

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122922\
 Data File : VU052611.D
 Acq On : 29 Dec 2022 17:51
 Operator : JC/MD
 Sample : N6216-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H0AA9

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\SFAMUTR122022WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU052611.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.360	3	6	26	rVB	69283	70600	5.90%	0.700%
2	1.601	70	81	95	rVB2	130318	169893	14.19%	1.685%
3	1.916	170	179	196	rVV	99475	135718	11.33%	1.346%
4	2.569	370	382	399	rBV	180610	295264	24.66%	2.929%
5	3.044	518	530	545	rBV4	10044	20693	1.73%	0.205%
6	4.433	945	962	979	rBV3	15411	39947	3.34%	0.396%
7	4.662	1012	1033	1098	rBV3	116146	562616	46.98%	5.581%
8	5.060	1141	1157	1180	rBV	156577	362799	30.30%	3.599%
9	5.459	1266	1281	1296	rVB4	14801	32251	2.69%	0.320%
10	5.723	1342	1363	1390	rBV2	321573	850191	71.00%	8.433%
11	5.896	1404	1417	1432	rVB3	43049	97344	8.13%	0.966%
12	6.247	1510	1526	1550	rBV	255063	489162	40.85%	4.852%
13	6.539	1603	1617	1631	rBV2	61967	118781	9.92%	1.178%
14	6.687	1648	1663	1689	rBV	210522	459327	38.36%	4.556%
15	6.803	1689	1699	1709	rVV2	32895	63243	5.28%	0.627%
16	6.861	1709	1717	1729	rVV3	36507	69697	5.82%	0.691%
17	7.070	1766	1782	1794	rVB8	23756	54013	4.51%	0.536%
18	7.247	1821	1837	1853	rVB5	45928	122553	10.23%	1.216%
19	7.379	1865	1878	1891	rVB3	31741	61954	5.17%	0.615%
20	7.469	1897	1906	1918	rVB3	7191	13506	1.13%	0.134%
21	7.562	1919	1935	1947	rBV	95544	185011	15.45%	1.835%
22	7.745	1978	1992	2002	rBV7	7771	16513	1.38%	0.164%
23	7.835	2011	2020	2027	rBV4	8322	16844	1.41%	0.167%
24	7.893	2027	2038	2054	rVV	362311	630348	52.64%	6.252%
25	8.176	2115	2126	2136	rBV	61884	106473	8.89%	1.056%
26	8.234	2136	2144	2164	rVB5	20154	45279	3.78%	0.449%
27	8.433	2191	2206	2214	rBV5	11865	30364	2.54%	0.301%
28	8.549	2227	2242	2256	rBV	526492	886609	74.04%	8.794%
29	8.636	2256	2269	2296	rBV2	584529	1197530	100.00%	11.878%
30	8.755	2298	2306	2312	rBV	24298	42143	3.52%	0.418%
31	8.928	2348	2360	2364	rBV10	7066	15650	1.31%	0.155%
32	9.063	2393	2402	2414	rVB8	10400	18590	1.55%	0.184%
33	9.163	2423	2433	2445	rBV6	19260	39251	3.28%	0.389%
34	9.337	2476	2487	2498	rBV9	5894	14097	1.18%	0.140%
35	9.414	2498	2511	2527	rVV	377212	627990	52.44%	6.229%
36	9.562	2549	2557	2565	rBV7	9743	16535	1.38%	0.164%

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37	10.022	2690	2700	2707	rBV8	10820	20514	1.71%	0.203%
38	10.234	2751	2766	2772	rBV10	6305	14306	1.19%	0.142%
39	10.752	2916	2927	2939	rBV	170627	275711	23.02%	2.735%
40	11.607	3185	3193	3209	rVB2	19225	32163	2.69%	0.319%
41	11.684	3209	3217	3227	rVB6	10614	15813	1.32%	0.157%
42	11.742	3228	3235	3243	rVB6	10296	15634	1.31%	0.155%
43	11.806	3243	3255	3275	rBV	392976	621383	51.89%	6.163%
44	12.060	3325	3334	3350	rBV4	13330	26529	2.22%	0.263%
45	12.189	3362	3374	3390	rBV	362330	586692	48.99%	5.819%
46	12.549	3473	3486	3502	rBV4	10392	19302	1.61%	0.191%
47	12.716	3530	3538	3546	rBV3	9445	14488	1.21%	0.144%
48	12.758	3546	3551	3564	rVB6	9849	16103	1.34%	0.160%
49	12.880	3578	3589	3598	rVV4	30022	56828	4.75%	0.564%
50	12.935	3598	3606	3613	rVV4	25112	41182	3.44%	0.408%
51	12.980	3614	3620	3630	rVB	14110	20431	1.71%	0.203%
52	13.112	3652	3661	3675	rVB	33176	49511	4.13%	0.491%
53	13.218	3682	3694	3703	rBV	12992	21559	1.80%	0.214%
54	13.321	3716	3726	3739	rVB2	33318	53391	4.46%	0.530%
55	13.626	3813	3821	3831	rVB2	8684	14686	1.23%	0.146%
56	13.877	3890	3899	3906	rBV4	14532	23368	1.95%	0.232%
57	14.057	3944	3955	3962	rVV3	10993	17249	1.44%	0.171%
58	14.115	3962	3973	3985	rVB8	7379	15448	1.29%	0.153%
59	14.266	4008	4020	4036	rBV9	10983	23369	1.95%	0.232%
60	14.349	4036	4046	4053	rBV4	7364	13502	1.13%	0.134%
61	14.661	4134	4143	4152	rBV3	16263	28189	2.35%	0.280%
62	14.803	4178	4187	4197	rVV3	20607	29919	2.50%	0.297%
63	14.870	4200	4208	4218	rVB5	12550	20220	1.69%	0.201%
64	15.021	4247	4255	4264	rBV4	8600	15427	1.29%	0.153%

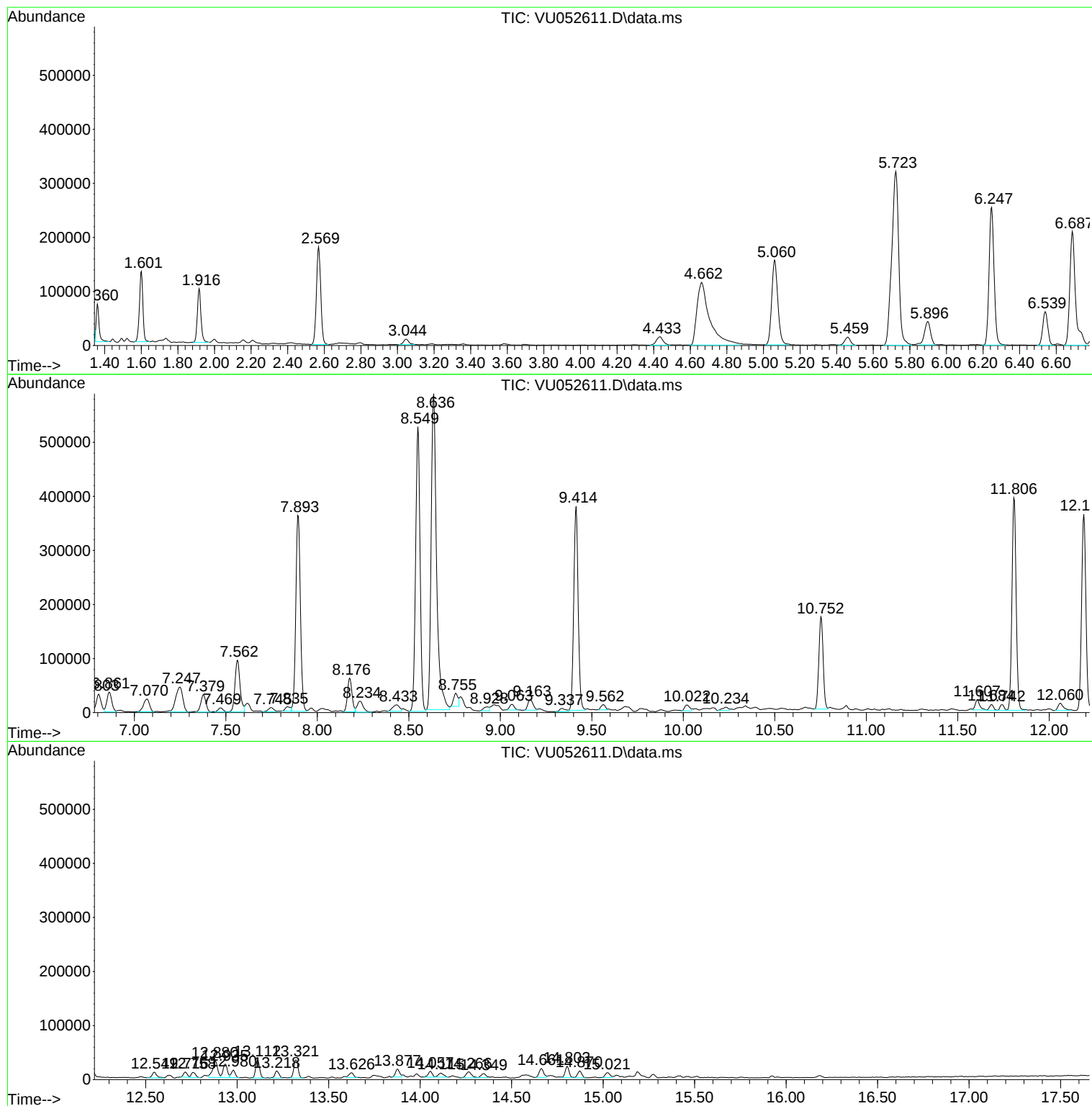
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Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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ClientSampleId :
H0AA9

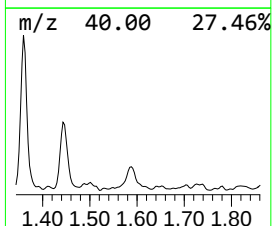
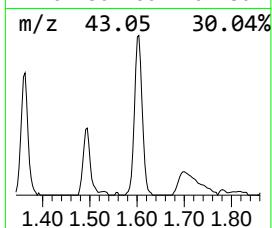
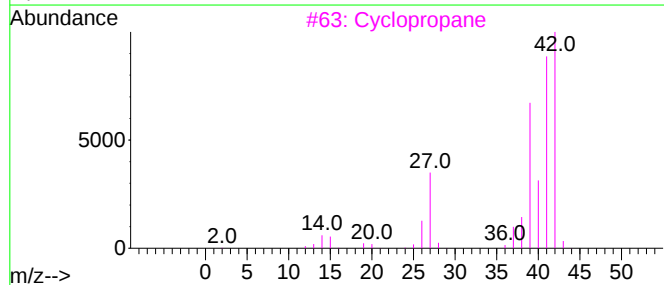
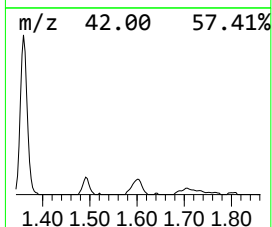
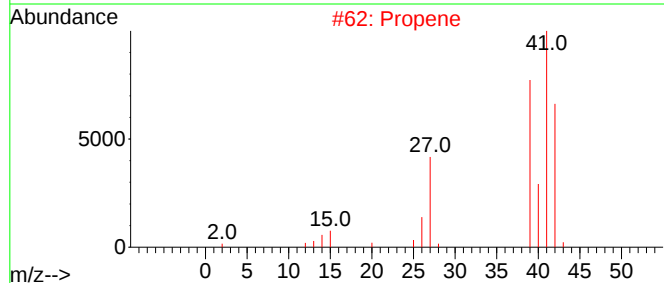
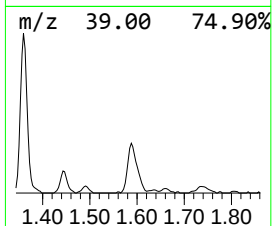
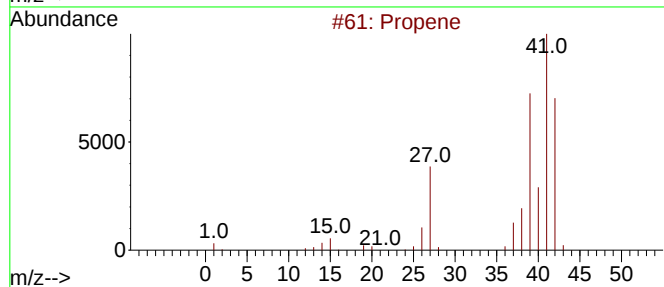
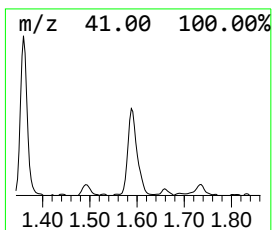
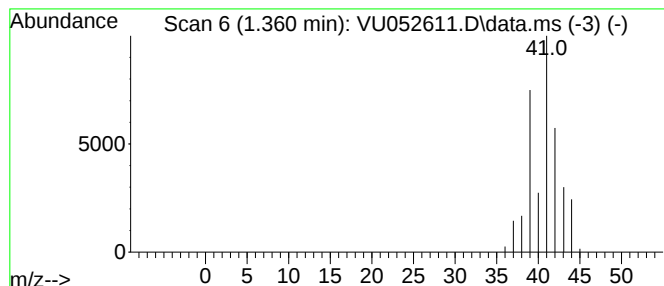
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.360	0.72 ug/L	70600	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	56
3			Cyclopropane	42	C3H6	000075-19-4	40
4			Cyclopropane	42	C3H6	000075-19-4	8
5			Cyclopropane	42	C3H6	000075-19-4	4



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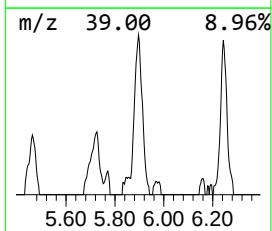
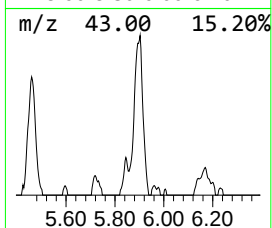
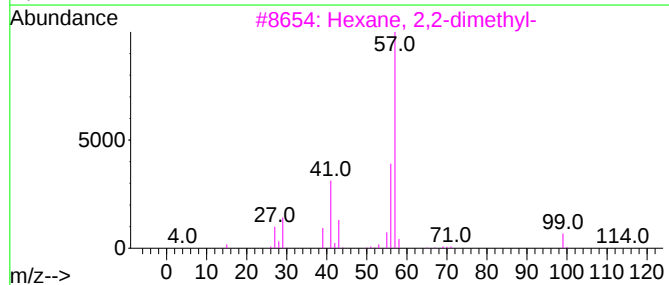
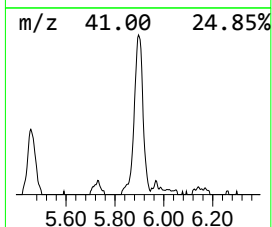
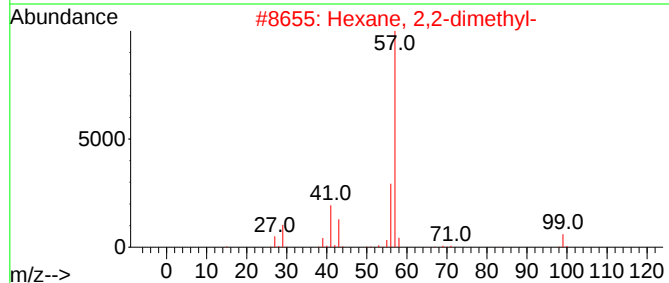
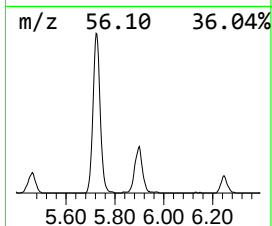
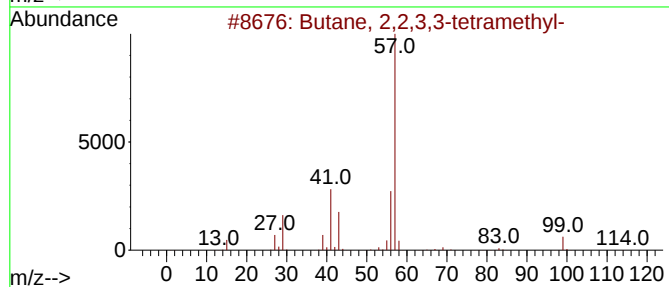
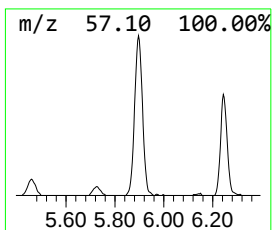
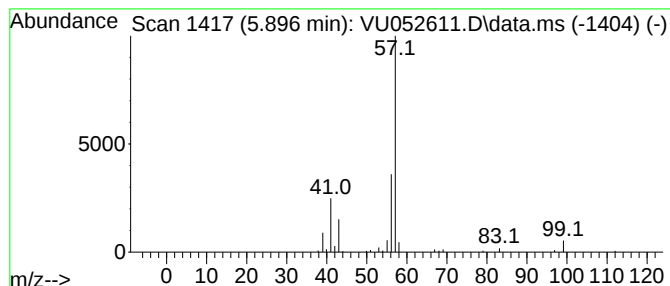
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.896	1.00 ug/L	97344	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



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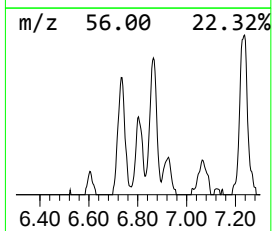
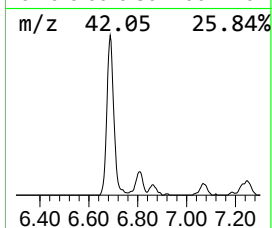
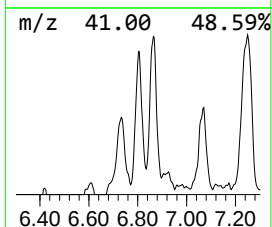
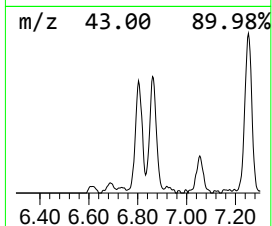
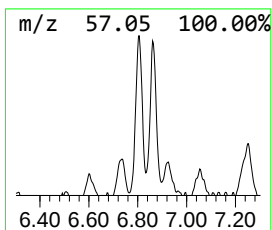
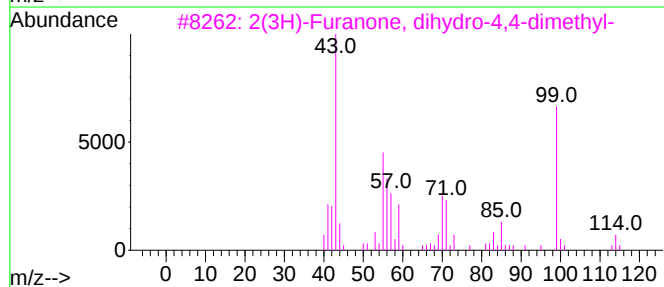
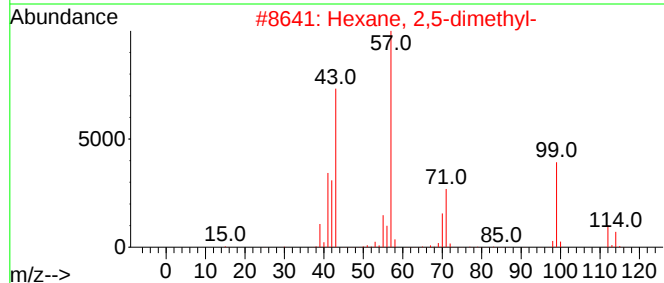
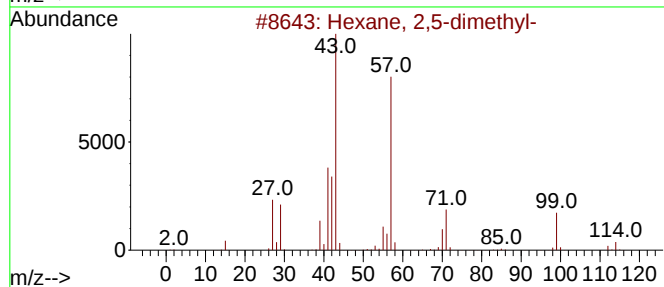
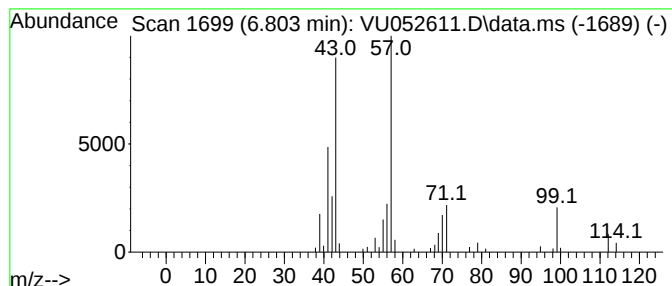
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.803	0.65 ug/L	63243	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	80
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	64
3			2(3H)-Furanone, dihydro-4,4-dime...	114	C6H10O2	013861-97-7	53
4			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	52
5			Heptane, 2-methyl-	114	C8H18	000592-27-8	50



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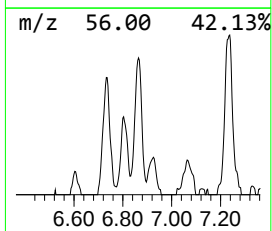
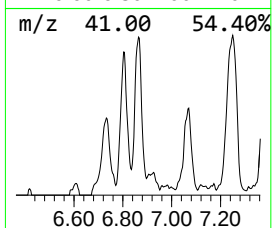
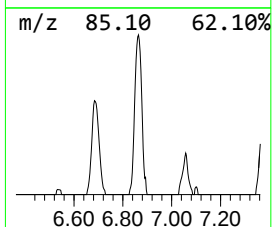
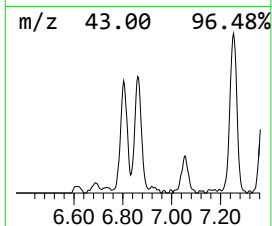
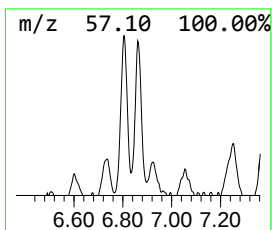
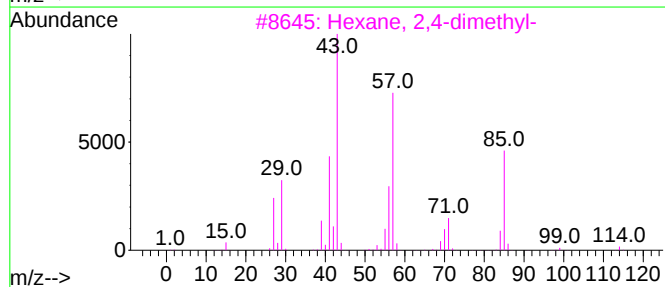
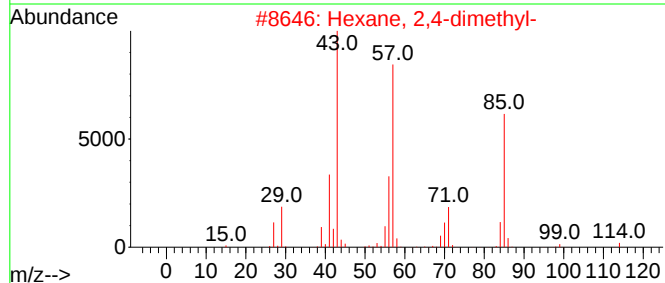
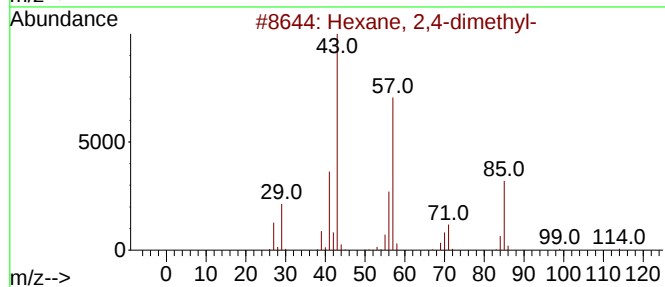
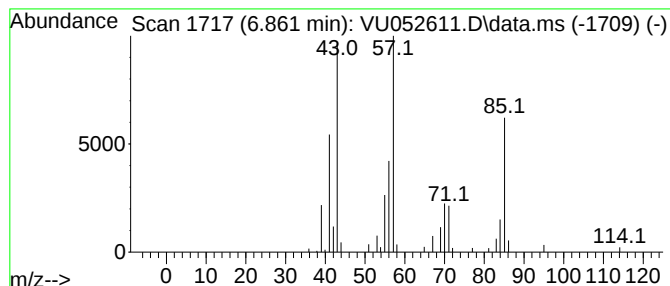
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.861	0.71 ug/L	69697	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	91
2	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	90
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	90
4	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	59
5	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	58



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ClientSampleId :
H0AA9

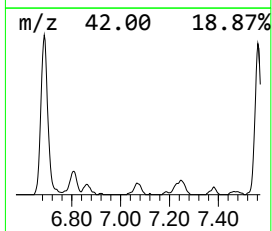
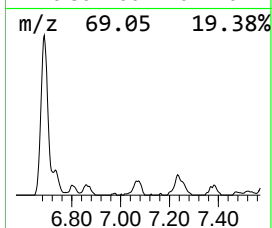
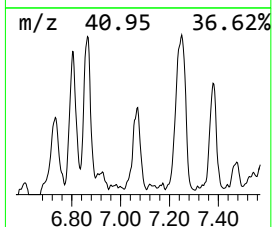
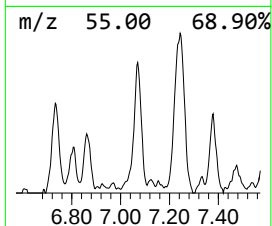
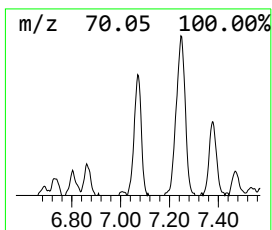
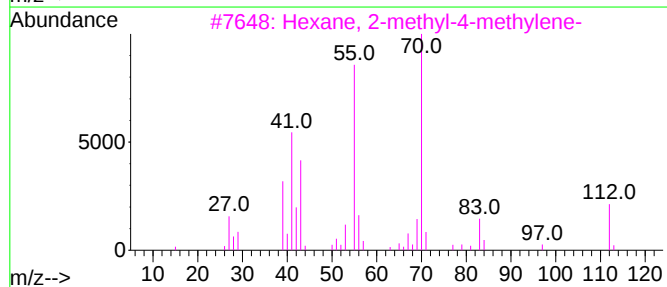
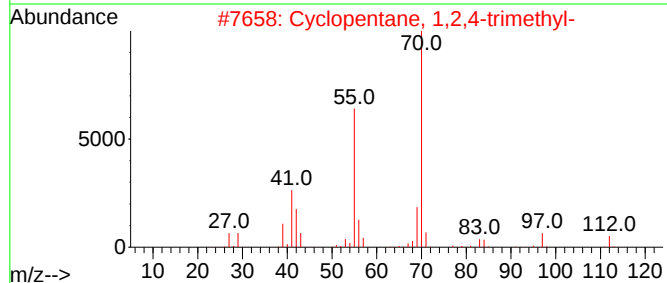
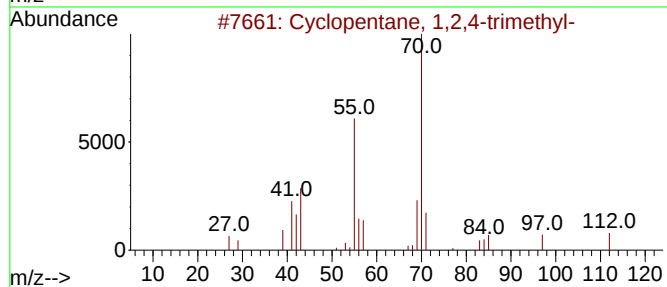
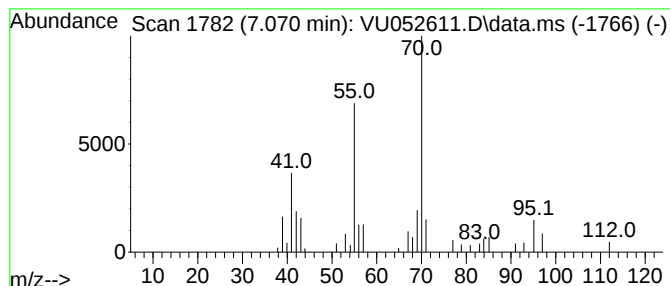
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic7.070 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.070	0.55 ug/L	54013	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	87
2			Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	68
3			Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	64
4			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	64
5			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122922\
Data File : VU052611.D
Acq On : 29 Dec 2022 17:51
Operator : JC/MD
Sample : N6216-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H0AA9

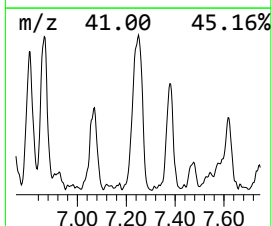
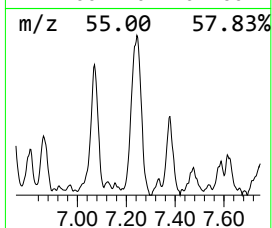
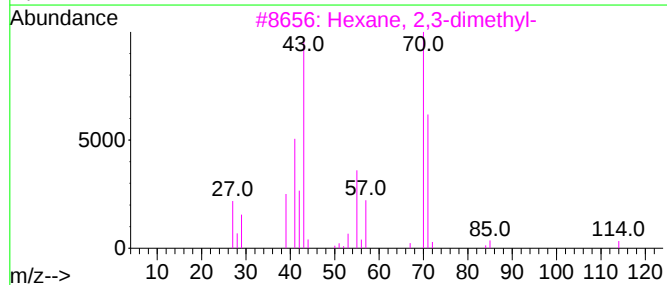
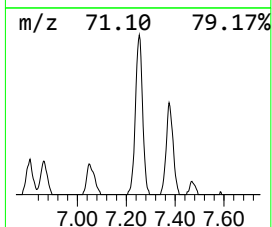
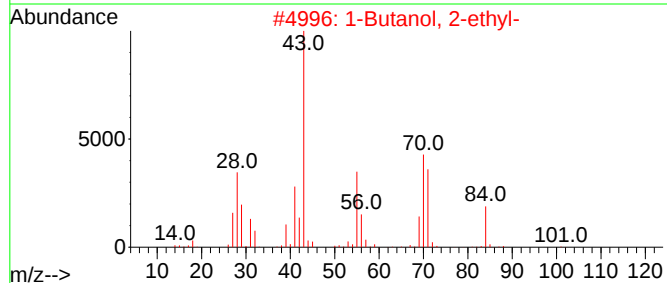
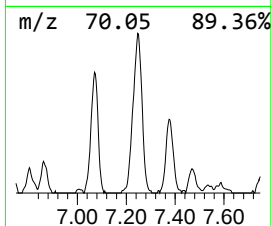
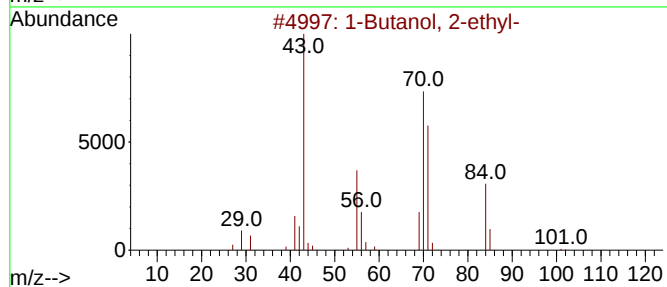
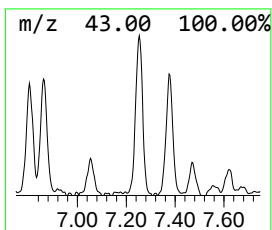
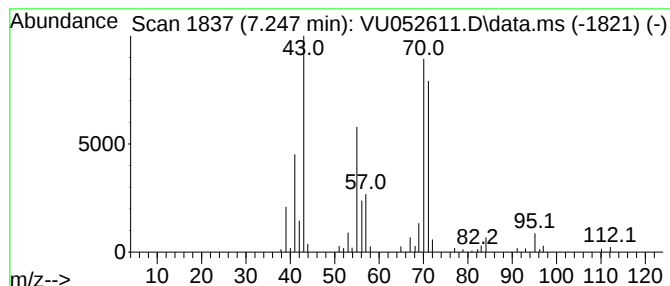
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1-Butanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.247	1.25 ug/L	122553	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	78
2		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	72
3		Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	72
4		1-Heptene, 4-methyl-	112	C8H16	013151-05-8	59
5		1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122922\
Data File : VU052611.D
Acq On : 29 Dec 2022 17:51
Operator : JC/MD
Sample : N6216-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

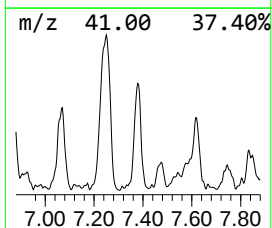
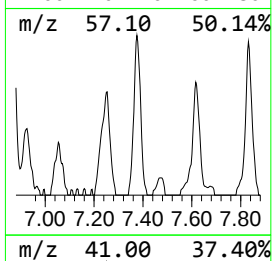
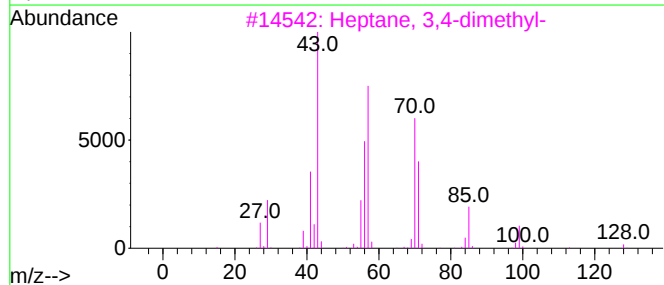
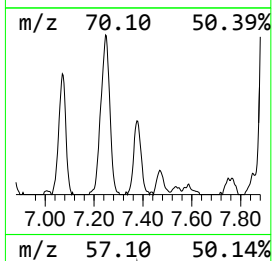
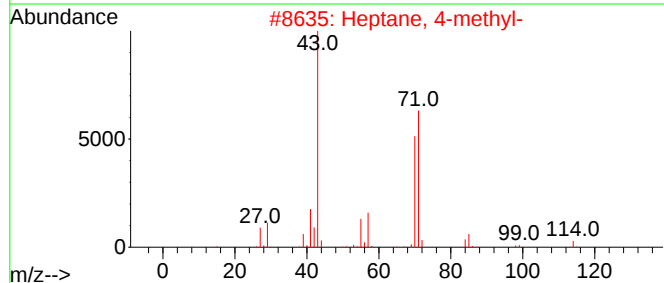
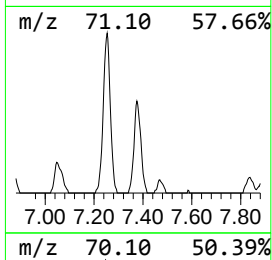
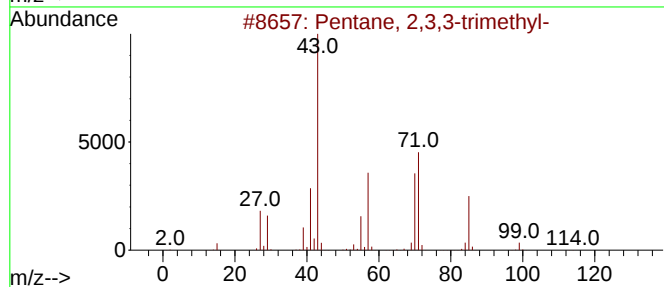
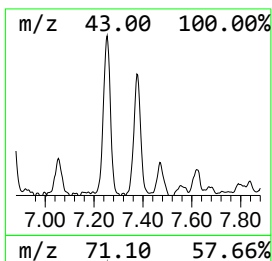
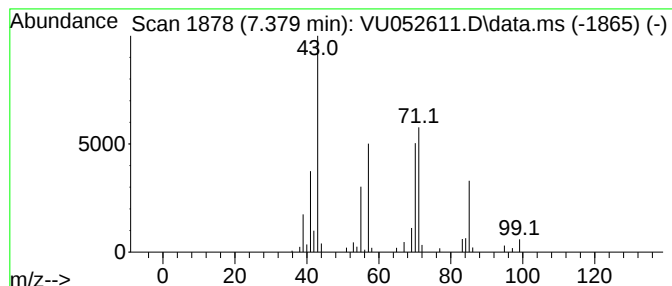
Instrument :
MSVOA_U
ClientSampleId :
H0AA9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.379	0.63 ug/L	61954	1,4-Difluorobenzene	6.247	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	86
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	59
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122922\
Data File : VU052611.D
Acq On : 29 Dec 2022 17:51
Operator : JC/MD
Sample : N6216-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H0AA9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.360	0.7	ug/L	70600	1	6.247	489162	5.0
(DEL) Alkane: S...	5.896	1.0	ug/L	97344	1	6.247	489162	5.0
(DEL) Alkane: S...	6.803	0.7	ug/L	63243	1	6.247	489162	5.0
(DEL) Alkane: S...	6.861	0.7	ug/L	69697	1	6.247	489162	5.0
(DEL) Alkane: C...	7.070	0.6	ug/L	54013	1	6.247	489162	5.0
1-Butanol, 2-et...	7.247	1.3	ug/L	122553	1	6.247	489162	5.0
(DEL) Alkane: S...	7.379	0.6	ug/L	61954	1	6.247	489162	5.0