LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

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: VU044299.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	94	rBV3	46580	64158	3.40%	0.792%
2	1.871	159	165	172	rBV	18224	23289	1.23%	0.288%
3	1.919	173	180	191	rVB	44359	59509	3.15%	0.735%
4	2.569	370	382	401	rVB2	81193	138953	7.36%	1.716%
5	3.359	614	628	647	rBV2	40484	80621	4.27%	0.996%
6	4.462	956	971	985	rBV3	10416	27211	1.44%	0.336%
7	4.675	1015	1037	1079	rBV2	789341	1886892	100.00%	23.299%
8	5.073	1145	1161	1181	rBV	78728	177998	9.43%	2.198%
9	5.732	1345	1366	1376	rBV2	165586	426554	22.61%	5.267%
10	6.256	1515	1529	1549	rBV	162086	303796	16.10%	3.751%
11	6.549	1607	1620	1636	rBV2	105222	196455	10.41%	2.426%
12	6.700	1653	1667	1682	rBV	104253	203663	10.79%	2.515%
13	7.572	1926	1938	1954	rBV2	54977	97921	5.19%	1.209%
14	7.903	2025	2041	2056	rBV	204885	361401	19.15%	4.463%
15	8.186	2117	2129	2142	rBV	34835	59318	3.14%	0.732%
16	8.645	2256	2272	2305	rBV	263092	535771	28.39%	6.616%
17	9.424	2500	2514	2518	rBV	230573	364148	19.30%	4.497%
18	10.764	2919	2931	2942	rBV	86172	136643	7.24%	1.687%
19	11.565	3164	3180	3190	rBV2	13144	21961	1.16%	0.271%
20	11.819	3247	3259	3281	rVB2	262830	520789	27.60%	6.431%
21	12.202	3362	3378	3400	rVB3	253080	522202	27.68%	6.448%
22	12.716	3523	3538	3549	rBV6	18573	32259	1.71%	0.398%
23	13.015	3618	3631	3645	rVB3	11244	20579	1.09%	0.254%
24	13.108	3649	3660	3674	rVB3	13619	22410	1.19%	0.277%
25	13.729	3841	3853	3860	rBV3	12488	19776	1.05%	0.244%
26	13.822	3874	3882	3897	rVB6	13431	26149	1.39%	0.323%
27	13.980	3920	3931	3963	rVB5	108885	252999	13.41%	3.124%
28	14.185	3980	3995	4010	rBV2	218226	367188	19.46%	4.534%
29	14.314	4025	4035	4048	rBV	128080	186775	9.90%	2.306%
30	14.398	4050	4061	4069	rVB10	13469	29160	1.55%	0.360%
31	14.459	4070	4080	4097	rBV	91233	147900	7.84%	1.826%
32	14.539	4097	4105	4111	rBV6	13993	23007	1.22%	0.284%
33	14.584	4111	4119	4133	rVB2	81645	125710	6.66%	1.552%
34	14.658	4133	4142	4152	rBV9	13926	28153	1.49%	0.348%
35	14.761	4165	4174	4183	rVB2	80748	114619	6.07%	1.415%
36	14.848	4191	4201	4211	rBV	150206	220458	11.68%	2.722%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

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	14.957	4225	4235	4248	rVB5	22264	37567	1.99%	0.464%
38	15.189	4299	4307	4326	rVV6	22963	53354	2.83%	0.659%
39	16.880	4822	4833	4845	rBV	50460	81310	4.31%	1.004%
40	17.018	4867	4876	4888	rBV	36105	56589	3.00%	0.699%
41	17.359	4974	4982	4994	rBV2	14384	23552	1.25%	0.291%
42	17.552	5033	5042	5053	rVB	12682	19691	1.04%	0.243%

Sum of corrected areas: 8098458

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Acq On : 02 Jul 2021 13:20
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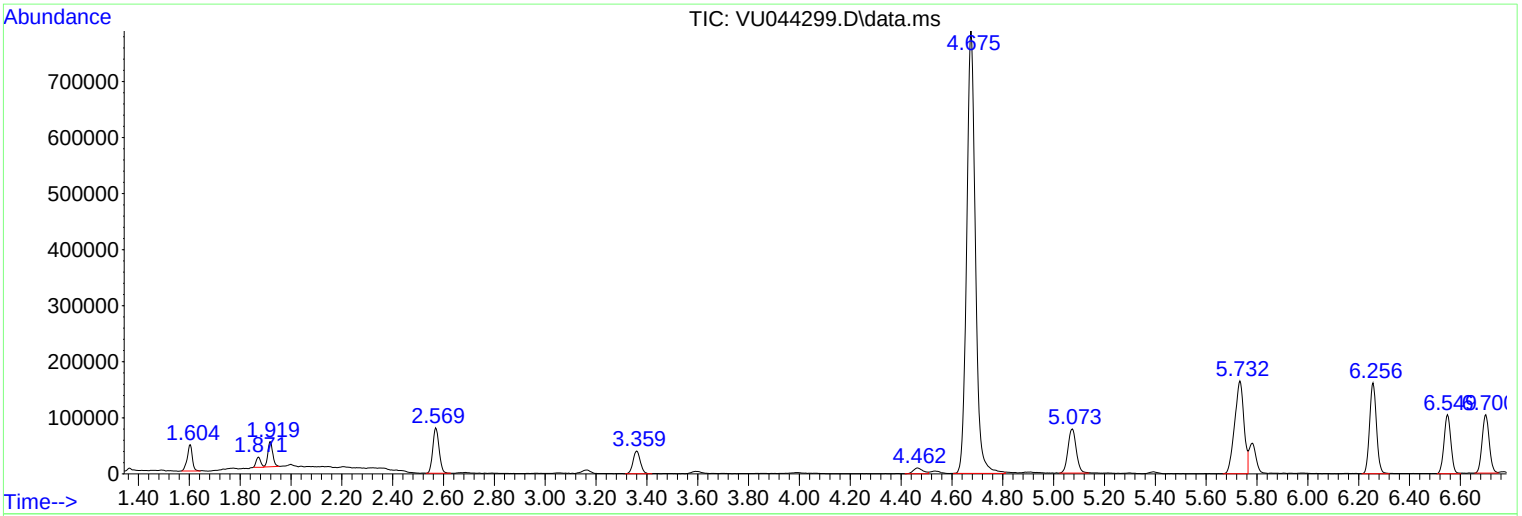
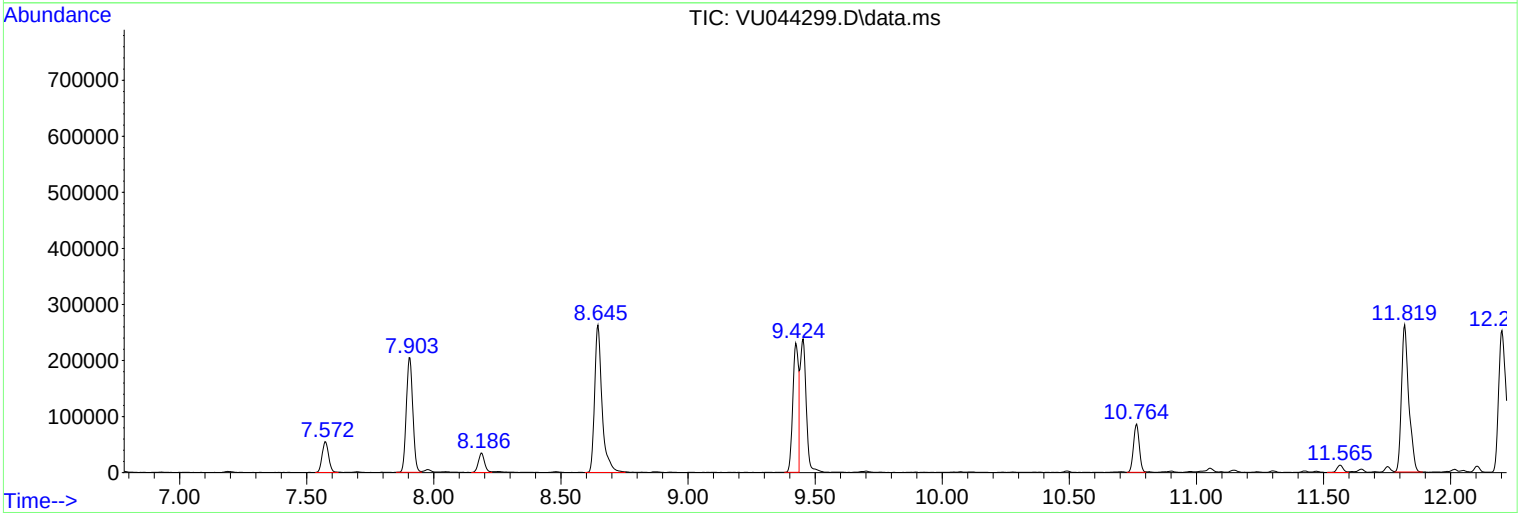
ALS Vial : 9 Sample Multiplier: 1

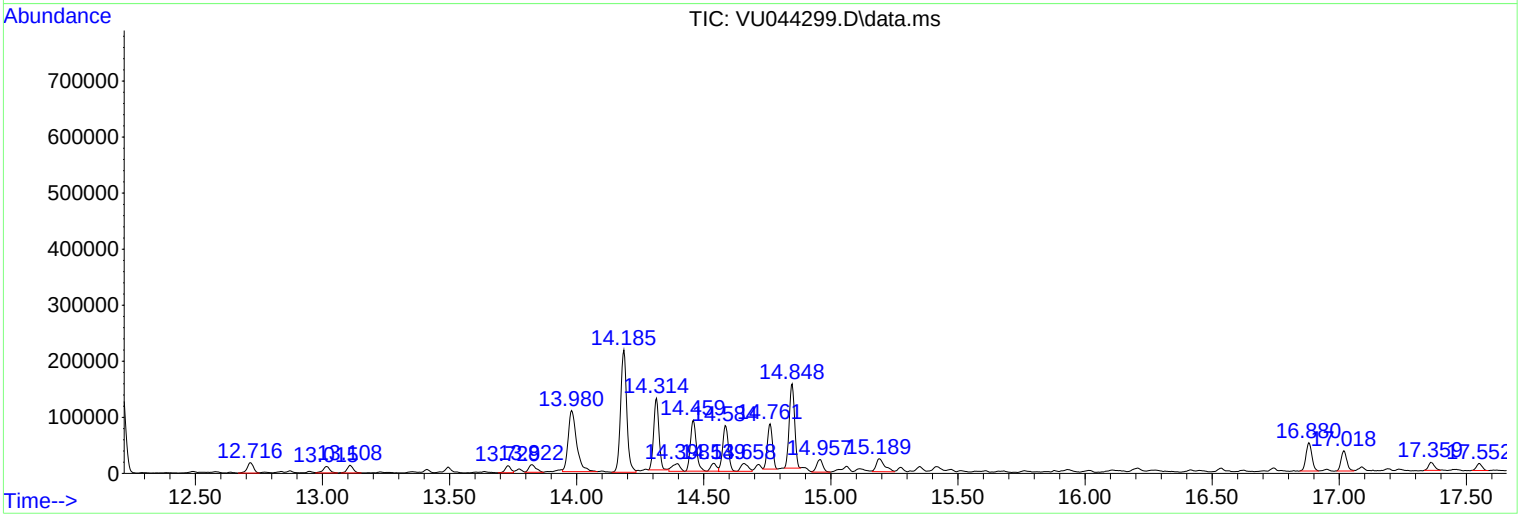
Instrument :
MSVOA_U
ClientSampleId :
DBK29

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\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

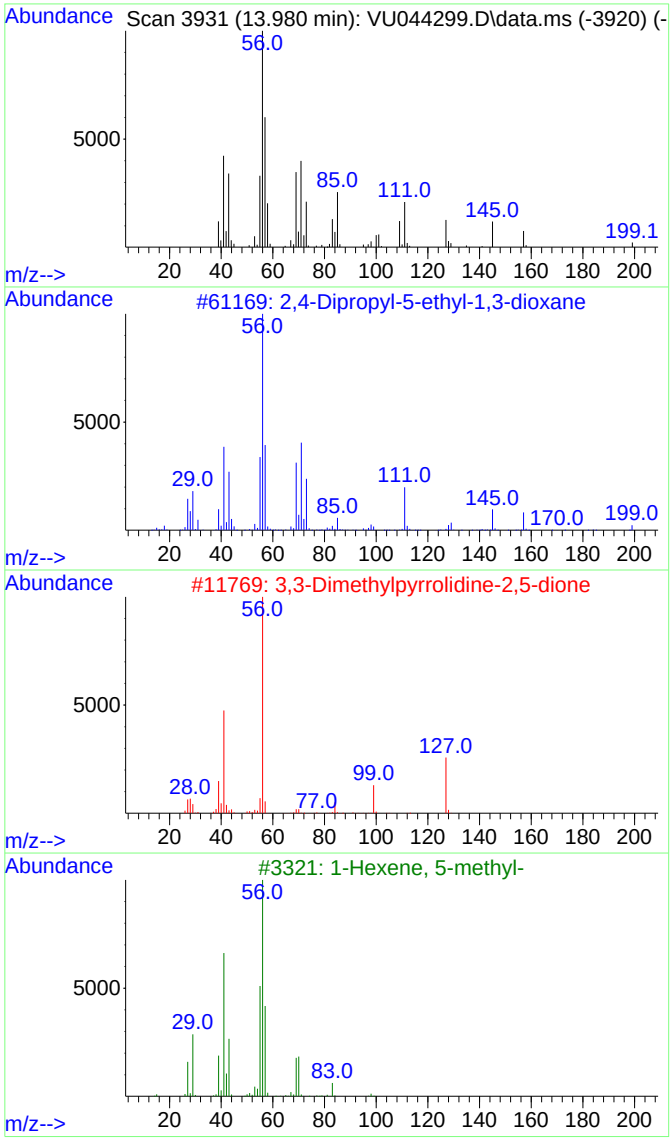
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

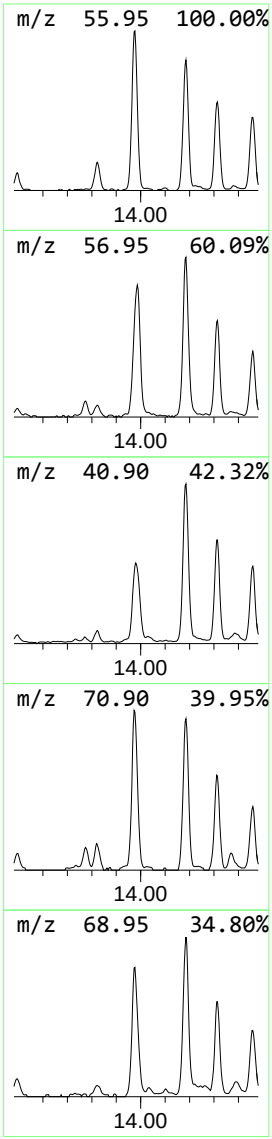
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	2.43 ug/L	252999	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	59
2	3,3-Dimethylpyrrolidine-2,5-dione	127	C6H9NO2	003437-29-4	25
3	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	22
4	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	22
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

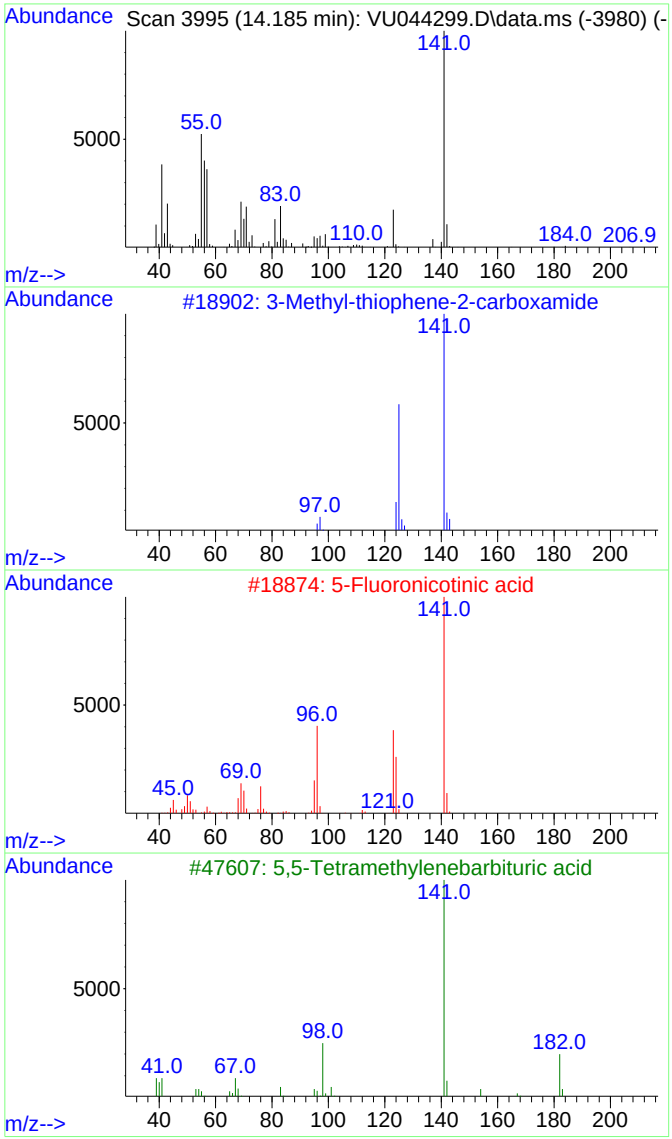
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

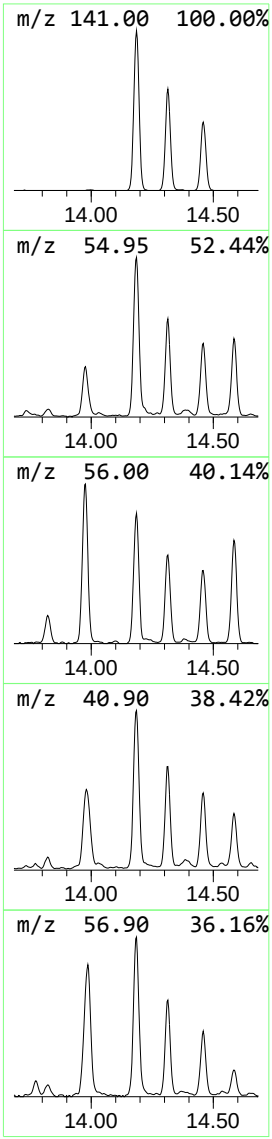
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-Methyl-thiophene-2-carbox... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.185	3.53 ug/L	367188	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-thiophene-2-carboxamide	141	C6H7NOS	076655-99-7	64
2	5-Fluoronicotinic acid	141	C6H4FNO2	000402-66-4	46
3	5,5-Tetramethylenebarbituric acid	182	C8H10N2O3	1000306-49-5	43
4	2,6-Difluorobenzoic acid, 2-meth...	214	C11H12F2O2	1000293-47-5	42
5	4-Amino-5-methyl-2(1H)-pyrimidin...	141	C5H7N3S	007390-56-9	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

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

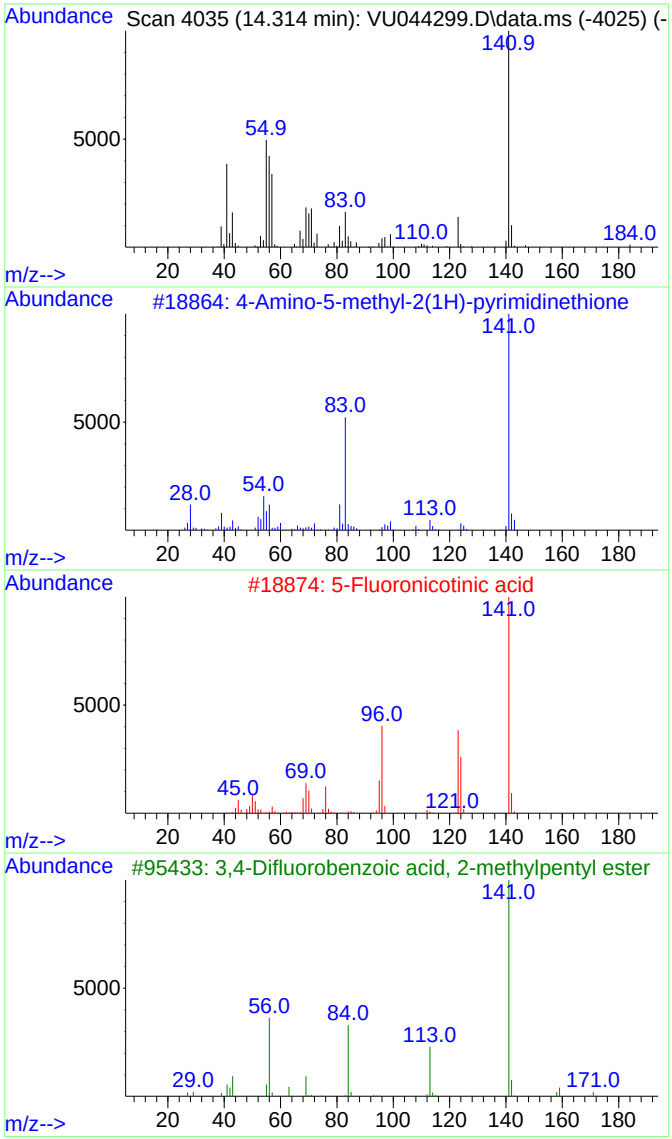
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

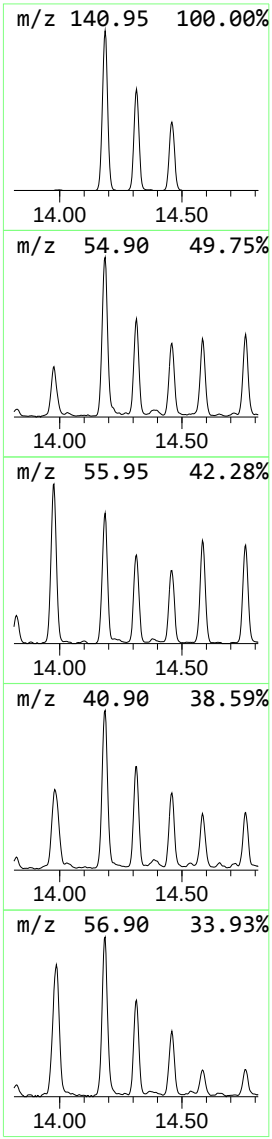
****

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.314	1.79 ug/L	186775	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	49
2	5-Fluoronicotinic acid	141	C6H4FNO2	000402-66-4	47
3	3,4-Difluorobenzoic acid, 2-meth...	242	C13H16F2O2	1000357-31-6	45
4	3,4-Difluorobenzoic acid, nonyl ...	284	C16H22F2O2	1000338-86-5	42
5	Silane, trimethyl-2-thienyl-	156	C7H12SSi	018245-28-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

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

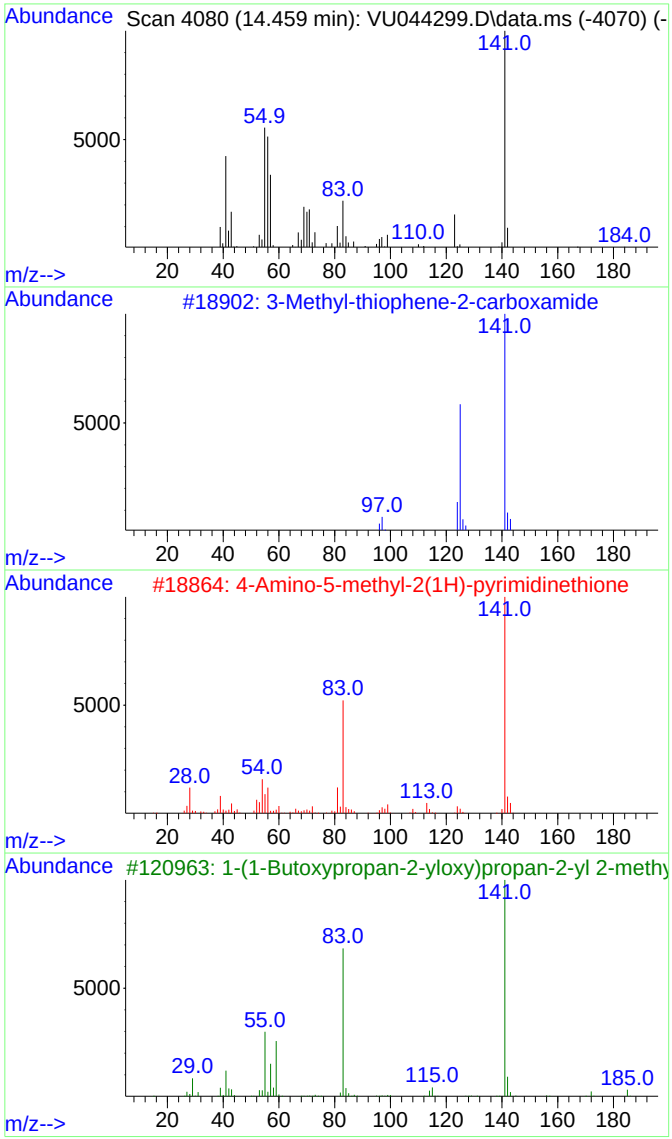
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

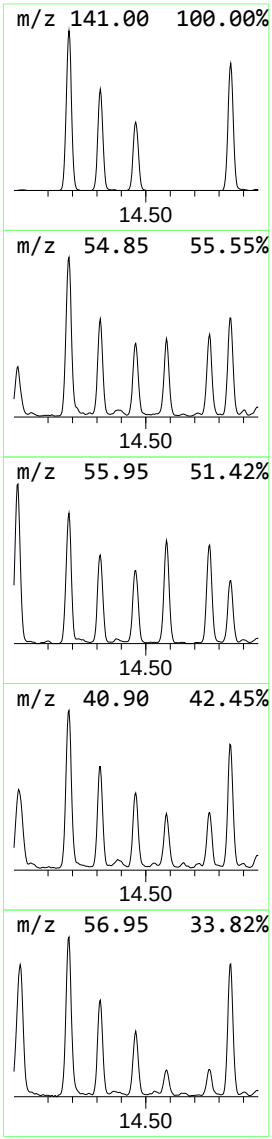
****

Peak Number 5 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.459	1.42 ug/L	147900	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methyl-thiophene-2-carboxamide	141	C6H7NOS	076655-99-7	72
2	4-Amino-5-methyl-2(1H)-pyrimidin...	141	C5H7N3S	007390-56-9	47
3	1-(1-Butoxypropan-2-yloxy)propan...	272	C15H28O4	1000367-11-0	47
4	Nonanoic acid, 2-methylpentyl ester	242	C15H30O2	1000360-66-6	42
5	5-Fluoronicotinic acid	141	C6H4FNO2	000402-66-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

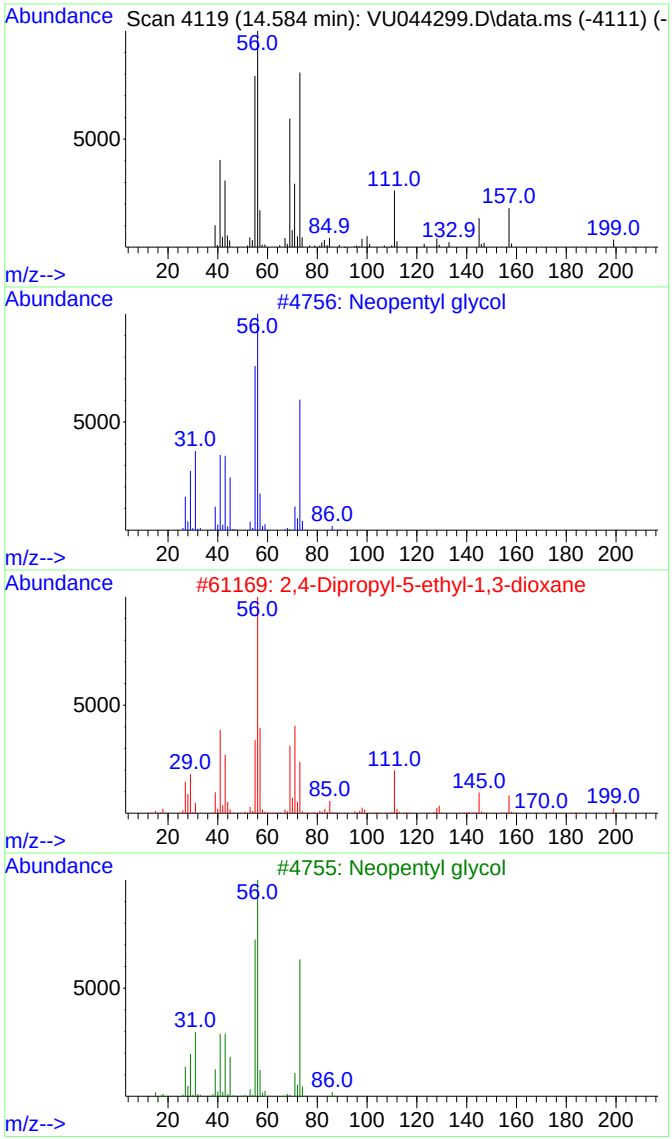
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

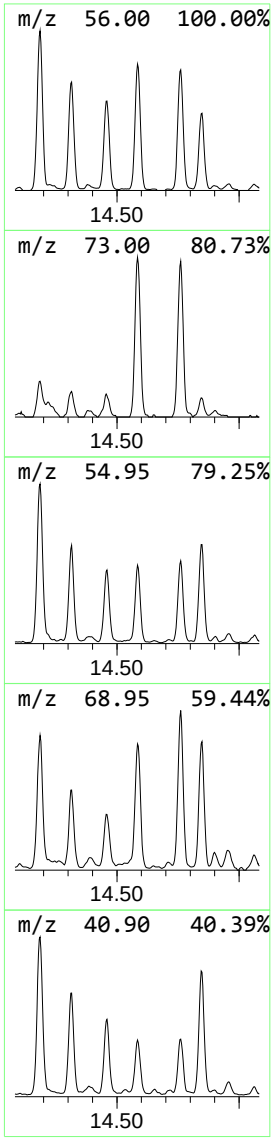
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Neopentyl glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.584	1.21 ug/L	125710	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neopentyl glycol	104	C5H12O2	000126-30-7	50
2	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	45
3	Neopentyl glycol	104	C5H12O2	000126-30-7	40
4	Nonane, 4-methylene-	140	C10H20	033717-91-8	38
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37





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Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

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

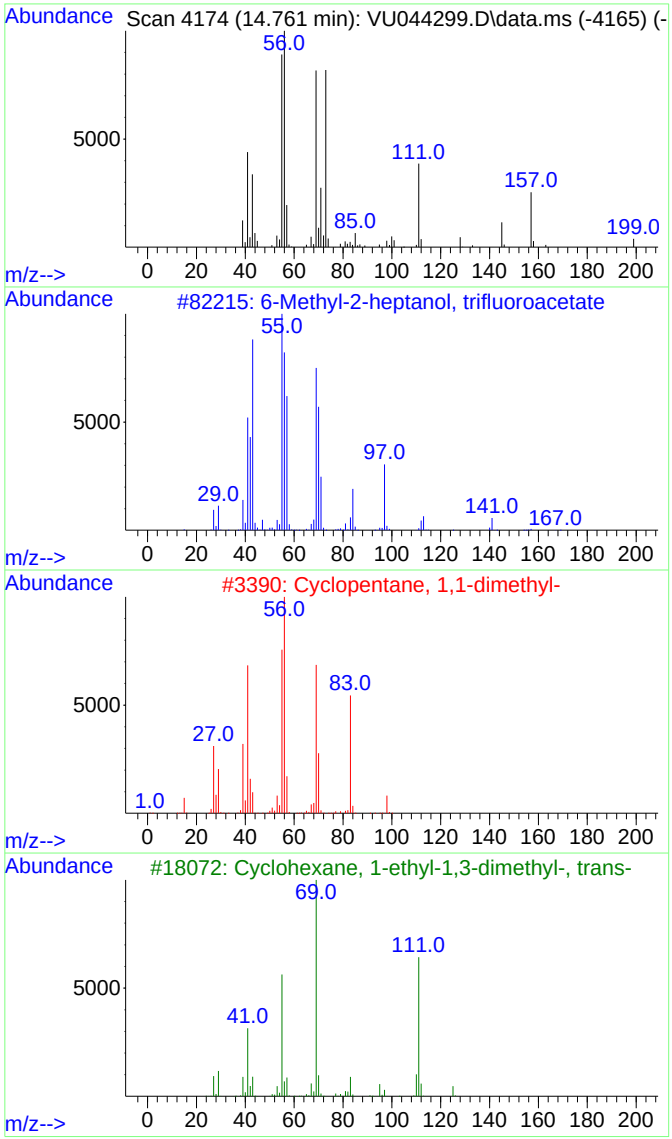
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

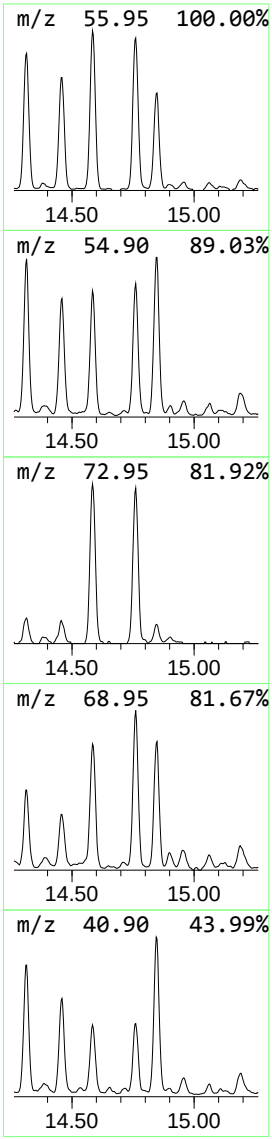
****

Peak Number 7 unknown-03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.761	1.10 ug/L	114619	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-Methyl-2-heptanol, trifluoroac...	226	C10H17F3O2	1000365-05-8	40
2	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	38
3	Cyclohexane, 1-ethyl-1,3-dimethy...	140	C10H20	062238-29-3	35
4	Cyclohexane, 1-ethyl-1,4-dimethy...	140	C10H20	062238-32-8	35
5	2-Dodecene, (Z)-	168	C12H24	007206-26-0	33





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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

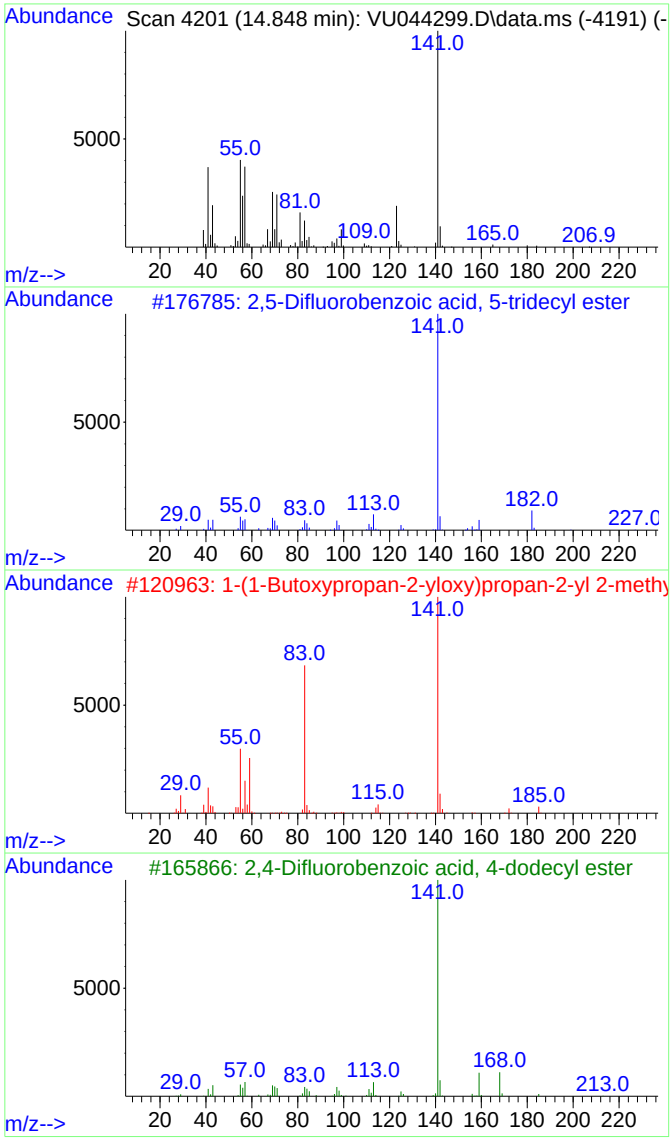
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

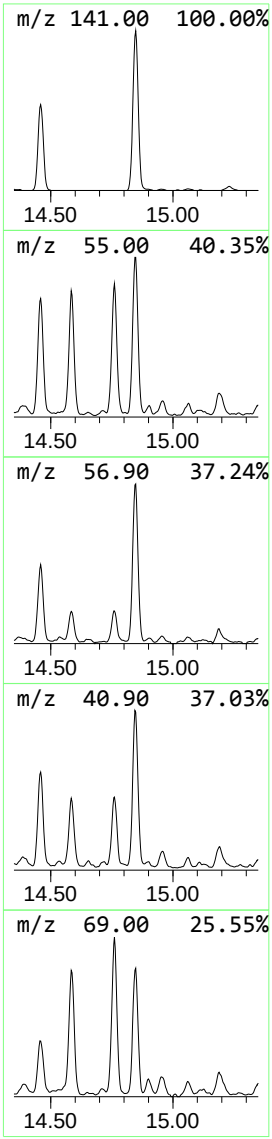
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2,5-Difluorobenzoic acid, 5... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.848	2.12 ug/L	220458	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Difluorobenzoic acid, 5-trid...	340	C20H30F2O2	1000338-47-6	50
2	1-(1-Butoxypropan-2-yloxy)propan...	272	C15H28O4	1000367-11-0	37
3	2,4-Difluorobenzoic acid, 4-dode...	326	C19H28F2O2	1000338-56-4	37
4	2,4-Difluorobenzoic acid, 3-dode...	326	C19H28F2O2	1000338-56-3	37
5	Nonanoic acid, pentafluorophenyl...	324	C15H17F5O2	1000360-66-5	33





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Data File : VU044299.D
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ALS Vial : 9 Sample Multiplier: 1

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

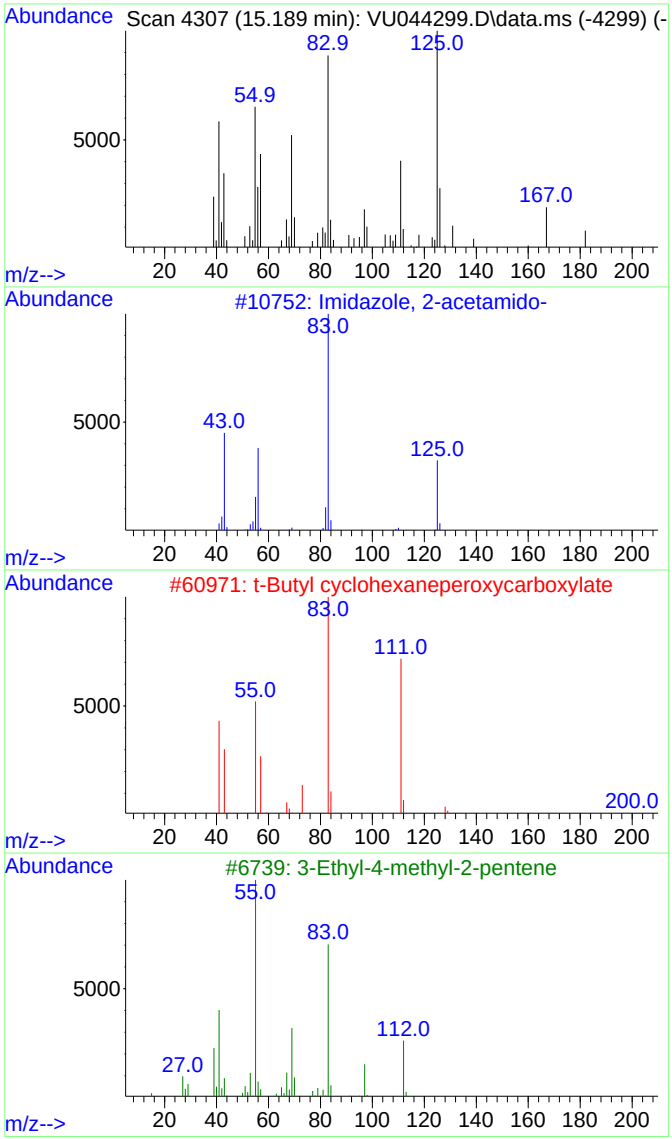
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

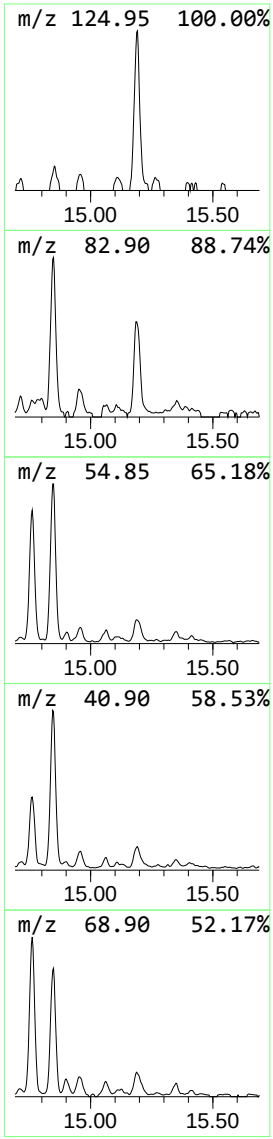
****

Peak Number 9 unknown-04 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.189	0.51 ug/L	53354	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazole, 2-acetamido-	125	C5H7N3O	052737-49-2	43
2	t-Butyl cyclohexaneperoxycarboxy...	200	C11H20O3	020396-49-0	35
3	3-Ethyl-4-methyl-2-pentene	112	C8H16	019780-68-8	30
4	Cyclohexanecarboxylic acid, 4-ni...	249	C13H15NO4	1000307-70-8	27
5	2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	25





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Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

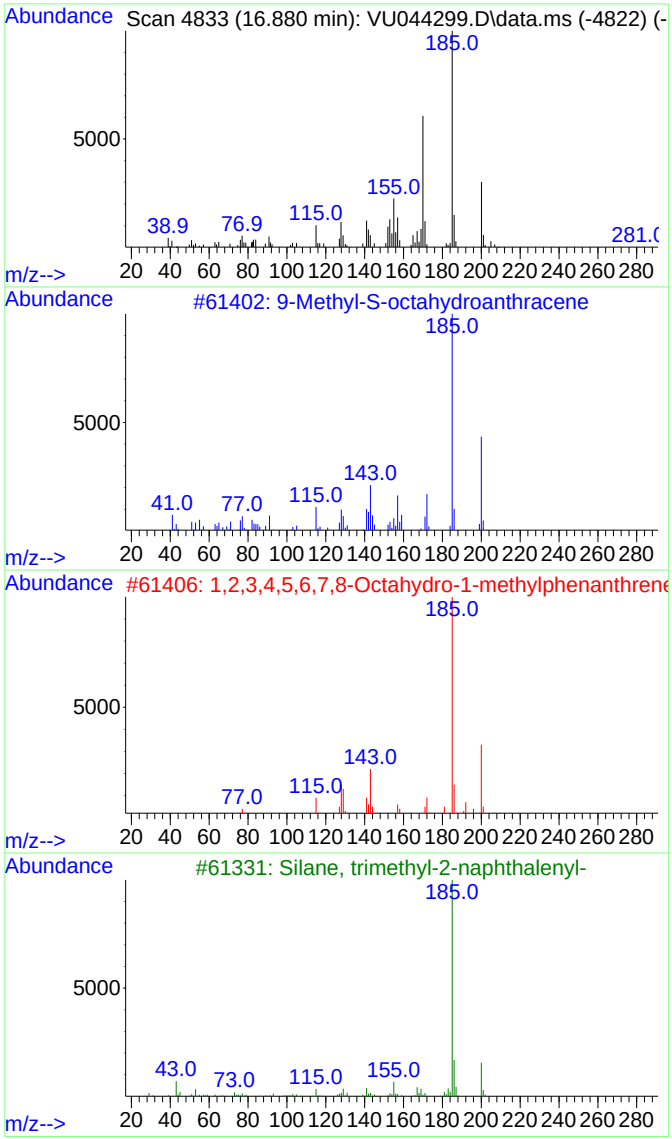
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

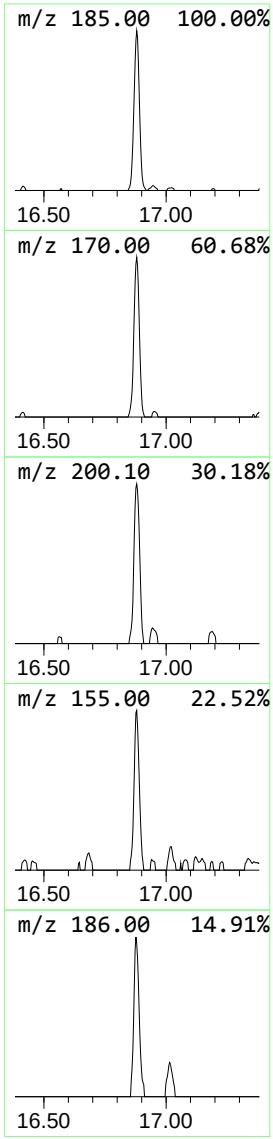
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 9-Methyl-S-octahydroanthracene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.880	0.78 ug/L	81310	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Methyl-S-octahydroanthracene	200	C15H20	004948-51-0	60
2	1,2,3,4,5,6,7,8-Octahydro-1-meth...	200	C15H20	1000080-19-4	55
3	Silane, trimethyl-2-naphthalenyl-	200	C13H16Si	018052-85-2	53
4	1H-Pyrazole, 5-(t-butyl)-3-phenyl-	200	C13H16N2	1000261-34-8	49
5	1-Methyl-1-n-pentyloxy-1-silacyc...	200	C11H24OSi	232270-61-0	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

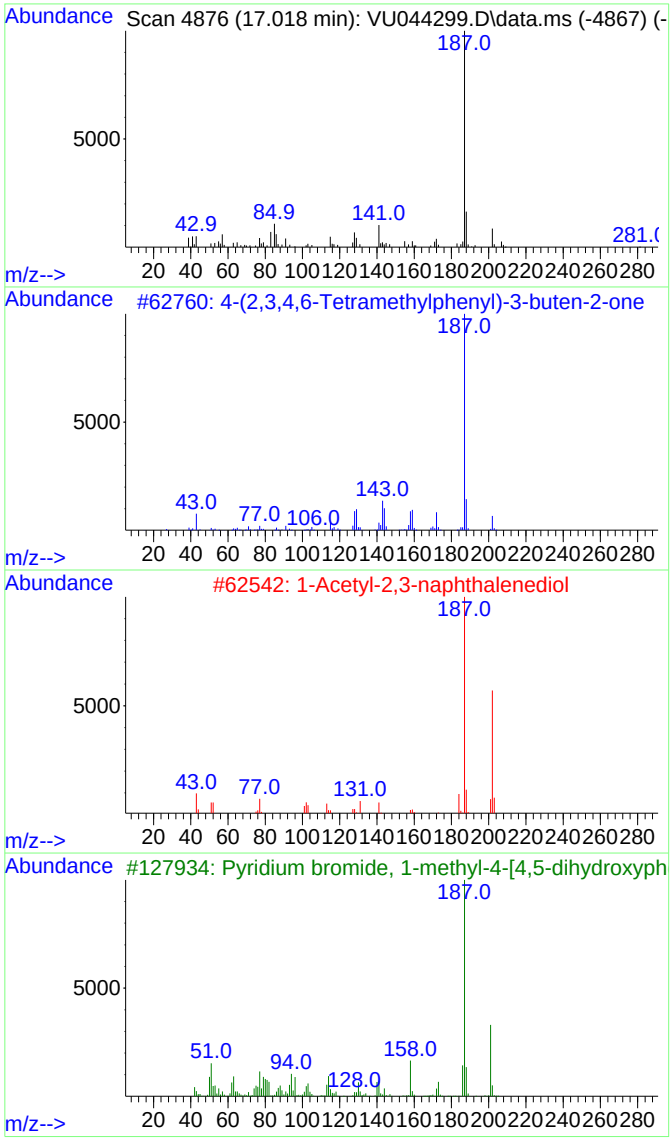
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

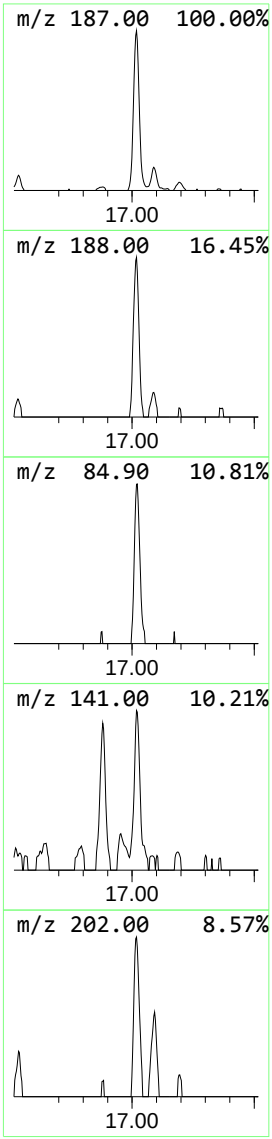
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 4-(2,3,4,6-Tetramethylpheny... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.018	0.54 ug/L	56589	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(2,3,4,6-Tetramethylphenyl)-3-...	202	C14H18O	094112-30-8	64
2	1-Acetyl-2,3-naphthalenediol	202	C12H10O3	091368-52-4	64
3	Pyridium bromide, 1-methyl-4-[4,...	281	C12H12BrNO2	1000124-80-7	50
4	1H-Indene, 4-butyl-2,3-dihydro-1...	202	C15H22	054889-53-1	46
5	1(2H)-Naphthalenone, 7-(1,1-dime...	202	C14H18O	022583-68-2	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070221\
Data File : VU044299.D
Acq On : 02 Jul 2021 13:20
Operator : SY/MD
Sample : M2914-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBK29

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
2,4-Dipropyl-5-...	13.980	2.4	ug/L	252999	3	11.819	520789	5.0
3-Methyl-thioph...	14.185	3.5	ug/L	367188	3	11.819	520789	5.0
unknown-01	14.314	1.8	ug/L	186775	3	11.819	520789	5.0
unknown-02	14.459	1.4	ug/L	147900	3	11.819	520789	5.0
Neopentyl glycol	14.584	1.2	ug/L	125710	3	11.819	520789	5.0
unknown-03	14.761	1.1	ug/L	114619	3	11.819	520789	5.0
2,5-Difluoroben...	14.848	2.1	ug/L	220458	3	11.819	520789	5.0
unknown-04	15.189	0.5	ug/L	53354	3	11.819	520789	5.0
9-Methyl-S-octa...	16.880	0.8	ug/L	81310	3	11.819	520789	5.0
4-(2,3,4,6-Tetr...	17.018	0.5	ug/L	56589	3	11.819	520789	5.0