

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021619\
 Data File : VU029509.D
 Acq On : 15 Feb 2019 20:30
 Operator : JC/SP
 Sample : K1494-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AL4

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	24	28	36	RBV3	8305	7932	1.16%	0.107%
2	1.386	85	92	105	RBV2	185826	264790	38.69%	3.564%
3	1.547	136	142	149	RBV5	10006	16121	2.36%	0.217%
4	1.682	177	184	196	RVB	80168	103523	15.12%	1.393%
5	2.273	358	368	377	RBV	184925	282223	41.23%	3.798%
6	2.321	377	383	398	RVB	39909	66285	9.68%	0.892%
7	2.447	410	422	440	RBV	26074	52287	7.64%	0.704%
8	2.836	531	543	568	RBV2	112432	236653	34.58%	3.185%
9	3.990	875	902	930	RBV2	137344	397142	58.02%	5.345%
10	4.193	951	965	1011	RBV2	85326	316768	46.28%	4.263%
11	4.646	1090	1106	1131	RBV	96524	245460	35.86%	3.303%
12	4.990	1199	1213	1230	RVB3	24625	59479	8.69%	0.800%
13	5.337	1297	1321	1342	RBV2	217040	588342	85.96%	7.918%
14	5.884	1477	1491	1511	RBV	200185	393012	57.42%	5.289%
15	6.331	1616	1630	1649	RBV	134252	275088	40.19%	3.702%
16	6.784	1755	1771	1781	RBV	224401	458123	66.93%	6.165%
17	7.228	1897	1909	1933	RBV2	74152	138087	20.17%	1.858%
18	7.562	2000	2013	2032	RBV	318149	560053	81.82%	7.537%
19	7.849	2090	2102	2117	RBV	46010	83706	12.23%	1.127%
20	8.177	2191	2204	2214	RBV3	6132	12559	1.83%	0.169%
21	8.312	2235	2246	2281	RBV	381214	684460	100.00%	9.211%
22	8.469	2287	2295	2308	RVB6	7240	12567	1.84%	0.169%
23	9.086	2475	2487	2511	RBV	295864	501276	73.24%	6.746%
24	10.029	2771	2780	2796	RBV3	9756	17625	2.58%	0.237%
25	10.430	2893	2905	2918	RBV	121067	191744	28.01%	2.580%
26	10.604	2949	2959	2970	RVB2	9785	16217	2.37%	0.218%
27	11.006	3074	3084	3095	RBV2	4453	8026	1.17%	0.108%
28	11.482	3220	3232	3259	RBV	322061	530480	77.50%	7.139%
29	11.752	3307	3316	3325	RBV5	4348	8464	1.24%	0.114%
30	11.858	3336	3349	3372	RBV	328135	551609	80.59%	7.424%
31	12.479	3528	3542	3551	RBV3	5780	12022	1.76%	0.162%
32	13.987	4000	4011	4024	RBV2	84041	129412	18.91%	1.742%
33	14.279	4095	4102	4113	RVB3	5562	8554	1.25%	0.115%
34	15.353	4426	4436	4449	RBV6	19528	32113	4.69%	0.432%

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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	16.337	4736	4742	4751	rbV8	4578	6915	1.01%	0.093%
36	16.427	4759	4770	4792	rbV2	87740	161425	23.58%	2.172%

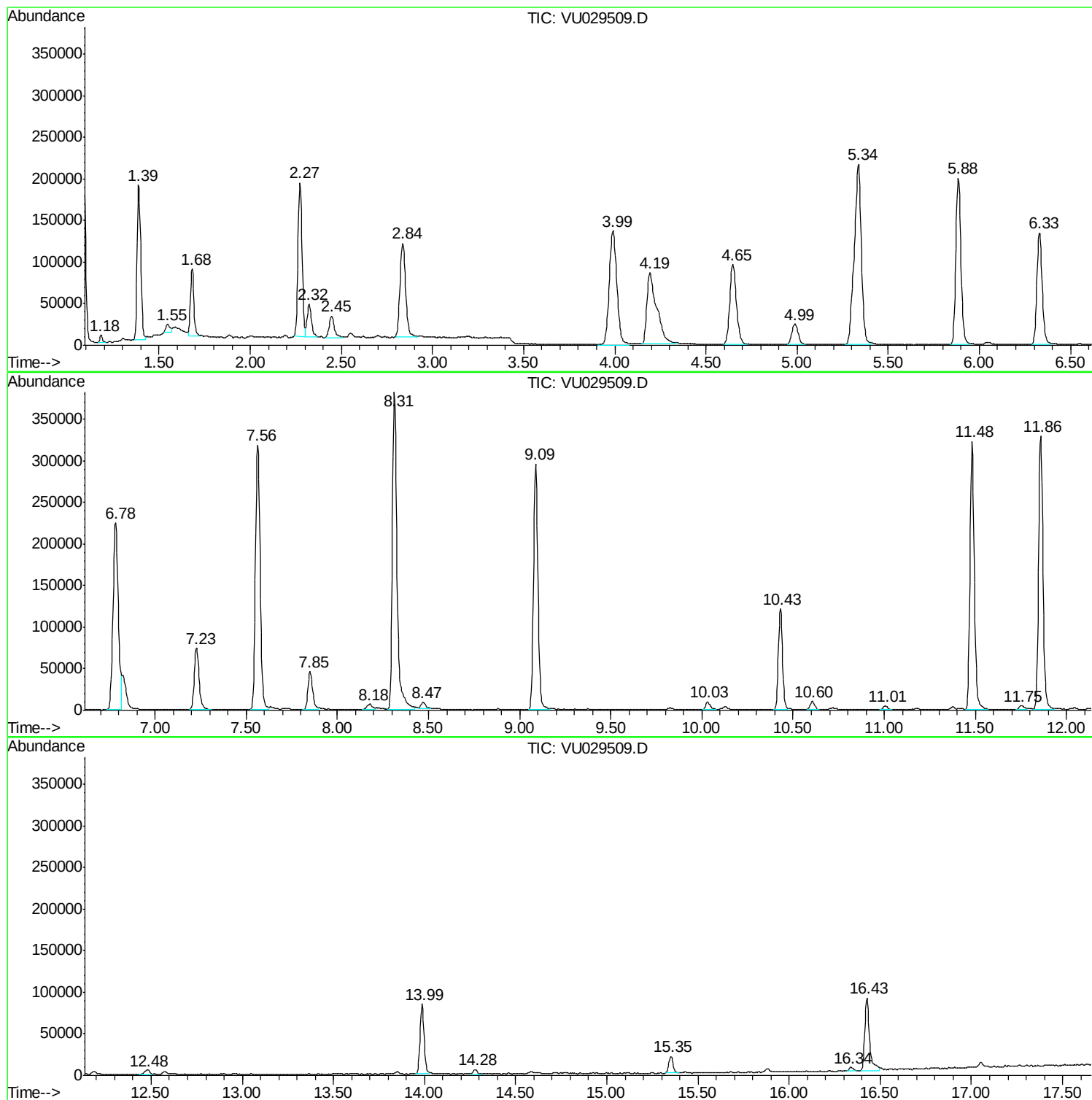
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Quant Title : TRACE VOA SOM01.0

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



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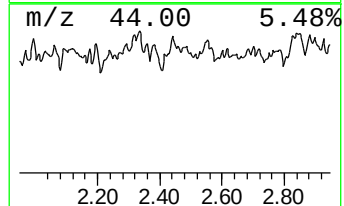
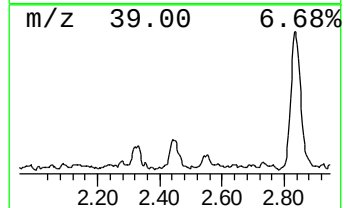
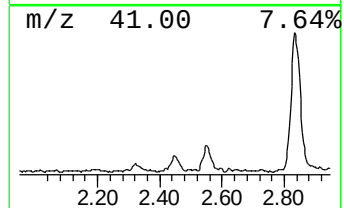
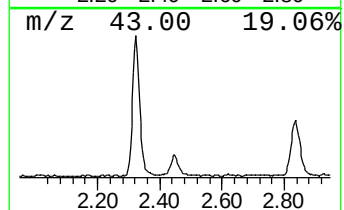
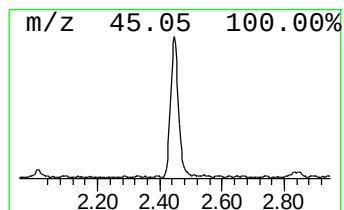
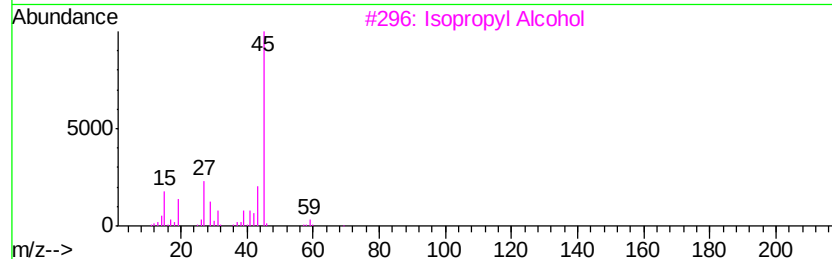
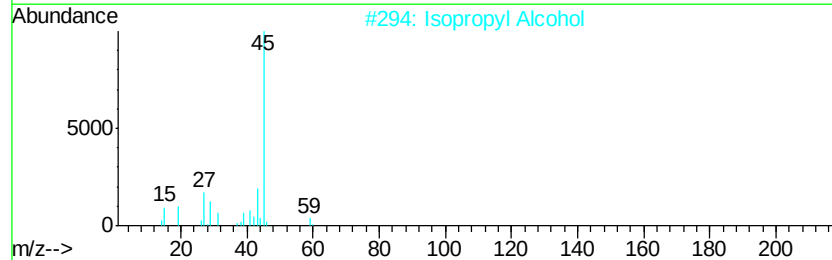
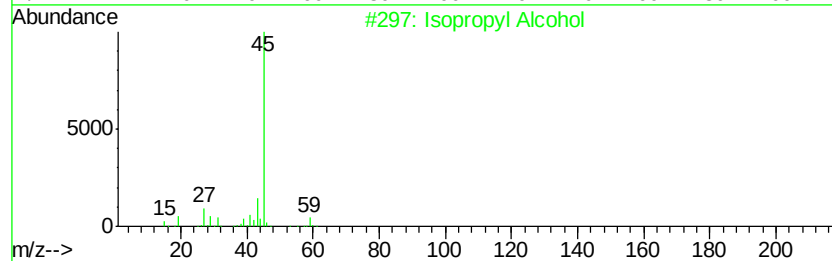
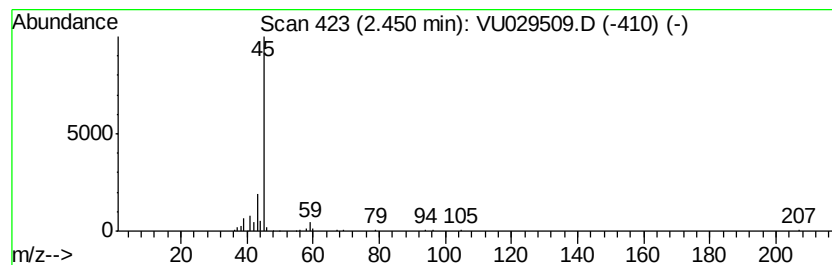
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	0.67 ug/L	52287	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	72
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	72
4		2-Pentanol	88	C5H12O	006032-29-7	56
5		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40



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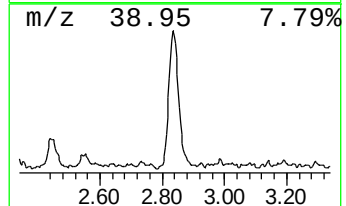
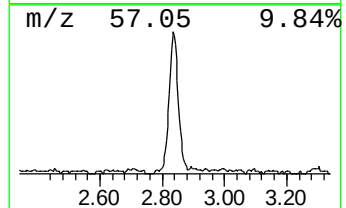
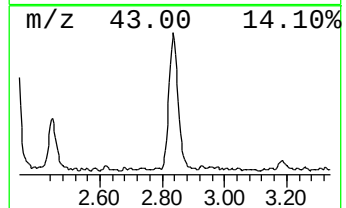
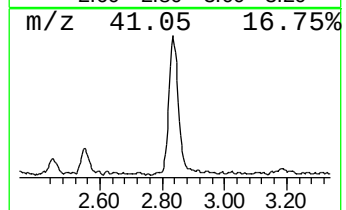
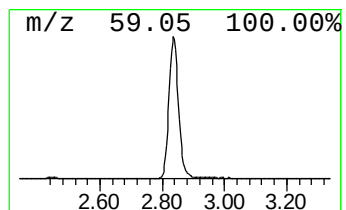
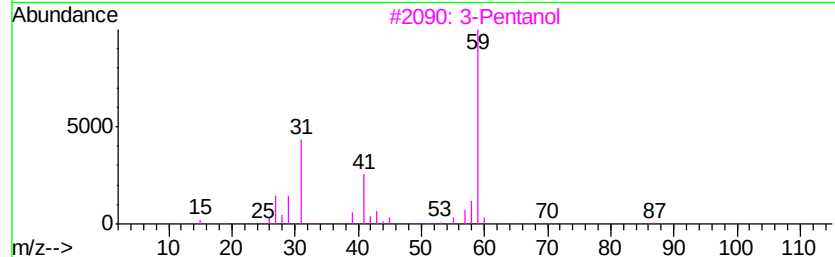
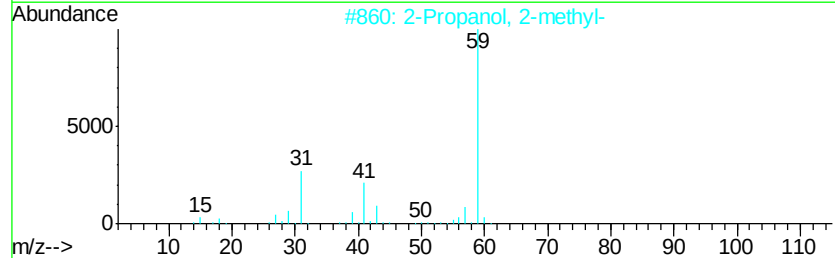
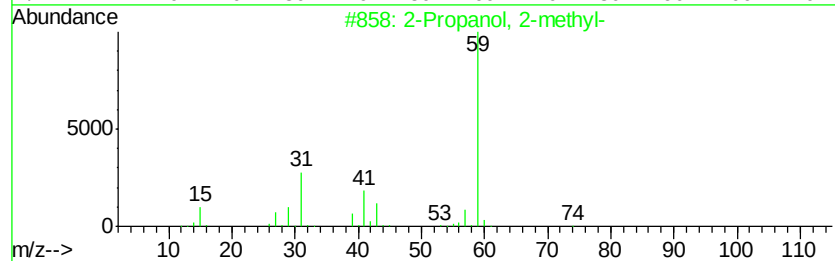
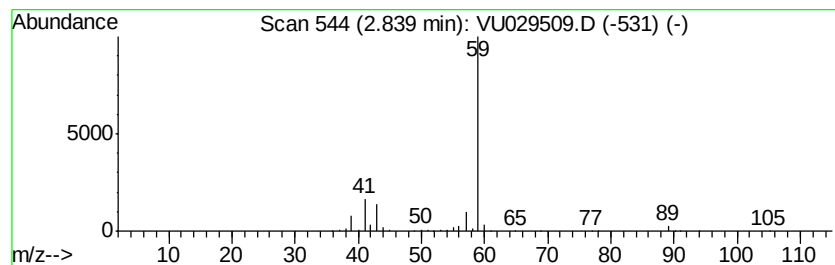
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	3.01 ug/L	236653	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3			3-Pentanol	88	C5H12O	000584-02-1	64
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
5			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	50



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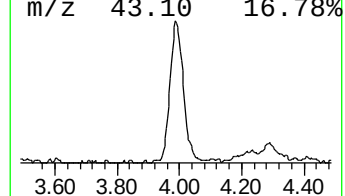
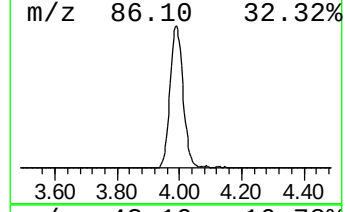
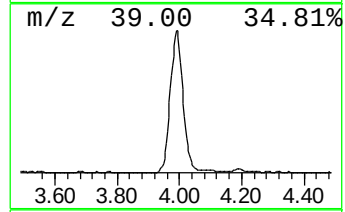
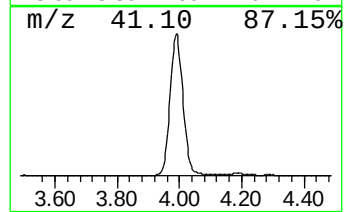
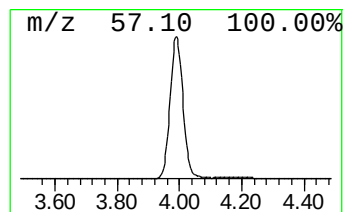
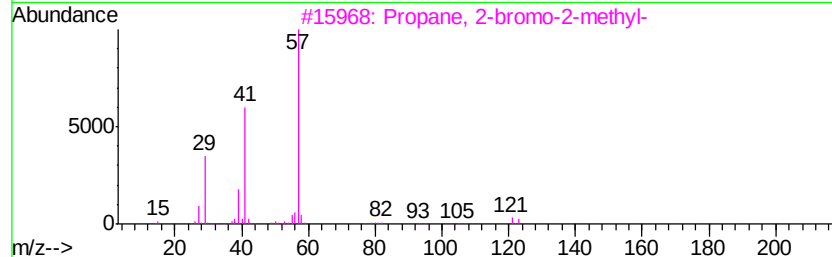
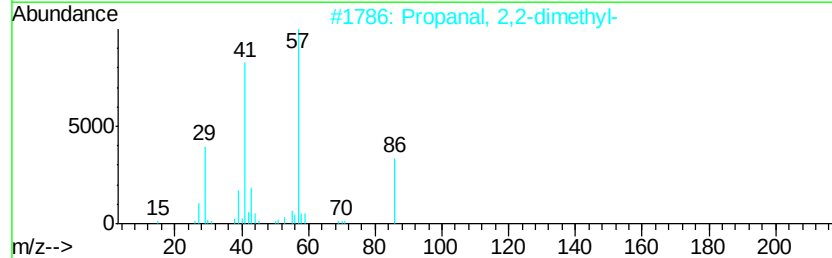
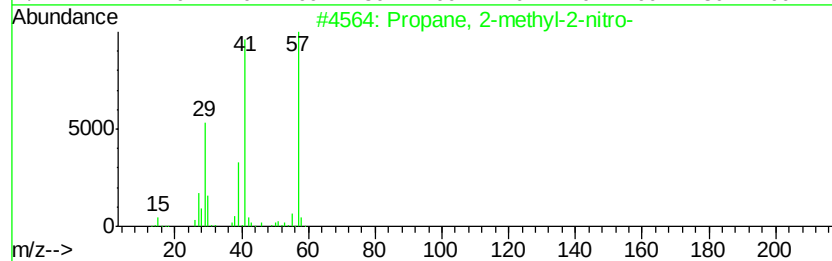
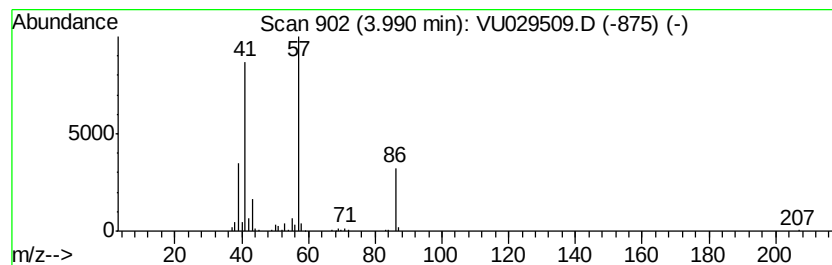
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Propane, 2-methyl-2-nitro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	5.05 ug/L	397142	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
2			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45
3			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	40
4			3-Pentanone	86	C5H10O	000096-22-0	40
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40



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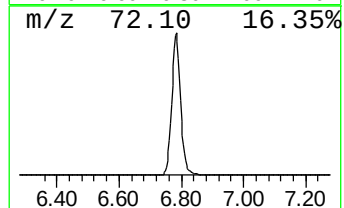
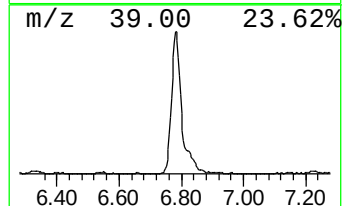
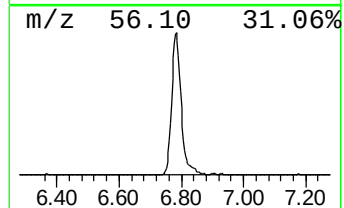
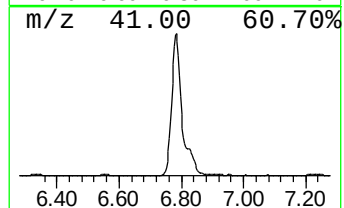
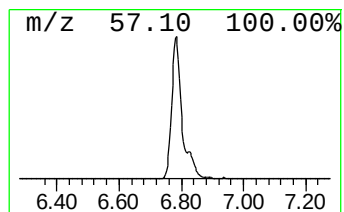
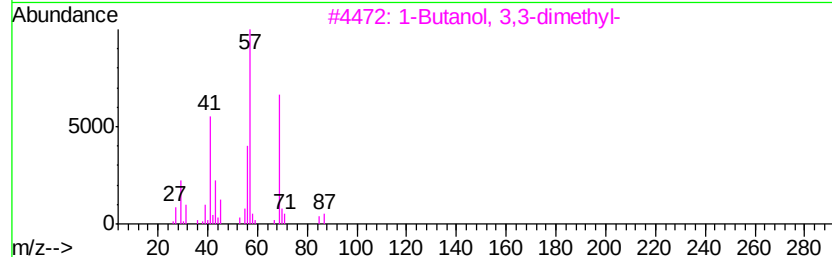
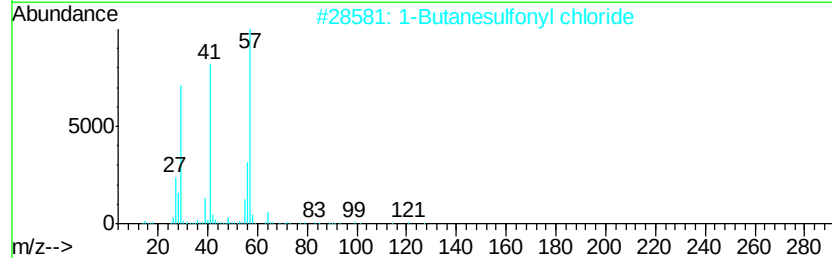
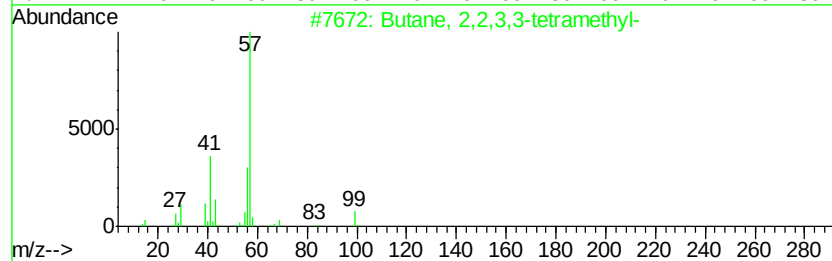
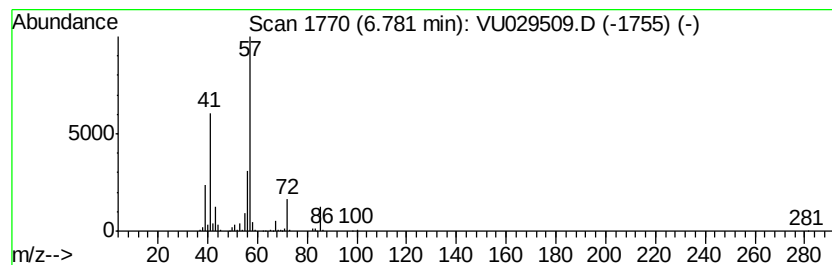
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	5.83 ug/L	458123	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
2			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	42
3			1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	40
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	37
5			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	36



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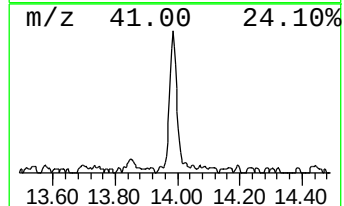
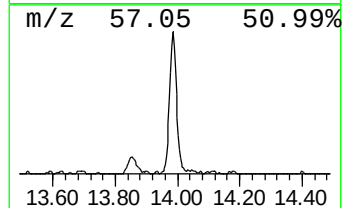
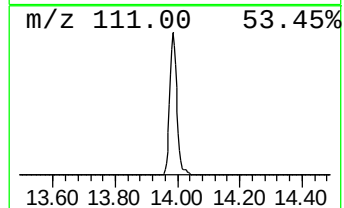
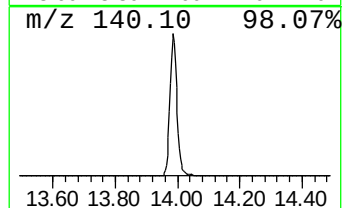
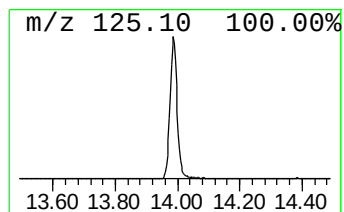
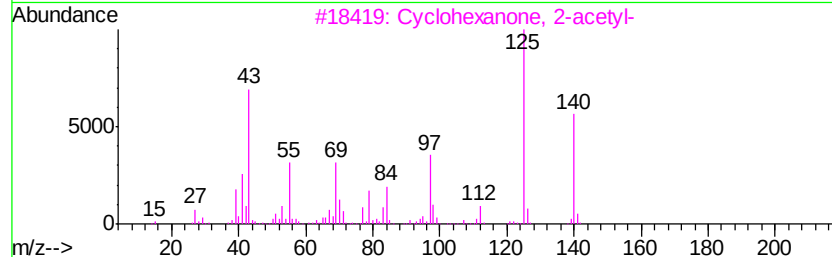
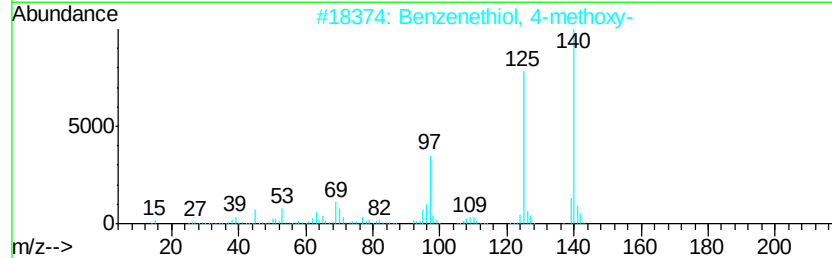
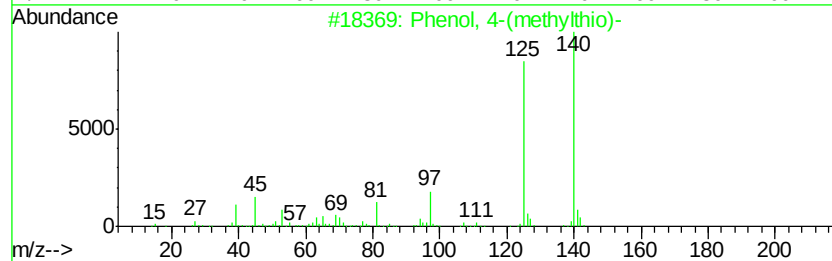
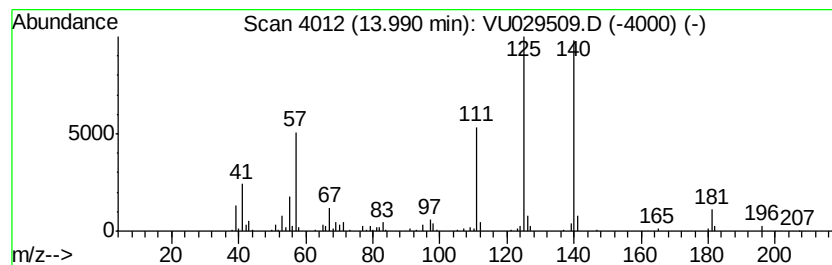
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 4-(methylthio)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	1.22 ug/L	129412	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Phenol, 4-(methylthio)-	140 C7H8OS	001073-72-9	64
2	Benzenethiol, 4-methoxy-	140 C7H8OS	000696-63-9	59
3	Cyclohexanone, 2-acetyl-	140 C8H12O2	000874-23-7	59
4	3-Amino-5-t-butylisoxazole	140 C7H12N2O	055809-36-4	58
5	Thiophene, 2,5-diethyl-	140 C8H12S	005069-23-8	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU021619\
Data File : VU029509.D
Acq On : 15 Feb 2019 20:30
Operator : JC/SP
Sample : K1494-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 12 Sample Multiplier: 1

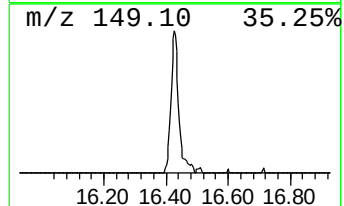
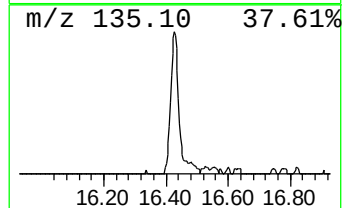
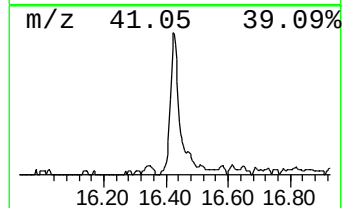
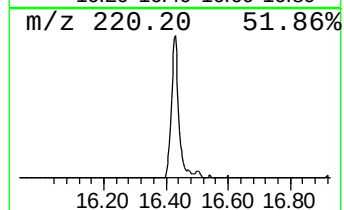
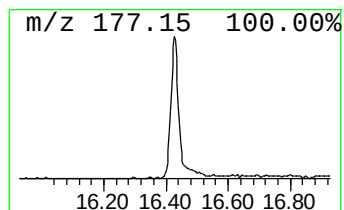
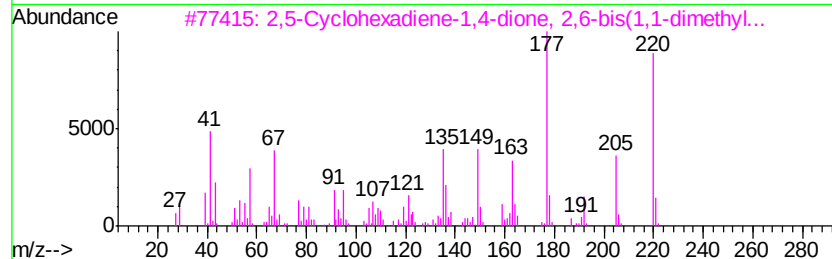
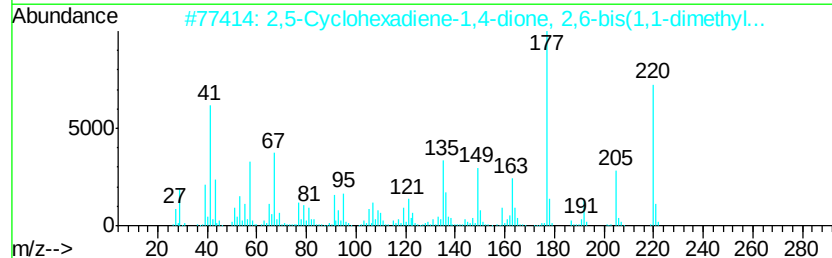
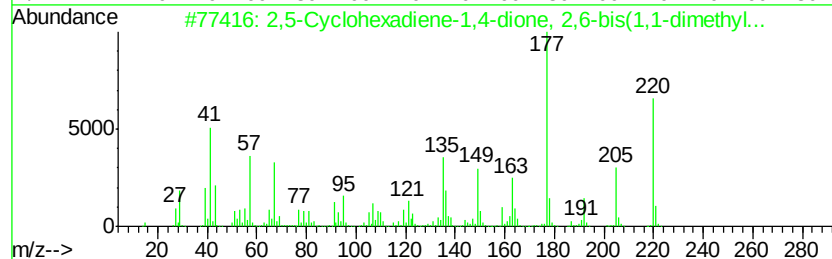
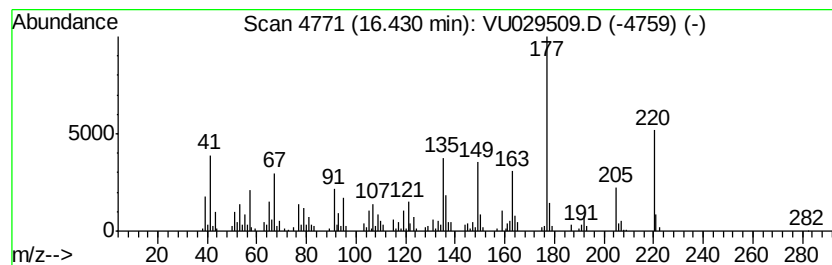
Instrument :
MSVOA_U
ClientSampleId :
C0AL4

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.43	1.52 ug/L	161425	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	93
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	76
4	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	62
5	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	55



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021619\
Data File : VU029509.D
Acq On : 15 Feb 2019 20:30
Operator : JC/SP
Sample : K1494-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AL4

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
Isopropyl Alcohol	2.45	0.7	ug/L	52287	1	5.88	393012	5.0
2-Propanol, 2-met...	2.84	3.0	ug/L	236653	1	5.88	393012	5.0
Propane, 2-methyl...	3.99	5.0	ug/L	397142	1	5.88	393012	5.0
(DEL) Alkane: Str...	6.78	5.8	ug/L	458123	1	5.88	393012	5.0
Phenol, 4-(methyl...	13.99	1.2	ug/L	129412	3	11.48	530480	5.0
2,5-Cyclohexadien...	16.43	1.5	ug/L	161425	3	11.48	530480	5.0