

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV111718\
 Data File : VV008588.D
 Acq On : 16 Nov 2018 18:19
 Operator : SY/MD
 Sample : J5988-04
 Misc : 25.0 mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0JF4

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_V\METHOD\SOMVTR111718WMA.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	1.119	5	9	17	rBV2	5532	5029	1.01%	0.088%
2	1.306	60	67	80	rBV2	142833	187915	37.74%	3.272%
3	1.586	147	154	165	rVB	42591	48278	9.70%	0.841%
4	2.135	315	325	336	rBV	92483	135812	27.28%	2.365%
5	2.206	336	347	364	rVB	27390	51711	10.39%	0.900%
6	2.357	385	394	408	rVB2	7970	23423	4.70%	0.408%
7	2.708	489	503	525	rVB2	32180	98963	19.88%	1.723%
8	3.746	806	826	845	rBV2	144888	395536	79.44%	6.887%
9	3.955	877	891	901	rBV	68256	177939	35.74%	3.098%
10	4.405	1013	1031	1053	rBV2	85074	207741	41.72%	3.617%
11	4.727	1111	1131	1153	rBV2	151246	373711	75.06%	6.507%
12	5.100	1228	1247	1271	rBV3	201736	478925	96.19%	8.339%
13	5.669	1406	1424	1440	rBV	196197	391843	78.70%	6.823%
14	5.833	1463	1475	1490	rBV3	5949	14081	2.83%	0.245%
15	6.122	1551	1565	1596	rVB	111665	227984	45.79%	3.970%
16	6.589	1693	1710	1720	rBV	112860	246358	49.48%	4.290%
17	7.032	1837	1848	1869	rBV	55149	103531	20.79%	1.803%
18	7.193	1884	1898	1912	rVB5	9116	18230	3.66%	0.317%
19	7.363	1935	1951	1967	rBV	233611	414539	83.26%	7.218%
20	7.666	2033	2045	2062	rBV2	35486	65503	13.16%	1.141%
21	7.987	2134	2145	2154	rBV3	9420	16641	3.34%	0.290%
22	8.138	2180	2192	2230	rBV	246279	497905	100.00%	8.670%
23	8.289	2233	2239	2250	rVB4	8038	14020	2.82%	0.244%
24	8.900	2415	2429	2450	rBV	264694	450355	90.45%	7.842%
25	9.855	2711	2726	2738	rBV3	10752	19757	3.97%	0.344%
26	9.949	2743	2755	2762	rVV2	3922	6777	1.36%	0.118%
27	10.264	2842	2853	2866	rBV	78898	126339	25.37%	2.200%
28	10.431	2894	2905	2916	rVB4	10465	17534	3.52%	0.305%
29	10.830	3021	3029	3036	rBV2	5250	8492	1.71%	0.148%
30	11.199	3138	3144	3150	rBV7	3480	5326	1.07%	0.093%
31	11.299	3163	3175	3199	rVB	240246	405617	81.46%	7.063%
32	11.582	3255	3263	3278	rBV4	5168	9054	1.82%	0.158%
33	11.675	3279	3292	3312	rVV	204366	337459	67.78%	5.876%
34	12.292	3473	3484	3497	rBV7	7263	14101	2.83%	0.246%

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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

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Title : TRACE VOA SOM01.0

35	12.399	3508	3517	3526	rBV8	4890	8102	1.63%	0.141%
36	13.315	3793	3802	3812	rBV8	3330	5455	1.10%	0.095%
37	13.807	3943	3955	3970	rBV	34068	52614	10.57%	0.916%
38	14.386	4124	4135	4145	rBV4	8874	14530	2.92%	0.253%
39	15.170	4370	4379	4390	rVB5	23352	34893	7.01%	0.608%
40	16.157	4679	4686	4697	rVB7	9847	15627	3.14%	0.272%
41	16.238	4704	4711	4722	rBV7	3870	5779	1.16%	0.101%
42	16.341	4740	4743	4747	rBV	17049	9593	1.93%	0.167%

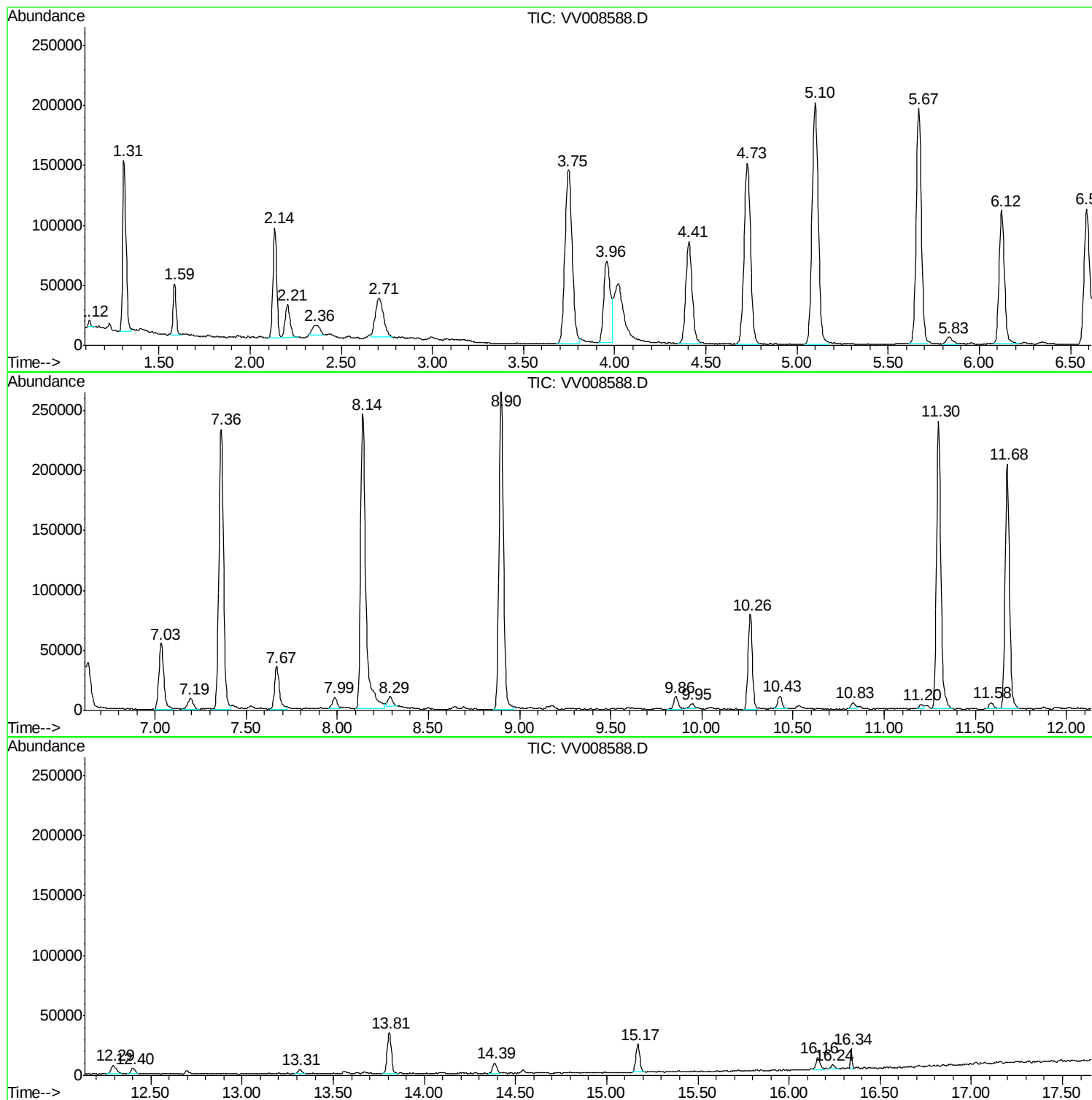
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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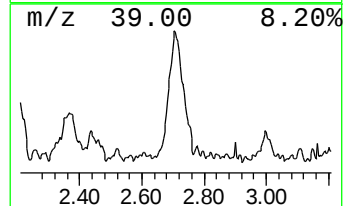
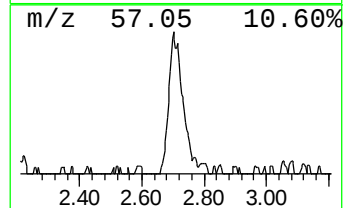
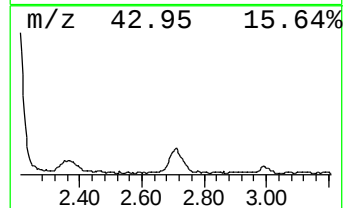
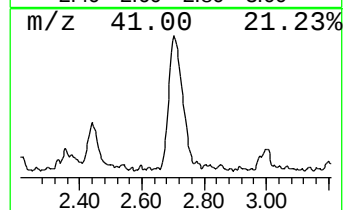
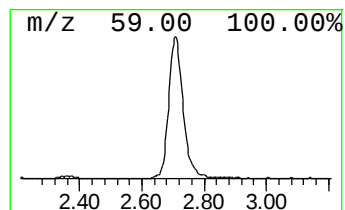
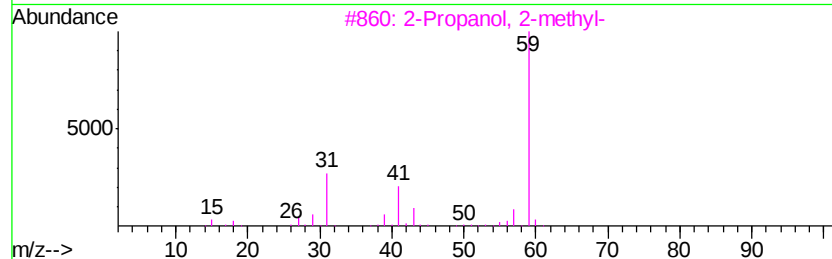
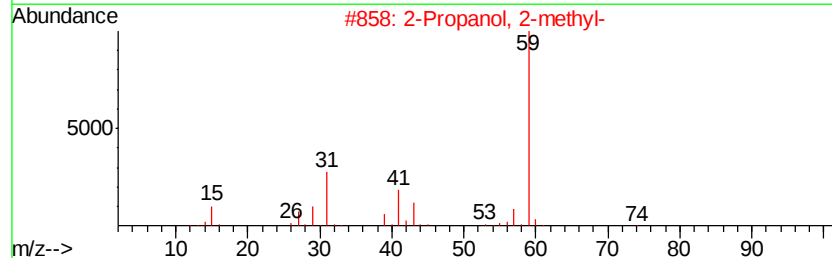
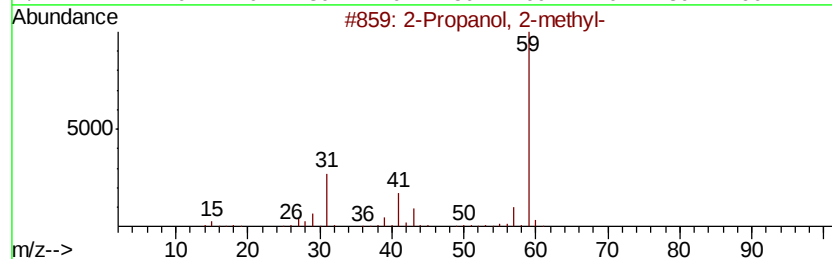
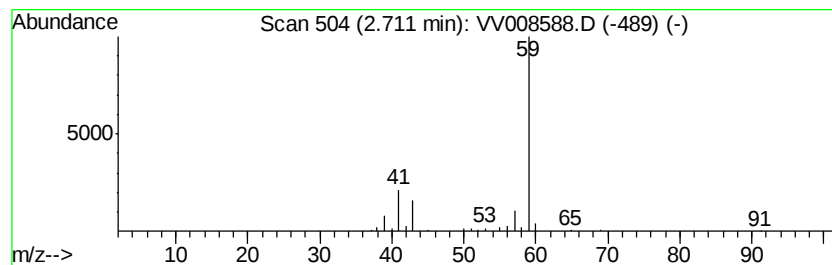
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR111718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.71	1.26 ug/L	98963	1,4-Difluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	72
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	56
3	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	56
4	3-Pentanol			88	C5H12O	000584-02-1	40
5	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	37



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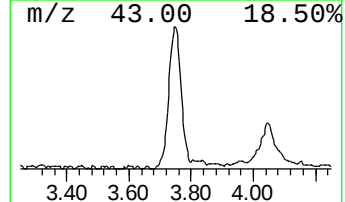
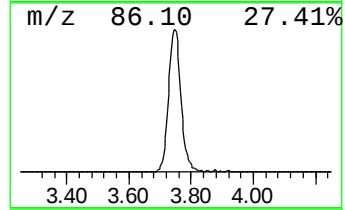
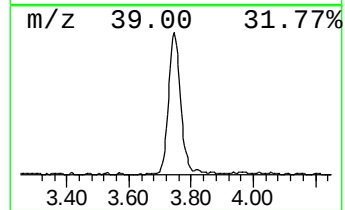
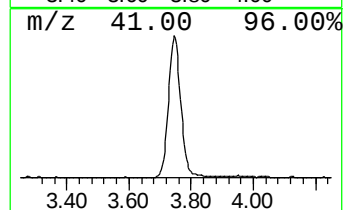
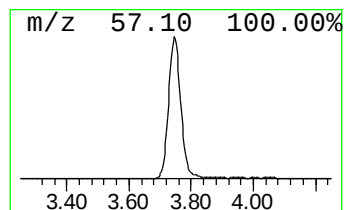
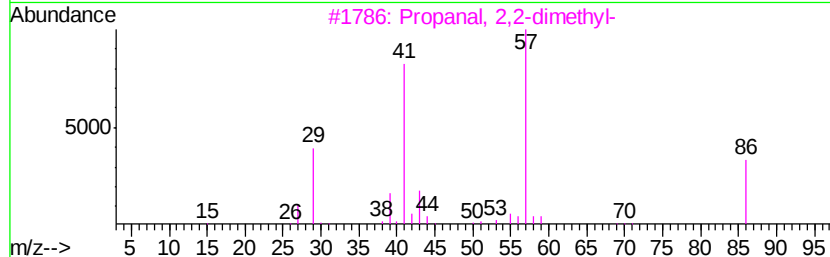
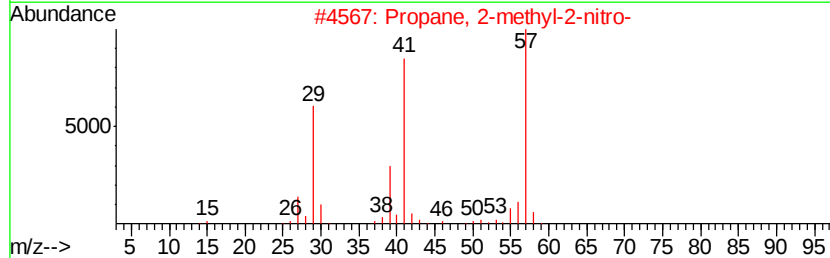
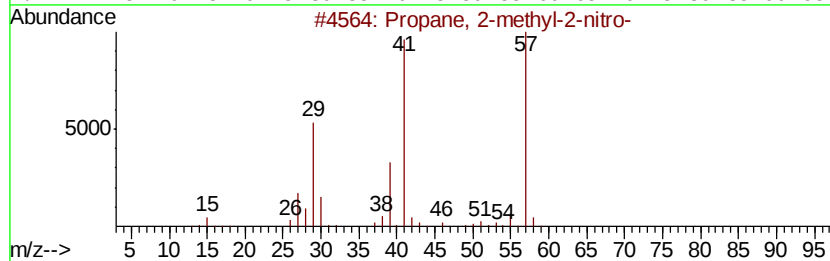
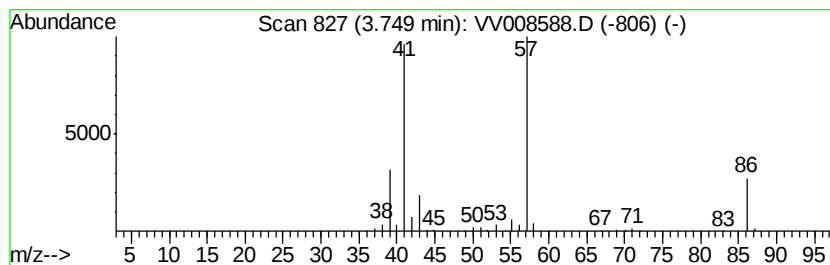
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.75	5.05 ug/L	395536	1,4-Difluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	50		
5	3-Pentanone	86	C5H10O	000096-22-0	42		



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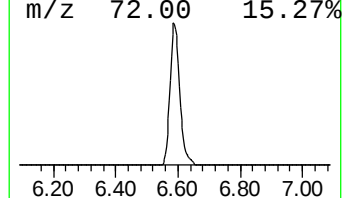
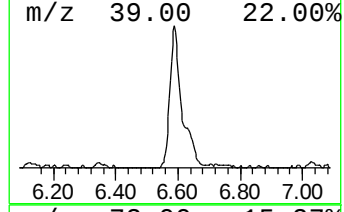
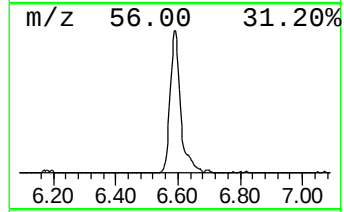
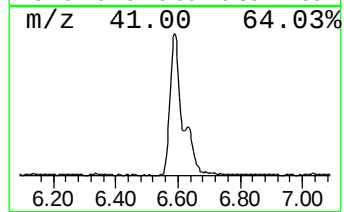
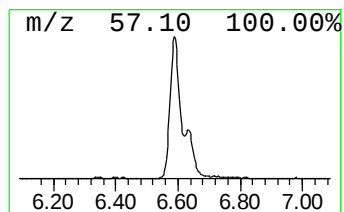
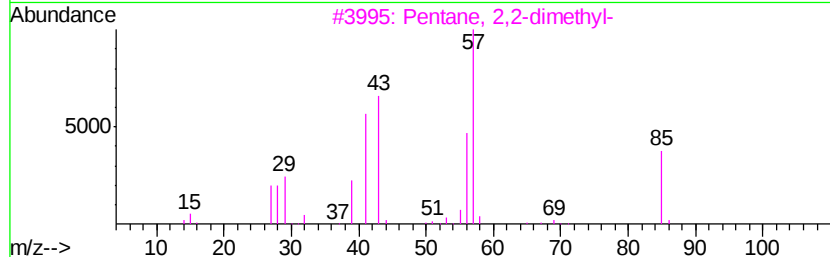
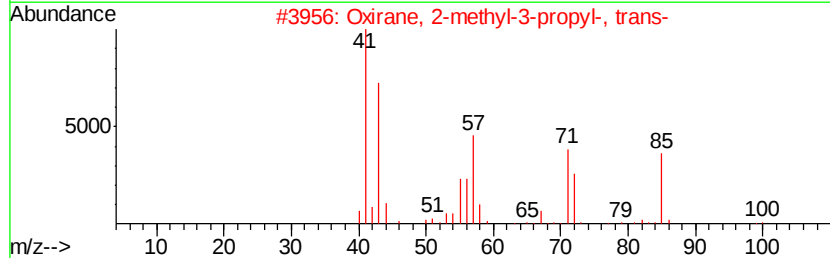
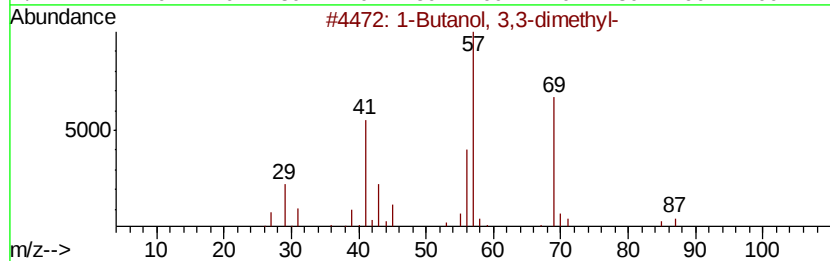
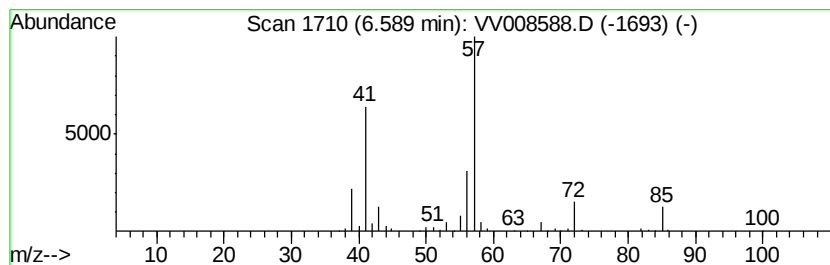
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	3.14 ug/L	246358	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	47
2		Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	43
3		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	40
4		1-Hexen-3-ol	100	C6H12O	004798-44-1	40
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38



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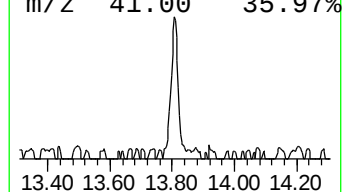
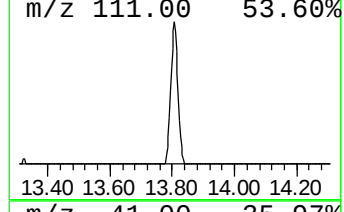
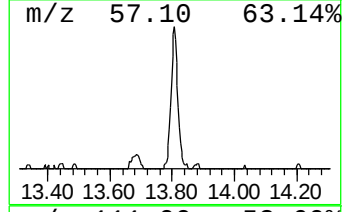
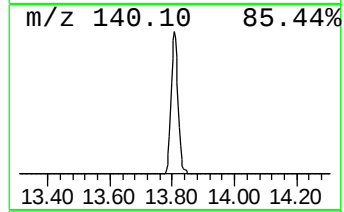
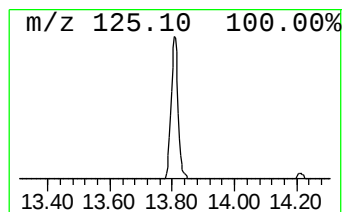
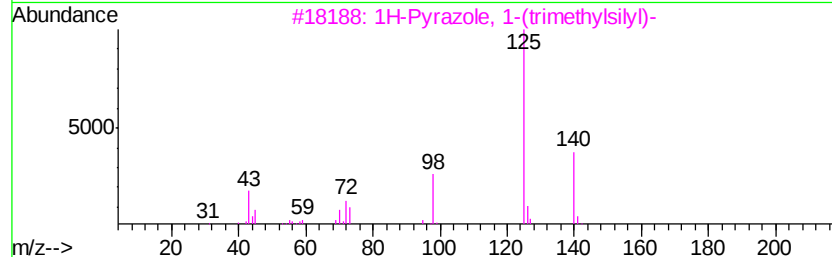
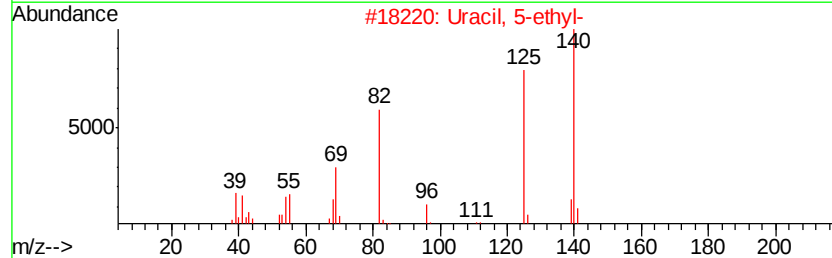
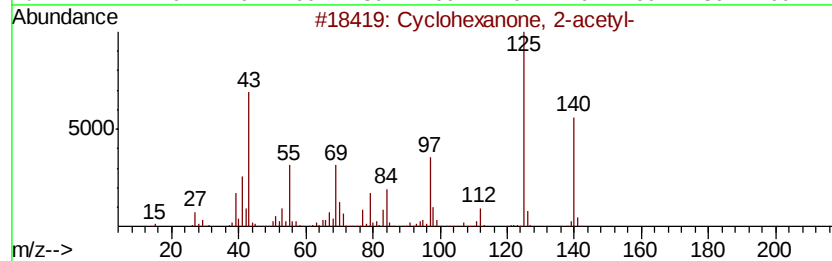
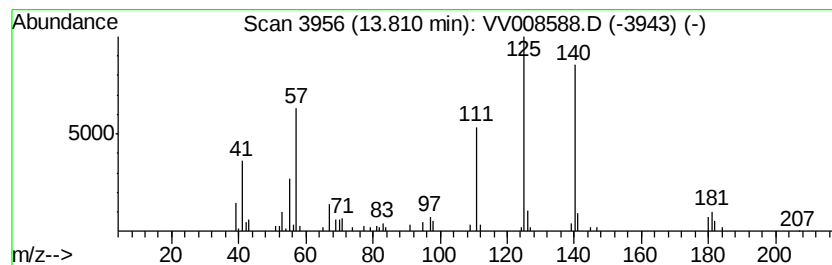
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexanone, 2-acetyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	0.65 ug/L	52614	1,4-Dichlorobenzene-d4	11.30

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2-acetyl-	140	C8H12O2	000874-23-7	59
2	Uracil, 5-ethyl-	140	C6H8N2O2	004212-49-1	58
3	1H-Pyrazole, 1-(trimethylsilyl)-	140	C6H12N2Si	018156-75-7	58
4	Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	53
5	Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	53



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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...	2.71	1.3	ug/L	98963	1	5.67	391843	5.0
Propane, 2-methyl...	3.75	5.0	ug/L	395536	1	5.67	391843	5.0
unknown-01	6.59	3.1	ug/L	246358	1	5.67	391843	5.0
Cyclohexanone, 2-...	13.81	0.7	ug/L	52614	3	11.30	405617	5.0