

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030722\
 Data File : VU047362.D
 Acq On : 07 Mar 2022 13:10
 Operator : SY/MD
 Sample : VIBLK008
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK008

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\SFAMUTR030422WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU047362.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	98	rBV	87316	100881	11.00%	1.131%
2	1.916	170	179	201	rBV	77035	104681	11.42%	1.174%
3	2.572	371	383	397	rBV	149039	244416	26.65%	2.740%
4	4.649	1012	1029	1078	rBV2	88832	339680	37.04%	3.808%
5	5.067	1143	1159	1180	rBV	143274	317365	34.61%	3.558%
6	5.729	1338	1365	1386	rBV2	285685	745166	81.26%	8.354%
7	6.253	1510	1528	1552	rBV	237133	451345	49.22%	5.060%
8	6.546	1607	1619	1632	rVB4	13524	26187	2.86%	0.294%
9	6.694	1650	1665	1684	rBV	182520	352518	38.44%	3.952%
10	7.568	1923	1937	1954	rBV	100107	174688	19.05%	1.958%
11	7.899	2027	2040	2059	rBV	361118	621788	67.80%	6.971%
12	8.182	2116	2128	2145	rBV	62763	109282	11.92%	1.225%
13	8.555	2234	2244	2256	rVB2	18735	31359	3.42%	0.352%
14	8.636	2256	2269	2312	rBV	479700	917032	100.00%	10.281%
15	9.417	2498	2512	2528	rBV	324782	544736	59.40%	6.107%
16	10.758	2917	2929	2946	rVB	165601	270296	29.48%	3.030%
17	10.893	2963	2971	2982	rVB2	7563	12308	1.34%	0.138%
18	11.813	3244	3257	3274	rBV	377879	595447	64.93%	6.676%
19	12.192	3360	3375	3390	rBV	388990	626420	68.31%	7.023%
20	13.430	3751	3760	3767	rBV2	10077	16215	1.77%	0.182%
21	13.587	3800	3809	3819	rBV3	7285	14820	1.62%	0.166%
22	14.047	3943	3952	3960	rBV9	6351	12516	1.36%	0.140%
23	14.192	3985	3997	4010	rBV3	21055	40849	4.45%	0.458%
24	14.449	4068	4077	4086	rBV	83323	113819	12.41%	1.276%
25	14.571	4111	4115	4125	rVB7	9729	11454	1.25%	0.128%
26	14.648	4133	4139	4153	rVB5	13378	23534	2.57%	0.264%
27	14.941	4223	4230	4235	rBV3	14897	23377	2.55%	0.262%
28	15.021	4249	4255	4260	rBV2	16382	21688	2.37%	0.243%
29	15.066	4261	4269	4277	rVB3	42642	66562	7.26%	0.746%
30	15.147	4287	4294	4304	rVB2	34535	53162	5.80%	0.596%
31	15.211	4304	4314	4325	rBV	125572	191330	20.86%	2.145%
32	15.401	4363	4373	4382	rBV	440788	620422	67.66%	6.956%
33	15.504	4397	4405	4415	rBV5	32414	61876	6.75%	0.694%
34	15.841	4503	4510	4518	rBV4	33422	58961	6.43%	0.661%
35	15.938	4534	4540	4544	rBV3	33297	40533	4.42%	0.454%
36	15.976	4544	4552	4565	rVV	271966	391086	42.65%	4.385%

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ClientSampleId :
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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\SFAMUTR030422WMA.M
Title : TRACE VOA SFAM1.0

37	16.050	4569	4575	4586	rVB3	57617	94460	10.30%	1.059%
38	16.291	4641	4650	4662	rVB	302267	421937	46.01%	4.730%
39	16.889	4828	4836	4846	rBV	35337	55396	6.04%	0.621%

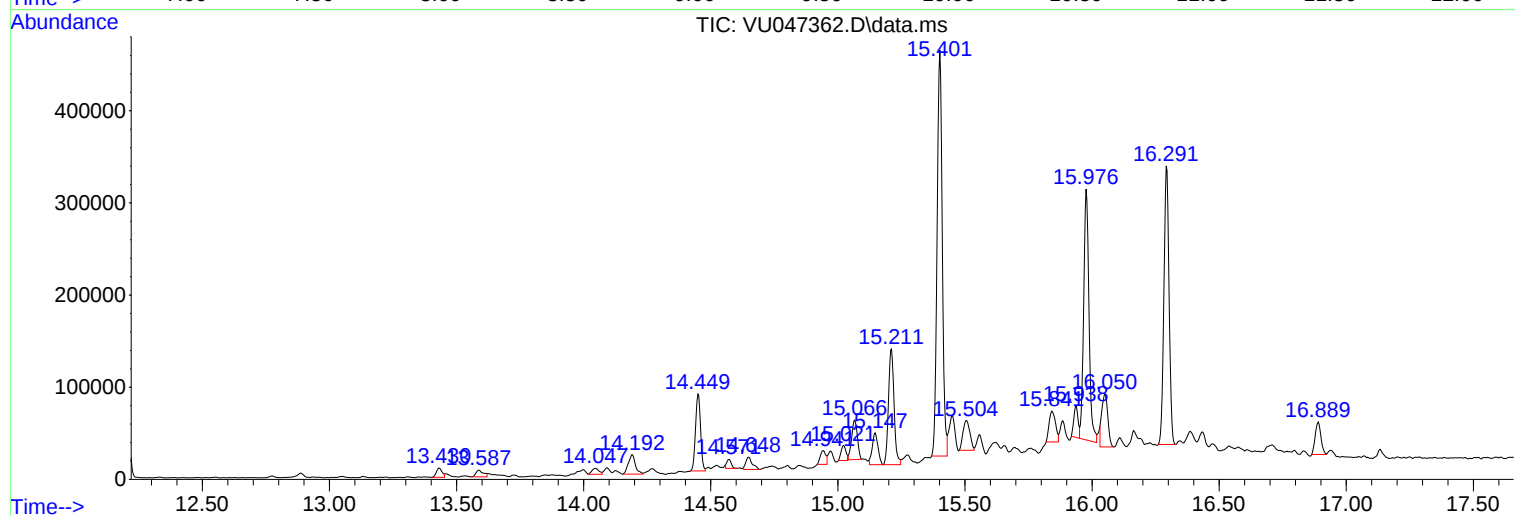
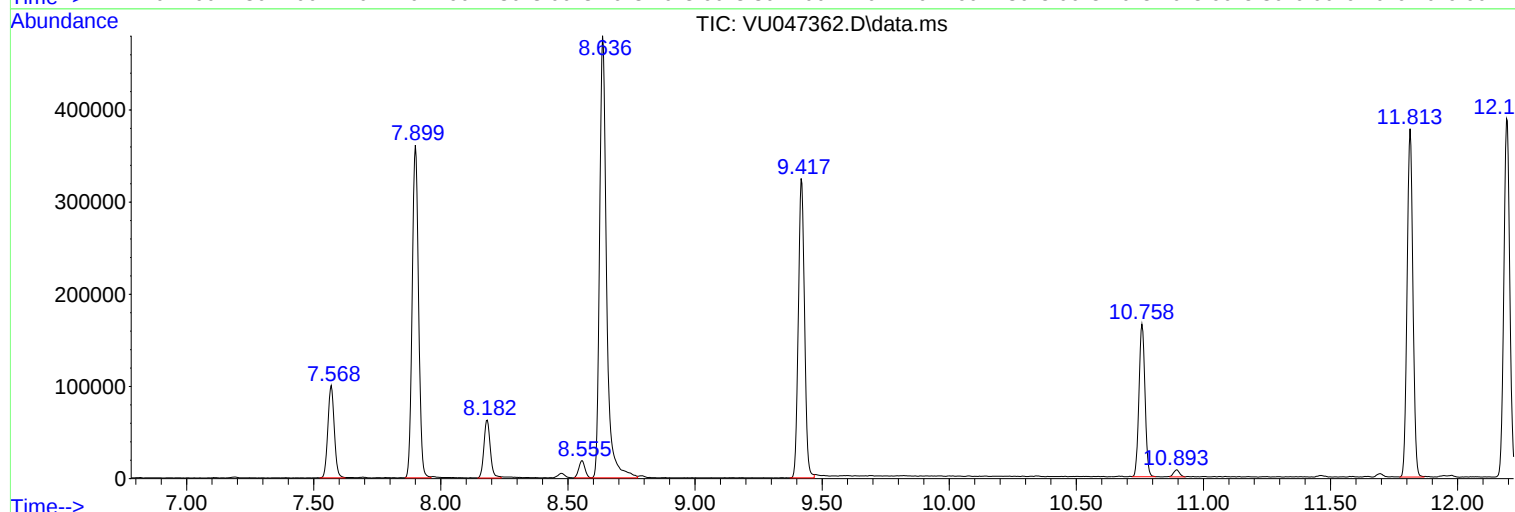
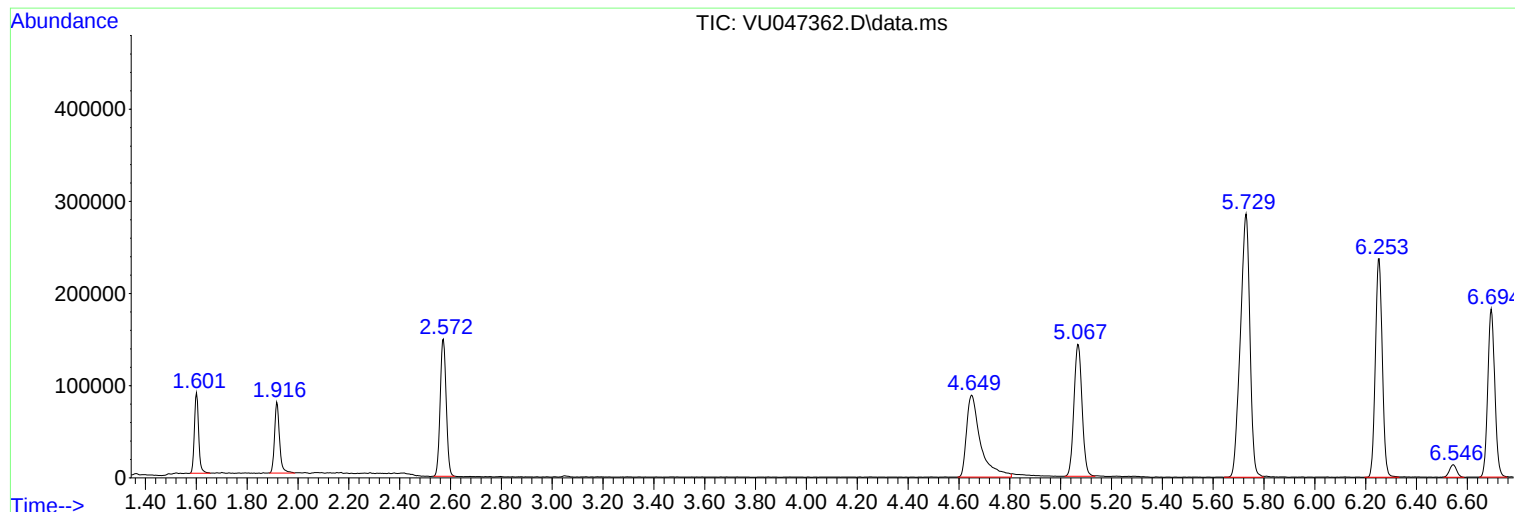
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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ClientSampleId :
VIBLK008

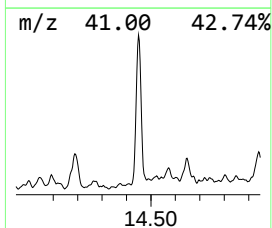
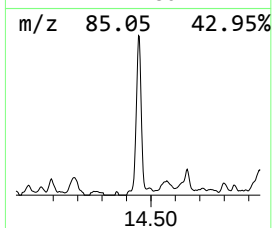
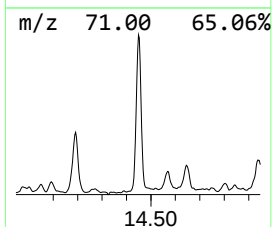
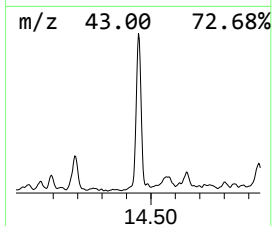
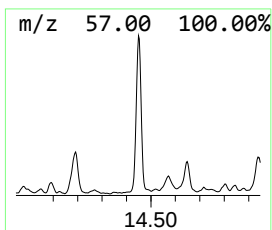
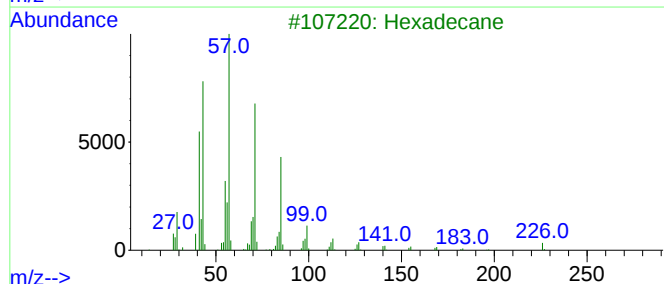
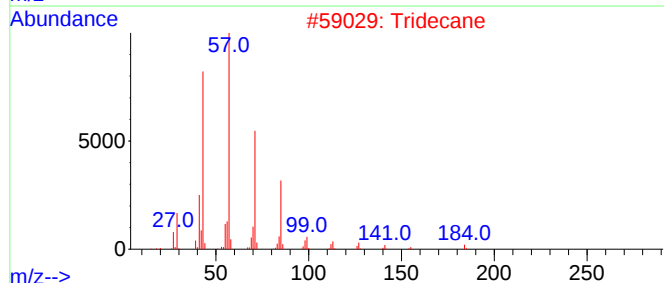
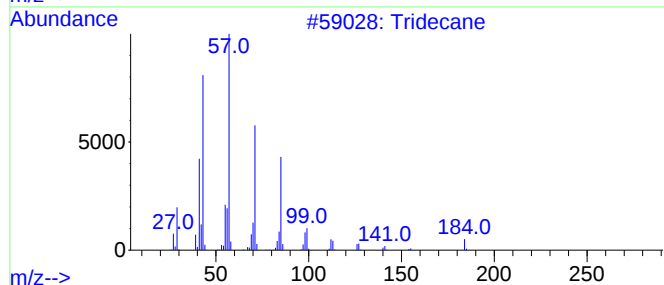
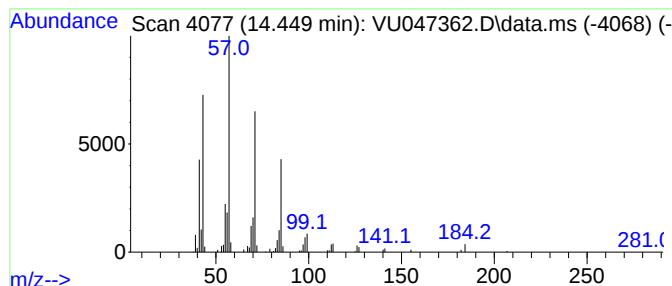
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.449	0.96 ug/L	113819	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane	184	C13H28	000629-50-5	96
2			Tridecane	184	C13H28	000629-50-5	91
3			Hexadecane	226	C16H34	000544-76-3	90
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5			Dodecane	170	C12H26	000112-40-3	86



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK008

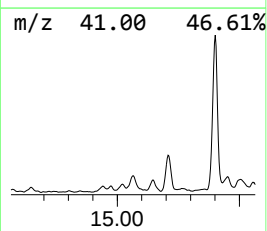
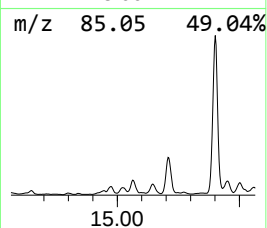
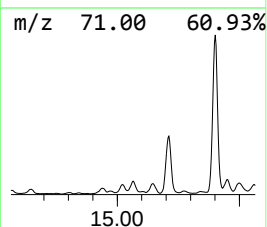
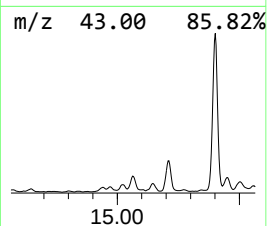
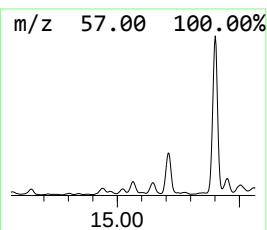
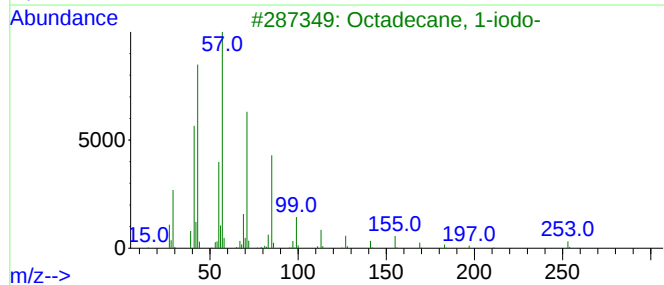
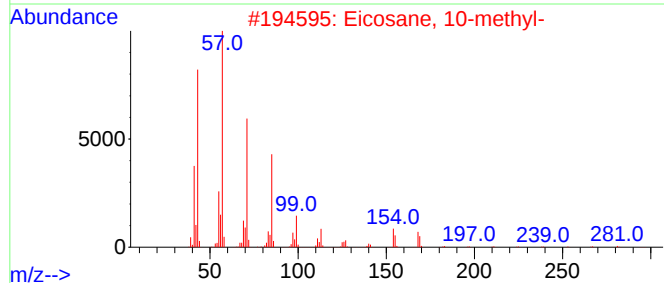
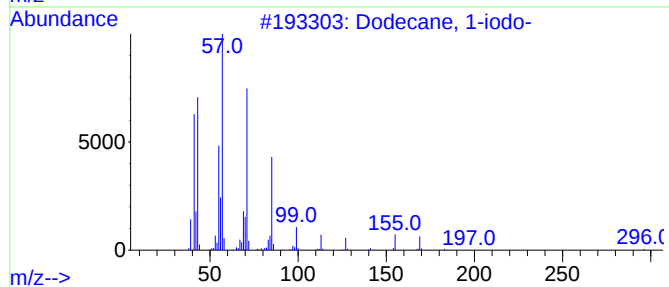
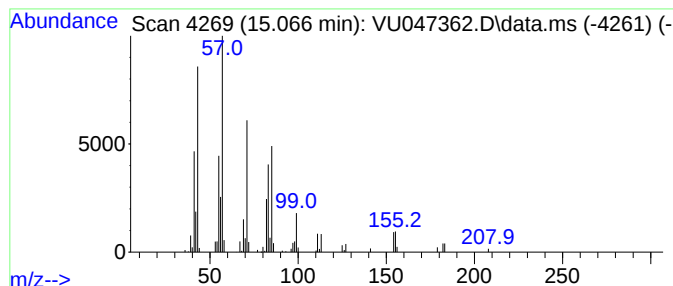
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Dodecane, 1-iodo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.066	0.56 ug/L	66562	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	52
2			Eicosane, 10-methyl-	296	C21H44	054833-23-7	52
3			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	49
4			Hexadecane	226	C16H34	000544-76-3	49
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	46



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK008

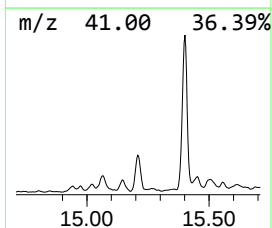
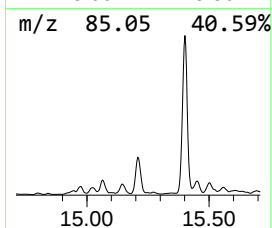
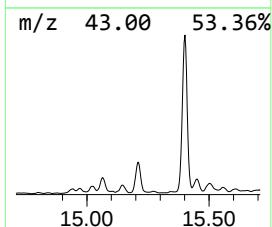
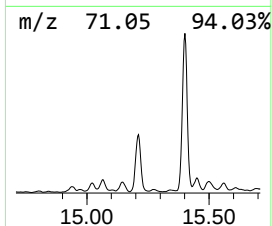
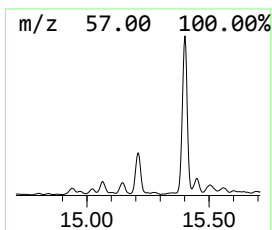
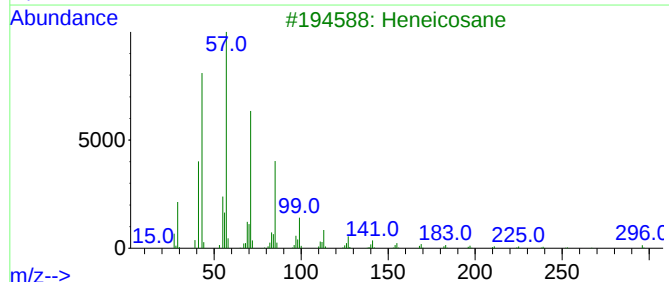
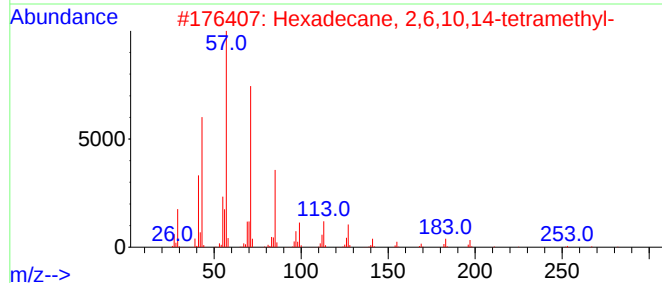
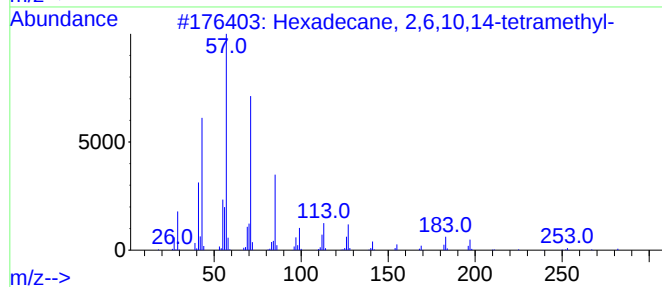
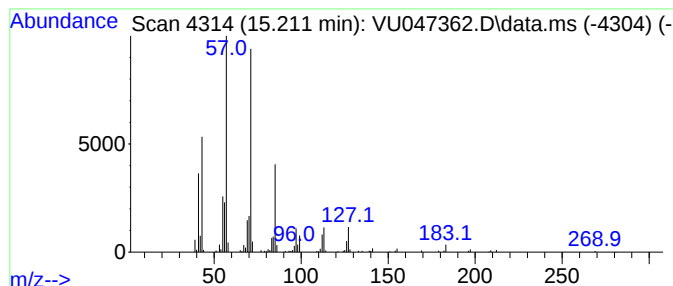
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.211	1.61 ug/L	191330	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
2			Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
3			Heneicosane	296	C21H44	000629-94-7	86
4			Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	80
5			Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44	018344-37-1	78



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Instrument :
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ClientSampleId :
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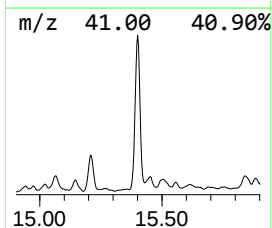
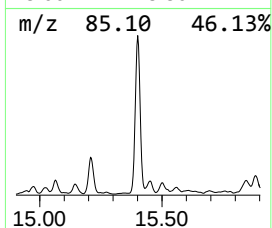
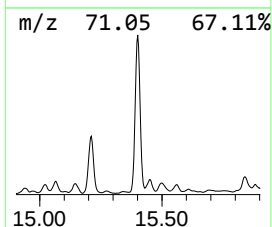
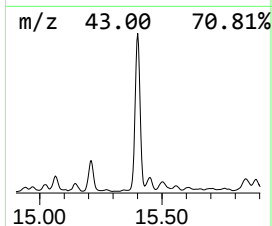
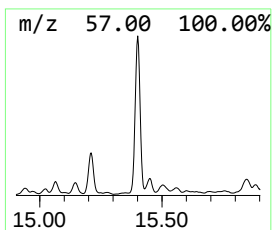
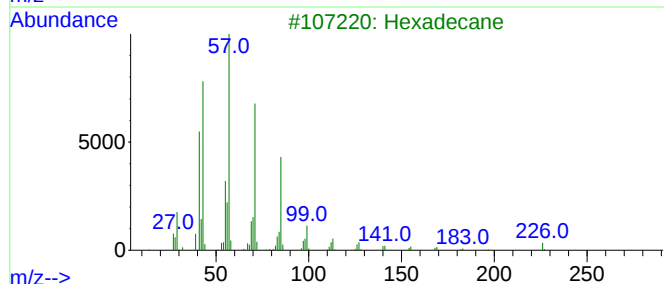
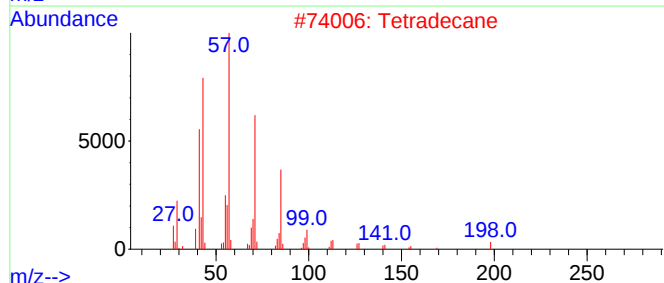
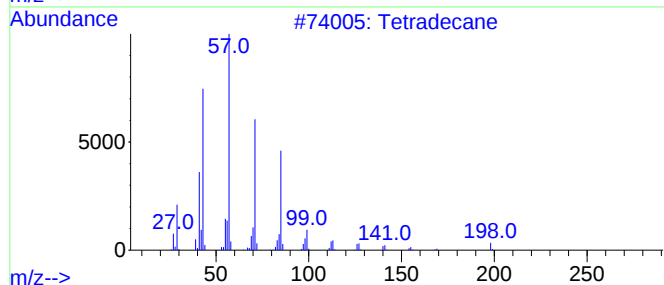
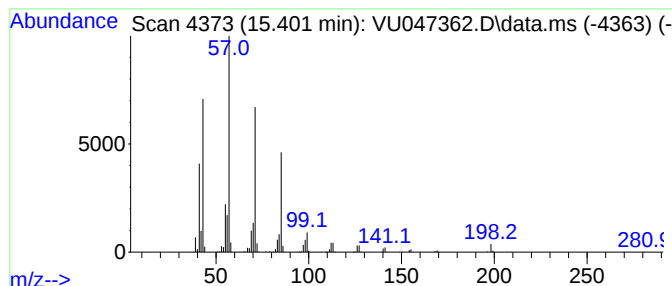
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.401	5.21 ug/L	620422	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	98
2			Tetradecane	198	C14H30	000629-59-4	97
3			Hexadecane	226	C16H34	000544-76-3	91
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	91
5			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	90



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VIBLK008

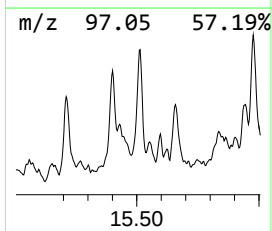
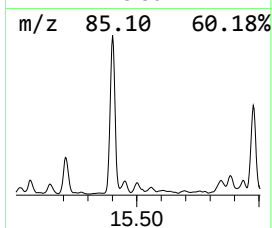
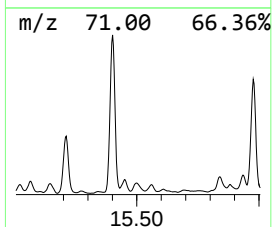
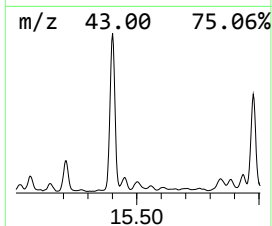
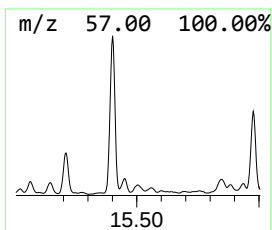
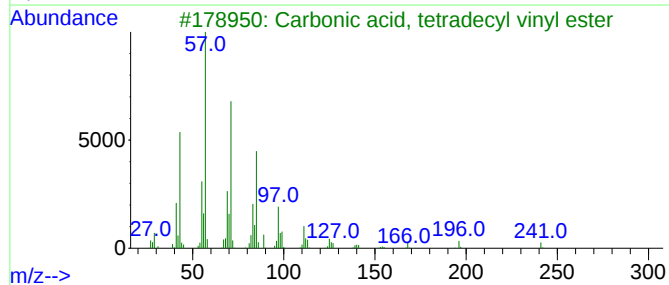
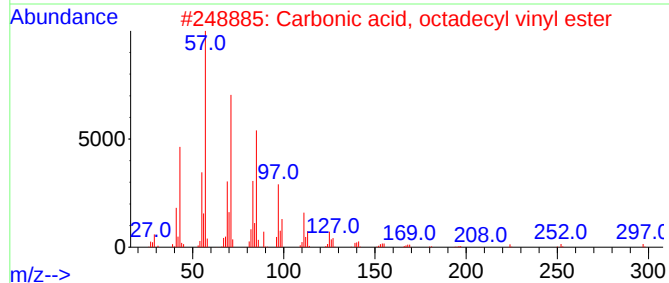
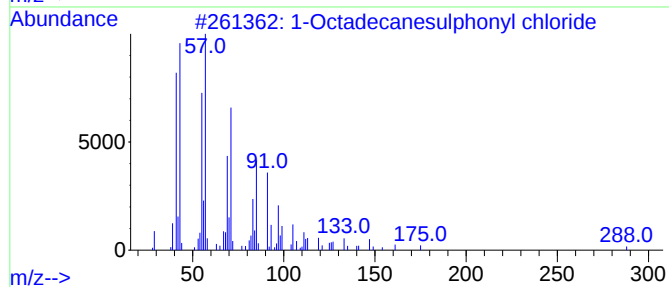
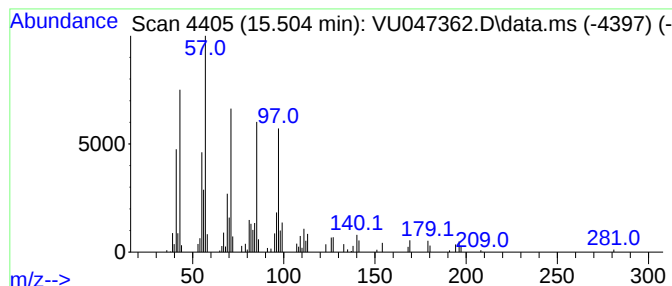
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1-Octadecanesulphonyl chloride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.504	0.52 ug/L	61876	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	64
2			Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	64
3			Carbonic acid, tetradecyl vinyl ...	284	C17H32O3	1000382-54-5	64
4			Tetratetracontane	619	C44H90	007098-22-8	58
5			Tritetracontane	605	C43H88	007098-21-7	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030722\
Data File : VU047362.D
Acq On : 07 Mar 2022 13:10
Operator : SY/MD
Sample : VIBLK008
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK008

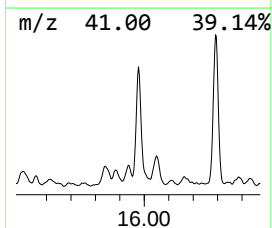
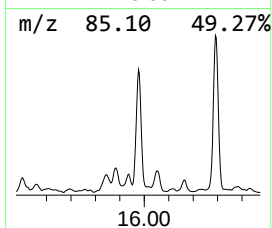
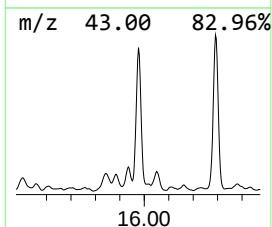
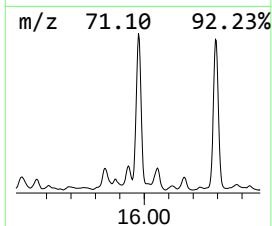
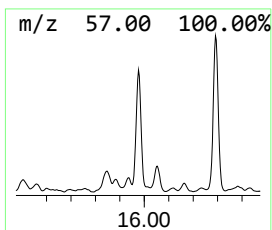
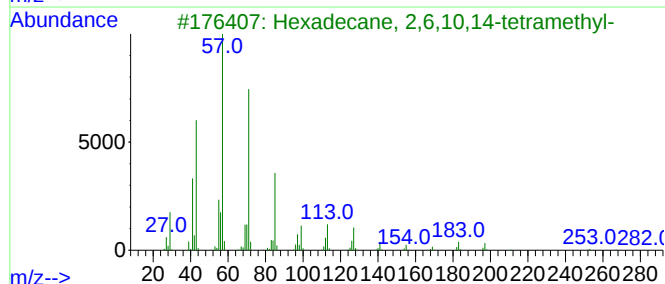
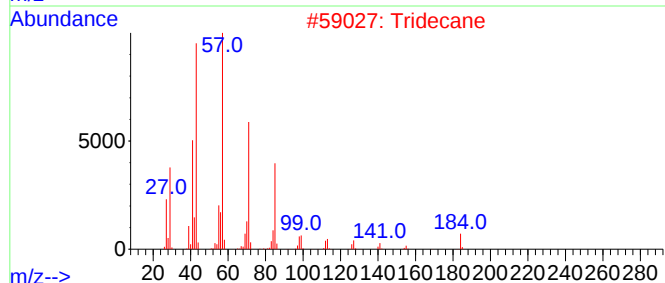
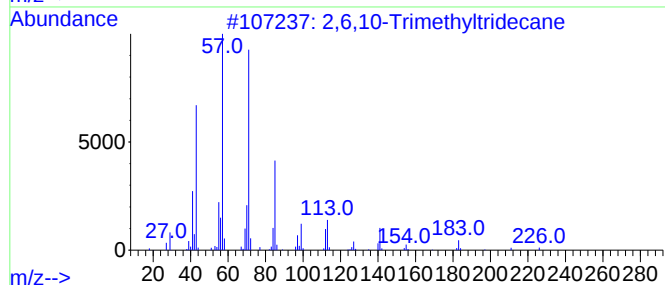
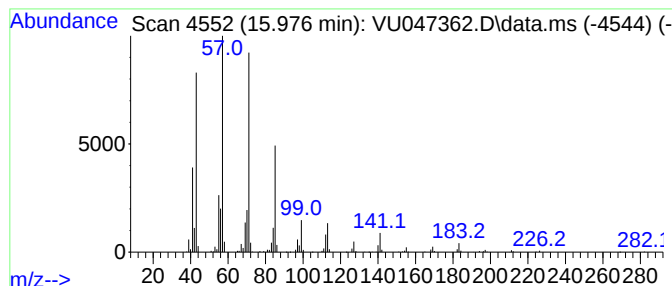
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.976	3.28 ug/L	391086	1,4-Dichlorobenzene-d4	11.813

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	97
2		Tridecane	184	C13H28	000629-50-5	90
3		Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
4		Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
5		Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030722\
Data File : VU047362.D
Acq On : 07 Mar 2022 13:10
Operator : SY/MD
Sample : VIBLK008
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK008

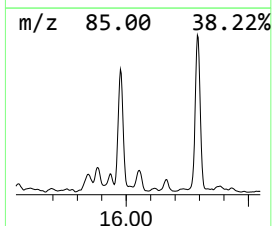
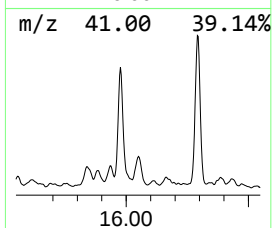
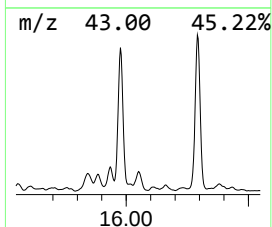
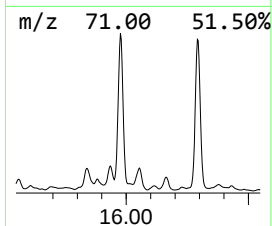
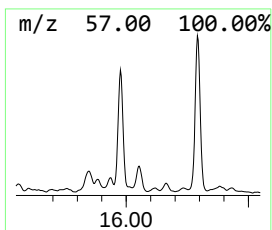
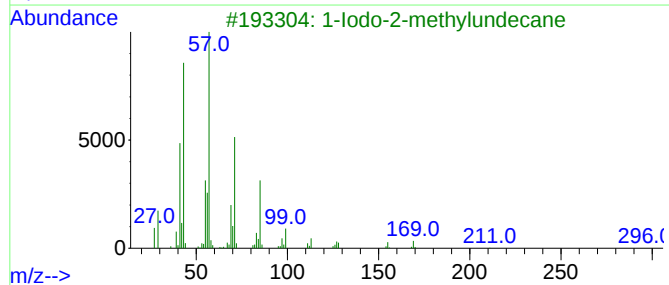
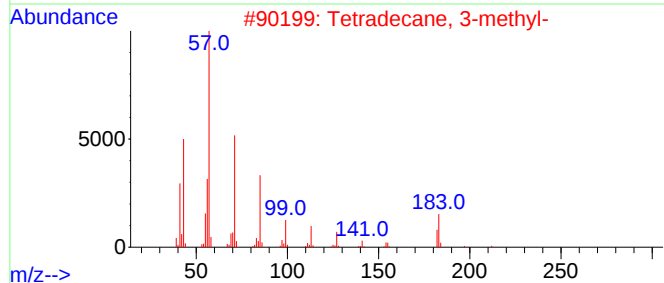
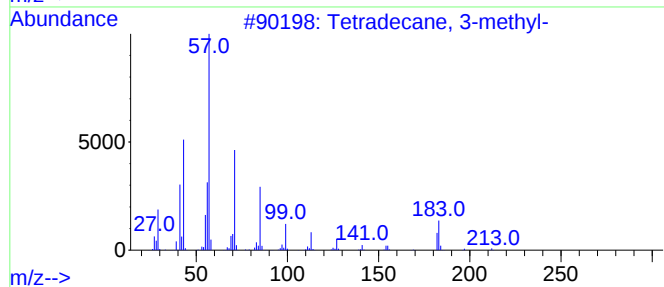
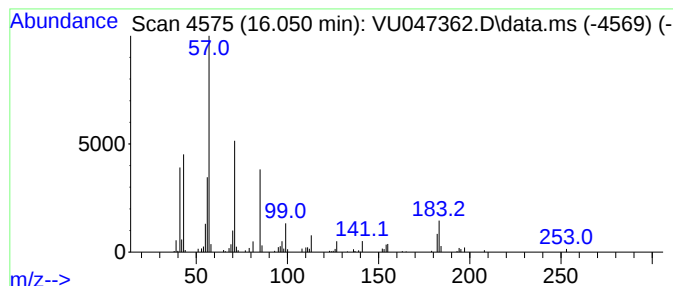
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.050	0.79 ug/L	94460	1,4-Dichlorobenzene-d4	11.813

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane, 3-methyl-	212	C15H32	018435-22-8	91
2		Tetradecane, 3-methyl-	212	C15H32	018435-22-8	83
3		1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80
4		Dodecane, 3-methyl-	184	C13H28	017312-57-1	72
5		Hexadecane	226	C16H34	000544-76-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030722\
Data File : VU047362.D
Acq On : 07 Mar 2022 13:10
Operator : SY/MD
Sample : VIBLK008
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK008

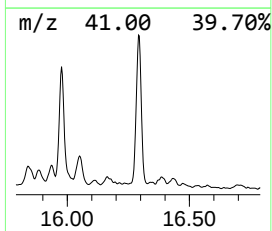
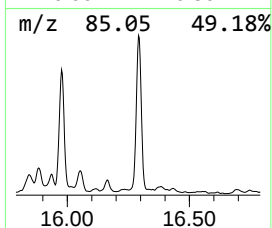
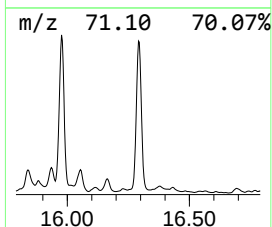
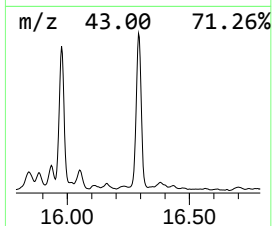
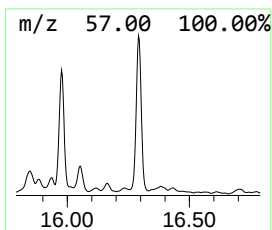
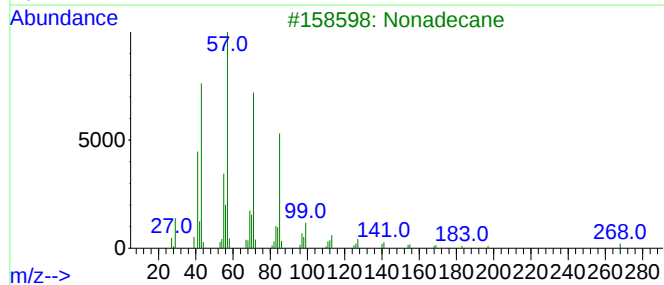
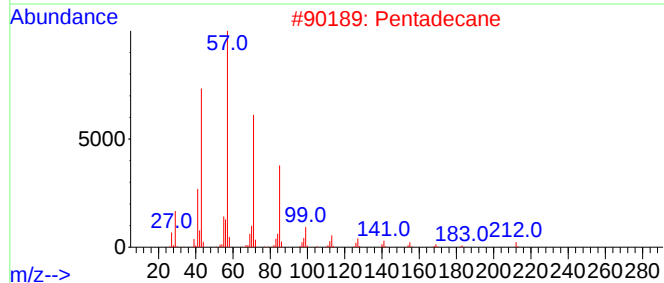
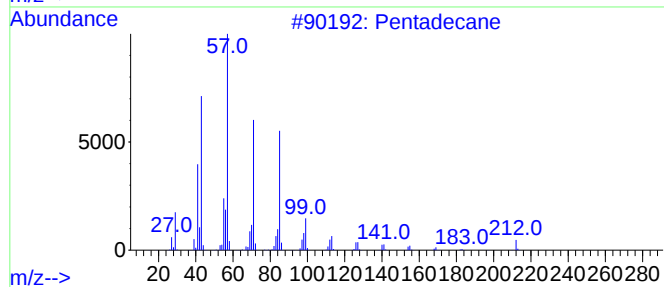
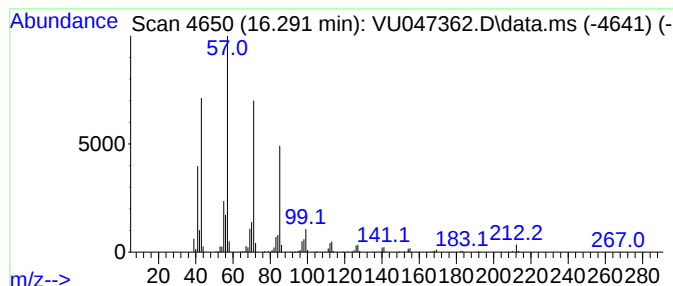
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.291	3.54 ug/L	421937	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	97
2			Pentadecane	212	C15H32	000629-62-9	93
3			Nonadecane	268	C19H40	000629-92-5	91
4			Pentadecane	212	C15H32	000629-62-9	91
5			Heptadecane	240	C17H36	000629-78-7	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030722\
 Data File : VU047362.D
 Acq On : 07 Mar 2022 13:10
 Operator : SY/MD
 Sample : VIBLK008
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK008

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.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...	14.449	1.0	ug/L	113819	3	11.813	595447	5.0
Dodecane, 1-iodo-	15.066	0.6	ug/L	66562	3	11.813	595447	5.0
(DEL) Alkane: S...	15.211	1.6	ug/L	191330	3	11.813	595447	5.0
(DEL) Alkane: S...	15.401	5.2	ug/L	620422	3	11.813	595447	5.0
1-Octadecanesul...	15.504	0.5	ug/L	61876	3	11.813	595447	5.0
(DEL) Alkane: S...	15.976	3.3	ug/L	391086	3	11.813	595447	5.0
(DEL) Alkane: S...	16.050	0.8	ug/L	94460	3	11.813	595447	5.0
(DEL) Alkane: S...	16.291	3.5	ug/L	421937	3	11.813	595447	5.0