LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

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\SFAMUTR072222WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU049942.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	18	rVB	63065	57693	2.22%	0.801%
2	1.601	70	81	90	rBV2	84824	105720	4.07%	1.467%
3	1.912	170	178	189	rVB	31965	41084	1.58%	0.570%
4	1.993	193	203	214	rVB	93186	128150	4.93%	1.778%
5	2.202	260	268	283	rVB	46897	67441	2.60%	0.936%
6	2.565	369	381	401	rBV	47519	87893	3.38%	1.220%
7	3.044	515	530	535	rBV3	13881	27857	1.07%	0.387%
8	3.083	535	542	550	rVV2	20312	40770	1.57%	0.566%
9	3.137	550	559	573	rVB	32785	64574	2.49%	0.896%
10	3.359	613	628	645	rVB3	20414	44598	1.72%	0.619%
11	3.851	751	781	815	rVB2	7470	37370	1.44%	0.519%
12	4.530	975	992	1010	rVB3	58054	141588	5.45%	1.965%
13	4.636	1010	1025	1067	rBV3	80160	296585	11.42%	4.115%
14	5.063	1140	1158	1173	rBV	66272	147884	5.69%	2.052%
15	5.388	1242	1259	1274	rBV3	64412	150139	5.78%	2.083%
16	5.726	1345	1364	1373	rBV2	118335	316721	12.19%	4.395%
17	5.777	1373	1380	1396	rVV2	74040	174276	6.71%	2.418%
18	6.250	1513	1527	1548	rBV	97354	183193	7.05%	2.542%
19	6.543	1606	1618	1631	rBV3	22176	41824	1.61%	0.580%
20	6.690	1650	1664	1675	rBV	82855	165540	6.37%	2.297%
21	6.761	1676	1686	1701	rVB3	56217	118281	4.55%	1.641%
22	7.565	1925	1936	1952	rBV	32793	60230	2.32%	0.836%
23	7.896	2029	2039	2054	rVB	116017	201391	7.75%	2.794%
24	8.182	2117	2128	2139	rBV2	20084	35136	1.35%	0.488%
25	8.552	2228	2243	2259	rBV	1535357	2597942	100.00%	36.048%
26	8.636	2259	2269	2303	rVB3	213391	539550	20.77%	7.487%
27	9.417	2497	2512	2532	rBV	138041	251481	9.68%	3.489%
28	9.697	2587	2599	2617	rBV	89957	155327	5.98%	2.155%
29	10.099	2708	2724	2742	rVB	64668	111423	4.29%	1.546%
30	10.484	2834	2844	2856	rVB	18063	27432	1.06%	0.381%
31	10.755	2916	2928	2940	rBV2	103146	184860	7.12%	2.565%
32	11.086	3022	3031	3046	rBV	34985	52998	2.04%	0.735%
33	11.292	3086	3095	3109	rBV2	20000	31569	1.22%	0.438%
34	11.468	3140	3150	3162	rBV	30861	46974	1.81%	0.652%
35	11.812	3242	3257	3273	rBV	144939	237892	9.16%	3.301%
36	12.192	3364	3375	3393	rBV	140778	233565	8.99%	3.241%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

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\SFAMUTR072222WMA.M
Title : TRACE VOA SFAM1.0

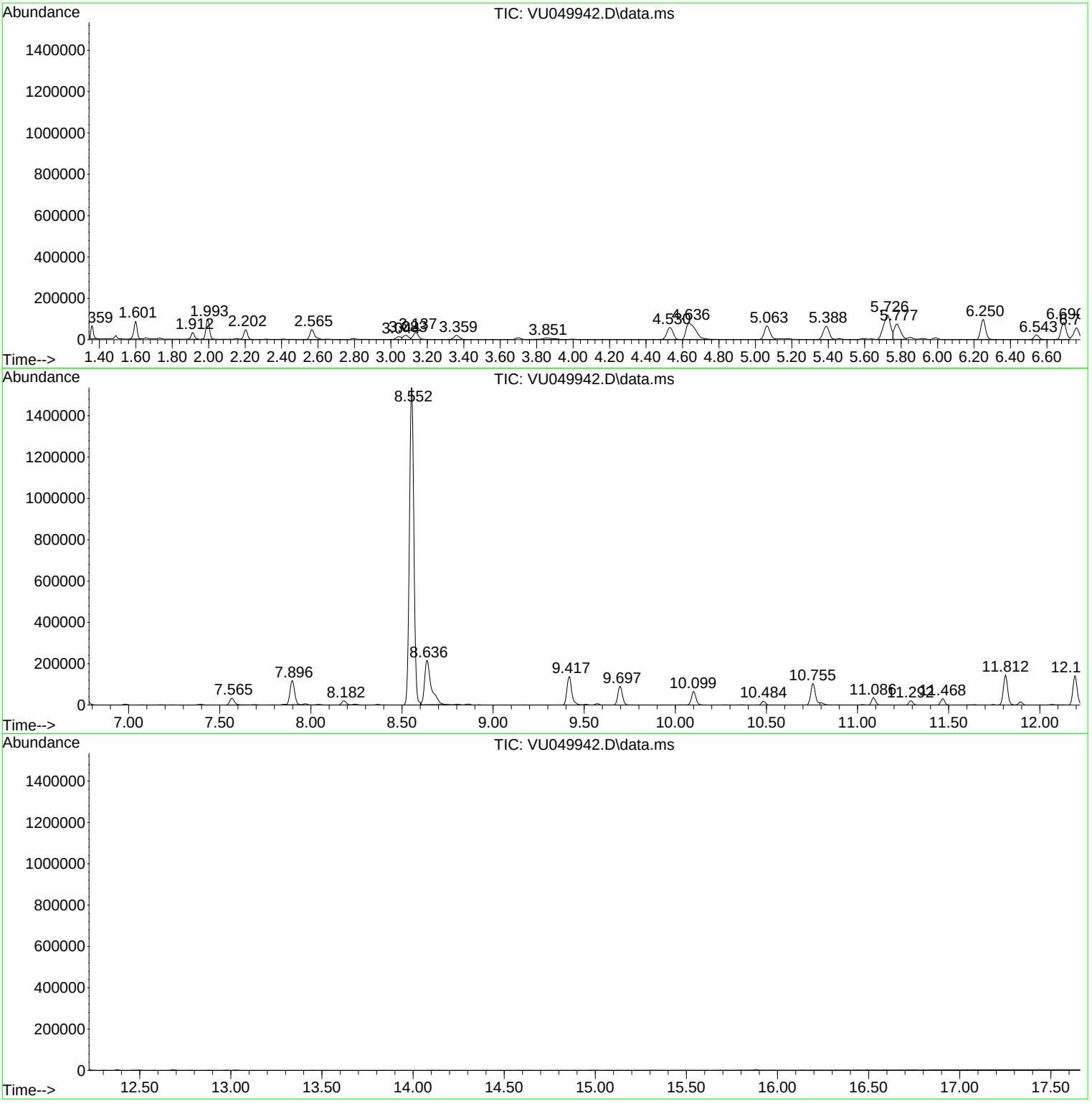
Sum of corrected areas: 7206951

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.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\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

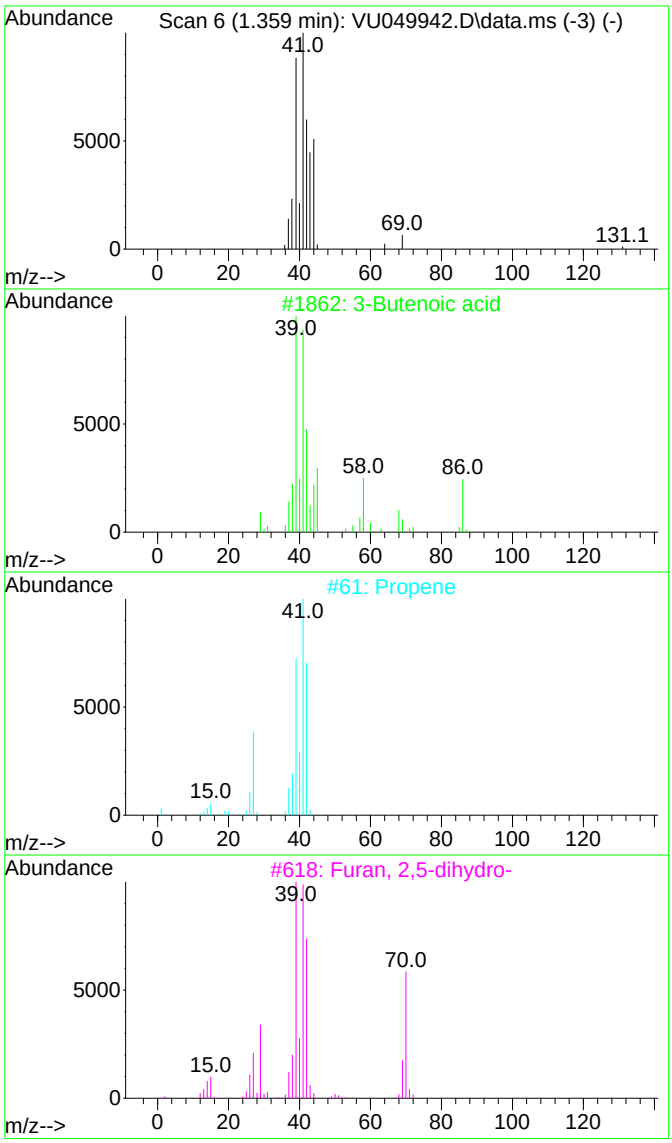
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

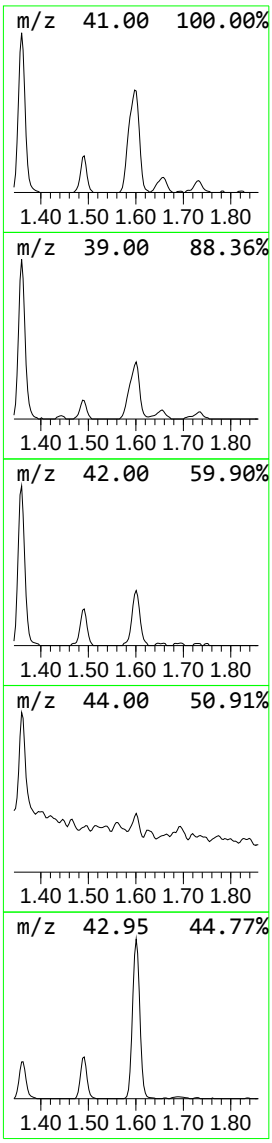
****

Peak Number 1 3-Butenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	1.57 ug/L	57693	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Butenoic acid	86	C4H6O2	000625-38-7	83
2	Propene	42	C3H6	000115-07-1	64
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	59
4	2-Butenal, (E)-	70	C4H6O	000123-73-9	56
5	2-Butenal	70	C4H6O	004170-30-3	56





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

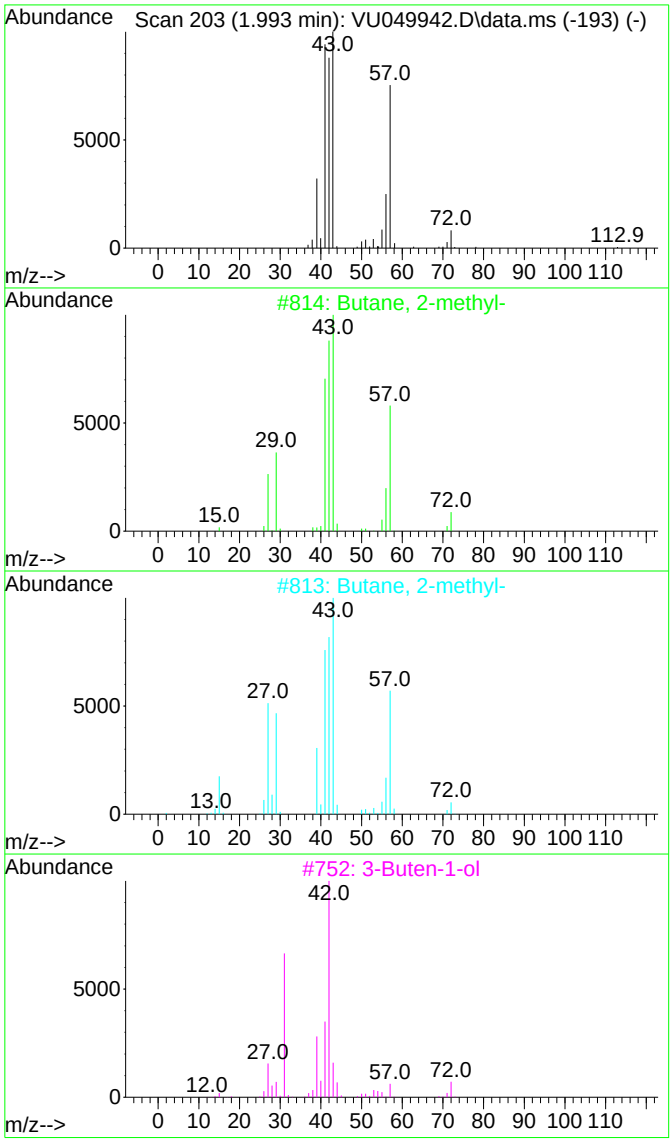
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

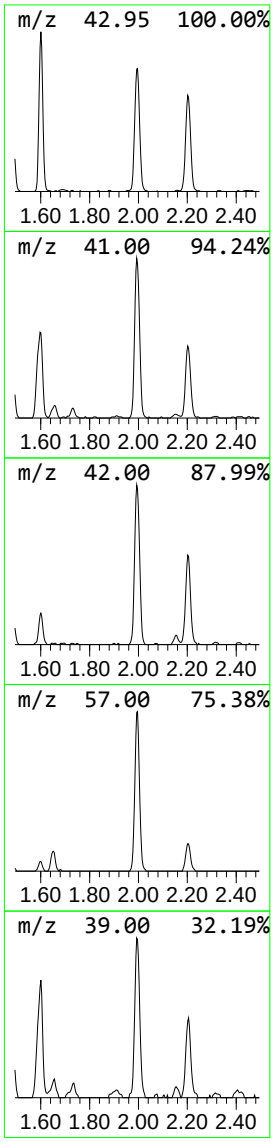
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.993	3.50 ug/L	128150	1,4-Difluorobenzene	6.250

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	78
3	3-Buten-1-ol	72	C4H8O	000627-27-0	43
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	36
5	Pentane	72	C5H12	000109-66-0	33





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

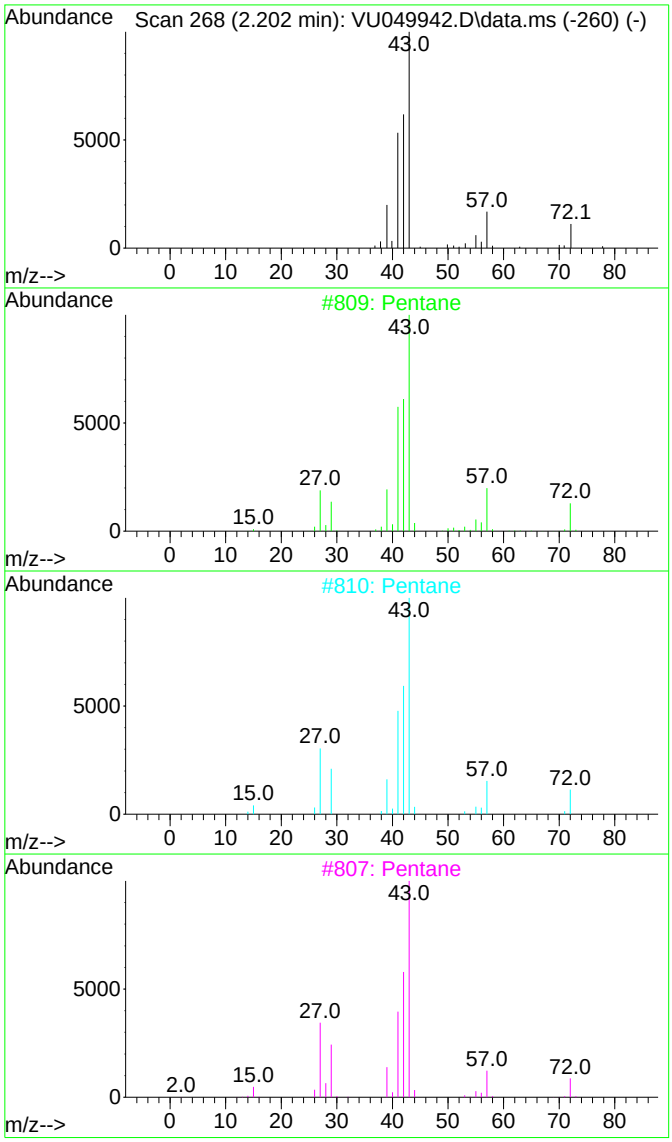
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

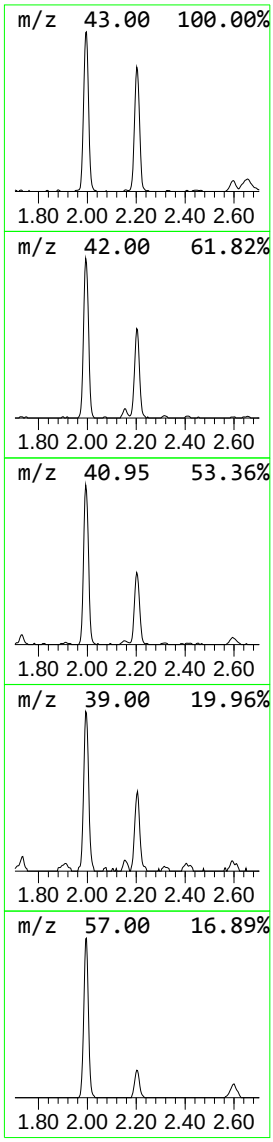
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.202	1.84 ug/L	67441	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	87
2	Pentane	72	C5H12	000109-66-0	86
3	Pentane	72	C5H12	000109-66-0	86
4	Pentane	72	C5H12	000109-66-0	86
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

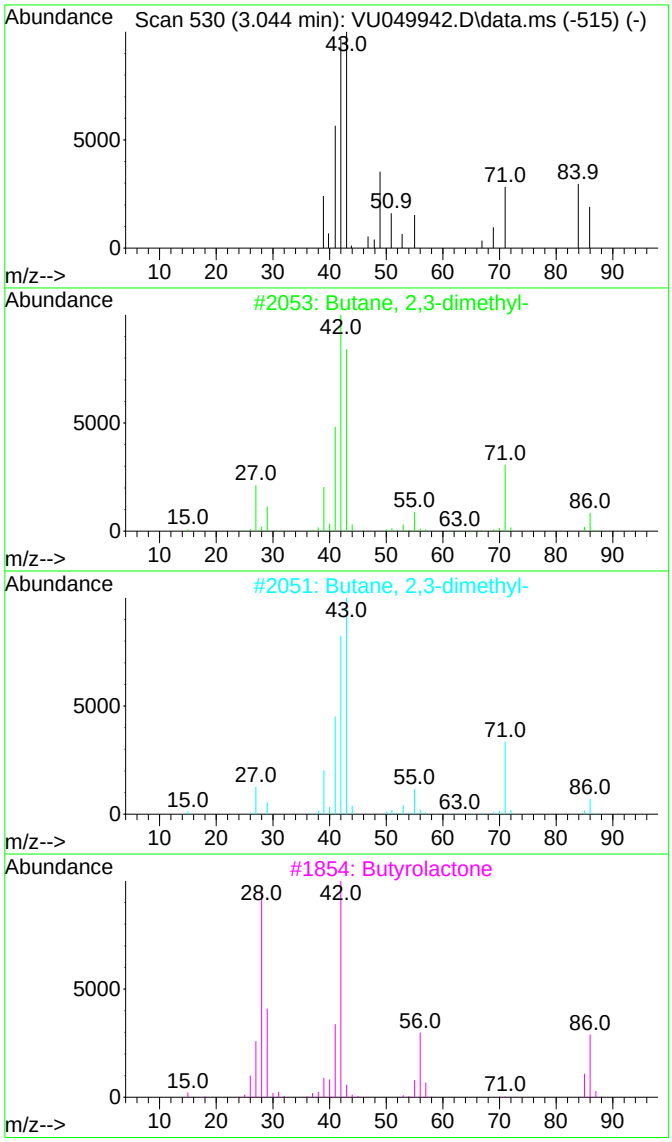
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

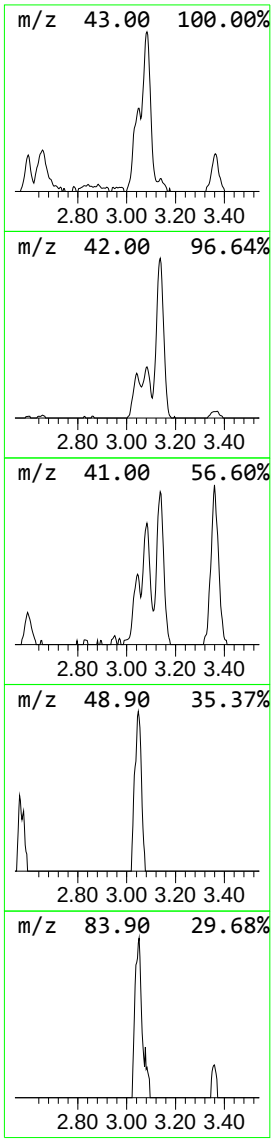
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.044	0.76 ug/L	27857	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	25
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	25
3	Butyrolactone	86	C4H6O2	000096-48-0	7
4	Butyrolactone	86	C4H6O2	000096-48-0	7
5	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

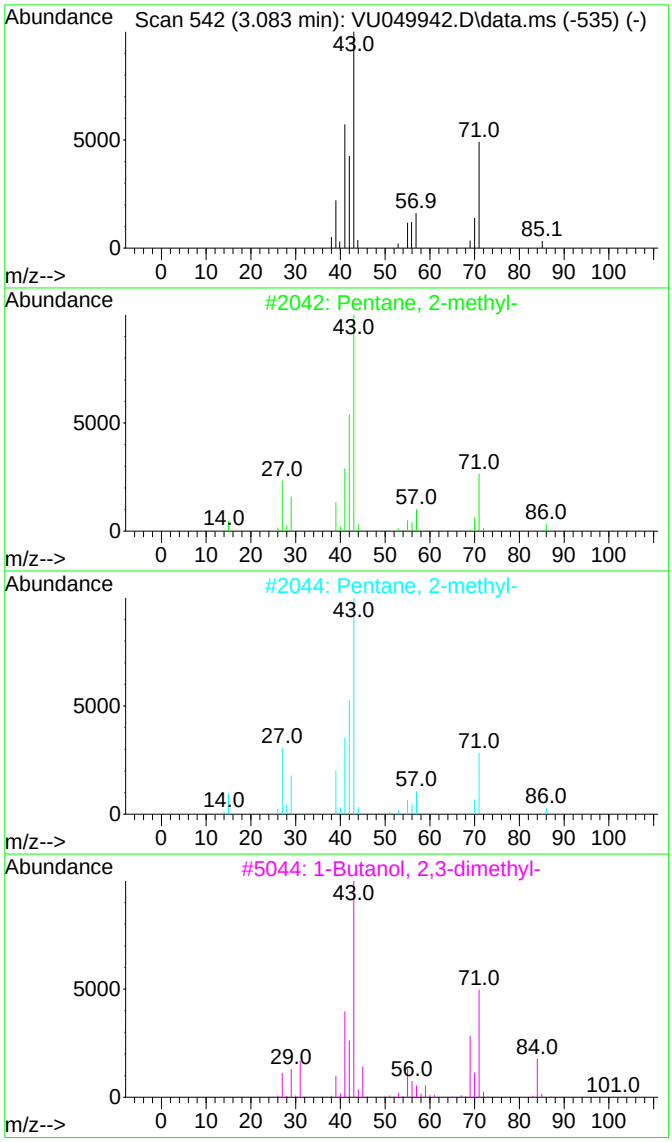
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

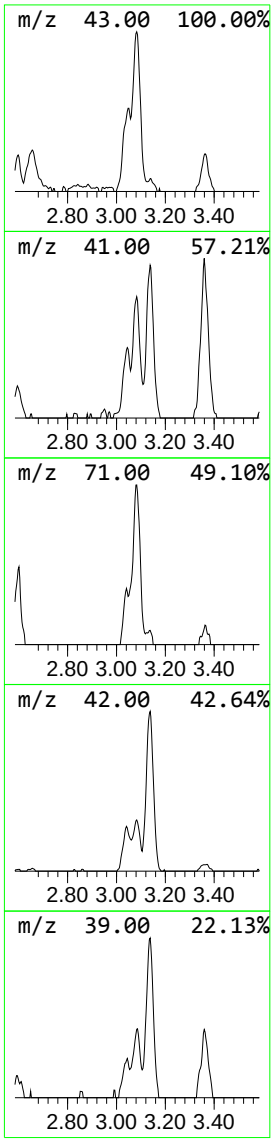
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.083	1.11 ug/L	40770	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	56
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	36
4	Hexane, 3-ethyl-	114	C8H18	000619-99-8	32
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

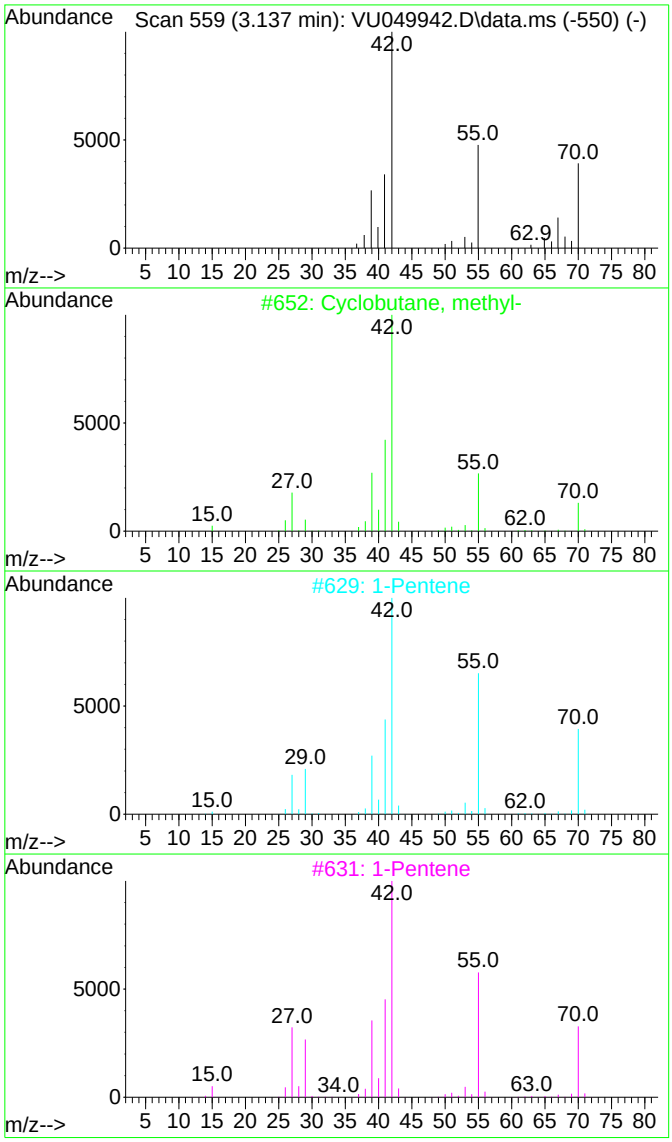
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

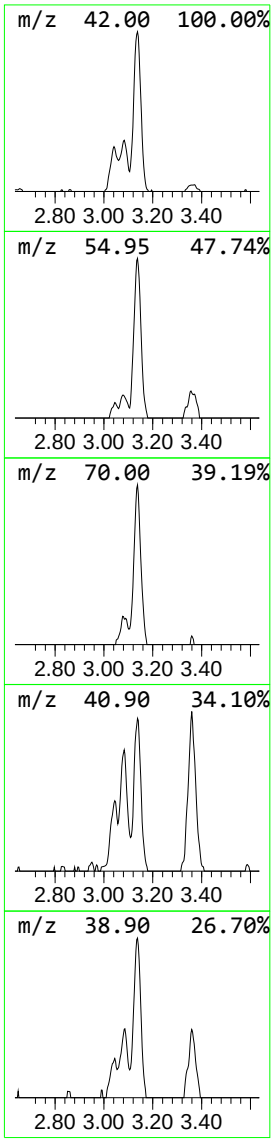
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Cyclic3.137 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.137	1.76 ug/L	64574	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
2	1-Pentene	70	C5H10	000109-67-1	59
3	1-Pentene	70	C5H10	000109-67-1	50
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	45
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

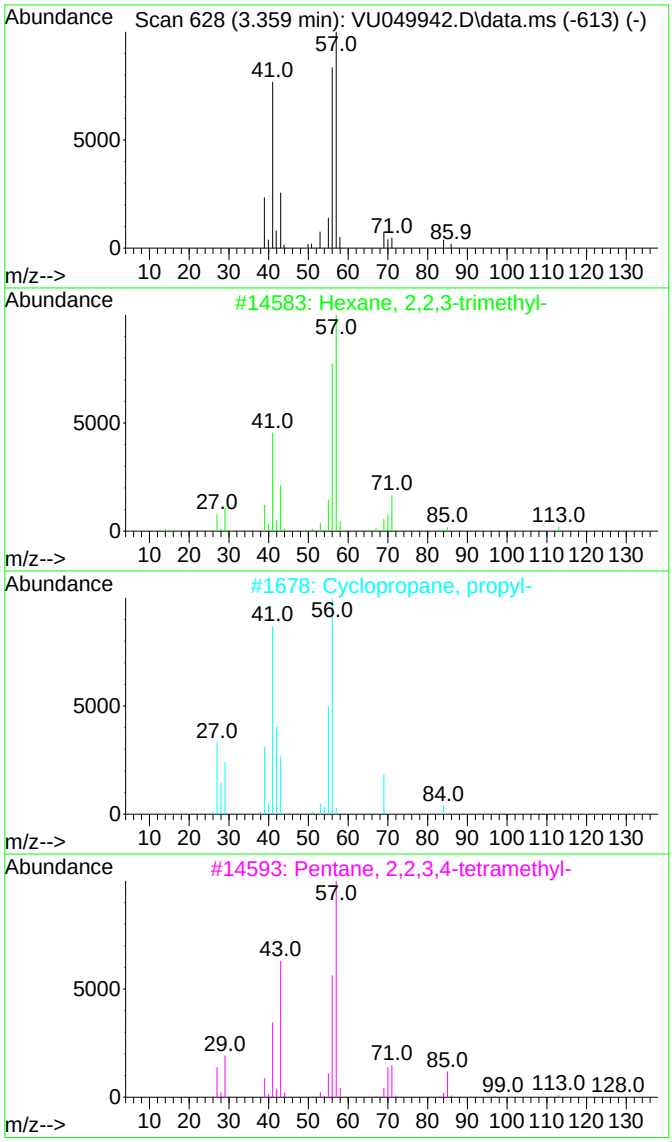
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

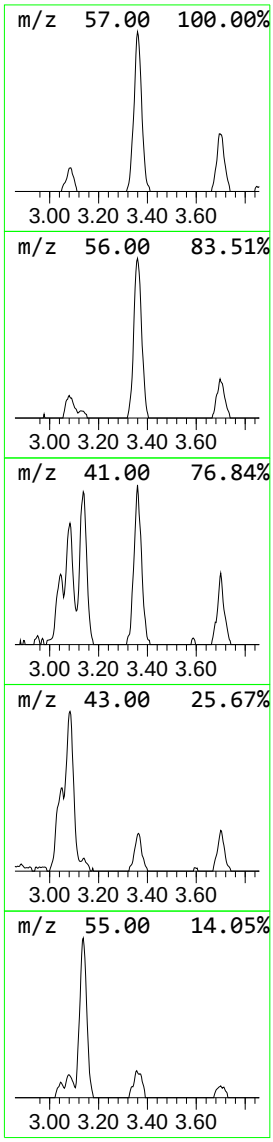
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.359	1.22 ug/L	44598	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	53
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	45
4	Pentane, 3-methyl-	86	C6H14	000096-14-0	40
5	Pentane, 3-methyl-	86	C6H14	000096-14-0	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

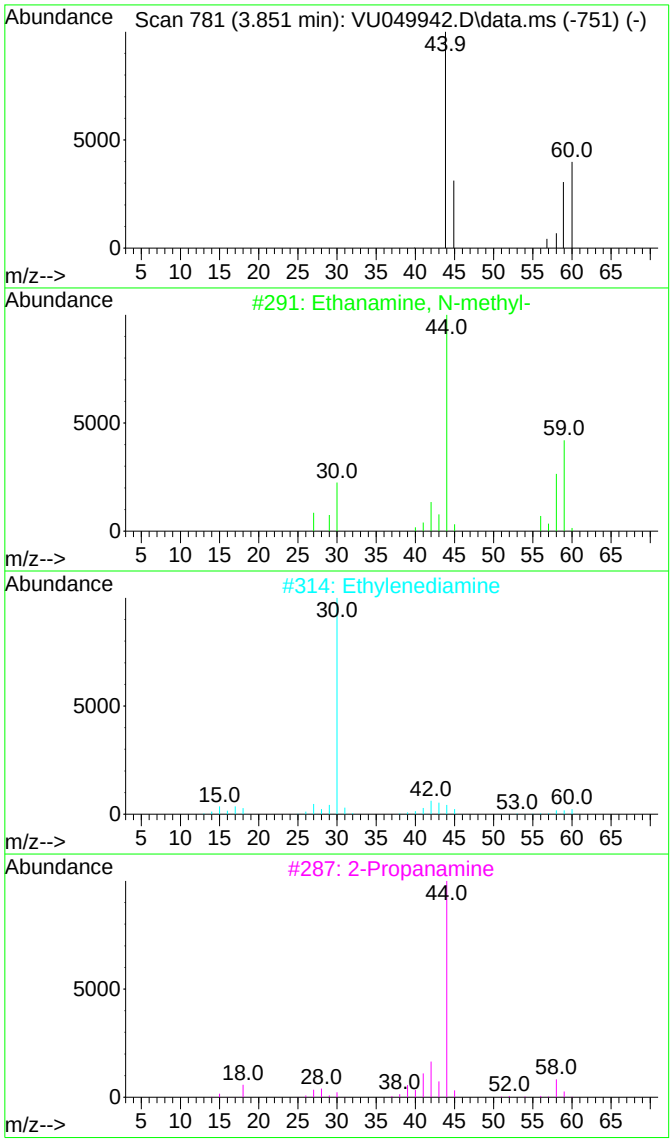
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

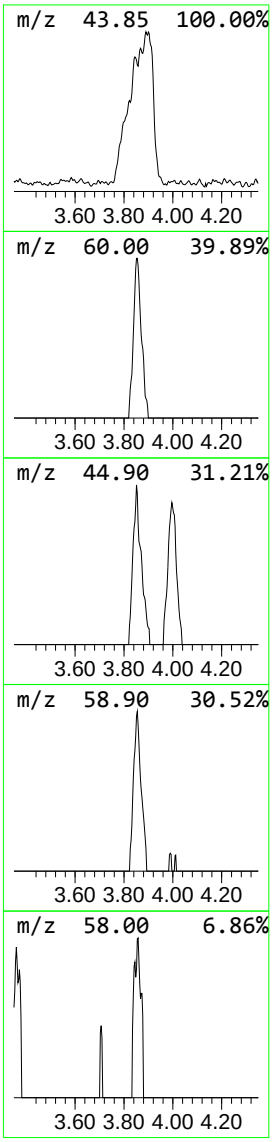
****

Peak Number 8 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.851	1.02 ug/L	37370	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanamine, N-methyl-	59	C3H9N	000624-78-2	7
2	Ethylenediamine	60	C2H8N2	000107-15-3	4
3	2-Propanamine	59	C3H9N	000075-31-0	3
4	2-Propanamine	59	C3H9N	000075-31-0	3
5	Ethylenediamine	60	C2H8N2	000107-15-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

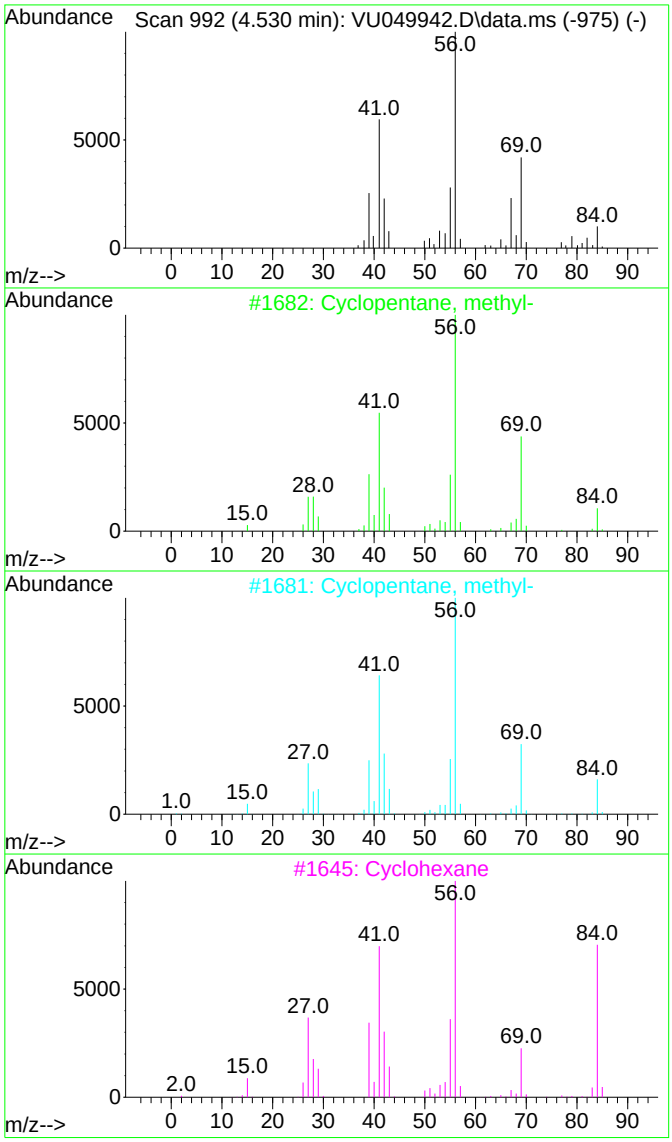
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

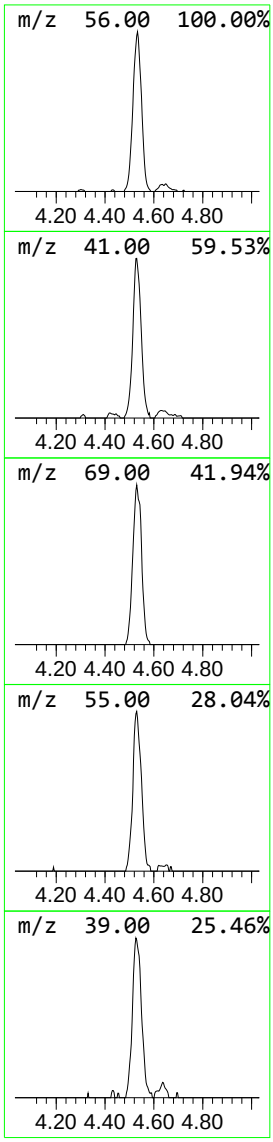
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (DEL) Alkane: Cyclic4.530 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.530	3.86 ug/L	141588	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	74
3	Cyclohexane	84	C6H12	000110-82-7	68
4	Cyclohexane	84	C6H12	000110-82-7	64
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

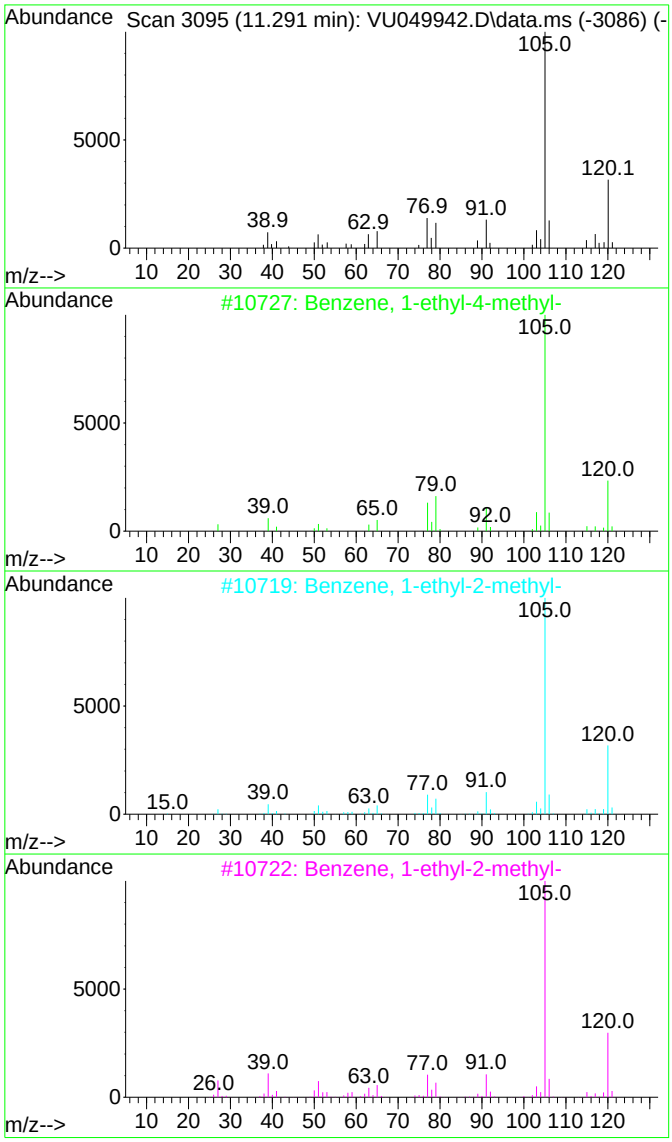
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.M
Quant Title : TRACE VOA SFAM1.0

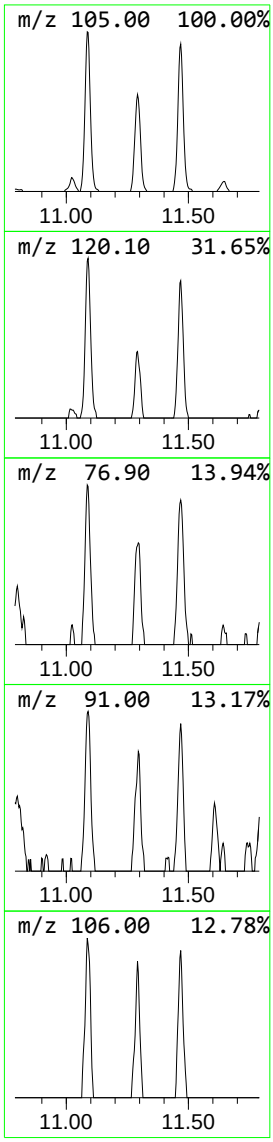
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Benzene, 1-ethyl-4-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	0.66 ug/L	31569	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072622\
Data File : VU049942.D
Acq On : 27 Jul 2022 04:12
Operator : SY/MD
Sample : N3879-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUH7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR072222WMA.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
3-Butenoic acid	1.359	1.6	ug/L	57693	1	6.250	183193	5.0
(DEL) Alkane: S...	1.993	3.5	ug/L	128150	1	6.250	183193	5.0
(DEL) Alkane: S...	2.202	1.8	ug/L	67441	1	6.250	183193	5.0
(DEL) Alkane: S...	3.044	0.8	ug/L	27857	1	6.250	183193	5.0
(DEL) Alkane: S...	3.083	1.1	ug/L	40770	1	6.250	183193	5.0
(DEL) Alkane: C...	3.137	1.8	ug/L	64574	1	6.250	183193	5.0
(DEL) Alkane: S...	3.359	1.2	ug/L	44598	1	6.250	183193	5.0
unknown-01	3.851	1.0	ug/L	37370	1	6.250	183193	5.0
(DEL) Alkane: C...	4.530	3.9	ug/L	141588	1	6.250	183193	5.0
Benzene, 1-ethy...	11.291	0.7	ug/L	31569	3	11.812	237892	5.0