

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040225\
 Data File : VN086204.D
 Acq On : 02 Apr 2025 13:21
 Operator : JC\MD
 Sample : Q1659-02 100X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 3809

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\82N031825W.M
 Title : SW846 8260

Signal : TIC: VN086204.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.006	3	9	26	rVB	1345762	2399800	100.00%	27.015%
2	2.271	49	54	55	rBV4	14639	26830	1.12%	0.302%
3	4.724	461	471	482	rVB2	18610	47795	1.99%	0.538%
4	8.229	1058	1067	1071	rBV	86036	203678	8.49%	2.293%
5	8.282	1071	1076	1090	rVB	166401	366790	15.28%	4.129%
6	8.635	1126	1136	1149	rBV2	90520	208518	8.69%	2.347%
7	9.141	1213	1222	1231	rBV	236763	474424	19.77%	5.341%
8	9.294	1231	1248	1262	rBV	492900	1164364	48.52%	13.107%
9	10.582	1459	1467	1480	rVB	326156	587845	24.50%	6.617%
10	11.876	1679	1687	1695	rBV	296048	529166	22.05%	5.957%
11	12.653	1796	1819	1842	rBV3	58002	305168	12.72%	3.435%
12	12.853	1846	1853	1860	rVB	256852	431167	17.97%	4.854%
13	13.706	1992	1998	2005	rBV3	18490	32076	1.34%	0.361%
14	13.794	2005	2013	2020	rVV	269006	464692	19.36%	5.231%
15	14.241	2080	2089	2097	rBV	623186	963522	40.15%	10.846%
16	14.488	2127	2131	2138	rVB2	39935	62878	2.62%	0.708%
17	15.511	2293	2305	2312	rVB2	37489	70419	2.93%	0.793%
18	15.641	2321	2327	2336	rVB9	11012	26432	1.10%	0.298%
19	16.005	2378	2389	2397	rBV	210134	399195	16.63%	4.494%
20	16.405	2450	2457	2464	rBV3	54412	118555	4.94%	1.335%

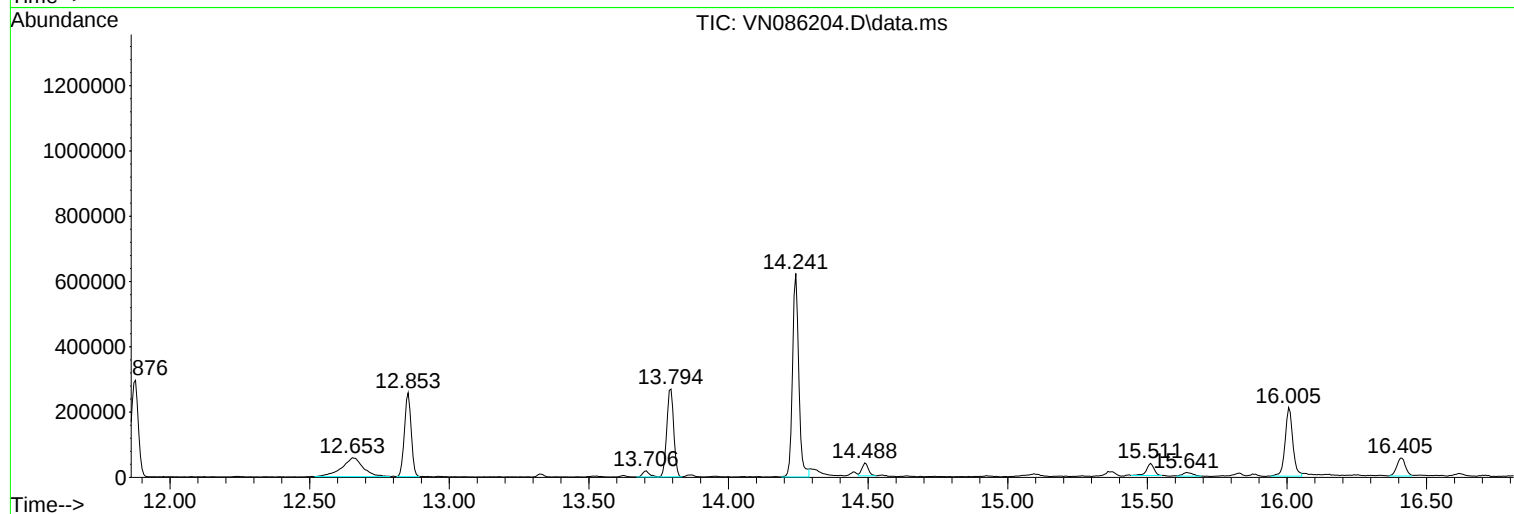
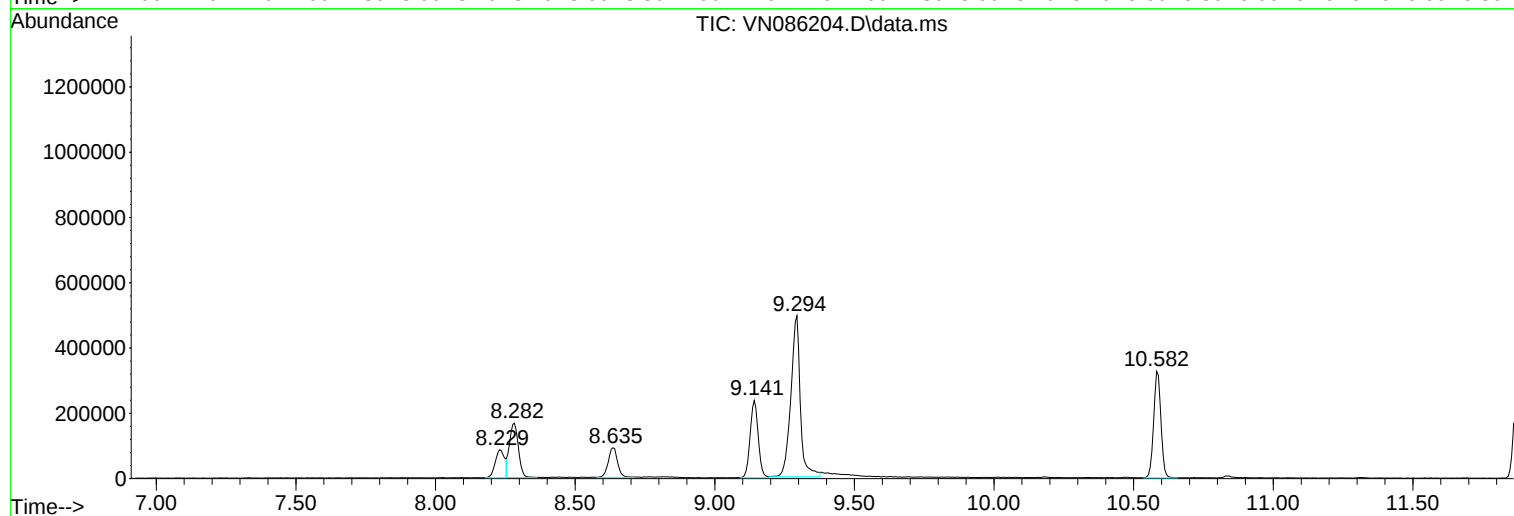
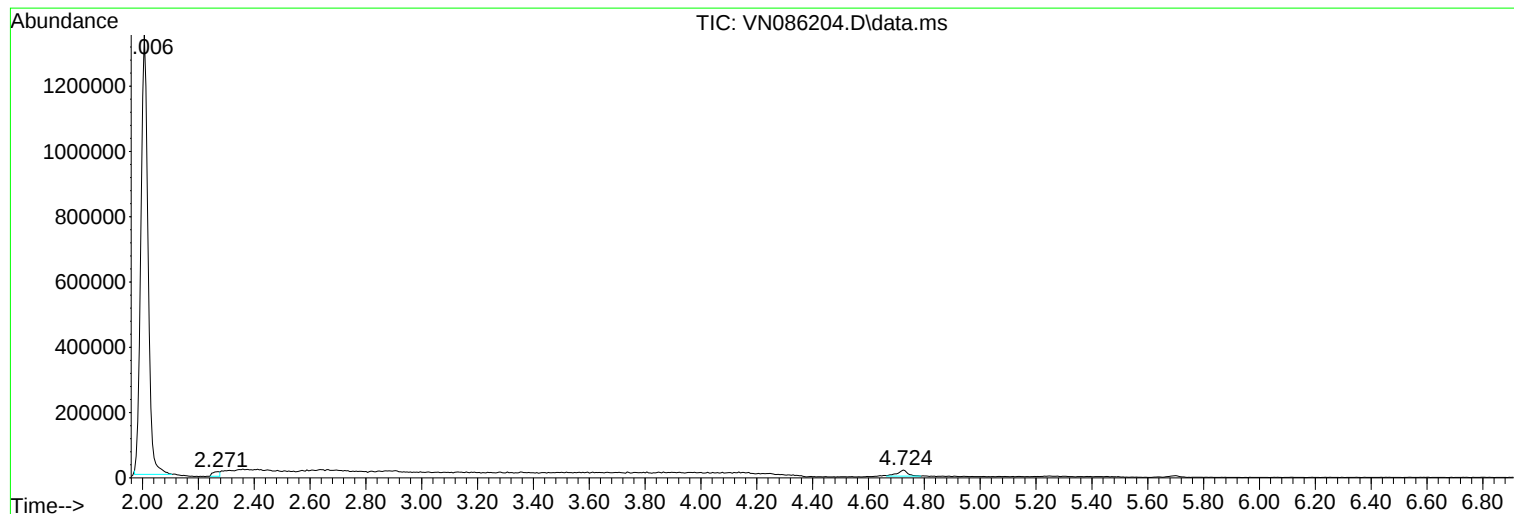
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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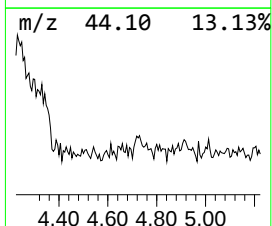
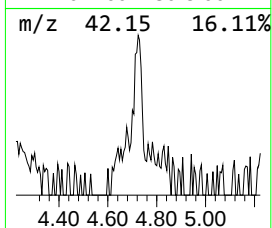
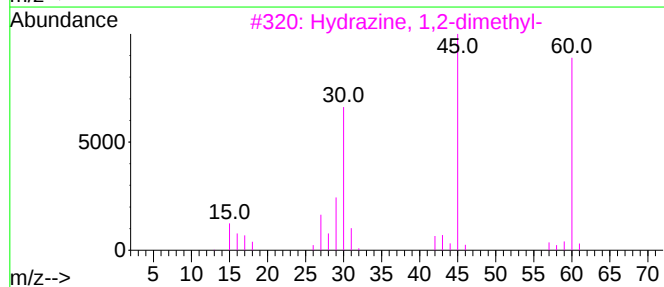
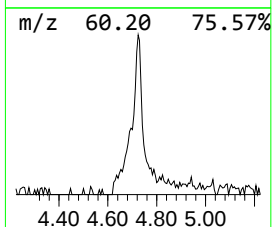
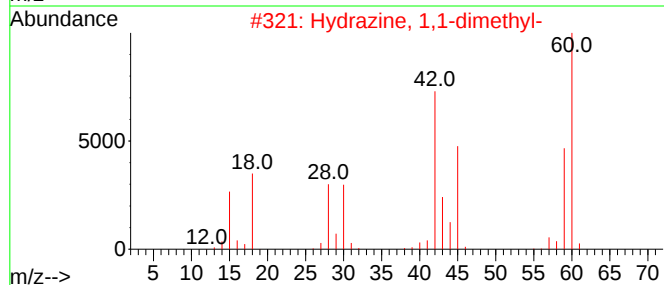
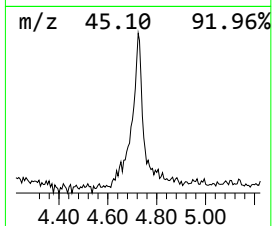
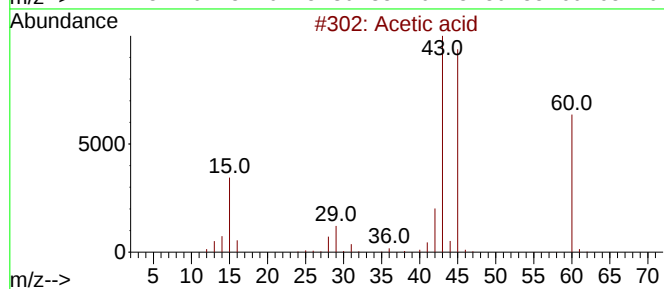
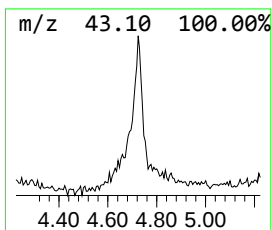
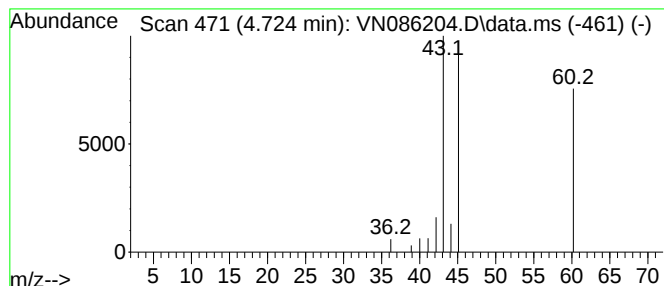
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Quant Title : SW846 8260

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

Peak Number 2 Acetic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.724	6.52 ug/l	47795	Pentafluorobenzene	8.282

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	5
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	5
4			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	4
5			Methane, nitroso-	45	CH3NO	000865-40-7	3



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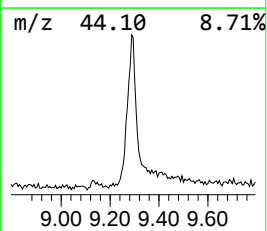
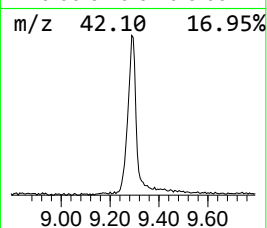
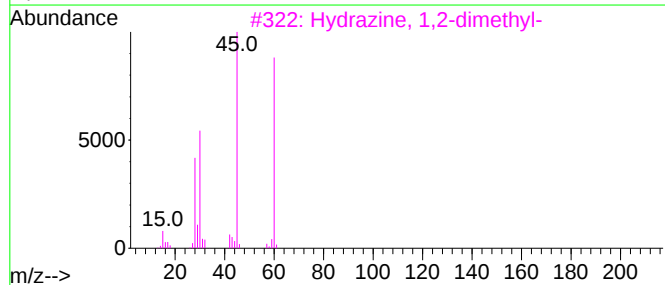
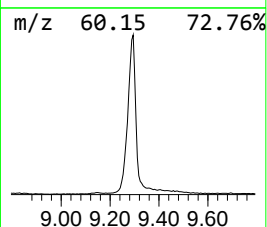
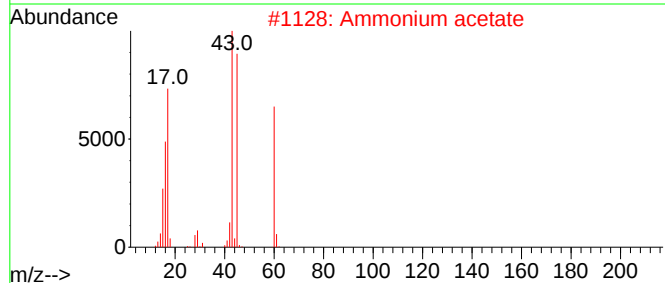
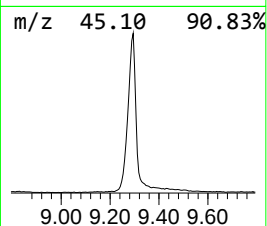
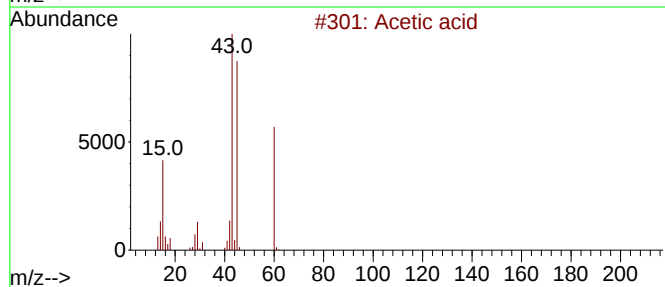
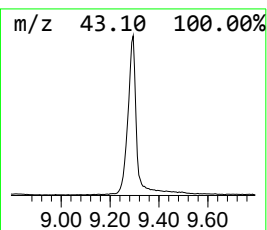
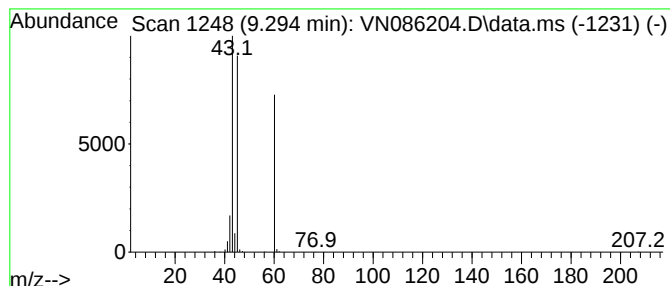
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ammonium acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.294	122.71 ug/l	1164360	1,4-Difluorobenzene	9.141

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			Ammonium acetate	77	C2H7NO2	000631-61-8	74
3			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			Carbonyl sulfide	60	COS	000463-58-1	5



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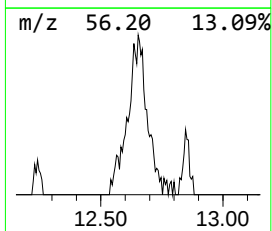
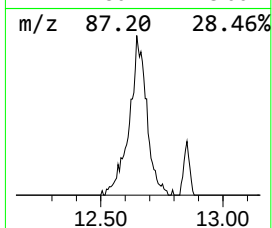
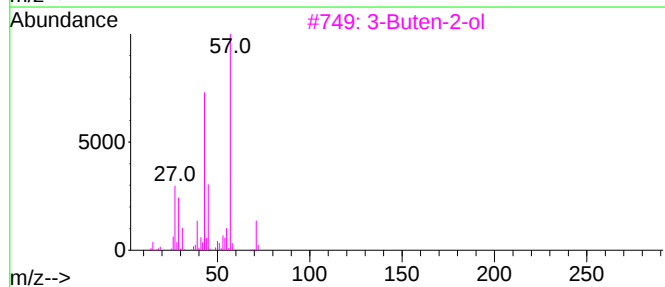
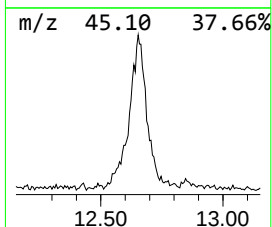
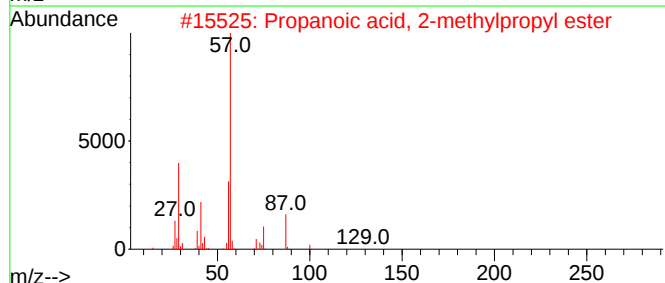
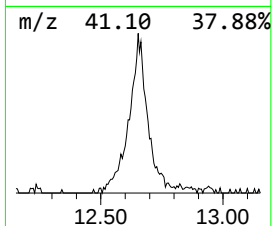
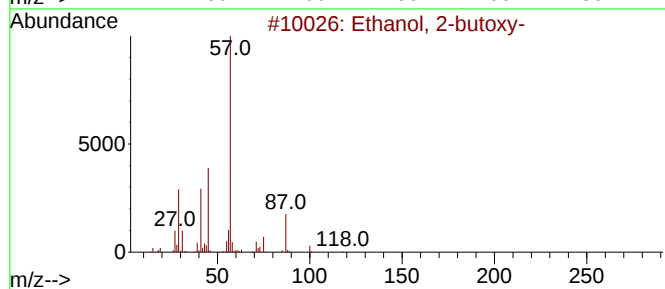
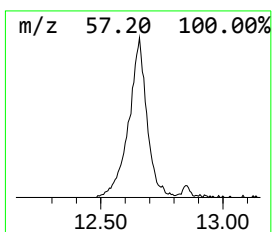
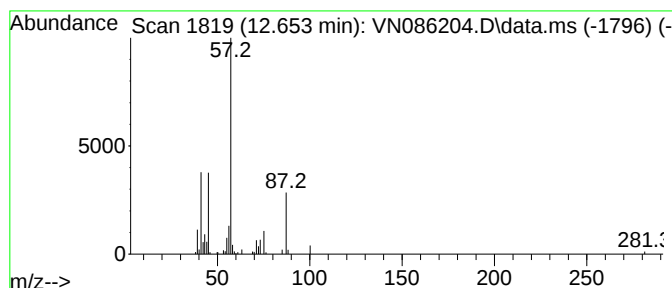
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Peak Number 4 Ethanol, 2-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.653	28.83 ug/l	305168	Chlorobenzene-d5	11.876

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2			Propanoic acid, 2-methylpropyl e...	130	C7H14O2	000540-42-1	38
3			3-Buten-2-ol	72	C4H8O	000598-32-3	35
4			Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	28
5			Propane, 1-methoxy-2,2-dimethyl-	102	C6H14O	001118-00-9	28



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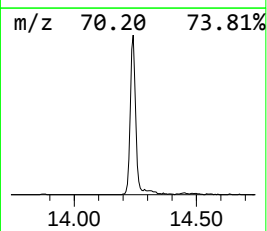
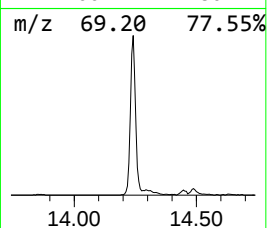
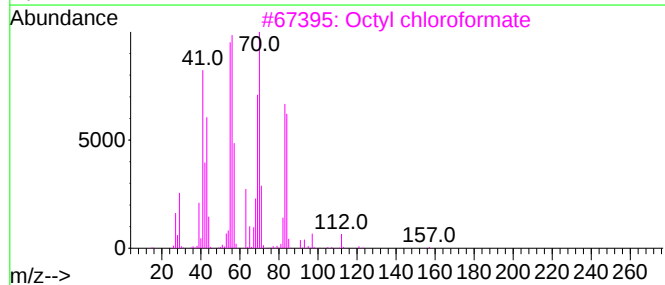
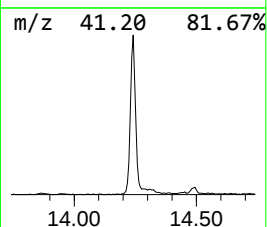
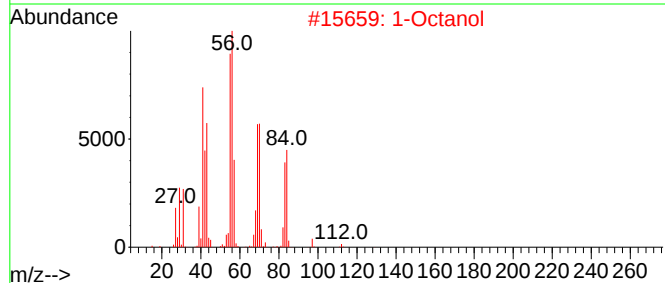
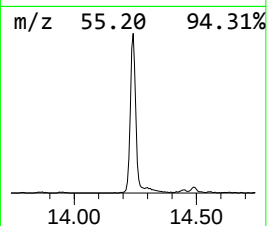
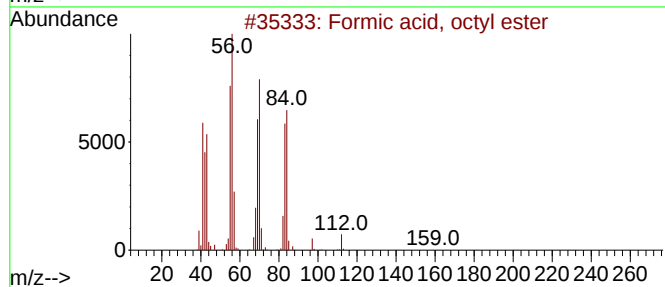
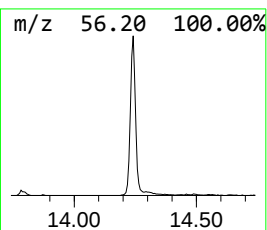
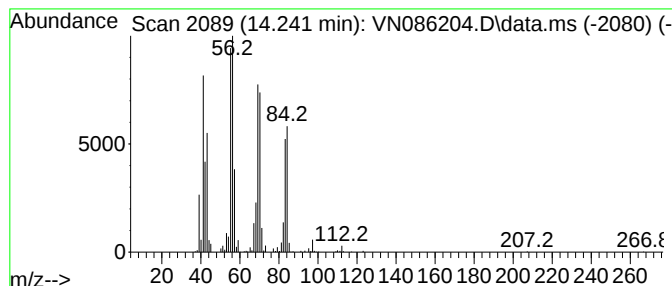
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Formic acid, octyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.241	103.67 ug/l	963522	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid, octyl ester	158	C9H18O2	000112-32-3	91
2			1-Octanol	130	C8H18O	000111-87-5	91
3			Octyl chloroformate	192	C9H17ClO2	007452-59-7	91
4			Cyclooctane	112	C8H16	000292-64-8	90
5			Pentafluoropropionic acid, octyl...	276	C11H17F5O2	001867-95-4	90



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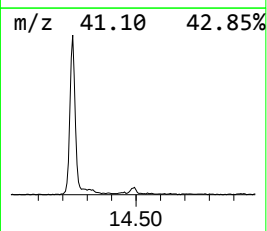
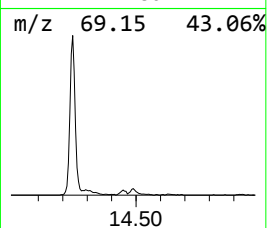
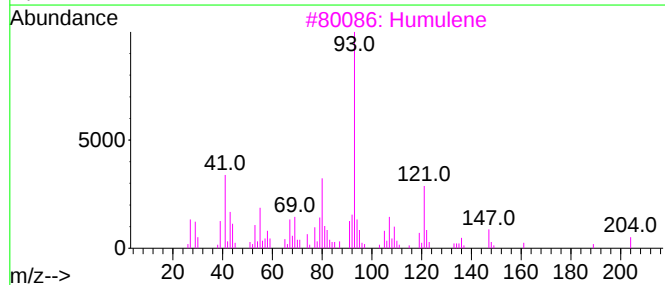
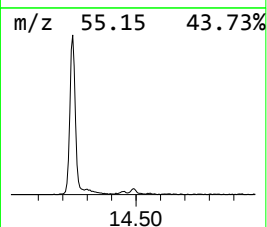
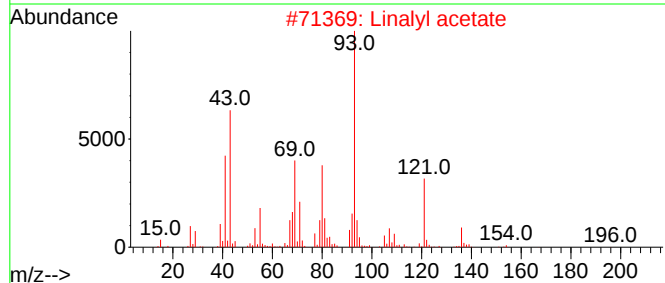
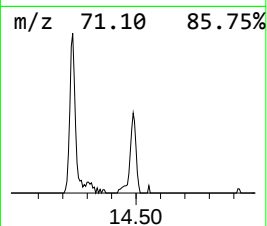
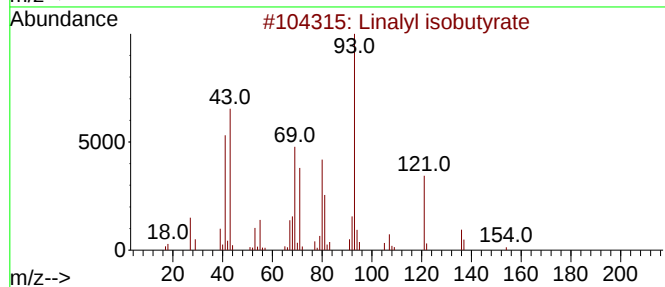
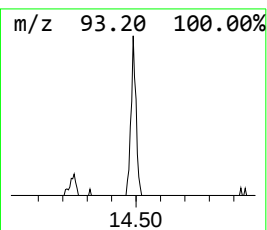
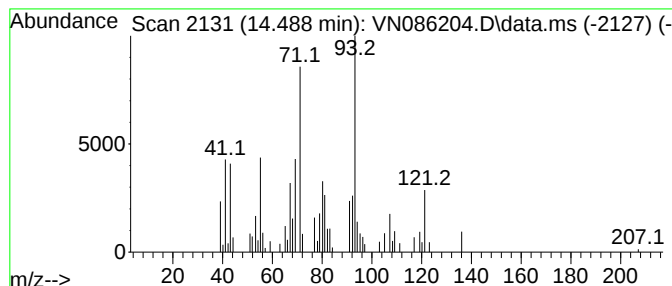
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Quant Title : SW846 8260

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

Peak Number 6 unknown14.488 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.488	6.77 ug/l	62878	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linalyl isobutyrate	224	C14H24O2	000078-35-3	47
2			Linalyl acetate	196	C12H20O2	000115-95-7	47
3			Humulene	204	C15H24	006753-98-6	47
4			Butanoic acid, 3-methyl-, 1-ethe...	238	C15H26O2	001118-27-0	46
5			.alpha.-Pinene	136	C10H16	000080-56-8	43



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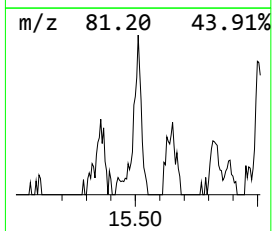
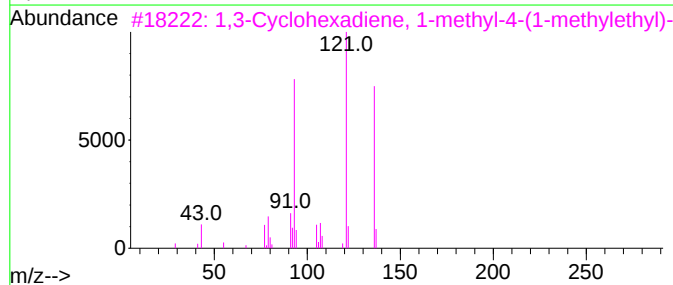
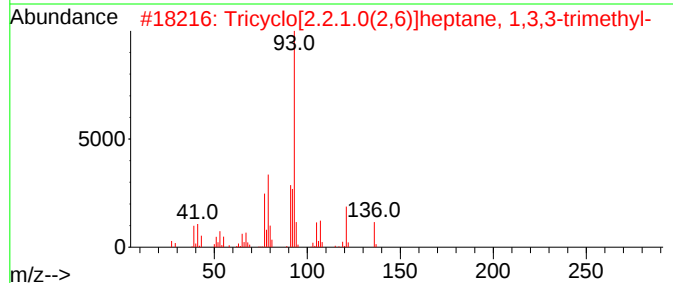
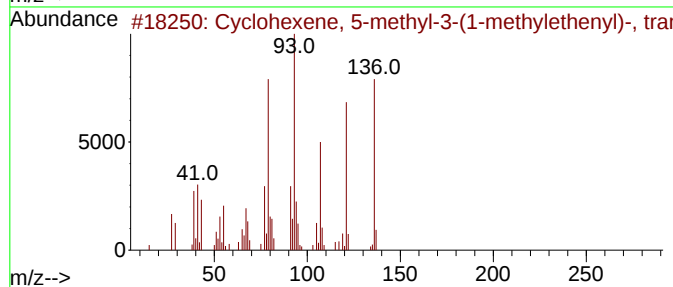
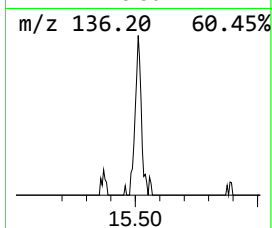
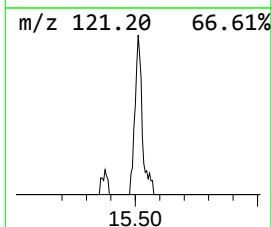
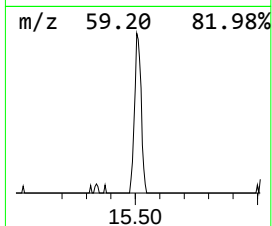
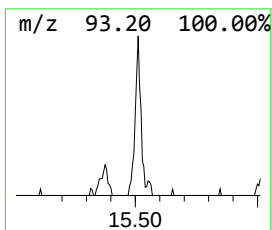
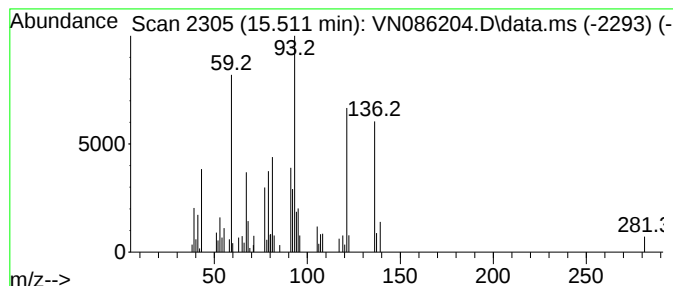
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Quant Title : SW846 8260

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

Peak Number 7 Cyclohexene, 5-methyl-3-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.511	7.58 ug/l	70419	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	60
2			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	60
3			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	55
4			(1R)-2,6,6-Trimethylbicyclo[3.1...	136	C10H16	007785-70-8	55
5			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040225\
Data File : VN086204.D
Acq On : 02 Apr 2025 13:21
Operator : JC\MD
Sample : Q1659-02 100X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

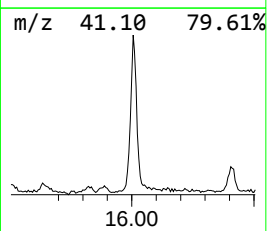
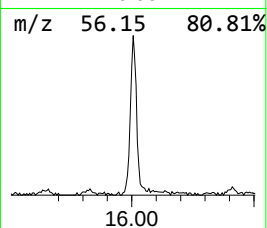
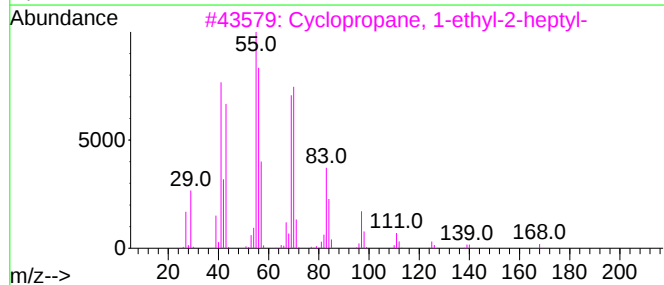
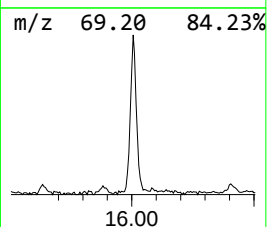
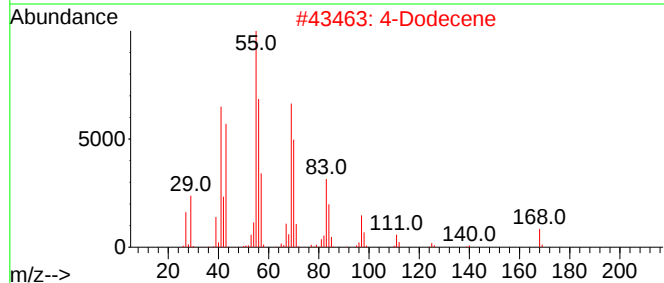
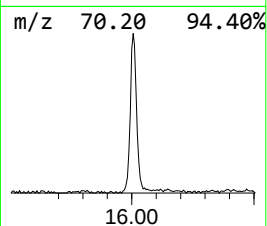
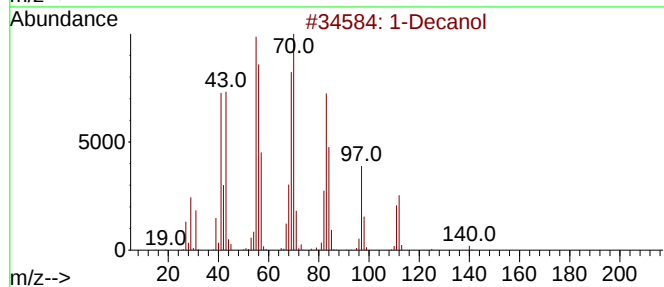
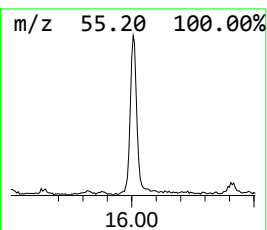
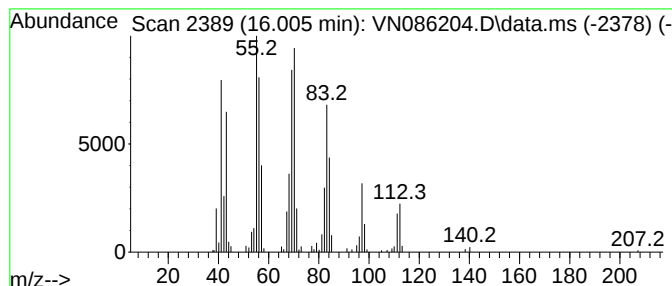
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Quant Title : SW846 8260

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

Peak Number 8 1-Decanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.006	42.95 ug/l	399195	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Decanol	158	C10H22O	000112-30-1	91
2			4-Dodecene	168	C12H24	002030-84-4	86
3			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	86
4			Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1010150-67-3	86
5			Cyclooctane	112	C8H16	000292-64-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040225\
Data File : VN086204.D
Acq On : 02 Apr 2025 13:21
Operator : JC\MD
Sample : Q1659-02 100X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

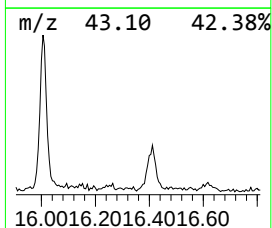
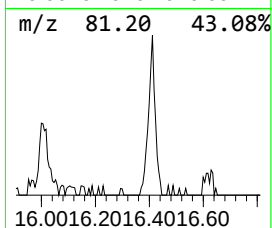
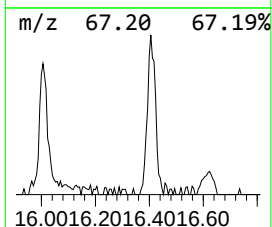
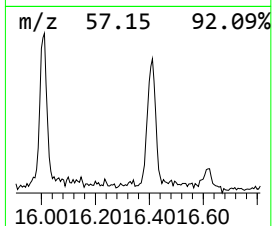
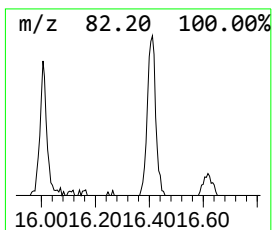
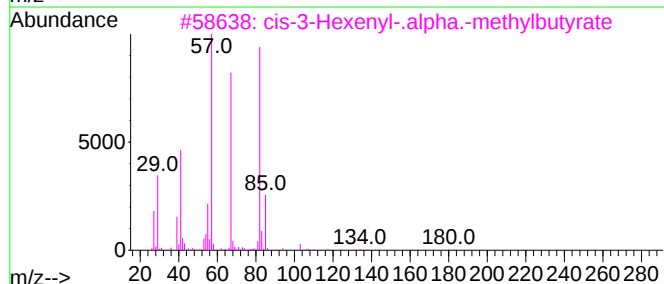
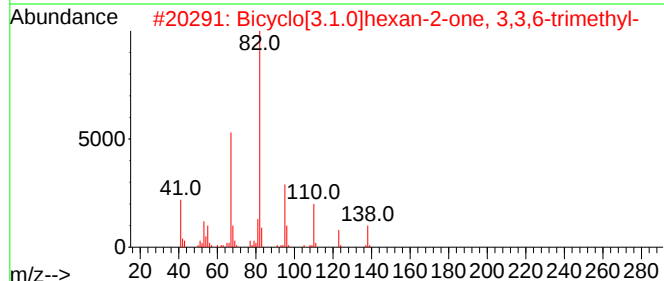
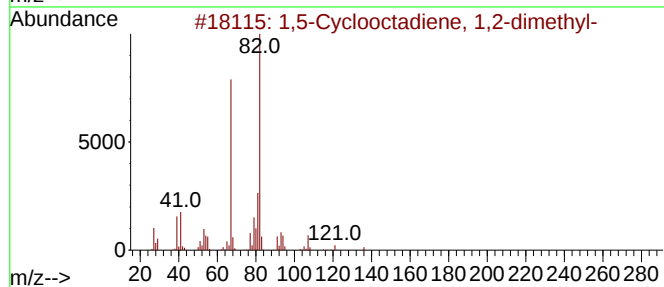
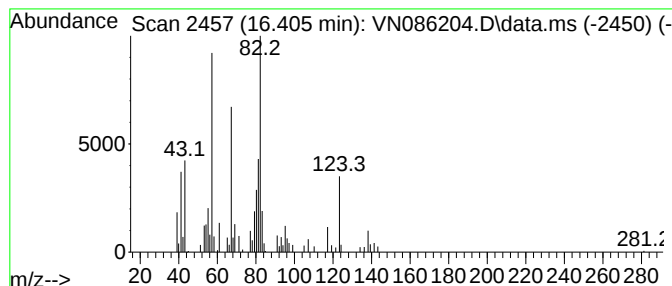
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Quant Title : SW846 8260

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

Peak Number 9 unknown16.405 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.405	12.76 ug/l	118555	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Cyclooctadiene, 1,2-dimethyl-	136	C10H16	006588-51-8	49
2			Bicyclo[3.1.0]hexan-2-one, 3,3,6...	138	C9H14O	053966-40-8	47
3			cis-3-Hexenyl-.alpha.-methylbuty...	184	C11H20O2	053398-85-9	47
4			2,4-Hexadiene	82	C6H10	000592-46-1	46
5			4-Methyl-1,3-pentadiene	82	C6H10	000926-56-7	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN040225\
Data File : VN086204.D
Acq On : 02 Apr 2025 13:21
Operator : JC\MD
Sample : Q1659-02 100X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
3809

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031825W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid	4.724	6.5	ug/l	47795	1	8.282	366790	50.0
Ammonium acetate	9.294	122.7	ug/l	1164360	2	9.141	474424	50.0
Ethanol, 2-butoxy-	12.653	28.8	ug/l	305168	3	11.876	529166	50.0
Formic acid, oc...	14.241	103.7	ug/l	963522	4	13.794	464692	50.0
unknown14.488	14.488	6.8	ug/l	62878	4	13.794	464692	50.0
Cyclohexene, 5-...	15.511	7.6	ug/l	70419	4	13.794	464692	50.0
1-Decanol	16.006	43.0	ug/l	399195	4	13.794	464692	50.0
unknown16.405	16.405	12.8	ug/l	118555	4	13.794	464692	50.0