

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN080222\
 Data File : VN073692.D
 Acq On : 02 Aug 2022 17:15
 Operator : JC\MD
 Sample : N3971-18
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-26R

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\82N072822W.M
 Title : SW846 8260

Signal : TIC: VN073692.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	47	58	62	rBV5	18385	45068	2.61%	0.393%
2	2.328	66	75	79	rBV2	45255	148311	8.57%	1.293%
3	2.399	82	87	93	rVV2	60184	106347	6.15%	0.927%
4	2.699	134	138	150	rVB5	30927	90125	5.21%	0.786%
5	3.081	196	203	217	rVB	139612	336134	19.43%	2.931%
6	4.234	392	399	410	rVB2	19211	57977	3.35%	0.506%
7	4.510	437	446	458	rBV	55401	177982	10.29%	1.552%
8	4.998	513	529	539	rBV3	21263	83146	4.81%	0.725%
9	7.339	920	927	937	rBV2	76757	187852	10.86%	1.638%
10	7.957	1019	1032	1037	rBV	267926	667529	38.58%	5.821%
11	8.016	1037	1042	1054	rVB	453454	1006620	58.19%	8.778%
12	8.375	1092	1103	1117	rBV	267501	636307	36.78%	5.549%
13	8.904	1184	1193	1206	rBV	642820	1325824	76.64%	11.561%
14	10.380	1435	1444	1459	rBV	953267	1730028	100.00%	15.086%
15	11.233	1582	1589	1601	rBV2	52646	102255	5.91%	0.892%
16	11.686	1654	1666	1681	rBV	945522	1662783	96.11%	14.499%
17	12.674	1826	1834	1844	rBV	774002	1285367	74.30%	11.208%
18	13.616	1985	1994	2004	rBV	982054	1600725	92.53%	13.958%
19	13.710	2004	2010	2019	rVB	130790	217692	12.58%	1.898%

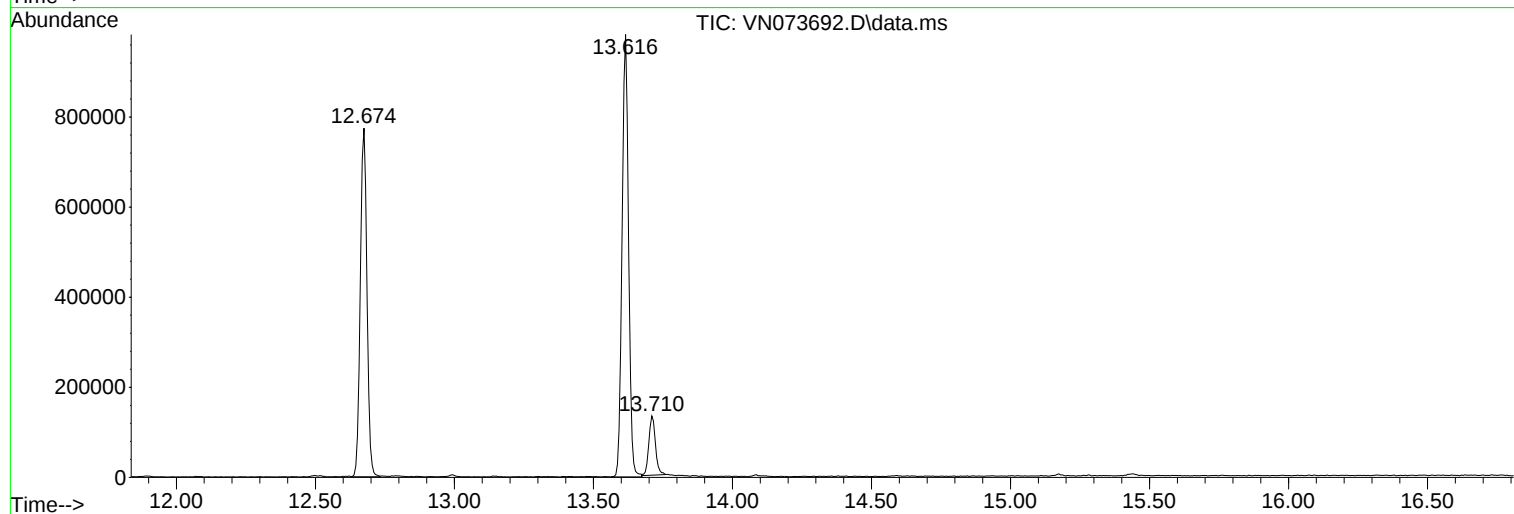
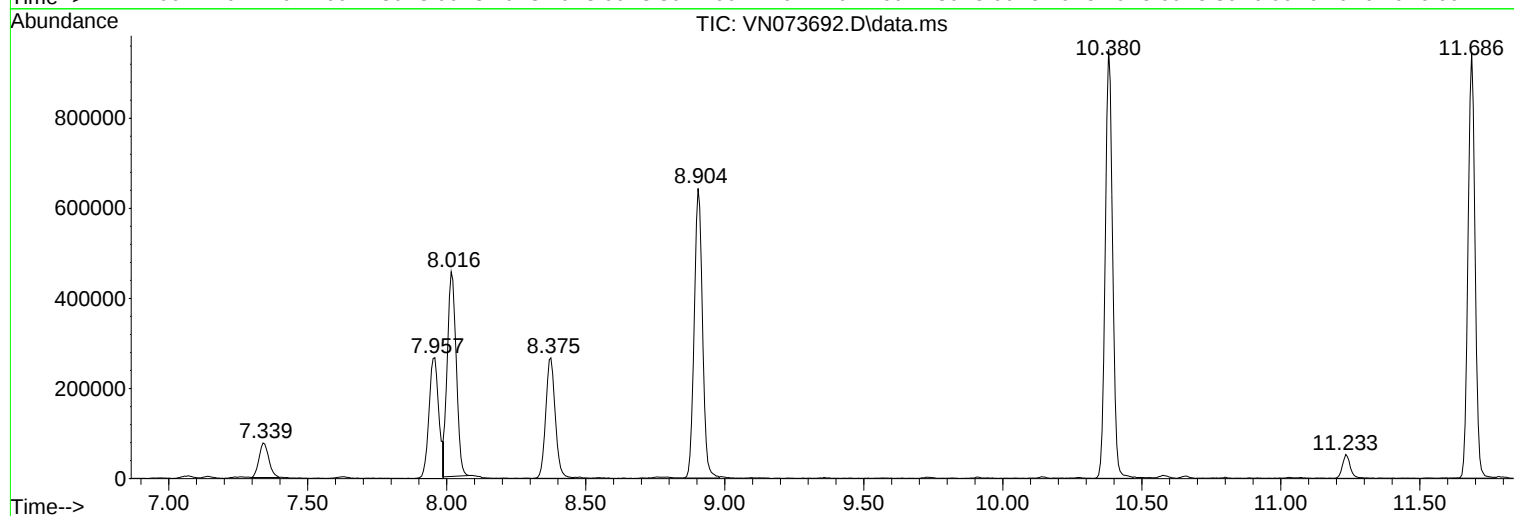
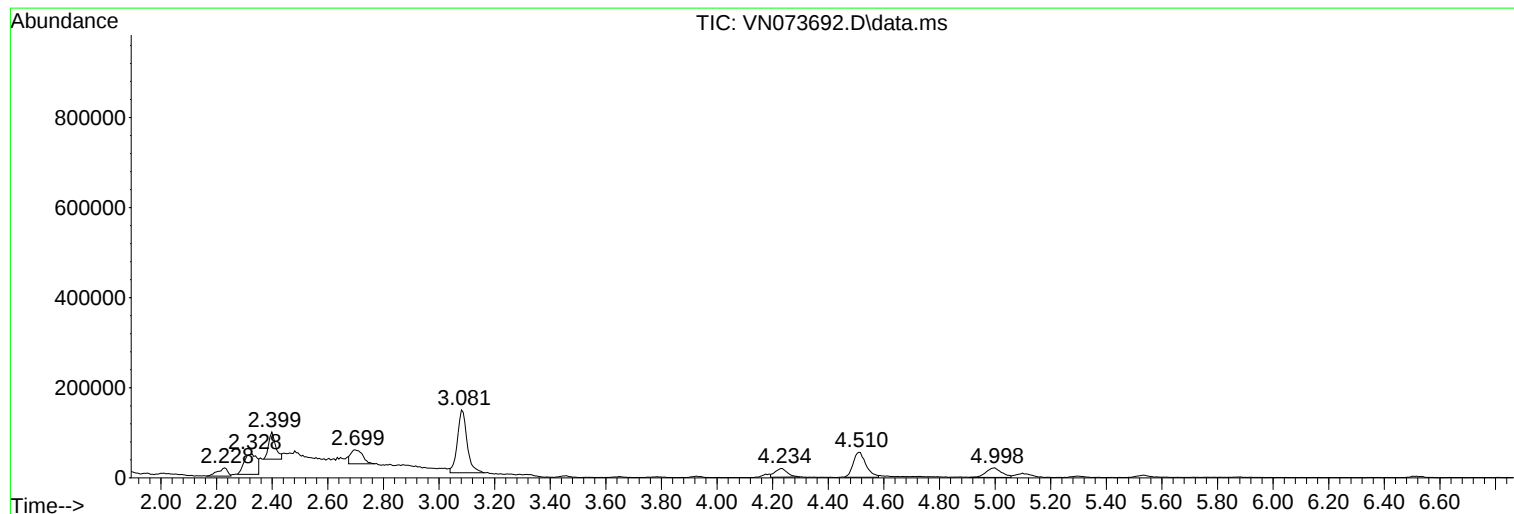
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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



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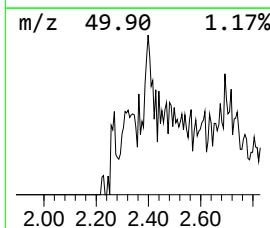
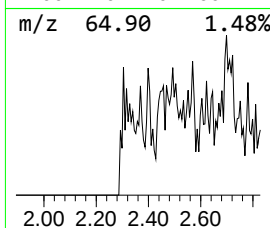
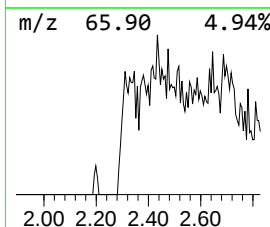
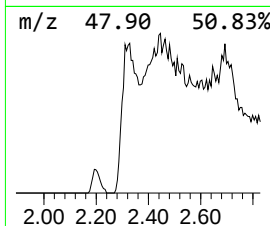
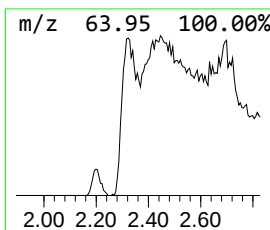
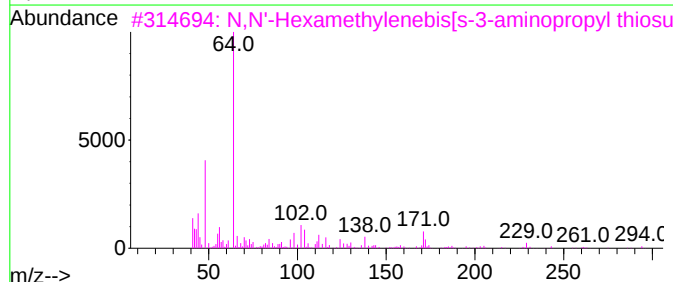
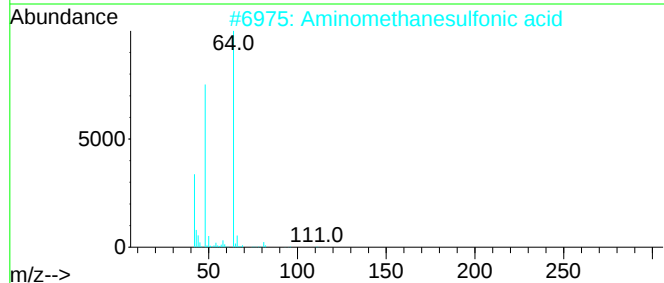
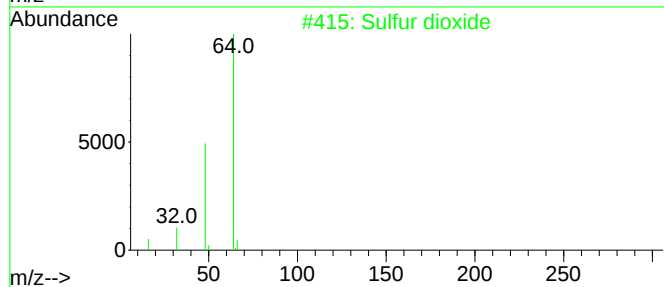
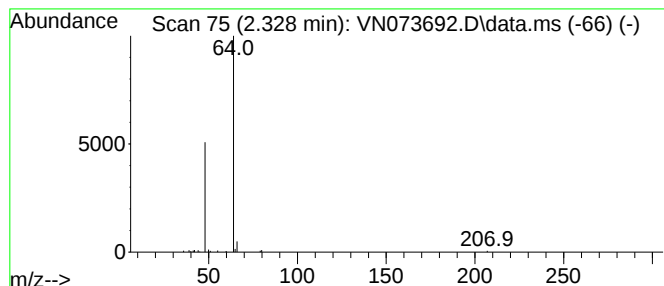
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.328	7.37 ug/l	148311	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	9
4			1,1,1,2,2,3,3,4,4,5,5-Undecaflu...	602	C10F22O2S	1000486-78-5	9
5			S-2-[4-Glutarimidobutylamino]eth...	324	C11H20N2O5S2	031701-78-7	9



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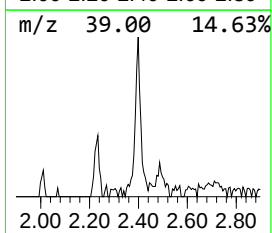
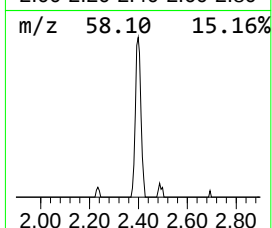
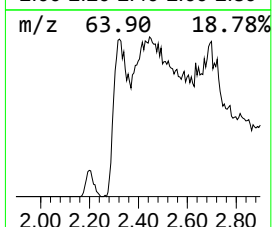
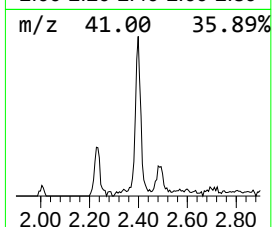
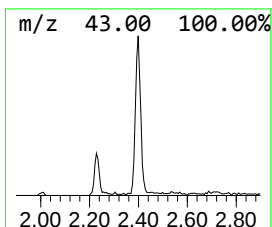
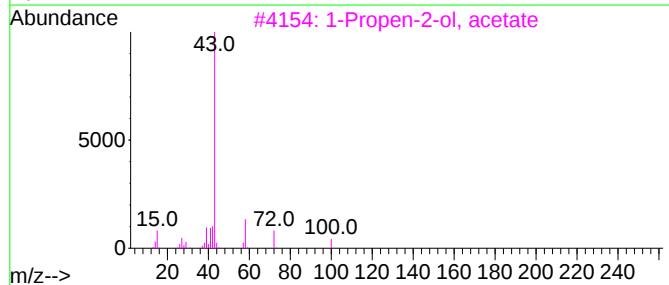
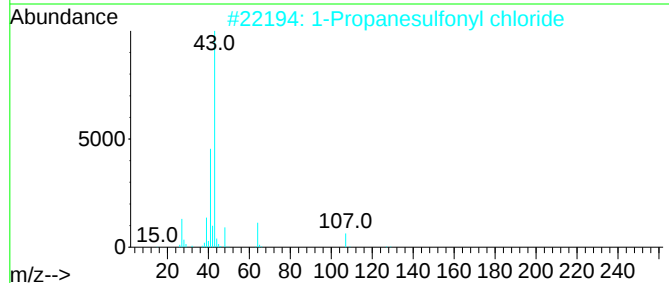
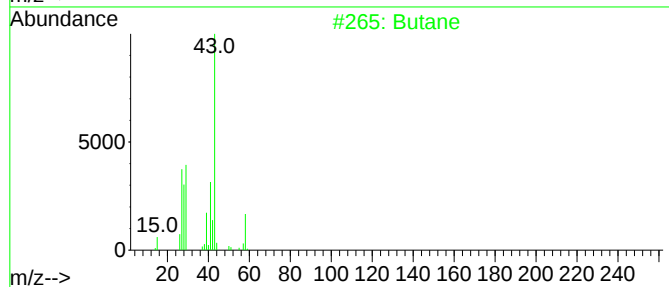
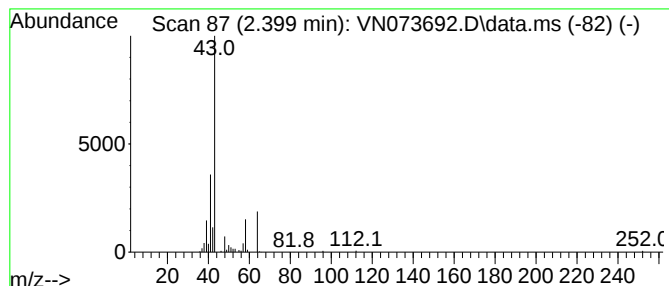
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N072822W.M
Quant Title : SW846 8260

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Peak Number 2 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.399	5.28 ug/l	106347	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	50
2			1-Propanesulfonyl chloride	142	C3H7ClO2S	010147-36-1	33
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4			Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9



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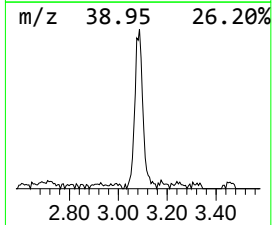
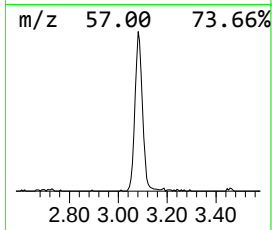
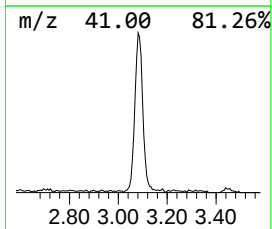
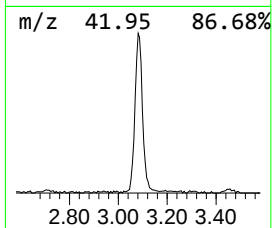
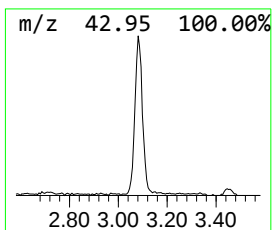
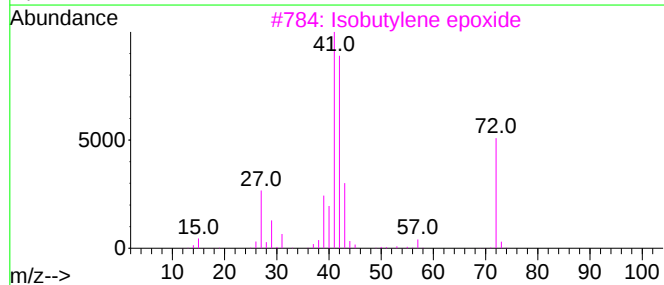
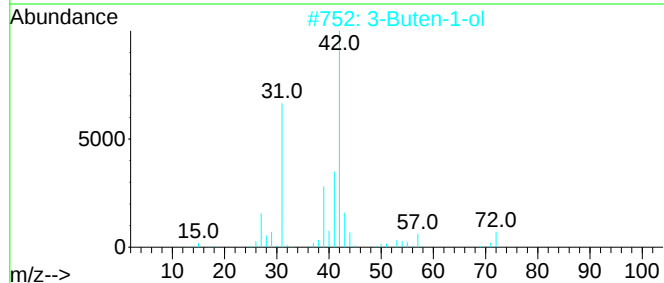
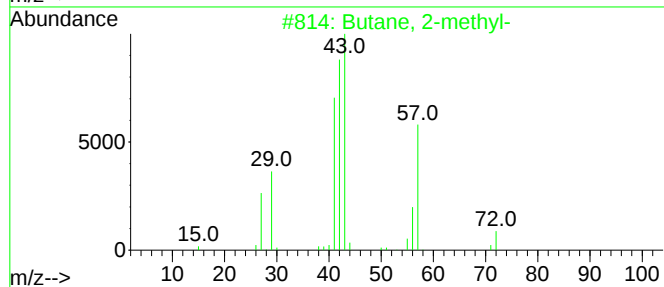
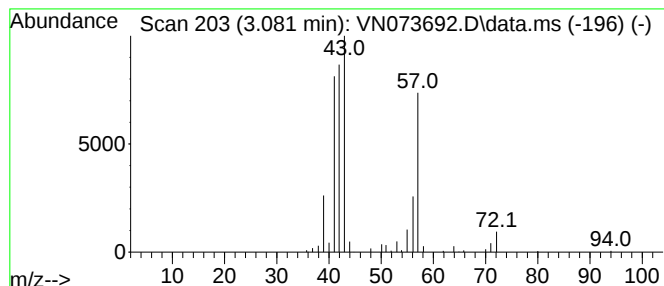
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.081	16.70 ug/l	336134	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			3-Buten-1-ol	72	C4H8O	000627-27-0	43
3			Isobutylene epoxide	72	C4H8O	000558-30-5	40
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	33
5			Pentane	72	C5H12	000109-66-0	28



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ALS Vial : 18 Sample Multiplier: 1

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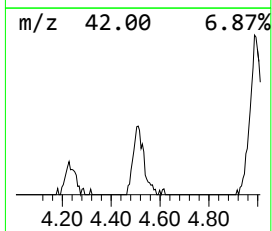
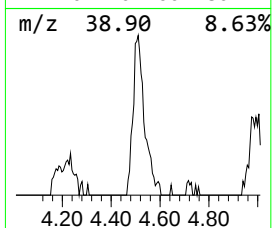
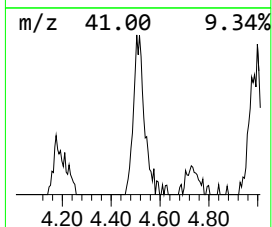
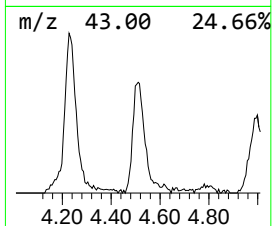
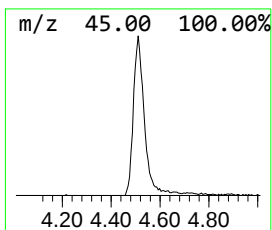
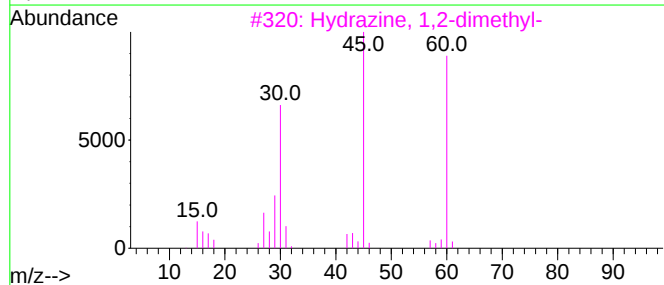
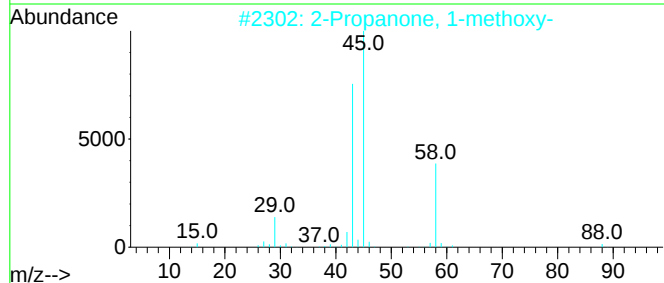
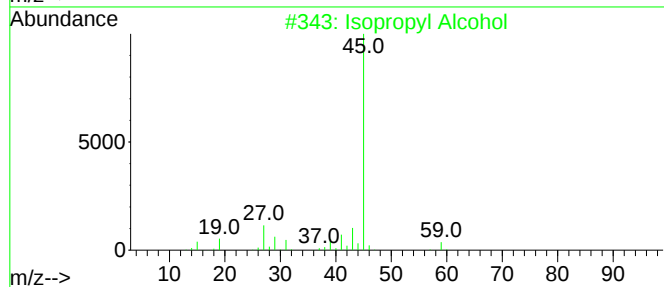
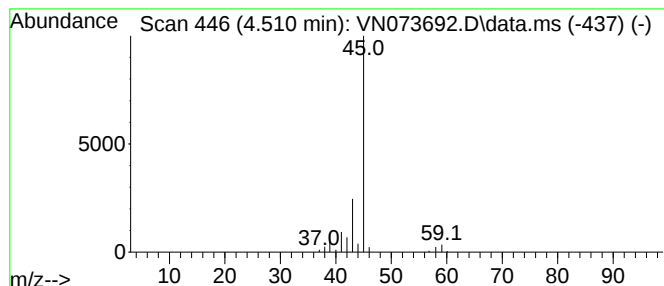
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	8.84 ug/l	177982	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4			4-Penten-2-ol	86	C5H10O	000625-31-0	9
5			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4



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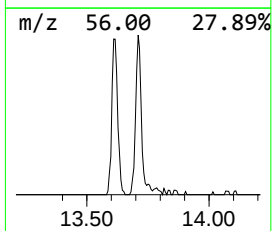
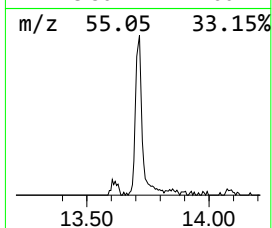
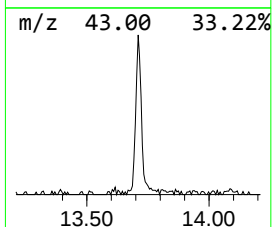
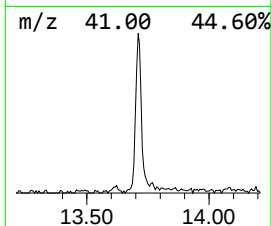
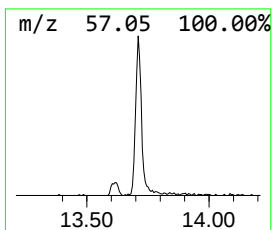
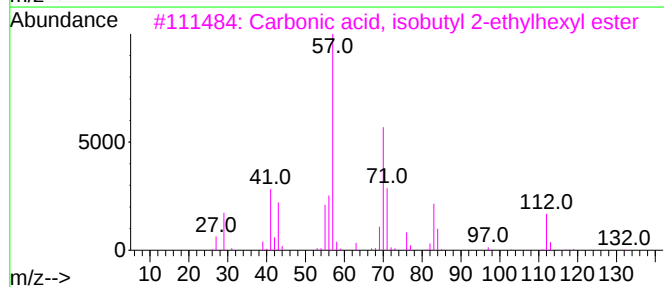
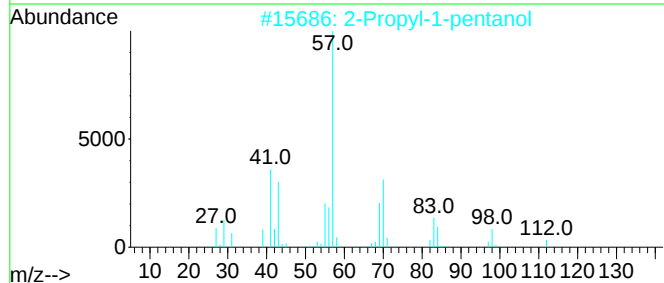
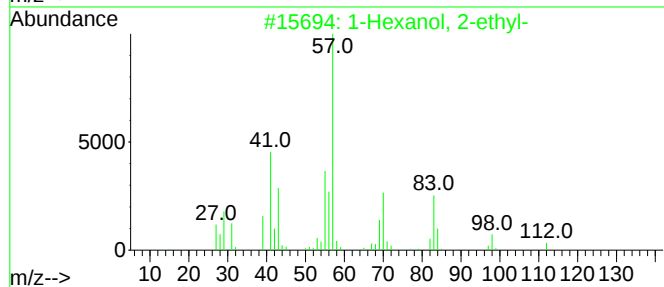
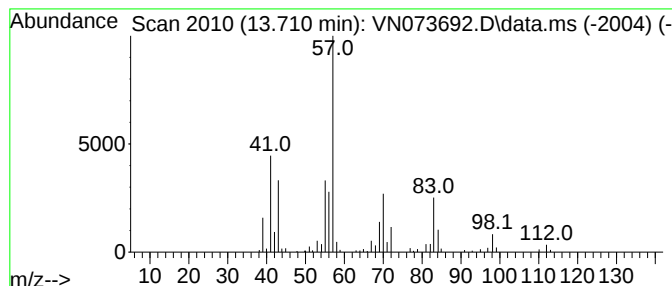
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Quant Title : SW846 8260

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.710	6.80 ug/l	217692	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	47
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.328	7.4	ug/l	148311	1	8.016	1006620	50.0
Butane	2.399	5.3	ug/l	106347	1	8.016	1006620	50.0
Butane, 2-methyl-	3.081	16.7	ug/l	336134	1	8.016	1006620	50.0
Isopropyl Alcohol	4.510	8.8	ug/l	177982	1	8.016	1006620	50.0
1-Hexanol, 2-et...	13.710	6.8	ug/l	217692	4	13.616	1600730	50.0