

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052620\
 Data File : VU038305.D
 Acq On : 26 May 2020 18:32
 Operator : JC/MD
 Sample : L2766-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4Y5

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	20491	26478	1.46%	0.168%
2	1.601	72	81	94	rBV2	256076	401550	22.12%	2.548%
3	1.700	104	112	125	rVB	59334	72115	3.97%	0.458%
4	1.932	175	184	197	rVB	117516	156728	8.63%	0.994%
5	2.591	373	389	399	rBV	239236	400265	22.05%	2.540%
6	2.649	399	407	426	rVB	186106	314561	17.33%	1.996%
7	3.208	564	581	610	rBV	339900	758486	41.78%	4.812%
8	3.620	695	709	725	rBV2	12307	27165	1.50%	0.172%
9	4.482	955	977	1005	rBV	697670	1815335	100.00%	11.518%
10	4.662	1018	1033	1051	rBV	247571	589834	32.49%	3.742%
11	4.742	1053	1058	1076	rVB	26078	52937	2.92%	0.336%
12	5.102	1155	1170	1190	rVB	224727	490278	27.01%	3.111%
13	5.424	1257	1270	1284	rBV6	13382	30816	1.70%	0.196%
14	5.761	1353	1375	1401	rBV2	438255	1164012	64.12%	7.385%
15	6.279	1516	1536	1564	rVV	390721	794838	43.78%	5.043%
16	6.420	1568	1580	1600	rVV2	32062	65616	3.61%	0.416%
17	6.723	1659	1674	1691	rBV2	280071	546734	30.12%	3.469%
18	7.157	1793	1809	1817	rBV	649728	1336484	73.62%	8.480%
19	7.591	1931	1944	1960	rBV	147463	261221	14.39%	1.657%
20	7.922	2033	2047	2061	rBV	556504	1004863	55.35%	6.376%
21	7.993	2063	2069	2080	rVV	34802	61986	3.41%	0.393%
22	8.202	2121	2134	2145	rBV	97409	168599	9.29%	1.070%
23	8.507	2218	2229	2240	rVB5	10999	25412	1.40%	0.161%
24	8.655	2261	2275	2287	rBV	745238	1316266	72.51%	8.351%
25	8.806	2313	2322	2333	rVB4	27174	41334	2.28%	0.262%
26	9.436	2504	2518	2551	rVB	565922	969774	53.42%	6.153%
27	10.359	2795	2805	2815	rBV4	22138	36693	2.02%	0.233%
28	10.462	2828	2837	2846	rVB2	12854	19759	1.09%	0.125%
29	10.771	2921	2933	2946	rBV	221343	351468	19.36%	2.230%
30	10.902	2964	2974	2987	rVB5	12662	22458	1.24%	0.142%
31	11.041	3005	3017	3030	rVB4	10707	20826	1.15%	0.132%
32	11.700	3212	3222	3231	rBV3	13326	19838	1.09%	0.126%
33	11.825	3249	3261	3279	rVB	621010	1019599	56.17%	6.469%
34	12.079	3324	3340	3361	rBV3	17037	41042	2.26%	0.260%

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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	3394	rVV	586048	929722	51.21%	5.899%
36	12.459	3449	3458	3467	rBV3	11657	18654	1.03%	0.118%
37	12.520	3467	3477	3487	rBV2	21714	35052	1.93%	0.222%
38	12.800	3553	3564	3572	rBV5	18632	31795	1.75%	0.202%
39	12.909	3587	3598	3611	rVB5	17273	27533	1.52%	0.175%
40	14.115	3962	3973	3985	rVB	72369	113924	6.28%	0.723%
41	14.352	4036	4047	4063	rBV	110321	178923	9.86%	1.135%

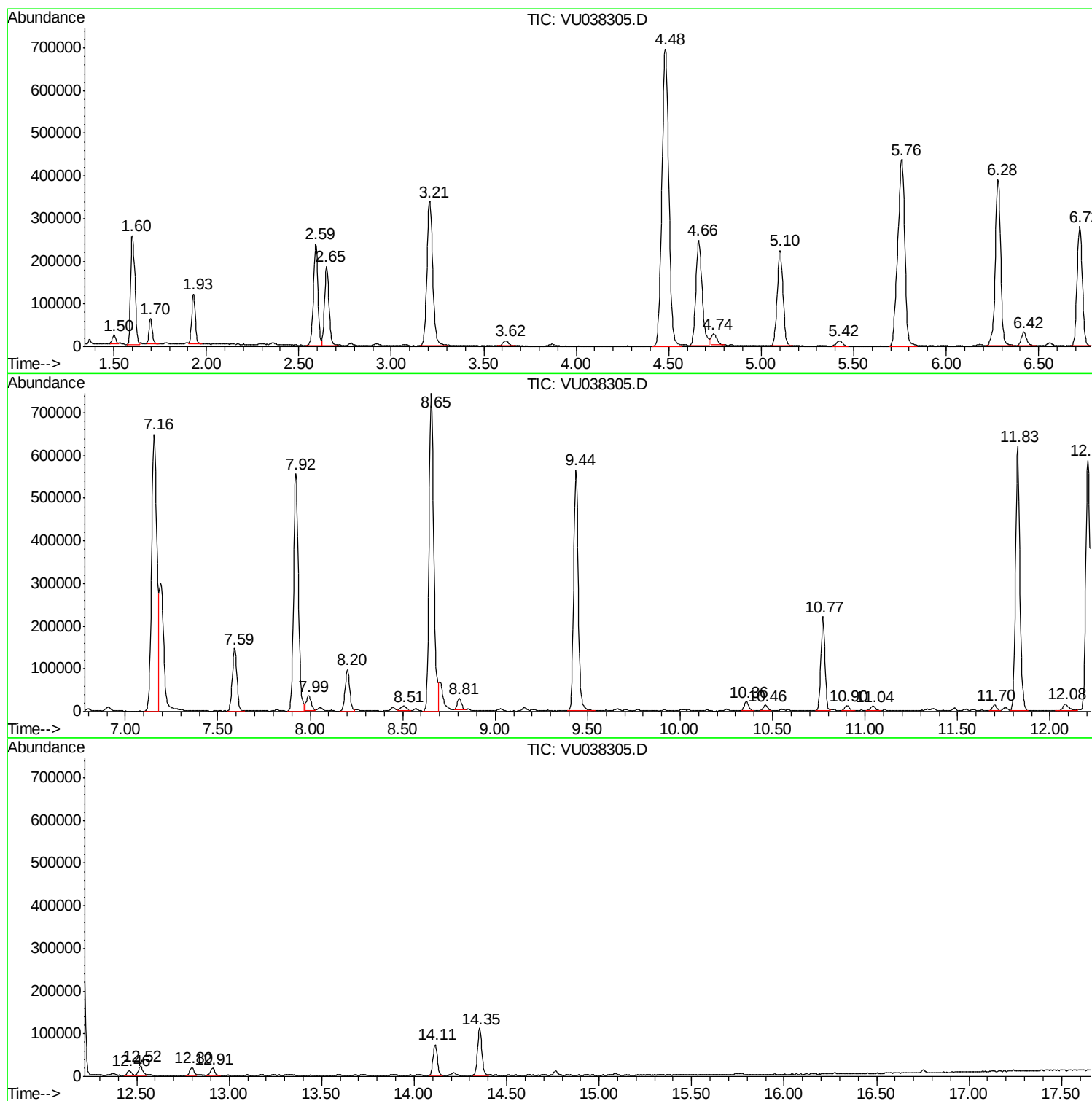
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Quant Title : TRACE VOA SOM01.0

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



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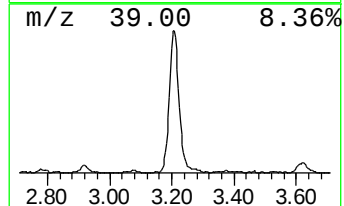
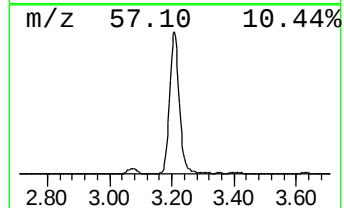
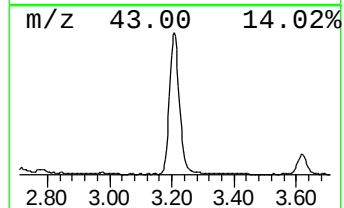
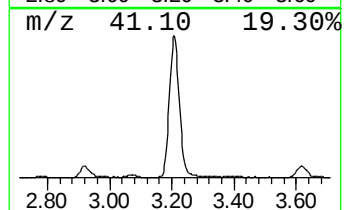
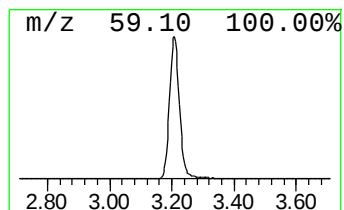
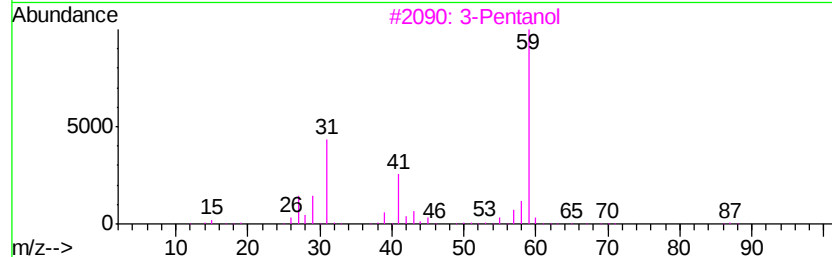
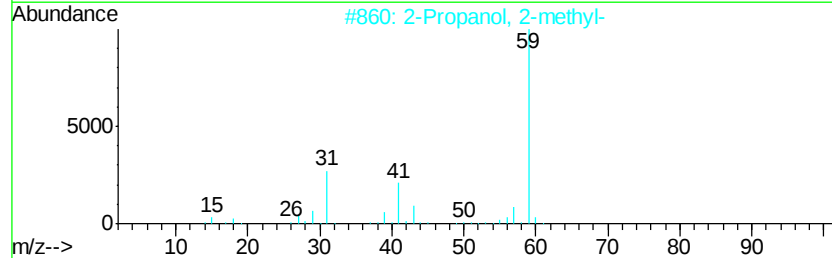
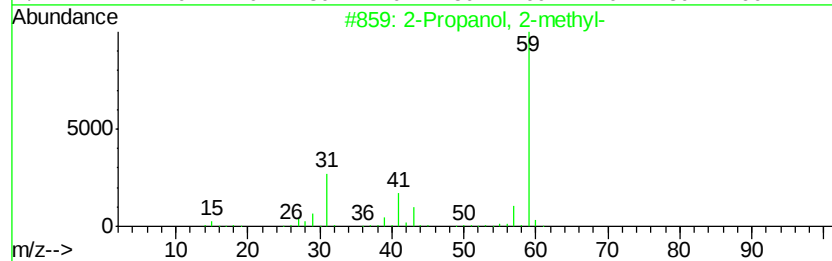
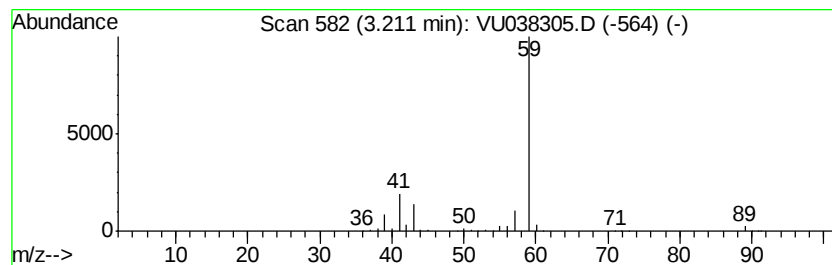
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	4.77 ug/L	758486	1,4-Difluorobenzene	6.28

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			3-Pentanol	88	C5H12O	000584-02-1	56
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
5			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	43



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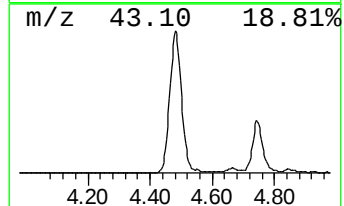
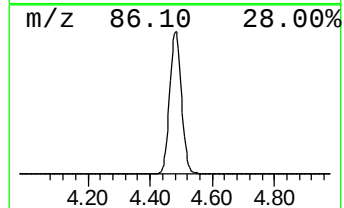
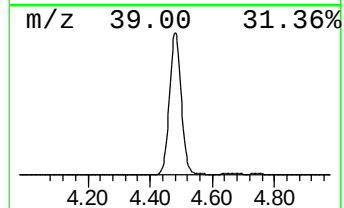
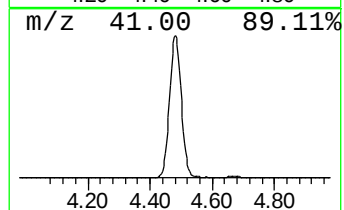
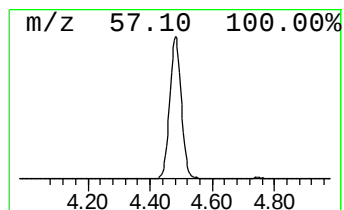
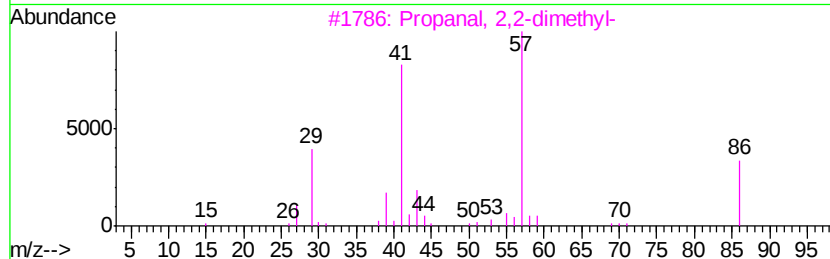
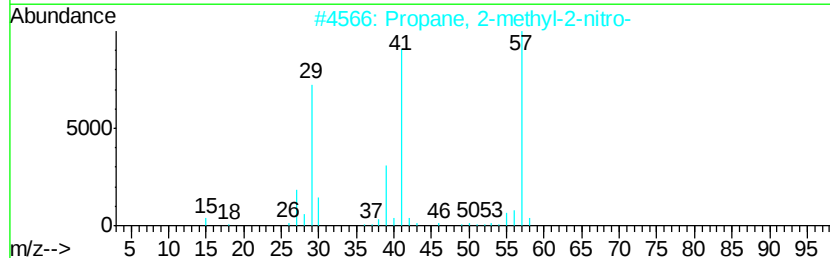
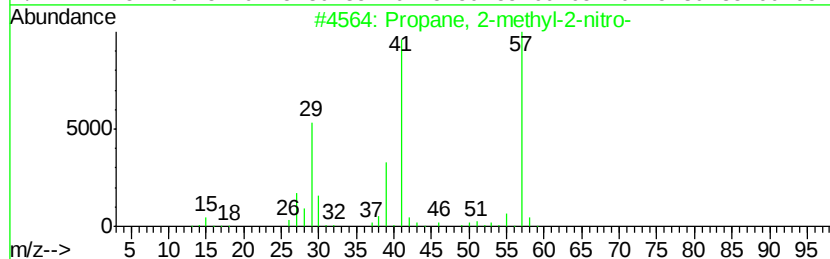
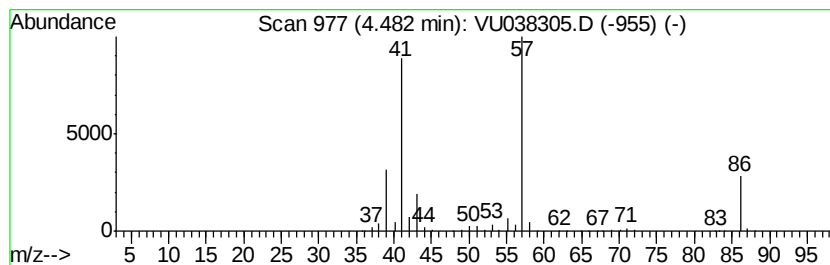
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 2-methyl-2-nitro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	11.42 ug/L	1815340	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	59		
2	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50		
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47		
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45		
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	45		



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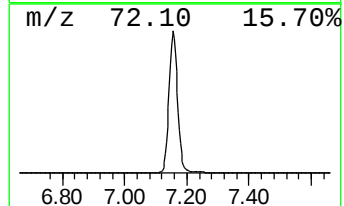
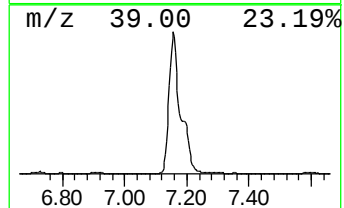
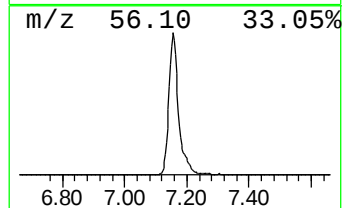
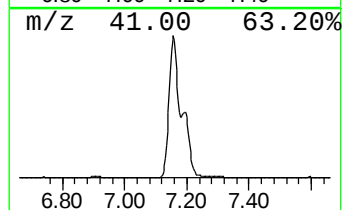
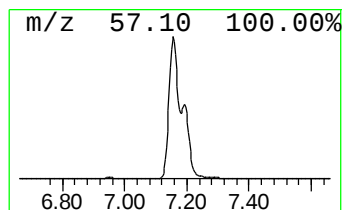
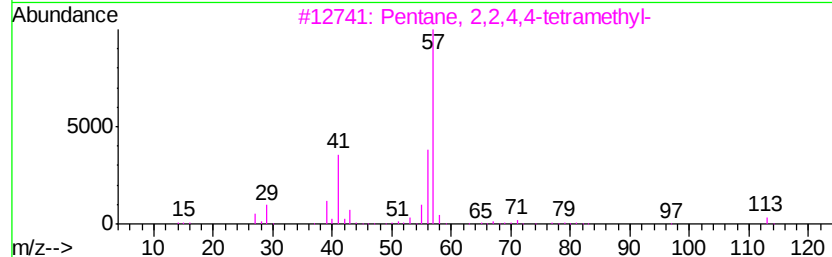
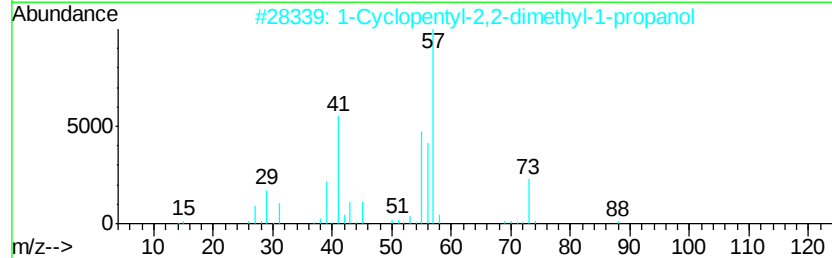
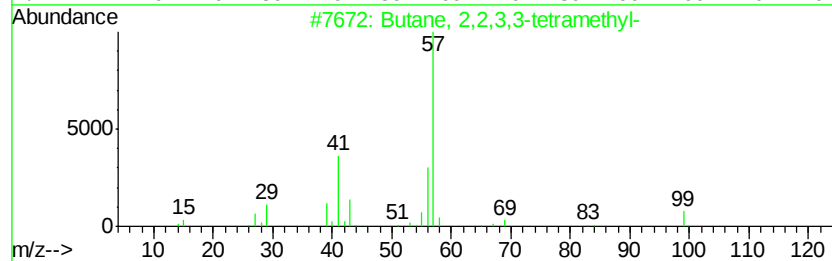
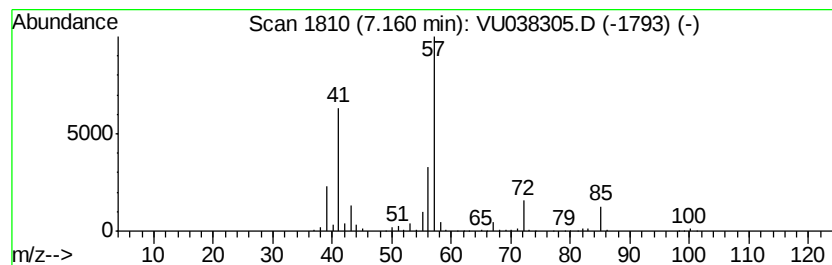
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	8.41 ug/L	1336480	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
2		1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	42
3		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42
4		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	42
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38



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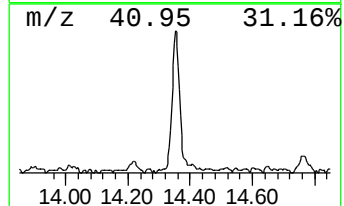
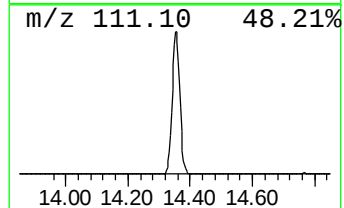
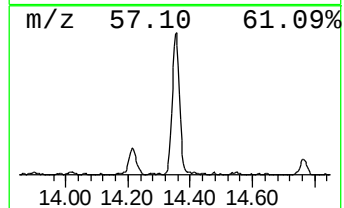
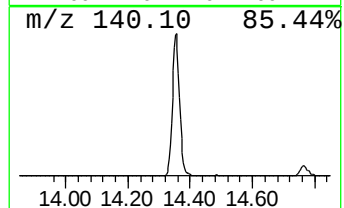
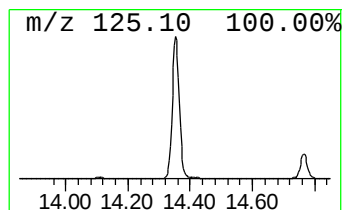
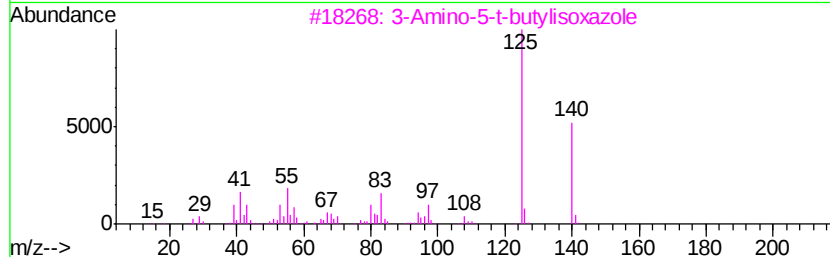
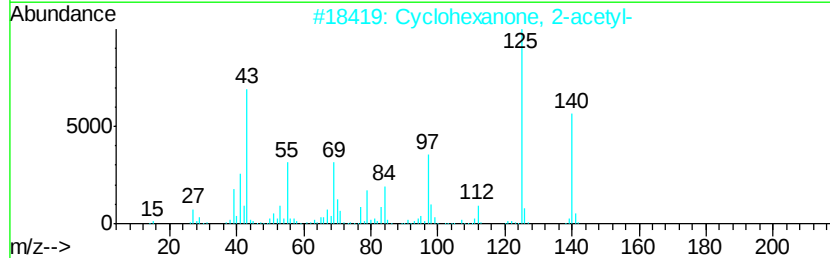
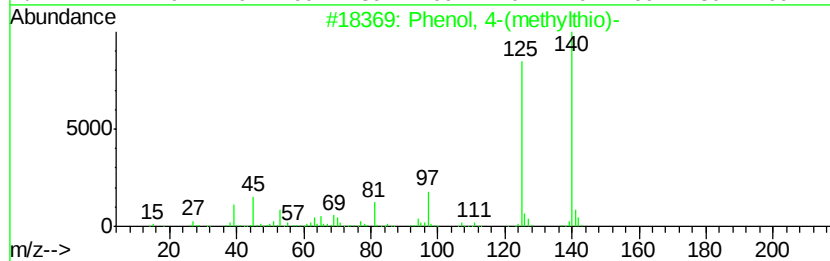
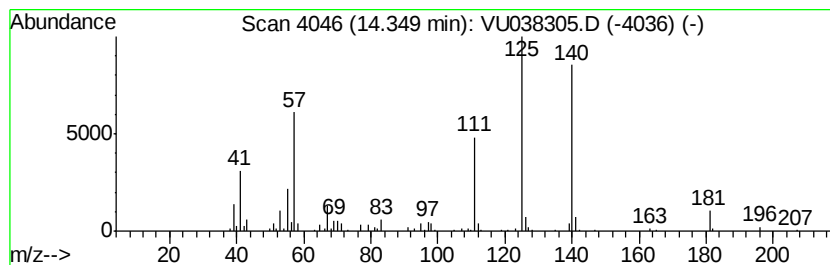
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenol, 4-(methylthio)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	0.88 ug/L	178923	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	64
2		Cyclohexanone, 2-acetyl-	140	C8H12O2	000874-23-7	59
3		3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	53
4		Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	53
5		2-Methoxyresorcinol	140	C7H8O3	029267-67-2	53



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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	4.8	ug/L	758486	1	6.28	794838	5.0
Propane, 2-methyl...	4.48	11.4	ug/L	1815340	1	6.28	794838	5.0
(DEL) Alkane: Str...	7.16	8.4	ug/L	1336480	1	6.28	794838	5.0
Phenol, 4-(methyl...	14.35	0.9	ug/L	178923	3	11.83	1019600	5.0