

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021819\
 Data File : VU029520.D
 Acq On : 18 Feb 2019 10:50
 Operator : JC/SP
 Sample : K1494-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 4 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	rBV2	8836	9018	1.22%	0.109%
2	1.386	85	92	106	rBV2	199195	278540	37.58%	3.363%
3	1.544	134	141	153	rBV3	12551	24155	3.26%	0.292%
4	1.682	176	184	194	rVB	81426	103126	13.91%	1.245%
5	2.273	358	368	377	rBV	190991	291184	39.28%	3.515%
6	2.322	377	383	396	rVB	44354	66945	9.03%	0.808%
7	2.444	413	421	434	rVB	22168	39508	5.33%	0.477%
8	2.833	530	542	561	rBV2	121434	254258	34.30%	3.070%
9	3.987	878	901	928	rBV2	155354	438488	59.16%	5.294%
10	4.190	948	964	1007	rBV2	95232	336722	45.43%	4.065%
11	4.643	1088	1105	1128	rBV	112735	274183	36.99%	3.310%
12	4.987	1196	1212	1230	rBV3	28784	69453	9.37%	0.838%
13	5.334	1298	1320	1341	rBV3	234807	643696	86.84%	7.771%
14	5.884	1475	1491	1514	rBV	244509	480905	64.88%	5.806%
15	6.042	1529	1540	1556	rBV6	3439	7555	1.02%	0.091%
16	6.328	1613	1629	1656	rBV2	150080	303451	40.94%	3.663%
17	6.781	1755	1770	1781	rBV	245591	508546	68.61%	6.139%
18	7.225	1897	1908	1926	rBV	86870	160626	21.67%	1.939%
19	7.563	1999	2013	2032	rBV	347862	606811	81.87%	7.326%
20	7.849	2092	2102	2119	rBV	52698	94468	12.74%	1.140%
21	8.177	2191	2204	2214	rBV3	9466	17928	2.42%	0.216%
22	8.312	2234	2246	2282	rBV	401362	741222	100.00%	8.948%
23	8.469	2287	2295	2303	rVV4	7706	12209	1.65%	0.147%
24	9.087	2475	2487	2509	rBV	360944	600966	81.08%	7.255%
25	10.029	2771	2780	2795	rBV7	11743	20936	2.82%	0.253%
26	10.431	2892	2905	2921	rBV	131819	210041	28.34%	2.536%
27	10.604	2945	2959	2969	rBV	18003	29841	4.03%	0.360%
28	11.006	3073	3084	3093	rBV3	4989	8316	1.12%	0.100%
29	11.482	3219	3232	3257	rBV	390395	632467	85.33%	7.635%
30	11.752	3305	3316	3332	rBV4	5561	12605	1.70%	0.152%
31	11.858	3337	3349	3370	rBV	341068	571801	77.14%	6.903%
32	12.186	3442	3451	3457	rBV2	5280	8341	1.13%	0.101%
33	12.476	3531	3541	3552	rBV2	7416	13198	1.78%	0.159%
34	12.575	3560	3572	3583	rBV6	5516	10808	1.46%	0.130%

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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	13.987	3999	4011	4026	rBV2	92362	145158	19.58%	1.752%
36	14.276	4086	4101	4116	rBV2	11408	21501	2.90%	0.260%
37	15.350	4423	4435	4451	rBV4	22057	37901	5.11%	0.458%
38	15.881	4592	4600	4609	rBV2	6321	11005	1.48%	0.133%
39	16.427	4759	4770	4781	rBV2	112408	185448	25.02%	2.239%

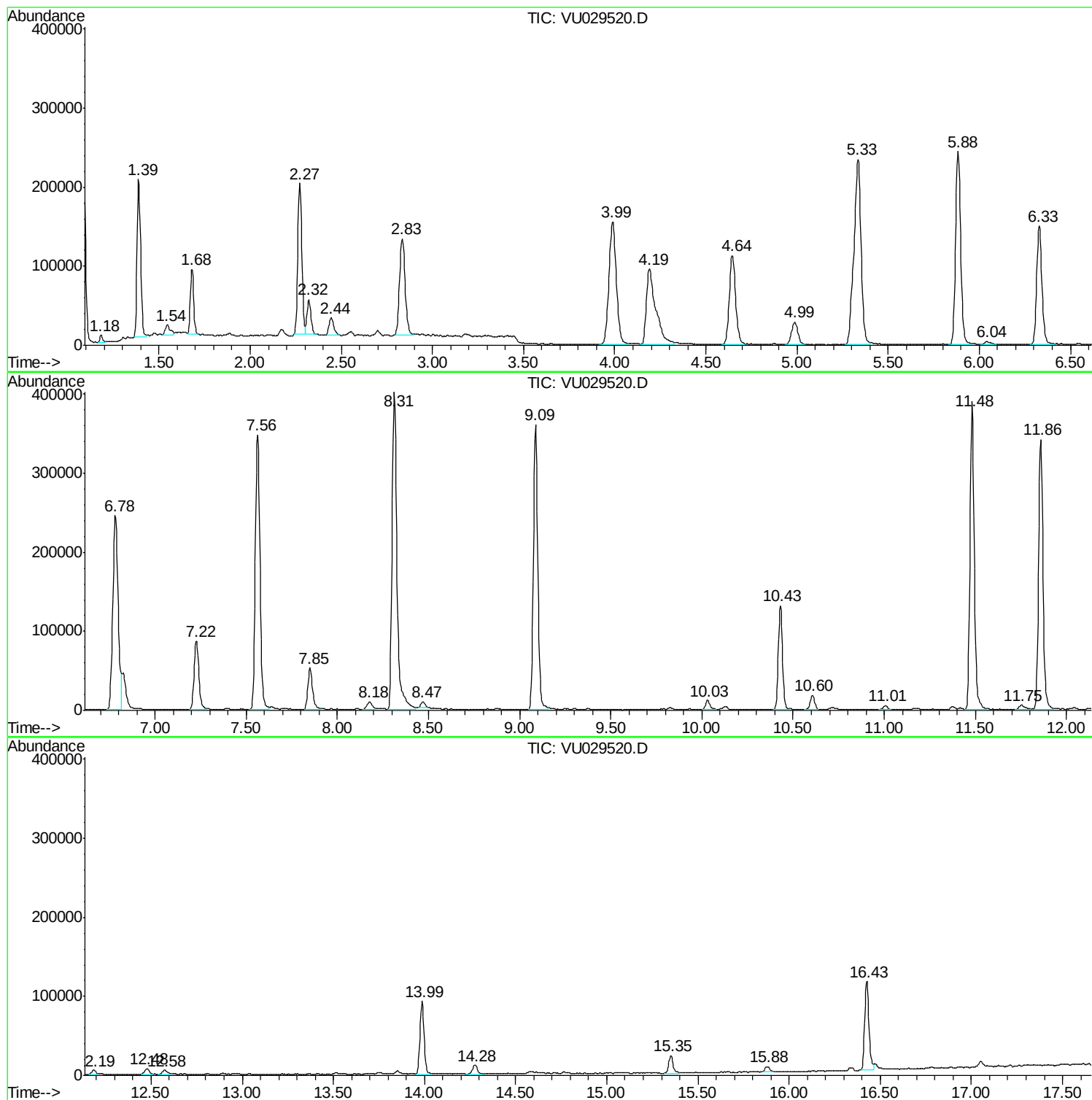
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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



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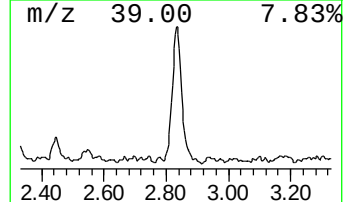
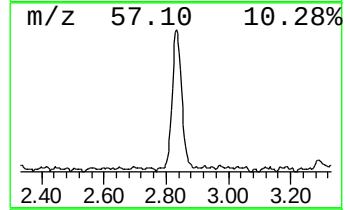
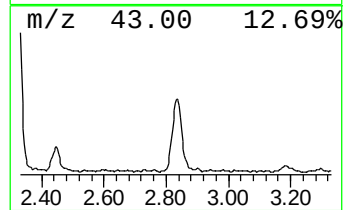
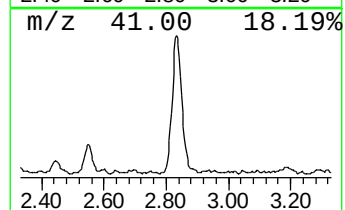
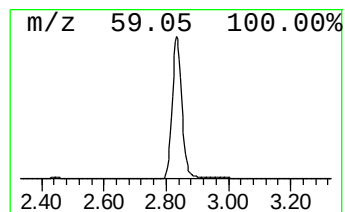
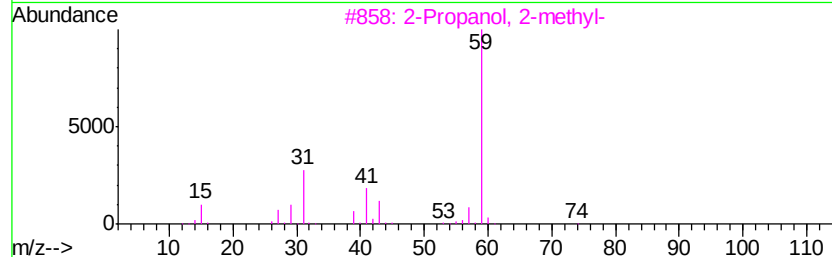
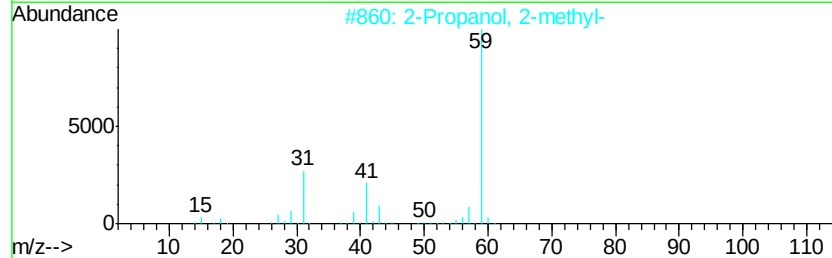
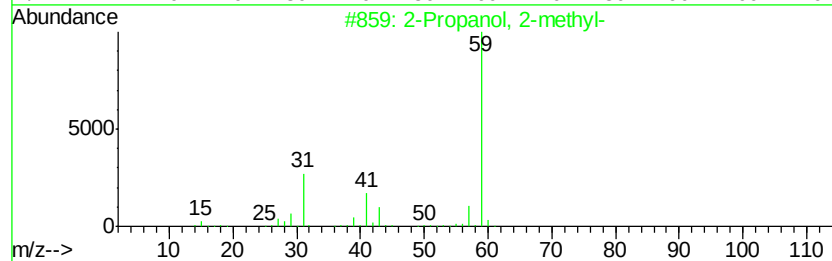
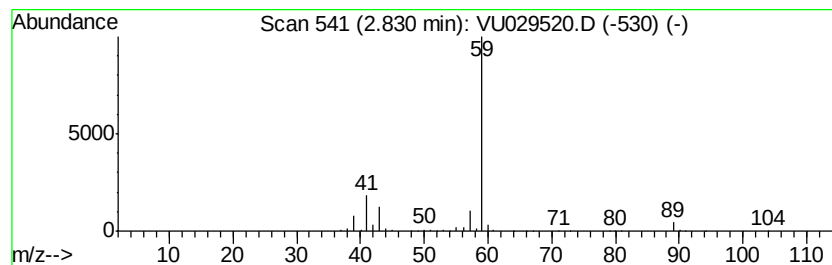
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	2.64 ug/L	254258	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	72
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
5			Ethanol, 2-ethoxy-	90	C4H10O2	000110-80-5	9



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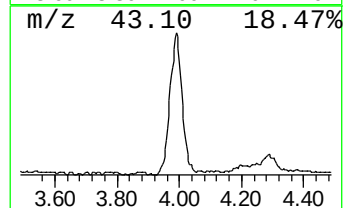
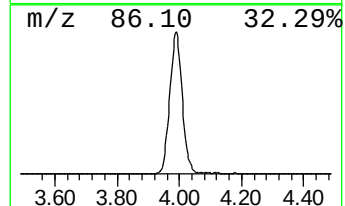
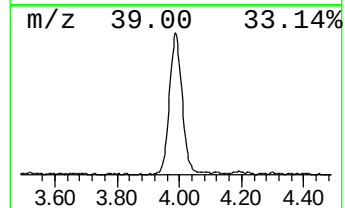
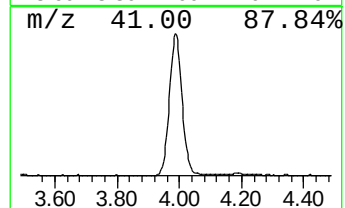
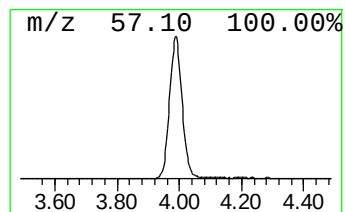
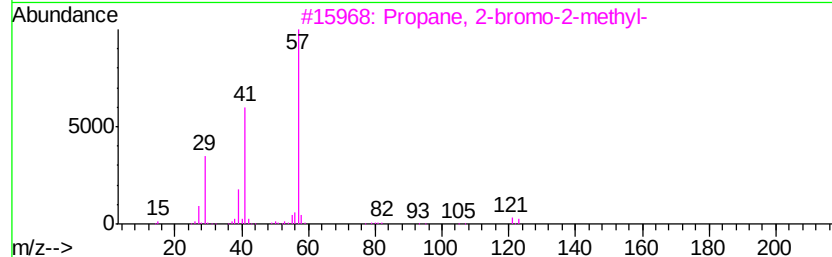
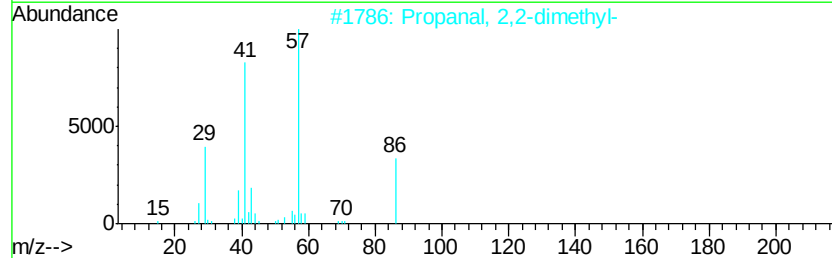
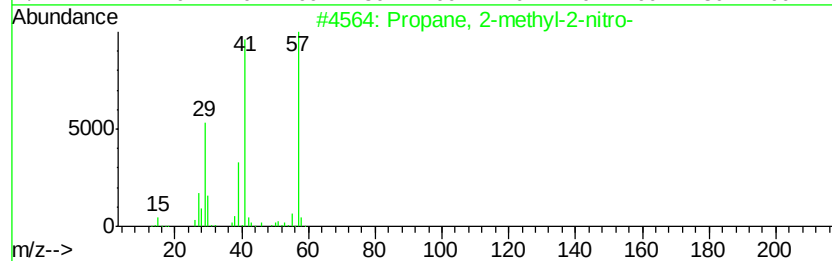
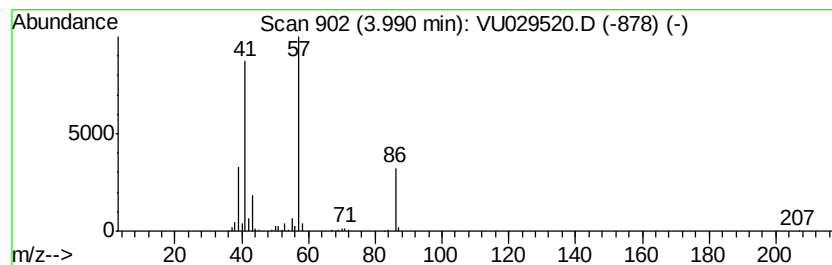
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.99	4.56 ug/L	438488	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	53
2	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45
3	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	42
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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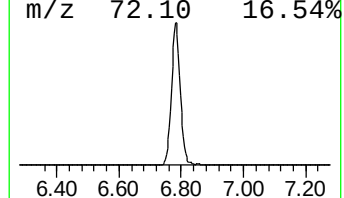
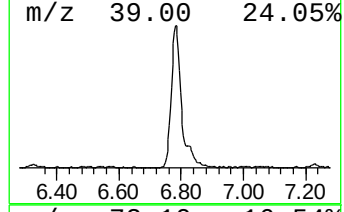
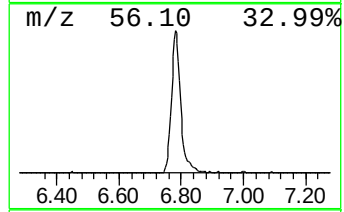
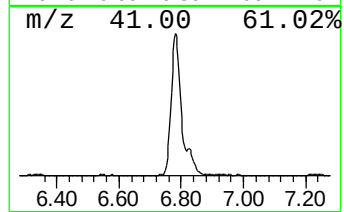
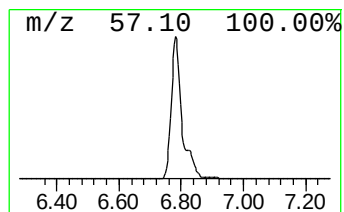
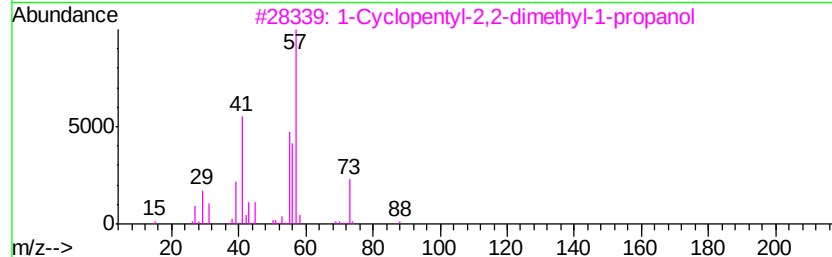
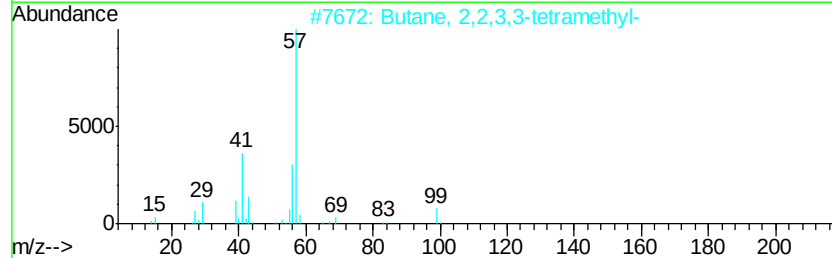
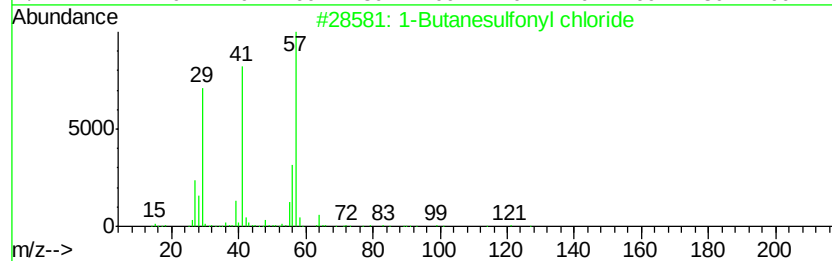
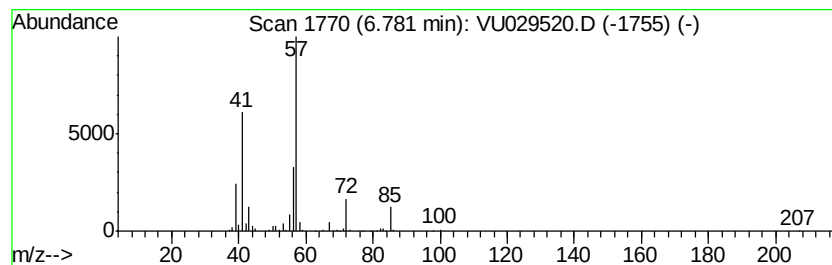
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.78	5.29 ug/L	508546	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
3		1-Cyclopentyl-2,2-dimethyl-1-propanol	156	C10H20O	337966-85-5	38
4		Methane, isocyanato-	57	C2H3NO	000624-83-9	38
5		3,4-Hexanedione, 2,2,5,5-tetramethyl-	185	C10H18O2	039950-93-1	37



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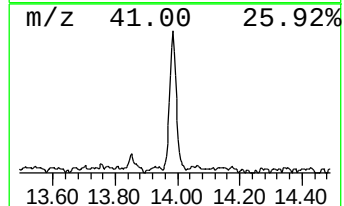
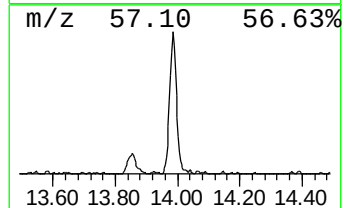
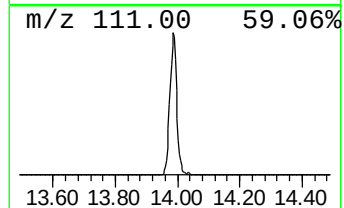
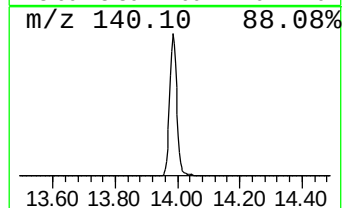
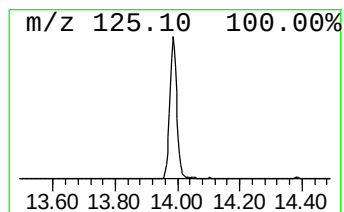
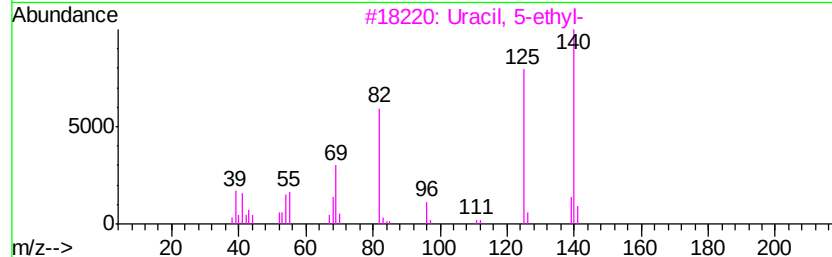
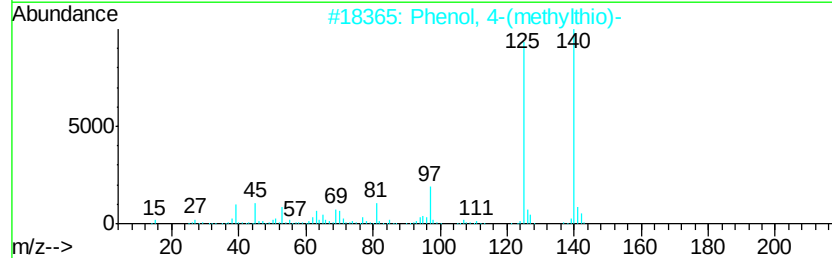
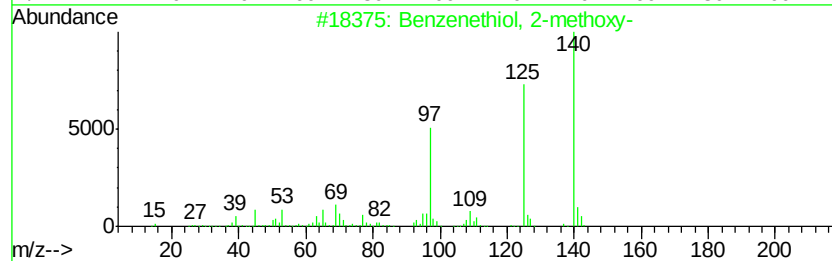
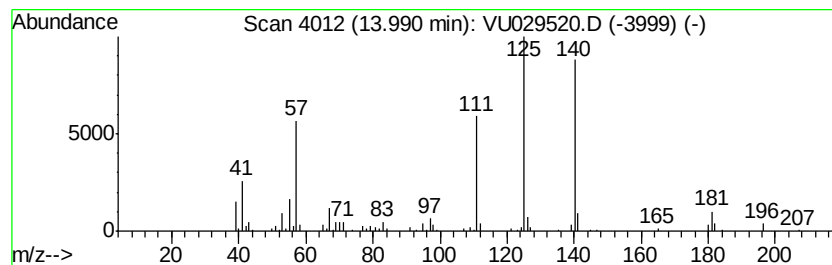
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenethiol, 2-methoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.99	1.15 ug/L	145158	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	59
2	Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	58
3	Uracil, 5-ethyl-	140	C6H8N2O2	004212-49-1	53
4	Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	53
5	Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	53



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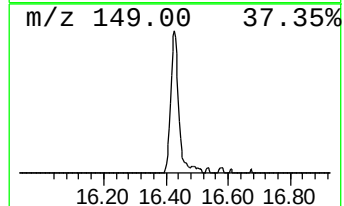
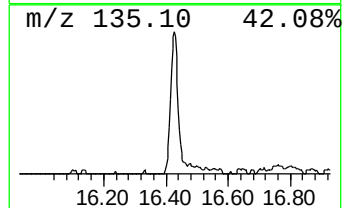
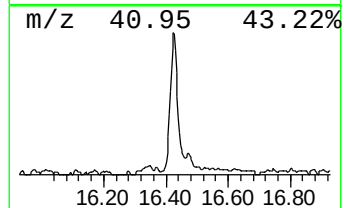
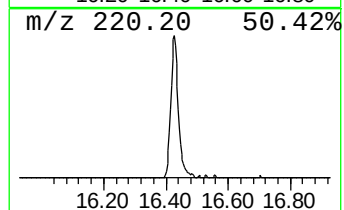
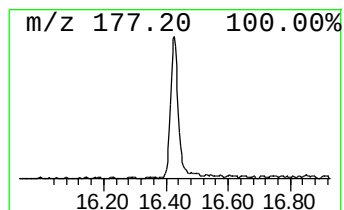
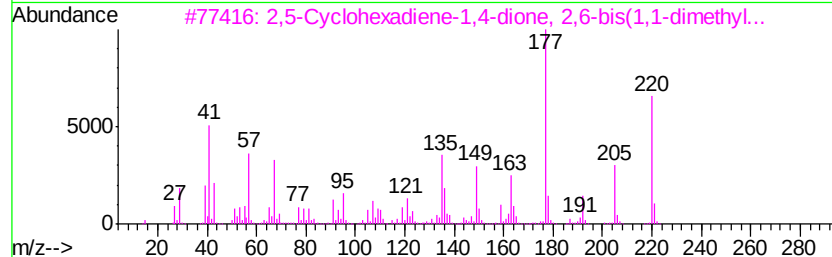
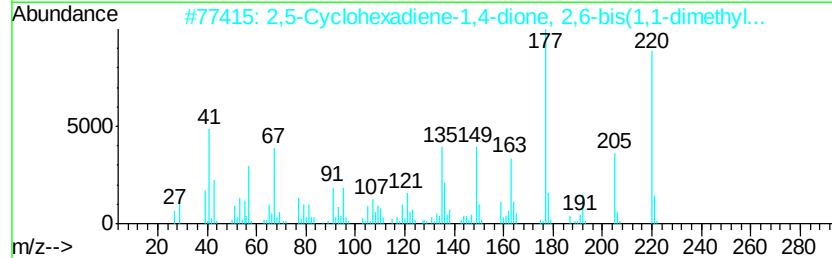
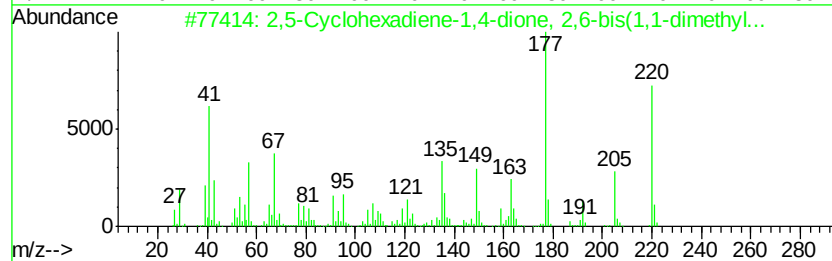
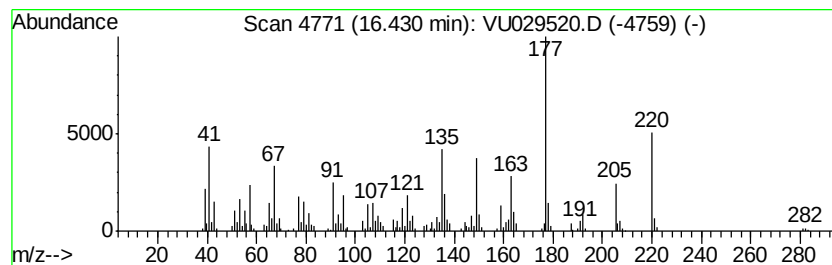
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021219WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.43	1.47 ug/L	185448	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	99
3		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	97
4		N-[4-(Ethyl-methyl-amino)-phenyl]...	192	C11H16N2O	099981-45-0	53
5		trans-.beta.-Ionone	192	C13H20O	000079-77-6	46



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU021819\
Data File : VU029520.D
Acq On : 18 Feb 2019 10:50
Operator : JC/SP
Sample : K1494-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 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
2-Propanol, 2-met...	2.83	2.6	ug/L	254258	1	5.88	480905	5.0
Propane, 2-methyl...	3.99	4.6	ug/L	438488	1	5.88	480905	5.0
unknown-01	6.78	5.3	ug/L	508546	1	5.88	480905	5.0
Benzenethiol, 2-m...	13.99	1.1	ug/L	145158	3	11.48	632467	5.0
2,5-Cyclohexadien...	16.43	1.5	ug/L	185448	3	11.48	632467	5.0