

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
 Data File : VX031421.D
 Acq On : 16 Sep 2022 19:32
 Operator : JC/MD
 Sample : N4645-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TOLL-MW-04

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\82X091422W.M
 Title : SW846 8260

Signal : TIC: VX031421.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	22	30	35	rBV2	21538	42953	5.79%	1.195%
2	1.368	43	46	52	rVB	31647	34168	4.61%	0.951%
3	1.599	73	84	95	rVB5	11768	43344	5.84%	1.206%
4	1.746	104	108	114	rVB3	9685	13091	1.76%	0.364%
5	3.111	323	332	343	rVB3	9908	25372	3.42%	0.706%
6	4.215	503	513	522	rBV4	4887	14557	1.96%	0.405%
7	4.489	549	558	571	rVB2	12197	35216	4.75%	0.980%
8	5.391	693	706	722	rBV	85537	247415	33.35%	6.886%
9	5.556	722	733	740	rVV	85851	244833	33.00%	6.814%
10	5.617	741	743	756	rVB3	20030	48780	6.57%	1.358%
11	5.958	789	799	814	rBV	95591	254188	34.26%	7.075%
12	6.251	837	847	858	rVB	30683	92642	12.49%	2.578%
13	6.763	917	931	943	rBV	133643	314354	42.37%	8.749%
14	7.495	1043	1051	1057	rBV5	4081	8134	1.10%	0.226%
15	7.604	1065	1069	1076	rVB2	3916	7848	1.06%	0.218%
16	7.988	1123	1132	1142	rBV	40232	78215	10.54%	2.177%
17	8.110	1142	1152	1161	rBV	57155	111213	14.99%	3.095%
18	8.653	1226	1241	1250	rBV	449403	741969	100.00%	20.651%
19	8.964	1287	1292	1299	rVB4	4696	8674	1.17%	0.241%
20	9.049	1299	1306	1311	rBV3	4460	7632	1.03%	0.212%
21	10.055	1465	1471	1478	rBV	289883	379934	51.21%	10.575%
22	11.079	1634	1639	1651	rBV	384359	489348	65.95%	13.620%
23	12.024	1789	1794	1803	rBV	275713	349030	47.04%	9.714%

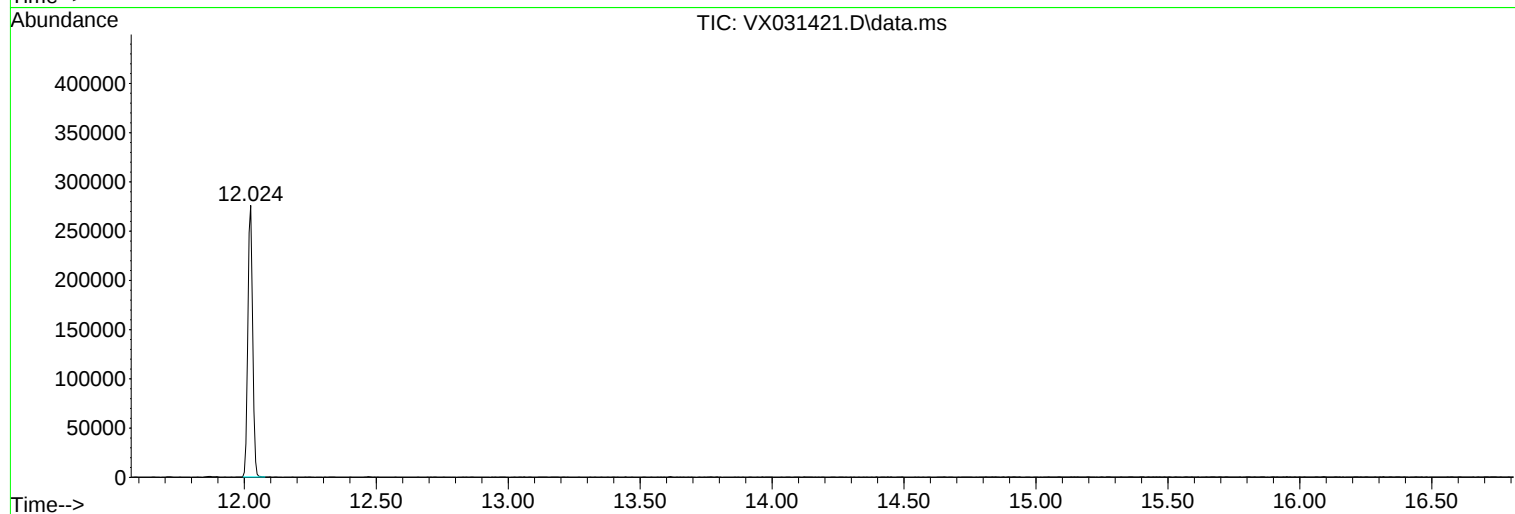
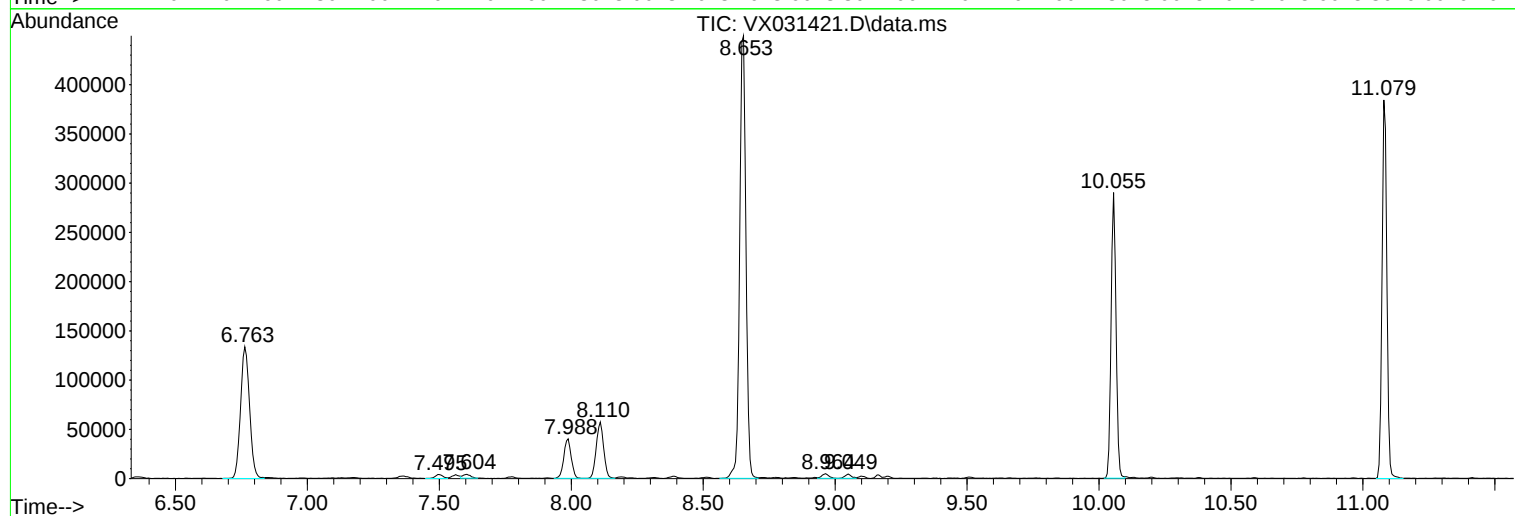
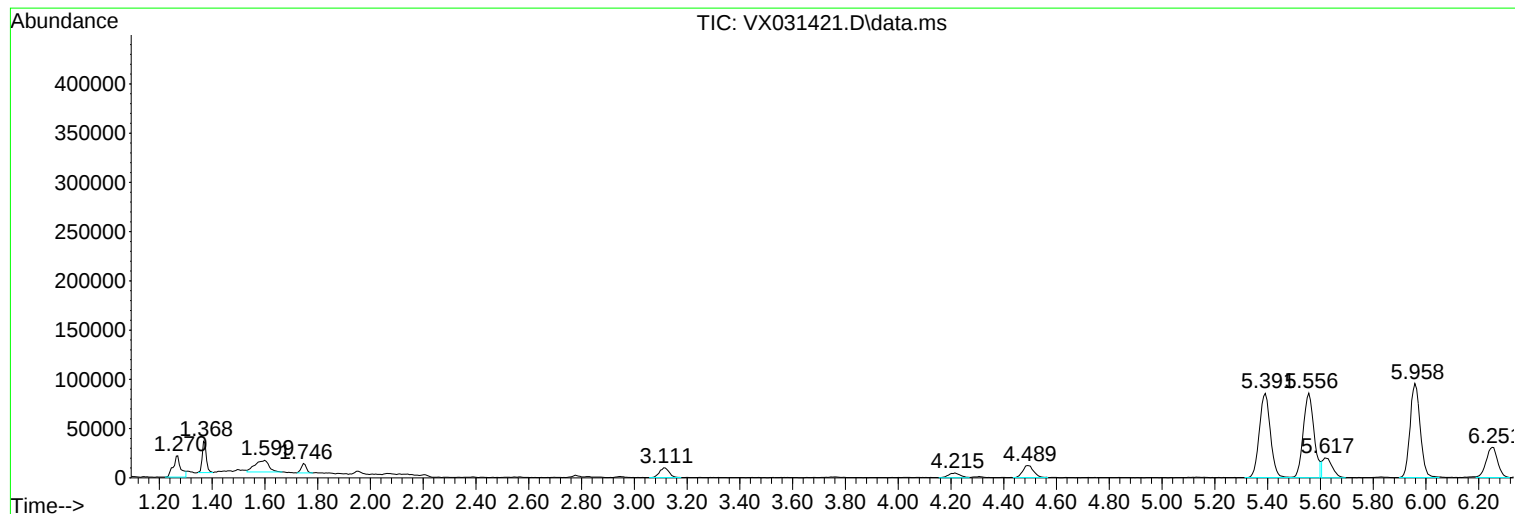
Sum of corrected areas: 3592910

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031421.D
Acq On : 16 Sep 2022 19:32
Operator : JC/MD
Sample : N4645-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031421.D
Acq On : 16 Sep 2022 19:32
Operator : JC/MD
Sample : N4645-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-04

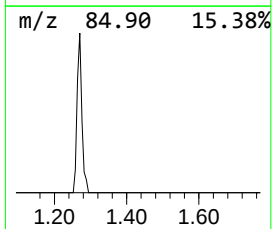
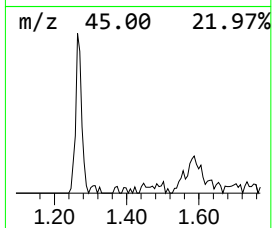
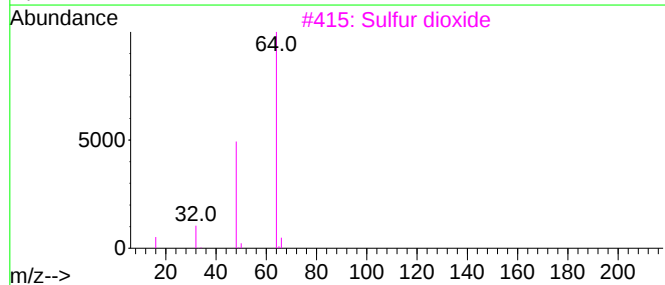
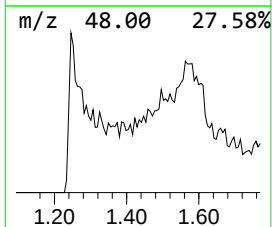
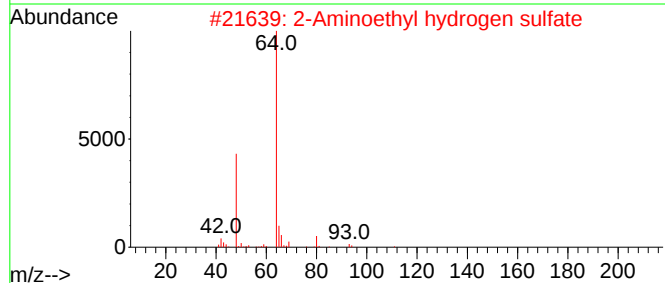
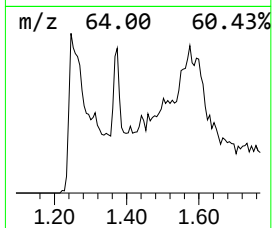
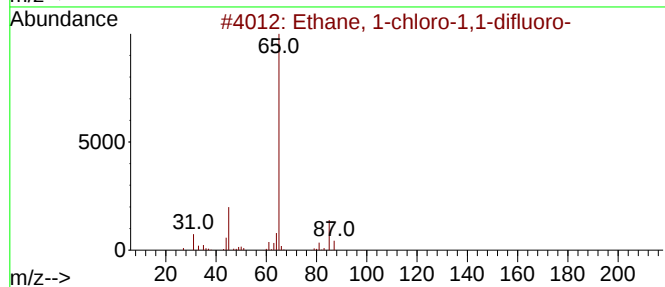
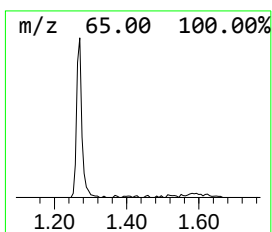
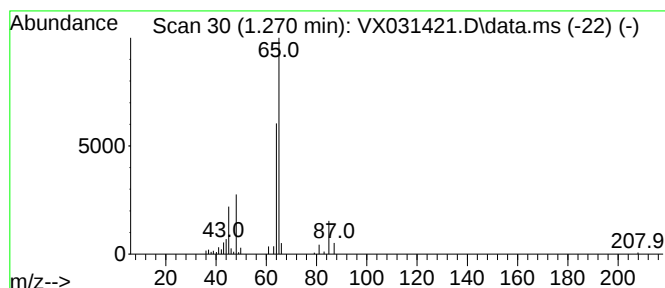
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown1.270 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	8.77 ug/l	42953	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	40
2			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	12
3			Sulfur dioxide	64	O2S	007446-09-5	10
4			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	10
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031421.D
Acq On : 16 Sep 2022 19:32
Operator : JC/MD
Sample : N4645-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-04

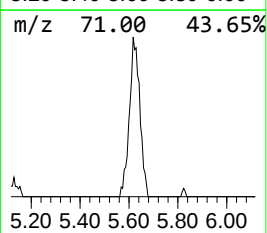
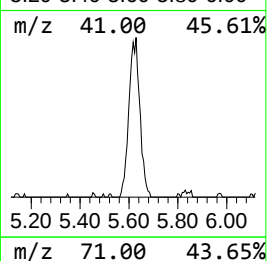
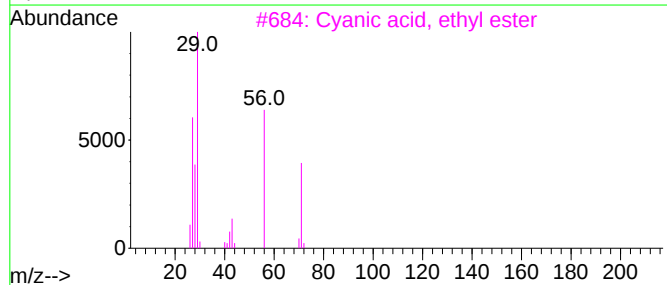
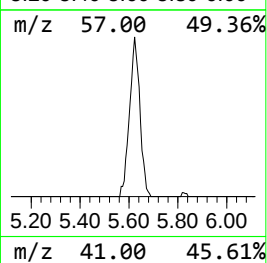
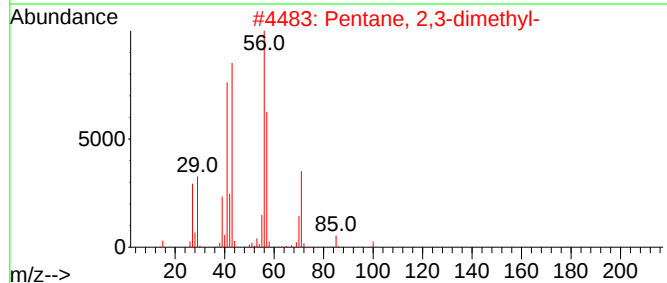
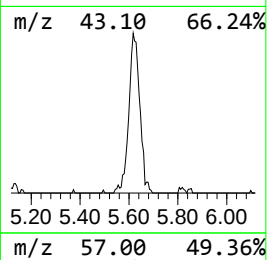
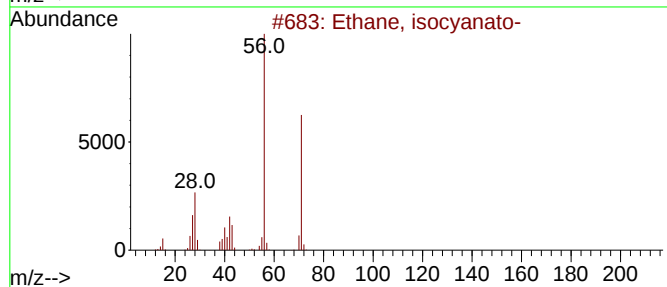
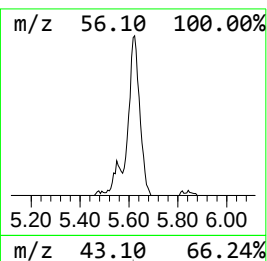
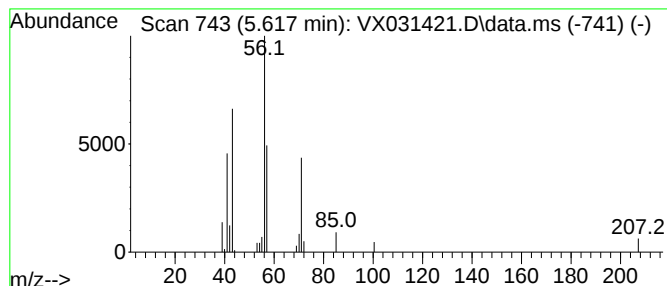
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 3 Ethane, isocyanato- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.617	9.96 ug/l	48780	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, isocyanato-	71	C3H5NO	000109-90-0	64
2			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	56
3			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	50
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
5			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031421.D
Acq On : 16 Sep 2022 19:32
Operator : JC/MD
Sample : N4645-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-04

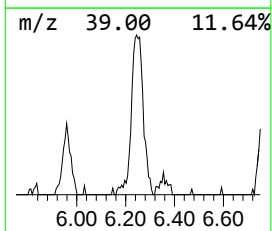
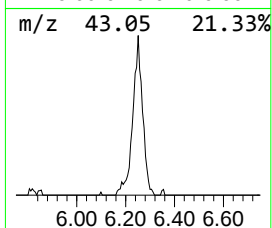
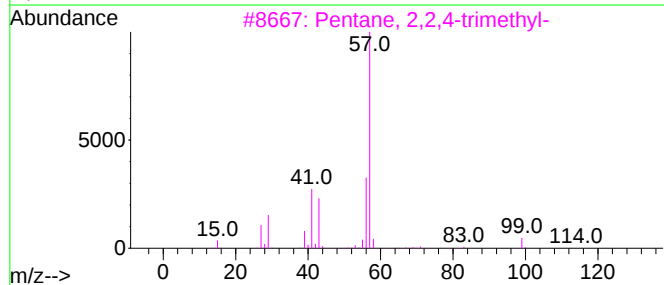
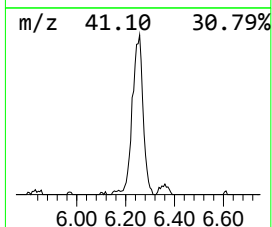
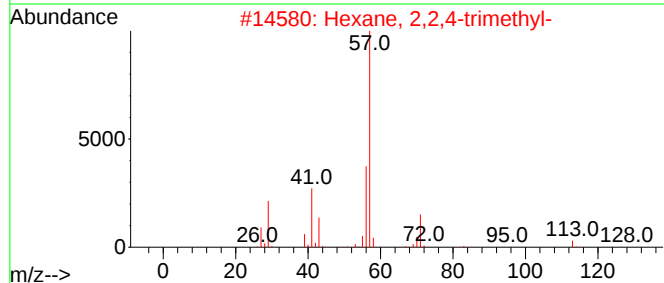
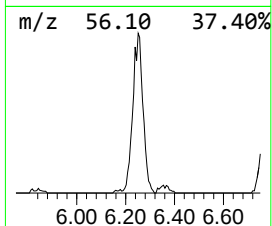
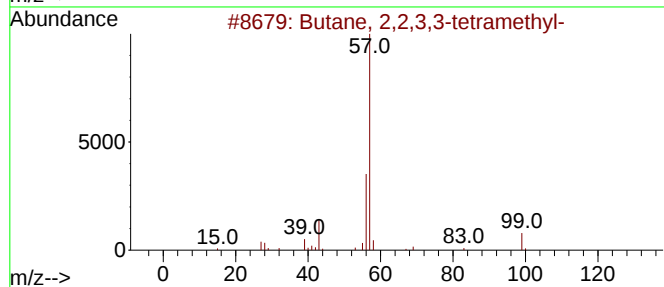
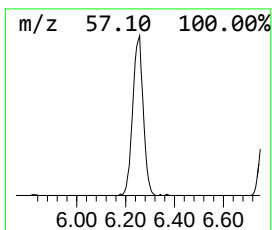
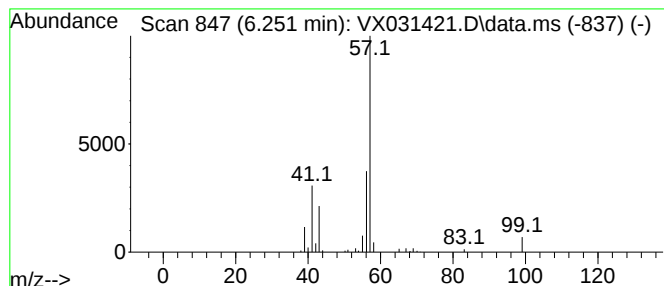
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 4 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	14.74 ug/l	92642	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	59
4			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031421.D
Acq On : 16 Sep 2022 19:32
Operator : JC/MD
Sample : N4645-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-04

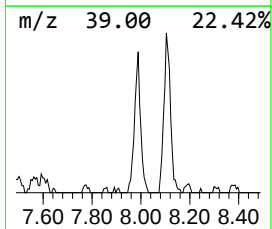
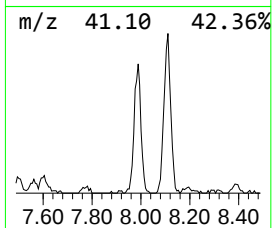
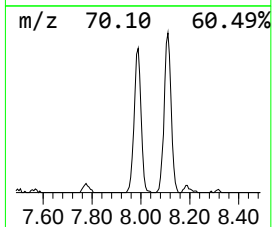
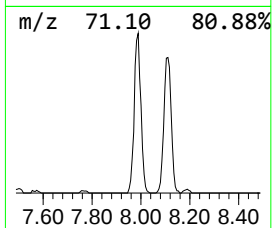
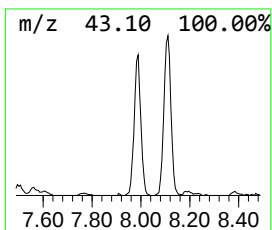
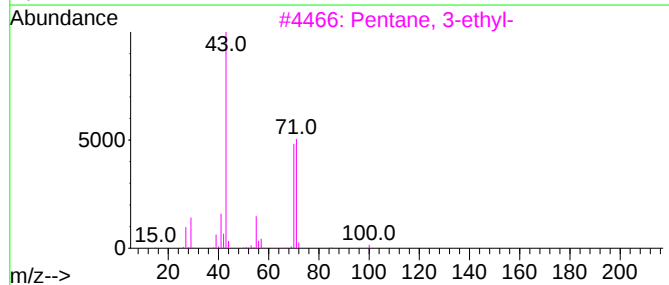
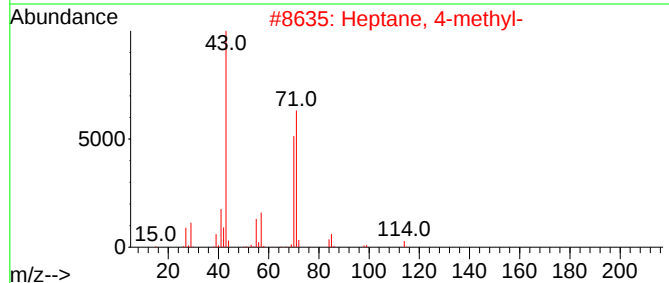
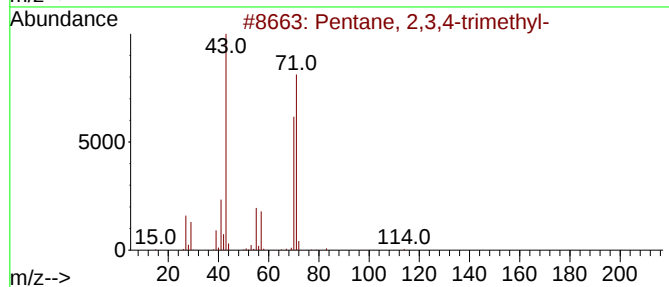
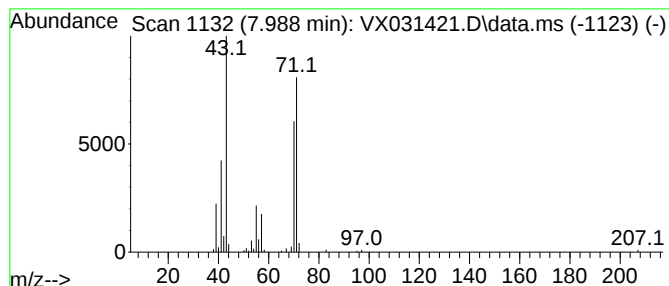
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	12.44 ug/l	78215	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	78
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	78
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	72
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031421.D
Acq On : 16 Sep 2022 19:32
Operator : JC/MD
Sample : N4645-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-04

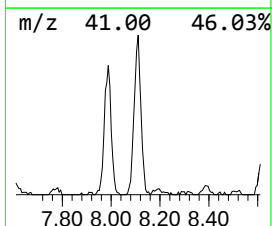
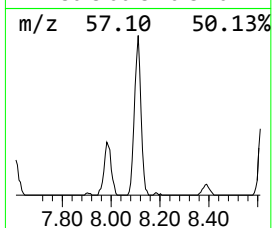
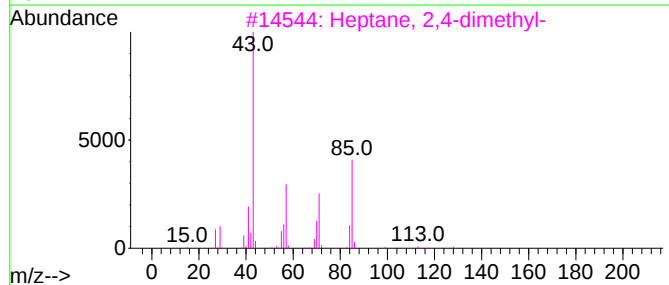
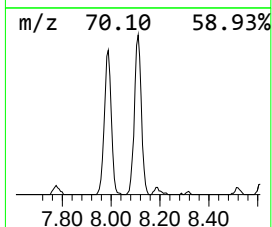
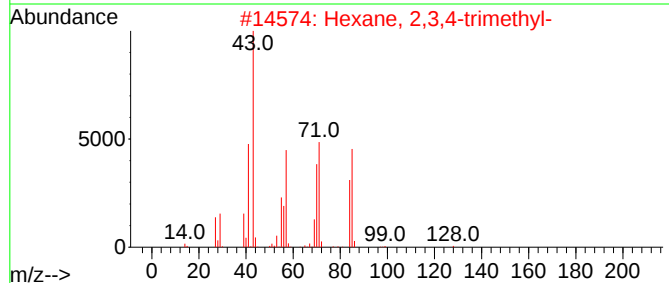
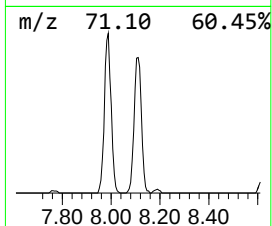
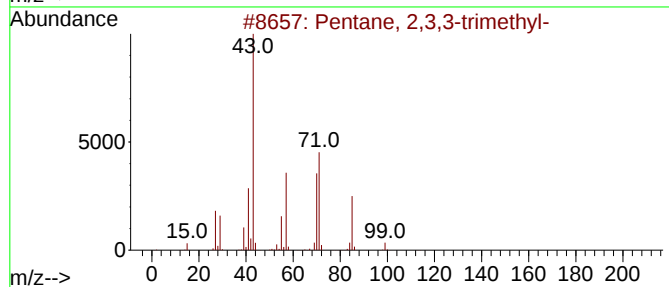
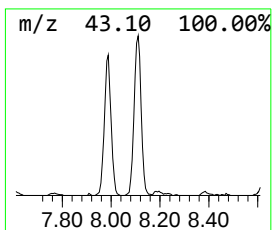
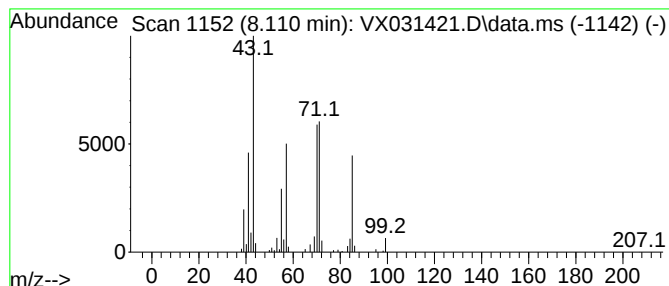
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 6 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	17.69 ug/l	111213	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	72
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031421.D
Acq On : 16 Sep 2022 19:32
Operator : JC/MD
Sample : N4645-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.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
unknown1.270	1.270	8.8	ug/l	42953	1	5.556	244833	50.0
Ethane, isocyan...	5.617	10.0	ug/l	48780	1	5.556	244833	50.0
Butane, 2,2,3,3...	6.251	14.7	ug/l	92642	2	6.763	314354	50.0
Pentane, 2,3,4-...	7.988	12.4	ug/l	78215	2	6.763	314354	50.0
Pentane, 2,3,3-...	8.110	17.7	ug/l	111213	2	6.763	314354	50.0