

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
 Data File : VU046864.D
 Acq On : 27 Jan 2022 12:27
 Operator : SY/MD
 Sample : N1260-07DL 5X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX8DL

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\SFAMUTR011822WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU046864.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	26	rVB	311176	332980	54.15%	5.850%
2	1.494	39	48	61	rVB3	18483	22022	3.58%	0.387%
3	1.600	71	81	97	rBV3	131106	225770	36.72%	3.967%
4	1.739	118	124	137	rVB	16471	20232	3.29%	0.355%
5	1.922	171	181	196	rBV	43134	67405	10.96%	1.184%
6	2.002	199	206	215	rVB3	13023	18478	3.00%	0.325%
7	2.163	247	256	263	rVV3	21885	29310	4.77%	0.515%
8	2.211	263	271	288	rVB3	17256	32430	5.27%	0.570%
9	2.420	327	336	345	rVB2	6539	10504	1.71%	0.185%
10	2.575	368	384	401	rBV2	115421	220612	35.88%	3.876%
11	3.192	563	576	589	rVB	5555	12158	1.98%	0.214%
12	3.366	618	630	645	rBV4	5079	11595	1.89%	0.204%
13	3.597	688	702	713	rBV8	3789	8525	1.39%	0.150%
14	3.877	775	789	805	rVB2	19218	44177	7.18%	0.776%
15	4.668	1012	1035	1091	rBV4	103177	369308	60.06%	6.489%
16	5.070	1144	1160	1186	rVB	86187	196237	31.91%	3.448%
17	5.321	1227	1238	1254	rBV5	5263	11702	1.90%	0.206%
18	5.729	1344	1365	1394	rBV2	165467	446139	72.55%	7.839%
19	6.253	1512	1528	1548	rBV	144968	279076	45.38%	4.903%
20	6.546	1606	1619	1633	rBV	210113	389494	63.34%	6.843%
21	6.694	1652	1665	1681	rBV	105716	205269	33.38%	3.607%
22	6.890	1714	1726	1736	rBV3	4001	7293	1.19%	0.128%
23	7.568	1925	1937	1956	rVB	48095	85245	13.86%	1.498%
24	7.902	2028	2041	2056	rBV	189015	334925	54.47%	5.885%
25	7.973	2056	2063	2076	rVB	6945	12338	2.01%	0.217%
26	8.182	2117	2128	2142	rBV	33812	54270	8.83%	0.954%
27	8.478	2209	2220	2233	rBV3	3800	8647	1.41%	0.152%
28	8.555	2233	2244	2259	rVB2	73875	129575	21.07%	2.277%
29	8.648	2259	2273	2299	rBV	300136	614911	100.00%	10.804%
30	8.793	2306	2318	2333	rBV2	43297	82400	13.40%	1.448%
31	9.420	2500	2513	2535	rBV	229694	383289	62.33%	6.734%
32	10.349	2793	2802	2816	rBV3	12680	20089	3.27%	0.353%
33	10.761	2918	2930	2945	rBV	105662	171576	27.90%	3.015%
34	10.896	2963	2972	2983	rBV2	5274	9468	1.54%	0.166%
35	11.690	3210	3219	3231	rVB3	18014	26099	4.24%	0.459%
36	11.816	3246	3258	3278	rVB	251381	398915	64.87%	7.009%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX8DL

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\SFAMUTR011822WMA.M
Title : TRACE VOA SFAM1.0

37	12.195	3364	3376	3393	rVB	203348	327415	53.25%	5.753%
38	12.889	3582	3592	3601	rBV2	44284	63994	10.41%	1.124%
39	14.735	4159	4166	4173	rVB5	6267	7707	1.25%	0.135%

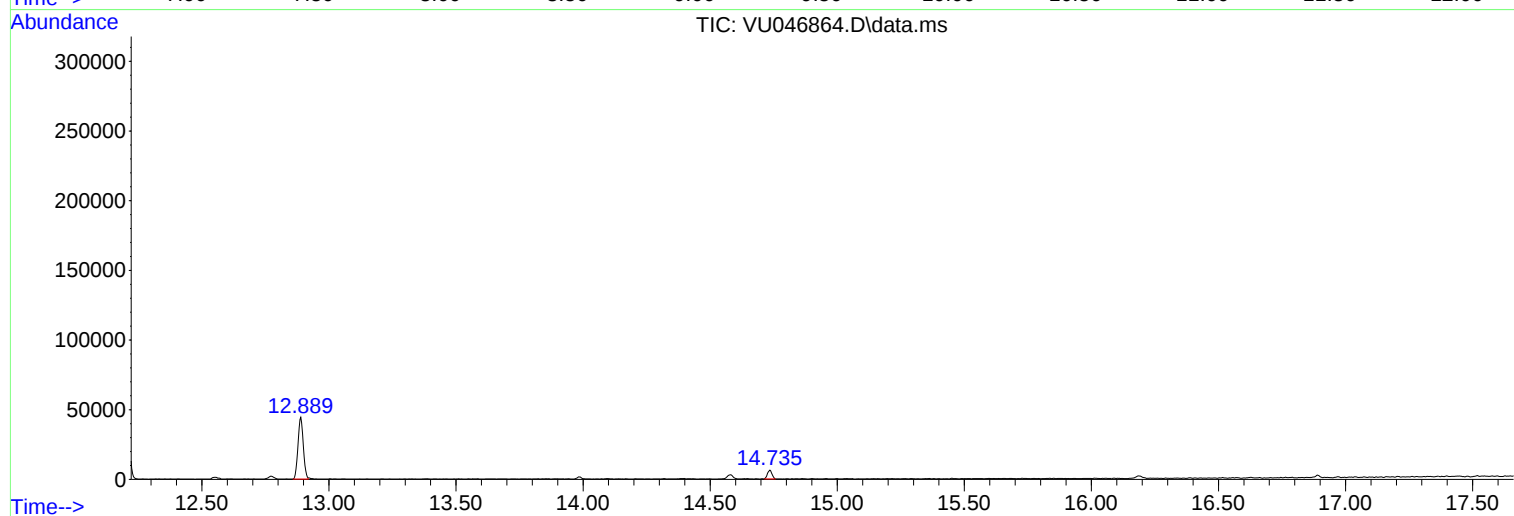
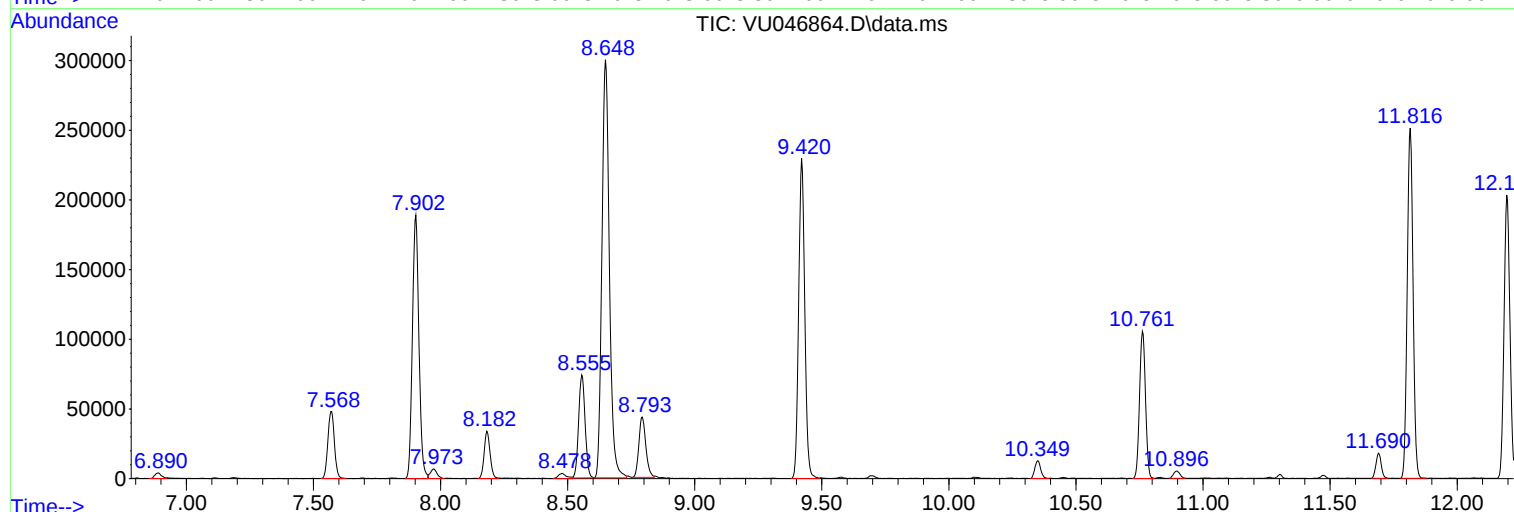
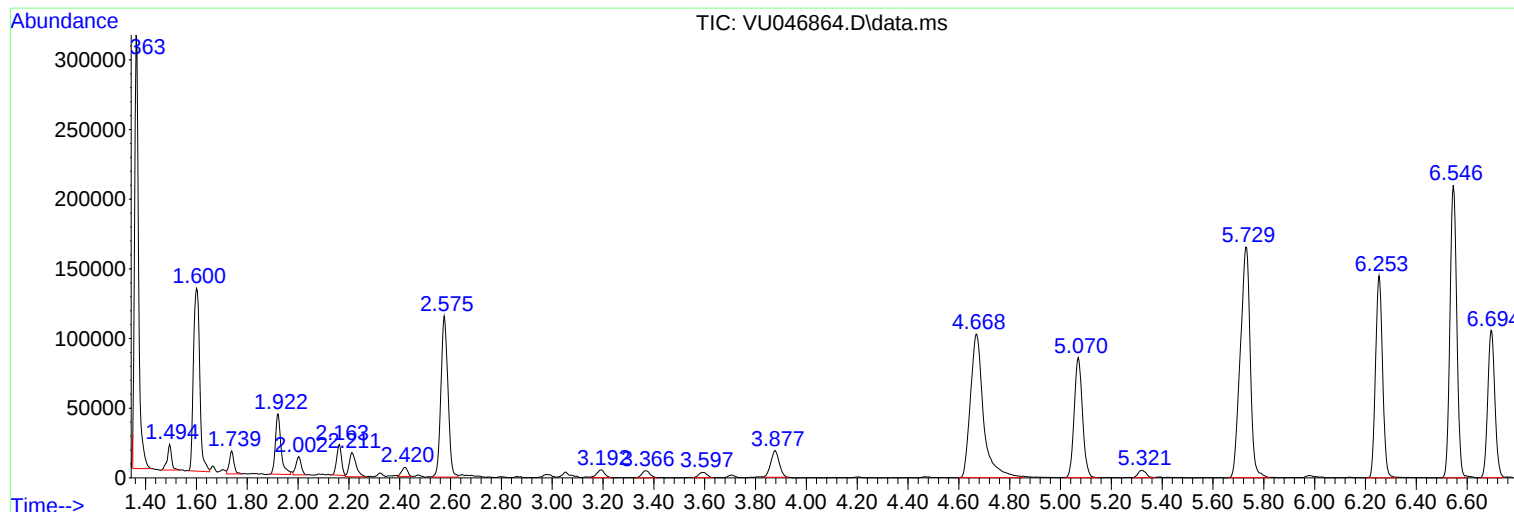
Sum of corrected areas: 5691579

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.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\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX8DL

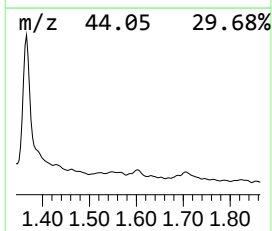
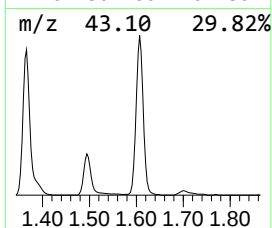
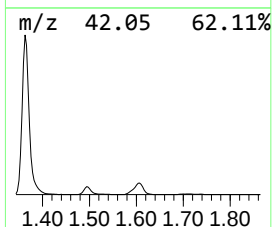
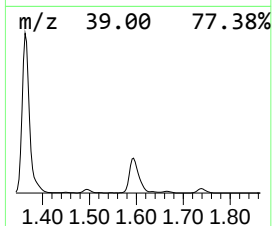
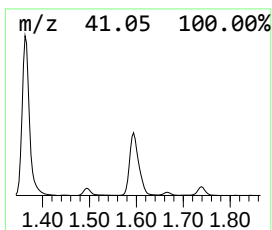
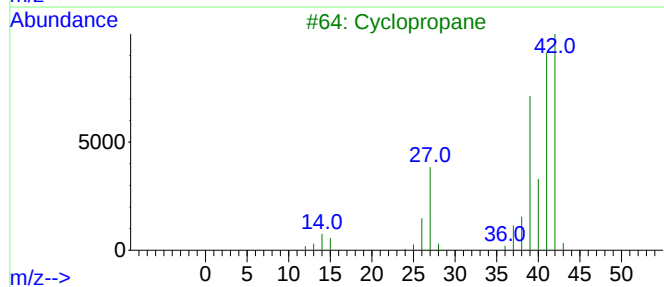
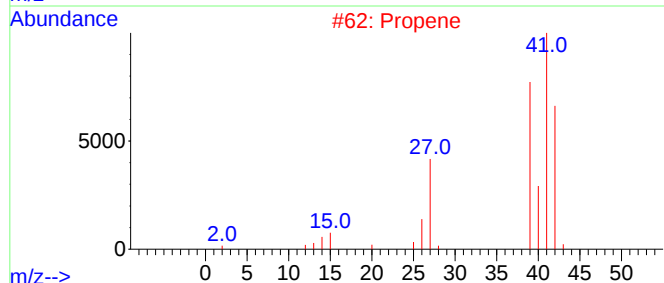
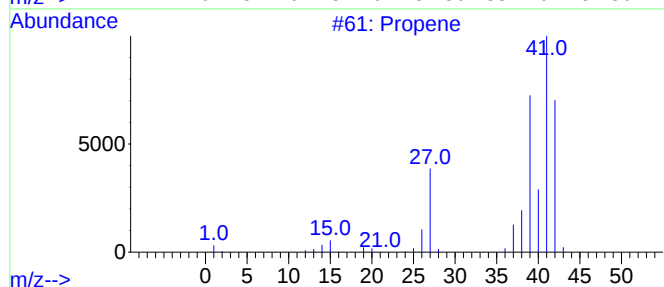
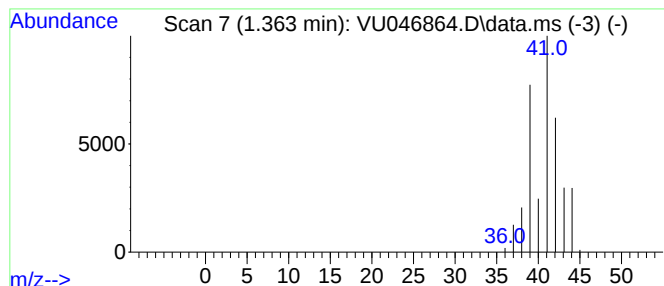
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.363	5.97 ug/L	332980	1,4-Difluorobenzene	6.253

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		Cyclopropane	42	C3H6	000075-19-4	9
5		Cyclopropene	40	C3H4	002781-85-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX8DL

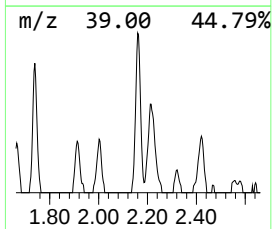
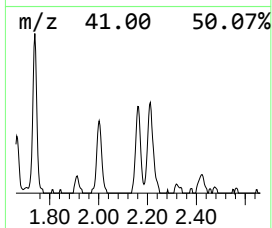
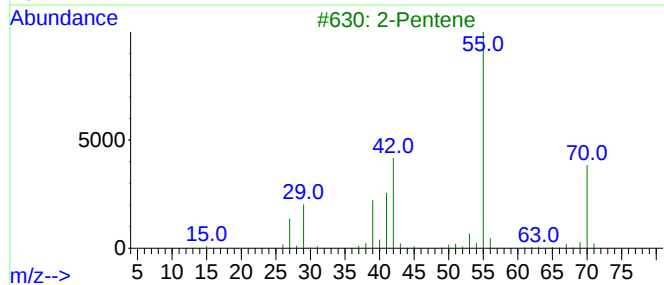
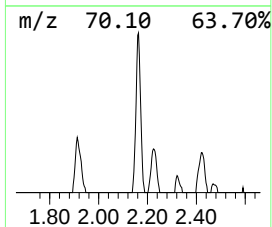
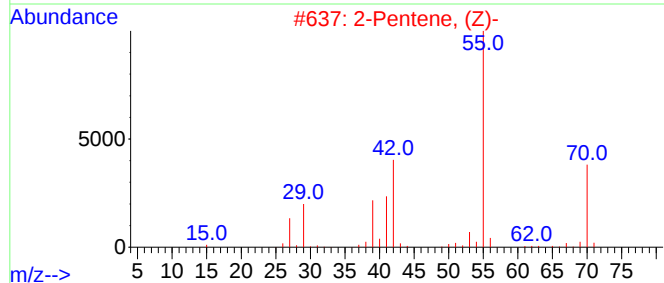
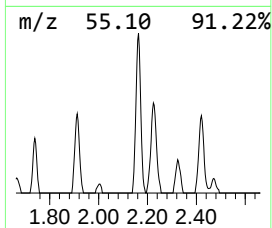
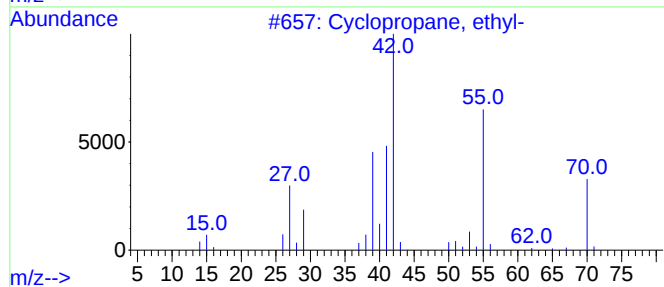
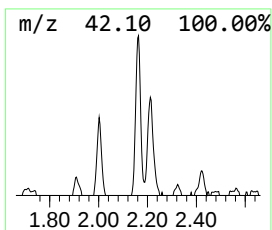
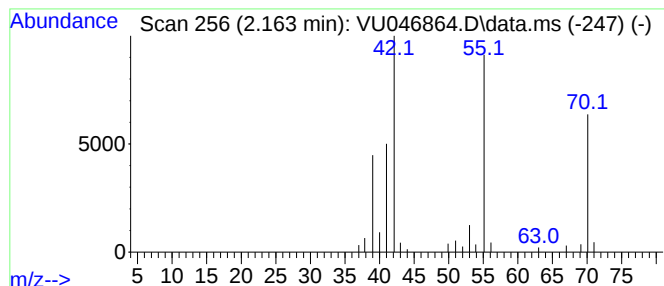
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Cyclic2.163 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.163	0.53 ug/L	29310	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropane, ethyl-	70	C5H10	001191-96-4	90
2			2-Pentene, (Z)-	70	C5H10	000627-20-3	83
3			2-Pentene	70	C5H10	000109-68-2	80
4			Cyclopropane, ethyl-	70	C5H10	001191-96-4	78
5			1-Pentene	70	C5H10	000109-67-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX8DL

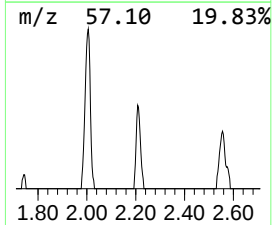
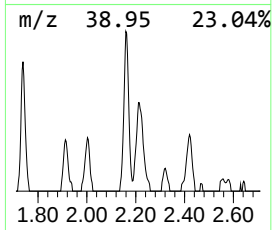
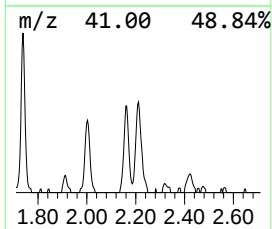
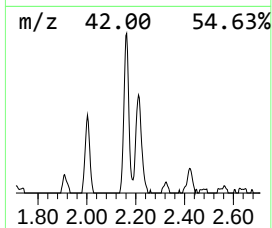
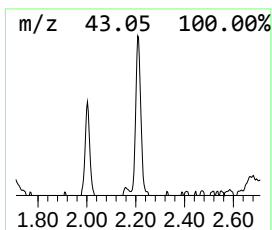
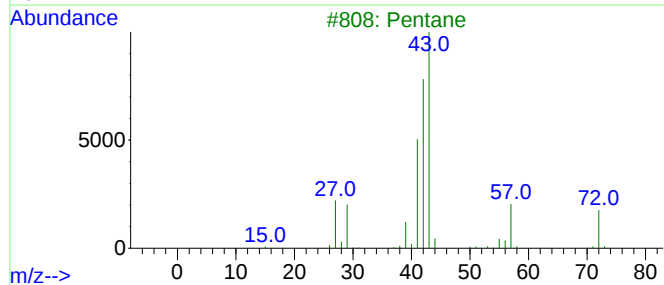
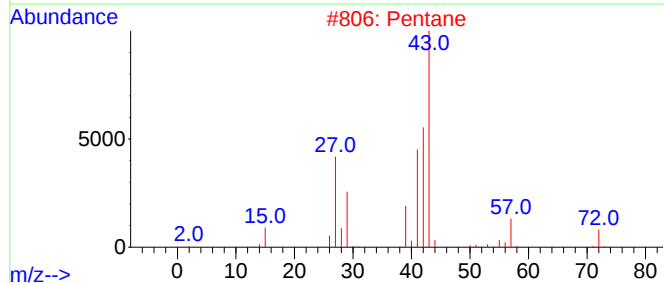
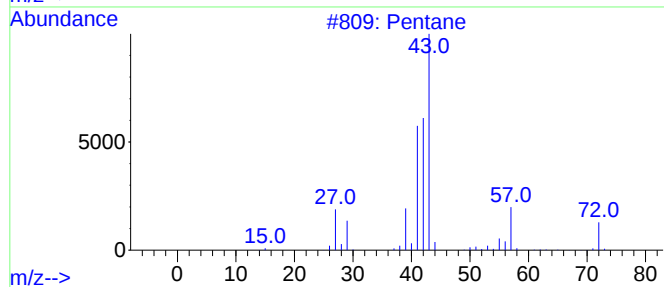
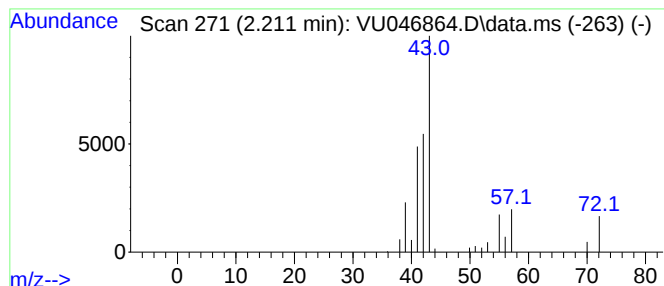
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	0.58 ug/L	32430	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	78
2	Pentane			72	C5H12	000109-66-0	78
3	Pentane			72	C5H12	000109-66-0	72
4	Butanal, 2,2-dimethyl-			100	C6H12O	002094-75-9	17
5	Methyl glyoxal			72	C3H4O2	000078-98-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX8DL

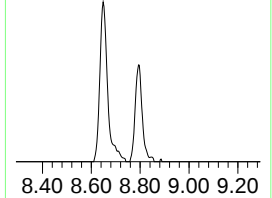
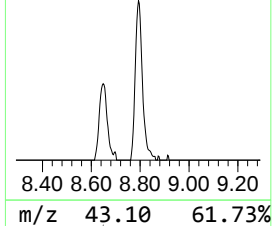
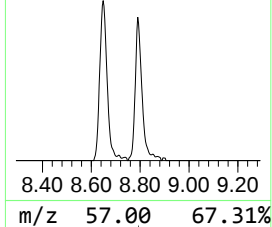
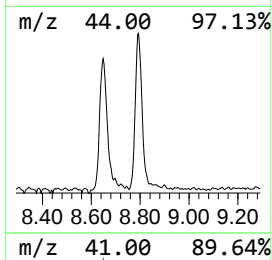
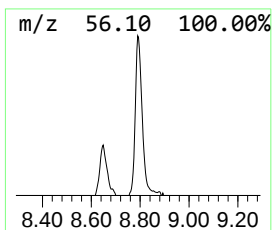
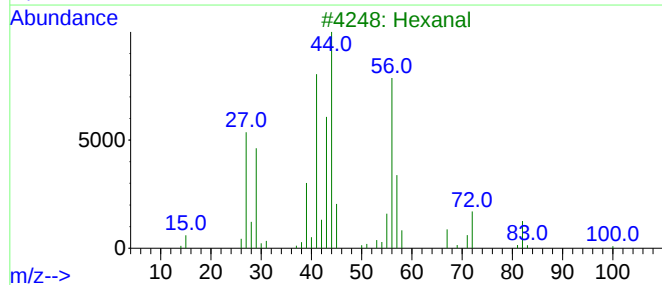
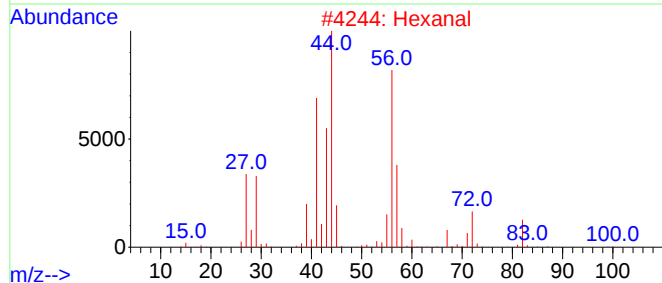
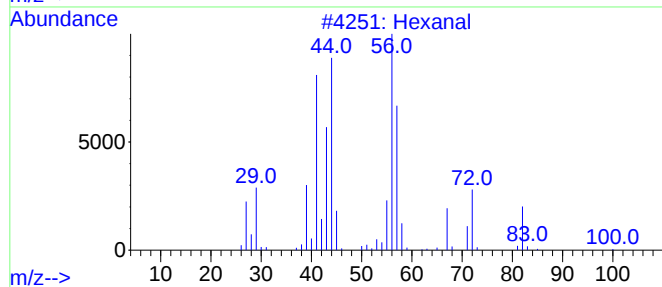
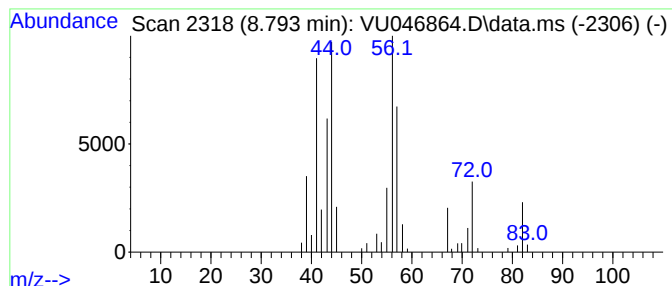
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.793	1.07 ug/L	82400	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	91
2	Hexanal			100	C6H12O	000066-25-1	78
3	Hexanal			100	C6H12O	000066-25-1	78
4	Hexanal			100	C6H12O	000066-25-1	78
5	Hexanal			100	C6H12O	000066-25-1	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX8DL

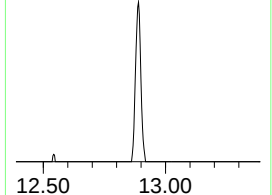
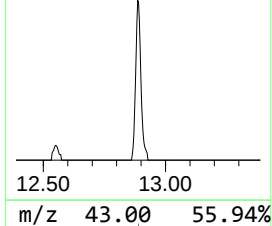
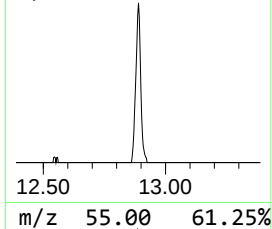
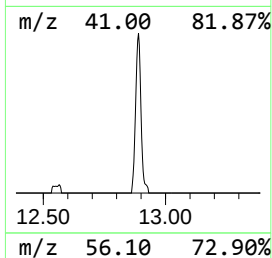
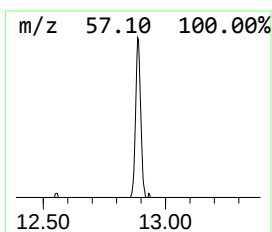
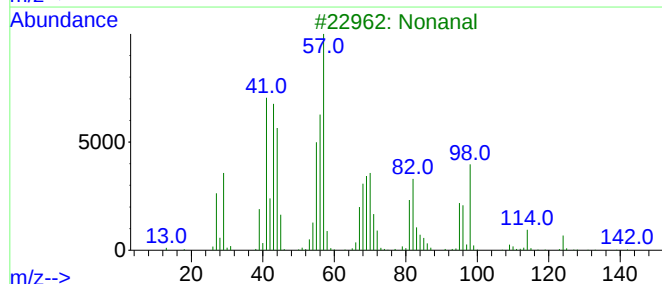
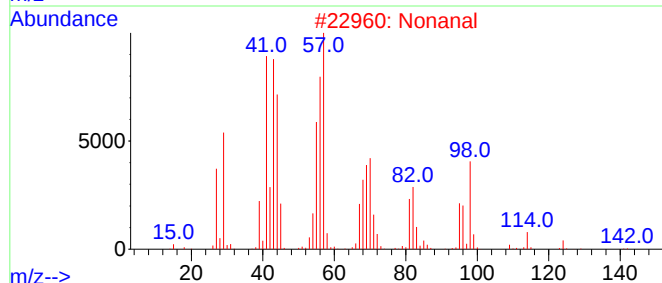
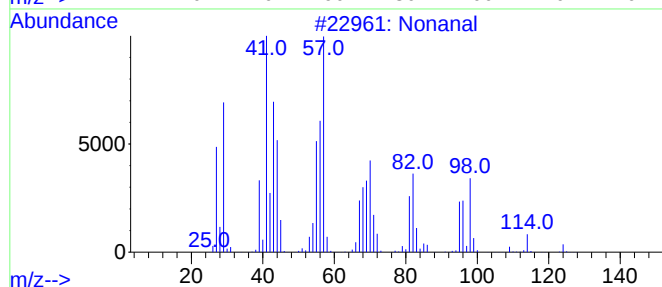
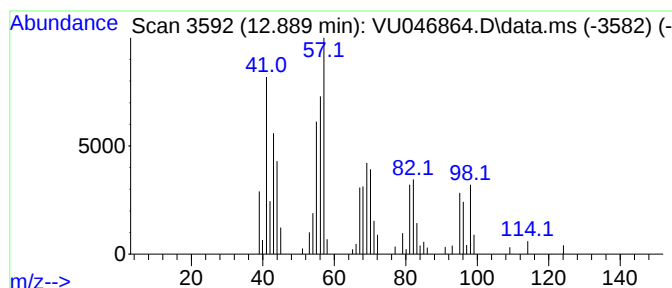
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.889	0.80 ug/L	63994	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	86
2			Nonanal	142	C9H18O	000124-19-6	83
3			Nonanal	142	C9H18O	000124-19-6	83
4			2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	35
5			2-Heptenol	114	C7H14O	1000429-19-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012722\
Data File : VU046864.D
Acq On : 27 Jan 2022 12:27
Operator : SY/MD
Sample : N1260-07DL 5X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.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
(DEL) Alkane: S...	1.363	6.0	ug/L	332980	1	6.253	279076	5.0
(DEL) Alkane: C...	2.163	0.5	ug/L	29310	1	6.253	279076	5.0
(DEL) Alkane: S...	2.211	0.6	ug/L	32430	1	6.253	279076	5.0
Hexanal	8.793	1.1	ug/L	82400	2	9.420	383289	5.0
Nonanal	12.889	0.8	ug/L	63994	3	11.816	398915	5.0