

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV111718\
 Data File : VV008587.D
 Acq On : 16 Nov 2018 17:54
 Operator : SY/MD
 Sample : J5987-08
 Misc : 25.0 mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 COL34

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	1.309	61	68	85	rVB2	156042	196560	43.02%	3.741%
2	1.585	148	154	162	rVB	40505	44932	9.83%	0.855%
3	2.135	315	325	337	rBV	88996	125232	27.41%	2.384%
4	2.209	338	348	363	rVB	22875	46497	10.18%	0.885%
5	2.714	490	505	536	rVB3	26334	97967	21.44%	1.865%
6	3.746	805	826	850	rBV2	137211	377456	82.61%	7.185%
7	3.958	876	892	905	rBV	58340	176635	38.66%	3.362%
8	4.405	1013	1031	1053	rBV2	78261	191865	41.99%	3.652%
9	4.727	1110	1131	1153	rBV	118016	287832	62.99%	5.479%
10	5.100	1227	1247	1269	rBV2	185224	441849	96.70%	8.410%
11	5.666	1407	1423	1447	rVB	186915	379526	83.06%	7.224%
12	5.833	1465	1475	1487	rBV5	5510	12035	2.63%	0.229%
13	6.122	1551	1565	1583	rBV	104139	210285	46.02%	4.003%
14	6.588	1695	1710	1719	rBV2	107630	219214	47.98%	4.173%
15	7.032	1835	1848	1862	rBV2	52277	93003	20.35%	1.770%
16	7.360	1938	1950	1969	rBV	215893	384266	84.10%	7.314%
17	7.666	2034	2045	2071	rBV	32867	62667	13.71%	1.193%
18	7.984	2133	2144	2153	rBV7	3370	7228	1.58%	0.138%
19	8.138	2181	2192	2218	rBV	230056	456931	100.00%	8.697%
20	8.289	2234	2239	2251	rVB6	7060	11705	2.56%	0.223%
21	8.897	2413	2428	2452	rBV	255506	430617	94.24%	8.197%
22	9.855	2718	2726	2740	rBV6	9767	16762	3.67%	0.319%
23	9.945	2746	2754	2760	rBV	3831	5337	1.17%	0.102%
24	10.264	2840	2853	2866	rBV	71824	114607	25.08%	2.181%
25	10.428	2896	2904	2914	rVB4	3007	5156	1.13%	0.098%
26	10.829	3019	3029	3038	rBV2	5737	10291	2.25%	0.196%
27	11.206	3136	3146	3149	rBV7	3947	5823	1.27%	0.111%
28	11.299	3163	3175	3202	rVB	227985	391440	85.67%	7.451%
29	11.592	3256	3266	3275	rBV8	2677	4880	1.07%	0.093%
30	11.675	3280	3292	3314	rBV	191189	310610	67.98%	5.912%
31	12.296	3474	3485	3500	rBV7	5611	12509	2.74%	0.238%
32	12.399	3510	3517	3530	rBV7	4394	6879	1.51%	0.131%
33	12.698	3600	3610	3617	rBV4	4433	6755	1.48%	0.129%
34	13.321	3795	3804	3816	rBV4	4210	7915	1.73%	0.151%

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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	13.562	3869	3879	3885	rBV3	3748	4655	1.02%	0.089%
36	13.807	3945	3955	3968	rBV2	33358	49128	10.75%	0.935%
37	14.386	4124	4135	4146	rBV4	7766	12017	2.63%	0.229%
38	15.170	4370	4379	4390	rBV5	17148	26396	5.78%	0.502%
39	16.160	4680	4687	4696	rBV8	5229	8157	1.79%	0.155%

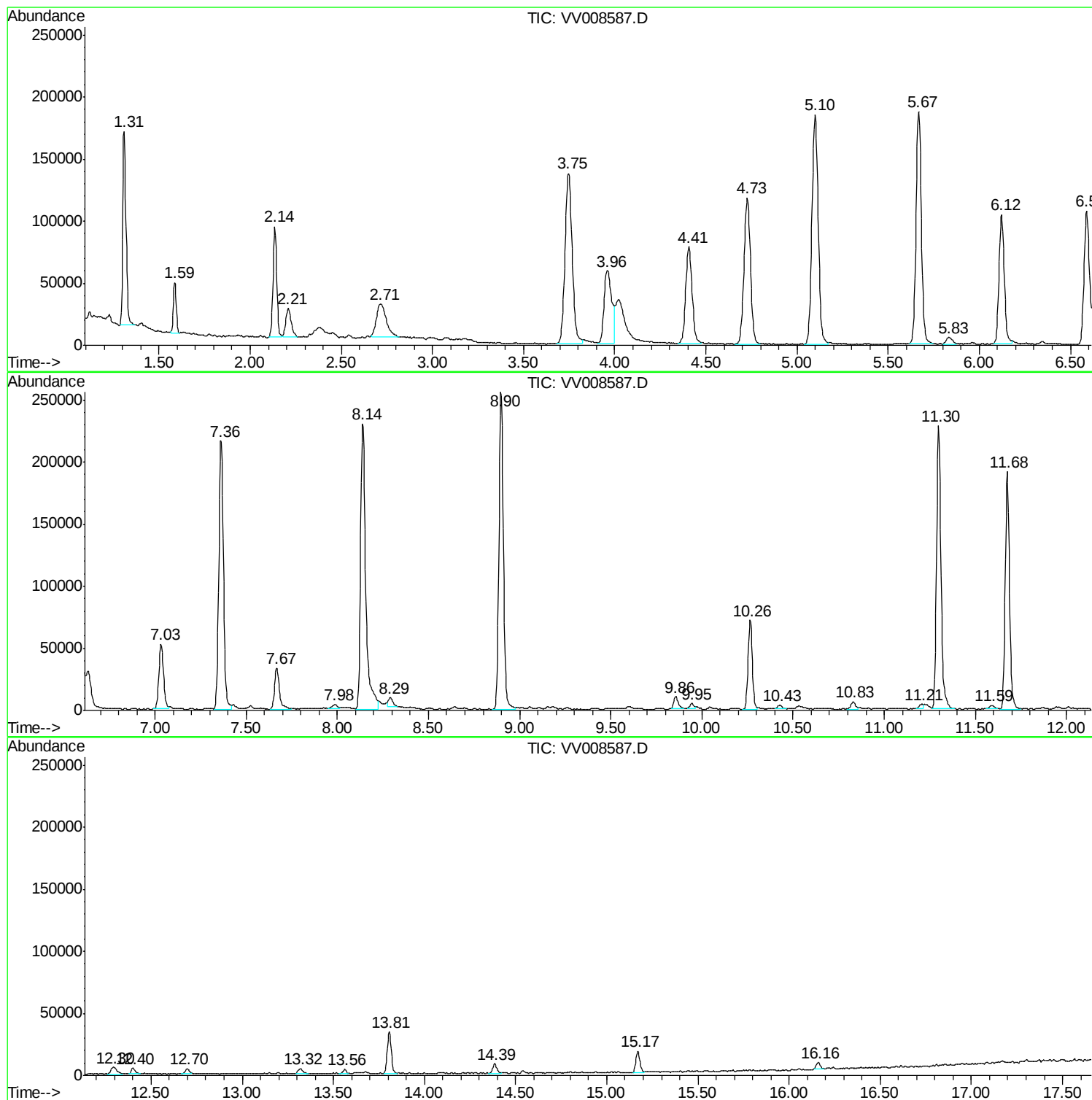
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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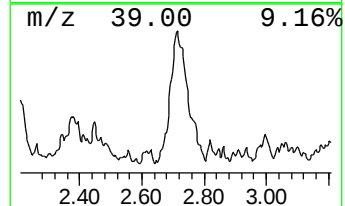
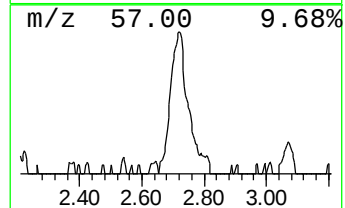
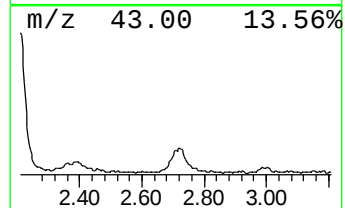
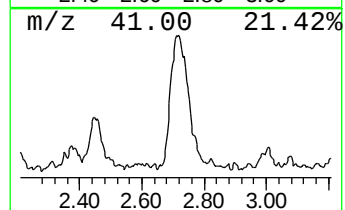
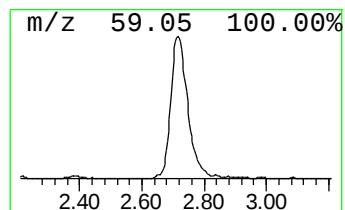
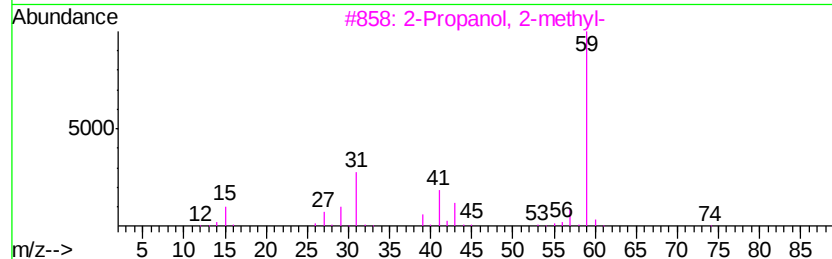
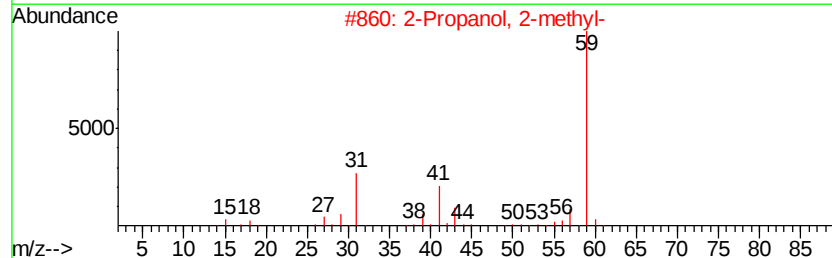
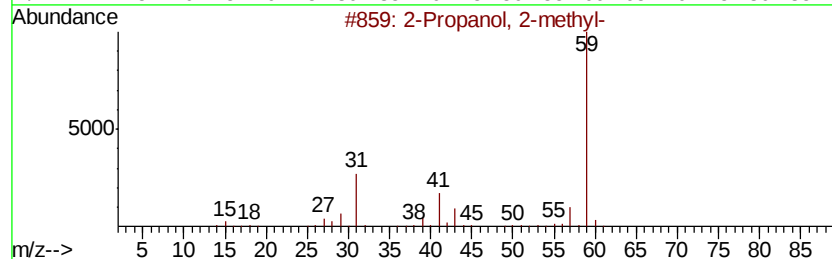
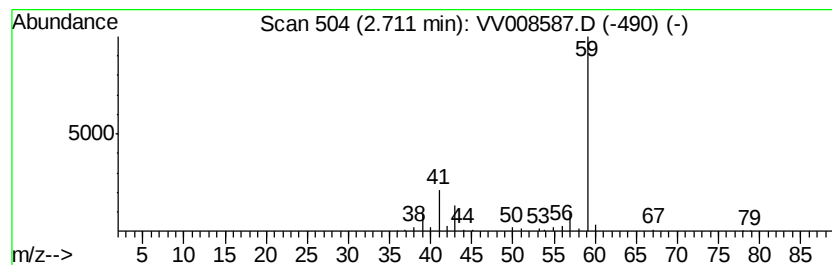
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.71	1.29 ug/L	97967	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	5-Hexyn-3-ol			98	C6H10O	019780-84-8	43
5	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	32



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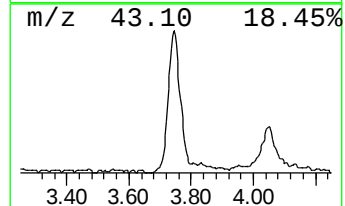
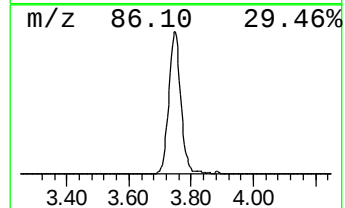
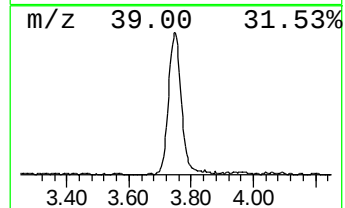
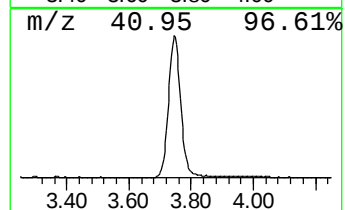
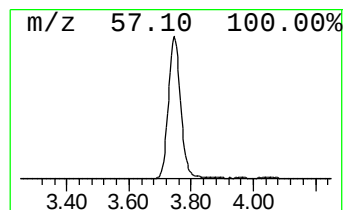
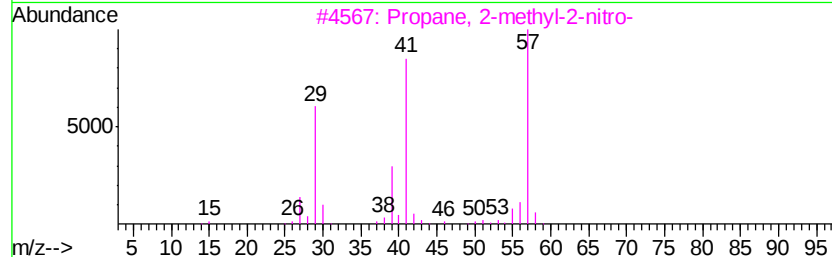
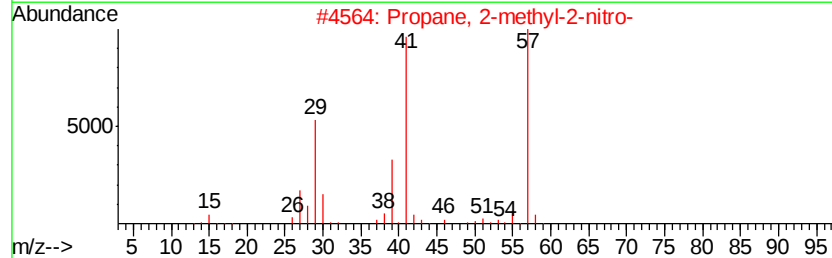
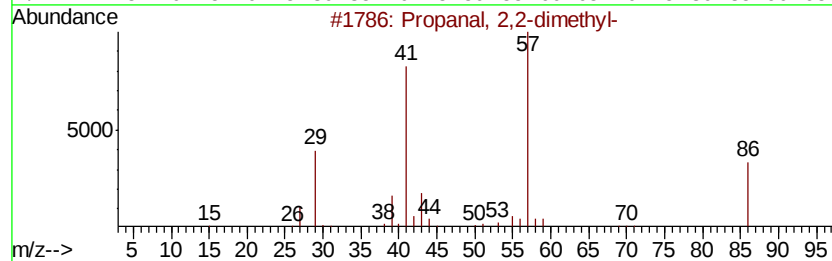
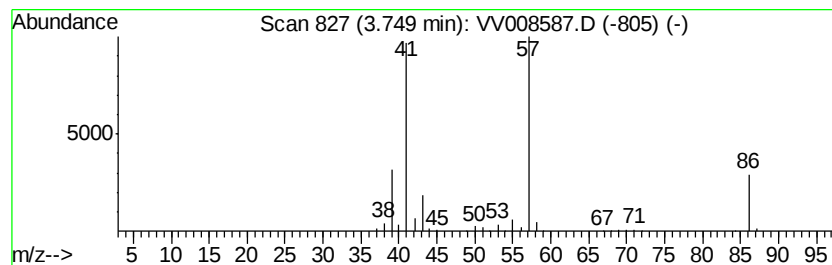
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.75	4.97 ug/L	377456	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
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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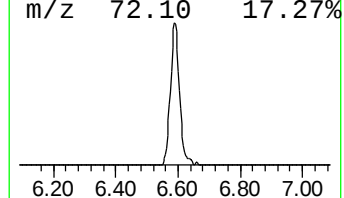
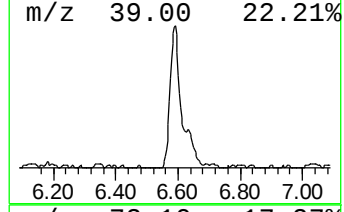
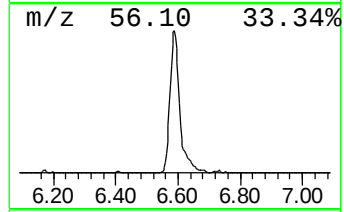
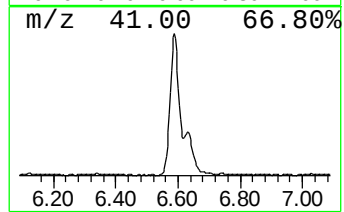
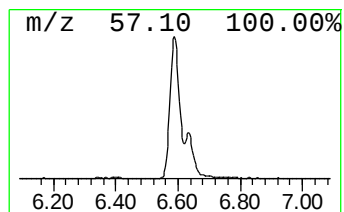
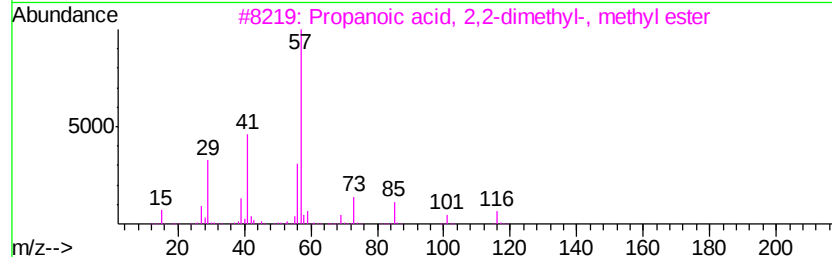
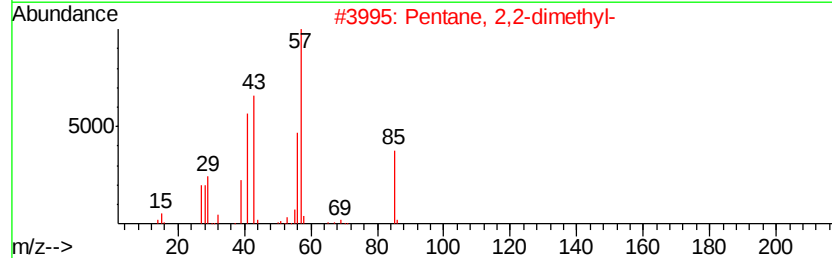
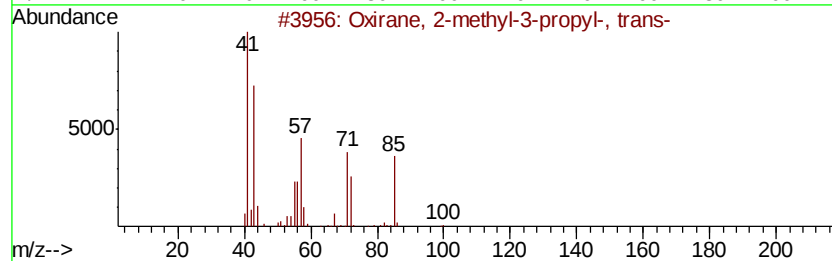
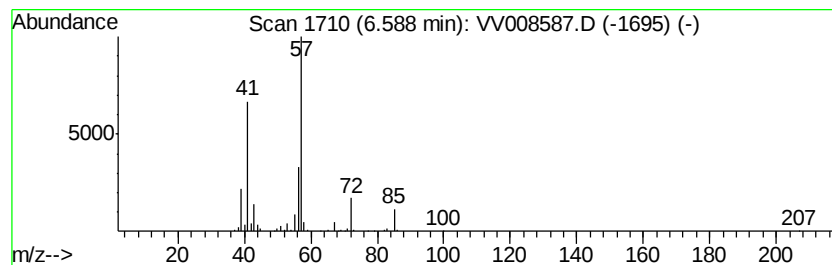
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	2.89 ug/L	219214	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	43
2		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	42
3		Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	40
4		1-Hexen-3-ol	100	C6H12O	004798-44-1	37
5		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	37



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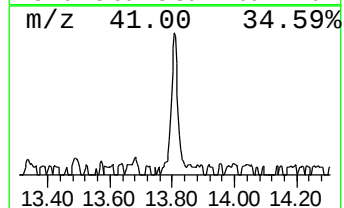
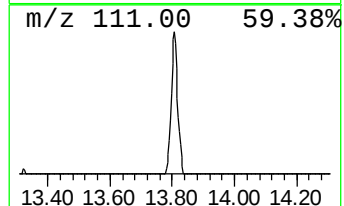
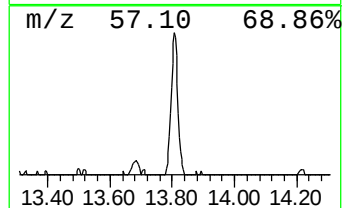
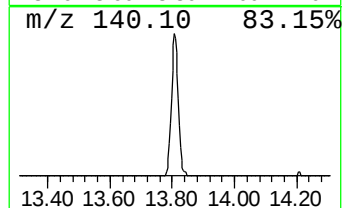
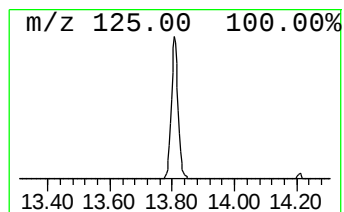
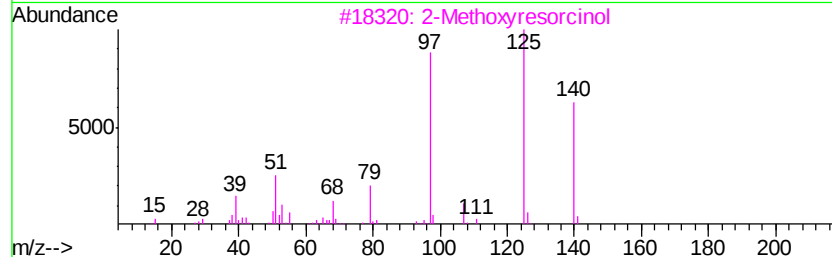
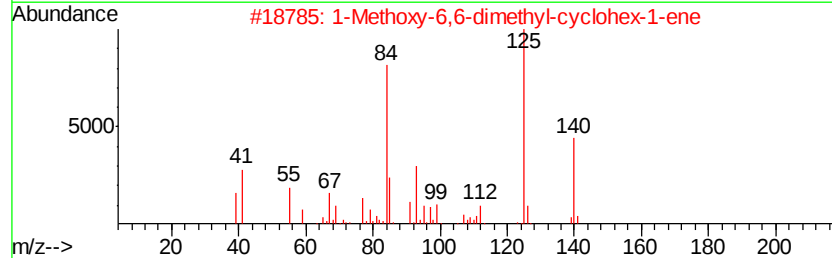
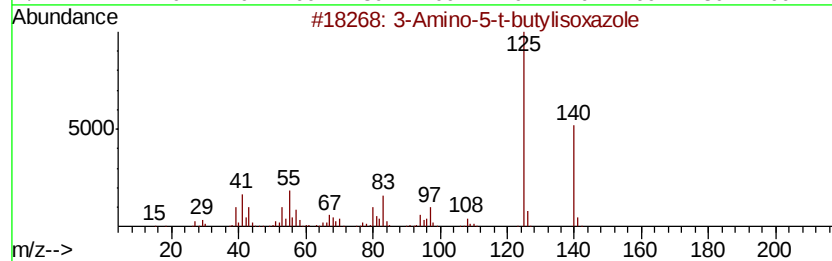
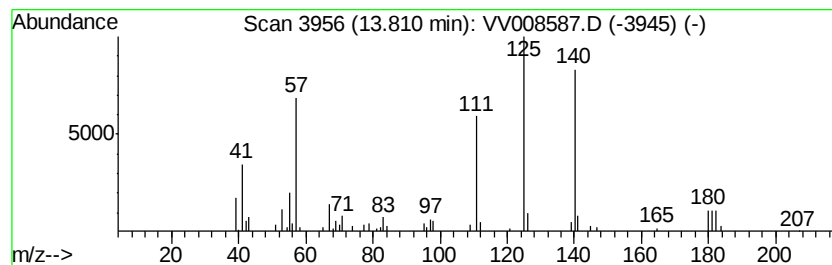
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Amino-5-t-butylisoxazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	0.63 ug/L	49128	1,4-Dichlorobenzene-d4	11.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		3-Amino-5-t-butylisoxazole	140 C7H12N2O	055809-36-4 58
2		1-Methoxy-6,6-dimethyl-cyclohex-...	140 C9H16O	073741-66-9 58
3		2-Methoxyresorcinol	140 C7H8O3	029267-67-2 58
4		Phenol, 4-(methylthio)-	140 C7H8OS	001073-72-9 53
5		1,4-Benzenediol, 2-methoxy-	140 C7H8O3	000824-46-4 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...	2.71	1.3	ug/L	97967	1	5.67	379526	5.0
Propanal, 2,2-dim...	3.75	5.0	ug/L	377456	1	5.67	379526	5.0
unknown-01	6.59	2.9	ug/L	219214	1	5.67	379526	5.0
3-Amino-5-t-butyl...	13.81	0.6	ug/L	49128	3	11.30	391440	5.0