LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210317059-01-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_X\Method\82X031621W.M
Title : SW846 8260

Signal : TIC: VX021311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.275	30	32	47	rVB	70937	122988	3.91%	0.743%
2	1.564	77	81	88	rBV	57618	62466	1.99%	0.378%
3	2.099	166	172	179	rBV	35913	58526	1.86%	0.354%
4	2.417	219	226	238	rBV	138733	247244	7.87%	1.495%
5	2.582	246	254	265	rVB	56571	106862	3.40%	0.646%
6	3.017	316	328	345	rBV	1350630	2922986	93.02%	17.670%
7	4.664	582	608	646	rBV	903294	3142313	100.00%	18.995%
8	5.088	668	680	701	rBV	330394	982218	31.26%	5.938%
9	5.464	733	744	756	rVV	55085	156083	4.97%	0.944%
10	5.623	760	771	786	rVB2	92451	263971	8.40%	1.596%
11	6.029	829	840	848	rBV	64216	168590	5.37%	1.019%
12	6.147	848	860	871	rVB4	46133	169313	5.39%	1.024%
13	6.306	879	887	897	rVB	22227	59707	1.90%	0.361%
14	6.829	965	976	991	rVV	139996	334052	10.63%	2.019%
15	8.618	1271	1280	1285	rVB2	15423	34218	1.09%	0.207%
16	8.694	1285	1293	1299	rBV	295354	454488	14.46%	2.747%
17	8.759	1299	1304	1313	rVB2	53560	90649	2.88%	0.548%
18	8.847	1313	1319	1324	rBV	35448	54459	1.73%	0.329%
19	9.418	1407	1416	1422	rBV	133535	194125	6.18%	1.173%
20	9.530	1430	1435	1441	rBV	22253	32014	1.02%	0.194%
21	10.094	1519	1531	1543	rBV	286049	456617	14.53%	2.760%
22	10.235	1550	1555	1561	rBV2	105056	159286	5.07%	0.963%
23	10.341	1568	1573	1579	rVB	100866	142285	4.53%	0.860%
24	10.683	1625	1631	1643	rVB	63886	94636	3.01%	0.572%
25	11.000	1678	1685	1691	rVB3	20093	36267	1.15%	0.219%
26	11.118	1699	1705	1711	rBV	220948	304295	9.68%	1.839%
27	11.418	1749	1756	1762	rVB2	20206	39726	1.26%	0.240%
28	11.542	1774	1777	1783	rVB	31458	40650	1.29%	0.246%
29	11.789	1815	1819	1823	rVB	41892	50941	1.62%	0.308%
30	11.924	1838	1842	1850	rVB	55009	70151	2.23%	0.424%
31	12.059	1859	1865	1872	rVB2	290672	425501	13.54%	2.572%
32	12.142	1872	1879	1883	rBV3	84284	133455	4.25%	0.807%
33	12.283	1894	1903	1913	rBV2	41344	85492	2.72%	0.517%
34	12.453	1927	1932	1939	rBV4	23413	42435	1.35%	0.257%
35	12.559	1946	1950	1952	rBV2	26344	35093	1.12%	0.212%
36	12.612	1956	1959	1964	rVB	54189	65171	2.07%	0.394%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210317059-01-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_X\Method\82X031621W.M
Title : SW846 8260

37	12.801	1984	1991	1996	rVV	123684	175253	5.58%	1.059%
38	12.942	2003	2015	2021	rBV	730294	1001432	31.87%	6.054%
39	13.001	2021	2025	2029	rVB2	40008	60937	1.94%	0.368%
40	13.206	2055	2060	2064	rBV3	18979	31665	1.01%	0.191%
41	13.254	2064	2068	2074	rVB4	32225	54635	1.74%	0.330%
42	13.324	2074	2080	2084	rVB4	22944	36935	1.18%	0.223%
43	13.371	2084	2088	2093	rBV	88315	125917	4.01%	0.761%
44	13.465	2100	2104	2107	rVB	31465	41426	1.32%	0.250%
45	13.512	2107	2112	2114	rBV2	137615	177599	5.65%	1.074%
46	13.548	2114	2118	2126	rVB	1069533	1428607	45.46%	8.636%
47	13.630	2126	2132	2141	rBV2	248016	371903	11.84%	2.248%
48	13.771	2151	2156	2159	rBV	140329	176758	5.63%	1.069%
49	13.812	2159	2163	2170	rVB	353102	457645	14.56%	2.766%
50	13.977	2183	2191	2196	rBV3	31585	75169	2.39%	0.454%
51	14.136	2212	2218	2230	rBV	196525	274267	8.73%	1.658%
52	14.677	2306	2310	2314	rVV	49353	60105	1.91%	0.363%
53	14.818	2327	2334	2340	rVB	43177	61598	1.96%	0.372%
54	16.277	2569	2582	2593	rBV9	11877	33343	1.06%	0.202%
55	16.383	2593	2600	2611	rVB	29582	58025	1.85%	0.351%

Sum of corrected areas: 16542492

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Operator : JC/MD
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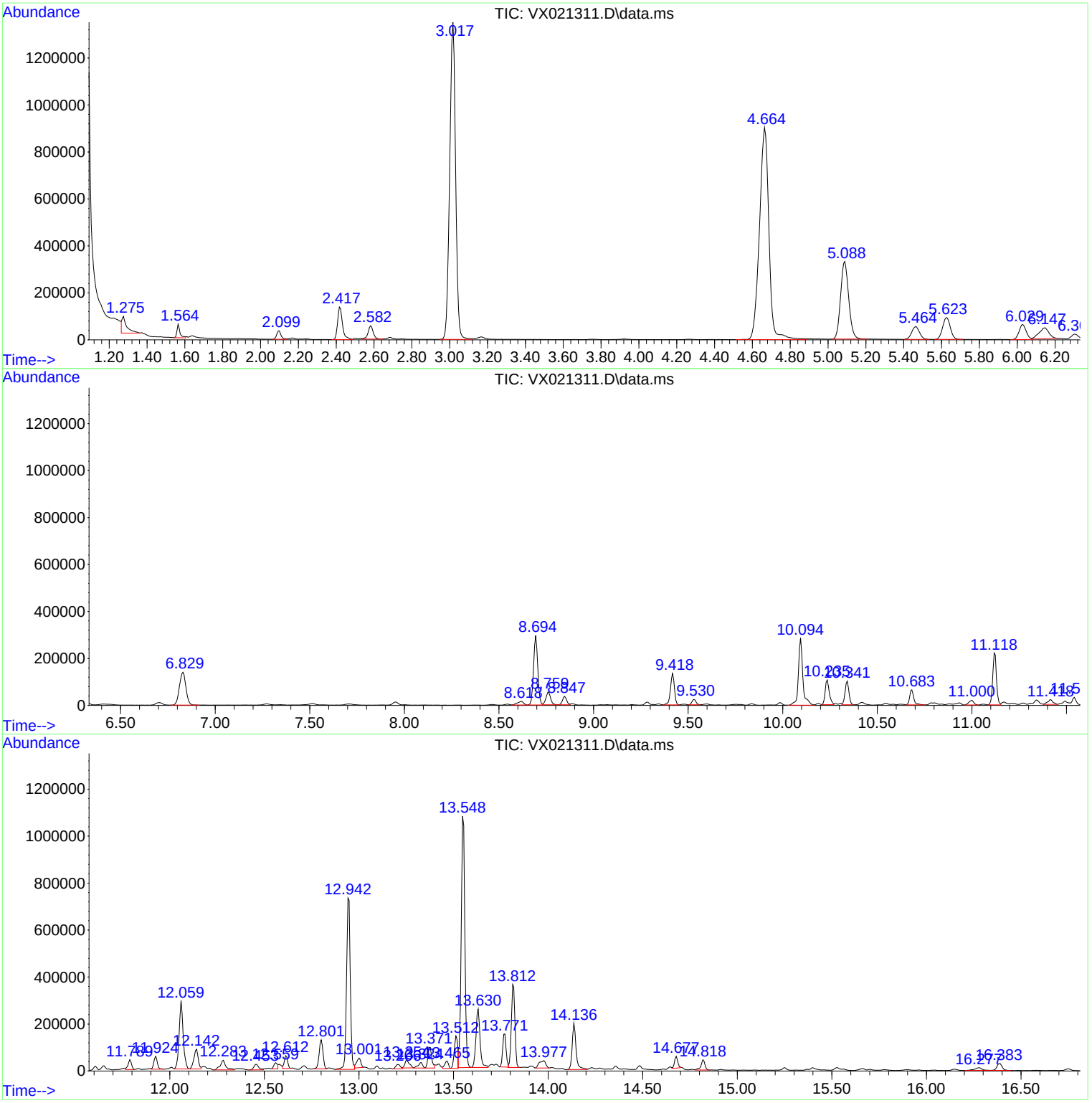
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210317059-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210317059-01-VOA

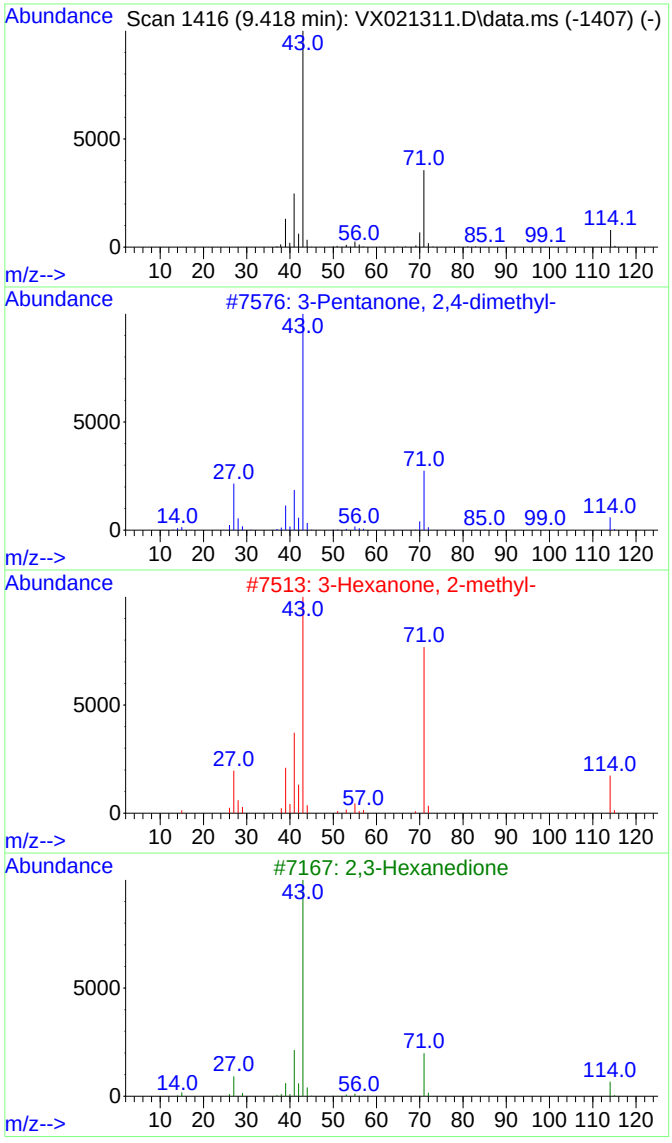
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

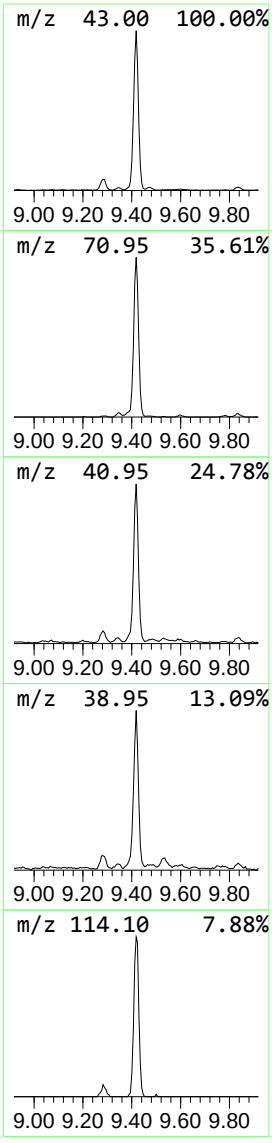
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.418	21.26 ug/l	194125	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	64
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	53
4	2,5-Hexanedione	114	C6H10O2	000110-13-4	50
5	4-Heptanone	114	C7H14O	000123-19-3	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210317059-01-VOA

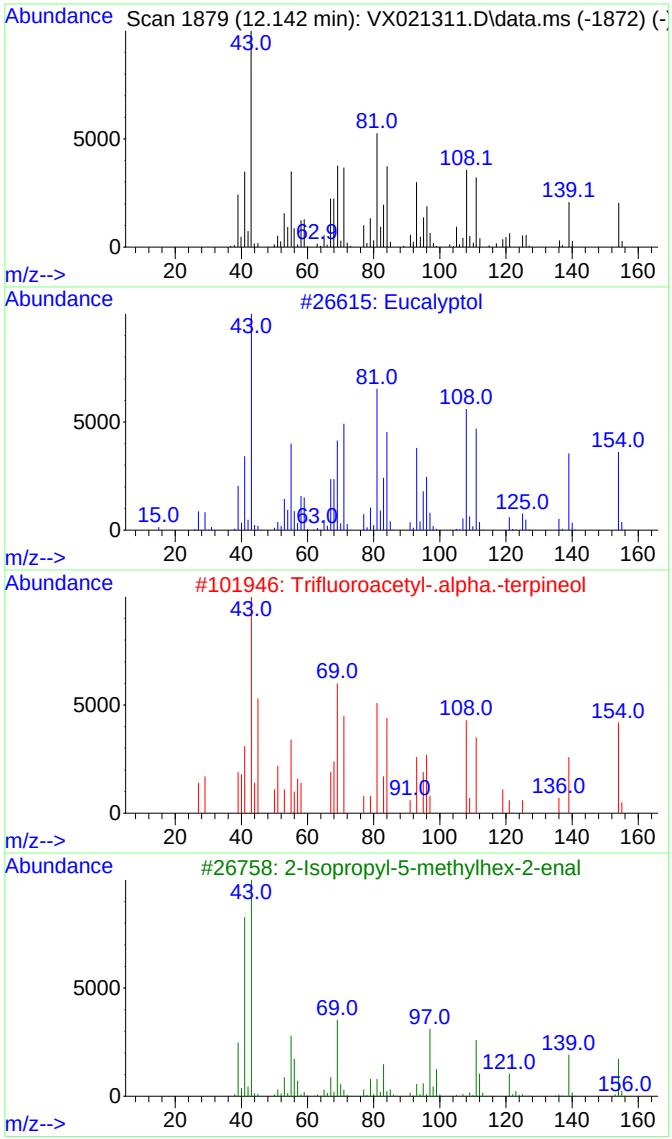
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

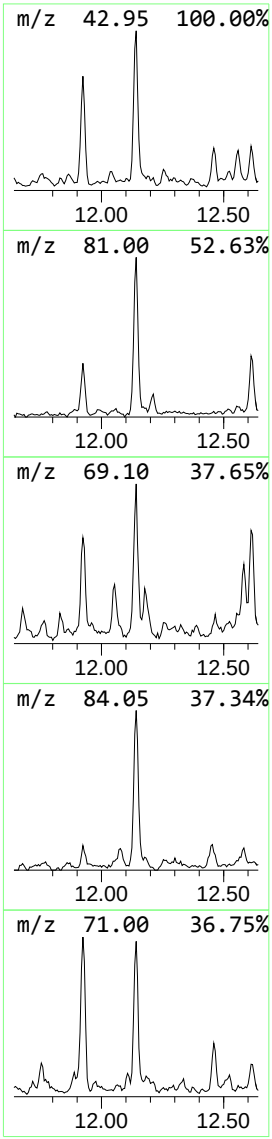
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.142	15.68 ug/l	133455	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	97
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	53
3	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	35
4	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	35
5	1-Cyclopentene-1-methanol, .alph...	154	C10H18O	056666-69-4	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210317059-01-VOA

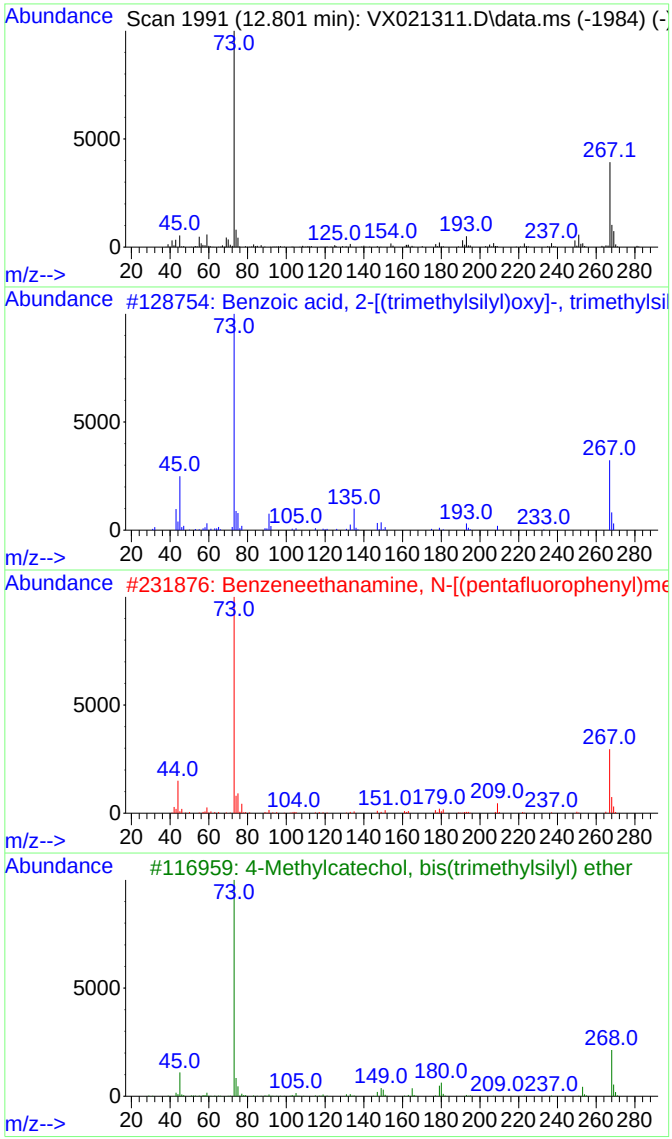
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

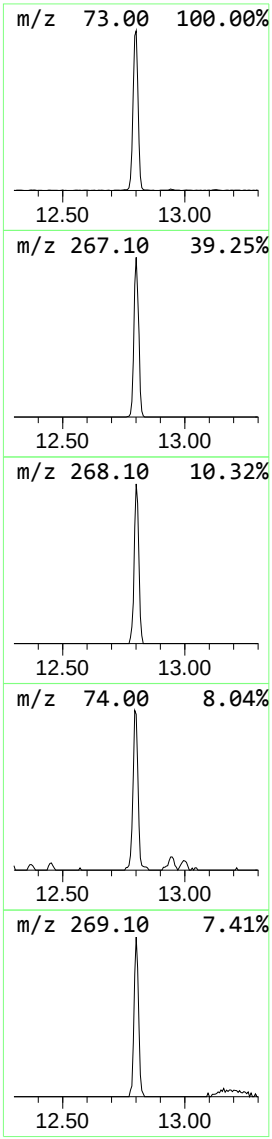
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzoic acid, 2-[(trimethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.801	20.59 ug/l	175253	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	72
2	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	45
3	4-Methylcatechol, bis(trimethyls...	268	C13H24O2Si2	1000332-79-9	22
4	Tetrasiloxane, 1,1,3,3,5,5,7,7-o...	282	C8H26O3Si4	001000-05-1	16
5	11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
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Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210317059-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

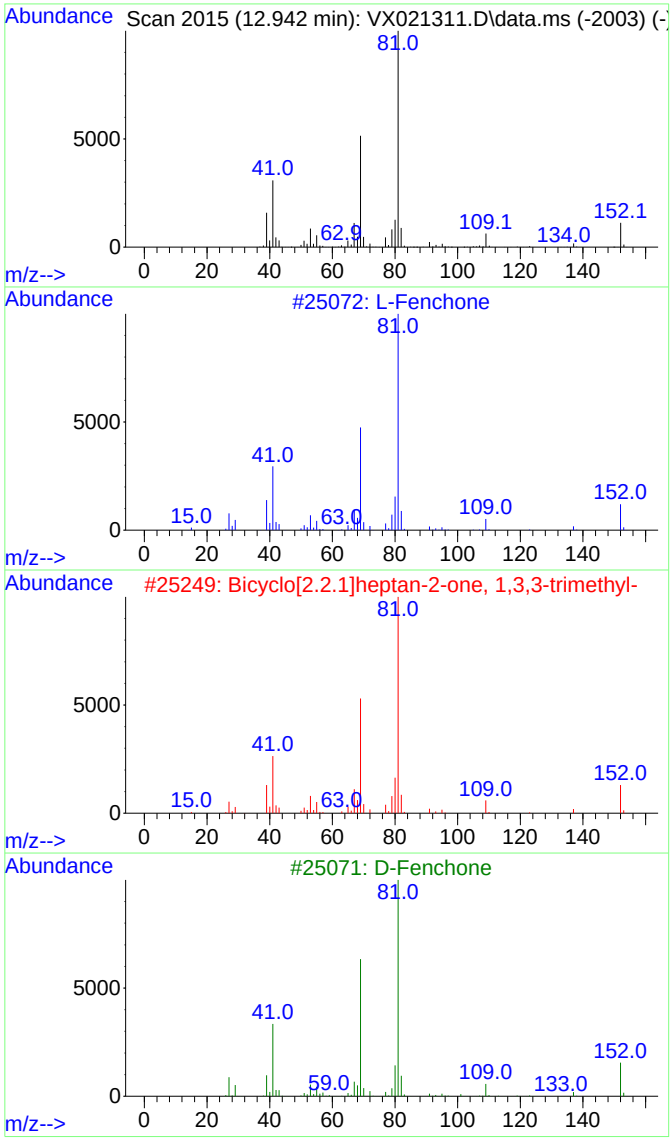
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

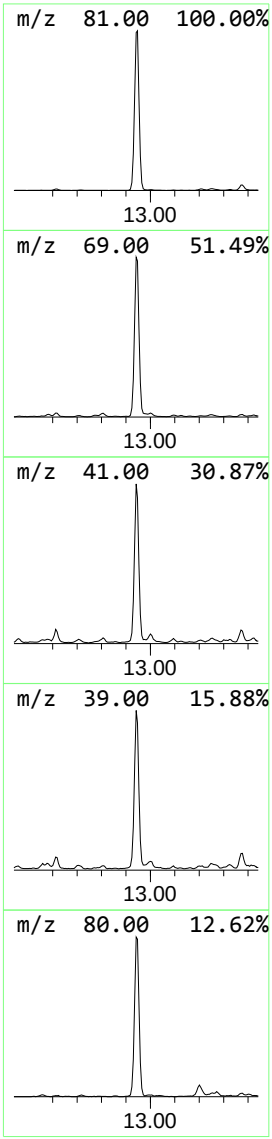
****

Peak Number 5 L-Fenchone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.942	117.68 ug/l	1001430	1,4-Dichlorobenzene-d4	12.059

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	2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	59
5	Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42





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Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210317059-01-VOA

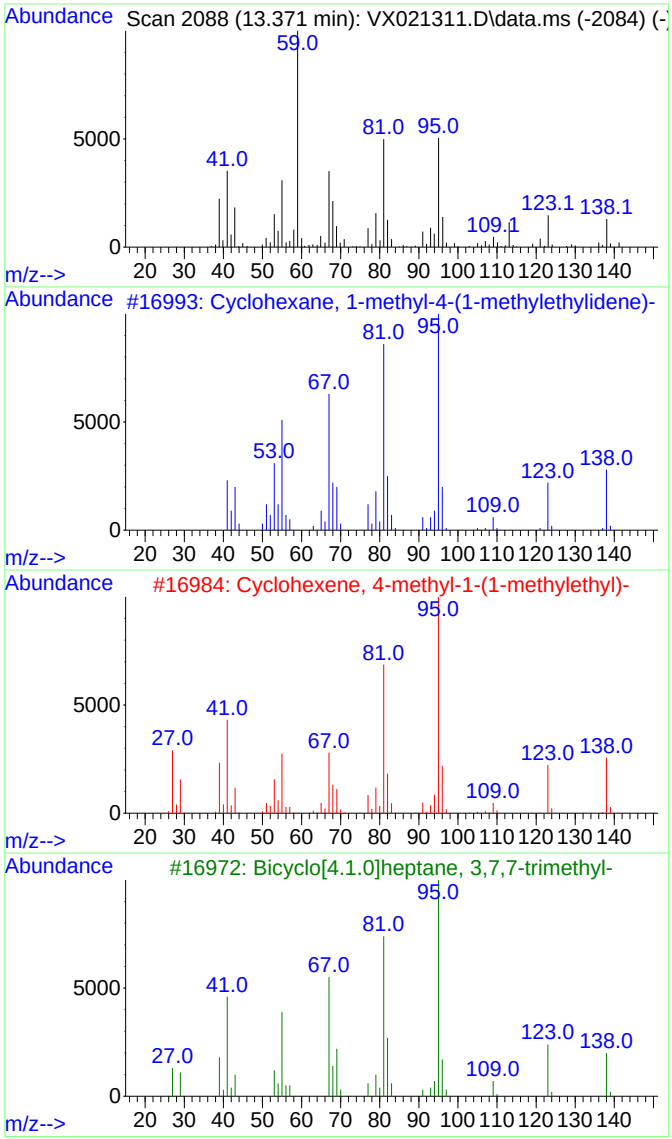
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

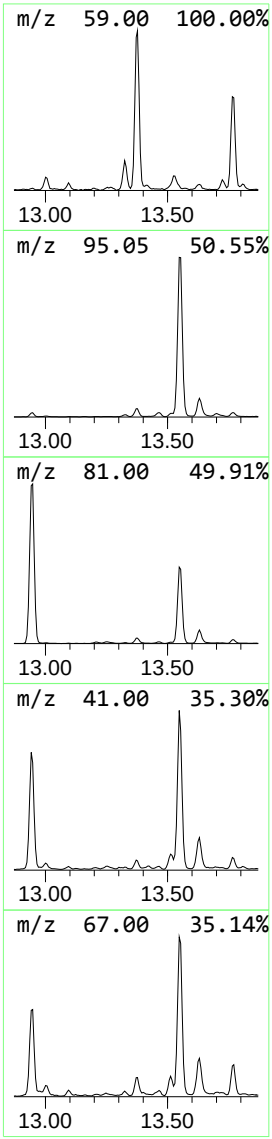
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclohexane, 1-methyl-4-(1-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.371	14.80 ug/l	125917	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001124-27-2	89
2	Cyclohexene, 4-methyl-1-(1-methy...	138	C10H18	000500-00-5	80
3	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	000554-59-6	46
4	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	018968-23-5	46
5	Cyclohexane, 1-methyl-3-(1-methy...	138	C10H18	024399-15-3	45





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Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

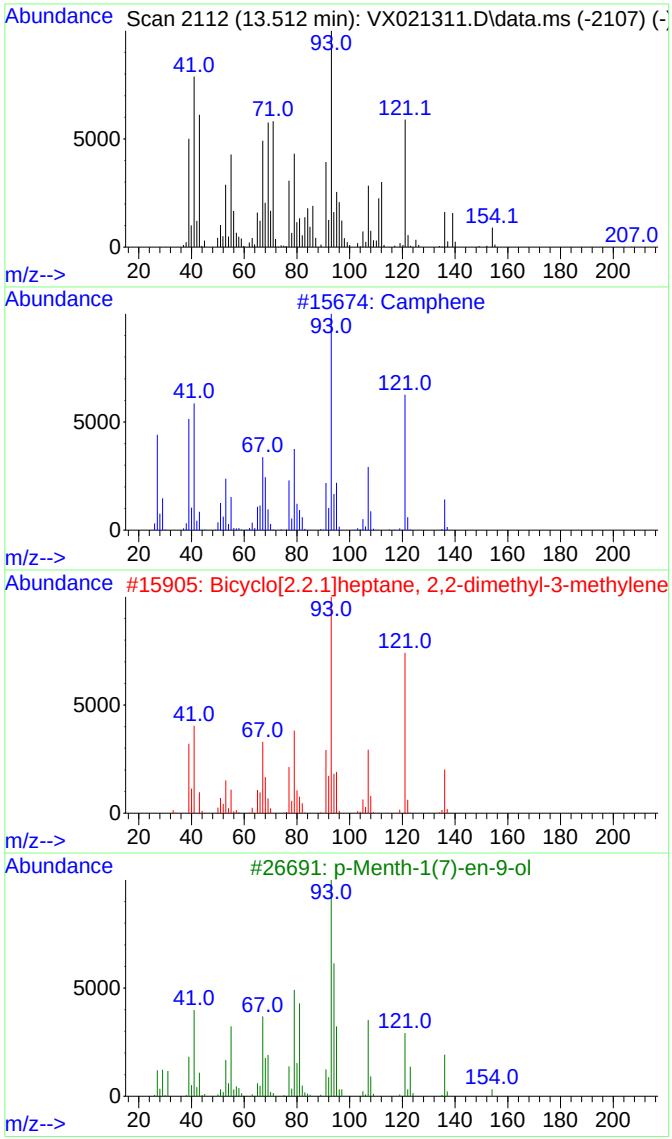
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

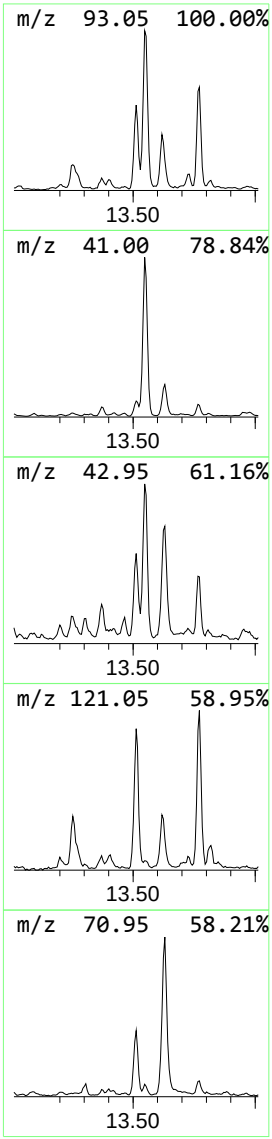
****

Peak Number 7 Camphene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	20.87 ug/l	177599	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Camphene	136	C10H16	000079-92-5	95
2	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	005794-04-7	83
3	p-Menth-1(7)-en-9-ol	154	C10H18O	029548-16-1	53
4	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	50
5	p-Menth-2-en-7-ol, trans-	154	C10H18O	019898-87-4	49





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Data File : VX021311.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210317059-01-VOA

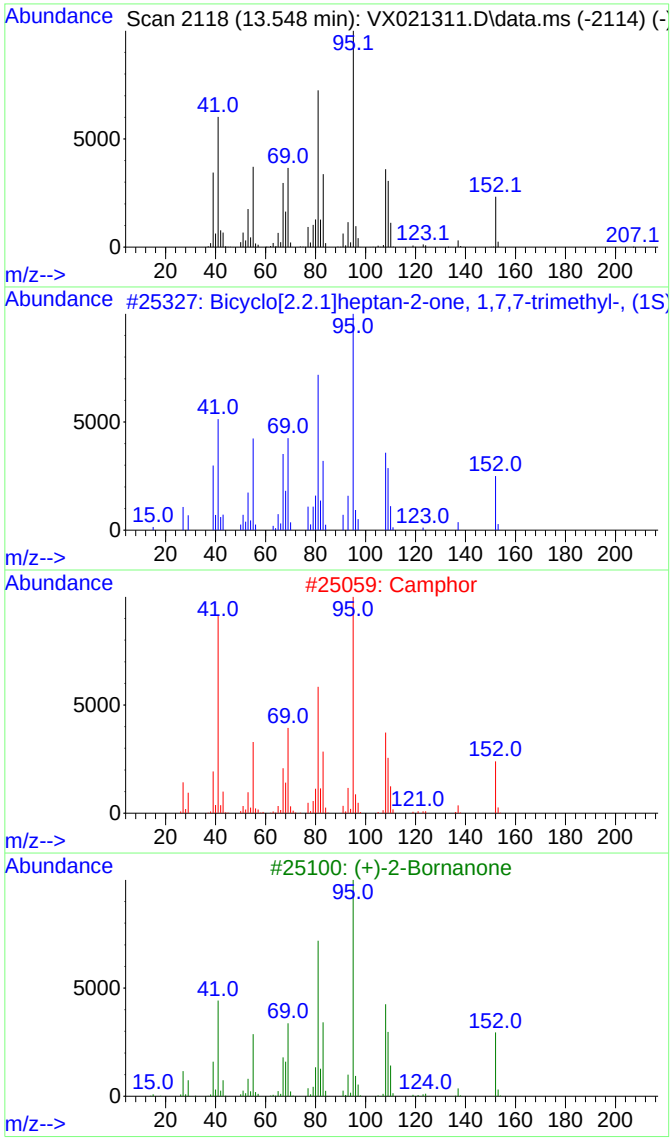
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

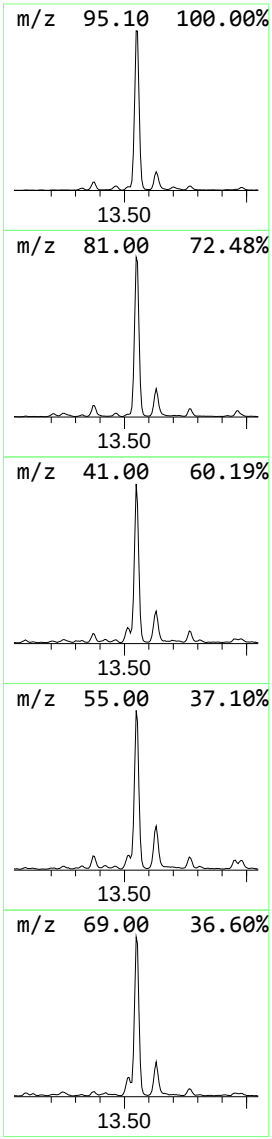
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.548	167.87 ug/l	1428610	1,4-Dichlorobenzene-d4	12.059

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	Camphor	152	C10H16O	000076-22-2	97
3	(+)-2-Bornanone	152	C10H16O	000464-49-3	97
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	64
5	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46





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Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210317059-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

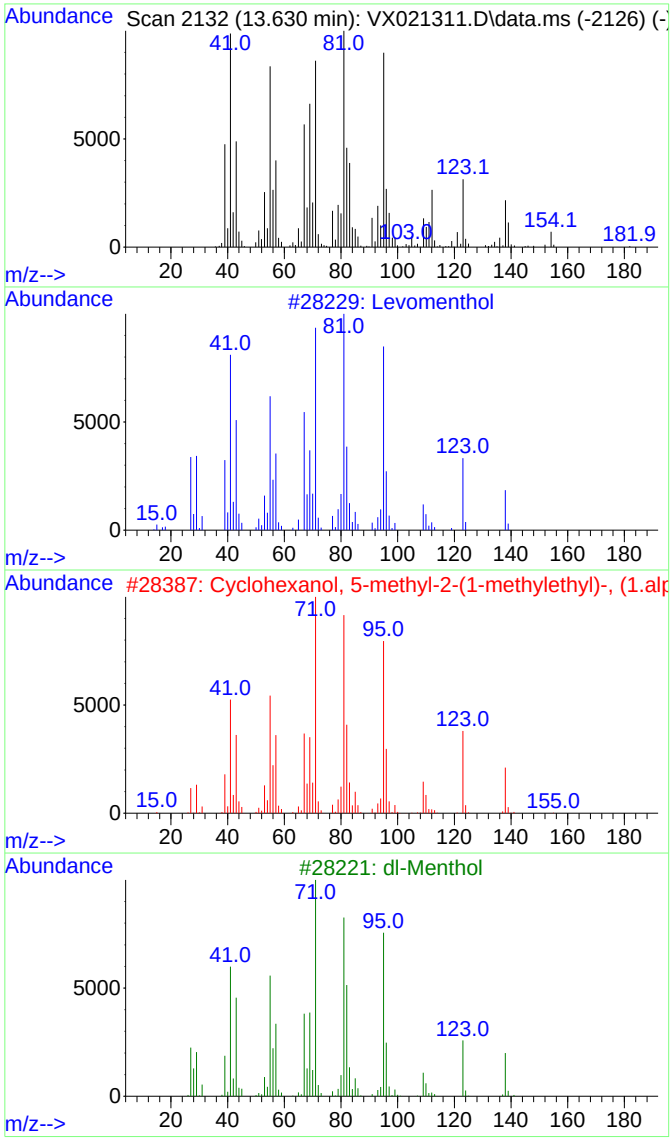
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

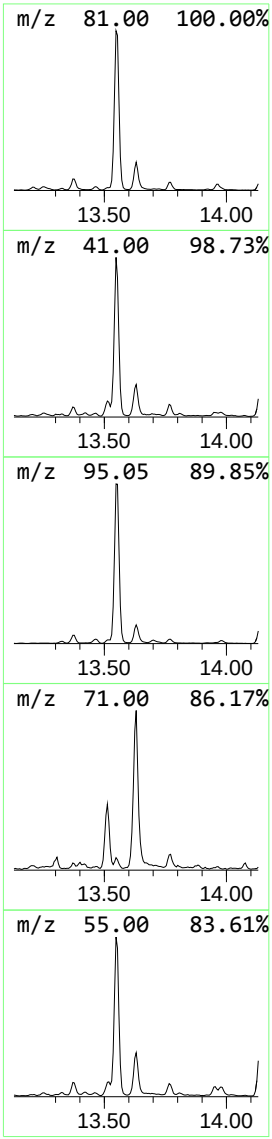
****

Peak Number 9 Levomenthol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.630	43.70 ug/l	371903	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Levomenthol	156	C10H20O	002216-51-5	87
2	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	74
3	dl-Menthol	156	C10H20O	000089-78-1	74
4	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	72
5	Bicyclo[4.1.0]heptane, 3,7,7-tri...	138	C10H18	002778-68-9	60





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
210317059-01-VOA

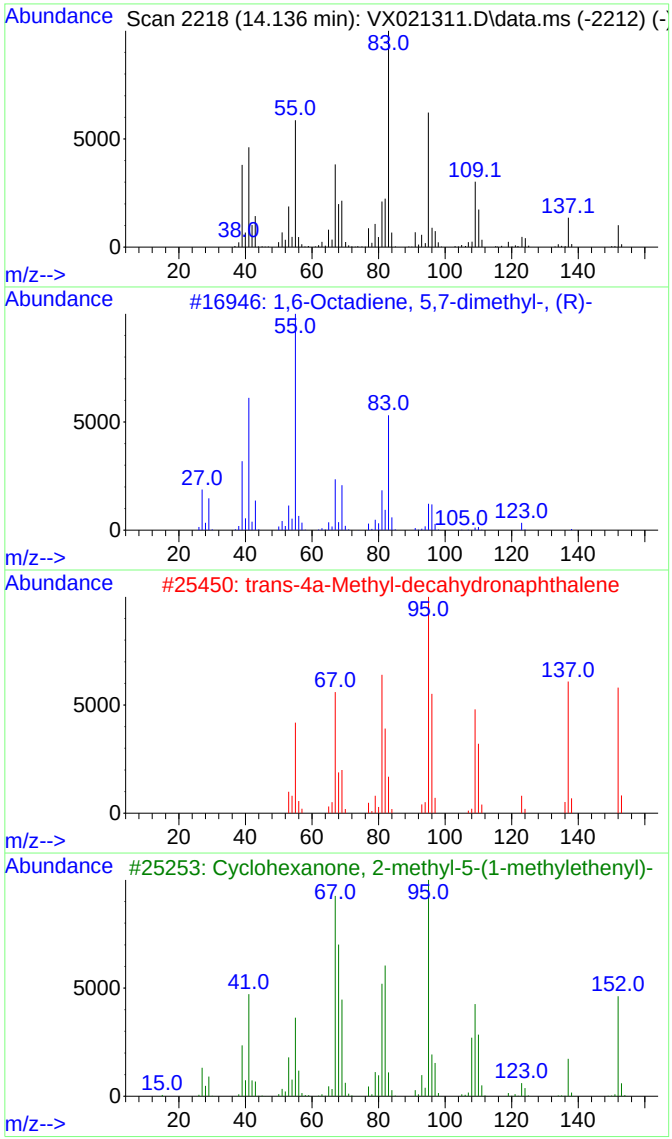
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.M
Quant Title : SW846 8260

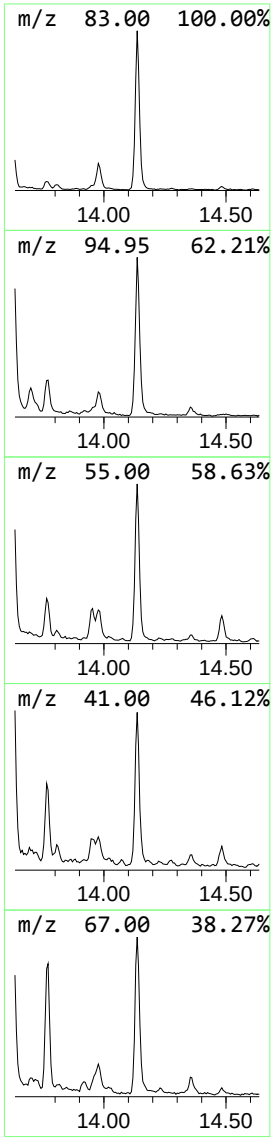
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1,6-Octadiene, 5,7-dimethyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.136	32.23 ug/l	274267	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	50
2	trans-4a-Methyl-decahydronaphtha...	152	C11H20	002547-27-5	46
3	Cyclohexanone, 2-methyl-5-(1-met...	152	C10H16O	007764-50-3	43
4	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	000764-13-6	38
5	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	018669-52-8	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032121\
Data File : VX021311.D
Acq On : 19 Mar 2021 18:47
Operator : JC/MD
Sample : M1716-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 210317059-01-VOA

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031621W.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-Pentanone, 2,...	9.418	21.3	ug/l	194125	3	10.094	456617	50.0
Eucalyptol	12.142	15.7	ug/l	133455	4	12.059	425501	50.0
Benzoic acid, 2...	12.801	20.6	ug/l	175253	4	12.059	425501	50.0
L-Fenchone	12.942	117.7	ug/l	1001430	4	12.059	425501	50.0
Cyclohexane, 1-...	13.371	14.8	ug/l	125917	4	12.059	425501	50.0
Camphene	13.512	20.9	ug/l	177599	4	12.059	425501	50.0
Bicyclo[2.2.1]h...	13.548	167.9	ug/l	1428610	4	12.059	425501	50.0
Levomenthol	13.630	43.7	ug/l	371903	4	12.059	425501	50.0
1,6-Octadiene, ...	14.136	32.2	ug/l	274267	4	12.059	425501	50.0