

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031622\
 Data File : VU047590.D
 Acq On : 16 Mar 2022 15:08
 Operator : SY/MD
 Sample : N1858-16RE
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNK2RE

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\SFAMUTR031422WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU047590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	22	rVB	109007	110064	4.48%	1.016%
2	1.494	40	48	73	rBV	169110	189231	7.71%	1.747%
3	1.604	73	82	93	rVV	1113266	1219088	49.66%	11.257%
4	1.655	93	98	117	rVB	35807	50207	2.05%	0.464%
5	1.919	171	180	194	rBV	41259	57232	2.33%	0.528%
6	1.999	194	205	223	rVB	1807775	2455053	100.00%	22.670%
7	2.208	262	270	284	rVB	28760	41280	1.68%	0.381%
8	2.572	367	383	405	rBV3	64303	139866	5.70%	1.292%
9	3.047	515	531	545	rBV3	10864	25409	1.03%	0.235%
10	3.144	545	561	586	rVB	310005	624878	25.45%	5.770%
11	4.536	975	994	1010	rBV	66138	157526	6.42%	1.455%
12	4.642	1010	1027	1070	rVV	72825	287781	11.72%	2.657%
13	5.067	1144	1159	1184	rVB	84873	185740	7.57%	1.715%
14	5.391	1244	1260	1279	rBV3	137737	309734	12.62%	2.860%
15	5.729	1345	1365	1370	rBV2	152504	380991	15.52%	3.518%
16	5.777	1370	1380	1405	rVV	839260	1735642	70.70%	16.027%
17	5.896	1406	1417	1435	rVB3	18667	41124	1.68%	0.380%
18	6.253	1514	1528	1549	rBV	152299	289142	11.78%	2.670%
19	6.694	1651	1665	1687	rBV	104552	203486	8.29%	1.879%
20	7.568	1924	1937	1957	rBV	50395	90380	3.68%	0.835%
21	7.899	2025	2040	2054	rBV	156009	272513	11.10%	2.516%
22	8.182	2114	2128	2144	rBV2	32486	55811	2.27%	0.515%
23	8.639	2257	2270	2307	rBV	329820	662957	27.00%	6.122%
24	9.417	2499	2512	2535	rBV	214220	367596	14.97%	3.394%
25	10.758	2914	2929	2944	rBV	114348	181119	7.38%	1.672%
26	11.812	3244	3257	3276	rBV	228821	365315	14.88%	3.373%
27	12.195	3361	3376	3391	rBV	202970	330201	13.45%	3.049%

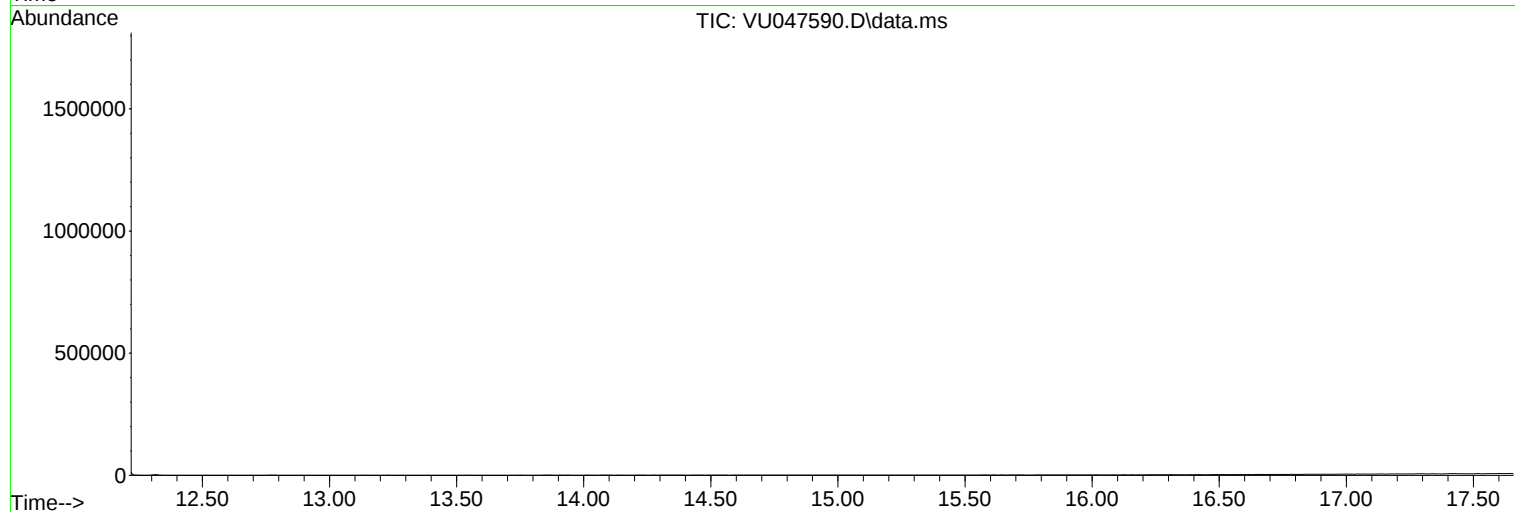
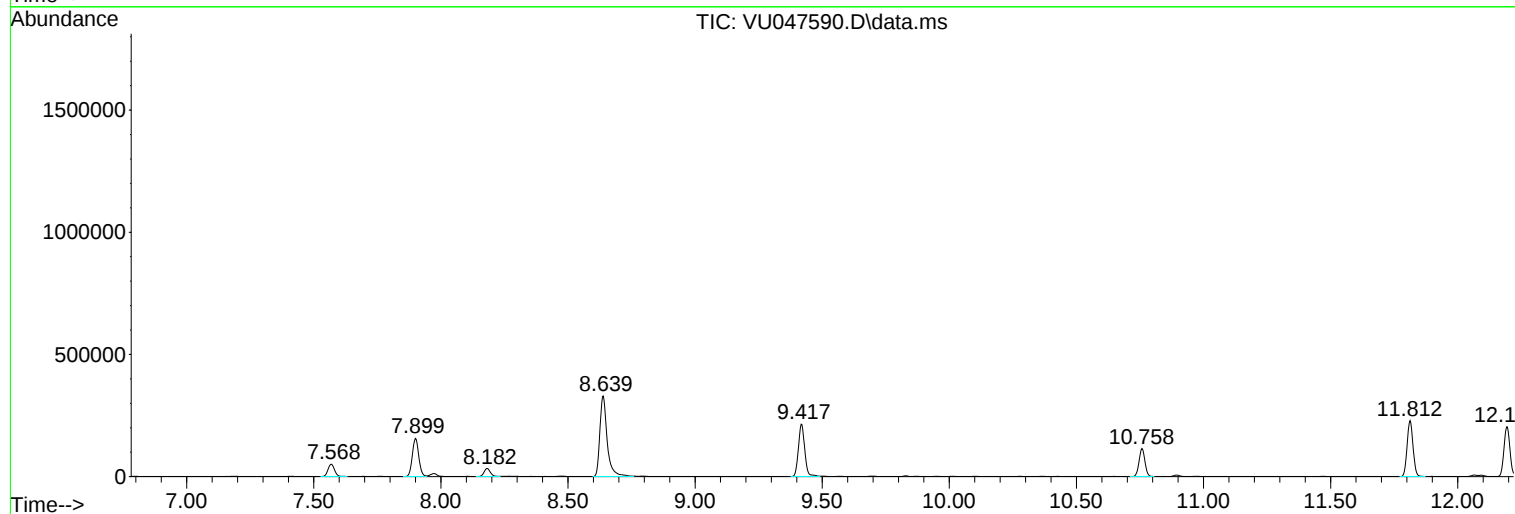
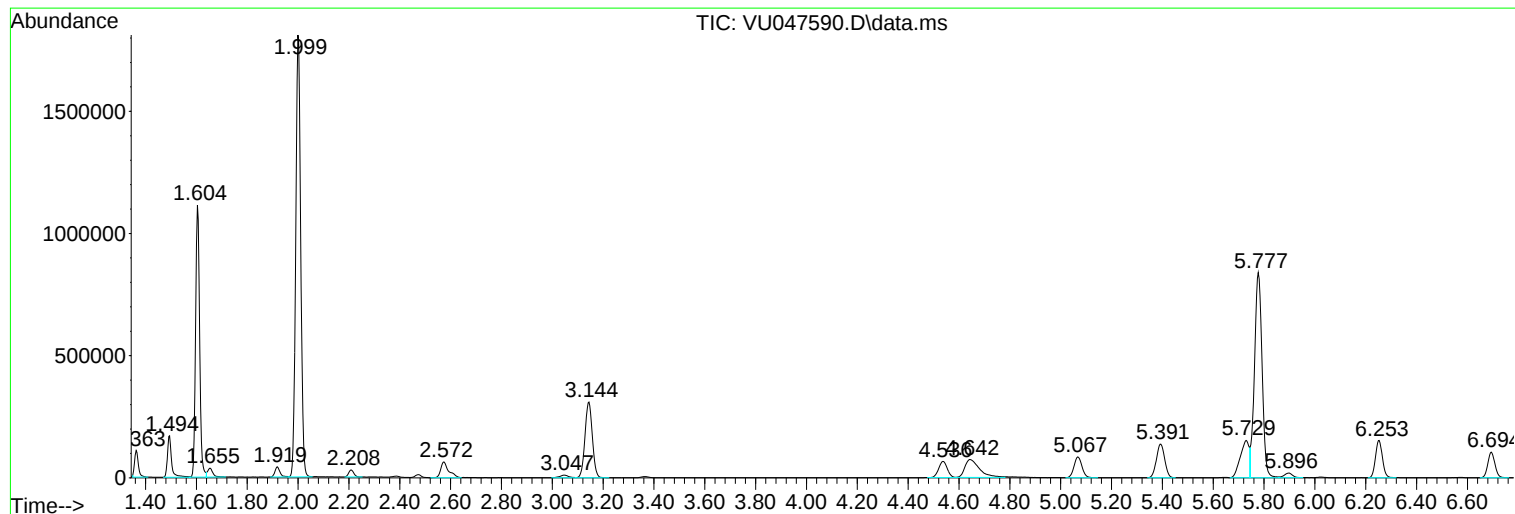
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ETNK2RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR031422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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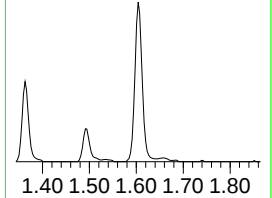
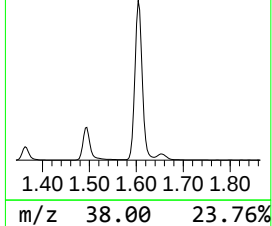
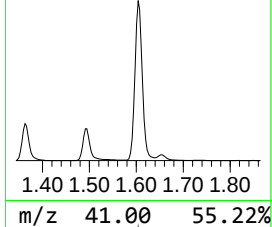
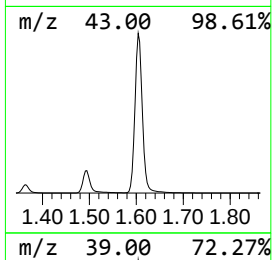
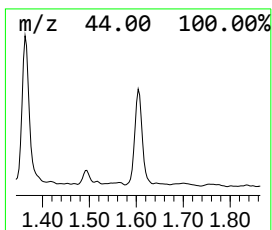
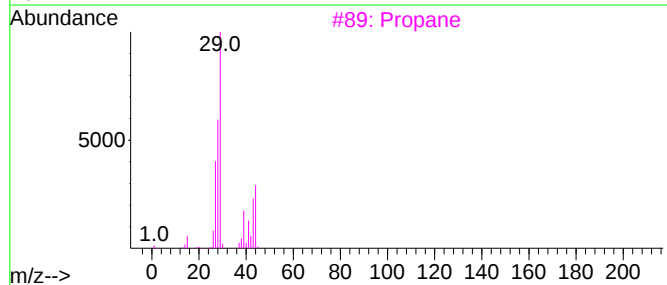
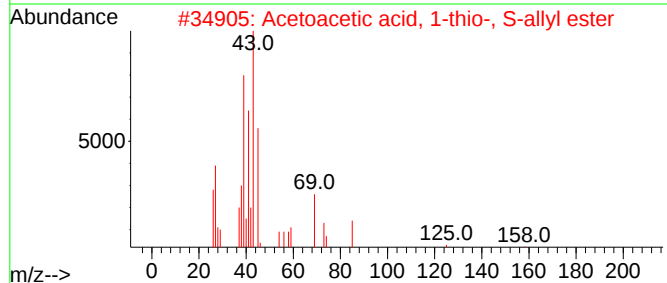
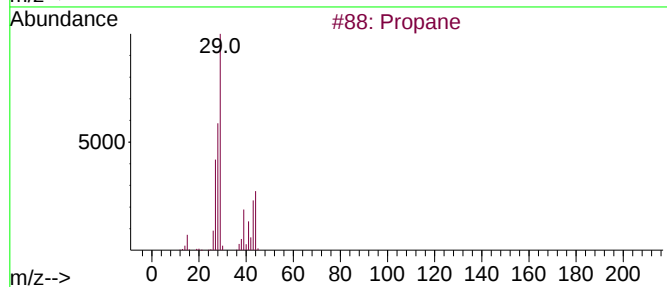
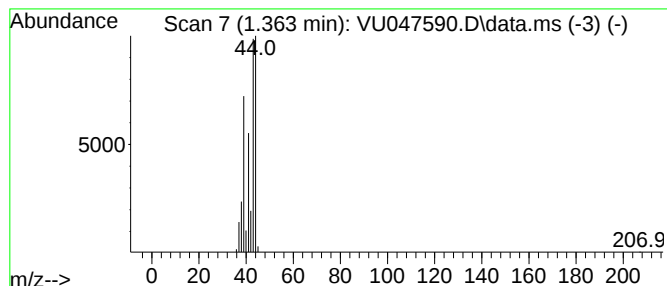
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.363	1.90 ug/L	110064	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Acetoacetic acid, 1-thio-, S-all...	158	C7H10O2S	015780-65-1	50
3			Propane	44	C3H8	000074-98-6	45
4			2-Hexynoic acid	112	C6H8O2	000764-33-0	39
5			2H-Pyran-2-one	96	C5H4O2	000504-31-4	28



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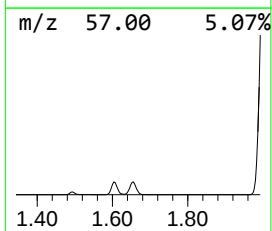
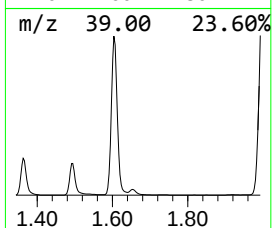
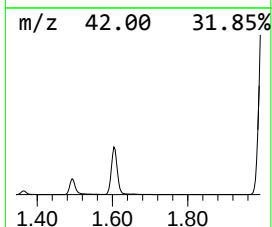
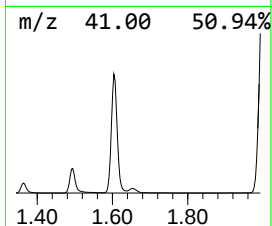
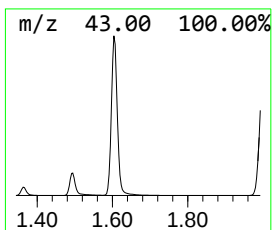
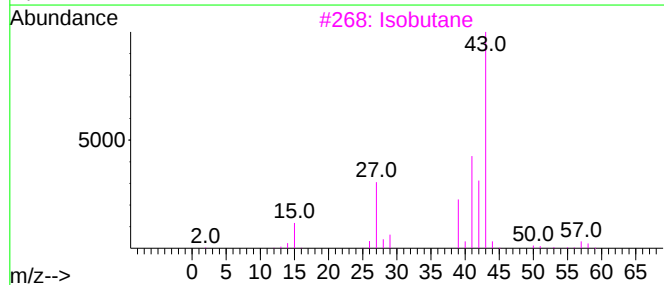
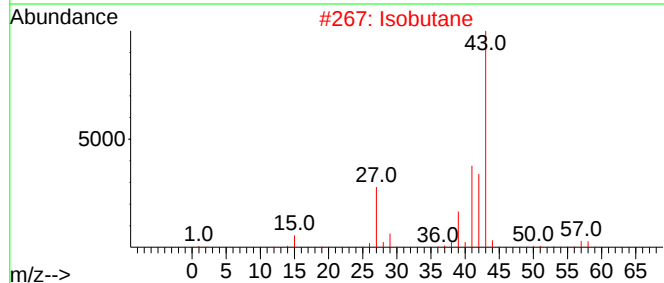
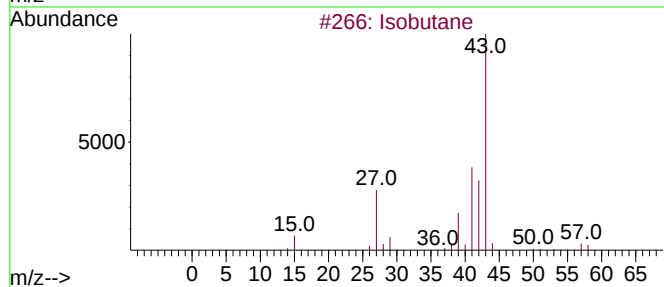
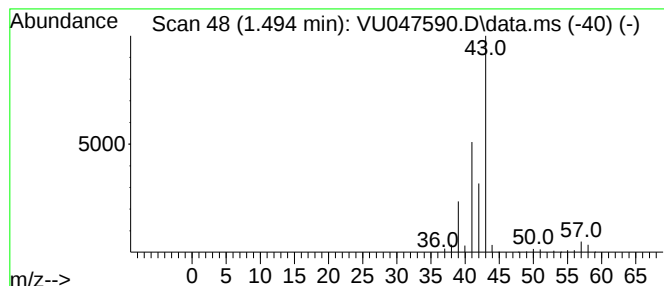
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR031422WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.494	3.27 ug/L	189231	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	72
2		Isobutane	58	C4H10	000075-28-5	72
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	64
5		Isobutane	58	C4H10	000075-28-5	45



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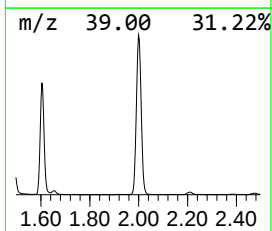
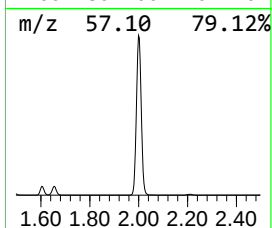
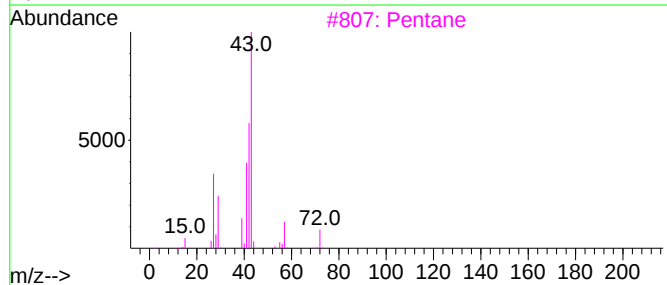
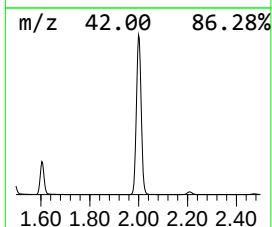
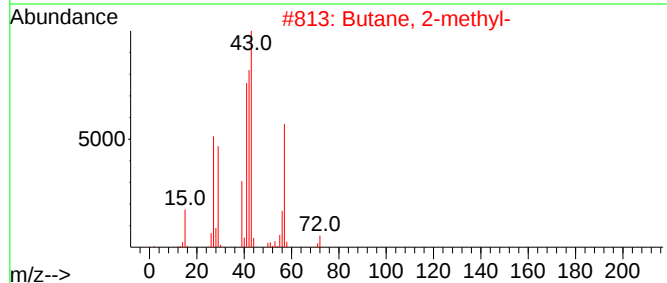
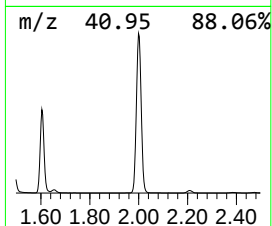
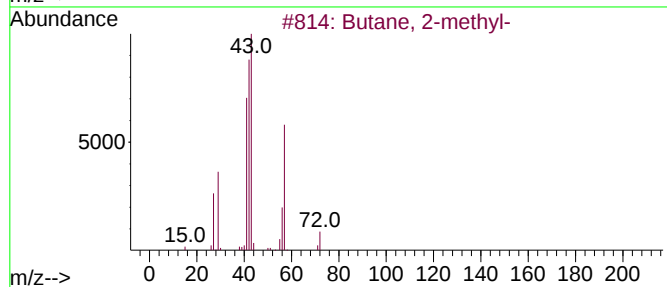
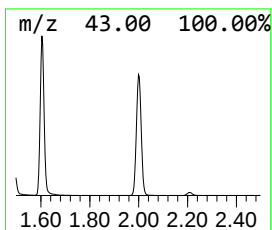
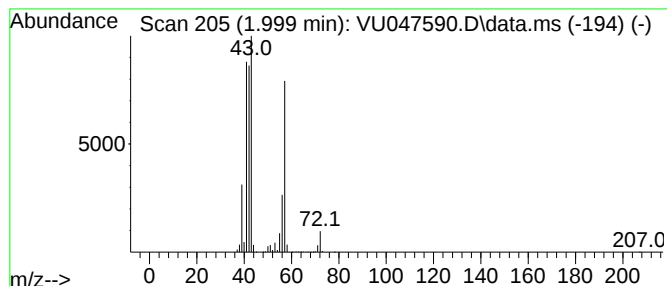
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.999	42.45 ug/L	2455050	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	87
2	Butane, 2-methyl-			72	C5H12	000078-78-4	86
3	Pentane			72	C5H12	000109-66-0	42
4	Oxirane, trimethyl-			86	C5H10O	005076-19-7	33
5	Pentane			72	C5H12	000109-66-0	32



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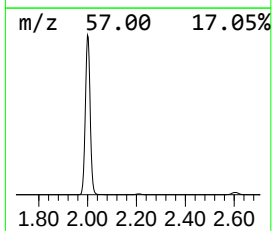
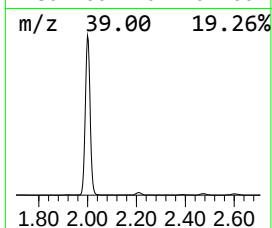
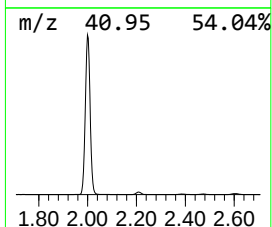
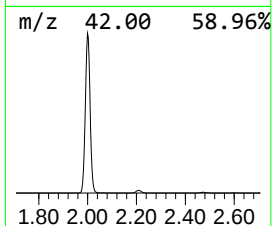
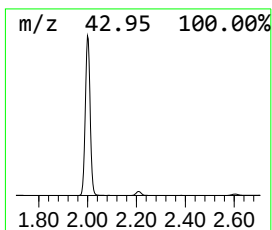
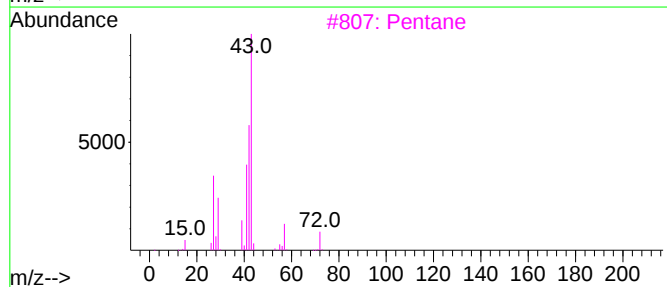
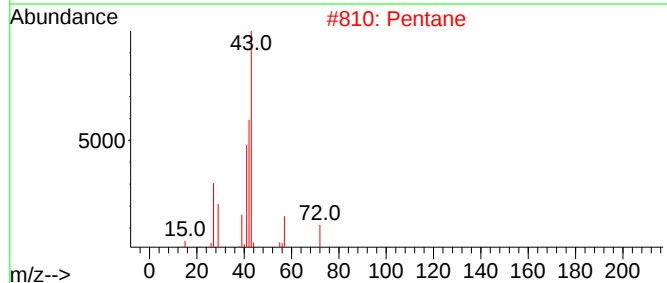
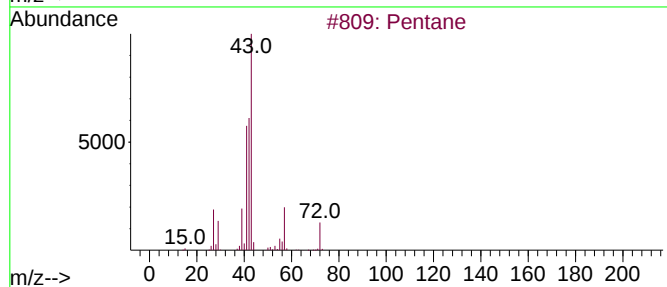
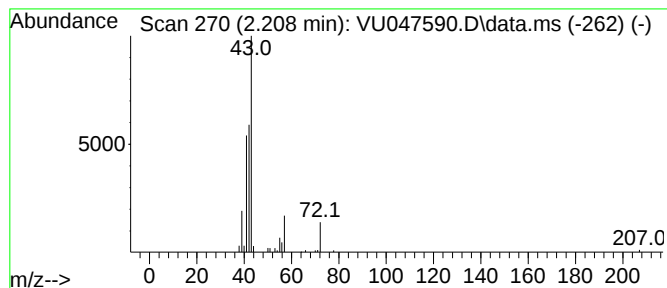
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.208	0.71 ug/L	41280	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	87
2	Pentane			72	C5H12	000109-66-0	86
3	Pentane			72	C5H12	000109-66-0	80
4	Pentane			72	C5H12	000109-66-0	80
5	Pentane			72	C5H12	000109-66-0	72



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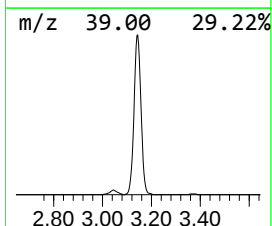
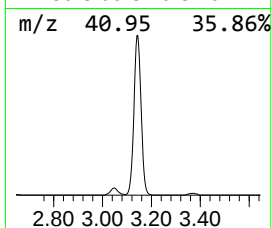
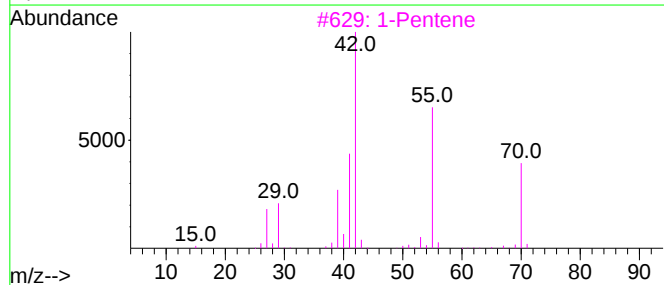
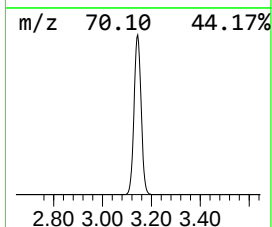
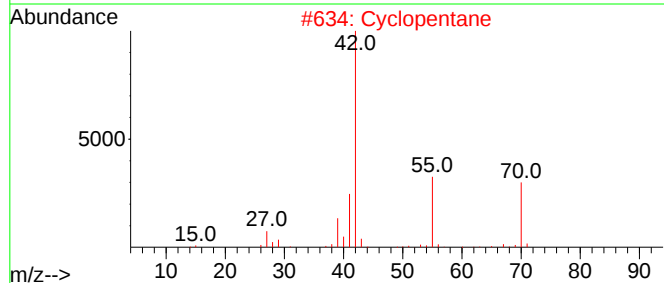
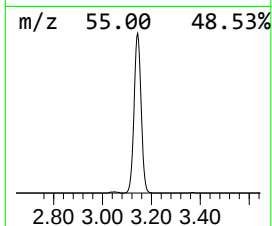
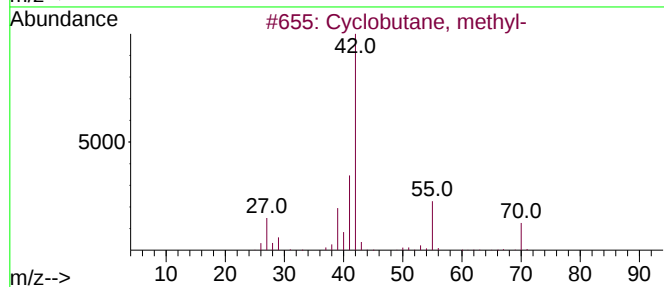
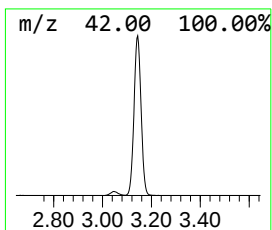
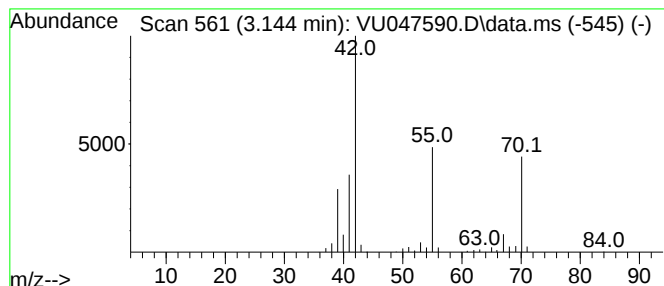
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic3.144 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.144	10.81 ug/L	624878	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2			Cyclopentane	70	C5H10	000287-92-3	80
3			1-Pentene	70	C5H10	000109-67-1	80
4			Cyclopentane	70	C5H10	000287-92-3	72
5			Cyclopentane	70	C5H10	000287-92-3	72



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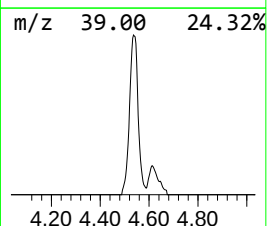
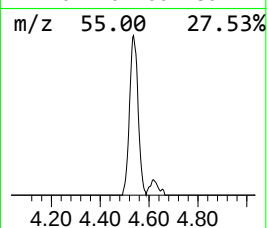
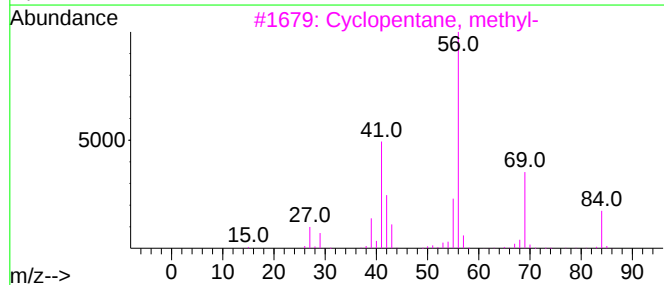
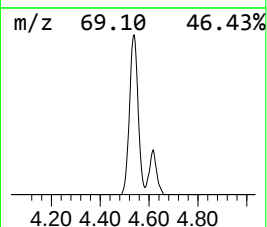
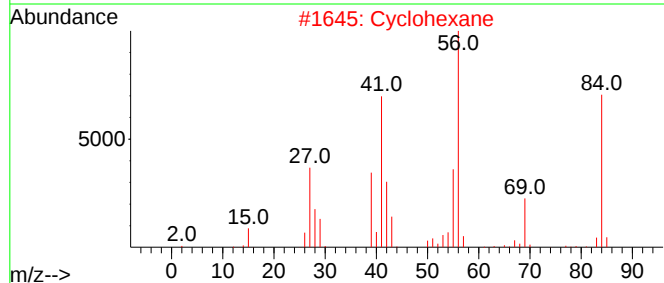
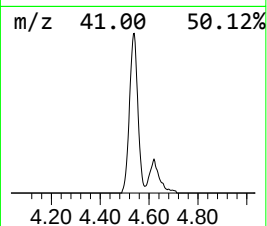
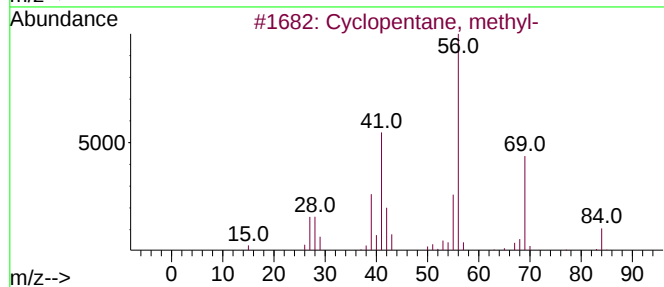
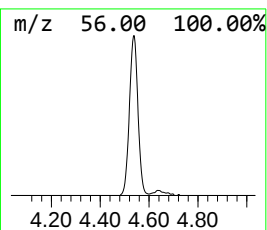
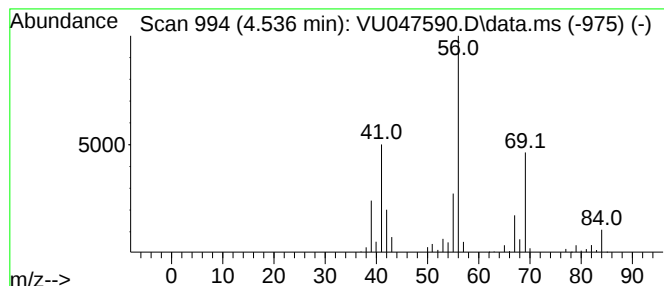
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Cyclic4.536 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.536	2.72 ug/L	157526	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2			Cyclohexane	84	C6H12	000110-82-7	74
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031622\
Data File : VU047590.D
Acq On : 16 Mar 2022 15:08
Operator : SY/MD
Sample : N1858-16RE
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNK2RE

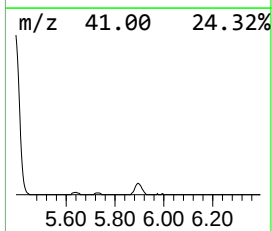
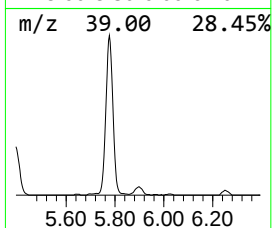
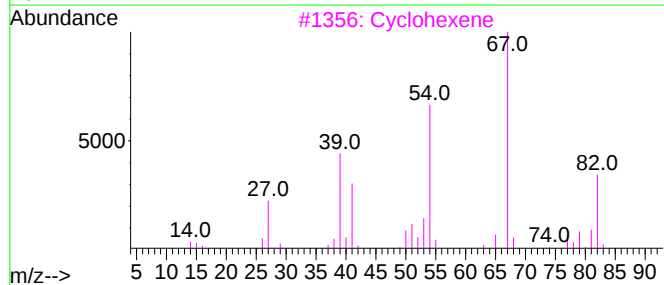
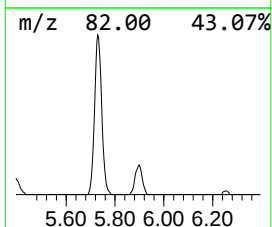
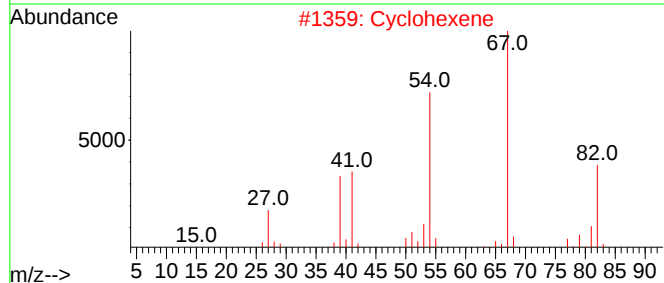
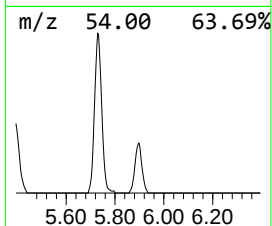
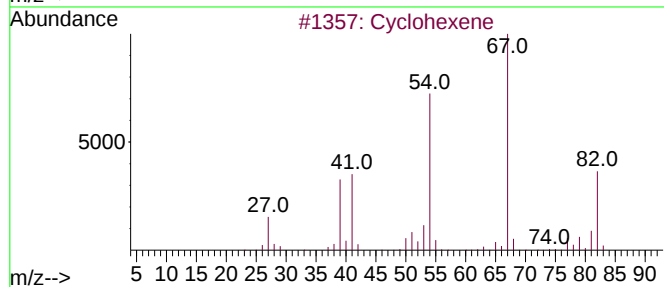
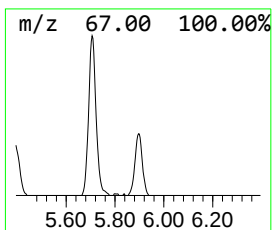
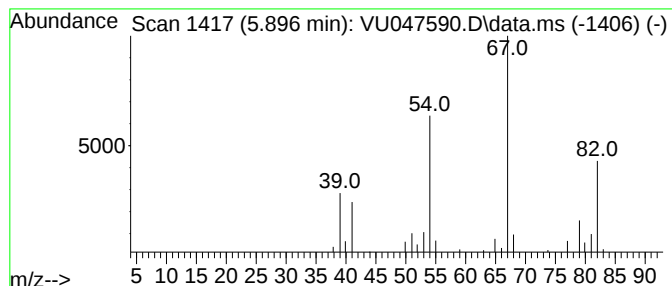
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Ethylenecyclobutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.896	0.71 ug/L	41124	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene	82	C6H10	000110-83-8	90
2			Cyclohexene	82	C6H10	000110-83-8	90
3			Cyclohexene	82	C6H10	000110-83-8	90
4			Cyclohexene	82	C6H10	000110-83-8	90
5			Ethylenecyclobutane	82	C6H10	001528-21-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU031622\
Data File : VU047590.D
Acq On : 16 Mar 2022 15:08
Operator : SY/MD
Sample : N1858-16RE
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNK2RE

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR031422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.363	1.9	ug/L	110064	1	6.253	289142	5.0
(DEL) Alkane: S...	1.494	3.3	ug/L	189231	1	6.253	289142	5.0
(DEL) Alkane: S...	1.999	42.5	ug/L	2455050	1	6.253	289142	5.0
(DEL) Alkane: S...	2.208	0.7	ug/L	41280	1	6.253	289142	5.0
(DEL) Alkane: C...	3.144	10.8	ug/L	624878	1	6.253	289142	5.0
(DEL) Alkane: C...	4.536	2.7	ug/L	157526	1	6.253	289142	5.0
Ethylidenecyclo...	5.896	0.7	ug/L	41124	1	6.253	289142	5.0