

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
 Data File : VN071381.D
 Acq On : 18 Mar 2022 18:43
 Operator : JC\MD
 Sample : N2015-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-03

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: VN071381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.234	35	42	44	rBV	225740	429608	4.91%	0.836%
2	2.263	44	47	63	rVB	264631	716210	8.18%	1.394%
3	2.434	71	76	85	rVB	207468	339527	3.88%	0.661%
4	3.128	188	194	202	rVB2	70787	168859	1.93%	0.329%
5	5.081	513	526	539	rBV2	62678	250127	2.86%	0.487%
6	5.616	603	617	632	rBV3	124523	446940	5.11%	0.870%
7	7.045	847	860	874	rBV2	581938	1776225	20.30%	3.456%
8	7.322	898	907	918	rVB4	38940	111112	1.27%	0.216%
9	7.845	988	996	1008	rVB3	38887	109619	1.25%	0.213%
10	8.022	1013	1026	1031	rBV	493871	1230586	14.06%	2.394%
11	8.086	1031	1037	1044	rVV	968088	2195406	25.09%	4.272%
12	8.175	1044	1052	1063	rVB	1192930	2930963	33.49%	5.703%
13	8.433	1088	1096	1109	rBV	569013	1308930	14.96%	2.547%
14	8.616	1109	1127	1138	rBV	3587104	8751353	100.00%	17.028%
15	8.704	1138	1142	1154	rVB5	84842	218506	2.50%	0.425%
16	8.963	1177	1186	1199	rBV	1437744	3064015	35.01%	5.962%
17	9.457	1257	1270	1275	rBV3	334134	859205	9.82%	1.672%
18	9.510	1275	1279	1286	rVV	152504	295610	3.38%	0.575%
19	9.592	1286	1293	1305	rVV	255825	534907	6.11%	1.041%
20	9.728	1305	1316	1324	rVV3	86447	240448	2.75%	0.468%
21	9.880	1334	1342	1353	rVB	2270294	4407870	50.37%	8.577%
22	10.010	1355	1364	1378	rVV	2775890	5670465	64.80%	11.033%
23	10.198	1389	1396	1403	rBV3	88403	173764	1.99%	0.338%
24	10.369	1418	1425	1430	rBV	496546	885496	10.12%	1.723%
25	10.439	1430	1437	1451	rVB	2349698	4275794	48.86%	8.320%
26	10.627	1458	1469	1477	rVB7	50852	174359	1.99%	0.339%
27	10.857	1502	1508	1511	rBV	116611	232362	2.66%	0.452%
28	11.127	1547	1554	1560	rBV3	47633	115686	1.32%	0.225%
29	11.739	1650	1658	1666	rBV	2056320	3711558	42.41%	7.222%
30	11.992	1693	1701	1711	rVB5	46101	113741	1.30%	0.221%
31	12.727	1815	1826	1835	rBV	1667797	2903269	33.18%	5.649%
32	13.668	1978	1986	1997	rBV	1540768	2649966	30.28%	5.156%
33	14.145	2061	2067	2074	rBV3	57290	101296	1.16%	0.197%

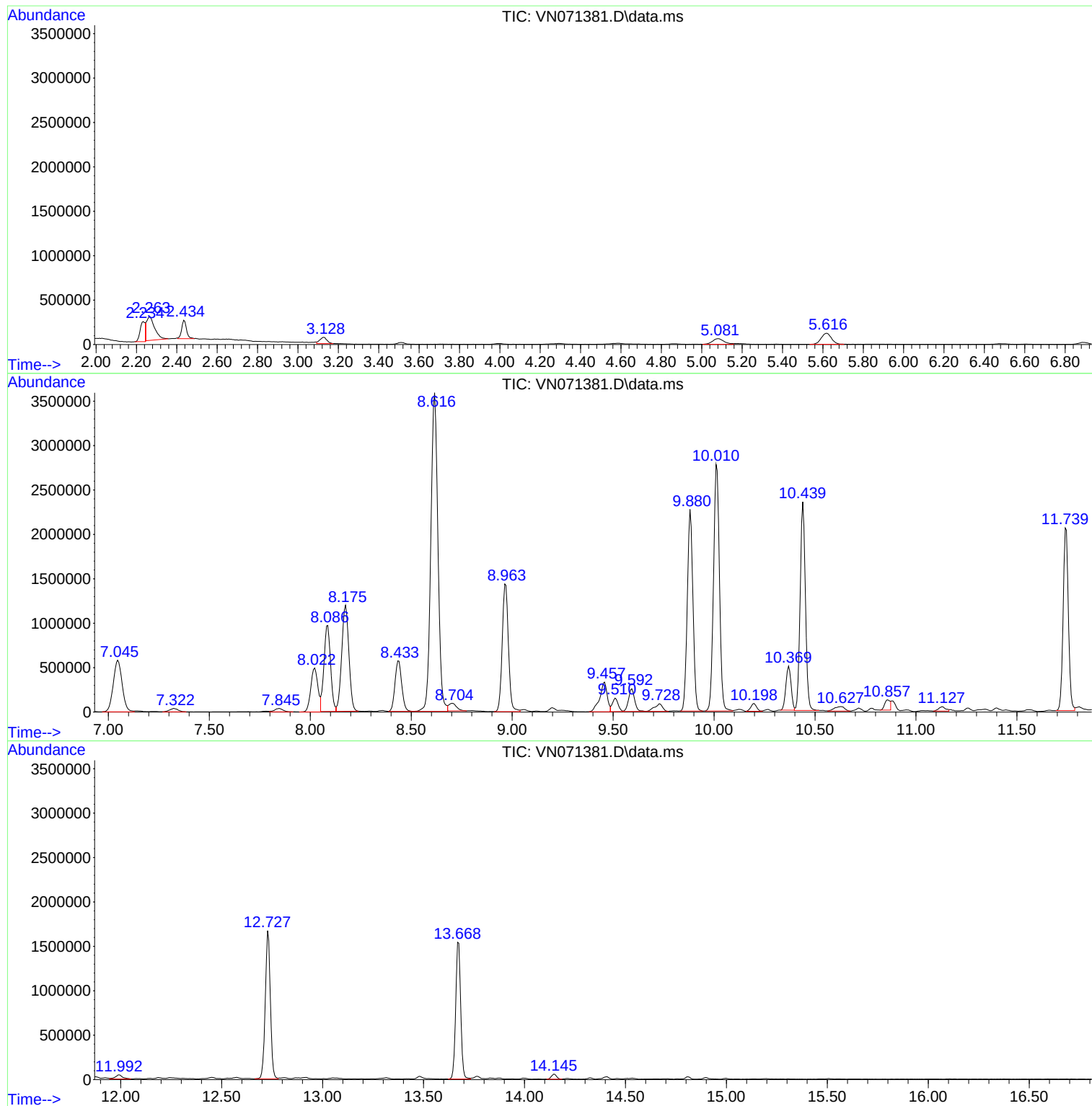
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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



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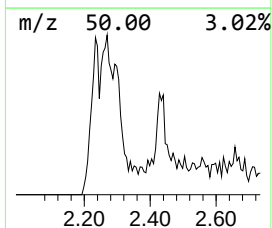
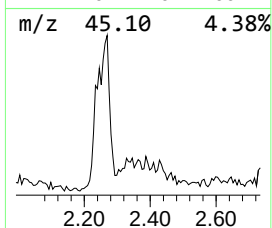
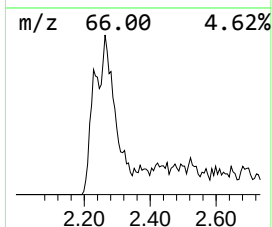
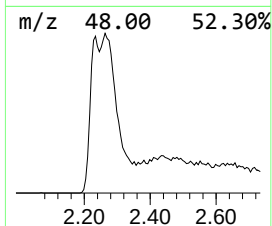
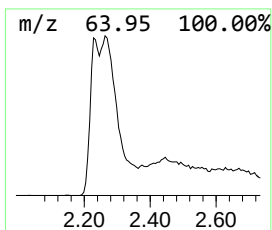
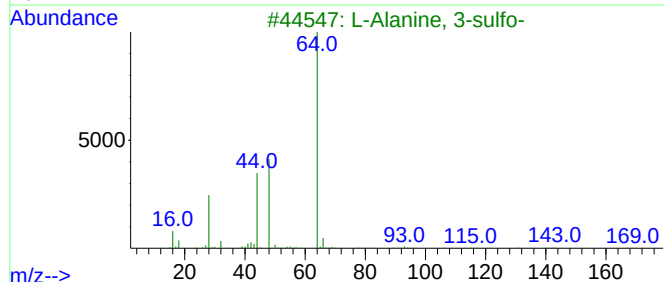
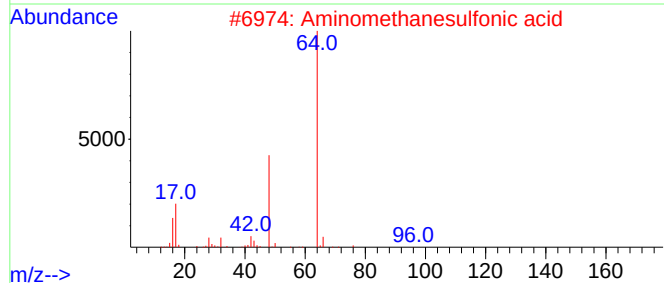
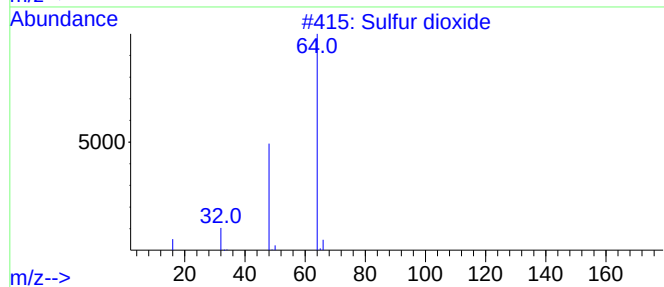
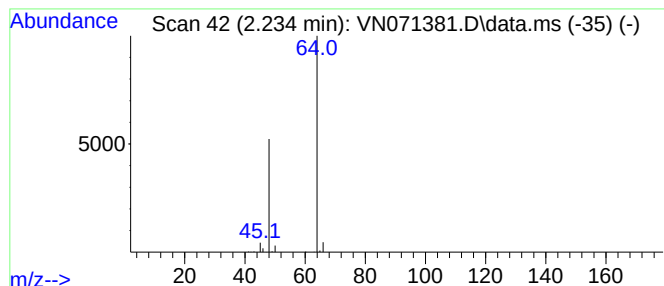
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	9.78 ug/l	429608	Pentafluorobenzene	8.086

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	7
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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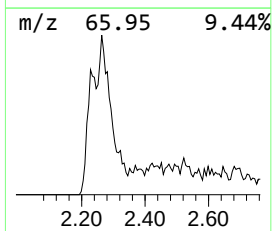
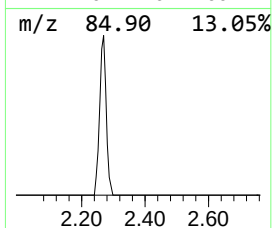
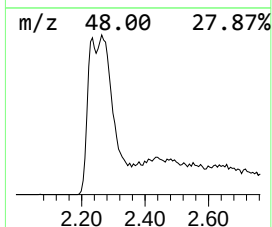
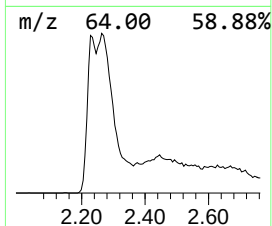
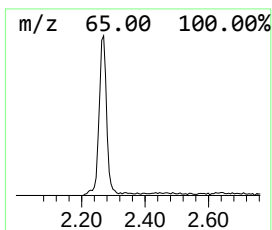
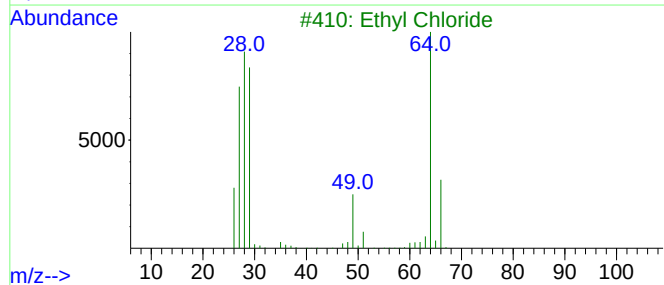
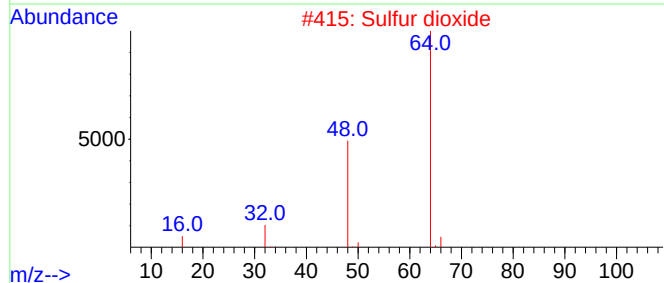
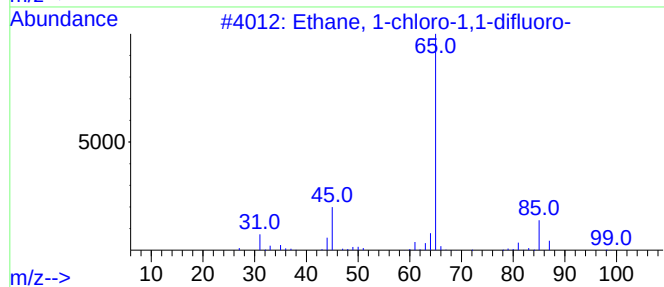
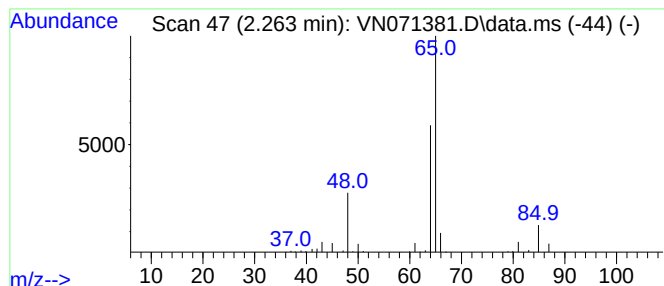
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown2.263 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	16.31 ug/l	716210	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	33
2			Sulfur dioxide	64	O2S	007446-09-5	7
3			Ethyl Chloride	64	C2H5Cl	000075-00-3	7
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4



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ALS Vial : 20 Sample Multiplier: 1

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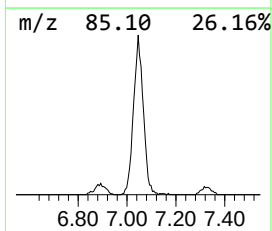
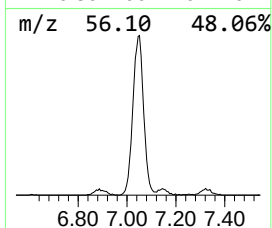
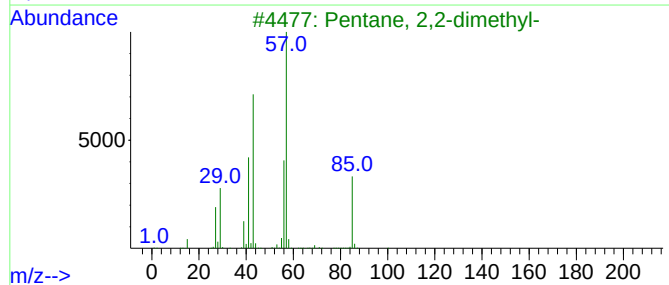
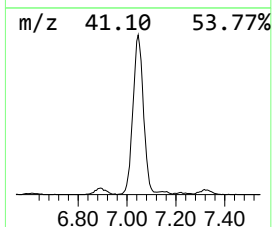
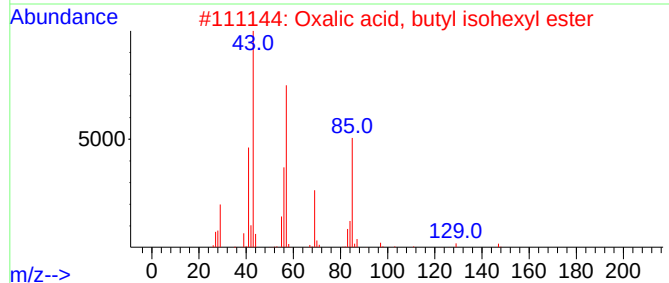
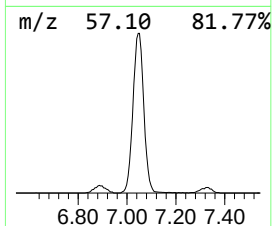
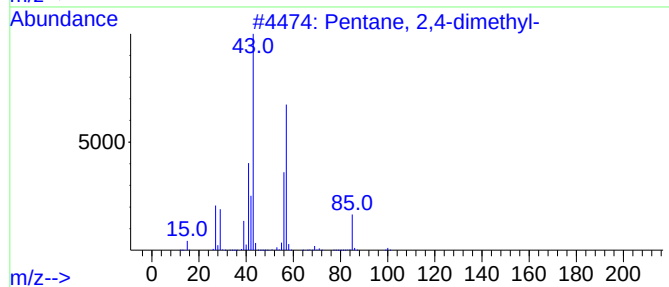
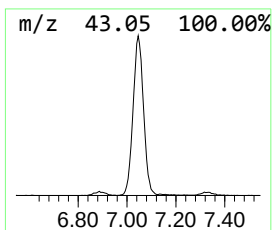
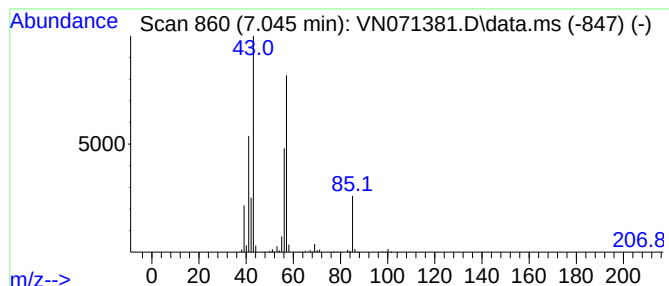
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.045	40.45 ug/l	1776230	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	64
3			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
4			Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	53
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	53



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Sample : N2015-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

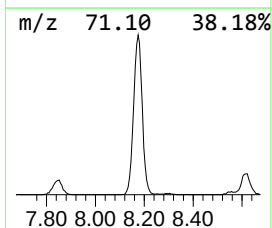
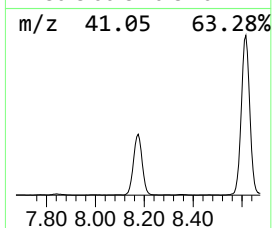
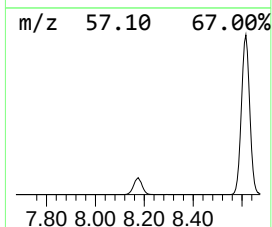
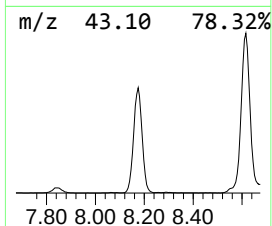
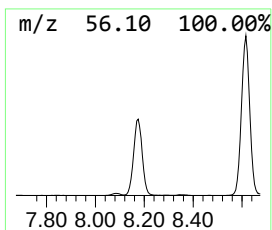
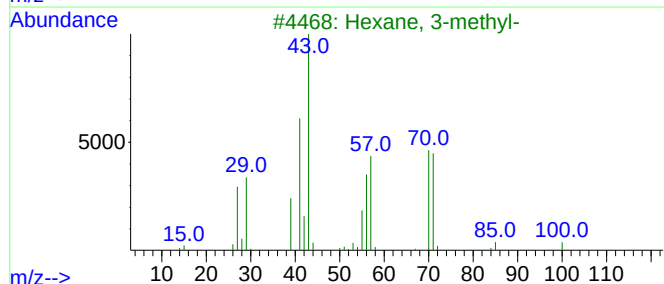
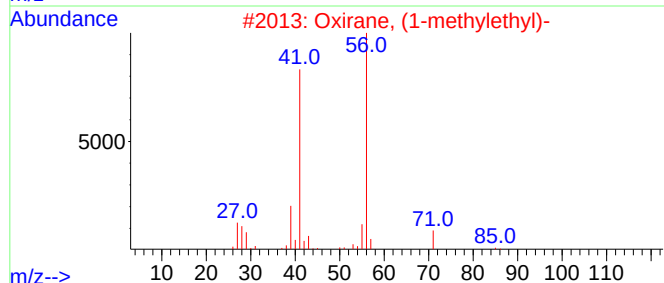
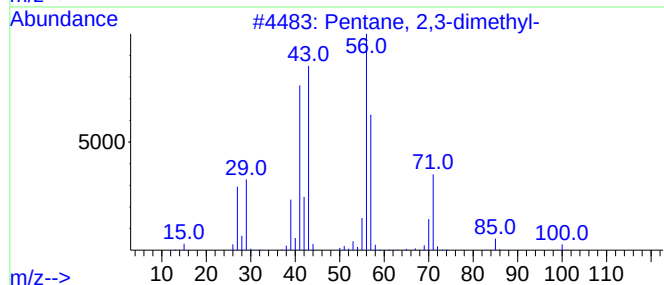
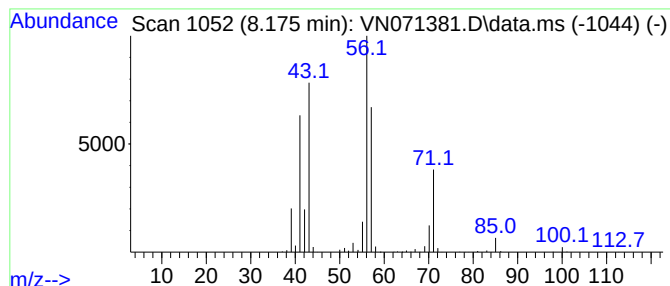
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.175	66.75 ug/l	2930960	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	43
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	42
5			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	38



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

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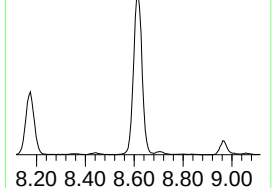
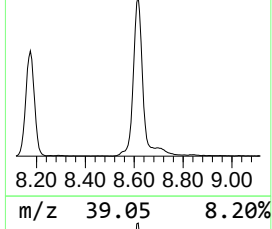
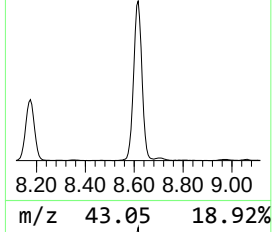
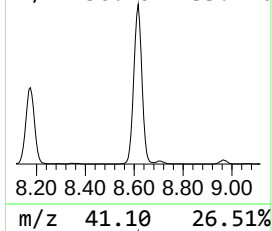
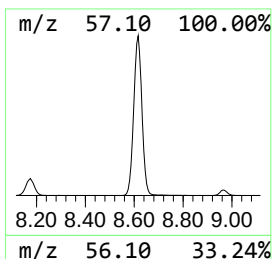
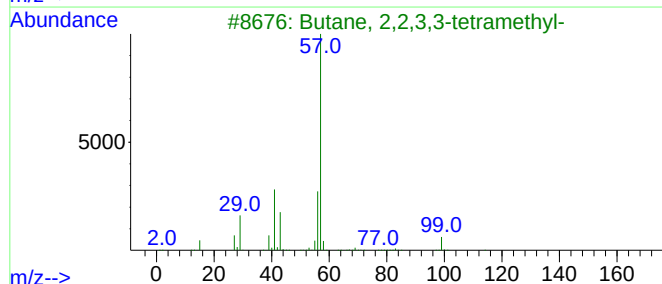
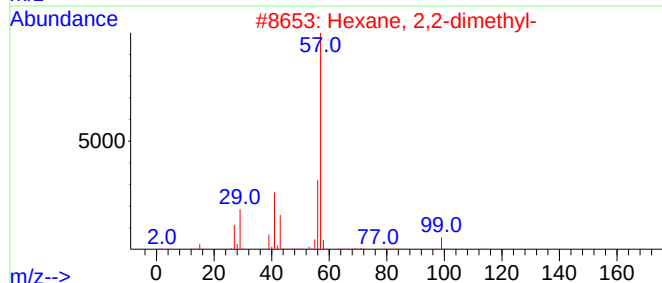
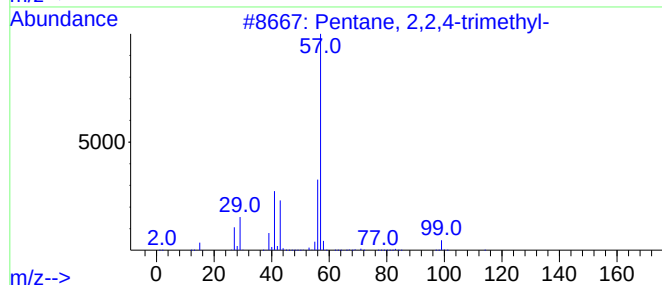
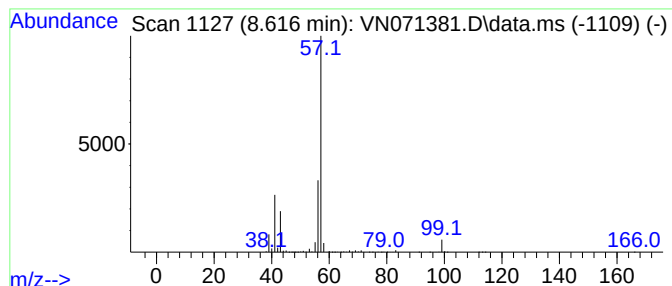
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.616	142.81 ug/l	8751350	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	59



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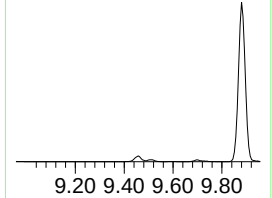
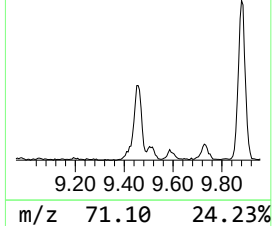
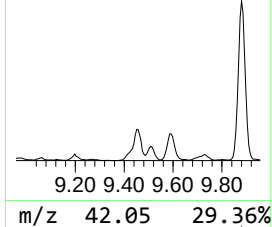
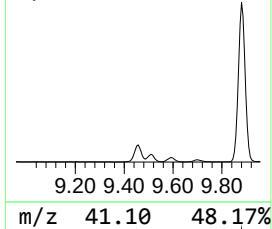
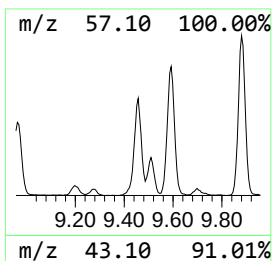
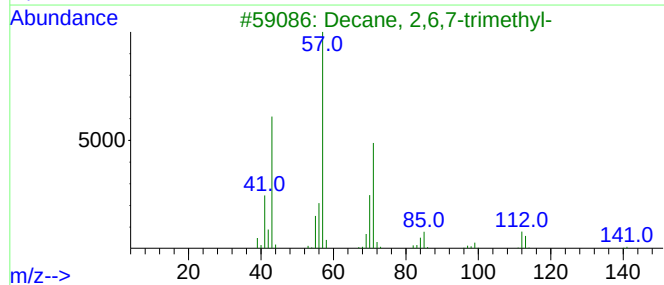
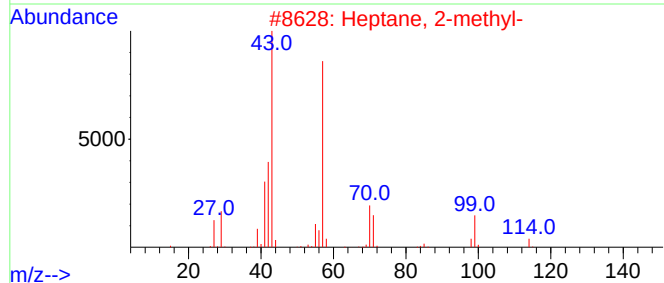
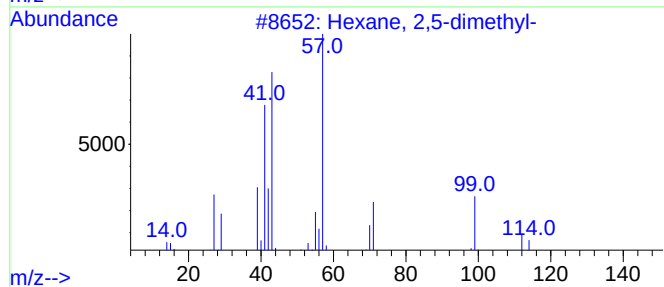
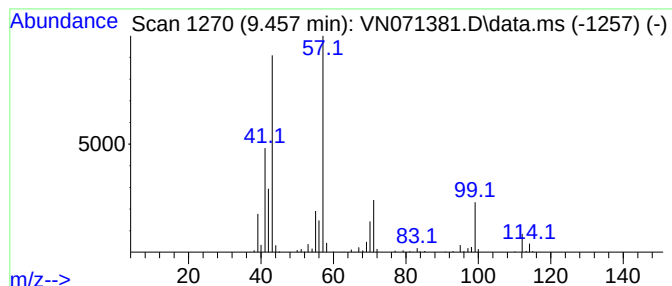
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Quant Title : SW846 8260

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

Peak Number 6 Hexane, 2,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.457	14.02 ug/l	859205	1,4-Difluorobenzene	8.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	91
2		Heptane, 2-methyl-	114	C8H18	000592-27-8	80
3		Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	53
4		Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	53
5		Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071381.D
Acq On : 18 Mar 2022 18:43
Operator : JC\MD
Sample : N2015-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

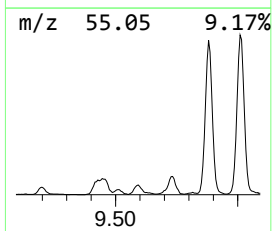
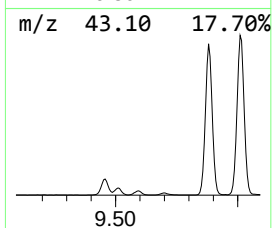
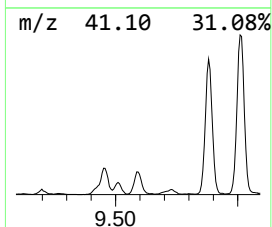
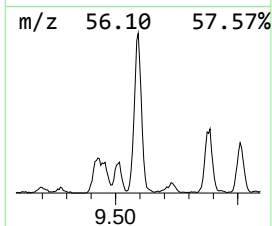
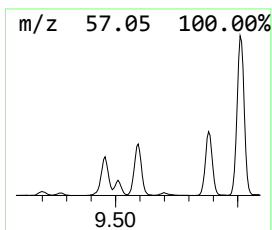
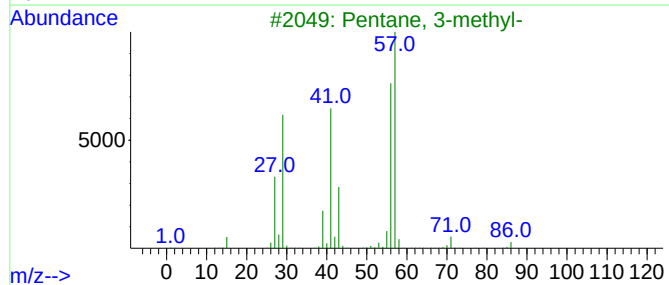
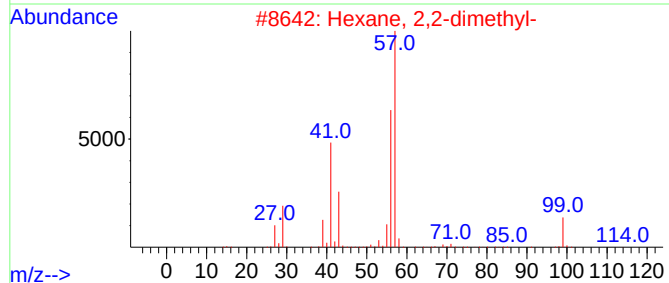
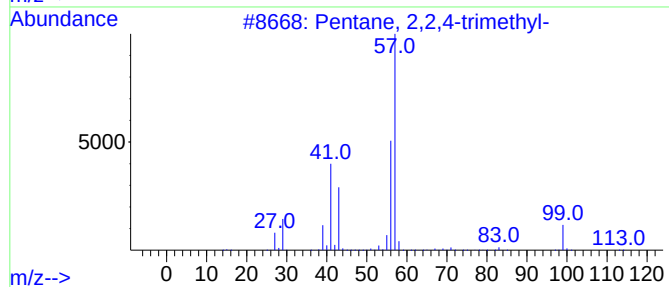
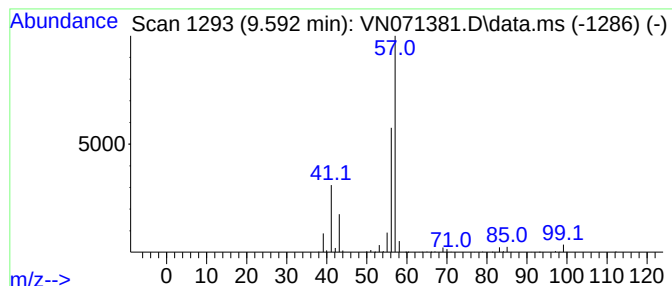
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Quant Title : SW846 8260

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

Peak Number 7 Hexane, 2,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.592	8.73 ug/l	534907	1,4-Difluorobenzene	8.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
3			Pentane, 3-methyl-	86	C6H14	000096-14-0	64
4			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	59
5			Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071381.D
Acq On : 18 Mar 2022 18:43
Operator : JC\MD
Sample : N2015-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

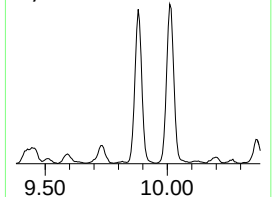
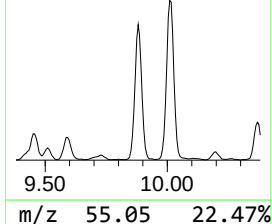
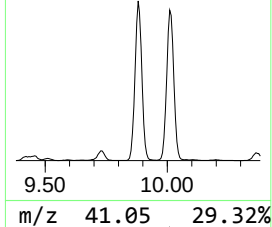
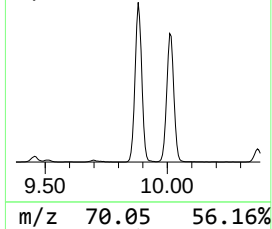
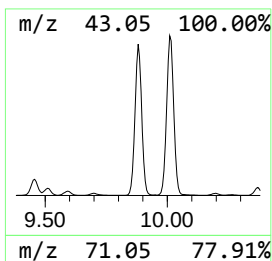
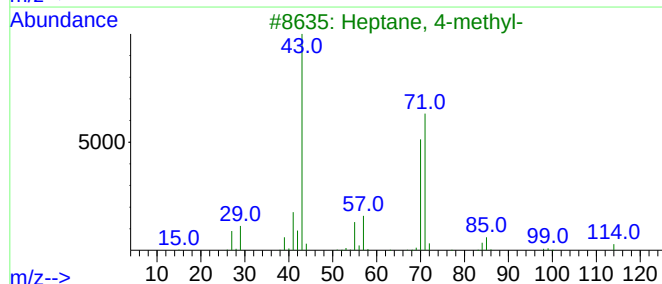
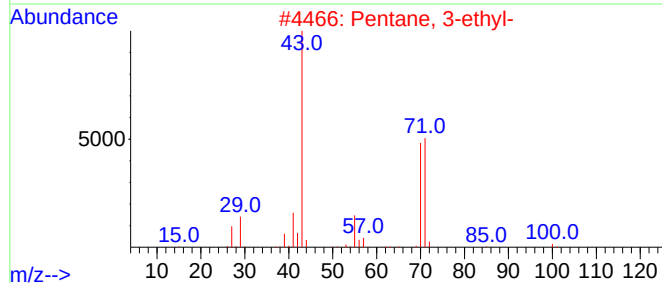
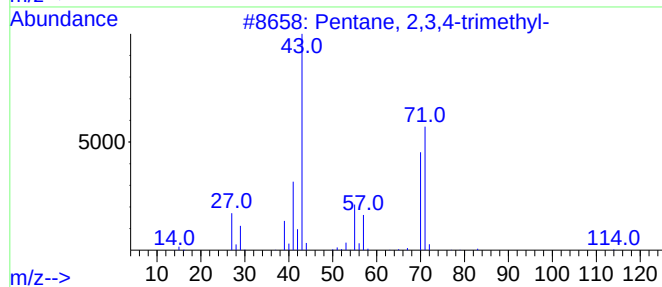
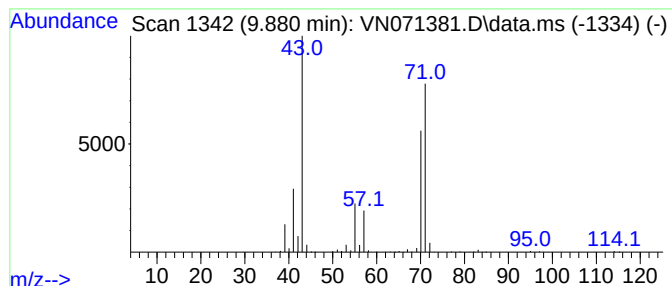
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Quant Title : SW846 8260

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

Peak Number 8 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.880	71.93 ug/l	4407870	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-methyl-	100	C7H16	000589-34-4	78
5			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071381.D
Acq On : 18 Mar 2022 18:43
Operator : JC\MD
Sample : N2015-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

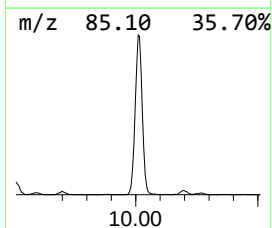
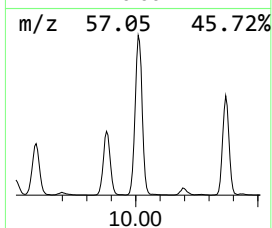
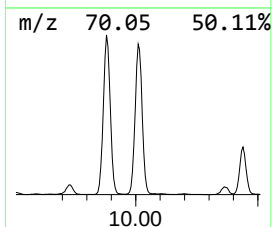
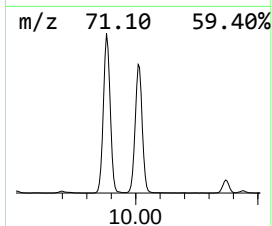
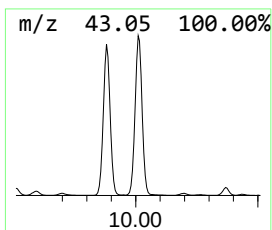
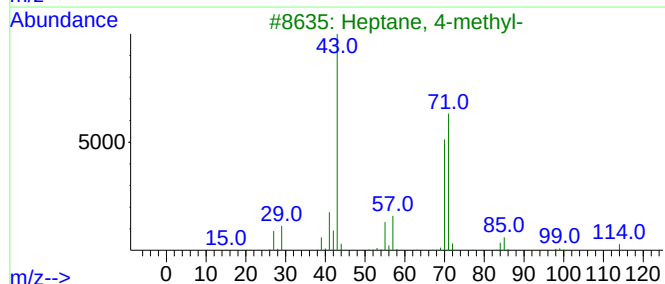
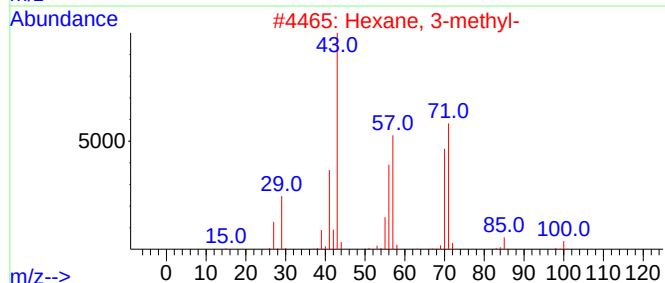
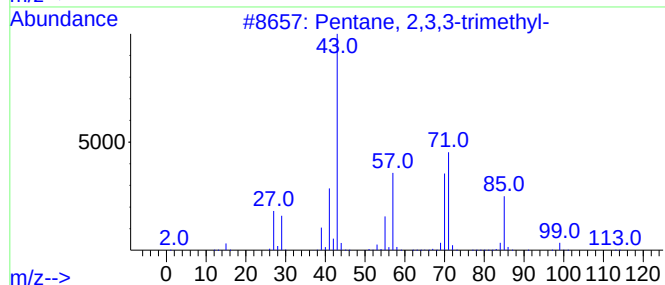
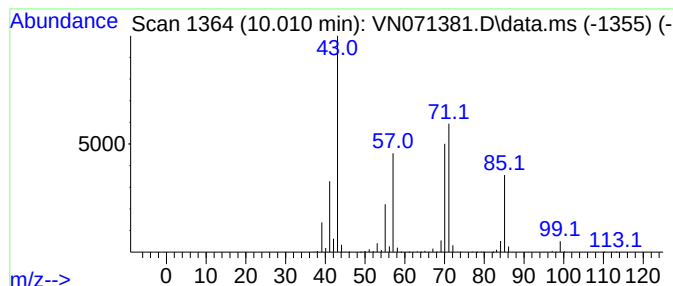
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.M
Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.010	92.53 ug/l	5670470	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			Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071381.D
Acq On : 18 Mar 2022 18:43
Operator : JC\MD
Sample : N2015-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

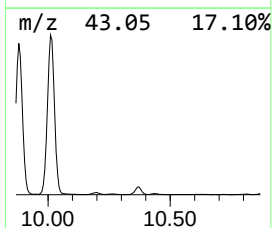
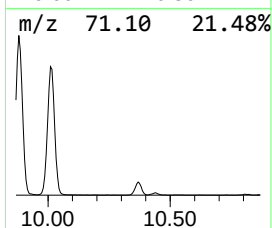
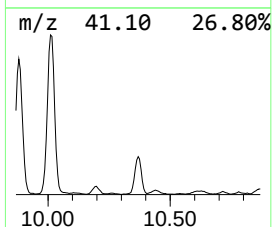
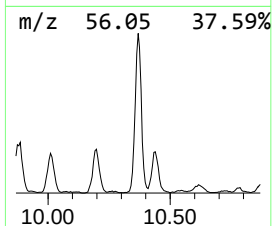
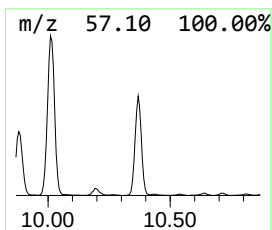
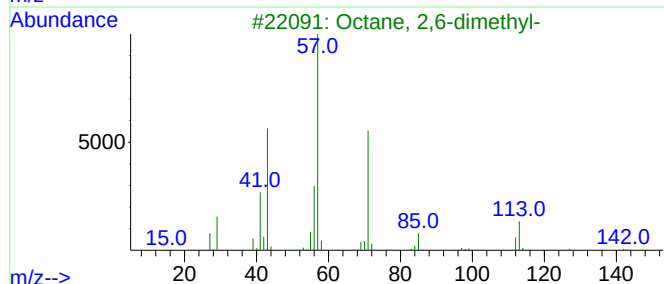
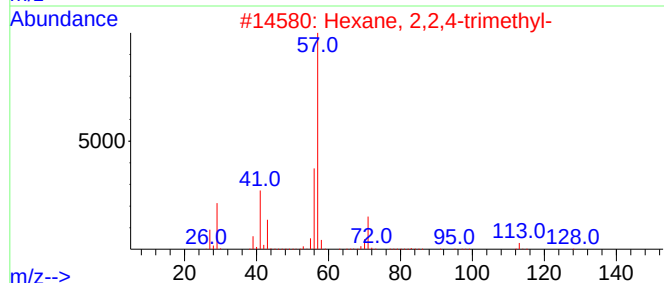
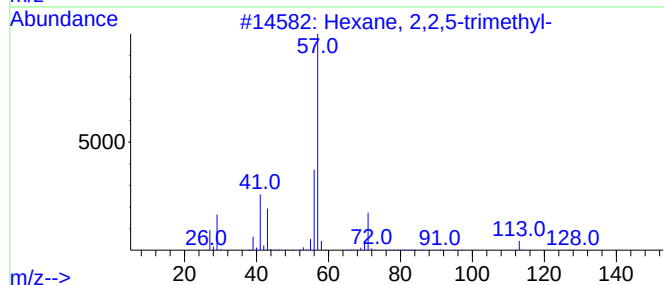
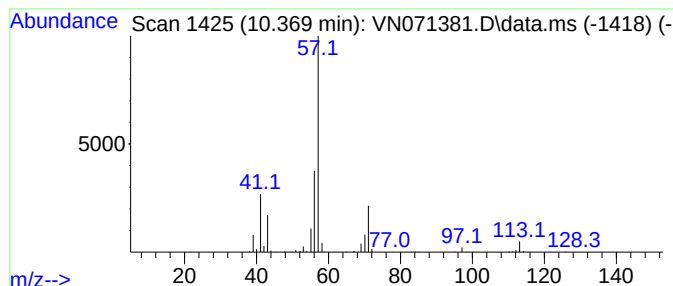
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Quant Title : SW846 8260

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

Peak Number 10 Hexane, 2,2,5-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.369	11.93 ug/l	885496	Chlorobenzene-d5	11.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	78
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	78
3			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	59
5			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031822\
Data File : VN071381.D
Acq On : 18 Mar 2022 18:43
Operator : JC\MD
Sample : N2015-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N030722W.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
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unknown2.263	2.263	16.3	ug/l	716210	1	8.086	2195410	50.0
Pentane, 2,4-di...	7.045	40.5	ug/l	1776230	1	8.086	2195410	50.0
Pentane, 2,3-di...	8.175	66.8	ug/l	2930960	1	8.086	2195410	50.0
Pentane, 2,2,4-...	8.616	142.8	ug/l	8751350	2	8.969	3064020	50.0
Hexane, 2,5-dim...	9.457	14.0	ug/l	859205	2	8.969	3064020	50.0
Hexane, 2,2-dim...	9.592	8.7	ug/l	534907	2	8.969	3064020	50.0
Pentane, 2,3,4-...	9.880	71.9	ug/l	4407870	2	8.969	3064020	50.0
Pentane, 2,3,3-...	10.010	92.5	ug/l	5670470	2	8.969	3064020	50.0
Hexane, 2,2,5-t...	10.369	11.9	ug/l	885496	3	11.739	3711560	50.0