LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050421\
Data File : VU043519.D
Acq On : 04 May 2021 14:35
Operator : SY/MD
Sample : M2195-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB3J2

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\SFAMUTR050321WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU043519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	19	rVB	37246	37971	4.02%	0.849%
2	1.446	27	33	41	rVB	26652	27096	2.87%	0.606%
3	1.491	41	47	54	rVB2	24821	25123	2.66%	0.562%
4	1.604	72	82	93	rBV2	68618	81797	8.67%	1.828%
5	1.916	172	179	191	rVB	36587	46203	4.90%	1.033%
6	1.996	197	204	214	rVB2	18375	25210	2.67%	0.564%
7	2.215	262	272	291	rVB4	15538	37818	4.01%	0.845%
8	2.472	342	352	362	rVB3	12988	20479	2.17%	0.458%
9	2.575	367	384	396	rBV	78496	130801	13.86%	2.924%
10	2.639	396	404	417	rVB	9081	15777	1.67%	0.353%
11	4.636	1010	1025	1046	rBV	75514	191237	20.27%	4.275%
12	5.073	1145	1161	1180	rBV	72817	162550	17.23%	3.633%
13	5.735	1345	1367	1392	rBV2	139997	387733	41.10%	8.667%
14	5.845	1392	1401	1413	rVB4	5129	11513	1.22%	0.257%
15	6.259	1515	1530	1545	rBV	121168	227498	24.11%	5.085%
16	6.700	1653	1667	1681	rBV	95660	183995	19.50%	4.113%
17	6.774	1681	1690	1707	rVB6	7904	15465	1.64%	0.346%
18	7.575	1925	1939	1951	rBV	48653	84856	8.99%	1.897%
19	7.906	2029	2042	2055	rBV	159610	271445	28.77%	6.067%
20	7.976	2055	2064	2075	rVB2	21529	35085	3.72%	0.784%
21	8.189	2119	2130	2142	rBV2	30118	49997	5.30%	1.118%
22	8.562	2232	2246	2259	rBV	559648	943472	100.00%	21.089%
23	8.642	2259	2271	2305	rVB	255158	476249	50.48%	10.645%
24	9.423	2503	2514	2530	rBV	179730	295771	31.35%	6.611%
25	9.578	2554	2562	2573	rVB2	6291	9599	1.02%	0.215%
26	9.700	2591	2600	2611	rBV2	11640	19071	2.02%	0.426%
27	10.764	2916	2931	2948	rBV	69581	109918	11.65%	2.457%
28	11.475	3142	3152	3164	rVB3	7186	10440	1.11%	0.233%
29	11.819	3246	3259	3274	rVB	171804	267726	28.38%	5.984%
30	12.070	3327	3337	3357	rBV2	9627	16244	1.72%	0.363%
31	12.201	3366	3378	3392	rVB	159633	255659	27.10%	5.715%

Sum of corrected areas: 4473798

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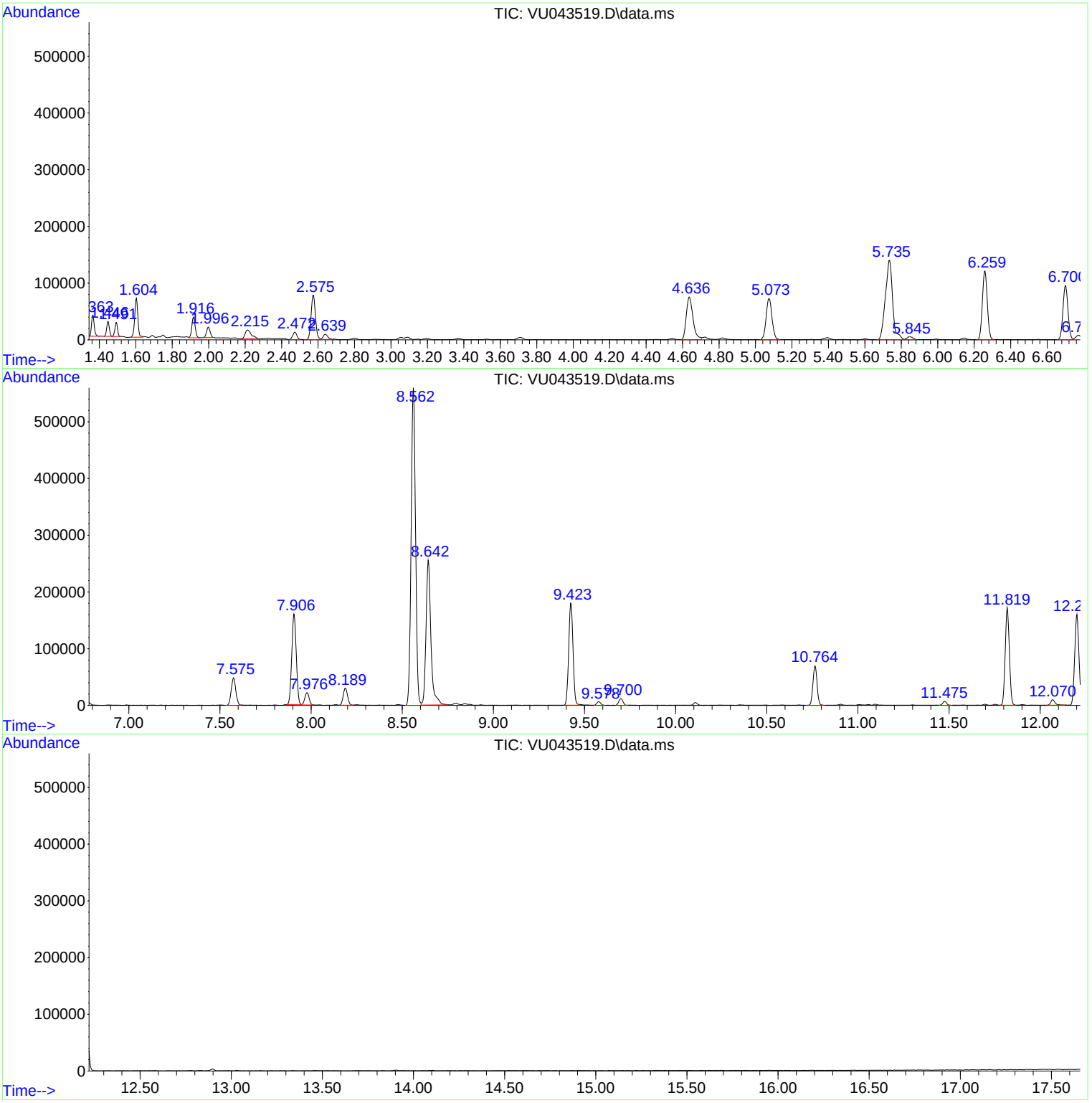
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GB3J2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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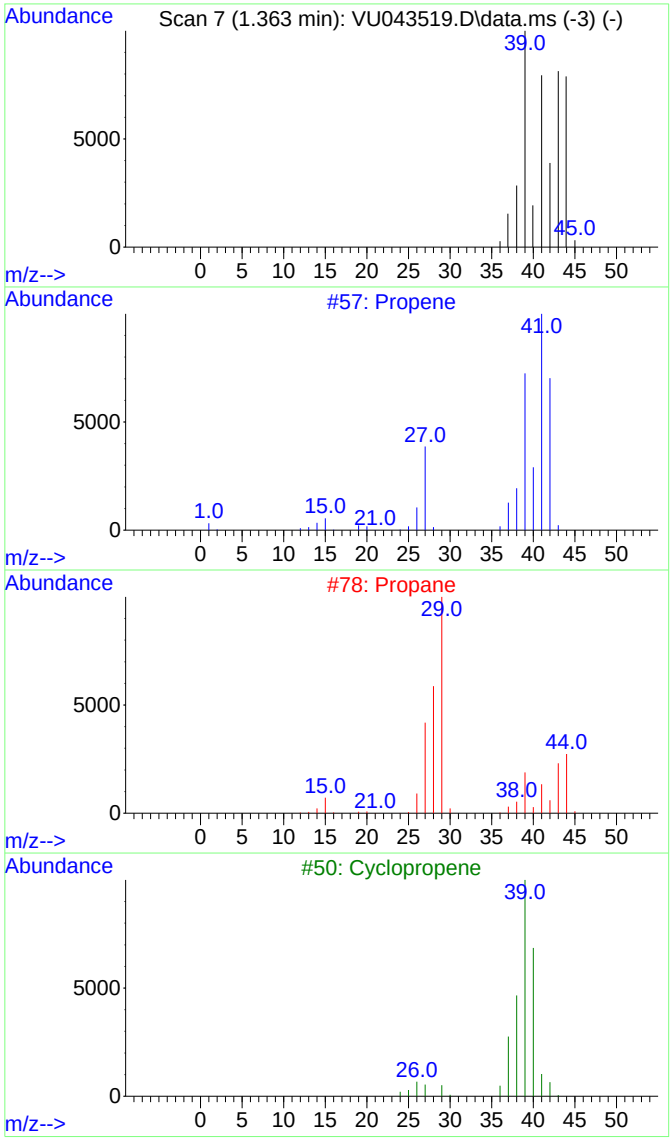
Quant Title : TRACE VOA SFAM1.0

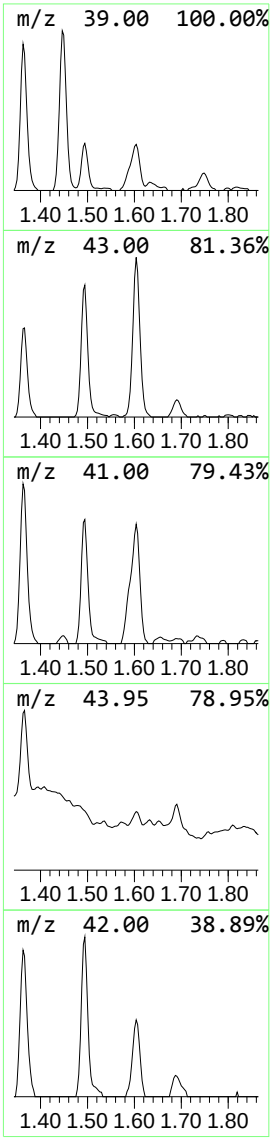
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.363	0.83 ug/L	37971	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	9
2	Propane	44	C3H8	000074-98-6	5
3	Cyclopropene	40	C3H4	002781-85-3	4
4	Propane	44	C3H8	000074-98-6	4
5	Propane	44	C3H8	000074-98-6	3





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Acq On : 04 May 2021 14:35
Operator : SY/MD
Sample : M2195-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB3J2

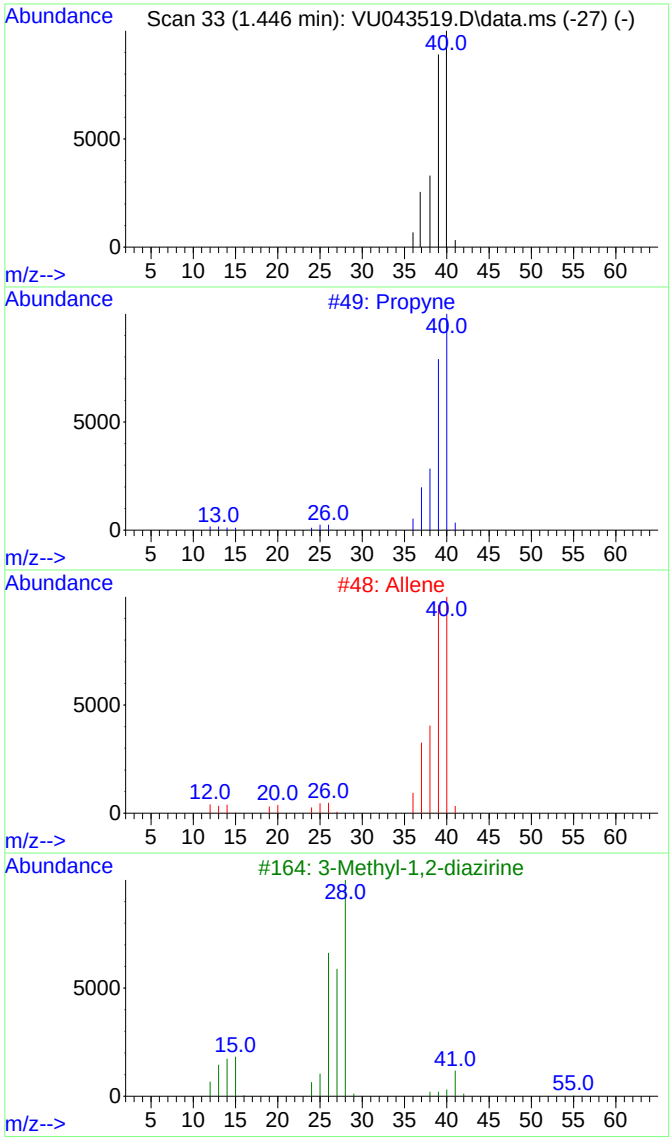
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

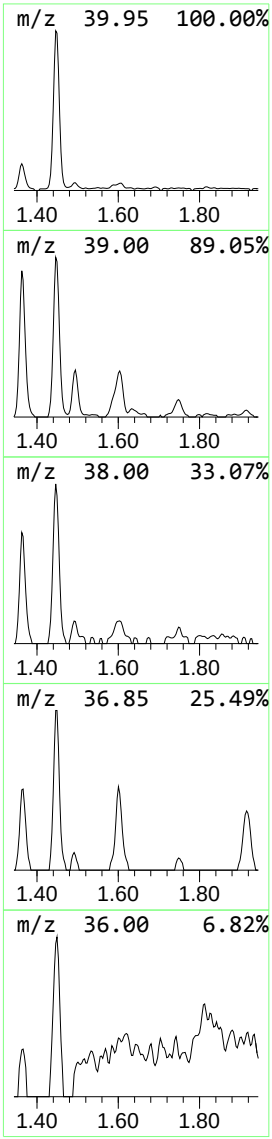
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propyne Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.446	0.60 ug/L	27096	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyne	40	C3H4	000074-99-7	90
2	Allene	40	C3H4	000463-49-0	90
3	3-Methyl-1,2-diazirine	56	C2H4N2	1000305-83-7	1
4	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	1
5	Ethane, nitro-	75	C2H5NO2	000079-24-3	1





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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB3J2

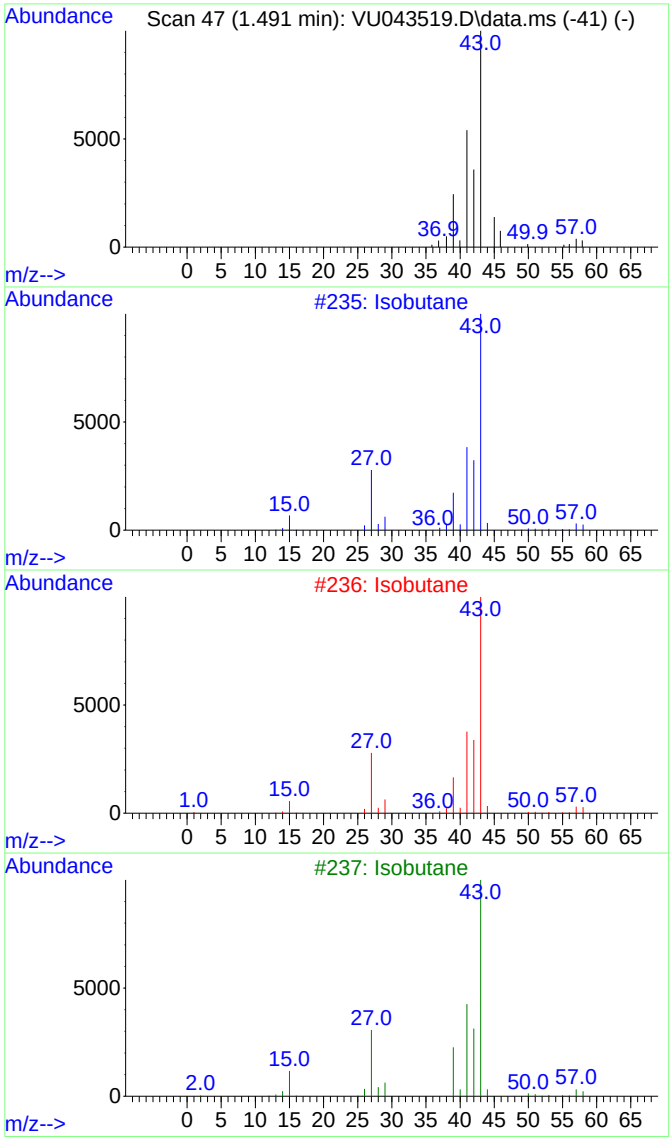
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

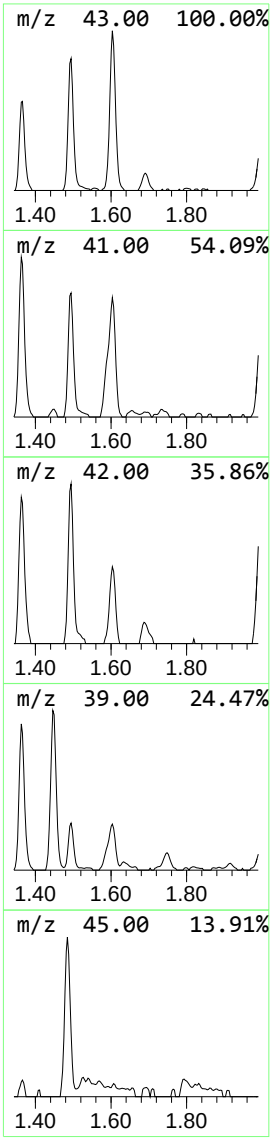
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	0.55 ug/L	25123	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	53
2	Isobutane	58	C4H10	000075-28-5	42
3	Isobutane	58	C4H10	000075-28-5	42
4	Isobutane	58	C4H10	000075-28-5	9
5	Propane, 1-chloro-2-methyl-	92	C4H9Cl	000513-36-0	9





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Operator : SY/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB3J2

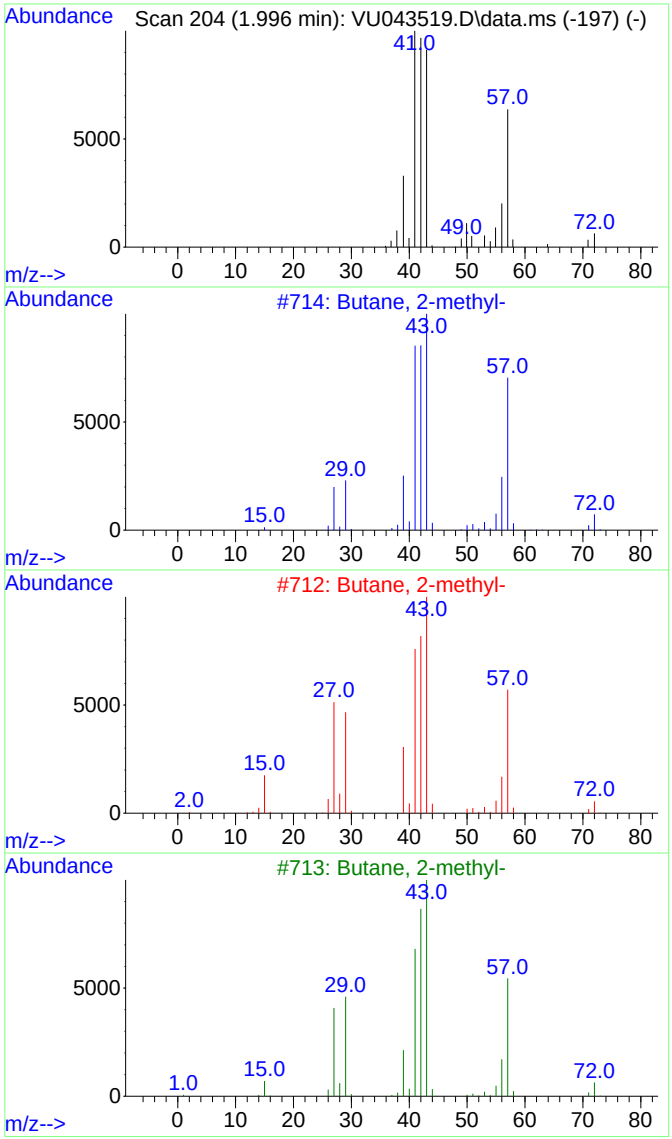
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

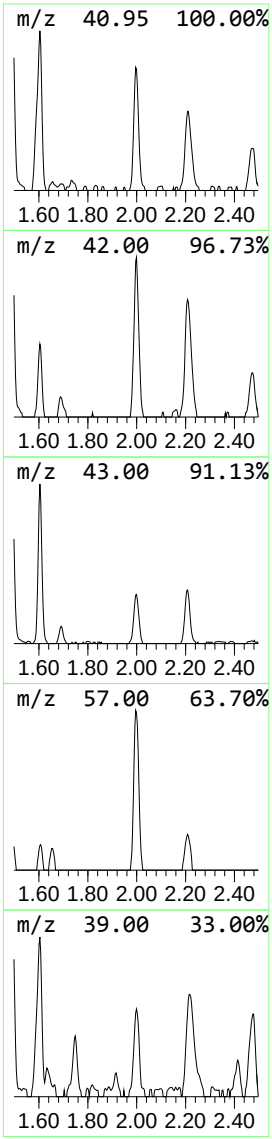
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	0.55 ug/L	25210	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	Butane, 2-methyl-	72	C5H12	000078-78-4	80
4	3-Buten-1-ol	72	C4H8O	000627-27-0	38
5	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36





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Operator : SY/MD
Sample : M2195-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB3J2

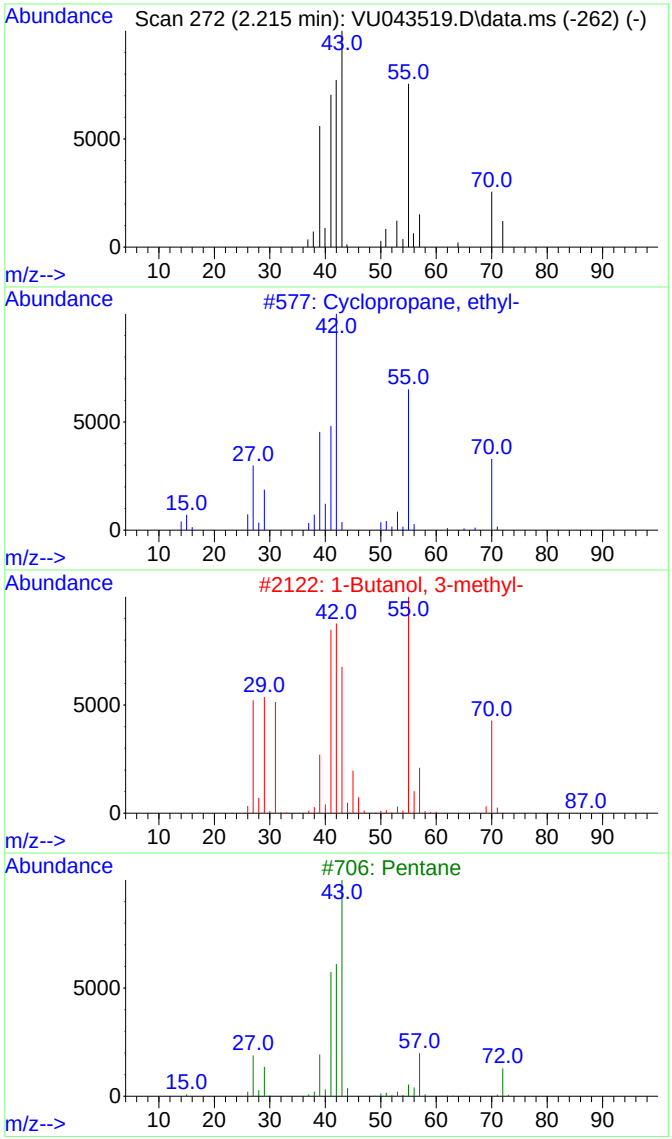
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR050321WMA.M
Quant Title : TRACE VOA SFAM1.0

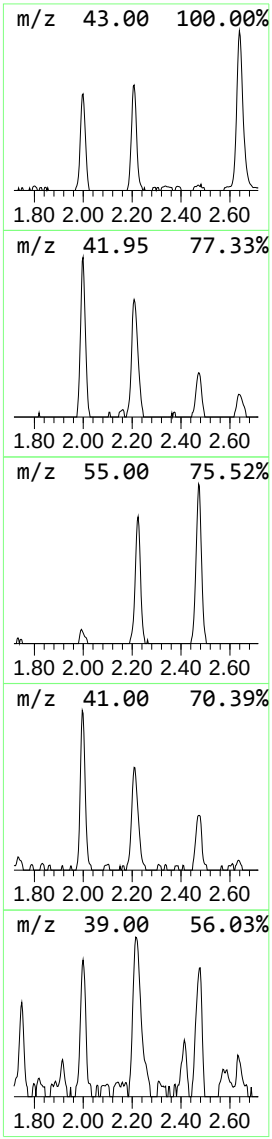
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic2.215 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	0.83 ug/L	37818	1,4-Difluorobenzene	6.259

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
2	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	50
3	Pentane	72	C5H12	000109-66-0	43
4	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	40
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	40





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.363	0.8	ug/L	37971	1	6.259	227498	5.0
Propyne	1.446	0.6	ug/L	27096	1	6.259	227498	5.0
(DEL) Alkane: S...	1.491	0.6	ug/L	25123	1	6.259	227498	5.0
(DEL) Alkane: S...	1.996	0.6	ug/L	25210	1	6.259	227498	5.0
(DEL) Alkane: C...	2.215	0.8	ug/L	37818	1	6.259	227498	5.0