

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_R\DATA\VR122118\
 Data File : VR026284.D
 Acq On : 21 Dec 2018 16:47
 Operator : SY/MD
 Sample : J6468-02
 Misc : 25mL/MSVOA_R/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_R
 ClientSampleId :
 C0JG0

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\SOMRTR121718WMA.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	1.776	13	16	21	rVB4	19423	33660	2.20%	0.228%
2	2.111	61	71	76	rBV	175320	391171	25.62%	2.655%
3	2.628	146	156	167	rBV2	103592	257786	16.88%	1.749%
4	3.607	305	317	328	rBV2	211816	710201	46.52%	4.820%
5	3.705	328	333	343	rVB	46586	126912	8.31%	0.861%
6	4.654	478	489	500	rBV2	49371	191017	12.51%	1.296%
7	6.406	768	777	794	rVB2	299615	944361	61.85%	6.409%
8	6.588	799	807	817	rVV2	70309	212179	13.90%	1.440%
9	6.686	819	823	830	rVB3	11109	26514	1.74%	0.180%
10	7.203	899	908	919	rBV	265393	675246	44.23%	4.583%
11	7.519	949	960	974	rBV4	413059	1172719	76.81%	7.959%
12	7.854	1007	1015	1032	rBV2	523386	1468859	96.21%	9.968%
13	8.462	1107	1115	1124	rBV	807591	1432580	93.83%	9.722%
14	8.900	1179	1187	1196	rBV	329045	630321	41.29%	4.278%
15	9.308	1247	1254	1263	rBV	324640	590251	38.66%	4.006%
16	9.685	1310	1316	1321	rBV	121566	199213	13.05%	1.352%
17	9.971	1356	1363	1370	rBV	819905	1256818	82.32%	8.529%
18	10.038	1370	1374	1377	rVB5	10272	19781	1.30%	0.134%
19	10.239	1402	1407	1412	rBV	58930	92965	6.09%	0.631%
20	10.385	1427	1431	1436	rBV2	12170	20119	1.32%	0.137%
21	10.591	1460	1465	1479	rBV	290667	473776	31.03%	3.215%
22	10.737	1486	1489	1495	rVB6	13671	22260	1.46%	0.151%
23	11.291	1573	1580	1587	rBV	1019862	1526745	100.00%	10.361%
24	12.015	1695	1699	1703	rVB7	14458	20835	1.36%	0.141%
25	12.118	1710	1716	1721	rBV4	12692	20197	1.32%	0.137%
26	12.307	1741	1747	1751	rBV3	27927	45637	2.99%	0.310%
27	12.362	1751	1756	1766	rVB	119458	186884	12.24%	1.268%
28	13.226	1891	1898	1906	rBV	751384	1034338	67.75%	7.020%
29	13.518	1939	1946	1955	rBV	425671	640986	41.98%	4.350%
30	13.706	1973	1977	1982	rBV	14851	23043	1.51%	0.156%
31	13.767	1982	1987	1992	rVB2	20031	34259	2.24%	0.232%
32	13.901	2006	2009	2013	rBV5	10725	18765	1.23%	0.127%
33	14.010	2022	2027	2032	rVB9	13168	23491	1.54%	0.159%
34	15.142	2207	2213	2224	rBV4	46688	98831	6.47%	0.671%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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	2282	2286	2294	rBV2	25615	51031	3.34%	0.346%
36	16.438	2417	2426	2433	rBV9	27576	61325	4.02%	0.416%

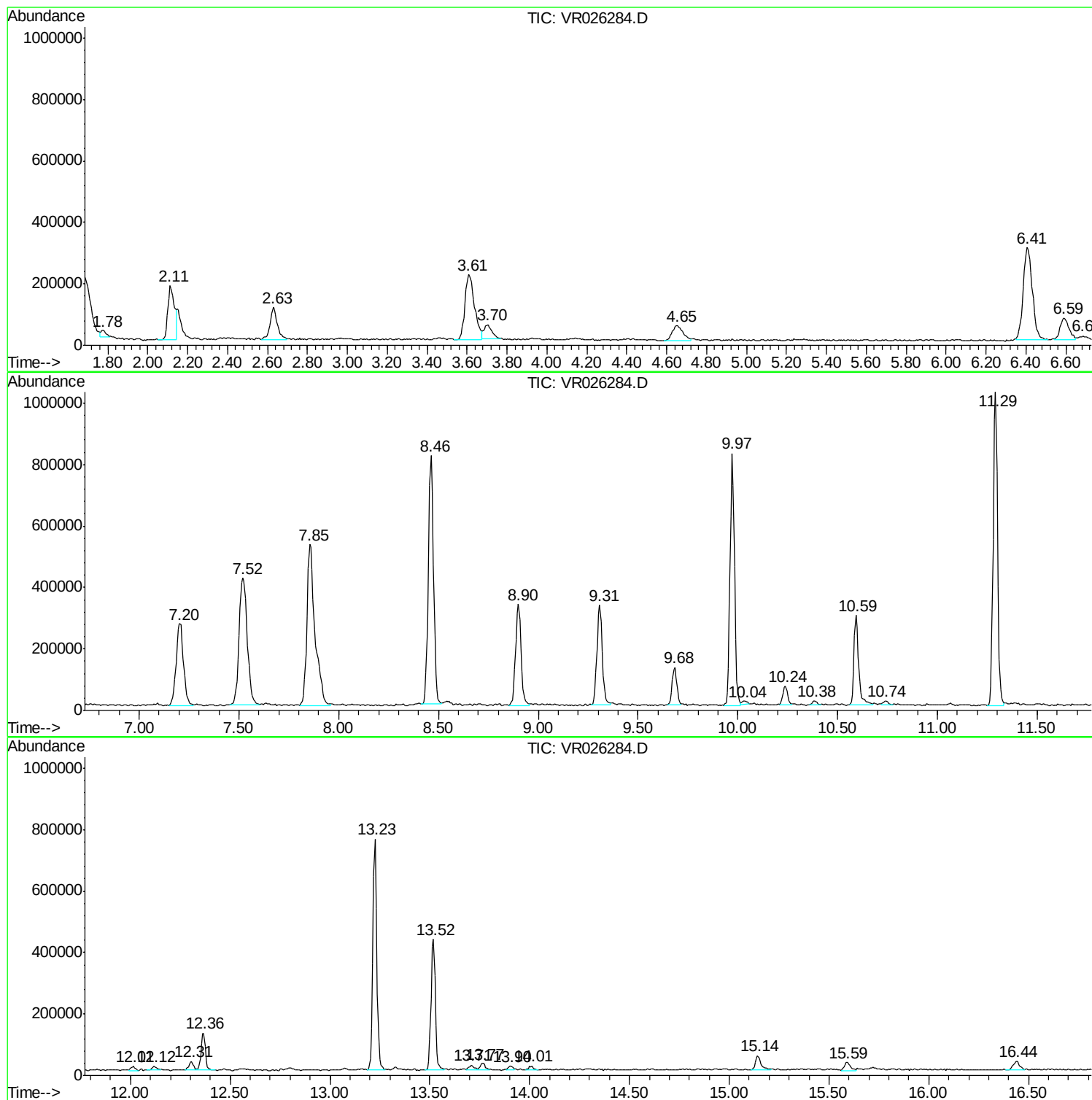
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Quant Title : TRACE VOA SOM01.0

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



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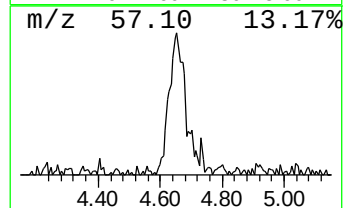
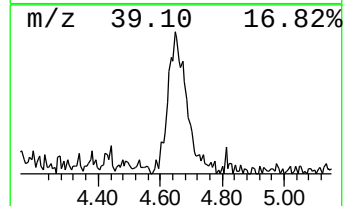
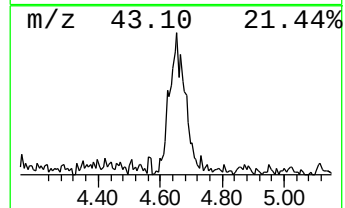
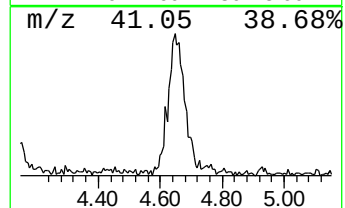
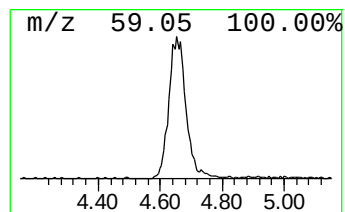
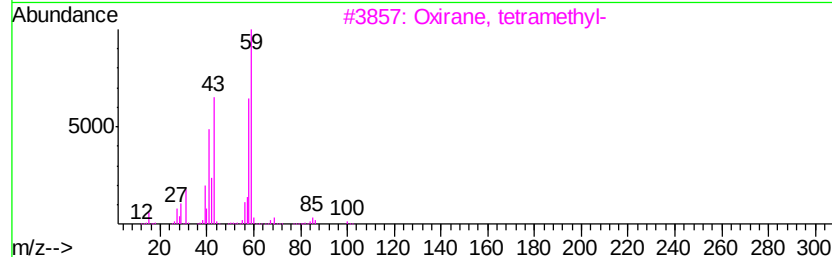
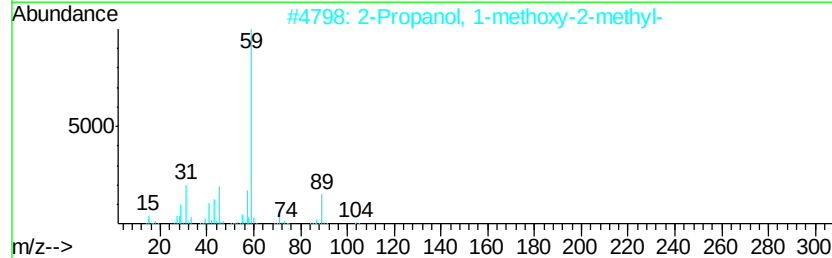
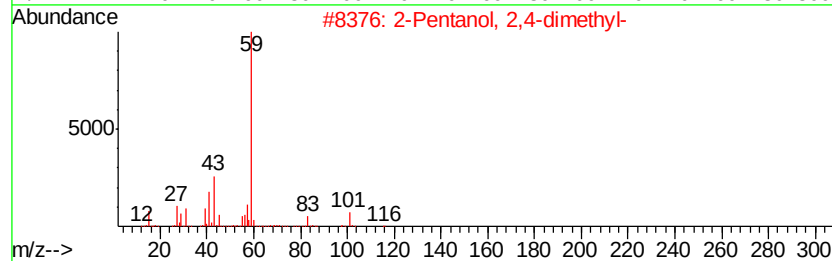
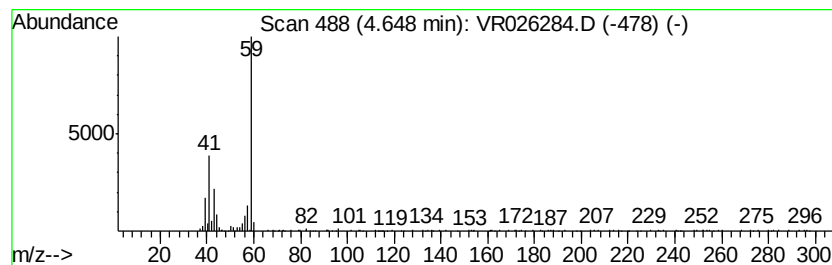
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanol, 2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.65	0.67 ug/L	191017	1,4-Difluorobenzene	8.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	56
2			2-Propanol, 1-methoxy-2-methyl-	104	C5H12O2	003587-64-2	56
3			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	40
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	40
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	40



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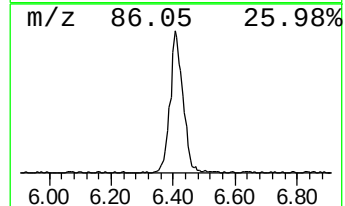
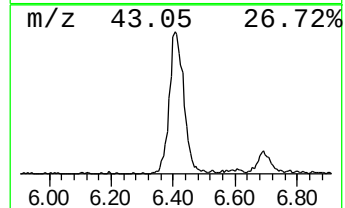
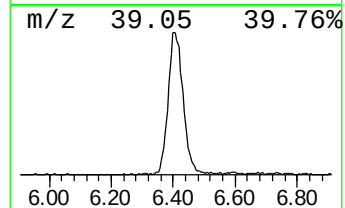
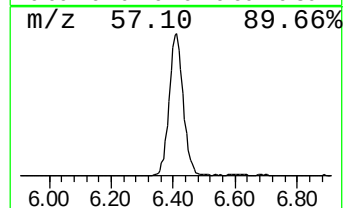
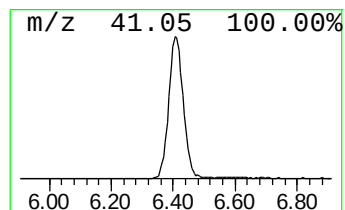
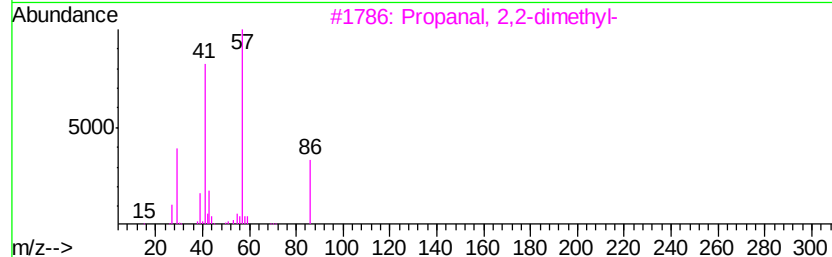
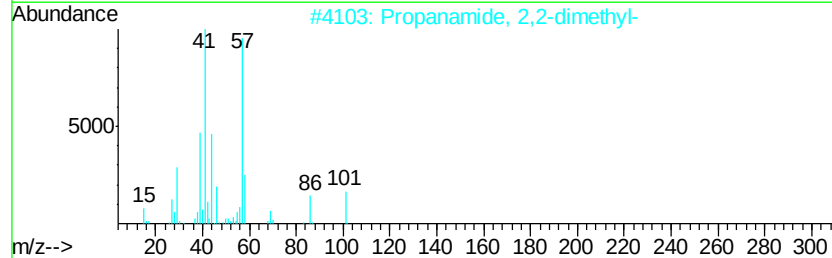
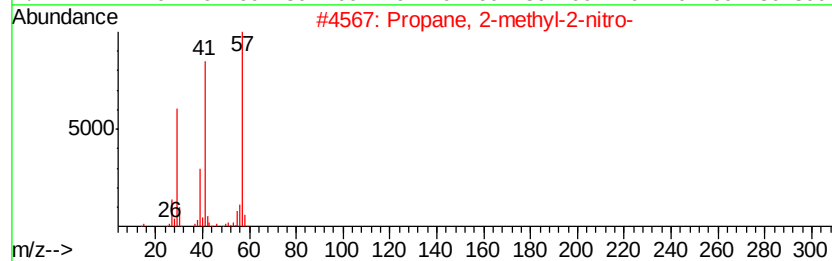
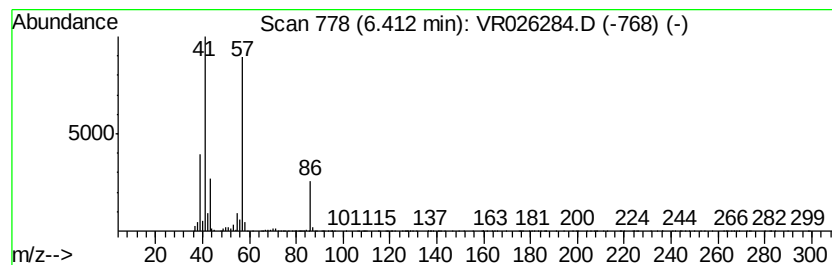
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	3.30 ug/L	944361	1,4-Difluorobenzene	8.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Propane, 2-methyl-2-nitro-	103 C4H9NO2	000594-70-7	53
2	Propanamide, 2,2-dimethyl-	101 C5H11NO	000754-10-9	50
3	Propanal, 2,2-dimethyl-	86 C5H10O	000630-19-3	43
4	4,4-Dimethyl-3-oxopentanenitrile	125 C7H11NO	059997-51-2	42
5	1,1-Diisobutoxy-butane	202 C12H26O2	013002-16-9	36



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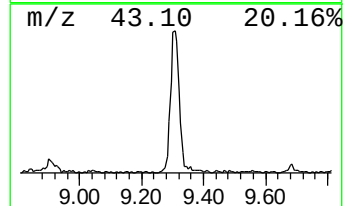
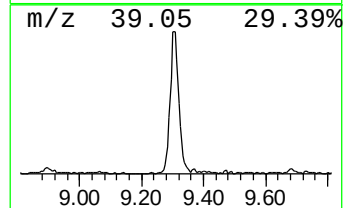
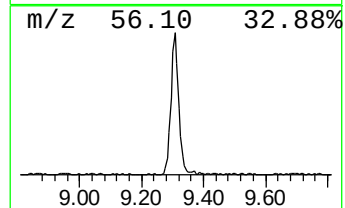
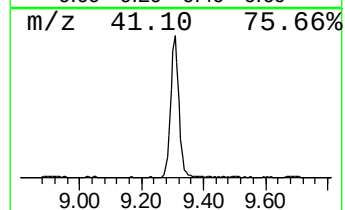
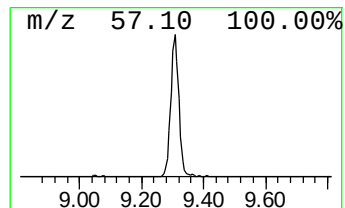
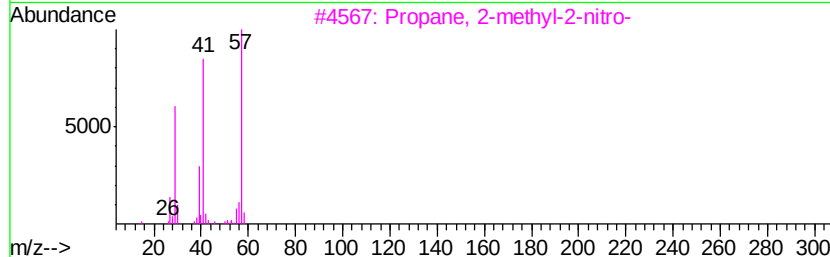
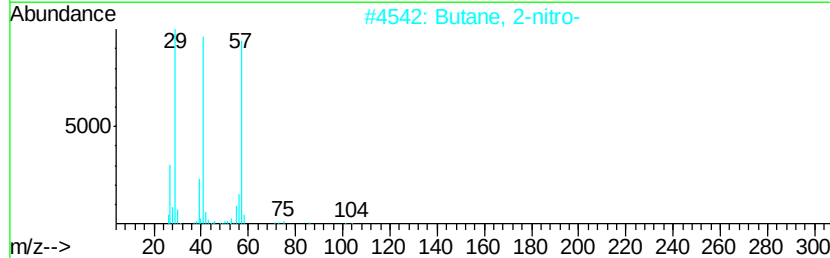
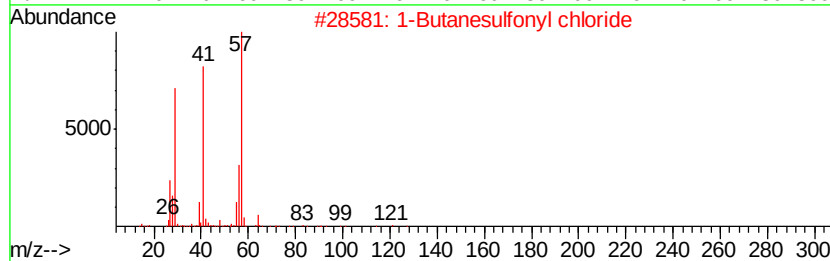
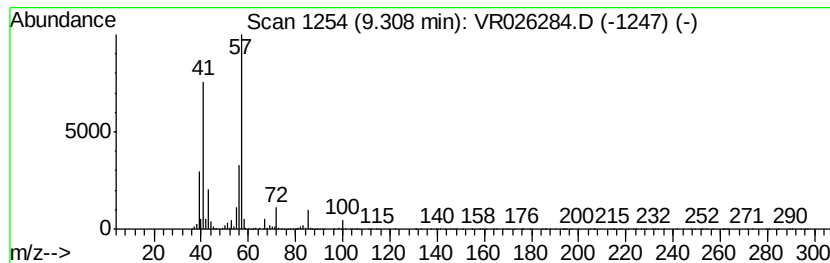
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.31	2.06 ug/L	590251	1,4-Difluorobenzene	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
2		Butane, 2-nitro-	103	C4H9NO2	000600-24-8	37
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	37
4		1-Butene	56	C4H8	000106-98-9	35
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanol, 2,4-d...	4.65	0.7	ug/L	191017	1	8.46	1432580	5.0
Propane, 2-methyl...	6.41	3.3	ug/L	944361	1	8.46	1432580	5.0
unknown-01	9.31	2.1	ug/L	590251	1	8.46	1432580	5.0