

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU053120\
 Data File : VU038420.D
 Acq On : 30 May 2020 17:57
 Operator : JC/MD
 Sample : L2766-16
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4Z9

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\SOMUTR053120WMA.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	1.498	42	49	56	rBV2	15379	18261	1.02%	0.118%
2	1.610	73	84	100	rBV2	163453	258051	14.42%	1.661%
3	1.707	106	114	132	rBV	50055	84321	4.71%	0.543%
4	1.932	176	184	196	rVB	116569	151320	8.46%	0.974%
5	2.594	375	390	402	rBV	250230	420911	23.53%	2.710%
6	2.681	402	417	457	rVB	120925	434810	24.30%	2.799%
7	3.308	571	612	613	rBV2	93025	388191	21.70%	2.499%
8	3.620	697	709	726	rVB4	12301	30405	1.70%	0.196%
9	3.877	774	789	805	rVB5	6858	18595	1.04%	0.120%
10	4.482	956	977	1014	rBV	676644	1789002	100.00%	11.518%
11	4.681	1023	1039	1059	rBV2	202875	671672	37.54%	4.324%
12	5.102	1152	1170	1189	rBV	218035	480282	26.85%	3.092%
13	5.758	1352	1374	1403	rBV2	435984	1156968	64.67%	7.449%
14	6.279	1516	1536	1563	rBV	406860	834779	46.66%	5.374%
15	6.424	1568	1581	1601	rBV2	32295	70203	3.92%	0.452%
16	6.723	1659	1674	1693	rBV	268371	519469	29.04%	3.344%
17	6.912	1721	1733	1741	rBV5	9834	19118	1.07%	0.123%
18	7.157	1792	1809	1817	rBV	608672	1261929	70.54%	8.125%
19	7.591	1931	1944	1963	rBV	146551	254883	14.25%	1.641%
20	7.922	2032	2047	2062	rBV	519030	936466	52.35%	6.029%
21	7.993	2062	2069	2081	rVV	32456	59177	3.31%	0.381%
22	8.202	2117	2134	2146	rBV	95885	169159	9.46%	1.089%
23	8.507	2217	2229	2241	rBV3	11714	25226	1.41%	0.162%
24	8.655	2261	2275	2312	rBV	852675	1637534	91.53%	10.543%
25	8.809	2312	2323	2333	rBV4	29738	48819	2.73%	0.314%
26	9.436	2503	2518	2551	rVB	592991	1006019	56.23%	6.477%
27	10.359	2795	2805	2819	rBV2	28718	45744	2.56%	0.295%
28	10.771	2921	2933	2945	rBV	224405	363063	20.29%	2.337%
29	11.041	3007	3017	3031	rVB4	10484	18666	1.04%	0.120%
30	11.700	3208	3222	3232	rBV7	14758	23696	1.32%	0.153%
31	11.825	3248	3261	3280	rVB	645566	1069781	59.80%	6.887%
32	12.083	3327	3341	3354	rBV5	8054	19430	1.09%	0.125%
33	12.205	3365	3379	3391	rBV	543371	885645	49.50%	5.702%
34	12.523	3467	3478	3490	rBV	21293	35408	1.98%	0.228%

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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	12.796	3553	3563	3574	rBV2	19879	32818	1.83%	0.211%
36	12.909	3588	3598	3607	rBV4	15115	22823	1.28%	0.147%
37	14.115	3961	3973	3988	rBV	70244	112732	6.30%	0.726%
38	14.352	4036	4047	4060	rBV2	97331	157001	8.78%	1.011%

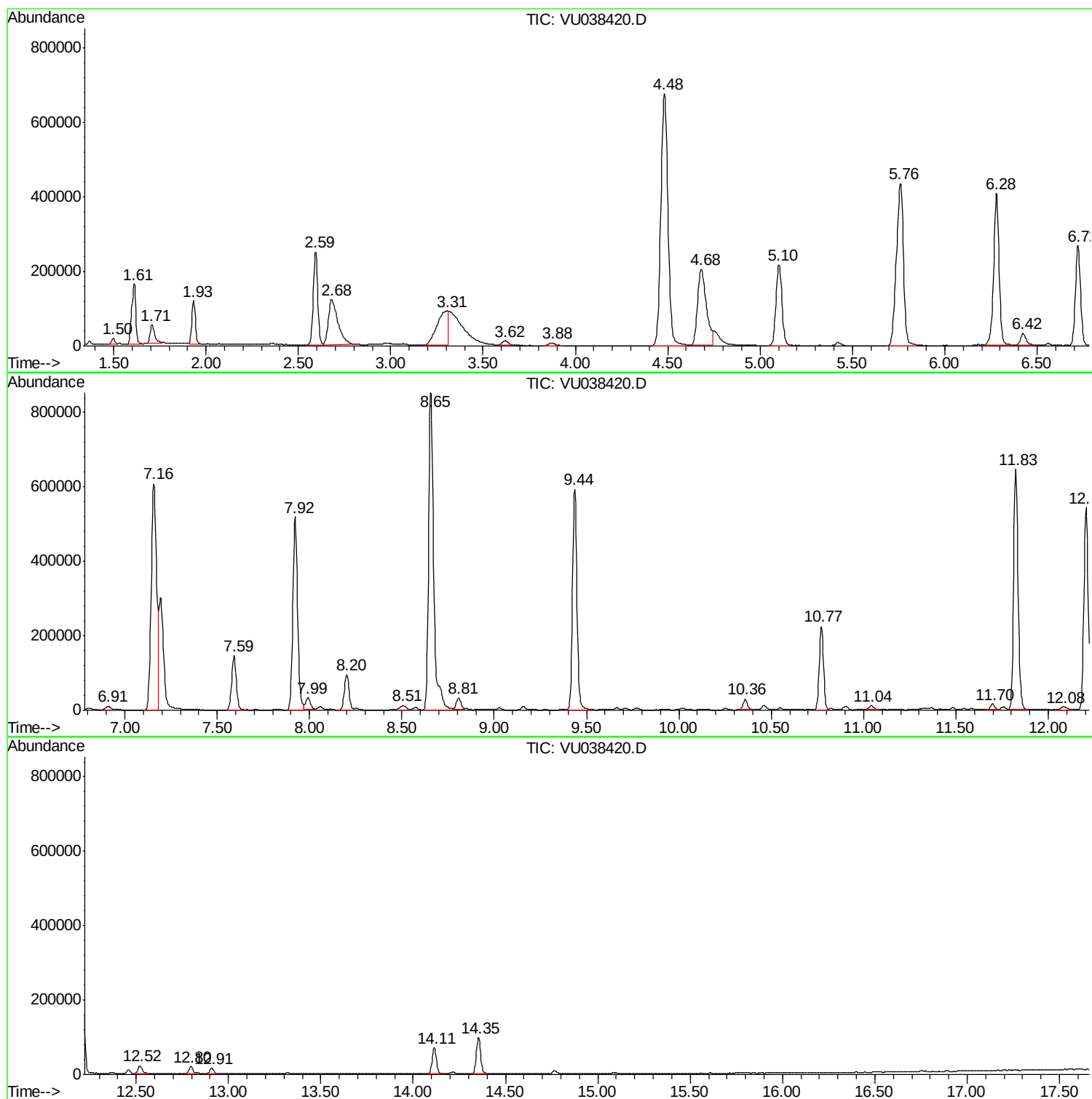
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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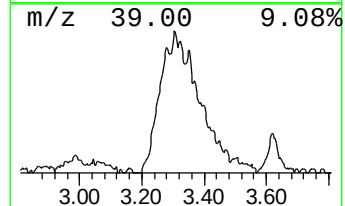
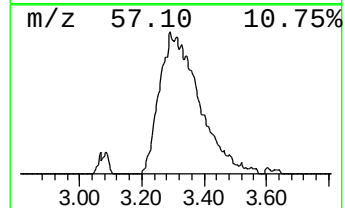
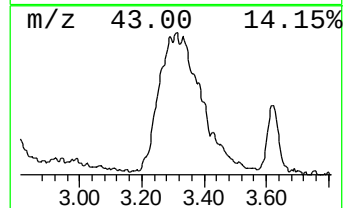
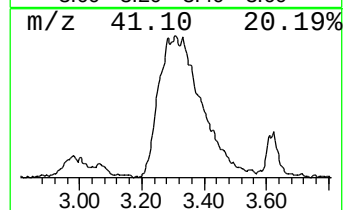
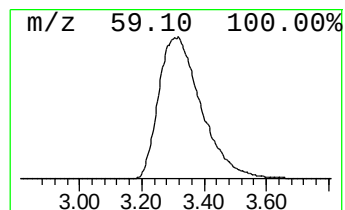
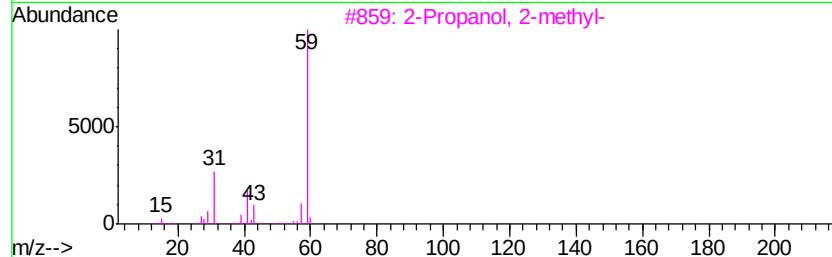
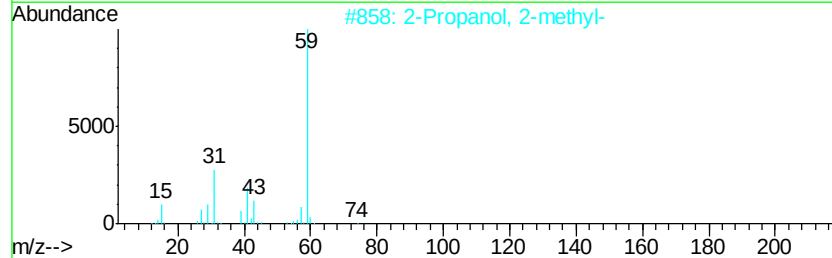
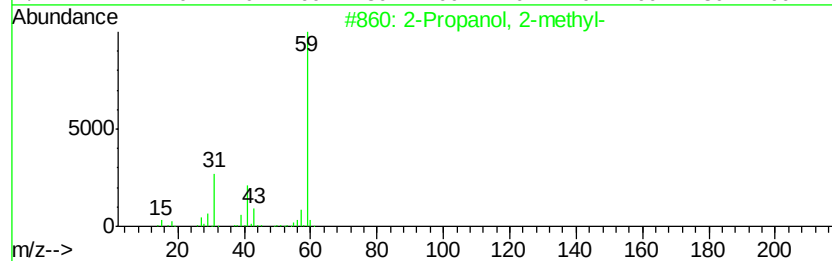
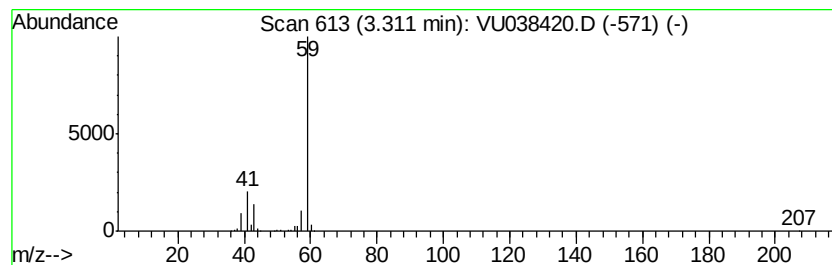
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.31	2.33 ug/L	388191	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
2		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4		3-Pentanol	88	C5H12O	000584-02-1	64
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43



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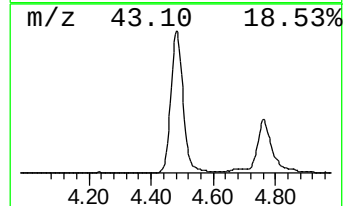
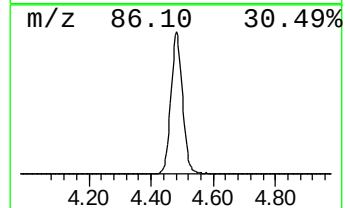
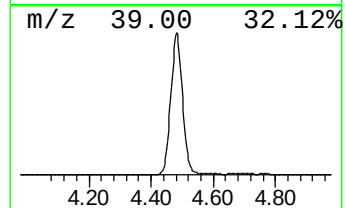
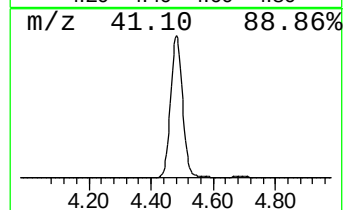
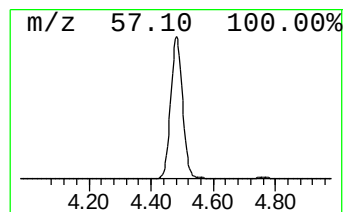
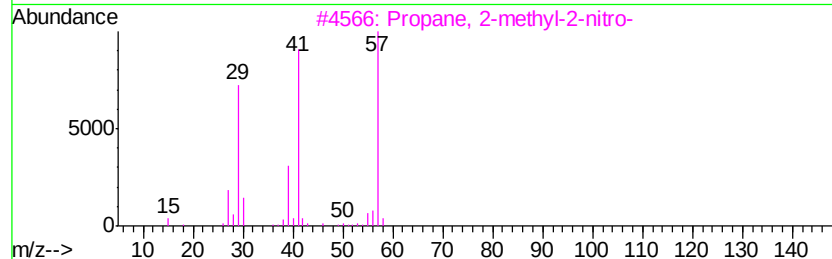
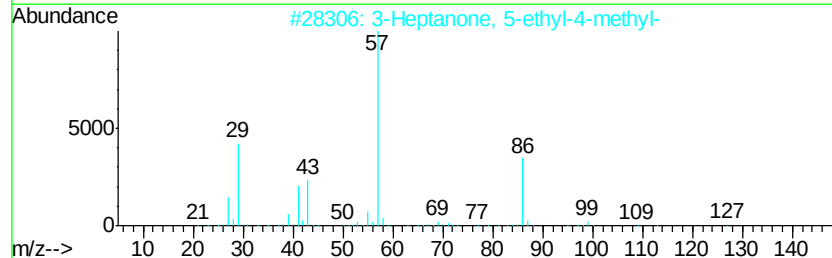
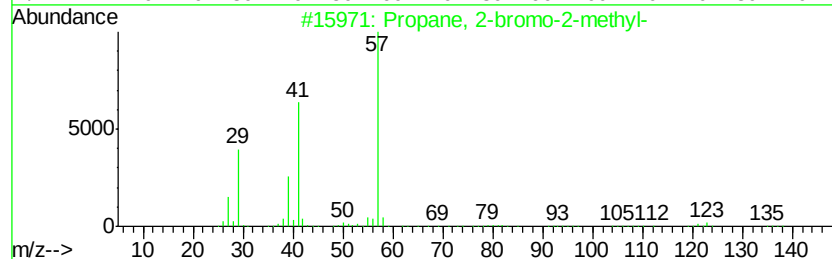
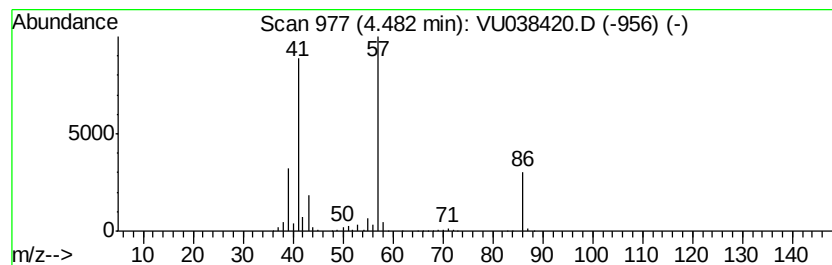
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR053120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Propane, 2-bromo-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	10.72 ug/L	1789000	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
2		3-Heptanone, 5-ethyl-4-methyl-	156	C10H20O	027607-63-2	50
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
4		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
5		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	45



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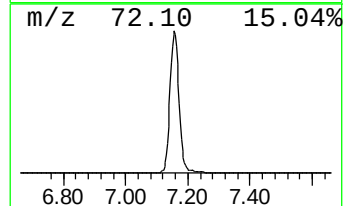
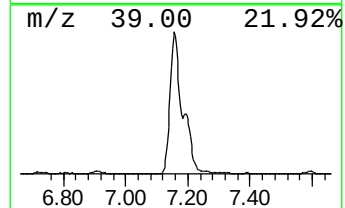
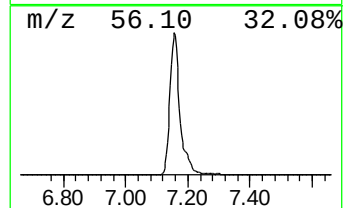
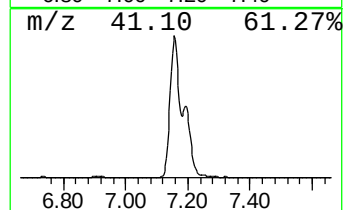
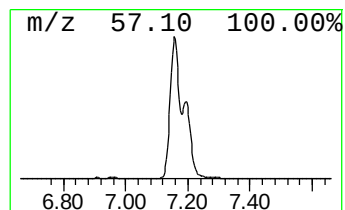
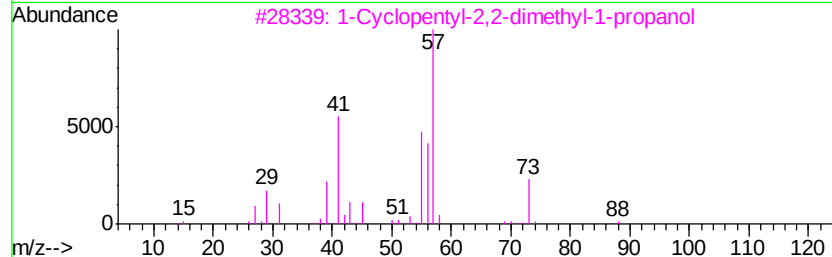
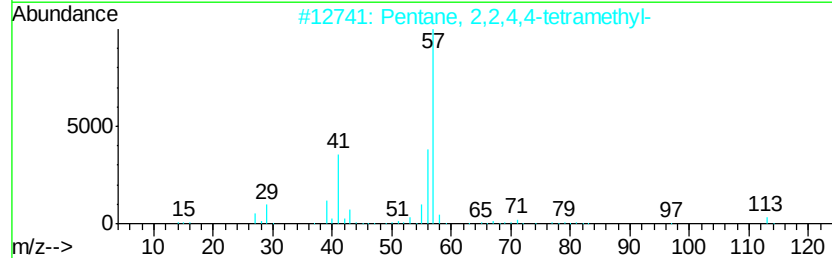
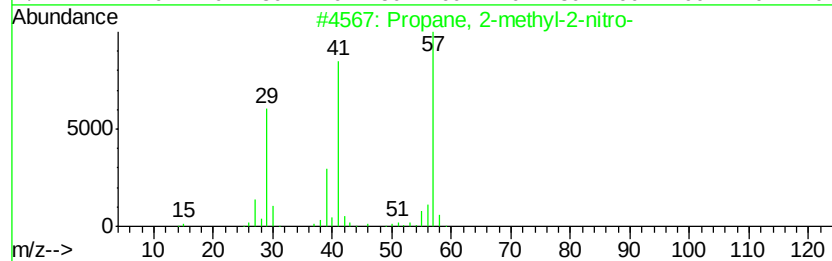
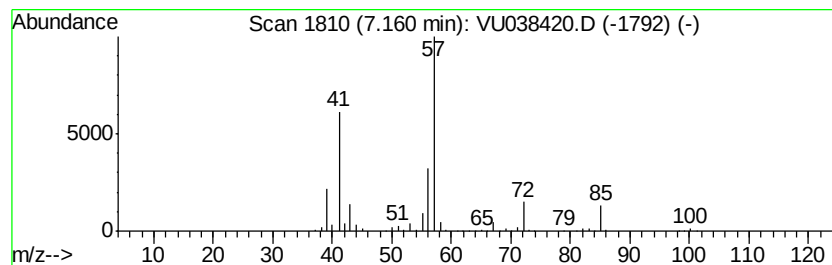
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	7.56 ug/L	1261930	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	37
2		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	36
3		1-Cyclopentyl-2,2-dimethyl-1-propanol	156	C10H20O	337966-85-5	36
4		Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	33
5		1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	33



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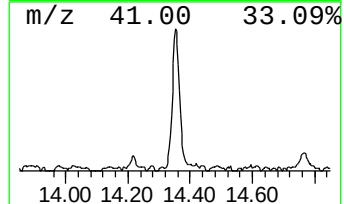
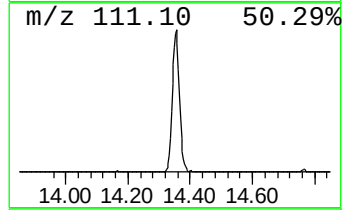
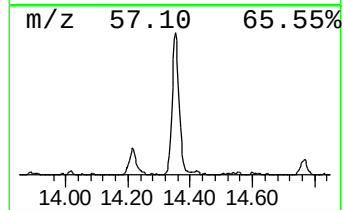
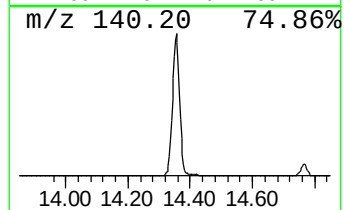
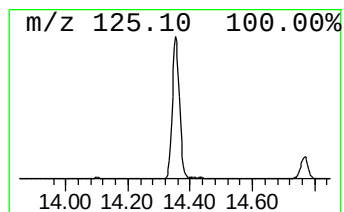
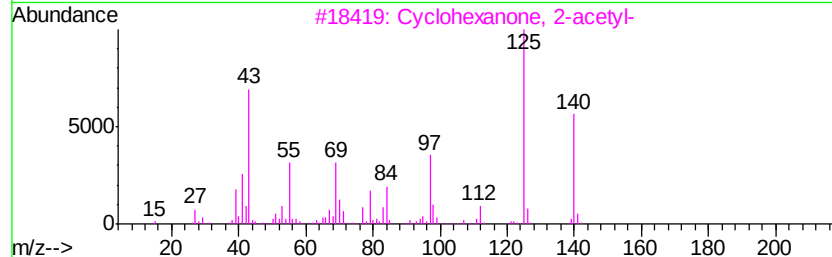
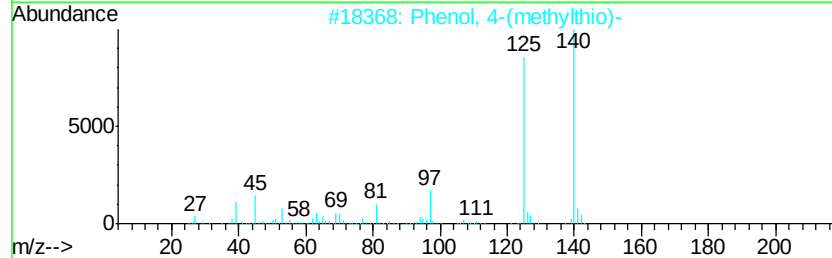
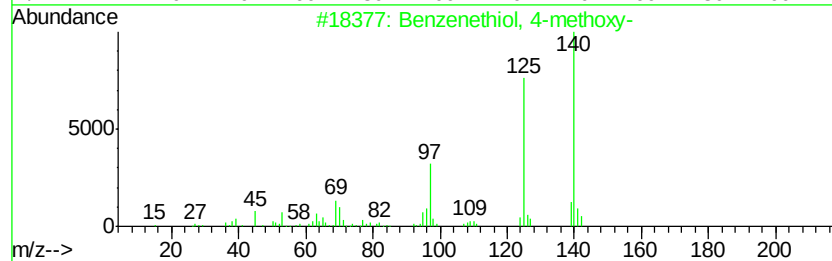
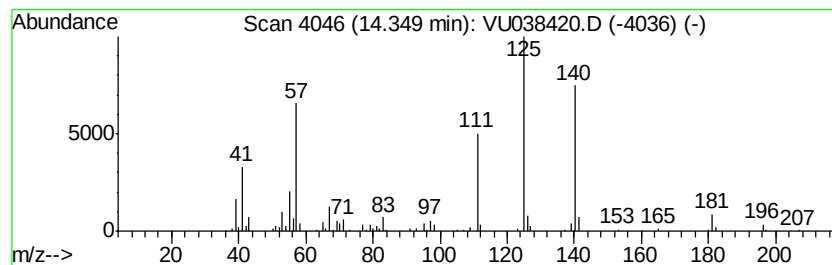
Instrument :
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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzenethiol, 4-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.35	0.73 ug/L	157001	1,4-Dichlorobenzene-d4		11.82	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	59
2		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
3		Cyclohexanone, 2-acetyl-	140	C8H12O2	000874-23-7	59
4		3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	53
5		3-tert-Butyl-2-pyrazolin-5-one	140	C7H12N2O	029211-68-5	53



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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...	3.31	2.3	ug/L	388191	1	6.28	834779	5.0
Propane, 2-bromo-...	4.48	10.7	ug/L	1789000	1	6.28	834779	5.0
unknown-01	7.16	7.6	ug/L	1261930	1	6.28	834779	5.0
Benzenethiol, 4-m...	14.35	0.7	ug/L	157001	3	11.82	1069780	5.0