

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
 Data File : VN071382.D
 Acq On : 18 Mar 2022 19:07
 Operator : JC\MD
 Sample : N2015-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 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_N\methods\82N030722W.M
 Title : SW846 8260

Signal : TIC: VN071382.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	35	41	44	rBV	175815	352366	8.14%	1.211%
2	2.263	44	47	61	rVB2	274659	706203	16.31%	2.426%
3	2.434	72	76	85	rVB2	128273	211143	4.88%	0.725%
4	3.122	187	193	204	rVB3	37156	97990	2.26%	0.337%
5	5.616	604	617	631	rBV3	61662	217635	5.03%	0.748%
6	7.045	847	860	874	rBV3	55906	184142	4.25%	0.633%
7	7.328	897	908	918	rBV	92608	251437	5.81%	0.864%
8	8.022	1014	1026	1031	rBV	517657	1280160	29.57%	4.398%
9	8.081	1031	1036	1044	rVV	1000216	2252757	52.04%	7.740%
10	8.175	1044	1052	1064	rVB	296505	743289	17.17%	2.554%
11	8.434	1087	1096	1111	rBV	599021	1375385	31.77%	4.726%
12	8.616	1111	1127	1138	rBV	511603	1395045	32.22%	4.793%
13	8.963	1178	1186	1198	rBV	1500479	3106139	71.75%	10.672%
14	9.457	1255	1270	1275	rBV5	60777	181112	4.18%	0.622%
15	9.510	1275	1279	1286	rVB3	40780	76514	1.77%	0.263%
16	9.592	1286	1293	1299	rBV2	45705	92840	2.14%	0.319%
17	9.728	1305	1316	1323	rVB8	15224	44962	1.04%	0.154%
18	9.881	1334	1342	1354	rVB	450568	888301	20.52%	3.052%
19	10.010	1354	1364	1378	rBV	608956	1255787	29.01%	4.315%
20	10.192	1389	1395	1402	rBV3	30376	64302	1.49%	0.221%
21	10.369	1418	1425	1430	rBV	95003	173726	4.01%	0.597%
22	10.439	1430	1437	1451	rVB	2420116	4329145	100.00%	14.874%
23	10.639	1461	1471	1478	rVB6	48234	113211	2.62%	0.389%
24	10.710	1478	1483	1491	rVB2	44067	79231	1.83%	0.272%
25	10.875	1503	1511	1519	rVB7	33060	105938	2.45%	0.364%
26	11.739	1649	1658	1678	rBV	2120639	3840810	88.72%	13.196%
27	12.727	1817	1826	1837	rBV	1730130	2913581	67.30%	10.010%
28	13.669	1977	1986	1998	rBV	1638054	2772183	64.04%	9.525%

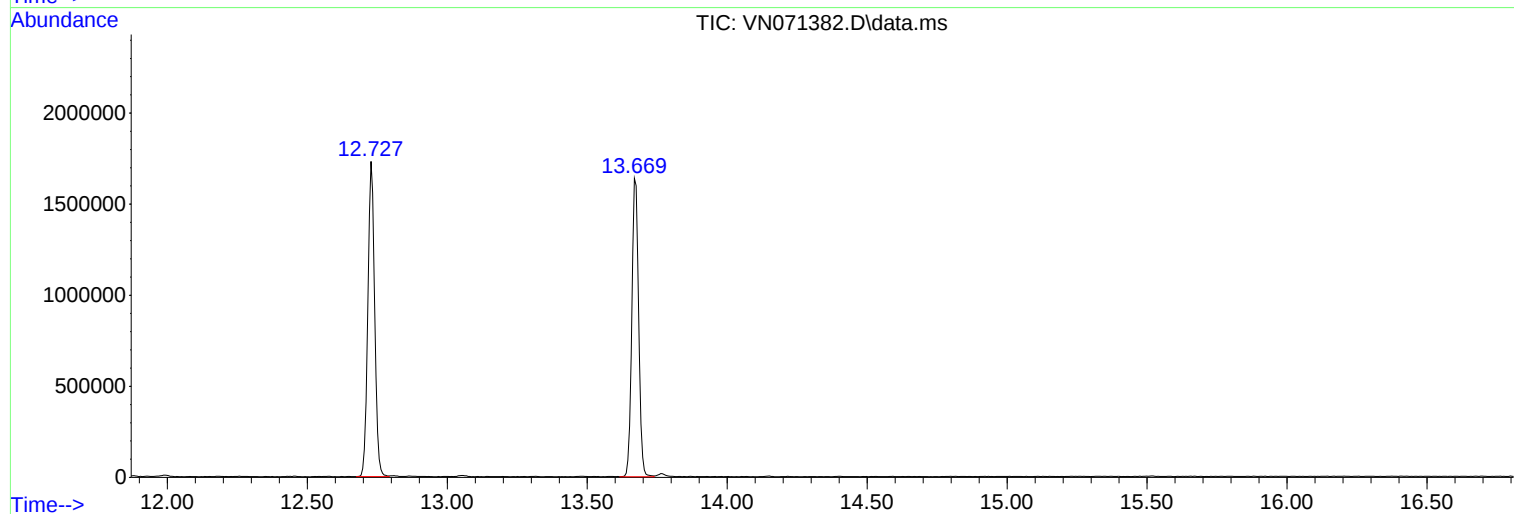
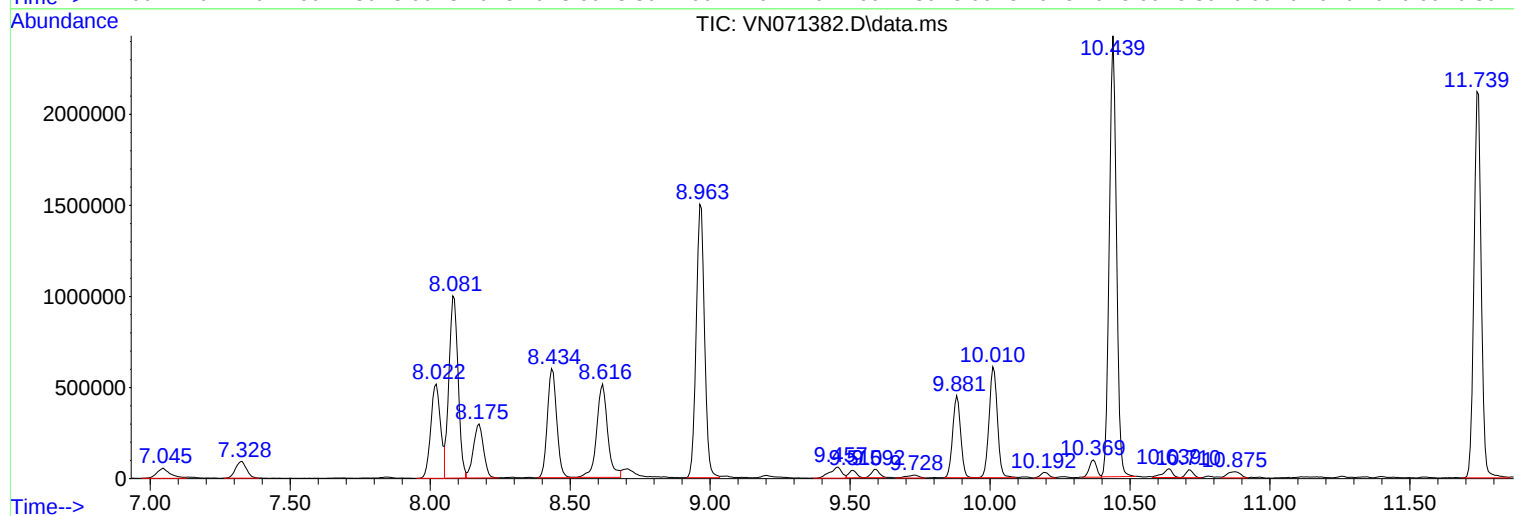
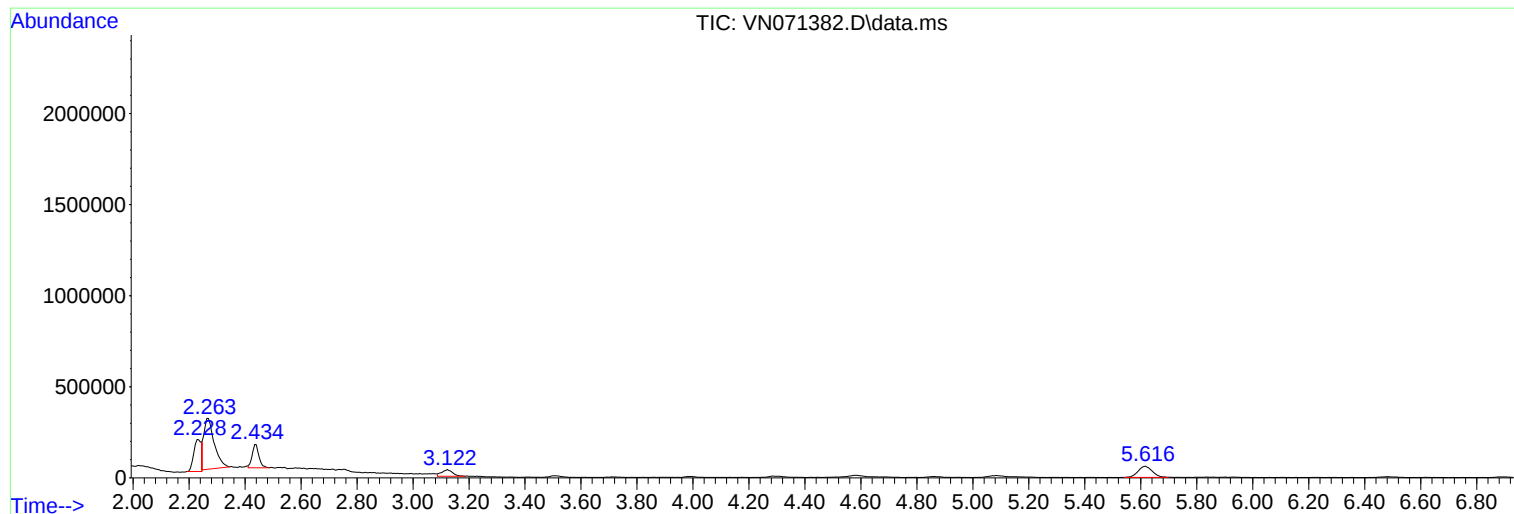
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ALS Vial : 21 Sample Multiplier: 1

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ClientSampleId :
TOLL-MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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



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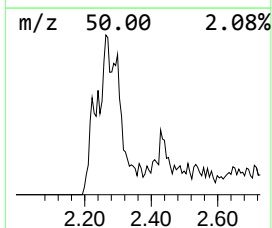
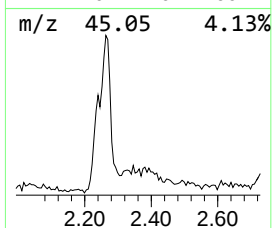
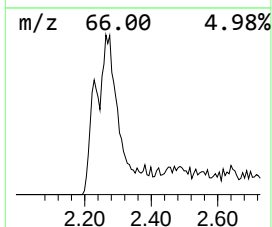
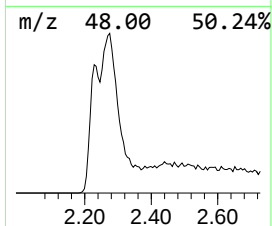
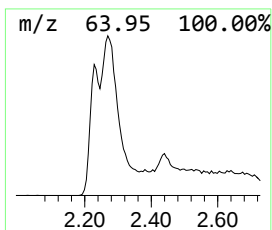
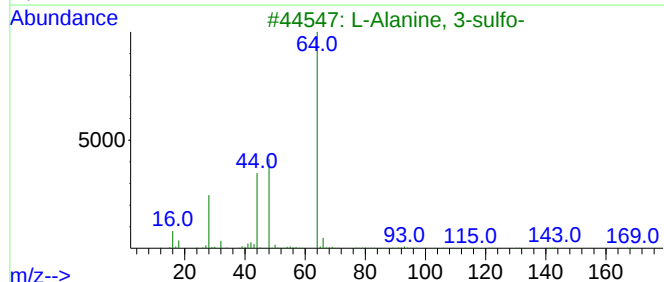
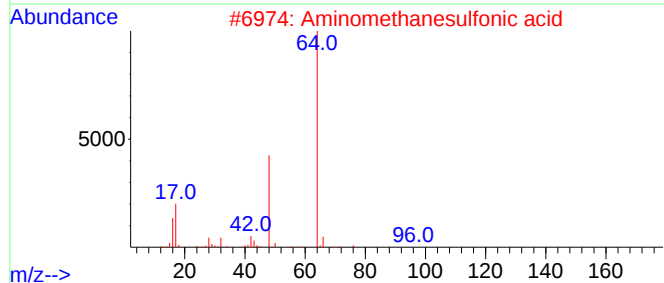
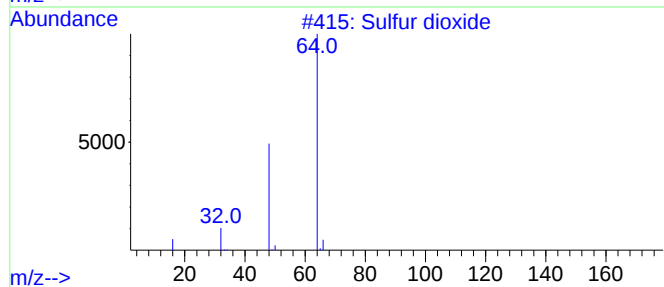
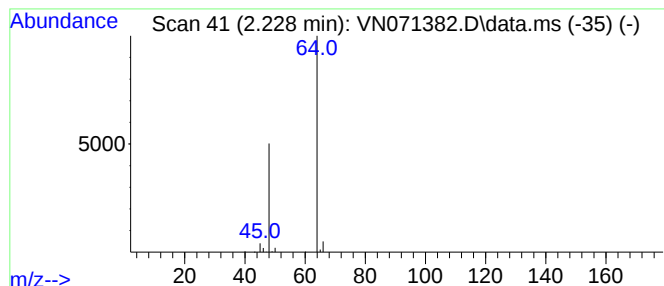
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	7.82 ug/l	352366	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
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



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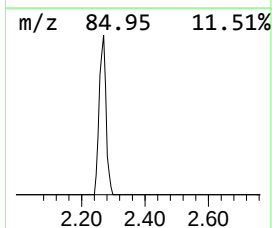
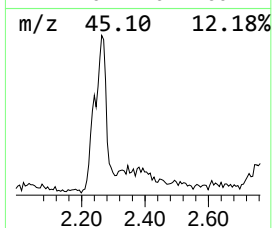
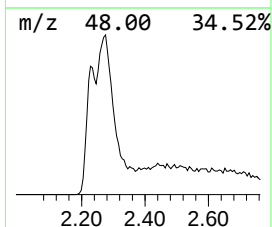
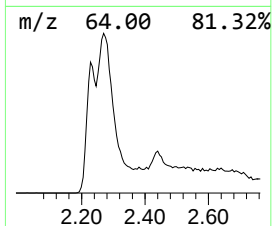
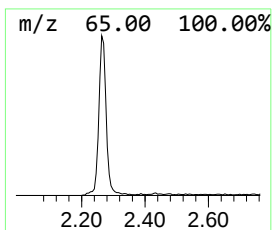
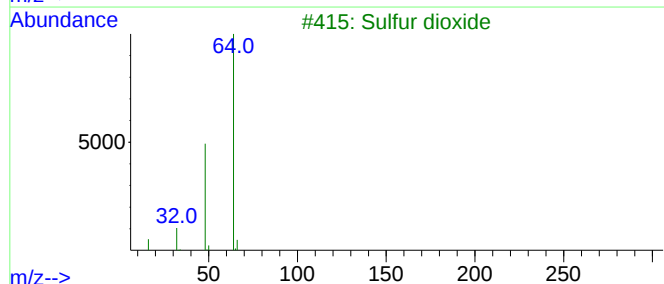
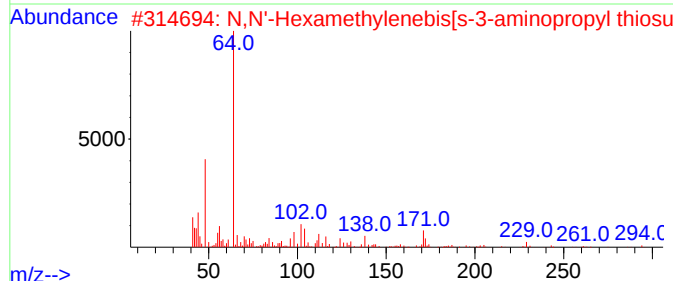
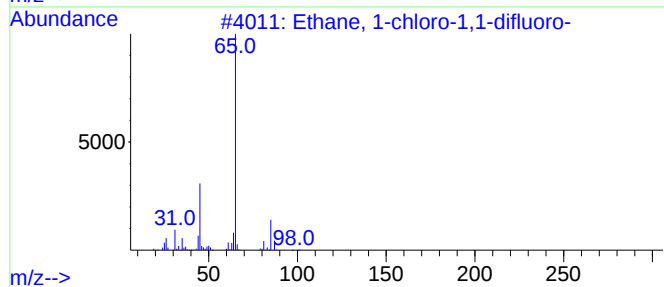
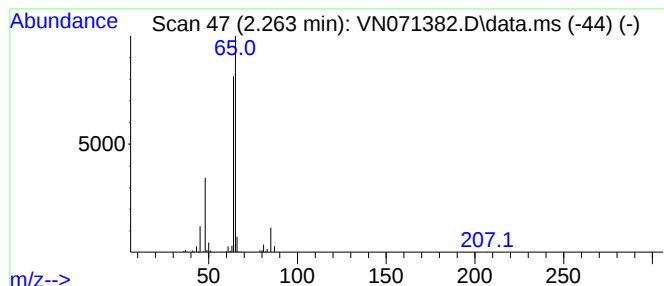
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.263 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	15.67 ug/l	706203	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	38
2			N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	32
3			Sulfur dioxide	64	O2S	007446-09-5	32
4			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	23
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	23



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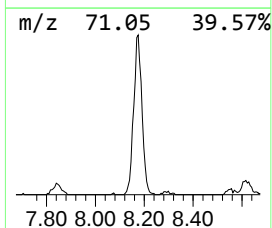
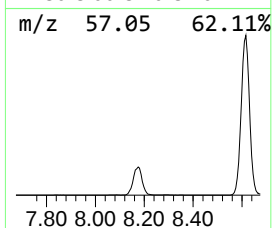
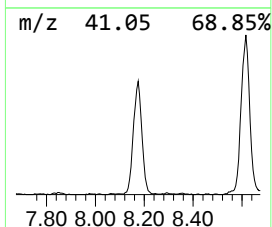
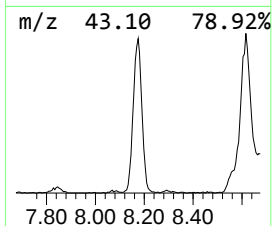
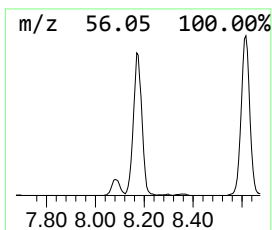
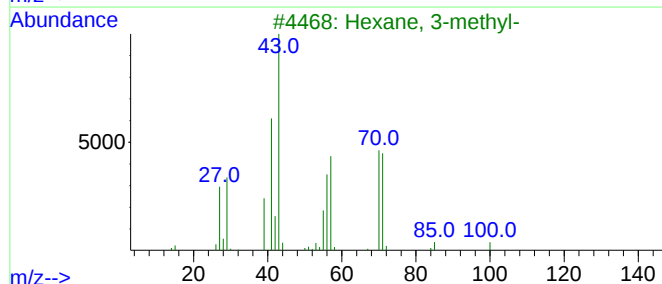
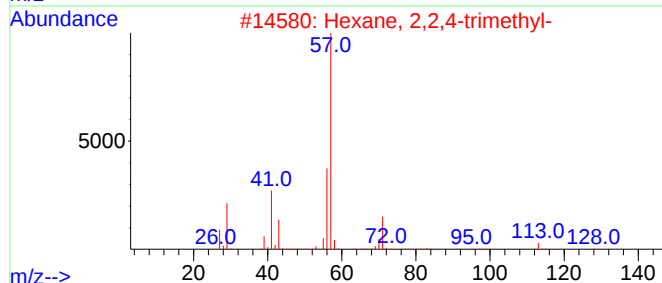
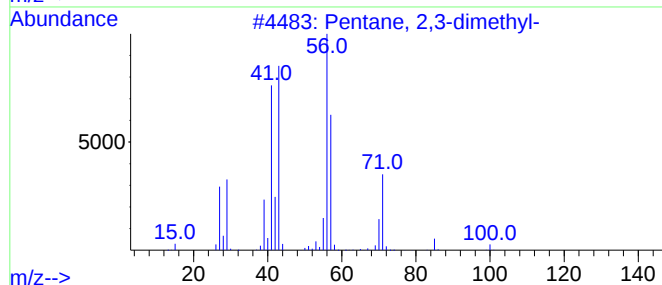
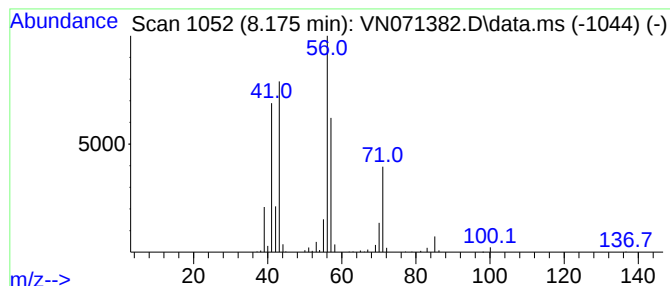
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	16.50 ug/l	743289	Pentafluorobenzene	8.087

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	38
4			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	38
5			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	38



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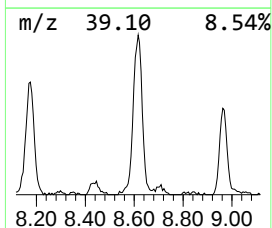
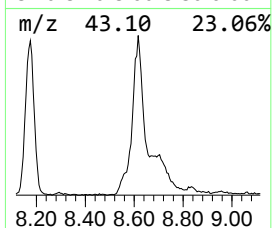
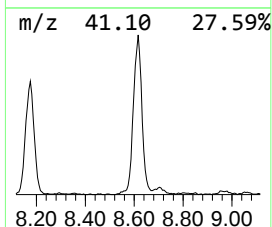
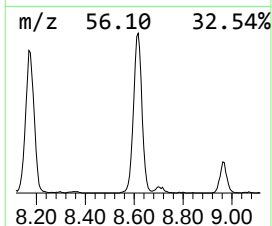
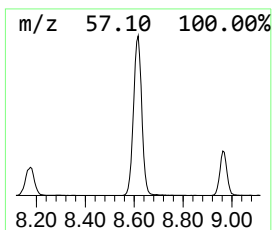
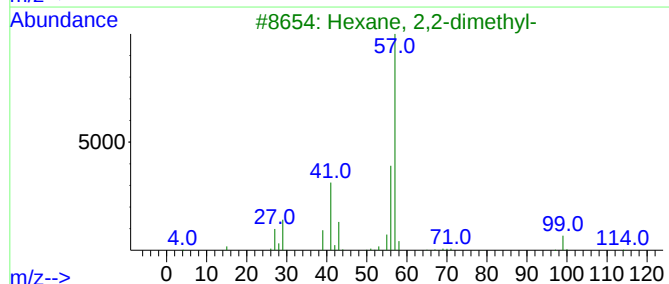
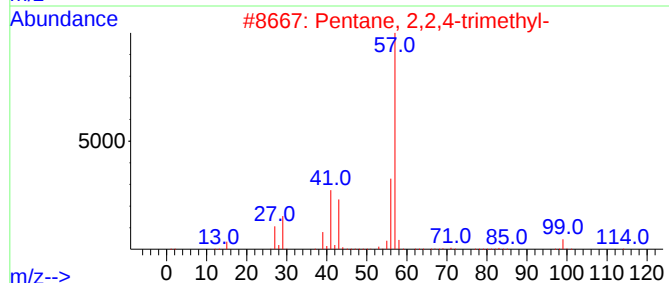
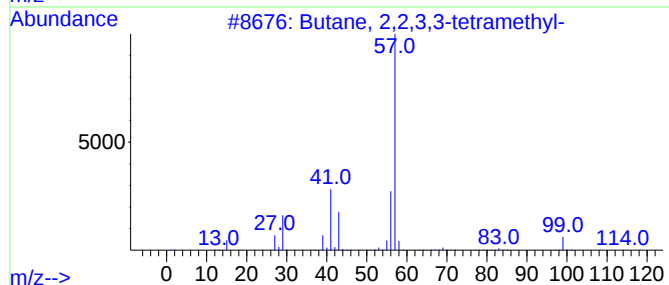
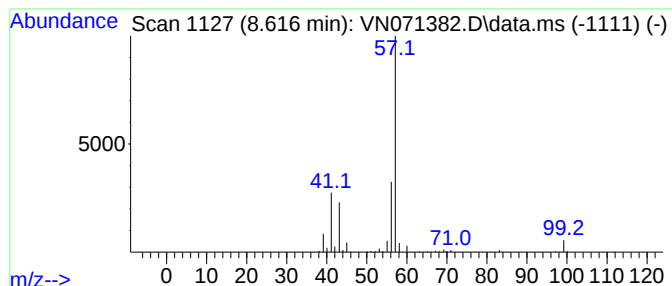
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Peak Number 4 Butane, 2,2,3,3-tetramethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	22.46 ug/l	1395050	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	64
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	53
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	53



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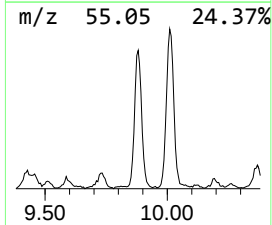
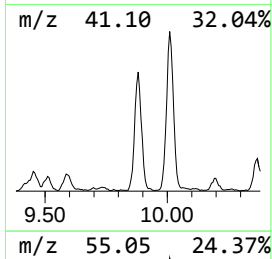
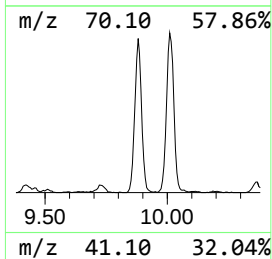
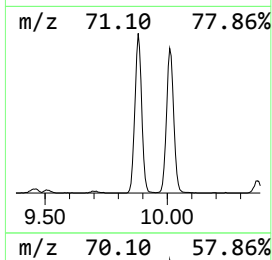
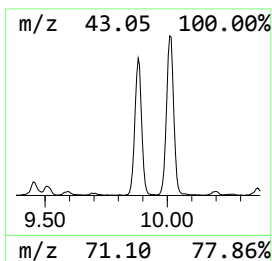
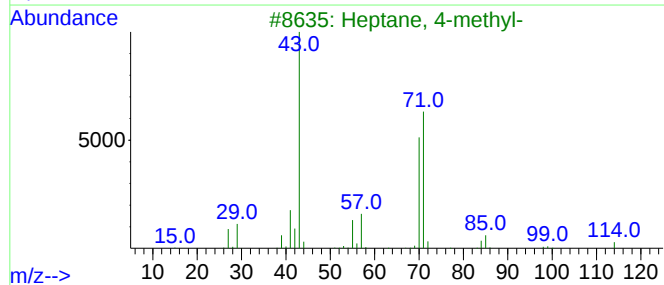
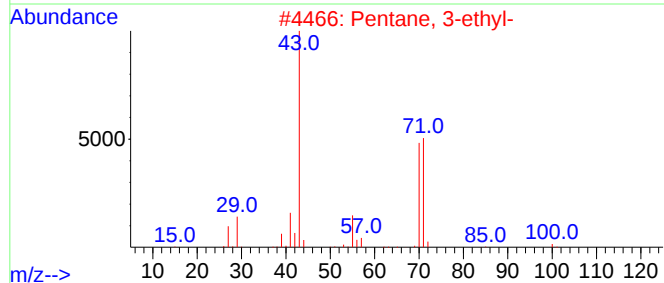
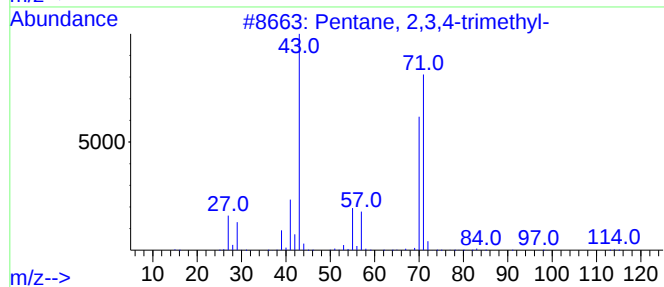
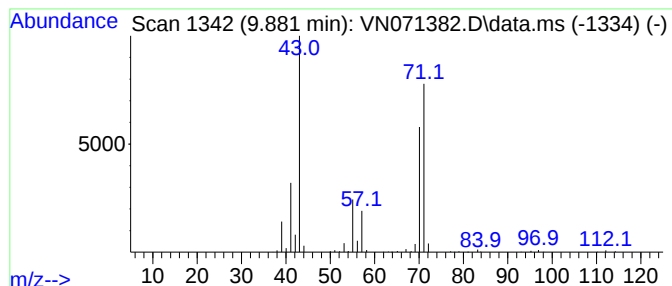
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.881	14.30 ug/l	888301	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	83
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	78



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TOLL-MW-04

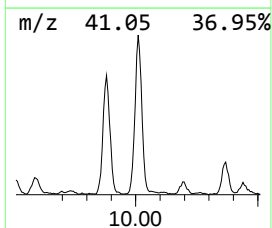
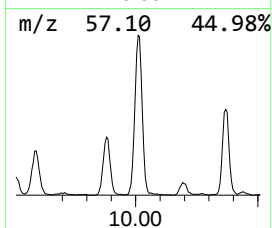
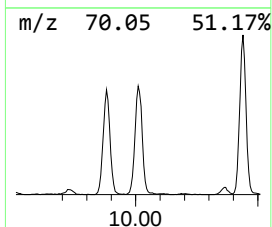
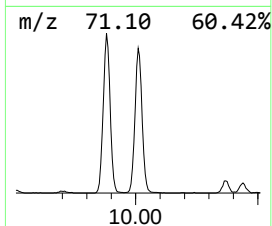
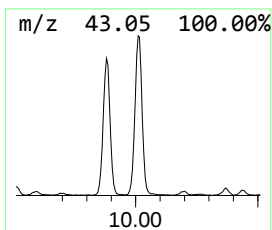
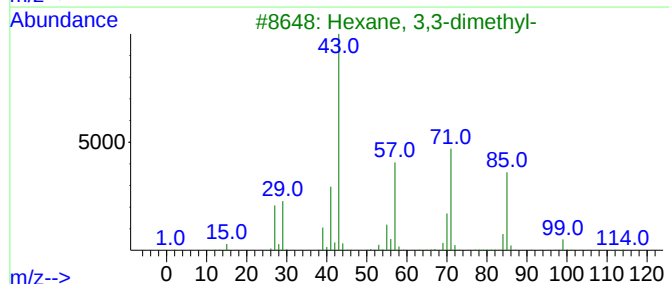
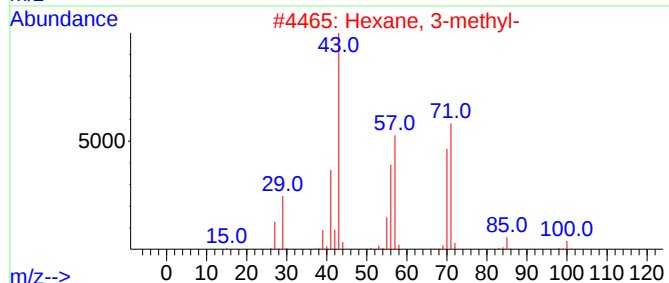
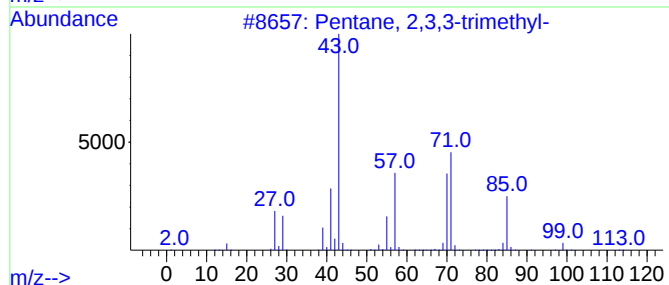
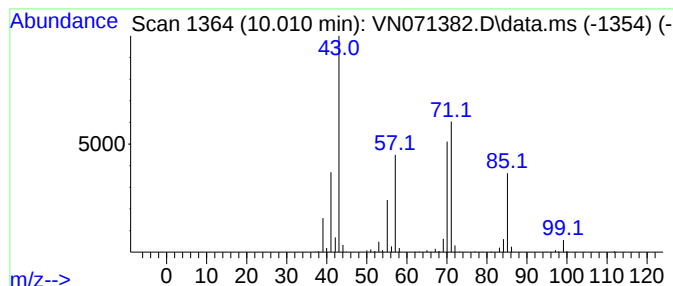
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	20.21 ug/l	1255790	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071382.D
Acq On : 18 Mar 2022 19:07
Operator : JC\MD
Sample : N2015-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-04

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.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	2.228	7.8	ug/l	352366	1	8.087	2252760	50.0
unknown2.263	2.263	15.7	ug/l	706203	1	8.087	2252760	50.0
Pentane, 2,3-di...	8.175	16.5	ug/l	743289	1	8.087	2252760	50.0
Butane, 2,2,3,3...	8.616	22.5	ug/l	1395050	2	8.969	3106140	50.0
Pentane, 2,3,4-...	9.881	14.3	ug/l	888301	2	8.969	3106140	50.0
Pentane, 2,3,3-...	10.010	20.2	ug/l	1255790	2	8.969	3106140	50.0