

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
 Data File : VU051521.D
 Acq On : 26 Oct 2022 23:34
 Operator : JC/MD
 Sample : N5300-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHAC1

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\SFAMUTR100722WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.395	12	17	27	rVB	25312	32896	1.09%	0.248%
2	1.472	32	41	52	rBV	127450	250819	8.30%	1.891%
3	1.597	74	80	86	rBV	131179	142354	4.71%	1.073%
4	1.909	170	177	194	rVB2	108995	190467	6.30%	1.436%
5	2.376	316	322	341	rVB	54711	94121	3.11%	0.710%
6	2.565	368	381	394	rBV	195341	318354	10.53%	2.400%
7	3.080	533	541	555	rVB2	36746	72452	2.40%	0.546%
8	3.183	561	573	588	rVB	13100	30483	1.01%	0.230%
9	3.359	611	628	647	rBV2	120763	272081	9.00%	2.051%
10	3.694	722	732	750	rVB5	14551	31950	1.06%	0.241%
11	3.877	755	789	791	rBV	19503	73883	2.44%	0.557%
12	3.990	808	824	847	rVB	205613	528858	17.49%	3.987%
13	4.530	973	992	1008	rBV2	124608	306379	10.13%	2.310%
14	4.617	1008	1019	1051	rBV	197741	489051	16.18%	3.687%
15	5.060	1140	1157	1182	rBV	183216	416212	13.77%	3.138%
16	5.385	1244	1258	1272	rBV6	16764	38362	1.27%	0.289%
17	5.723	1341	1363	1376	rBV2	364833	967325	32.00%	7.292%
18	6.247	1513	1526	1549	rBV	302278	592720	19.60%	4.468%
19	6.690	1649	1664	1679	rBV	224609	448421	14.83%	3.380%
20	7.565	1923	1936	1952	rBV2	88405	155494	5.14%	1.172%
21	7.896	2026	2039	2054	rBV	384758	666512	22.05%	5.024%
22	8.179	2115	2127	2141	rBV2	55201	94271	3.12%	0.711%
23	8.633	2255	2268	2296	rBV2	591636	1122977	37.14%	8.465%
24	9.443	2498	2520	2551	rBV2	1369157	3023358	100.00%	22.791%
25	9.690	2582	2597	2611	rBV4	17798	35617	1.18%	0.268%
26	10.755	2913	2928	2939	rBV	205221	329917	10.91%	2.487%
27	10.883	2955	2968	2982	rBV7	19043	39515	1.31%	0.298%
28	11.028	3005	3013	3026	rVB2	31027	53011	1.75%	0.400%
29	11.812	3245	3257	3275	rVV2	438004	1037081	34.30%	7.818%
30	12.092	3326	3344	3357	rBV	119358	204522	6.76%	1.542%
31	12.192	3362	3375	3398	rVV2	424629	797903	26.39%	6.015%
32	12.301	3399	3409	3423	rVB3	20762	34716	1.15%	0.262%
33	12.861	3575	3583	3597	rVB3	63337	106262	3.51%	0.801%
34	12.970	3611	3617	3626	rVB2	26456	40248	1.33%	0.303%
35	13.025	3626	3634	3650	rVB2	22782	39395	1.30%	0.297%
36	14.086	3953	3964	3980	rBV	37130	70314	2.33%	0.530%

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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\SFAMUTR100722WMA.M
Title : TRACE VOA SFAM1.0

37	16.883	4826	4834	4844	rBV2	47616	69844	2.31%	0.527%
38	17.095	4892	4900	4913	rVB	29479	47457	1.57%	0.358%

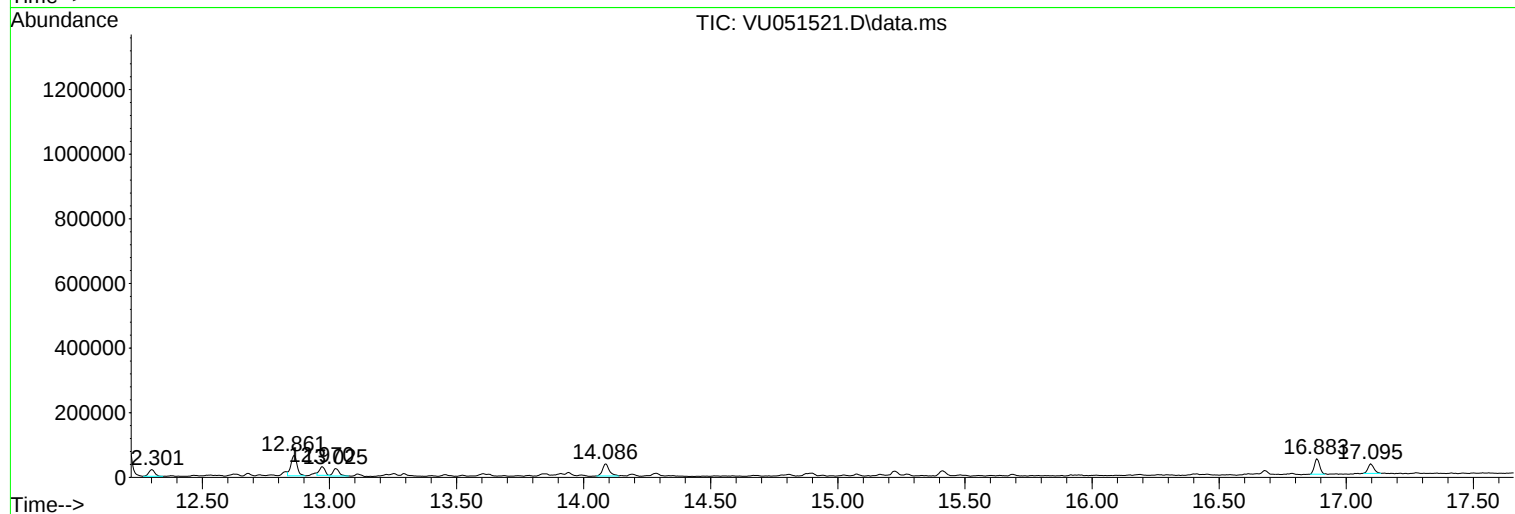
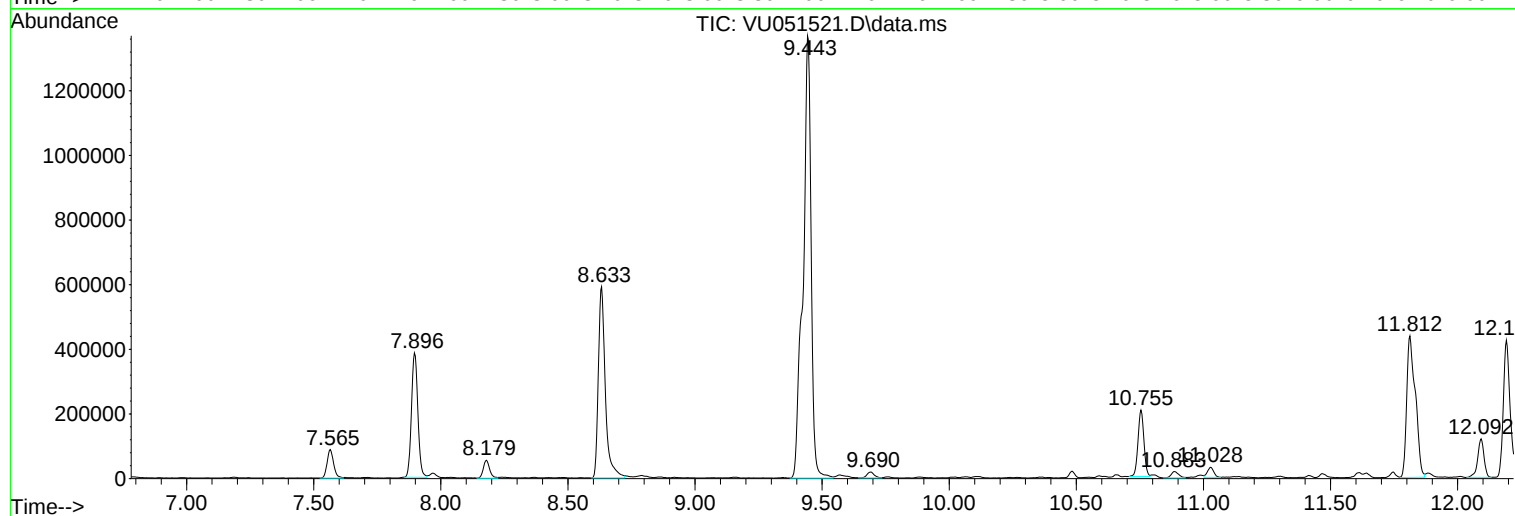
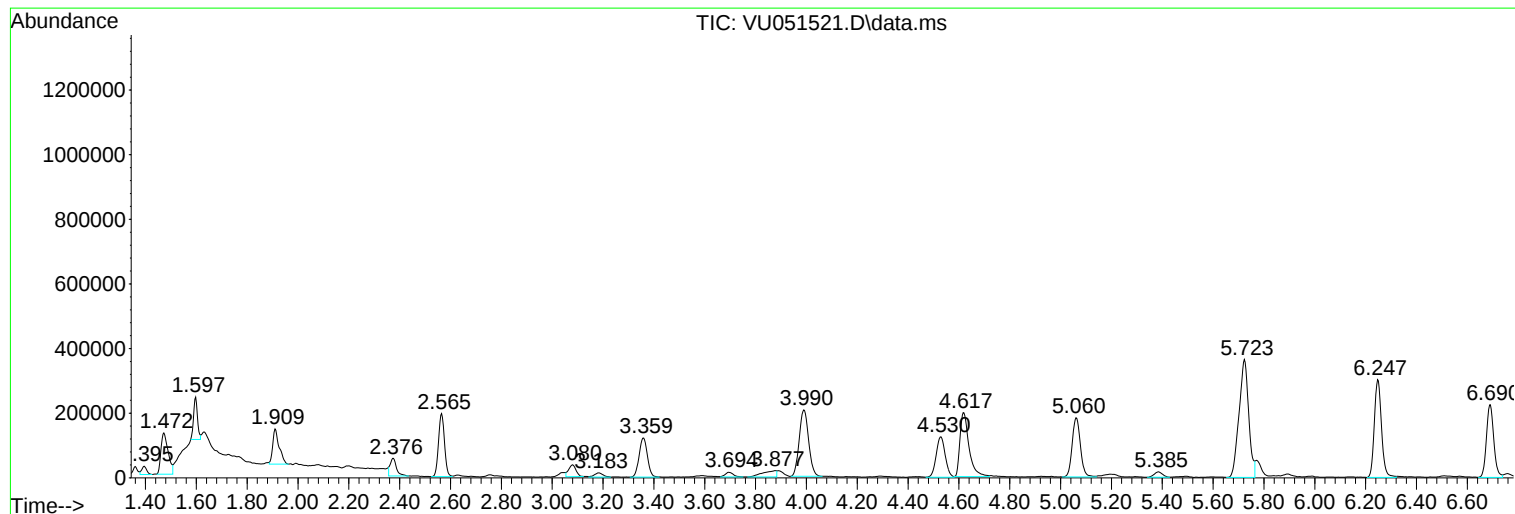
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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ClientSampleId :
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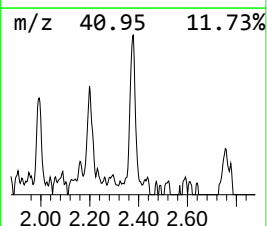
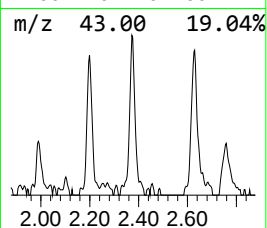
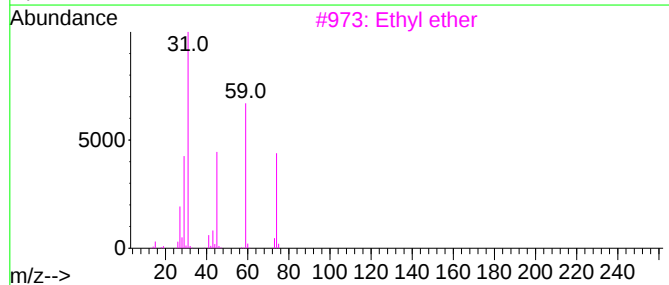
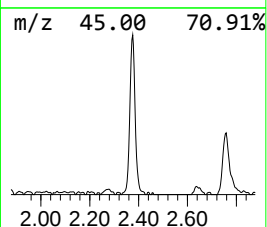
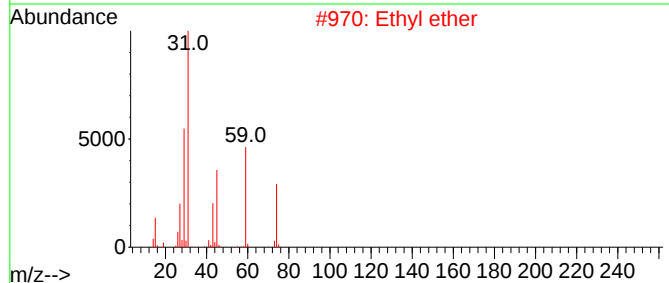
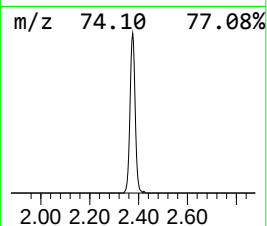
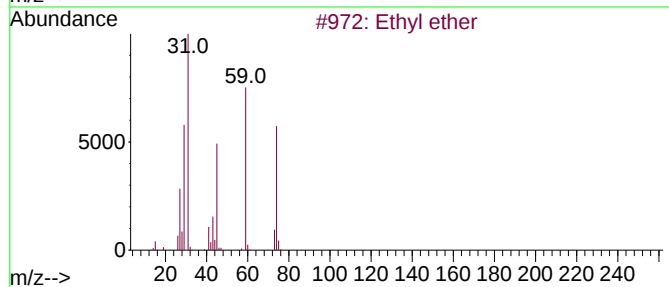
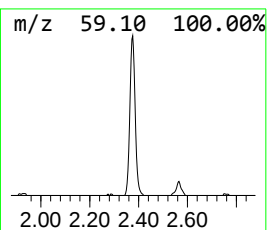
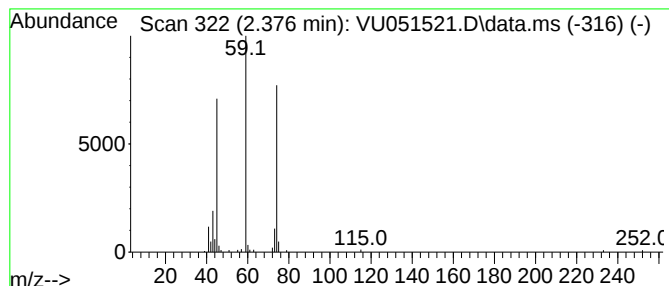
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Ethyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.376	0.79 ug/L	94121	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl ether			74	C4H10O	000060-29-7	90
2	Ethyl ether			74	C4H10O	000060-29-7	90
3	Ethyl ether			74	C4H10O	000060-29-7	90
4	Ethyl ether			74	C4H10O	000060-29-7	78
5	Ethyl ether			74	C4H10O	000060-29-7	72



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAC1

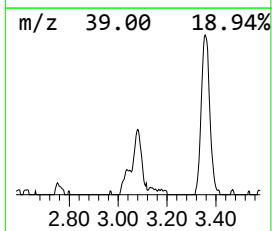
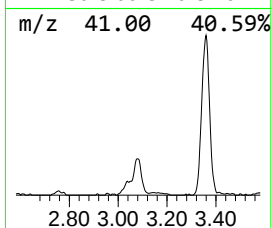
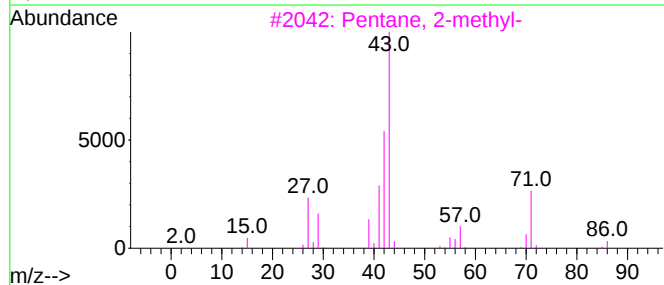
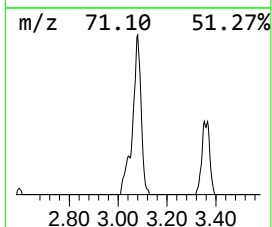
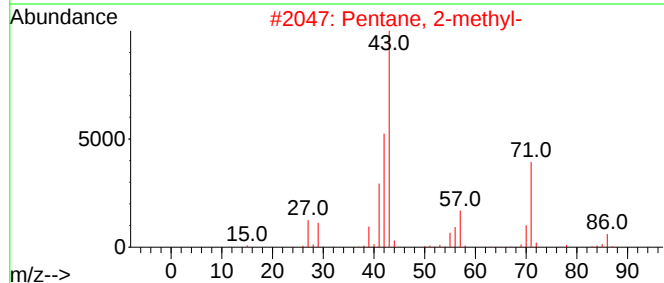
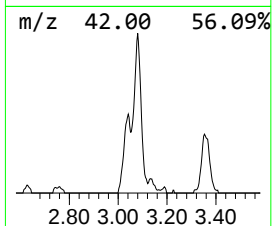
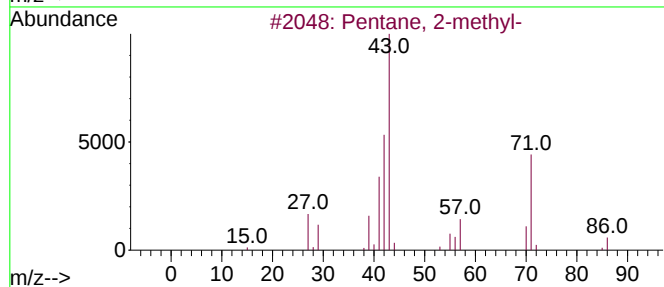
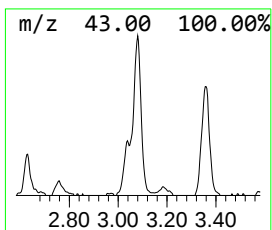
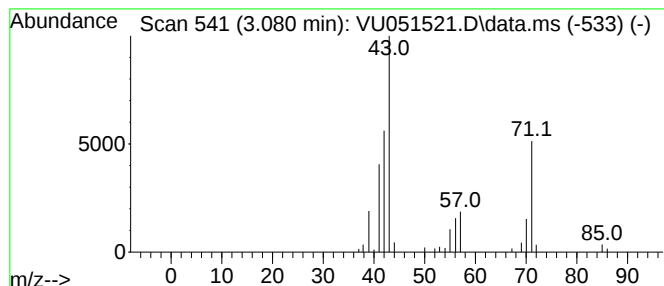
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.080	0.61 ug/L	72452	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2-methyl-	86	C6H14	000107-83-5	86
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	78
3		Pentane, 2-methyl-	86	C6H14	000107-83-5	72
4		Pentane, 2-methyl-	86	C6H14	000107-83-5	72
5		Pentane, 2-methyl-	86	C6H14	000107-83-5	56



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ALS Vial : 29 Sample Multiplier: 1

Instrument :
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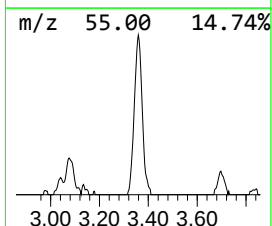
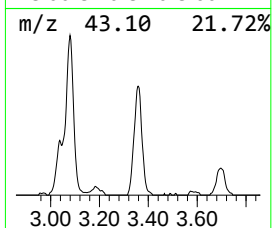
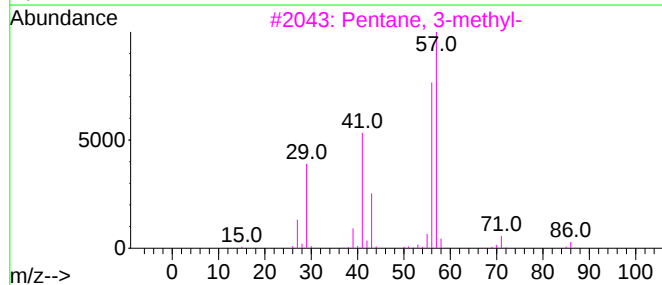
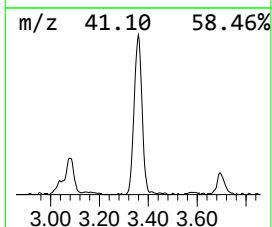
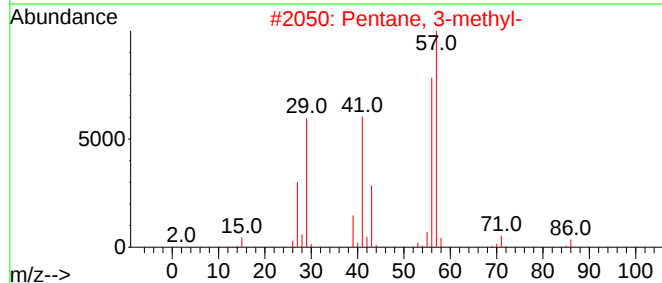
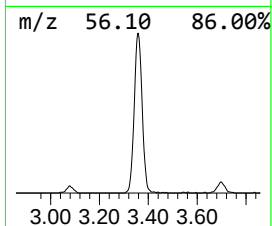
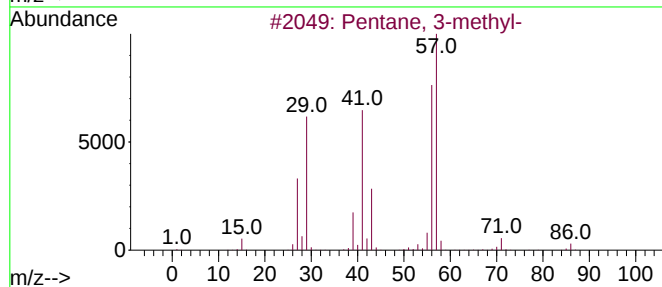
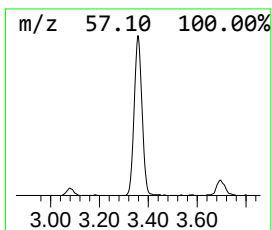
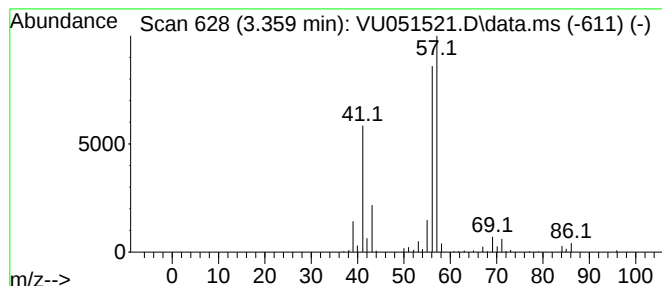
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.359	2.30 ug/L	272081	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2			Pentane, 3-methyl-	86	C6H14	000096-14-0	86
3			Pentane, 3-methyl-	86	C6H14	000096-14-0	86
4			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	74
5			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	56



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Sample : N5300-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAC1

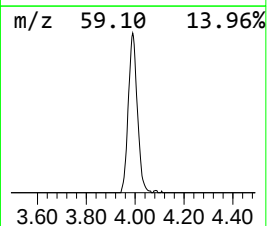
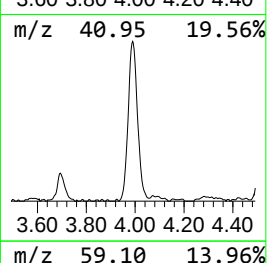
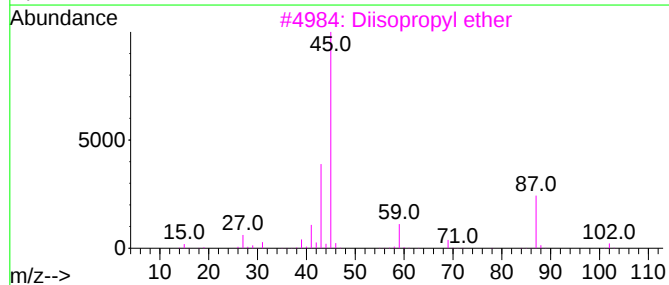
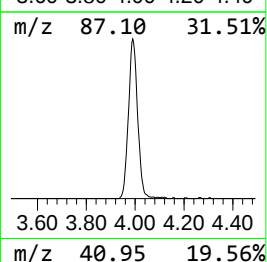
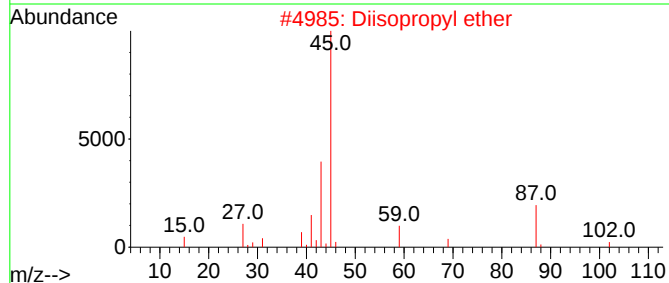
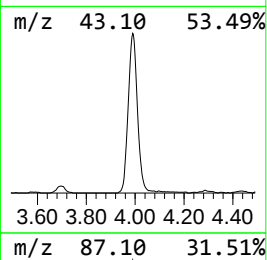
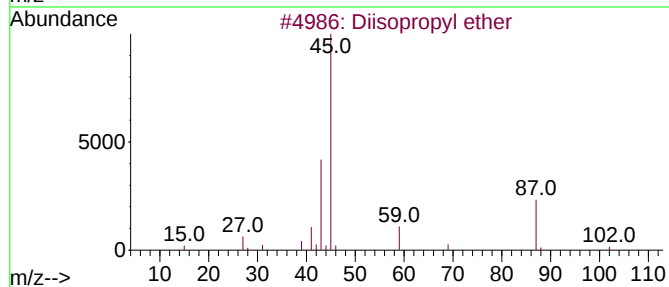
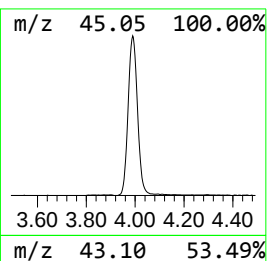
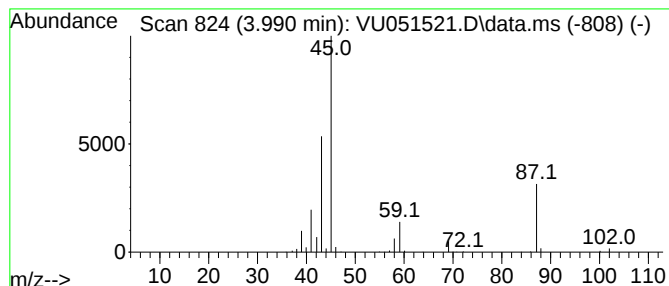
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Diisopropyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.990	4.46 ug/L	528858	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Diisopropyl ether	102	C6H14O	000108-20-3	90
2		Diisopropyl ether	102	C6H14O	000108-20-3	80
3		Diisopropyl ether	102	C6H14O	000108-20-3	80
4		Diisopropyl ether	102	C6H14O	000108-20-3	78
5		Diisopropyl ether	102	C6H14O	000108-20-3	78



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Instrument :
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ClientSampleId :
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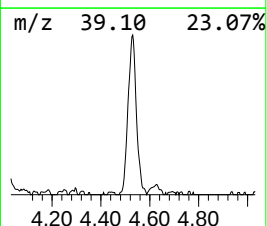
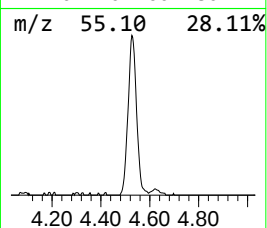
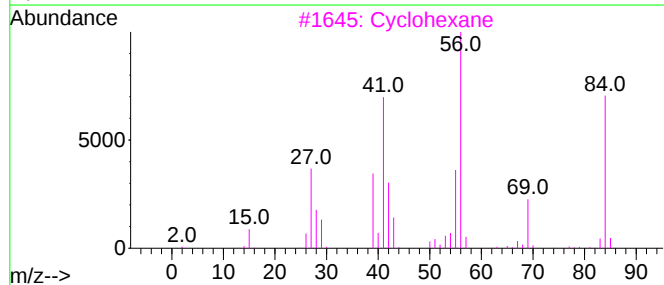
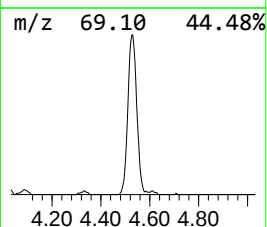
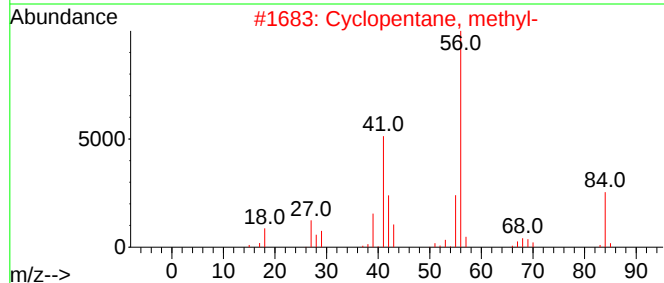
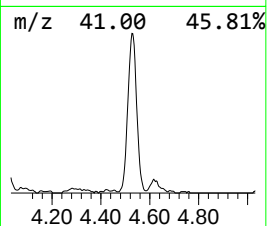
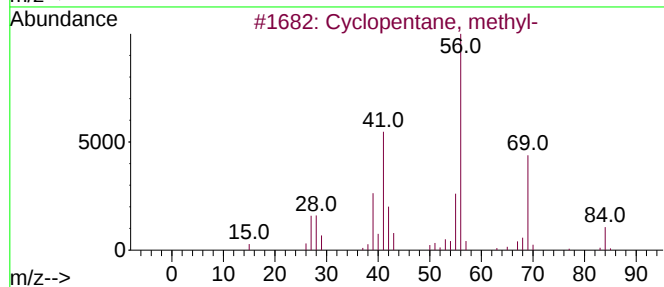
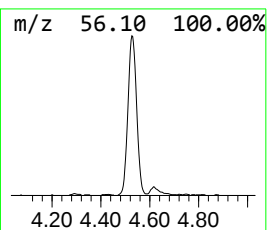
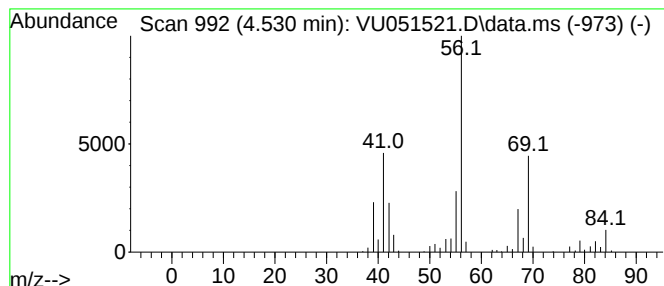
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Cyclic4.530 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.530	2.58 ug/L	306379	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	64
3			Cyclohexane	84	C6H12	000110-82-7	64
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	53
5			Cyclohexane	84	C6H12	000110-82-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051521.D
Acq On : 26 Oct 2022 23:34
Operator : JC/MD
Sample : N5300-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAC1

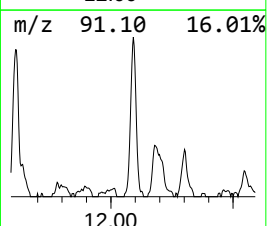
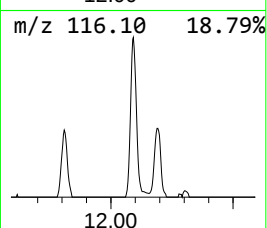
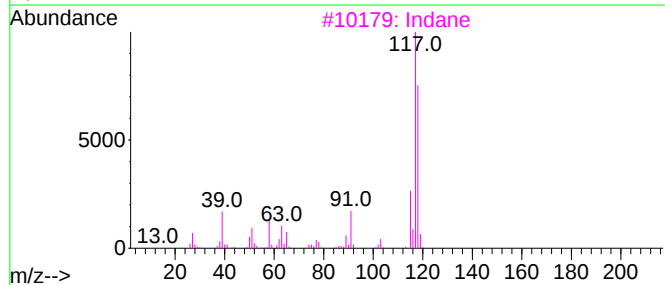
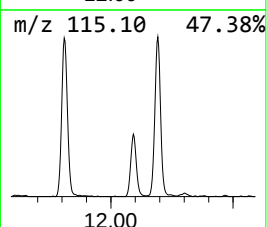
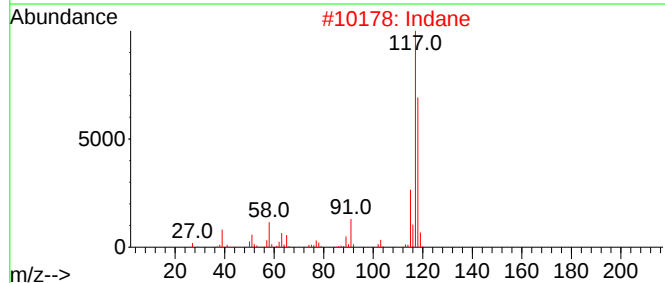
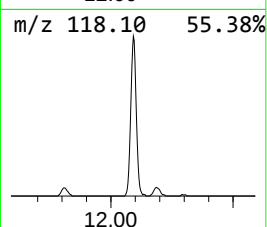
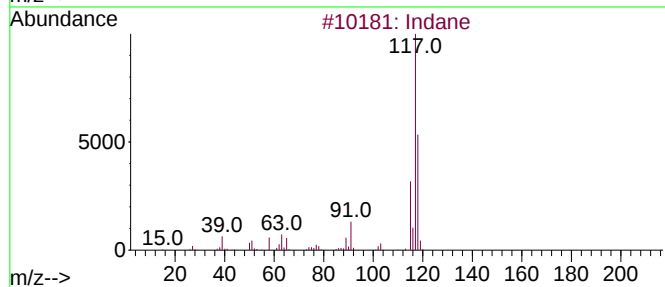
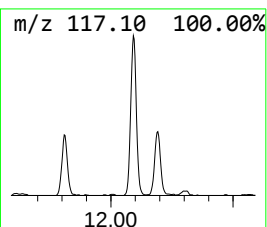
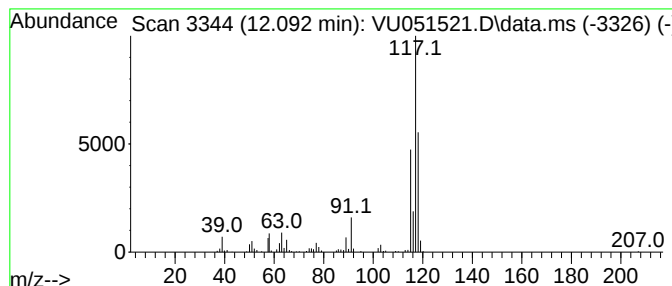
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	0.99 ug/L	204522	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane			118	C9H10	000496-11-7	93
2	Indane			118	C9H10	000496-11-7	76
3	Indane			118	C9H10	000496-11-7	76
4	3-Bromo-1-phenyl-1-propene			196	C9H9Br	004392-24-9	64
5	Indane-5-carboxylic acid			162	C10H10O2	065898-38-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051521.D
Acq On : 26 Oct 2022 23:34
Operator : JC/MD
Sample : N5300-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAC1

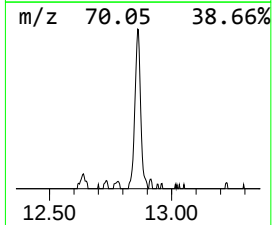
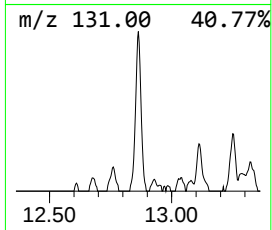
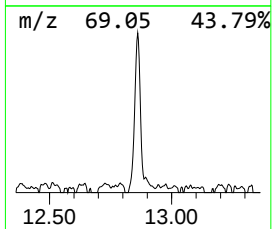
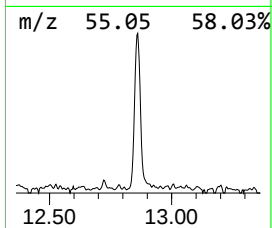
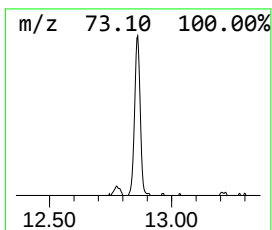
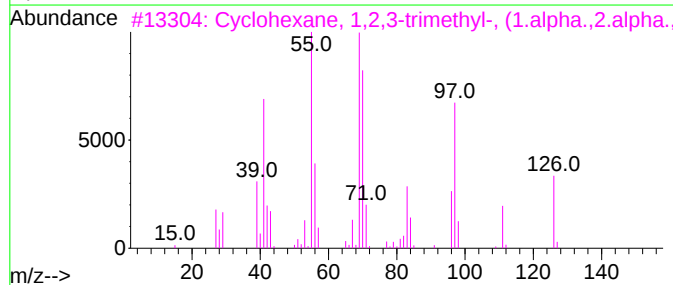
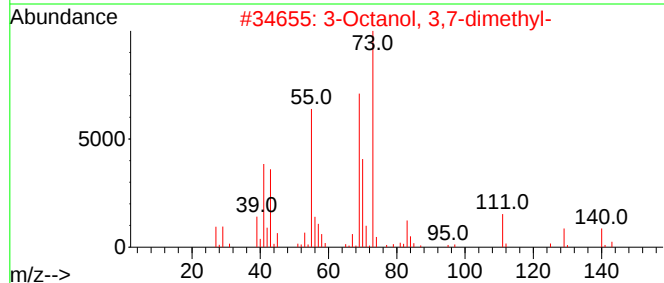
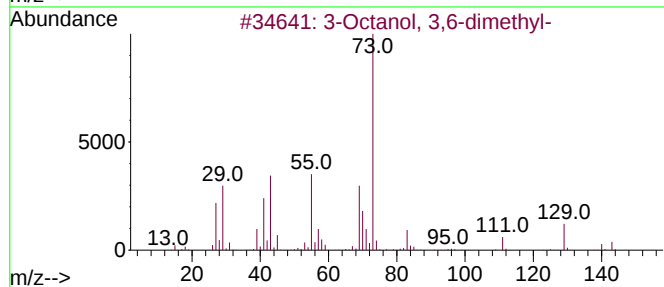
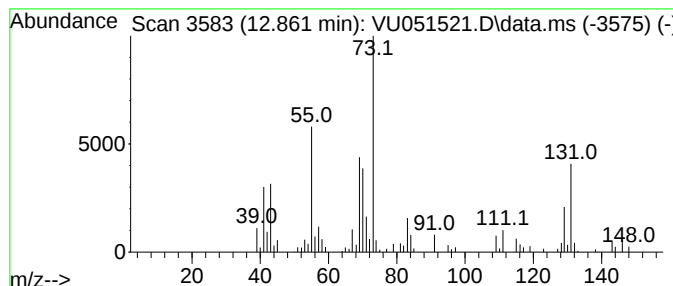
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 unknown-01 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.861	0.51 ug/L	106262	1,4-Dichlorobenzene-d4	11.812

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octanol, 3,6-dimethyl-	158	C10H22O	000151-19-9	27
2		3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	25
3		Cyclohexane, 1,2,3-trimethyl-, (...)	126	C9H18	001839-88-9	14
4		2-Bromostearic acid, trimethylsi...	434	C21H43BrO2Si	1000472-44-2	12
5		3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051521.D
Acq On : 26 Oct 2022 23:34
Operator : JC/MD
Sample : N5300-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAC1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.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
Sulfur dioxide	1.472	2.1	ug/L	250819	1	6.247	592720	5.0
Ethyl ether	2.376	0.8	ug/L	94121	1	6.247	592720	5.0
(DEL) Alkane: S...	3.080	0.6	ug/L	72452	1	6.247	592720	5.0
(DEL) Alkane: S...	3.359	2.3	ug/L	272081	1	6.247	592720	5.0
Diisopropyl ether	3.990	4.5	ug/L	528858	1	6.247	592720	5.0
(DEL) Alkane: C...	4.530	2.6	ug/L	306379	1	6.247	592720	5.0
Indane	12.092	1.0	ug/L	204522	3	11.812	1037080	5.0
unknown-01	12.861	0.5	ug/L	106262	3	11.812	1037080	5.0