

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
 Data File : VV027675.D
 Acq On : 01 Sep 2022 18:34
 Operator : SY/MD
 Sample : N4366-07DL 5X
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F5E76DL

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\SFAMVTR083122WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV027675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.207	46	52	56	rBV2	12671	11772	1.86%	0.174%
2	1.297	70	80	88	rBV	112320	120443	19.05%	1.784%
3	1.336	90	92	104	rVB2	10904	11968	1.89%	0.177%
4	1.558	154	161	172	rVV	80693	90781	14.36%	1.344%
5	1.622	174	181	192	rVB	72217	86385	13.66%	1.279%
6	2.098	318	329	345	rBV	175617	291403	46.09%	4.315%
7	2.484	435	449	464	rBV2	105751	220805	34.92%	3.270%
8	2.561	467	473	488	rVB2	21988	41649	6.59%	0.617%
9	2.751	516	532	562	rBV	236691	460943	72.90%	6.826%
10	3.529	762	774	777	rBV	5052	8574	1.36%	0.127%
11	3.654	794	813	828	rBV2	56707	146550	23.18%	2.170%
12	3.908	880	892	903	rBV2	96816	255150	40.36%	3.778%
13	4.346	1011	1028	1056	rBV2	120484	321690	50.88%	4.764%
14	4.735	1136	1149	1169	rBV3	58230	145354	22.99%	2.153%
15	5.024	1226	1239	1264	rBV2	285863	632261	100.00%	9.363%
16	5.194	1280	1292	1306	rVB2	115351	264973	41.91%	3.924%
17	5.596	1404	1417	1446	rVB	176382	367028	58.05%	5.435%
18	5.895	1493	1510	1526	rBV3	54556	117464	18.58%	1.740%
19	6.063	1546	1562	1587	rBV	155473	350946	55.51%	5.197%
20	6.239	1604	1617	1626	rBV8	6070	12613	1.99%	0.187%
21	6.291	1626	1633	1643	rVB8	3953	7460	1.18%	0.110%
22	6.448	1670	1682	1694	rVB5	6560	12843	2.03%	0.190%
23	6.545	1700	1712	1721	rBV4	4455	11623	1.84%	0.172%
24	6.670	1735	1751	1767	rVB2	55958	121811	19.27%	1.804%
25	6.792	1774	1789	1806	rBV2	64470	135050	21.36%	2.000%
26	7.008	1841	1856	1880	rBV2	63026	122285	19.34%	1.811%
27	7.275	1928	1939	1946	rBV8	5706	11941	1.89%	0.177%
28	7.333	1946	1957	1979	rVB	275277	486740	76.98%	7.208%
29	7.641	2045	2053	2071	rVB	35574	69251	10.95%	1.026%
30	7.796	2092	2101	2109	rVB9	5690	8001	1.27%	0.118%
31	7.853	2109	2119	2128	rBV	13211	22943	3.63%	0.340%
32	7.985	2152	2160	2169	rVB7	4675	7951	1.26%	0.118%
33	8.114	2189	2200	2229	rBV2	227016	486393	76.93%	7.203%
34	8.522	2316	2327	2337	rVB9	6441	10531	1.67%	0.156%
35	8.860	2421	2432	2450	rBV	226835	379915	60.09%	5.626%
36	9.107	2500	2509	2515	rBV8	5303	8540	1.35%	0.126%

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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

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Title : TRACE VOA SFAM1.0

37	10.220	2843	2855	2871	rBV	92511	151244	23.92%	2.240%
38	11.249	3164	3175	3196	rBV	198810	314520	49.75%	4.658%
39	11.625	3278	3292	3308	rBV	216401	350521	55.44%	5.191%
40	12.548	3570	3579	3590	rVB6	6228	9734	1.54%	0.144%
41	12.754	3636	3643	3652	rVB3	9237	13404	2.12%	0.198%
42	13.310	3808	3816	3830	rVB5	5097	8867	1.40%	0.131%
43	15.914	4606	4626	4631	rBV5	13831	42406	6.71%	0.628%

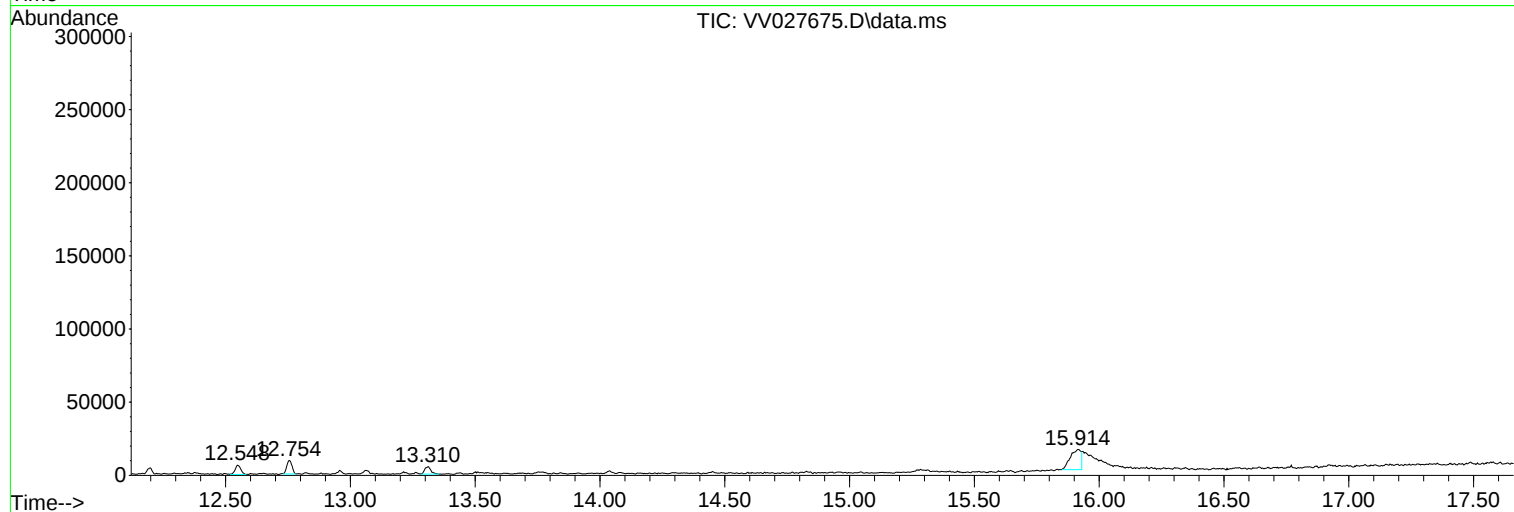
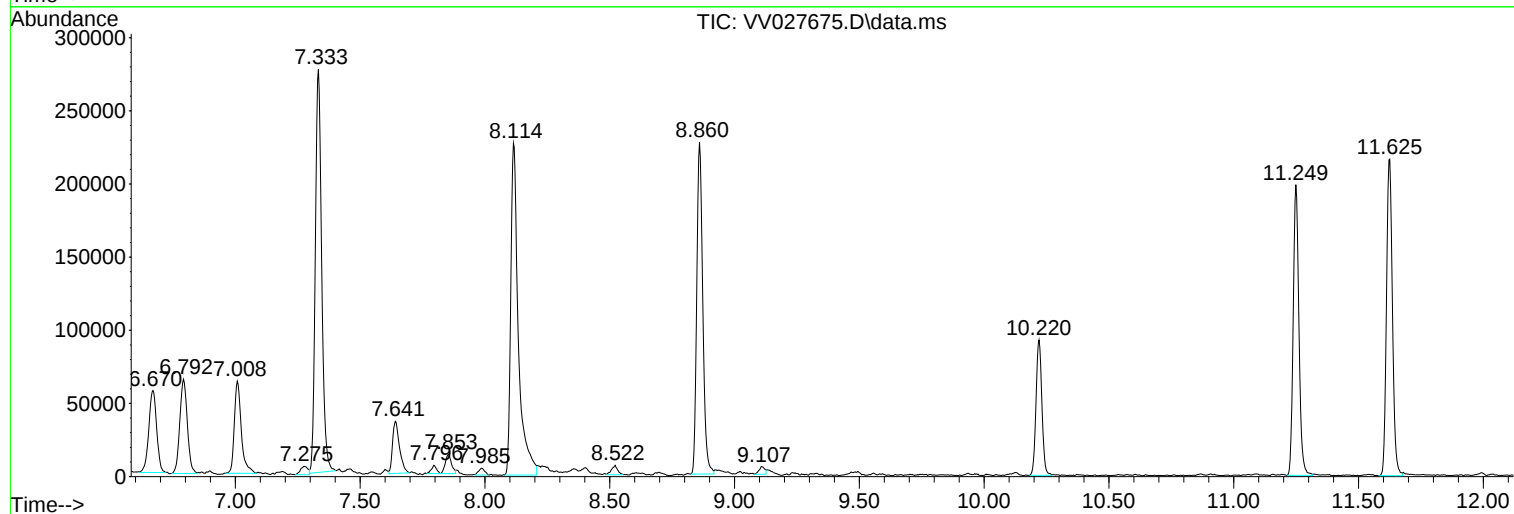
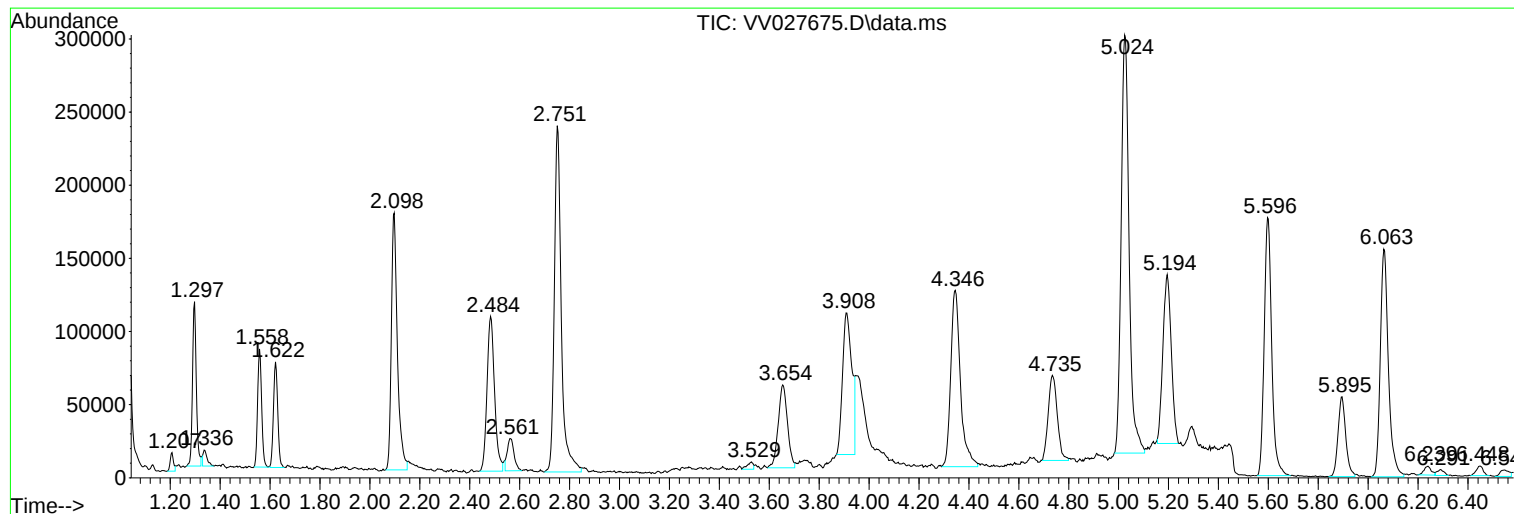
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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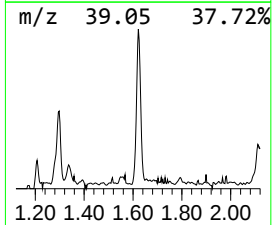
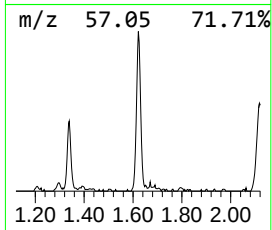
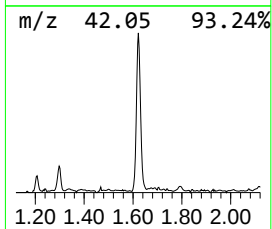
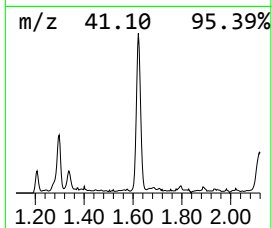
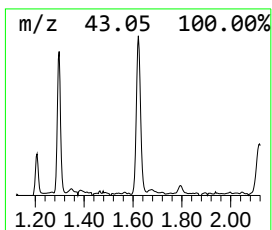
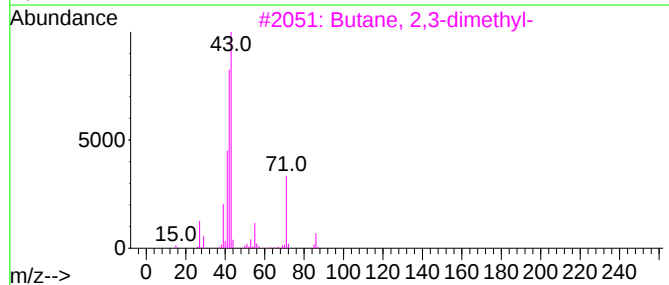
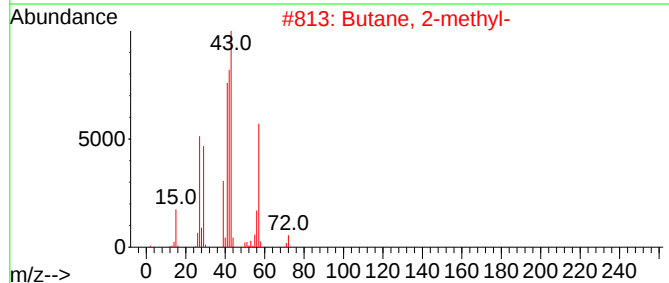
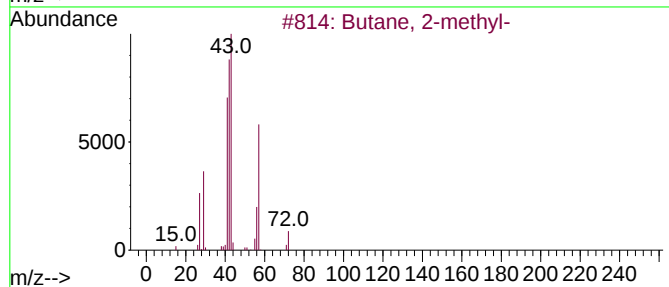
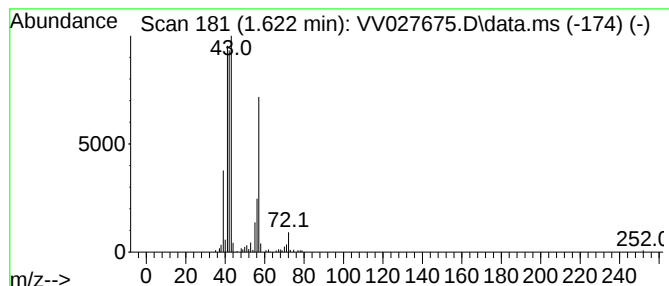
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.622	1.18 ug/L	86385	1,4-Difluorobenzene	5.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-		72	C5H12	000078-78-4	90	
2	Butane, 2-methyl-		72	C5H12	000078-78-4	80	
3	Butane, 2,3-dimethyl-		86	C6H14	000079-29-8	33	
4	Pentane		72	C5H12	000109-66-0	33	
5	Butane, 2-chloro-3-methyl-		106	C5H11Cl	000631-65-2	28	



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Instrument :
MSVOA_V
ClientSampleId :
F5E76DL

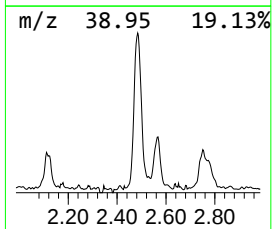
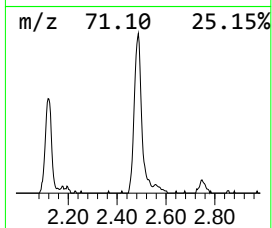
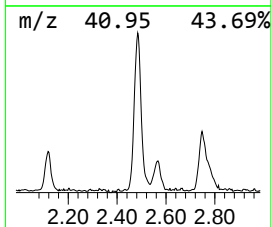
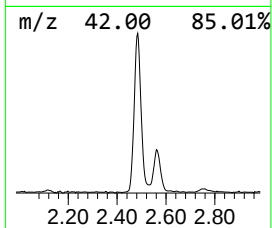
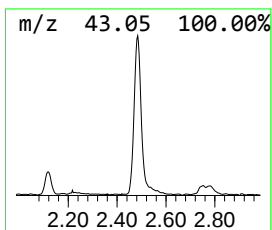
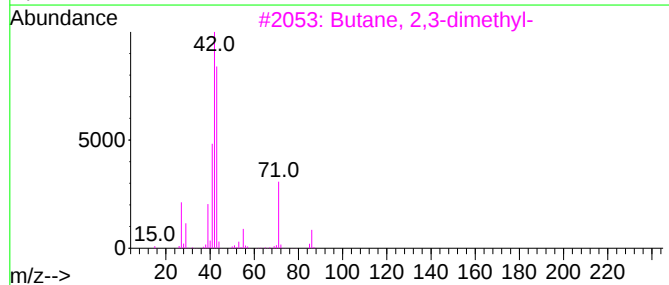
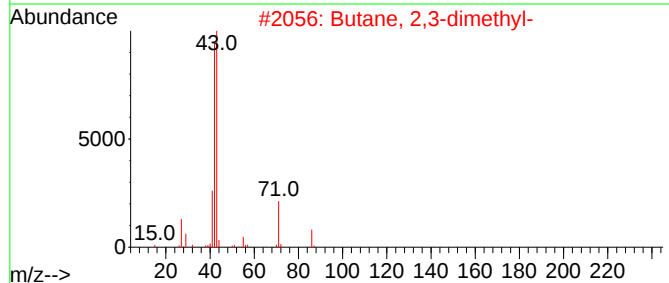
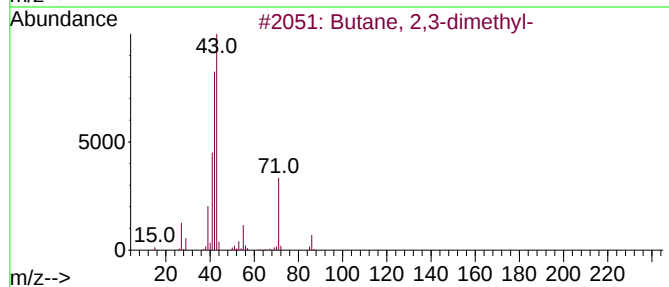
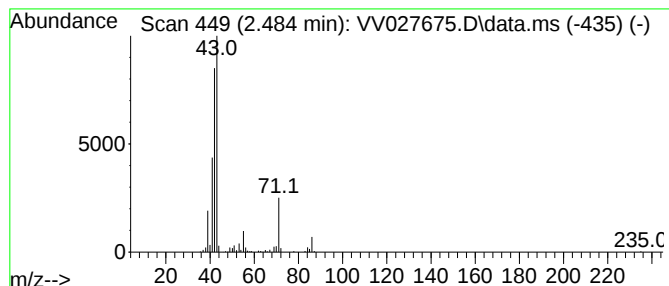
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.484	3.01 ug/L	220805	1,4-Difluorobenzene	5.596

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
4		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	78
5		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	78



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Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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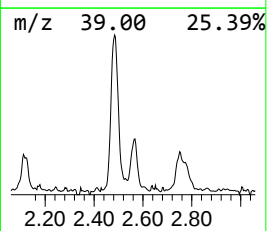
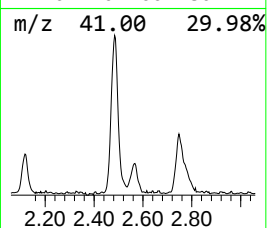
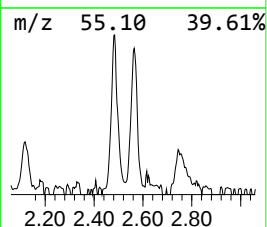
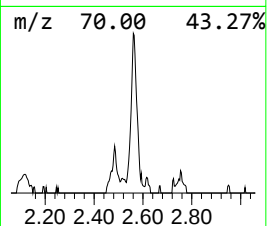
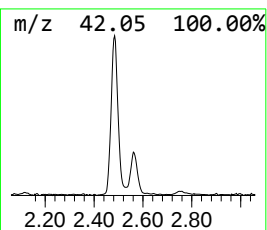
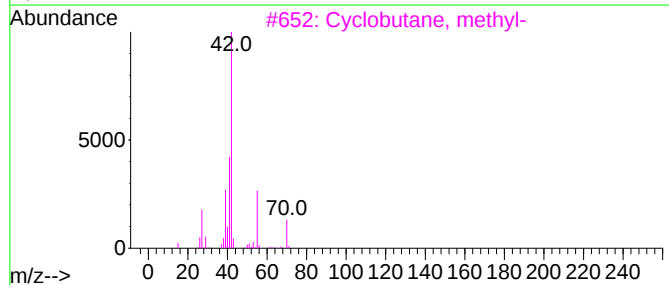
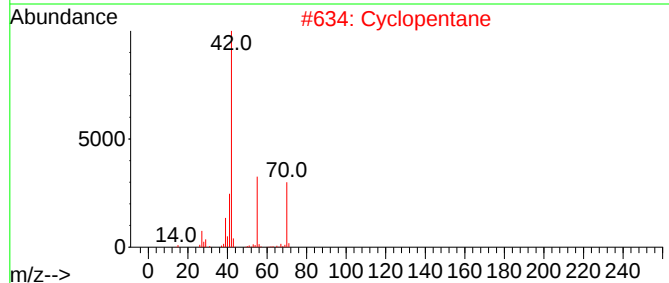
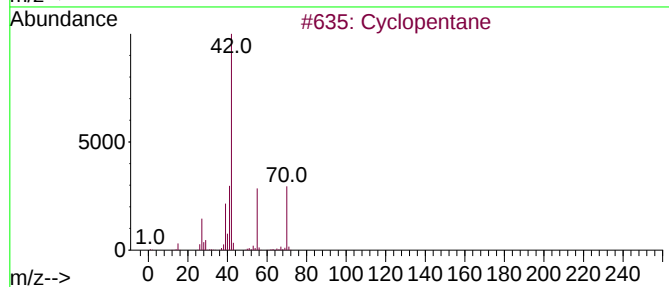
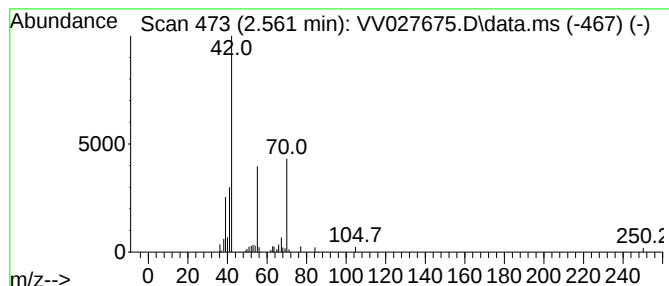
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Cyclic2.561 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.561	0.57 ug/L	41649	1,4-Difluorobenzene	5.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane	70	C5H10	000287-92-3	80
2			Cyclopentane	70	C5H10	000287-92-3	72
3			Cyclobutane, methyl-	70	C5H10	000598-61-8	50
4			1-Pentene	70	C5H10	000109-67-1	50
5			Cyclopropane, ethyl-	70	C5H10	001191-96-4	45



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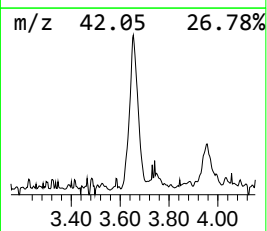
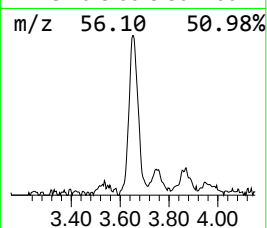
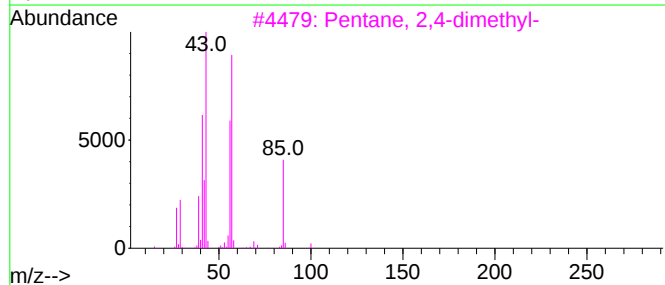
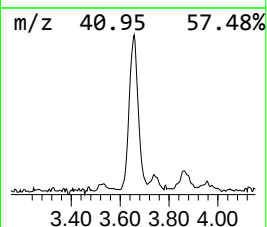
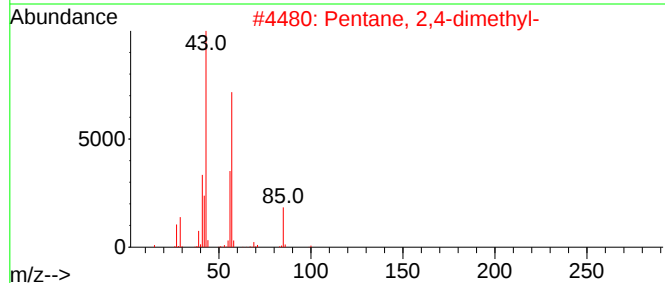
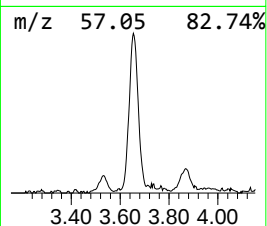
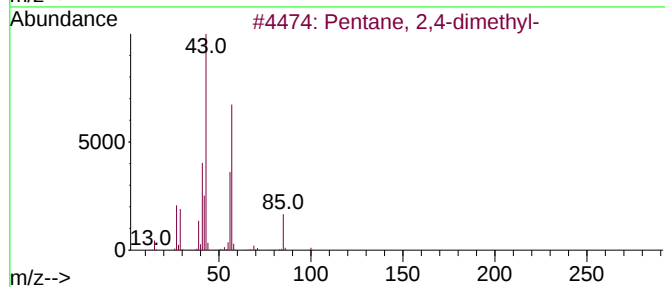
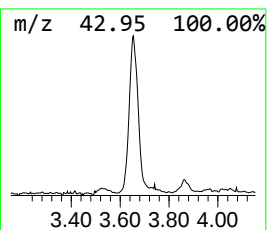
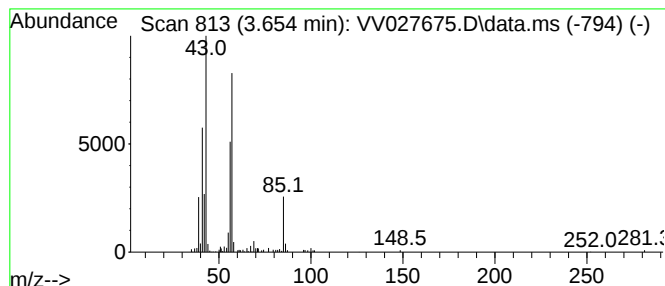
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.654	2.00 ug/L	146550	1,4-Difluorobenzene	5.596

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	87
2		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	78
3		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	74
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
5		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53



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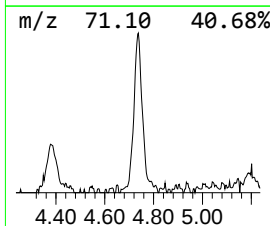
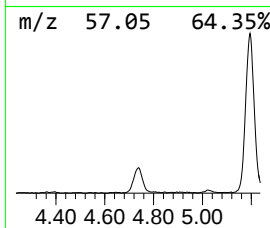
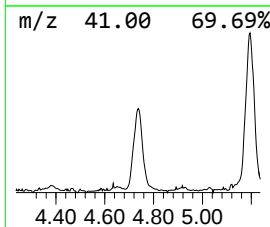
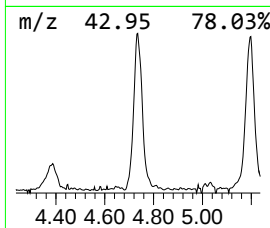
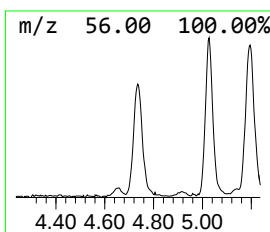
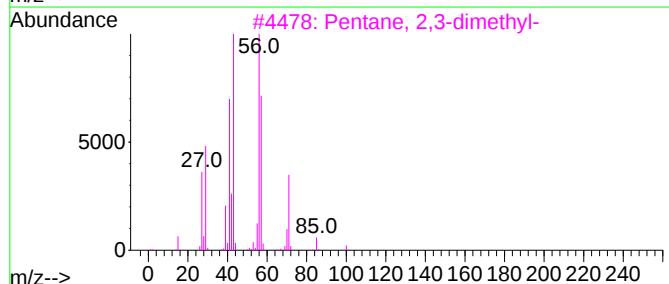
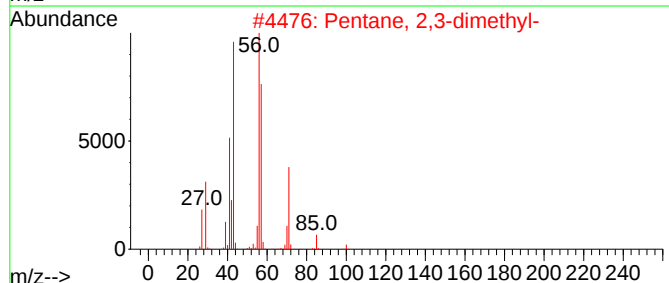
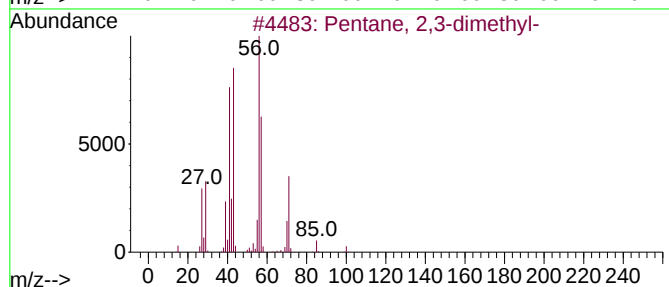
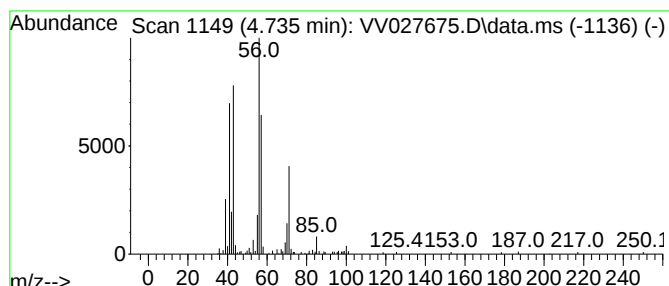
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.735	1.98 ug/L	145354	1,4-Difluorobenzene	5.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
3			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	64
4			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	50
5			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027675.D
Acq On : 01 Sep 2022 18:34
Operator : SY/MD
Sample : N4366-07DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

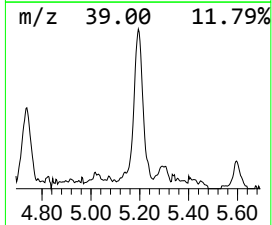
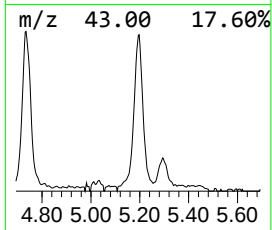
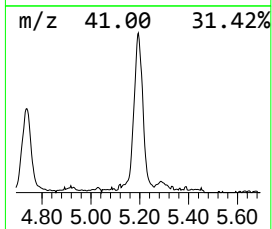
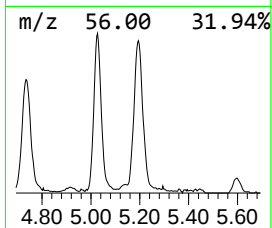
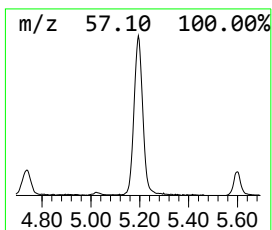
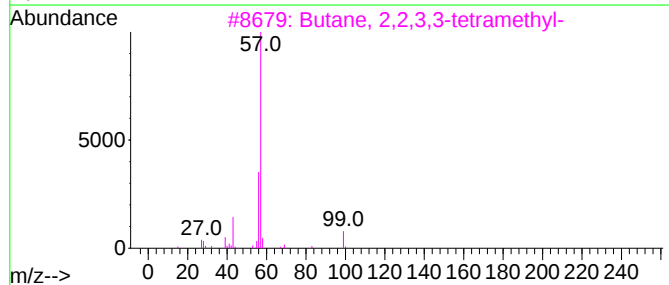
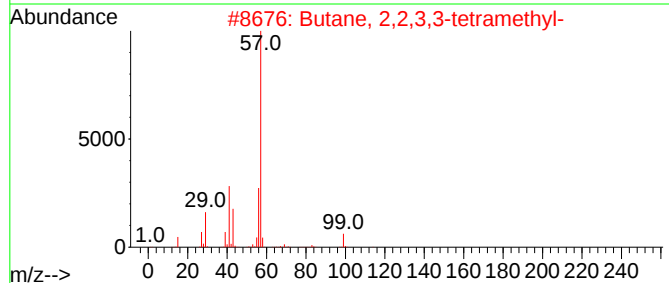
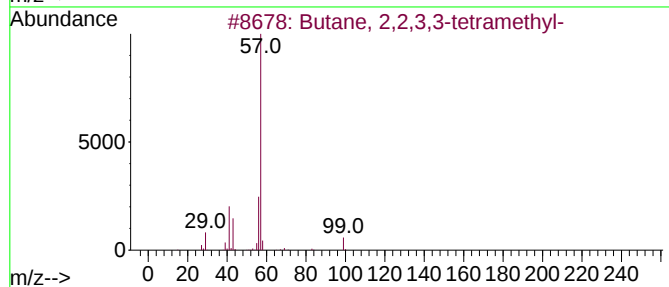
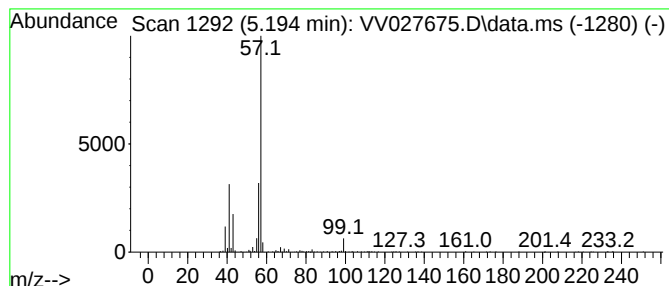
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ClientSampleId :
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.194	3.61 ug/L	264973	1,4-Difluorobenzene	5.596	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
4	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027675.D
Acq On : 01 Sep 2022 18:34
Operator : SY/MD
Sample : N4366-07DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

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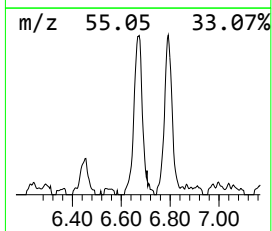
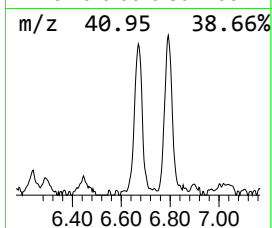
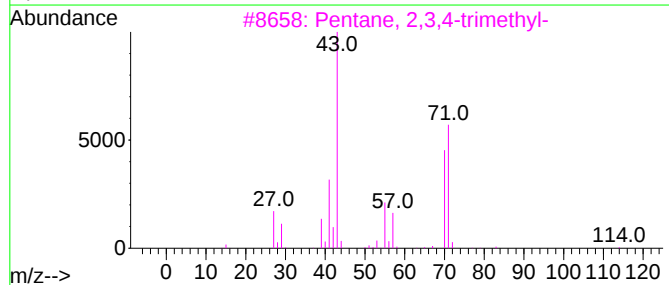
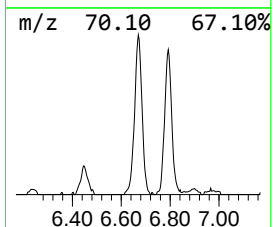
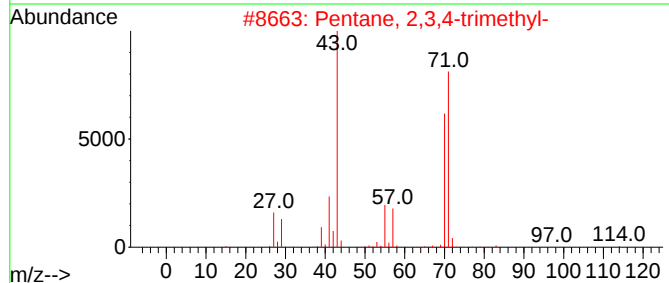
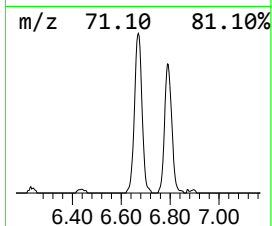
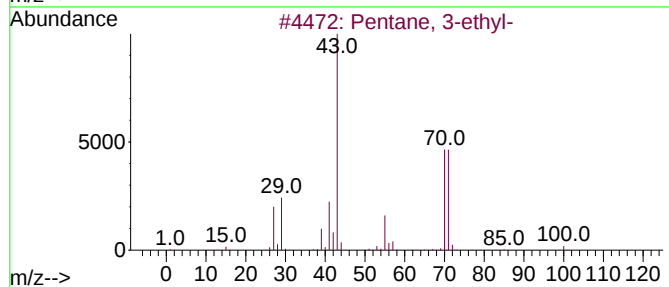
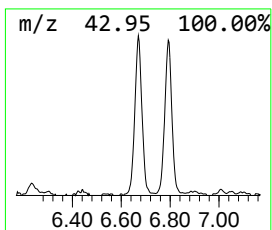
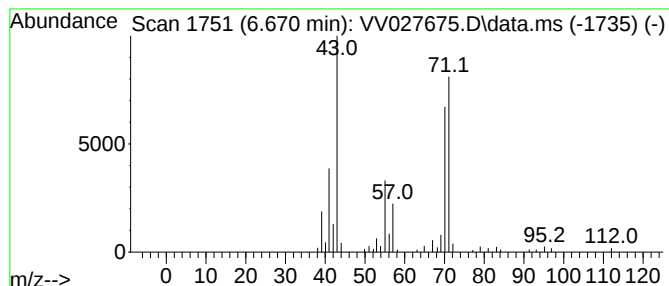
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.670	1.66 ug/L	121811	1,4-Difluorobenzene	5.596

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
2		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
4		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
5		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027675.D
Acq On : 01 Sep 2022 18:34
Operator : SY/MD
Sample : N4366-07DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

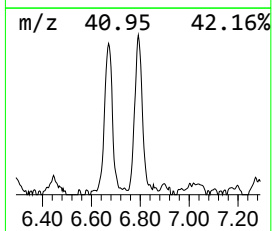
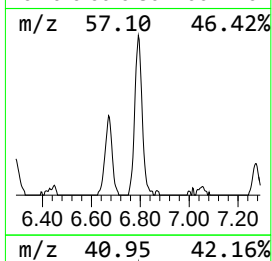
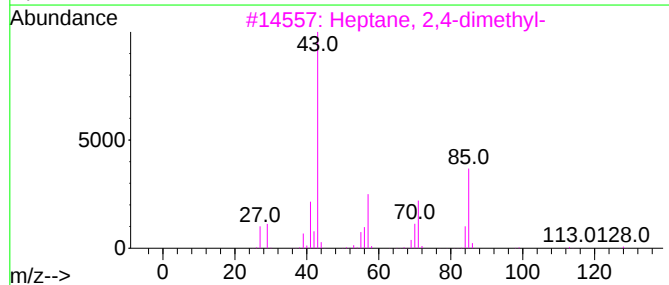
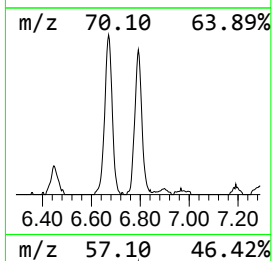
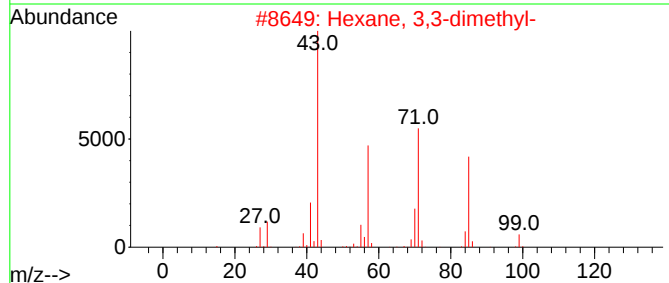
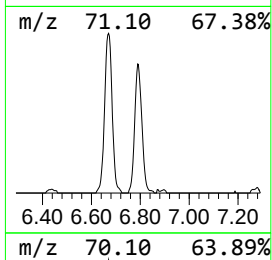
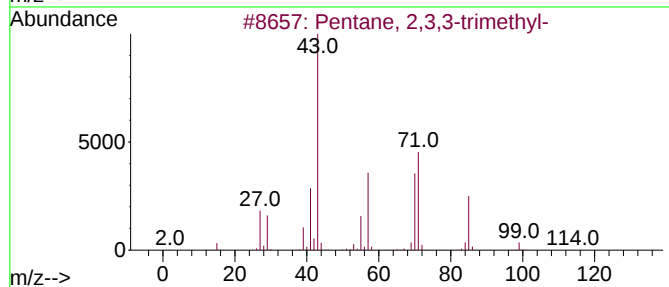
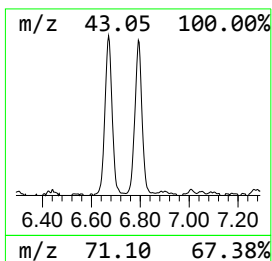
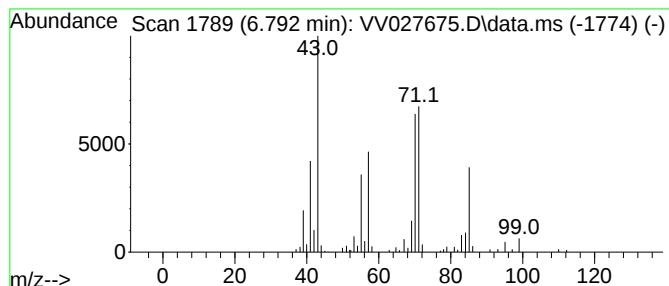
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.792	1.84 ug/L	135050	1,4-Difluorobenzene	5.596	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	59
4	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027675.D
Acq On : 01 Sep 2022 18:34
Operator : SY/MD
Sample : N4366-07DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E76DL

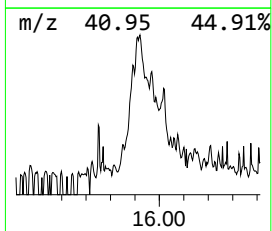
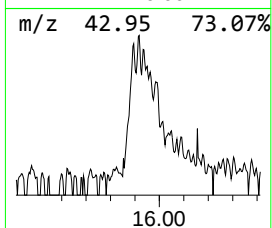
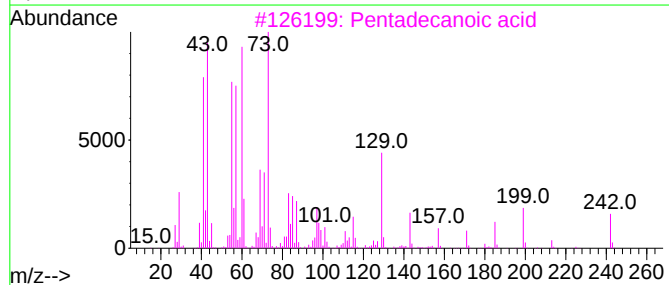
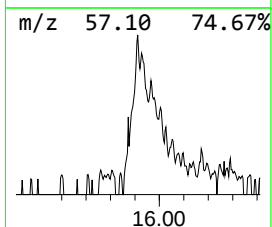
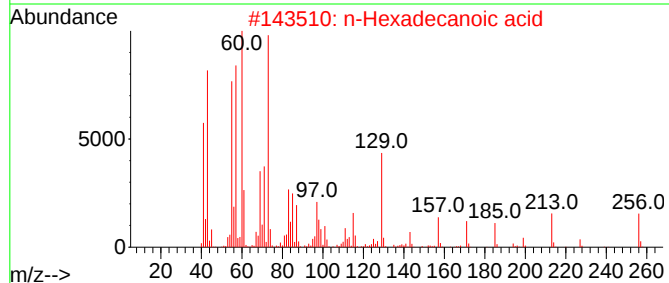
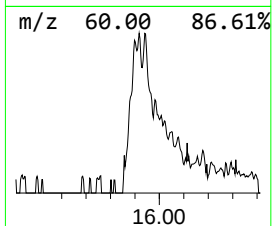
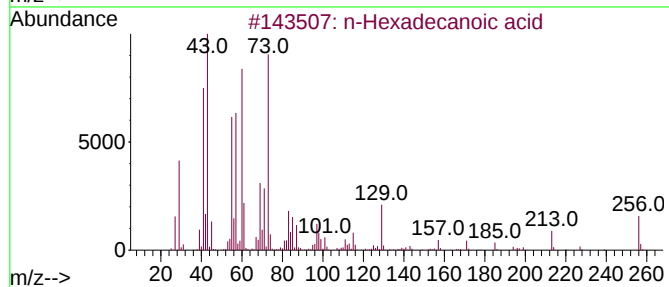
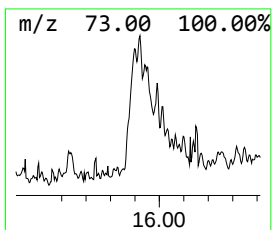
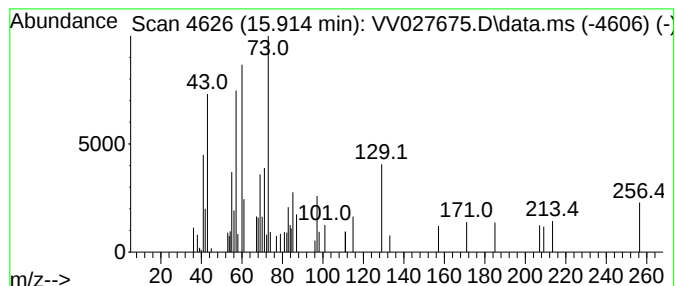
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.914	0.67 ug/L	42406	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Dodecanoic acid	200	C12H24O2	000143-07-7	72
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027675.D
Acq On : 01 Sep 2022 18:34
Operator : SY/MD
Sample : N4366-07DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E76DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

						--Internal Standard--			
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(DEL) Alkane: S...	2.484	3.0	ug/L	220805	1	5.596	367028	5.0	
(DEL) Alkane: C...	2.561	0.6	ug/L	41649	1	5.596	367028	5.0	
(DEL) Alkane: S...	3.654	2.0	ug/L	146550	1	5.596	367028	5.0	
(DEL) Alkane: S...	4.735	2.0	ug/L	145354	1	5.596	367028	5.0	
(DEL) Alkane: S...	5.194	3.6	ug/L	264973	1	5.596	367028	5.0	
(DEL) Alkane: S...	6.670	1.7	ug/L	121811	1	5.596	367028	5.0	
(DEL) Alkane: S...	6.792	1.8	ug/L	135050	1	5.596	367028	5.0	
n-Hexadecanoic ...	15.914	0.7	ug/L	42406	3	11.249	314520	5.0	