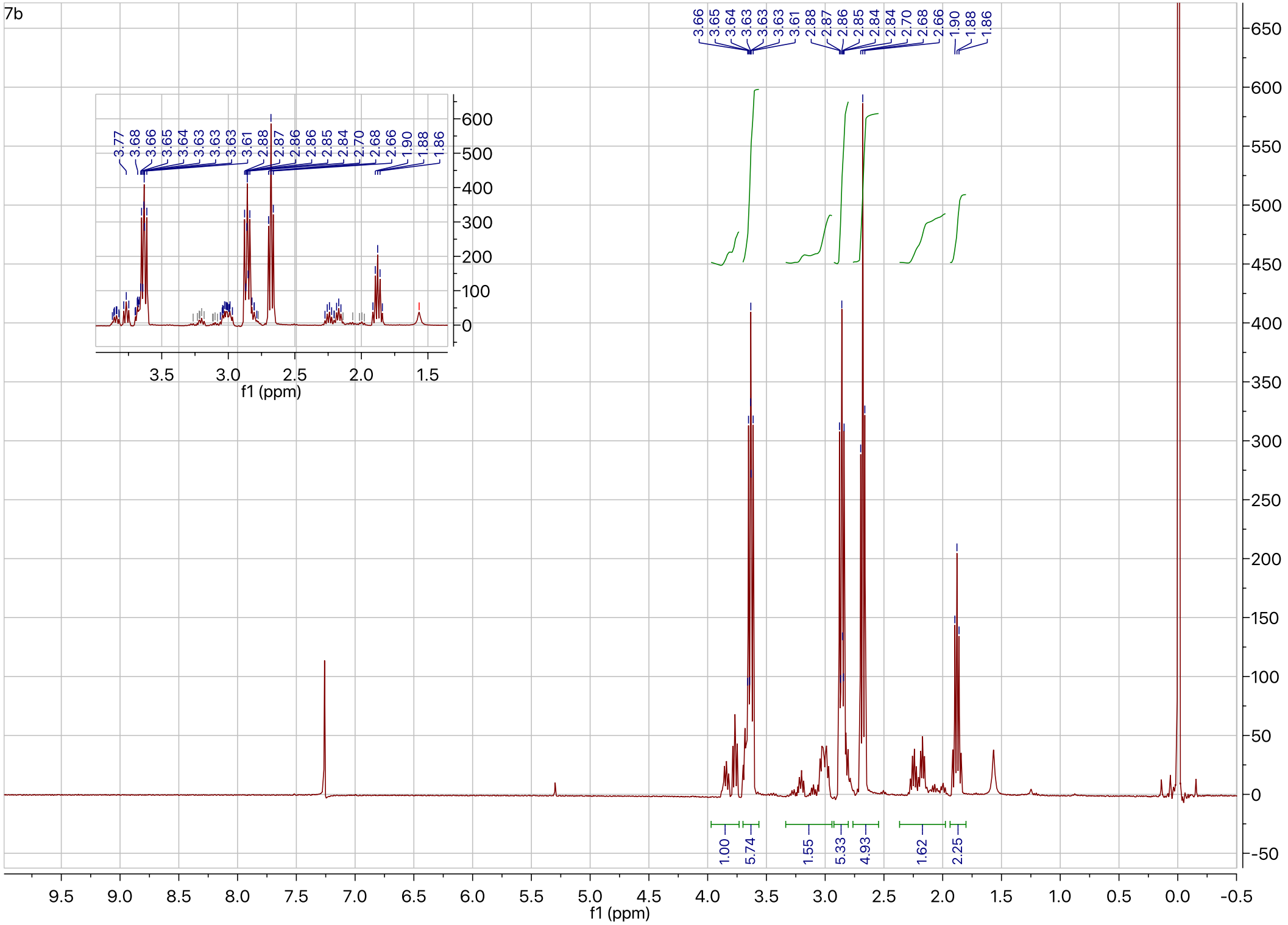

Compound 7a
7.26
3.66
3.64
3.62
2.92
2.90
2.88
2.79
2.78
1.00
1.03
1.09
f1 (ppm)
1.00
1.02
f1 (ppm)

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Instrument : VE002
Sample Name :

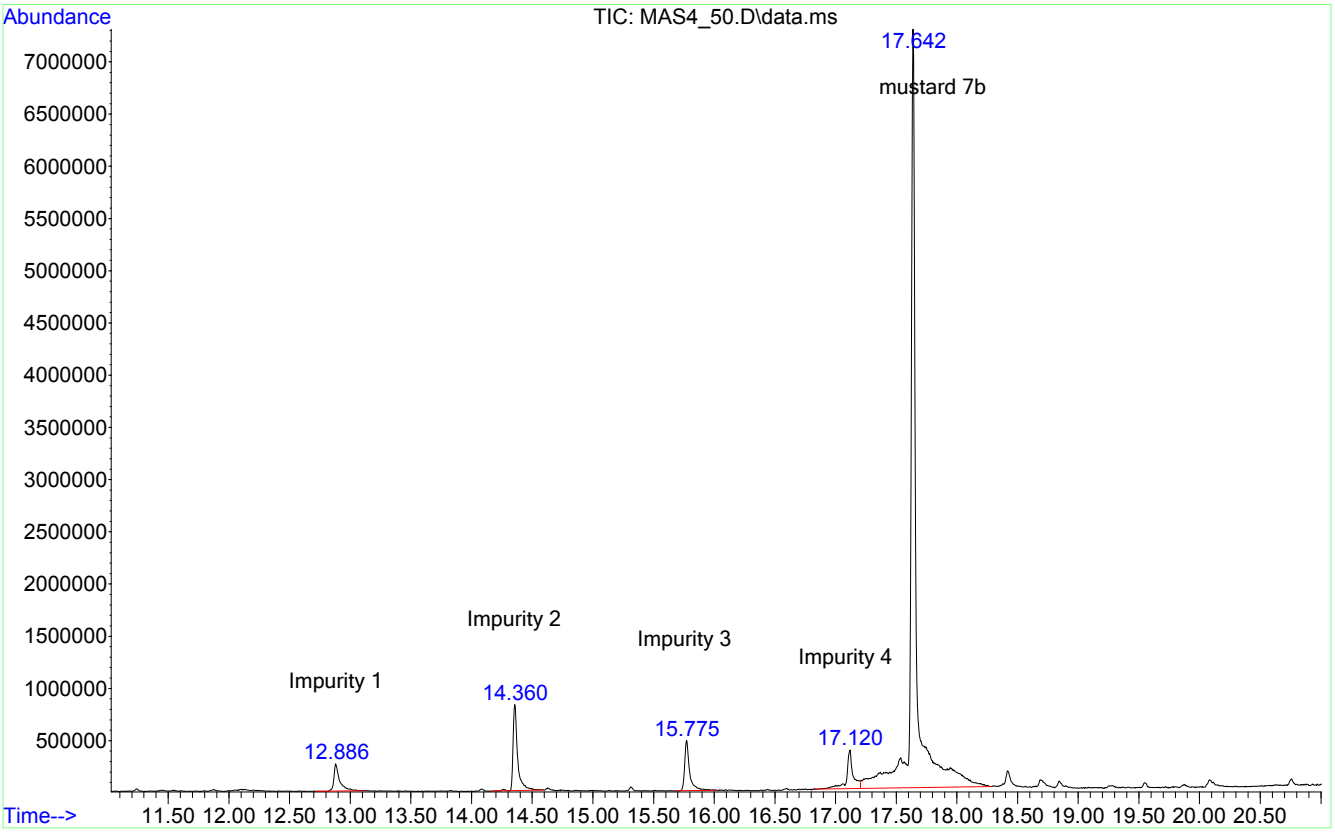


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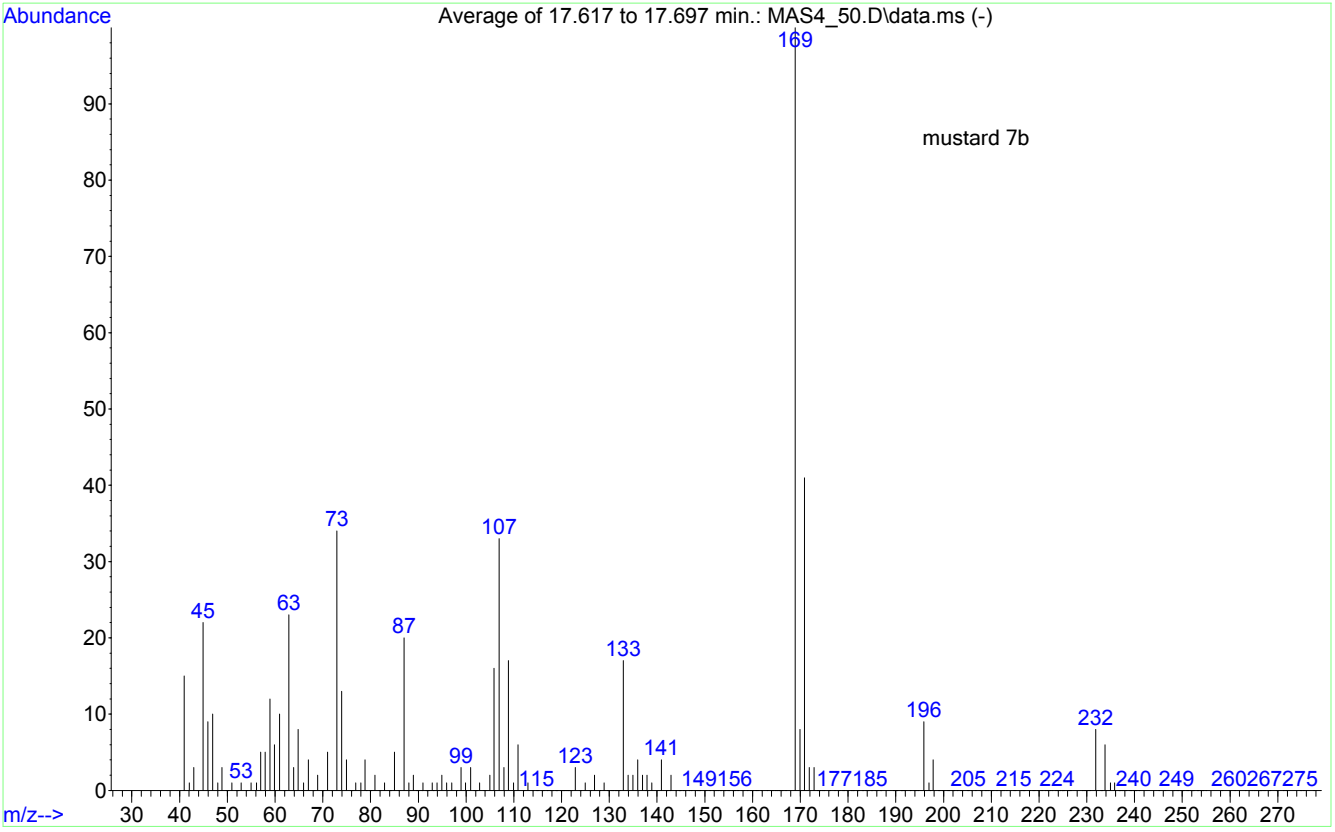


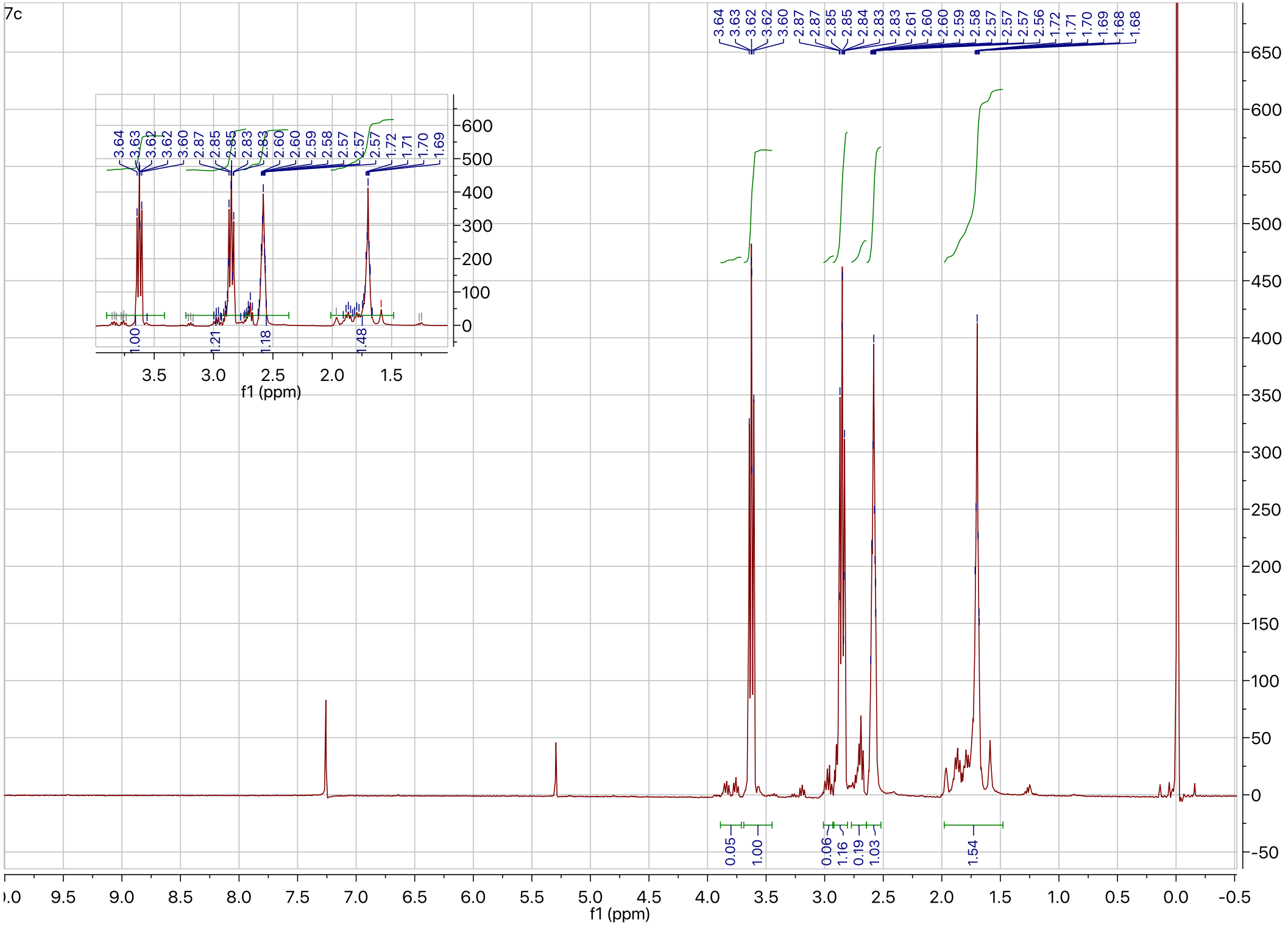

7b
3.66
3.65
3.64
3.63
3.63
3.63
3.61
2.88
2.87
2.86
2.85
2.84
2.84
2.70
2.68
2.66
1.90
1.88
1.86
1.00
5.74
1.55
5.33
4.93
1.62
2.25
f1 (ppm)
3.77
3.68
3.66
3.65
3.64
3.63
3.63
3.63
3.61
2.88
2.87
2.86
2.86
2.85
2.84
2.70
2.68
2.66
1.90
1.88
1.86
f1 (ppm)

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Instrument : VE032
Sample Name :

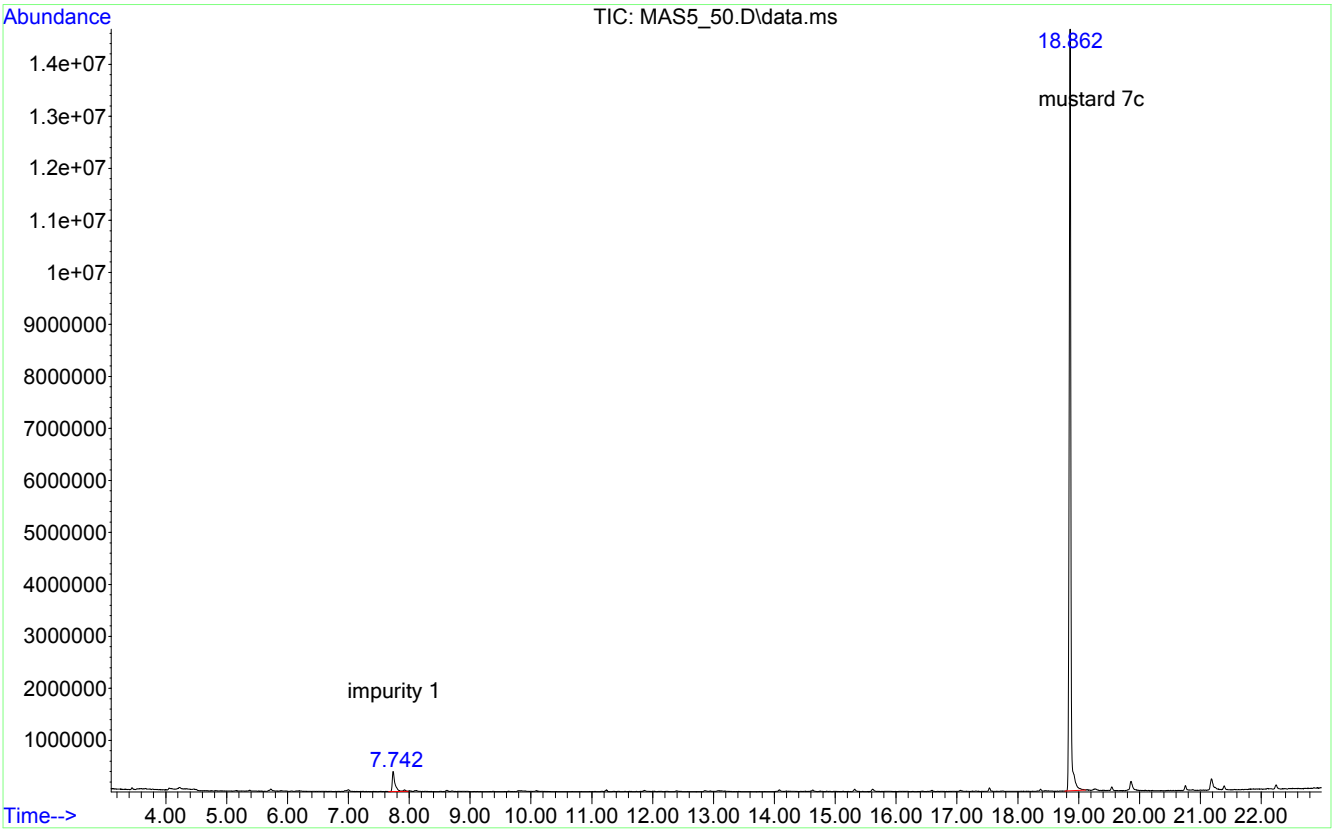


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Instrument : VE032
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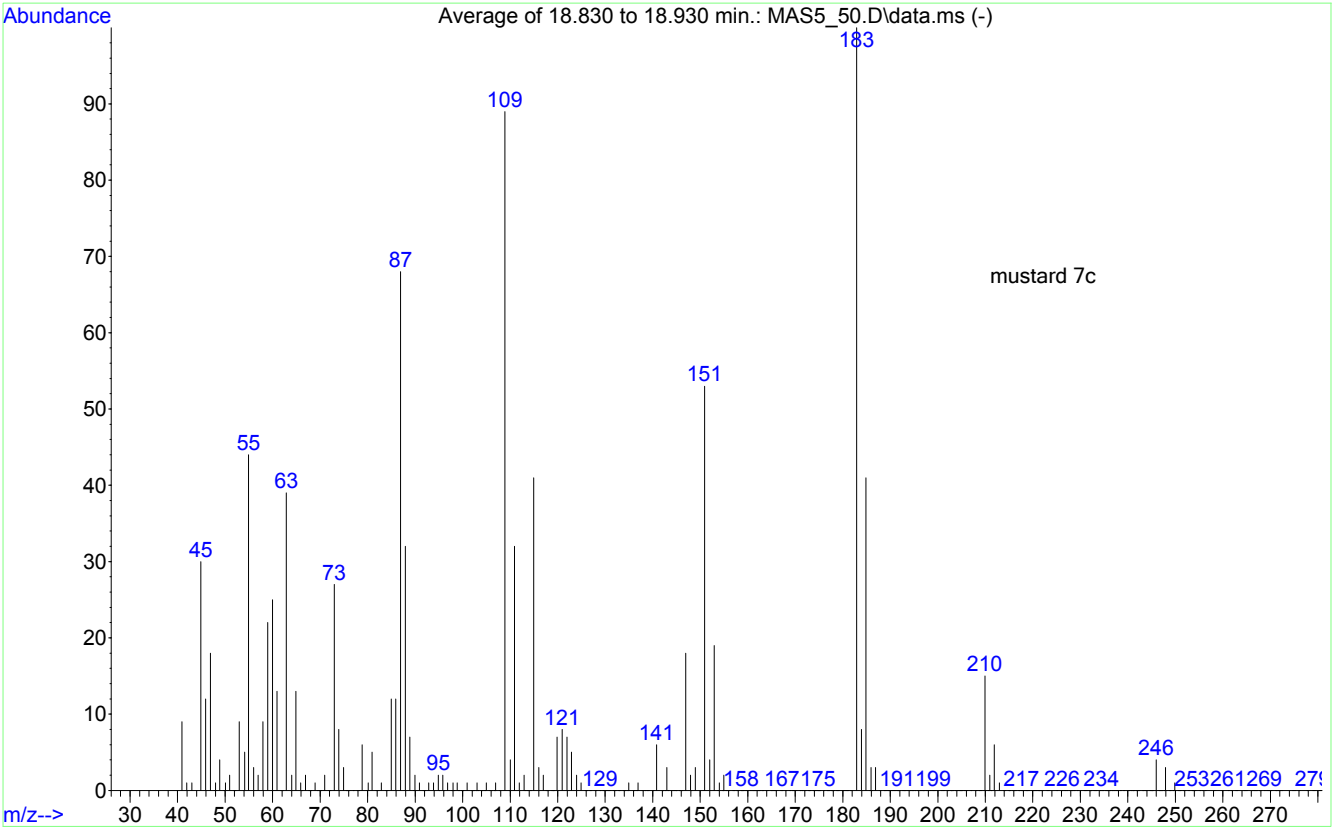


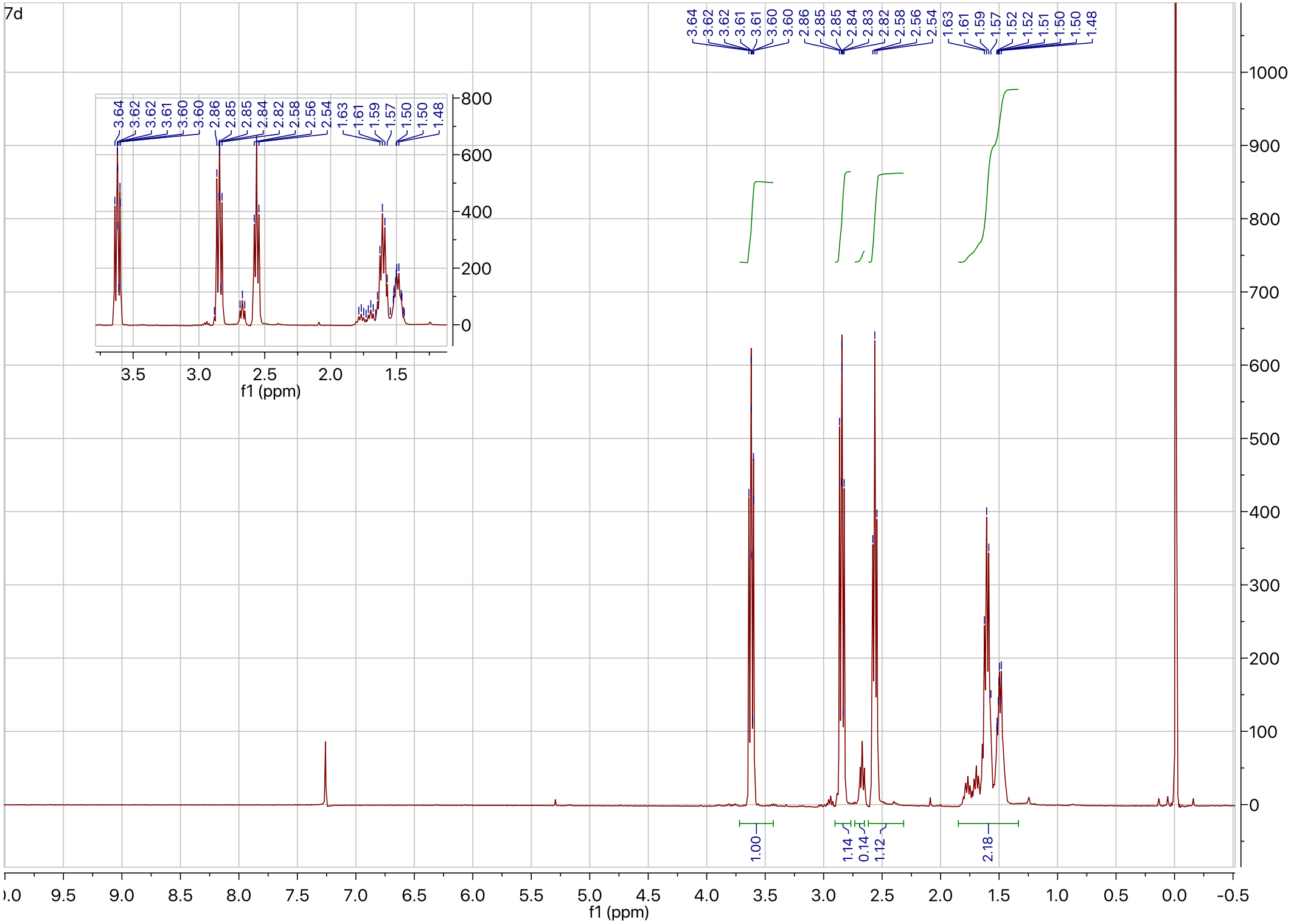

7c
3.64
3.63
3.62
3.62
3.60
2.87
2.87
2.85
2.85
2.84
2.83
2.83
2.61
2.60
2.60
2.59
2.58
2.57
2.57
2.57
2.56
1.72
1.71
1.70
1.69
1.68
1.68
1.00
1.21
1.18
1.48
f1 (ppm)
0.05
1.00
0.06
1.16
0.19
1.03
1.54
f1 (ppm)

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Instrument : VE032
Sample Name :

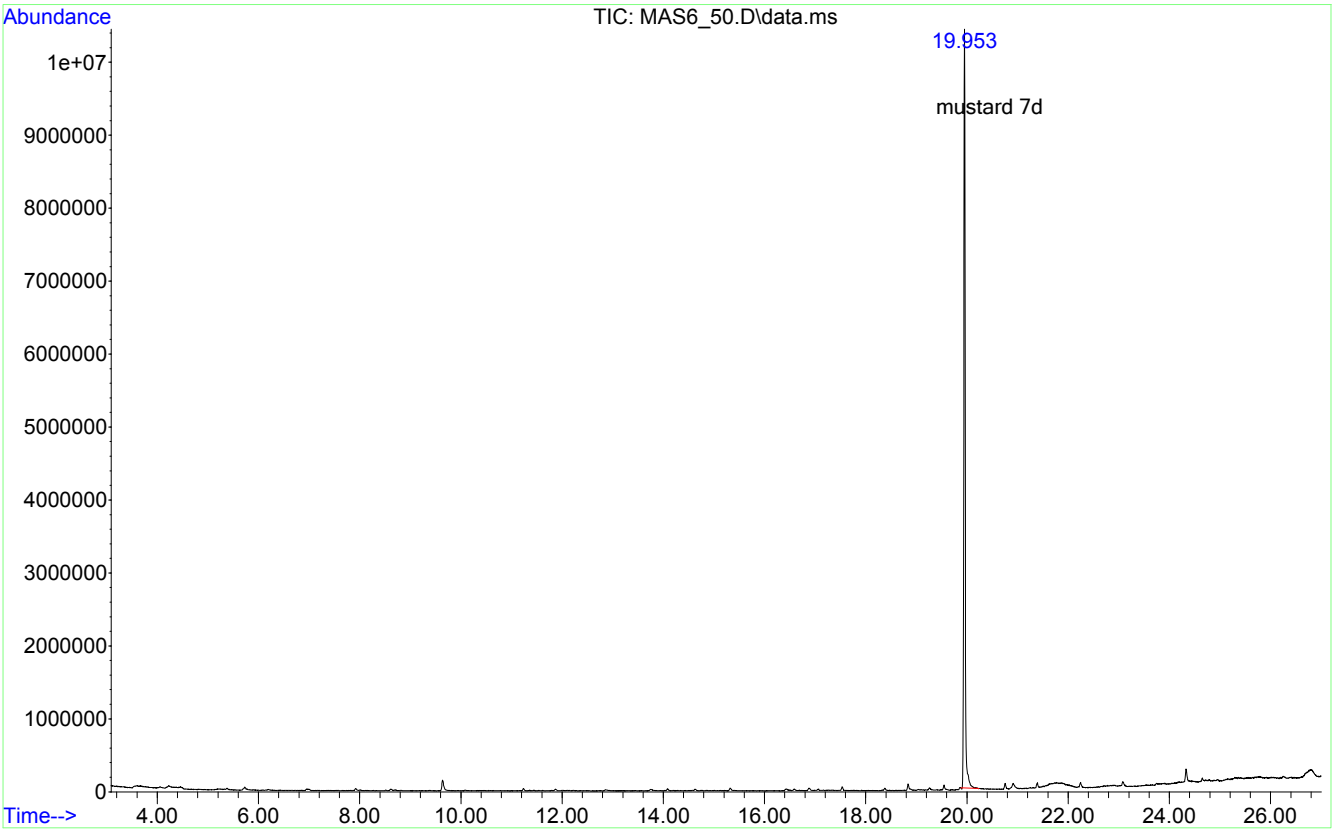


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Instrument : VE032
Sample Name :

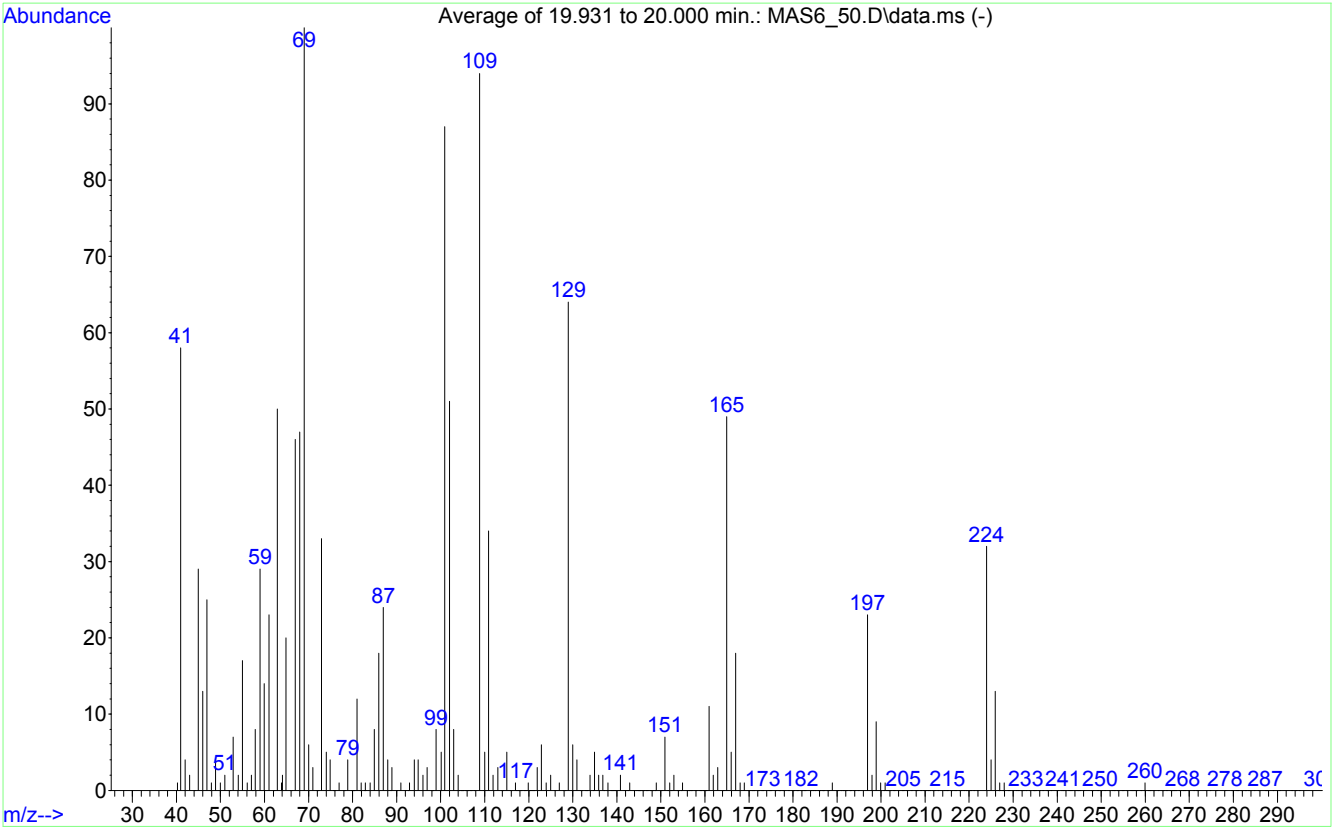


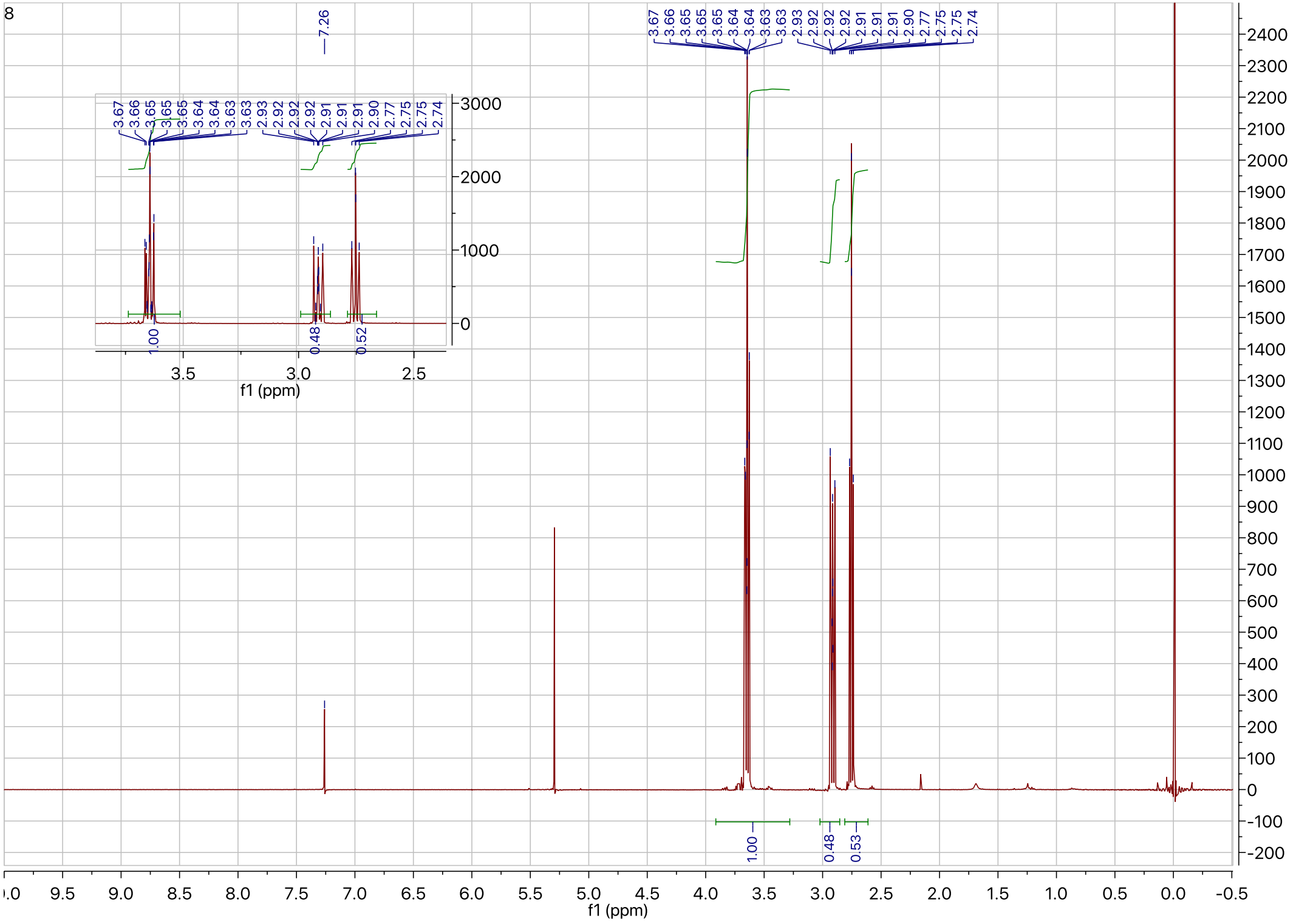

7d
3.64
3.62
3.62
3.61
3.61
3.60
3.60
2.86
2.85
2.85
2.84
2.83
2.82
2.58
2.56
2.54
1.63
1.61
1.59
1.57
1.52
1.52
1.51
1.50
1.50
1.48
1.00
1.14
0.14
1.12
2.18
f1 (ppm)

File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\MAS6_50.D
Date Acquired : 10 Dec 2012 11:59 Method File : 32PT.M
Instrument : VE032
Sample Name :

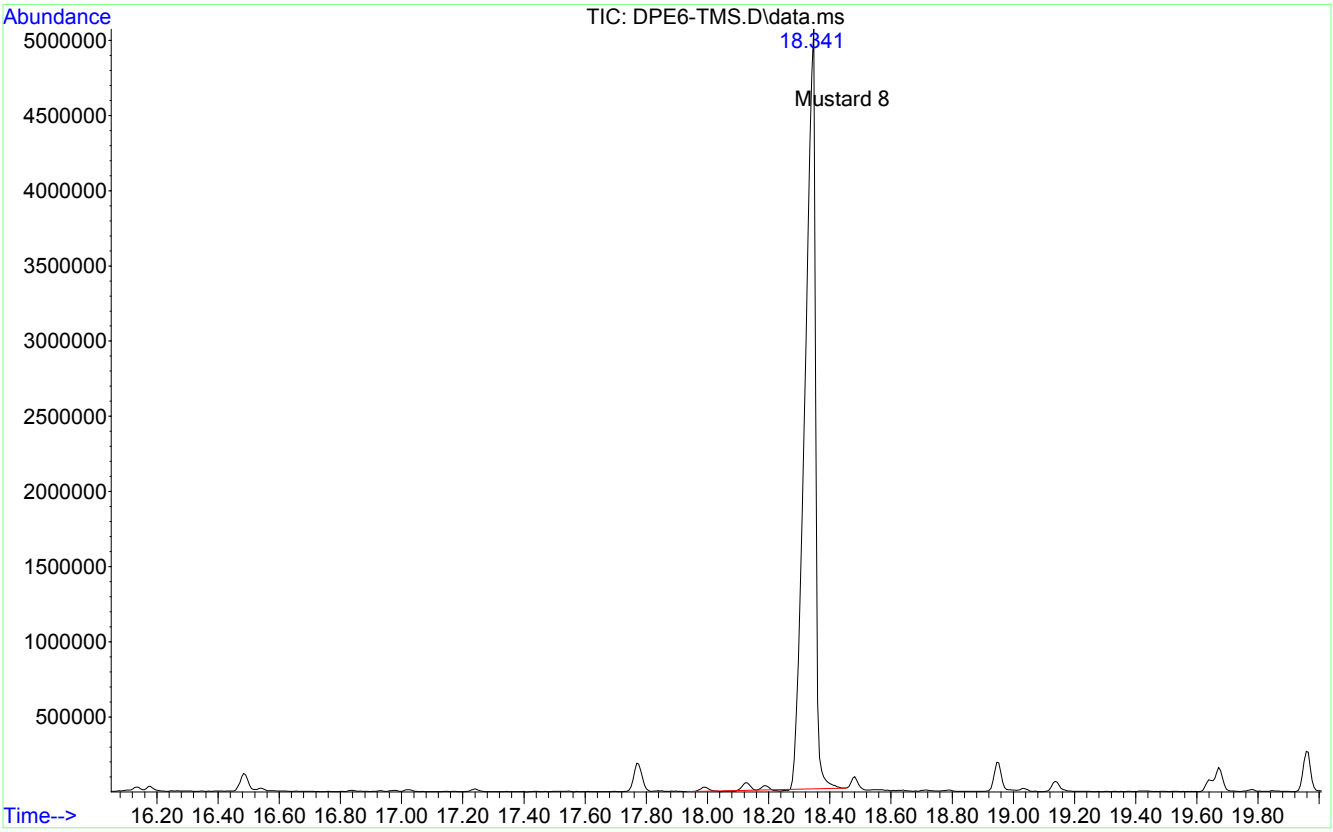


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Instrument : VE032
Sample Name :

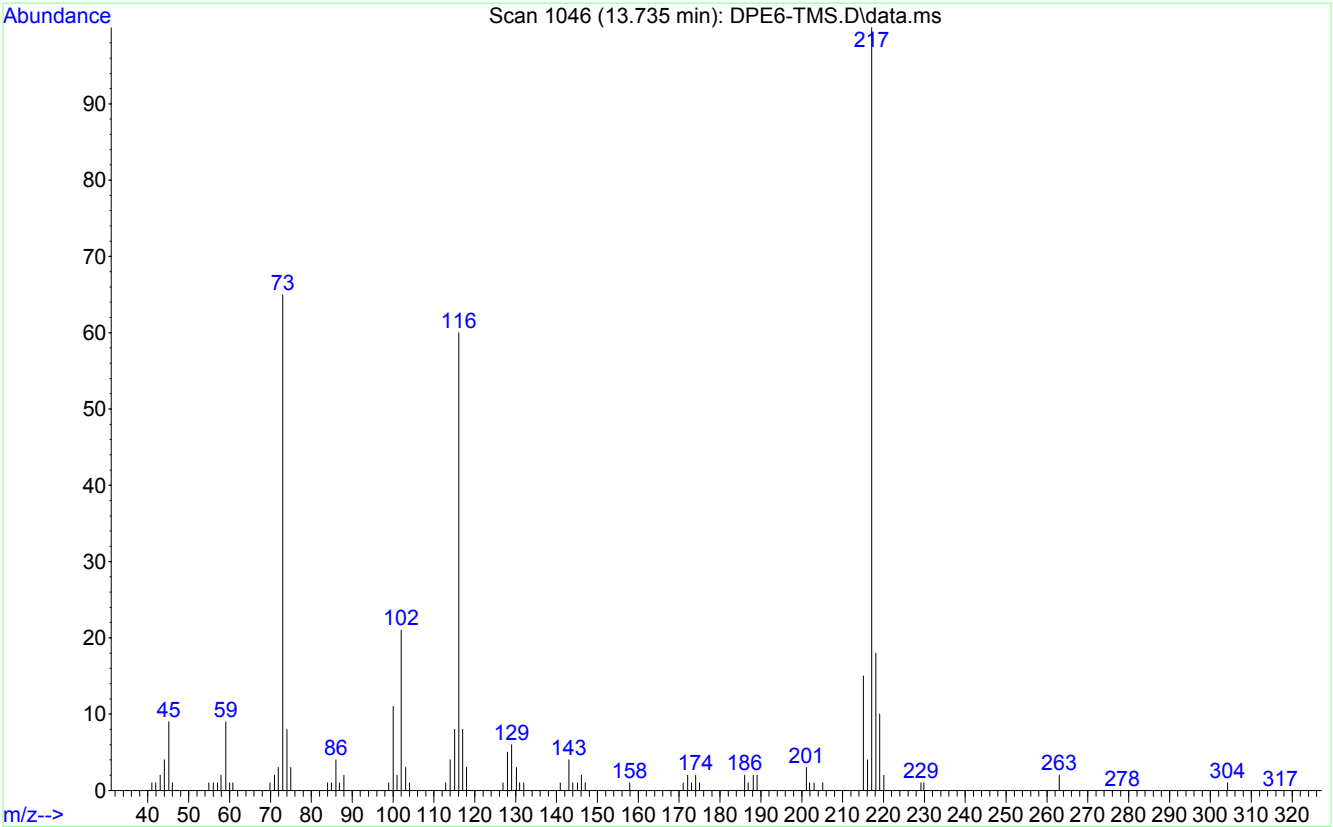



8
7.26
3.67
3.66
3.65
3.65
3.65
3.64
3.64
3.63
3.63
2.93
2.92
2.92
2.92
2.91
2.91
2.91
2.90
2.77
2.75
2.75
2.74
1.00
0.48
0.52
0.53
f1 (ppm)

File : F:\MOSTAZAS descontaminacion\20150063\GC-MS-EI-0991\DPE6-TMS.D
Date Acquired : 9 Mar 2015 12:02 Method File : 35PTMS.M
Instrument : VE002
Sample Name : DPE6-TMS



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Instrument : VE002
Sample Name : DPE6-TMS

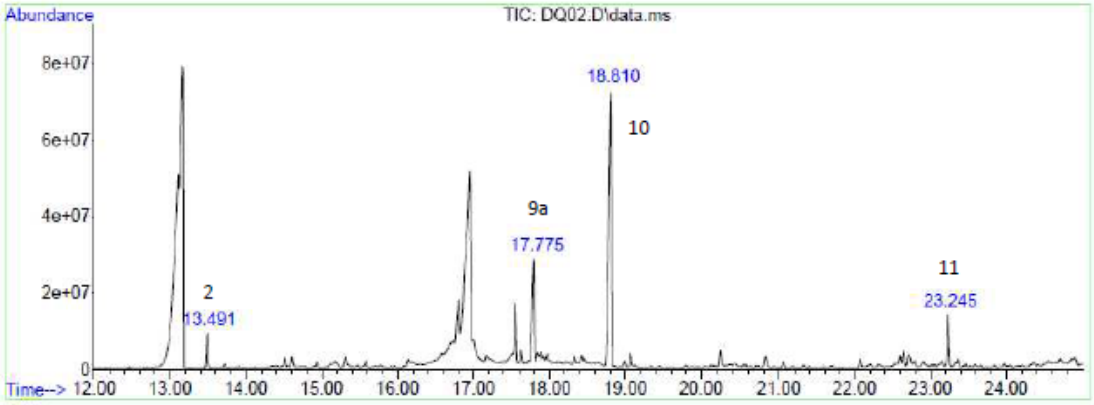


Experimental data

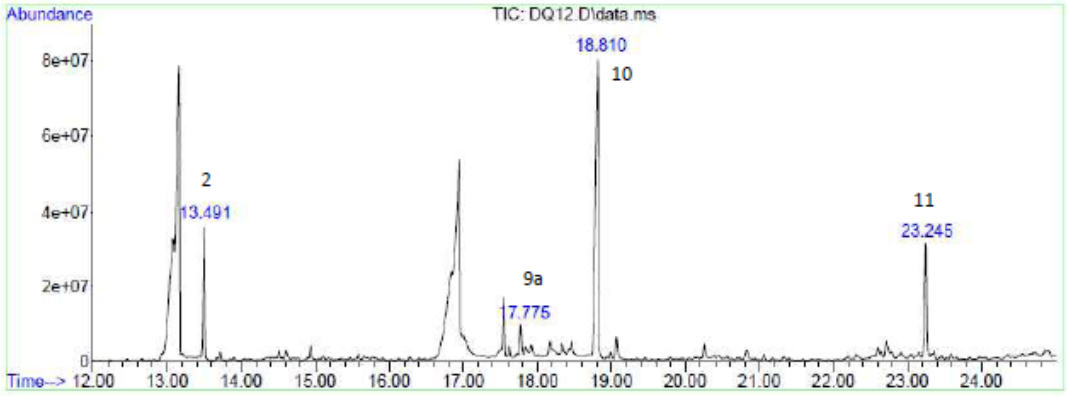
*Compounds **2**, **9**, **10-12** were silylated with BSTFA in order to be observed in the chromatographic columns used in this study.

<u>Main degradation products observed in the decontamination of **7a** with **RM21**</u>

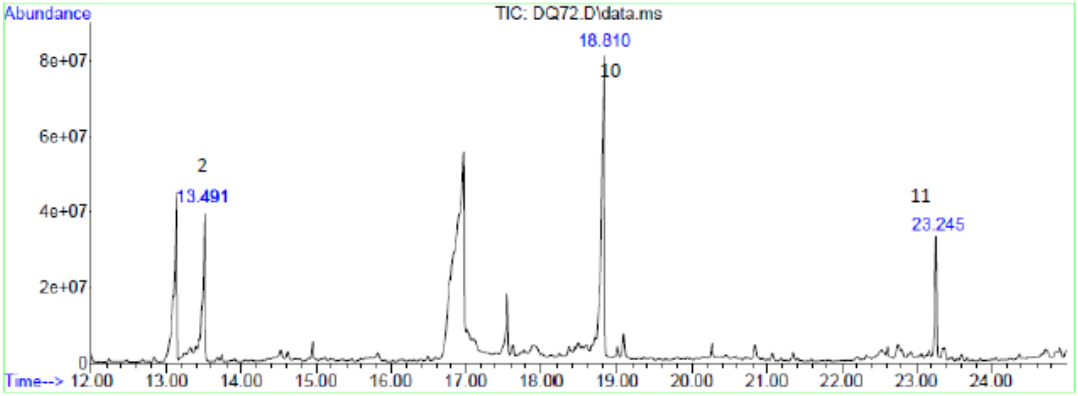
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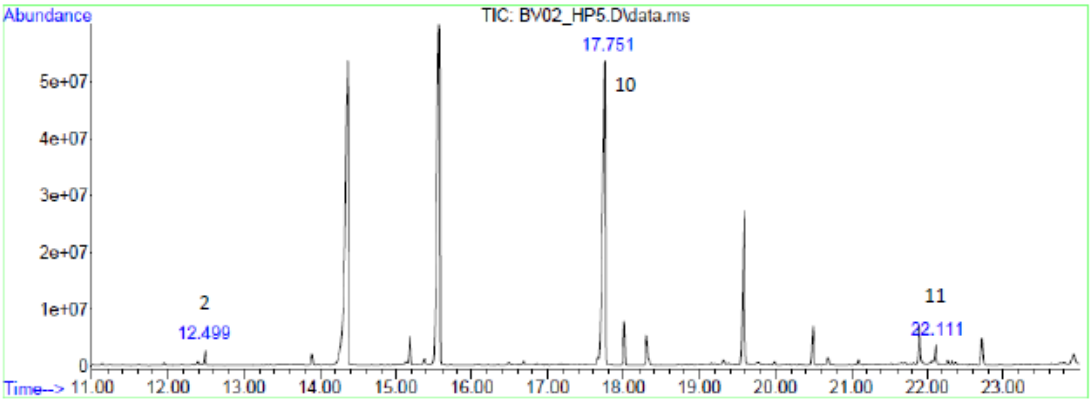
t = 24 hours



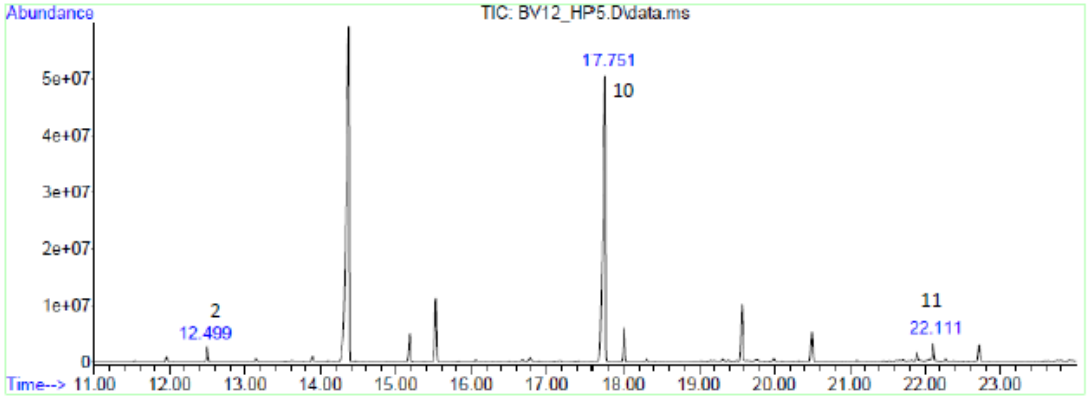
t = 7 days



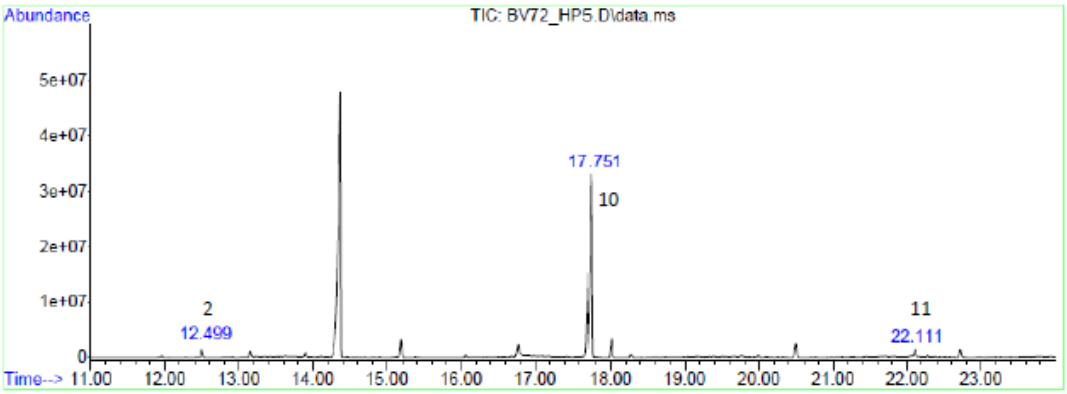
Main degradation products observed in the decontamination of **7a** with **RM31**
t = 90 min.



t = 24 hours

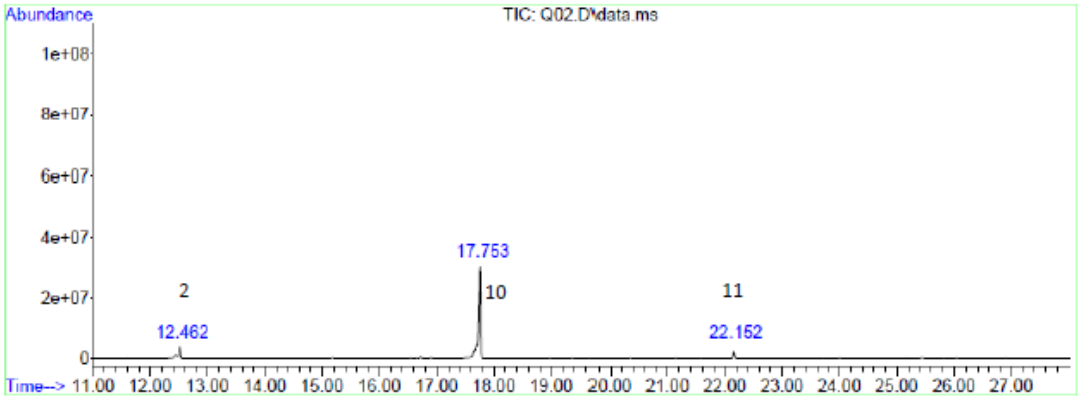


t = 7 days

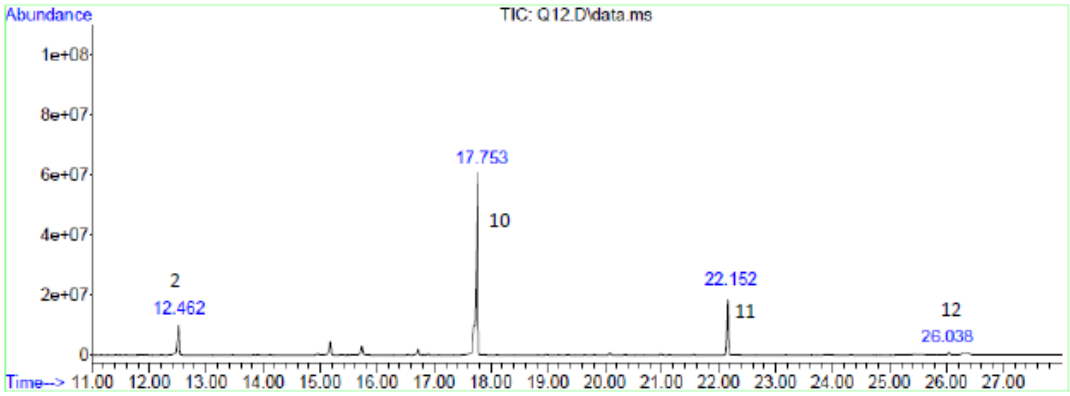


Main degradation products observed in the decontamination of **7a** with **BX24**

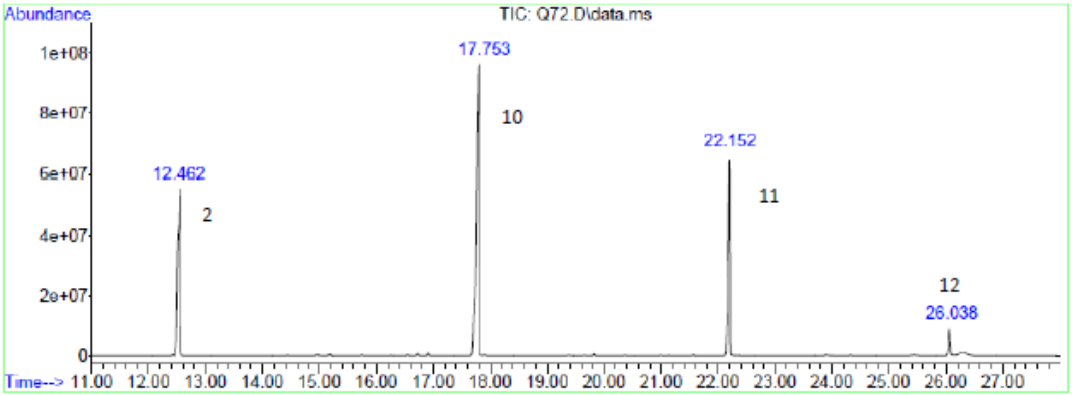
t = 90 min.



t = 24 hours

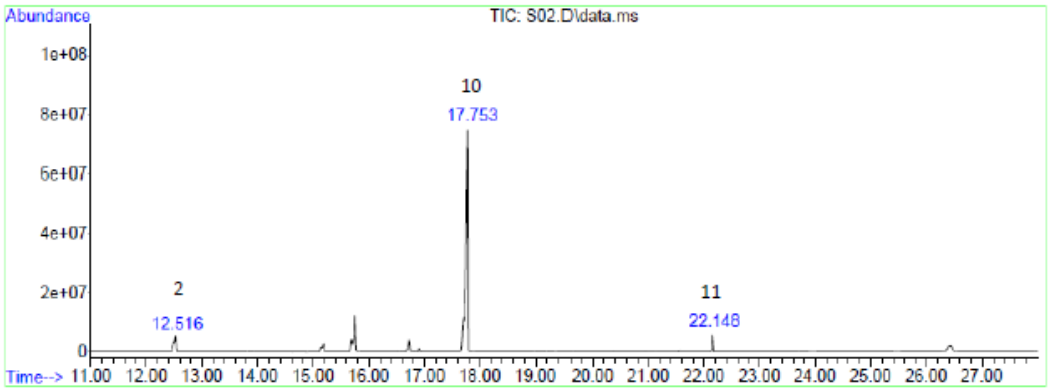


t = 7 days

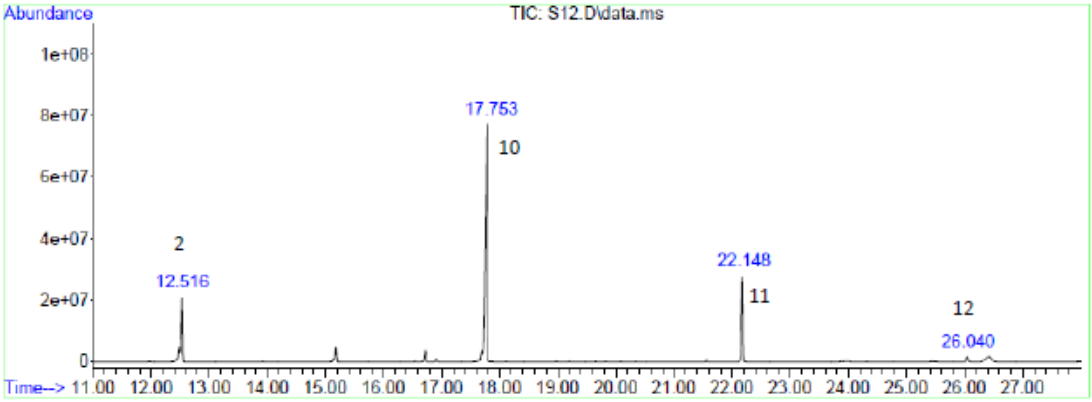


Main degradation products observed in the decontamination of **7a** with **BX29**

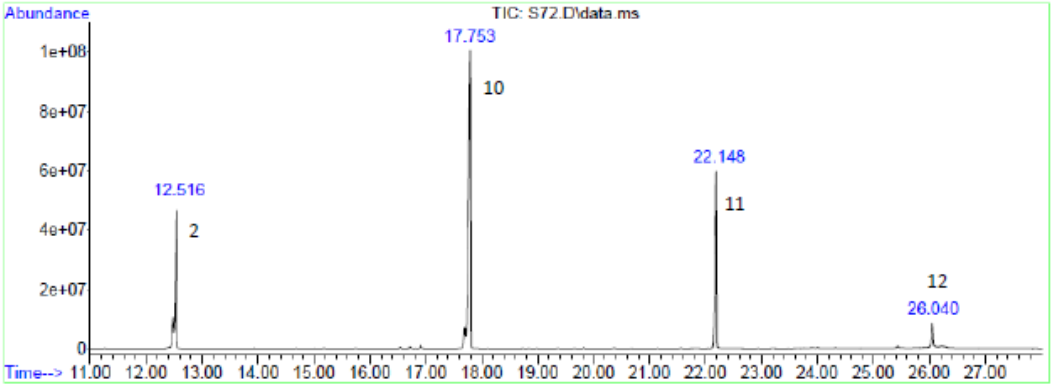
t = 90 min.



t = 24 hours

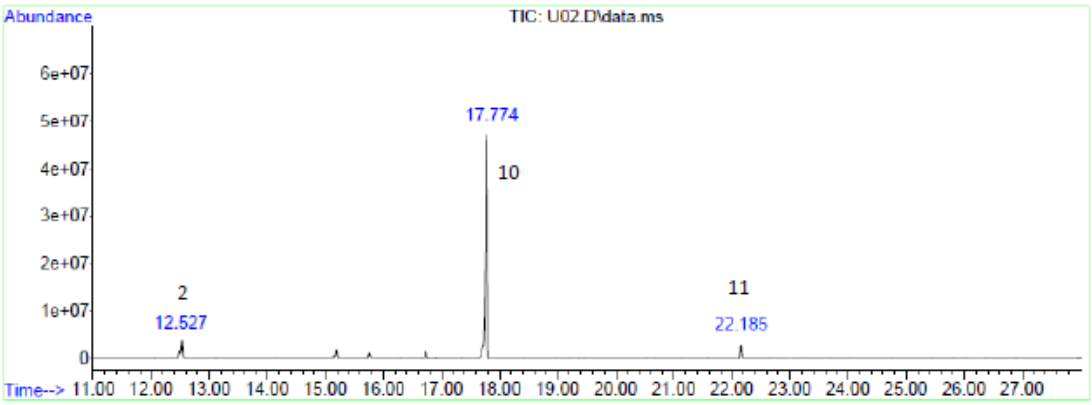


t = 7 days

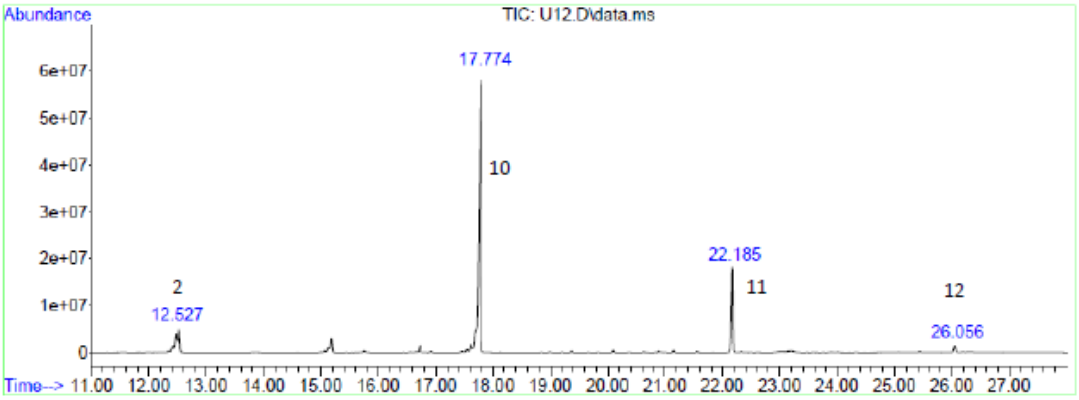


Main degradation products observed in the decontamination of **7a** with **BX40**

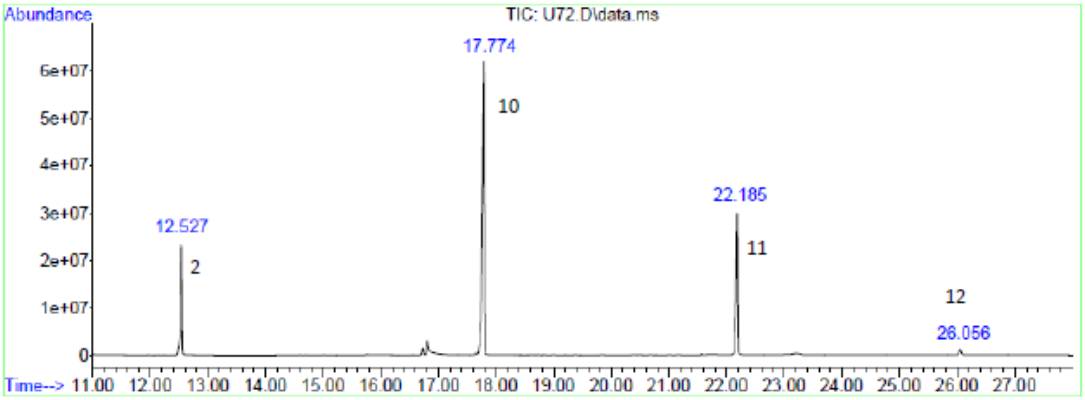
t = 90 min.



t = 24 hours

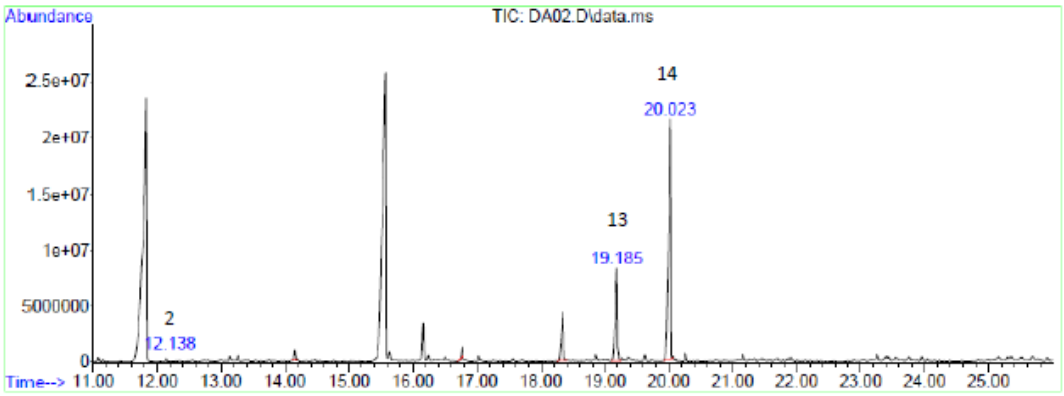


t = 7 days

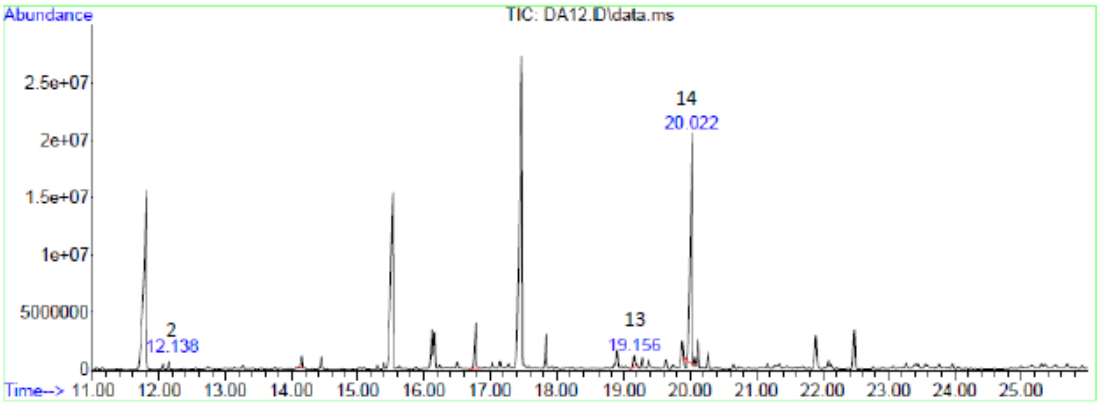


Chemicals **2**, **13** and **14** were silylated with BSTFA in order to be observed in the chromatographic columns used in this study.

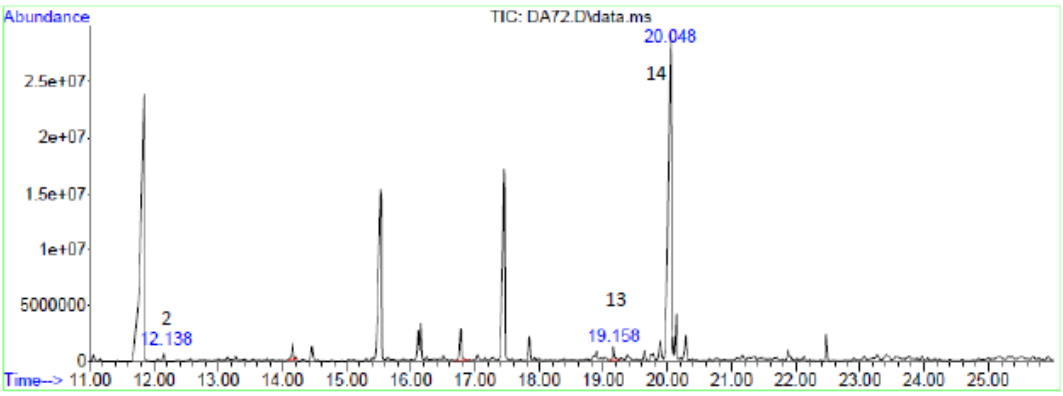
<u>Main degradation products observed in the decontamination of **8** with **RM21**</u>
t = 90 min.



t = 24 hours

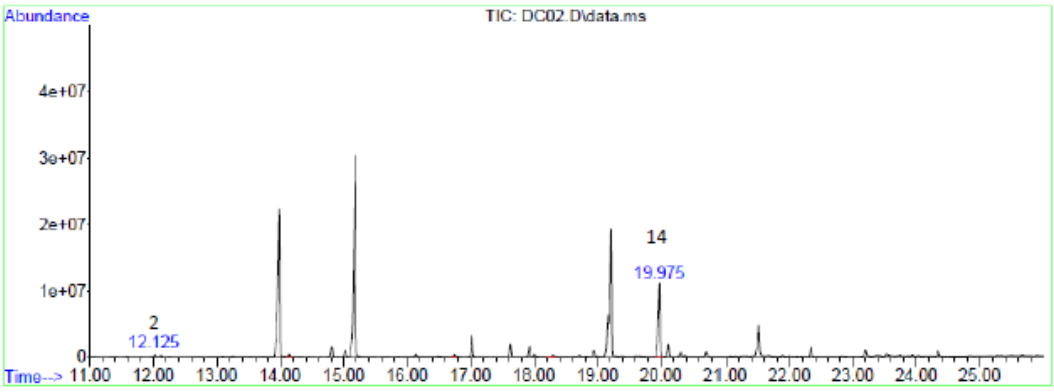


t = 7 days

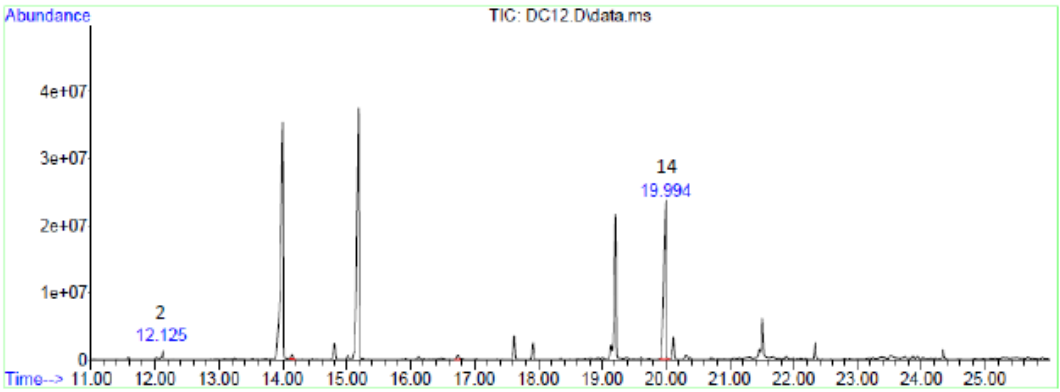


Main degradation products observed in the decontamination of **8** with **RM31**

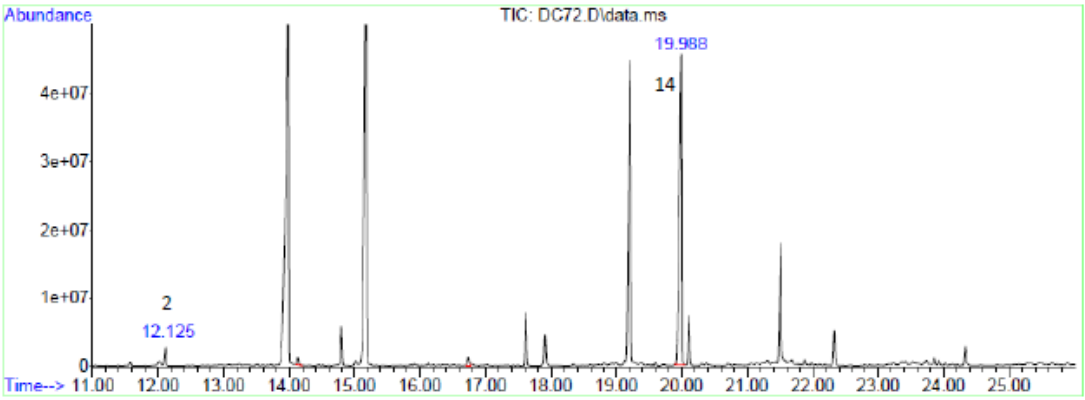
t = 90 min.



t = 24 hours

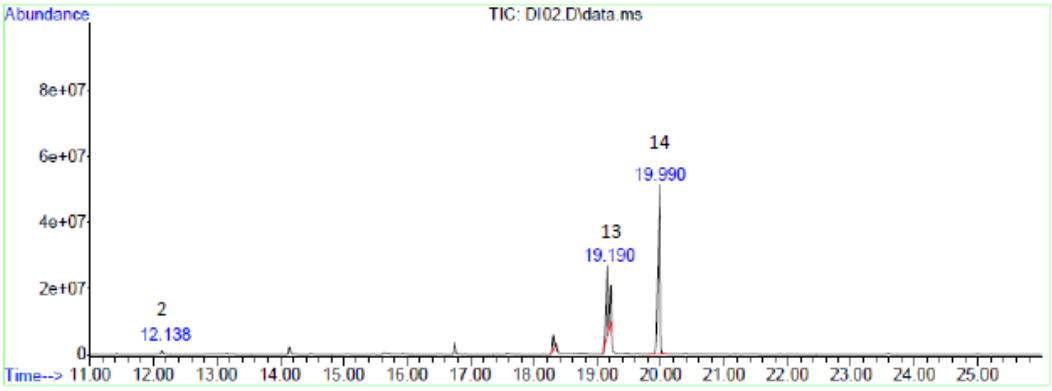


t = 7 days

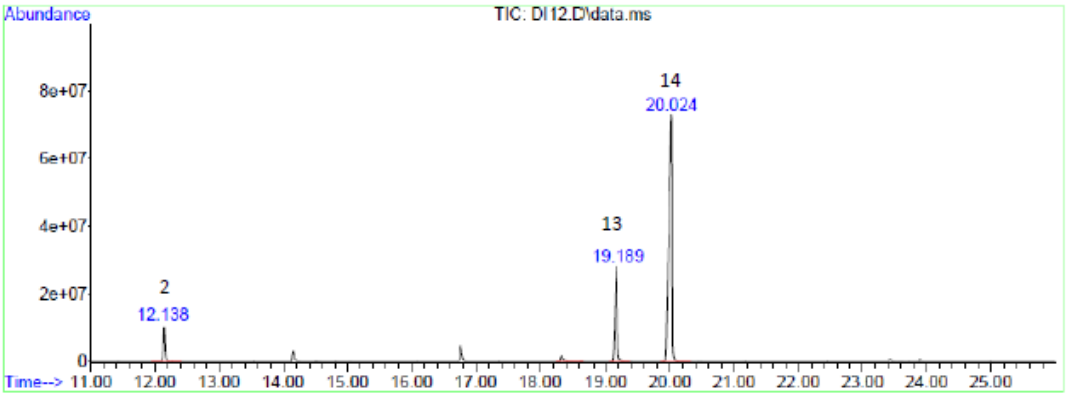


Main degradation products observed in the decontamination of **8** with **BX24**

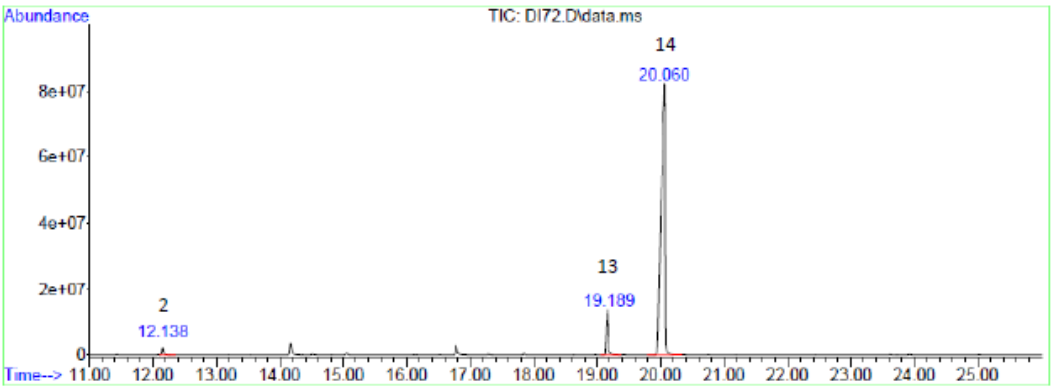
t = 90 min.



t = 24 hours

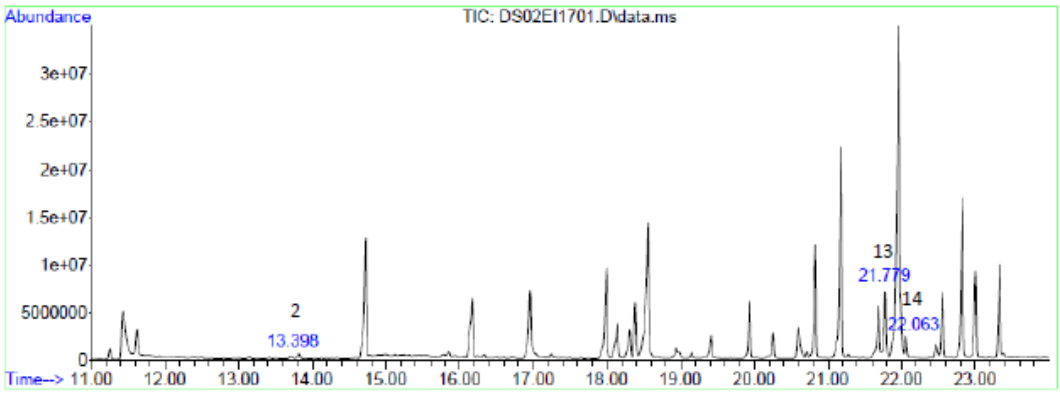


t = 7 days

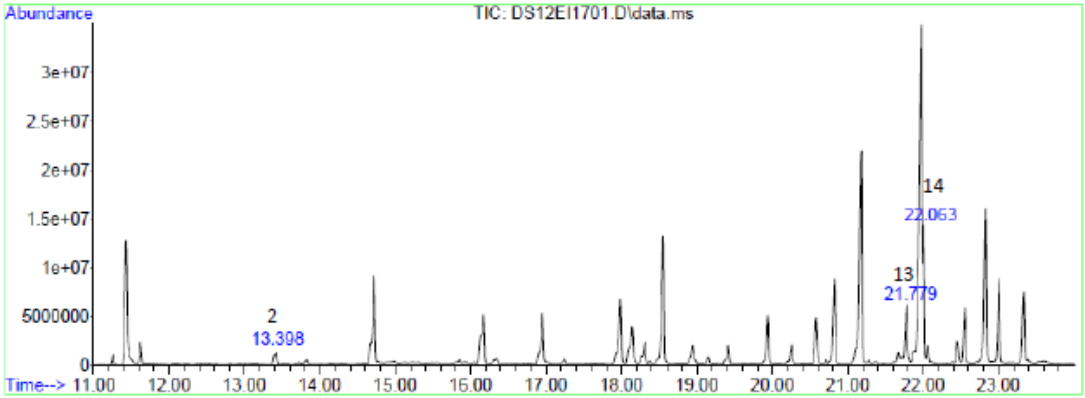


Main degradation products observed in the decontamination of **8** with **BX29**

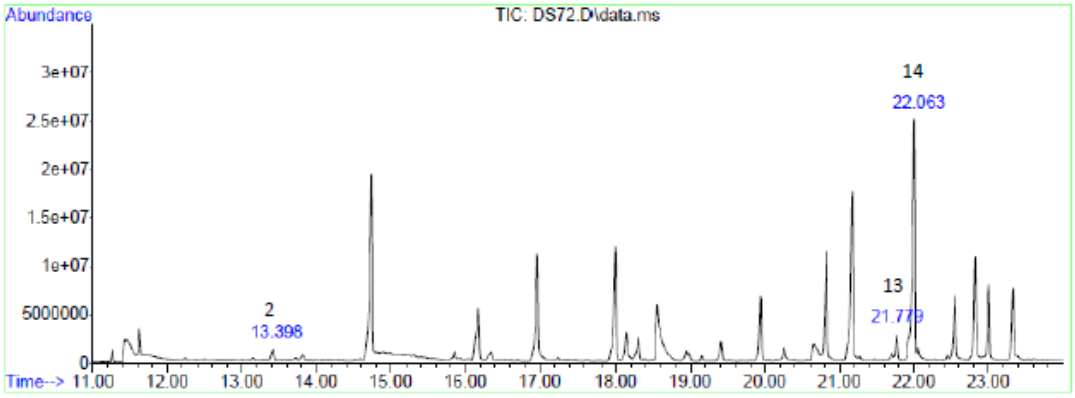
t = 90 min.



t = 24 hours



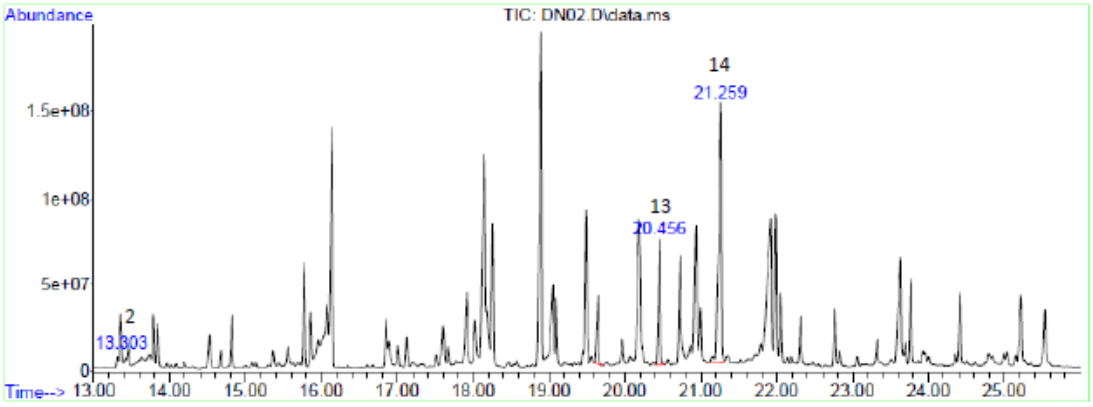
t = 7 days



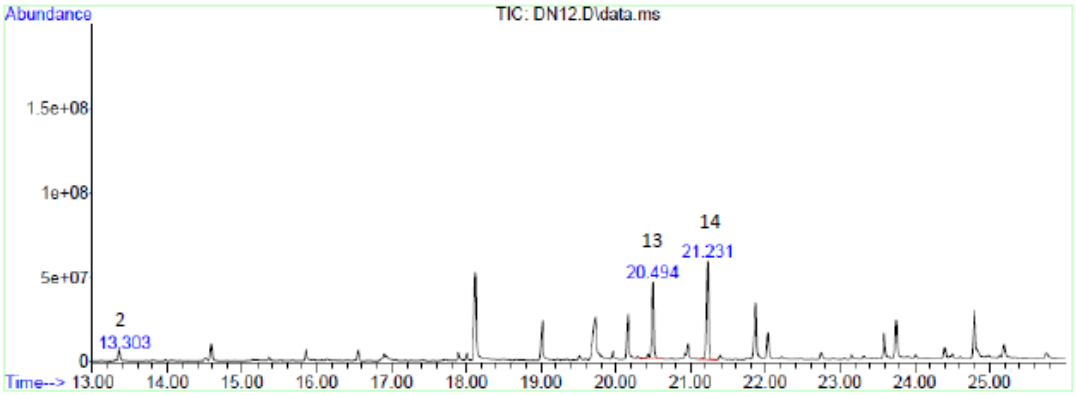
Retention times are different in relation to other experiments because the study with this decontaminant was carried out in a 1701 column instead of a HP5 column.

Main degradation products observed in the decontamination of **8** with **BX40**

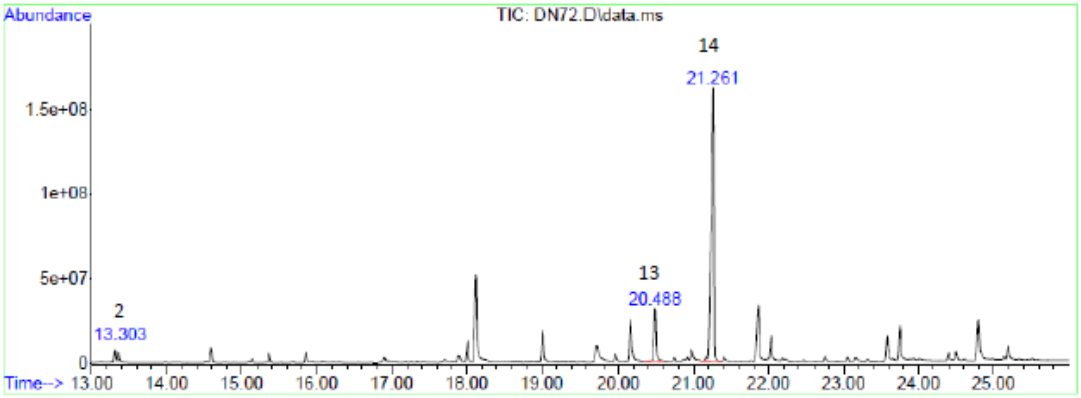
t = 90 min.



t = 24 hours

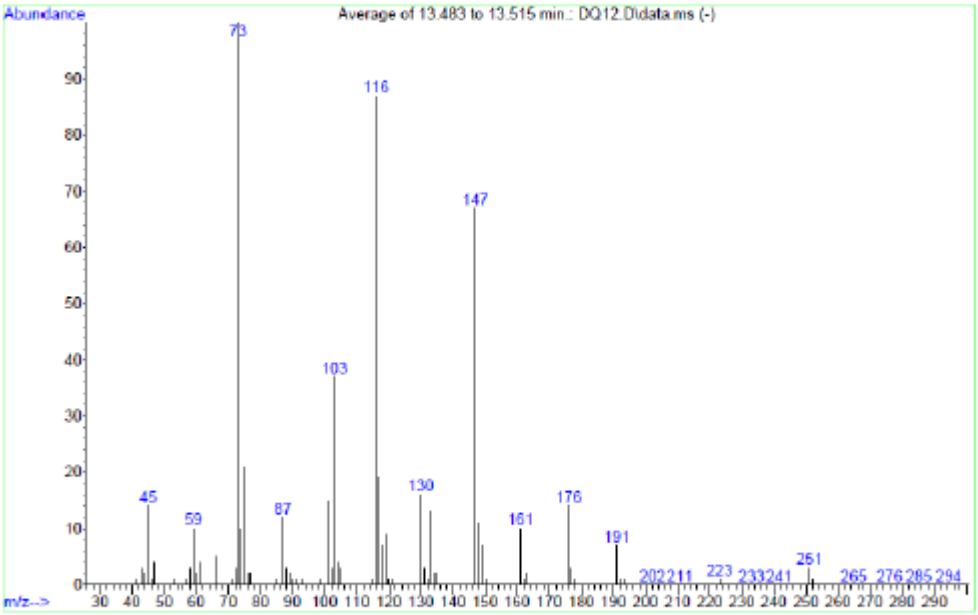


t = 7 days



GC-MS-EI of compound **2** (silylated)

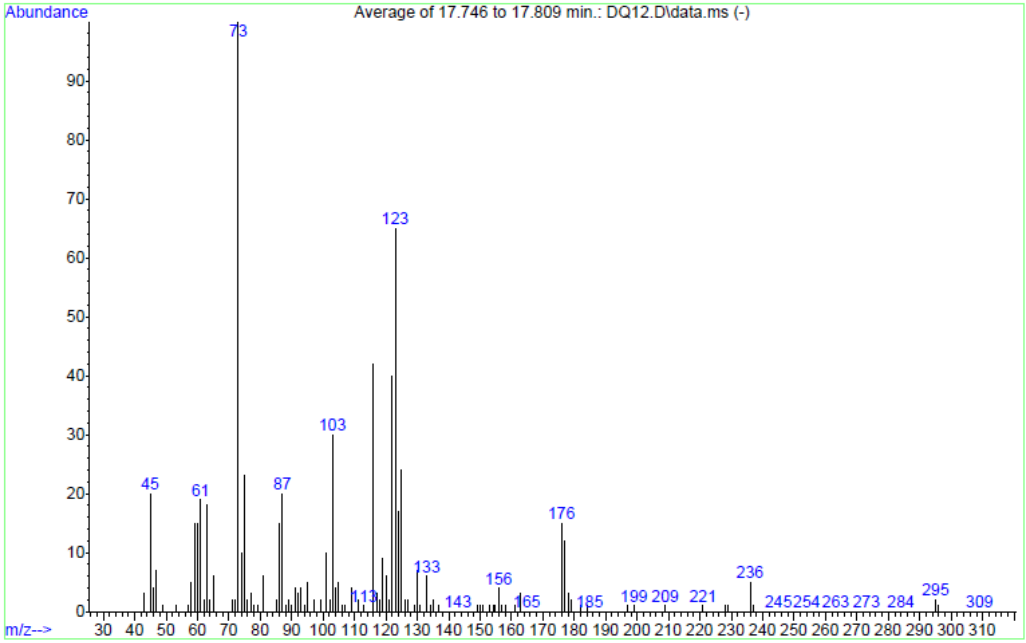
MS(EI,70eV) *m/z* (%B): 266($M^{\cdot+}$,no se observa), 251(3), 191(6), 176(12), 161(9), 147(66), 130(15), 116(84), 103(35), 87(12), 73(100), 59(10), 45(14)



MS(CI,NH_3) *m/z* (%B): 284$[M+NH_4]^+$(31), 267$[M+H]^+$(21), 177{$[(M+H]-(CH_3)_3SiOH\}^+$(100), 90$[(CH_3)_3Si(NH_3)]^+$(15)

GC-MS-EI of compound **9** (silylated)

MS(EI,70eV) *m/z* (%B): 272(M ,no se observa), 236(5), 176(13), 123(62), 116(41), 103(28), 87(18), 73(100)

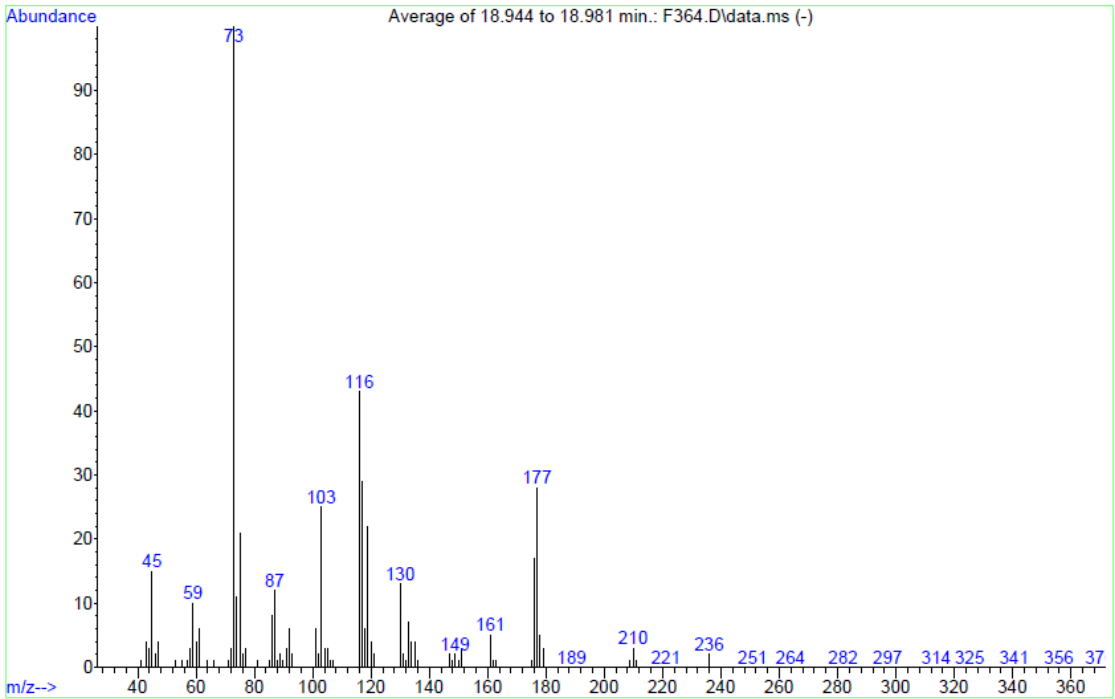


GC-MS-CI-NH_3 of compound **9**(silylated)

MS(CI,NH_3) *m/z* (%B): 290$[M+NH_4]^+$(100), 183$\{[M+H]-(CH_3)_3SiOH\}^+$(94), 155$\{[M+H]-(CH_3)_3SiOCH_2\text{-}CH_3\}^+$(25), 90$[(CH_3)_3Si(NH_3)]^+$(15)

GC-MS-EI of compound **10** (silylated)

MS(EI,70eV) *m/z* (%B): 326(M ,no se observa), 236(3), 210(4), 177(28), 148(3), 147(4), 133(6), 117(30), 116(44), 103(24), 87(12), 73(100), 59(10), 45(16)

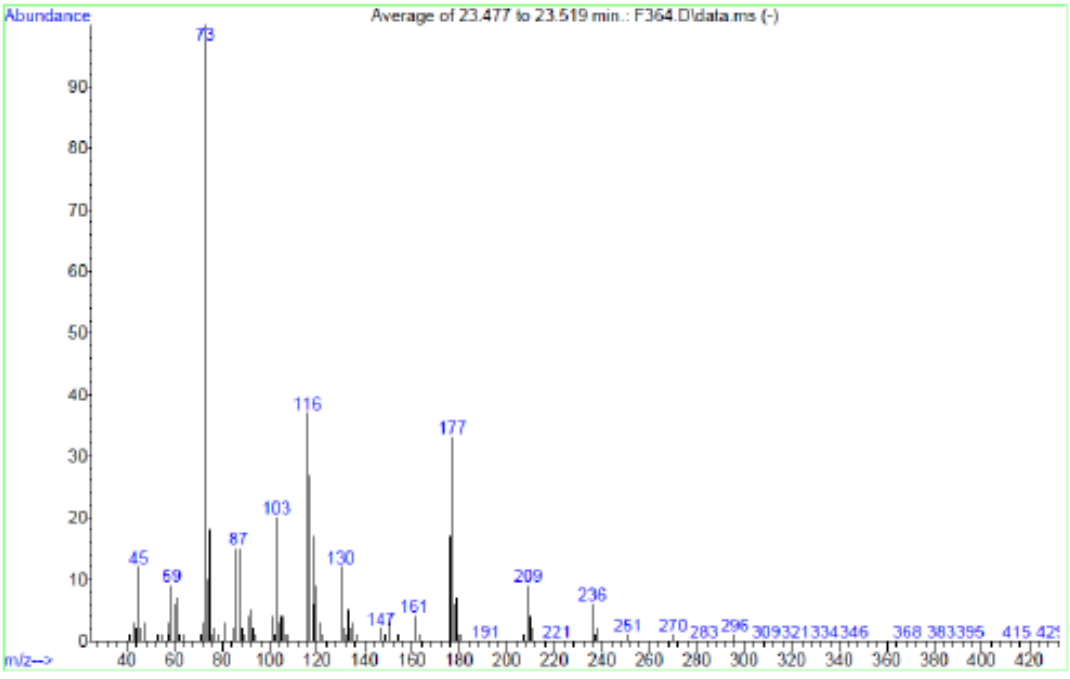


GC-MS-CI-NH_3 of chemical **10**(silylated)

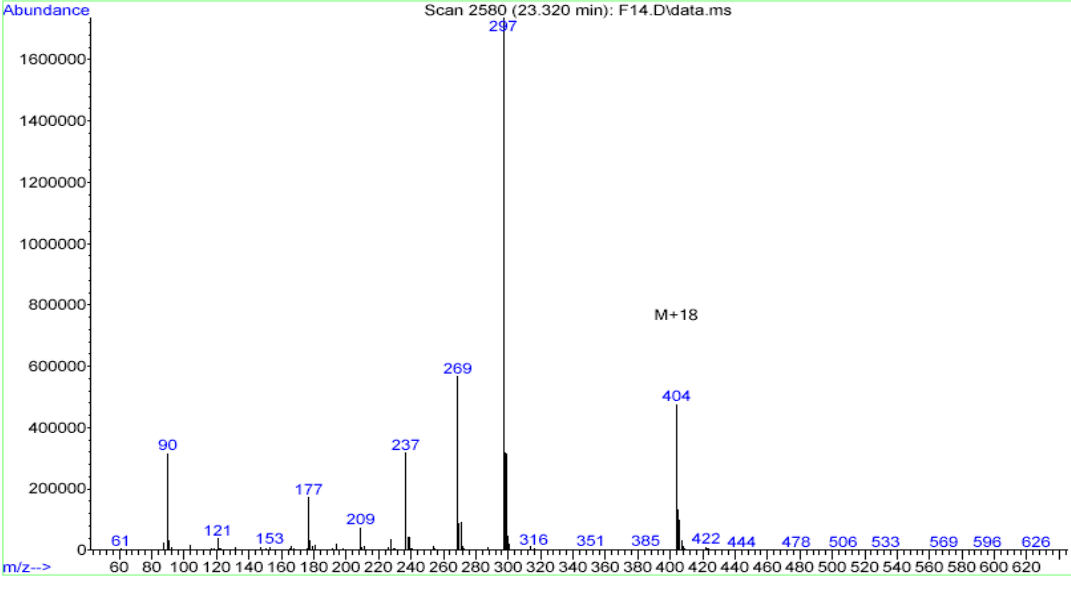
MS(CI,NH_3) *m/z* (%B): 344$[M+NH_4]^+$(46), 237{$[M+H]$- $(CH_3)_3SiOH\}^+$(35), 209{$[M+H]$-$(CH_3)_3SiOCH_2$-$CH_3\}^+$(68), 90$[(CH_3)_3Si(NH_3)]^+$(100)

GC-MS-EI of chemical **11**(silylated)

MS(EI,70eV) *m/z* (%B): 386($M^{\bullet+}$, no se observa), 296 (1), 236(6), 209(9), 177(33), 130(12), 116(38), 103(20), 87(15), 73(100)



GC-MS-CI-NH_3 of chemical **11**(silylated)



Cartesian Coordinates and Energies (in Hartree) of all optimized species. In brackets the values of the imaginary frequency for TS

15+OH E = -1183.66462

6	-0.361590000	0.686890000	0.156890000
6	-0.409835000	1.797970000	1.110004000
1	0.161071000	0.895910000	-0.809766000
1	-0.461018000	-0.328824000	0.530827000
1	0.080117000	2.729931000	0.836439000
1	-0.522772000	1.609128000	2.174175000
16	-2.024554000	1.567944000	0.200751000
6	-1.883143000	2.761398000	-1.212411000
1	-2.670373000	2.453931000	-1.905638000
1	-0.887203000	2.559801000	-1.651389000
6	-2.059841000	4.202577000	-0.754725000
1	-3.073146000	4.392645000	-0.389654000
1	-1.361762000	4.456843000	0.045429000
16	-1.836801000	5.366927000	-2.160803000
6	-0.070962000	5.128587000	-2.608599000
1	0.114950000	4.102471000	-2.939809000
1	0.085730000	5.803008000	-3.456633000
6	0.904570000	5.472095000	-1.491025000
1	0.786217000	4.766624000	-0.657204000
1	0.707627000	6.483924000	-1.107988000
8	2.219572000	5.374117000	-2.046906000
1	2.847930000	5.456369000	-1.315698000
8	0.839065000	1.849071000	-2.233270000
1	0.206872000	1.450846000	-2.849462000

TS16-1 E = -1183.64885 (-215.56)

6	-0.521081000	0.628406000	-0.311858000
6	-0.236285000	1.729563000	0.602863000
1	-0.213514000	0.689946000	-1.358884000
1	-0.662961000	-0.365350000	0.102226000
1	0.261086000	2.614288000	0.210786000
1	-0.053208000	1.521344000	1.654187000
16	-2.060430000	1.738755000	0.223042000
6	-2.115438000	2.969810000	-1.159354000
1	-3.037667000	2.759508000	-1.705646000
1	-1.263628000	2.748652000	-1.805224000
6	-2.085411000	4.395612000	-0.615600000
1	-3.019012000	4.638136000	-0.101850000
1	-1.266023000	4.535236000	0.093151000
16	-1.927019000	5.625210000	-1.971590000
6	-0.174038000	5.395838000	-2.462433000
1	0.020632000	4.341181000	-2.677790000
1	-0.065857000	5.949695000	-3.399963000
6	0.822082000	5.917615000	-1.434434000
1	0.714251000	5.372097000	-0.486817000
1	0.628866000	6.981138000	-1.234318000
8	2.127743000	5.720363000	-1.984665000
1	2.768387000	5.982115000	-1.308252000
8	1.529105000	0.023082000	-1.791879000
1	1.108387000	-0.849878000	-1.808077000

10 E = -1183.75541

6	-0.553218000	-0.140756000	-0.646630000
6	-0.400887000	0.923107000	0.432909000
1	-0.829659000	0.323257000	-1.603553000
1	-1.354765000	-0.839831000	-0.369041000
1	0.411131000	1.610035000	0.177609000
1	-0.144502000	0.449636000	1.385779000
16	-1.941171000	1.862558000	0.762567000
6	-2.117133000	2.865344000	-0.769604000
1	-3.117668000	3.302589000	-0.693988000
1	-2.111598000	2.203469000	-1.639321000
6	-1.057800000	3.956263000	-0.898674000
1	-1.084664000	4.617019000	-0.029191000
1	-0.056749000	3.522909000	-0.977829000
16	-1.361378000	4.930072000	-2.439291000
6	0.243392000	5.800757000	-2.591844000
1	1.055230000	5.068935000	-2.528329000
1	0.257498000	6.232050000	-3.597627000
6	0.440730000	6.900329000	-1.556360000
1	0.406848000	6.477988000	-0.542388000
1	-0.369534000	7.638818000	-1.638632000
8	1.714909000	7.496587000	-1.818359000
1	1.868139000	8.162656000	-1.133569000
8	0.706841000	-0.810456000	-0.753463000
1	0.623694000	-1.468995000	-1.457690000

TS16-2 E = -1183.64058 (-439.098)

6	-0.854560000	0.819976000	0.539092000
6	0.232277000	1.484211000	1.272466000
1	-1.074177000	1.134119000	-0.477809000
1	-1.094807000	-0.211479000	0.778881000
1	0.786602000	2.281510000	0.783868000
1	0.771459000	0.928533000	2.033733000
16	-1.456463000	2.016228000	1.824402000
6	-1.690280000	3.773746000	0.537875000
1	-2.753679000	3.664017000	0.394537000
1	-1.060797000	3.420443000	-0.266122000
6	-1.163427000	4.879687000	1.423325000
1	-0.153886000	4.649204000	1.776456000
1	-1.100315000	5.788956000	0.828555000
16	-2.143508000	5.217619000	2.942694000
6	-3.789457000	5.661341000	2.262422000
1	-4.248122000	4.790645000	1.785097000
1	-4.388067000	5.906896000	3.145886000
6	-3.778079000	6.844230000	1.300882000
1	-3.261368000	6.566248000	0.373867000
1	-3.249674000	7.694967000	1.756643000
8	-5.148556000	7.172943000	1.034773000
1	-5.161864000	7.715462000	0.234120000
8	-2.125090000	5.159691000	-1.274130000
1	-1.274122000	5.617132000	-1.215455000

2 + thiirane E = -1183.73354

6	-0.224614000	0.630523000	0.726827000
6	0.782226000	1.636193000	1.113698000
1	-1.109749000	0.962187000	0.191443000
1	0.114792000	-0.371897000	0.480478000
1	0.605430000	2.675634000	0.849515000
1	1.826904000	1.338570000	1.138771000

16	-0.227419000	1.017900000	2.535897000
6	-2.264977000	3.664682000	0.189825000
1	-2.807850000	2.756973000	0.470269000
1	-1.358640000	3.358963000	-0.356435000
6	-1.825275000	4.422111000	1.437916000
1	-1.133410000	3.790832000	2.004378000
1	-1.287275000	5.334601000	1.162298000
16	-3.145129000	4.821169000	2.654697000
6	-4.190619000	6.057588000	1.787195000
1	-4.669450000	5.594150000	0.923869000
1	-4.964221000	6.323754000	2.514854000
6	-3.444584000	7.314145000	1.360242000
1	-2.692124000	7.069380000	0.599080000
1	-2.921238000	7.753853000	2.221627000
8	-4.420596000	8.217900000	0.829602000
1	-3.943051000	8.977239000	0.466899000
8	-3.139360000	4.404589000	-0.664389000
1	-2.697027000	5.238228000	-0.881321000

13 E = -1721.93563

6	-1.481509000	3.166327000	-1.090478000
1	-2.176487000	3.901815000	-0.672932000
1	-1.962023000	2.703263000	-1.964432000
6	-0.170960000	3.847098000	-1.492202000
1	0.313576000	4.247989000	-0.597931000
1	0.509361000	3.137950000	-1.972247000
16	-0.519769000	5.204752000	-2.685903000
6	1.191283000	5.709887000	-3.105379000
1	1.768446000	4.824118000	-3.389792000
1	1.105741000	6.352437000	-3.987066000
6	1.893422000	6.463553000	-1.983227000
1	1.966390000	5.831528000	-1.087592000
1	1.312358000	7.357646000	-1.715698000
8	3.195183000	6.815149000	-2.463277000
1	3.662748000	7.247853000	-1.734830000
6	-4.218988000	1.360125000	0.630870000
6	-0.677172000	0.983674000	-0.506052000
6	-3.346385000	0.626766000	1.633585000
1	-3.672204000	1.633626000	-0.268432000
6	-0.742385000	-0.035766000	0.619162000
1	-1.186763000	0.608124000	-1.404654000
1	0.379713000	1.151133000	-0.760366000
1	-3.956885000	0.240661000	2.453739000
1	-2.637507000	1.345737000	2.053501000
1	-0.103461000	-0.886351000	0.362685000
1	-0.353505000	0.404918000	1.542409000
8	-1.283002000	2.198560000	-0.062849000
16	-2.385738000	-0.790278000	0.957699000
1	-4.657961000	2.250941000	1.084441000
17	-5.640544000	0.338056000	0.078018000

TS20-1 E = -1721.90281 (-139.352)

6	-0.447754000	3.416532000	0.211245000
1	-0.422776000	3.394134000	1.304773000
1	0.567208000	3.222967000	-0.147425000
16	-0.946484000	5.148199000	-0.183835000
6	-1.247785000	5.112513000	-1.995637000
1	-2.005495000	4.361206000	-2.226081000
1	-1.669561000	6.097985000	-2.222548000

6	0.003885000	4.873548000	-2.836123000
1	0.474731000	3.930649000	-2.551958000
1	0.728140000	5.683706000	-2.673597000
8	-0.322539000	4.744380000	-4.224360000
1	-0.739596000	5.572344000	-4.504930000
8	-1.096026000	2.100916000	-1.676835000
6	-1.381112000	2.327382000	-0.294719000
1	-2.431301000	2.618528000	-0.158005000
1	-1.211250000	1.400927000	0.274445000
6	-2.154854000	1.496639000	-2.398230000
1	-3.084006000	2.073767000	-2.278803000
1	-2.342020000	0.469454000	-2.051953000
6	-1.699481000	1.501491000	-3.854491000
1	-1.503146000	2.520912000	-4.197826000
1	-0.796671000	0.900195000	-3.981797000
16	-3.009840000	0.814084000	-4.947069000
6	-2.619181000	-1.145852000	-4.792233000
1	-3.554353000	-1.683230000	-4.873426000
1	-2.020650000	-1.292219000	-3.902709000
6	-2.068124000	-0.458890000	-5.945055000
1	-1.003543000	-0.246089000	-5.977708000
1	-2.544580000	-0.612907000	-6.909570000
17	-1.552100000	-3.680442000	-5.382107000

17 + Cl E = -1721.90316

6	-0.440732000	3.416215000	0.212376000
1	-0.411566000	3.386418000	1.305586000
1	0.572393000	3.222838000	-0.151555000
16	-0.937442000	5.151448000	-0.169699000
6	-1.247302000	5.126995000	-1.980299000
1	-2.006898000	4.377888000	-2.211886000
1	-1.669501000	6.114077000	-2.199213000
6	0.000480000	4.891980000	-2.827734000
1	0.473169000	3.948251000	-2.549447000
1	0.725014000	5.701911000	-2.665413000
8	-0.331858000	4.767853000	-4.215069000
1	-0.750713000	5.596442000	-4.491074000
8	-1.093985000	2.111805000	-1.681225000
6	-1.378352000	2.332586000	-0.297797000
1	-2.427421000	2.626679000	-0.159542000
1	-1.211491000	1.402605000	0.266308000
6	-2.157206000	1.522661000	-2.408152000
1	-3.079306000	2.111872000	-2.294041000
1	-2.359446000	0.497486000	-2.064870000
6	-1.689015000	1.525961000	-3.860732000
1	-1.479936000	2.544415000	-4.199795000
1	-0.792875000	0.914138000	-3.983539000
16	-2.996183000	0.864353000	-4.971852000
6	-2.704094000	-1.050517000	-4.789232000
1	-3.643754000	-1.576902000	-4.899430000
1	-2.121670000	-1.248292000	-3.898048000
6	-2.073624000	-0.446910000	-5.950065000
1	-1.001542000	-0.275603000	-5.949044000
1	-2.532695000	-0.588952000	-6.924417000
17	-1.595950000	-3.706509000	-5.394287000

TS20-2 E = -1721.90281 (-385.503)

6	-0.447754000	3.416532000	0.211245000

1	-0.422776000	3.394134000	1.304773000
1	0.567208000	3.222967000	-0.147425000
16	-0.946484000	5.148199000	-0.183835000
6	-1.247785000	5.112513000	-1.995637000
1	-2.005495000	4.361206000	-2.226081000
1	-1.669561000	6.097985000	-2.222548000
6	0.003885000	4.873548000	-2.836123000
1	0.474731000	3.930649000	-2.551958000
1	0.728140000	5.683706000	-2.673597000
8	-0.322539000	4.744380000	-4.224360000
1	-0.739596000	5.572344000	-4.504930000
8	-1.096026000	2.100916000	-1.676835000
6	-1.381112000	2.327382000	-0.294719000
1	-2.431301000	2.618528000	-0.158005000
1	-1.211250000	1.400927000	0.274445000
6	-2.154854000	1.496639000	-2.398230000
1	-3.084006000	2.073767000	-2.278803000
1	-2.342020000	0.469454000	-2.051953000
6	-1.699481000	1.501491000	-3.854491000
1	-1.503146000	2.520912000	-4.197826000
1	-0.796671000	0.900195000	-3.981797000
16	-3.009840000	0.814084000	-4.947069000
6	-2.619181000	-1.145852000	-4.792233000
1	-3.554353000	-1.683230000	-4.873426000
1	-2.020650000	-1.292219000	-3.902709000
6	-2.068124000	-0.458890000	-5.945055000
1	-1.003543000	-0.246089000	-5.977708000
1	-2.544580000	-0.612907000	-6.909570000
17	-1.552100000	-3.680442000	-5.382107000

19 + Cl E = -1721.91188

6	-1.658992000	2.811718000	-1.668165000
1	-2.625989000	3.309941000	-1.620943000
1	-1.605119000	2.201671000	-2.570335000
6	-0.493321000	3.764918000	-1.501778000
1	-0.575401000	4.279514000	-0.542194000
1	0.451621000	3.215165000	-1.535947000
16	-0.521717000	4.971676000	-2.892767000
6	1.215535000	5.552268000	-2.828581000
1	1.885654000	4.688936000	-2.886281000
1	1.355834000	6.152554000	-3.732592000
6	1.526578000	6.388998000	-1.593917000
1	1.359967000	5.797139000	-0.683054000
1	0.856475000	7.259538000	-1.556276000
8	2.895589000	6.789103000	-1.698040000
1	3.107638000	7.297539000	-0.902548000
6	-2.932176000	1.762454000	0.252852000
6	-0.959210000	0.568972000	-0.813407000
6	-2.668626000	1.159065000	1.609889000
1	-3.606233000	1.177906000	-0.372792000
6	-0.563897000	-0.120116000	0.471539000
1	-1.664866000	-0.003996000	-1.418603000
1	-0.079289000	0.844873000	-1.394839000
1	-3.636927000	1.125736000	2.116489000
1	-1.985189000	1.793205000	2.181509000
1	-0.060983000	-1.053208000	0.203267000
1	0.136468000	0.502451000	1.034992000
8	-1.625259000	1.875084000	-0.500734000
16	-2.005756000	-0.544170000	1.520800000

1	-3.280945000	2.788410000	0.344492000
17	-6.048585000	2.107056000	1.303229000

19 + OH E = -1337.46077

6	-2.126384000	3.365449000	-1.643636000
1	-3.128818000	2.986520000	-1.430432000
1	-1.700089000	2.922200000	-2.558416000
6	-2.084840000	4.879224000	-1.653173000
1	-2.948575000	5.211989000	-2.237973000
1	-2.209484000	5.294112000	-0.650100000
16	-0.647272000	5.665820000	-2.496185000
6	0.796320000	4.962123000	-1.610974000
1	0.795708000	3.876875000	-1.732391000
1	1.669696000	5.348295000	-2.145586000
6	0.856201000	5.354314000	-0.141772000
1	-0.098904000	5.139517000	0.350229000
1	1.043339000	6.433000000	-0.049127000
8	1.912560000	4.595771000	0.460732000
1	1.874023000	4.751516000	1.415252000
6	-1.889159000	2.839378000	0.806546000
6	-0.576351000	1.524693000	-0.894180000
6	-0.834139000	2.698501000	1.882528000
1	-2.620438000	2.027625000	0.807020000
6	0.585509000	1.307238000	0.041112000
1	-1.350928000	0.757708000	-0.813736000
1	-0.260286000	1.684616000	-1.946991000
1	-1.340978000	2.740960000	2.850112000
1	-0.119009000	3.521927000	1.827960000
1	1.090376000	0.385595000	-0.260941000
1	1.293458000	2.137244000	-0.030952000
8	-1.243199000	2.834529000	-0.538904000
16	0.072169000	1.108459000	1.794542000
1	-2.388459000	3.804642000	0.880239000
8	-0.199126000	2.266025000	-3.759885000
1	-0.006729000	3.211724000	-3.700006000

TS21-1 E =-1337.46552 (-483.843)

6	-2.129178000	3.476005000	-1.100779000
1	-3.206904000	3.645854000	-1.110737000
1	-1.817835000	3.153004000	-2.097570000
6	-1.381844000	4.717667000	-0.609020000
1	-2.043566000	5.353647000	-0.017094000
1	-0.546431000	4.444139000	0.037241000
16	-0.764659000	5.762717000	-1.989043000
6	0.580618000	4.684635000	-2.638202000
1	0.200070000	3.665369000	-2.758973000
1	0.809766000	5.065602000	-3.637979000
6	1.852030000	4.656146000	-1.777884000
1	1.585450000	4.451064000	-0.727709000
1	2.316356000	5.651575000	-1.791611000
8	2.770114000	3.704619000	-2.274308000
1	2.423028000	2.764598000	-1.959563000
6	-2.921892000	1.331018000	-0.258492000
6	-0.223552000	1.707509000	-0.549999000
6	-2.695936000	0.300917000	0.827163000
1	-2.905048000	0.893982000	-1.261880000
6	0.008201000	0.755656000	0.583281000
1	-0.474981000	1.331228000	-1.531172000
1	0.259877000	2.663772000	-0.486267000

1	-3.522160000	-0.414552000	0.796460000
1	-2.694413000	0.783858000	1.808550000
1	1.010415000	0.347974000	0.448171000
1	-0.029748000	1.289566000	1.536785000
8	-1.878465000	2.358398000	-0.176719000
16	-1.152396000	-0.661053000	0.611902000
1	-3.873571000	1.843885000	-0.094635000
8	1.909801000	1.456610000	-1.494810000
1	1.595850000	1.090779000	-2.333937000

14 E = -1337.55385

6	-2.298447000	3.506969000	-1.207468000
1	-3.314494000	3.765816000	-1.538821000
1	-1.791860000	3.013648000	-2.048679000
6	-1.548043000	4.761924000	-0.771924000
1	-2.192610000	5.418217000	-0.181265000
1	-0.696234000	4.490160000	-0.144022000
16	-0.942881000	5.758944000	-2.190431000
6	0.441718000	4.686072000	-2.751847000
1	0.087850000	3.652402000	-2.816001000
1	0.691741000	5.010777000	-3.765931000
6	1.677339000	4.748297000	-1.849307000
1	1.388121000	4.609833000	-0.798238000
1	2.152024000	5.731463000	-1.932970000
8	2.639891000	3.772318000	-2.241409000
1	2.239351000	2.903776000	-2.023848000
6	-3.079862000	1.429209000	-0.344439000
6	0.856024000	1.704517000	-0.060144000
6	-2.501299000	0.272744000	0.456509000
1	-3.069063000	1.182920000	-1.414451000
6	0.408655000	0.415137000	0.619944000
1	0.058807000	2.448914000	-0.019036000
1	1.730254000	2.099403000	0.467334000
1	-3.231485000	-0.542139000	0.470728000
1	-2.319821000	0.573207000	1.493128000
1	1.238056000	-0.298459000	0.635715000
1	0.115785000	0.617694000	1.655072000
8	-2.334756000	2.617625000	-0.092025000
16	-0.961485000	-0.482134000	-0.224201000
1	-4.129789000	1.584757000	-0.050569000
8	1.277928000	1.487077000	-1.415879000
1	0.480791000	1.326295000	-1.944355000

TS21-2 E = -1337.44090 (-233.035)

6	-1.873734000	3.157027000	-1.464429000
1	-2.940971000	3.239244000	-1.316184000
1	-1.601254000	2.457496000	-2.243648000
6	-1.113340000	4.466478000	-1.381756000
1	-1.826881000	5.289259000	-1.402979000
1	-0.573680000	4.529142000	-0.431942000
16	0.109803000	4.675467000	-2.744863000
6	1.593595000	5.175847000	-1.787701000
1	1.802174000	4.438868000	-1.004512000
1	2.424639000	5.148316000	-2.499992000
6	1.483094000	6.568270000	-1.181131000
1	0.636858000	6.609807000	-0.480400000
1	1.294009000	7.304424000	-1.975689000
8	2.716074000	6.837476000	-0.506249000
1	2.631544000	7.704634000	-0.085443000

6	-2.499573000	1.433607000	0.375217000
6	-0.115820000	1.695590000	-0.259416000
6	-2.191850000	0.993745000	1.790911000
1	-2.575203000	0.599887000	-0.328031000
6	0.417124000	1.287863000	1.096992000
1	-0.237831000	0.852161000	-0.944025000
1	0.525356000	2.453333000	-0.709487000
1	-3.006512000	0.349599000	2.132145000
1	-2.137419000	1.864095000	2.450706000
1	1.407989000	0.847862000	0.956727000
1	0.513360000	2.165889000	1.741879000
8	-1.438599000	2.345682000	-0.108934000
16	-0.637686000	0.029038000	1.911865000
1	-3.410113000	2.032875000	0.354140000
8	-2.827717000	4.015544000	-3.595825000
1	-2.528984000	4.931105000	-3.514041000

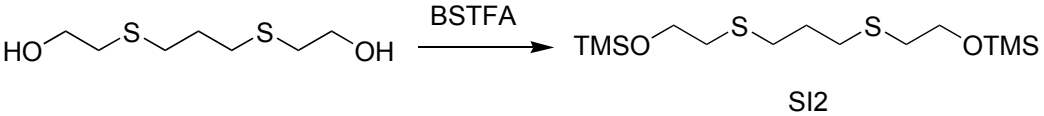
2 + 1,4-thioxane 6 E = -1337.54801

6	-2.311786000	3.446695000	-2.579049000
1	-3.294300000	3.534710000	-2.090486000
1	-1.924373000	2.444865000	-2.371308000
6	-1.390933000	4.505212000	-1.987365000
1	-1.810129000	5.501924000	-2.157927000
1	-1.301481000	4.347473000	-0.909425000
16	0.303796000	4.410784000	-2.713471000
6	1.281996000	5.057509000	-1.305796000
1	1.037039000	4.485209000	-0.406382000
1	2.331370000	4.870643000	-1.554637000
6	1.066173000	6.544132000	-1.053544000
1	0.008082000	6.738890000	-0.828491000
1	1.328196000	7.118653000	-1.953718000
8	1.896946000	6.908251000	0.054025000
1	1.721784000	7.838947000	0.252122000
6	-1.682637000	2.416560000	1.085144000
6	0.314061000	1.706481000	-0.026727000
6	-1.866393000	1.161911000	1.931391000
1	-2.247030000	2.327572000	0.145900000
6	0.423064000	0.349647000	0.659092000
1	-0.235349000	1.614456000	-0.973199000
1	1.315101000	2.090080000	-0.246460000
1	-2.928306000	0.992744000	2.129949000
1	-1.344983000	1.272949000	2.887293000
1	0.911703000	-0.369296000	-0.004279000
1	1.013685000	0.438409000	1.576289000
8	-0.304924000	2.691559000	0.808489000
16	-1.234122000	-0.336830000	1.071578000
1	-2.056305000	3.286991000	1.633910000
8	-2.436373000	3.536275000	-3.999755000
1	-2.773765000	4.420661000	-4.205000000

Degradation of 7b with decontaminats



SI1

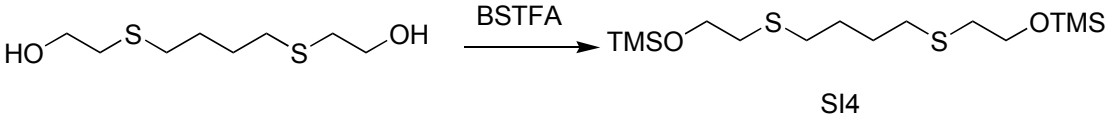


SI2

Degradation of 7c with decontaminats



SI3



SI4

Degradation of 7d with decontaminats

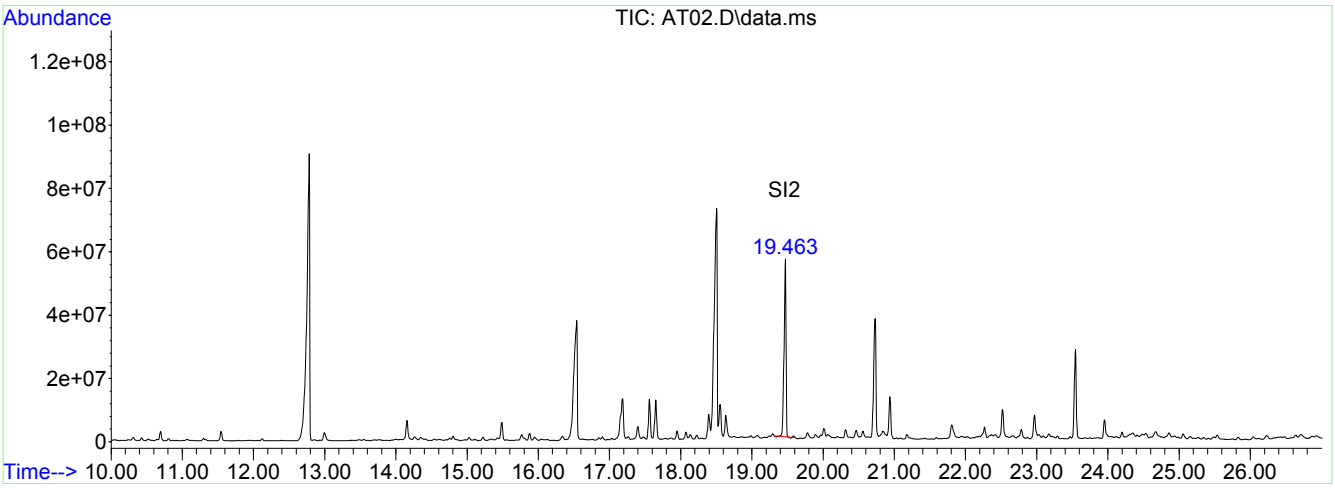


SI5

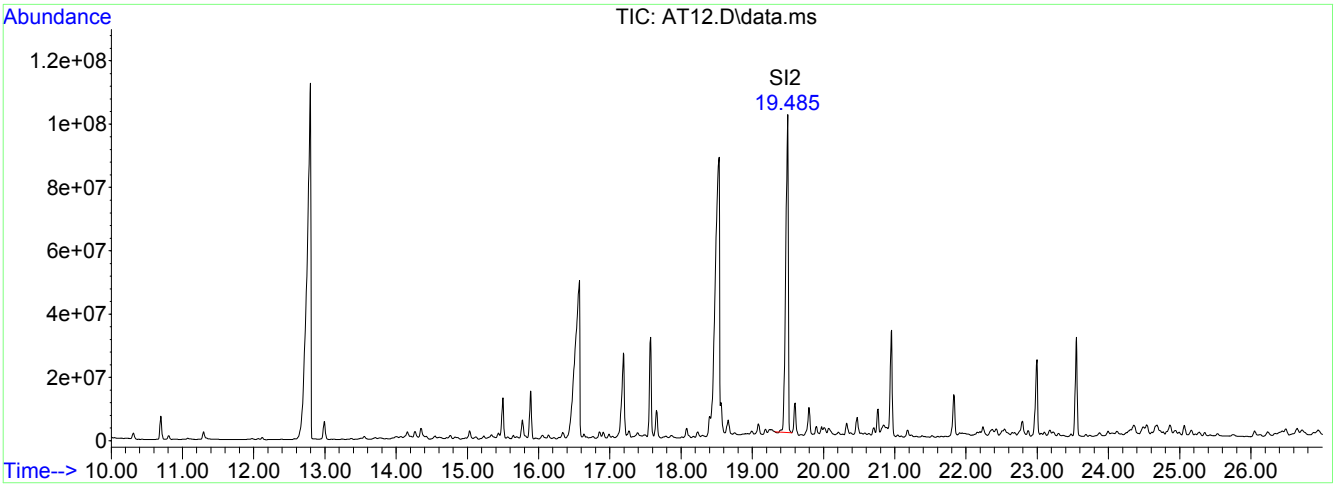


SI6

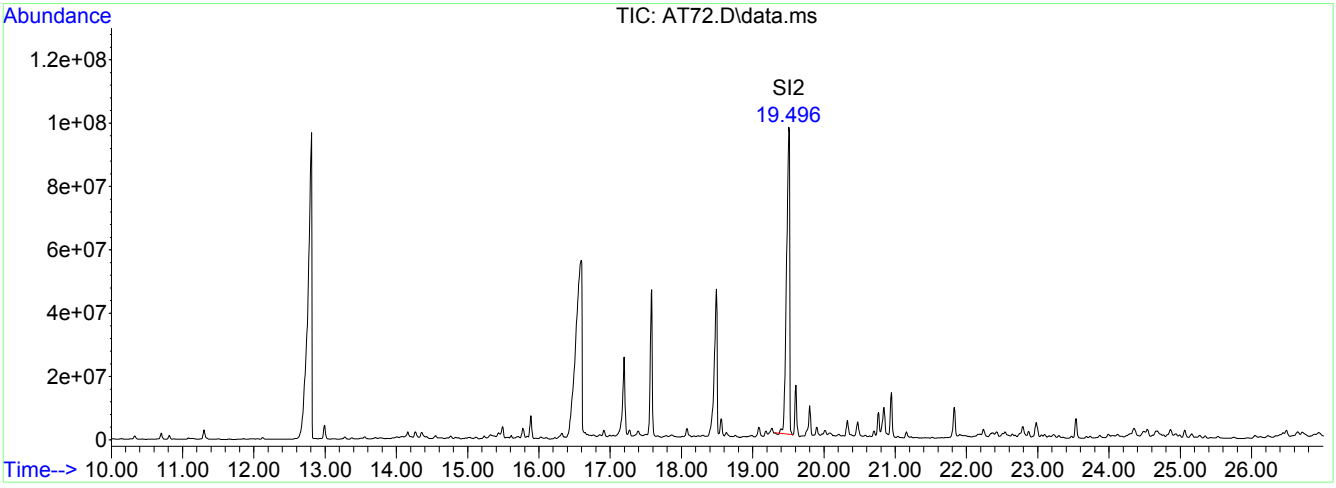
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AT02.D
Date Acquired : 8 Feb 2013 11:21 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AT02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AT12.D
Date Acquired : 11 Feb 2013 11:09 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AT12

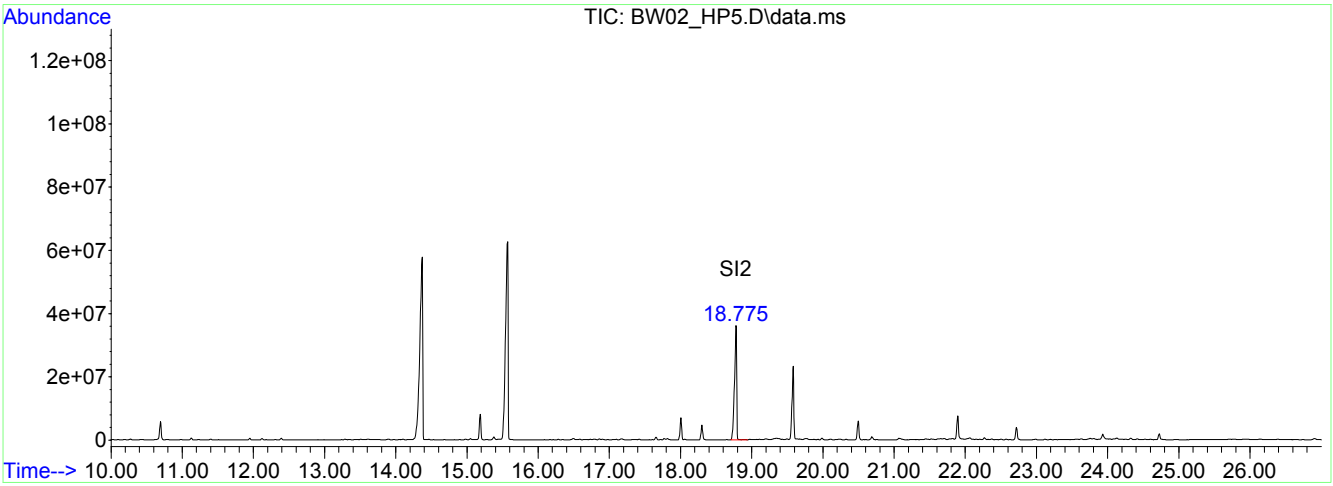


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AT72.D
Date Acquired : 15 Feb 2013 17:58 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AT72

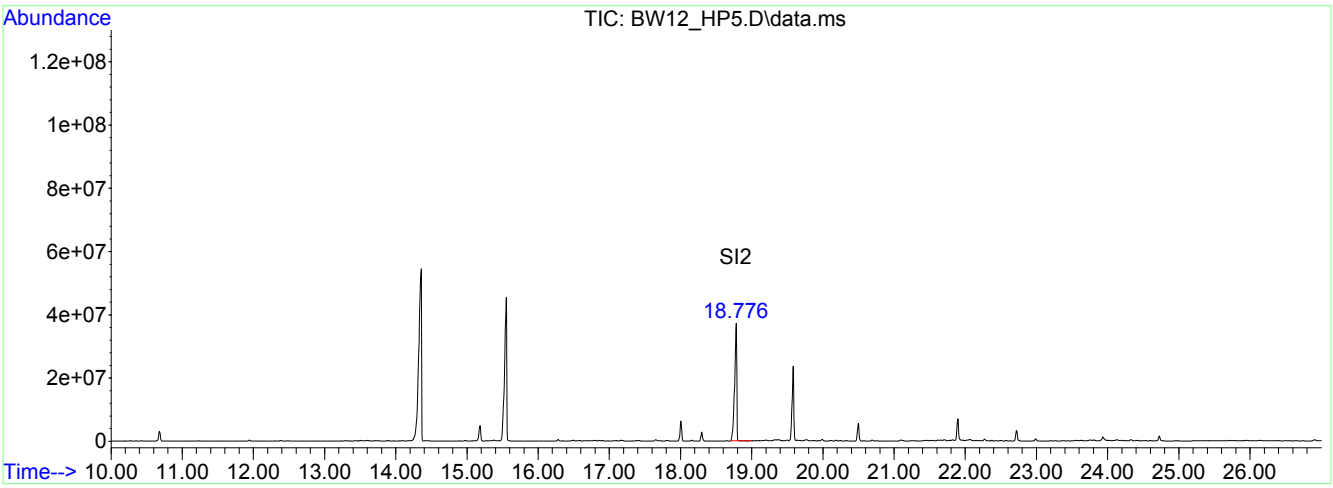


RM21-7b
90 minutes
24 hours
7 days

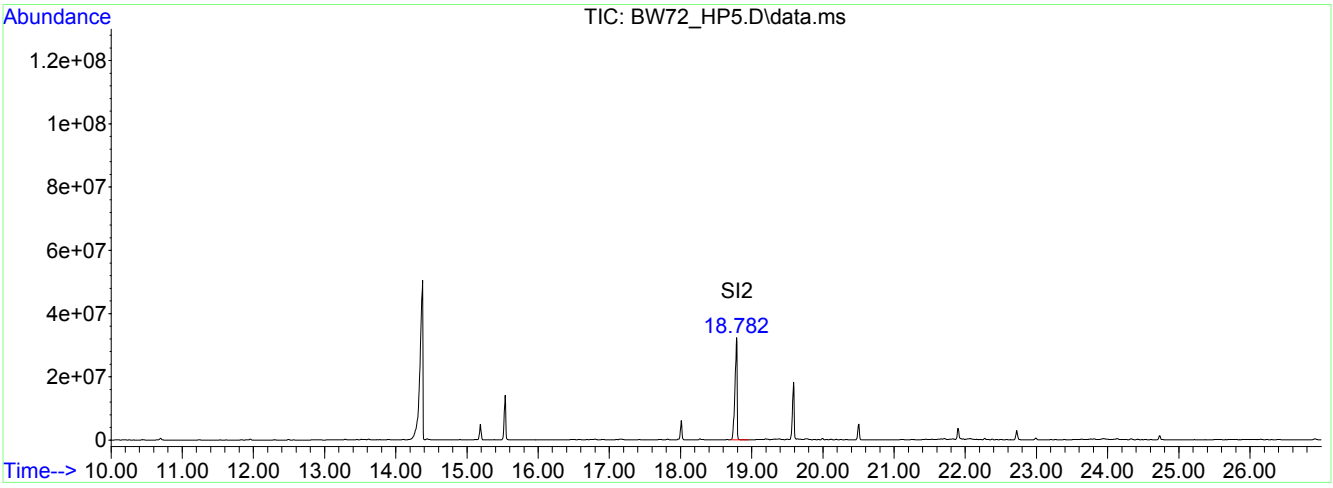
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BW02_HP5.D
Date Acquired : 15 Jul 2013 12:30 Method File : 32PTEITMS.M
Instrument : VE002
Sample Name : BW02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BW12_HP5.D
Date Acquired : 15 Jul 2013 21:16 Method File : 32PTEITMS.M
Instrument : VE002
Sample Name : BW12

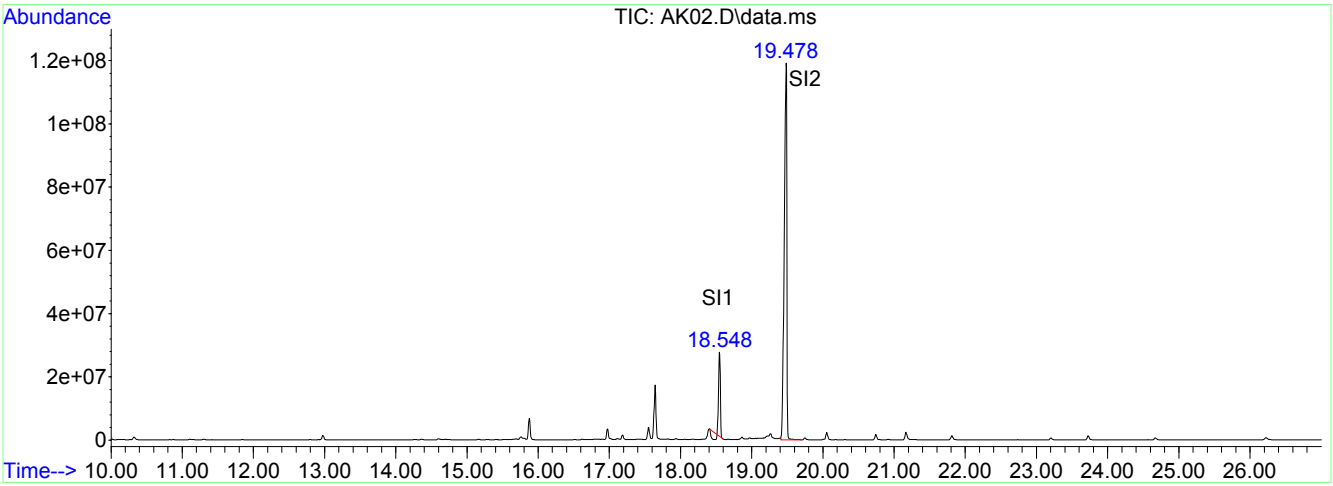


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BW72_HP5.D
Date Acquired : 16 Jul 2013 20:17 Method File : 32PTEI.M
Instrument : VE002
Sample Name : BW72

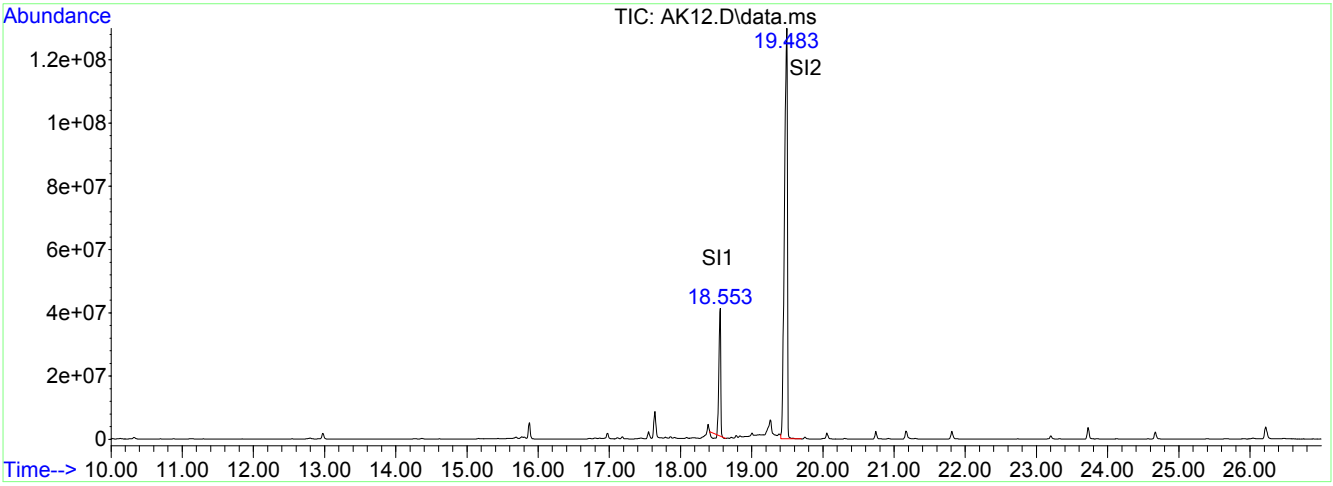


RM31-7b
90 minutes
24 hours
7 days

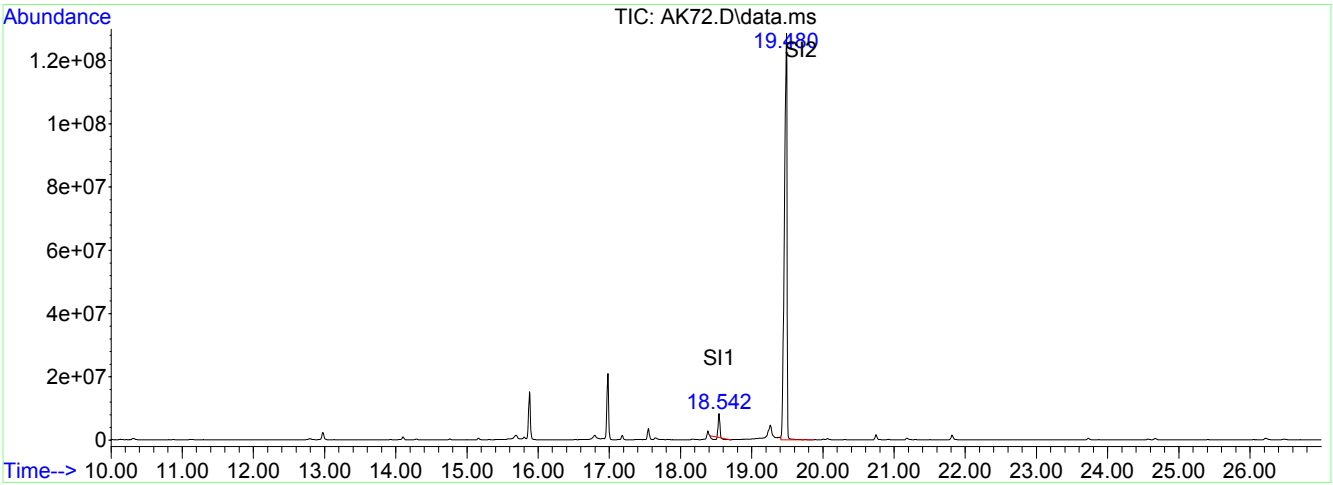
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AK02.D
Date Acquired : 16 Jan 2013 18:17 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AK02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AK12.D
Date Acquired : 17 Jan 2013 16:43 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AK12

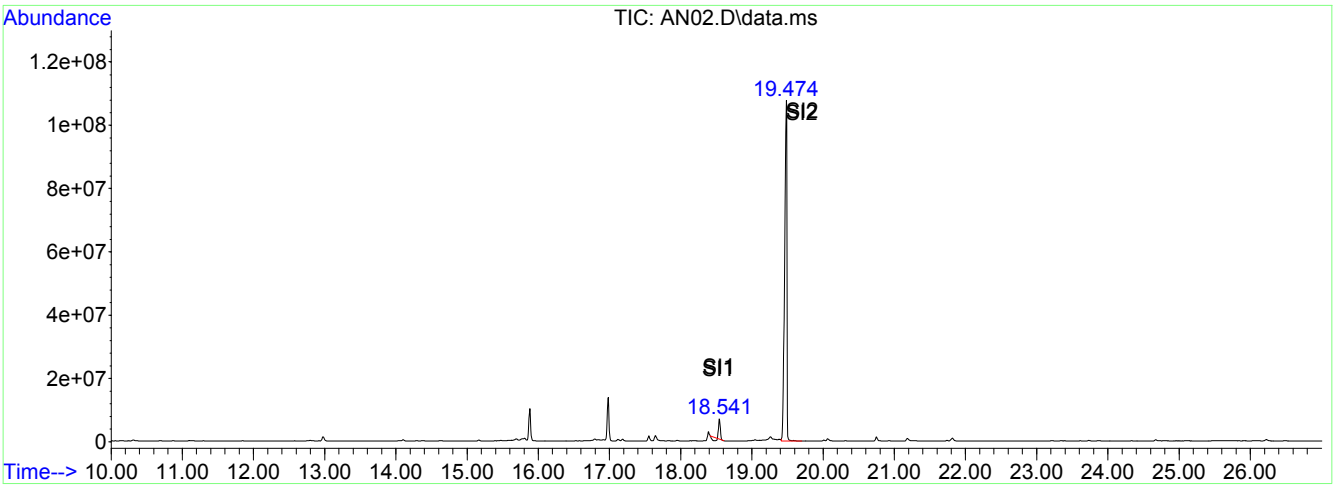


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AK72.D
Date Acquired : 23 Jan 2013 17:03 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AK72

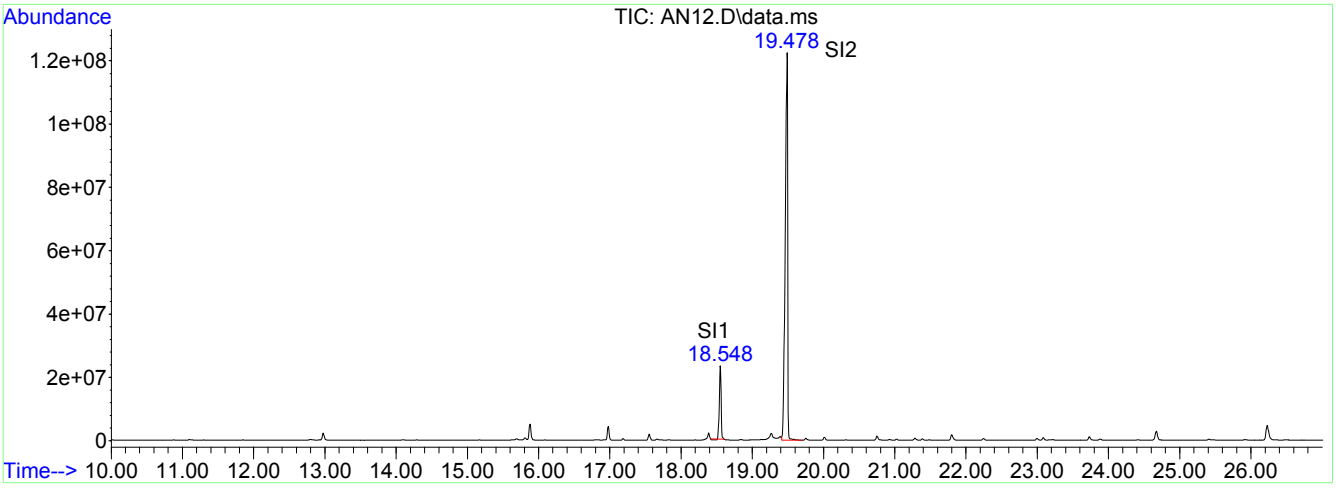


BX24-7b
90 minutes
24 hours
7 days

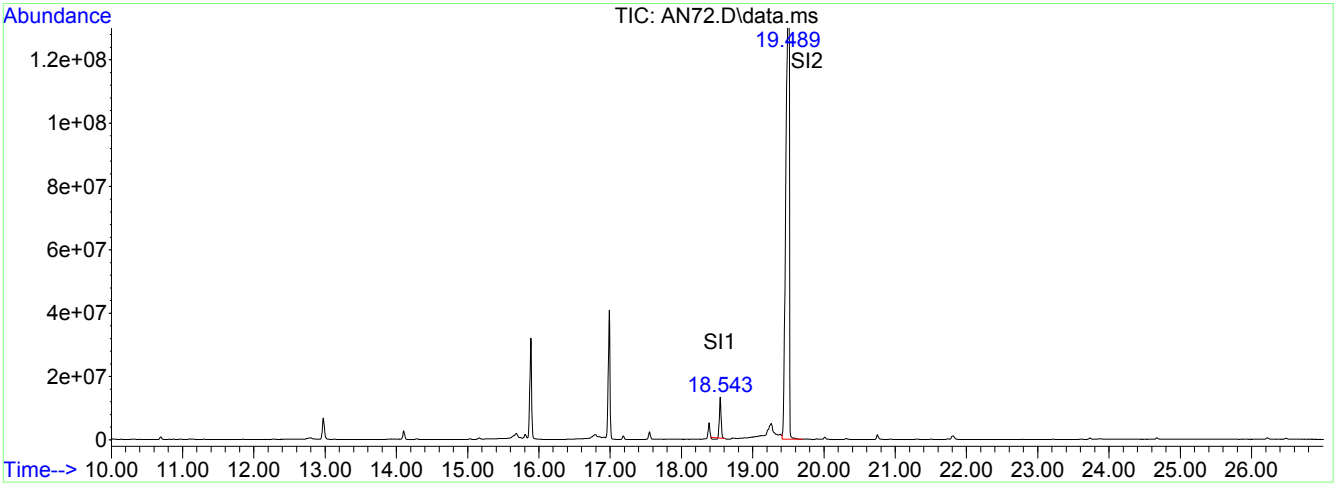
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AN02.D
Date Acquired : 25 Jan 2013 11:51 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AN02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AN12.D
Date Acquired : 25 Jan 2013 21:34 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AN12

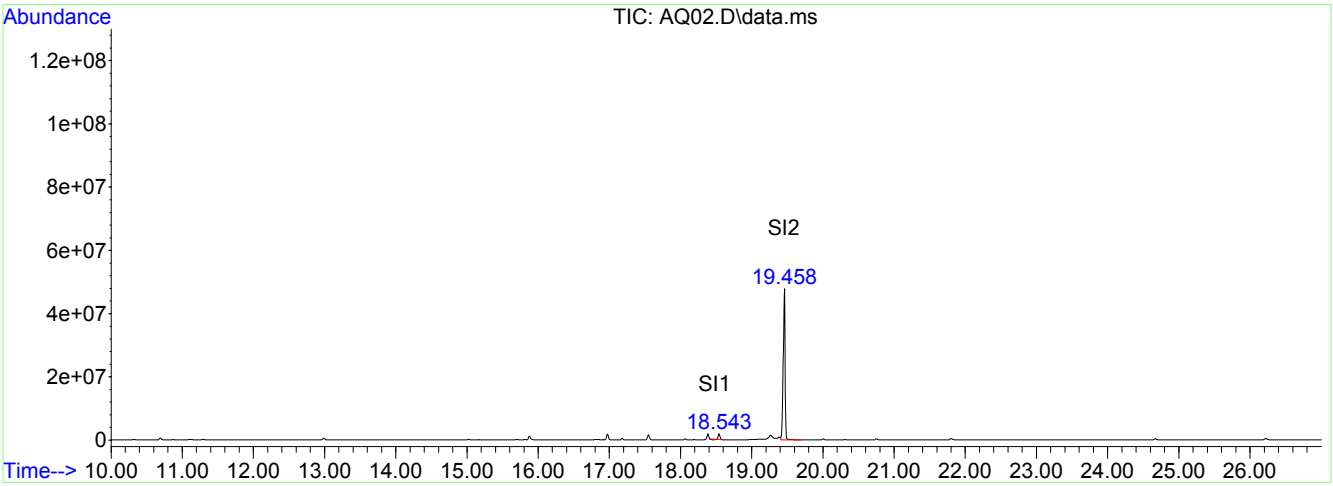


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AN72.D
Date Acquired : 1 Feb 2013 11:32 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AN72

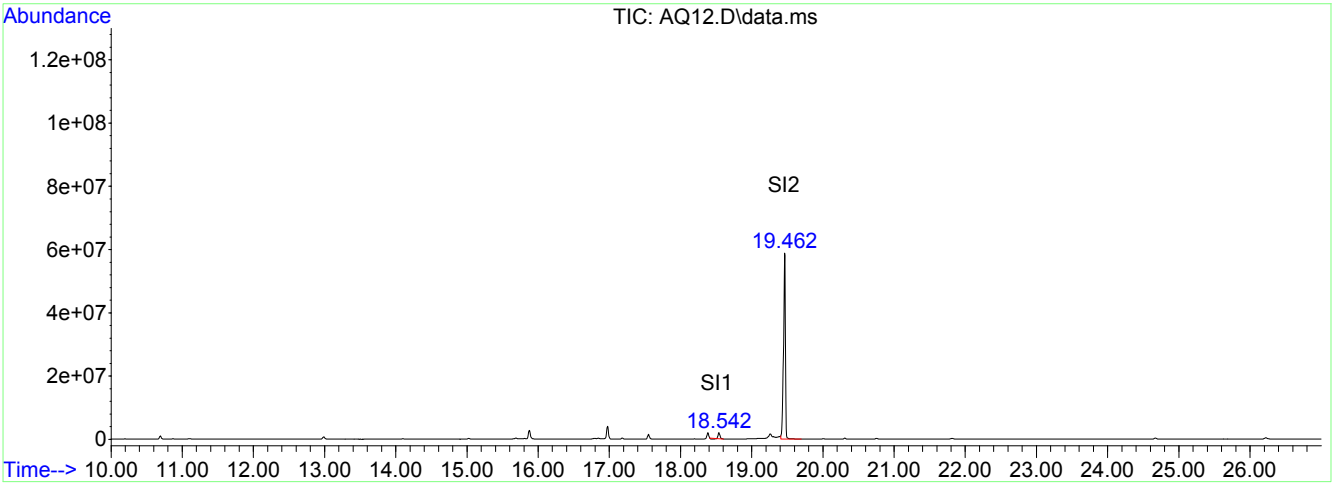


BX29-7b
90 minutes
24 hours
7 days

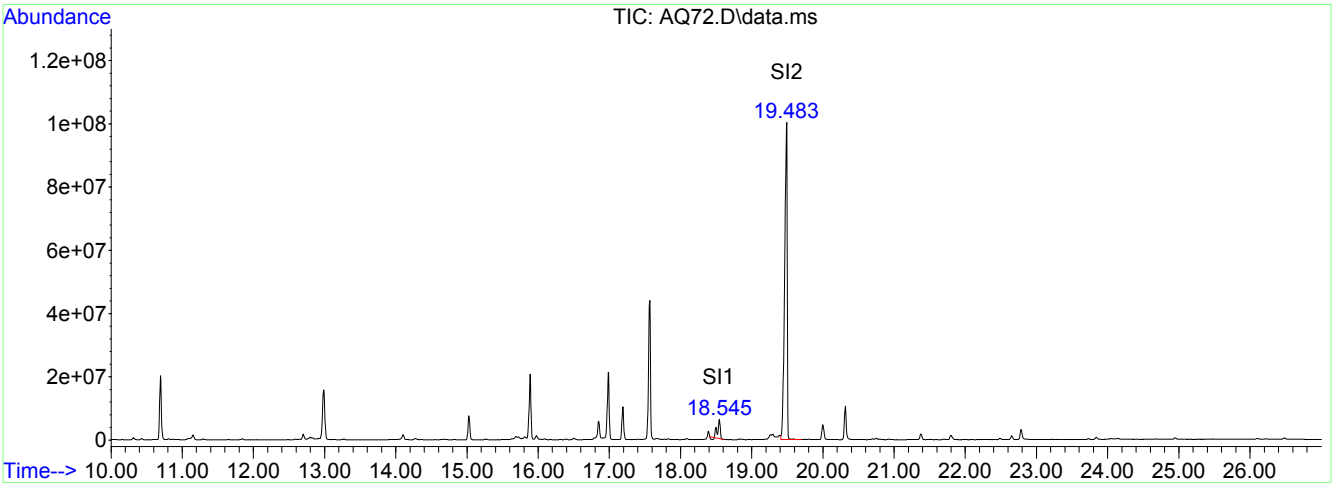
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AQ02.D
Date Acquired : 6 Feb 2013 11:54 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AQ02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AQ12.D
Date Acquired : 7 Feb 2013 14:48 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AQ12

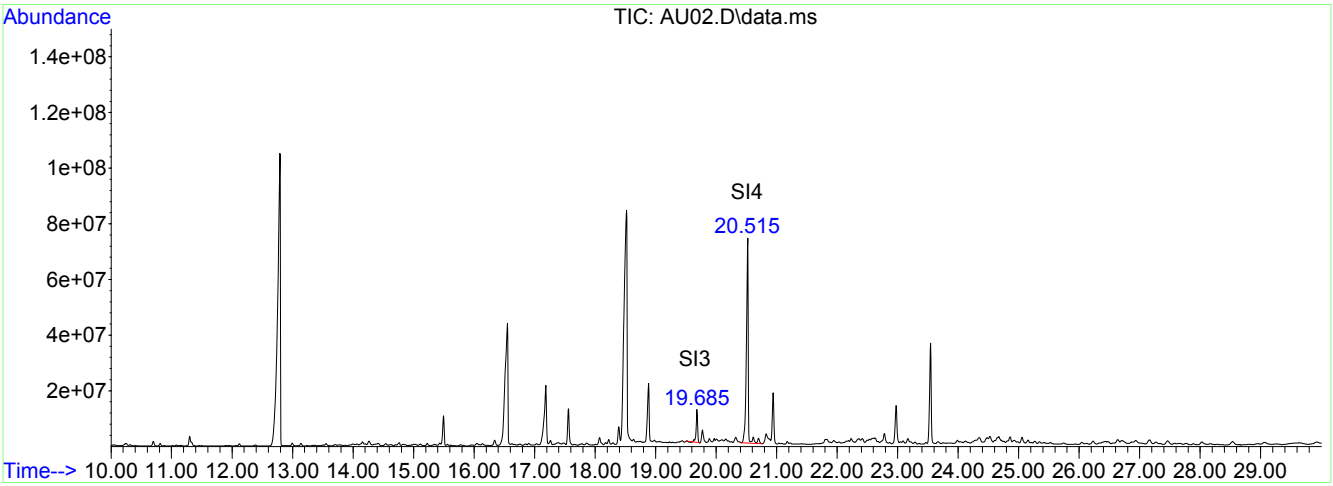


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AQ72.D
Date Acquired : 13 Feb 2013 17:23 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AQ72

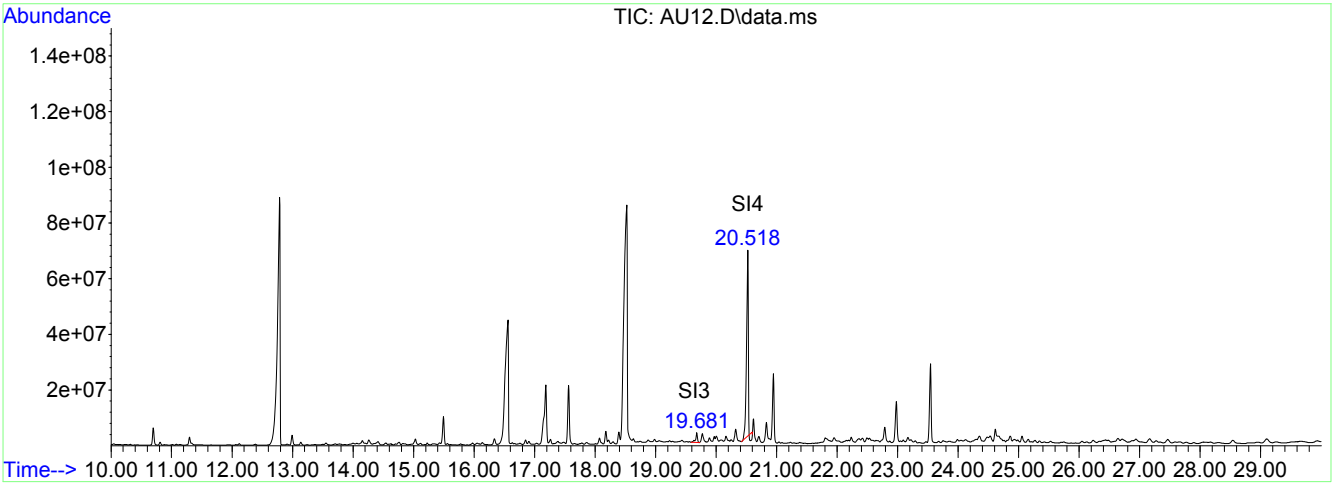


BX40-7b
90 minutes
24 hours
7 days

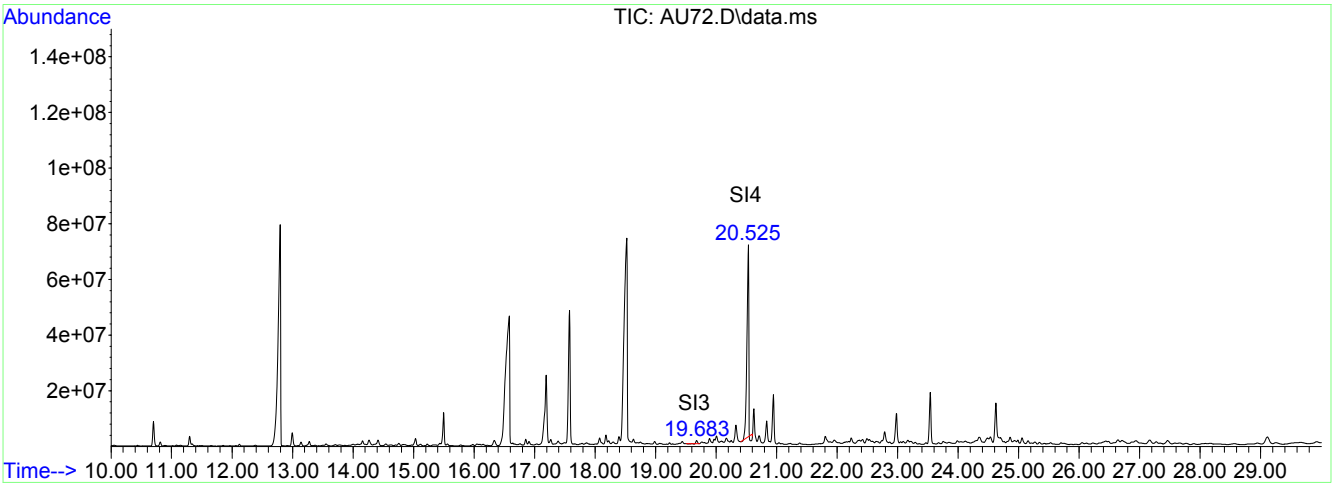
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AU02.D
Date Acquired : 8 Feb 2013 14:35 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AU02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AU12.D
Date Acquired : 11 Feb 2013 11:50 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AU12

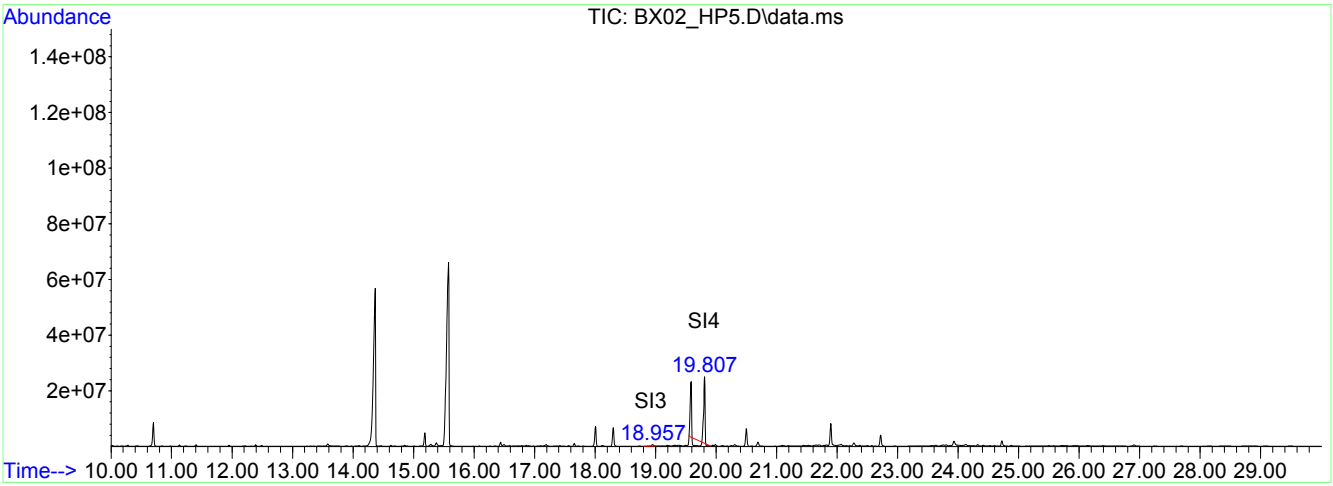


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AU72.D
Date Acquired : 15 Feb 2013 18:39 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AU72

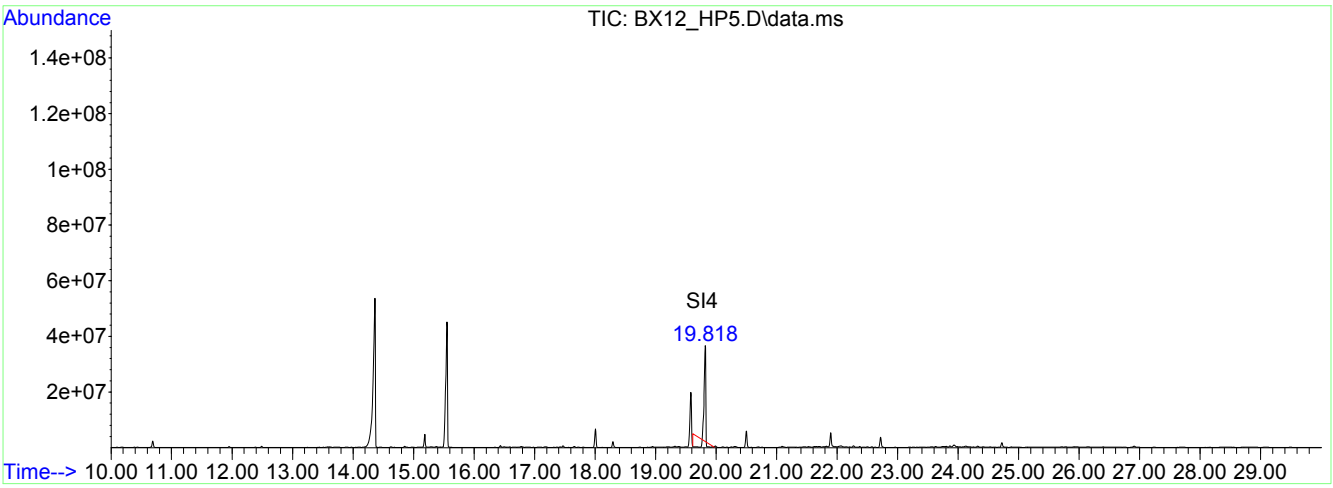


RM21-7c
90 minutes
24 hours
7 days

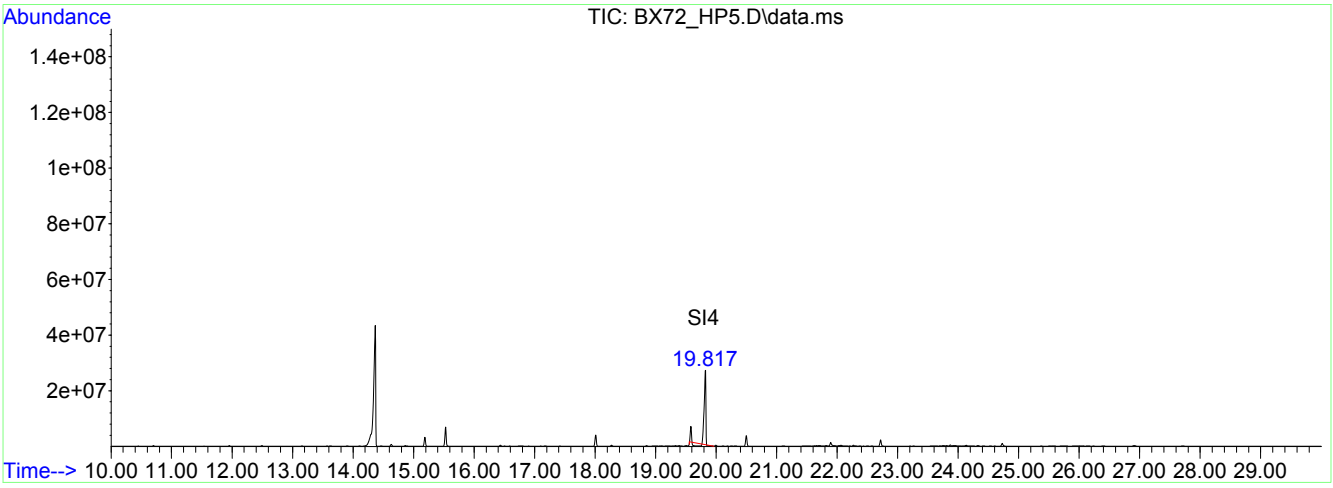
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BX02_HP5.D
Date Acquired : 15 Jul 2013 13:14 Method File : 32PTEITMS.M
Instrument : VE002
Sample Name : BX02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BX12_HP5.D
Date Acquired : 15 Jul 2013 21:59 Method File : 32PTEITMS.M
Instrument : VE002
Sample Name : BX12

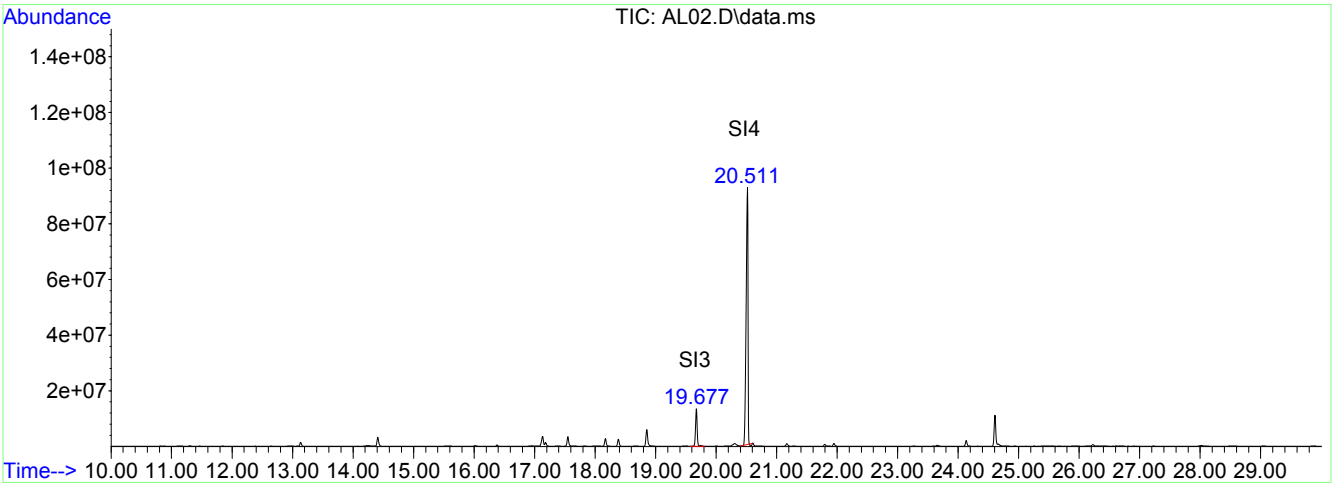


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BX72_HP5.D
Date Acquired : 16 Jul 2013 21:01 Method File : 32PTEI.M
Instrument : VE002
Sample Name : BX72

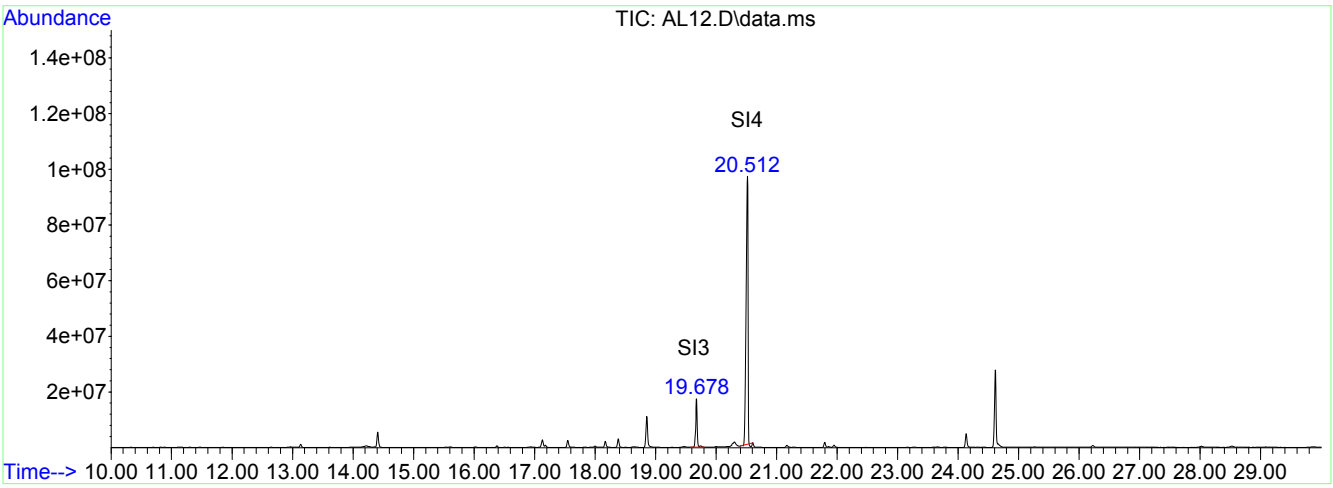


RM31-7c
90 minutes
24 hours
7 days

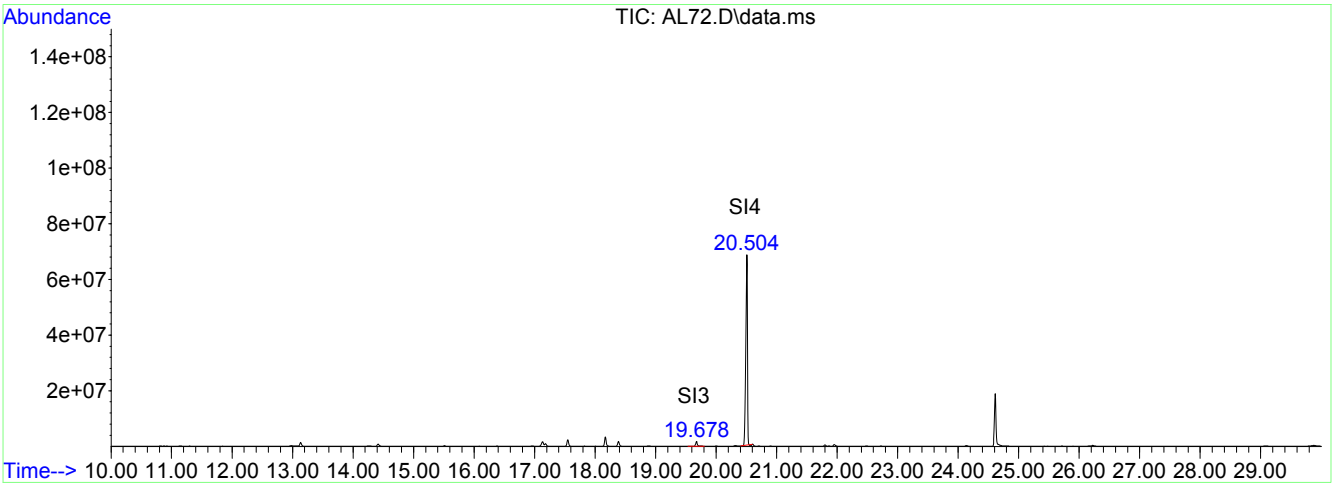
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AL02.D
Date Acquired : 16 Jan 2013 19:39 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AL02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AL12.D
Date Acquired : 17 Jan 2013 18:08 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AL12

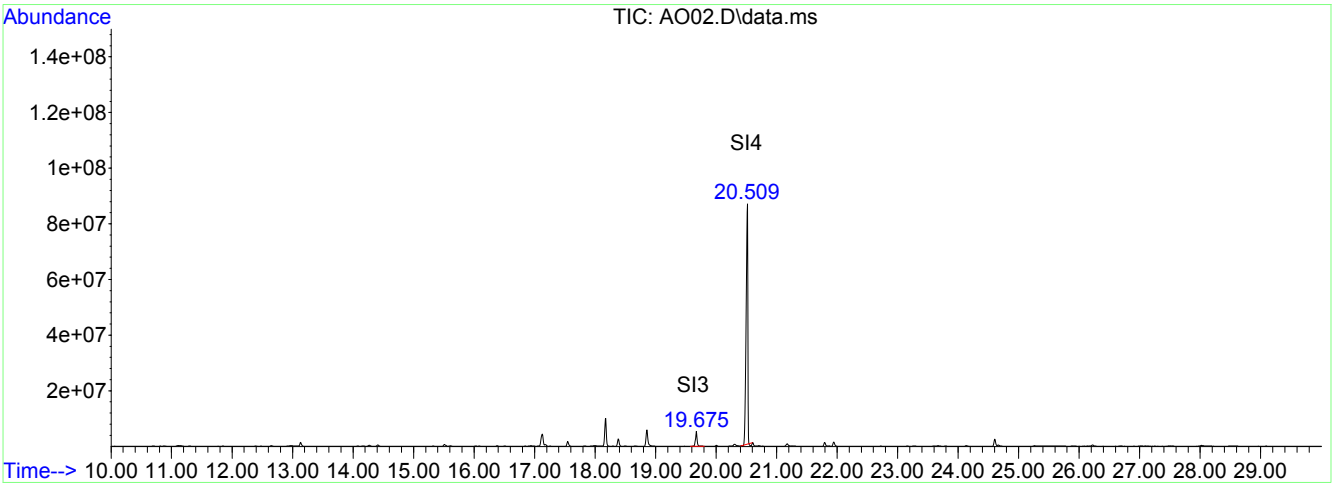


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AL72.D
Date Acquired : 23 Jan 2013 18:26 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AL72

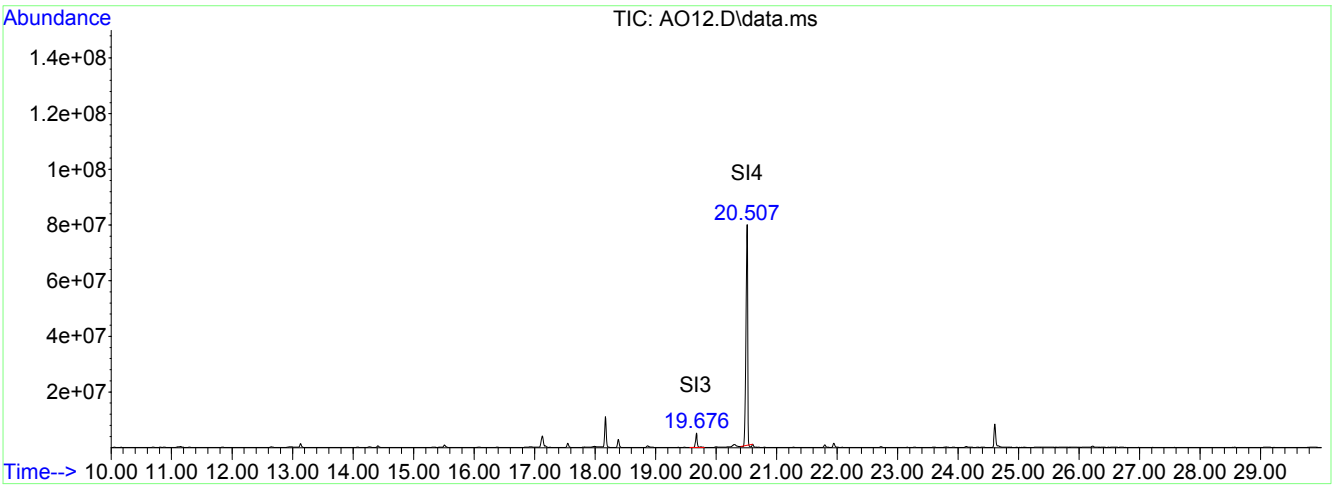


BX24-7c
90 minutes
24 hours
7 days

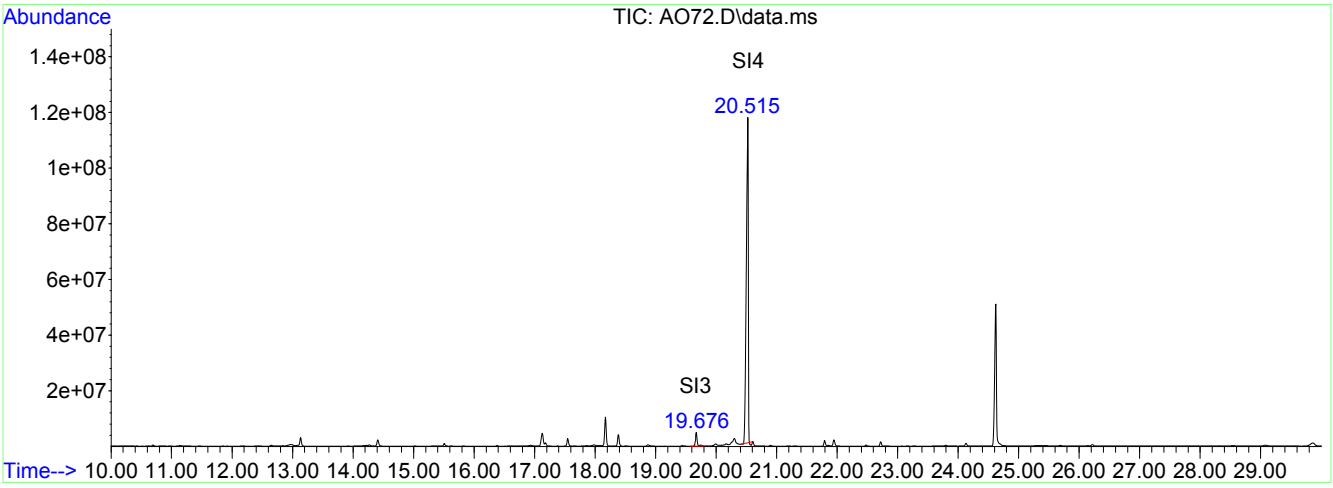
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AO02.D
Date Acquired : 25 Jan 2013 13:13 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AO02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AO12.D
Date Acquired : 25 Jan 2013 22:58 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AO12

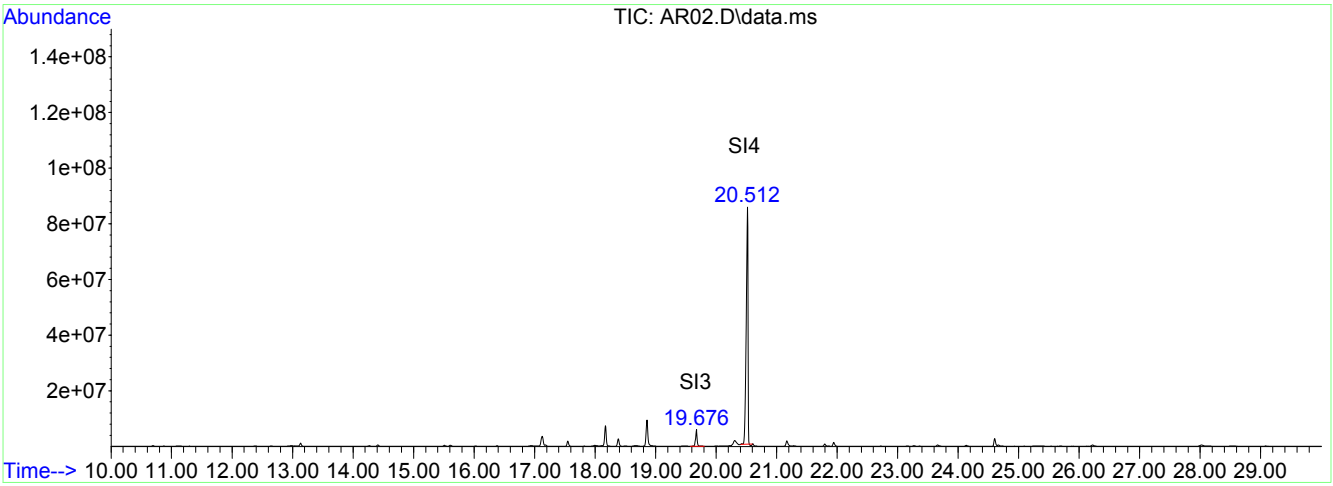


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AO72.D
Date Acquired : 1 Feb 2013 12:57 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AO72

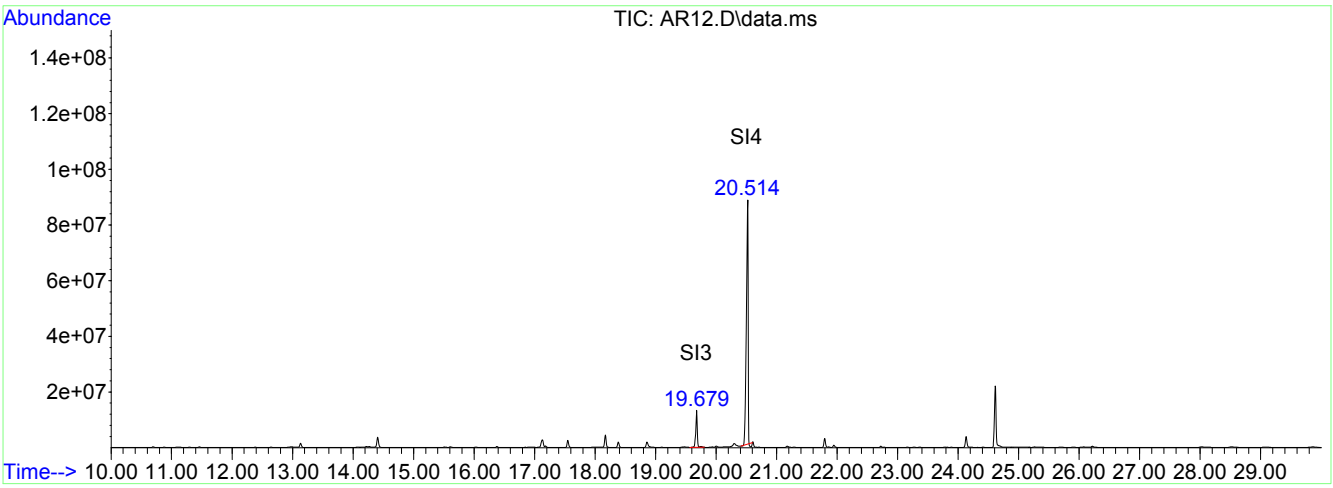


BX29-7c
90 minutes
24 hours
7 days

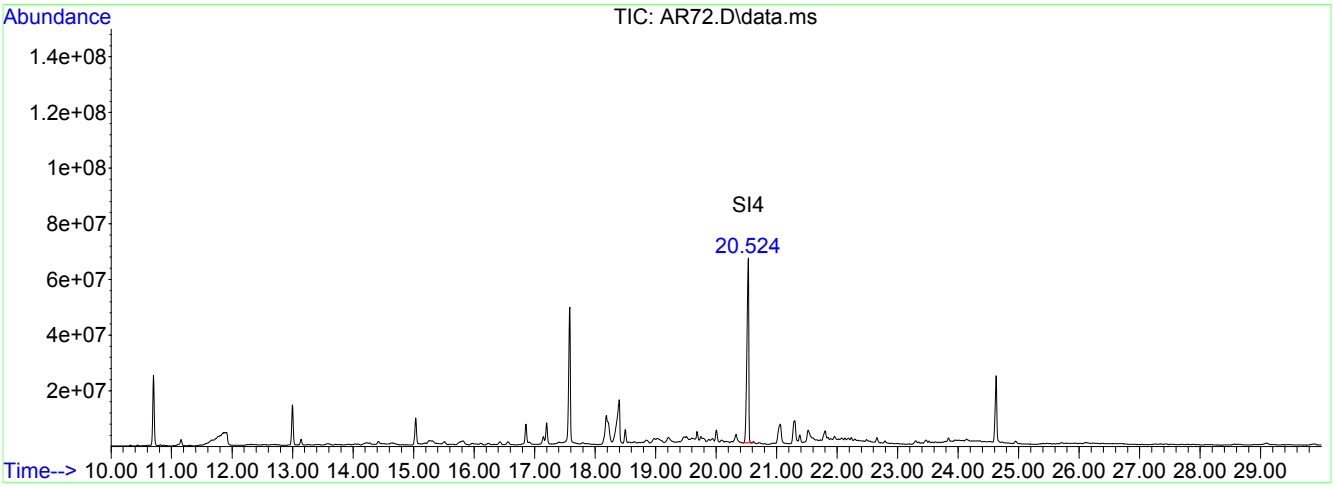
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AR02.D
Date Acquired : 6 Feb 2013 12:37 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AR02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AR12.D
Date Acquired : 7 Feb 2013 15:32 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AR12

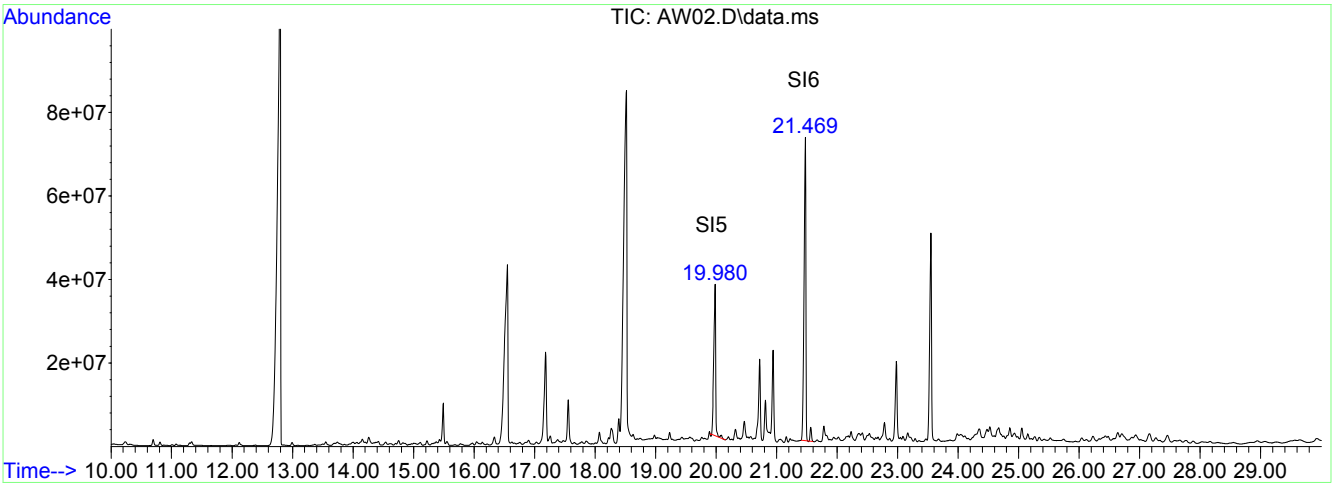


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AR72.D
Date Acquired : 15 Feb 2013 11:47 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AR72

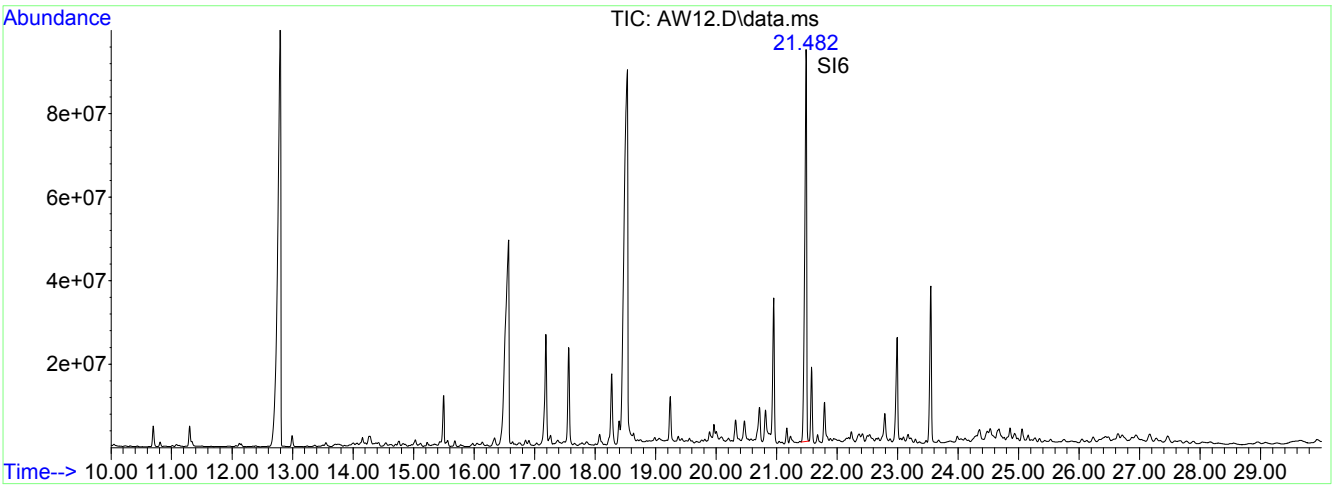


BX40-7c
90 minutes
24 hours
7 days

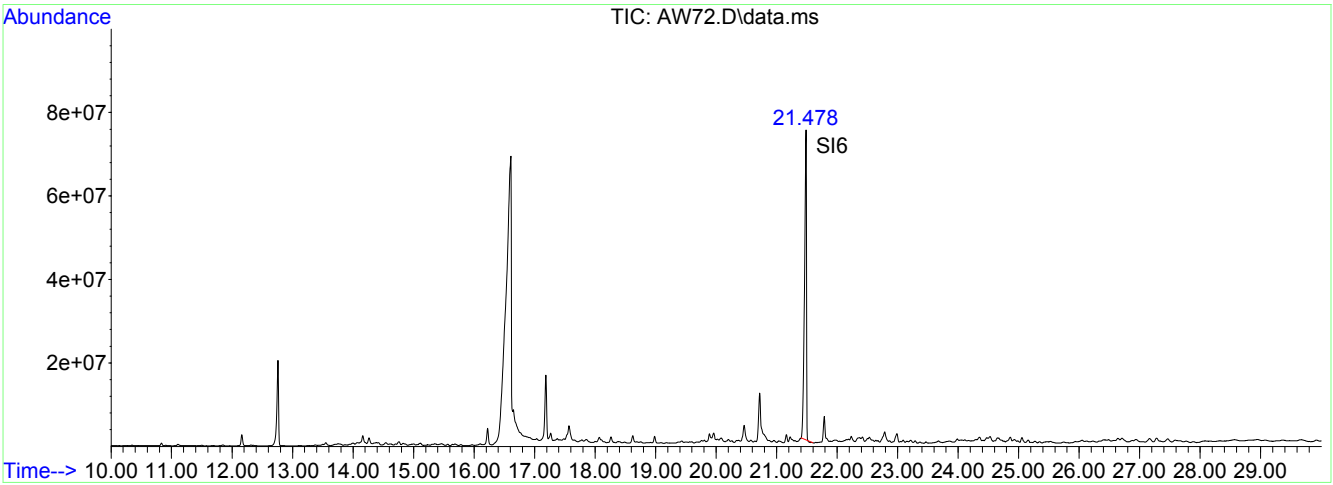
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AW02.D
Date Acquired : 8 Feb 2013 15:18 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AW02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AW12.D
Date Acquired : 11 Feb 2013 12:31 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AW12

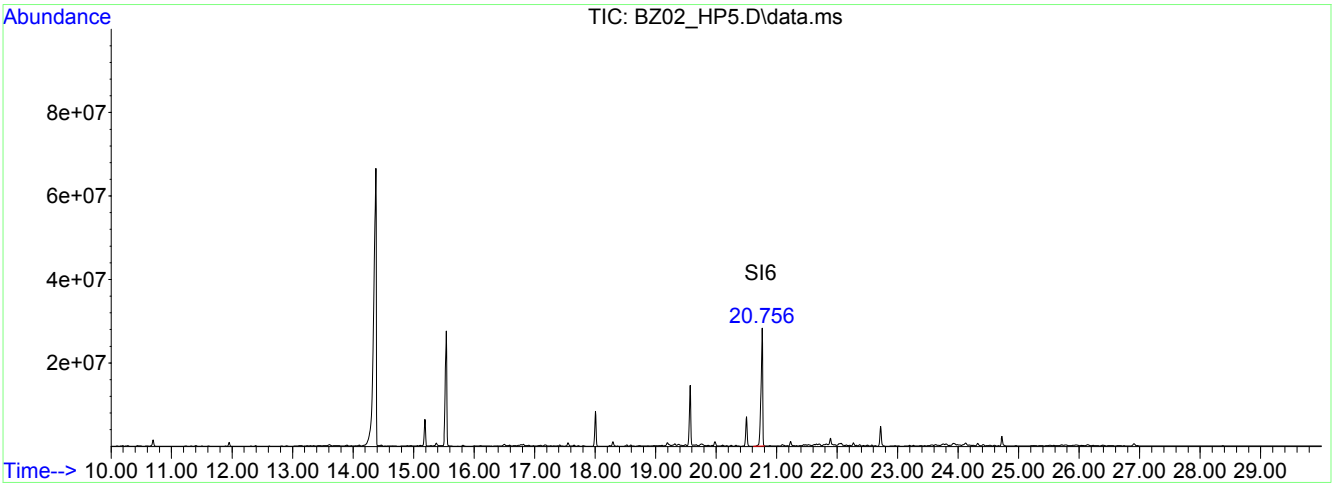


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AW72.D
Date Acquired : 15 Feb 2013 19:20 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AW72

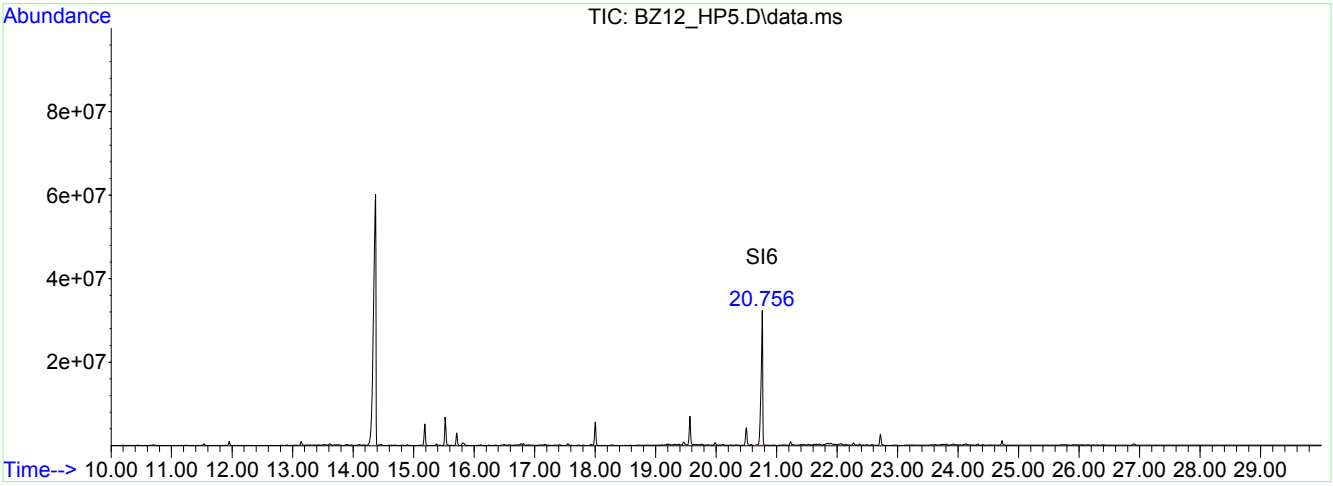


RM21-7d
90 minutes
24 hours
7 days

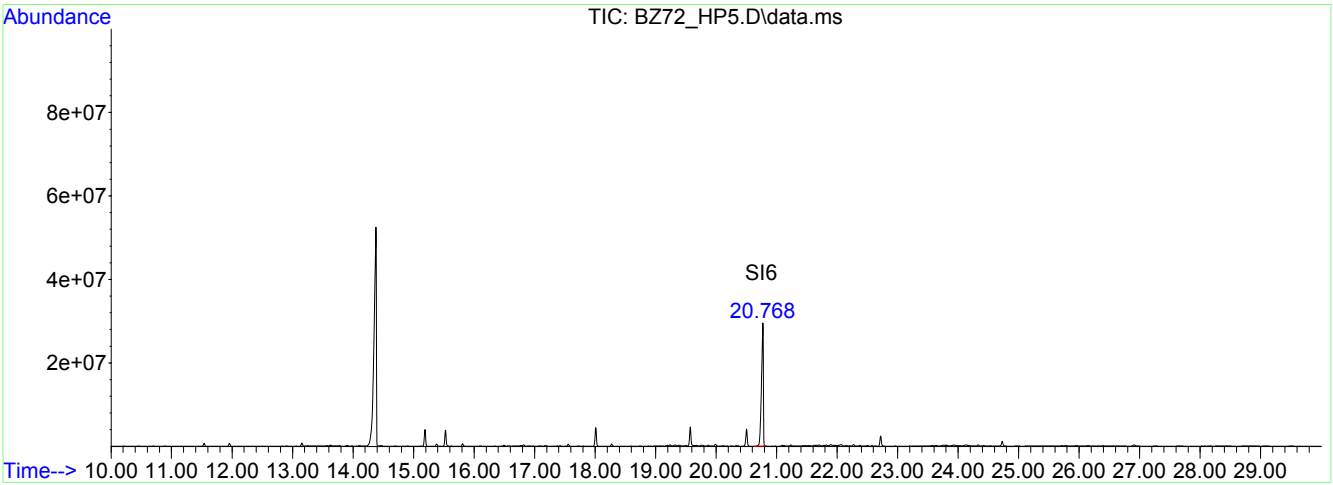
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BZ02_HP5.D
Date Acquired : 15 Jul 2013 13:59 Method File : 32PTEITMS.M
Instrument : VE002
Sample Name : BZ02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BZ12_HP5.D
Date Acquired : 15 Jul 2013 22:42 Method File : 32PTEITMS.M
Instrument : VE002
Sample Name : BZ12

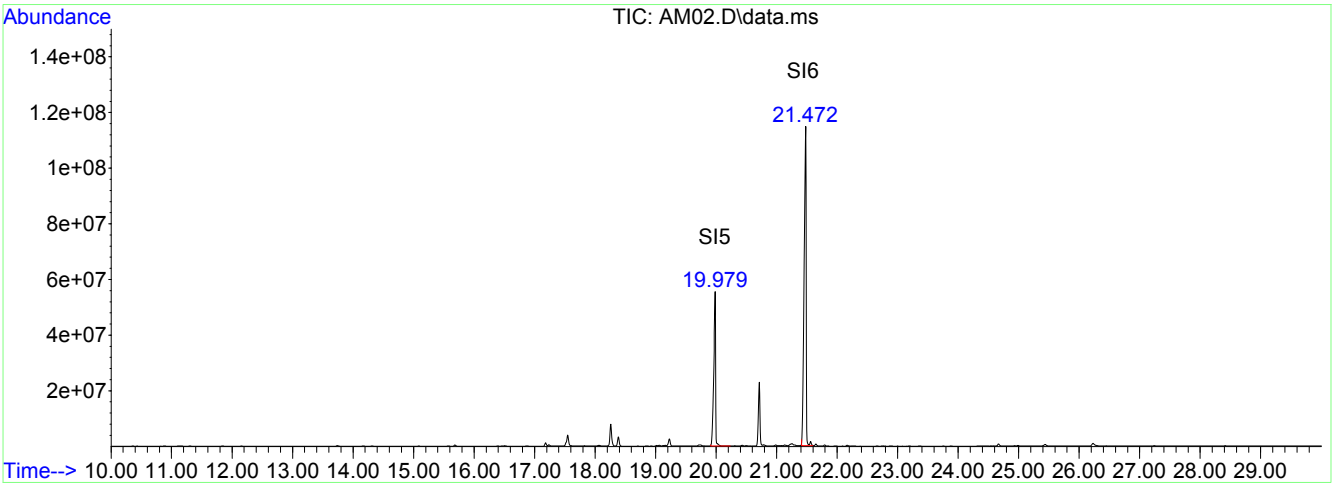


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\BZ72_HP5.D
Date Acquired : 16 Jul 2013 21:45 Method File : 32PTEI.M
Instrument : VE002
Sample Name : BZ72

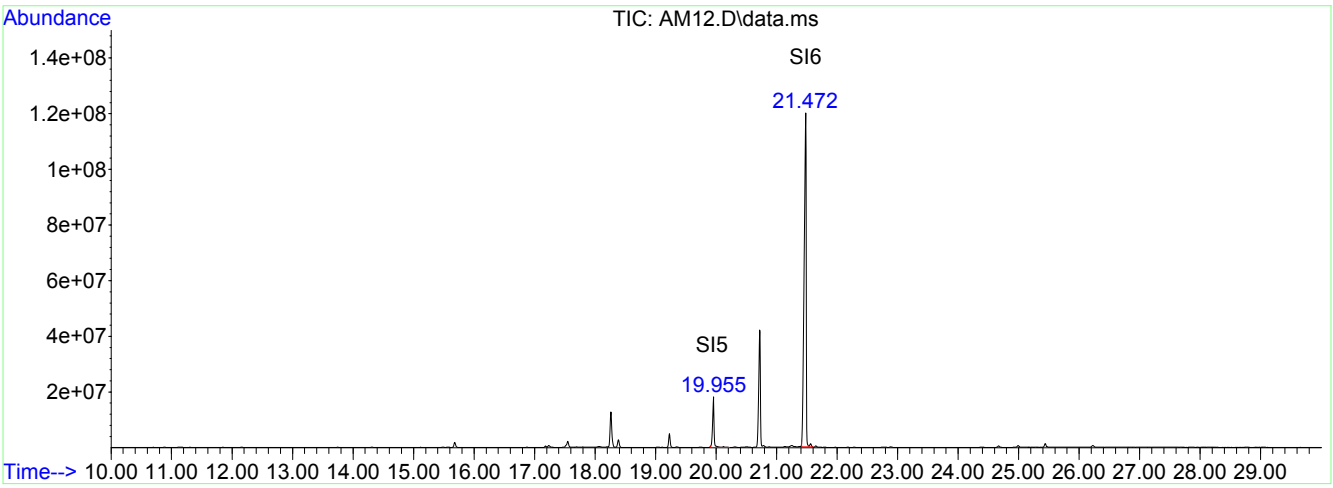


RM31-7d
90 minutes
24 hours
7 days

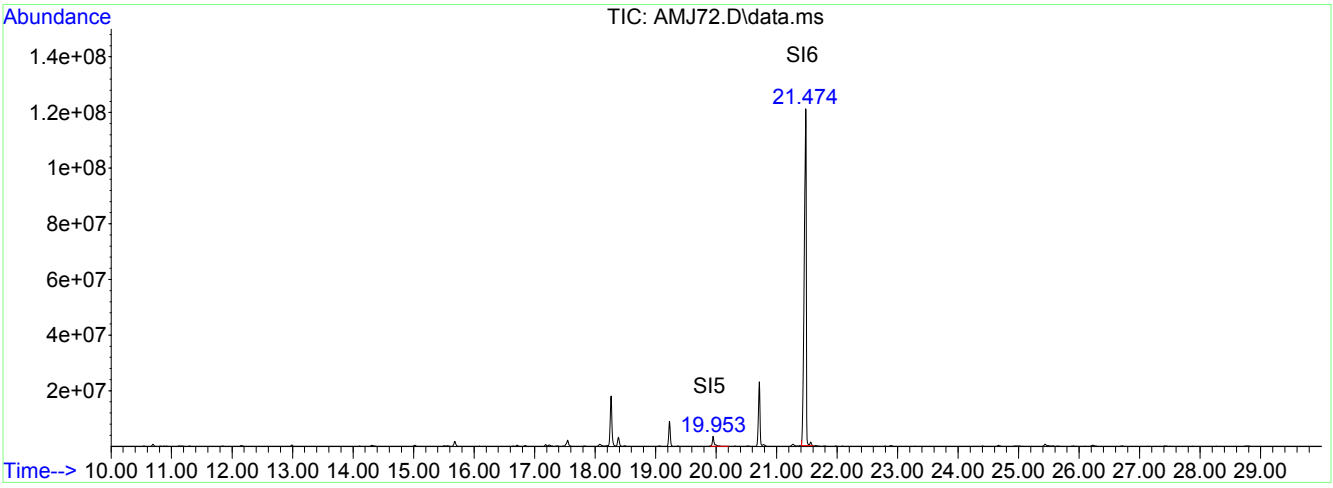
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AM02.D
Date Acquired : 16 Jan 2013 21:02 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AM02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AM12.D
Date Acquired : 17 Jan 2013 19:33 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AM12

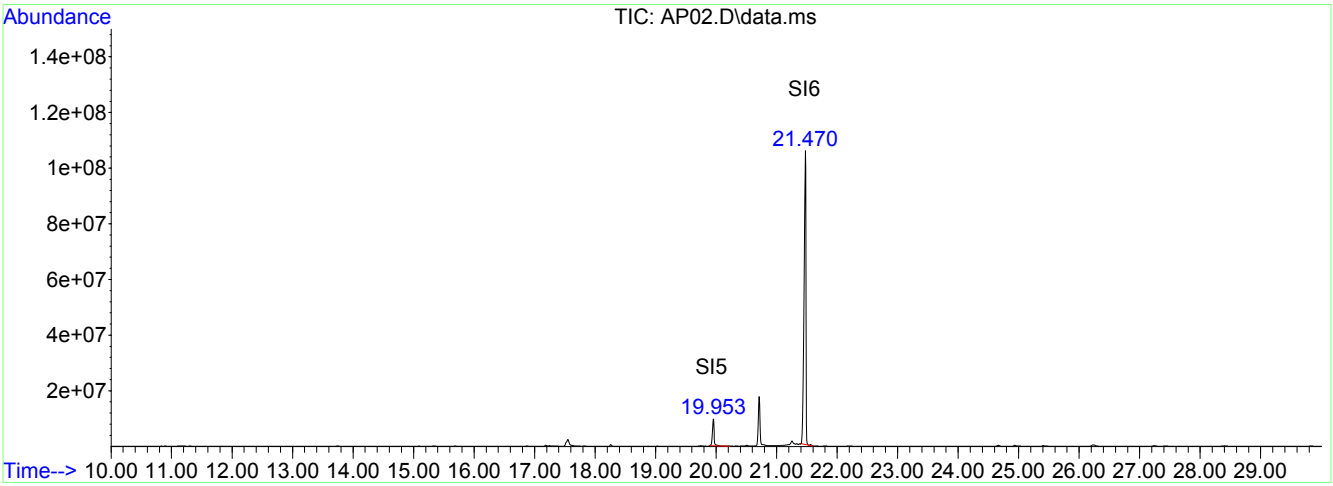


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AMJ72.D
Date Acquired : 23 Jan 2013 19:48 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AM72

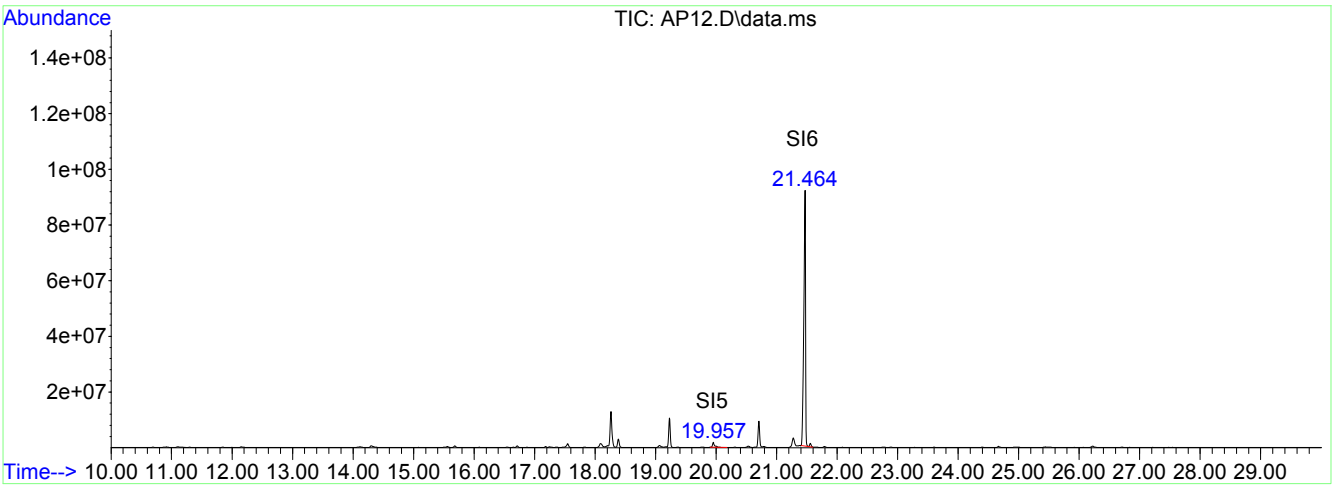


BX24-7d
90 minutes
24 hours
7 days

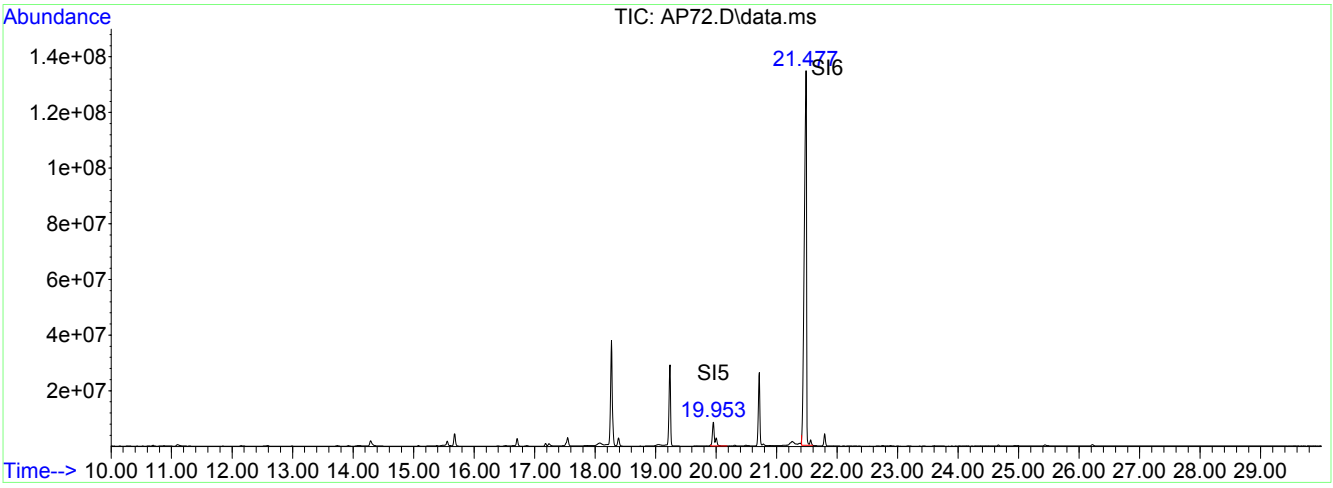
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AP02.D
Date Acquired : 25 Jan 2013 14:37 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AP02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AP12.D
Date Acquired : 26 Jan 2013 00:20 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AP12

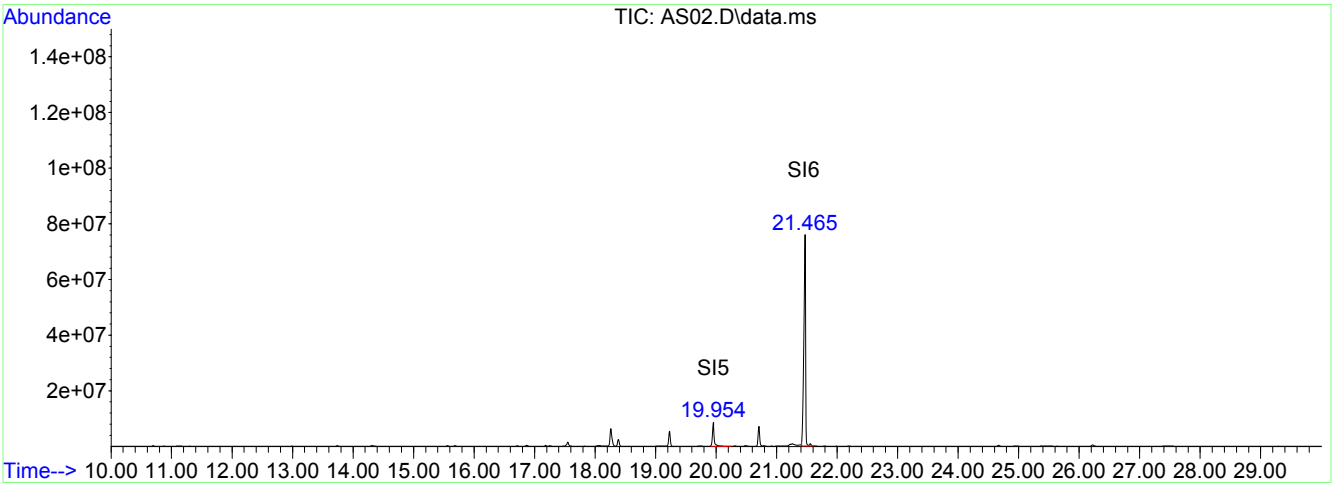


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AP72.D
Date Acquired : 1 Feb 2013 14:24 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AP72

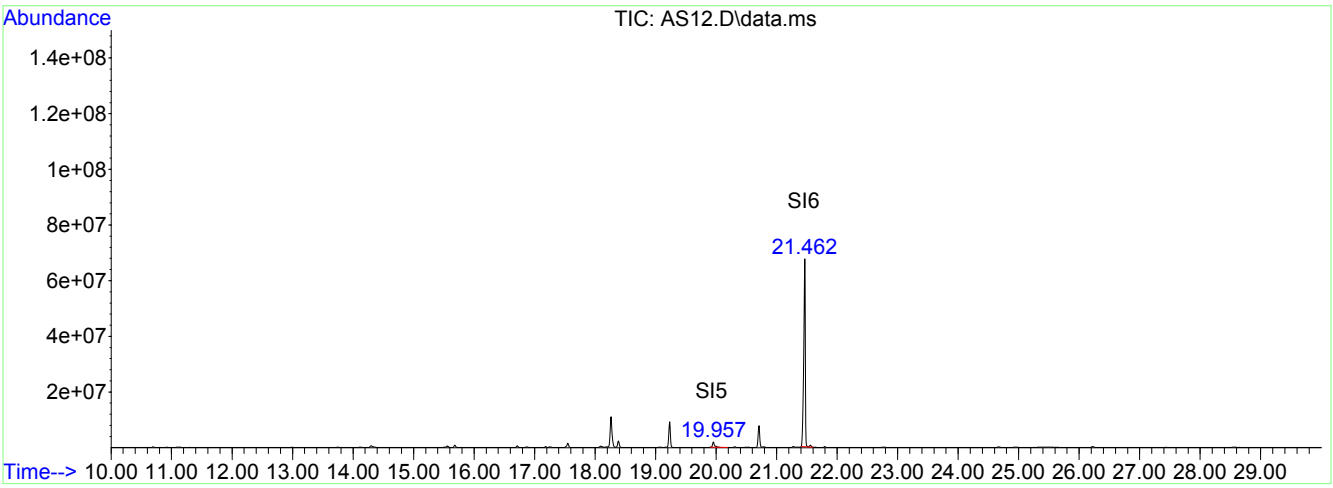


BX29-7d
90 minutes
24 hours
7 days

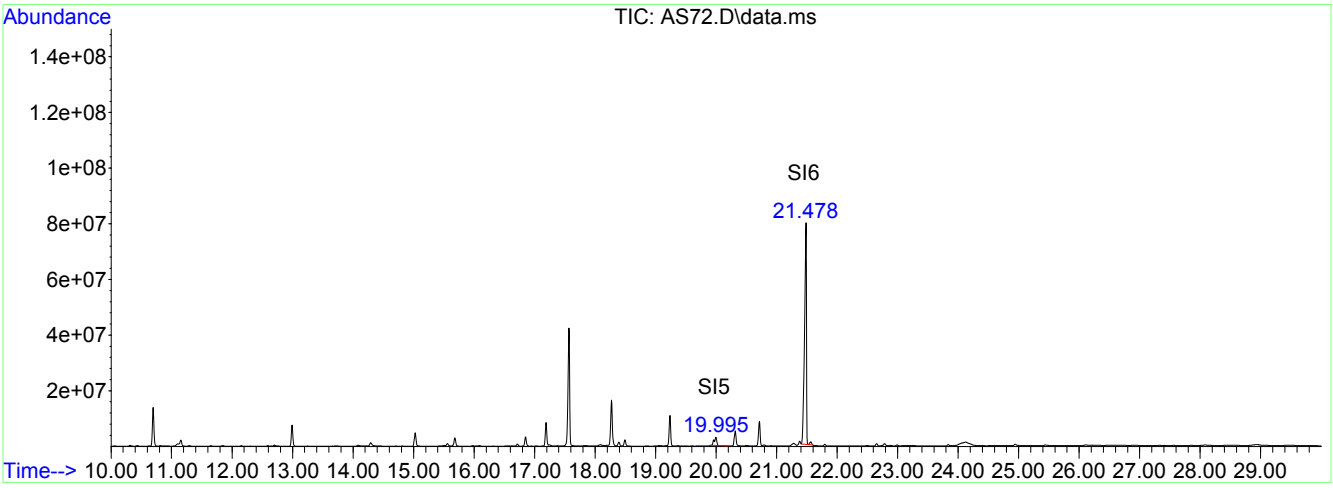
File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AS02.D
Date Acquired : 6 Feb 2013 13:21 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AS02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AS12.D
Date Acquired : 7 Feb 2013 16:17 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AS12

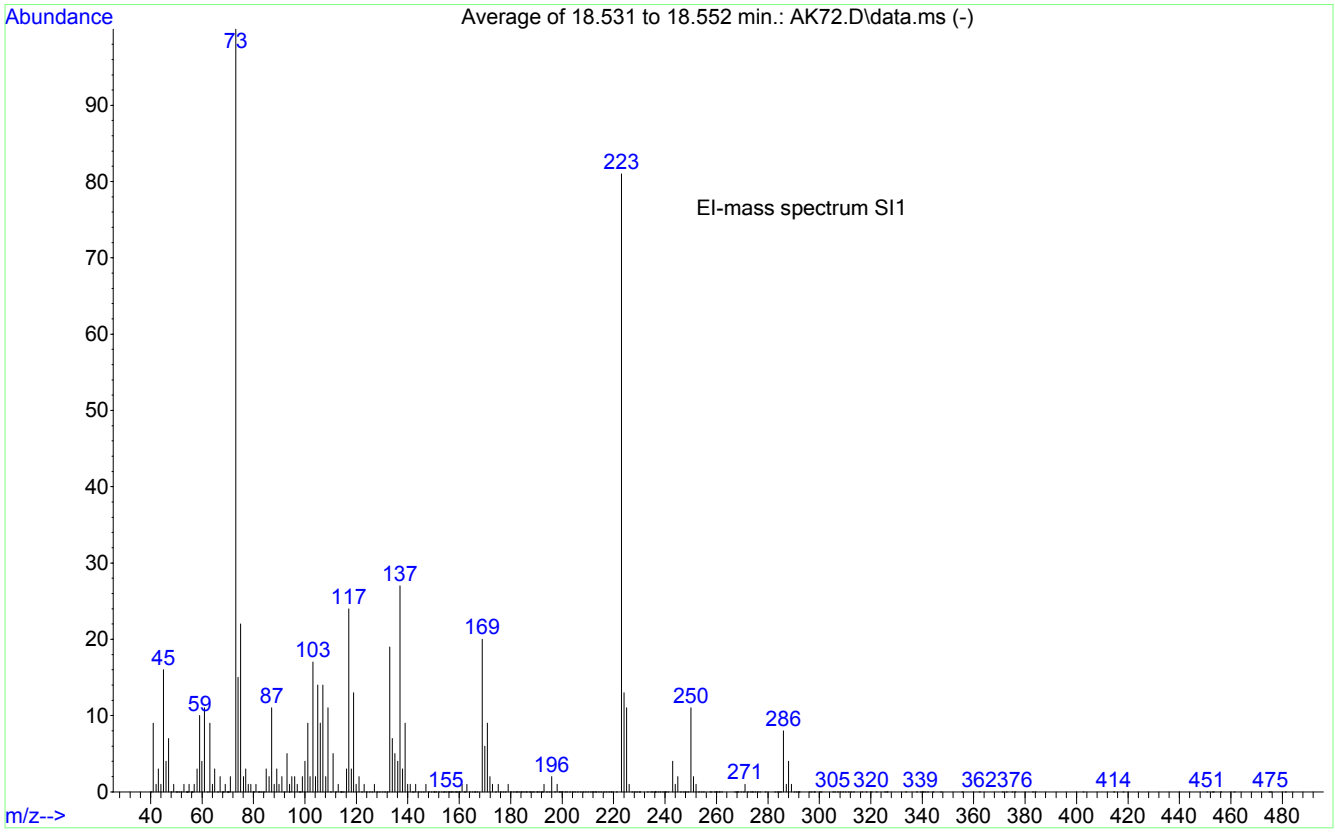


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AS72.D
Date Acquired : 15 Feb 2013 12:27 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AS72

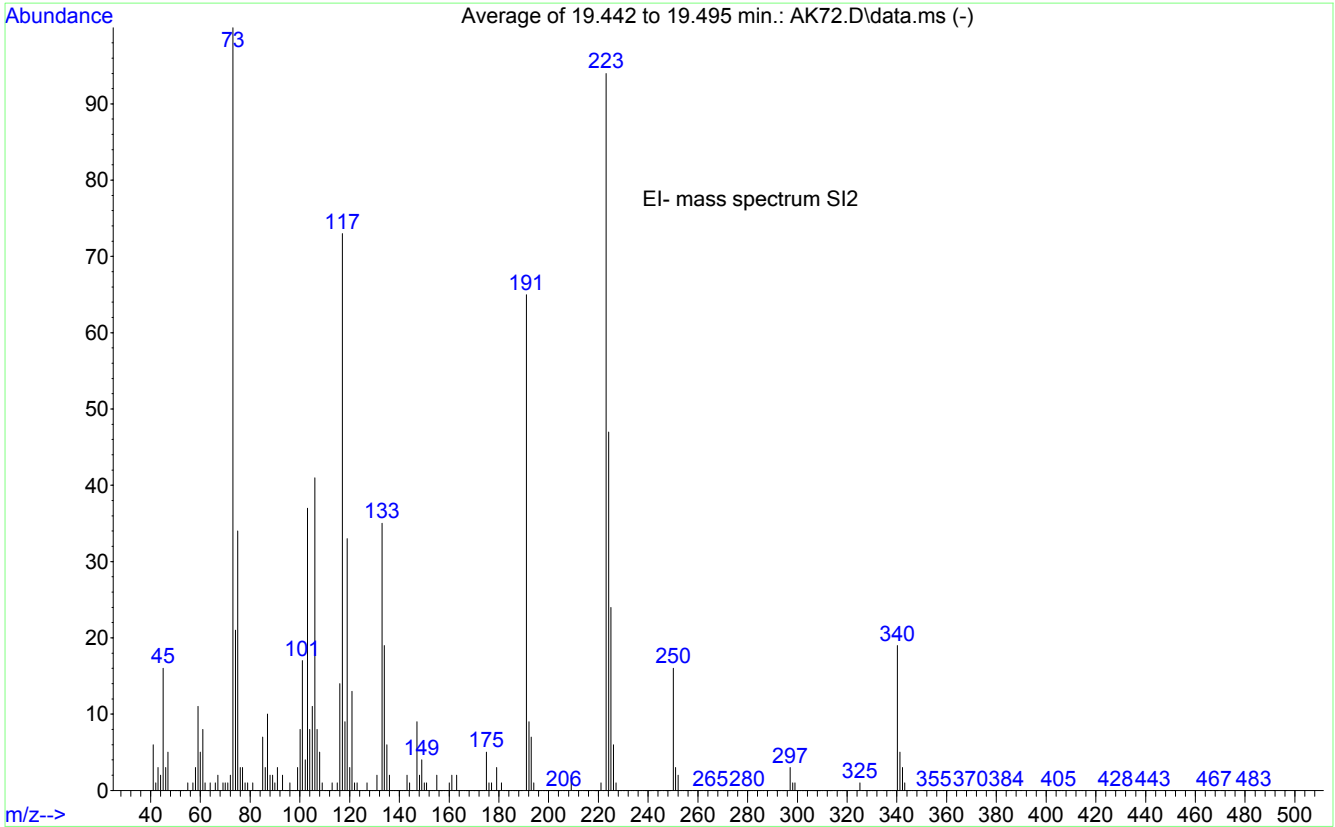


BX40-7d
90 minutes
24 hours
7 days

File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AK72.D
Date Acquired : 23 Jan 2013 17:03 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AK72

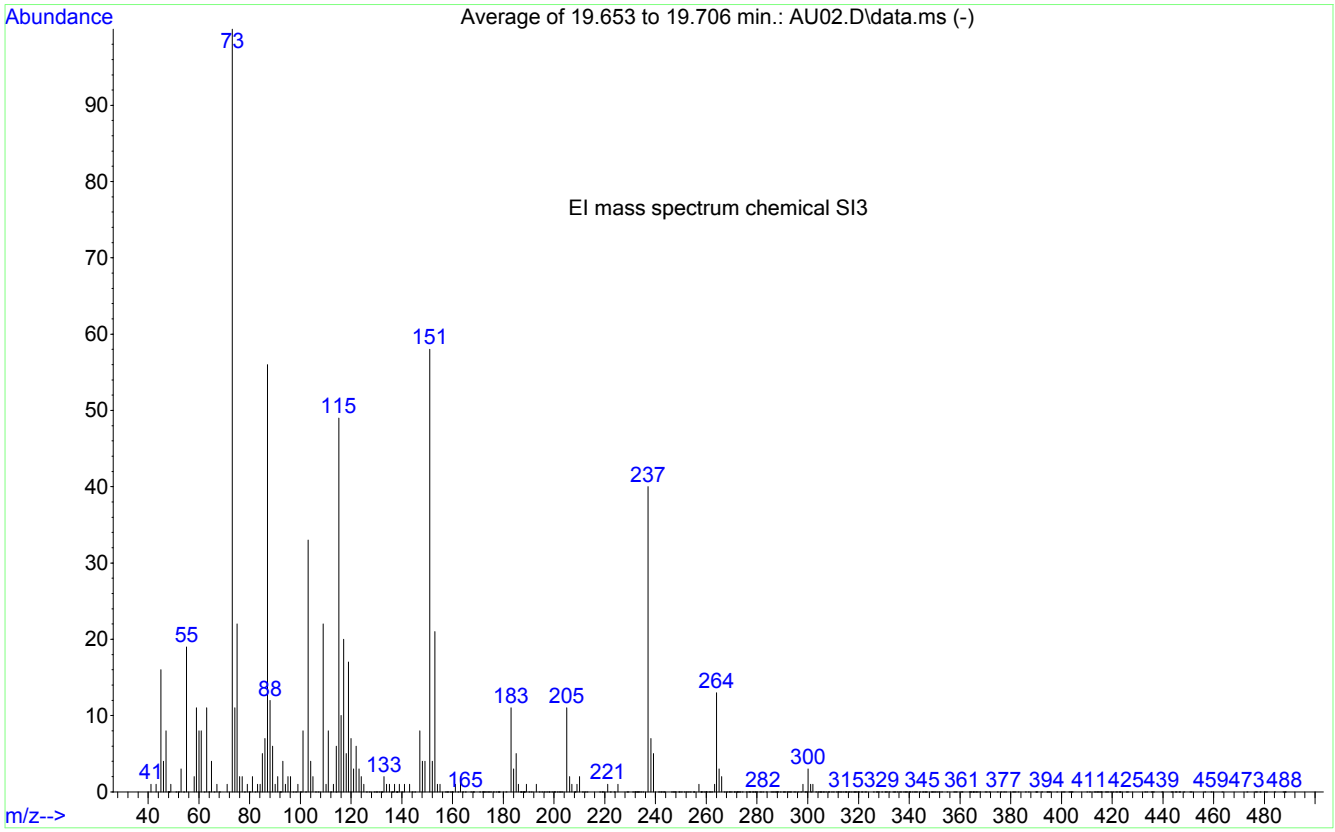


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AK72.D
Date Acquired : 23 Jan 2013 17:03 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AK72

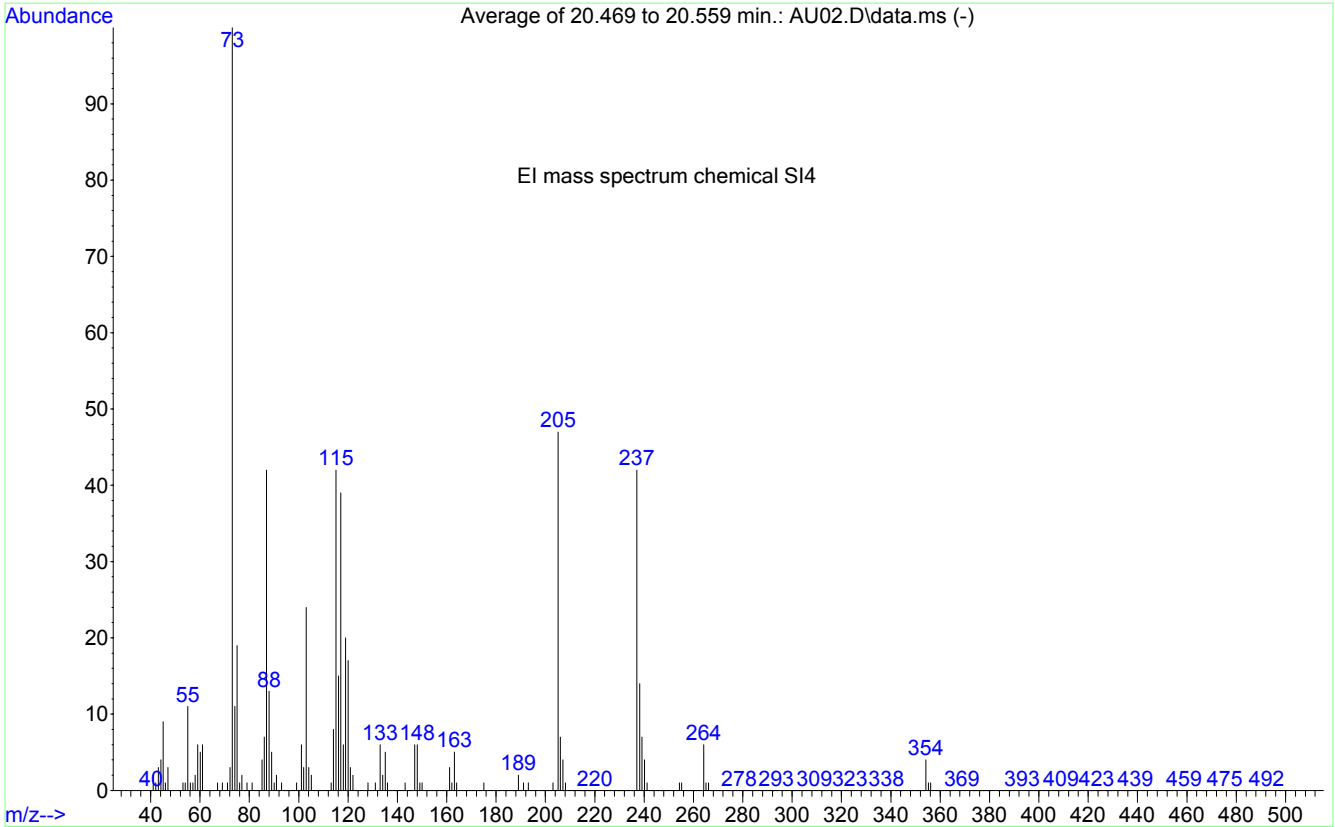


EI mass spectra SI1 and SI2
EI mass spectrum SI1
EI mass spectrum SI2

File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AU02.D
Date Acquired : 8 Feb 2013 14:35 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AU02

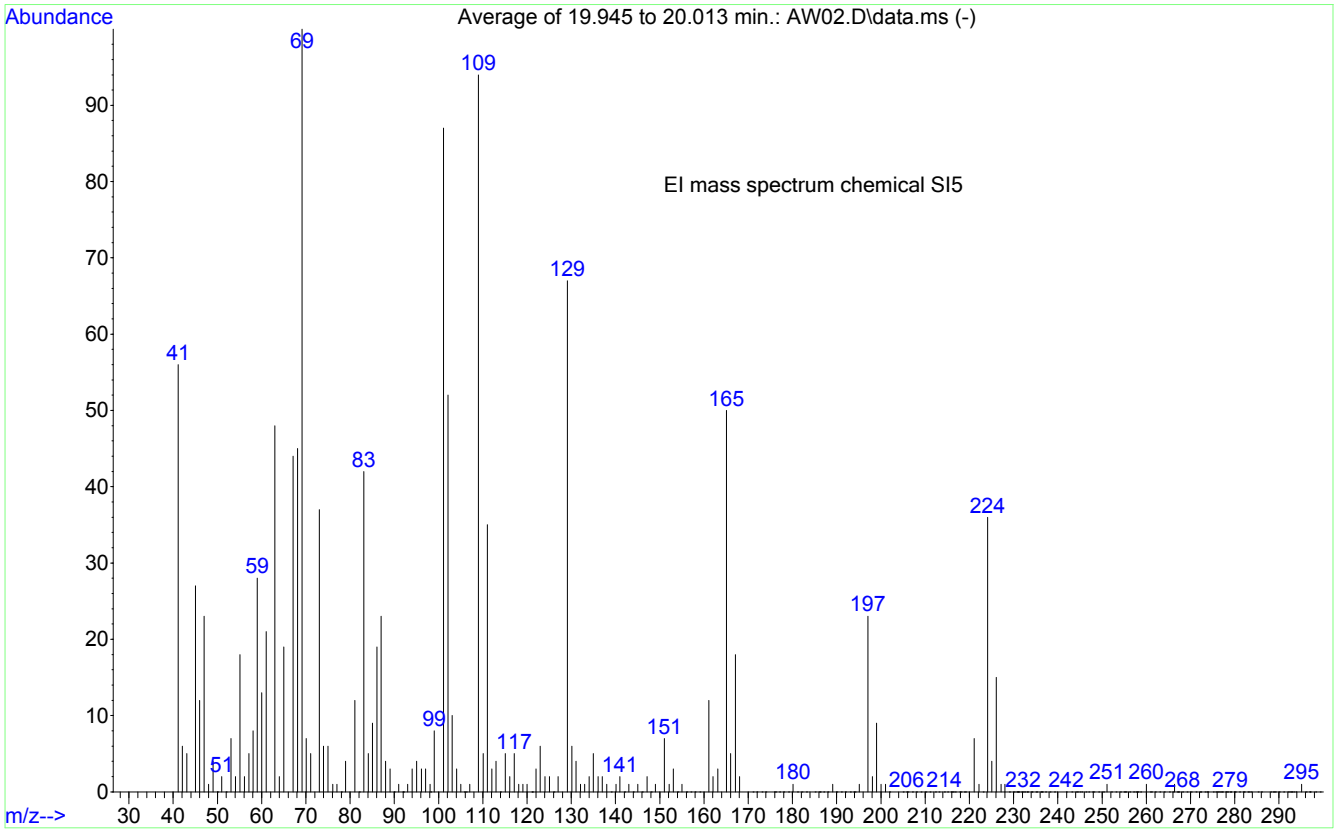


File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AU02.D
Date Acquired : 8 Feb 2013 14:35 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AU02

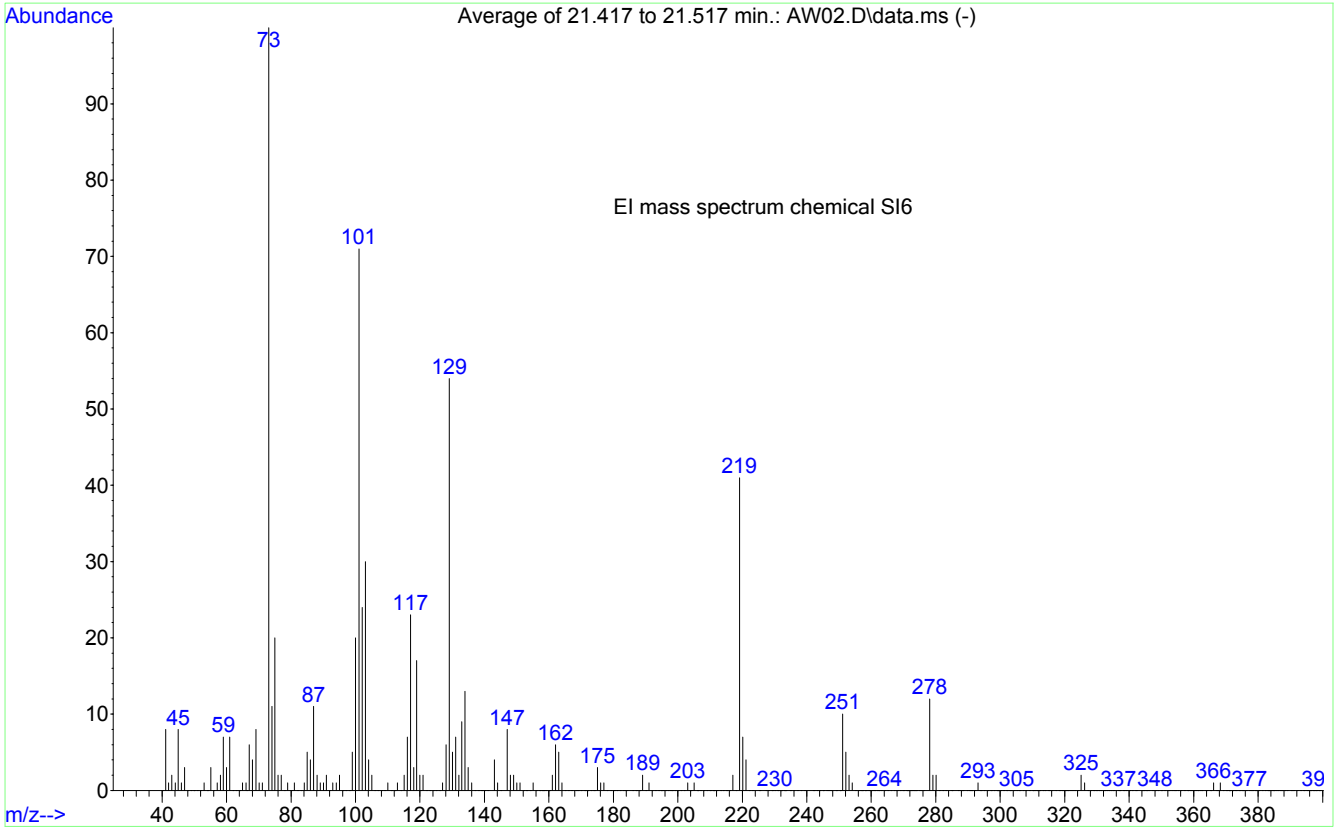


EI mass spectra degradation products chemical 7c
SI3
SI4

File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AW02.D
Date Acquired : 8 Feb 2013 15:18 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AW02



File : F:\MOSTAZAS descontaminacion\120366-MS-EI\20120366\AW02.D
Date Acquired : 8 Feb 2013 15:18 Method File : 32PTMSEI.M
Instrument : VE032
Sample Name : AW02



EI mass spectra degradation products chemical 7d
SI5
SI6