LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

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\SFAMUTR062121WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU044280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	71	82	99	rBV3	101898	203308	2.62%	0.345%
2	2.571	373	383	402	rVB2	122216	207141	2.67%	0.352%
3	3.362	618	629	642	rBV	47386	91930	1.19%	0.156%
4	3.616	697	708	723	rVB	43638	96697	1.25%	0.164%
5	4.497	958	982	1025	rBV	333772	990635	12.78%	1.682%
6	4.703	1031	1046	1089	rVB2	86140	292144	3.77%	0.496%
7	5.092	1152	1167	1194	rVB	95689	216788	2.80%	0.368%
8	5.745	1349	1370	1377	rBV3	201118	481337	6.21%	0.817%
9	5.793	1377	1385	1404	rVB	311250	625315	8.07%	1.062%
10	6.269	1518	1533	1549	rBV	184619	351215	4.53%	0.596%
11	6.710	1658	1670	1684	rBV	119973	224992	2.90%	0.382%
12	7.581	1927	1941	1955	rBV	64856	113351	1.46%	0.192%
13	7.909	2022	2043	2057	rBV	239649	417861	5.39%	0.709%
14	8.648	2258	2273	2313	rBV	319802	603966	7.79%	1.025%
15	8.890	2336	2348	2365	rVB	50022	83107	1.07%	0.141%
16	9.426	2502	2515	2532	rBV2	256139	556568	7.18%	0.945%
17	9.603	2556	2570	2579	rBV	71084	115373	1.49%	0.196%
18	9.700	2579	2600	2612	rBV4	411530	916851	11.83%	1.557%
19	10.491	2833	2846	2859	rBV	58083	100599	1.30%	0.171%
20	10.713	2903	2915	2924	rBV	536051	844039	10.89%	1.433%
21	10.764	2924	2931	2940	rVB	84759	130734	1.69%	0.222%
22	10.912	2970	2977	2986	rVB	51317	78571	1.01%	0.133%
23	10.970	2986	2995	3007	rBV3	50787	81362	1.05%	0.138%
24	11.098	3026	3035	3045	rVB2	265697	417538	5.39%	0.709%
25	11.153	3045	3052	3066	rVB2	48664	79631	1.03%	0.135%
26	11.561	3164	3179	3187	rBV6	39967	91798	1.18%	0.156%
27	11.729	3222	3231	3240	rBV	240699	380987	4.92%	0.647%
28	11.848	3249	3268	3288	rVB	4770328	7748987	100.00%	13.156%
29	11.947	3290	3299	3305	rVV	177223	275257	3.55%	0.467%
30	11.983	3306	3310	3317	rVV3	91185	137015	1.77%	0.233%
31	12.047	3320	3330	3339	rVV	919136	1464463	18.90%	2.486%
32	12.102	3339	3347	3358	rVB2	559933	883723	11.40%	1.500%
33	12.198	3365	3377	3385	rBV2	303642	556570	7.18%	0.945%
34	12.262	3391	3397	3406	rVB	233406	360124	4.65%	0.611%
35	12.385	3428	3435	3448	rVB4	116737	196396	2.53%	0.333%
36	12.455	3448	3457	3473	rVB4	88500	158063	2.04%	0.268%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
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Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

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\SFAMUTR062121WMA.M
Title : TRACE VOA SFAM1.0

37	12.581	3486	3496	3506	rBV2	440773	682223	8.80%	1.158%
38	12.732	3533	3543	3561	rVB2	369390	812212	10.48%	1.379%
39	12.835	3561	3575	3583	rBV2	492587	997528	12.87%	1.694%
40	12.873	3584	3587	3598	rVB4	104609	148070	1.91%	0.251%
41	12.947	3598	3610	3616	rBV2	211412	373634	4.82%	0.634%
42	13.018	3616	3632	3644	rVB	2224240	3887177	50.16%	6.600%
43	13.108	3646	3660	3673	rBV	2202158	3377585	43.59%	5.734%
44	13.182	3674	3683	3690	rBV2	104500	161873	2.09%	0.275%
45	13.262	3694	3708	3724	rVB2	260484	625641	8.07%	1.062%
46	13.356	3725	3737	3741	rBV4	124271	236819	3.06%	0.402%
47	13.410	3748	3754	3762	rVB3	271869	411498	5.31%	0.699%
48	13.462	3762	3770	3773	rBV3	176038	238266	3.07%	0.405%
49	13.494	3774	3780	3789	rVV	527287	790645	10.20%	1.342%
50	13.539	3789	3794	3803	rVB	104503	149099	1.92%	0.253%
51	13.667	3826	3834	3846	rBV4	224294	391505	5.05%	0.665%
52	13.738	3846	3856	3874	rVB2	920338	1687088	21.77%	2.864%
53	13.828	3874	3884	3894	rBV2	459673	719693	9.29%	1.222%
54	13.876	3894	3899	3910	rVB4	60025	90551	1.17%	0.154%
55	13.976	3915	3930	3953	rBV	4047640	6986231	90.16%	11.861%
56	14.095	3960	3967	3978	rVB6	111483	212802	2.75%	0.361%
57	14.195	3979	3998	4020	rVB10	202100	814573	10.51%	1.383%
58	14.327	4029	4039	4047	rBV	384126	616461	7.96%	1.047%
59	14.381	4047	4056	4069	rVV2	494459	1013272	13.08%	1.720%
60	14.442	4070	4075	4085	rVB2	277388	386674	4.99%	0.656%
61	14.536	4095	4104	4111	rBV3	153858	248414	3.21%	0.422%
62	14.584	4111	4119	4133	rVB	769692	1113846	14.37%	1.891%
63	14.658	4135	4142	4161	rVB6	131970	301451	3.89%	0.512%
64	14.761	4162	4174	4181	rBV	873305	1391608	17.96%	2.363%
65	14.851	4195	4202	4209	rBV2	75768	105623	1.36%	0.179%
66	14.899	4209	4217	4228	rVB2	96322	161352	2.08%	0.274%
67	15.105	4274	4281	4284	rVV3	86125	121729	1.57%	0.207%
68	15.134	4285	4290	4296	rVV2	157832	242537	3.13%	0.412%
69	15.185	4297	4306	4318	rVB	1841883	2863782	36.96%	4.862%
70	15.269	4327	4332	4342	rVB2	137000	208695	2.69%	0.354%
71	15.368	4349	4363	4369	rBV6	339735	710105	9.16%	1.206%
72	15.410	4370	4376	4384	rVB	308683	474909	6.13%	0.806%
73	15.542	4408	4417	4420	rBV3	90918	139001	1.79%	0.236%
74	15.655	4442	4452	4472	rVB	305091	678458	8.76%	1.152%
75	15.754	4474	4483	4490	rVV	71581	119367	1.54%	0.203%
76	15.809	4492	4500	4527	rVB2	124368	285324	3.68%	0.484%

LSC Area Percent Report

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Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Title : TRACE VOA SFAM1.0

77	15.992	4550	4557	4572	rVB5	72607	144168	1.86%	0.245%
78	16.072	4573	4582	4586	rBV3	82915	128194	1.65%	0.218%
79	16.111	4587	4594	4604	rVB	129774	218326	2.82%	0.371%
80	16.204	4614	4623	4640	rVB4	227514	507816	6.55%	0.862%
81	16.391	4672	4681	4701	rVB3	242852	446102	5.76%	0.757%
82	16.674	4761	4769	4775	rBV2	51500	84919	1.10%	0.144%
83	16.828	4806	4817	4839	rVB6	110464	268336	3.46%	0.456%
84	16.944	4847	4853	4864	rVB	51372	84076	1.08%	0.143%
85	17.018	4865	4876	4891	rVB	650864	985259	12.71%	1.673%
86	17.166	4914	4922	4935	rVV2	48809	87307	1.13%	0.148%
87	17.236	4936	4944	4949	rVV2	52678	86835	1.12%	0.147%
88	17.272	4950	4955	4968	rVB	66465	102772	1.33%	0.174%
89	17.442	4999	5008	5035	rVB6	80837	204072	2.63%	0.346%

Sum of corrected areas: 58899939

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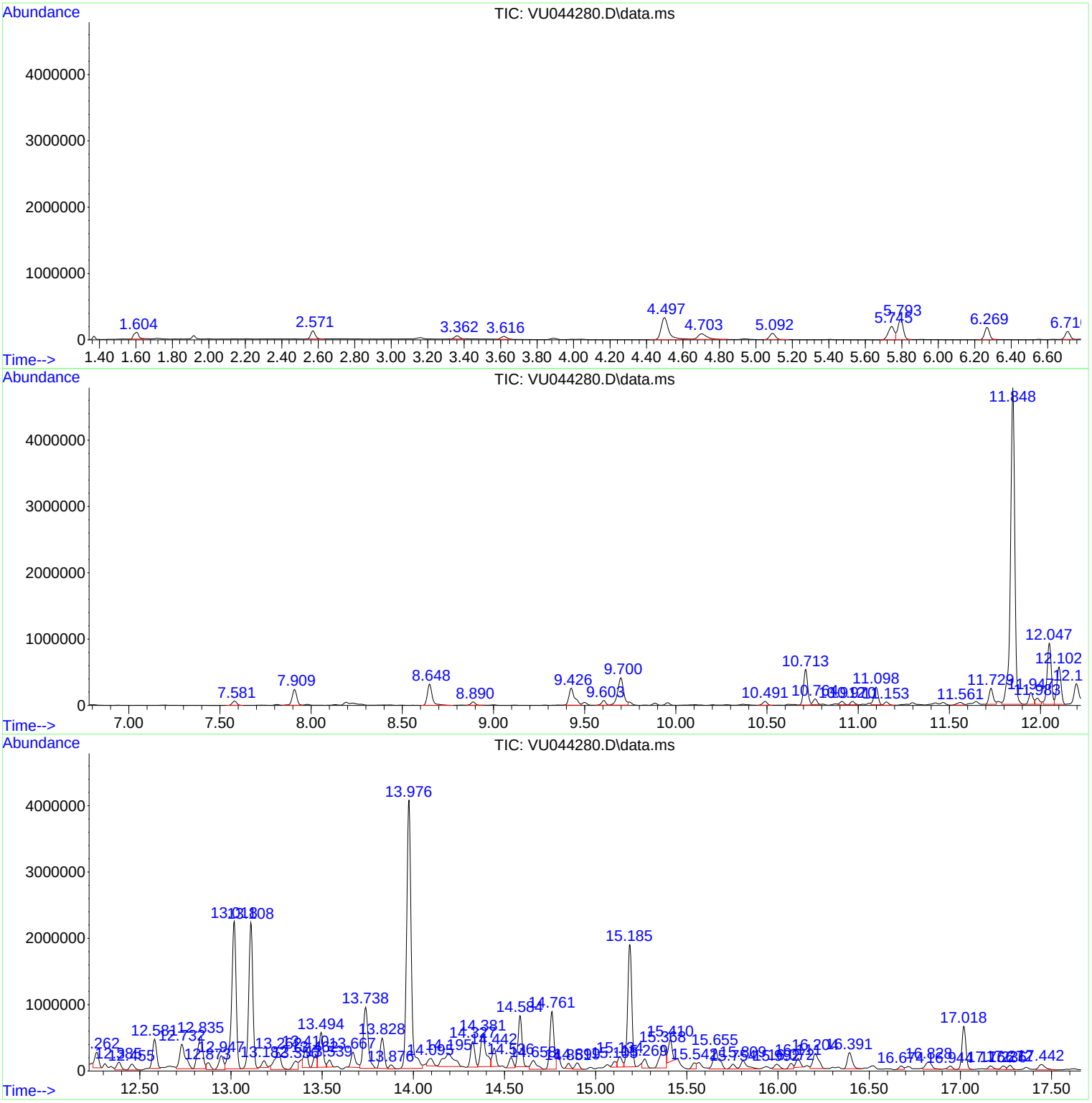
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

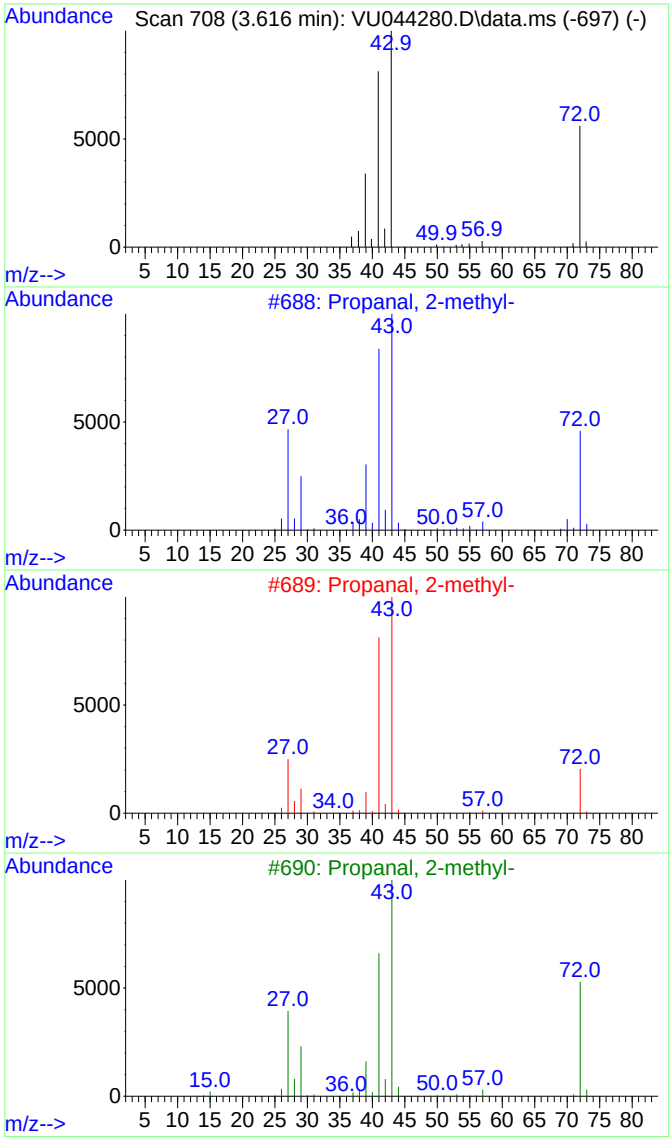
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

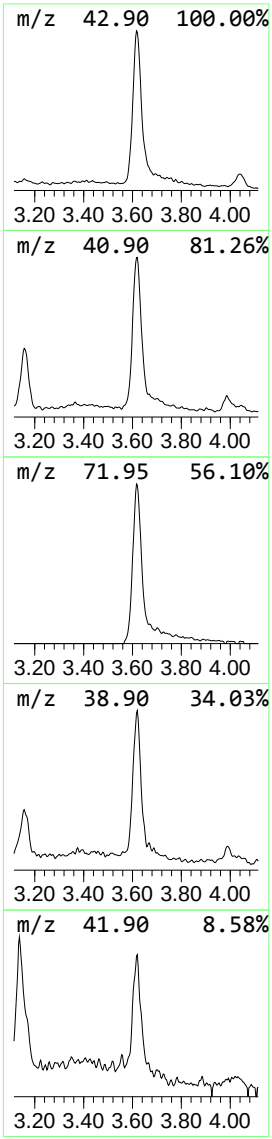
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propanal, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.616	1.38 ug/L	96697	1,4-Difluorobenzene	6.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	90
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	86
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	78
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	64
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

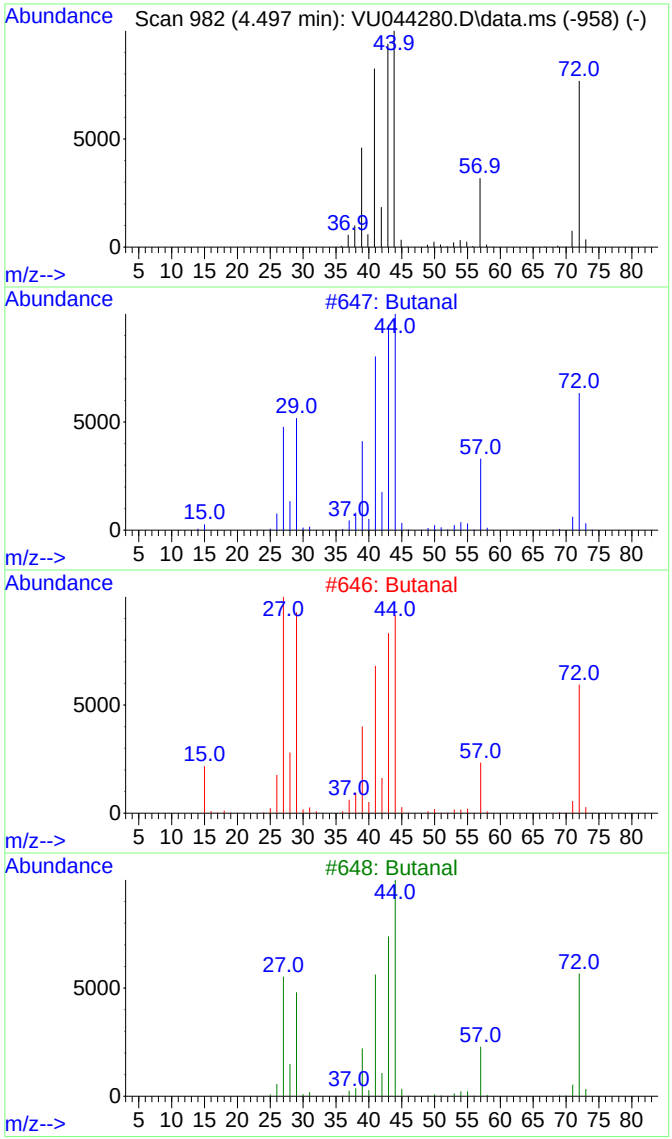
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

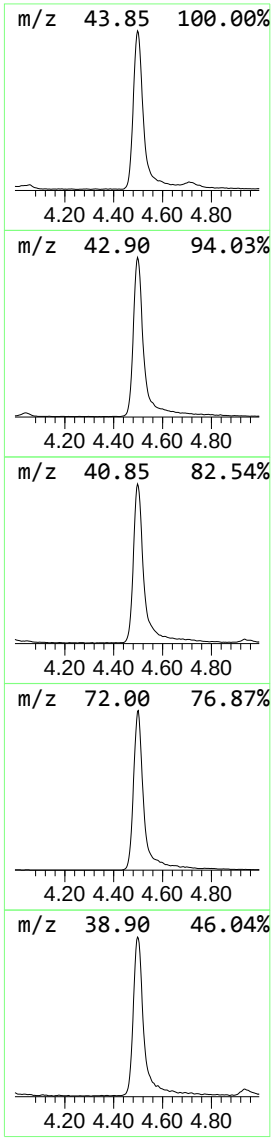
****

Peak Number 2 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.497	14.10 ug/L	990635	1,4-Difluorobenzene	6.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Butanal	72	C4H8O	000123-72-8	91
3	Butanal	72	C4H8O	000123-72-8	72
4	Butanal	72	C4H8O	000123-72-8	72
5	Ethene, ethoxy-	72	C4H8O	000109-92-2	58





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

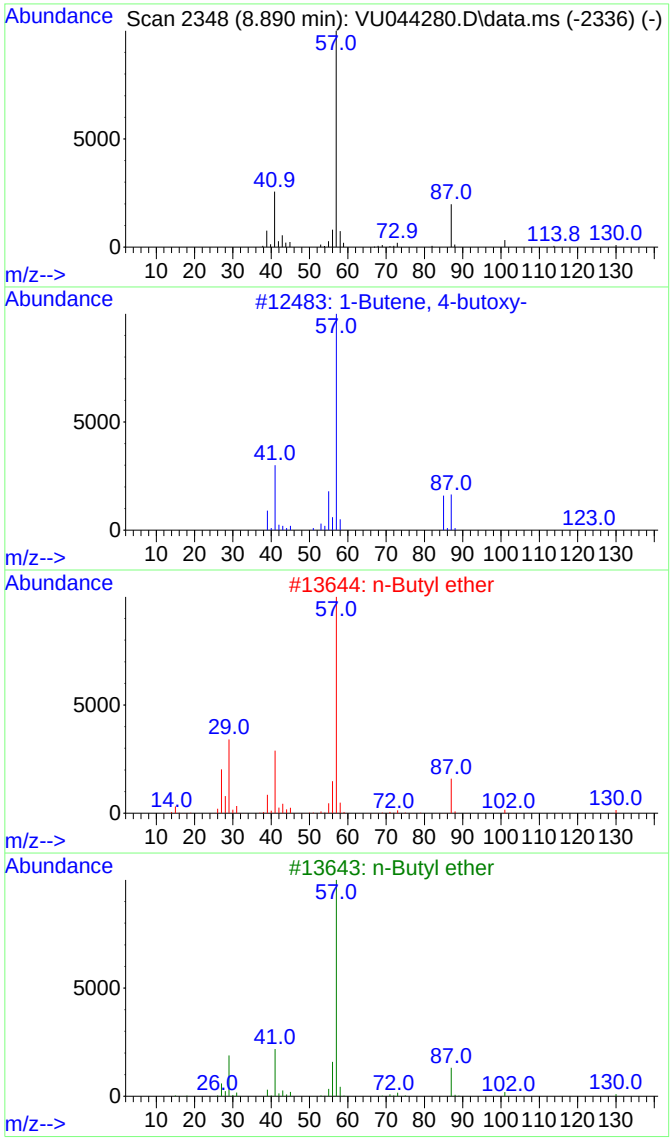
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

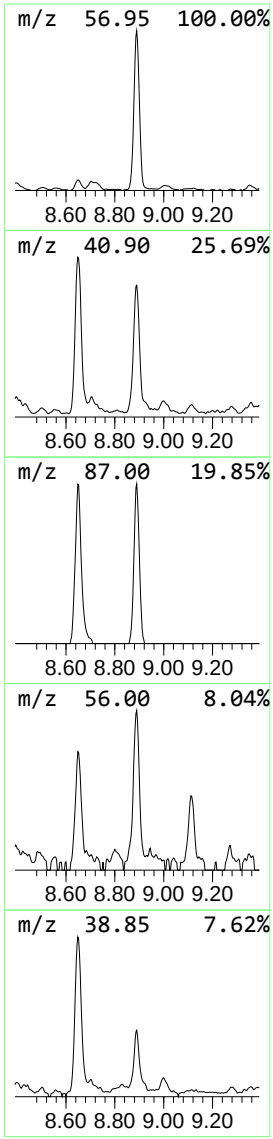
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Butene, 4-butoxy- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.890	0.75 ug/L	83107	Chlorobenzene-d5	9.426

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	64
2	n-Butyl ether	130	C8H18O	000142-96-1	56
3	n-Butyl ether	130	C8H18O	000142-96-1	53
4	Isobutyl ether	130	C8H18O	000628-55-7	50
5	n-Butyl ether	130	C8H18O	000142-96-1	42





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

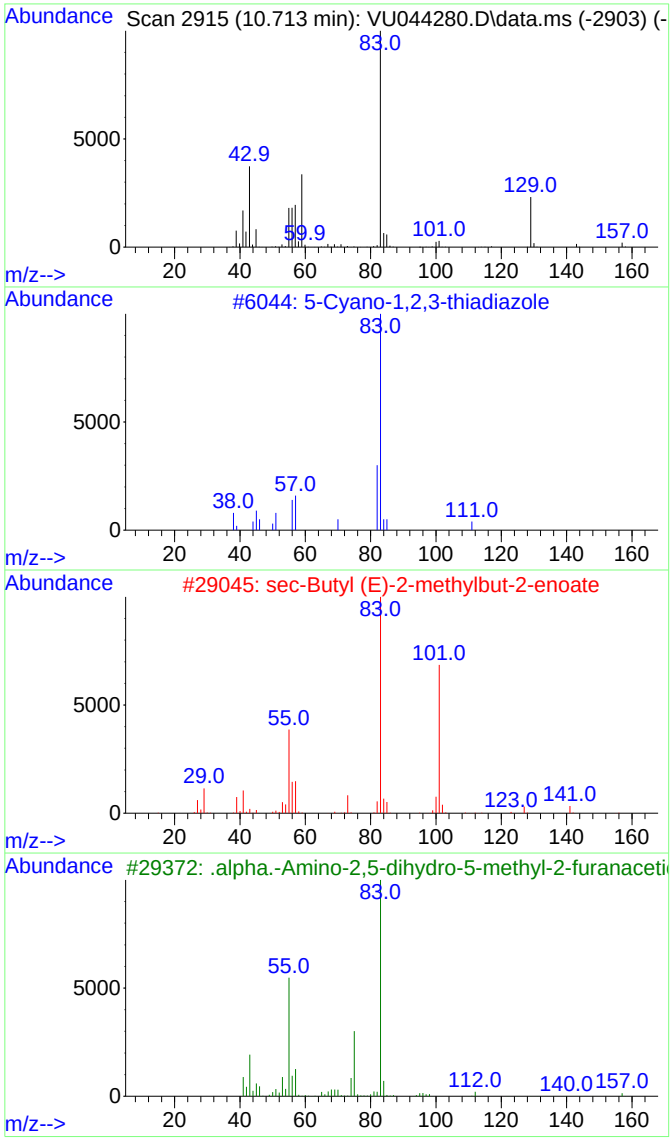
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

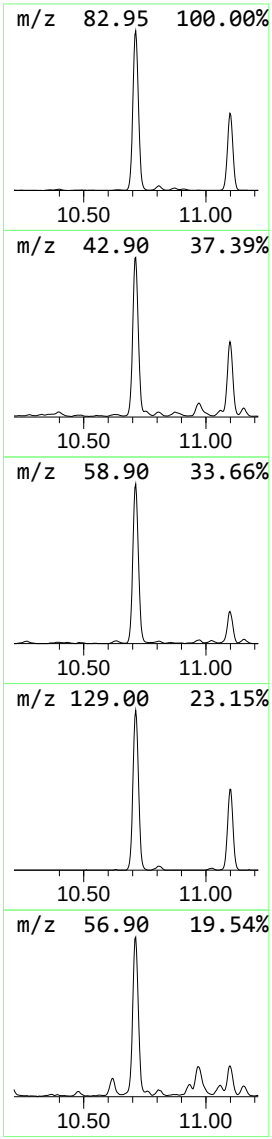
****

Peak Number 5 unknown-01 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.713	0.54 ug/L	844039	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	40
2	sec-Butyl (E)-2-methylbut-2-enoate	156	C9H16O2	1000373-72-7	33
3	.alpha.-Amino-2,5-dihydro-5-meth...	157	C7H11NO3	018455-25-9	33
4	Bis(2-ethylhexyl) hydrogen phosp...	306	C16H35O3P	003658-48-8	28
5	1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	9





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Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

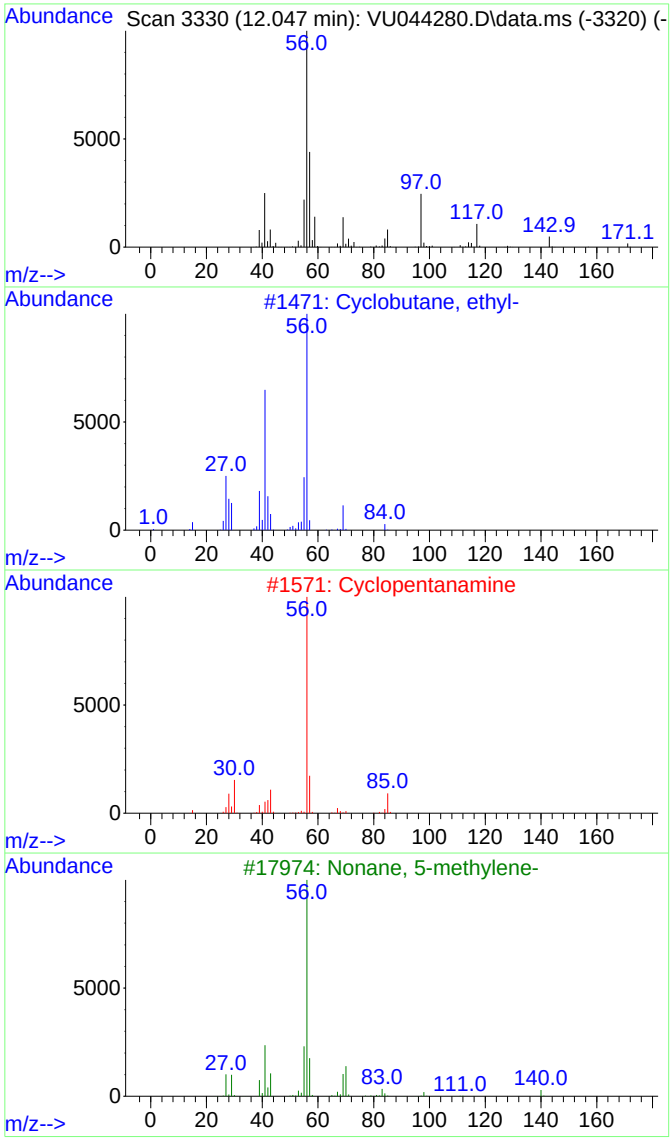
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

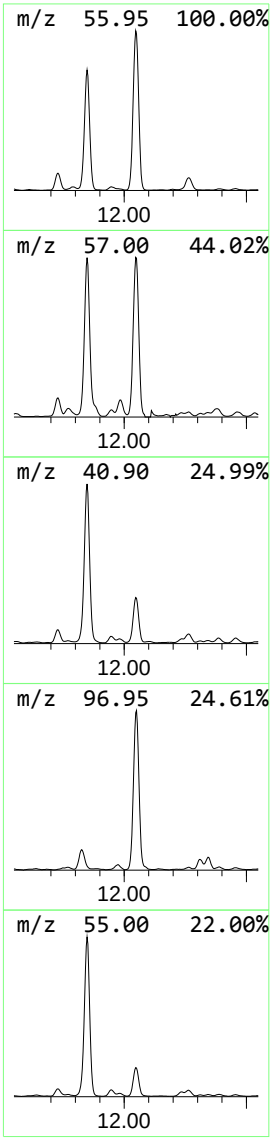
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Cyclic12.047 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.047	0.94 ug/L	1464460	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, ethyl-	84	C6H12	004806-61-5	47
2	Cyclopentanamine	85	C5H11N	001003-03-8	38
3	Nonane, 5-methylene-	140	C10H20	006795-79-5	33
4	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	33
5	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
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Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

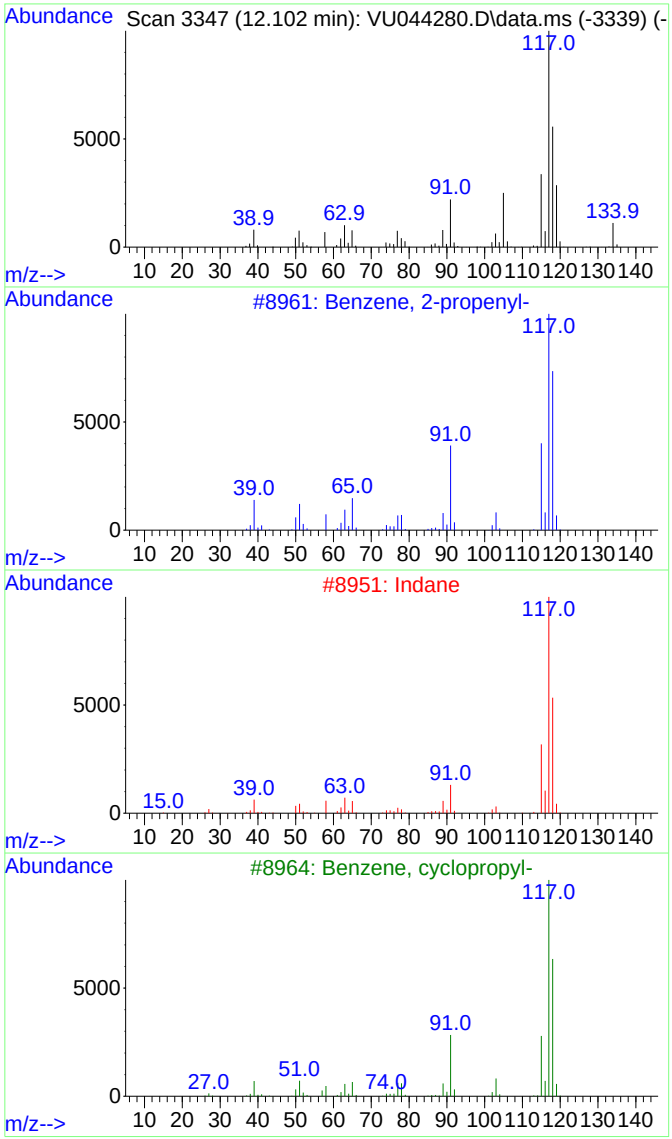
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

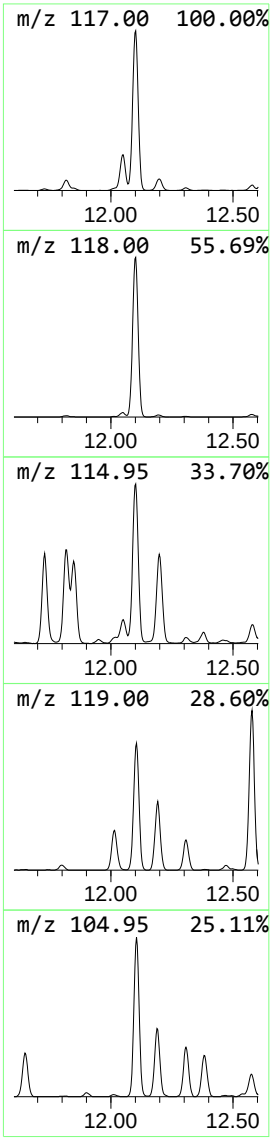
****

Peak Number 7 Benzene, 2-propenyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.102	0.57 ug/L	883723	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
2	Indane	118	C9H10	000496-11-7	64
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	64
5	Benzene, 1-propenyl-	118	C9H10	000637-50-3	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

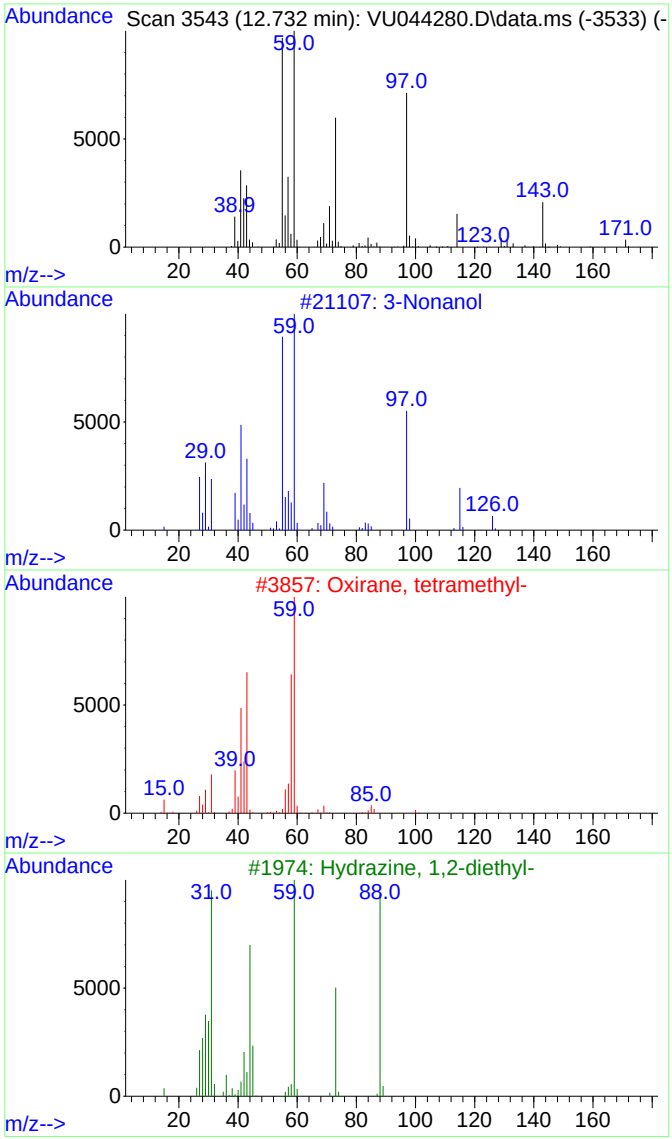
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

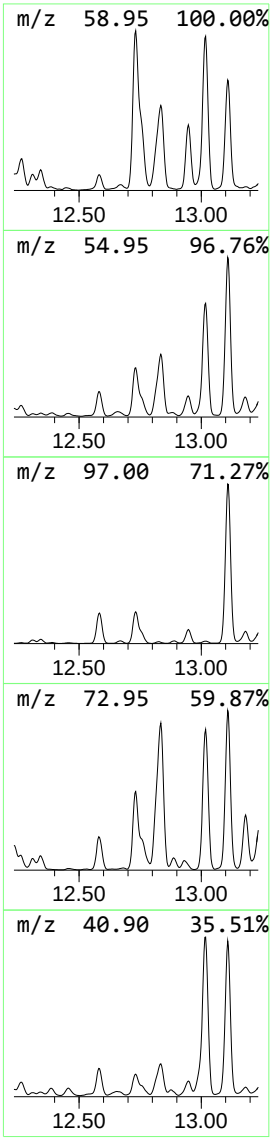
****

Peak Number 8 3-Nonanol Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.732	0.52 ug/L	812212	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Nonanol	144	C9H20O	000624-51-1	50
2	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	35
3	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	32
4	3-Hexanol	102	C6H14O	000623-37-0	32
5	3-Nonanol	144	C9H20O	000624-51-1	32





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

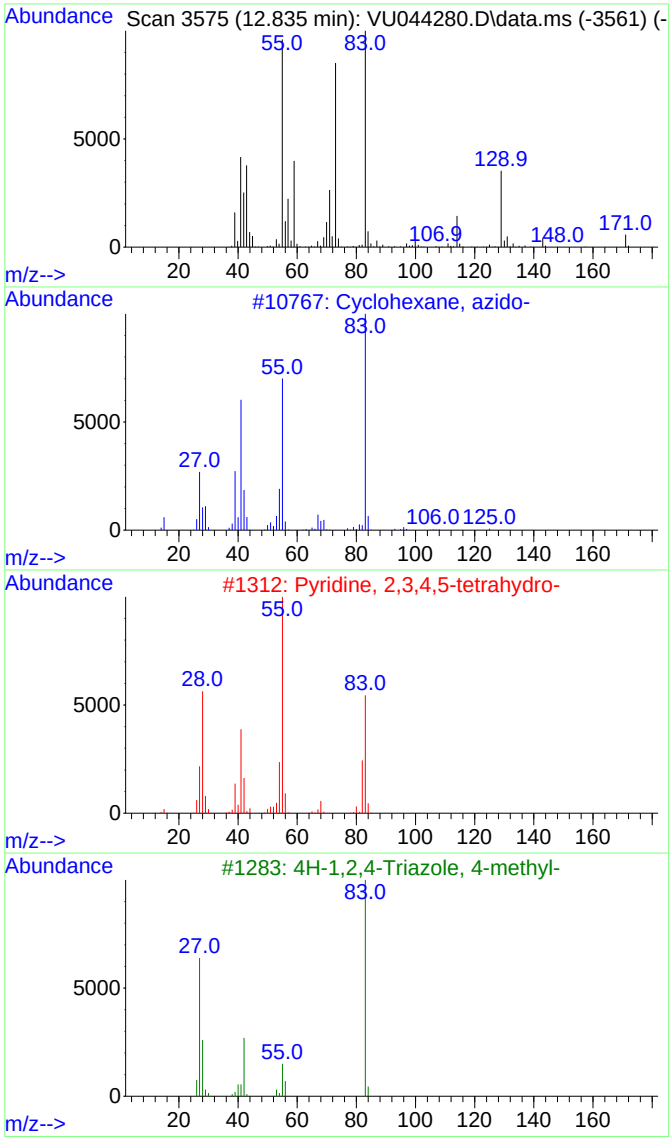
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

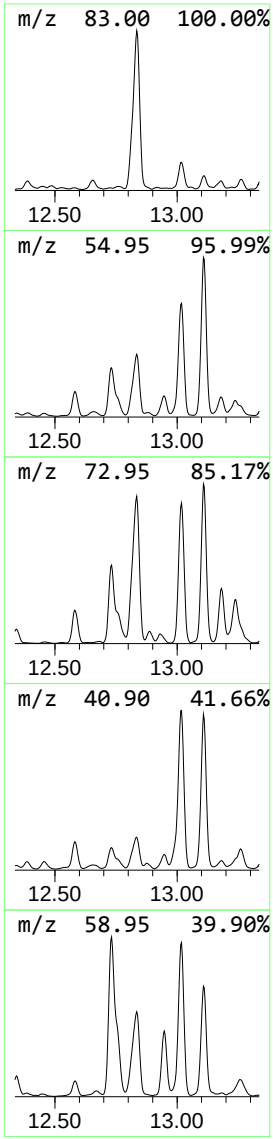
****

Peak Number 9 unknown-02 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.835	0.64 ug/L	997528	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, azido-	125	C6H11N3	019573-22-9	38
2	Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	35
3	4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	27
4	1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	27
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	27





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

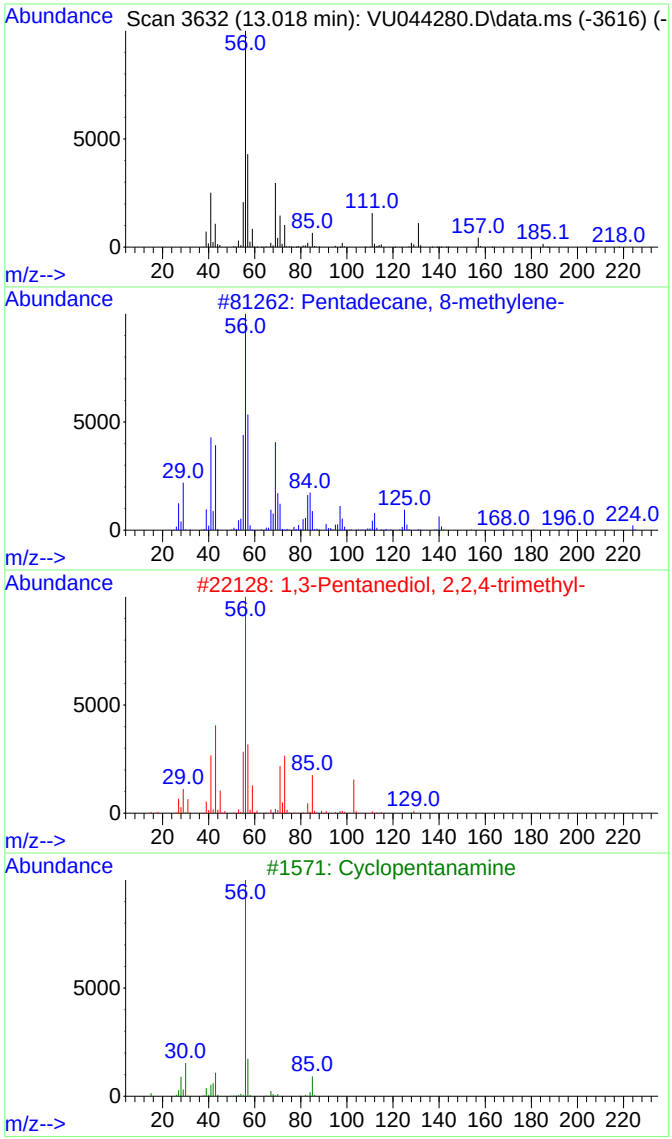
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

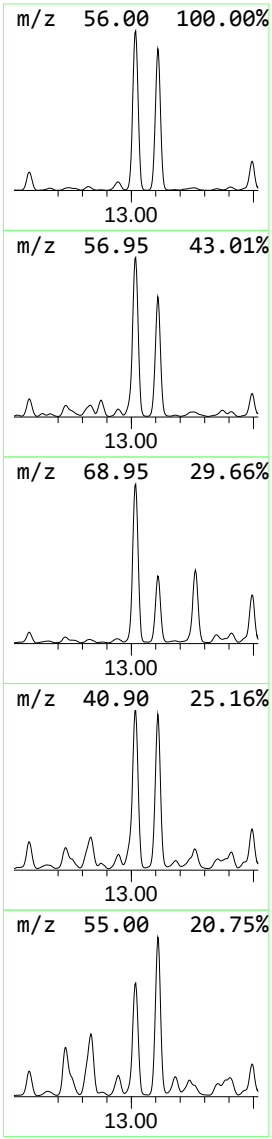
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.018	2.51 ug/L	3887180	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	42
2	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	42
3	Cyclopentanamine	85	C5H11N	001003-03-8	40
4	Cyclopentane, (1,1-dimethylethyl)-	126	C9H18	003875-52-3	38
5	Cyclobutane, 1,2,3,4-tetramethyl-	112	C8H16	069531-57-3	37





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

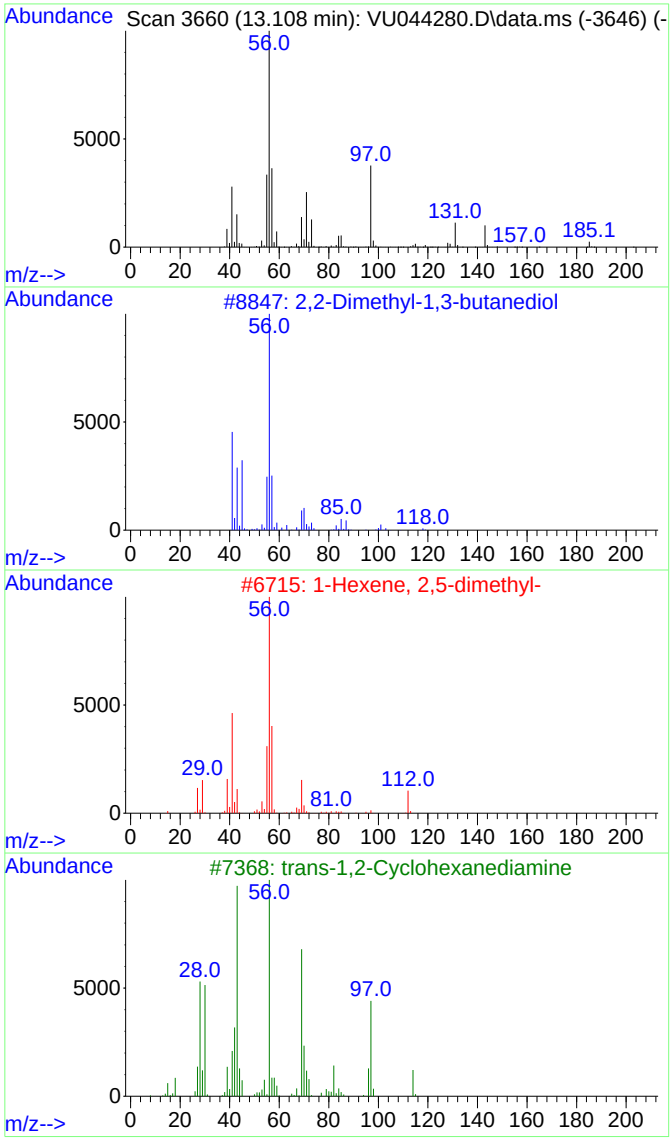
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

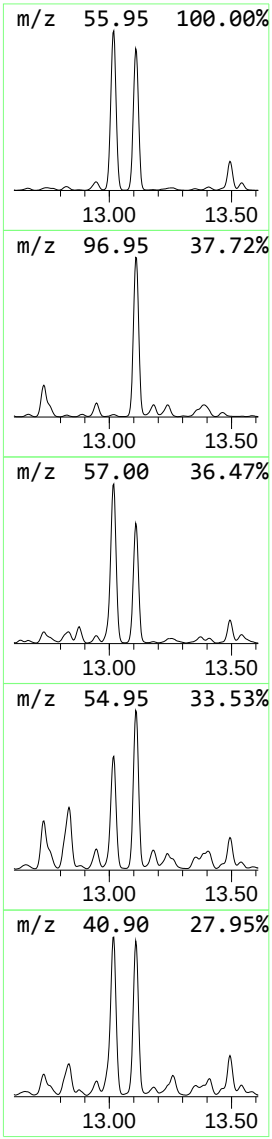
****

Peak Number 11 unknown-03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.108	2.18 ug/L	3377590	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	47
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
3	trans-1,2-Cyclohexanediamine	114	C6H14N2	001121-22-8	33
4	1,2-Cyclohexanediamine	114	C6H14N2	000694-83-7	33
5	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	23





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

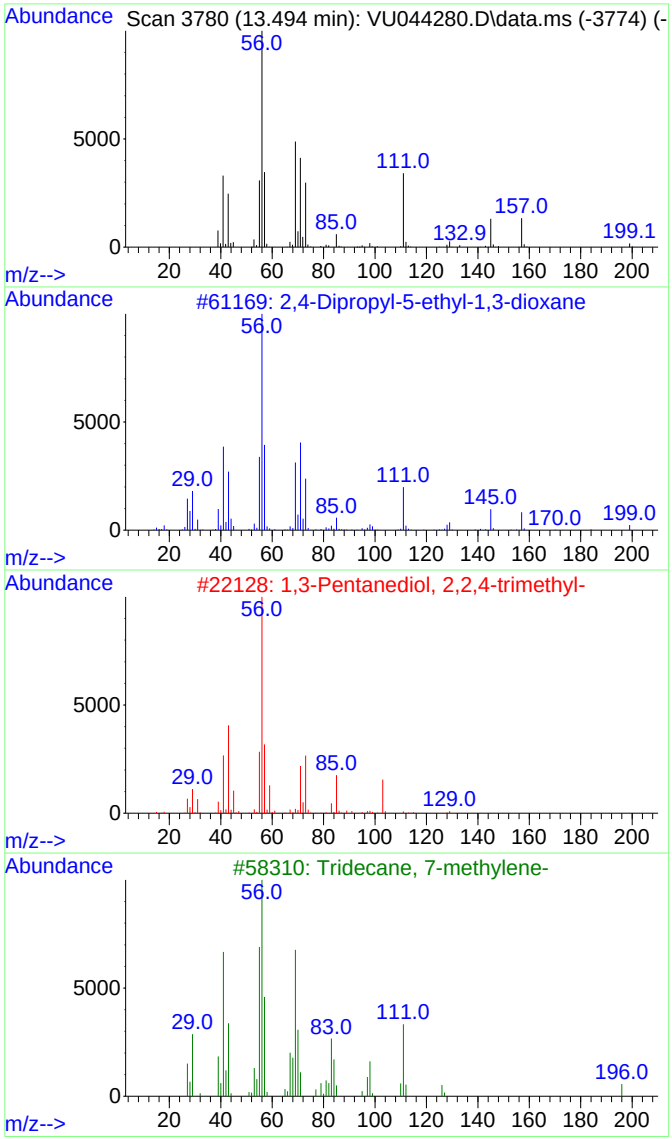
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

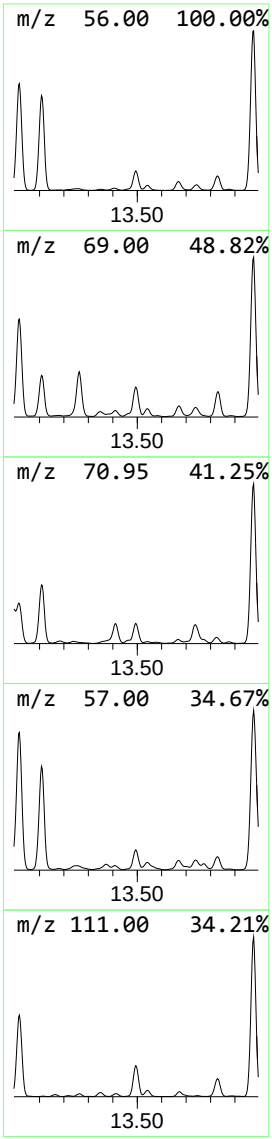
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.494	0.51 ug/L	790645	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	64
2	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	38
3	Tridecane, 7-methylene-	196	C14H28	019780-80-4	28
4	2H-Pyran-2-one, tetrahydro-3,5-d...	128	C7H12O2	003290-57-1	25
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	17





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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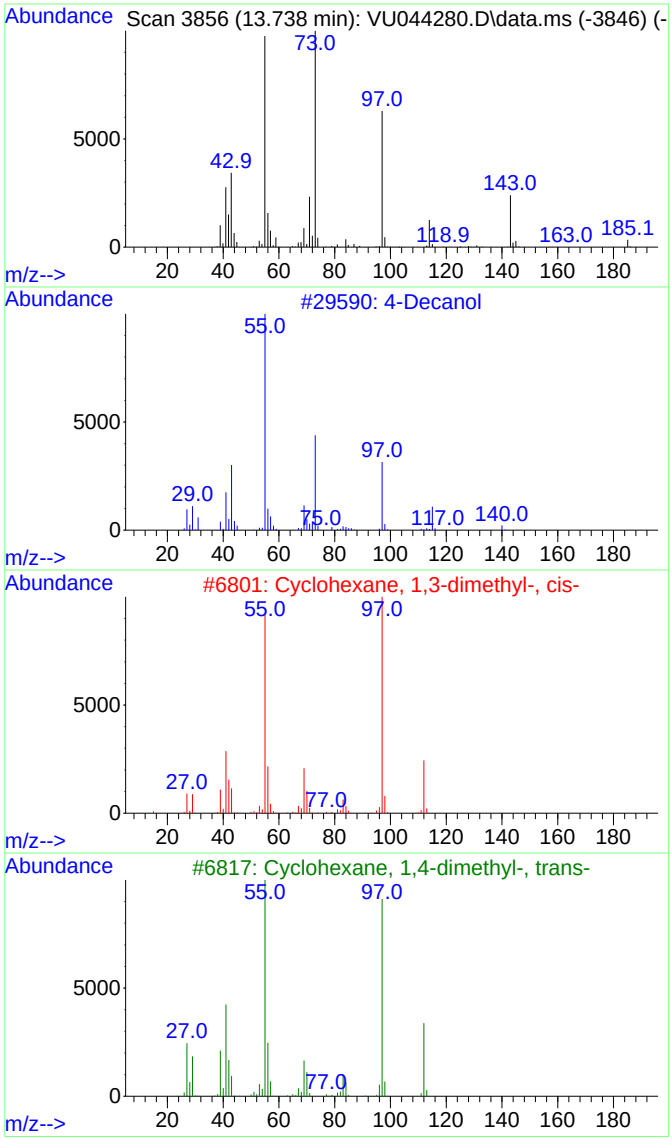
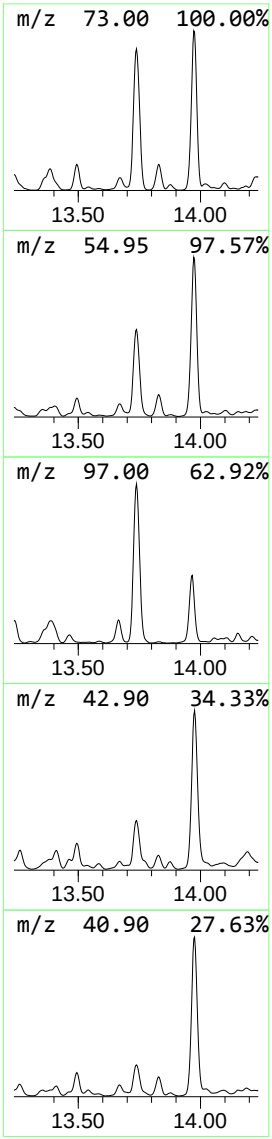
Peak Number 13 unknown-04 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.738	1.09 ug/L	1687090	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Decanol	158	C10H22O	002051-31-2	43
2	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	35
3	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	002207-04-7	27
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	27
5	Sulfurous acid, cyclohexylmethyl...	388	C22H44O3S	1000309-22-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

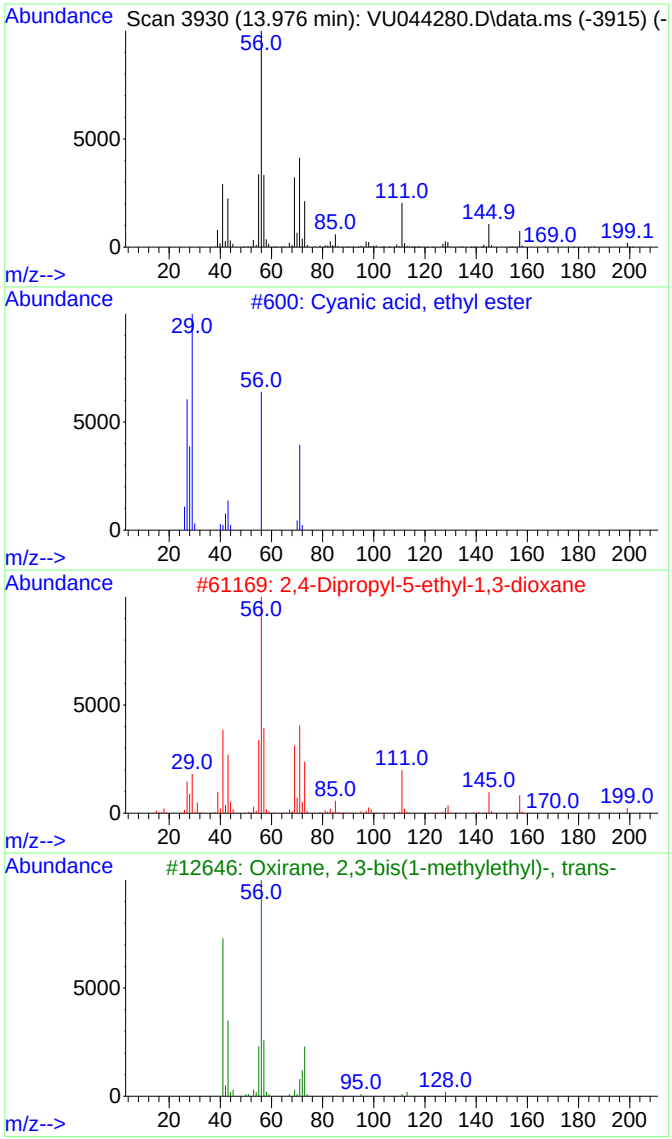
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

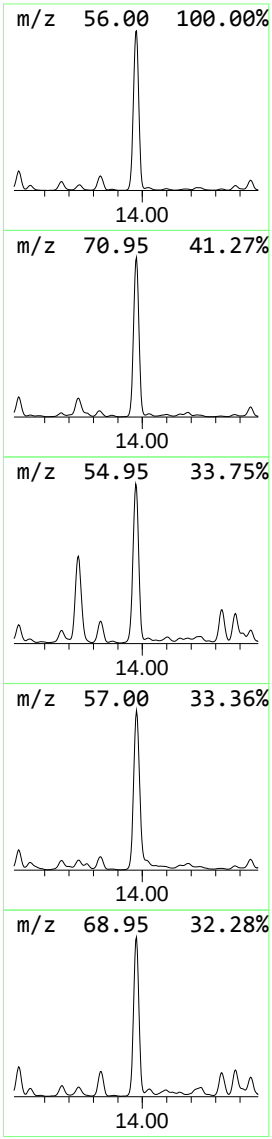
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 Cyanic acid, ethyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.976	4.51 ug/L	6986230	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	52
2	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	47
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37
4	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	33
5	2-Methyl-1-nonene	140	C10H20	002980-71-4	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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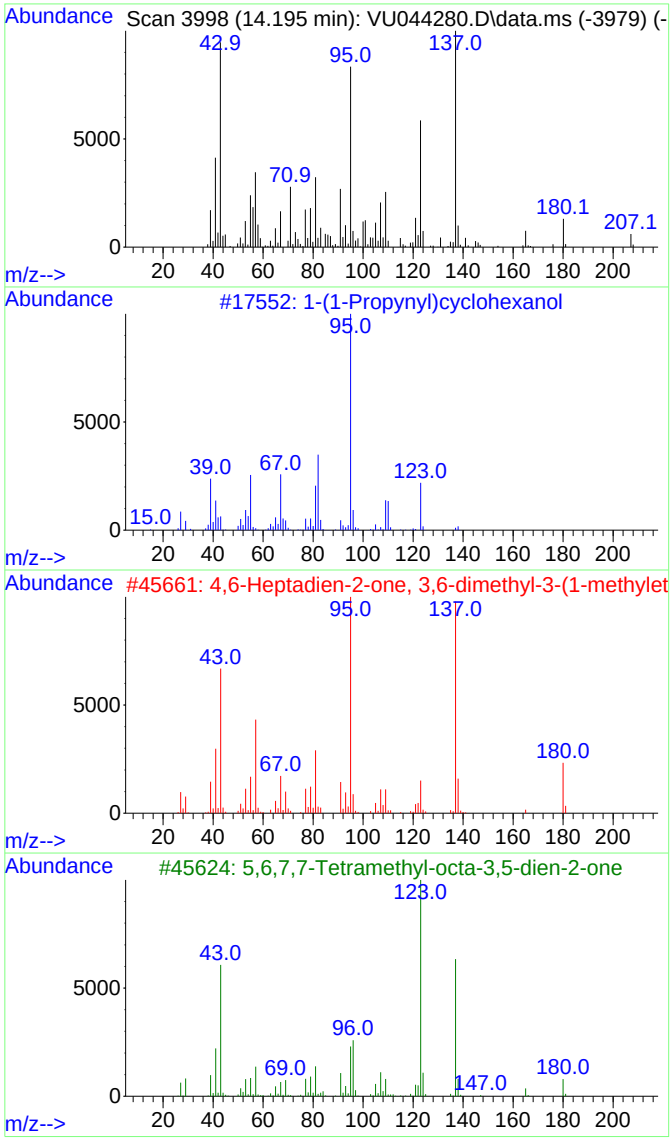
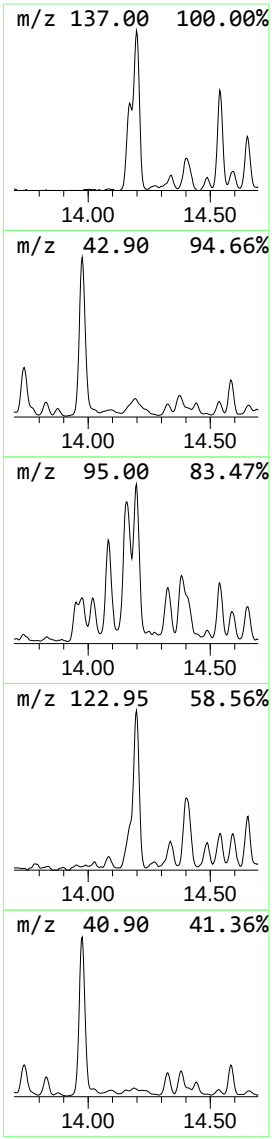
Peak Number 15 unknown-05 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.195	0.53 ug/L	814573	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-Propynyl)cyclohexanol	138	C9H14O	000697-37-0	46
2	4,6-Heptadien-2-one, 3,6-dimethy...	180	C12H20O	077822-50-5	46
3	5,6,7,7-Tetramethyl-octa-3,5-die...	180	C12H20O	1000190-70-9	43
4	2-Pentenoic acid, 3-methyl-5-(2,...	236	C15H24O2	1000196-81-2	38
5	2-Cyclohexen-1-one, 5-bromo-4,4-...	202	C8H11BrO	1000327-26-6	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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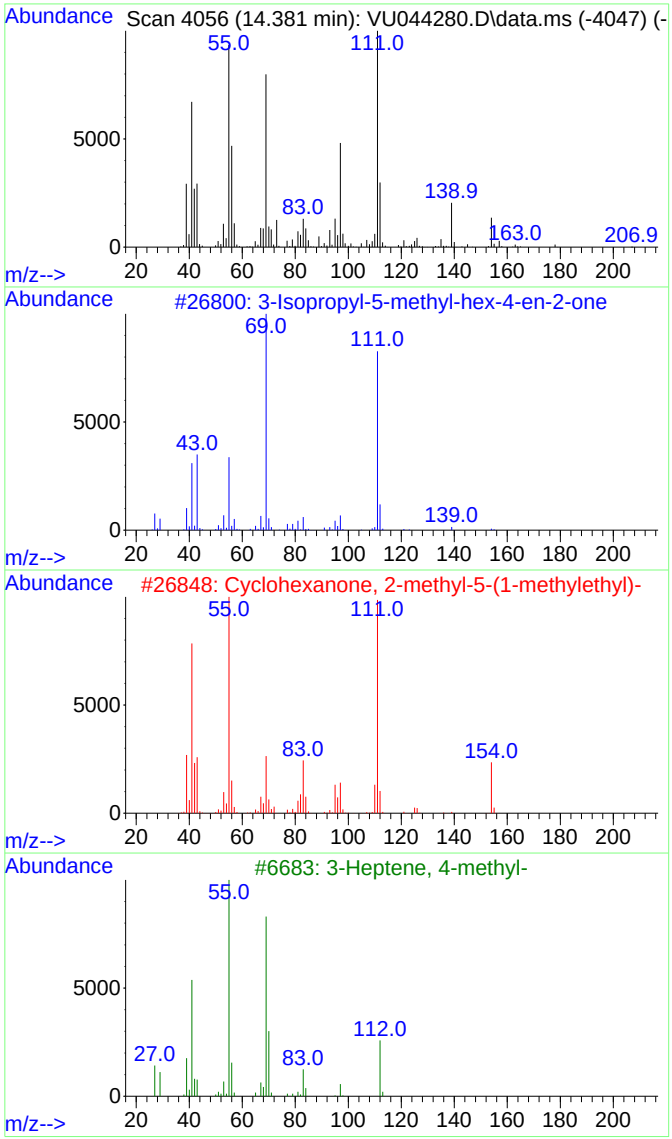
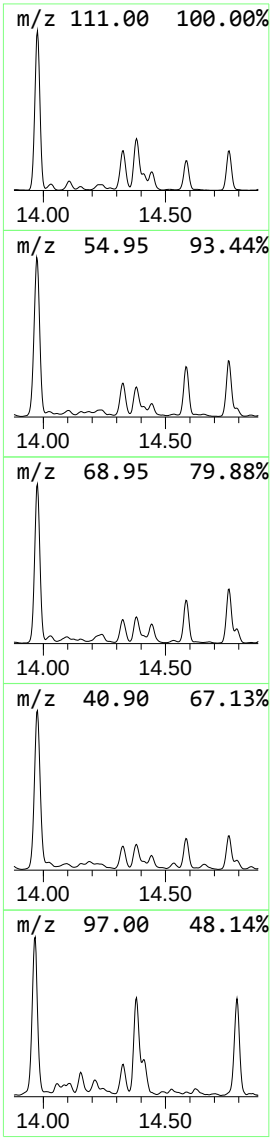
Peak Number 16 unknown-06 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.381	0.65 ug/L	1013270	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Isopropyl-5-methyl-hex-4-en-2-one	154	C10H18O	077142-85-9	49
2	Cyclohexanone, 2-methyl-5-(1-met...	154	C10H18O	059471-80-6	38
3	3-Heptene, 4-methyl-	112	C8H16	004485-16-9	30
4	3-Octene, (E)-	112	C8H16	014919-01-8	25
5	3-Octene, (Z)-	112	C8H16	014850-22-7	25





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Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

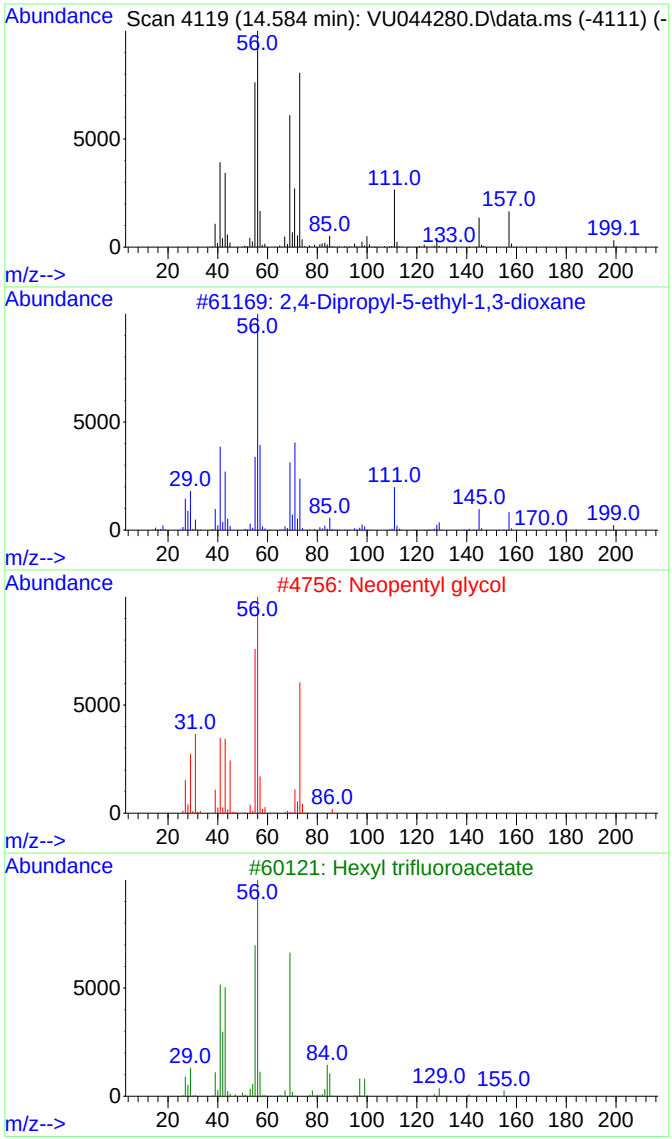
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

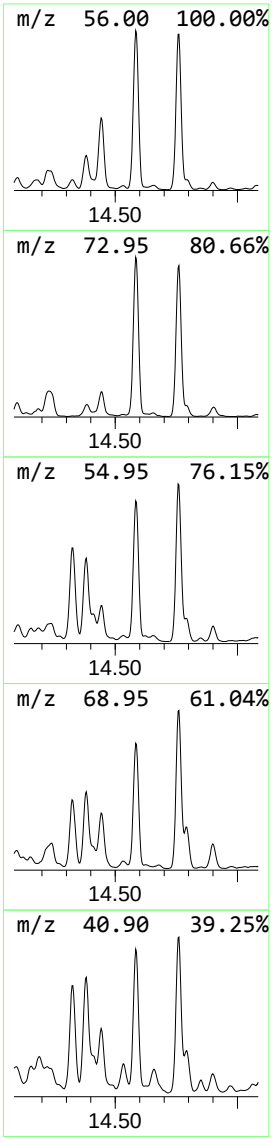
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 unknown-07 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.584	0.72 ug/L	1113850	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	45
2	Neopentyl glycol	104	C5H12O2	000126-30-7	38
3	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	38
4	Neopentyl glycol	104	C5H12O2	000126-30-7	33
5	Nonane, 4-methylene-	140	C10H20	033717-91-8	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

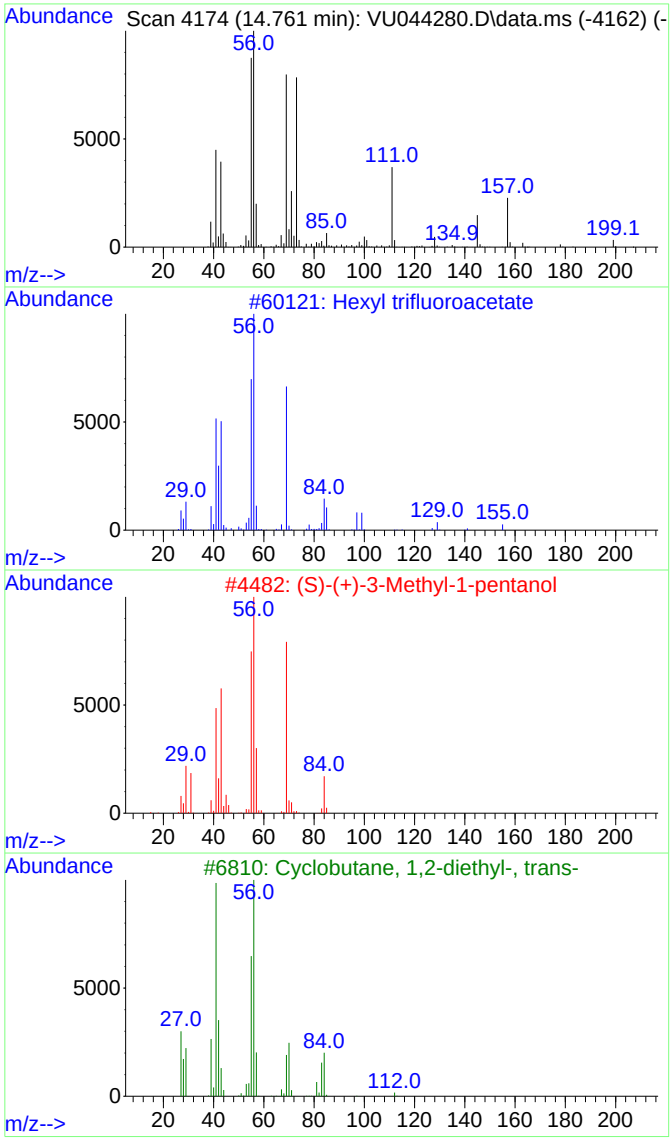
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

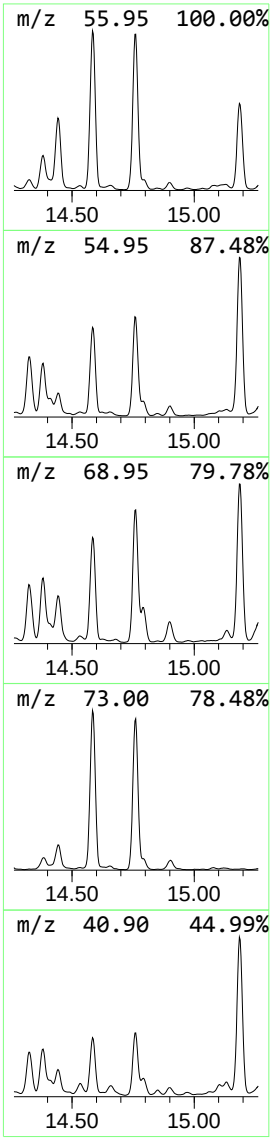
****

Peak Number 18 unknown-08 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.761	0.90 ug/L	1391610	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexyl trifluoroacetate	198	C8H13F3O2	000400-61-3	40
2	(S)-(+)-3-Methyl-1-pentanol	102	C6H14O	042072-39-9	33
3	Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	27
4	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	25
5	Undecanol-4	172	C11H24O	004272-06-4	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

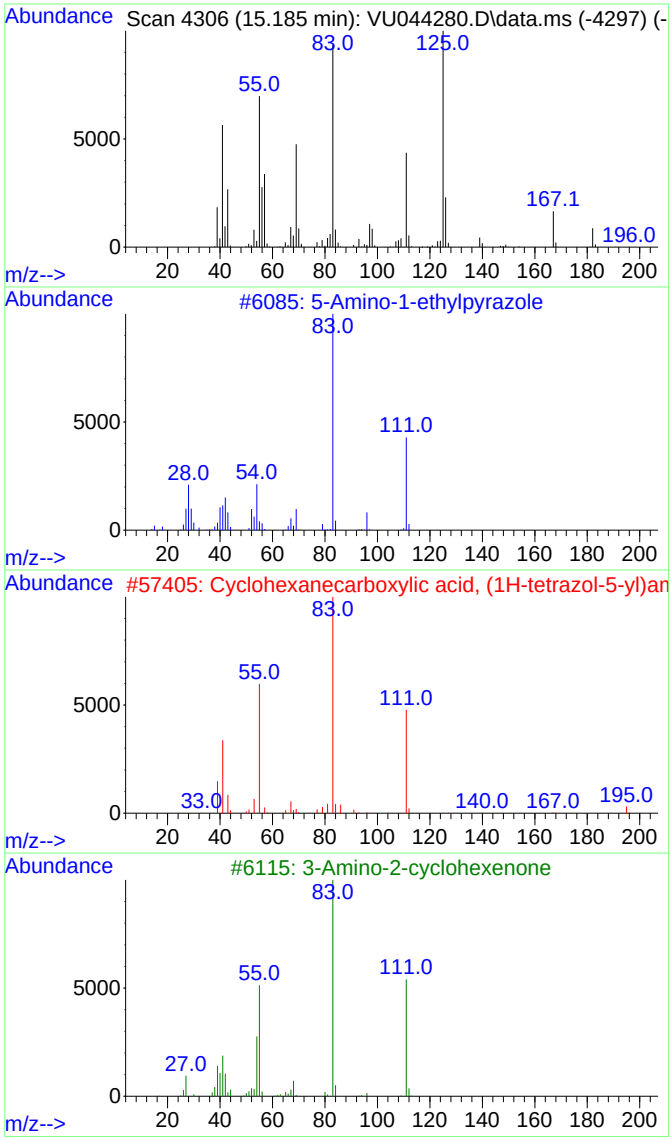
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

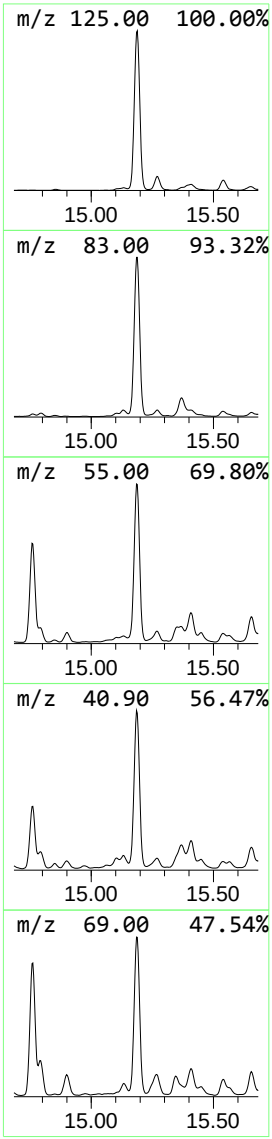
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 unknown-09 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.185	1.85 ug/L	2863780	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	35
2	Cyclohexanecarboxylic acid, (1H-...	195	C8H13N5O	1000310-78-1	35
3	3-Amino-2-cyclohexenone	111	C6H9NO	005220-49-5	35
4	5-Amino-1-ethylpyrazole	111	C5H9N3	003528-58-3	35
5	Cyclohexane, propyl-	126	C9H18	001678-92-8	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

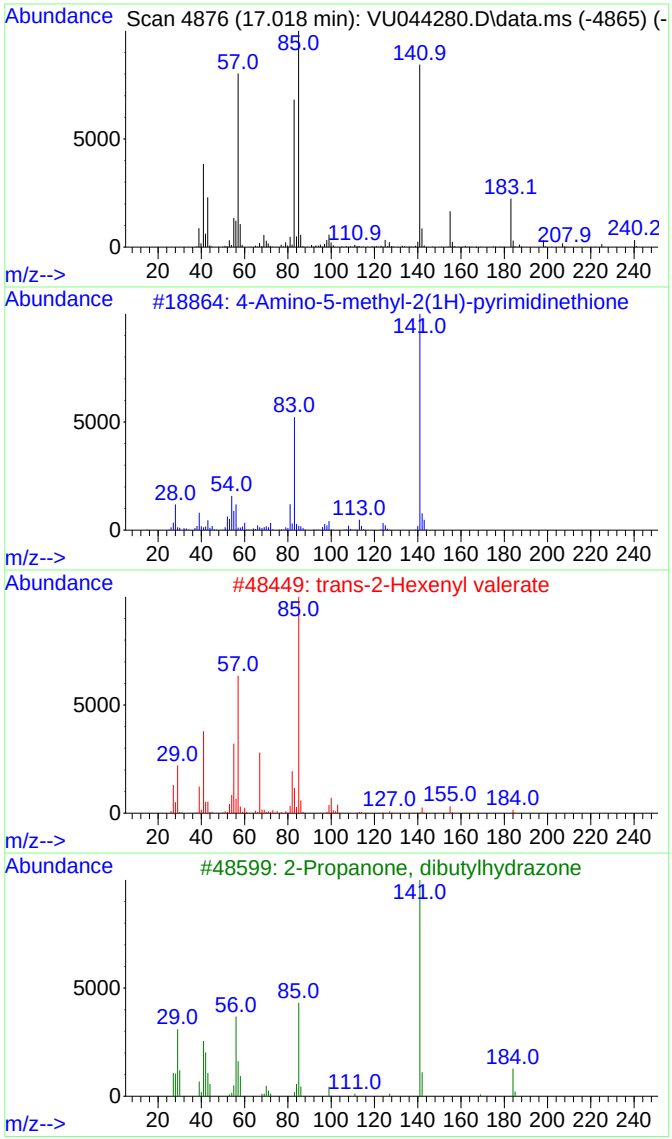
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

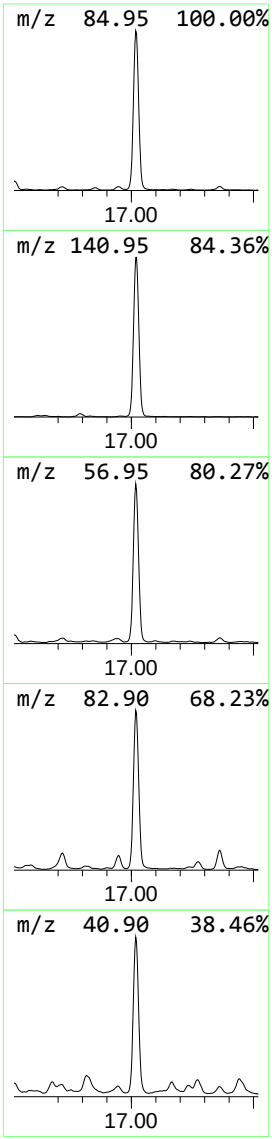
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 unknown-10 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.018	0.64 ug/L	985259	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Amino-5-methyl-2(1H)-pyrimidin...	141	C5H7N3S	007390-56-9	35
2	trans-2-Hexenyl valerate	184	C11H20O2	056922-74-8	35
3	2-Propanone, dibutylhydrazone	184	C11H24N2	067660-52-0	27
4	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	22
5	3,4-Difluorobenzoic acid, 7-tetr...	354	C21H32F2O2	1000338-61-0	22





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044280.D
Acq On : 01 Jul 2021 12:44
Operator : SY/MD
Sample : M2905-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
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
Propanal, 2-met...	3.616	1.4	ug/L	96697	1	6.269	351215	5.0
Butanal	4.497	14.1	ug/L	990635	1	6.269	351215	5.0
1-Butene, 4-but...	8.890	0.8	ug/L	83107	2	9.426	556568	5.0
unknown-01	10.713	0.5	ug/L	844039	3	11.819	7748990	5.0
(DEL) Alkane: C...	12.047	0.9	ug/L	1464460	3	11.819	7748990	5.0
Benzene, 2-prop...	12.102	0.6	ug/L	883723	3	11.819	7748990	5.0
3-Nonanol	12.732	0.5	ug/L	812212	3	11.819	7748990	5.0
unknown-02	12.835	0.6	ug/L	997528	3	11.819	7748990	5.0
(DEL) Alkane: S...	13.018	2.5	ug/L	3887180	3	11.819	7748990	5.0
unknown-03	13.108	2.2	ug/L	3377590	3	11.819	7748990	5.0
2,4-Dipropyl-5-...	13.494	0.5	ug/L	790645	3	11.819	7748990	5.0
unknown-04	13.738	1.1	ug/L	1687090	3	11.819	7748990	5.0
Cyanic acid, et...	13.976	4.5	ug/L	6986230	3	11.819	7748990	5.0
unknown-05	14.195	0.5	ug/L	814573	3	11.819	7748990	5.0
unknown-06	14.381	0.7	ug/L	1013270	3	11.819	7748990	5.0
unknown-07	14.584	0.7	ug/L	1113850	3	11.819	7748990	5.0
unknown-08	14.761	0.9	ug/L	1391610	3	11.819	7748990	5.0
unknown-09	15.185	1.9	ug/L	2863780	3	11.819	7748990	5.0
unknown-10	17.018	0.6	ug/L	985259	3	11.819	7748990	5.0