

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062022\
 Data File : VN072966.D
 Acq On : 20 Jun 2022 17:05
 Operator : JC\MD
 Sample : N3370-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TOLL-MW-07

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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: VN072966.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	56	60	64	rVB2	14107	19478	1.26%	0.166%
2	2.410	78	89	91	rBV4	10453	24509	1.58%	0.209%
3	4.992	517	528	532	rBV4	9156	27100	1.75%	0.232%
4	5.292	568	579	585	rBV3	7521	22797	1.47%	0.195%
5	5.534	611	620	638	rBV3	30951	110784	7.14%	0.947%
6	6.963	854	863	875	rBV3	12945	37601	2.42%	0.321%
7	7.251	902	912	920	rBV4	10393	27980	1.80%	0.239%
8	7.951	1021	1031	1036	rBV	226066	548003	35.31%	4.683%
9	8.016	1036	1042	1051	rVV	449273	1026131	66.12%	8.769%
10	8.104	1051	1057	1066	rVB2	82896	199464	12.85%	1.705%
11	8.369	1093	1102	1114	rBV2	232266	545332	35.14%	4.660%
12	8.545	1121	1132	1145	rBV	283150	682636	43.98%	5.834%
13	8.898	1184	1192	1207	rBV	603493	1262301	81.33%	10.788%
14	9.357	1265	1270	1278	rBV6	7409	17672	1.14%	0.151%
15	9.522	1289	1298	1309	rBV	26293	53418	3.44%	0.457%
16	9.816	1340	1348	1361	rBV	195119	387758	24.98%	3.314%
17	9.945	1361	1370	1383	rVV	281909	571494	36.82%	4.884%
18	10.127	1395	1401	1407	rBV5	11649	23624	1.52%	0.202%
19	10.304	1426	1431	1436	rBV2	19177	31162	2.01%	0.266%
20	10.374	1436	1443	1459	rVB	816703	1501878	96.77%	12.835%
21	10.798	1504	1515	1524	rVB10	22737	80830	5.21%	0.691%
22	11.680	1656	1665	1674	rBV	862955	1511965	97.42%	12.921%
23	11.780	1678	1682	1691	rVB6	11393	23690	1.53%	0.202%
24	11.892	1693	1701	1705	rBV2	10415	21314	1.37%	0.182%
25	12.668	1824	1833	1842	rBV	729900	1223278	78.82%	10.454%
26	13.304	1936	1941	1948	rVB	16622	30817	1.99%	0.263%
27	13.609	1985	1993	2005	rBV	914101	1552015	100.00%	13.264%
28	14.080	2068	2073	2080	rBV4	19496	39080	2.52%	0.334%
29	14.339	2110	2117	2124	rBV7	8507	17751	1.14%	0.152%
30	14.745	2182	2186	2192	rBV5	12319	18515	1.19%	0.158%
31	15.433	2296	2303	2309	rVB	19948	38344	2.47%	0.328%
32	16.527	2483	2489	2494	rBV3	10438	22664	1.46%	0.194%

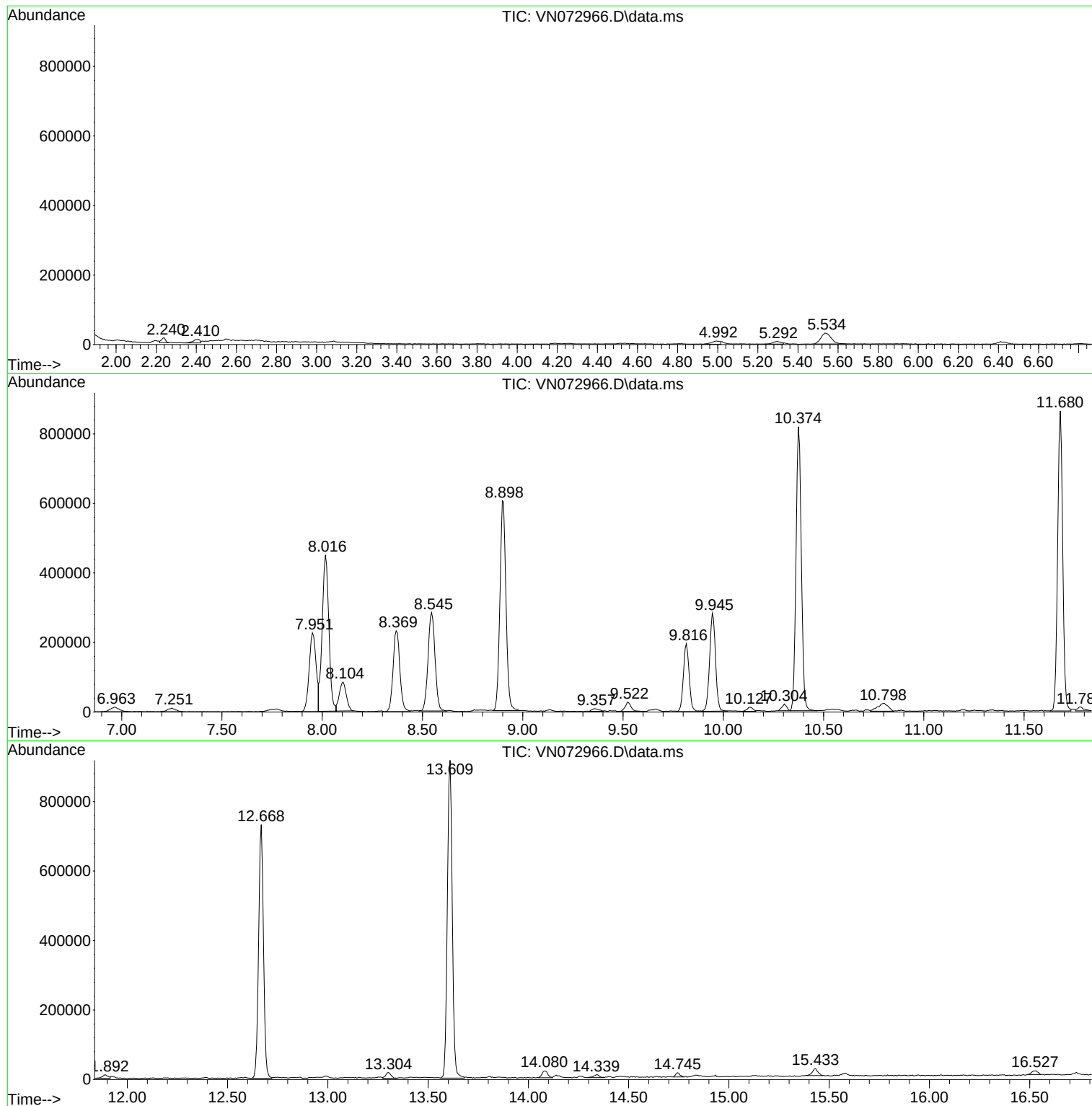
Sum of corrected areas: 11701385

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Instrument :
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ClientSampleId :
TOLL-MW-07

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



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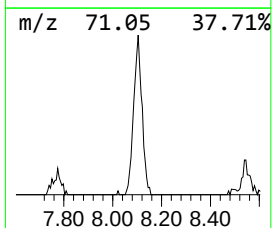
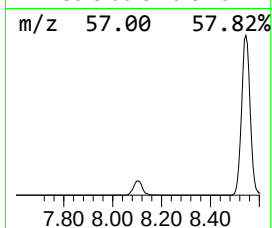
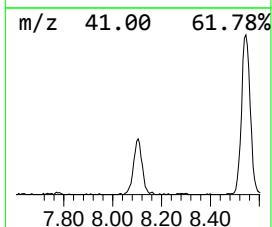
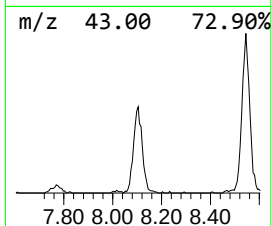
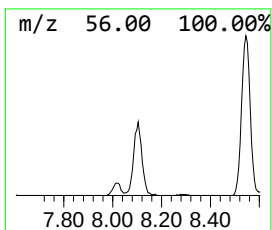
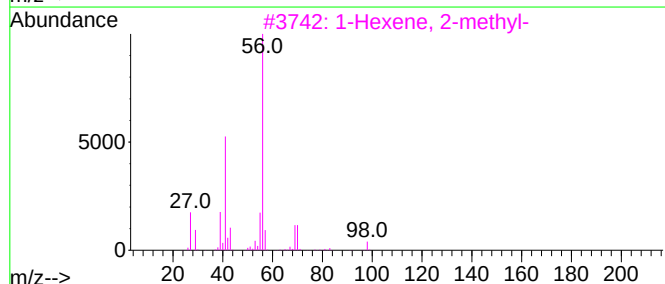
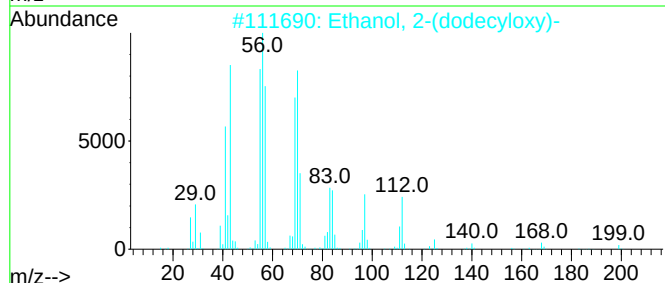
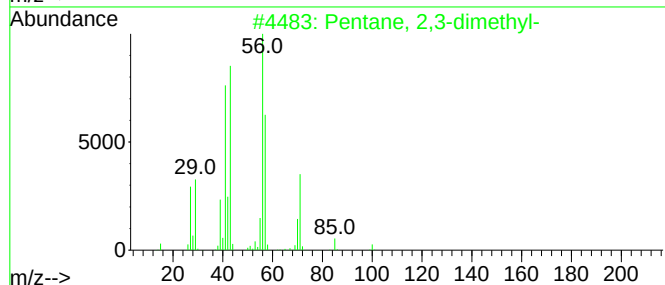
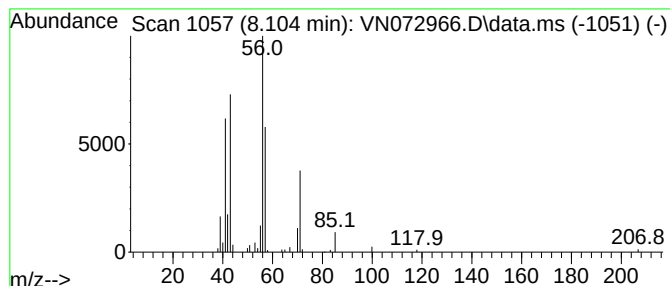
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Pentane, 2,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.104	9.72 ug/l	199464	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90
2			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	56
3			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	50
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
5			Cyclopentanamine	85	C5H11N	001003-03-8	42



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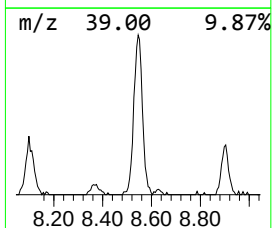
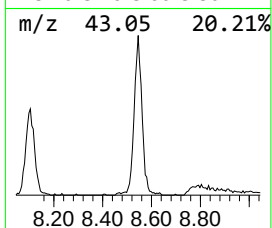
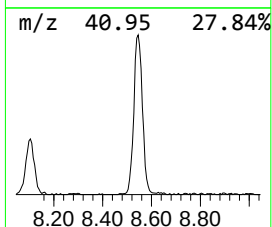
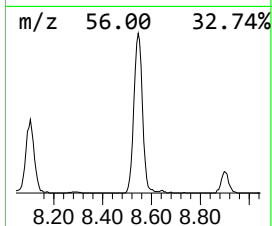
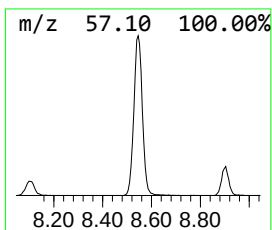
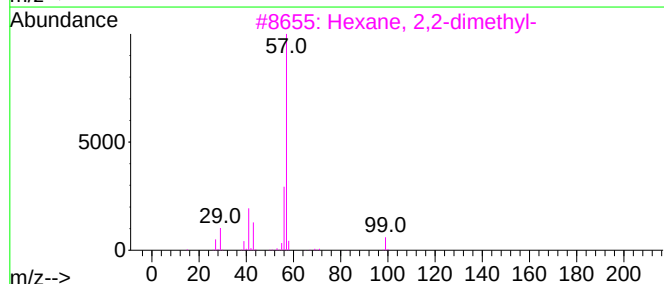
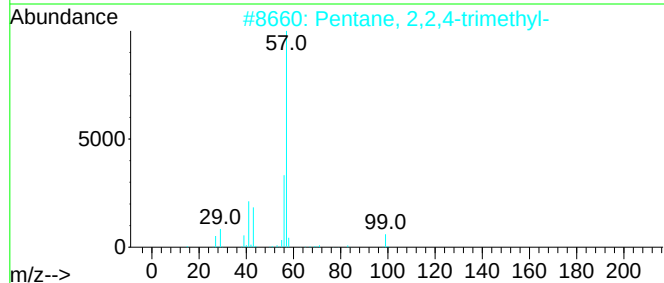
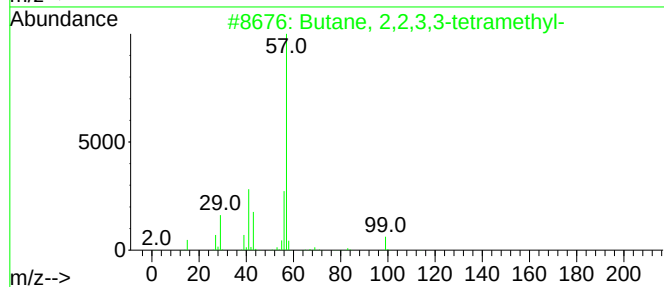
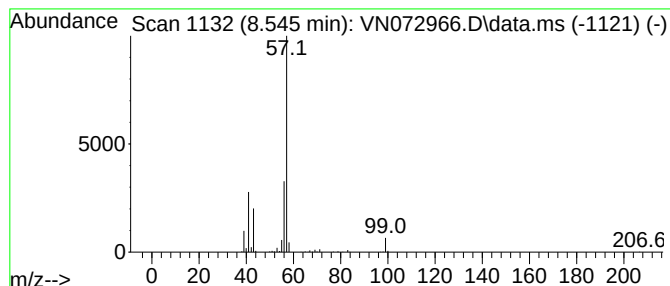
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	27.04 ug/l	682636	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	64
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



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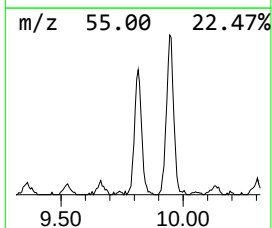
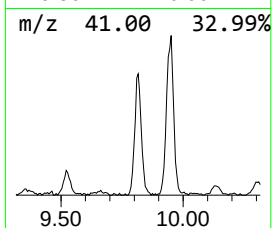
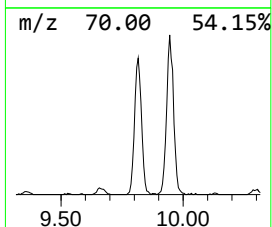
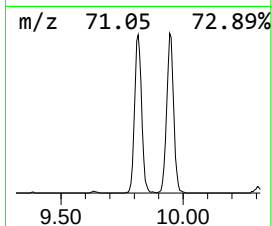
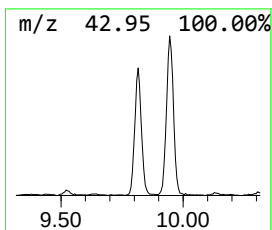
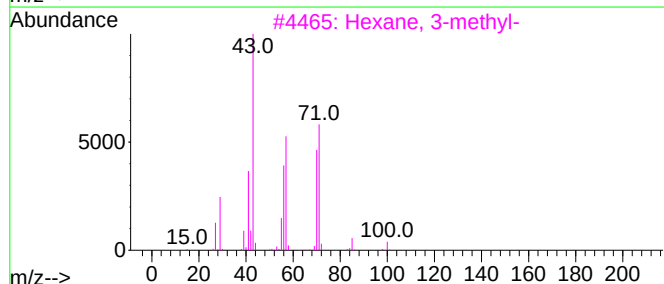
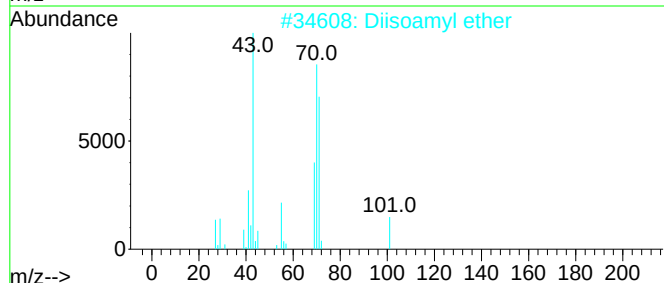
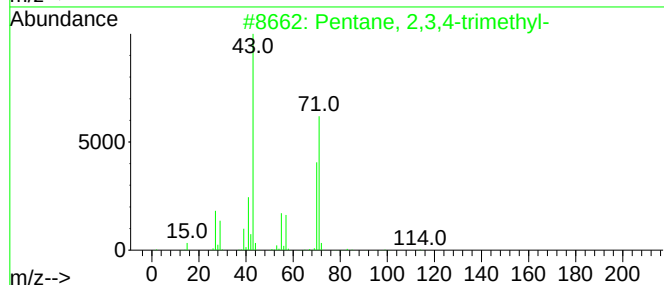
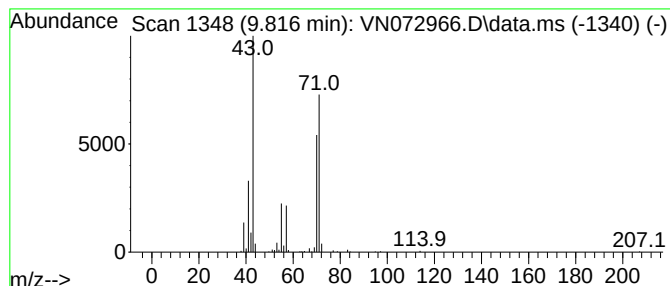
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061722W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.816	15.36 ug/l	387758	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Diisooamyl ether	158	C10H22O	000544-01-4	83
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	78
4			Pentane, 3-ethyl-	100	C7H16	000617-78-7	74
5			Heptane, 4-methyl-	114	C8H18	000589-53-7	74



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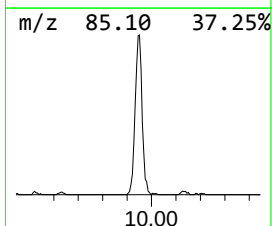
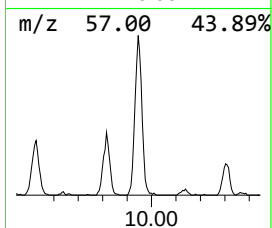
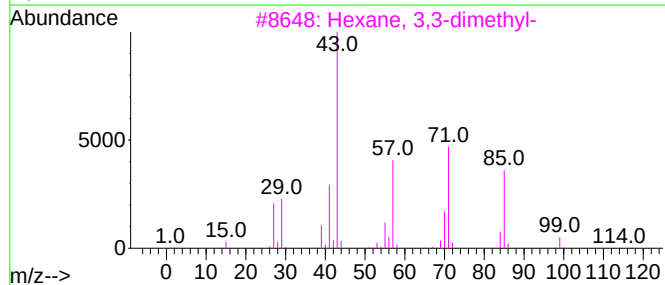
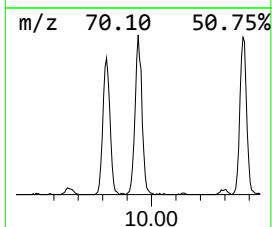
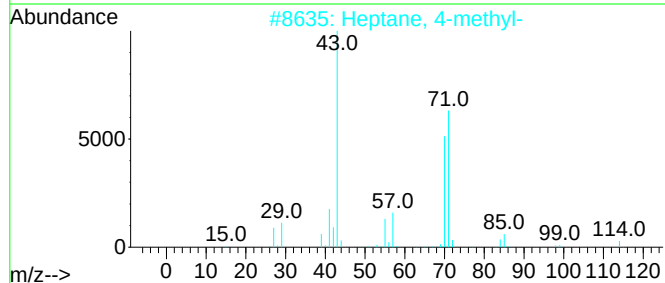
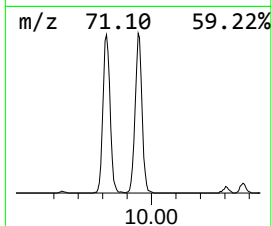
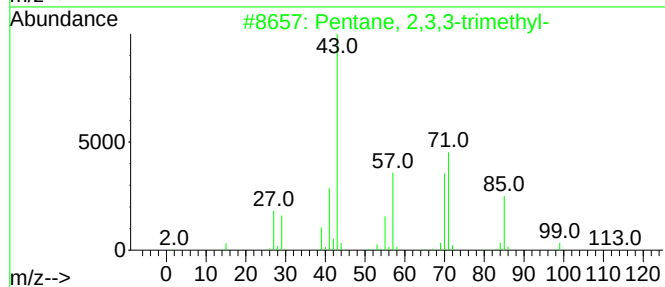
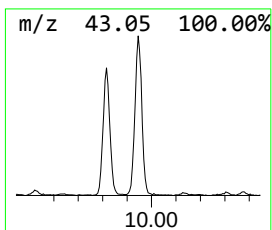
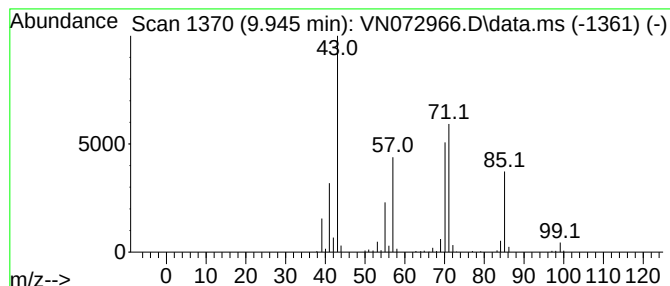
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.945	22.64 ug/l	571494	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Heptane, 4-methyl-	114	C8H18	000589-53-7	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			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	50



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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
Pentane, 2,3-di...	8.104	9.7	ug/l	199464	1	8.016	1026130	50.0
Butane, 2,2,3,3...	8.545	27.0	ug/l	682636	2	8.898	1262300	50.0
Pentane, 2,3,4-...	9.816	15.4	ug/l	387758	2	8.898	1262300	50.0
Pentane, 2,3,3-...	9.945	22.6	ug/l	571494	2	8.898	1262300	50.0