

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
 Data File : VU051518.D
 Acq On : 26 Oct 2022 22:18
 Operator : JC/MD
 Sample : N5300-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHA92

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\SFAMUTR100722WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	34	43	51	rBV2	33968	65860	5.90%	0.462%
2	1.597	74	80	112	rVB2	140167	246955	22.13%	1.731%
3	1.909	170	177	194	rVB	109681	153926	13.79%	1.079%
4	2.565	369	381	395	rBV	189941	307424	27.54%	2.154%
5	3.179	562	572	583	rBV2	6653	14662	1.31%	0.103%
6	3.874	759	788	810	rVB	17543	86367	7.74%	0.605%
7	3.993	813	825	839	rVB3	6330	14934	1.34%	0.105%
8	4.620	1006	1020	1050	rBV	191155	475021	42.56%	3.329%
9	5.060	1141	1157	1176	rBV	191184	424566	38.04%	2.975%
10	5.723	1342	1363	1371	rBV2	386480	992953	88.96%	6.959%
11	5.771	1371	1378	1401	rVB	488880	987485	88.47%	6.920%
12	6.247	1508	1526	1552	rBV	332273	642807	57.59%	4.505%
13	6.690	1649	1664	1681	rBV	238964	473887	42.46%	3.321%
14	7.565	1925	1936	1959	rBV	92908	163476	14.65%	1.146%
15	7.896	2021	2039	2056	rBV	409297	724274	64.89%	5.076%
16	8.179	2116	2127	2145	rBV	56251	96907	8.68%	0.679%
17	8.632	2252	2268	2302	rBV	577851	1116161	100.00%	7.822%
18	9.417	2499	2512	2549	rBV	491894	910946	81.61%	6.384%
19	9.571	2549	2560	2574	rVB	37520	62370	5.59%	0.437%
20	9.690	2586	2597	2610	rBV	56536	91771	8.22%	0.643%
21	10.105	2714	2726	2739	rBV3	27389	49821	4.46%	0.349%
22	10.484	2833	2844	2855	rBV3	15356	24717	2.21%	0.173%
23	10.610	2872	2883	2890	rBV9	6423	11382	1.02%	0.080%
24	10.755	2915	2928	2954	rVB	210737	342249	30.66%	2.398%
25	10.896	2959	2972	2989	rVB4	18950	43023	3.85%	0.302%
26	11.095	3025	3034	3043	rBV10	7811	12171	1.09%	0.085%
27	11.465	3139	3149	3162	rBV	60262	95710	8.57%	0.671%
28	11.809	3244	3256	3274	rBV	457686	762511	68.32%	5.344%
29	11.893	3274	3282	3293	rVB2	22283	38511	3.45%	0.270%
30	12.092	3323	3344	3357	rBV	113746	207386	18.58%	1.453%
31	12.192	3362	3375	3400	rVB	406132	680399	60.96%	4.768%
32	12.478	3452	3464	3469	rBV3	32485	58274	5.22%	0.408%
33	12.513	3469	3475	3486	rVV2	36955	68439	6.13%	0.480%
34	12.568	3487	3492	3499	rVV4	9550	14387	1.29%	0.101%
35	12.626	3502	3510	3519	rVB4	6051	12353	1.11%	0.087%
36	12.774	3544	3556	3568	rBV8	10309	22387	2.01%	0.157%

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37	13.028	3627	3635	3644	rBV4	7624	12806	1.15%	0.090%
38	13.195	3678	3687	3694	rBV9	12771	19192	1.72%	0.134%
39	13.291	3710	3717	3729	rVB2	15376	23741	2.13%	0.166%
40	13.452	3757	3767	3778	rBV3	20400	34134	3.06%	0.239%
41	13.513	3778	3786	3796	rVB6	13525	21742	1.95%	0.152%
42	13.626	3807	3821	3834	rVB5	19010	36468	3.27%	0.256%
43	13.796	3860	3874	3882	rVV10	14959	32679	2.93%	0.229%
44	13.851	3882	3891	3905	rVB3	48213	79151	7.09%	0.555%
45	13.944	3909	3920	3927	rBV5	35812	65365	5.86%	0.458%
46	13.992	3928	3935	3944	rVB4	31730	48689	4.36%	0.341%
47	14.086	3951	3964	3980	rBV	660028	1094465	98.06%	7.670%
48	14.205	3989	4001	4016	rVB	28004	65386	5.86%	0.458%
49	14.282	4019	4025	4046	rVB	9527	23691	2.12%	0.166%
50	14.899	4207	4217	4225	rBV3	84686	140770	12.61%	0.987%
51	14.941	4225	4230	4236	rVV3	27382	40301	3.61%	0.282%
52	14.976	4237	4241	4253	rVB8	22910	34637	3.10%	0.243%
53	15.073	4255	4271	4280	rBV3	76440	142624	12.78%	0.999%
54	15.221	4306	4317	4329	rBV	364200	613564	54.97%	4.300%
55	15.330	4345	4351	4362	rVB8	10644	20126	1.80%	0.141%
56	15.407	4364	4375	4392	rVV	375566	633309	56.74%	4.438%
57	15.954	4536	4545	4556	rBV3	13463	22186	1.99%	0.155%
58	16.147	4599	4605	4612	rVB2	11243	14523	1.30%	0.102%
59	16.262	4631	4641	4651	rBV3	23881	49622	4.45%	0.348%
60	16.407	4669	4686	4693	rBV4	50037	106323	9.53%	0.745%
61	16.449	4694	4699	4712	rVB3	29973	51090	4.58%	0.358%
62	16.610	4740	4749	4753	rBV6	12602	22335	2.00%	0.157%
63	16.674	4766	4769	4779	rVB8	9484	13955	1.25%	0.098%
64	16.780	4790	4802	4813	rBV6	16094	39533	3.54%	0.277%
65	16.886	4826	4835	4844	rVB3	39357	60931	5.46%	0.427%
66	17.095	4889	4900	4911	rBV2	117960	209750	18.79%	1.470%

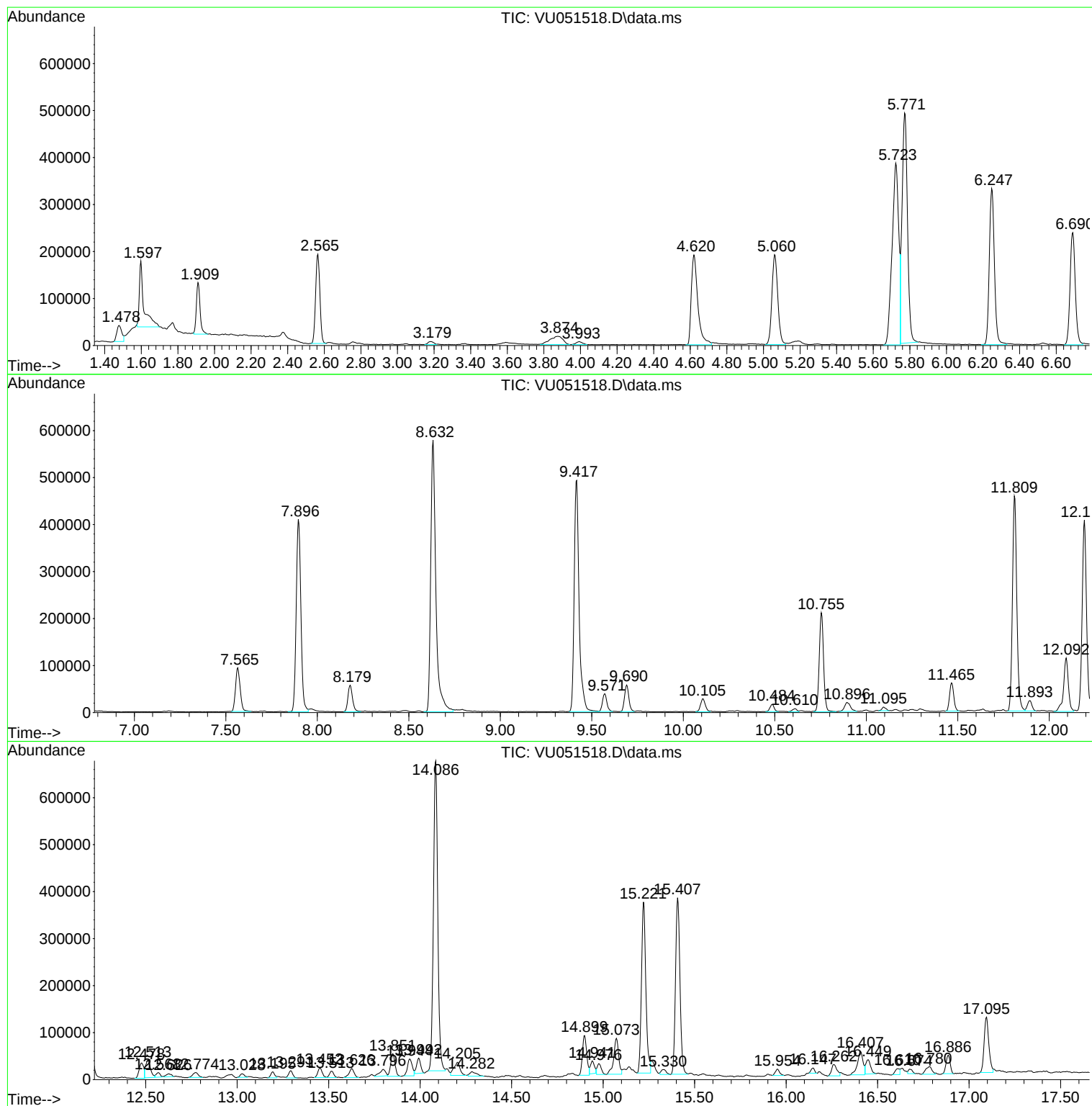
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ClientSampleId :
BHA92

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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BHA92

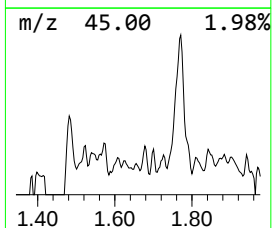
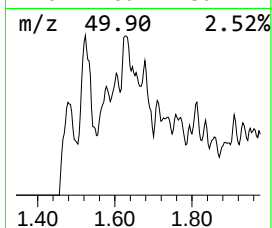
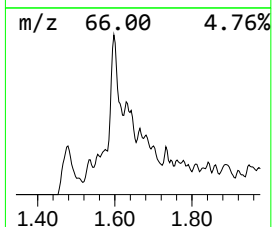
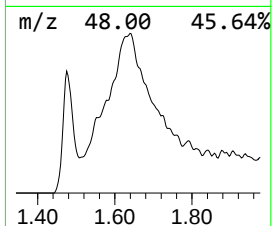
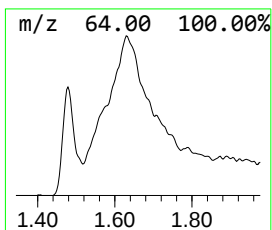
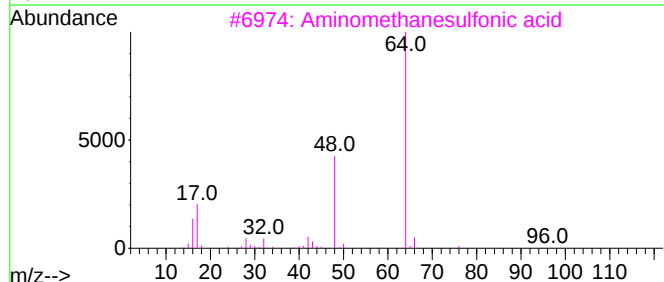
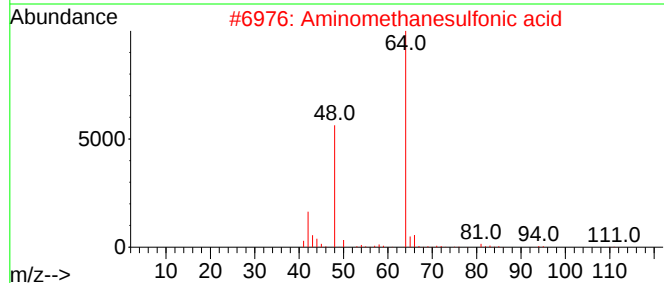
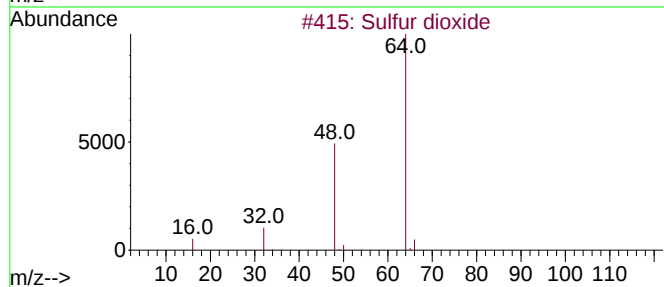
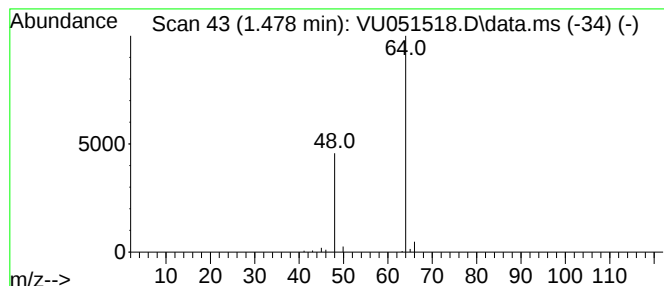
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.478	0.51 ug/L	65860	1,4-Difluorobenzene	6.247

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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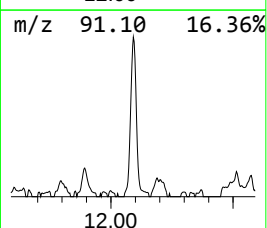
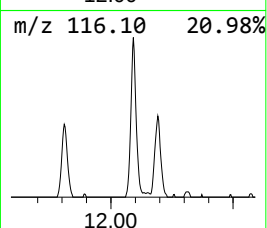
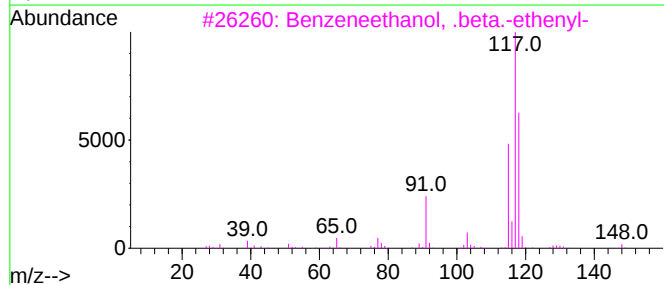
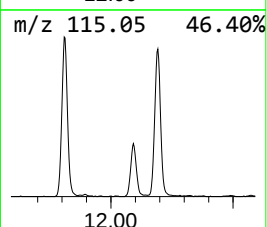
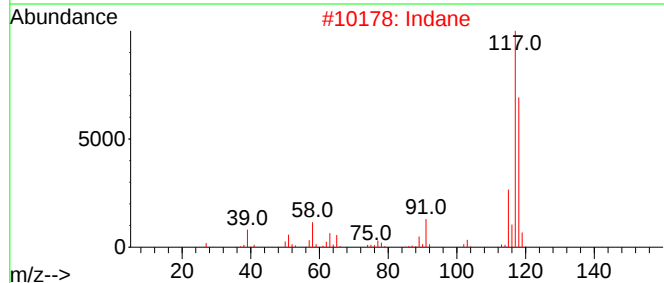
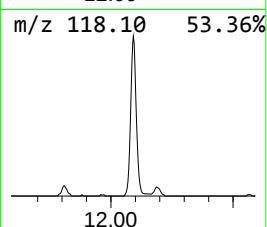
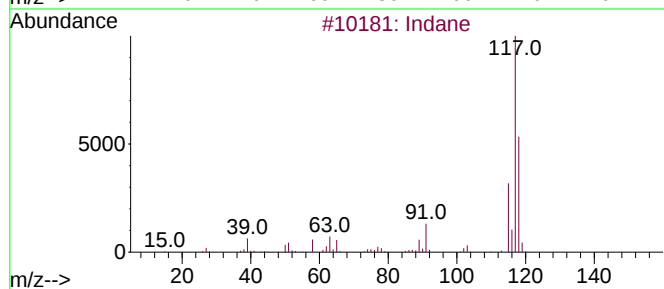
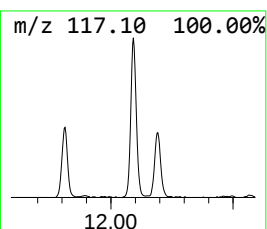
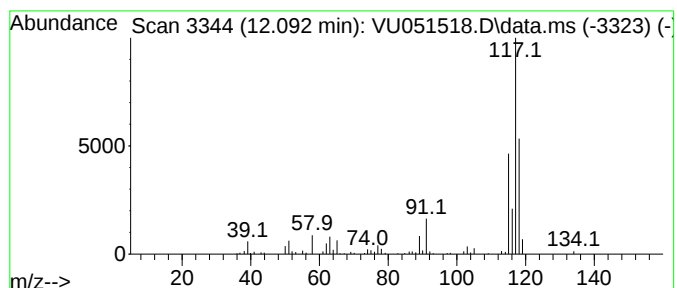
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	1.36 ug/L	207386	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane			118	C9H10	000496-11-7	76
2	Indane			118	C9H10	000496-11-7	70
3	Benzeneethanol, .beta.-ethenyl-			148	C10H12O	006052-63-7	64
4	Indane			118	C9H10	000496-11-7	55
5	7-Methylenecycloocta-1,3,5-triene			118	C9H10	002570-13-0	53



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ALS Vial : 26 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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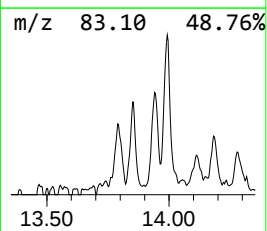
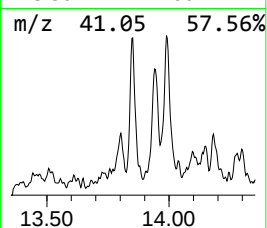
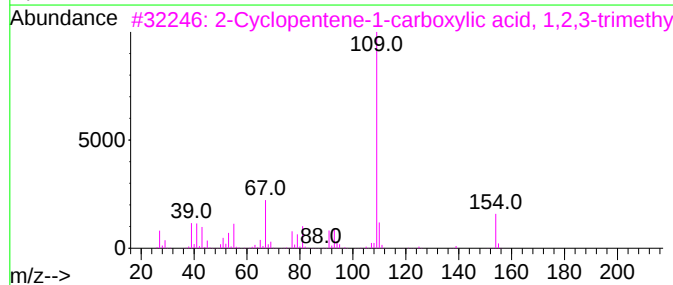
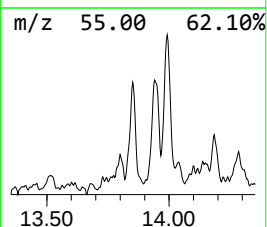
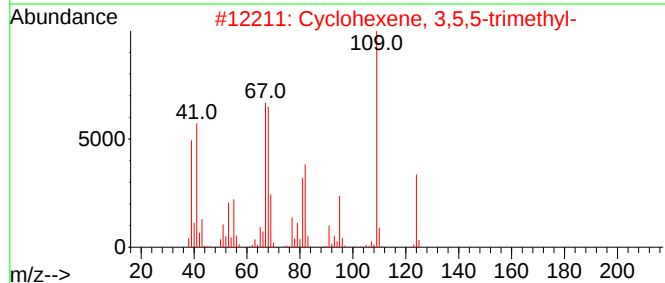
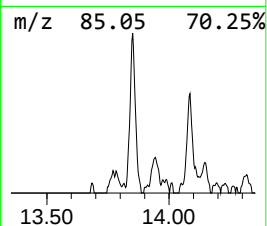
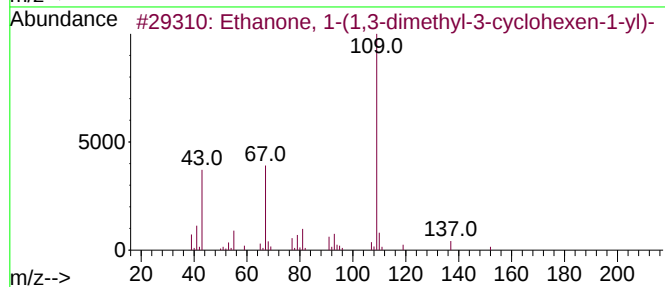
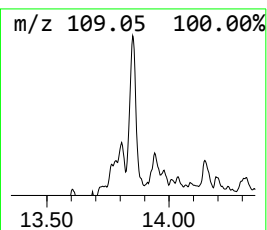
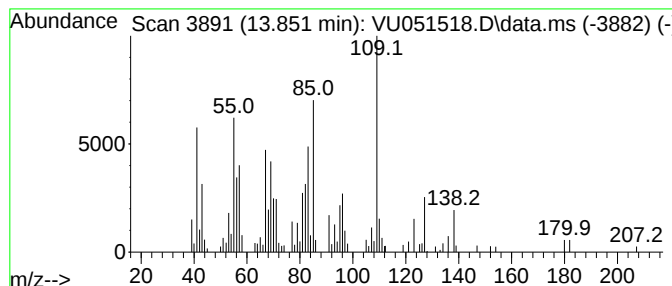
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 unknown-01 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.851	0.52 ug/L	79151	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(1,3-dimethyl-3-cycl...	152	C10H16O	051733-68-7	38
2			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	38
3			2-Cyclopentene-1-carboxylic acid...	154	C9H14O2	006894-69-5	35
4			2-(5-Methyl-furan-2-yl)-propiona...	138	C8H10O2	1000193-72-3	25
5			3,5-Dimethyl-4-propyl-1H-pyrazole	138	C8H14N2	081328-51-0	25



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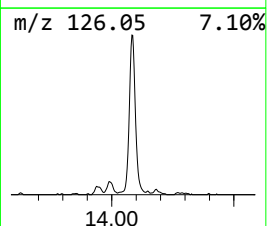
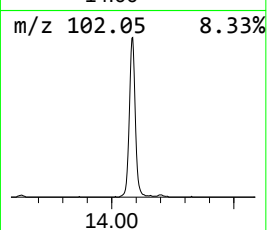
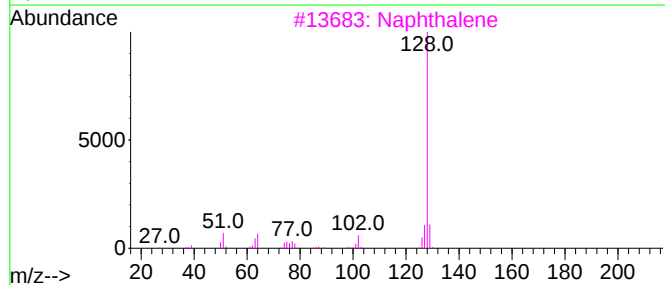
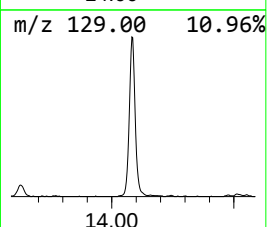
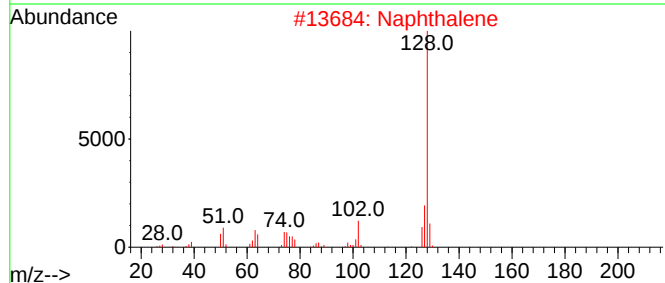
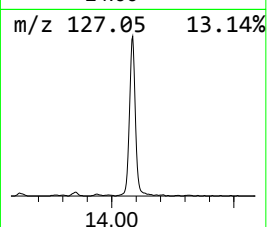
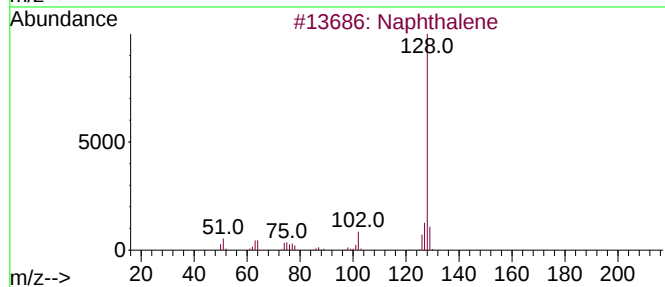
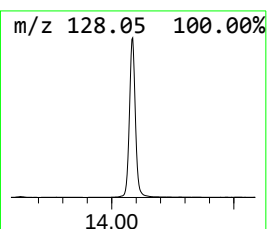
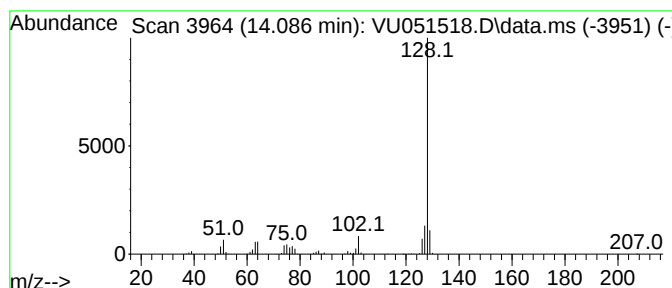
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
14.086	7.18 ug/L	1094470	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	94
3			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	93
5			Azulene	128	C10H8	000275-51-4	91



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Acq On : 26 Oct 2022 22:18
Operator : JC/MD
Sample : N5300-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

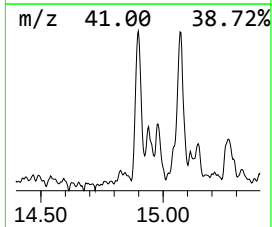
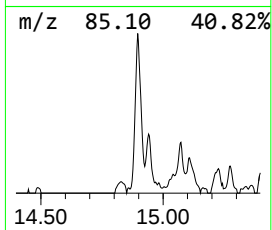
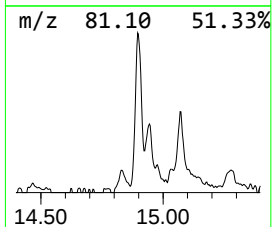
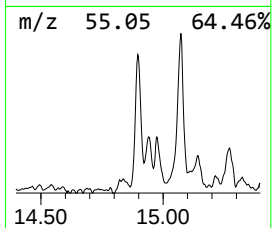
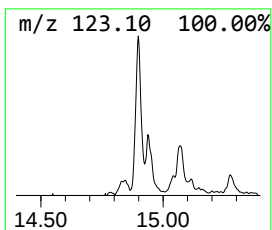
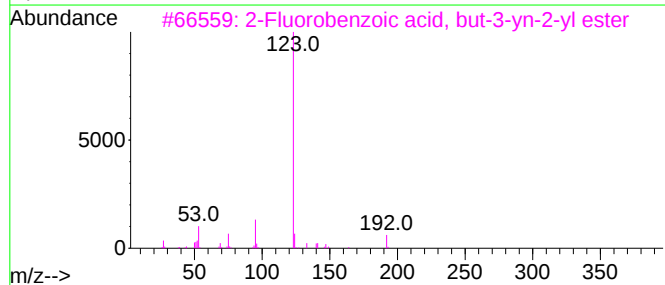
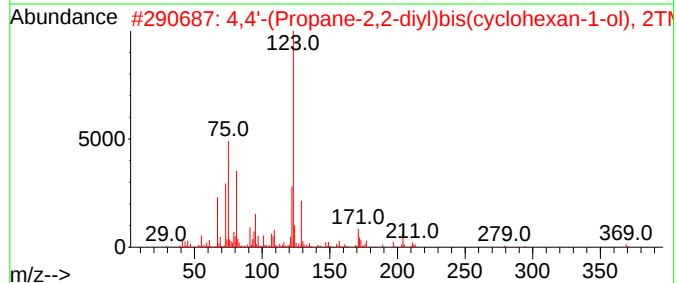
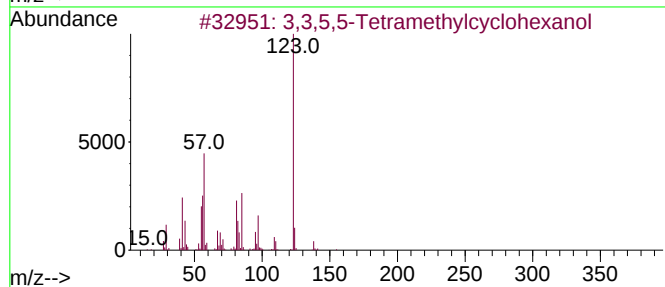
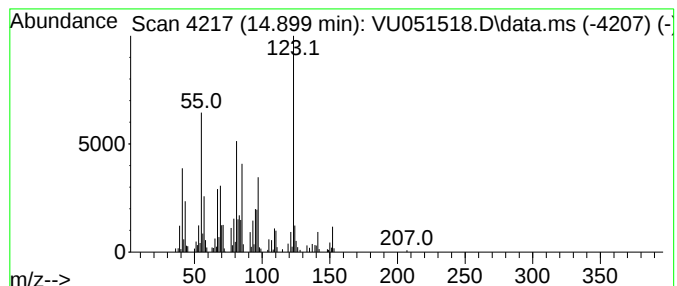
Instrument :
MSVOA_U
ClientSampleId :
BHA92

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 3,3,5,5-Tetramethylcyclohex... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
14.899	0.92 ug/L	140770	1,4-Dichlorobenzene-d4	11.809		
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3,3,5,5-Tetramethylcyclohexanol		156	C10H20O	002650-40-0	53
2	4,4'-(Propane-2,2-diyl)bis(cyclo...		384	C21H44O2Si2	1000496-96-0	43
3	2-Fluorobenzoic acid, but-3-yn-2...		192	C11H9FO2	1000299-16-1	38
4	Benzoic acid, octadecyl ester		374	C25H42O2	010578-34-4	35
5	5-Amino-1,3,3-trimethylcyclohexa...		562	C18H20F14N2O2	1000454-05-8	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051518.D
Acq On : 26 Oct 2022 22:18
Operator : JC/MD
Sample : N5300-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA92

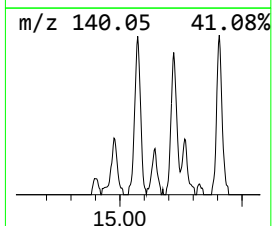
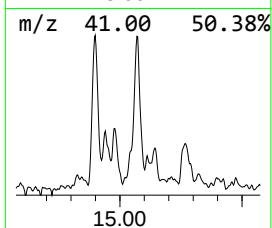
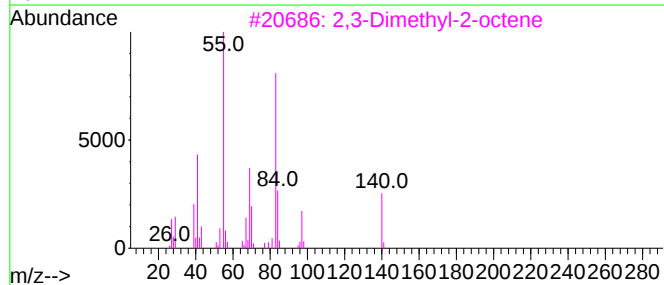
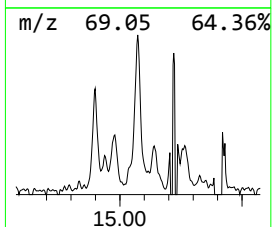
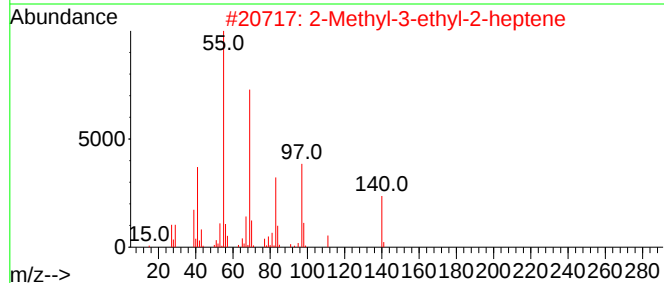
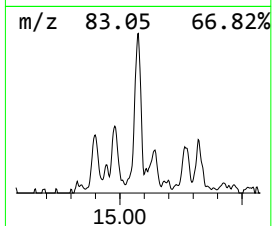
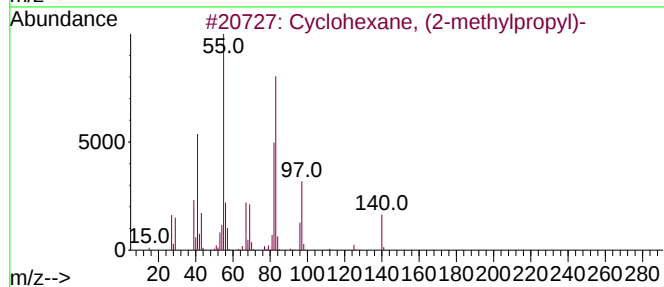
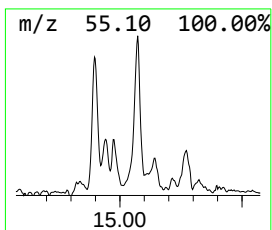
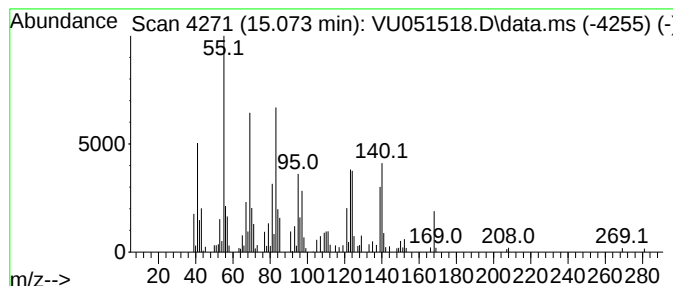
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Cyclic15.073 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.073	0.94 ug/L	142624	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	38
2			2-Methyl-3-ethyl-2-heptene	140	C10H20	019780-61-1	38
3			2,3-Dimethyl-2-octene	140	C10H20	019781-18-1	35
4			Cyclopropane, 1,1,2-trimethyl-3-...	140	C10H20	041977-43-9	30
5			Spiro[2.3]hexane-5-carboxylic ac...	278	C18H30O2	1000152-25-7	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051518.D
Acq On : 26 Oct 2022 22:18
Operator : JC/MD
Sample : N5300-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA92

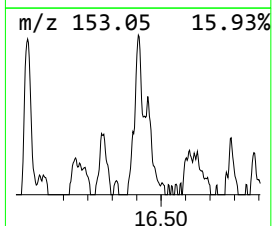
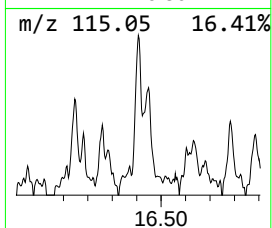
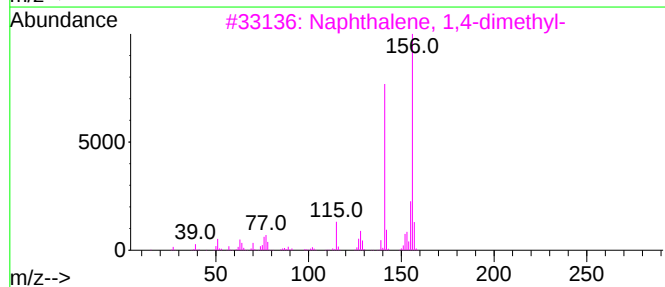
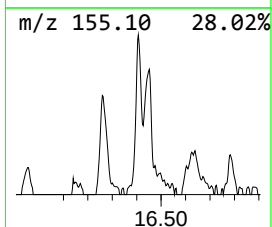
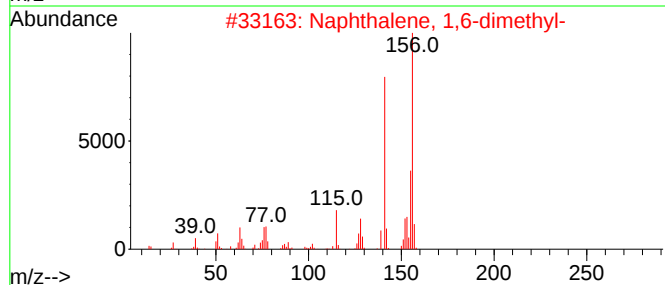
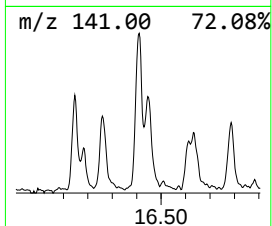
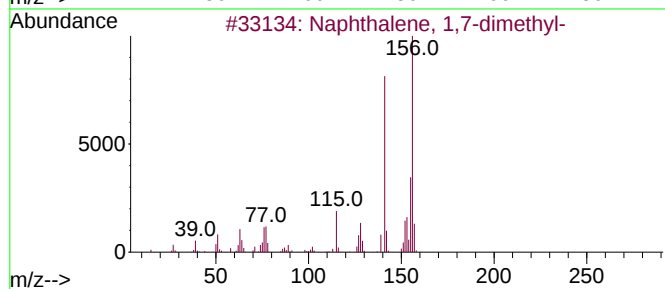
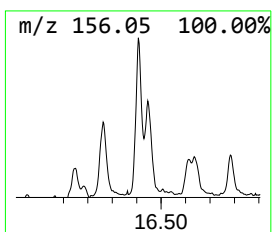
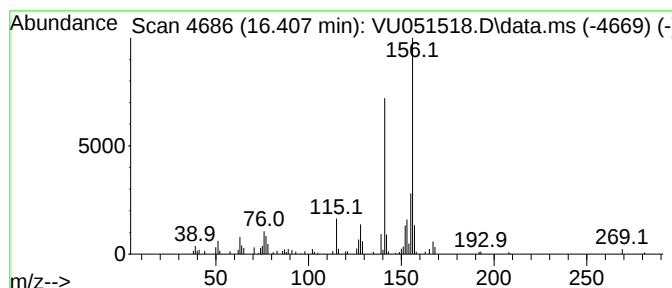
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 Naphthalene, 1,7-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.407	0.70 ug/L	106323	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	98
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051518.D
Acq On : 26 Oct 2022 22:18
Operator : JC/MD
Sample : N5300-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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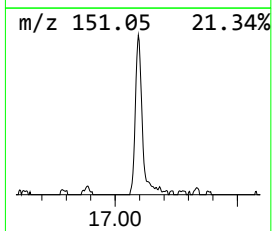
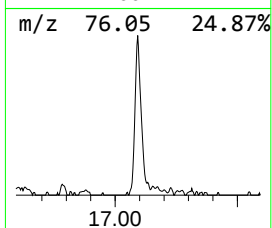
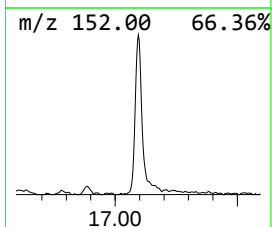
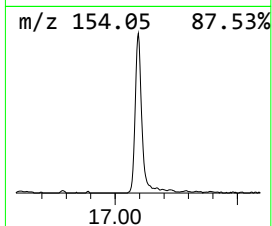
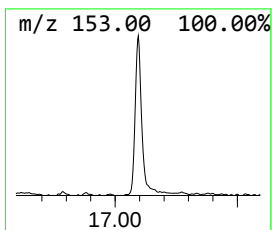
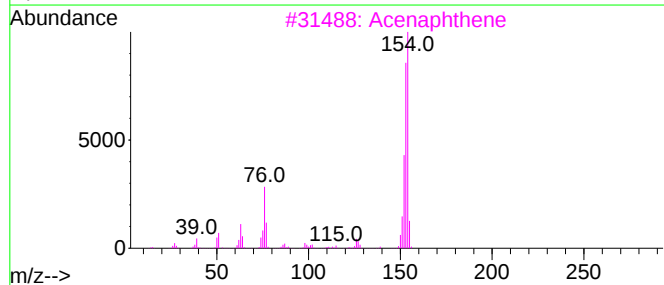
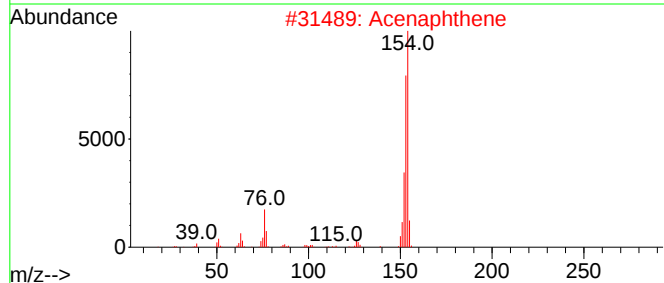
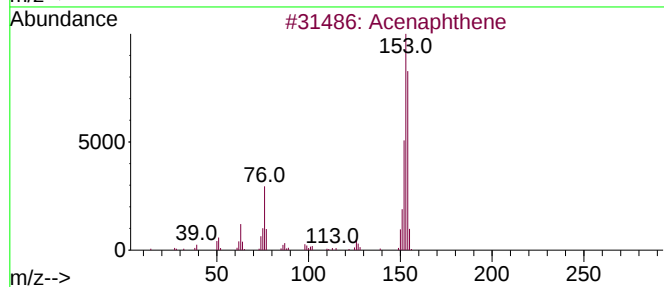
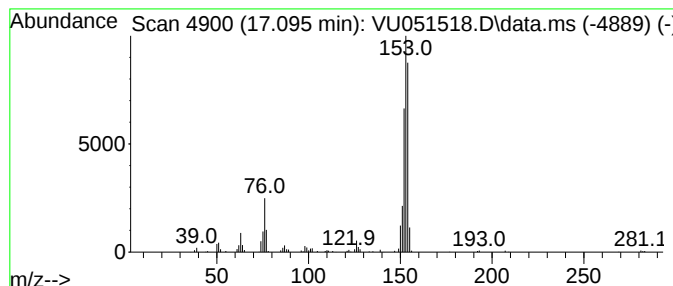
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.095	1.38 ug/L	209750	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	96
2			Acenaphthene	154	C12H10	000083-32-9	68
3			Acenaphthene	154	C12H10	000083-32-9	59
4			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	58
5			Acenaphthene	154	C12H10	000083-32-9	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051518.D
Acq On : 26 Oct 2022 22:18
Operator : JC/MD
Sample : N5300-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA92

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.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
Sulfur dioxide	1.478	0.5	ug/L	65860	1	6.247	642807	5.0
Indane	12.092	1.4	ug/L	207386	3	11.809	762511	5.0
unknown-01	13.851	0.5	ug/L	79151	3	11.809	762511	5.0
Azulene	14.086	7.2	ug/L	1094470	3	11.809	762511	5.0
3,3,5,5-Tetrame...	14.899	0.9	ug/L	140770	3	11.809	762511	5.0
(DEL) Alkane: C...	15.073	0.9	ug/L	142624	3	11.809	762511	5.0
Naphthalene, 1,...	16.407	0.7	ug/L	106323	3	11.809	762511	5.0
Hexa-2,4-diyne-1...	17.095	1.4	ug/L	209750	3	11.809	762511	5.0