LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

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\SFAMUTR122022WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU052563.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	26	rVB	670033	621730	50.68%	6.942%
2	1.491	40	47	54	rBV2	43141	45806	3.73%	0.511%
3	1.591	69	78	95	rBV3	323317	543529	44.31%	6.068%
4	1.662	95	100	105	rVV	11291	12410	1.01%	0.139%
5	1.732	116	122	132	rVB	41891	49707	4.05%	0.555%
6	1.912	164	178	194	rVB2	97243	146338	11.93%	1.634%
7	1.996	196	204	215	rVB	37924	52698	4.30%	0.588%
8	2.157	245	254	262	rBV	83681	116113	9.47%	1.296%
9	2.211	262	271	288	rVB3	64649	133220	10.86%	1.487%
10	2.417	322	335	345	rBV	27808	47723	3.89%	0.533%
11	2.568	369	382	396	rBV	148466	242492	19.77%	2.707%
12	2.980	493	510	520	rBV6	11125	32875	2.68%	0.367%
13	3.044	522	530	537	rBV2	9673	16236	1.32%	0.181%
14	3.137	550	559	571	rVB3	10058	19580	1.60%	0.219%
15	3.363	616	629	641	rVB2	8825	19098	1.56%	0.213%
16	3.584	682	698	719	rVB4	25422	65918	5.37%	0.736%
17	3.697	719	733	750	rBV3	10396	23008	1.88%	0.257%
18	4.192	874	887	902	rBV5	6154	15570	1.27%	0.174%
19	4.639	1008	1026	1064	rBV2	155990	521696	42.53%	5.825%
20	5.060	1141	1157	1181	rVB	150599	339718	27.69%	3.793%
21	5.723	1341	1363	1393	rBV2	305040	839362	68.42%	9.371%
22	6.022	1447	1456	1469	rVB9	8086	18009	1.47%	0.201%
23	6.247	1512	1526	1551	rBV	230037	450868	36.75%	5.034%
24	6.687	1649	1663	1682	rBV	209029	409938	33.42%	4.577%
25	7.562	1920	1935	1956	rBV	95792	172380	14.05%	1.925%
26	7.893	2022	2038	2053	rBV	335294	590291	48.12%	6.590%
27	7.964	2053	2060	2069	rVB3	9946	17168	1.40%	0.192%
28	8.176	2115	2126	2149	rVB2	60710	108686	8.86%	1.213%
29	8.549	2233	2242	2253	rVB4	22106	37217	3.03%	0.416%
30	8.632	2253	2268	2302	rBV	655399	1226726	100.00%	13.696%
31	8.784	2306	2315	2329	rVB4	17340	32714	2.67%	0.365%
32	9.414	2498	2511	2538	rBV	331921	554348	45.19%	6.189%
33	9.690	2586	2597	2610	rBV	16967	28229	2.30%	0.315%
34	10.099	2712	2724	2735	rBV3	25608	42267	3.45%	0.472%
35	10.751	2915	2927	2940	rBV	177755	282530	23.03%	3.154%
36	11.806	3243	3255	3275	rBV	318904	504791	41.15%	5.636%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

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\SFAMUTR122022WMA.M
Title : TRACE VOA SFAM1.0

37	12.189	3361	3374	3392	rBV	343076	552330	45.02%	6.167%
38	12.883	3581	3590	3604	rBV5	14735	23389	1.91%	0.261%

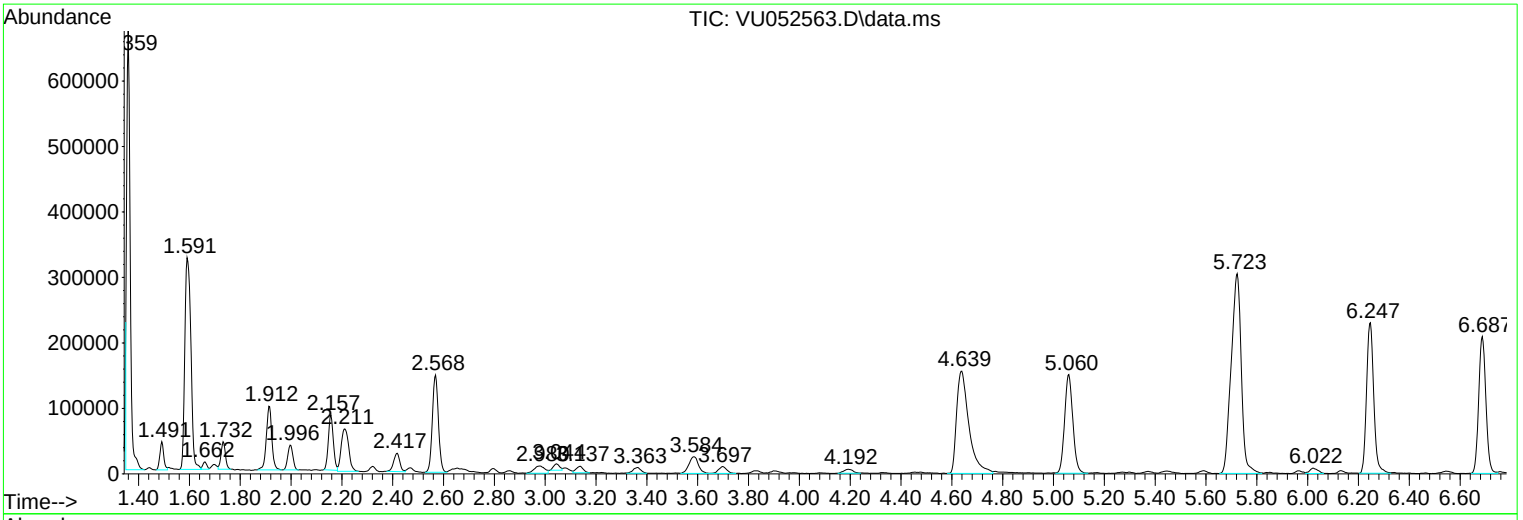
Sum of corrected areas: 8956708

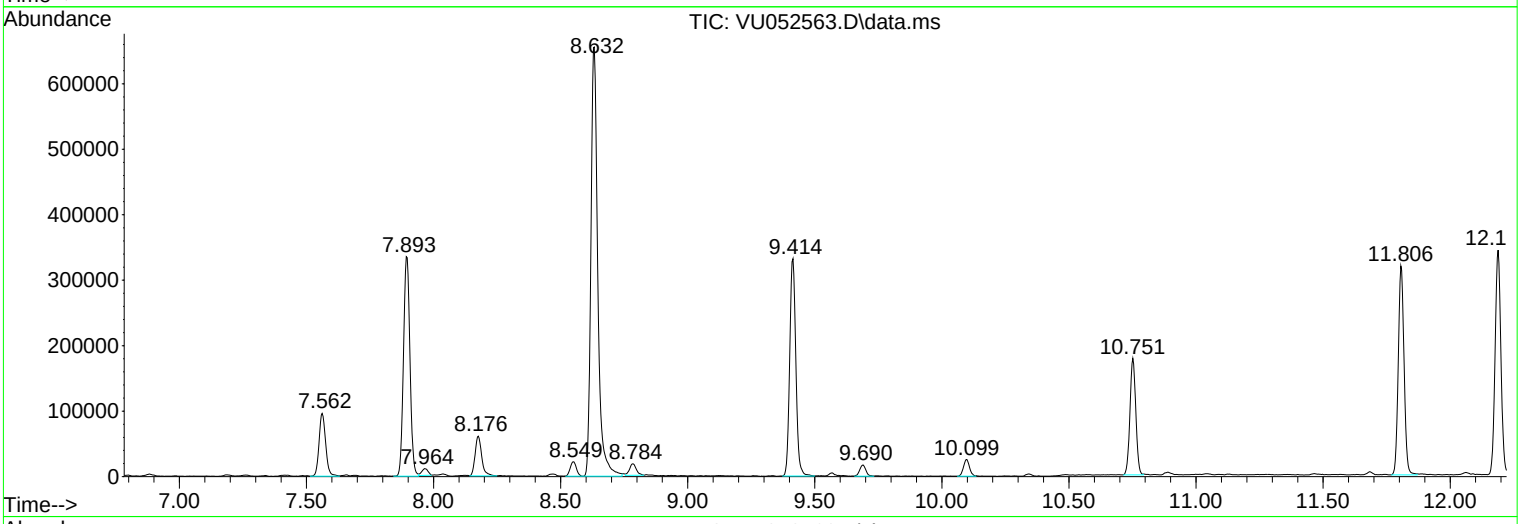
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

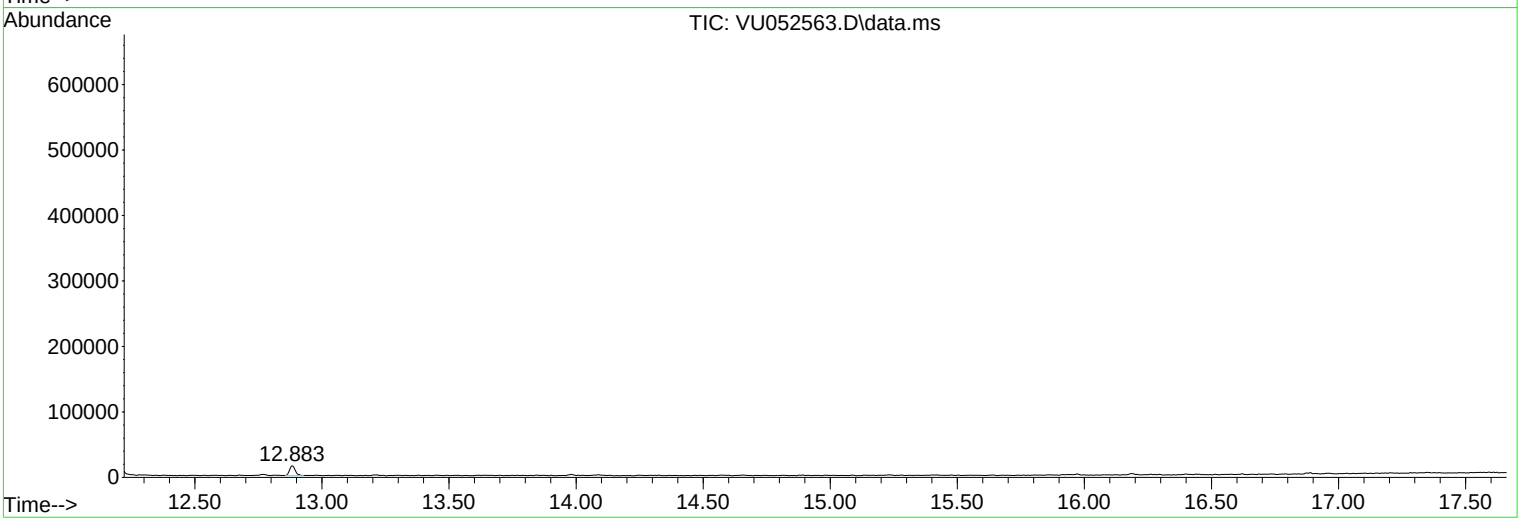
Instrument :
MSVOA_U
ClientSampleId :
GBQD1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

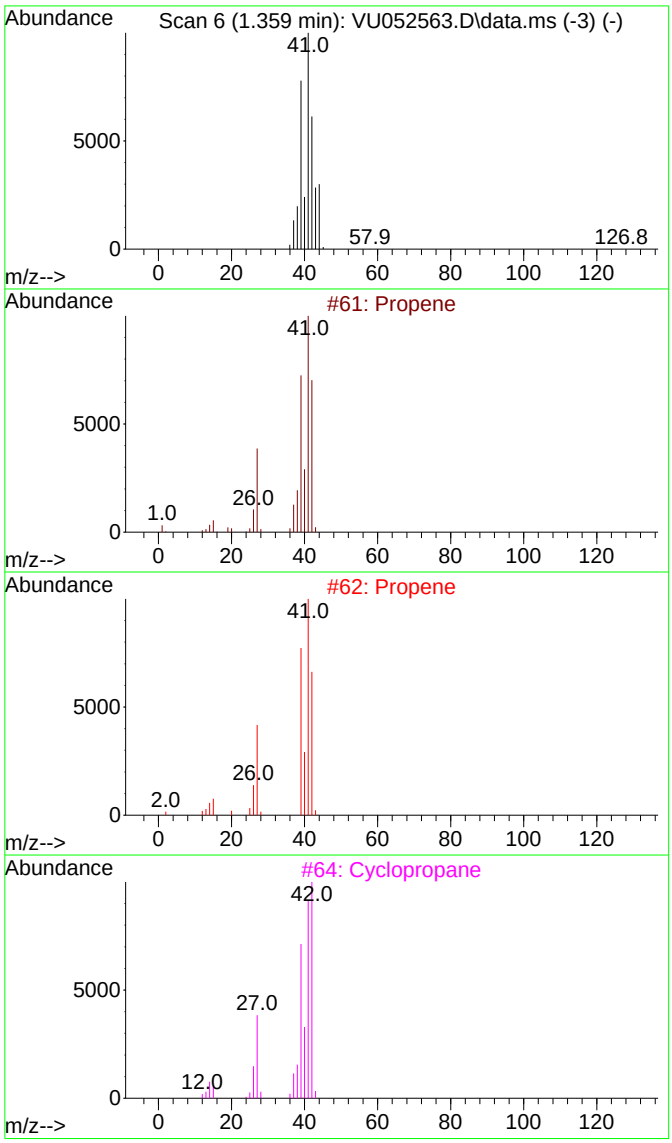
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

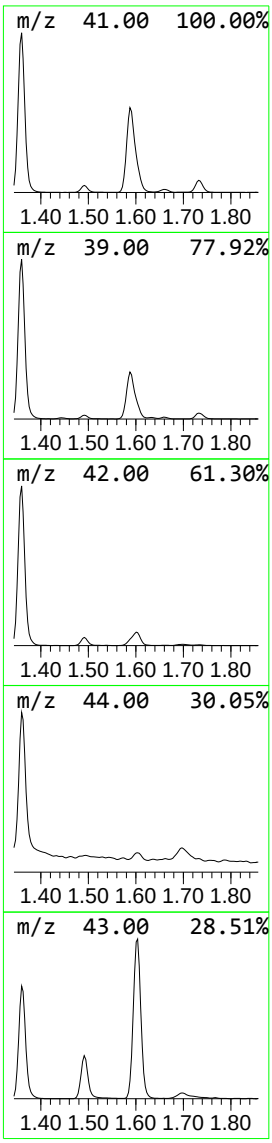
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	6.89 ug/L	621730	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropane	42	C3H6	000075-19-4	9
4	Cyclopropene	40	C3H4	002781-85-3	9
5	Cyclopropane	42	C3H6	000075-19-4	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

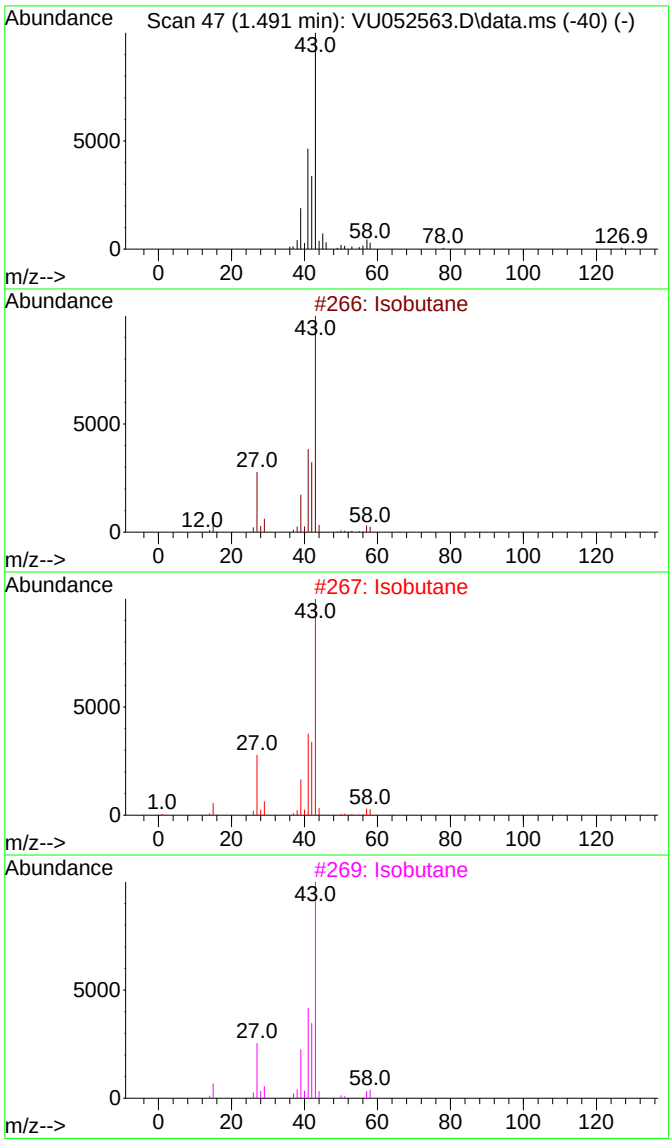
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

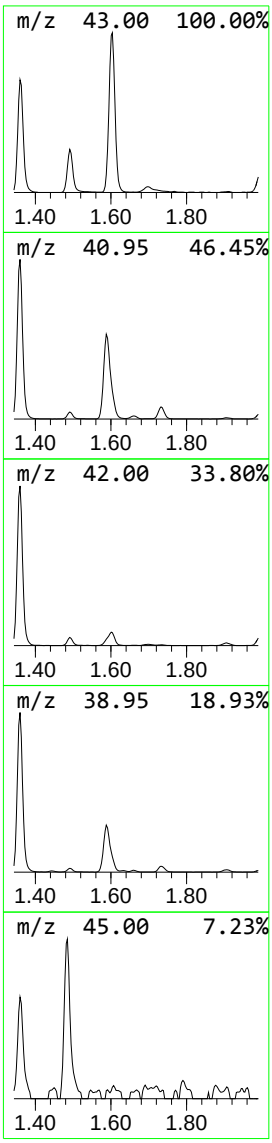
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	0.51 ug/L	45806	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	64
2	Isobutane	58	C4H10	000075-28-5	64
3	Isobutane	58	C4H10	000075-28-5	59
4	Isobutane	58	C4H10	000075-28-5	59
5	Isobutane	58	C4H10	000075-28-5	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

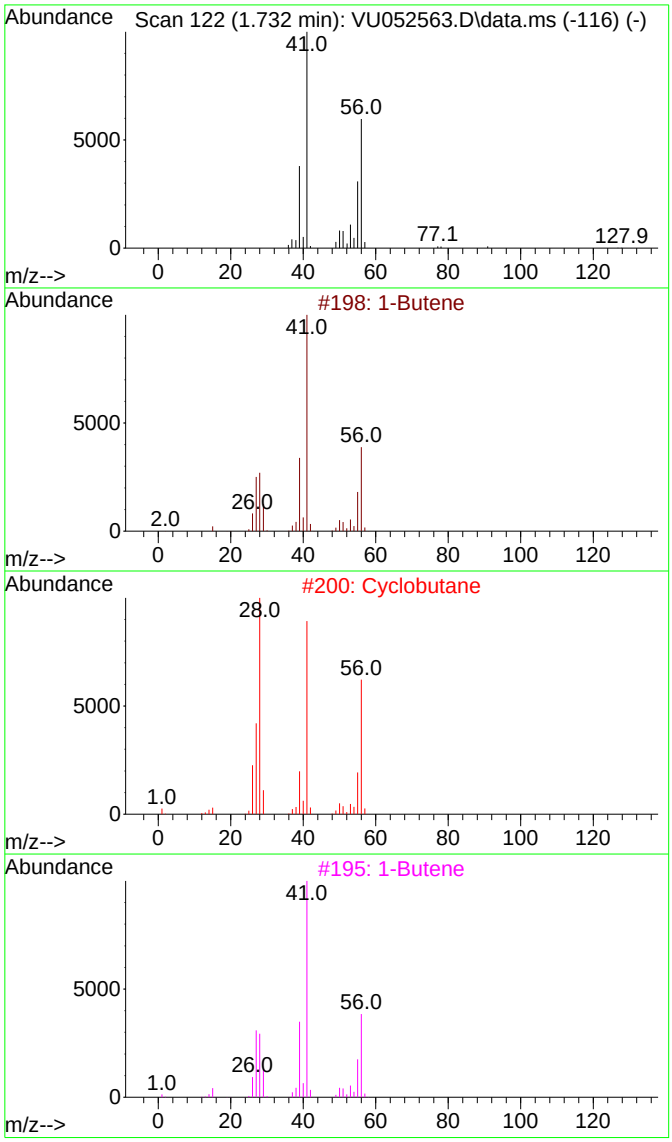
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

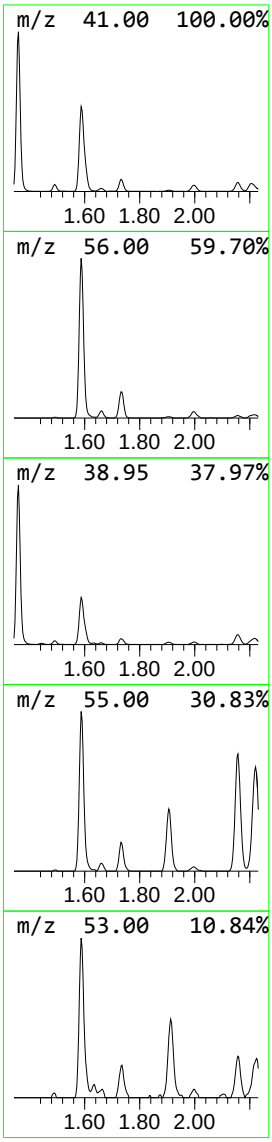
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.732	0.55 ug/L	49707	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene	56	C4H8	000106-98-9	87
2	Cyclobutane	56	C4H8	000287-23-0	86
3	1-Butene	56	C4H8	000106-98-9	80
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	80
5	2-Butene, (Z)-	56	C4H8	000590-18-1	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

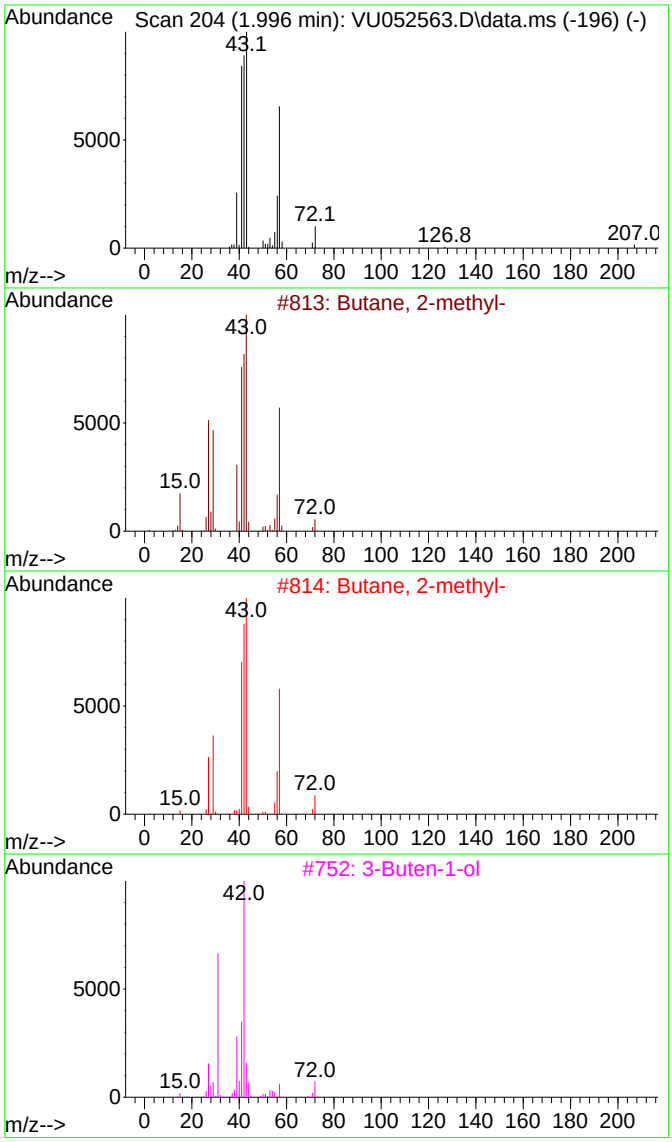
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

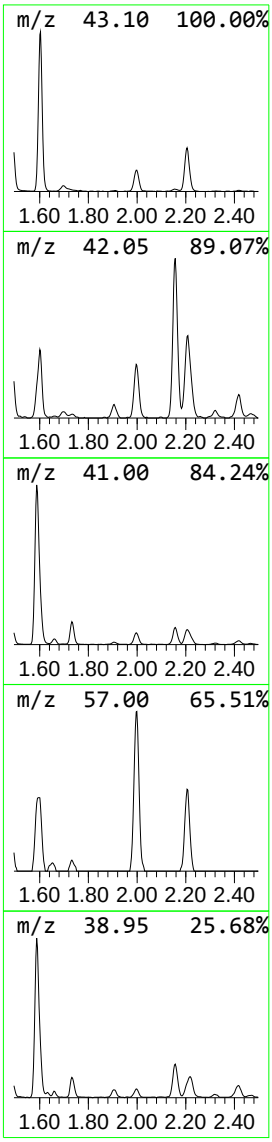
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	0.58 ug/L	52698	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	86
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	Pentane	72	C5H12	000109-66-0	33
5	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

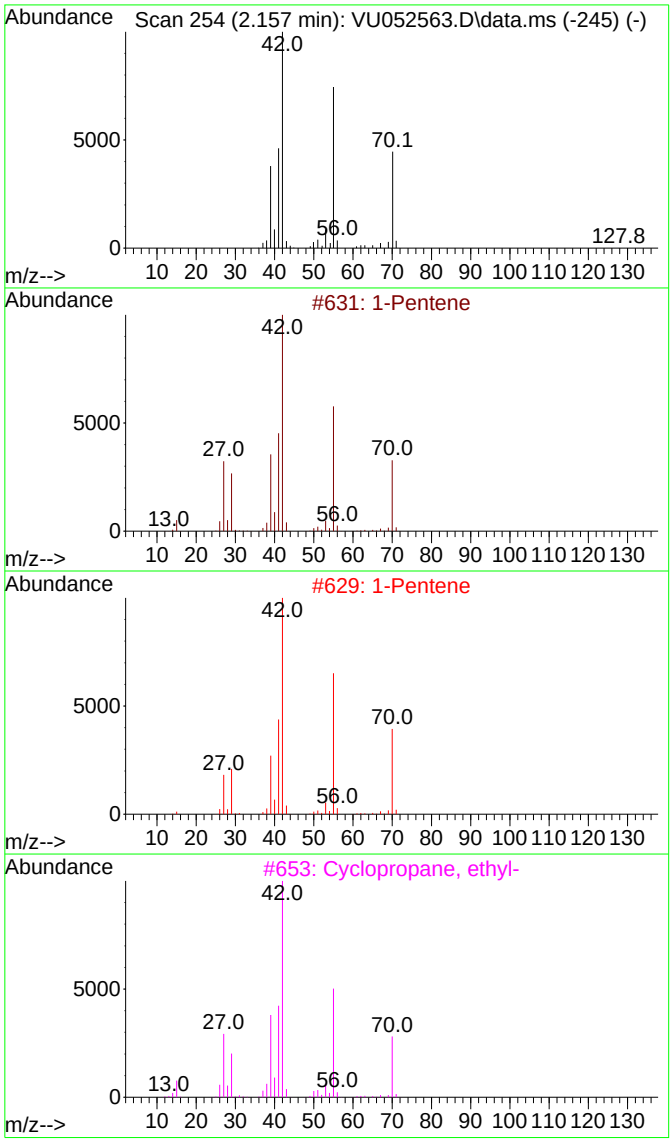
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

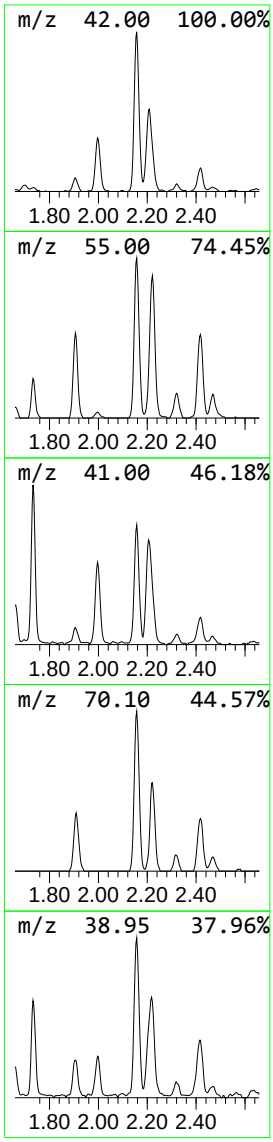
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.157	1.29 ug/L	116113	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	91
2	1-Pentene	70	C5H10	000109-67-1	91
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	87
4	Cyclopentane	70	C5H10	000287-92-3	80
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

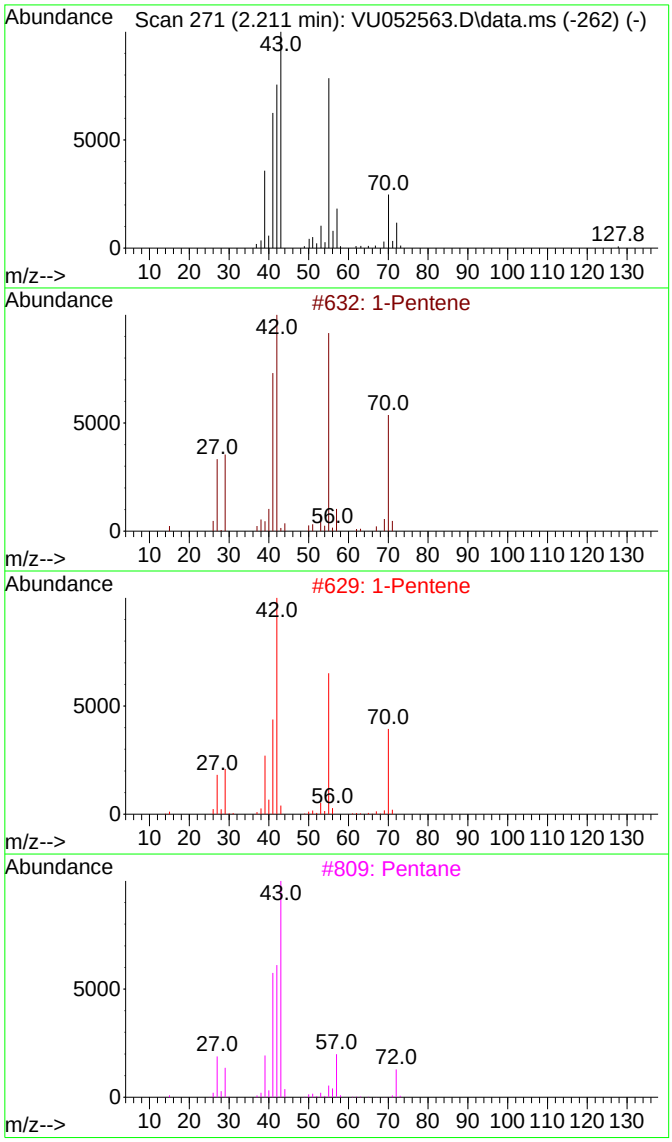
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

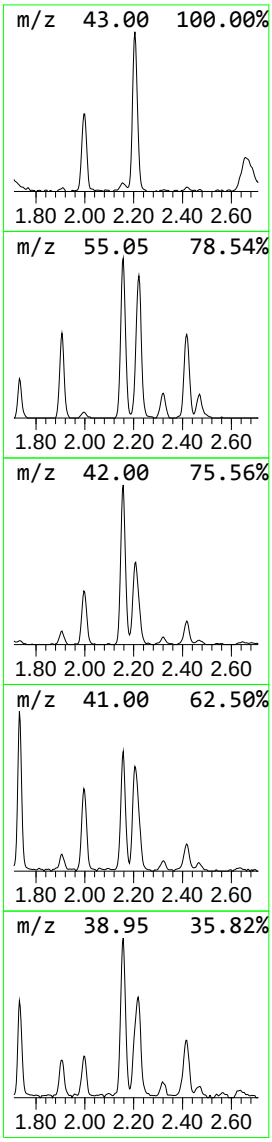
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	1.48 ug/L	133220	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	62
2	1-Pentene	70	C5H10	000109-67-1	59
3	Pentane	72	C5H12	000109-66-0	58
4	Pentane	72	C5H12	000109-66-0	53
5	1-Pentene	70	C5H10	000109-67-1	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

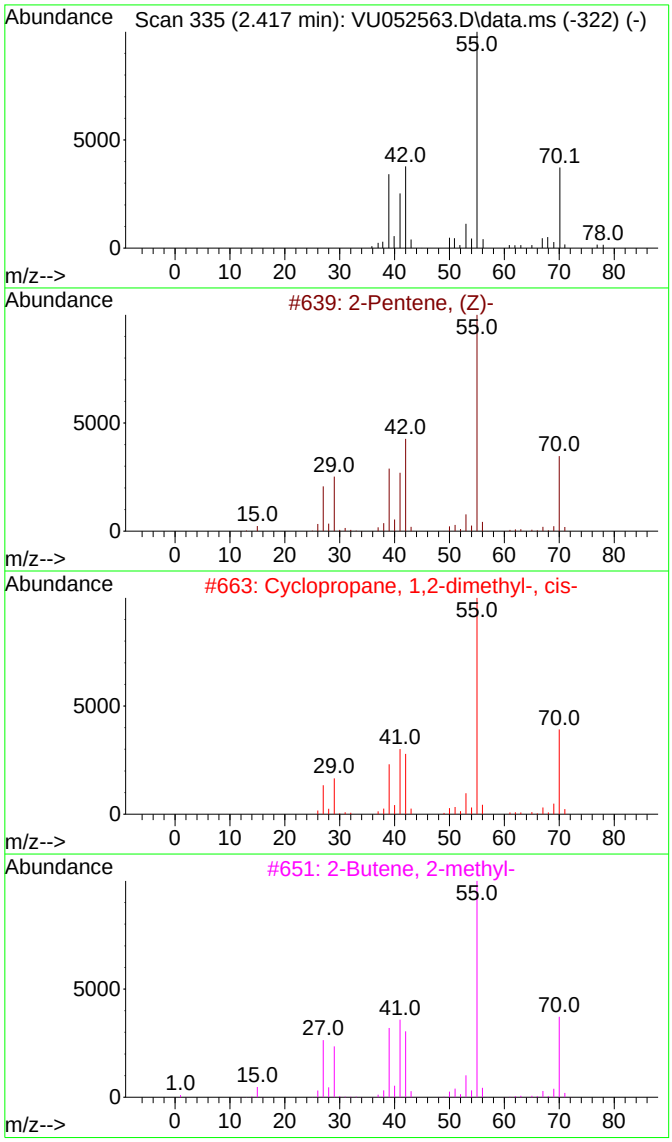
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

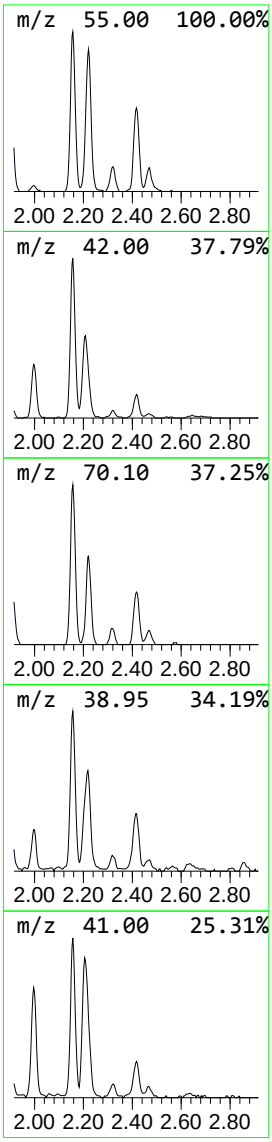
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.417	0.53 ug/L	47723	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-	70	C5H10	000627-20-3	87
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	86
3	2-Butene, 2-methyl-	70	C5H10	000513-35-9	86
4	2-Methyl-1-butene	70	C5H10	000563-46-2	80
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	80





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

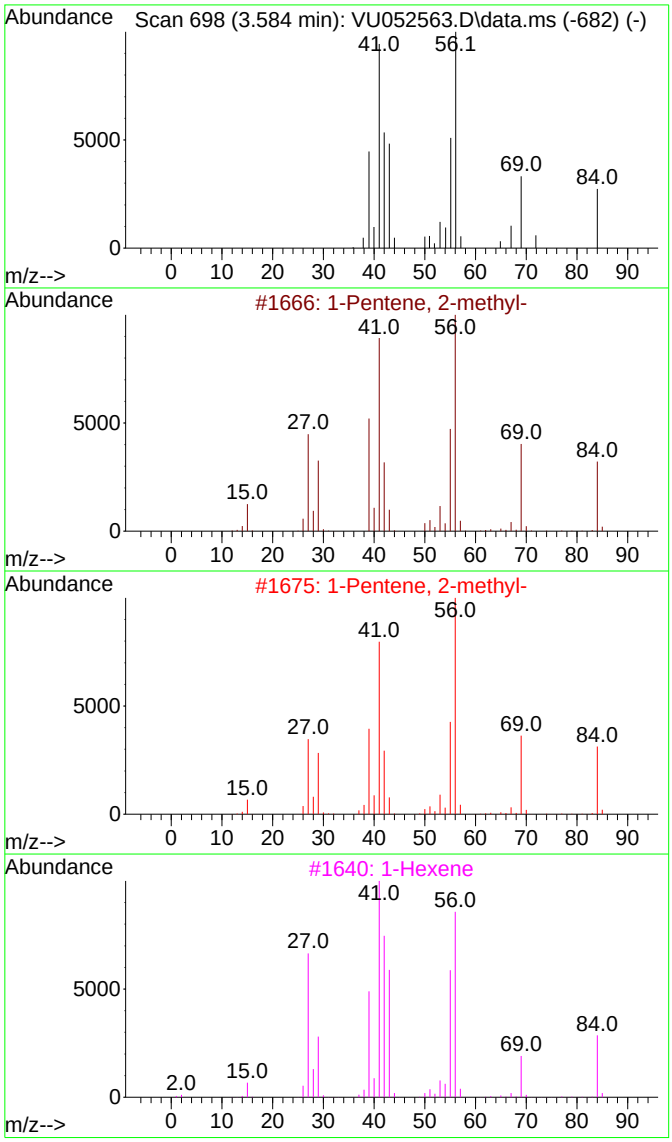
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

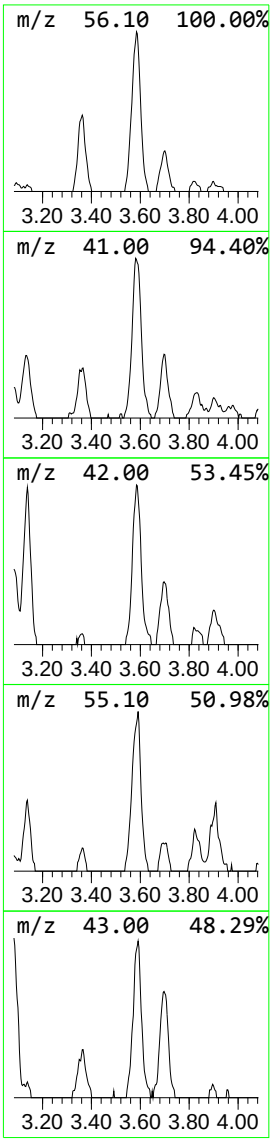
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.584	0.73 ug/L	65918	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	83
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	81
3	1-Hexene	84	C6H12	000592-41-6	76
4	1-Hexene	84	C6H12	000592-41-6	64
5	3-Hexene, (E)-	84	C6H12	013269-52-8	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122722\
Data File : VU052563.D
Acq On : 27 Dec 2022 14:41
Operator : JC/MD
Sample : N6171-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBQD1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.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...	1.359	6.9	ug/L	621730	1	6.247	450868	5.0
(DEL) Alkane: S...	1.491	0.5	ug/L	45806	1	6.247	450868	5.0
(DEL) Alkane: S...	1.732	0.6	ug/L	49707	1	6.247	450868	5.0
(DEL) Alkane: S...	1.996	0.6	ug/L	52698	1	6.247	450868	5.0
(DEL) Alkane: S...	2.157	1.3	ug/L	116113	1	6.247	450868	5.0
(DEL) Alkane: S...	2.211	1.5	ug/L	133220	1	6.247	450868	5.0
(DEL) Alkane: S...	2.417	0.5	ug/L	47723	1	6.247	450868	5.0
(DEL) Alkane: S...	3.584	0.7	ug/L	65918	1	6.247	450868	5.0