

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110923\
 Data File : VU056150.D
 Acq On : 09 Nov 2023 19:16
 Operator : MD/SY
 Sample : 05339-18
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GCDK3

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\SFAMUTR110723WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU056150.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.583	82	91	103	rVB	148170	174366	2.47%	0.959%
2	1.901	180	190	207	rBV	112097	162026	2.29%	0.891%
3	2.551	378	392	410	rBV2	247982	421159	5.96%	2.316%
4	4.650	1031	1045	1055	rBV2	89750	201882	2.86%	1.110%
5	4.724	1056	1068	1100	rVB2	62563	269515	3.81%	1.482%
6	5.052	1153	1170	1193	rBV2	231511	567303	8.02%	3.120%
7	5.711	1356	1375	1390	rBV2	490301	1141323	16.14%	6.277%
8	6.242	1527	1540	1552	rBV	375253	737922	10.44%	4.058%
9	6.531	1614	1630	1666	rBV	3598541	7070180	100.00%	38.882%
10	6.685	1666	1678	1708	rVB	267092	560749	7.93%	3.084%
11	7.283	1852	1864	1889	rVB2	57001	145350	2.06%	0.799%
12	7.560	1938	1950	1975	rBV	128444	248043	3.51%	1.364%
13	7.891	2040	2053	2091	rBV	419792	1028567	14.55%	5.657%
14	8.177	2131	2142	2160	rBV	73641	135698	1.92%	0.746%
15	8.547	2244	2257	2276	rBV2	65240	131369	1.86%	0.722%
16	8.647	2276	2288	2305	rBV	402568	858548	12.14%	4.722%
17	8.721	2306	2311	2329	rVB3	57699	132394	1.87%	0.728%
18	9.415	2514	2527	2553	rBV	503984	1091638	15.44%	6.003%
19	10.753	2931	2943	2960	rBV2	165239	284133	4.02%	1.563%
20	11.450	3151	3160	3173	rVB2	69872	113265	1.60%	0.623%
21	11.695	3224	3236	3246	rBV	138311	232126	3.28%	1.277%
22	11.811	3259	3272	3284	rBV	660172	1099045	15.54%	6.044%
23	11.939	3299	3312	3316	rBV2	94314	157682	2.23%	0.867%
24	11.968	3317	3321	3337	rVB	132846	193684	2.74%	1.065%
25	12.190	3372	3390	3404	rVB	535409	1025630	14.51%	5.640%

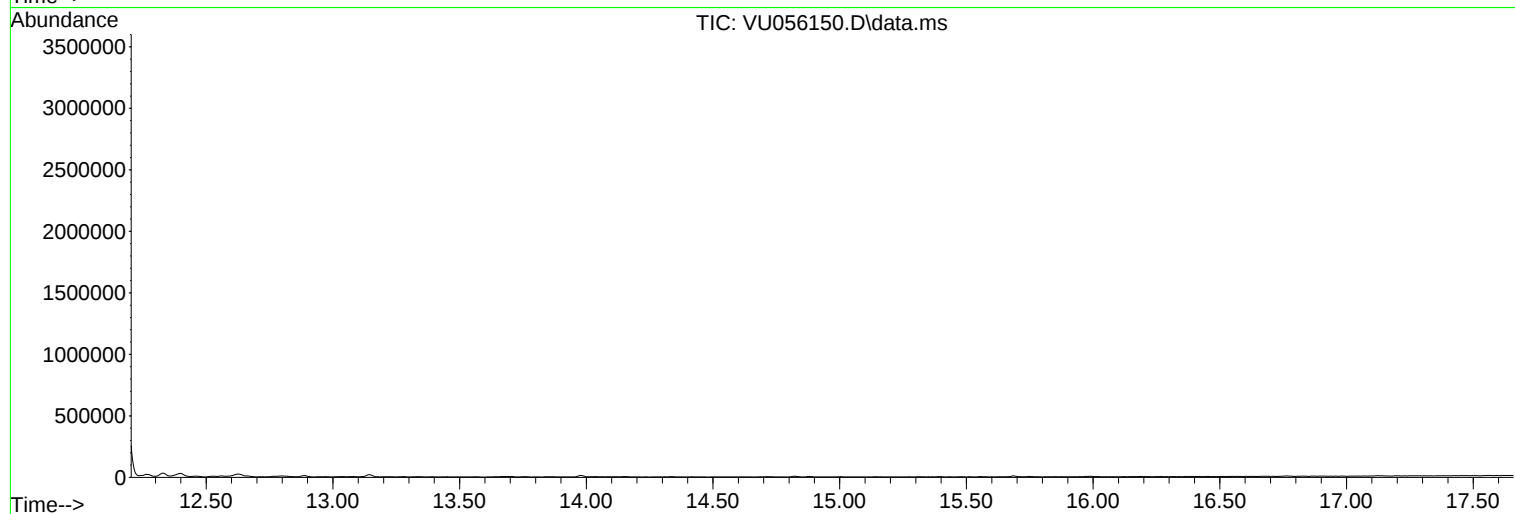
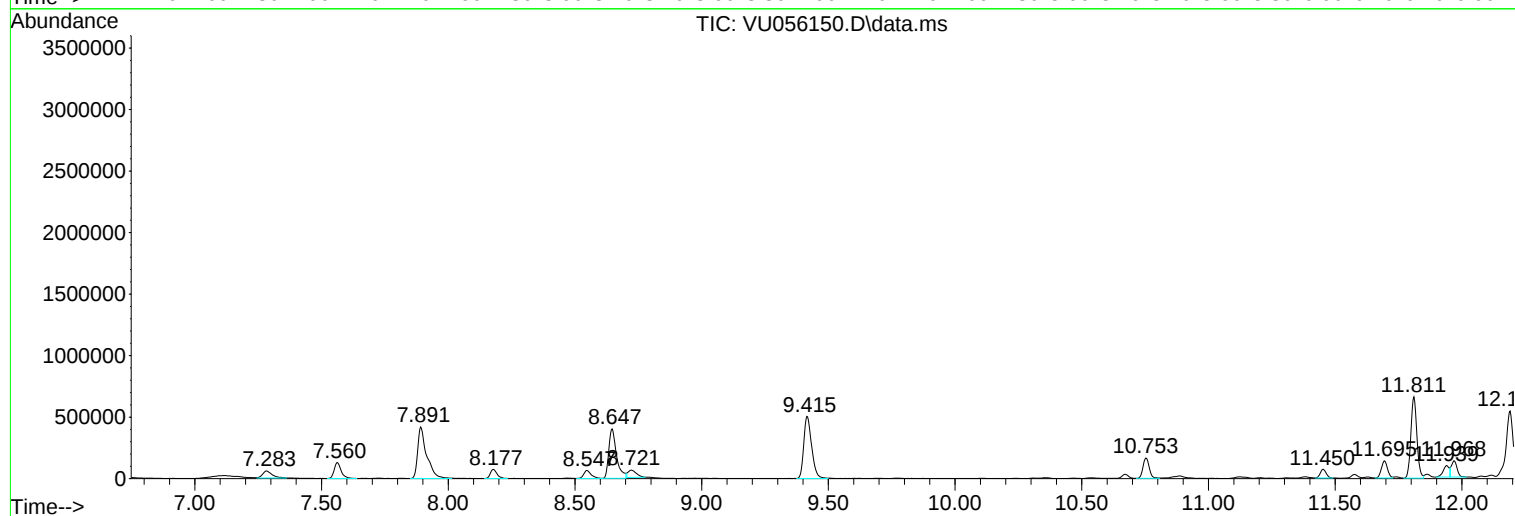
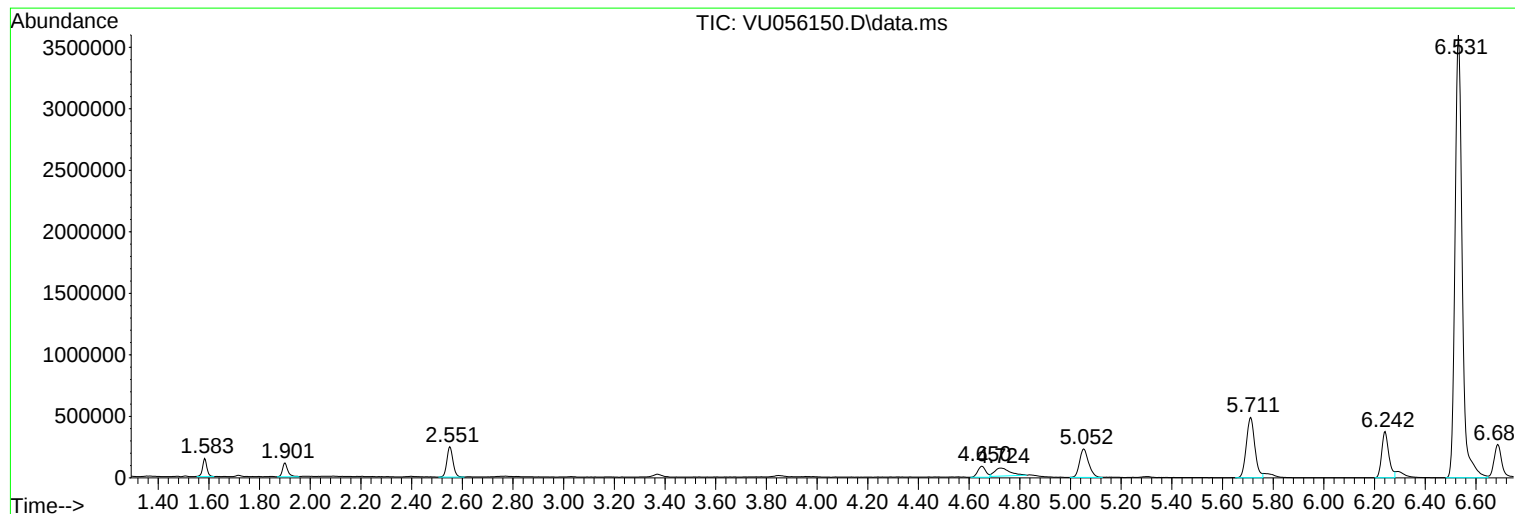
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GCDK3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR110723WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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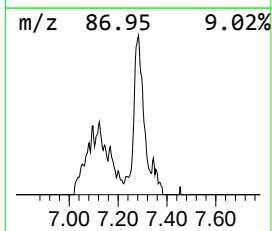
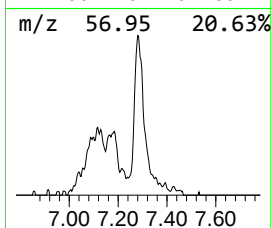
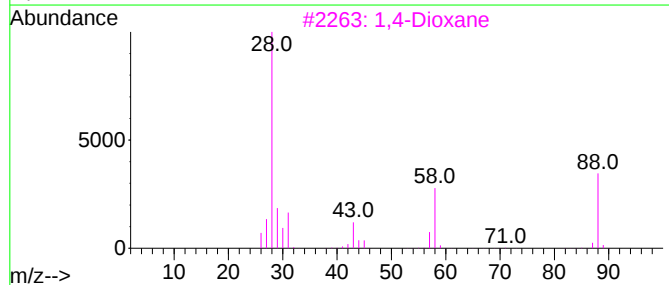
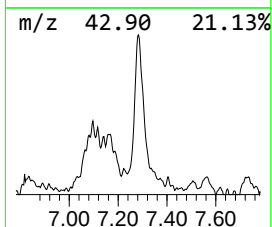
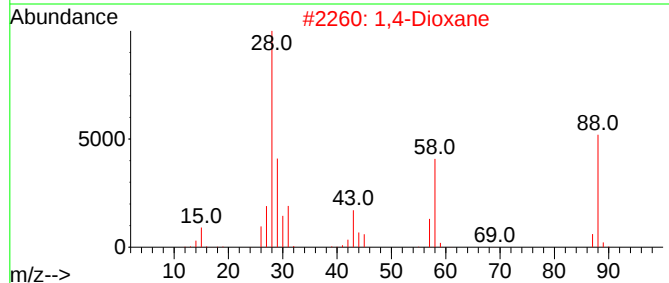
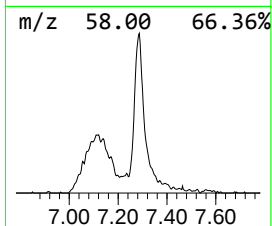
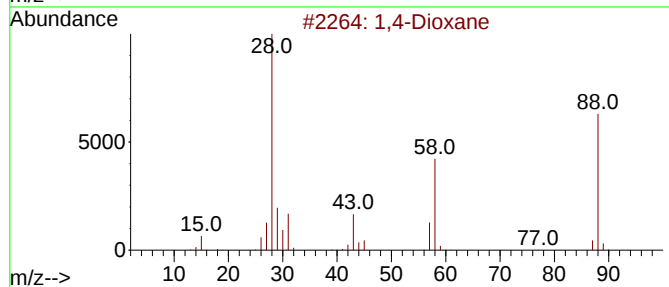
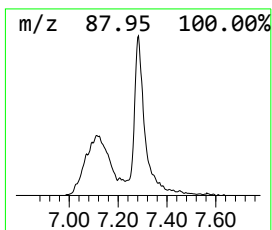
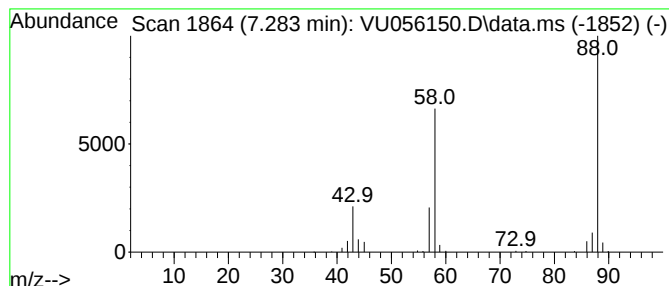
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR110723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 1,4-Dioxane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.283	0.98 ug/L	145350	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane			88	C4H8O2	000123-91-1	86
2	1,4-Dioxane			88	C4H8O2	000123-91-1	86
3	1,4-Dioxane			88	C4H8O2	000123-91-1	83
4	1,4-Dioxane			88	C4H8O2	000123-91-1	72
5	1,4-Dioxane			88	C4H8O2	000123-91-1	72



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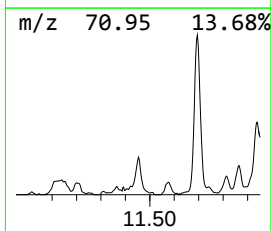
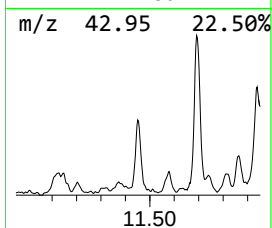
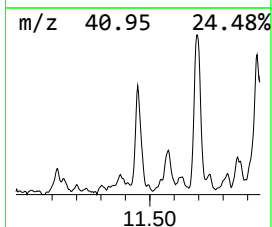
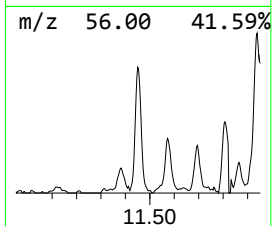
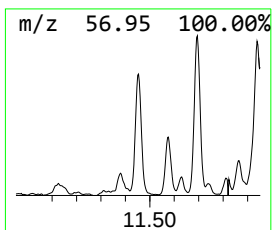
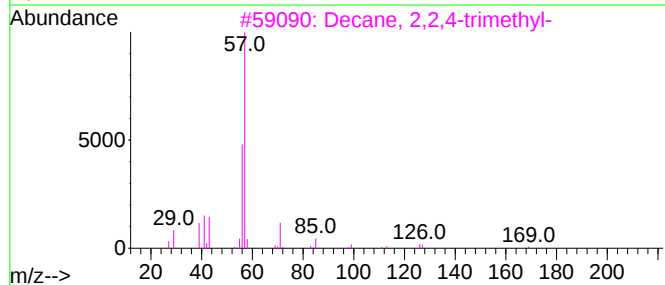
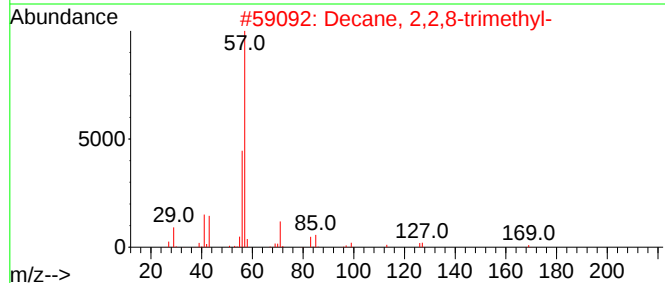
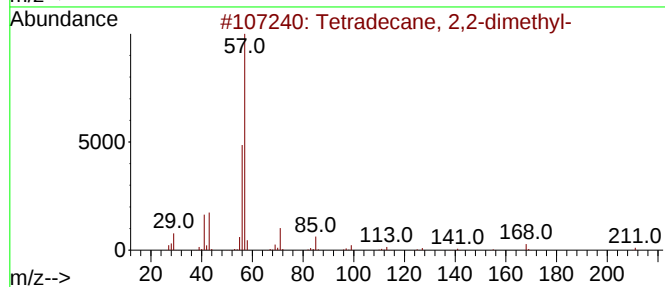
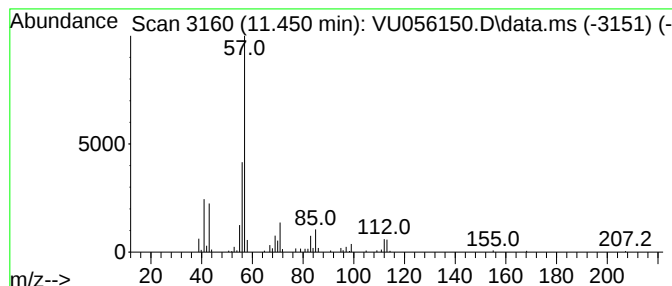
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR110723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.451	0.52 ug/L	113265	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	72
2			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	72
3			Decane, 2,2,4-trimethyl-	184	C13H28	062237-98-3	72
4			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	64



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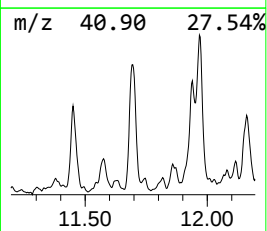
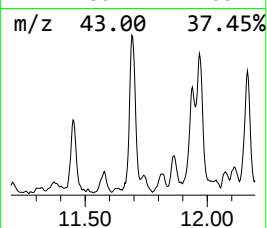
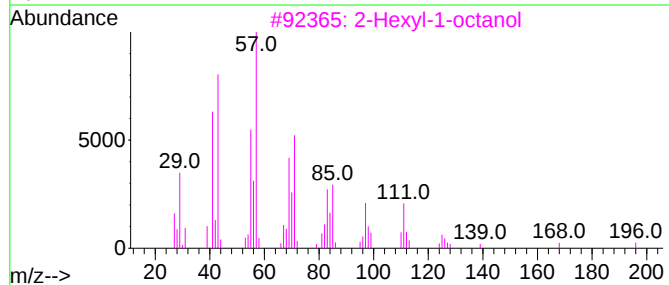
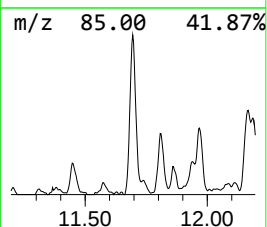
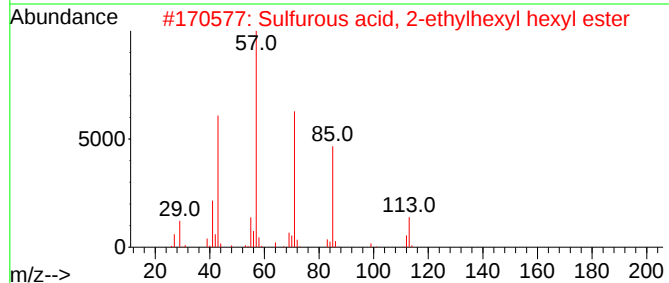
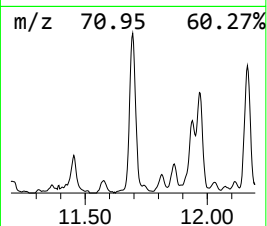
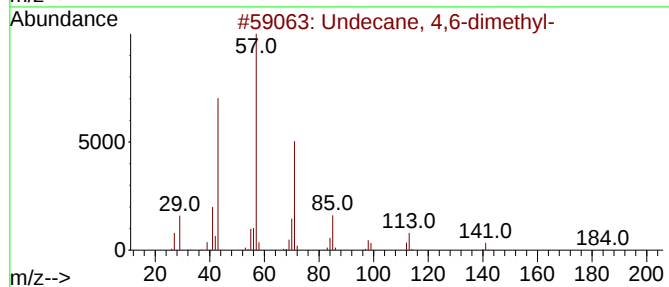
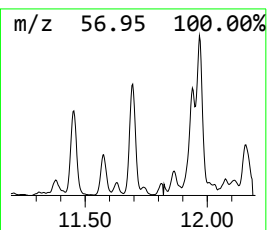
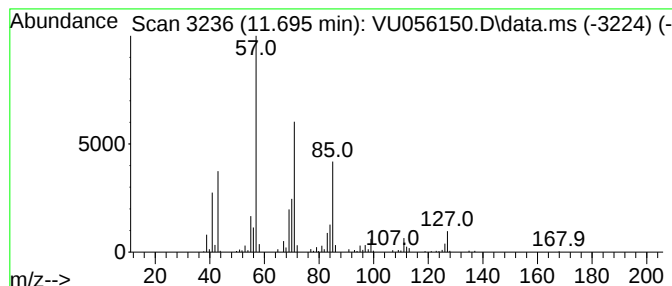
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR110723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.695	1.06 ug/L	232126	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59
2			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
3			2-Hexyl-1-octanol	214	C14H30O	019780-79-1	53
4			Tridecane, 6-methyl-	198	C14H30	013287-21-3	50
5			2-Decanol, 2-methylpropionate	228	C14H28O2	1000447-30-4	47



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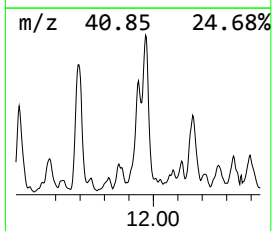
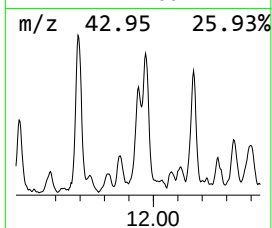
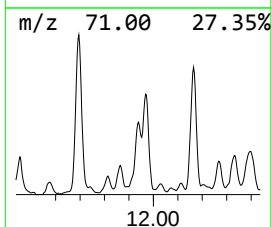
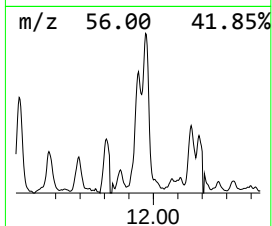
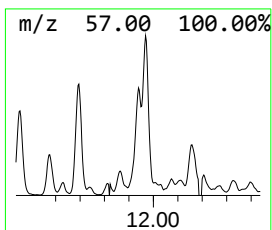
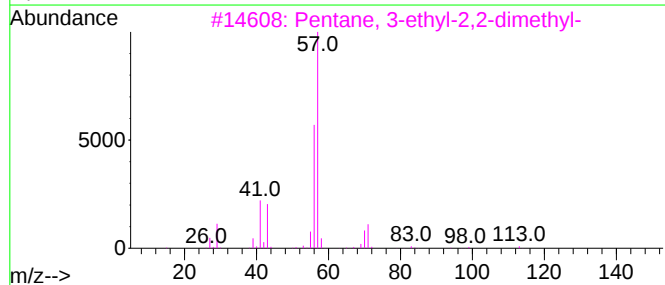
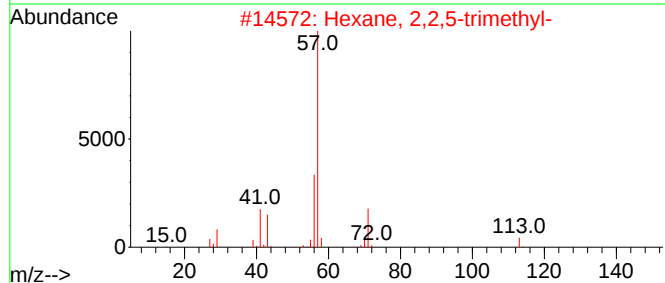
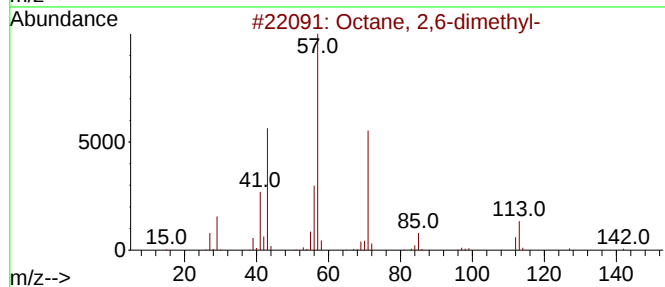
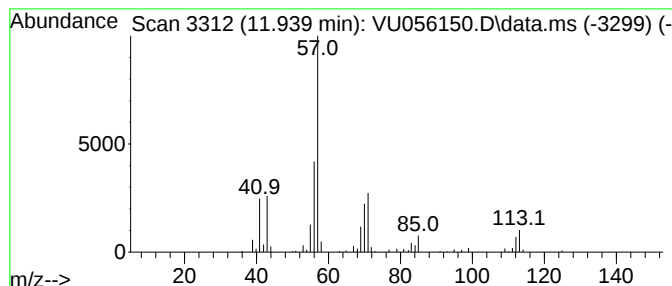
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.939	0.72 ug/L	157682	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	59
2			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	53
3			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50
4			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	50
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	50



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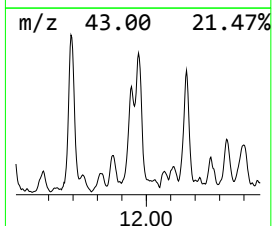
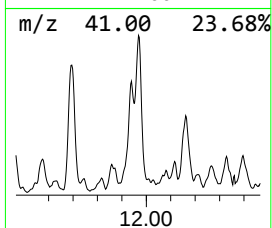
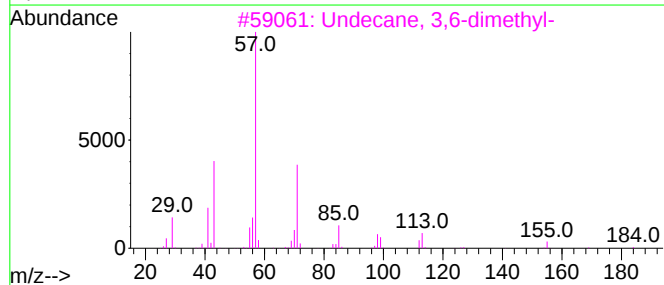
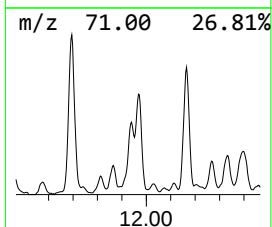
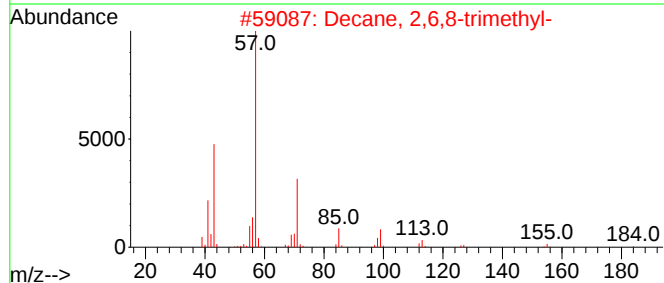
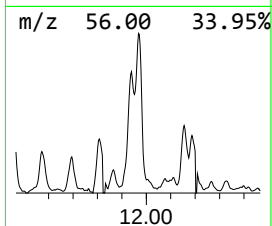
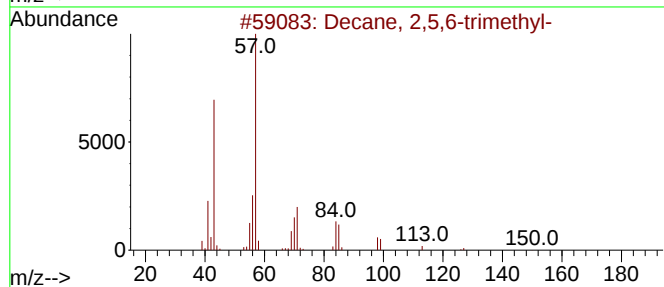
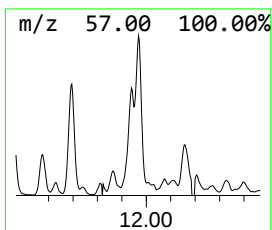
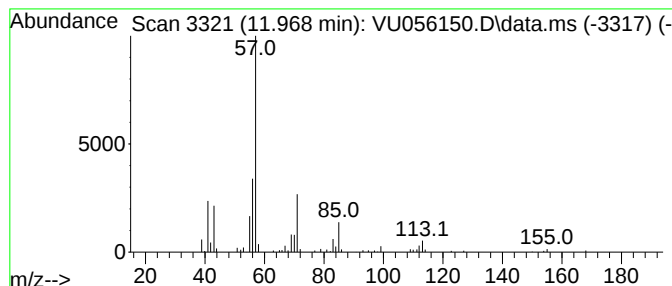
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.968	0.88 ug/L	193684	1,4-Dichlorobenzene-d4	11.811

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	64
2		Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	64
3		Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	53
4		Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
5		Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,4-Dioxane	7.283	1.0	ug/L	145350	1	6.242	737922	5.0
(DEL) Alkane: S...	11.451	0.5	ug/L	113265	3	11.811	1099050	5.0
(DEL) Alkane: S...	11.695	1.1	ug/L	232126	3	11.811	1099050	5.0
(DEL) Alkane: S...	11.939	0.7	ug/L	157682	3	11.811	1099050	5.0
(DEL) Alkane: S...	11.968	0.9	ug/L	193684	3	11.811	1099050	5.0