

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021022\
 Data File : VV024584.D
 Acq On : 10 Feb 2022 21:33
 Operator : SY/MD
 Sample : N1475-02
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F4M04

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_V\Method\SFAMVTR020922WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV024584.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	52	64	67	rBV4	3739	7209	1.62%	0.151%
2	1.307	73	83	95	rVB2	84320	98645	22.16%	2.065%
3	1.577	159	167	180	rBV	69985	79927	17.95%	1.673%
4	2.114	324	334	348	rBV	131789	183519	41.22%	3.842%
5	3.966	899	910	912	rBV6	15947	24016	5.39%	0.503%
6	4.359	1015	1032	1053	rVB2	79550	193758	43.52%	4.056%
7	5.056	1233	1249	1275	rBV2	197536	445195	100.00%	9.319%
8	5.635	1403	1429	1456	rBV	138936	287599	64.60%	6.020%
9	6.088	1548	1570	1587	rBV	105766	217945	48.95%	4.562%
10	6.606	1716	1731	1755	rBV3	26518	59114	13.28%	1.237%
11	6.998	1843	1853	1872	rBV	53575	99251	22.29%	2.078%
12	7.323	1938	1954	1973	rBV	229806	405551	91.10%	8.489%
13	7.403	1973	1979	1987	rVB	4513	7099	1.59%	0.149%
14	7.500	2002	2009	2020	rBV6	2644	4933	1.11%	0.103%
15	7.632	2040	2050	2064	rBV	30641	53573	12.03%	1.121%
16	7.950	2138	2149	2161	rBV5	4579	9593	2.15%	0.201%
17	8.104	2188	2197	2242	rBV	180587	407091	91.44%	8.522%
18	8.857	2415	2431	2463	rBV	222966	373393	83.87%	7.816%
19	9.104	2500	2508	2519	rVB	16745	26428	5.94%	0.553%
20	9.236	2536	2549	2560	rBV8	4008	9310	2.09%	0.195%
21	9.390	2583	2597	2607	rBV	11867	20309	4.56%	0.425%
22	9.821	2723	2731	2744	rBV7	2381	4927	1.11%	0.103%
23	10.149	2828	2833	2841	rVV8	4311	6438	1.45%	0.135%
24	10.217	2844	2854	2870	rVB	64412	100803	22.64%	2.110%
25	10.435	2914	2922	2934	rBV2	5439	9487	2.13%	0.199%
26	10.513	2934	2946	2956	rBV7	4487	8321	1.87%	0.174%
27	11.156	3135	3146	3155	rBV8	4233	7086	1.59%	0.148%
28	11.249	3164	3175	3194	rVB	248771	384822	86.44%	8.055%
29	11.529	3251	3262	3281	rBV	225538	406850	91.39%	8.517%
30	11.625	3282	3292	3315	rVB	202199	333923	75.01%	6.990%
31	11.776	3331	3339	3348	rBV	9506	14014	3.15%	0.293%
32	12.345	3507	3516	3525	rBV6	6022	9234	2.07%	0.193%
33	13.066	3733	3740	3750	rVB6	3453	5404	1.21%	0.113%
34	13.432	3847	3854	3864	rBV6	3699	5918	1.33%	0.124%
35	13.631	3905	3916	3932	rBV	105320	158187	35.53%	3.311%
36	13.754	3942	3954	3965	rVB6	3870	6890	1.55%	0.144%

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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_V\Method\SFAMVTR020922WMA.M
 Title : TRACE VOA SFAM1.0

37	14.098	4050	4061	4071	rVB5	3305	6833	1.53%	0.143%
38	14.435	4153	4166	4186	rBV5	7235	17583	3.95%	0.368%
39	14.721	4247	4255	4264	rVB4	5089	7154	1.61%	0.150%
40	14.889	4298	4307	4314	rBV2	6567	8544	1.92%	0.179%
41	14.979	4327	4335	4341	rBV5	5821	8150	1.83%	0.171%
42	15.024	4341	4349	4358	rVV6	6680	10894	2.45%	0.228%
43	15.114	4369	4377	4387	rVB7	9590	15120	3.40%	0.317%
44	15.561	4507	4516	4528	rBV2	34442	50617	11.37%	1.060%
45	15.770	4574	4581	4590	rVB4	5841	7335	1.65%	0.154%
46	16.181	4696	4709	4719	rBV8	12588	20384	4.58%	0.427%
47	16.307	4735	4748	4759	rBV	101116	148760	33.41%	3.114%

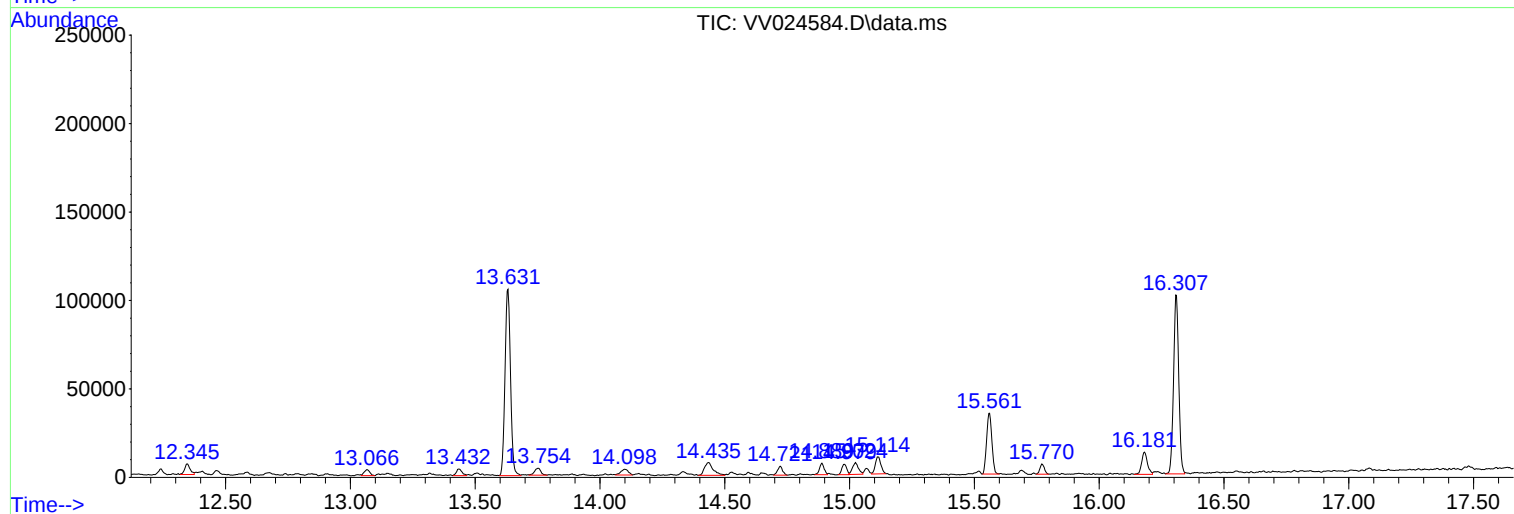
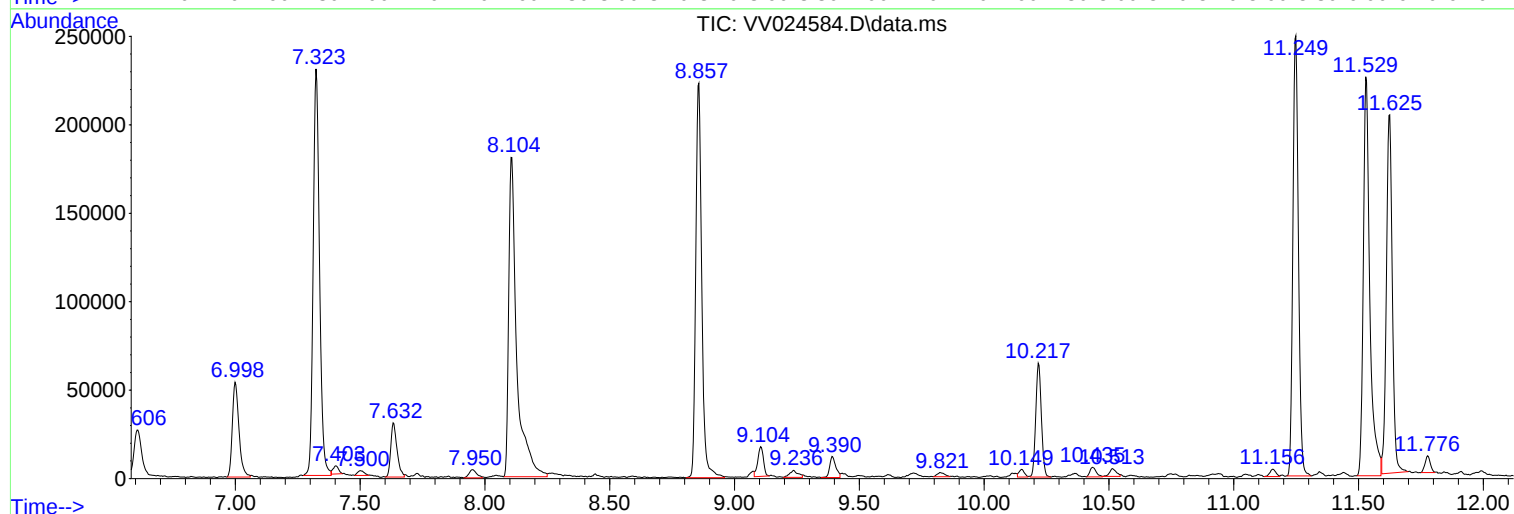
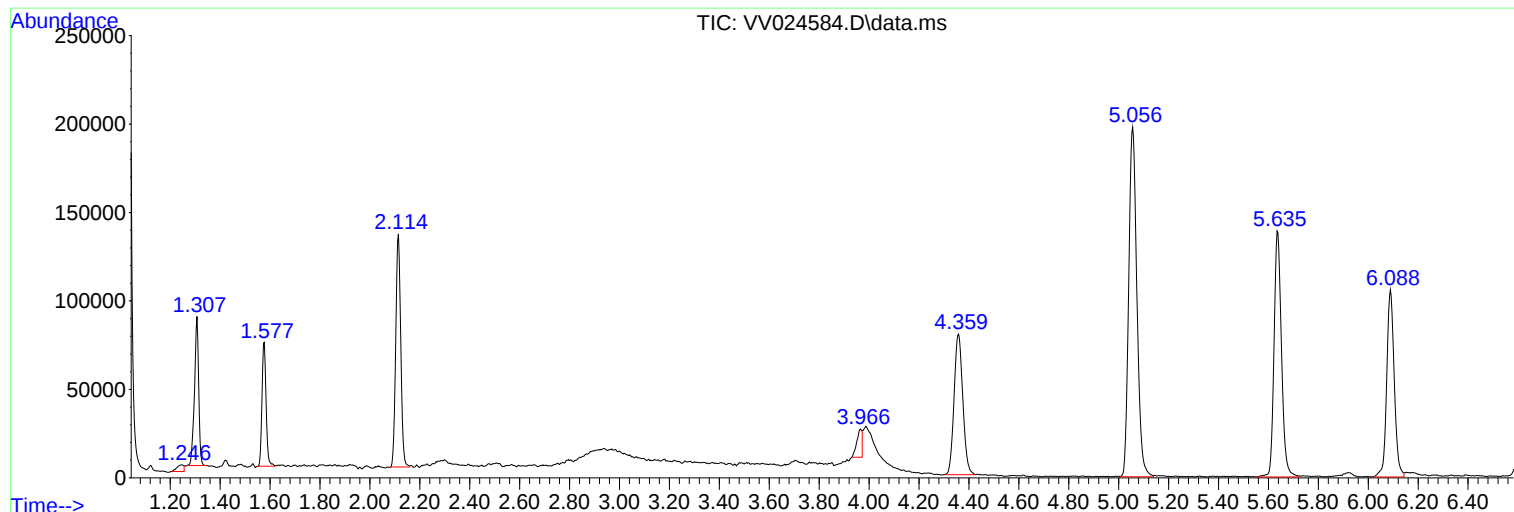
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020922WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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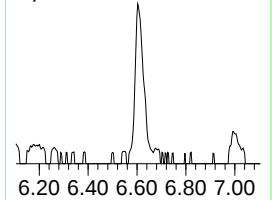
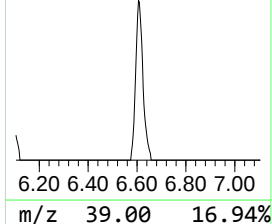
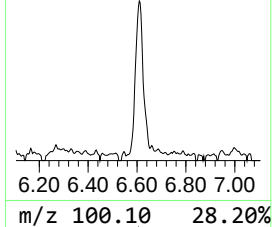
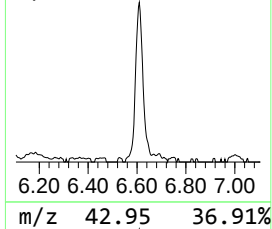
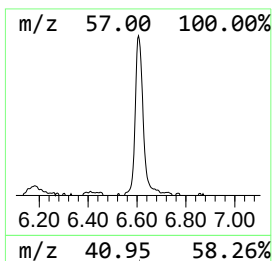
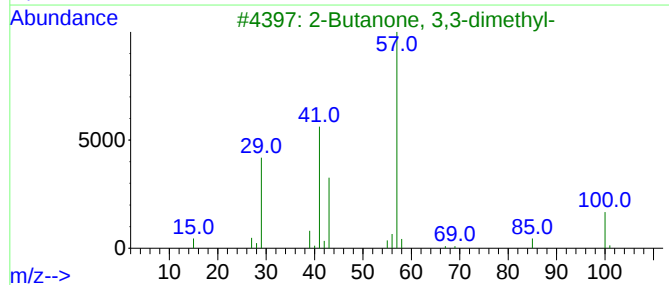
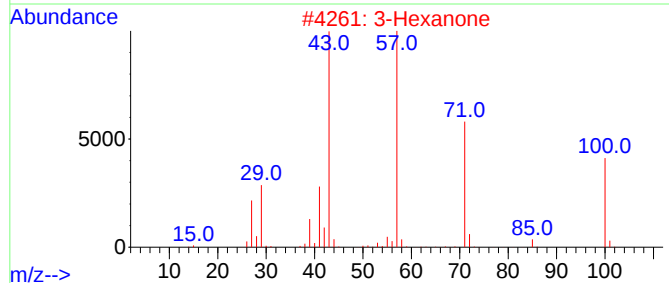
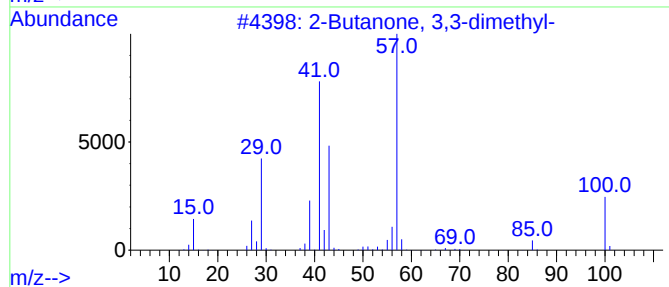
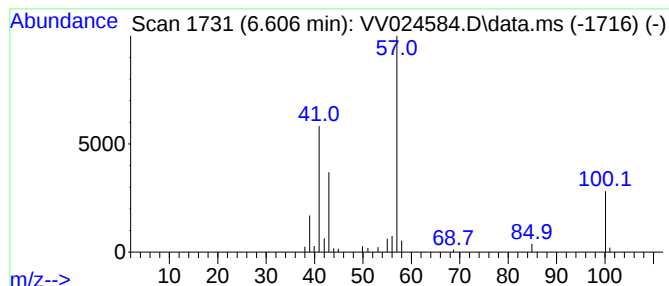
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.606	1.03 ug/L	59114	1,4-Difluorobenzene	5.635

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72	
2	3-Hexanone	100	C6H12O	000589-38-8	72	
3	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64	
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59	
5	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59	



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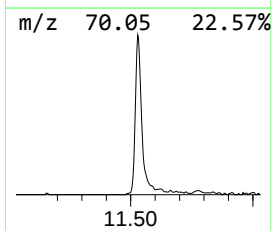
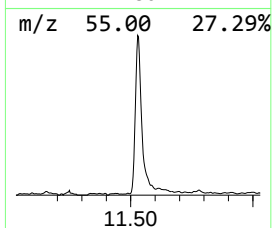
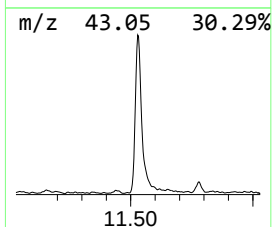
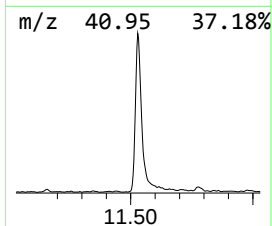
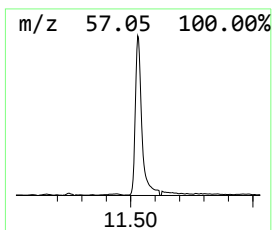
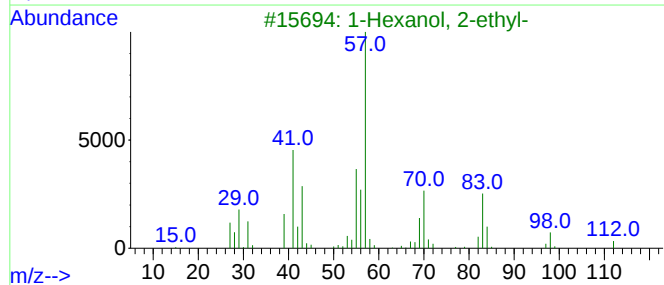
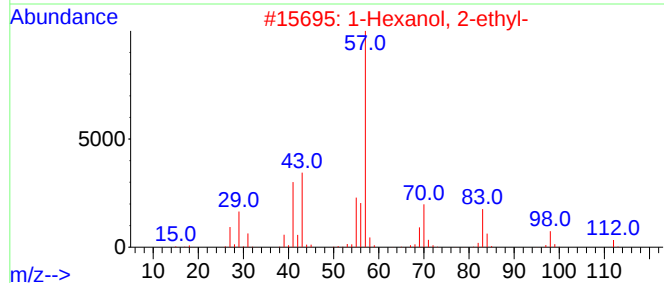
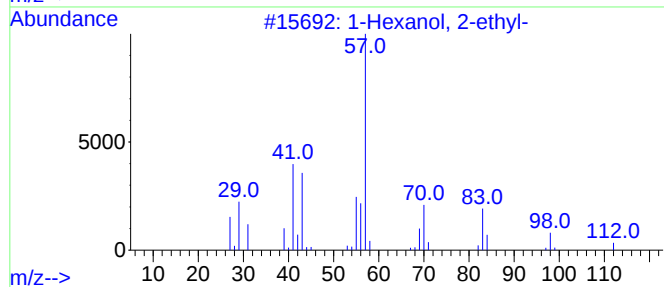
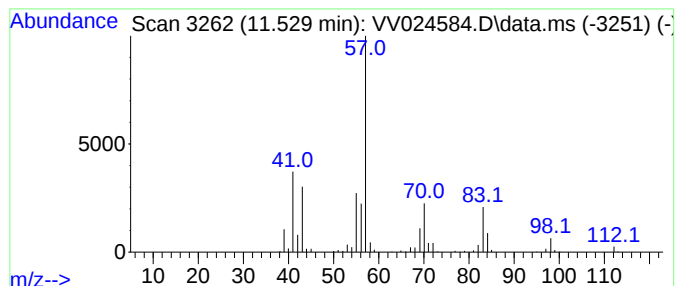
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	5.29 ug/L	406850	1,4-Dichlorobenzene-d4	11.249

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	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59



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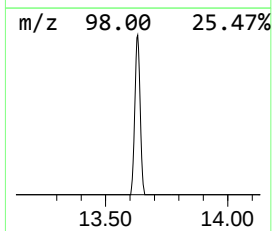
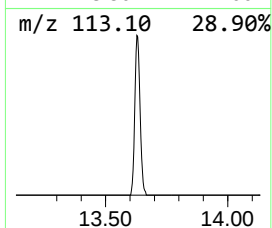
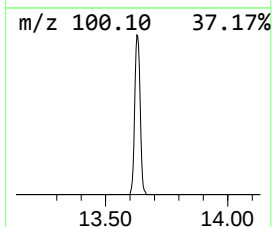
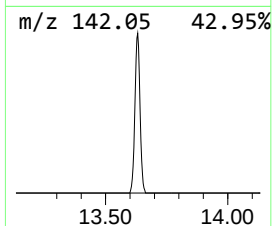
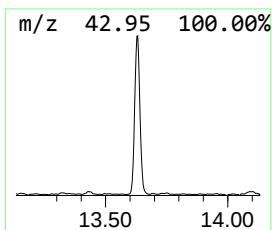
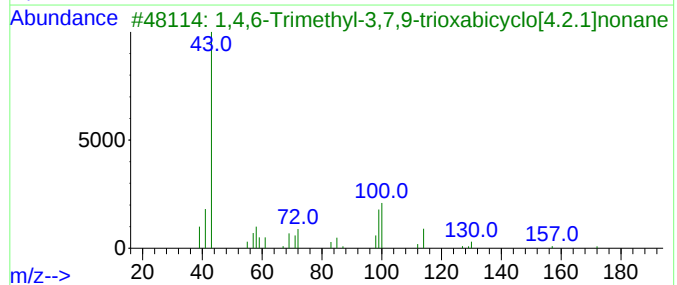
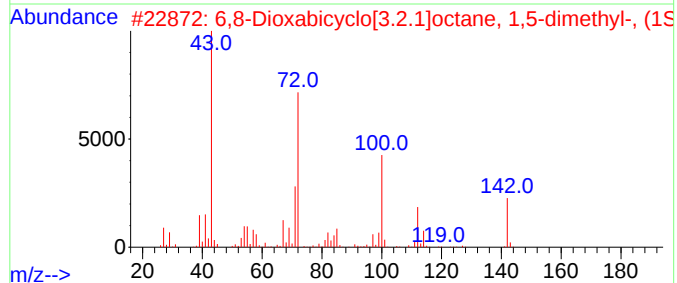
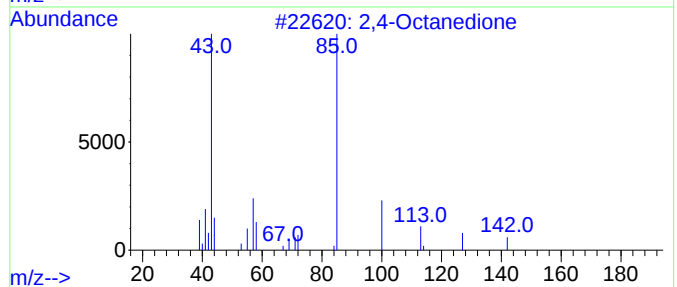
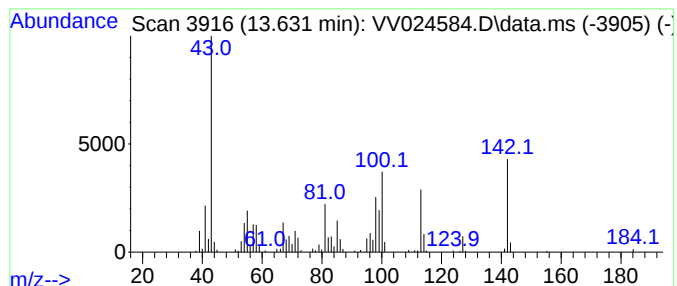
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020922WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
13.632	2.06 ug/L	158187	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	43
2			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	25
3			1,4,6-Trimethyl-3,7,9-trioxabicy...	172	C9H16O3	062759-58-4	12
4			5-Undecanone, 2-methyl-	184	C12H24O	050639-02-6	12
5			trans-1,4,6-Trimethyl-3,7,9-trio...	172	C9H16O3	062759-59-5	12



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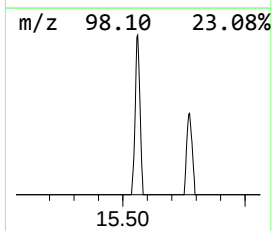
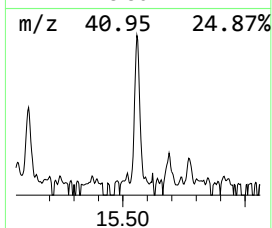
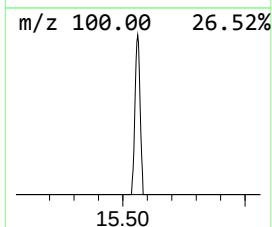
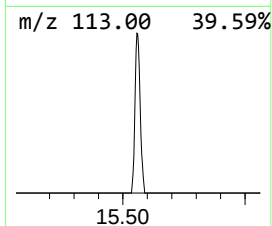
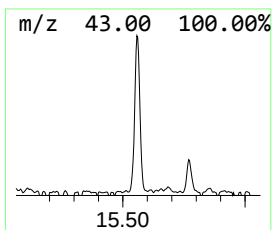
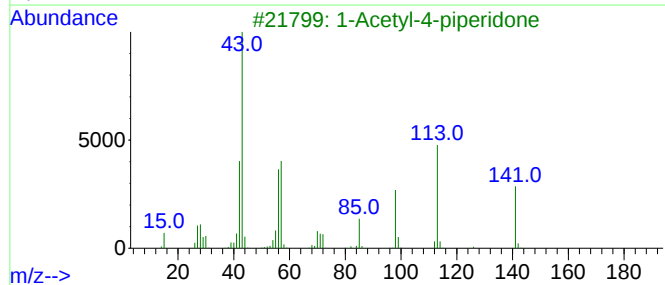
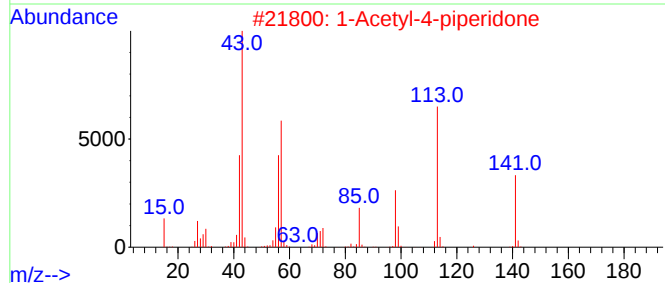
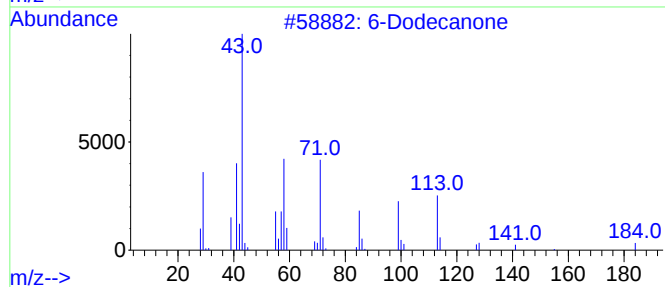
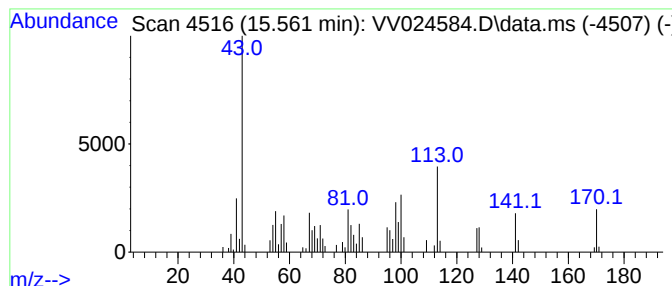
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.561	0.66 ug/L	50617	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Dodecanone	184	C12H24O	006064-27-3	35
2			1-Acetyl-4-piperidone	141	C7H11NO2	032161-06-1	35
3			1-Acetyl-4-piperidone	141	C7H11NO2	032161-06-1	35
4			7-Heptadecanone	254	C17H34O	006064-42-2	16
5			Cyclohexanemethylamine	113	C7H15N	003218-02-8	14



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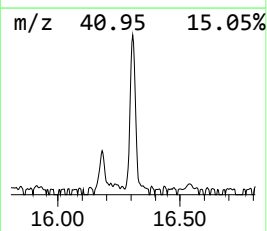
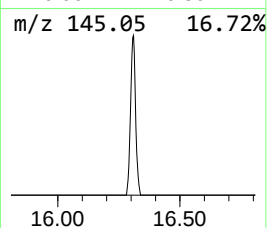
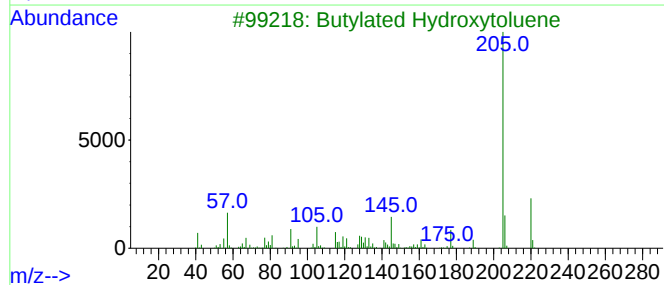
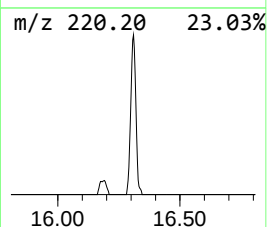
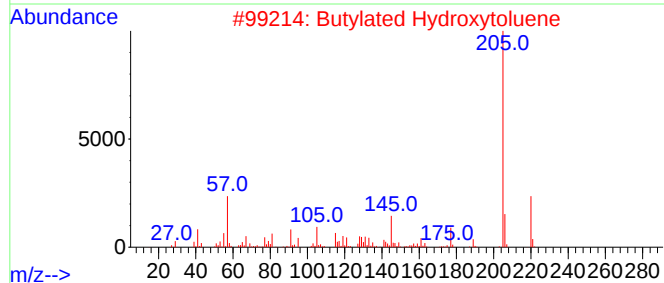
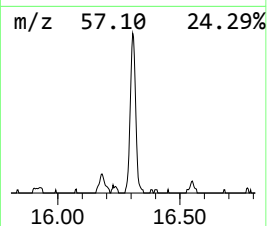
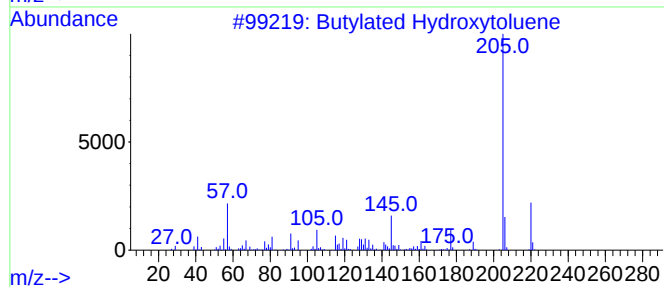
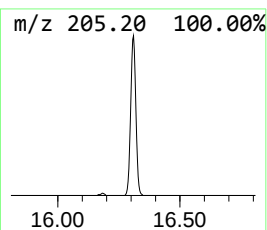
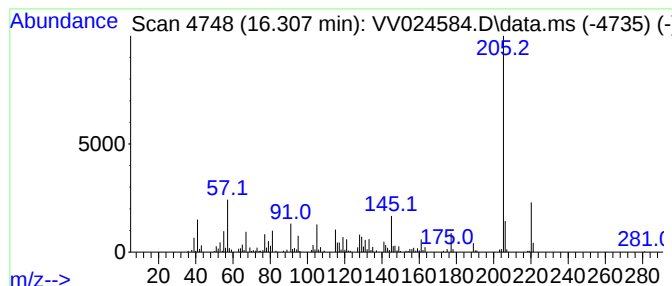
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.307	1.93 ug/L	148760	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV021022\
Data File : VV024584.D
Acq On : 10 Feb 2022 21:33
Operator : SY/MD
Sample : N1475-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F4M04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR020922WMA.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-Butanone, 3,3...	6.606	1.0	ug/L	59114	1	5.635	287599	5.0
1-Hexanol, 2-et...	11.529	5.3	ug/L	406850	3	11.249	384822	5.0
unknown-01	13.632	2.1	ug/L	158187	3	11.249	384822	5.0
unknown-02	15.561	0.7	ug/L	50617	3	11.249	384822	5.0
Butylated Hydro...	16.307	1.9	ug/L	148760	3	11.249	384822	5.0