LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051322\
Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

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\82X051222W.M
Title : SW846 8260

Signal : TIC: VX028715.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	51	rBV	411116	1515020	18.06%	4.196%
2	2.380	204	212	217	rBV	385308	643032	7.66%	1.781%
3	2.538	229	238	251	rBV	310994	713455	8.50%	1.976%
4	5.391	692	706	722	rBV	181031	531526	6.34%	1.472%
5	5.556	722	733	748	rVB	280774	792795	9.45%	2.196%
6	5.958	788	799	810	rBV	198556	507577	6.05%	1.406%
7	6.763	921	931	947	rBV	468537	1111749	13.25%	3.079%
8	8.574	1221	1228	1234	rBV	54667	93860	1.12%	0.260%
9	8.653	1234	1241	1247	rVV	950720	1517620	18.09%	4.203%
10	8.720	1247	1252	1260	rVB	139942	215889	2.57%	0.598%
11	9.031	1297	1303	1314	rBV	85966	141209	1.68%	0.391%
12	10.055	1465	1471	1483	rVB	1174030	1557917	18.57%	4.315%
13	10.305	1505	1512	1518	rVB	86348	124031	1.48%	0.344%
14	10.506	1540	1545	1554	rBV	131265	171673	2.05%	0.475%
15	11.079	1634	1639	1651	rVB	1070268	1356705	16.17%	3.758%
16	11.378	1683	1688	1694	rBV	59471	120312	1.43%	0.333%
17	11.750	1745	1749	1759	rVB	133513	186563	2.22%	0.517%
18	12.024	1789	1794	1800	rVB	1144792	1404134	16.74%	3.889%
19	12.103	1800	1807	1813	rBV2	391837	621711	7.41%	1.722%
20	12.219	1821	1826	1833	rBV	7065583	8389658	100.00%	23.237%
21	12.317	1838	1842	1848	rVB3	164092	303758	3.62%	0.841%
22	12.530	1873	1877	1879	rBV	79883	105607	1.26%	0.292%
23	12.555	1879	1881	1884	rVV	85754	96577	1.15%	0.267%
24	12.615	1887	1891	1894	rVB	118355	141478	1.69%	0.392%
25	12.701	1900	1905	1913	rBV4	40613	93182	1.11%	0.258%
26	12.792	1913	1920	1923	rBV3	61718	123151	1.47%	0.341%
27	12.859	1926	1931	1938	rVV2	666797	991420	11.82%	2.746%
28	12.920	1938	1941	1944	rVV	112770	147567	1.76%	0.409%
29	12.969	1944	1949	1956	rVV2	473997	766500	9.14%	2.123%
30	13.067	1960	1965	1968	rVV	466078	770163	9.18%	2.133%
31	13.103	1968	1971	1973	rVV	1763978	2324351	27.70%	6.438%
32	13.128	1973	1975	1985	rVV3	1845357	3550732	42.32%	9.834%
33	13.213	1985	1989	1995	rVV	763661	1102323	13.14%	3.053%
34	13.292	1999	2002	2007	rVB2	262753	344800	4.11%	0.955%
35	13.420	2020	2023	2033	rVB	181932	266899	3.18%	0.739%
36	13.512	2033	2038	2041	rBV3	106858	159033	1.90%	0.440%

LSC Area Percent Report

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Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

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\82X051222W.M
Title : SW846 8260

37	13.585	2046	2050	2057	rVB4	58517	100049	1.19%	0.277%
38	13.731	2070	2074	2078	rBV2	310560	521068	6.21%	1.443%
39	13.774	2078	2081	2088	rVB	333445	464991	5.54%	1.288%
40	13.859	2088	2095	2097	rBV2	146386	246276	2.94%	0.682%
41	13.890	2097	2100	2104	rVV	159134	195485	2.33%	0.541%
42	14.036	2121	2124	2128	rVB	108854	115344	1.37%	0.319%
43	14.231	2150	2156	2163	rVB	159892	262290	3.13%	0.726%
44	14.481	2193	2197	2206	rVB4	126130	209186	2.49%	0.579%
45	14.615	2215	2219	2221	rBV	127399	177083	2.11%	0.490%
46	14.640	2221	2223	2226	rVV	126466	138107	1.65%	0.383%
47	14.755	2239	2242	2245	rBV	138258	158291	1.89%	0.438%
48	15.182	2308	2312	2314	rBV	80999	107192	1.28%	0.297%
49	15.213	2314	2317	2320	rVB2	76197	96747	1.15%	0.268%
50	15.487	2357	2362	2367	rBV2	128527	210591	2.51%	0.583%
51	16.377	2503	2508	2516	rVB2	54285	98501	1.17%	0.273%

Sum of corrected areas: 36105178

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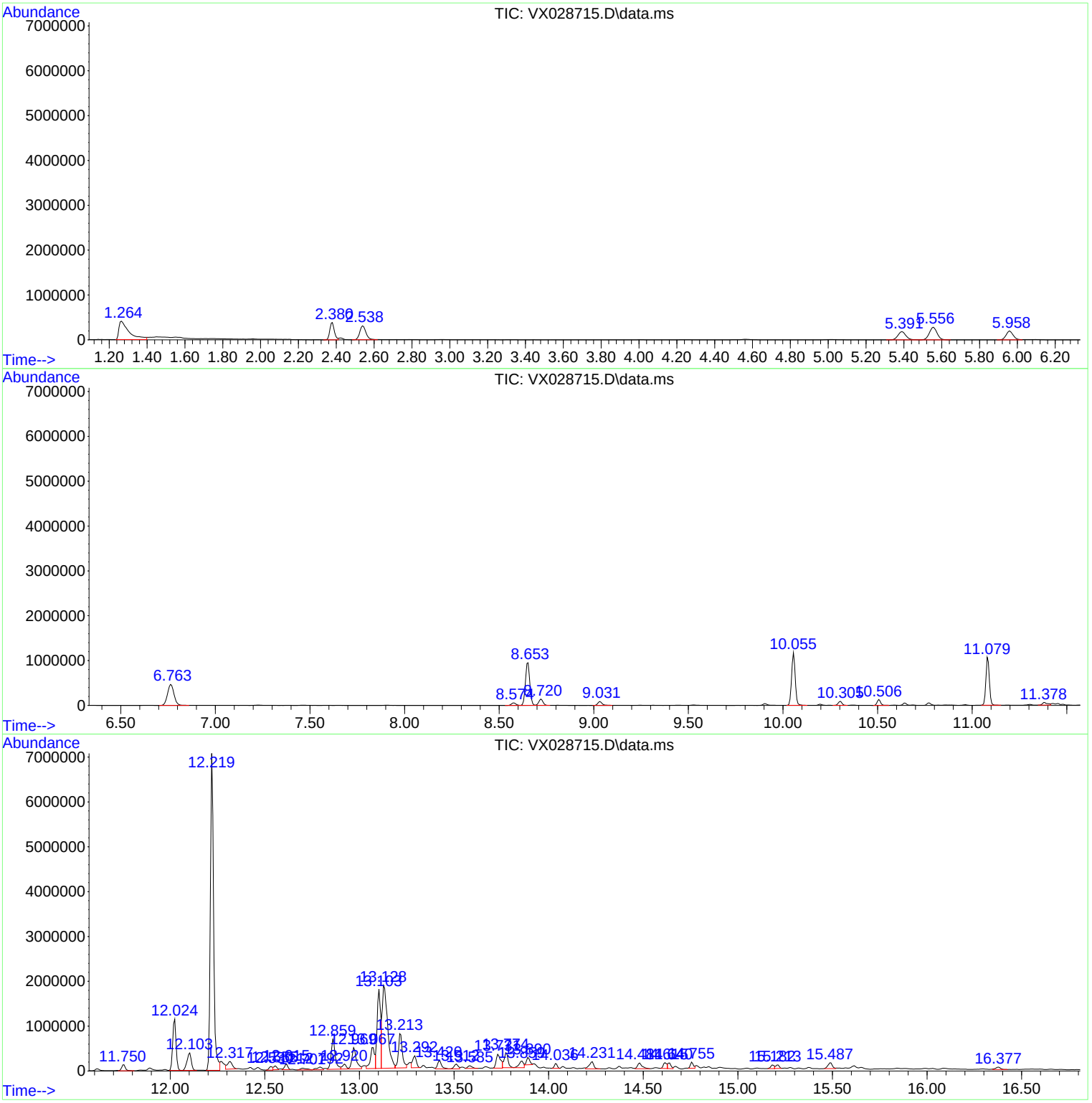
Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

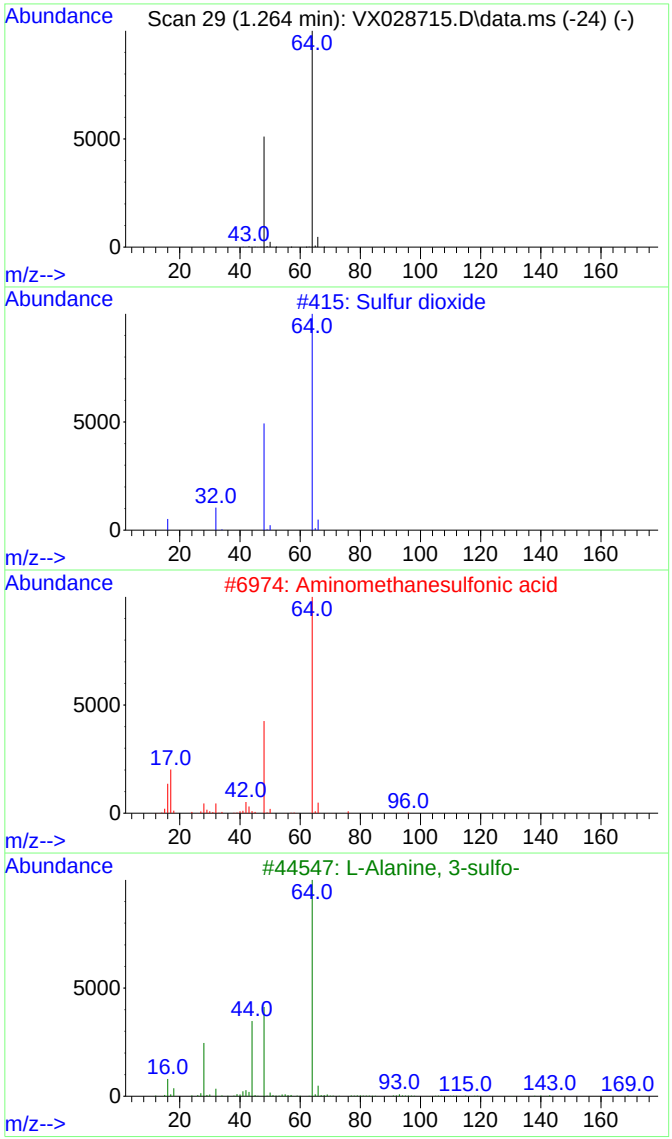
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

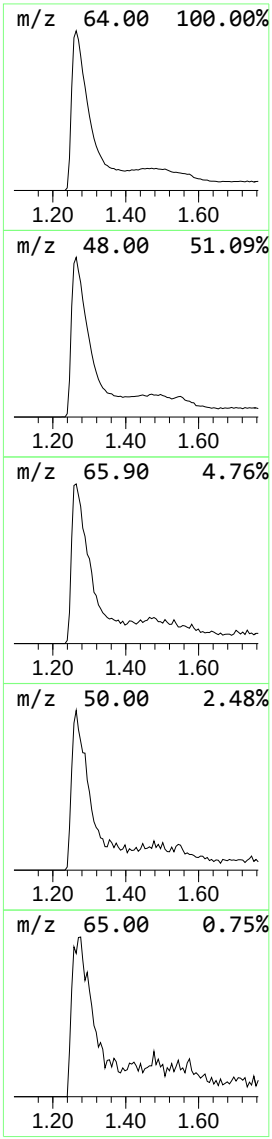
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	95.55 ug/l	1515020	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

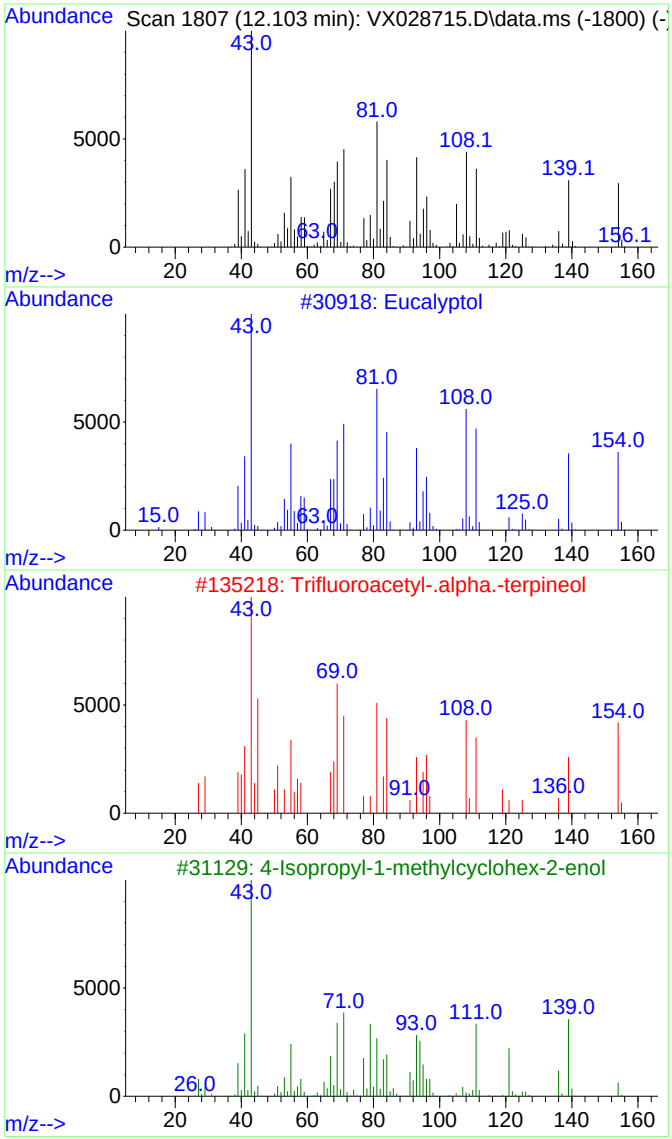
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

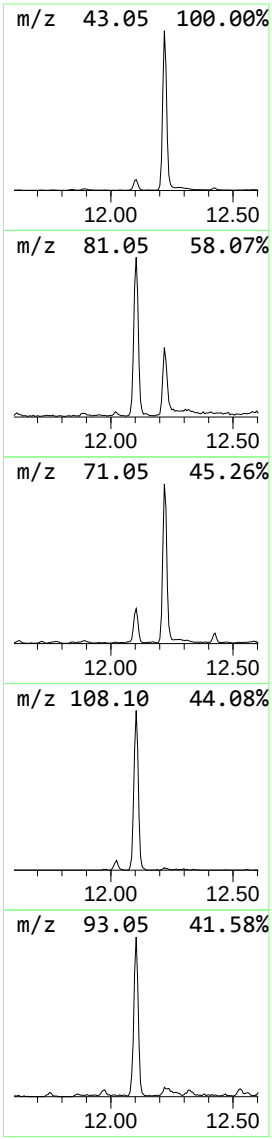
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.103	22.14 ug/l	621711	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	98
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	43
3	4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	35
4	5-Isopropyl-2-methylbicyclo[3.1....	154	C10H18O	000546-79-2	32
5	2-Cyclohexen-1-ol, 1-methyl-4-(1...	154	C10H18O	029803-81-4	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051322\
Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

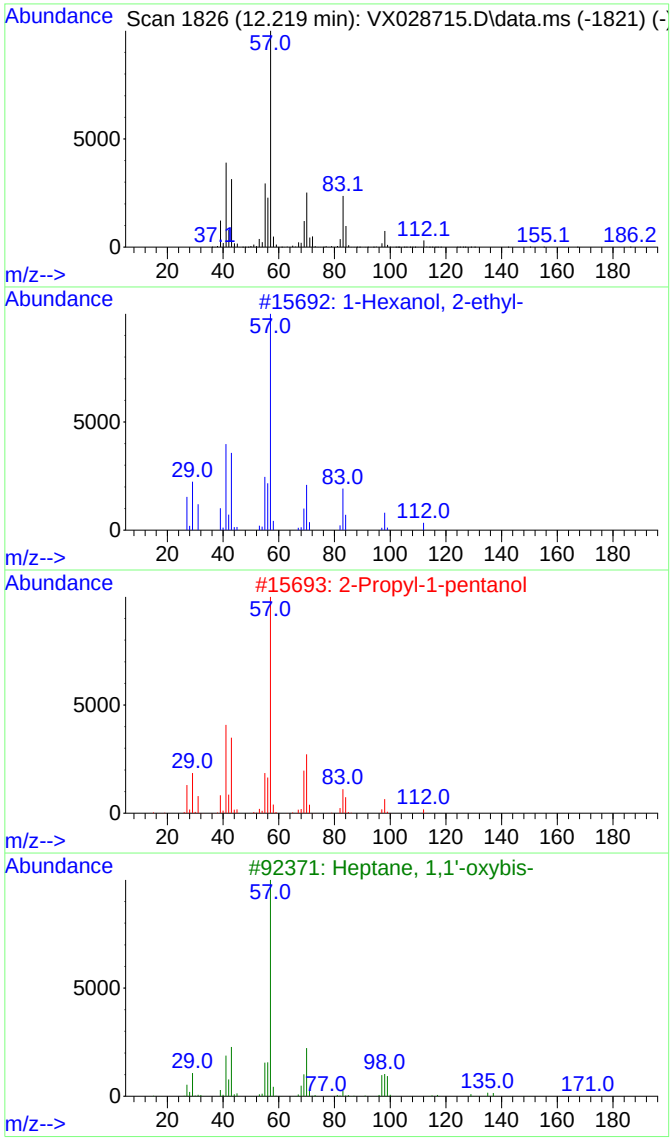
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

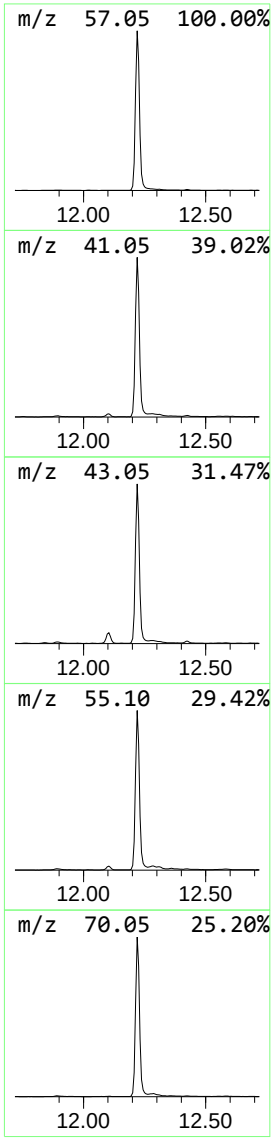
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	298.75 ug/l	8389660	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	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051322\
Data File : VX028715.D
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Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

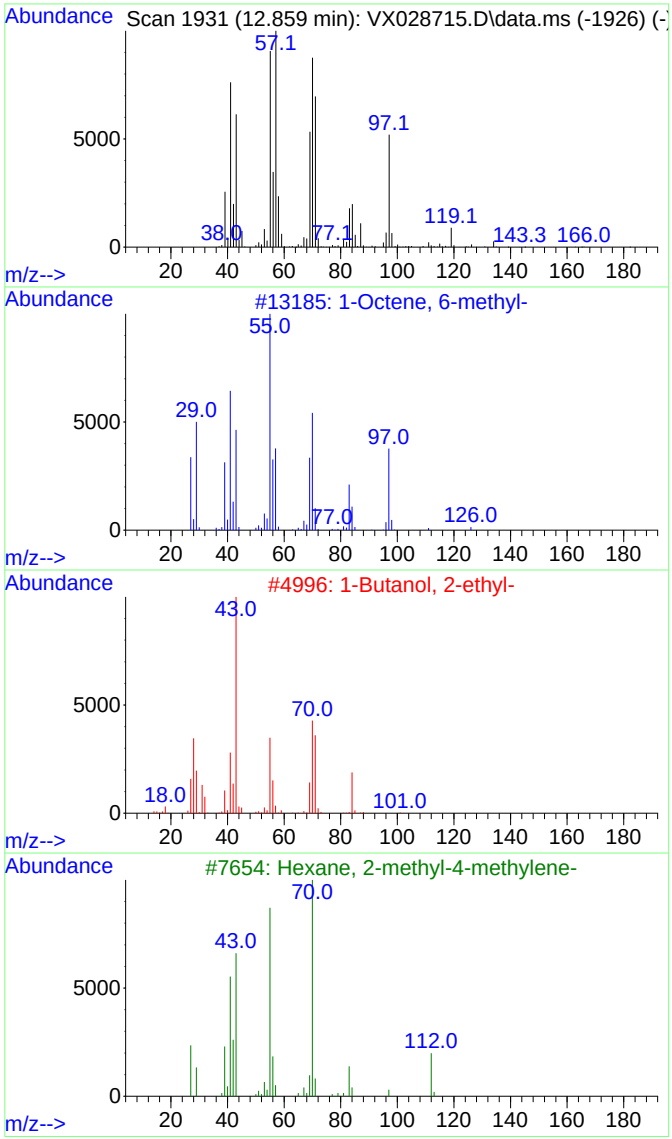
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

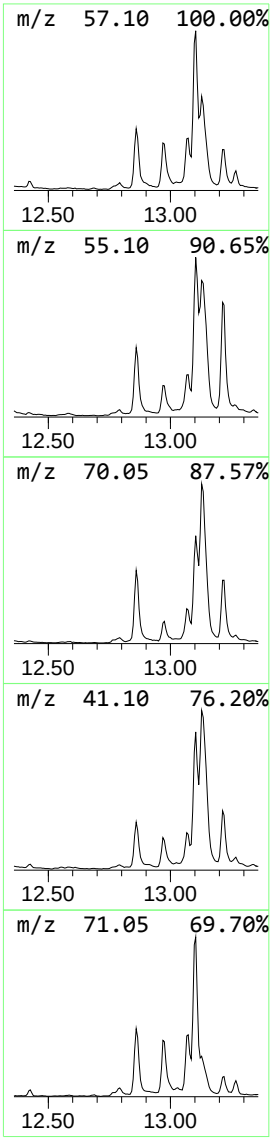
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	35.30 ug/l	991420	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	52
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	47
3	Hexane, 2-methyl-4-methylene-	112	C8H16	003404-80-6	43
4	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	35
5	Diisoamyl ether	158	C10H22O	000544-01-4	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051322\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

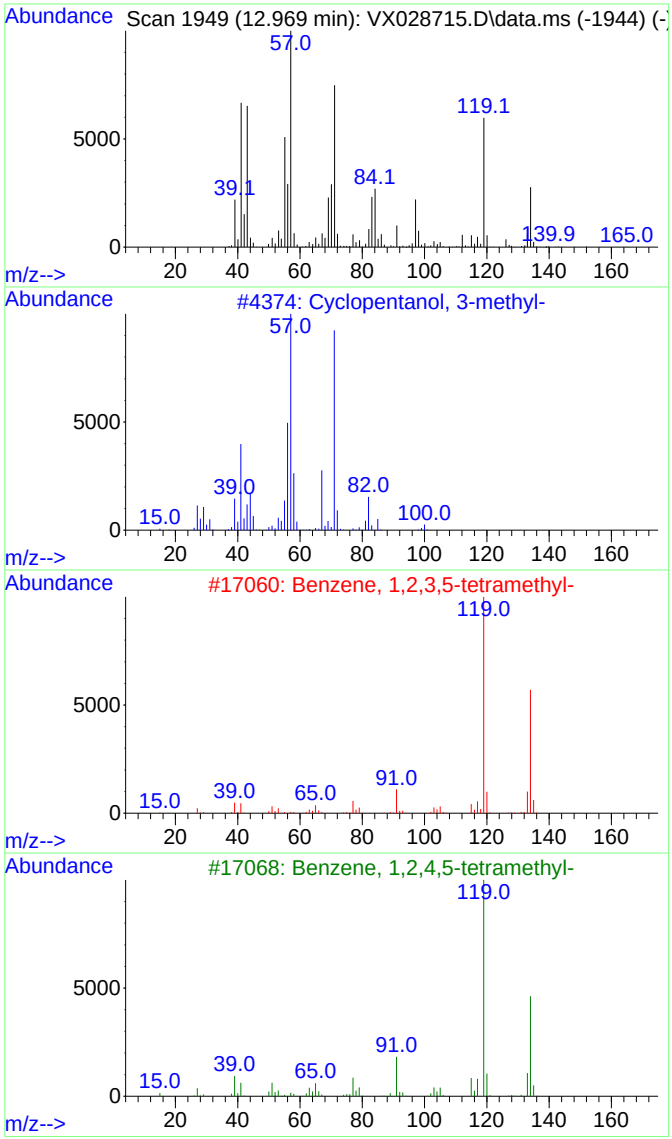
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

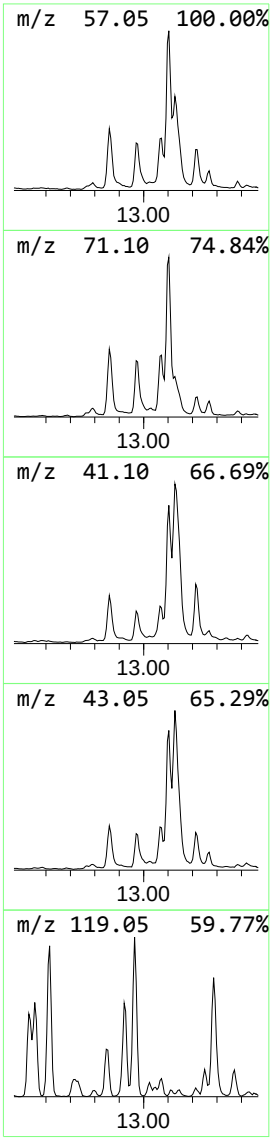
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown12.969 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.969	27.29 ug/l	766500	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanol, 3-methyl-	100	C6H12O	018729-48-1	30
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	25
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	25
4	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	25
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	25





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ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
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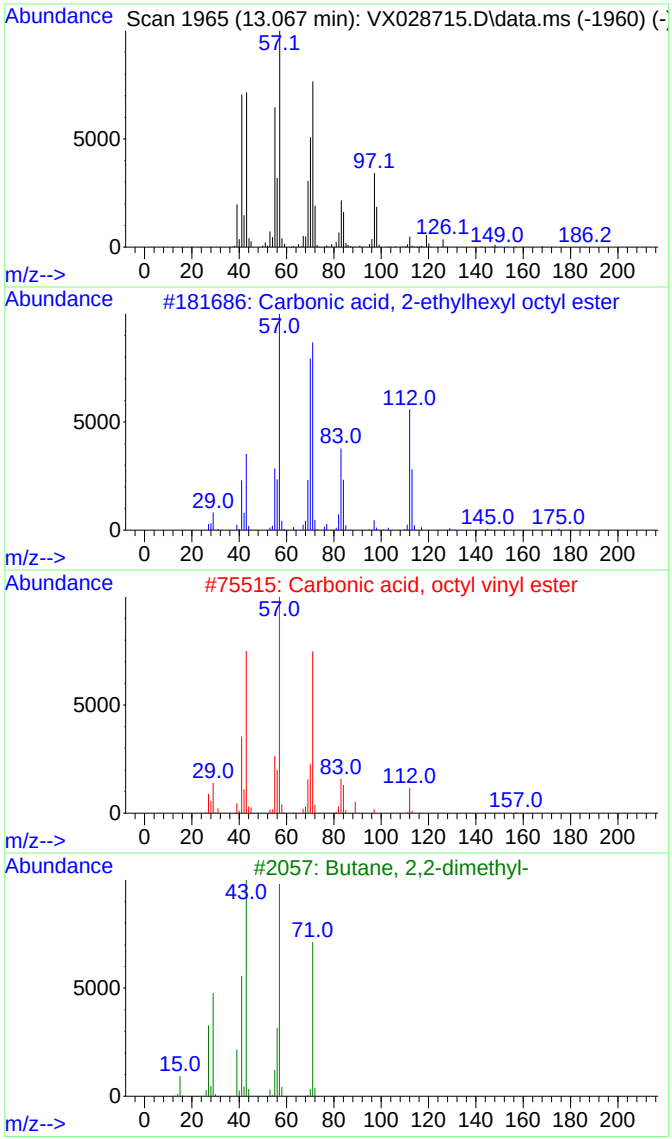
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

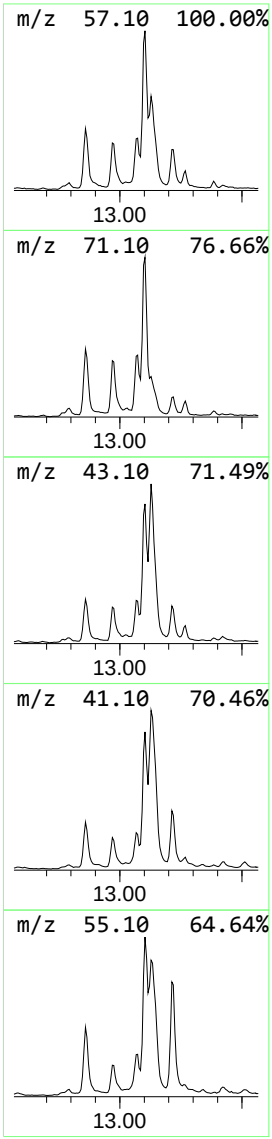
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown13.067 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.067	27.42 ug/l	770163	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2-ethylhexyl octy...	286	C17H34O3	1000383-13-5	47
2	Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	47
3	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
4	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	38
5	1-Hexanethiol, 2-ethyl-	146	C8H18S	007341-17-5	35





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ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

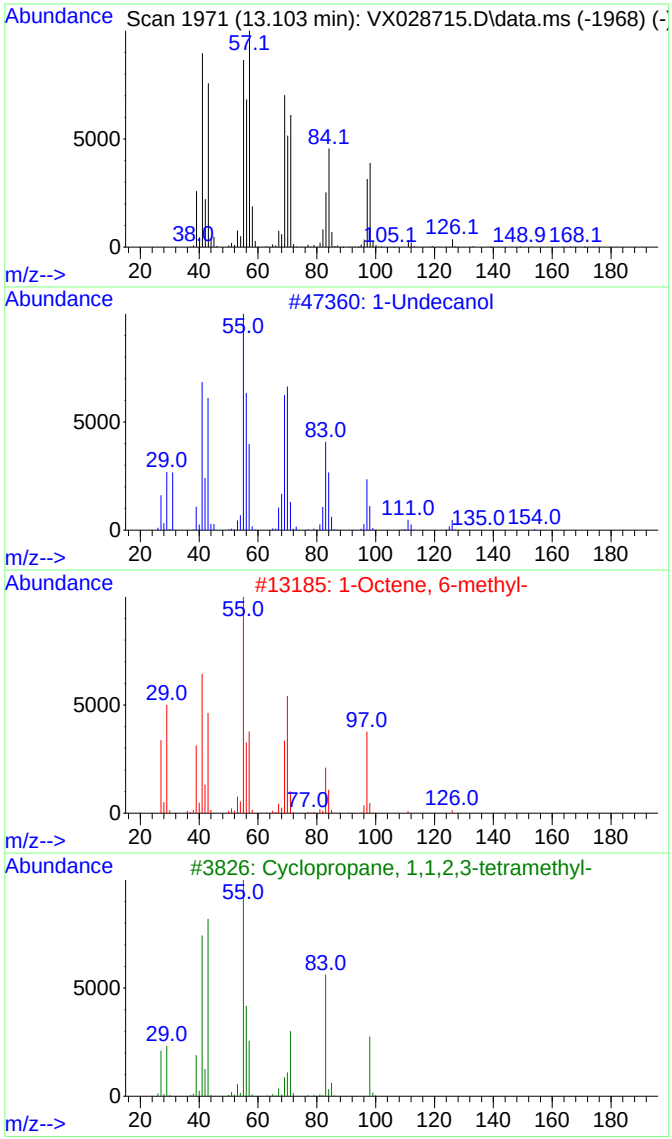
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

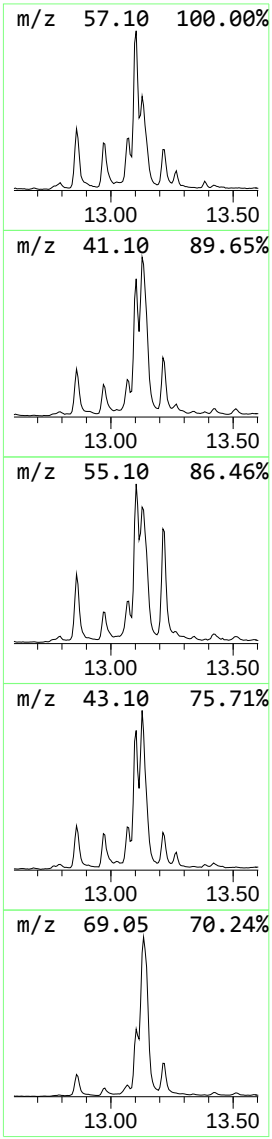
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 unknown13.103 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	82.77 ug/l	2324350	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Undecanol	172	C11H24O	000112-42-5	43
2	1-Octene, 6-methyl-	126	C9H18	013151-10-5	38
3	Cyclopropane, 1,1,2,3-tetramethyl-	98	C7H14	074752-93-5	38
4	1-Heptene, 3-methyl-	112	C8H16	004810-09-7	38
5	Cyclooctane, methyl-	126	C9H18	001502-38-1	38





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Data File : VX028715.D
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Operator : JC/MD
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ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

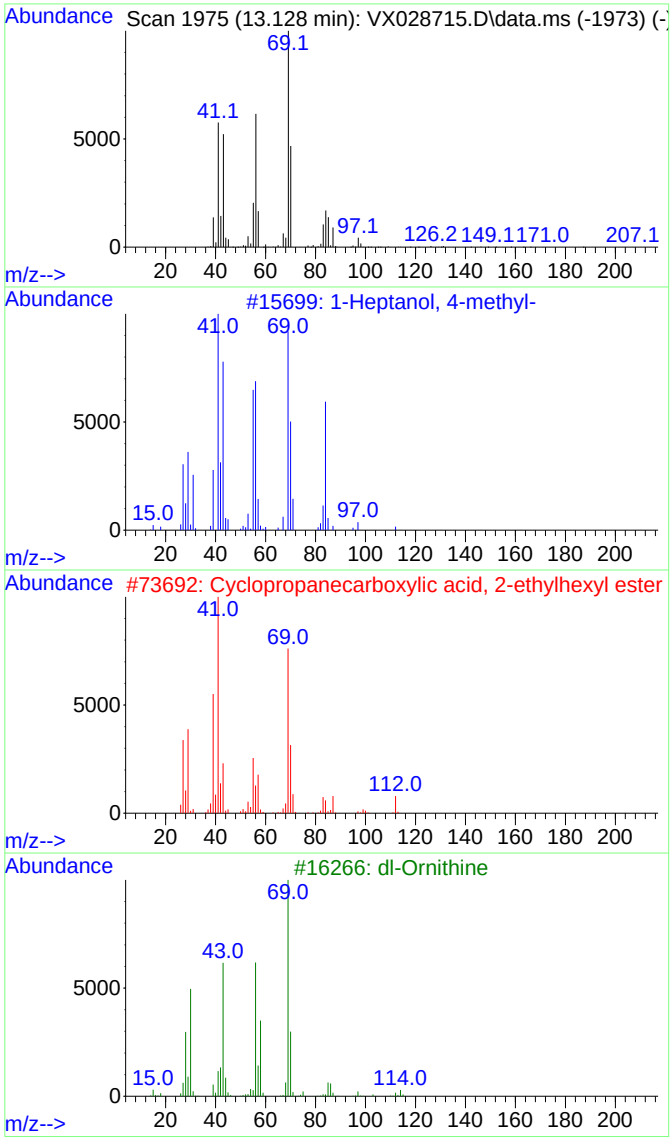
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

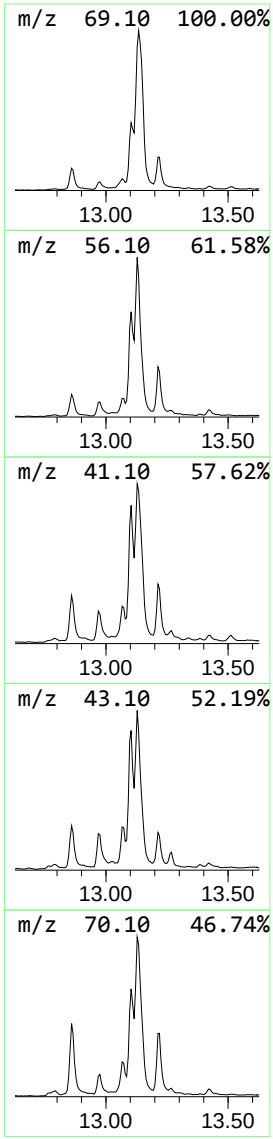
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Heptanol, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.128	126.44 ug/l	3550730	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	50
2	Cyclopropanecarboxylic acid, 2-e...	198	C12H22O2	103604-31-5	50
3	dl-Ornithine	132	C5H12N2O2	000616-07-9	45
4	3-Methylpentyl acetate	144	C8H16O2	035897-13-3	42
5	3-Ethyl-4-methylpentan-1-ol	130	C8H18O	038514-13-5	38





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Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

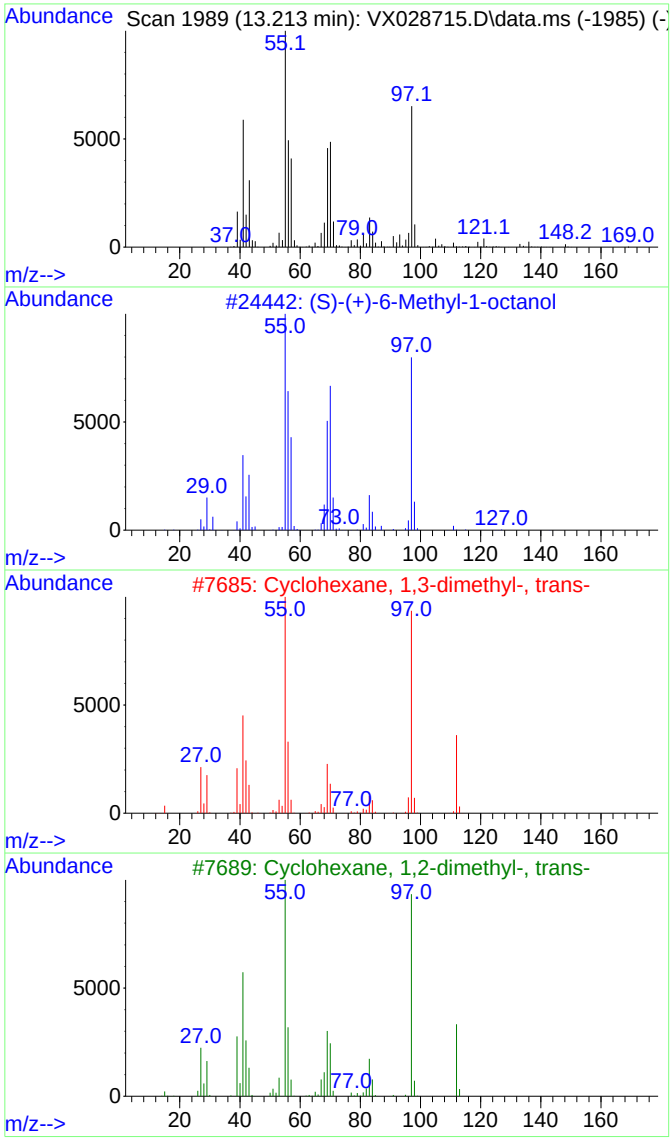
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

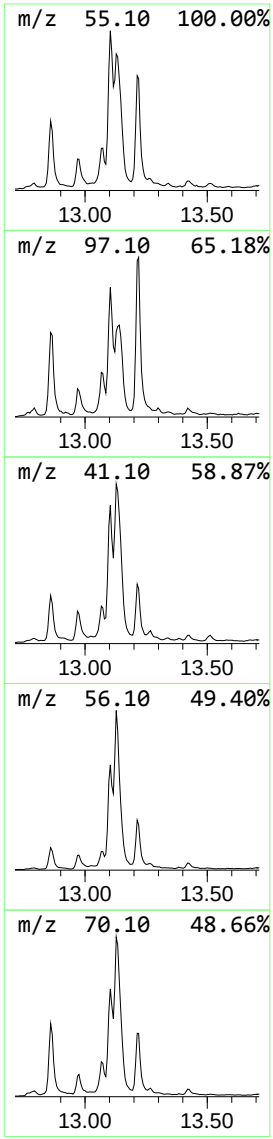
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 (S)-(+)-6-Methyl-1-octanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.213	39.25 ug/l	1102320	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-6-Methyl-1-octanol	144	C9H20O	110453-78-6	91
2	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	59
3	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	50
4	Cyclohexane, 1,1-dimethyl-	112	C8H16	000590-66-9	50
5	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	000624-29-3	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051322\
Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

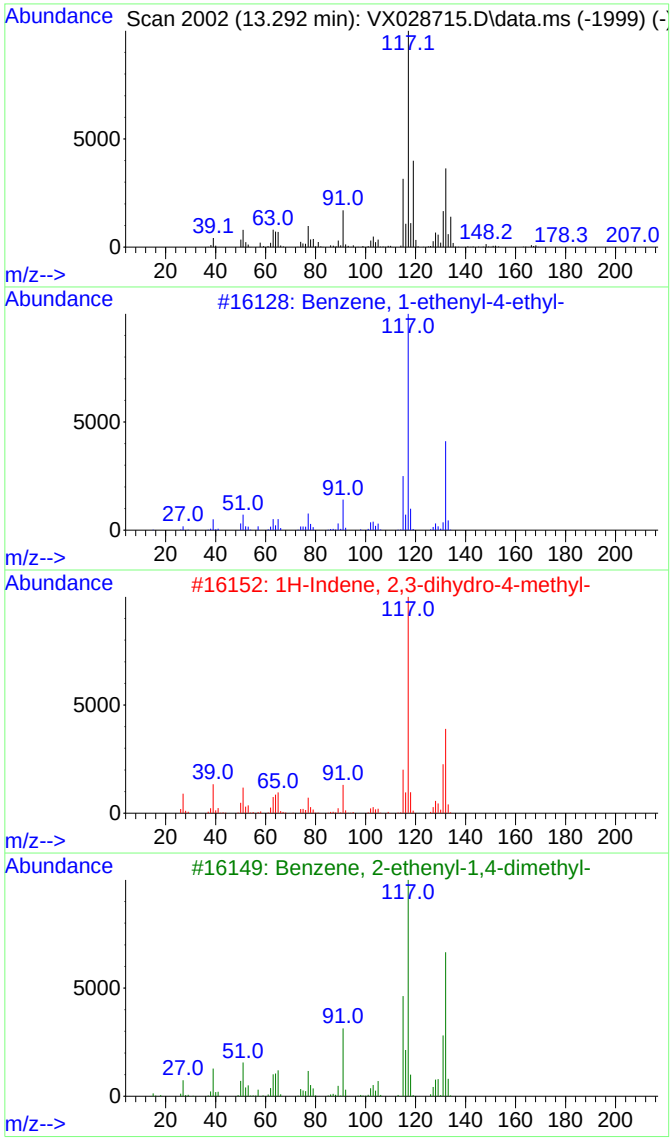
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

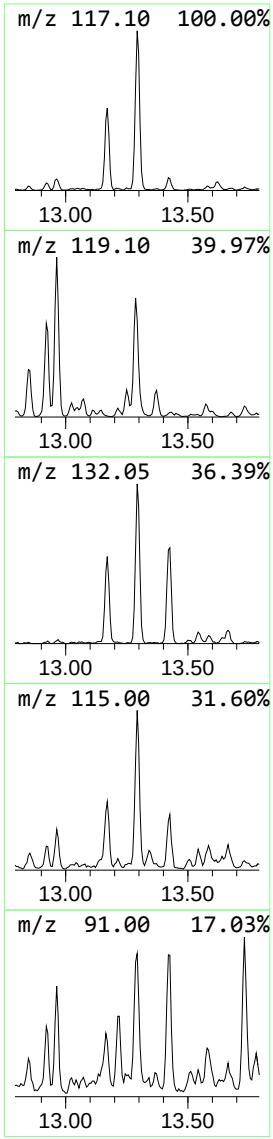
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	12.28 ug/l	344800	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	93
2	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	92
3	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	89
5	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051322\
Data File : VX028715.D
Acq On : 14 May 2022 06:27
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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
Sulfur dioxide	1.264	95.5	ug/l	1515020	1	5.556	792795	50.0
Eucalyptol	12.103	22.1	ug/l	621711	4	12.024	1404130	50.0
1-Hexanol, 2-et...	12.219	298.8	ug/l	8389660	4	12.024	1404130	50.0
1-Octene, 6-met...	12.859	35.3	ug/l	991420	4	12.024	1404130	50.0
unknown12.969	12.969	27.3	ug/l	766500	4	12.024	1404130	50.0
unknown13.067	13.067	27.4	ug/l	770163	4	12.024	1404130	50.0
unknown13.103	13.103	82.8	ug/l	2324350	4	12.024	1404130	50.0
1-Heptanol, 4-m...	13.128	126.4	ug/l	3550730	4	12.024	1404130	50.0
(S)-(+)-6-Methy...	13.213	39.3	ug/l	1102320	4	12.024	1404130	50.0
Benzene, 1-ethe...	13.292	12.3	ug/l	344800	4	12.024	1404130	50.0