

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041522\
 Data File : VV025565.D
 Acq On : 15 Apr 2022 14:09
 Operator : SY/MD
 Sample : N2356-10DL 100X
 Misc : 25mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GBDS8DL

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\SFAMVTR040822WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV025565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.220	50	56	61	rBV	15308	14645	1.85%	0.246%
2	1.314	75	85	97	rBV	181695	184660	23.32%	3.106%
3	1.574	158	166	176	rBV	85719	99907	12.62%	1.680%
4	1.638	177	186	203	rVV	169623	213997	27.03%	3.599%
5	1.812	232	240	253	rVB2	23717	35057	4.43%	0.590%
6	1.909	263	270	282	rVB	12732	18796	2.37%	0.316%
7	2.031	300	308	318	rVB2	28913	41668	5.26%	0.701%
8	2.114	324	334	357	rVB	159490	243014	30.69%	4.087%
9	2.507	440	456	463	rBV5	23624	59247	7.48%	0.996%
10	2.584	473	480	496	rVB3	17404	32843	4.15%	0.552%
11	2.767	523	537	555	rBV2	16644	33462	4.23%	0.563%
12	3.677	807	820	833	rBV7	3810	10434	1.32%	0.175%
13	3.767	833	848	865	rVB4	18527	45910	5.80%	0.772%
14	3.902	879	890	922	rBV	48905	170274	21.50%	2.864%
15	4.352	1013	1030	1060	rBV	92462	237476	29.99%	3.994%
16	4.680	1117	1132	1145	rBV5	15748	40333	5.09%	0.678%
17	4.764	1147	1158	1181	rVB6	11114	31100	3.93%	0.523%
18	5.050	1232	1247	1255	rBV2	206810	495439	62.57%	8.332%
19	5.101	1255	1263	1285	rVB	368171	791840	100.00%	13.317%
20	5.236	1297	1305	1323	rVB5	15153	40766	5.15%	0.686%
21	5.320	1324	1331	1344	rVB5	4669	10533	1.33%	0.177%
22	5.619	1413	1424	1454	rBV	181066	374264	47.27%	6.294%
23	5.915	1504	1516	1530	rBV8	7786	16529	2.09%	0.278%
24	6.072	1550	1565	1593	rBV	118524	261774	33.06%	4.402%
25	6.658	1734	1747	1758	rBV4	9591	19418	2.45%	0.327%
26	6.777	1771	1784	1799	rBV3	18668	41075	5.19%	0.691%
27	6.989	1839	1850	1871	rBV2	48737	93928	11.86%	1.580%
28	7.317	1941	1952	1971	rBV	231923	409238	51.68%	6.882%
29	7.625	2040	2048	2071	rBV	27845	49698	6.28%	0.836%
30	8.092	2183	2193	2222	rBV	175676	372814	47.08%	6.270%
31	8.854	2418	2430	2462	rBV	279182	466646	58.93%	7.848%
32	9.149	2513	2522	2536	rVB4	6479	11385	1.44%	0.191%
33	10.217	2841	2854	2868	rBV	70483	112975	14.27%	1.900%
34	10.381	2891	2905	2915	rVB3	10625	20093	2.54%	0.338%
35	11.249	3164	3175	3192	rBV	276249	431975	54.55%	7.265%
36	11.529	3251	3262	3276	rVB2	21228	34674	4.38%	0.583%

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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\SFAMVTR040822WMA.M
Title : TRACE VOA SFAM1.0

37	11.622	3280	3291	3308	rBV	210805	341130	43.08%	5.737%
38	12.117	3435	3445	3452	rBV2	7332	10808	1.36%	0.182%
39	12.249	3473	3486	3496	rBV	10895	17309	2.19%	0.291%
40	14.040	4035	4043	4052	rVB2	5790	9075	1.15%	0.153%

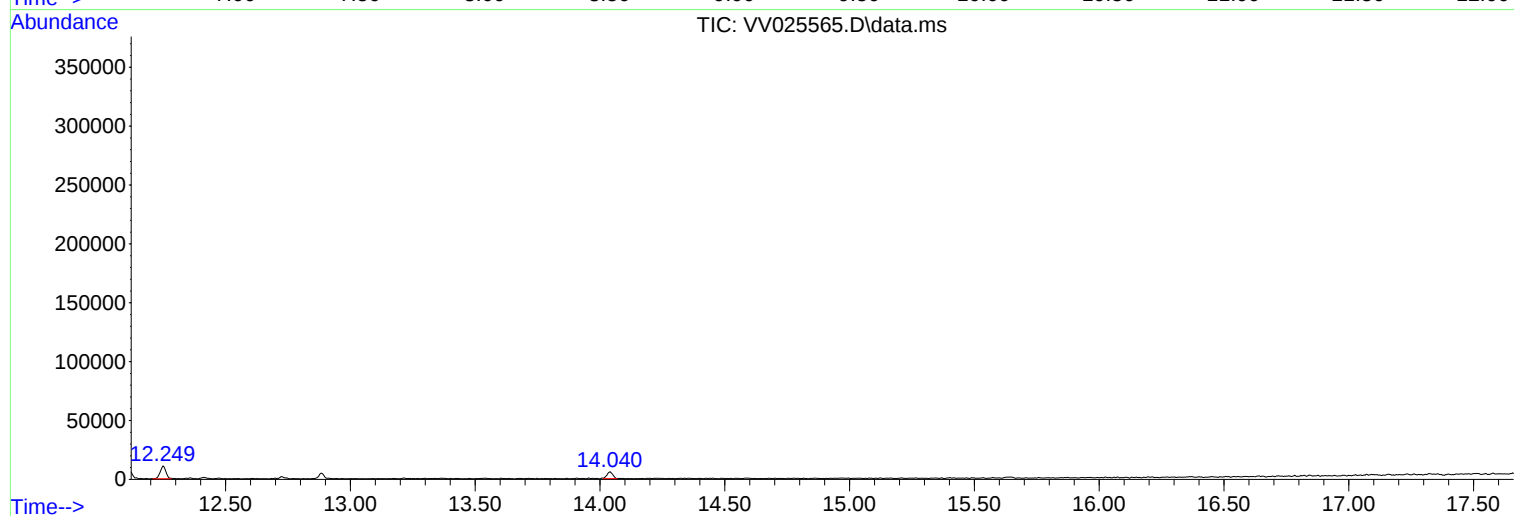
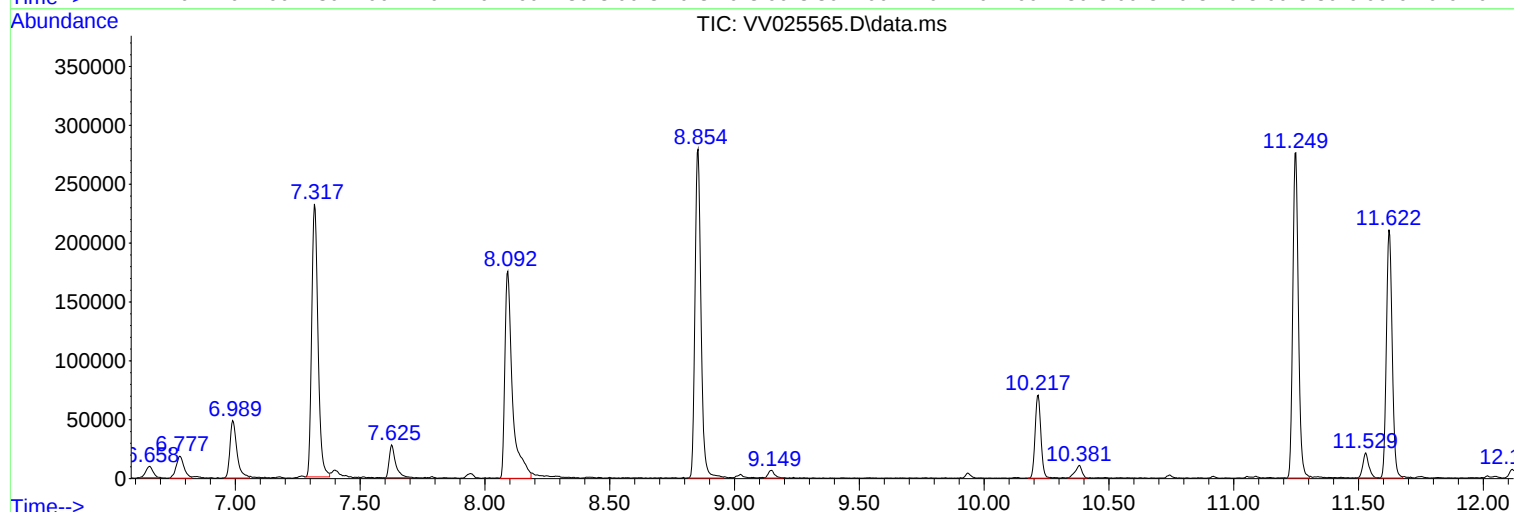
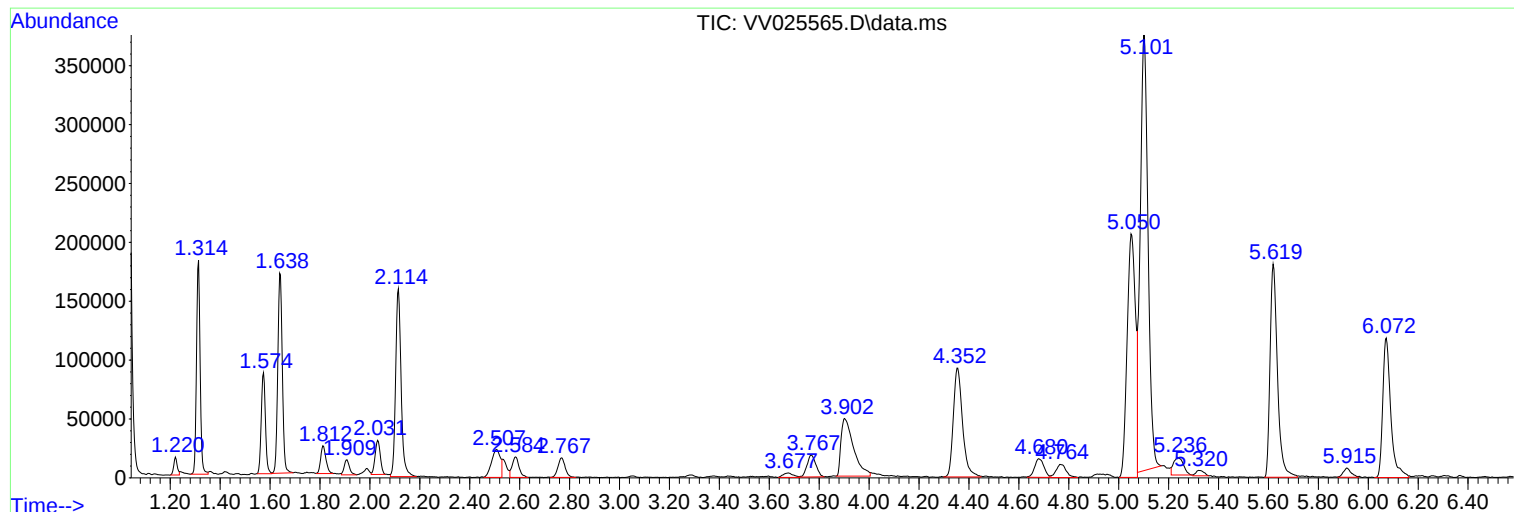
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR040822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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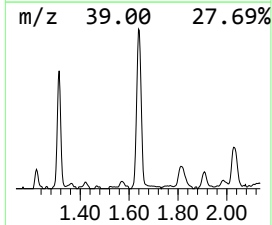
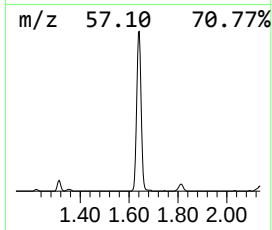
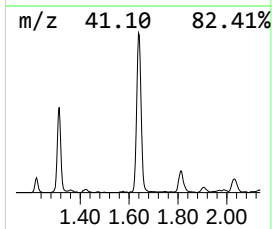
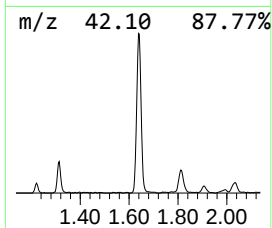
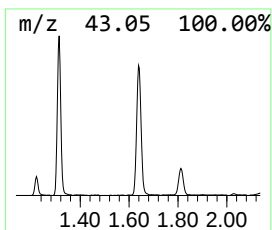
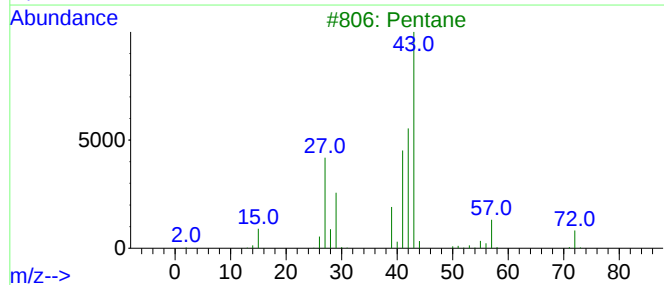
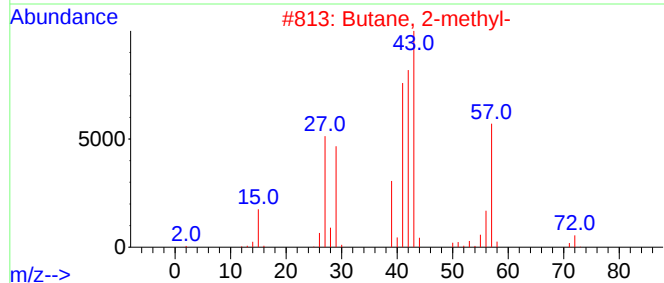
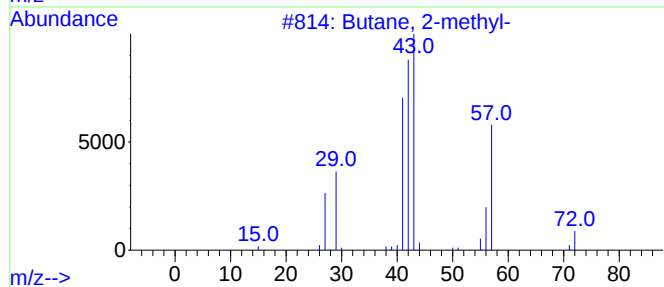
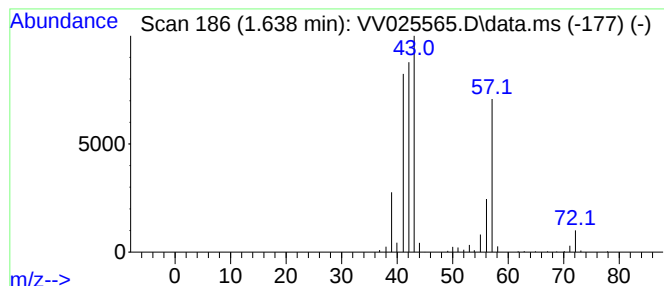
Instrument :
MSVOA_V
ClientSampleId :
GBDS8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR040822WMA.M
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 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.638	2.86 ug/L	213997	1,4-Difluorobenzene	5.619	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	Pentane	72	C5H12	000109-66-0	59
4	Pentane	72	C5H12	000109-66-0	47
5	3-Buten-1-ol	72	C4H8O	000627-27-0	47



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Instrument :
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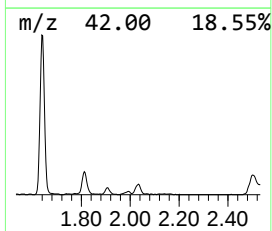
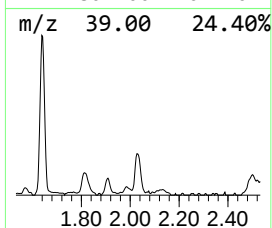
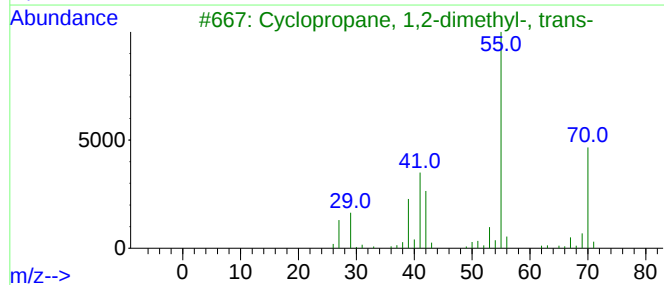
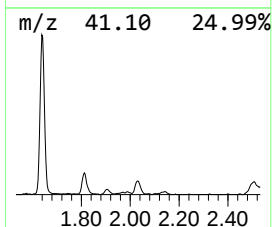
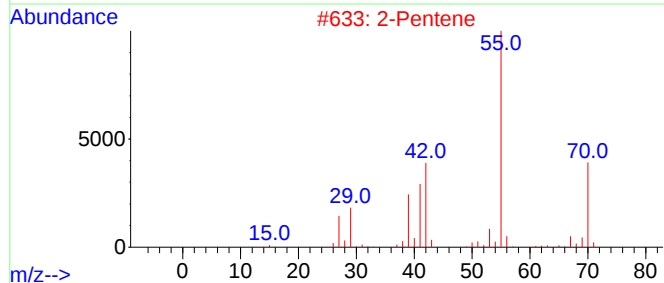
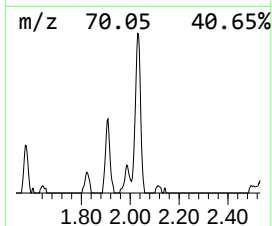
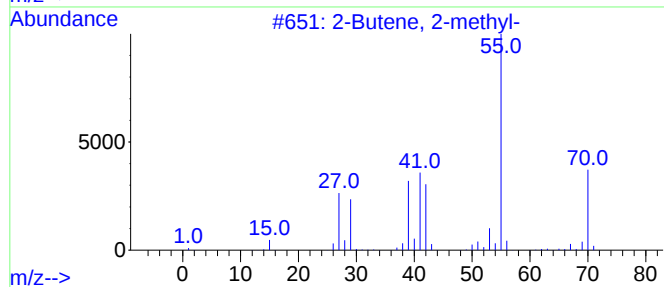
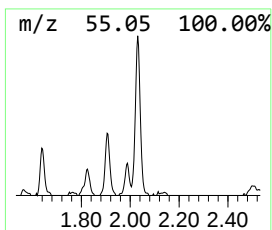
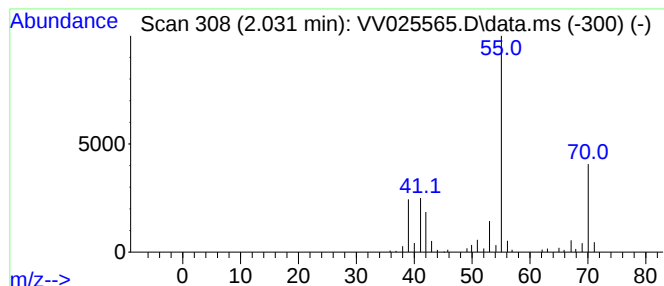
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR040822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.031	0.56 ug/L	41668	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	86	
2	2-Pentene	70	C5H10	000109-68-2	80	
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	80	
4	2-Butene, 2-methyl-	70	C5H10	000513-35-9	80	
5	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	72	



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Instrument :
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ClientSampleId :
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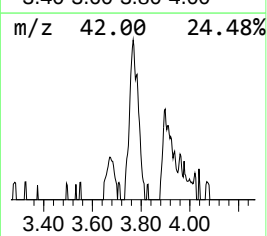
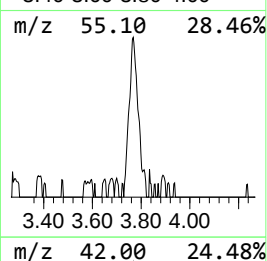
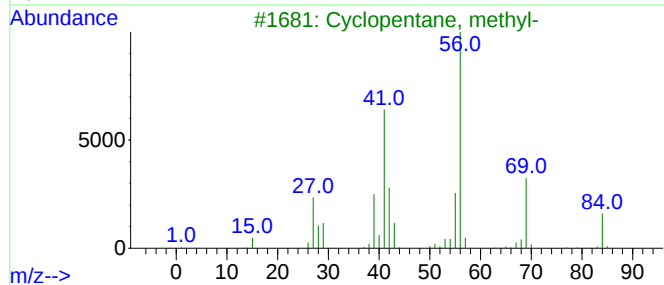
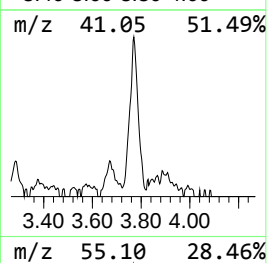
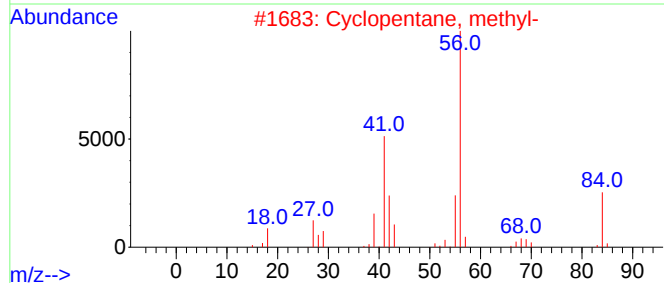
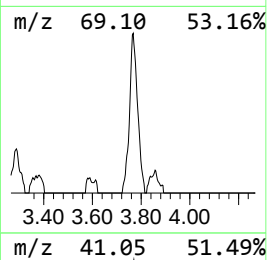
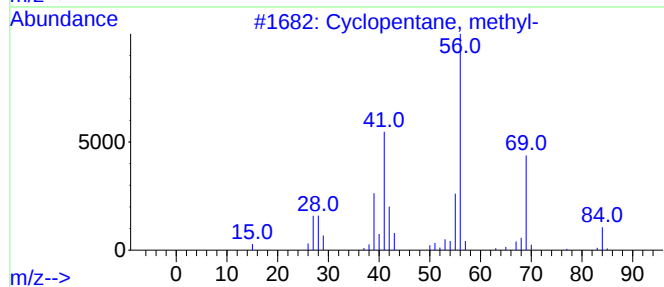
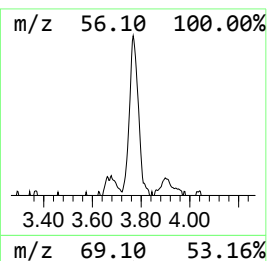
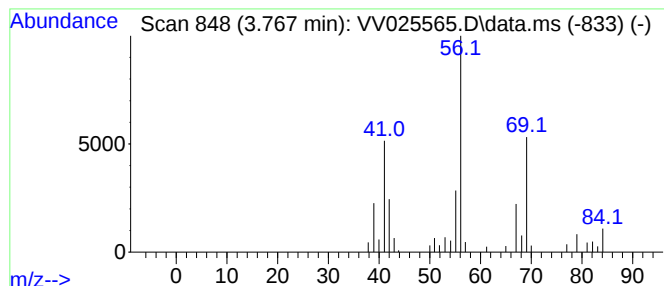
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR040822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Cyclic3.767 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.767	0.61 ug/L	45910	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	76
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	53
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	53
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	52
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	49



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ALS Vial : 8 Sample Multiplier: 1

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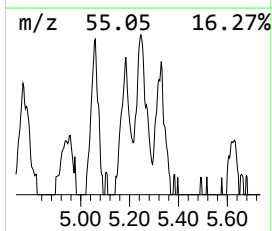
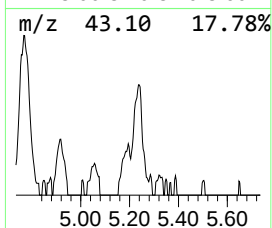
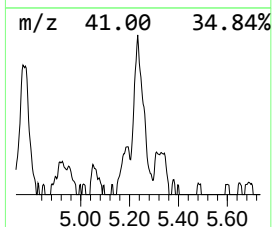
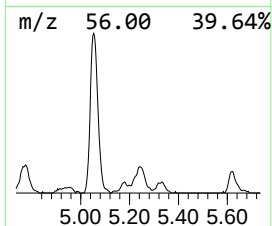
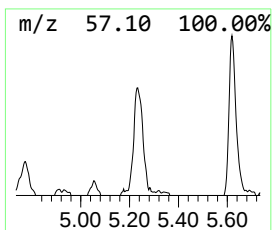
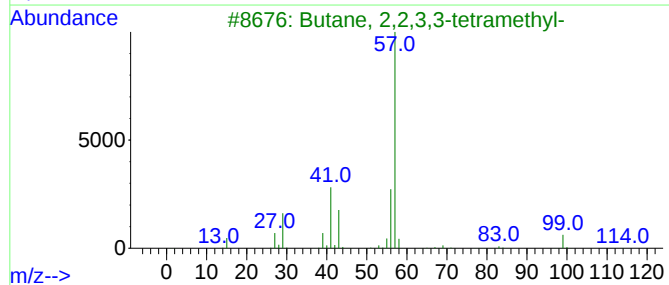
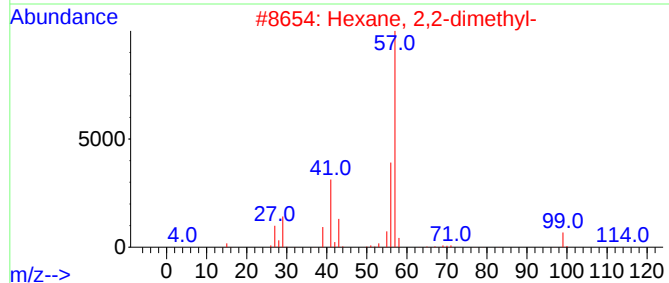
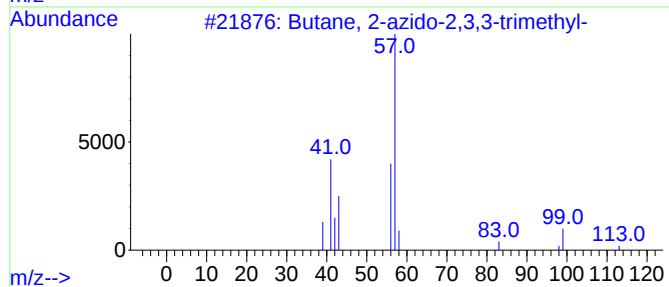
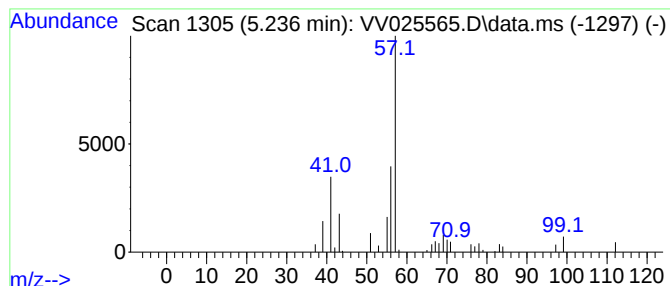
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.236	0.54 ug/L	40766	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-azido-2,3,3-trimethyl-	141	C7H15N3	051677-41-9	38
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	33
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	33
4			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	33
5			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	22



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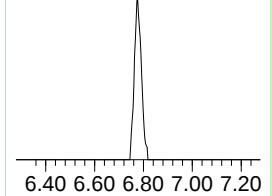
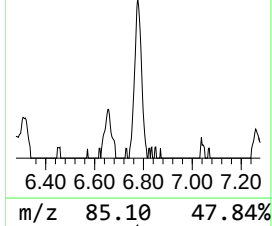
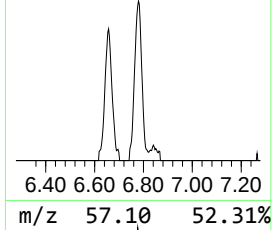
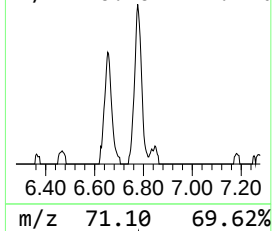
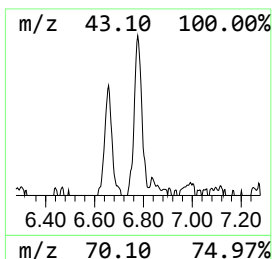
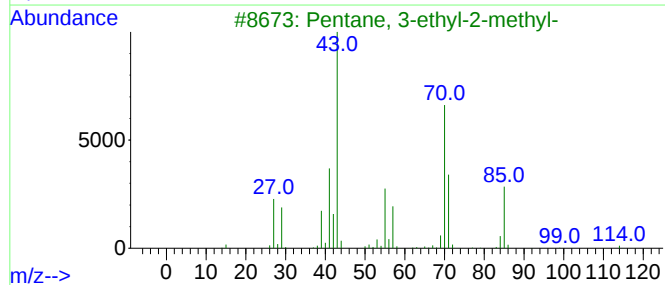
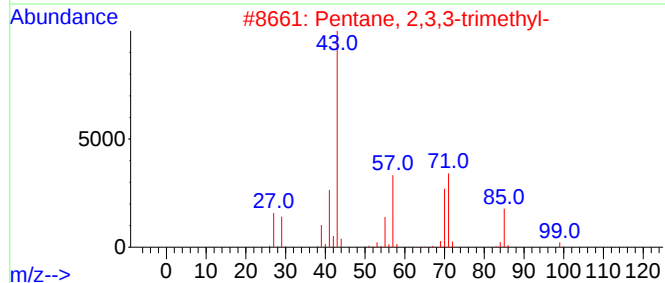
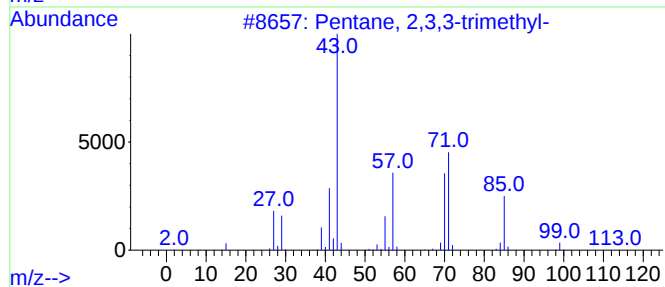
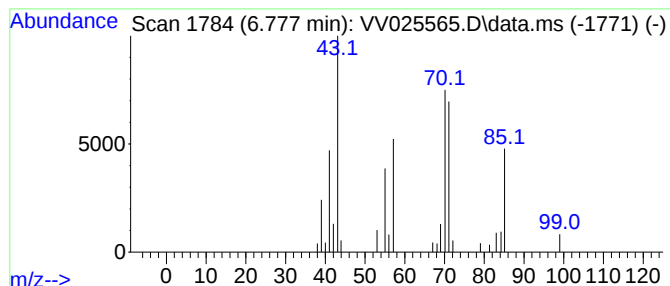
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR040822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.777	0.55 ug/L	41075	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
3			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	64
4			Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	56
5			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041522\
Data File : VV025565.D
Acq On : 15 Apr 2022 14:09
Operator : SY/MD
Sample : N2356-10DL 100X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
GBDS8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR040822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.638	2.9	ug/L	213997	1	5.619	374264	5.0
(DEL) Alkane: S...	2.031	0.6	ug/L	41668	1	5.619	374264	5.0
(DEL) Alkane: C...	3.767	0.6	ug/L	45910	1	5.619	374264	5.0
unknown-01	5.236	0.5	ug/L	40766	1	5.619	374264	5.0
(DEL) Alkane: S...	6.777	0.6	ug/L	41075	1	5.619	374264	5.0