LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

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\82X031023W.M
Title : SW846 8260

Signal : TIC: VX034653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	20	rVB3	9306	15800	1.05%	0.103%
2	1.252	23	27	31	rBV3	13138	25371	1.68%	0.166%
3	1.355	31	44	49	rBV2	38654	95038	6.29%	0.622%
4	1.569	71	79	83	rVB6	23209	50406	3.34%	0.330%
5	2.050	155	158	168	rVB	15104	26831	1.78%	0.176%
6	2.288	193	197	205	rVB	19073	31886	2.11%	0.209%
7	2.374	205	211	228	rVB	499376	814667	53.92%	5.335%
8	2.532	230	237	245	rVB2	22149	46514	3.08%	0.305%
9	2.953	299	306	314	rVB3	7640	17083	1.13%	0.112%
10	4.550	559	568	583	rBV	196032	554238	36.68%	3.629%
11	5.007	633	643	664	rBV3	44294	151630	10.04%	0.993%
12	5.385	693	705	720	rBV	154138	447479	29.62%	2.930%
13	5.550	720	732	746	rVB	263028	758901	50.23%	4.970%
14	5.958	786	799	817	rBV	179308	484665	32.08%	3.174%
15	6.635	902	910	920	rBV2	10269	27638	1.83%	0.181%
16	6.763	920	931	947	rVV	417460	1011172	66.92%	6.622%
17	7.464	1039	1046	1058	rVB	24131	54855	3.63%	0.359%
18	7.647	1070	1076	1088	rVB2	12464	29930	1.98%	0.196%
19	8.574	1223	1228	1233	rBV2	17479	29326	1.94%	0.192%
20	8.647	1233	1240	1247	rVV	902266	1425883	94.37%	9.337%
21	8.720	1247	1252	1259	rVB	75432	122092	8.08%	0.800%
22	8.805	1260	1266	1271	rBV	47839	76678	5.07%	0.502%
23	9.305	1344	1348	1357	rVB	85269	125357	8.30%	0.821%
24	9.433	1364	1369	1379	rBV	97088	143001	9.46%	0.936%
25	9.519	1379	1383	1392	rVV	21178	35571	2.35%	0.233%
26	9.641	1392	1403	1412	rVV3	9177	21783	1.44%	0.143%
27	10.055	1465	1471	1484	rVB	914766	1249377	82.69%	8.181%
28	10.299	1507	1511	1519	rVB2	9638	16157	1.07%	0.106%
29	10.506	1539	1545	1551	rBV	29699	42124	2.79%	0.276%
30	10.640	1561	1567	1570	rBV4	20611	34077	2.26%	0.223%
31	10.683	1570	1574	1583	rVB	65725	90377	5.98%	0.592%
32	10.768	1584	1588	1594	rBV	51380	67189	4.45%	0.440%
33	11.079	1634	1639	1645	rBV	765334	983136	65.07%	6.438%
34	11.134	1645	1648	1652	rVB	12847	16786	1.11%	0.110%
35	11.238	1659	1665	1669	rBV	17499	28339	1.88%	0.186%
36	11.299	1669	1675	1680	rVV	45828	58876	3.90%	0.386%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

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\82X031023W.M
Title : SW846 8260

37	11.360	1680	1685	1693	rBV	139370	181254	12.00%	1.187%
38	11.604	1721	1725	1731	rVV	122949	182414	12.07%	1.195%
39	11.756	1747	1750	1754	rBV	36563	49168	3.25%	0.322%
40	11.841	1760	1764	1769	rBV2	42940	59827	3.96%	0.392%
41	11.969	1782	1785	1788	rBV3	23679	29435	1.95%	0.193%
42	12.024	1788	1794	1801	rVB	915476	1186589	78.53%	7.770%
43	12.104	1801	1807	1821	rVB	394443	526065	34.82%	3.445%
44	12.219	1821	1826	1836	rBV	232969	476263	31.52%	3.119%
45	12.451	1862	1864	1870	rVB3	29752	43610	2.89%	0.286%
46	12.689	1900	1903	1911	rVB2	35395	48999	3.24%	0.321%
47	12.774	1911	1917	1918	rBV3	112917	164576	10.89%	1.078%
48	12.792	1918	1920	1927	rVB2	76077	123288	8.16%	0.807%
49	12.859	1927	1931	1939	rBV	138988	312504	20.68%	2.046%
50	12.975	1946	1950	1957	rBV5	76448	194784	12.89%	1.276%
51	13.079	1961	1967	1968	rVV3	130655	221651	14.67%	1.451%
52	13.109	1968	1972	1991	rVB5	374794	1510957	100.00%	9.894%
53	13.512	2030	2038	2046	rVB2	132313	230008	15.22%	1.506%
54	13.591	2046	2051	2061	rVB4	92983	169731	11.23%	1.111%
55	13.774	2079	2081	2090	rVB2	35476	69258	4.58%	0.454%
56	14.231	2150	2156	2165	rVB5	27744	55177	3.65%	0.361%
57	14.481	2194	2197	2206	rVB8	19937	36906	2.44%	0.242%
58	14.585	2209	2214	2217	rBV6	25939	57276	3.79%	0.375%
59	14.640	2220	2223	2227	rVB2	13992	19802	1.31%	0.130%
60	14.786	2243	2247	2251	rBV5	34452	61939	4.10%	0.406%
61	15.615	2378	2383	2387	rBV4	9211	15211	1.01%	0.100%
62	16.328	2494	2500	2507	rVB2	16851	34006	2.25%	0.223%

Sum of corrected areas: 15270931

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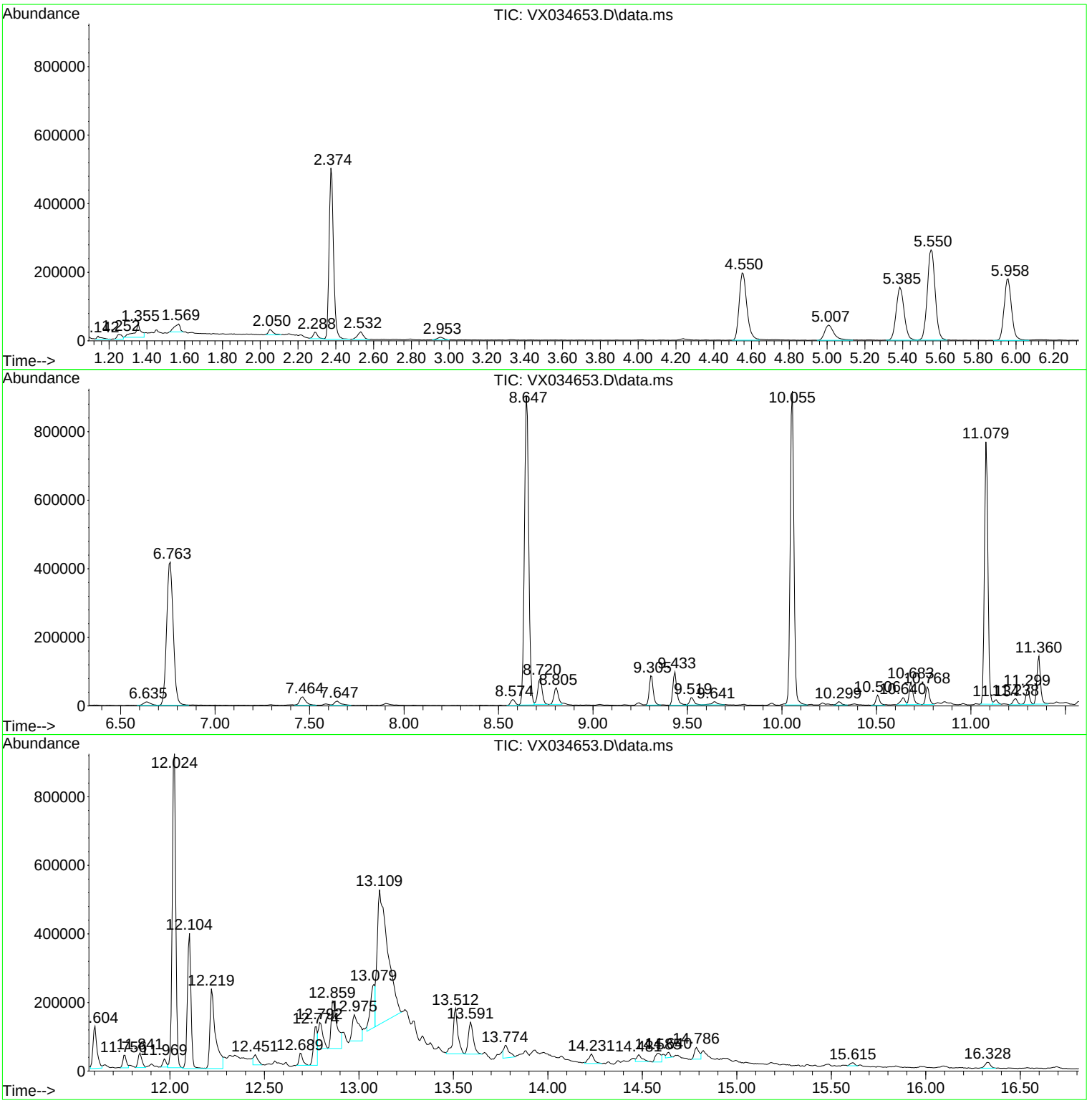
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

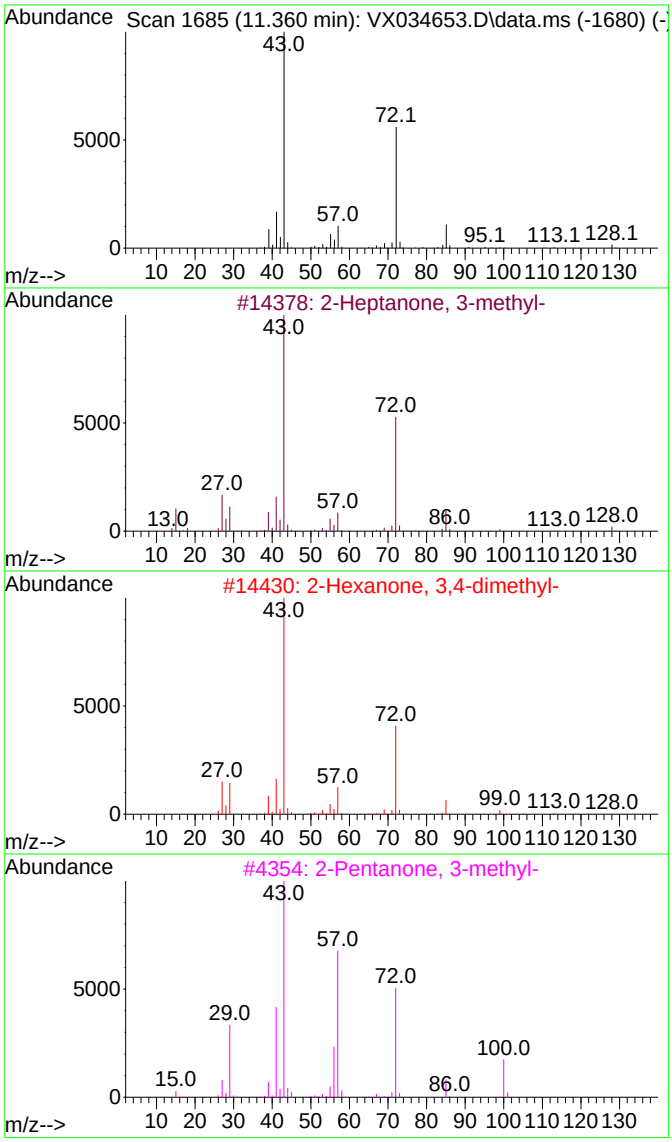
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

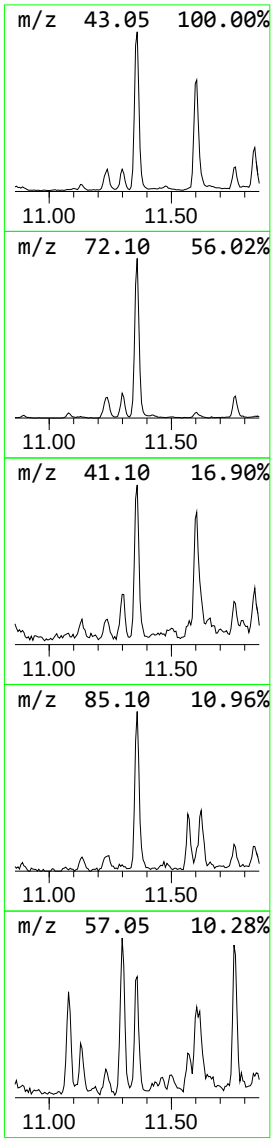
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Heptanone, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.360	7.64 ug/l	181254	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	91
2	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	53
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	38
4	4-Fluorobuphedrone	195	C11H14FNO	1368599-12-5	37
5	1-Propene, 1-methoxy-	72	C4H8O	007319-16-6	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

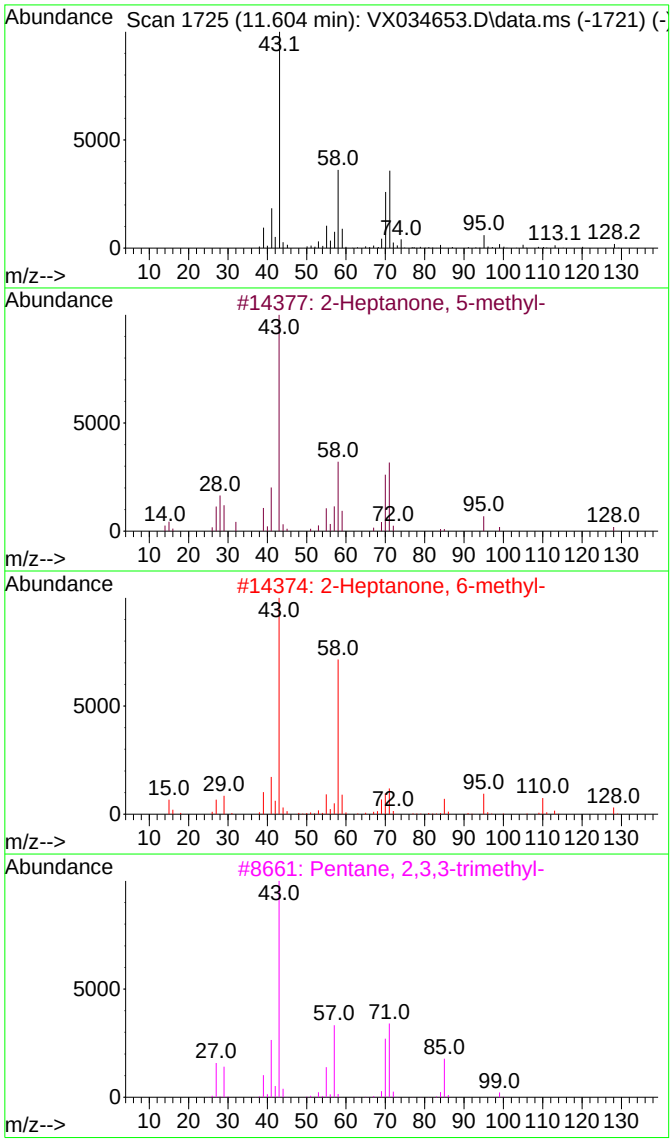
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

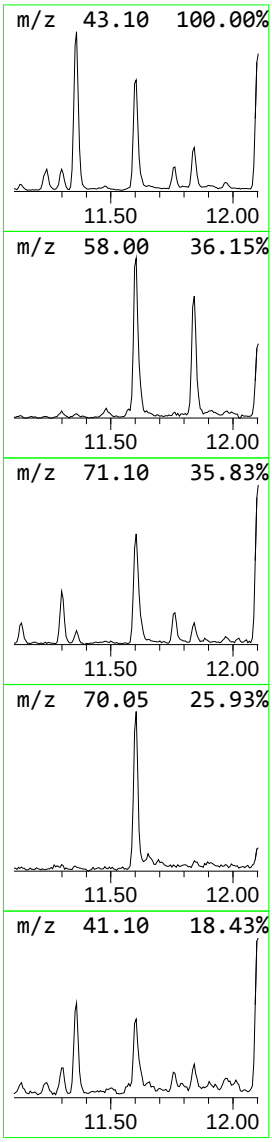
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Heptanone, 5-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.604	7.69 ug/l	182414	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 5-methyl-	128	C8H16O	018217-12-4	91
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	43
3	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	40
4	4-Decanone	156	C10H20O	000624-16-8	40
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

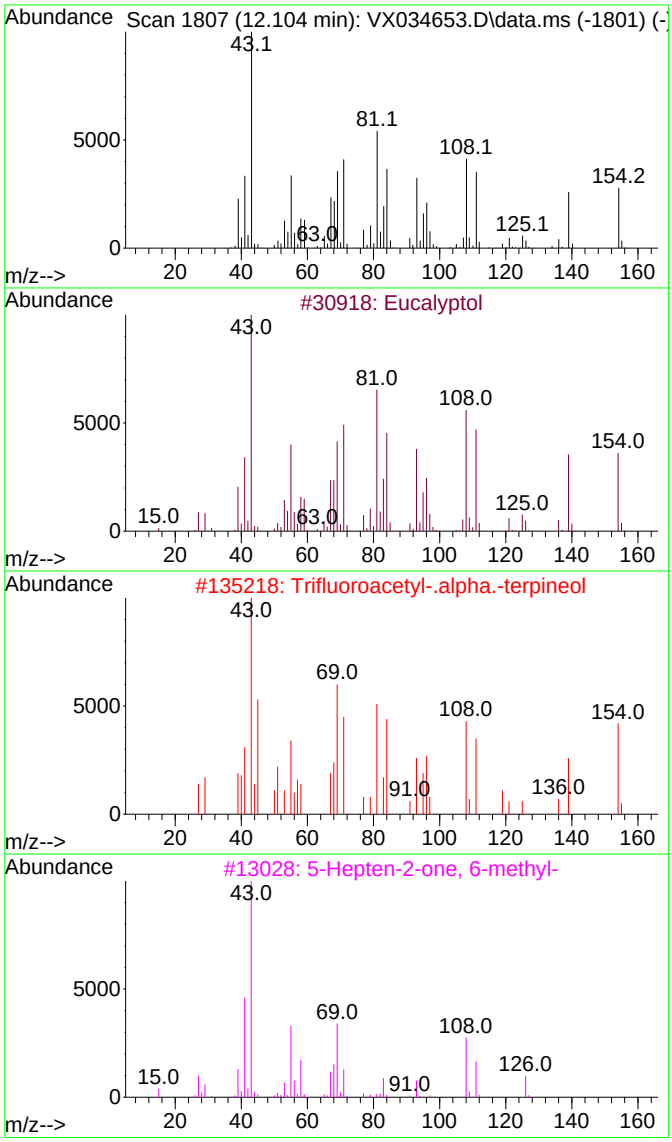
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

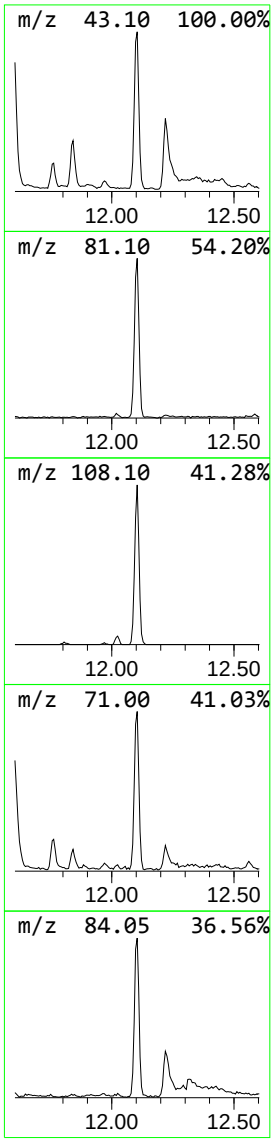
****

Peak Number 3 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	22.17 ug/l	526065	1,4-Dichlorobenzene-d4	12.024

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	64
3	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	25
4	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5	Sulfurous acid, 2-pentyl propyl ...	194	C8H18O3S	1000309-15-1	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

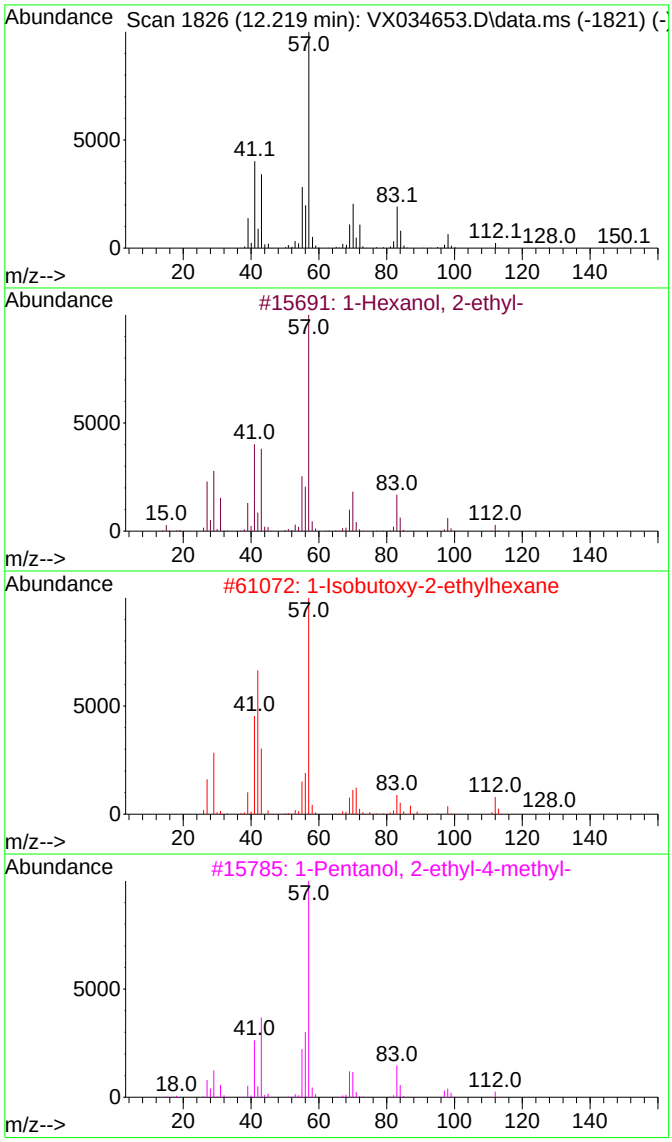
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

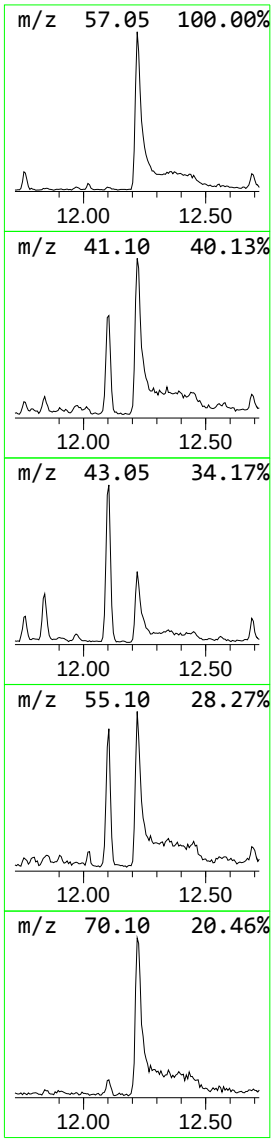
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	20.07 ug/l	476263	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	78
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
5	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

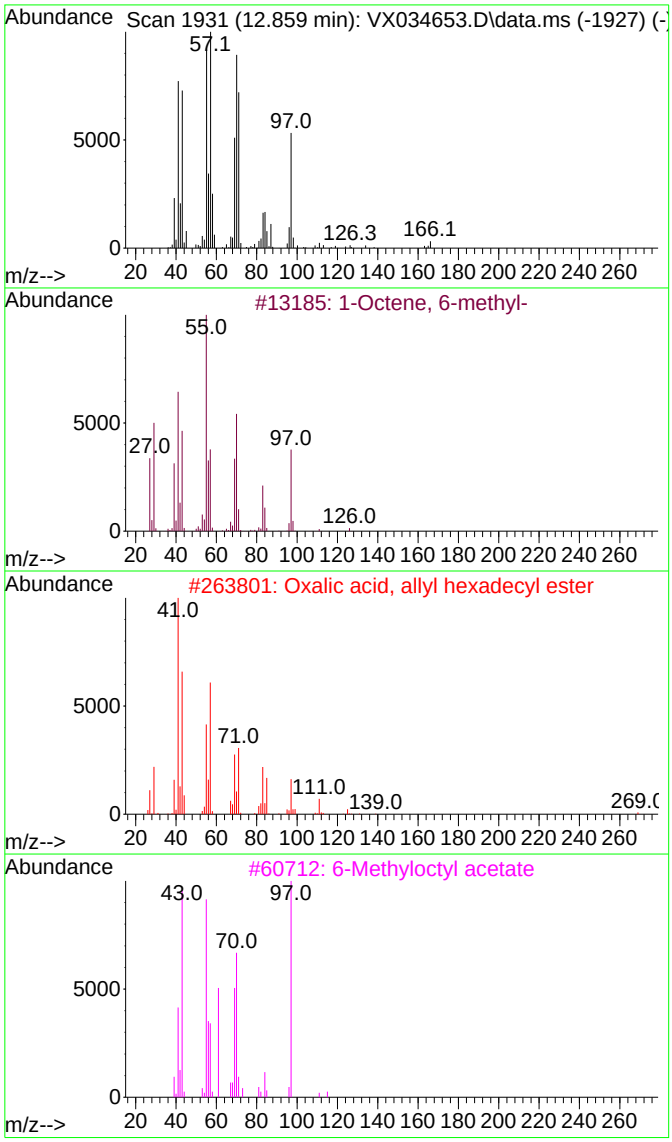
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

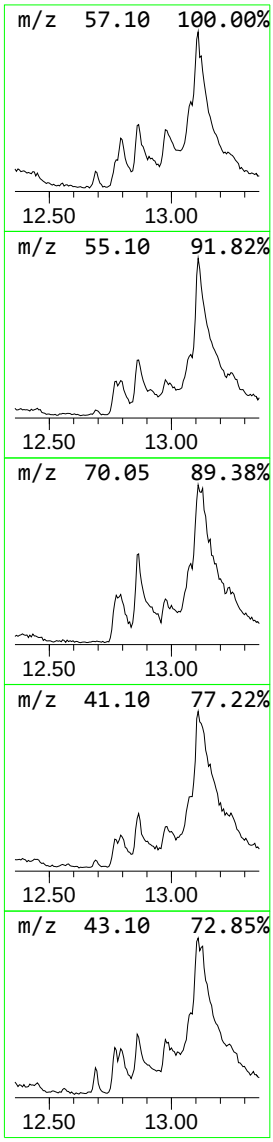
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Octene, 6-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.860	13.17 ug/l	312504	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octene, 6-methyl-	126	C9H18	013151-10-5	58
2	Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	43
3	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	35
4	2-Nonene, 3-methyl-, (E)-	140	C10H20	017003-99-5	35
5	2-Propen-1-amine, N-ethyl-	85	C5H11N	002424-02-4	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

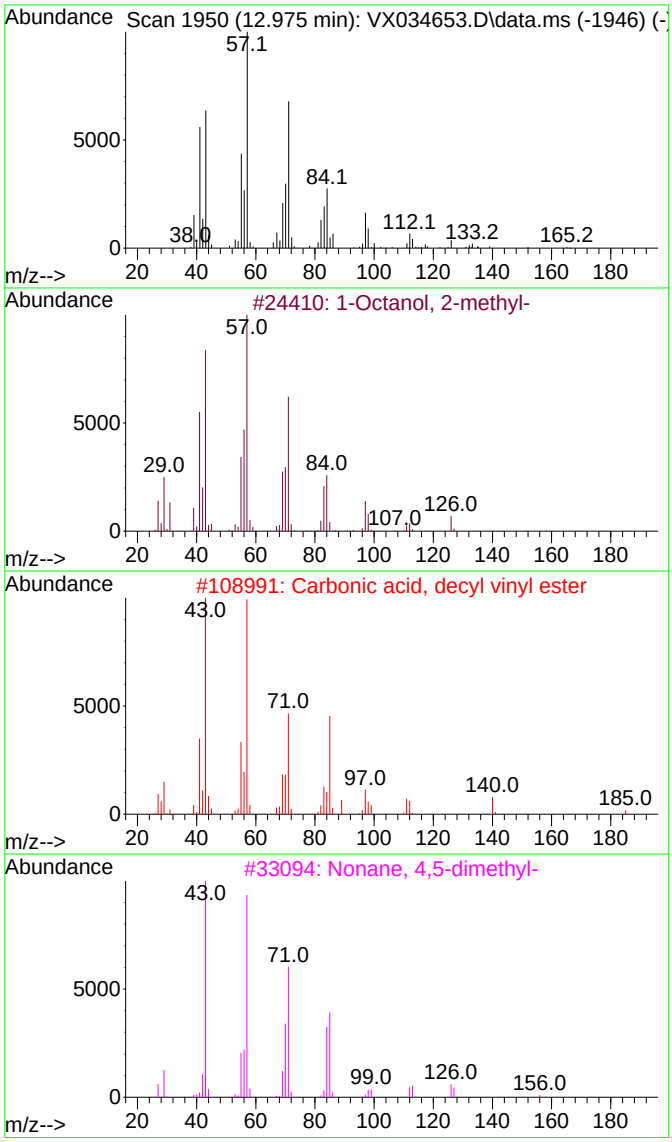
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

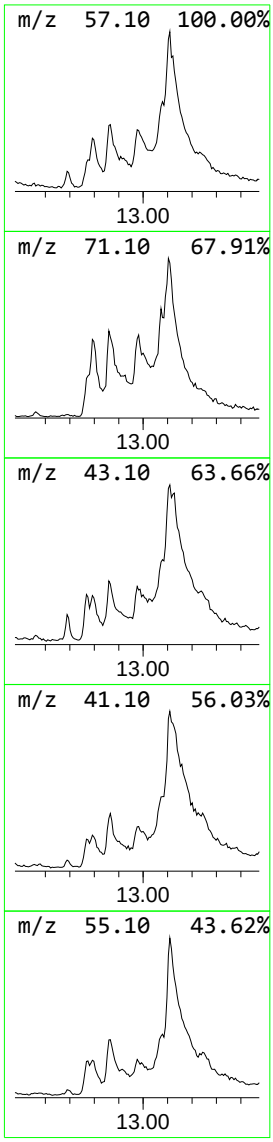
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Octanol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	8.21 ug/l	194784	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	72
2	Carbonic acid, decyl vinyl ester	228	C13H24O3	1000383-25-7	59
3	Nonane, 4,5-dimethyl-	156	C11H24	017302-23-7	53
4	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	50
5	Propionic acid, 3-mercapto-, iso...	218	C11H22O2S	077916-53-1	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

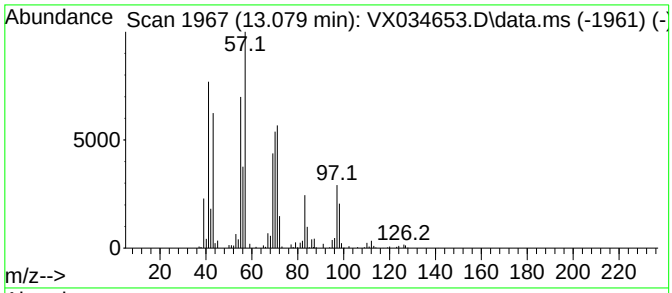
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

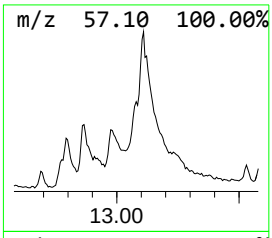
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

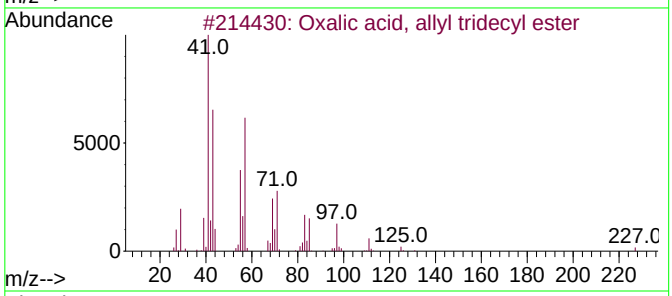
****
Peak Number 7 unknown13.079 Concentration Rank 6

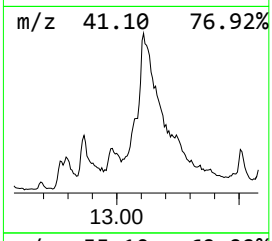
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.079	9.34 ug/l	221651	1,4-Dichlorobenzene-d4	12.024

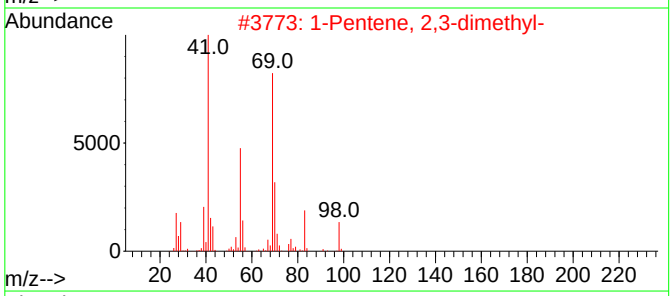
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl tridecyl ester	312	C18H32O4	1000309-24-1	47
2	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	43
3	Cyclohexane, 1,2,3-trimethyl-	126	C9H18	001678-97-3	38
4	2-Decenal, (E)-	154	C10H18O	003913-81-3	35
5	4-Methyl-3-heptanol, pentafluoro...	276	C11H17F5O2	1000365-51-7	35

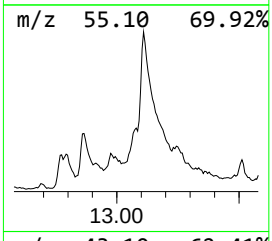


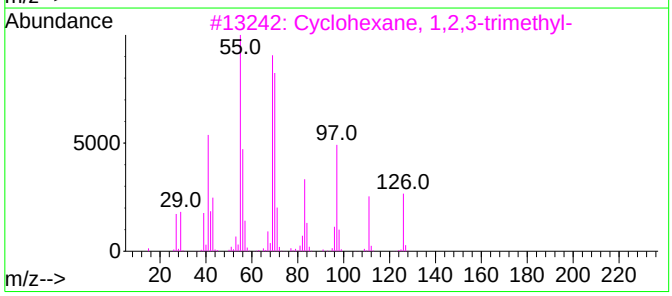


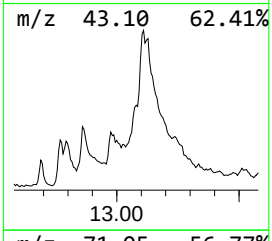


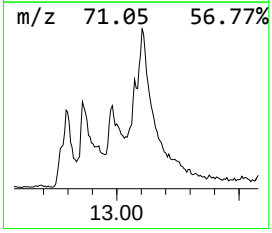












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

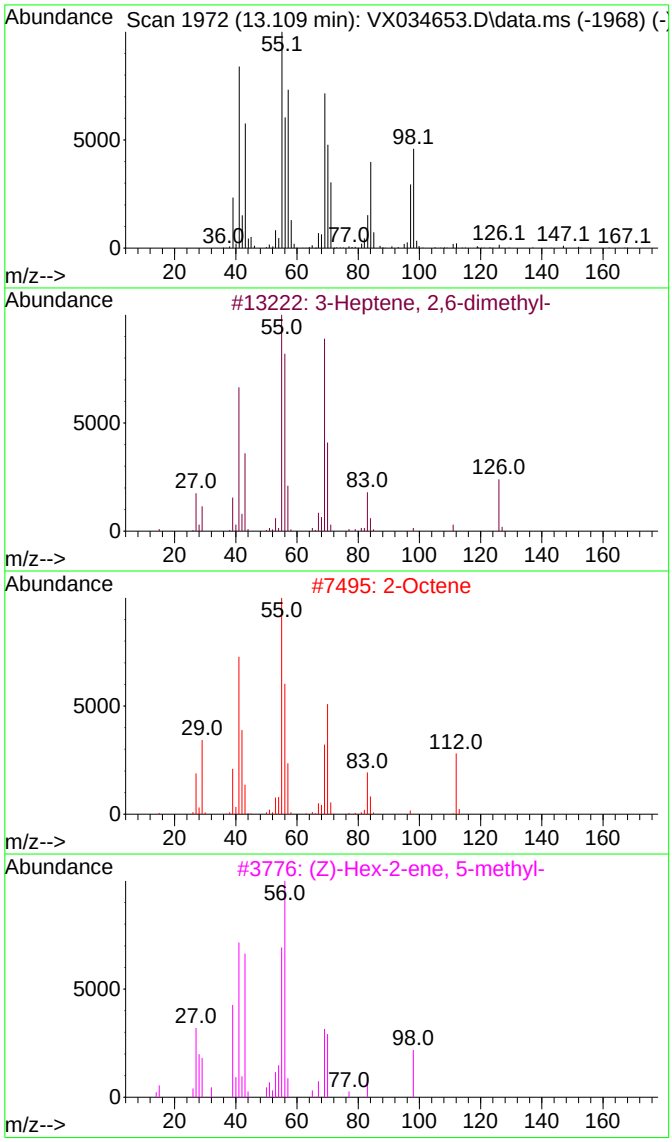
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

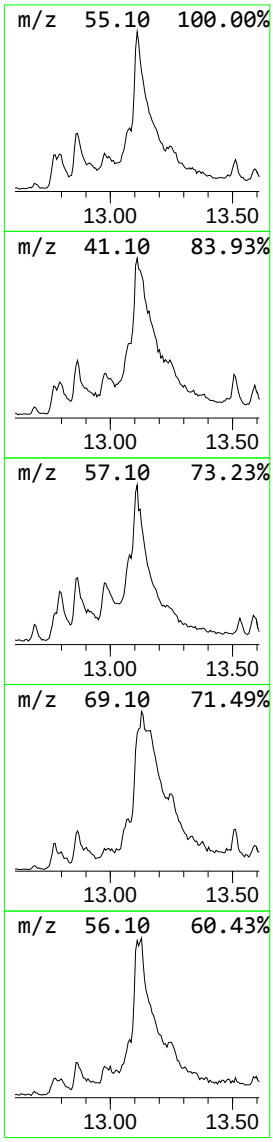
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown13.109 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.109	63.67 ug/l	1510960	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	43
2	2-Octene	112	C8H16	000111-67-1	43
3	(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	35
4	3-Hexene, (E)-	84	C6H12	013269-52-8	22
5	Cyclohexane	84	C6H12	000110-82-7	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

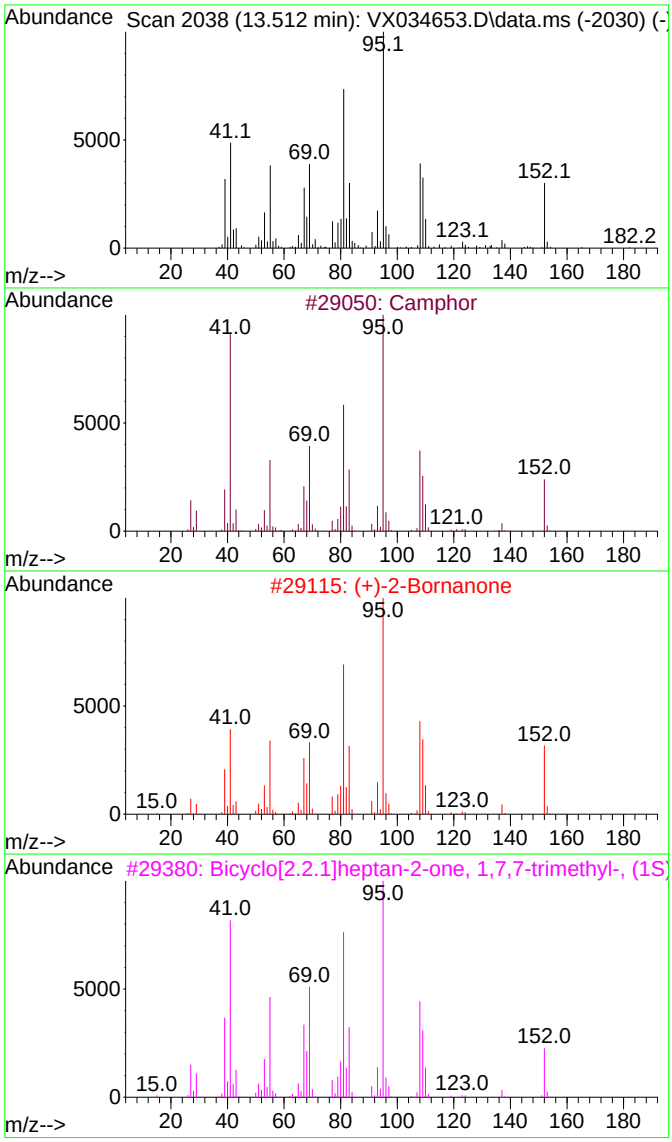
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

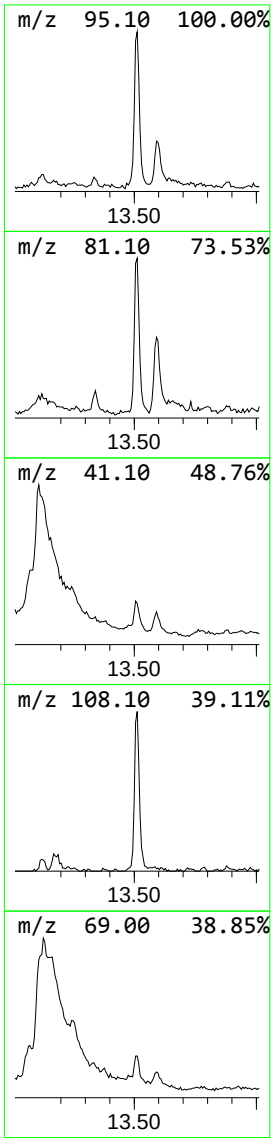
****

Peak Number 9 Camphor Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	9.69 ug/l	230008	1,4-Dichlorobenzene-d4	12.024

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	97
4	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	000529-00-0	38
5	2,4-Decadienal, (E,Z)-	152	C10H16O	025152-83-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

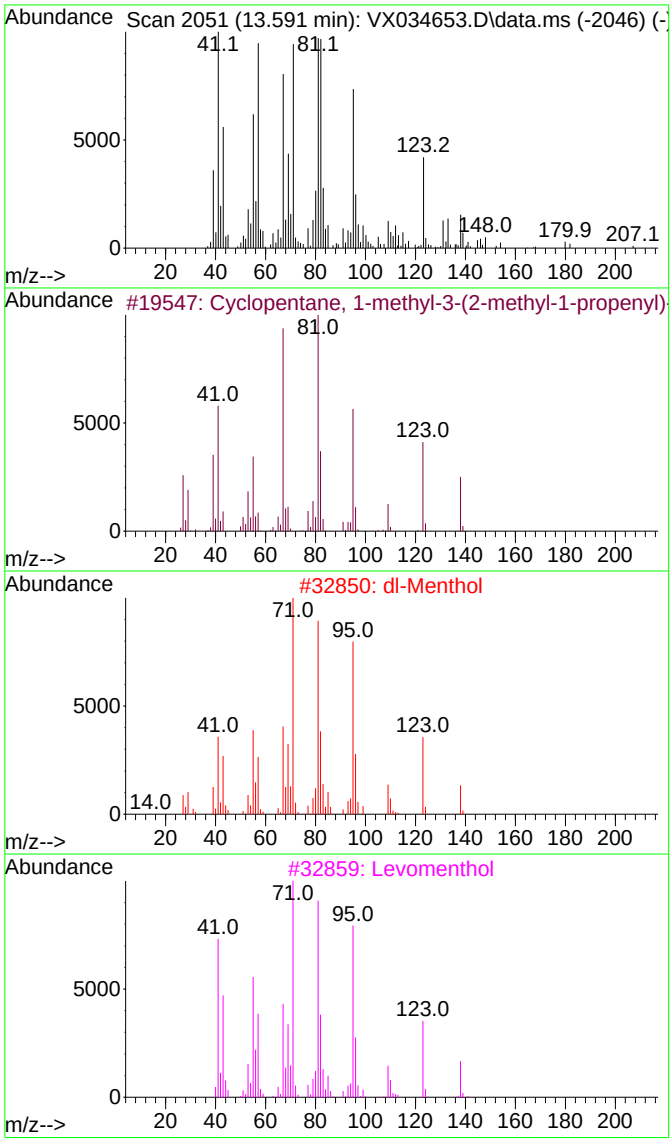
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

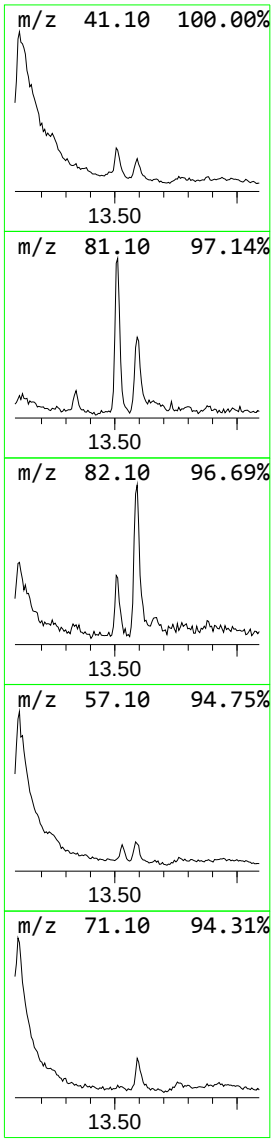
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Cyclopentane, 1-methyl-3-(2... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	7.15 ug/l	169731	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1-methyl-3-(2-meth...	138	C10H18	075873-01-7	64
2	dl-Menthol	156	C10H20O	000089-78-1	58
3	Levomenthol	156	C10H20O	002216-51-5	58
4	Cyclopentene, 1-pentyl-	138	C10H18	004291-98-9	55
5	Cyclohexane, (2-methyl-1-propenyl)-	138	C10H18	089656-98-4	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
Data File : VX034653.D
Acq On : 21 Mar 2023 14:40
Operator : JC/MD
Sample : 02013-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Heptanone, 3-...	11.360	7.6	ug/l	181254	4	12.024	1186590	50.0
2-Heptanone, 5-...	11.604	7.7	ug/l	182414	4	12.024	1186590	50.0
Eucalyptol	12.104	22.2	ug/l	526065	4	12.024	1186590	50.0
1-Hexanol, 2-et...	12.219	20.1	ug/l	476263	4	12.024	1186590	50.0
1-Octene, 6-met...	12.860	13.2	ug/l	312504	4	12.024	1186590	50.0
1-Octanol, 2-me...	12.975	8.2	ug/l	194784	4	12.024	1186590	50.0
unknown13.079	13.079	9.3	ug/l	221651	4	12.024	1186590	50.0
unknown13.109	13.109	63.7	ug/l	1510960	4	12.024	1186590	50.0
Camphor	13.512	9.7	ug/l	230008	4	12.024	1186590	50.0
Cyclopentane, 1...	13.591	7.2	ug/l	169731	4	12.024	1186590	50.0