

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111922\
 Data File : VV029183.D
 Acq On : 19 Nov 2022 20:14
 Operator : SY/MD
 Sample : N5694-09
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BHB45

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: VV029183.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.108	15	21	39	rBV	233994	235719	22.41%	1.933%
2	1.217	48	55	61	rBV	63223	62923	5.98%	0.516%
3	1.307	75	83	100	rVB	165688	190190	18.08%	1.559%
4	1.394	101	110	133	rBV	51967	181483	17.25%	1.488%
5	1.568	157	164	178	rVB	131167	153405	14.58%	1.258%
6	2.108	322	332	348	rBV2	273657	422719	40.19%	3.466%
7	2.764	525	536	554	rBV2	17385	38231	3.63%	0.313%
8	3.188	653	668	689	rBV	78967	169584	16.12%	1.390%
9	3.905	874	891	936	rBV2	348974	1051839	100.00%	8.623%
10	4.343	1007	1027	1059	rBV2	160613	414652	39.42%	3.400%
11	4.603	1094	1108	1124	rBV5	6838	17445	1.66%	0.143%
12	5.043	1229	1245	1279	rBV2	385932	988977	94.02%	8.108%
13	5.613	1409	1422	1459	rBV	341492	719157	68.37%	5.896%
14	5.918	1501	1517	1545	rBV2	61340	134609	12.80%	1.104%
15	6.066	1550	1563	1593	rBV	207989	442012	42.02%	3.624%
16	6.986	1838	1849	1878	rBV	91046	178655	16.99%	1.465%
17	7.310	1939	1950	1967	rBV	471583	847713	80.59%	6.950%
18	7.391	1968	1975	1997	rVB	27518	60509	5.75%	0.496%
19	7.622	2036	2047	2067	rBV2	47884	93178	8.86%	0.764%
20	8.088	2180	2192	2241	rBV	346624	792732	75.37%	6.499%
21	8.847	2413	2428	2452	rBV	499662	832031	79.10%	6.821%
22	9.014	2472	2480	2493	rVB2	15425	25394	2.41%	0.208%
23	9.137	2505	2518	2540	rBV	50875	94361	8.97%	0.774%
24	9.542	2634	2644	2669	rBV2	28832	59152	5.62%	0.485%
25	10.210	2832	2852	2870	rBV	147807	238382	22.66%	1.954%
26	10.445	2916	2925	2944	rBV2	10668	24440	2.32%	0.200%
27	10.535	2944	2953	2964	rVB2	10854	16540	1.57%	0.136%
28	10.911	3060	3070	3083	rBV	37453	59621	5.67%	0.489%
29	11.169	3141	3150	3162	rBV2	21988	38164	3.63%	0.313%
30	11.239	3162	3172	3192	rVV	521572	823244	78.27%	6.749%
31	11.329	3192	3200	3211	rVB2	13112	20844	1.98%	0.171%
32	11.519	3245	3259	3278	rBV	246998	410304	39.01%	3.364%
33	11.616	3278	3289	3310	rVB	457958	747453	71.06%	6.128%
34	11.735	3316	3326	3349	rVB	195024	320747	30.49%	2.630%
35	12.008	3400	3411	3418	rBV4	6340	10972	1.04%	0.090%
36	12.108	3431	3442	3452	rBV2	17428	27170	2.58%	0.223%

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Stop Thrs : 0

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Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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37	12.355	3510	3519	3529	rBV2	21956	35224	3.35%	0.289%
38	12.461	3542	3552	3563	rBV6	18329	40332	3.83%	0.331%
39	12.718	3622	3632	3646	rVB2	14234	21781	2.07%	0.179%
40	12.876	3671	3681	3692	rVV2	20364	30804	2.93%	0.253%
41	13.037	3722	3731	3746	rVB4	15302	25950	2.47%	0.213%
42	13.490	3858	3872	3895	rBV	431101	691138	65.71%	5.666%
43	13.612	3899	3910	3925	rBV	95091	152010	14.45%	1.246%
44	14.567	4196	4207	4215	rBV2	8857	15298	1.45%	0.125%
45	14.622	4215	4224	4236	rVV	63050	97986	9.32%	0.803%
46	14.805	4270	4281	4293	rBV	44476	74492	7.08%	0.611%
47	15.358	4444	4453	4463	rVB3	6960	11542	1.10%	0.095%
48	15.657	4540	4546	4558	rVB8	6352	10696	1.02%	0.088%
49	15.802	4583	4591	4598	rBV5	7331	10960	1.04%	0.090%
50	16.471	4790	4799	4812	rBV2	19838	34594	3.29%	0.284%

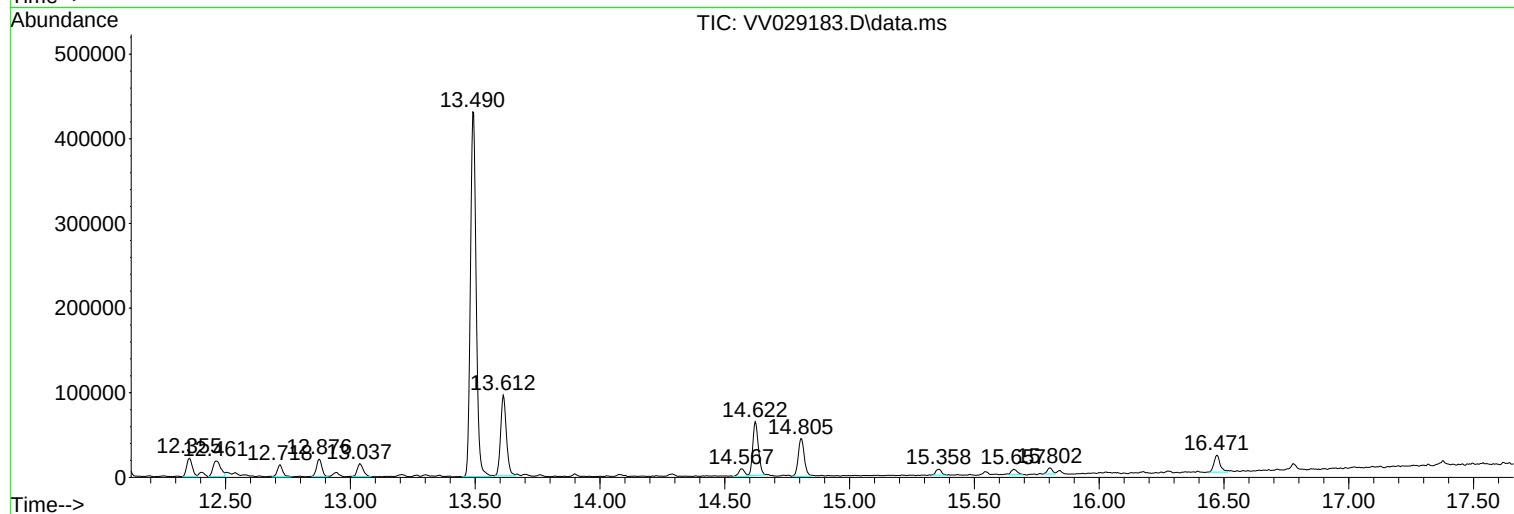
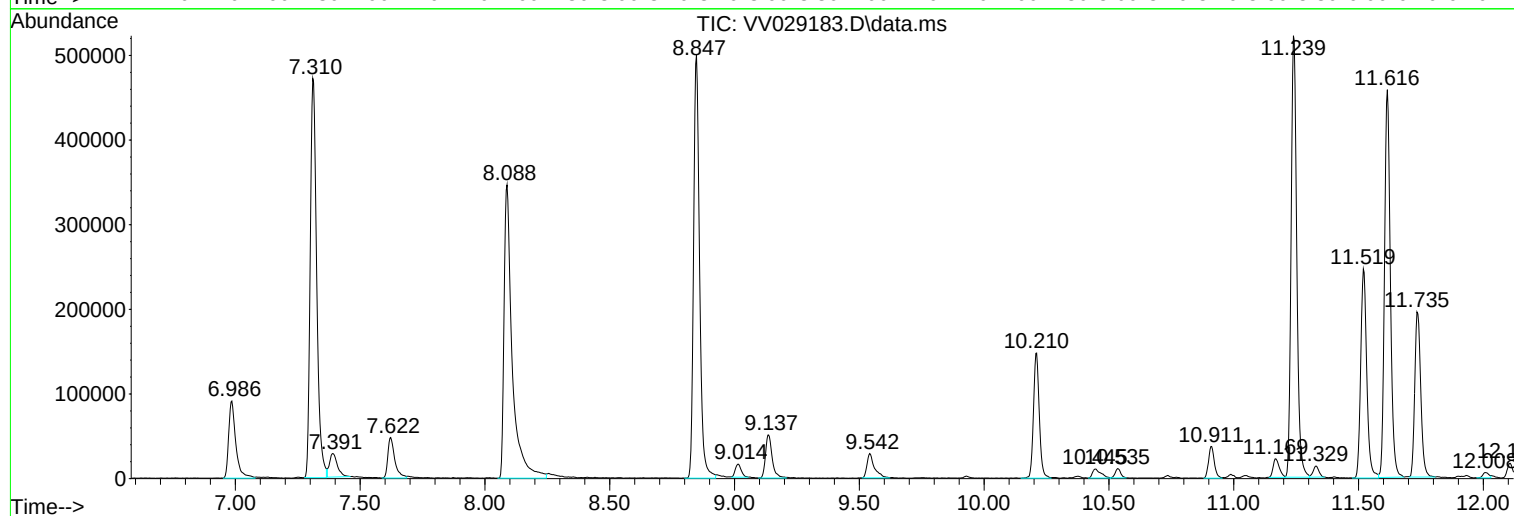
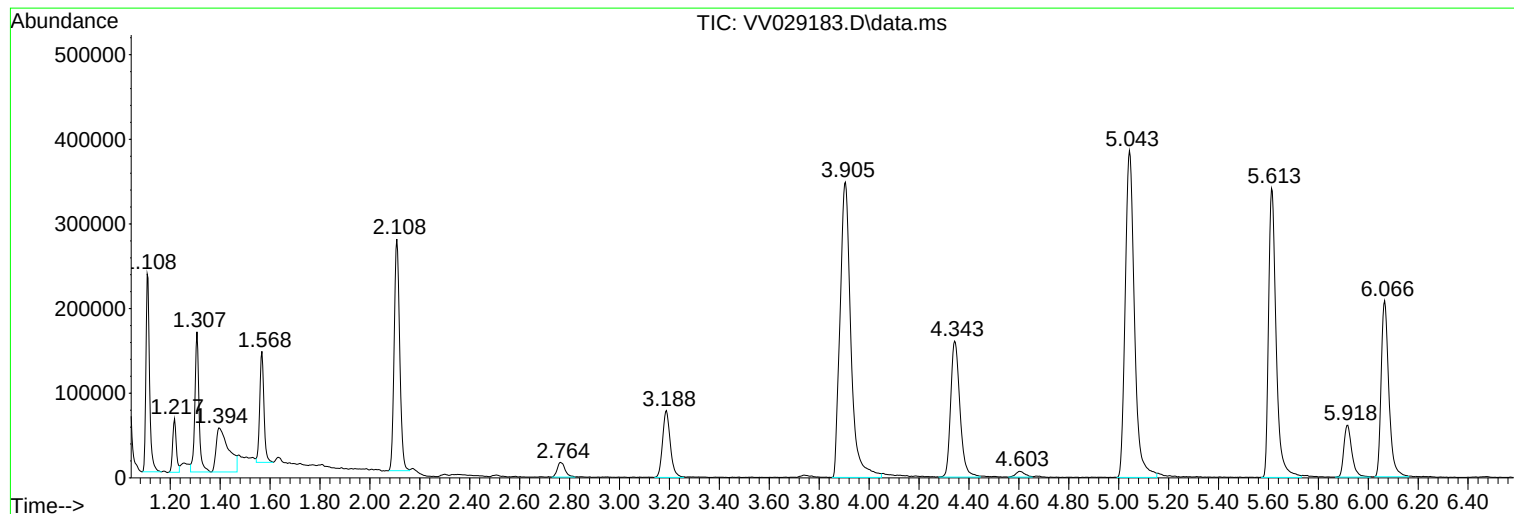
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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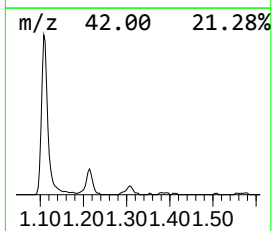
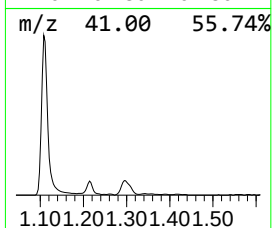
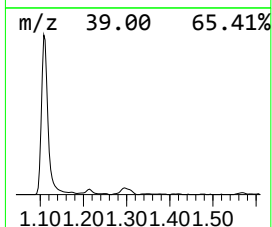
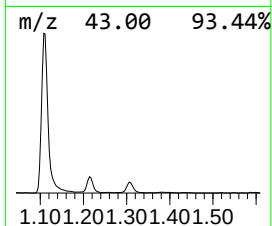
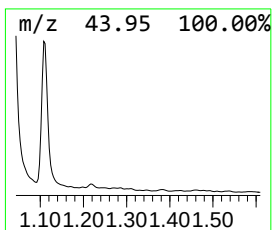
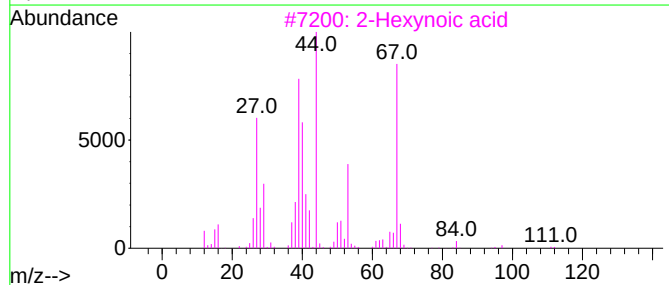
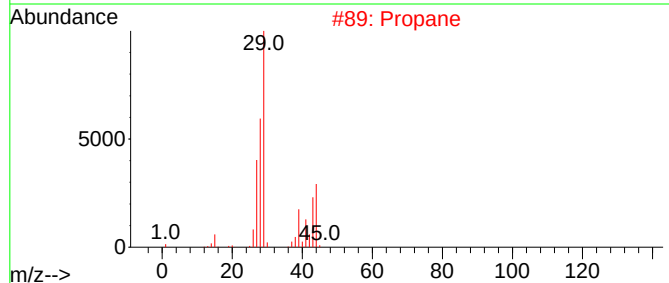
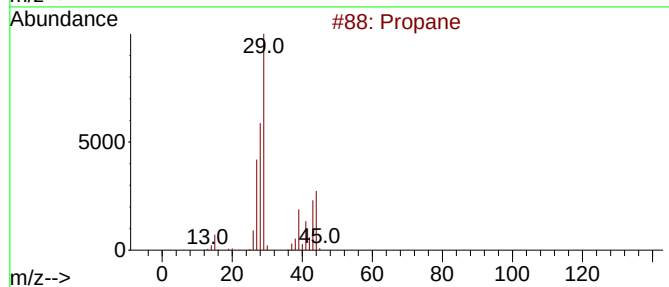
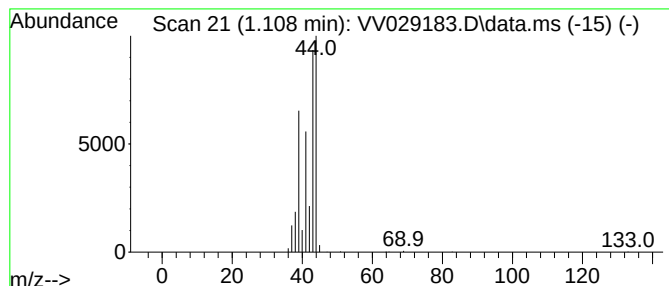
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.108	1.64 ug/L	235719	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Propane	44	C3H8	000074-98-6	83
3			2-Hexynoic acid	112	C6H8O2	000764-33-0	38
4			2-Butenal, (E)-	70	C4H6O	000123-73-9	17
5			2-Butenal	70	C4H6O	004170-30-3	17



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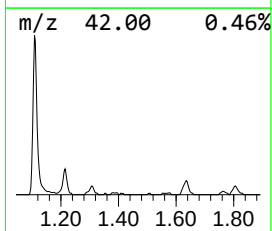
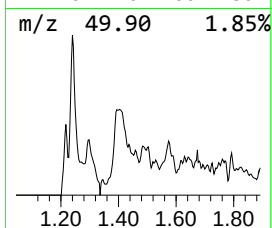
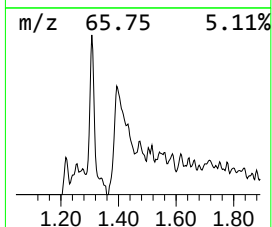
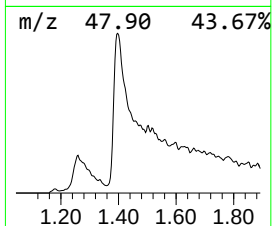
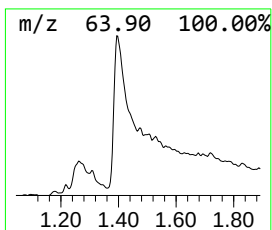
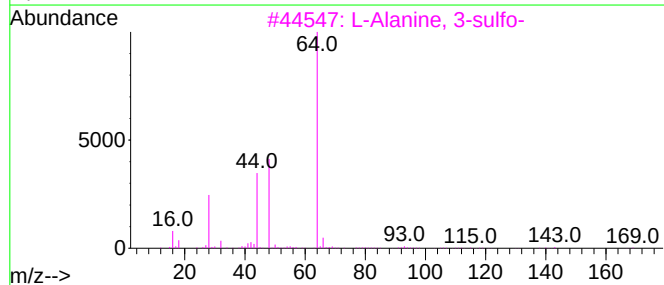
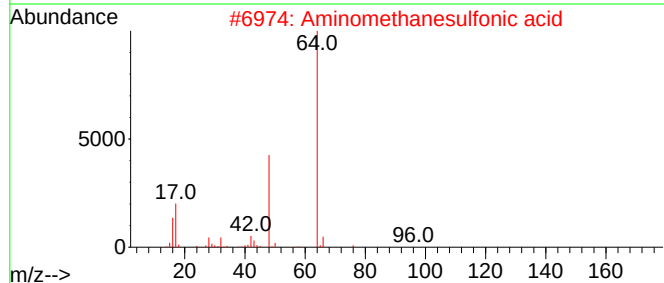
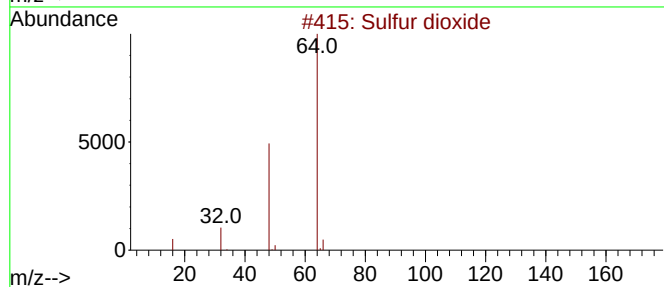
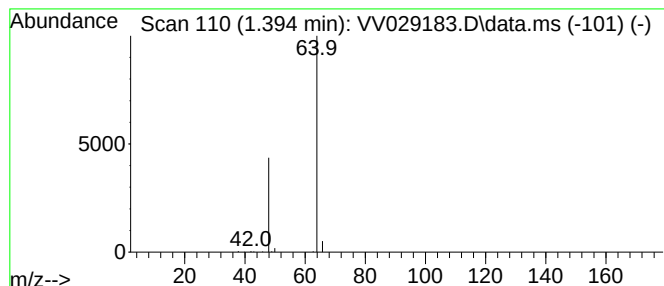
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.394	1.26 ug/L	181483	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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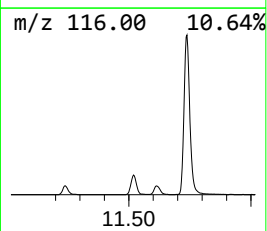
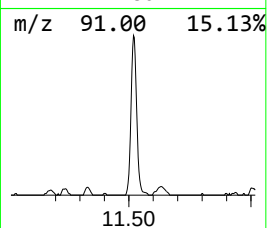
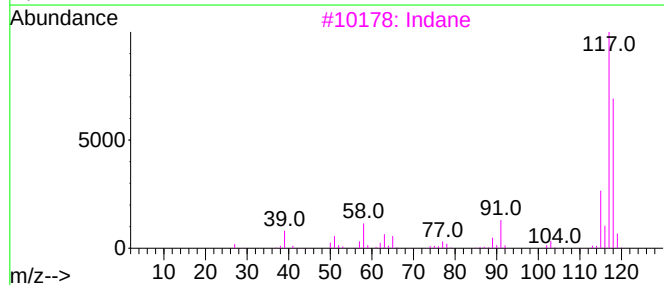
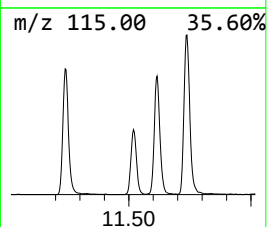
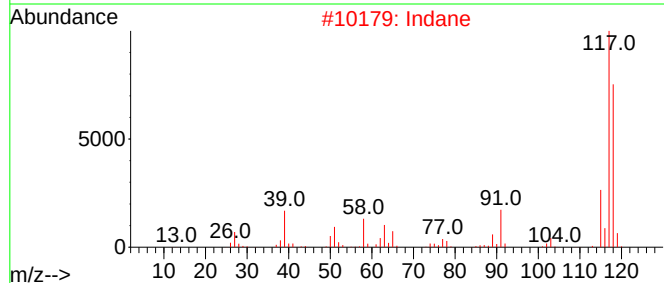
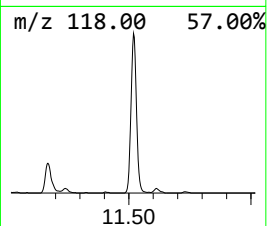
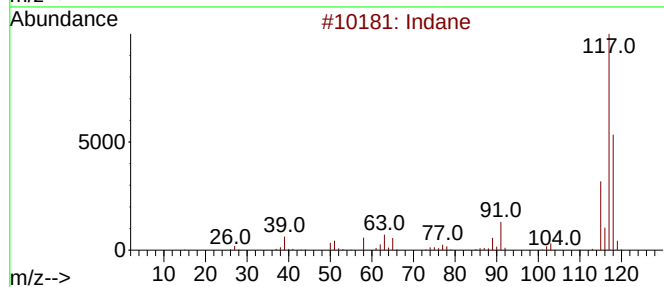
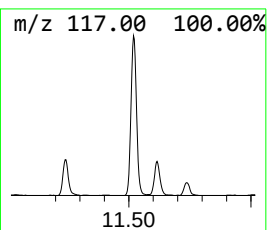
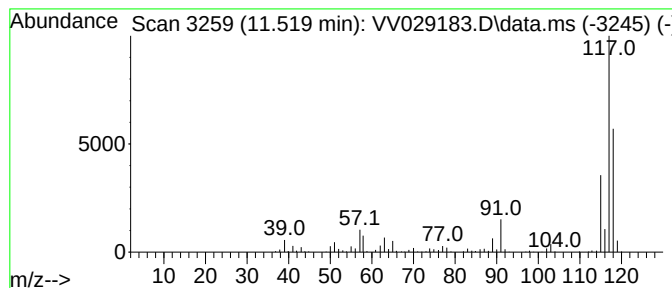
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.519	2.49 ug/L	410304	1,4-Dichlorobenzene-d4	11.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane			118	C9H10	000496-11-7	95
2	Indane			118	C9H10	000496-11-7	90
3	Indane			118	C9H10	000496-11-7	90
4	Benzene, 1-ethenyl-4-methyl-			118	C9H10	000622-97-9	74
5	Benzene, cyclopropyl-			118	C9H10	000873-49-4	74



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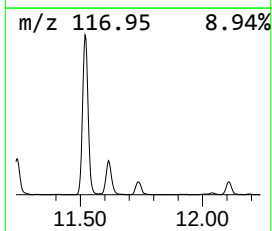
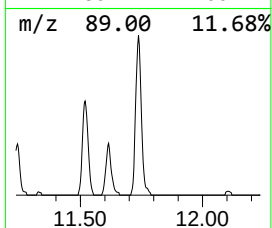
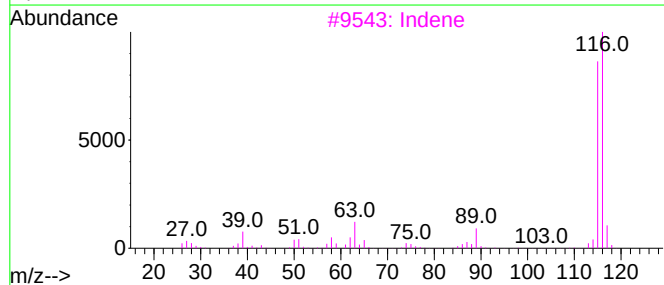
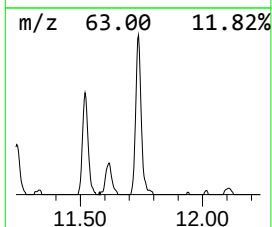
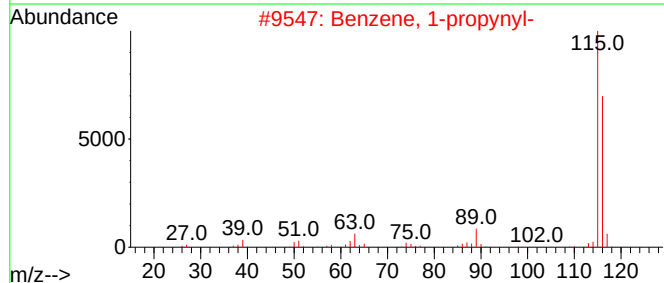
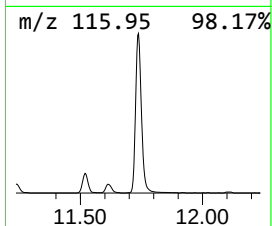
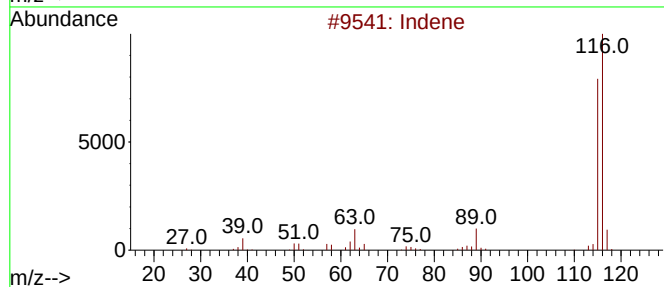
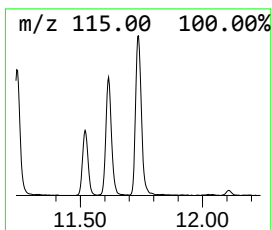
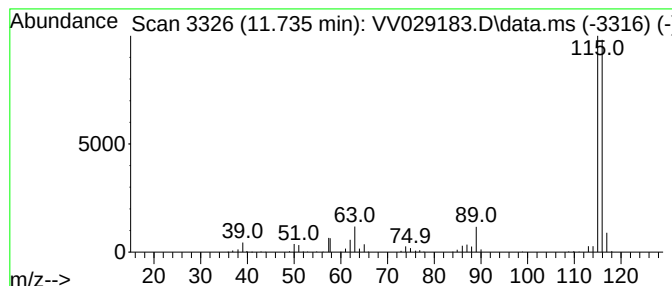
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Indene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.735	1.95 ug/L	320747	1,4-Dichlorobenzene-d4	11.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3			Indene	116	C9H8	000095-13-6	94
4			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5			3-Methylphenylacetylene	116	C9H8	000766-82-5	91



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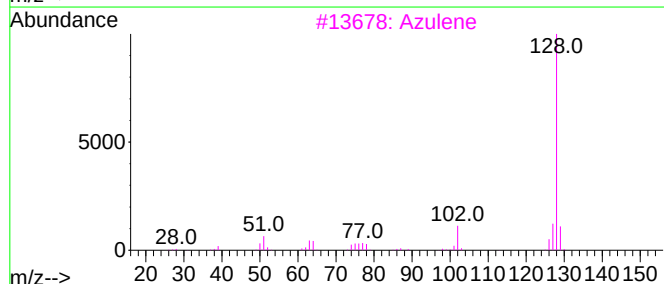
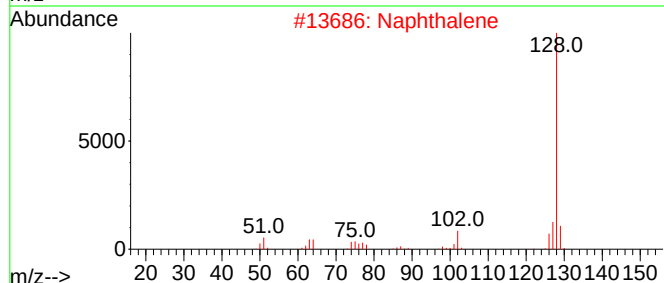
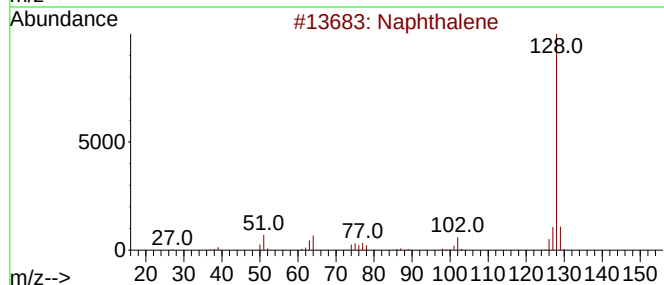
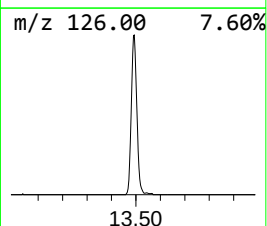
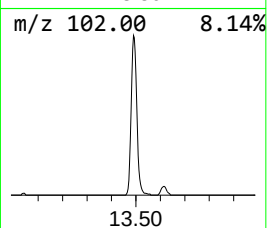
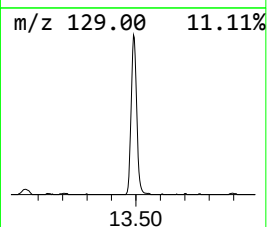
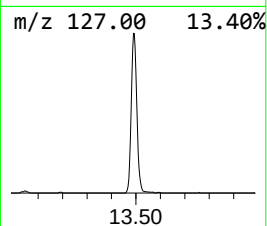
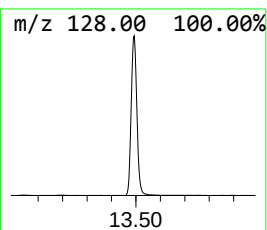
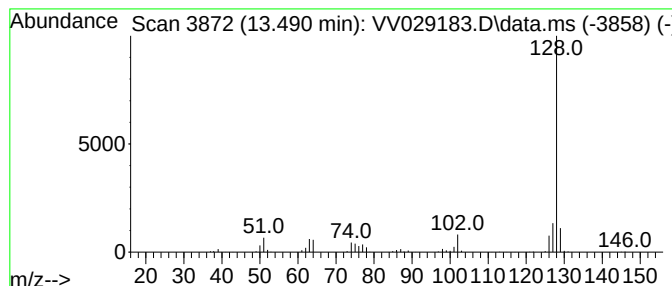
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.490	4.20 ug/L	691138	1,4-Dichlorobenzene-d4	11.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	95
3			Azulene	128	C10H8	000275-51-4	94
4			Naphthalene	128	C10H8	000091-20-3	94
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111922\
Data File : VV029183.D
Acq On : 19 Nov 2022 20:14
Operator : SY/MD
Sample : N5694-09
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BHB45

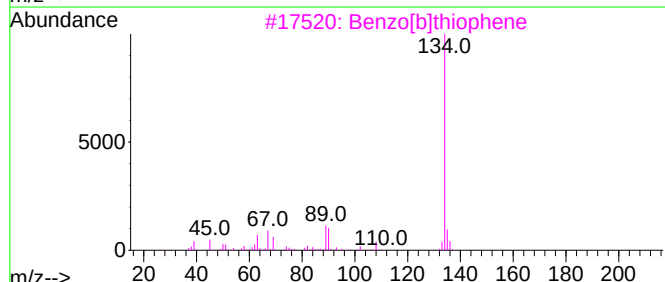
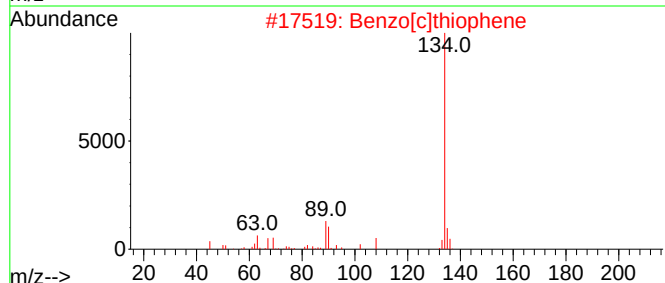
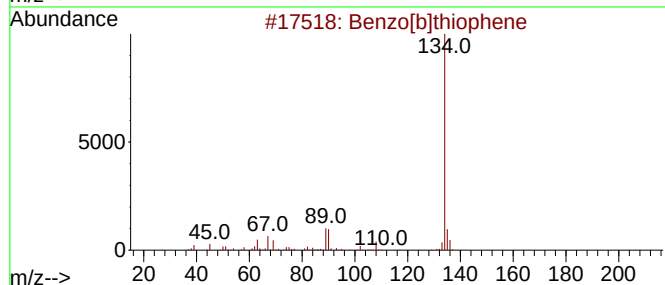
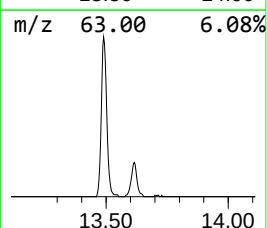
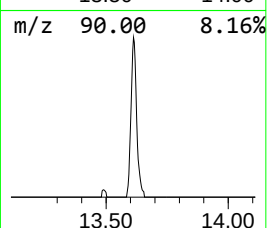
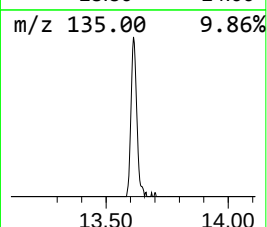
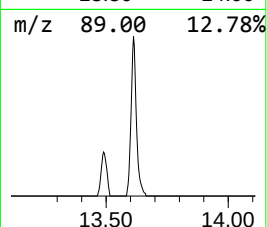
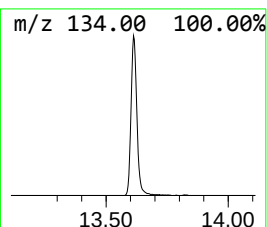
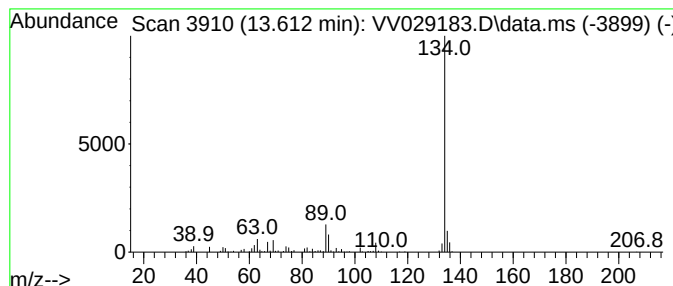
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Benzo[b]thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.612	0.92 ug/L	152010	1,4-Dichlorobenzene-d4	11.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene	134	C8H6S	000095-15-8	94
2			Benzo[c]thiophene	134	C8H6S	000270-82-6	94
3			Benzo[b]thiophene	134	C8H6S	000095-15-8	94
4			Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	91
5			Benzo[b]thiophene	134	C8H6S	000095-15-8	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111922\
Data File : VV029183.D
Acq On : 19 Nov 2022 20:14
Operator : SY/MD
Sample : N5694-09
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BHB45

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
(DEL) Alkane: S...	1.108	1.6	ug/L	235719	1	5.613	719157	5.0
Sulfur dioxide	1.394	1.3	ug/L	181483	1	5.613	719157	5.0
Indane	11.519	2.5	ug/L	410304	3	11.243	823244	5.0
Indene	11.735	2.0	ug/L	320747	3	11.243	823244	5.0
Azulene	13.490	4.2	ug/L	691138	3	11.243	823244	5.0
Benzo[b]thiophene	13.612	0.9	ug/L	152010	3	11.243	823244	5.0