

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061622\
 Data File : VU049215.D
 Acq On : 16 Jun 2022 19:34
 Operator : SY/MD
 Sample : N3285-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4P6

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\SFAMUTR061422WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU049215.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	22	rVB2	37720	35904	6.60%	0.818%
2	1.481	41	44	49	rVB	7978	6410	1.18%	0.146%
3	1.591	67	78	88	rBV2	59880	84144	15.46%	1.917%
4	1.784	133	138	150	rVB	19618	25929	4.76%	0.591%
5	1.906	170	176	185	rVB	40165	48323	8.88%	1.101%
6	2.559	369	379	392	rVB	82977	134818	24.77%	3.071%
7	2.681	405	417	427	rBV2	37818	76264	14.01%	1.737%
8	3.041	506	529	550	rBV	53821	115608	21.24%	2.633%
9	3.870	772	787	801	rBV2	18874	43512	8.00%	0.991%
10	3.960	802	815	832	rVB6	6311	17350	3.19%	0.395%
11	4.687	1024	1041	1058	rBV	44044	166706	30.63%	3.797%
12	5.063	1144	1158	1175	rBV	77509	171747	31.56%	3.912%
13	5.722	1344	1363	1395	rBV2	162524	415833	76.41%	9.471%
14	6.250	1513	1527	1546	rVB	157496	296987	54.57%	6.764%
15	6.690	1652	1664	1681	rBV	100366	196710	36.15%	4.480%
16	6.796	1689	1697	1715	rVB4	3679	10069	1.85%	0.229%
17	7.176	1802	1815	1823	rBV6	3293	7623	1.40%	0.174%
18	7.565	1925	1936	1953	rBV	52296	91506	16.81%	2.084%
19	7.806	1996	2011	2026	rBV5	23083	62337	11.45%	1.420%
20	7.896	2027	2039	2053	rVV	190651	330554	60.74%	7.529%
21	7.970	2054	2062	2075	rVV2	13522	24871	4.57%	0.566%
22	8.179	2117	2127	2140	rBV2	31538	52294	9.61%	1.191%
23	8.250	2140	2149	2162	rVV2	6500	12769	2.35%	0.291%
24	8.475	2209	2219	2229	rBV3	3835	8018	1.47%	0.183%
25	8.639	2258	2270	2307	rBV	250329	544224	100.00%	12.396%
26	9.417	2500	2512	2532	rBV	215027	358657	65.90%	8.169%
27	9.693	2585	2598	2609	rBV2	8056	12754	2.34%	0.290%
28	10.758	2918	2929	2943	rVB	82930	133662	24.56%	3.044%
29	10.893	2957	2971	2982	rBV3	8775	13680	2.51%	0.312%
30	11.812	3244	3257	3276	rBV	229661	368055	67.63%	8.383%
31	12.060	3319	3334	3351	rBV	57435	106739	19.61%	2.431%
32	12.195	3364	3376	3398	rVB	187140	312782	57.47%	7.124%
33	12.545	3476	3485	3498	rBV6	4236	9143	1.68%	0.208%
34	12.950	3600	3611	3622	rBV2	10918	17508	3.22%	0.399%
35	13.291	3704	3717	3724	rBV10	6107	9806	1.80%	0.223%
36	13.513	3775	3786	3797	rVB6	5808	10431	1.92%	0.238%

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ALS Vial : 25 Sample Multiplier: 1

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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_U\Method\SFAMUTR061422WMA.M
Title : TRACE VOA SFAM1.0

37	13.741	3843	3857	3865	rBV8	5354	9552	1.76%	0.218%
38	16.770	4788	4799	4812	rBV5	26666	47197	8.67%	1.075%

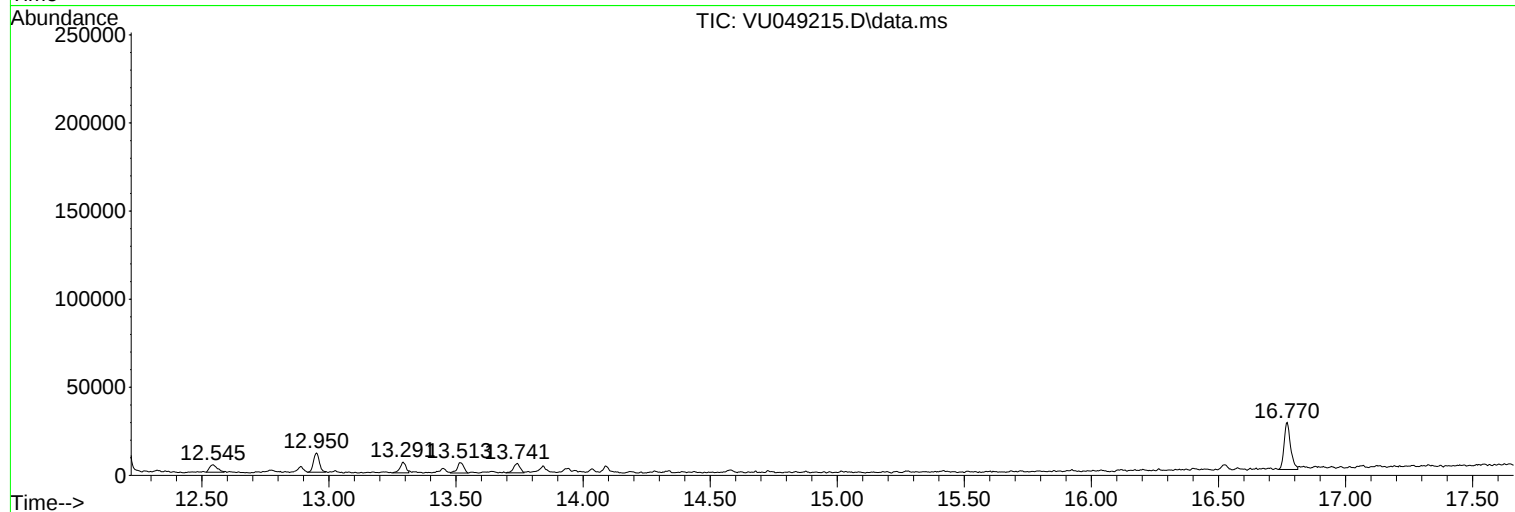
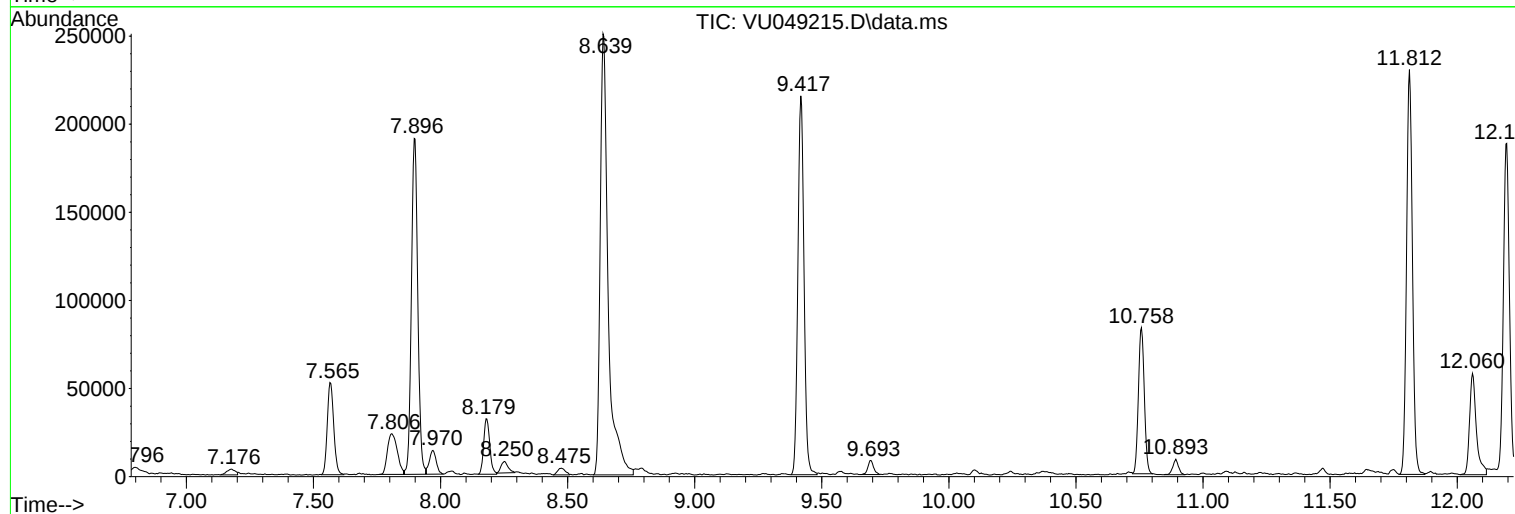
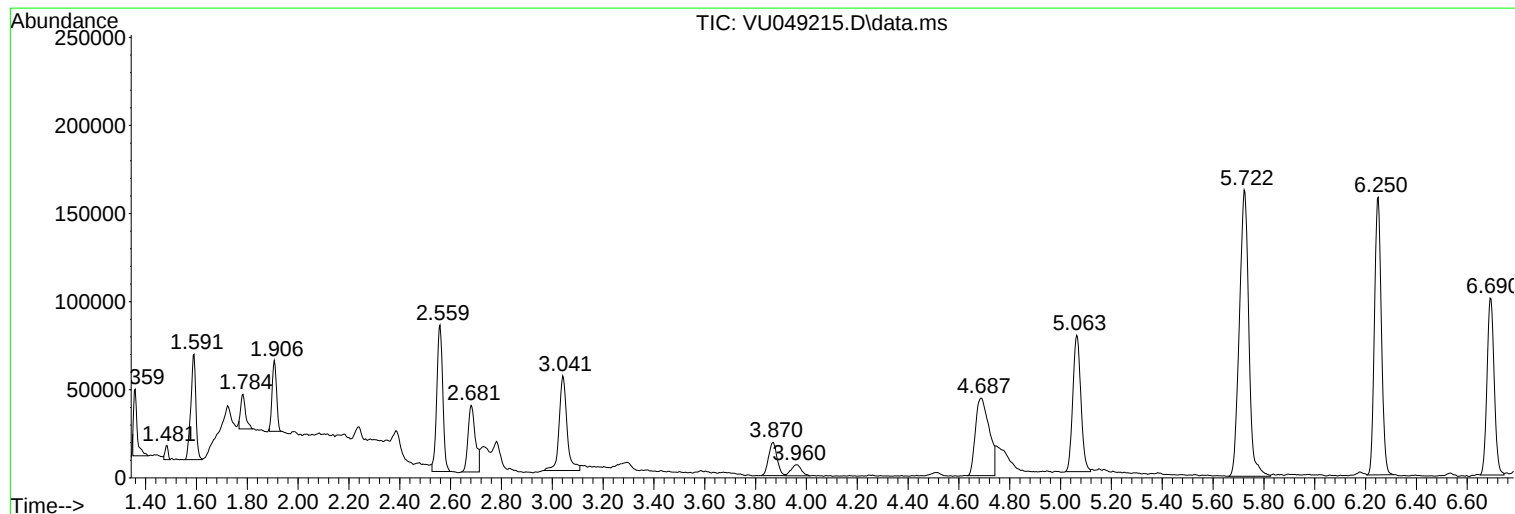
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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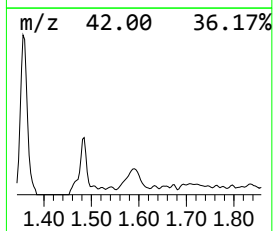
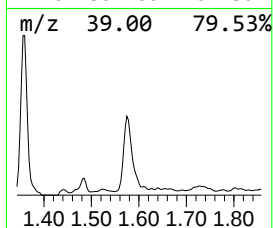
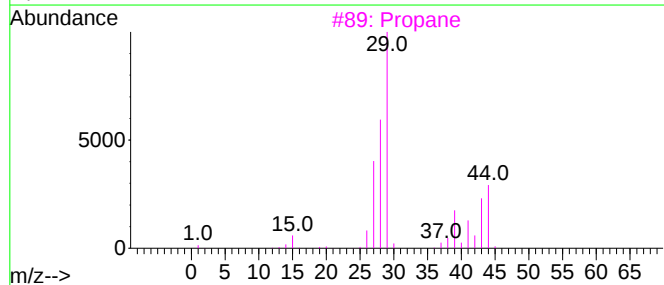
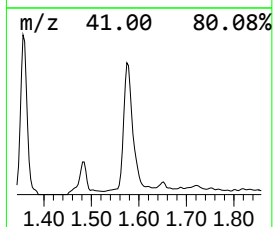
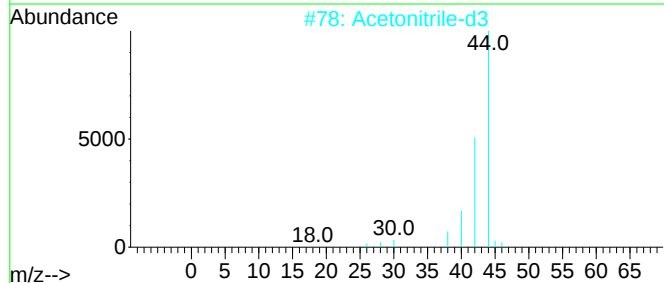
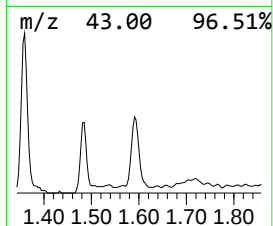
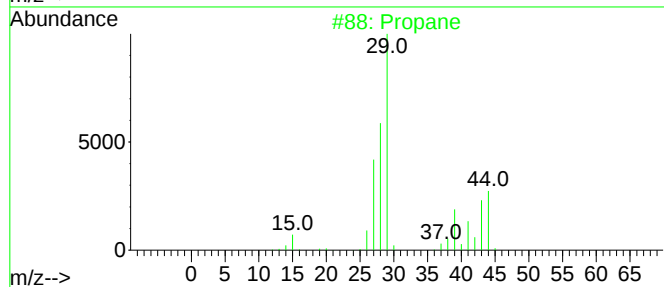
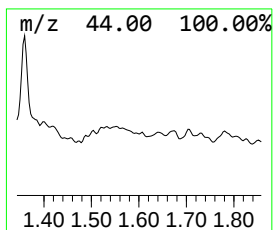
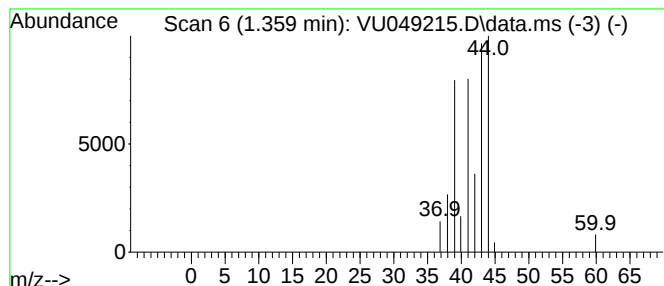
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	0.60 ug/L	35904	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	74
2			Acetonitrile-d3	44	C2D3N	002206-26-0	9
3			Propane	44	C3H8	000074-98-6	9
4			Propane	44	C3H8	000074-98-6	5
5			Propene	42	C3H6	000115-07-1	4



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
MSVOA_U
ClientSampleId :
EW4P6

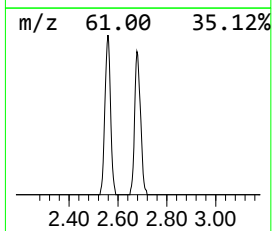
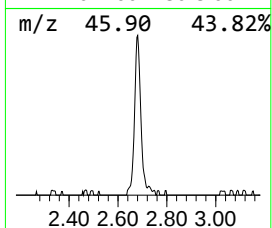
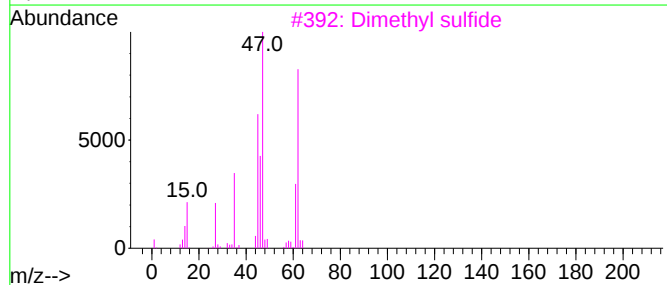
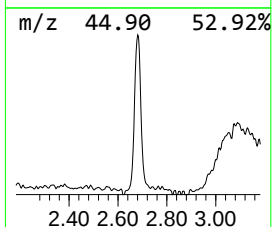
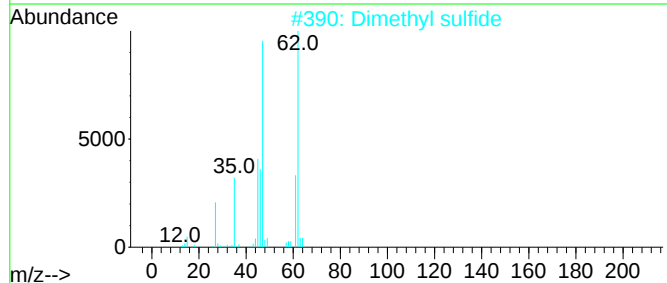
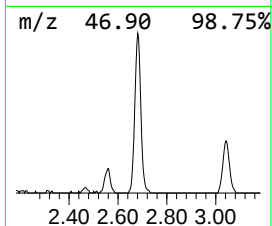
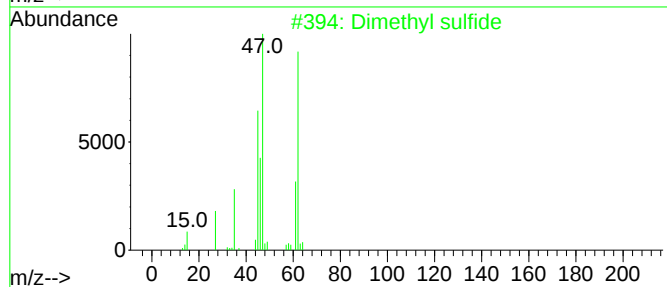
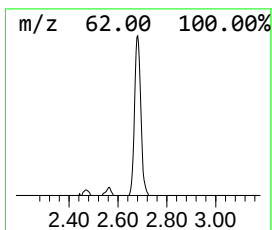
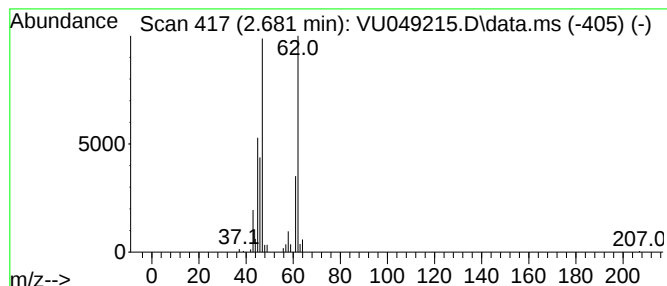
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.681	1.28 ug/L	76264	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Dimethyl sulfide	62	C2H6S	000075-18-3	94
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	90
5			Dimethyl sulfide	62	C2H6S	000075-18-3	87



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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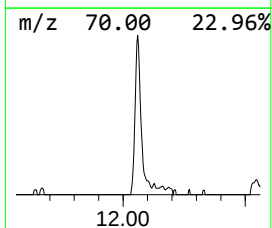
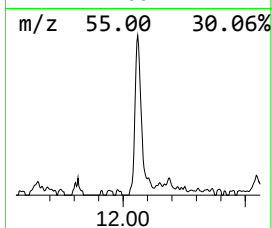
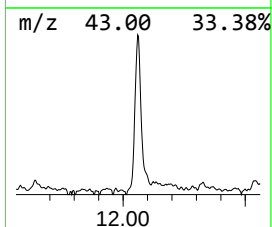
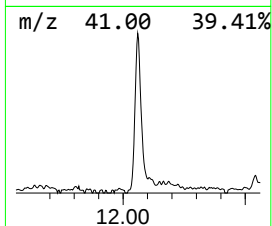
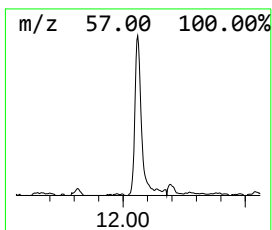
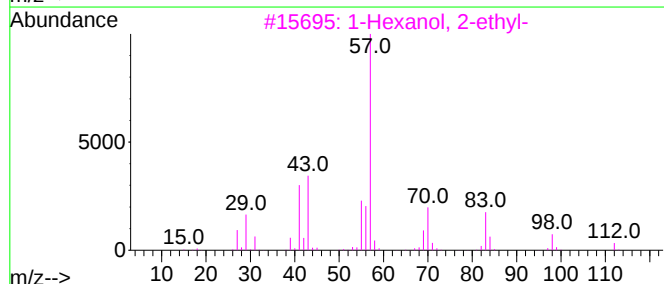
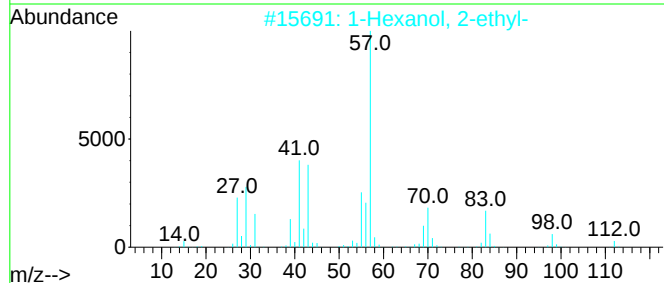
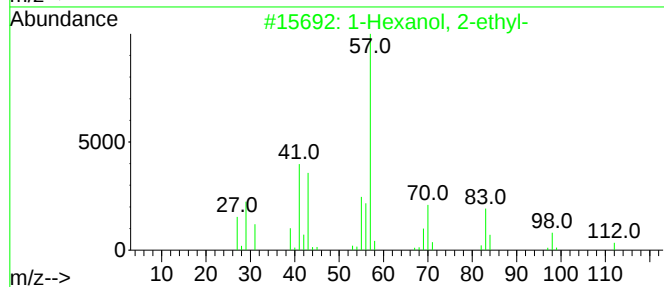
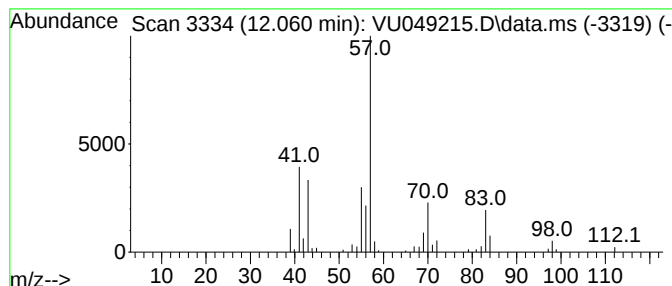
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	1.45 ug/L	106739	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
5			3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	47



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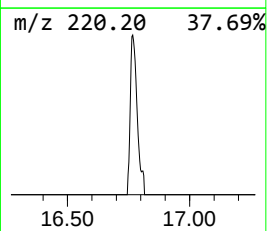
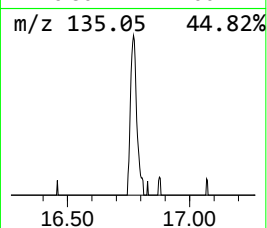
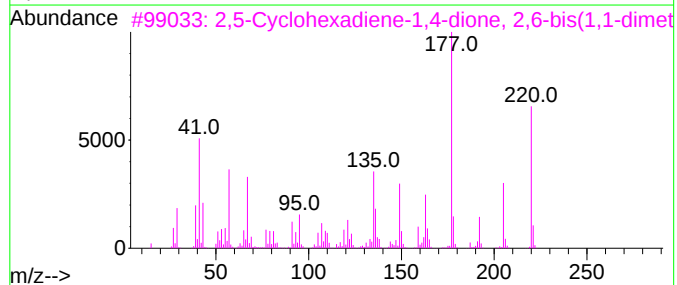
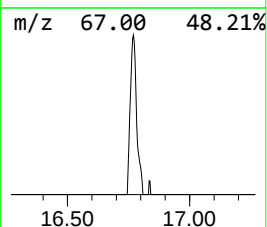
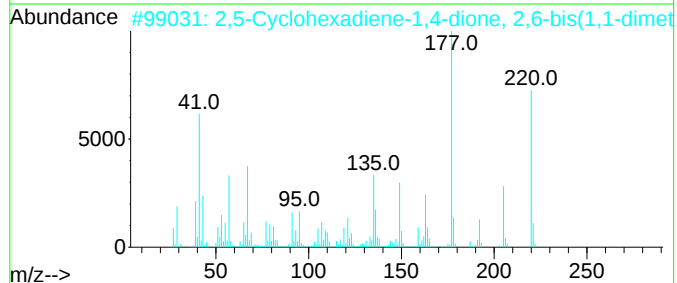
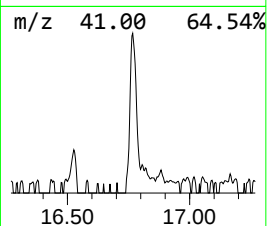
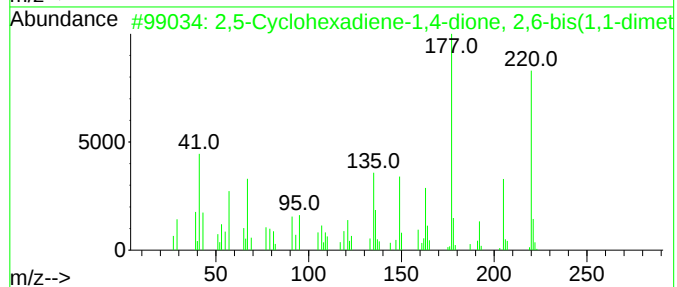
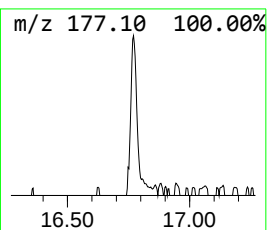
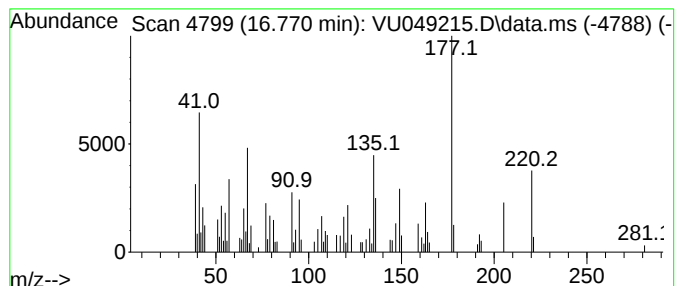
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.770	0.64 ug/L	47197	1,4-Dichlorobenzene-d4	11.812

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	97		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	95		
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	86		



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.359	0.6	ug/L	35904	1	6.250	296987	5.0
Dimethyl sulfide	2.681	1.3	ug/L	76264	1	6.250	296987	5.0
1-Hexanol, 2-et...	12.060	1.5	ug/L	106739	3	11.812	368055	5.0
2,5-Cyclohexadi...	16.770	0.6	ug/L	47197	3	11.812	368055	5.0