

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122823\
 Data File : VU057353.D
 Acq On : 29 Dec 2023 00:01
 Operator : MD/SY
 Sample : 06020-16
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH7Y2

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\SFAMUTR122723WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	84	95	105	rBV2	146429	211553	23.08%	2.539%
2	1.702	117	128	144	rBV	157301	324896	35.45%	3.899%
3	1.911	185	193	207	rVB	110001	149601	16.32%	1.796%
4	2.560	381	395	411	rBV	207933	342051	37.32%	4.105%
5	2.695	421	437	438	rBV	13549	27086	2.96%	0.325%
6	3.181	578	588	606	rVB3	7957	17810	1.94%	0.214%
7	4.438	962	979	1001	rBV5	22801	73948	8.07%	0.888%
8	4.672	1029	1052	1093	rBV2	58470	316521	34.53%	3.799%
9	5.058	1150	1172	1209	rBV	191172	517720	56.49%	6.214%
10	5.721	1356	1378	1407	rBV2	346545	916541	100.00%	11.000%
11	6.245	1521	1541	1564	rVB	299936	587332	64.08%	7.049%
12	6.685	1661	1678	1699	rBV	220686	445638	48.62%	5.349%
13	6.788	1701	1710	1716	rBV3	8144	13907	1.52%	0.167%
14	6.881	1730	1739	1756	rBV4	10808	22132	2.41%	0.266%
15	7.123	1803	1814	1826	rBV6	4352	9519	1.04%	0.114%
16	7.563	1935	1951	1974	rBV	94661	175214	19.12%	2.103%
17	7.894	2040	2054	2068	rBV	364200	646832	70.57%	7.763%
18	7.968	2068	2077	2098	rVB	60056	113395	12.37%	1.361%
19	8.177	2130	2142	2160	rBV2	58015	104597	11.41%	1.255%
20	8.473	2221	2234	2250	rBV4	5883	14337	1.56%	0.172%
21	8.573	2250	2265	2269	rBV	6840	15758	1.72%	0.189%
22	8.637	2273	2285	2322	rVV3	327299	868296	94.74%	10.421%
23	8.785	2323	2331	2348	rVB3	42409	83383	9.10%	1.001%
24	9.415	2514	2527	2552	rBV	423098	730945	79.75%	8.773%
25	9.566	2568	2574	2590	rVB3	8384	14778	1.61%	0.177%
26	9.692	2604	2613	2630	rVB	26236	49097	5.36%	0.589%
27	10.097	2732	2739	2748	rBV3	8458	14343	1.56%	0.172%
28	10.235	2772	2782	2802	rVB	49695	87016	9.49%	1.044%
29	10.753	2927	2943	2957	rBV	155837	259156	28.28%	3.110%
30	10.891	2978	2986	2997	rVB2	14284	24296	2.65%	0.292%
31	11.807	3259	3271	3290	rBV	357230	586788	64.02%	7.043%
32	12.190	3378	3390	3405	rBV2	332042	547886	59.78%	6.576%
33	17.469	5026	5032	5043	rBV2	10161	19474	2.12%	0.234%

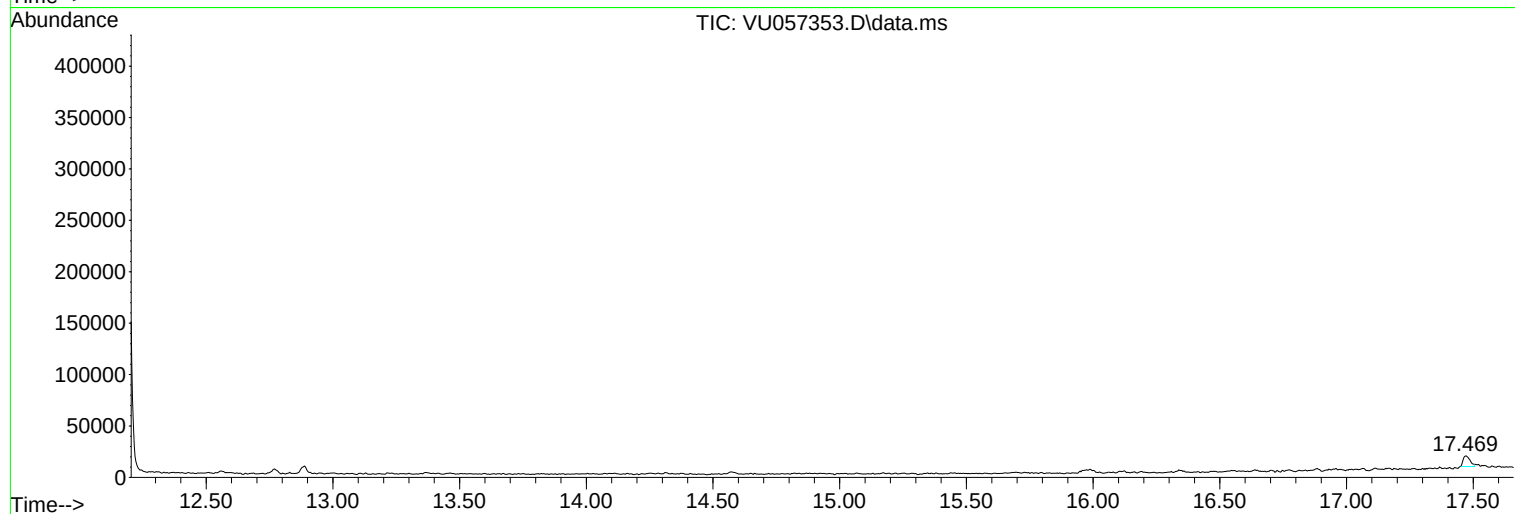
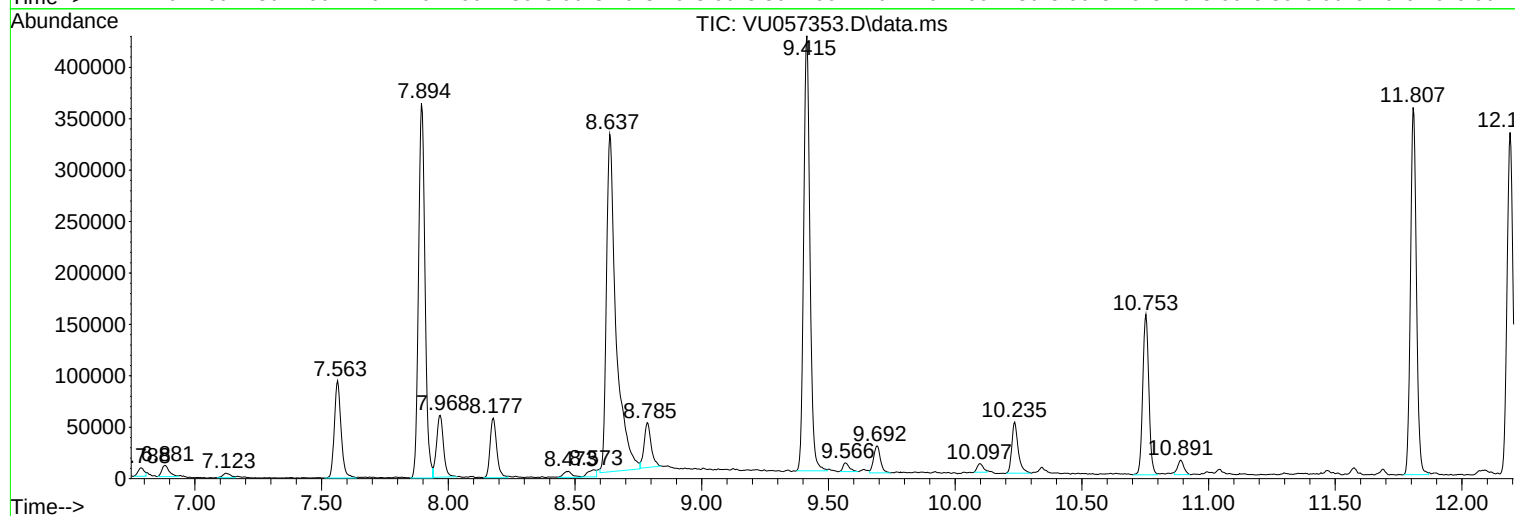
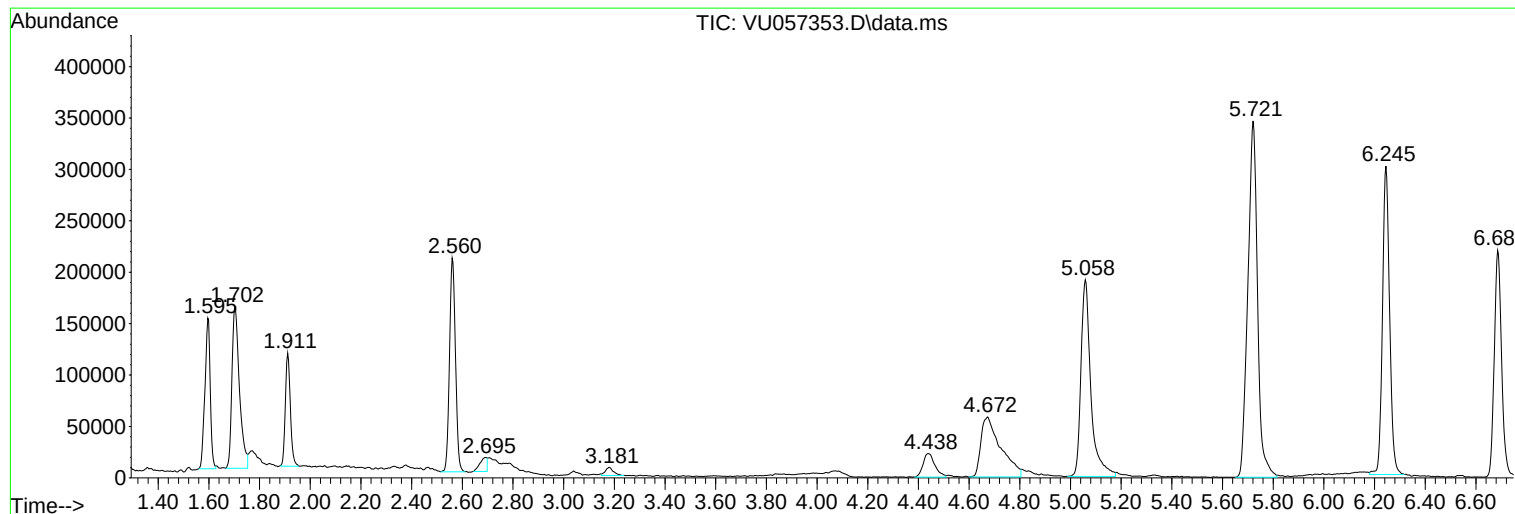
Sum of corrected areas: 8331846

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122823\
Data File : VU057353.D
Acq On : 29 Dec 2023 00:01
Operator : MD/SY
Sample : 06020-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH7Y2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.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\VU122823\
Data File : VU057353.D
Acq On : 29 Dec 2023 00:01
Operator : MD/SY
Sample : 06020-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH7Y2

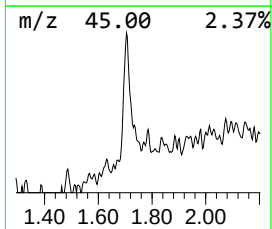
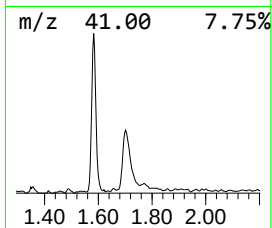
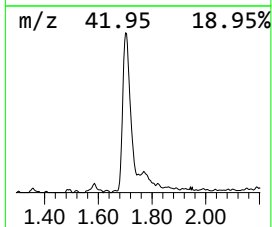
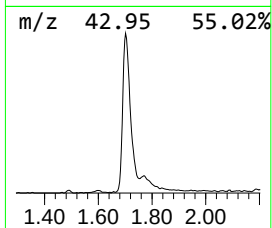
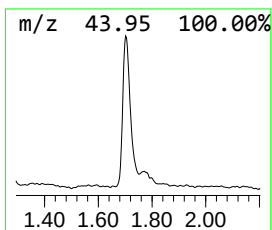
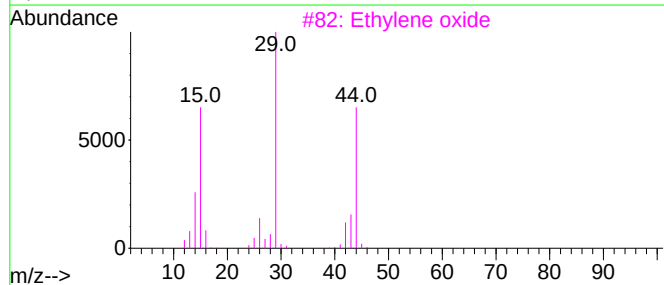
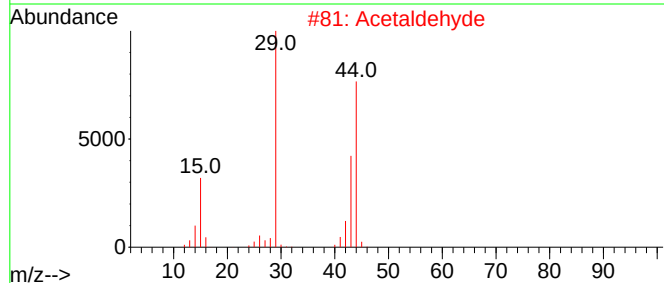
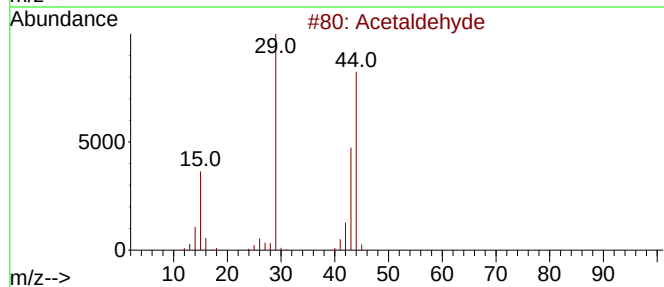
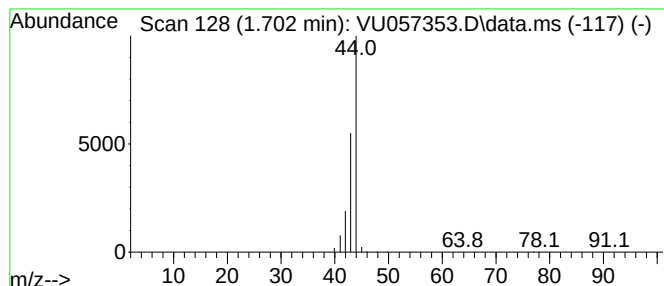
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.702	2.77 ug/L	324896	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122823\
Data File : VU057353.D
Acq On : 29 Dec 2023 00:01
Operator : MD/SY
Sample : 06020-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH7Y2

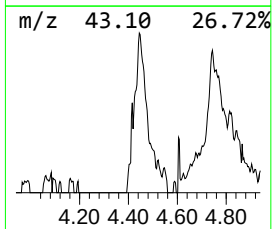
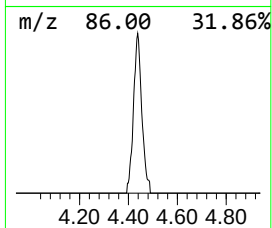
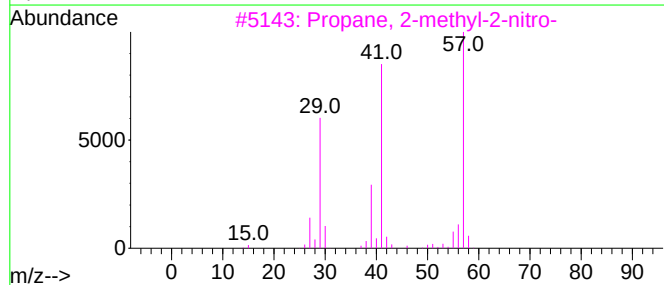
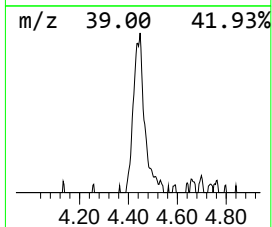
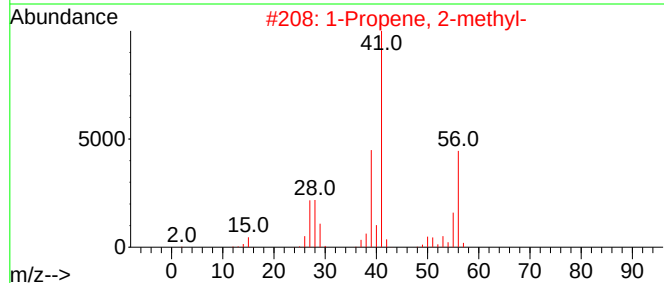
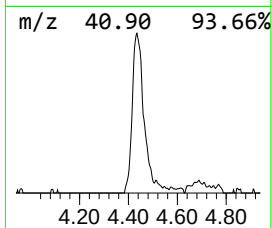
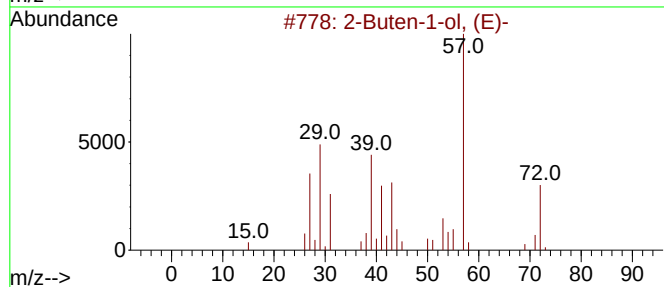
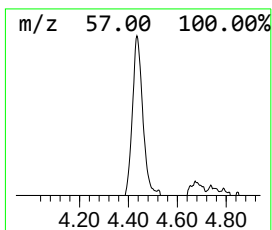
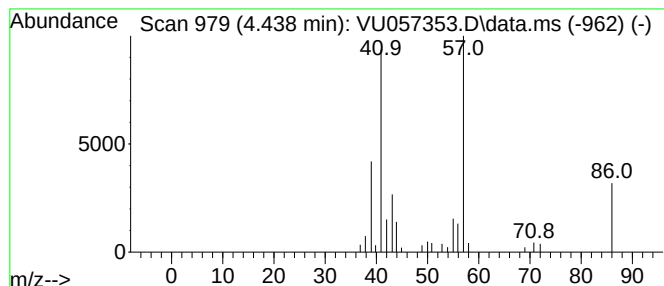
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.438	0.63 ug/L	73948	1,4-Difluorobenzene	6.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	47
2		1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
3		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40
4		1-Propene, 2-methyl-	56	C4H8	000115-11-7	37
5		Butanal, 2-methyl-	86	C5H10O	000096-17-3	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122823\
Data File : VU057353.D
Acq On : 29 Dec 2023 00:01
Operator : MD/SY
Sample : 06020-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH7Y2

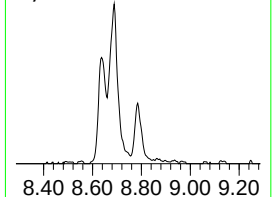
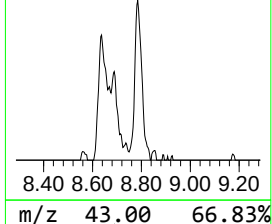
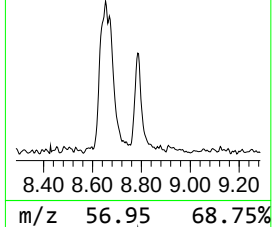
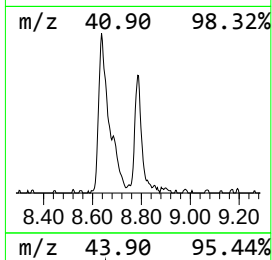
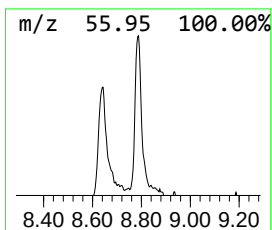
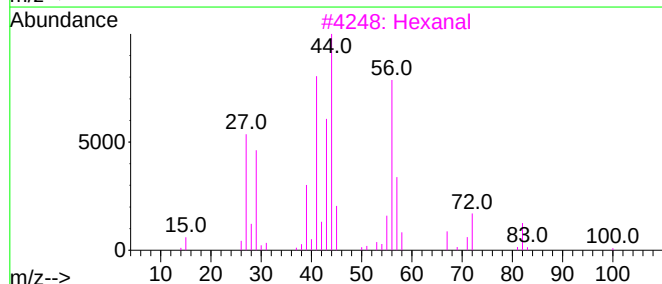
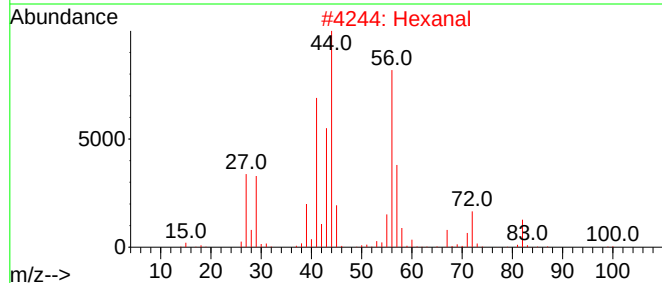
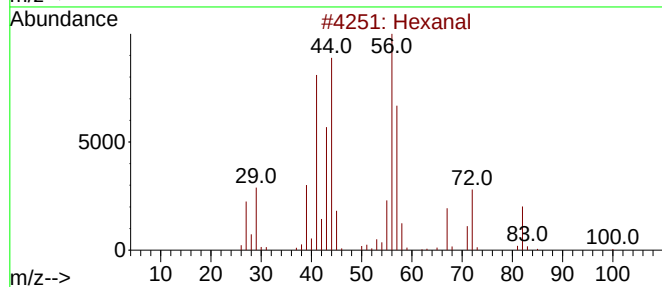
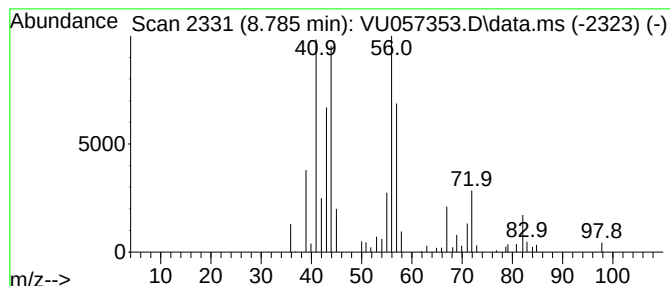
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	0.57 ug/L	83383	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	83
2	Hexanal			100	C6H12O	000066-25-1	78
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122823\
Data File : VU057353.D
Acq On : 29 Dec 2023 00:01
Operator : MD/SY
Sample : 06020-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH7Y2

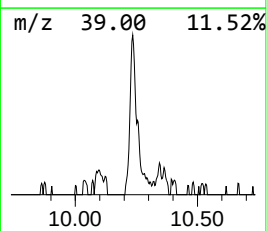
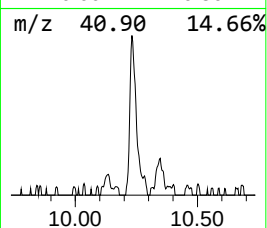
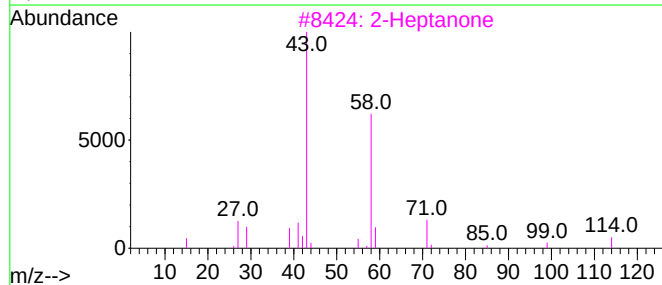
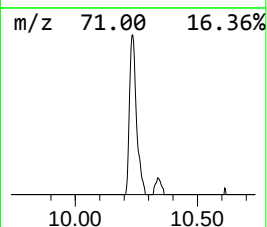
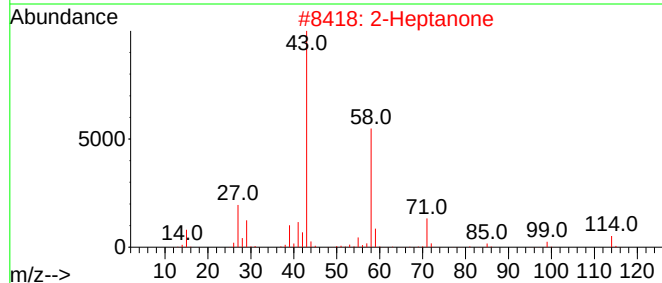
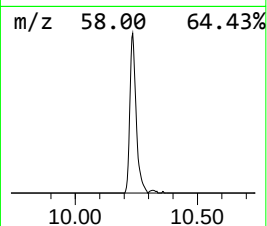
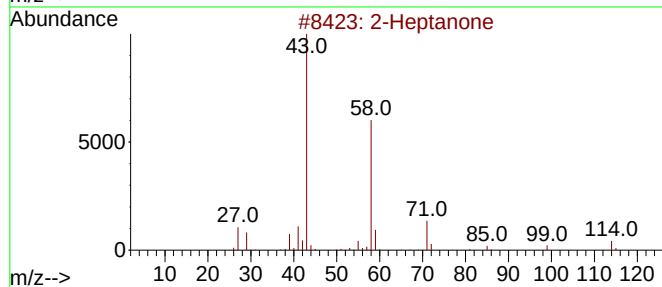
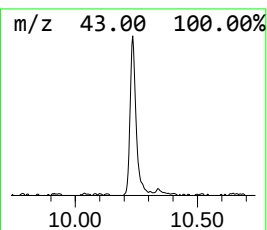
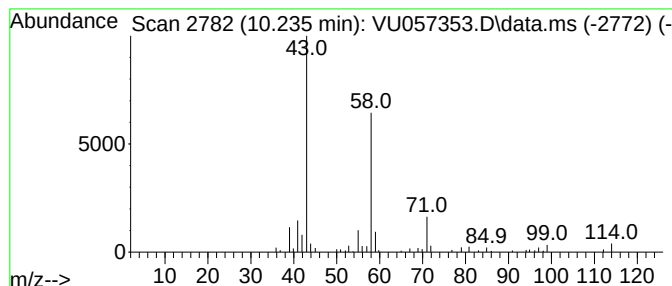
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.235	0.60 ug/L	87016	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	90
2	2-Heptanone			114	C7H14O	000110-43-0	86
3	2-Heptanone			114	C7H14O	000110-43-0	86
4	2-Heptanone			114	C7H14O	000110-43-0	72
5	2-Heptanone			114	C7H14O	000110-43-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122823\
Data File : VU057353.D
Acq On : 29 Dec 2023 00:01
Operator : MD/SY
Sample : 06020-16
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH7Y2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.702	2.8	ug/L	324896	1	6.245	587332	5.0
unknown-02	4.438	0.6	ug/L	73948	1	6.245	587332	5.0
Hexanal	8.785	0.6	ug/L	83383	2	9.415	730945	5.0
2-Heptanone	10.235	0.6	ug/L	87016	2	9.415	730945	5.0