

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100422\
 Data File : VV028324.D
 Acq On : 04 Oct 2022 13:03
 Operator : SY/MD
 Sample : N4730-12RE
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EXFS5RE

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_V\Method\SFAMVTR100322WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV028324.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	17	20	41	rVB3	11776	23061	3.61%	0.406%
2	1.304	74	82	97	rBV2	221448	241958	37.91%	4.261%
3	1.384	97	107	147	rBV	92206	422067	66.13%	7.433%
4	1.564	156	163	179	rVB	79167	100303	15.72%	1.766%
5	2.101	321	330	351	rVB	149305	233051	36.52%	4.104%
6	2.757	523	534	556	rVB3	7942	16994	2.66%	0.299%
7	3.905	878	891	924	rBV2	130561	415157	65.05%	7.312%
8	4.342	1010	1027	1053	rBV2	99235	252031	39.49%	4.439%
9	5.043	1229	1245	1280	rBV2	231114	638223	100.00%	11.240%
10	5.612	1411	1422	1441	rBV	158886	323845	50.74%	5.703%
11	5.915	1506	1516	1533	rBV4	14340	29522	4.63%	0.520%
12	6.066	1550	1563	1594	rBV	134802	280613	43.97%	4.942%
13	6.985	1838	1849	1871	rBV2	57977	114541	17.95%	2.017%
14	7.313	1939	1951	1971	rBV	246291	440163	68.97%	7.752%
15	7.622	2035	2047	2066	rBV2	35503	67557	10.59%	1.190%
16	8.088	2182	2192	2225	rBV	310759	612666	96.00%	10.790%
17	8.850	2414	2429	2450	rBV	256171	427826	67.03%	7.535%
18	10.213	2839	2853	2870	rBV2	118037	187842	29.43%	3.308%
19	10.381	2895	2905	2912	rBV2	4180	6474	1.01%	0.114%
20	11.246	3162	3174	3199	rBV	248073	391997	61.42%	6.904%
21	11.529	3253	3262	3280	rBV2	26005	51244	8.03%	0.902%
22	11.619	3280	3290	3305	rVV	252246	400979	62.83%	7.062%

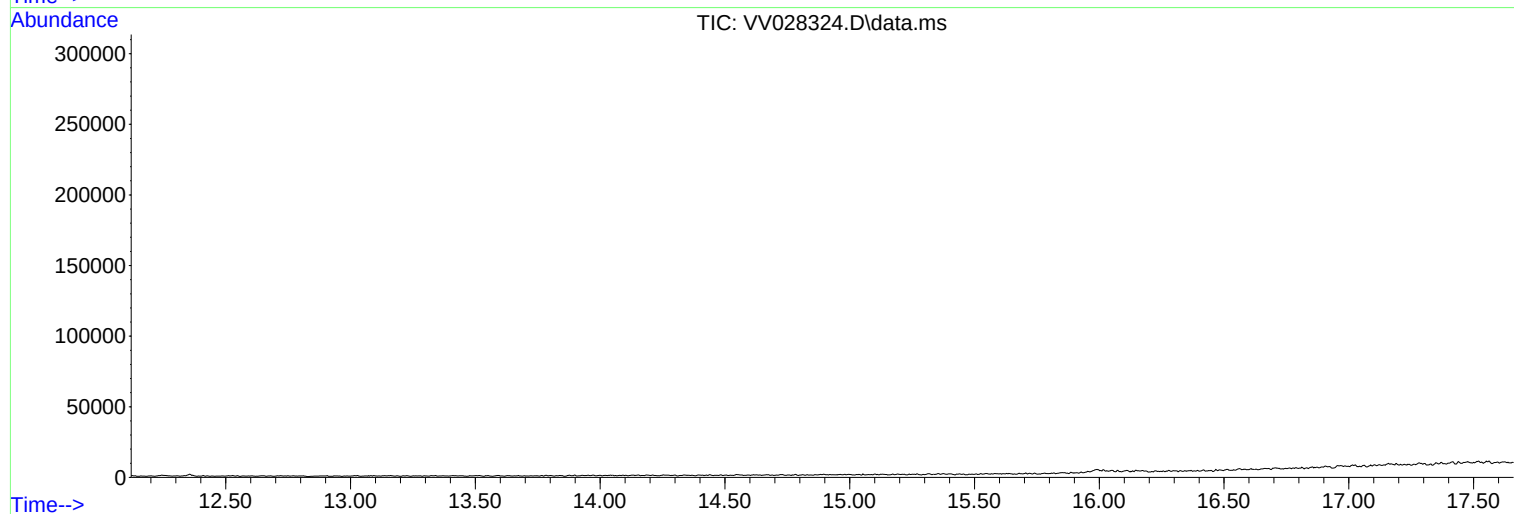
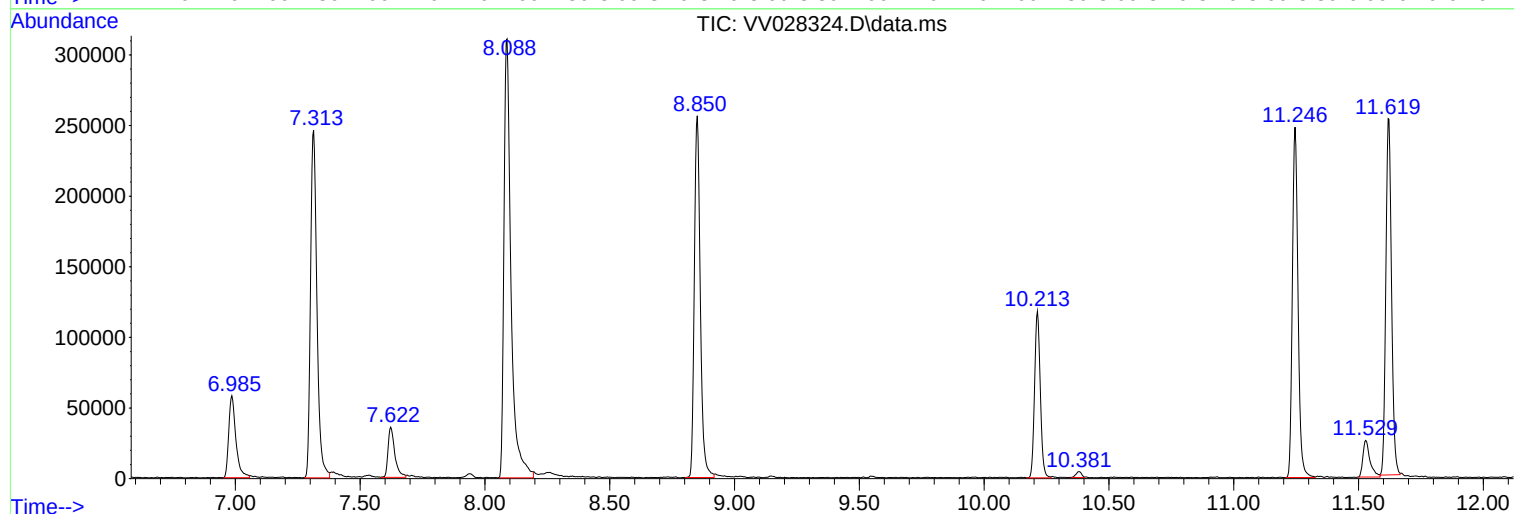
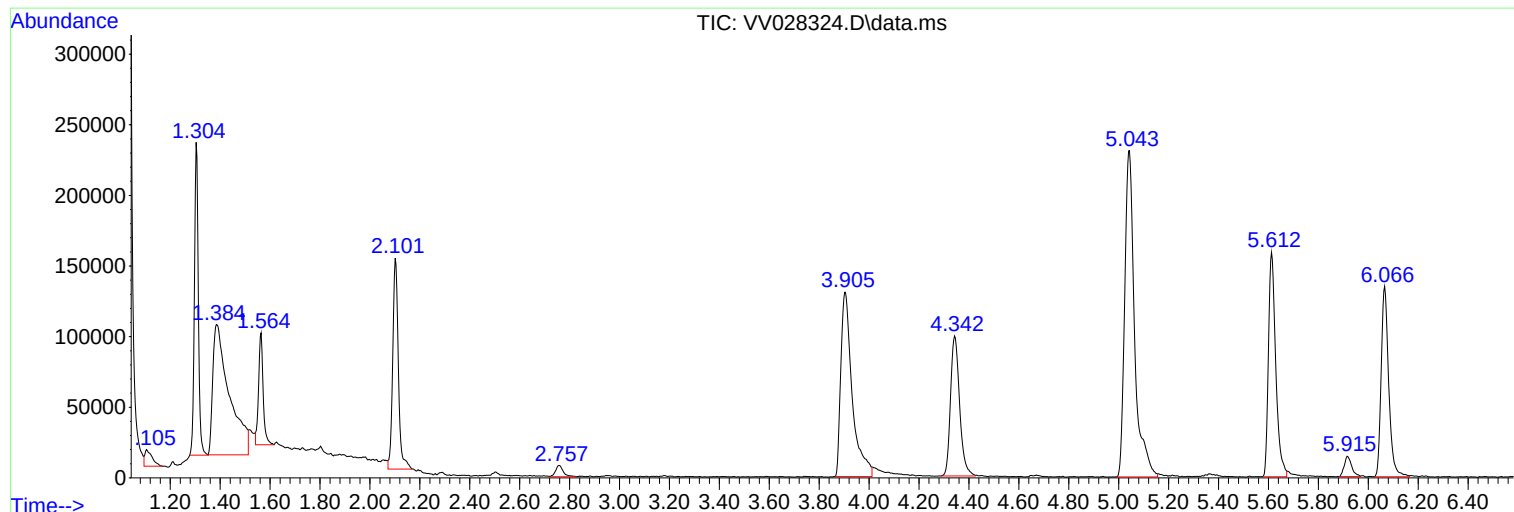
Sum of corrected areas: 5678114

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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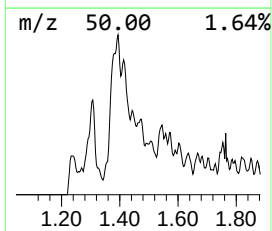
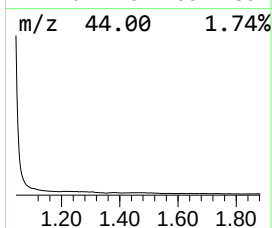
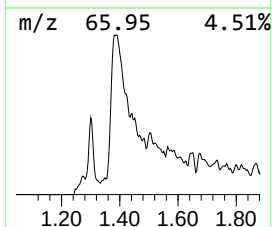
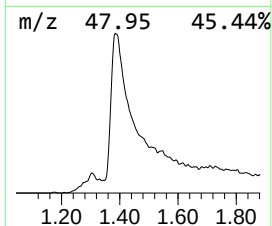
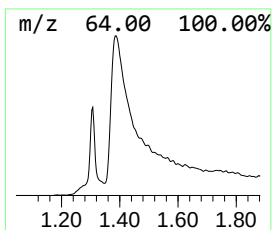
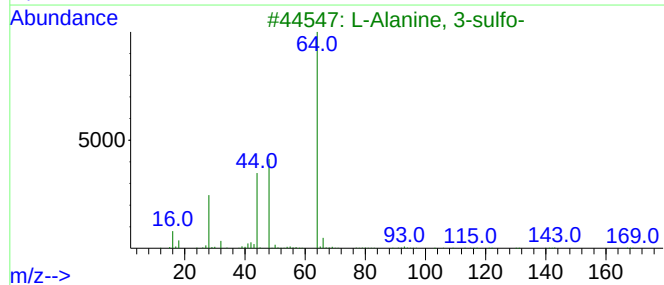
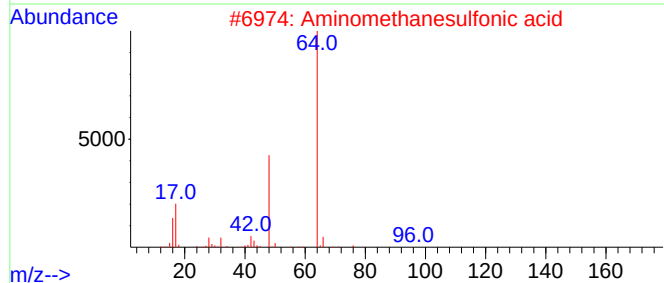
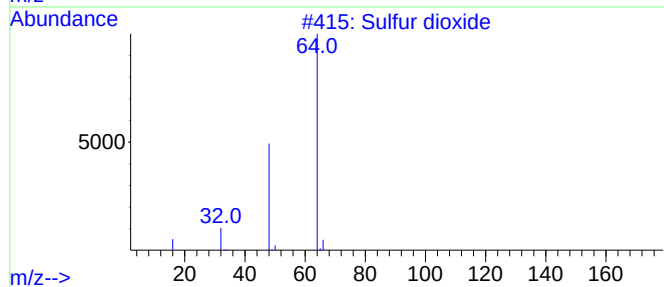
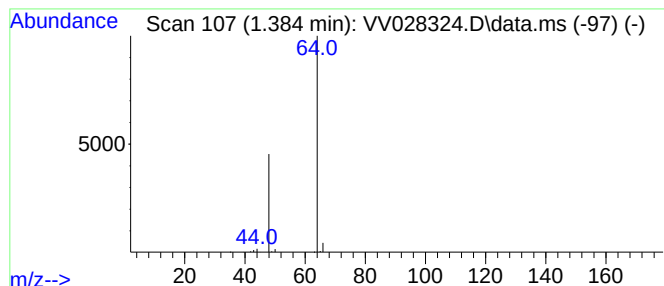
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.384	6.52 ug/L	422067	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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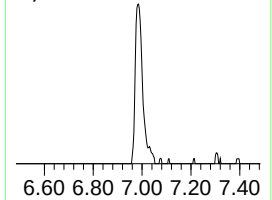
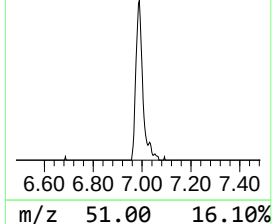
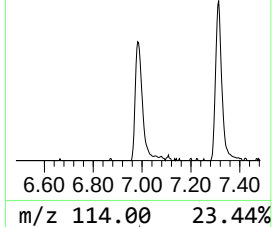
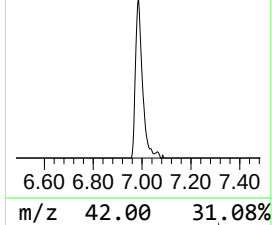
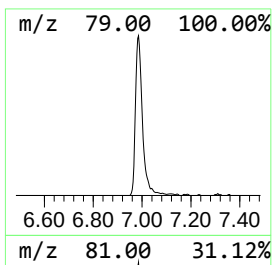
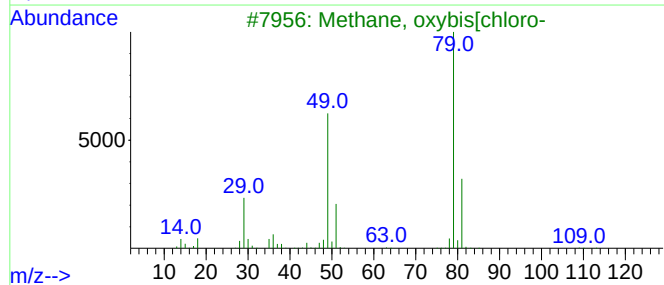
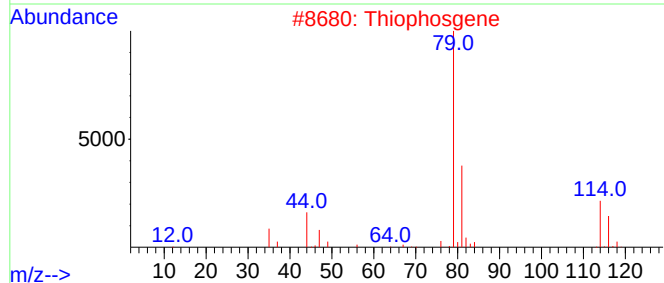
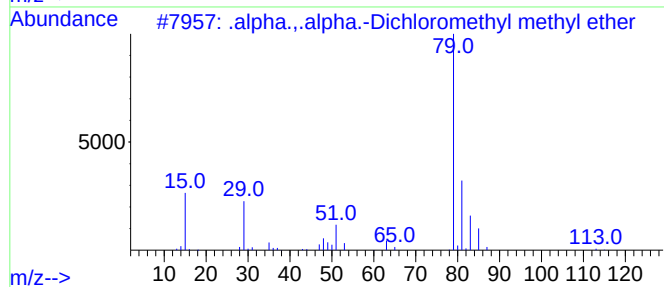
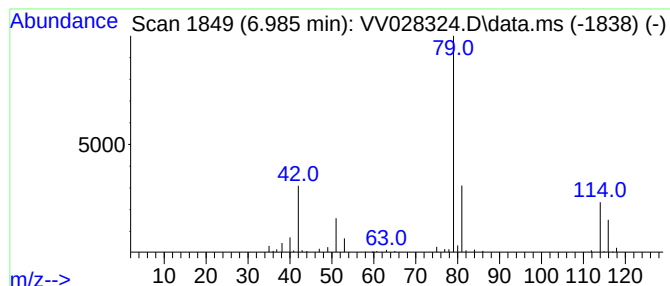
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 .alpha.,.alpha.-Dichloromet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.985	1.77 ug/L	114541	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	.	.alpha.,.alpha.-Dichloromethyl m...	114	C2H4Cl2O	004885-02-3	50
2			Thiophosgene	114	CCl2S	000463-71-8	45
3			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	40
4			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	33
5			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	28



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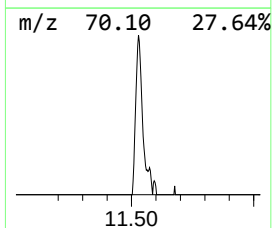
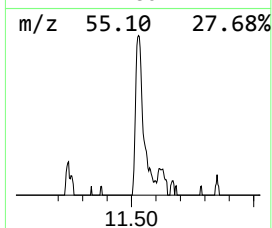
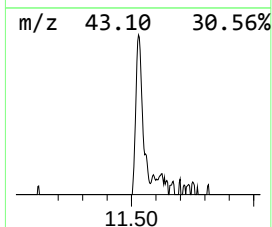
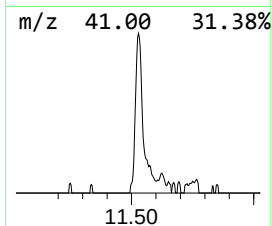
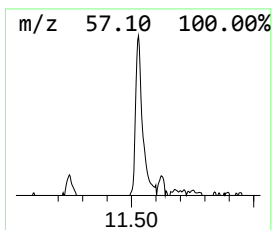
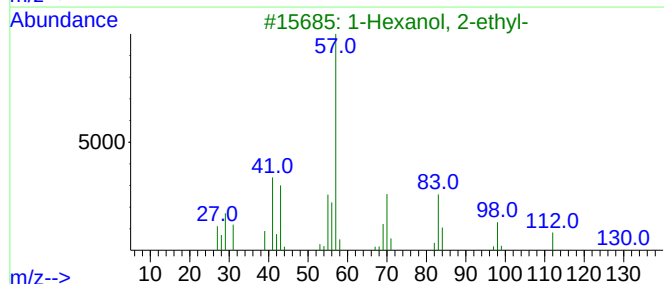
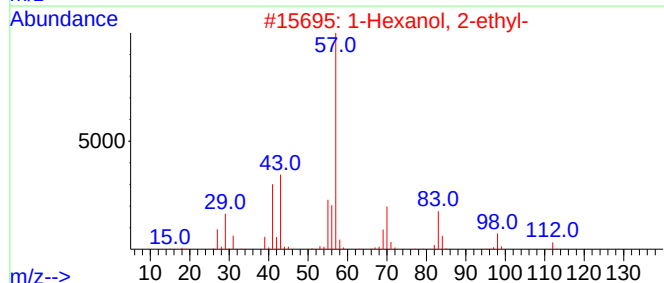
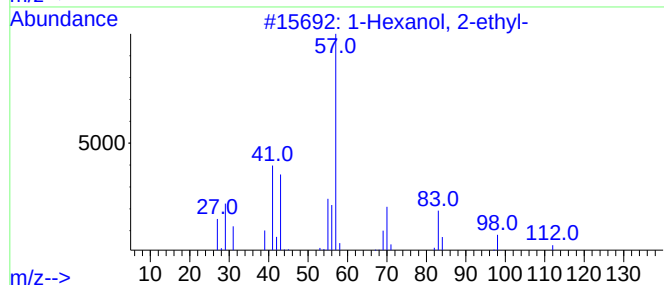
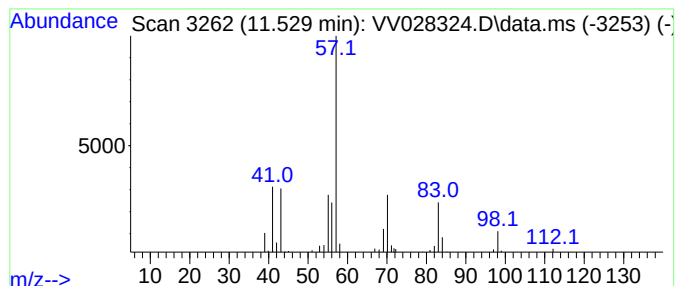
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.528	0.65 ug/L	51244	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.384	6.5	ug/L	422067	1	5.612	323845	5.0
.alpha.,.alpha....	6.985	1.8	ug/L	114541	1	5.612	323845	5.0
1-Hexanol, 2-et...	11.528	0.7	ug/L	51244	3	11.246	391997	5.0