

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
 Data File : VV011293.D
 Acq On : 07 Jun 2019 17:38
 Operator : SY/MD
 Sample : K3197-13
 Misc : 25ML/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F9P57

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	24	rVB2	18998	21905	3.09%	0.342%
2	1.312	60	69	76	rBV2	86921	112772	15.90%	1.763%
3	1.421	99	103	116	rVB	25425	34237	4.83%	0.535%
4	1.579	146	152	162	rVB	66421	77711	10.96%	1.215%
5	2.122	312	321	334	rVB	147166	204153	28.79%	3.192%
6	2.309	374	379	388	rVB	17522	24591	3.47%	0.384%
7	2.470	423	429	440	rBV3	7128	13359	1.88%	0.209%
8	2.650	479	485	496	rVB2	11520	22462	3.17%	0.351%
9	2.781	502	526	527	rBV2	20231	59661	8.41%	0.933%
10	3.762	806	831	845	rBV4	18257	63491	8.95%	0.993%
11	3.981	884	899	940	rBV2	38528	205074	28.92%	3.206%
12	4.396	1010	1028	1046	rBV	95750	233474	32.93%	3.650%
13	5.090	1224	1244	1269	rBV2	235994	566878	79.95%	8.863%
14	5.662	1406	1422	1440	rBV	201808	410244	57.86%	6.414%
15	6.071	1538	1549	1552	rBV5	13436	20709	2.92%	0.324%
16	6.116	1553	1563	1594	rVB2	131699	279714	39.45%	4.373%
17	6.341	1625	1633	1646	rVB9	5296	11668	1.65%	0.182%
18	6.630	1717	1723	1734	rVB4	10672	20169	2.84%	0.315%
19	7.029	1833	1847	1860	rBV	59459	110375	15.57%	1.726%
20	7.357	1936	1949	1967	rBV	265908	460486	64.94%	7.200%
21	7.666	2031	2045	2059	rBV2	35910	63665	8.98%	0.995%
22	8.138	2181	2192	2206	rBV	284013	528559	74.54%	8.264%
23	8.289	2230	2239	2255	rVB8	12906	27006	3.81%	0.422%
24	8.894	2415	2427	2443	rBV	293836	487870	68.81%	7.628%
25	9.145	2493	2505	2515	rBV	73068	115925	16.35%	1.812%
26	9.257	2533	2540	2550	rVB10	5366	10283	1.45%	0.161%
27	9.428	2582	2593	2603	rBV10	3689	7095	1.00%	0.111%
28	9.752	2686	2694	2706	rVB2	13271	22386	3.16%	0.350%
29	9.855	2717	2726	2733	rBV9	7801	14474	2.04%	0.226%
30	10.260	2841	2852	2864	rBV	87857	139667	19.70%	2.184%
31	10.553	2934	2943	2955	rBV2	11562	20274	2.86%	0.317%
32	11.083	3098	3108	3121	rBV2	20863	39507	5.57%	0.618%
33	11.196	3136	3143	3155	rVB6	20373	33844	4.77%	0.529%
34	11.292	3162	3173	3187	rBV	269856	433751	61.17%	6.782%

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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

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

35	11.575	3247	3261	3279	rBV	391253	709057	100.00%	11.086%
36	11.669	3281	3290	3312	rVB	256222	430736	60.75%	6.734%
37	12.042	3400	3406	3420	rVB	3976	7402	1.04%	0.116%
38	12.279	3468	3480	3489	rBV	50569	85853	12.11%	1.342%
39	12.392	3504	3515	3527	rBV3	28061	43639	6.15%	0.682%
40	13.482	3845	3854	3864	rBV9	10001	16504	2.33%	0.258%
41	13.681	3906	3916	3928	rVB7	12043	20687	2.92%	0.323%
42	15.167	4367	4378	4388	rBV7	7029	12034	1.70%	0.188%
43	16.234	4699	4710	4724	rBV3	60254	117359	16.55%	1.835%
44	16.360	4741	4749	4758	rBV3	36639	55372	7.81%	0.866%

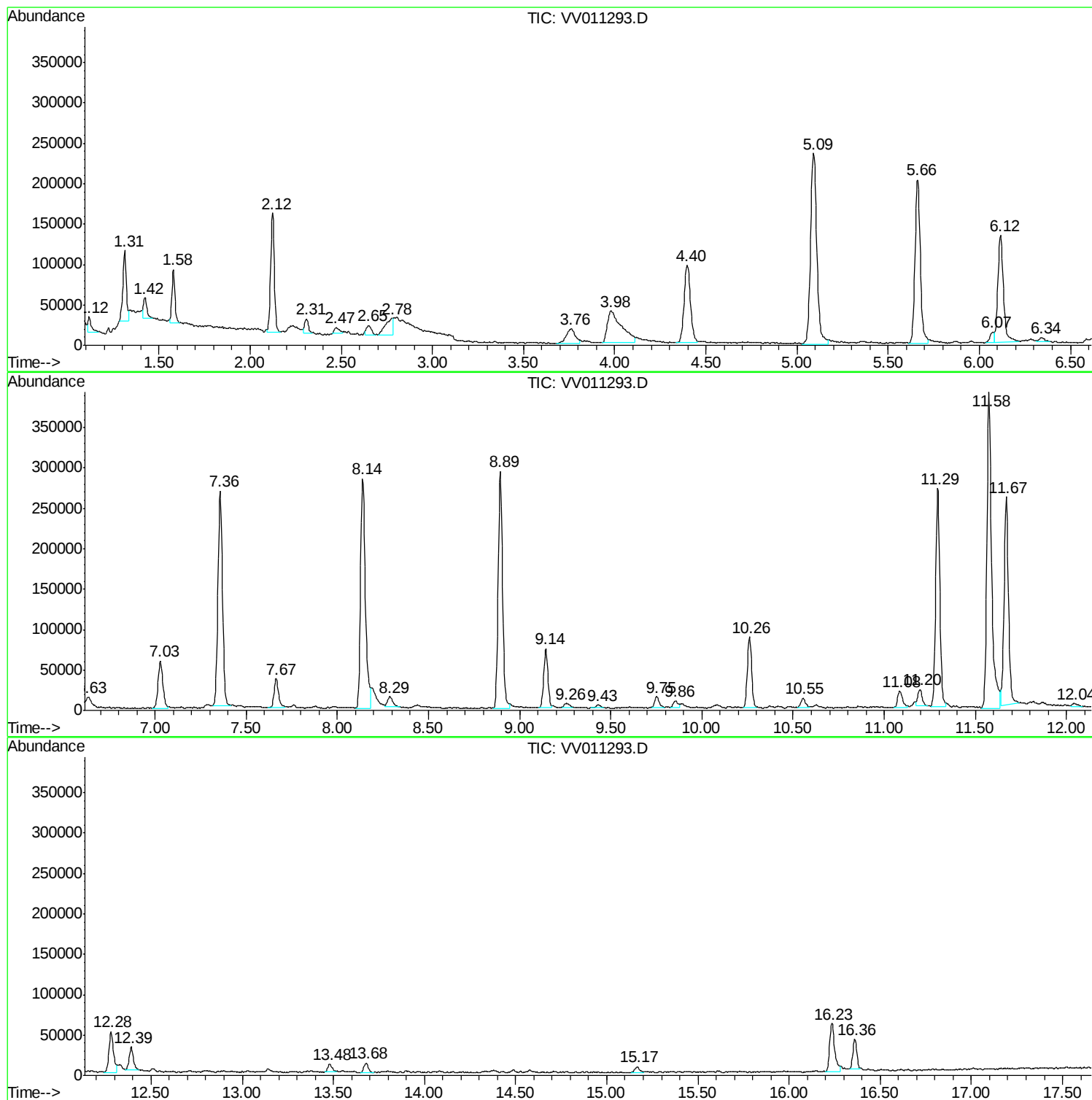
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR060419WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
MSVOA_V
ClientSampleId :
F9P57

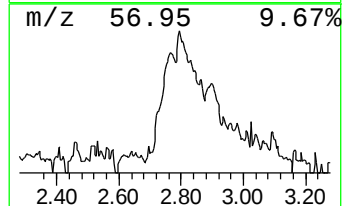
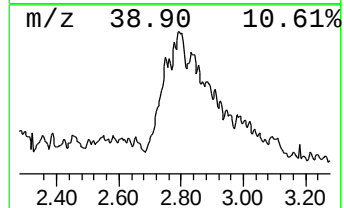
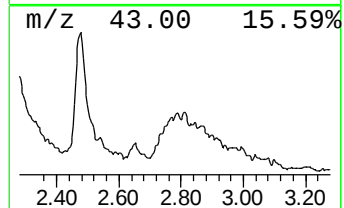
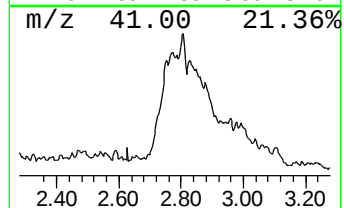
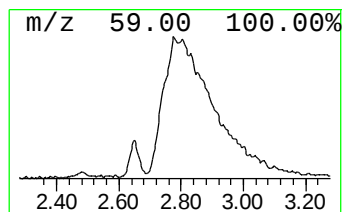
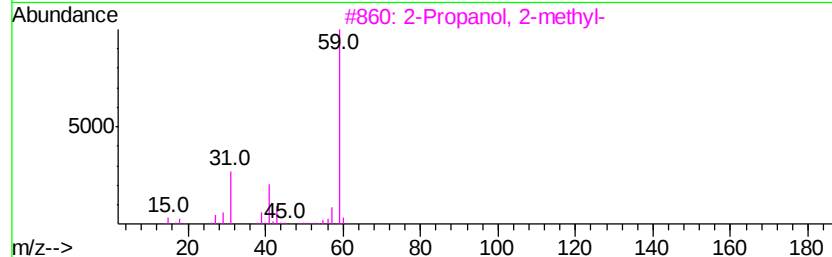
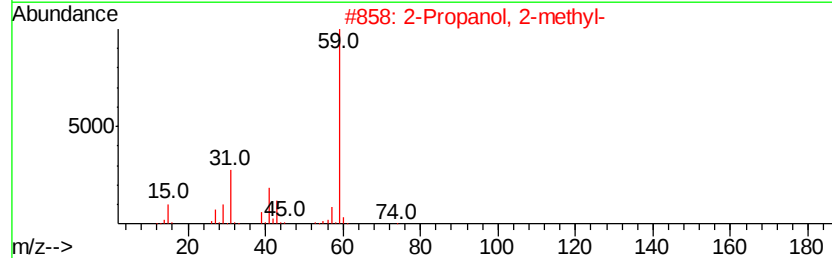
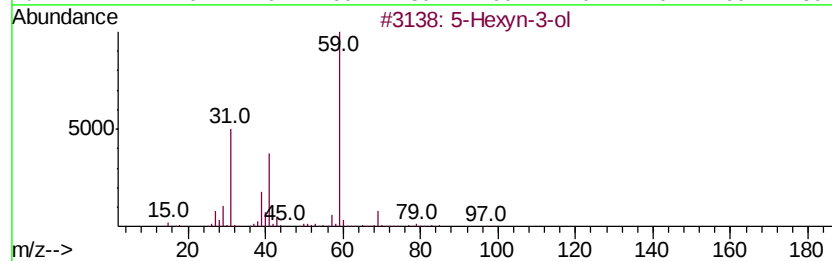
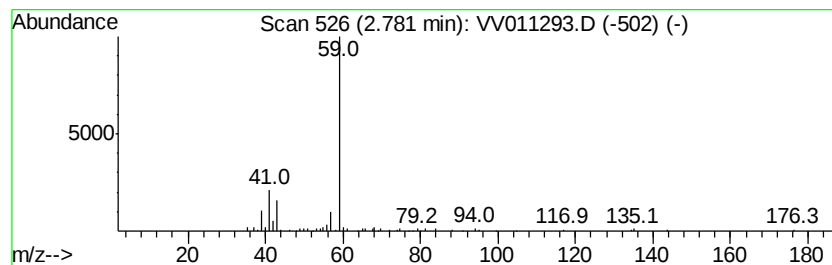
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.78	0.73 ug/L	59661	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Hexyn-3-ol	98	C6H10O	019780-84-8	39
2		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39
3		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39
4		d-Ribo-tetrofuranose, 4-c-cyclop...	200	C10H16O4	030571-50-7	17
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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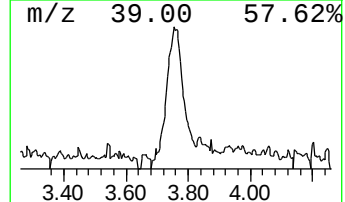
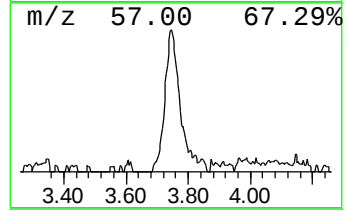
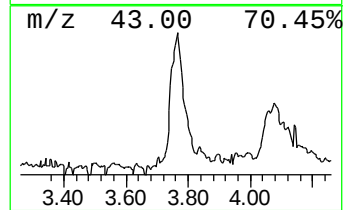
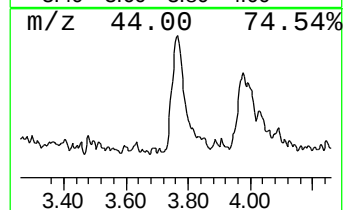
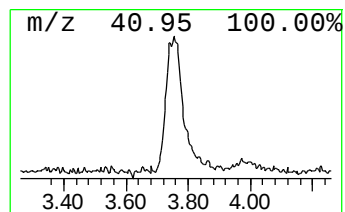
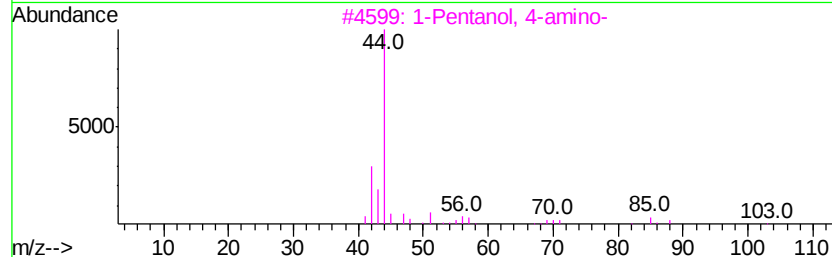
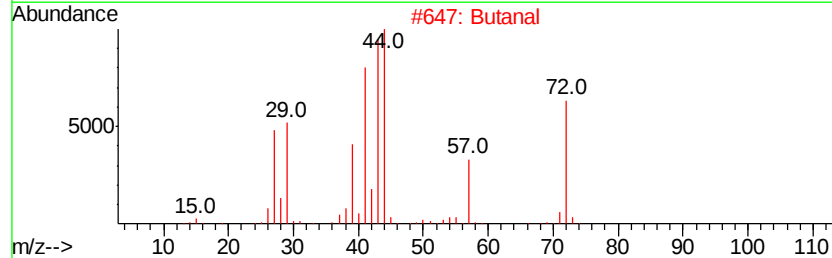
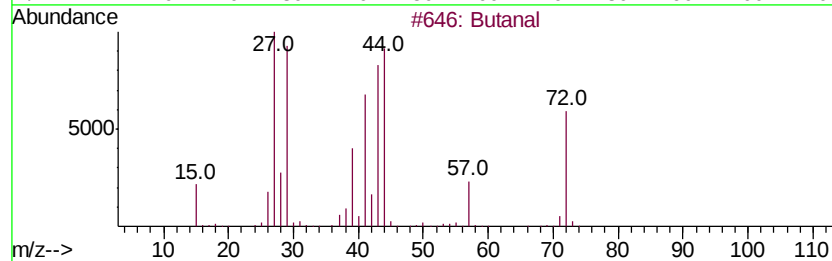
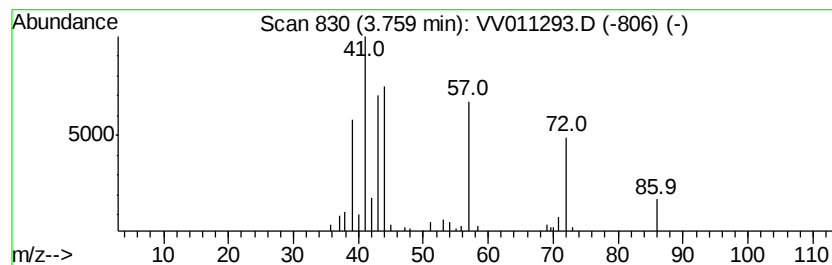
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	0.77 ug/L	63491	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	58
2		Butanal	72	C4H8O	000123-72-8	49
3		1-Pentanol, 4-amino-	103	C5H13NO	000927-55-9	47
4		Butanal	72	C4H8O	000123-72-8	43
5		Butanal	72	C4H8O	000123-72-8	43



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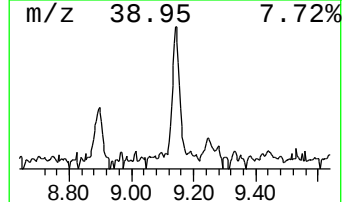
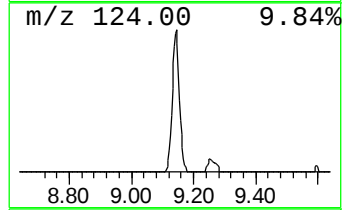
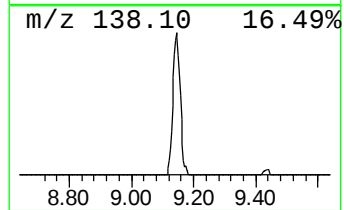
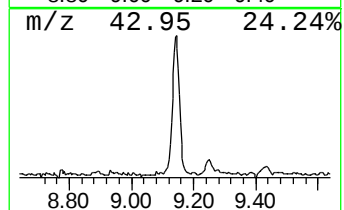
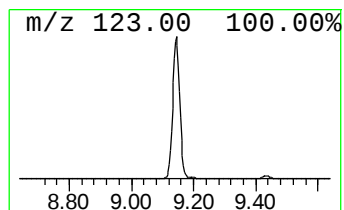
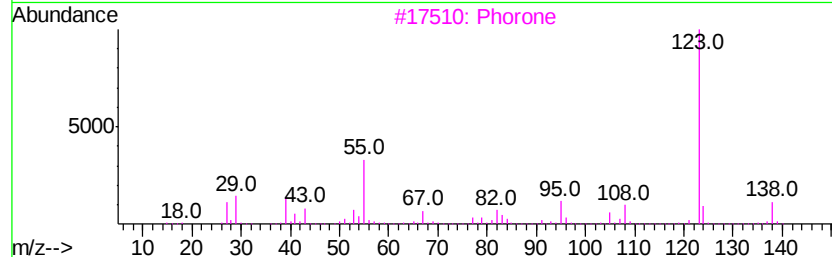
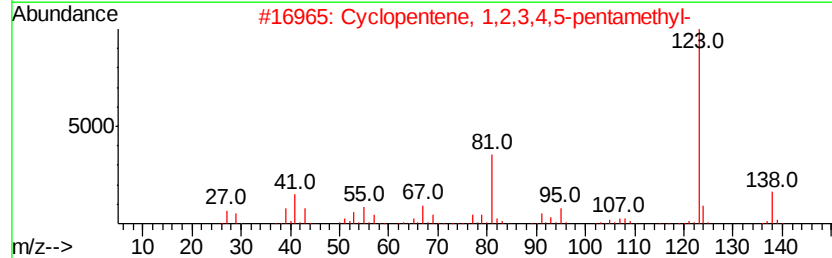
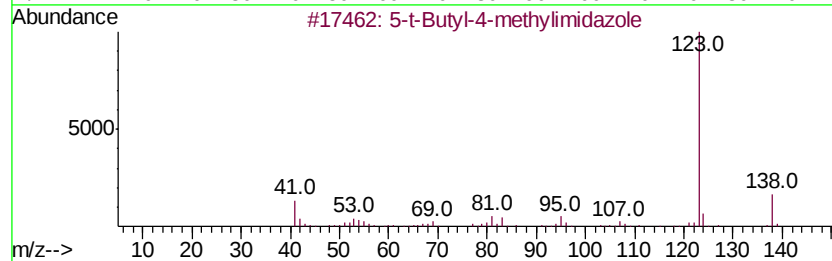
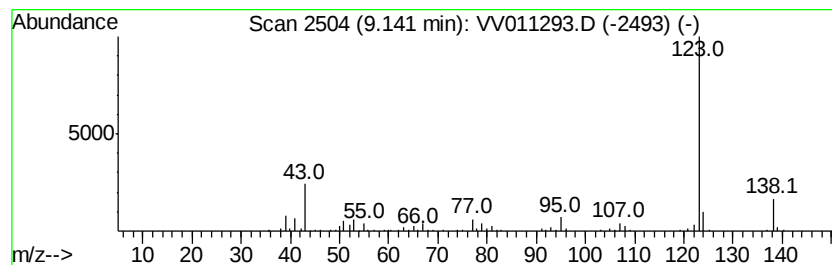
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.14	1.19 ug/L	115925	Chlorobenzene-d5	8.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	90
2		Cyclopentene, 1,2,3,4,5-pentamet...	138	C10H18	1000154-28-6	87
3		Phorone	138	C9H14O	000504-20-1	78
4		Cyclopentene, 1,2,3,3,4-pentamet...	138	C10H18	197390-29-7	78
5		3-Pyridinol, 2,6-dimethyl-	123	C7H9NO	001122-43-6	59



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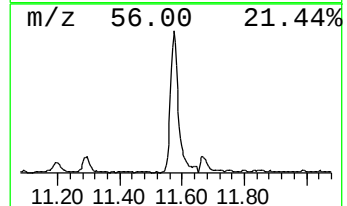
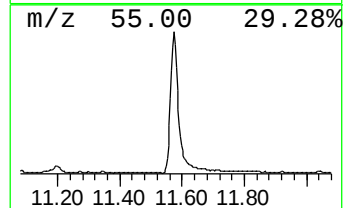
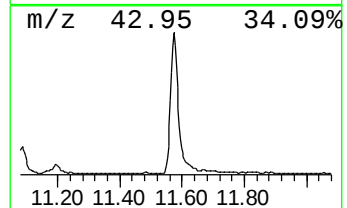
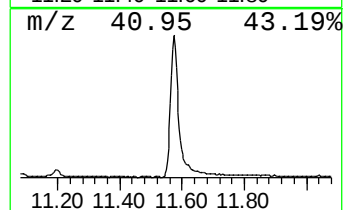
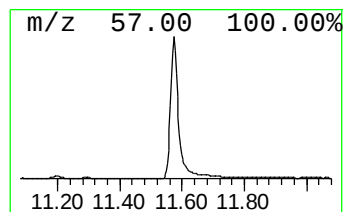
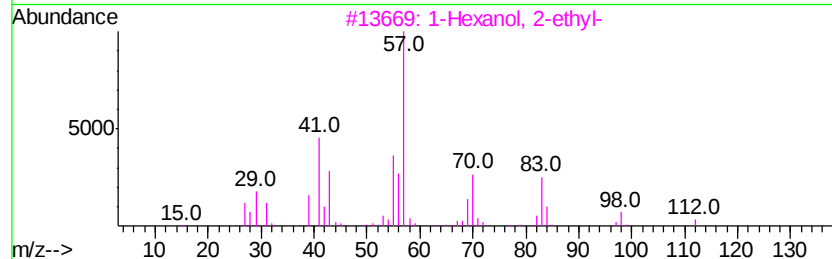
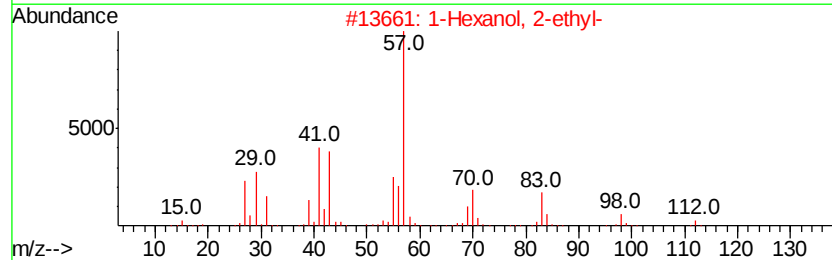
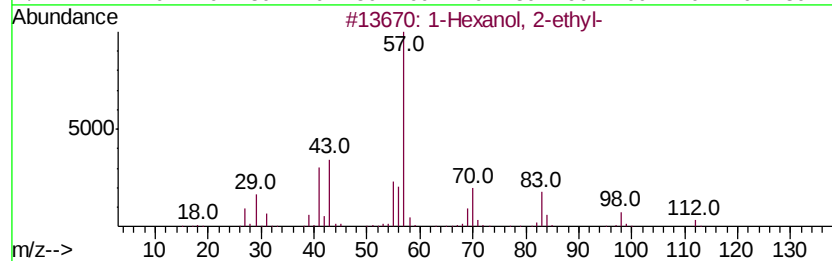
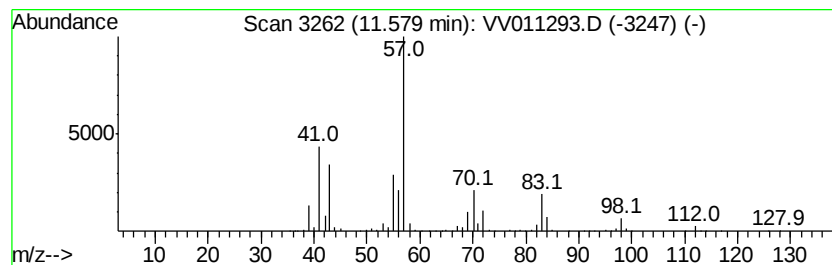
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	8.17 ug/L	709057	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	78
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
5		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53



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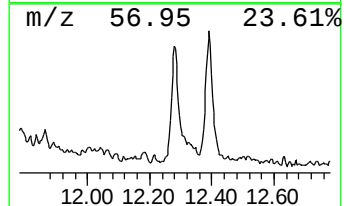
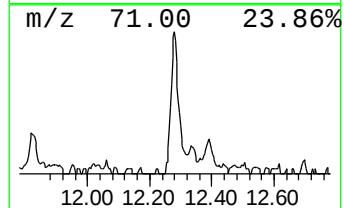
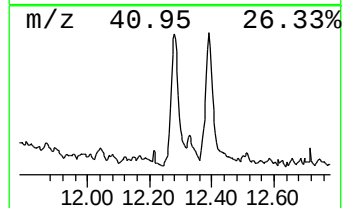
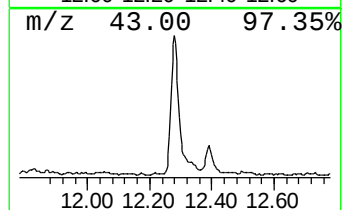
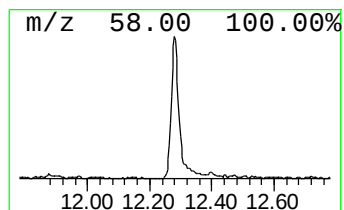
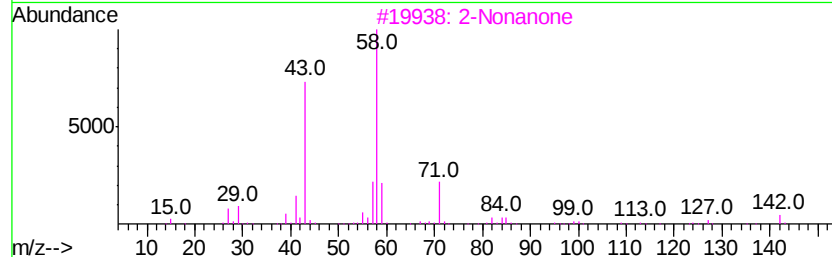
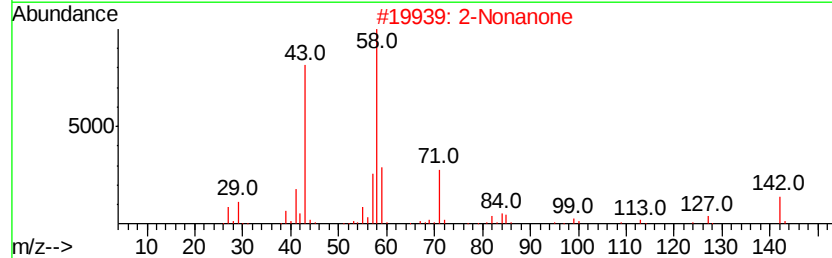
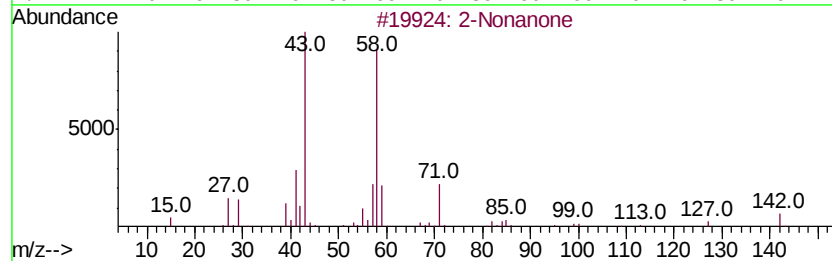
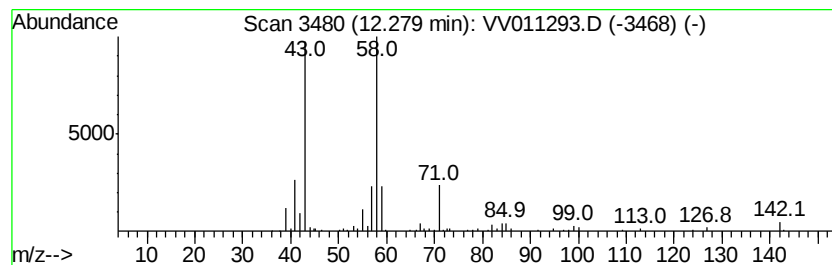
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2-Nonanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.28	0.99 ug/L	85853	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Nonanone	142	C9H18O	000821-55-6	91
2		2-Nonanone	142	C9H18O	000821-55-6	87
3		2-Nonanone	142	C9H18O	000821-55-6	87
4		2-Nonanone	142	C9H18O	000821-55-6	78
5		2-Heptanone	114	C7H14O	000110-43-0	72



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011293.D
Acq On : 07 Jun 2019 17:38
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

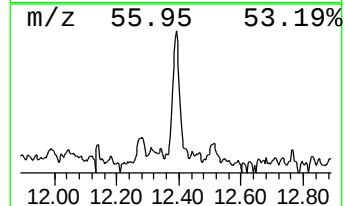
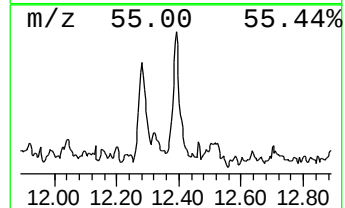
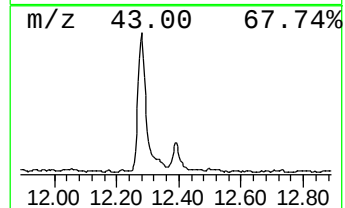
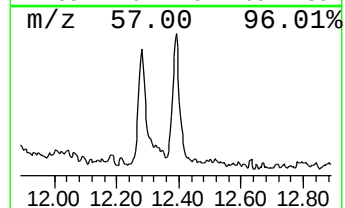
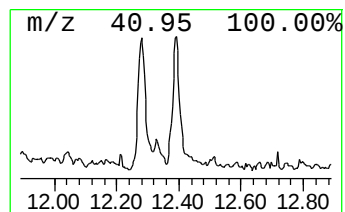
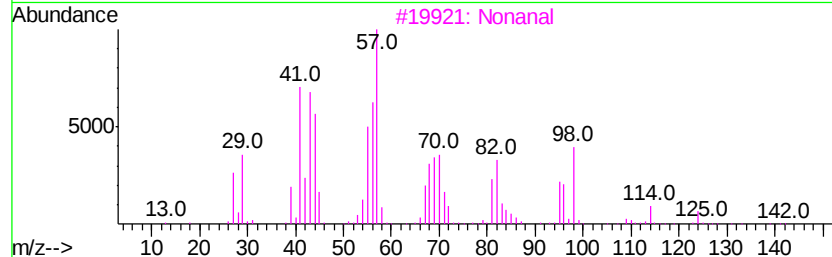
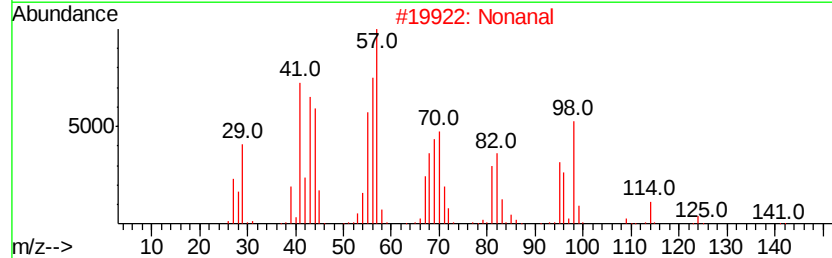
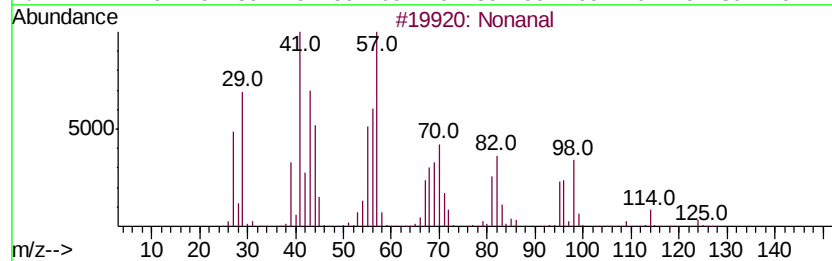
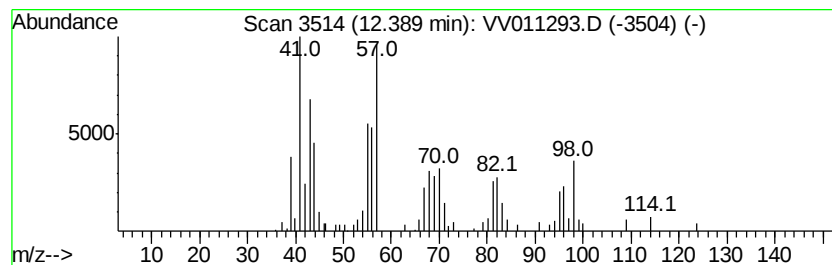
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Nonanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.39	0.50 ug/L	43639	1,4-Dichlorobenzene-d4	11.29
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonanal		142 C9H18O	000124-19-6 91
2	Nonanal		142 C9H18O	000124-19-6 90
3	Nonanal		142 C9H18O	000124-19-6 86
4	1,3-Cyclohexanediamine		114 C6H14N2	003385-21-5 43
5	trans-2-Undecen-1-ol		170 C11H22O	075039-84-8 27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011293.D
Acq On : 07 Jun 2019 17:38
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P57

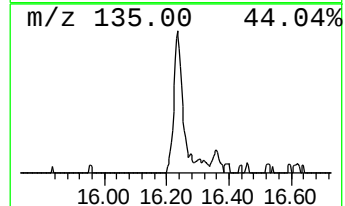
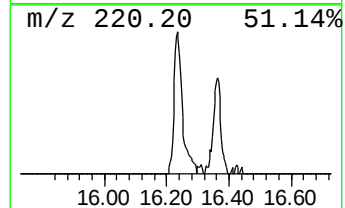
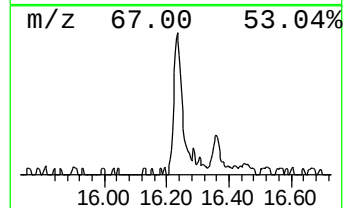
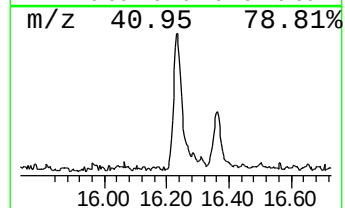
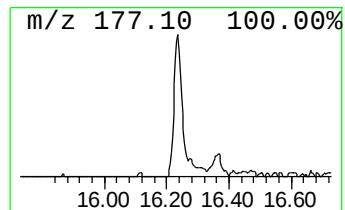
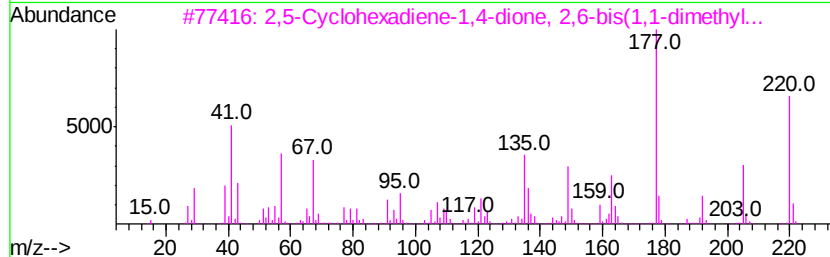
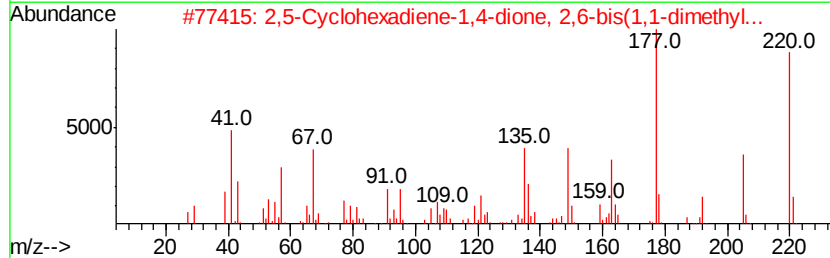
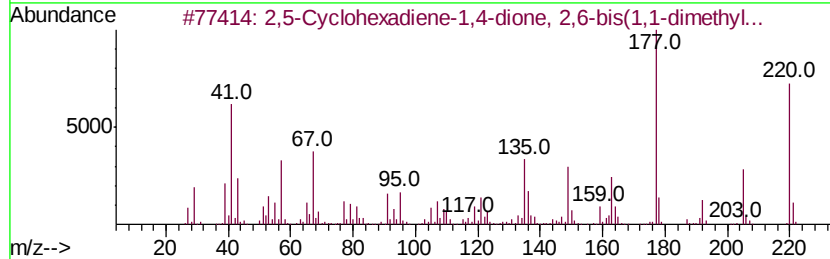
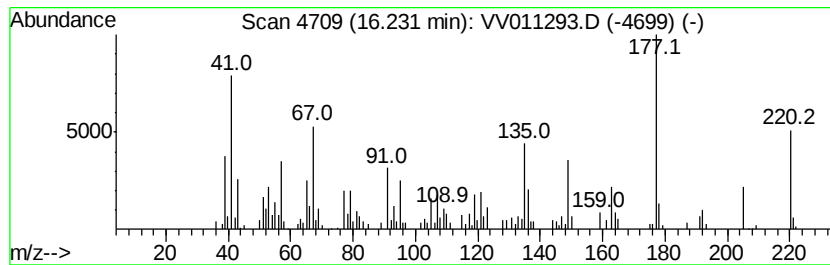
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.23	1.35 ug/L	117359	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	97
3		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
4		Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	46
5		Thiocoumarin, 4,4,6,8-tetramethyl-	220	C13H16OS	1000128-90-3	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060619\
Data File : VV011293.D
Acq On : 07 Jun 2019 17:38
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P57

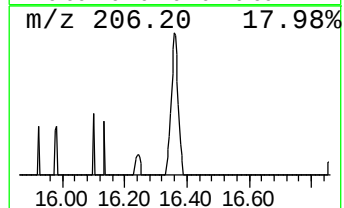
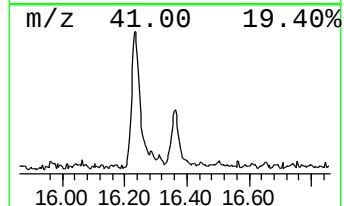
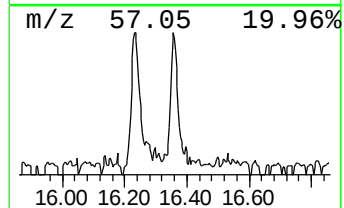
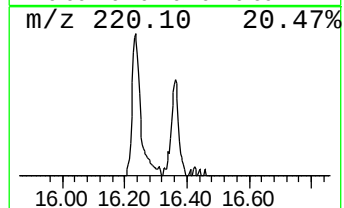
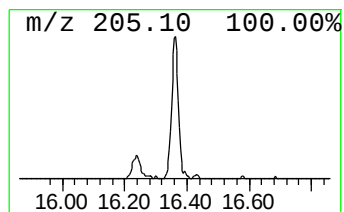
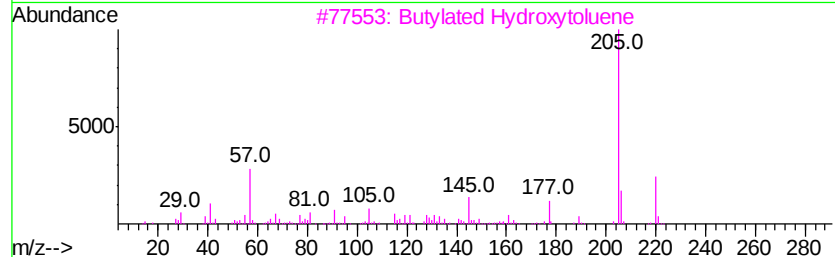
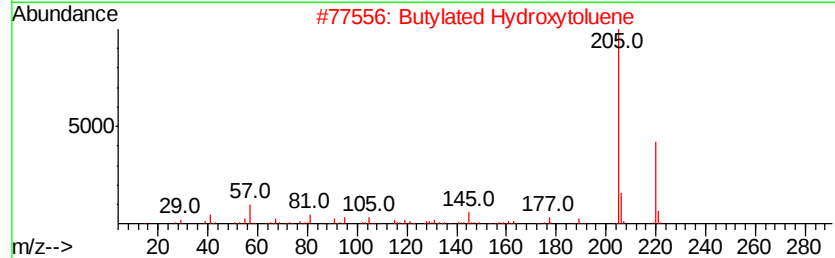
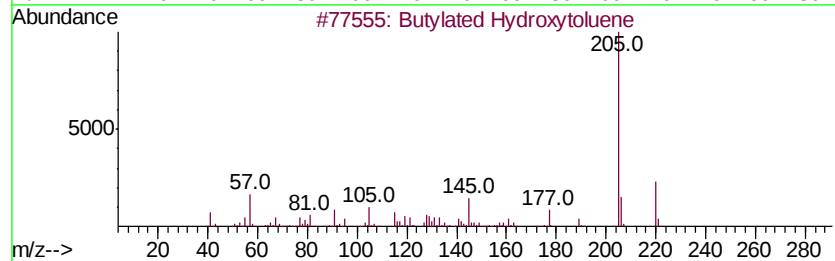
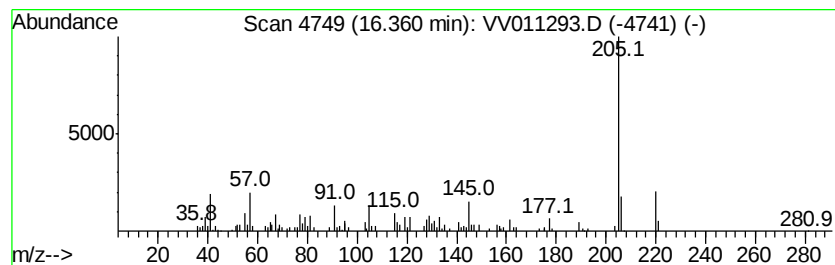
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Butylated Hydroxytoluene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	0.64 ug/L	55372	1,4-Dichlorobenzene-d4	11.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	97
2	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	94
3	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	93
4	Butylated		Hydroxytoluene	220	C15H24O	000128-37-0	93
5	Phenol, 4,6-di(1,1-dimethylethyl...			220	C15H24O	000616-55-7	87



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060619\
Data File : VV011293.D
Acq On : 07 Jun 2019 17:38
Operator : SY/MD
Sample : K3197-13
Misc : 25ML/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F9P57

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
unknown-01	2.78	0.7	ug/L	59661	1	5.66	410244	5.0
Butanal	3.76	0.8	ug/L	63491	1	5.66	410244	5.0
5-t-Butyl-4-methy...	9.14	1.2	ug/L	115925	2	8.89	487870	5.0
1-Hexanol, 2-ethyl-	11.58	8.2	ug/L	709057	3	11.29	433751	5.0
2-Nonanone	12.28	1.0	ug/L	85853	3	11.29	433751	5.0
Nonanal	12.39	0.5	ug/L	43639	3	11.29	433751	5.0
2,5-Cyclohexadien...	16.23	1.4	ug/L	117359	3	11.29	433751	5.0
Butylated Hydroxy...	16.36	0.6	ug/L	55372	3	11.29	433751	5.0