

Data Path : Z:\VOASRV\HPCHEM1\MSVOA R\DATA\VR100118\
 Data File : VR025910.D
 Acq On : 1 Oct 2018 14:02
 Operator : SY/MD
 Sample : J5114-03
 Misc : 25mL/MSVOA R/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_R
 ClientSampleId :
 C0J68

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

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_R\METHODS\SOMRTR092718WMA.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	2.111	65	71	74	rBV	122387	235843	14.65%	1.461%
2	2.634	149	157	169	rVB	103042	255612	15.87%	1.583%
3	3.632	307	321	330	rBV2	184402	765094	47.51%	4.740%
4	3.705	330	333	341	rVB	48838	101621	6.31%	0.630%
5	3.942	365	372	383	rVB	25615	71269	4.43%	0.441%
6	4.654	479	489	501	rBV3	41513	156241	9.70%	0.968%
7	6.406	766	777	792	rBV2	249789	809158	50.25%	5.013%
8	6.594	798	808	816	rBV2	101829	311108	19.32%	1.927%
9	6.698	819	825	832	rVB	34729	95681	5.94%	0.593%
10	7.203	898	908	922	rVB	274476	701052	43.53%	4.343%
11	7.513	948	959	974	rBV	473041	1416163	87.94%	8.773%
12	7.854	1004	1015	1030	rBV2	581807	1594706	99.03%	9.879%
13	8.462	1107	1115	1123	rVV	807186	1529032	94.95%	9.472%
14	8.541	1124	1128	1134	rVB6	12108	26271	1.63%	0.163%
15	8.900	1179	1187	1198	rVB	368152	711919	44.21%	4.410%
16	9.302	1246	1253	1263	rBV	263523	504042	31.30%	3.122%
17	9.679	1309	1315	1325	rBV	153228	254440	15.80%	1.576%
18	9.971	1356	1363	1370	rBV	893211	1424869	88.48%	8.827%
19	10.238	1401	1407	1414	rVB	73574	114581	7.12%	0.710%
20	10.384	1424	1431	1433	rBV8	10707	19347	1.20%	0.120%
21	10.591	1457	1465	1476	rBV	484374	794148	49.32%	4.920%
22	10.737	1485	1489	1493	rBV5	19504	26992	1.68%	0.167%
23	11.285	1573	1579	1593	rBV	1031160	1610338	100.00%	9.976%
24	12.015	1695	1699	1704	rBV5	21622	34921	2.17%	0.216%
25	12.124	1712	1717	1720	rBV2	11896	21299	1.32%	0.132%
26	12.301	1741	1746	1751	rBV3	16379	29942	1.86%	0.185%
27	12.362	1751	1756	1763	rVB	131897	207391	12.88%	1.285%
28	12.800	1823	1828	1832	rVB2	11631	23669	1.47%	0.147%
29	13.219	1891	1897	1905	rBV	834331	1160459	72.06%	7.189%
30	13.511	1939	1945	1956	rVB	471819	708562	44.00%	4.389%
31	13.706	1973	1977	1981	rBV	11373	19471	1.21%	0.121%
32	13.907	2003	2010	2013	rBV3	18453	28870	1.79%	0.179%
33	14.004	2022	2026	2032	rVB8	14039	25073	1.56%	0.155%
34	15.142	2205	2213	2221	rBV3	59061	106886	6.64%	0.662%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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	15.586	2277	2286	2296	rBV2	80252	159757	9.92%	0.990%
36	16.438	2419	2426	2435	rBV7	41223	86798	5.39%	0.538%

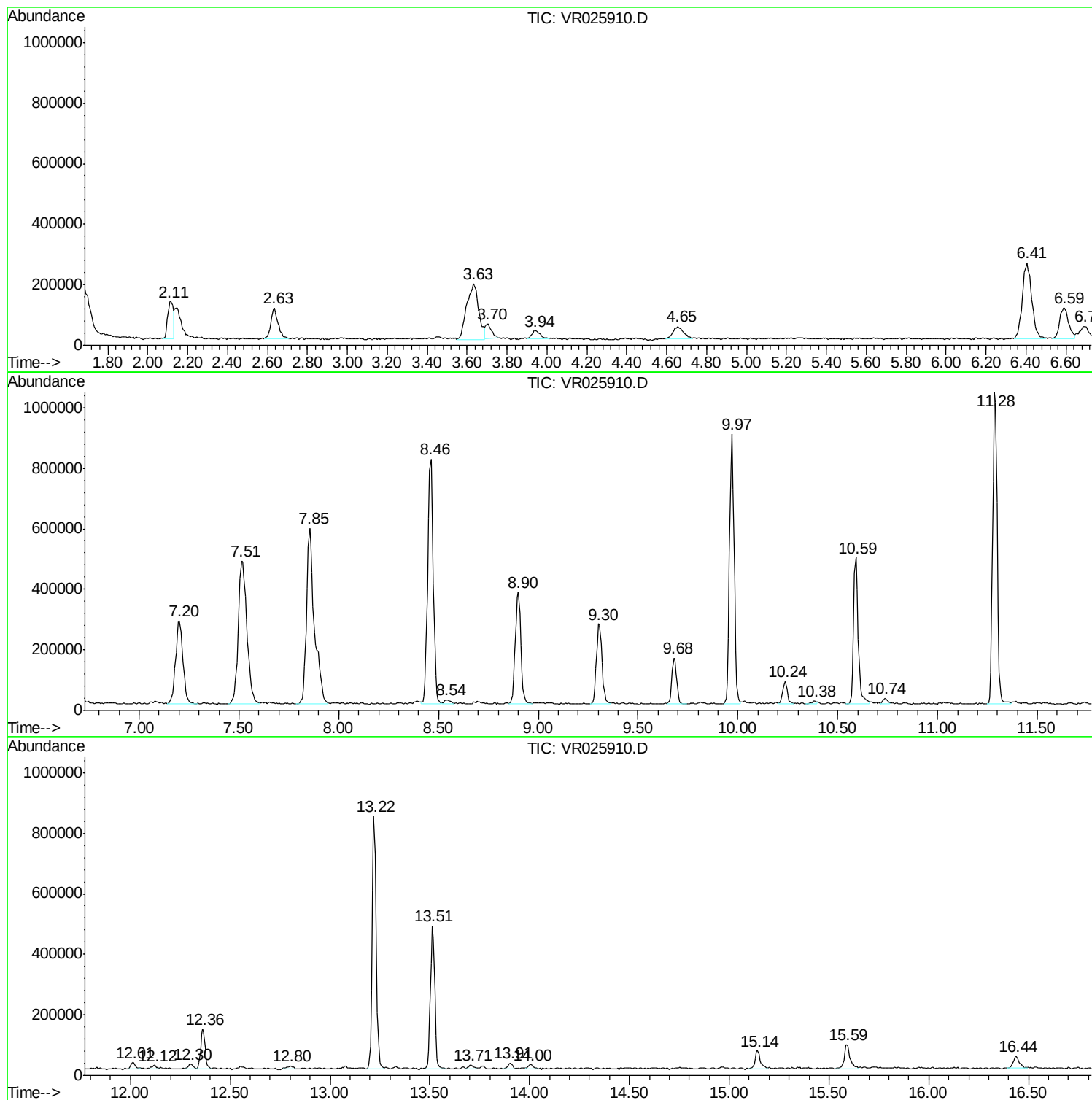
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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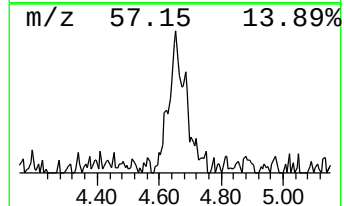
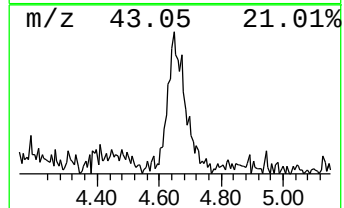
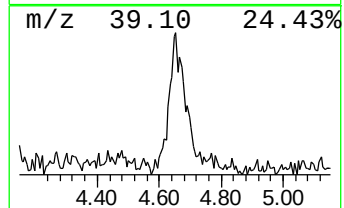
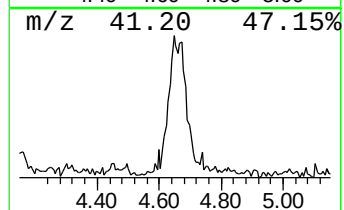
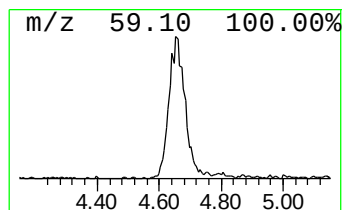
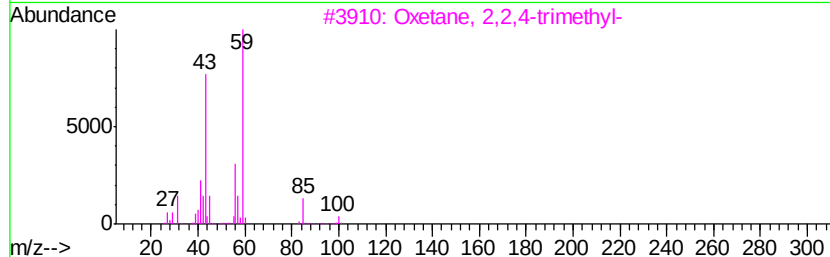
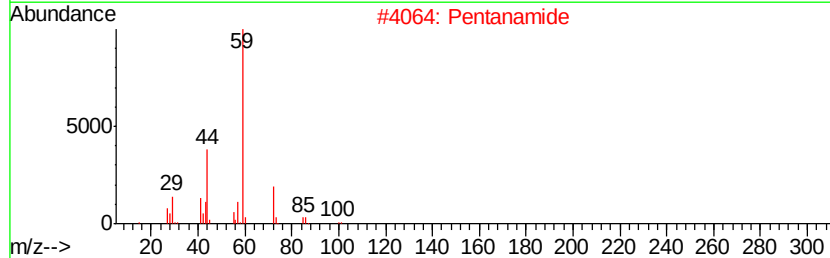
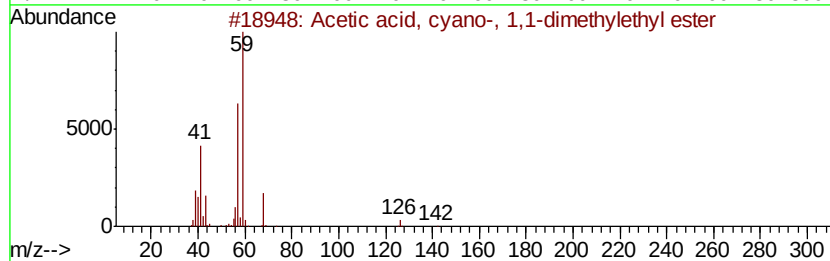
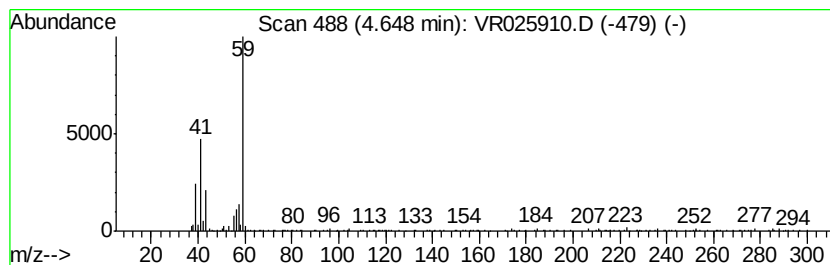
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	0.51 ug/L	156241	1,4-Difluorobenzene	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	45
2		Pentanamide	101	C5H11NO	000626-97-1	45
3		Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	45
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	40
5		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40



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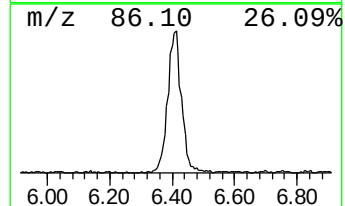
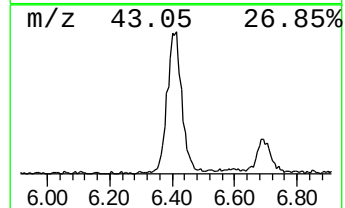
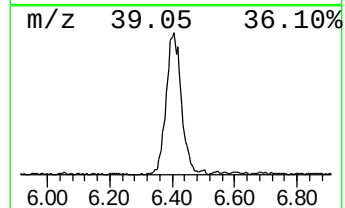
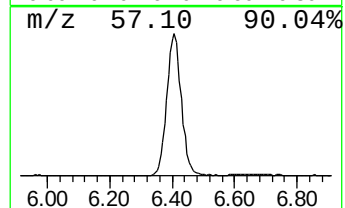
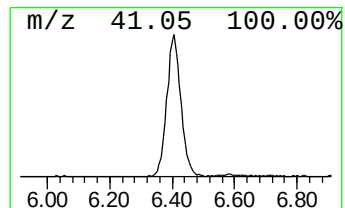
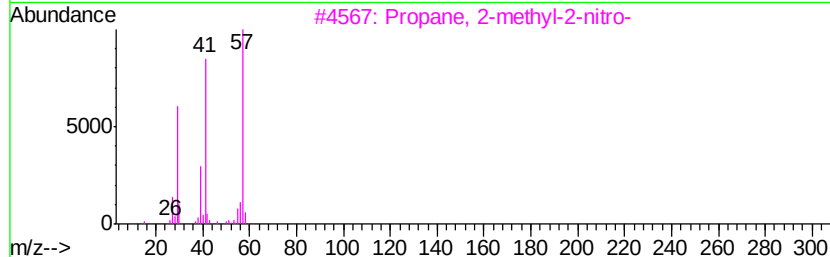
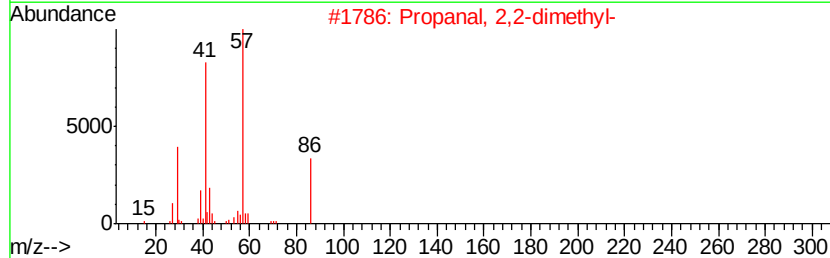
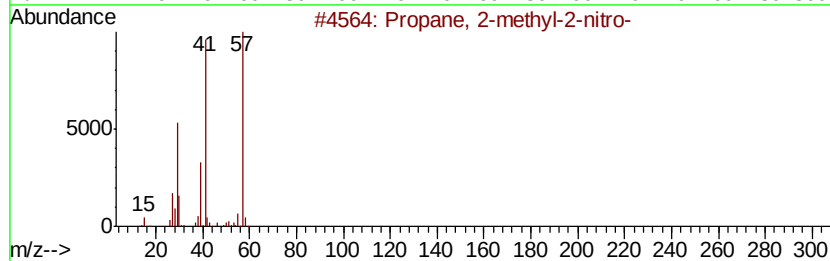
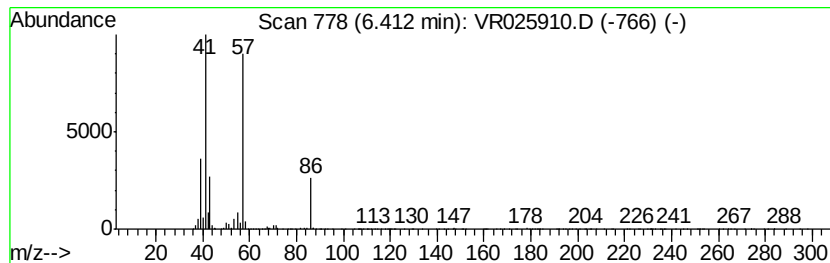
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR092718WMA.M
Quant Title : TRACE VOA SOM01.0

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.
6.41	2.65 ug/L	809158	1,4-Difluorobenzene	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
2		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	50
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
4		4,4-Dimethyl-3-oxopentanenitrile	125	C7H11NO	059997-51-2	38
5		Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	28



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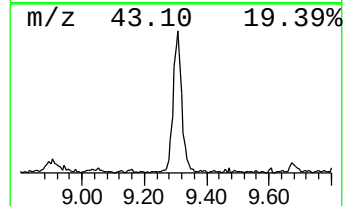
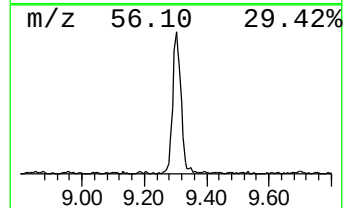
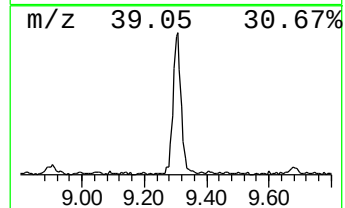
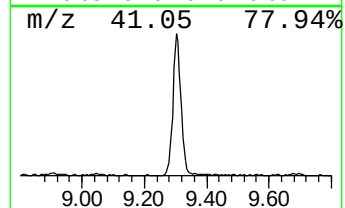
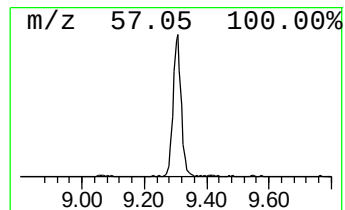
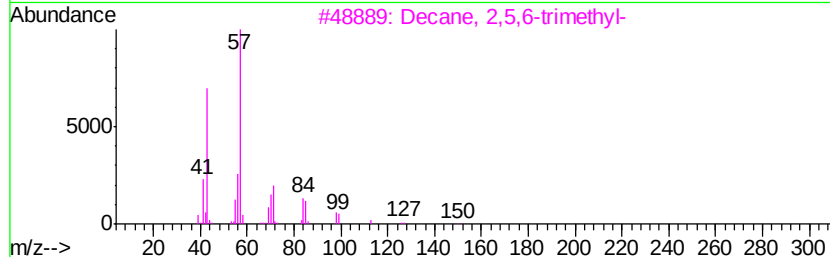
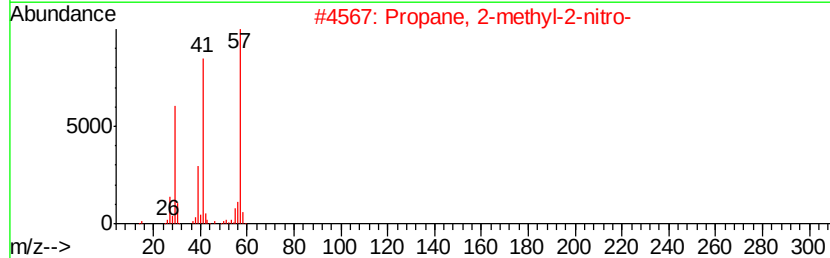
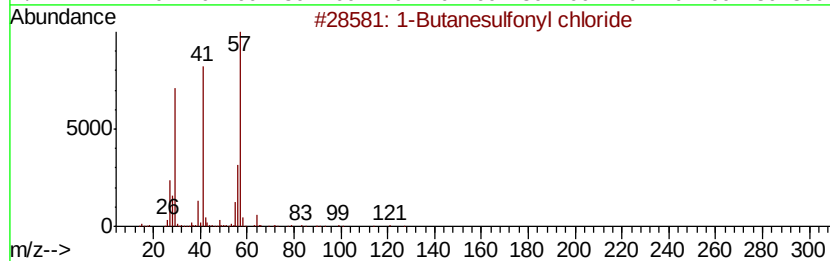
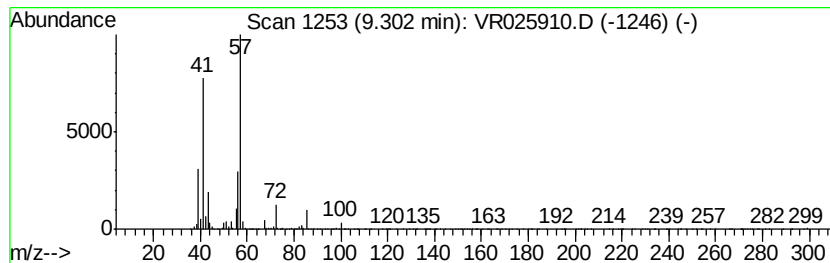
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.30	1.65 ug/L	504042	1,4-Difluorobenzene	8.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
2			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
3			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	37
4			Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	36
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	35



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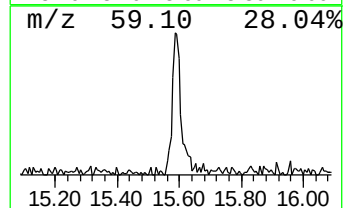
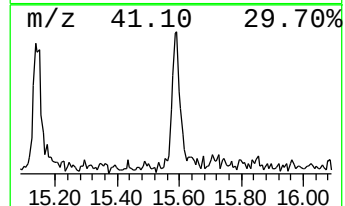
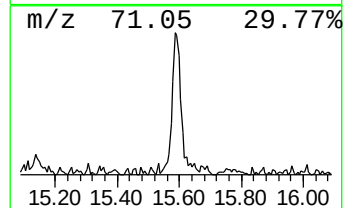
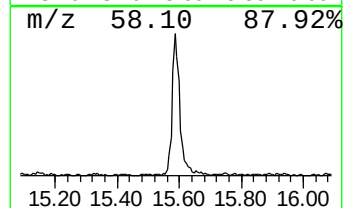
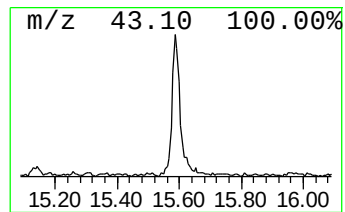
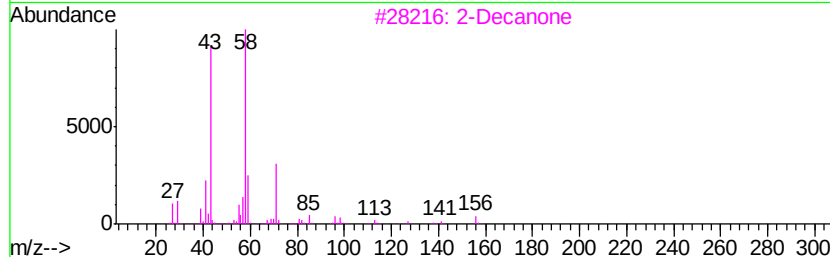
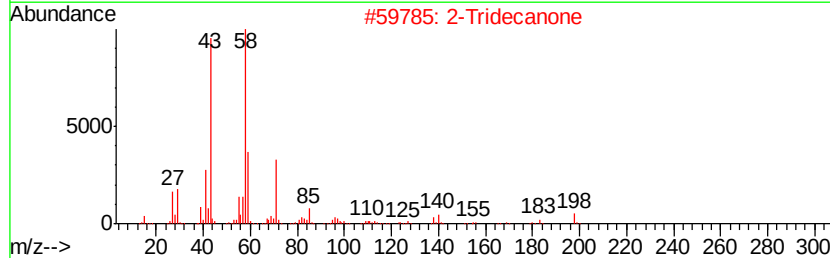
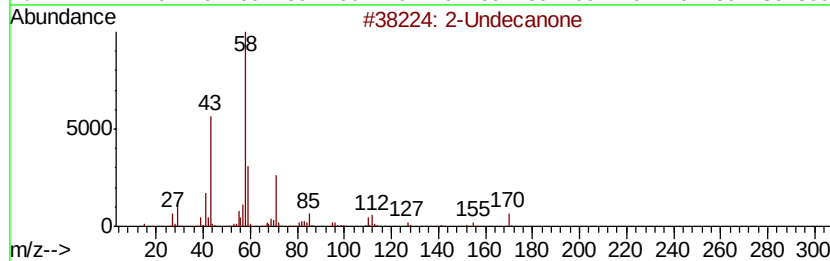
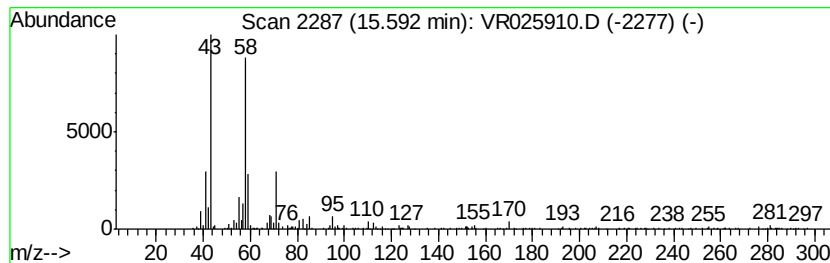
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Undecanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	0.69 ug/L	159757	1,4-Dichlorobenzene-d4	13.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Undecanone	170	C11H22O	000112-12-9	87
2		2-Tridecanone	198	C13H26O	000593-08-8	72
3		2-Decanone	156	C10H20O	000693-54-9	72
4		2-Tridecanone	198	C13H26O	000593-08-8	72
5		Butanimidamide	86	C4H10N2	000107-90-4	64



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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
unknown-01	4.65	0.5	ug/L	156241	1	8.46	1529030	5.0
Propane, 2-methyl...	6.41	2.6	ug/L	809158	1	8.46	1529030	5.0
unknown-02	9.30	1.6	ug/L	504042	1	8.46	1529030	5.0
2-Undecanone	15.59	0.7	ug/L	159757	3	13.22	1160460	5.0