

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU012121\  
 Data File : VU042155.D  
 Acq On : 21 Jan 2021 16:57  
 Operator : SY/MD  
 Sample : M1170-19  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampled :  
 BFT99

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % of largest Peak  
 Start Thrs: 0.1 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\_U\METHOD\SOMUTR012021WMA.M  
 Title : TRACE VOA SOM01.0

Signal : TIC: VU042155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	71	81	92	rVB	47889	56391	3.43%	1.036%
2	1.916	172	179	190	rVB	37572	47498	2.89%	0.873%
3	2.572	371	383	399	rBV	84495	138131	8.40%	2.538%
4	4.456	953	969	983	rBV5	6356	17236	1.05%	0.317%
5	4.649	1013	1029	1074	rBV2	48627	180610	10.99%	3.318%
6	5.073	1146	1161	1181	rBV2	76504	183975	11.19%	3.380%
7	5.732	1345	1366	1391	rBV2	144249	383092	23.31%	7.038%
8	6.256	1515	1529	1554	rBV	142450	266737	16.23%	4.901%
9	6.549	1596	1620	1641	rBV	849468	1643618	100.00%	30.197%
10	6.700	1654	1667	1686	rVB2	94195	182636	11.11%	3.355%
11	7.115	1786	1796	1809	rBV2	9599	17535	1.07%	0.322%
12	7.575	1924	1939	1957	rBV	54737	98847	6.01%	1.816%
13	7.906	2026	2042	2059	rBV	181646	311865	18.97%	5.730%
14	8.186	2116	2129	2141	rBV	35994	61740	3.76%	1.134%
15	8.559	2235	2245	2258	rVB2	32809	53740	3.27%	0.987%
16	8.642	2258	2271	2306	rBV	245625	496532	30.21%	9.122%
17	8.796	2309	2319	2335	rVB7	12529	30128	1.83%	0.554%
18	9.423	2502	2514	2546	rVB	195094	325821	19.82%	5.986%
19	9.771	2610	2622	2642	rVB	35855	67425	4.10%	1.239%
20	10.349	2793	2802	2813	rBV3	11095	17119	1.04%	0.315%
21	10.764	2920	2931	2948	rVB	73123	117986	7.18%	2.168%
22	11.697	3211	3221	3232	rBV2	22912	34839	2.12%	0.640%
23	11.819	3247	3259	3273	rVB	206105	323652	19.69%	5.946%
24	12.201	3365	3378	3393	rVB	184125	291072	17.71%	5.348%
25	12.896	3584	3594	3608	rBV	63538	94756	5.77%	1.741%

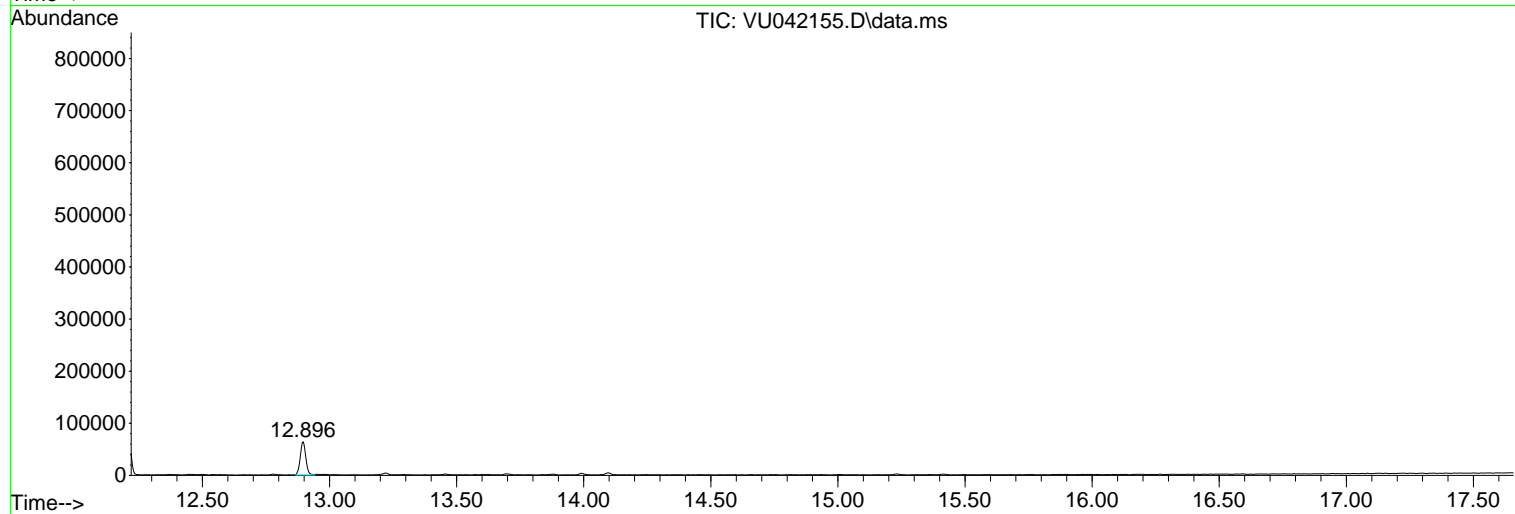
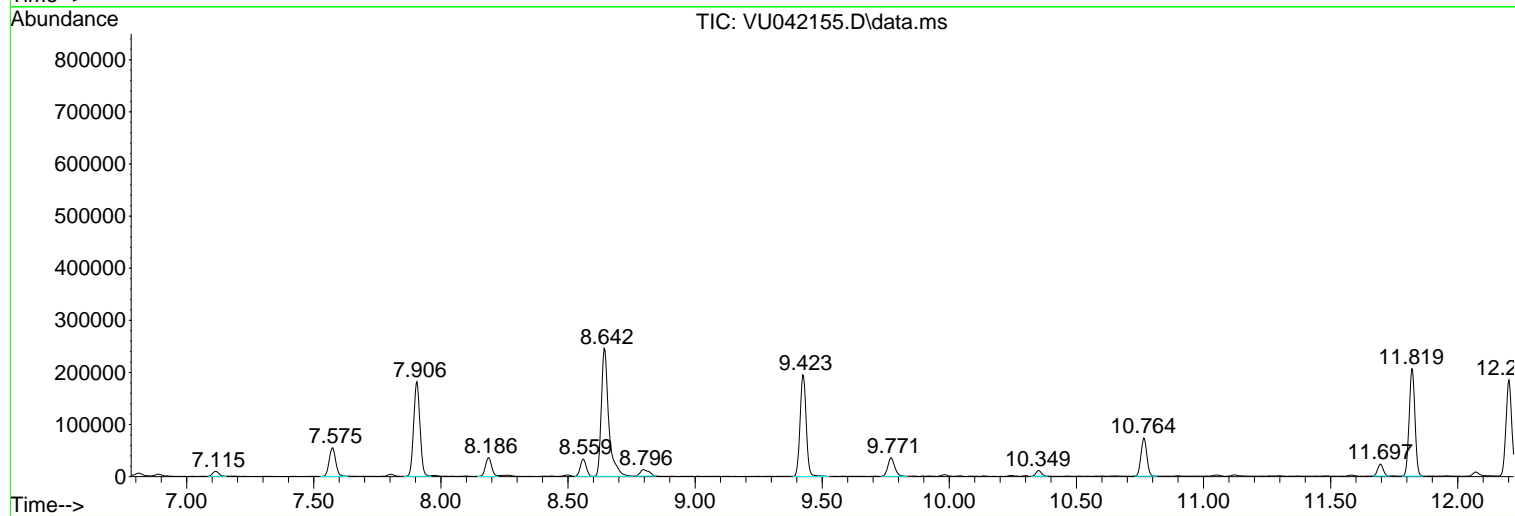
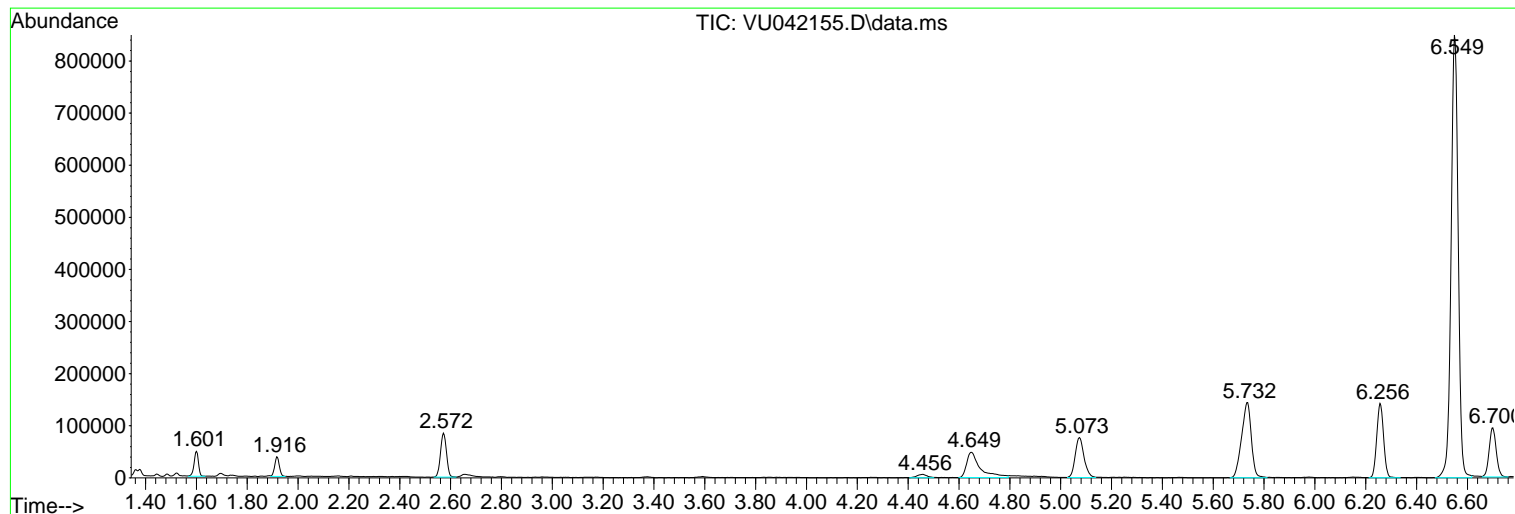
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ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampled :  
BFT99

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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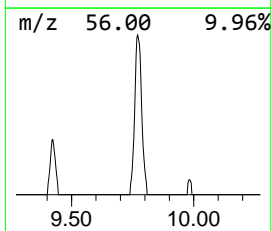
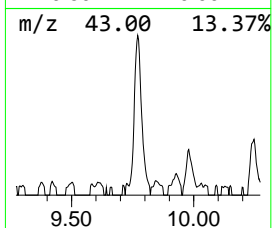
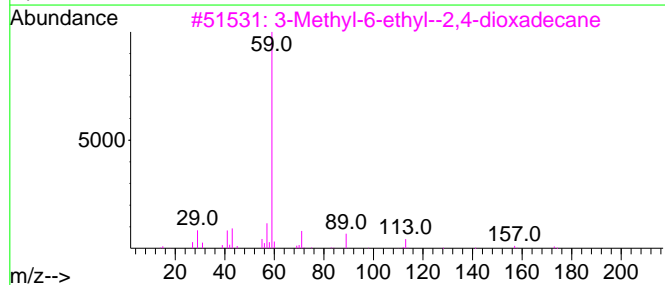
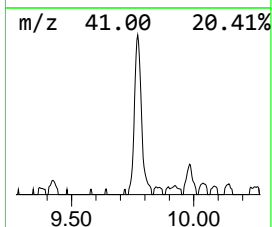
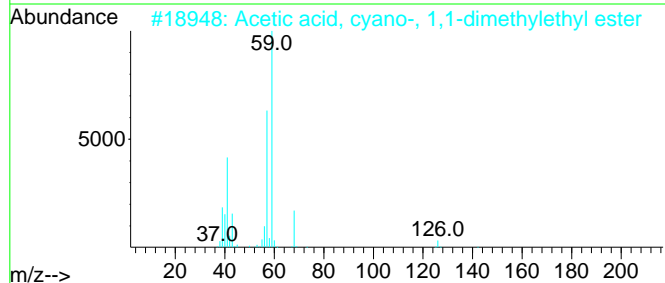
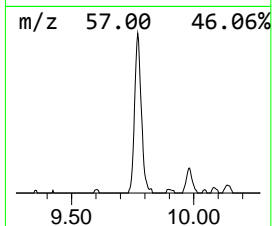
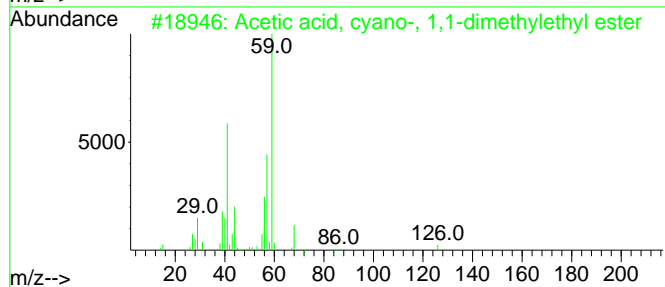
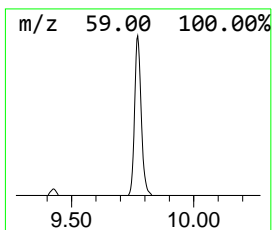
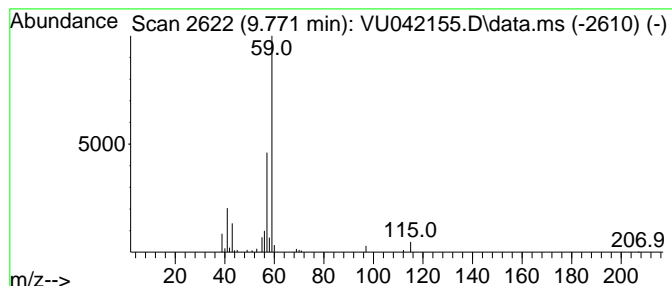
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
 Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 2 Acetic acid, cyano-, 1,1-di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.771	1.03 ug/L	67425	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11N02	001116-98-9	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11N02	001116-98-9	50
3			3-Methyl-6-ethyl--2,4-dioxadecane	188	C11H24O2	1000334-83-2	9
4			2,3-Dimethyl-4-penten-2-ol	114	C7H14O	019781-52-3	9
5			2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	9



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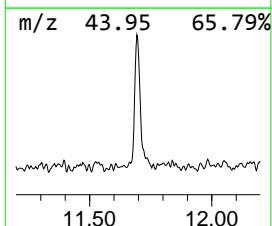
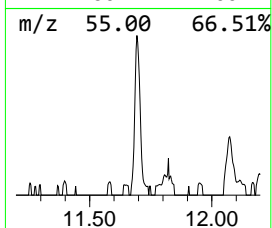
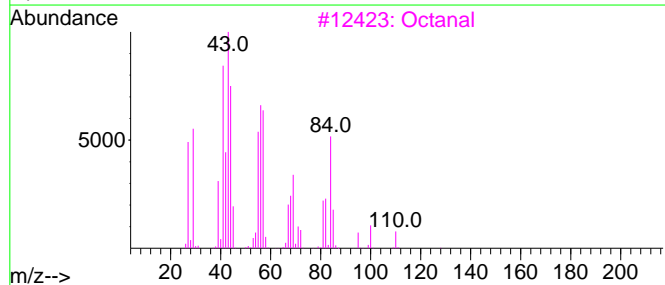
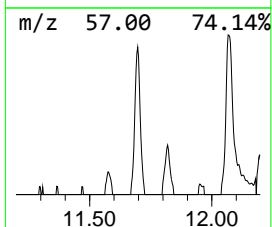
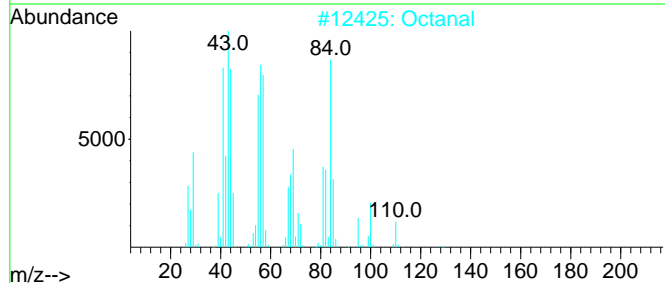
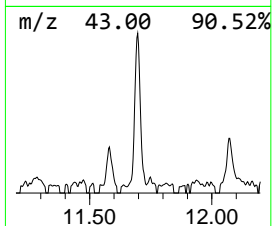
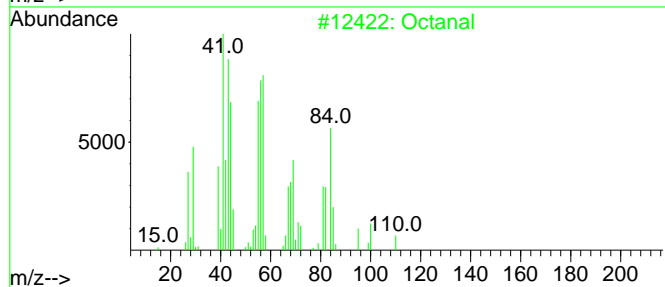
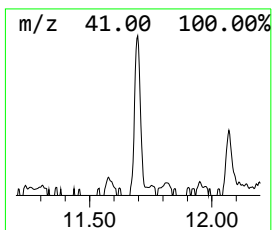
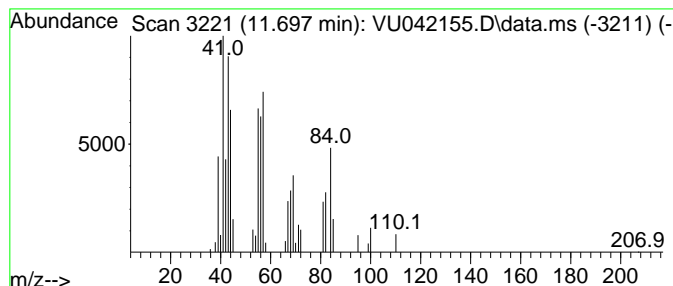
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 Peak Number 3 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.697	0.54 ug/L	34839	1,4-Dichlorobenzene-d4	11.822

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octanal	128	C8H16O	000124-13-0	91
2		Octanal	128	C8H16O	000124-13-0	90
3		Octanal	128	C8H16O	000124-13-0	87
4		Octanal	128	C8H16O	000124-13-0	72
5		Octanal	128	C8H16O	000124-13-0	53



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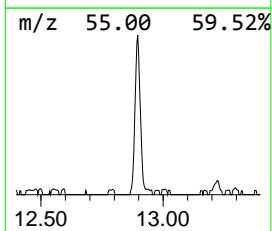
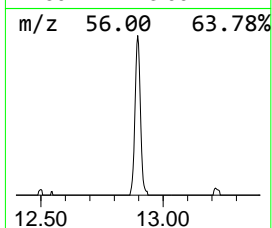
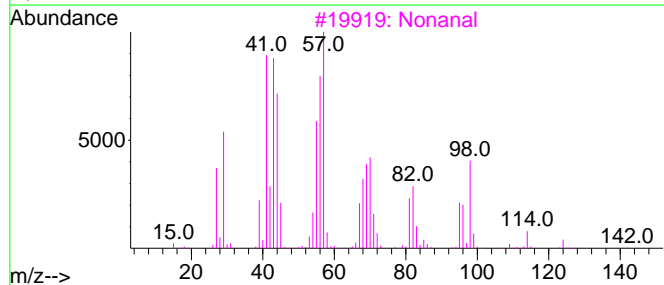
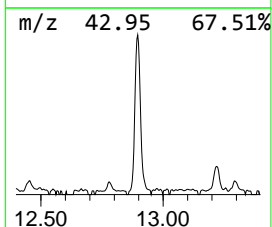
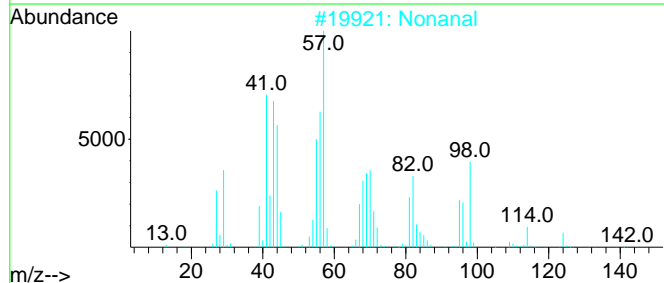
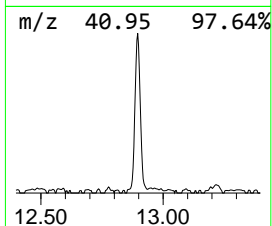
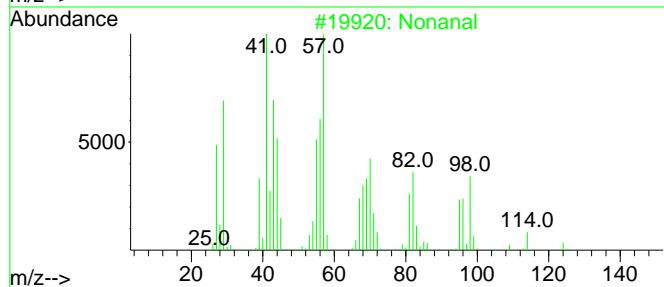
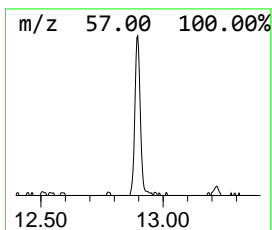
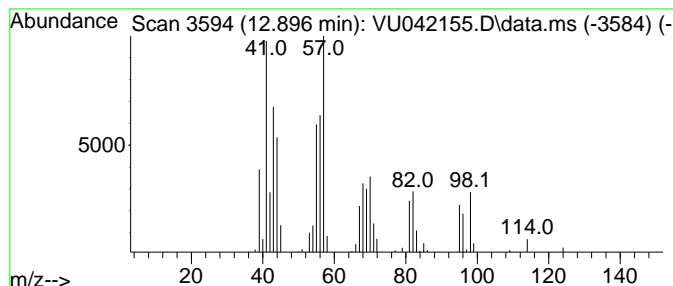
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR012021WMA.M  
 Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.896	1.46 ug/L	94756	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	90
3			Nonanal	142	C9H18O	000124-19-6	72
4			2-Nonen-1-ol, (Z)-	142	C9H18O	041453-56-9	47
5			2-Heptene	98	C7H14	000592-77-8	30



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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, cy...	9.771	1.0	ug/L	67425	2	9.423	325821	5.0
Octanal	11.697	0.5	ug/L	34839	3	11.822	323652	5.0
Nonanal	12.896	1.5	ug/L	94756	3	11.822	323652	5.0