

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
 Data File : VV011234.D
 Acq On : 05 Jun 2019 17:16
 Operator : SY/MD
 Sample : K3197-06
 Misc : 25ML/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9P47

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\SOMVTR060419WMA.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	3	8	19	rVB	60187	55232	7.30%	0.700%
2	1.238	36	46	51	rBV	376505	756965	100.00%	9.598%
3	1.579	147	152	164	rVB	84861	100504	13.28%	1.274%
4	2.123	313	321	332	rVB	189952	263615	34.83%	3.342%
5	2.316	375	381	386	rBV2	6495	8708	1.15%	0.110%
6	2.650	478	485	498	rVB2	19122	36592	4.83%	0.464%
7	3.984	883	900	922	rBV	42078	183115	24.19%	2.322%
8	4.399	1011	1029	1053	rBV	109620	272389	35.98%	3.454%
9	5.090	1229	1244	1262	rBV2	276917	642625	84.89%	8.148%
10	5.663	1407	1422	1445	rBV	203148	419275	55.39%	5.316%
11	6.116	1539	1563	1583	rBV2	152389	327971	43.33%	4.158%
12	6.634	1713	1724	1737	rBV2	13216	27253	3.60%	0.346%
13	7.029	1834	1847	1863	rBV2	74578	136411	18.02%	1.730%
14	7.357	1935	1949	1967	rVV	322531	573292	75.74%	7.269%
15	7.431	1967	1972	1988	rVB6	9918	21235	2.81%	0.269%
16	7.666	2035	2045	2057	rBV	42114	73954	9.77%	0.938%
17	8.138	2180	2192	2203	rBV	302245	551853	72.90%	6.997%
18	8.190	2204	2208	2222	rVB	53220	98023	12.95%	1.243%
19	8.894	2414	2427	2454	rBV	300639	520540	68.77%	6.600%
20	9.142	2496	2504	2512	rBV2	15257	22250	2.94%	0.282%
21	9.428	2585	2593	2604	rBV2	17562	29638	3.92%	0.376%
22	9.646	2654	2661	2669	rVB2	6561	9855	1.30%	0.125%
23	9.749	2678	2693	2709	rBV	86692	151032	19.95%	1.915%
24	9.855	2718	2726	2732	rBV7	8228	13803	1.82%	0.175%
25	9.881	2732	2734	2749	rVB7	6940	11837	1.56%	0.150%
26	10.193	2822	2831	2841	rVB2	12306	20283	2.68%	0.257%
27	10.261	2841	2852	2867	rVB	97679	154779	20.45%	1.962%
28	10.476	2908	2919	2931	rBV	19064	32720	4.32%	0.415%
29	10.556	2936	2944	2955	rVB10	8628	16281	2.15%	0.206%
30	10.984	3065	3077	3088	rVB10	3883	8331	1.10%	0.106%
31	11.084	3097	3108	3126	rBV	206637	336931	44.51%	4.272%
32	11.293	3162	3173	3193	rVB	294366	474309	62.66%	6.014%
33	11.482	3227	3232	3245	rVB9	5751	10139	1.34%	0.129%
34	11.572	3249	3260	3279	rBV2	22864	49803	6.58%	0.631%

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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	11.669	3279	3290	3307	rVB	286685	462865	61.15%	5.869%
36	11.826	3331	3339	3346	rBV	6822	11278	1.49%	0.143%
37	12.039	3394	3405	3418	rVB	7190	14404	1.90%	0.183%
38	12.280	3470	3480	3491	rBV	159234	251608	33.24%	3.190%
39	12.389	3504	3514	3527	rBV2	62029	98201	12.97%	1.245%
40	12.508	3544	3551	3562	rVB2	7993	13904	1.84%	0.176%
41	13.486	3844	3855	3863	rBV10	6424	10975	1.45%	0.139%
42	13.678	3905	3915	3926	rBV2	47409	74718	9.87%	0.947%
43	15.164	4370	4377	4387	rBV10	9711	16206	2.14%	0.205%
44	15.611	4508	4516	4524	rVB9	8497	12360	1.63%	0.157%
45	16.238	4699	4711	4731	rBV3	122169	250013	33.03%	3.170%
46	16.363	4739	4750	4762	rVB	174518	258867	34.20%	3.282%

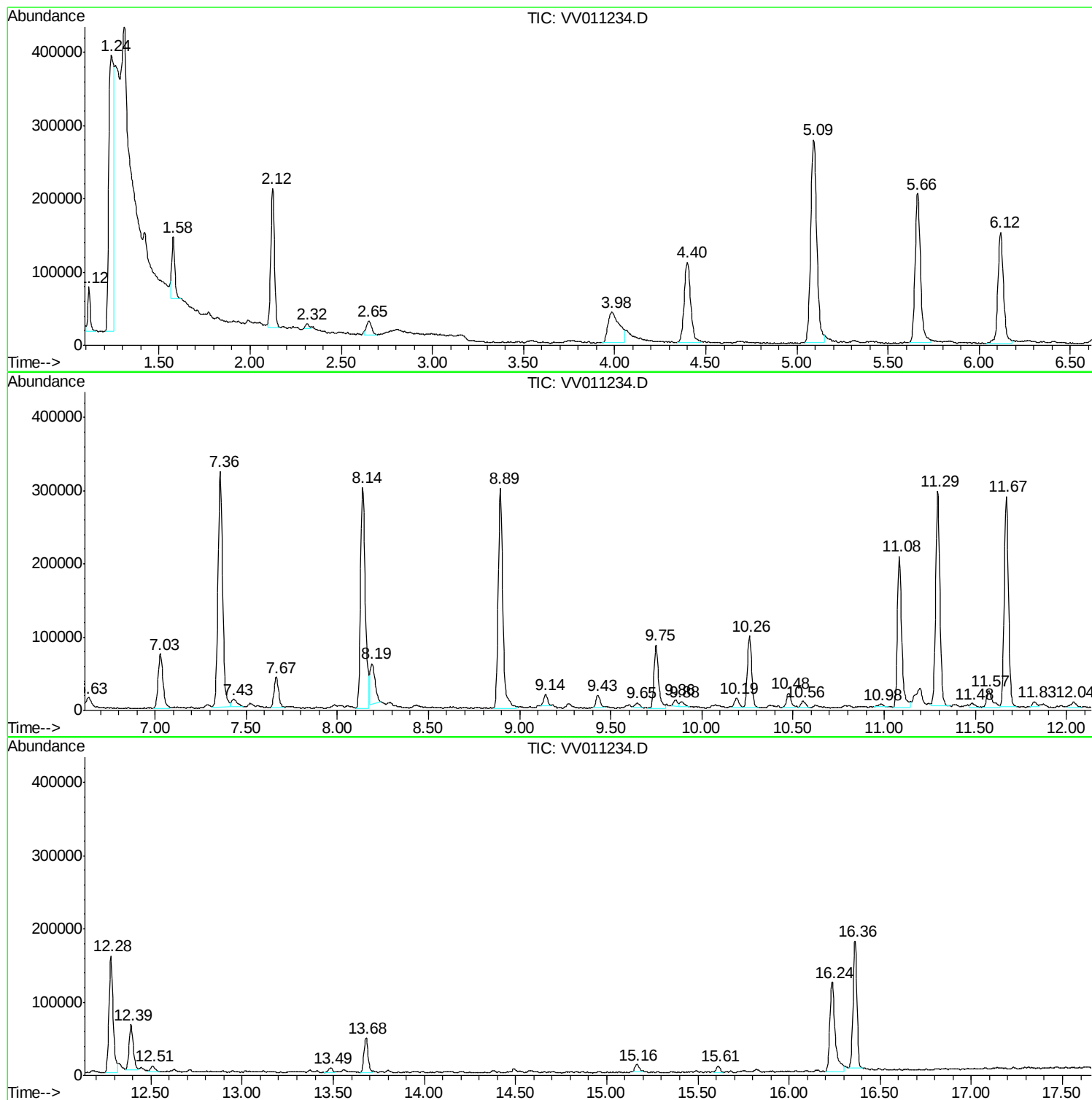
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MSVOA_V
ClientSampled :
F9P47

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
MSVOA_V
ClientSampleId :
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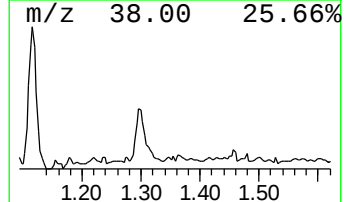
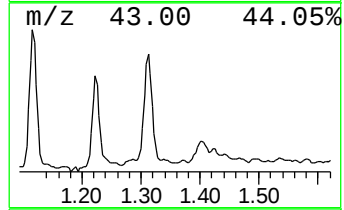
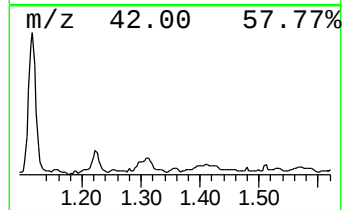
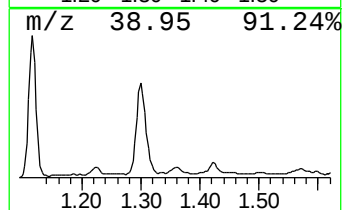
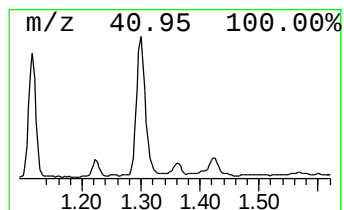
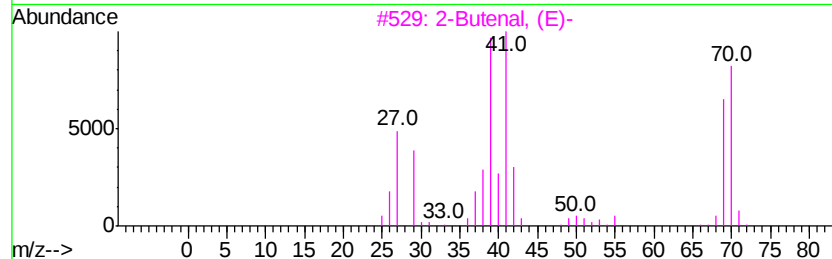
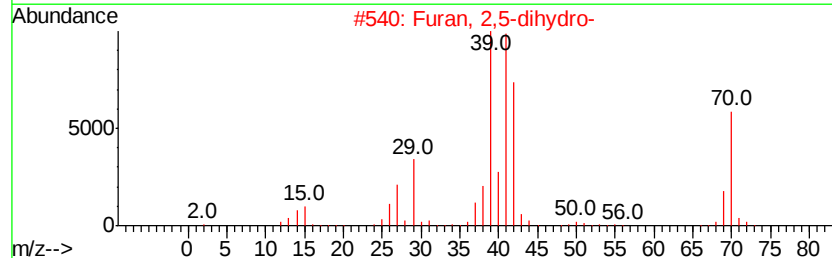
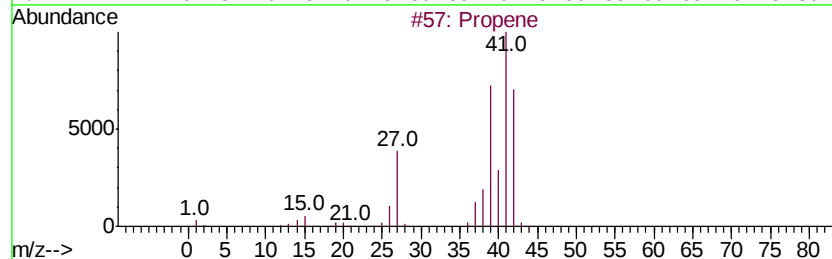
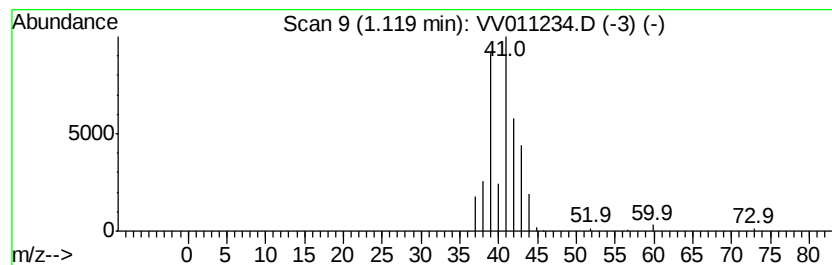
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Cyclic1.12 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	0.66 ug/L	55232	1,4-Difluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	78
2			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	64
3			2-Butenal, (E)-	70	C4H6O	000123-73-9	64
4			2-Butenal	70	C4H6O	004170-30-3	56
5			Propene	42	C3H6	000115-07-1	42



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ClientSampleId :
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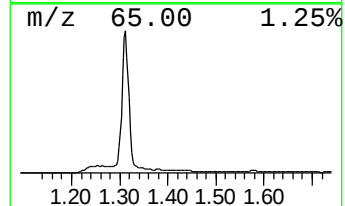
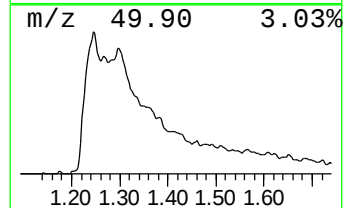
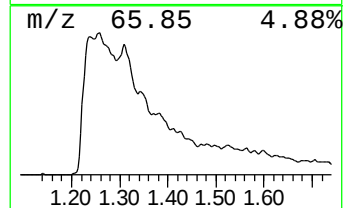
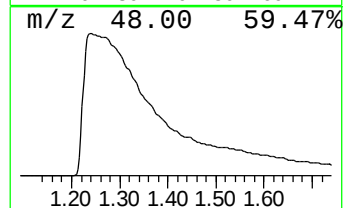
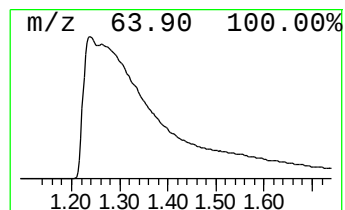
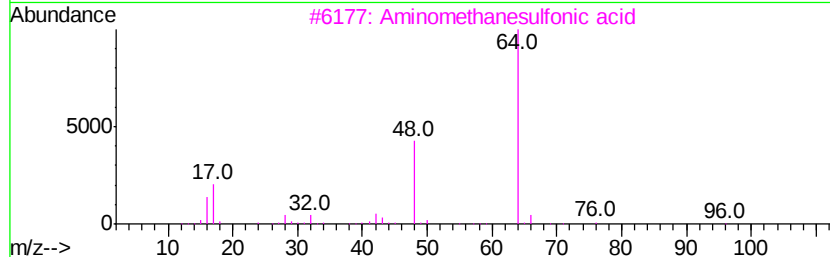
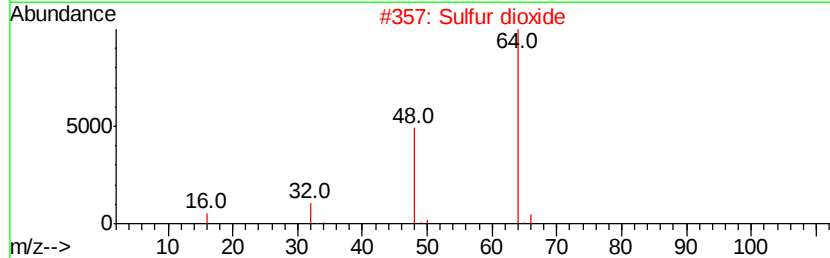
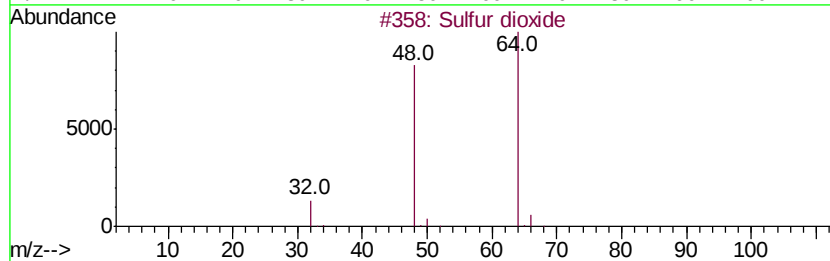
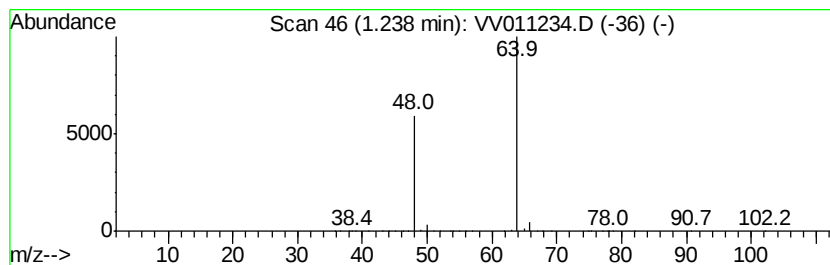
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.24	9.03 ug/L	756965	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfur dioxide	64	O2S	007446-09-5	83
2		Sulfur dioxide	64	O2S	007446-09-5	83
3		Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	74
4		L-Alanine, 3-sulfo-	169	C3H7N05S	000498-40-8	9
5		Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	9



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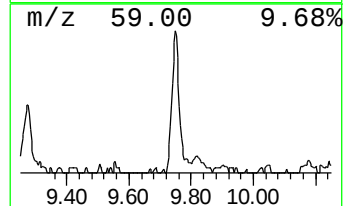
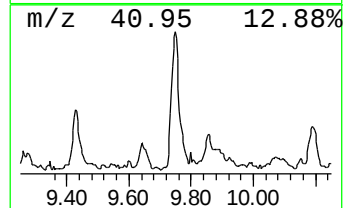
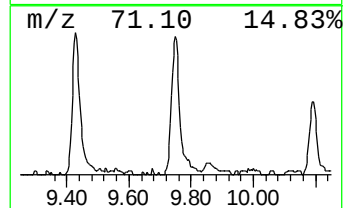
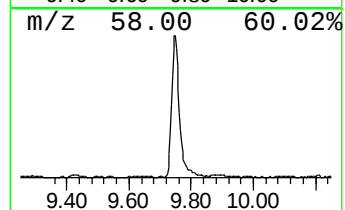
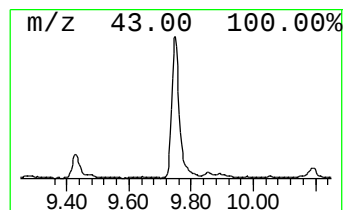
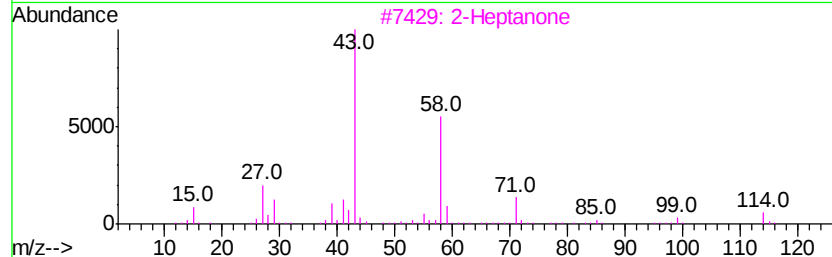
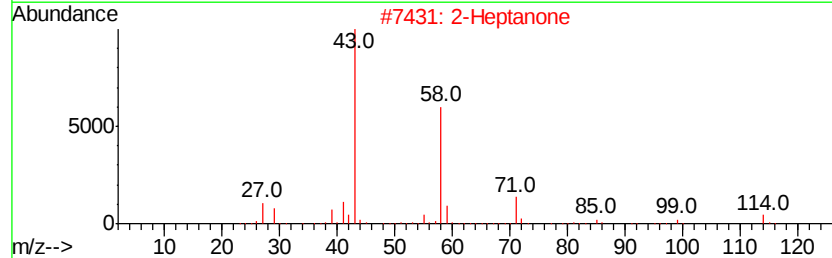
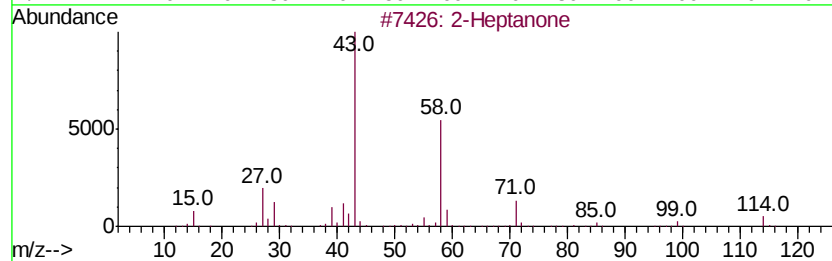
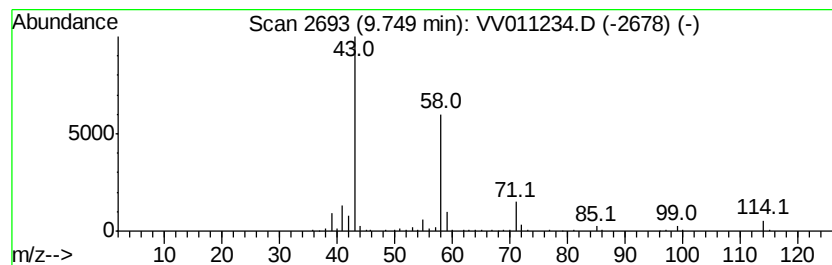
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 2-Heptanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	1.45 ug/L	151032	Chlorobenzene-d5	8.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Heptanone	114	C7H14O	000110-43-0	91
3			2-Heptanone	114	C7H14O	000110-43-0	91
4			2-Heptanone	114	C7H14O	000110-43-0	83
5			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64



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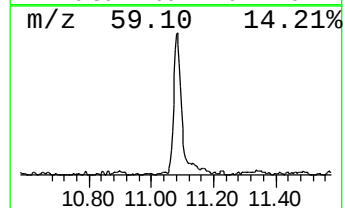
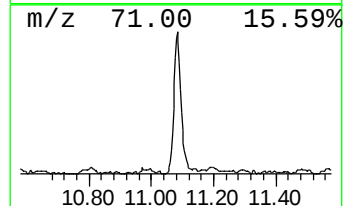
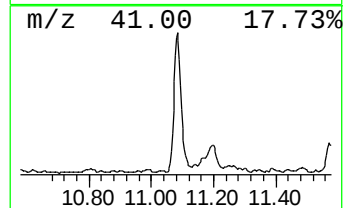
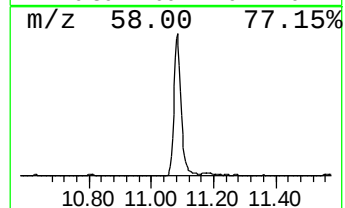
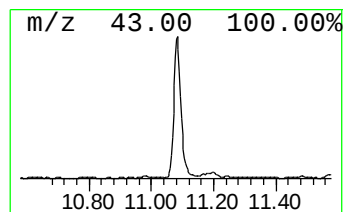
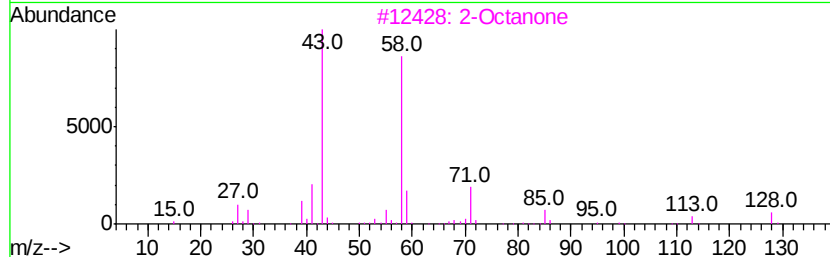
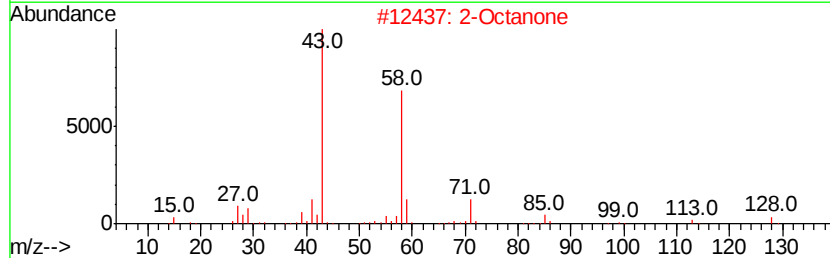
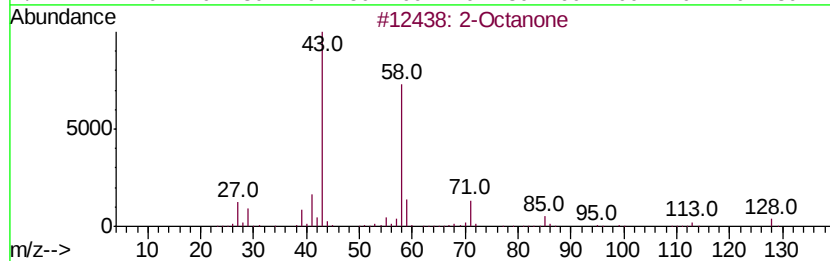
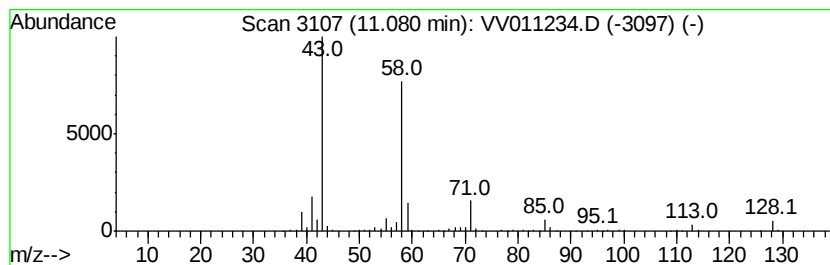
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	3.55 ug/L	336931	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Octanone	128	C8H16O	000111-13-7	94
2		2-Octanone	128	C8H16O	000111-13-7	94
3		2-Octanone	128	C8H16O	000111-13-7	94
4		2-Octanone	128	C8H16O	000111-13-7	90
5		2-Octanone	128	C8H16O	000111-13-7	90



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ALS Vial : 1 Sample Multiplier: 1

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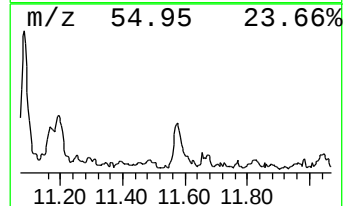
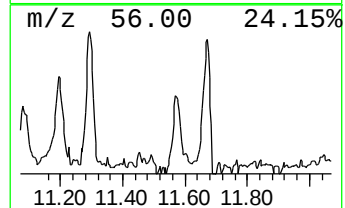
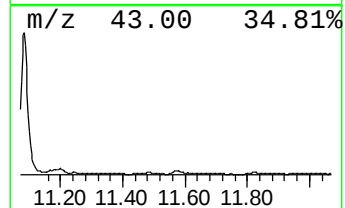
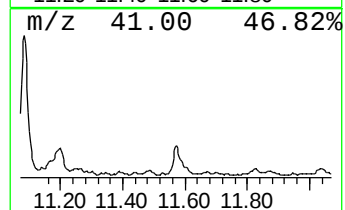
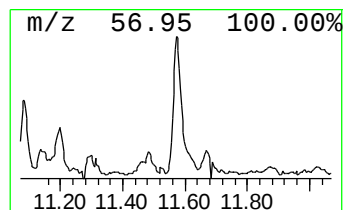
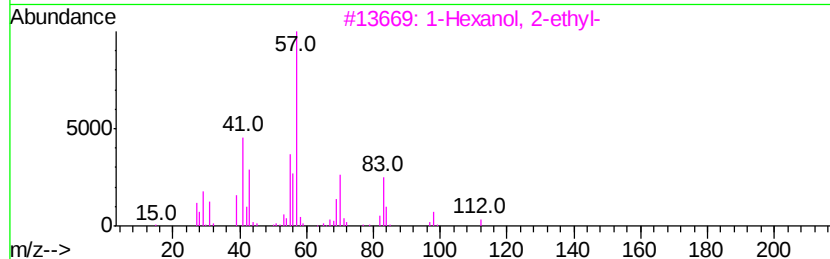
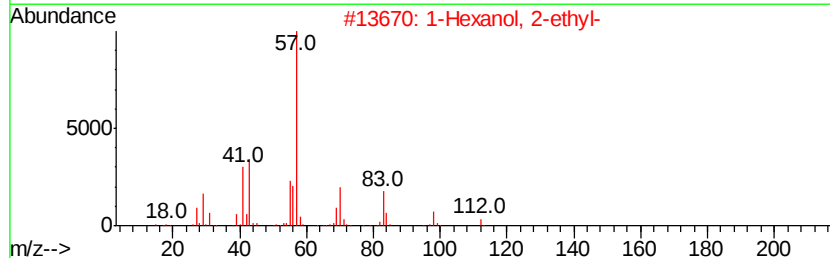
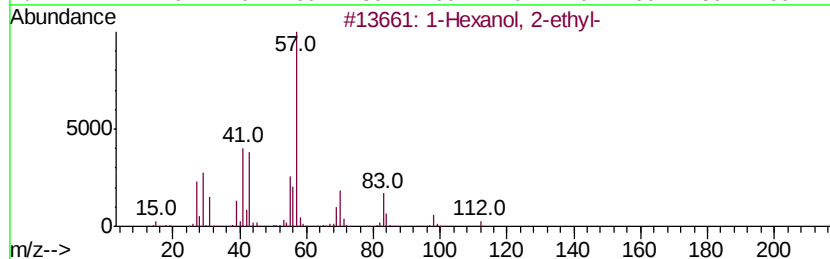
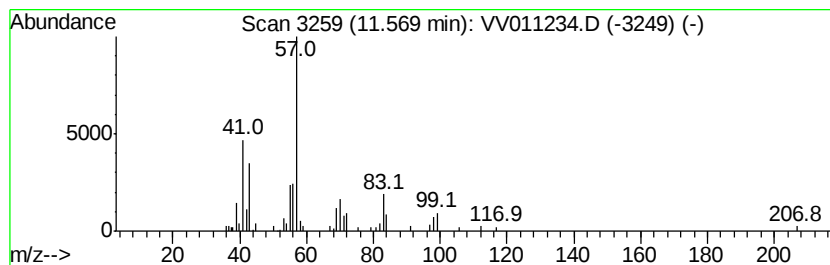
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	0.53 ug/L	49803	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
4		2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	1000365-51-1	50
5		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011234.D
Acq On : 05 Jun 2019 17:16
Operator : SY/MD
Sample : K3197-06
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P47

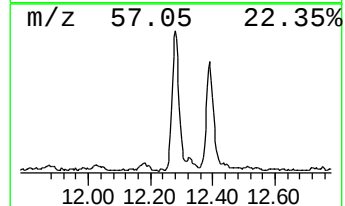
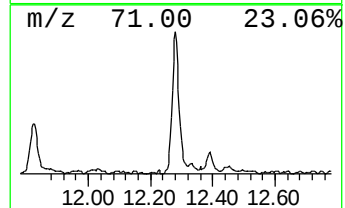
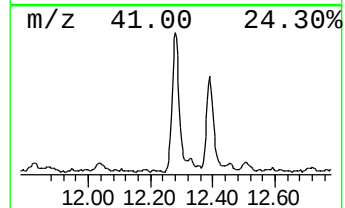
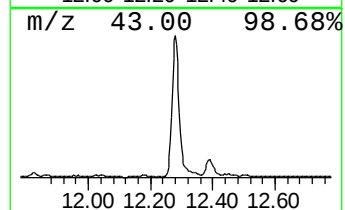
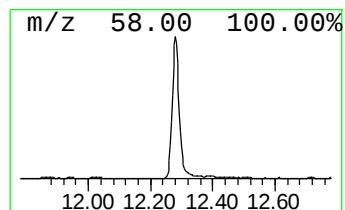
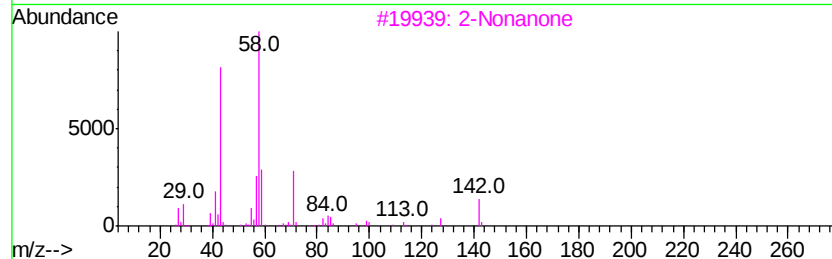
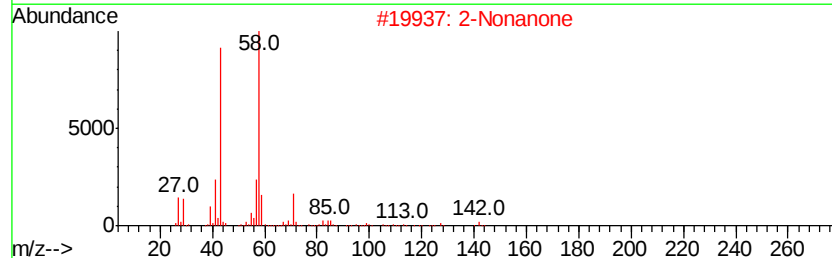
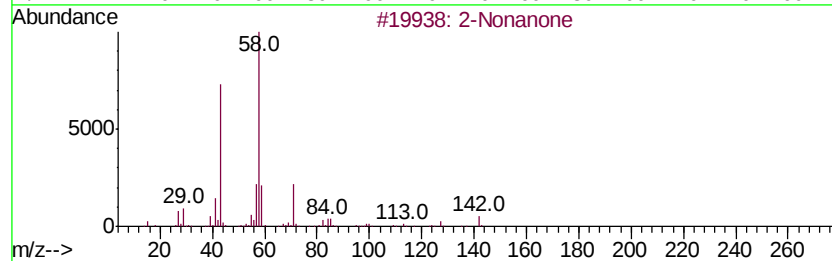
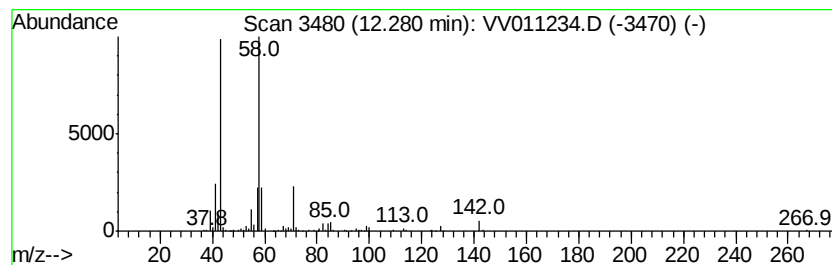
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 2-Nonanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	2.65 ug/L	251608	1,4-Dichlorobenzene-d4	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone		142	C9H18O	000821-55-6	97
2	2-Nonanone		142	C9H18O	000821-55-6	91
3	2-Nonanone		142	C9H18O	000821-55-6	91
4	2-Octanone		128	C8H16O	000111-13-7	78
5	2-Heptanone		114	C7H14O	000110-43-0	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011234.D
Acq On : 05 Jun 2019 17:16
Operator : SY/MD
Sample : K3197-06
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P47

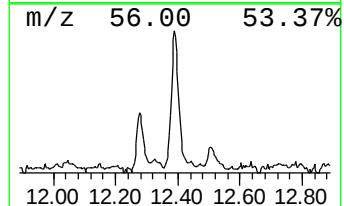
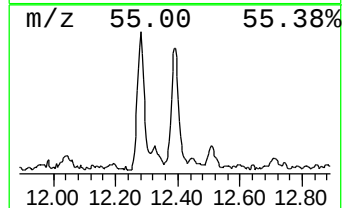
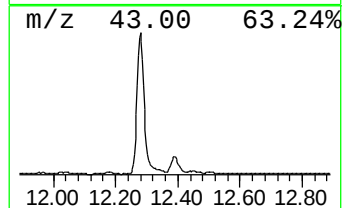
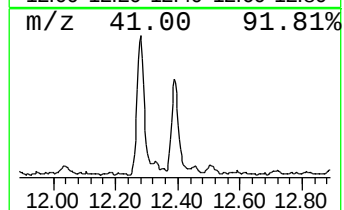
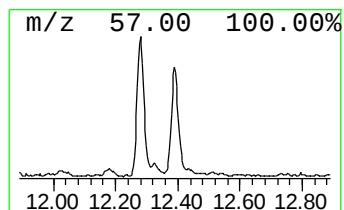
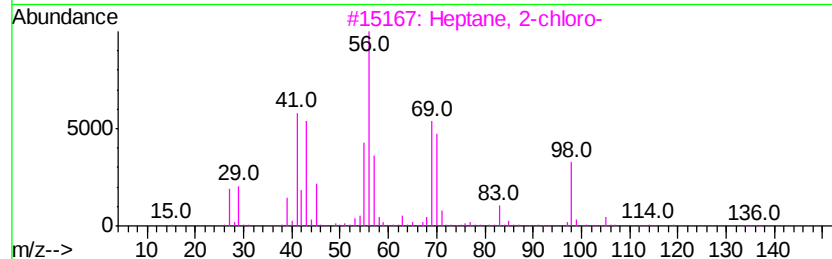
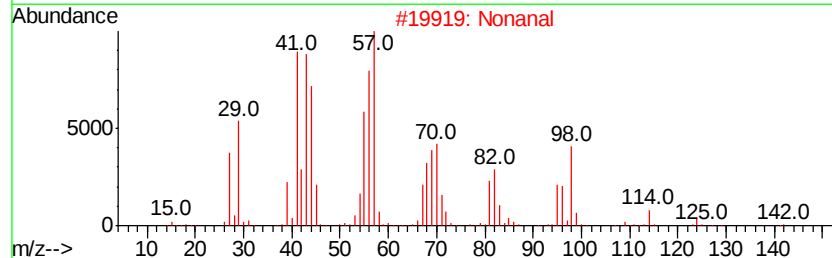
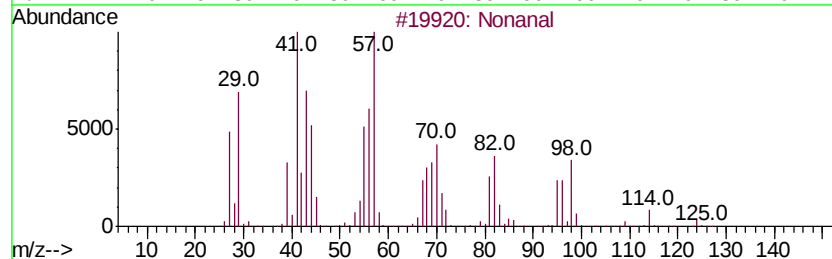
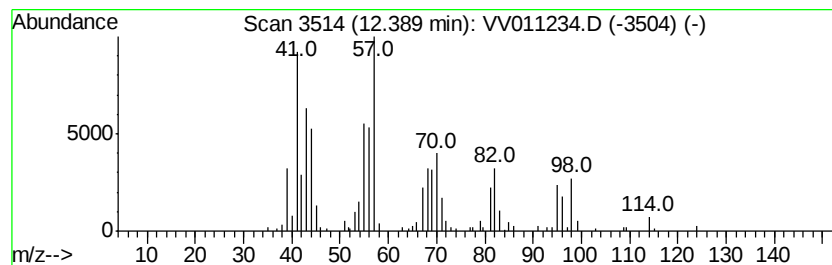
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Nonanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	1.04 ug/L	98201	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	83
3		Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27
4		Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27
5		Octane, 2-chloro-	148	C8H17Cl	000628-61-5	22



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011234.D
Acq On : 05 Jun 2019 17:16
Operator : SY/MD
Sample : K3197-06
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

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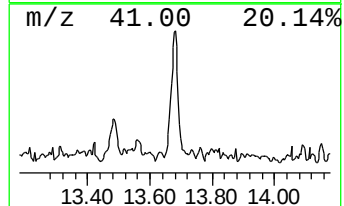
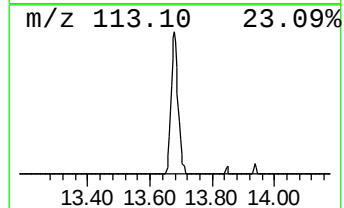
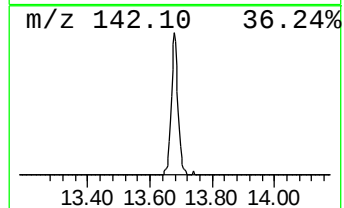
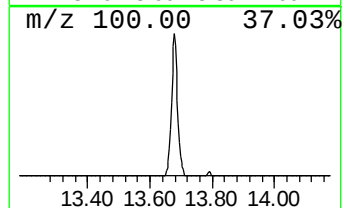
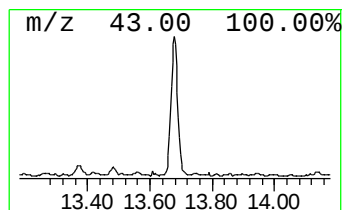
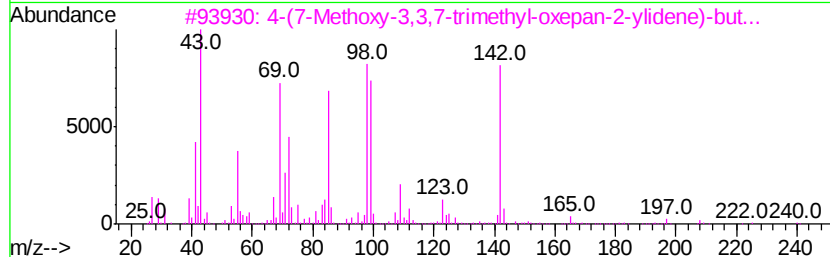
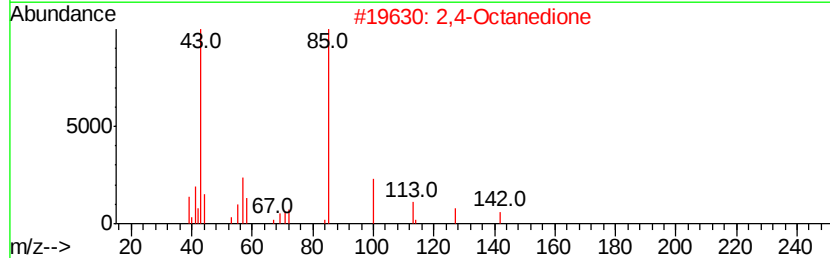
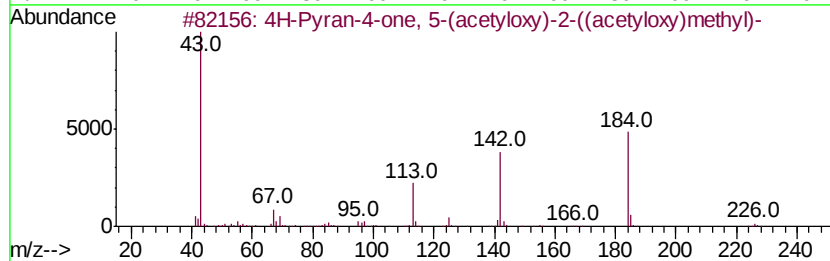
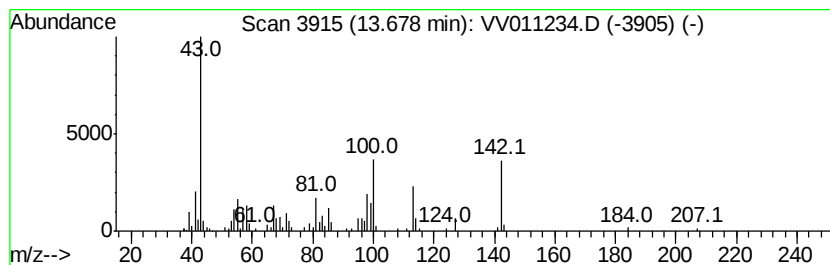
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	0.79 ug/L	74718	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	27
2		2,4-Octanedione	142	C8H14O2	014090-87-0	25
3		4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	16
4		6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	12
5		Pyrrolidine, 1-(1-oxo-2,5-octade...	333	C22H39NO	056666-48-9	12



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011234.D
Acq On : 05 Jun 2019 17:16
Operator : SY/MD
Sample : K3197-06
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

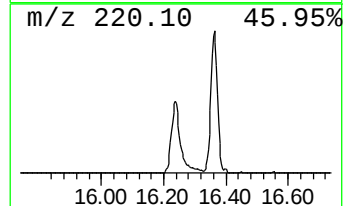
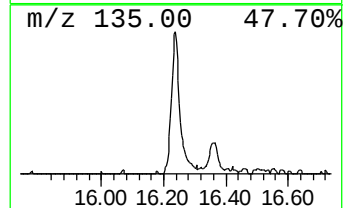
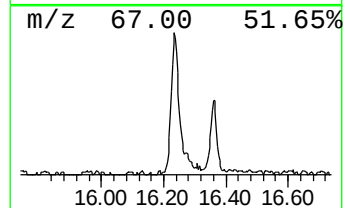
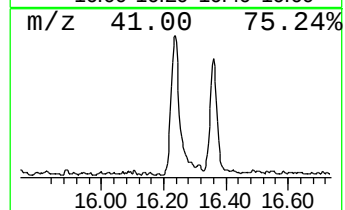
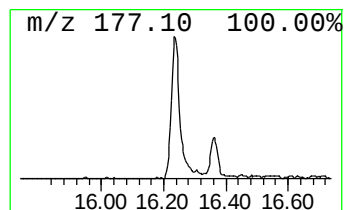
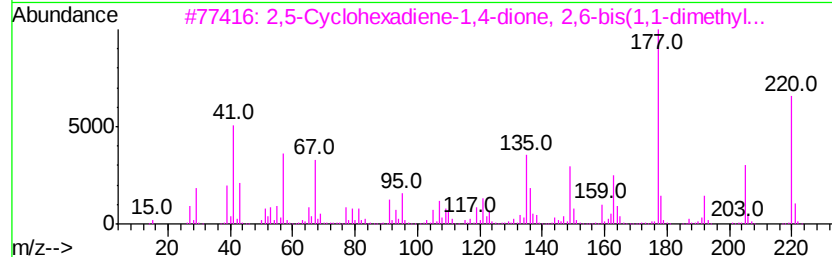
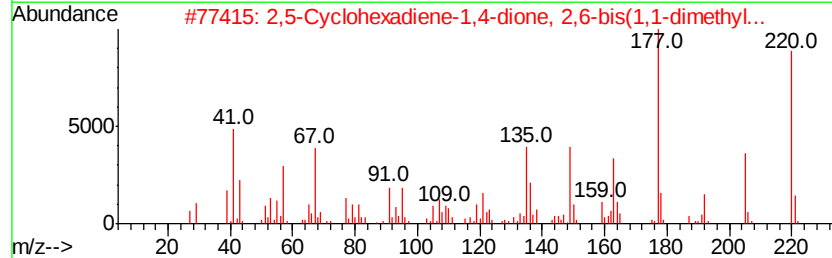
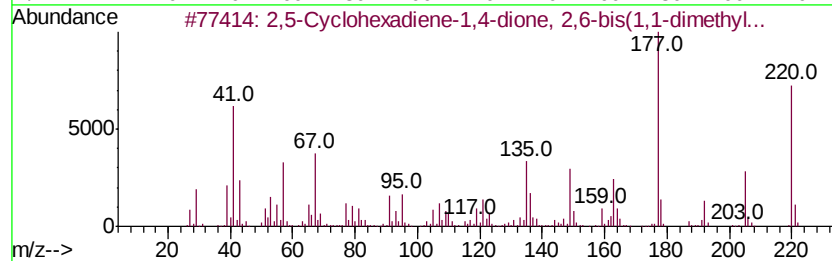
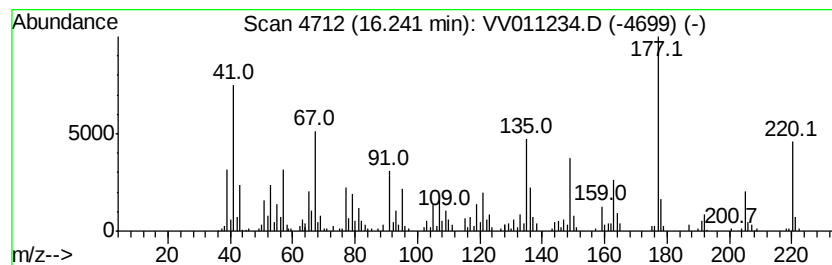
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.24	2.64 ug/L	250013	1,4-Dichlorobenzene-d4	11.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
4	2H-1-Benzopyran, 3,5,6,8a-tetra...	192	C13H20O	041678-29-9	44
5	4-Propylbenzaldehyde diethyl acetal	222	C14H22O2	089557-35-7	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011234.D
Acq On : 05 Jun 2019 17:16
Operator : SY/MD
Sample : K3197-06
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P47

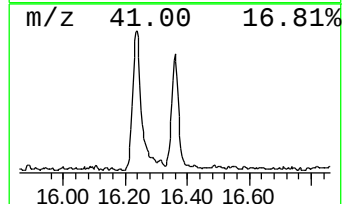
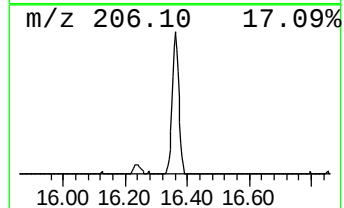
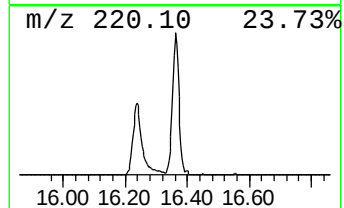
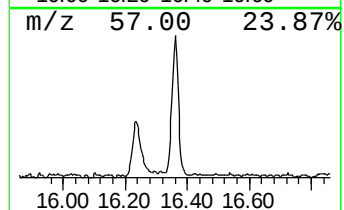
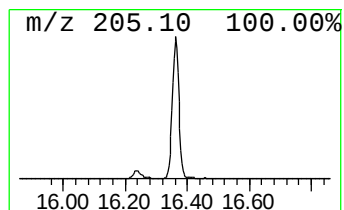
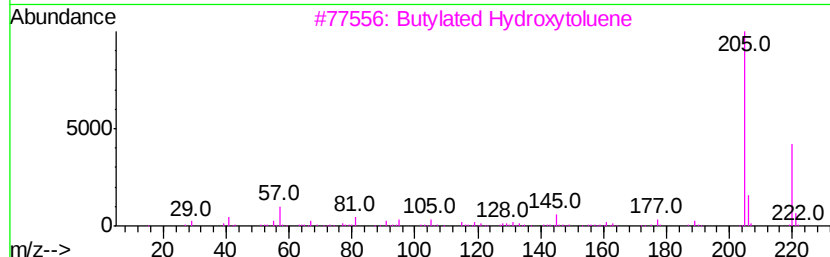
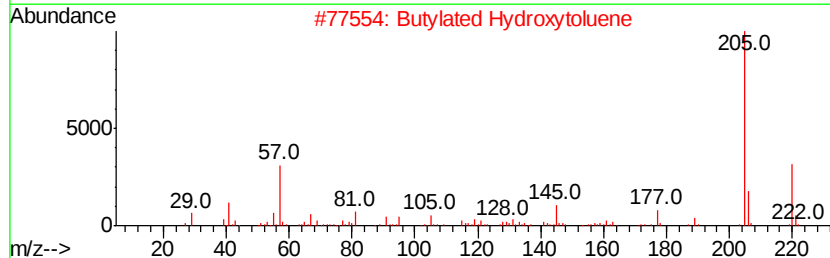
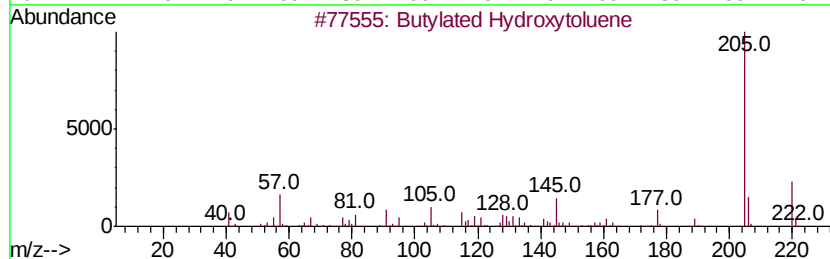
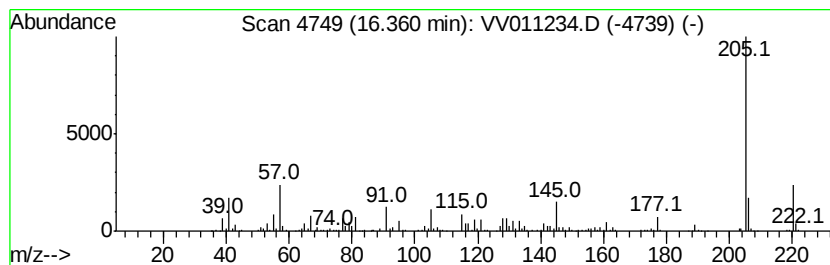
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	2.73 ug/L	258867	1,4-Dichlorobenzene-d4	11.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	98
2	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	95
3	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	94
4	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	93
5	Phenol, 2,4,6-tris(1-methylethyl)-			220	C15H24O	002934-07-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060519\
Data File : VV011234.D
Acq On : 05 Jun 2019 17:16
Operator : SY/MD
Sample : K3197-06
Misc : 25ML/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P47

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.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	0.7	ug/L	55232	1	5.66	419275	5.0
Sulfur dioxide	1.24	9.0	ug/L	756965	1	5.66	419275	5.0
2-Heptanone	9.75	1.5	ug/L	151032	2	8.89	520540	5.0
2-Octanone	11.08	3.5	ug/L	336931	3	11.29	474309	5.0
1-Hexanol, 2-ethyl-	11.57	0.5	ug/L	49803	3	11.29	474309	5.0
2-Nonanone	12.28	2.6	ug/L	251608	3	11.29	474309	5.0
Nonanal	12.39	1.0	ug/L	98201	3	11.29	474309	5.0
unknown-01	13.68	0.8	ug/L	74718	3	11.29	474309	5.0
2,5-Cyclohexadien...	16.24	2.6	ug/L	250013	3	11.29	474309	5.0
Butylated Hydroxy...	16.36	2.7	ug/L	258867	3	11.29	474309	5.0