

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074530.D
 Acq On : 17 Sep 2022 00:06
 Operator : JC\MD
 Sample : N4549-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-47

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

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M

Title : SW846 8260

Signal : TIC: VN074530.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	59	rBV	230575	438496	21.57%	3.244%
2	2.687	131	136	137	rBV	55609	77919	3.83%	0.576%
3	5.263	559	574	575	rBV4	28092	65459	3.22%	0.484%
4	5.281	575	577	588	rVB2	29134	59721	2.94%	0.442%
5	5.528	609	619	633	rVB4	48474	180788	8.89%	1.337%
6	6.410	761	769	772	rBV4	12691	31745	1.56%	0.235%
7	7.228	900	908	920	rVB2	44278	129848	6.39%	0.961%
8	7.951	1022	1031	1036	rBV	279140	658395	32.39%	4.871%
9	8.016	1036	1042	1051	rVB	430288	975795	48.01%	7.219%
10	8.369	1093	1102	1113	rBV	331727	748223	36.81%	5.535%
11	8.904	1183	1193	1202	rBV	712559	1460964	71.88%	10.808%
12	10.139	1395	1403	1414	rBV2	39039	89441	4.40%	0.662%
13	10.380	1434	1444	1453	rBV	1121287	2032506	100.00%	15.037%
14	10.580	1471	1478	1484	rVV2	182061	325256	16.00%	2.406%
15	10.657	1485	1491	1499	rVB2	196414	343225	16.89%	2.539%
16	11.027	1543	1554	1558	rBV6	13017	25344	1.25%	0.187%
17	11.527	1632	1639	1646	rBV3	16293	34179	1.68%	0.253%
18	11.686	1654	1666	1677	rBV	1147099	1991087	97.96%	14.730%
19	11.804	1681	1686	1691	rVB6	9990	20709	1.02%	0.153%
20	12.516	1803	1807	1814	rVB4	13645	22356	1.10%	0.165%
21	12.674	1826	1834	1844	rBV	926986	1548925	76.21%	11.459%
22	13.615	1987	1994	2002	rBV	1123828	1862939	91.66%	13.782%
23	13.710	2008	2010	2016	rVB5	18476	27934	1.37%	0.207%
24	13.945	2043	2050	2055	rVB8	20329	36569	1.80%	0.271%
25	14.080	2070	2073	2080	rVB8	16384	29062	1.43%	0.215%
26	14.268	2097	2105	2108	rBV9	20319	53253	2.62%	0.394%
27	14.404	2124	2128	2132	rBV5	14853	21974	1.08%	0.163%
28	14.762	2183	2189	2194	rBV9	12753	26428	1.30%	0.196%
29	14.874	2202	2208	2215	rVB10	14166	24701	1.22%	0.183%
30	15.127	2246	2251	2260	rBV10	17217	40273	1.98%	0.298%
31	15.498	2309	2314	2317	rBV7	16310	26107	1.28%	0.193%
32	15.574	2320	2327	2332	rBV5	22479	45732	2.25%	0.338%
33	16.551	2487	2493	2495	rBV7	10278	22122	1.09%	0.164%
34	16.739	2519	2525	2531	rVB7	15353	39643	1.95%	0.293%

Sum of corrected areas: 13517118

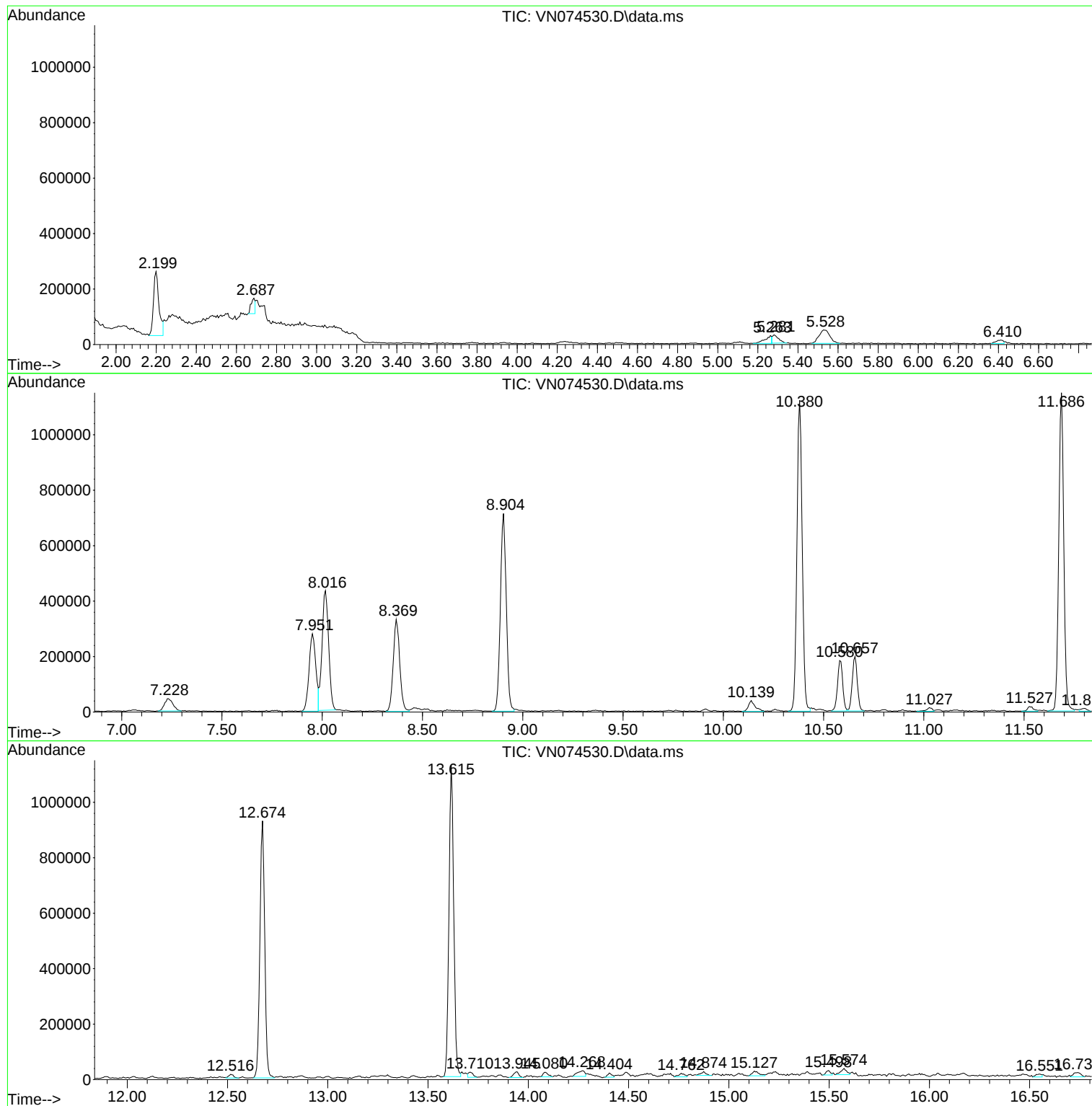
Instrument :
MSVOA_N
ClientSampleId :
MW-47

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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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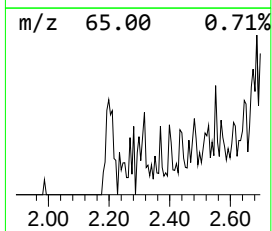
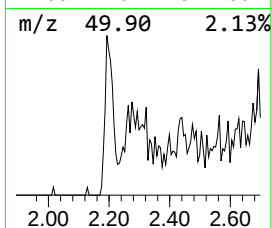
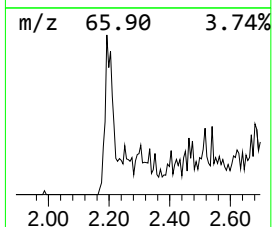
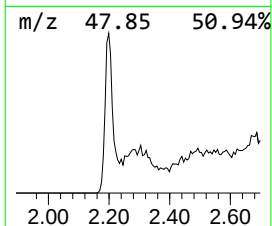
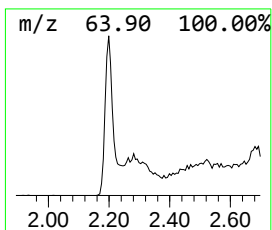
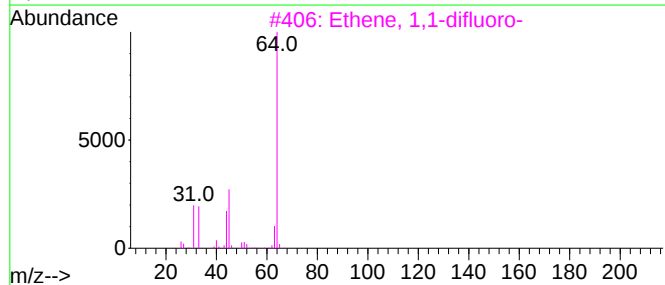
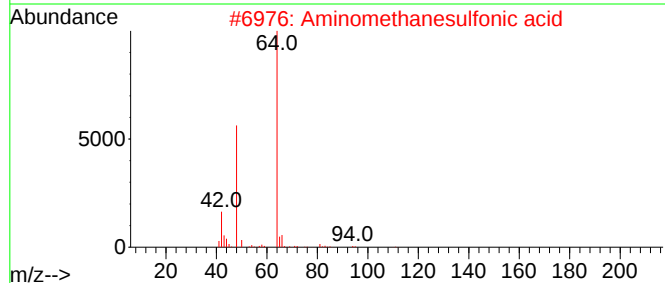
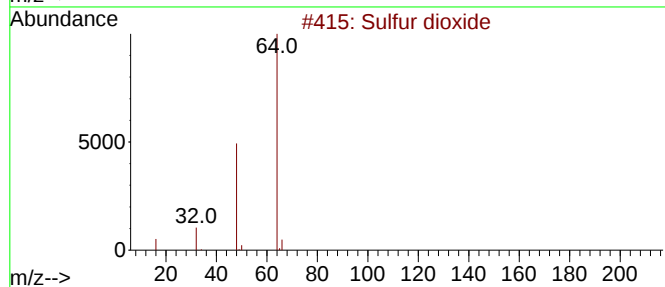
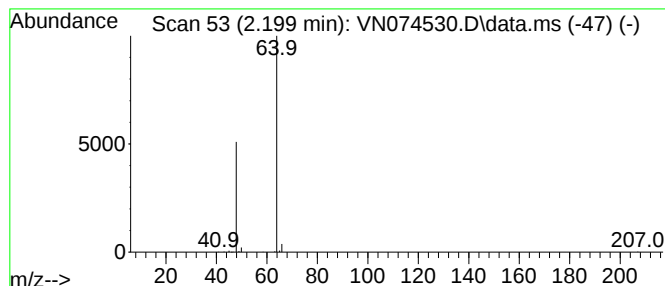
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	22.47 ug/l	438496	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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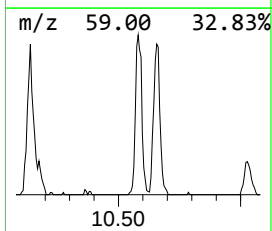
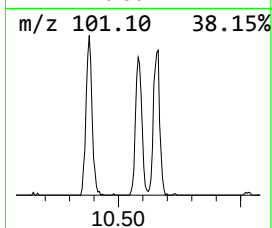
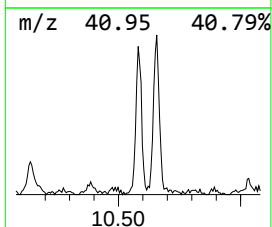
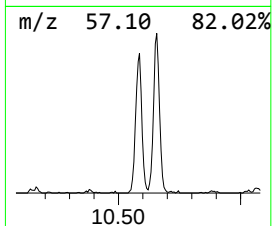
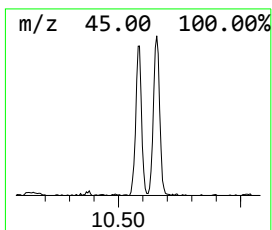
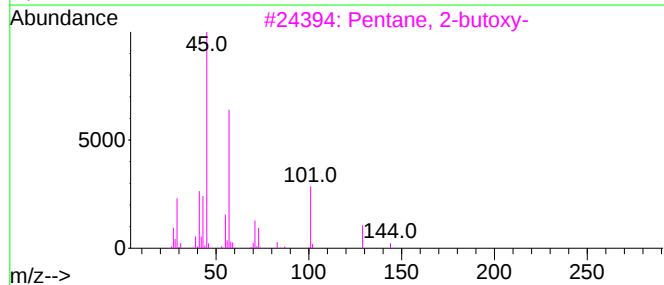
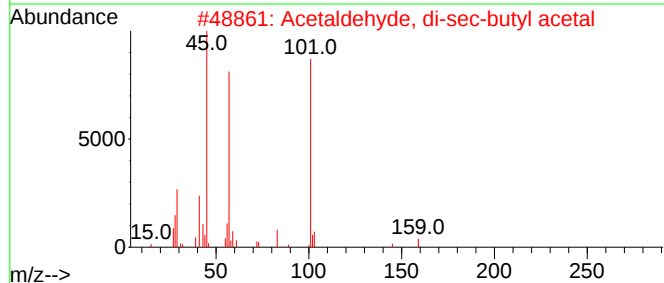
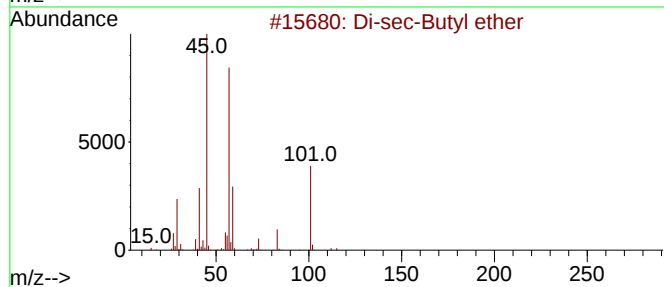
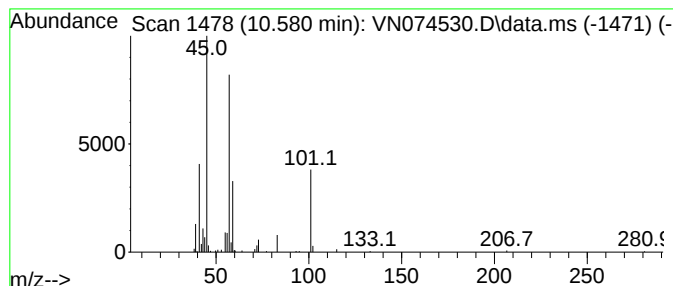
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Peak Number 3 Di-sec-Butyl ether Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	8.17 ug/l	325256	Chlorobenzene-d5	11.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2			Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	72
3			Pentane, 2-butoxy-	144	C9H20O	062238-02-2	72
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			Butane, 1,1'-[ethylidenebis(oxy)]...	174	C10H22O2	000871-22-7	38



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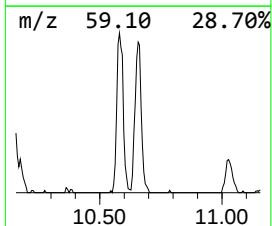
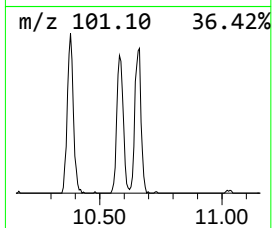
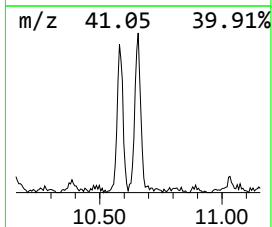
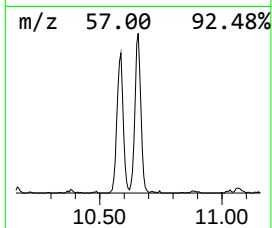
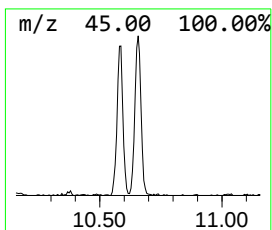
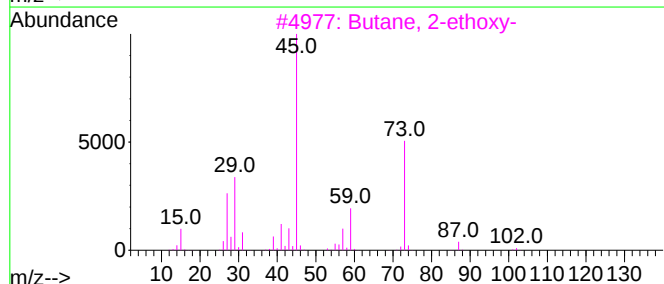
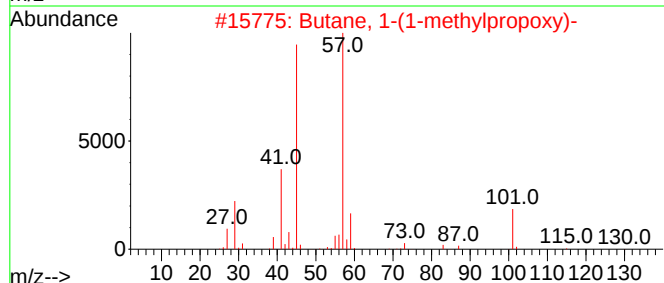
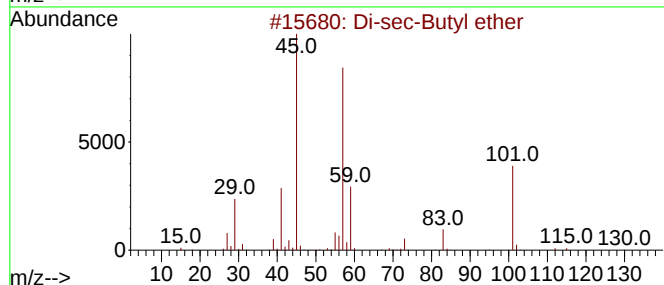
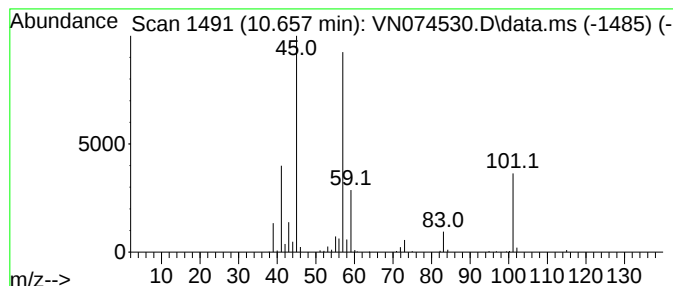
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 1-(1-methylpropoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.657	8.62 ug/l	343225	Chlorobenzene-d5	11.686	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	72
3	Butane, 2-ethoxy-	102	C6H14O	002679-87-0	36
4	Boronic acid, ethyl-, diethyl ester	130	C6H15B02	053907-92-9	36
5	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	33



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ALS Vial : 36 Sample Multiplier: 1

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	22.5	ug/l	438496	1	8.016	975795	50.0
Di-sec-Butyl ether	10.580	8.2	ug/l	325256	3	11.686	1991090	50.0
Butane, 1-(1-me...	10.657	8.6	ug/l	343225	3	11.686	1991090	50.0