

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083022\
 Data File : VV027605.D
 Acq On : 30 Aug 2022 23:26
 Operator : SY/MD
 Sample : N4366-06DL 5X
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F5E75DL

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: VV027605.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.214	48	54	59	rBV2	13498	13434	2.56%	0.196%
2	1.307	74	83	91	rBV	93088	102705	19.55%	1.496%
3	1.346	91	95	103	rVB	10676	11305	2.15%	0.165%
4	1.564	156	163	176	rVV	63704	73800	14.05%	1.075%
5	1.632	176	184	194	rVB	90857	112809	21.47%	1.643%
6	2.105	321	331	352	rBV2	128333	240121	45.70%	3.497%
7	2.178	352	354	375	rVB2	6964	14543	2.77%	0.212%
8	2.497	438	453	468	rBV2	180791	375414	71.45%	5.467%
9	2.574	468	477	496	rVB2	29860	59826	11.39%	0.871%
10	2.757	521	534	551	rBV	274120	495089	94.23%	7.210%
11	2.838	551	559	575	rVB9	7224	19567	3.72%	0.285%
12	3.664	797	816	832	rBV2	53697	145647	27.72%	2.121%
13	3.754	835	844	858	rVB10	5442	13545	2.58%	0.197%
14	3.905	865	891	913	rBV3	136824	426700	81.21%	6.214%
15	4.346	1012	1028	1057	rBV2	90102	254371	48.41%	3.705%
16	4.674	1118	1130	1139	rBV9	4827	11358	2.16%	0.165%
17	4.760	1141	1157	1177	rVV2	60917	157528	29.98%	2.294%
18	4.937	1201	1212	1215	rBV8	4071	5464	1.04%	0.080%
19	5.043	1226	1245	1276	rBV2	195485	525408	100.00%	7.652%
20	5.230	1288	1303	1316	rBV2	123146	303112	57.69%	4.414%
21	5.616	1411	1423	1457	rBV	182422	403887	76.87%	5.882%
22	5.915	1499	1516	1537	rBV2	57566	131263	24.98%	1.912%
23	6.069	1550	1564	1595	rBV2	115478	283052	53.87%	4.122%
24	6.255	1612	1622	1630	rBV10	5798	11274	2.15%	0.164%
25	6.304	1630	1637	1647	rVB9	3904	7222	1.37%	0.105%
26	6.461	1674	1686	1697	rBV7	7647	16972	3.23%	0.247%
27	6.651	1727	1745	1764	rBV2	64665	144815	27.56%	2.109%
28	6.773	1768	1783	1804	rVV2	71633	157813	30.04%	2.298%
29	6.989	1839	1850	1872	rBV	44938	93508	17.80%	1.362%
30	7.265	1925	1936	1942	rBV	6136	13203	2.51%	0.192%
31	7.317	1942	1952	1973	rVB	201940	361951	68.89%	5.271%
32	7.628	2040	2049	2066	rVB3	24455	51570	9.82%	0.751%
33	7.786	2090	2098	2107	rVB7	5017	7638	1.45%	0.111%
34	7.844	2107	2116	2126	rBV4	16092	29331	5.58%	0.427%
35	7.976	2148	2157	2167	rBV4	4558	7956	1.51%	0.116%
36	8.091	2183	2193	2229	rBV	172042	434036	82.61%	6.321%

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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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37	8.387	2280	2285	2294	rVB7	4937	7436	1.42%	0.108%
38	8.509	2311	2323	2335	rBV7	8090	15331	2.92%	0.223%
39	8.850	2418	2429	2448	rBV	274521	463254	88.17%	6.747%
40	9.104	2499	2508	2518	rBV10	6302	12507	2.38%	0.182%
41	9.477	2615	2624	2640	rVB10	3435	8555	1.63%	0.125%
42	10.217	2840	2854	2871	rBV	78810	132016	25.13%	1.923%
43	11.249	3163	3175	3191	rBV	238039	373461	71.08%	5.439%
44	11.625	3278	3292	3308	rBV	177348	289321	55.07%	4.214%
45	12.194	3461	3469	3477	rVB4	5171	7645	1.46%	0.111%
46	12.551	3570	3580	3592	rVB3	8002	12656	2.41%	0.184%
47	12.754	3635	3643	3653	rBV4	11520	17816	3.39%	0.259%
48	13.307	3809	3815	3825	rVB3	6414	9198	1.75%	0.134%

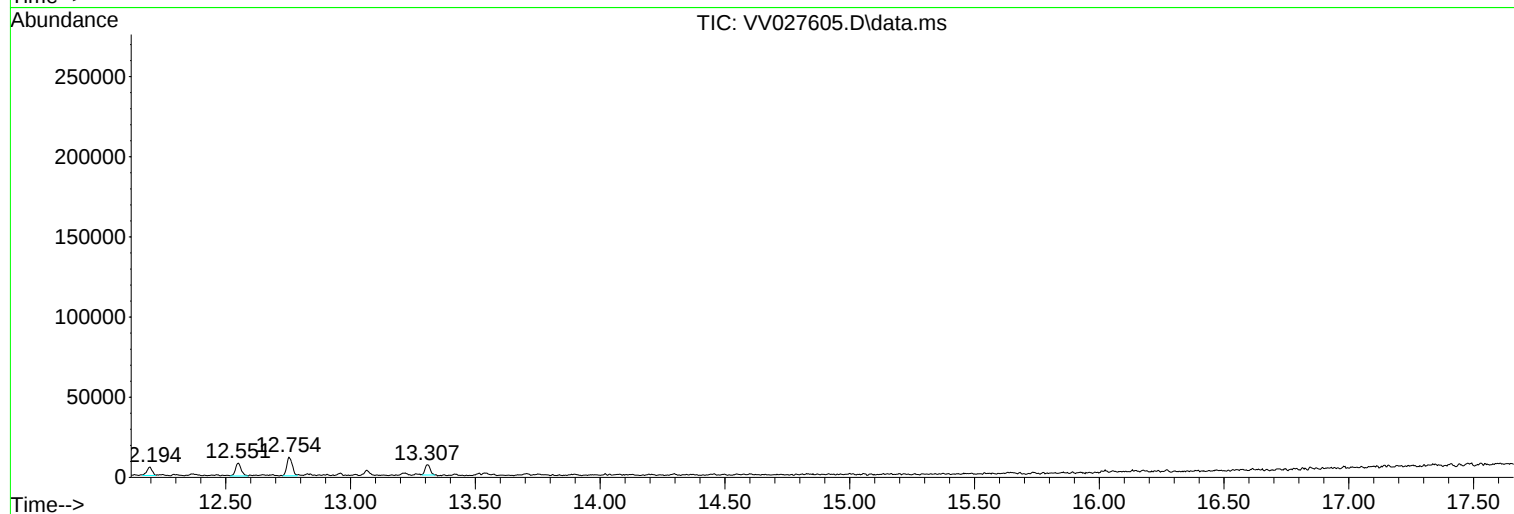
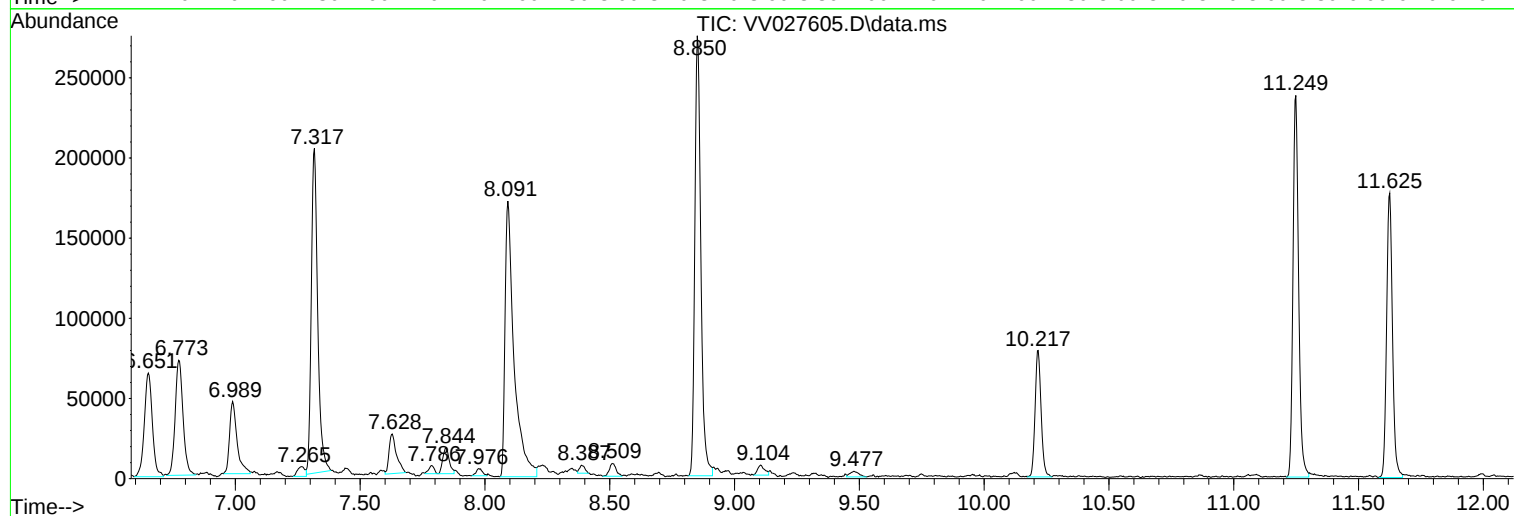
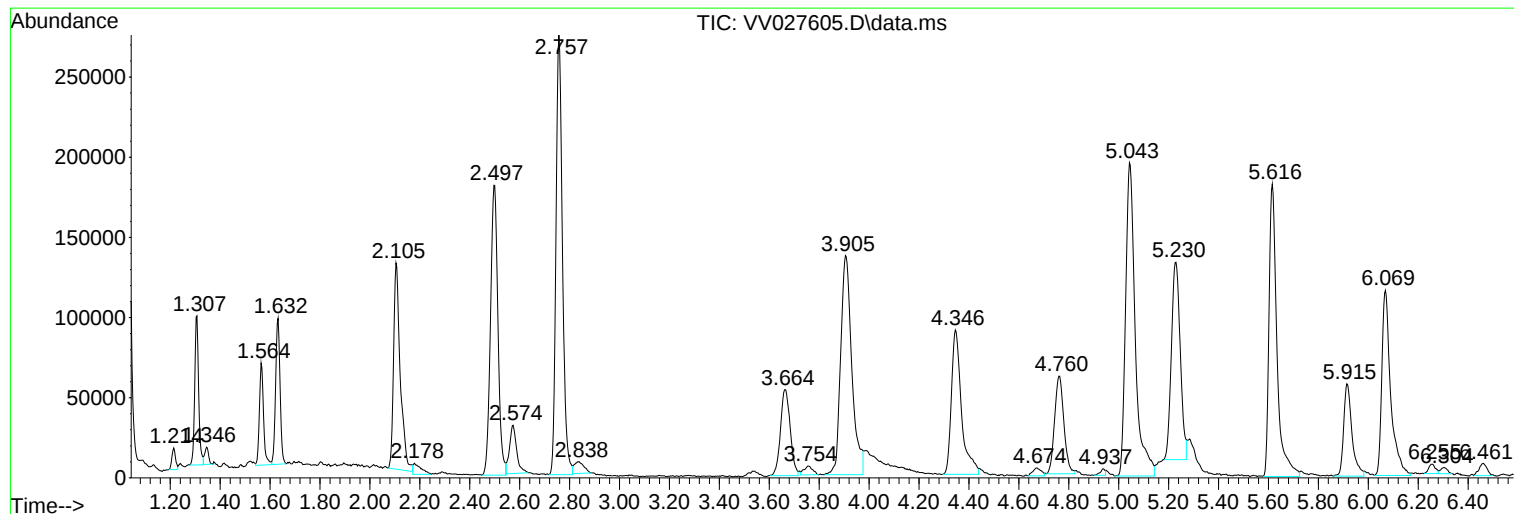
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F5E75DL

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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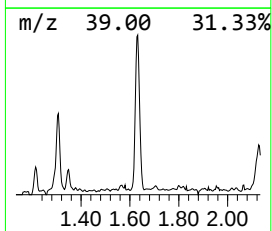
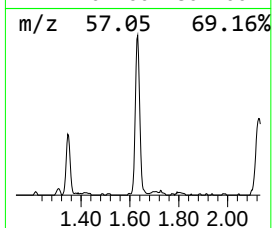
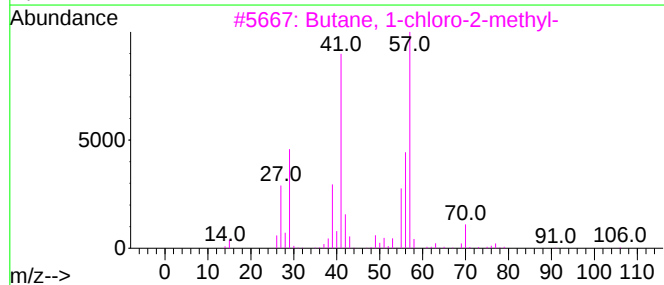
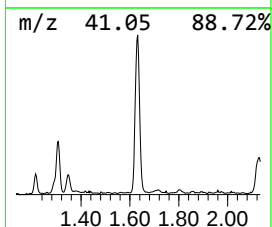
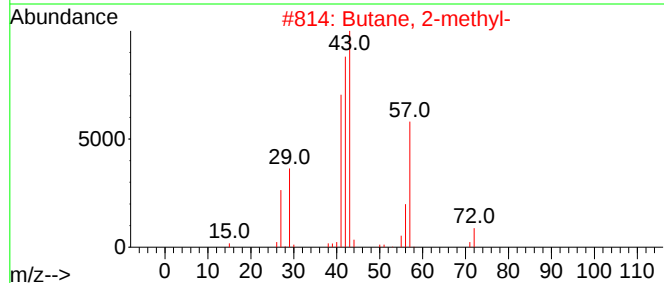
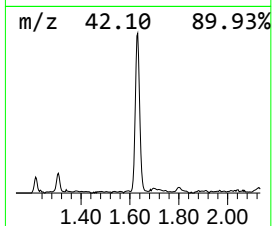
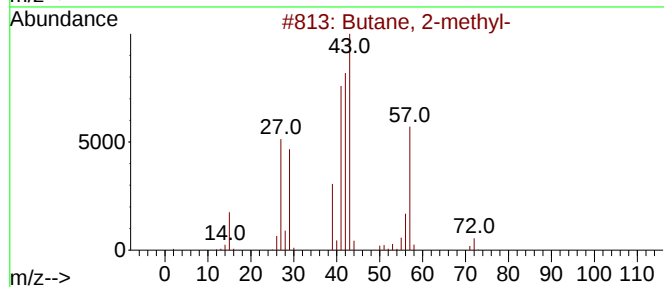
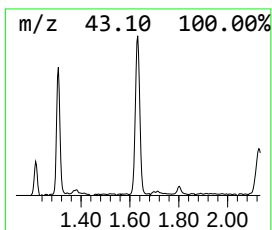
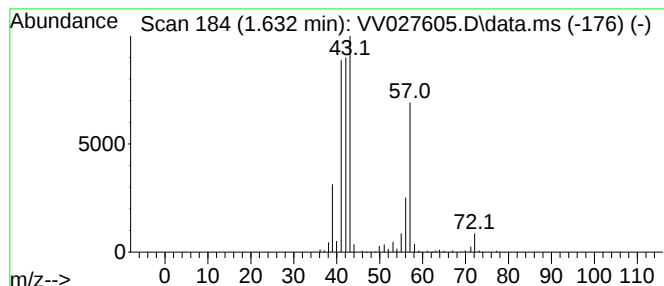
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Quant Title : TRACE VOA SFAM1.0

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.
1.632	1.40 ug/L	112809	1,4-Difluorobenzene	5.616

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	86
3		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
4		1-Propene, 2-methyl-	56	C4H8	000115-11-7	14
5		Methane, isocyanato-	57	C2H3NO	000624-83-9	9



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ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E75DL

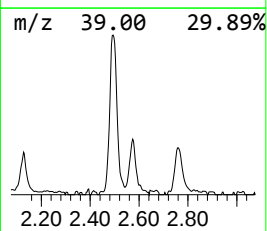
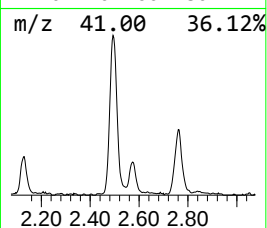
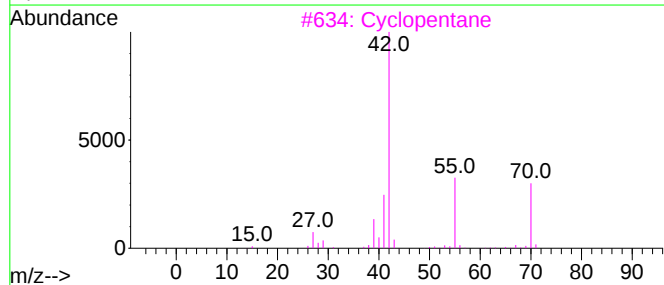
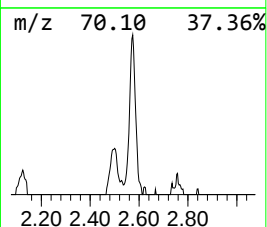
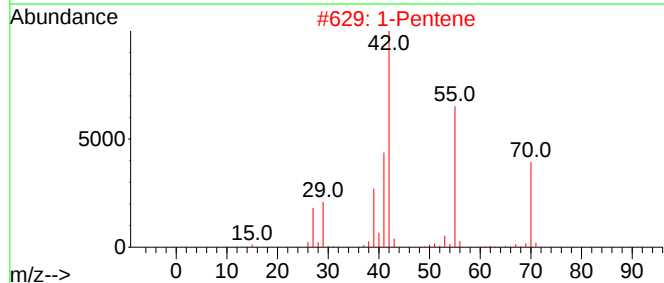
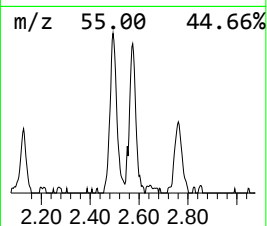
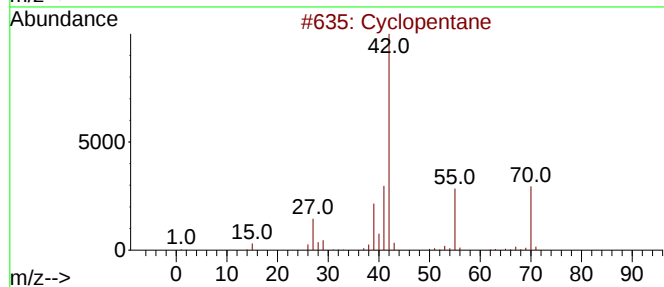
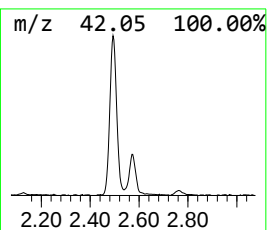
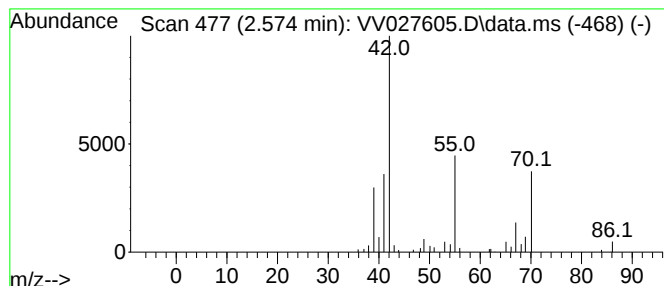
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Cyclic2.574 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.574	0.74 ug/L	59826	1,4-Difluorobenzene	5.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane	70	C5H10	000287-92-3	64
2		1-Pentene	70	C5H10	000109-67-1	64
3		Cyclopentane	70	C5H10	000287-92-3	64
4		Cyclopentane	70	C5H10	000287-92-3	64
5		Cyclobutane, methyl-	70	C5H10	000598-61-8	59



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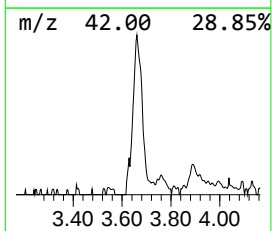
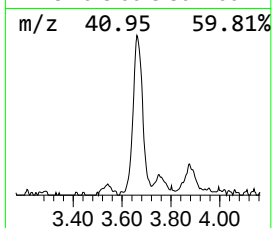
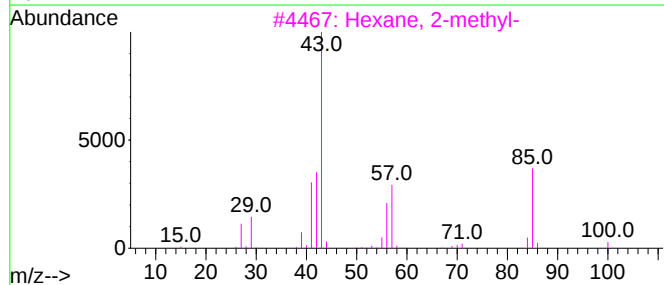
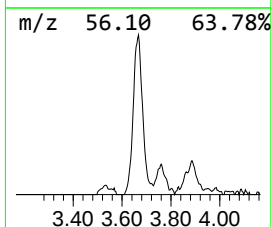
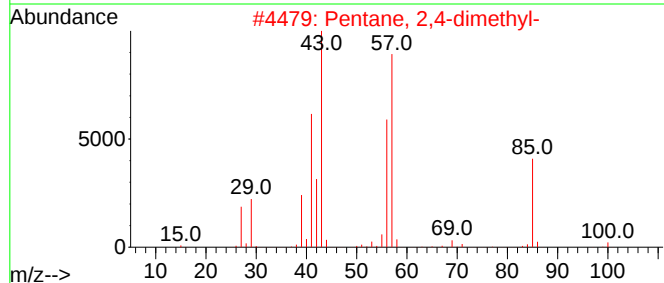
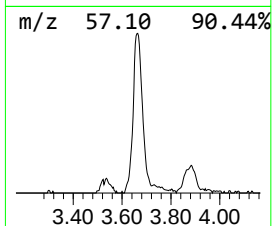
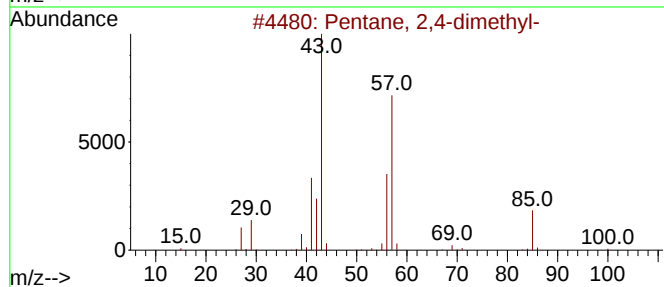
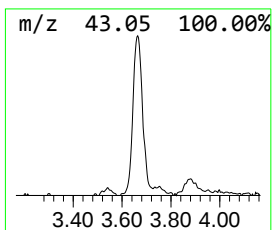
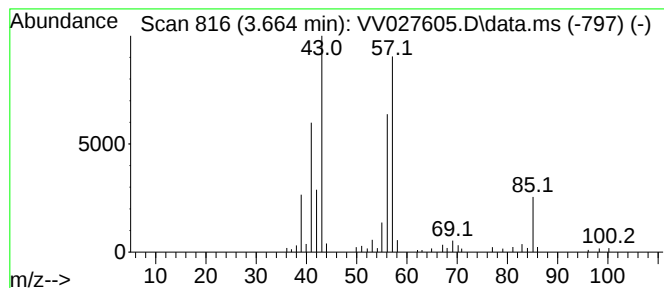
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR081922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.664	1.80 ug/L	145647	1,4-Difluorobenzene	5.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	78
2		Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	64
3		Hexane, 2-methyl-	100	C7H16	000591-76-4	64
4		1-Pentene, 4-methyl-	84	C6H12	000691-37-2	58
5		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53



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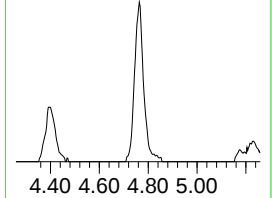
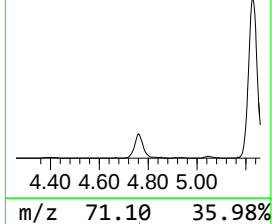
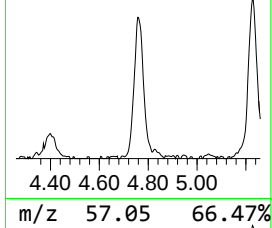
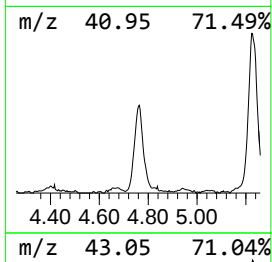
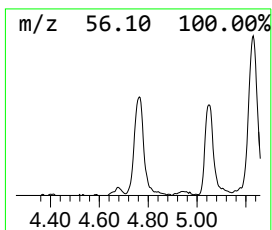
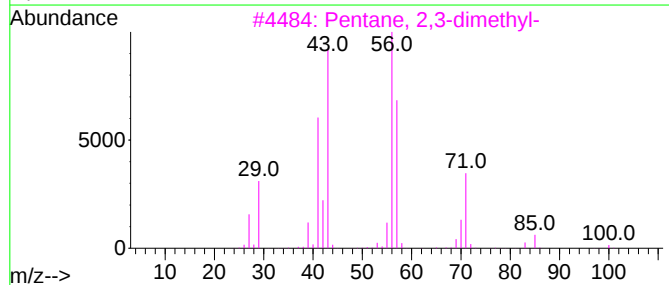
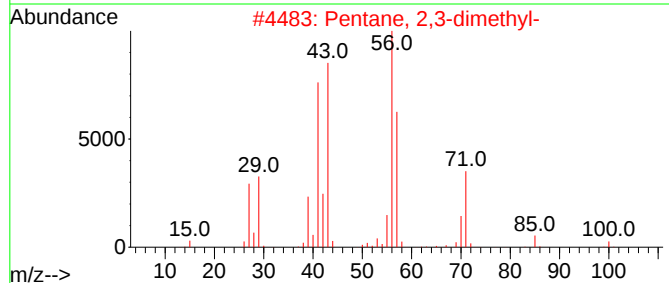
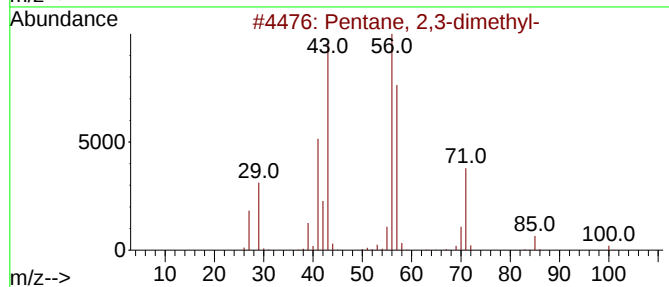
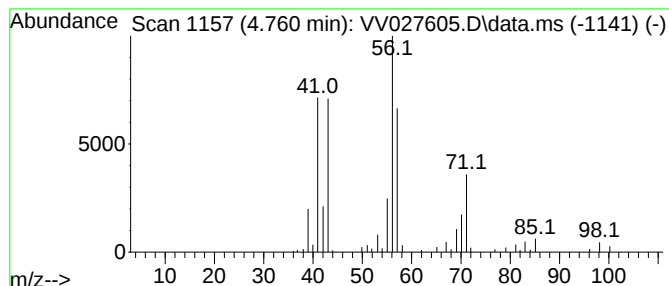
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.760	1.95 ug/L	157528	1,4-Difluorobenzene	5.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
3		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
4		Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	83
5		Octane, 3-methyl-	128	C9H20	002216-33-3	72



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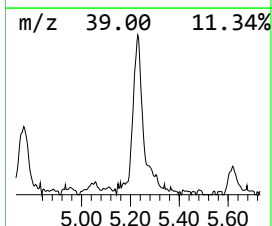
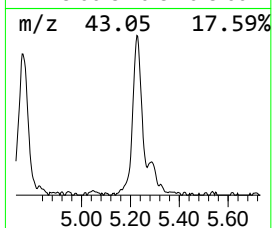
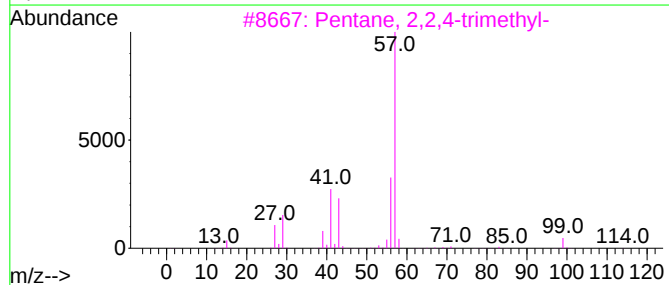
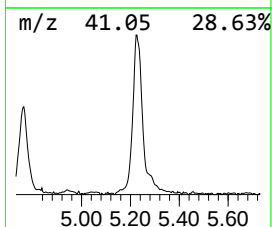
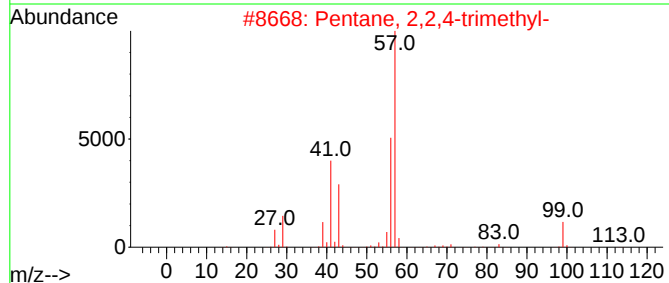
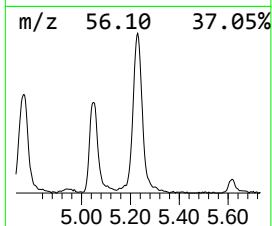
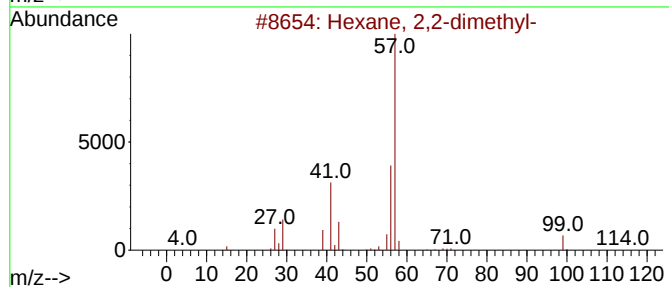
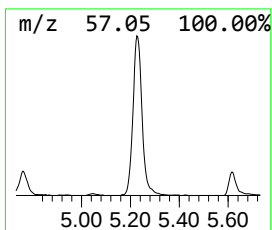
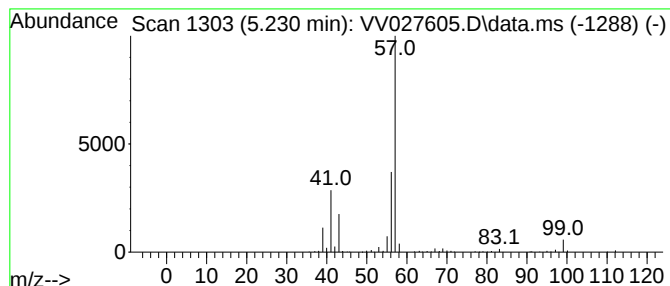
Instrument :
MSVOA_V
ClientSampleId :
F5E75DL

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.230	3.75 ug/L	303112	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	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
4	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083022\
Data File : VV027605.D
Acq On : 30 Aug 2022 23:26
Operator : SY/MD
Sample : N4366-06DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E75DL

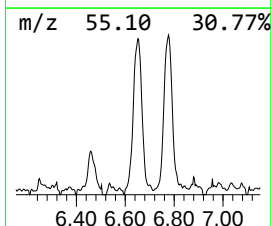
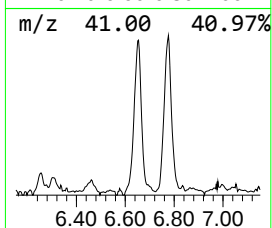
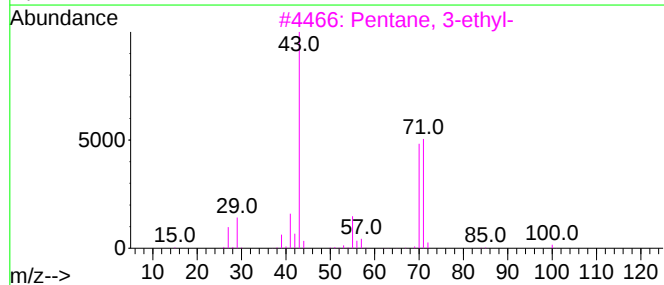
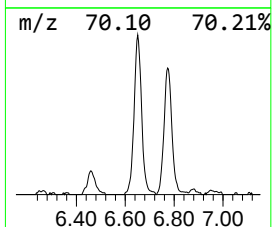
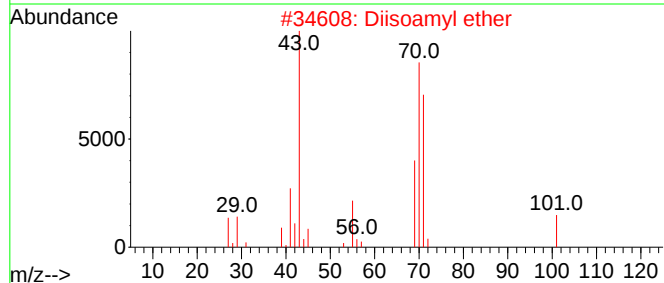
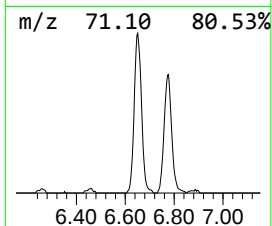
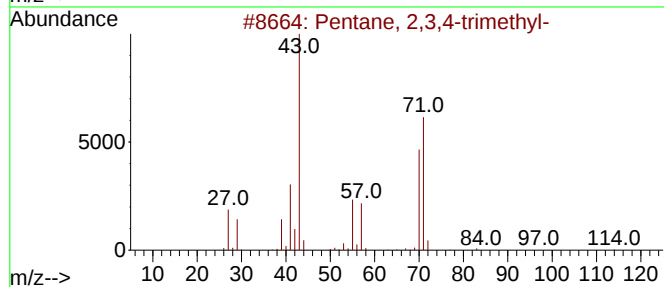
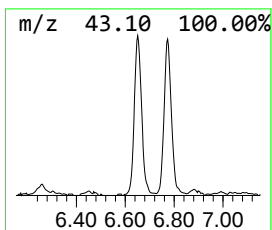
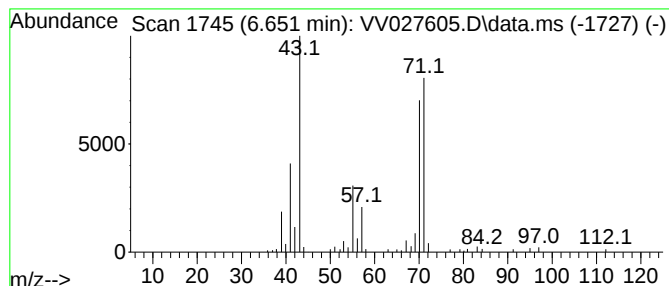
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.651	1.79 ug/L	144815	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	78
2		Diisoamyl ether	158	C10H22O	000544-01-4	78
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083022\
Data File : VV027605.D
Acq On : 30 Aug 2022 23:26
Operator : SY/MD
Sample : N4366-06DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

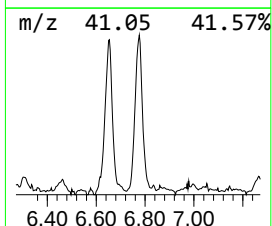
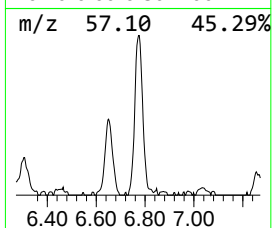
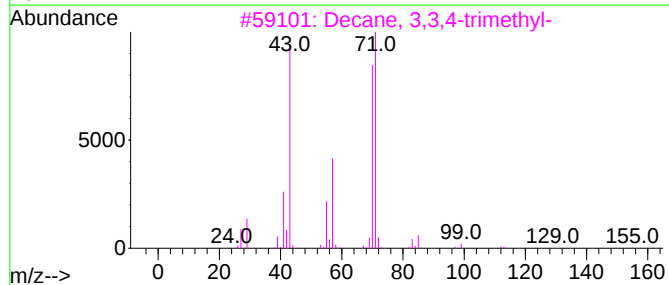
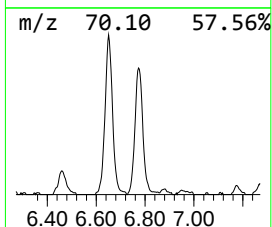
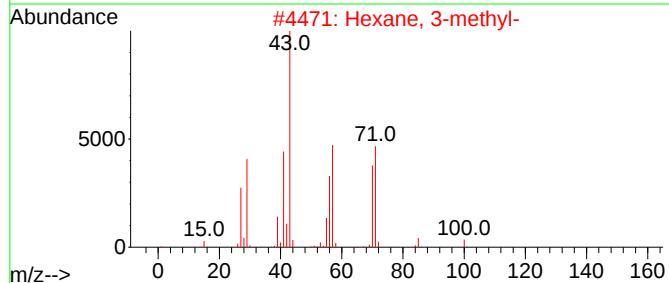
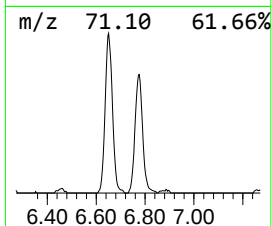
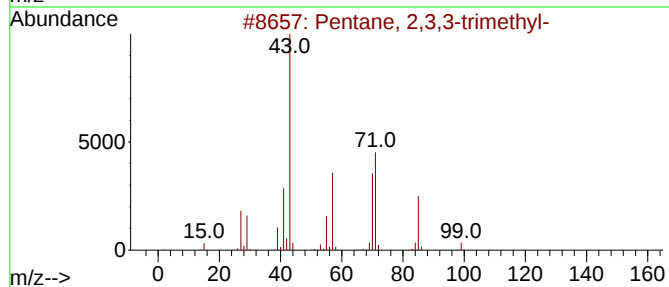
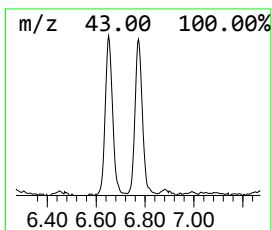
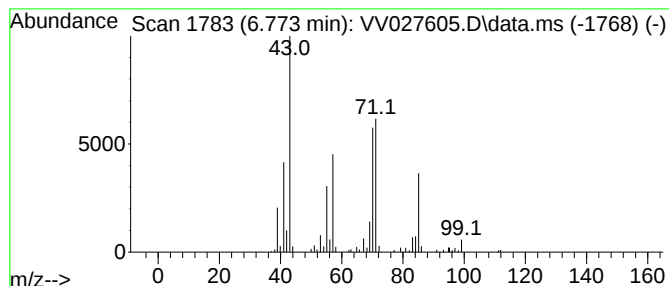
Instrument :
MSVOA_V
ClientSampleId :
F5E75DL

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.773	1.95 ug/L	157813	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	64
2	Hexane, 3-methyl-	100	C7H16	000589-34-4	59
3	Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
4	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	59
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV083022\
Data File : VV027605.D
Acq On : 30 Aug 2022 23:26
Operator : SY/MD
Sample : N4366-06DL 5X
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5E75DL

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

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

					--Internal Standard--			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.632	1.4	ug/L	112809	1	5.616	403887	5.0
(DEL) Alkane: C...	2.574	0.7	ug/L	59826	1	5.616	403887	5.0
(DEL) Alkane: S...	3.664	1.8	ug/L	145647	1	5.616	403887	5.0
(DEL) Alkane: S...	4.760	2.0	ug/L	157528	1	5.616	403887	5.0
(DEL) Alkane: S...	5.230	3.8	ug/L	303112	1	5.616	403887	5.0
(DEL) Alkane: S...	6.651	1.8	ug/L	144815	1	5.616	403887	5.0
(DEL) Alkane: S...	6.773	2.0	ug/L	157813	1	5.616	403887	5.0