LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

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\82X050420W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.471	60	63	73	rVB	150736	172709	2.21%	0.332%
2	2.087	158	164	173	rBV	424307	649426	8.31%	1.248%
3	2.416	212	218	232	rVB	996570	1602560	20.50%	3.078%
4	2.685	255	262	271	rBV	64702	123340	1.58%	0.237%
5	3.916	456	464	477	rBV	38323	103244	1.32%	0.198%
6	4.635	571	582	593	rBV	135247	386496	4.94%	0.742%
7	5.471	706	719	730	rBV	126431	368278	4.71%	0.707%
8	5.629	735	745	759	rVB	227970	644238	8.24%	1.238%
9	6.038	797	812	821	rBV	140349	373517	4.78%	0.718%
10	6.708	911	922	933	rBV	73497	187754	2.40%	0.361%
11	6.830	933	942	955	rVV	362762	856786	10.96%	1.646%
12	7.513	1047	1054	1067	rVB	110353	215798	2.76%	0.415%
13	8.622	1229	1236	1241	rBV	61339	97667	1.25%	0.188%
14	8.696	1241	1248	1254	rBV	768019	1184625	15.16%	2.276%
15	9.476	1371	1376	1383	rVB	96027	133306	1.71%	0.256%
16	10.098	1468	1478	1490	rVV	796440	1099697	14.07%	2.112%
17	10.622	1559	1564	1571	rBV	62618	97967	1.25%	0.188%
18	10.805	1589	1594	1599	rBV	112011	141077	1.80%	0.271%
19	11.122	1640	1646	1651	rBV	691068	852817	10.91%	1.638%
20	11.659	1728	1734	1737	rBV	96132	117530	1.50%	0.226%
21	11.799	1750	1757	1761	rVB	121442	154613	1.98%	0.297%
22	11.878	1766	1770	1775	rVV	388683	453735	5.81%	0.872%
23	12.061	1795	1800	1807	rVB	872250	1121945	14.35%	2.155%
24	12.146	1807	1814	1820	rBV	5794469	7815923	100.00%	15.014%
25	12.256	1827	1832	1841	rBV	1149331	1526840	19.53%	2.933%
26	12.384	1849	1853	1858	rVB	82545	108855	1.39%	0.209%
27	12.494	1867	1871	1878	rVB2	59596	92583	1.18%	0.178%
28	12.622	1884	1892	1904	rBV4	212049	444352	5.69%	0.854%
29	12.725	1905	1909	1915	rVB	68639	85524	1.09%	0.164%
30	12.805	1917	1922	1925	rBV	211004	238874	3.06%	0.459%
31	12.860	1925	1931	1934	rVV3	117446	187339	2.40%	0.360%
32	13.012	1951	1956	1967	rBV	1846821	2597917	33.24%	4.991%
33	13.109	1968	1972	1974	rVV	2257486	2685041	34.35%	5.158%
34	13.140	1974	1977	1993	rVB	4034233	5592187	71.55%	10.742%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

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\82X050420W.M
Title : SW846 8260

35	13.463	2025	2030	2039	rBV	4860611	6076081	77.74%	11.672%
36	13.548	2039	2044	2052	rVV	3025679	4217571	53.96%	8.102%
37	13.634	2054	2058	2066	rVB2	199106	316678	4.05%	0.608%
38	13.744	2072	2076	2078	rBV	976161	1196367	15.31%	2.298%
39	13.786	2081	2083	2096	rVV	1351650	1905247	24.38%	3.660%
40	13.896	2097	2101	2104	rVV	1133781	1555832	19.91%	2.989%
41	13.926	2104	2106	2119	rVB	1436134	2060547	26.36%	3.958%
42	14.146	2138	2142	2147	rVB	191868	221351	2.83%	0.425%
43	14.237	2152	2157	2164	rBV	398625	646460	8.27%	1.242%
44	14.445	2187	2191	2195	rBV	341640	379933	4.86%	0.730%
45	14.487	2195	2198	2201	rBV	128366	173343	2.22%	0.333%
46	14.524	2201	2204	2214	rVB	112214	196590	2.52%	0.378%
47	14.609	2214	2218	2221	rBV	102940	158494	2.03%	0.304%
48	14.731	2235	2238	2251	rVB	90255	174470	2.23%	0.335%
49	14.835	2251	2255	2267	rVB2	97974	174063	2.23%	0.334%
50	15.298	2326	2331	2345	rBV	42935	89594	1.15%	0.172%

Sum of corrected areas: 52057181

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
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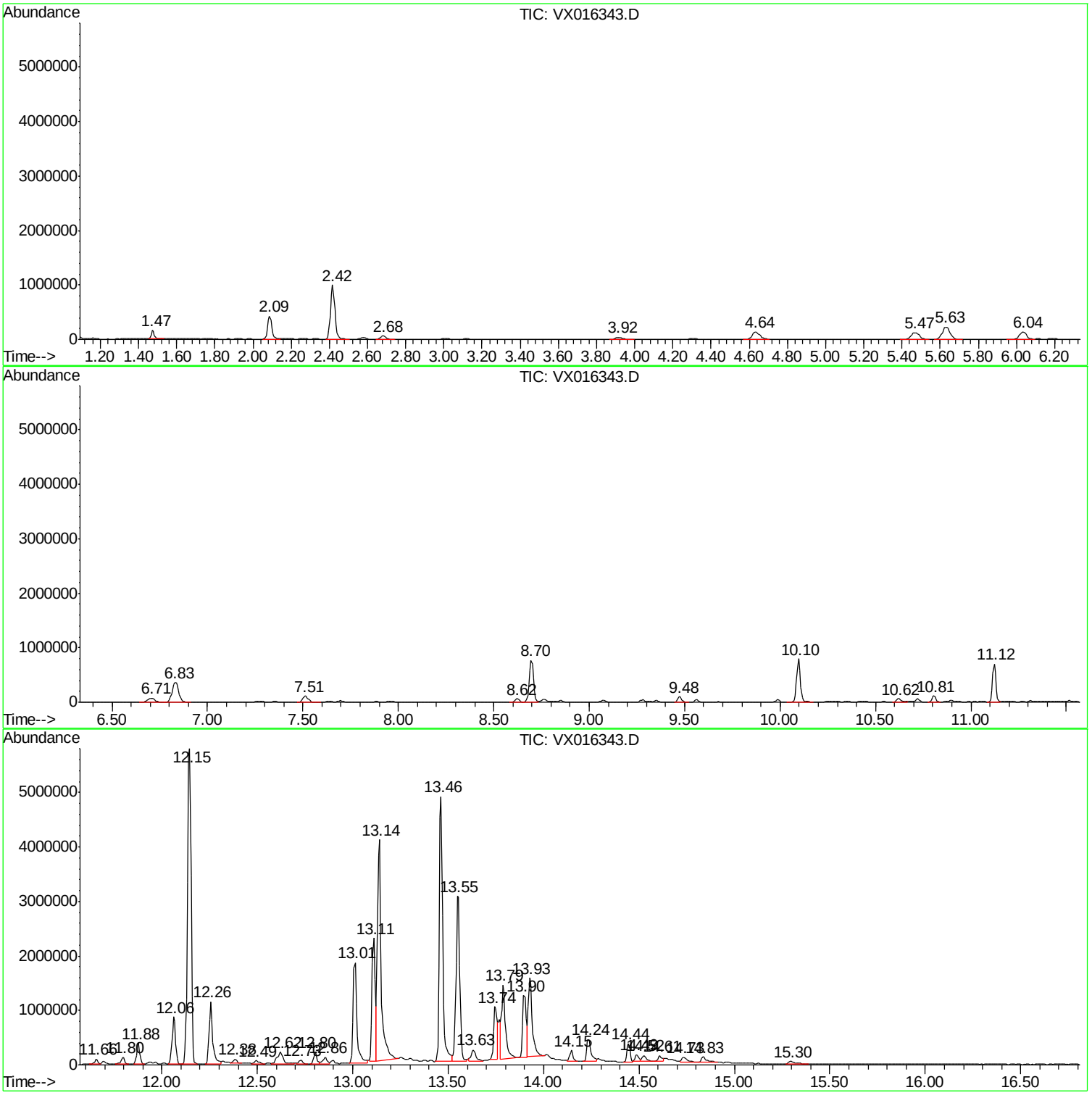
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

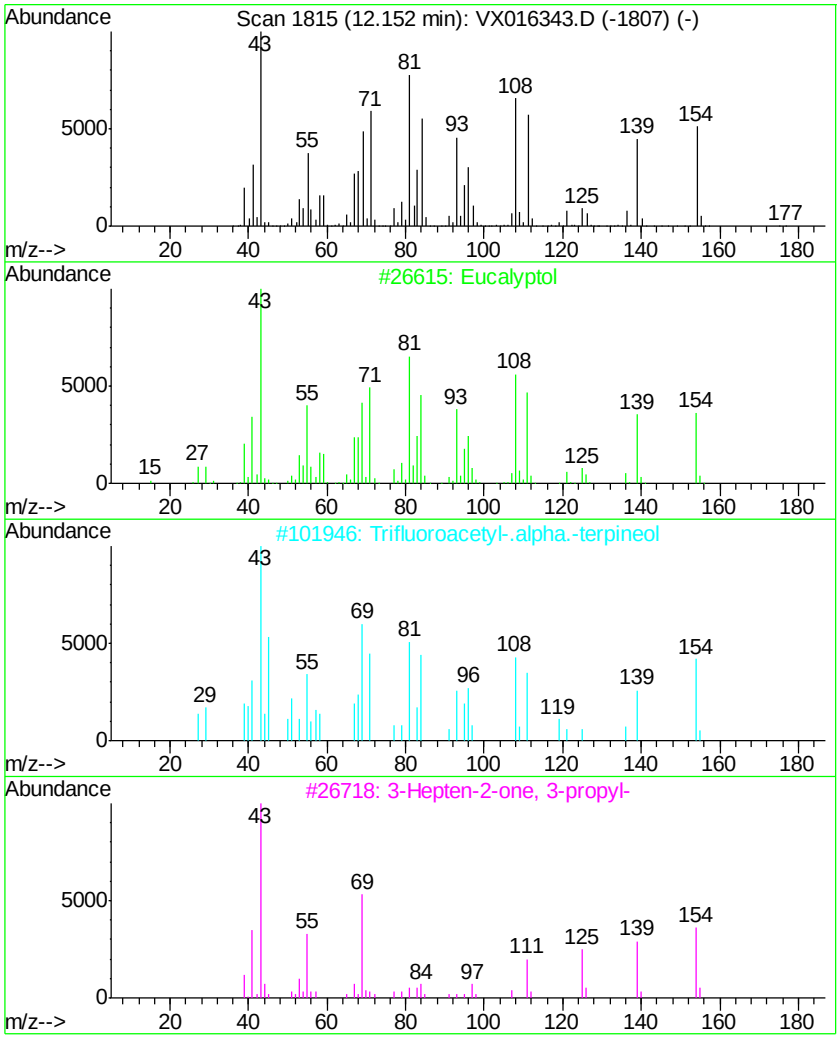
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

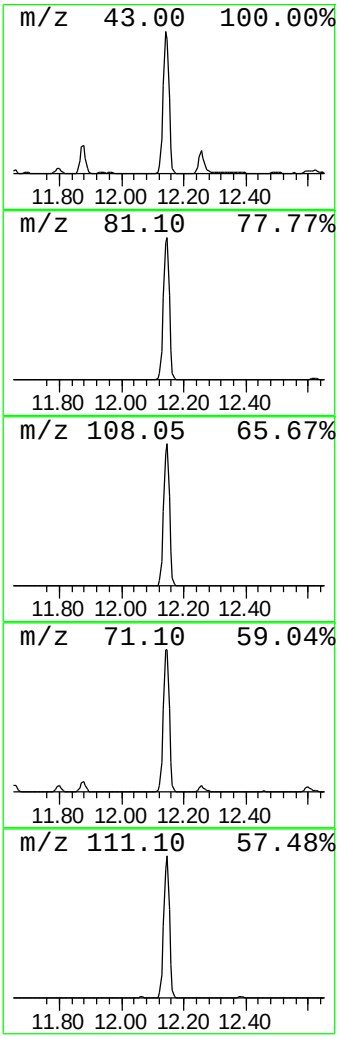
****

Peak Number 1 Eucalyptol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.15	348.32 ug/l	7815920	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	52
3	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
4	Cyclohexene, 3-methyl-	96	C7H12	000591-48-0	25
5	Cyclohexene, 1-methyl-	96	C7H12	000591-49-1	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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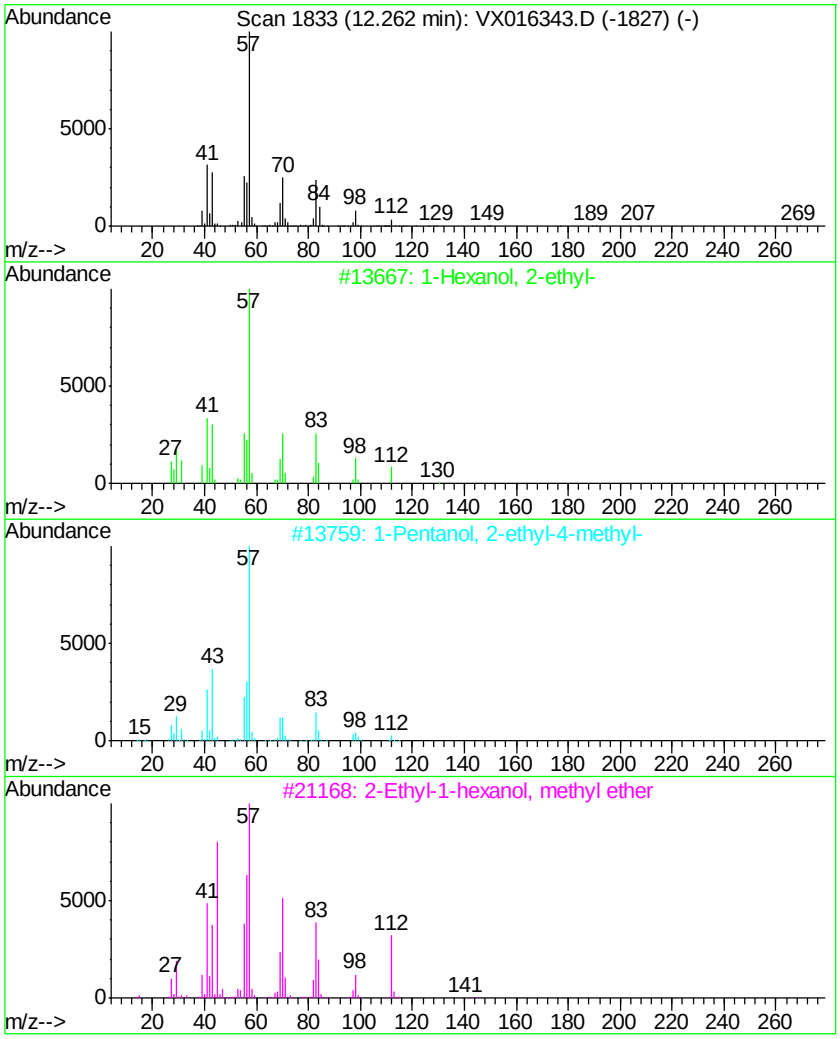
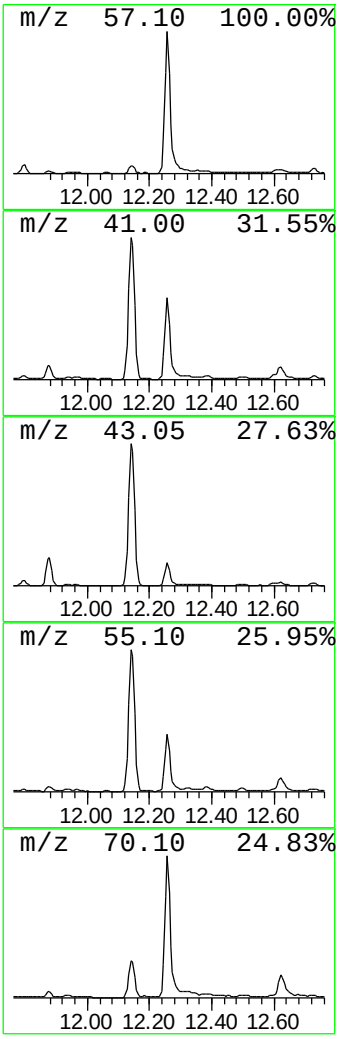
Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	68.04 ug/l	1526840	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	45





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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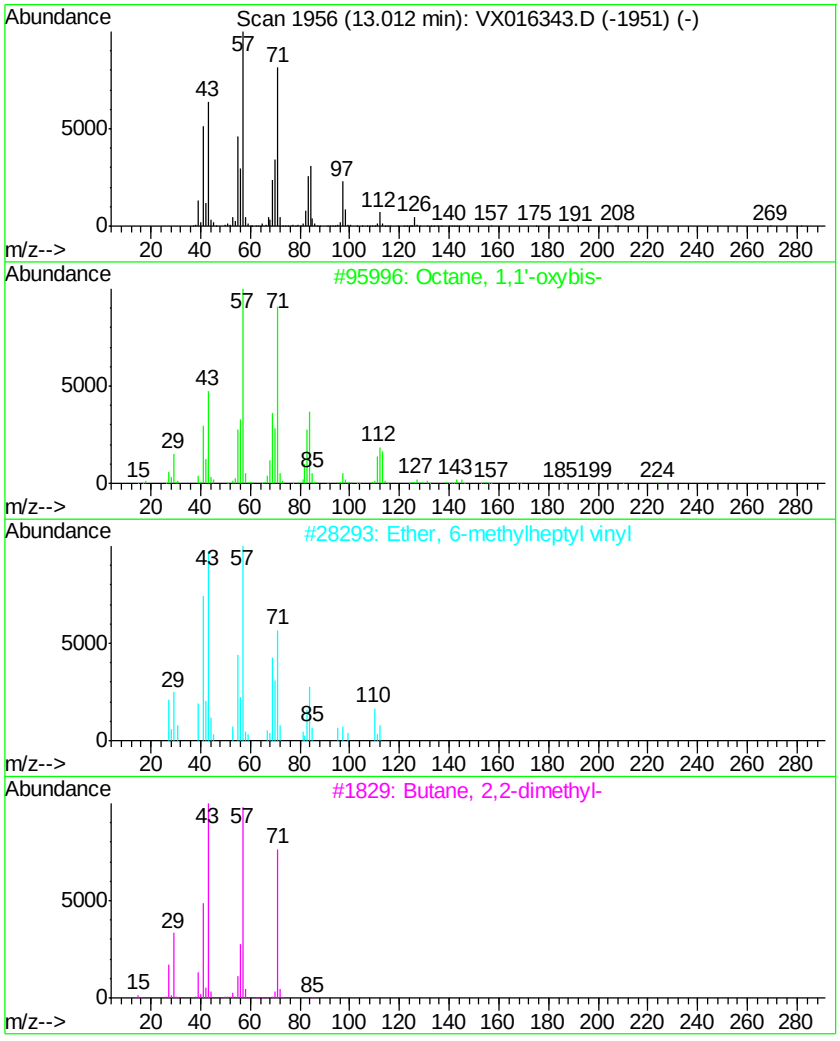
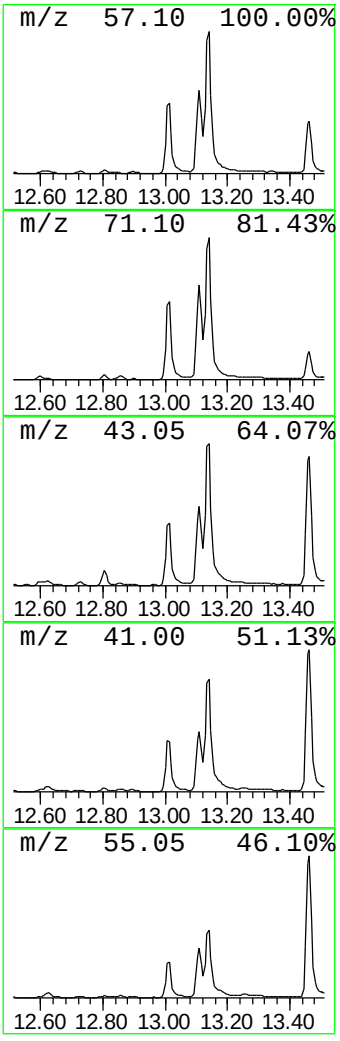
Peak Number 3 Octane, 1,1'-oxybis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	115.78 ug/l	2597920	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	72
2	Ether, 6-methylheptyl vinyl	156	C10H20O	010573-35-0	72
3	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43
4	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43
5	1-Fluorononane	146	C9H19F	000463-18-3	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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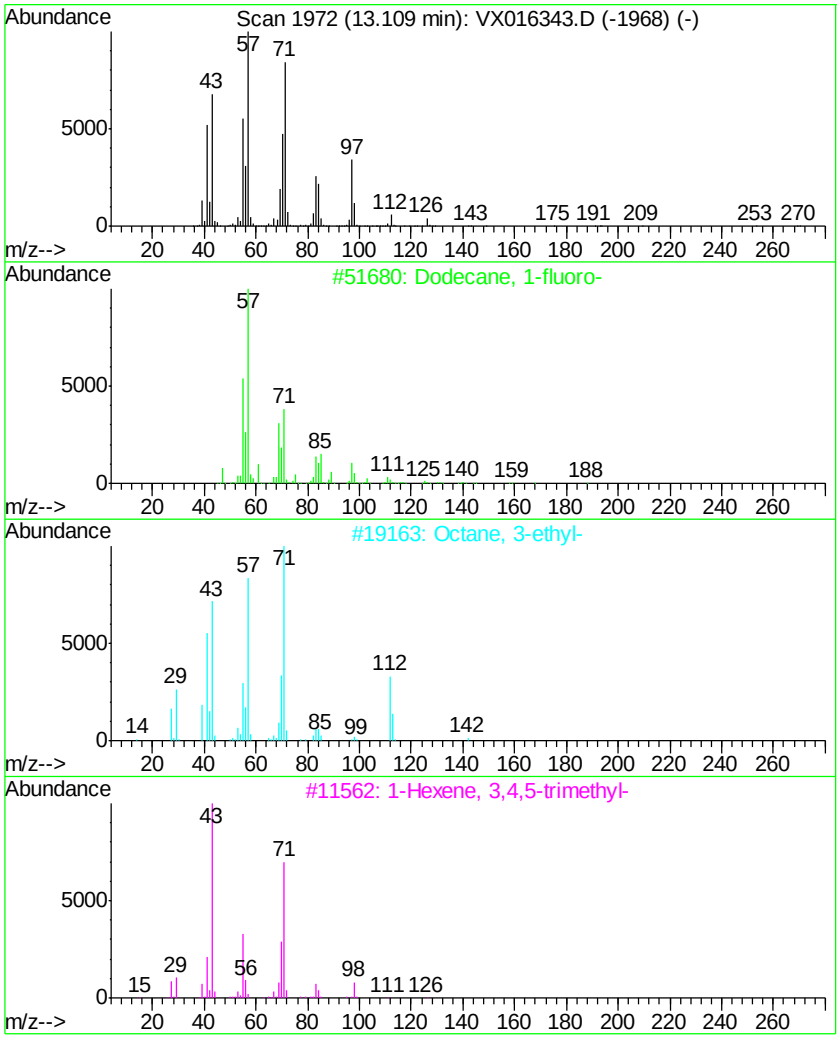
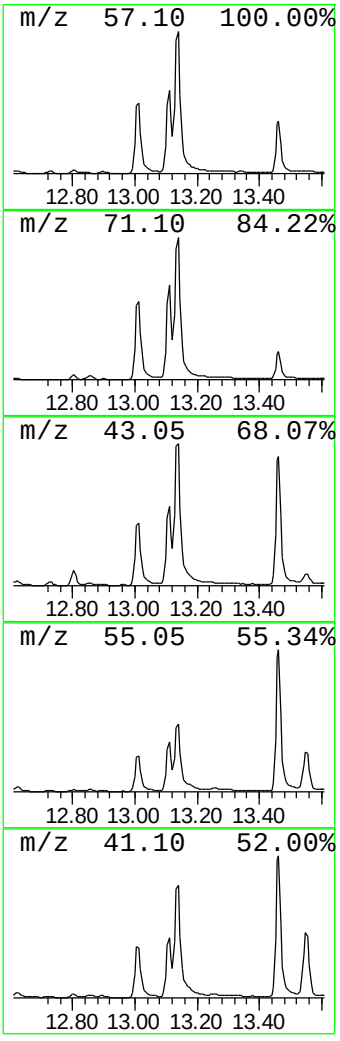
Peak Number 4 Dodecane, 1-fluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.11	119.66 ug/l	2685040	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-fluoro-	188	C12H25F	000334-68-9	64
2	Octane, 3-ethyl-	142	C10H22	005881-17-4	47
3	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	47
4	Sulfurous acid, butyl octyl ester	250	C12H26O3S	1000309-17-5	47
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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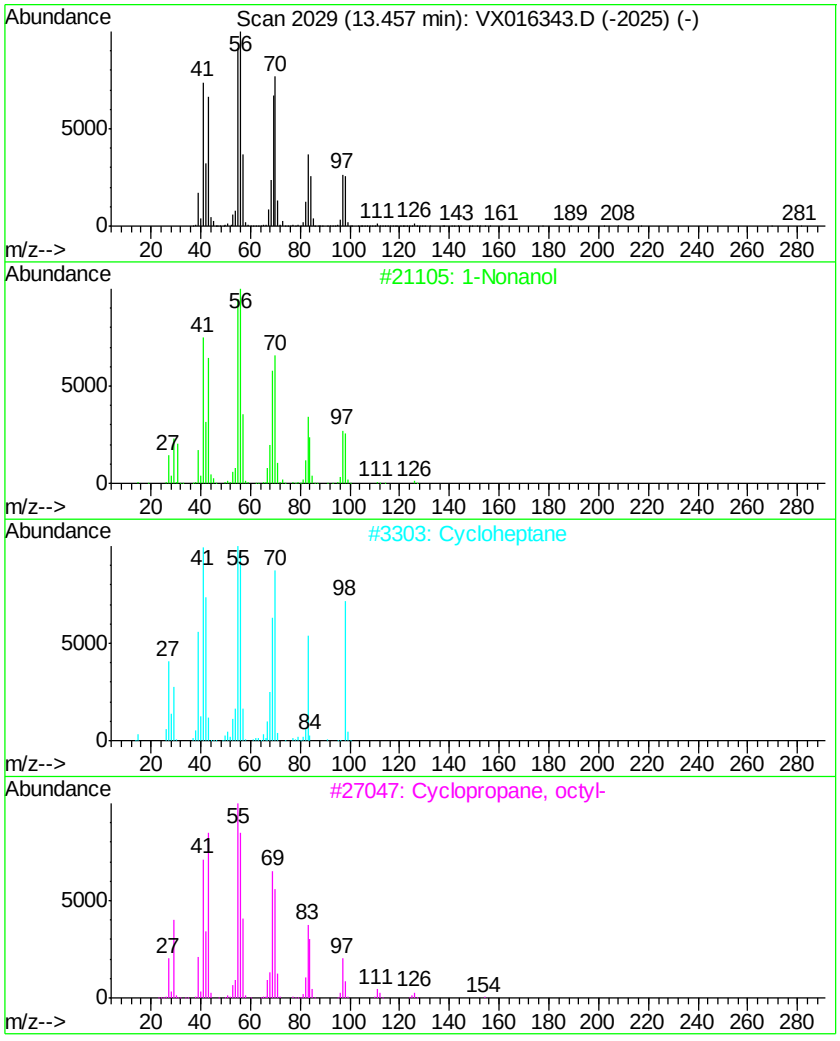
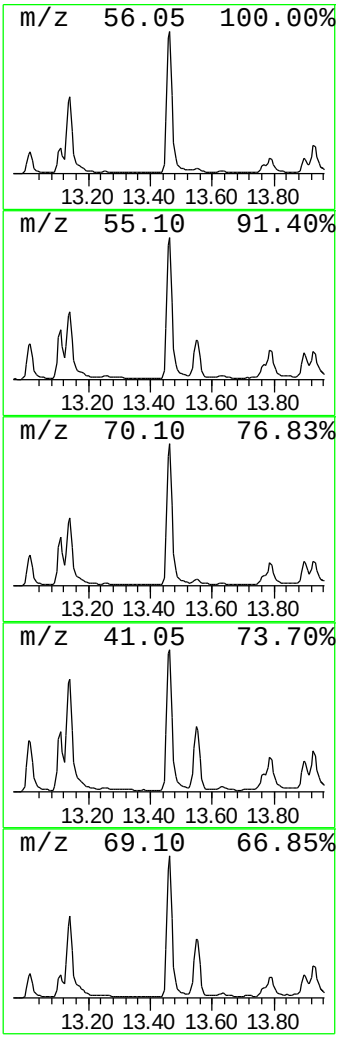
Peak Number 6 1-Nonanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	270.78 ug/l	6076080	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cycloheptane	98	C7H14	000291-64-5	87
3	Cyclopropane, octyl-	154	C11H22	001472-09-9	87
4	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	78
5	1-Octanol	130	C8H18O	000111-87-5	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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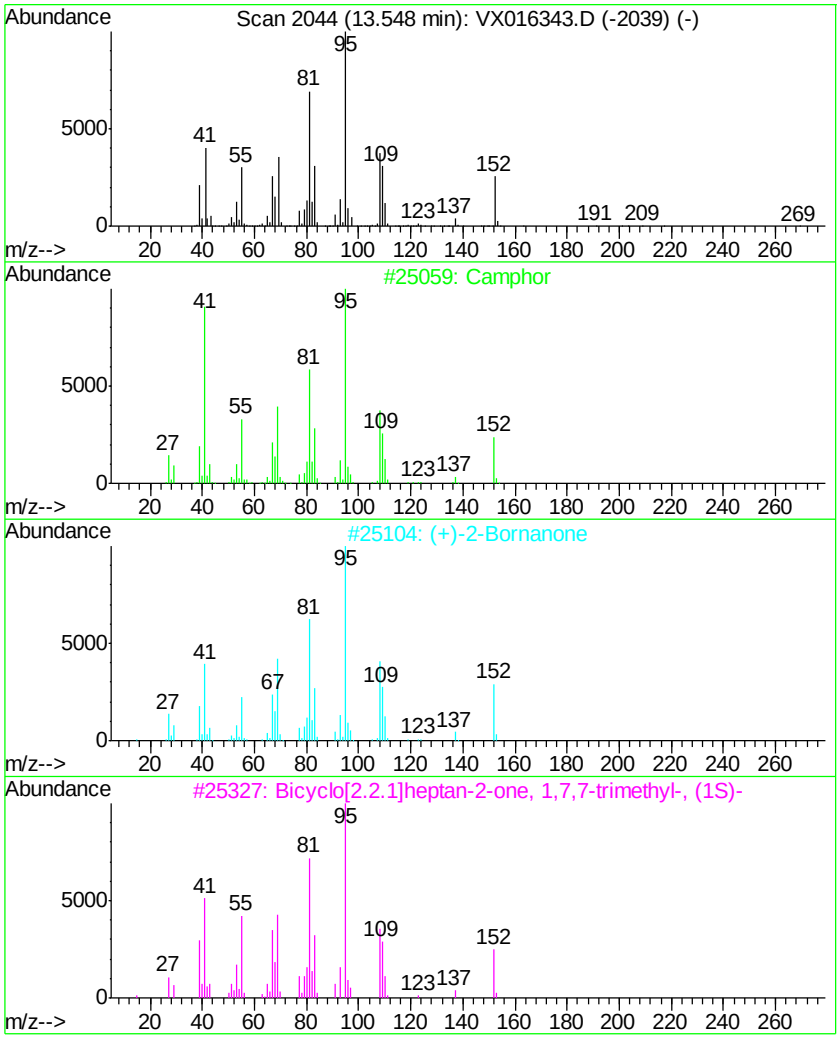
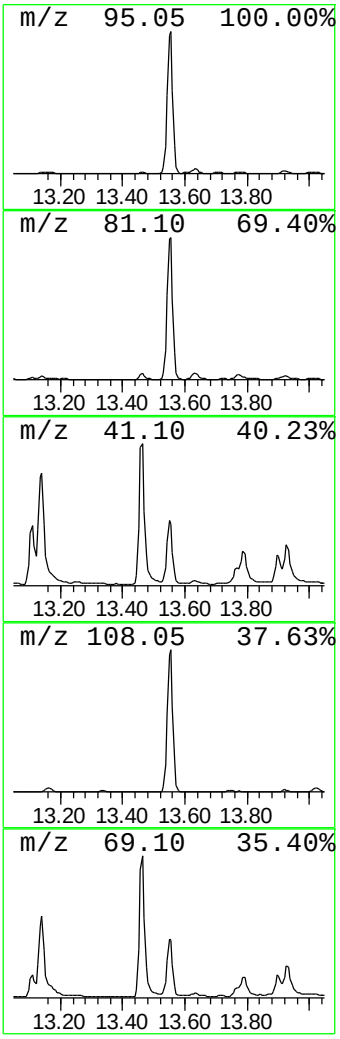
Peak Number 7 Camphor Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	187.96 ug/l	4217570	1,4-Dichlorobenzene-d4	12.06

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	98
3	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
4	5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	58
5	Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	46





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Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

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

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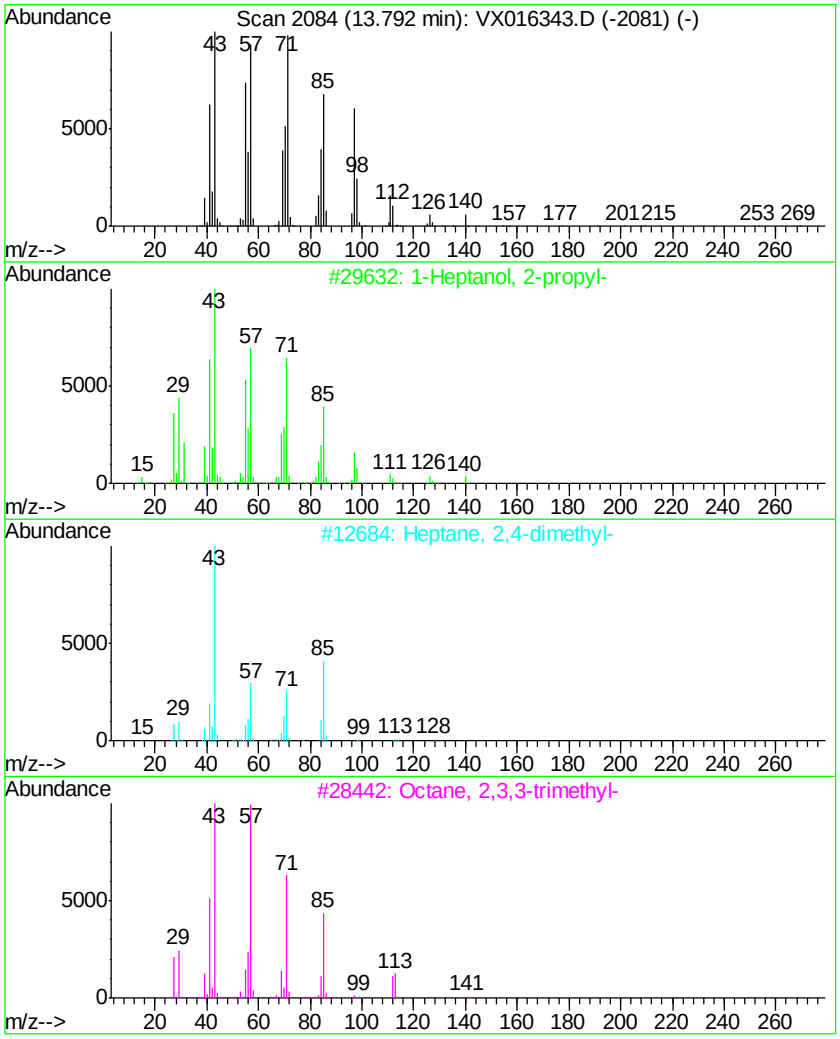
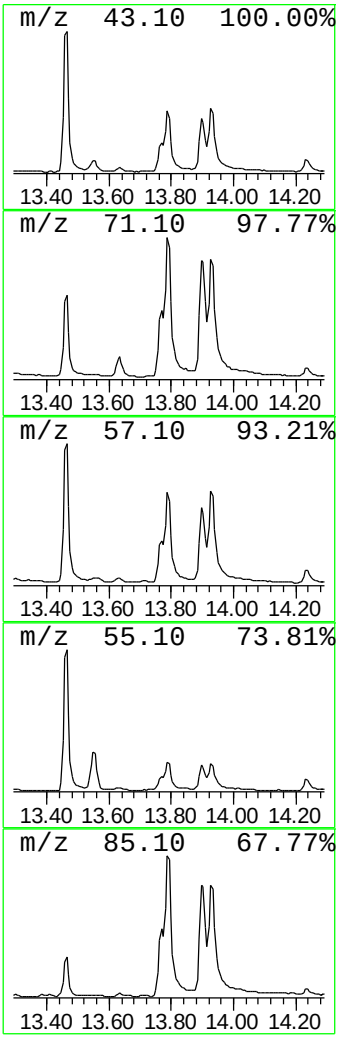
Peak Number 8 1-Heptanol, 2-propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	84.91 ug/l	1905250	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	64
2	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	58
3	Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	47
4	Octane	114	C8H18	000111-65-9	38
5	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

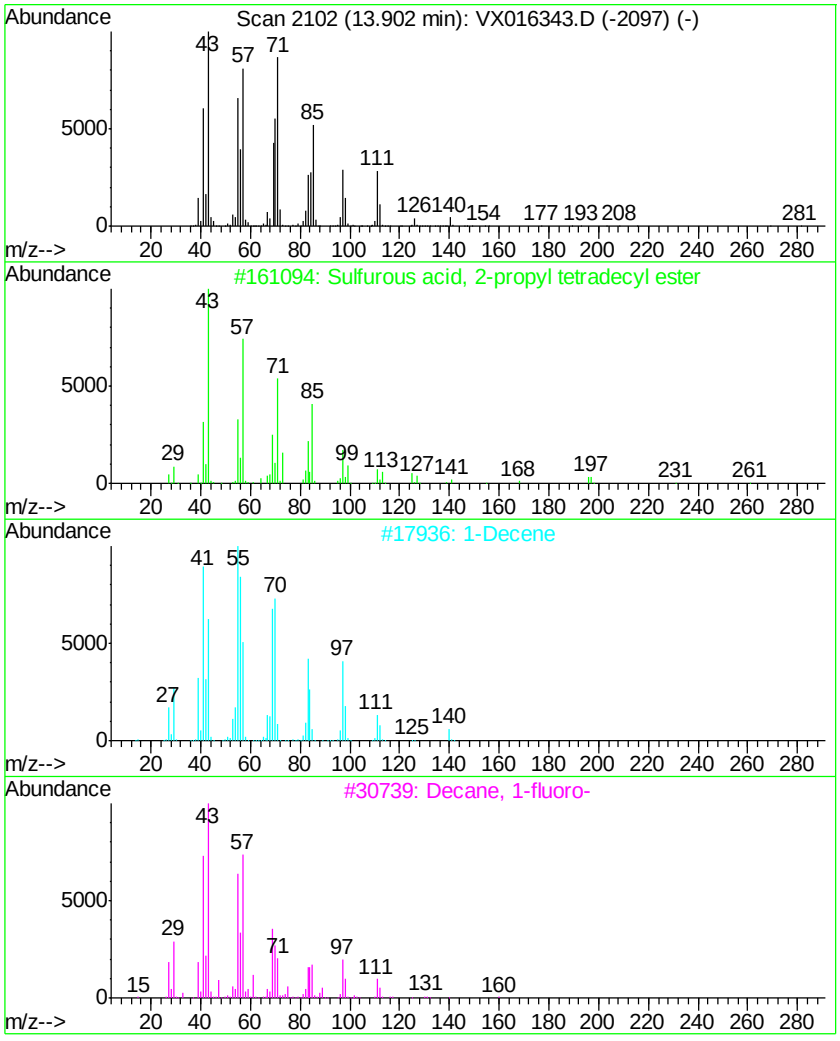
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

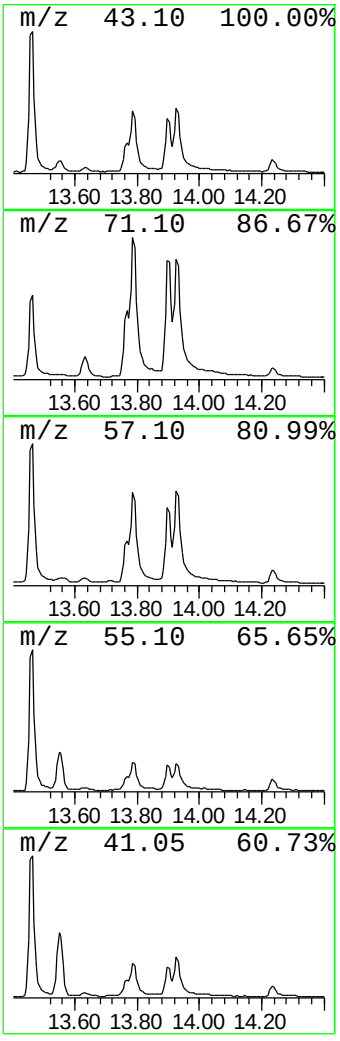
****

Peak Number 9 Sulfurous acid, 2-propyl te... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	69.34 ug/l	1555830	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	50
2	1-Decene	140	C10H20	000872-05-9	46
3	Decane, 1-fluoro-	160	C10H21F	000334-56-5	43
4	2-Methyl-1-undecanol	186	C12H26O	010522-26-6	38
5	Octane	114	C8H18	000111-65-9	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

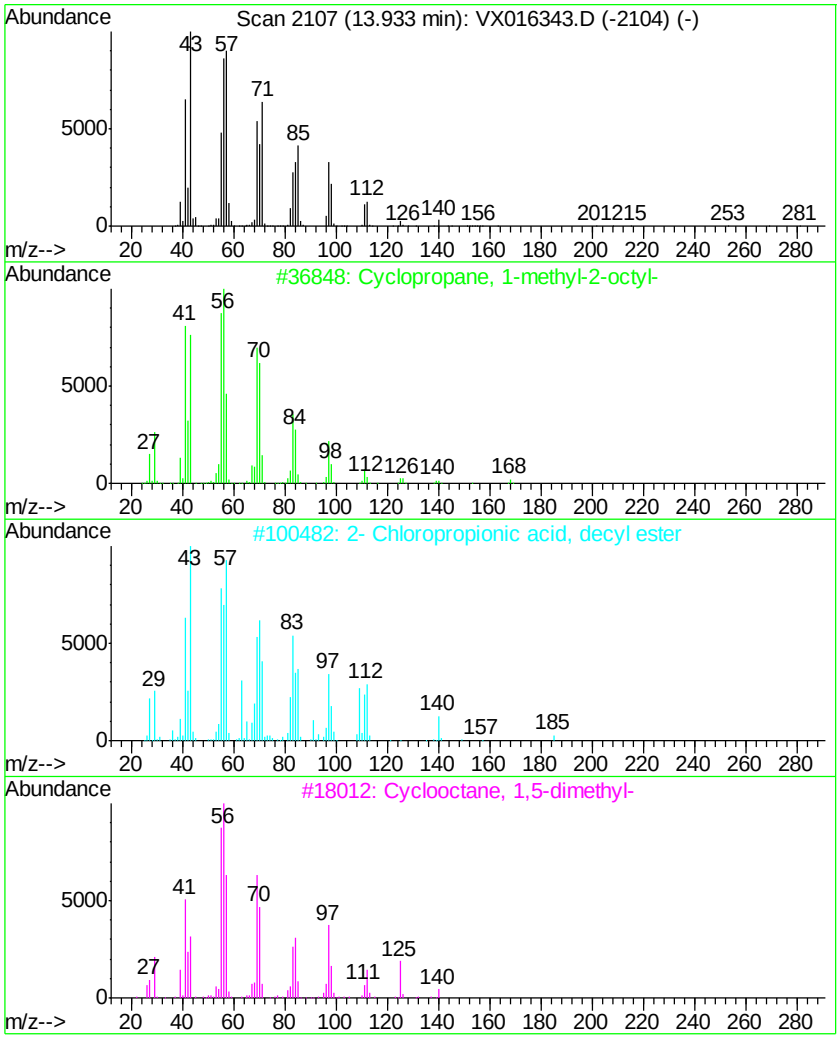
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

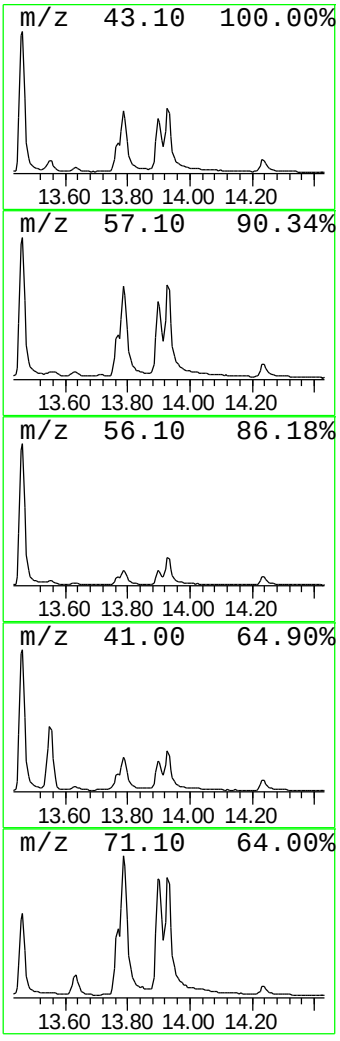
****

Peak Number 10 Cyclopropane, 1-methyl-2-oc... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	91.83 ug/l	2060550	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	64
2	2- Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	50
3	Cyclooctane, 1,5-dimethyl-	140	C10H20	021328-57-4	49
4	Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1000150-67-3	49
5	Cyclopropane, 1,2-dimethyl-3-pen...	140	C10H20	062238-10-2	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016343.D
Acq On : 19 May 2020 18:27
Operator : JC/SP
Sample : L2663-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1366

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.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
Eucalyptol	12.15	348.3	ug/l	7815920	4	12.06	1121950	50.0
1-Hexanol, 2-ethyl-	12.26	68.0	ug/l	1526840	4	12.06	1121950	50.0
Octane, 1,1'-oxybis-	13.01	115.8	ug/l	2597920	4	12.06	1121950	50.0
Dodecane, 1-fluoro-	13.11	119.7	ug/l	2685040	4	12.06	1121950	50.0
1-Nonanol	13.46	270.8	ug/l	6076080	4	12.06	1121950	50.0
Camphor	13.55	188.0	ug/l	4217570	4	12.06	1121950	50.0
1-Heptanol, 2-pro...	13.79	84.9	ug/l	1905250	4	12.06	1121950	50.0
Sulfurous acid, 2...	13.90	69.3	ug/l	1555830	4	12.06	1121950	50.0
Cyclopropane, 1-m...	13.93	91.8	ug/l	2060550	4	12.06	1121950	50.0