

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017026.D
 Acq On : 22 Jun 2020 18:58
 Operator : SY/MD
 Sample : L3067-05
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXG2

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\SOMVTR061720WMA.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	1.113	3	7	15	rVB2	24518	22566	3.05%	0.266%
2	1.315	62	70	81	rVB2	130981	135411	18.29%	1.595%
3	1.438	92	108	123	rBV2	38139	161075	21.75%	1.897%
4	1.576	145	151	166	rVB	88051	115386	15.58%	1.359%
5	1.785	213	216	224	rVB3	8433	8559	1.16%	0.101%
6	2.119	311	320	331	rBV	167227	233835	31.58%	2.754%
7	2.775	513	524	533	rBV2	58707	99999	13.50%	1.178%
8	2.984	579	589	600	rVB2	4417	9201	1.24%	0.108%
9	3.206	648	658	671	rVB	30617	67337	9.09%	0.793%
10	3.319	680	693	706	rVB2	21424	48539	6.55%	0.572%
11	3.939	870	886	928	rBV3	235169	733644	99.07%	8.640%
12	4.376	1003	1022	1044	rVB	134158	328692	44.39%	3.871%
13	5.071	1216	1238	1246	rBV3	318659	740530	100.00%	8.721%
14	5.122	1247	1254	1277	rVB	337838	713819	96.39%	8.406%
15	5.640	1400	1415	1434	rBV	238289	476787	64.38%	5.615%
16	5.939	1496	1508	1522	rBV	9519	24281	3.28%	0.286%
17	6.093	1536	1556	1573	rBV	168788	352805	47.64%	4.155%
18	6.347	1625	1635	1643	rVB6	7318	13789	1.86%	0.162%
19	6.778	1758	1769	1774	rBV10	6059	9749	1.32%	0.115%
20	6.958	1815	1825	1832	rBV4	8933	17023	2.30%	0.200%
21	7.010	1832	1841	1856	rVB2	65957	116896	15.79%	1.377%
22	7.167	1877	1890	1900	rBV3	21435	42596	5.75%	0.502%
23	7.338	1929	1943	1960	rBV	373746	655899	88.57%	7.724%
24	7.643	2026	2038	2056	rBV	39975	76478	10.33%	0.901%
25	8.113	2173	2184	2218	rBV2	347952	665185	89.83%	7.834%
26	8.871	2404	2420	2440	rBV	356935	588530	79.47%	6.931%
27	9.756	2683	2695	2710	rBV2	50287	85912	11.60%	1.012%
28	9.955	2747	2757	2766	rBV2	11411	18149	2.45%	0.214%
29	10.238	2833	2845	2856	rBV	121267	196988	26.60%	2.320%
30	10.299	2856	2864	2871	rVB6	6398	11985	1.62%	0.141%
31	10.376	2879	2888	2900	rBV5	16354	25594	3.46%	0.301%
32	10.502	2917	2927	2936	rBV5	18245	29209	3.94%	0.344%
33	11.270	3152	3166	3182	rBV	375434	589702	79.63%	6.945%
34	11.550	3243	3253	3271	rVB	118570	198641	26.82%	2.339%

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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	11.646	3271	3283	3300	rBV	391123	653698	88.27%	7.698%
36	11.942	3365	3375	3384	rBV6	8872	16546	2.23%	0.195%
37	12.135	3425	3435	3444	rVB9	4958	9176	1.24%	0.108%
38	12.315	3482	3491	3503	rBV3	12569	22372	3.02%	0.263%
39	12.910	3666	3676	3683	rBV7	7525	11515	1.55%	0.136%
40	13.485	3845	3855	3862	rBV6	17416	33280	4.49%	0.392%
41	13.627	3888	3899	3911	rBV3	49538	83207	11.24%	0.980%
42	13.833	3950	3963	3974	rBV3	8895	16313	2.20%	0.192%
43	14.026	4017	4023	4031	rVB5	11756	17869	2.41%	0.210%
44	14.460	4150	4158	4170	rVB5	7152	12523	1.69%	0.147%

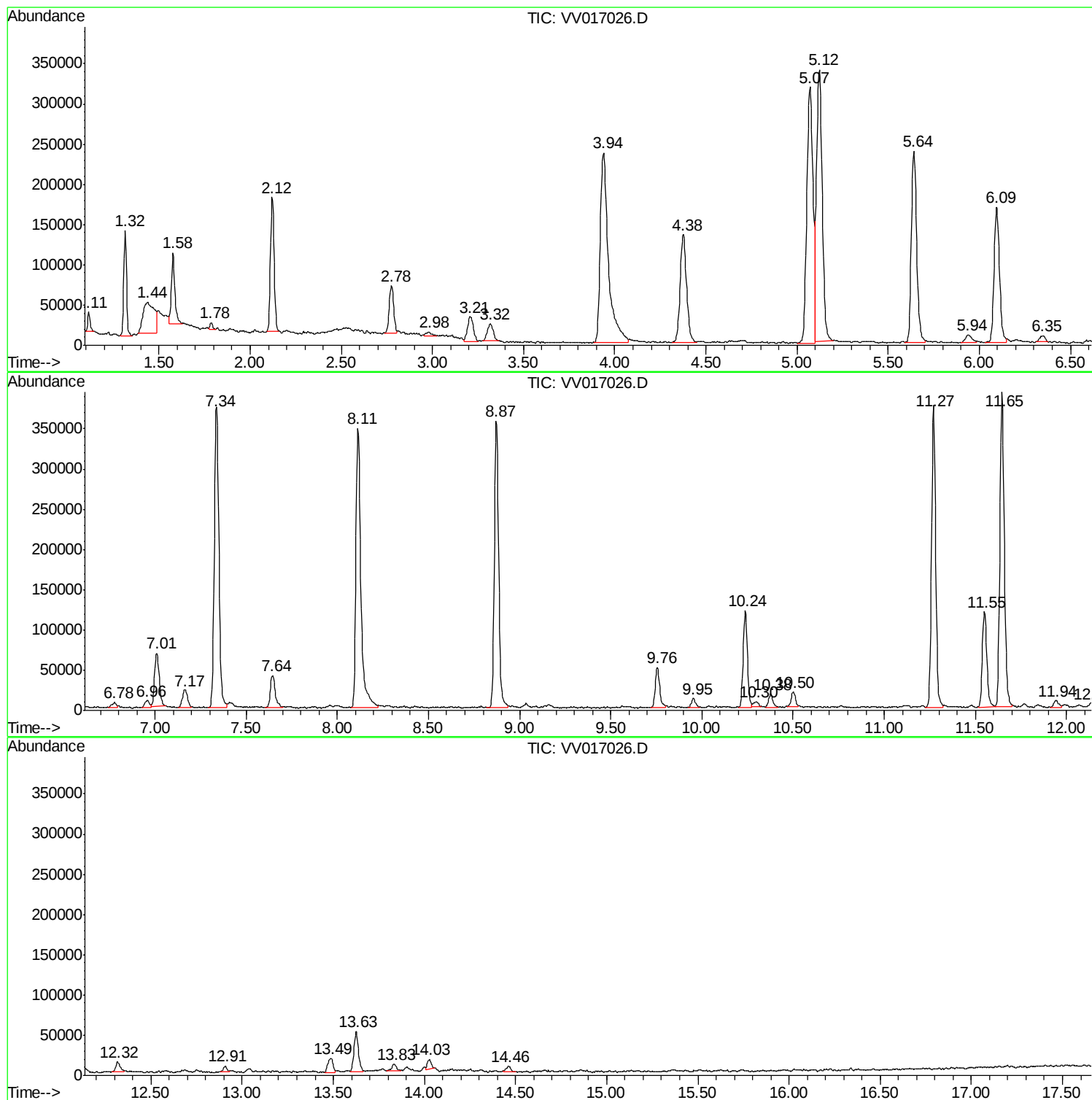
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Quant Title : TRACE VOA SOM01.0

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



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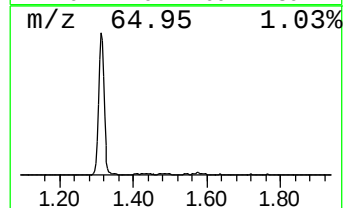
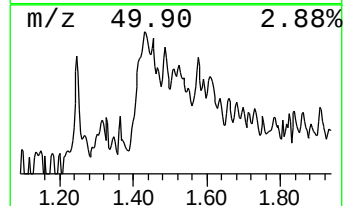
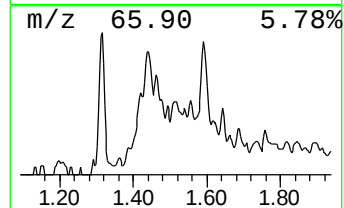
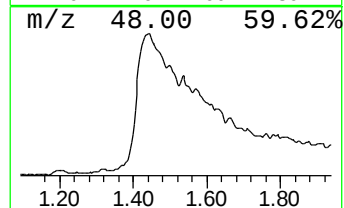
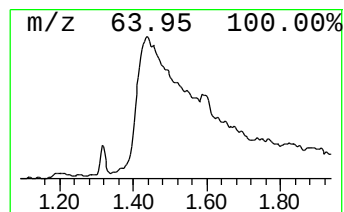
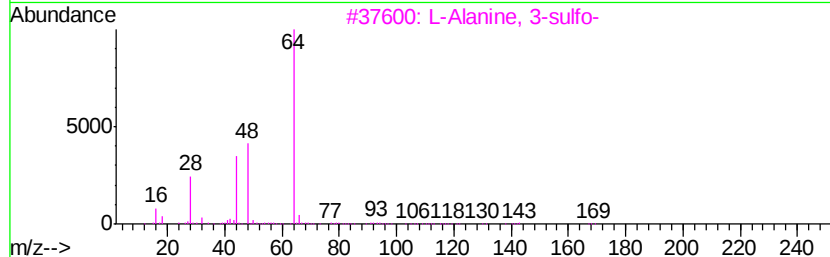
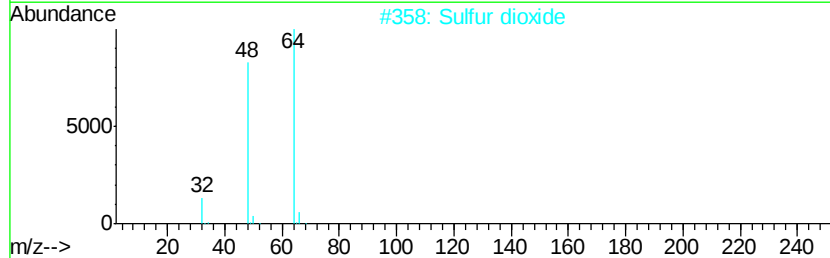
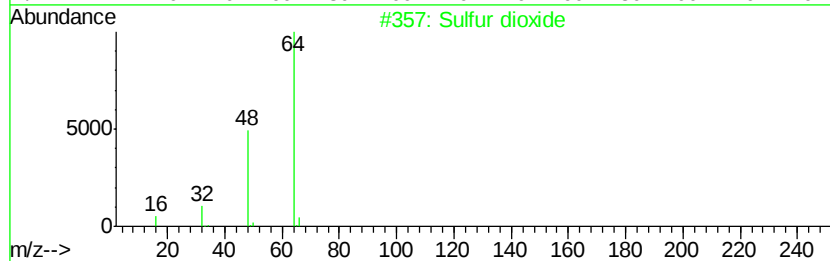
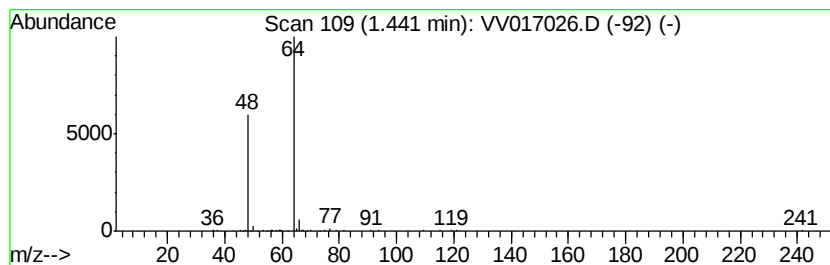
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.44	1.69 ug/L	161075	1,4-Difluorobenzene	5.64
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 02S	007446-09-5	90
2	Sulfur dioxide	64 02S	007446-09-5	74
3	L-Alanine, 3-sulfo-	169 C3H7N05S	000498-40-8	64
4	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	64
5	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	64



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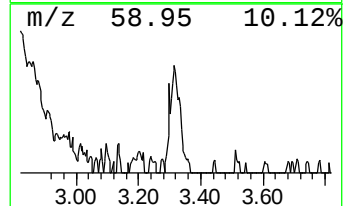
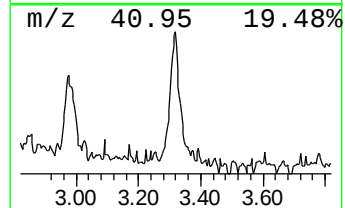
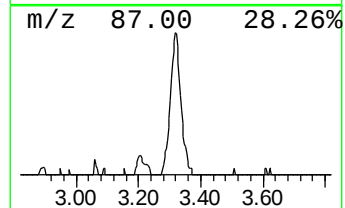
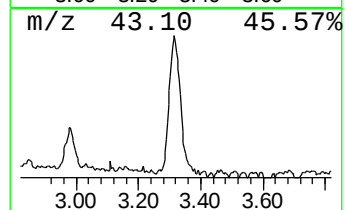
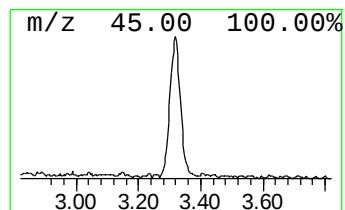
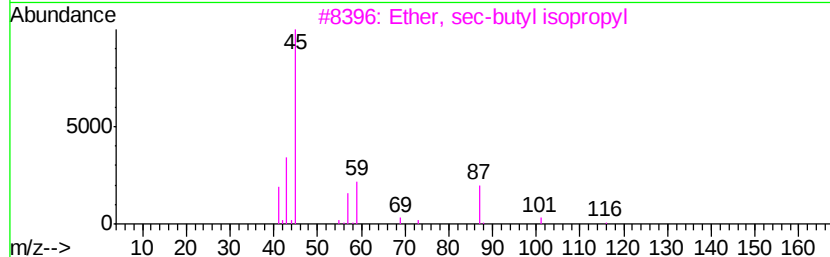
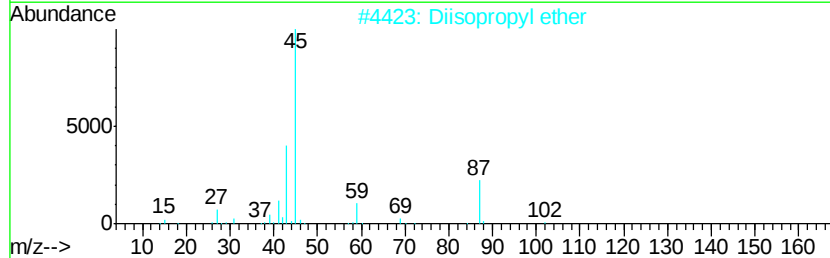
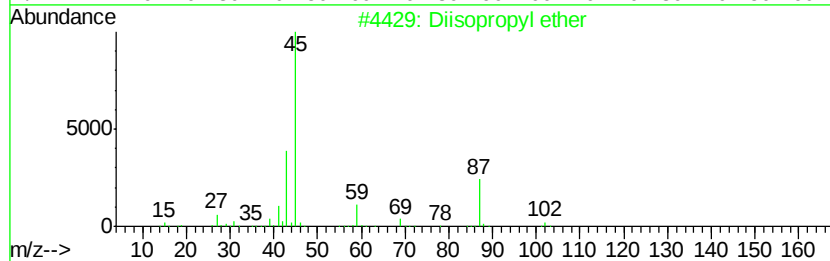
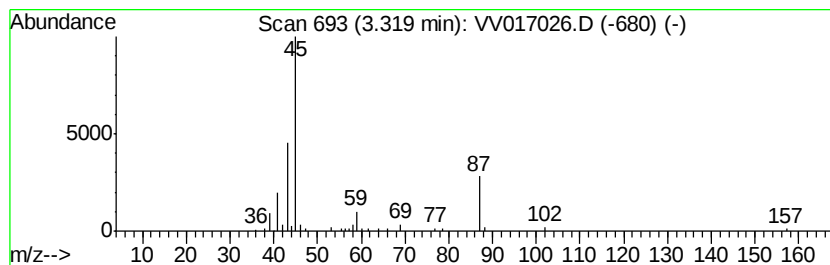
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Diisopropyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.32	0.51 ug/L	48539	1,4-Difluorobenzene	5.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl ether	102	C6H14O	000108-20-3	91
2	Diisopropyl ether	102	C6H14O	000108-20-3	78
3	Ether, sec-butyl isopropyl	116	C7H16O	018641-81-1	72
4	Diisopropyl ether	102	C6H14O	000108-20-3	64
5	Propane, 2,2'-[ethylidenebis(oxy...	146	C8H18O2	004285-59-0	56



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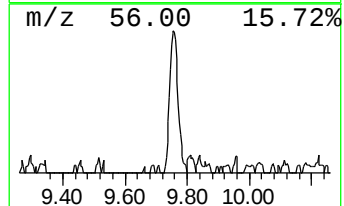
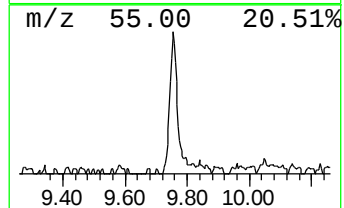
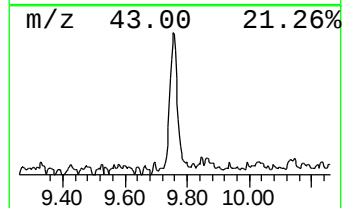
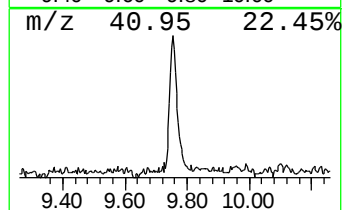
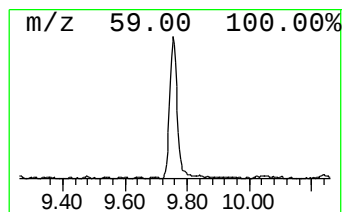
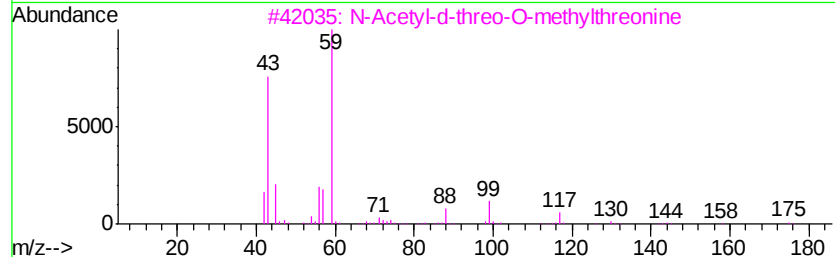
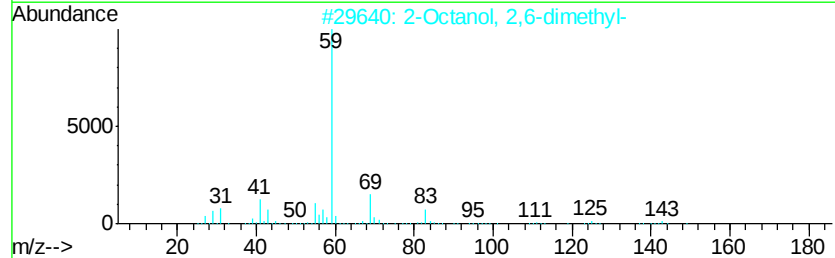
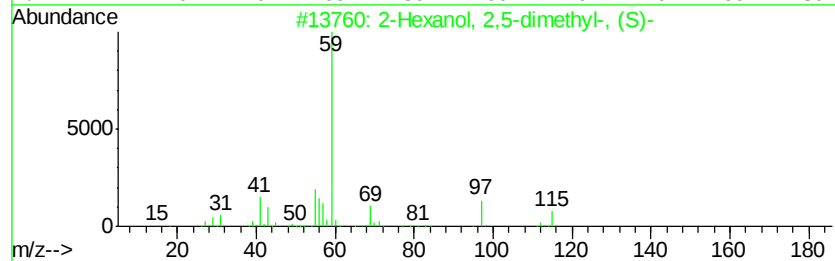
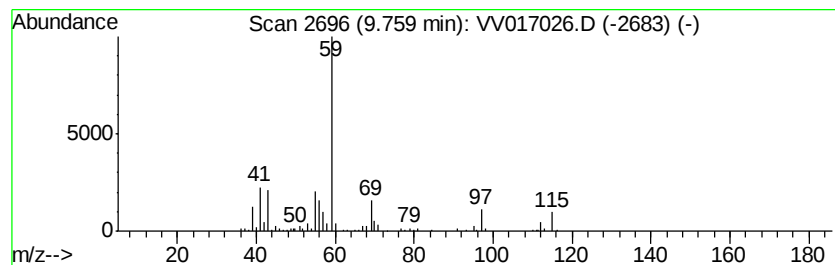
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	0.73 ug/L	85912	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	72
2			2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	64
3			N-Acetyl-d-threo-O-methylthreonine	175	C7H13NO4	1000214-70-5	53
4			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50
5			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	50



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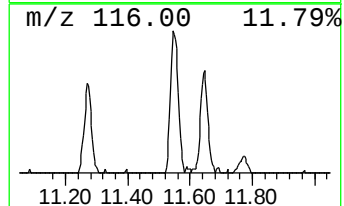
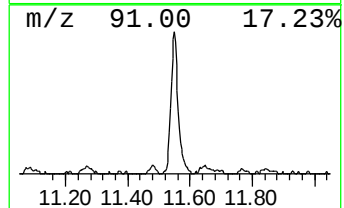
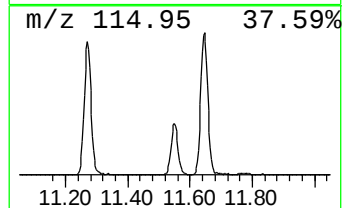
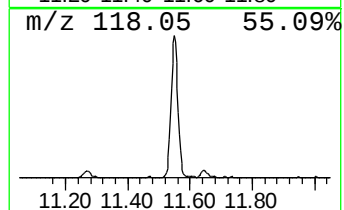
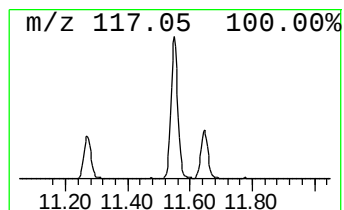
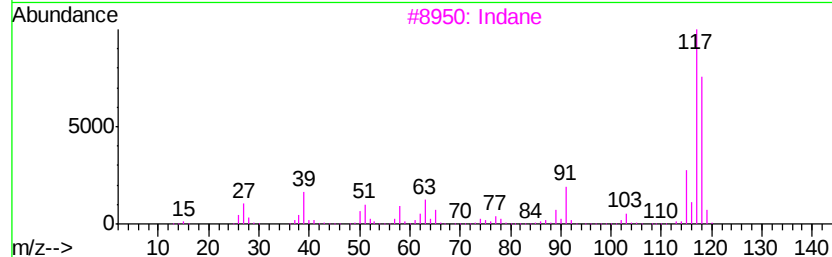
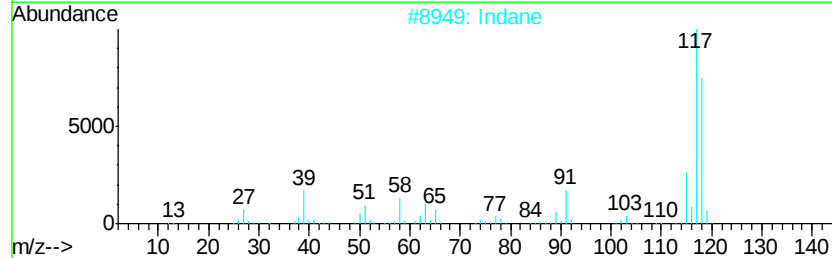
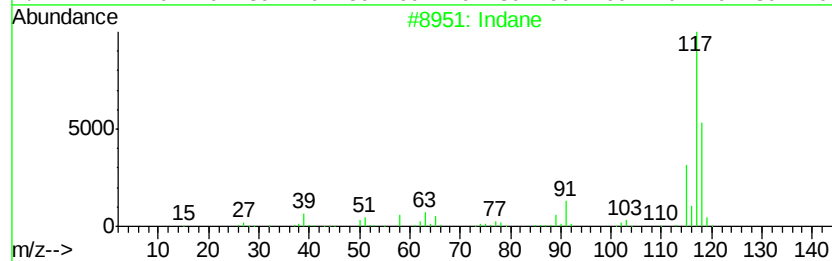
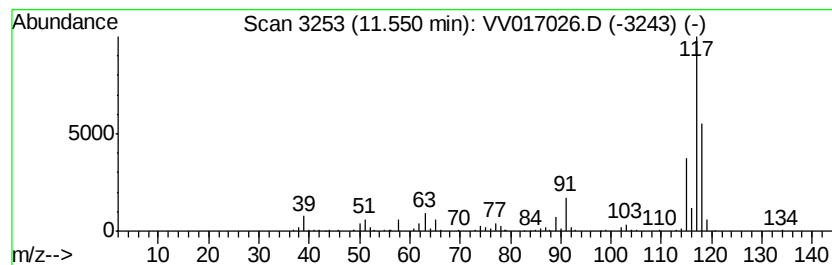
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	1.68 ug/L	198641	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Indane	118	C9H10	000496-11-7	95
2		Indane	118	C9H10	000496-11-7	91
3		Indane	118	C9H10	000496-11-7	90
4		Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	83
5		Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83



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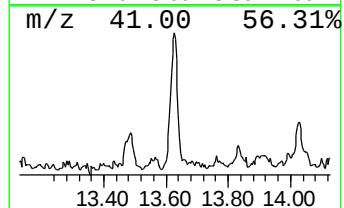
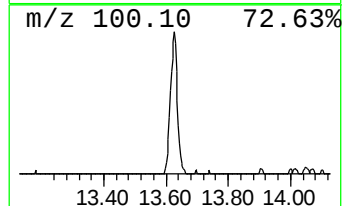
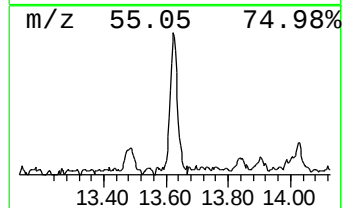
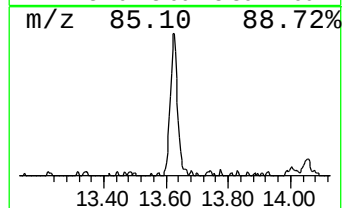
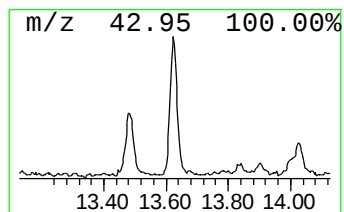
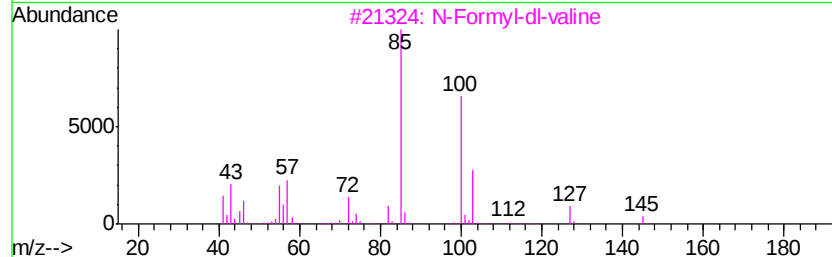
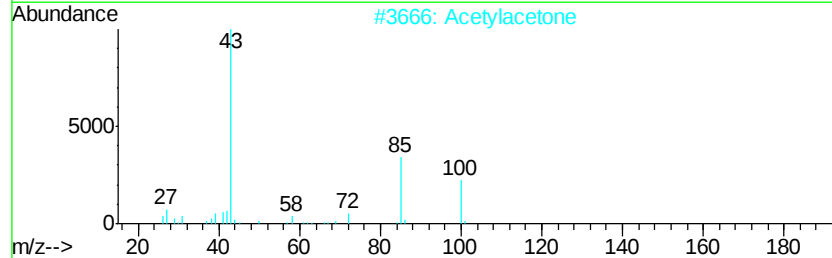
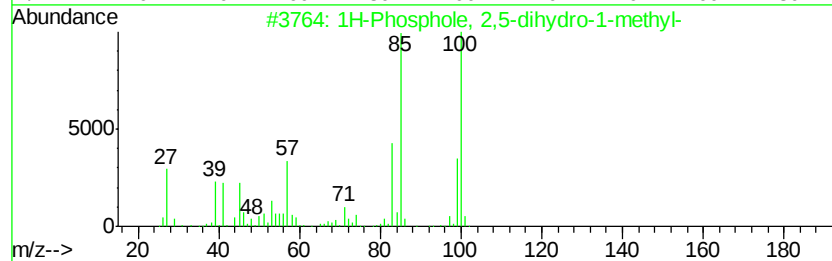
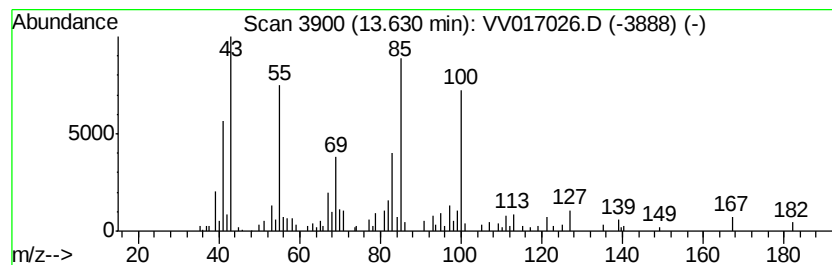
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 1H-Phosphole, 2,5-dihydro-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	0.71 ug/L	83207	1,4-Dichlorobenzene-d4	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Phosphole, 2,5-dihydro-1-methyl-	100	C5H9P	000872-37-7	74
2		Acetylacetone	100	C5H8O2	000123-54-6	47
3		N-Formyl-dl-valine	145	C6H11NO3	004289-96-7	47
4		Propionaldehyde, ethylhydrazone	100	C5H12N2	007422-92-6	47
5		7-Methyloctane-2,4-dione, enol form	156	C9H16O2	000999-05-3	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV062320\
Data File : VV017026.D
Acq On : 22 Jun 2020 18:58
Operator : SY/MD
Sample : L3067-05
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXG2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.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
Sulfur dioxide	1.44	1.7	ug/L	161075	1	5.64	476787	5.0
Diisopropyl ether	3.32	0.5	ug/L	48539	1	5.64	476787	5.0
2-Hexanol, 2,5-di...	9.76	0.7	ug/L	85912	2	8.87	588530	5.0
Indane	11.55	1.7	ug/L	198641	3	11.27	589702	5.0
1H-Phosphole, 2,5...	13.63	0.7	ug/L	83207	3	11.27	589702	5.0