

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV122319\
 Data File : VV014176.D
 Acq On : 23 Dec 2019 22:43
 Operator : SY/MD
 Sample : K6404-16
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFE05

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.116	5	8	27	rVB2	1046740	1551144	100.00%	11.839%
2	1.187	28	30	36	rVV2	77820	70073	4.52%	0.535%
3	1.225	38	42	45	rBV2	86573	61381	3.96%	0.468%
4	1.283	59	60	63	rVB2	33100	17475	1.13%	0.133%
5	1.319	63	71	77	rVB2	271557	346587	22.34%	2.645%
6	1.393	91	94	98	rVB2	32149	24524	1.58%	0.187%
7	1.479	114	121	134	rBV	420245	491712	31.70%	3.753%
8	1.582	147	153	165	rVB	162192	199847	12.88%	1.525%
9	1.788	214	217	222	rVB	25591	19823	1.28%	0.151%
10	2.000	279	283	291	rVB8	22538	28516	1.84%	0.218%
11	2.055	291	300	311	rVV	154251	215457	13.89%	1.644%
12	2.132	314	324	334	rVV	264200	393138	25.35%	3.001%
13	2.184	335	340	350	rVB	25015	40054	2.58%	0.306%
14	2.322	371	383	395	rBV	136820	209672	13.52%	1.600%
15	2.987	586	590	604	rVB	8624	17796	1.15%	0.136%
16	3.730	804	821	839	rBV2	26358	71698	4.62%	0.547%
17	3.926	870	882	913	rBV2	111345	303364	19.56%	2.315%
18	4.396	1013	1028	1048	rBV3	220960	535236	34.51%	4.085%
19	5.093	1225	1245	1269	rBV2	443831	1108059	71.43%	8.457%
20	5.659	1405	1421	1443	rBV	430006	864410	55.73%	6.598%
21	6.113	1545	1562	1582	rBV	250844	524427	33.81%	4.003%
22	7.026	1832	1846	1865	rBV	103346	196740	12.68%	1.502%
23	7.357	1936	1949	1965	rBV	507799	886433	57.15%	6.766%
24	7.431	1966	1972	1984	rVB3	16963	31660	2.04%	0.242%
25	7.563	2002	2013	2024	rBV	46001	83645	5.39%	0.638%
26	7.662	2034	2044	2059	rBV	63072	108365	6.99%	0.827%
27	8.132	2178	2190	2218	rBV	387893	854087	55.06%	6.519%
28	8.283	2229	2237	2250	rVB2	30971	55829	3.60%	0.426%
29	8.891	2412	2426	2451	rBV	670911	1107203	71.38%	8.451%
30	10.254	2831	2850	2866	rVB	180726	309632	19.96%	2.363%
31	11.196	3134	3143	3155	rBV10	19497	36028	2.32%	0.275%
32	11.289	3159	3172	3190	rBV	676069	1059232	68.29%	8.085%
33	11.392	3195	3204	3213	rVB7	25339	44553	2.87%	0.340%
34	11.665	3277	3289	3308	rBV	509360	808690	52.14%	6.172%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

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Title : TRACE VOA SOM01.0

35	11.804	3322	3332	3346	rBV	119557	185781	11.98%	1.418%
36	12.389	3504	3514	3534	rBV2	95877	160583	10.35%	1.226%
37	12.919	3671	3679	3687	rVB	15282	22846	1.47%	0.174%
38	13.202	3754	3767	3778	rBV9	19097	40089	2.58%	0.306%
39	13.926	3981	3992	4000	rBV9	8200	15962	1.03%	0.122%

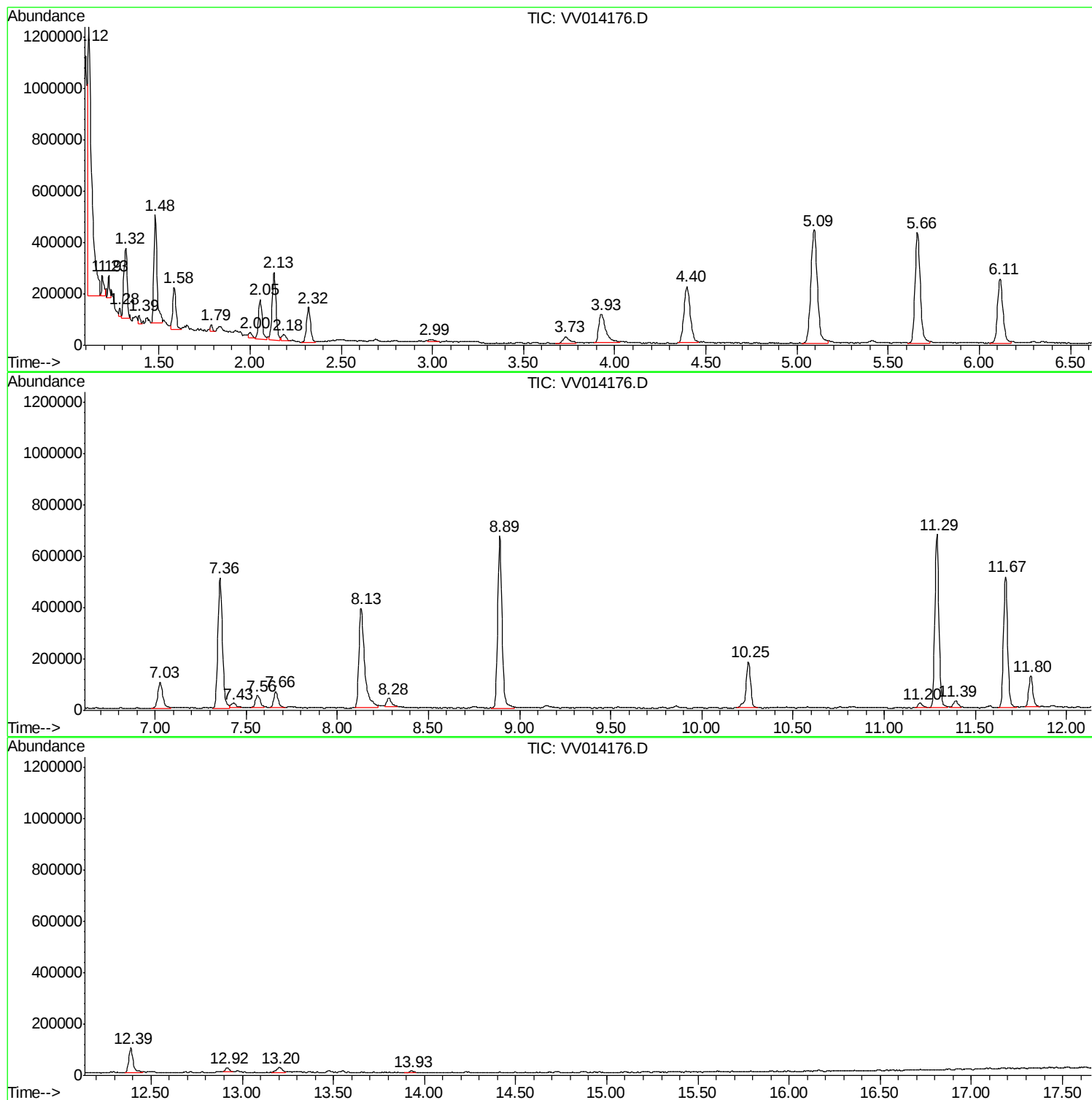
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Quant Title : TRACE VOA SOM01.0

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



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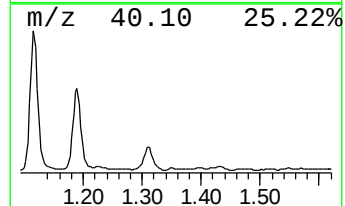
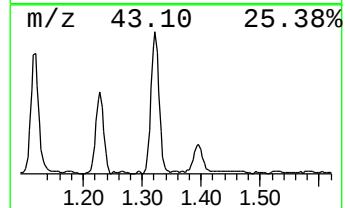
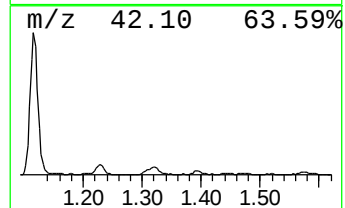
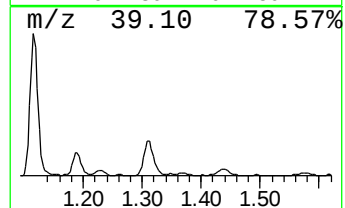
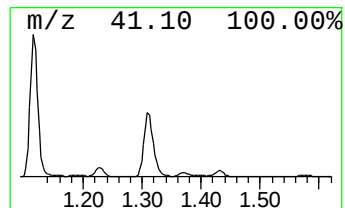
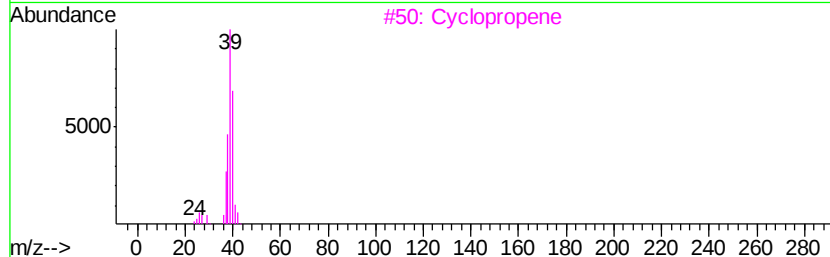
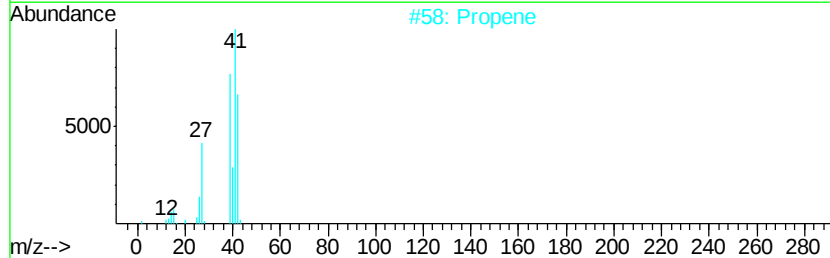
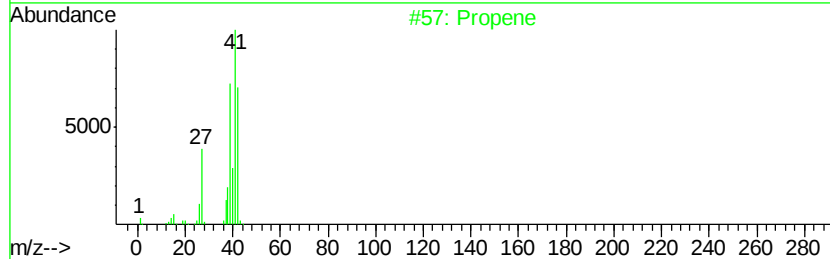
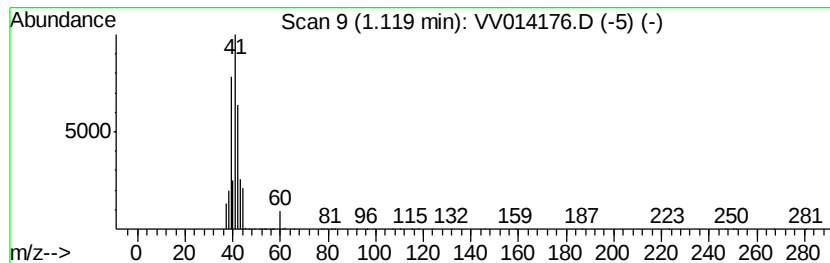
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Cyclic1.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	8.97 ug/L	1551140	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propene	42	C3H6	000115-07-1	90
2		Propene	42	C3H6	000115-07-1	42
3		Cyclopropene	40	C3H4	002781-85-3	9
4		Cyclopropane	42	C3H6	000075-19-4	9
5		Cyclopropane	42	C3H6	000075-19-4	9



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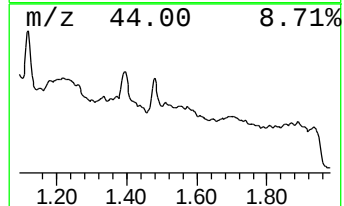
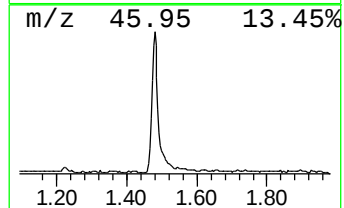
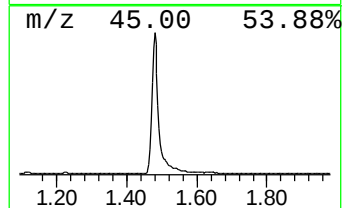
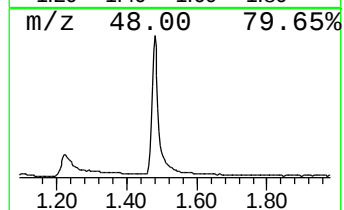
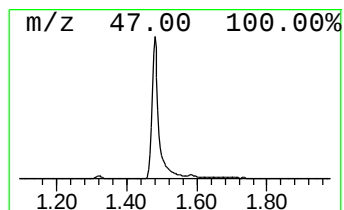
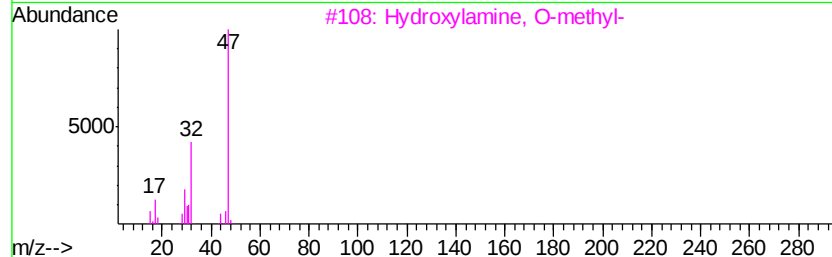
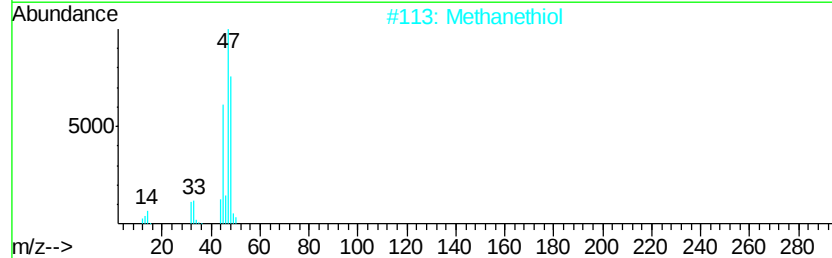
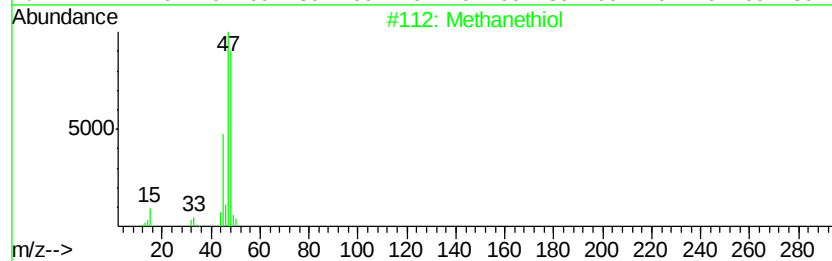
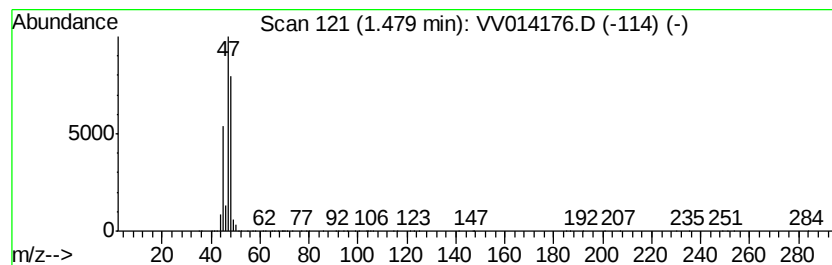
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	2.84 ug/L	491712	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethiol	48	CH4S	000074-93-1	90
2		Methanethiol	48	CH4S	000074-93-1	90
3		Hvdroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4		Hvdroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5		Ethane, fluoro-	48	C2H5F	000353-36-6	4



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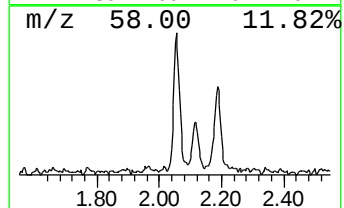
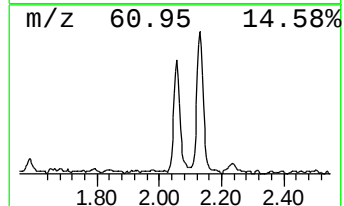
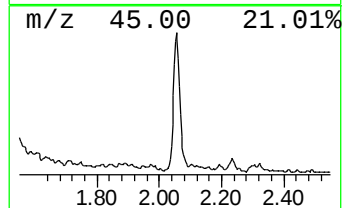
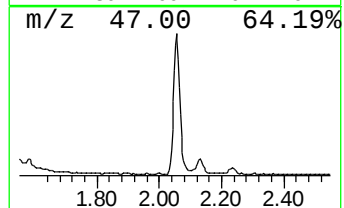
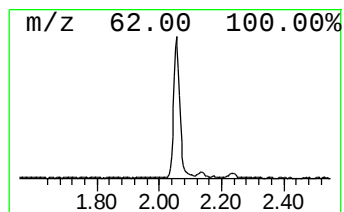
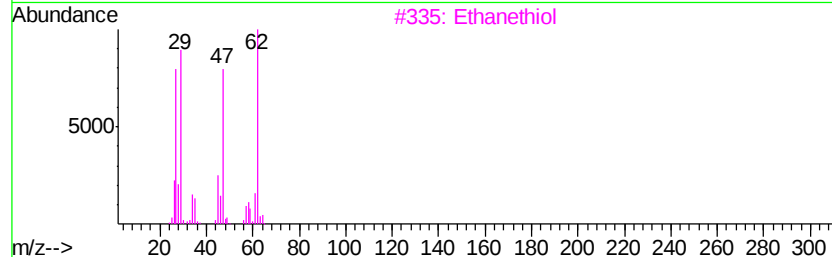
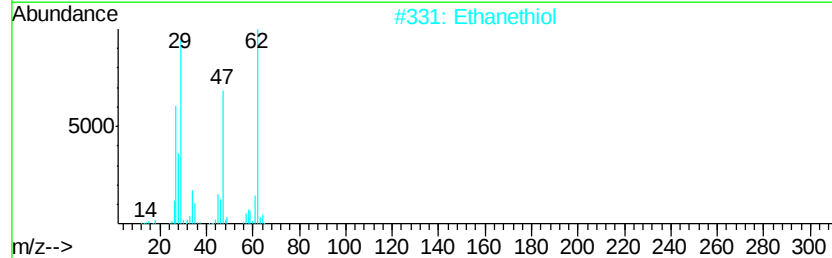
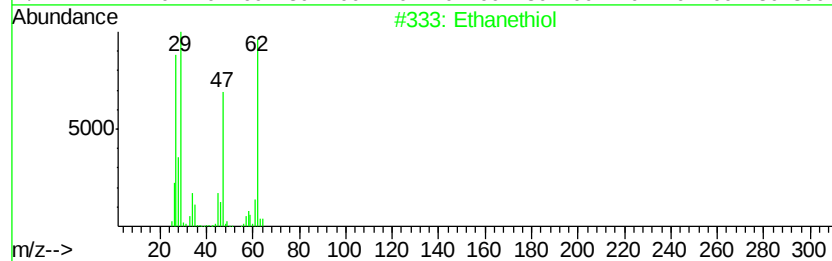
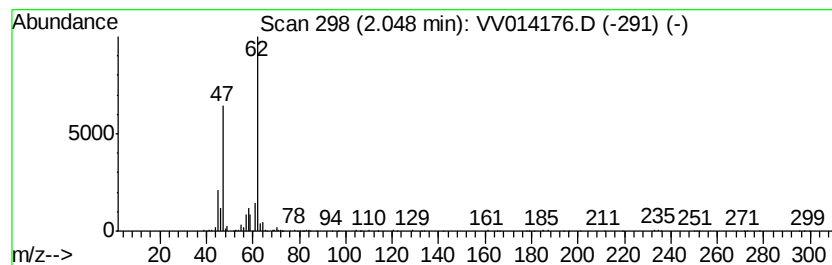
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	1.25 ug/L	215457	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanethiol	62	C2H6S	000075-08-1	91
2		Ethanethiol	62	C2H6S	000075-08-1	91
3		Ethanethiol	62	C2H6S	000075-08-1	91
4		Ethanethiol	62	C2H6S	000075-08-1	91
5		Ethanethiol	62	C2H6S	000075-08-1	90



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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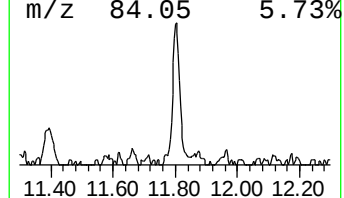
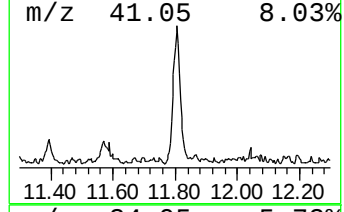
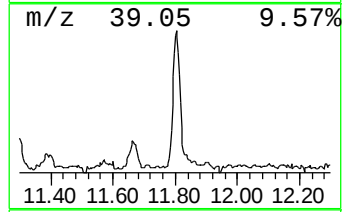
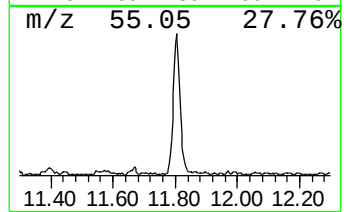
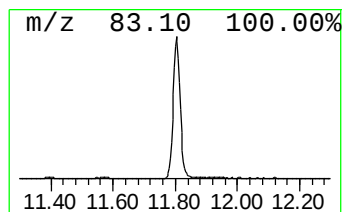
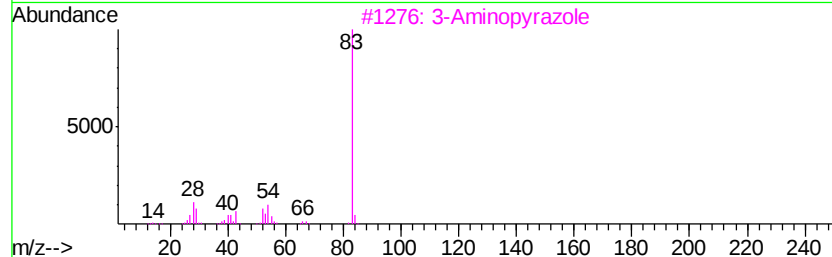
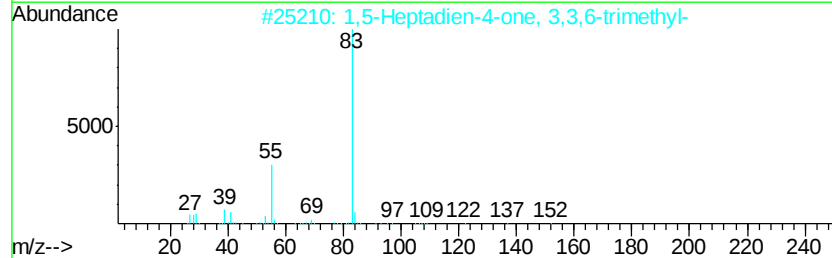
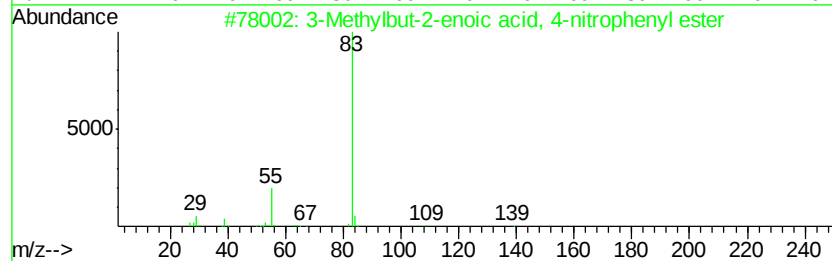
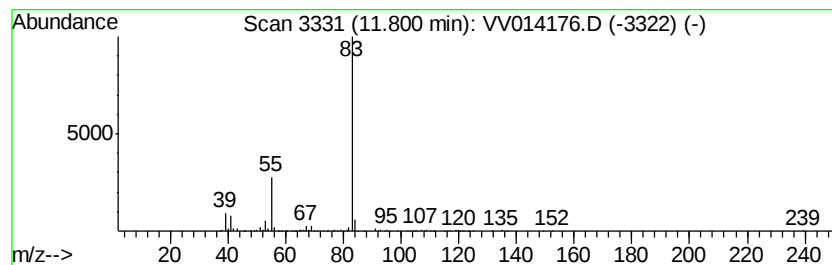
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 3-Methylbut-2-enoic acid, 4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	0.88 ug/L	185781	1,4-Dichlorobenzene-d4	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Methylbut-2-enoic acid, 4-nitr...	221	C11H11N04	1000307-59-8	72
2		1,5-Heptadien-4-one, 3,3,6-trime...	152	C10H16O	000546-49-6	72
3		3-Aminopyrazole	83	C3H5N3	001820-80-0	72
4		1-Imidazol-1-yl-3-methylbut-2-en...	150	C8H10N2O	061985-22-6	56
5		4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	56



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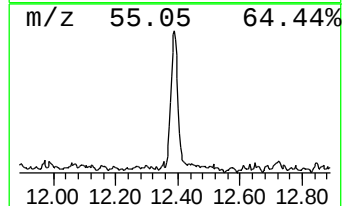
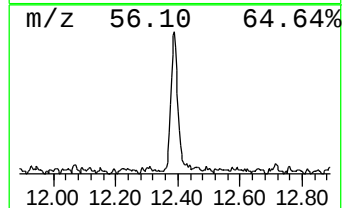
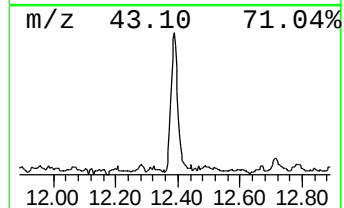
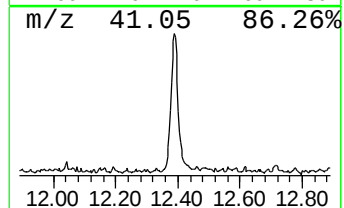
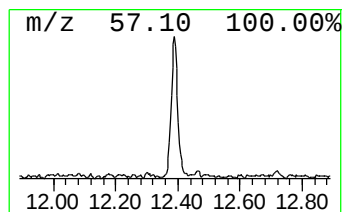
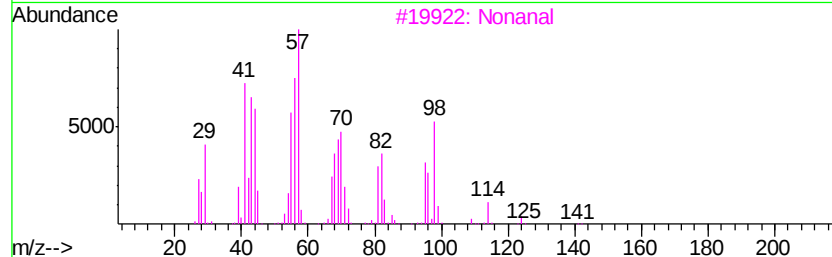
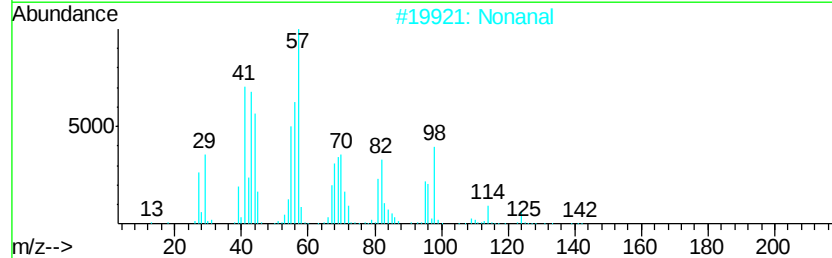
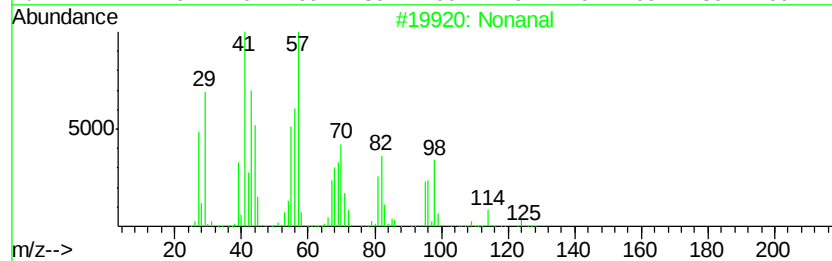
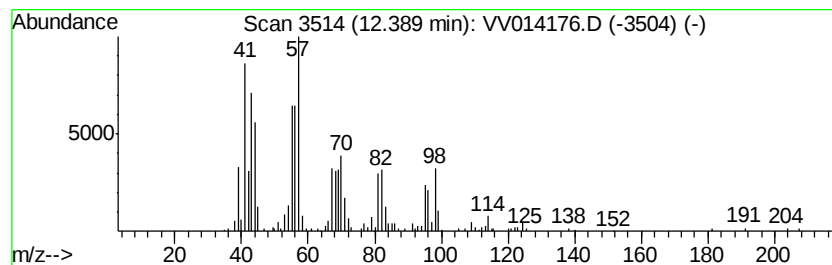
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Peak Number 6 Nonanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	0.76 ug/L	160583	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	91
2		Nonanal	142	C9H18O	000124-19-6	90
3		Nonanal	142	C9H18O	000124-19-6	86
4		Cycloheptane	98	C7H14	000291-64-5	38
5		1-Octene, 3,7-dimethyl-	140	C10H20	004984-01-4	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV122319\
Data File : VV014176.D
Acq On : 23 Dec 2019 22:43
Operator : SY/MD
Sample : K6404-16
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFE05

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR122319WMA.M
Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.12	9.0	ug/L	1551140	1	5.66	864410	5.0
Methanethiol	1.48	2.8	ug/L	491712	1	5.66	864410	5.0
Ethanethiol	2.05	1.3	ug/L	215457	1	5.66	864410	5.0
3-Methylbut-2-eno...	11.80	0.9	ug/L	185781	3	11.29	1059230	5.0
Nonanal	12.39	0.8	ug/L	160583	3	11.29	1059230	5.0