LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 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: VX028744.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	50	rBV	389222	1430776	18.38%	4.352%
2	2.374	205	211	217	rBV	379859	628140	8.07%	1.911%
3	2.532	228	237	252	rBV	380141	697192	8.96%	2.121%
4	5.391	693	706	718	rBV	163202	477050	6.13%	1.451%
5	5.556	722	733	750	rVB	248856	703749	9.04%	2.141%
6	5.958	788	799	810	rBV2	173898	462235	5.94%	1.406%
7	6.763	921	931	945	rBV	419845	1003577	12.90%	3.053%
8	8.574	1221	1228	1234	rBV	55128	92491	1.19%	0.281%
9	8.653	1234	1241	1247	rVV	865500	1378124	17.71%	4.192%
10	8.720	1247	1252	1263	rVB	136140	209936	2.70%	0.639%
11	9.031	1297	1303	1319	rBV	81526	137718	1.77%	0.419%
12	10.055	1462	1471	1482	rBV	945786	1280811	16.46%	3.896%
13	10.299	1506	1511	1518	rVB	72429	100305	1.29%	0.305%
14	10.506	1540	1545	1554	rBV	114812	148558	1.91%	0.452%
15	10.768	1583	1588	1594	rBV	55849	79779	1.03%	0.243%
16	11.079	1631	1639	1651	rVB	903811	1173765	15.08%	3.570%
17	11.378	1683	1688	1691	rBV	53937	80409	1.03%	0.245%
18	11.756	1745	1750	1759	rVB	141300	193899	2.49%	0.590%
19	12.024	1789	1794	1800	rVB	1047187	1267768	16.29%	3.856%
20	12.104	1800	1807	1813	rBV3	371568	591261	7.60%	1.798%
21	12.219	1821	1826	1833	rBV	6730011	7782677	100.00%	23.673%
22	12.317	1839	1842	1847	rVB3	160242	235906	3.03%	0.718%
23	12.530	1873	1877	1879	rBV	79643	99958	1.28%	0.304%
24	12.555	1879	1881	1885	rVV	82434	97553	1.25%	0.297%
25	12.616	1887	1891	1894	rVB	124613	139076	1.79%	0.423%
26	12.701	1900	1905	1913	rBV2	37897	80745	1.04%	0.246%
27	12.792	1913	1920	1925	rBV3	54475	127239	1.63%	0.387%
28	12.860	1926	1931	1938	rVV2	615966	910811	11.70%	2.770%
29	12.920	1938	1941	1945	rVV	102763	147502	1.90%	0.449%
30	12.969	1945	1949	1956	rVV2	417420	706837	9.08%	2.150%
31	13.073	1960	1966	1968	rVV	448772	686610	8.82%	2.088%
32	13.103	1968	1971	1973	rVV2	1699911	2158690	27.74%	6.566%
33	13.134	1973	1976	1986	rVV3	1703691	3410512	43.82%	10.374%
34	13.219	1986	1990	1996	rVV	691842	991650	12.74%	3.016%
35	13.292	1999	2002	2007	rVB2	230934	316407	4.07%	0.962%
36	13.420	2019	2023	2032	rVB	166662	245906	3.16%	0.748%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 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	13.512	2033	2038	2042	rBV2	101788	158582	2.04%	0.482%
38	13.585	2046	2050	2056	rVB2	53274	89859	1.15%	0.273%
39	13.731	2070	2074	2079	rBV2	294362	541794	6.96%	1.648%
40	13.774	2079	2081	2088	rVB	309088	397740	5.11%	1.210%
41	13.859	2089	2095	2098	rBV3	137571	233906	3.01%	0.711%
42	13.896	2098	2101	2105	rVV	156562	201660	2.59%	0.613%
43	14.231	2147	2156	2165	rVB	144642	248437	3.19%	0.756%
44	14.481	2193	2197	2207	rVB3	114861	186478	2.40%	0.567%
45	14.615	2215	2219	2221	rBV	87703	122485	1.57%	0.373%
46	14.640	2221	2223	2226	rVB	90369	93595	1.20%	0.285%
47	14.756	2239	2242	2244	rBV	81024	84968	1.09%	0.258%
48	15.182	2308	2312	2315	rBV	59258	90629	1.16%	0.276%
49	15.487	2357	2362	2367	rBV3	86759	150072	1.93%	0.456%

Sum of corrected areas: 32875827

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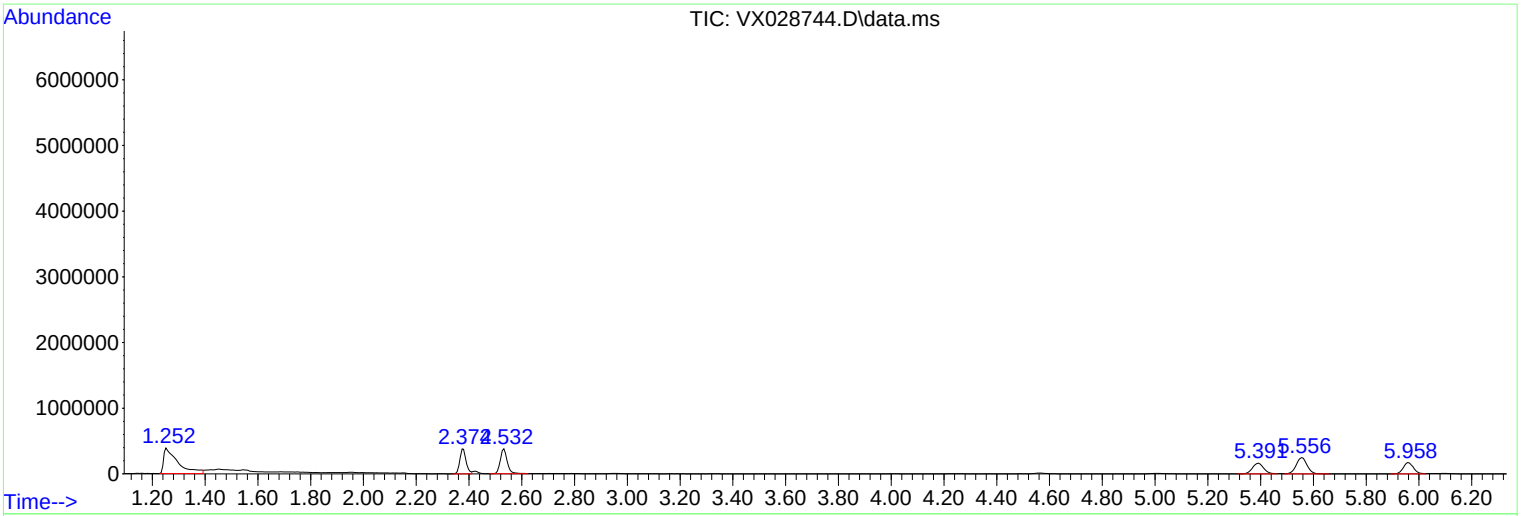
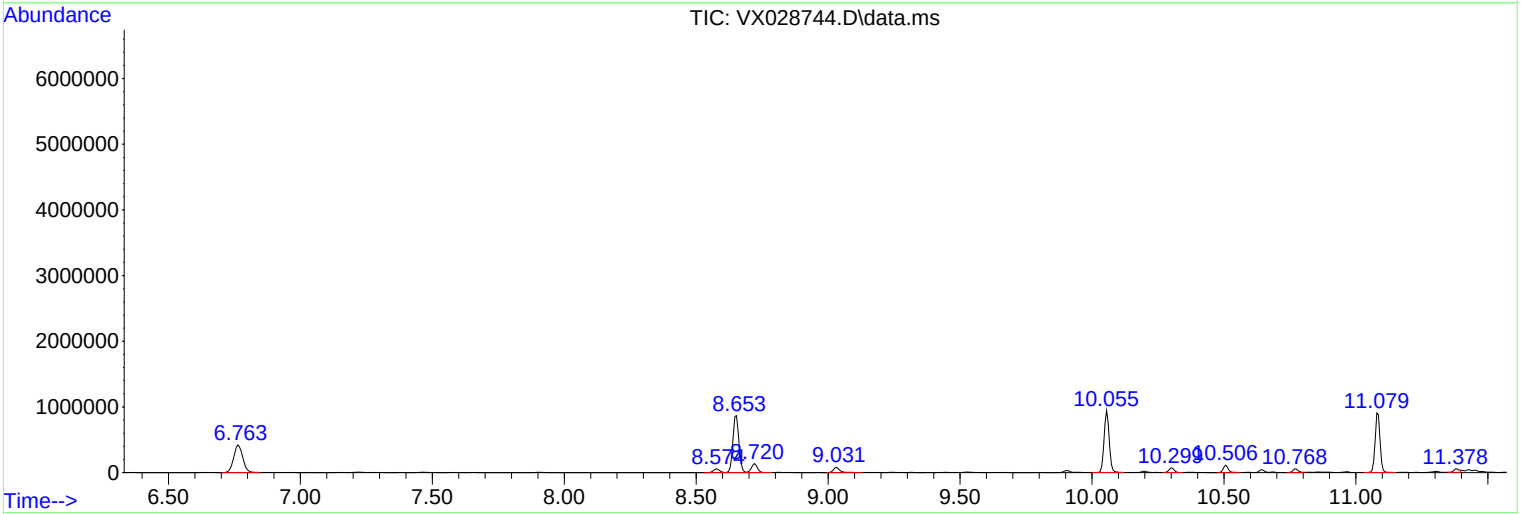
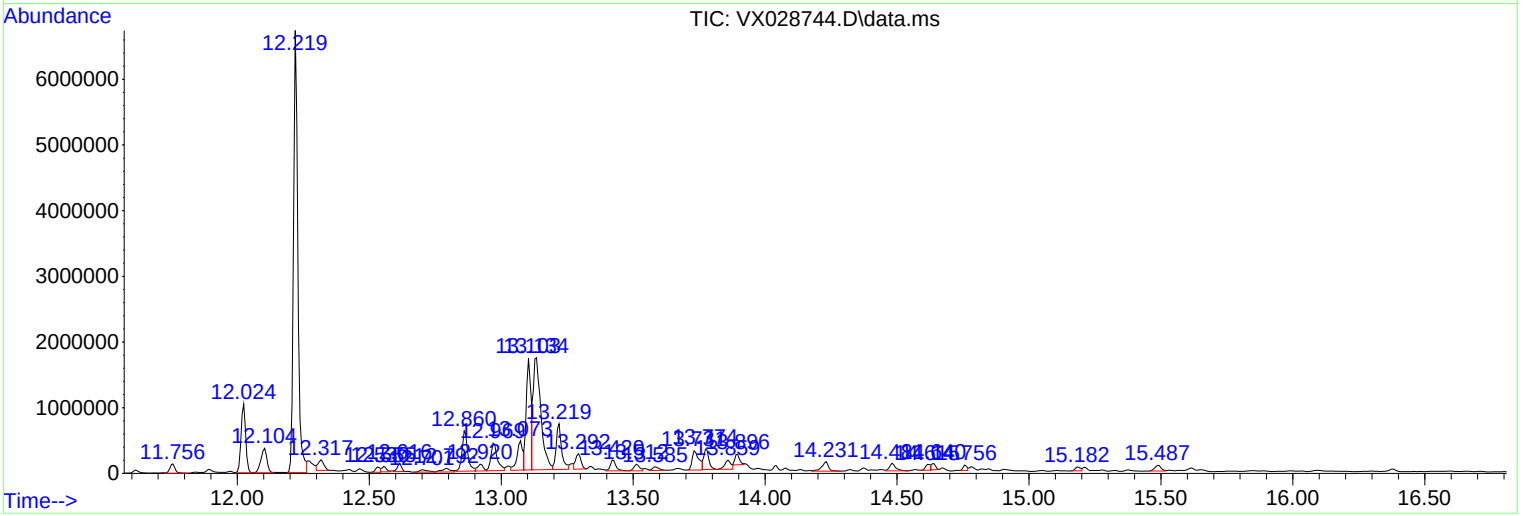
MSVOA_X
ClientSampleId :
BUR-1148

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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Acq On : 16 May 2022 20:12
Operator : JC/MD
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ALS Vial : 27 Sample Multiplier: 1

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MSVOA_X
ClientSampleId :
BUR-1148

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

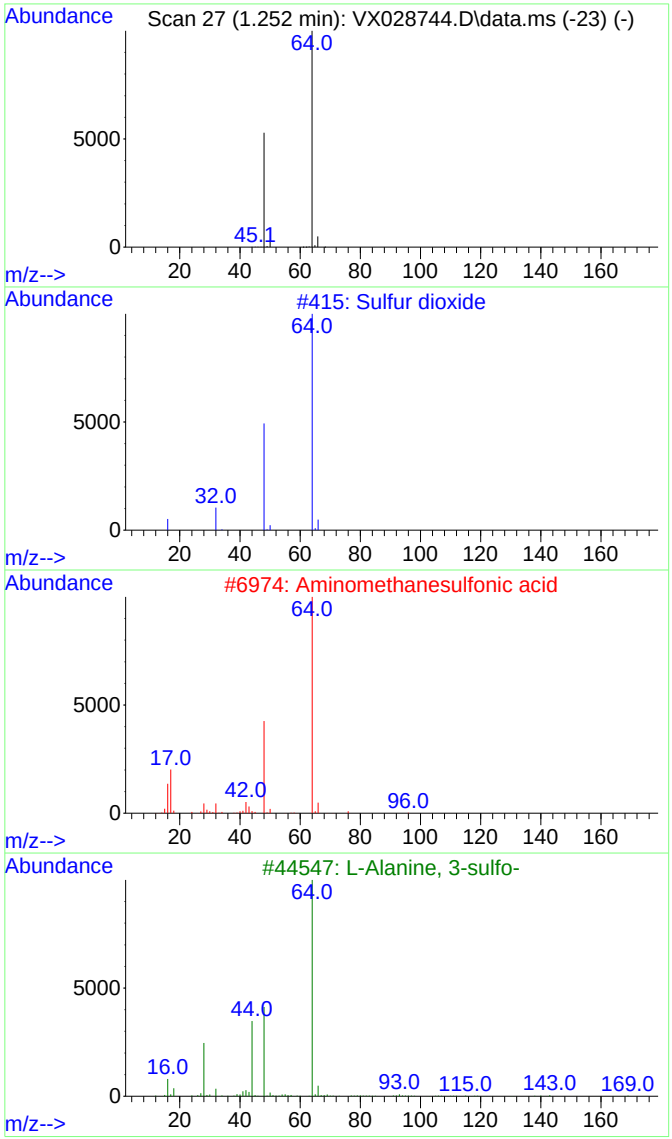
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

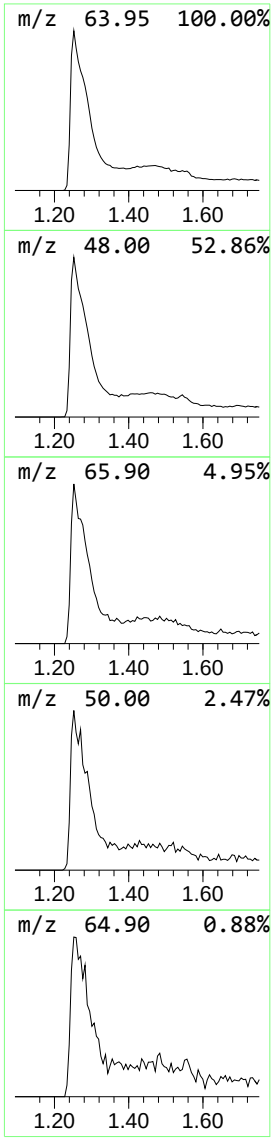
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	101.65 ug/l	1430780	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
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	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

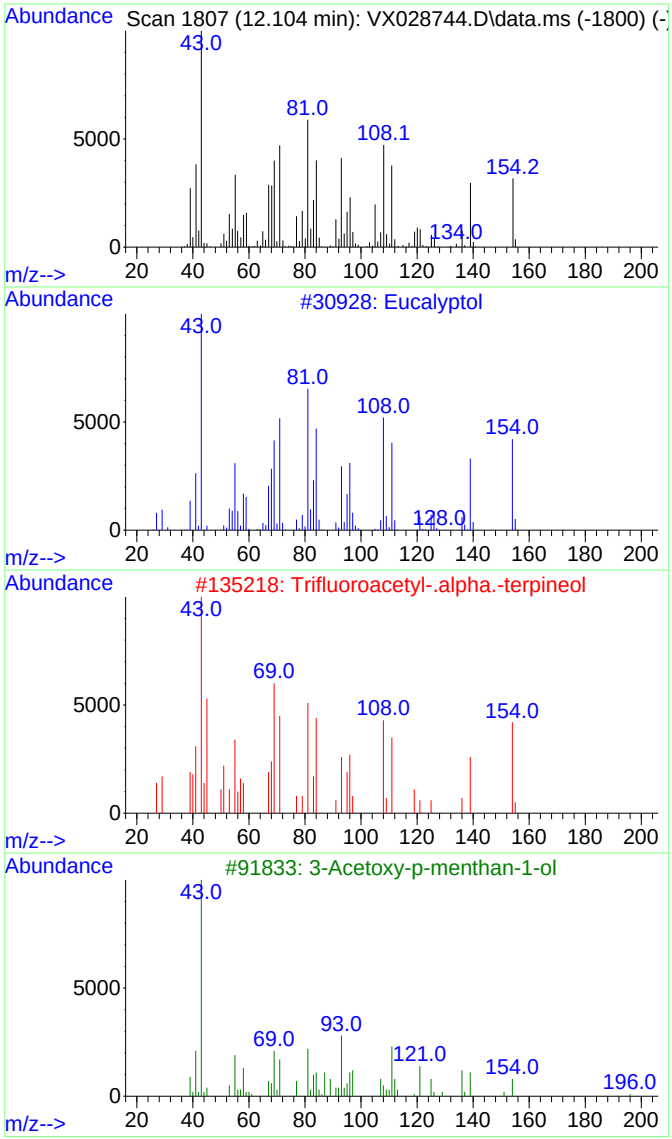
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

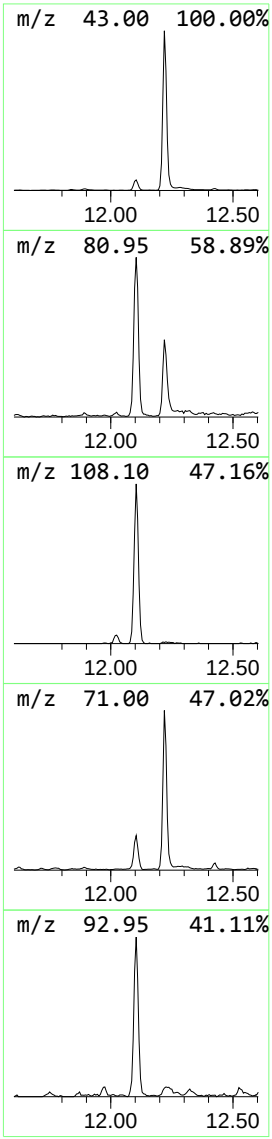
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Eucalyptol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.104	23.32 ug/l	591261	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	59
3	3-Acetoxy-p-menthan-1-ol	214	C12H22O3	058315-86-9	35
4	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5	5-Isopropyl-2-methylbicyclo[3.1....	154	C10H18O	000546-79-2	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

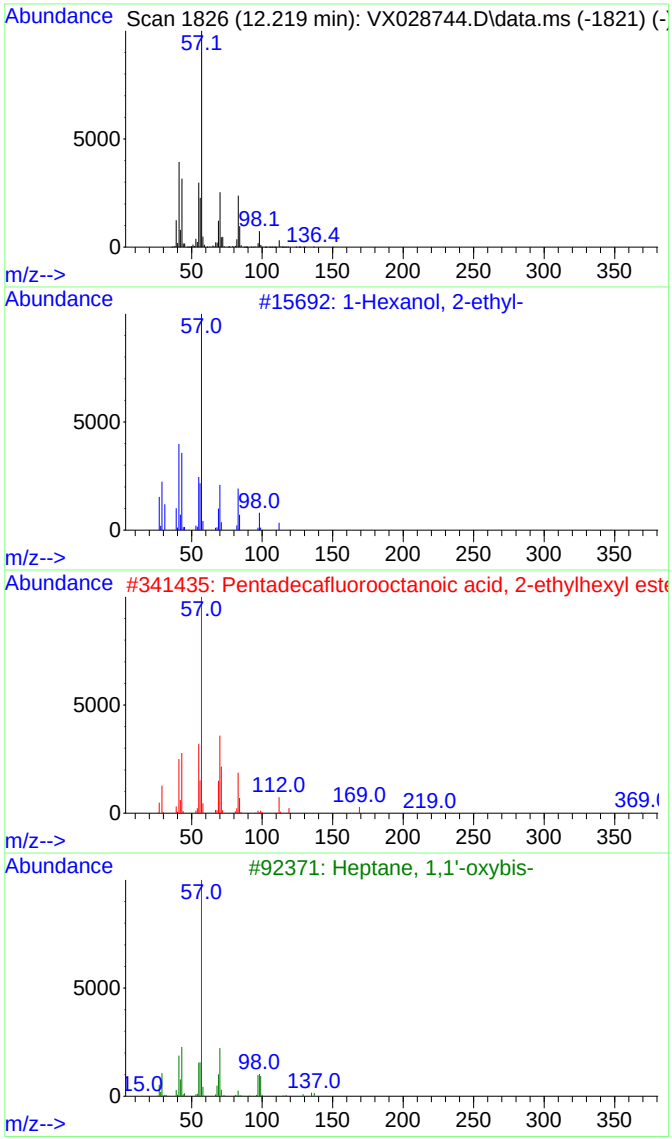
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

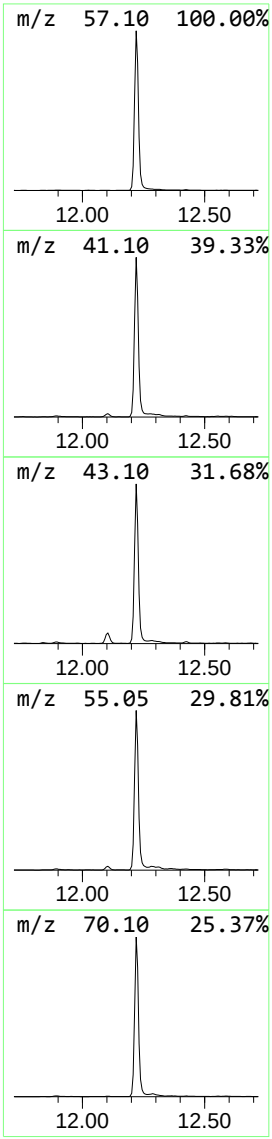
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	306.94 ug/l	7782680	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	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	53
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
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ALS Vial : 27 Sample Multiplier: 1

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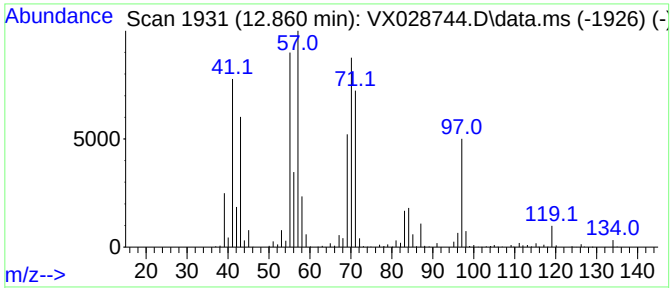
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

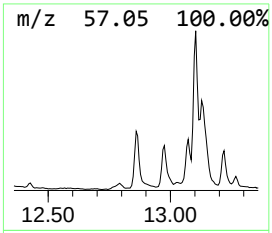
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

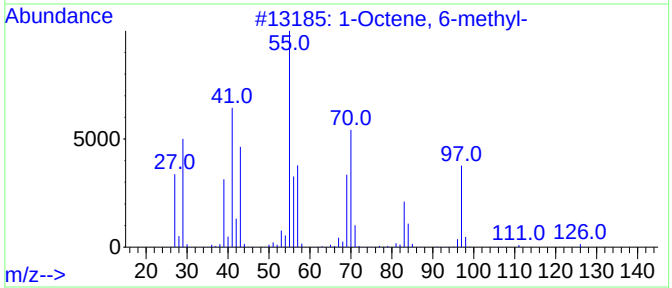
****
Peak Number 4 1-Octene, 6-methyl- Concentration Rank 6

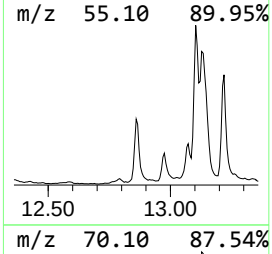
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.860	35.92 ug/l	910811	1,4-Dichlorobenzene-d4	12.024

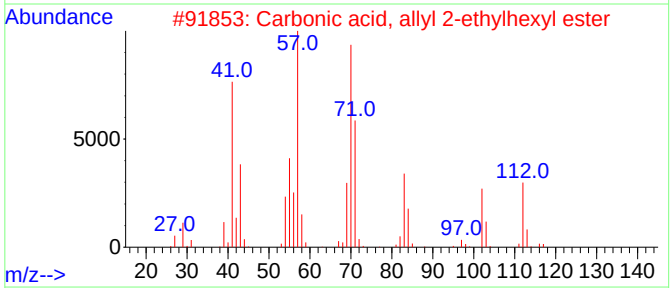
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octene, 6-methyl-	126	C9H18	013151-10-5	58
2	Carbonic acid, allyl 2-ethylhexy...	214	C12H22O3	1000357-80-6	53
3	Carbonic acid, isobutyl 2-methyl...	188	C10H20O3	1000331-39-8	47
4	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	47
5	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	43

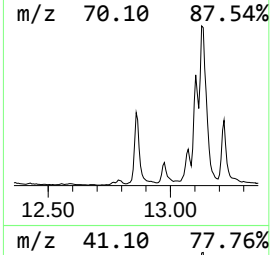


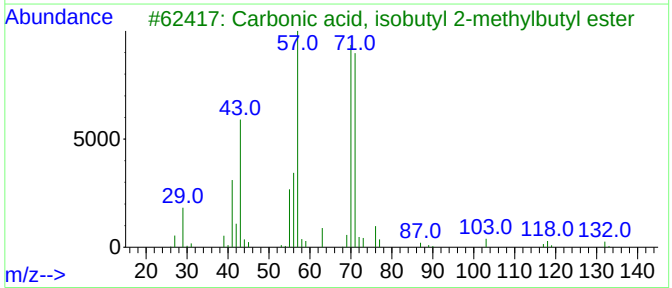


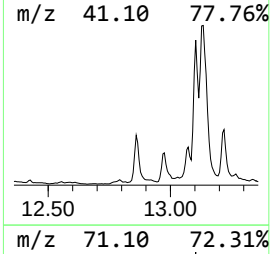


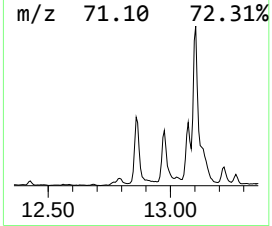












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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

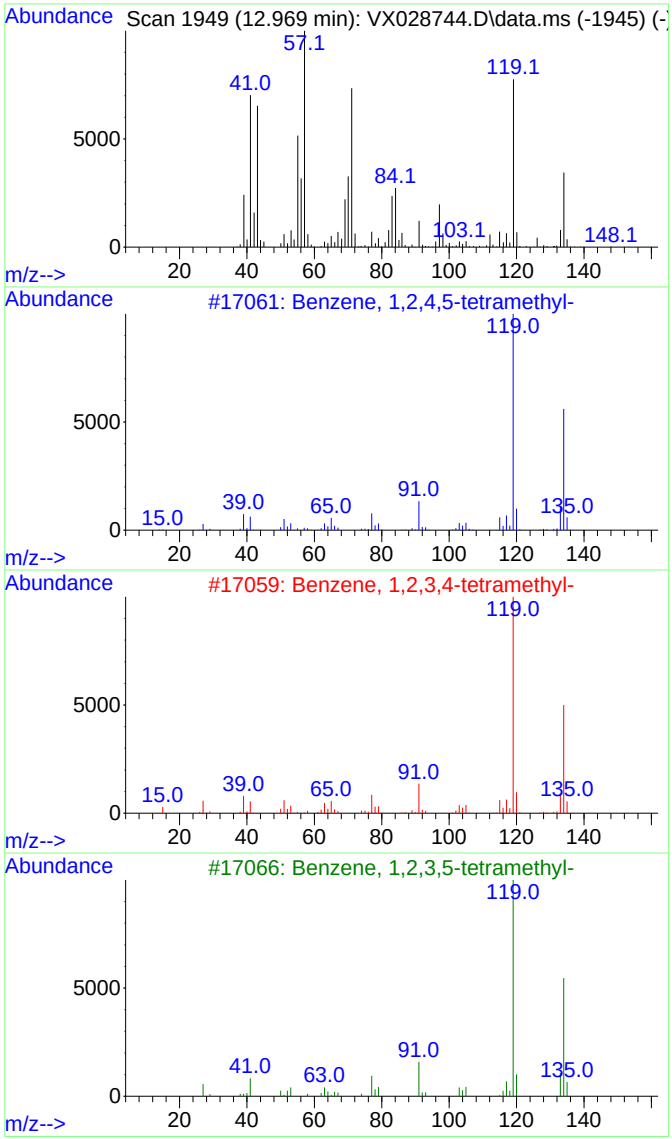
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

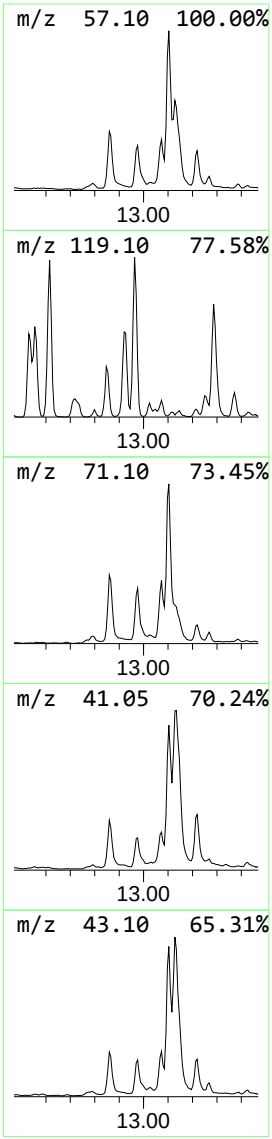
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.969	27.88 ug/l	706837	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	78
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	78
3	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	78
4	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	74
5	o-Cymene	134	C10H14	000527-84-4	72





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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

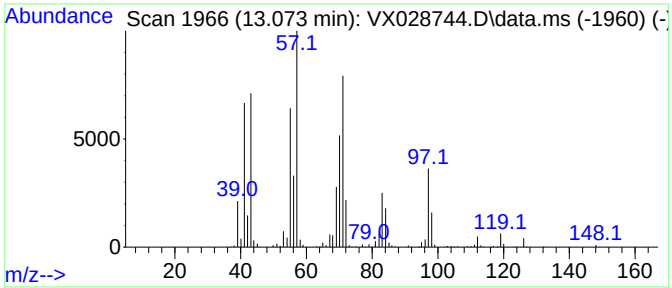
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

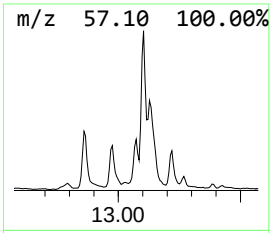
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

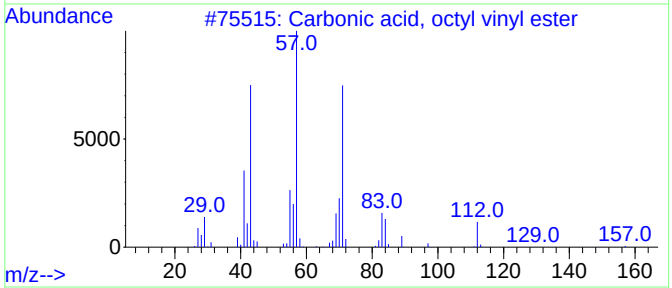
****
Peak Number 6 Carbonic acid, octyl vinyl ... Concentration Rank 8

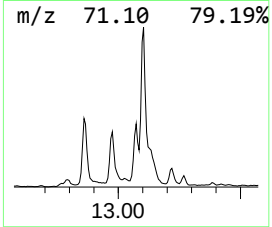
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.073	27.08 ug/l	686610	1,4-Dichlorobenzene-d4	12.024

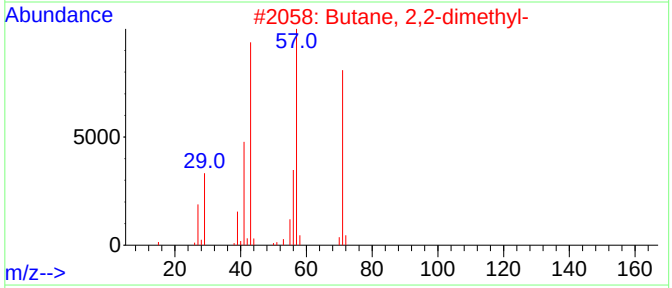
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octyl vinyl ester	200	C11H20O3	1000383-25-5	50
2	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
3	1-Hexanethiol, 2-ethyl-	146	C8H18S	007341-17-5	35
4	1-Octene, 6-methyl-	126	C9H18	013151-10-5	35
5	1-Eicosanol	298	C20H42O	000629-96-9	27

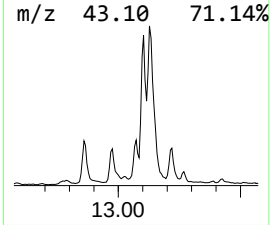


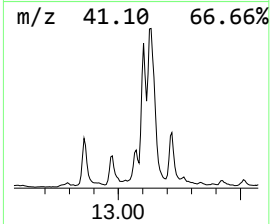


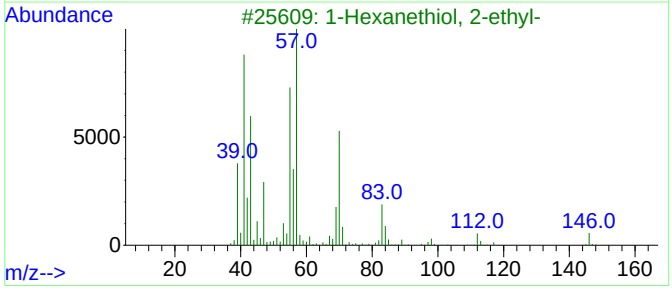


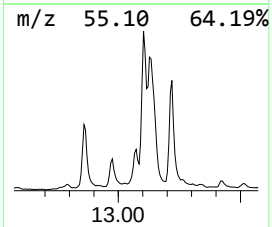












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

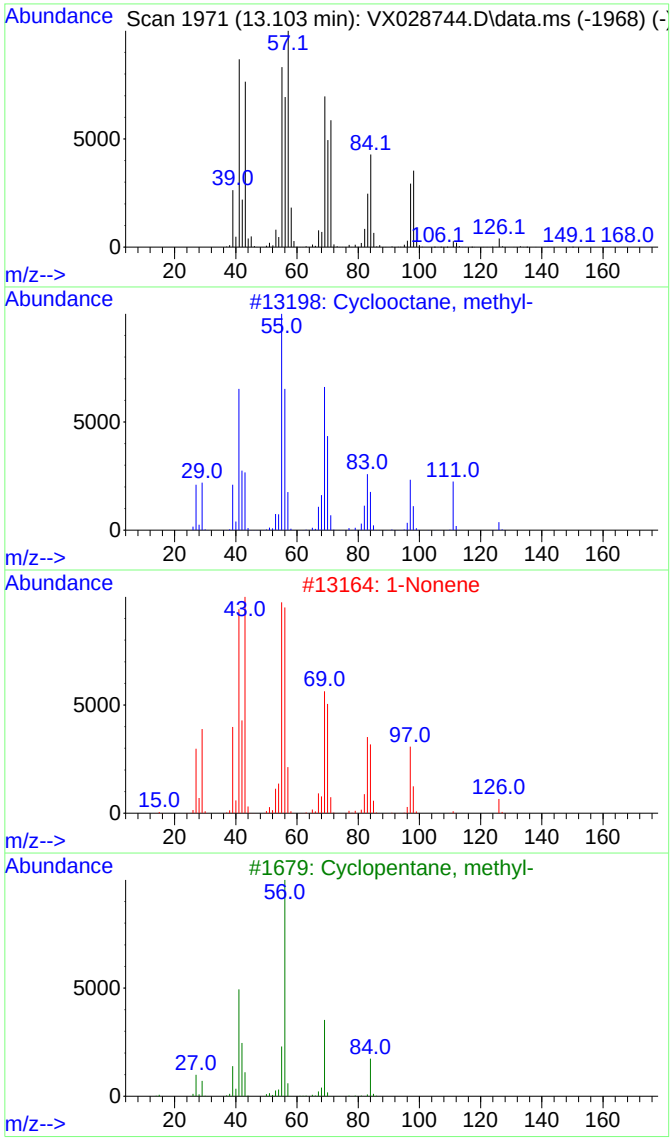
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

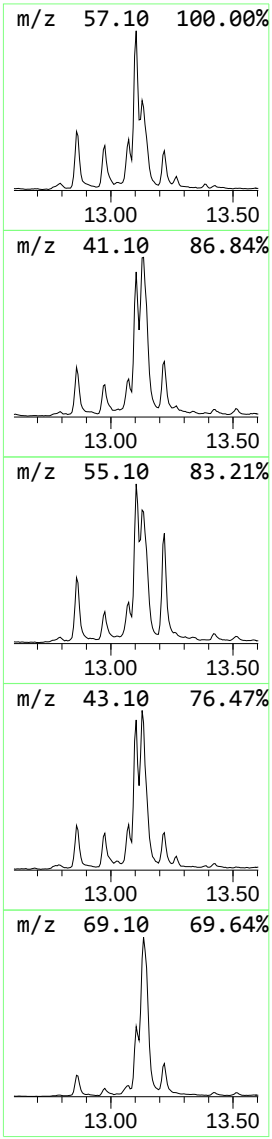
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	85.14 ug/l	2158690	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclooctane, methyl-	126	C9H18	001502-38-1	43
2	1-Nonene	126	C9H18	000124-11-8	38
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	30
4	(R)-(+)-3-Aminoquinuclidine	126	C7H14N2	123536-15-2	30
5	3-Heptene, (E)-	98	C7H14	014686-14-7	30





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

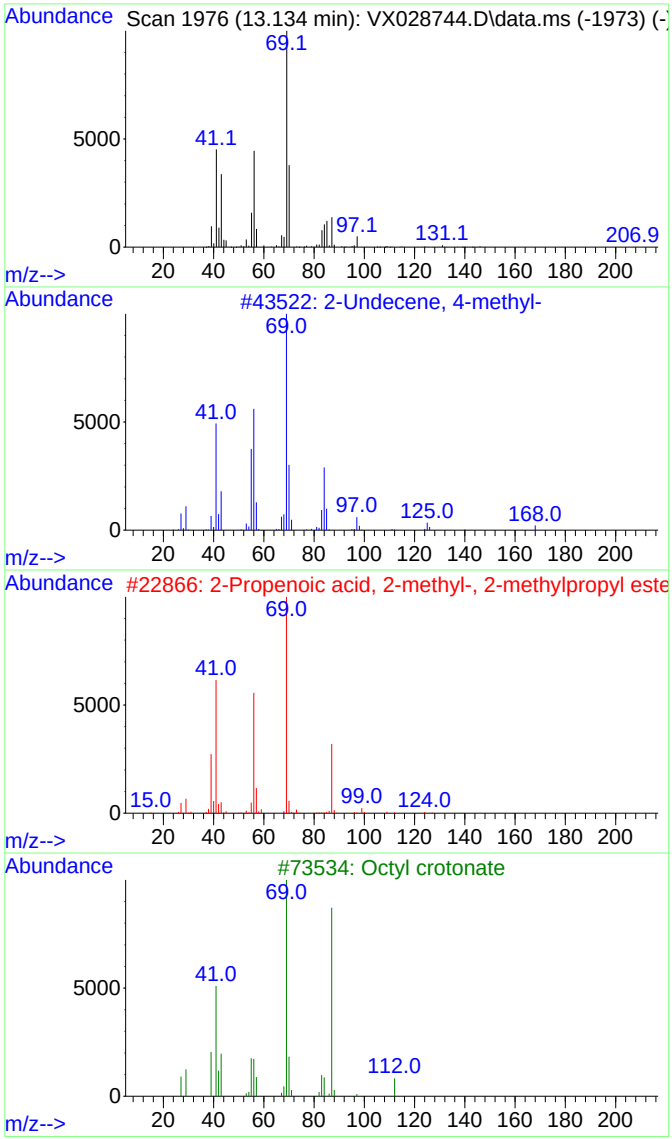
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

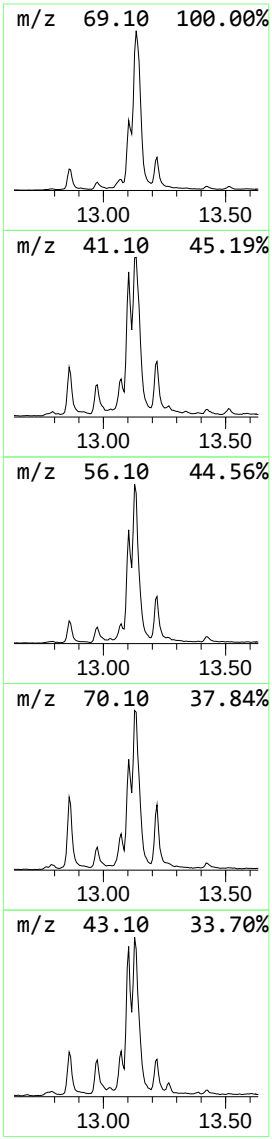
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 2-Undecene, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.134	134.51 ug/l	3410510	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Undecene, 4-methyl-	168	C12H24	091695-32-8	64
2	2-Propenoic acid, 2-methyl-, 2-m...	142	C8H14O2	000097-86-9	53
3	Octyl crotonate	198	C12H22O2	1000429-17-5	50
4	Cyclopropane, 1,2-dimethyl-1-pen...	140	C10H20	062238-04-4	50
5	1-Hexene, 3,3-dimethyl-	112	C8H16	003404-77-1	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

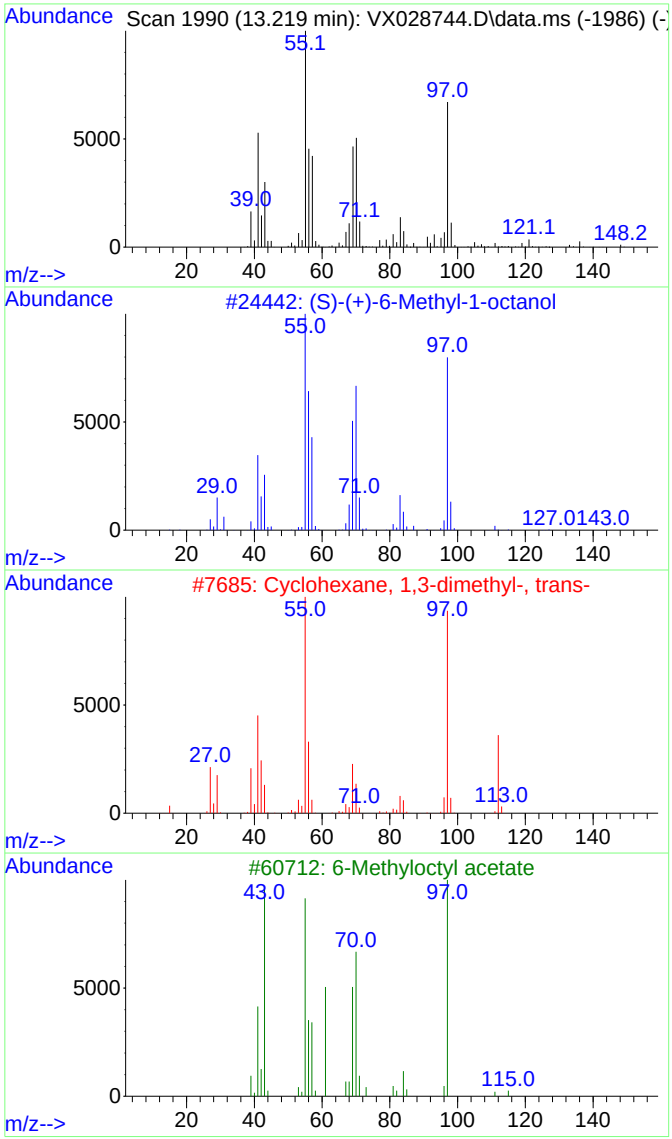
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

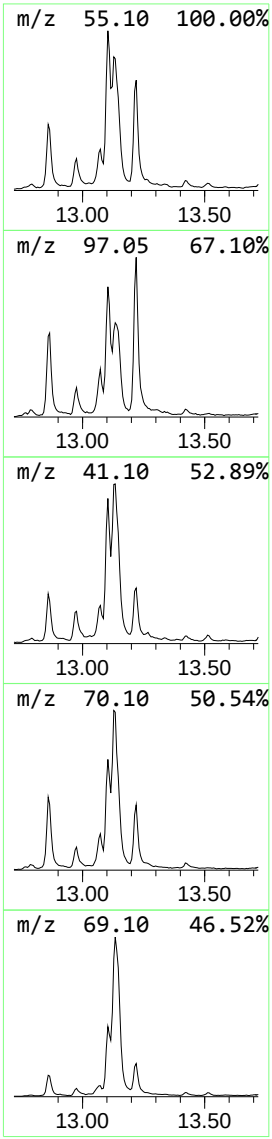
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.219	39.11 ug/l	991650	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	6-Methyloctyl acetate	186	C11H22O2	1000439-66-5	50
4	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	50
5	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BUR-1148

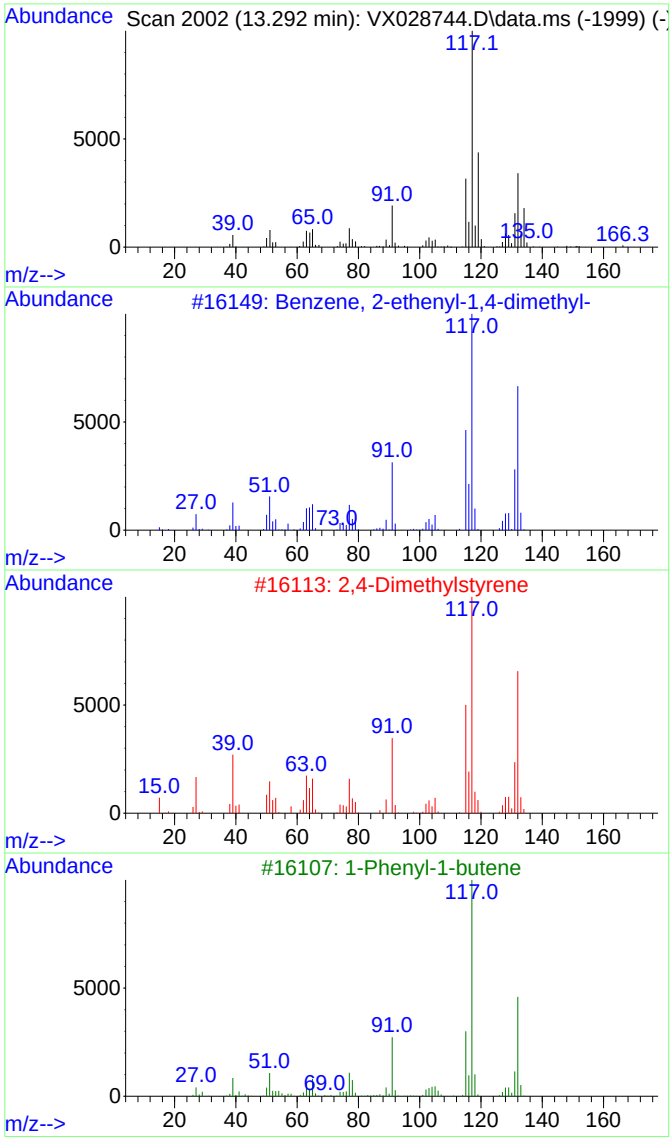
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

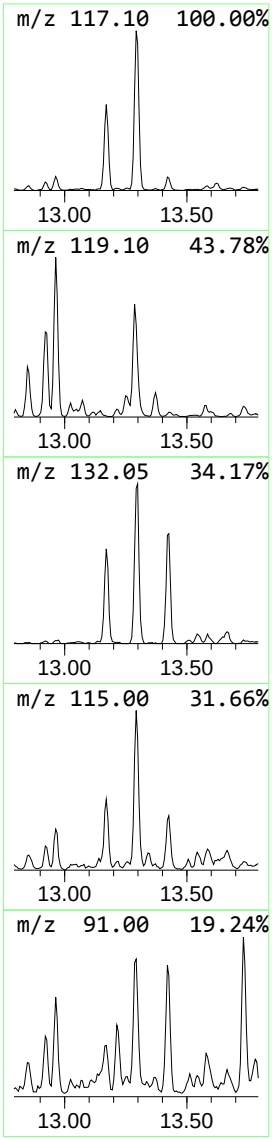
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	12.48 ug/l	316407	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	95
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	94
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	76
5	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051622\
Data File : VX028744.D
Acq On : 16 May 2022 20:12
Operator : JC/MD
Sample : N2813-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 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	1.252	101.7	ug/l	1430780	1	5.556	703749	50.0
Eucalyptol	12.104	23.3	ug/l	591261	4	12.024	1267770	50.0
1-Hexanol, 2-et...	12.219	306.9	ug/l	7782680	4	12.024	1267770	50.0
1-Octene, 6-met...	12.860	35.9	ug/l	910811	4	12.024	1267770	50.0
Benzene, 1,2,4,...	12.969	27.9	ug/l	706837	4	12.024	1267770	50.0
Carbonic acid, ...	13.073	27.1	ug/l	686610	4	12.024	1267770	50.0
unknown13.103	13.103	85.1	ug/l	2158690	4	12.024	1267770	50.0
2-Undecene, 4-m...	13.134	134.5	ug/l	3410510	4	12.024	1267770	50.0
(S)-(+)-6-Methy...	13.219	39.1	ug/l	991650	4	12.024	1267770	50.0
Benzene, 2-ethe...	13.292	12.5	ug/l	316407	4	12.024	1267770	50.0