

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052620\
 Data File : VU038306.D
 Acq On : 26 May 2020 18:56
 Operator : JC/MD
 Sample : L2766-02
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4Y6

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\SOMUTR050720WMA.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	1.501	43	50	57	rBV2	20266	25369	1.38%	0.159%
2	1.601	71	81	97	rBV2	262037	413602	22.49%	2.589%
3	1.700	104	112	121	rVB	59563	69116	3.76%	0.433%
4	1.932	175	184	195	rVB	121473	157931	8.59%	0.988%
5	2.591	373	389	399	rBV	241580	404789	22.01%	2.534%
6	2.652	399	408	427	rVB	187622	315857	17.17%	1.977%
7	3.208	564	581	610	rBV	344125	766416	41.67%	4.797%
8	3.617	690	708	723	rBV3	12329	28729	1.56%	0.180%
9	4.481	955	977	1010	rBV	706735	1839169	100.00%	11.511%
10	4.662	1018	1033	1050	rBV	245074	584589	31.79%	3.659%
11	4.742	1054	1058	1078	rVB2	27387	51976	2.83%	0.325%
12	5.102	1152	1170	1191	rBV	231439	505040	27.46%	3.161%
13	5.424	1257	1270	1283	rBV6	12697	28044	1.52%	0.176%
14	5.761	1350	1375	1404	rBV2	452629	1193512	64.89%	7.470%
15	6.279	1515	1536	1555	rBV	368609	742643	40.38%	4.648%
16	6.420	1566	1580	1602	rBV3	33107	68966	3.75%	0.432%
17	6.723	1659	1674	1690	rBV	286731	559288	30.41%	3.500%
18	7.157	1789	1809	1817	rBV	658254	1358075	73.84%	8.500%
19	7.591	1930	1944	1962	rBV	151667	266947	14.51%	1.671%
20	7.922	2031	2047	2062	rBV	573293	1022962	55.62%	6.403%
21	7.993	2063	2069	2080	rVV3	34063	60942	3.31%	0.381%
22	8.202	2116	2134	2145	rBV	102697	176914	9.62%	1.107%
23	8.504	2218	2228	2241	rVB5	12519	26287	1.43%	0.165%
24	8.655	2261	2275	2287	rBV	800533	1394686	75.83%	8.729%
25	8.806	2313	2322	2332	rBV3	25133	39176	2.13%	0.245%
26	9.436	2505	2518	2539	rBV	530930	899760	48.92%	5.631%
27	10.359	2794	2805	2816	rBV4	23196	37475	2.04%	0.235%
28	10.462	2825	2837	2848	rVB	12206	21237	1.15%	0.133%
29	10.771	2921	2933	2947	rBV	228289	373660	20.32%	2.339%
30	10.902	2963	2974	2985	rVB3	14223	23975	1.30%	0.150%
31	11.041	3007	3017	3029	rVB2	10297	18852	1.03%	0.118%
32	11.700	3208	3222	3230	rBV5	14453	24027	1.31%	0.150%
33	11.825	3248	3261	3281	rVB	590043	977920	53.17%	6.121%
34	12.079	3327	3340	3351	rBV3	15605	31830	1.73%	0.199%

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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\SOMUTR050720WMA.M
Title : TRACE VOA SOM01.0

35	12.205	3364	3379	3398	rBV	599110	972238	52.86%	6.085%
36	12.459	3448	3458	3467	rBV4	11933	19153	1.04%	0.120%
37	12.520	3469	3477	3486	rBV2	21797	34864	1.90%	0.218%
38	12.796	3553	3563	3579	rBV4	21032	39537	2.15%	0.247%
39	12.909	3589	3598	3612	rVB2	19364	31006	1.69%	0.194%
40	14.115	3962	3973	3985	rBV	79035	130220	7.08%	0.815%
41	14.352	4035	4047	4061	rBV	125675	202194	10.99%	1.265%
42	14.764	4165	4175	4186	rVB	11908	19153	1.04%	0.120%
43	16.751	4786	4793	4810	rVB	10581	19315	1.05%	0.121%

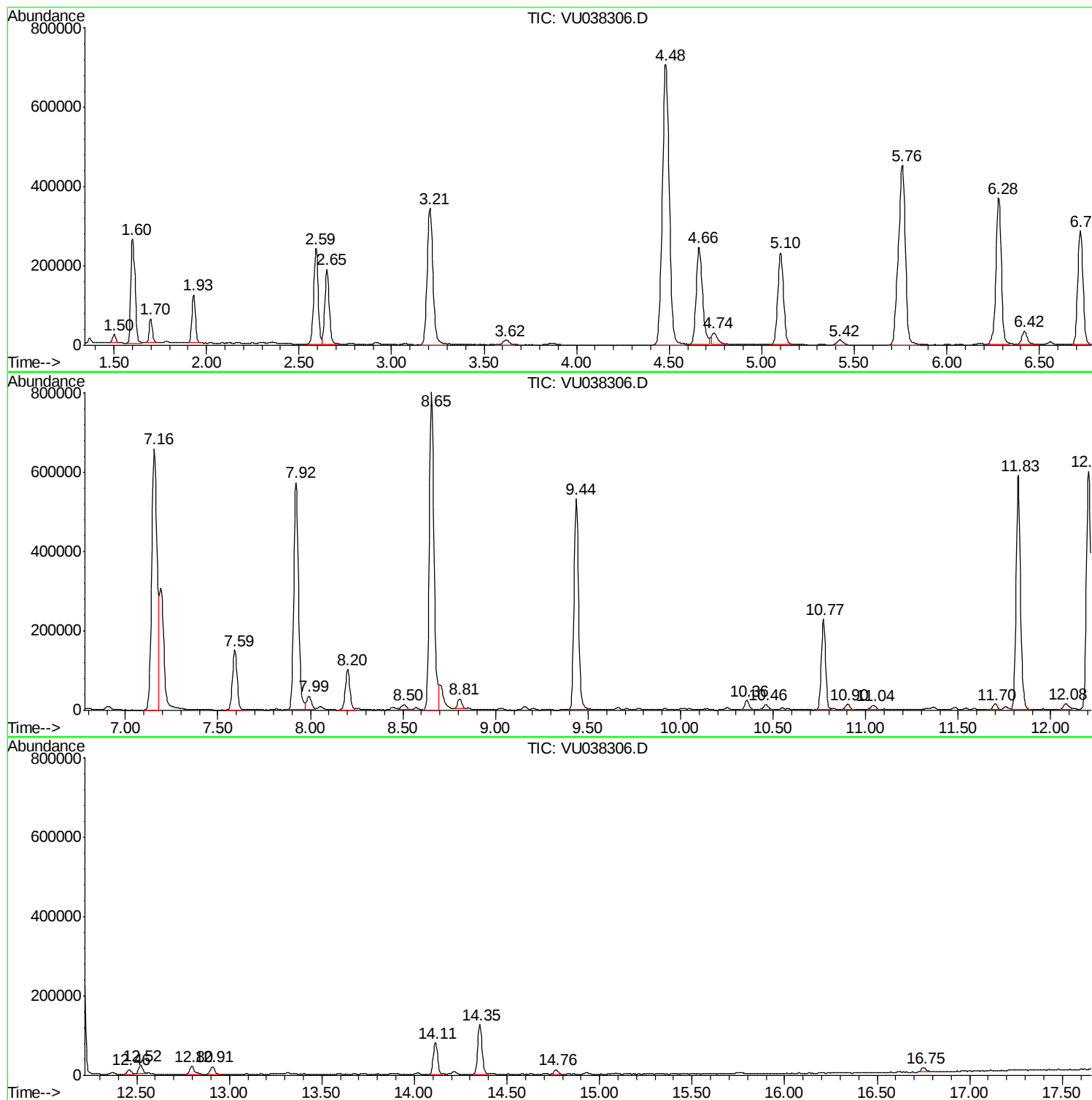
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
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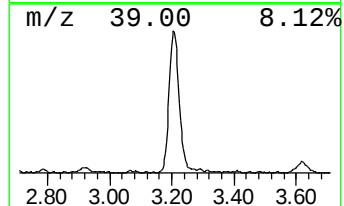
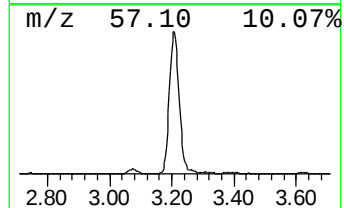
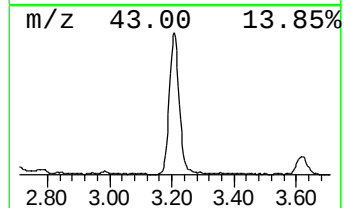
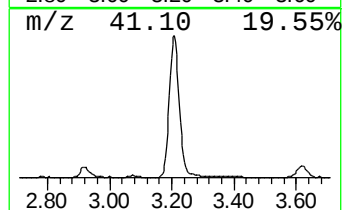
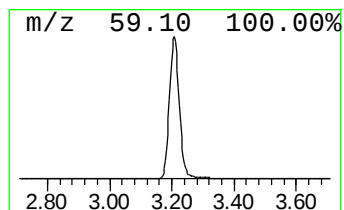
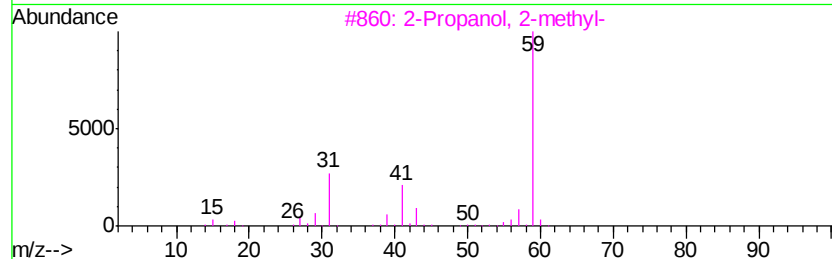
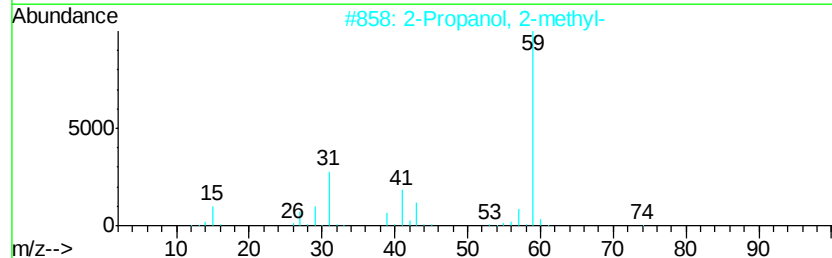
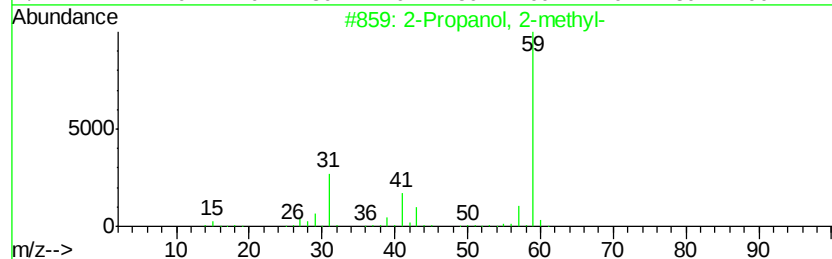
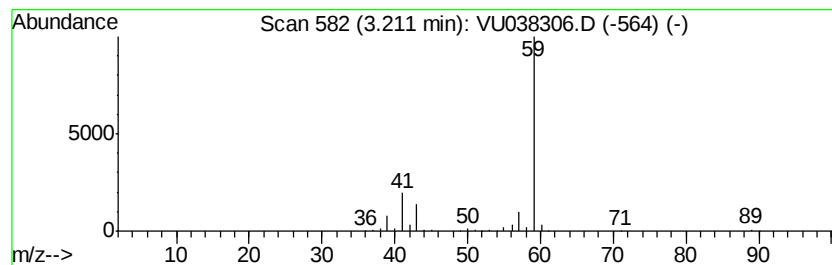
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.21	5.16 ug/L	766416	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	78
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	43
5			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9



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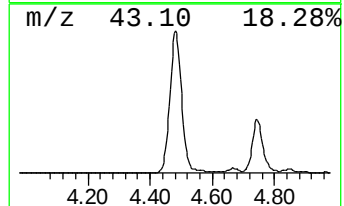
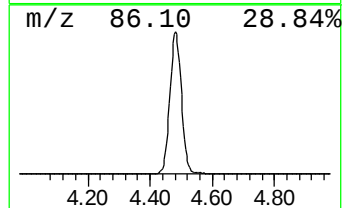
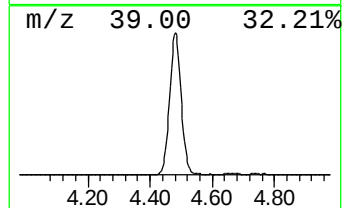
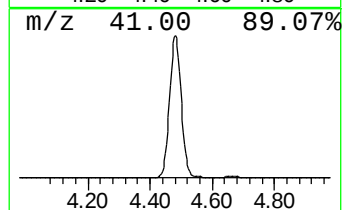
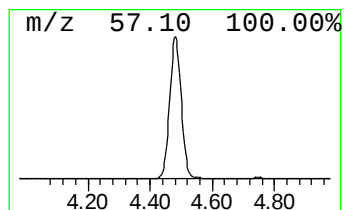
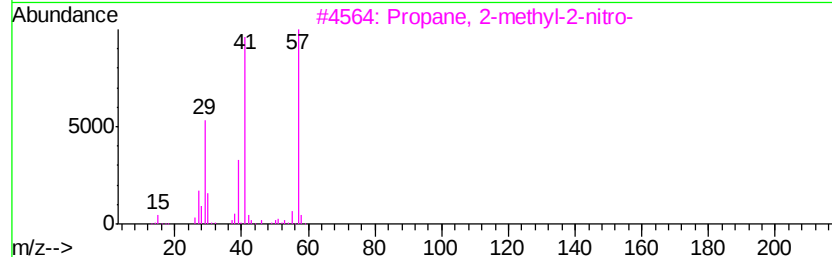
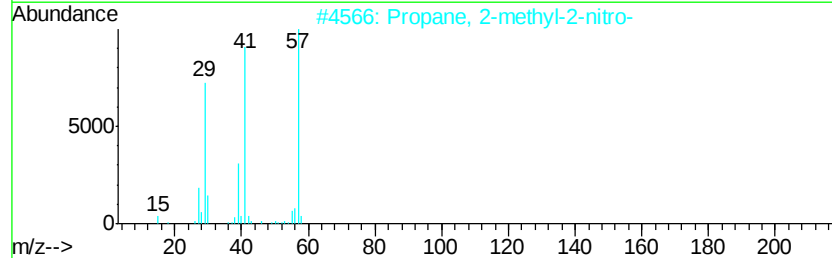
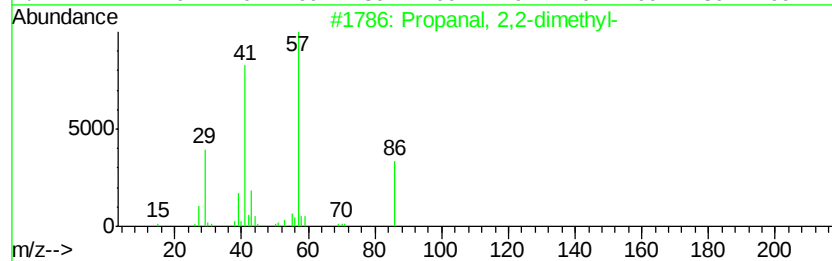
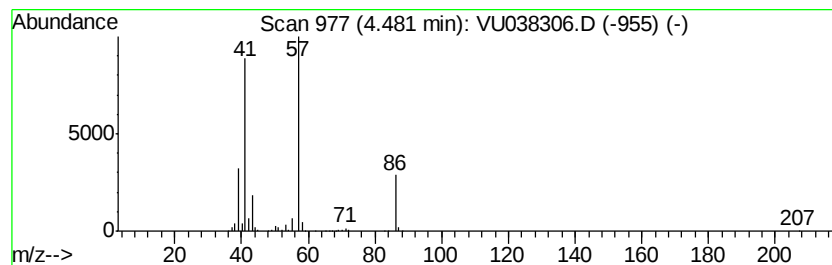
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	12.38 ug/L	1839170	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
5		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	42



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ALS Vial : 1 Sample Multiplier: 1

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ClientSampled :
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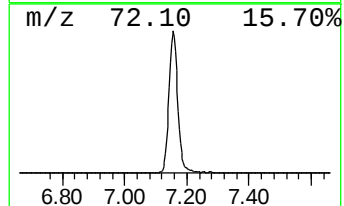
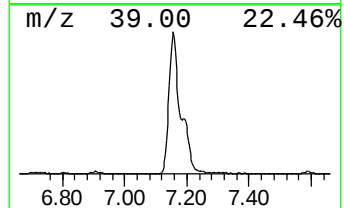
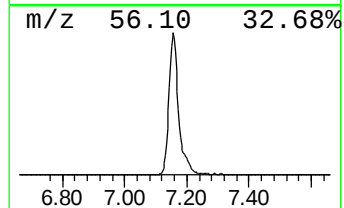
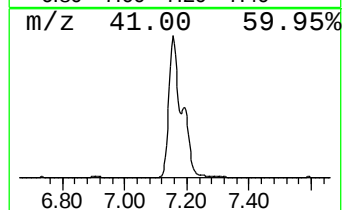
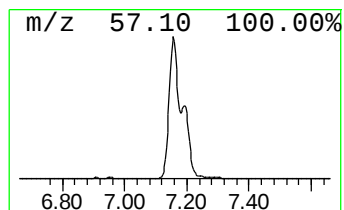
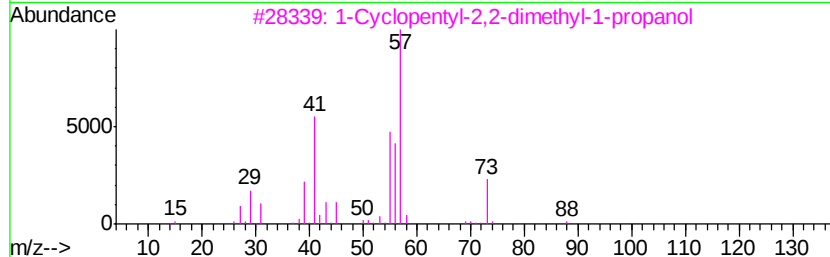
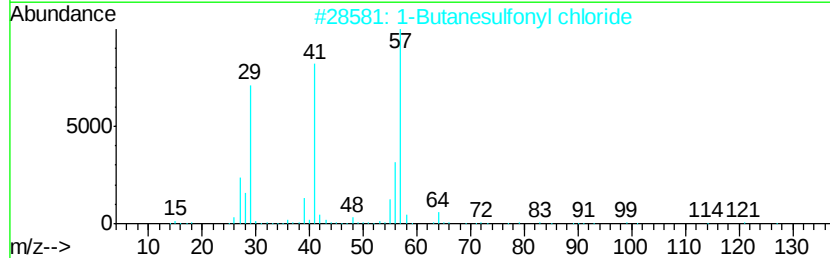
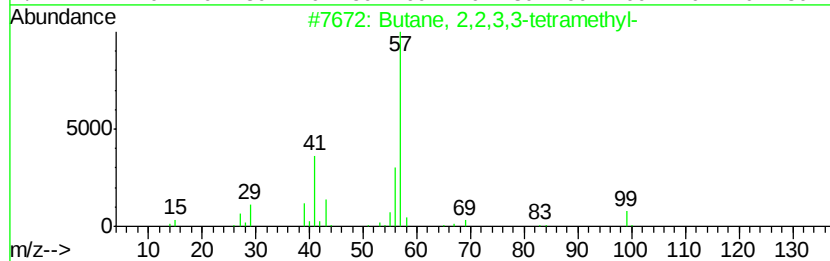
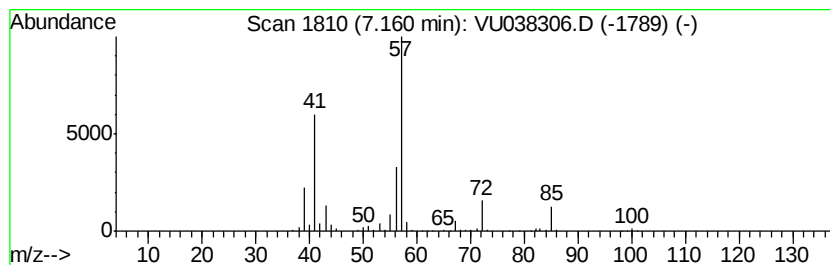
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	9.14 ug/L	1358080	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
2			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
3			1-Cyclopentyl-2,2-dimethyl-1-propanol	156	C10H20O	337966-85-5	38
4			1-Hexen-3-ol	100	C6H12O	004798-44-1	38
5			1-Hexen-3-ol	100	C6H12O	004798-44-1	38



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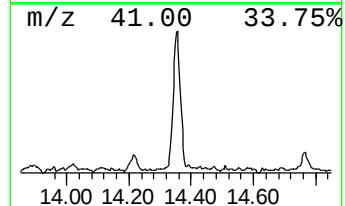
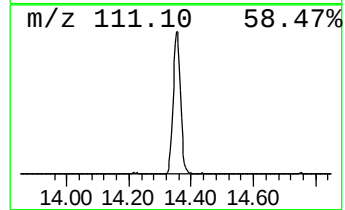
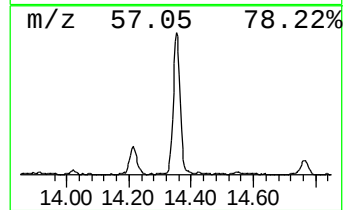
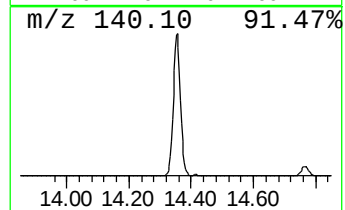
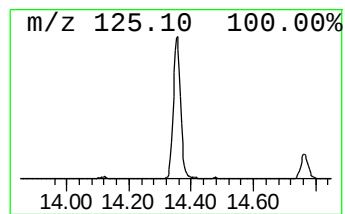
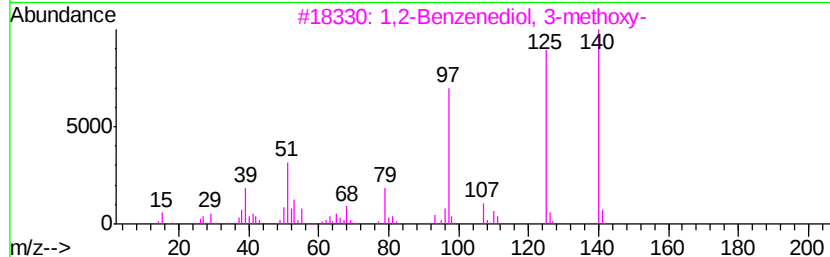
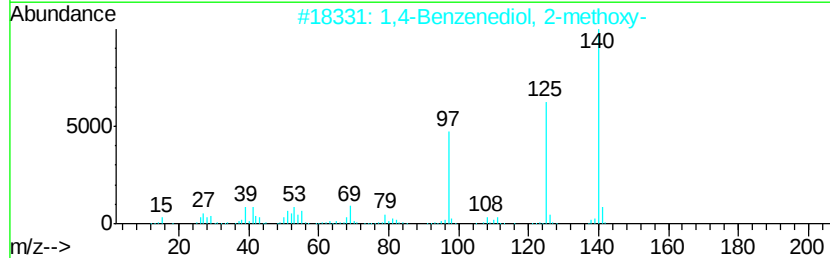
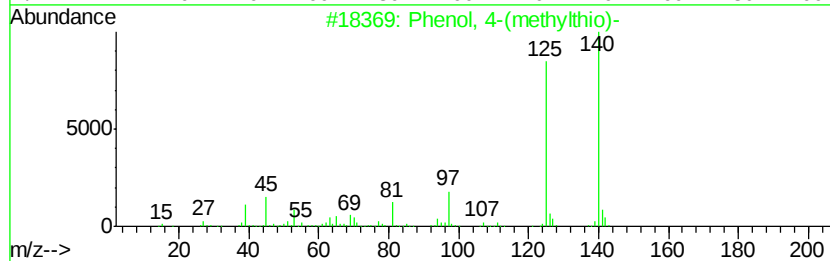
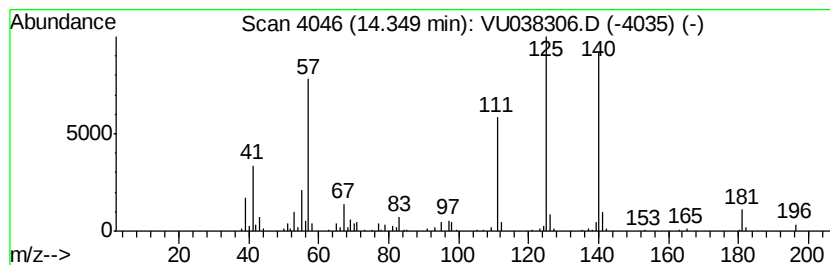
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Phenol, 4-(methylthio)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	1.03 ug/L	202194	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	58
2		1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	53
3		1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	53
4		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	53
5		3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	50



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.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...	3.21	5.2	ug/L	766416	1	6.28	742643	5.0
Propanal, 2,2-dim...	4.48	12.4	ug/L	1839170	1	6.28	742643	5.0
(DEL) Alkane: Str...	7.16	9.1	ug/L	1358080	1	6.28	742643	5.0
Phenol, 4-(methyl...	14.35	1.0	ug/L	202194	3	11.83	977920	5.0