

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
 Data File : VU052557.D
 Acq On : 27 Dec 2022 12:21
 Operator : JC/MD
 Sample : N6169-10
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQA1

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: VU052557.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	27	rVB	990535	905215	82.46%	8.425%
2	1.491	40	47	65	rBV	69938	78353	7.14%	0.729%
3	1.591	69	78	94	rBV3	420378	729196	66.42%	6.787%
4	1.662	94	100	105	rVV	12635	12289	1.12%	0.114%
5	1.733	116	122	131	rVB	56306	64275	5.85%	0.598%
6	1.913	164	178	194	rVV2	90798	135990	12.39%	1.266%
7	1.996	196	204	218	rVB	66091	90346	8.23%	0.841%
8	2.157	245	254	262	rBV	101658	141219	12.86%	1.314%
9	2.212	262	271	288	rVB2	101797	205315	18.70%	1.911%
10	2.318	295	304	314	rBV2	10702	16774	1.53%	0.156%
11	2.417	323	335	344	rBV	35804	58762	5.35%	0.547%
12	2.469	344	351	366	rVB2	16702	28763	2.62%	0.268%
13	2.569	366	382	395	rBV	133020	223032	20.32%	2.076%
14	2.639	397	404	424	rVB	9252	23446	2.14%	0.218%
15	2.797	442	453	464	rBV2	12921	22873	2.08%	0.213%
16	2.980	494	510	518	rBV6	12001	32804	2.99%	0.305%
17	3.044	521	530	550	rVV6	33541	91294	8.32%	0.850%
18	3.134	552	558	578	rVB4	7402	15877	1.45%	0.148%
19	3.353	611	626	646	rBV	185845	374262	34.09%	3.483%
20	3.585	682	698	716	rVB4	32974	85723	7.81%	0.798%
21	3.700	719	734	750	rVB3	15177	33277	3.03%	0.310%
22	4.192	868	887	899	rBV6	8161	20102	1.83%	0.187%
23	4.658	1006	1032	1059	rBV2	292730	1038704	94.62%	9.668%
24	5.060	1141	1157	1182	rVB	127906	287747	26.21%	2.678%
25	5.591	1312	1322	1331	rVB4	5644	11178	1.02%	0.104%
26	5.723	1341	1363	1396	rBV2	256241	714378	65.07%	6.649%
27	5.964	1427	1438	1446	rBV3	5897	11185	1.02%	0.104%
28	6.022	1447	1456	1474	rVB5	8755	20375	1.86%	0.190%
29	6.244	1512	1525	1552	rBV	196248	390915	35.61%	3.638%
30	6.539	1602	1617	1634	rBV2	149110	288252	26.26%	2.683%
31	6.684	1647	1662	1681	rBV	173801	340364	31.00%	3.168%
32	7.562	1921	1935	1949	rBV	80927	144046	13.12%	1.341%
33	7.893	2020	2038	2053	rBV	284600	487947	44.45%	4.542%
34	7.964	2053	2060	2070	rVB	13844	21983	2.00%	0.205%
35	8.176	2114	2126	2144	rBV2	52761	92070	8.39%	0.857%
36	8.549	2229	2242	2255	rBV	457333	765284	69.71%	7.123%

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Min Area: 3 % of largest Peak

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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

37	8.629	2255	2267	2300	rVV	592441	1097795	100.00%	10.218%
38	8.787	2308	2316	2333	rVB10	7082	14809	1.35%	0.138%
39	9.414	2499	2511	2533	rBV	272944	461502	42.04%	4.295%
40	9.687	2583	2596	2611	rBV2	15533	26829	2.44%	0.250%
41	10.096	2711	2723	2737	rBV2	19742	33227	3.03%	0.309%
42	10.751	2914	2927	2942	rBV	160546	255717	23.29%	2.380%
43	11.806	3243	3255	3269	rBV	255948	399623	36.40%	3.720%
44	12.189	3358	3374	3397	rBV	274379	450810	41.07%	4.196%

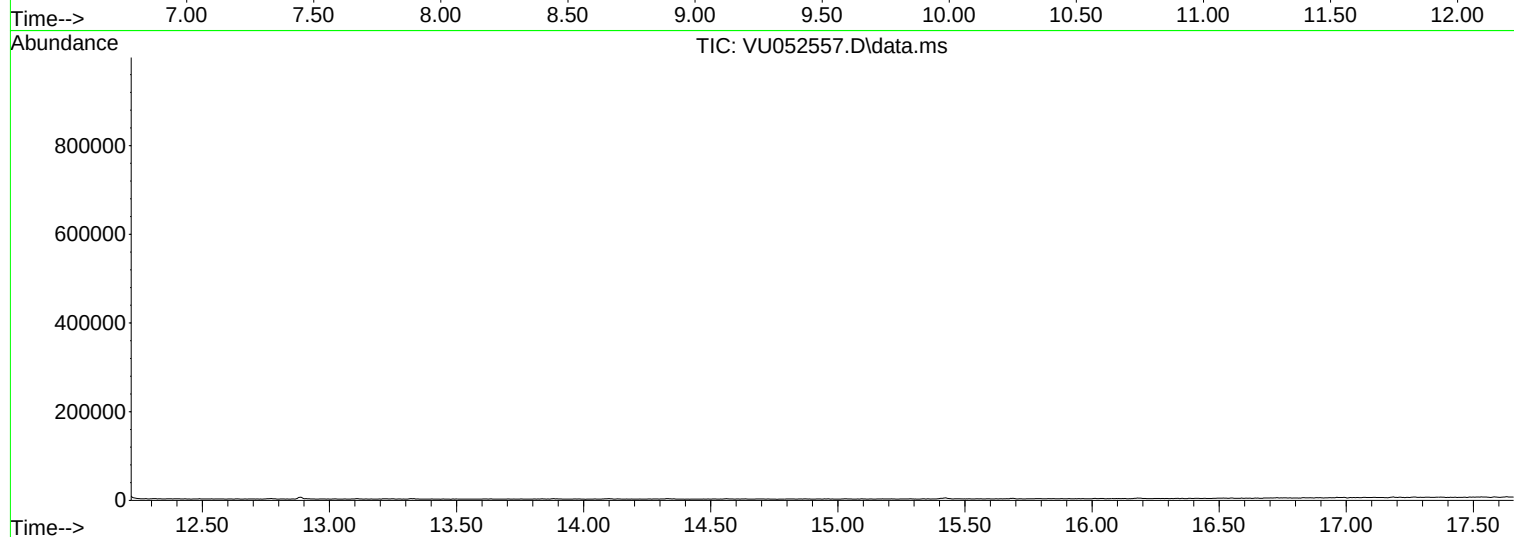
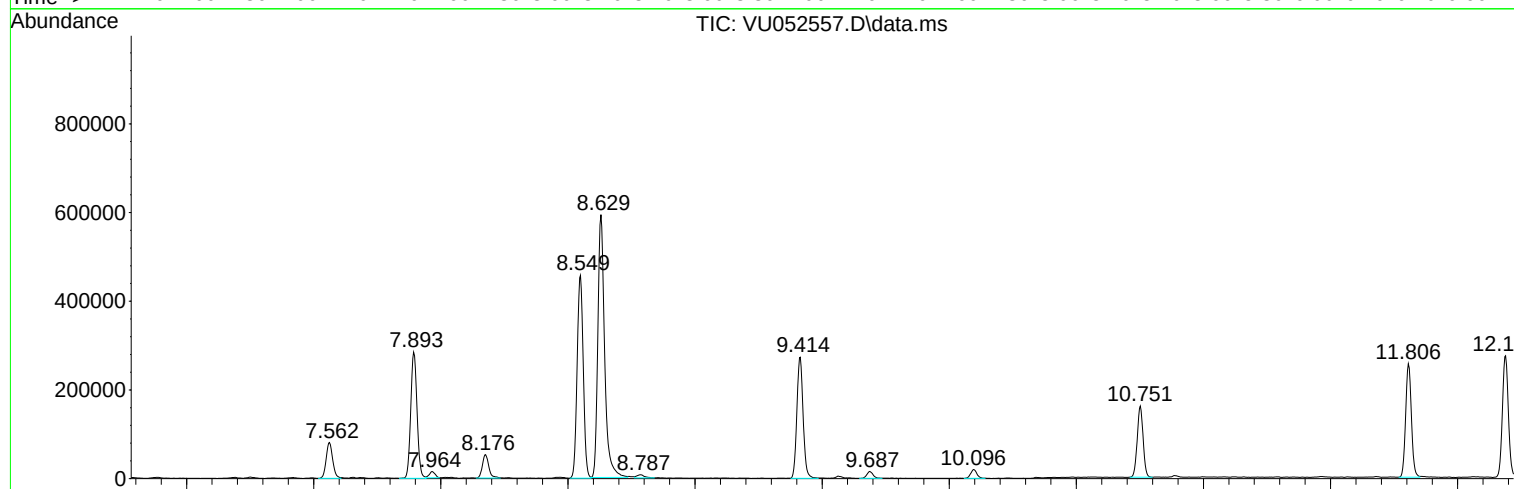
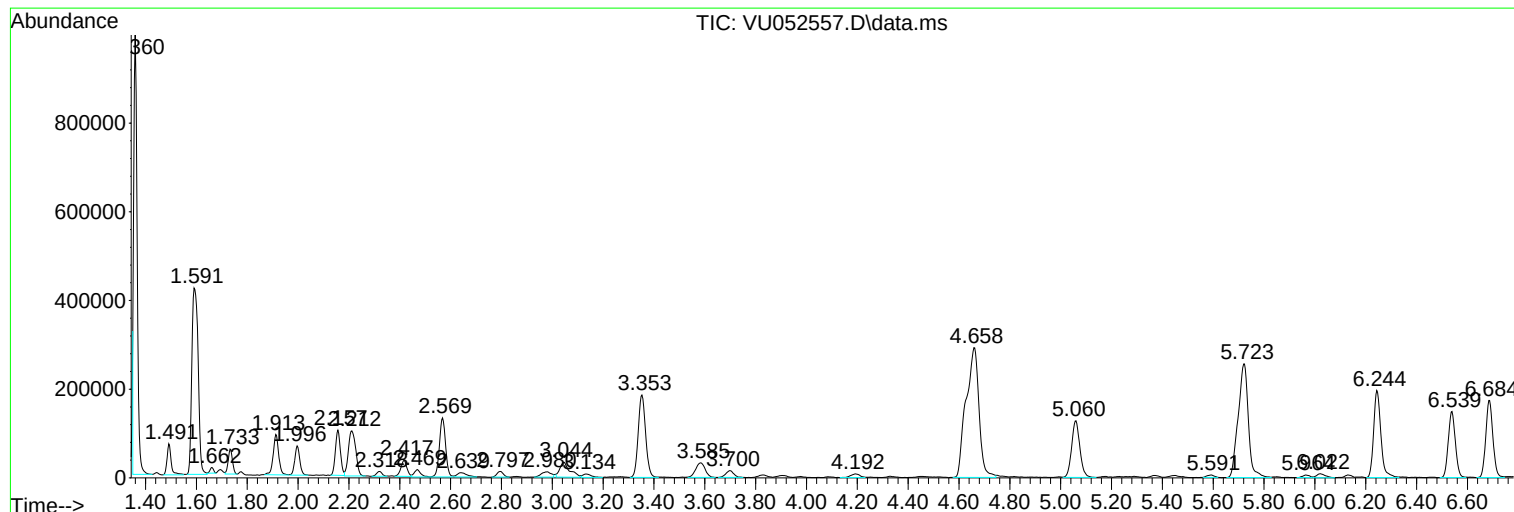
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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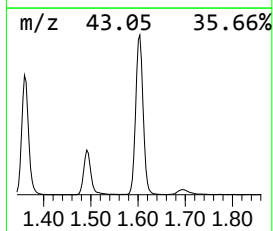
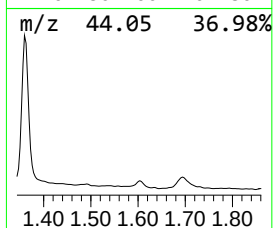
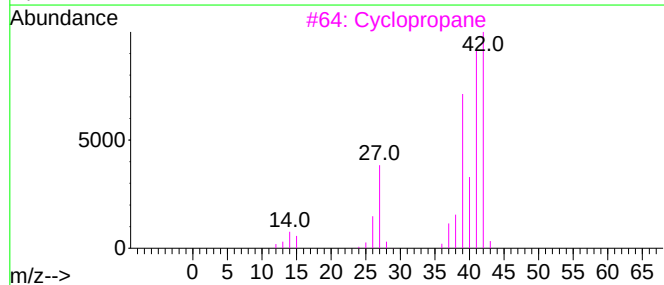
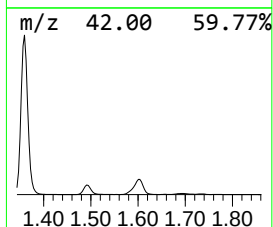
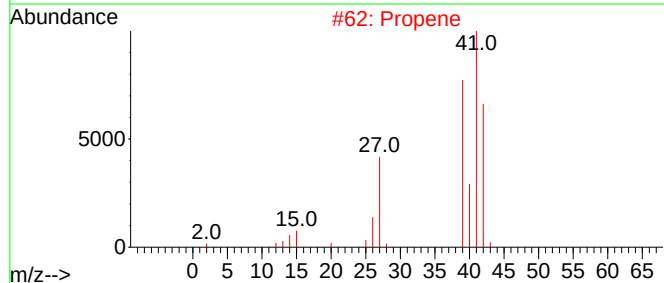
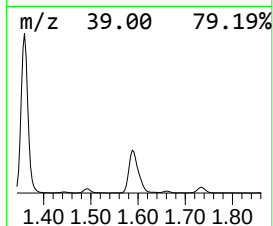
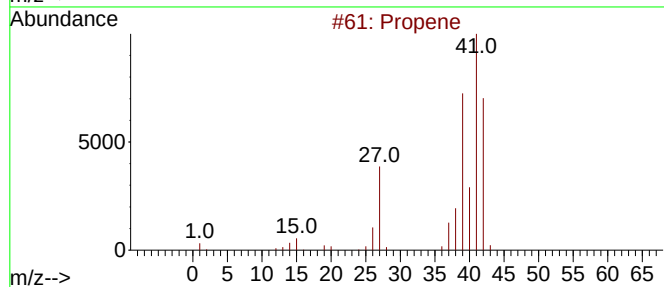
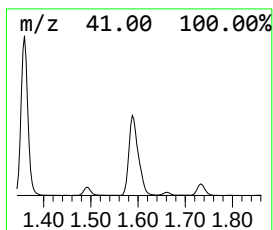
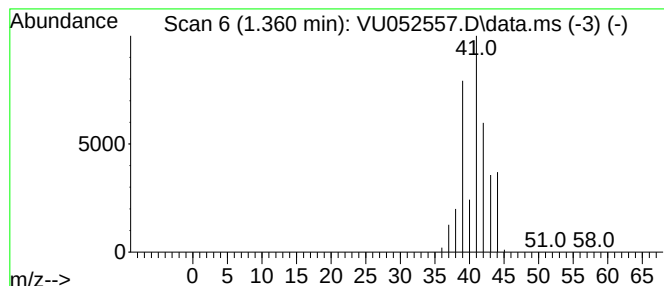
Instrument :
MSVOA_U
ClientSampleId :
GBQA1

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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.360	11.58 ug/L	905215	1,4-Difluorobenzene	6.244	
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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Sample : N6169-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA1

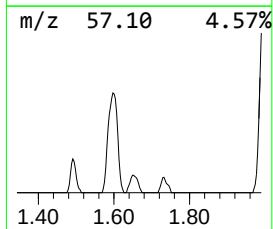
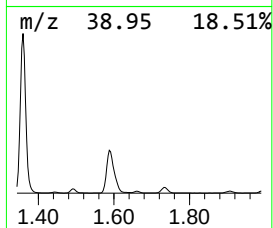
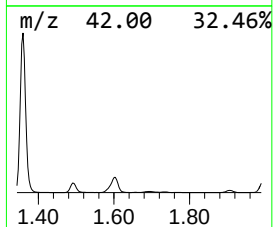
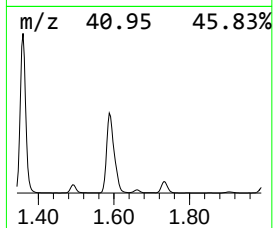
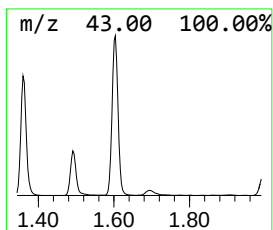
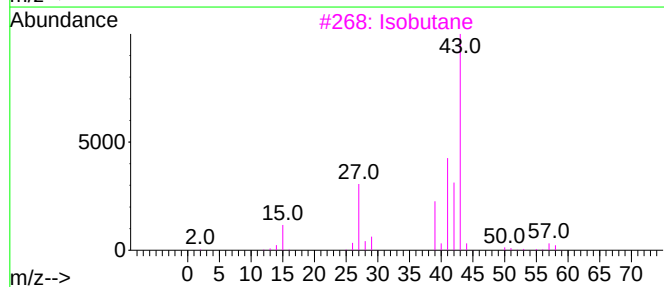
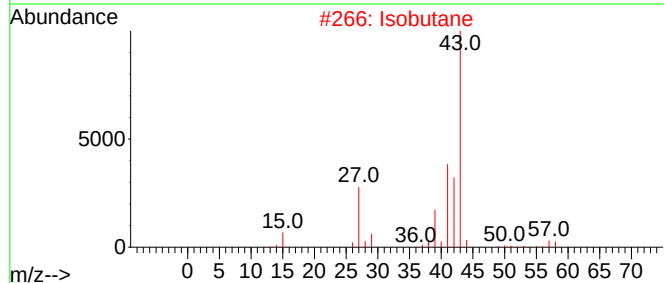
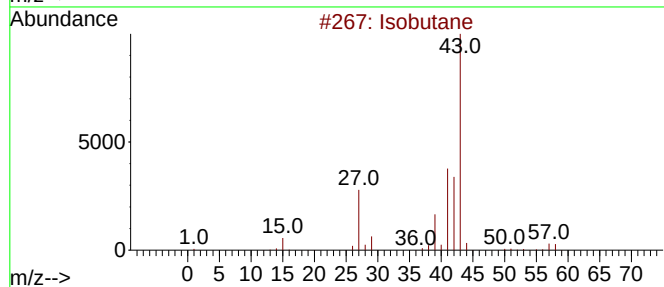
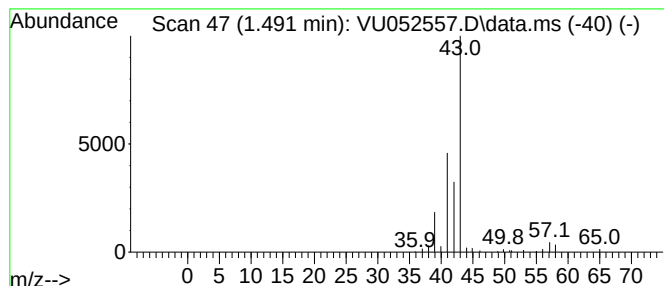
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	1.00 ug/L	78353	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	72
2			Isobutane	58	C4H10	000075-28-5	64
3			Isobutane	58	C4H10	000075-28-5	50
4			Isobutane	58	C4H10	000075-28-5	7
5			Isobutane	58	C4H10	000075-28-5	5



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Sample : N6169-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA1

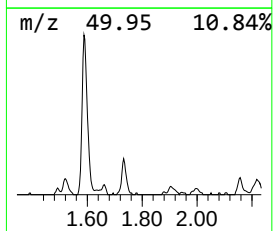
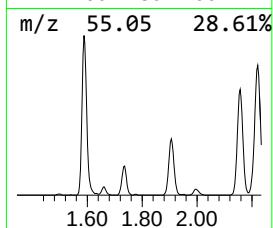
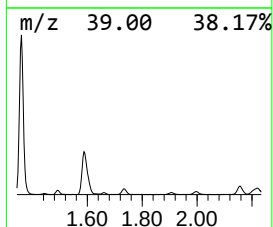
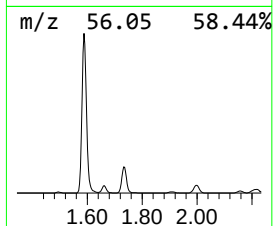
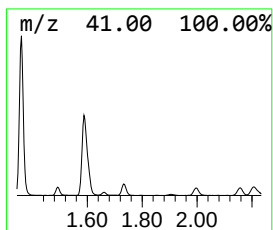
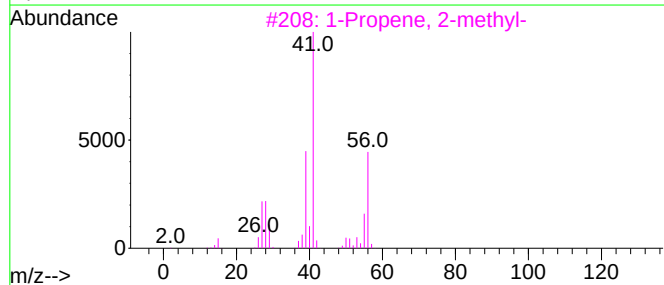
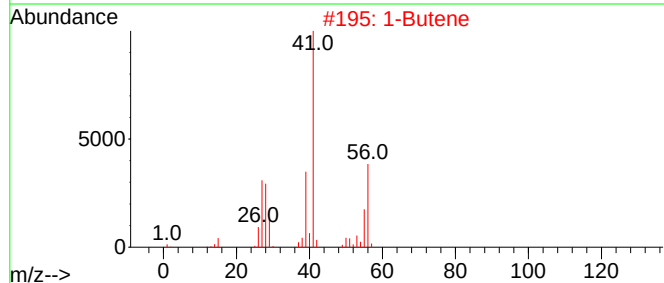
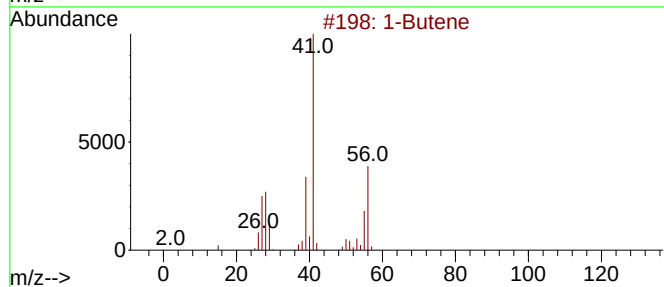
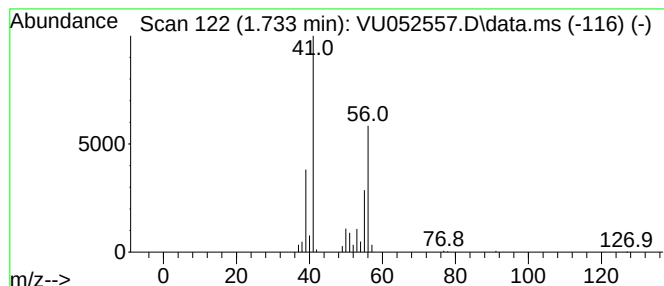
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.733	0.82 ug/L	64275	1,4-Difluorobenzene	6.244

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	87
3	1-Propene, 2-methyl-		56	C4H8	000115-11-7	87
4	1-Butene		56	C4H8	000106-98-9	86
5	2-Butene, (Z)-		56	C4H8	000590-18-1	86



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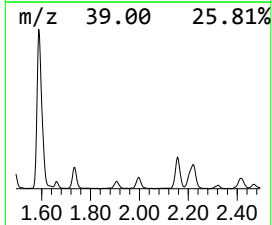
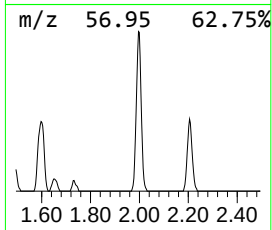
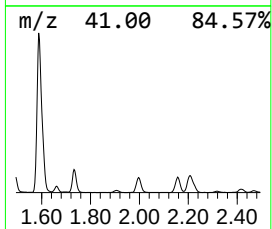
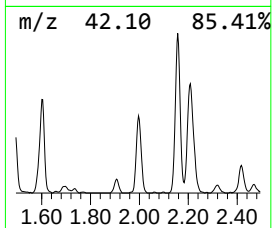
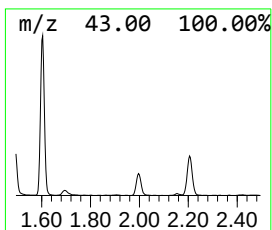
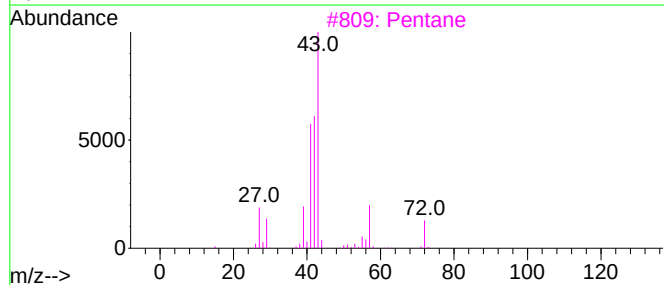
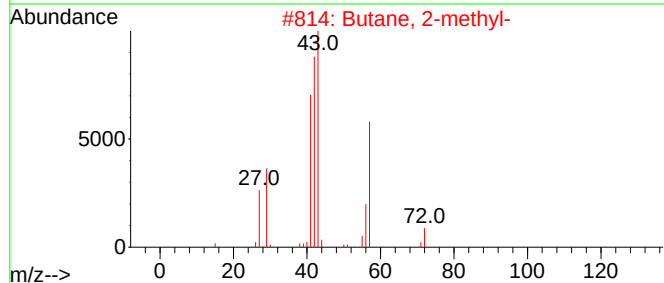
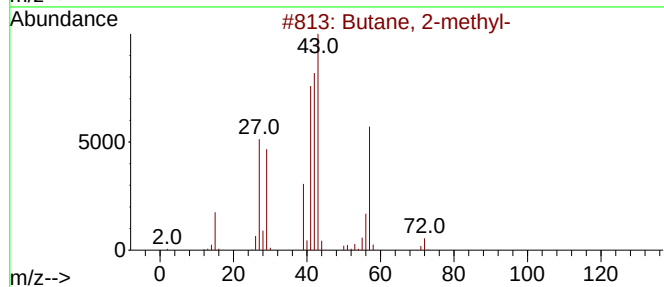
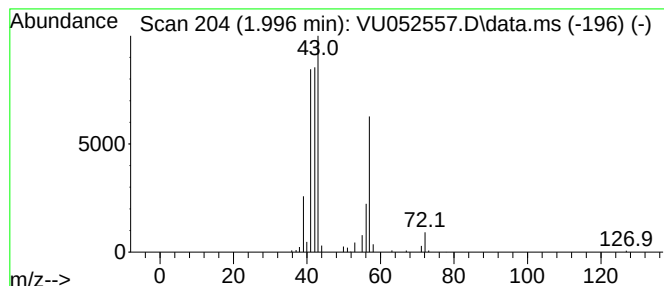
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Quant Title : TRACE VOA SFAM1.0

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.
1.996	1.16 ug/L	90346	1,4-Difluorobenzene	6.244

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	87
3	Pentane			72	C5H12	000109-66-0	43
4	Butane, 2,3-dimethyl-			86	C6H14	000079-29-8	36
5	3-Buten-1-ol			72	C4H8O	000627-27-0	28



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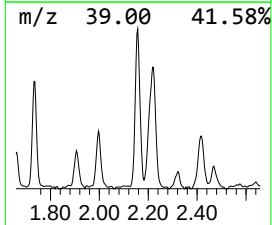
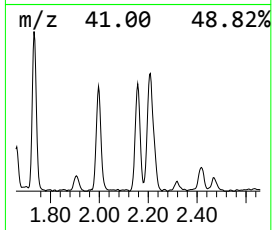
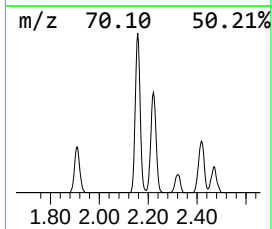
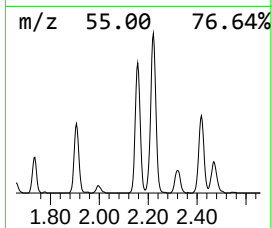
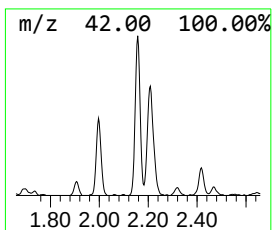
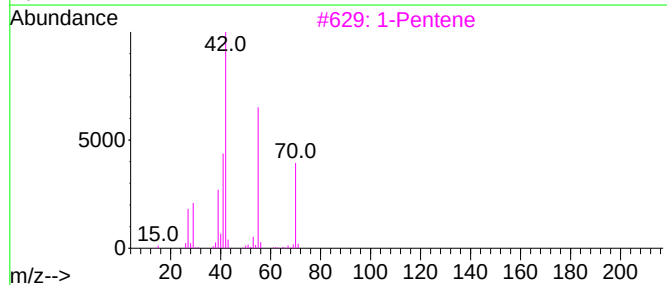
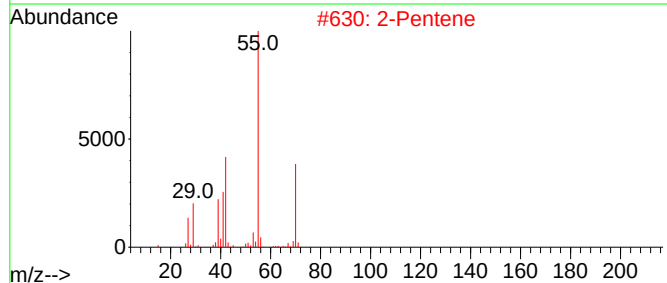
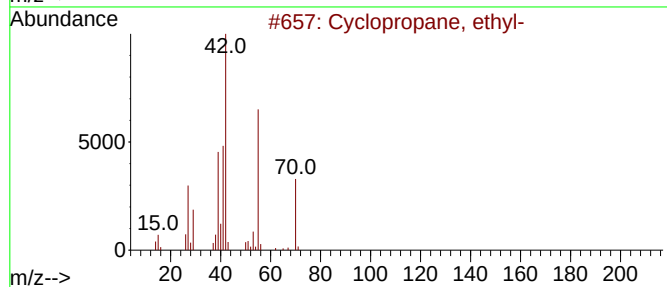
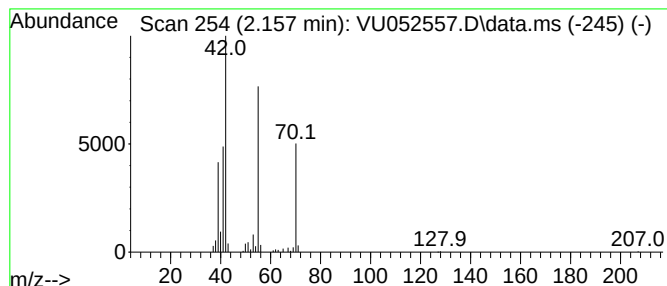
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic2.157 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	1.81 ug/L	141219	1,4-Difluorobenzene	6.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	90
2			2-Pentene	70	C5H10	000109-68-2	80
3			1-Pentene	70	C5H10	000109-67-1	68
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	64
5			2(3H)-Furanone, dihydro-3,5-dime...	114	C6H10O2	005145-01-7	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052557.D
Acq On : 27 Dec 2022 12:21
Operator : JC/MD
Sample : N6169-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA1

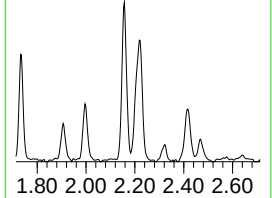
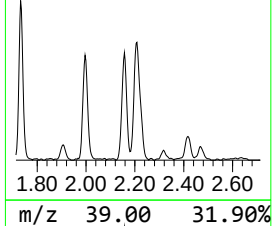
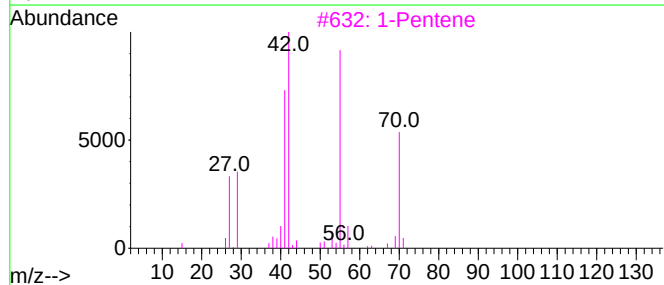
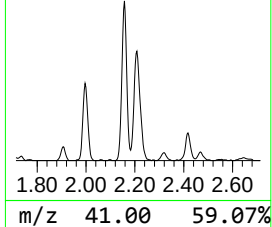
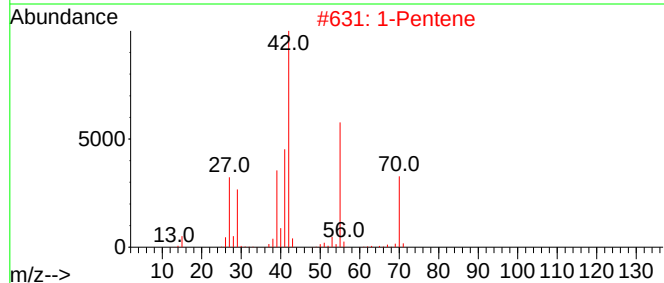
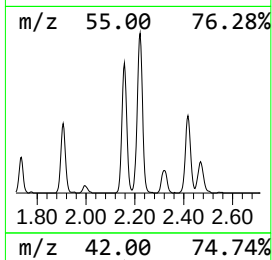
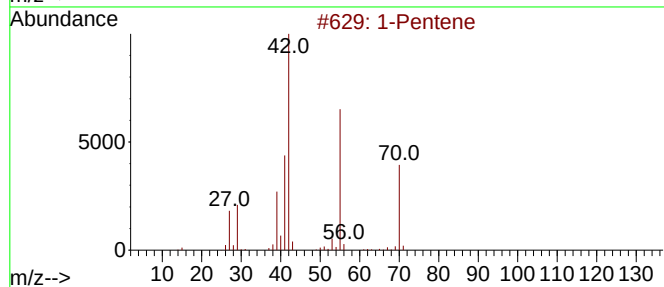
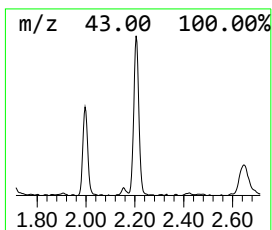
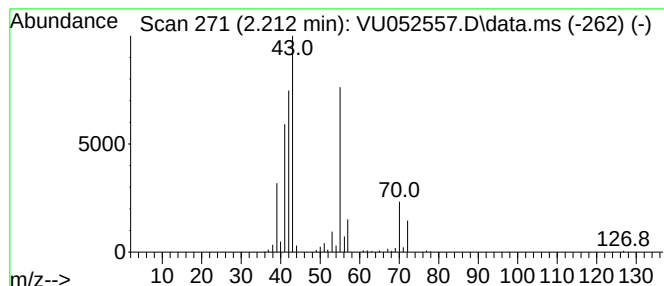
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.212	2.63 ug/L	205315	1,4-Difluorobenzene	6.244

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene	70	C5H10	000109-67-1	59
2		1-Pentene	70	C5H10	000109-67-1	58
3		1-Pentene	70	C5H10	000109-67-1	58
4		Pentane	72	C5H12	000109-66-0	53
5		Cyclopropane, ethyl-	70	C5H10	001191-96-4	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052557.D
Acq On : 27 Dec 2022 12:21
Operator : JC/MD
Sample : N6169-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQA1

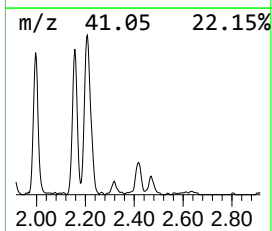
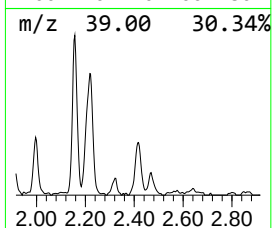
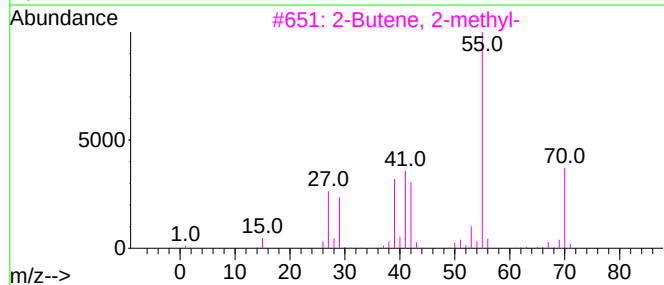
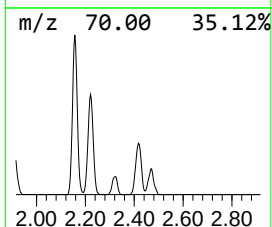
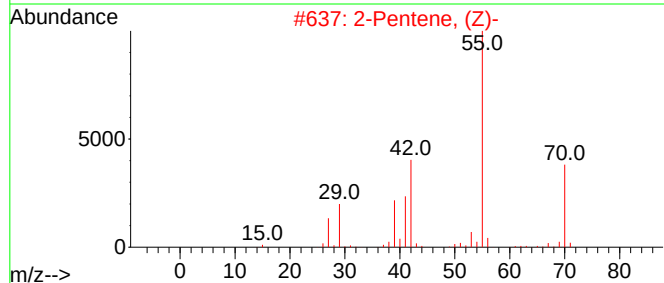
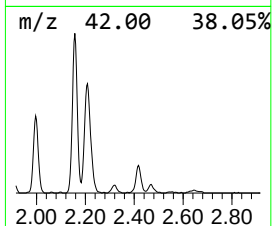
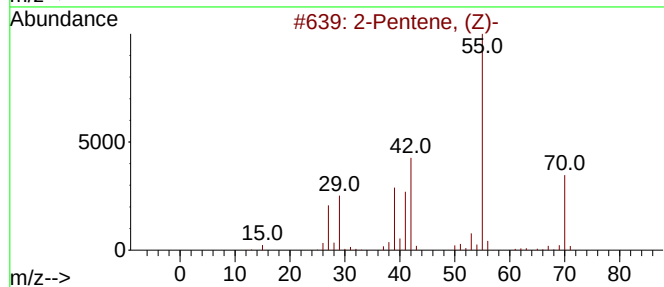
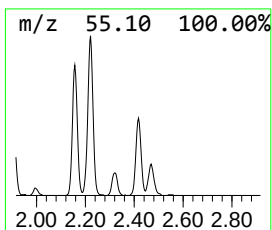
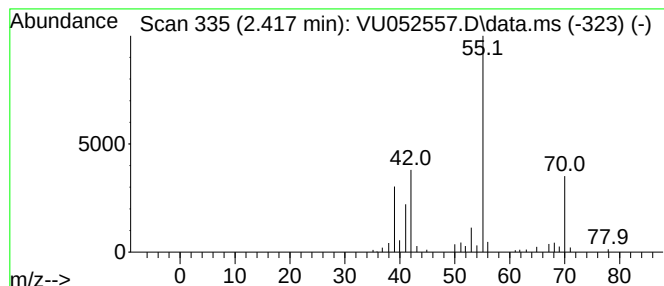
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.417	0.75 ug/L	58762	1,4-Difluorobenzene	6.244

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentene, (Z)-	70	C5H10	000627-20-3	90
2		2-Pentene, (Z)-	70	C5H10	000627-20-3	90
3		2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
4		2-Pentene, (E)-	70	C5H10	000646-04-8	86
5		2-Pentene	70	C5H10	000109-68-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052557.D
Acq On : 27 Dec 2022 12:21
Operator : JC/MD
Sample : N6169-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

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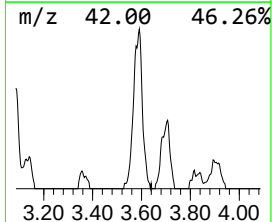
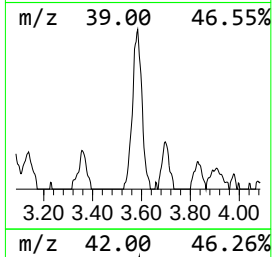
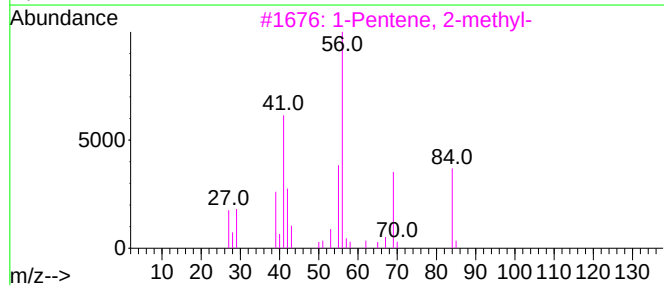
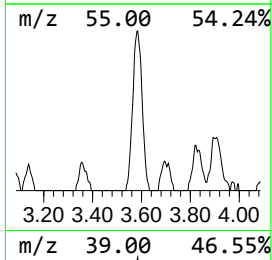
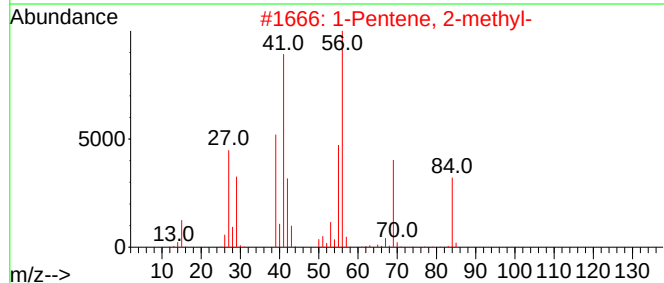
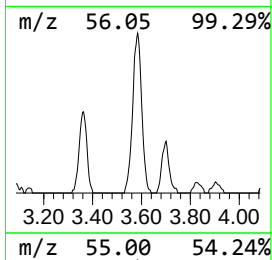
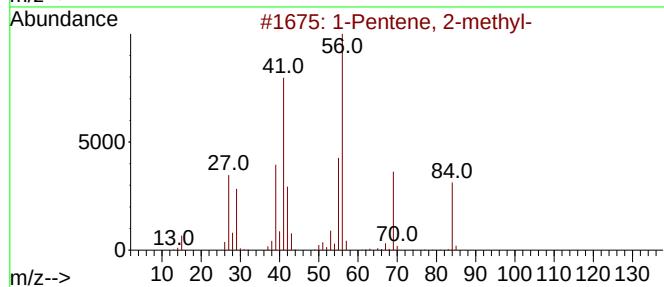
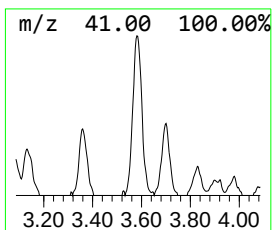
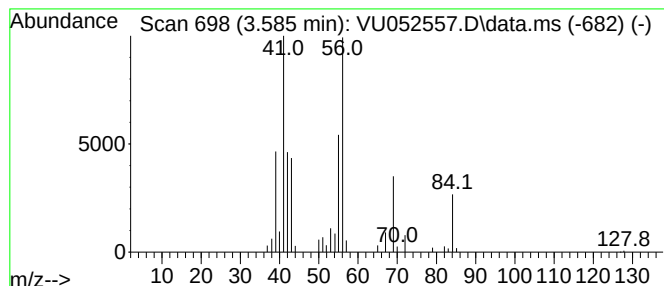
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.585	1.10 ug/L	85723	1,4-Difluorobenzene	6.244

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	87
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	87
3		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	81
4		1-Hexene	84	C6H12	000592-41-6	58
5		1-Hexene	84	C6H12	000592-41-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
 Data File : VU052557.D
 Acq On : 27 Dec 2022 12:21
 Operator : JC/MD
 Sample : N6169-10
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBQA1

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	1.0	ug/L	78353	1	6.244	390915	5.0
(DEL) Alkane: S...	1.733	0.8	ug/L	64275	1	6.244	390915	5.0
(DEL) Alkane: S...	1.996	1.2	ug/L	90346	1	6.244	390915	5.0
(DEL) Alkane: C...	2.157	1.8	ug/L	141219	1	6.244	390915	5.0
(DEL) Alkane: S...	2.212	2.6	ug/L	205315	1	6.244	390915	5.0
(DEL) Alkane: S...	2.417	0.8	ug/L	58762	1	6.244	390915	5.0
(DEL) Alkane: S...	3.585	1.1	ug/L	85723	1	6.244	390915	5.0