LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038610.D
Acq On : 27 Oct 2023 18:08
Operator : JC/MD
Sample : 05107-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

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\82X100523W.M
Title : SW846 8260

Signal : TIC: VX038610.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.374	205	211	226	rBV	743483	1212764	3.04%	0.571%
2	4.550	556	568	600	rBV	626879	1754776	4.40%	0.827%
3	5.385	694	705	719	rBV	161574	474015	1.19%	0.223%
4	5.550	722	732	749	rVV	217995	626737	1.57%	0.295%
5	5.958	789	799	817	rBV	160464	427918	1.07%	0.202%
6	6.763	921	931	946	rBV	343187	831107	2.08%	0.392%
7	8.647	1234	1240	1247	rBV	818435	1309544	3.29%	0.617%
8	8.720	1247	1252	1260	rVB	332225	524763	1.32%	0.247%
9	9.433	1363	1369	1379	rBV	507885	740364	1.86%	0.349%
10	10.055	1462	1471	1485	rBV	826492	1173334	2.94%	0.553%
11	11.079	1634	1639	1645	rBV	857862	1110170	2.78%	0.523%
12	11.360	1679	1685	1691	rVB	455083	600707	1.51%	0.283%
13	11.598	1719	1724	1731	rBV	2532435	3320161	8.33%	1.565%
14	11.841	1759	1764	1769	rBV	6058402	7511777	18.84%	3.540%
15	11.896	1769	1773	1782	rVV2	882300	1624291	4.07%	0.765%
16	12.024	1789	1794	1800	rVB	1046563	1369161	3.43%	0.645%
17	12.104	1801	1807	1813	rBV	11492865	14451555	36.25%	6.810%
18	12.219	1820	1826	1832	rBV2	519122	947165	2.38%	0.446%
19	12.286	1832	1837	1839	rBV3	788374	1268881	3.18%	0.598%
20	12.457	1859	1865	1872	rVB5	155789	399978	1.00%	0.188%
21	12.555	1876	1881	1885	rBV2	317373	473611	1.19%	0.223%
22	12.768	1909	1916	1918	rBV	12882567	15401440	38.64%	7.258%
23	12.792	1918	1920	1927	rVV2	8281174	10932064	27.42%	5.151%
24	12.872	1927	1933	1938	rVV	27244753	39862974	100.00%	18.784%
25	12.927	1938	1942	1946	rVV	1425748	3016189	7.57%	1.421%
26	12.975	1946	1950	1957	rVV	7927692	14689191	36.85%	6.922%
27	13.030	1957	1959	1961	rVV	2804077	3409565	8.55%	1.607%
28	13.073	1961	1966	1969	rVV3	8008229	15731559	39.46%	7.413%
29	13.109	1969	1972	1975	rVV2	17867139	28337102	71.09%	13.353%
30	13.140	1975	1977	1987	rVV2	16245001	27252906	68.37%	12.842%
31	13.219	1987	1990	2008	rVB	2701242	4199665	10.54%	1.979%
32	13.512	2033	2038	2047	rVV	3764961	4841786	12.15%	2.282%
33	13.603	2048	2053	2061	rVB	1426967	1723977	4.32%	0.812%
34	13.884	2092	2099	2109	rBV2	355814	662553	1.66%	0.312%

Sum of corrected areas: 212213750

Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

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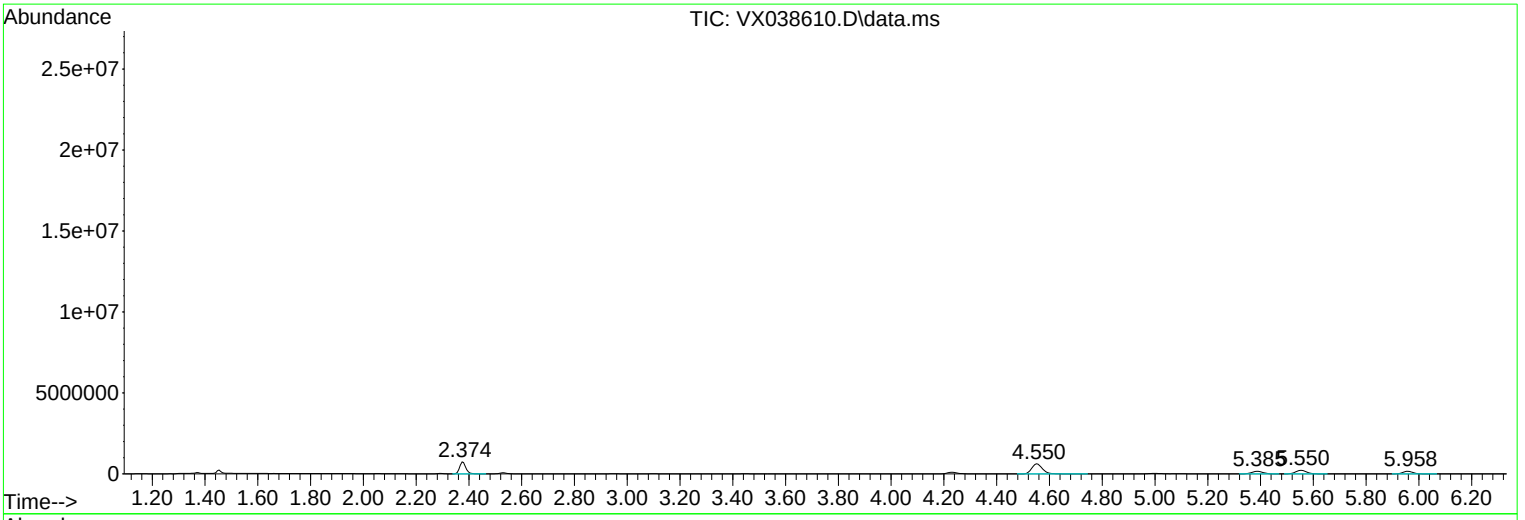
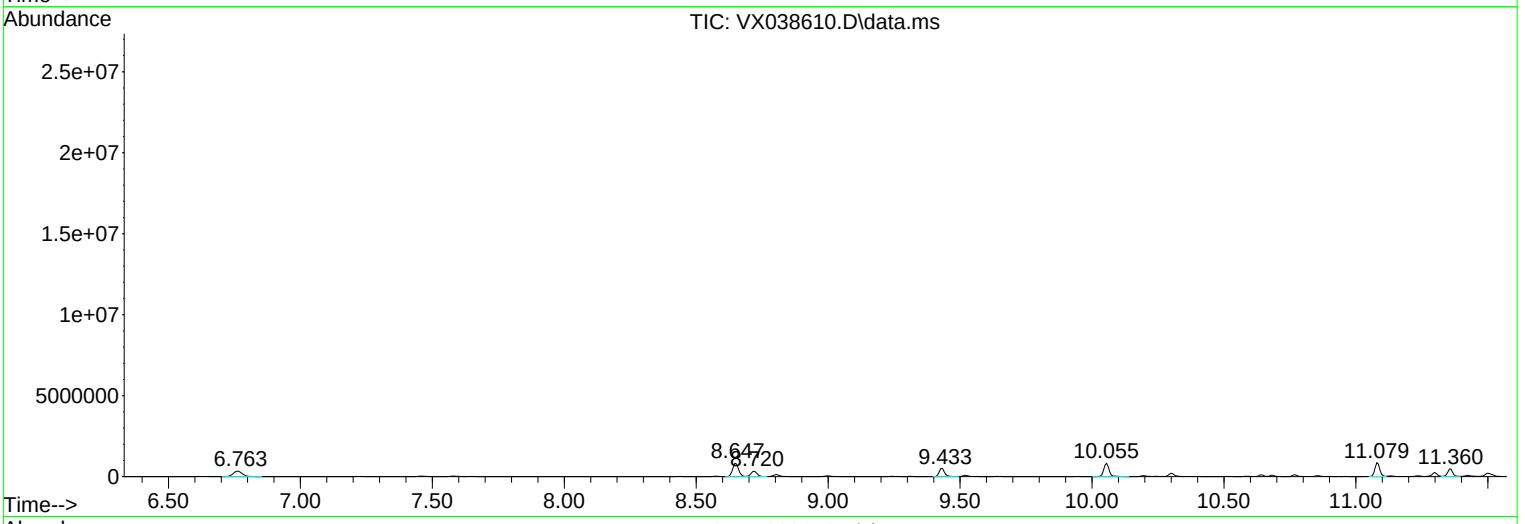
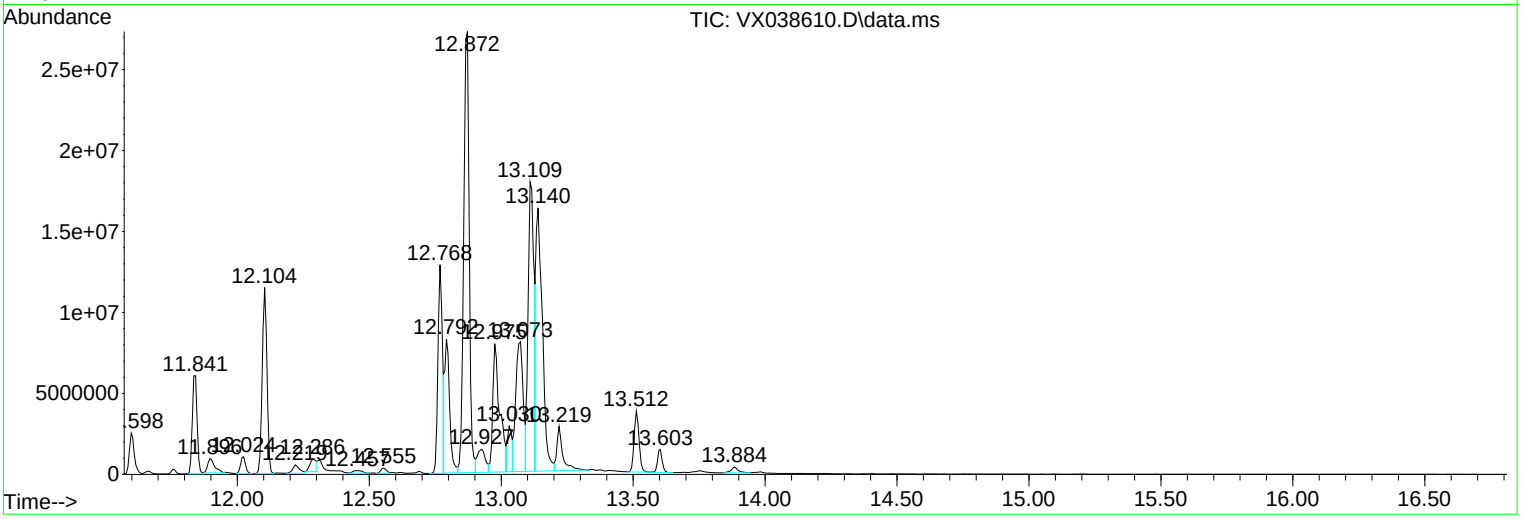
Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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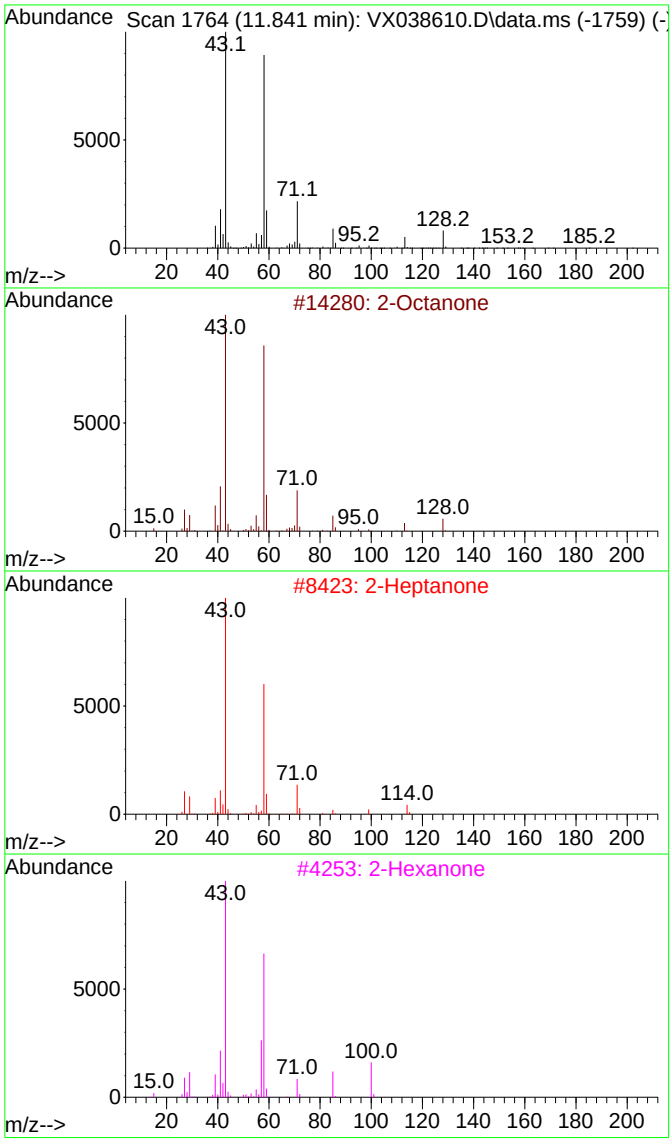
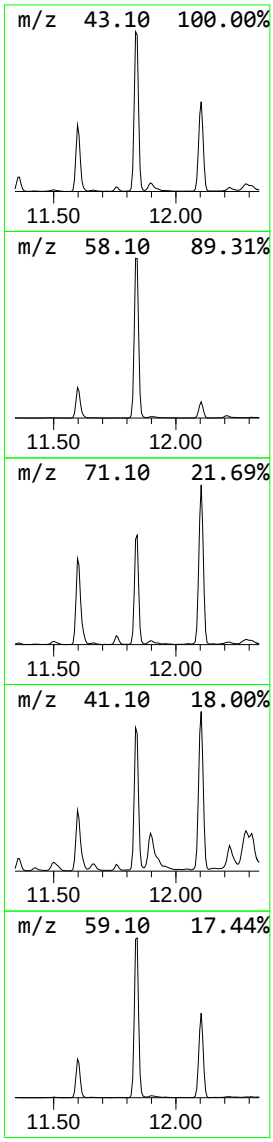
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Octanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.841	274.32 ug/l	7511780	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	94
2	2-Heptanone	114	C7H14O	000110-43-0	72
3	2-Hexanone	100	C6H12O	000591-78-6	64
4	2-Dodecanone	184	C12H24O	006175-49-1	56
5	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	56





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ClientSampleId :
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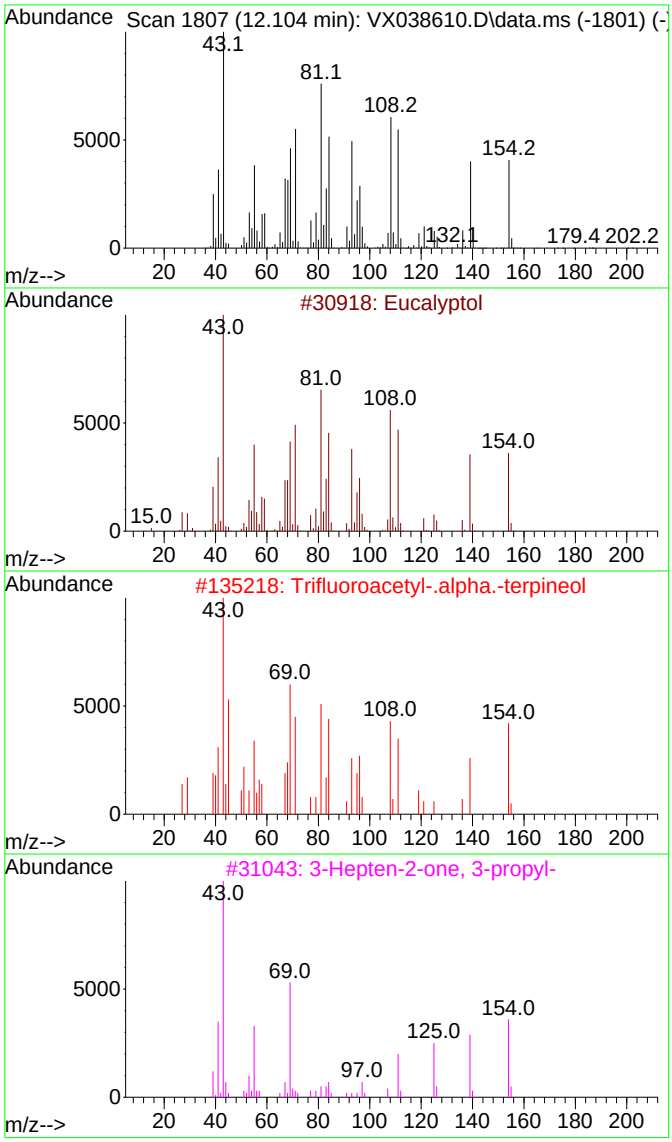
Quant Title : SW846 8260

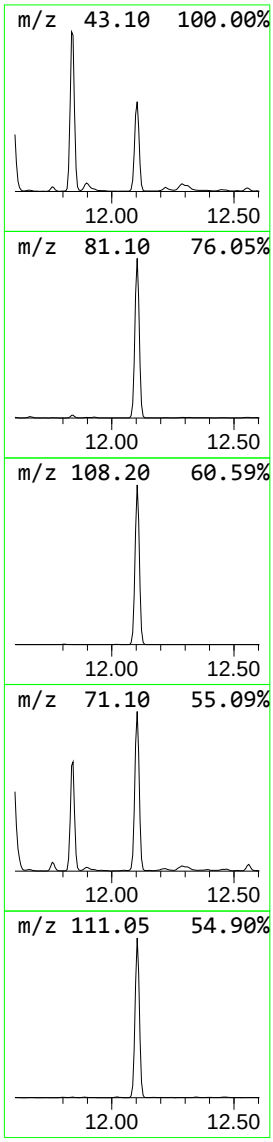
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Eucalyptol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	527.75 ug/l	14451600	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	58
3	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
4	1,4-Hexadiene, 5-methyl-	96	C7H12	000763-88-2	25
5	1,4-Hexadiene, 4-methyl-	96	C7H12	001116-90-1	25





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

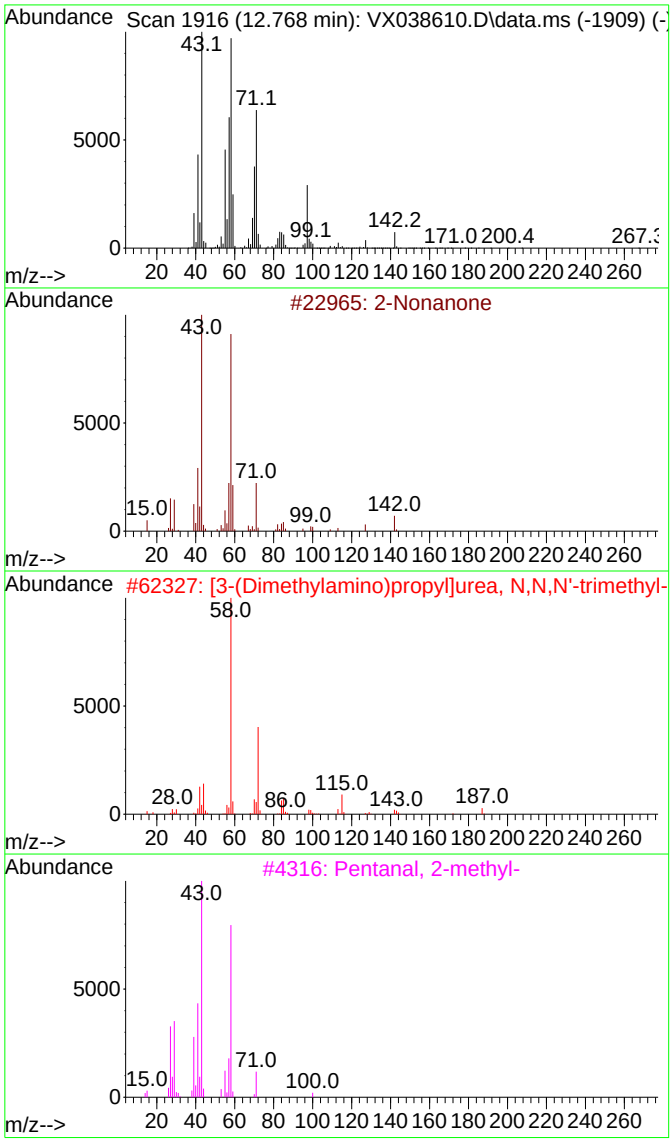
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

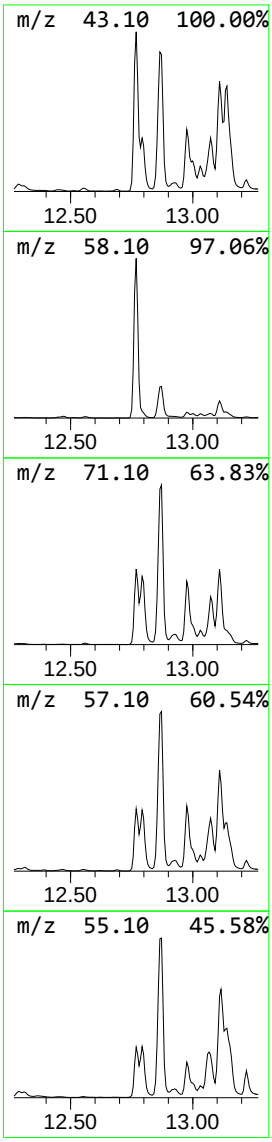
****

Peak Number 3 2-Nonanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.768	562.44 ug/l	15401400	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	91
2	[3-(Dimethylamino)propyl]urea, N...	187	C9H21N3O	1593933-50-6	38
3	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	35
4	2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	22
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	22





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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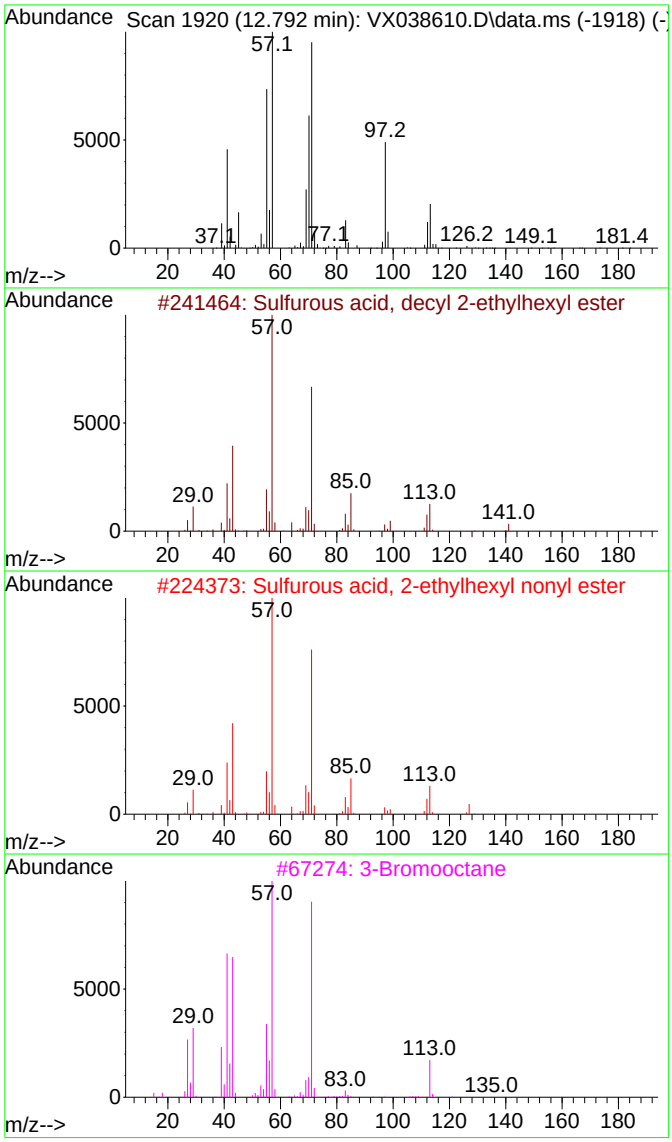
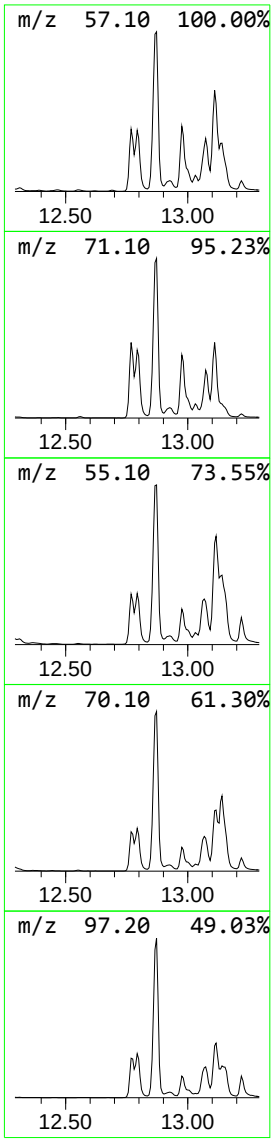
****
Peak Number 4 Sulfurous acid, decyl 2-eth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.793	399.23 ug/l	10932100	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	50
2	Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	47
3	3-Bromooctane	192	C8H17Br	000999-64-4	43
4	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	43
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	43





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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

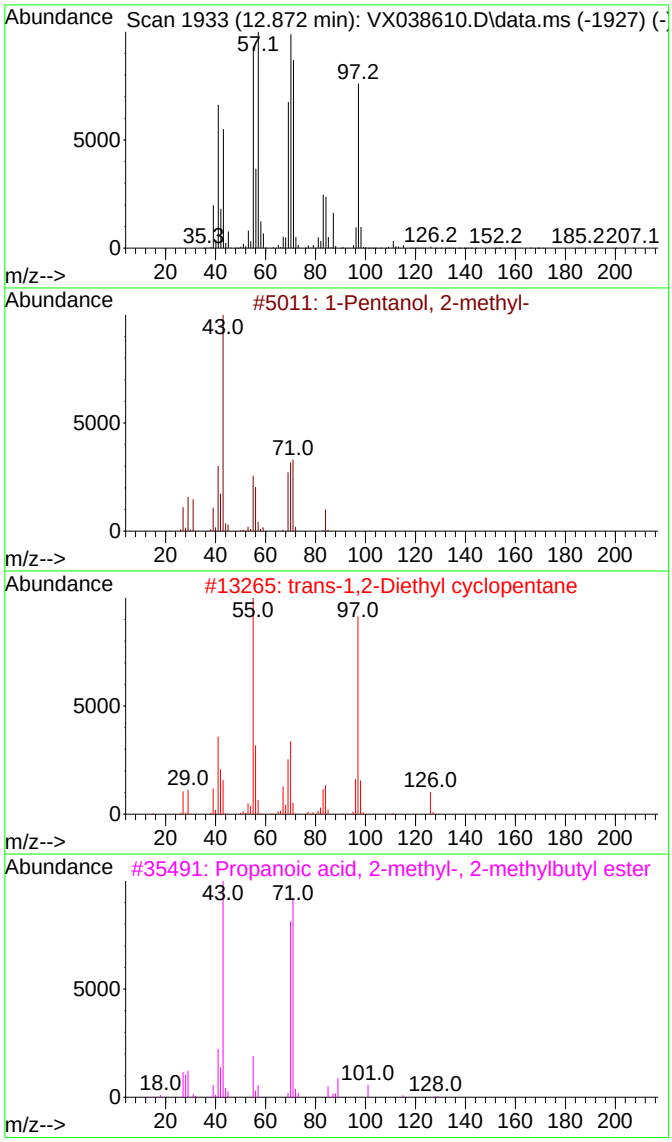
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

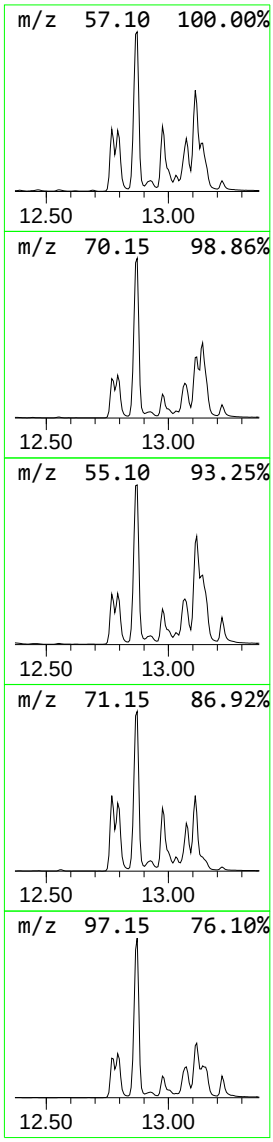
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown12.872 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.872	1455.74 ug/l	39863000	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	43
2	trans-1,2-Diethyl cyclopentane	126	C9H18	000932-40-1	38
3	Propanoic acid, 2-methyl-, 2-met...	158	C9H18O2	002445-69-4	35
4	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	27
5	Cyclohexane, 1,4-dimethyl-	112	C8H16	000589-90-2	27





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MSVOA_X
ClientSampleId :
AQ-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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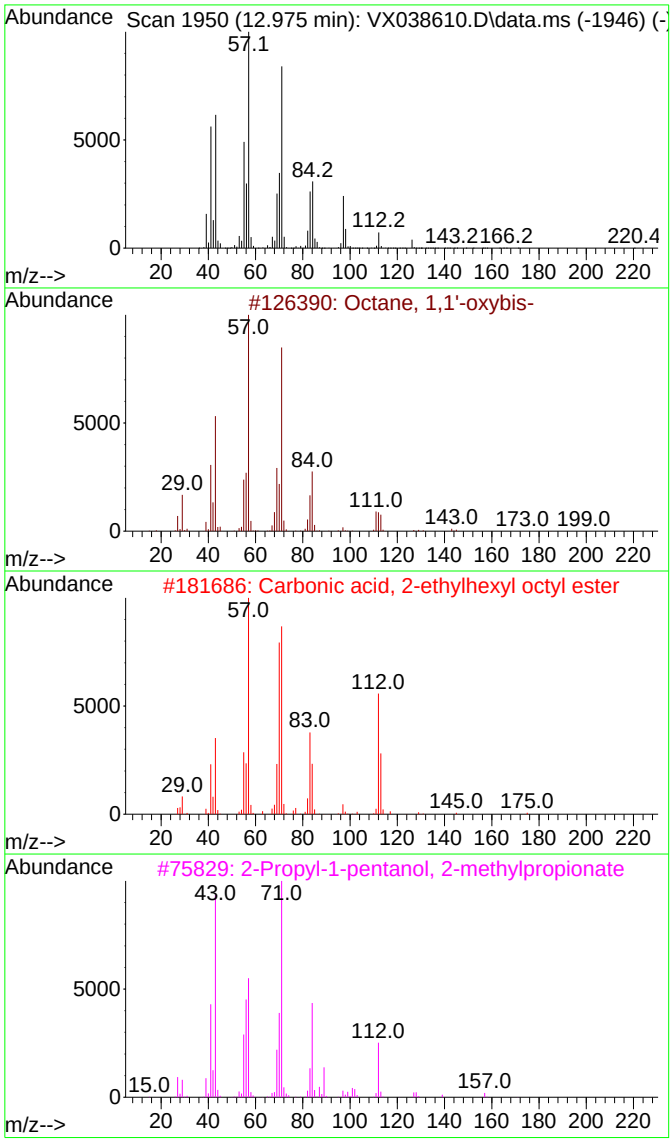
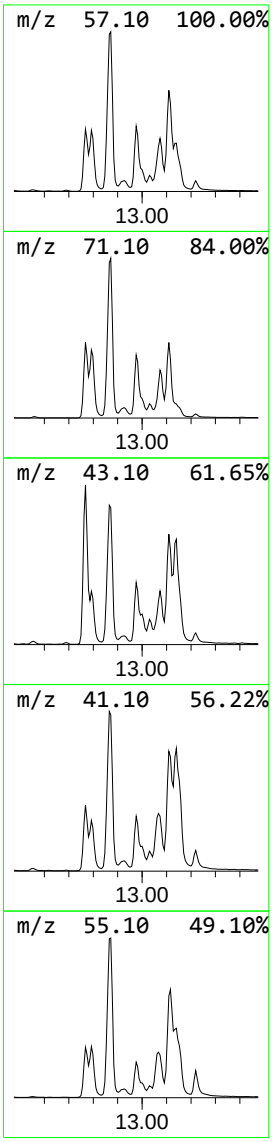
****
Peak Number 6 Octane, 1,1'-oxybis- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.975	536.43 ug/l	14689200	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	64
2	Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	53
3	2-Propyl-1-pentanol, 2-methylpro...	200	C12H24O2	1000447-36-4	53
4	Oxalic acid, 2-ethylhexyl hexyl ...	286	C16H30O4	1000309-38-9	53
5	Undecane, 5-methyl-	170	C12H26	001632-70-8	50





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Sample : 05107-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

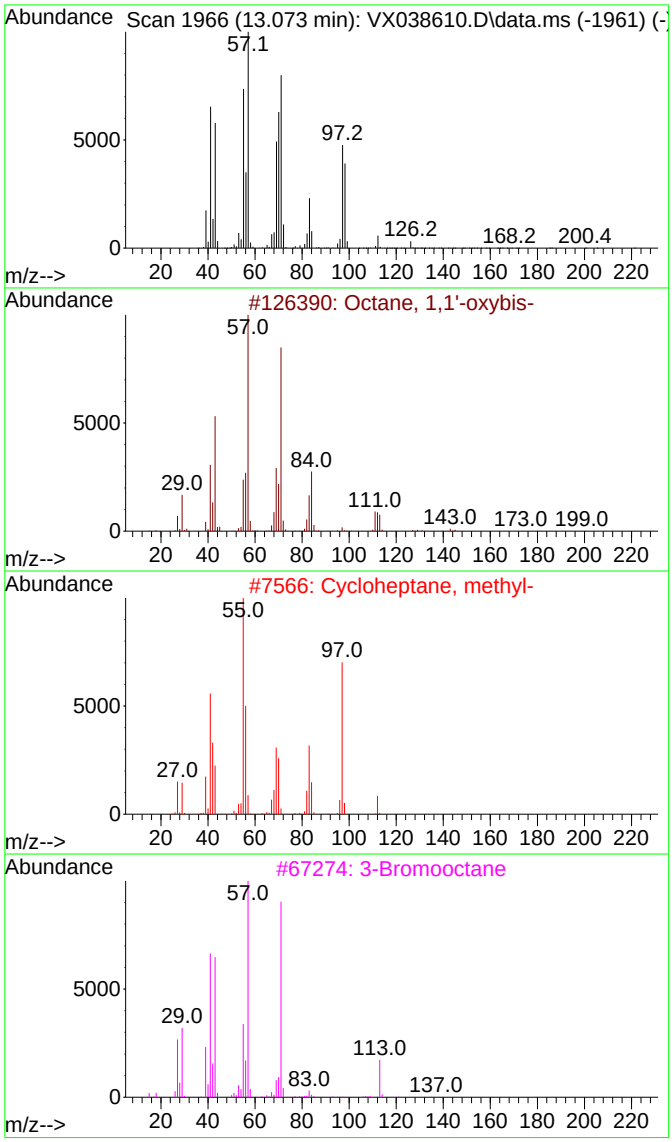
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

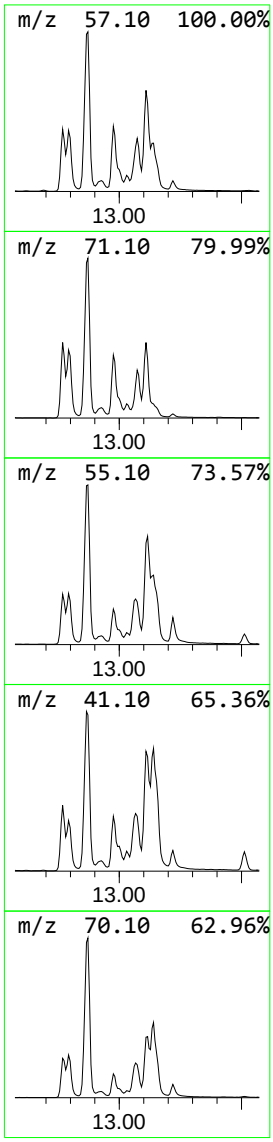
****

Peak Number 7 unknown13.073 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.073	574.50 ug/l	15731600	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	38
2	Cycloheptane, methyl-	112	C8H16	004126-78-7	38
3	3-Bromooctane	192	C8H17Br	000999-64-4	27
4	Methylamine, N-(1-butylpentylide...	155	C10H21N	010599-81-2	27
5	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	27





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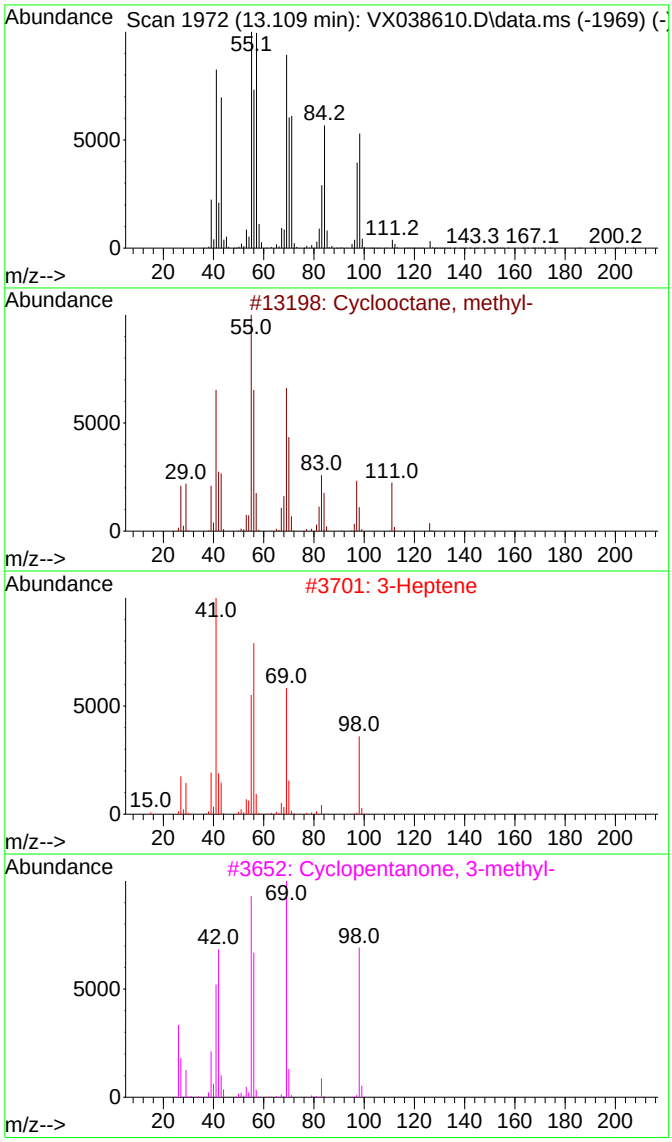
Quant Title : SW846 8260

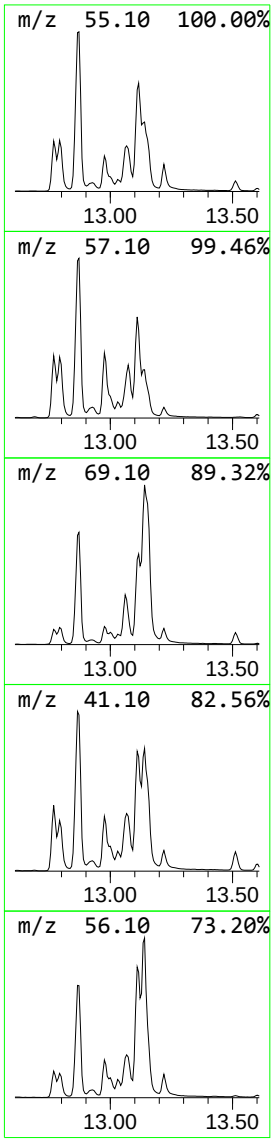
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclooctane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.110	1034.83 ug/l	28337100	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, methyl-	126	C9H18	001502-38-1	53
2	3-Heptene	98	C7H14	000592-78-9	43
3	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	43
4	Cycloheptane	98	C7H14	000291-64-5	43
5	2-Pentene, 3-ethyl-	98	C7H14	000816-79-5	38





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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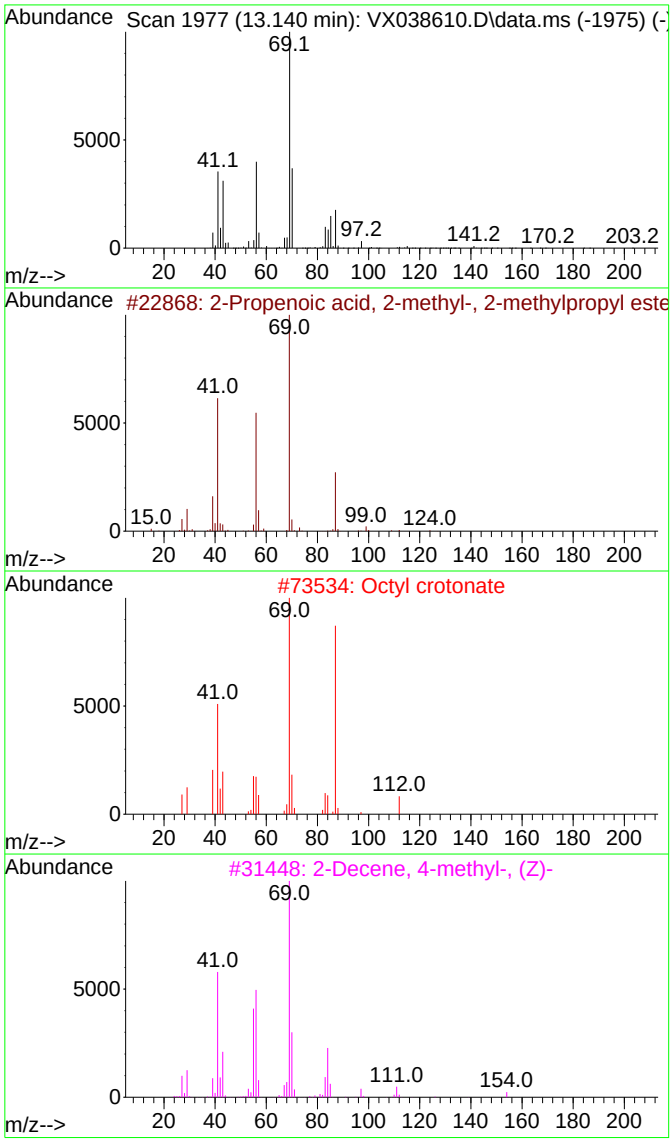
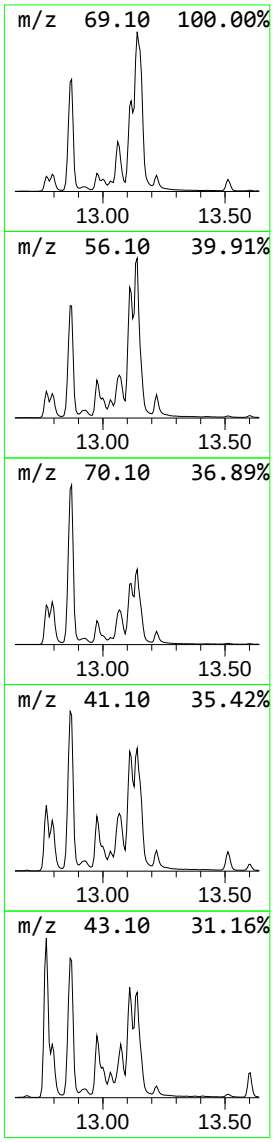
****
Peak Number 9 2-Propenoic acid, 2-methyl-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	995.24 ug/l	27252900	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 2-methyl-, 2-m...	142	C8H14O2	000097-86-9	53
2	Octyl crotonate	198	C12H22O2	1000429-17-5	40
3	2-Decene, 4-methyl-, (Z)-	154	C11H22	074630-30-1	40
4	2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	38
5	4-Pentenoic acid, 2-methyl-, tri...	296	C19H36O2	1000406-11-6	34





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038610.D
Acq On : 27 Oct 2023 18:08
Operator : JC/MD
Sample : 05107-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

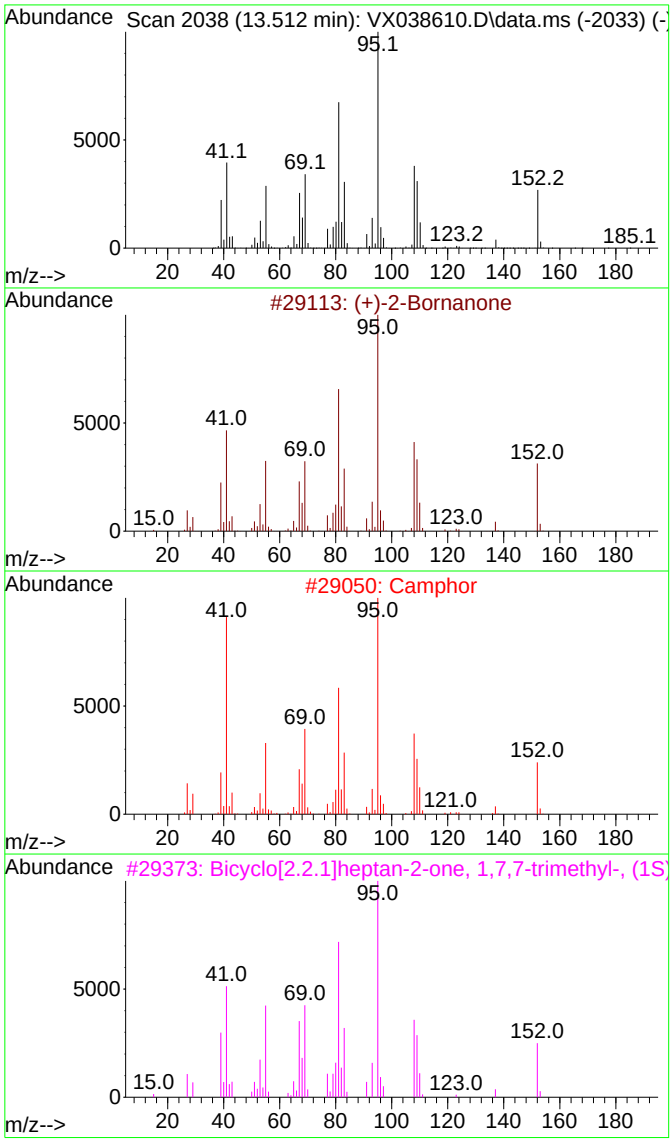
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.M
Quant Title : SW846 8260

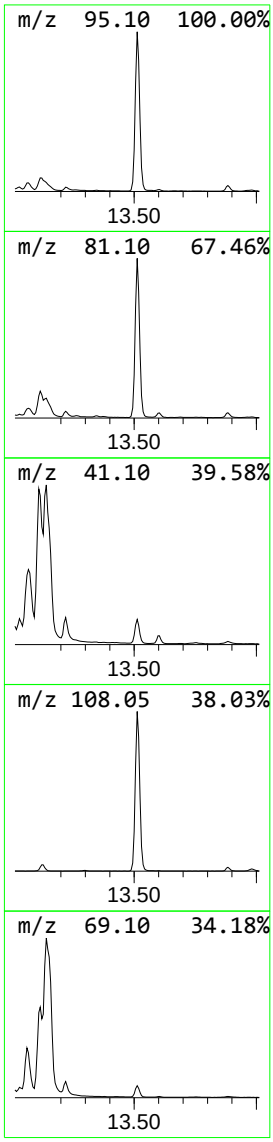
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 (+)-2-Bornanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.512	176.82 ug/l	4841790	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-2-Bornanone	152	C10H16O	000464-49-3	98
2	Camphor	152	C10H16O	000076-22-2	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	2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102723\
Data File : VX038610.D
Acq On : 27 Oct 2023 18:08
Operator : JC/MD
Sample : 05107-16
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AQ-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100523W.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-Octanone	11.841	274.3	ug/l	7511780	4	12.024	1369160	50.0
Eucalyptol	12.104	527.8	ug/l	14451600	4	12.024	1369160	50.0
2-Nonanone	12.768	562.4	ug/l	15401400	4	12.024	1369160	50.0
Sulfurous acid,...	12.793	399.2	ug/l	10932100	4	12.024	1369160	50.0
unknown12.872	12.872	1455.7	ug/l	39863000	4	12.024	1369160	50.0
Octane, 1,1'-ox...	12.975	536.4	ug/l	14689200	4	12.024	1369160	50.0
unknown13.073	13.073	574.5	ug/l	15731600	4	12.024	1369160	50.0
Cyclooctane, me...	13.110	1034.8	ug/l	28337100	4	12.024	1369160	50.0
2-Propenoic aci...	13.140	995.2	ug/l	27252900	4	12.024	1369160	50.0
(+)-2-Bornanone	13.512	176.8	ug/l	4841790	4	12.024	1369160	50.0