

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
 Data File : VX021230.D
 Acq On : 16 Mar 2021 03:51
 Operator : JC/MD
 Sample : M1666-05 50X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-89-90

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\82X031521W.M
 Title : SW846 8260

Signal : TIC: VX021230.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	62	66	73	rBV	31055	35474	7.89%	1.111%
2	1.599	79	87	90	rVB6	4202	9113	2.03%	0.285%
3	2.093	167	171	176	rBV3	3704	5784	1.29%	0.181%
4	2.422	221	227	231	rBV	20561	33305	7.41%	1.043%
5	2.458	231	233	240	rVB3	4295	7010	1.56%	0.220%
6	2.581	246	254	262	rBV	15562	28627	6.37%	0.896%
7	4.299	539	546	557	rVB7	1494	4573	1.02%	0.143%
8	5.464	731	744	758	rBV	53476	153298	34.11%	4.800%
9	5.629	761	772	789	rBV	80808	225529	50.19%	7.062%
10	6.029	830	840	854	rBV	60870	162163	36.09%	5.078%
11	6.829	964	976	988	rBV	139128	328092	73.01%	10.273%
12	7.270	1044	1051	1066	rBV3	2166	6178	1.37%	0.193%
13	8.694	1286	1293	1301	rBV	282422	449388	100.00%	14.071%
14	8.764	1301	1305	1312	rVB	9144	16697	3.72%	0.523%
15	10.094	1525	1531	1547	rBV	305197	411791	91.63%	12.894%
16	10.876	1658	1664	1671	rBV2	7283	9970	2.22%	0.312%
17	11.029	1681	1690	1700	rBV	99729	177444	39.49%	5.556%
18	11.118	1700	1705	1714	rVB	263866	341479	75.99%	10.693%
19	12.059	1860	1865	1873	rVB	313178	385670	85.82%	12.076%
20	12.253	1893	1898	1909	rBV	14735	27624	6.15%	0.865%
21	12.341	1909	1913	1923	rVB7	3752	7212	1.60%	0.226%
22	12.618	1953	1960	1972	rBV	116229	151138	33.63%	4.733%
23	12.794	1985	1990	1995	rBV3	4812	6040	1.34%	0.189%
24	12.853	1996	2000	2005	rBV	19338	24396	5.43%	0.764%
25	13.553	2114	2119	2124	rBV4	3460	5671	1.26%	0.178%
26	14.677	2303	2310	2313	rBV3	5539	9076	2.02%	0.284%
27	14.824	2332	2335	2340	rVB3	5202	7658	1.70%	0.240%
28	15.006	2364	2366	2373	rVB7	3989	5667	1.26%	0.177%
29	15.465	2440	2444	2449	rVB3	10066	14516	3.23%	0.455%
30	15.524	2450	2454	2461	rVV	10046	17557	3.91%	0.550%
31	15.665	2473	2478	2481	rBV2	15967	24475	5.45%	0.766%
32	15.700	2481	2484	2488	rVV2	7037	9543	2.12%	0.299%
33	15.795	2495	2500	2506	rVB4	11969	20368	4.53%	0.638%
34	16.148	2554	2560	2567	rBV	25421	47382	10.54%	1.484%
35	16.330	2586	2591	2592	rBV4	5481	8177	1.82%	0.256%
36	16.659	2645	2647	2654	rVB7	4536	7161	1.59%	0.224%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021230.D
Acq On : 16 Mar 2021 03:51
Operator : JC/MD
Sample : M1666-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-89-90

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\82X031521W.M
Title : SW846 8260

37	16.777	2662	2667	2669	rBV4	5101	8365	1.86%	0.262%
----	--------	------	------	------	------	------	------	-------	--------

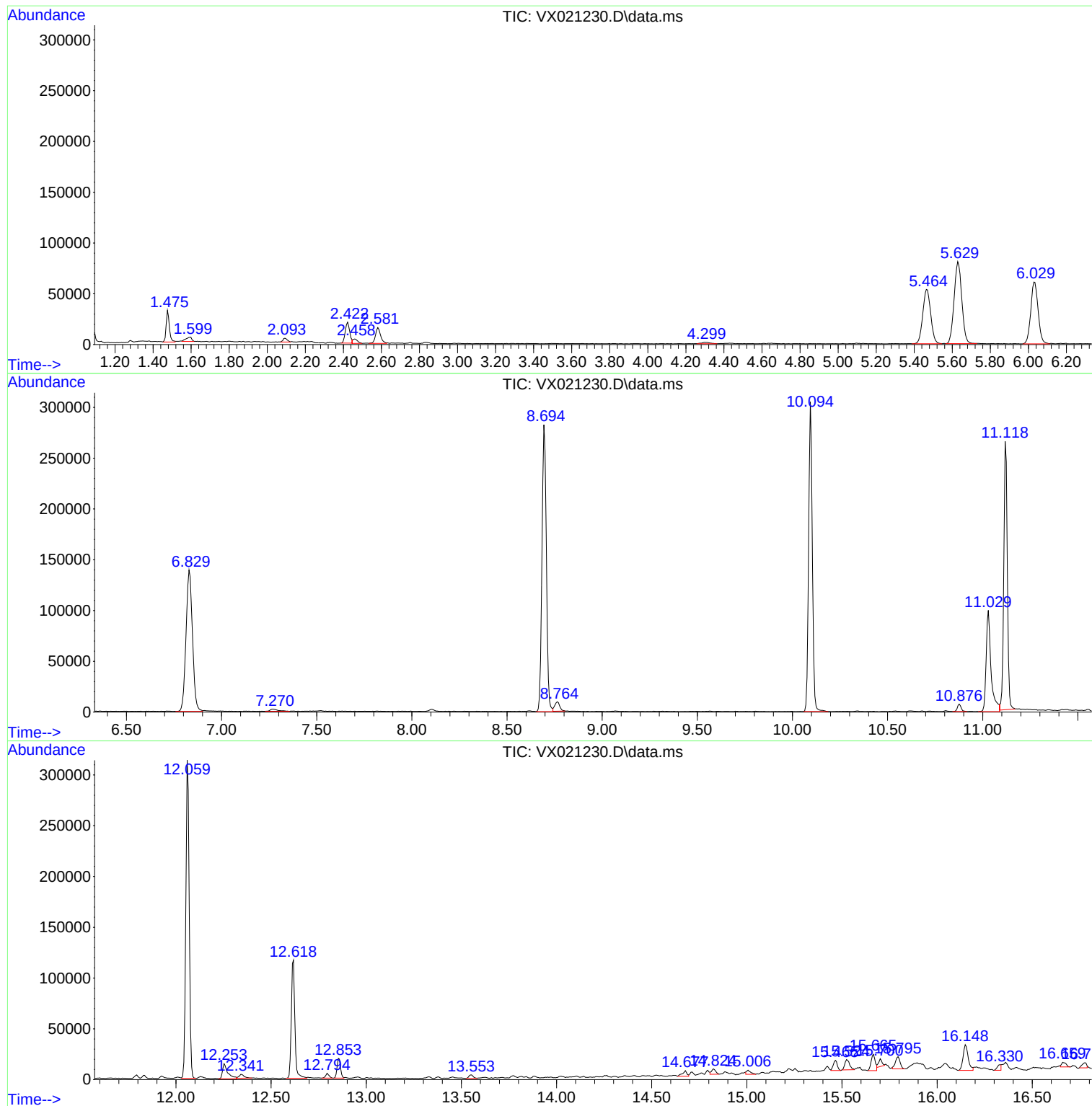
Sum of corrected areas: 3193611

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021230.D
Acq On : 16 Mar 2021 03:51
Operator : JC/MD
Sample : M1666-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-89-90

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021230.D
Acq On : 16 Mar 2021 03:51
Operator : JC/MD
Sample : M1666-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-89-90

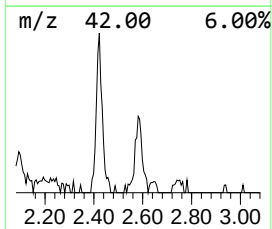
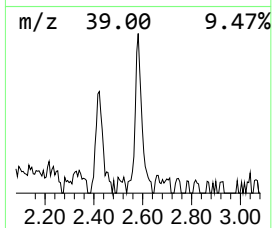
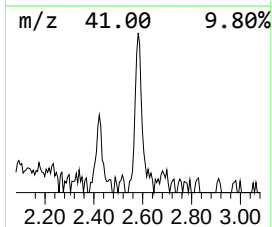
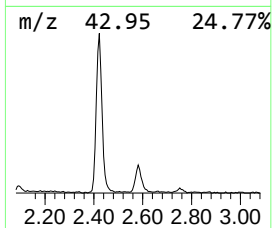
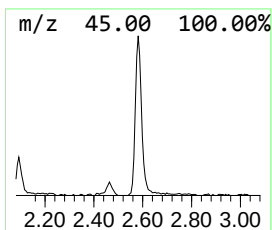
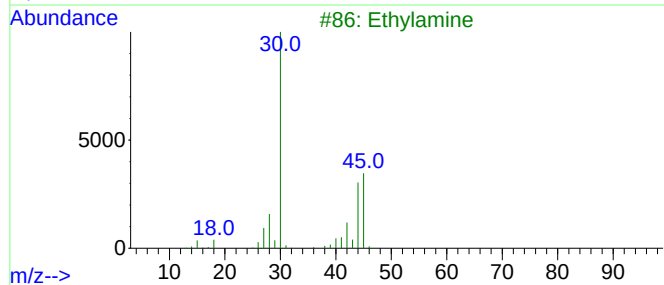
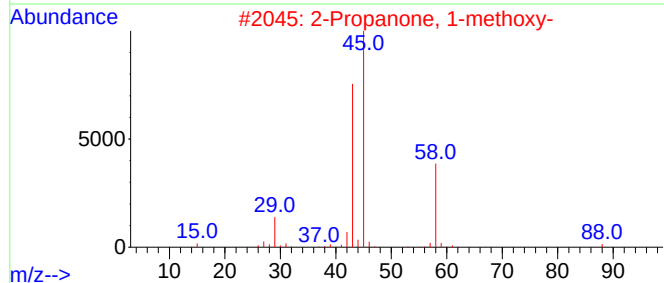
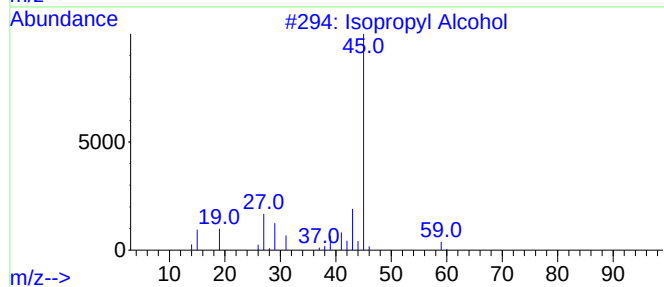
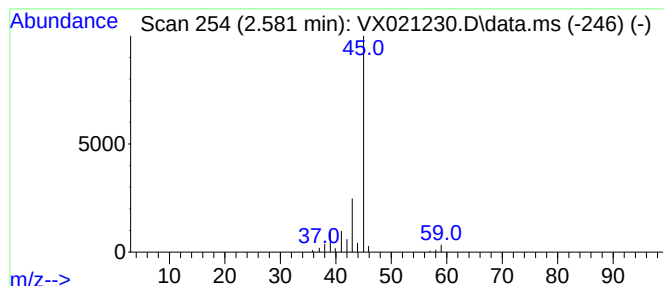
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.581	6.35 ug/l	28627	Pentafluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9
3			Ethylamine	45	C2H7N	000075-04-7	5
4			Formamide	45	CH3NO	000075-12-7	4
5			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021230.D
Acq On : 16 Mar 2021 03:51
Operator : JC/MD
Sample : M1666-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-89-90

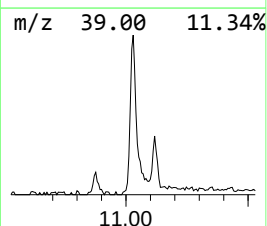
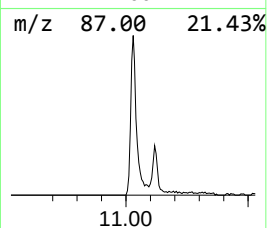
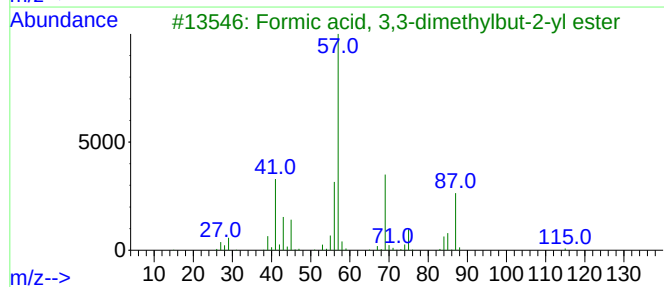
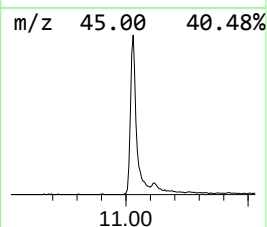
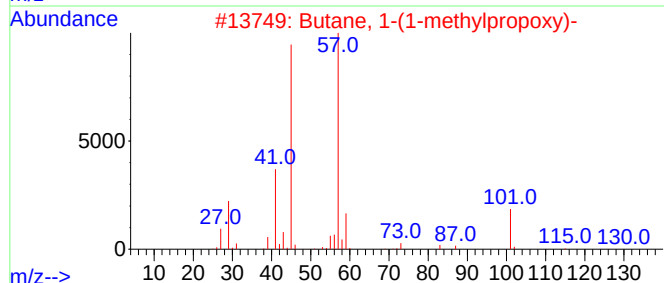
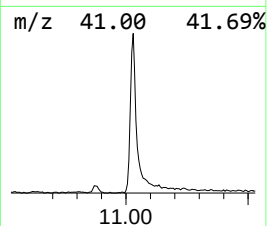
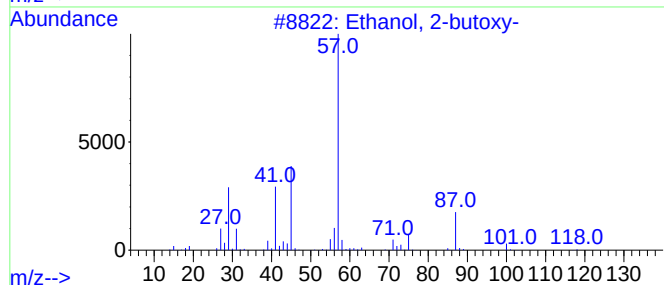
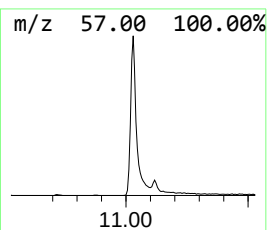
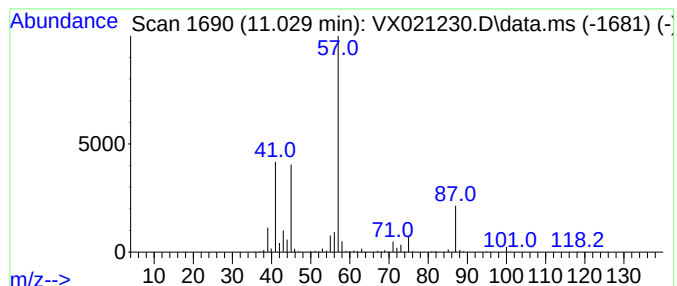
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.029	21.55 ug/l	177444	Chlorobenzene-d5	10.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3			Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	39
4			1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	32
5			Propane, 1-methoxy-2,2-dimethyl-	102	C6H14O	001118-00-9	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021230.D
Acq On : 16 Mar 2021 03:51
Operator : JC/MD
Sample : M1666-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-89-90

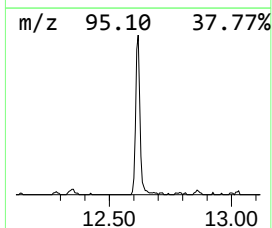
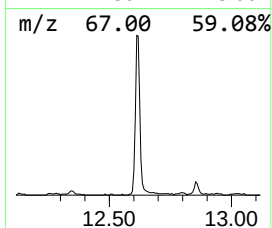
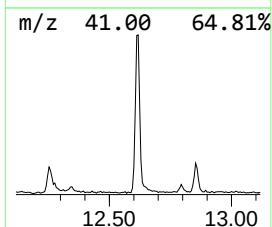
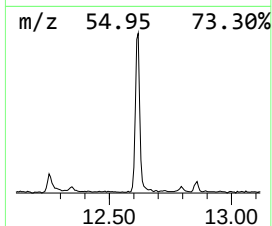
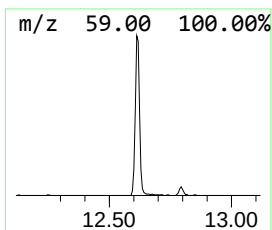
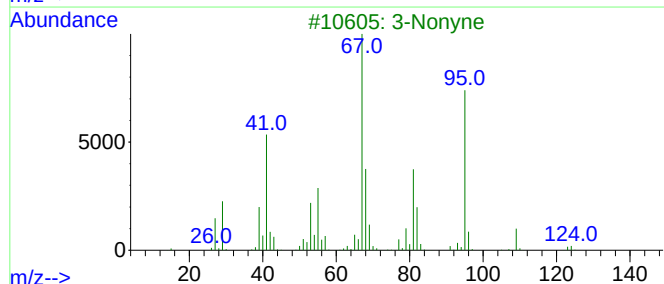
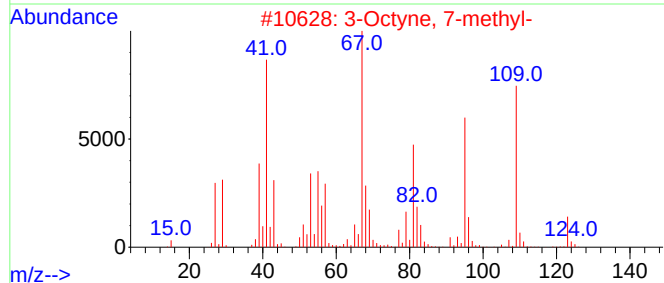
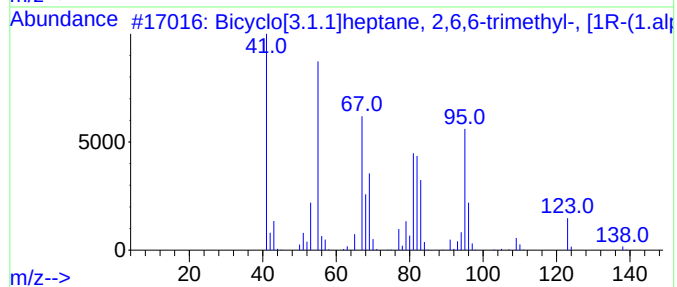
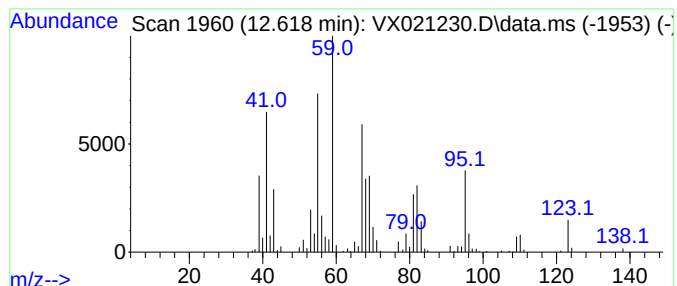
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.618 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.618	19.59 ug/l	151138	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004795-86-2	43
2			3-Octyne, 7-methyl-	124	C9H16	037050-06-9	38
3			3-Nonyne	124	C9H16	020184-89-8	30
4			3-Hexanol	102	C6H14O	000623-37-0	27
5			2-Propenoic acid, undec-10-enyl ...	224	C14H24O2	020763-72-8	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021230.D
Acq On : 16 Mar 2021 03:51
Operator : JC/MD
Sample : M1666-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-89-90

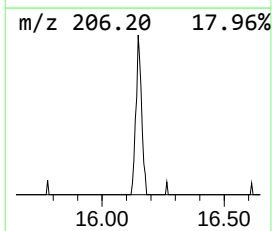
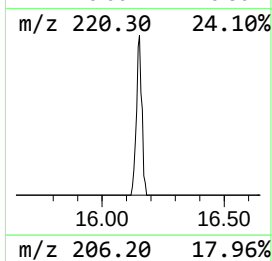
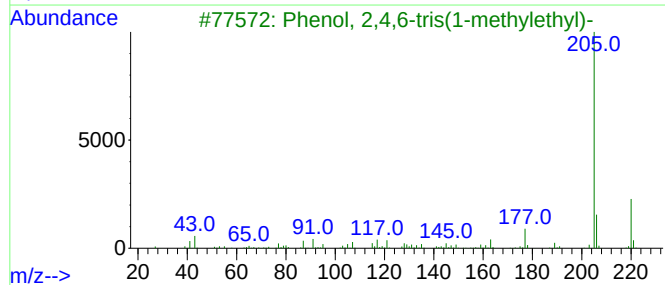
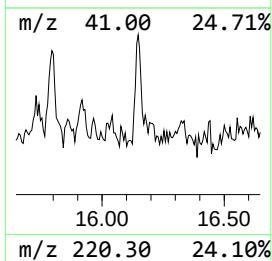
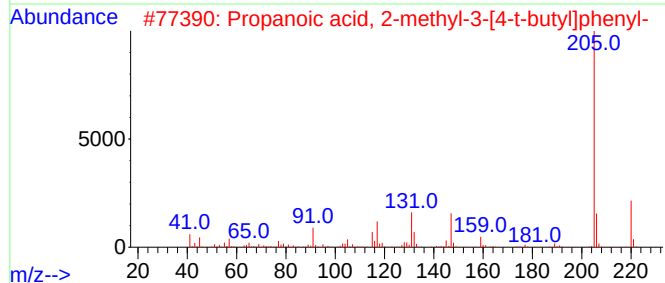
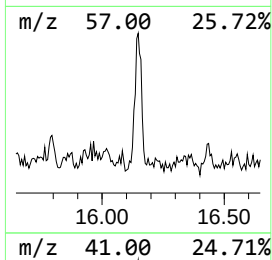
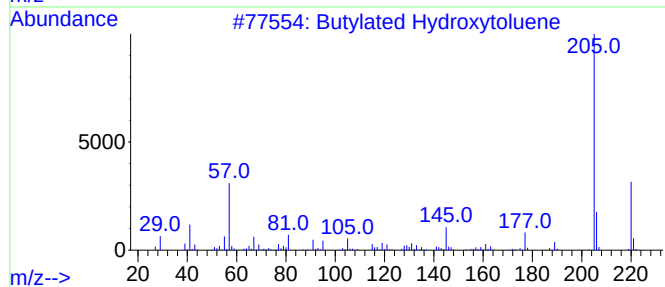
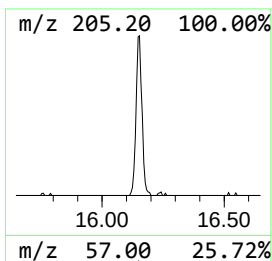
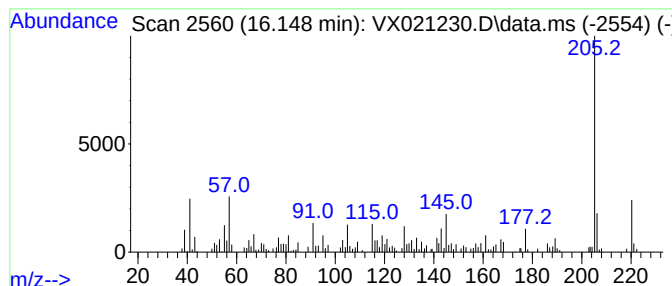
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.148	6.14 ug/l	47382	1,4-Dichlorobenzene-d4	12.059

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
2			Propanoic acid, 2-methyl-3-[4-t...	220	C14H20O2	1000131-87-0	64
3			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	64
4			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	58
5			2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021230.D
Acq On : 16 Mar 2021 03:51
Operator : JC/MD
Sample : M1666-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-89-90

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.581	6.3	ug/l	28627	1	5.629	225529	50.0
Ethanol, 2-butoxy-	11.029	21.6	ug/l	177444	3	10.094	411791	50.0
unknown12.618	12.618	19.6	ug/l	151138	4	12.059	385670	50.0
Butylated Hydro...	16.148	6.1	ug/l	47382	4	12.059	385670	50.0