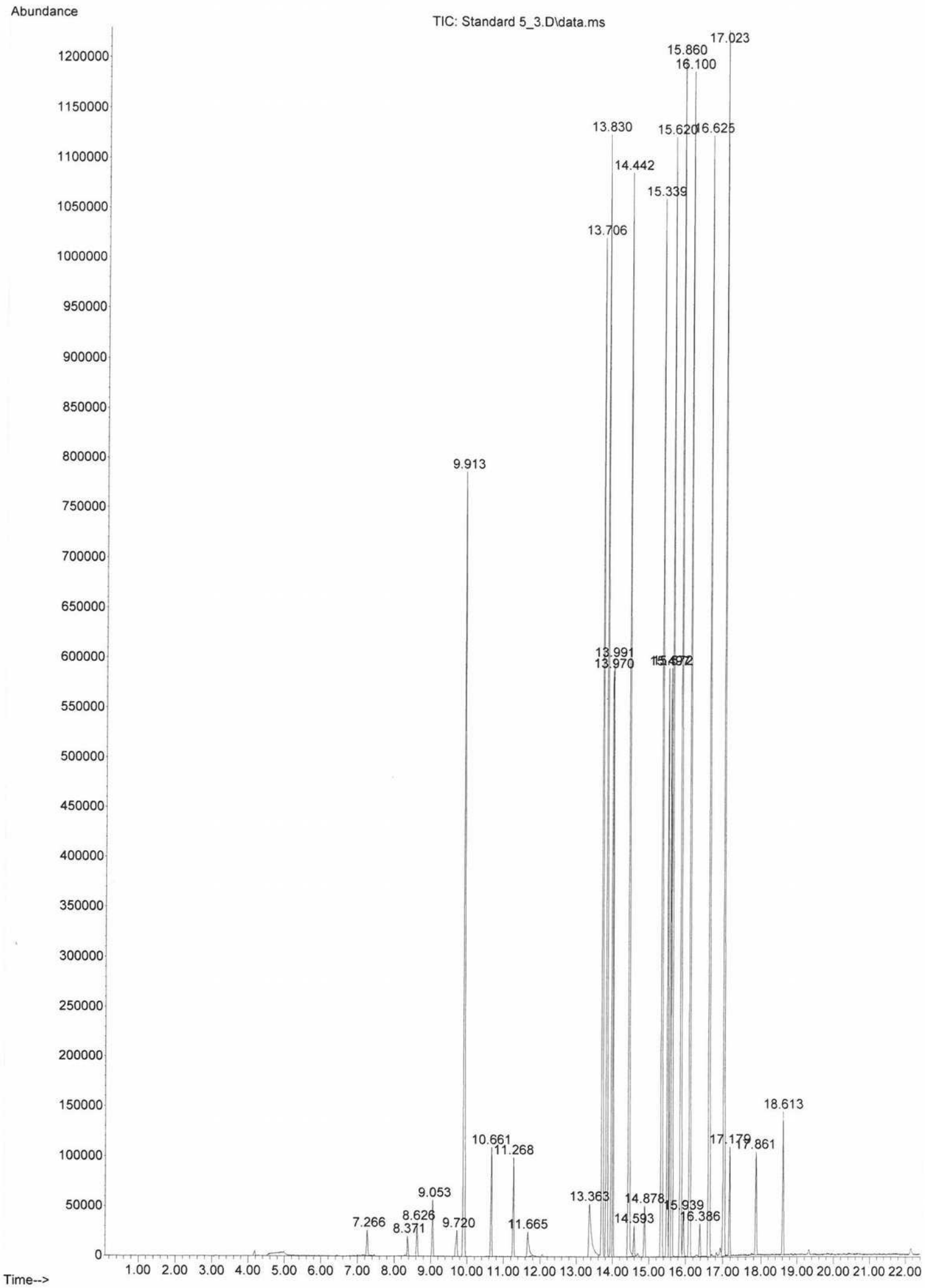
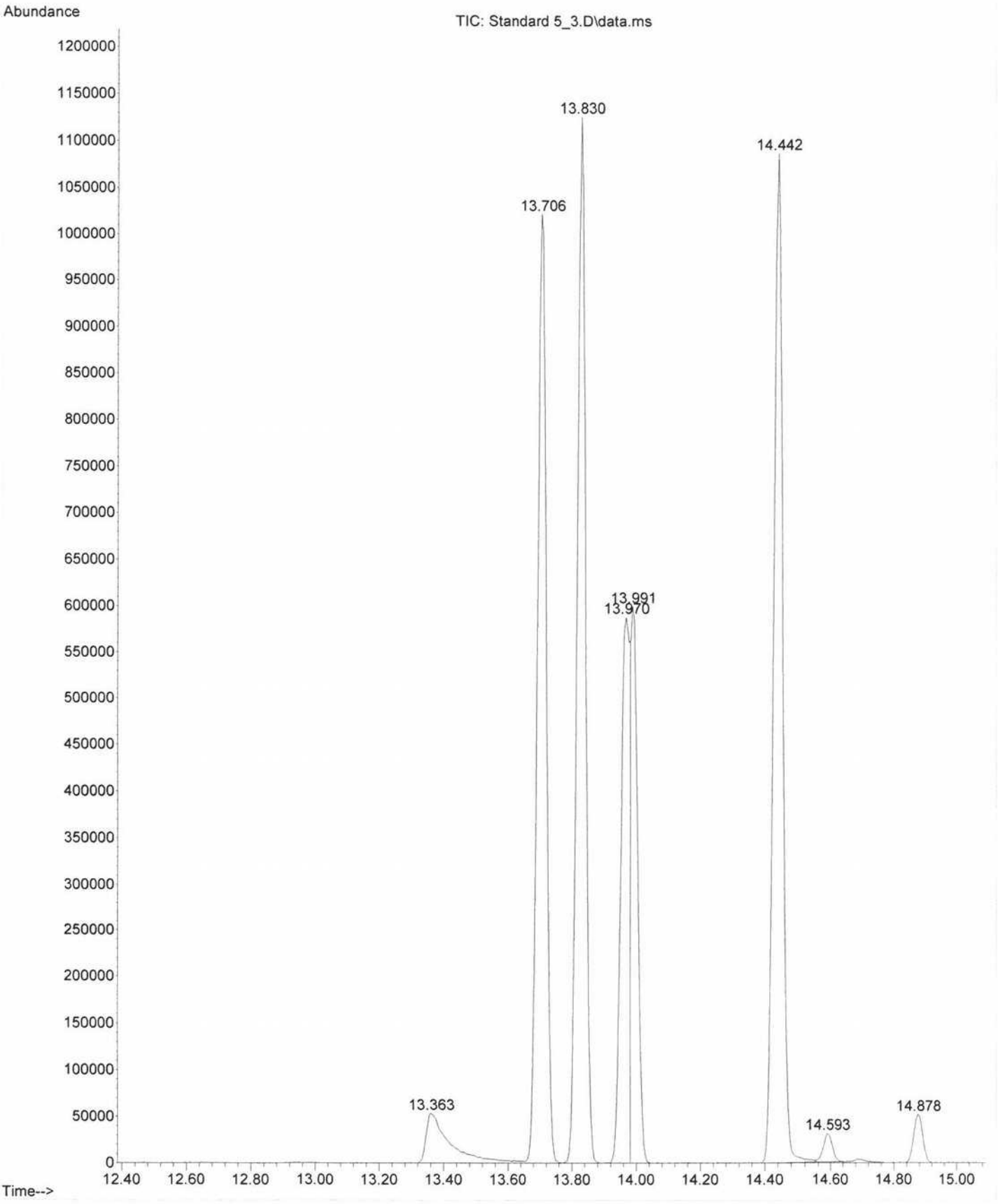
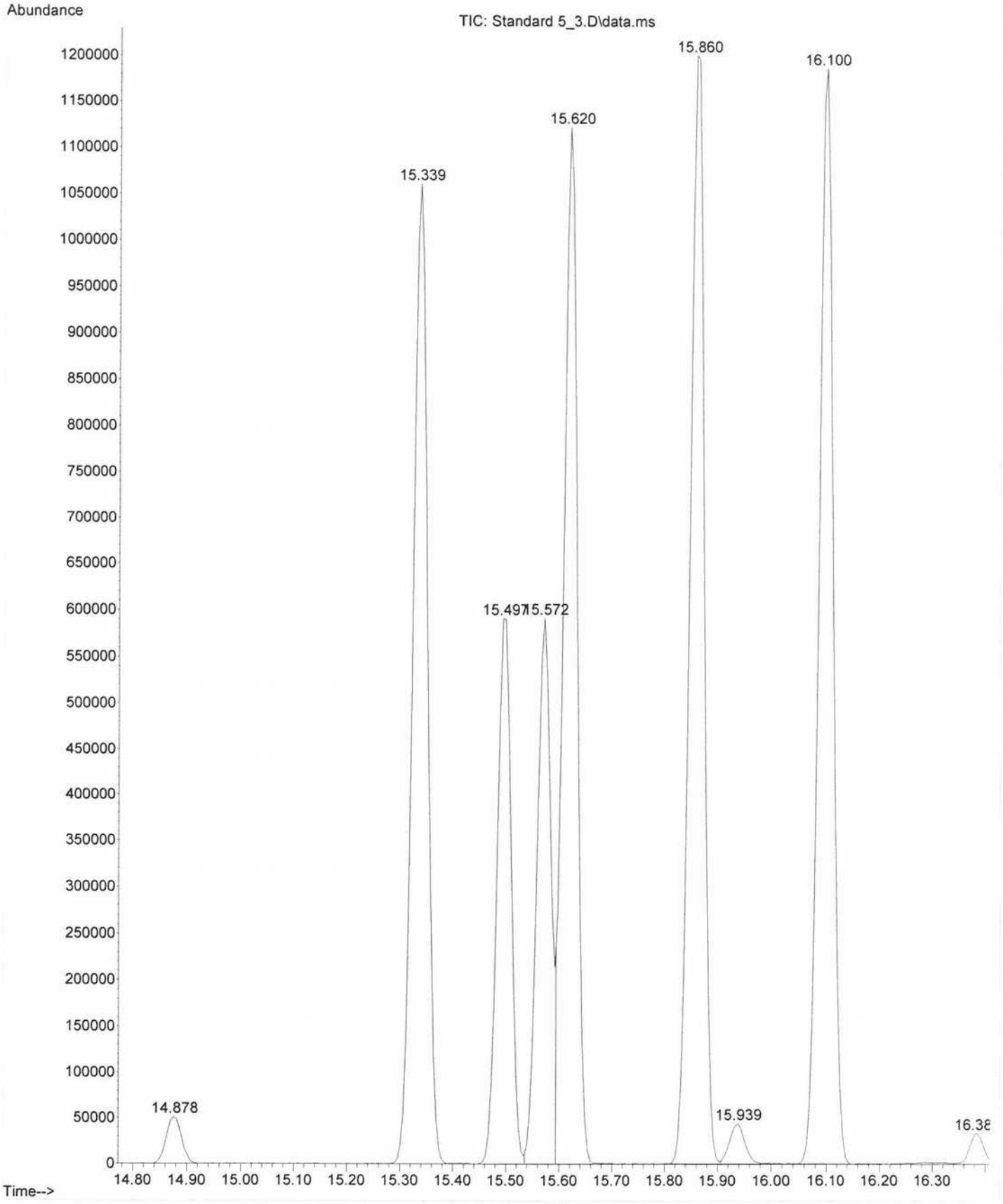

Abundance
TIC: Standard 5_3.D\data.ms
1200000
1150000
1100000
1050000
1000000
950000
900000
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
17.023
15.860
16.100
13.830
15.620
16.625
14.442
15.339
13.706
9.913
13.991
13.970
18.613
10.661
11.268
17.179
17.861
9.053
13.363
14.878
15.939
16.386
7.266
8.626
8.371
9.720
11.665
14.593
1.00 2.00 3.00 4.00 5.00 6.00 7.00 8.00 9.00 10.00 11.00 12.00 13.00 14.00 15.00 16.00 17.00 18.00 19.00 20.00 21.00 22.00
Time-->

File :C:\MassHunter\Data\Jaytee HS\Standard 5_3.D
Operator :
Acquired : 27 Oct 2020 13:34 using AcqMethod AAHeadspace.M
Instrument : Adler and Allen
Sample Name: Sample 1
Misc Info :
Vial Number: 1



File :C:\MassHunter\Data\Jaytee HS\Standard 5_3.D
Operator :
Acquired : 27 Oct 2020 13:34 using AcqMethod AAHeadspace.M
Instrument : Adler and Allen
Sample Name: Sample 1
Misc Info :
Vial Number: 1



Library Search Report

Data Path : C:\MassHunter\Data\Jaytee HS\
Data File : Standard 5_3.D
Acq On : 27 Oct 2020 13:34
Operator :
Sample : Sample 1
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: C:\DATABASE\NIST14-MAINLIB.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	7.266	0.21	C:\DATABASE\NIST14-MAINLIB.L			
			Methylene chloride	18037	000075-09-2	72
			1,16-Cyclocorynan-17-oic acid, 19, 20-didehydro-, methyl ester, (16S, 19E)-	54064	006393-66-4	9
			Methane-d, trichloro-	54063	000865-49-6	9
2	8.371	0.15	C:\DATABASE\NIST14-MAINLIB.L			
			1-Propene, 1-methoxy-	39641	007319-16-6	9
			Isobutylene epoxide	2310	000558-30-5	9
			Formaldehyde, dimethylhydrazone	39666	002035-89-4	9
3	8.626	0.24	C:\DATABASE\NIST14-MAINLIB.L			
			Pentanoic acid, 3-methyl-4-oxo-	8681	006628-79-1	9
			1-Propene, 1-(methylthio)-, (Z)-	17248	052195-40-1	5
			Ethyl Acetate	8290	000141-78-6	4
4	9.053	0.43	C:\DATABASE\NIST14-MAINLIB.L			
			Trichloromethane	52864	000067-66-3	91
			Methane, oxybis[dichloro-	52863	020524-86-1	9
			2-Propanone, 1,1,3,3-tetrachloro-	52872	000632-21-3	9
5	9.720	0.27	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	31471	000107-06-2	90
			Ethene, chloro-	86	000075-01-4	9
			Phosphine, ethyl-	31446	000593-68-0	5
6	9.913	5.88	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	48131	000071-43-2	91
			2,4,6-Cycloheptatrien-1-one	48228	000539-80-0	83
			Benzenemethanesulfonic acid, 2-hydroxy-, .gamma.-sultone	48229	010284-44-3	78
7	10.661	0.80	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	115116	000079-01-6	95
			N-Methyl-N'-acetylthiourea	116250	072886-35-2	10
			1,3-Oxathiane, 4,6-dimethyl-, cis-	116337	022452-25-1	9
8	11.268	0.71	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	8057	000108-10-1	78
			2-Hexanone	8092	000591-78-6	50
			N-Allyl-N,N-dimethylamine	27860	002155-94-4	40
9	11.665	0.30	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	48576	000110-86-1	90
			methanesulfonamide, N-(5-chloro-2-pyridinyl)-N-(methylsulfonyl)-	48569	000000-00-0	83
			1-Ethylpyridinium bromide	48568	001906-79-2	83
10	13.363	1.00	C:\DATABASE\NIST14-MAINLIB.L			
			5-Bromo-2-nitrophenylacetic acid	48126	124840-61-5	64
			1H-1,2,4-Triazole-3-carboxaldehyde, 5-(4-pyridinyl)-	31598	042786-73-2	64
			Dimethyl Sulfoxide	31596	000067-68-5	50
11	13.706	7.42	C:\DATABASE\NIST14-MAINLIB.L			

Data Path : C:\MassHunter\Data\Jaytee HS\
Data File : Standard 5_3.D
Acq On : 27 Oct 2020 13:34
Operator :
Sample : Sample 1
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: C:\DATABASE\NIST14-MAINLIB.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			[redacted]	89478	000108-90-7	91
			Phenol, 4-fluoro-	89493	000371-41-5	9
			2-Benzoylamino-1-cyclohexylamino-2-phenylethane	89592	000000-00-0	9
12	13.830	7.74	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	61070	000100-41-4	91
			p-Xylene	61097	000106-42-3	64
			Ethyl 2-(benzylamino)-2-(2-chloroacetamido)-3,3,3-trifluoropropionat	61079	339352-59-9	59
13	13.970	3.87	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	61097	000106-42-3	97
			Benzene, 1,3-dimethyl-	61096	000108-38-3	97
			o-Xylene	61100	000095-47-6	93
14	13.991	3.62	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	61096	000108-38-3	97
			p-Xylene	61097	000106-42-3	95
			o-Xylene	61100	000095-47-6	93
15	14.442	7.67	C:\DATABASE\NIST14-MAINLIB.L			
			Benzene, 1,3-dimethyl-	61096	000108-38-3	97
			[redacted]	61100	000095-47-6	97
			p-Xylene	61097	000106-42-3	95
16	14.593	0.23	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	19575	000108-94-1	80
			3-Heptene	2988	000592-78-9	64
			Cyclopentanone, 2-methyl-	4710	001120-72-5	59
17	14.878	0.37	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	52870	000079-34-5	95
			Ethane, 1,2,2-trichloro-1,1-difluoro-	52875	000354-21-2	43
			Trichloromethane	52864	000067-66-3	40
18	15.339	7.60	C:\DATABASE\NIST14-MAINLIB.L			
			Benzene, bromo-	47489	000108-86-1	91
			Pyridine, 2,6-dibromo-	204043	000626-05-1	50
			Benzenesulfonic acid	46900	000098-11-3	47
19	15.497	4.04	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	80898	000620-14-4	95
			Benzene, 1-ethyl-2-methyl-	80895	000611-14-3	94
			Benzene, 1,2,3-trimethyl-	80888	000526-73-8	91
20	15.572	3.88	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	80905	000622-96-8	94
			Benzene, 1-ethyl-2-methyl-	80895	000611-14-3	94
			Mesitylene	80908	000108-67-8	91
21	15.620	7.66	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	80908	000108-67-8	97
			Benzene, 1,2,3-trimethyl-	80888	000526-73-8	94
			Benzene, 1,2,4-trimethyl-	80868	000095-63-6	91

Library Search Report

Data Path : C:\MassHunter\Data\Jaytee HS\
Data File : Standard 5_3.D
Acq On : 27 Oct 2020 13:34
Operator :
Sample : Sample 1
Misc :
ALS Vial : 1 Sample Multiplier: 1

Search Libraries: C:\DATABASE\NIST14-MAINLIB.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
22	15.860	8.40	C:\DATABASE\NIST14-MAINLIB.L			
			Benzene, 1,2,4-trimethyl-	80868	000095-63-6	90
			Benzene, 1,2,3-trimethyl-	80888	000526-73-8	90
			Benzene, 1-ethyl-3-methyl-	80898	000620-14-4	90
23	15.939	0.32	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	65955	000062-53-3	94
			Glutaconaldehyde dianilide	66671	005608-83-3	90
			Pyridine, 4-methyl-	65960	000108-89-4	78
24	16.100	8.04	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	80908	000108-67-8	97
			Benzene, 1,2,3-trimethyl-	80888	000526-73-8	95
			Benzene, 1,2,4-trimethyl-	80868	000095-63-6	91
25	16.386	0.22	C:\DATABASE\NIST14-MAINLIB.L			
			Benzene, 1-methyl-3-(1-methylethyl)-	100340	000535-77-3	91
			1,3,5-Cycloheptatriene, 3,7,7-trim ethyl-	99545	003479-89-8	91
			Benzene, 1,2,4,5-tetramethyl-	100339	000095-93-2	91
26	16.625	7.78	C:\DATABASE\NIST14-MAINLIB.L			
			Benzene, 1-ethyl-3-methyl-	80898	000620-14-4	95
			Benzene, 1,2,3-trimethyl-	80888	000526-73-8	94
			Mesitylene	80908	000108-67-8	91
27	17.023	8.82	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	134512	000095-50-1	97
			Benzene, 1,3-dichloro-	134513	000541-73-1	96
			Benzene, 1,4-dichloro-	134514	000106-46-7	91
28	17.179	0.69	C:\DATABASE\NIST14-MAINLIB.L			
			Undecane	24369	001120-21-4	87
			Octatetracontane, 1-iodo-	25330	040710-70-1	86
			Carbonic acid, octadecyl prop-1-en -2-yl ester	24212	000000-00-0	86
29	17.861	0.73	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	47241	000098-95-3	91
			Hydrazine, phenylsulfinyl-	46571	017420-03-0	36
			N-(2-Benzyloxy-ethyl)-benzenesulfo namide	46846	000000-00-0	17
30	18.613	0.92	C:\DATABASE\NIST14-MAINLIB.L			
			[redacted]	24230	000112-40-3	97
			Carbonic acid, octadecyl prop-1-en -2-yl ester	24212	000000-00-0	86
			Carbonic acid, tetradecyl vinyl es ter	25286	000000-00-0	86

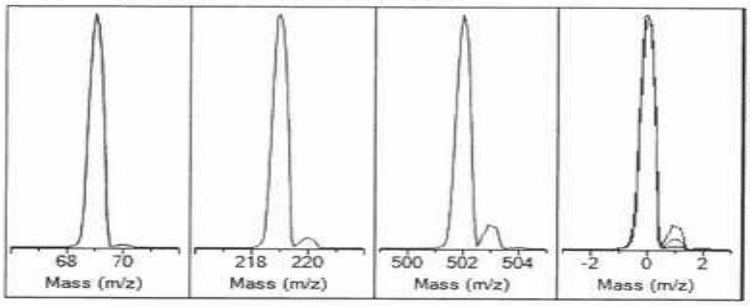
Autotune - 5975

Tune timestamp: 27/10/2020 13:01 (UTC+00:00)

C:\MASSHUNTER\GCMS\1\5975\ATUNE.U

Adler and Allen

US90432216

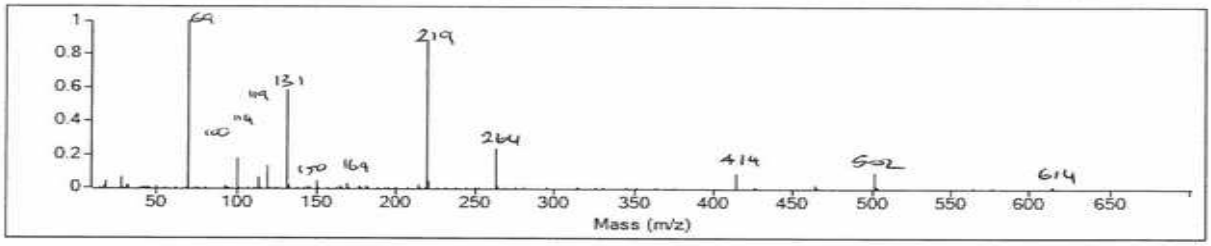


Ion Polarity	Pos	PFTBA	Open
Emission	34.6	Mass Gain	-879
Electron Energy	70.3	Mass Offset	-38
Filament	1	Amu Gain	1454
Repeller	21.84	Amu Offset	121.19
Ion Focus	90.2	Width219	-0.004
Entrance Lens	25.5	DC Polarity	Pos
Ent Lens Offset	18.82	HED Enable	On
		EM Volts	1612 ✓
		Scan Speed	3
JetClean Flow Actual/[Setpoint]	0.00 [0.00]	Averages	3

Actual m/z		Abund	Rel Abund		Pw50
69.00	✓	429,773	100.0%	✓	0.60
219.00	✓	372,559	86.7%	✓	0.61
502.00	✓	42,633	9.9%	✓	0.59

Temperatures and Pressures			
MS Source	230	Turbo Speed	100.0
MS Quad	150	Hi Vac	1.60e-05

Low	High	Step	Speed	Threshold	Peaks	Base	Abundance	Total Ion
10.00	701.00	0.10	3	100	137	69.00	407,040	1,543,145



Target m/z	Actual m/z	Abund	Rel Abund	Iso m/z	Iso Abund	Iso Ratio	
69.00	69.00	407,040	100.0%	70.00	4,517	1.1%	✓
219.00	219.00	360,064	88.5%	220.00	16,081	4.5%	✓
502.00	502.00	39,256	9.6%	503.00	3,718	9.5%	✓

Air/Water Check: H20 ~3.9% ✓ N2 ~6.7% ✓ O2 ~1.9% ✓ CO2 ~0.5% ✓ N2/H20 ~172.3% ✓

Column(1) Flow: 0.00 Column(2): 1.01 ml/min Interface Temp: 280

Ramp Criteria:

Ion Focus maximum 90 volts using ion 502; Electron Multiplier Gain 167876.719

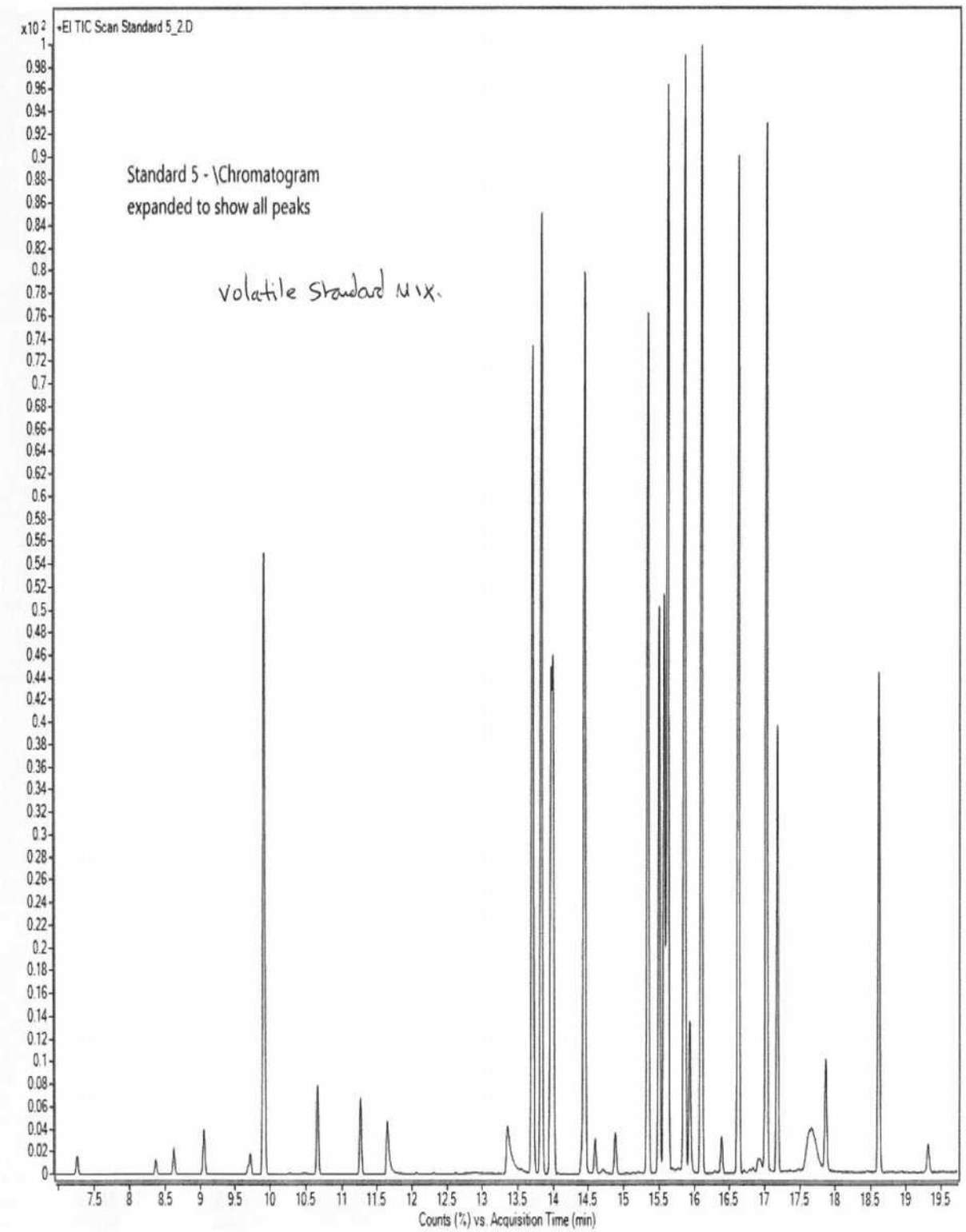
Repeller maximum 35 volts using ion 219; Gain Factor 1.6788

Mass Gain Values(Scan Speed): -880(3) -875(2) -861(1) -830(0) -778(FS1) -735(FS2)

TARGET MASS:	50	69	131	219	414	502	1050
Amu Offset	121.2	121.2	121.2	121.2	121.2	121.2	121.2
Entrance Lens Offset	18.8	18.8	18.8	18.8	18.8	18.8	18.8

Agilent 5975C
Inert XL MSD

Report Created: 27/10/2020 13:02 (UTC+00:00)


x10 2
+EI TIC Scan Standard 5_2.D
Standard 5 - \Chromatogram
expanded to show all peaks
Volatile Standard Mix.
Counts (%) vs. Acquisition Time (min)