

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021720\
 Data File : VU036808.D
 Acq On : 17 Feb 2020 14:30
 Operator : JC/MD
 Sample : L1537-10
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AR0

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\SOMUTR021220WMA.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	1.600	73	81	99	rBV2	140358	203452	43.21%	4.115%
2	1.700	105	112	122	rVB	10877	13769	2.92%	0.278%
3	1.932	175	184	199	rVB	56272	73665	15.64%	1.490%
4	2.591	377	389	401	rBV	90641	147483	31.32%	2.983%
5	2.658	401	410	426	rVB	21495	37178	7.90%	0.752%
6	2.793	439	452	468	rBV	33648	64973	13.80%	1.314%
7	3.221	568	585	610	rBV2	103840	238439	50.64%	4.822%
8	4.488	960	979	1004	rBV	110199	284241	60.36%	5.749%
9	4.677	1021	1038	1060	rBV4	106420	282492	59.99%	5.713%
10	5.105	1154	1171	1189	rBV	80761	179121	38.04%	3.623%
11	5.430	1256	1272	1283	rBV5	6134	13167	2.80%	0.266%
12	5.764	1355	1376	1403	rBV2	176605	450562	95.68%	9.112%
13	6.285	1519	1538	1558	rBV	151997	284815	60.48%	5.760%
14	6.726	1659	1675	1696	rBV	111490	215739	45.81%	4.363%
15	7.163	1796	1811	1840	rBV2	158643	355479	75.49%	7.189%
16	7.594	1932	1945	1969	rBV	53733	96756	20.55%	1.957%
17	7.925	2035	2048	2064	rBV	216191	374604	79.55%	7.576%
18	8.063	2084	2091	2104	rVB4	2891	4963	1.05%	0.100%
19	8.208	2124	2136	2151	rBV2	31345	55168	11.72%	1.116%
20	8.664	2265	2278	2307	rBV	233987	470892	100.00%	9.523%
21	8.812	2316	2324	2335	rVB3	6700	11672	2.48%	0.236%
22	9.439	2506	2519	2555	rVB	205693	350431	74.42%	7.087%
23	10.372	2799	2809	2818	rBV4	8521	13150	2.79%	0.266%
24	10.777	2922	2935	2952	rVB	80226	128295	27.25%	2.595%
25	11.832	3251	3263	3279	rVB	172466	284537	60.43%	5.755%
26	12.086	3333	3342	3352	rBV4	3163	4782	1.02%	0.097%
27	12.211	3369	3381	3395	rBV	178354	289827	61.55%	5.862%
28	12.532	3471	3481	3492	rBV2	3680	6358	1.35%	0.129%
29	14.359	4041	4049	4061	rVB3	5639	8533	1.81%	0.173%

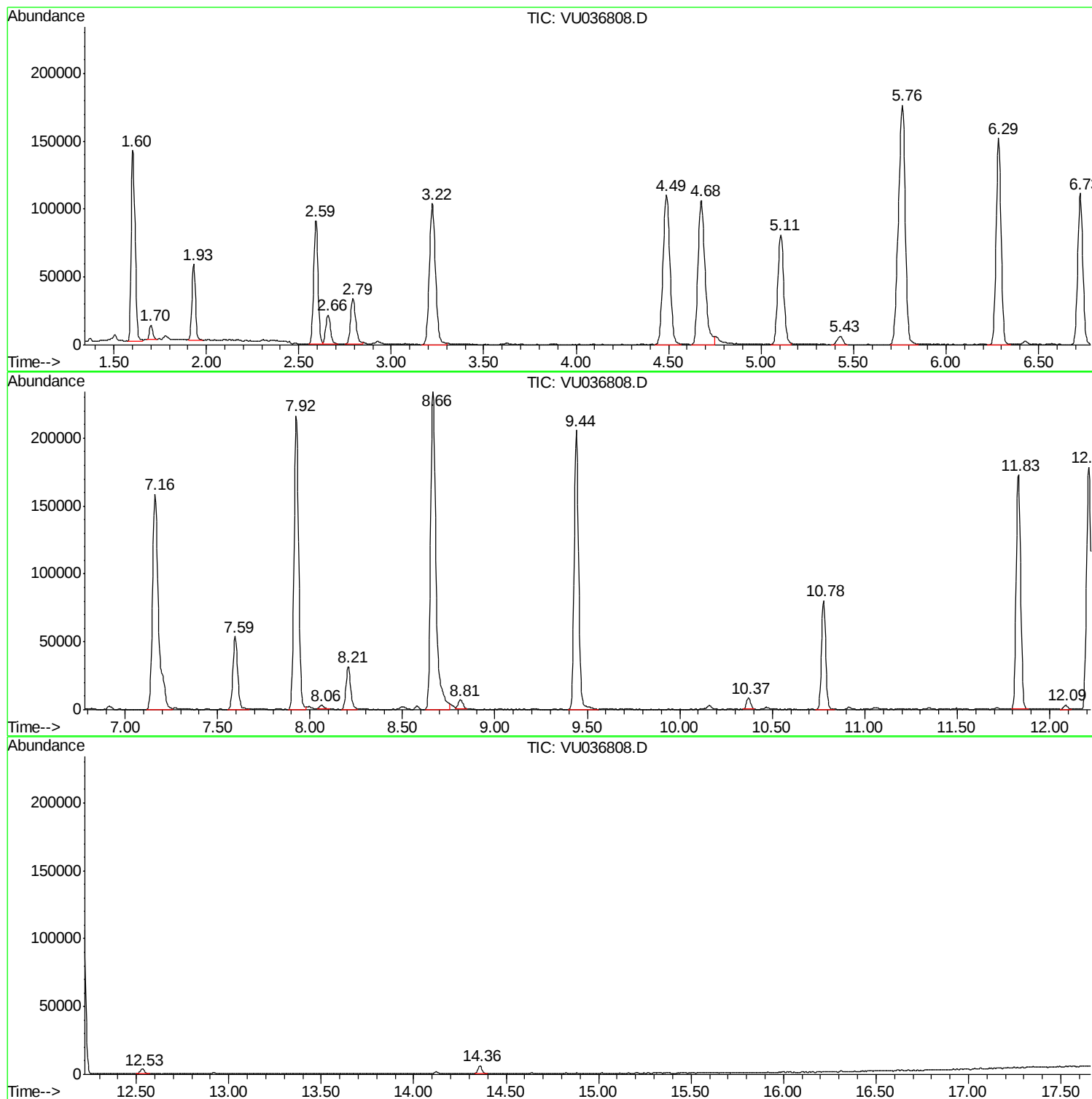
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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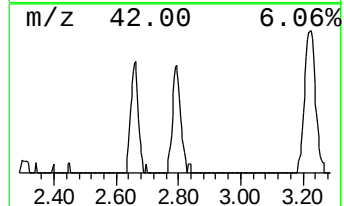
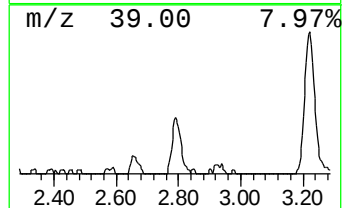
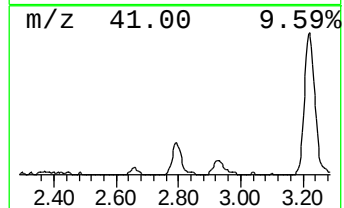
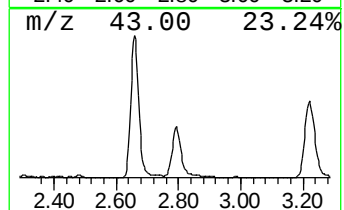
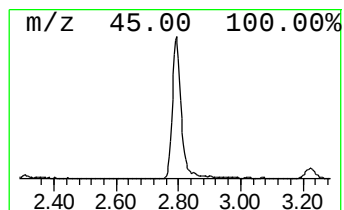
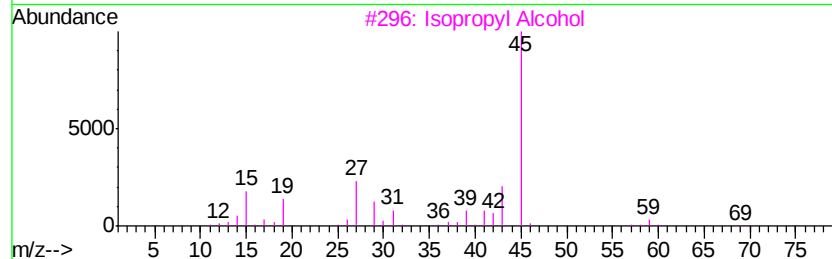
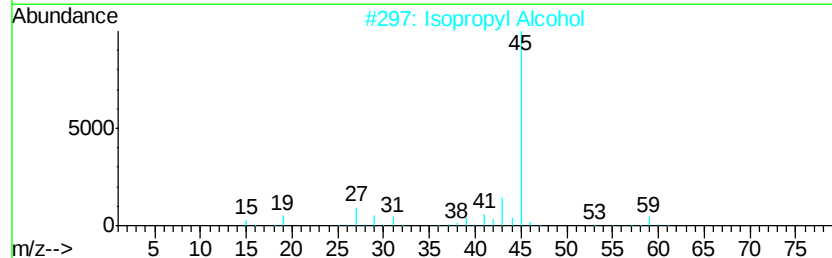
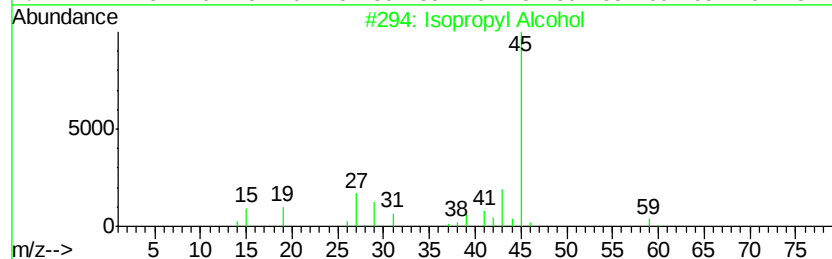
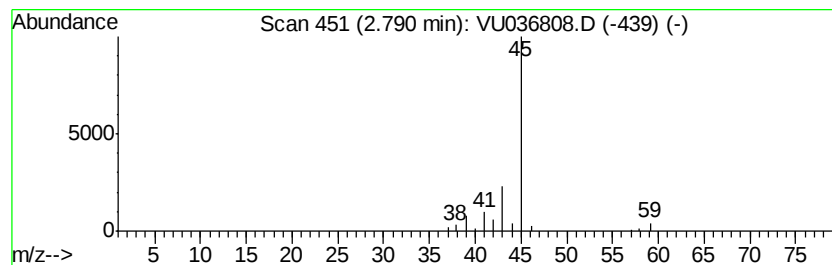
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021220WMA.M
Quant Title : TRACE VOA SOM01.0

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.
2.79	1.14 ug/L	64973	1,4-Difluorobenzene	6.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	43
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Formamide	45	CH3NO	000075-12-7	4



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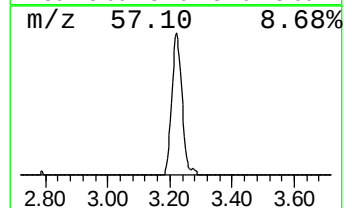
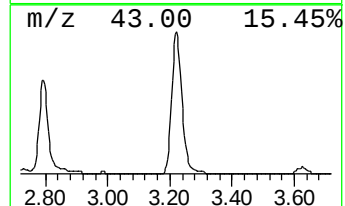
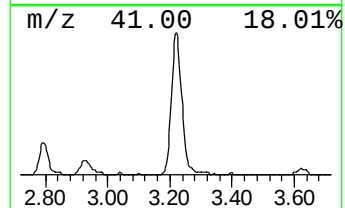
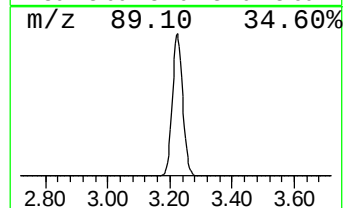
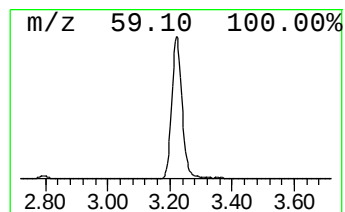
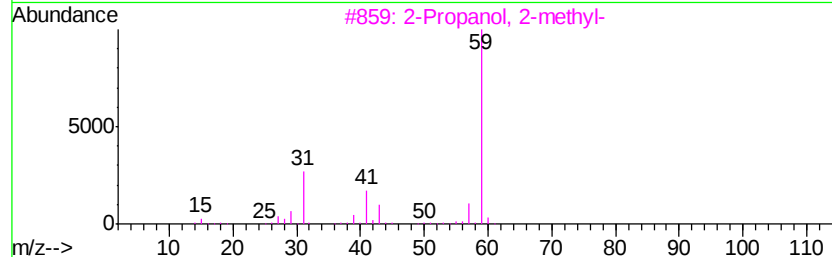
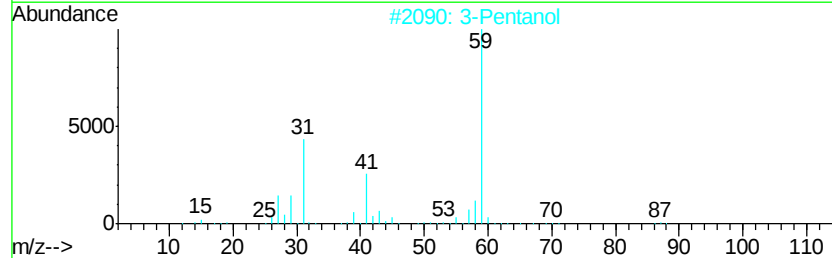
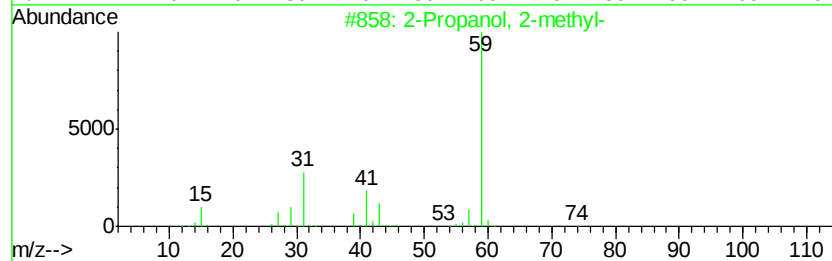
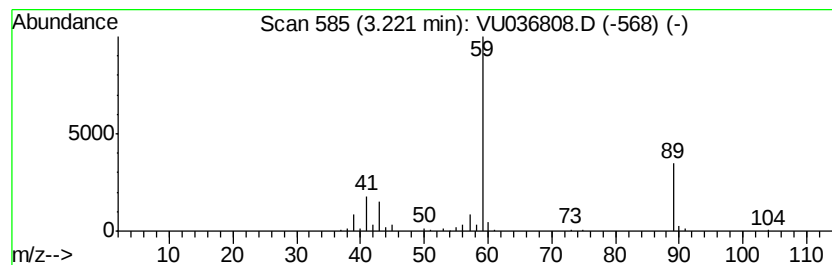
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021220WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.22	4.19 ug/L	238439	1,4-Difluorobenzene	6.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol,	2-methyl-	74	C4H10O	000075-65-0	42	
2	3-Pentanol		88	C5H12O	000584-02-1	42	
3	2-Propanol,	2-methyl-	74	C4H10O	000075-65-0	42	
4	2-Propanol,	2-methyl-	74	C4H10O	000075-65-0	42	
5	3-Pentanol		88	C5H12O	000584-02-1	42	



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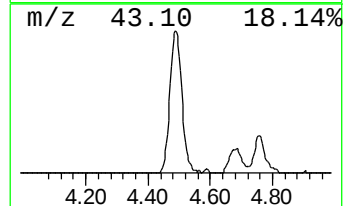
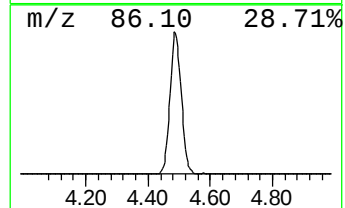
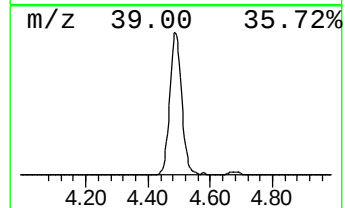
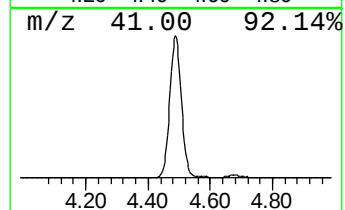
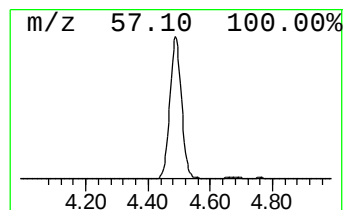
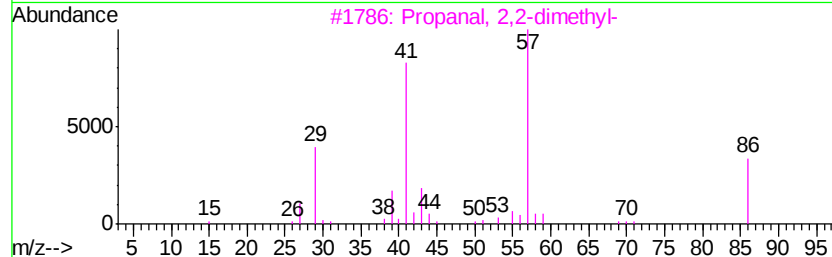
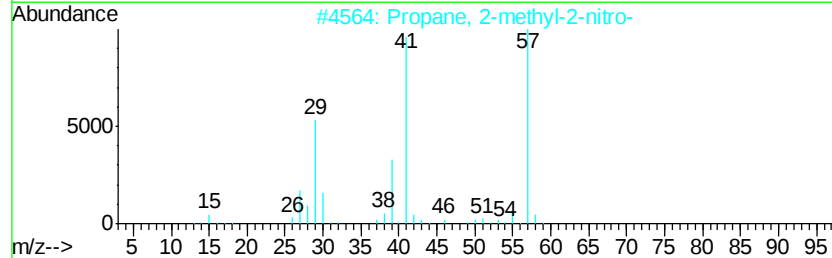
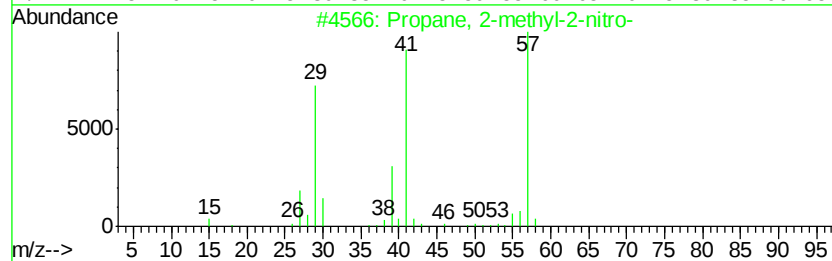
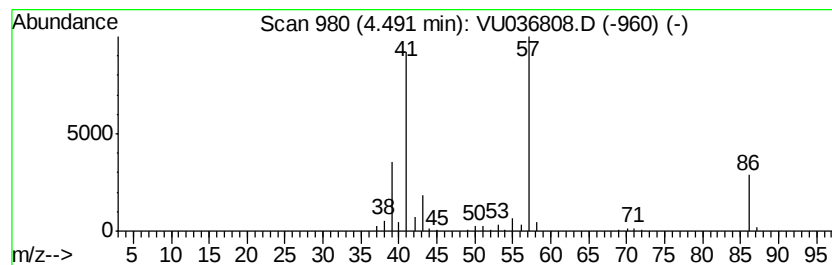
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 2-methyl-2-nitro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	4.99 ug/L	284241	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	50
4		3-Pentanone	86	C5H10O	000096-22-0	42
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40



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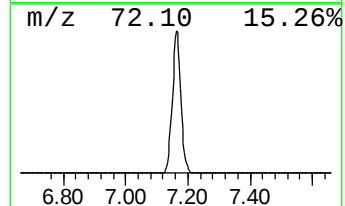
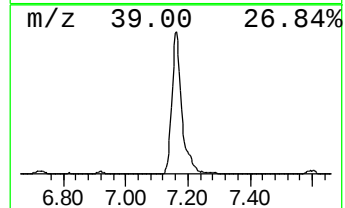
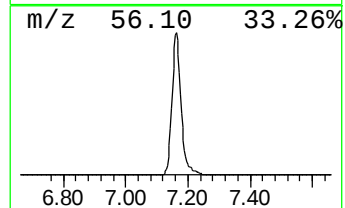
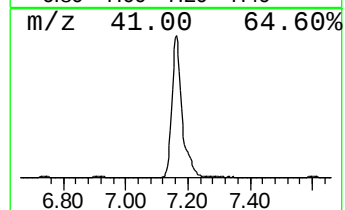
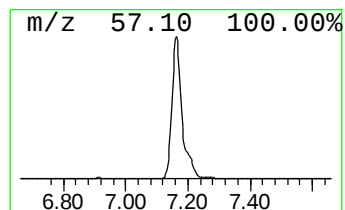
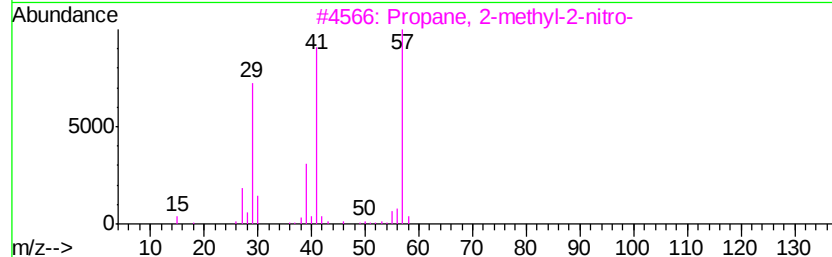
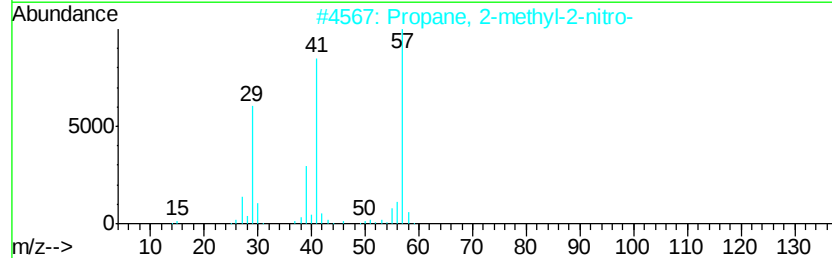
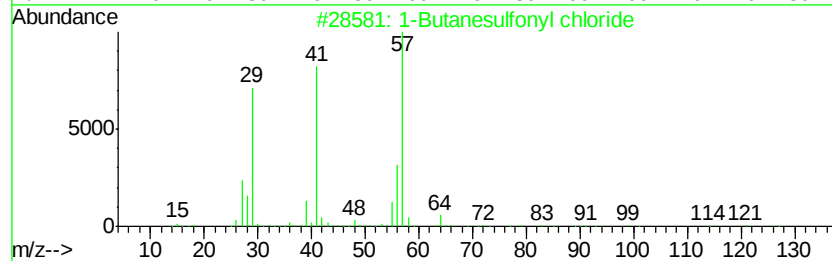
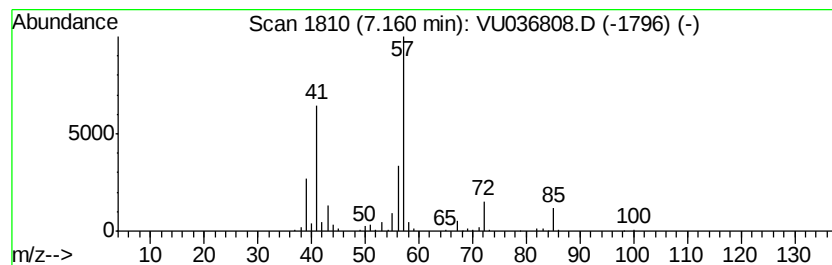
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	6.24 ug/L	355479	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	33
5		1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.79	1.1	ug/L	64973	1	6.29	284815	5.0
unknown-01	3.22	4.2	ug/L	238439	1	6.29	284815	5.0
Propane, 2-methyl...	4.49	5.0	ug/L	284241	1	6.29	284815	5.0
unknown-02	7.16	6.2	ug/L	355479	1	6.29	284815	5.0