

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
 Data File : VN072984.D
 Acq On : 21 Jun 2022 15:31
 Operator : JC\MD
 Sample : N3379-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 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\82N061722W.M
 Title : SW846 8260

Signal : TIC: VN072984.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	54	60	67	rVB2	38089	51442	1.69%	0.258%
2	2.405	81	88	96	rBV	64341	112863	3.70%	0.566%
3	3.087	195	204	214	rBV3	21722	51864	1.70%	0.260%
4	4.998	517	529	541	rBV3	26449	101584	3.33%	0.510%
5	5.540	608	621	634	rBV3	51567	188921	6.19%	0.948%
6	6.969	850	864	877	rBV	208009	635879	20.85%	3.191%
7	7.251	901	912	921	rVB5	17029	47376	1.55%	0.238%
8	7.769	984	1000	1012	rBV4	20399	70495	2.31%	0.354%
9	7.951	1021	1031	1036	rBV	213607	516477	16.93%	2.592%
10	8.016	1036	1042	1049	rVV	417489	959822	31.47%	4.816%
11	8.104	1049	1057	1072	rVB2	455884	1149632	37.69%	5.769%
12	8.369	1094	1102	1116	rBV	217671	515581	16.90%	2.587%
13	8.545	1116	1132	1143	rVV	1273091	3050106	100.00%	15.305%
14	8.639	1143	1148	1157	rVB3	23020	54911	1.80%	0.276%
15	8.904	1184	1193	1203	rBV	579502	1202498	39.42%	6.034%
16	9.392	1263	1276	1280	rBV2	103423	270724	8.88%	1.358%
17	9.445	1280	1285	1292	rVV3	50816	107576	3.53%	0.540%
18	9.528	1292	1299	1310	rVB	98537	213304	6.99%	1.070%
19	9.669	1310	1323	1329	rBV5	33366	93694	3.07%	0.470%
20	9.816	1340	1348	1358	rBV	854585	1674968	54.92%	8.405%
21	9.945	1360	1370	1384	rVV	1166541	2383985	78.16%	11.963%
22	10.133	1394	1402	1408	rBV2	36331	73006	2.39%	0.366%
23	10.304	1419	1431	1437	rBV	147235	279112	9.15%	1.401%
24	10.375	1437	1443	1457	rVB	786786	1470164	48.20%	7.377%
25	10.563	1466	1475	1484	rVB7	25872	86840	2.85%	0.436%
26	10.657	1484	1491	1496	rVV7	15992	32596	1.07%	0.164%
27	10.716	1496	1501	1505	rVV3	16233	32523	1.07%	0.163%
28	10.798	1505	1515	1525	rVV6	55583	194607	6.38%	0.977%
29	11.192	1575	1582	1587	rBV7	18871	36939	1.21%	0.185%
30	11.680	1657	1665	1674	rBV	828070	1462638	47.95%	7.339%
31	11.927	1701	1707	1714	rVB3	21339	40450	1.33%	0.203%
32	12.669	1825	1833	1841	rBV	684951	1152059	37.77%	5.781%
33	13.416	1955	1960	1967	rVB2	19921	34780	1.14%	0.175%
34	13.610	1985	1993	2007	rBV	871563	1486506	48.74%	7.459%
35	14.080	2067	2073	2080	rBV3	32634	61387	2.01%	0.308%
36	14.345	2109	2118	2124	rVV6	15243	31309	1.03%	0.157%

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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\82N061722W.M
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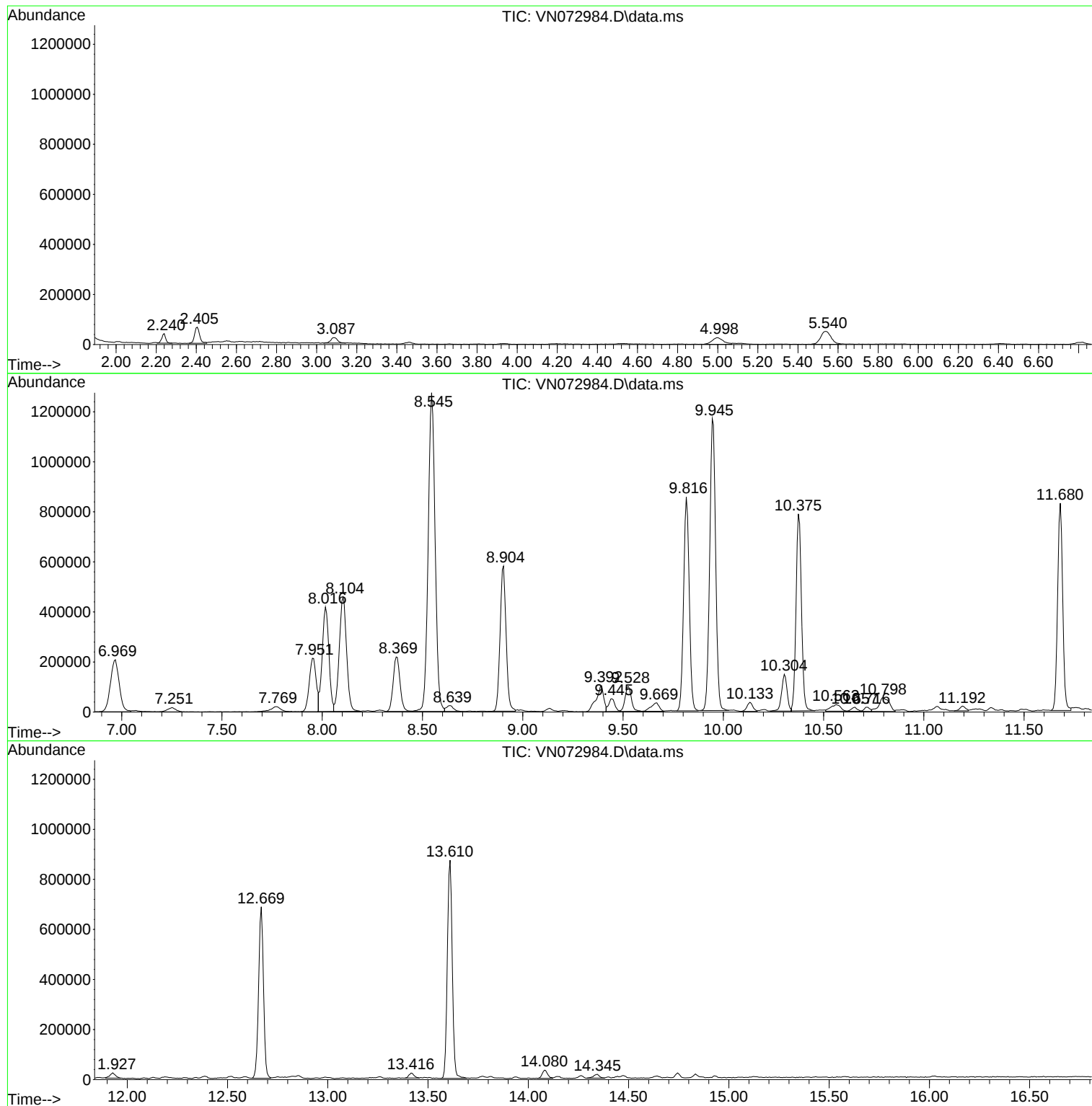
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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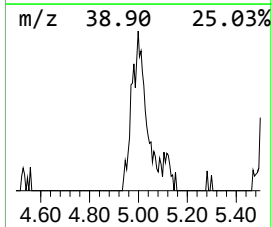
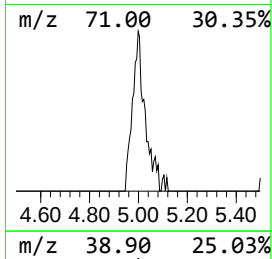
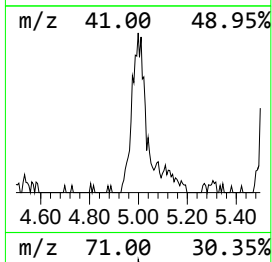
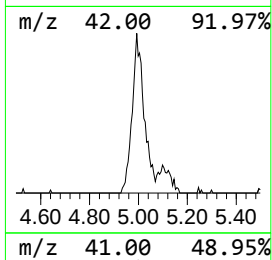
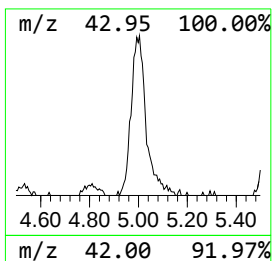
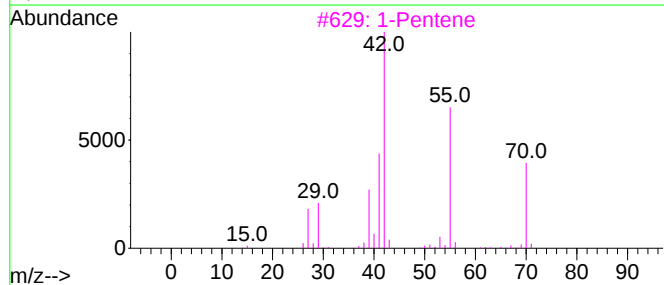
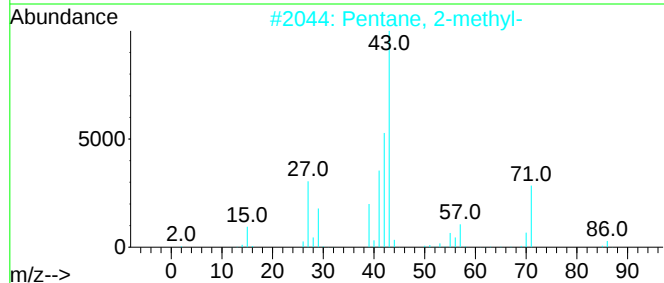
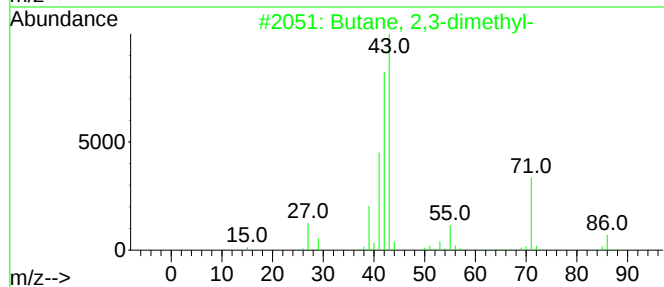
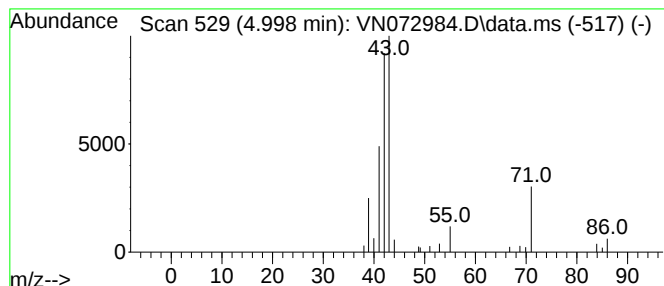
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Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.998	5.29 ug/l	101584	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3			1-Pentene	70	C5H10	000109-67-1	28
4			Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	9
5			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	9



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Instrument :
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ClientSampleId :
TOLL-MW-03

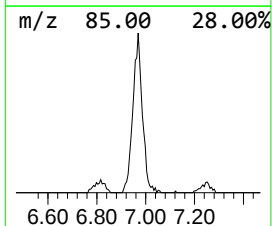
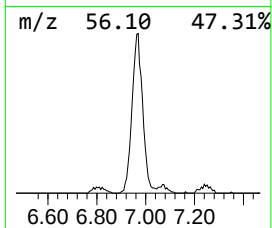
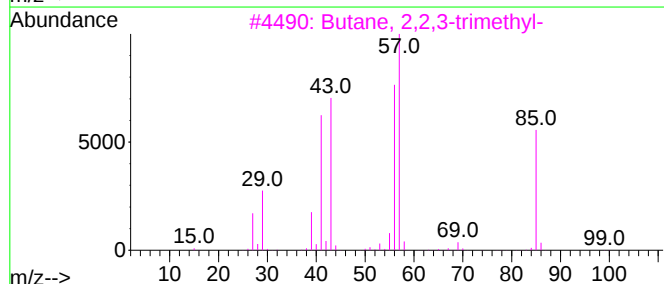
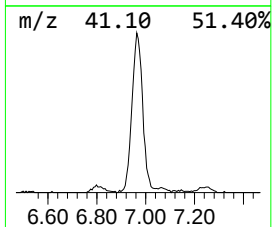
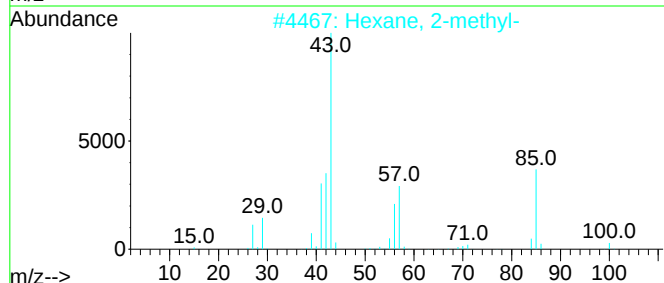
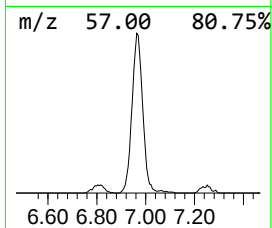
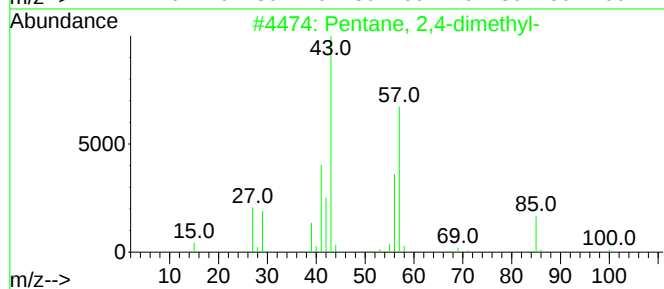
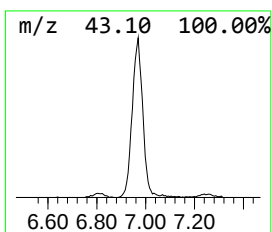
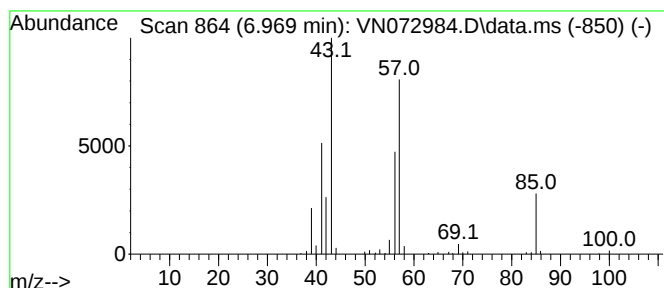
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.969	33.12 ug/l	635879	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	91
2			Hexane, 2-methyl-	100	C7H16	000591-76-4	64
3			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
4			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	53
5			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	50



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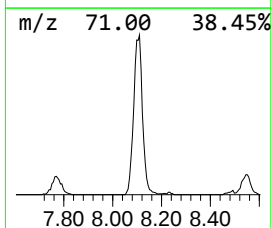
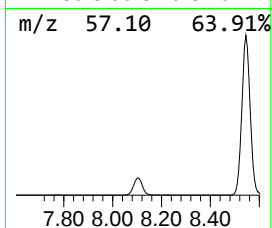
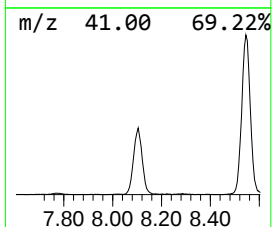
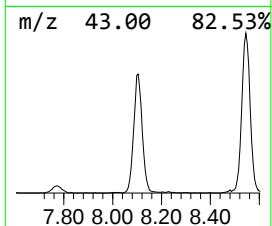
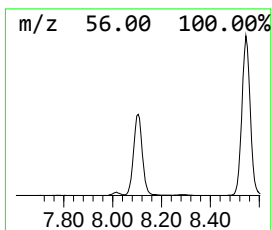
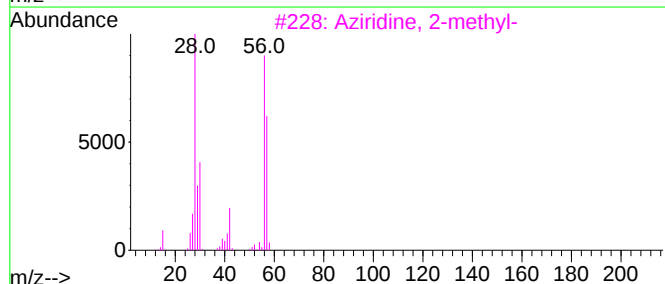
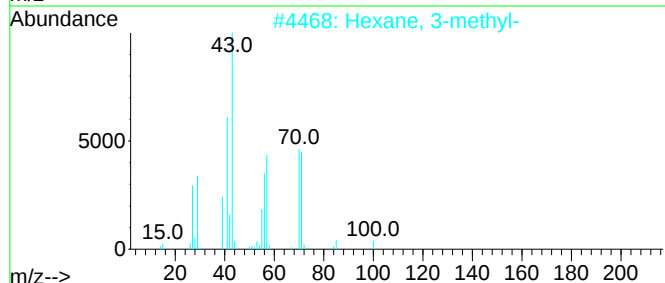
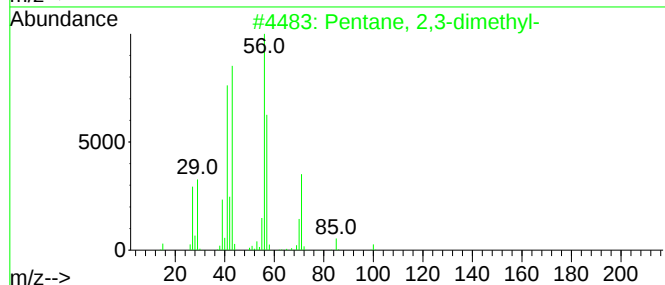
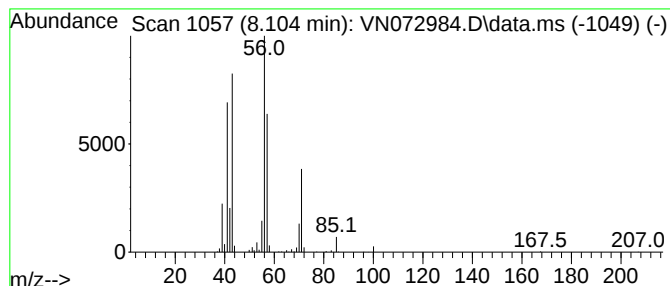
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	59.89 ug/l	1149630	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	95
2			Hexane, 3-methyl-	100	C7H16	000589-34-4	43
3			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	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 : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

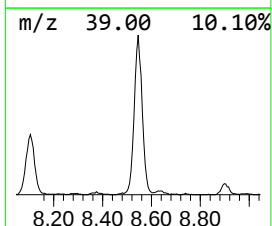
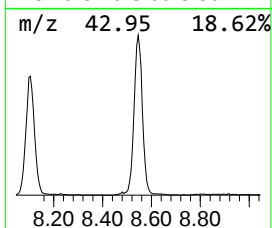
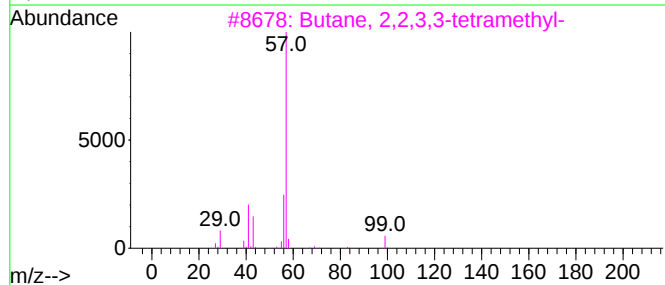
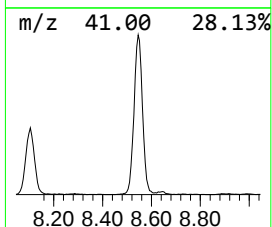
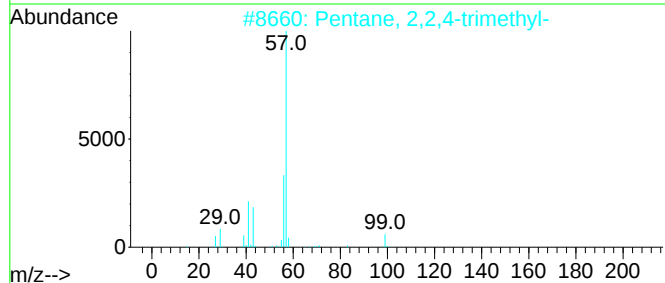
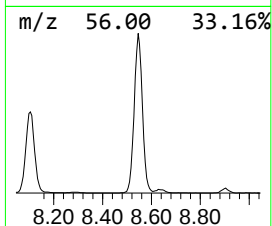
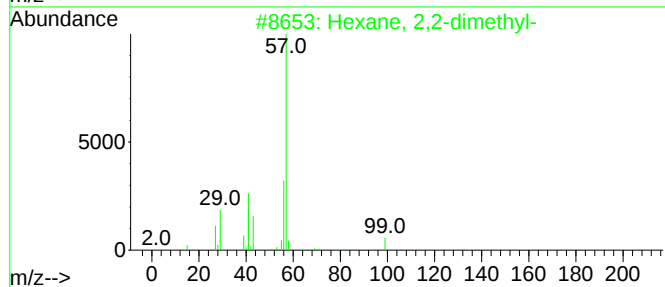
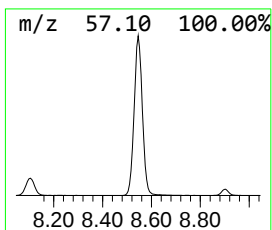
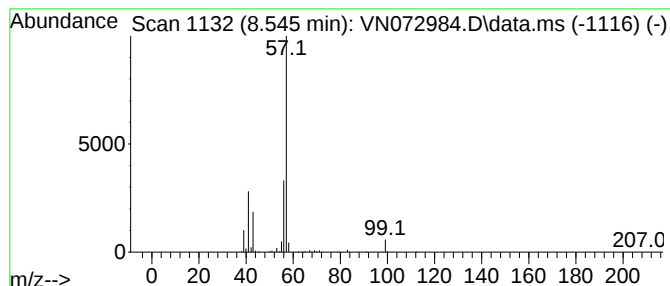
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

Peak Number 4 Hexane, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	126.82 ug/l	3050110	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
3			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	72
5			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	50



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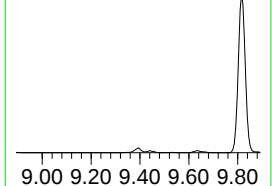
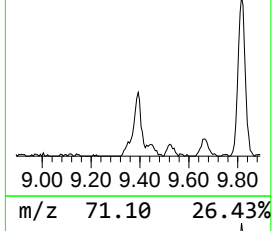
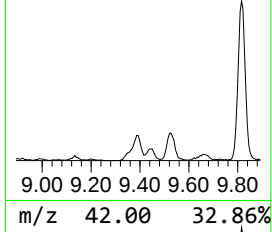
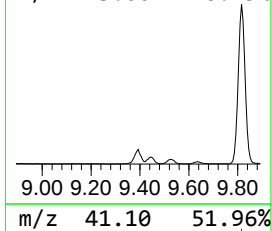
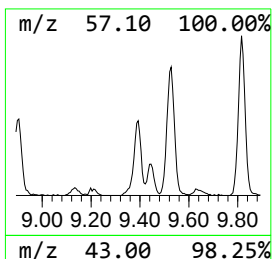
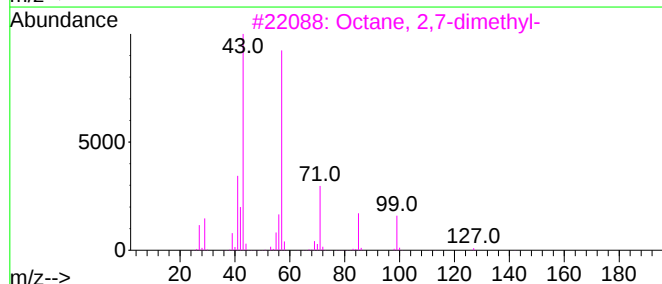
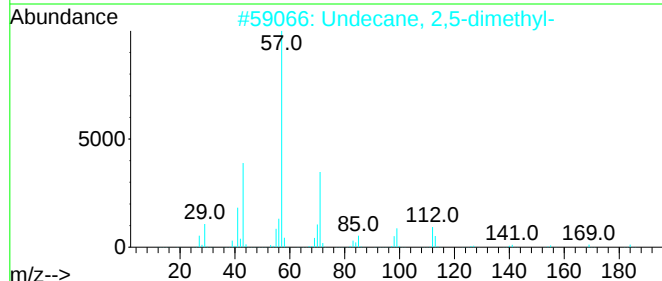
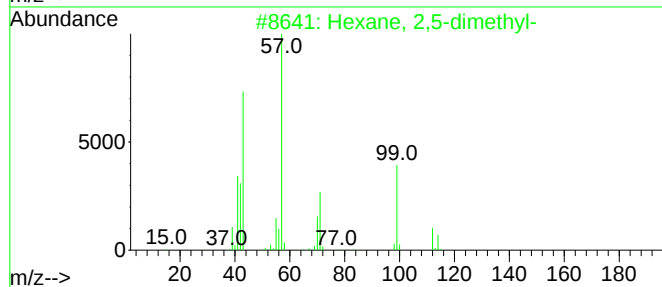
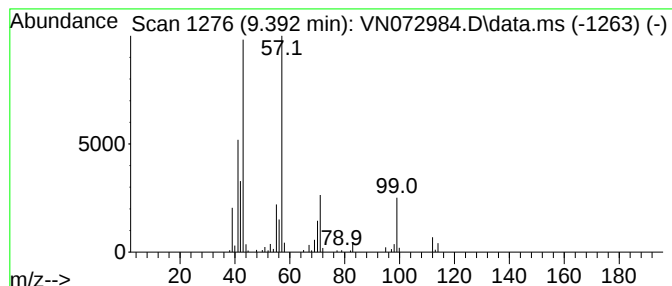
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.392	11.26 ug/l	270724	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	90
2			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	47
3			Octane, 2,7-dimethyl-	142	C10H22	001072-16-8	47
4			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	47
5			Heptane, 2-methyl-	114	C8H18	000592-27-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072984.D
Acq On : 21 Jun 2022 15:31
Operator : JC\MD
Sample : N3379-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

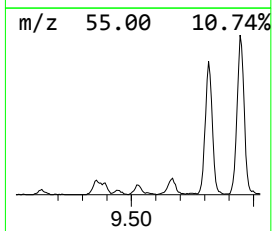
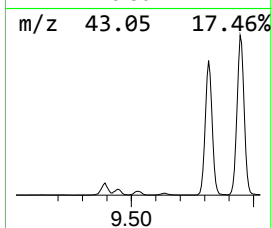
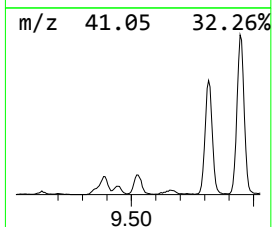
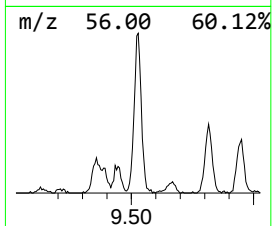
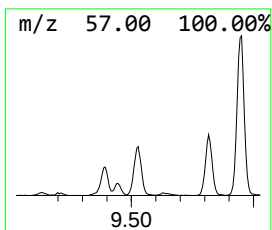
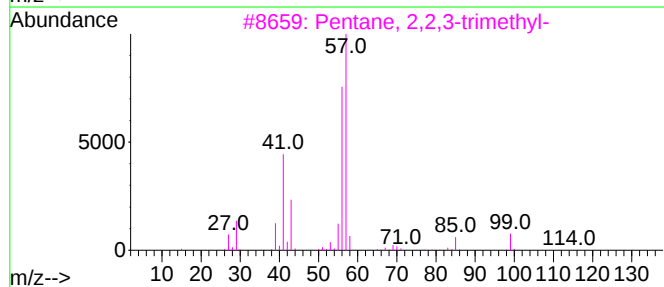
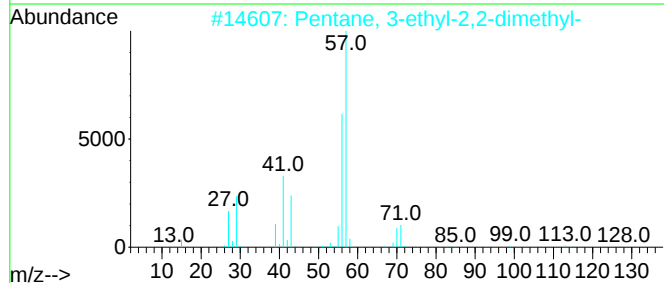
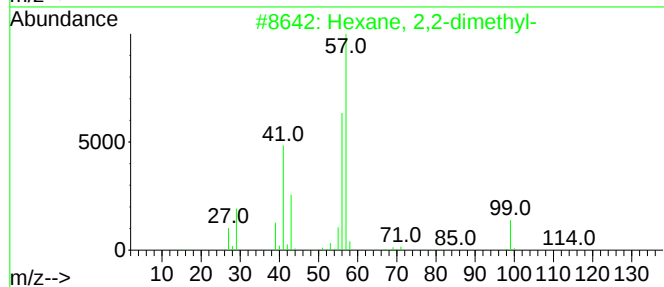
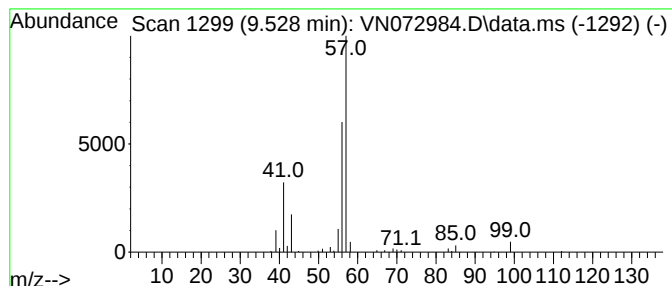
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Quant Title : SW846 8260

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

Peak Number 6 Pentane, 3-ethyl-2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.528	8.87 ug/l	213304	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
3			Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	64
4			Heptane, 2,2,4-trimethyl-	142	C10H22	014720-74-2	64
5			Pentane, 3-methyl-	86	C6H14	000096-14-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072984.D
Acq On : 21 Jun 2022 15:31
Operator : JC\MD
Sample : N3379-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

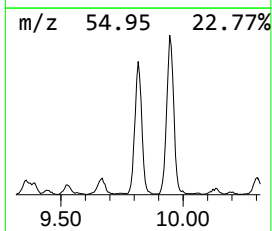
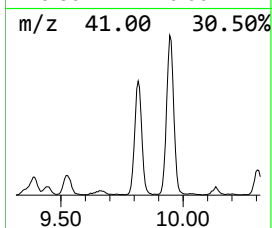
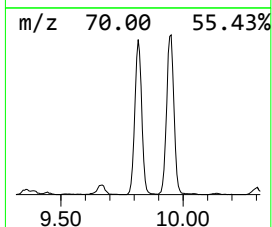
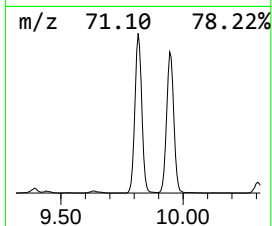
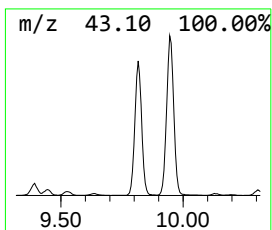
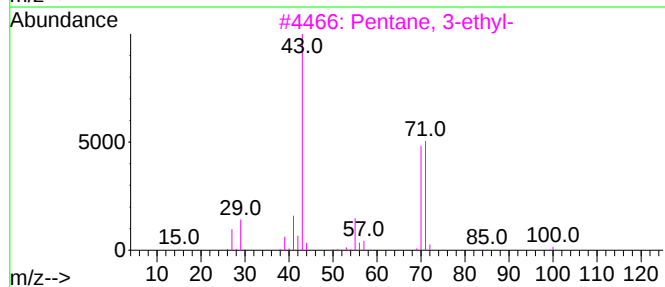
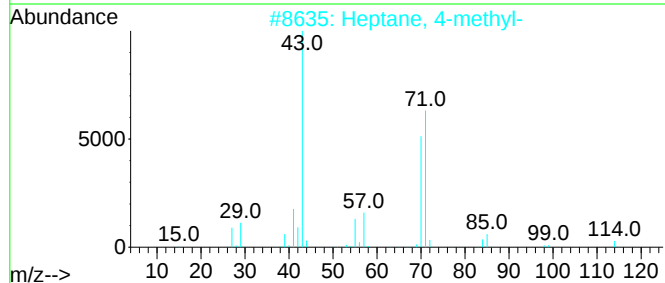
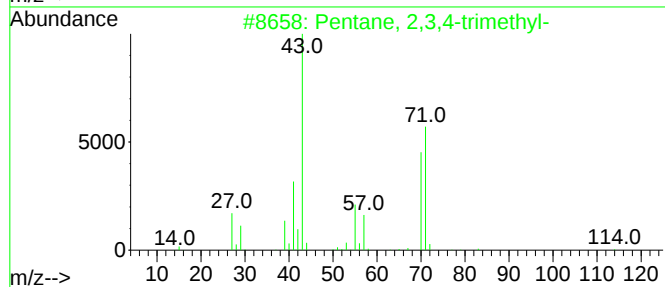
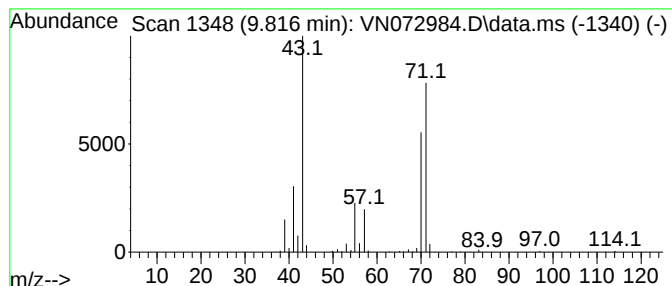
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	69.65 ug/l	1674970	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3			Pentane, 3-ethyl-	100	C7H16	000617-78-7	74
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74
5			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072984.D
Acq On : 21 Jun 2022 15:31
Operator : JC\MD
Sample : N3379-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

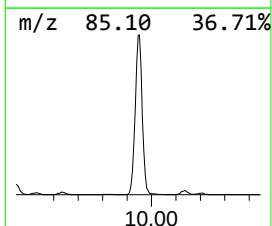
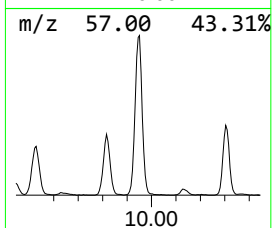
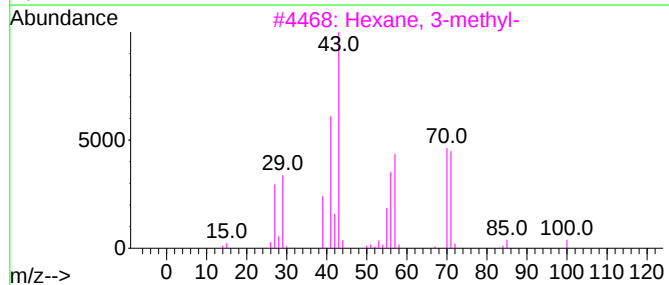
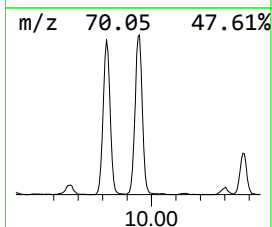
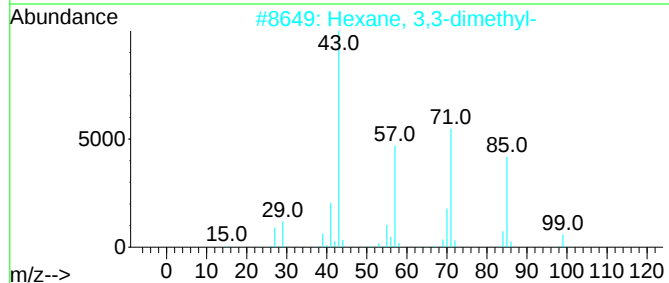
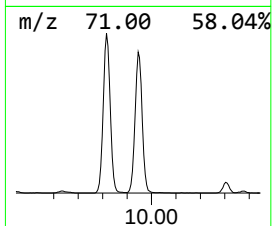
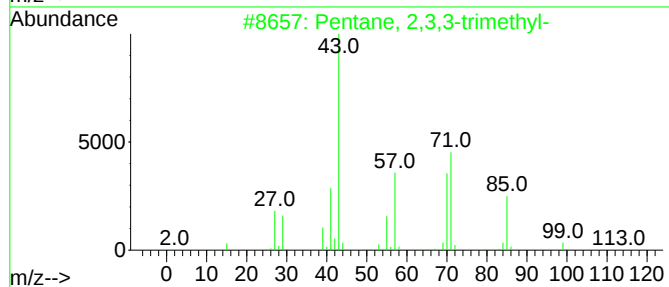
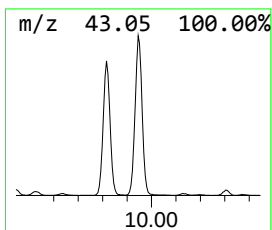
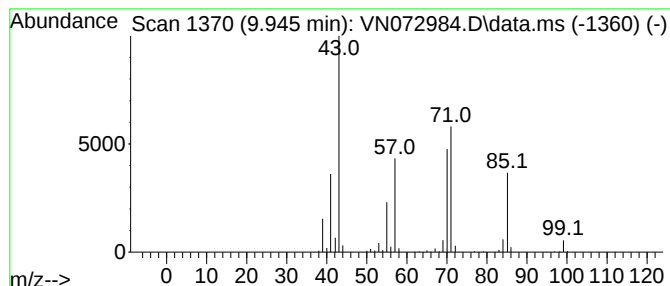
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	99.13 ug/l	2383990	1,4-Difluorobenzene	8.904

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072984.D
Acq On : 21 Jun 2022 15:31
Operator : JC\MD
Sample : N3379-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

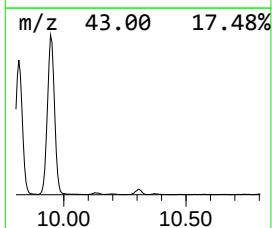
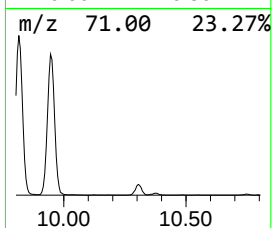
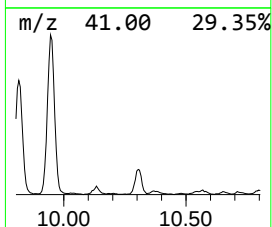
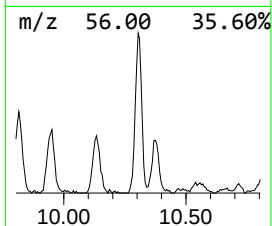
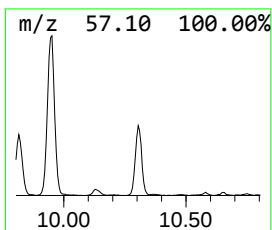
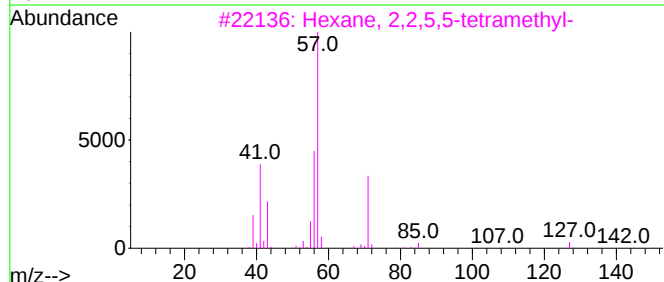
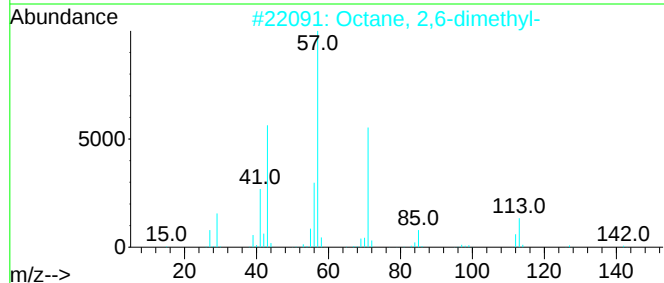
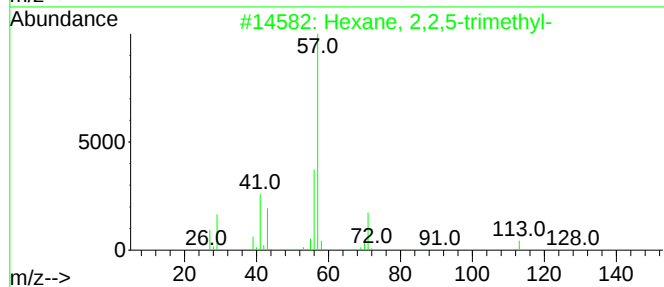
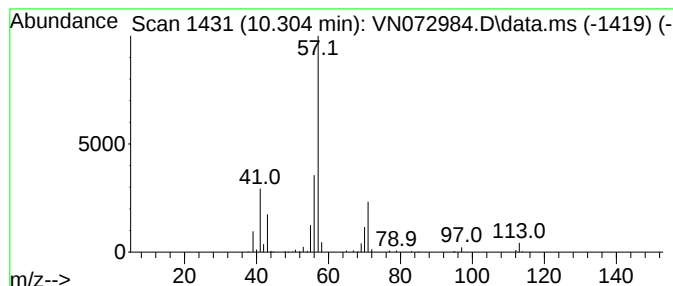
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Quant Title : SW846 8260

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

Peak Number 9 Hexane, 2,2,5-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.304	9.54 ug/l	279112	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	72
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	56
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
4			Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	47
5			Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072984.D
Acq On : 21 Jun 2022 15:31
Operator : JC\MD
Sample : N3379-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

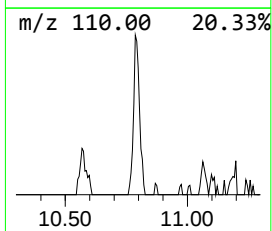
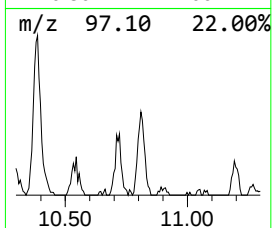
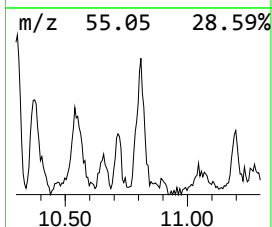
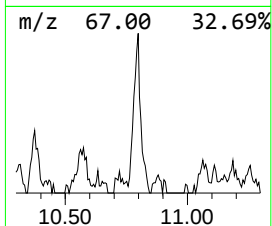
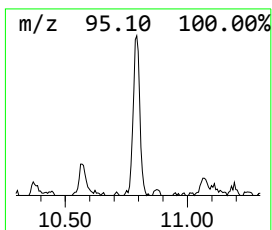
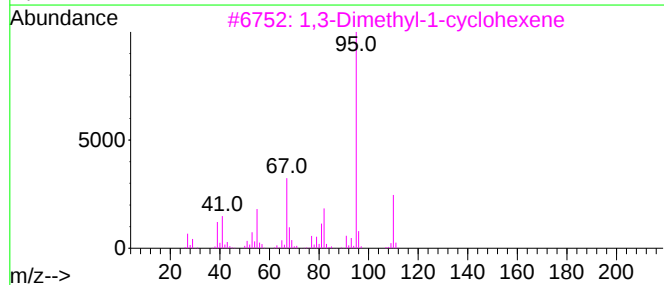
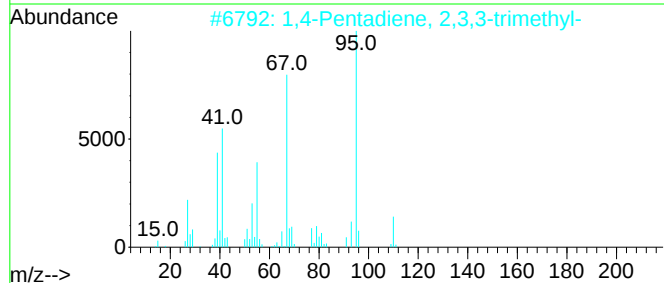
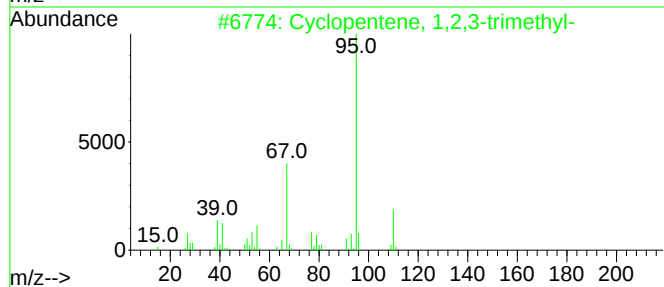
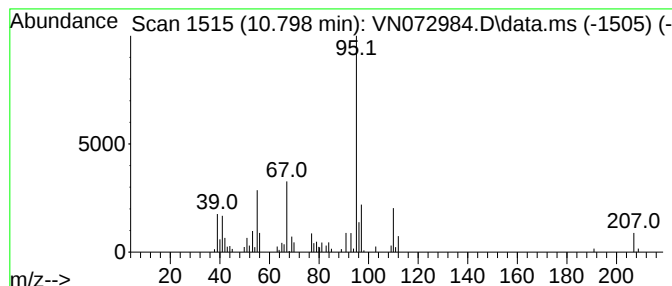
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Quant Title : SW846 8260

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

Peak Number 10 Cyclopentene, 1,2,3-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.798	6.65 ug/l	194607	Chlorobenzene-d5	11.680

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	76
2			1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	64
3			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	64
4			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	64
5			2(1H)-Pyridinone	95	C5H5NO	000142-08-5	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062122\
Data File : VN072984.D
Acq On : 21 Jun 2022 15:31
Operator : JC\MD
Sample : N3379-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOLL-MW-03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.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
Butane, 2,3-dim...	4.998	5.3	ug/l	101584	1	8.016	959822	50.0
Pentane, 2,4-di...	6.969	33.1	ug/l	635879	1	8.016	959822	50.0
Pentane, 2,3-di...	8.104	59.9	ug/l	1149630	1	8.016	959822	50.0
Hexane, 2,2-dim...	8.545	126.8	ug/l	3050110	2	8.904	1202500	50.0
Hexane, 2,5-dim...	9.392	11.3	ug/l	270724	2	8.904	1202500	50.0
Pentane, 3-ethy...	9.528	8.9	ug/l	213304	2	8.904	1202500	50.0
Pentane, 2,3,4-...	9.816	69.7	ug/l	1674970	2	8.904	1202500	50.0
Pentane, 2,3,3-...	9.945	99.1	ug/l	2383990	2	8.904	1202500	50.0
Hexane, 2,2,5-t...	10.304	9.5	ug/l	279112	3	11.680	1462640	50.0
Cyclopentene, 1...	10.798	6.7	ug/l	194607	3	11.680	1462640	50.0