

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111323\
 Data File : VU056290.D
 Acq On : 14 Nov 2023 07:47
 Operator : MD/SY
 Sample : 05372-20
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GCDR4

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\SFAMUTR111323WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU056290.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.460	44	53	69	rBV	567198	890089	96.87%	10.182%
2	1.599	89	96	109	rVB	92253	121700	13.24%	1.392%
3	1.911	186	193	204	rVB	72181	95269	10.37%	1.090%
4	2.451	353	361	377	rVB2	33379	58793	6.40%	0.673%
5	2.563	383	396	407	rBV	167537	280142	30.49%	3.205%
6	2.628	407	416	445	rVB	136522	282212	30.71%	3.228%
7	2.817	452	475	476	rBV5	34187	80844	8.80%	0.925%
8	3.869	792	802	816	rBV	7224	17669	1.92%	0.202%
9	4.621	1020	1036	1057	rBV	106091	325143	35.39%	3.719%
10	5.058	1154	1172	1191	rBV	157377	350632	38.16%	4.011%
11	5.721	1358	1378	1409	rBV2	298602	780006	84.89%	8.923%
12	6.245	1528	1541	1571	rBV	358210	704639	76.69%	8.060%
13	6.544	1624	1634	1647	rBV4	10898	19776	2.15%	0.226%
14	6.685	1661	1678	1697	rBV	186449	364750	39.70%	4.172%
15	6.782	1700	1708	1724	rVV2	6480	13988	1.52%	0.160%
16	7.158	1807	1825	1840	rBV2	29022	60743	6.61%	0.695%
17	7.563	1939	1951	1968	rBV	85819	153942	16.75%	1.761%
18	7.894	2041	2054	2076	rBV	351320	642946	69.97%	7.355%
19	8.177	2131	2142	2157	rBV2	49479	86301	9.39%	0.987%
20	8.553	2247	2259	2271	rBV5	6979	11900	1.30%	0.136%
21	8.631	2271	2283	2299	rBV	385853	736265	80.13%	8.422%
22	9.412	2512	2526	2562	rBV	516366	918871	100.00%	10.511%
23	10.135	2744	2751	2765	rVB4	5557	9884	1.08%	0.113%
24	10.753	2930	2943	2963	rBV	137817	223476	24.32%	2.556%
25	11.807	3258	3271	3292	rBV	481451	798937	86.95%	9.139%
26	12.065	3332	3351	3371	rBV2	46216	126191	13.73%	1.444%
27	12.187	3378	3389	3420	rVB	328755	575452	62.63%	6.583%
28	16.881	4841	4849	4856	rBV4	8939	11382	1.24%	0.130%

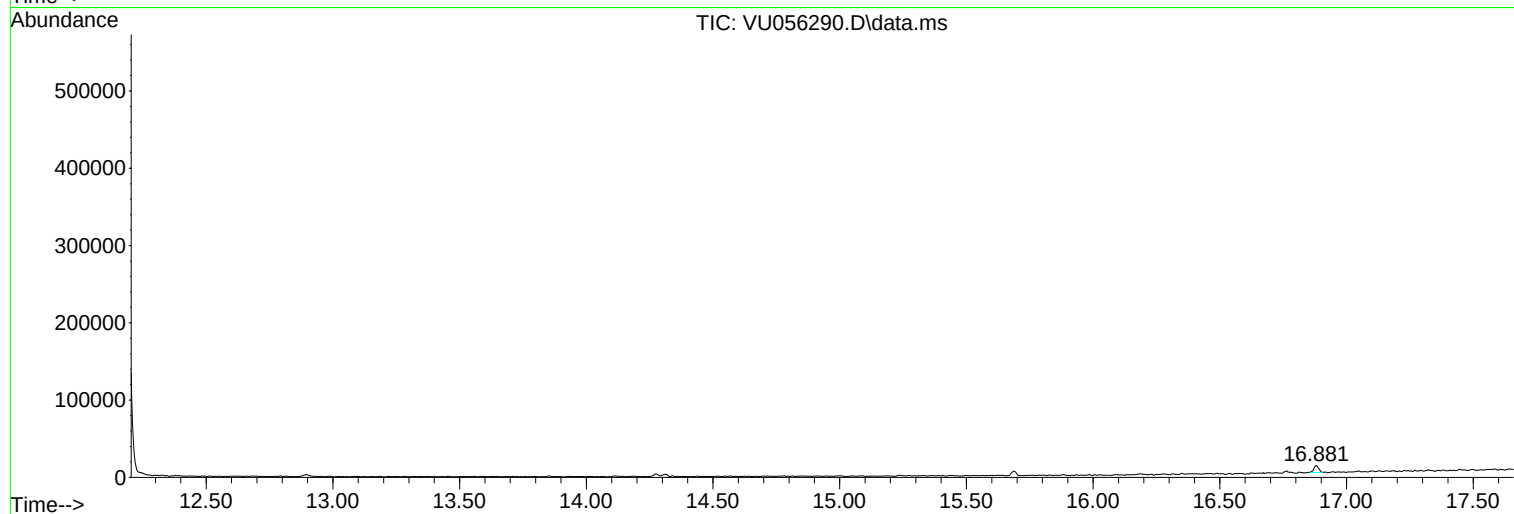
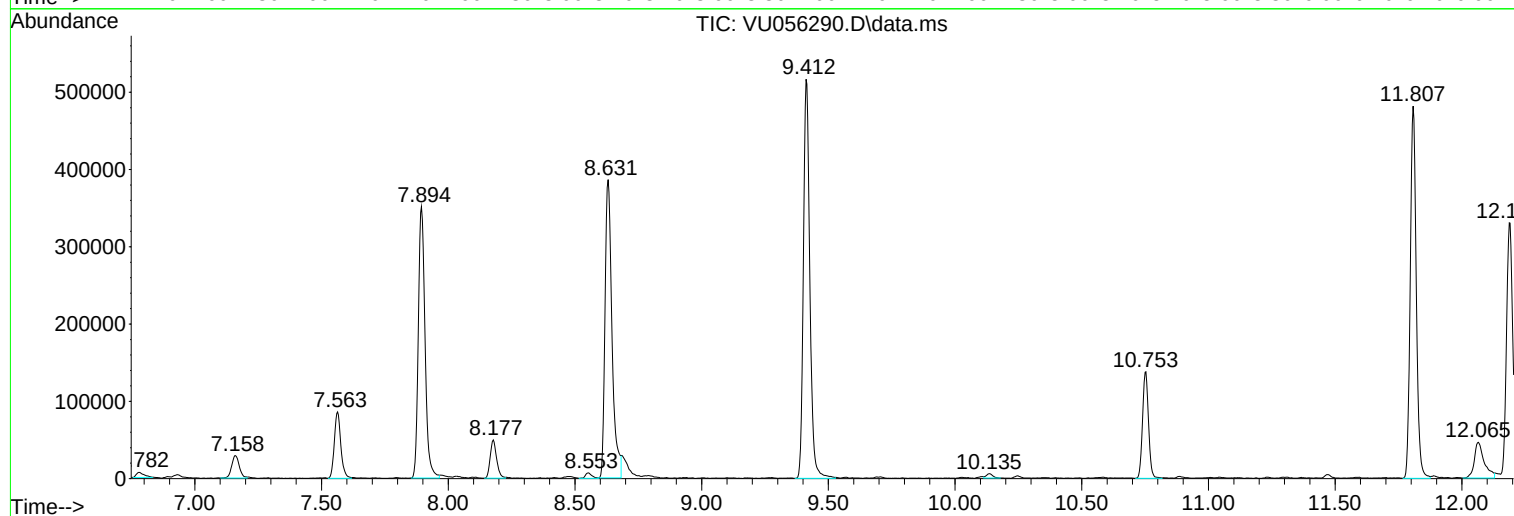
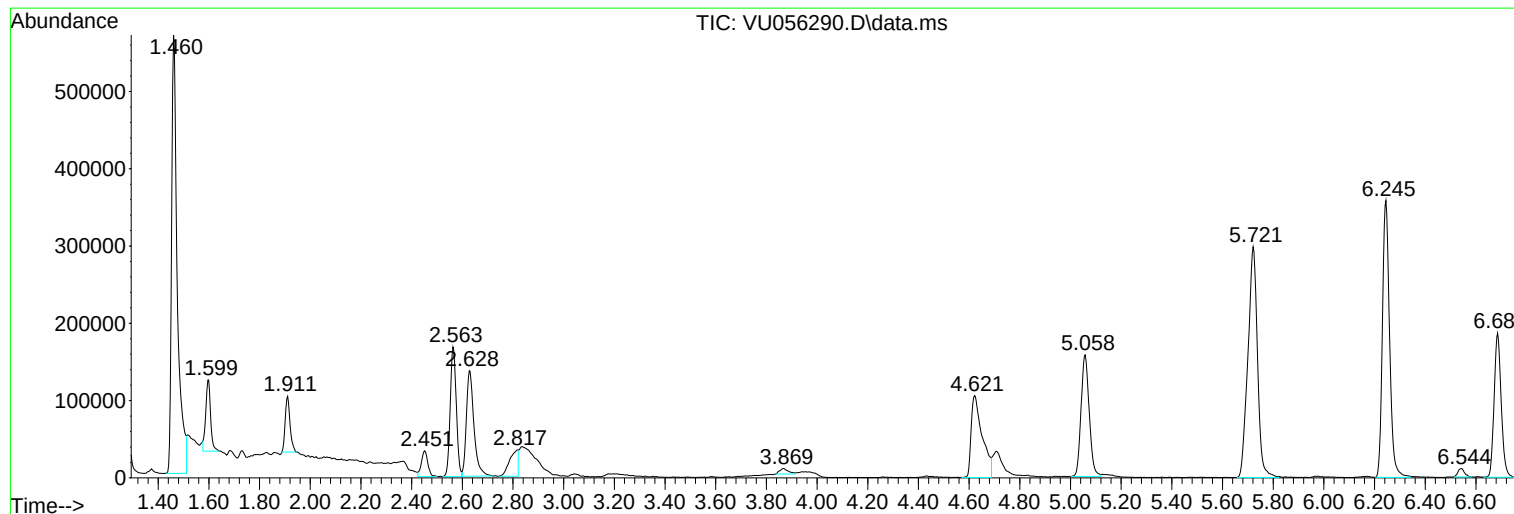
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ClientSampleId :
GCDR4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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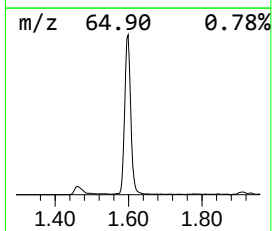
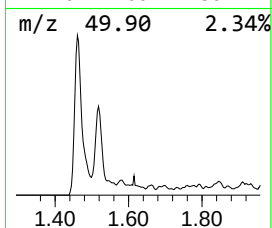
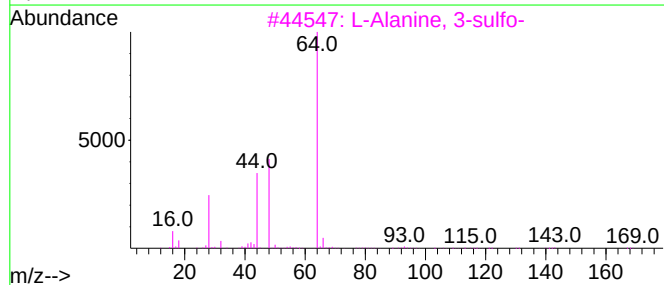
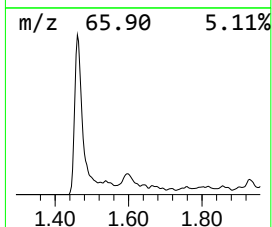
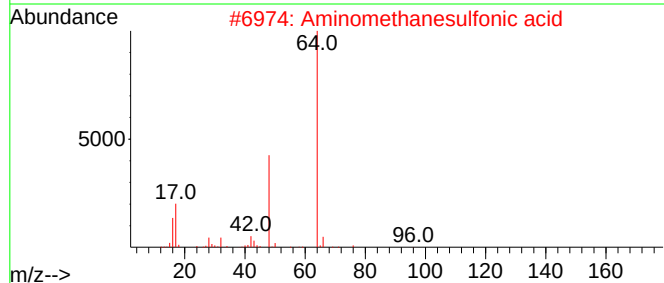
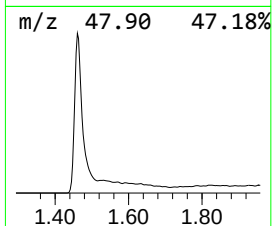
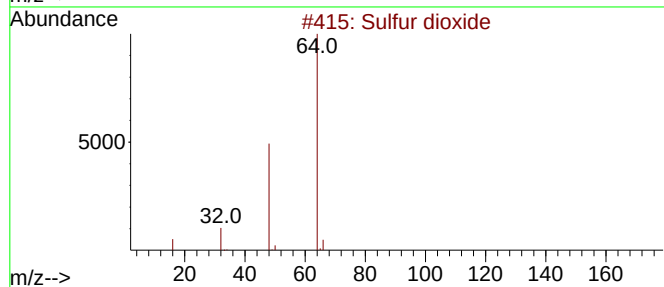
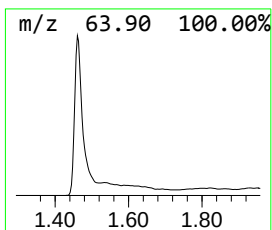
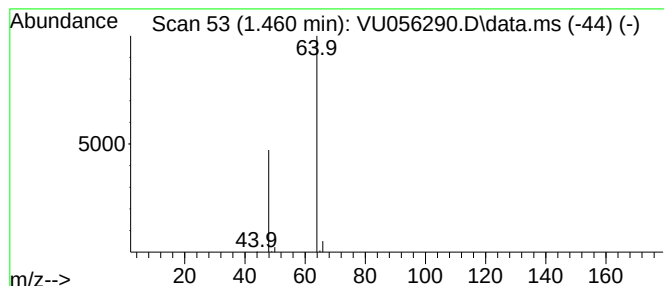
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.460	6.32 ug/L	890089	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
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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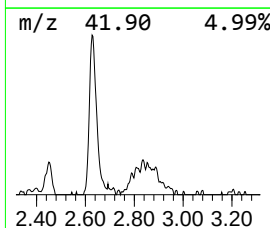
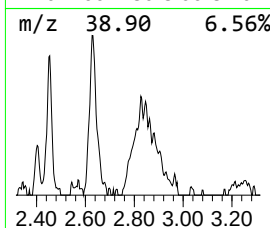
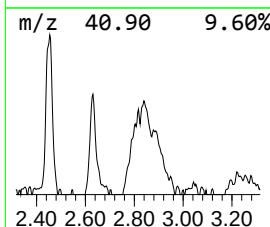
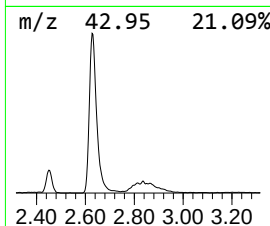
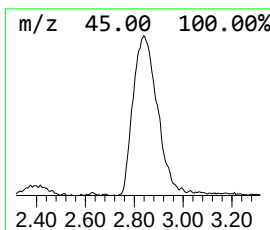
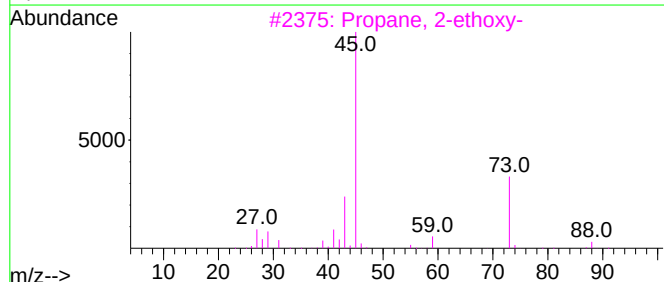
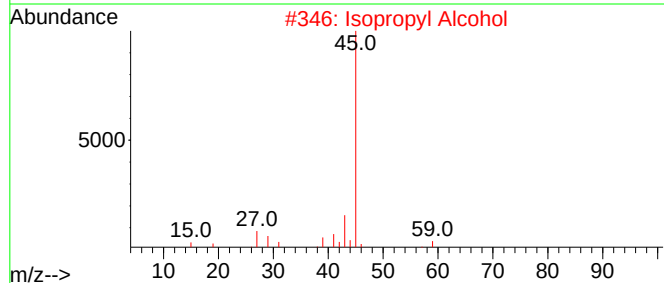
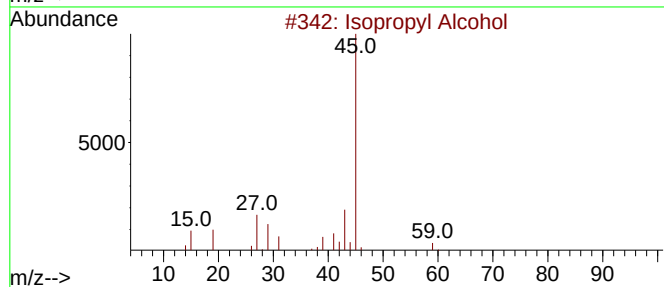
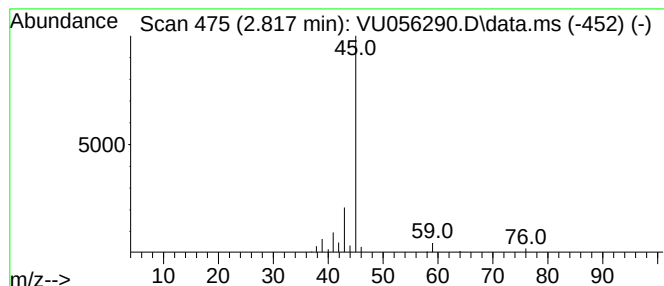
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.817	0.57 ug/L	80844	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9



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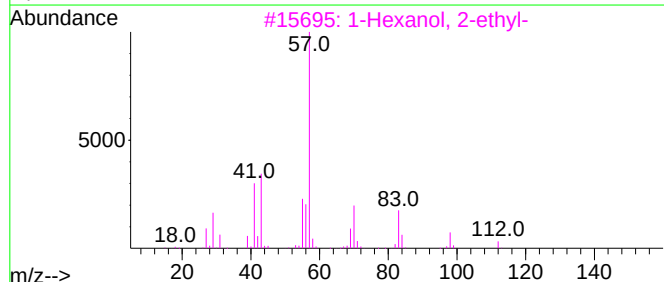
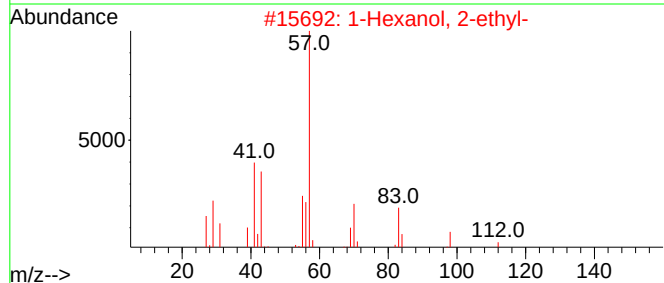
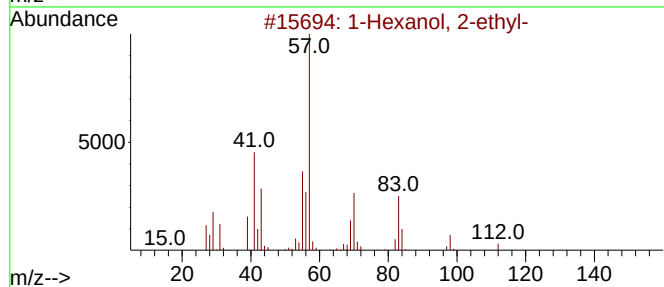
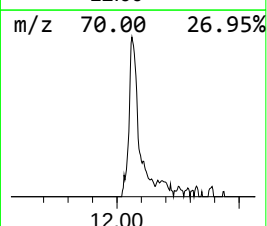
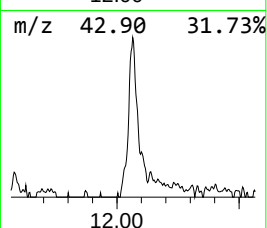
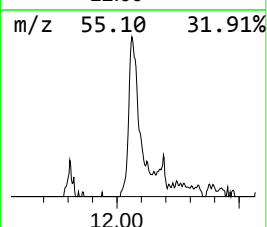
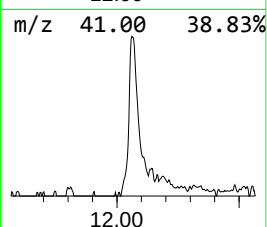
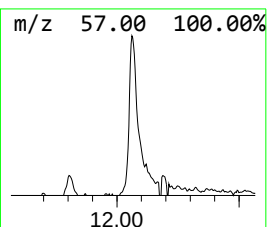
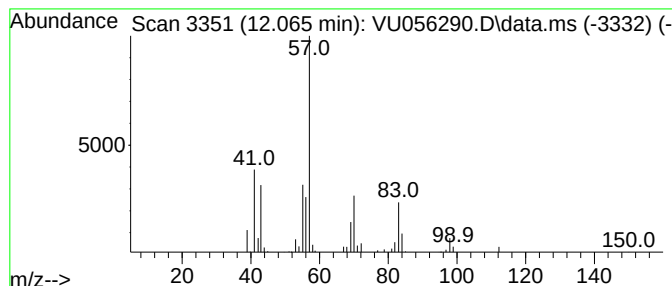
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.065	0.79 ug/L	126191	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72



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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	1.460	6.3	ug/L	890089	1	6.245	704639	5.0
Isopropyl Alcohol	2.817	0.6	ug/L	80844	1	6.245	704639	5.0
1-Hexanol, 2-et...	12.065	0.8	ug/L	126191	3	11.807	798937	5.0