

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111622\
 Data File : VV029032.D
 Acq On : 16 Nov 2022 21:44
 Operator : SY/MD
 Sample : N5604-10
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 H46G3

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: VV029032.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	37	rVB	237506	233248	22.62%	2.113%
2	1.301	72	81	90	rBV3	206197	324121	31.43%	2.937%
3	1.352	90	97	104	rVB2	29808	39100	3.79%	0.354%
4	1.413	109	116	147	rBV3	78421	258279	25.05%	2.340%
5	1.542	151	156	157	rVV2	40870	36911	3.58%	0.334%
6	1.564	158	163	178	rVB	111942	145432	14.10%	1.318%
7	1.764	219	225	232	rBV	24712	29995	2.91%	0.272%
8	1.815	233	241	255	rVB4	36796	60829	5.90%	0.551%
9	1.899	260	267	274	rBV	24266	30681	2.98%	0.278%
10	1.947	276	282	286	rVV2	18081	24173	2.34%	0.219%
11	1.976	287	291	299	rVV2	23327	29146	2.83%	0.264%
12	2.024	300	306	316	rVB2	18131	26938	2.61%	0.244%
13	2.105	321	331	348	rVB	221524	335046	32.49%	3.036%
14	2.474	423	446	468	rBV2	39105	107122	10.39%	0.971%
15	2.571	468	476	494	rVB3	10524	24436	2.37%	0.221%
16	2.761	520	535	550	rBV4	20974	42549	4.13%	0.386%
17	2.937	579	590	609	rBV3	8926	23782	2.31%	0.215%
18	3.188	660	668	686	rVV3	10366	32403	3.14%	0.294%
19	3.272	687	694	708	rVB3	8542	15903	1.54%	0.144%
20	3.439	733	746	760	rBV7	6375	16696	1.62%	0.151%
21	3.580	778	790	803	rVB6	5722	12310	1.19%	0.112%
22	3.757	832	845	856	rBV4	6677	14986	1.45%	0.136%
23	3.905	881	891	916	rBV2	40644	161104	15.62%	1.460%
24	4.343	1012	1027	1053	rBV	151375	390416	37.86%	3.538%
25	4.670	1115	1129	1143	rVV6	9419	24755	2.40%	0.224%
26	4.757	1143	1156	1180	rVB7	13701	44132	4.28%	0.400%
27	4.934	1204	1211	1225	rVB10	5260	12740	1.24%	0.115%
28	5.043	1229	1245	1281	rBV2	367048	1031182	100.00%	9.343%
29	5.224	1291	1301	1317	rVB3	18478	48373	4.69%	0.438%
30	5.310	1318	1328	1339	rVV4	9623	20964	2.03%	0.190%
31	5.371	1340	1347	1369	rVB4	7324	18667	1.81%	0.169%
32	5.613	1411	1422	1456	rBV	270839	627201	60.82%	5.683%
33	5.947	1510	1526	1544	rBV5	35080	84187	8.16%	0.763%
34	6.066	1549	1563	1593	rBV	200834	447956	43.44%	4.059%
35	6.458	1675	1685	1699	rVB4	9022	18914	1.83%	0.171%
36	6.558	1699	1716	1717	rBV6	10098	20357	1.97%	0.184%

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37	6.648	1731	1744	1763	rVB4	17234	44469	4.31%	0.403%
38	6.770	1767	1782	1798	rBV4	30957	73128	7.09%	0.663%
39	6.982	1831	1848	1884	rBV	102133	221242	21.46%	2.005%
40	7.159	1888	1903	1906	rBV	4864	10346	1.00%	0.094%
41	7.262	1920	1935	1937	rBV6	10035	15977	1.55%	0.145%
42	7.310	1939	1950	1966	rVV	470454	848445	82.28%	7.688%
43	7.387	1966	1974	1986	rVB	74553	126746	12.29%	1.148%
44	7.622	2039	2047	2065	rVB2	48527	111001	10.76%	1.006%
45	7.783	2092	2097	2105	rVB3	10091	14530	1.41%	0.132%
46	7.838	2105	2114	2137	rVB2	30163	71119	6.90%	0.644%
47	8.088	2181	2192	2225	rBV	301766	765250	74.21%	6.934%
48	8.342	2263	2271	2279	rBV3	11661	21223	2.06%	0.192%
49	8.506	2310	2322	2337	rVB5	17559	34649	3.36%	0.314%
50	8.847	2417	2428	2458	rBV	385236	677108	65.66%	6.135%
51	9.008	2469	2478	2498	rBV	71267	121190	11.75%	1.098%
52	9.133	2498	2517	2537	rVB	128550	240699	23.34%	2.181%
53	9.481	2615	2625	2634	rVB9	5049	11052	1.07%	0.100%
54	9.538	2634	2643	2662	rBV	59431	98377	9.54%	0.891%
55	9.927	2753	2764	2781	rBV2	14959	30374	2.95%	0.275%
56	10.011	2781	2790	2800	rVB2	18946	29909	2.90%	0.271%
57	10.207	2838	2851	2871	rVB	148330	248103	24.06%	2.248%
58	10.355	2888	2897	2912	rVB4	6942	15760	1.53%	0.143%
59	10.445	2912	2925	2930	rBV3	15666	25592	2.48%	0.232%
60	10.735	3006	3015	3027	rVB4	8306	15127	1.47%	0.137%
61	10.911	3060	3070	3085	rVB2	14155	22568	2.19%	0.204%
62	11.188	3147	3156	3162	rBV5	6890	10448	1.01%	0.095%
63	11.243	3162	3173	3192	rVV	405077	655710	63.59%	5.941%
64	11.329	3192	3200	3214	rVB2	18794	32001	3.10%	0.290%
65	11.532	3250	3263	3270	rBV6	30950	65731	6.37%	0.596%
66	11.616	3279	3289	3312	rVB	478390	812158	78.76%	7.359%
67	11.815	3340	3351	3361	rBV	22329	36219	3.51%	0.328%
68	11.905	3368	3379	3384	rBV2	19341	30058	2.91%	0.272%
69	12.008	3402	3411	3428	rVB	29681	50097	4.86%	0.454%
70	12.107	3433	3442	3450	rBV3	15615	24872	2.41%	0.225%
71	12.300	3493	3502	3512	rBV5	6046	10932	1.06%	0.099%
72	12.403	3527	3534	3543	rVV	18956	27170	2.63%	0.246%
73	12.458	3543	3551	3563	rVB	22887	34768	3.37%	0.315%
74	12.873	3671	3680	3689	rVB3	28117	44283	4.29%	0.401%
75	13.259	3792	3800	3806	rBV6	7516	10830	1.05%	0.098%
76	13.603	3897	3907	3916	rBV2	28079	42991	4.17%	0.390%

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77	13.696	3924	3936	3949	rBV2	26987	45556	4.42%	0.413%
78	14.098	4046	4061	4081	rVB7	14870	37740	3.66%	0.342%
79	14.213	4083	4097	4107	rBV6	10982	20361	1.97%	0.184%
80	14.287	4107	4120	4131	rVB5	15762	29685	2.88%	0.269%
81	14.419	4153	4161	4175	rBV7	11139	22329	2.17%	0.202%
82	14.603	4209	4218	4232	rBV3	27659	56924	5.52%	0.516%
83	14.673	4232	4240	4254	rVB4	27780	53137	5.15%	0.481%
84	14.754	4254	4265	4275	rBV5	9201	16752	1.62%	0.152%
85	14.869	4292	4301	4306	rBV8	12277	20449	1.98%	0.185%
86	14.905	4306	4312	4324	rVV9	11568	20023	1.94%	0.181%
87	14.995	4326	4340	4349	rBV8	9741	23065	2.24%	0.209%
88	15.149	4380	4388	4401	rVB8	7127	16366	1.59%	0.148%
89	15.326	4428	4443	4460	rVB4	13472	39615	3.84%	0.359%
90	15.406	4460	4468	4476	rBV9	9422	15246	1.48%	0.138%
91	15.548	4504	4512	4518	rBV8	6875	11496	1.11%	0.104%
92	15.808	4584	4593	4598	rBV9	6097	10461	1.01%	0.095%

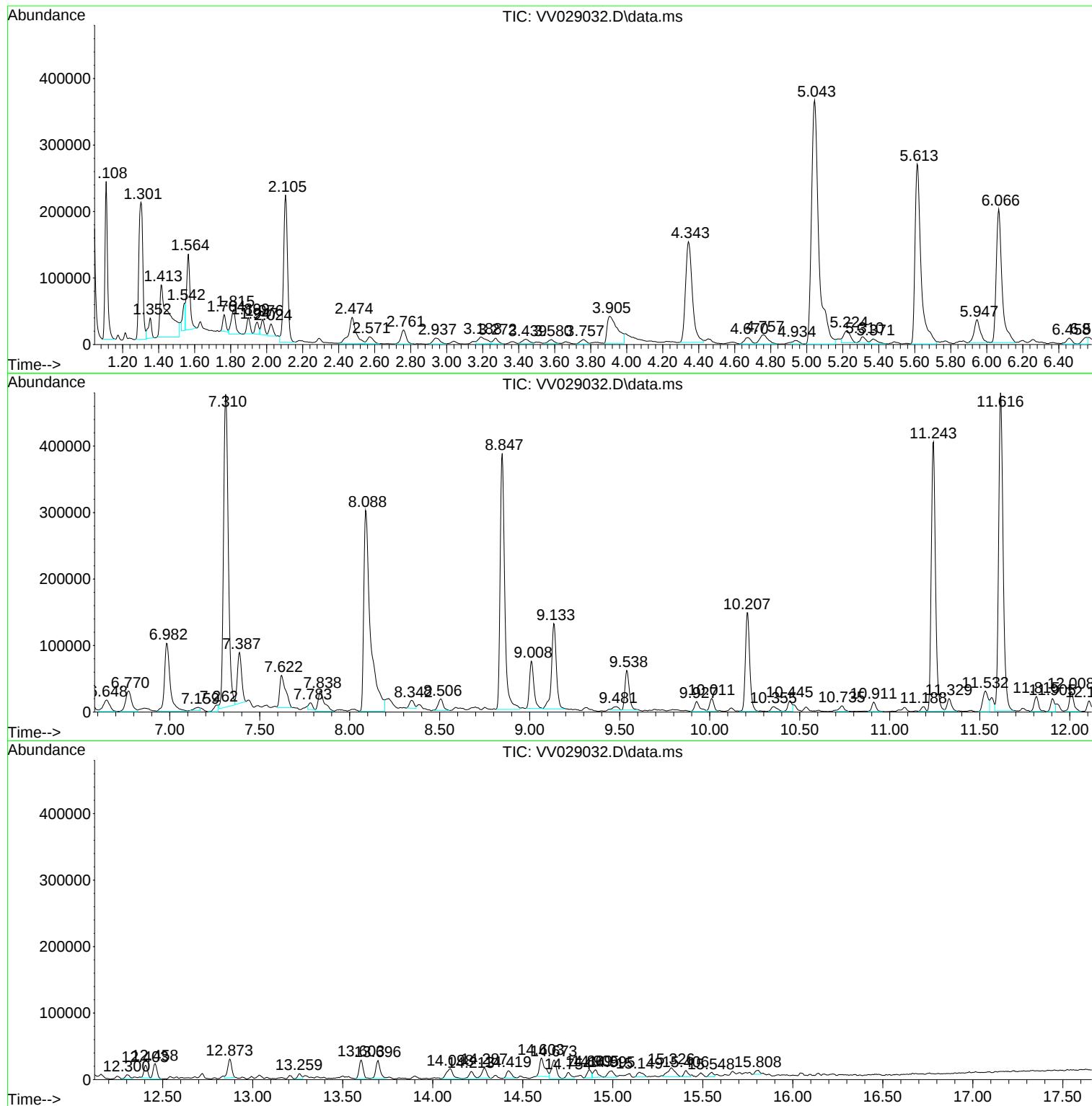
Sum of corrected areas: 11036491

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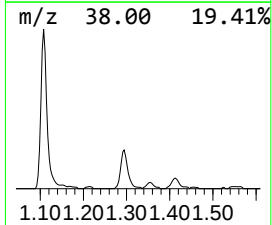
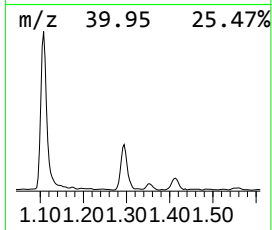
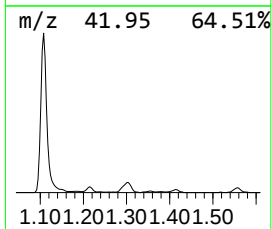
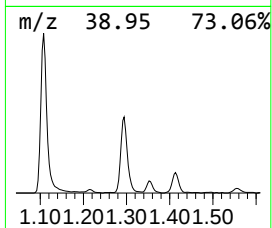
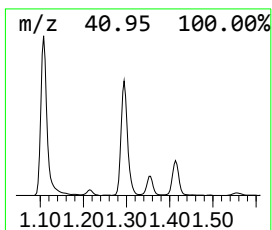
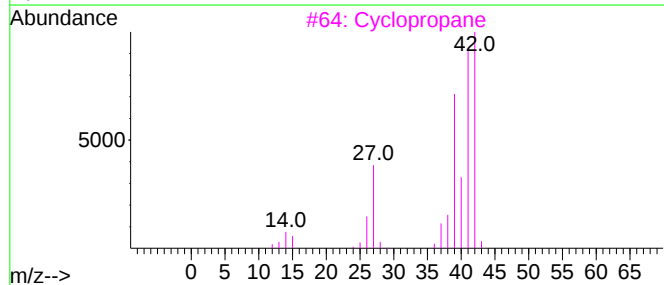
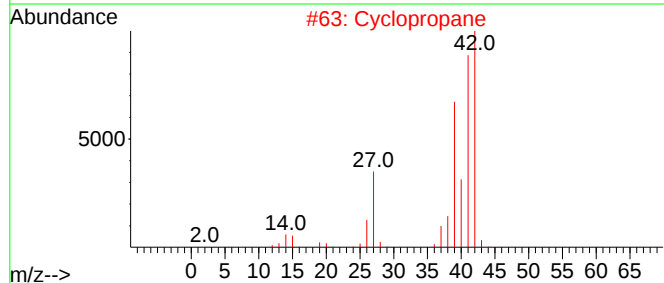
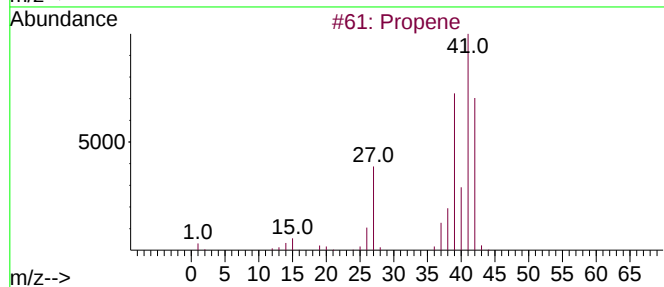
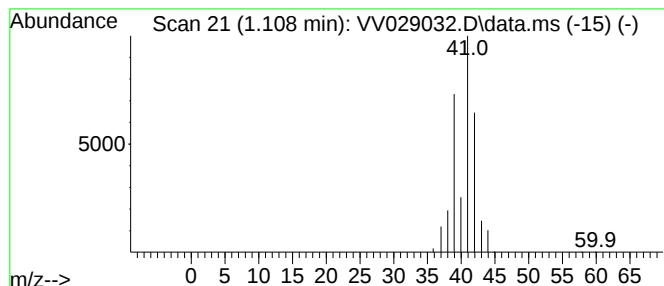
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.108	1.86 ug/L	233248	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	47
3			Cyclopropane	42	C3H6	000075-19-4	38
4			Cyclopropene	40	C3H4	002781-85-3	37
5			Propene	42	C3H6	000115-07-1	16



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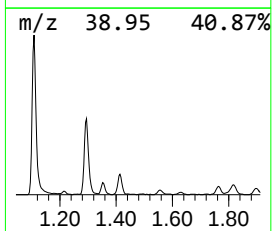
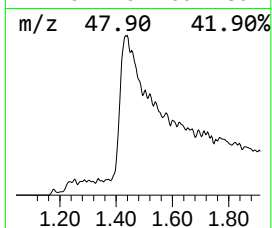
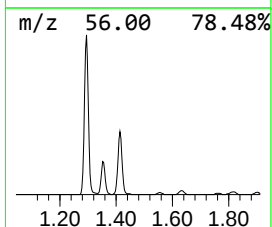
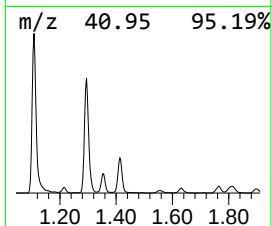
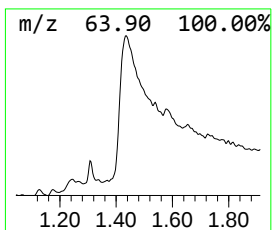
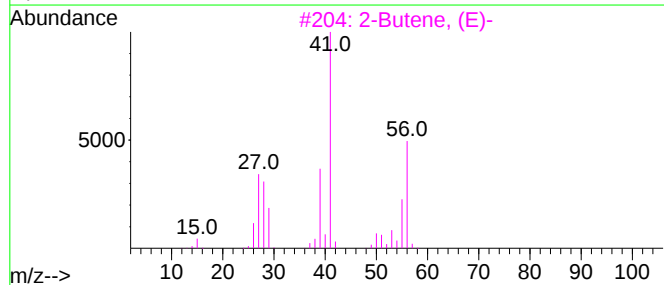
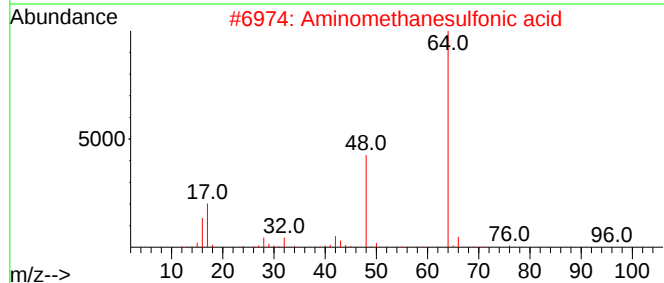
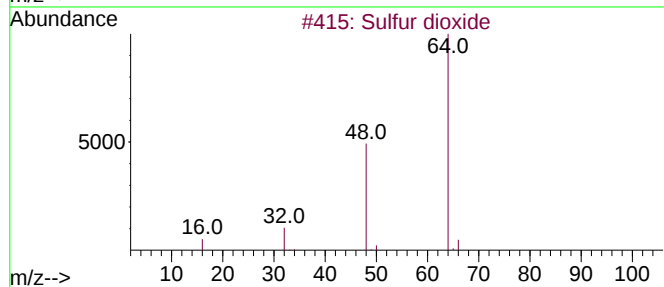
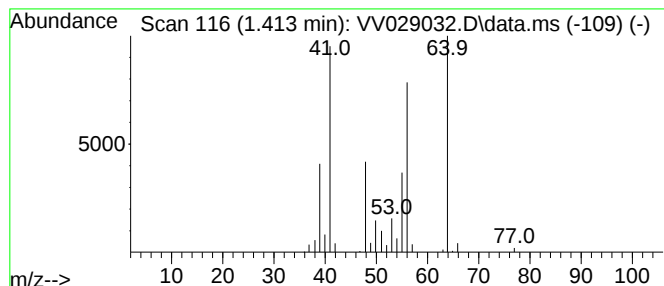
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.413	2.06 ug/L	258279	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	40
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	33
3			2-Butene, (E)-	56	C4H8	000624-64-6	15
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	11
5			2-Butene, (Z)-	56	C4H8	000590-18-1	11



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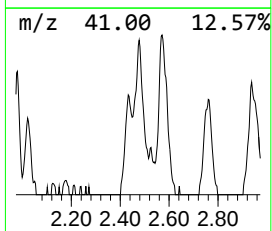
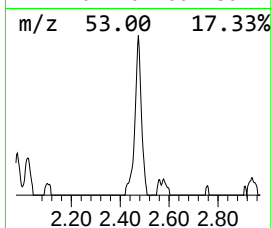
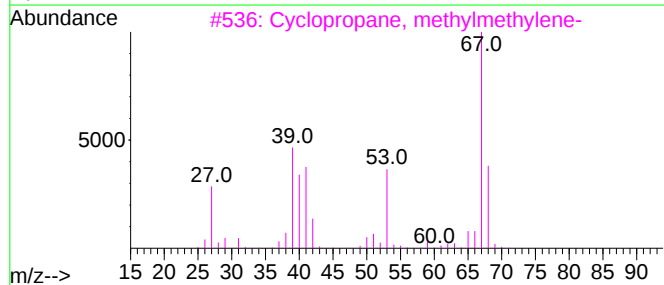
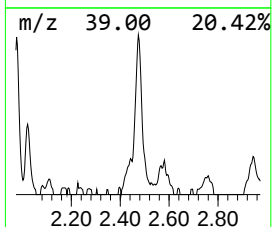
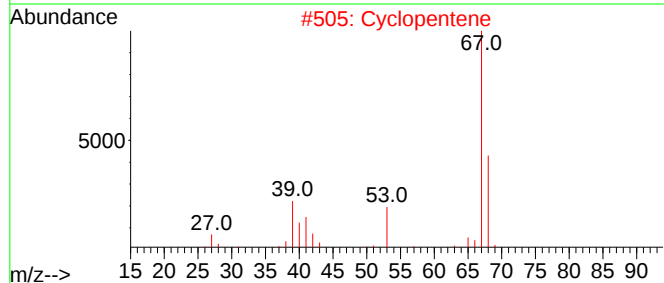
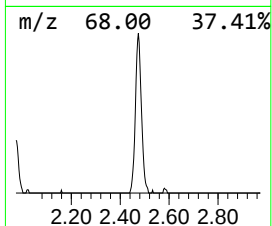
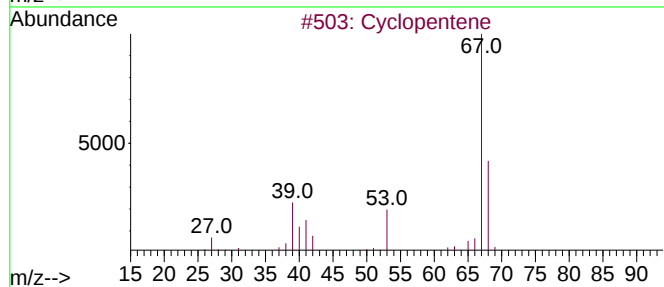
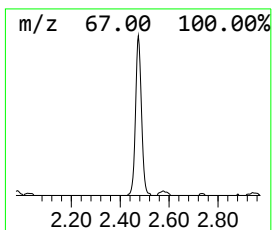
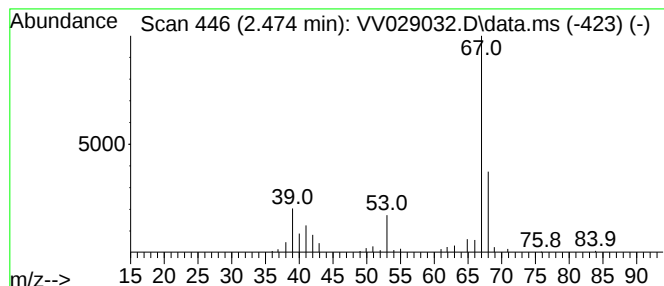
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Cyclopentene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.474	0.85 ug/L	107122	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene	68	C5H8	000142-29-0	91
2			Cyclopentene	68	C5H8	000142-29-0	91
3			Cyclopropane, methylmethylene-	68	C5H8	018631-84-0	91
4			Cyclopentene	68	C5H8	000142-29-0	91
5			Cyclopentene	68	C5H8	000142-29-0	91



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H46G3

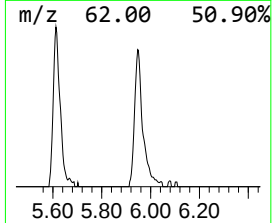
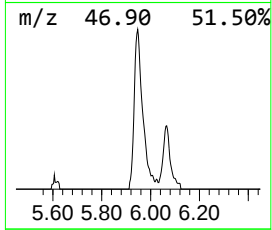
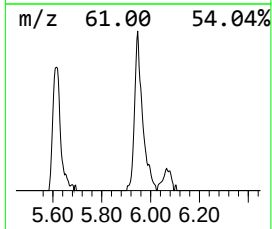
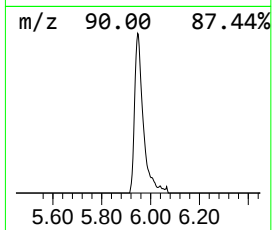
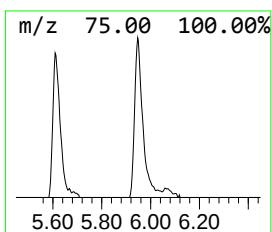
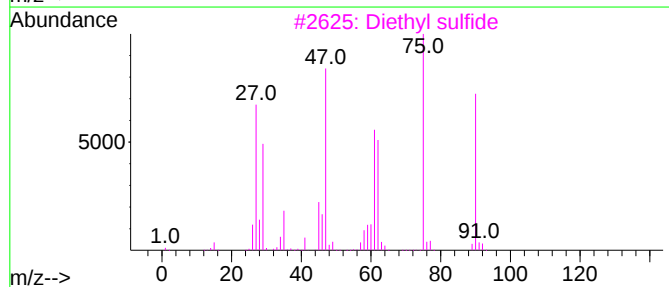
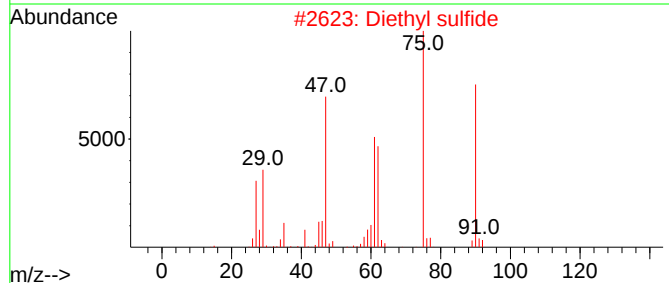
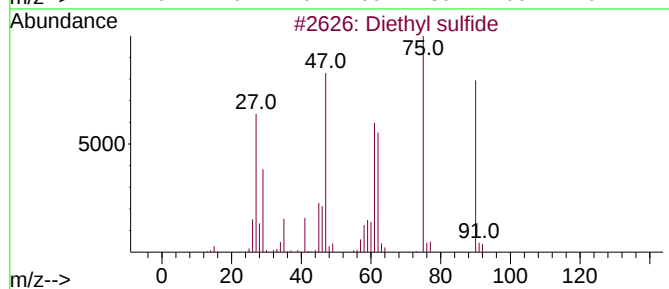
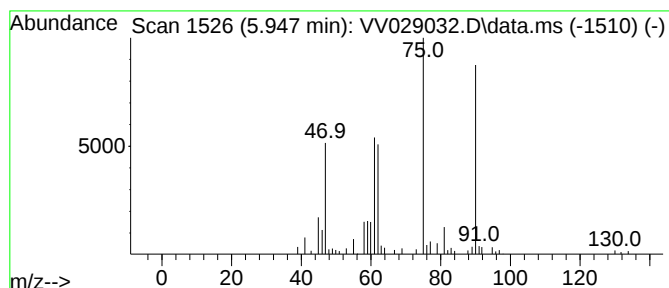
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Diethyl sulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.947	0.67 ug/L	84187	1,4-Difluorobenzene	5.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl sulfide	90	C4H10S	000352-93-2	95
2	Diethyl sulfide	90	C4H10S	000352-93-2	91
3	Diethyl sulfide	90	C4H10S	000352-93-2	91
4	Diethyl sulfide	90	C4H10S	000352-93-2	91
5	Sulfur diimide, dimethyl-	90	C2H6N2S	013849-02-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111622\
Data File : VV029032.D
Acq On : 16 Nov 2022 21:44
Operator : SY/MD
Sample : N5604-10
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
H46G3

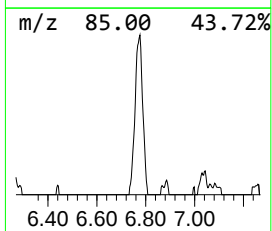
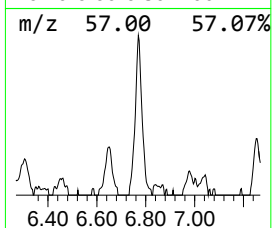
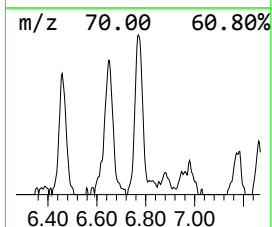
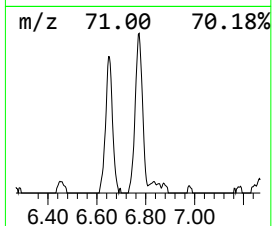
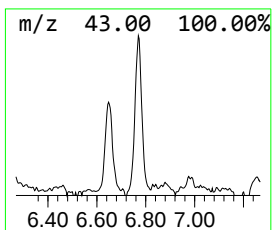
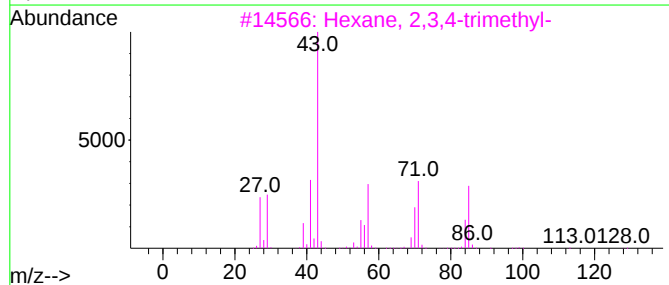
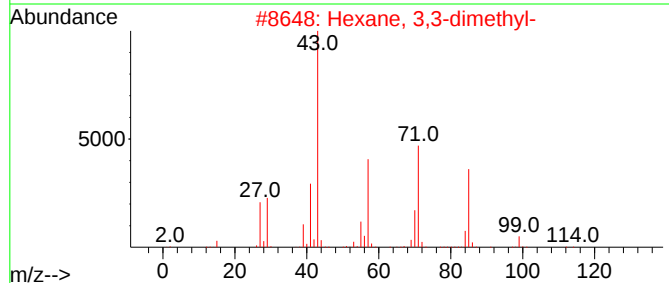
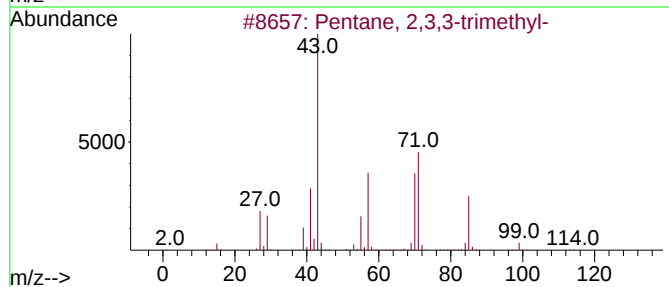
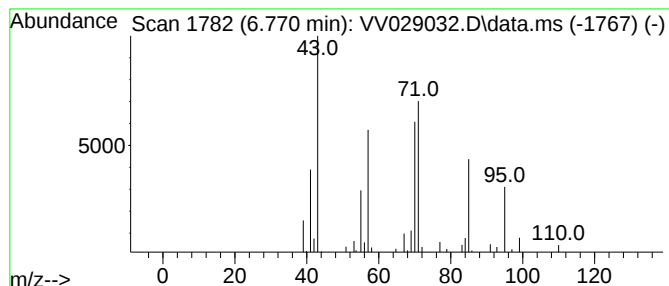
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.770	0.58 ug/L	73128	1,4-Difluorobenzene	5.613

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	59
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	47
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	47
4	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	47
5	Hexadecane	226	C16H34	000544-76-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111622\
Data File : VV029032.D
Acq On : 16 Nov 2022 21:44
Operator : SY/MD
Sample : N5604-10
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
H46G3

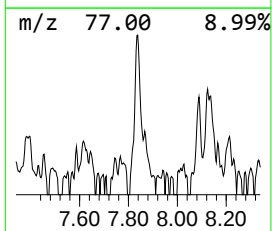
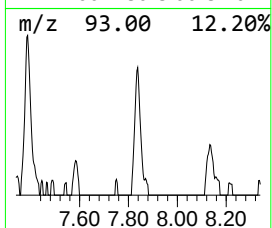
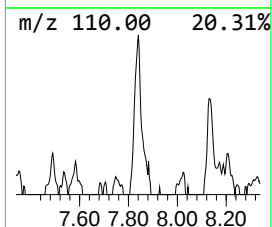
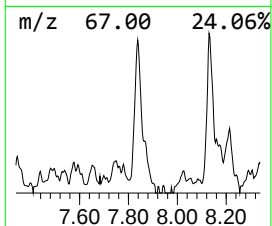
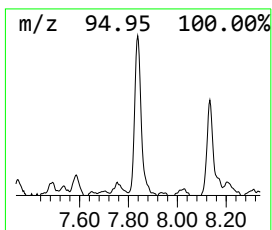
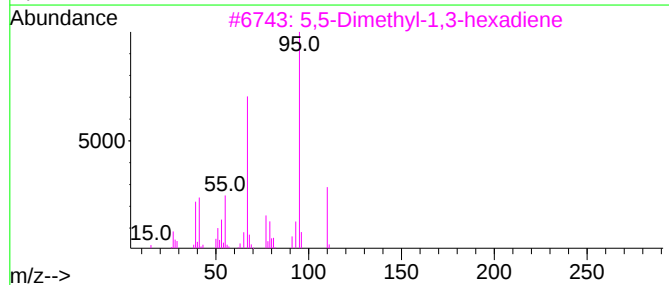
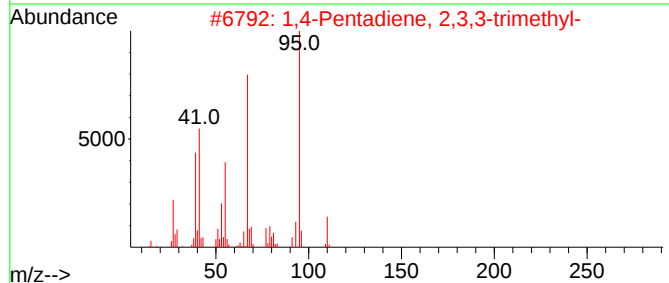
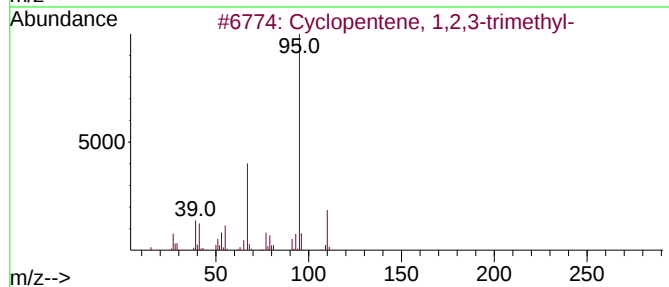
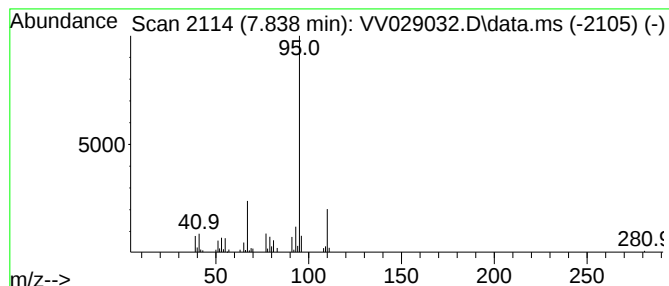
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.838	0.53 ug/L	71119	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	91
2			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	91
3			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	90
4			1-(3H-Imidazol-4-yl)-ethanone	110	C5H6N2O	061985-25-9	72
5			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111622\
Data File : VV029032.D
Acq On : 16 Nov 2022 21:44
Operator : SY/MD
Sample : N5604-10
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
H46G3

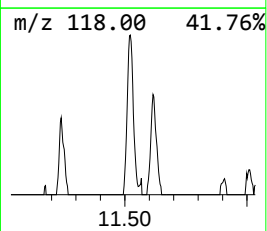
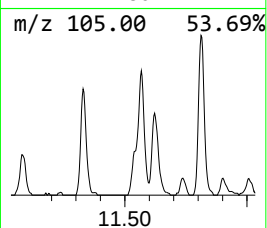
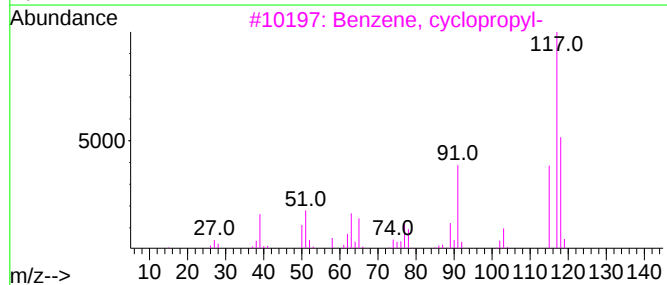
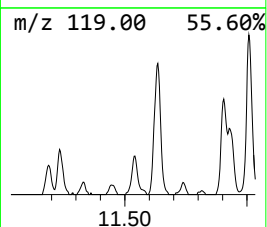
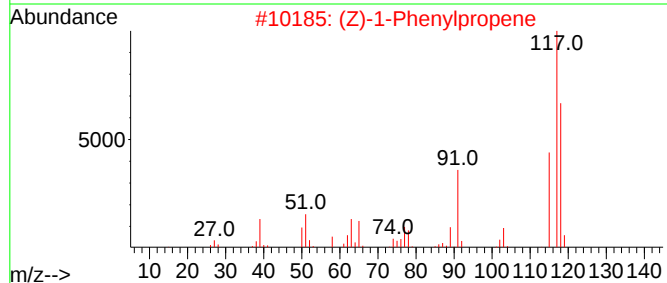
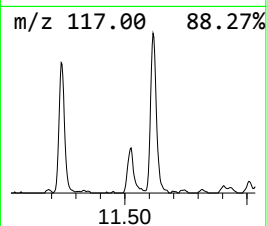
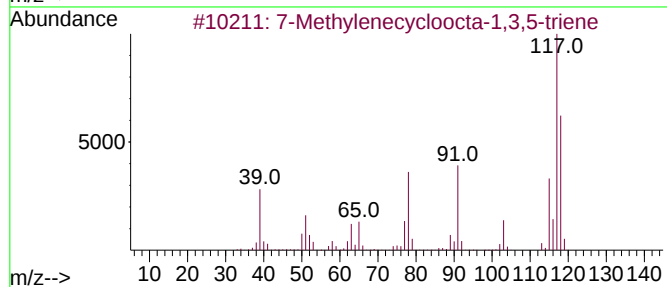
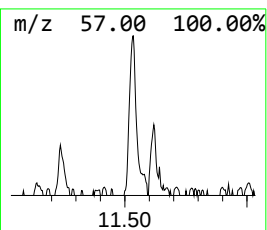
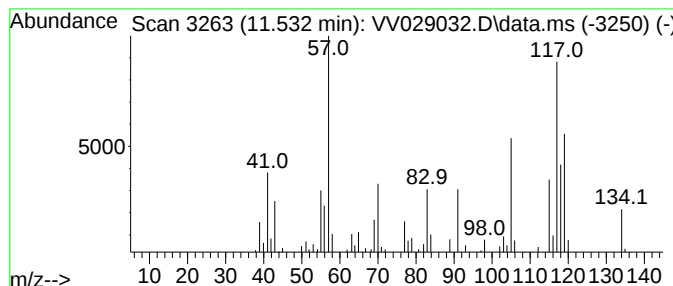
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 7-Methylenecycloocta-1,3,5-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.532	0.50 ug/L	65731	1,4-Dichlorobenzene-d4	11.243

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		7-Methylenecycloocta-1,3,5-triene	118	C9H10	002570-13-0	50
2		(Z)-1-Phenylpropene	118	C9H10	000766-90-5	50
3		Benzene, cyclopropyl-	118	C9H10	000873-49-4	50
4		Deltacyclene	118	C9H10	007785-10-6	45
5		Indane	118	C9H10	000496-11-7	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111622\
Data File : VV029032.D
Acq On : 16 Nov 2022 21:44
Operator : SY/MD
Sample : N5604-10
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
H46G3

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	1.9	ug/L	233248	1	5.613	627201	5.0
unknown-01	1.413	2.1	ug/L	258279	1	5.613	627201	5.0
Cyclopentene	2.474	0.8	ug/L	107122	1	5.613	627201	5.0
Diethyl sulfide	5.947	0.7	ug/L	84187	1	5.613	627201	5.0
(DEL) Alkane: S...	6.770	0.6	ug/L	73128	1	5.613	627201	5.0
Cyclopentene, 1...	7.838	0.5	ug/L	71119	2	8.847	677108	5.0
7-Methylenecycl...	11.532	0.5	ug/L	65731	3	11.243	655710	5.0