

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051823\
 Data File : VU054179.D
 Acq On : 18 May 2023 20:53
 Operator : JC/MD
 Sample : 02844-13
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBX07

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\SFAMUTR051823WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU054179.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	21	rVB2	68041	66090	13.47%	1.478%
2	1.485	35	45	65	rBV2	53064	167067	34.06%	3.737%
3	1.597	70	80	92	rVB2	66587	127929	26.08%	2.861%
4	1.912	171	178	192	rVB	44530	61693	12.58%	1.380%
5	2.565	367	381	394	rBV	101695	168673	34.39%	3.773%
6	2.642	394	405	431	rVB2	24427	64872	13.23%	1.451%
7	3.041	523	529	541	rVB5	5569	10300	2.10%	0.230%
8	3.848	770	780	800	rVB4	14525	35587	7.26%	0.796%
9	4.629	1010	1023	1058	rBV	45061	141469	28.84%	3.164%
10	4.806	1068	1078	1105	rVB3	17708	44410	9.05%	0.993%
11	5.057	1141	1156	1186	rVB	86443	208335	42.48%	4.660%
12	5.385	1244	1258	1270	rVB4	8434	17582	3.58%	0.393%
13	5.719	1341	1362	1387	rBV2	169909	431155	87.91%	9.644%
14	6.243	1512	1525	1546	rBV2	207549	399949	81.55%	8.946%
15	6.536	1607	1616	1629	rBV7	6009	10914	2.23%	0.244%
16	6.684	1645	1662	1683	rBV2	98454	195795	39.92%	4.379%
17	7.562	1923	1935	1959	rBV2	50871	89847	18.32%	2.010%
18	7.893	2026	2038	2053	rBV	213551	366121	74.65%	8.189%
19	7.967	2053	2061	2075	rVB	13233	23234	4.74%	0.520%
20	8.176	2114	2126	2141	rBV2	30449	50833	10.36%	1.137%
21	8.629	2256	2267	2302	rBV2	172142	336487	68.61%	7.526%
22	8.928	2350	2360	2374	rBV4	4505	9416	1.92%	0.211%
23	9.414	2498	2511	2532	rBV	284968	490464	100.00%	10.970%
24	10.751	2915	2927	2943	rVB	70300	113696	23.18%	2.543%
25	11.806	3243	3255	3275	rBV	302115	481232	98.12%	10.764%
26	12.063	3325	3335	3358	rBV3	11838	31798	6.48%	0.711%
27	12.189	3361	3374	3391	rVV	189070	314522	64.13%	7.035%
28	17.282	4952	4958	4966	rVB2	8429	11375	2.32%	0.254%

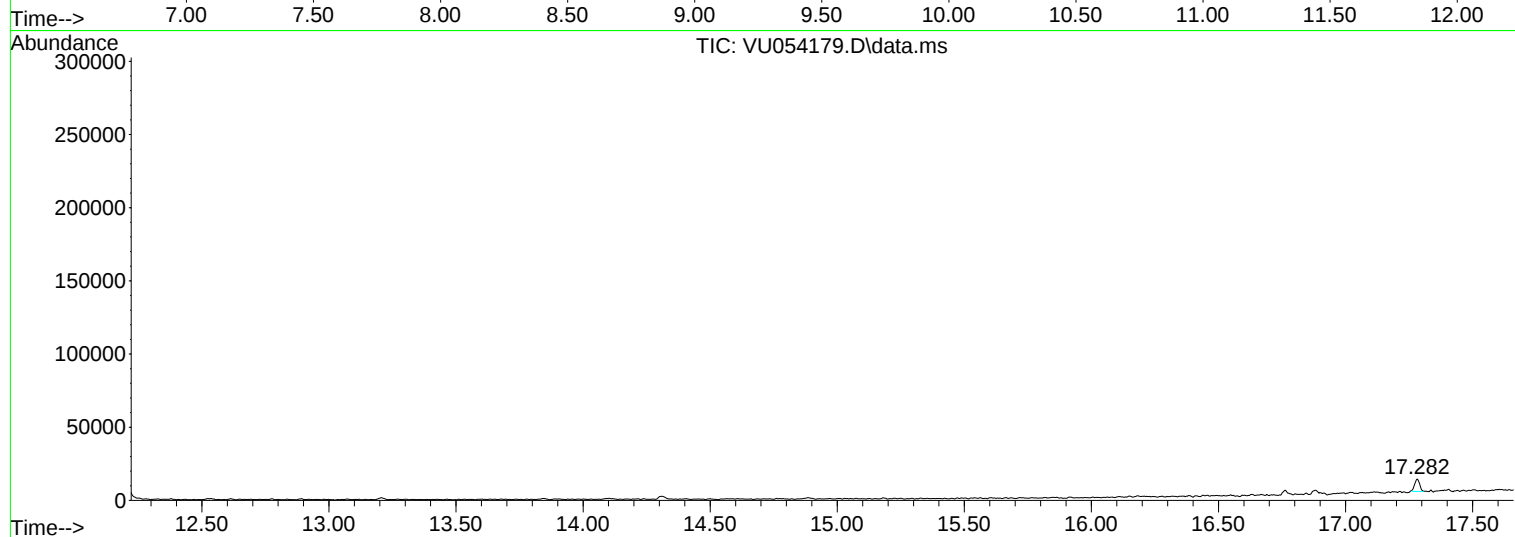
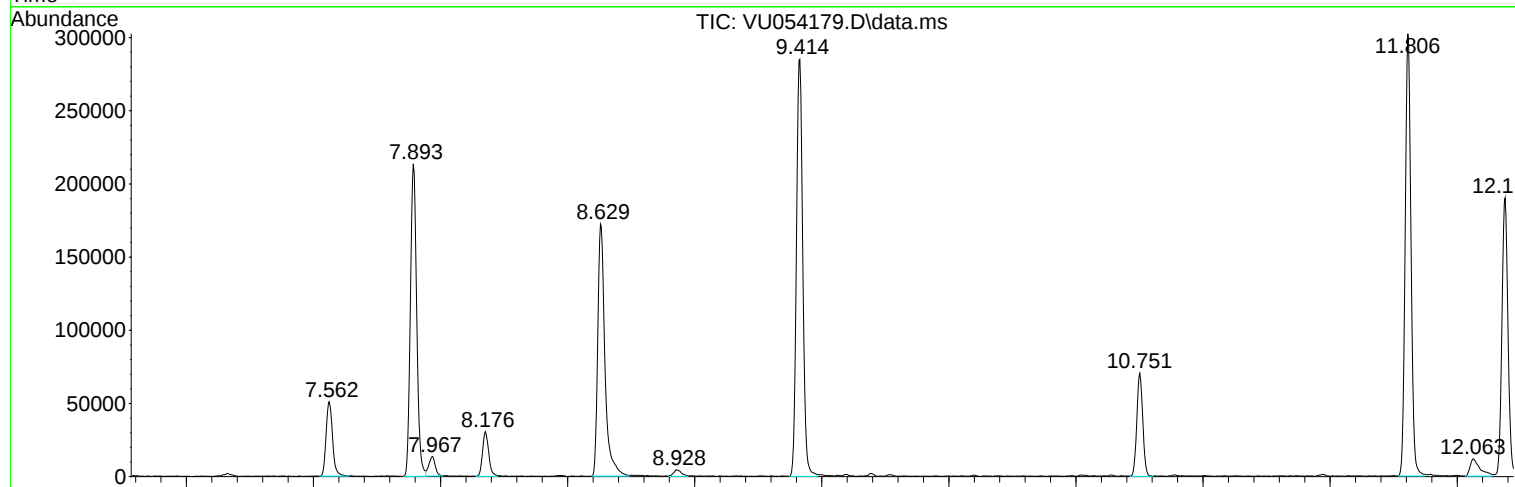
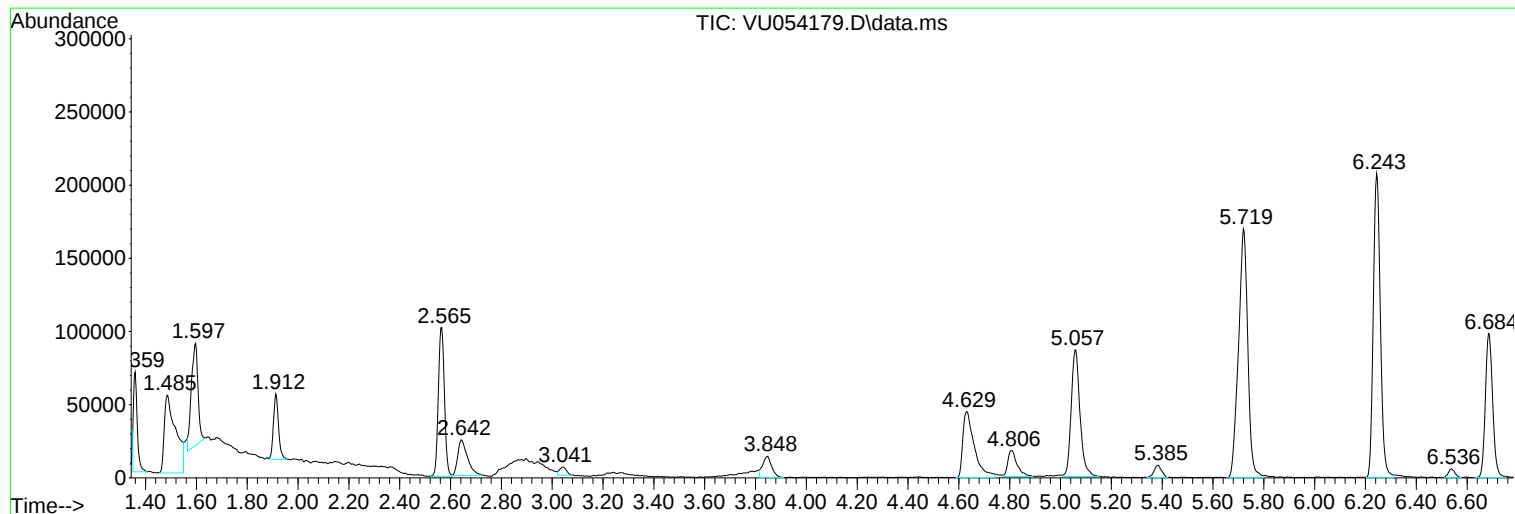
Sum of corrected areas: 4470845

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR051823WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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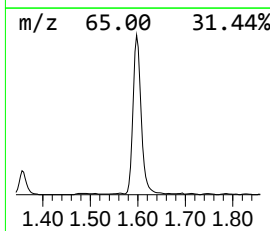
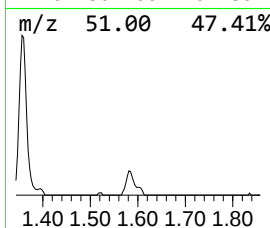
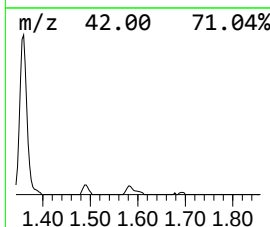
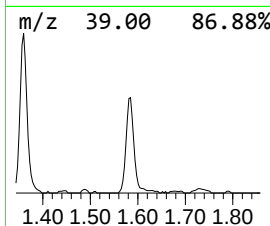
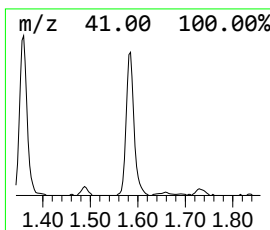
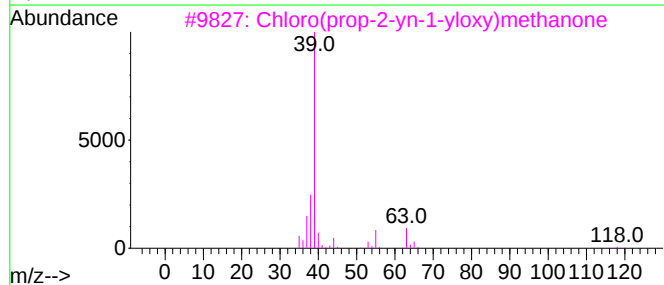
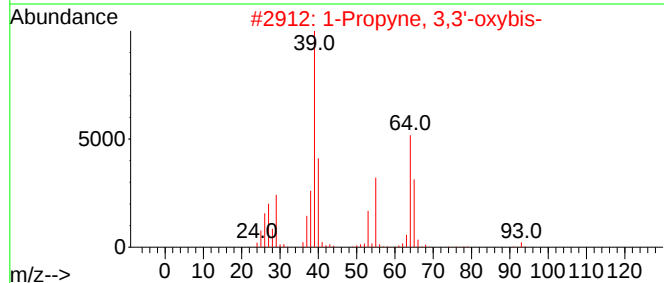
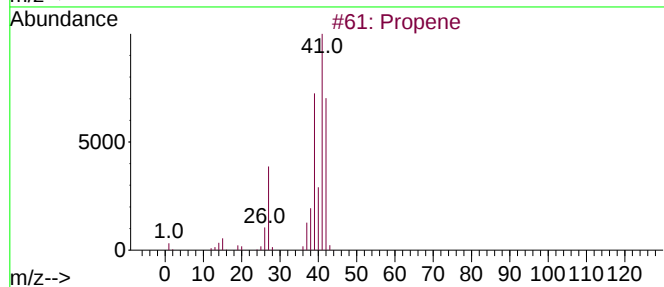
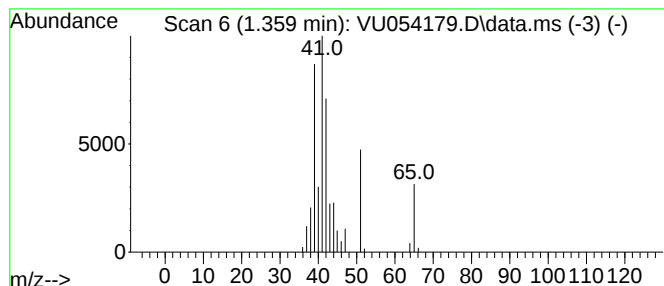
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR051823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	0.83 ug/L	66090	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	72
2			1-Propyne, 3,3'-oxybis-	94	C6H6O	006921-27-3	45
3			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	38
4			Propene	42	C3H6	000115-07-1	38
5			Cyclopropane	42	C3H6	000075-19-4	10



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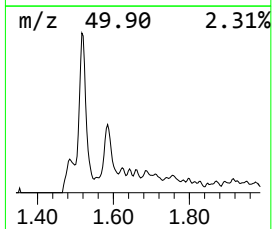
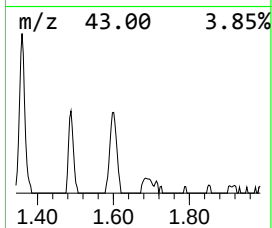
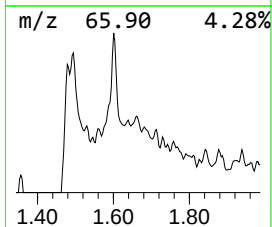
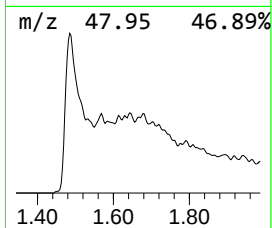
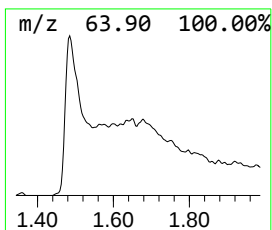
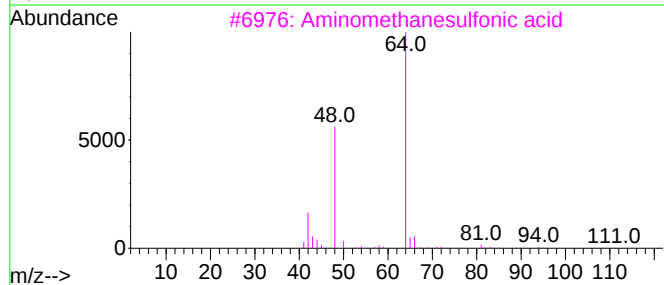
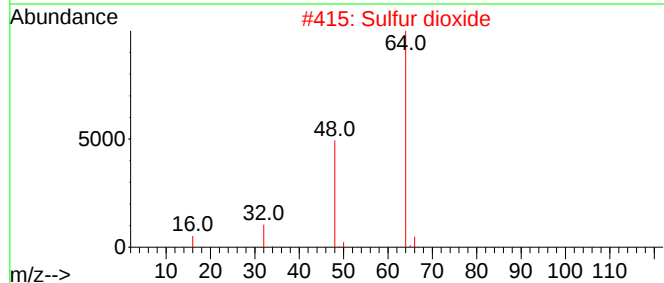
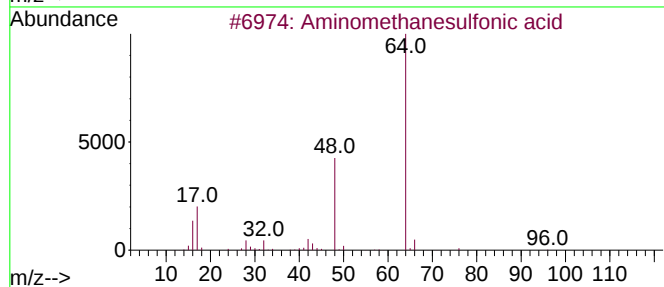
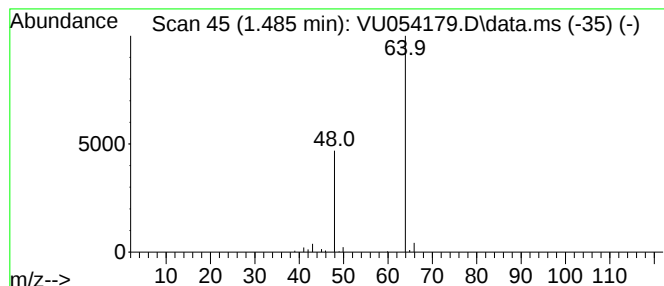
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.485	2.09 ug/L	167067	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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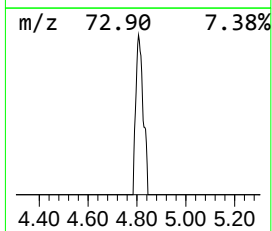
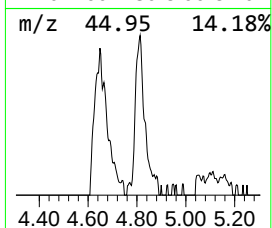
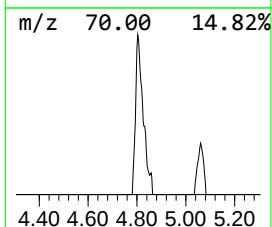
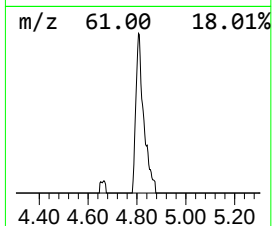
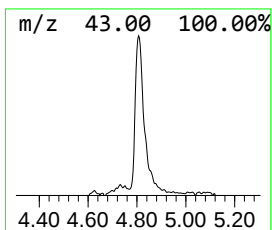
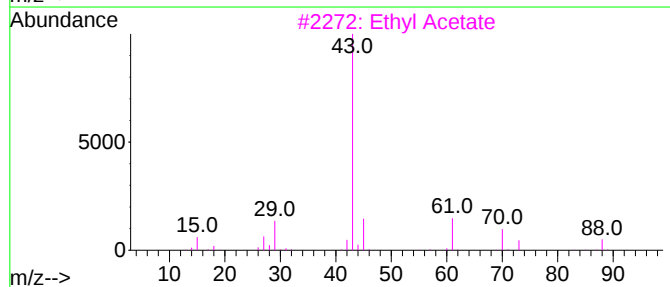
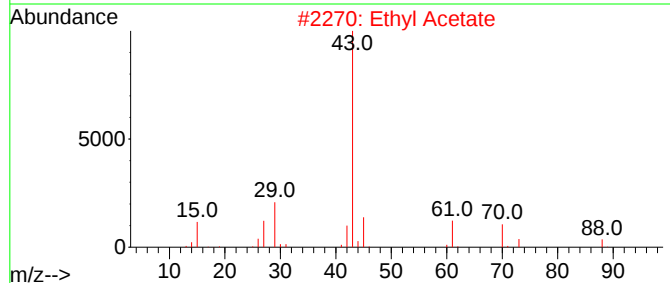
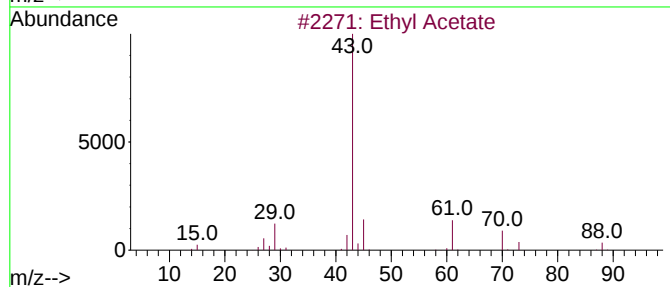
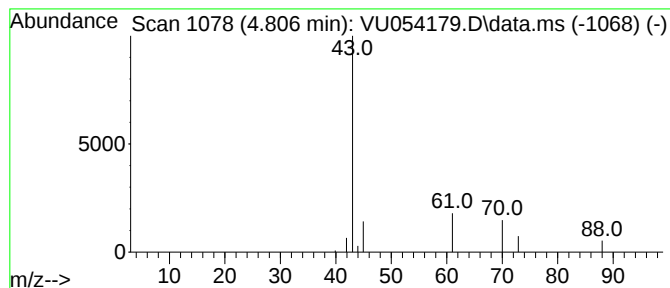
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.806	0.56 ug/L	44410	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	83
4			Ethyl Acetate	88	C4H8O2	000141-78-6	83
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	78



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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
(DEL) Alkane: S...	1.359	0.8	ug/L	66090	1	6.243	399949	5.0
Aminomethanesul...	1.485	2.1	ug/L	167067	1	6.243	399949	5.0
Ethyl Acetate	4.806	0.6	ug/L	44410	1	6.243	399949	5.0