

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
 Data File : VV028914.D
 Acq On : 12 Nov 2022 07:29
 Operator : SY/MD
 Sample : N5590-13
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GBMY4

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\SFAMVTR111122WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV028914.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.101	16	19	30	rVB4	7315	9245	1.05%	0.096%
2	1.301	70	81	96	rBV	115504	144027	16.43%	1.493%
3	1.420	110	118	128	rBV	38414	47514	5.42%	0.493%
4	1.587	162	170	185	rVV	105721	133771	15.26%	1.387%
5	2.153	336	346	361	rBV	202391	285801	32.60%	2.963%
6	2.310	377	395	397	rBV	37515	87860	10.02%	0.911%
7	2.545	458	468	479	rVB	66055	104576	11.93%	1.084%
8	3.960	892	908	915	rBV3	31979	78362	8.94%	0.812%
9	4.172	967	974	999	rVB	33565	101714	11.60%	1.054%
10	4.394	1026	1043	1062	rBV2	148672	354509	40.44%	3.675%
11	5.072	1238	1254	1280	rBV2	346501	761435	86.85%	7.894%
12	5.622	1414	1425	1444	rBV	264854	507472	57.89%	5.261%
13	5.915	1503	1516	1535	rVB2	91168	181647	20.72%	1.883%
14	6.088	1554	1570	1587	rBV	233673	489077	55.79%	5.070%
15	6.156	1587	1591	1607	rVB	11787	17521	2.00%	0.182%
16	6.722	1762	1767	1785	rBV	37383	72162	8.23%	0.748%
17	7.027	1851	1862	1881	rBV	94906	167596	19.12%	1.737%
18	7.349	1949	1962	1981	rBV	506911	876675	100.00%	9.088%
19	7.654	2048	2057	2080	rBV	47622	85977	9.81%	0.891%
20	8.127	2192	2204	2246	rBV	357136	848483	96.78%	8.796%
21	8.866	2422	2434	2453	rBV	473541	779810	88.95%	8.084%
22	9.937	2760	2767	2780	rVB2	5219	8826	1.01%	0.091%
23	10.220	2844	2855	2871	rVB	160893	251330	28.67%	2.605%
24	11.088	3113	3125	3133	rBV9	6399	11800	1.35%	0.122%
25	11.246	3163	3174	3197	rBV	486688	768651	87.68%	7.968%
26	11.522	3249	3260	3273	rBV4	29487	52883	6.03%	0.548%
27	11.619	3277	3290	3315	rVB	433408	712335	81.25%	7.385%
28	12.040	3407	3421	3436	rBV4	34585	67273	7.67%	0.697%
29	12.641	3598	3608	3615	rBV7	13209	23805	2.72%	0.247%
30	12.876	3673	3681	3695	rVB5	6975	12098	1.38%	0.125%
31	12.975	3698	3712	3725	rBV6	11074	22905	2.61%	0.237%
32	13.053	3725	3736	3743	rBV6	6122	9798	1.12%	0.102%
33	13.374	3827	3836	3845	rBV7	9475	20377	2.32%	0.211%
34	13.458	3854	3862	3874	rVB7	6016	11006	1.26%	0.114%
35	13.596	3894	3905	3911	rBV7	6498	12023	1.37%	0.125%
36	13.686	3925	3933	3944	rVB7	15242	26040	2.97%	0.270%

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37	13.741	3944	3950	3962	rVB7	6705	11259	1.28%	0.117%
38	13.914	3996	4004	4019	rVB4	52265	94702	10.80%	0.982%
39	13.991	4019	4028	4048	rVB3	68061	113414	12.94%	1.176%
40	14.130	4057	4071	4086	rBV8	26471	75298	8.59%	0.781%
41	14.200	4086	4093	4104	rVV5	20260	35139	4.01%	0.364%
42	14.271	4105	4115	4127	rVV3	93117	200146	22.83%	2.075%
43	14.326	4129	4132	4139	rVV	30602	43330	4.94%	0.449%
44	14.371	4141	4146	4159	rVV3	28759	57646	6.58%	0.598%
45	14.432	4159	4165	4178	rVB6	13308	22885	2.61%	0.237%
46	14.731	4250	4258	4267	rBV2	11317	17505	2.00%	0.181%
47	15.644	4534	4542	4550	rBV9	6344	10961	1.25%	0.114%
48	15.760	4568	4578	4590	rBV2	111360	169636	19.35%	1.759%
49	16.168	4694	4705	4721	rBV4	52532	95557	10.90%	0.991%
50	16.297	4734	4745	4761	rBV	355737	525613	59.96%	5.449%
51	17.081	4984	4989	5000	rVB	18869	26867	3.06%	0.279%

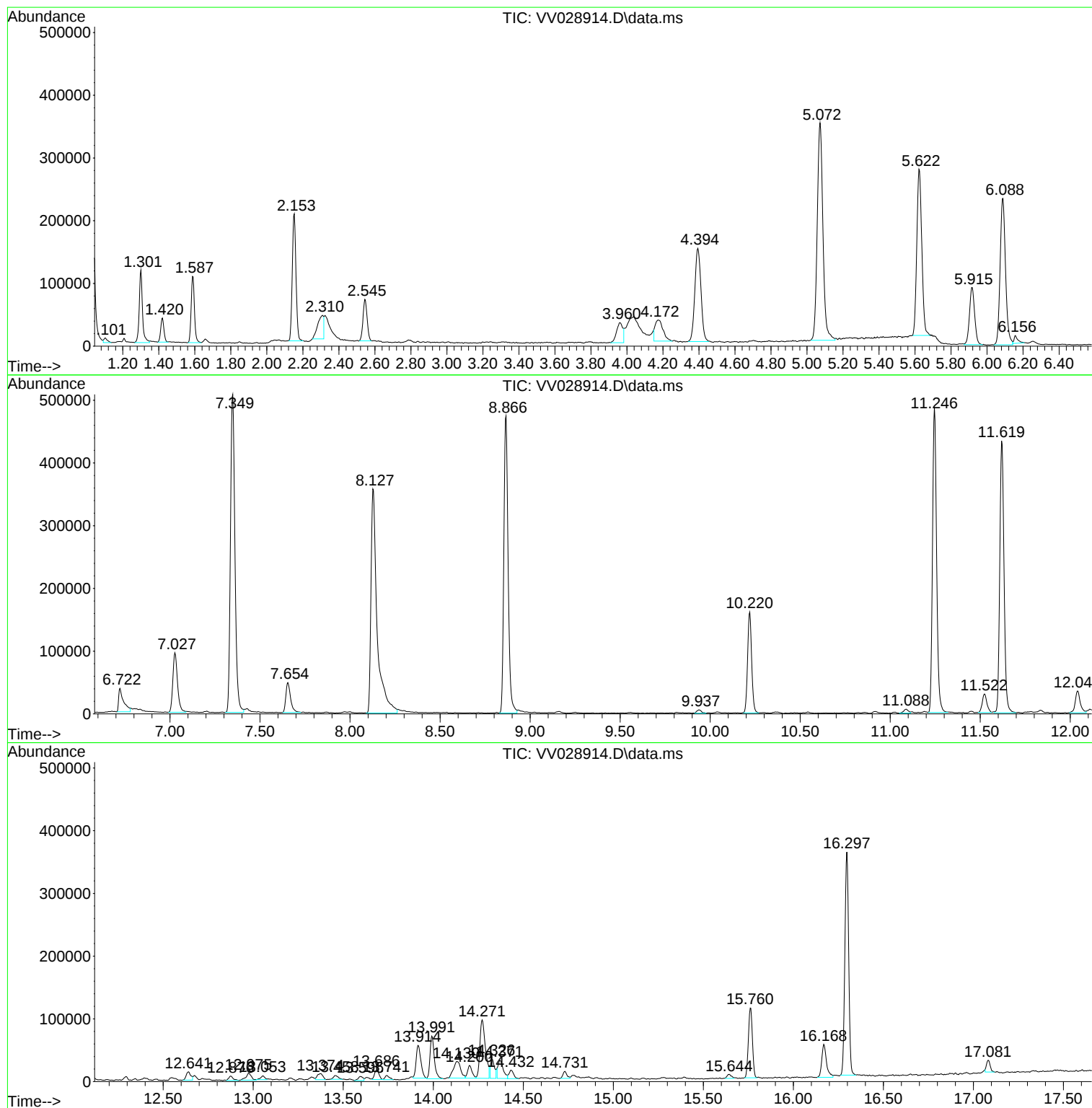
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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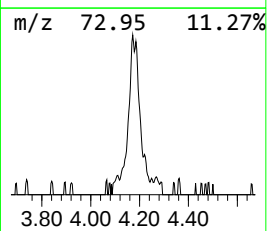
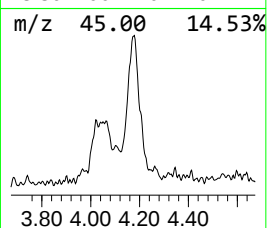
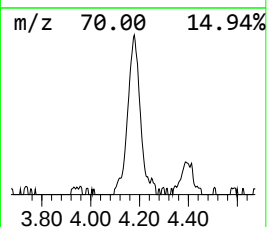
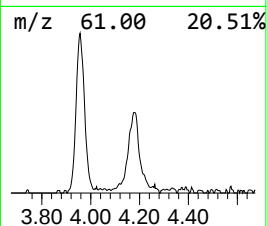
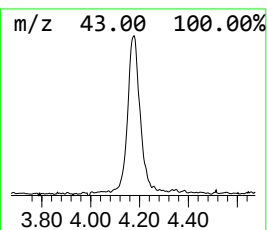
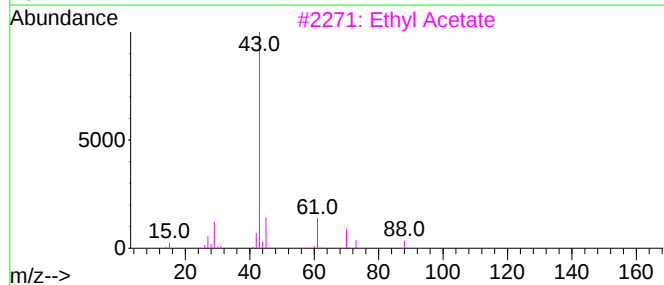
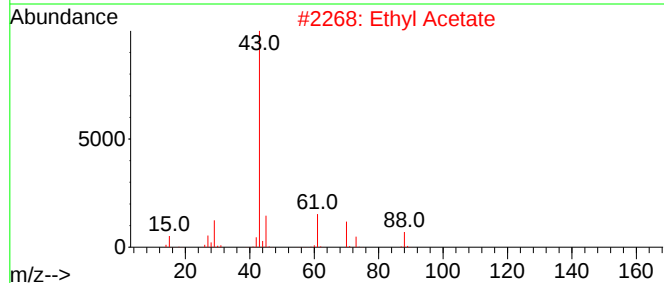
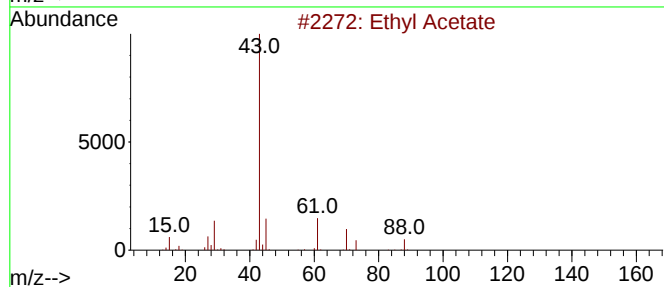
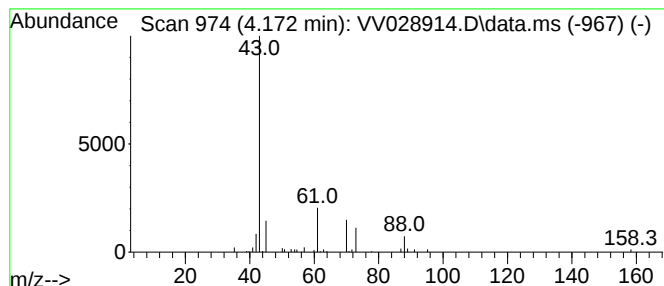
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Ethyl Acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.172	1.00 ug/L	101714	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	72
2			Ethyl Acetate	88	C4H8O2	000141-78-6	64
3			Ethyl Acetate	88	C4H8O2	000141-78-6	58
4			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	43
5			n-Propyl acetate	102	C5H10O2	000109-60-4	37



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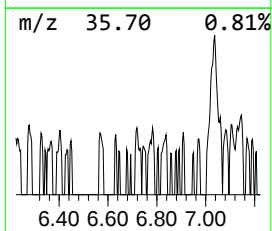
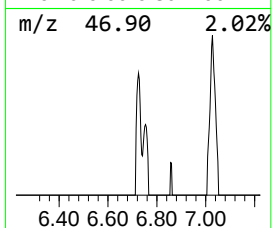
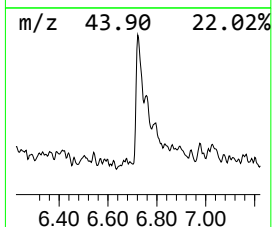
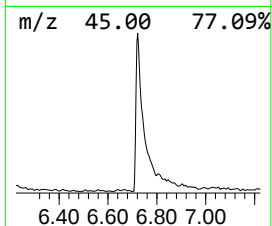
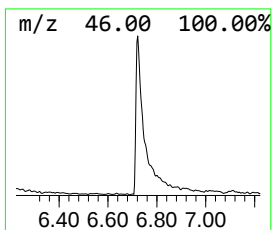
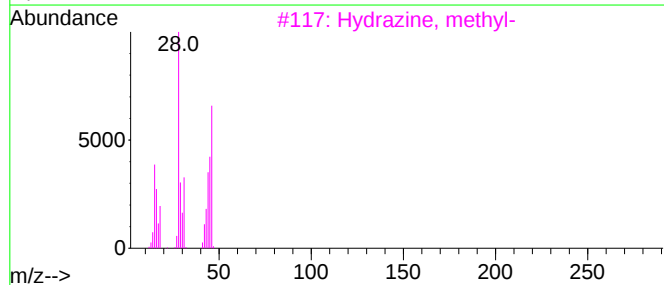
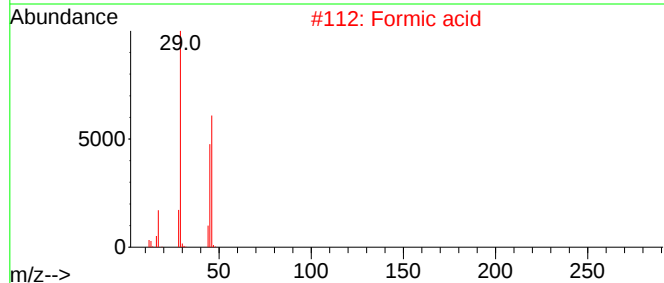
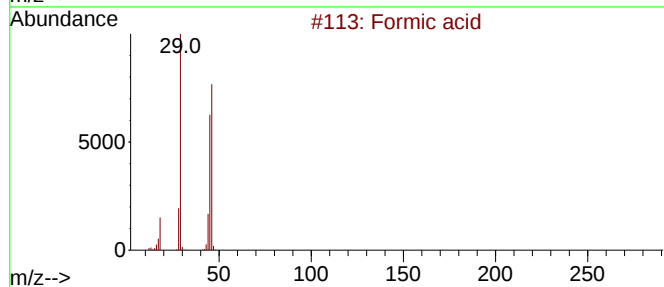
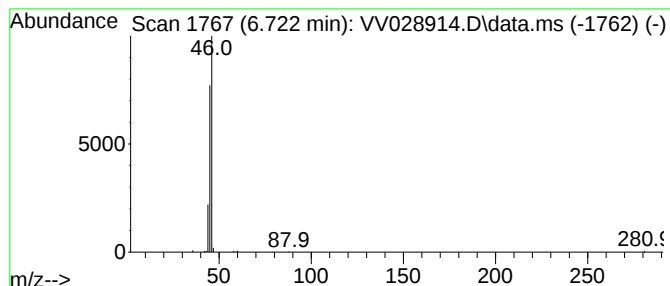
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Formic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.722	0.71 ug/L	72162	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid	46	CH2O2	000064-18-6	78
2			Formic acid	46	CH2O2	000064-18-6	64
3			Hydrazine, methyl-	46	CH6N2	000060-34-4	9
4			Hydrazine, methyl-	46	CH6N2	000060-34-4	9
5			Ethene, fluoro-	46	C2H3F	000075-02-5	9



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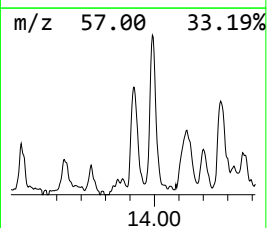
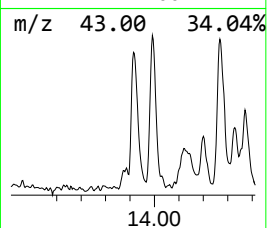
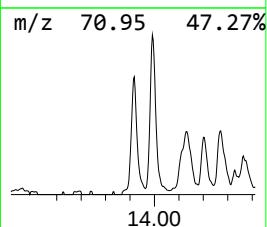
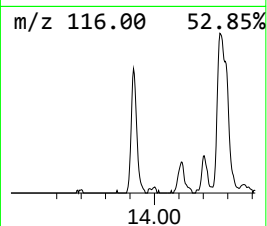
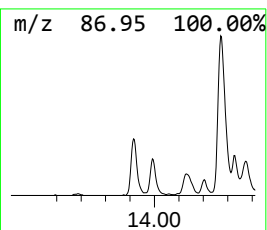
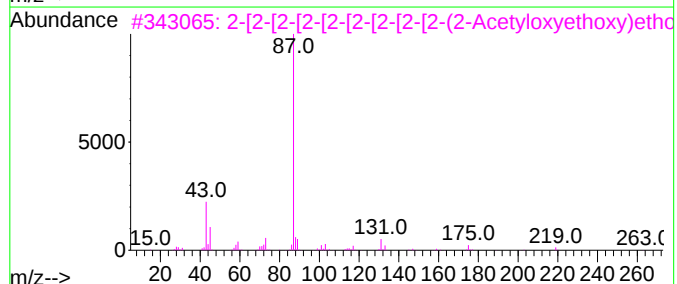
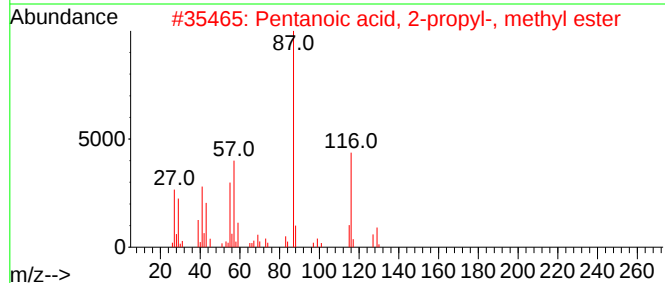
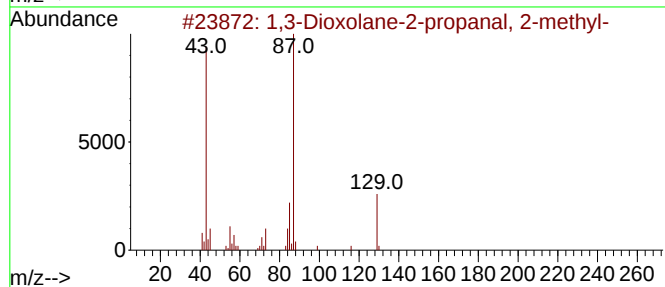
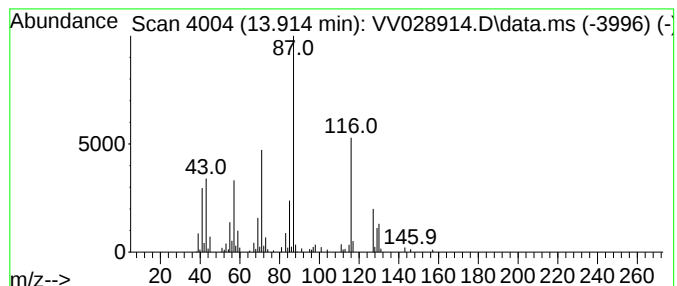
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.914	0.62 ug/L	94702	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane-2-propanal, 2-methyl-	144	C7H12O3	024108-29-0	38
2			Pentanoic acid, 2-propyl-, methyl...	158	C9H18O2	022632-59-3	38
3			2-[2-[2-[2-[2-[2-[2-(2-Ace...	542	C24H46O13	1000351-90-4	27
4			Tetraethylene glycol, diacetate	278	C12H22O7	022790-12-1	14
5			2-Pentanone, 1,3-dimethoxy-3-met...	160	C8H16O3	056830-17-2	12



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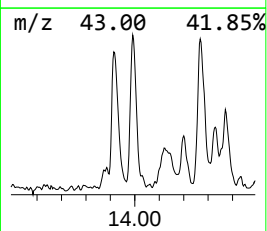
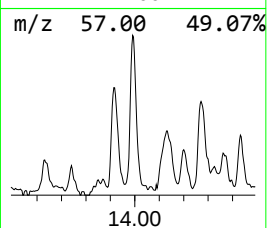
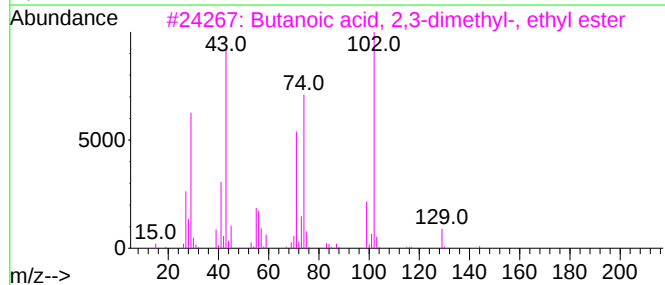
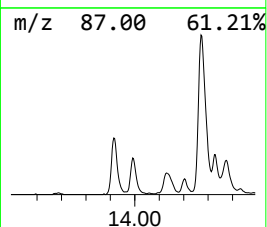
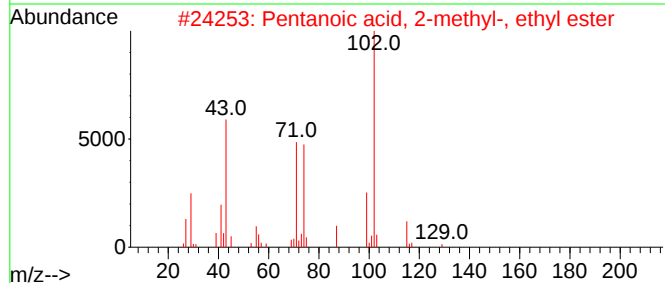
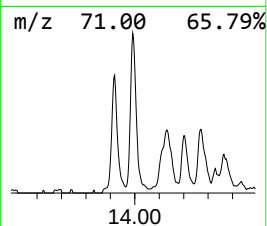
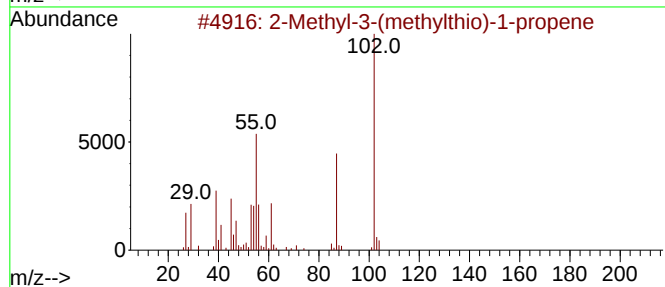
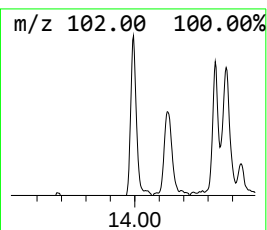
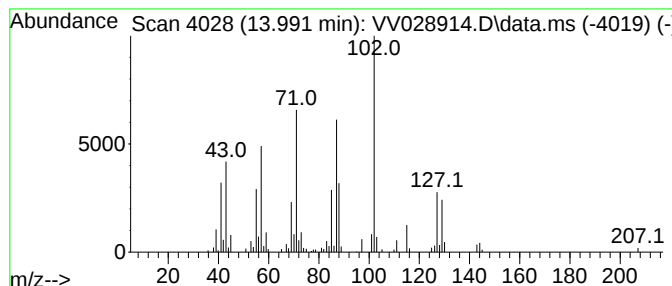
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.992	0.74 ug/L	113414	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methyl-3-(methylthio)-1-propene	102	C5H10S	052326-10-0	38
2			Pentanoic acid, 2-methyl-, ethyl...	144	C8H16O2	039255-32-8	38
3			Butanoic acid, 2,3-dimethyl-, et...	144	C8H16O2	054004-42-1	35
4			2-Imidazolidinethione	102	C3H6N2S	000096-45-7	25
5			3-Ethyl-4-methyl-3-heptanol	158	C10H22O	066719-39-9	22



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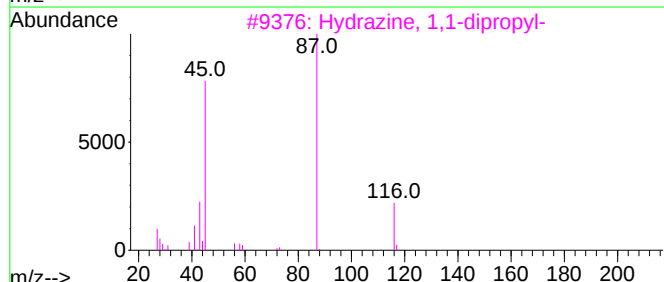
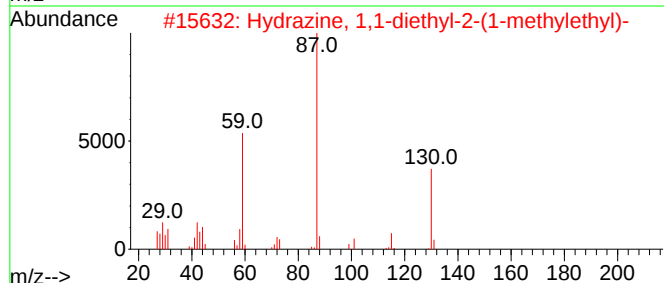
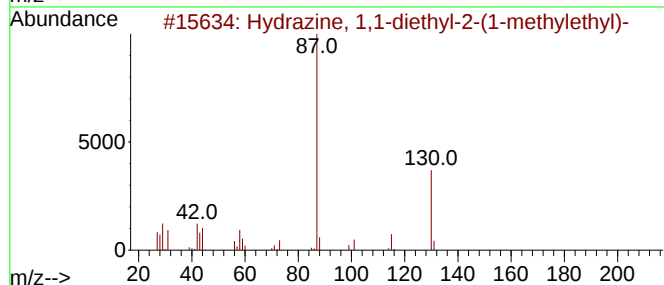
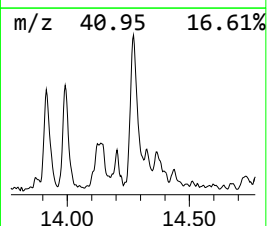
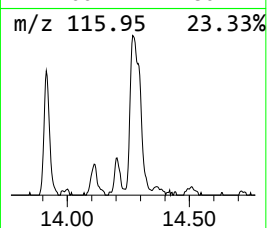
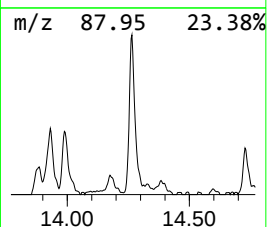
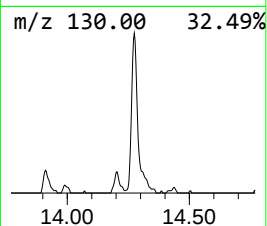
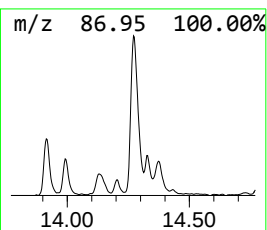
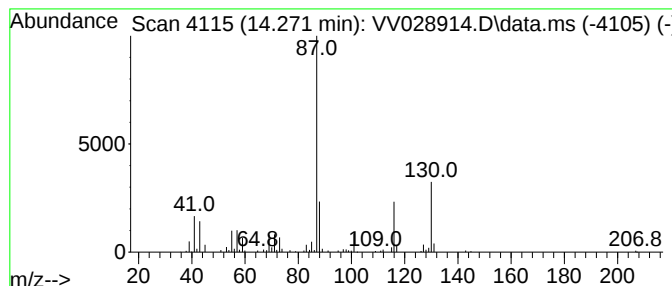
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Hydrazine, 1,1-diethyl-2-(1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.271	1.30 ug/L	200146	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	53
2			Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	53
3			Hydrazine, 1,1-dipropyl-	116	C6H16N2	004986-50-9	46
4			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	42
5			2-[2-[2-[2-[2-[2-[2-[2-(2-Ace...	542	C24H46O13	1000351-90-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
Data File : VV028914.D
Acq On : 12 Nov 2022 07:29
Operator : SY/MD
Sample : N5590-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBMY4

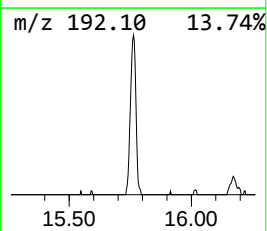
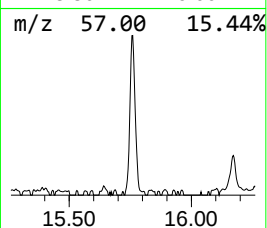
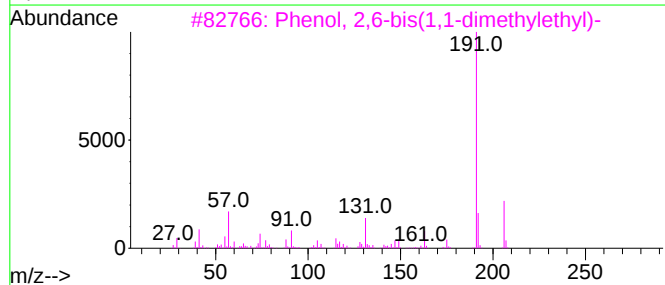
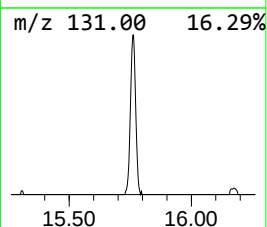
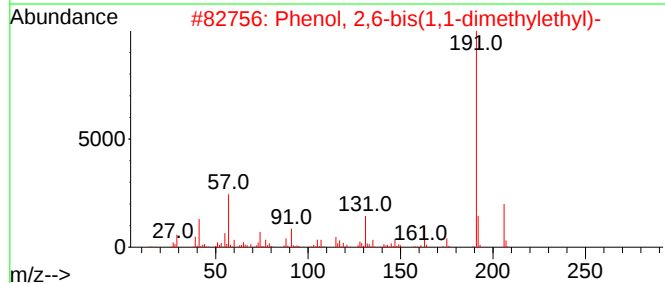
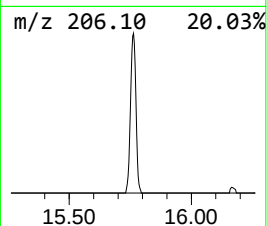
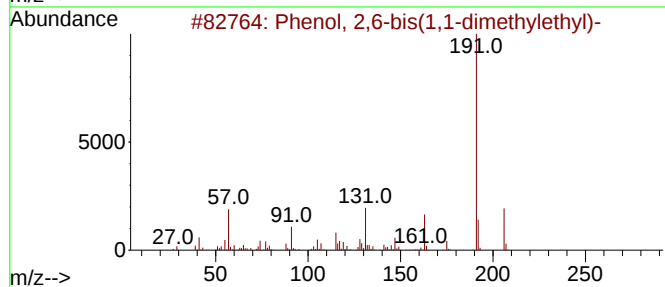
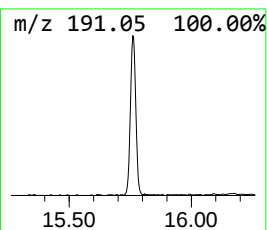
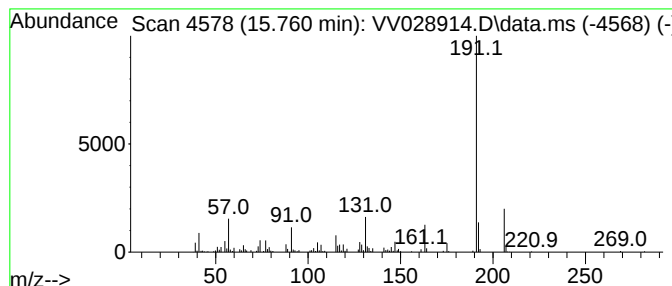
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.760	1.10 ug/L	169636	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	98
2			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
3			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
4			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
5			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
Data File : VV028914.D
Acq On : 12 Nov 2022 07:29
Operator : SY/MD
Sample : N5590-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBMY4

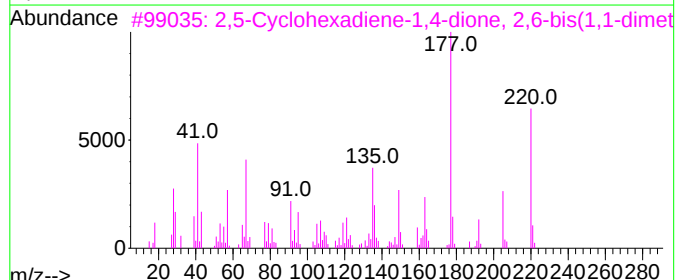
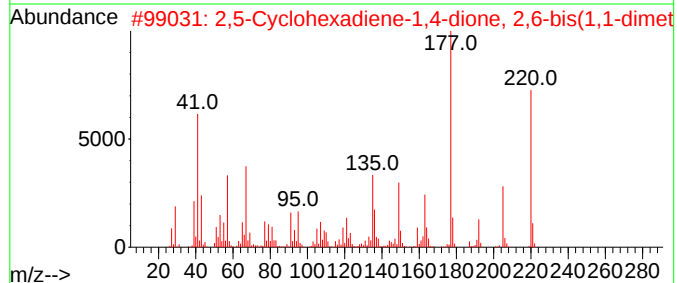
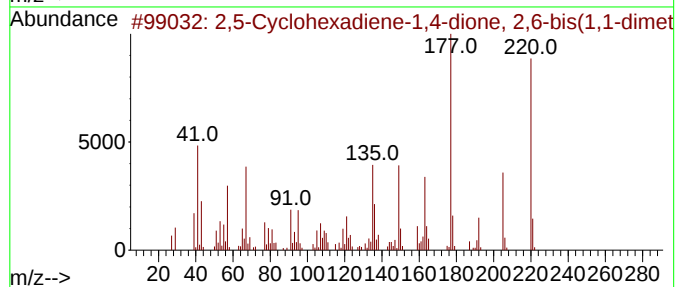
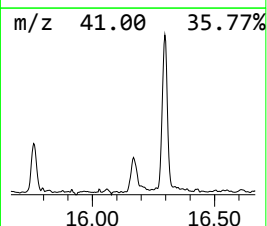
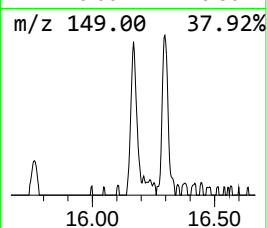
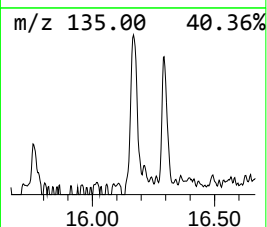
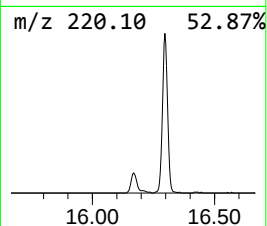
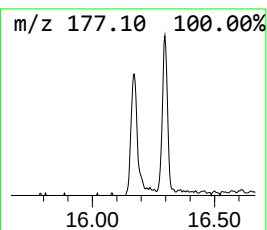
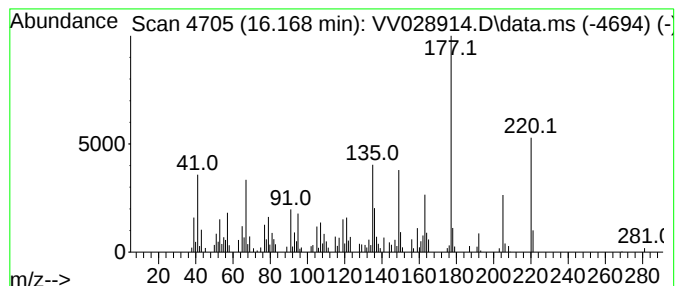
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.168	0.62 ug/L	95557	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	98		
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	94		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	92		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
Data File : VV028914.D
Acq On : 12 Nov 2022 07:29
Operator : SY/MD
Sample : N5590-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBMY4

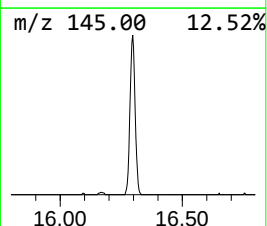
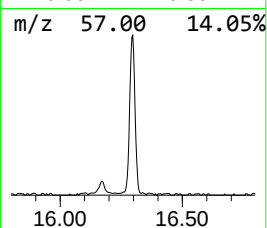
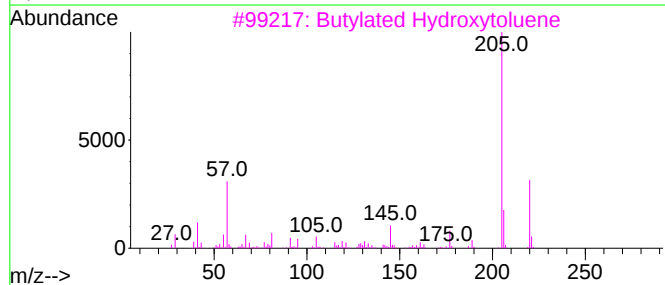
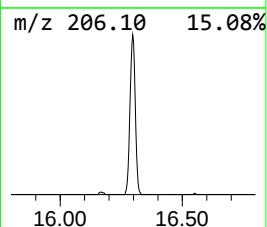
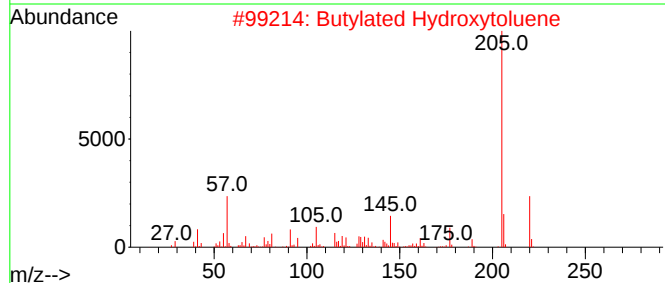
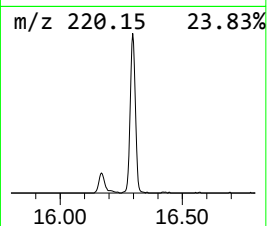
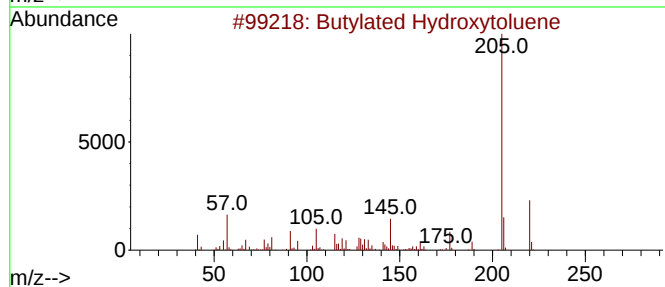
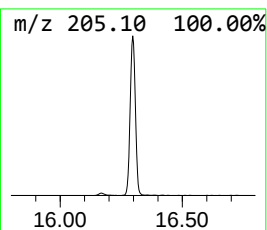
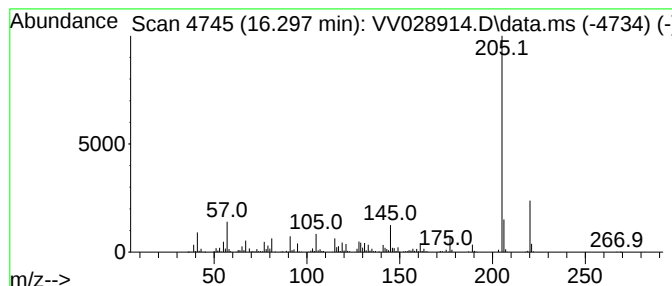
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.297	3.42 ug/L	525613	1,4-Dichlorobenzene-d4	11.246

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	96
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
Data File : VV028914.D
Acq On : 12 Nov 2022 07:29
Operator : SY/MD
Sample : N5590-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 48 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBMY4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.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
Ethyl Acetate	4.172	1.0	ug/L	101714	1	5.622	507472	5.0
Formic acid	6.722	0.7	ug/L	72162	1	5.622	507472	5.0
unknown-01	13.914	0.6	ug/L	94702	3	11.246	768651	5.0
unknown-02	13.992	0.7	ug/L	113414	3	11.246	768651	5.0
Hydrazine, 1,1-...	14.271	1.3	ug/L	200146	3	11.246	768651	5.0
Phenol, 2,6-bis...	15.760	1.1	ug/L	169636	3	11.246	768651	5.0
2,5-Cyclohexadi...	16.168	0.6	ug/L	95557	3	11.246	768651	5.0
Butylated Hydro...	16.297	3.4	ug/L	525613	3	11.246	768651	5.0