

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_R\DATA\VR122118\
 Data File : VR026285.D
 Acq On : 21 Dec 2018 17:20
 Operator : SY/MD
 Sample : J6468-22
 Misc : 25mL/MSVOA_R/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_R
 ClientSampleId :
 C0JJ1

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	2.117	65	72	74	rBV	90019	178166	10.27%	1.169%
2	2.147	74	77	89	rVB	105921	223377	12.88%	1.466%
3	2.628	146	156	166	rBV2	116675	283251	16.33%	1.859%
4	3.607	306	317	328	rBV2	231039	827751	47.73%	5.433%
5	3.705	329	333	342	rVB	45878	111892	6.45%	0.734%
6	4.660	479	490	501	rBV4	48144	178460	10.29%	1.171%
7	6.406	766	777	792	rBV2	258303	835551	48.18%	5.484%
8	6.588	795	807	819	rBV	87685	273826	15.79%	1.797%
9	7.203	896	908	920	rBV	306615	795407	45.87%	5.221%
10	7.519	949	960	975	rBV2	185513	535495	30.88%	3.515%
11	7.860	1006	1016	1030	rBV2	626569	1734114	100.00%	11.382%
12	8.462	1107	1115	1125	rBV	812738	1472893	84.94%	9.667%
13	8.900	1179	1187	1196	rBV	390198	751516	43.34%	4.933%
14	9.308	1245	1254	1264	rBV	290551	541119	31.20%	3.552%
15	9.685	1309	1316	1326	rBV	145502	260052	15.00%	1.707%
16	9.971	1354	1363	1372	rBV	976930	1521461	87.74%	9.986%
17	10.239	1402	1407	1414	rBV	75202	122878	7.09%	0.807%
18	10.385	1426	1431	1436	rVB3	15155	22913	1.32%	0.150%
19	10.591	1458	1465	1472	rBV	364562	569869	32.86%	3.740%
20	10.737	1486	1489	1495	rVB8	12687	22202	1.28%	0.146%
21	11.291	1573	1580	1588	rBV	1016151	1529809	88.22%	10.041%
22	12.015	1695	1699	1706	rBV10	13577	22662	1.31%	0.149%
23	12.118	1711	1716	1720	rBV2	13874	20579	1.19%	0.135%
24	12.301	1740	1746	1751	rBV2	23702	38607	2.23%	0.253%
25	12.362	1751	1756	1763	rVB	140837	220375	12.71%	1.446%
26	13.226	1892	1898	1908	rVV	755045	1034395	59.65%	6.789%
27	13.518	1939	1946	1957	rBV	510481	762066	43.95%	5.002%
28	13.761	1982	1986	1993	rVB3	16676	30433	1.75%	0.200%
29	13.901	2004	2009	2015	rBV3	11954	21899	1.26%	0.144%
30	14.004	2022	2026	2032	rVB9	12822	27553	1.59%	0.181%
31	15.142	2207	2213	2221	rBV4	51712	96978	5.59%	0.637%
32	15.586	2281	2286	2292	rBV2	39079	73375	4.23%	0.482%
33	15.720	2304	2308	2313	rVB8	10805	19852	1.14%	0.130%
34	16.438	2419	2426	2433	rBV9	33488	74787	4.31%	0.491%

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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

Method : Z:\VOASRV\HPCHEM1\MSVOA_R\METHODS\SOMRTR121718WMA.M
Title : TRACE VOA SOM01.0

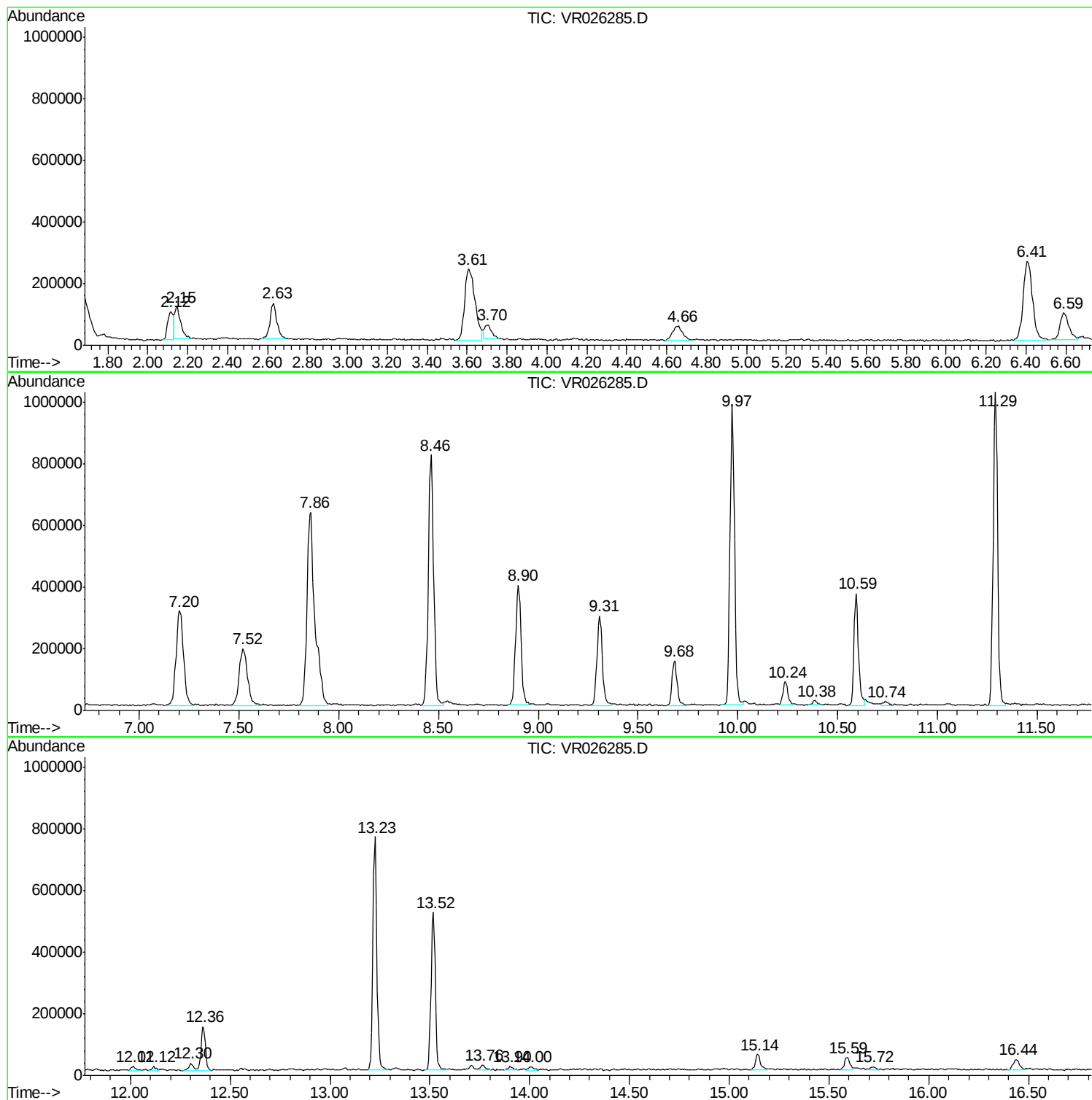
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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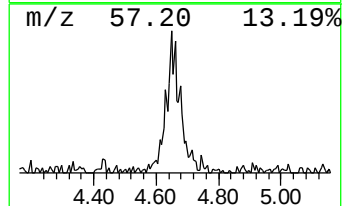
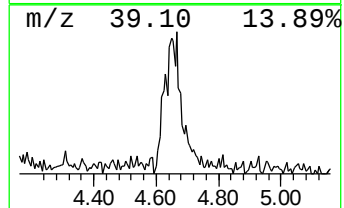
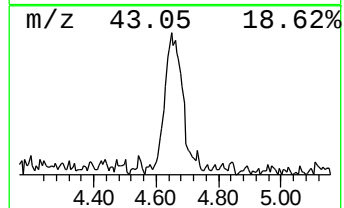
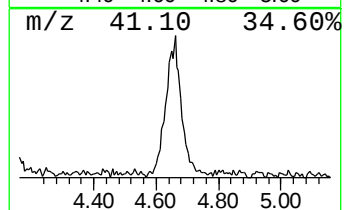
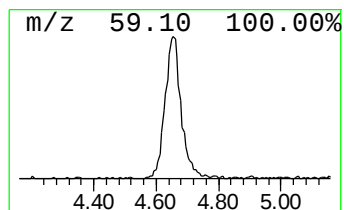
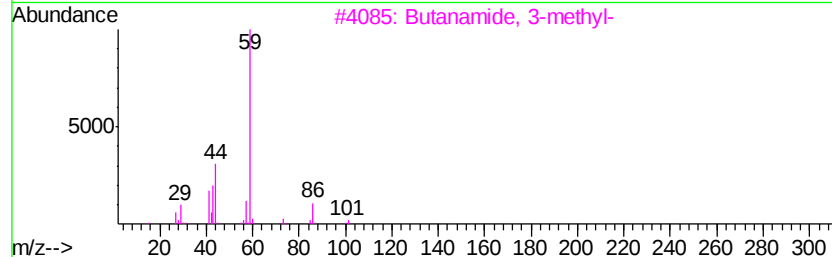
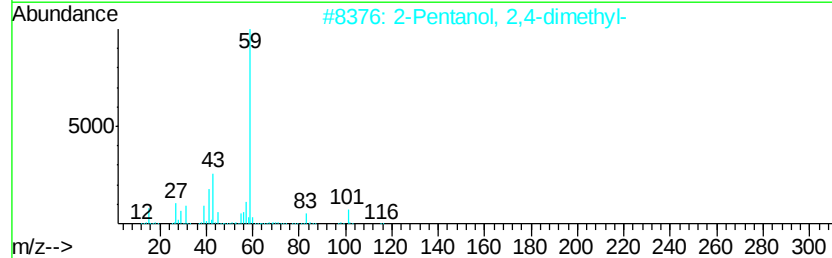
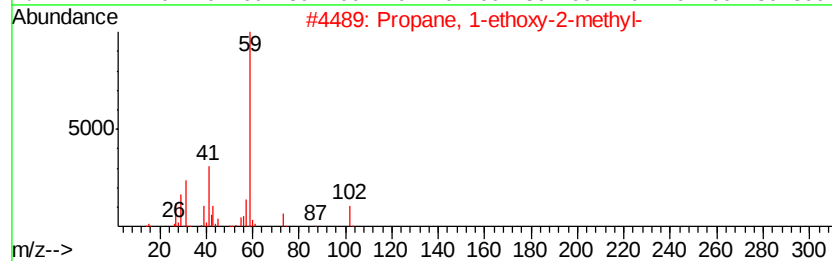
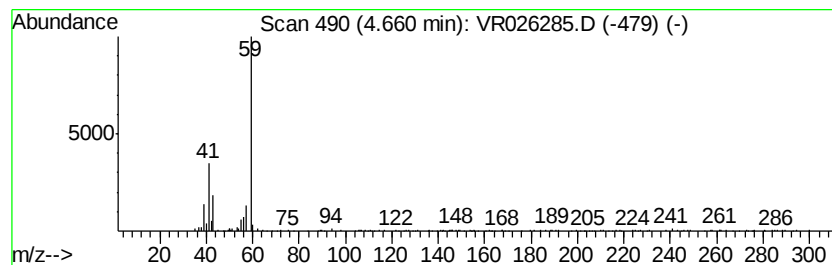
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 1-ethoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	0.61 ug/L	178460	1,4-Difluorobenzene	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	56
2		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40
3		Butanamide, 3-methyl-	101	C5H11NO	000541-46-8	40
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	40



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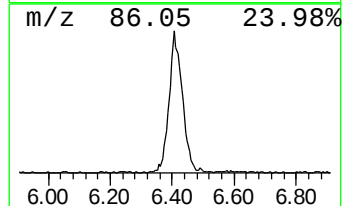
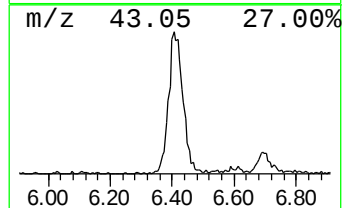
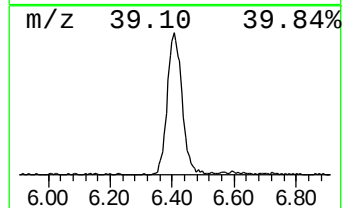
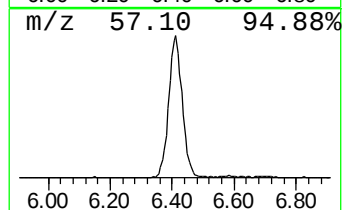
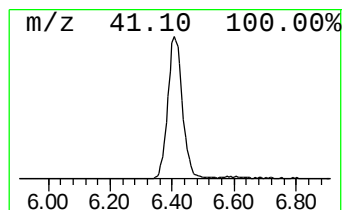
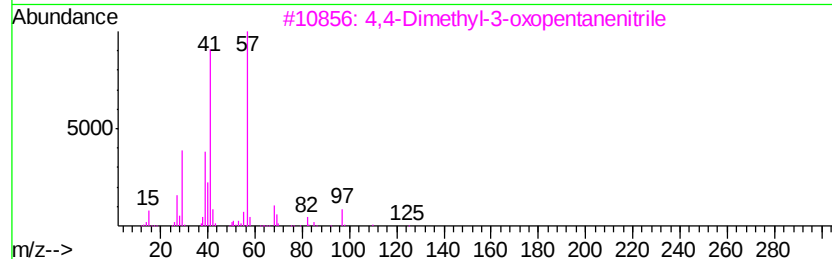
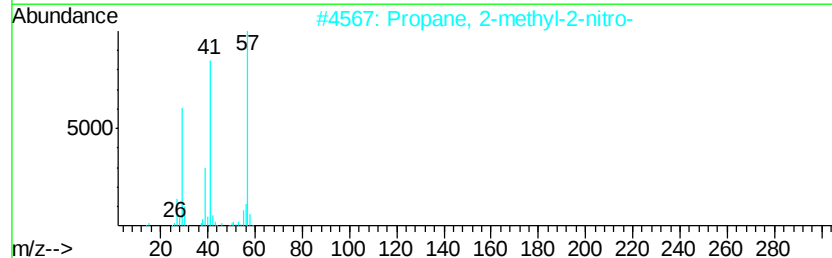
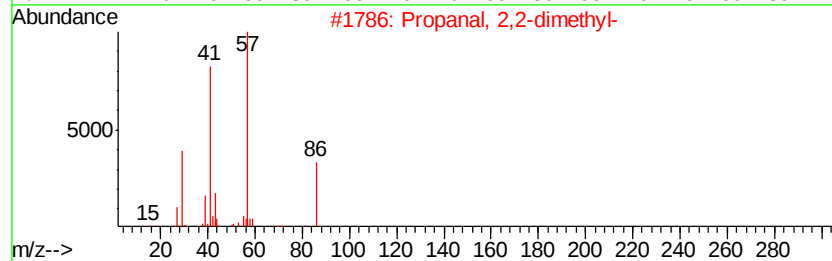
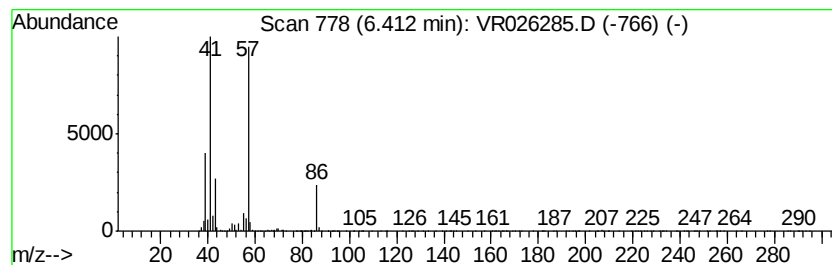
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.41	2.84 ug/L	835551	1,4-Difluorobenzene	8.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	43
2		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	42
3		4,4-Dimethyl-3-oxopentanenitrile	125	C7H11NO	059997-51-2	42
4		1,1-Diisobutoxy-butane	202	C12H26O2	013002-16-9	38
5		n-Hexane	86	C6H14	000110-54-3	35



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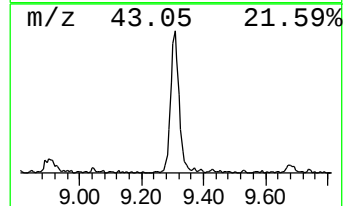
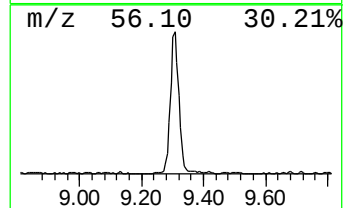
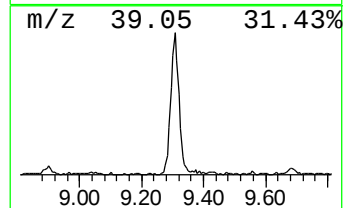
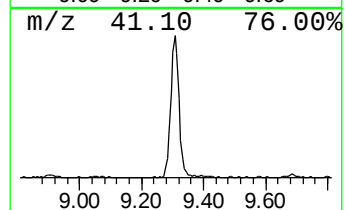
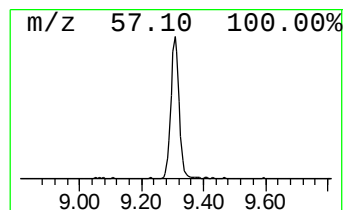
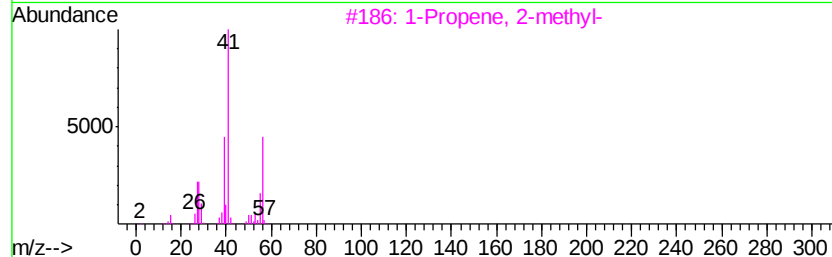
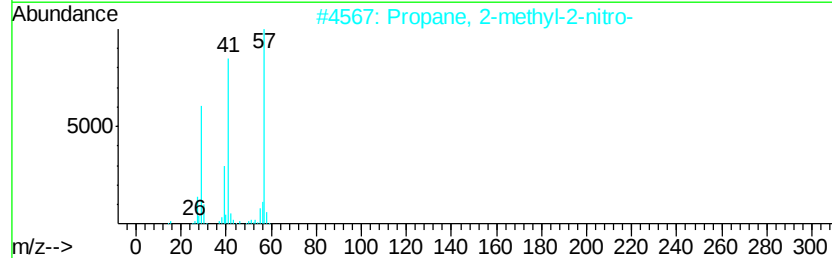
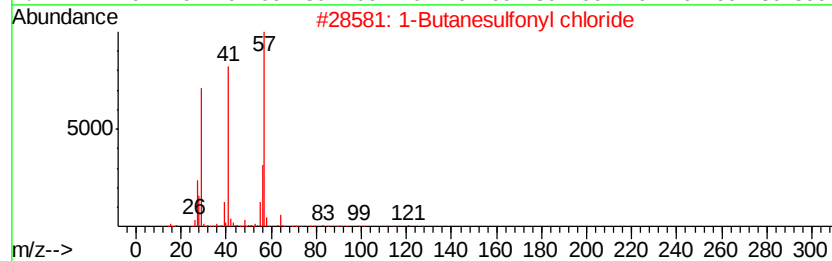
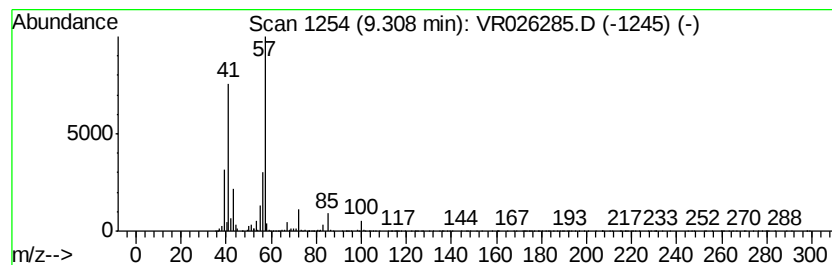
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.31	1.84 ug/L	541119	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		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
3		1-Propene, 2-methyl-	56	C4H8	000115-11-7	35
4		2-Butene, (Z)-	56	C4H8	000590-18-1	35
5		2-Butene, (E)-	56	C4H8	000624-64-6	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1-ethoxy...	4.66	0.6	ug/L	178460	1	8.46	1472890	5.0
unknown-01	6.41	2.8	ug/L	835551	1	8.46	1472890	5.0
unknown-02	9.31	1.8	ug/L	541119	1	8.46	1472890	5.0