

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
 Data File : VV011237.D
 Acq On : 05 Jun 2019 18:35
 Operator : SY/MD
 Sample : K3197-09
 Misc : 25ML/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9P50

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	6	8	19	rVB2	14969	15952	2.42%	0.216%
2	1.312	60	69	82	rBV	125415	200804	30.46%	2.714%
3	1.579	146	152	161	rVB	77508	88046	13.36%	1.190%
4	2.126	313	322	333	rVB	186488	260873	39.58%	3.526%
5	2.312	372	380	391	rVB	87450	127300	19.31%	1.721%
6	3.756	813	829	847	rBV10	8812	27656	4.20%	0.374%
7	3.984	886	900	935	rBV2	43412	221976	33.68%	3.000%
8	4.399	1011	1029	1050	rBV	104179	264671	40.15%	3.577%
9	5.093	1226	1245	1268	rBV2	277714	659161	100.00%	8.909%
10	5.662	1408	1422	1442	rBV	202531	412107	62.52%	5.570%
11	6.074	1540	1550	1551	rBV5	8911	11024	1.67%	0.149%
12	6.116	1552	1563	1585	rVB	147607	308935	46.87%	4.176%
13	6.248	1595	1604	1624	rBV4	7224	20815	3.16%	0.281%
14	6.633	1716	1724	1740	rVB3	14345	29967	4.55%	0.405%
15	7.029	1836	1847	1863	rBV	79095	145205	22.03%	1.963%
16	7.357	1931	1949	1968	rBV	329051	577756	87.65%	7.809%
17	7.666	2034	2045	2064	rBV	45416	83069	12.60%	1.123%
18	8.138	2181	2192	2203	rBV	346619	622045	94.37%	8.408%
19	8.289	2232	2239	2252	rVB8	10582	20319	3.08%	0.275%
20	8.431	2273	2283	2296	rBV7	5652	14675	2.23%	0.198%
21	8.894	2415	2427	2450	rBV	310053	519038	78.74%	7.015%
22	9.145	2495	2505	2516	rBV2	33533	52364	7.94%	0.708%
23	9.264	2532	2542	2544	rBV9	6483	8823	1.34%	0.119%
24	9.431	2583	2594	2607	rBV2	14155	24080	3.65%	0.325%
25	9.749	2681	2693	2709	rBV	92424	160138	24.29%	2.164%
26	9.852	2719	2725	2753	rVB	12227	29501	4.48%	0.399%
27	10.190	2822	2830	2841	rVB10	6689	11122	1.69%	0.150%
28	10.260	2841	2852	2864	rBV2	106780	169275	25.68%	2.288%
29	10.476	2909	2919	2929	rBV2	10743	18811	2.85%	0.254%
30	10.553	2930	2943	2954	rVB4	14297	25347	3.85%	0.343%
31	10.627	2959	2966	2976	rBV5	5770	8533	1.29%	0.115%
32	10.781	3005	3014	3018	rBV7	4848	7279	1.10%	0.098%
33	10.981	3063	3076	3096	rBV	33311	56652	8.59%	0.766%
34	11.083	3096	3108	3121	rBV	55659	93439	14.18%	1.263%

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 Integrator: RTE
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 Sampling : 1
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 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

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35	11.196	3131	3143	3153	rVB6	16867	28944	4.39%	0.391%
36	11.292	3163	3173	3188	rVB	292156	467851	70.98%	6.323%
37	11.575	3249	3261	3279	rBV	248325	453523	68.80%	6.130%
38	11.669	3280	3290	3310	rVB	301556	496048	75.25%	6.705%
39	11.823	3330	3338	3343	rBV5	4431	7859	1.19%	0.106%
40	11.865	3343	3351	3367	rVB3	15276	33311	5.05%	0.450%
41	12.042	3403	3406	3415	rVB9	6250	7622	1.16%	0.103%
42	12.183	3441	3450	3456	rBV10	5155	8096	1.23%	0.109%
43	12.280	3471	3480	3490	rBV	44962	76018	11.53%	1.027%
44	12.389	3506	3514	3526	rVB2	31692	48418	7.35%	0.654%
45	12.508	3546	3551	3562	rVB2	5261	9078	1.38%	0.123%
46	13.112	3731	3739	3757	rVB2	22241	37157	5.64%	0.502%
47	13.479	3844	3853	3865	rBV2	9849	19174	2.91%	0.259%
48	13.678	3906	3915	3927	rBV	44584	70017	10.62%	0.946%
49	13.800	3946	3953	3961	rBV9	5317	7757	1.18%	0.105%
50	14.141	4045	4059	4064	rBV9	4441	8102	1.23%	0.110%
51	15.167	4367	4378	4388	rBV9	8802	17080	2.59%	0.231%
52	15.611	4510	4516	4527	rVB9	8288	12565	1.91%	0.170%
53	16.238	4698	4711	4732	rBV3	92086	186491	28.29%	2.521%
54	16.363	4740	4750	4760	rVB	71548	106765	16.20%	1.443%

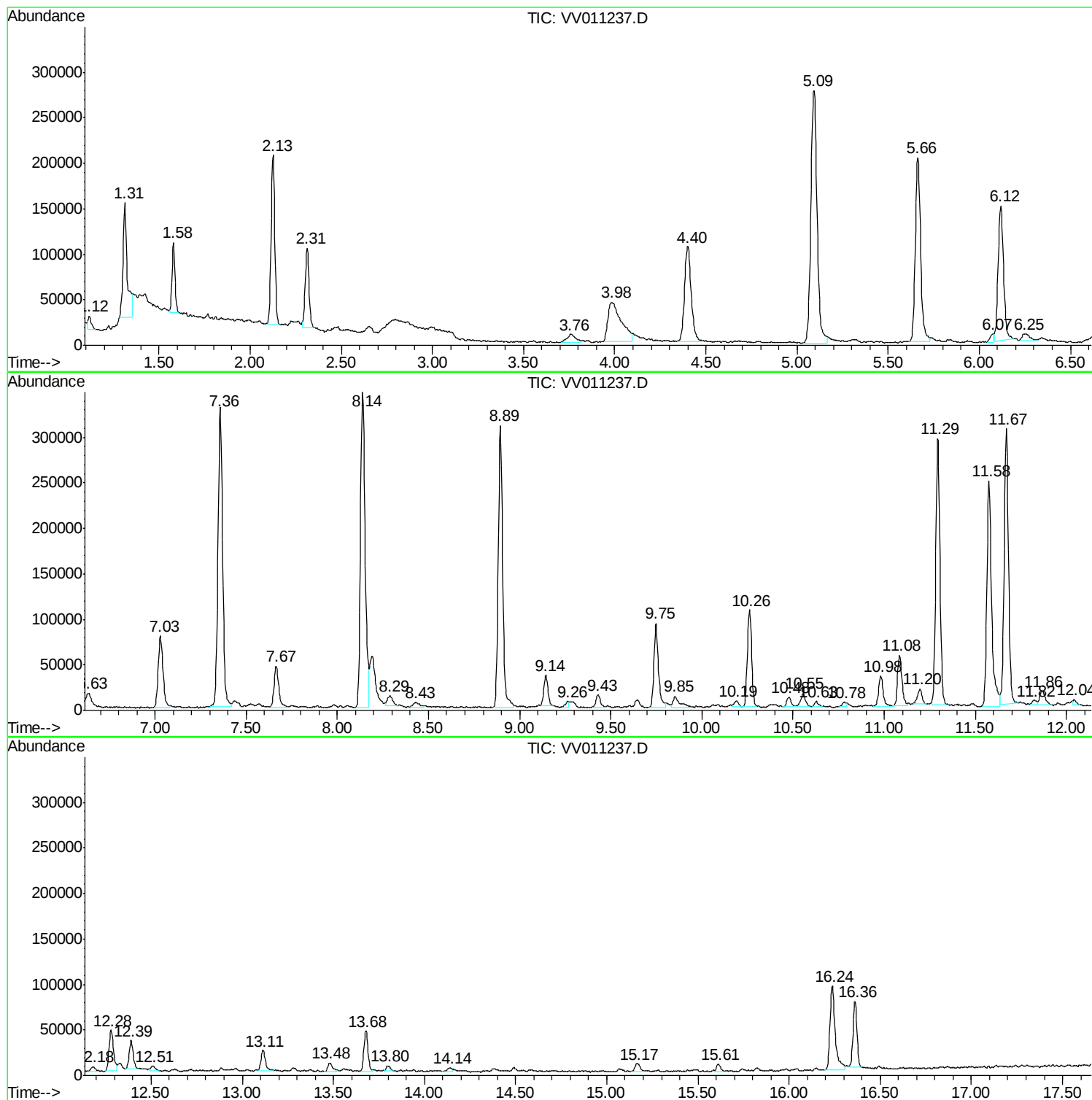
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ClientSampled :
F9P50

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



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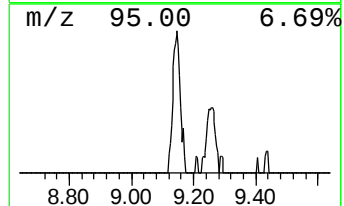
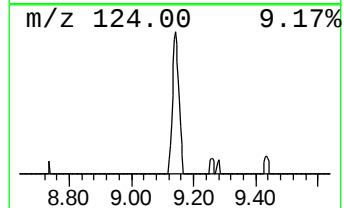
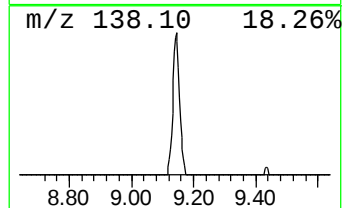
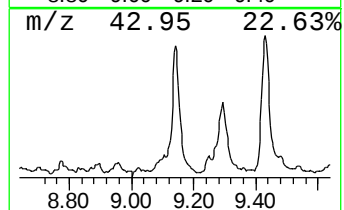
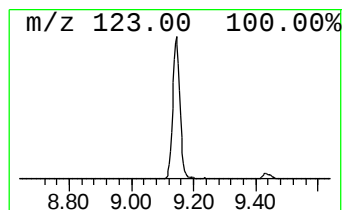
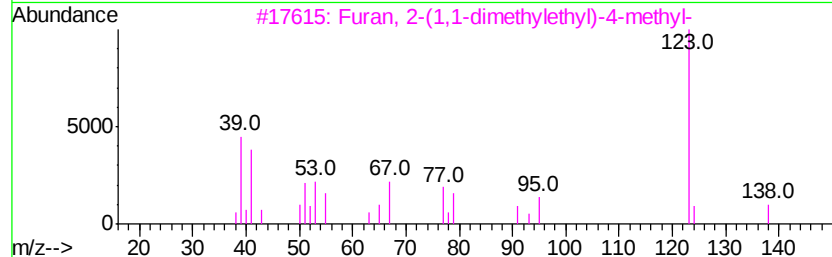
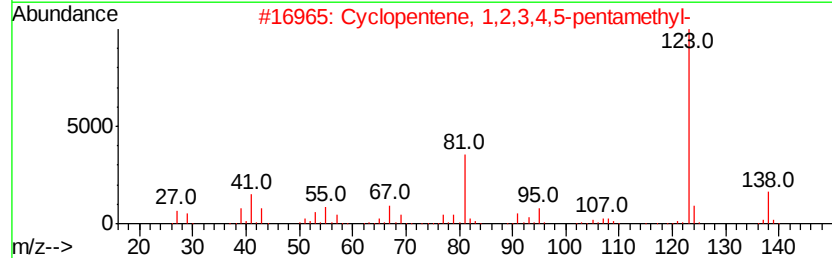
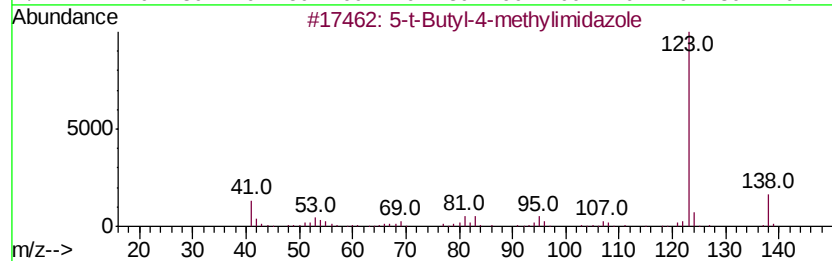
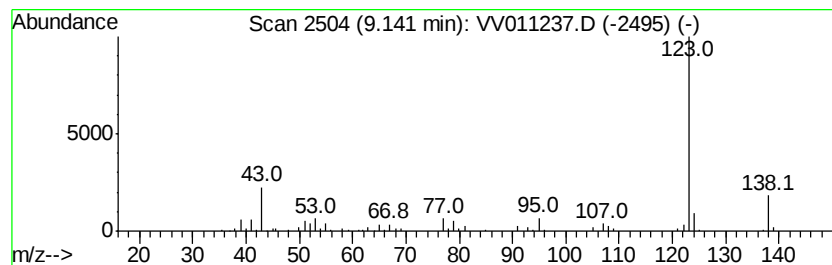
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 5-t-Butyl-4-methylimidazole Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.14	0.50 ug/L	52364	Chlorobenzene-d5	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	91
2		Cyclopentene, 1,2,3,4,5-pentamet...	138	C10H18	1000154-28-6	87
3		Furan, 2-(1,1-dimethylethyl)-4-m...	138	C9H14O	006141-68-0	72
4		Ethanone, 1-(4-fluorophenyl)-	138	C8H7FO	000403-42-9	64
5		4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	000461-98-3	64



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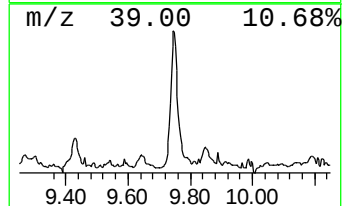
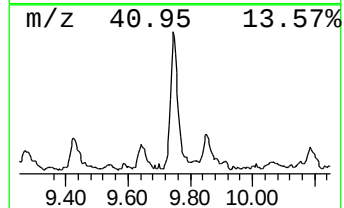
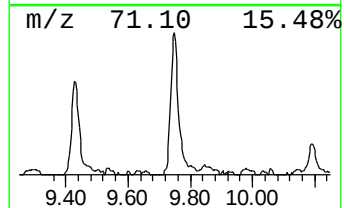
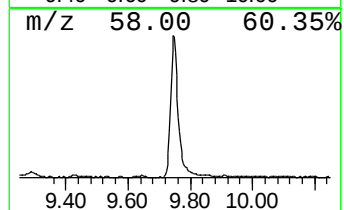
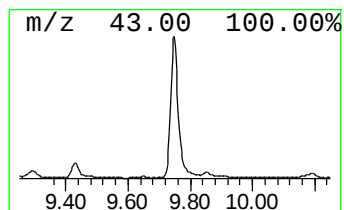
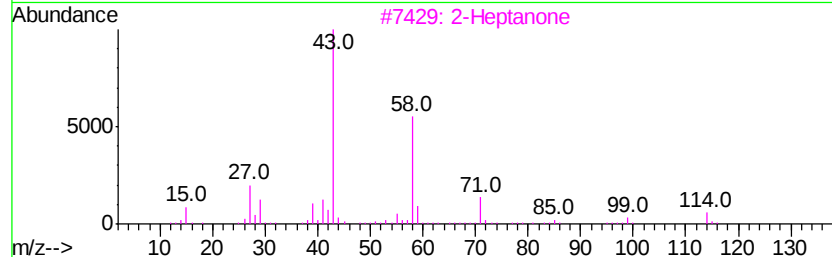
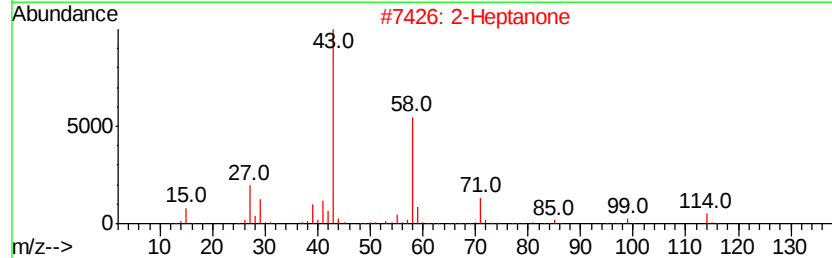
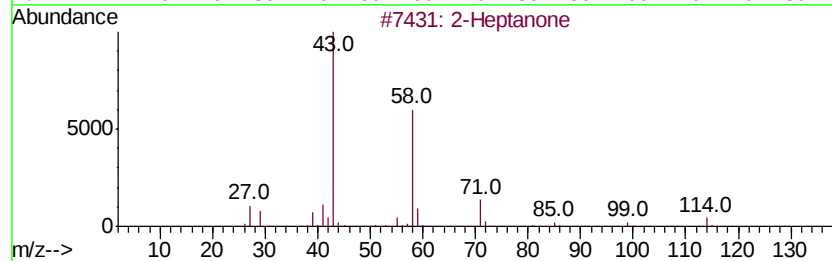
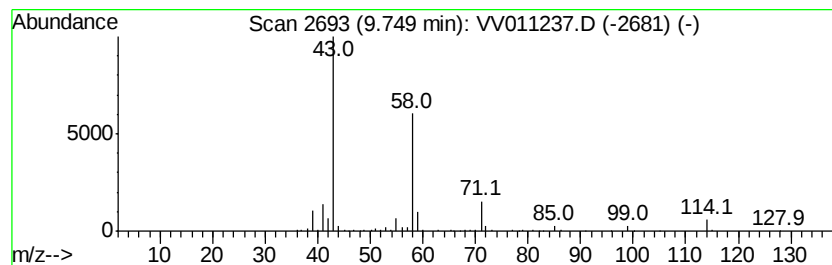
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	1.54 ug/L	160138	Chlorobenzene-d5	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	83
5		2-Heptanone	114	C7H14O	000110-43-0	80



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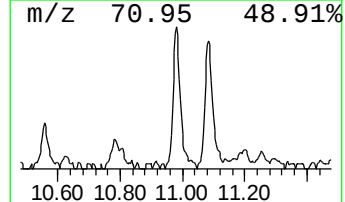
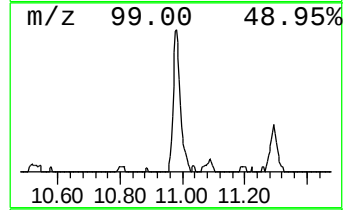
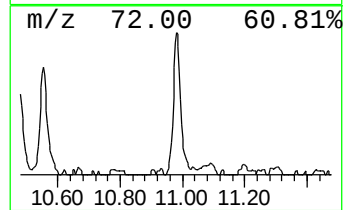
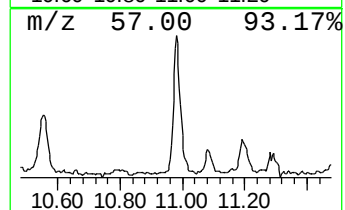
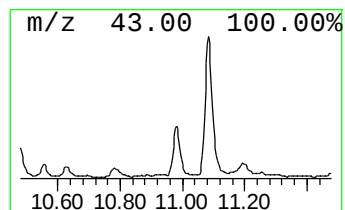
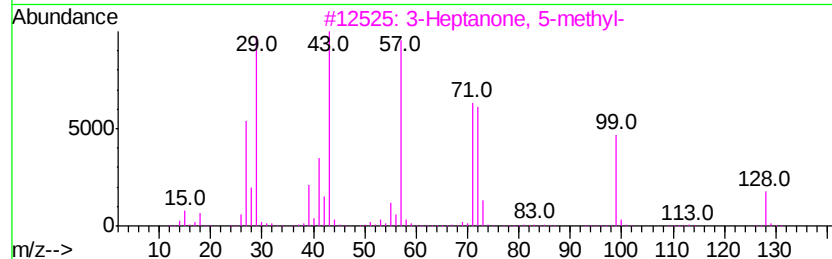
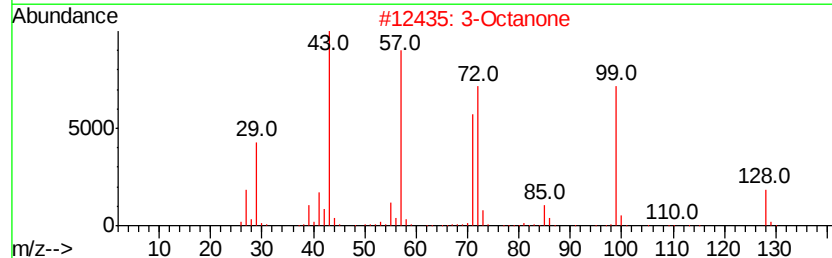
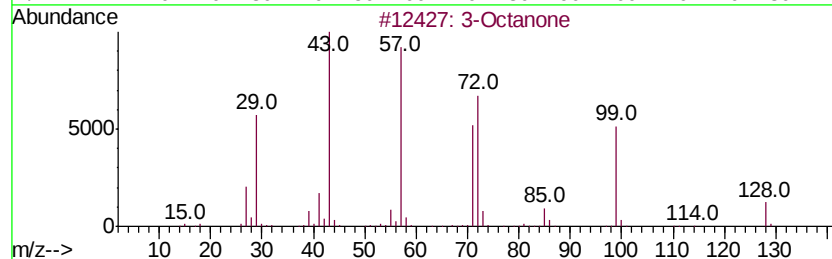
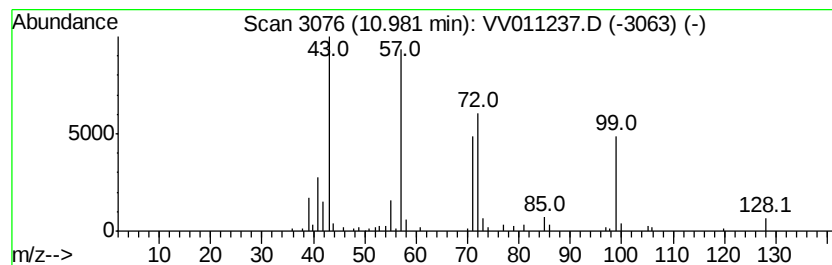
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 3-Octanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	0.61 ug/L	56652	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Octanone	128	C8H16O	000106-68-3	91
2		3-Octanone	128	C8H16O	000106-68-3	91
3		3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	56
4		3-Octanone	128	C8H16O	000106-68-3	50
5		3-Octanone	128	C8H16O	000106-68-3	47



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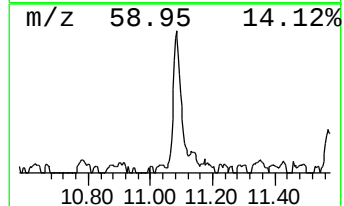
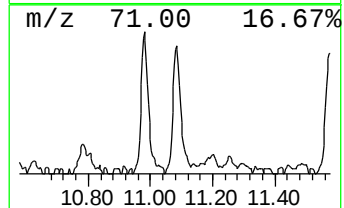
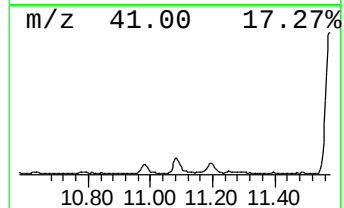
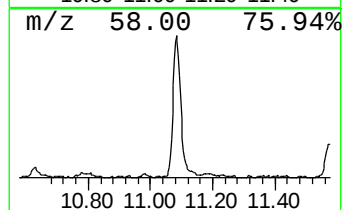
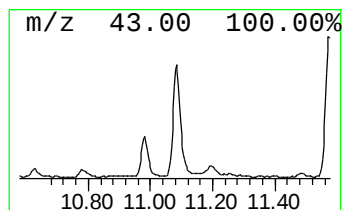
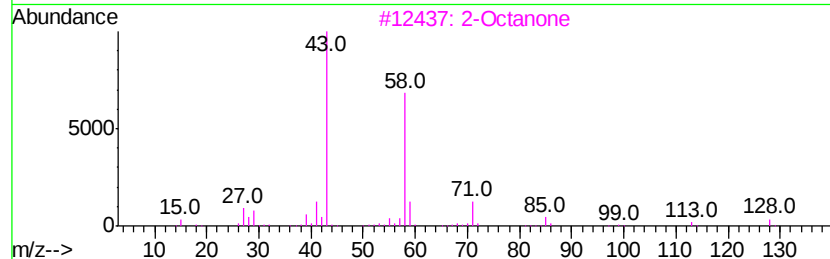
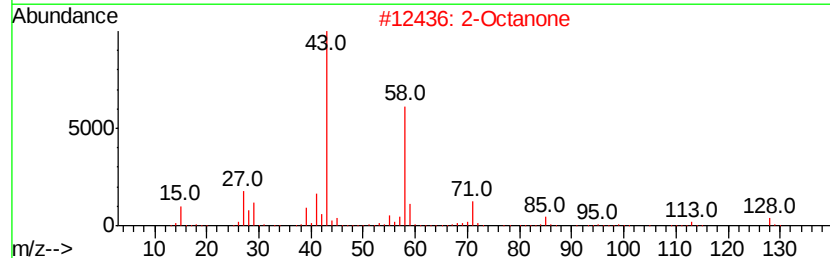
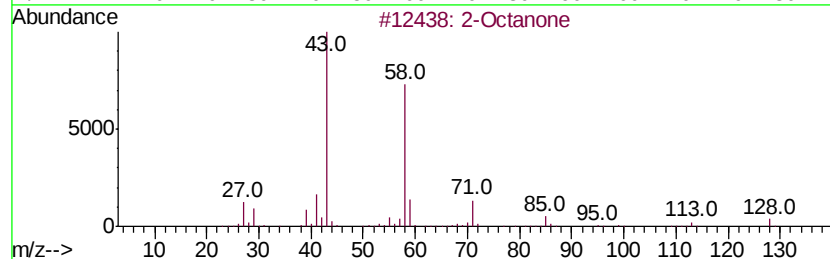
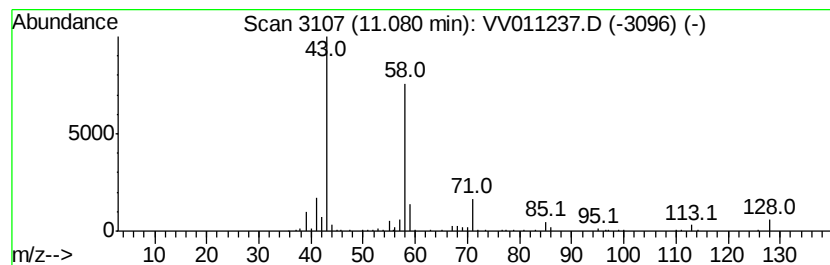
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 2-Octanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	1.00 ug/L	93439	1,4-Dichlorobenzene-d4	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone		128	C8H16O	000111-13-7	91
2	2-Octanone		128	C8H16O	000111-13-7	91
3	2-Octanone		128	C8H16O	000111-13-7	91
4	2-Octanone		128	C8H16O	000111-13-7	91
5	2-Octanone		128	C8H16O	000111-13-7	83



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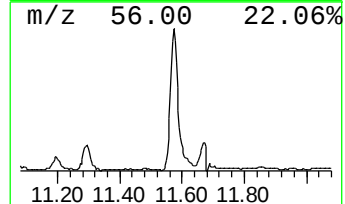
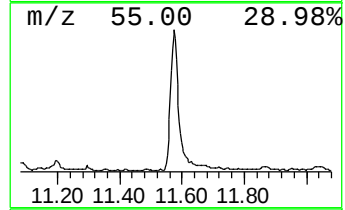
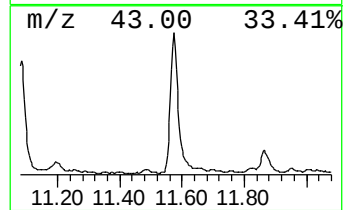
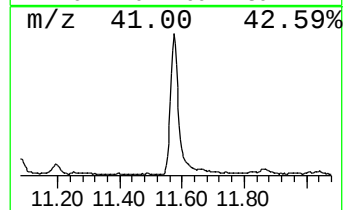
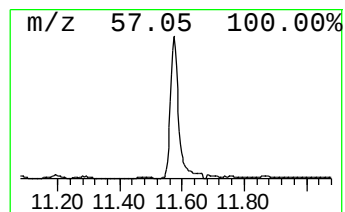
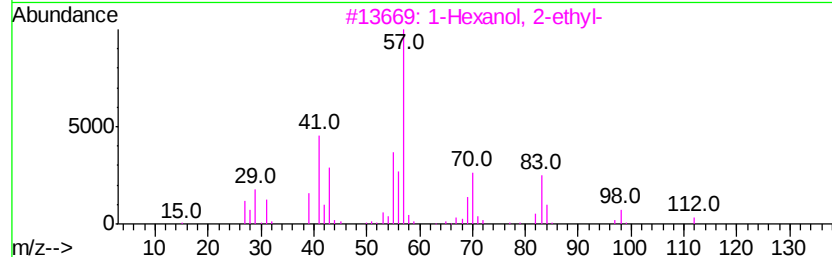
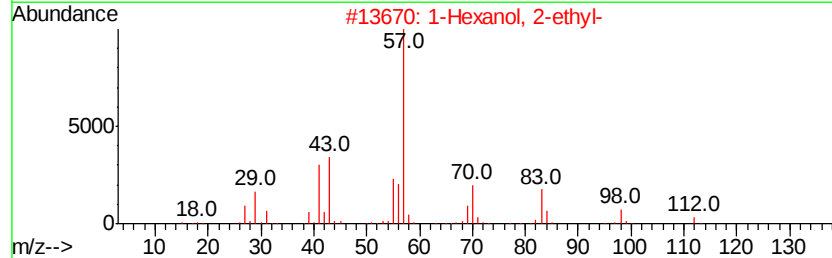
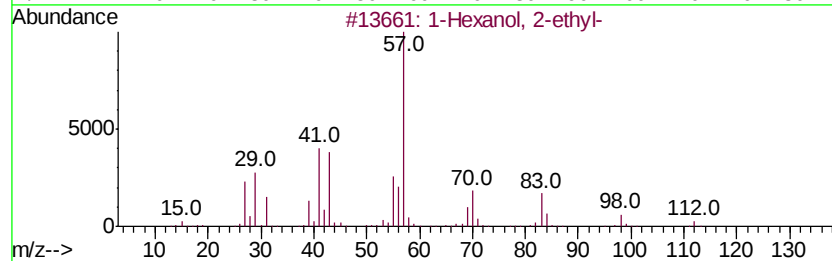
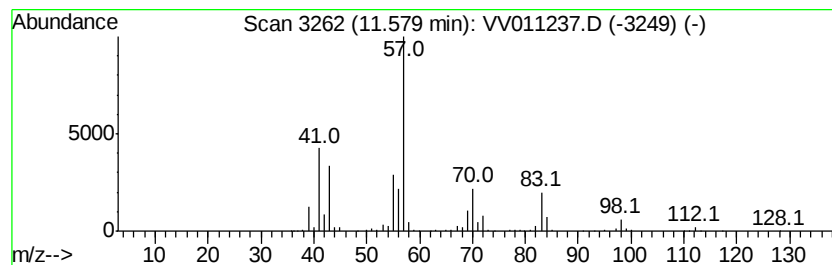
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	4.85 ug/L	453523	1,4-Dichlorobenzene-d4	11.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	83
2	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	64
5	Chloroacetic acid, 2-ethylhexyl ...	206 C10H19ClO2	005345-58-4	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011237.D
Acq On : 05 Jun 2019 18:35
Operator : SY/MD
Sample : K3197-09
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P50

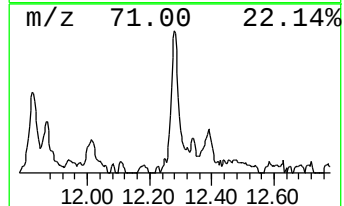
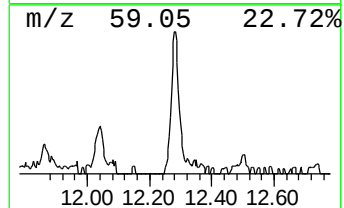
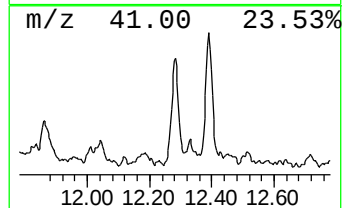
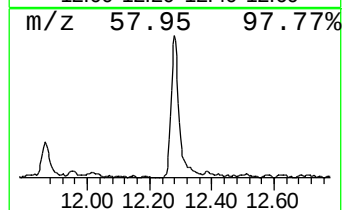
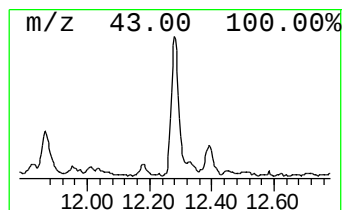
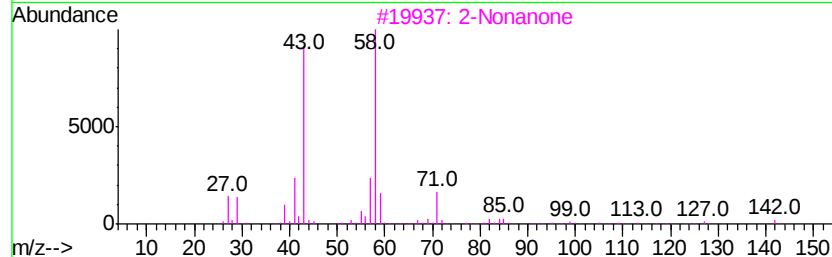
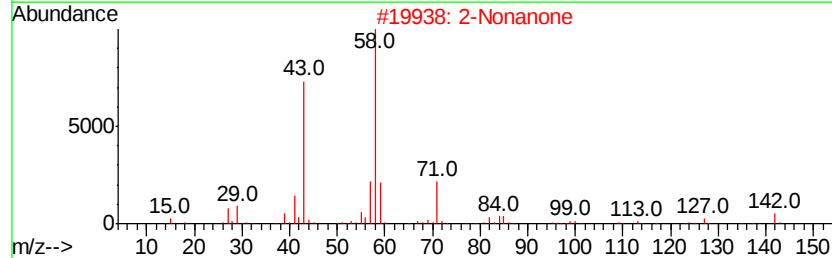
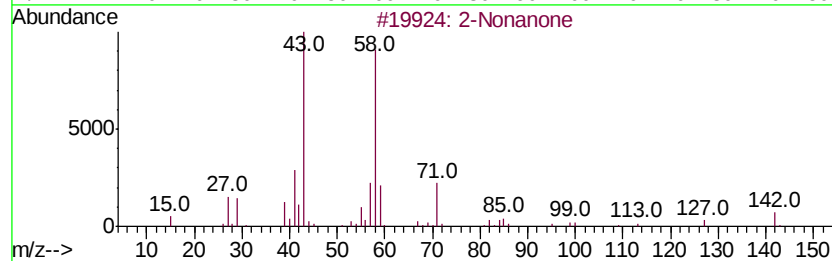
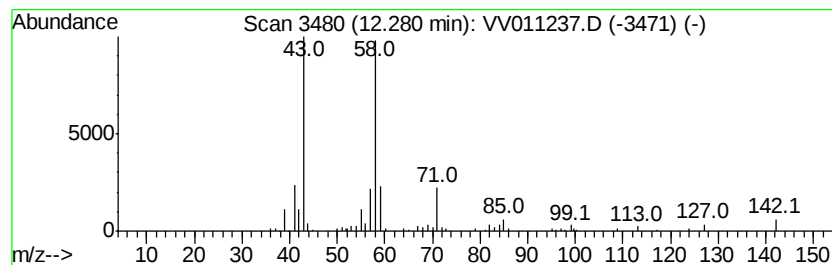
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 2-Nonanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	0.81 ug/L	76018	1,4-Dichlorobenzene-d4	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone		142	C9H18O	000821-55-6	95
2	2-Nonanone		142	C9H18O	000821-55-6	93
3	2-Nonanone		142	C9H18O	000821-55-6	80
4	2-Nonanone		142	C9H18O	000821-55-6	78
5	Pentanal, 2-methyl-		100	C6H12O	000123-15-9	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011237.D
Acq On : 05 Jun 2019 18:35
Operator : SY/MD
Sample : K3197-09
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P50

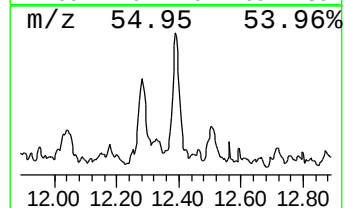
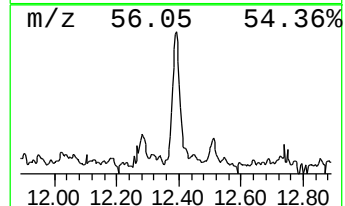
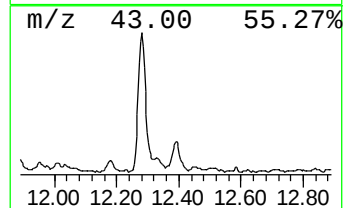
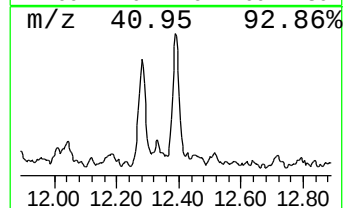
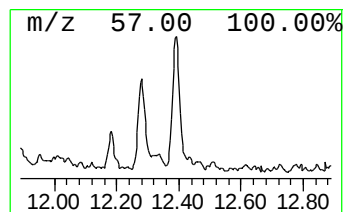
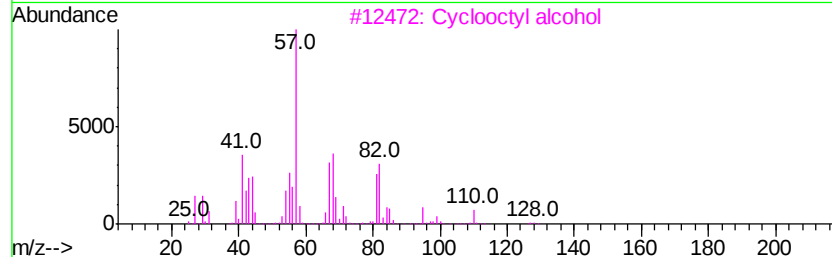
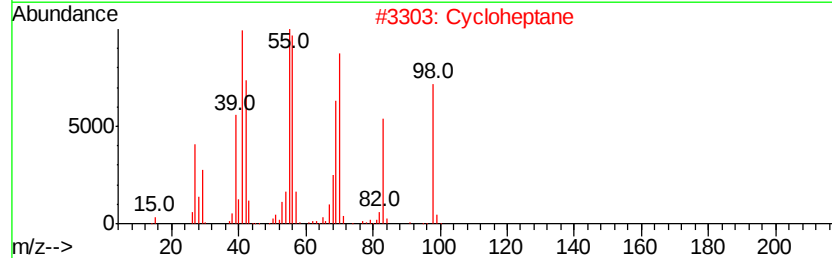
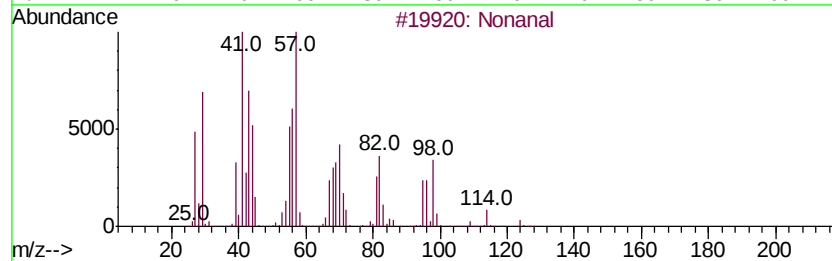
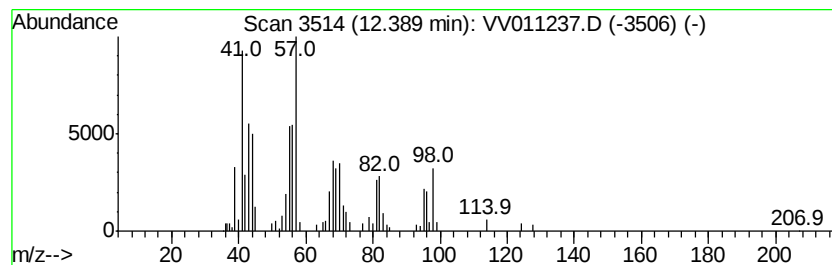
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Nonanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	0.52 ug/L	48418	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	91
2		Cycloheptane	98	C7H14	000291-64-5	30
3		Cyclooctyl alcohol	128	C8H16O	000696-71-9	30
4		Cycloheptane	98	C7H14	000291-64-5	27
5		2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011237.D
Acq On : 05 Jun 2019 18:35
Operator : SY/MD
Sample : K3197-09
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

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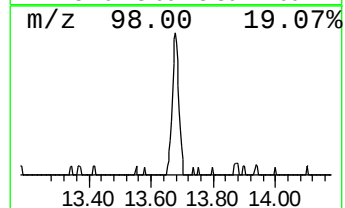
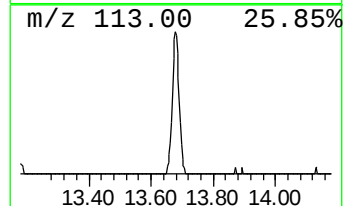
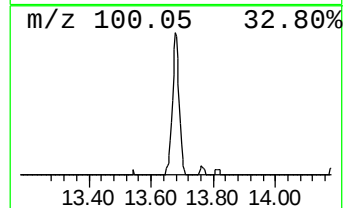
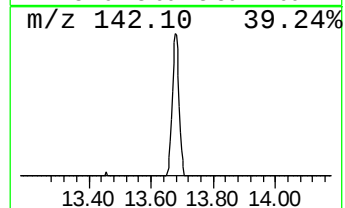
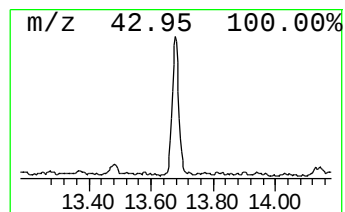
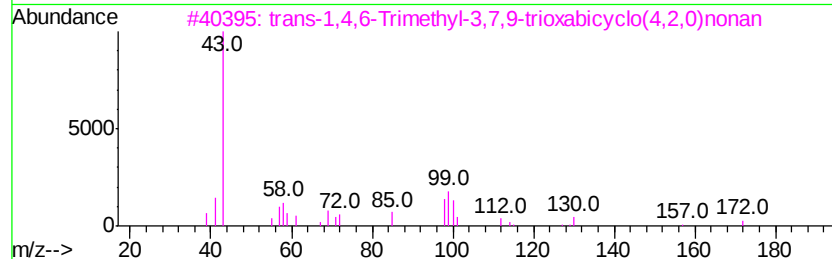
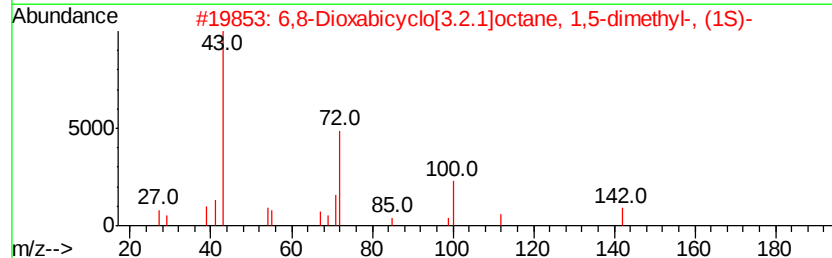
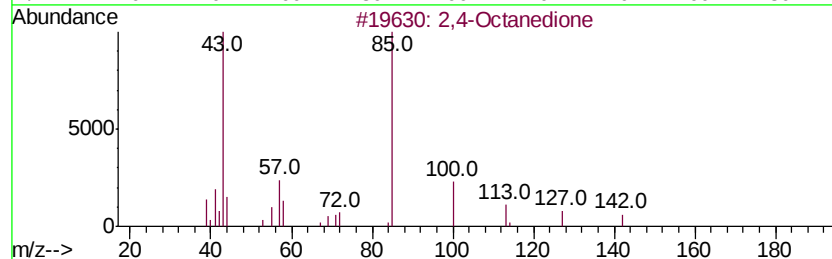
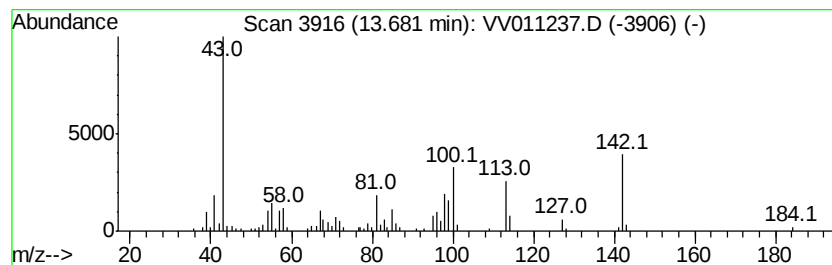
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 2,4-Octanedione Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	0.75 ug/L	70017	1,4-Dichlorobenzene-d4	11.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	50
2			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	32
3			trans-1,4,6-Trimethyl-3,7,9-trio...	172	C9H16O3	062759-59-5	16
4			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	12
5			Pentanoic Acid, 2,2,2-trifluoro...	184	C7H11F3O2	1000376-54-2	12



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011237.D
Acq On : 05 Jun 2019 18:35
Operator : SY/MD
Sample : K3197-09
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

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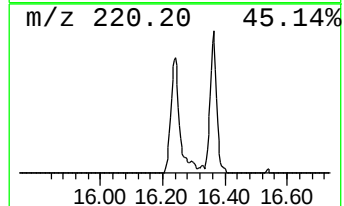
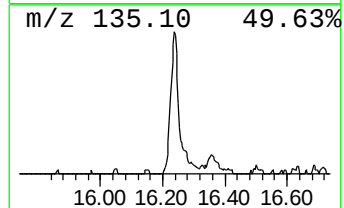
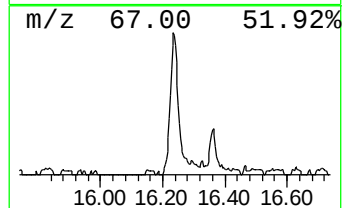
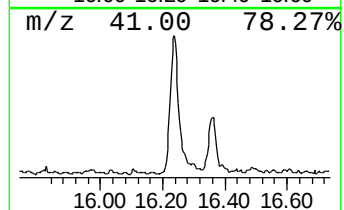
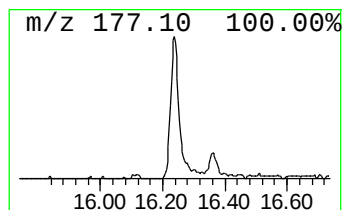
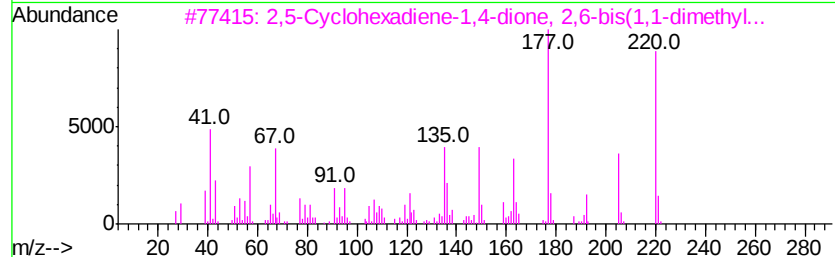
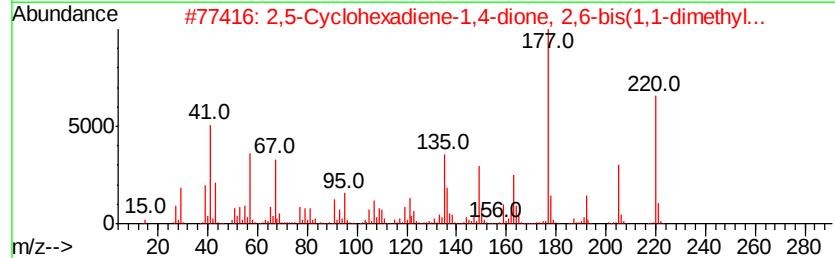
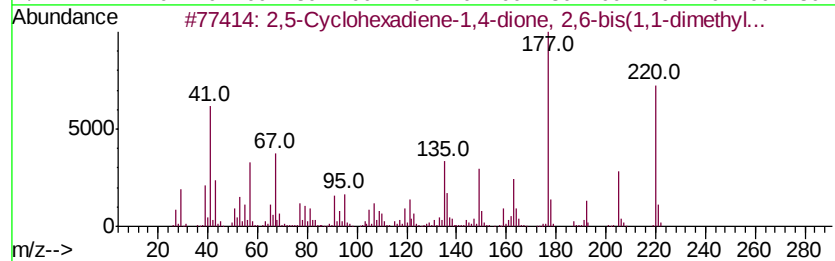
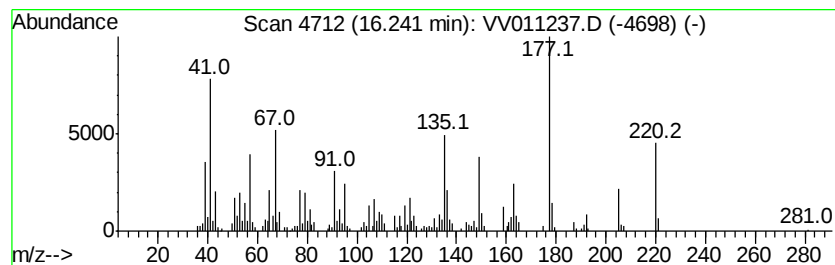
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.24	1.99 ug/L	186491	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	95
4			Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	43
5			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	35



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011237.D
Acq On : 05 Jun 2019 18:35
Operator : SY/MD
Sample : K3197-09
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

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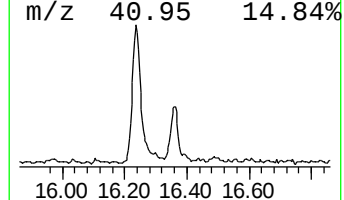
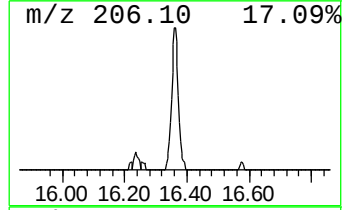
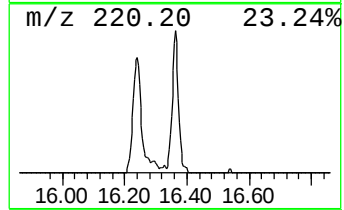
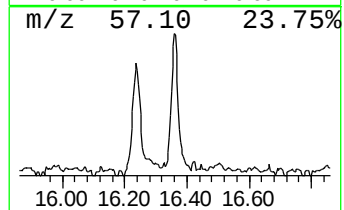
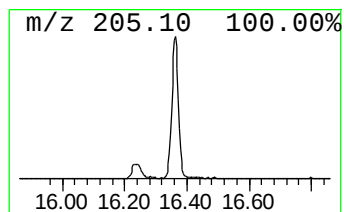
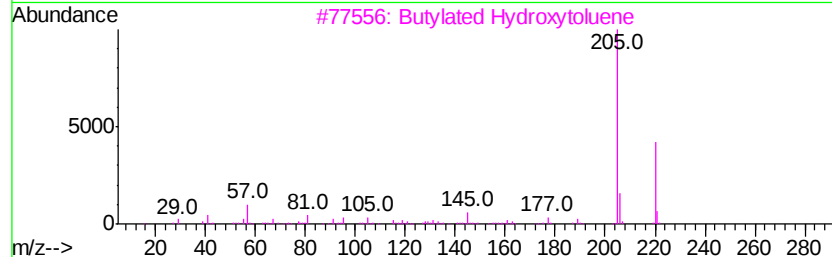
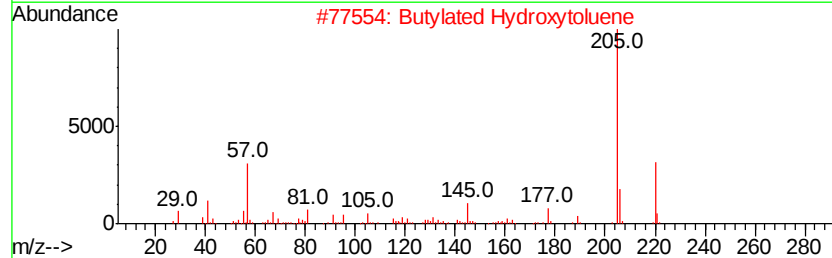
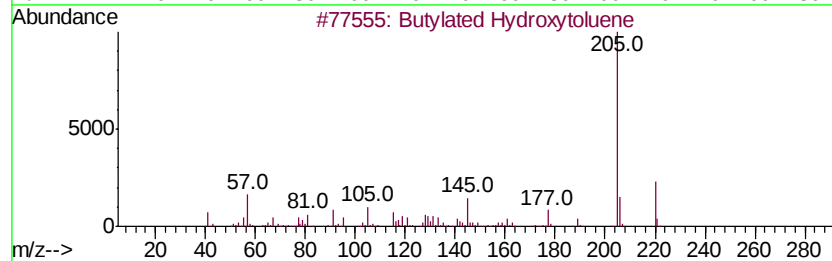
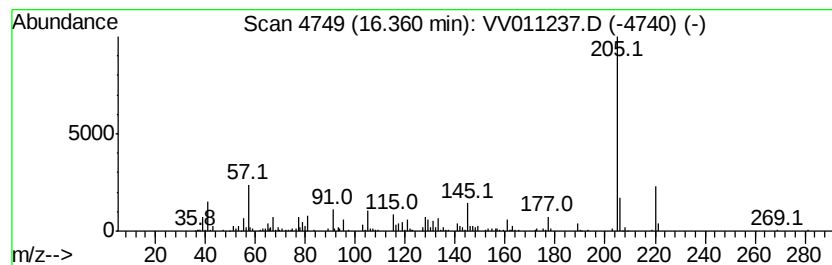
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 Butylated Hydroxytoluene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	1.14 ug/L	106765	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	91
5		Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	81



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060519\
Data File : VV011237.D
Acq On : 05 Jun 2019 18:35
Operator : SY/MD
Sample : K3197-09
Misc : 25ML/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P50

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
5-t-Butyl-4-methy...	9.14	0.5	ug/L	52364	2	8.89	519038	5.0
2-Heptanone	9.75	1.5	ug/L	160138	2	8.89	519038	5.0
3-Octanone	10.98	0.6	ug/L	56652	3	11.29	467851	5.0
2-Octanone	11.08	1.0	ug/L	93439	3	11.29	467851	5.0
1-Hexanol, 2-ethyl-	11.58	4.8	ug/L	453523	3	11.29	467851	5.0
2-Nonanone	12.28	0.8	ug/L	76018	3	11.29	467851	5.0
Nonanal	12.39	0.5	ug/L	48418	3	11.29	467851	5.0
2,4-Octanedione	13.68	0.8	ug/L	70017	3	11.29	467851	5.0
2,5-Cyclohexadien...	16.24	2.0	ug/L	186491	3	11.29	467851	5.0
Butylated Hydroxy...	16.36	1.1	ug/L	106765	3	11.29	467851	5.0