LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 210505078-02-VOA

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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\82U050621W.M
Title : SW846 8260

Signal : TIC: VU043587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	38	44	51	rBV	51503	52677	1.58%	0.267%
2	1.523	51	57	72	rVB	81556	114945	3.44%	0.582%
3	1.838	149	155	183	rVB	27522	58925	1.76%	0.298%
4	2.626	386	400	429	rBV	720093	1308635	39.16%	6.624%
5	2.758	430	441	467	rVB	363702	675583	20.22%	3.420%
6	2.890	474	482	499	rVB	17465	33658	1.01%	0.170%
7	3.182	555	573	605	rBV	1565985	3341632	100.00%	16.914%
8	4.639	1005	1026	1038	rBV	1096679	2697949	80.74%	13.656%
9	4.706	1038	1047	1068	rVB	529060	1180521	35.33%	5.975%
10	4.980	1118	1132	1143	rBV2	228692	495535	14.83%	2.508%
11	5.054	1143	1155	1188	rVB	769502	1691517	50.62%	8.562%
12	5.298	1216	1231	1244	rBV	125271	262886	7.87%	1.331%
13	5.382	1244	1257	1279	rVB	187851	384224	11.50%	1.945%
14	5.710	1344	1359	1373	rBV2	160593	323840	9.69%	1.639%
15	5.787	1373	1383	1389	rVV4	19396	43688	1.31%	0.221%
16	5.832	1390	1397	1421	rVB2	31800	66977	2.00%	0.339%
17	6.256	1514	1529	1544	rBV	292594	542104	16.22%	2.744%
18	7.153	1800	1808	1825	rVB7	15178	35480	1.06%	0.180%
19	7.783	1991	2004	2024	rBV4	18348	45347	1.36%	0.230%
20	7.906	2024	2042	2057	rVV	486753	845195	25.29%	4.278%
21	8.034	2073	2082	2098	rVB	32947	58227	1.74%	0.295%
22	8.639	2253	2270	2280	rBV	47605	82532	2.47%	0.418%
23	9.423	2482	2514	2534	rBV	419848	733435	21.95%	3.712%
24	9.578	2551	2562	2578	rBV2	46002	76682	2.29%	0.388%
25	9.697	2581	2599	2610	rVV	40959	73403	2.20%	0.372%
26	10.002	2682	2694	2713	rBV3	15738	33738	1.01%	0.171%
27	10.108	2717	2727	2745	rVB3	23554	44542	1.33%	0.225%
28	10.639	2877	2892	2904	rBV	354967	557981	16.70%	2.824%
29	11.819	3244	3259	3275	rVB	423973	703084	21.04%	3.559%
30	11.922	3279	3291	3301	rBV4	45421	79168	2.37%	0.401%
31	12.536	3474	3482	3500	rVB2	32675	57119	1.71%	0.289%
32	12.780	3548	3558	3569	rVB	80756	128672	3.85%	0.651%
33	12.957	3595	3613	3626	rBV	348914	571616	17.11%	2.893%
34	13.523	3778	3789	3804	rBV	113490	201284	6.02%	1.019%
35	13.638	3817	3825	3834	rVB5	21651	34235	1.02%	0.173%
36	13.703	3834	3845	3848	rBV6	51685	85272	2.55%	0.432%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 210505078-02-VOA

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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\82U050621W.M
Title : SW846 8260

37	13.745	3848	3858	3876	rVV	832078	1388229	41.54%	7.027%
38	13.854	3879	3892	3912	rVV5	150167	293258	8.78%	1.484%
39	14.040	3940	3950	3958	rBV3	42159	69049	2.07%	0.349%
40	14.092	3958	3966	3981	rVB	87464	144518	4.32%	0.731%
41	14.516	4087	4098	4115	rBV	77736	139400	4.17%	0.706%

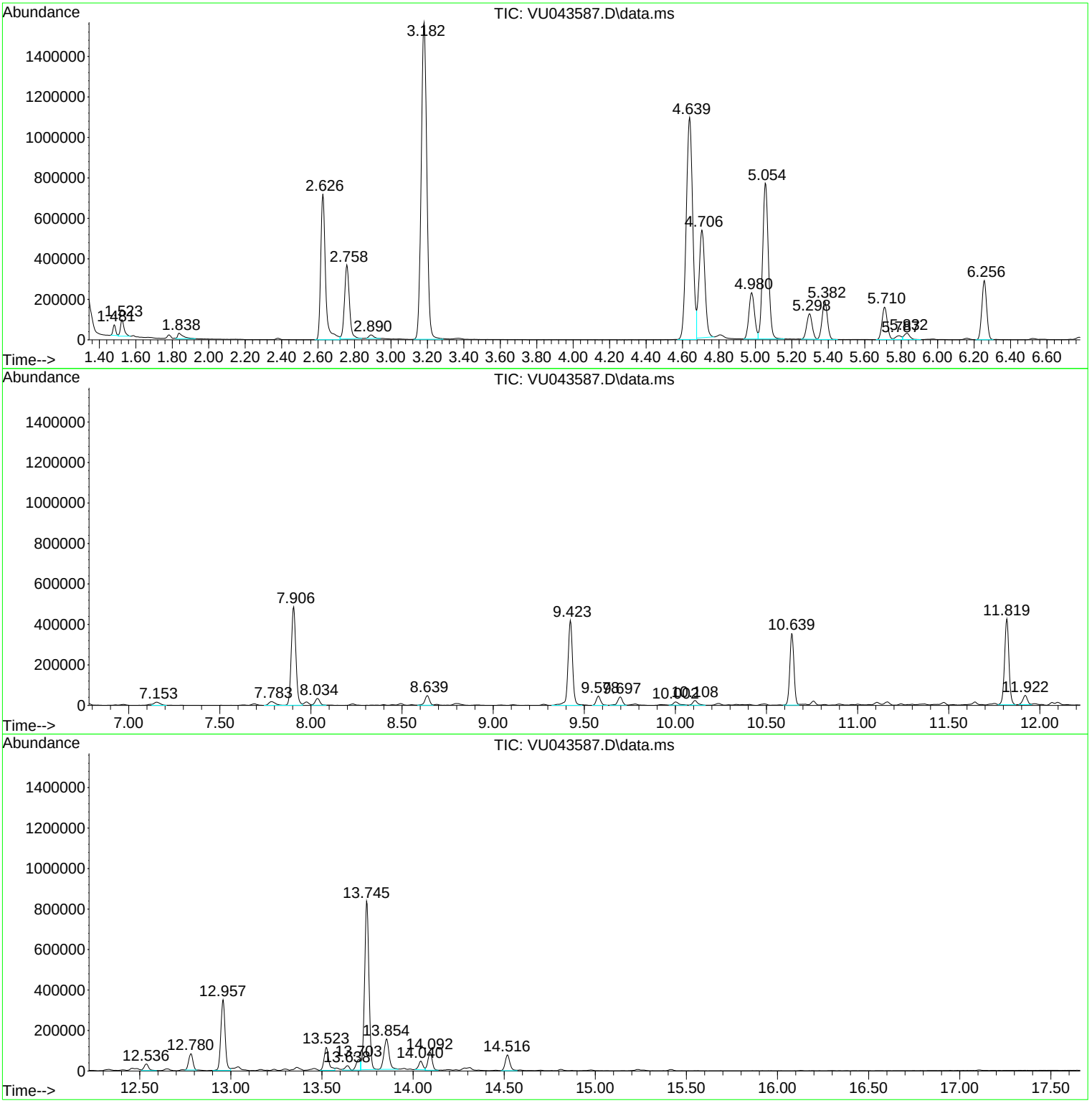
Sum of corrected areas: 19756762

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

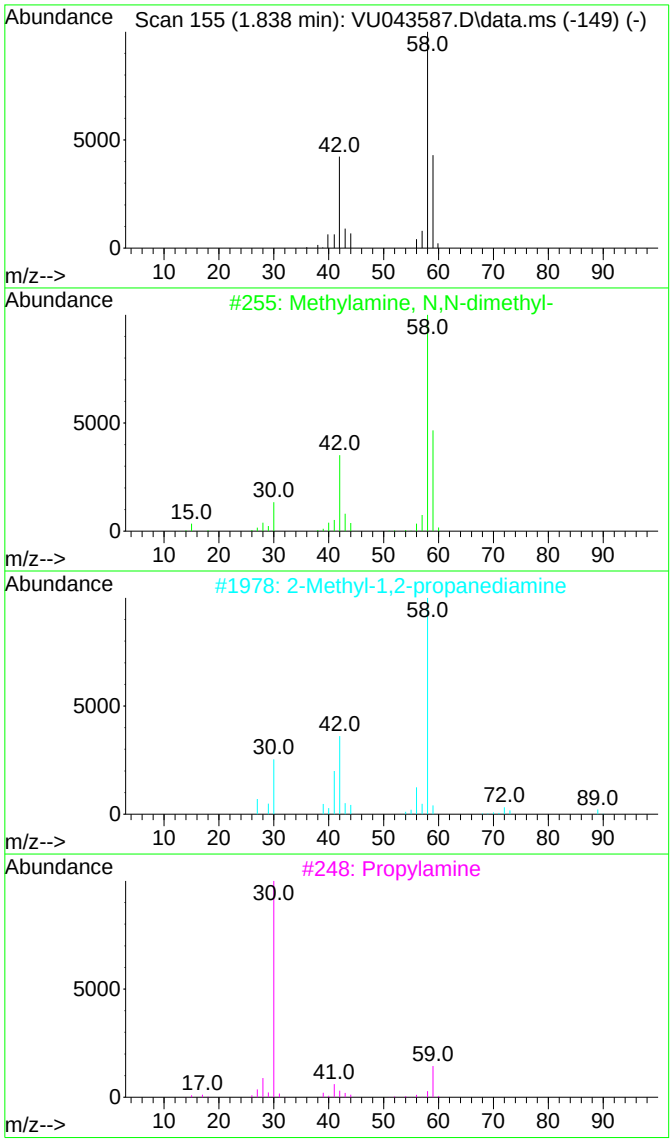
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

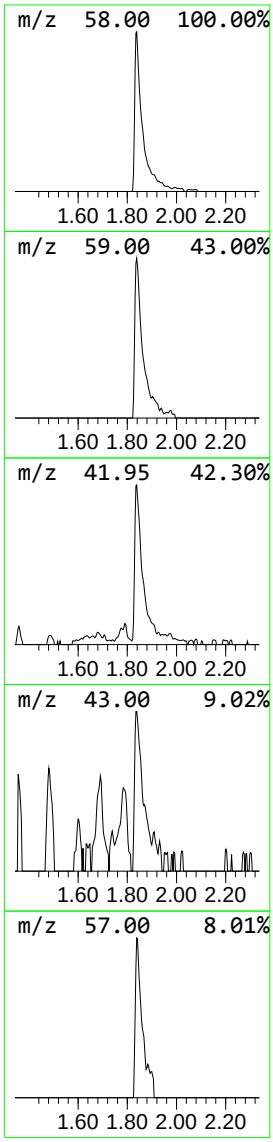
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Methylamine, N,N-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.838	7.67 ug/l	58925	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	90
2	2-Methyl-1,2-propanediamine	88	C4H12N2	000811-93-8	9
3	Propylamine	59	C3H9N	000107-10-8	7
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	4
5	Propylene oxide	58	C3H6O	000075-56-9	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

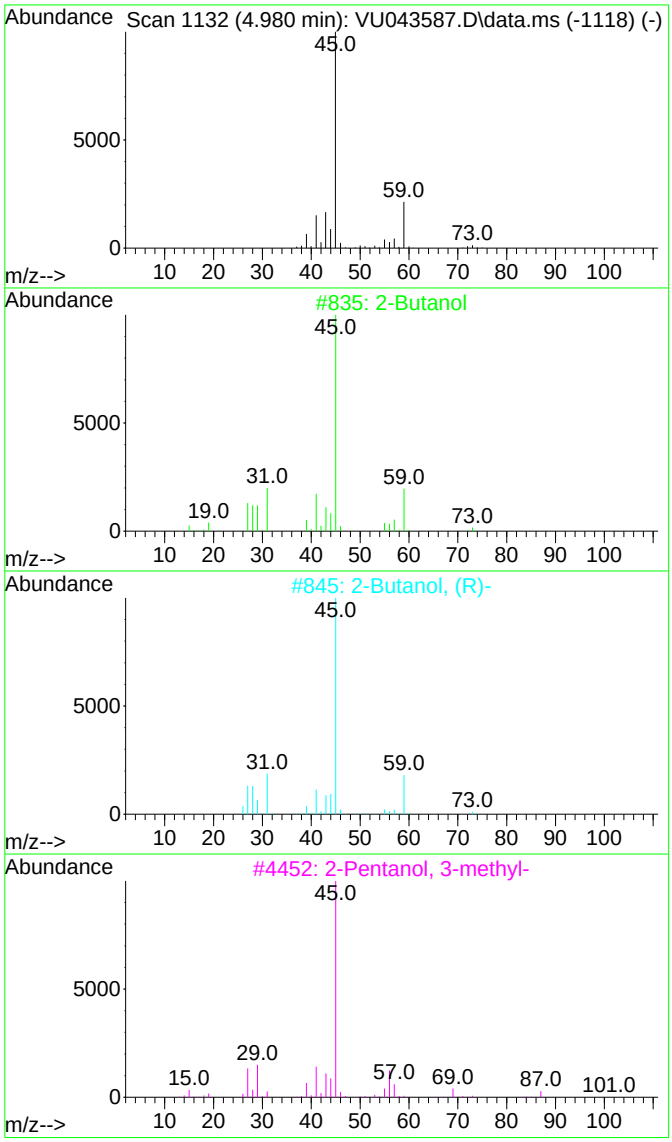
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

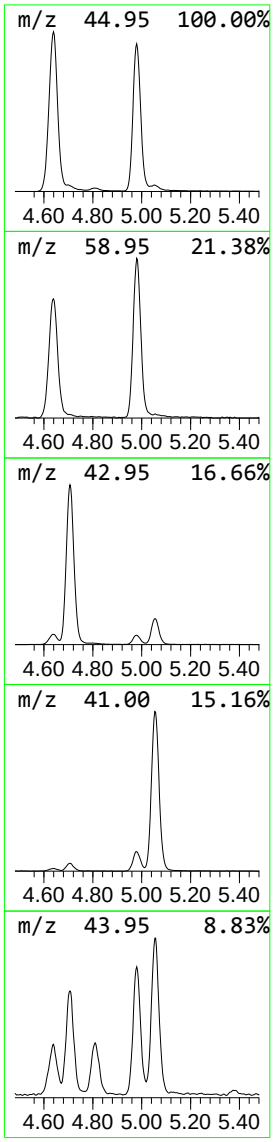
****

Peak Number 4 2-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.980	64.49 ug/l	495535	Pentafluorobenzene	5.382

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol	74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-	74	C4H10O	014898-79-4	83
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	42
5	2-Hexanol	102	C6H14O	000626-93-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 210505078-02-VOA

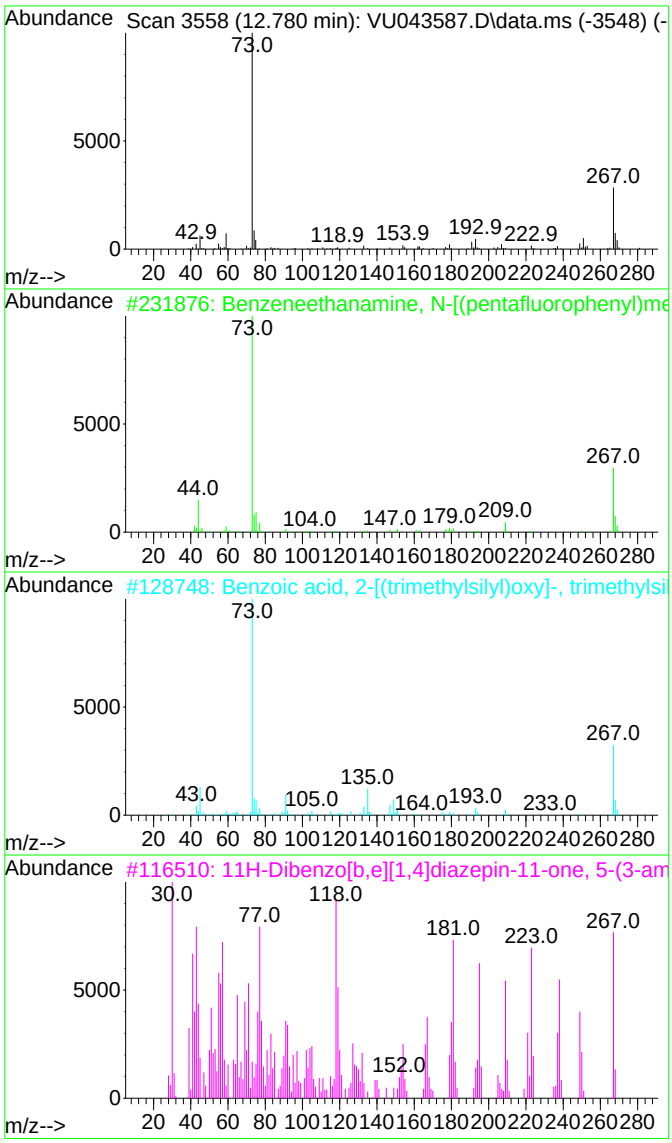
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

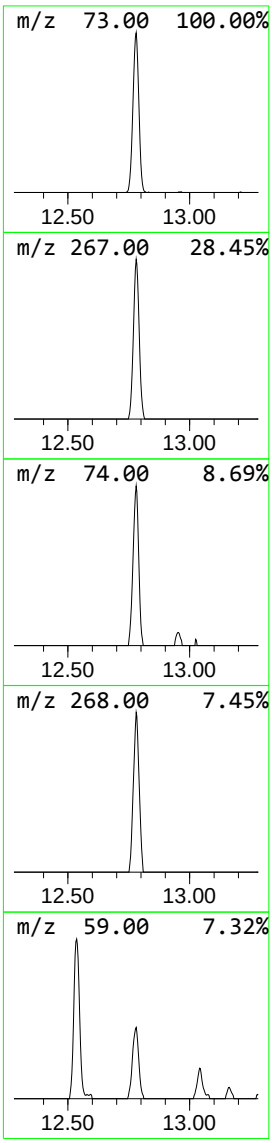
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzeneethanamine, N-[(pent... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.780	9.15 ug/l	128672	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	50
2	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	45
3	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	22
4	4-Methylcatechol, bis(trimethyls...	268	C13H24O2Si2	1000332-79-9	12
5	Cyclopropene, 3,3-diphenyl-1-tri...	264	C18H20Si	173595-34-1	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

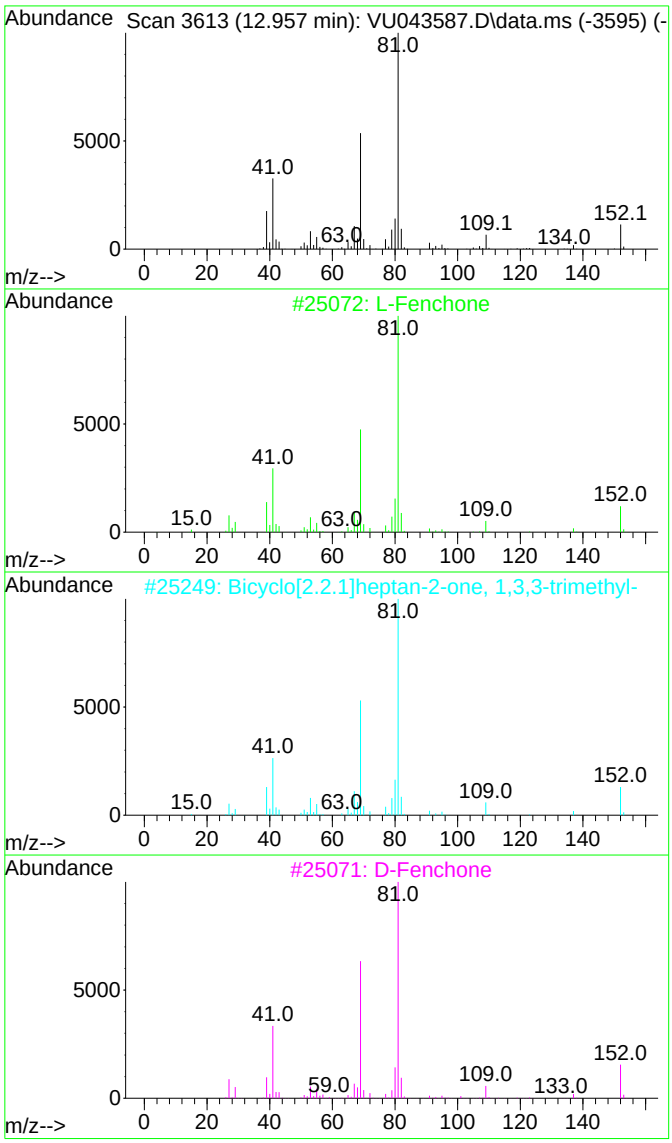
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

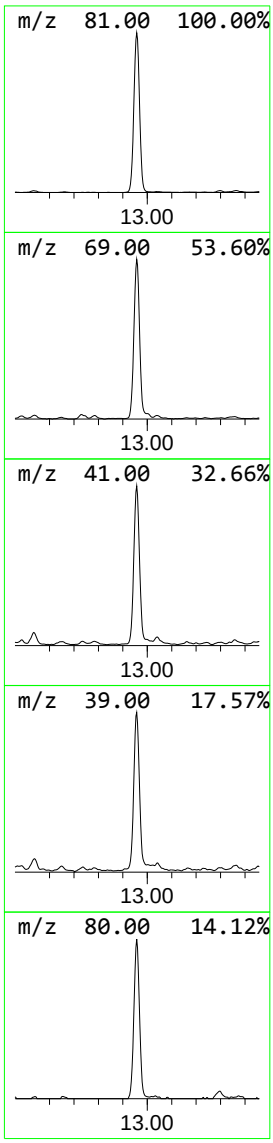
****

Peak Number 6 L-Fenchone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.957	40.65 ug/l	571616	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Fenchone	152	C10H16O	007787-20-4	95
2	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
3	D-Fenchone	152	C10H16O	004695-62-9	91
4	2-Cyclopentene-1-carboxylic acid...	140	C8H12O2	068317-73-7	53
5	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

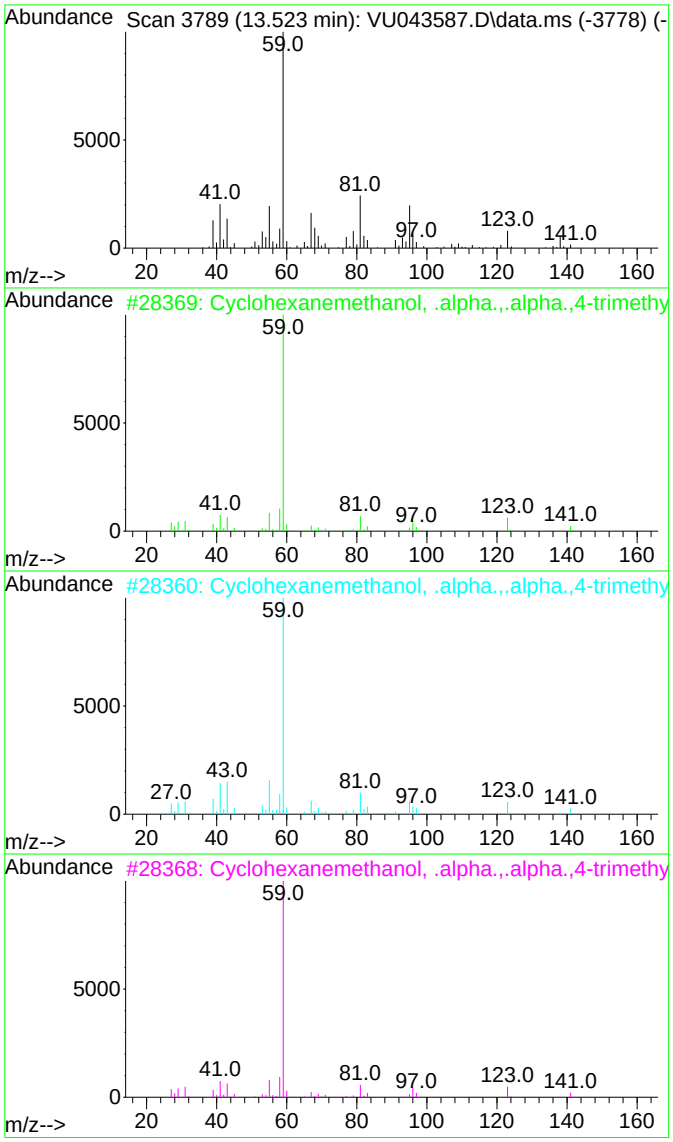
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

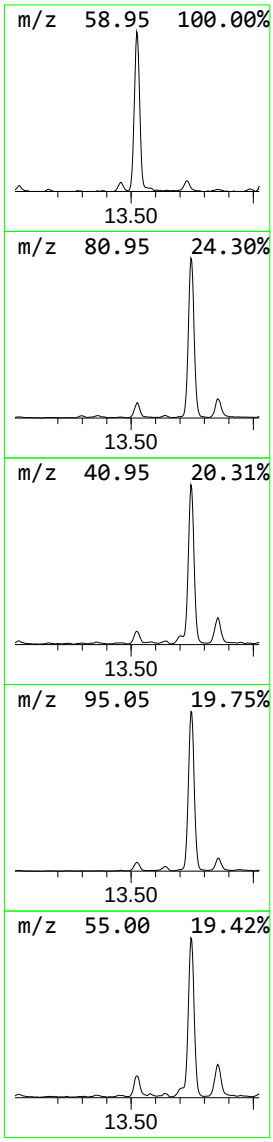
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexanemethanol, .alpha... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.523	14.31 ug/l	201284	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	53
2	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	53
3	Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	007322-63-6	40
4	2-(3,4-Dibromo-4-methylcyclohexy...	312	C10H18Br2O	110202-13-6	38
5	2-Hydroxy-2-methylundec-5-en-3-one	198	C12H22O2	1000191-46-2	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

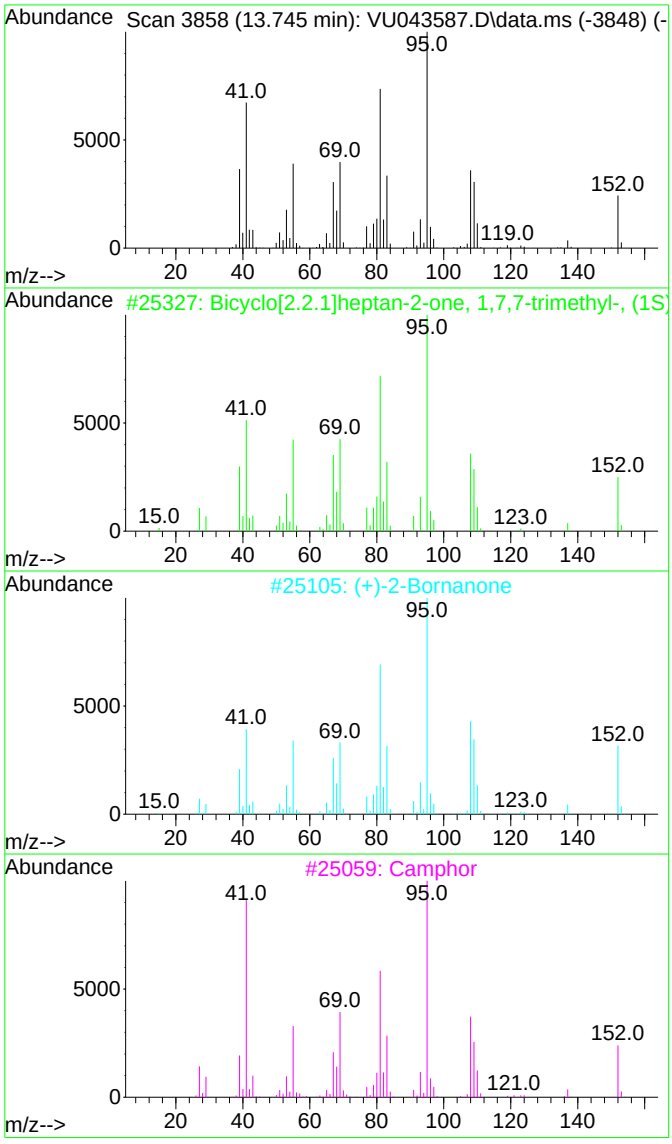
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

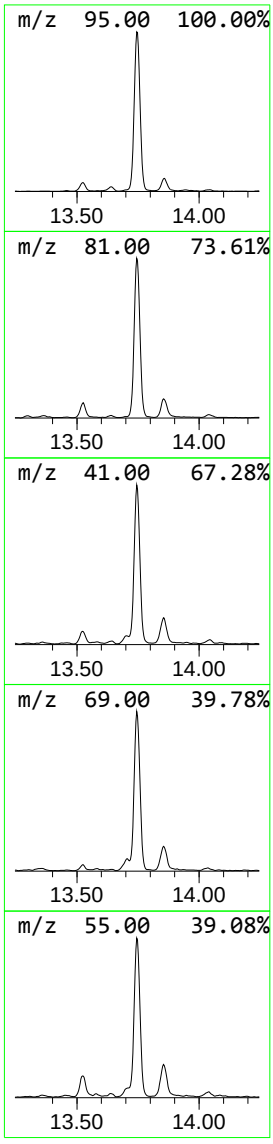
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	98.72 ug/l	1388230	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3	Camphor	152	C10H16O	000076-22-2	97
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	50
5	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	46





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Sample : M2313-01
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

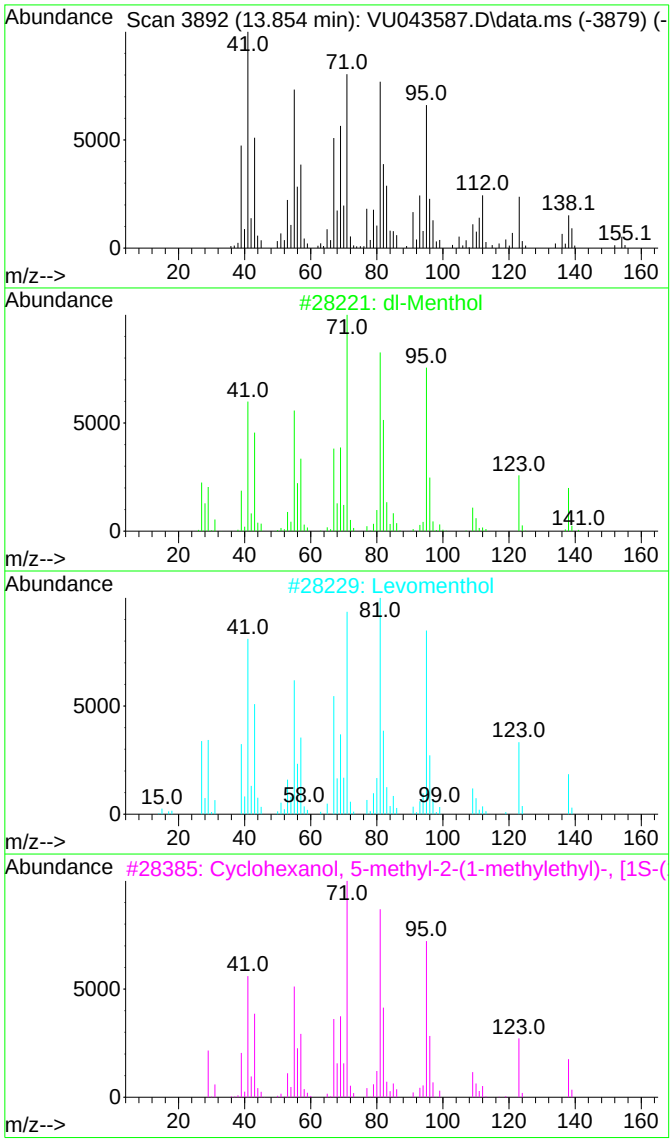
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

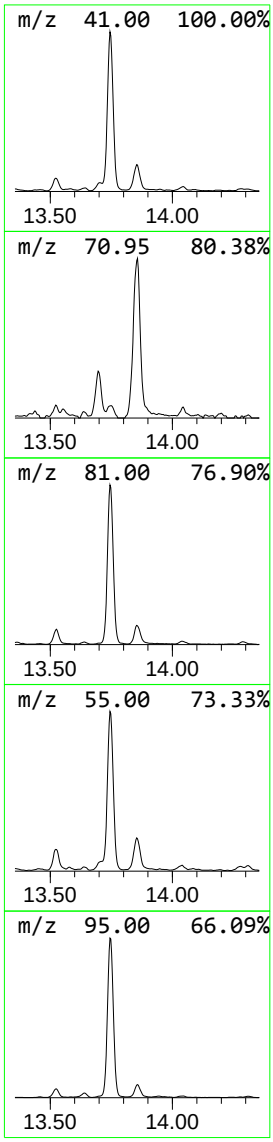
****

Peak Number 9 dl-Menthol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.854	20.86 ug/l	293258	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Menthol	156	C10H20O	000089-78-1	80
2	Levomenthol	156	C10H20O	002216-51-5	80
3	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	80
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	74
5	Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
210505078-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

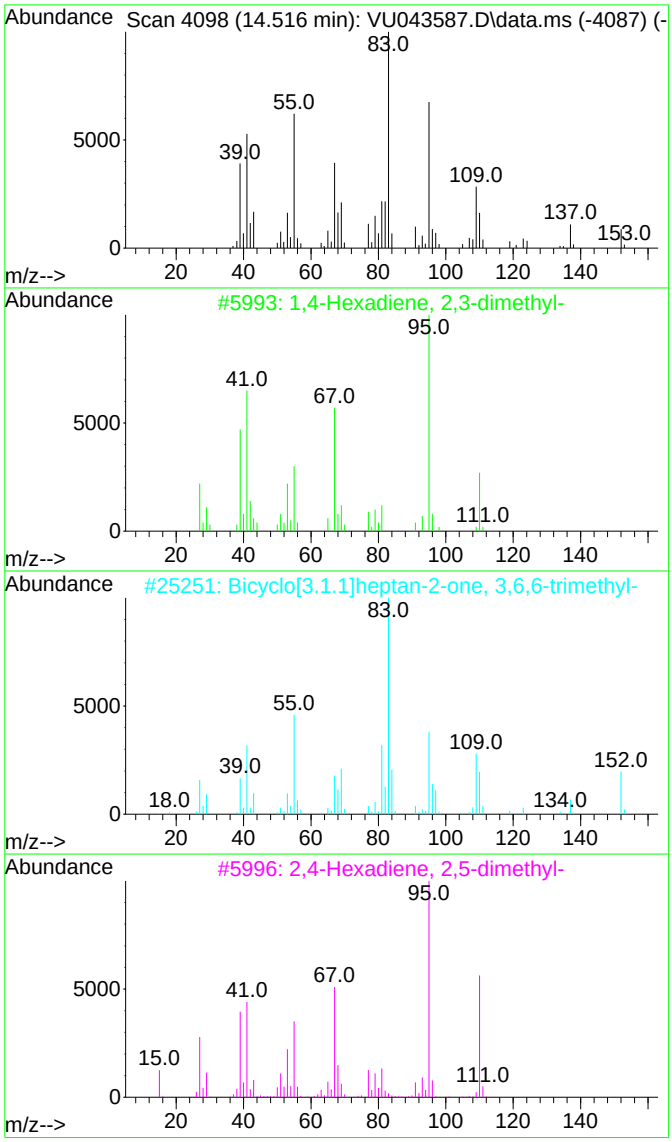
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

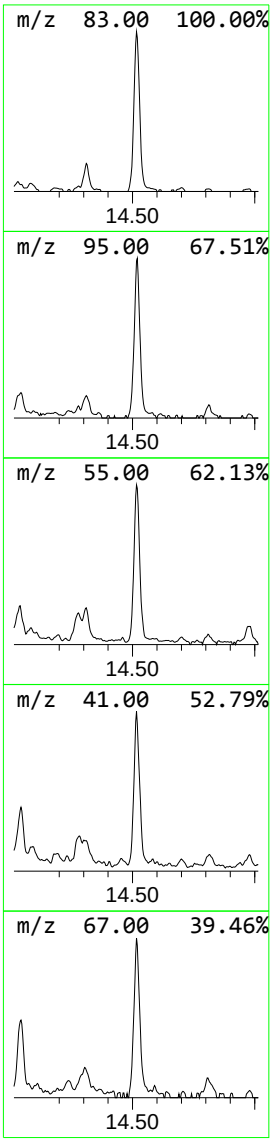
****

Peak Number 10 unknown14.516 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.516	9.91 ug/l	139400	1,4-Dichlorobenzene-d4	11.819

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	45
2	Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	38
3	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	38
4	1,3-Hexadiene, 2,5-dimethyl-	110	C8H14	029253-64-3	25
5	Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050621\
Data File : VU043587.D
Acq On : 06 May 2021 16:46
Operator : SY/MD
Sample : M2313-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : 210505078-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U050621W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Methylamine, N,...	1.838	7.7	ug/l	58925	1	5.382	384224	50.0
2-Butanol	4.980	64.5	ug/l	495535	1	5.382	384224	50.0
Benzeneethanami...	12.780	9.2	ug/l	128672	4	11.819	703084	50.0
L-Fenchone	12.957	40.6	ug/l	571616	4	11.819	703084	50.0
Cyclohexanemeth...	13.523	14.3	ug/l	201284	4	11.819	703084	50.0
Bicyclo[2.2.1]h...	13.745	98.7	ug/l	1388230	4	11.819	703084	50.0
dl-Menthol	13.854	20.9	ug/l	293258	4	11.819	703084	50.0
unknown14.516	14.516	9.9	ug/l	139400	4	11.819	703084	50.0