

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060519\
 Data File : VV011235.D
 Acq On : 05 Jun 2019 17:42
 Operator : SY/MD
 Sample : K3197-07
 Misc : 25ML/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9P48

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	5	8	21	rVB2	16246	19038	2.86%	0.268%
2	1.312	45	69	92	rBV2	181074	664539	100.00%	9.361%
3	1.579	146	152	167	rVB	79813	94219	14.18%	1.327%
4	2.126	313	322	332	rVB	186726	258096	38.84%	3.636%
5	2.309	373	379	389	rVB	28039	39547	5.95%	0.557%
6	2.656	478	487	497	rVB2	14713	27810	4.18%	0.392%
7	3.987	880	901	941	rBV	40735	224354	33.76%	3.160%
8	4.399	1012	1029	1055	rBV	105871	265122	39.90%	3.735%
9	5.090	1226	1244	1272	rBV2	277369	660165	99.34%	9.300%
10	5.663	1405	1422	1445	rBV	210810	430846	64.83%	6.069%
11	6.116	1546	1563	1586	rBV	147001	307816	46.32%	4.336%
12	6.637	1714	1725	1739	rVB2	9783	20133	3.03%	0.284%
13	7.029	1835	1847	1863	rBV2	76032	139318	20.96%	1.963%
14	7.286	1914	1927	1935	rBV3	15984	31790	4.78%	0.448%
15	7.357	1935	1949	1968	rVV	321870	567503	85.40%	7.994%
16	7.666	2032	2045	2058	rBV2	43678	76330	11.49%	1.075%
17	8.138	2180	2192	2204	rBV	306694	561979	84.57%	7.917%
18	8.286	2230	2238	2245	rBV	4762	6999	1.05%	0.099%
19	8.894	2415	2427	2454	rBV	318009	532290	80.10%	7.498%
20	9.145	2496	2505	2512	rBV	11992	18885	2.84%	0.266%
21	9.273	2532	2545	2554	rBV	5313	11801	1.78%	0.166%
22	9.431	2584	2594	2606	rBV3	10261	18456	2.78%	0.260%
23	9.749	2677	2693	2709	rBV	52572	97540	14.68%	1.374%
24	9.855	2717	2726	2732	rBV9	7425	12579	1.89%	0.177%
25	9.887	2733	2736	2749	rVB9	6148	10080	1.52%	0.142%
26	10.260	2841	2852	2870	rVB	96733	157560	23.71%	2.220%
27	10.476	2909	2919	2926	rBV	8330	13901	2.09%	0.196%
28	10.556	2935	2944	2950	rBV6	6798	10230	1.54%	0.144%
29	11.084	3097	3108	3126	rBV	106936	182186	27.42%	2.566%
30	11.174	3129	3136	3138	rBV3	8302	9468	1.42%	0.133%
31	11.293	3162	3173	3194	rVB	296429	484379	72.89%	6.823%
32	11.575	3253	3261	3271	rBV4	11337	19449	2.93%	0.274%
33	11.672	3279	3291	3308	rVB	283600	453244	68.20%	6.385%
34	12.042	3398	3406	3417	rVB	5561	9854	1.48%	0.139%

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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	12.280	3470	3480	3492	rBV	80694	136050	20.47%	1.917%
36	12.389	3506	3514	3527	rVB3	21465	35273	5.31%	0.497%
37	12.508	3545	3551	3563	rVB3	6949	11055	1.66%	0.156%
38	13.482	3846	3854	3861	rBV10	5399	8917	1.34%	0.126%
39	13.678	3906	3915	3929	rBV2	39464	60954	9.17%	0.859%
40	15.170	4366	4379	4390	rBV2	10710	21205	3.19%	0.299%
41	15.607	4507	4515	4525	rBV2	6393	10548	1.59%	0.149%
42	16.234	4697	4710	4734	rBV2	90147	186348	28.04%	2.625%
43	16.360	4738	4749	4764	rVB2	122687	190872	28.72%	2.689%

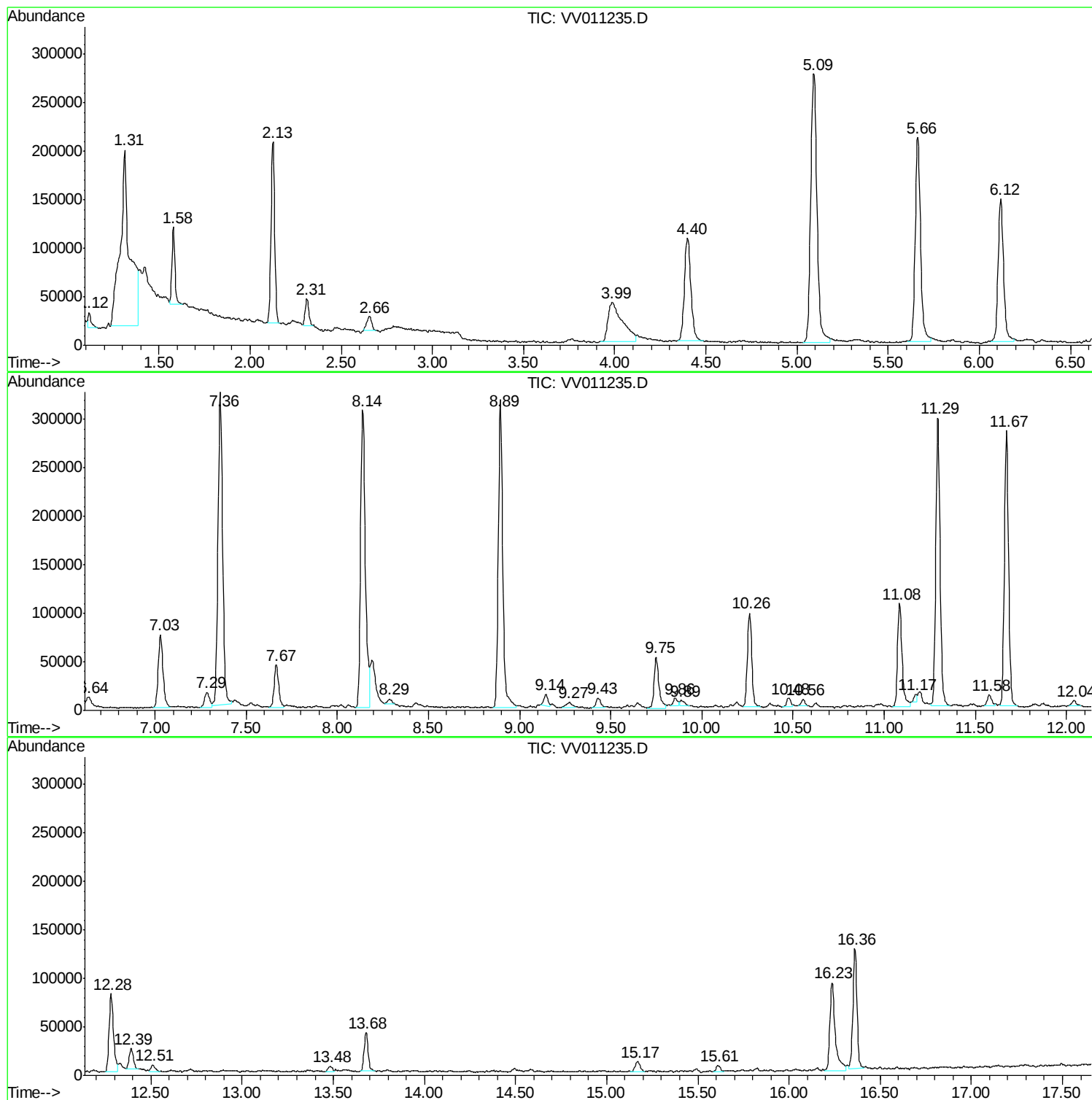
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
MSVOA_V
ClientSampleId :
F9P48

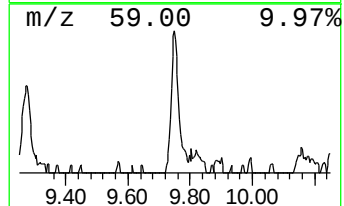
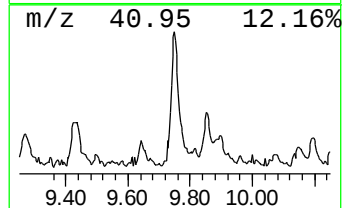
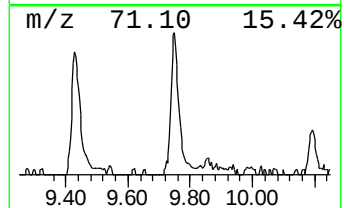
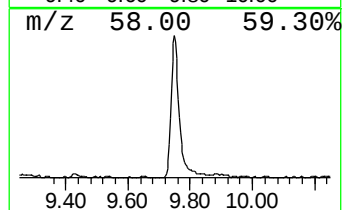
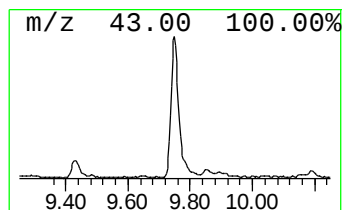
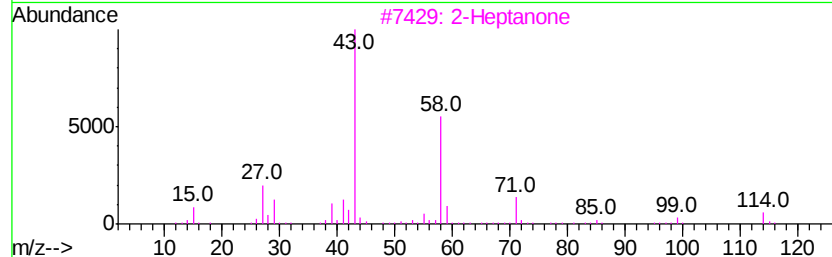
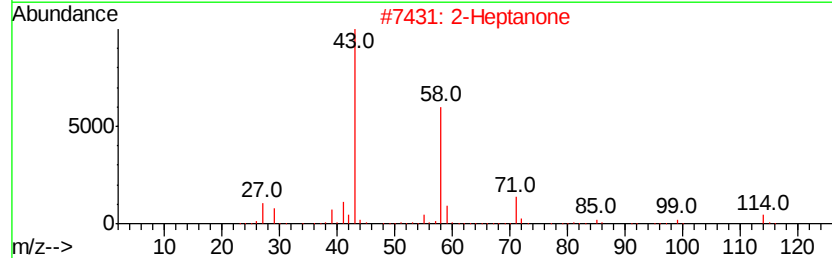
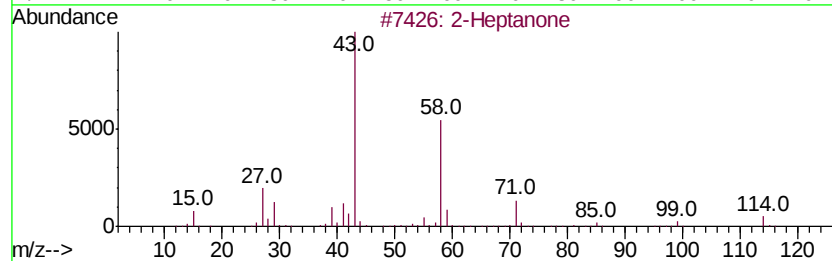
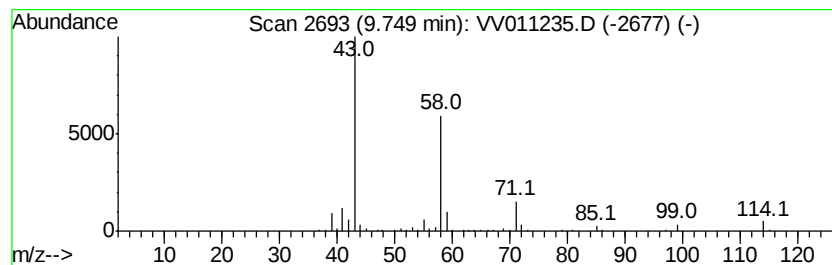
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	0.92 ug/L	97540	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	86
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	86



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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampled :
F9P48

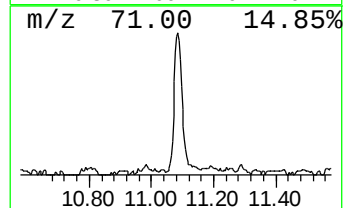
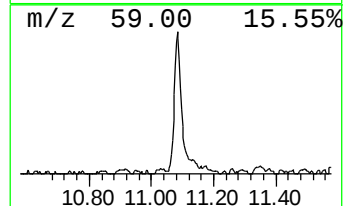
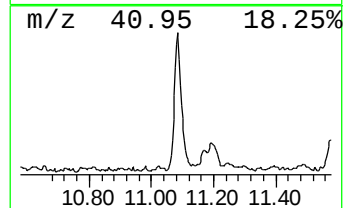
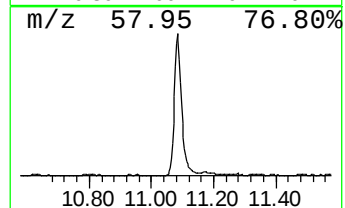
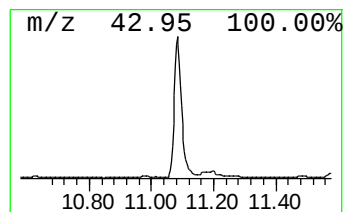
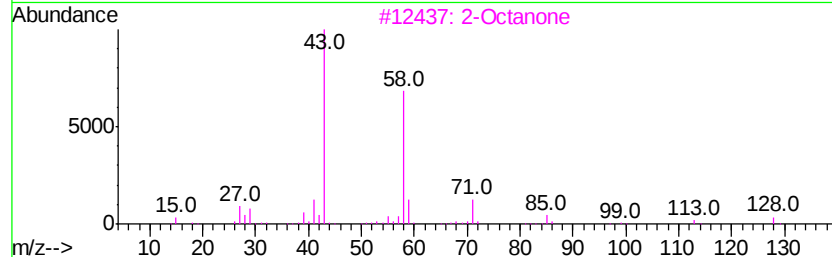
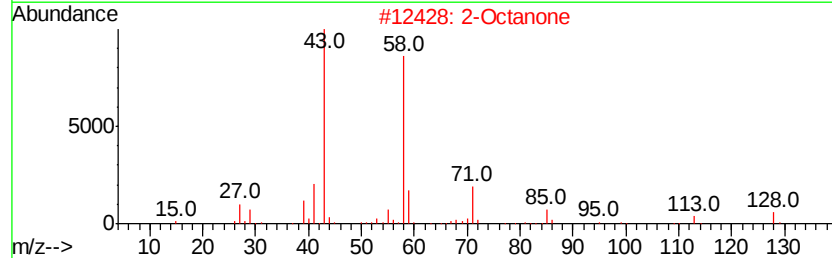
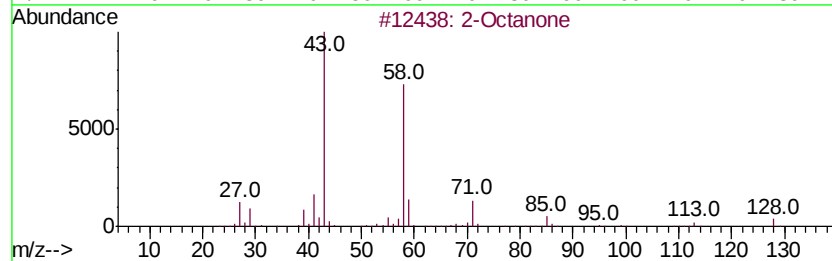
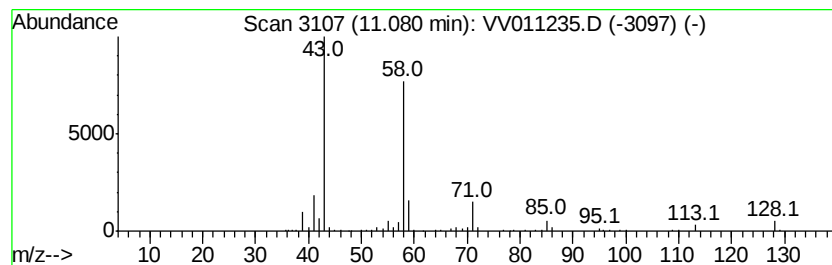
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.08	1.88 ug/L	182186	1,4-Dichlorobenzene-d4	11.30

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	91
5		2-Octanone	128	C8H16O	000111-13-7	90



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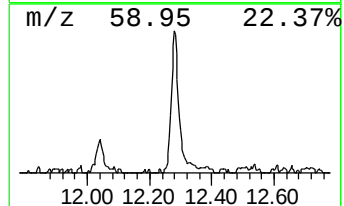
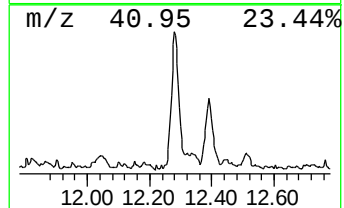
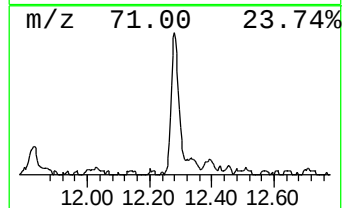
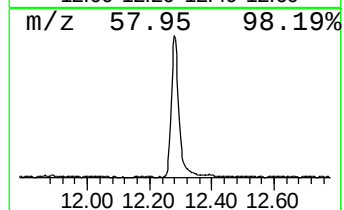
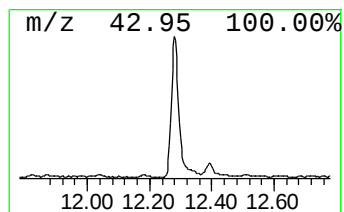
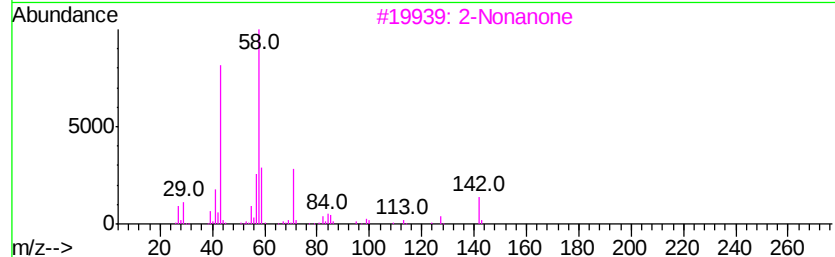
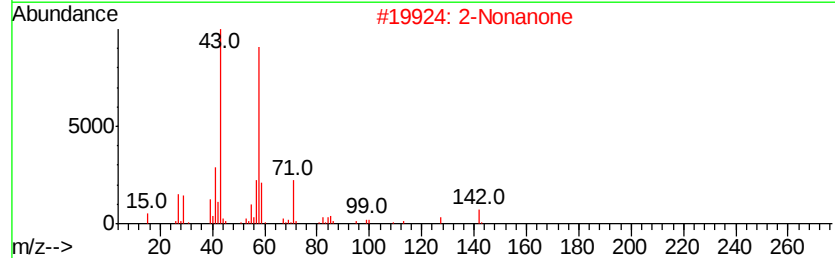
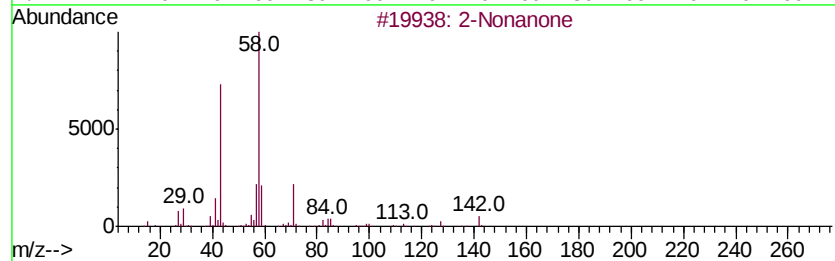
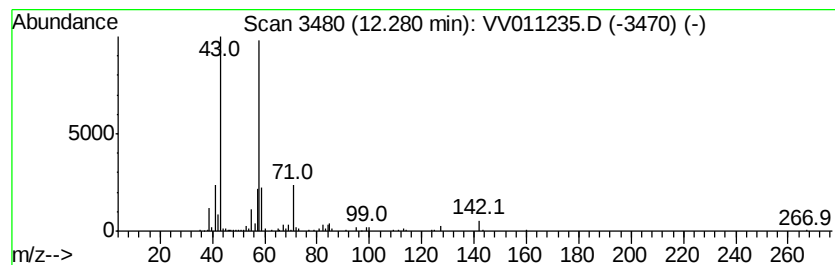
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 2-Nonanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	1.40 ug/L	136050	1,4-Dichlorobenzene-d4	11.30

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	95
3	2-Nonanone		142	C9H18O	000821-55-6	91
4	2-Decanone		156	C10H20O	000693-54-9	64
5	Pentanal, 2-methyl-		100	C6H12O	000123-15-9	59



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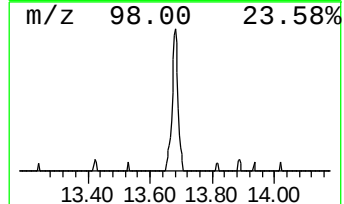
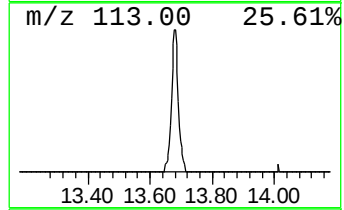
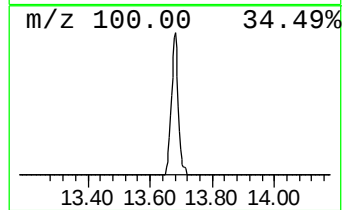
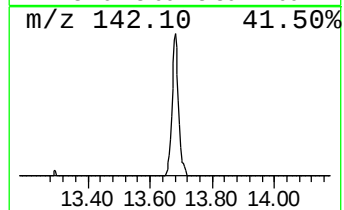
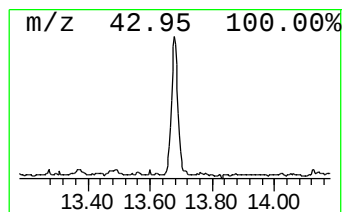
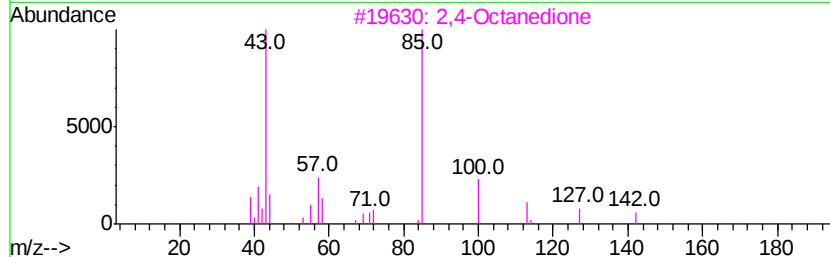
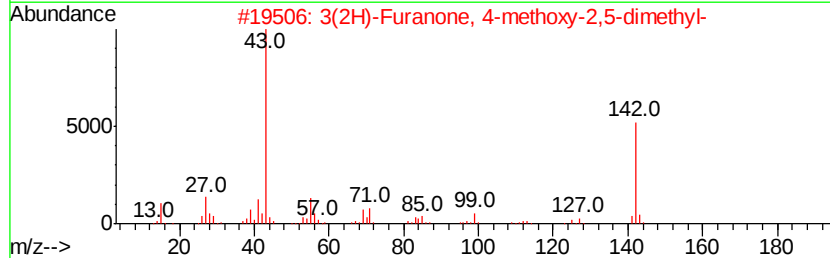
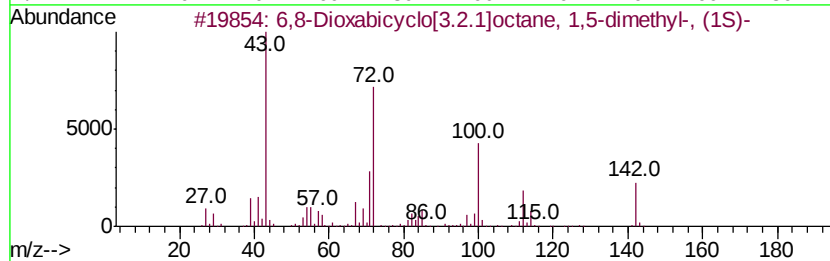
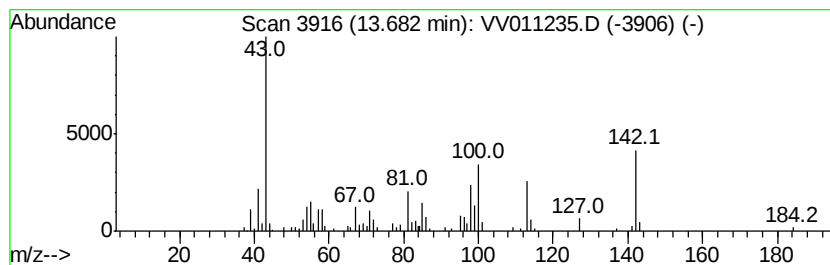
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	0.63 ug/L	60954	1,4-Dichlorobenzene-d4	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	27
2		3(2H)-Furanone, 4-methoxy-2,5-di...	142	C7H10O3	004077-47-8	27
3		2,4-Octanedione	142	C8H14O2	014090-87-0	25
4		6-Dodecanone	184	C12H24O	006064-27-3	16
5		4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	16



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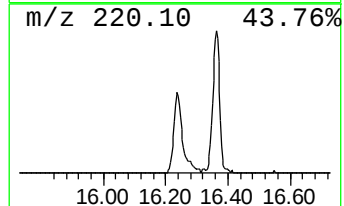
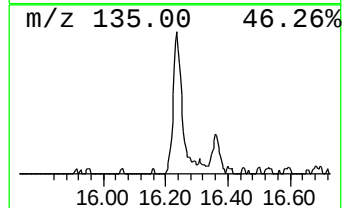
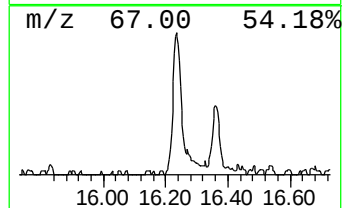
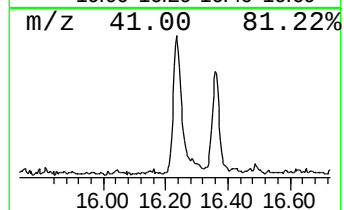
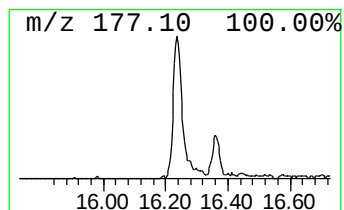
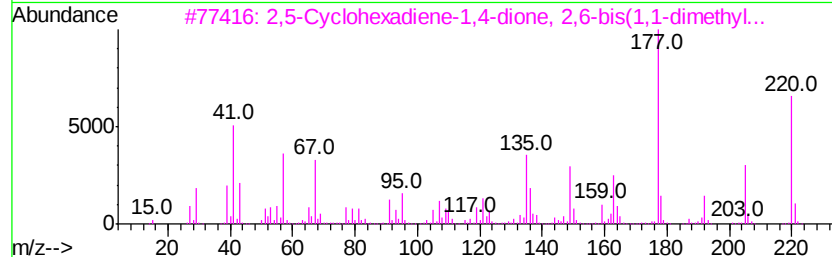
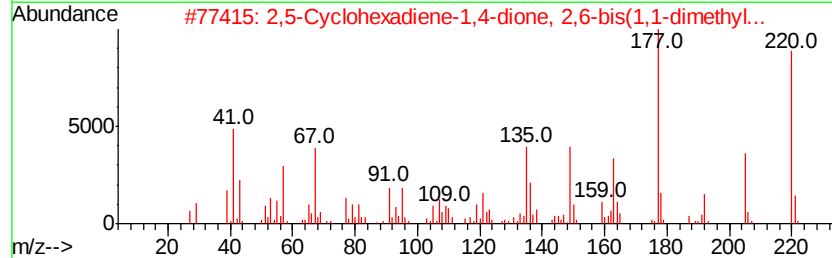
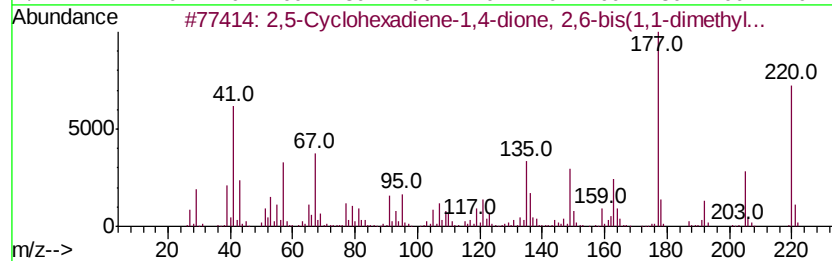
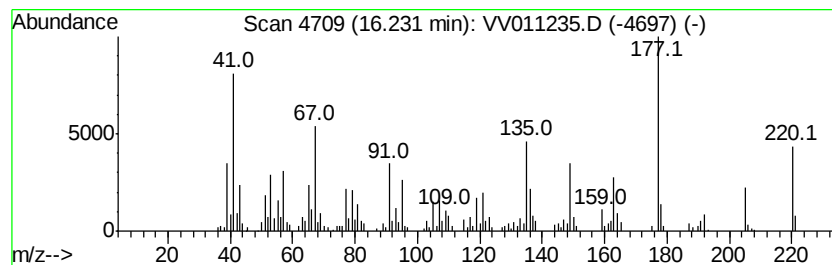
Instrument :
MSVOA_V
ClientSampleId :
F9P48

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 6 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.23	1.92 ug/L	186348	1,4-Dichlorobenzene-d4	11.30		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2		000719-22-2	98
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	87
4	Thiocoumarin, 4,4,6,8-tetramethyl-	220	C13H16OS		1000128-90-3	38
5	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS		1000128-90-2	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060519\
Data File : VV011235.D
Acq On : 05 Jun 2019 17:42
Operator : SY/MD
Sample : K3197-07
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P48

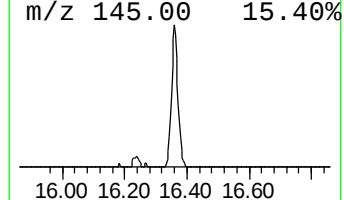
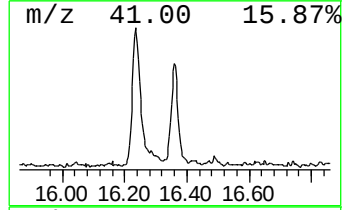
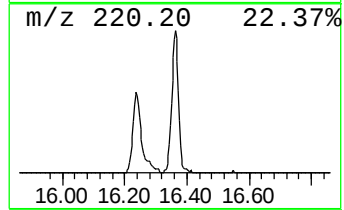
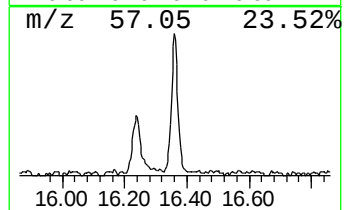
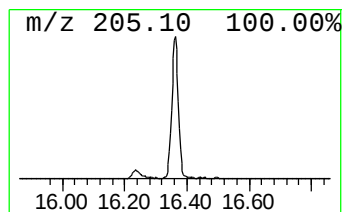
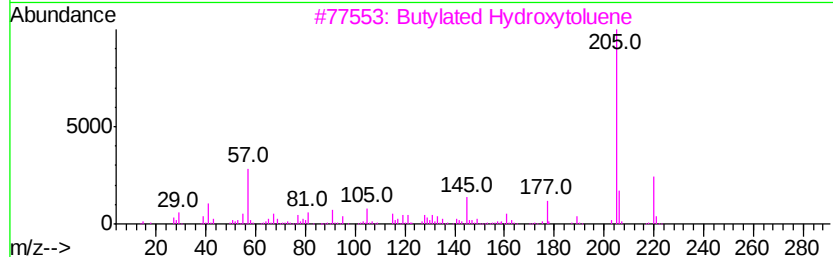
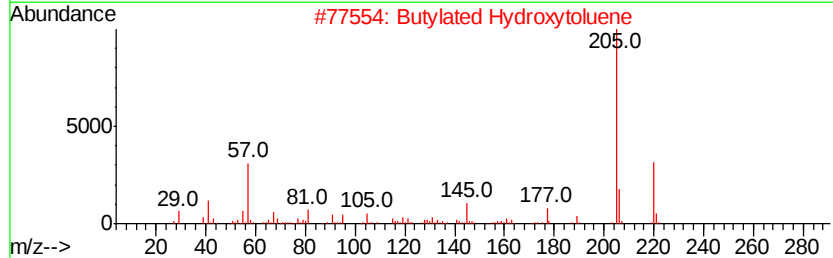
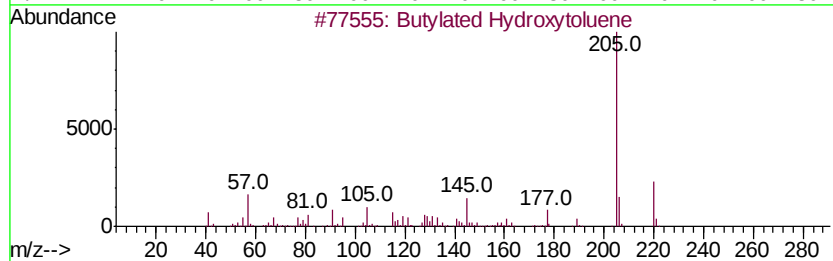
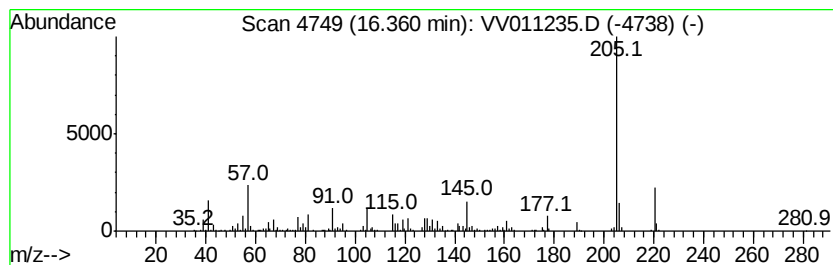
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	1.97 ug/L	190872	1,4-Dichlorobenzene-d4	11.30

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	97
3	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	96
4	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 2,4,6-tris(1-methylethyl)-		220	C15H24O	002934-07-8	87



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060519\
Data File : VV011235.D
Acq On : 05 Jun 2019 17:42
Operator : SY/MD
Sample : K3197-07
Misc : 25ML/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P48

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
2-Heptanone	9.75	0.9	ug/L	97540	2	8.89	532290	5.0
2-Octanone	11.08	1.9	ug/L	182186	3	11.30	484379	5.0
2-Nonanone	12.28	1.4	ug/L	136050	3	11.30	484379	5.0
unknown-01	13.68	0.6	ug/L	60954	3	11.30	484379	5.0
2,5-Cyclohexadien...	16.23	1.9	ug/L	186348	3	11.30	484379	5.0
Butylated Hydroxy...	16.36	2.0	ug/L	190872	3	11.30	484379	5.0