

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
 Data File : VU045951.D
 Acq On : 23 Nov 2021 13:20
 Operator : SY/MD
 Sample : M4755-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AY5

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\SFAMUTR111521WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU045951.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.588	69	77	94	rBV2	75726	132351	18.81%	2.349%
2	1.710	104	115	125	rBV4	3152	7409	1.05%	0.132%
3	1.916	171	179	191	rVB	39470	51028	7.25%	0.906%
4	2.571	371	383	396	rBV	83545	135796	19.30%	2.410%
5	2.671	396	414	463	rVV	27000	125687	17.86%	2.231%
6	3.144	550	561	570	rBV3	4341	8481	1.21%	0.151%
7	3.311	570	613	619	rBV	28309	139243	19.79%	2.472%
8	4.443	945	965	987	rBV	265496	703674	100.00%	12.491%
9	4.649	1011	1029	1046	rBV	45077	154405	21.94%	2.741%
10	5.070	1143	1160	1175	rBV	66696	150492	21.39%	2.671%
11	5.729	1345	1365	1389	rBV2	136068	354283	50.35%	6.289%
12	6.253	1508	1528	1548	rVV	123701	244441	34.74%	4.339%
13	6.394	1561	1572	1593	rBV3	17746	39077	5.55%	0.694%
14	6.694	1652	1665	1684	rBV	84038	164403	23.36%	2.918%
15	7.134	1786	1802	1807	rBV	214641	418453	59.47%	7.428%
16	7.568	1925	1937	1955	rBV2	44907	78160	11.11%	1.387%
17	7.902	2026	2041	2059	rBV	169732	304990	43.34%	5.414%
18	8.034	2072	2082	2093	rVV2	6598	11792	1.68%	0.209%
19	8.182	2115	2128	2142	rBV2	29003	49551	7.04%	0.880%
20	8.491	2211	2224	2235	rBV3	6255	12934	1.84%	0.230%
21	8.639	2256	2270	2282	rBV	214344	404874	57.54%	7.187%
22	9.420	2501	2513	2545	rVB	176058	295642	42.01%	5.248%
23	10.761	2919	2930	2941	rBV	73588	118884	16.89%	2.110%
24	10.893	2960	2971	2983	rBV5	4870	8216	1.17%	0.146%
25	11.031	3005	3014	3027	rVB3	4483	8089	1.15%	0.144%
26	11.745	3228	3236	3246	rBV5	5394	8309	1.18%	0.147%
27	11.815	3246	3258	3274	rVB	186084	297440	42.27%	5.280%
28	12.063	3323	3335	3355	rBV2	31727	68152	9.69%	1.210%
29	12.195	3365	3376	3396	rVB	169961	275788	39.19%	4.895%
30	12.504	3462	3472	3486	rVV2	7188	14406	2.05%	0.256%
31	12.889	3583	3592	3606	rVB4	5189	7341	1.04%	0.130%
32	14.176	3982	3992	4003	rBV2	4789	7805	1.11%	0.139%
33	14.317	4025	4036	4048	rBV	27616	43444	6.17%	0.771%
34	14.725	4154	4163	4175	rVB	9020	13848	1.97%	0.246%
35	15.044	4242	4262	4274	rBV2	325079	482922	68.63%	8.572%
36	15.137	4287	4291	4300	rVB3	5634	7308	1.04%	0.130%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Title : TRACE VOA SFAM1.0

37	15.696	4452	4465	4484	rBV2	118715	189075	26.87%	3.356%
38	16.683	4760	4772	4784	rBV2	24270	38816	5.52%	0.689%
39	16.773	4789	4800	4808	rVV2	32827	49550	7.04%	0.880%
40	16.818	4808	4814	4826	rVB9	4415	7057	1.00%	0.125%

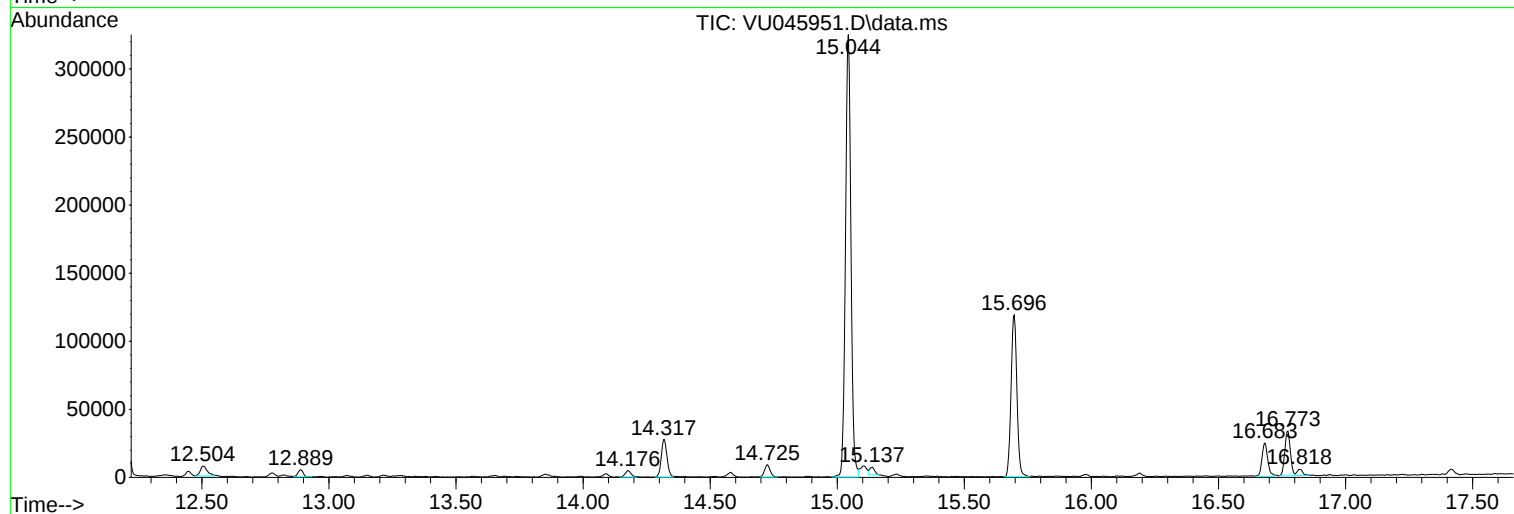
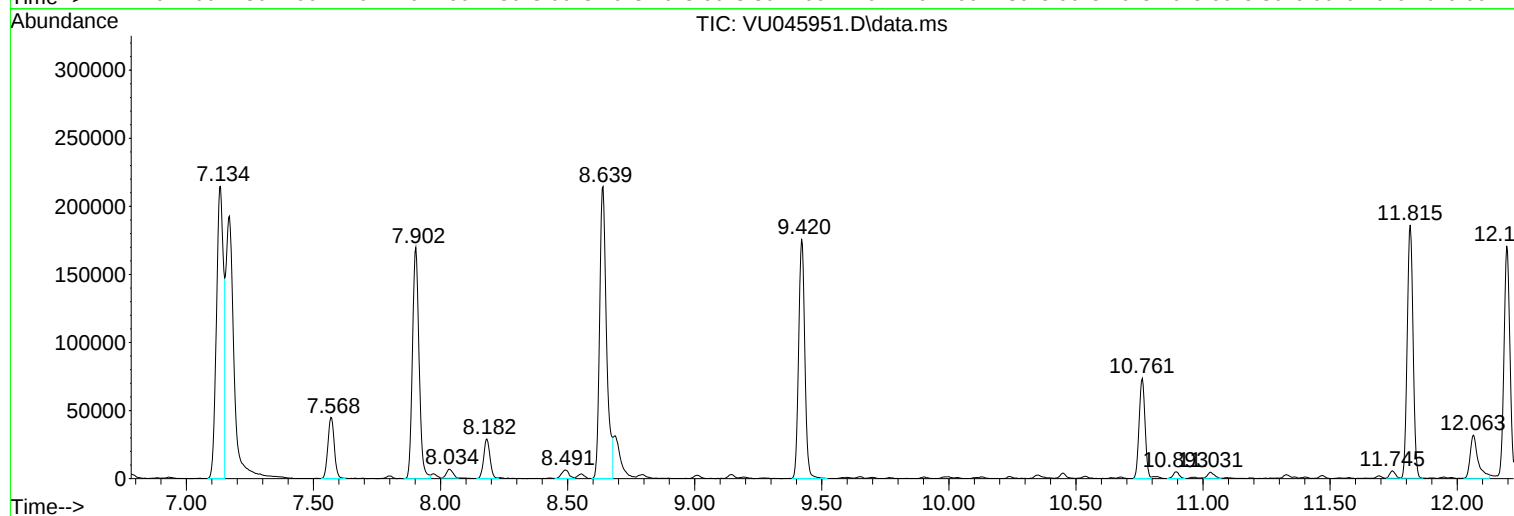
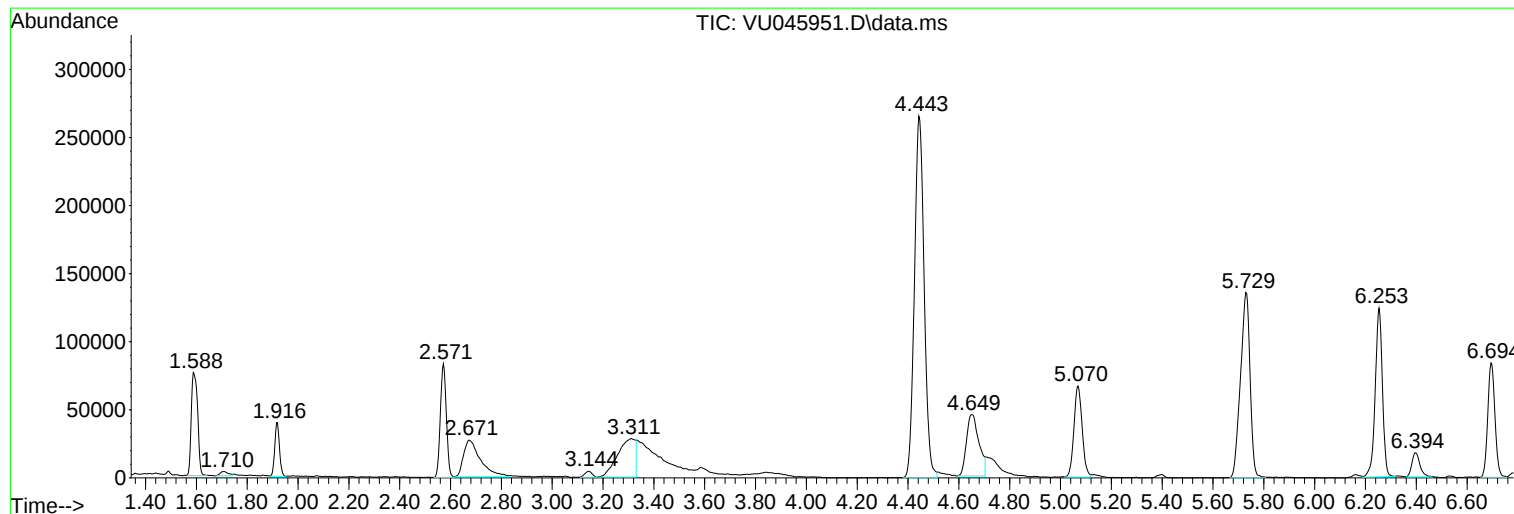
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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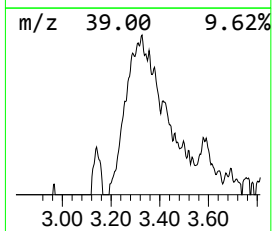
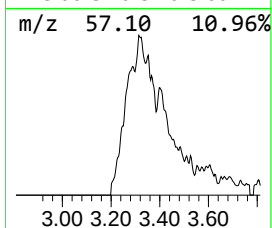
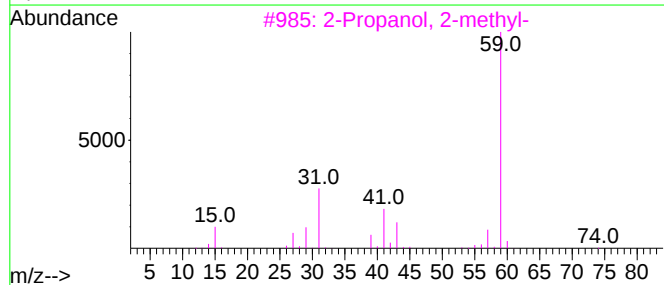
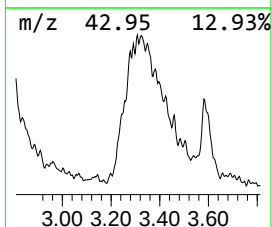
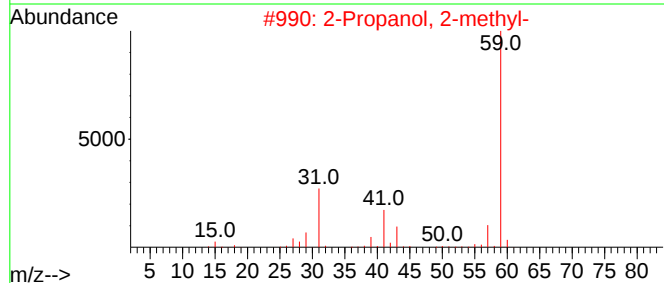
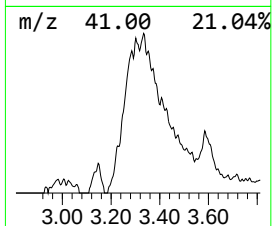
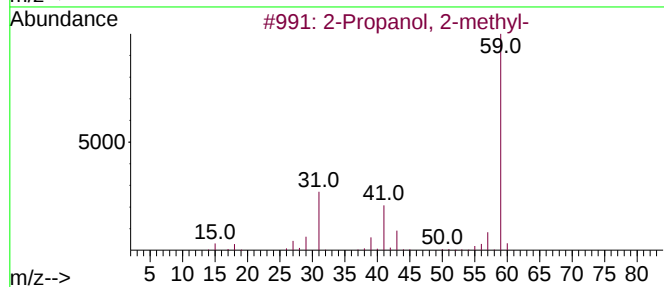
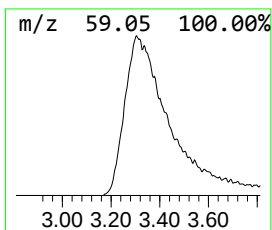
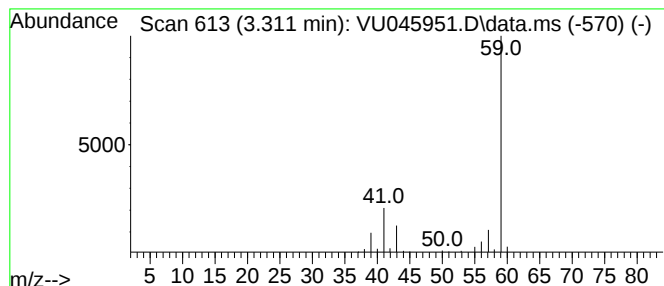
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.311	2.85 ug/L	139243	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	72
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	56
3	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	40
4	Propanoic acid, 2-hydroxy-2-methyl-			104	C4H8O3	000594-61-6	38
5	3-Pentanol			88	C5H12O	000584-02-1	9



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Instrument :
MSVOA_U
ClientSampleId :
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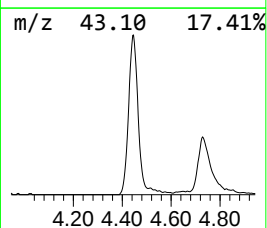
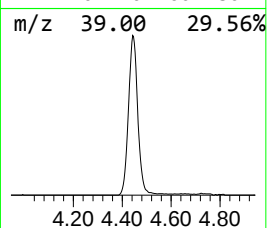
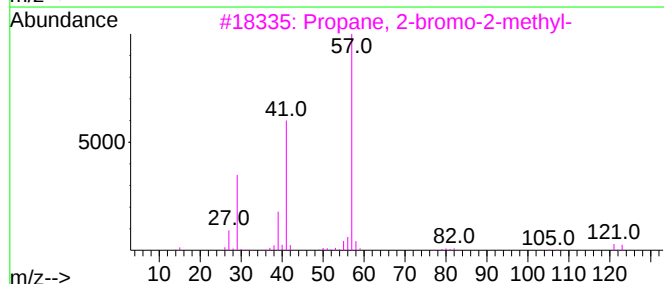
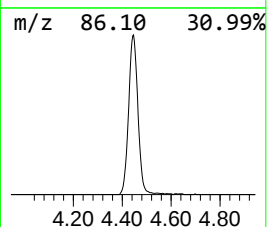
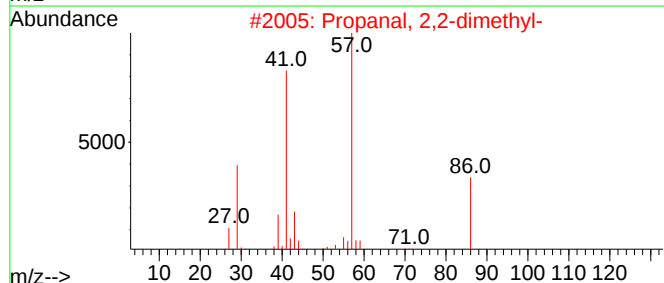
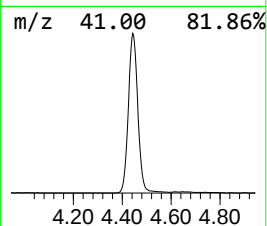
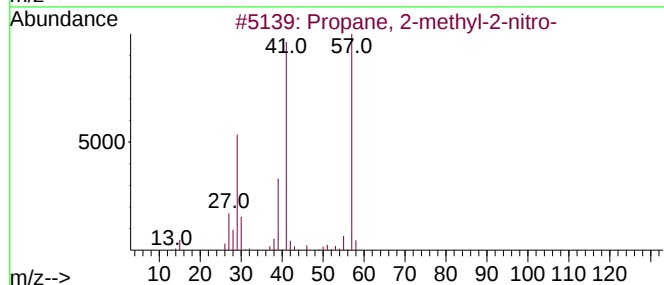
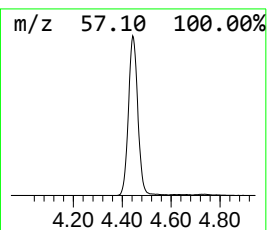
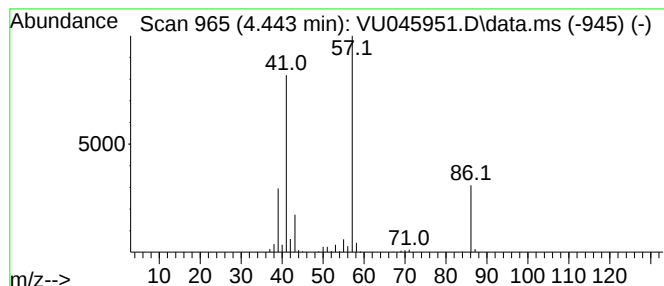
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propane, 2-methyl-2-nitro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.443	14.39 ug/L	703674	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
2			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45
3			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	42
4			3-Pentanone	86	C5H10O	000096-22-0	42
5			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	42



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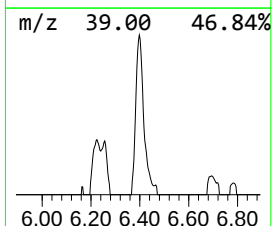
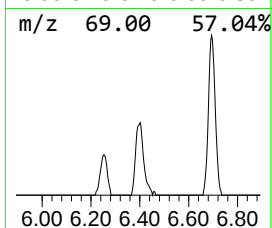
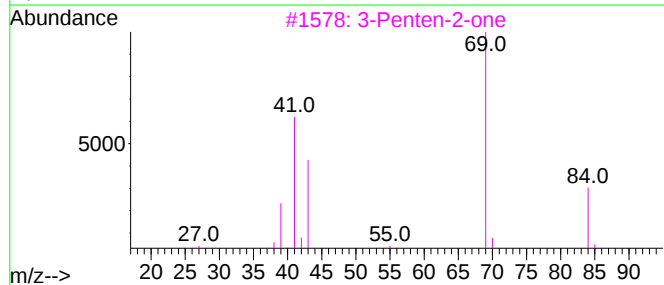
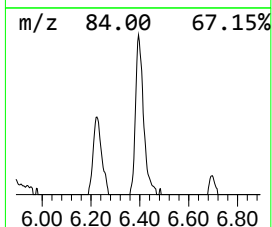
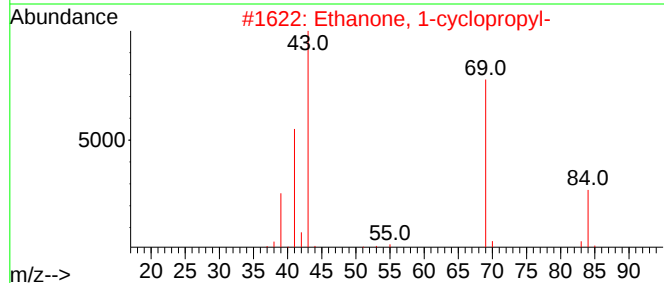
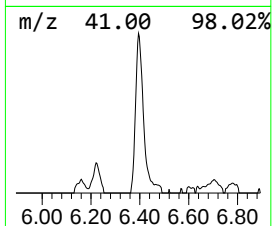
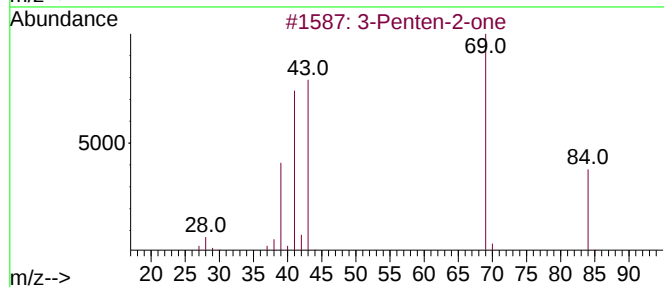
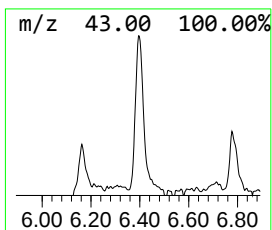
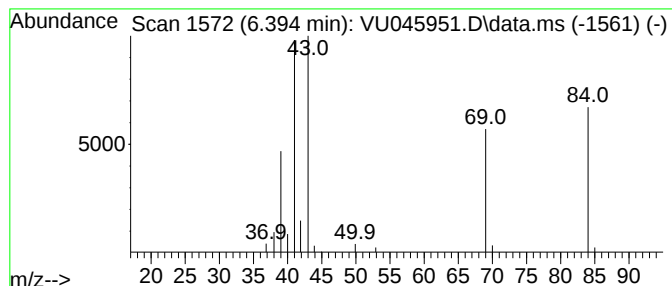
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 3-Penten-2-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.394	0.80 ug/L	39077	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one	84	C5H8O	000625-33-2	90
2			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	83
3			3-Penten-2-one	84	C5H8O	000625-33-2	72
4			3-Penten-2-one	84	C5H8O	000625-33-2	64
5			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	53



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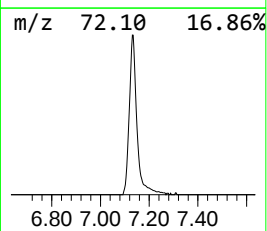
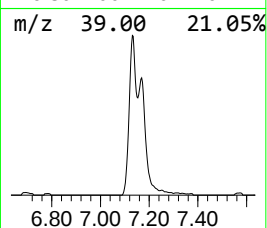
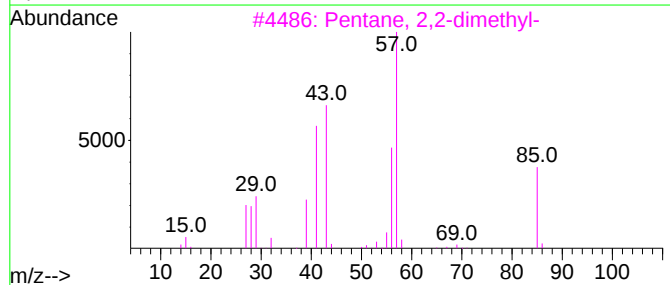
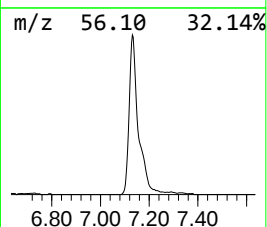
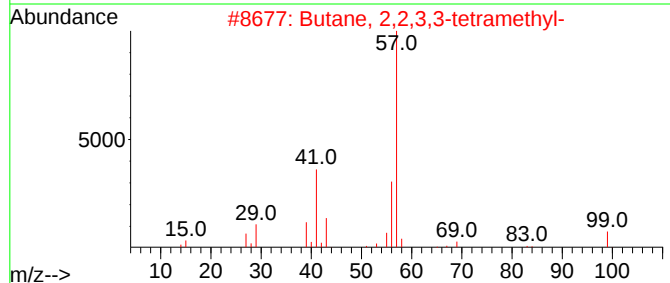
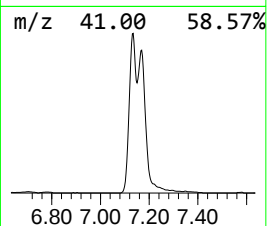
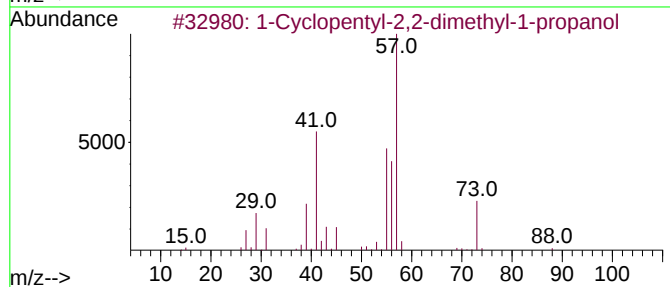
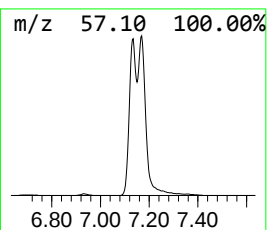
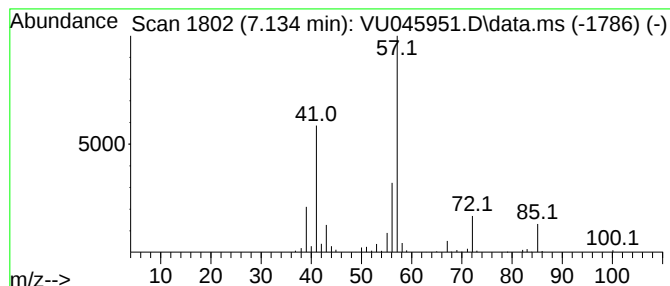
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.134	8.56 ug/L	418453	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	42
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	38
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
5			Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	33



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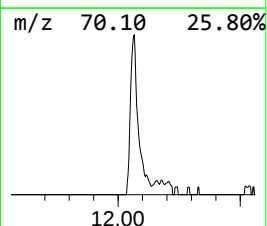
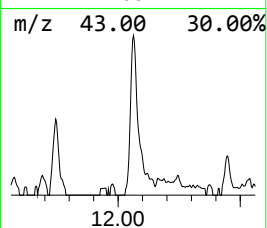
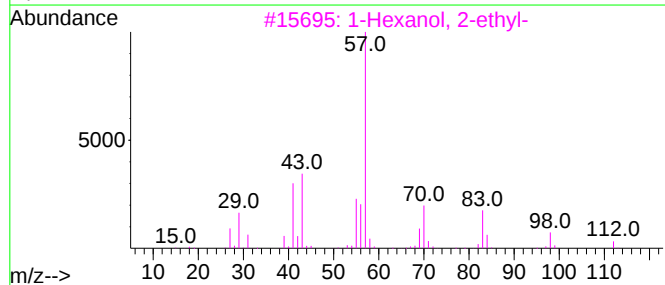
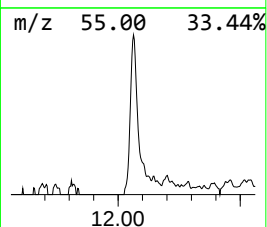
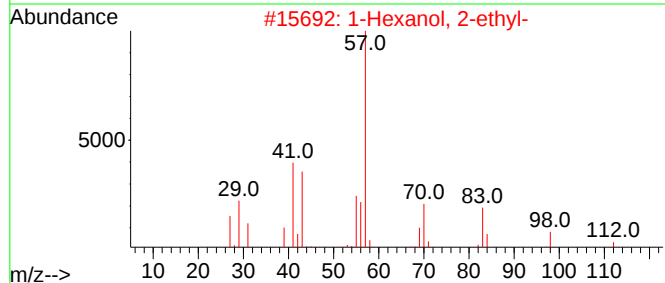
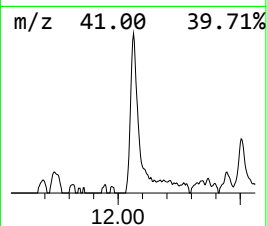
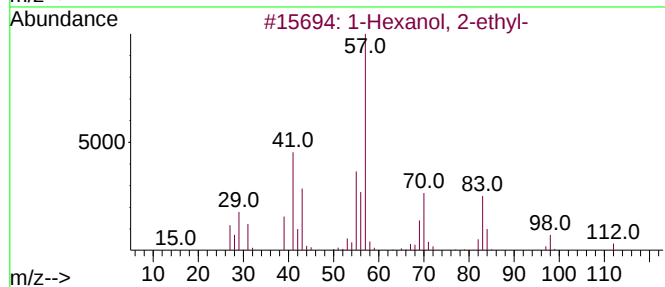
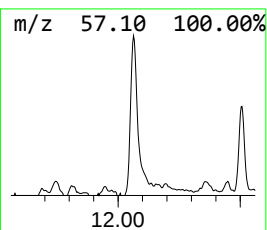
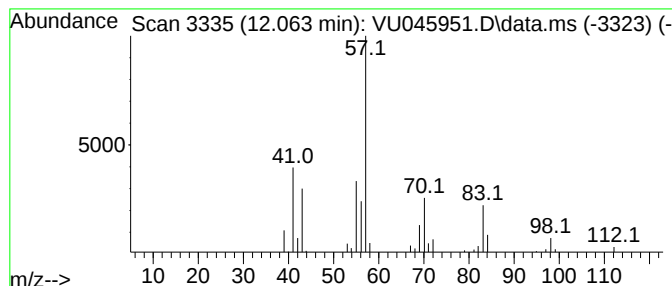
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	1.15 ug/L	68152	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
Data File : VU045951.D
Acq On : 23 Nov 2021 13:20
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

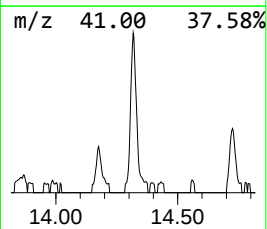
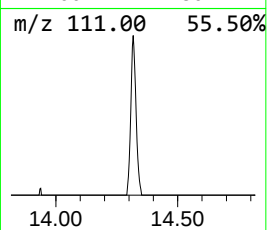
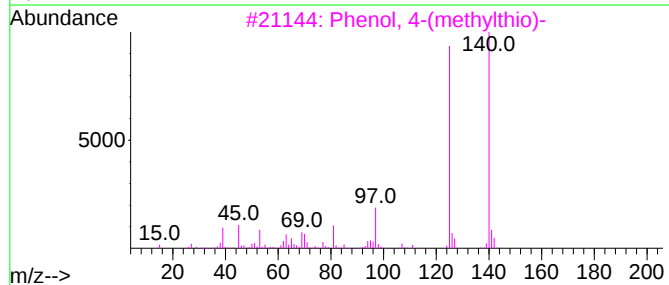
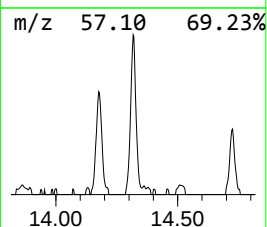
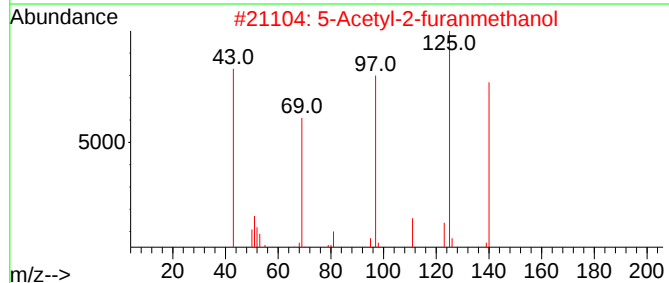
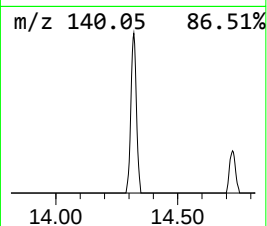
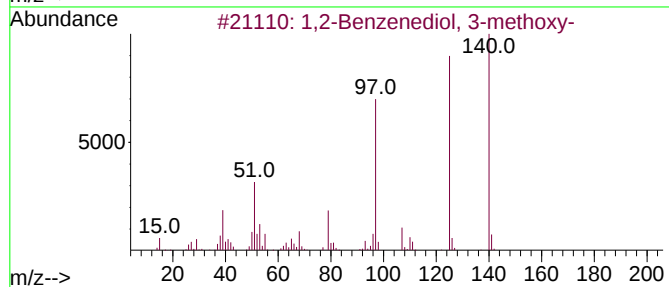
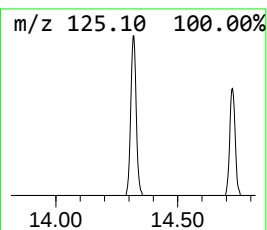
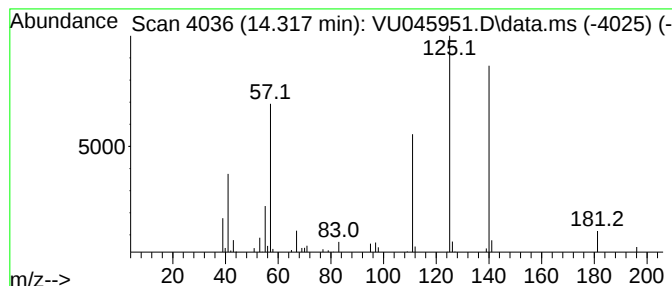
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1,2-Benzenediol, 3-methoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.317	0.73 ug/L	43444	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
2			5-Acetyl-2-furanmethanol	140	C7H8O3	055087-82-6	59
3			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
4			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
5			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
Data File : VU045951.D
Acq On : 23 Nov 2021 13:20
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

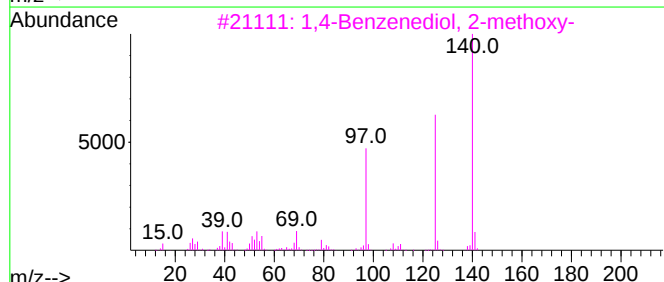
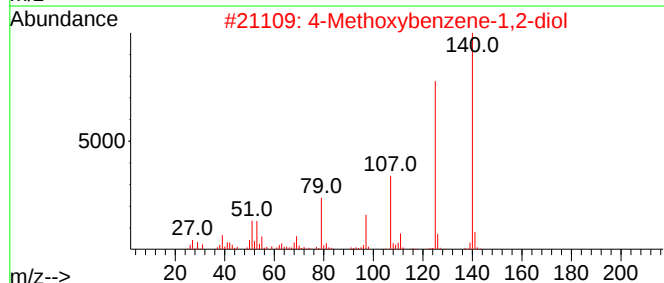
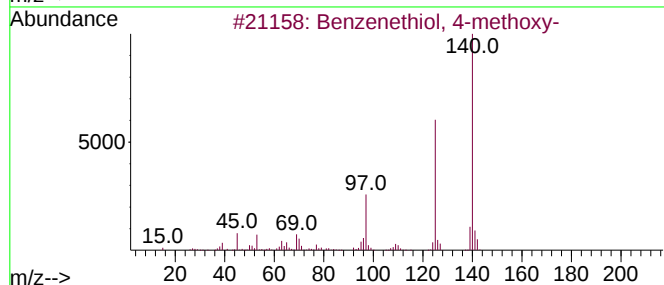
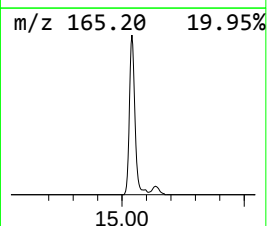
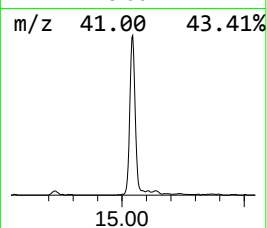
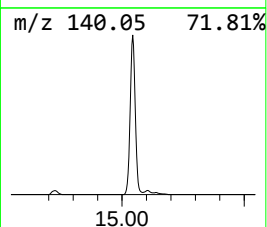
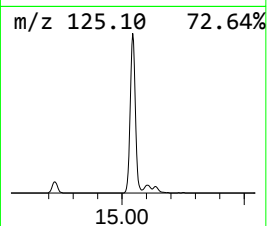
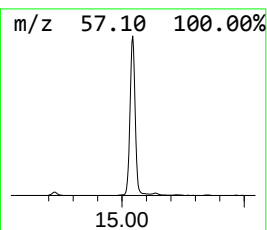
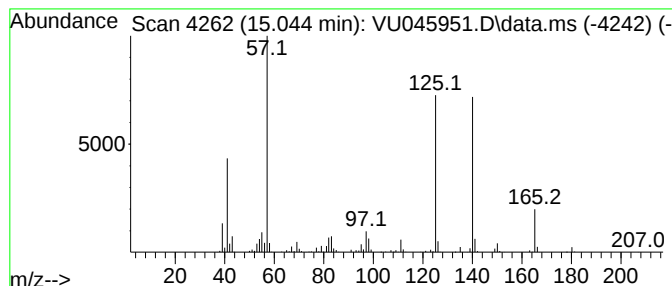
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Benzenethiol, 4-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.044	8.12 ug/L	482922	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	50
2			4-Methoxybenzene-1,2-diol	140	C7H8O3	003934-97-2	50
3			1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	50
4			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	50
5			1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
Data File : VU045951.D
Acq On : 23 Nov 2021 13:20
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

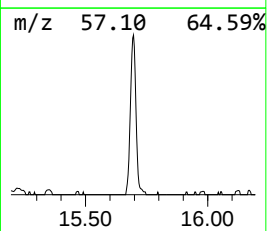
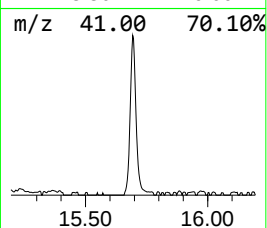
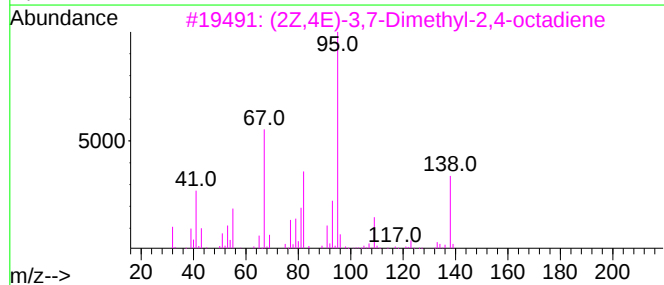
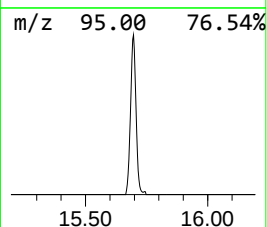
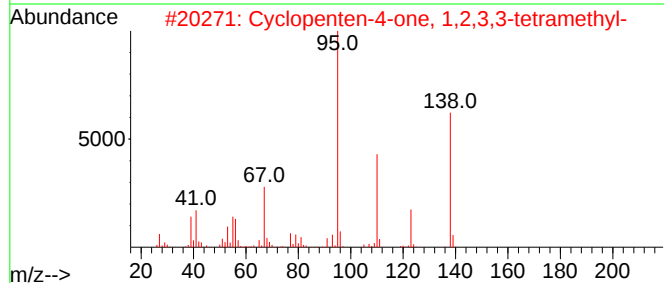
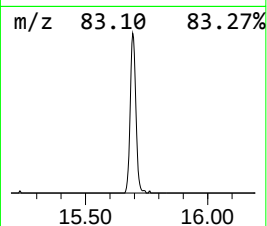
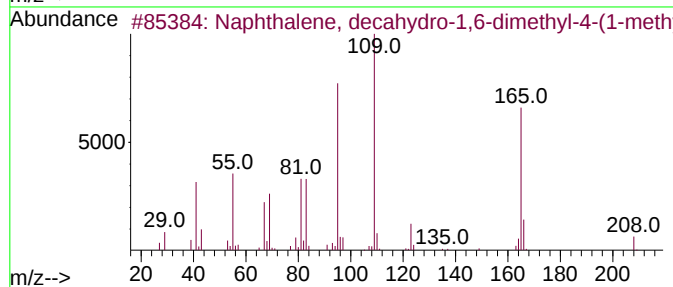
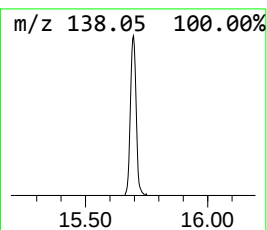
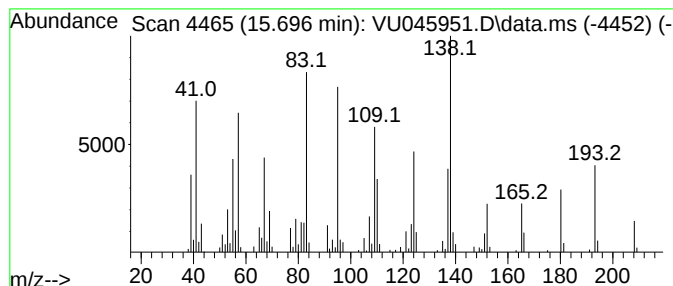
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.696	3.18 ug/L	189075	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-1,6-dimet...	208	C15H28	029788-41-8	38
2			Cyclopenten-4-one, 1,2,3,3-tetra...	138	C9H14O	1000163-38-6	30
3			(2Z,4E)-3,7-Dimethyl-2,4-octadiene	138	C10H18	1000374-08-4	30
4			4-Acetyl-1-methylcyclohexene	138	C9H14O	006090-09-1	25
5			Cyclopentanecarboxylic acid, 3-m...	278	C18H30O2	1000152-25-8	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
Data File : VU045951.D
Acq On : 23 Nov 2021 13:20
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

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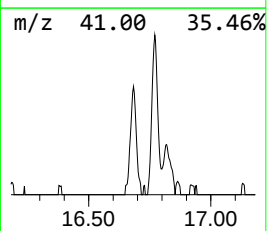
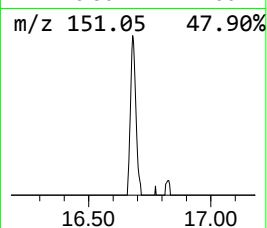
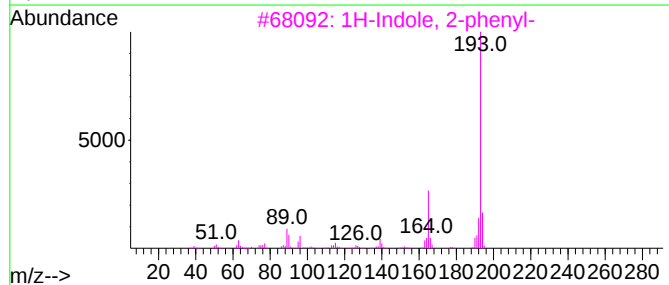
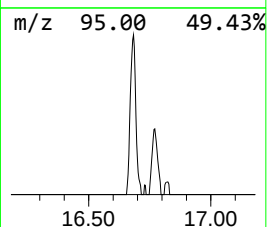
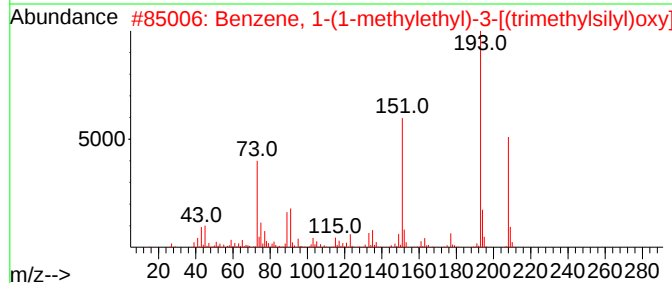
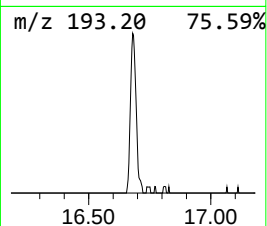
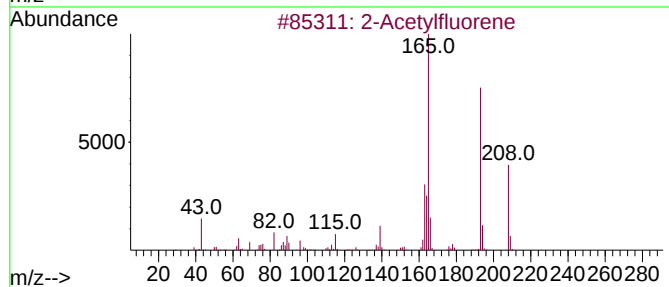
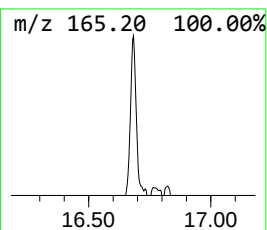
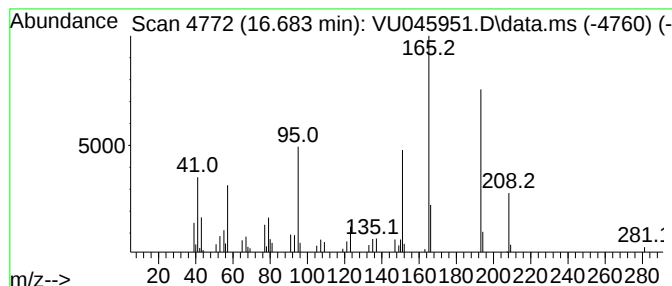
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 2-Acetylfluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.683	0.65 ug/L	38816	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Acetylfluorene	208	C15H12O	000781-73-7	52
2			Benzene, 1-(1-methylethyl)-3-[(t...	208	C12H20OSi	025237-76-7	50
3			1H-Indole, 2-phenyl-	193	C14H11N	000948-65-2	47
4			9-Phenanthrenamine	193	C14H11N	000947-73-9	43
5			Acetic acid, (5-formyl-2-methoxy...	208	C11H12O4	099865-67-5	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
Data File : VU045951.D
Acq On : 23 Nov 2021 13:20
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

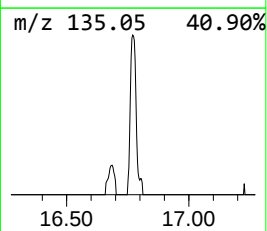
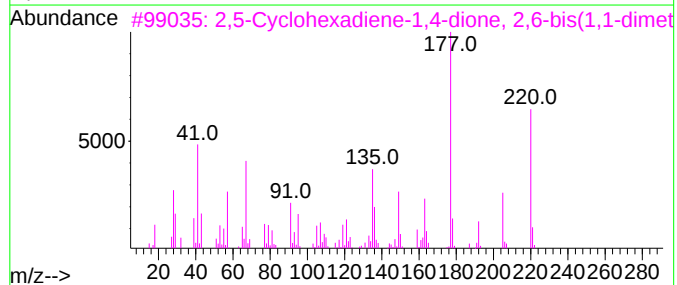
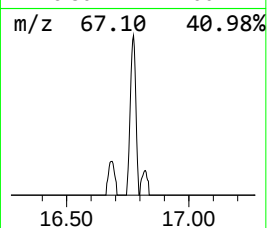
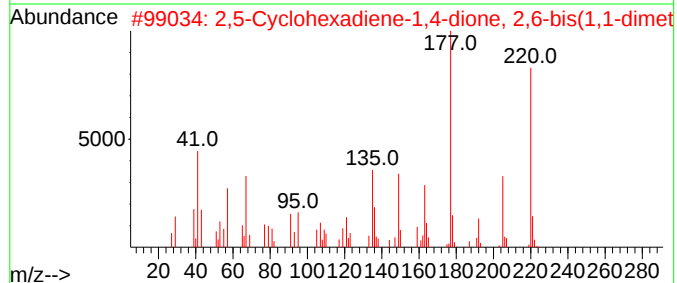
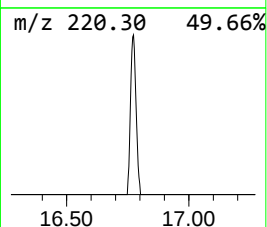
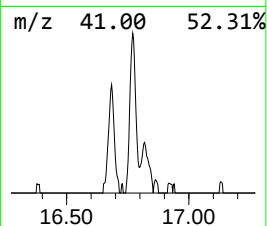
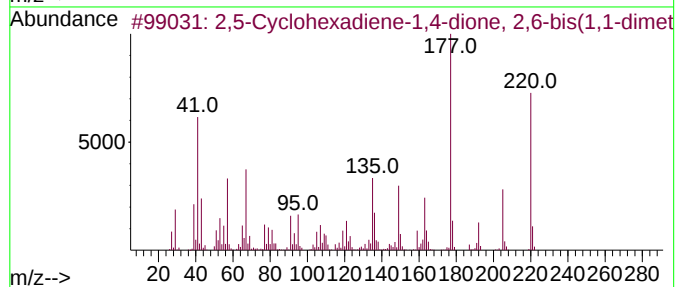
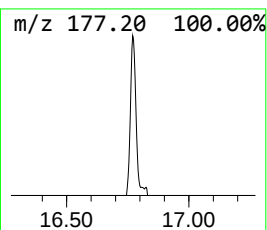
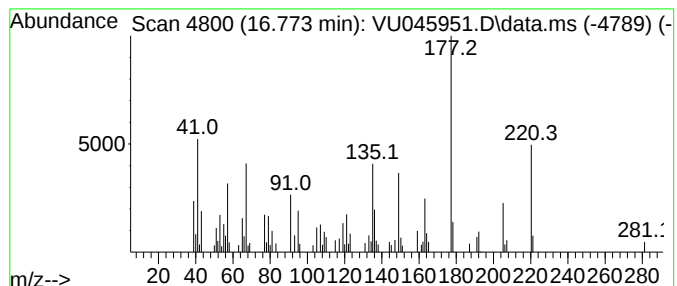
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.773	0.83 ug/L	49550	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	99		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	98		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	98		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	98		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	93		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112321\
Data File : VU045951.D
Acq On : 23 Nov 2021 13:20
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-m...	3.311	2.9	ug/L	139243	1	6.253	244441	5.0
Propane, 2-meth...	4.443	14.4	ug/L	703674	1	6.253	244441	5.0
3-Penten-2-one	6.394	0.8	ug/L	39077	1	6.253	244441	5.0
unknown-01	7.134	8.6	ug/L	418453	1	6.253	244441	5.0
1-Hexanol, 2-et...	12.063	1.1	ug/L	68152	3	11.816	297440	5.0
1,2-Benzenediol...	14.317	0.7	ug/L	43444	3	11.816	297440	5.0
Benzenethiol, 4...	15.044	8.1	ug/L	482922	3	11.816	297440	5.0
unknown-02	15.696	3.2	ug/L	189075	3	11.816	297440	5.0
2-Acetylfluorene	16.683	0.7	ug/L	38816	3	11.816	297440	5.0
2,5-Cyclohexadi...	16.773	0.8	ug/L	49550	3	11.816	297440	5.0