LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001988.D
Acq On : 25 May 2018 20:10
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.075	76	80	90	rBV	3156423	3844274	12.78%	4.976%
2	1.325	115	121	144	rBV	660079	2763326	9.19%	3.577%
3	1.490	144	148	161	rVV	511354	984029	3.27%	1.274%
4	2.172	245	260	263	rBV	11772342	30081061	100.00%	38.933%
5	2.270	271	276	301	rVB	424719	1033842	3.44%	1.338%
6	2.636	322	336	346	rBV2	240936	1093966	3.64%	1.416%
7	4.032	554	565	575	rBV	466139	1156886	3.85%	1.497%
8	4.721	668	678	692	rBV	227664	649423	2.16%	0.841%
9	4.873	694	703	716	rVB	265389	755551	2.51%	0.978%
10	5.513	796	808	823	rBV	268014	774517	2.57%	1.002%
11	5.672	823	834	851	rVB	304108	853549	2.84%	1.105%
12	6.074	889	900	921	rVB	298302	787472	2.62%	1.019%
13	6.867	1020	1030	1044	rBV	473582	1102283	3.66%	1.427%
14	7.342	1100	1108	1121	rBV	1776444	3514176	11.68%	4.548%
15	8.720	1328	1334	1343	rVB	1359036	2097629	6.97%	2.715%
16	10.116	1557	1563	1571	rBV	983213	1342196	4.46%	1.737%
17	11.098	1719	1724	1727	rBV	274934	323364	1.07%	0.419%
18	11.140	1727	1731	1736	rVB	1193131	1528199	5.08%	1.978%
19	11.951	1851	1864	1868	rBV2	148460	341854	1.14%	0.442%
20	12.085	1880	1886	1893	rBV	1194785	1540485	5.12%	1.994%
21	12.305	1914	1922	1927	rBV	755917	966748	3.21%	1.251%
22	12.372	1929	1933	1941	rVB3	196307	310219	1.03%	0.402%
23	12.463	1944	1948	1953	rVV	245112	346966	1.15%	0.449%
24	12.640	1972	1977	1979	rBV	281637	353744	1.18%	0.458%
25	12.670	1979	1982	1986	rVB	538829	646702	2.15%	0.837%
26	12.762	1993	1997	2003	rBV3	385359	681158	2.26%	0.882%
27	12.878	2012	2016	2023	rVB3	196537	395825	1.32%	0.512%
28	12.981	2023	2033	2037	rBV2	531411	921799	3.06%	1.193%
29	13.091	2047	2051	2056	rVB3	175717	302006	1.00%	0.391%
30	13.201	2066	2069	2075	rBV4	269032	406738	1.35%	0.526%
31	13.317	2083	2088	2090	rBV2	254712	344744	1.15%	0.446%
32	13.353	2090	2094	2099	rVV3	1523911	2376050	7.90%	3.075%
33	13.408	2099	2103	2109	rVB2	1227083	1539471	5.12%	1.993%
34	13.481	2109	2115	2122	rBV7	159482	414522	1.38%	0.537%

LSC Area Percent Report

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Data File : VX001988.D
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Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Title : SW846 8260

35	13.646	2138	2142	2146	rBV3	282404	466423	1.55%	0.604%
36	13.737	2153	2157	2161	rVB4	328114	557357	1.85%	0.721%
37	13.859	2174	2177	2182	rVB3	288957	410007	1.36%	0.531%
38	13.914	2182	2186	2192	rBV4	264181	451720	1.50%	0.585%
39	13.993	2192	2199	2202	rBV3	373457	643771	2.14%	0.833%
40	14.042	2202	2207	2212	rVV4	306399	530600	1.76%	0.687%
41	14.225	2230	2237	2241	rBV7	142779	339407	1.13%	0.439%
42	14.280	2241	2246	2254	rVV4	378751	943476	3.14%	1.221%
43	14.371	2257	2261	2267	rVV4	352404	680142	2.26%	0.880%
44	14.432	2267	2271	2276	rVB3	228228	361026	1.20%	0.467%
45	14.548	2286	2290	2293	rBV2	360491	533582	1.77%	0.691%
46	14.841	2334	2338	2343	rBV2	411885	636298	2.12%	0.824%
47	14.957	2352	2357	2358	rBV3	211990	305374	1.02%	0.395%
48	15.036	2366	2370	2376	rVB4	305791	556226	1.85%	0.720%
49	15.121	2381	2384	2389	rBV2	390069	547152	1.82%	0.708%
50	15.243	2399	2404	2409	rBV4	321041	723128	2.40%	0.936%
51	15.402	2425	2430	2434	rBV	521592	761640	2.53%	0.986%
52	15.560	2451	2456	2461	rBV2	229470	429292	1.43%	0.556%
53	15.694	2473	2478	2482	rBV	284088	501241	1.67%	0.649%
54	15.731	2482	2484	2491	rVB	214331	310568	1.03%	0.402%

Sum of corrected areas: 77263204

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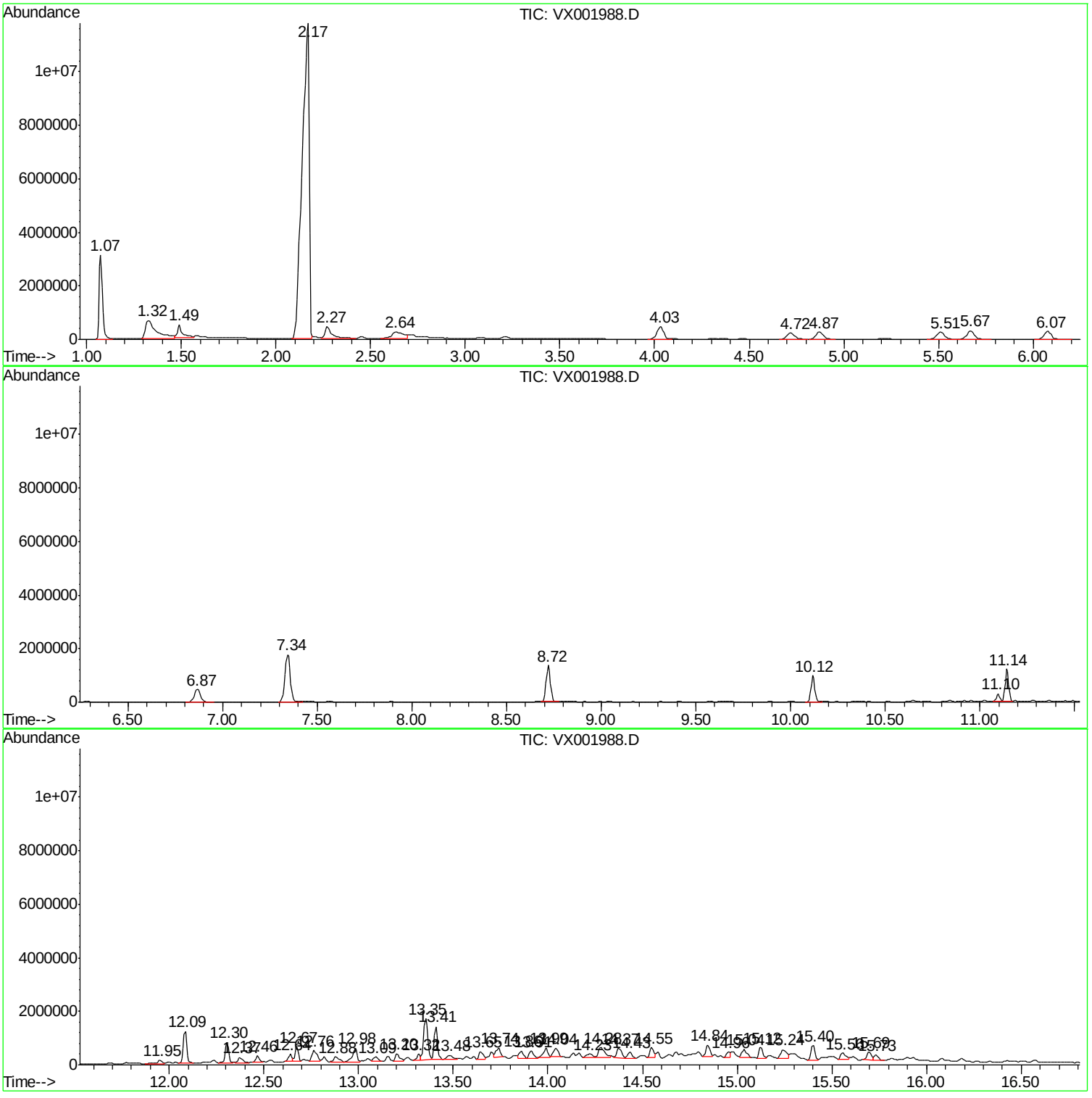
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001988.D
Acq On : 25 May 2018 20:10
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
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Quant Title : SW846 8260

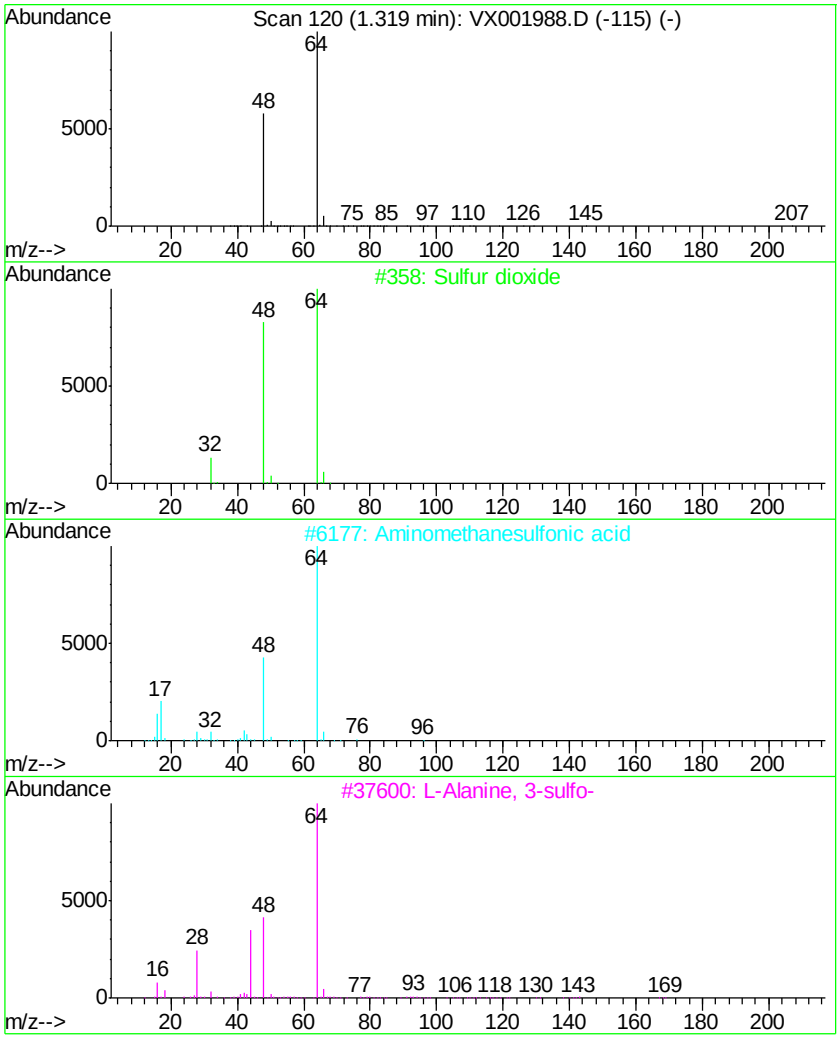
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

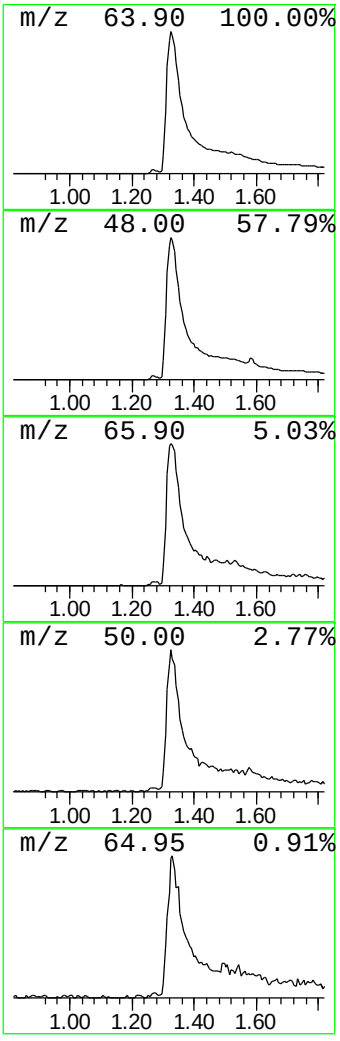
****

Peak Number 2 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	161.87 ug/l	2763330	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX052518\
Data File : VX001988.D
Acq On : 25 May 2018 20:10
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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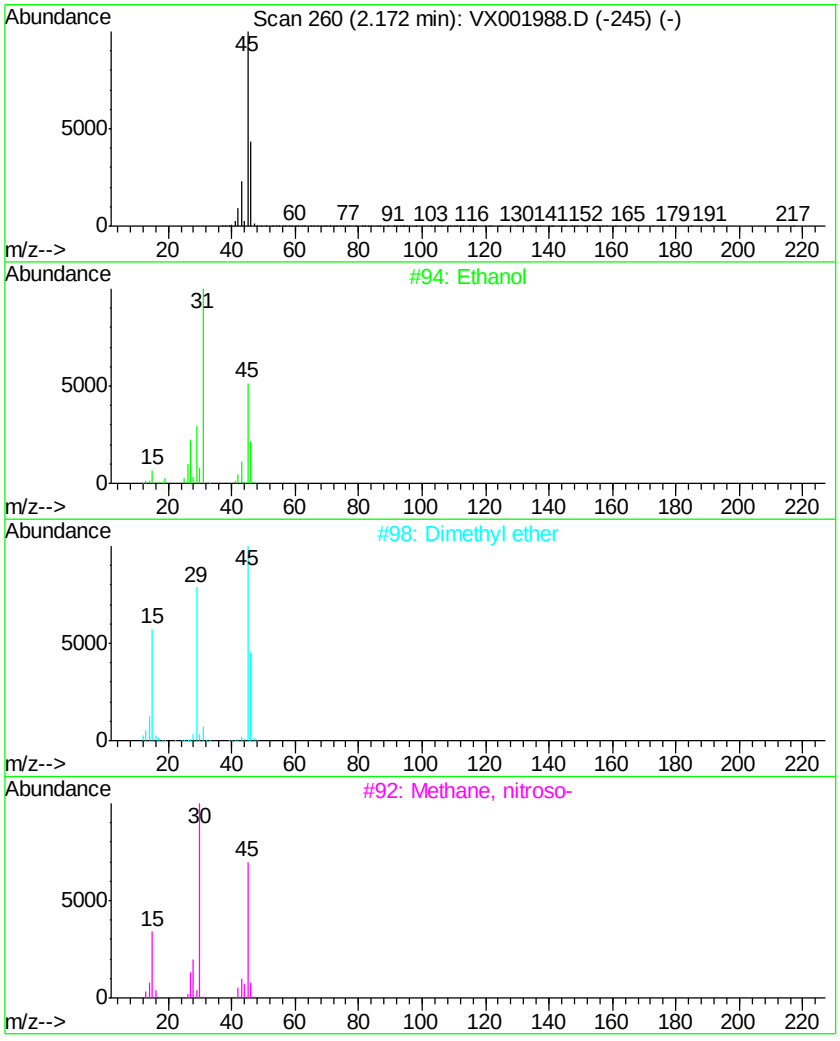
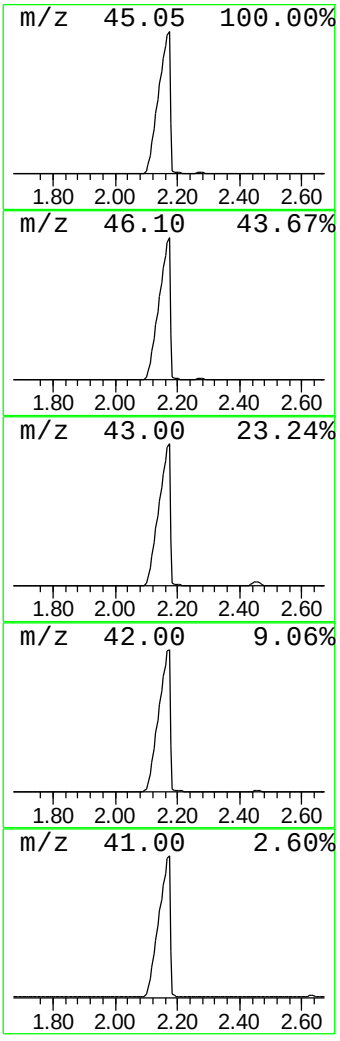
Peak Number 4 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	1762.12 ug/l	30081100	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	86
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001988.D
Acq On : 25 May 2018 20:10
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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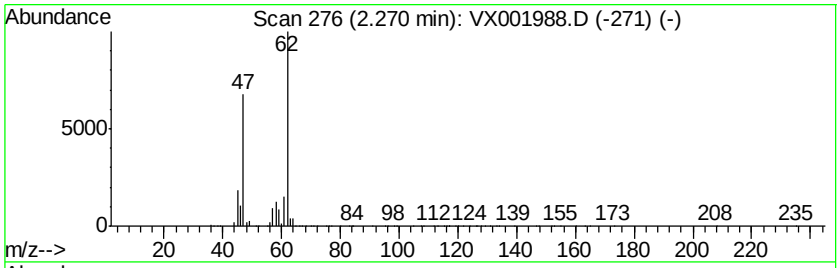
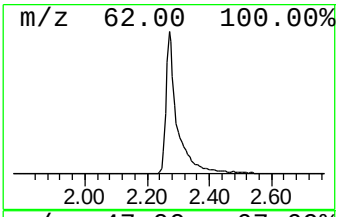
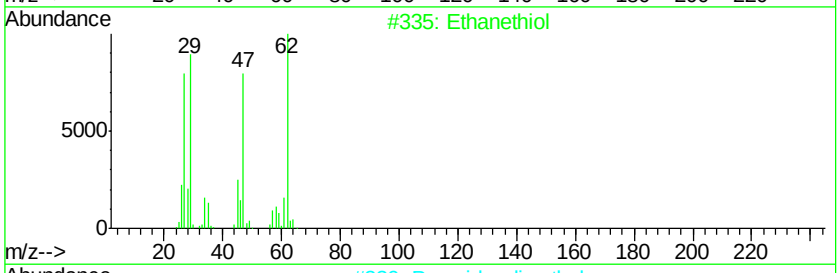
Peak Number 5 Ethanethiol Concentration Rank 7

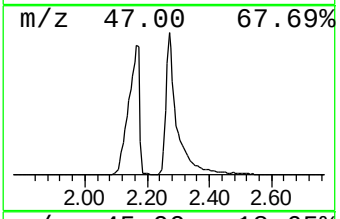
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	60.56 ug/l	1033840	Pentafluorobenzene	5.67

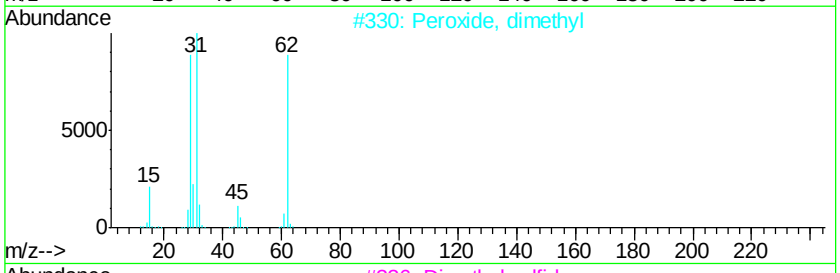
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol	62	C2H6S	000075-08-1	91
2	Peroxide, dimethyl	62	C2H6O2	000690-02-8	72
3	Dimethyl sulfide	62	C2H6S	000075-18-3	64
4	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	43
5	Ethene, chloro-	62	C2H3Cl	000075-01-4	39

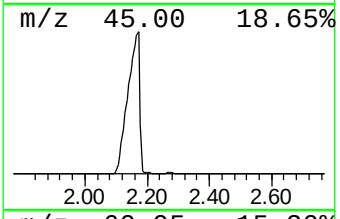


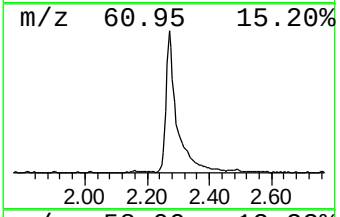


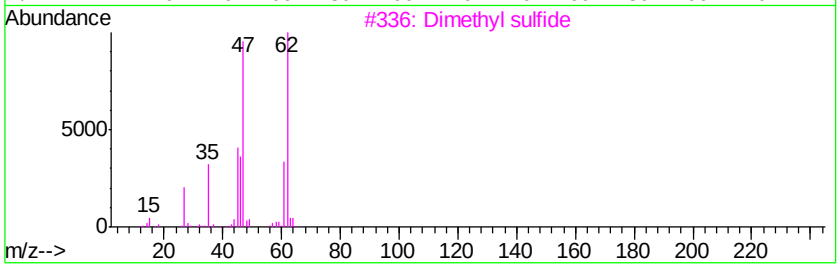


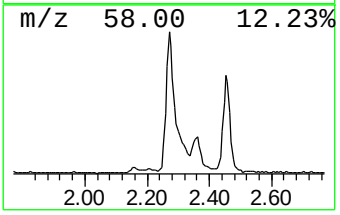












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ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

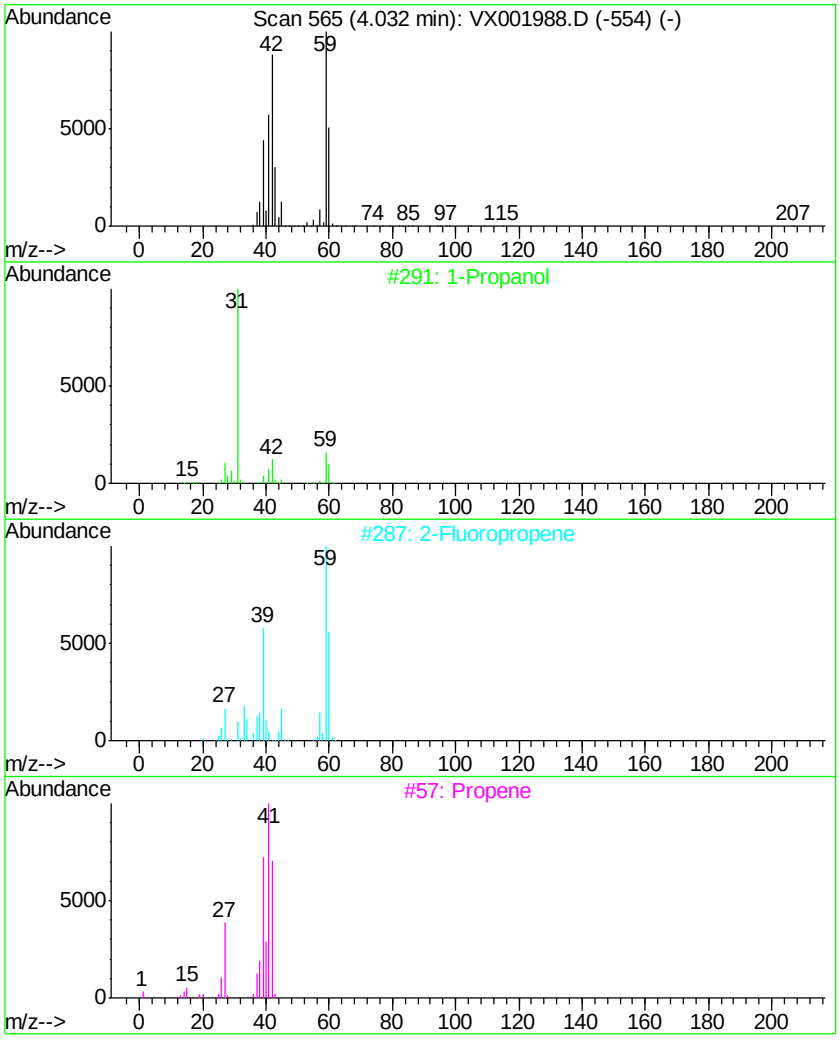
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

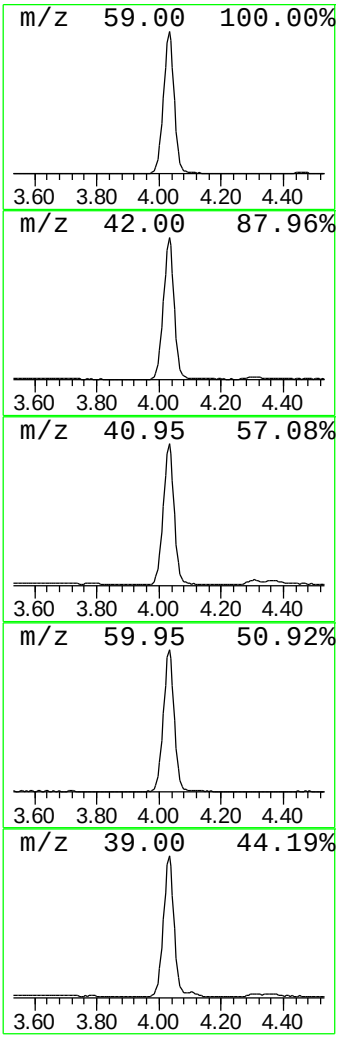
****

Peak Number 6 1-Propanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	67.77 ug/l	1156890	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	59
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Propene	42	C3H6	000115-07-1	25
4	Cyclopropane	42	C3H6	000075-19-4	25
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7





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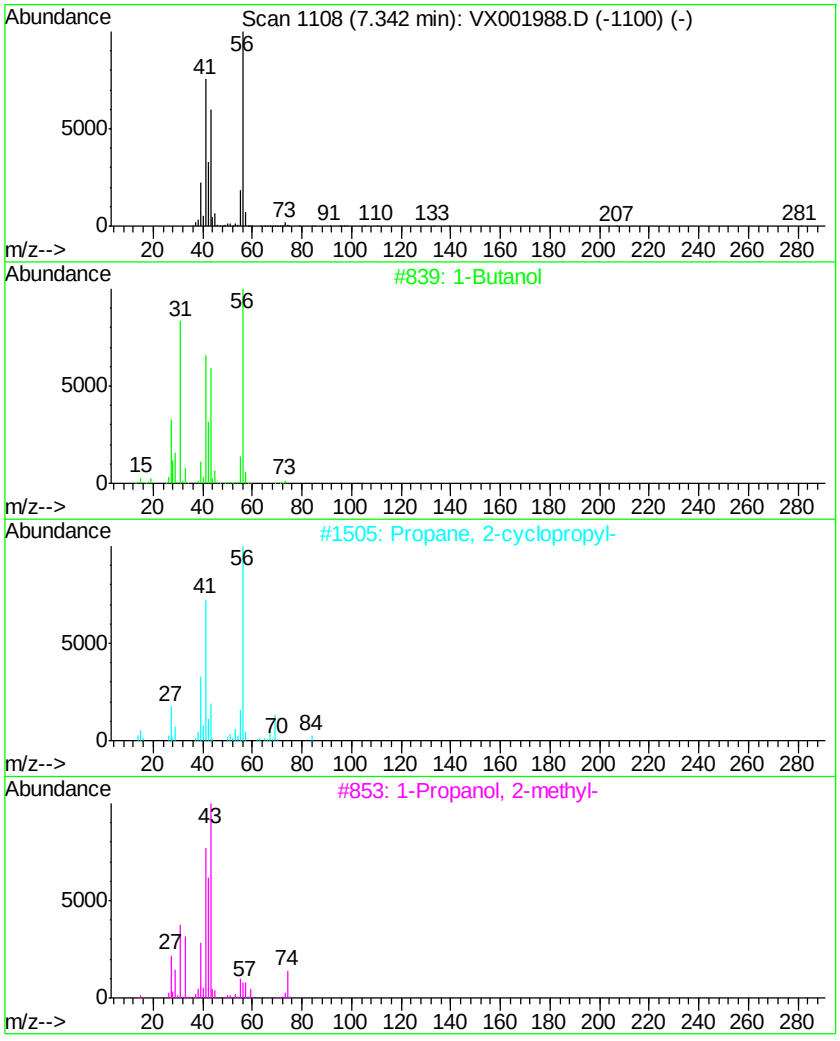
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

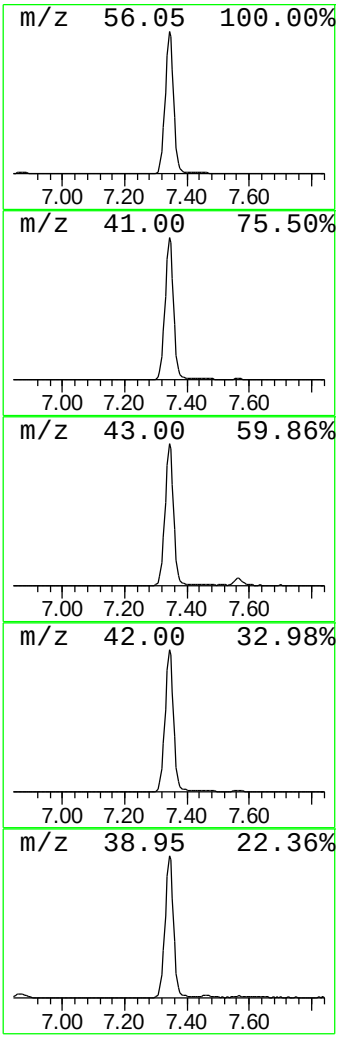
****

Peak Number 7 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	159.40 ug/l	3514180	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	12
4	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9
5	Isobutylene epoxide	72	C4H8O	000558-30-5	9





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Sample : J3064-04
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ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

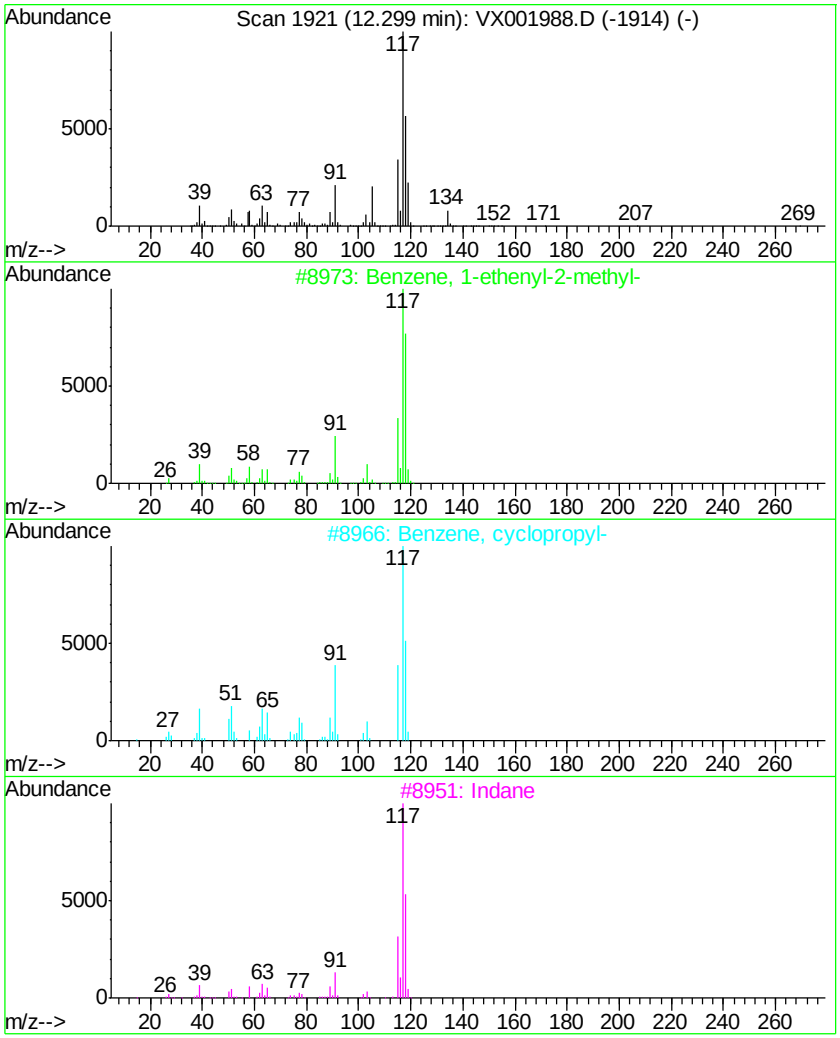
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

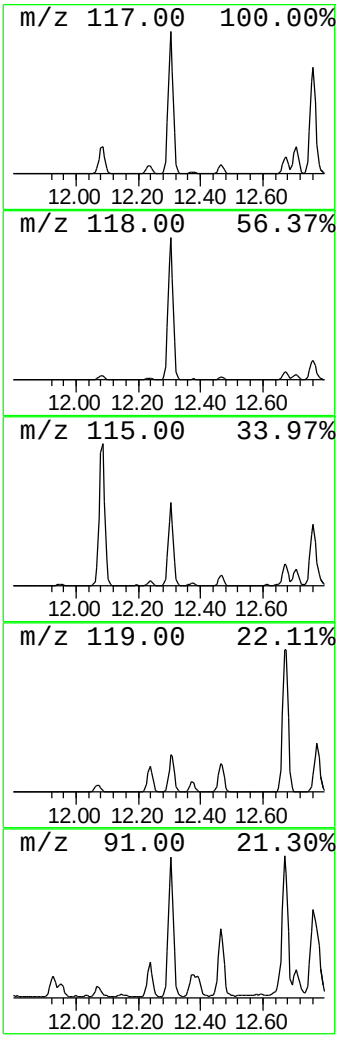
****

Peak Number 8 Benzene, 1-ethenyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	31.38 ug/l	966748	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	91
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3	Indane	118	C9H10	000496-11-7	64
4	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	50
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	50





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001988.D
Acq On : 25 May 2018 20:10
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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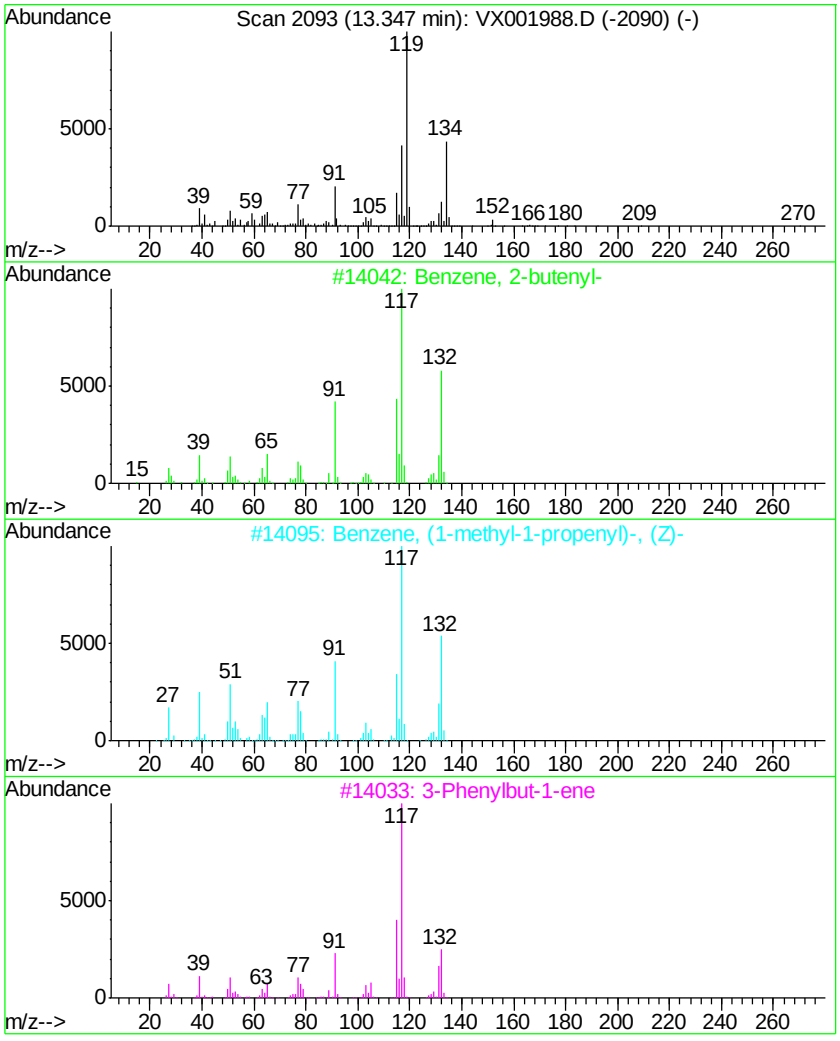
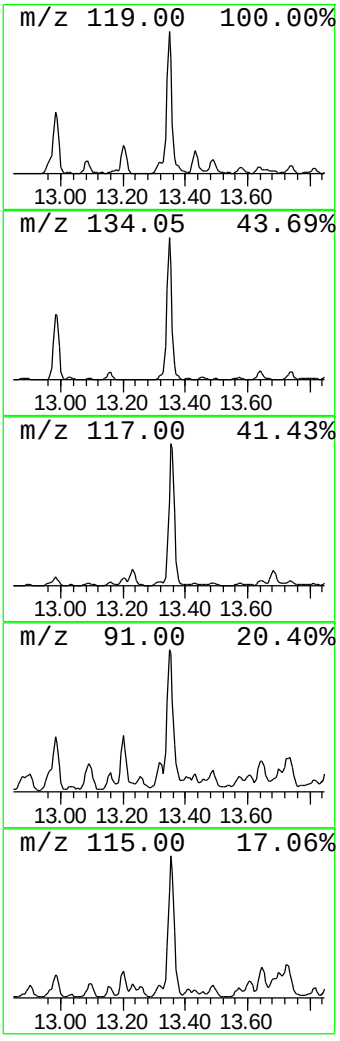
Peak Number 9 Benzene, 2-butenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	77.12 ug/l	2376050	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-butenyl-	132	C10H12	001560-06-1	64
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	64
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	60
4	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	50
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	50





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001988.D
Acq On : 25 May 2018 20:10
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

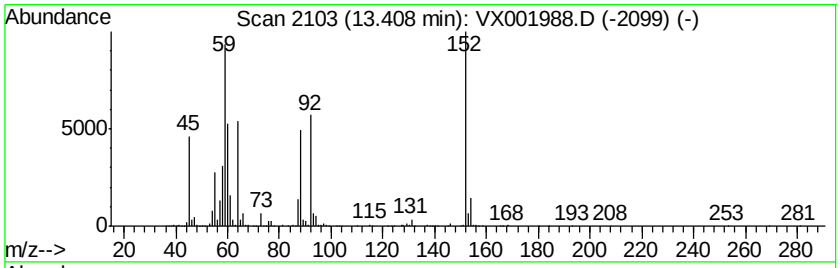
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

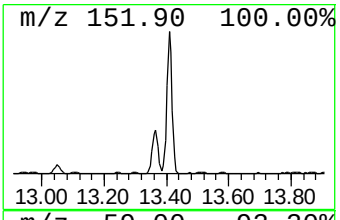
****

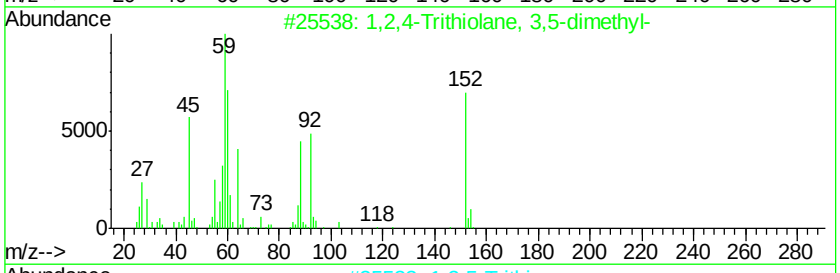
Peak Number 10 1,2,4-Trithiolane, 3,5-dime... Concentration Rank 9

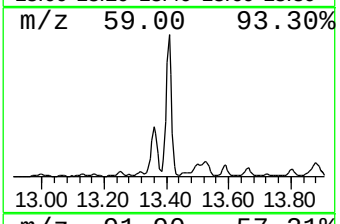
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.41	49.97 ug/l	1539470	1,4-Dichlorobenzene-d4	12.09

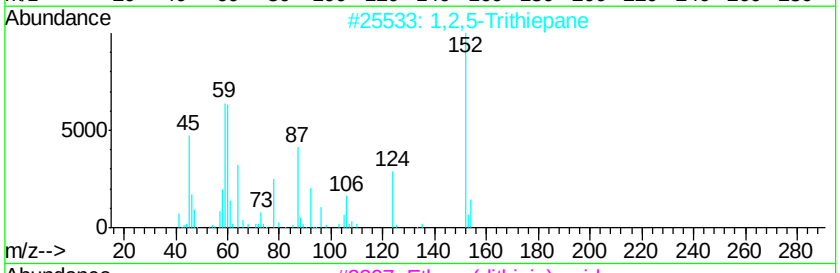
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	96
2	1,2,5-Trithiepane	152	C4H8S3	006576-93-8	38
3	Ethane(dithioic) acid	92	C2H4S2	000594-03-6	22
4	1,3,5-Trithiocycloheptane	152	C4H8S3	081451-19-6	12
5	Thiirane, 2,3-dimethyl-, trans-	88	C4H8S	005955-98-6	12

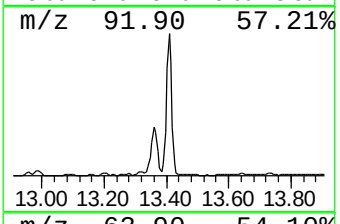


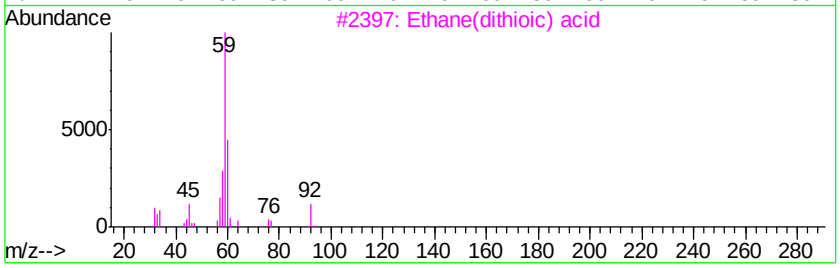


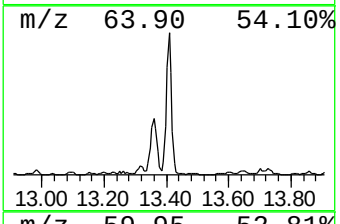


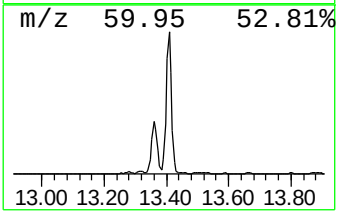












Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX052518\
Data File : VX001988.D
Acq On : 25 May 2018 20:10
Operator : JC/MD
Sample : J3064-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-02

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X052418W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.32	161.9	ug/l	2763330	1	5.67	853549	50.0
Ethanol	2.17	1762.1	ug/l	30081100	1	5.67	853549	50.0
Ethanethiol	2.27	60.6	ug/l	1033840	1	5.67	853549	50.0
1-Propanol	4.03	67.8	ug/l	1156890	1	5.67	853549	50.0
1-Butanol	7.34	159.4	ug/l	3514180	2	6.87	1102280	50.0
Benzene, 1-etheny...	12.30	31.4	ug/l	966748	4	12.09	1540490	50.0
Benzene, 2-butenyl-	13.35	77.1	ug/l	2376050	4	12.09	1540490	50.0
1,2,4-Trithiolane...	13.41	50.0	ug/l	1539470	4	12.09	1540490	50.0