

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082522\
 Data File : VV027510.D
 Acq On : 25 Aug 2022 21:56
 Operator : SY/MD
 Sample : N4367-02
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F5E82

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\SFAMVTR081922WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV027510.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	73	82	97	rBV	52734	62278	10.55%	1.151%
2	1.564	155	163	174	rBV	49389	60314	10.22%	1.114%
3	1.632	178	184	191	rVB2	9641	12288	2.08%	0.227%
4	2.105	321	331	346	rVB	114203	177169	30.02%	3.273%
5	2.494	436	452	467	rBV2	63692	124997	21.18%	2.309%
6	2.571	467	476	489	rVB5	3600	7718	1.31%	0.143%
7	2.764	525	536	554	rVB5	8862	18599	3.15%	0.344%
8	3.664	796	816	835	rBV3	69686	184119	31.20%	3.402%
9	3.908	882	892	910	rBV	17414	51166	8.67%	0.945%
10	4.346	1012	1028	1050	rBV	65793	174788	29.62%	3.229%
11	4.674	1112	1130	1141	rBV5	10822	26391	4.47%	0.488%
12	4.760	1141	1157	1173	rBV2	219805	552681	93.66%	10.211%
13	4.947	1201	1215	1230	rVB9	5177	13747	2.33%	0.254%
14	5.047	1230	1246	1275	rBV2	143905	375787	63.68%	6.943%
15	5.230	1279	1303	1325	rBV	227864	590096	100.00%	10.902%
16	5.616	1411	1423	1450	rBV	143585	316903	53.70%	5.855%
17	6.069	1547	1564	1593	rBV	83203	214833	36.41%	3.969%
18	6.194	1593	1603	1613	rVV3	18711	40901	6.93%	0.756%
19	6.256	1613	1622	1630	rVV3	17120	36844	6.24%	0.681%
20	6.304	1630	1637	1654	rVB4	8489	18695	3.17%	0.345%
21	6.458	1671	1685	1699	rBV7	10587	24333	4.12%	0.450%
22	6.651	1726	1745	1766	rBV	107489	234037	39.66%	4.324%
23	6.773	1766	1783	1801	rBV	94765	210363	35.65%	3.887%
24	6.989	1832	1850	1873	rBV2	37162	90154	15.28%	1.666%
25	7.175	1900	1908	1921	rVB9	4597	9642	1.63%	0.178%
26	7.262	1921	1935	1942	rBV5	21429	44000	7.46%	0.813%
27	7.313	1942	1951	1975	rVB	155521	290141	49.17%	5.361%
28	7.628	2042	2049	2070	rVB3	16663	43153	7.31%	0.797%
29	7.786	2084	2098	2108	rBV4	8685	16513	2.80%	0.305%
30	7.841	2108	2115	2122	rBV4	9395	14920	2.53%	0.276%
31	8.091	2181	2193	2227	rBV	100307	271199	45.96%	5.011%
32	8.509	2312	2323	2333	rVB7	4257	6740	1.14%	0.125%
33	8.850	2419	2429	2447	rBV	213192	366166	62.05%	6.765%
34	10.217	2843	2854	2871	rBV	53784	88099	14.93%	1.628%
35	10.384	2895	2906	2915	rVB4	6072	9607	1.63%	0.177%
36	11.059	3107	3116	3121	rBV3	5405	8957	1.52%	0.165%

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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_V\Method\SFAMVTR081922WMA.M
Title : TRACE VOA SFAM1.0

37	11.085	3121	3124	3132	rVB3	5089	6354	1.08%	0.117%
38	11.249	3164	3175	3202	rBV	199682	319712	54.18%	5.907%
39	11.622	3280	3291	3309	rBV	135384	224282	38.01%	4.144%
40	12.114	3434	3444	3455	rBV2	8676	13099	2.22%	0.242%
41	15.512	4490	4501	4513	rBV3	20131	30362	5.15%	0.561%
42	16.702	4863	4871	4881	rBV2	20965	30345	5.14%	0.561%

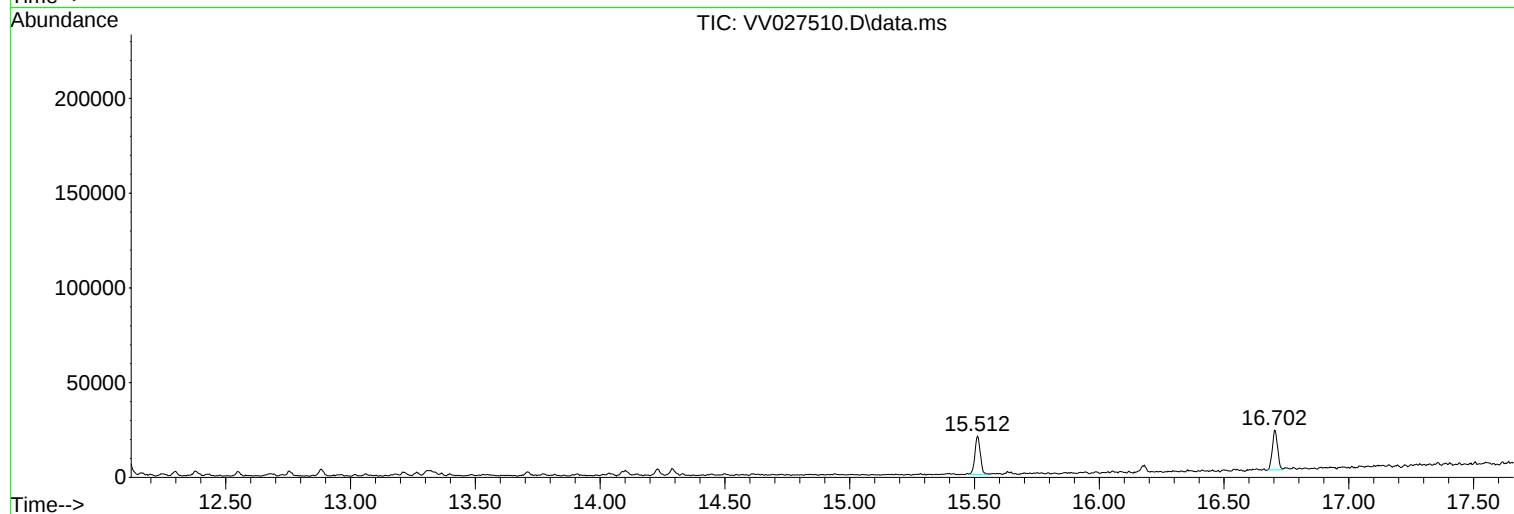
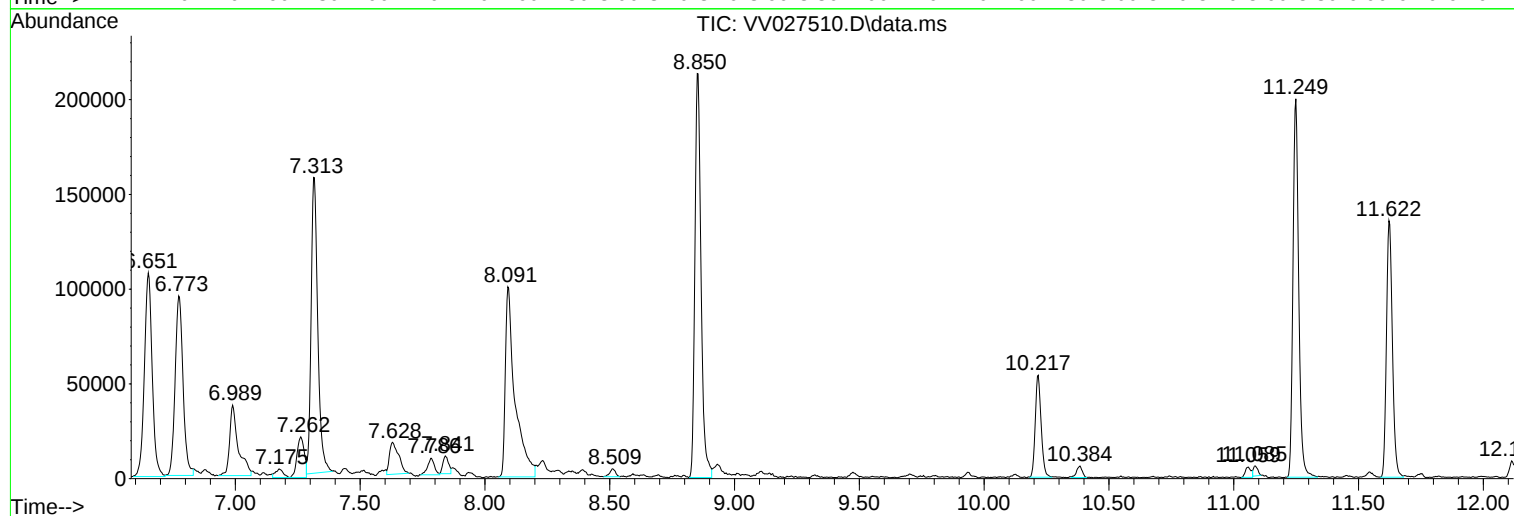
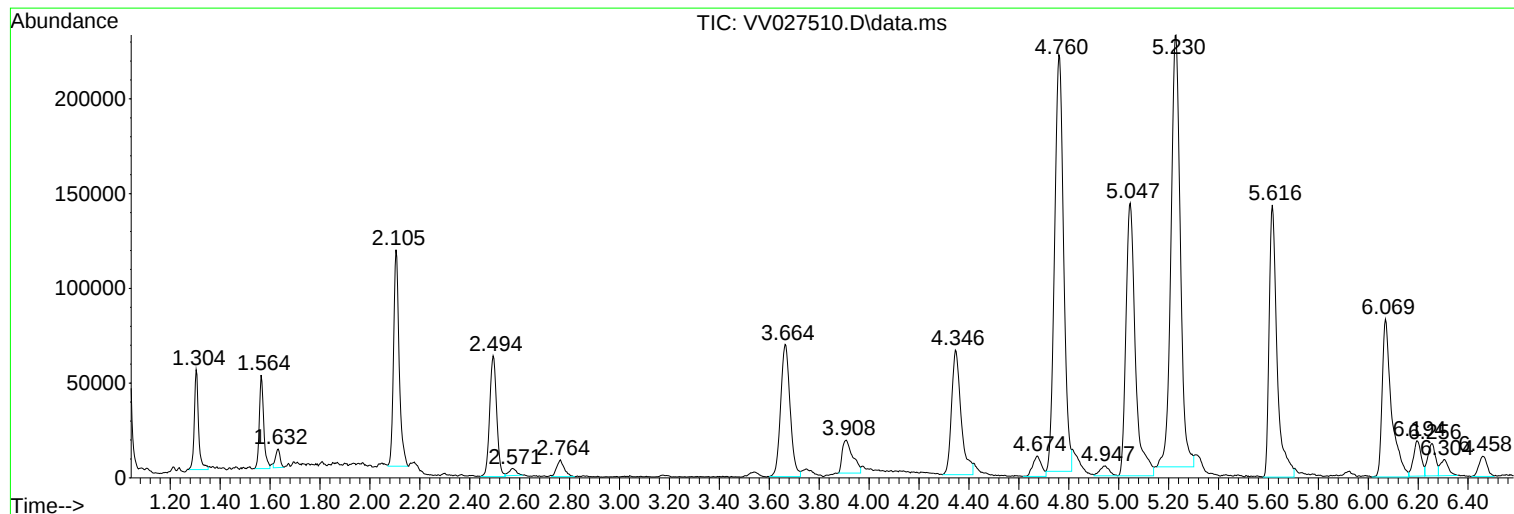
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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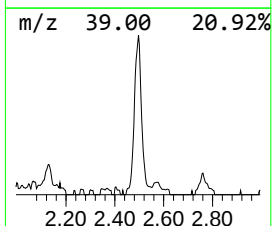
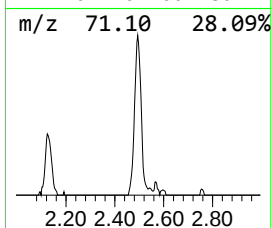
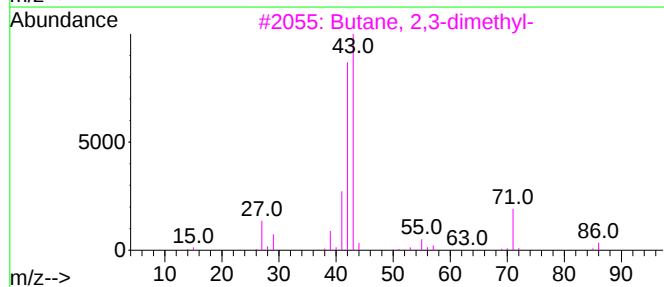
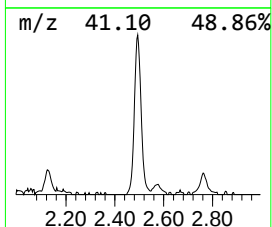
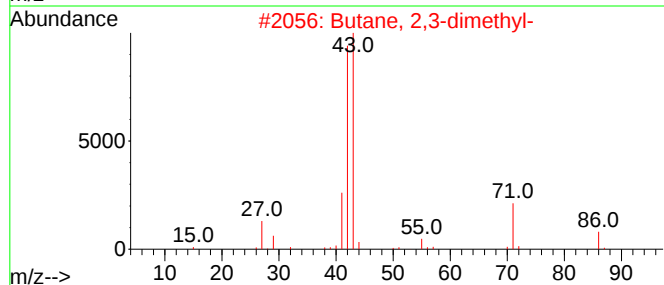
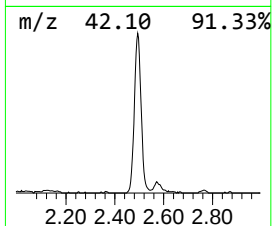
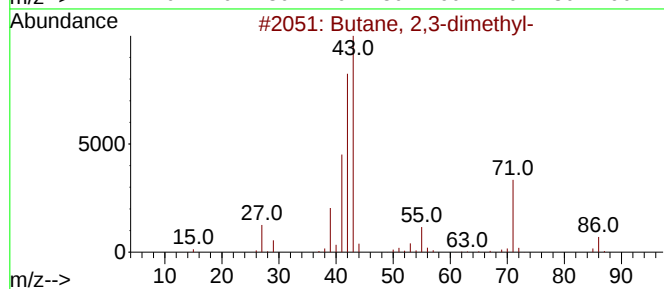
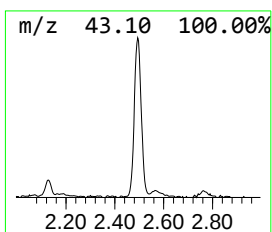
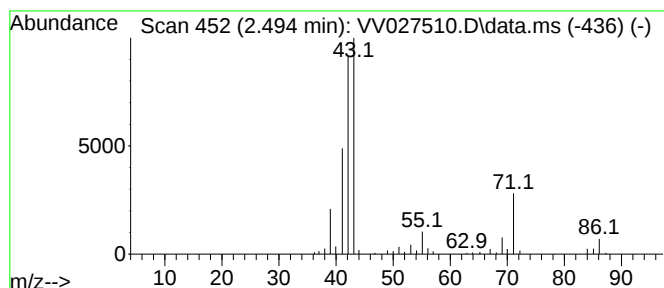
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.494	1.97 ug/L	124997	1,4-Difluorobenzene	5.616

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	80
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64



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Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E82

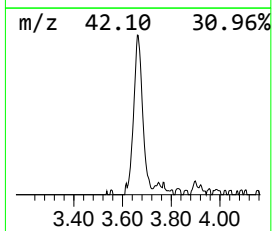
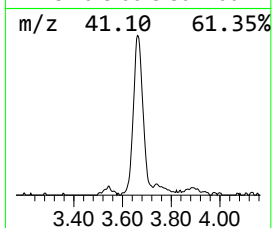
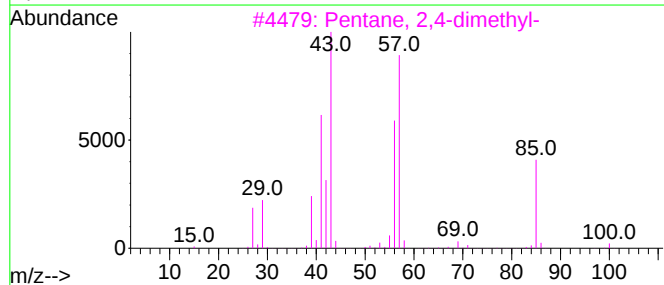
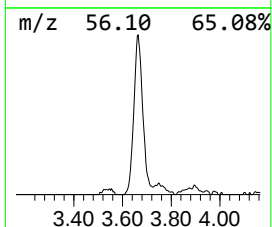
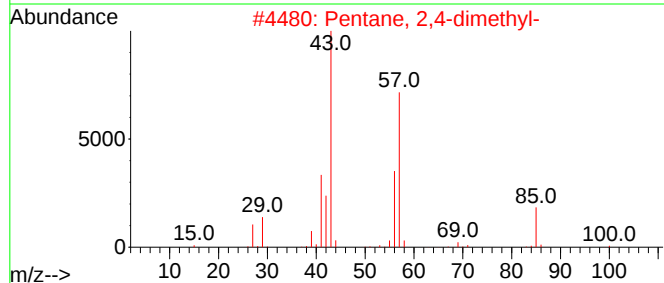
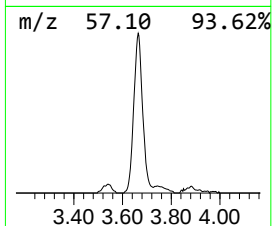
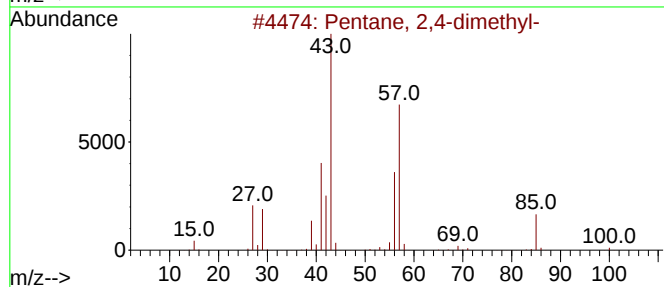
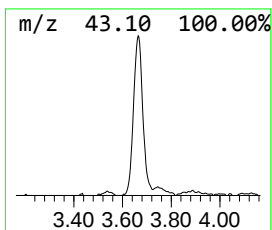
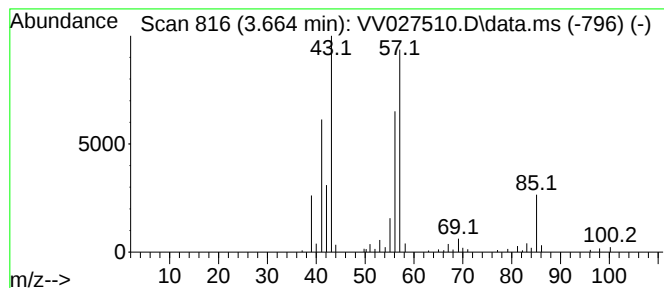
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.664	2.90 ug/L	184119	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	83
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	64
5			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53



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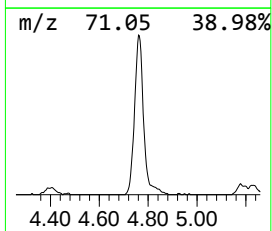
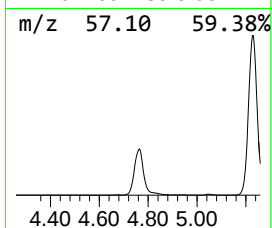
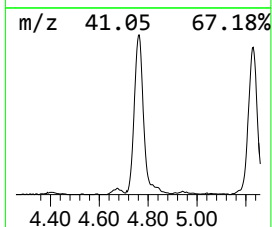
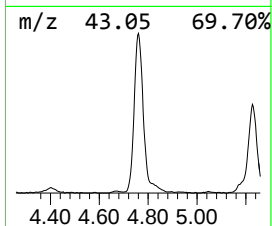
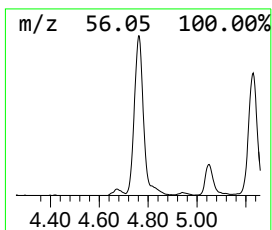
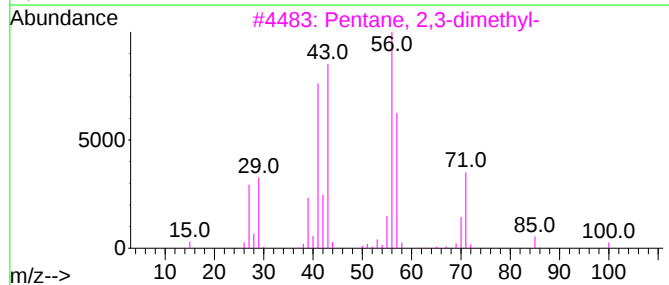
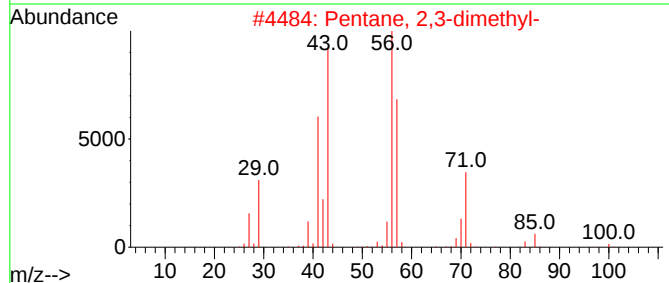
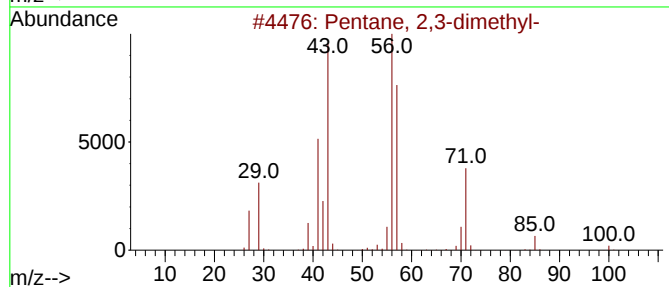
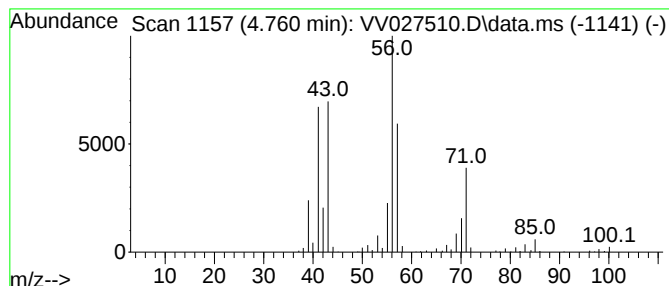
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.760	8.72 ug/L	552681	1,4-Difluorobenzene	5.616

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	91
3		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
4		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	72
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	47



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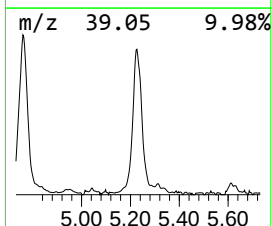
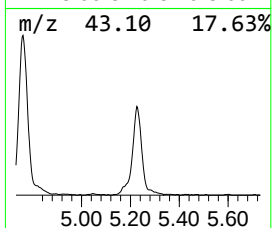
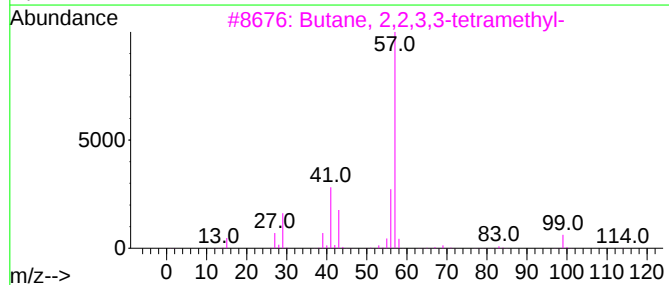
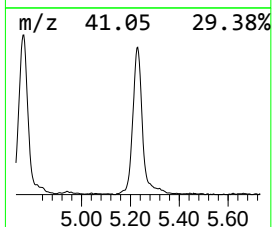
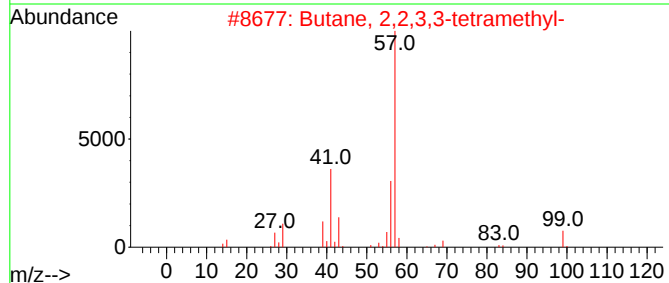
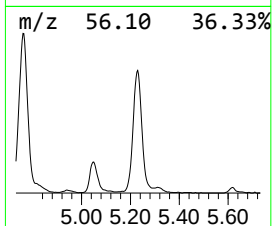
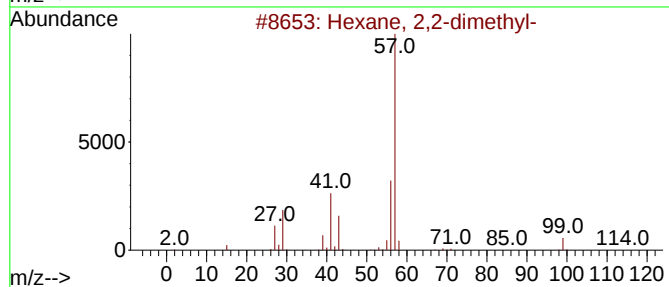
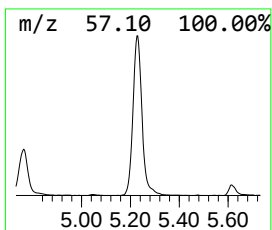
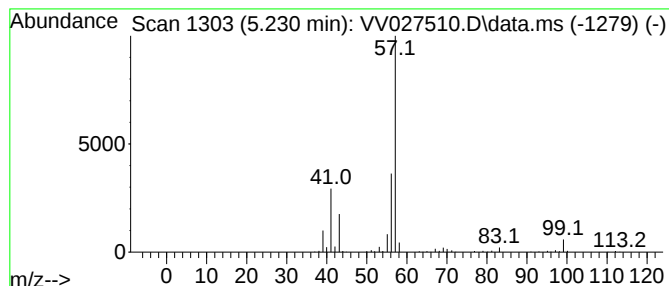
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.230	9.31 ug/L	590096	1,4-Difluorobenzene	5.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
4		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
5		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64



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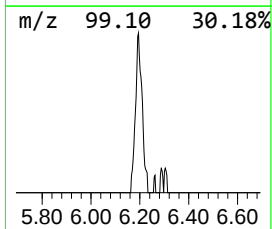
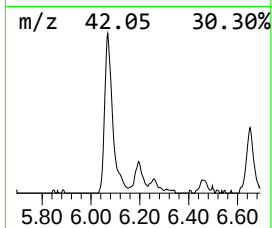
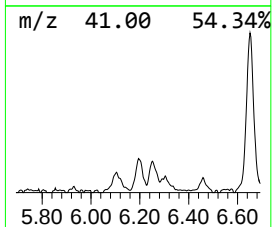
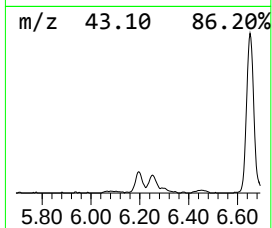
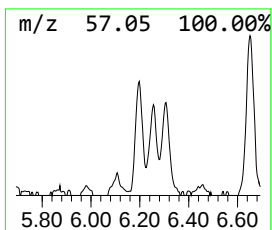
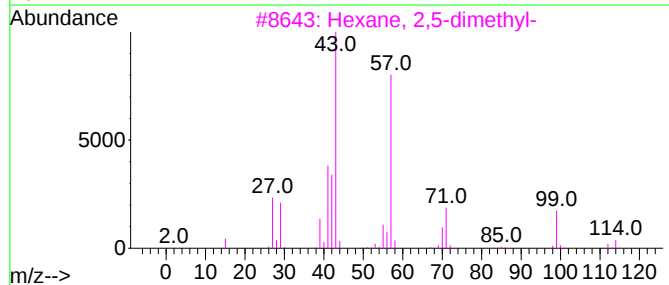
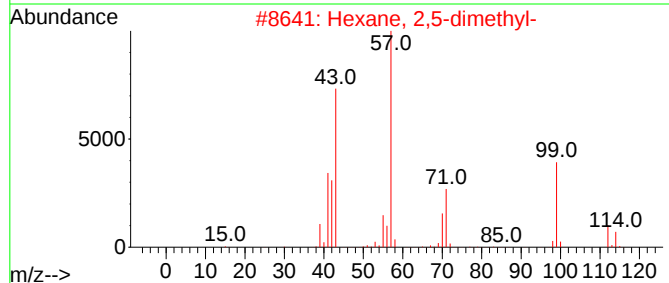
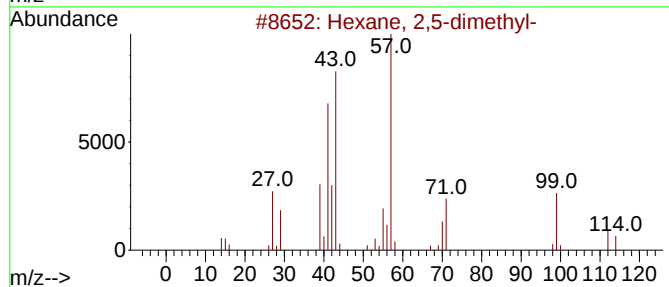
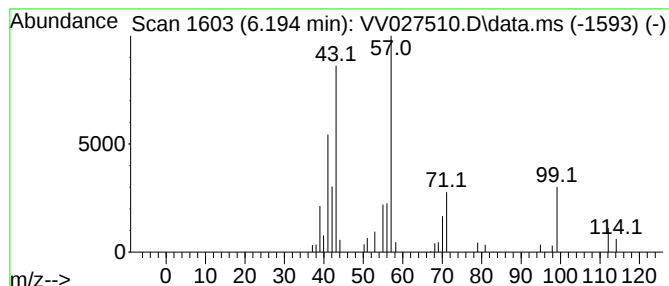
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.194	0.65 ug/L	40901	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	81
2			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	58
3			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	49
4			2(3H)-Furanone, dihydro-4,4-dime...	114	C6H10O2	013861-97-7	43
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082522\
Data File : VV027510.D
Acq On : 25 Aug 2022 21:56
Operator : SY/MD
Sample : N4367-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E82

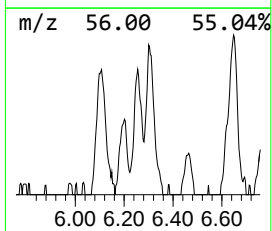
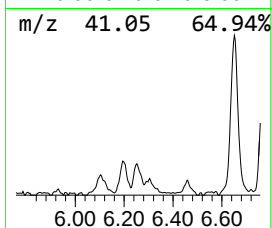
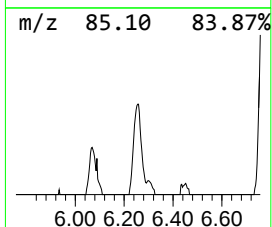
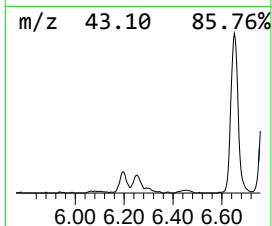
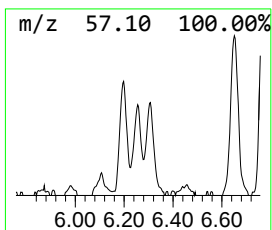
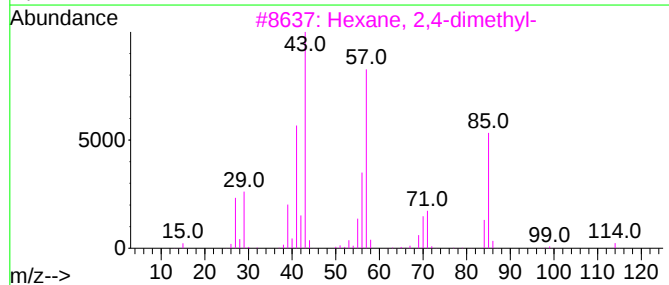
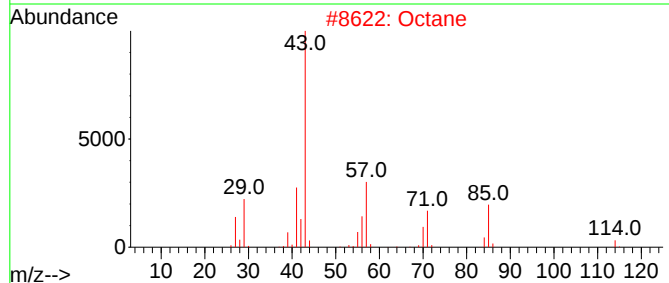
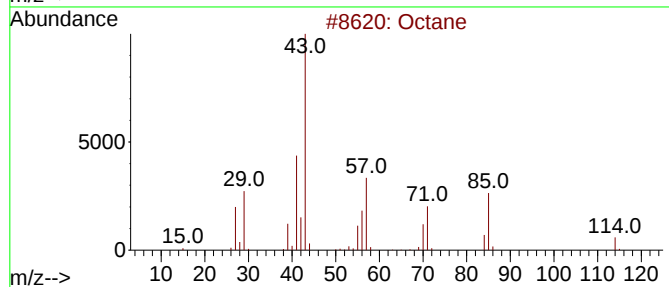
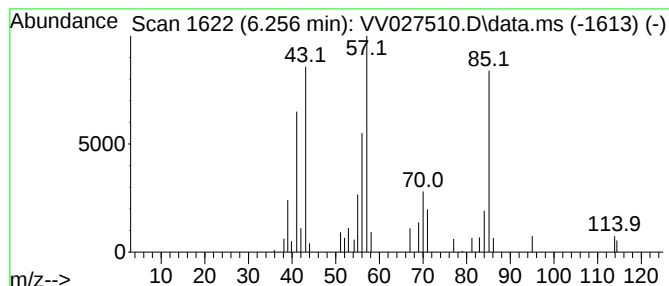
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.256	0.58 ug/L	36844	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane			114	C8H18	000111-65-9	80
2	Octane			114	C8H18	000111-65-9	80
3	Hexane, 2,4-dimethyl-			114	C8H18	000589-43-5	72
4	Octane			114	C8H18	000111-65-9	72
5	Octane			114	C8H18	000111-65-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082522\
Data File : VV027510.D
Acq On : 25 Aug 2022 21:56
Operator : SY/MD
Sample : N4367-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E82

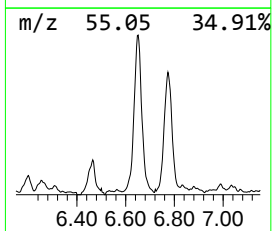
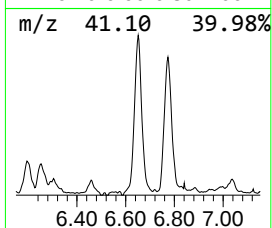
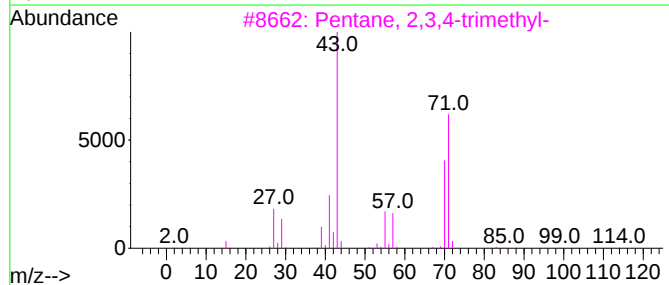
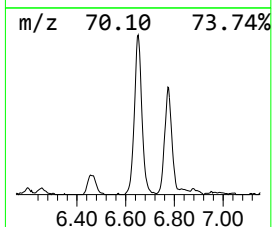
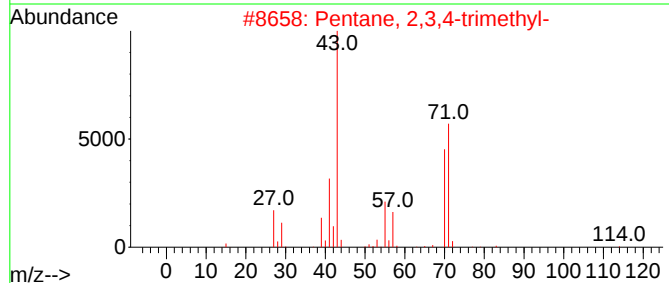
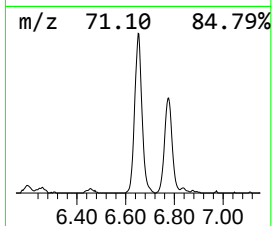
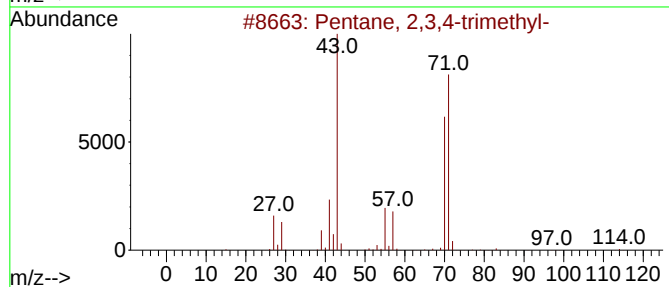
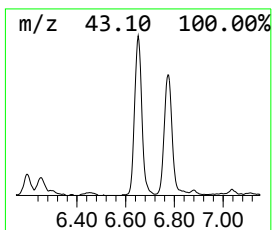
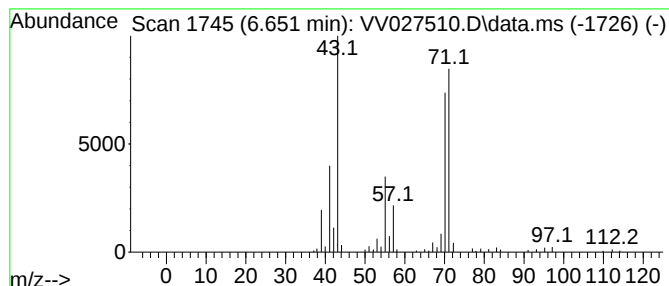
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Quant Title : TRACE VOA SFAM1.0

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.
6.651	3.69 ug/L	234037	1,4-Difluorobenzene	5.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	87
3		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	80
4		Diisoamyl ether	158	C10H22O	000544-01-4	78
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082522\
Data File : VV027510.D
Acq On : 25 Aug 2022 21:56
Operator : SY/MD
Sample : N4367-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E82

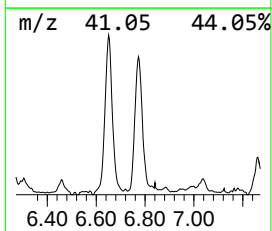
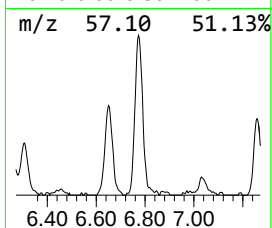
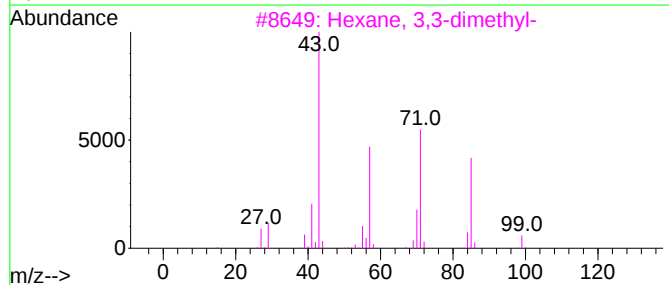
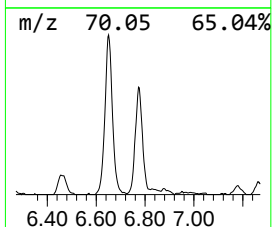
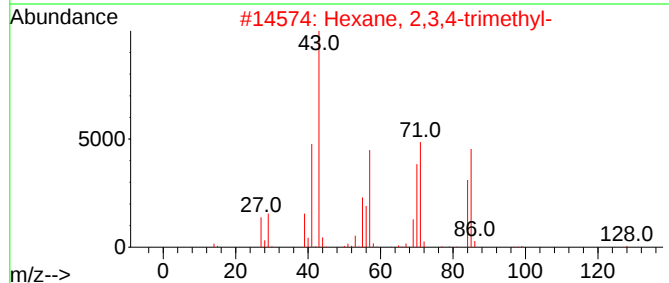
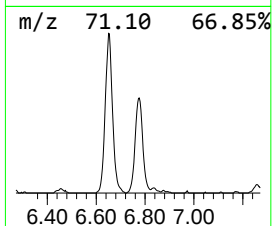
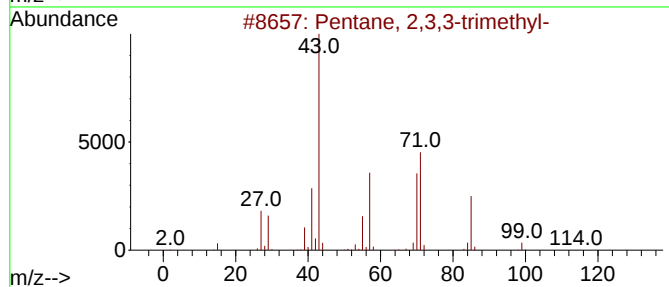
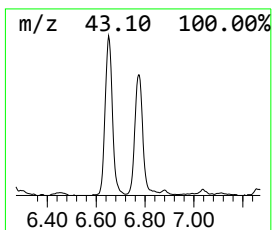
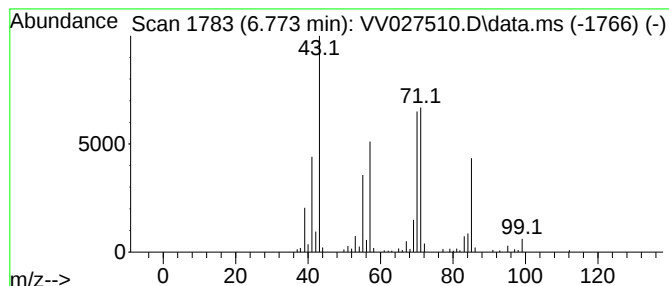
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.773	3.32 ug/L	210363	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	59
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082522\
Data File : VV027510.D
Acq On : 25 Aug 2022 21:56
Operator : SY/MD
Sample : N4367-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E82

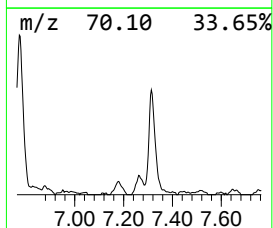
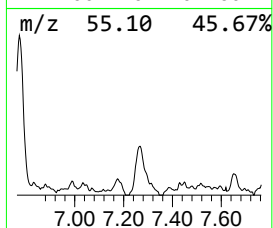
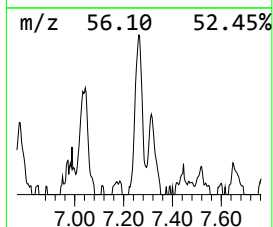
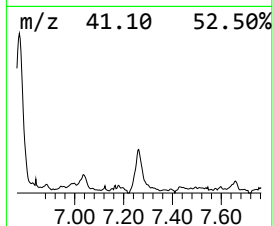
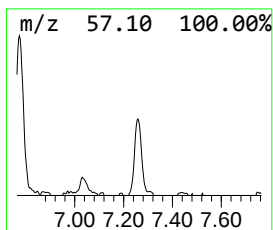
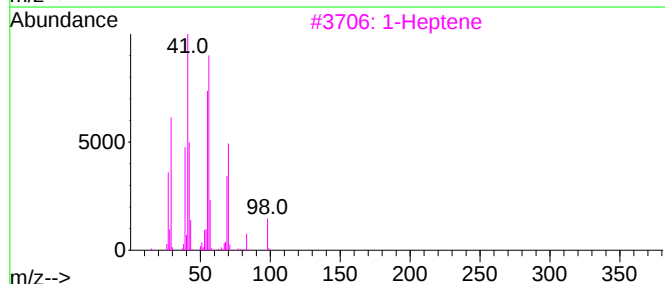
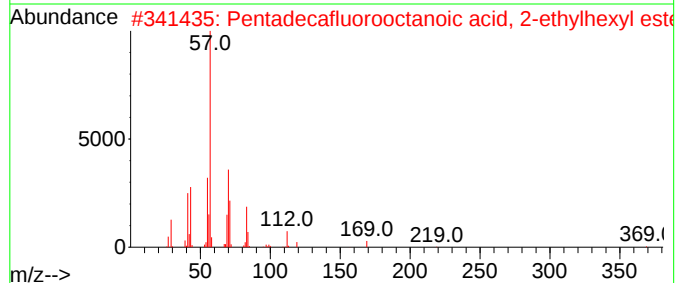
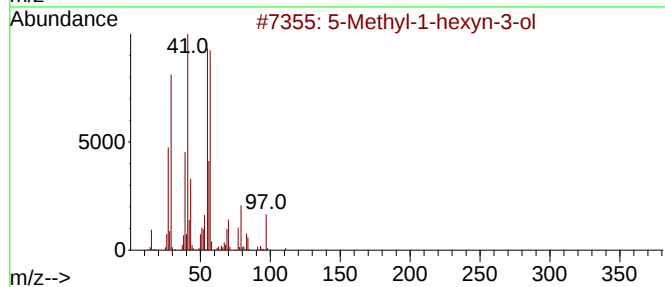
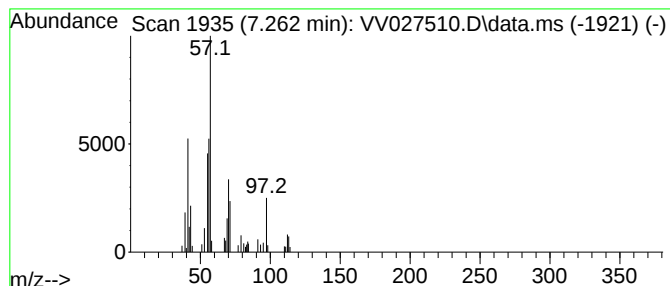
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 5-Methyl-1-hexyn-3-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.262	0.60 ug/L	44000	Chlorobenzene-d5	8.850

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Methyl-1-hexyn-3-ol	112	C7H12O	061996-79-0	50
2		Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	43
3		1-Heptene	98	C7H14	000592-76-7	38
4		1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	38
5		Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082522\
Data File : VV027510.D
Acq On : 25 Aug 2022 21:56
Operator : SY/MD
Sample : N4367-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E82

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	2.494	2.0	ug/L	124997	1	5.616	316903	5.0
(DEL) Alkane: S...	3.664	2.9	ug/L	184119	1	5.616	316903	5.0
(DEL) Alkane: S...	4.760	8.7	ug/L	552681	1	5.616	316903	5.0
(DEL) Alkane: S...	5.230	9.3	ug/L	590096	1	5.616	316903	5.0
(DEL) Alkane: S...	6.194	0.7	ug/L	40901	1	5.616	316903	5.0
(DEL) Alkane: S...	6.256	0.6	ug/L	36844	1	5.616	316903	5.0
(DEL) Alkane: S...	6.651	3.7	ug/L	234037	1	5.616	316903	5.0
(DEL) Alkane: S...	6.773	3.3	ug/L	210363	1	5.616	316903	5.0
5-Methyl-1-hexy...	7.262	0.6	ug/L	44000	2	8.850	366166	5.0