LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065851.D
Acq On : 12 Feb 2021 20:26
Operator : JC/MD
Sample : M1386-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 210210007-02-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_N\methods\82N012521W.M
Title : SW846 8260

Signal : TIC: VN065851.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.981	67	75	90	rVB2	30697	47673	1.89%	0.353%
2	3.779	619	634	648	rBV3	18215	48518	1.93%	0.359%
3	4.039	698	715	732	rVB2	8180	26070	1.03%	0.193%
4	4.759	901	939	979	rBV	474579	1678132	66.59%	12.423%
5	6.795	1546	1572	1631	rBV	827745	2520082	100.00%	18.655%
6	7.171	1670	1689	1719	rBV2	250353	688704	27.33%	5.098%
7	7.547	1789	1806	1818	rBV	87642	219738	8.72%	1.627%
8	7.621	1818	1829	1859	rVB	148368	348716	13.84%	2.581%
9	7.988	1926	1943	1958	rBV3	111322	272379	10.81%	2.016%
10	8.081	1959	1972	1976	rBV5	15443	36347	1.44%	0.269%
11	8.225	2001	2017	2040	rVB9	10300	33451	1.33%	0.248%
12	8.412	2061	2075	2091	rBV	11568	26964	1.07%	0.200%
13	8.547	2102	2117	2134	rBV	261353	544784	21.62%	4.033%
14	9.952	2539	2554	2564	rBV3	14827	29769	1.18%	0.220%
15	10.058	2573	2587	2599	rBV	436166	807738	32.05%	5.979%
16	10.122	2599	2607	2614	rVV	38343	72544	2.88%	0.537%
17	10.161	2614	2619	2631	rVV	27211	48108	1.91%	0.356%
18	10.688	2766	2783	2802	rBV	103416	192400	7.63%	1.424%
19	10.843	2813	2831	2843	rBV5	17112	43376	1.72%	0.321%
20	11.376	2984	2997	3018	rBV	424206	751426	29.82%	5.563%
21	11.479	3018	3029	3046	rVB2	53381	103400	4.10%	0.765%
22	11.589	3047	3063	3073	rBV	75482	146958	5.83%	1.088%
23	11.917	3154	3165	3180	rBB	57682	98938	3.93%	0.732%
24	12.373	3295	3307	3329	rVB	323486	568056	22.54%	4.205%
25	13.010	3491	3505	3515	rBV	35582	62536	2.48%	0.463%
26	13.135	3533	3544	3553	rBV3	48585	80024	3.18%	0.592%
27	13.312	3588	3599	3612	rVV	387561	701562	27.84%	5.193%
28	13.376	3613	3619	3628	rVB2	57835	89751	3.56%	0.664%
29	13.515	3654	3662	3681	rVB	25102	55293	2.19%	0.409%
30	13.788	3732	3747	3757	rVV5	69028	153166	6.08%	1.134%
31	13.849	3757	3766	3777	rVB	133095	220381	8.74%	1.631%
32	13.990	3804	3810	3820	rVB4	18325	30233	1.20%	0.224%
33	14.190	3856	3872	3891	rBV	541707	927506	36.80%	6.866%
34	14.267	3891	3896	3914	rVB10	11669	26448	1.05%	0.196%
35	14.454	3945	3954	3961	rBV9	19331	34468	1.37%	0.255%
36	14.540	3974	3981	3994	rVB8	19437	39840	1.58%	0.295%

LSC Area Percent Report

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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 210210007-02-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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Title : SW846 8260

37	14.614	3994	4004	4014	rBV2	59415	97619	3.87%	0.723%
38	14.708	4028	4033	4041	rVB6	19066	28032	1.11%	0.208%
39	14.772	4041	4053	4056	rBV4	58037	103980	4.13%	0.770%
40	14.814	4057	4066	4075	rVV	476927	831948	33.01%	6.159%
41	14.862	4075	4081	4098	rVB5	168334	301901	11.98%	2.235%
42	15.097	4140	4154	4170	rVB	148780	272234	10.80%	2.015%
43	15.431	4247	4258	4273	rVB2	49846	97574	3.87%	0.722%

Sum of corrected areas: 13508767

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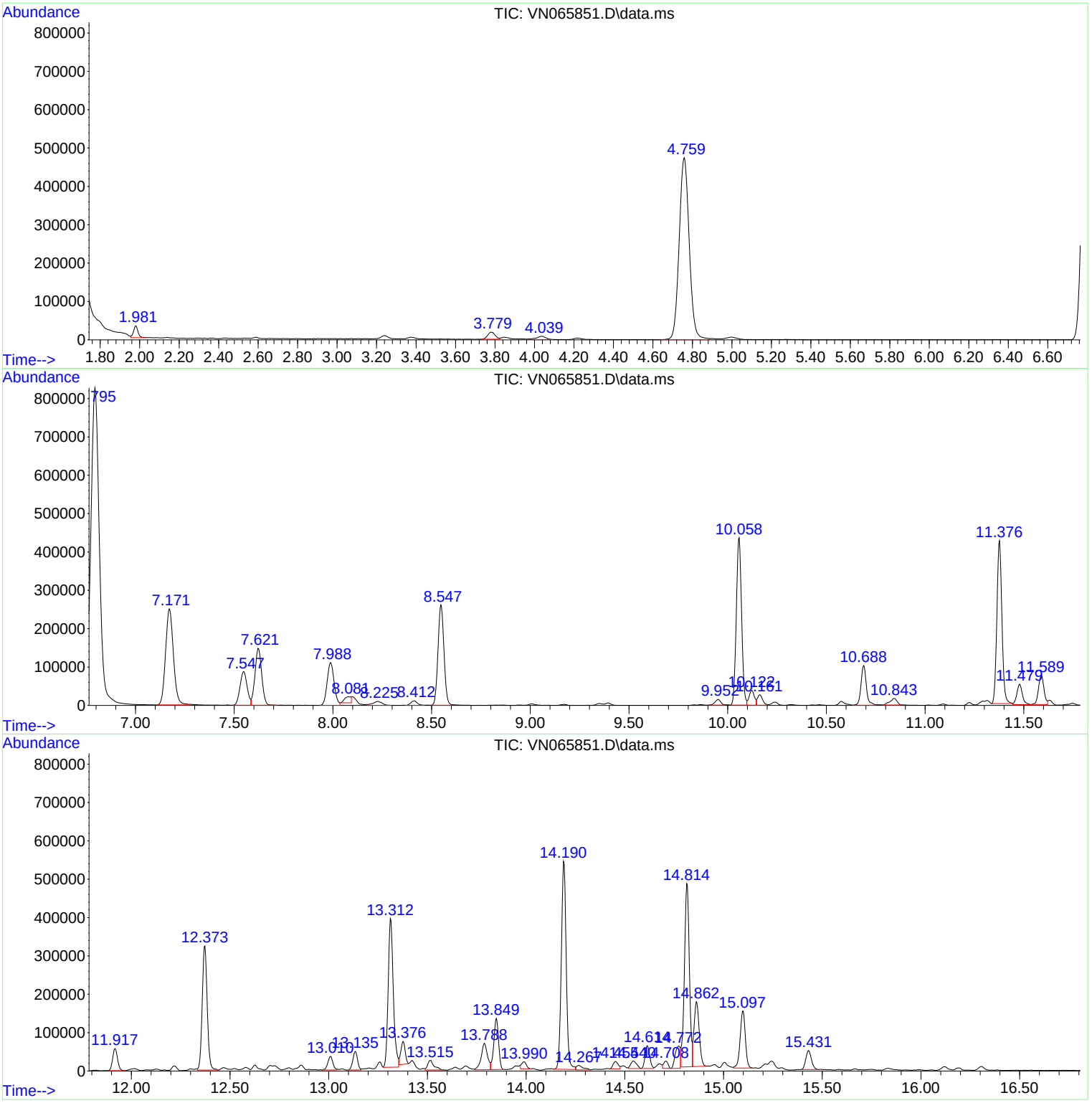
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065851.D
Acq On : 12 Feb 2021 20:26
Operator : JC/MD
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

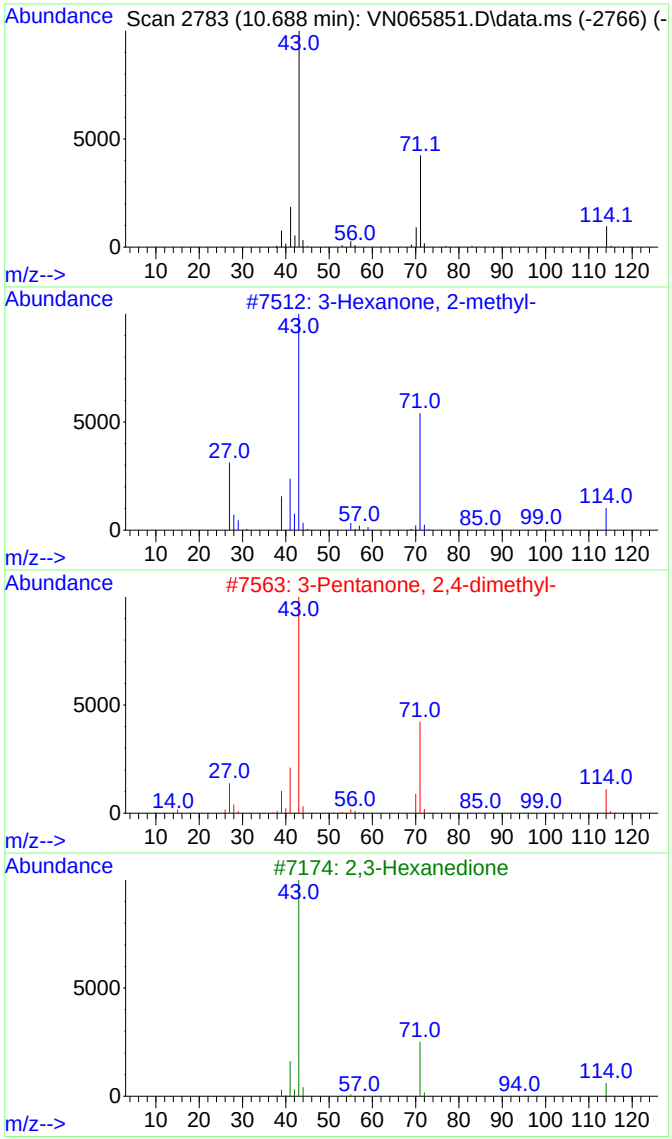
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

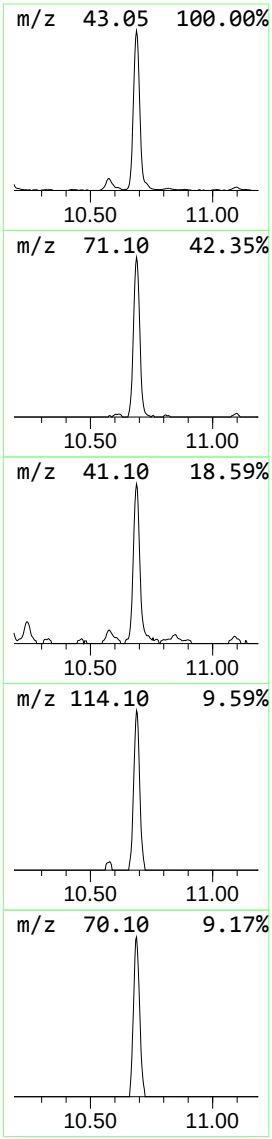
****

Peak Number 2 3-Hexanone, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.688	12.80 ug/l	192400	Chlorobenzene-d5	11.377

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
2	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
4	4-Heptanone	114	C7H14O	000123-19-3	53
5	1,4-Dioxin, 2,3-dihydro-5,6-dime...	114	C6H10O2	025465-18-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065851.D
Acq On : 12 Feb 2021 20:26
Operator : JC/MD
Sample : M1386-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

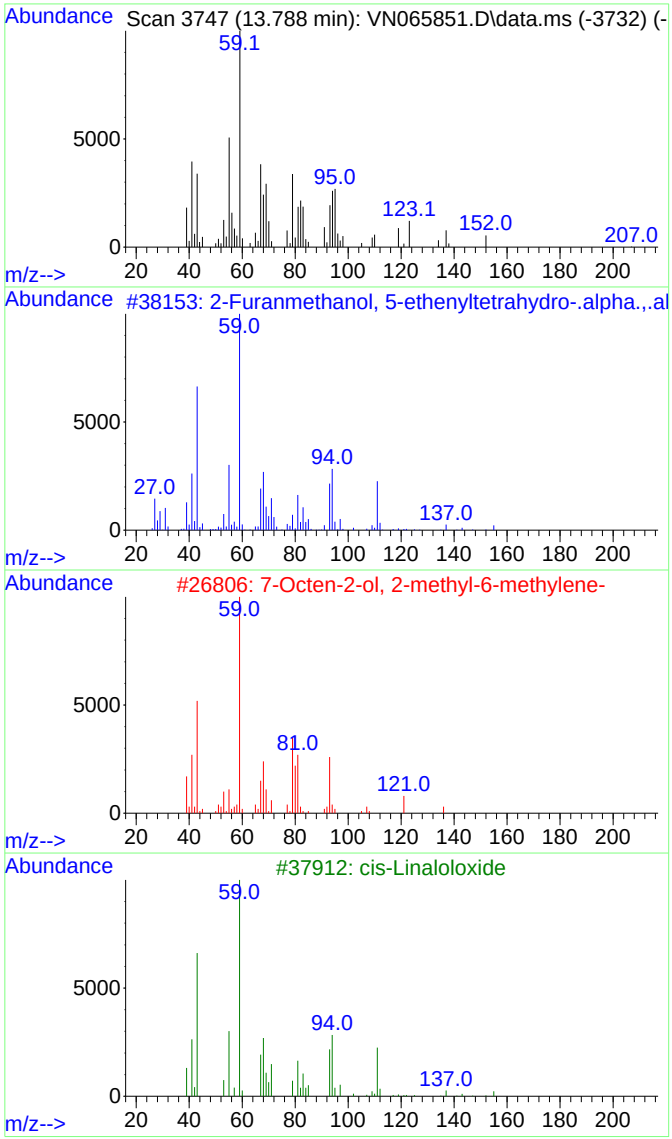
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

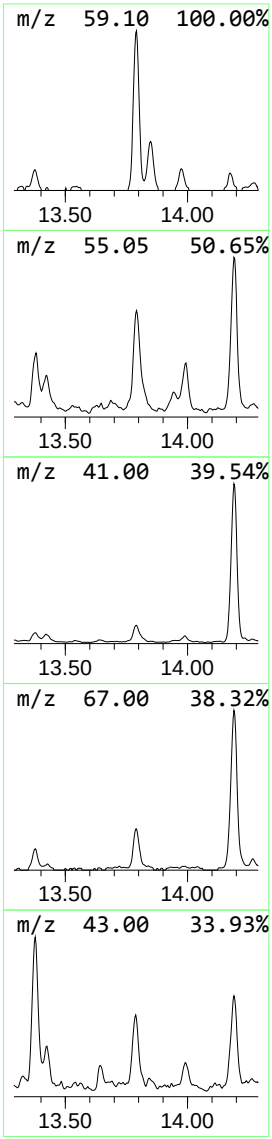
****

Peak Number 3 unknown13.788 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.788	10.92 ug/l	153166	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furanmethanol, 5-ethenyltetrah...	170	C10H18O2	005989-33-3	47
2	7-Octen-2-ol, 2-methyl-6-methylene-	154	C10H18O	000543-39-5	47
3	cis-Linaloloxide	170	C10H18O2	1000121-97-4	38
4	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	32
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065851.D
Acq On : 12 Feb 2021 20:26
Operator : JC/MD
Sample : M1386-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

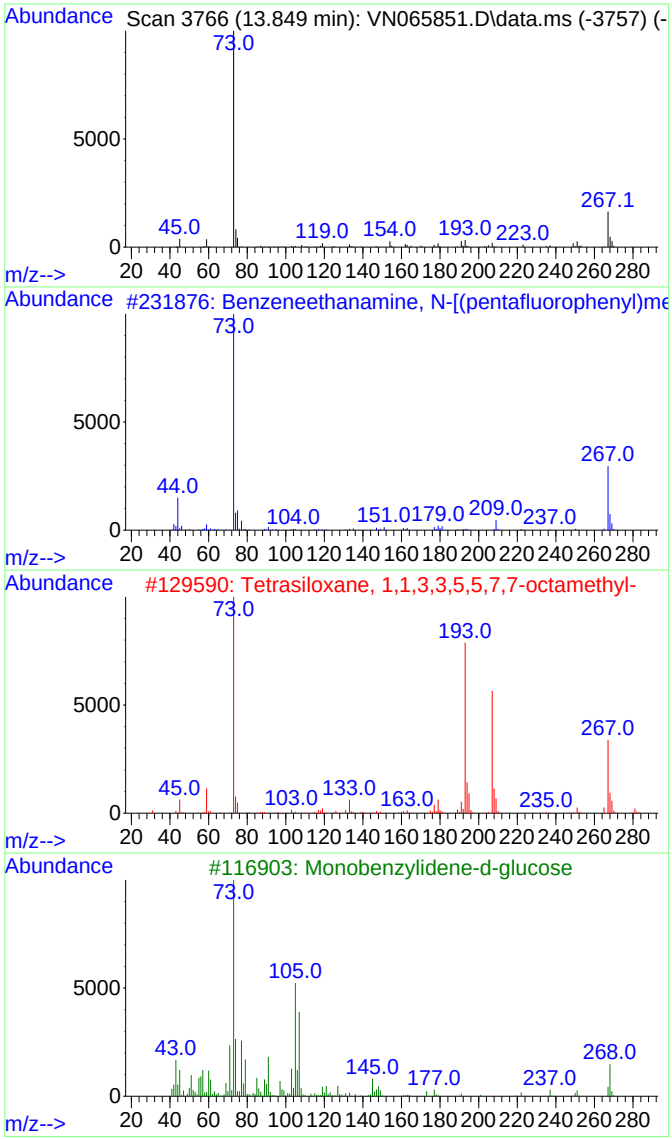
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

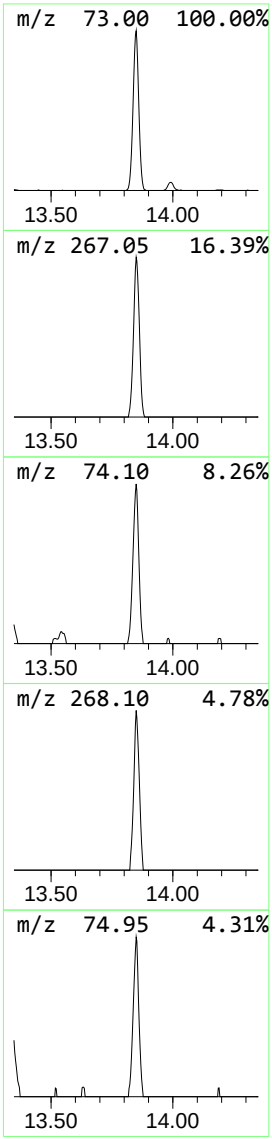
****

Peak Number 4 unknown13.849 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.849	15.71 ug/l	220381	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	47
2	Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	38
3	Monobenzylidene-d-glucose	268	C13H16O6	1000127-04-3	37
4	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	33
5	Cyclopropene, 3,3-diphenyl-1-tri...	264	C18H20Si	173595-34-1	23





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Acq On : 12 Feb 2021 20:26
Operator : JC/MD
Sample : M1386-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

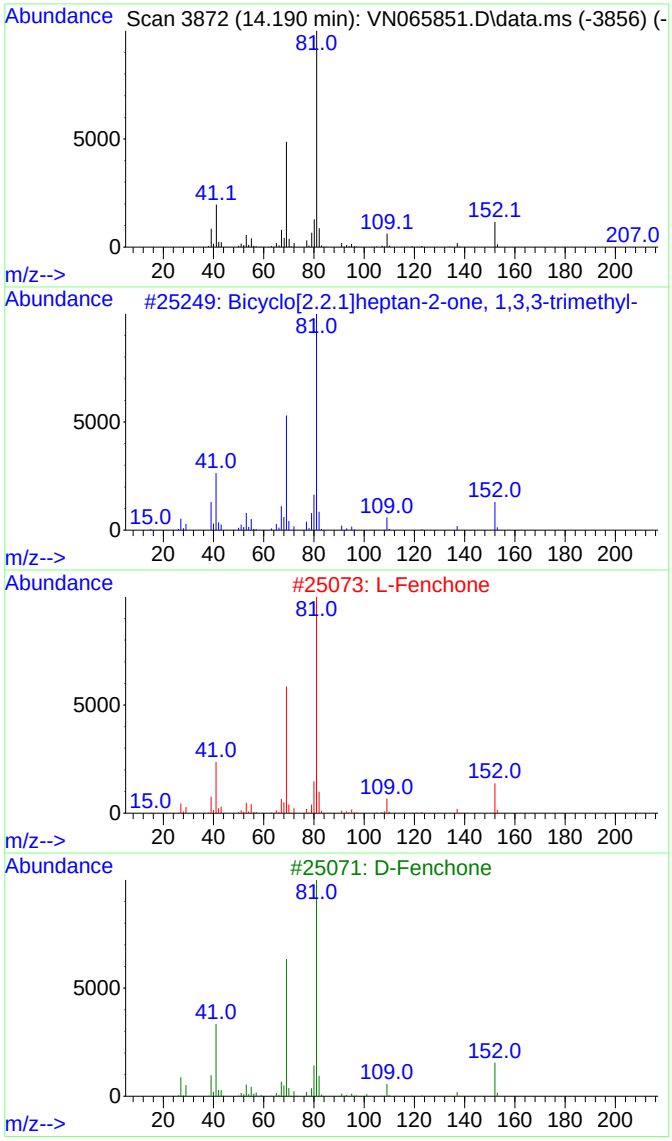
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

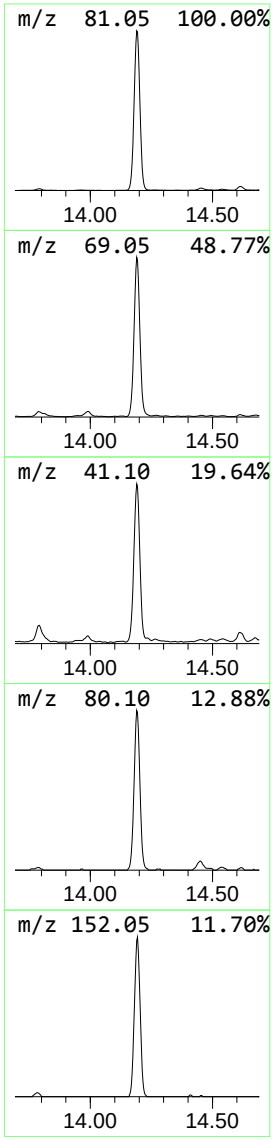
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.190	66.10 ug/l	927506	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	95
2	L-Fenchone	152	C10H16O	007787-20-4	95
3	D-Fenchone	152	C10H16O	004695-62-9	94
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	45
5	1-[4-(4-tert-Butyl-spirocyclohex...	371	C20H28F3NO2	1000301-43-3	36





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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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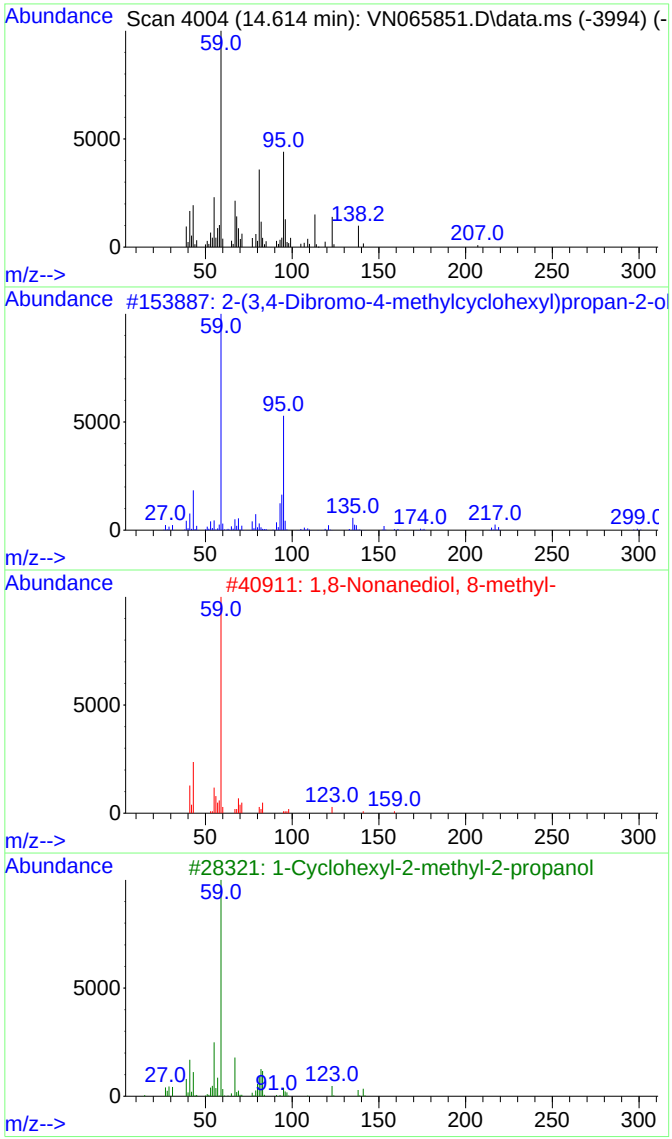
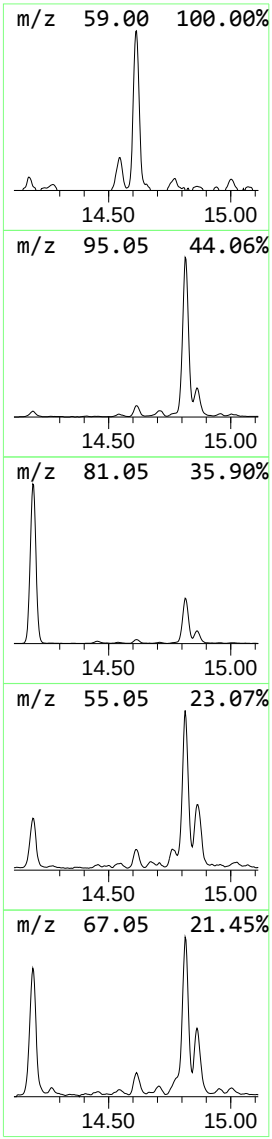
****

Peak Number 6 unknown14.614 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.614	6.96 ug/l	97619	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(3,4-Dibromo-4-methylcyclohexy...	312	C10H18Br2O	110202-13-6	40
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	35
3	1-Cyclohexyl-2-methyl-2-propanol	156	C10H20O	005531-30-6	33
4	2-Methyl-2-nonanol	158	C10H22O	010297-57-1	27
5	2-Dodecanol, 2-methyl-	200	C13H28O	001653-37-8	27





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TIC Library : C:\DATABASE\NIST11.L
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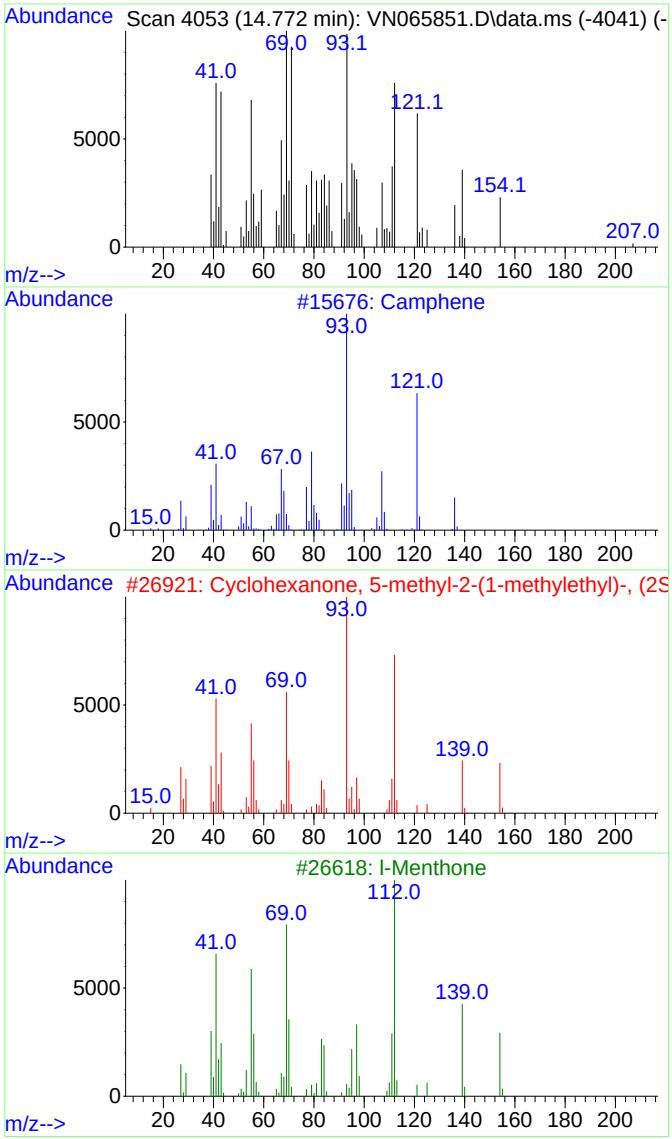
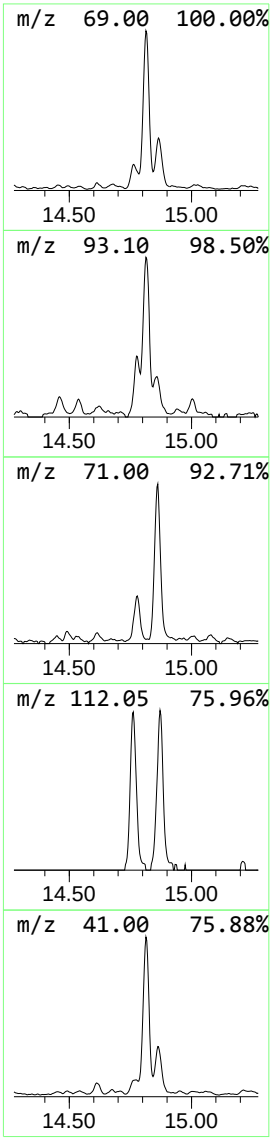
Peak Number 7 Camphene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.772	7.41 ug/l	103980	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphene	136	C10H16	000079-92-5	53
2	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	018309-28-9	46
3	l-Menthone	154	C10H18O	014073-97-3	38
4	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	35
5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	35





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Quant Title : SW846 8260

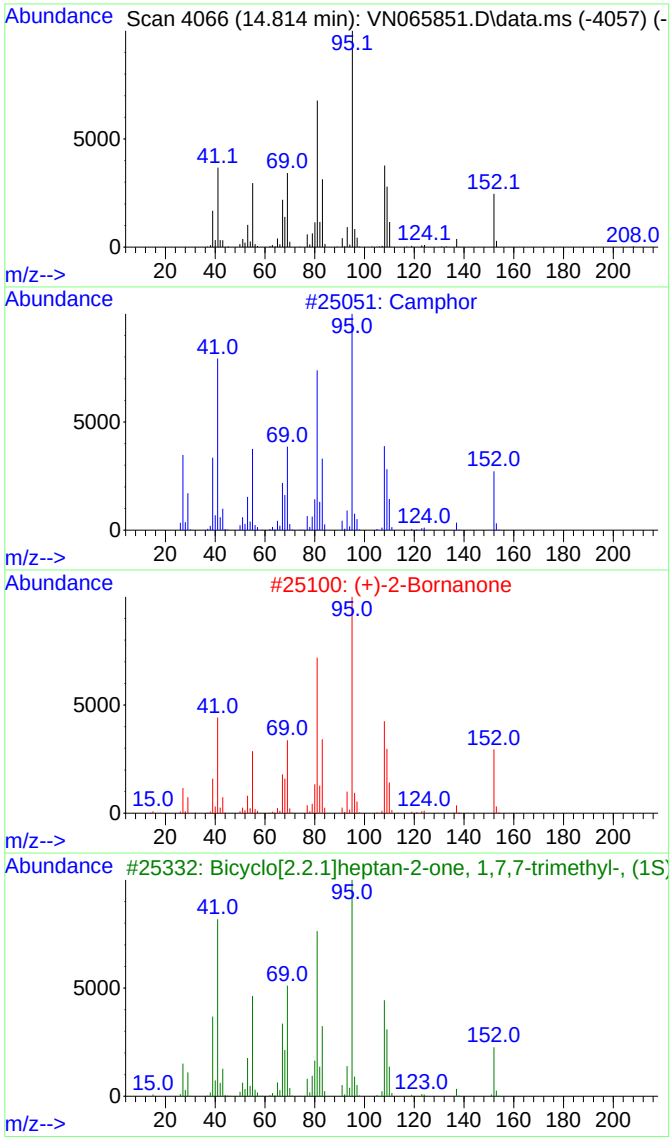
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

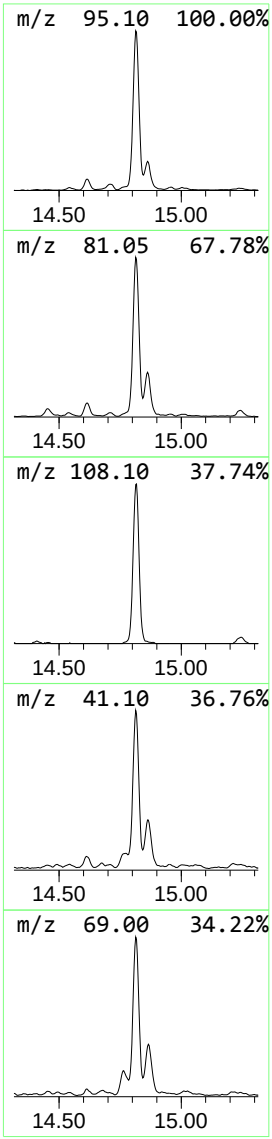
****

Peak Number 8 Camphor Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.814	59.29 ug/l	831948	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphor	152	C10H16O	000076-22-2	98
2	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	81
4	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	41
5	Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1000142-17-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065851.D
Acq On : 12 Feb 2021 20:26
Operator : JC/MD
Sample : M1386-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

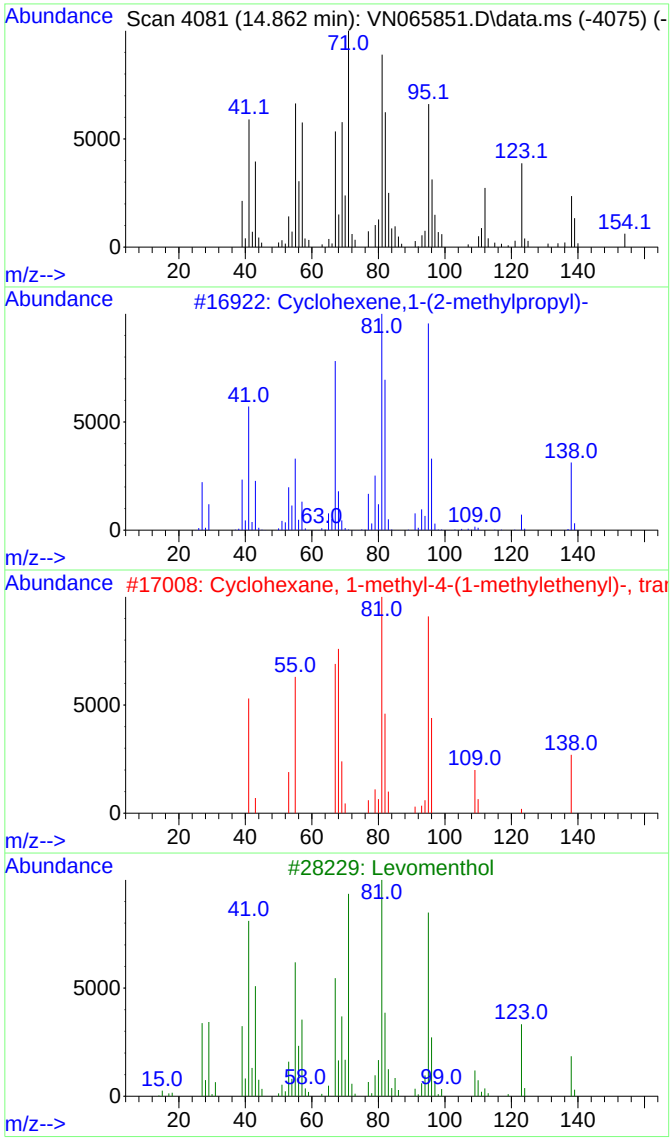
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

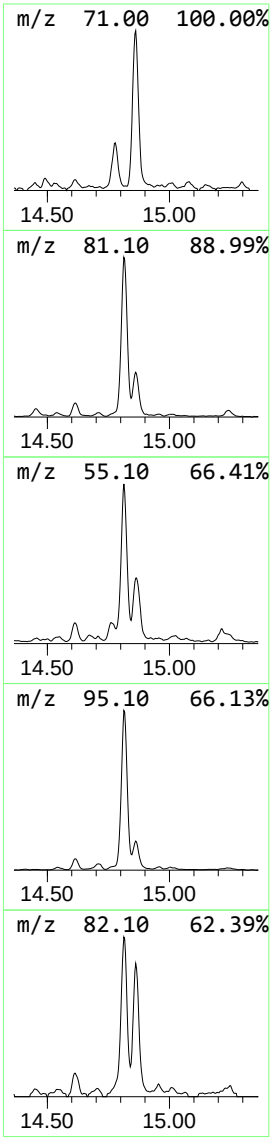
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclohexene,1-(2-methylprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.862	21.52 ug/l	301901	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene,1-(2-methylpropyl)-	138	C10H18	003983-03-7	78
2	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-25-0	70
3	Levomenthol	156	C10H20O	002216-51-5	64
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	59
5	6-Octen-1-ol, 3,7-dimethyl-, pro...	212	C13H24O2	000141-14-0	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065851.D
Acq On : 12 Feb 2021 20:26
Operator : JC/MD
Sample : M1386-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
210210007-02-VOA

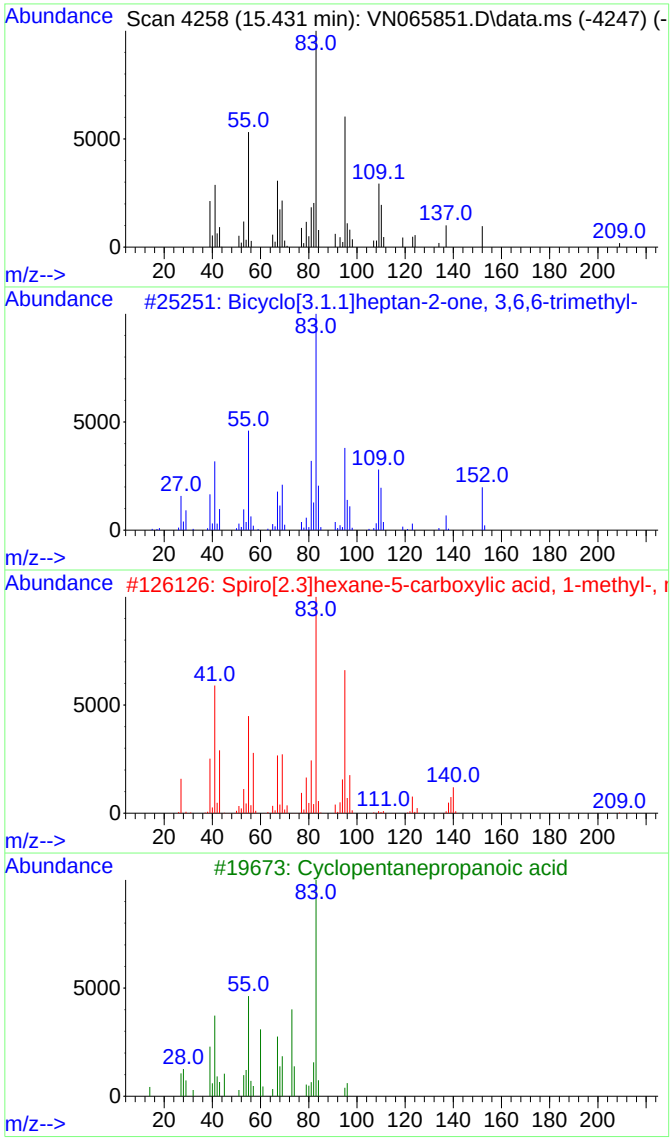
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.M
Quant Title : SW846 8260

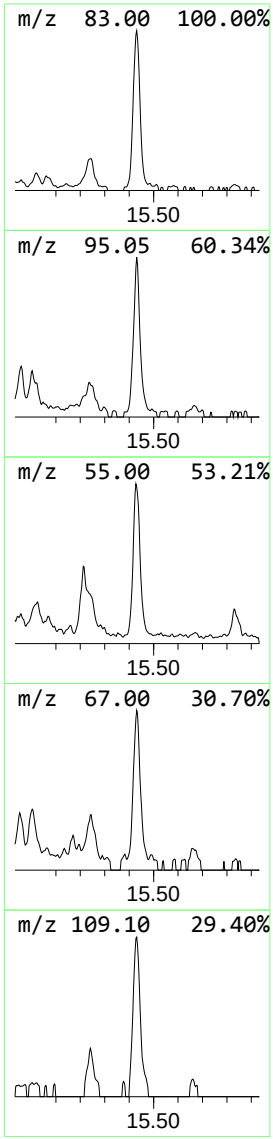
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Bicyclo[3.1.1]heptan-2-one,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.431	6.95 ug/l	97574	1,4-Dichlorobenzene-d4	13.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[3.1.1]heptan-2-one, 3,6,...	152	C10H16O	016022-08-5	64
2	Spiro[2.3]hexane-5-carboxylic ac...	278	C18H30O2	1000152-25-7	47
3	Cyclopentanepropanoic acid	142	C8H14O2	000140-77-2	43
4	Carbonic acid, butyl undec-10-en...	270	C16H30O3	1000314-63-8	35
5	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN021221\
Data File : VN065851.D
Acq On : 12 Feb 2021 20:26
Operator : JC/MD
Sample : M1386-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 210210007-02-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012521W.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
3-Hexanone, 2-m...	10.688	12.8	ug/l	192400	3	11.377	751426	50.0
unknown13.788	13.788	10.9	ug/l	153166	4	13.312	701562	50.0
unknown13.849	13.849	15.7	ug/l	220381	4	13.312	701562	50.0
Bicyclo[2.2.1]h...	14.190	66.1	ug/l	927506	4	13.312	701562	50.0
unknown14.614	14.614	7.0	ug/l	97619	4	13.312	701562	50.0
Camphene	14.772	7.4	ug/l	103980	4	13.312	701562	50.0
Camphor	14.814	59.3	ug/l	831948	4	13.312	701562	50.0
Cyclohexene,1-(...	14.862	21.5	ug/l	301901	4	13.312	701562	50.0
Bicyclo[3.1.1]h...	15.431	7.0	ug/l	97574	4	13.312	701562	50.0