

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
 Data File : VX033333.D
 Acq On : 08 Dec 2022 18:59
 Operator : JC/MD
 Sample : N5906-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-23R

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\82X120722W.M
 Title : SW846 8260

Signal : TIC: VX033333.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	23	29	43	rBV2	23511	68357	10.16%	1.775%
2	2.343	200	206	212	rBV2	6701	12899	1.92%	0.335%
3	2.782	272	278	284	rBV2	3970	8774	1.30%	0.228%
4	3.117	325	333	340	rVB2	4210	9990	1.48%	0.259%
5	4.306	520	528	539	rVV4	2369	6822	1.01%	0.177%
6	4.422	539	547	559	rVB7	2693	7900	1.17%	0.205%
7	5.385	694	705	719	rBV	51832	152626	22.68%	3.962%
8	5.556	722	733	758	rVB	167869	484856	72.05%	12.587%
9	5.958	789	799	808	rBV	40804	108516	16.13%	2.817%
10	6.044	808	813	821	rVB2	7711	19521	2.90%	0.507%
11	6.245	827	846	861	rBV3	17312	58598	8.71%	1.521%
12	6.763	920	931	942	rBV	245251	583950	86.78%	15.159%
13	7.982	1124	1131	1140	rVB4	3654	8015	1.19%	0.208%
14	8.110	1146	1152	1156	rBV3	5659	11919	1.77%	0.309%
15	8.427	1199	1204	1211	rBV2	5092	8796	1.31%	0.228%
16	8.507	1211	1217	1227	rVB	12198	21542	3.20%	0.559%
17	8.647	1229	1240	1248	rBV	161010	261861	38.91%	6.798%
18	8.842	1265	1272	1281	rBV2	11638	20556	3.05%	0.534%
19	8.958	1281	1291	1299	rVB3	16248	27653	4.11%	0.718%
20	9.043	1300	1305	1311	rBV2	16680	27352	4.06%	0.710%
21	10.055	1459	1471	1478	rBV	492187	672920	100.00%	17.469%
22	10.146	1482	1486	1490	rVV3	6050	8617	1.28%	0.224%
23	10.195	1490	1494	1499	rVB	19202	24137	3.59%	0.627%
24	11.079	1634	1639	1649	rBV	287958	362935	53.93%	9.422%
25	11.305	1673	1676	1681	rVB	10522	13327	1.98%	0.346%
26	12.024	1788	1794	1801	rBV	490643	617748	91.80%	16.037%
27	12.244	1825	1830	1837	rBV	20165	27072	4.02%	0.703%
28	12.317	1837	1842	1850	rVB2	6981	11017	1.64%	0.286%
29	12.616	1884	1891	1893	rBV	11317	14255	2.12%	0.370%
30	12.646	1893	1896	1900	rVV	14268	17592	2.61%	0.457%
31	12.701	1900	1905	1912	rVB4	5112	9237	1.37%	0.240%
32	12.920	1935	1941	1946	rVB	5976	8664	1.29%	0.225%
33	13.170	1969	1982	1990	rBV6	10849	27513	4.09%	0.714%
34	13.292	1997	2002	2007	rVV2	9659	13910	2.07%	0.361%
35	13.664	2053	2063	2068	rVB2	19716	35353	5.25%	0.918%
36	13.774	2073	2081	2091	rVB	18883	30444	4.52%	0.790%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033333.D
Acq On : 08 Dec 2022 18:59
Operator : JC/MD
Sample : N5906-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23R

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\82X120722W.M
Title : SW846 8260

37	14.640	2219	2223	2226	rVV	11546	14993	2.23%	0.389%
38	14.780	2241	2246	2250	rBV	15689	21548	3.20%	0.559%
39	15.615	2374	2383	2386	rBV4	5718	10276	1.53%	0.267%

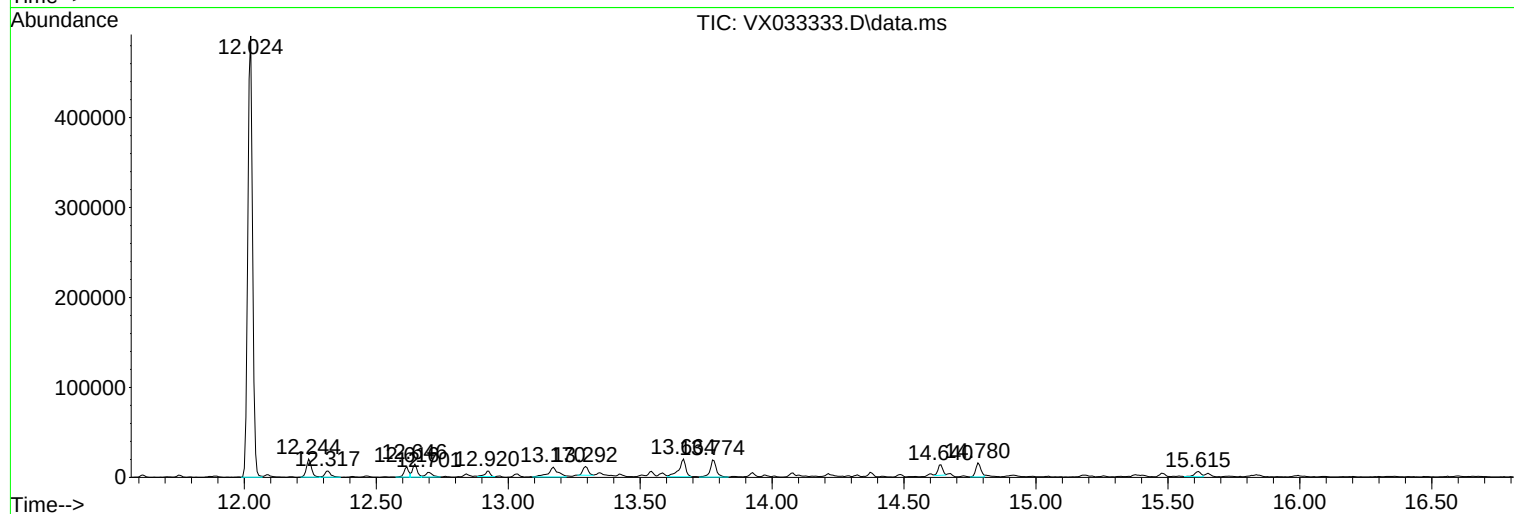
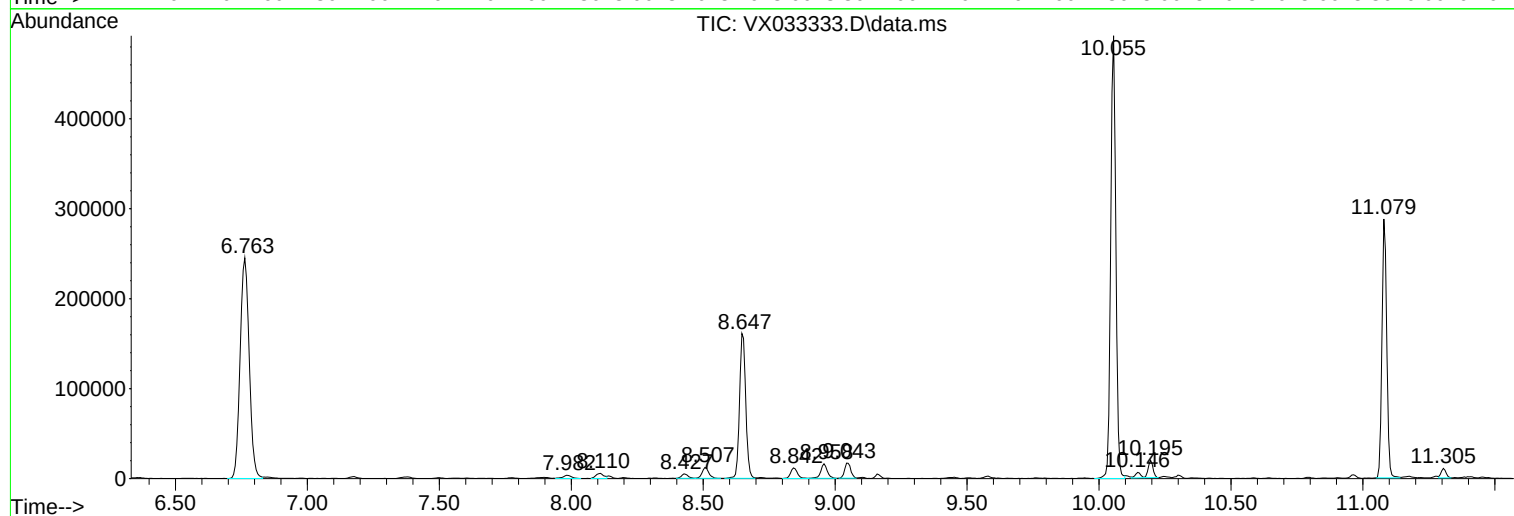
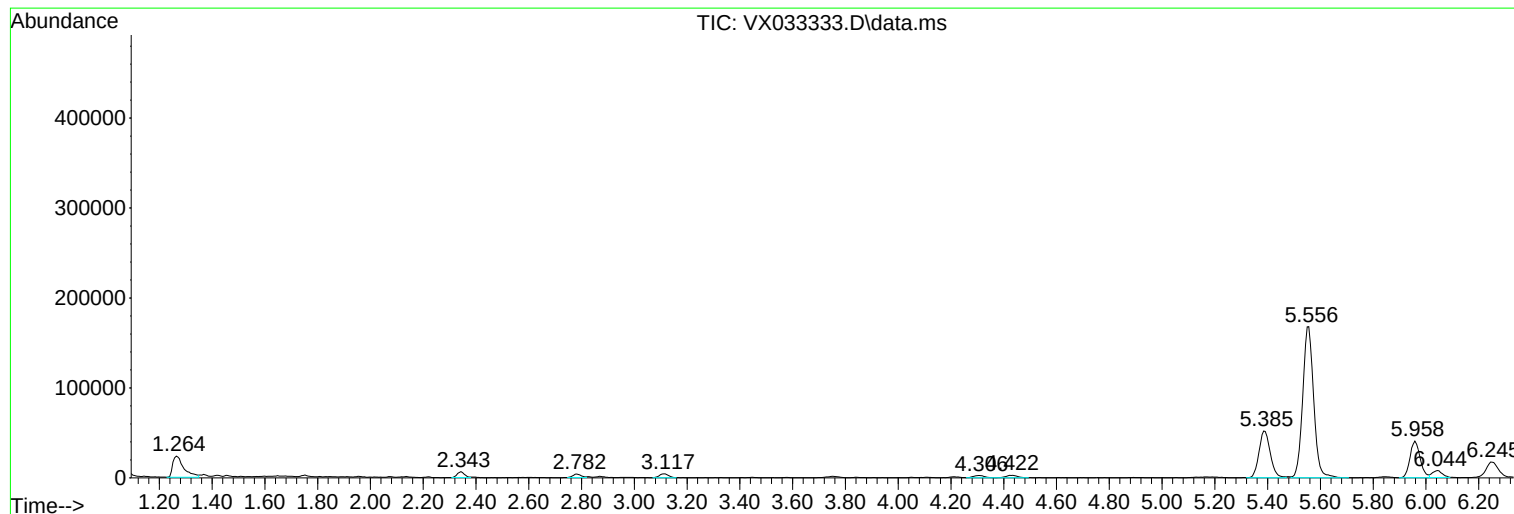
Sum of corrected areas: 3852061

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033333.D
Acq On : 08 Dec 2022 18:59
Operator : JC/MD
Sample : N5906-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033333.D
Acq On : 08 Dec 2022 18:59
Operator : JC/MD
Sample : N5906-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23R

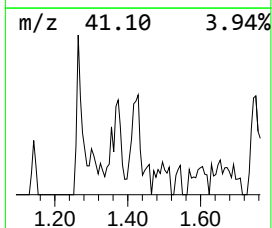
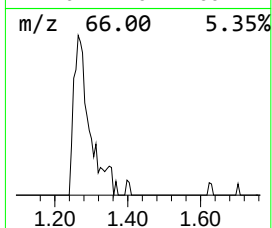
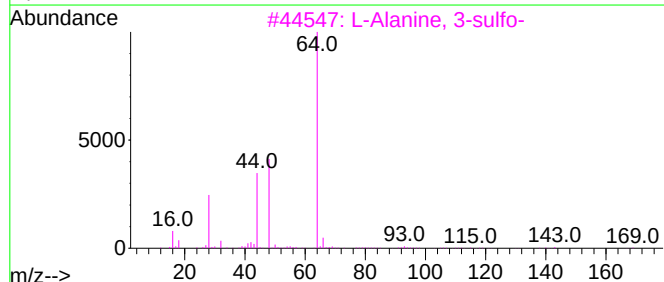
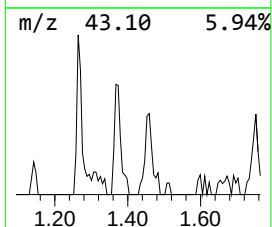
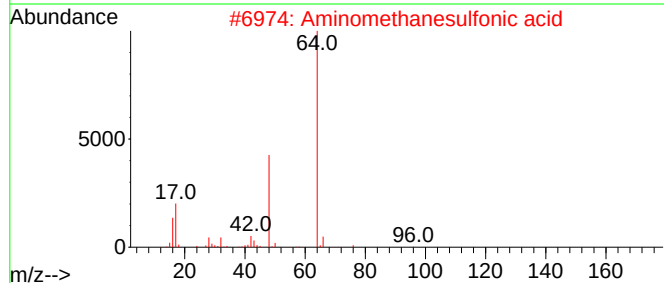
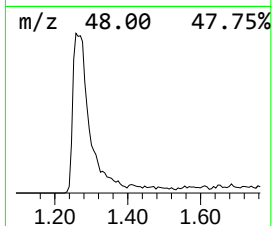
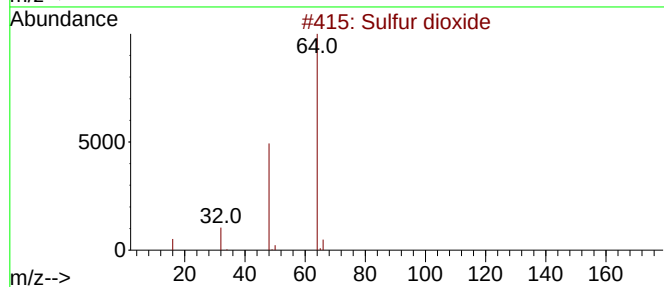
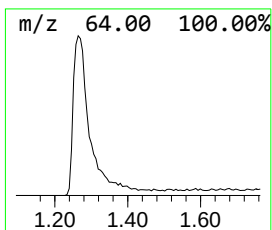
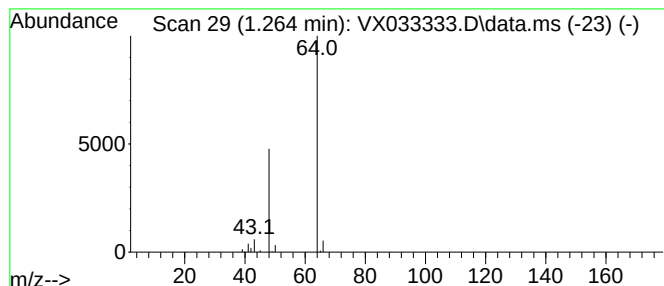
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	7.05 ug/l	68357	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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033333.D
Acq On : 08 Dec 2022 18:59
Operator : JC/MD
Sample : N5906-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23R

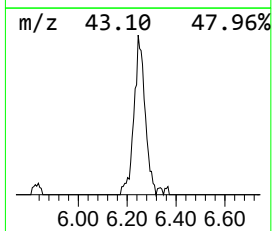
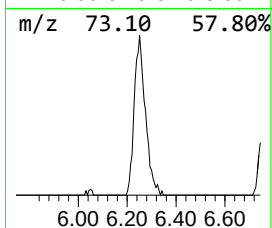
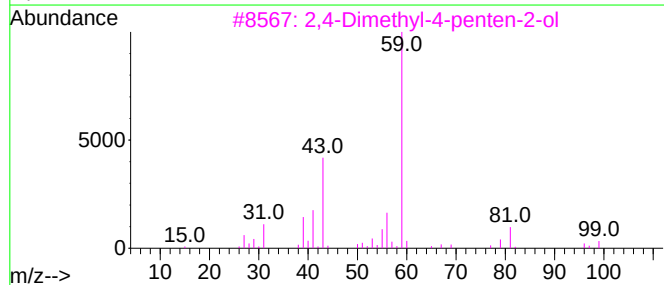
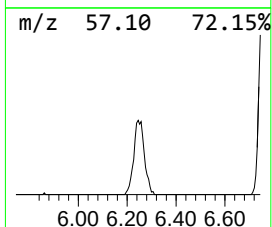
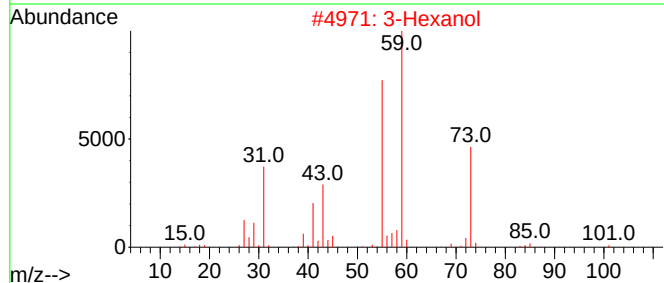
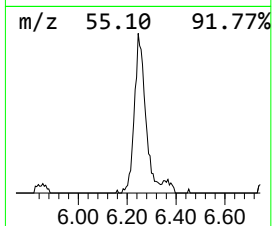
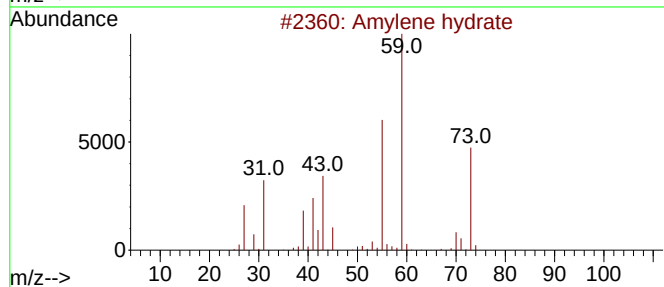
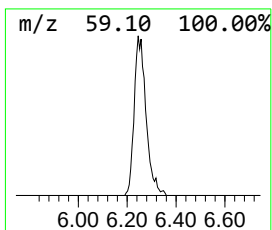
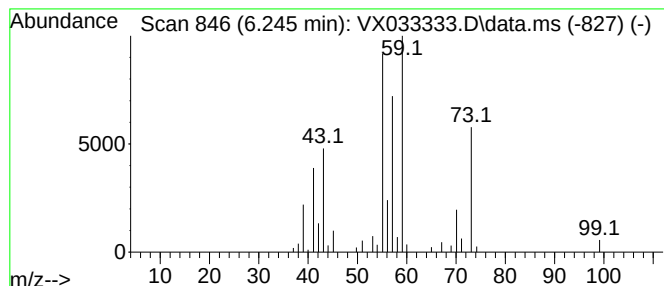
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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

Peak Number 2 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.245	5.02 ug/l	58598	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	53
2			3-Hexanol	102	C6H14O	000623-37-0	42
3			2,4-Dimethyl-4-penten-2-ol	114	C7H14O	019781-53-4	38
4			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	36
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120822\
Data File : VX033333.D
Acq On : 08 Dec 2022 18:59
Operator : JC/MD
Sample : N5906-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-23R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.264	7.0	ug/l	68357	1	5.556	484856	50.0
Amylene hydrate	6.245	5.0	ug/l	58598	2	6.763	583950	50.0