

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
 Data File : VU044270.D
 Acq On : 30 Jun 2021 19:15
 Operator : SY/MD
 Sample : M2905-14
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBK37

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\SFAMUTR062121WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU044270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	73	82	89	rBV	59448	74901	11.16%	1.131%
2	1.919	173	180	196	rVB	54448	73235	10.91%	1.106%
3	2.575	369	384	400	rBV	105247	177109	26.39%	2.675%
4	3.363	618	629	641	rBV2	6298	11981	1.79%	0.181%
5	3.594	685	701	714	rBV4	3043	7569	1.13%	0.114%
6	4.459	956	970	990	rBV2	19012	49639	7.40%	0.750%
7	4.652	1013	1030	1064	rBV3	63330	243499	36.29%	3.678%
8	5.073	1145	1161	1180	rBV	102525	226092	33.69%	3.415%
9	5.732	1344	1366	1392	rBV2	204787	538085	80.19%	8.127%
10	6.256	1510	1529	1552	rBV	183715	350125	52.18%	5.288%
11	6.549	1607	1620	1635	rBV2	116475	222127	33.10%	3.355%
12	6.700	1652	1667	1686	rBV	130529	254775	37.97%	3.848%
13	7.571	1926	1938	1954	rBV	68327	123557	18.41%	1.866%
14	7.906	2028	2042	2056	rBV	266932	462347	68.90%	6.983%
15	8.185	2116	2129	2150	rBV2	44217	80711	12.03%	1.219%
16	8.642	2256	2271	2316	rBV	296075	671009	100.00%	10.135%
17	9.327	2475	2484	2492	rBV6	4670	7666	1.14%	0.116%
18	9.423	2501	2514	2528	rBV	259980	430018	64.09%	6.495%
19	9.497	2528	2537	2555	rVB2	18653	37690	5.62%	0.569%
20	9.684	2581	2595	2623	rVB4	15384	38245	5.70%	0.578%
21	9.828	2628	2640	2653	rVV	59720	106259	15.84%	1.605%
22	10.709	2904	2914	2921	rBV	21026	33175	4.94%	0.501%
23	10.764	2921	2931	2953	rVB	104328	175264	26.12%	2.647%
24	10.970	2985	2995	3004	rBV3	4521	8086	1.21%	0.122%
25	11.099	3027	3035	3045	rBV3	6481	9960	1.48%	0.150%
26	11.729	3218	3231	3242	rBV4	5882	13001	1.94%	0.196%
27	11.819	3247	3259	3265	rBV	298847	510152	76.03%	7.705%
28	11.983	3305	3310	3318	rVV4	4894	7170	1.07%	0.108%
29	12.047	3319	3330	3342	rVV2	52783	85730	12.78%	1.295%
30	12.102	3342	3347	3355	rVB2	4872	6851	1.02%	0.103%
31	12.198	3364	3377	3390	rBV	278197	454117	67.68%	6.859%
32	12.262	3390	3397	3408	rVB4	6083	11322	1.69%	0.171%
33	12.584	3487	3497	3506	rBV3	10426	16243	2.42%	0.245%
34	12.732	3533	3543	3548	rBV3	7674	12782	1.90%	0.193%
35	12.835	3562	3575	3584	rBV5	9964	20958	3.12%	0.317%
36	12.951	3597	3611	3616	rBV8	3832	7537	1.12%	0.114%

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37	13.015	3618	3631	3646	rVB	66736	111602	16.63%	1.686%
38	13.108	3646	3660	3676	rBV2	55569	90189	13.44%	1.362%
39	13.465	3761	3771	3774	rBV5	5530	8280	1.23%	0.125%
40	13.494	3774	3780	3788	rVV2	11274	16723	2.49%	0.253%
41	13.738	3849	3856	3864	rVB4	6852	10124	1.51%	0.153%
42	13.828	3875	3884	3893	rVV9	4254	7531	1.12%	0.114%
43	13.976	3914	3930	3940	rBV2	90023	163019	24.29%	2.462%
44	14.082	3955	3963	3975	rVB5	7794	14073	2.10%	0.213%
45	14.153	3977	3985	3992	rBV4	9057	14618	2.18%	0.221%
46	14.327	4025	4039	4047	rBV4	14019	25060	3.73%	0.379%
47	14.381	4048	4056	4064	rBV3	13023	20997	3.13%	0.317%
48	14.584	4111	4119	4131	rVB6	5127	8070	1.20%	0.122%
49	14.758	4165	4173	4179	rBV5	8742	12998	1.94%	0.196%
50	14.790	4179	4183	4194	rVB8	6572	10495	1.56%	0.159%
51	15.134	4283	4290	4293	rBV6	8156	11623	1.73%	0.176%
52	15.185	4297	4306	4317	rVB2	56609	99888	14.89%	1.509%
53	15.368	4354	4363	4367	rBV8	5433	9445	1.41%	0.143%
54	15.407	4368	4375	4383	rVV2	18450	30462	4.54%	0.460%
55	15.536	4407	4415	4419	rBV5	6752	9383	1.40%	0.142%
56	15.561	4421	4423	4438	rVB9	6709	11217	1.67%	0.169%
57	15.655	4442	4452	4459	rBV3	10317	19632	2.93%	0.297%
58	15.803	4491	4498	4509	rVV5	9689	17204	2.56%	0.260%
59	15.992	4547	4557	4570	rVB9	9557	18820	2.80%	0.284%
60	16.069	4573	4581	4586	rBV5	10455	16515	2.46%	0.249%
61	16.108	4587	4593	4603	rVB	14707	25820	3.85%	0.390%
62	16.201	4614	4622	4641	rVB5	33968	77297	11.52%	1.167%
63	16.394	4672	4682	4698	rVB5	32432	61941	9.23%	0.936%
64	16.671	4761	4768	4776	rBV8	6799	10986	1.64%	0.166%
65	16.822	4805	4815	4827	rVB7	12250	26885	4.01%	0.406%
66	16.947	4845	4854	4865	rVB9	5985	10330	1.54%	0.156%
67	17.018	4866	4876	4890	rBV2	44744	72209	10.76%	1.091%
68	17.442	5001	5008	5025	rVB10	9374	18388	2.74%	0.278%

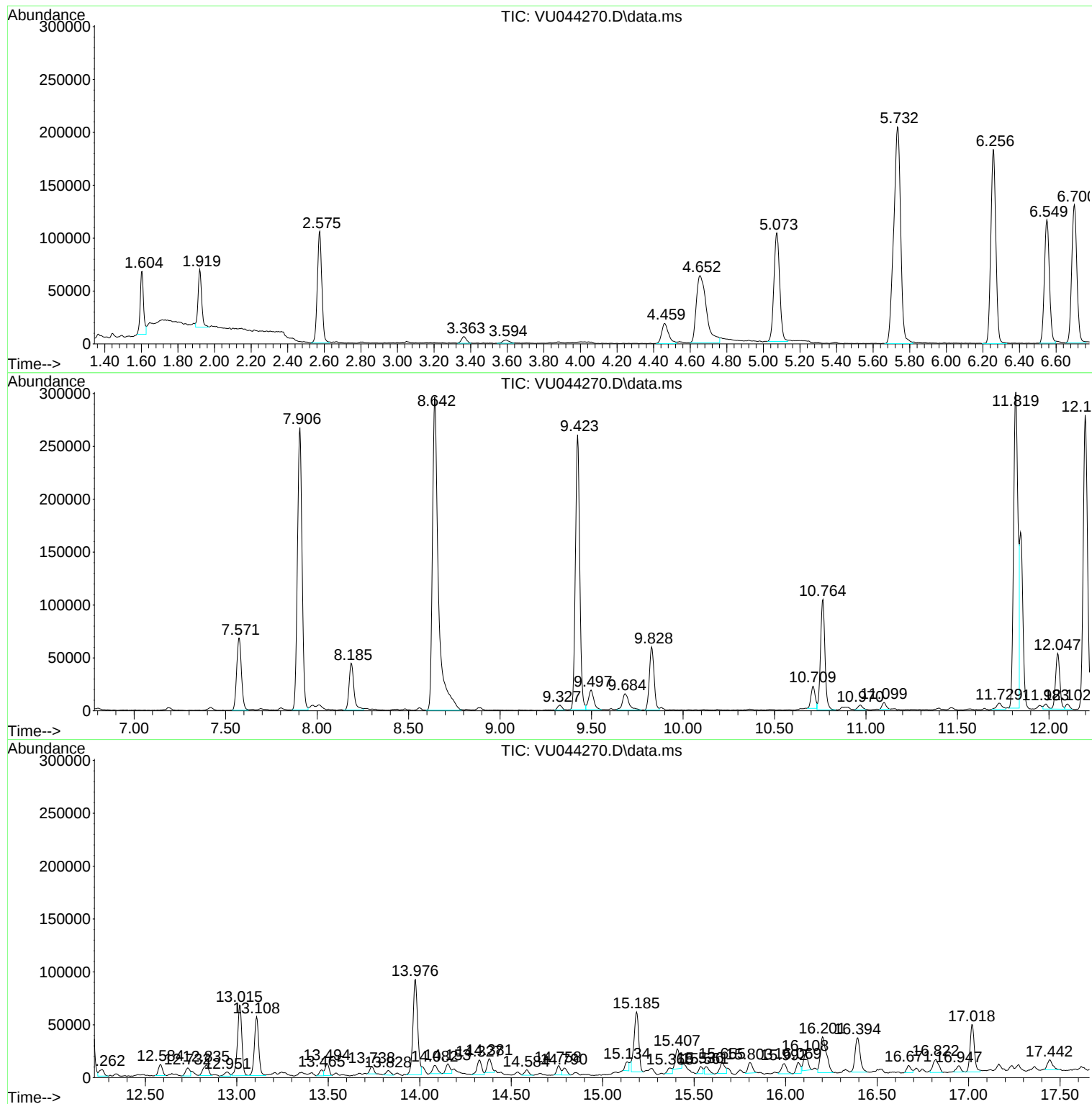
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DBK37

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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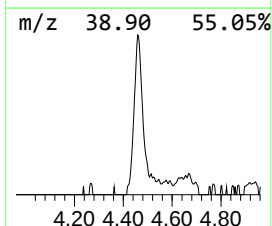
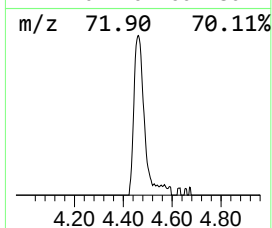
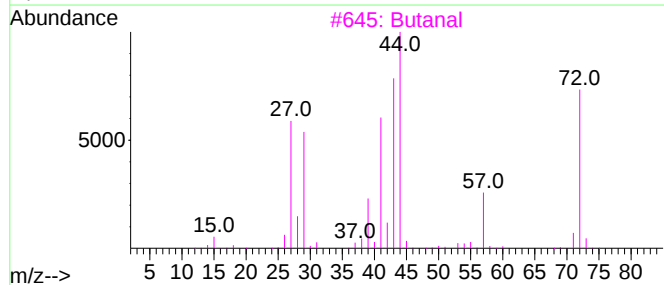
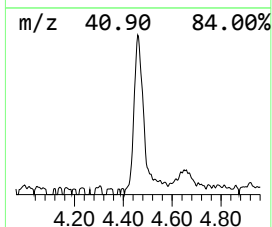
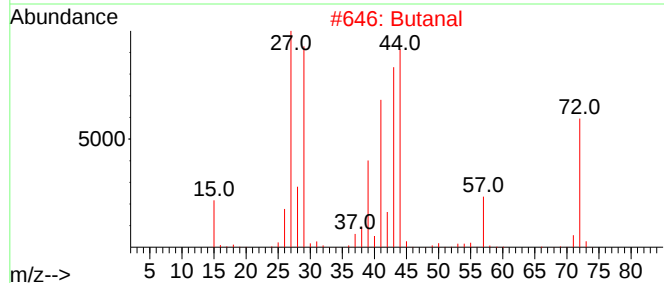
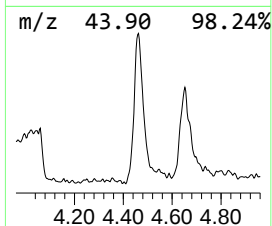
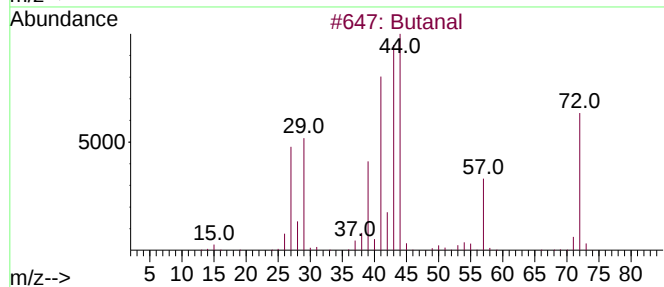
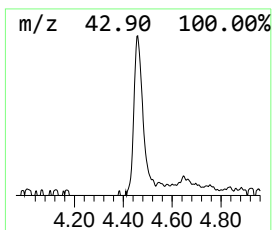
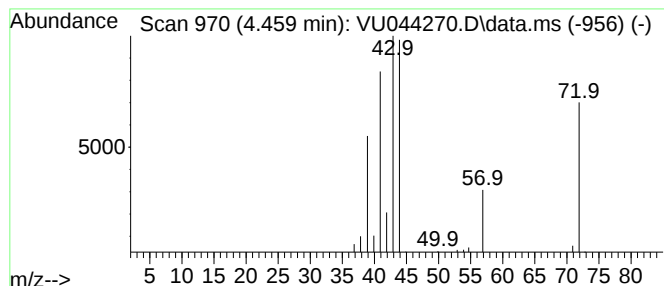
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.459	0.71 ug/L	49639	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Butanal	72	C4H8O	000123-72-8	91
3			Butanal	72	C4H8O	000123-72-8	50
4			Butanal	72	C4H8O	000123-72-8	50
5			Ethene, ethoxy-	72	C4H8O	000109-92-2	38



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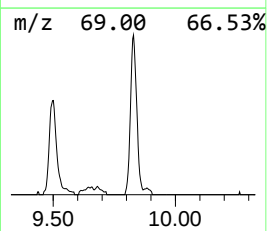
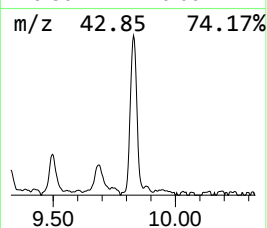
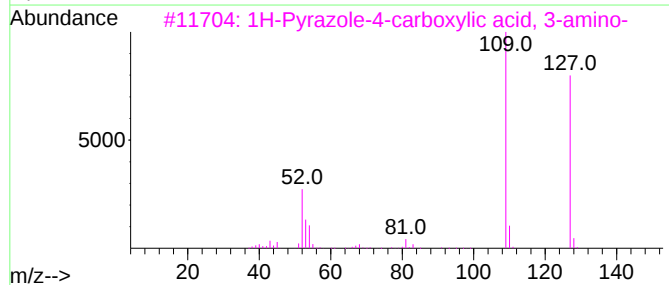
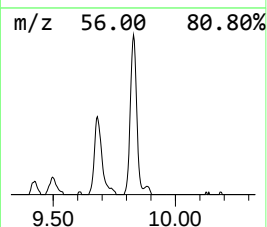
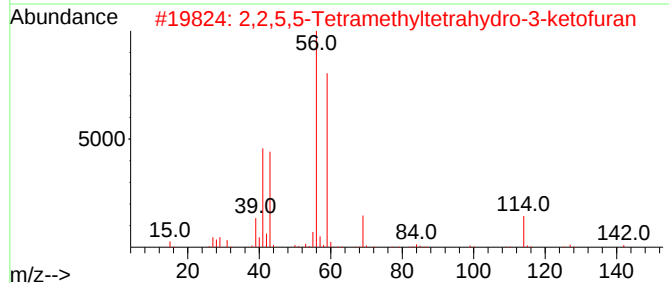
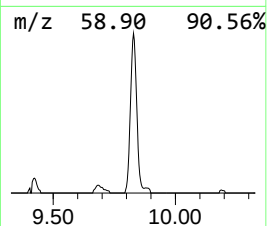
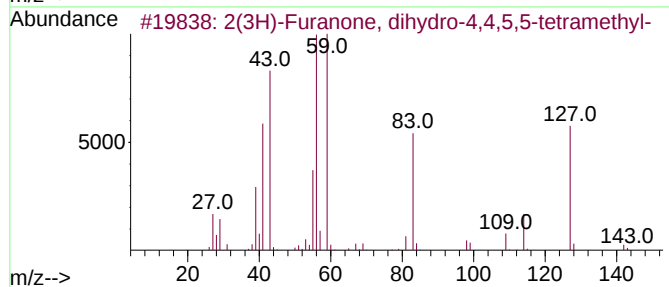
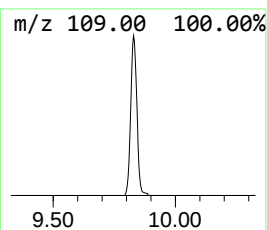
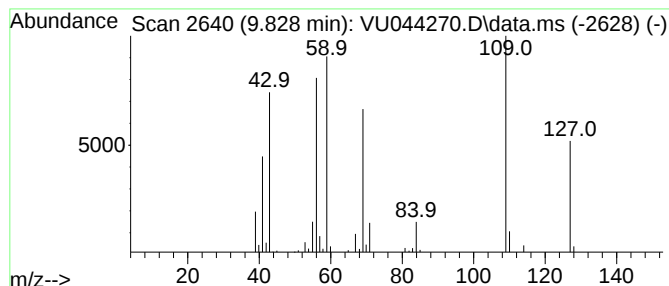
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.828	1.24 ug/L	106259	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-4,4,5,5-...	142	C8H14O2	016466-24-3	40		
2	2,2,5,5-Tetramethyltetrahydro-3-...	142	C8H14O2	005455-94-7	32		
3	1H-Pyrazole-4-carboxylic acid, 3-...	127	C4H5N3O2	041680-34-6	27		
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	14		
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	10		



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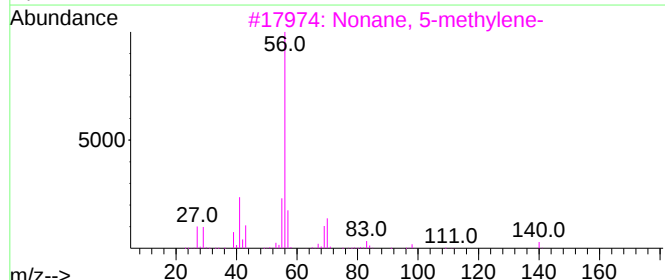
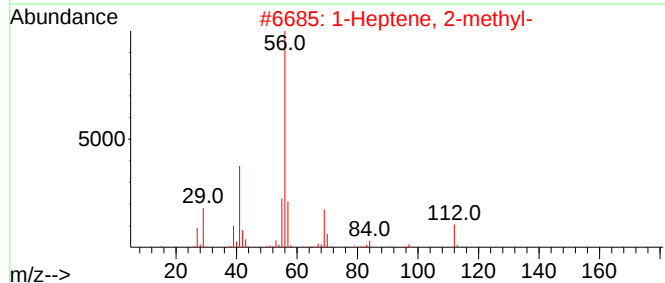
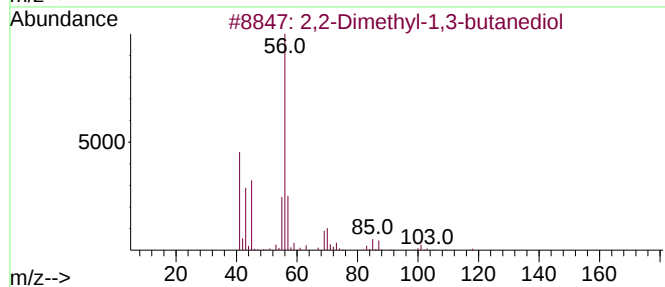
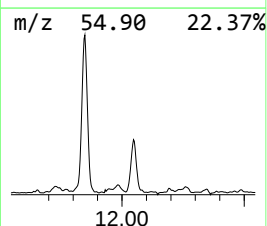
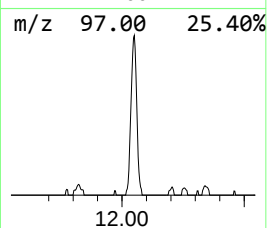
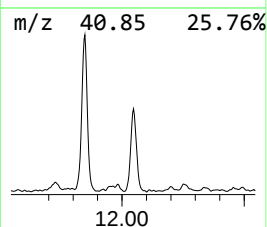
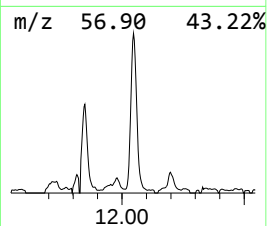
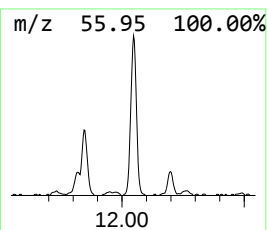
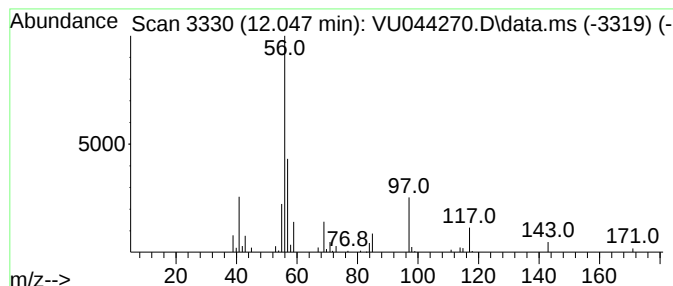
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,2-Dimethyl-1,3-butanediol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.047	0.84 ug/L	85730	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	50
2			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	33
3			Nonane, 5-methylene-	140	C10H20	006795-79-5	33
4			Ethyl isocyanoacetate	113	C5H7NO2	002999-46-4	28
5			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	28



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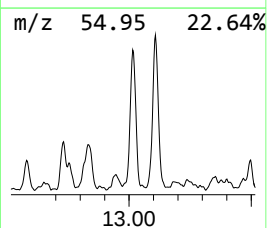
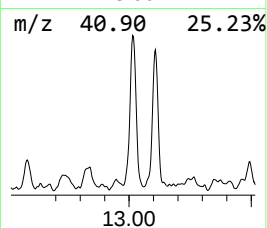
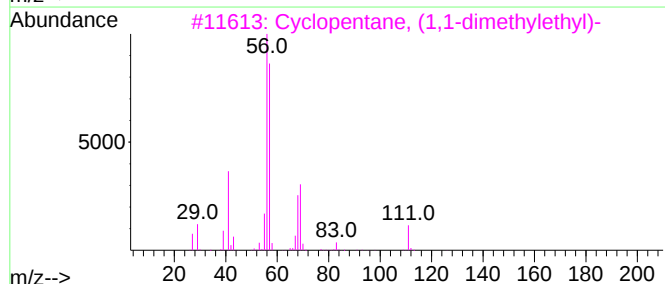
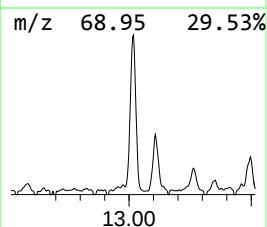
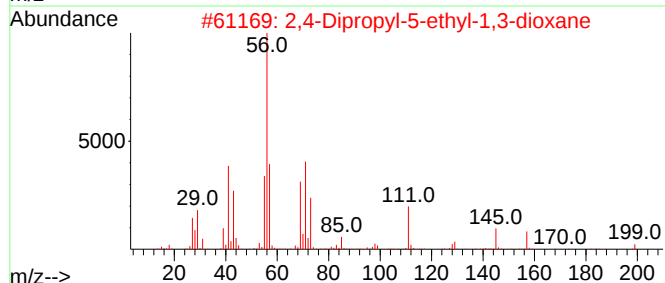
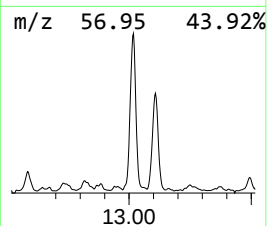
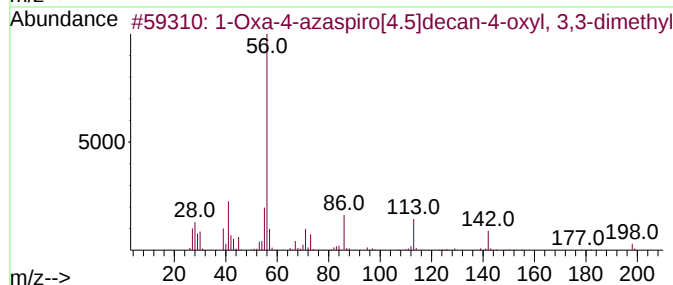
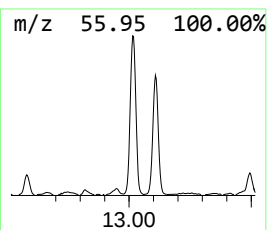
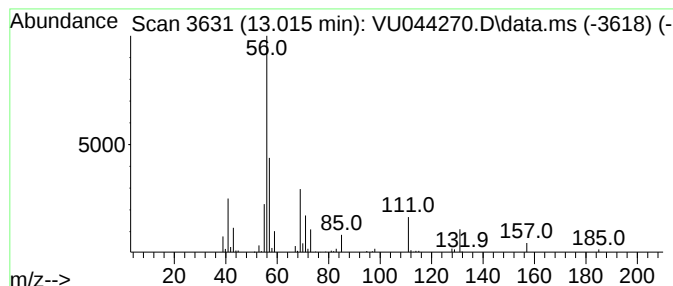
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Oxa-4-azaspiro[4.5]decan-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.015	1.09 ug/L	111602	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Oxa-4-azaspiro[4.5]decan-4-oxy...	198	C10H16NO3	1000115-84-0	50
2			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	43
3			Cyclopentane, (1,1-dimethylethyl)-	126	C9H18	003875-52-3	38
4			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
Data File : VU044270.D
Acq On : 30 Jun 2021 19:15
Operator : SY/MD
Sample : M2905-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK37

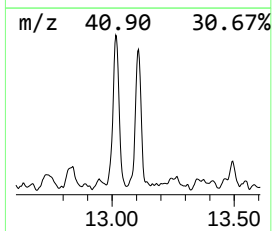
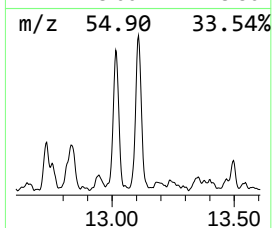
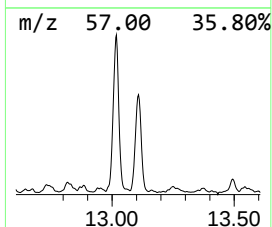
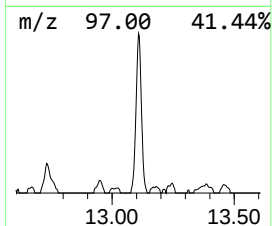
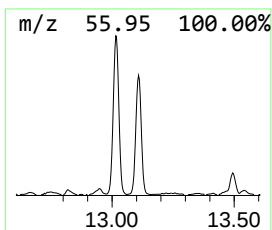
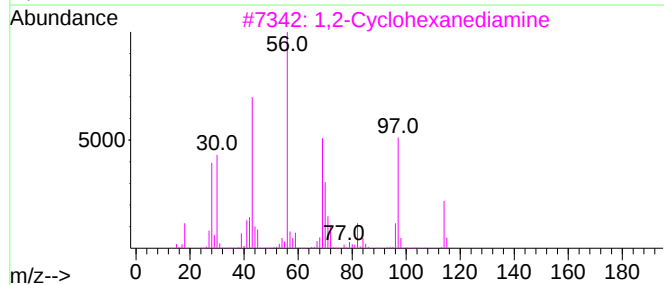
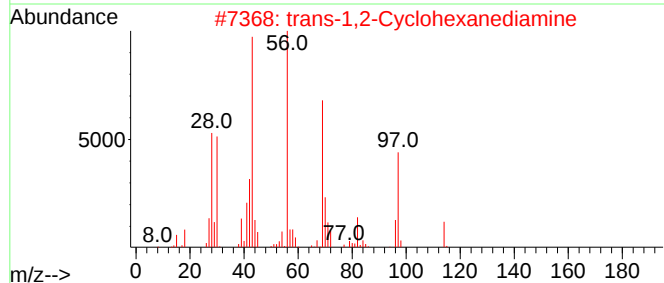
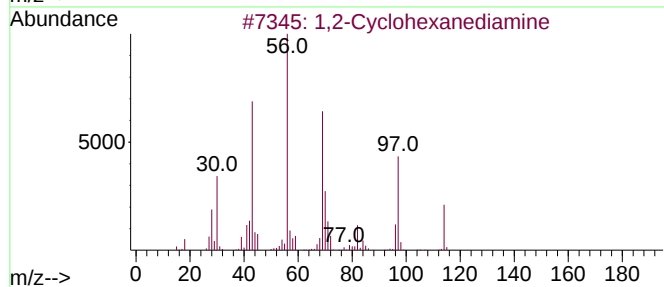
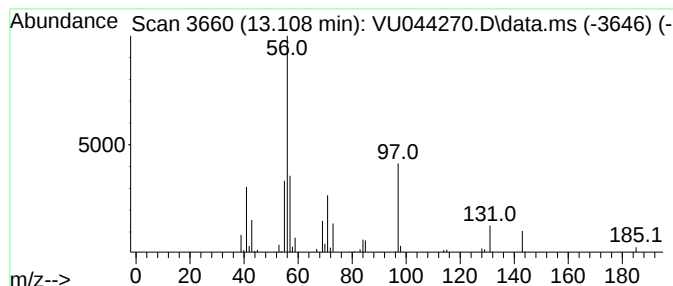
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.108	0.88 ug/L	90189	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Cyclohexanediamine	114	C6H14N2	000694-83-7	38
2			trans-1,2-Cyclohexanediamine	114	C6H14N2	001121-22-8	38
3			1,2-Cyclohexanediamine	114	C6H14N2	000694-83-7	38
4			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
Data File : VU044270.D
Acq On : 30 Jun 2021 19:15
Operator : SY/MD
Sample : M2905-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK37

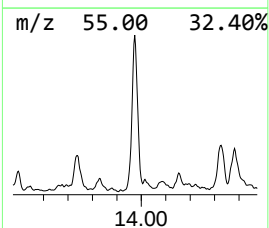
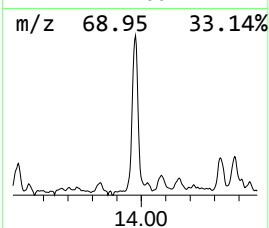
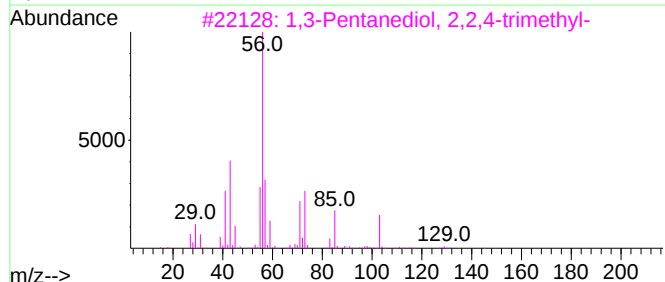
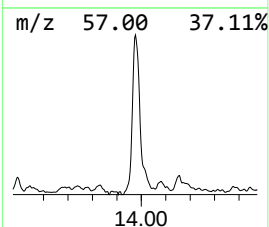
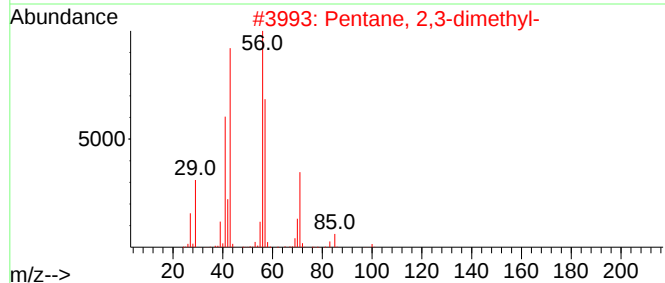
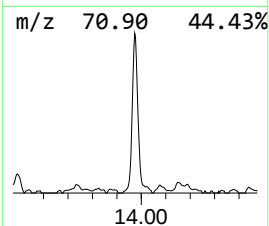
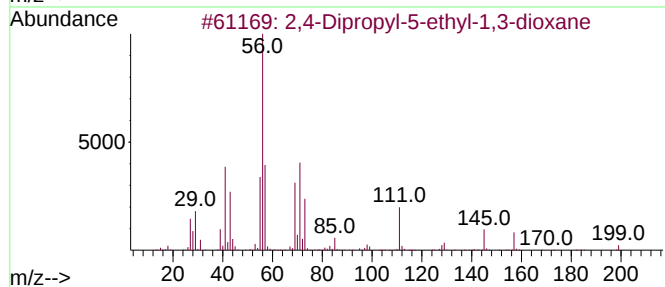
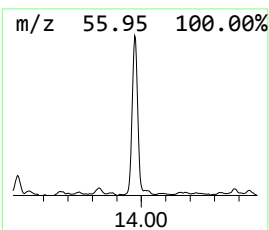
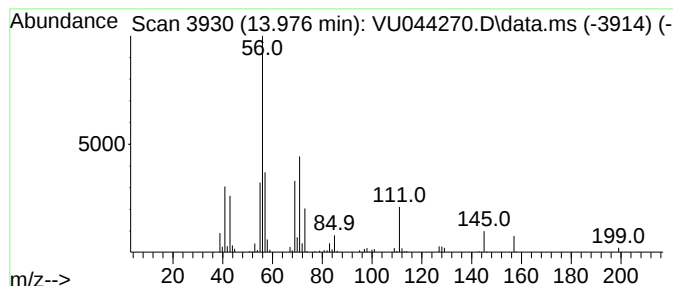
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.976	1.60 ug/L	163019	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	47		
2	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	33		
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	28		
4	Cyclobutane, 1,2,3,4-tetramethyl-	112	C8H16	069531-57-3	27		
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
Data File : VU044270.D
Acq On : 30 Jun 2021 19:15
Operator : SY/MD
Sample : M2905-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK37

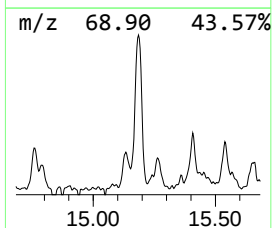
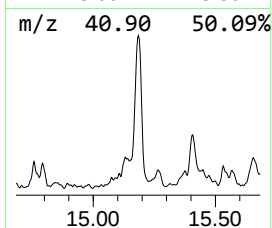
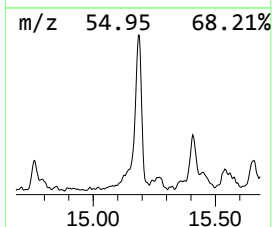
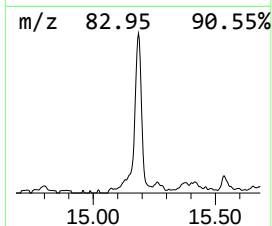
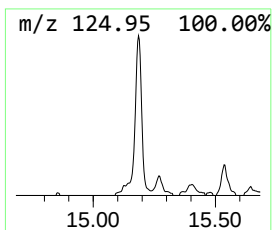
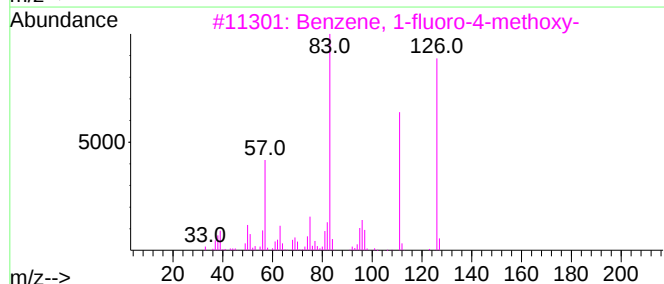
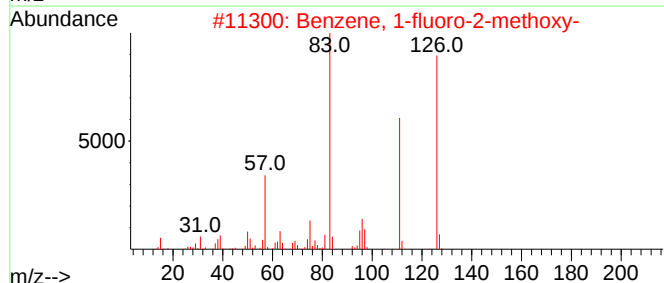
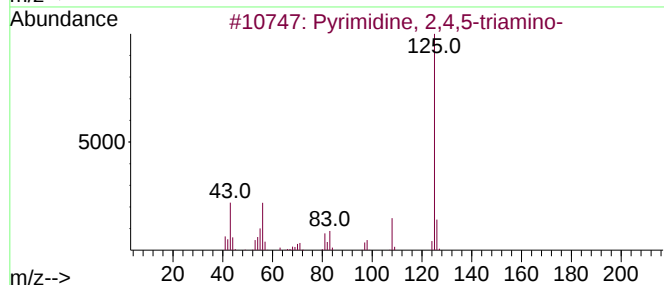
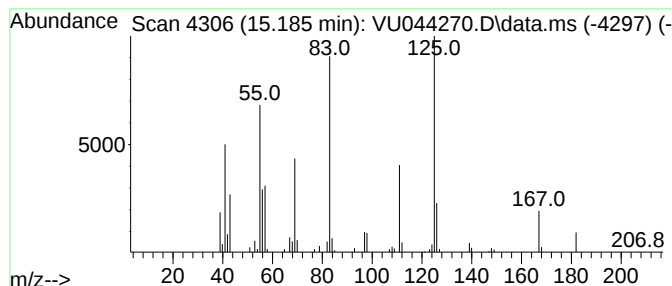
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown-04 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.185	0.98 ug/L	99888	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrimidine, 2,4,5-triamino-	125	C4H7N5	003546-50-7	38
2			Benzene, 1-fluoro-2-methoxy-	126	C7H7FO	000321-28-8	38
3			Benzene, 1-fluoro-4-methoxy-	126	C7H7FO	000459-60-9	38
4			3-Amino-2-cyclohexenone	111	C6H9NO	005220-49-5	30
5			5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
Data File : VU044270.D
Acq On : 30 Jun 2021 19:15
Operator : SY/MD
Sample : M2905-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK37

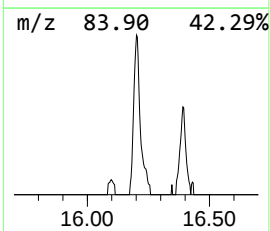
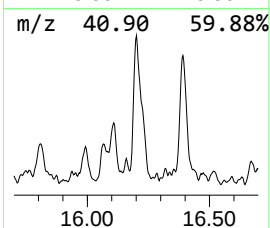
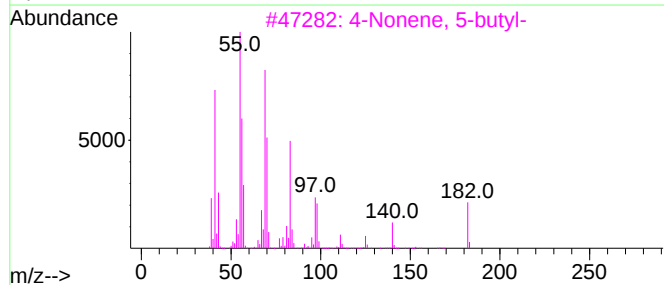
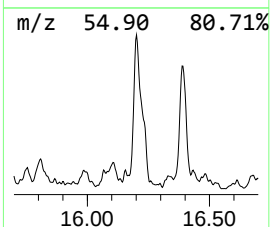
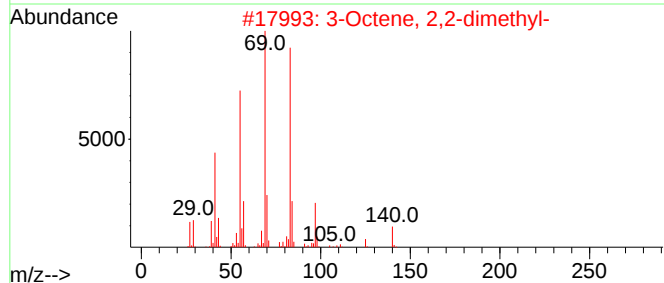
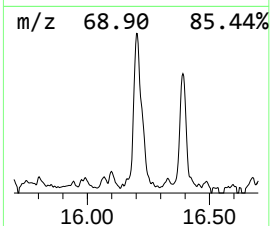
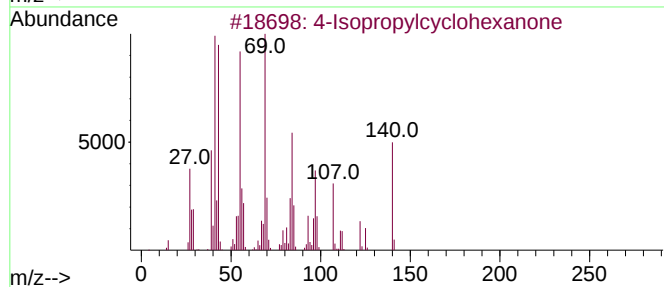
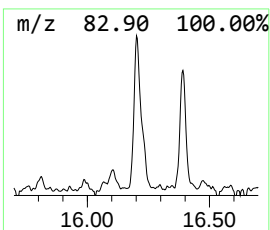
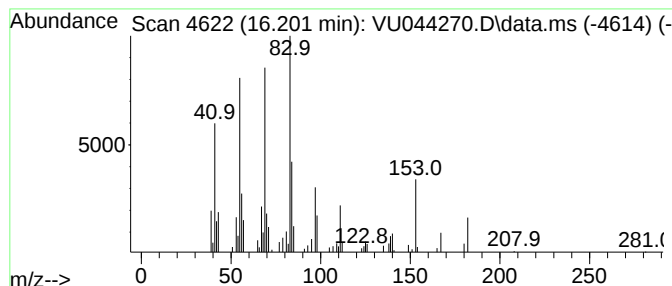
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 4-Isopropylcyclohexanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.201	0.76 ug/L	77297	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Isopropylcyclohexanone	140	C9H16O	005432-85-9	55
2			3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	52
3			4-Nonene, 5-butyl-	182	C13H26	007367-38-6	46
4			Cyclobutanecarboxylic acid, 6-et...	240	C15H28O2	1000282-61-1	43
5			2-Pentene, 3-methyl-	84	C6H12	000922-61-2	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
Data File : VU044270.D
Acq On : 30 Jun 2021 19:15
Operator : SY/MD
Sample : M2905-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK37

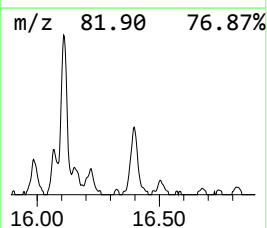
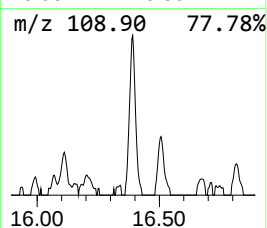
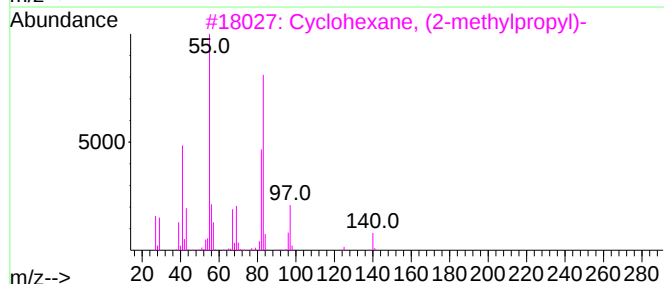
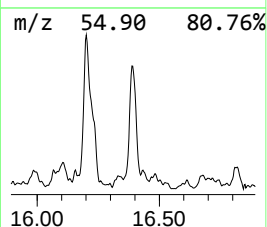
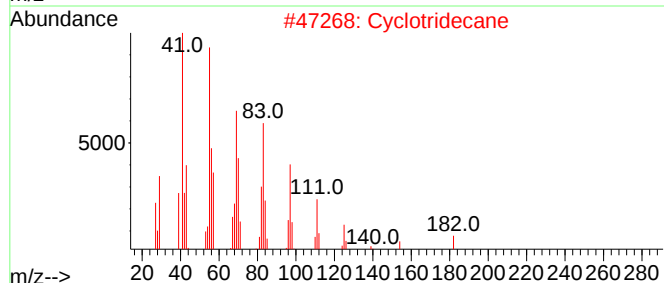
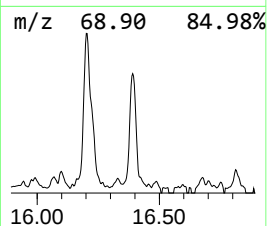
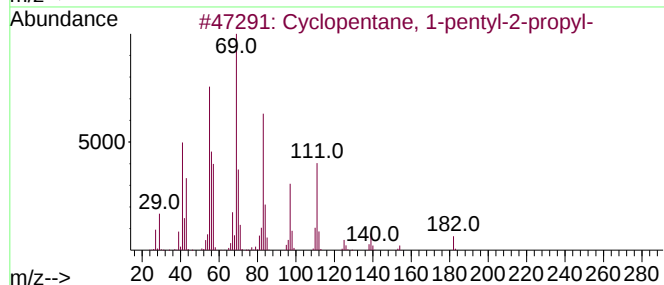
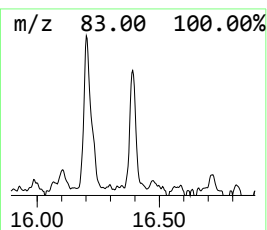
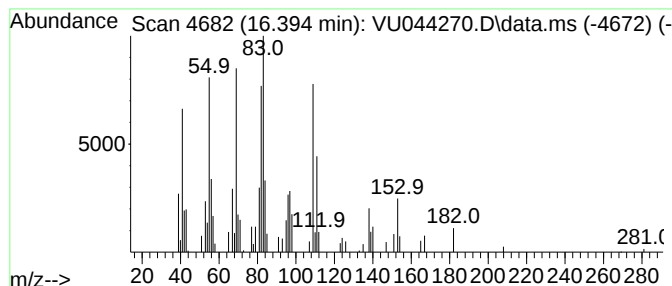
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 (DEL) Alkane: Cyclic16.394 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.394	0.61 ug/L	61941	1,4-Dichlorobenzene-d4	11.819

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	38
2		Cyclotridecane	182	C13H26	000295-02-3	30
3		Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	30
4		Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	25
5		Cyclopentane, (2-methylpropyl)-	126	C9H18	003788-32-7	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
Data File : VU044270.D
Acq On : 30 Jun 2021 19:15
Operator : SY/MD
Sample : M2905-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK37

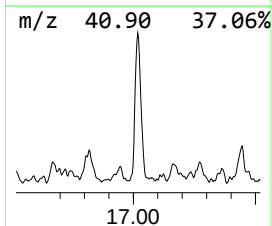
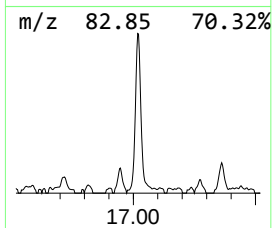
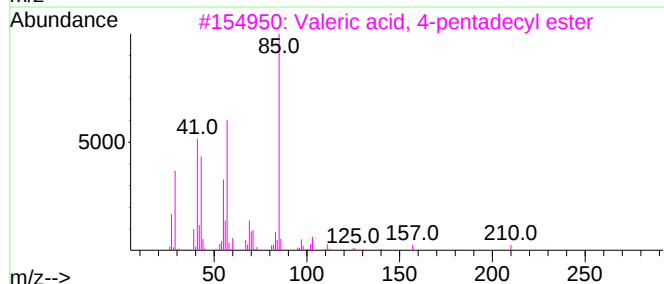
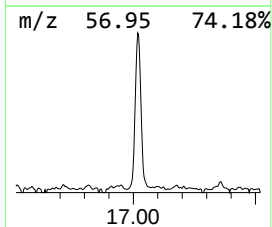
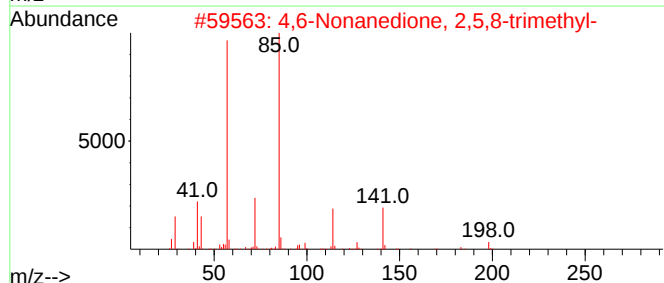
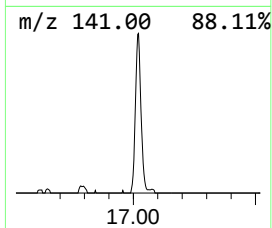
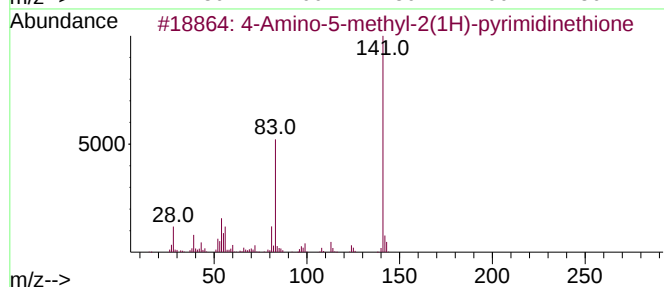
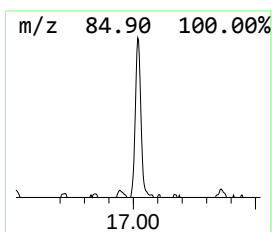
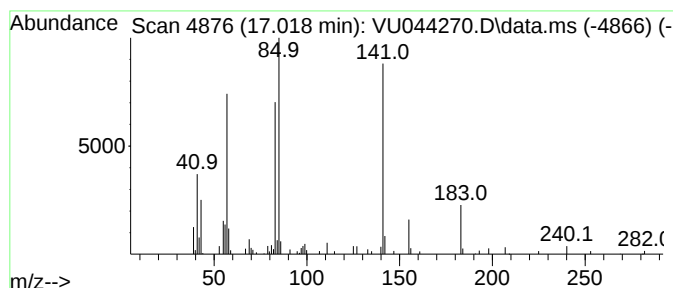
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown-05 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.018	0.71 ug/L	72209	1,4-Dichlorobenzene-d4	11.819

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Amino-5-methyl-2(1H)-pyrimidin...	141	C5H7N3S	007390-56-9	35
2		4,6-Nonanedione, 2,5,8-trimethyl-	198	C12H22O2	1000162-14-3	30
3		Valeric acid, 4-pentadecyl ester	312	C20H40O2	1000281-99-4	27
4		Sulfurous acid, butyl isohexyl e...	222	C10H22O3S	1000309-17-2	27
5		trans-2-Hexenyl valerate	184	C11H20O2	056922-74-8	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU063021\
Data File : VU044270.D
Acq On : 30 Jun 2021 19:15
Operator : SY/MD
Sample : M2905-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK37

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown-01	9.828	1.2	ug/L	106259	2	9.423	430018	5.0
2,2-Dimethyl-1,...	12.047	0.8	ug/L	85730	3	11.819	510152	5.0
1-Oxa-4-azaspir...	13.015	1.1	ug/L	111602	3	11.819	510152	5.0
unknown-02	13.108	0.9	ug/L	90189	3	11.819	510152	5.0
unknown-03	13.976	1.6	ug/L	163019	3	11.819	510152	5.0
unknown-04	15.185	1.0	ug/L	99888	3	11.819	510152	5.0
4-Isopropylcycl...	16.201	0.8	ug/L	77297	3	11.819	510152	5.0
(DEL) Alkane: C...	16.394	0.6	ug/L	61941	3	11.819	510152	5.0
unknown-05	17.018	0.7	ug/L	72209	3	11.819	510152	5.0