

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU112719\
 Data File : VU035892.D
 Acq On : 27 Nov 2019 13:21
 Operator : JC/SP
 Sample : K6057-14
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AB3

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\SOMUTR112119WMA.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	1.372	4	10	16	rBV3	19322	21874	1.30%	0.148%
2	1.613	75	85	95	rBV2	232858	404547	24.00%	2.743%
3	1.703	109	113	126	rVB	26378	31931	1.89%	0.217%
4	1.935	177	185	197	rVB	188942	237529	14.09%	1.611%
5	2.594	375	390	402	rBV	271215	459100	27.23%	3.113%
6	2.668	403	413	442	rVB	95099	174619	10.36%	1.184%
7	2.806	445	456	477	rBV	58167	115465	6.85%	0.783%
8	3.234	572	589	625	rBV2	361419	880491	52.23%	5.971%
9	4.501	962	983	1014	rBV2	536580	1418645	84.15%	9.620%
10	4.694	1026	1043	1086	rBV3	253649	786601	46.66%	5.334%
11	5.115	1157	1174	1200	rBV	252614	572716	33.97%	3.884%
12	5.433	1260	1273	1291	rVB2	41851	91512	5.43%	0.621%
13	5.771	1357	1378	1405	rBV2	498620	1312528	77.86%	8.901%
14	6.292	1523	1540	1566	rBV	303616	601407	35.67%	4.078%
15	6.732	1663	1677	1701	rBV	311837	635969	37.72%	4.313%
16	7.176	1797	1815	1845	rBV	687940	1685813	100.00%	11.432%
17	7.603	1933	1948	1969	rBV	141191	277480	16.46%	1.882%
18	7.935	2037	2051	2067	rBV	539761	979131	58.08%	6.640%
19	8.214	2124	2138	2163	rBV	81535	172703	10.24%	1.171%
20	8.684	2269	2284	2323	rBV	454013	1433365	85.03%	9.720%
21	8.825	2323	2328	2344	rVB7	14064	30295	1.80%	0.205%
22	9.449	2506	2522	2560	rBV	449565	860784	51.06%	5.837%
23	10.388	2802	2814	2829	rBV8	9800	22739	1.35%	0.154%
24	10.787	2926	2938	2956	rBV	235251	405171	24.03%	2.748%
25	11.841	3254	3266	3281	rBV	300551	527923	31.32%	3.580%
26	12.221	3369	3384	3404	rVB2	325164	566757	33.62%	3.843%
27	12.536	3471	3482	3491	rBV2	11111	17917	1.06%	0.122%
28	14.343	4035	4044	4055	rVB3	13278	21255	1.26%	0.144%

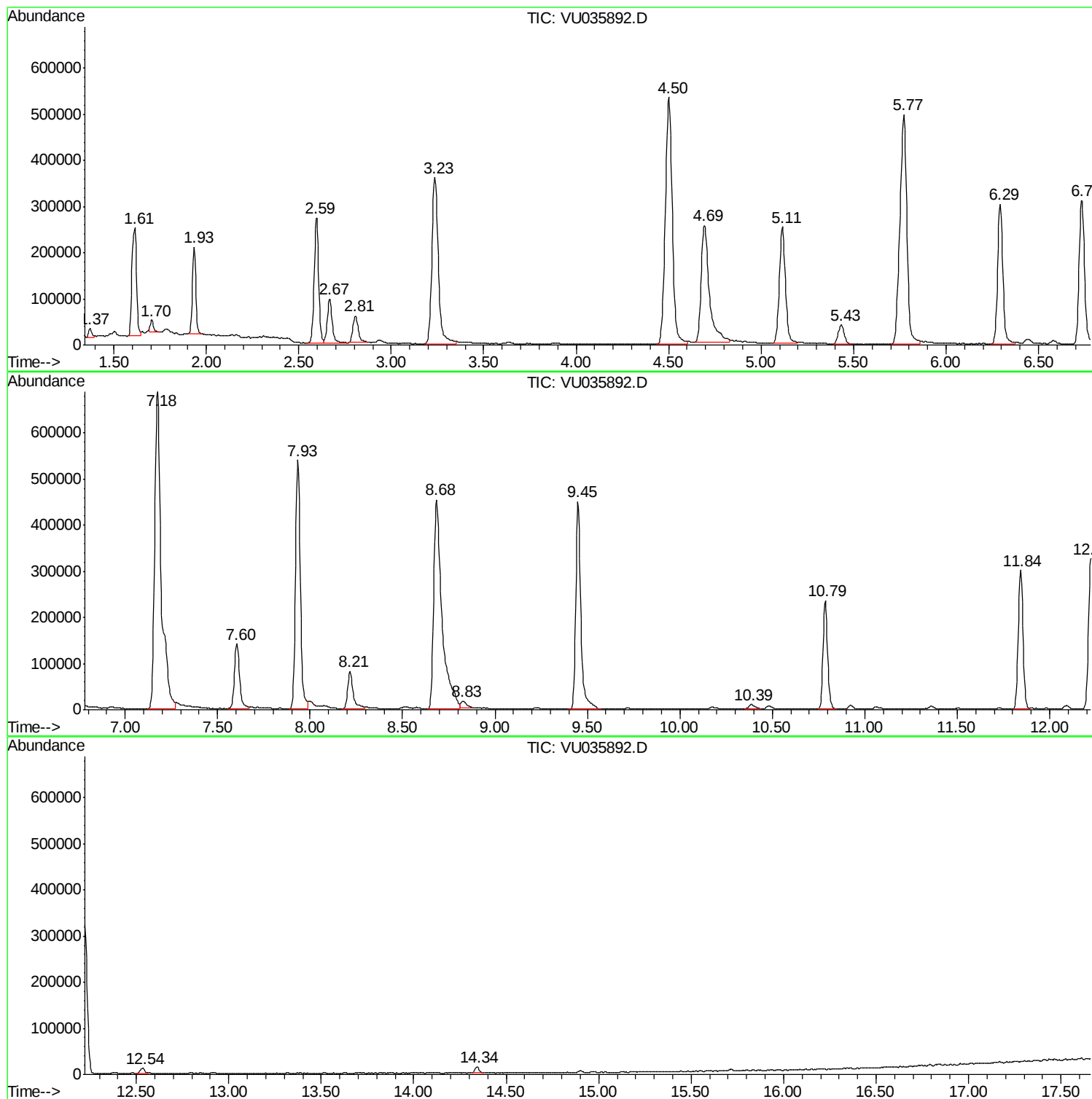
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Quant Title : TRACE VOA SOM01.0

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



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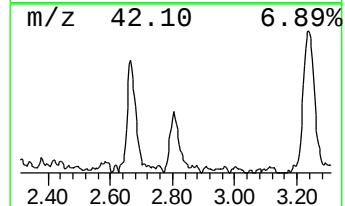
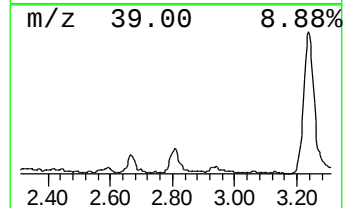
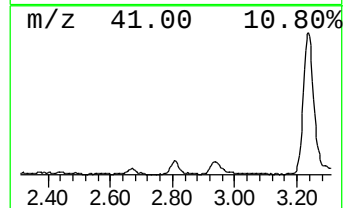
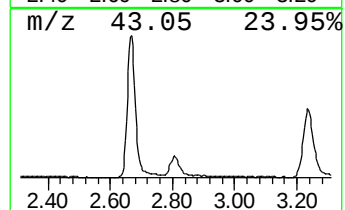
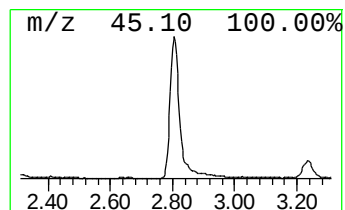
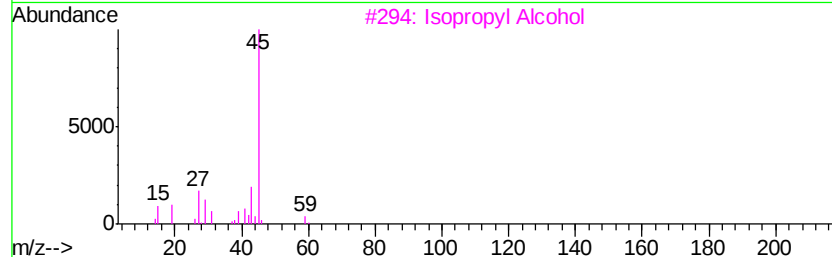
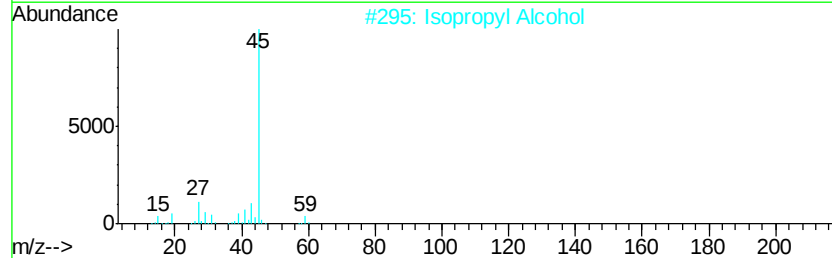
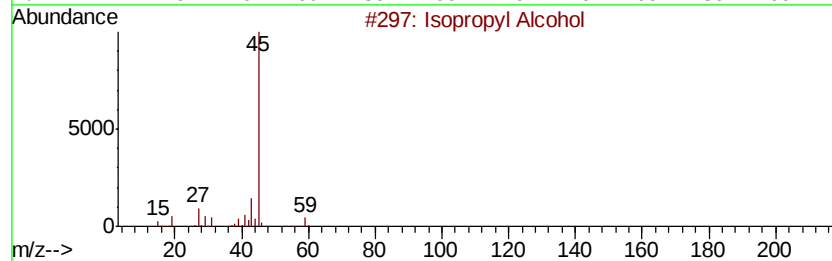
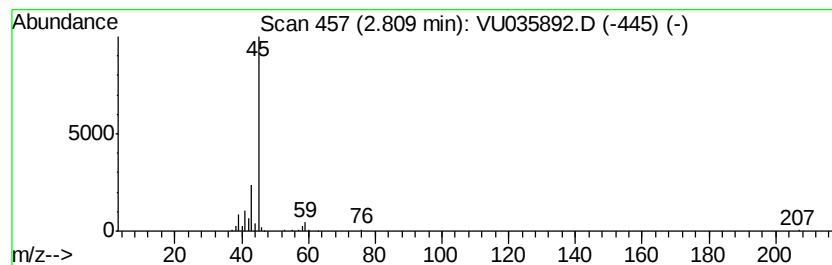
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.81	0.96 ug/L	115465	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	80
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	80
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4		Isopropyl Alcohol	60	C3H8O	000067-63-0	72
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40



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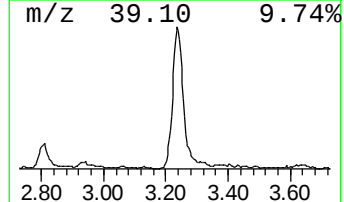
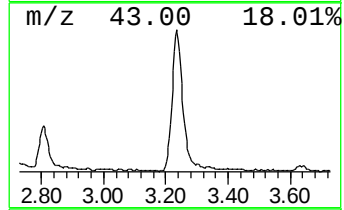
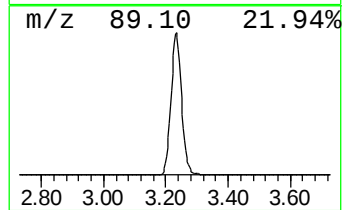
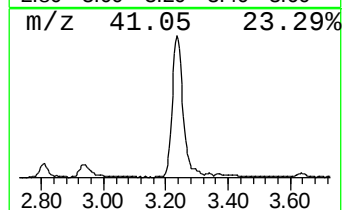
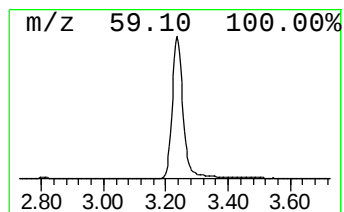
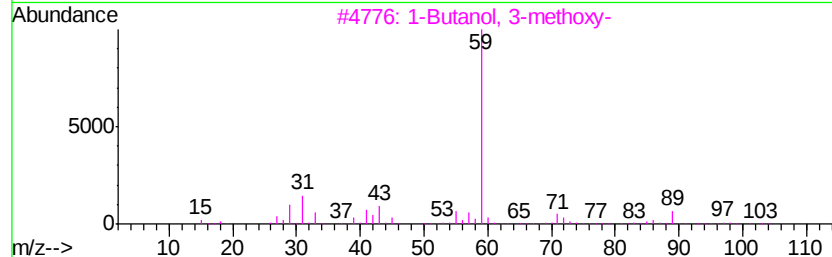
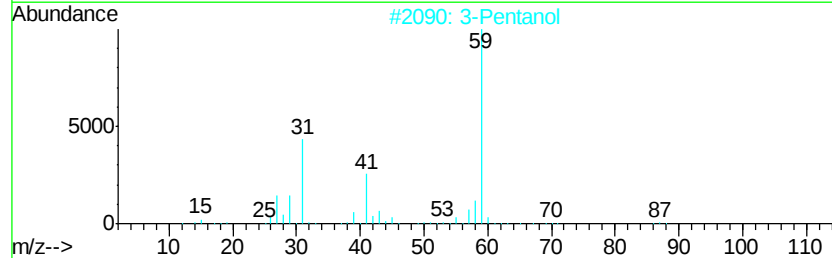
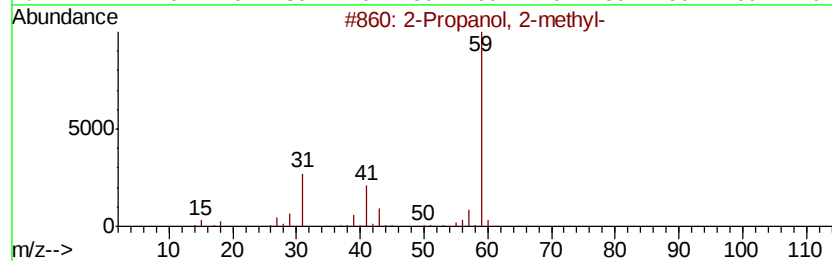
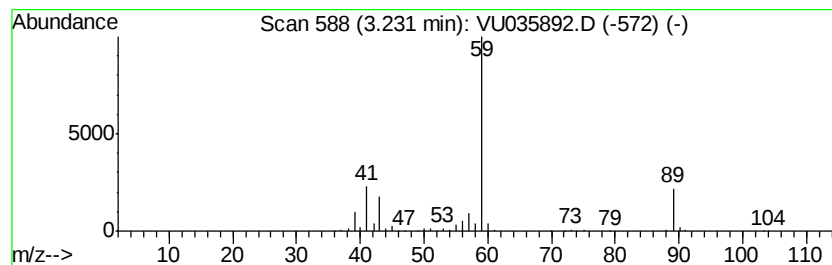
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	7.32 ug/L	880491	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	45	
2	3-Pentanol	88	C5H12O	000584-02-1	42	
3	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	39	
4	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38	
5	3-Pentanol	88	C5H12O	000584-02-1	36	



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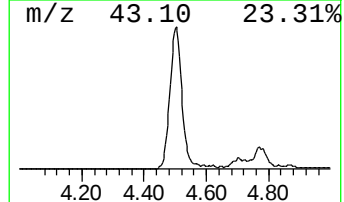
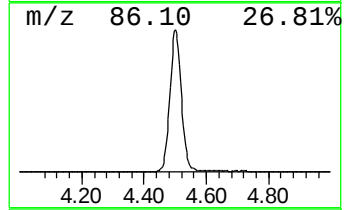
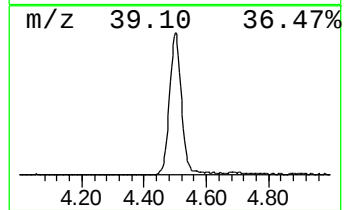
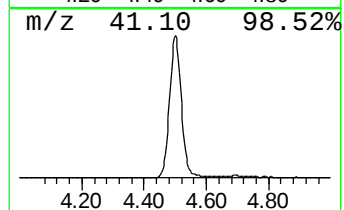
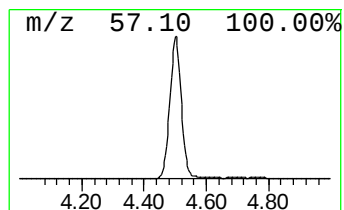
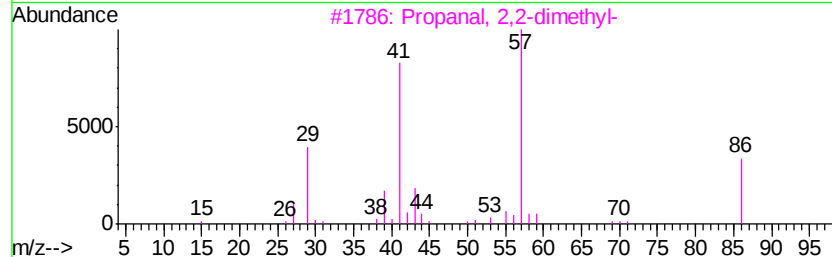
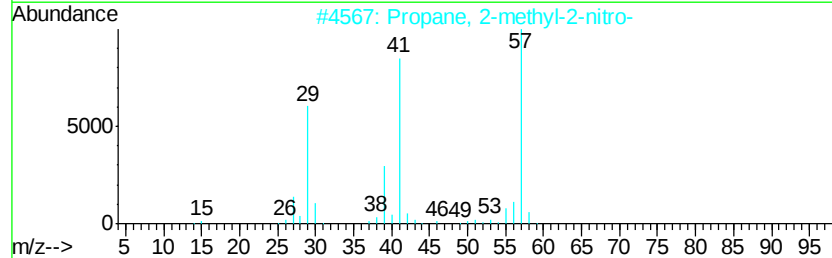
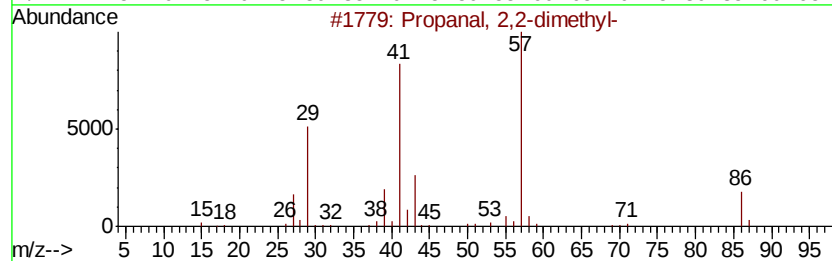
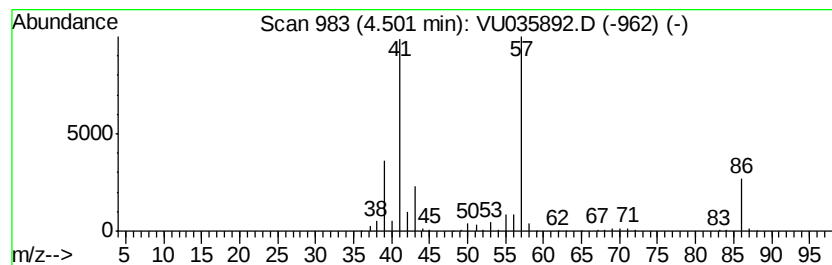
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanal, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.50	11.79 ug/L	1418650	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	72
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	42



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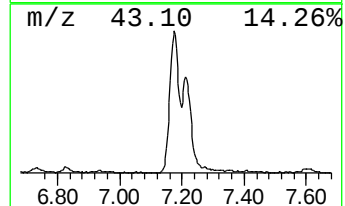
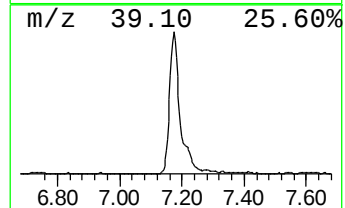
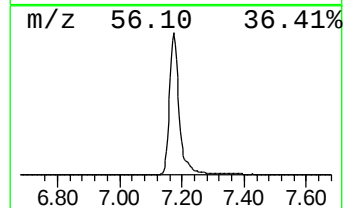
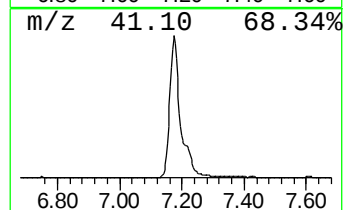
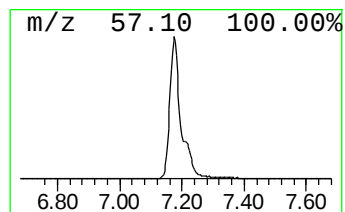
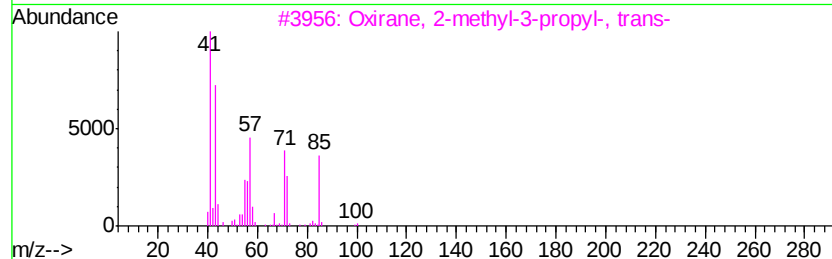
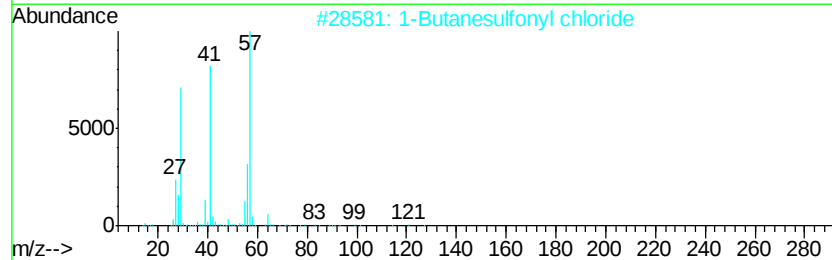
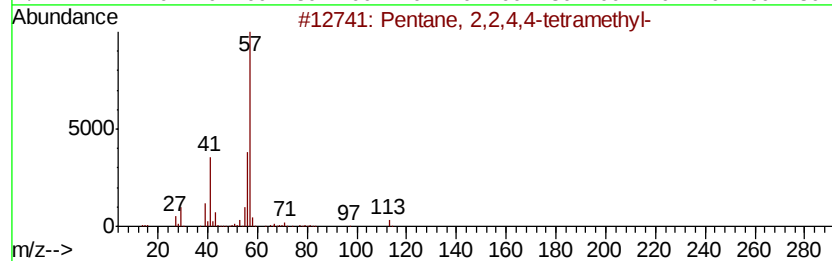
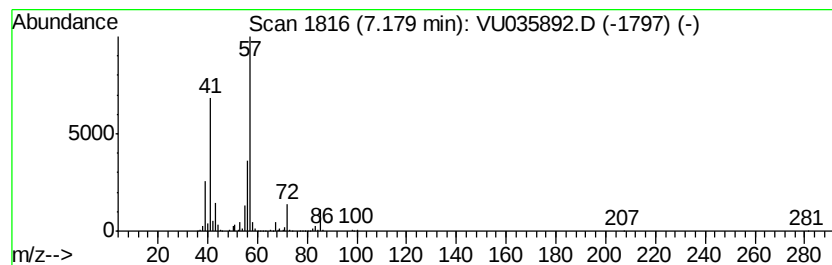
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Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.18	14.02 ug/L	1685810	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	50
2		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
3		Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	38
4		Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	36
5		3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	33



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.81	1.0	ug/L	115465	1	6.29	601407	5.0
unknown-01	3.23	7.3	ug/L	880491	1	6.29	601407	5.0
Propanal, 2,2-dim...	4.50	11.8	ug/L	1418650	1	6.29	601407	5.0
(DEL) Alkane: Str...	7.18	14.0	ug/L	1685810	1	6.29	601407	5.0