

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
 Data File : VU052565.D
 Acq On : 27 Dec 2022 15:27
 Operator : JC/MD
 Sample : N6171-16
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQD2

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: VU052565.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	27	rVB	884186	810412	67.91%	8.711%
2	1.491	40	47	62	rBV	59008	64760	5.43%	0.696%
3	1.594	69	79	95	rBV3	372217	643951	53.96%	6.921%
4	1.694	104	110	116	rBV	14564	22307	1.87%	0.240%
5	1.732	116	122	133	rVB	49028	61751	5.17%	0.664%
6	1.912	169	178	190	rVB2	92865	130083	10.90%	1.398%
7	1.996	196	204	218	rVB	55465	78658	6.59%	0.845%
8	2.157	244	254	262	rBV	87722	123100	10.32%	1.323%
9	2.208	262	270	294	rVB3	78930	153293	12.85%	1.648%
10	2.321	298	305	317	rVB	9802	14797	1.24%	0.159%
11	2.417	323	335	344	rBV3	29908	49826	4.18%	0.536%
12	2.568	367	382	396	rBV	141169	237649	19.91%	2.554%
13	2.642	396	405	425	rVB2	11758	35367	2.96%	0.380%
14	2.793	441	452	466	rVB	13608	22265	1.87%	0.239%
15	2.973	496	508	519	rBV6	10050	27666	2.32%	0.297%
16	3.044	522	530	537	rBV	10076	16450	1.38%	0.177%
17	3.137	551	559	571	rVB3	8642	18221	1.53%	0.196%
18	3.362	618	629	642	rVB3	11262	23630	1.98%	0.254%
19	3.584	682	698	720	rVB3	26898	67091	5.62%	0.721%
20	3.697	722	733	746	rVB4	12891	27822	2.33%	0.299%
21	4.189	875	886	899	rVB6	5846	13431	1.13%	0.144%
22	4.449	948	967	980	rBV6	7832	23464	1.97%	0.252%
23	4.632	1007	1024	1067	rBV	167588	517727	43.38%	5.565%
24	5.060	1142	1157	1179	rVB2	138401	312936	26.22%	3.364%
25	5.722	1341	1363	1392	rBV3	284830	786854	65.93%	8.457%
26	6.018	1447	1455	1472	rVB10	6667	15246	1.28%	0.164%
27	6.137	1480	1492	1501	rBV6	6735	13837	1.16%	0.149%
28	6.247	1512	1526	1551	rBV	221435	431268	36.14%	4.635%
29	6.687	1649	1663	1680	rBV2	191827	375616	31.47%	4.037%
30	6.880	1711	1723	1735	rBV2	10819	21663	1.82%	0.233%
31	7.562	1923	1935	1949	rBV	87210	157840	13.23%	1.697%
32	7.893	2025	2038	2053	rBV	314303	546105	45.76%	5.870%
33	7.967	2053	2061	2069	rVB2	14648	23816	2.00%	0.256%
34	8.176	2115	2126	2143	rBV	58204	100310	8.41%	1.078%
35	8.552	2232	2243	2252	rVB3	12881	21049	1.76%	0.226%
36	8.629	2254	2267	2298	rBV	646820	1193382	100.00%	12.827%

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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

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37	8.783	2305	2315	2329	rVB2	54210	90993	7.62%	0.978%
38	9.414	2497	2511	2530	rBV	312666	527657	44.22%	5.671%
39	9.690	2584	2597	2608	rBV	20348	33394	2.80%	0.359%
40	10.095	2713	2723	2745	rVB3	27895	52809	4.43%	0.568%
41	10.340	2788	2799	2808	rBV6	12298	19844	1.66%	0.213%
42	10.751	2914	2927	2941	rBV	172904	273751	22.94%	2.942%
43	11.684	3208	3217	3231	rBV4	14668	23393	1.96%	0.251%
44	11.806	3244	3255	3274	rBV	297945	478682	40.11%	5.145%
45	12.057	3324	3333	3354	rBV3	15007	31343	2.63%	0.337%
46	12.188	3362	3374	3391	rBV	319150	522700	43.80%	5.618%
47	12.883	3580	3590	3601	rBV3	39572	65537	5.49%	0.704%

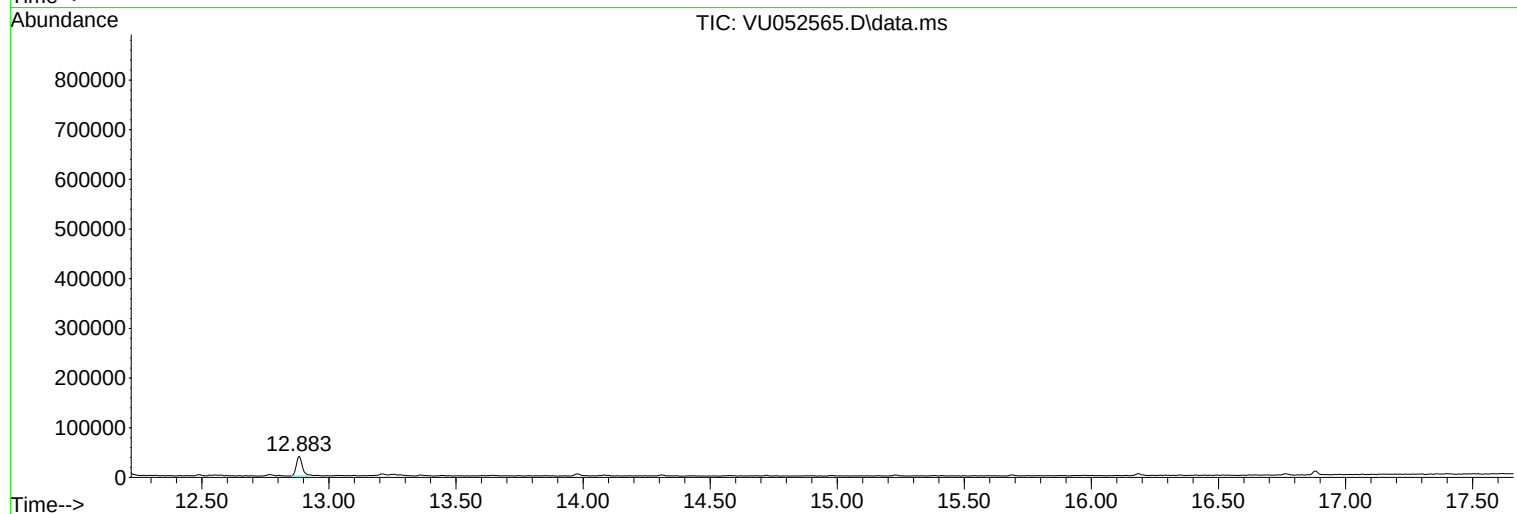
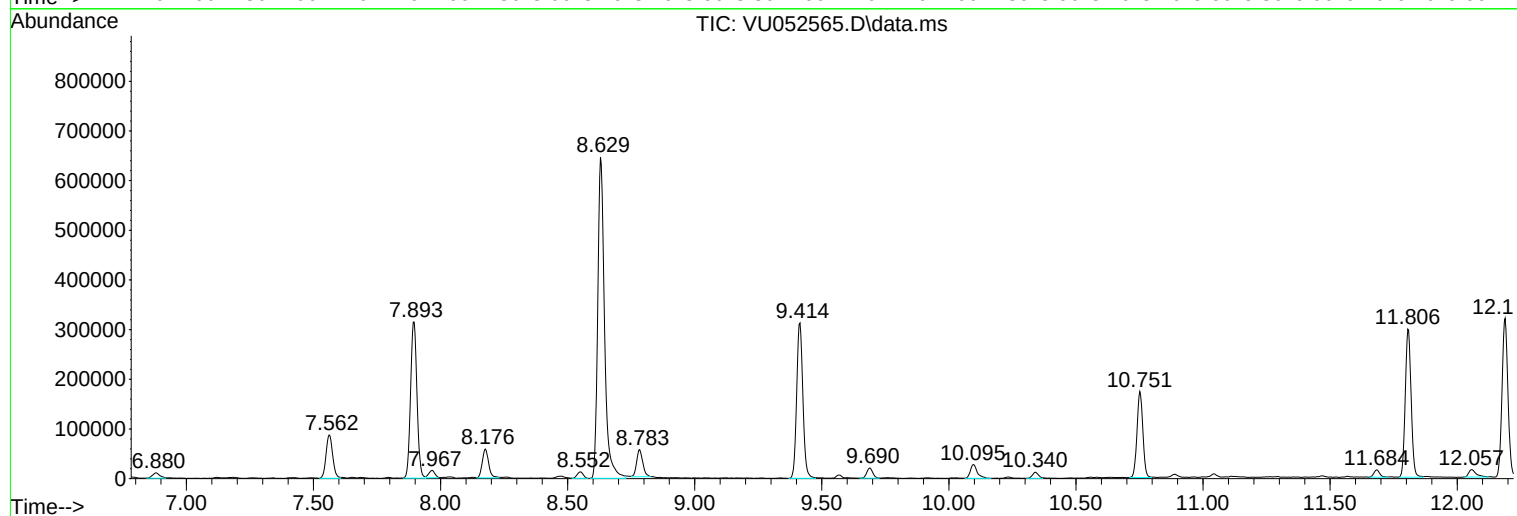
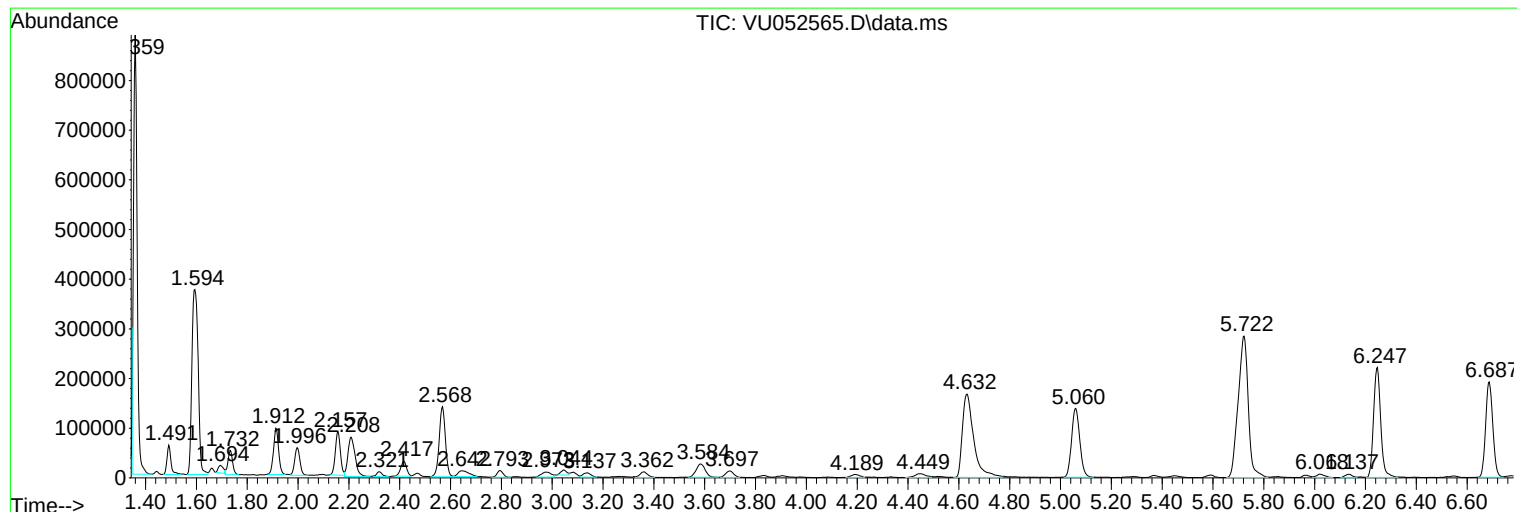
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
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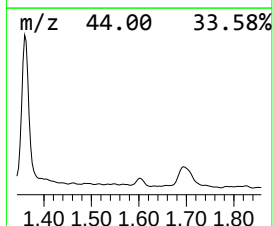
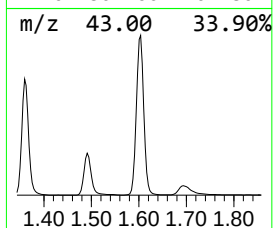
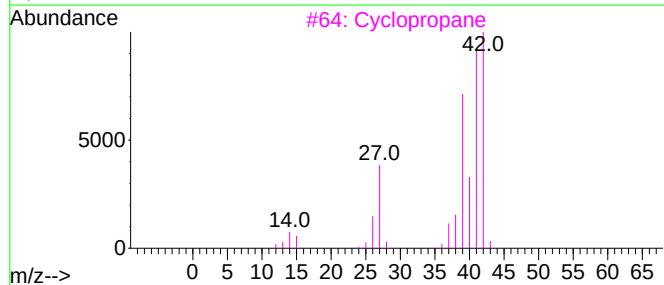
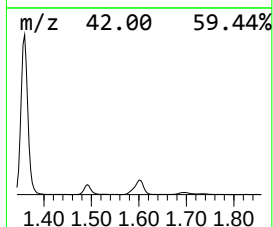
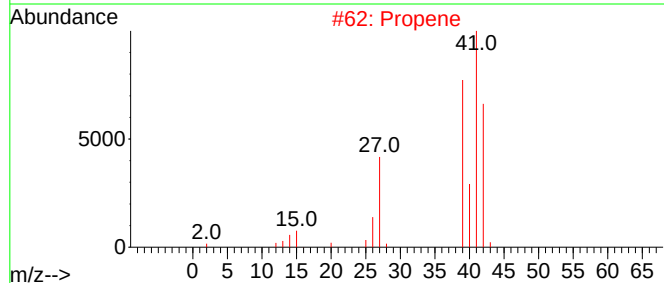
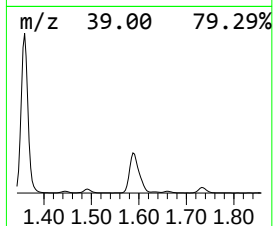
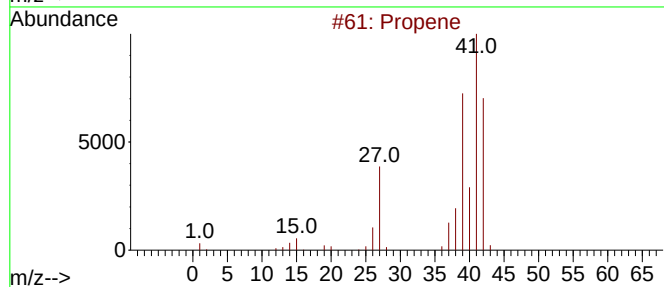
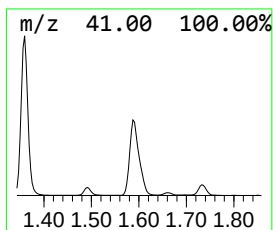
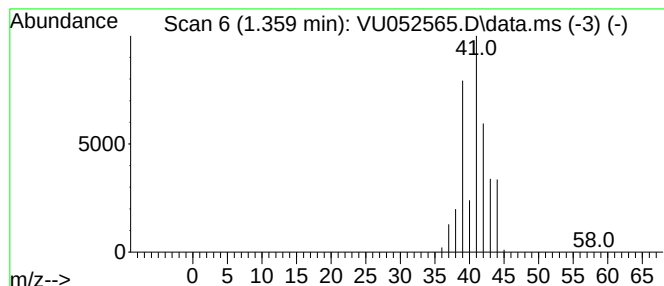
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	9.40 ug/L	810412	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	42
3			Cyclopropane	42	C3H6	000075-19-4	9
4			Cyclopropene	40	C3H4	002781-85-3	9
5			Cyclopropane	42	C3H6	000075-19-4	7



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
MSVOA_U
ClientSampleId :
GBQD2

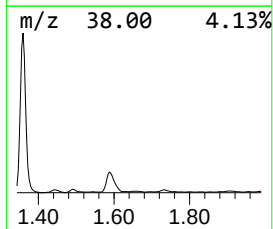
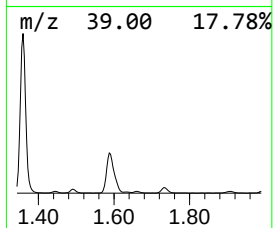
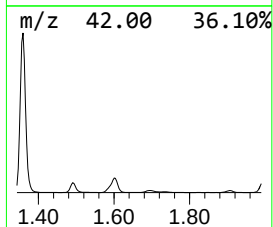
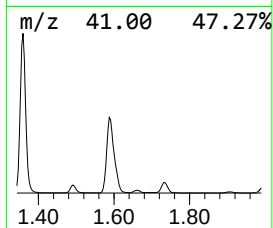
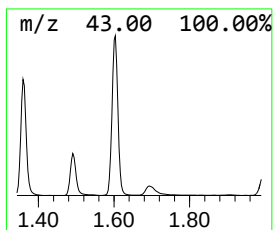
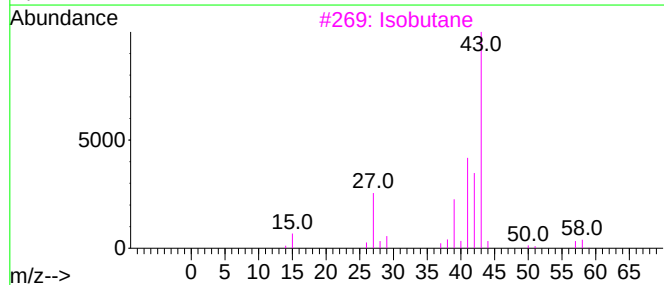
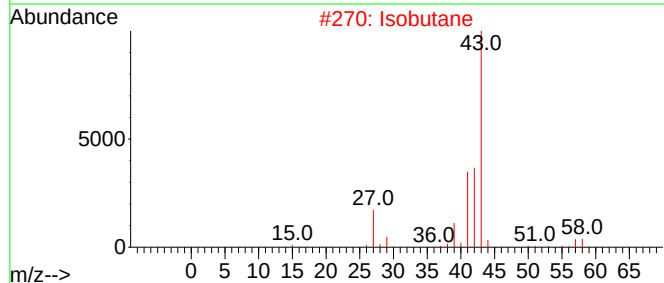
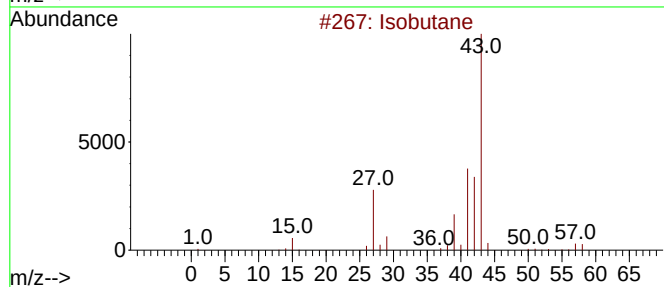
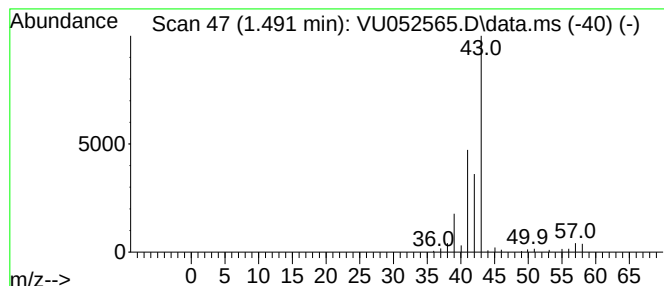
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	0.75 ug/L	64760	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	64
2		Isobutane	58	C4H10	000075-28-5	64
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	64
5		Isobutane	58	C4H10	000075-28-5	50



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Sample : N6171-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

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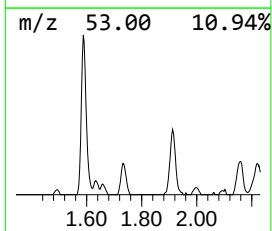
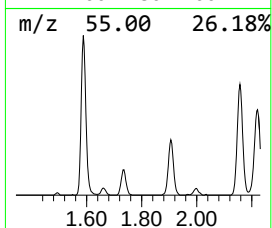
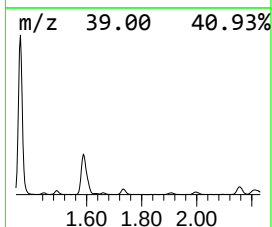
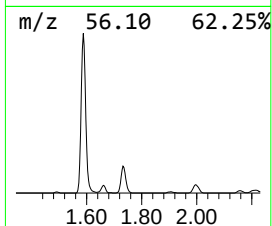
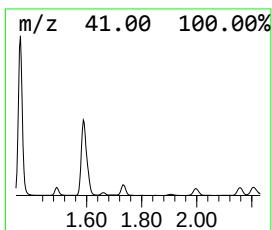
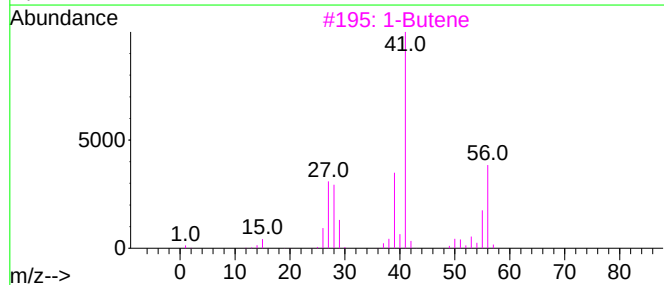
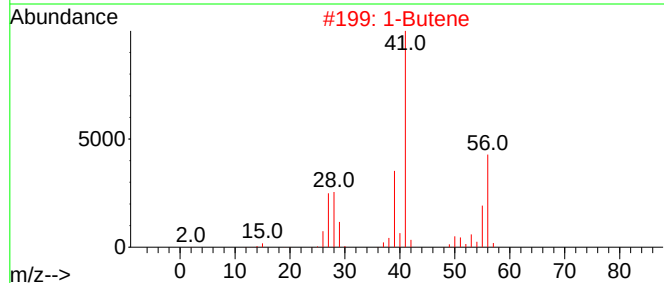
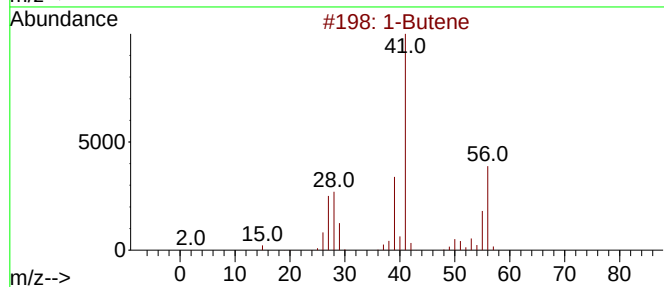
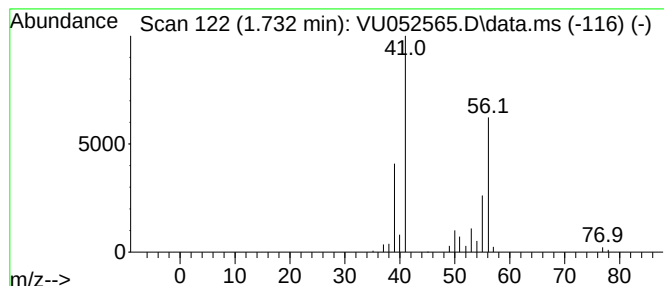
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.732	0.72 ug/L	61751	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Butene	56	C4H8	000106-98-9	87
2		1-Butene	56	C4H8	000106-98-9	86
3		1-Butene	56	C4H8	000106-98-9	86
4		2-Butene, (Z)-	56	C4H8	000590-18-1	86
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	86



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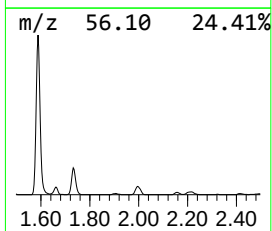
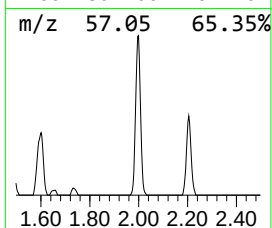
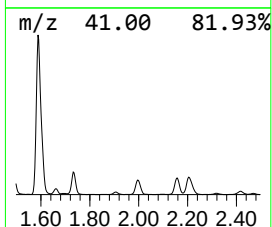
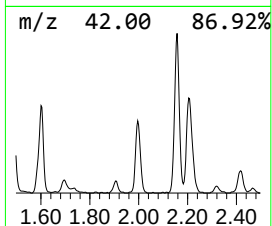
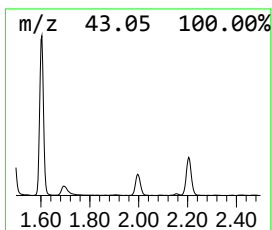
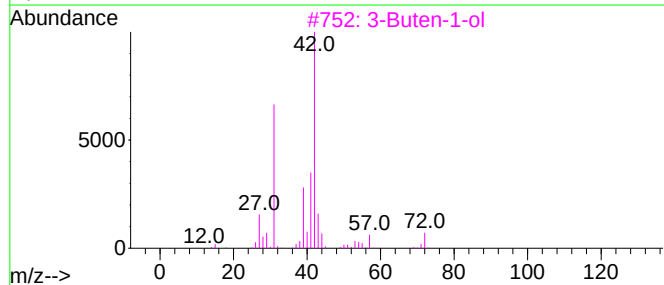
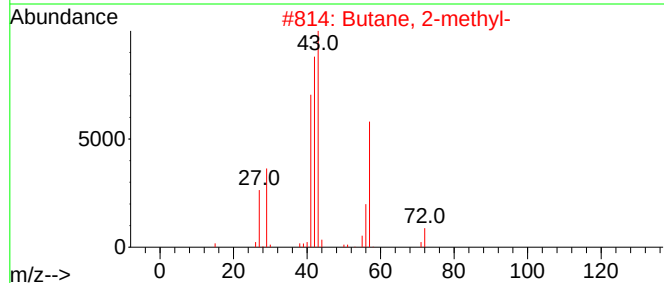
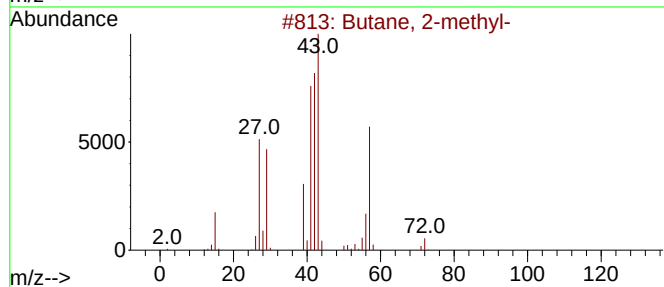
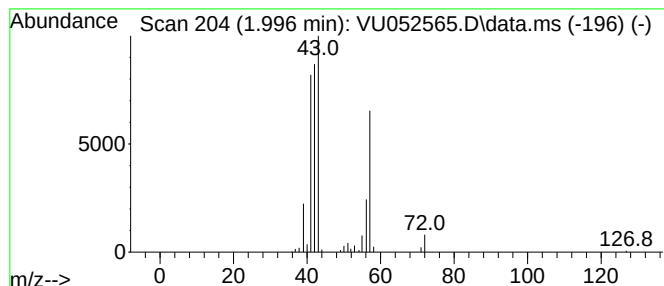
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	0.91 ug/L	78658	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	90
2	Butane, 2-methyl-			72	C5H12	000078-78-4	90
3	3-Buten-1-ol			72	C4H8O	000627-27-0	43
4	1-Propene, 2-methyl-			56	C4H8	000115-11-7	10
5	1-Butene			56	C4H8	000106-98-9	10



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ClientSampleId :
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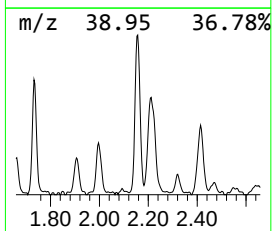
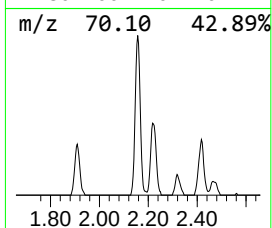
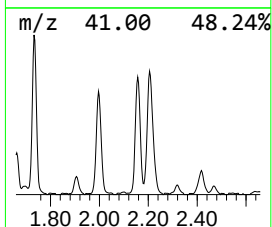
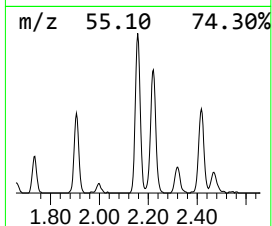
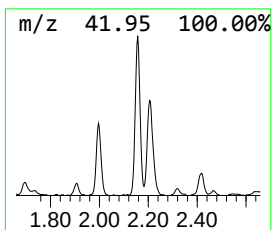
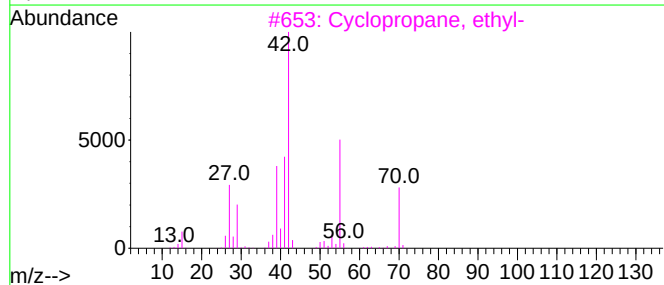
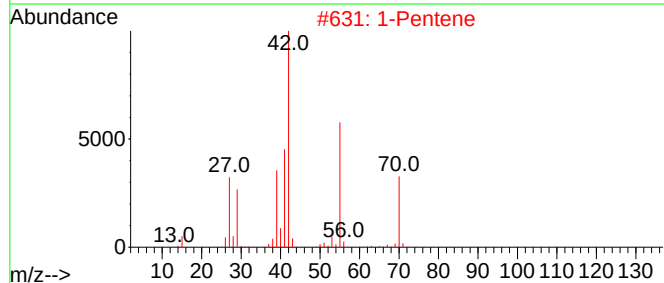
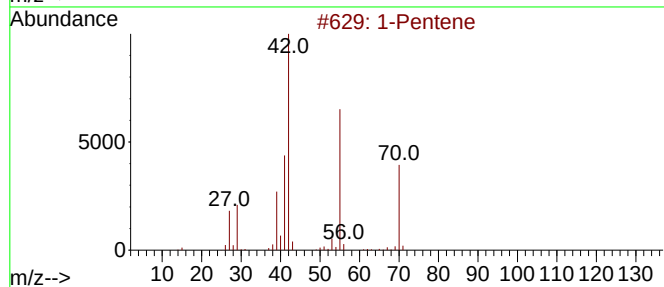
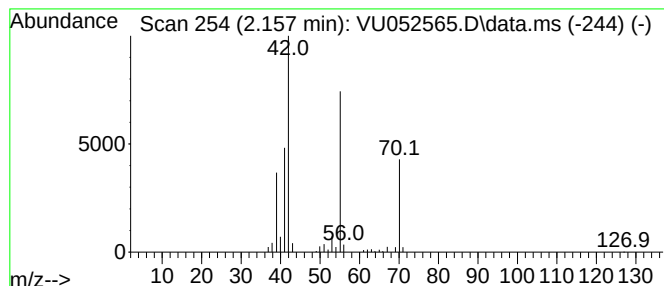
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	1.43 ug/L	123100	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene	70	C5H10	000109-67-1	91
2			1-Pentene	70	C5H10	000109-67-1	91
3			Cyclopropane, ethyl-	70	C5H10	001191-96-4	91
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	86
5			Cyclopentane	70	C5H10	000287-92-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052565.D
Acq On : 27 Dec 2022 15:27
Operator : JC/MD
Sample : N6171-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD2

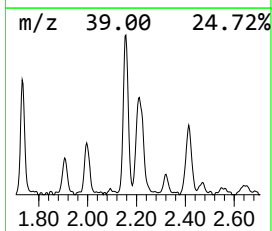
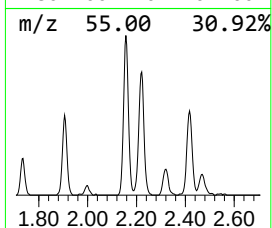
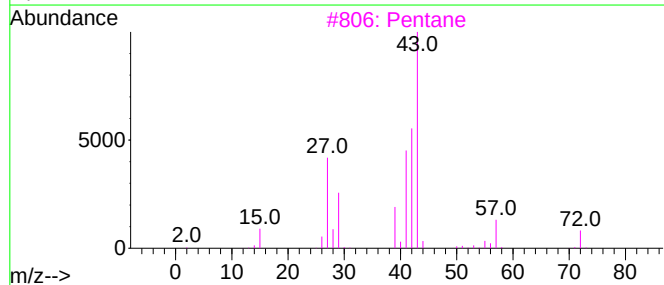
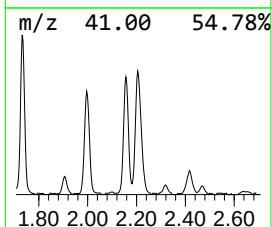
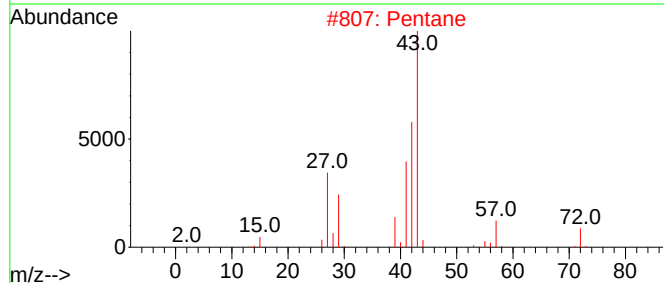
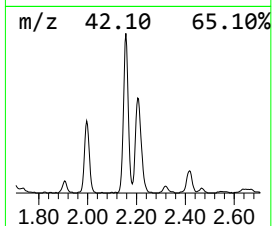
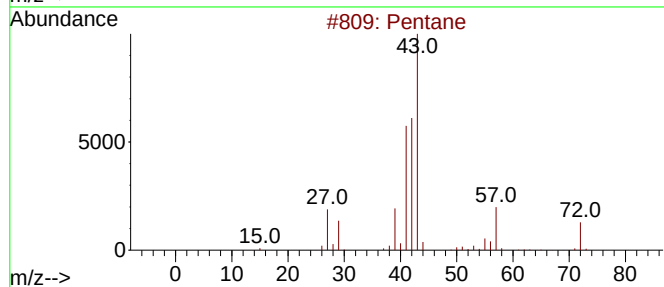
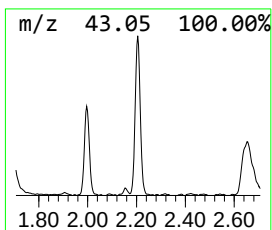
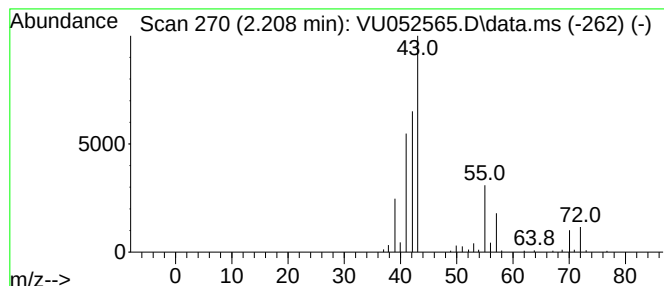
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.208	1.78 ug/L	153293	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	87
2	Pentane			72	C5H12	000109-66-0	72
3	Pentane			72	C5H12	000109-66-0	72
4	Pentane			72	C5H12	000109-66-0	72
5	Pentane			72	C5H12	000109-66-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052565.D
Acq On : 27 Dec 2022 15:27
Operator : JC/MD
Sample : N6171-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

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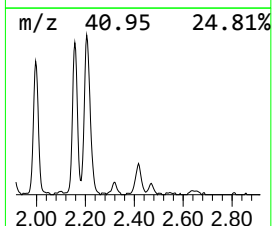
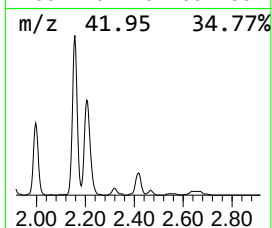
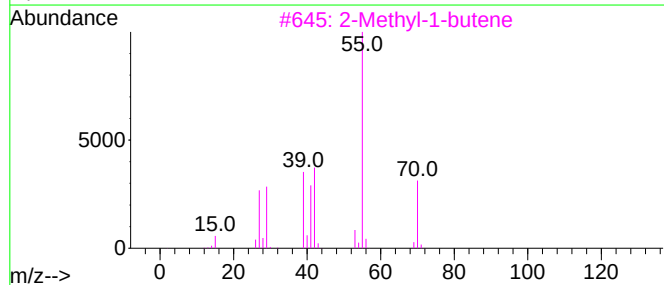
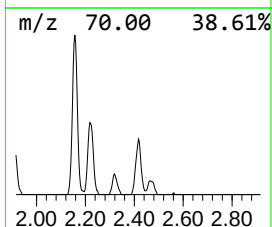
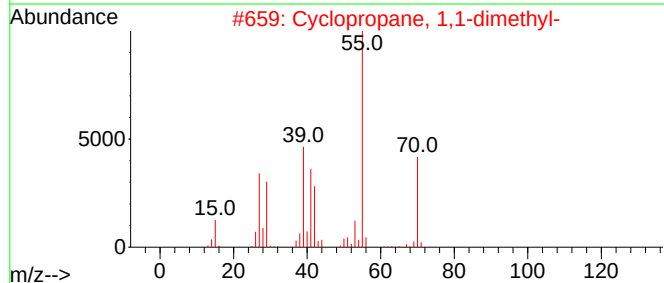
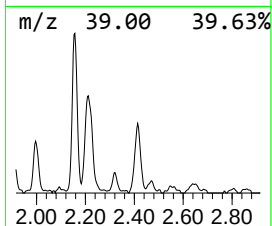
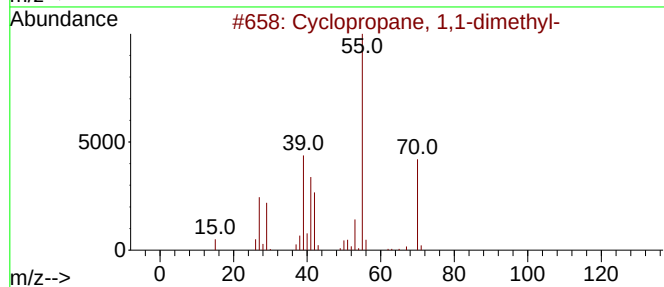
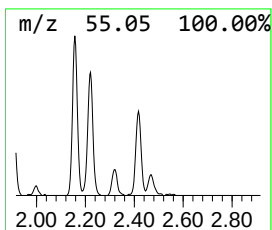
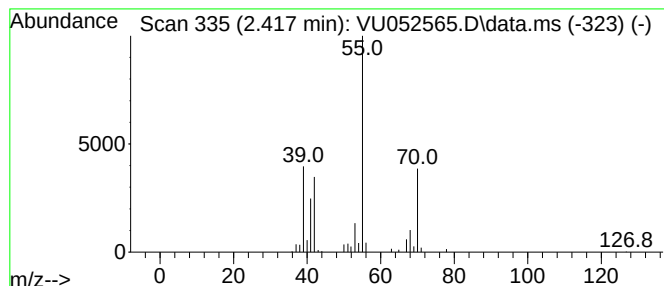
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Cyclic2.417 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.417	0.58 ug/L	49826	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	86
2			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
3			2-Methyl-1-butene	70	C5H10	000563-46-2	80
4			2-Butene, 2-methyl-	70	C5H10	000513-35-9	72
5			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052565.D
Acq On : 27 Dec 2022 15:27
Operator : JC/MD
Sample : N6171-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

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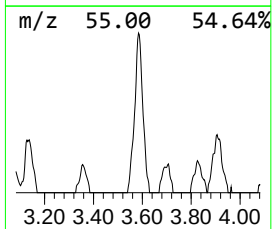
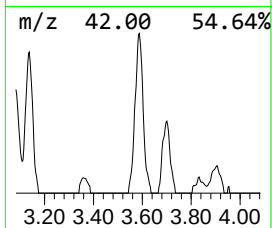
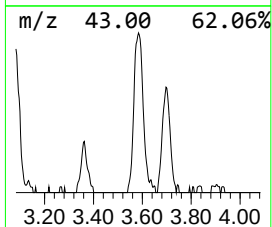
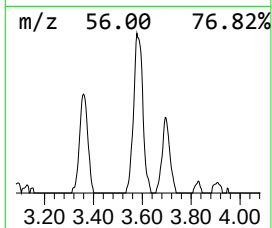
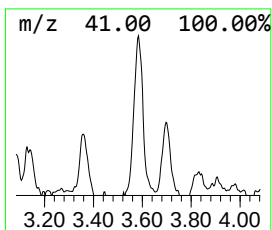
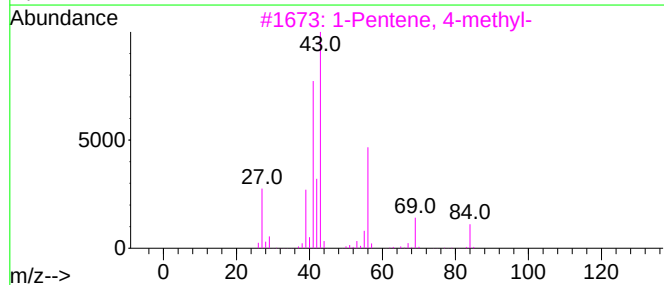
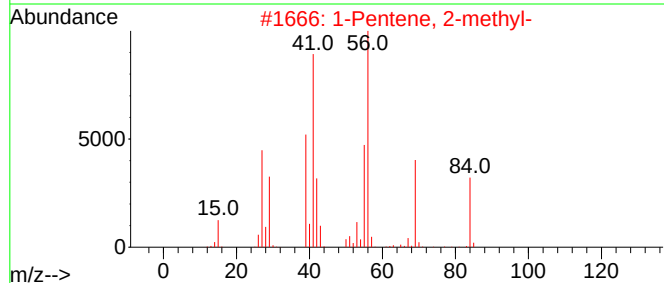
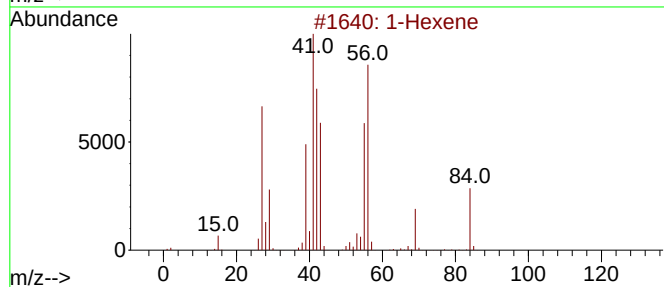
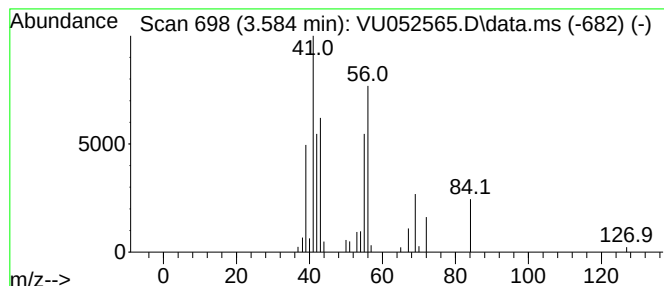
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.584	0.78 ug/L	67091	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene			84	C6H12	000592-41-6	90
2	1-Pentene, 2-methyl-			84	C6H12	000763-29-1	64
3	1-Pentene, 4-methyl-			84	C6H12	000691-37-2	64
4	1-Hexene			84	C6H12	000592-41-6	58
5	1-Pentene, 4-methyl-			84	C6H12	000691-37-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052565.D
Acq On : 27 Dec 2022 15:27
Operator : JC/MD
Sample : N6171-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

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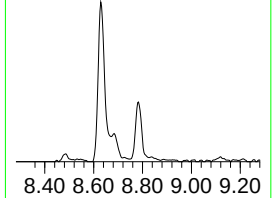
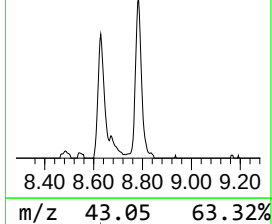
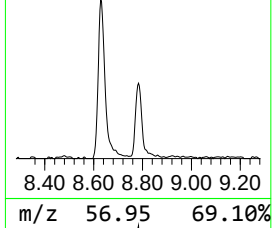
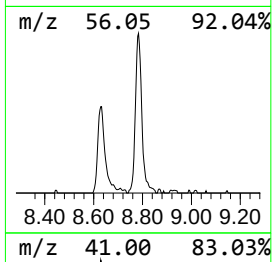
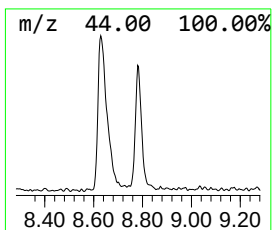
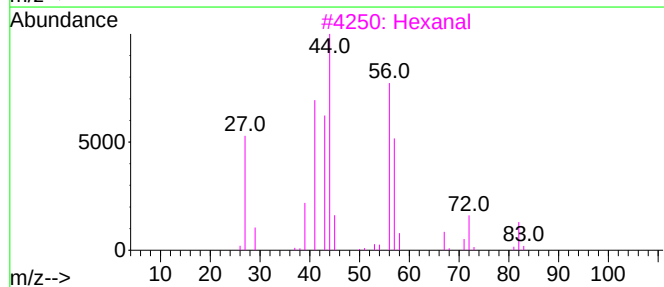
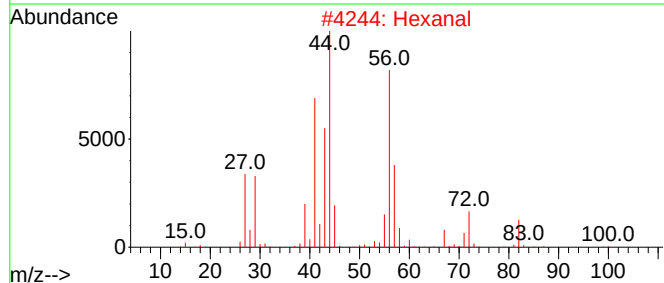
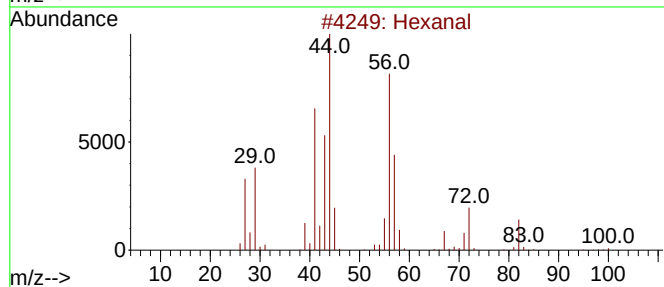
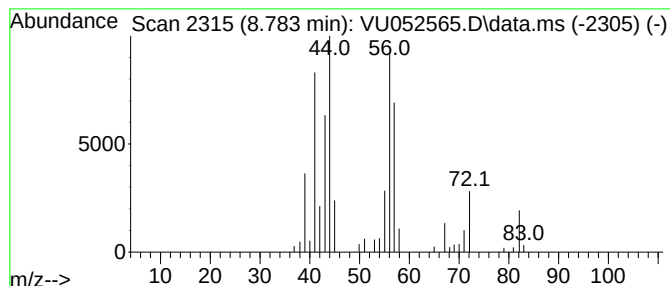
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.783	0.86 ug/L	90993	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	83
2	Hexanal			100	C6H12O	000066-25-1	83
3	Hexanal			100	C6H12O	000066-25-1	78
4	Hexanal			100	C6H12O	000066-25-1	72
5	Hexanal			100	C6H12O	000066-25-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052565.D
Acq On : 27 Dec 2022 15:27
Operator : JC/MD
Sample : N6171-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

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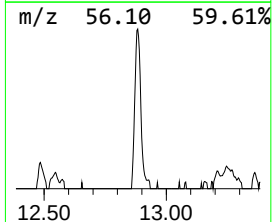
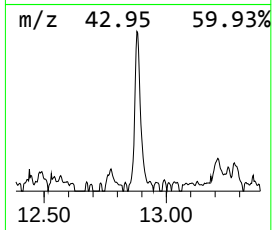
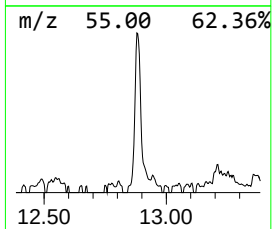
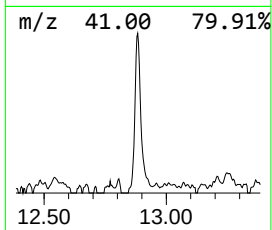
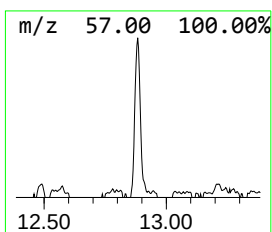
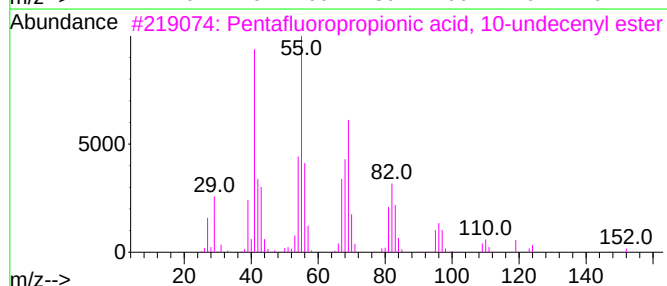
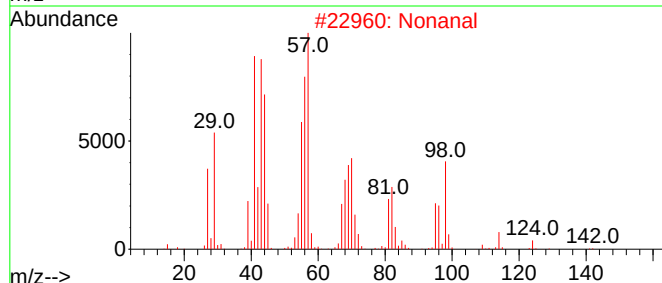
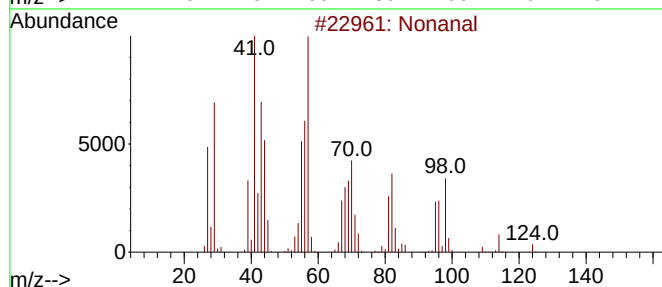
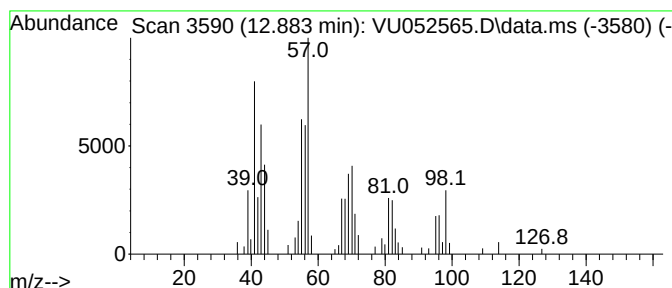
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 Nonanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.883	0.68 ug/L	65537	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	90
2			Nonanal	142	C9H18O	000124-19-6	90
3			Pentafluoropropionic acid, 10-un...	316	C14H21F5O2	1000280-07-1	38
4			Heptane, 4-chloro-	134	C7H15Cl	000998-95-8	35
5			2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052565.D
Acq On : 27 Dec 2022 15:27
Operator : JC/MD
Sample : N6171-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD2

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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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(DEL) Alkane: S...	1.491	0.8	ug/L	64760	1	6.247	431268	5.0
(DEL) Alkane: S...	1.732	0.7	ug/L	61751	1	6.247	431268	5.0
(DEL) Alkane: S...	1.996	0.9	ug/L	78658	1	6.247	431268	5.0
(DEL) Alkane: S...	2.157	1.4	ug/L	123100	1	6.247	431268	5.0
(DEL) Alkane: S...	2.208	1.8	ug/L	153293	1	6.247	431268	5.0
(DEL) Alkane: C...	2.417	0.6	ug/L	49826	1	6.247	431268	5.0
(DEL) Alkane: S...	3.584	0.8	ug/L	67091	1	6.247	431268	5.0
Hexanal	8.783	0.9	ug/L	90993	2	9.414	527657	5.0
Nonanal	12.883	0.7	ug/L	65537	3	11.809	478682	5.0