

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072122\
 Data File : VX030144.D
 Acq On : 20 Jul 2022 19:55
 Operator : JC/MD
 Sample : N3775-03 200X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 M-R-2

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\82X071222W.M
 Title : SW846 8260

Signal : TIC: VX030144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.557	72	77	81	rBV6	9425	15706	1.58%	0.272%
2	5.391	695	706	720	rBV	107363	321944	32.30%	5.567%
3	5.556	720	733	746	rBV	190445	539957	54.18%	9.338%
4	5.964	789	800	817	rBV	122625	338236	33.94%	5.849%
5	6.769	922	932	944	rBV	310569	741777	74.43%	12.828%
6	8.653	1232	1241	1250	rBV	637741	996676	100.00%	17.236%
7	10.055	1465	1471	1483	rBV	643621	857046	85.99%	14.821%
8	11.085	1634	1640	1648	rBV	459934	594009	59.60%	10.272%
9	12.024	1788	1794	1801	rBV	615424	747887	75.04%	12.933%
10	12.225	1823	1827	1837	rBV2	9857	23588	2.37%	0.408%
11	13.689	2062	2067	2075	rBV2	12370	19233	1.93%	0.333%
12	14.048	2115	2126	2131	rBV3	51218	104281	10.46%	1.803%
13	14.103	2131	2135	2145	rVB2	101274	143996	14.45%	2.490%
14	14.219	2145	2154	2158	rBV5	32763	70851	7.11%	1.225%
15	14.323	2165	2171	2176	rBV2	95092	179064	17.97%	3.097%
16	14.371	2176	2179	2181	rVV	28356	43230	4.34%	0.748%
17	14.402	2181	2184	2189	rVB2	31930	45177	4.53%	0.781%

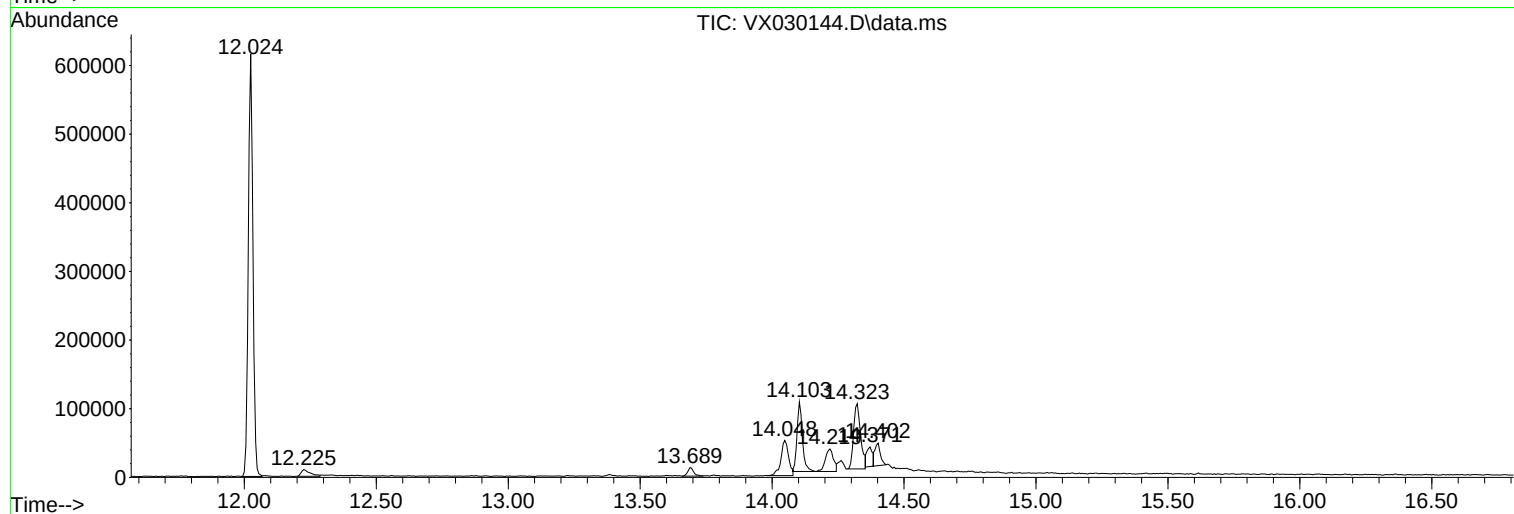
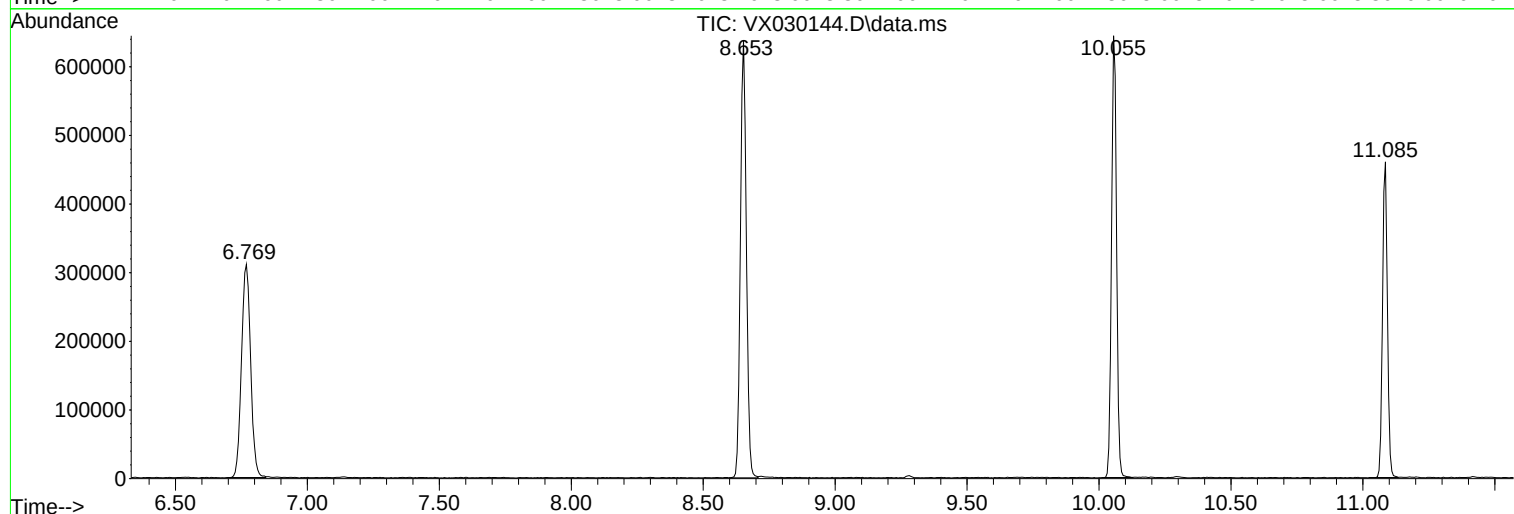
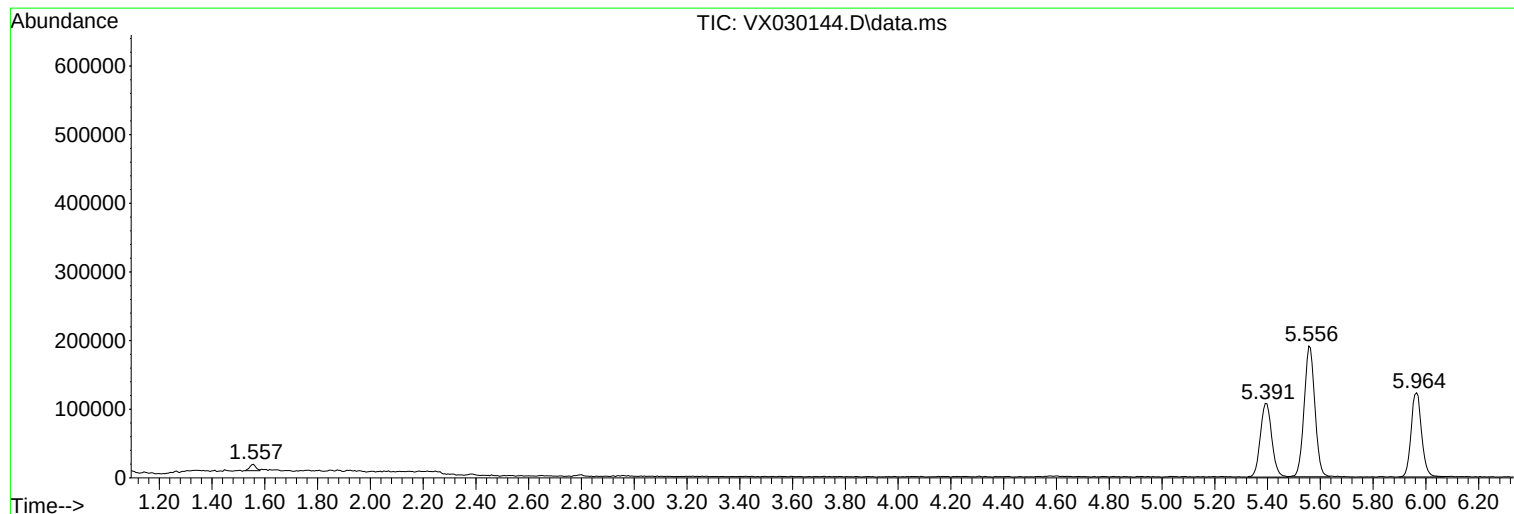
Sum of corrected areas: 5782658

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.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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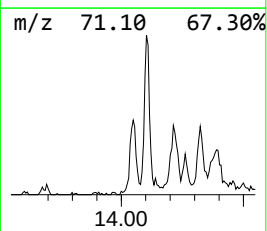
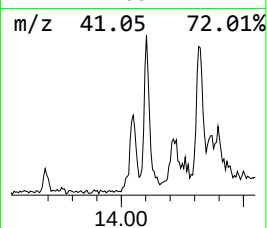
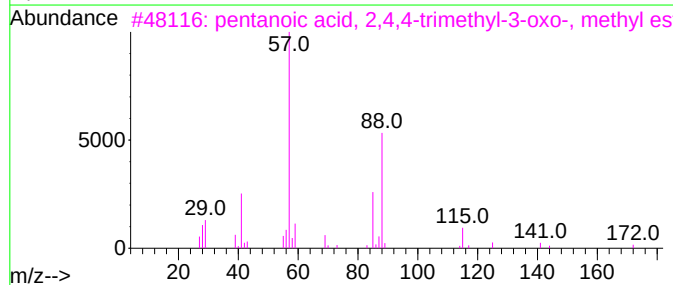
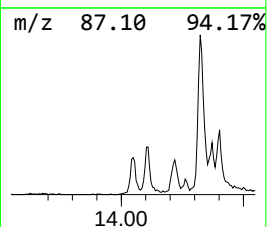
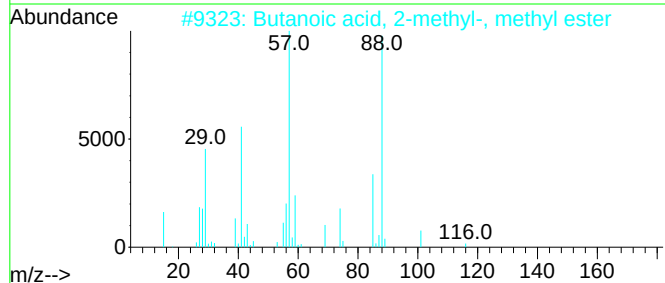
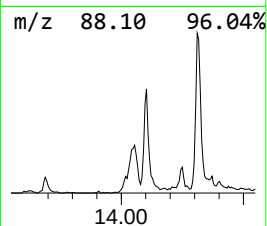
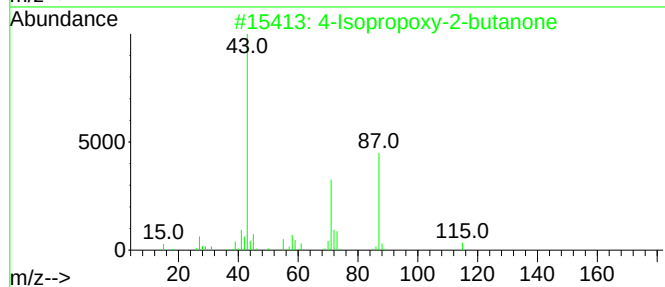
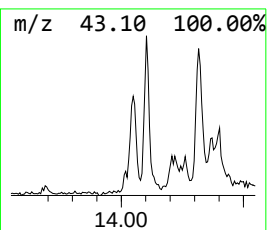
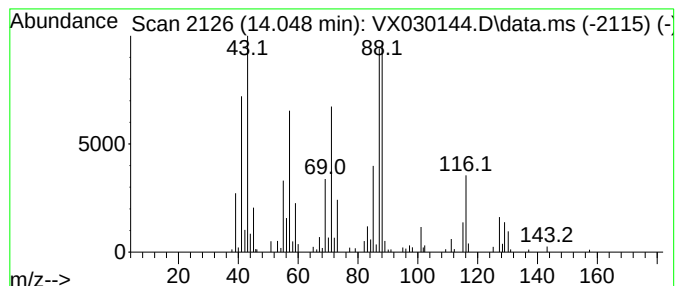
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown14.048 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.048	6.97 ug/l	104281	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Isopropoxy-2-butanone	130	C7H14O2	032541-58-5	35
2			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	35
3			pentanoic acid, 2,4,4-trimethyl-...	172	C9H16O2	1000404-62-8	27
4			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	25
5			Butanoic acid, 2-methyl-3-oxo-, ...	130	C6H10O3	017094-21-2	25



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MSVOA_X
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M-R-2

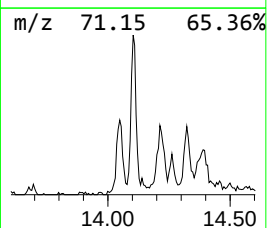
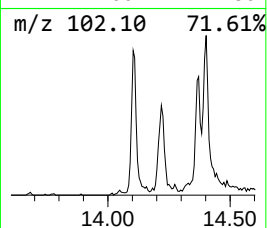
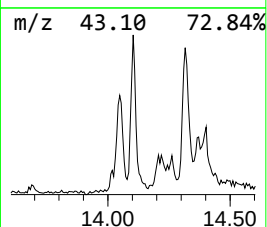
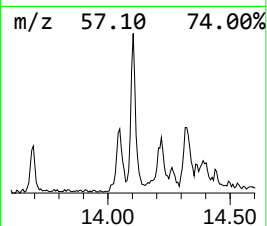
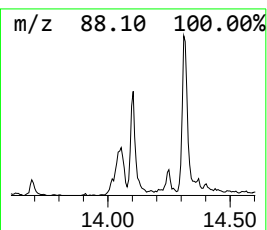
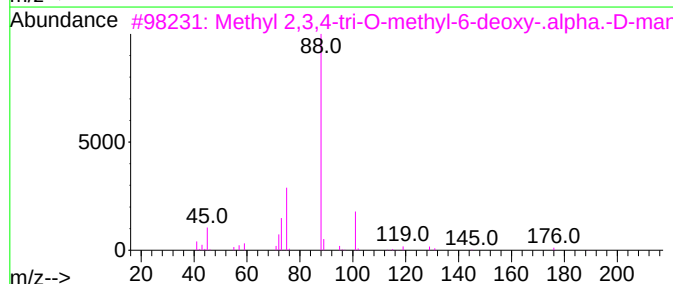
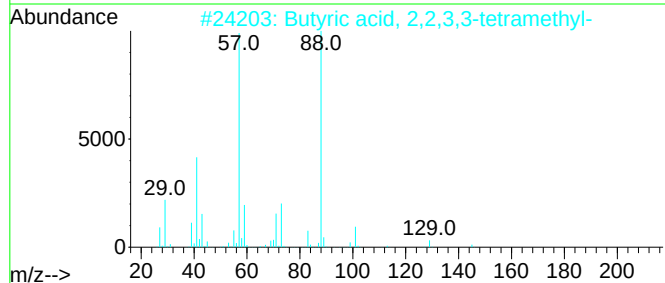
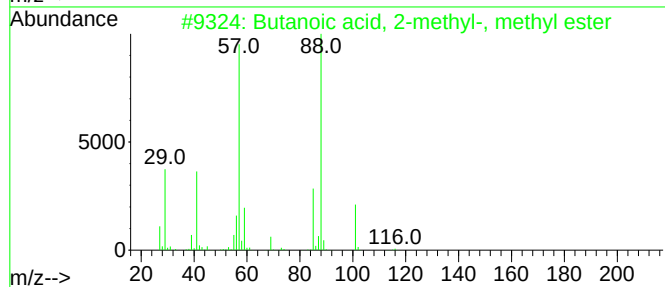
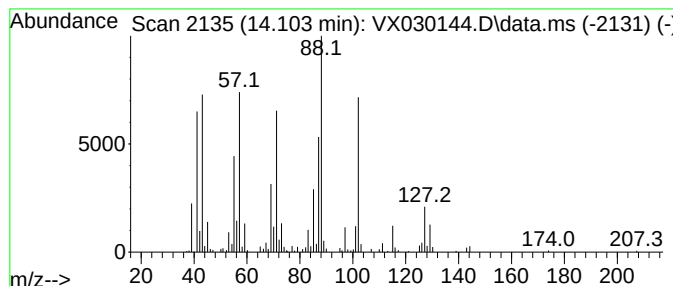
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X071222W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown14.103 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.103	9.63 ug/l	143996	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	27
2			Butyric acid, 2,2,3,3-tetramethyl-	144	C8H16O2	030407-41-1	27
3			Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	22
4			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	15
5			Acetaldehyde isopentyl propyl ac...	174	C10H22O2	1000431-62-2	14



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ClientSampleId :
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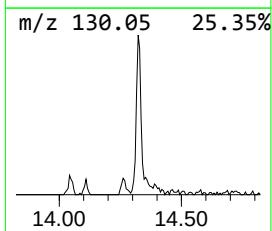
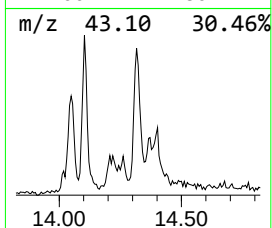
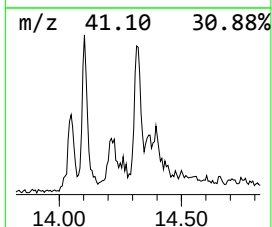
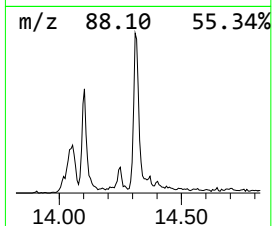
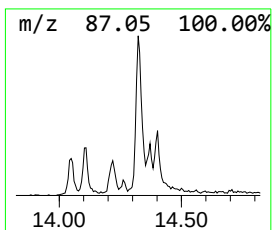
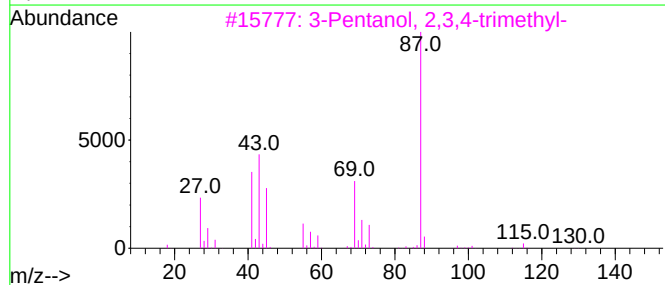
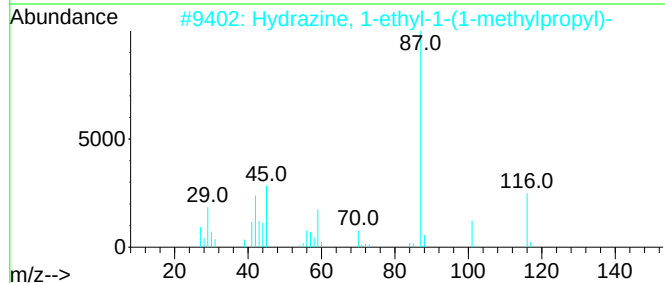
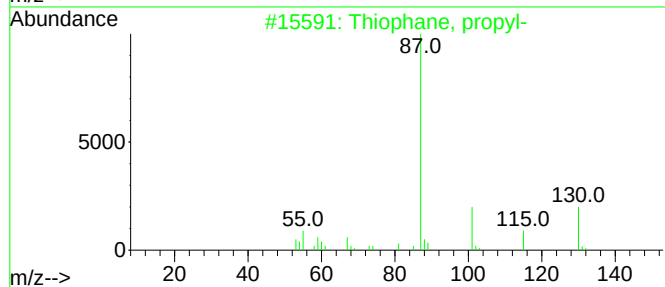
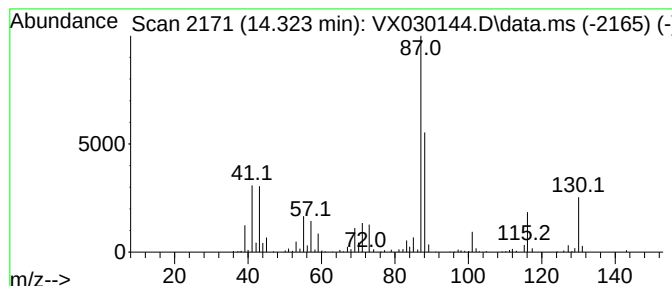
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Quant Title : SW846 8260

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

Peak Number 3 unknown14.323 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.323	11.97 ug/l	179064	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophane, propyl-	130	C7H14S	001551-34-4	43
2			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	38
3			3-Pentanol, 2,3,4-trimethyl-	130	C8H18O	003054-92-0	38
4			Neodecanoic acid	172	C10H20O2	026896-20-8	38
5			2,3-Di-O-methyl-D-xylopyranose	178	C7H14O5	018186-26-0	38



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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
unknown14.048	14.048	7.0	ug/l	104281	4	12.024	747887	50.0
unknown14.103	14.103	9.6	ug/l	143996	4	12.024	747887	50.0
unknown14.323	14.323	12.0	ug/l	179064	4	12.024	747887	50.0