

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
 Data File : VX030370.D
 Acq On : 03 Aug 2022 15:00
 Operator : JC/MD
 Sample : N3988-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 63022-E

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\82X072522W.M
 Title : SW846 8260

Signal : TIC: VX030370.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.385	206	213	225	rVB	98646	169035	1.14%	0.268%
2	3.574	401	408	421	rBV	112230	257368	1.74%	0.408%
3	5.391	694	706	718	rBV2	99690	292225	1.97%	0.463%
4	5.562	723	734	745	rVB	99853	287966	1.94%	0.456%
5	5.964	788	800	805	rBV	121935	320758	2.17%	0.508%
6	6.043	805	813	834	rVB	1681899	4443317	29.99%	7.036%
7	6.354	853	864	881	rBV2	98648	291405	1.97%	0.461%
8	6.769	919	932	942	rBV3	238011	835912	5.64%	1.324%
9	7.805	1093	1102	1114	rBV	1451957	2474738	16.70%	3.919%
10	8.555	1219	1225	1234	rBV	270885	432383	2.92%	0.685%
11	8.652	1234	1241	1246	rBV	499286	769445	5.19%	1.218%
12	8.726	1246	1253	1270	rVB	3889502	6172372	41.66%	9.775%
13	8.957	1285	1291	1297	rBV	372190	525410	3.55%	0.832%
14	9.250	1333	1339	1345	rBV	320774	452191	3.05%	0.716%
15	9.378	1357	1360	1366	rVB	139439	195826	1.32%	0.310%
16	9.488	1372	1378	1383	rBV	760169	979717	6.61%	1.551%
17	9.579	1389	1393	1407	rVB	456389	613866	4.14%	0.972%
18	9.914	1443	1448	1456	rBV	1099130	1391147	9.39%	2.203%
19	10.055	1463	1471	1479	rBV	394389	569534	3.84%	0.902%
20	10.195	1489	1494	1500	rBV	736703	936384	6.32%	1.483%
21	10.305	1504	1512	1523	rVV	3764170	5071764	34.23%	8.032%
22	10.646	1563	1568	1581	rVB	4429319	5762688	38.90%	9.126%
23	11.085	1634	1640	1645	rBV	409844	511052	3.45%	0.809%
24	11.384	1682	1689	1696	rBV	401455	656530	4.43%	1.040%
25	11.451	1696	1700	1712	rVB	371442	483665	3.26%	0.766%
26	11.615	1722	1727	1735	rBV	252926	351088	2.37%	0.556%
27	11.756	1742	1750	1755	rBV	1885412	2413387	16.29%	3.822%
28	11.963	1779	1784	1789	rBV	176198	234518	1.58%	0.371%
29	12.024	1789	1794	1798	rVV	541087	674102	4.55%	1.068%
30	12.091	1798	1805	1808	rVV	556898	700733	4.73%	1.110%
31	12.243	1822	1830	1838	rBV	252697	381368	2.57%	0.604%
32	12.414	1853	1858	1864	rBV	1956040	2349253	15.86%	3.720%
33	12.804	1911	1922	1927	rBV	1156132	1801895	12.16%	2.853%
34	12.951	1939	1946	1957	rVB2	281455	519564	3.51%	0.823%
35	13.292	1993	2002	2006	rBV2	121052	182397	1.23%	0.289%
36	13.426	2019	2024	2031	rVV	143544	186269	1.26%	0.295%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

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\82X072522W.M
Title : SW846 8260

37	13.713	2066	2071	2076	rVB2	371919	462190	3.12%	0.732%
38	13.780	2076	2082	2087	rVV	11704599	14814964	100.00%	23.461%
39	13.828	2087	2090	2093	rVV3	154501	214805	1.45%	0.340%
40	13.871	2093	2097	2102	rVB	518927	656028	4.43%	1.039%
41	14.639	2218	2223	2234	rVB	1106838	1380702	9.32%	2.186%
42	14.779	2241	2246	2253	rBV	738301	927086	6.26%	1.468%

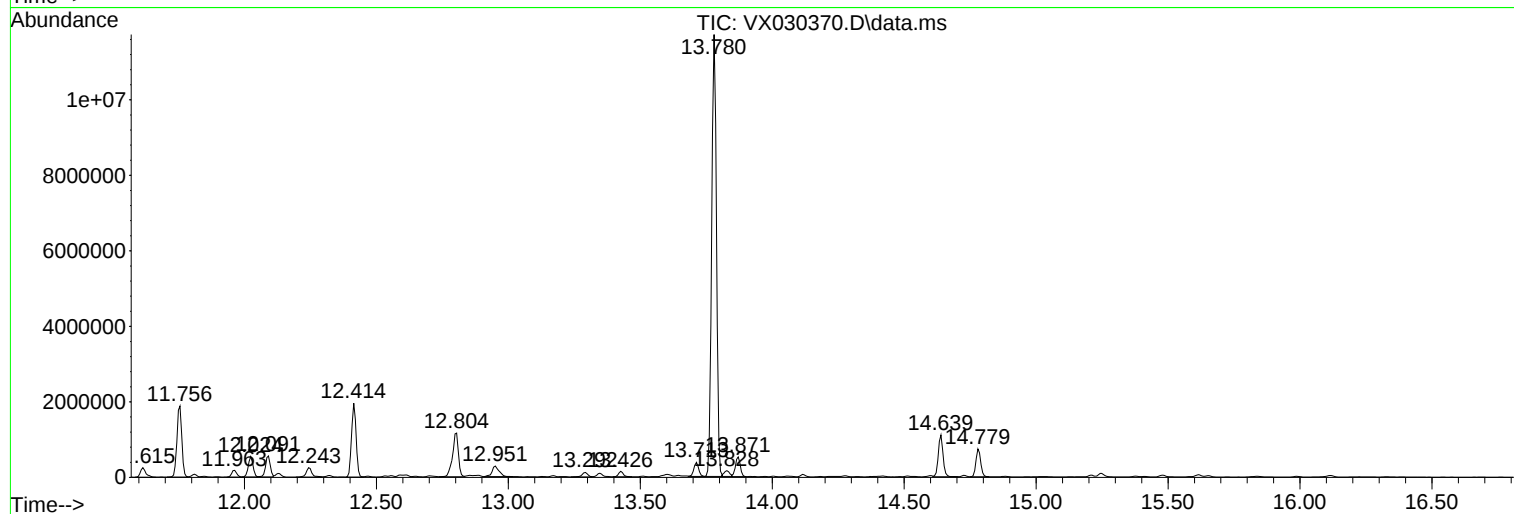
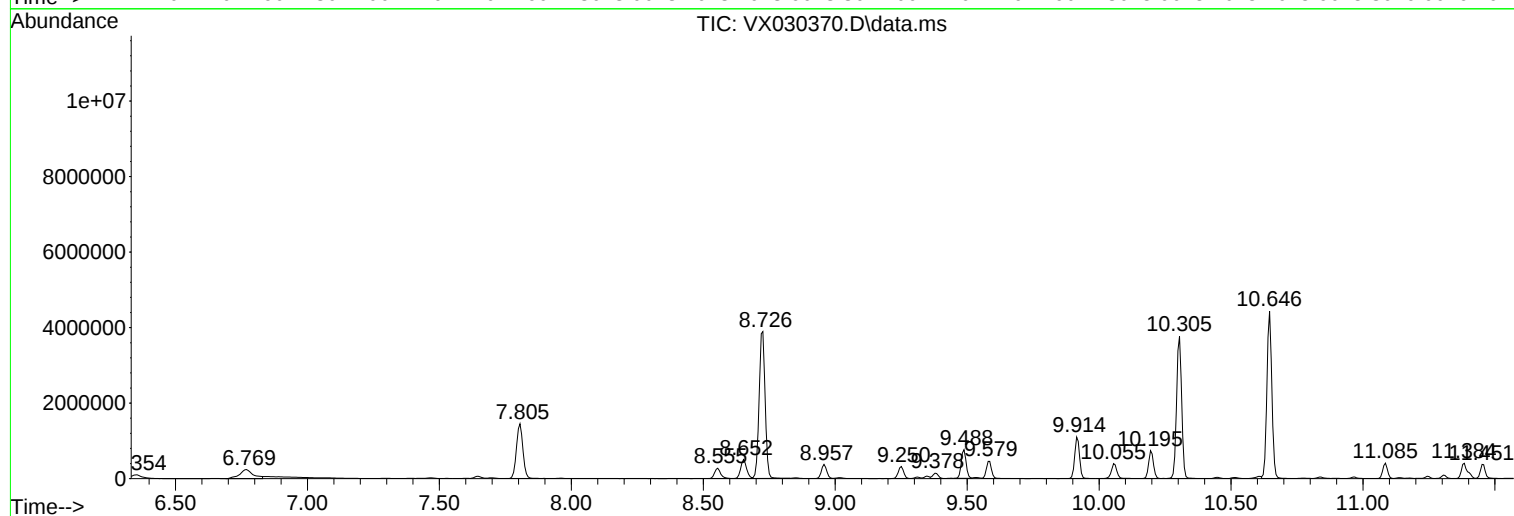
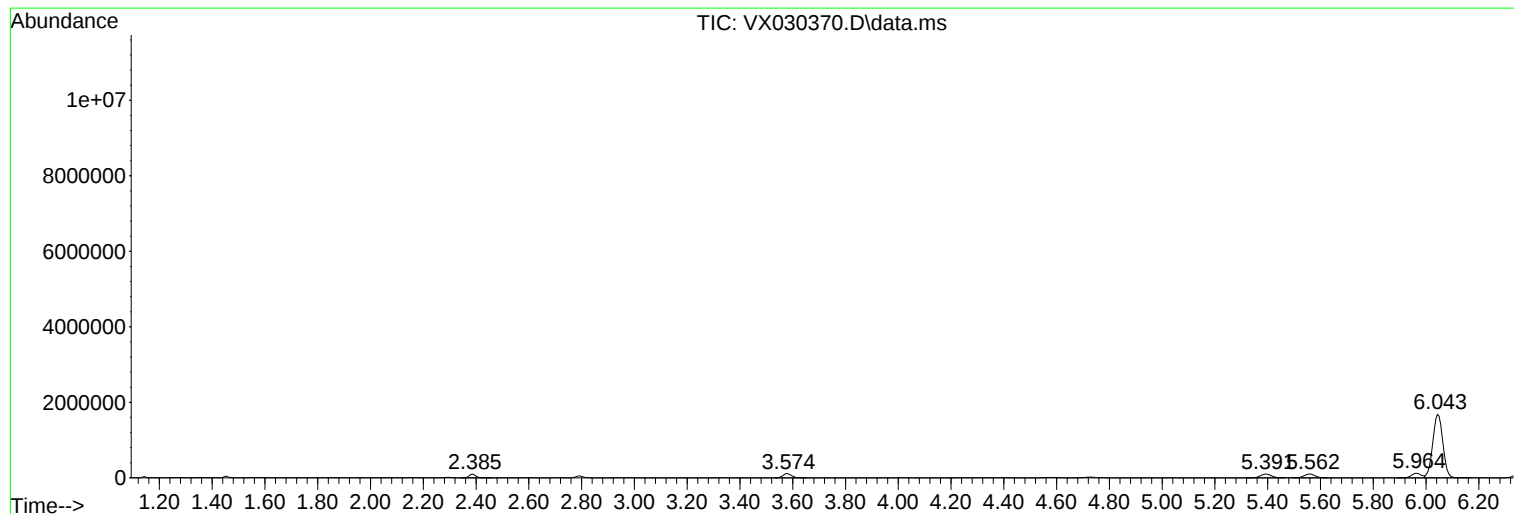
Sum of corrected areas: 63147047

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

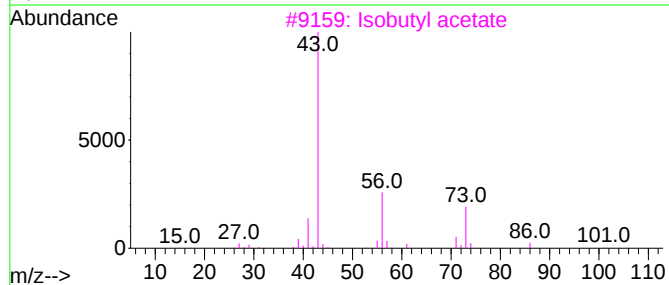
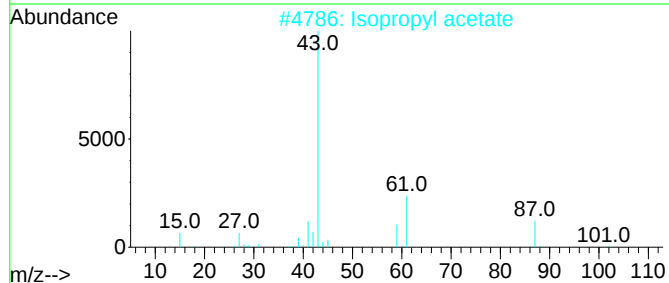
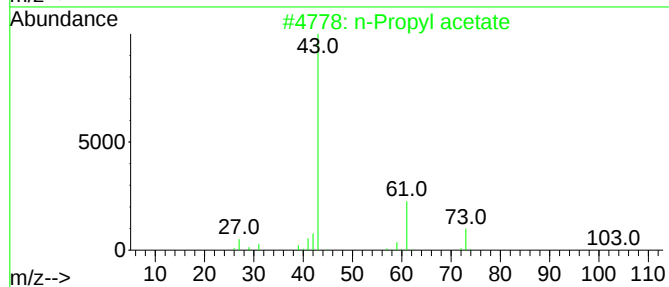
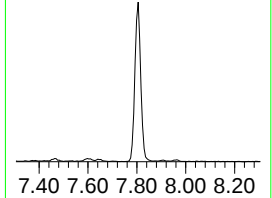
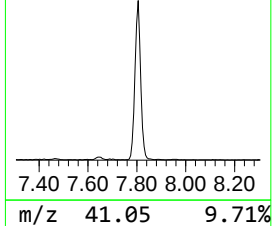
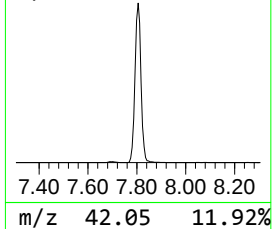
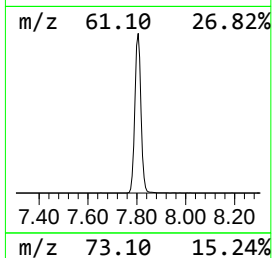
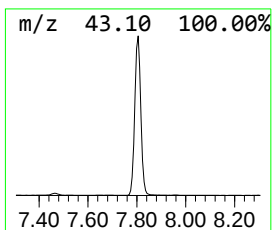
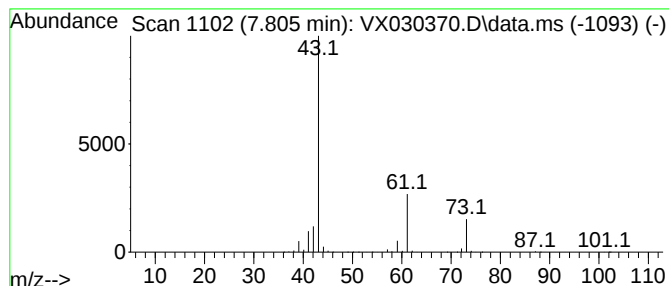
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.805	148.03 ug/l	2474740	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	36
3			Isobutyl acetate	116	C6H12O2	000110-19-0	9
4			Isobutylamine	73	C4H11N	000078-81-9	7
5			1-Butanamine	73	C4H11N	000109-73-9	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

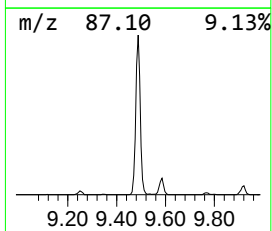
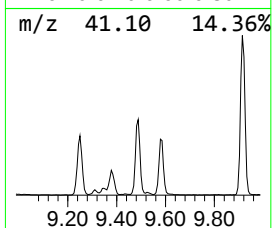
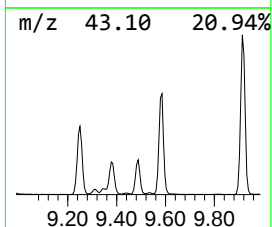
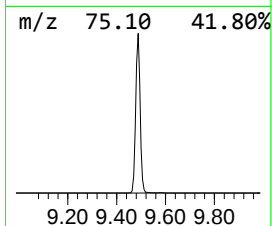
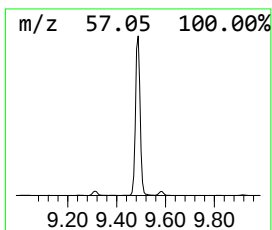
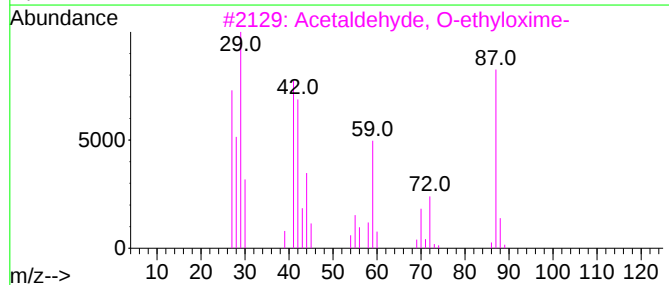
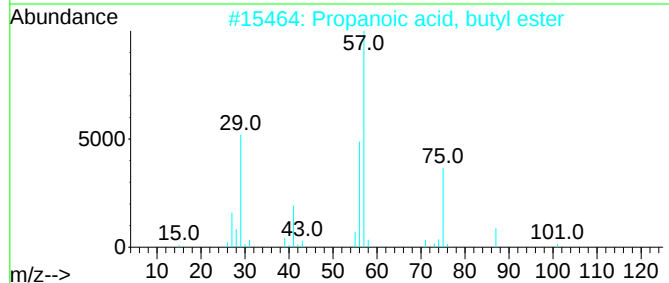
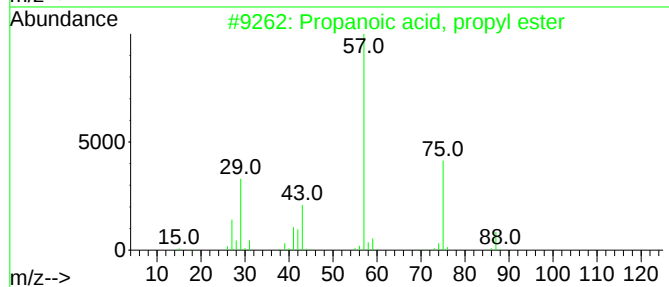
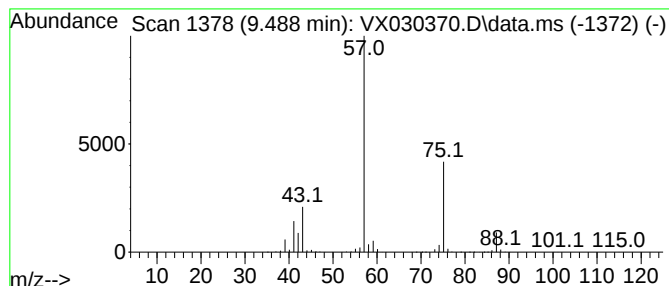
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 2 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.488	86.01 ug/l	979717	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	56
3			Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	9
4			Isobutyl ether	130	C8H18O	000628-55-7	9
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

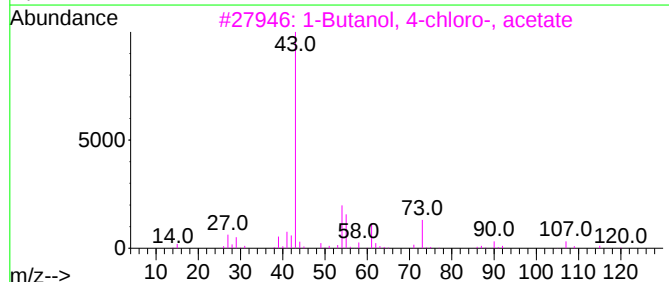
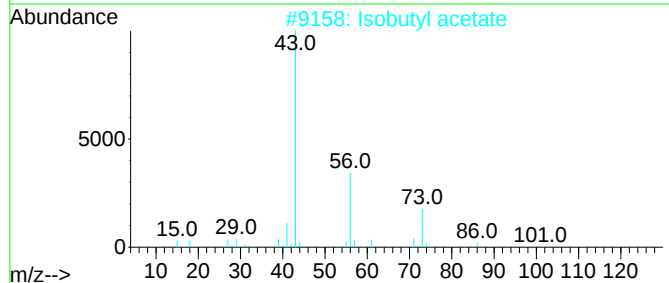
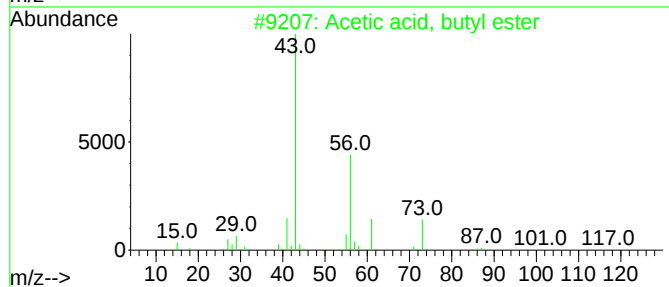
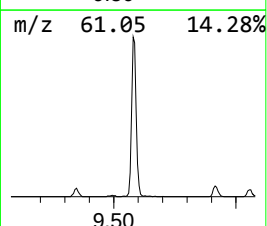
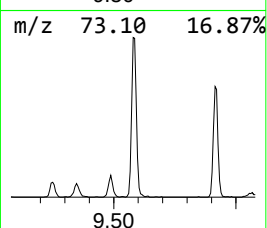
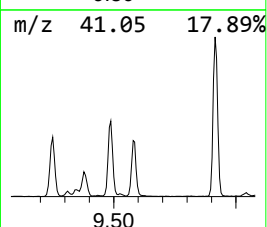
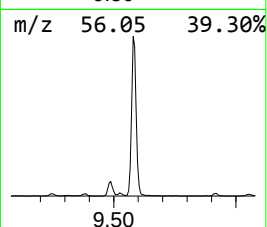
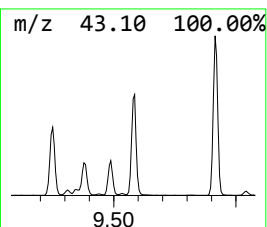
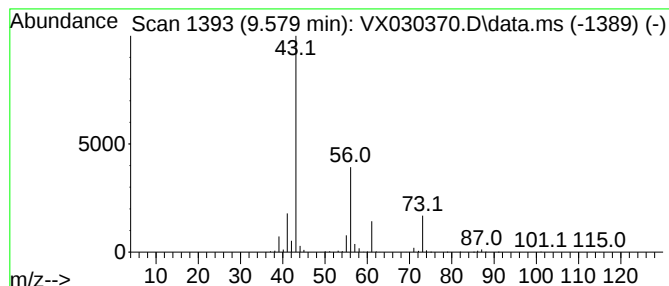
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	53.89 ug/l	613866	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	39
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

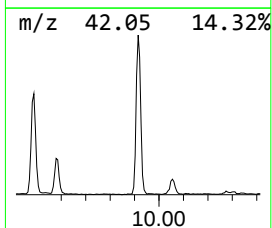
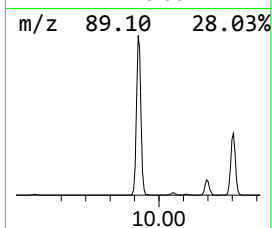
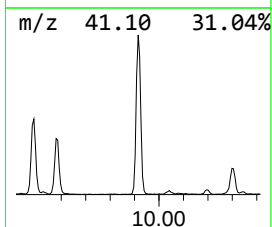
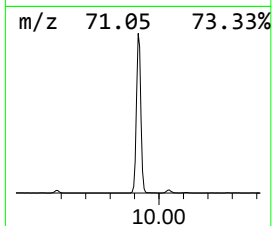
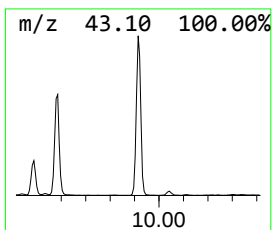
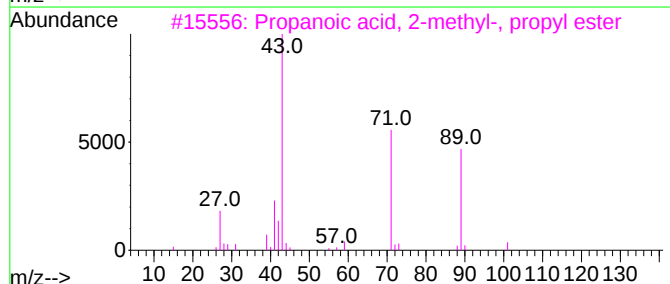
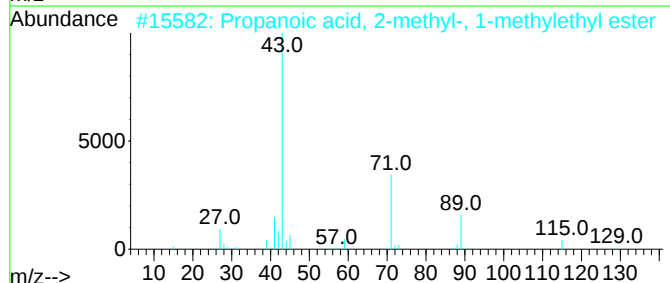
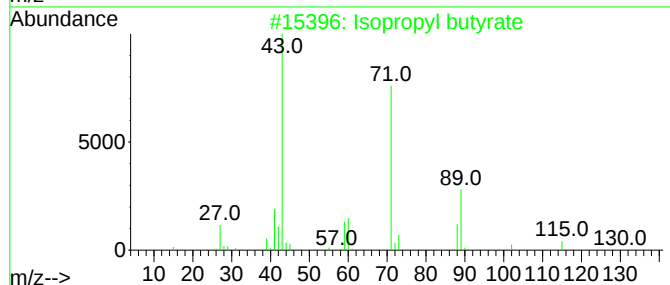
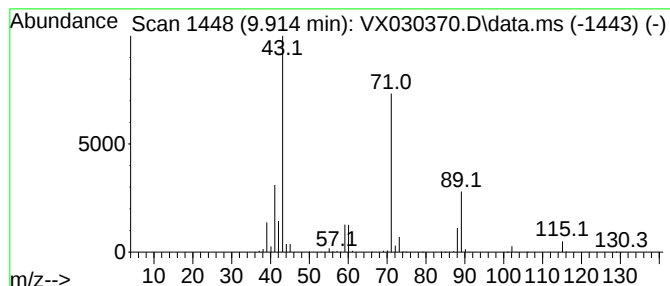
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 4 Isopropyl butyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.914	122.13 ug/l	1391150	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	64
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

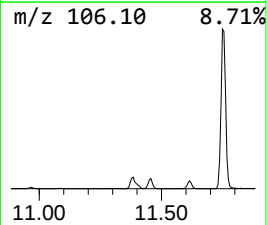
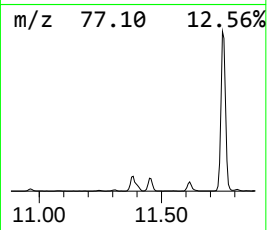
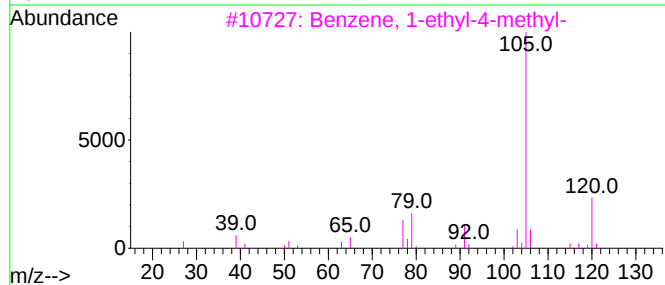
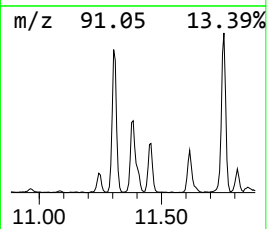
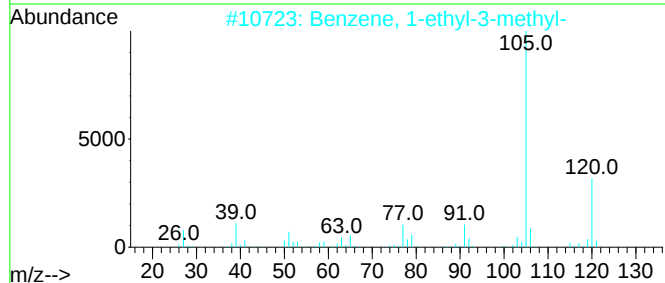
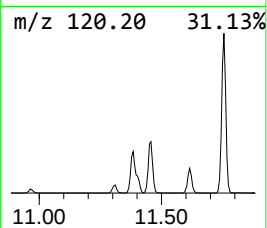
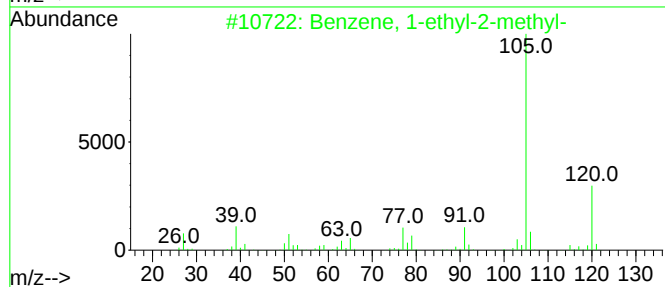
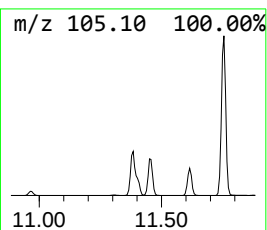
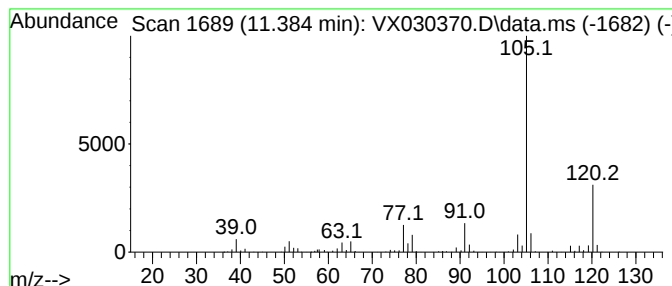
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.384	48.70 ug/l	656530	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

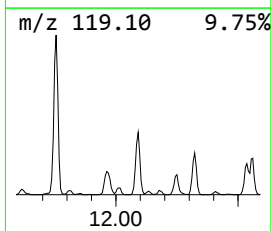
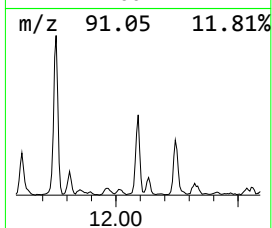
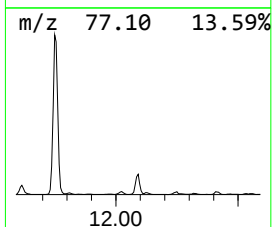
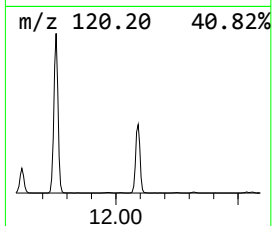
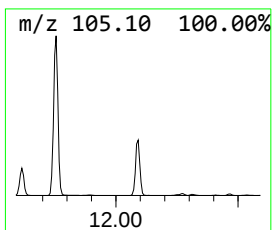
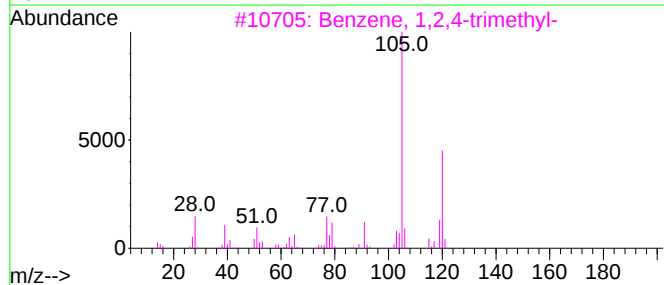
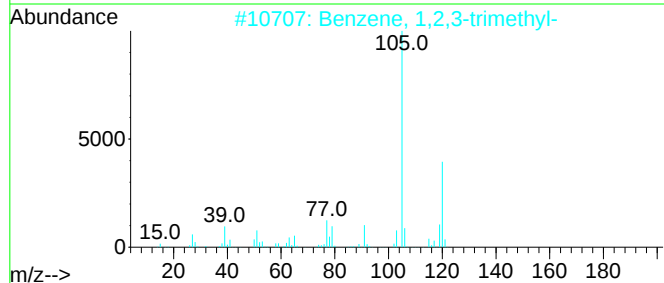
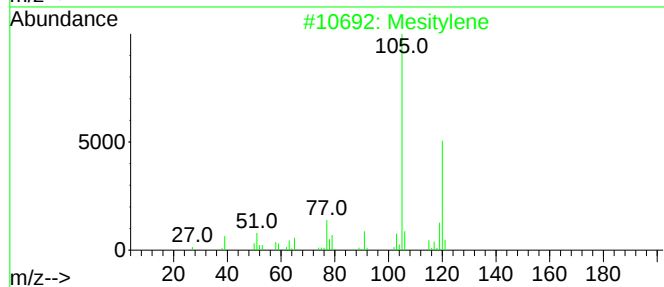
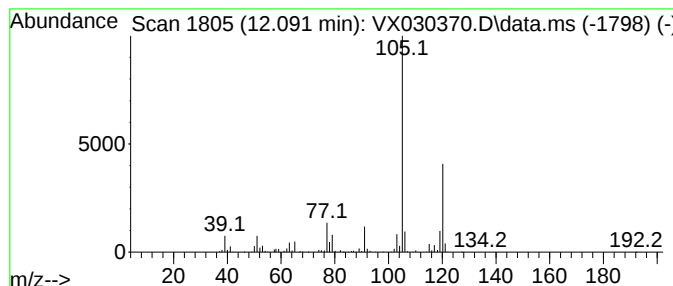
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 6 Mesitylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	51.98 ug/l	700733	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

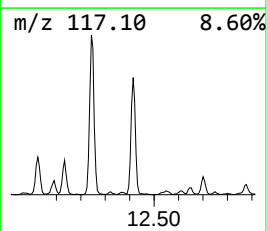
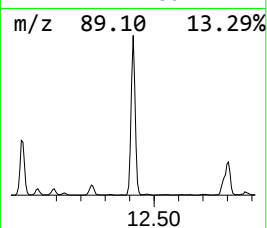
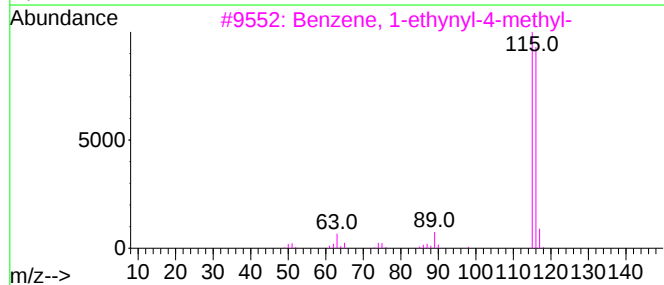
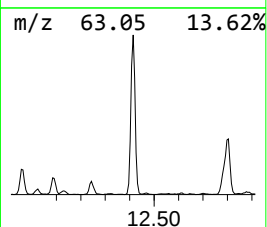
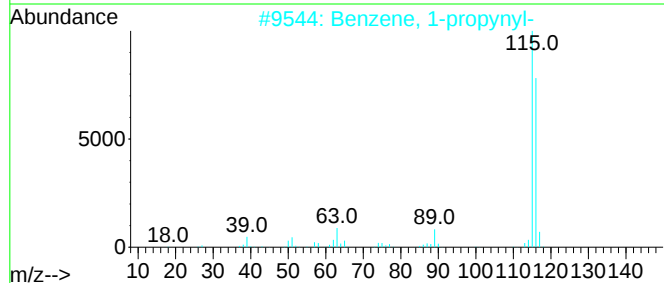
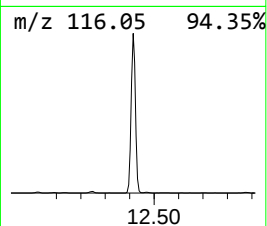
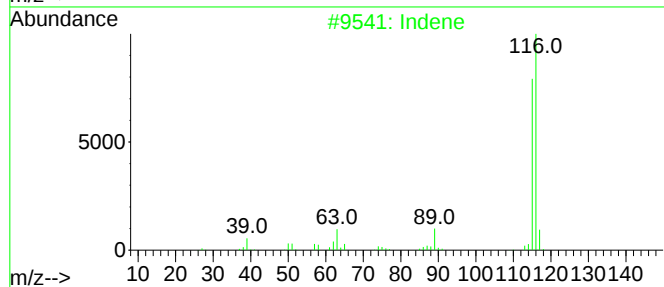
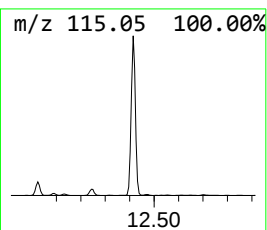
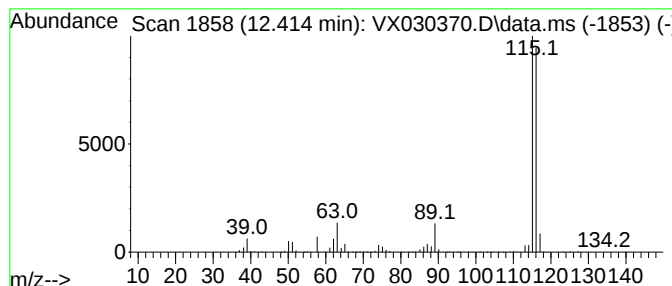
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 7 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.414	174.25 ug/l	2349250	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

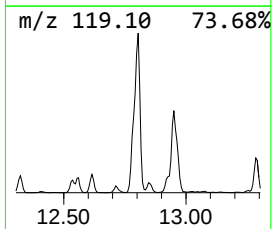
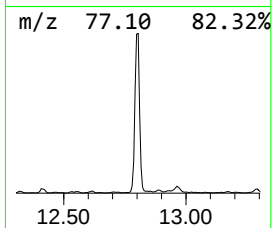
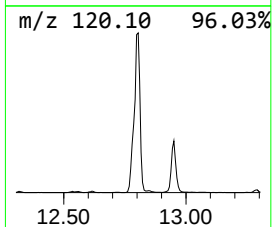
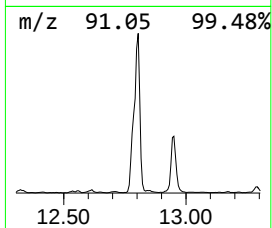
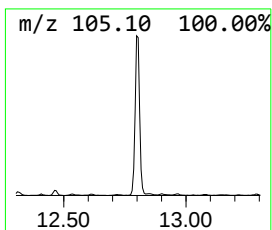
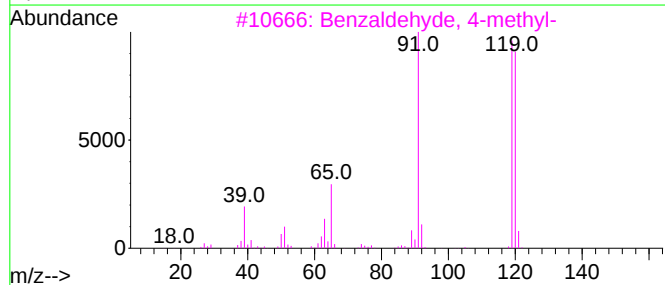
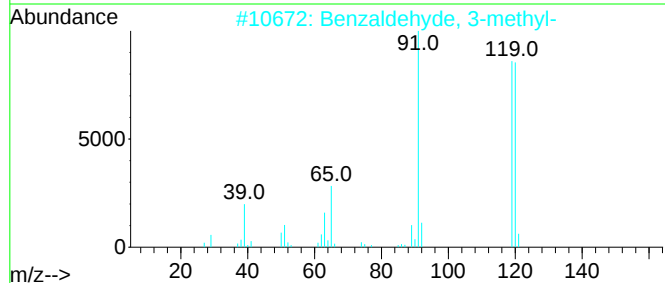
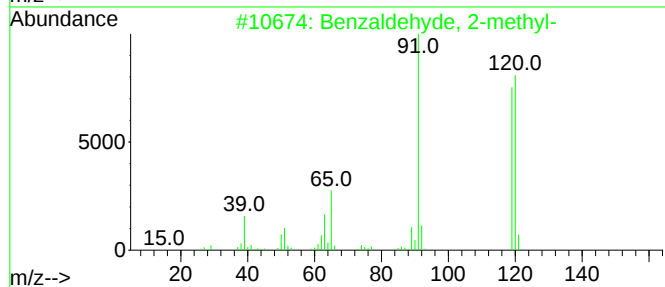
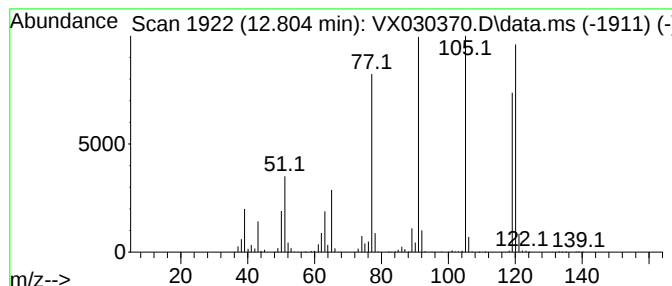
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 8 Benzaldehyde, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.804	133.65 ug/l	1801900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 2-methyl-	120	C8H8O	000529-20-4	95
2			Benzaldehyde, 3-methyl-	120	C8H8O	000620-23-5	95
3			Benzaldehyde, 4-methyl-	120	C8H8O	000104-87-0	90
4			Phthalan	120	C8H8O	000496-14-0	55
5			4-Vinylphenol	120	C8H8O	002628-17-3	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

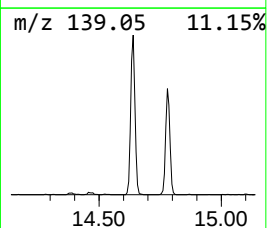
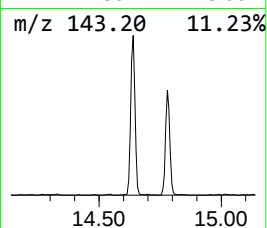
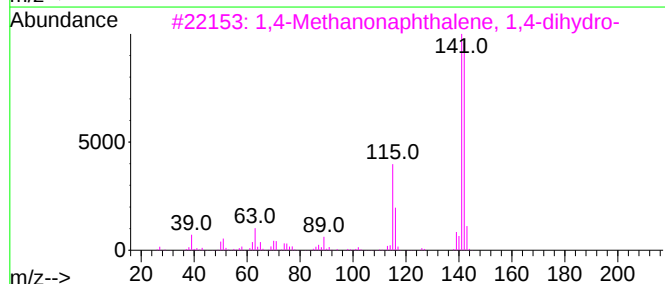
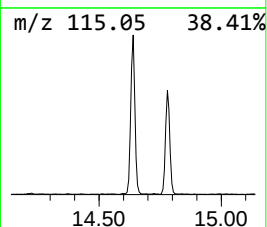
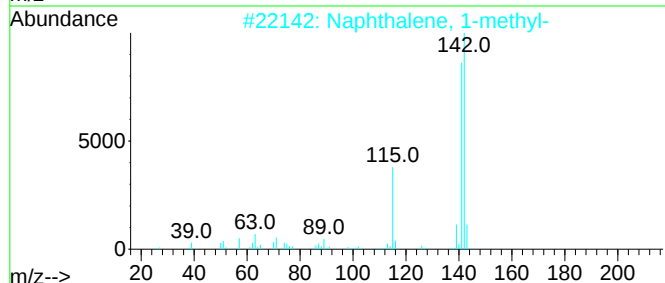
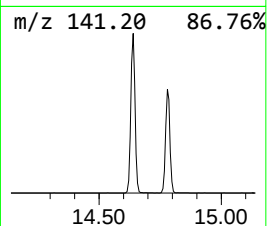
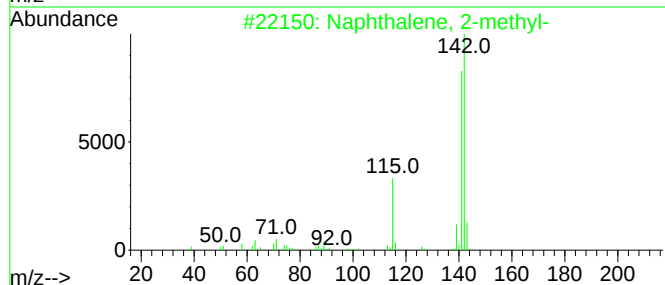
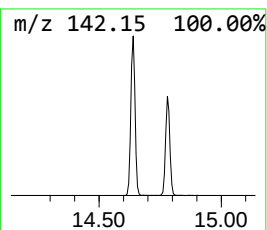
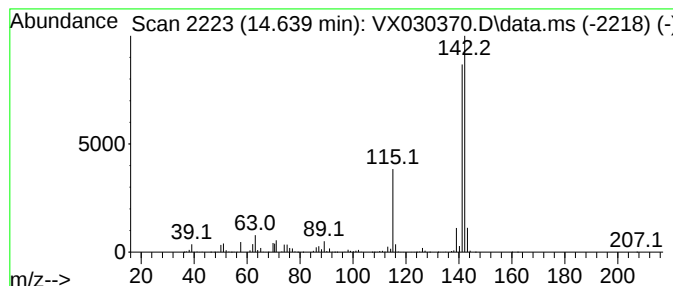
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 9 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.639	102.41 ug/l	1380700	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

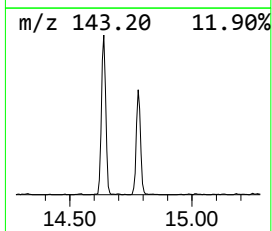
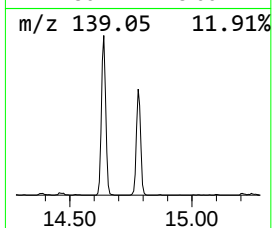
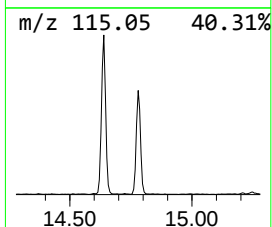
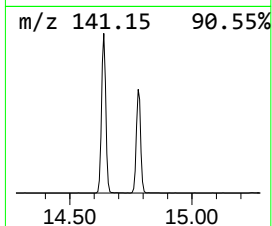
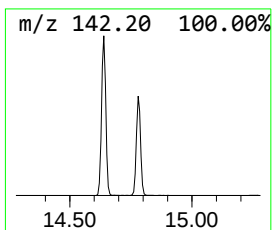
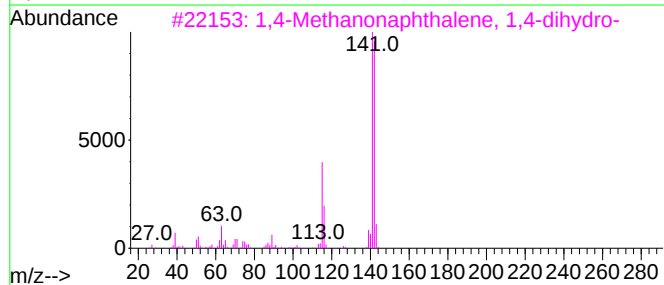
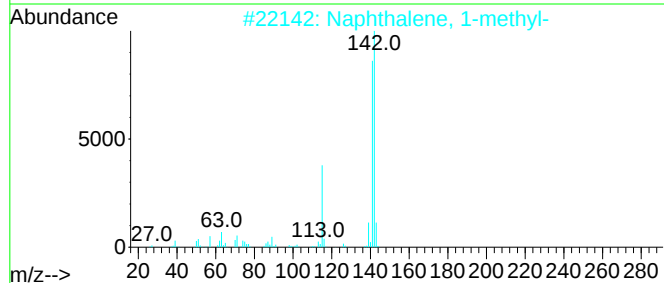
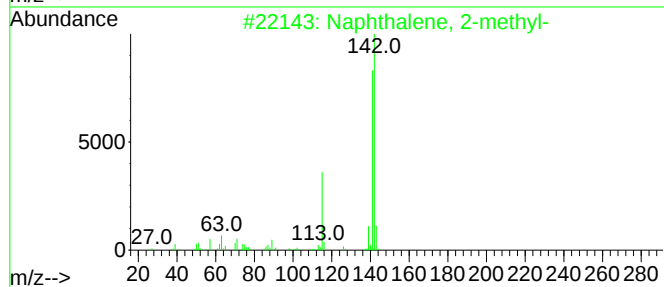
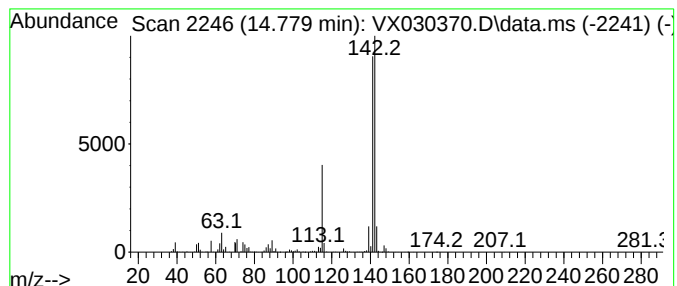
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.M
Quant Title : SW846 8260

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

Peak Number 10 1,4-Methanonaphthalene, 1,4... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.779	68.76 ug/l	927086	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
4		Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5		Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080322\
Data File : VX030370.D
Acq On : 03 Aug 2022 15:00
Operator : JC/MD
Sample : N3988-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
63022-E

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072522W.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
n-Propyl acetate	7.805	148.0	ug/l	2474740	2	6.769	835912	50.0
Propanoic acid,...	9.488	86.0	ug/l	979717	3	10.055	569534	50.0
Acetic acid, bu...	9.579	53.9	ug/l	613866	3	10.055	569534	50.0
Isopropyl butyrate	9.914	122.1	ug/l	1391150	3	10.055	569534	50.0
Benzene, 1-ethy...	11.384	48.7	ug/l	656530	4	12.024	674102	50.0
Mesitylene	12.091	52.0	ug/l	700733	4	12.024	674102	50.0
Indene	12.414	174.3	ug/l	2349250	4	12.024	674102	50.0
Benzaldehyde, 2...	12.804	133.7	ug/l	1801900	4	12.024	674102	50.0
Naphthalene, 1-...	14.639	102.4	ug/l	1380700	4	12.024	674102	50.0
1,4-Methanonaph...	14.779	68.8	ug/l	927086	4	12.024	674102	50.0