

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052720\
 Data File : VU038313.D
 Acq On : 27 May 2020 12:18
 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	42	50	56	rBV3	25278	32522	1.74%	0.201%
2	1.601	72	81	95	rBV2	246350	389725	20.81%	2.407%
3	1.700	105	112	126	rVB	59964	72599	3.88%	0.448%
4	1.932	175	184	196	rVB	117377	152123	8.12%	0.940%
5	2.591	374	389	399	rBV	232167	391466	20.90%	2.418%
6	2.652	399	408	435	rVB	185753	326674	17.44%	2.018%
7	3.215	563	583	608	rBV	330687	762678	40.73%	4.711%
8	3.616	694	708	722	rBV4	12491	29591	1.58%	0.183%
9	4.481	956	977	1000	rBV2	716376	1872726	100.00%	11.567%
10	4.661	1017	1033	1052	rBV	248399	598058	31.94%	3.694%
11	4.745	1052	1059	1083	rVB2	26549	63321	3.38%	0.391%
12	5.102	1153	1170	1188	rBV	223602	488417	26.08%	3.017%
13	5.424	1255	1270	1284	rVB5	13438	31113	1.66%	0.192%
14	5.761	1351	1375	1404	rBV2	442671	1161915	62.04%	7.177%
15	6.279	1517	1536	1561	rVV	402244	808492	43.17%	4.994%
16	6.420	1568	1580	1596	rBV	33990	69313	3.70%	0.428%
17	6.722	1659	1674	1691	rBV	279164	547986	29.26%	3.385%
18	7.157	1793	1809	1816	rBV	678662	1339420	71.52%	8.273%
19	7.591	1930	1944	1961	rBV	148464	265528	14.18%	1.640%
20	7.922	2031	2047	2062	rBV	542074	989880	52.86%	6.114%
21	7.989	2063	2068	2080	rVV2	35600	61745	3.30%	0.381%
22	8.202	2122	2134	2146	rBV	99389	171568	9.16%	1.060%
23	8.494	2217	2225	2241	rVB5	16405	37707	2.01%	0.233%
24	8.655	2260	2275	2287	rBV	816513	1414123	75.51%	8.735%
25	8.806	2313	2322	2333	rBV3	28639	41655	2.22%	0.257%
26	9.436	2504	2518	2553	rVB	570926	987970	52.76%	6.103%
27	10.359	2794	2805	2820	rBV5	25616	41132	2.20%	0.254%
28	10.771	2918	2933	2947	rBV	223775	366962	19.60%	2.267%
29	10.902	2961	2974	2986	rVB4	36966	60145	3.21%	0.372%
30	11.044	3007	3018	3029	rVB5	11266	21818	1.17%	0.135%
31	11.700	3210	3222	3232	rBV4	14925	22874	1.22%	0.141%
32	11.825	3249	3261	3283	rVB	649167	1071529	57.22%	6.619%
33	12.082	3330	3341	3353	rBV4	12620	27880	1.49%	0.172%
34	12.205	3365	3379	3398	rBV	584431	948808	50.66%	5.861%

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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	12.459	3448	3458	3468	rBV3	12196	19735	1.05%	0.122%
36	12.523	3468	3478	3487	rBV2	25731	41892	2.24%	0.259%
37	12.796	3552	3563	3573	rBV4	31119	54429	2.91%	0.336%
38	12.909	3590	3598	3612	rVB5	21091	31697	1.69%	0.196%
39	14.114	3961	3973	3985	rBV	85175	137315	7.33%	0.848%
40	14.356	4037	4048	4062	rBV	135682	215127	11.49%	1.329%
41	14.767	4166	4176	4189	rBV2	11992	19928	1.06%	0.123%

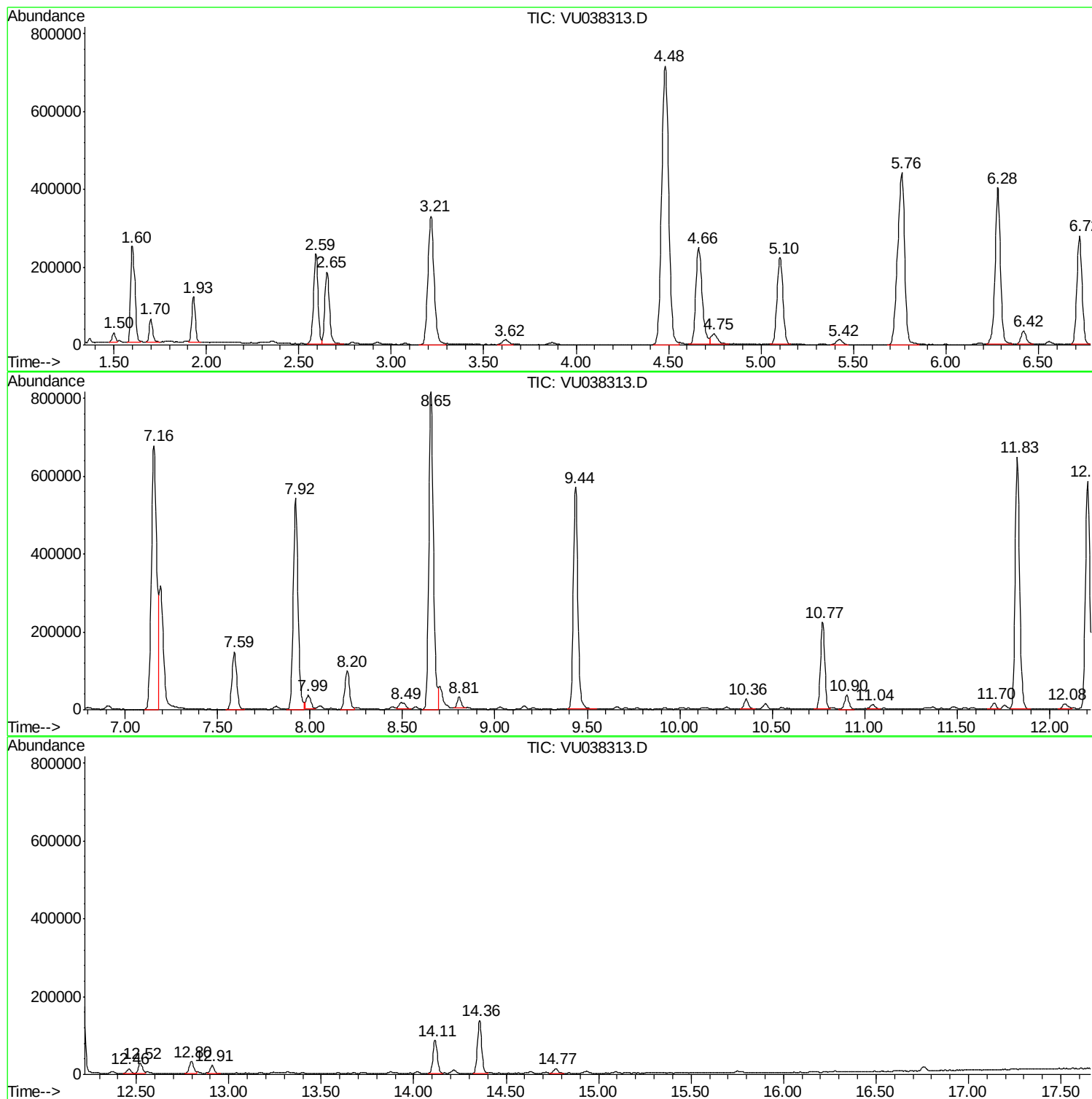
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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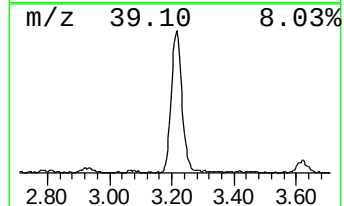
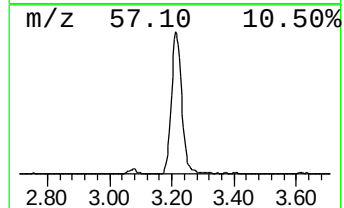
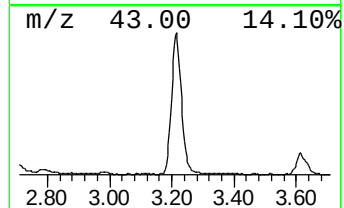
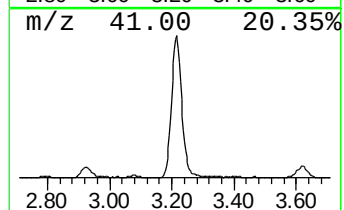
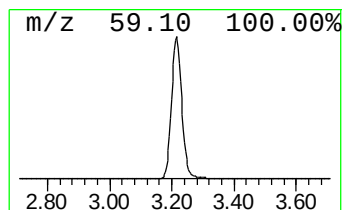
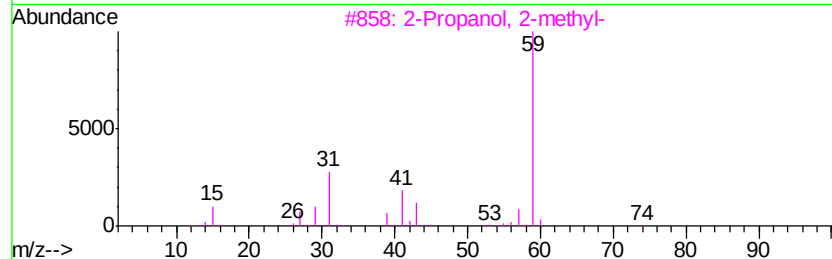
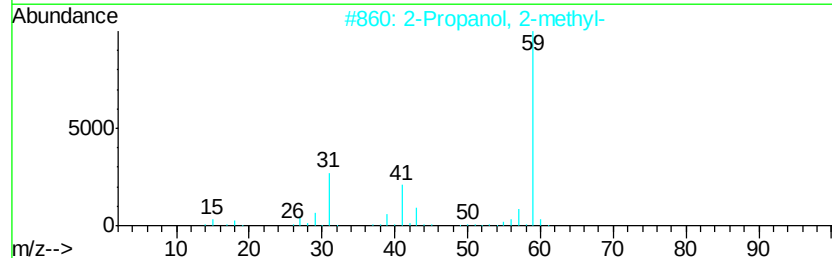
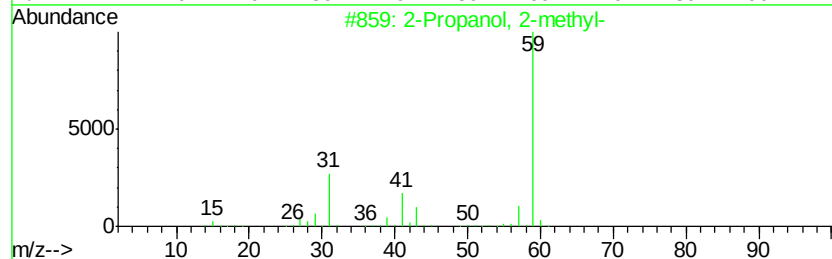
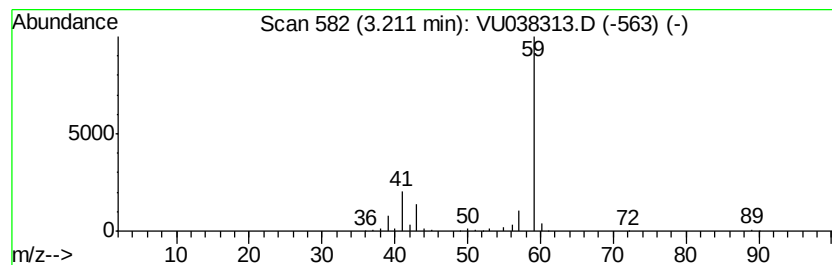
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.21	4.72 ug/L	762678	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			4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	9



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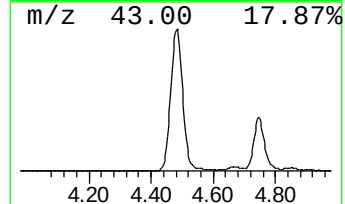
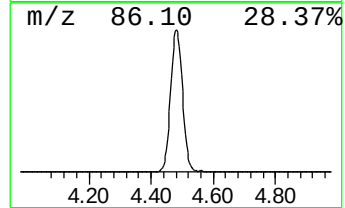
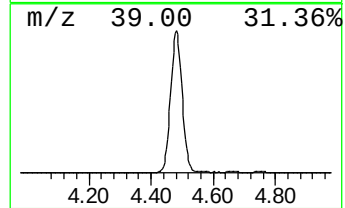
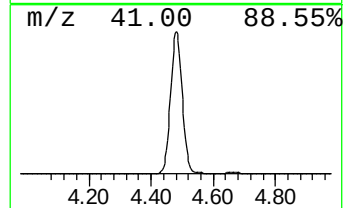
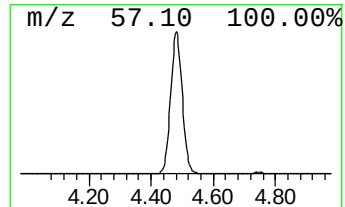
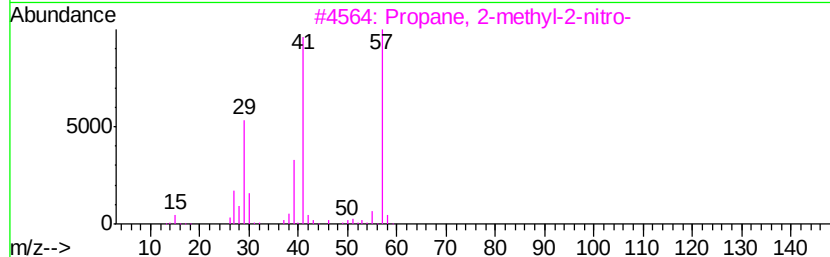
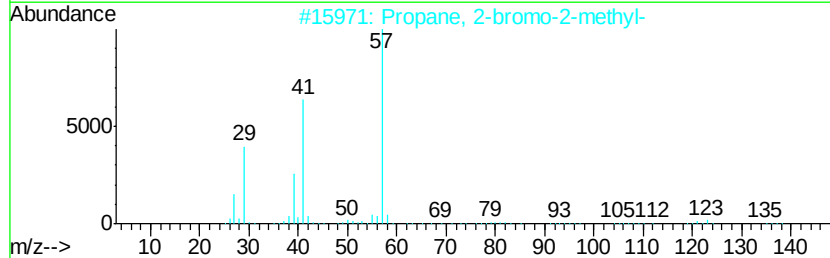
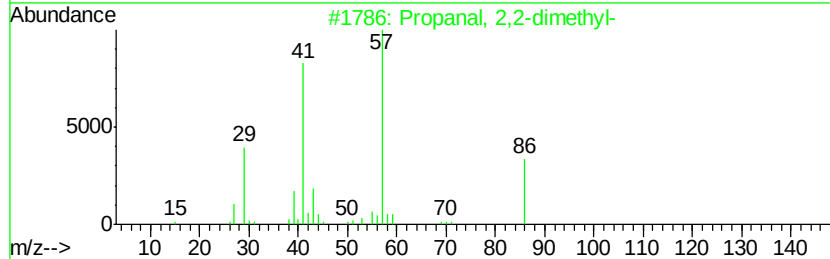
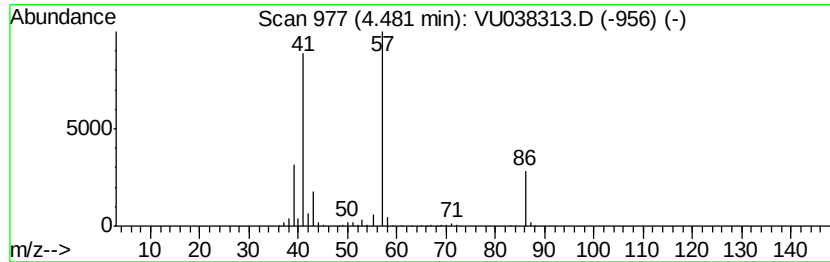
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	11.58 ug/L	1872730	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	59
2		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	59
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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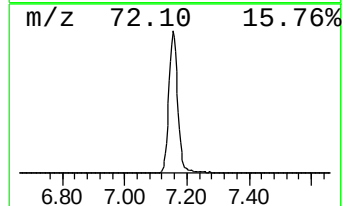
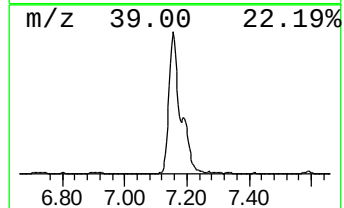
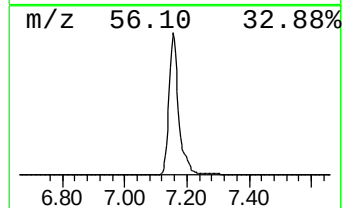
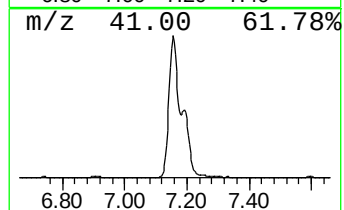
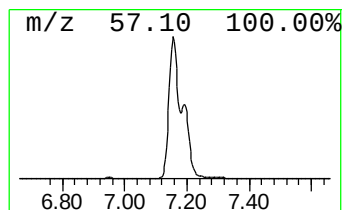
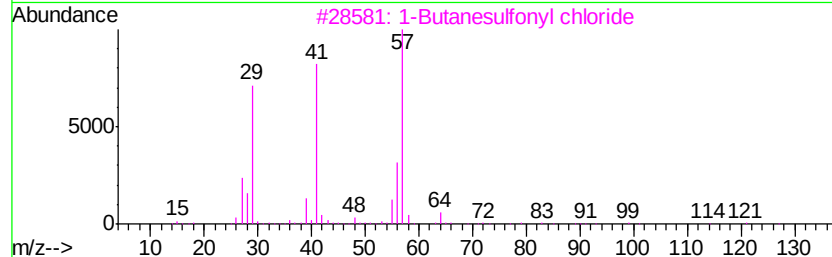
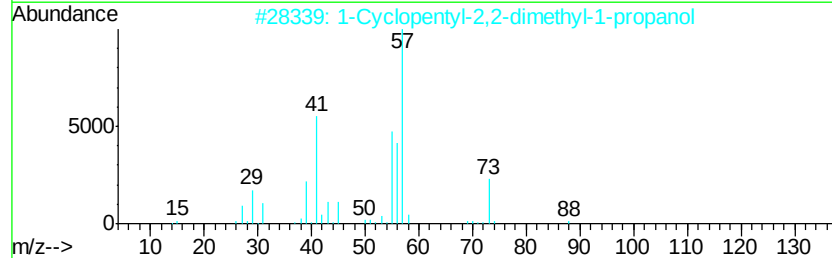
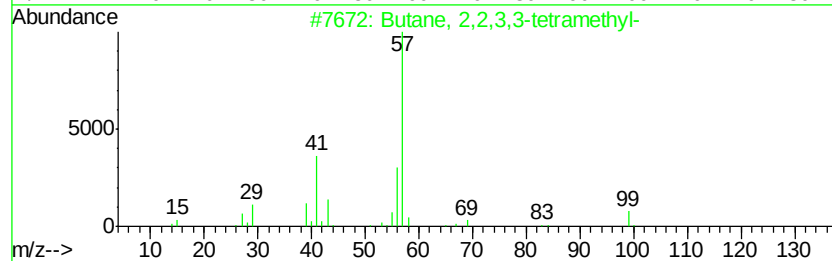
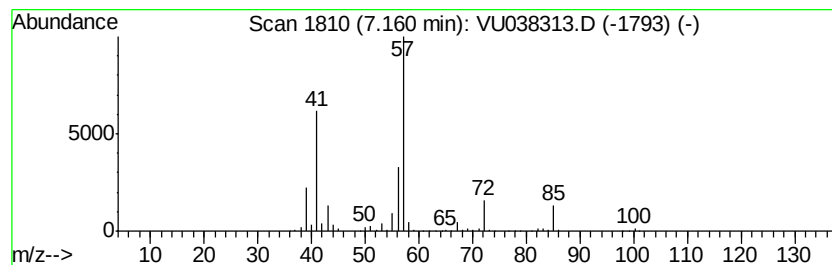
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Quant Title : TRACE VOA SOM01.0

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	8.28 ug/L	1339420	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-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	40
3	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
4	1-Hexen-3-ol	100	C6H12O	004798-44-1	37
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	36



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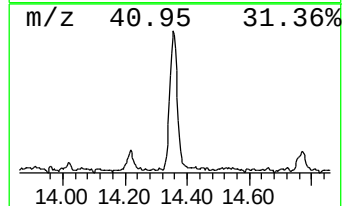
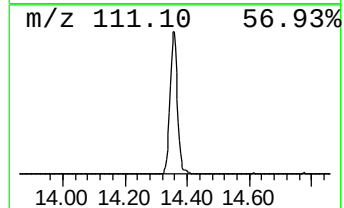
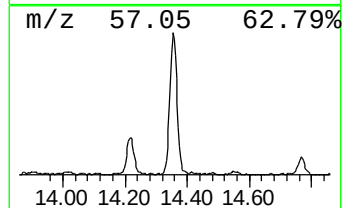
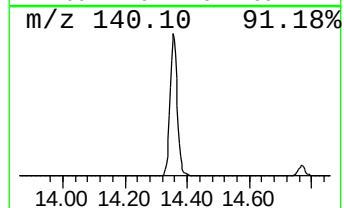
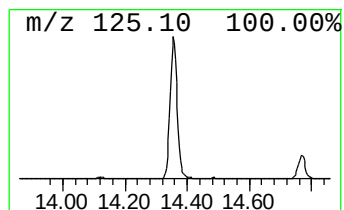
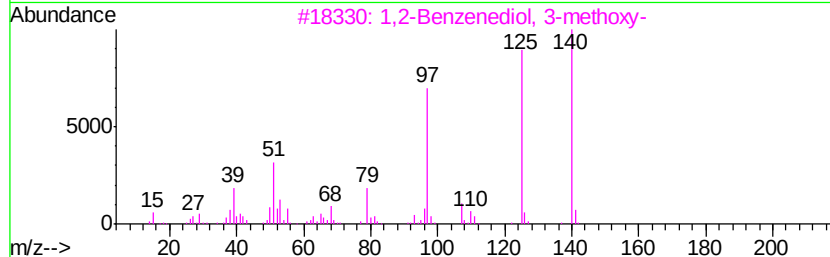
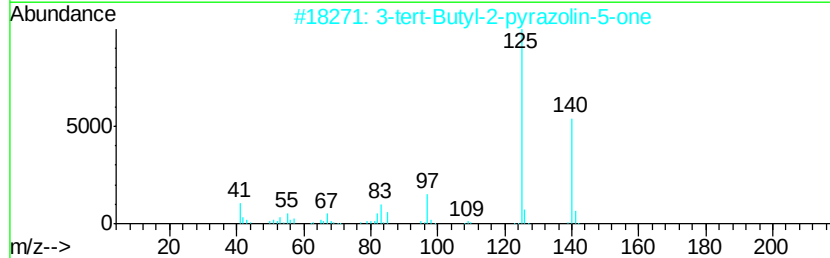
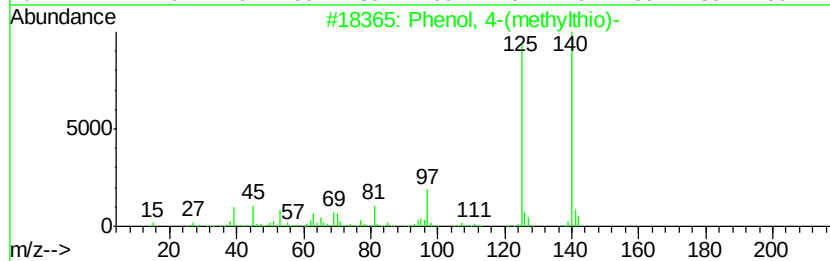
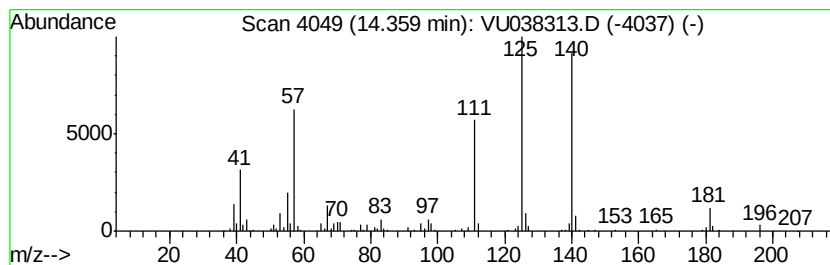
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	1.00 ug/L	215127	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		3-tert-Butyl-2-pyrazolin-5-one	140	C7H12N2O	029211-68-5	58
3		1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	53
4		Thiophene, 2,5-diethyl-	140	C8H12S	005069-23-8	53
5		3-Amino-5-t-butyliisoxazole	140	C7H12N2O	055809-36-4	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...	3.21	4.7	ug/L	762678	1	6.28	808492	5.0
Propanal, 2,2-dim...	4.48	11.6	ug/L	1872730	1	6.28	808492	5.0
(DEL) Alkane: Str...	7.16	8.3	ug/L	1339420	1	6.28	808492	5.0
Phenol, 4-(methyl...	14.36	1.0	ug/L	215127	3	11.83	1071530	5.0