

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052220\
 Data File : VU038280.D
 Acq On : 22 May 2020 16:20
 Operator : JC/MD
 Sample : L2724-18
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4W4

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	1.491	41	47	65	rBV5	24515	50888	2.38%	0.275%
2	1.604	71	82	92	rBV2	187653	342740	16.00%	1.851%
3	1.697	104	111	123	rVB	49663	63883	2.98%	0.345%
4	1.925	174	182	200	rVB	143275	187880	8.77%	1.015%
5	2.588	373	388	399	rBV	279312	465045	21.71%	2.512%
6	2.652	399	408	432	rVB	159767	300417	14.03%	1.623%
7	3.224	566	586	620	rBV	291157	866947	40.48%	4.683%
8	3.613	693	707	725	rVB4	11520	27860	1.30%	0.150%
9	4.478	953	976	1004	rBV	813103	2141667	100.00%	11.568%
10	4.661	1017	1033	1051	rBV	304371	753532	35.18%	4.070%
11	5.099	1150	1169	1190	rBV	256942	573747	26.79%	3.099%
12	5.423	1254	1270	1285	rBV2	36053	81643	3.81%	0.441%
13	5.758	1352	1374	1404	rBV2	526164	1375687	64.23%	7.431%
14	6.279	1515	1536	1562	rBV	463711	927959	43.33%	5.012%
15	6.417	1568	1579	1599	rBV2	37202	76748	3.58%	0.415%
16	6.722	1656	1674	1692	rBV	331354	649506	30.33%	3.508%
17	7.157	1792	1809	1817	rBV	787470	1605224	74.95%	8.671%
18	7.591	1931	1944	1960	rBV	177690	305957	14.29%	1.653%
19	7.925	2033	2048	2062	rBV	618896	1143848	53.41%	6.179%
20	7.992	2063	2069	2081	rVV	44325	81414	3.80%	0.440%
21	8.205	2119	2135	2146	rBV	113483	198610	9.27%	1.073%
22	8.501	2217	2227	2241	rVB3	20917	48411	2.26%	0.261%
23	8.658	2262	2276	2288	rBV	907353	1600430	74.73%	8.645%
24	8.809	2313	2323	2332	rBV4	27260	45846	2.14%	0.248%
25	9.439	2505	2519	2553	rVB	648013	1122991	52.44%	6.066%
26	10.362	2794	2806	2818	rBV3	26691	43299	2.02%	0.234%
27	10.465	2830	2838	2846	rBV	14045	22058	1.03%	0.119%
28	10.774	2922	2934	2947	rBV	259405	417134	19.48%	2.253%
29	10.906	2962	2975	2988	rBV2	38562	63761	2.98%	0.344%
30	11.044	3010	3018	3030	rVB2	13636	25471	1.19%	0.138%
31	11.336	3094	3109	3117	rBV4	13622	28063	1.31%	0.152%
32	11.703	3209	3223	3233	rBV4	12947	21730	1.01%	0.117%
33	11.828	3249	3262	3282	rVB	701349	1170548	54.66%	6.323%
34	12.086	3331	3342	3353	rBV5	13353	28309	1.32%	0.153%

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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	12.208	3367	3380	3396	rBV	651343	1053695	49.20%	5.692%
36	12.465	3449	3460	3470	rBV6	13021	23179	1.08%	0.125%
37	12.529	3470	3480	3491	rBV	28644	46204	2.16%	0.250%
38	12.809	3556	3567	3589	rBV5	18182	38322	1.79%	0.207%
39	12.918	3589	3601	3610	rBV4	20206	31633	1.48%	0.171%
40	14.124	3965	3976	3987	rBV	81720	132348	6.18%	0.715%
41	14.365	4036	4051	4068	rBV	120976	196365	9.17%	1.061%
42	15.108	4269	4282	4301	rBV2	34231	60884	2.84%	0.329%
43	15.764	4476	4486	4502	rBV4	37344	71235	3.33%	0.385%

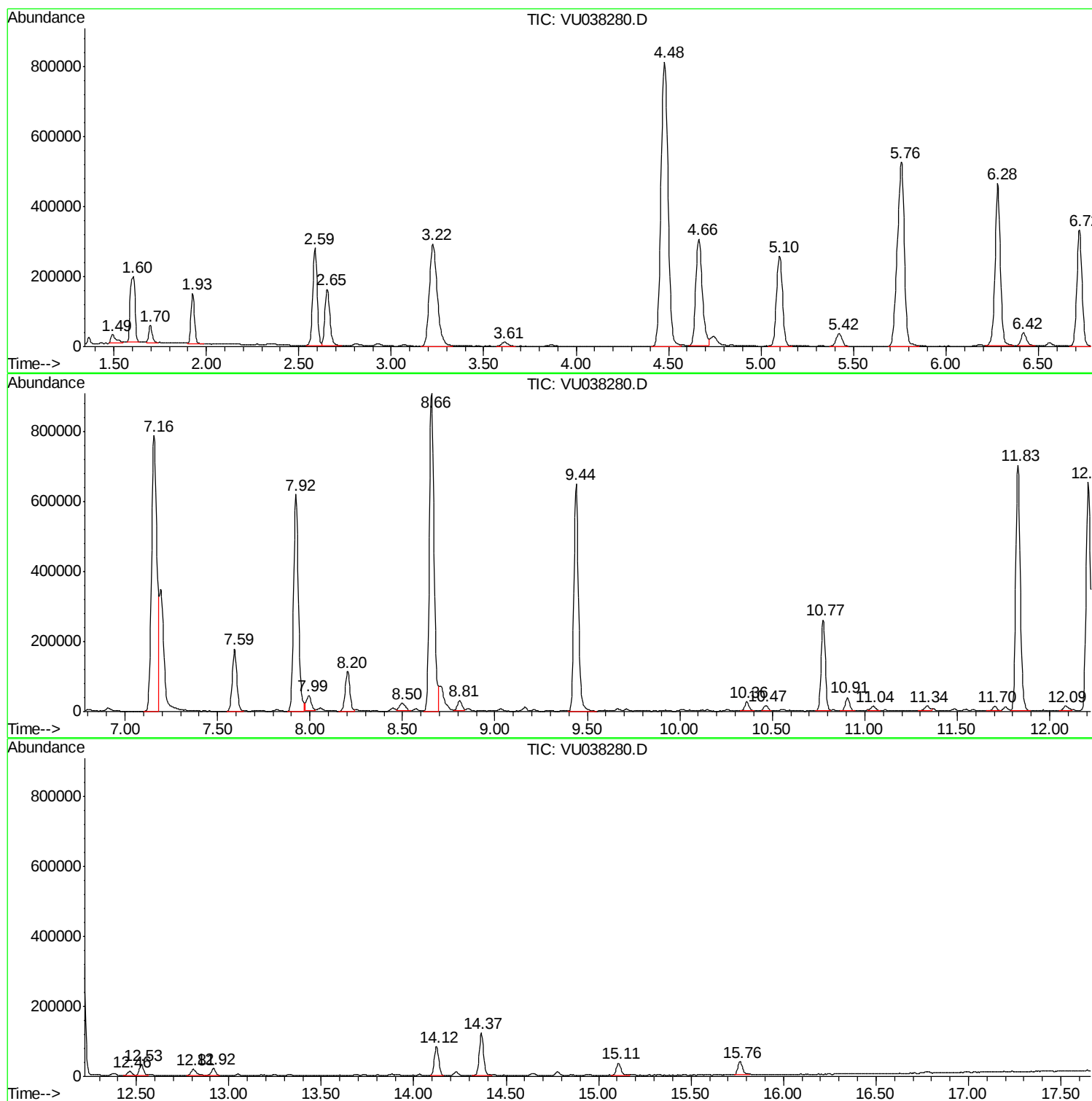
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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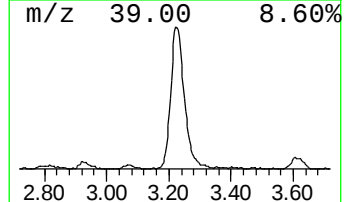
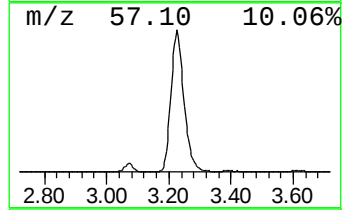
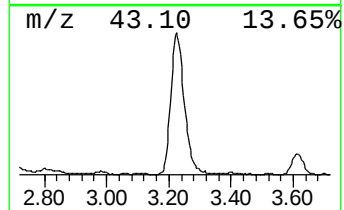
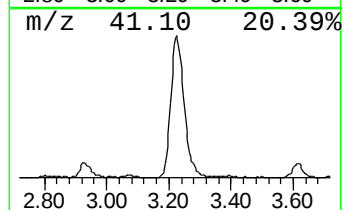
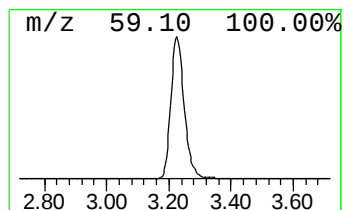
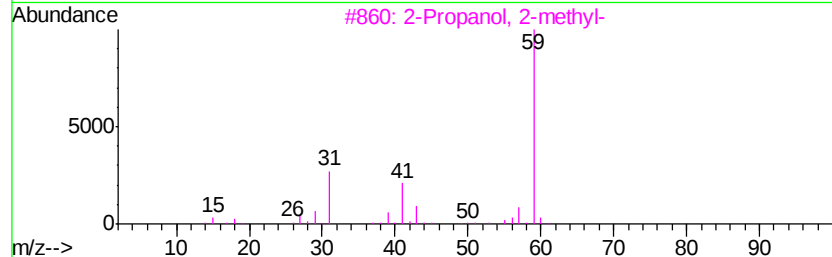
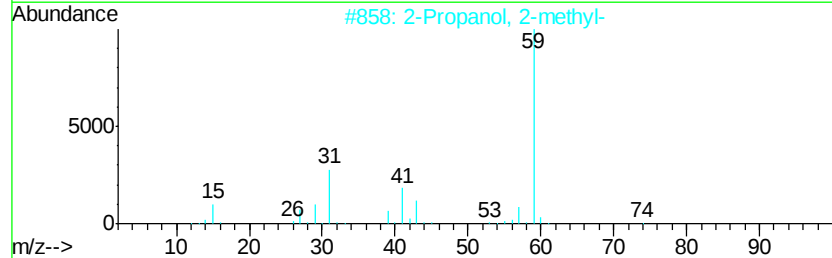
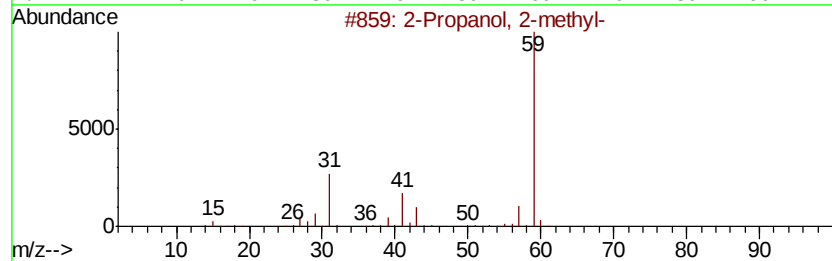
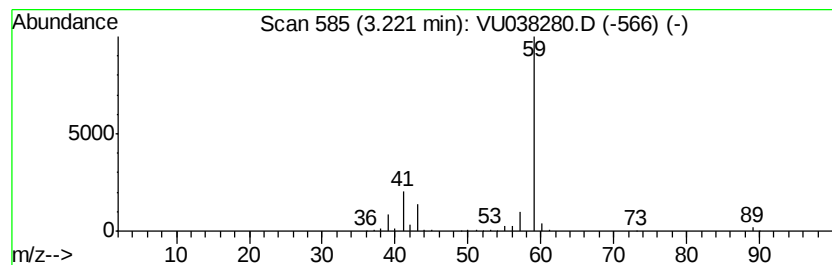
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.22	4.67 ug/L	866947	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	3-Pentanol			88	C5H12O	000584-02-1	56
5	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	43



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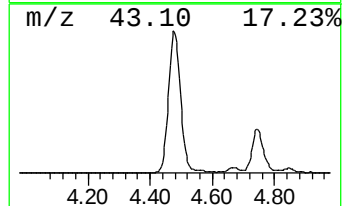
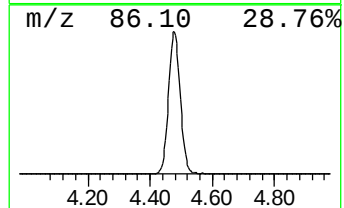
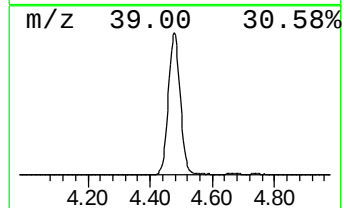
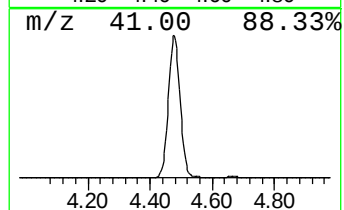
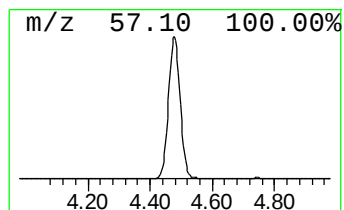
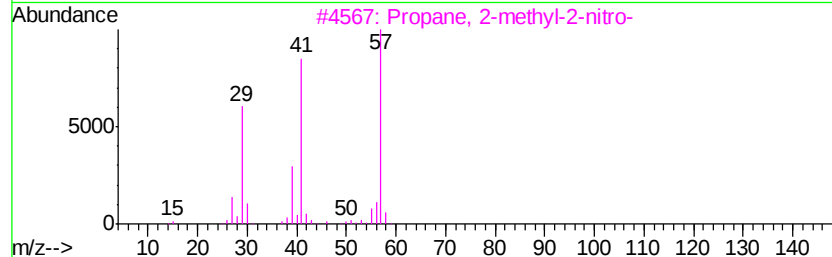
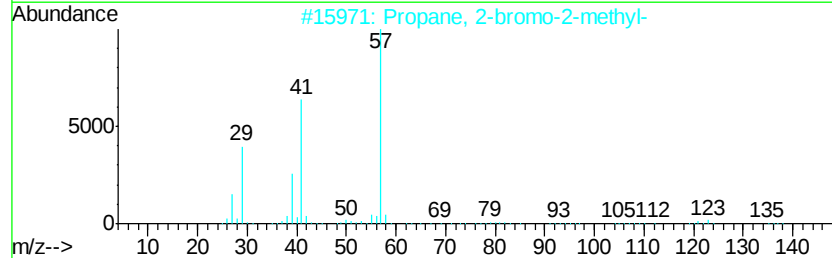
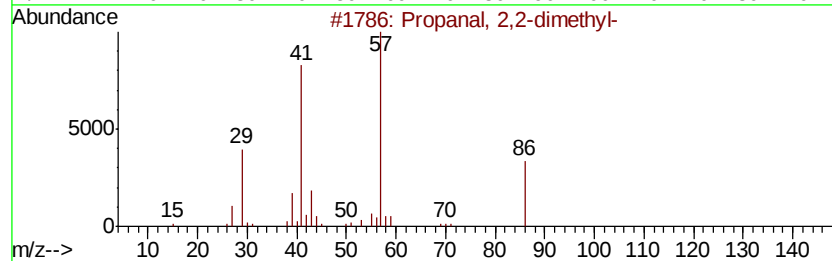
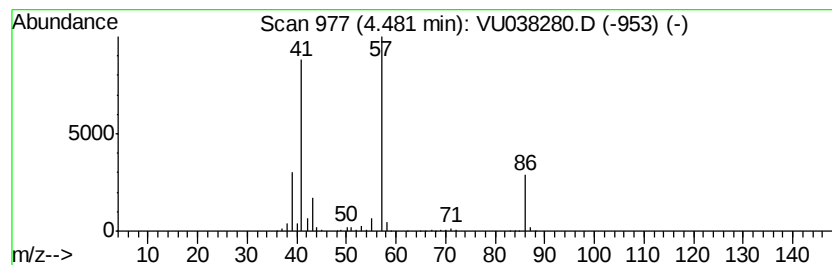
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	11.54 ug/L	2141670	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
3			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	45



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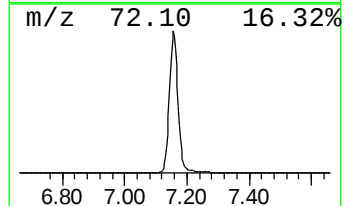
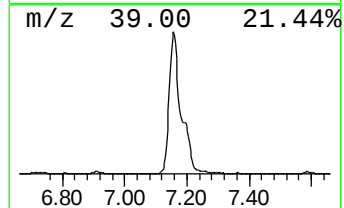
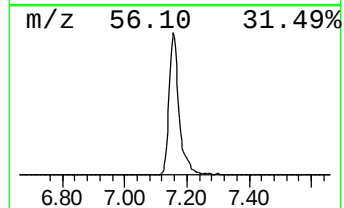
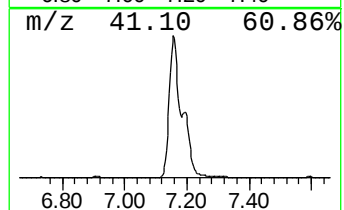
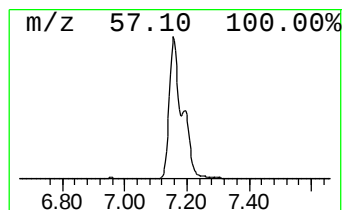
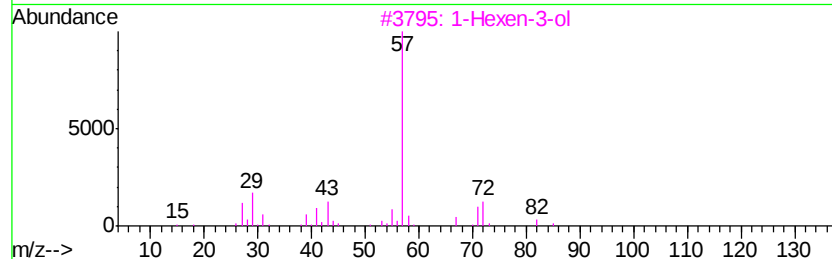
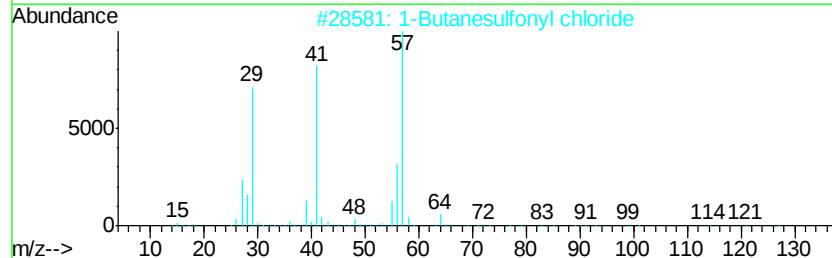
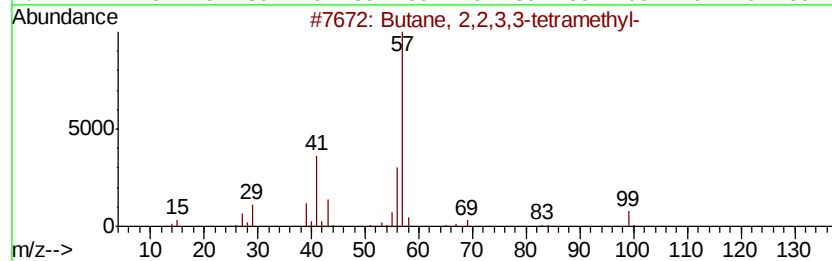
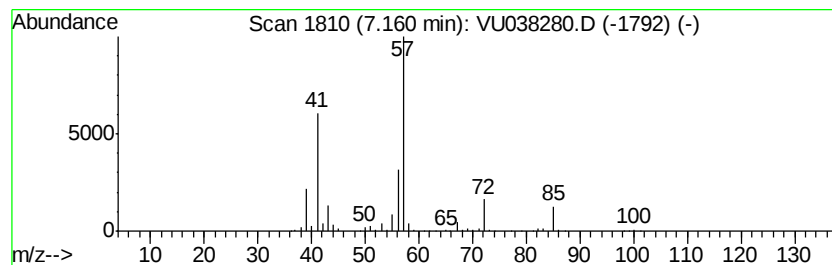
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Quant Title : TRACE VOA SOM01.0

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	8.65 ug/L	1605220	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-Hexen-3-ol	100	C6H12O	004798-44-1	38
4			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	38
5			1-Hexen-3-ol	100	C6H12O	004798-44-1	38



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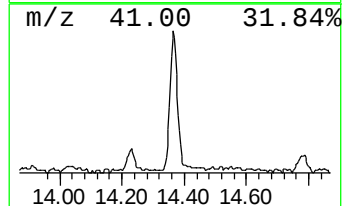
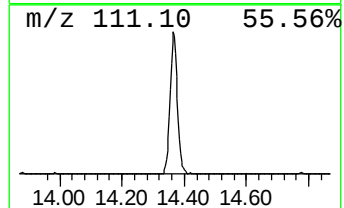
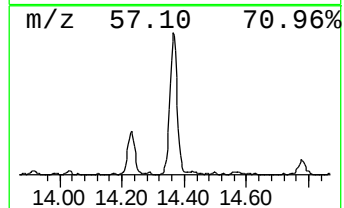
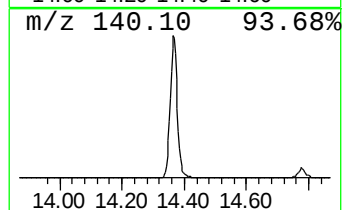
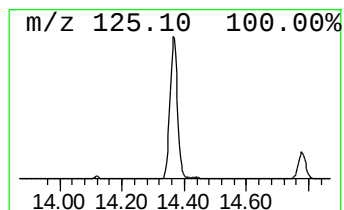
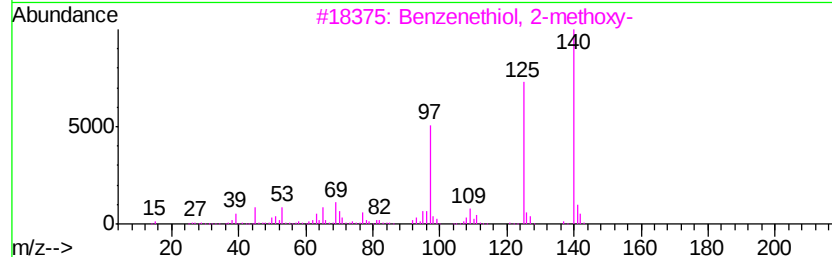
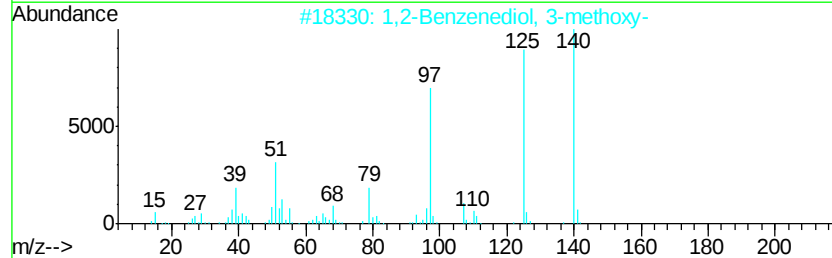
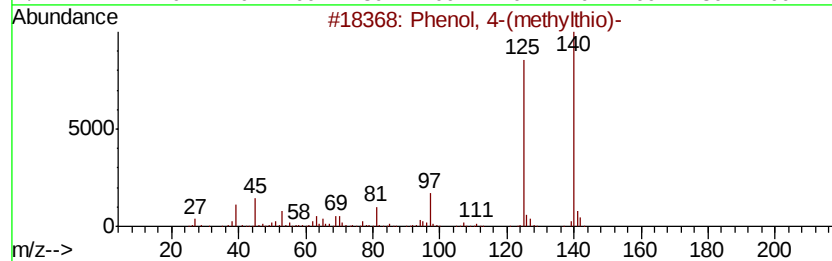
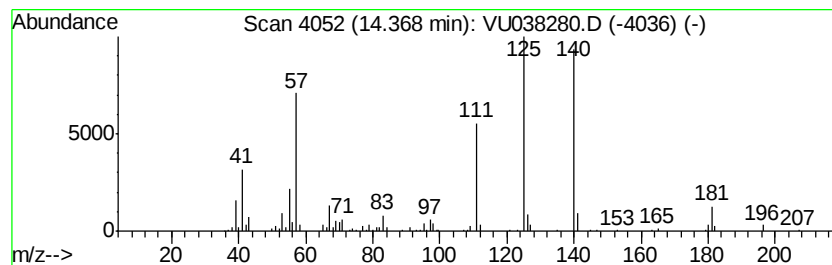
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.37	0.84 ug/L	196365	1,4-Dichlorobenzene-d4	11.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	64
2	1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
3	Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	59
4	Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	59
5	3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	59



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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...	3.22	4.7	ug/L	866947	1	6.28	927959	5.0
Propanal, 2,2-dim...	4.48	11.5	ug/L	2141670	1	6.28	927959	5.0
(DEL) Alkane: Str...	7.16	8.7	ug/L	1605220	1	6.28	927959	5.0
Phenol, 4-(methyl...	14.37	0.8	ug/L	196365	3	11.83	1170550	5.0