

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
 Data File : VX029674.D
 Acq On : 21 Jun 2022 20:03
 Operator : JC/MD
 Sample : N3398-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ORA-021

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\82X061822W.M
 Title : SW846 8260

Signal : TIC: VX029674.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	43	rBV	427729	750623	51.37%	5.500%
2	2.075	155	162	173	rBV	114667	228650	15.65%	1.675%
3	2.294	192	198	206	rVB2	9067	16175	1.11%	0.119%
4	2.380	206	212	226	rBV	311180	504142	34.50%	3.694%
5	2.544	229	239	252	rBV	36401	81228	5.56%	0.595%
6	2.965	299	308	321	rBV	24380	58038	3.97%	0.425%
7	3.331	361	368	382	rVB2	6300	15546	1.06%	0.114%
8	4.233	504	516	539	rBV	424412	1174542	80.38%	8.607%
9	4.562	559	570	583	rBV	95794	268377	18.37%	1.967%
10	5.013	633	644	657	rBV4	20104	66798	4.57%	0.489%
11	5.391	695	706	721	rBV	137437	396469	27.13%	2.905%
12	5.556	721	733	753	rVB	253906	718163	49.15%	5.262%
13	5.964	788	800	813	rBV	142190	385179	26.36%	2.822%
14	6.123	819	826	840	rVB4	10694	29863	2.04%	0.219%
15	6.763	921	931	946	rBV	382532	919962	62.96%	6.741%
16	7.214	998	1005	1016	rBV	50164	115839	7.93%	0.849%
17	7.464	1039	1046	1054	rBV2	9044	19730	1.35%	0.145%
18	7.580	1058	1065	1072	rVV	73971	143992	9.85%	1.055%
19	7.647	1072	1076	1090	rVB2	12624	28746	1.97%	0.211%
20	8.580	1222	1229	1234	rBV2	9798	16661	1.14%	0.122%
21	8.653	1234	1241	1248	rVV	777021	1208829	82.73%	8.858%
22	8.720	1248	1252	1257	rVV	60938	95957	6.57%	0.703%
23	8.769	1257	1260	1270	rVB2	36122	62248	4.26%	0.456%
24	8.964	1287	1292	1298	rBV2	8651	15229	1.04%	0.112%
25	9.238	1334	1337	1343	rBV2	13441	21606	1.48%	0.158%
26	9.537	1382	1386	1395	rVB2	10172	18726	1.28%	0.137%
27	10.055	1461	1471	1483	rBV	765571	1057310	72.36%	7.748%
28	10.159	1483	1488	1492	rBV	32127	46316	3.17%	0.339%
29	10.305	1505	1512	1521	rVB3	13396	26595	1.82%	0.195%
30	10.506	1540	1545	1555	rVB	42171	57210	3.92%	0.419%
31	10.683	1571	1574	1581	rVB	22013	27071	1.85%	0.198%
32	10.756	1581	1586	1593	rBV2	108569	162227	11.10%	1.189%
33	11.085	1634	1640	1645	rBV	599061	779171	53.33%	5.710%
34	11.134	1645	1648	1652	rVB	28821	35420	2.42%	0.260%
35	11.482	1701	1705	1714	rVB	30808	45038	3.08%	0.330%
36	11.573	1714	1720	1723	rBV	49228	68363	4.68%	0.501%

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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

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37	11.604	1723	1725	1733	rVB3	45385	64982	4.45%	0.476%
38	11.756	1745	1750	1755	rBV	12991	19081	1.31%	0.140%
39	11.835	1758	1763	1765	rVV2	22183	32184	2.20%	0.236%
40	11.872	1765	1769	1779	rVV2	48700	83456	5.71%	0.612%
41	11.969	1779	1785	1789	rVV7	6889	15801	1.08%	0.116%
42	12.024	1789	1794	1801	rVB	810830	999120	68.38%	7.321%
43	12.219	1821	1826	1837	rBV	1173914	1461161	100.00%	10.707%
44	12.305	1837	1840	1855	rVB6	38622	90076	6.16%	0.660%
45	12.567	1879	1883	1885	rBV3	12777	18159	1.24%	0.133%
46	12.597	1885	1888	1892	rVB5	12667	17227	1.18%	0.126%
47	12.817	1919	1924	1928	rBV7	19709	27001	1.85%	0.198%
48	12.890	1931	1936	1938	rBV4	14102	23846	1.63%	0.175%
49	12.981	1947	1951	1958	rVB5	31359	48304	3.31%	0.354%
50	13.042	1958	1961	1964	rVB2	23658	24502	1.68%	0.180%
51	13.292	1996	2002	2007	rVB5	40167	77790	5.32%	0.570%
52	13.347	2007	2011	2014	rBV3	24840	33244	2.28%	0.244%
53	13.390	2014	2018	2020	rBV	51510	67287	4.61%	0.493%
54	13.414	2020	2022	2025	rVB4	18933	22201	1.52%	0.163%
55	13.500	2033	2036	2042	rVB8	9601	16869	1.15%	0.124%
56	13.603	2047	2053	2056	rBV7	15174	30519	2.09%	0.224%
57	13.701	2062	2069	2072	rBV4	29936	65037	4.45%	0.477%
58	13.737	2072	2075	2078	rVV2	49732	77077	5.28%	0.565%
59	13.774	2078	2081	2084	rVV2	54580	81818	5.60%	0.600%
60	13.841	2088	2092	2099	rVV	92887	155653	10.65%	1.141%
61	13.914	2099	2104	2111	rVB4	37830	70173	4.80%	0.514%
62	14.073	2127	2130	2132	rBV4	11932	15242	1.04%	0.112%
63	14.103	2133	2135	2138	rVB3	14802	15220	1.04%	0.112%
64	14.188	2145	2149	2151	rBV3	14224	21549	1.47%	0.158%
65	14.268	2158	2162	2165	rVB5	12485	18377	1.26%	0.135%
66	14.438	2187	2190	2193	rVV2	17217	22016	1.51%	0.161%
67	14.475	2193	2196	2198	rVV4	13826	18561	1.27%	0.136%
68	14.505	2198	2201	2207	rVB5	21023	38772	2.65%	0.284%
69	14.615	2216	2219	2221	rBV2	19565	19320	1.32%	0.142%
70	14.792	2244	2248	2252	rVB3	12181	21928	1.50%	0.161%
71	15.109	2296	2300	2302	rBV3	14344	18338	1.26%	0.134%
72	15.487	2358	2362	2370	rVB6	17264	39353	2.69%	0.288%
73	15.615	2379	2383	2386	rBV3	11327	17763	1.22%	0.130%
74	15.652	2386	2389	2395	rVB3	16435	25890	1.77%	0.190%
75	15.987	2439	2444	2449	rVB8	8547	15309	1.05%	0.112%
76	16.377	2501	2508	2516	rBV6	19477	50581	3.46%	0.371%

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ClientSampleId :
ORA-021

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\82X061822W.M
Title : SW846 8260

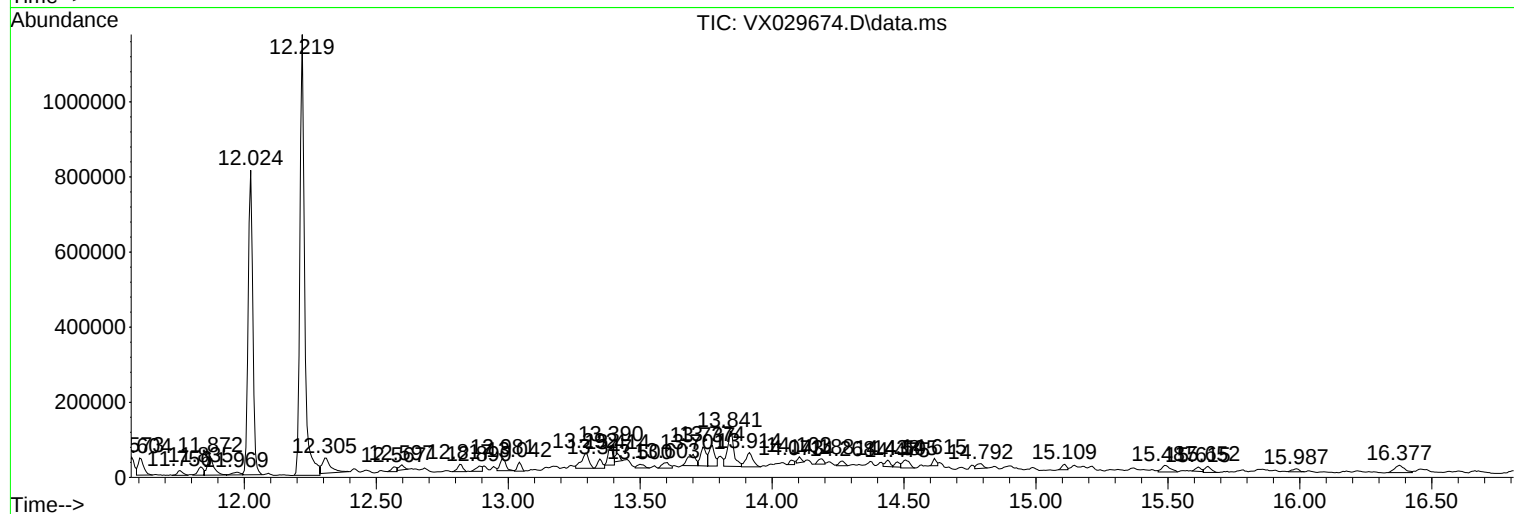
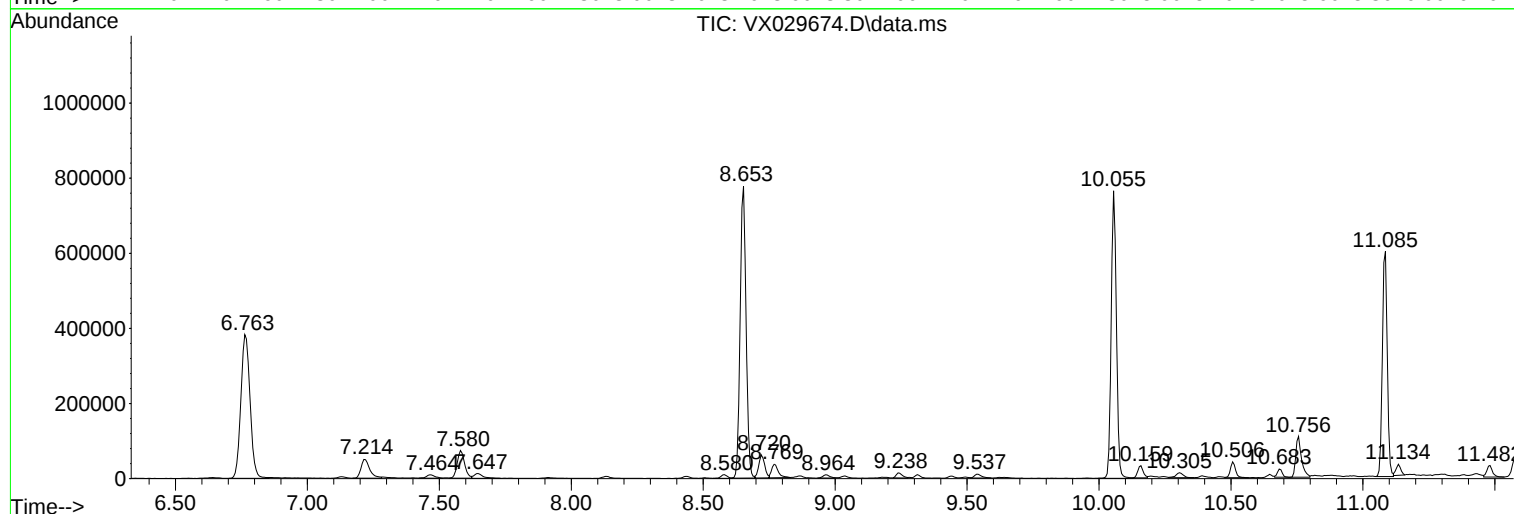
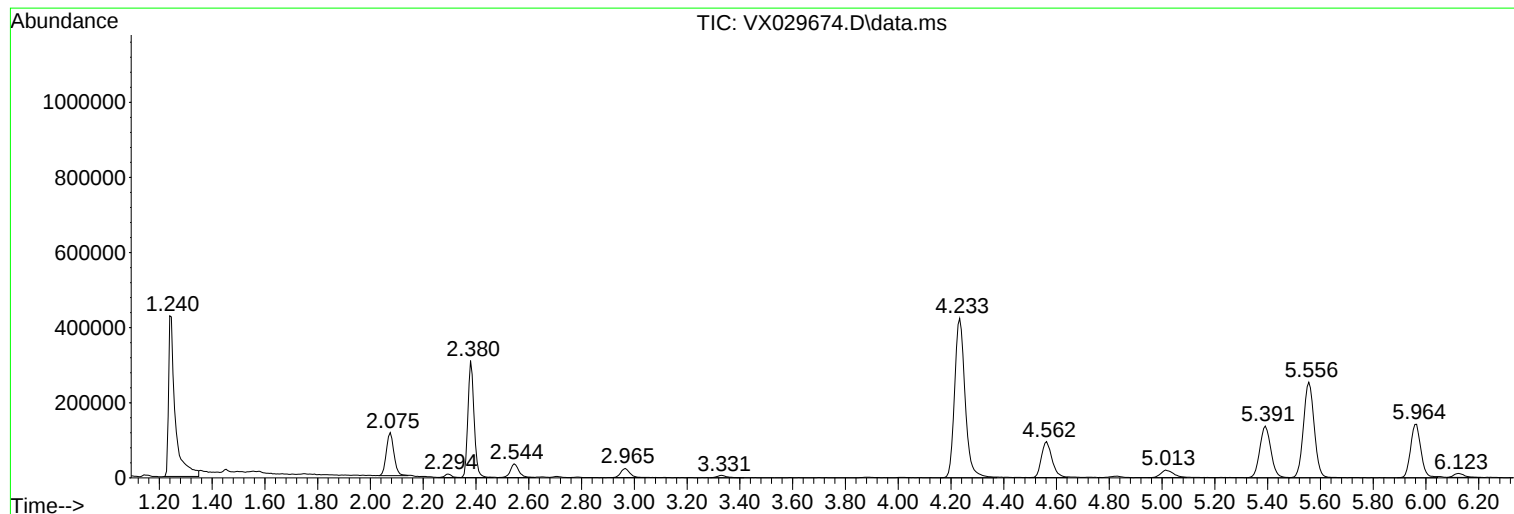
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
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Instrument :
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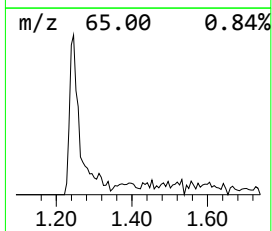
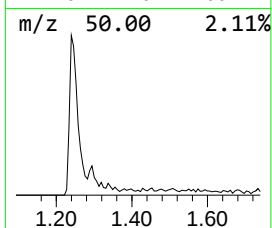
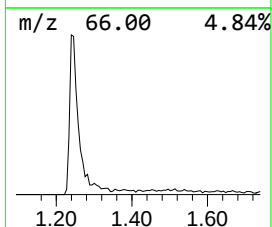
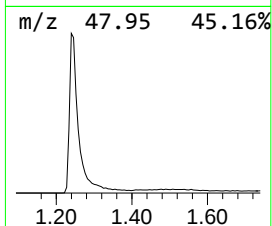
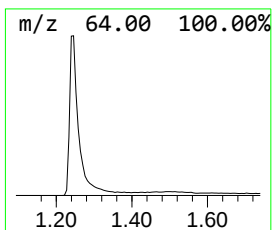
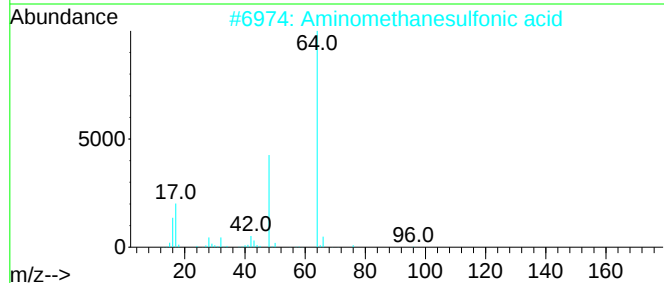
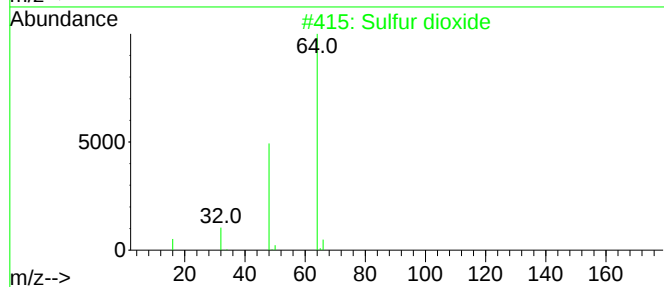
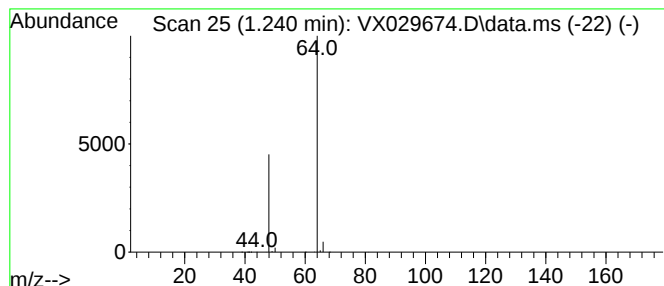
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Quant Title : SW846 8260

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.
1.240	52.26 ug/l	750623	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			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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Instrument :
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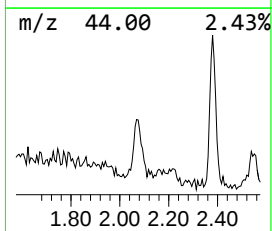
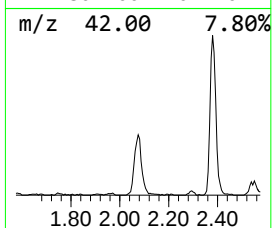
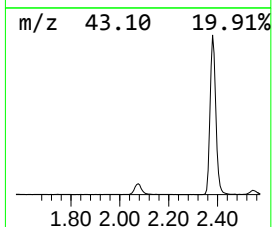
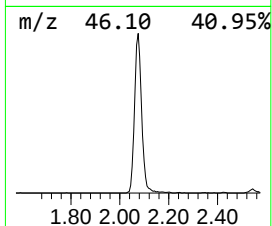
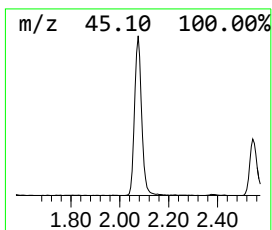
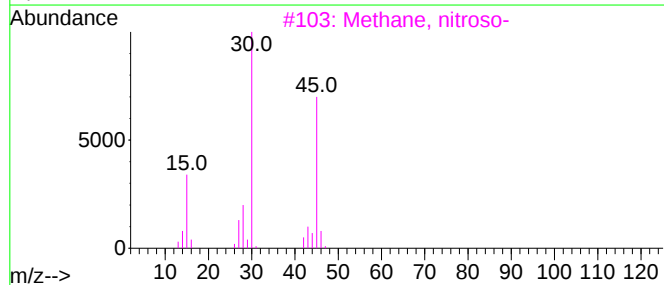
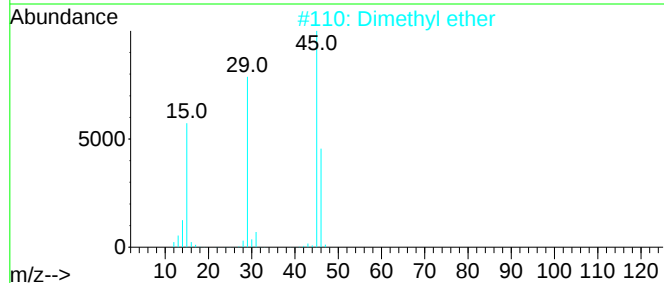
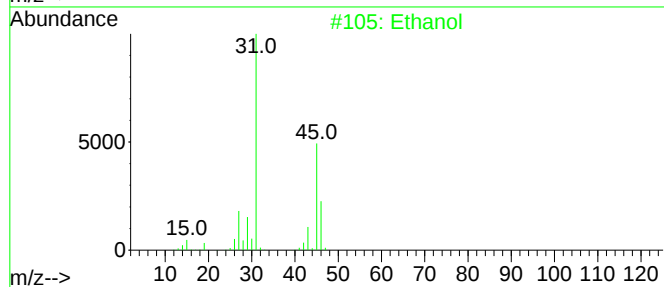
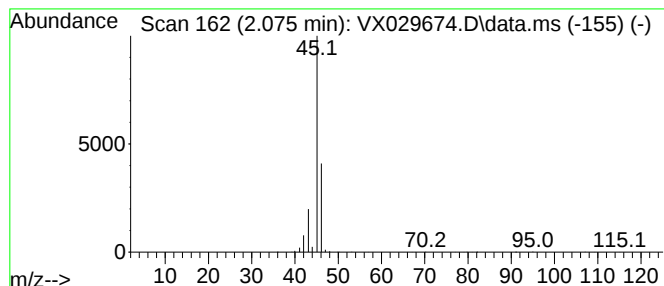
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.075	15.92 ug/l	228650	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	78
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			L-Lactic acid	90	C3H6O3	000079-33-4	4



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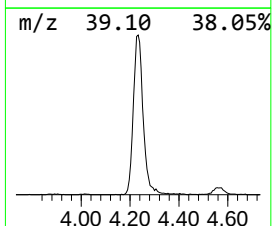
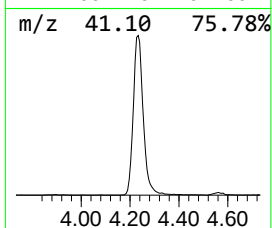
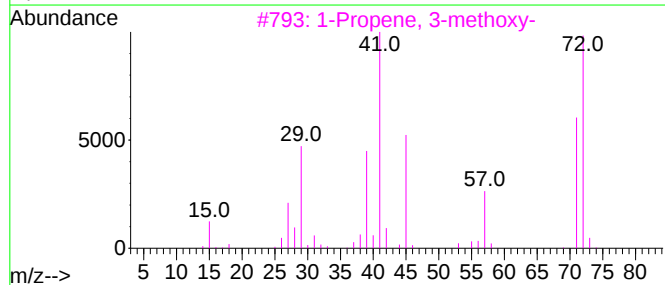
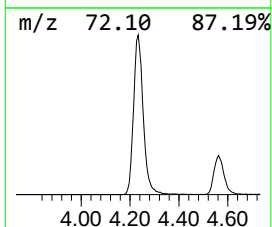
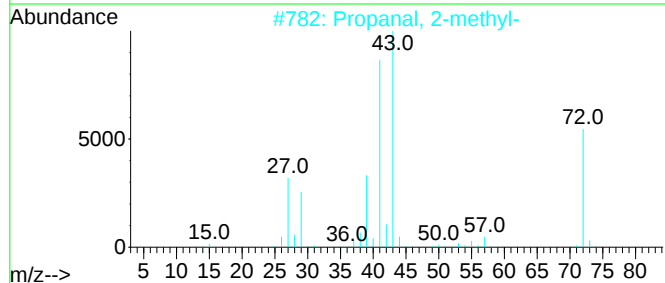
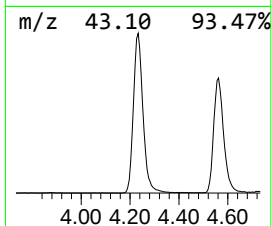
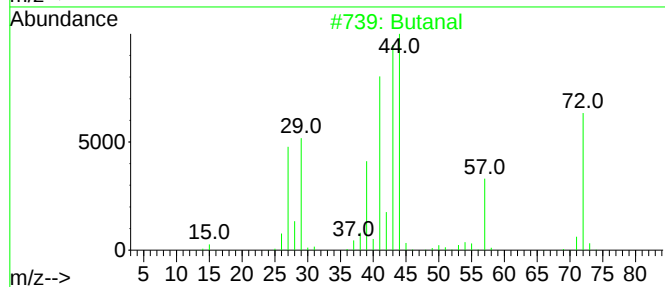
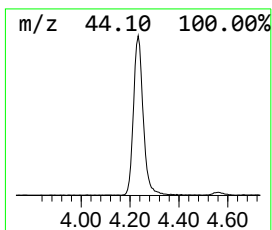
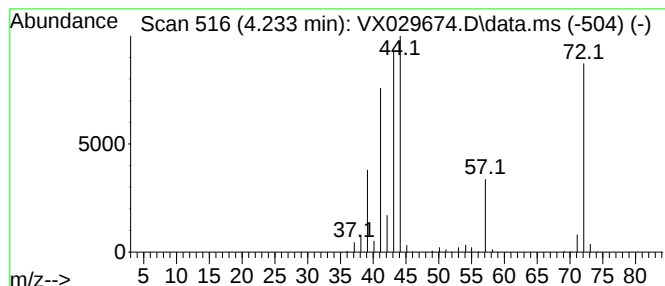
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 3 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	81.77 ug/l	1174540	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
4			Isobutylene epoxide	72	C4H8O	000558-30-5	35
5			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	32



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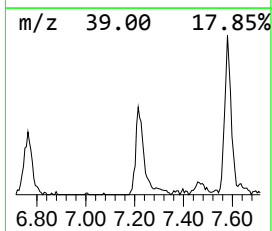
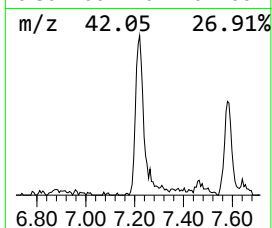
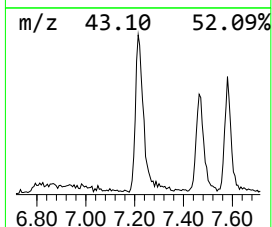
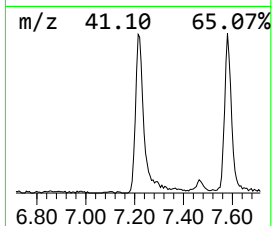
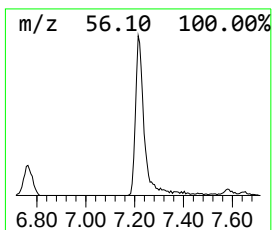
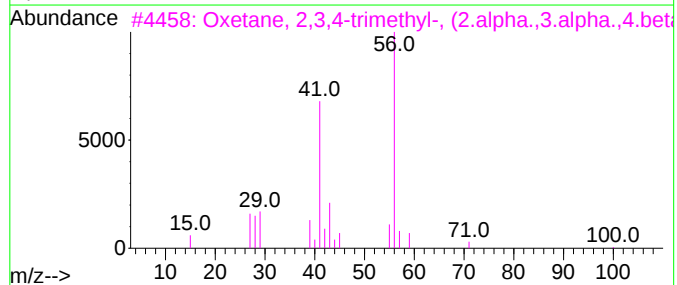
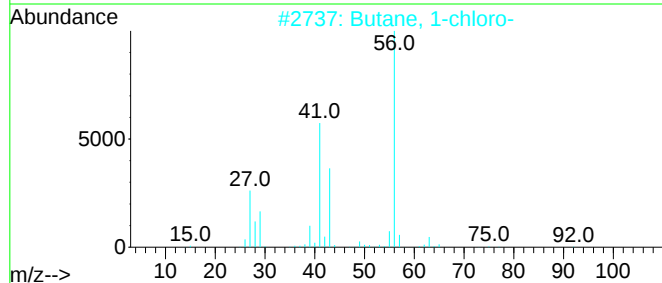
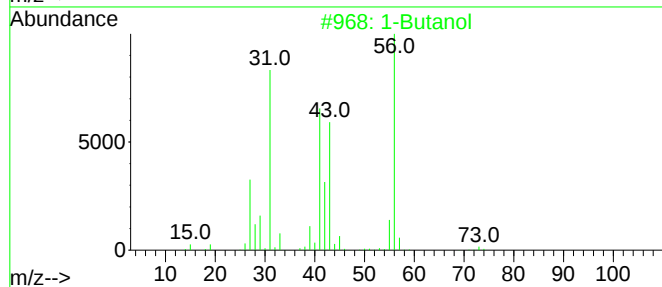
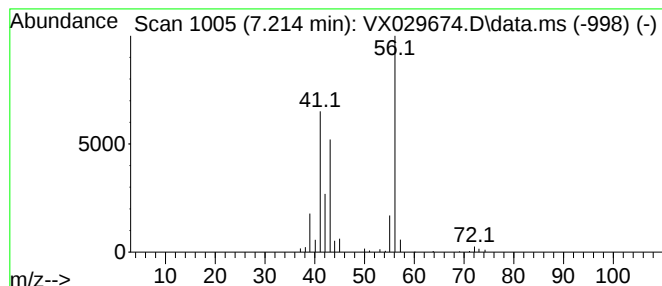
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Quant Title : SW846 8260

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

Peak Number 4 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	6.30 ug/l	115839	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
3			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	38
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029674.D
Acq On : 21 Jun 2022 20:03
Operator : JC/MD
Sample : N3398-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-021

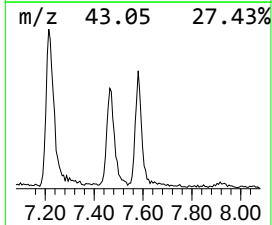
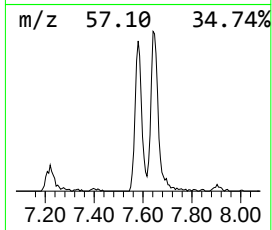
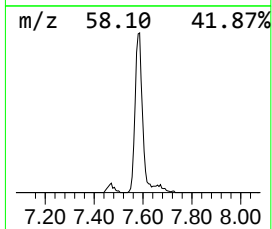
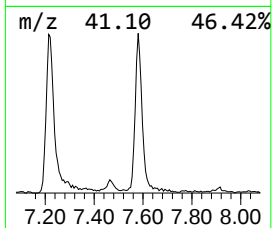
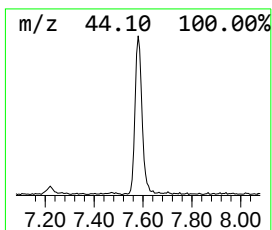
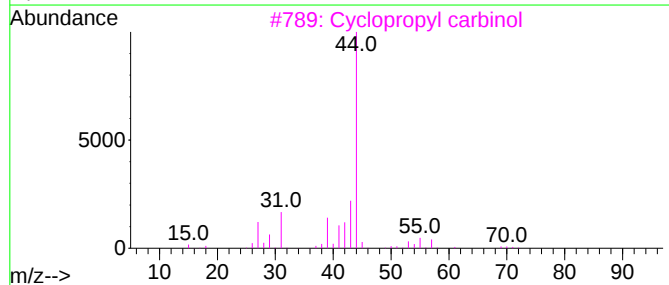
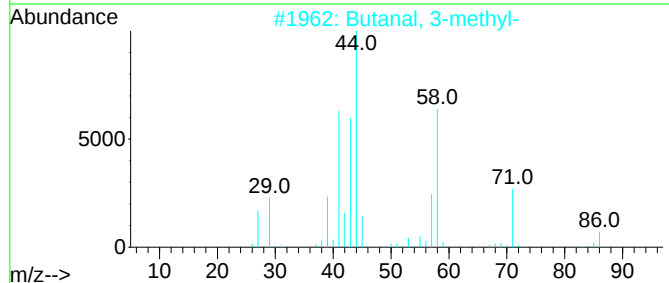
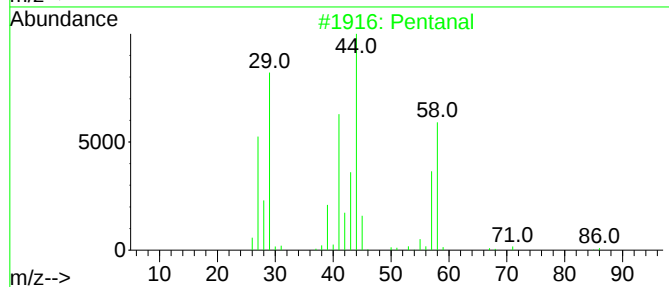
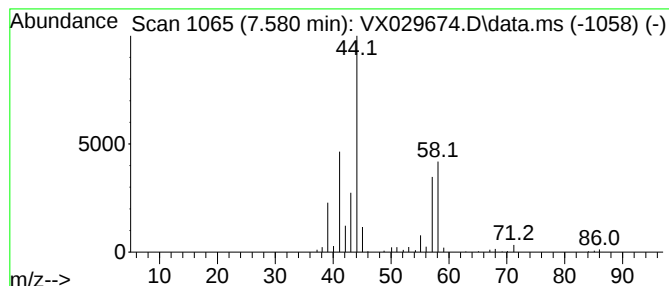
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Quant Title : SW846 8260

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

Peak Number 5 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.580	7.83 ug/l	143992	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	91
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	33
4			2-Propanamine	59	C3H9N	000075-31-0	9
5			Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029674.D
Acq On : 21 Jun 2022 20:03
Operator : JC/MD
Sample : N3398-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-021

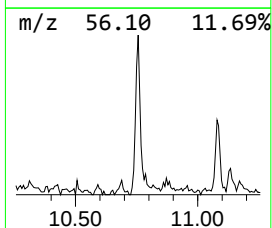
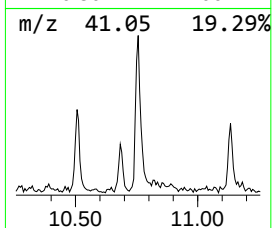
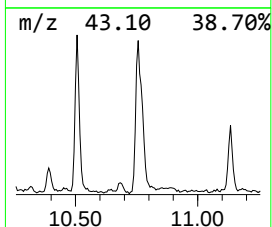
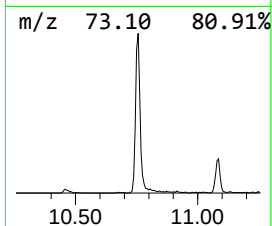
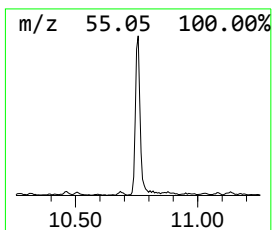
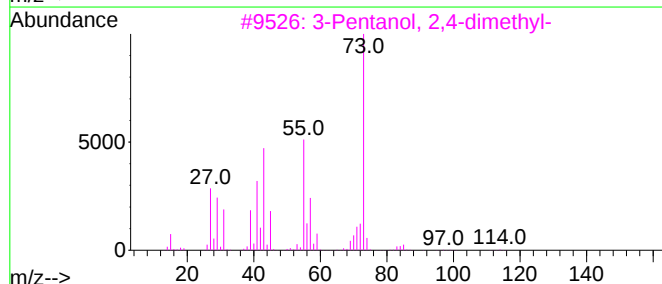
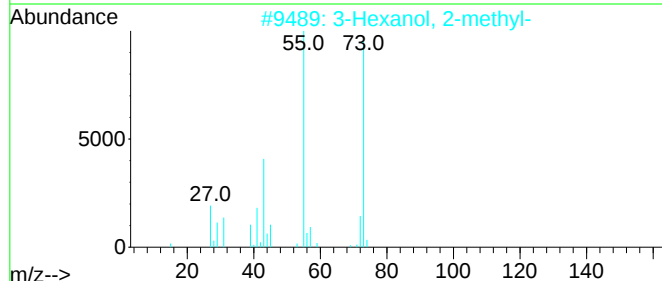
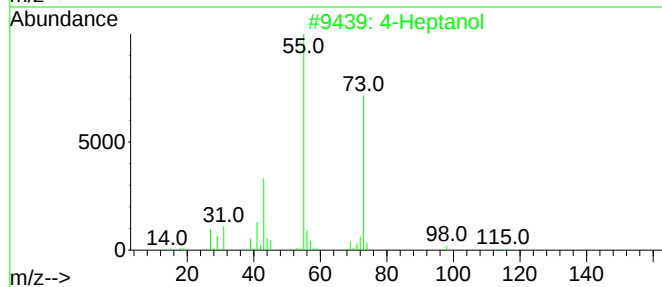
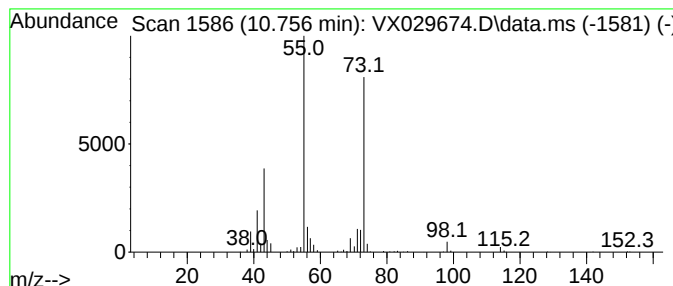
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Quant Title : SW846 8260

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

Peak Number 6 4-Heptanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	7.67 ug/l	162227	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanol	116	C7H16O	000589-55-9	78
2			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	53
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	38
4			4,5-Octanediol	146	C8H18O2	022607-10-9	36
5			5-Ethyl-4-nonanol	172	C11H24O	019780-73-5	33



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029674.D
Acq On : 21 Jun 2022 20:03
Operator : JC/MD
Sample : N3398-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-021

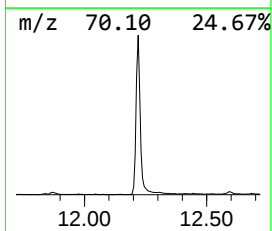
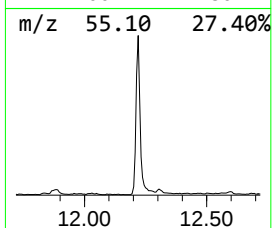
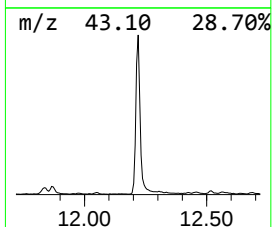
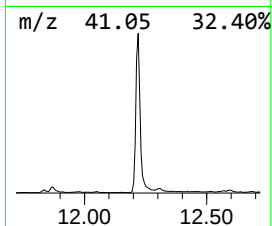
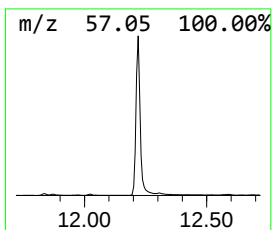
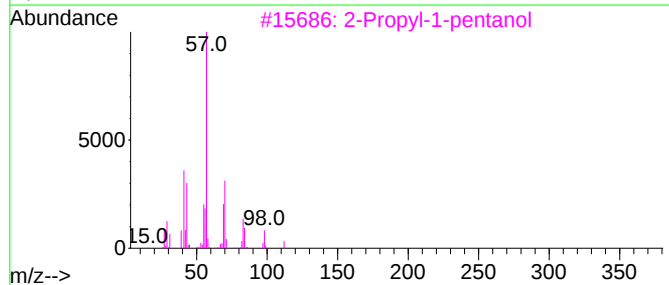
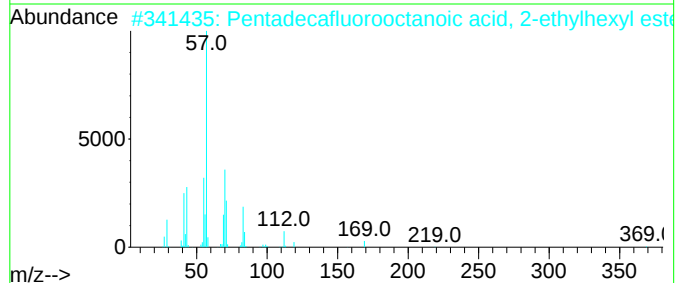
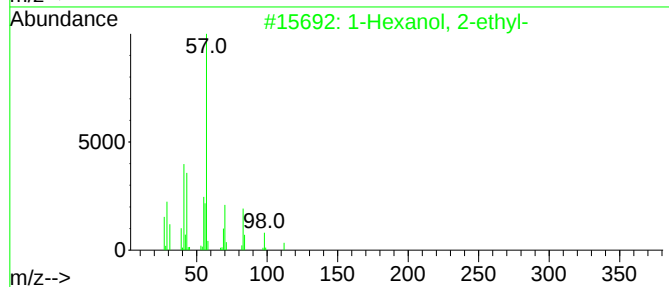
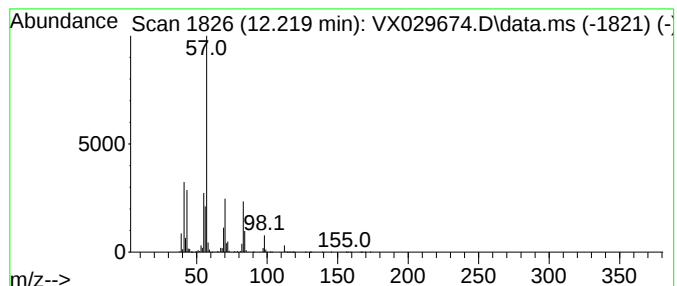
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Quant Title : SW846 8260

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	73.12 ug/l	1461160	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			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029674.D
Acq On : 21 Jun 2022 20:03
Operator : JC/MD
Sample : N3398-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-021

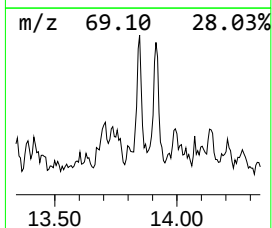
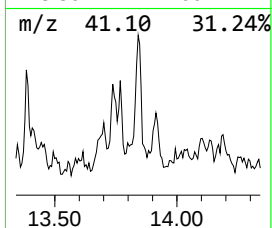
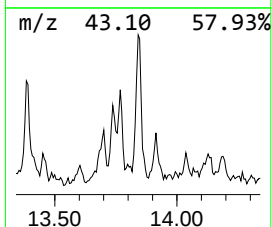
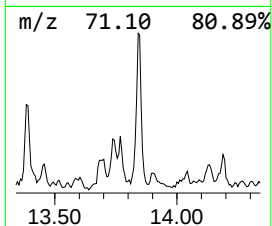
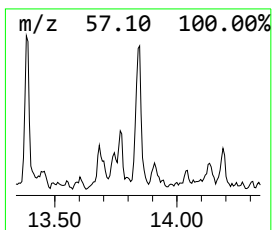
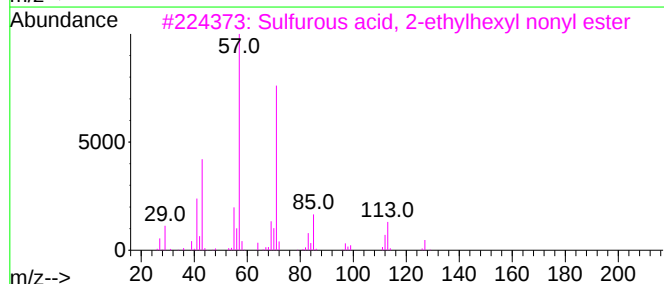
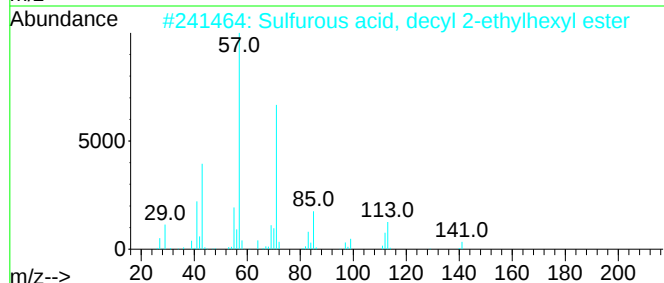
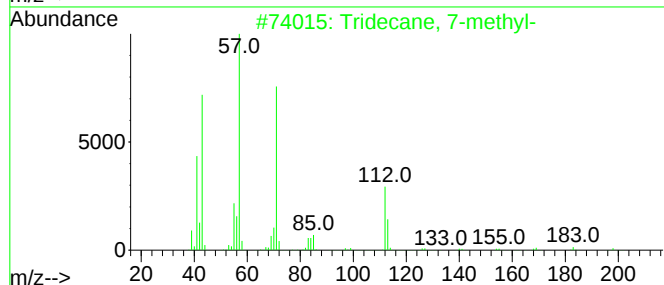
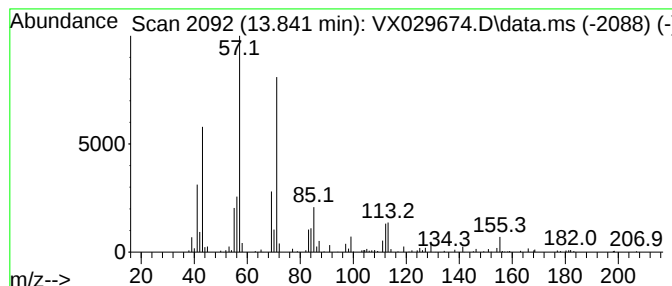
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

Peak Number 8 Tridecane, 7-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.841	7.79 ug/l	155653	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecane, 7-methyl-	198	C14H30	026730-14-3	76
2			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	72
3			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	72
4			Decyl octyl ether	270	C18H38O	1000406-38-3	72
5			Tridecane, 2-methyl-	198	C14H30	001560-96-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029674.D
Acq On : 21 Jun 2022 20:03
Operator : JC/MD
Sample : N3398-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-021

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	52.3	ug/l	750623	1	5.556	718163	50.0
Ethanol	2.075	15.9	ug/l	228650	1	5.556	718163	50.0
Butanal	4.233	81.8	ug/l	1174540	1	5.556	718163	50.0
1-Butanol	7.214	6.3	ug/l	115839	2	6.769	919962	50.0
Pentanal	7.580	7.8	ug/l	143992	2	6.769	919962	50.0
4-Heptanol	10.756	7.7	ug/l	162227	3	10.055	1057310	50.0
1-Hexanol, 2-et...	12.219	73.1	ug/l	1461160	4	12.024	999120	50.0
Tridecane, 7-me...	13.841	7.8	ug/l	155653	4	12.024	999120	50.0