

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
 Data File : VU045891.D
 Acq On : 19 Nov 2021 13:48
 Operator : SY/MD
 Sample : M4755-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 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: VU045891.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	68	77	92	rBV2	87801	133649	19.86%	2.655%
2	1.700	104	112	132	rBV2	3676	9867	1.47%	0.196%
3	1.916	171	179	194	rVB	31995	41892	6.22%	0.832%
4	2.572	371	383	396	rBV	63212	103179	15.33%	2.050%
5	2.671	396	414	460	rBV2	22592	118031	17.54%	2.345%
6	3.141	548	560	571	rBV3	4487	9101	1.35%	0.181%
7	3.273	572	601	602	rBV3	20421	53268	7.91%	1.058%
8	4.443	945	965	1000	rBV	249138	673049	100.00%	13.372%
9	4.649	1014	1029	1048	rBV2	38297	139210	20.68%	2.766%
10	5.067	1140	1159	1178	rBV	56331	131901	19.60%	2.621%
11	5.729	1345	1365	1387	rBV2	113316	296558	44.06%	5.892%
12	6.250	1508	1527	1547	rBV	108124	214784	31.91%	4.267%
13	6.395	1560	1572	1596	rBV	15691	35047	5.21%	0.696%
14	6.694	1652	1665	1683	rBV	74184	144087	21.41%	2.863%
15	7.131	1786	1801	1807	rBV	201504	404935	60.16%	8.045%
16	7.568	1923	1937	1949	rBV	38044	65436	9.72%	1.300%
17	7.899	2028	2040	2056	rBV	134020	239431	35.57%	4.757%
18	8.034	2073	2082	2096	rVB2	6130	11461	1.70%	0.228%
19	8.182	2117	2128	2138	rBV	24094	40701	6.05%	0.809%
20	8.488	2210	2223	2234	rBV4	5844	10963	1.63%	0.218%
21	8.636	2256	2269	2308	rVV	198668	428384	63.65%	8.511%
22	9.420	2500	2513	2529	rBV	162545	271736	40.37%	5.399%
23	10.758	2918	2929	2940	rBV	67180	108559	16.13%	2.157%
24	11.031	3004	3014	3027	rVB2	4101	7590	1.13%	0.151%
25	11.742	3225	3235	3246	rBV4	4743	7457	1.11%	0.148%
26	11.812	3246	3257	3272	rVB	170941	269546	40.05%	5.355%
27	12.063	3323	3335	3362	rBV2	26256	60768	9.03%	1.207%
28	12.195	3364	3376	3390	rVB	145534	234344	34.82%	4.656%
29	12.504	3462	3472	3487	rVV2	6428	12579	1.87%	0.250%
30	14.317	4025	4036	4051	rBV2	24102	36073	5.36%	0.717%
31	14.722	4153	4162	4172	rVB	10169	15746	2.34%	0.313%
32	15.041	4243	4261	4275	rBV2	269360	420864	62.53%	8.362%
33	15.137	4284	4291	4306	rVB2	20938	33918	5.04%	0.674%
34	15.693	4453	4464	4481	rBV	107014	170031	25.26%	3.378%
35	16.680	4761	4771	4782	rBV3	22189	35172	5.23%	0.699%
36	16.770	4790	4799	4809	rBV3	30761	44000	6.54%	0.874%

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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

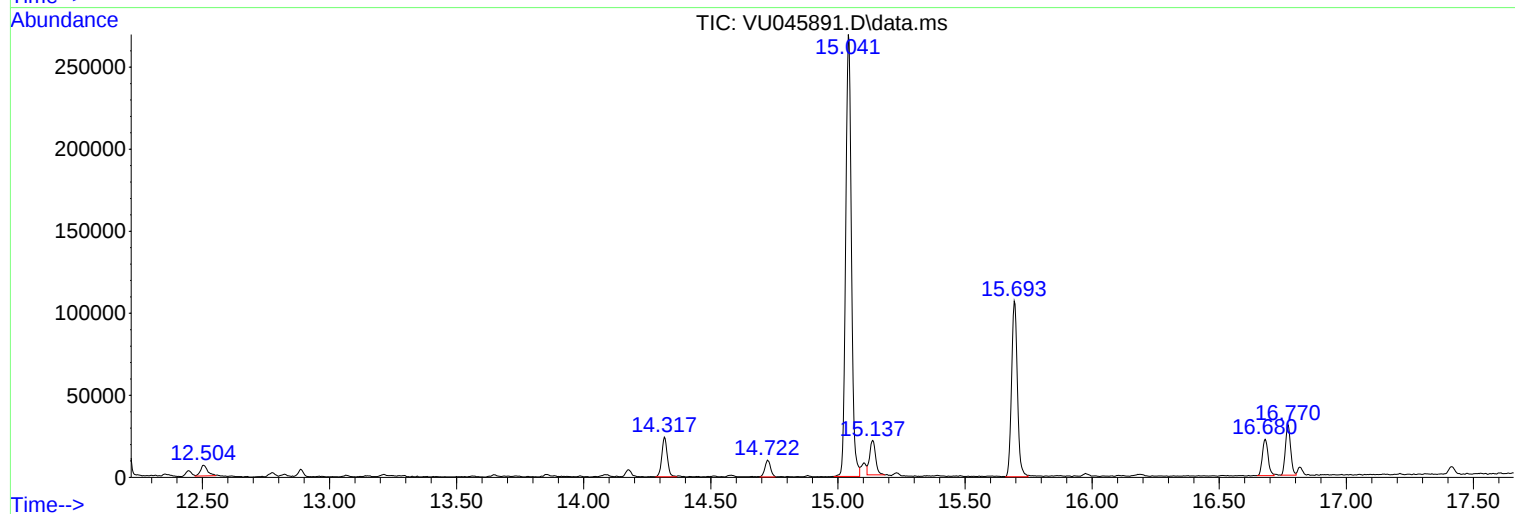
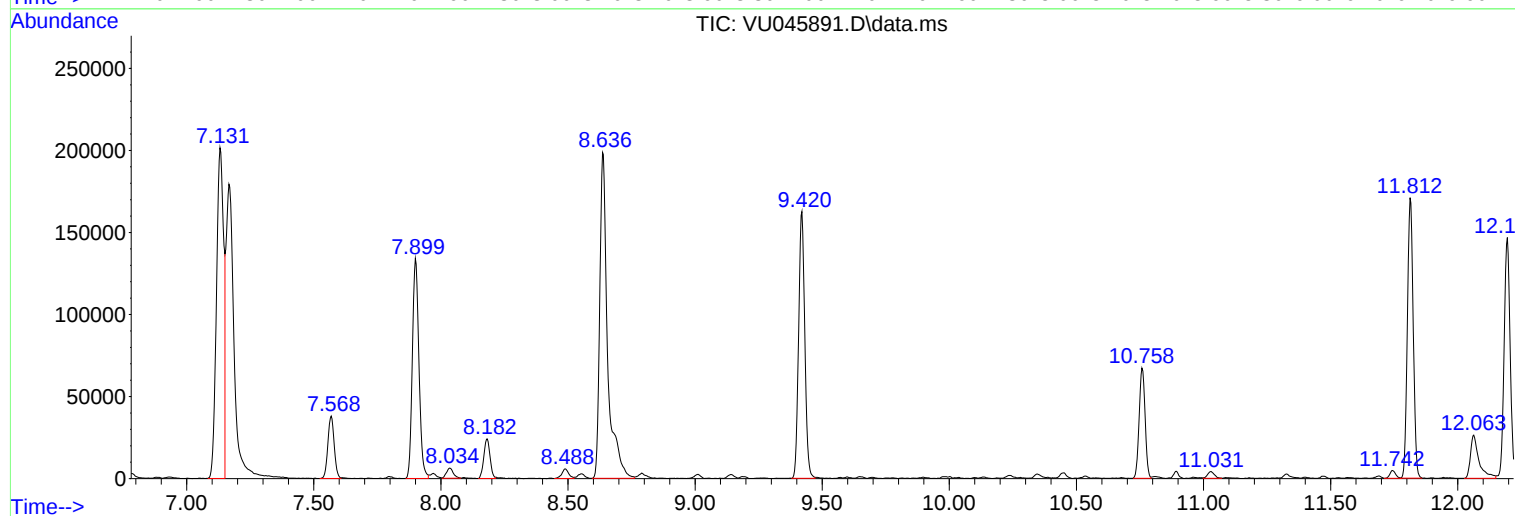
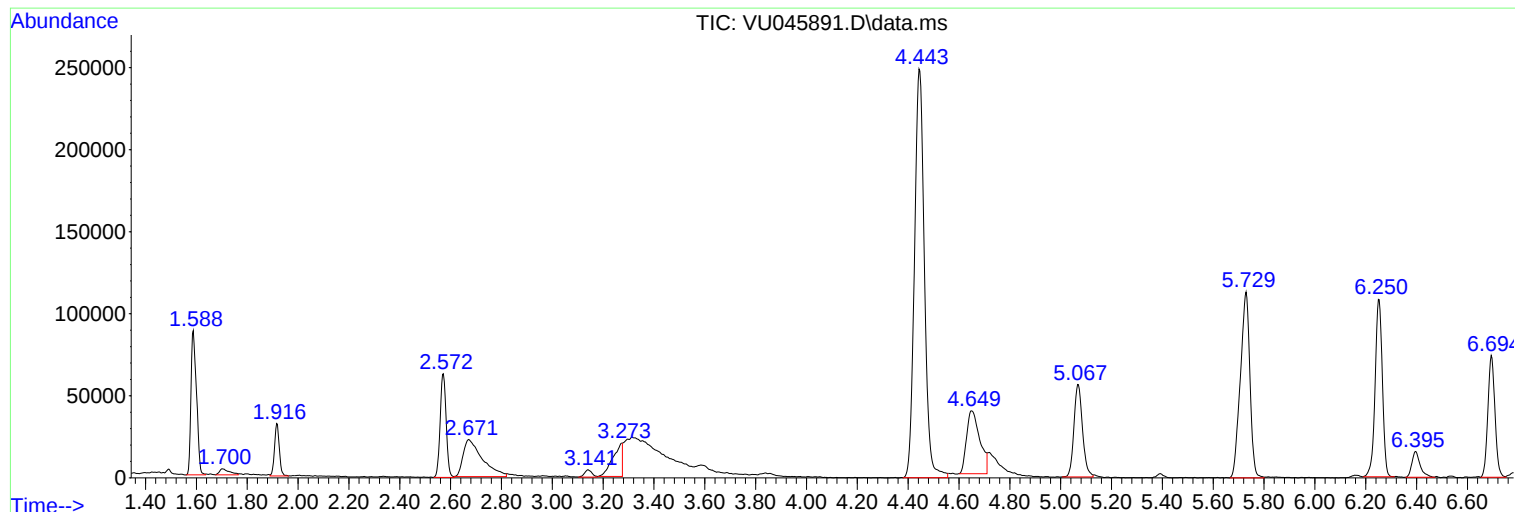
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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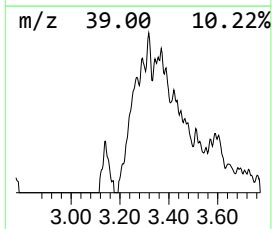
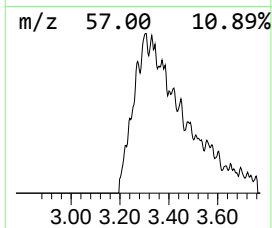
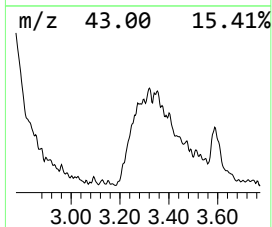
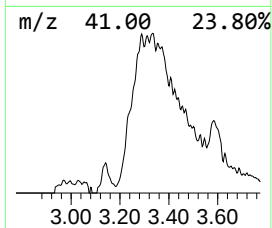
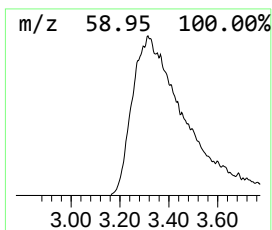
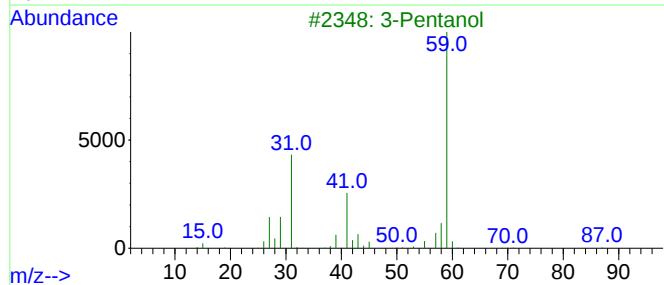
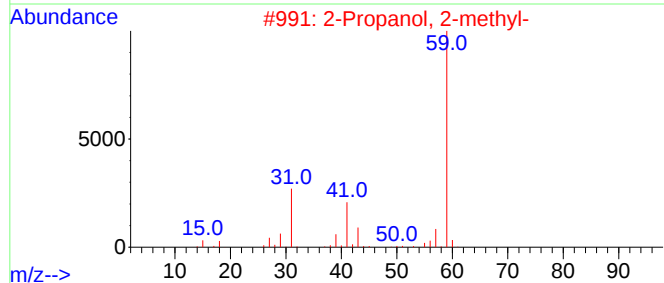
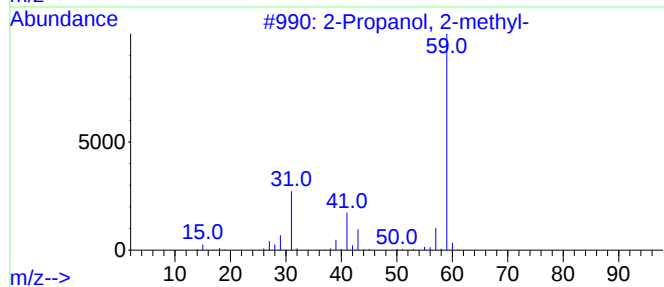
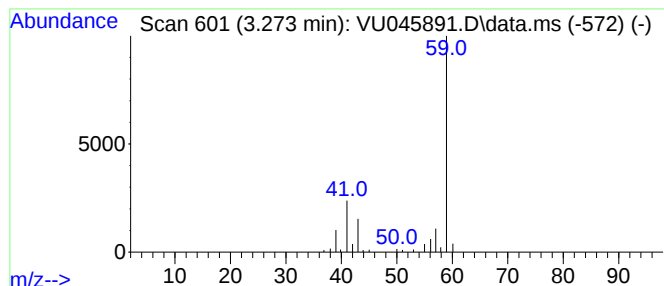
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.273	1.24 ug/L	53268	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	64
2	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	64
3	3-Pentanol		88	C5H12O	000584-02-1	56
4	3-Pentanol		88	C5H12O	000584-02-1	40
5	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	9



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

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

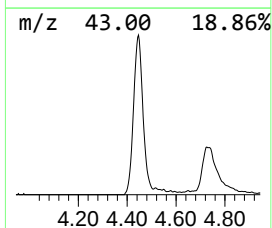
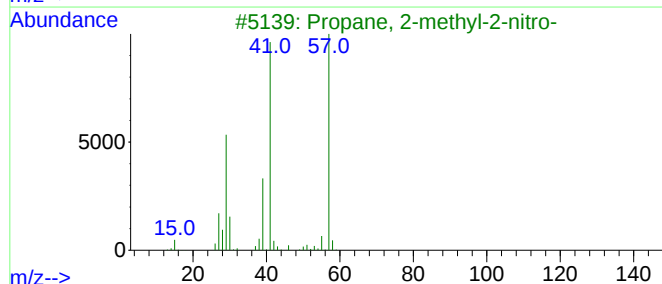
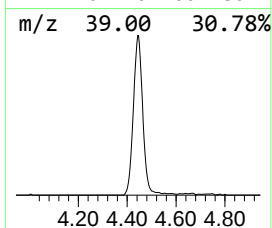
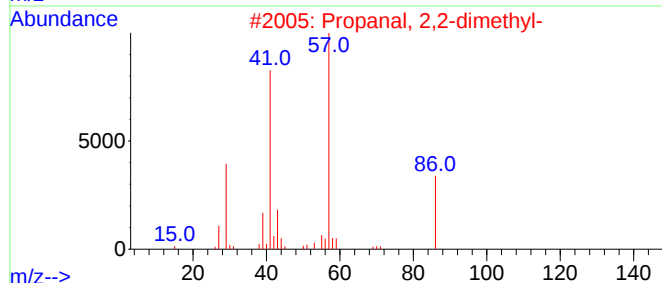
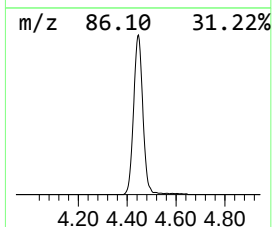
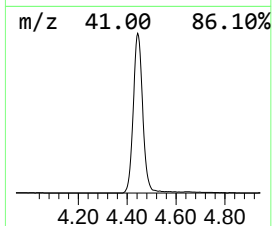
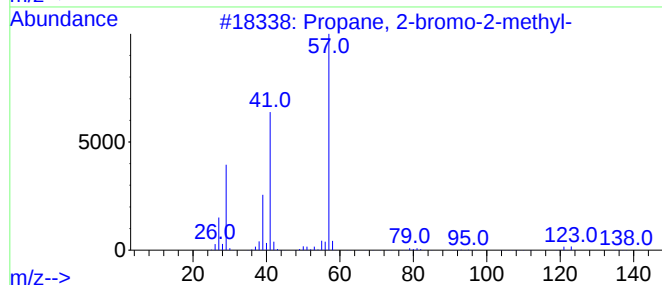
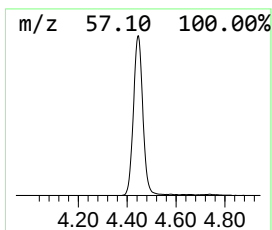
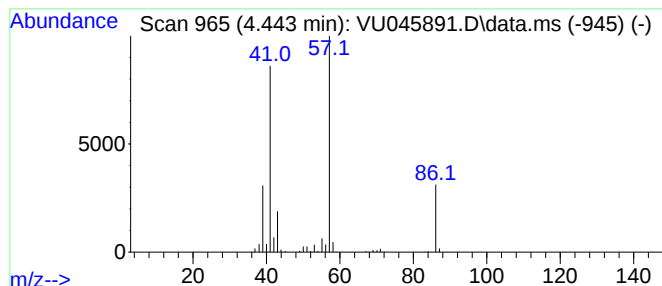
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.443	15.67 ug/L	673049	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	53
2			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	53
3			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
4			3-Heptanone, 5-ethyl-4-methyl-	156	C10H20O	027607-63-2	42
5			3-Pentanone	86	C5H10O	000096-22-0	42



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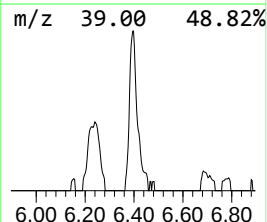
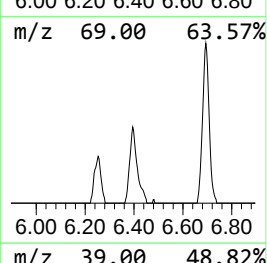
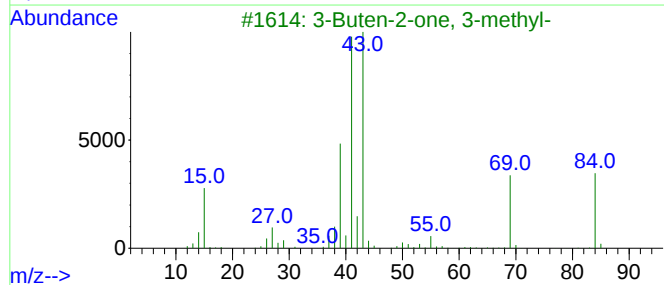
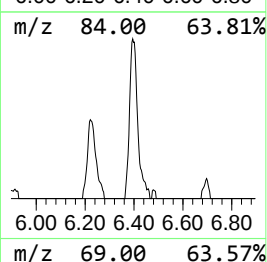
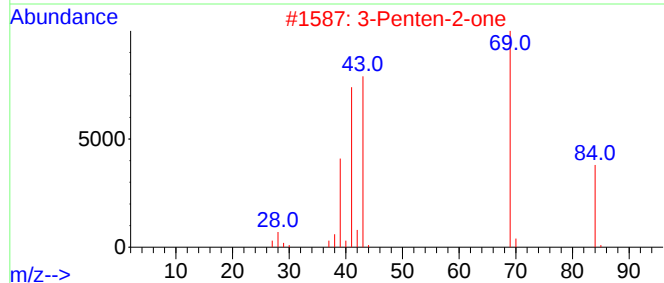
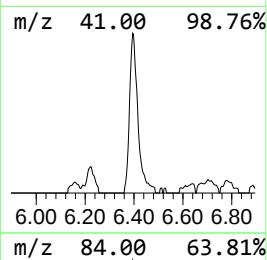
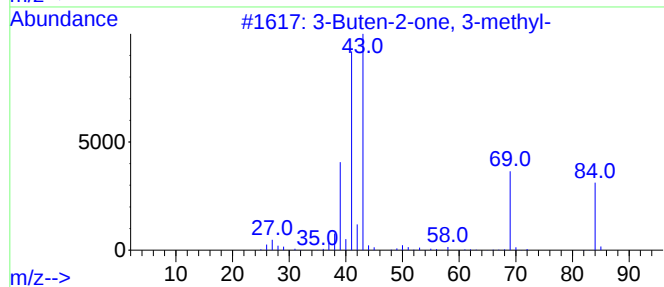
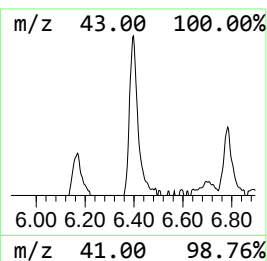
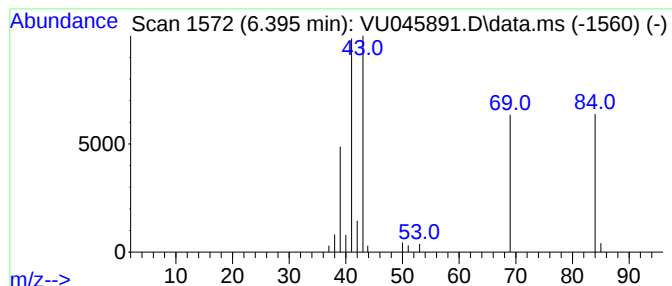
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 3-Buten-2-one, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.395	0.82 ug/L	35047	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	90
2			3-Penten-2-one	84	C5H8O	000625-33-2	72
3			3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	64
4			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	64
5			Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	53



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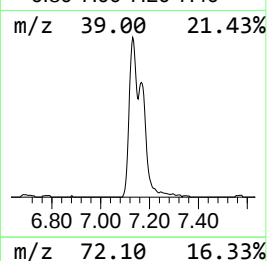
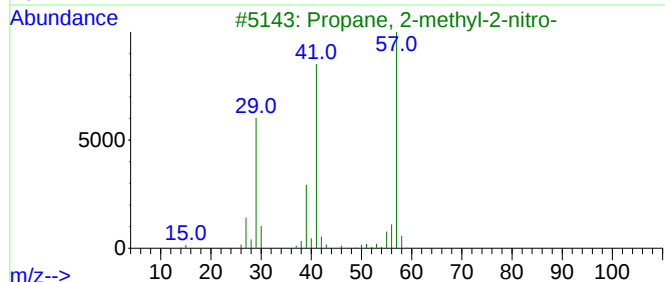
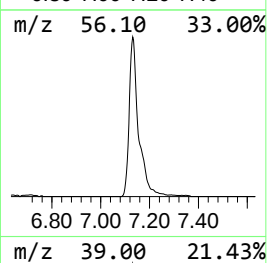
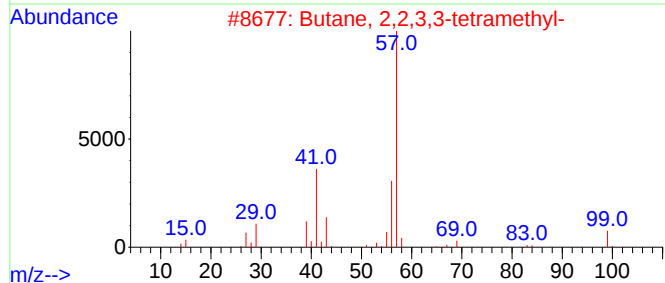
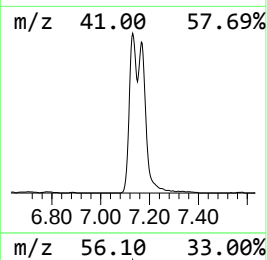
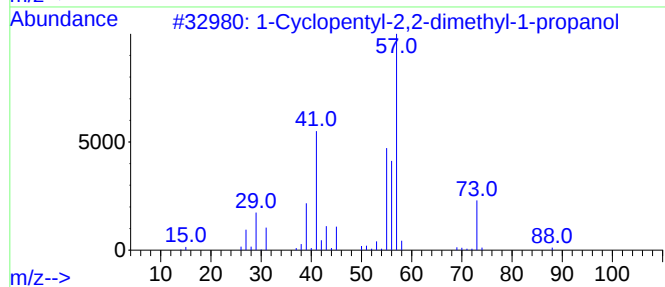
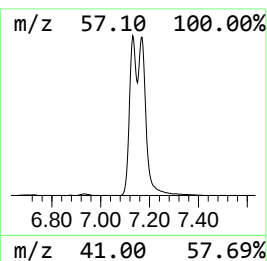
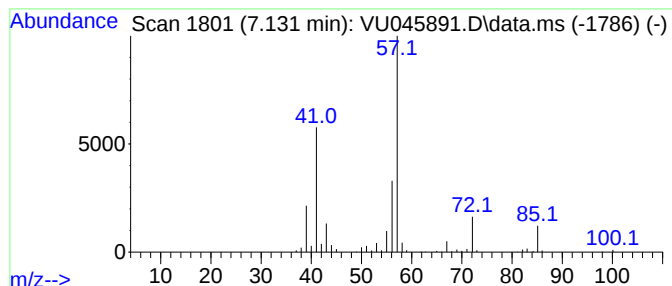
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
7.131	9.43 ug/L	404935	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			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
4			1-Hexen-3-ol	100	C6H12O	004798-44-1	37
5			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	36



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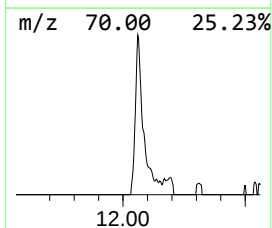
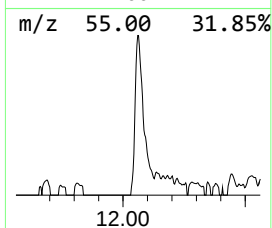
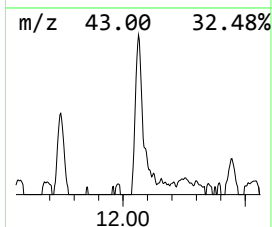
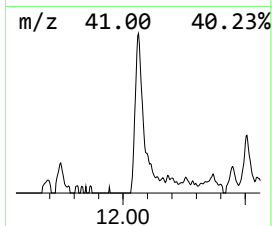
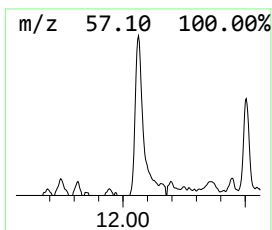
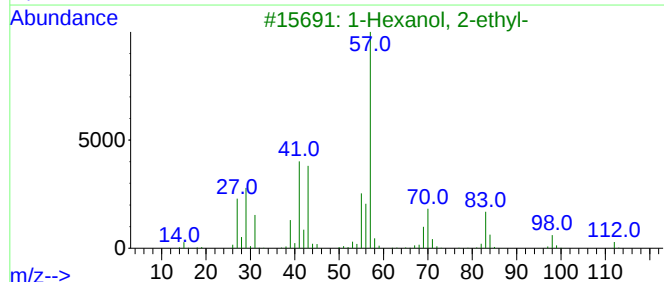
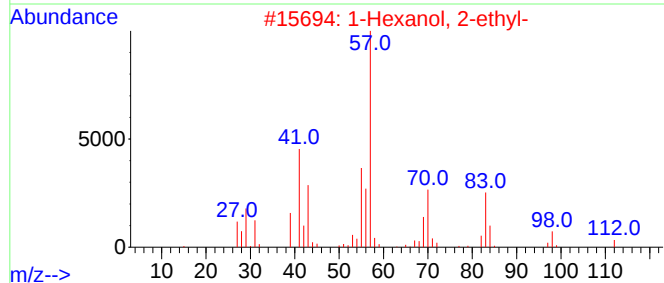
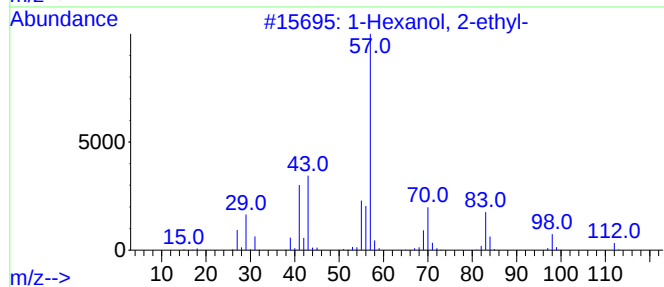
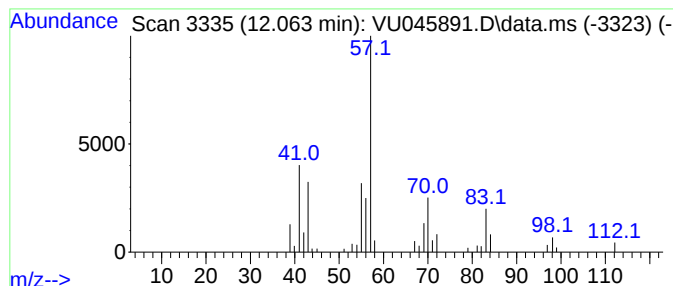
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111521WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	1.13 ug/L	60768	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	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
Data File : VU045891.D
Acq On : 19 Nov 2021 13:48
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

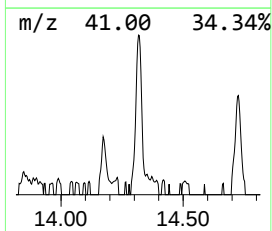
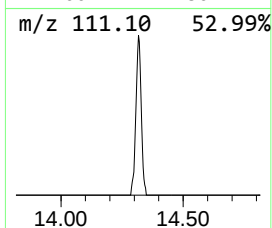
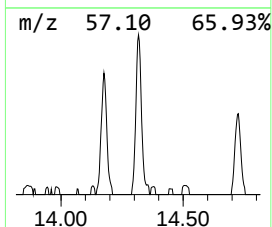
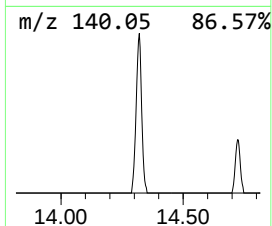
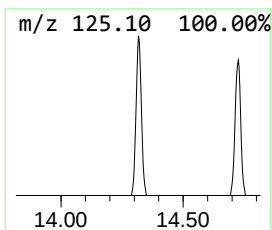
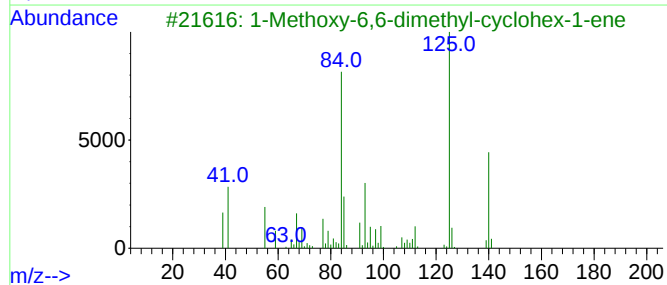
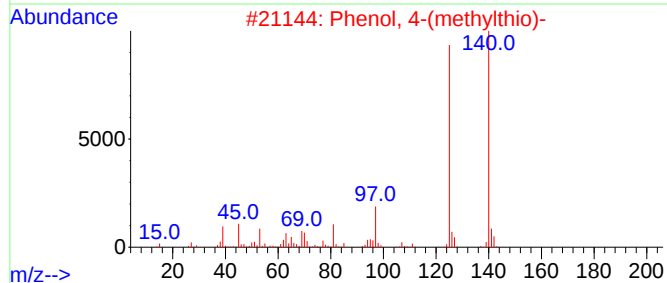
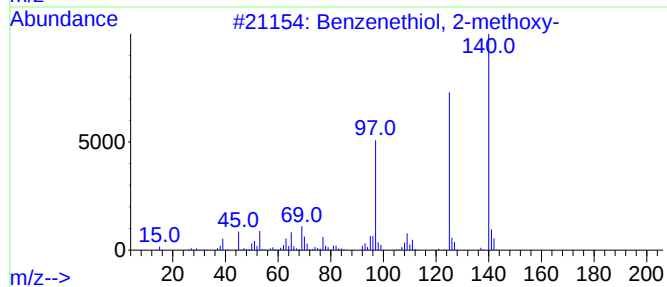
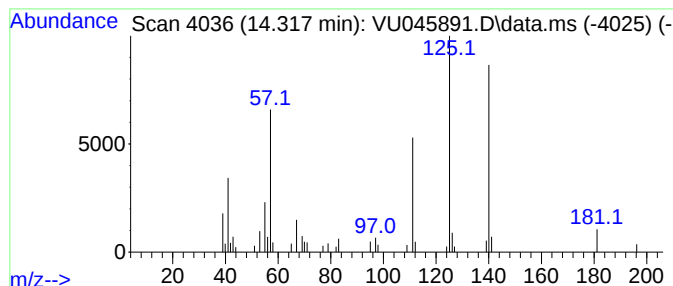
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Benzenethiol, 2-methoxy- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.317	0.67 ug/L	36073	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	59
2			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
3			1-Methoxy-6,6-dimethyl-cyclohex-...	140	C9H16O	073741-66-9	59
4			1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
5			2-Methoxyresorcinol	140	C7H8O3	029267-67-2	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
Data File : VU045891.D
Acq On : 19 Nov 2021 13:48
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

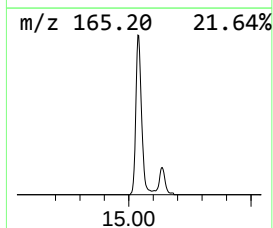
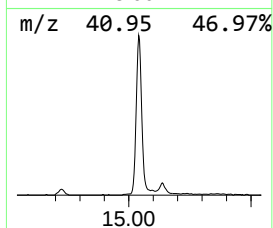
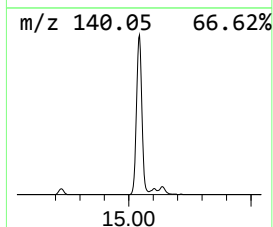
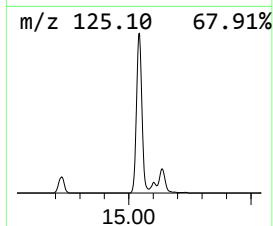
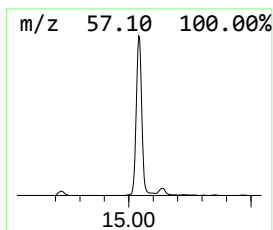
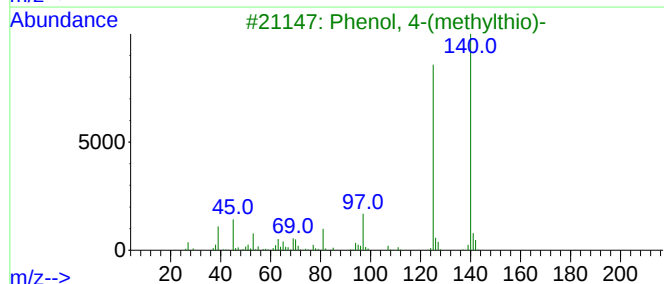
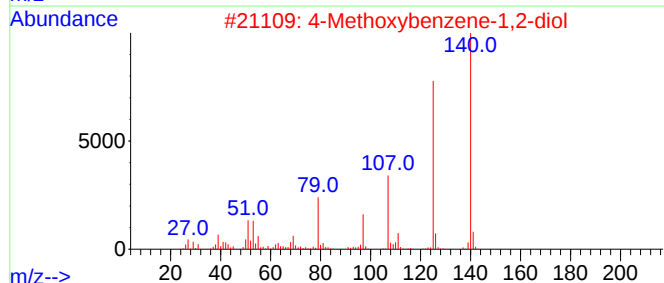
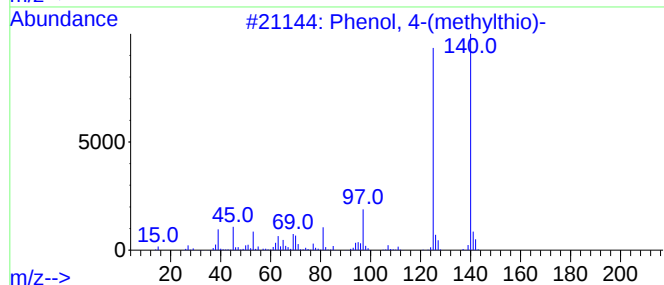
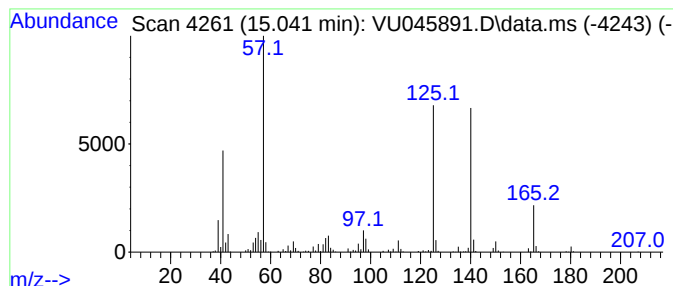
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Phenol, 4-(methylthio)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.041	7.81 ug/L	420864	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	52
2			4-Methoxybenzene-1,2-diol	140	C7H8O3	003934-97-2	52
3			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	52
4			Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	50
5			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
Data File : VU045891.D
Acq On : 19 Nov 2021 13:48
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

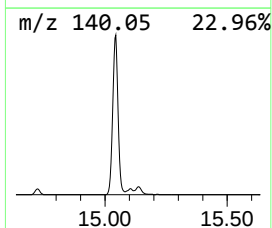
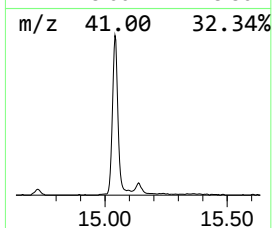
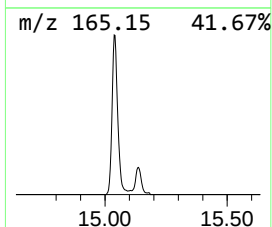
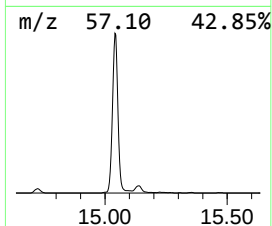
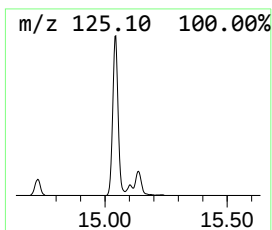
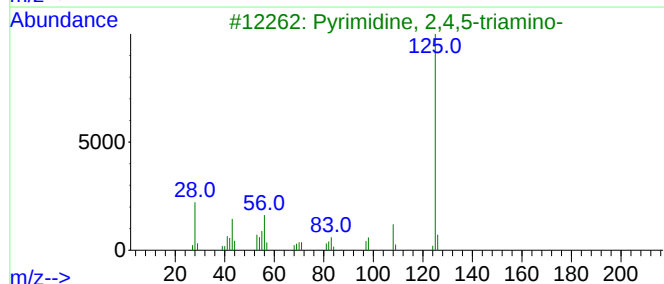
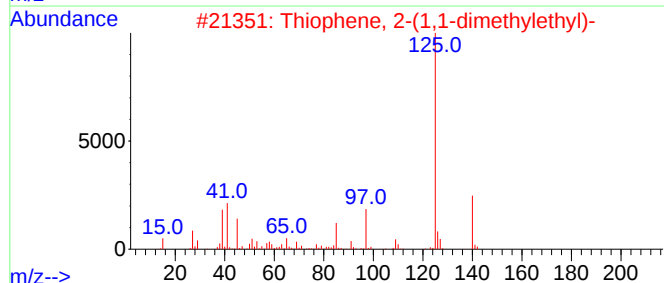
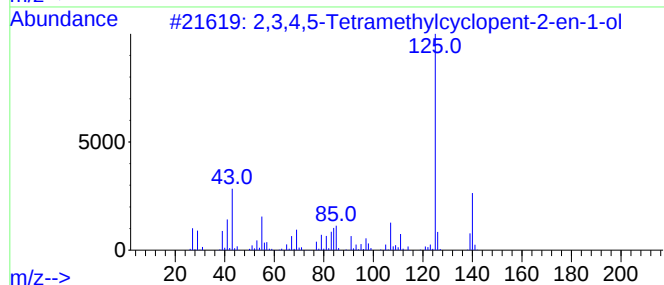
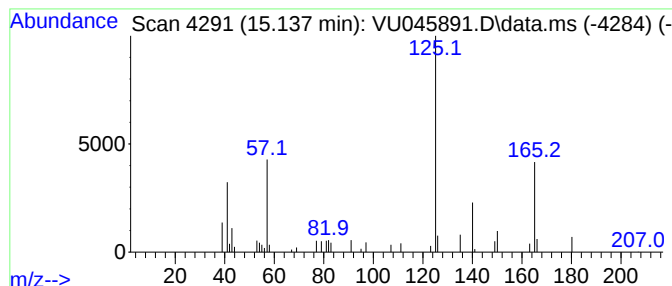
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 unknown-02 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.137	0.63 ug/L	33918	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3,4,5-Tetramethylcyclopent-2-e...	140	C9H16O	082061-20-9	43		
2	Thiophene, 2-(1,1-dimethylethyl)-	140	C8H12S	001689-78-7	25		
3	Pyrimidine, 2,4,5-triamino-	125	C4H7N5	003546-50-7	25		
4	2,4,6-Pyrimidinetriamine	125	C4H7N5	001004-38-2	25		
5	2,2,3,3-Tetramethylcyclopropanec...	232	C15H20O2	1000221-98-5	17		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
Data File : VU045891.D
Acq On : 19 Nov 2021 13:48
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

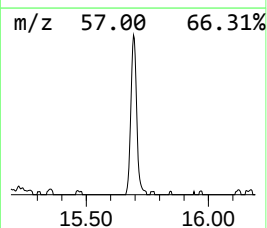
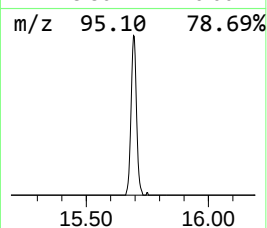
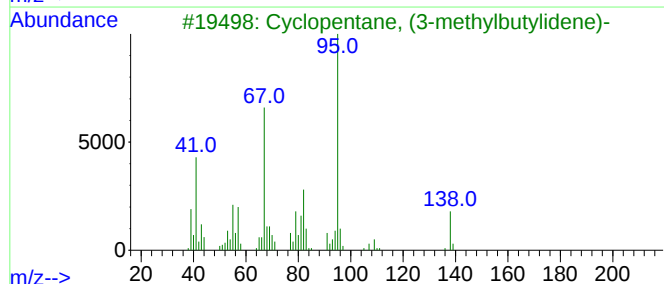
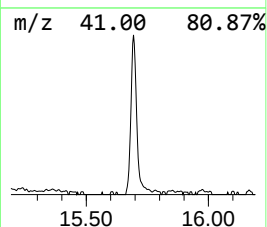
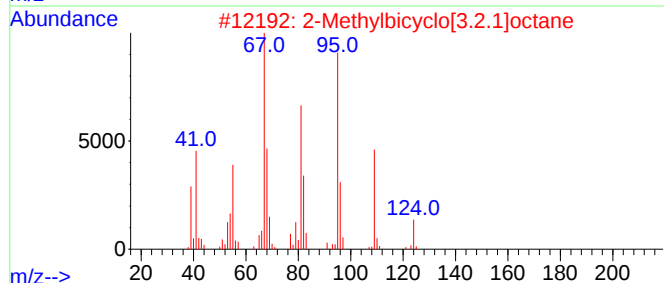
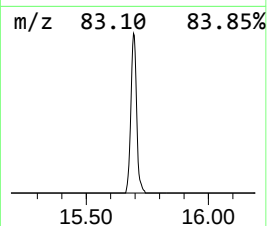
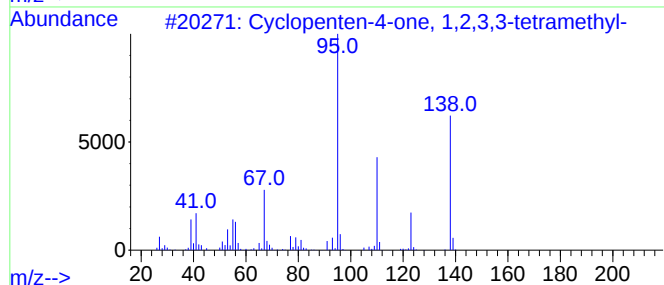
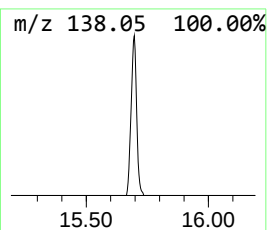
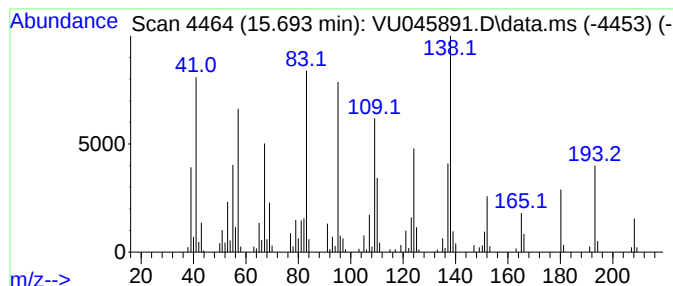
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 unknown-03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.693	3.15 ug/L	170031	1,4-Dichlorobenzene-d4	11.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopenten-4-one, 1,2,3,3-tetra...	138	C9H14O	1000163-38-6	38
2		2-Methylbicyclo[3.2.1]octane	124	C9H16	1010215-28-0	25
3		Cyclopentane, (3-methylbutylidene)-	138	C10H18	053366-51-1	25
4		Allyl 2,4-hexadienoate	152	C9H12O2	1000431-58-3	25
5		Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	20



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
Data File : VU045891.D
Acq On : 19 Nov 2021 13:48
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

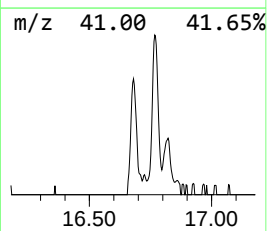
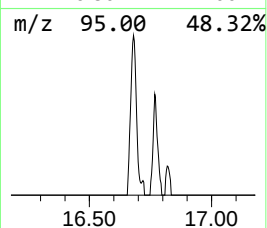
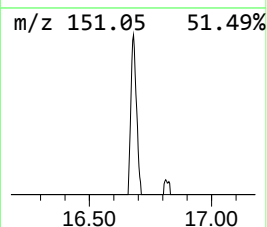
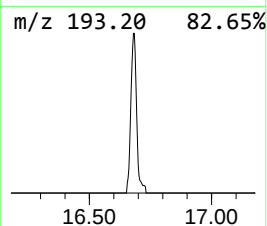
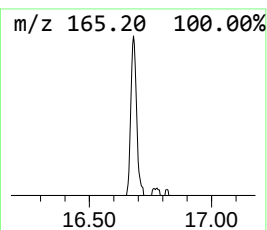
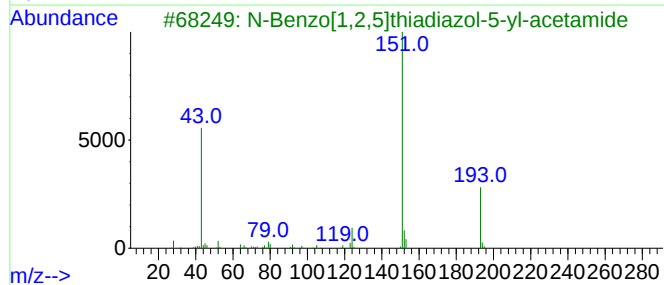
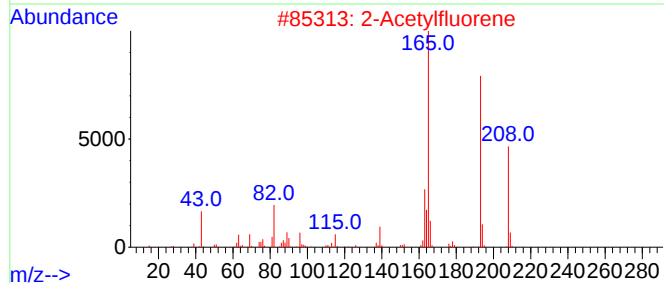
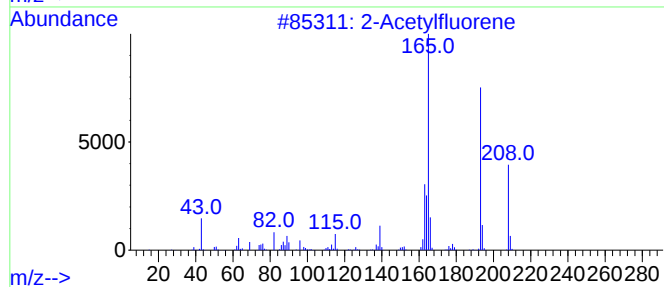
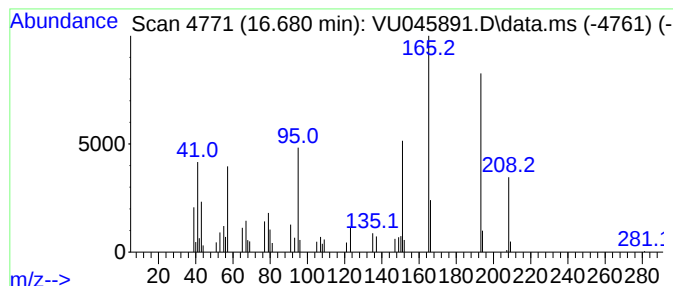
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2-Acetylfluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.680	0.65 ug/L	35172	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			2-Acetylfluorene	208	C15H12O	000781-73-7	49
3			N-Benzo[1,2,5]thiadiazol-5-yl-ac...	193	C8H7N3OS	021110-91-8	30
4			4',6'-Dimethoxy-2',3'-dimethylac...	208	C12H16O3	1010244-80-3	30
5			Anthracene, 9-methoxy-	208	C15H12O	002395-96-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
Data File : VU045891.D
Acq On : 19 Nov 2021 13:48
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AY5

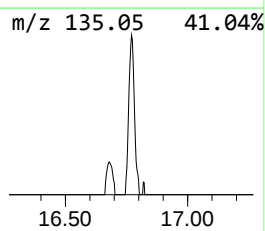
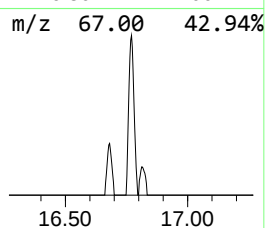
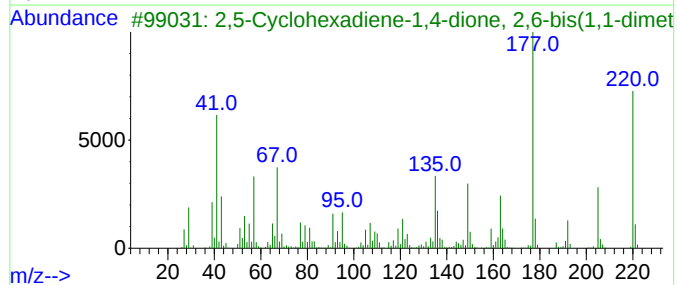
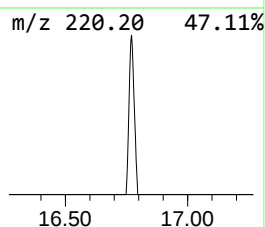
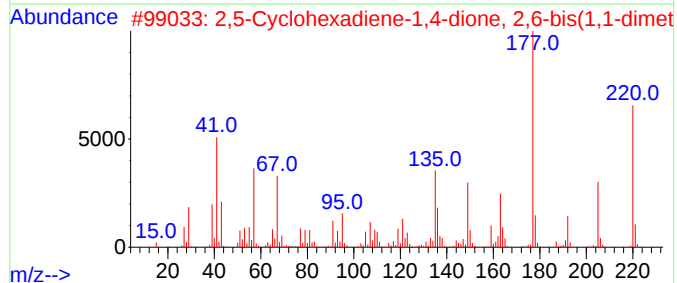
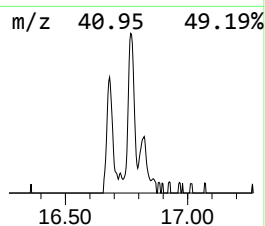
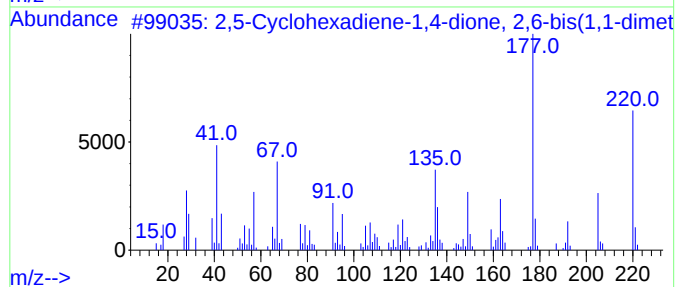
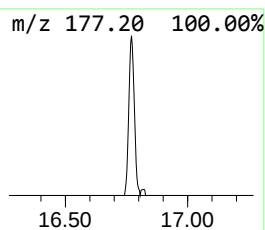
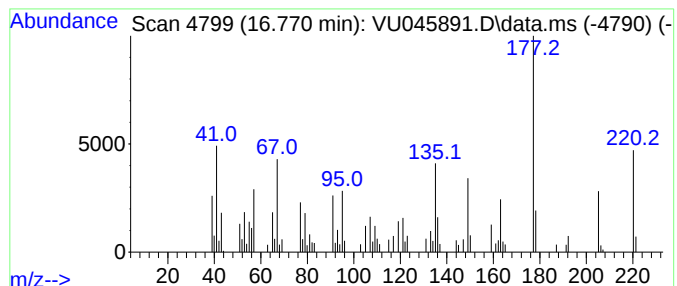
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.770	0.82 ug/L	44000	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	93
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	93
4			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	89
5			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111921\
Data File : VU045891.D
Acq On : 19 Nov 2021 13:48
Operator : SY/MD
Sample : M4755-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 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...	3.273	1.2	ug/L	53268	1	6.253	214784	5.0
Propane, 2-brom...	4.443	15.7	ug/L	673049	1	6.253	214784	5.0
3-Buten-2-one, ...	6.395	0.8	ug/L	35047	1	6.253	214784	5.0
unknown-01	7.131	9.4	ug/L	404935	1	6.253	214784	5.0
1-Hexanol, 2-et...	12.063	1.1	ug/L	60768	3	11.816	269546	5.0
Benzenethiol, 2...	14.317	0.7	ug/L	36073	3	11.816	269546	5.0
Phenol, 4-(meth...	15.041	7.8	ug/L	420864	3	11.816	269546	5.0
unknown-02	15.137	0.6	ug/L	33918	3	11.816	269546	5.0
unknown-03	15.693	3.1	ug/L	170031	3	11.816	269546	5.0
2-Acetylfluorene	16.680	0.7	ug/L	35172	3	11.816	269546	5.0
2,5-Cyclohexadi...	16.770	0.8	ug/L	44000	3	11.816	269546	5.0