

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
 Data File : VU029449.D
 Acq On : 14 Feb 2019 11:49
 Operator : JC/SP
 Sample : K1387-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0JJ8

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_U\METHOD\SOMUTR021219WMA.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	1.180	23	28	40	rBV3	12883	14523	2.22%	0.208%
2	1.302	60	66	78	rBV	44775	44947	6.86%	0.643%
3	1.386	84	92	111	rBV2	416346	500919	76.44%	7.167%
4	1.473	114	119	129	rVB	7797	9868	1.51%	0.141%
5	1.547	136	142	153	rBV3	9927	14015	2.14%	0.201%
6	1.679	176	183	194	rVB	75076	91952	14.03%	1.316%
7	2.061	298	302	313	rVB	7226	11245	1.72%	0.161%
8	2.273	357	368	377	rBV	174087	263242	40.17%	3.766%
9	2.322	377	383	396	rVB	43433	70449	10.75%	1.008%
10	2.444	412	421	440	rVB	47765	88689	13.53%	1.269%
11	2.836	530	543	560	rBV	98100	204154	31.15%	2.921%
12	3.990	883	902	923	rBV2	62363	178216	27.20%	2.550%
13	4.193	950	965	975	rBV	87349	239763	36.59%	3.430%
14	4.646	1088	1106	1127	rBV2	101159	245554	37.47%	3.513%
15	4.987	1195	1212	1234	rBV	96957	232864	35.54%	3.332%
16	5.338	1294	1321	1351	rBV2	207439	572122	87.31%	8.186%
17	5.884	1473	1491	1513	rBV	217597	435610	66.47%	6.233%
18	6.328	1614	1629	1651	rBV	131304	263118	40.15%	3.765%
19	6.784	1754	1771	1781	rBV	57774	122768	18.73%	1.757%
20	7.225	1895	1908	1927	rBV	74677	138885	21.19%	1.987%
21	7.563	2000	2013	2030	rBV	295378	515776	78.71%	7.380%
22	7.849	2092	2102	2120	rBV	45575	82714	12.62%	1.183%
23	8.177	2188	2204	2216	rBV3	9582	19704	3.01%	0.282%
24	8.312	2235	2246	2288	rBV	364711	655307	100.00%	9.376%
25	8.469	2288	2295	2304	rVB6	5715	8094	1.24%	0.116%
26	9.087	2475	2487	2511	rBV	311579	521648	79.60%	7.464%
27	10.029	2770	2780	2796	rBV5	7570	13792	2.10%	0.197%
28	10.431	2891	2905	2917	rBV2	113534	182554	27.86%	2.612%
29	10.604	2949	2959	2969	rBV4	14232	23963	3.66%	0.343%
30	11.482	3220	3232	3259	rBV	347805	568070	86.69%	8.128%
31	11.749	3304	3315	3331	rBV3	7372	15592	2.38%	0.223%
32	11.858	3337	3349	3367	rBV	307377	505188	77.09%	7.228%
33	12.463	3526	3537	3539	rBV2	10473	13406	2.05%	0.192%
34	13.987	4000	4011	4024	rBV2	42742	67324	10.27%	0.963%

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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_U\METHOD\SOMUTR021219WMA.M
Title : TRACE VOA SOM01.0

35	14.279	4092	4102	4112	rVB	4915	8442	1.29%	0.121%
36	14.575	4184	4194	4201	rBV6	5111	10062	1.54%	0.144%
37	15.646	4516	4527	4537	rBV6	9755	18332	2.80%	0.262%
38	16.340	4734	4743	4754	rBV6	8931	16287	2.49%	0.233%

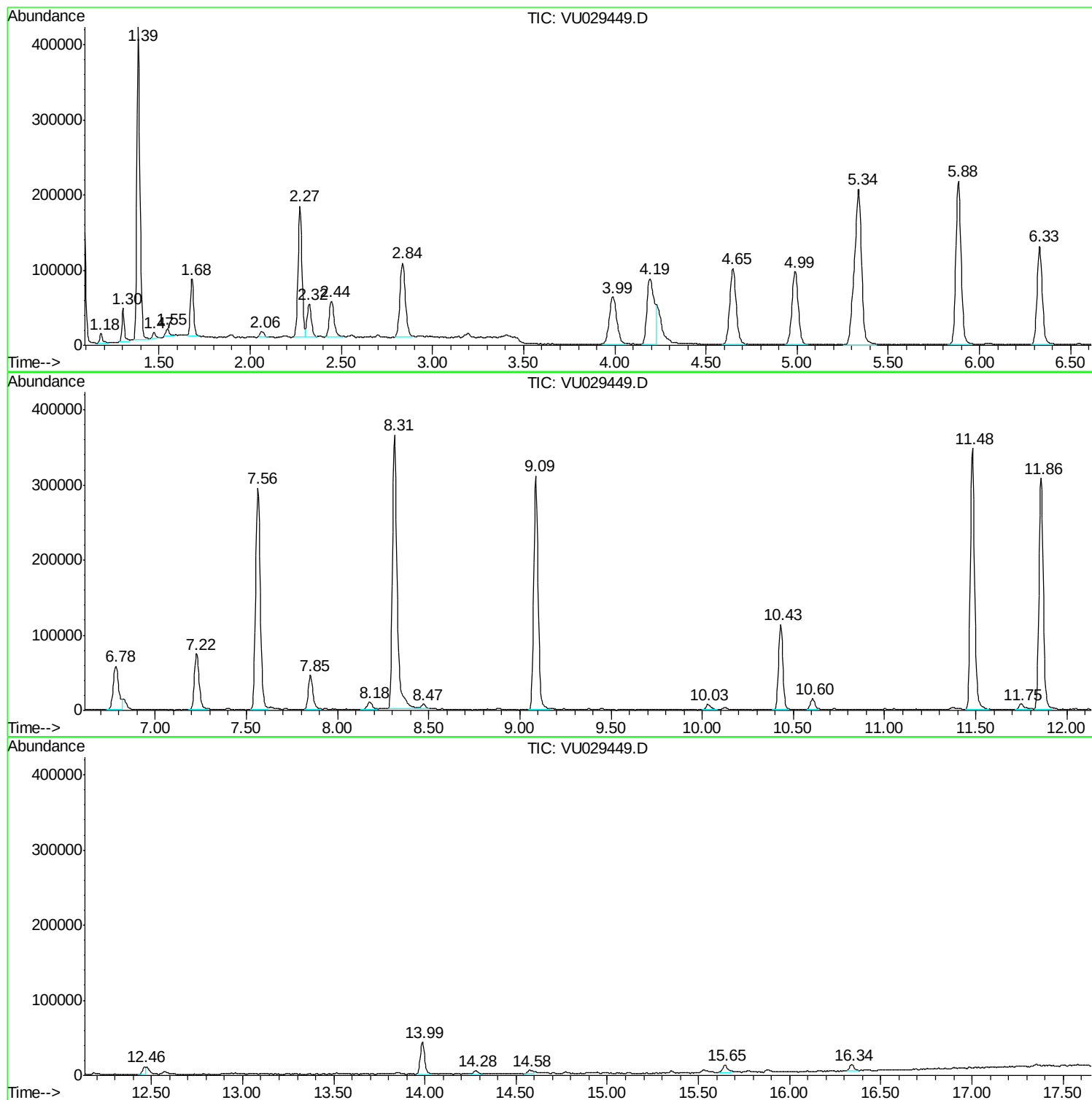
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Quant Title : TRACE VOA SOM01.0

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



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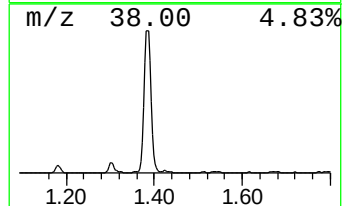
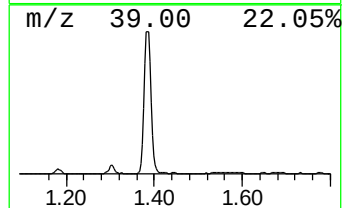
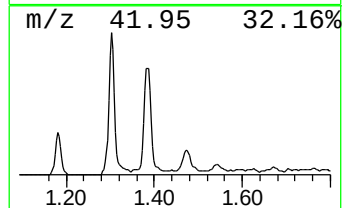
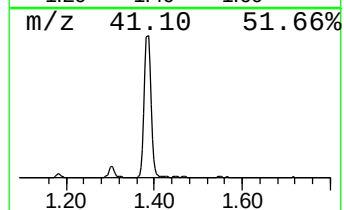
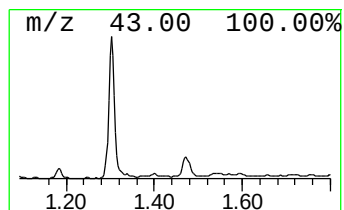
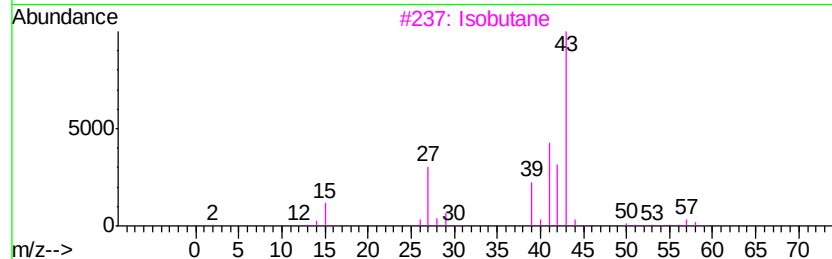
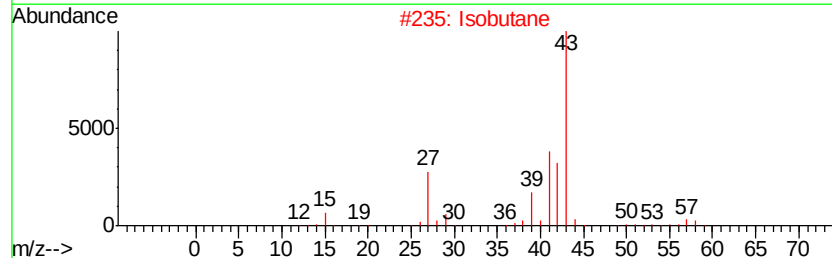
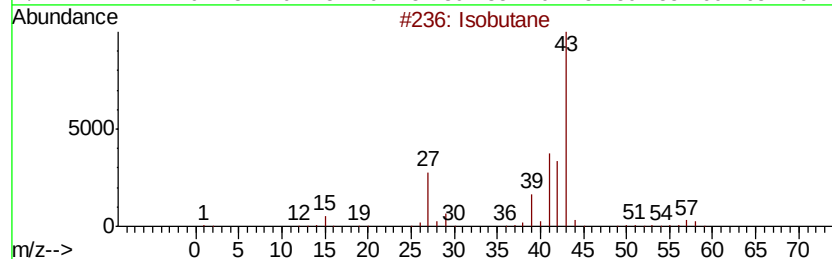
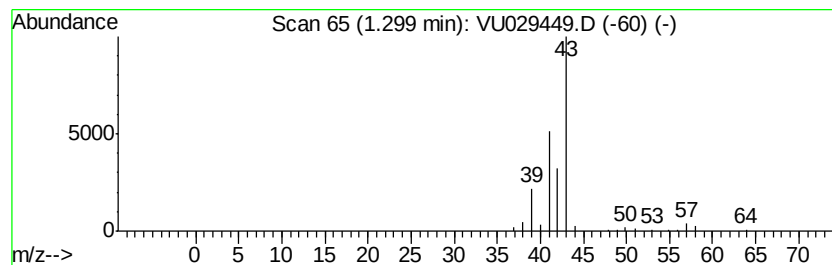
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	0.52 ug/L	44947	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isobutane	58	C4H10	000075-28-5	80
2		Isobutane	58	C4H10	000075-28-5	72
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	59
5		Isobutyl nitrite	103	C4H9NO2	000542-56-3	28



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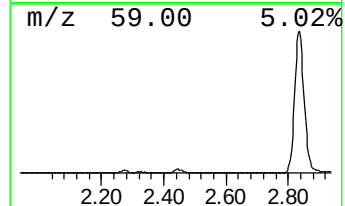
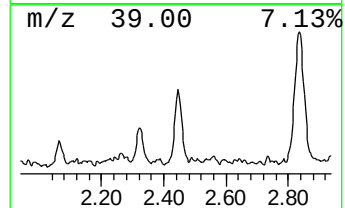
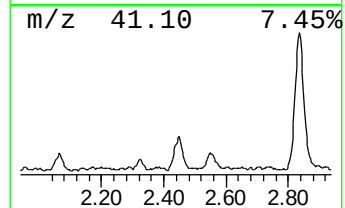
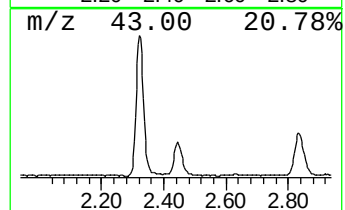
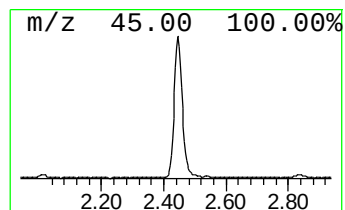
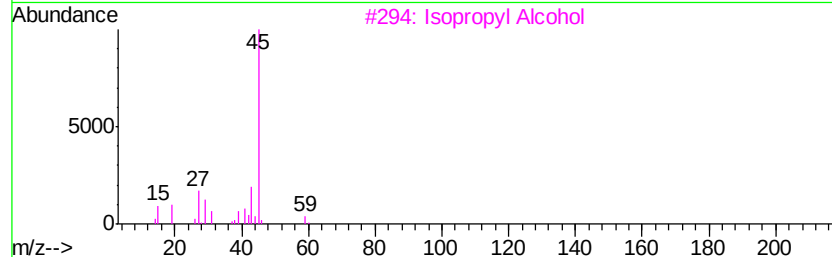
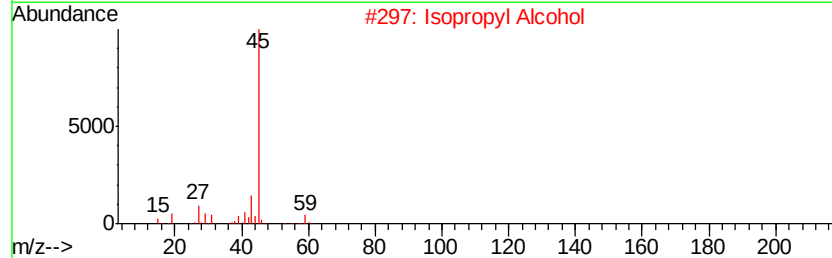
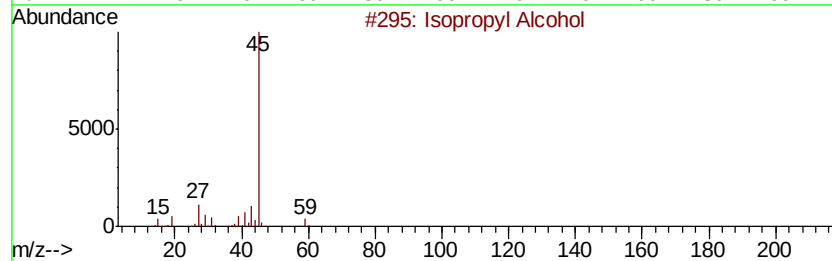
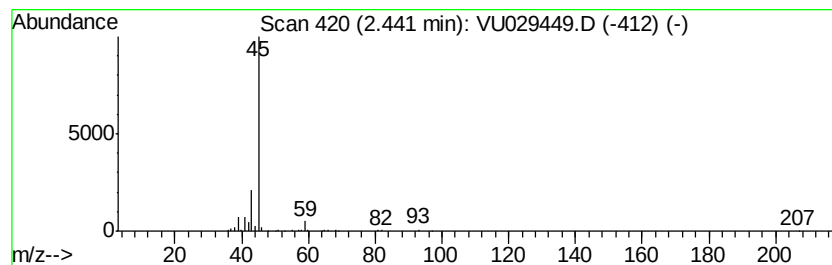
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.44	1.02 ug/L	88689	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
5		Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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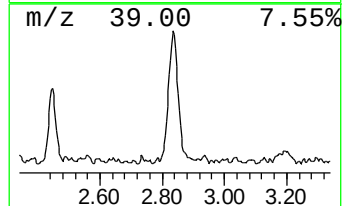
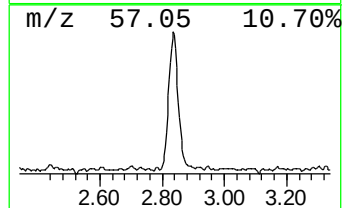
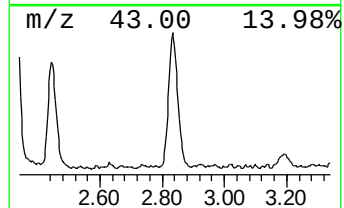
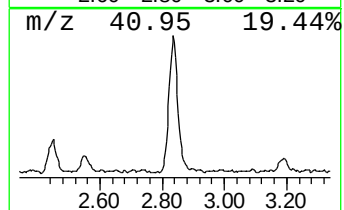
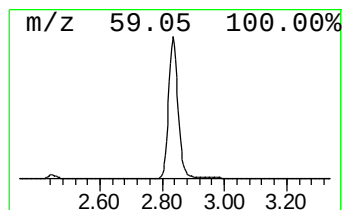
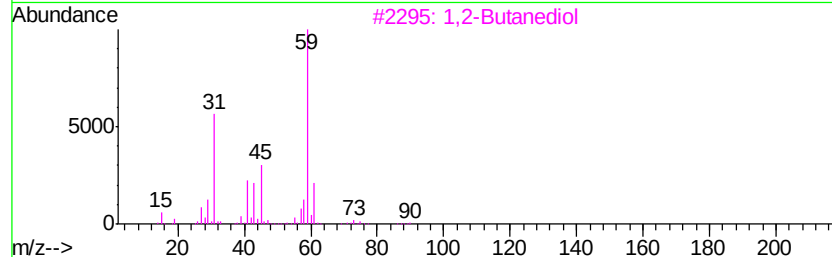
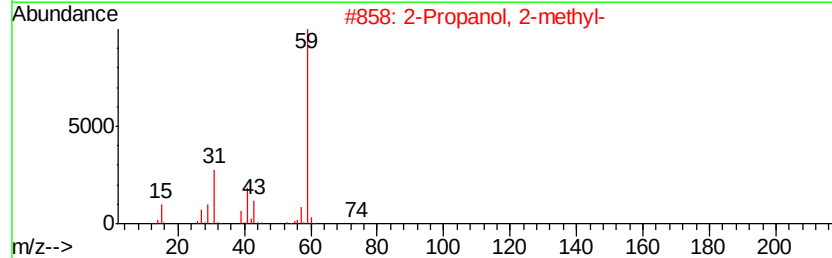
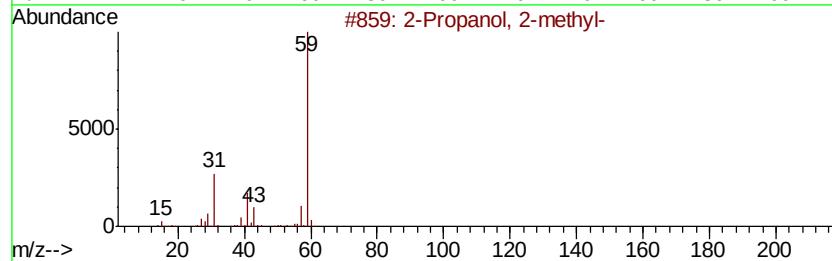
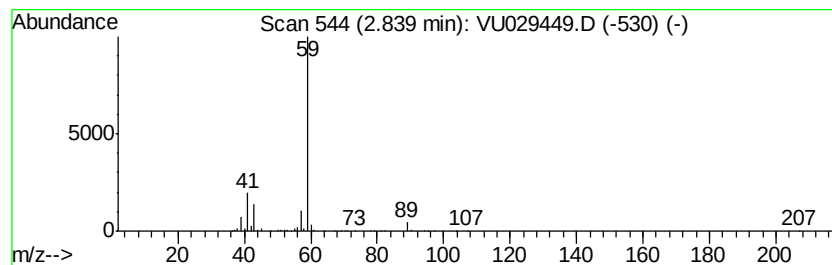
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 2-Propanol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	2.34 ug/L	204154	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	78
2		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3		1,2-Butanediol	90	C4H10O2	000584-03-2	56
4		3-Pentanol	88	C5H12O	000584-02-1	50
5		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	40



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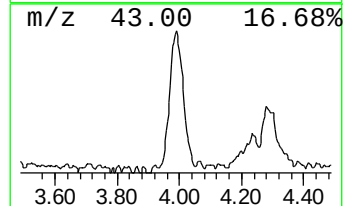
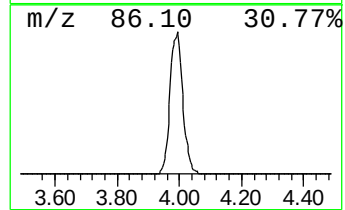
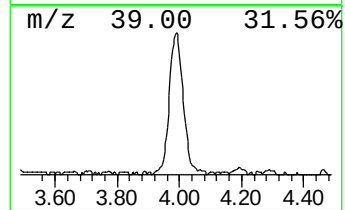
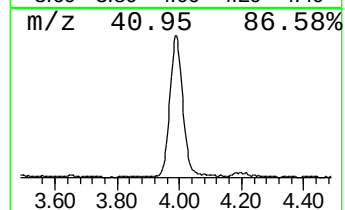
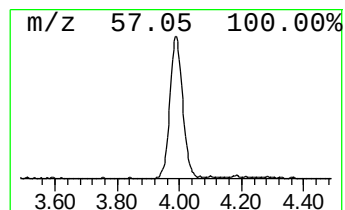
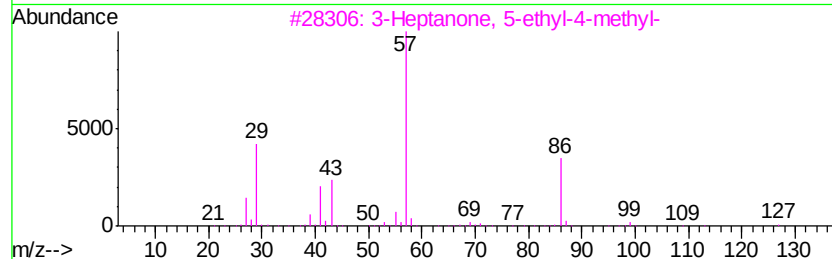
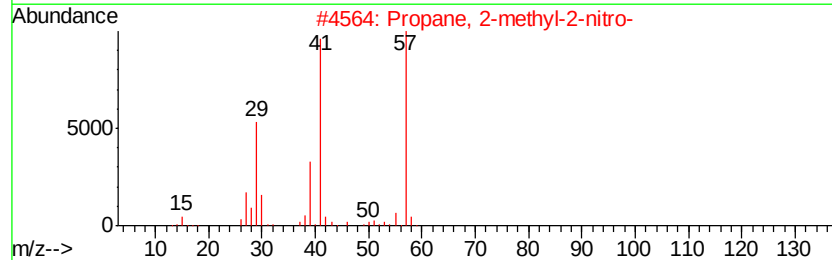
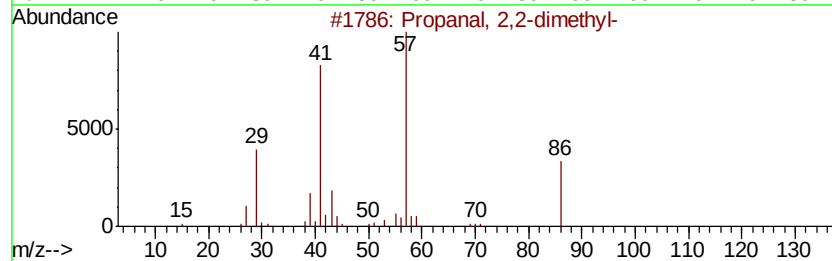
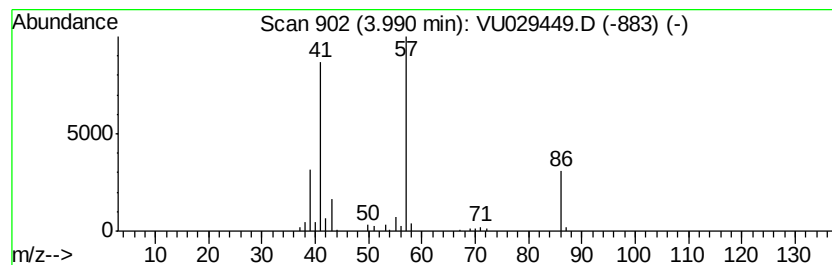
Instrument :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Propanal, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	2.05 ug/L	178216	1,4-Difluorobenzene	5.88
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Propanal, 2,2-dimethyl-	86 C5H10O	000630-19-3	64
2	Propane, 2-methyl-2-nitro-	103 C4H9NO2	000594-70-7	53
3	3-Heptanone, 5-ethyl-4-methyl-	156 C10H20O	027607-63-2	50
4	Propane, 2-methyl-2-nitro-	103 C4H9NO2	000594-70-7	47
5	3-Pentanone	86 C5H10O	000096-22-0	40



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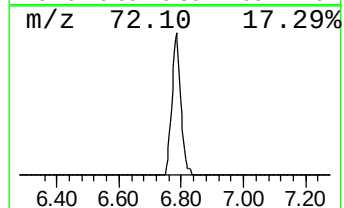
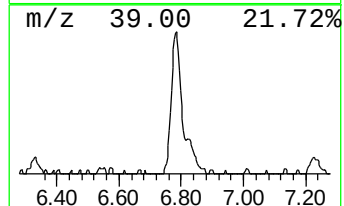
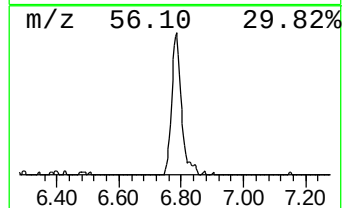
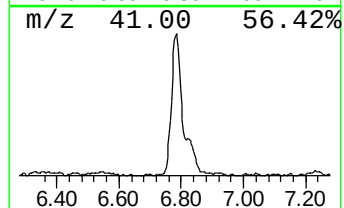
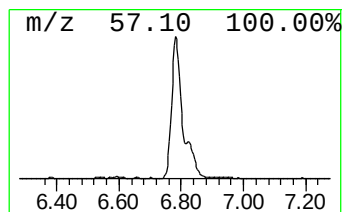
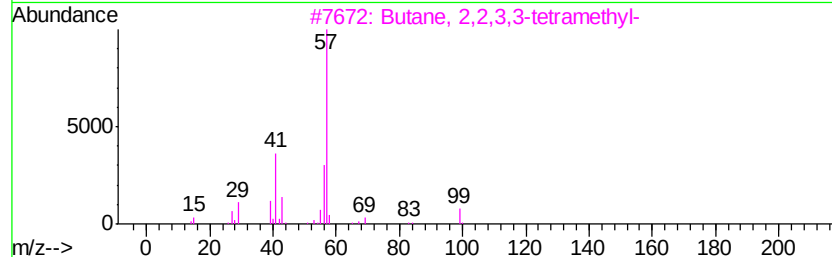
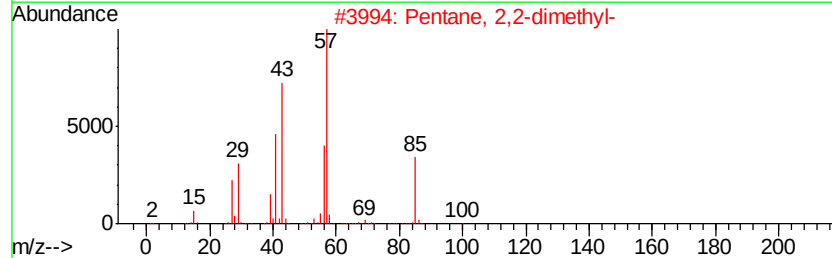
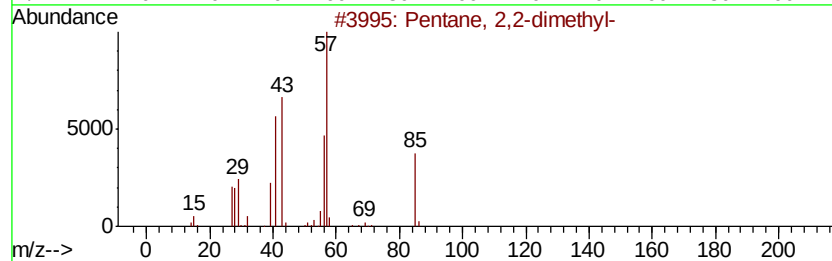
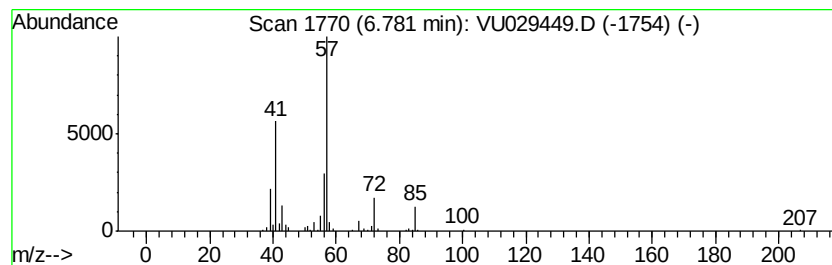
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	1.41 ug/L	122768	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	45
2		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	42
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
4		1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	38
5		1-Hepten-3-ol	114	C7H14O	004938-52-7	37



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029449.D
Acq On : 14 Feb 2019 11:49
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

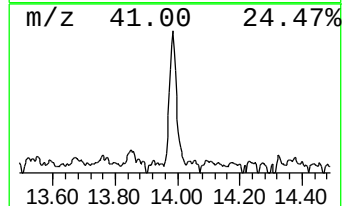
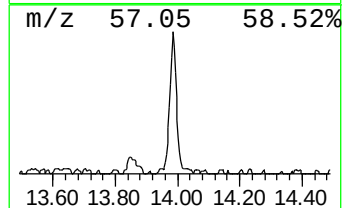
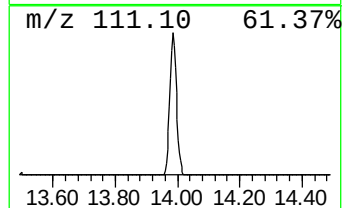
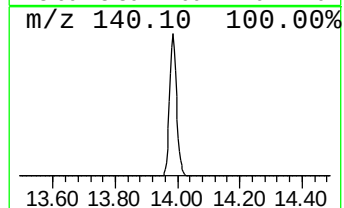
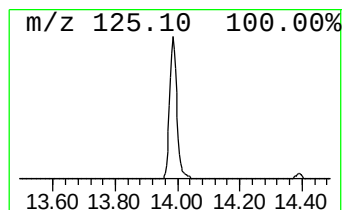
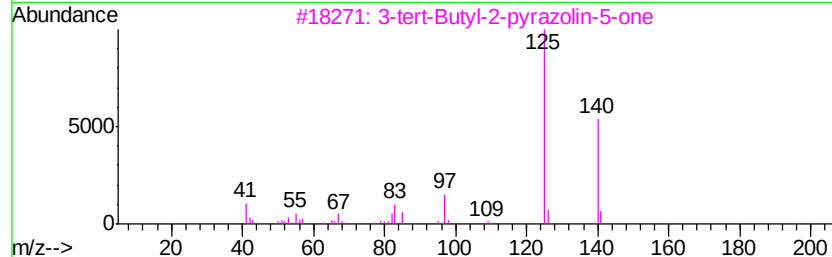
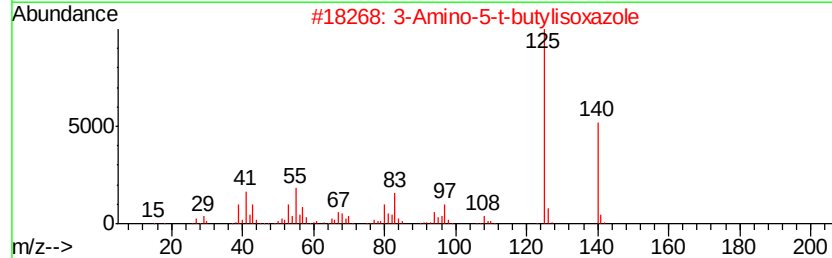
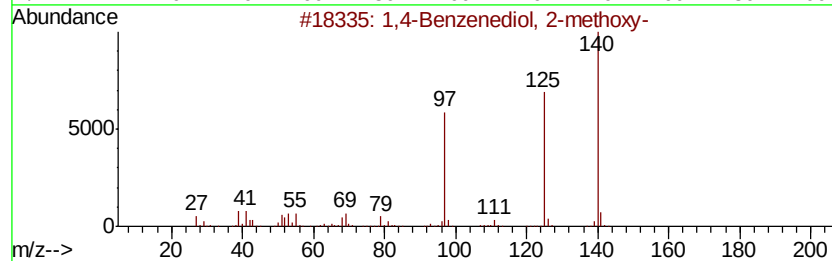
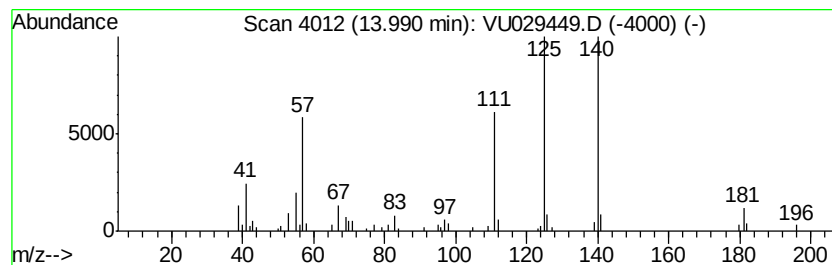
Instrument :
MSVOA_U
ClientSampleId :
C0JJ8

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 1,4-Benzenediol, 2-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	0.59 ug/L	67324	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1,4-Benzenediol, 2-methoxy-	140 C7H8O3	000824-46-4	58
2	3-Amino-5-t-butylisoxazole	140 C7H12N2O	055809-36-4	58
3	3-tert-Butyl-2-pyrazolin-5-one	140 C7H12N2O	029211-68-5	58
4	Benzenethiol, 4-methoxy-	140 C7H8OS	000696-63-9	53
5	1,2-Benzenediol, 3-methoxy-	140 C7H8O3	000934-00-9	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021419\
Data File : VU029449.D
Acq On : 14 Feb 2019 11:49
Operator : JC/SP
Sample : K1387-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0JJ8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.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: Str...	1.30	0.5	ug/L	44947	1	5.88	435610	5.0
Isopropyl Alcohol	2.44	1.0	ug/L	88689	1	5.88	435610	5.0
2-Propanol, 2-met...	2.84	2.3	ug/L	204154	1	5.88	435610	5.0
Propanal, 2,2-dim...	3.99	2.0	ug/L	178216	1	5.88	435610	5.0
(DEL) Alkane: Str...	6.78	1.4	ug/L	122768	1	5.88	435610	5.0
1,4-Benzenediol, ...	13.99	0.6	ug/L	67324	3	11.48	568070	5.0