

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
 Data File : VX031424.D
 Acq On : 16 Sep 2022 20:42
 Operator : JC/MD
 Sample : N4645-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TOLL-MW-07

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: VX031424.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	23	30	42	rBV3	20975	84912	11.99%	2.607%
2	1.569	74	79	80	rBV2	7952	12086	1.71%	0.371%
3	3.117	325	333	343	rBV2	12548	28219	3.98%	0.866%
4	5.391	694	706	721	rBV	82854	239608	33.82%	7.357%
5	5.556	721	733	743	rBV	84320	240145	33.90%	7.373%
6	5.958	787	799	811	rBV	93466	242426	34.22%	7.443%
7	6.251	835	847	859	rBV2	30439	89826	12.68%	2.758%
8	6.763	921	931	944	rBV	129724	306186	43.22%	9.401%
9	7.988	1124	1132	1141	rVB	25902	52054	7.35%	1.598%
10	8.110	1141	1152	1160	rBV	34906	69088	9.75%	2.121%
11	8.653	1228	1241	1250	rBV	454337	708458	100.00%	21.752%
12	10.055	1465	1471	1483	rBV	282567	372315	52.55%	11.431%
13	11.079	1634	1639	1646	rBV	361551	470201	66.37%	14.437%
14	12.024	1789	1794	1803	rBV	278673	341478	48.20%	10.484%

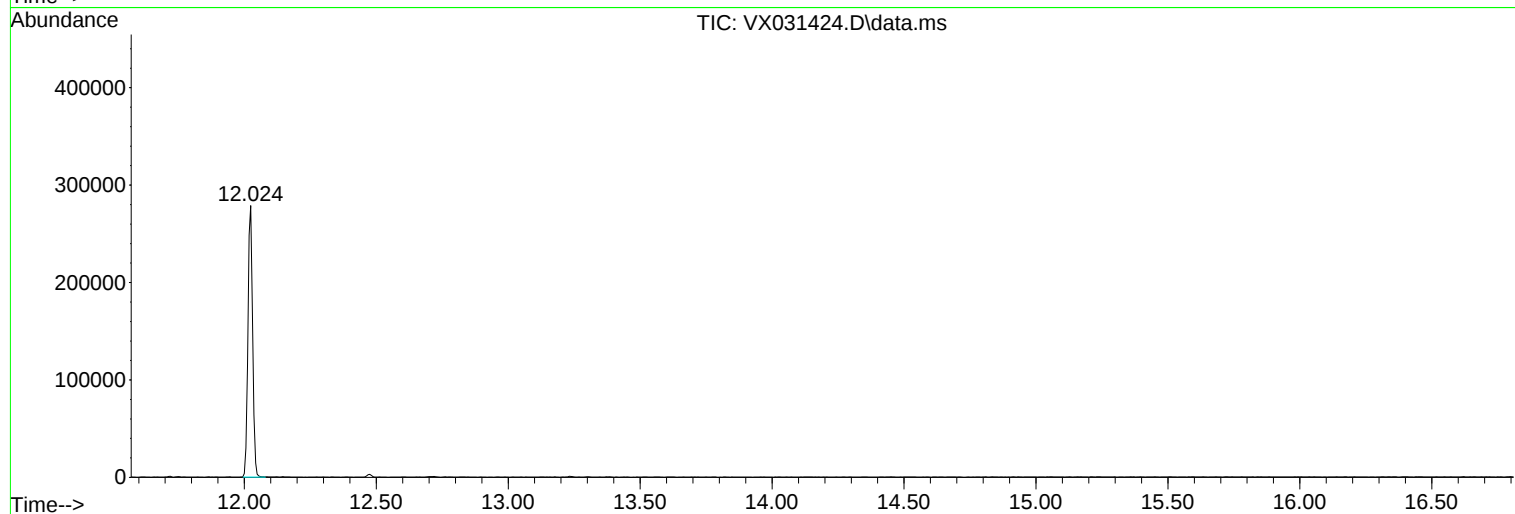
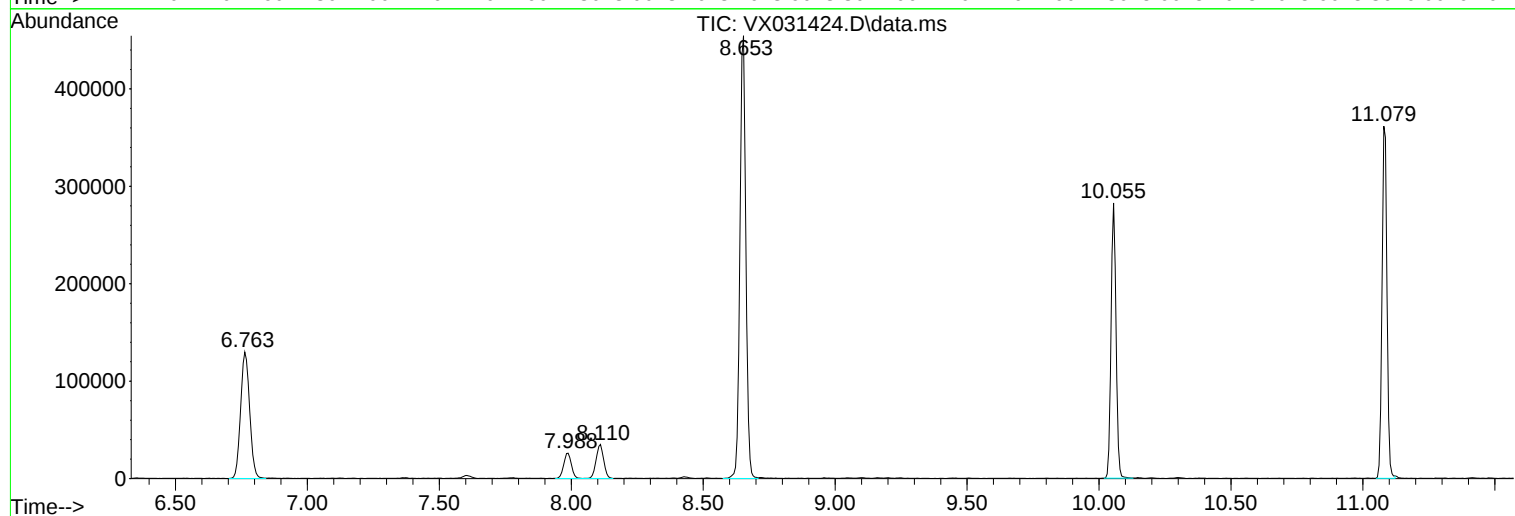
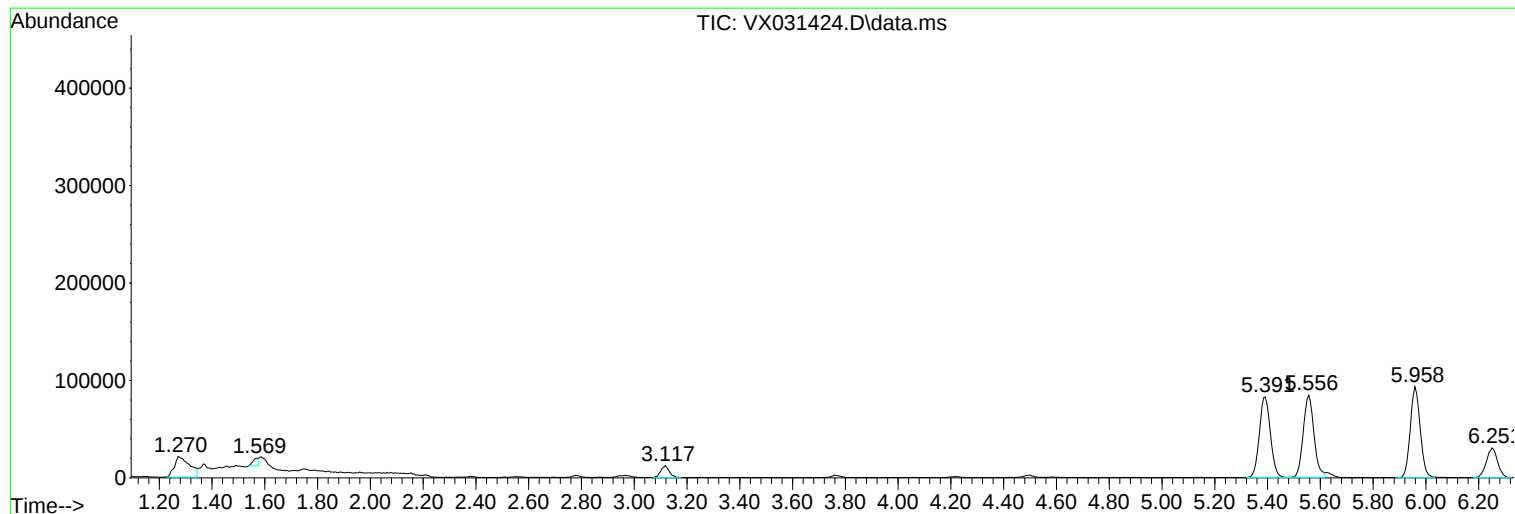
Sum of corrected areas: 3257002

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031424.D
Acq On : 16 Sep 2022 20:42
Operator : JC/MD
Sample : N4645-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-07

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 : VX031424.D
Acq On : 16 Sep 2022 20:42
Operator : JC/MD
Sample : N4645-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-07

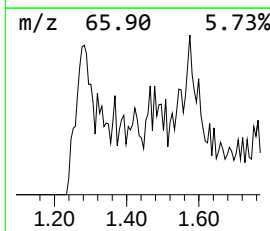
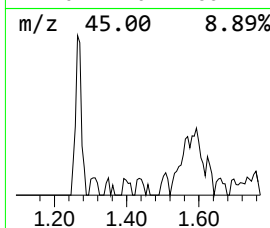
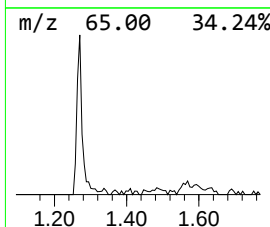
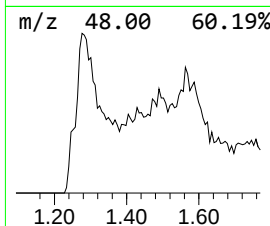
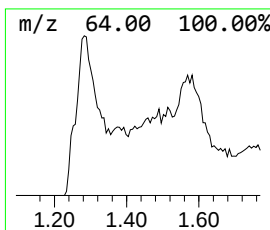
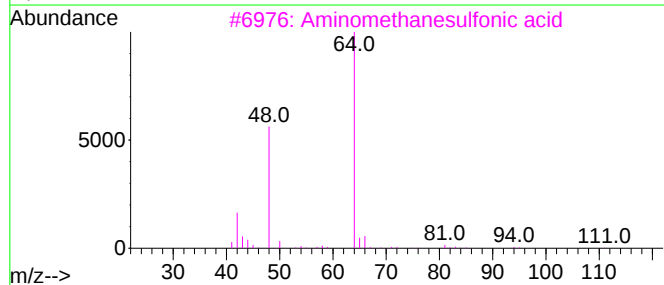
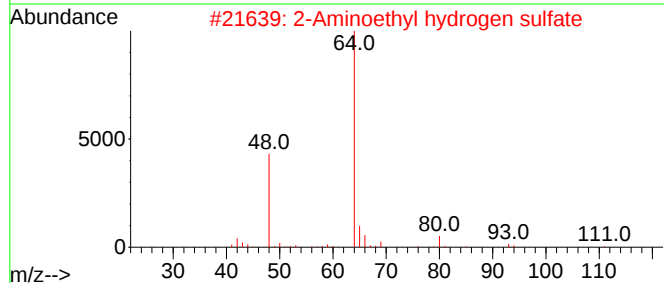
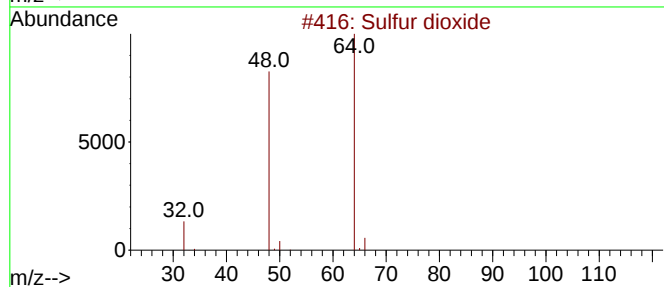
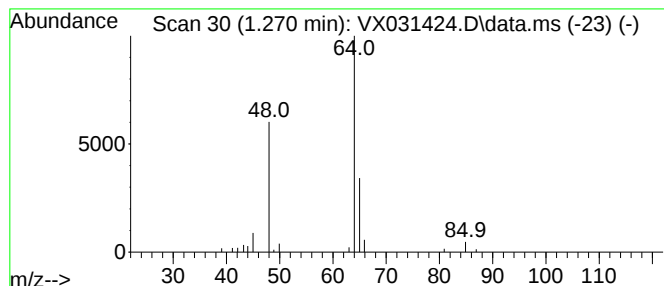
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	17.68 ug/l	84912	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	78
2			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	78
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031424.D
Acq On : 16 Sep 2022 20:42
Operator : JC/MD
Sample : N4645-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-07

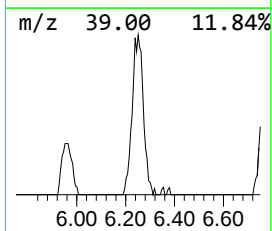
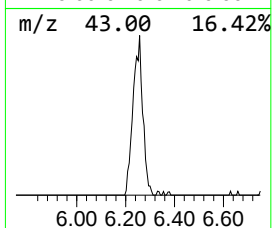
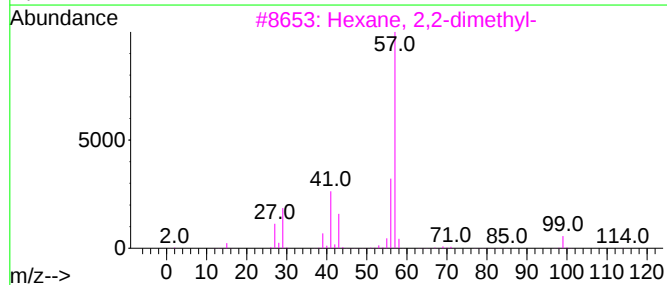
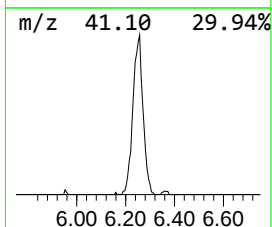
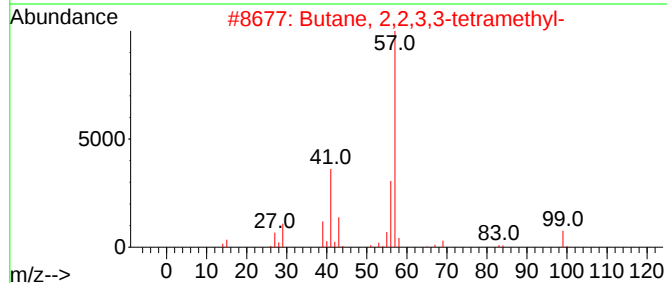
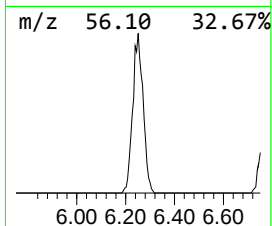
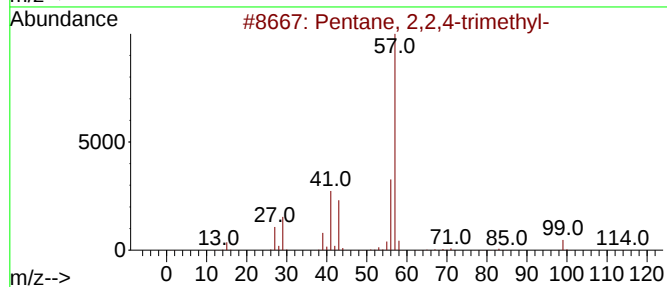
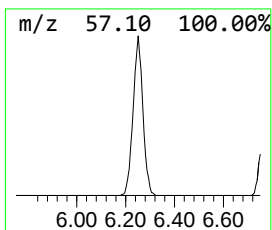
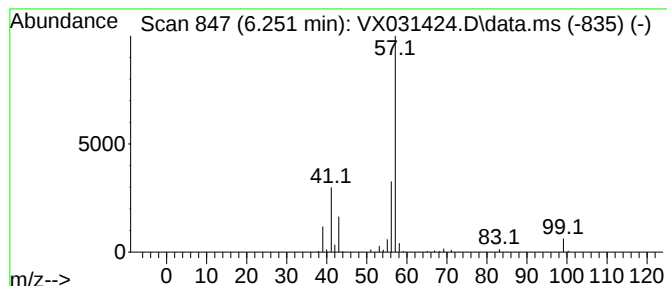
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	14.67 ug/l	89826	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	59
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031424.D
Acq On : 16 Sep 2022 20:42
Operator : JC/MD
Sample : N4645-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-07

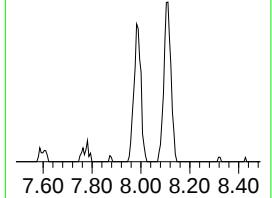
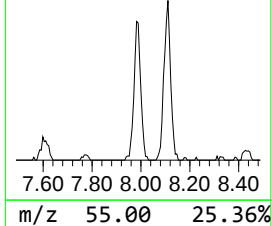
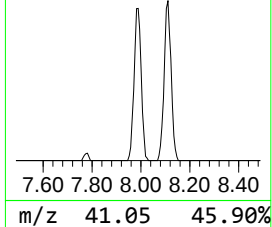
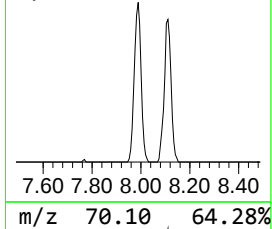
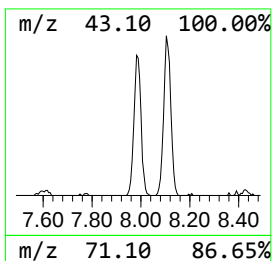
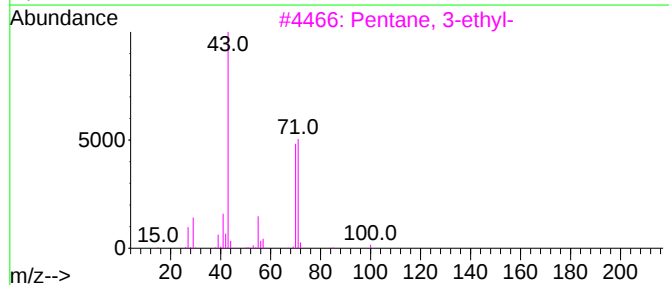
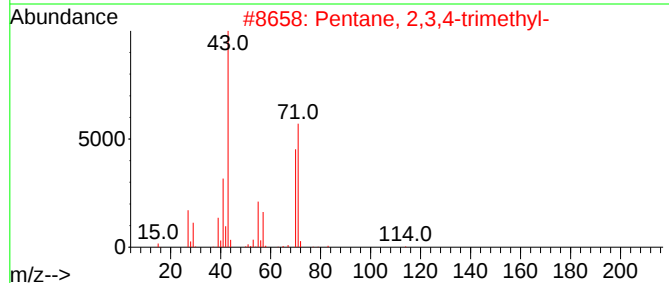
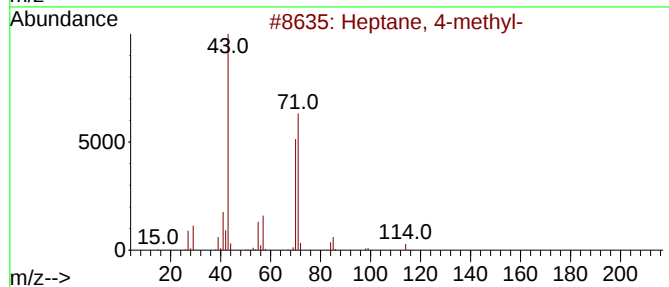
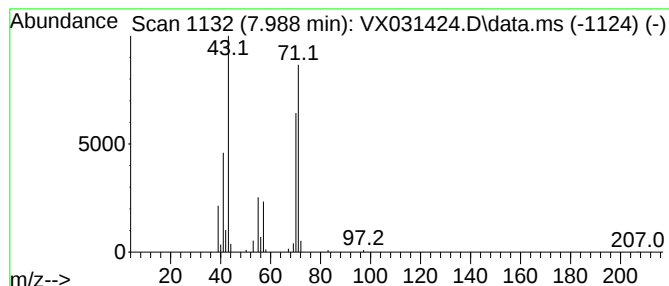
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

Peak Number 3 Heptane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	8.50 ug/l	52054	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
2			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031424.D
Acq On : 16 Sep 2022 20:42
Operator : JC/MD
Sample : N4645-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-07

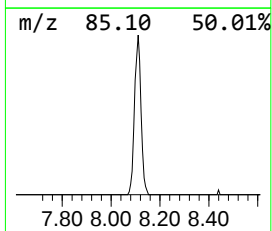
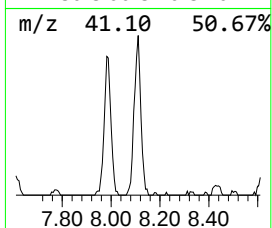
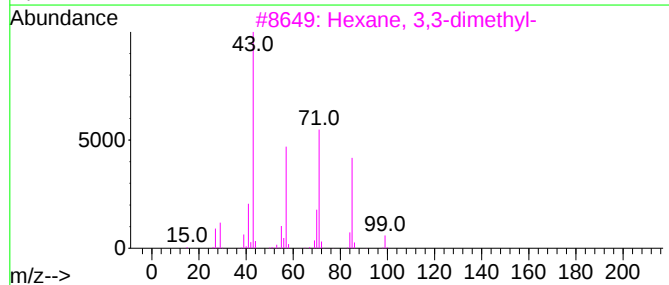
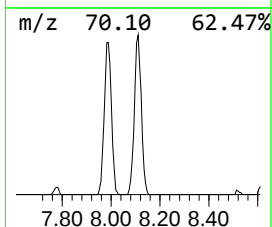
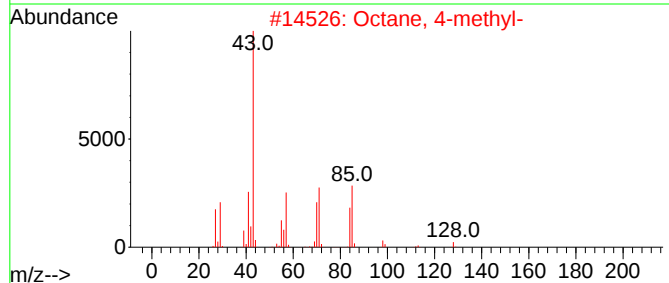
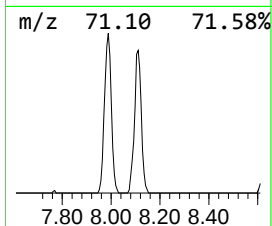
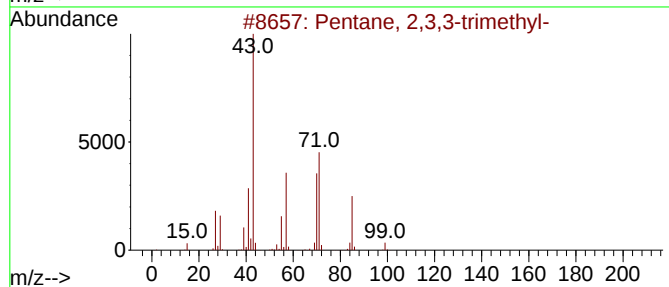
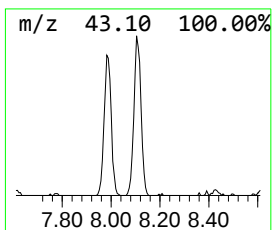
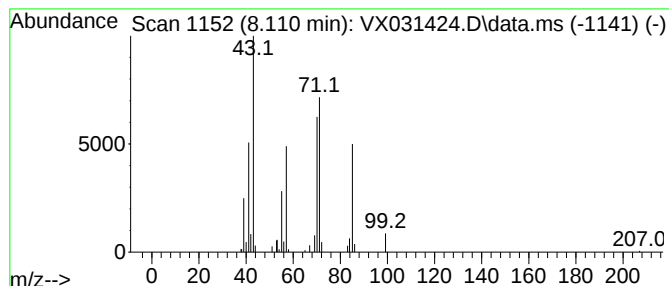
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091422W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	11.28 ug/l	69088	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	90
2			Octane, 4-methyl-	128	C9H20	002216-34-4	72
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4			Heptane, 4-methyl-	114	C8H18	000589-53-7	53
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091622\
Data File : VX031424.D
Acq On : 16 Sep 2022 20:42
Operator : JC/MD
Sample : N4645-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TOLL-MW-07

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
Sulfur dioxide	1.270	17.7	ug/l	84912	1	5.556	240145	50.0
Pentane, 2,2,4-...	6.251	14.7	ug/l	89826	2	6.763	306186	50.0
Heptane, 4-methyl-	7.988	8.5	ug/l	52054	2	6.763	306186	50.0
Pentane, 2,3,3-...	8.110	11.3	ug/l	69088	2	6.763	306186	50.0