

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052720\
 Data File : VU038314.D
 Acq On : 27 May 2020 12:41
 Operator : JC/MD
 Sample : L2749-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4W6

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	1.597	72	80	99	rBV2	258715	405391	21.45%	2.509%
2	1.700	105	112	125	rVB	46228	55664	2.95%	0.345%
3	1.932	175	184	197	rVB	121063	158856	8.41%	0.983%
4	2.594	374	390	400	rBV	233440	394397	20.87%	2.441%
5	2.658	400	410	437	rVB	155818	290509	15.37%	1.798%
6	3.227	568	587	624	rBV	280119	790294	41.82%	4.892%
7	3.616	692	708	725	rBV4	11325	27826	1.47%	0.172%
8	4.481	952	977	1012	rBV	727869	1889907	100.00%	11.698%
9	4.665	1019	1034	1052	rBV	256283	630650	33.37%	3.904%
10	5.102	1153	1170	1194	rVB	228481	499825	26.45%	3.094%
11	5.423	1252	1270	1290	rBV3	22237	52354	2.77%	0.324%
12	5.761	1353	1375	1407	rBV2	451966	1192993	63.12%	7.384%
13	6.282	1516	1537	1555	rBV	369408	720382	38.12%	4.459%
14	6.420	1568	1580	1597	rBV2	34106	68642	3.63%	0.425%
15	6.722	1657	1674	1692	rBV	289789	562391	29.76%	3.481%
16	7.157	1793	1809	1817	rBV	696717	1438019	76.09%	8.901%
17	7.591	1932	1944	1965	rBV	157831	273125	14.45%	1.691%
18	7.922	2030	2047	2061	rBV	566450	1016668	53.79%	6.293%
19	7.992	2062	2069	2080	rVV	37387	69861	3.70%	0.432%
20	8.201	2121	2134	2146	rBV	101204	179315	9.49%	1.110%
21	8.504	2216	2228	2241	rVB4	14259	32848	1.74%	0.203%
22	8.655	2260	2275	2287	rBV	855267	1470440	77.80%	9.102%
23	8.806	2314	2322	2332	rVB4	26331	38992	2.06%	0.241%
24	9.436	2504	2518	2543	rBV	520582	879004	46.51%	5.441%
25	10.359	2795	2805	2818	rVB3	24738	39665	2.10%	0.246%
26	10.462	2828	2837	2846	rVB	13466	20983	1.11%	0.130%
27	10.771	2919	2933	2945	rBV	236921	381283	20.17%	2.360%
28	10.902	2961	2974	2986	rVB3	22199	37533	1.99%	0.232%
29	11.041	3001	3017	3028	rVB4	13024	24760	1.31%	0.153%
30	11.700	3207	3222	3231	rBV3	13639	22810	1.21%	0.141%
31	11.825	3249	3261	3281	rVB	575982	961799	50.89%	5.953%
32	12.079	3330	3340	3351	rBV3	15026	28956	1.53%	0.179%
33	12.205	3363	3379	3393	rBV	602510	963469	50.98%	5.964%
34	12.462	3448	3459	3467	rBV4	12014	19179	1.01%	0.119%

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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	12.520	3468	3477	3486	rBV2	27315	42786	2.26%	0.265%
36	12.796	3554	3563	3573	rBV2	19910	33519	1.77%	0.207%
37	12.909	3590	3598	3610	rVB3	20685	30229	1.60%	0.187%
38	14.114	3960	3973	3984	rBV	83513	132409	7.01%	0.820%
39	14.356	4031	4048	4066	rBV	142087	231615	12.26%	1.434%
40	14.764	4166	4175	4188	rBV3	12304	20435	1.08%	0.126%
41	16.754	4785	4794	4802	rBV5	15765	25853	1.37%	0.160%

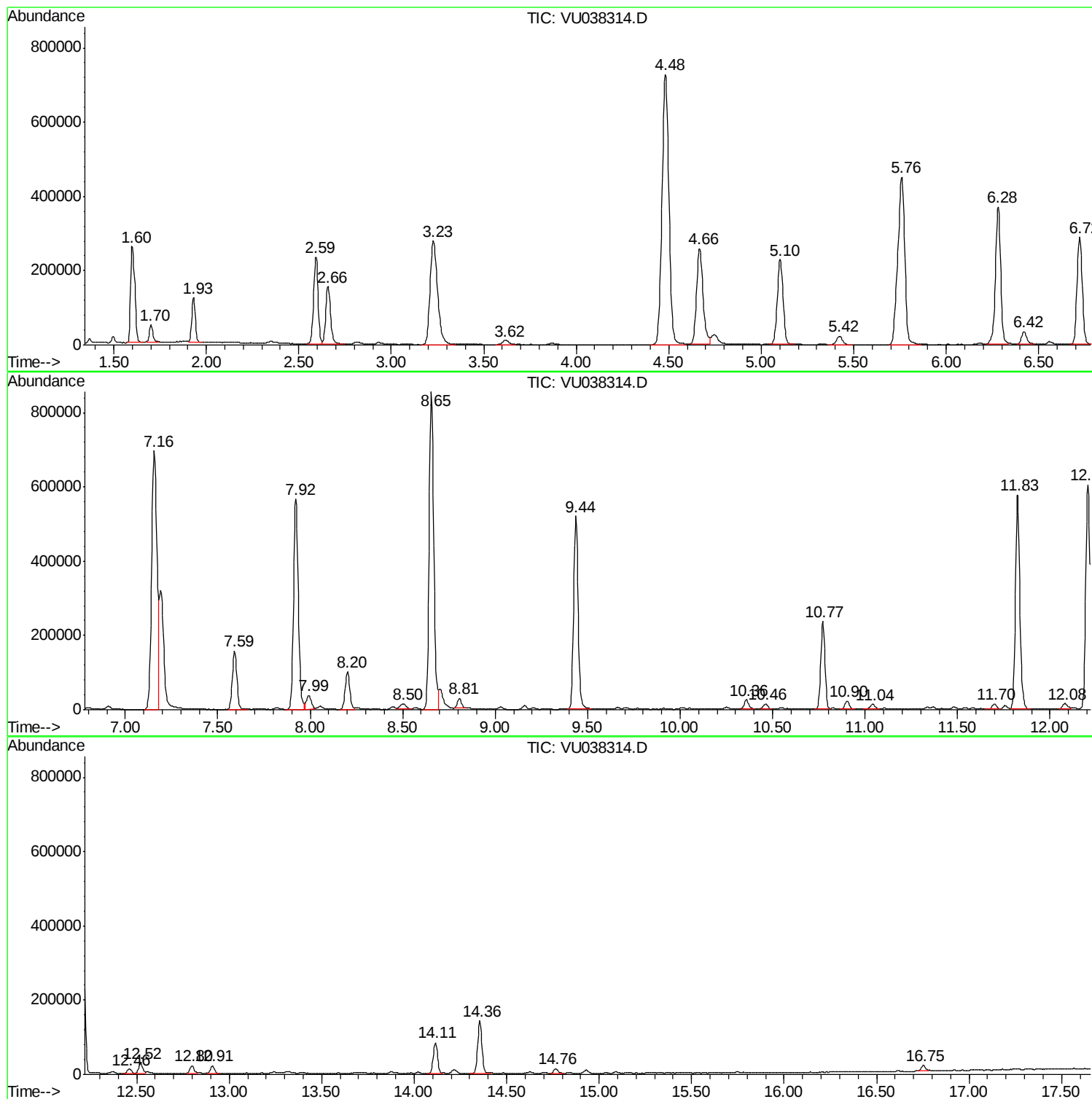
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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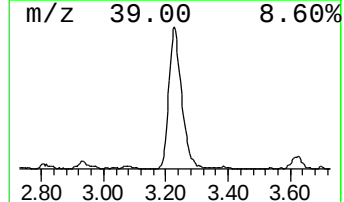
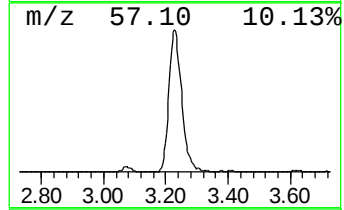
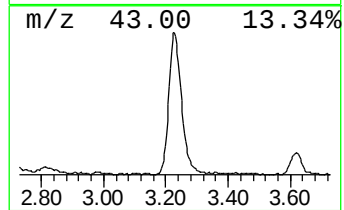
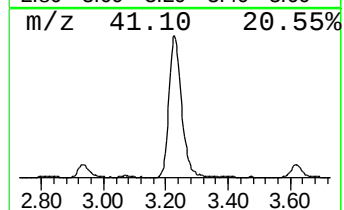
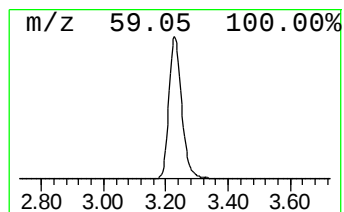
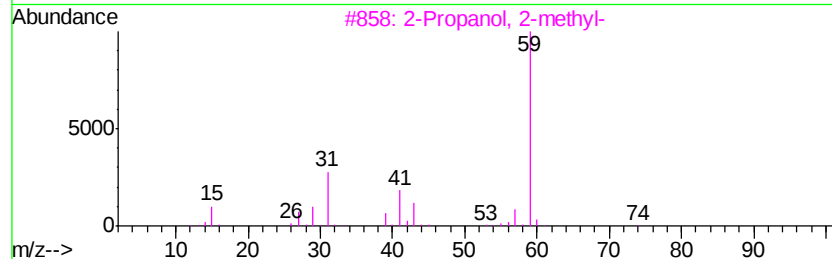
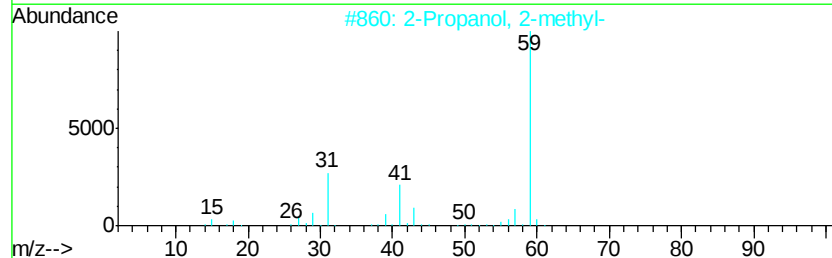
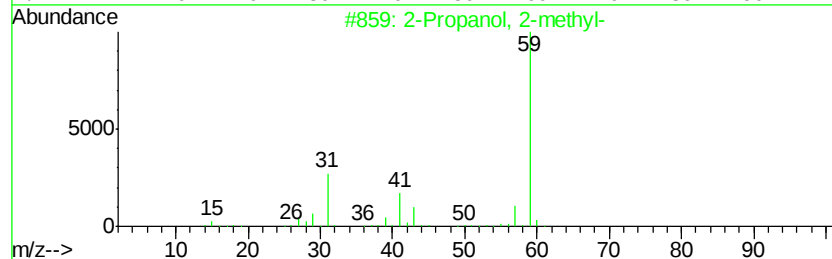
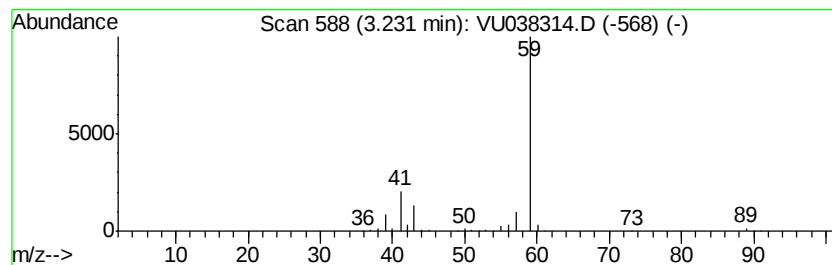
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.23	5.49 ug/L	790294	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	78
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	37



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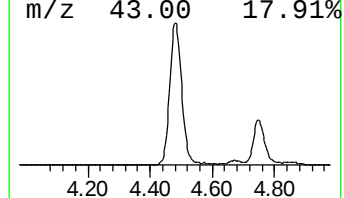
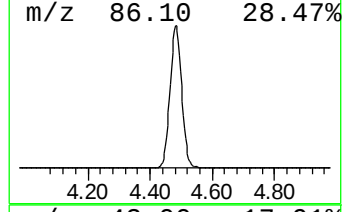
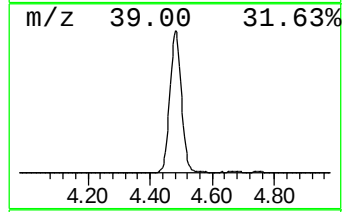
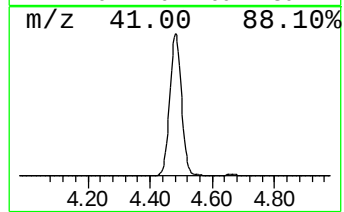
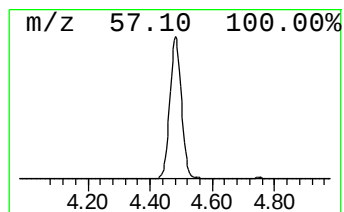
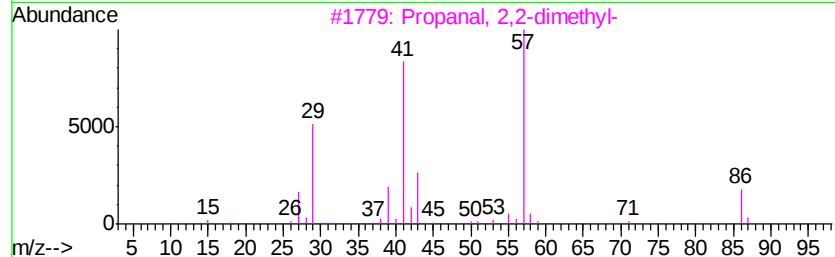
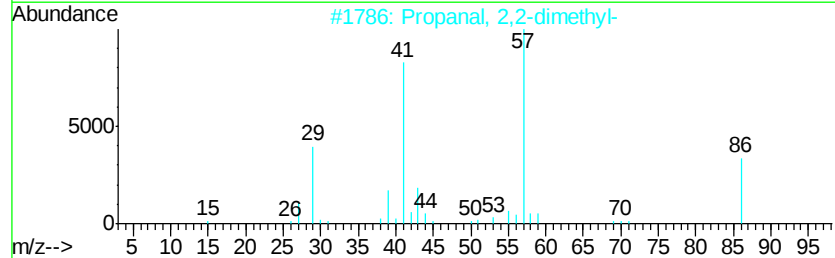
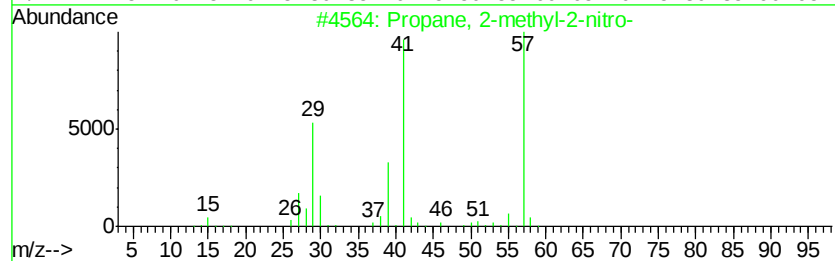
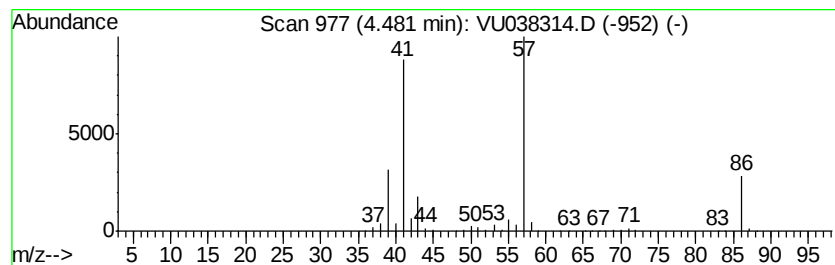
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	13.12 ug/L	1889910	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	50
2		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45
4		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	45
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40



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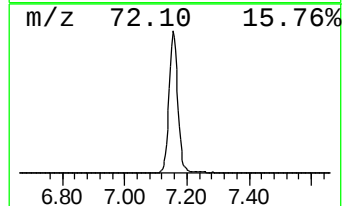
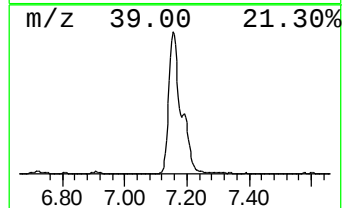
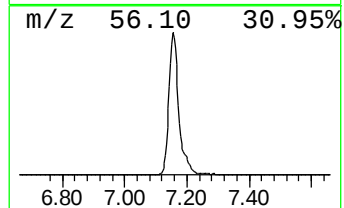
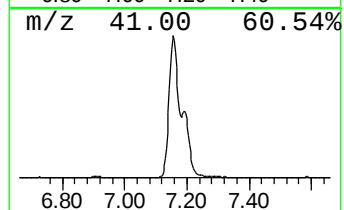
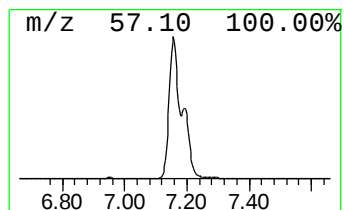
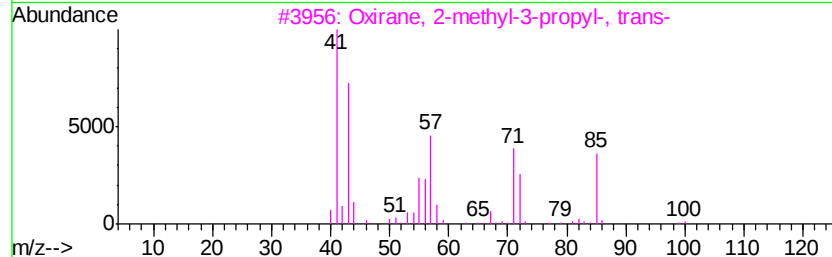
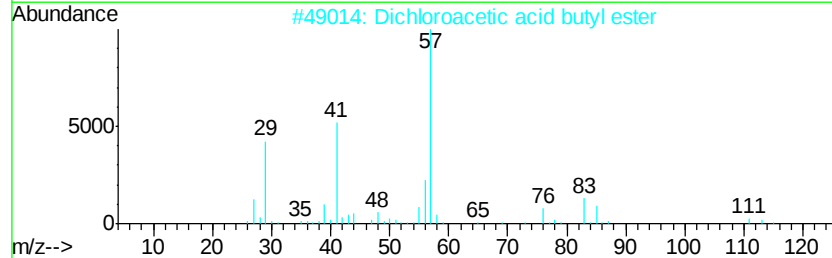
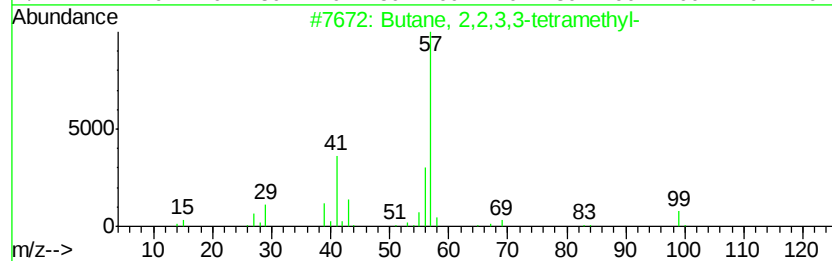
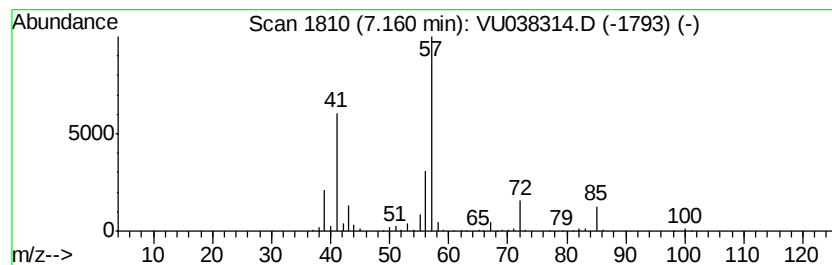
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	9.98 ug/L	1438020	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			Dichloroacetic acid butyl ester	184	C6H10Cl2O2	029003-73-4	38
3			Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	37
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	33
5			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	28



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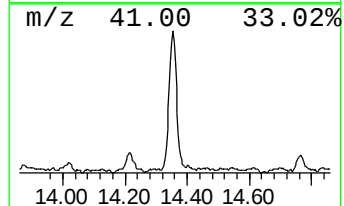
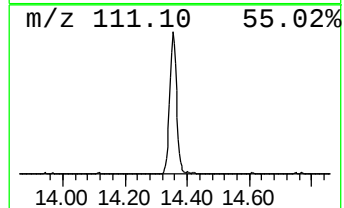
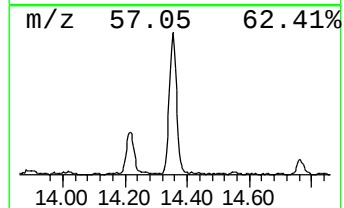
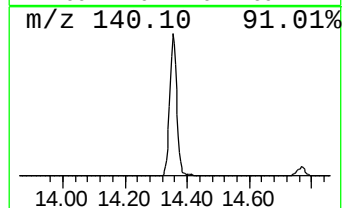
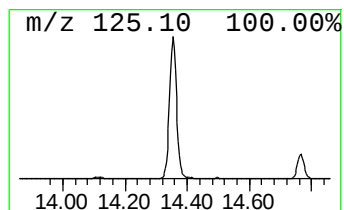
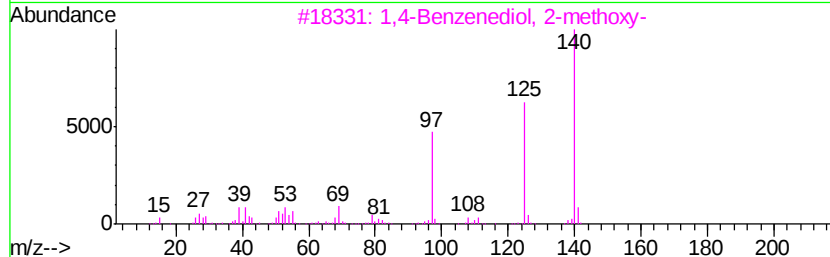
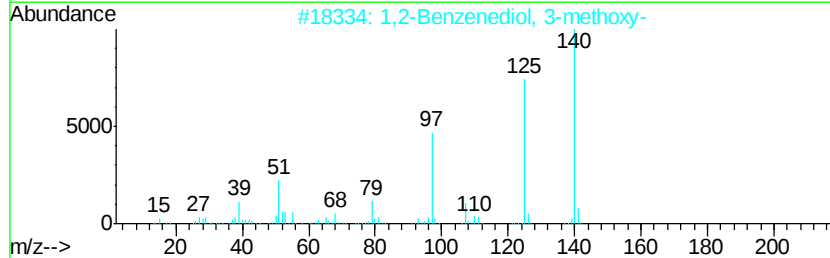
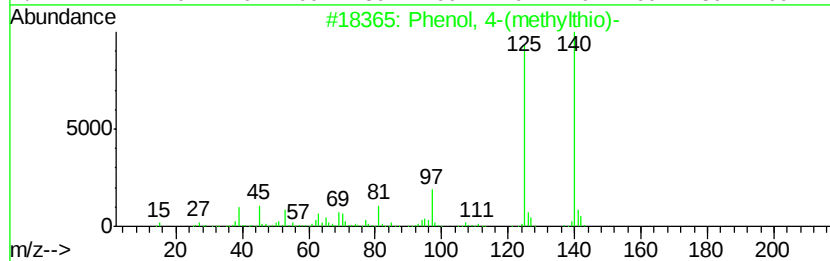
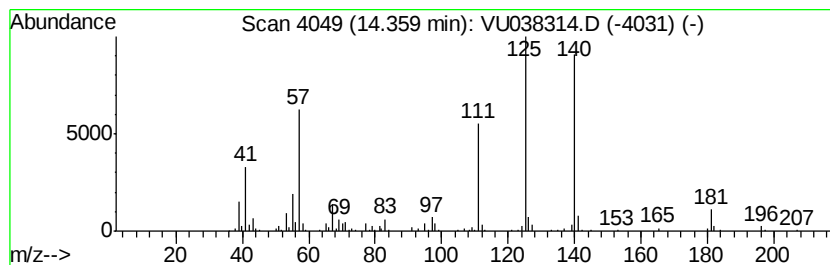
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.36	1.20 ug/L	231615	1,4-Dichlorobenzene-d4	11.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
2	1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
3	1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	59
4	Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	59
5	Uracil, 5-ethyl-	140	C6H8N2O2	004212-49-1	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...	3.23	5.5	ug/L	790294	1	6.28	720382	5.0
Propane, 2-methyl...	4.48	13.1	ug/L	1889910	1	6.28	720382	5.0
(DEL) Alkane: Str...	7.16	10.0	ug/L	1438020	1	6.28	720382	5.0
Phenol, 4-(methyl...	14.36	1.2	ug/L	231615	3	11.83	961799	5.0