

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120722\
 Data File : VX033297.D
 Acq On : 07 Dec 2022 21:28
 Operator : JC/MD
 Sample : N5911-01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A3594TOG

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_X\Method\82X120722W.M
 Title : SW846 8260

Signal : TIC: VX033297.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.282	26	32	42	rBV	15605	58279	4.83%	1.183%
2	1.459	57	61	69	rVB	10681	14257	1.18%	0.289%
3	2.148	158	174	206	rVV2	178983	1206485	100.00%	24.481%
4	2.989	302	312	328	rVB3	3690	13897	1.15%	0.282%
5	5.099	646	658	678	rBV	51131	157380	13.04%	3.193%
6	5.385	694	705	720	rBV2	59682	175093	14.51%	3.553%
7	5.556	722	733	747	rVV	156159	443847	36.79%	9.006%
8	5.958	789	799	813	rBV2	46518	124050	10.28%	2.517%
9	6.763	921	931	945	rBV	232318	549245	45.52%	11.145%
10	7.824	1096	1105	1115	rBV	20307	39698	3.29%	0.806%
11	8.647	1234	1240	1249	rBV	175282	285188	23.64%	5.787%
12	10.055	1465	1471	1481	rBV	458866	618885	51.30%	12.558%
13	11.079	1634	1639	1651	rVB	325509	409413	33.93%	8.307%
14	12.024	1788	1794	1803	rBV	464339	588966	48.82%	11.951%
15	12.219	1821	1826	1832	rBV	13060	21958	1.82%	0.446%
16	13.378	2011	2016	2025	rBV	43083	61718	5.12%	1.252%
17	14.048	2122	2126	2131	rVB2	24114	37411	3.10%	0.759%
18	14.103	2131	2135	2143	rVB	31725	43569	3.61%	0.884%
19	14.213	2146	2153	2157	rBV5	14553	29659	2.46%	0.602%
20	14.316	2166	2170	2175	rVV3	20495	36490	3.02%	0.740%
21	14.359	2175	2177	2181	rVV2	8182	12803	1.06%	0.260%

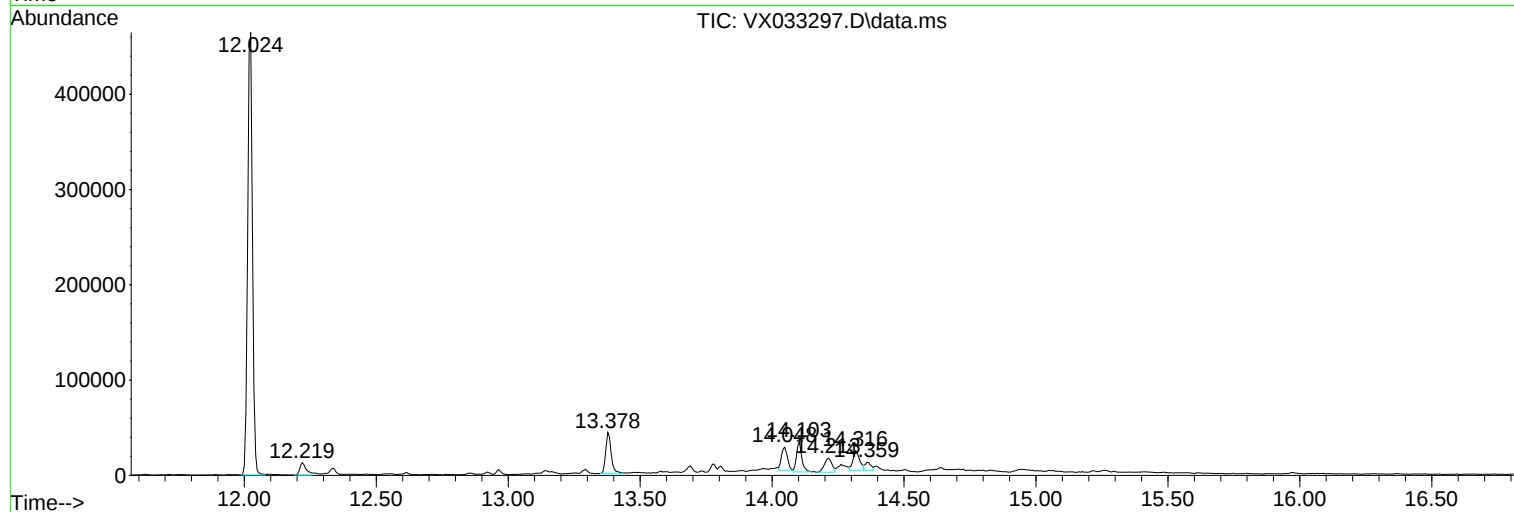
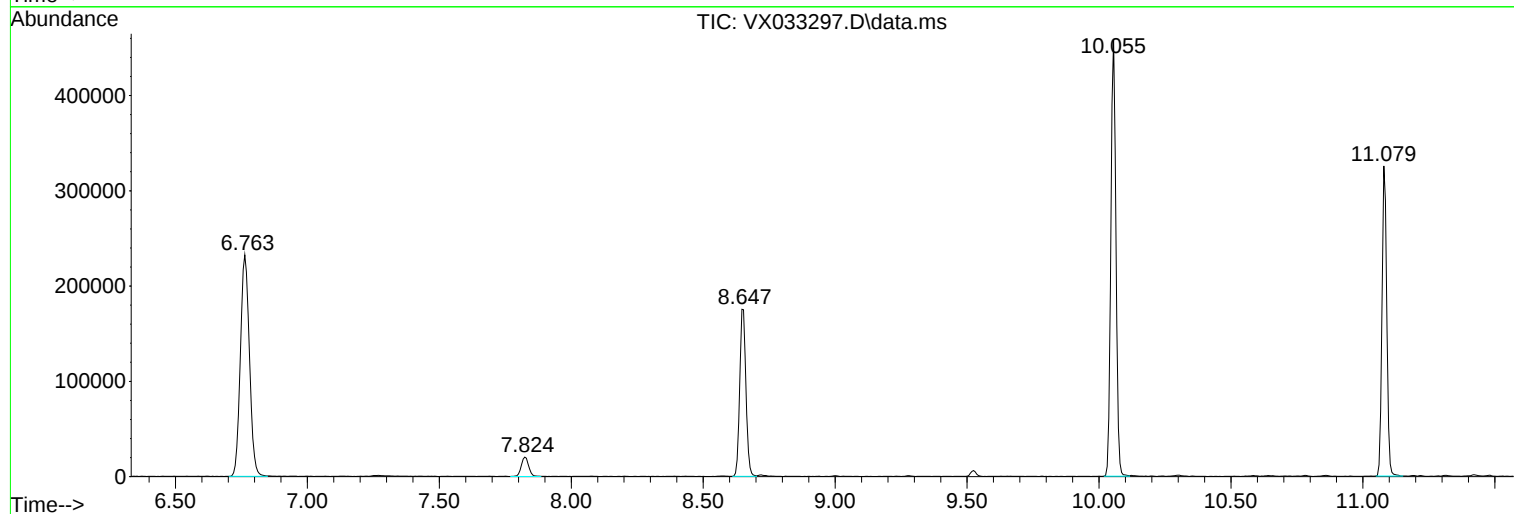
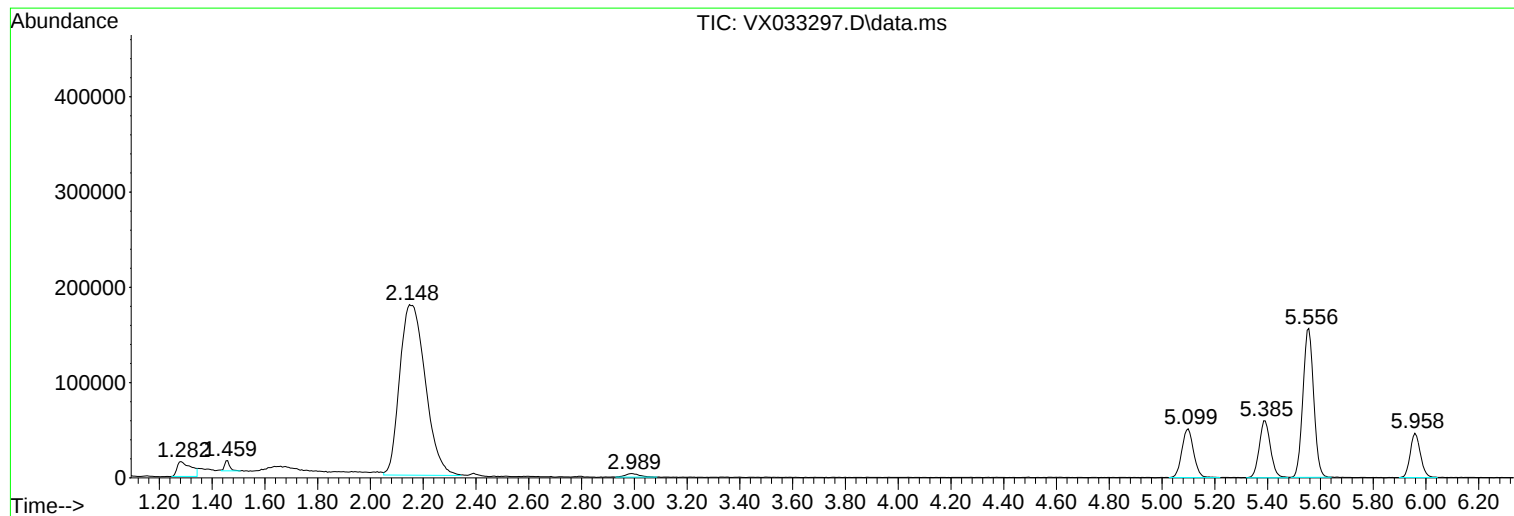
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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



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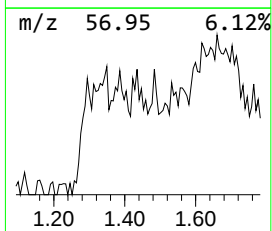
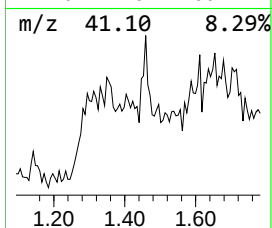
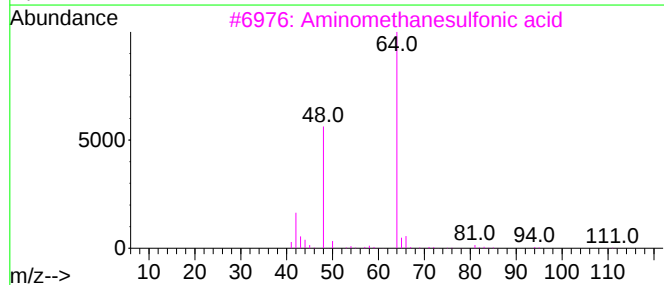
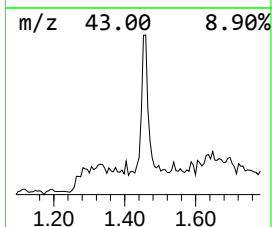
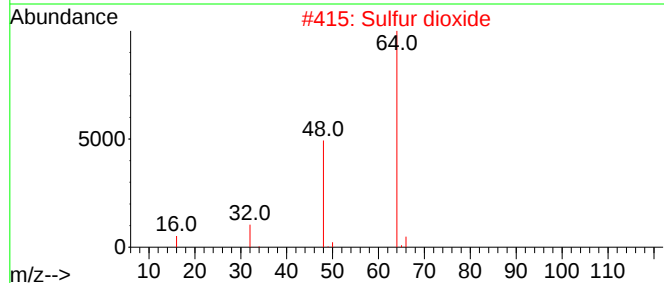
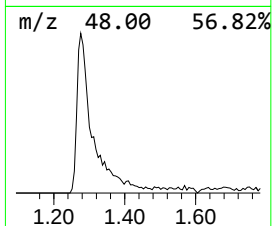
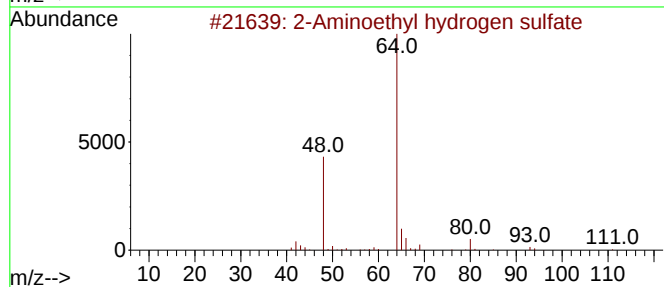
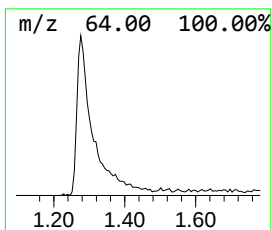
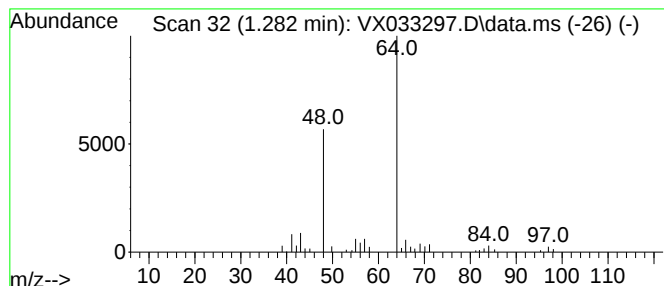
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Aminoethyl hydrogen sulfate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.282	6.57 ug/l	58279	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	83
2			Sulfur dioxide	64	O2S	007446-09-5	78
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	43
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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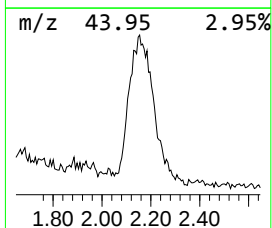
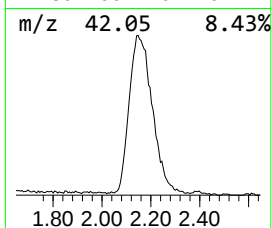
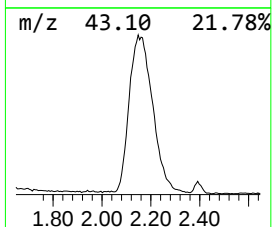
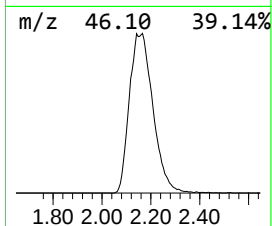
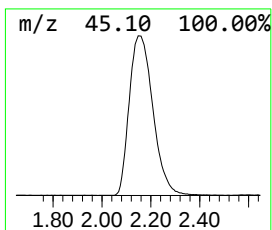
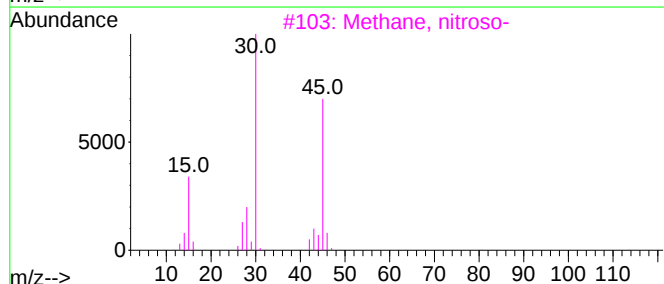
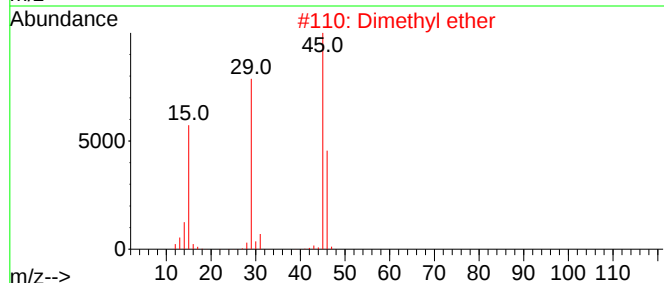
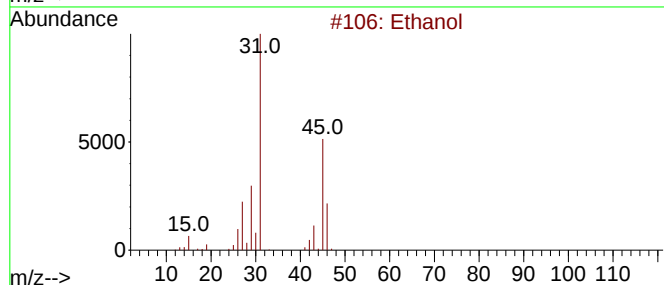
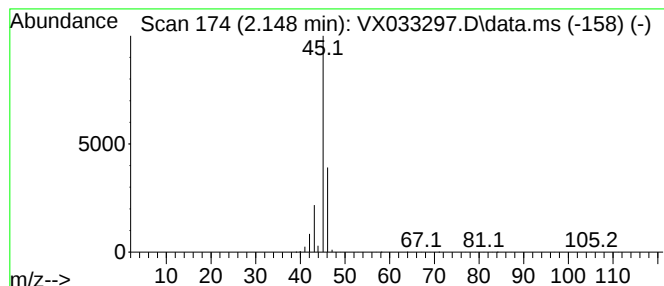
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Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.148	135.91 ug/l	1206490	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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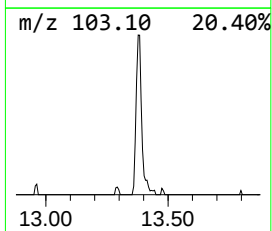
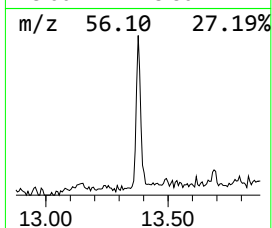
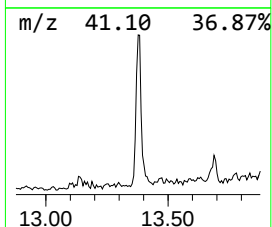
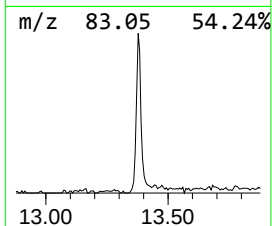
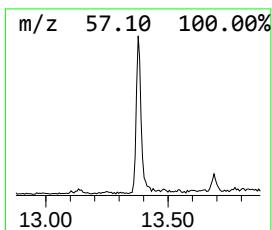
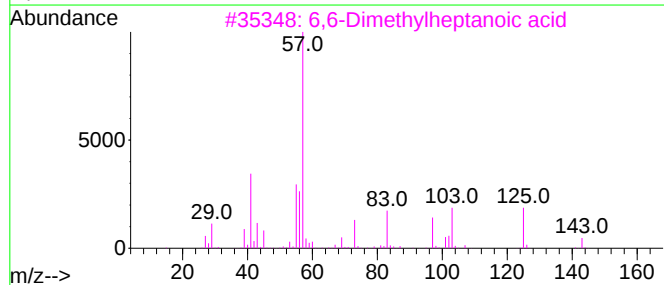
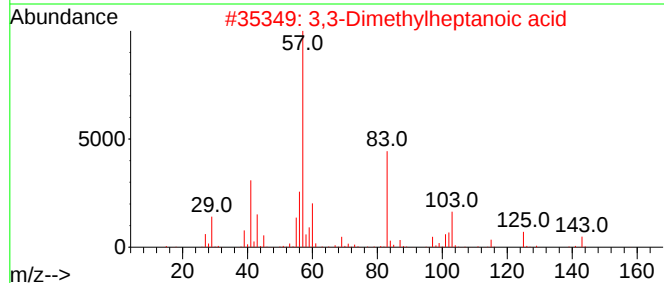
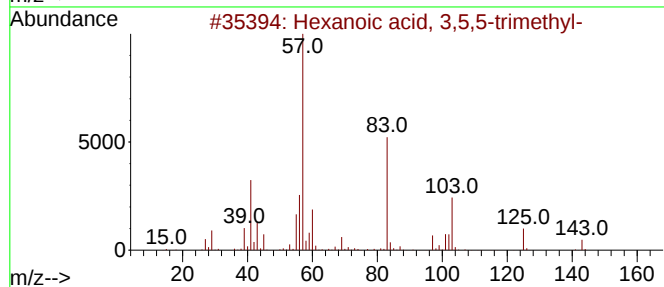
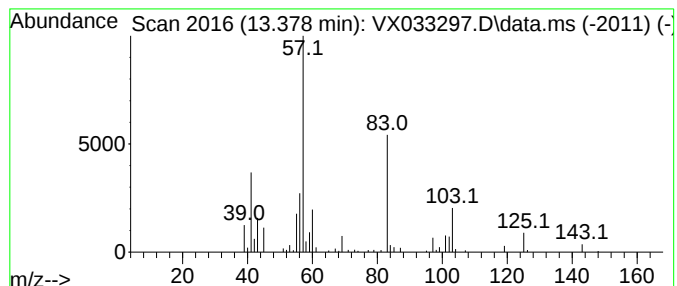
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Peak Number 3 Hexanoic acid, 3,5,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.378	5.24 ug/l	61718	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	91
2			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	90
3			6,6-Dimethylheptanoic acid	158	C9H18O2	015898-92-7	47
4			Hexanoyl chloride, 3,5,5-trimethyl-	176	C9H17ClO	036727-29-4	37
5			Propanoic acid, 2,2-dimethyl-, h...	200	C12H24O2	017660-61-6	35



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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
2-Aminoethyl hy...	1.282	6.6	ug/l	58279	1	5.556	443847	50.0
Ethanol	2.148	135.9	ug/l	1206490	1	5.556	443847	50.0
Hexanoic acid, ...	13.378	5.2	ug/l	61718	4	12.024	588966	50.0